

**PROPOSAL FOR A DOCTOR OF PHILOSOPHY PROGRAM IN
CHEMISTRY ON THE INDIANAPOLIS CAMPUS**

**DEPARTMENT OF CHEMISTRY AND CHEMICAL BIOLOGY
PURDUE SCHOOL OF SCIENCE**

INSTITUTION: Indiana University – Purdue University, Indianapolis (IUPUI)

SCHOOL: Science

DEPARTMENT: Chemistry and Chemical Biology

DEGREE PROGRAM TITLE: Chemistry

FORM OF RECOGNITION TO BE AWARDED/DEGREE CODE: Doctor of Philosophy (Ph.D.)

SUGGESTED CIP CODE: 400501

LOCATION OF PROGRAM/CAMPUS CODE: Indianapolis, IUPUI

PROJECTED DATE OF IMPLEMENTATION: August 2011

**DATE PROPOSAL WAS APPROVED BY
INSTITUTIONAL BOARD OF TRUSTEES:**

**SIGNATURE OF AUTHORIZING
INSTITUTIONAL OFFICER**

**DATE RECEIVED BY COMMISSION FOR
HIGHER EDUCATION**

COMMISSION ACTION (DATE)

A. ABSTRACT

Doctor of Philosophy (Ph.D.) in Chemistry

To be offered by the Purdue School of Science on the
Indiana University – Purdue University Indianapolis (IUPUI) campus

Objectives:

This proposal was prepared at the request of the Indiana Commission of Higher Education (ICHE). The objective of the proposal is to convert a well-established Purdue Ph.D. program in chemistry to a Purdue Ph.D. program in chemistry that is site-approved for Indianapolis (IUPUI). The Department of Chemistry & Chemical Biology at IUPUI has graduated a total of 318 graduate students since 1973 (273 Purdue M.S. degrees and, since 1986, 45 Ph.D. degrees). We have been training Ph.D. students for twenty-five years with 43 of 45 graduates earning the Purdue University Ph.D. degree, and two earning Indiana University degrees. The vast majority have gone on to successful careers in science, with destinations including academic institutions, industrial laboratories, and non-profit organizations. Our productivity in graduate degrees, while currently attributed to Purdue University, already exceeds the expected ICHE standards for productivity of graduate degrees. As an already mature program, strategic growth is cautiously expected in the future.

At present, by arrangement with our departmental counterpart at Purdue University West Lafayette (PUWL), the program is entirely delivered on the Indianapolis campus. However, its graduates are attributed to the graduate school at PUWL. An objective of the proposed degree is to train productive researchers that contribute to the economic development of central Indiana and beyond. Our program makes a Purdue graduate degree accessible to many Indiana residents, or place-bound students, that would otherwise be unable to take advantage of opportunities to advance their graduate education. A final objective for this research-focused Purdue Ph.D. program in the Department of Chemistry & Chemical Biology is to meet our expanded research faculty's own expertise to provide students with training in the latest research and investigative techniques to advance our scientific and technological frontiers. In addition, by selective and distinctive specialization, we are able to drive increased research collaboration across campus, enhancing externally funded scholarship at IUPUI. Historically, the Department has successfully attracted major funding from Federal agencies that have recognized that our program meets national needs for training in the sciences, a critical challenge to achieve global competitiveness in science and technology.

Clientele to be Served:

The program will continue to serve highly qualified, research-motivated baccalaureate and master's degree holders from Indiana, the U.S., and beyond.

Curriculum:

Our proposed Purdue Indianapolis Ph.D. program will require the traditional 90 credit hours of registration and the Graduate Advisory Committee of each student will determine the course work component. After decades of close ties to the Purdue West Lafayette Ph.D. program in chemistry, our curriculum has evolved to accommodate a range of student backgrounds and needs, as well as our regional requirements. The diversity of the research opportunities available in our program has demonstrated a capacity to attract excellent students, and allowed them to achieve scientific success in a variety of collaborative research endeavors. Students will typically enroll in at least 20 credit hours of course work. In parallel with the PUWL Ph.D. program, students will be required to present two one-hour seminars on topics unrelated to their research during the Oral Candidacy Examination and a Formal Seminar Presentation. These experiences will appear as two separate credit hours of CHEM 69500, Seminar, on Plans of Study and on transcripts.

Most students will enter the program with undergraduate and/or masters degrees in chemistry; we also seek talented and highly motivated students from allied fields including biochemistry, biology, chemical engineering, and other programs who have sufficient preparation to enable their success in the program. The blending of rich curricular backgrounds with ours has led to a distinctive, successful program producing capable students strongly impacting our scientific workforce needs in Indiana and elsewhere.

Employment Possibilities:

Our students have gone on to prominent postdoctoral appointments at research universities and, ultimately, have taken permanent positions in academia or in government and industrial laboratories (see Section C2 and accompanying table). Other graduates have gone directly into industry. In general, Ph.D. programs do not necessarily funnel graduates to local employers. That said, it is notable that a significant number of our graduates remain in the greater central Indiana workforce.

A. Program Description

1. Program description and objectives

The prime objective of this proposal is to recognize that we currently have an established Purdue Ph.D. program in chemistry at IUPUI, and to confirm this by converting that program to one that is site-approved for Indianapolis (IUPUI). The Department of Chemistry & Chemical Biology is a key contributor to research and learning on the IUPUI campus, an urban research university that has been designated by the Indiana University System as its “Health & Life Sciences” campus. It provides the course work foundation for undergraduate health programs, as well as the undergraduate degree programs that feed into professional programs and health-related graduate programs on campuses statewide. The Department is also the setting for an assemblage of externally funded research programs with strengths in sub-

disciplines that emphasize basic chemical research. The Ph.D. program currently provides training in the highest degree offered by institutions of higher education and complements the advanced degree programs in the professional schools on campus. The Department of Chemistry & Chemical Biology has been training Ph.D. students for twenty-five years with the vast majority earning the Purdue University Ph.D. in Chemistry, a degree awarded on the West Lafayette campus despite the fact that *100% of the course work and research is completed at IUPUI*. The Department of Chemistry & Chemical Biology of the Purdue School of Science is in the midst of a hiring initiative that will bring additional research-focused faculty members on board. Allowing IUPUI to retain rightful ownership of the degrees awarded by establishing a Purdue Ph.D. program that awards degrees in Indianapolis will prove to be more attractive to prospective new faculty. Further, as we undergo expansion, it will facilitate increased research collaboration across campus, and will make IUPUI more competitive for external funding. The latter is particularly important, as the present system has been seen to be confusing to grant reviewers.

The research focus of IUPUI has generated economic benefits for central Indiana. Since 1980, external funding for the Department exceeds \$22 million and there is an auxiliary impact from additional millions from allied goods and services accompanying this figure. The graduate programs (45 Ph.D. and 273 M.S. graduates since 1986 and 1973, respectively) have made a significant contribution to this research enterprise. Right now, there are thirteen full time and many hourly individuals supported by external funding. Our chemistry research programs are contributing at ever-increasing levels to the transformation of the Indiana economy and its emphasis on the life sciences. The availability of Ph.D. students is essential in the recruiting of high-caliber research faculty and in the completion of the work contracted for in funded proposals.

The proposed program will be structured much like the Purdue West Lafayette Ph.D. program in the Purdue Department of Chemistry, the one in which we have been participating. The program is structured similarly to most Ph.D. programs in chemistry in that it is research intensive and requires 90 credit hours of registration. This program is characterized by an extensive research element that is closely monitored by a Graduate Advisory Committee. Our primary academic objective is to produce Ph.D. graduates who are trained in the latest technologies and techniques, who have the foundational skills to direct an independent program of research and who are competitive for positions in academia, industry and government.

2. Admission requirements, student clientele, and student financial support

All applicants must have earned, at the minimum, a four-year baccalaureate degree from a U.S. institution or an equivalent degree from a foreign institution. For admission, applicants must complete an online application and submit the Graduate Student Questionnaire, a personal statement, and original transcripts from all institutions previously attended. A minimum cumulative GPA 3.0 (on a 4.0 scale) is required for admission. Applicants must also arrange for letters of recommendation from three individuals who can evaluate the applicant's past work and comment on the applicant's potential for success at the graduate level. International applicants must also submit their official general GRE and TOEFL scores unless their undergraduate

degrees were earned from U.S. institutions or select international institutions where instruction was delivered exclusively in English.

The program will serve highly qualified, research-motivated baccalaureate and masters degree holders from Indiana and beyond. Applicants will be expected to have completed basic course work in biology, chemistry, physics, and mathematics for admission. Because the curriculum (see Section B3) is built for maximum flexibility, deficiencies can be addressed while in the program. The primary traits we seek in applicants are intellectual and research ability and motivation. We can adjust for academic background within the program through supplementary course work and tutorials. Our history is that approximately 26% of our Ph.D. students come from IUPUI B.S. and M.S. programs in Chemistry. This serves to the benefit of place-bound students in Indiana that may otherwise be unable to pursue a graduate degree elsewhere.

The Admissions Committee, comprised of graduate faculty members from the Department of Chemistry & Chemical Biology, reviews completed applications. The committee screens for GPAs of at least 3.0 in all degrees completed, supportive letters of recommendation, and a commitment to a research career as evidenced by previous research experience and/or a strong motivation for research revealed in the personal statement section of the online application. For international students, competitive GRE scores and minimum TOEFL scores (Paper 550, Computer 213, and Internet-based Testing (iBT) 79 with minimum sub-scores of 19 reading, 16 listening, 22 speaking and 18 writing) are required. These are also our current admission criteria. It should be noted that they are equal to and, in some cases, more stringent than those at PUWL. Applicants we wish to pursue are normally interviewed on campus unless this is not feasible (e.g. overseas or international); these students will be interviewed by phone or by Skype. The number of students admitted each year will be dependent on the quality of the applicant pool, the level of available institutional and faculty support, and the number of available laboratory openings. We anticipate recruiting an average of five to six students a year initially. Our program has traditionally been highly selective; graduate students are selected for their potential success as researchers.

Under our current arrangement with the PUWL Ph.D. program, students recommended for admission at IUPUI receive administrative approval from the Purdue West Lafayette Department of Chemistry. When the Chemistry & Chemical Biology Ph.D. is site-approved for IUPUI, admissions will be handled on the Indianapolis campus by the faculty of the Chemistry Ph.D. program as currently carried out; however, administrative approval will also be granted in Indianapolis, using the same criteria used by the PUWL Department of Chemistry.

Student support will be derived from institutional, departmental and faculty sources. At the institutional level there are competitive first-year fellowships and block grants to schools (distributed to departments) for one-year fellowships. In addition, there are funds to support graduate Teaching Assistants (TAs). Students whose native language is not English must pass a language test administered by the Department of English before they can be assigned to teaching. Our department has regularly supported 5-6 Ph.D. or thesis M.S. students as TAs, particularly during the first year of their degree program and another 3-4 on internal research fellowships. The department has recently

received additional funds through the IUPUI School of Science to support another 4-6 Ph.D. students. These students are critical to our teaching mission as they lead laboratory sections of courses in our growing undergraduate program. Finally, a number of students are supported on faculty research grants as Research Assistants (RAs). Faculty routinely include graduate support lines in their federal grant proposals. Recently, the School of Science has taken over the costs of most of the tuition for graduate students. This is critical for the support of the research faculty recently hired and those who will come on board in the future. Current support for TA or RA positions is a stipend of \$21,000 for Ph.D. and M.S. students. With respect to the teaching and research duties of our students, both TAs and RAs receive tuition remission and paid health insurance premiums.

3. The program curriculum

Program requirements include selecting a Research Advisor, passing five Cumulative Exams, establishing a Graduate Advisory Committee, submitting a Plan of Study, passing an Oral Candidacy Exam, satisfactorily presenting a Formal Seminar, submitting a Research Progress Report, and submitting and defending a thesis. To provide degree consistency, the Purdue Indianapolis Ph.D. in Chemistry will be operated and managed in the same way as the current Purdue West Lafayette Ph.D. in Chemistry. Students who continue on from an IUPUI M.S. degree may select a Research Advisor at the outset of the Ph.D. and begin the other program requirements. Students new to IUPUI will commonly interview with prospective mentors early in the first fall semester and from that experience will select a Research Advisor as soon as feasible, but before the beginning of the second semester.

Cumulative examinations are started during the first month of the Ph.D. program, consistent with the system at PUWL. Notably, since 1993, IUPUI Chemistry faculty have been invited to write and grade cumulative examinations for PUWL students and administer PUWL-authored exams to our Ph.D. students. As our faculty and graduate student composition has changed and will continue to do so, we expect that the subdisciplinary foci of the examinations will change over time. Students take cumulative exams until they have succeeded in passing five sub-discipline tests in 20 opportunities.

Within six months of passing the fifth and final cumulative exam, Ph.D. students establish a Graduate Advisory Committee. The Committee is comprised of the Research Advisor, one member of the graduate faculty from the student's area of focus, and one member of the graduate faculty from outside the student's area of focus. Two members of the Committee must be from the Department of Chemistry & Chemical Biology. Under the current Ph.D. arrangement, the Committee is comprised of two faculty members from the IUPUI Department of Chemistry & Chemical Biology and two members of the Purdue West Lafayette Graduate Faculty (one as a thesis reader and one that participates fully in the thesis reading, oral exams and defense). The proposed Ph.D. program would not require a committee member from the Purdue West Lafayette Graduate Faculty. Based on experience it would seem that this is an onerous task for PUWL faculty, although one could be invited based on an expertise match with the student's research area. The Graduate Advisor meets with the student and

establishes a Plan of Study, subject to the approval of the Graduate Advisory Committee and the Graduate School. This document lists all courses and seminars the student is to complete. Research credits are not listed. Submission of this document to the Graduate School also establishes the membership of the Graduate Advisory Committee.

Six months after the Plan of Study has been approved, the Oral Candidacy Exam takes place. The Graduate Advisory Committee functions as the examining committee. This exam is an oral exam that is a defense of a written original research proposal and the student's research progress. The Committee will receive the comprehensive research proposal and the progress report two weeks before the exam. Passing this exam officially admits the student to candidacy for the Ph.D.

The Graduate Advisory Committee will meet with the student annually to help direct the research and to monitor progress. A written progress report, due at that meeting, will be filed with the department. The Graduate Advisory Committee will also serve as the thesis examining committee at the end of program.

The Plan of Study will list a set of courses that will support and facilitate the research area and two seminar experiences (CHEM 69500, Seminar), where the student delivers one-hour presentations on subjects inside and outside of the research area. The overall expectation of the Purdue Indianapolis Ph.D. program in chemistry is one that is heavily research-oriented with the thesis and publications derived from the research being the primary outcomes. Because there are no core requirements, the course work component of the Ph.D. can be individually crafted. This is particularly important in chemistry, a discipline that covers a wide range of sub-disciplines from theoretical to experimental chemistry: physical, organic, inorganic, and analytical chemistry; biochemistry, and chemical education. Finding an acceptable core to serve all of these areas would not be possible. The minimum number of credit hours needed to qualify for full-time status for domestic (international) students at IUPUI is six (eight), six (eight) and one (one) credit for fall, spring and a summer semester, respectively. Below is a sample Plan of Study for a student entering the program with a B.S. degree; a plan for an entering M.S. student would be expected to contain transferred coursework, approved by the Director of Graduate Studies on consultation with appropriate departmental faculty.

First Semester:	CHEM 62100 Advanced Analytical Chemistry	3 cr. hrs.
	CHEM 69600 Special Topics: Biomaterials	3 cr. hrs.
Second Semester:	CHEM 69600 Special Topics: Analytical Spectroscopy	3 cr. hrs.
	CHEM 65100 Special Topics: Advanced Organic Chemistry	3 cr. hrs.
Third Semester:	CHEM 53300 Introductory Biochemistry	3 cr. hrs.
	CHEM 69600 Special Topics: Bioanalytical Chemistry	3 cr. hrs.
Fifth Semester:	CHEM 69500 Seminar	1 cr. hr.
Sixth Semester:	CHEM 69500 Seminar	1 cr. hr.

The Ph.D. requires 90 credit hours of course work and research. Students who enter the Ph.D. program with an M.S. degree can apply a maximum of 30 credit hours toward the 90 credit hours required for the Ph.D. degree. Specific requirements for the Ph.D. degree are summarized below (these align with the requirements currently employed at PUWL):

1. Select Research Advisor and Graduate Advisory Committee
2. Cumulative Exams (details given below)
3. An approved Plan of Study form submitted by the end of the third semester
 - a. 20 credit hours of approved graduate courses including:
 - i. 9 credit hours in a major area of concentration
 - ii. 9 credit hours outside the major area, in at least two other areas
 - iii. Among items 3a(i) and 3a(ii), 12 credit hours must be 600-level courses.
 - iv. 2 credits of CHEM 69500 Seminar
4. Written Research Report:
 - a. During the 4th semester each student will provide a written research report to the Graduate Advisory Committee describing research progress and future plans.
5. Oral Candidacy Examination (details given below).
6. Formal Literature Seminar:
 - a. Before the end of the 6th semester students must present a Formal Literature Seminar. His/her Graduate Advisory Committee and the faculty member in charge of the seminar program must approve the timing and content of the seminar.
7. 69900 Ph.D. Thesis Research
8. A thesis approved by the student's Graduate Advisory Committee
9. Defense of thesis

In addition to the above formal requirements, from their 3rd semester on, Ph.D. students are expected to participate in the Departmental Poster Session held every fall semester; this important event serves partially as a progress review for thesis students and also assists in developing presentation skills and preparation for the final thesis defense. Students admitted in January are expected to participate on or before their 4th semester in residence.

Cumulative Examinations

Ten Cumulative Examinations are offered each academic year. The student must pass five cumulative examinations by the end of the 4th semester (summer semesters are not counted). All students take the exam in a preannounced sitting, scheduled at the beginning of each academic year, when they write responses to as many of the offered sub-discipline tests as they wish to attempt. Traditionally, cumulative examinations are given once each month on Saturday mornings from 10:00 am to 12:00 noon in LD 326T. Occasionally, topics are posted. The Graduate Advisor will provide information on a topic as it is received. Students continue to take cumulative exams until they have succeeded in passing five sub-discipline tests within 20 or fewer opportunities. The counting of opportunities begins at the first sitting, normally the first semester of the

Ph.D. program, and runs contiguously thereafter. A hiatus from cumulative exams occurs during the summer semester.

Faculty members write individual questions, evaluate the responses, and set the passing level. Our faculty have shared examination responsibilities during the collaborative period thus ensuring expertise in appropriate levels of expectation. IUPUI Chemistry & Chemical Biology faculty will be administering and grading their students' cumes.

Oral Candidacy Examination and Research Summary

The Oral Candidacy Examination consists of an Original Proposal (OP) and a summary of the student's dissertation research and must be taken after the cumulative examinations have been completed but no later than the end of the fifth semester. The OP must originate with the student and not be related to their doctoral research.

The Original Proposal should include a concise statement of the problem or hypothesis to be tested, a statement of its significance and originality, why the proposal is superior to previous approaches (if applicable), how it is proposed to attack the problem, what difficulties can be expected in the course of the project and their solutions, and what will be accomplished by addressing the project. Although the student is expected to have a complete knowledge of the area(s) related to the OP, the written OP should not include an extensive review of the area but should outline a research program as opposed to a single experiment. The Original Proposal is to be the student's own work; consultation with any faculty member is not permitted.

The Research Summary should consist of a statement of research already accomplished as well as a discussion of directions that further research might take.

The Oral Examination will consist of a presentation by the student and discussion of the OP and Research Summary. Members of the committee are free to interrupt the student at any time and probe, by detailed questioning, the depth of the student's understanding of the proposed research.

4. Form of recognition

The degree offered would be a Purdue University Doctor of Philosophy (Ph.D.) in Chemistry through the Purdue University Graduate School. The degree would be offered exclusively on the Indianapolis campus, in a manner similar to the long-standing relationship with PUWL on undergraduate degrees.

At the time of degree creation, campus administration will identify an appropriate CIP code that will be approved by the Indiana Commission of Higher Education.

The diploma will read Doctor of Philosophy in Chemistry, Purdue University School of Science, Indianapolis.

5. List program faculty and administrators

Tenure -Track Faculty

Name	Rank	PhD	Postdoctoral
Haibo Ge, Ph.D.	Asst. Professor	University of Kansas	The Scripps Research Institute
John Goodpaster, Ph.D.	Asst. Professor	Michigan State University	National Institute of Standards and Technology (NIST)
Lei Li, Ph.D.	Asst. Professor	The Johns Hopkins University	University of Michigan
Eric Long, Ph.D.	Professor	University of Virginia	California Institute of Technology
David Malik, Ph.D.	Chancellor's Professor, Executive Vice-Chancellor, Indiana University Northwest	University of California, San Diego	University of Illinois
Michael McLeish, Ph.D.	Assoc. Professor	La Trobe University, Melbourne, Australia	University of California, Berkeley
Robert Minto, Ph.D.	Assoc. Professor, Director of Graduate Admissions	University of California, Berkeley	The Johns Hopkins University
Barry Muhoberac, Ph.D.	Assoc. Professor	University of Virginia	University of Texas Health Science Center at San Antonio
Christoph Naumann, Ph.D.	Assoc. Professor	Technical University of Munich, Germany	MPI for Polymer Research Mainz, Germany
David Nurok, Ph.D.	Assoc. Professor Emeritus	University of Cape Town, South Africa	AE and CI, North Rand, South Africa
Martin O'Donnell, Ph.D.	Chancellor's Professor, Director of Graduate Studies	Yale University	Université Catholique de Louvain, Belgium
Kyungsoo Oh, Ph.D.	Asst. Professor	University of Sussex, U.K.	University of Pennsylvania
Jingzhi Pu, Ph.D.	Asst. Professor	University of Minnesota	Harvard University
Rajesh Sardar, Ph.D.	Asst. Professor	The City University of New York, College of Staten Island	University of North Carolina
Jay Siegel, Ph.D.	Professor, Chair of Chemistry and Chemical Biology, Director of Forensic & Investigative Sciences Program	George Washington University	Virginia Bureau of Forensic Sciences
Pratibha Varma-Nelson, Ph.D.	Professor, Director of Center for Teaching and Learning	University of Illinois, Chicago	Stritch School of Medicine, Loyola University

Research Faculty (Non-Tenure Track)

Name	Rank	PhD	1st postdoctoral
Brenda Blacklock, Ph.D.	Asst. Research Professor	University of Alberta, Canada	The Johns Hopkins University
Donald Boyd, Ph.D.	Research Professor	Harvard University	Cornell University
Tax Georgiadis, Ph.D.	Asst. Research Professor	University of California, Los Angeles	Columbia University
Malea Kneen, Ph.D.	Asst. Research Professor	The University of Melbourne, Australia	University of California, San Francisco
James McCarthy, Ph.D.	Research Professor	University of Utah	Dow Chemical Co.
William Scott, Ph.D.	Research Professor	University of California, Los Angeles	Rockefeller University

Associate Research Faculty

Name	Rank	PhD	1st postdoctoral
Millie Georgiadis Ph.D.	Assoc. Professor, IUSM	University of California, Los Angeles	Columbia University
Samy Meroueh Ph.D.	Asst. Professor, IUSM	Wayne State University	Wayne State University

Curriculum Vitae for all faculty participating in training Ph.D. students and administering the proposed Ph.D. program can be found in Appendix C.

Although still below the high point of 18 tenure-track faculty in the mid-1990s, our faculty numbers have been partially restored in recent years (including four faculty hires in the last two years). Our Strategic Plan indicates additional research and teaching efforts will be needed. Two current faculty members, Drs. Jay Siegel and Martin O'Donnell, are approaching normal retirement age and will likely be replaced within three years. In addition, the opening of a new building in 2013 will provide the additional research space necessary to further increase the number of Chemistry & Chemical Biology faculty. Overall, an increase of one to two faculty per year is anticipated over the next five-year window. Concomitantly, additional Ph.D. students will be needed to drive faculty research and to provide instructional support for the large and growing undergraduate teaching mission at IUPUI.

In addition to the full-time faculty, Chemistry & Chemical Biology has two jointly appointed (official IUPUI appointments) faculty members whose primary appointments are at the IU School of Medicine (IUSM). These individuals also hold special graduate certification with the Purdue Graduate School that allows them to serve as outside members of Ph.D. and thesis M.S. committees.

6. Needed learning resources

Since we have been engaged in Ph.D. training for twenty-five years, we do not anticipate a need for additional learning resources. We have at our disposal excellent libraries on campus as well as online resources to successfully operate all aspects of Ph.D. training in Indianapolis. Other technical resources are available through core facilities in the School of Science, at the IUSM, and through Indiana University Bloomington. In addition, the Indiana Clinical and Translational Sciences Institute provides access to core facilities at Purdue University West Lafayette, at Indiana University Bloomington, and at the University of Notre Dame.

7. Other program strengths

In addition to covering all of the essentials of a sound undergraduate curriculum, offering an array of appropriate service courses, and delivering highly respected thesis and non-thesis Purdue M.S. degrees, the department has developed an extensive externally supported research program over the past 30 years. In 1999, we identified Life Science Chemistry as the organizational theme on which, where possible, we would concentrate our hires, while maintaining sufficient breadth to continue to support the aforementioned offerings. Beyond the strengths of individual research programs, departmental research expertise has evolved over time. This resulted in the formation of the Integrated Nanosystem Development Institute and the Center for Membrane Biosciences, centers of excellence incorporated as IUPUI Signature Centers that include other faculty on campus spanning departments in science and the professional schools, and throughout the central Indiana academic community. The Chemical Synthesis & Organic Drug Lead Development Core is operated through Chemistry and Chemical Biology to provide core facilities that allow departmental expertise to be more fully shared with the School of Medicine and local industry. There

are several faculty members in the department participating in other campus centers such as the Center for Computational Biology & Bioinformatics and the Indiana University Cancer Center. Several facilities centers provide research capabilities necessary for vibrant chemical research on the IUPUI campus, including the Nanoscale Imaging Center, and the Chemistry and Chemical Biology Nuclear Magnetic Resonance (NMR) and High-Resolution Mass Spectrometry (HRMS) Cores. The focus and expertise for science on both the atomic and molecular scales clearly gives us a distinction on campus that is fully compatible with the research goals in the Schools of Medicine as well as other programs, such as Engineering.

The Department of Chemistry & Chemical Biology has had a long-term commitment to including undergraduate students in the research enterprise. The presence of undergraduate students as active participants in research is a distinctive feature of the research environment in Chemistry & Chemical Biology and provides opportunities for graduate students to gain experience in mentoring and directing research projects.

B. Program Rationale

1. Institutional factors

IUPUI has identified itself as the urban research university of Indiana. Given the presence of a contingent of large health schools on campus, the Indiana University system has labeled IUPUI as the Health & Life Sciences campus in the state. Furthermore, the IUPUI Vision Statement is very clear about the future direction of the institution. The IUPUI Vision is:

“to be the best urban research university by conducting world-class research, scholarship, and creative activities that develop knowledge and contribute to the economic growth and social advancement of Indiana and the nation and benefit humanity as a whole.”

This vision together with the natural maturation of the IUPUI campus makes Indianapolis-based doctoral programs not just an aspiration but also a pressing need to fulfill the research and educational enterprise of central Indiana, the home of many life and health sciences industries. Building the research capacity of the Purdue School of Science at IUPUI has been on the agenda for at least 35 years. The Department of Chemistry & Chemical Biology began offering the M.S. degree in the early 1970s and admitted its first Ph.D. student in the mid 1980s. We are not new to this endeavor but we are on the cusp of a major expansion. The current hiring rate with more new positions planned will build the faculty and enhance external funding. Our new building (2013) will address the space shortage. With the growth of the undergraduate student population, the recruitment of more research-oriented faculty, and the increased external grant income, the Dean of the School of Science envisions a doubling of the Chemistry & Chemical Biology graduate student (thesis M.S. and Ph.D.) population in the next three years. A Ph.D program entirely delivered on the Indianapolis campus can only help make this vision a reality.

On a campus where many schools train a wide variety of health care professionals, a vital Department of Chemistry & Chemical Biology is a key element. At IUPUI, Chemistry & Chemical Biology provides fundamental education for students seeking admission to nursing, dental hygiene, physical therapy, and a number of other health-related programs in the Schools of Medicine, Dentistry, Engineering and Technology, Nursing, and Health & Rehabilitative Sciences. In addition, we train students at the baccalaureate and masters levels for application to medical and dental schools on campus as well as for programs in pharmacy, optometry and veterinary medicine elsewhere in the state. These responsibilities along with those associated with providing service courses to the general undergraduate population and graduating undergraduate majors who have the intention of joining the life sciences work force make our programs among the fastest growing on the IUPUI campus.

Our concept of the Urban Research University does not limit research to professional schools but rather raises the expectations across campus in order to elevate all units and provide multiple opportunities for cross-fertilization through collaboration. Our commitment to research is made clear in all of our hires. In order for us to be able to recruit top faculty talent and in order for them to be successful, we must have a robust, high quality graduate program at the Ph.D. level. We have already seen the impact of such programs over the past twenty-five years on faculty productivity, external funding success, and the overall intellectual climate of the department. We are also aware of the impact that these scientists-in-training can have as teaching assistants in our undergraduate laboratory courses. Indeed, they are essential to educating our undergraduate students yet, at the same time, they obtain their own teaching experience and credentials.

Our hope is to have this proposal approved for implementation as soon as possible. The new program will seamlessly replace our current one, so it will not impact other IUPUI units or those elsewhere in the state. The resources needed will be the same except for those associated with our plans for growth. We intend to generate these resources through increased enrollments and external funding success.

2. Student demand

We project admitting six to eight new Ph.D. students each year for the next two to three years. Beyond that our target number for recruitment will depend on faculty expansion that will accelerate when the new building opens. Because we have grown in the number of faculty with active research programs and in external funding that includes graduate student support lines, we anticipate that we will and must double the number of annual admissions. We foresee a Ph.D. program that emphasizes the quality of the student experience. We anticipate a steady-state enrollment of around 30 Ph.D. students plus a cohort of thesis-based M.S. students.

We have data on Ph.D. students thus far trained in chemistry as well as the students currently enrolled in the program. The vast majority of our graduates have gone on to successful careers in higher education and industrial or governmental positions. Below is a list of our Ph.D. graduates to date. One of the students was an Indiana University

Ph.D. student who, because of medical reasons, completed all the research for his doctoral thesis at IUPUI under the direction of one of our faculty.

Last	First	Degree Date	Last Known Position
Bennett (IU)	William	1986	Adv ChemTech, Louisville, KY – Sr. Scientist
Carfagna (IU)	Mark	1990	Eli Lilly, Indianapolis, IN
Steinmetz	Curtis	1991	Ctr. Ocean-Land-Atmospheric Studies, MD – Dir. Info. Sys.
Wu	Shengde	1992	Proctor & Gamble, Cincinnati, OH – Sr. Scientist
Parish	Carol	1994	Univ. of Richmond – Professor
Shen	Peidong	1994	Stanford Univ. – Genome Tech Center, Res. Assoc.
Liu	Shanghao	1995	Yale Univ. – Postdoctoral
Thompson	David	1995	Los Alamos National Lab
Peterson	Michael	1996	Duke University – Senior Analyst, Dept. of Chemistry
Stout	Joyce	1996	Eli Lilly, Indianapolis
Eason	Paula	1997	Meso Scale Technologies, Gaithersburg, MD
Lawin	Laurie	1997	Innovative Surface Technologies, St. Paul, MN – Scientist
Speelman	Brent	1997	Purdue Univ. – Postdoctoral
Ewing	Gregory	1997	Deceased
Roach	Steven	1997	Unknown
Liang	Qi	1997	NIST, MD – Staff Scientist
Ananias	Davina	1998	Roche Diagnostics, Indianapolis, IN
Huang	Xiaofen	1998	South China Univ. of Technology, PRC
de Oliveira	Glenisson	1998	Rhode Island College – Professor and Chair
Gao	Yang	1998	Genentech, San Francisco, CA – Sr. Scientist
Mattison	Kevin	1999	Malvern Instr., Westborough, MA – Principal Scientist
Hemkin	Sheryl	1999	Kenyon College – Assoc. Professor
Borts	David	1999	Univ. of North Carolina – Research Asst. Professor
Wang	Yingfan	1999	Univ. of Alabama – Postdoctoral
Chin	Frederick	2000	Stanford Univ. – Instructor, Radiology
Jalaie	Mehran	2000	Pfizer, La Jolla, CA
Turner	Jeffrey	2000	Roche Diagnostics, Indianapolis, IN
Cooper	Jeremy	2001	Wake Forest Univ. – Visiting Professor
Uhrhammer	Darrell	2001	Evert Software Systems, Chaska, MN – Scientist
Schefzick	Sabine	2002	Pfizer, La Jolla, CA

Chenoweth	Kimberly	2002	Smith College – Visiting Professor
Claussen	Craig	2003	Seradyn, Indianapolis, IN
Lecher	Carl	2003	Marian College – Assoc. Professor
Deverall	Miranda	2005	Roche Diagnostics, Indianapolis, IN
Seyrek	Emek	2005	Univ. Geneva, Switzerland - Lecturer
Murcia	Michael	2006	Nalco, Naperville, IL – Sr. Research Chemist
Lewis	Mark	2007	Entrepreneur, CA
Garg	Sumit	2008	Argonne Natl Lab – Postdoctoral
Kimble-Hill	Ann	2008	IU School of Medicine – Postdoctoral
Denton	Ryan	2009	IUPUI, Chemistry – Academic Specialist
Novotny	Allyson	2009	Univ. of Indianapolis – Asst. Professor
Trobaugh	Corey	2009	Cummins Automotive, Columbus, IN
Cissell	Kyle	2010	TransGenex Nanobiotech, Tampa, FL – Research Scientist
Goulding	Ann	2010	IUPUI, Chemistry – Instructor
Minner	Daniel	2010	IUPUI, Chemistry – Postdoctoral

3. Transferability

Generally, this is not a critical issue for Ph.D. students. We have admitted a few students who began Ph.D. work elsewhere and have allowed relevant course work to transfer.

4. Access to graduate and professional programs

The Ph.D. degree is a terminal degree for most students, therefore, this is not a common concern.

5. Demand and employment factors

Based on the success of our graduates (see above table in Section C2) over the past two and a half decades, we are confident that future graduates will continue to find excellent positions in industry, government and academia. To date 45 students have earned their Ph.D. degrees in chemistry at IUPUI. Forty-three have done so under the Purdue University West Lafayette Ph.D. and two under Indiana University Ph.D. programs. The summary of the placement outcomes for these graduates include sixteen who are in academic positions, eighteen who work in industry, and three who has found laboratory or management positions in government. Of the total, thirteen are presently employed in Indiana.

6. Regional, state and national factors

There are several chemistry Ph.D. programs in Indiana with the largest being at Purdue University West Lafayette (PUWL), the program through which we are now operating. The others are at Indiana University Bloomington (IUB) and the University of Notre Dame. The IUPUI campus also has a chemistry-related “life science” Ph.D. program in the School of Medicine as well as a biochemistry doctoral program, PUWL has both an agricultural biochemistry and medicinal chemistry and molecular pharmacology faculty and IUB has a Molecular and Cellular Biochemistry department. Each of these programs has a focus that makes each program different in some but not in all ways. For example, organic chemists may be on staff in most departments and each of these faculty will direct research in some aspect of organic chemistry. However, at other levels and in certain chemistry sub-disciplines, clear distinctions emerge. In most traditional chemistry programs, the six core areas include analytical, biological, chemical education, inorganic, organic and theoretical/physical chemistry.

PUWL Chemistry is subdivided into the six common core areas plus chemical biology and materials chemistry. Recently, it has been focusing its research into three strategic areas:

1. Drug Discovery and Disease Detection: this area includes natural product synthesis, chemical biology, human trials, target selection and validation, combinatorial chemistry, biomarker identification and detection, drug delivery, structure-based drug design, and chemical sensing and imaging.
2. Energy/Catalysis: this area includes solar/hydrogen, biofuels, organometallic synthesis, battery research, fuel cells, and hydrogen storage.
3. Soft Materials: this area includes membranes, DNA nanostructures, peptide assemblies and composite materials, carbohydrates, and chemical sensing and imaging.

IUB Chemistry has identified 26 research clusters and a program in Quantitative and Chemical Biology has been initiated recently. They participate in three interdisciplinary doctoral degrees in chemical physics, biochemistry, and a combined MD/Ph.D. program. Doctoral programs within their department, however, lie in the following six traditional areas:

1. Analytical Chemistry
2. Biological Chemistry
3. Inorganic Chemistry
4. Materials Chemistry
5. Organic Chemistry
6. Physical Chemistry

The **University of Notre Dame Department of Chemistry and Biochemistry** lists 13 research specialties, which are broadly represented in the following four fields of study:

1. Organic Chemistry
2. Physical Chemistry
3. Inorganic Chemistry
4. Analytical Chemistry

The **IU Schools of Medicine and Dentistry and the Purdue programs listed from departments outside of Chemistry** have research areas in the standard basic sciences with the obvious emphases on the appropriate applied areas of human health or agricultural science.

Chemistry at IUPUI, while relatively small compared to these long-standing programs, is growing in terms of faculty count and has Ph.D. opportunities in several areas including membrane biophysics, metabolic biochemistry, nucleic acids chemistry, protein chemistry, synthetic organic and medicinal chemistry, inorganic chemistry, combinatorial chemistry and analytical chemistry. As already mentioned, our major focal area is in Life Science Chemistry. This focus is synergistic with, and complementary to, research being done in biology, physics, medicine, dentistry and engineering on the IUPUI campus. In campus Signature Centers, there are labs working on bio-renewable products, structure and dynamics of membrane systems, nanotechnology, and tobacco cessation research.

There are Indianapolis-area residents with strong interests in graduate education who cannot relocate outside of the city for personal reasons. Many students are excited by the atomic/ molecular level understanding of matter that is a central attribute of the chemical sciences. That interest cannot be satisfied by campus Ph.D. programs in the professional schools and, for those students, we are the only option. It is notable that at least eight of our Ph.D. graduates and four of our current students had/have such issues.

D. Program Implementation and Evaluation

There are no special steps we must take to implement the program. It will be operated in the same way as the current Purdue West Lafayette program except for the need to pass applications through the PUWL Department of Chemistry for administrative approval and the necessity of PUWL faculty representation on students' Graduate Advisory Committees. Students in the current program will migrate to the new program provided they are not too far along in their studies and provided that there are no burdensome procedures required.

The program will be evaluated using the following parameters:

1. Number of applicants and admitted students
2. Number of students attending

3. Number of students supported on grants and from institutional sources
4. Profiles of attendees (GPAs, GRE scores, graduate degrees, previous institutions attended)
5. Student performance in course work
6. Student performance on Cumulative Exams
7. Student research productivity (number of publications, presentations)
8. Awards and other special recognition
9. Time to degree
10. Number of graduates
11. Student placement: Number placed and quality of placements

Monitoring the above parameters will be the responsibilities of the Department Chair, the Director of Graduate Studies and the Chemistry & Chemical Biology Graduate Admissions Committee. Each year in early fall the recruiting data (Items 1 and 2) from the previous year will be collected and summarized. Historical data (Item 4) on matriculating students will also be compiled at that time. Each annual cohort will be followed through graduation to collect the information for items 9 and 10. Pass rates on the Cumulative Exams will be collected for the previous year in the summer (Item 6). Course work performance will be monitored semester by semester (Item 5). Data regarding student research productivity, awards and placement will be followed for three to five years post-graduation to capture program productivity that appears after leaving and to allow for a long-term view of career trajectory (Items 7, 8 and 11). We will also monitor annually the proportion of institutionally and grant-supported students (Item 3). It is an important measure of program effectiveness that institutional commitment and external research funding success be in balance.

We are prepared to change whatever is necessary if student performance does not measure up to expectations. What follows are steps that may be taken in cases where there are multiple examples of poor performance. In cases where the data indicate poor to mediocre performance on Cumulative Exams we will review students' academic history, preparatory materials made available to students, and courses taken prior to the exam. Solutions could involve changes in preparatory materials, changes within courses or among courses selected, and requiring more background of students admitted to certain areas of study. In cases of poor classroom performance, we will also consider instructional effectiveness and examination materials. In some cases, a change of instructor may be the best remedy. We will annually report the publications and other achievements of our students in order to publicly display expectations to all faculty mentors and students. This is a subtle way to support the notion that productivity (Item 7 above) is a critical outcome of the training. To this point in our history of Ph.D. training there have been no recurring problems with exams or courses that have required curricular or instructor changes.

E. Tabular Information

1. **Table 1: Enrollment and Completion Data**
2. **Tables 2A and 2B: Cost and Revenue Data**
3. **New Program Proposal Summary**

TABLE 3:
NEW ACADEMIC DEGREE PROGRAM PROPOSAL SUMMARY
26 January 2011

I. Prepared by Institution

Institution/Location: Indiana University-Purdue University Indianapolis
 Program: Ph.D. in Chemistry
 Proposed CIP Code: 400501
 Base Budget Year: 2010-11

	Year 1 2011-12	Year 2 2012-13	Year 3 2013-14	Year 4 2014-15	Year 5 2015-16
Enrollment Projections (Headcount)	18	21	24	27	30
Enrollment Projections (FTE)	14	16	18	20	23
Degree Completion Projection	3	3	3	3	6
New State Funds Requested (Actual)	\$ 0	\$ 0	\$ 0	\$ 0	\$ 0
New State Funds Requested (Increases)	\$ 0	\$ 0	\$ 0	\$ 0	\$ 0

II. Prepared by Commission for Higher Education

New State Funds to be Considered for Recommendation (Actual)	\$ _____	\$ _____	\$ _____	\$ _____	\$ _____
New State Funds to be Considered for Recommendation (Increases)	\$ _____	\$ _____	\$ _____	\$ _____	\$ _____

CHE Code: _____
 Campus Code: _____
 County Code: _____
 Degree Level: _____
 CIP Code: _____

Comment: _____

Campus: Indiana University-Purdue University Indianapolis
 Program: Ph.D. in Chemistry
 Date: 26 January 2011

TABLE 1: PROGRAM ENROLLMENTS AND COMPLETIONS
 Annual Totals by Fiscal Year (Use SIS Definitions)

	Year 1 2011-12	Year 2 2012-13	Year 3 2013-14	Year 4 2014-15	Year 5 2015-16
A. Program Credit Hours Generated					
1. Existing Courses	288	324	378	432	486
2. New Courses	36	54	54	54	54
Total	324	378	432	486	540
B. Full-time Equivalents (FTEs)					
1. Generated by Full-time Students	14	16	18	20	23
2. Generated by Part-time Students	0	0	0	0	0
Total	14	16	18	20	23
3. On-Campus Transfers	11	11	11	11	11
4. New-to-Campus	2	5	7	9	11
C. Program Majors (Headcounts)					
1. Full-time Students	18	21	24	27	30
2. Part-time Students	0	0	0	0	0
Total	18	21	24	27	30
3. On-Campus Transfers	15	15	15	15	15
4. New-to-Campus	3	6	9	12	15
5. In-State	6	7	8	9	10
6. Out-of-State	12	14	16	18	20
D. Program Completions	3	3	3	3	6

Campus: Indiana University-Purdue University Indianapolis
Program: Ph.D. in Chemistry
Date: 26 January 2011

TABLE 2A:
TOTAL DIRECT PROGRAM COSTS AND SOURCES OF PROGRAM REVENUE

	Year 1		Year 2		Year 3		Year 4		Year 5	
	FTE	2011-12	FTE	2012-13	FTE	2013-14	FTE	2014-15	FTE	2015-16
A. Total Direct Program Costs										
1. Existing Departmental Faculty Resources	2.2	\$ 198,000	2.2	\$ 198,000	2.2	\$ 198,000	2.2	\$ 198,000	2.2	\$ 198,000
2. Other Existing Resources		40,000		40,000		40,000		40,000		40,000
3. Incremental Resources (Table 2B)		61,100		122,300		183,400		244,600		305,700
TOTAL		\$ 299,100		\$ 360,300		\$ 421,400		\$ 482,600		\$ 543,700
B. Sources of Program Revenue										
1. Reallocation		\$ 238,000		\$ 238,000		\$ 238,000		\$ 238,000		\$ 238,000
2. New-to-Campus Student Fees		40,100		80,300		120,400		160,600		200,700
3. Other (Non-State): External Research Grants		21,000		42,000		63,000		84,000		105,000
4. New State Appropriations										
a. Enrollment Change Funding		0		0		0		0		0
b. Other State Funds		0		0		0		0		0
TOTAL		\$ 299,100		\$ 360,300		\$ 421,400		\$ 482,600		\$ 543,700

Campus: Indiana University-Purdue University Indianapolis
Program: Ph.D. in Chemistry
Date: 26 January 2011

TABLE 2B:
DETAIL ON INCREMENTAL OR
OUT-OF-POCKET DIRECT PROGRAM COSTS

	Year 1		Year 2		Year 3		Year 4		Year 5	
	FTE	2011-12	FTE	2012-13	FTE	2013-14	FTE	2014-15	FTE	2015-16
1. Personnel Services										
a. Faculty	0.0	0	0.0	0	0.0	0	0.0	0	0.0	0
b. Support Staff	0.0	0	0.0	0	0.0	0	0.0	0	0.0	0
c. Graduate Teaching Assistants	0.5	21,000	1.0	42,000	1.5	63,000	2.0	84,000	2.5	105,000
Total Personnel Services		21,000		42,000		63,000		84,000		105,000
2. Supplies and Expense										
a. General Supplies and Expense		0		0		0		0		0
b. Recruiting		0		0		0		0		0
c. Travel		0		0		0		0		0
d. Library Acquisitions		0		0		0		0		0
Total Supplies and Expense		0		0		0		0		0
3. Equipment										
a. New Equipment Necessary for Program										
b. Routine Replacement										
Total Equipment		0		0		0		0		0
4. Facilities		0		0		0		0		0
5. Student Assistance										
a. Graduate Fee Scholarships		40,100		80,300		120,400		160,600		200,700
b. Fellowships										
Total Student Assistance		40,100		80,300		120,400		160,600		200,700
Total Incremental Direct Costs	\$	61,100	\$	122,300	\$	183,400	\$	244,600	\$	305,700

Appendix A

Graduate Course Descriptions for IUPUI Chemistry & Chemical Biology

Course Title:	Introductory Biochemistry
Course Number:	53300
Home School:	School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours:	3
Prerequisites:	C342 or equivalent
Description:	A rigorous one-semester introduction to biochemistry.
Course Title:	Inorganic Chemistry
Course Number:	54200
Home School:	School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours:	3
Prerequisites:	C362 or equivalent or consent of instructor
Description:	A survey of the chemistry of main group and transition elements in which descriptive chemistry is wedded to qualitative theories of bonding and structure.
Course Title:	Intermediate Physical Chemistry
Course Number:	57500
Home School:	School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours:	3
Prerequisites:	C362 or equivalent
Description:	Quantum theory of atoms and molecules, theories of chemical bonding, molecular spectroscopy, methods for determining molecular structure, and electrical and magnetic properties.
Course Title:	Special Assignments
Course Number:	59900
Home School:	School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours:	1-4
Prerequisites:	Consent of instructor
Description:	Directed reading or special work not included in other courses.
Course Title:	Advanced Analytical Chemistry
Course Number:	62100
Home School:	School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours:	3
Prerequisites:	C311 and C410
Description:	A critical survey of recent developments in chemical and instrumental methods of analysis.

Course Title: Chromatic Methods of Analysis
Course Number: 62900
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: C410 or equivalent or consent of instructor.
Description: Principles and practice of modern gas and liquid chromatography are developed from an integrated point of view. Emphasis is placed on those features useful in practical analytical separations. Instrumentation is described and evaluated using chemical examples from recent literature. Although column techniques are emphasized, thin-layer chromatography and electrophoresis methods also are described. Offered in alternate years.

Course Title: Biochemistry: Structural Aspects
Course Number: 63400
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: C311, C342, C361, and C362 or equivalent.
Description: Chemistry of materials of biochemical interest: carbohydrates, lipids, proteins, amino acids, nucleic acids, porphyrins, biochemistry of blood.

Course Title: Biochemical Mechanisms
Course Number: 63600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: One year of physical chemistry and 651.
Description: The chemical basis of enzymatic catalysis with particular emphasis on catalytic interactions important in aqueous media.

Course Title: Advanced Inorganic Chemistry
Course Number: 64100
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: C430 or 542 or equivalent or consent of instructor.
Description: Survey of main group and transition metal chemistry. Main group special topics, bonding and structure of boron hydrides. Coordination chemistry, bonding models in coordination compounds. Transition metal organometallic chemistry, ligand types and reactivity patterns. Survey of inorganic NMR spectroscopy.

Course Title: Advanced Organic Chemistry
Course Number: 65100
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: C342 or equivalent
Description: Modern structural organic chemistry, including introductions to molecular orbital theory and reaction mechanisms. Prerequisite: a year's course in organic chemistry.

Course Title: Synthetic Organic Chemistry
Course Number: 65200
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: 651 or 657
Description: An advanced treatment of methods for preparing major types of organic functionalities and bonds, stressing stereochemical control and involving mechanisms for understanding the reactions employed.

Course Title: Reaction Mechanisms
Course Number: 65700
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: C342 or equivalent or consent of instructor.
Description: Modern structural organic chemistry, introduction to physical organic chemistry, mechanisms of representative reactions, and methods used for understanding reactivity in organic transformation.

Course Title: Quantum Chemistry
Course Number: 67200
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: One year of physical chemistry
Description: Basic principles of classical and quantum mechanics, exact solutions for simple systems, approximation methods, atomic structure, spectroscopy, application of group theory, theory of molecular binding.

Course Title: Chemical Kinetics
Course Number: 67500
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 2-3
Prerequisites: One year of physical chemistry
Description: Experimental and theoretical considerations of chemical reaction rates and mechanisms.

Course Title: Statistical Thermodynamics
Course Number: 68200
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Prerequisites: C362 or equivalent.
Description: Application of statistical mechanics to the description of imperfect gases, liquids, and solutions; to order-disorder phenomena in solids and surfaces; and to absolute reaction rate theory.

Course Title: Seminar
Course Number: 69500
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 0-1
Description: Groups meeting for review and discussion of important current literature in analytical, biological, inorganic, organic, and physical chemistry. Each graduate student is required to attend the seminar of his or her major subject.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Solid-Phase Synthesis and Combinatorial Chemistry: Theory and Practice
This course will explore how the tools of solid-phase synthesis and combinatorial chemistry are being used to solve a wide variety of problems requiring chemical solutions. Examples range from medicinal chemistry and drug discovery to new catalyst creation, from new "chiral selectors" to new biochemical probes. The course will focus on the rationale for employing a combinatorial approach in chemical discovery. It will teach the basics of solid-phase organic chemistry, and the methodology, equipment, and analytical technology employed to use it as a tool to rapidly and effectively carry out a combinatorial approach to problem solving.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Seminars in Nucleic Acid Chemistry
Discussions of the bio-organic chemistry of DNA and RNA including their chemical syntheses, structures, enzymatic manipulation, and analyses of ligand (drug, metal ion, and protein) binding.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Bioinorganic Chemistry
This course aims to understand biological problems via the inorganic chemistry approaches. Inorganic elements are essential to the life processes. During the course, the role of naturally occurring inorganic elements in biology will be studied. How metals are introduced into biological systems as probes and drugs will be addressed as well. Specific topics include oxygen transportation, electron transfer, metal toxicity and control as well as metallodrugs.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Biomimetic Chemistry
This highly interdisciplinary graduate-level course offers an introduction into the fascinating world of biomimetic systems considered from the perspectives of chemistry, biology, physics, and engineering. The course provides a basic overview of the fundamental principles of molecular assembly of polymers and biomolecules into supramolecular systems and discusses corresponding scientific and technological applications.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Chemical Analysis of Alcohol & Drugs
This course will focus on the analysis and identification of commonly abused chemicals such as ethanol, inhalants, controlled substances and prescription drugs. The history, legal issues, synthesis, chemical / physical properties, and laboratory analysis of these materials will be discussed. Special topics will also include source determination by isotope ratio mass spectrometry, impurity profiling or genetic analysis, newly introduced analytical methods such as desorption ionization techniques in mass spectrometry and investigations of the mechanisms for canine detection of drugs. An optional laboratory section will also be offered in which students will complete practical exercises utilizing spectroscopy, chromatography and mass spectrometry that reflect common practice in forensic science laboratories.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Biosynthesis and Physiology
Intermediary metabolism, biosynthesis and regulation.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Organometallics
This course covers a number of notable advances in the field of organometallic chemistry, and the particular emphasis will be made in the use of transition metals in synthetic organic chemistry. *The formation of carbon-carbon and carbon-heteroatom (O, N, S) bonds* will be examined through detailed reaction mechanisms and extensive synthetic examples.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Instrumental Analysis-Trace Evidence
This course will focus on the use of instrumental techniques to analyze trace evidence types such as ink, fibers, paint, adhesives, tape, ignitable liquids, and explosives. A separate lab section will include practical laboratory exercises utilizing spectroscopy, chromatography and mass spectrometry that reflect common practice in forensic science laboratories. Special topics will also include current research such as pattern recognition techniques, novel sampling methods, and provenance determination.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Drug Discovery
This one semester course will explore the strategies and chemistry underlying drug discovery. The student will also learn the chemical and biochemical basis of drug action for a representative series of drugs. Traditional screening and lead modification approaches will be discussed, along with the latest developments in drug discovery based on "rational" computer-assisted design, combinatorial technology, and biotechnology. The student should have taken a graduate level organic chemistry course and have a basic understanding of organic reaction mechanisms, amino acids and proteins. Taking the course without this background requires permission of the instructor. Previous coursework in biochemistry would also be helpful but is not essential.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Bioanalytical Chemistry
Introduction to concepts in biosensors and biosensing. The discussion topics include optical, electrochemical and novel biosensors, microarrays, SPR, proteomics, hybridization, immunoassays, reporters and labels, and nanotechnology.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Organic Spectroscopy
Application of modern analytical techniques including 1- and 2-D nuclear magnetic resonance (NMR) spectroscopy, infrared spectroscopy, and mass spectrometry to the rational identification of organic structures.

Course Title: Special Topics in Chemistry
Course Number: 69600
Home School: School of Science, Dept. of Chemistry and Chemical Biology
Credit Hours: 3
Description: Introduction to Medicinal and Agricultural Chemistry
Topics will include the physiochemical properties of drugs and agrochemicals; drug structure and metabolisms; and enzymes, receptors and DNA as drug targets. Several Case studies of commonly used pharmaceuticals will be presented.

Appendix B

Demand and Employment Analysis

Rather than speculate or project demand for this program, we will rely on our experience with Ph.D. training in Chemistry & Chemical Biology at IUPUI. It is not typical to expect that a Ph.D. program will have significant local impact on the region in terms of permanent employment. Rather the Ph.D. is a global degree with recipients most frequently seeking high-level positions wherever they exist, sometimes including opportunities in other countries. Despite this we note that thirteen of our forty-five Ph.D. graduates are currently employed in Indiana. These are listed in sections C2 and C5 along with out-of-state faculty, governmental and industrial positions taken by the rest of our graduates. We are confident that such success in placement of our graduates, both locally and beyond, will continue even as our program grows.

Appendix C
Faculty Curriculum Vitae

Haibo Ge, Ph.D
Assistant Professor

Chemistry & Chemical Biology
IUPUI
402 N. Blackford St.
Indianapolis, IN 46202

Phone: 317-274-6876(office)
317-274-9830(lab)
Fax: 317-274-4701
Email: geh@iupui.edu

Education:

Postdoctoral Fellow, Advisor: Professor Dale L. Boger, October 2006~May 2009.
Department of Chemistry, The Scripps Research Institute

Ph.D., Medicinal Chemistry, Advisor: Professor Gunda I. Georg, August 2006.
Department of Medicinal Chemistry, University of Kansas
Thesis: "Novel Paclitaxel Analogues for Brain Delivery"

M.S., Medicinal Chemistry, Advisor: Professor Erhua Wang, May 2001.
Department of Medicinal Chemistry, China Pharmaceutical University
Thesis: "Design and Synthesis of the Insulin Sensitizer Rosiglitazone and Its Analogues"

Research Experience:

Assistant Professor, Department of Chemistry & Chemical Biology, Indiana University Purdue University-Indianapolis, August 2009~now

Palladium-catalyzed C-H functionalization: investigation of novel transformations and new substrates. Our current focus is decarboxylative cross-coupling reactions.

Total synthesis and structure-activity relationship (SAR) study of Ascochlorin for estrogen-receptor negative breast cancers. We collaborate with Prof. Qi-Zhuang Ye at Indiana University School of Medicine for biological studies on this project.

Research Associate, The Scripps Research Institute, October 2006~May 2009

Research Advisor: Professor Dale L. Boger

- Completed the total synthesis of [Dap²]-ramoplanin A2 aglycon
- Investigated and obtained conditions of the macrocyclization step for the total synthesis of [Dap², Cys¹²]-ramoplanin A2 aglycon dimer

Graduate Research Assistant, University of Kansas, August 2002~August 2006

Research Advisor: Professor Gunda I. Georg

- Developed a highly efficient kinetic resolution method for syntheses of paclitaxel analogues and applied this method to the preparation of designed paclitaxel analogues aimed to reduce Pgp interaction
- Developed a palladium (II)-catalyzed direct arylation of enamines and applied this methodology to the total syntheses of (+)-ipalbidine and (+)-antofine
- Designed and synthesized analogues of TH-5-188, a male contraceptive lead compound

Research Scientist, China Pharmaceutical University, June 2001~July 2002

- Developed a practical synthesis of darbufelone, a COX-2 inhibitor, and prepared this compound on a kilogram scale

Graduate Research Assistant, China Pharmaceutical University, August 1998~May 2001

Research Advisor: Professor Erhua Wang

- Developed a practical synthesis of rosiglitazone, a PPAR γ activator, and prepared this compound on a kilogram scale without chromatography.
- Investigated structure-activity relationship of rosiglitazone with PPAR γ activation by designing and synthesizing a series of rosiglitazone analogues

Teaching Experience:

Courses: Organic Chemistry II (C342, undergraduate course), Spring 2010 (Global Score: 3.86), Fall 2010, Spring 2011; Synthetic Organic Chemistry (C352, graduate course), Fall 2011
Research Mentor – Mingzong Li, Postdoctoral researcher, IUPUI, August 2009~August 2010
Research Mentor – Liangxi Li, Postdoctoral researcher, IUPUI, September 2009~January 2010
Research Mentor – Ping Fang, Postdoctoral researcher, IUPUI, March 2010~now
Research Mentor – Cong Wang, Postdoctoral researcher, IUPUI, August 2010~now
Research Mentor – Jinmin Miao, Graduate student, IUPUI, August 2010~now
Research Mentor – Tommy Lynch, Undergraduate student, IUPUI, August 2009~December 2010
Research Mentor – Zachary J. Funk, Undergraduate student, IUPUI, August 2009~May 2010
Research Mentor – Kong Ni, Undergraduate student, IUPUI, August 2010~November 2010

Service Activities:

Graduate Student Recruiting Committee, 2009, 2010
Organic Coordinator Searching Committee, 2009
Analytical Faculty Searching Committee, 2009
Organic Chemistry Search Committee, 2010
Faculty Peer Review Committee, 2010

Award: Thieme Chemistry Journal Award, 2011

Selected Publications:

10. Li, M.; Wang, C.; Ge, H. Pd(II)-Catalyzed Decarboxylative Cross-Coupling of Potassium Aryltrifluoroborates with α -Oxocarboxylic Acids at Room Temperature. In preparation.
9. Ge, H.; Li, M.; Wang, C.; Fang, P. Pd(II)-Catalyzed Decarboxylative Cross-Coupling of Potassium Phenyltrifluoroborates with Oxamic Acids. In preparation.
8. Li, M.; Li, L.; Ge, H. Direct C3-Alkenylation of Quinolones via Palladium-Catalyzed C-H Functionalization with Low Catalyst Loading. *Advanced Synthesis & Catalysis* **2010**, 352, 2445-2449.
7. Fang, P.; Li, M.; Ge, H. Room Temperature Palladium-Catalyzed Decarboxylative *ortho*-Acylation of Acetanilides with α -Oxocarboxylic Acids. *Journal of the American Chemical Society* **2010**, 132, 11898-11899.
6. Li, M.; Ge, H. Decarboxylative Acylation of Arenes with α -Oxocarboxylic Acids via Palladium-Catalyzed C-H Activation. *Organic Letters* **2010**, 12, 3464-3467.
5. Ge, H.; Wang, J.; Kayser, M.; Himes, R. H.; Gunda I. Georg. Synthesis, Tubulin Assembly, and Antiproliferative Activity of 10-O-Acetyl-5'-hydroxybutitaxel. *Bioorganic & Medicinal Chemistry Letters* **2008**, 18, 6165-6167.
4. Turunen, B. J.; Ge, H.; Oyeturji, J.; Vasandani, V.; Desino, K.; Audus, K. L.; Himes, R. H.; Gunda I. Georg. Paclitaxel Succinate Analogues: Anionic and Amide Introduction As a Strategy to Impart Blood-Brain Barrier Permeability. *Bioorganic & Medicinal Chemistry Letters* **2008**, 18, 5971-5974.
3. Ge, H.; Niphakis, M. J.; Georg, G. I. Palladium (II) Catalyzed Direct Arylation of Enaminones Using Organotrifluoroborates. *Journal of the American Chemical Society* **2008**, 130, 3708-3709.
2. Ge, H.; Spletstoser, J. T.; Yang, Y.; Kayser M.; Georg, G. I. Synthesis of Docetaxel and Butitaxel Analogues Through Kinetic Resolution of Racemic β -Lactams with 7-O-Triethylsilylbaccatin III. *Journal of Organic Chemistry* **2007**, 72, 756-759.
1. Ge, H.; Vasandani, V.; Huff, J. K.; Audus, K. L.; Himes, R. H.; Seelig, A.; Georg, G. I. Synthesis and Interactions of 7-Deoxy-, 10-Deacetoxy- and 10-Deacetoxy-7-deoxypaclitaxel with NCI/ADR-RES Cancer Cells and Bovine Brain Microvessel Endothelial Cells. *Bioorganic & Medicinal Chemistry Letters* **2006**, 16, 433-36.

Patent:

Peng, Y.; Li, Q.; Liu, X.; Yang, X.; Ge, H.; Chen, X. Method for Preparing of 1-Methoxy-2,3,6-O-tribenzoyl-4-deoxy-4-fluoro- α -D-glucose. CN 101245086, 2008.



John V. Goodpaster, Ph.D.

Department of Chemistry and Chemical Biology
Forensic and Investigative Sciences (FIS) Program
Indiana University Purdue University Indianapolis (IUPUI)
402 North Blackford Street, LD 326
Indianapolis, IN 46202
(317) 274-6881
goodpaster@chem.iupui.edu

EDUCATION

B.A., Chemistry (Certified by the American Chemical Society)
Gustavus Adolphus College, St. Peter, MN (1995)
Graduated *summa cum laude*

M.S., Criminal Justice (Specialization in Forensic Science)
Michigan State University, East Lansing, MI (2000)
Advisor: Jay A. Siegel, Ph.D.
Thesis: *Forensic Analysis of Soil Based on Its Organic Content*

Ph.D., Analytical Chemistry
Michigan State University, East Lansing, MI (2000)
Advisor: Victoria L. McGuffin, Ph.D.
Dissertation: *Fundamental Studies and Analytical Applications of Selective Fluorescence Quenching*

National Research Council Post-Doctoral Associate
National Institute of Standards and Technology (NIST), Gaithersburg, MD (2001-2002)
Advisor: Bruce A. Benner, Ph.D.
Project: *Chemical Analysis of Hair Surface Components*

ACADEMIC APPOINTMENTS

8/07 – present *Assistant Professor*
Department of Chemistry and Chemical Biology
Forensic and Investigative Sciences (FIS) Program
Indiana University Purdue University Indianapolis (IUPUI)
Indianapolis, IN

OTHER APPOINTMENTS AND PROFESSIONAL CONSULTANTSHIPS

8/02 – 7/07 *Forensic Chemist*
Forensic Science Laboratory - Washington
Bureau of Alcohol, Tobacco, Firearms and Explosives (ATF)
Ammendale, MD

1/08 – present *Consultant (Explosives Analysis and Detection)*
Goodpaster Forensic Consulting, LLC
Zionsville, IN

PROFESSIONAL ORGANIZATIONS

American Chemical Society (ACS), 1995 – present
American Academy of Forensic Sciences (AAFS), 1996 – present
Midwestern Association of Forensic Scientists (MAFS), 2007 – present

HONORS AND AWARDS

National Merit Scholarship (1991 – 1995)
ACS Division of Analytical Chemistry Undergraduate Award (1994)
FBI Honors Internship (1994)
Phi Beta Kappa (1994)
National Science Foundation Graduate Research Fellowship (1996 – 1999)
American Society of Crime Laboratory Directors Scholarship (1996)
Kenan Award Symposium (1998)
ACS Division of Analytical Chemistry Graduate Fellowship (1999 – 2000)
United States Department of Commerce Certificate of Appreciation (2002)
United States Department of Treasury Certificate of Award (2003)
Gustavus Adolphus College First Decade Award Nominee (2005)
Purdue School of Science Mentoring Citation (2008)

GRANTS AND CONTRACTS

1. “Causes, Effects and Mitigation of the Microbial Degradation of Ignitable Liquids”, Research Support Funds Grant, Office of Research and Sponsored Programs, IUPUI, 8/08 – 8/09, \$35,000, PI.
2. “Evaluation of the Odor Compounds Sensed by Explosive-Detecting Canines”, Technical Support Working Group, Combating Terrorism Technical Support Office, Department of Defense, 4/09 – 11/10, \$477,964, PI.
3. Matching Funds for “Evaluation of the Odor Compounds Sensed by Explosive-Detecting Canines”, Venture Fund, IUPUI Solution Center, 9/09 – 9/10, \$5,000, PI.
4. “Discrimination of Dyed Cotton Fibers Based on UV-visible Microspectrophotometry and Multivariate Statistical Analysis”, Midwest Forensics Resource Center, 1/10 – 9/10, \$55,000, PI.
5. “Development of a Sampling System to Stabilize Ignitable Liquid Residues in Fire Debris”, 10/10 – 10/12, \$239,025, PI.

6. “Evaluation of Statistical Measures for Fiber Comparisons: Interlaboratory Studies and Forensic Databases”, National Institute of Justice, 10/10 – 10/12, \$139,848 (\$489,049 total), co-PI.

TEACHING ASSIGNMENTS (* = Team taught, ** = Newly developed course)

Term	Course
Fall 2007	FIS 401: Forensic Chemistry I*
Spring 2008	FIS 206: Concepts in Forensic Science II*
	FIS 404: Forensic Chemistry II*
Fall 2008	CHEM 696: Chemical Analysis of Alcohol and Drugs (Lecture)**
	CHEM 696: Chemical Analysis of Alcohol and Drugs (Lab)**
Spring 2009	CHEM 696: Instrumental Analysis of Trace Evidence (Lecture)**
	CHEM 696: Instrumental Analysis of Trace Evidence (Lab)**
Fall 2009, Fall 2010	FIS 511: Forensic Chemistry I (Lecture)**
	FIS 511: Forensic Chemistry I (Lab)**
Spring 2010, Spring 2011	FIS 512: Forensic Chemistry II (Lecture)**
	FIS 512: Forensic Chemistry II (Lab)**

PROFESSIONAL SERVICE

Guest Editor, “Forensic Analysis”, *Analytical and Bioanalytical Chemistry* (2003)
 Guest Editor, “Explosives Analysis”, *Analytical and Bioanalytical Chemistry* (2009)

Peer Reviewer, *Journal of Forensic Sciences* (Fall 2007 – present)
 Peer Reviewer, *Analytical and Bioanalytical Chemistry* (Fall 2007 – present)
 Peer Reviewer, *Applied Spectroscopy* (Fall 2009 – present)
 Peer Reviewer, *Rapid Communications in Mass Spectrometry* (Fall 2009 – present)

UNIVERSITY SERVICE

Undergraduate Teaching Committee
 Department of Chemistry and Chemical Biology (Fall 2007 – Spring 2009)

Assessment Committee
 Purdue School of Science (Fall 2007 – Spring 2009)

Graduate Education Committee
Purdue School of Science (Fall 2009 – present)

GRADUATE ADVISEES

1. Elisa Liszewski (M.S. Forensic Science, 2010)
2. Erica Lotspeich (M.S. Forensic Science, 2010)
3. Cheryl Szudlarek (M.S. Forensic Science)
4. Kelley Kitts (M.S. Forensic Science)
5. Dee Ann Turner (Ph.D. Chemistry)
6. Christina Rainey (Ph.D. Chemistry)

GRADUATE COMMITTEES

1. Julie Barrett (M.S. Chemistry, 2008)
2. Lilyvet Rivas (M.S. Chemistry, 2008)

UNDERGRADUATE AND HIGH SCHOOL RESEARCH STUDENTS

1. Nicholas Estrada (Fall 2007)
2. Brandon Kocher (Fall 2007 – Spring 2008)
3. Samantha Weatherall
4. Benjamin Routon
5. Emily Smith
6. Katiana Whitaker
7. Suzanne Hakeem
8. Michelle Jordan
9. Neoshia Roemer
10. Justyne Kondos
11. Sean Campbell
12. Jason Hull (M.S. Student)
13. John Lawrence
14. Kevin Line (HS Student/Project SEED)
15. Josh Cummins
16. Alejandra Flores
17. Paige Conder
18. Aaron Todd

OTHER PROFESSIONAL ACTIVITIES

EXTERNAL TRAINING PROVIDED

“Explosives: Synthesis, Properties and Evidence” for the Indiana State Police Bomb Squad, Muscatatuck Urban Training Center, Butlerville, IN (9/20/07)

“Laboratory Analysis of Explosives Evidence”, for *State and Local Post-Blast Investigation*, sponsored by the Bureau of Alcohol, Tobacco, Firearms and Explosives (ATF), Naval Surface Weapons Center, Crane Division, Crane, IN (10/24/07)

“Putting the Pipe Back in Pipe Bomb” and “Instrumental Analysis of Low Explosives” for *Analysis of Low Explosives*, sponsored by the Midwest Forensics Resource Center, East Lansing, MI (6/25/08)

Coordinated presentation and exhibit on the clandestine synthesis of peroxide explosives for an FBI-sponsored event on Weapons of Mass Destruction held at Raytheon, Indianapolis, IN (8/13-14/08)

“Putting the Pipe Back in Pipe Bomb” and “IUPUI Pipe Bomb Study” for the Indiana State Police Bomb Squad, Pendleton, IN (11/12/08)

“The Use of Multivariate Statistics in Trace Evidence Investigations” at the *National Institute of Justice Trace Evidence Symposium*, Clearwater Beach, FL (8/4/09)

“Putting the Pipe Back in Pipe Bomb” and “IUPUI Pipe Bomb Study” for the Indiana State Police Bomb Squad, Muscatatuck Urban Training Center, Butlerville, IN (10/1/09)

“Chemometrics for Forensic Scientists: The Good, the Bad, and the Misleading” at the 62nd Annual Meeting of the American Academy of Forensic Sciences, Seattle, WA (2/23/10)

“Explosions and Explosives” for the Indianapolis Fire Department, Fire Investigation Section, Indianapolis, IN (5/18/10)

“Applications of Statistics to the Analysis of Alcohol and Drugs” and “Probability-Based Sampling Methods” for the Indiana State Police Laboratory, Indianapolis, IN (5/19/10)

“Pipe Bombs” for the Indianapolis Fire Department, Fire Investigation Section, Indianapolis, IN (6/22/10)

COURTROOM EXPERIENCE

The People of the State of New York v. Sammie Boyd
County Court, County of Erie, Buffalo, NY (5/21/04)

United States of America v. Andre Henry
United States District Court, Eastern District of Pennsylvania (2/15/07)

United States of America v. Daniel Wayne Osbourne
United States District Court, District of Montana (2/26/07)

PEER-REVIEWED PUBLICATIONS

1. J.V. Goodpaster, J.F. Harrison, V.L. McGuffin; "Ab Initio Study of Polycyclic Aromatic Hydrocarbons in Their Ground and Excited States," *J. Phys. Chem. A* 102, 3372-3381 (1998).
2. J.V. Goodpaster, V.L. McGuffin; "Rapid and Accurate Determination of Stern-Volmer Quenching Constants," *Appl. Spectrosc.* 53, 1000-1007 (1999).
3. J.V. Goodpaster, V.L. McGuffin; "Selective Fluorescence Quenching of Polycyclic Aromatic Compounds by Aliphatic Amines," *Anal. Chem.* 72, 1072-1077 (2000).
4. J.V. Goodpaster, V.L. McGuffin; "Fluorescence Quenching as a Novel Indirect Detection Method for Nitrated Explosives," *Anal. Chem.* 73, 2004-2011 (2001).
5. J.V. Goodpaster, V.L. McGuffin; "Separation of Nitramine and Nitroaromatic Explosives by Capillary Liquid Chromatography," *J. Liq. Chromatogr. Relat. Technol.* 24, 1965-1978 (2001).
6. J.V. Goodpaster, S.B. Howerton, V.L. McGuffin; "Forensic Analysis of Commercial Petroleum Products Using Selective Fluorescence Quenching," *J. Forensic Sci.* 46, 1358-1371 (2001).
7. S.B. Howerton, J.V. Goodpaster, V.L. McGuffin; "Characterization of Polycyclic Aromatic Hydrocarbons in Environmental Samples by Selective Fluorescence Quenching," *Anal. Chim. Acta* 459, 61-73 (2002).
8. J.V. Goodpaster, J.F. Harrison, V.L. McGuffin; "Ab Initio Study of Selective Fluorescence Quenching of Polycyclic Aromatic Hydrocarbons," *J. Phys. Chem. A*, 106, 10645-10654 (2002).
9. J.V. Goodpaster, J.J. Bishop, B.A. Benner, Jr.; "Forensic Analysis of Hair Surface Components Using Off-Line Extraction and Large Volume Injection," *J. Sep. Sci.*, 26, 137-141 (2003).
10. J.V. Goodpaster, B.C. Drumheller, B.A. Benner, Jr.; "Evaluation of Extraction Techniques for the Forensic Analysis of Human Scalp Hair Using Gas Chromatography/Mass Spectrometry (GC/MS)," *J. Forensic Sci.*, 48, 299-306 (2003).
11. B.A. Benner, Jr., J.V. Goodpaster, J.A. DeGrasse, L.A. Tully, B.C. Levin; "Characterization of Surface Organic Components of Human Hair by On-Line Supercritical Fluid Extraction - Gas Chromatography-Mass Spectrometry: A Feasibility Study and Comparison with Human Identification Using Mitochondrial DNA Sequences," *J. Forensic Sci.*, 48, 554-563 (2003).
12. J.V. Goodpaster, R.O. Keto; "Identification of Ascorbic Acid and Its Degradation Products in Black Powder Substitutes," *J. Forensic Sci.*, 49, 523-528 (2004).
13. J.V. Goodpaster, A.B. Sturdevant, K.L. Andrews, L. Brun-Conti; "Identification and Comparison of Electrical Tapes Using Instrumental and Statistical Techniques: I. Microscopic Surface Texture and Elemental Composition," *J. Forensic Sci.*, 52, 610-629 (2007).

14. J.V. Goodpaster, A.B. Sturdevant, K.L. Andrews, E.M. Briley, L. Brun-Conti; "Identification and Comparison of Electrical Tapes Using Instrumental and Statistical Techniques: II. Organic Composition of the Tape Backing and Adhesive," *J. Forensic Sci.* 54, 328-338 (2009).
15. D.A. Turner, J.V. Goodpaster; "Effects of Microbial Degradation on Ignitable Liquids in Soil," *Anal. Bioanal. Chem.*, 394, 363-371 (2009).
16. J.V. Goodpaster, E.A. Liszewski; "Forensic Analysis of Dyed Textile Fibers," *Anal. Bioanal. Chem.*, 394, 2009-2018 (2009).
17. J.A. Barrett, J.A. Siegel, J.V. Goodpaster; "Forensic Discrimination of Dyed Hair Color: I. UV-visible microspectrophotometry," *J. Forensic Sci.*, 55, 323-333 (2010).
18. E.A. Liszewski, S. Lewis, J. Siegel, J.V. Goodpaster, "Characterization of Automotive Paint Clear Coats by Ultraviolet Absorption Microspectrophotometry with Subsequent Chemometric Analysis," *Appl. Spectrosc.* 64, 1122-1125 (2010).
19. J.A. Barrett, J.A. Siegel, J.V. Goodpaster; "Forensic Discrimination of Dyed Hair Color: II. Multi-variate Statistical Analysis," *J. Forensic Sci.* (in press).
20. B.J. Routon, B.B. Kocher, J.V. Goodpaster "Discriminating Hodgdon Pyrodex and Triple Seven Using Gas Chromatography-Mass Spectrometry," *J. Forensic Sci.* (in press).
21. D.A. Turner, J.V. Goodpaster; "The Effect of Microbial Degradation on the Chromatographic Profiles of Tiki Torch Fuel, Lamp Oil and Turpentine" *J. Forensic Sci.* (in press).

OTHER PUBLICATIONS

1. V.L. McGuffin, J.V. Goodpaster; "Polycyclic Aromatic Compounds, Fluorescence Quenching," *Encyclopedia of Environmental Analysis and Remediation*, John Wiley and Sons: New York (1998), pp. 3814-3831.
2. S. Balou, J.V. Goodpaster, W. MacCrehan, D. Reeder, "Forensic Analysis," *Anal. Bioanal. Chem.* 376, 148 (2003) (*Guest Editor*).
3. P.A. Dreifuss, J.V. Goodpaster; "Atmospheric Pressure Ionization LC/MS Methods for the Analysis of Black Powder Substitutes," *Proceedings of the 8th International Symposium on the Analysis and Detection of Explosives*, Garbutt, D., Pilon, P., Lightfoot, P., Editors, 168-180 (2004).
4. J.V. Goodpaster; "Household Items that Contain Explosive Compounds: A Guide for Explosive-Detecting Canine Handlers," *The Detonator*, 34(2), 42-46 (March/April 2007).
5. J.V. Goodpaster, Book Review of "Trace Quantitative Analysis by Mass Spectrometry" by Robert K. Boyd, Cecilia Basic and Robert A. Bethem for *Journal of the American Chemical Society*, 130, 13183 (2008).
6. J.V. Goodpaster; "Does Amount Matter? Current Research Into the Concept of Odor Availability for Explosives-Detecting Canines," *The Detonator*, 36(5), 64-65 (2009).
7. D.S. Moore, J.V. Goodpaster; "Explosives analysis," *Anal. Bioanal. Chem.*, 395, 245-246 (2009) (*Guest Editor*).

8. J.V. Goodpaster, Book Review of "Quantification in GC and LC: A Practical Guide to Good Chromatographic Data" by H-J Kuss, S. Kromidas, editors for *Journal of Forensic Sciences*, 55, 1407 (2010).

PRESENTATIONS (* = Invited Speaker)

1. J.V. Goodpaster, V.L. McGuffin, "Multiwavelength Fluorescence and Fluorescence Quenching Detection in Capillary Separations," *Pittcon 1997*, Atlanta, GA (3/17/97).
2. J.V. Goodpaster, V.L. McGuffin, "Selective Fluorescence Quenching for the Analysis of Petroleum Products and Nitrated Explosives," *Pittcon 1998*, New Orleans, LA (3/4/98).
3. * J.V. Goodpaster, "Selective Fluorescence Quenching: Theory, Experiment and Application," *8th Annual Kenan Award Symposium*, Union Carbide Corporation, South Charleston, WV (4/1/98).
4. J.V. Goodpaster, V.L. McGuffin, "Forensic Applications of Fluorescence and Fluorescence Quenching Detection in Liquid Chromatography," *AAFS Annual Meeting*, Orlando, FL (2/19/99).
5. J.V. Goodpaster, V.L. McGuffin, "Fluorescence Quenching Detection for Liquid Chromatography," *FACSS 1999*, Vancouver, BC (10/25/99).
6. J.V. Goodpaster, B.C. Drumheller, B.A. Benner, Jr., "Extraction and Chemical Analysis of Human Scalp Hair as a Novel Trace Evidence Technique," *Annual Meeting of the Midwestern Association of Forensic Scientists*, Bloomington, MN (9/27/01).
7. * J.V. Goodpaster, "Evidence That Never Lies: Analytical Chemistry Applied to Human Hair," Department of Chemistry, Gustavus Adolphus College, St. Peter, MN (9/28/01).
8. * J.V. Goodpaster, "Research in the Field of Forensic Science," *AAFS Annual Meeting (Young Forensic Scientists Forum)*, Atlanta, GA (2/12/02).
9. J.V. Goodpaster, B.C. Drumheller, B.A. Benner, Jr., "Chemical Analysis of Organic Material on the Surface of Human Scalp Hair as a Basis for Forensic Comparisons," *AAFS Annual Meeting*, Atlanta, GA (2/16/02).
10. J.V. Goodpaster, B.A. Benner, Jr., "Limitations of the Retention Gap Technique for the Injection of Large Sample Volumes in Capillary Gas Chromatography/Mass Spectrometry," *Pittcon 2002*, New Orleans, LA (3/18/02).
11. * J.V. Goodpaster, "A New Alternative for Forensic Hair Comparisons: Chemical Analysis of Hair Surface Components Using GC/MS," *Washington Chromatography Discussion Group*, Rockville, MD (4/19/02).
12. J.V. Goodpaster, R.O. Keto, "Identification of Organic Components in Intact and Burned Black Powder Substitutes Using GC/MS," *AAFS Annual Meeting*, Dallas, TX (2/20/04).
13. * J.V. Goodpaster, P.A. Dreifuss, "Novel Analyses of Black Powder Substitutes and Their Post-Blast Residues by Reversed Phase ESI LC/MS," *17th Sanibel Conference on Mass Spectrometry*, Clearwater Beach, FL (1/29/05).
14. * J.V. Goodpaster, "Living CSI: Separating Fact from Fiction," *Homecoming 2005*, Gustavus Adolphus College, St. Peter, MN (10/8/05).

15. * J.V. Goodpaster, "Designing Instrumental and Statistical Solutions to Explosive Problems," Department of Chemistry, Gustavus Adolphus College, St. Peter, MN (2/24/06).
16. * J.V. Goodpaster, "The Role of Instrumental and Chemometric Analysis in Explosives Investigations," Department of Chemistry and Chemical Biology, IUPUI, Indianapolis, IN (10/11/06).
17. J.V. Goodpaster, "From 'Fuzzy Math' to Functional Tool: The Role of Chemometric Analysis in the Identification and Comparison of Black Electrical Tape," *Annual Meeting of the Midwestern Association of Forensic Scientists*, Indianapolis, IN (10/12/06).
18. * J.V. Goodpaster, "The Utility of Derivatization in the Analysis of Explosives and Fire Debris," Department of Forensic Science, Virginia Commonwealth University, Richmond, VA (1/31/07).
19. * J.V. Goodpaster, "Improving the Analysis and Detection of Explosives Through Instrumental and Statistical Techniques," Naval Surface Weapons Center, Crane Division, Crane, IN (9/13/07).
20. * J.V. Goodpaster, "Preventing, Investigating and Reconstructing Explosive Incidents, The Chemist's Role," Butler University, Indianapolis, IN (1/22/08).
21. * J.V. Goodpaster, "The Role of a Chemist in an Explosives Investigation," *ACS Career Night* (Hosted By the Chapter of Student Affiliates of the American Chemical Society at IUPUI (Chemistry Club), IUPUI, Indianapolis, IN (9/23/08).
22. * J.V. Goodpaster, "Chemometric Analysis as a Means to Differentiate Class Evidence," *FACSS*, Reno, NV (10/1/08).
23. D.A. Turner, J.V. Goodpaster, "The Effects of Microbial Degradation on Ignitable Liquids," *Annual Meeting of the Midwestern Association of Forensic Scientists*, Des Moines, IA (10/2/08).
24. * J.V. Goodpaster, "Coming Apart at the Seams: The Anatomy of a Pipe Bomb Explosion," *IUPUI Cutting Edge Lecture Series*, IUPUI, Indianapolis, IN (10/22/08).
25. * J.V. Goodpaster, "Beating the Bugs: The Destruction of Ignitable Liquids by Microbes in Fire Debris Evidence," Department of Biology, University of Indianapolis, Indianapolis, IN (11/6/08).
26. L. Rivas, J.A. Siegel, J.V. Goodpaster, "Analysis of Pigmented Inks by Pyrolysis Gas Chromatography-Mass Spectrometry," *AAFS Annual Meeting*, Denver, CO (2/19/09).
27. E.A. Liszewski, J.A. Siegel, J.V. Goodpaster, E. Duckworth, B. Cline, A. Trantham, "Analysis of Automotive Paint Clear Coats by UV-Visible Microspectrophotometry, Raman Spectroscopy, and FTIR," *AAFS Annual Meeting*, Denver, CO (2/19/09).
28. J.N. Cummins, N. Roemer, B.J. Routon, E.J. Smith, K.M. Whitaker, J.V. Goodpaster, "Coming Apart at the Seams: The Anatomy of a Pipe Bomb Explosion," *AAFS Annual Meeting*, Denver, CO (2/20/09).
29. J. Barrett, J.A. Siegel, J.V. Goodpaster, "Forensic Discrimination of Red Hair Dyes by UV-visible Microspectrophotometry," *AAFS Annual Meeting*, Denver, CO (2/20/09).
30. D.A. Turner, J.V. Goodpaster, "The Effect of Microbial Degradation on Ignitable Liquids," *AAFS Annual Meeting*, Denver, CO (2/20/09).

31. * J.V. Goodpaster, "What Do Explosives Smell Like? Understanding Canine Detection of Energetic Materials," Manchester College, North Manchester, IN (4/13/09).
32. * J.V. Goodpaster, "Applications of Multi-variate Statistics to Forensic Science," *Central Regional Meeting of the American Chemical Society (CERMACS)*, Cleveland, OH (5/20/09).
33. E.H. Lotspeich, J.V. Goodpaster, "Evaluation of the Odor Compounds Sensed by Explosive-Detecting Canines," *Central Regional Meeting of the American Chemical Society (CERMACS)*, Cleveland, Ohio (5/20/09).
34. J. N. Cummins, N.R. Roemer, J.V. Goodpaster, "The Lethal Potential of the American IED: Velocity, Momentum and Kinetic Energy Measurements of Pipe Bomb Container Fragments" *Central Regional Meeting of the American Chemical Society (CERMACS)*, Cleveland, OH (5/20/09).
35. J.H. Kennedy, J.V. Goodpaster, E.A. Lotspeich, J.M. Wiseman, "Analysis of Post – Blast Pipe Bomb Fragments using DESI-Mass Spectrometry" (poster) *ASMS Conference on Mass Spectrometry and Allied Techniques*, Philadelphia, PA (6/2/09).
36. G. Koehler, M. Alsheikh, R. Wilson, J. Rohloff, S. Randall, J. Goodpaster, "Comparative Analysis of Protein and Transcripts Associated with Cold Response in Cultivated Strawberry," *Plant Biology 2009*, Honolulu, HI (7/19/09).
37. J.V. Goodpaster, "Analysis of Trace Evidence Using Microspectrophotometry and Multivariate Statistics," *NIJ Trace Evidence Symposium*, Clearwater Beach, FL (8/7/09).
38. D.A. Turner, J.V. Goodpaster, "Multivariate Statistical Analysis of the Effects of Weathering and Microbial Degradation of Ignitable Liquids Used in Incendiary Devices," *Joint Forensic Association Meeting*, Orlando, FL (10/22/09).
39. N.R. Roemer, E. Lotspeich, J.Cummins, J.V. Goodpaster, "Does Amount Matter?: Modeling the Escape of Explosive Vapors from Perforated Containers," *Joint Forensic Association Meeting*, Orlando, FL (10/23/09).
40. E.H. Lotspeich, Neoshia Roemer, J.V. Goodpaster, "Demonstrating Explosive Odor Availability by Headspace Analysis" (poster), *Joint Forensic Association Meeting*, Orlando, FL (10/20/09).
41. D.A. Turner, J.V. Goodpaster, "Chemical Agents for Use in Preserving Fire Debris Evidence," *AAFS Annual Meeting*, Seattle, WA (2/25/10).
42. E.H. Lotspeich, Neoshia Roemer, J.V. Goodpaster, "Odor Availability and Its Effect on Canine Detection of Explosives," *AAFS Annual Meeting*, Seattle, WA (2/26/10).
43. E.A. Liszewski, J.A. Siegel, J.V. Goodpaster, "Improved Methods for the Discrimination of Automotive Paint Clear Coats," *AAFS Annual Meeting*, Seattle, WA (2/26/10).
44. * J.V. Goodpaster, "'What Do Explosives Smell Like?' Characterizing the Volatile Compounds Available to Explosive-Detecting Canines Using Gas and Liquid Chromatography," *Keynote Speaker at the 31st Annual Spring Symposium of the Minnesota Chromatography Forum*, Minneapolis, MN (5/13/10).
45. S.W. Lewis, N. Karslake, E.A. Liszewski, W. van Bronswijk, J.V. Goodpaster, J. Siegel, "Characterization of Automotive Paint Clear Coats by UV-Visible Microspectrophotometry and ATR-FT-IR with Subsequent Chemometric Analysis,"

Australian and New Zealand Forensic Science Society 20th International Symposium on the Forensic Sciences, Sydney, Australia (9/10).

46. J.V. Goodpaster, E.A. Liszewski, C.Szkudlarek, "To What Extent Can Microspectrophotometry Discriminate Red Cotton Fibers?"_ *Annual Meeting of the Midwestern Association of Forensic Scientists*, Kansas City, MO (10/1/10).

Biographical Sketch

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and other significant contributors in the order listed on Form Page 2.

Follow this format for each person. **DO NOT EXCEED FOUR PAGES.**

NAME Li, Lei	POSITION TITLE Assistant Professor		
eRA COMMONS USER NAME: LILEI2			
EDUCATION/TRAINING (<i>Begin with baccalaureate or other initial professional education, such as</i>			
INSTITUTION AND LOCATION	DEGREE (if applicable)	YEAR(s)	FIELD OF STUDY
Peking University, Beijing, P.R. China	B.S.	09/91-07/96	chemistry
Peking University, Beijing, P.R. China	M.S.	09/96-07/99	organometallic chemistry
The Johns Hopkins University, Baltimore, MD	Ph.D.	08/99-10/05	bioinorganic chemistry
University of Michigan, Ann Arbor, MI		11/05-07/09	enzymology
Indiana University-Purdue University Indianapolis		08/09	biochemistry

A. Positions and Honors.

Positions and Employment

- 2009- **Assistant Professor**
Department of Chemistry and Chemical Biology, Indiana University-Purdue University, Indianapolis
Indianapolis, IN
- 2005-09 **Postdoctoral Fellow** in Biochemistry/Enzymology Mentor: Dr. E. Neil G. Marsh
Department of Chemistry, University of Michigan, Ann Arbor, MI
Research project: *Mechanistic Studies of Benzylsuccinate Synthase, a Glycyl Radical Enzyme Involved in Toluene Degradation*
- 1999-05 **Ph.D.** in Bioinorganic Chemistry Advisor: Dr. Kenneth D. Karlin
Department of Chemistry, The Johns Hopkins University, Baltimore, MD
Thesis: *Copper-Dioxygen Complex Mediated Aliphatic C-H Bond and DNA Nucleobase Oxidation*
(DNA cleavage studies were carried out under the guidance of Prof. Steven E. Rokita at University of Maryland, College Park)
- 1996-99 **M.S.** in Organometallic Chemistry Advisors: Dr. Xianglin Jin & Kaluo Tang
Department of Chemistry, Peking University, Beijing, P.R. China
Thesis: *Synthesis and Physical Property Analysis of Molybdenum and Tungsten Metallafullerenes*
- 1991-96 **B.S.** in Chemistry Advisors: Dr. Xianglin Jin & Kaluo Tang
Department of Chemistry, Peking University, Beijing, P.R. China
Thesis: *Synthesis of Cu, Ag Clusters by CS₂-insertion Reaction*

Professional Societies

- 2001- The American Chemical Society
2009- The Associate Faculty Member, Small molecule chemistry Section, Faculty of 1000 Biology

Honors

- 2001 Outstanding Invention of the Year (Life Science) University of Maryland, College Park, MD

Award title: *Novel copper complexes being tested as anti-cancer agents*

This award is given by the University of Maryland annually. The three winning inventions (physical science, information science and life science) in 2001 were selected from a pool of 97 applicants by an independent panel based on creativity, novelty and potential overall benefit to society.

- 1992 GuangHua Award Peking University, Beijing, China
This award is given to top 10% students by Peking University annually.

B. Peer-reviewed publications (in chronological order).

- 1) Zhang, T.-Q; Li, J.-L.; Gao, P.; Gong, Q.-H.; Tang, K.-L.;* Jin, X.-L.; Zheng, S.-J.; **Li, L.** "Enhanced Optical Limiting Performance of a Novel Molybdenum Complex of Fullerene" *Optics Communications* 1998, 150, 201-204.
- 2) Zanello, P.; Laschi, F.; Fontani, M.; Mealli, C.; Ienco, A.; Tang, K.-L.;* Jin, X.-L.; **Li, L.** "Redox Behavior of the Molybdenum and Tungsten Metallofullerenes $M(\eta^2-C_{60})(CO)_2(phen)(dbm)$ ($M = Mo$ or W ; $phen = 1,10$ -Phenanthroline; $dbm =$ Dibutyl Maleate): (Spectro)Electrochemistry and Theoretical Considerations" *Journal of the Chemical Society, Dalton Transactions* 1999, 6, 965-970.
- 3) Liu, C.-L.; Zhao, G.-Z.; Gong, Q.H.; Tang, K.-L.;* Jin, X.-L.; Cui, P.; **Li, L.** "Optical Limiting Property of Molybdenum Complex of Fullerene C_{70} " *Optics Communications* 2000, 309-313.
- 4) Zanello, P.; Laschi, F.; Cinquantini, A.; Fontani, M.; Tang, K.-L.;* Jin, X.-L.; **Li, L.** "The Redox Behavior of the Family $C_{60}[Mo(CO)_2(phen)(dbm)]_n$ ($n = 1-3$) – A Comparison with the Analog $(\eta^2-C_{70})Mo(CO)_2(phen)(dbm)$ ($phen = 1,10$ -Phenanthroline; $dbm =$ Dibutyl Maleate)" *European Journal of Inorganic Chemistry* 2000, 6, 1345-1350.
- 5) Tang K.-L.; Jin X.-L.; Cui P.; Zheng S.-J.; **Li, L.**; Xie X.-J.* "Study on Isomerization of the Ligand Dibutyl Maleate" *ACTA CHIMICA SINICA* 2001, 59, 1628-1632.
- 6) Cui, P.; **Li, L.**; Tank, K.-L.; Jin, X.-L.* "The Crystal Structure of the Molybdenum Complex of C_{70} Fullerene $Mo(\eta^2-C_{70})(CO)_2(phen)(dbm) \cdot 2C_3H_8O \cdot 2.5H_2O$ " *Journal of Chemical Research, Synopses* 2001, 6, 240-242.
- 7) **Li, L.**; Karlin, K. D.* Rokita, S. E.* "Changing Selectivity of DNA Oxidation from Deoxyribose to Guanine by Ligand Design and a New Binuclear Copper Complex" *Journal of the American Chemical Society*, 2005, 127, 520-521.
- 8) **Li, L.**; Sarjeant, A. A.; Vance, M. A.; Zakharov, L. V.; Rheingold, A. L.; Solomon, E. I.; Karlin, K. D.* "Exogenous Nitrile Substrate Hydroxylation by a New Dicopper-hydroperoxide Complex" *Journal of the American Chemical Society*, 2005, 127, 15360-15361.
[Highlighted in the Science magazine on "Highlights of Recent Literature, Editor's Choice" section, *Science*, 2005, 310, 591].
- 9) **Li, L.**; Sarjeant, A. A.; Karlin, K. D.* "Reactivity study of a hydroperoxodicopper(II) complex: hydroxylation, dehydrogenation, and ligand cross-link reactions" *Inorganic Chemistry*, 2006, 45, 7160-7172.

- 10) **Li, L.**; Telser, J.; Murthy, N. N.; Zakharov, L. V.; Yap, G; Rheingold, A. L.; Karlin, K.D.*; Rokita, S. E.* “Targeted guanine oxidation by a dinuclear copper(II) complex at single stranded/double stranded DNA junctions” *Inorganic Chemistry*, 2006, 45, 7144-7159.
- 11) **Li, L.**; Marsh, E. N. G.* “Deuterium Isotope Effects in the Unusual Addition of Toluene to Fumarate Catalyzed by Benzylsuccinate Synthase” *Biochemistry*, **2006**, 45, 13932-13938.
- 12) **Li, L.**; Marsh, E. N. G.* “Mechanism of Benzylsuccinate Synthase Probed by Substrate and Isotope Exchange” *Journal of the American Chemical Society*, **2006**, 128, 16056-16057.
- 13) **Li, L.**; Paterson, D. P.; Lin, B.; Coschigano, P. W.; Marsh, E. N. G.* “The Subunit Structure of Benzylsuccinate Synthase” *Biochemistry*, **2009**, 48, 1284–1292.
- 14) Lucas, H. R.; **Li, L.**; Sarjeant, A. A.; Vance, M. A.; Milligan, A. E.; Solomon, E. I.; Karlin, K. D. * “Aliphatic C-H Bond Oxidations Initiated by a μ -1,2-Peroxo-dicopper(II) Complex” *Journal of the American Chemical Society*, **2009**, 131, 3230–3245.
- 15) Marsh, E. N. G.*; Paterson, D.; **Li, L.*** “Adenosyl radical: reagent and catalyst in enzyme reactions” *ChemBioChem*, **2010**, 11, 604-621
- 16) Lin, G.; **Li, L.*** “Revealing the spore photoproduct (SP) formation via isotope labeling” (**hot paper** as the Editor’s choice) *Angewandte Chemie International Edition, ASAP*
- 17) Yang, L.; [†] Lin, G.; [†] Liu, D.; Dria, K. J.; Telser, J.; **Li, L.*** Probing the reaction mechanism of spore photoproduct lyase (SPL) via diastereoselectively labeled dinucleotide SP TpT substrates” *Submitted*. ([†] These authors contribute equally to this work)
- 18) Liu D. and **Li, L.*** “A cyclobutane pyrimidine dimer (CPD) analog formed between thymine and toluene via photolysis” *Submitted*.
(* correspondent authors)

C. Research Support.

Ongoing Research Support

- R00 ES017177 (NIH Pathway to Independence (PI) Award) 08/01/09 – 07/31/12 NIH/NIEHS

Enzyme Catalysis of Toluene Degradation and Unusual DNA Photoproduct Repair

This study is to investigate the structure and mechanism of the adenosylmethionine (SAM)-dependent radical enzymes, benzylsuccinate synthase (BSS) at K99 phase and spore photoproduct lyase (SPL) at R00 phase, as model systems to study radical-mediated enzymatic catalysis

Responsibility on project: P.I.

- IUPUI Startup Fund 08/01/2009 – 07/31/2012

CURRICULUM VITAE

(Fall 2010)

ERIC C. LONG

DEPARTMENT OF CHEMISTRY & CHEMICAL BIOLOGY
PURDUE SCHOOL OF SCIENCE, INDIANA UNIVERSITY–PURDUE UNIVERSITY INDIANAPOLIS
402 NORTH BLACKFORD STREET, INDIANAPOLIS, INDIANA 46202-3274

PERSONAL

Birth Date: November 20th, 1962

Citizenship: U.S.A.

Contact Information: e-mail elong@iupui.edu; phone (317) 274-6888

Web Directory: <http://www.chem.iupui.edu/Faculty/Long/>

RESEARCH INTERESTS

Biological & Bioorganic Chemistry: Molecular recognition and modification of nucleic acids by natural products, peptides, and anti-tumor agents; expedited discovery and analysis of nucleic acid-targeted agents.

EDUCATION

1980 - 1984

Bachelor of Science in Biochemistry (ACS-Certified),
Albright College, Reading, Pennsylvania; Awarded May 1984.

1984 - 1988

Doctor of Philosophy, University of Virginia, Department of Chemistry;
Awarded January 1989 (defended August 1988); Dissertation Title: *Mechanistic Studies of Metallo-Bleomycins & Their Interaction with Oligonucleotides*.
Advisor: Professor Sidney M. Hecht

1988 - 1991

Fellow of The Jane Coffin Childs Memorial Fund for Medical Research,
California Institute of Technology, Division of Chemistry & Chemical Engineering and
Columbia University, Department of Chemistry, with Prof. Jacqueline K. Barton

ACADEMIC & ADMINISTRATIVE APPOINTMENTS

2002 - Present

Professor of Chemistry, Department of Chemistry & Chemical Biology,
Purdue School of Science, Indiana University–Purdue University Indianapolis
(Associate Professor 1997-2002, Assistant Professor 1991-1997)

2008 – Present

Director, IU Simon Cancer Center Core Facility for Chemical Synthesis & Drug Lead
Development, IU School of Medicine, IUPUI

2000 - 2009

Associate Chair, Department of Chemistry & Chemical Biology,
Purdue School of Science, Indiana University–Purdue University Indianapolis

2007 - 2008

Interim Chair, Department of Chemistry & Chemical Biology,
Purdue School of Science, Indiana University–Purdue University Indianapolis

2005 - Present

Affiliate Member, Indiana University Simon Cancer Center (Full Member, Experimental & Developmental Therapeutics Program 2005-2006)

2002 - Present

Full Member, Indiana University Graduate School (Associate Member 1991-2002)

1991 - 2001

Member, Medical Biophysics Program, Indiana University Medical & Graduate Schools

1988 - 1991

Research Fellow, Department of Chemistry, Columbia University and Division of Chemistry & Chemical Engineering, the California Institute of Technology

1984 - 1988

Teaching & Research Assistant, Department of Chemistry, University of Virginia

CONSULTING**2009 - Present**

Microbiotix, Inc., Worcester, MA.

PROFESSIONAL ORGANIZATION MEMBERSHIPS

American Chemical Society:

Divisions of Biological, Inorganic & Organic Chemistry.

American Association for the Advancement of Science

The American Peptide Society

AWARDS/HONORS

- | | |
|--------------------|--|
| 2006 | ACS, Division of Biological Chemistry, Travel Award Mentor (for M.A. Lewis) |
| 2004 | Japan Society for the Promotion of Science, Invitation Fellowship Award |
| 2004 | Sabbatical Leave (spring) |
| 2002 | Trustees Teaching Award – Indiana University |
| 2001 | Trustees Teaching Award – Indiana University |
| 1999 | Purdue School of Science Teaching Award |
| 1999 | Teaching Excellence Recognition Award – Indiana University |
| 1997 | Teaching Excellence Recognition Award – Indiana University |
| 1992 | Purdue Research Foundation Summer Faculty Fellow |
| 1989 - 1991 | Jane Coffin Childs Memorial Fund for Medical Research Fellowship |
| 1989 | American Cancer Society Postdoctoral Fellowship (declined by awardee) |
| 1989 | NIH-Individual Research Service Award (declined by awardee) |
| 1988 | Centre National De La Recherche Scientifique Fellowship, Laboratoire De Chimie De Coordination, Toulouse, France (declined by awardee) |
| 1987 - 1988 | Dupont Fellowship, University of Virginia |
| 1986 - 1987 | Dean's Fellowship, University of Virginia |
| 1984 | MDS Laboratories Award for Undergraduate Research |
| 1980 - 1984 | Albright College Trustee Grant Award |

BIOGRAPHICAL ENTRIES

American Men & Women of Science, 1997 - Present.

Who's Who in the Midwest, 1994 - Present.

Who's Who in the West, 23rd Edition, 1992.

Who's Who in Science and Engineering, 1994 - Present.

PROFESSIONAL SERVICE OF NOTE

- Editorial: *Editor* – ACS Symposium Series Volume 1012: *Bioinorganic Chemistry: Cellular Systems & Synthetic Models* (co-edited with M. J. Baldwin) (May, 2009)
- Associate Editor* – *Current Bioactive Compounds* (2008 – Present)
- Editorial Advisory Board* – *Current Organic Synthesis* (2009-Present)
- Editorial Advisory Board* – *The Open Natural Products Journal* (2007 – Present)
- Associate Editor* – *International Journal of Biological Chemistry* (2006 – 2008)
- Invited Expert Analyst* – *Chemtracts: Inorganic Chemistry* (1991-2003)
- Meeting Organization: *Co-Chair*, Biological Chemistry Division, American Chemical Society 36th Central Regional Meeting (Indianapolis, IN, June 2-4, 2004).
- Symposium Co-organizer*, Biological Chemistry Division, American Chemical Society 36th Central Regional Meeting (Indianapolis, IN, June 2-4, 2004). Sessions Organized: Nucleic Acid Structure & Chemistry I, Nucleic Acid Structure & Chemistry II, Biological Chemistry General Session, and Biological Chemistry Poster Session.
- Symposium Chair*, Symposium on Metal-Containing Polymeric Materials, ACS 1994 Fall Meeting, Washington, D.C.
- Proposal Reviewing: *Temporary Member*, NIH SBCA Study Section (June, 2009)
- Member*, NIH Biological Chemistry Special Emphasis Panel ZRG-1 BCMB-U 02S (June, 2009)
- Temporary Member*, NIH SBCB Study Section (October, 2005)
- Temporary Member*, NIH Metallobiochemistry Study Section (June 1998, June 1999, and February 2002)
- National Science Foundation
- Manuscript Reviewing: *Biochemistry, Bioorganic & Medicinal Chemistry, Bioorganic & Medicinal Chemistry Letters, Journal of the American Chemical Society, Journal of Inorganic Biochemistry, Journal of Biological Inorganic Chemistry, Nucleic Acids Research*

RECENT DEPARTMENT, SCHOOL, & UNIVERSITY SERVICE OF NOTE

Departmental Committees/Appointments

Interim Department Chair
Associate Department Chair
Director of Graduate Programs
*Chair, Graduate Admissions/Recruitment Committee (past and **current**)*
Chair, Graduate Policies Committee
Undergraduate Curriculum Committee
*Executive Committee (elected and *ad hoc*) (past and **current**)*
Seminar Chair
Tenure-Track Faculty Search & Screen Committees–
(Chair, '02-'03, '03-'04, '04-'05, '05-'06, '07-'08, '08-'09, '09-'10)
Search Committee–Department Chair '07-'08
Chair, 2006 Department Planning/Direction Sub-Group

School of Science Committees

Department of Biology, Chair Search Committee (2009-2010)
*Promotion and Tenure-Unit Committee (past and **current**)*
Search Committee: Associate Dean for Research & Graduate Education
Ad Hoc Graduate Affairs Committee
School of Science Steering Committee
School of Science Graduate Affairs Committee
Research & Graduate Education Strategic Planning Team

School of Medicine Committees

Small Molecule Working Group
*Core Consortium (**current**)*
*Indiana CTSI Preclinical Development Team ('08-'09 - **current**)*
*Faculty Mentoring Committee (**current**)*
Medical Biophysics Steering Committee
*CTSI Core Grant Review Committee (**current**)*

University Committees

Sabbatical Leaves Committee
External Review Committee, IUPUI Department of Biology
Research Support Fund Grants (RSFG) Standing Committee (2005 – 2008)
Intercampus Applied Research Program (IARP) Review Committee (2007 – 2008)
Graduate Affairs Committee (Purdue School of Science Representative)
IUPUI Office for Professional Development – Grant Advisory Panel

RECENT TEACHING

Chem 485: *Biosynthesis & Physiology* (Spring, 2011)
Chem 486: *Biological Chemistry Laboratory*
Chem 484: *Introductory Biological Chemistry*
Chem 533: *Introductory Biological Chemistry*
Chem 696: *Special Topics: Metabolism* (Spring, 2011)
Chem 696: *Special Topics: Seminars in Nucleic Acid Chemistry* (Fall, 2010)

RESEARCH GRANTS, FELLOWSHIPS, AND CONTRACTS

External

"The Influence of Carbohydrates on DNA Recognition" E. C. Long, \$67,500 (The Jane Coffin Childs Memorial Fund for Medical Research), July 1, 1989 - June 30, 1992.

"An Investigation into the Role of Carbohydrates in DNA Recognition" E. C. Long, \$45,000 (American Cancer Society), July 1, 1989 - June 30, 1991. Declined by Grantee.

"Studies on Carbohydrate-Containing Rh-Complexes with DNA" E. C. Long, \$26,000 (National Institutes of Health-Individual National Research Service Award), June 1, 1989 - May 31, 1991. Declined by Grantee.

"Stabilization of DNA Recognition Helices Through Strategically-Placed Metal Binding Sites" E. C. Long, \$21,000 (The Petroleum Research Fund-American Chemical Society) June 1, 1992 - August 31, 1994.

"Purchase of Macromolecular Modeling Equipment" D. J. Malik, P. L. Dubin, W. K. Fife, K. B. Lipkowitz, E. C. Long (Co-PI), and M. Zeldin, \$78,011 (National Science Foundation) January 1, 1993 - December 31, 1995.

"Capillary Electrophoresis in the Analytical and Biological Chemistry Laboratory" J. J. Breen and E. C. Long (Co-PI), \$39,870 (National Science Foundation) July 1, 1994 - June 30, 1996.

"DNA Recognition by β -Turn Peptides and Peptidomimetics" E. C. Long, \$521,486 (National Institutes of Health GM 50557) August 1, 1994 - July 31, 2000.

"A Phosphoimager for Molecular Biology Research" P. L. Crowell, E. C. Long (Co-PI), S. J. Rhodes, and J. C. Watson, \$73,972 (National Science Foundation) September 15, 1999 - August 31, 2000.

"Collaborative Agreement with ComChem Technologies, Inc." M. J. O'Donnell and E. C. Long (Co-PI), \$5,980 (ComChem Technologies, Inc.) May 1, 2000 - April 30, 2001.

"Metallopeptide-DNA Recognition & Reactivity" E. C. Long, \$720,486 (National Institutes of Health GM 63821) April 1, 2001 - March 31, 2006.

"Graduate Assistance in Areas of National Need Fellowship Program" D. J. Malik and E. C. Long (Co-PI), \$546,732 (U.S. Department of Education) August 15, 2001 - August 14, 2005.

"Binding and Reaction of Novel Modified Metallopeptides with DNA" E. C. Long (Fellow) and M. Chikira (Host), ~ \$20,000 (Japan Society for the Promotion of Science, Invitation Fellowship for Research in Japan - Short Term); awarded: August 1, 2003 used: March 15, 2004 - April 30, 2004.

"Acquisition of a 500 MHz NMR Spectrometer" F. A. Schultz (PI), E. C. Long, R. E. Minto, M. J. O'Donnell, Z.-Y. Zhang (Co-PIs), \$516,500 (NSF Major Research Instrumentation) August 1, 2006 - July 31, 2007.

"Quantifying Kidney Filtration Function with Quantum Dot Nanoprobes" W. Yu (PI) and C. A. Naumann, E. C. Long and B. Molitoris (Co-investigators), \$568,125 (National Institutes of Health R21 DK077051-01) May 1, 2007 – April 30, 2010.

"Microbiotix, Inc. Contract Research" E. C. Long (PI), \$11,880 (Microbiotix, Inc.) June 9, 2008 – September 30, 2008; Renewed 2010 (\$32,447). **ACTIVE**

"ApeX Therapeutics Contract Research Project" E. C. Long (PI, on behalf of Synthesis Core), \$21,000 (ApeX Therapeutics). **ACTIVE**

"Dual Targeting of p53 and DNA Repair Pathways for Treatment of Brain Cancer" K. Pollok (PI), E. C. Long Co-Investigator (5%) *et al.*, \$1,927,000 (National Institutes of Health R01 CA138798) July 1, 2010 – June 31, 2015. **ACTIVE**

"Structural Studies of DNA-Bound Bleomycin: Recognition & Reactivity" E.C. Long (PI) and M.M. Georgiadis (co-PI); National Institutes of Health (GM); submission planned Spring 2011.

Internal

"The Role of Conformational Change in DNA Binding by the Transcriptional Regulator GCN4" E. C. Long, \$10,000 (The American Cancer Society, Institutional) July 1, 1992 - June 30, 1993.

"Metal Ion-Controlled DNA Binding by the Transcriptional Regulator GCN4" E. C. Long, \$6,000 (IUPUI Faculty Development Grant) 1992 - 1993.

"Mechanistic Studies of Conformational-Controlled DNA binding by the Protein GCN4 Through the Use of Strategically-Placed Metal Chelating Domains" E. C. Long, \$5,000 (Purdue Research Foundation) Summer, 1992.

"Cellular and Biomolecular Spectroscopy" L. J. Janski, N. D. Lees, E. C. Long (Co-PI) and D. J. Malik, \$251,094 (IUPUI Research Investment Fund).

"Metallopeptide-DNA Interactions" E. C. Long, \$23,332 (Purdue Research Foundation) August 1, 1996 - July 31, 1998.

"Binding and Cleavage of HIV-1 TAR RNA by Fe•Bleomycin" E. C. Long, \$3,000 (IUPUI Office for Professional Development) May 26, 2000 - May 25, 2001.

"Selective Cleavage of HIV RNAs by Bleomycin" E. C. Long, \$26,140 (Purdue Research Foundation) May 1, 2001 – December 31, 2004.

"Investigation of Kidney Filtration Function Using Quantum Dots and Intravital Microscopy" W. Yu, C. Naumann, Co-PIs, E. C. Long, B. Molitoris, Co-Investigators, \$60,000 (IUPUI Office of Research & Sponsored Programs NIH Roadmap Initiative Grant). April, 2005 – June, 2006.

"Development of a High-Throughput, High-Resolution 'New Pathway to Discovery' of Specific Drug-DNA Interactions" E. C. Long, M. M. Georgiadis, Co-PIs, \$60,000 (IUPUI Office of Research & Sponsored Programs NIH Roadmap Initiative). April, 2005 – June, 2006.

"HT-HR Analyses of Site-Selective Bulged DNA and siRNA Binding Ligands" E. C. Long, PI, \$35,000 (IUPUI Office of Research & Sponsored Programs Research Support Funds Grant) May 1, 2007 – April 30, 2008.

"Dual Targeting of p53 and DNA Repair Pathways for Treatment of Brain Cancer" K. Pollok (PI), E. C. Long (Co-Investigator) *et al.*, \$35,000 (IUPUI Office of Research & Sponsored Programs Research Support Funds Grant) **ACTIVE**.

PUBLICATIONS

Journal Articles

1. G. M. Ehrenfeld, J. B. Shipley, D. C. Heimbrook, H. Sugiyama, E. C. Long, J. H. van Boom, G. A. van der Marel, N. J. Oppenheimer, and S. M. Hecht* "Copper-Dependent Cleavage of DNA by Bleomycin" *Biochemistry* **1987**, 26, 931-942.
2. D. C. Heimbrook, S. A. Carr, M. A. Mentzer, E. C. Long, and S. M. Hecht* "Mechanism of Oxidation of *cis*-Stilbene by Fe-Bleomycin" *Inorganic Chemistry* **1987**, 26, 3835-3836.
3. E. C. Long and S. M. Hecht* "Direct Comparison of Oxygen Transfer by Fe-Bleomycin and Zn-Bleomycin" *Tetrahedron Letters* **1988**, 29, 6413-6416.
4. R. B. Van Atta, E. C. Long, S. M. Hecht*, G. A. van der Marel, and J. H. van Boom "Electrochemical Activation of Oxygenated Fe-Bleomycin" *Journal of the American Chemical Society* **1989**, 111, 2722-2724.
5. A. M. Pyle, E. C. Long, and J. K. Barton* "Shape-Selective Targeting of DNA by (Phenanthrenequinone diimine)rhodium(III) Photocleaving Agents" *Journal of the American Chemical Society* **1989**, 111, 4520-4522.
6. E. C. Long, S. M. Hecht*, G. A. van der Marel, and J. H. van Boom "Interaction of Bleomycin with a Methylated DNA Oligonucleotide" *Journal of the American Chemical Society* **1990**, 112, 5272-5276.
7. E. C. Long and J. K. Barton* "On Demonstrating DNA Intercalation" *Accounts of Chemical Research* **1990**, 23, 271-273.
8. B. J. Carter, E. deVroom, E. C. Long, G. A. van der Marel, J. H. van Boom, and S. M. Hecht* "Site-Specific Cleavage of RNA by Fe(II)-Bleomycin" *Proceedings of the National Academy of Sciences, U.S.A.* **1990**, 87, 9373-9377.
9. E. C. Long and J. K. Barton* review & analysis of: "Chiral Symmetry Breaking in Na Chlorate Crystallization" *Chemtracts-Inorganic Chemistry* **1991**, 3, 1-3.
10. E. C. Long* review & analysis of: "Peptide Architecture. Design of Stable α -Helical Metallopeptides via a Novel Exchange-Intert Rh(III) Complex" *Chemtracts-Inorganic Chemistry* **1991**, 3, 203-205.

11. E. C. Long* review & analysis of: "Self-Assembly of Porphyrins on Nucleic Acids and Polypeptides" *Chemtracts-Inorganic Chemistry* **1991**, 3, 377-380.
12. Y. Kim, E. C. Long, J. K. Barton*, and C. M. Lieber "Imaging of Oligonucleotide-Metal Complexes by Scanning Tunneling Microscopy" *Langmuir* **1992**, 8, 496-500.
13. A. Sitlani, E. C. Long, A. M. Pyle, and J. K. Barton* "DNA Photocleavage by Phenanthrene-quinone Diimine Complexes of Rhodium(III): Shape-Selective Recognition and Reaction" *Journal of the American Chemical Society* **1992**, 114, 2303-2312.
14. D. F. Shullenberger and E. C. Long* review & analysis of: "Efficient Catalytic Cleavage of RNA by Lanthanide(III) Macrocyclic Complexes: Toward Synthetic Nucleases for In Vivo Application" *Chemtracts-Inorganic Chemistry* **1992**, 4, 262-265.
15. E. C. Long* "The DNA Helical Biopolymer: A Template for the Binding, Assembly, and Reactivity of Metal Ions and Complexes" *Journal of Inorganic and Organometallic Polymers* **1993**, 3, 3-39. (invited)
16. D. F. Shullenberger and E. C. Long* "Design and Synthesis of a DNA-Cleaving Metallopeptide" *Bioorganic & Medicinal Chemistry Letters* **1993**, 3, 333-336.
17. D. F. Shullenberger, P. D. Eason, and E. C. Long* "Design and Synthesis of a Versatile DNA-Cleaving Metallopeptide Structural Domain" *Journal of the American Chemical Society* **1993**, 115, 11038-11039.
18. X. Huang, D. F. Shullenberger, and E. C. Long* "Aromatic Stacking and Bending of the DNA Helix by the Individual Repeat Units of the Carboxy-Terminal Domain of RNA Polymerase II" *Biochemical & Biophysical Research Communications* **1994**, 198, 712-719.
19. D. C. Ananias and E. C. Long*, analysis of: A Novel Zinc-Finger Based DNA Cutter: Biosynthetic Design and Highly Selective DNA Cleavage" *Chemtracts-Inorganic Chemistry* **1994**, 6, 56-59.
20. P. D. Eason and E. C. Long*, analysis of: "Iron(II) Bleomycin-Mediated Degradation of a DNA-RNA Heteroduplex" *Chemtracts-Inorganic Chemistry* **1994**, 6, 121-124.
21. X. Huang and E. C. Long* "Chemoenzymatic Synthesis and Incorporation of L-2-Quinoxalylalanine into a Tandem β -Turn Peptide Motif" *Bioorganic & Medicinal Chemistry Letters* **1995**, 5, 1937-1940.
22. Q. Liang, P. D. Eason, and E. C. Long* "Metallopeptide-DNA Interactions: Site-Selectivity Based on Amino Acid Composition and Chirality" *Journal of the American Chemical Society* **1995**, 117, 9625-9631.
23. J. R. Dobbins, N. Murali, and E. C. Long* "Structural Redesign and Stabilization of the Overlapping β -Turns of RNA Polymerase II" *International Journal of Peptide & Protein Research* **1996**, 47, 260-268.

24. D. C. Ananias and E. C. Long* "DNA Strand Scission by Dioxygen + Light-Activated Co(II)-Metallopeptides" *Inorganic Chemistry* **1997**, 36, 2469-2471.
25. Q. Liang, D. C. Ananias, and E. C. Long* "Ni(II)•Xaa-Xaa-His Induced DNA Cleavage: Deoxyribose Modification by a Common "Activated" Intermediate Derived from KHSO₅, MMPP, or H₂O₂" *Journal of the American Chemical Society* **1998**, 120, 248-257.
26. I. J. Brittain, X. Huang, and E. C. Long* "Selective Recognition and Cleavage of RNA Loop Structures by Ni(II)•Xaa-Gly-His Metallopeptides" *Biochemistry* **1998**, 37, 12113-12120.
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50. K. M. Elpers, M. J. O'Donnell, W. L. Scott, and E. C. Long* "Synthesis of Amino-Pyrimidine- and Pyridine-Containing Ni(II)•Xaa-Xaa-Pyr Metallopeptides and Their Potential Interactions with DNA" Third Annual Indiana Local Section of the American Chemical Society Poster Session, October 15, 2002.
51. M. A. Lewis, C. A. Claussen, and E. C. Long* "High Throughput DNA Recognition Screening by Combinatorial Libraries of Ni(II)•Xaa-Xaa-His Metallopeptides" Fourth Annual Indiana Local Section of the American Chemical Society Poster Session, October 8, 2003.

52. Y.-Y. Fang, B. D. Ray, K. B. Lipkowitz and E. C. Long* "Theoretical and Experimental Studies of DNA Binding and Recognition by Ni(II)•Xaa-Xaa-His Metallopeptides" Fourth Annual Indiana Local Section of the American Chemical Society Poster Session, October 8, 2003.
53. M. S. Dearry, Y.-Y. Fang, and E. C. Long* "DNA Recognition and Binding by Ni(II)•Xaa-Gly-His Metallopeptides Containing Proline and Modified Proline Residues" Fourth Annual Indiana Local Section of the American Chemical Society Poster Session, October 8, 2003.
54. K. M. Diaz, X. Deng, M. J. O'Donnell, W. L. Scott and E. C. Long* "Synthesis of Amino-Pyrimidine- and Pyridine-Containing Ni(II)•Metallopeptides and Their Potential Interactions with DNA" Fourth Annual Indiana Local Section of the American Chemical Society Poster Session, October 8, 2003.
55. M. A. Lewis, C. A. Claussen and E. C. Long* "High Throughput DNA Recognition Screening of Ni(II)•Xaa-Xaa-His Metallopeptides" *Abstracts of Papers* 227th National Meeting of the American Chemical Society, Anaheim, CA.; American Chemical Society: Washington, D. C., 2004: INOR 656, March 28-April 1, 2004.
56. M. Chikira, M. Ito, H. Honma, S. Hirosawa and E. C. Long "Interaction of Cu(II) Complexes of Histidine-Containing Peptides with DNA" *Proceedings of the 84th Annual Meeting of the Chemical Society of Japan*, March 26-29, 2004, Kobe, Japan.
57. C. A. Claussen, Y.-Y. Fang, B. D. Ray, K. B. Lipkowitz and E. C. Long "DNA Recognition by Ni(II)-Gly-Gly-His Derived Metallopeptides" *Abstracts*, 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, United States, June 2-4 (2004), INV-160.
58. K. M. Diaz, X. Deng, M. J. O'Donnell, W. L. Scott and E. C. Long "Synthesis of Amino-Pyrimidine- and Amino-Pyridine-Containing Ni(II)-Metallopeptides and Their Potential Interactions with DNA" *Abstracts*, 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, United States, June 2-4 (2004), GEN-197.
59. Y.-Y. Fang, B. D. Ray, K. B. Lipkowitz, E. C. Long "Theoretical and Experimental Studies of DNA Binding and Recognition by Ni(II)-Xaa-Xaa-His Metallopeptides" *Abstracts*, 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, United States, June 2-4 (2004), GEN-195.
60. M. A. Lewis, C. A. Claussen and E. C. Long "High-Throughput DNA Recognition Screening of Ni(II)-Xaa-Xaa-His Metallopeptides" *Abstracts*, 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, United States, June 2-4 (2004), GEN-192.
61. M. S. Wall, Y.-Y. Fang, E. C. Long "DNA Recognition and Binding by Ni(II)-Xaa-Gly-His Metallopeptides Containing Proline and Modified Proline Residues" *Abstracts*, 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, United States, June 2-4 (2004), GEN-190.

62. Y.-Y. Fang, C. A. Claussen, B. D. Ray, K. B. Lipkowitz and E. C. Long "Theoretical and Experimental Studies of DNA Minor Groove Recognition by Ni(II)•Gly-Gly-His-Derived Metallopeptides" *Abstracts of Papers 228th National Meeting of the American Chemical Society, Philadelphia, PA.; American Chemical Society: Washington, D. C., 2004: BIOL 47, August 22-26, 2004.*
63. M. A. Lewis, C. A. Claussen and E. C. Long "Examining the DNA Site-Selectivity of Ni(II)•Gly-Gly-His-Derived Metallopeptides via High-Throughput Fluorescent Intercalator Displacement" *Abstracts of Papers 228th National Meeting of the American Chemical Society, Philadelphia, PA.; American Chemical Society: Washington, D. C., 2004: BIOL 48, August 22-26, 2004.*
64. M. A. Lewis, K. D. Goodwin, M. M. Georgiadis and E. C. Long "DNA-Dependent Cu(II)•Xaa-Xaa-His Metal-Peptide Dissociation" *Abstracts, 12th International Conference on Bio-Inorganic Chemistry (ICBIC-12), July 31-August 5, 2005.* Published online at: <http://www.umich.edu/~icbic/ICBIC-12-Abstracts.htm>
65. M. A. Lewis, K. M. Williams, and E. C. Long "(δ)-Orn-Linked Cu(II)• or Ni(II)•Gly-Gly-His-Like 'Tandem-Array' Metal Binding Oligopeptides" *Abstracts, 12th International Conference on Bio-Inorganic Chemistry (ICBIC-12), July 31-August 5, 2005.* Published online at: <http://www.umich.edu/~icbic/ICBIC-12-Abstracts.htm>
66. A. M. Zins and E. C. Long (2005) "Interaction of Libraries of Cu(II)•Gly-Gly-His-Derived Metallopeptides and their Apo-Peptides with 2-Aminopurine-Labeled HIV-1 TAR" *Abstracts, 6th Annual Indiana Local Section American Chemical Society Poster Session, 5A, October 10, 2005.*
67. K. M. Williams, M. A. Lewis, and E. C. Long (2005) "Orn-Linked Cu(II)• or Ni(II)•Gly-Gly-His-Like 'Tandem Array' Metal binding oligopeptides" *Abstracts, 6th Annual Indiana Local Section American Chemical Society Poster Session, 21B, October 10, 2005.*
68. D. L. Shaw, C. A. Naumann, and E. C. Long (2005) "Sonochemical Synthesis, Shelling, and Biofunctionalization of 'Quantum Dots' for Quantitative *in vivo* Imaging Applications" *Abstracts, 6th Annual Indiana Local Section American Chemical Society Poster Session, 24B, October 10, 2005.*
69. M. A. Lewis, K. D. Goodwin, M. M. Georgiadis, and E. C. Long (2005) "DNA-Dependent Cu(II)•Xaa-Xaa-His Metal-Peptide Dissociation" *Abstracts, 6th Annual Indiana Local Section American Chemical Society Poster Session, 30B, October 10, 2005.*
70. M. A. Lewis and E. C. Long (2006) "Fluorescent Intercalator Displacement Analyses of the DNA Binding Site-Selectivities of Peptide-Derived Anti-Cancer Natural Products: Netropsin, Actinomycin, and Bleomycin" *IU Cancer Research Day, May 10, 2006.*

71. K. D. Goodwin, M. A. Lewis, M. M Georgiadis, and E. C. Long (2006) "A High-Throughput, High-Resolution Strategy for the Rapid Structural Elucidation of Site-Selective DNA Binding Agents" *IU Cancer Research Day*, May 10, 2006.
72. K. D. Goodwin, M. A. Lewis, M. M Georgiadis, and E. C. Long (2006) "A High-Throughput, High-Resolution Strategy for the Structural Elucidation of Site-Selective DNA Binding and Damaging Agents" *8th Annual Midwest DNA Repair Symposium*, IU School of Medicine, IUPUI, May 20-21, 2006.
73. D. T. Hall IV, M. A. Lewis and E. C. Long (2006) "Fluorescent Intercalator Displacement Analyses of Site-Selective DNA Binding by Chromomycin" *2006 CIC Summer Research Opportunities Program (SROP) Conference*, University of Illinois, Urbana-Champaign, July 21-23, 2006.
74. K. D. Goodwin, M. A. Lewis, E. C. Long, and M. M. Georgiadis (2006) "Crystallographic Studies of the Co(III)•Bleomycin-DNA Complex" *American Cancer Society Annual Meeting*, University of Michigan, November 2006.
75. M. A. Lewis, K. D. Goodwin, M. M. Georgiadis, and E. C. Long (2006) "High-Throughput, High-Resolution Strategy for the Rapid Structural Elucidation of Site-Selective DNA Binding Agents" *Abstracts of Papers 232nd National Meeting of the American Chemical Society*, San Francisco, CA.; American Chemical Society: Washington, D. C., 2006: BIOL 122, September 9-14, 2006.
76. Y.-Y. Fang, E. C. Long, V. R. Morris, and W. M. Southerland (2006) "Molecular Dynamics Simulations of the Orientation of Netropsin-DNA Binding" *Abstracts of Papers 232nd National Meeting of the American Chemical Society*, San Francisco, CA.; American Chemical Society: Washington, D. C., 2006: BIOL 136, September 9-14, 2006.
77. H. Hamada, R. Nagane, M. Chikira and E. C. Long (2006) "Interaction of Cu(II) Complexes of Histidine-Containing Tri- or Tetra-Peptides with DNA (III)" *Abstracts 45th Annual Meeting of the Society of Electron Spin Science and Technology*, November 14-16, Kyoto, Japan.
78. K. D. Goodwin, M. A. Lewis, E. C. Long and M. M. Georgiadis (2007) "A new approach to an old problem: The crystal structure of a DNA-Co(III)•bleomycin-B₂ complex" *Abstracts of Papers, CERMACS 2007*, Central Regional Meeting of the American Chemical Society, Covington, KY, May 20-23.
79. Eric C. Long, Millie M. Georgiadis, Kristie D. Goodwin and Mark A. Lewis (2007) "A new approach to analyzing DNA binding agents leading to the crystal structure of a DNA-Co(III)•bleomycin-B₂ complex" *Abstracts of Papers, CERMACS 2007*, Central Regional Meeting of the American Chemical Society, Covington, KY, May 20-23 (invited presentation).
80. K. D. Goodwin, M. A. Lewis, E. C. Long and M. M. Georgiadis (2007) "A new approach to an old problem: The crystal structure of a DNA-Co(III)•bleomycin-B₂ complex" *Albany 2007: The 15th Conversation*, State University of New York at Albany, Albany, NY, June 19-23. Abstract published in *Journal of Biomolecular Structure and Dynamics* **2007**, 24 (6), 674.

81. A. Luckenbill and E. C. Long* (2007) "(Lys)_n-(δ)-Orn-Gly-His Metallopeptides and their Interactions with DNA" *CIC Conference*, Purdue University-West Lafayette, July 27-29.
82. L. S. Glass, M. M. Georgiadis and E. C. Long (2008) "High-Throughput Discovery and Analysis of Nucleic Acid Binding Ligands: Towards the Rapid Development of New DNA-Targeted Chemotherapeutics" *Consortium for Urban Education Life and Health Sciences Research Showcase*, IUPUI, Indianapolis, IN, March 18th.
83. L. S. Glass, M. M. Georgiadis, and E. C. Long (2008) "High-Throughput Discovery and Analysis of Nucleic Acid Binding Ligands: Towards the Rapid Development of New DNA-Targeted Chemotherapeutics" *Abstract Book-Indiana University Melvin and Bren Simon Cancer Center-Cancer Research Day 2008*, Basic Science, page 10, IUPUI, Indianapolis, IN, May 7.
84. M. M. Georgiadis, K. D. Goodwin, M. A. Lewis and E. C. Long (2008) "Crystal Structures of DNA-Bound Co(III)•Bleomycins" [*Acta Cryst.* **2008**, A64, C156] MS.93.4 *Online Abstract Book*, XXI Congress and General Assembly of the International Union of Crystallography (IUCr2008) 23-31 August, Osaka, Japan.
85. LaTeca S. Glass, E. C. Long and Millie M. Georgiadis (2008) "High-Throughput, High-Resolution Strategy Approach to the Analysis of DNA Binding Compounds" *2008 Biochemistry & Molecular Biology Research Day* Indiana University School of Medicine, IUPUI, Indianapolis, IN, October 2.
86. LaTeca S. Glass, E. C. Long and Millie M. Georgiadis (2008) "High-Throughput, High-Resolution Strategy Approach to the Analysis of DNA Binding Compounds" *NOBCCHE Midwest Regional Conference*, Eli Lilly & Co. Corporate Center, Indianapolis, IN, October 23-25.
87. LaTeca S. Glass, Eric C. Long and Millie M. Georgiadis (2009) "Expedited Approaches to the Discovery and Analysis of DNA Binding Ligands" *IUPUI Research Day*, IUPUI, Indianapolis, IN, April 24, 2009.
88. LaTeca S. Glass, Eric C. Long and Millie M. Georgiadis (2009) "Expedited Approaches to the Discovery and Analysis of DNA Binding Ligands" *Abstract Book 2009 Indiana University Melvin and Bren Simon Cancer Center Cancer Research Day*, IUPUI, Indianapolis, IN, May 6, 2009.
89. Tax M. Georgiadis and Eric C. Long (2009) "IUPUI/IUSCC Chemical Synthesis and Organic Drug Lead Development Core: Services and Expertise" *Abstract Book-2009 Indiana University Melvin and Bren Simon Cancer Center Cancer Research Day*, IUPUI, Indianapolis, IN, May 6, 2009.
90. T. J. Opperman, J. B. Li, M. A. Lewis, C. Houseweart, D. Aiello, J. D. Williams, N. P. Peet, D. T. Moir, E. C. Long, and T. L. Bowlin (2009) "DNA Binding Activity of Novel Bis-Indole Antibiotics" *49th Interscience Conference on Antimicrobial Agents and Chemotherapy (ICAAC)*, San Francisco, CA, September 12-15, 2009.

91. Tax M. Georgiadis and Eric C. Long (2009) "IUPUI/IUSCC Chemical Synthesis and Organic Drug Lead Development Core: Services and Expertise" *Purdue CTSI Retreat*, Purdue University-West Lafayette, West Lafayette, IN, September 24, 2009.
92. Tax M. Georgiadis and Eric C. Long (2009) "IUPUI/IUSCC Chemical Synthesis and Organic Drug Lead Development Core: Services and Expertise" *Abstracts, 10th Annual Indiana Local Section American Chemical Society Poster Session*, poster 15, October 15, 2009.
93. ICDDT '10
94. H. Wang, S. Cai, B. J. Bailey, A. L. Sinn, J. M. Silver, R. E. Minto, T. M. Georgiadis, E. C. Long, J. N. Sarkaria, L. B. Mayo, K. E. Pollok (2010) "Modulation of Temozolomide-Mediated DNA Damage in Glioblastoma Multiforme by the HDM2 Antagonist, Nutlin3" [abstract]. In: *Proceedings of the 101st Annual Meeting of the American Association for Cancer Research*; 2010 Apr 17-21; Washington, DC. Philadelphia (PA): AACR; 2010. p#. Abstract nr 5373.
95. M. Garner and E. C. Long MedChem Abstract
96. S. Henkes and E. C. Long MedChem Abstract
97. T. M. Georgiadis and E. C. Long MedChem Abstract
98. M. Garner and E. C. Long ACS Local Abstract
99. S. Henkes and E. C. Long ACS Local Abstract
100. T. M. Georgiadis and E. C. Long ACS Local Abstract.
101. T. M. Georgiadis and E. C. Long TechPoint Innovation Summit Abstract.
102. E. C. Long* and M. M. Georgiadis (2010) "Expedited Studies of DNA-Ligand Recognition: Groove Binders to Bleomycins" *Abstracts: Pacificchem 2010*, Honolulu, Hawaii, December 15-29.

* Primary Authors/ Authors to whom correspondence should be addressed.

Invited Lectures

1. "The Interaction of Rhodium(III) complexes of Phenanthrenequinone Diimine with DNA: Mechanism and Applications," Department of Chemistry, Bowling Green State University, Spring, 1991.
2. "The Interaction of Rhodium(III) complexes of Phenanthrenequinone Diimine with DNA: Mechanism and Applications," Department of Chemistry, IUPUI, Spring, 1991.

3. "The Interaction of Rhodium(III) complexes of Phenanthrenequinone Diimine with DNA: Mechanism and Applications," Department of Chemistry, SUNY-Albany, Spring, 1991.
4. "The Interaction of Rhodium(III) complexes of Phenanthrenequinone Diimine with DNA: Mechanism and Applications," Department of Chemistry, IUPUI, September, 1991.
5. "Design and Synthesis of a Versatile Metallopeptide Structural Domain," Symposium on Metal-Containing Polymeric Materials, 207th American Chemical Society 1994 Fall Meeting, Washington, D.C.
6. "Incorporation of Square-Planar Metal Binding Sites into Protein Polymeric Structures" Department of Physics, IUPUI, September, 1994.
7. "Metallopeptide-DNA Recognition" Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, IUPUI, April, 1995.
8. "Sequence-Selective Interactions of Metallopeptides with DNA" Department of Biology, IUPUI, November, 1995.
9. "Sequence-Selective Interactions of Metallopeptides with DNA" Department of Chemistry, University of Toledo, March 13, 1996.
10. "Sequence-Selective Interactions of Metallopeptides with DNA" Departments of Chemistry and Biology (joint departmental lecture), Wittenberg University, October 28, 1996.
11. "Ni(II)•Xaa-Xaa-His Metallopeptide-Nucleic Acid Interactions: DNA Sequence-Selectivity & Mechanism of Strand Scission" Department of Chemistry, The Ohio State University, April, 1999.
12. "Ni(II)•Xaa-Xaa-His Metallopeptide-Nucleic Acid Interactions: DNA Sequence-Selectivity & Mechanism of Strand Scission" Department of Chemistry, Indiana University-Bloomington, April 7, 2000.
13. "Ni(II)•Xaa-Xaa-His Metallopeptide-Nucleic Acid Interactions: DNA Sequence-Selectivity & Mechanism of Strand Scission" Department of Chemistry, Wayne State University, April 21, 2000.
14. "M(II)•Xaa-Xaa-His Metallopeptide – Nucleic Acid Interactions" Symposium on Recent Advances in the Interactions of Metal Complexes with Nucleic Acids and Their Components, 220th National Meeting of the American Chemical Society, Washington, D. C., August 20, 2000.
15. "M(II)•Xaa-Xaa-His Metallopeptide - Nucleic Acid Interactions" Joint Departments of Biology & Chemistry Inaugural Biochemistry & Molecular Biology Program Lecturer, Illinois State University, September 29th, 2000.
16. "Ni(II)•Xaa-Xaa-His Metallopeptide-Nucleic Acid Interactions" Department of Chemistry, Indiana State University, September 11, 2001(!)

17. "Sequence-Selective DNA Recognition and Binding by Combinatorial Libraries of Ni(II)•Xaa-Xaa-His Metallopeptides Incorporating L- and D-Amino Acids" (C. A. Claussen, presenting, E. C. Long, co-authoring) 2002 Gordon Research Conference-7th Annual Graduate Research Seminar: Bioinorganic Chemistry, January 24-27, 2002, Ventura, CA.
18. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides" Department of Chemistry, University of Cincinnati, February 17, 2004.
19. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides" Department of Chemistry, Chuo University, Tokyo, Japan, March 18, 2004.
20. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides" Department of Chemistry, Kyoto University, Kyoto, Japan, March 29th, 2004.
21. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides" Department of Chemistry, Ochanomizu University, Tokyo, Japan, April 15, 2004.
22. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides" Department of Chemistry, The University of Tokyo, April 19th, 2004.
23. "Analysis of Small Molecule-DNA Binding Site-Selectivity and Affinity through Fluorescent Intercalator Displacement" Department of Chemistry, Chuo University, Tokyo, Japan, April 23, 2004.
24. "DNA Recognition by Ni(II)-Gly-Gly-His Derived Metallopeptides" (C. A. Claussen, presenting, with co-authors Y.-Y. Fang, B. D. Ray, K. B. Lipkowitz and E. C. Long) Symposium on Nucleic Acid Structure and Chemistry, 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, June 2-4, 2004.
25. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides and Other Minor Groove-Targeted Agents" Department of Chemistry, Indiana University-Purdue University Fort Wayne (IPFW), November 4th, 2005.
26. "DNA Recognition by Ni(II)•Gly-Gly-His Derived Metallopeptides and Other Minor Groove-Targeted Agents" Department of Chemistry, Purdue University-West Lafayette, October 17th, 2006.
27. "A New Approach to Analyzing DNA Binding Agents Leading to the Crystal Structure of a DNA-Co(III)•Bleomycin-B₂ Complex" (with co-authors M. M. Georgiadis, K. D. Goodwin and M. A. Lewis) Symposium on Bioinorganic Chemistry, CERMACS 2007, Central Regional Meeting of the American Chemical Society, Covington, KY, May 20-23.
28. "Studies of DNA-Ligand Recognition: From Peptides to Drugs (and Back Again?)" Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, IUPUI, September 15th, 2008.

29. "Studies of DNA-Ligand Recognition: From Peptides to Drugs" *Hecht Symposium*, Department of Chemistry, University of Virginia, April 4th, 2009.
30. "Expedited Studies of DNA-Ligand Recognition: From Peptides to Drugs" Department of Biochemistry, University of Missouri-Columbia, October 2, 2009.
31. "Expedited Studies of DNA-Ligand Recognition: From Peptides to Drugs" Microbiotix, Inc., Worcester, MA, October 28, 2009.
32. "An Overview of the Chemical Synthesis & Organic Drug Lead Development Core at IUPUI" (Tax M. Georgiadis, presenting) Experimental & Developmental Therapeutics Group Meeting, IU School of Medicine, November 16, 2009.
33. "Expedited Studies of DNA-Ligand Recognition: From Peptides to Drugs" Department of Chemistry, University of Wyoming, March 26, 2010.
34. "Expedited Studies of DNA-Ligand Recognition: Groove Binders to Bleomycins" Symposium on Molecular Recognition of Nucleic Acids: Biological Applications-Pacifichem 2010, Honolulu, Hawaii, scheduled: December 17, 2010.

PRESS RELEASES, COMMENTARIES, & NEWS MEDIA HIGHLIGHTS

- Publication of: "Novel Small Molecule Inhibitor of Apurinic/ Apyrimidinic Endonuclease 1 Blocks Proliferation and Reduces Viability of Glioblastoma Cells" (*Journal of Pharmacology & Experimental Therapeutics* **2010**, 334, 988-998) was featured on MDLinx.com and summarized by their physician-editor as follows: "Bapat A et al. – AR03 is chemically distinct from the previously reported small molecule inhibitors of Ape1. AR03 is a novel small molecule inhibitor of Ape1, which may have potential as an oncotherapeutic drug for treating glioblastoma and other cancers."
- Publication of: "Crystal Structure of DNA-Bound Co(III)•Bleomycin-B₂: Insights on Intercalation and Minor Groove Binding" (*Proceedings of the National Academy of Sciences, U.S.A.* **2008**, 105, 5052-5056) resulted in IUSCC, IU, and IUPUI press releases. These releases were picked up by numerous news agencies (*Science Daily, News-Medical.Net, Medical News Today, MedicExchange.com, BiologyNews.net*, and others) and featured by *Spectroscopy NOW*. A video interview for *MedStar TV* was also prepared for release to the Discovery Channel Network.

This publication was listed also by the "Faculty of 1000-Biology" (see: *Faculty of 1000 Biology: evaluations for Goodwin KD et al. Proc Natl Acad Sci U S A* 2008 Apr 1 105 (13):5052-6 <http://www.f1000biology.com/article/id/1107090/evaluation>) and also resulted in a "Spotlight" Article in *ACS Chemical Biology* (see: "Crystallizing DNA Cleavage" *ACS Chemical Biology* **2008**, 3, 258; <http://pubs.acs.org/doi/full/10.1021/cb800093f>)

- Publication of: "Facile Sonochemical Synthesis of Highly Luminescent ZnS-Shelled CdSe Quantum Dots" (03/31/06) resulted in an IUPUI News Release on 04/03/06: http://www.iupui.edu/news/releases/060403_quantum_dots.htm.

This IUPUI release was also picked up by *United Press International*: <http://www.upi.com/NewsTrack/view.php?StoryID=20060403-063844-5751r> and highlighted in *Science Daily*: “New way to synthesize quantum dots created” <http://www.sciencedaily.com/upi/index.php?feed=Science&article=UPI-1-20060403-18571600-bc-us-quantumdots.xml> Further news coverage also occurred in the *IUI Home Pages* at <http://www.homepages.indiana.edu/2006/05-12/story.php?id=664>

This publication was also cited as the #2 “Most-Accessed” Full paper in *Chemistry of Materials* for the period April-June, 2006 and #9 “Most-Accessed” paper for the year 2006 see:

http://pubs.acs.org/journals/cmater/promo/most/most_accessed/2006.html

- Research of Prof. Long’s Group was highlighted on the radio show “*Our Town Indy*” WIBC, Indianapolis, Spring, 2001.
- Presentation of: “Design and Synthesis of a Versatile DNA-Cleaving Metallopeptide Structural Domain” at the 206th National Meeting (Fall, 1993) resulted in a *Press Release* by the ACS News Service.
- Presentation of: “Design and Synthesis of Metal Binding DNA Recognition Helices” at the 205th ACS National Meeting (Spring, 1993) resulted in a *Press Release* by the ACS News Service.
- Publication of: “On Demonstrating DNA Intercalation” was highlighted in the Articles Alert section of *The Scientist*, November 26, 1990.
- Publication of: “Shape-Selective Targeting of DNA by (Phenanthrenequinone diimine)rhodium(III) Photocleaving Agents” prompted the release of a news article in *Chemical and Engineering News* (June 12, 1989, pg 22).

GRADUATE DEGREES AWARDED OR PENDING AS MAJOR PROFESSOR:

PhD & MS Thesis Students (Full-Time Research Group Members)

1. Xiaofen Huang, “*The Mechanism of DNA Binding by Synthetic Peptides Derived from the Carboxy-Terminal Domain of RNA Polymerase II*” (M.S., Chemistry, 1995). Xiaofen elected to continue PhD studies at IUPUI upon completion of his degree.
2. John R. Dobbins, “*Conversion of DNA Binding Proteins into DNA Binding Drugs: Structural Redesign of the Overlapping β -Turns of RNA Polymerase II*” (M.S., Chemistry, 1995). John is employed by Eli Lilly & Co., Indianapolis, IN.
3. Qi Liang, “*DNA Recognition by Metallopeptides of the Form Ni(II)•Xaa-Xaa-His: Binding Selectivity and Mechanism of Strand Scission*” (Ph.D., Chemistry, 1997). Qi pursued a post-doctoral position at the Massachusetts Institute of Technology with Prof. Peter C. Dedon upon completion of her degree.
4. Paula Denney Eason, “*Design of Ni(II)•Metallopeptides and Their Interaction with DNA*” (Ph.D., Chemistry, 1997). Paula pursued a post-doctoral position at the California Institute of Technology and the Massachusetts Institute of Technology with Prof. Barbara Imperiali upon completion of her degree.

5. Isabelle J. Brittain, *"Metallopeptide-Induced Cleavage of HIV-1 TAR RNA and tRNA^{Phe}"* (M.S., Chemistry, 1998). Jodie was employed by Eli Lilly & Co., Indianapolis, IN, upon completion of her degree.
6. Davina C. Ananias, *"Selective DNA Cleavage by Cobalt Metallopeptides"* (Ph.D., Chemistry, 1998). Vina pursued a position with Roche Diagnostics, Indianapolis, IN upon completion of her degree.
7. Xiaofen Huang, *"DNA Binding and Recognition by Synthetic Peptides and Metallopeptides"* (Ph.D., Chemistry, 1998). Xiaofen pursued a post-doctoral position with Prof. Ed Skibo at Arizona State University upon completion of his degree.
8. Jessica L. Combs, *"HIV-1 TAR RNA Binding by Fe(II)•Bleomycin"* (M.S., Chemistry, 2002). Jessica was employed by Eli Lilly & Co., Indianapolis, IN upon completion of her degree.
9. Craig A. Claussen, *"DNA Recognition and Binding by Combinatorial Libraries of Ni(II)•Xaa-Xaa-His Metallopeptides"* (Ph.D., Chemistry, 2003). Craig was employed by Roche Diagnostics, Inc., Indianapolis, IN upon completion of his studies.
10. David L. Shaw, *"Sonochemical Synthesis of CdSe/ZnS Core-Shell Nanocrystals and Their Surface Modification with Amino Acids and Peptides"* (M.S., Chemistry, 2007). David was employed by MiraVista Laboratories, Indianapolis upon completion of his studies.
11. Katie M. Williams, *"(δ)-Orn-Linked Cu(II)• and Ni(II)•Gly-Gly-His-Like 'Tandem-Array' Metal Binding Oligopeptides"* (M.S., Chemistry, 2007). Katie was employed by Baxter Pharmaceutical Solutions LLC, Bloomington, IN upon completion of her studies.
12. Mark A. Lewis, *"DNA Targeting by Metallopeptides: A Comparison to Peptide-Derived Natural Products"* (Ph.D., Chemistry, 2007). Mark was appointed as an Instructor at Venture County Community College, Ventura, CA, upon defense of his degree.
13. Amanda "Mandi" Zins, *"Peptide and Cobalt Metallopeptide Interactions with HIV-1 TAR RNA"* (M.S., Chemistry, 2007). Mandi was employed by Cook Pharmica LLC, Bloomington, IN upon completion of her degree.
14. LaTeca Glass, *"Expedited Approaches to the Discovery and Study of Novel DNA Binding Ligands"* (M.S., Chemistry, 2009; co-directed with M. M. Georgiadis).
15. Jessica (Bo) Li, *"Design, Synthesis and Analysis of DNA Minor Groove Binding Amino Acid-Phenylbenzimidazole Conjugates"* (M.S., Chemistry, 2009).
16. TianXiu Wang, *"DNA Recognition and Cleavage by Phenyl-Benzimidazole Modified Gly-Gly-His Derived Metallopeptides"* (M.S., Chemistry, 2010; defended 2009).
17. Matt Garner, *"DNA-Targeted Phenylbenzimidazole-Amino Acid Conjugates"* (current M.S. Thesis Student)
18. Sarah Henkes, *"Fluorescent Intercalator Displacement Analyses of Metallobleomycin"* (current M.S. Thesis Student)

MS Non-Thesis Research Students

1. Steve Bandy, *"DNA Cleavage by Co(III) Derivatives of Gly-Gly-His"* (M.S., Chemistry, 1993).
2. Joel Calvin, *"Synthesis of a Metallopeptide Structural Domain"* (M.S., Chemistry, 1994).
3. Kris Samaddar, *"DNA Alkylation by Ni(II)•Gly-Gly-His-Tyr"* (M.S., Chemistry, 1997).
4. Dean Hale, *"Capillary Electrophoresis of Protein Digests"* (M.S., Chemistry, 1999).
5. Jeff Buehrer, *"DNA Alkylation by Tyr-Containing Ni(II)•Xaa-Xaa-His Metallopeptides"* (M.S., Chemistry, 2001).
6. Kathryn M. Elpers, *"Synthesis of Amino-Pyrimidine and Amino-Pyridine-Containing Metallopeptides via UPS Chemistry Protocols"* full time graduate student converted to part time (M.S., Chemistry, 2005).
7. Thomas (Zack) Gunter, *"Chromatographic Separation and Purification of Synthetic Enantiomers of Nutlin 3"* (current MS non-thesis student, Fall, 2009).

DIRECTION OF UNDERGRADUATE RESEARCH PROJECTS

1. Jeff Turner, *"DNA Cleavage by Amide-Containing Metallopeptides"* (1992 – 1993).
2. Mike Krentscher, *"Computer Modeling of a Metal-Modified Homeodomain Protein"* (1993 – 1994).
3. Margo Gembolis, *"Survey of β -Turn Peptide Motifs"* (1993).
4. Janet Ananias, *"Purification of (δ)-Orn-Gly-His Metallopeptides"* (1994).
5. Steven Ernest, *"Capillary Electrophoresis of Protein Digests"* (1995).
6. Becky Hadfield, *"Cleavage of DNA by Tri- and Tetra-Glycine Ni(II) Metallopeptides"* (1996).
7. Laura Flodin, *"RNA Binding by Metallopeptides"* (1997 – 1998; Summer Undergraduate Research Award Recipient).
8. Amy Latham, *"DNA Cleavage by Pro-Containing Metallopeptides"* (1998 – 1999).
9. Melissa Dearry, *"DNA Binding and Cleavage by Lys-Containing Metallopeptides"* (1998 – 1999).
10. Olga Adelfinskaya, *"Modeling DNA Binding Metallopeptides"* (1998 – 1999).
11. Daniel T. Hall IV, *"HT-FID Analysis of Chromomycin"* (Summer 2006, IU Cancer Center Summer Research Program).

12. Amanda Luckenbill, *"Synthesis of Lys-Conjugated (δ)-Orn-Gly-His Metallopeptides"* (2006 – 2008; UIOP Fellow, Summer 2007).
13. Jeffrey Weber, *"High-Throughput Discovery and Analysis of DNA Binding Ligands"* (2007 – 2008).
14. Darrell Money, *"Synthesis and Analysis of Biomedically-Relevant Targets"* (Senior Capstone Student, 2009-2010)

DIRECTION OF POST-DOCTORAL RESEARCH PROJECTS

1. Dr. Daniel Shullenberger, *"Design and Synthesis of Nucleic Acid Modifying Metallopeptide Structural Domains"* (1992-1993). Dr. Shullenberger became an Assistant Professor of Chemistry at St. Francis College upon leaving IUPUI.
2. Dr. N. Murali, *"Determination of the Structure of Tandem β -Turns through NMR Spectroscopy"* (1993 – 1994). Dr. Murali became an Assistant Scholar/Scientist at the National High Magnetic Field Laboratory, Tallahassee, FL upon leaving IUPUI.
3. Dr. Ya-Yin Fang, *"Simulations of DNA Binding Ni(II)•Xaa-Xaa-His Metallopeptides"* (2001 – 2003). Dr. Fang is presently a Research Assistant Professor within the Department of Biochemistry & Molecular Biology, Howard University.
4. Dr. Zhongliang Zhu *"HT-HR Analyses of Minor Groove-Targeted DNA Binding Agents"* (June 2006 – May 2007; co-directed with M. M. Georgiadis).

ACTIVE RESEARCH COLLABORATORS (WITHIN THE LAST THREE YEARS)

1. Prof. Millie Georgiadis, *Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, IUPUI.* (Crystallization and structural analyses of DNA-bound natural products and synthetic ligands).
2. Prof. W. David Wilson, *Department of Chemistry, Georgia State University* (Analyses of site-selective minor groove binding compounds).
3. Prof. Makoto Chikira, *Department of Applied Chemistry, Chuo University, Tokyo, Japan.* (Fiber EPR studies of DNA-bound metallopeptides).
4. Prof. Christoph Naumann, *Department of Chemistry & Chemical Biology, IUPUI* (Development of peptide-conjugated quantum-dots).
5. Prof. Ya-Yin Fang, *Department of Biochemistry & Molecular Biology, Howard University College of Medicine* (Computational studies of DNA-targeted molecules).
6. Dr. Weiming Yu, *Northwestern University* (*in vivo* analyses of peptide-coated quantum dot imaging probes).
7. Dr. Tim Opperman, *Microbiotix, Inc.* Worcester, MA (FID analyses of synthetic DNA minor groove binding compounds).

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PROFESSIONAL EXPERIENCE

Interim Executive Vice Chancellor for Academic Affairs, Indiana University Northwest, Gary, IN, January, 2009 - present

University Director, *Faculty Colloquium on Excellence in Teaching* (FACET: IU Teaching Academy), Indiana University (system), 2006 - present

Chancellor's Professor, IUPUI, 2002 – present

Professor of Chemistry, IUPUI, 1995 – present

Founding Faculty Member, *University College* at IUPUI, 1997 – present.

Full Member, Indiana University Graduate School, 1991 – present.

Associate Executive Vice President, Indiana University (system), 2006 – 2009.

Chairman, Department of Chemistry, IUPUI, 1990–2000

Founding Faculty Member, *School of Informatics*, Indiana University (joint Bloomington and Indianapolis School), 1999 – 2000.

Director of Graduate Programs, Department of Chemistry, IUPUI, 1987–91.

Associate Professor of Chemistry, 1986–1995, Assistant Professor of Chemistry, 1980 – 1986.

Post-doctoral Research Associate, University of Illinois, 1977–1980.

Post-graduate Research Chemist/Lecturer, University of California, San Diego, 1976 – 1977.

EDUCATION AND SPECIAL TRAINING

B.S., Chemistry, California State University, East Bay, 1968.

M.S., Applied Mathematics (with Physics Cognate), California State University, East Bay, 1969.

Ph.D., Physical Chemistry, University of California, San Diego, 1976.

Chairing the Academic Department, American Council on Education, Washington, DC (June, 1991)

Achieving Excellence through Collaborative Problem Solving: Effective Facilitation, A Critical Tool, Angotti Weber and Associates (May 13-14, 1996).

Certificate, *Management Development Program*, Graduate School of Education, Harvard University (Summer, 1996)

HONORS/AWARDS/CITATIONS

American Chemical Society Outstanding Service Award, Indiana Section, American Chemical Society (2007)

Tonya Conour Faculty Service Award, Indiana University Purdue University Indianapolis (2007)

Favorite Professor Award, IUPUI Intercollegiate Athletics Department (2005)

American Chemical Society Certificate of Recognition, National Regional Meeting Office, American Chemical Society, Washington, DC (2004)

American Chemical Society Service Award, Indiana Section, American Chemical Society (2004)

9/26/08

Favorite Professor Award, IUPUI Intercollegiate Athletics Department (2004)
Trustees' Teaching Award, Indiana University (2003)
P.A. Mack Charter Fellow, FACET, Indiana University (2003-4)
Outstanding Educator Award, IUPUI Intercollegiate Athletics Department, Women's Volleyball Team Award (2003-4).
Faculty Learning Community Fellow, IUPUI (2003-4)
Excellence in Teaching Award, IUPUI Intercollegiate Athletics Department, Women's Volleyball Team Award (2002-3).
Chancellor's Professorship, Indiana University Purdue University Indianapolis (2002)
Trustees' Teaching Award, Indiana University (2002)
Excellence in Teaching Award, IUPUI Intercollegiate Athletics Department, Women's Tennis Team Award (2001 and 2002).
Excellence in Teaching Award, IUPUI Intercollegiate Athletics Department, Women's Basketball Team Award (2001 and 2002).
Teaching Excellence Recognition Award, Indiana University – Purdue University Indianapolis (1999).
Certificate of Appreciation, National Society of Black Engineers - Indiana (1998).
Teaching Excellence Recognition Award, Indiana University – Purdue University Indianapolis (1998).
Member, Faculty Colloquium on Excellence in Teaching Award (FACET), Indiana University System (1994).
The IUPUI Chancellor's Award for Excellence in Teaching, Indiana University–Purdue University at Indianapolis (1993).
The President's Award, Indiana University (1990).
Loren T. Jones Faculty Award, Purdue University School of Science, Indiana University – Purdue University at Indianapolis (1983).
Summer Faculty Fellowship, Indiana University–Purdue University at Indianapolis (1981).
Excellence-in-Teaching Award, Department of Chemistry, University of California, San Diego (1970).

BIOGRAPHICAL REFERENCES

Who's Who in the World, Marquis Publications, Twenty-fourth Edition, 2007
Who's Who in America, Marquis Publications, Fifty-ninth, Sixtieth (Diamond Anniversary), and Seventieth Editions, 2005 - 2007
Who's Who in American Education, Marquis Publications, Sixth Edition, 2004.
Who's Who in Science and Engineering, Marquis Publications, Fifth Edition, 1999 and Millennium Edition, 2000.
Who's Who in Education, Marquis Publications, 1995.
Who's Who in the Midwest, Marquis Publications, 22nd Edition, 1990.
Who's Who in Technology Today, Marquis Publications, Fifth and Sixth Editions, 1986 and 1989.
American Men and Women in Science, R. R. Bowker, Seventeenth to Twenty-third Editions, 1986-2007.
Who's Who in Frontier Science and Technology, Marquis Publications, First Edition, 1984.

PROFESSIONAL ACTIVITIES

Society/Association Memberships:

American Chemical Society (ACS), since 1969.
American Physical Society (APS), Life Member, since 1971.
International Union of Pure and Applied Chemistry, Affiliate Member, since 2002.
Sigma Xi, since 1978
Member, Alliance of Distinguished and Titled Professors, Indiana University, since 2002.

Membership on Editorial/Advisory Boards

Member, Advisory Board, *in Chemistry*, American Chemical Society, 2001-2007.

Co-editor, *Journal of the Scholarship of Teaching and Learning*, 2004 – present; online journal: <http://www.iupui.edu/%7Ejosotl/>

Professional Society Committees and Offices Held and Other Appointments:

National Positions (calendar year dates)

Past Chair, Board of Directors, ACS Central Regional Board, 2006-2007. Chair-elect, 2003-2004; Chair, 2004 - 6.

Member, German Academic Exchange (DAAD) – American Chemical Society International Research Experiences Fellowship Selection Committee, 2007 and 2008

Member and Vice Chair, Society Committee on Education (SocEd), American Chemical Society, *Associate Member*: 1998-99, *Full Member*: 2000-2008, *Vice Chair*: 2004-6.

Member: Executive Committee, Society Committee on Education, 2000-05.

Chair: SocEd Sub-committee on Colleges, Universities and Continuing Education (Sub-B), 2000-2003.

Member: Task Force on the Society Committee on Education Strategic Plan, 2000.

Member, ACS Faculty Status Working Group, SocEd, 2008.

Liaison, International Activities Committee from Society Committee on Education, 2006 - 2008

Member, Task Force on “ACS Guidelines for Chemistry Programs in Two-Year Colleges”, American Chemical Society, 2007-2009

Councilor, American Chemical Society (ACS), 1996-2006. Elected member of the Society governing body representing the Indiana Section.

Member, Task Force on “Scholarship in the Chemical Sciences and Engineering”, American Chemical Society, 2006 - 2007

Delegation Member, Project Kaleidoscope Delegation to China: Pro-Conference on Sino-U.S. Undergraduate STEM Reform, Fall, 2005.

Society Committee on Education Liaison to Committee on Meetings and Expositions, American Chemical Society, 2003

Member, Regional Activities Coordination Team, American Chemical Society, 2005-6.

Member, Organizing Committee, Invitational Meeting on Graduate Education, 1999.

Member, Presidential Task Force on Exploring the Molecular Vision (Re-evaluation of Undergraduate Education in Chemistry), SocEd Task Force and Organizing Committee, 2002-2005.

Team Member, Second Annual ACS Legislative Summit on Government Educational and Research Programs, Office of Legal and Governmental Affairs, Washington, DC (April, 2003)

Chair: ACS *ad hoc* Committee on Student Affiliate Chapter Review, Awards, and Grants, 2000-03, 2005.

Member, Task Force on Graduate Education, Society Committee on Education, American Chemical Society, 1998-99.

Member, Task Force on Academic Professional Guidelines, Committee on Economic and Professional Affairs, American Chemical Society, 1999.

Member (National ACS), General Chemistry Sub-Committee, American Chemical Society Examinations Committee, 1985-1989.

Regional and State Positions

General Chair, American Chemical Society, 36th ACS Central Regional Meeting, Indianapolis, IN (IUPUI), June 2 – 4, 2004

Member, Executive Committee, and *Higher Education Coordinator in Chemistry*, Project SEAM, Central Indiana Educational Service Center, 2001-2004

Chair, American Chemical Society Education Committee (Indiana), 1982-84, 1992-98, and 2005-08

Member, Executive Committee, ACS Indiana Section, 1982-89, 1994-present

Chair, Technical Program Committee, American Chemical Society 1991 23rd Central – 24th Great Lakes Joint Regional Meeting: May 29-30, 1991

Chair, Site Selection Committee, American Chemical Society 1991 23rd Central–24th Great Lakes Joint Regional Meeting

Editor, *The Accelerator Newsletter*, ACS (Indiana), 1986-1989

Section Chairman, ACS (Indiana), 1986. *Chairman-Elect*, ACS (Indiana), 1985

Member, ACS Education Committee (Indiana), 1981, 1982, 1983, 1984, and 1985;

Judge, ACS Award Science Fair, 1986

Member, Advisory Committee, Indianapolis Public Schools/IUPUI Television Project (1983-1984)

Major University Service***Current Appointments***

- *Co-Chair*, 2007 - present; *Steering Committee Member*, 2005 - present, Alliance of Distinguished and Titled Professors, Indiana University
- *Member* (2009 - present), *ex officio Member* (2006 – 2009), Academic Leadership Council, Indiana University.
- *Member*, FACET Steering Committee, Indiana University System-wide Teaching Honorary (1999-present)

Past Appointments

- *Member*, Board of Directors, University Faculty Club, 2006 - 2009
- *Co-Chair*, Research Collaborations Initiative, Indiana University - HBCU STEM Initiative, 2006 - 2009.
- *Member*, Indiana Commission on Higher Education Academic Policy Group, Indiana University, 2007 - 2009
- *Member*, Joint Committee to Review Indiana University Promotion and Tenure Procedures, A joint committee commissioned by the President and University Faculty Council Co-Chairs, 2008
- *Member*, Commission on Health, Indiana University, 2002 - 2008.
- *Member*, Preparing Future Faculty Oversight Committee, 2005 - 2008
- *Chair*, School of Science Promotion and Tenure Committee (Unit), IUPUI, 2005-7; Vice Chair, 2004-5; Member, 2003-7; Chair, 2005-7.
- *Member*, Bepko Scholars Selection Committee, 2005 - 2007
- *Chair and Member*, Budgetary Affairs Committee, University College, Chair (1998-2000), Member (2000-2007)
- *Member*, IUPUI Research Support Fund Grant (RSFG) Review Panel, 2006-7
- *Co-Chair*, Faculty Compensation and Benefits Committee, University Faculty Council, 2005-06
- *Chair*, Fringe Benefits Committee, IUPUI Faculty Council (2005-06)
- *Member*, Campus Promotion and Tenure Committee, IUPUI, 2005-6
- *Member*, *ad hoc* Campus Fiscal Futures Group, IUPUI, 2005 – 2006
- *Member*, Nominating Committee, IUPUI Faculty Council (2002-2006)

- *Member*, Task Force on Selection, FACET, Indiana University, 2005-6.
- *Campus Liaison*, Faculty Colloquium on Excellence in Teaching (FACET), Indiana University, Indianapolis Campus, 2002 - 2006
- *Member*, Gateway Group, Indiana University Purdue University Indianapolis, 2004 – 2006
- *Co-chair*, University Faculty Council (Indiana University System), Facilities and Finance Committee, 2002-05
- *Member*, Campus Distinguished and Outstanding Scholarships Committee, (1998-2005)
- *Chair, ad hoc* Promotion and Tenure Guidelines Revision Committee, School of Science, 2003-2005
- *Chair and Member*, Campus Budgetary Affairs Committee, IUPUI Faculty Council, Chair (2002-2005), Member (2000-2005)
- *Member*, Campus Team on “Organizing for Campus Success in a Climate of Restricted Resources: Student Learning, Faculty Vitality and Fiscal Reality (Project on the Future of Higher Education)”, American Association for Higher Education, Baltimore, MD, October, 2004 and continuing 2004-05.
- *Member*, Campus Financial Planning Advisory Committee, IUPUI, 2003 - 2004
- *Member*, Executive Committee, University College (2000-2003)
- *Member*, Dean’s Administrative Review Committee: Dean Scott Evenbeck, University College, 2001-2002
- *Member*, Dean’s Administrative Review Committee: Dean Paul Bippen, IUPUI Columbus, 2001-2002
- *Co-Chair*, Task Force on Campus Mission (Indiana University System-wide Task Force), Faculty Colloquium on Excellence in Teaching, (1999-2000)
- *Chair and Member*, Chancellor’s Convocation Committee, Chair (1997, 1998), Member (1996-99).
- *Member*, Campus Team at “AAHE Summer Academy: Organizing for Learning”, Quality Initiatives, American Association for Higher Education, with D. A. Ford, N. D. Lees, T. Mullen, and R. Turner, Snowbird, Utah (July, 1997).
- *Member*, Peer Review of Teaching Initiative, American Association of Higher Education, IUPUI Campus Team: Chemistry, 1995-98
- *Campus Faculty Representative*, Teaching Capacity Model Committee, Indiana University Board of Trustees and System, 1995
- *Chairman*, University Graduate Affairs Committee (Indianapolis), Indiana University Graduate School and Purdue University Graduate School, 1991-95
- *Member*, Chancellor’s Award for Excellence in Teaching Selection Committee, 1994
- *Presenter*, “The Role of External Funding on Teaching Quality and Effectiveness,” Indiana University Board of Trustees, January, 1994.
- *President*, Purdue School of Science Faculty Assembly, Indiana University–Purdue University at Indianapolis, 1990-1991. Resigned second year of elected term due to administrative appointment.
- *Chair*, Dean’s Administrative Advisory Committee, School of Science, 1985
- *Chair*, Faculty Council Athletic Affairs Committee, Indiana University Purdue University Indianapolis, 1983-85.
- *Chairman*, Search and Screen Committee, Department of Chemistry, 1980-81 and 1982-83

Major University Reports

- *The Purdue University School of Science in Indianapolis Criteria, Standards and Documentation Guidelines for Promotion, Tenure, and Reappointment* (27-page report), Indiana University Purdue University Indianapolis, 2005. Chair of *ad hoc* Revision Committee.

- *Department of Chemistry: 1995, A Report on Activities and Progress* (External Review Document, 130 pp.), Indiana University Purdue University at Indianapolis, 1995. Principal Author.
- *Undergraduate Research at IUPUI*, Dean of the Faculties, 1993 (principal author). Published in *Research and Scholarly Activity*, September, 1993.
- *ad hoc Teaching Evaluation Committee Final Report*, School of Science, IUPUI, 1990 and revised edition, 1994, 40 pp. (Committee member and Report Co-author)
- *Long Range Report–1987, Department of Chemistry*, IUPUI, (Committee member)
- *Task Force for Strategic Planning on University Computing Resources*, IUPUI, 1986 (Committee member)

Internal/External Departmental Reviewing Activities/Consulting

- *Primary External Reviewer*, External Review for the Department of Chemistry, Roger Williams University, RI (April, 2007)
- *Consultant*, McGraw-Hill Publishers, 2005
- *Consultant*, Metropolitan School District of Perry Township, 2002-03
- *Consultant*, Indianapolis Public Schools, 2001-3
- *Primary External Reviewer*, External Review Committee for the Department of Chemistry, University of Nebraska, Omaha (February, 1997)
- *Member*, Review Team for the Department of Mathematical Sciences, IUPUI (Spring, 1995).

Proposal and Journal Article Reviewing Activities:

Reviewer, U.S. Department of Education, Fund to Improve Post-Secondary Education, 2007

Review Panel Member, U.S. Department of Education, Graduate Assistance in Areas of National Need, 2002-2003

Review scientific proposals for: National Science Foundation, American Chemical Society: Petroleum Research Fund

Indiana University System Proposals, Institutional Award Nominees, and numerous Scholarship and internal Grant committees

Referee for the following journals:

The Journal on Scholarship of Teaching and Learning

Chemical Physics (Elsevier)

Chemical Physics Letters (Elsevier)

Journal of Chemical Information and Computational Science (ACS)

Journal of Chemical Physics (American Institute of Physics)

Journal of Quantitative Spectroscopy and Radiative Transfer

THEOCHEM

MEETINGS/SYMPOSIA ORGANIZED

1. *XXII Midwest Theoretical Chemistry Conference*, Co-organizer, Indiana University – Purdue University at Indianapolis (May 11-13, 1989).
2. *Workshop in Computational Chemistry and Molecular Graphics*, Co-organizer, Indiana University – Purdue University at Indianapolis (November 4, 1989).
3. *American Chemical Society 1991 Joint Great Lakes–Central Regional Meeting*, Technical Program Chairman, Indiana University–Purdue University at Indianapolis (May, 1991).
4. *Symposium to Recognize Excellence in Science and Mathematics Teaching: Chemistry*, Organizer, Indiana University–Purdue University at Indianapolis (October 2, 1991).

5. *Faculty Development Workshop: Implementing a Successful Tutoring Program*, Organizer and Presenter, Indiana University–Purdue University at Indianapolis (March, 1992).
6. *Funding through the GAANN Program of the U.S. Department of Education*, Local Meeting Organizer, IUPUI (November 3, 1993).
7. *IUPUI: Programs and Scholarship after 25 Years*, American Chemical Society Meeting (Indiana Section), Organizer and Presenter (March 10, 1994).
8. *Multiple Measures of Teaching Excellence/Peer Review*, Teaching Effectiveness Interest Group, Indiana University–Purdue University at Fort Wayne, Co-organizer and Presenter (September 17, 1994)
9. *American Chemical Society High School Chemistry Scholarship Examination Teachers' Meeting*, The American Chemical Society Meeting (Indiana Section), Organizer and Presenter (April 22, 1995).
10. *American Chemical Society High School Chemistry Scholarship Examination Teachers' Meeting*, The American Chemical Society Meeting (Indiana Section), Organizer and Presenter (April 13, 1996).
11. *XXIX Midwest Theoretical Chemistry Conference*, Co-organizer, Indiana University–Purdue University at Indianapolis (May 29 - June 1, 1996).
12. *Surprises and Strategies for New Administrators*, Co-organizer and Presenter, Faculty Development Office, Indiana University Purdue University Indianapolis (November, 1996).
13. *Chancellor's Convocation*, Co-organizer, Indiana University Purdue University Indianapolis (November, 1996).
14. *American Chemical Society High School Chemistry Scholarship Examination Teachers' Meeting*, The American Chemical Society Meeting (Indiana Section), Organizer and Presenter (April 26, 1997).
15. *Faculty Convocation for Excellence in Teaching*, "In Search of Teaching Excellence: Illustrating and Capturing the Elements," Chairman, Organizing Committee, Indiana University System (FACET), Four Winds Conference Center, Bloomington, IN (May 16-18, 1997).
16. *Chancellor's Convocation: The Collaborative Department*, Chair, Organizing Committee, Indiana University Purdue University Indianapolis (1998).
17. *American Chemical Society High School Chemistry Scholarship Examination Teachers' Meeting*, The American Chemical Society Meeting (Indiana Section), Organizer and Presenter (April 18, 1998).
18. *Chancellor's Convocation: Post-tenure Review*, Member, Organizing Committee, Indiana University Purdue University Indianapolis (Fall, 1998).
19. *American Chemical Society Invitational Conference on Graduate Education*, Member, Organizing Committee, ACS Committee on Education, Washington, DC, Invitational Meeting, February, 1999.
20. *American Chemical Society Peer Review of Student Affiliate Chapters*, Co-organizer, American Chemical Society, Washington, DC, July, 2001.
21. *American Chemical Society Invitational Conference: Exploring the Molecular Vision*, Member, Organizing Committee, ACS Committee on Education, Washington, DC, Invitational Meeting, June 27-29, 2003.
22. Symposium organized: *Symposium on Peer Led Team Learning: New Approaches, Different Results?* (full day symposium) at the 227th Spring National Meeting of the American Chemical Society, Anaheim, March, 2004.
23. *36th Central Regional American Chemical Society Meeting*, General Chair, Indianapolis, IN, June 2-4, 2004.
24. *Chemistry Enterprise 2015: A Conversation with ACS President-Elect William Carroll*, Indiana Section ACS, Eli Lilly and Company, Indianapolis, IN, November 10, 2004
25. *ACS High School Chemistry Scholarship Examination*, IUPUI, April 9, 2005
26. *ACS High School Chemistry Scholarship Examination*, IUPUI, April 15, 2006

27. Symposium organized: *A Decade of Peer-Led Team Learning* (full day symposium), 232nd Fall National Meeting of the American Chemical Society, San Francisco, September, 2006
28. *ACS High School Chemistry Scholarship Examination*, IUPUI, April 14, 2007
29. Science Café: *Are all stem cells alike? Who cares if they aren't?* American Chemical Society, Faculty Club, IUPUI, December 5, 2007
30. *ACS High School Chemistry Scholarship Examination*, IUPUI, April 26, 2008
31. *HBCU-IU STEM Initiative: Research Collaborations in Cancer, Diabetes, and Obesity Planning Meeting*, IUPUI, July 23, 2008

INVITED LECTURES, MEETING PRESENTATIONS, AND ABSTRACTS

1. *Toward a Convergent Perturbation Theory*, Department of Chemistry, Virginia Polytechnic University, Blacksburg, VA, 1977.
2. *Diffraction Scattering from a Corrugated Surface*, Department of Chemistry, University of Portland, Portland, OR, 1977
3. *Toward a Convergent Perturbation Theory*, Department of Chemistry, Amherst College, 1977.
4. *Application of Finite Element Method to Inelastic Scattering*, Midwest Theoretical Conference (Battelle Columbus Laboratories, May, 1978).
5. *Close Encounters of Argon and Methane*, Midwest Theoretical Conference (Battelle Columbus Laboratories, May 1978).
6. *Bound State Resonances in Argon-Methane Cross Sections*, Midwest Theoretical Conference (Purdue University, 1979).
7. *Theoretical Aspects of Argon-Methane Scattering*, Department of Chemistry, Indiana University Purdue University Indianapolis, March, 1980
8. *Theoretical Aspects of Argon-Methane Scattering*, Max Plank-Institut für Strömungsforschung, Göttingen, West Germany, April, 1980.
9. *On the Determination of the Ar-CH₄ Interaction Potential*, NATO Advanced Study Institute, Cortona, Italy (September, 1980).
10. *Energy Transfer in Polyatomic Molecules*, Department of Physics, Indiana University – Purdue University at Indianapolis, December, 1982.
11. *Polyatomic Interactions: Energy Transfer and Potential Energy Surfaces*, Physical Chemistry Divisional Seminar, Purdue University (West Lafayette), March 23, 1983.
12. *Determination of Excellence in Chemistry: Competitive Achievement Examinations*, CHEMED83 (Butler University, August, 1983, invited lecture).
13. *New Variants of the Finite Element Method for Scattering Problems*, ACS Spring National Meeting, April 8-13, 1984, St. Louis, MO.
14. *The American Chemical Society High School Chemistry Scholarship Examination*, Annual ACS High School Teachers' Committee Meeting (invited lecture, May, 1984).
15. *Propagating Finite Element Methods in Scattering*, Midwest Theoretical Conference (Southern Illinois University, May, 1984).
16. *Atomic and Molecular Energy Transfer*, University of Wisconsin (River Falls), May 25, 1984.
17. *Internuclear Potential Energy Surfaces: Determination and Role in Energy Transfer*, University of Cincinnati, February 28, 1985.

18. *Vibrational Motion Effects on Molecular Polarizabilities and Hyperpolarizabilities and the Influences of Applied Electric Fields and Field Gradients*, Conference on the Dynamics of Molecular Collisions (Snowbird, Utah, July, 1985).
19. *Internuclear Potential Energy: Influences of Electric Fields and Electric Field Gradients on Molecular Interactions*, University of California (San Diego), July, 1985.
20. *Vibrational Motion Effects on Molecular Polarizabilities and Hyperpolarizabilities and the Influences of Applied Electric Fields and Field Gradients*, American Chemical Society Fall National Meeting (September 8-13, 1985, Chicago, IL).
21. *Internuclear Potential Energy Surfaces: The Influence of Applied Electric Fields and Electric Field Gradients*, Indiana University (Bloomington), October 17, 1985.
22. *Hydrogen Bonding Effects on the Vibrational Transitions of Hydrogen Fluoride*, Midwest Theoretical Conference (Indiana University, May 15-17, 1986).
23. *Multivariate Approximants for Power Series Expansions of the Energy in Applied Electric Fields*, Midwest Theoretical Conference (Indiana University, May 15-17, 1986).
24. *Vibrational Spectroscopy of Diatomic Molecules in Static Electric Fields. An ab initio study of HF*, 1987 American Conference on Theoretical Chemistry (Gull Lake, MN, July 25-31, 1987).
25. *Molecular Vibrations and Electric Fields*, Xavier University (Cincinnati, OH), October 26, 1988.
26. *Quantum Mechanics in Molecular Modeling and Molecular Graphics*, Workshop in Computational Chemistry and Molecular Graphics, (IUPUI, November 4, 1989).
27. *Faculty Development Workshop: New Administrator Workshop*, Invited Presenter, Indiana University–Purdue University at Indianapolis (March, 1992).
28. *Workshop on Responsibility-Centered Management: A View From the Chair*, Indiana University–Purdue University at Indianapolis (November, 1992). Invited Presenter.
29. *Teaching Effectiveness: Assessment and Rewards*, Tenth Annual Conference, Academic Chairpersons: Selecting, Motivating, Evaluating, and Rewarding Faculty (Kansas State University), Orlando, FL (February 1-3, 1993). Invited panelist and presenter.
30. *National Science Foundation Invitational Workshop on Teaching Science Laboratories via Distance*, “Academic Issues: Curriculum Development, Accreditation, Pedagogical Integrity,” Invited Presenter and Moderator (October, 1993).
31. *External Funding: Its Impact on the Educational Mission*, Indiana University Board of Trustees (January 19, 1994).
32. *Expectations for Faculty in US Higher Education: Roles and Rewards* in “International Higher Education Administration Seminar,” United States Information Agency, IUPUI (January 25, 1994). Invited panelist.
33. *Faculty Development Workshop: New Administrator Workshop*, “Issues in Leadership,” Invited Presenter, Indiana University–Purdue University (March, 1994).
34. *Faculty Forum: Report on the IUPUI Team on AAHE Faculty Roles and Rewards*, Presenter and Panelist, IUPUI (March, 1994).
35. *Multiple Measures of Teaching Excellence*, Indiana University–Purdue University at Fort Wayne (September 17, 1994).
36. *Rewards and Motivation for Evaluating Teaching: Chairs’ Perspective*, Indiana University–Purdue University at Fort Wayne, with Richard Turner (September 17, 1994).
37. *Implementing A Teaching Evaluation Program*, Indiana University–Purdue University at Fort Wayne (September 17, 1994).

38. *Expectations for Faculty in U.S. Higher Education: Research*, International Higher Education Administration Seminar, United States Information Agency (USIA) and Indiana University, IUPUI (February 3, 1995). Invited panelist.
39. *Departments in Transition*, Twelfth Annual Conference, Academic Chairpersons: Selecting, Motivating, Evaluating, and Rewarding Faculty (Kansas State University), with N. D. Lees, Orlando, FL (February 8-10, 1995). Invited presenter.
40. *Through the Eyes of a Scientist: Big and Small*, 111th Annual Meeting, Indiana Academy of Science, Keynote Speaker: Junior Academy (Middle and High Schools), Indianapolis, November 3, 1995. Invited.
41. *Faculty Workload and Accountability*, at “Conference on Faculty Roles and Rewards”, American Association for Higher Education, with N.D. Lees, Atlanta, GA (January 18-21, 1996).
42. *Evaluating the Teaching Capacity of Academic Departments*, Faculty Roles and Rewards, American Association for Higher Education, with V. Borden, W. Plater, and J. Kremer, Atlanta, GA (January 18-21, 1996).
43. *Faculty Work: Approaches to Accountability*, Thirteenth Annual Conference, Academic Chairpersons: Approaches to Accountability (Kansas State University), with N. D. Lees, Orlando, FL (February 7-9, 1996). Invited Workshop Organizer/ Presenter.
44. *Edward C. Moore Symposium: Effectiveness of External Reviews*, Campus Colloquium, Indiana University–Purdue University Indianapolis (March, 1996). Invited.
45. *External Peer Review of Course Content: A New Dimension in Evaluating Teaching Excellence*, in “Symposium on The Scholarship of Teaching Chemistry”, Division of Chemical Education, American Chemical Society Fall National Meeting, Orlando, Florida (August 25-29, 1996). Invited.
46. *Faculty Development Program: Surprises and Strategies for New Administrators*, Presenter and Co-organizer, Indiana University Purdue University Indianapolis (November, 1996).
47. *Program Review: A Mechanism for Enhancing Academic Opportunity in an Era of Change*, in “Fifth AAHE Conference on Faculty Roles and Rewards,” American Association for Higher Education, with N.D. Lees, San Diego, CA (January 18-21, 1997). Invited.
48. *Of Mutual Benefit: Faculty and Students Document their Teaching and Learning*, in “Fifth AAHE Conference on Faculty Roles and Rewards,” American Association for Higher Education, San Diego, CA (January 18-21, 1997). Invited Workshop Presenter.
49. *Program Review: A Mechanism for Enhancing Academic Opportunity in an Era of Change*, Fourteenth Annual Conference, Academic Chairpersons: Changing Answers to Recurring Questions (Kansas State University), with N. D. Lees, Orlando, FL (February 12-14, 1997). Invited Workshop Organizer/Presenter.
50. *The Pedagogical Colloquium in Hiring in a Science Department*, in the American Association for Higher Education Teaching Initiative Program on Pedagogical Colloquia, Stanford University (February 21-22, 1997). Invited.
51. *Institutional Data for Program Review: Making a Difference at the Departmental Level*, at the Indiana Association of Institutional Researchers Annual Meeting, with Karen Black, Seasons Lodge Conference Center, Nashville, IN (March 20-21, 1997). Invited.
52. *Professional Development of Chairs*, in “AAHE Summer Academy: Organizing for Learning”, Quality Initiatives, American Association for Higher Education, with N. D. Lees and R. Turner, Snowbird, Utah (July, 1997). Invited.

53. *Strategies and Surprises on the Teaching Frontline*, in “New Faculty Teaching Workshop”, Faculty Development Office, Indiana University Purdue University Indianapolis (August, 1997). Invited.
54. *Progress in Building a Community of Chairs*, in “Campus Higher Education Series: A Conversation with Margaret Miller, President of the American Association for Higher Education,” IUPUI (October, 1997). Panel Discussion.
55. *Master Teachers in Action*, Faculty Development Workshop, IUPUI (December, 1997). Invited Presenter.
56. *Establishing A Campus Chair Community*, in “Sixth AAHE Conference on Faculty Roles and Rewards,” American Association for Higher Education, with N.D. Lees, T. Mullen, D. Ford, and R. Turner, Orlando, FL (January, 1998). Invited Program Brief.
57. *Workshop on Chair Development*, in “Sixth Annual AAHE Conference on Faculty Roles and Rewards,” American Association for Higher Education, with N.D. Lees, T. Mullen, D. Ford, and R. Turner, Orlando, FL (January, 1998). Invited.
58. *Establishing A Campus Chair Community*, Fifteenth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February, 1998).
59. *Community Engagement and Faculty Roles and Rewards*, “Universities as Citizens” Colloquium, Midwest Campus Compact, Respondent to Eugene Rice, Program Director, AAHE, Indianapolis, IN (February 6, 1998).
60. *Practical Considerations In The Use of On-line Testing For Introductory Chemistry Courses* in “Innovations in Teaching”, Division of Chemical Education, American Chemical Society National Meeting, Dallas, TX (April, 1998).
61. *The Chair and Faculty as Representatives to the Departmental Constituencies Can Lead to Change* in “Seventh Annual AAHE Conference on Faculty Roles and Rewards,” American Association for Higher Education, with N.D. Lees, San Diego, CA (January, 1999).
62. *Representing the Department Effectively to its Constituencies: Precursors to Change*, Sixteenth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February, 1999). Invited.
63. *Faculty Evaluation: Applications of Workload-Based Measures for Merit Pay and Post-tenure Review*, Seventeenth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February, 2000). Invited.
64. *AAHE Issues and the Department Chair: What can we expect?*, in “Strength in Numbers: Uniting the Fronts of Higher Education,” American Chemical Society Spring National Meeting, San Francisco, CA (March, 2000). Invited.
65. *Computational Chemistry and its Role in Graduate Research*, Department of Chemistry, Indiana University Northwest, Gary, IN (April 5, 2000).
66. *Green Chemistry*, Carmel Rotary Club, Carmel, IN, October 13, 2000.
67. *Preparing New Chairs*, Eighteenth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February, 2001). Invited.
68. *Integrating Illustrative Demonstrations with Science Instruction*, Professional Development Workshops, Department of Curriculum and Instruction, Indianapolis Public Schools, June 19, 2001. Invited.
69. *Effective Recitations*, Teaching Assistant and Part-time Faculty Workshop, Department of Chemistry, IUPUI, August 16, 2001

70. *Art of successful student placement in general chemistry*, in “Research in Chemical Education Symposium”, American Chemical Society 222nd National Meeting, Chicago, IL (August 30, 2001).
71. *Tips to the Department Chair*, Nineteenth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February, 2002). Invited.
72. Discussion and roundtable on “Tips to the Department Chair”, Nineteenth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February, 2002). Invited expanded presentation.
73. *Using Chemistry in Science Instruction*, Professional Development Workshops, Department of Curriculum and Instruction, Indianapolis Public Schools, July 9, 2002. Invited.
74. *Peer-Led Team Learning in a Large Urban University*, 17th International Union on Pure and Applied Chemistry International Conference on Chemical Education, Beijing, China (August, 2002).
75. *Improving the Transition from Secondary to Higher Education in a Large Urban Public University: Recognizing the Role of PLTL* in “Recent Developments in Student-Centered Teaching Methods: Problem-based Learning, Peer-led Team Learning, etc.”, American Chemical Society 224th National Meeting, Boston, MA (August, 2002).
76. *Bridging the Curriculum Gap: Across Campuses and with K-12*, in “The Courage to Question”, 89th Annual Meeting of the Association of American Universities and the 59th Annual Meeting of the American Conference of Academic Dean, with S. Evenbeck, D. Williams, A. Gavrín, Seattle, WA (January 23, 2003).
77. *Chair Leadership Beyond the Department*, Twentieth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February 5, 2003). Invited presentation.
78. *What are the new frontiers and interfaces of chemistry that impact upon our discipline?* in “ACS Presidential Event: Exploring the Molecular Vision Symposium”, American Chemical Society 226th National Meeting, New York, NY (September 9, 2003)
79. *PLTL: Issues in Sustainability*, Peer-led Team Learning National Leadership Conference, City College of New York, October 9-12, 2003. Invited Panel Member.
80. *Peer-led Team Learning in an Urban Institution: Improving the Transition from Secondary to Higher Education*, PLTL National Leadership Conference, City College of New York, October 10, 2003
81. *Using the External Review Process Wisely: Fostering Improvement and Understanding*, Pre-Conference Workshop, Academic Chairpersons Conference, with N. D. Lees and L. J. Janski, February 2, 2004. Invited Workshop.
82. *Creating External Partnerships to Enhance Department Relevance, Image and Fiscal Stability*, Twenty-first Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), with N. D. Lees, Orlando, FL (February 5, 2004). Invited presentation.
83. *Understanding Student Success using PLTL*, Department of Chemistry, Boston University, February 23, 2004. Invited.
84. *Peer-Led Team Learning: An Urban University Success Story*, Department of Chemistry, Providence College, Providence, RI, February 26, 2004. Invited.
85. *Maximizing Student Success via Peer-led Team Learning*, Moore Symposium, with Susan Holladay, Indiana University - Purdue University, Indianapolis, IN, March 5, 2004

86. *Faculty Colloquium on Excellence in Teaching*, Moore Symposium, with Robert Orr, Indiana University - Purdue University, Indianapolis, IN, March 5, 2004
87. *Creating a culture for PLTL: Selling the faculty and administration*, in “Peer-led Team Learning - New Approaches, Different Results?”, American Chemical Society 227th National Meeting, Anaheim, CA, March, 2004
88. *Maximizing Student Success using Peer-led Team Learning*, DePauw University – Wabash College, Phi Lambda Upsilon Award Program, April 2, 2004
89. *Exploring the Molecular Vision: What are the new frontiers and interfaces of chemistry that impact upon our discipline?* 18th Biennial Conference on Chemical Education, Ames, IA, July, 2004. Invited.
90. *Peer-led Team Learning in an Urban Public Institution: Demographic Challenges*, 18th Biennial Conference on Chemical Education, Ames, IA, July, 2004. Invited.
91. *Society Committee on Education Conference Report: Exploring the Molecular Vision*, Morton Hoffman, Maureen Scharberg, David Malik, Joseph Heppert, Alan Elzerman, 18th Biennial Conference on Chemical Education, Ames, IA, July, 2004.
92. *Maximizing Student Success through Peer-led Team Learning*, International Union on Pure and Applied Chemistry Conference on Chemical Education, Istanbul, Turkey, August, 2004
93. *Exploring the Molecular Vision: How can you excel in the future workforce?*, with Morton Hoffman, Maureen Scharberg, David Malik, and Alan Elzerman, 228th American Chemical Society National Meeting, Philadelphia, August, 2004.
94. *Peer-led Team Learning in an Urban Public Institution: Demographic Challenges*, Cleveland State University, Cleveland, OH, September 10, 2004. Invited.
95. *PLTL as a De-Centralized Project*, National Peer-led Team Learning Leadership Conference, Downer’s Grove, Illinois, October 8 – 10, 2004. Invited.
96. *Strategies for Improved Learning in Large General Chemistry Courses*, 40th International Union on Pure and Applied Chemistry Congress, Beijing, China, August 14 – 19, 2005
97. *Large Lecture Classroom Strategies: Student Response Systems*, Indiana University Kokomo, October 3, 2005. Invited
98. *Peer Led Team Learning and Other 21st Century Pedagogies*, Project Kaleidoscope: Sino-U.S. Undergraduate STEM Education Reform Conference, Wuhan University, Wuhan, China, November 2 – 4, 2005. Invited Plenary Speaker.
99. *Ten Tips for College Success*, Chemistry Club, IUPUI, February 16, 2006.
100. *Ten Tips for College Success*, Campus Honors Orientation Program, IUPUI, April 28, 2006.
101. *Can we predict the PLTL Leaders gains from personality inventories? An Analysis of the dimensions of PLTL Leader growth in academic and personal growth*, with Shilpi Bhargav, Shannon Sykes and Mark Hoyert. 19th Biennial Conference on Chemical Education, West Lafayette, IN, July 30 – August 3, 2006
102. *PLTL Orientation Sessions: Making Students Successful Leaders*, with Shilpi Bhargav, Shannon Sykes, and Bonnie Stevenson. 19th Biennial Conference on Chemical Education, West Lafayette, IN, July 30 – August 3, 2006
103. *Peer-led Team Learning Leaders: Contrasts in learning gains and perceived values of course interventions*, with Shannon Sykes and Shilpi Bhargav. 19th Biennial Conference on Chemical Education, West Lafayette, IN, July 30 – August 3, 2006
104. *PLTL Leaders: Transforming students into scholars*, with Shilpi Bhargav, Shannon Sykes, and Bonnie Stevenson, 232nd American Chemical Society National Meeting, San Francisco, CA, September 10 – 14, 2006.

105. *ACS Exam Measures of Impact of PLTL*, with J. A. Kampmeier and A. Fraiman, 232nd American Chemical Society National Meeting, San Francisco, CA, September 10 – 14, 2006.
106. *Tools and Processes: Understanding Methods of Inquiry and Dissemination*, with C. Hostetter, B. Pescosolido, D. Pace, Indiana University (Bloomington), October 26, 2006
107. *Excursions in the Scholarship of Teaching and Learning: Precursors to Publication*, IUPUI, November 8, 2006
108. *Quick Hits for SOTL: A Brief Orientation to Actual Issues in the Process of Scholarly Inquiry*, with C. Hostetter, B. Pescosolido, D. Pace, 3rd International Society for the Scholarship of Teaching and Learning Conference, Washington, DC, November 9-12, 2006
109. *Strategies for Maximizing Learning in Gateway Chemistry Courses*, Department of Chemistry, University of Toledo, November 15, 2006. Invited.
110. *Science, Technology, Engineering and Mathematics Opportunities at Indiana University*, in “The IU-HBCU STEM Initiative”, Jackson State University (Jackson, MS), February 4, 2007
111. *Interacting with the Dean*, with N. D. Lees, Twenty-fourth Annual Conference, Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education (Kansas State University), Orlando, FL, February 7, 2007. Invited presentation.
112. *Peer-Led Team Learning: An Active Learning Paradigm For Improved Student Success*, with Shannon Sykes, Bonnie Stevenson, and Stephanie So, FACET Retreat and Conference, IUPUI, May 18, 2007.
113. *An Introduction to SOTL: A Brief Orientation to Actual Issues in the Process of Scholarly Inquiry*, with Carol Hostetter, in “2007 Preparing Future Faculty Summer Institute”, IUPUI, June 15, 2007.
114. *Identifying Elements of Success for New University Students*, in “First Generation Bridge Scholars Program”, Faculty Panel, IUPUI, August 10, 2007.
115. *Accountability and the Department*, with N. D. Lees, Twenty-fifth Annual Conference, Academic Chairpersons, The Academic Department (Kansas State University), Orlando, FL, February 7, 2008.
116. *Transforming Classroom Problems into Researchable Questions: A Toolbox for Understanding the Scholarship of Teaching and Learning*, with Carol Hostetter and Bernice Pescosolido, FACET Retreat and Conference, French Lick Resort, May 16 – 18, 2008
117. *The Manuscript Review Process in a Teaching and Learning Journal*, Scholarship of Teaching and Learning Workshop, Western Michigan University, Kalamazoo, MI, May 30, 2008. Invited
118. *One-On-One Advice on Manuscripts and the Peer-Review Process*, Scholarship of Teaching and Learning Workshop, Western Michigan University, Kalamazoo, MI, May 30, 2008. Invited.
119. *Peer-led Team Learning: An Active Learning Paradigm for Improved Student Success*, “Ready, Set, Go! Engaging Students” Active Learning Symposium, Center for Teaching and Learning, Indiana University Purdue University Indianapolis, September 26, 2008. Invited.
120. *Changing the Faculty Paradigm*. Associate Faculty and Lecturer Conference, Indiana University FACET, October 25-26, 2008. Invited plenary. *Hass Birky Lecture Prelude*.
121. *Investments in Teaching: Making it all Pay Off*, Lilly House Event: “What’s Good Teaching?”, Marten House Meeting Center, November 7, 2008.
122. *SoTL Publication and Faculty Roles and Rewards*, in “The SoTL Life Cycle: From Germination to Dissemination Series”, Indiana University Purdue University Indianapolis, November 17, 2008. Invited.
123. *Partnering for Promotion: Excellence in Teaching*, Office for Women “Partnering for Promotion” Series, Indiana University Purdue University Indianapolis, January 29, 2009. Invited.

124. *Facilitating and Enhancing Research & Scholarship*, with N. D. Lees, Kansas State University Twenty-sixth Annual Academic Chairpersons Conference “What is on the Horizon?”, Orlando, FL, February 11-13, 2009. Invited.
125. *Advice for Department Chairs*, with N. D. Lees and Gautam Vemuri, Kansas State University Twenty-sixth Annual Academic Chairpersons Conference “What is on the Horizon?”, Orlando, FL, February 11-13, 2009. Invited.

MEETING PRESIDINGS AND OTHER SPECIAL INVITATIONS

Edward C. Moore Teaching Symposium, Charles J. Sykes Panel Discussion Moderator, “Are We Sacrificing Teaching for Prestige,” IUPUI, April 19, 1991.

Molecular, Electrical, Optical and Magnetic Properties and Interactions II, Presider, American Chemical Society Joint Central-Great Lakes Regional Meeting (IUPUI, May 29-31, 1991).

The Syllabus as a Tool for Imagination and Creativity, with Lee Shulman. Organized and presided over a Joint Faculty Colloquium of the School of Science and the School of Engineering and Technology (1994).

Networking Departmental Chairs, Forum on Faculty Roles and Rewards, American Association for Higher Education, Atlanta, GA (January 18-21, 1996). Invited Panel Co-coordinator.

Concerns of Departmental Chairs, Forum on Faculty Roles and Rewards, American Association for Higher Education, Orlando, FL (January 30, 1998). Invited Panel Facilitator

Workshop on Graduate Education in the Chemical Sciences: Issues for the 21st Century, Chemical Sciences Roundtable, National Research Council, December, 1999. Invited Participant.

American Chemical Society Peer Review of Student Affiliate Chapters, Overall Presider, American Chemical Society, Washington, DC, July, 2000.

Award Presenter, National Awards for ACS Student Affiliate Chapters, American Chemical Society, National Meeting, Orlando, April 7, 2002

American Chemical Society Peer Review of Student Affiliate Chapters, Overall Presider, American Chemical Society, Washington, DC, July, 2002.

Award Presenter, National Awards for ACS Student Affiliate Chapters, American Chemical Society, National Meeting, New Orleans, March 23, 2003

American Chemical Society Peer Review of Student Affiliate Chapters, Overall Presider, American Chemical Society, Washington, DC, August, 2003.

“Symposium on Peer-led Team Learning: New Approaches, New Results?” Presider, ACS National Meeting, Anaheim, CA, March 28, 2004

Award Presenter, National Awards for ACS Student Affiliate Chapters, American Chemical Society, National Meeting, Anaheim, CA, March 28, 2004

Award Presenter, National Awards for ACS Student Affiliate Chapters, American Chemical Society, National Meeting, Atlanta, GA, March 26, 2006

EXTERNALLY FUNDED PROPOSALS AND SUPPORT

National Science Foundation International Travel Grant, NATO Advanced Study Institute, Cortona, Italy, \$1,015 (September, 1980).

Research Corporation, Theoretical Interactions of Atoms and Polyatomic Molecules, \$3,700 (November, 1981).

Moore Foundation, ACS High School Scholarship Fund, \$500 (March, 1983) and \$600 (May, 1984).

American Chemical Society, Petroleum Research Fund, Energy Transfer in van der Waals Systems, \$15,000 (May, 1984).

American Chemical Society, Petroleum Research Fund, The Effects of Applied Electric Fields on Molecules and Weakly Bound Systems, \$20,000 (January, 1988).

Lilly Research Laboratories, Lilly Graduate Fellowship Program, co-principal investigator with Peter Rabideau, \$24,000 (March, 1988).

Lilly Research Laboratories, Lilly Graduate Fellowship Program, \$12,000 (December, 1990).

Lilly Research Laboratories, Lilly Graduate Fellowship Program, \$45,000 (December, 1991).

U.S. Department of Education, Graduate Assistance in Areas of National Need: Chemistry Fellowship Program, \$521,729 (February, 1992-August, 1995).

National Science Foundation, Macromolecular Modeling, Principal Investigator with other Co-PI's, \$111,000 (June, 1993).

E. Lilly and Company, Industrial Co-op Program, \$33,400 (1997-1999)

Project SEAM, Multi-institutional cooperative grant, Lilly Endowment, Project Director, Chemistry Program, \$105,000 (2001-4). Non-competitive.

U.S. Department of Education, Graduate Assistance in Areas of National Need: Chemistry Fellowship Program, with co-Principal Investigator: Eric C. Long, \$546,732 (April, 2001 – August, 2005).

INTERNALLY FUNDED PROPOSALS AND SUPPORT

University Research Operations Committee, Indiana University – Purdue University Indianapolis, \$12,000 (1981).

Grant-in-Aid of Research (IUPUI), Incorporation of Resonance Information in Determination of Potential Energy Surfaces, \$1200 (May, 1983).

Center for Innovative Computing Applications, Molecular Graphics and Computational Chemistry, co-principal investigator with K. Lipkowitz, \$19,500 (May, 1989).

Research Investment Fund, Computational Molecular and Biomolecular Science Facility, with several co-PIs, \$161,938 (July, 1992).

Research Investment Fund, SOS Spectroscopy Facility: Acquisition CD Spectrometer, Joint Biology-Chemistry Proposal, Chemistry funding: \$91,000 (December, 1993).

Research Investment Fund, Acquisition of Instruments for Molecular Structure Laboratory, with several other co-PI's, \$100,000 (April, 1994).

Research Investment Fund, Extending Computational Possibilities to Complex Biological Systems and Materials Sciences, \$170,700 (April, 1998).

University College, Peer-led Team Learning Workshop Program, \$8,000 (July, 2002).

Dedicated Tuition Fund (Commitment to Excellence Fund), Student-to-Student Scholar Program, \$150,000 annual grant (June, 2003 - present). Base budget allocation annually and, as of 2008-9, totals \$900,000.

University College, Peer-led Team Learning Workshop Program, \$10,000 (September, 2003).

University College, Peer-led Team Learning Workshop Program, \$10,000 (February, 2005).

PUBLICATIONS

1. Variational Bounds on the Radius of Convergence of the Born Series. David J. Malik and John H. Weare, *Chemical Physics*, **1**, 313-318 (1973).
2. Method of Averaging Wavefunction Corrections in Scattering Theory. David J. Malik and John H. Weare, *Journal of Chemical Physics*, **62**, 1044-1057 (1975).
3. Applications of Perturbation Theory to Atom-surface Diffraction. Karen L. Wolfe, David J. Malik, and John H. Weare, *Journal of Chemical Physics*, **67**, 1031-1041 (1977).
4. Method of Averaging Wavefunction Corrections in Scattering Theory. Inelastic Results. David J. Malik and John H. Weare, *Journal of Chemical Physics*, **67**, 2758-2764 (1977).
5. Accuracy and Convergence of Higher Order Distorted Wave Perturbation Theory. David J. Malik and John H. Weare, *Chemical Physics*, **32**, 153-160 (1978).
6. Rotational Compound State Resonances for an Argon and Methane Scattering System. Leslie N. Smith, David J. Malik, and Don Secrest, *Journal of Chemical Physics*, **71**, 4502-4514 (1979).
7. On Quantal Bound State Solutions and Potential Energy Surface Fitting. A Comparison of the Finite Element, Numerov-Cooley, and Finite Difference Method. David J. Malik, J. Eccles, and D. Secrest, *Journal of Computational Physics*, **38**, 157-184 (1980).
8. Potential Anisotropic Effects on Inelastic Differential Cross Sections. David J. Malik, D. Secrest, and U. Buck, *Chemical Physics Lett.* **75**, 465-467 (1980).
9. On the Argon-Methane Interaction from Scattering Data. U. Buck, J. Schleusener, David J. Malik, and D. Secrest, *Journal of Chemical Physics*, **74**, 1707-1717 (1981).
10. Systems for the Numerical Solution for the Radial Schrödinger Equation. Joseph Eccles and David J. Malik, *QCPE* **13**, 407, pp. 1-21 (1981).
11. An Approximate Method for Estimating Multiquantum Transition Probabilities in Molecular Collisions. Michael E. Coltrin and David J. Malik, *Chemical Physics Letters*, **85**, 567-571 (1982).
12. College Chemistry in a High School Environment. David J. Malik, *Journal of Chemical Education*, **60**, 967 (1983).
13. A Recursive Algorithm for the Finite Element Method in Scattering Theory. Rebecca B. Love and David J. Malik, *Chemical Physics*, **93**, 445-451 (1985).
14. Vibrational Motion Effects on Molecular Polarizabilities. Shifts in Vibrational Transition Frequencies and Transition Moments of Lithium Hydride from Applied Electrical Fields. David J. Malik and Clifford E. Dykstra, *Journal of Chemical Physics*, **83**, 6307-6315 (1985).
15. The Hydrogen Bonding Influence on Polarizability and Hyperpolarizability. A Derivative Hartree-Fock Study of the Electrical Properties of Hydrogen Fluoride and Hydrogen Fluoride Dimer. Clifford E. Dykstra, S. Liu, and David J. Malik, *Journal of Molecular Structure*, **135**, 357-368 (1986).
16. Conformational Analysis of the Covalent Pirkle Chiral Stationary Phases. Kenneth B. Lipkowitz, David J. Malik, and Thomas Darden, *Tetrahedron Lett.* **27**, 1759-1762 (1986).
17. Electrical Effects on the Vibrational Transitions of Hydrogen Fluoride Due to Hydrogen Bonding and Applied Fields. Shi-yi Liu, Clifford E. Dykstra, and David J. Malik, *Chemical Physics Lett.* **130**, 403-409 (1986).
18. Effects of Non-uniform Electric Fields on the Convergence Behavior of Energy Expansions. Raima Larter and David J. Malik, *Chemical Physics*, **112**, 301-305 (1987).

19. Derivative Numerov-Cooley Theory. A Method for Finding Vibrational State Properties of Diatomic Molecules. Clifford E. Dykstra and David J. Malik, *Journal of Chemical Physics*, **87**, 2806-2811 (1987).
20. Contour Diagrams for the Presentation of Separation Quality in Two-dimensional Thin Layer Chromatography. James E. Steinbrunner, David J. Malik and David Nurok, *Journal of High Resol. Chrom. and Chrom. Commun.* **10**, 560-563 (1987).
21. Vibrational Spectroscopy of Diatomic Molecules in Static Electric Fields. An *ab initio* Study of HF. David J. Malik, *Journal of Chemical Physics*, **88**, 2624-2629 (1988).
22. *ab initio* Determination of Molecular Electrical Properties and of Electrical Effects on Vibrational Spectra. Clifford E. Dykstra, S. Liu and David J. Malik, *Advances in Chemical Physics*, **75**, 37-117 (1989). Review article.
23. Book Review: Basic Principles and Applications of Molecular Quantum Mechanics, *Journal of the American Chemical Society*, **112**, 4093 (1990).
24. "Properties of Molecules by Direct Calculation," Clifford E. Dykstra, Joseph D. Augspurger, Bernard Kirtman, and David J. Malik in *Reviews in Computational Chemistry*, Kenny B. Lipkowitz and Donald B. Boyd, Eds., pp. 83-118 (VCH Publishers, New York, 1990). Invited.
25. Book Review: Atoms and Quanta, *Journal of the American Chemical Society*, **113**, 2802-2803 (1991).
26. "Teaching Effectiveness: Assessment and Rewards," John Kremer, John Hazer and David J. Malik in *Academic Chairpersons: Selecting, Motivating, Evaluating, and Rewarding Faculty*, Vol. 41, W. E. Cashin, Ed., National Issues in Higher Education, Kansas State University, 1993, p. 304-312.
27. "Fostering Elements of Change in the Department," David J. Malik and N. Douglas Lees, *The Department Chair*, (Anker Publishing, Spring, 1995). Invited.
28. "Departments in Transition: The Role of Faculty and Program Evaluation," David J. Malik and N. Douglas Lees, in *Academic Chairpersons: The Many Faces of Evaluation*, Vol. 45, W. E. Cashin, Ed., National Issues in Higher Education, Kansas State University, 1995, pp. 108-118.
29. "Peer Review of Teaching: External Review of Course Content," David J. Malik, *Innovative Higher Education* **20**(4), 277-286 (1996).
30. "Faculty Work: Approaches to Accountability," N. Douglas Lees and David J. Malik, in *Academic Chairpersons: The Many Faces of Evaluation*, Vol. 46, W. E. Cashin, Ed., National Issues in Higher Education, Kansas State University, 1996, p. 151-162.
31. "External Review of Teaching: A New Effort in the Chemistry Department at IUPUI," David J. Malik, in *Making Teaching Community Property: A Menu for Peer Collaboration and Peer Review*, Pat Hutchings, Ed., American Association for Higher Education Teaching Initiative, 1996, pp. 93-96.
32. "Maintaining Balance in Teaching Loads," David J. Malik and N. Douglas Lees, *The Department Chair*, Vol. 7, pp. 11-13 (Anker Publishing, Winter, 1997). Invited.
33. "Program Review: A Mechanism for Enhancing Academic Opportunity in an Era of Change," David J. Malik and N. D. Lees, *Academic Chairpersons: Changing Answers to Recurring Questions*, Vol. 47, W. E. Cashin, Ed., National Issues in Higher Education, Kansas State University, 1997, pp. 163-172.
34. "Can External Program Review Catalyze Departmental Change?," N. Douglas Lees and David J. Malik, *The Department Chair*, Vol. 7, pp. 13-14 (Anker Publishing, Summer, 1997). Invited.

35. *Book Review*: “Exploring Aspects of Computational Chemistry: Concepts” and “Exploring Aspects of Computational Chemistry: Exercises”, *J. Molec. Structure (Theochem)* 434 (1998) 265.
36. “Creating a Community of Chairs”, Richard C. Turner, N. Douglas Lees, E. Theodore Mullen, David J. Malik, and David A. Ford, *The Department Chair*, Vol. 9 (2), pp. 9-10 (Anker Publishing, Fall, 1998). Invited.
37. “Establishing a Campus Chair Community: Collaboration for Change”, N. Douglas Lees and David J. Malik, *Academic Chairpersons: The Cornerstone of Higher Education*, Vol. 48, National Issues in Higher Education, Kansas State University, 1998, pp. 122-128.
38. “Creating a Link between Accountability and Department Improvement,” N. Douglas Lees and David J. Malik, *The Department Chair*, Vol. 10 (1), pp. 1, 18-19 (1999)
39. “Representing the Department Effectively to its Constituencies: Precursors to Change”, David J. Malik and N. Douglas Lees, *Academic Chairpersons: The Cornerstone of Higher Education*, Vol. 49, National Issues in Higher Education, Kansas State University, 1999, pp. 165-174.
40. “Faculty Evaluation And The Role Of The Chair: Applications Of Workload-Based Models For Merit Pay And Post-Tenure Review”, N. Douglas Lees and David J. Malik, in *Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education*, Vol. 50, National Issues in Higher Education, Kansas State University, 2000, pp. 143-152.
41. “Making Faculty Evaluation Count,” David J. Malik and N. Douglas Lees, *The Department Chair*, Vol. 11 (2), pp. 6-8 (2000). Cited on American Council of Education Chair resource site: <http://www.acenet.edu/resources/chairs/>
42. “Preparing New Chairs”, N. Douglas Lees and David J. Malik, in *Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education*, Vol. 51, National Issues in Higher Education, Kansas State University, 2001, pp. 93-100.
43. “Move over faculty development: Let chairs train chairs,” N. Douglas Lees and David J. Malik, *The Department Chair*, Vol. 12 (2), pp. 10-12 (2001).
44. “Tips to the Department Chair,” David J. Malik and N. Douglas Lees, in *Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education*, Vol. 52, National Issues in Higher Education, Kansas State University, 2002, pp. 123-132.
45. “Is Graduate School for Me?”, *In Chemistry*, **12**(2), 2-3 (2002). Invited Editorial.
46. “Strategies for Successful Chairing. Public Work,” N. Douglas Lees and David J. Malik, *The Department Chair*, **13** (3), 13-15 (Winter, 2003). Invited article.
47. “Strategies for Successful Chairing. Private Work and Scholarship,” David J. Malik and N. Douglas Lees, *The Department Chair*, **13** (4), 1-3 (Spring, 2003). Invited article.
48. “Peer-led Team Learning in an Urban University”, *Chinese Journal of Chemical Education*, **24**, 37-39 (2003)
49. “Chair Leadership beyond the Department,” N. Douglas Lees and David J. Malik, in *Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education*, Vol. 53, National Issues in Higher Education, Kansas State University, 2003, pp. 163-172.
50. “Global Leadership and the Department Chair.” David J. Malik and N. Douglas Lees, *The Department Chair: A Resource for Academic Administrators*, **14** (3), 1-3 (2004)
51. “Creating External Partnerships to Enhance Department Relevance, Image and Fiscal Stability,” in *Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education*, Vol. 54, National Issues in Higher Education, Kansas State University, 2004, with N. D. Lees, 12 pp.

52. “Collaborative External Partnerships: Improving Department Finances and Image,” N. Douglas Lees and David J. Malik, *The Department Chair: A Resource for Academic Administrators*, **16** (2), 18 – 20 (2005). Invited article.
53. “Considering decentralization: Possible directions for peer-led team learning,” David J. Malik, *et al.*, *Progressions: Peer Led Team Learning*, Winter 2005
54. “Interacting with the Dean,” in *Academic Chairpersons, The Academic Department: The Cornerstone of Higher Education*, Vol. 57, National Issues in Higher Education, Kansas State University, 2007, with N. D. Lees, 8 pp.
55. “Working Effectively with the Dean,” David J. Malik and N. Douglas Lees, *The Department Chair: A Resource for Academic Administrators*, **18** (3), 1 - 3 (2008). Invited article. Cited and re-distributed by “Tomorrow’s Professor”, entry #846. <http://cgi.stanford.edu/%7Edept-ctl/cgi-bin/tomprof/postings.php>
56. “Accountability and the Role of the Department Chair,” in *Academic Chairpersons Conference Proceedings. Defining Department Leadership: Engaging Academic Communities for Success*, Twenty-fifth Annual Conference, February 6-8, 2008, Orlando, FL, with N. D. Lees, 9 pp.
57. “The Accountability Movement: Its Role, Opportunities and Meaning for Chairs”, David J. Malik and N. Douglas Lees, *The Department Chair: A Resource for Academic Administrators*, **19** (3), 3 – 5 (2009). Invited article. Cited and re-distributed by “Tomorrow’s Professor”, entry #924.
58. “Advice For Department Chairs,” in *Academic Chairpersons Conference Proceedings* of the Twenty-sixth Annual Conference (Orlando, FL), February 11-13, 2009, with N. Douglas Lees and Gautam Vemuri.
59. “Facilitating and Enhancing Research and Scholarship” in *Academic Chairpersons Conference Proceedings* of the Twenty-sixth Annual Conference (Orlando, FL), February 11-13, 2009, with N. Douglas Lees.
60. “Essentials of Chairing Academic Departments”, N. Douglas Lees, David J. Malik, and G. Vemuri, in *The Department Chair: A Resource for Academic Administrators*, Fall, 2009 (invited and in press).

EDUCATION MATERIALS AND CURRICULAR PUBLICATIONS

1. *Natural Science Laboratory Experiments*, with Brian Bowen, John Weare and Bruno Zimm, published by the Department of Chemistry, University of California (1972).
2. *General Chemistry Examination*. Member, Authoring Committee. American Chemical Society Division of Chemical Education (ACS DivCHED Examinations Institute, University of South Florida, 1987).
3. *General Chemistry Examination*. Member, Authoring Committee. American Chemical Society Division of Chemical Education (ACS DivCHED Examinations Institute, Oklahoma State University, Stillwater, OK, 1989).
4. *First-Term General Chemistry Examination*. Member, Authoring Committee. American Chemical Society Division of Chemical Education (ACS DivCHED Examinations Institute, Oklahoma State University, Stillwater, OK, 1989).
5. *General Chemistry Examination: Brief Test for Year Course*. Member, Authoring Committee. American Chemical Society Division of Chemical Education (ACS DivCHED Examinations Institute, Oklahoma State University, Stillwater, OK, 1990).
6. *Peer-Led Team Learning Manual for Chemistry C105*, Malik, *et al.*, Hayden-McNeil, 2004

7. *Peer-Led Team Learning Manual for Chemistry C105*, Malik, *et al.*, Hayden-McNeil, 2005
8. *The ‘Go Far’ Project*, in “The Scholarship of Teaching and Learning at IUPUI”, with Mark Hoyert, Center on Integrating Learning, IUPUI, 2005.
9. *Experimental Chemistry I Laboratory Manual*, Anliker, *et al.*, Ninth Edition, Hayden-McNeil (2006)
10. *PLTL Workbook: Principles of Chemistry I*, Malik, *et al.*, Hayden-McNeil, 2007 Edition (Summer, 2006)
11. *PLTL Workbook: Principles of Chemistry I*, Malik, *et al.*, Hayden-McNeil, 2009 Edition (Summer, 2008)
12. *Experimental Chemistry I Laboratory Manual*, Anliker, *et al.*, Tenth Edition, Hayden-McNeil (2008)
13. *ACS Guidelines for Chemistry Programs in Two-Year Colleges*, American Chemical Society, Washington, DC (2009), member of authoring task force.

CURRICULUM VITAE OF MICHAEL J. McLEISH Ph.D.

CONTACT DETAILS:

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EDUCATION:

Undergraduate

B.Sc. (Hons.) Chemistry Department, La Trobe University, Melbourne, Australia 1978.
Honours Thesis Title: "Synthesis of Heterocyclic Annellated Furoxans".
Research advisor: Bela Ternai

Graduate

Ph.D., Chemistry Department, La Trobe University, Melbourne, Australia 1984.
Thesis Title: "Mechanisms of the Decomposition of Aryl Diazonium Salts".
Research advisor: Trevor J. Broxton

Post-doctoral training:

Post-doctoral Research, Biochemistry Department, University of California at Berkeley, 1983-4.
Mechanistic studies on aspartate aminotransferase
Research advisor: Jack F. Kirsch

AWARDS AND SCHOLARSHIPS:

Undergraduate: Senior Government Scholarship, Commonwealth University Scholarship, Victorian Teaching Scholarship.

Graduate: La Trobe University Research Scholarship.

Post-Doctoral: CSIRO Postdoctoral Fellowship, Australian National Research Fellowship.

POSITIONS AND APPOINTMENTS:

1984	Tutor, Victorian College of Pharmacy Ltd., Australia.
1985	Visiting Lecturer, Chemistry Department, University of Papua New Guinea.
1985–88	National Research Fellow, Victorian College of Pharmacy Ltd., Australia.
1988–1994	Lecturer in Medicinal Chemistry, Victorian College of Pharmacy, Monash University, Australia.
1994	Visiting Professor, Department of Medicinal Chemistry, University of Kansas
1994–98	Senior Lecturer in Medicinal Chemistry, Victorian College of Pharmacy, Monash University, Australia.
1996–97	Sabbatical leave with Prof. George L. Kenyon, College of Pharmacy, University of California, San Francisco
1998–2004	Associate Research Scientist, College of Pharmacy, University of Michigan.
2004–2008	Research Scientist, College of Pharmacy, University of Michigan.
2008–	Associate Professor, Department of Chemistry & Chemical Biology, IUPUI

PROFESSIONAL AND UNIVERSITY ACTIVITIES:

PROFESSIONAL SERVICE

Current Member: American Chemical Society, American Society for Biochemistry and Molecular Biology.

Editorial Board: Enzyme Research

Ad hoc journal reviewing: Archives of Biochemistry and Biophysics, Biochemistry, Biochimica et Biophysica Acta, Bioorganic Chemistry, Biopolymers, Biotechnology Progress, Biotechnology & Bioengineering, Comparative Biochemistry and Physiology, FEBS Letters, FEBS Journal, Journal of the American Chemical Society, Journal of Biological Chemistry, Journal of Medicinal Chemistry, Journal of Peptide Research, Nature Chemical Biology, Protein & Peptide Letters, Protein Science, The Protein Journal, Talanta, Bioresource Technology, Angewandte Chemie.

Member of grant review panels:

National Science Foundation CHE/MCB review panel (March 2009).

National Science Foundation CLP review panel (November 2009).

Ad hoc grants reviewing: Australian Research Council (ARC), the National Science Foundation (NSF) and the German-Israeli Foundation (GIF).

Service to national organizations:

Committee member of Royal Australian Chemical Institute (RACI) Medicinal & Agricultural Chemistry Division, 1988-1998.

Conference organization:

Member, Organizing Committee for the 9th RACI Med & Ag Conference, 1991.

Member, Organizing Committee for the 12th RACI Med & Ag Conference, 1999.

Organizer of the inaugural Indiana Medicinal Chemistry Symposium to be held October 2010

UNIVERSITY SERVICE

Faculty committees (Indiana University-Purdue University, Indianapolis):

Member, School of Science Library committee, 2008-2009

Member, SELB research laboratories committee, 2008-

Chair, SELB core facilities committee; 2008-

Chair, Chemistry department faculty search committees (2); 2008-2009

Member, Chemistry Department Executive Committee; 2010

Faculty committees (University of Michigan):

Member, Animal Care & Safety committee, College of Pharmacy, University of Michigan; 2001-2005

Member, Research Resources committee, College of Pharmacy, University of Michigan; 2005-2008

Member, Graduate Admissions committee Medicinal Chemistry Department, University of Michigan; 2005-2008

Faculty committees (Monash University/Victorian College of Pharmacy):

Member, Research and Graduate Studies committee, 2002-2008

Member: Library committee, Search committee for Chair of Medicinal Chemistry, Pharmacy Course Review committee, various *ad hoc* committees.

COMMUNITY SERVICE

Pike High School "Ask the expert" day, 2009-2010

RACI Chemists in schools program, 1988-1998.

RESEARCH ACTIVITIES

My primary research interests lie in the areas of mechanistic enzymology and chemical biology. This includes structure-function analysis, rational design of enzyme inhibitors, evolution of the substrate specificity of enzymes, re-engineering of enzymes for organic synthesis, bioremediation and biofuel production, and the evolution of new enzymatic pathways.

RESEARCH FUNDING

Active

IUPUI Startup funds: 8/1/2008 -

Recently completed

NSF Frontiers in Integrative Biology, “How organisms adapt to new enzymes and pathways” MJ McLeish, P.I. (with GA Petsko, D Ringe and JJ Collins, co-P.Is.), 09/1/2004 - 08/30/2010 (33% effort, \$170,000 annual direct costs). Total costs: \$4.25M.

Australian Research Council; “Innovative Approaches to Membrane Protein Crystallography & Drug Discovery” MJ McLeish, co-investigator (JL Martin, University of Queensland, P.I.), 01/01/2006 - 12/31/2008 (5% effort only).

NIH RO1HL34193, “Design of Inhibitors of Epinephrine Biosynthesis” MJ McLeish, co-investigator (GL Grunewald, University of Kansas, P.I.), 08/01/2001 - 07/31/2006 (10% effort, \$56,000 annual direct costs)

NIH RO1GM40570; “Restructuring catalysis in the mandelate pathway” MJ McLeish, co-investigator (with GL Kenyon; J Gerlt, University of Illinois, P.I.), 06/01/2000 - 05/31/2002, (10% effort, \$131,864, total costs).

PUBLICATIONS

Contributions to peer-reviewed journals(reverse chronological order):

1. Pratt, R. F., and **McLeish, M. J.** (2010) The structural relationship between the active sites of β -lactam-recognizing and amidase signature enzymes: convergent evolution?, *Biochemistry*, **49**, 9688–9697.
2. Drinkwater, N., Vu, H., Lovell, K. M., Criscione, K. R., Collins, B., Prisinzano, T. E., Poulsen, S.-A., **McLeish, M. J.**, Grunewald, G. L., and Martin, J. L. (2010) Fragment-screening by X-ray crystallography, mass spectrometry and isothermal titration calorimetry to identify PNMT inhibitors, *Biochemical Journal*, **431**, 51-61.
3. Brandt, G. S., Kneen, M. M., Petsko, G. A., Ringe, D., and **McLeish, M. J.** (2010) Active-site engineering of benzaldehyde lyase shows that a point mutation can confer both new reactivity and susceptibility to mechanism-based inhibition, *Journal of the American Chemical Society* **132**, 438-439.
4. Yep, A., and **McLeish, M. J.** (2009) Evolution of a benzoylformate decarboxylase variant with enhanced pyruvate decarboxylase activity, *Biochemistry* **48**, 8387-8395.
5. Drinkwater, N., Gee, C. L., Puri, M., Criscione, K. R., **McLeish, M. J.**, Grunewald, G. L., and Martin, J. L. (2009) Molecular recognition of physiological substrate noradrenaline by the adrenaline synthesising enzyme PNMT and factors influencing its methyltransferase activity, *Biochemical Journal* **422**, 463-471.
6. Georgieva, P., Wu, Q., **McLeish, M. J.**, and Himo, F. (2009) The reaction mechanism of phenylethanolamine N-Methyltransferase: A density functional theory study, *Biochimica et Biophysica Acta - Proteins and Proteomics* **1794**, 1831-1837.
7. Wang, P. F., Yep, A., Kenyon, G. L., and **McLeish, M. J.** (2009) Using directed evolution to probe the substrate specificity of mandelamide hydrolase, *Protein Engineering, Design and Selection* **22**, 103-110.
8. Brandt, G. S., Kneen, M. M., Chakraborty, S., Baykal, A. T., Nemeria, N., Yep, A., Ruby, D. I., Petsko, G., Kenyon, G. L., **McLeish, M. J.**, Jordan, F., and Ringe, D. (2009) Snapshot of a reaction intermediate: analysis of benzoylformate decarboxylase in complex with a benzoylphosphonate inhibitor *Biochemistry* **48**, 3247-3257.
9. Chakraborty, S., Nemeria, N., Brandt, G. S., Kneen, M. M., Yep, A., **McLeish, M. J.**, Kenyon, G. L., Petsko, G., Ringe, D., and Jordan, F. (2009) Detection and time-course of formation of all thiamin diphosphate-bound

- covalent intermediates derived from a chromophoric substrate analogue on benzoylformate decarboxylase., *Biochemistry* 48, 981-994.
10. Wu, Q., Caine, J. M., Thomson, S. A., Slavica, M., Grunewald, G. L., and **McLeish, M. J.** (2009) Time-dependent inactivation of human phenylethanolamine *N*-methyltransferase by 7-isothiocyanatotetrahydroisoquinoline, *Bioorganic and Medicinal Chemistry Letters* 19, 1071-1074.
 11. Brandt, G., Nemeria, N., Chakraborty, S., **McLeish, M. J.**, Yep, A., Kenyon, G. L., Petsko, G., Jordan, F., and Ringe, D. (2008) Probing the active center of benzaldehyde lyase with substitutions and the pseudo-substrate analogue benzoylphosphonic acid methyl ester, *Biochemistry* 47, 7734-7743.
 12. Chakraborty, S., Nemeria, N., Yep, A., **McLeish, M. J.**, Kenyon, G. L., and Jordan, F. (2008) The mechanism of benzaldehyde lyase studied via thiamin diphosphate-bound Intermediates and kinetic isotope effects *Biochemistry* 47, 3800-3809.
 13. Yep, A., Kenyon, G. L., and **McLeish, M. J.** (2008) Saturation mutagenesis of putative catalytic residues of benzoylformate decarboxylase provides a challenge to the accepted mechanism, *Proceedings of the National Academy of Sciences USA* 105, 5733-5738.
 14. Yeung, C. K., Kenyon, G. L., and **McLeish, M. J.** (2008) Physical, kinetic and spectrophotometric studies of a NAD(P)⁺-dependent benzaldehyde dehydrogenase from *Pseudomonas putida* ATCC 12633, *Biochimica et Biophysica Acta - Proteins and Proteomics*, 1248-1255.
 15. Nemeria, N., Korotchkina, L., **McLeish, M. J.**, Kenyon, G. L., Patel, M. S., and Jordan, F. (2007) Elucidation of the chemistry of enzyme-bound thiamin diphosphate prior to substrate binding: defining internal equilibria among tautomeric and ionization states, *Biochemistry* 46, 10739-10744.
 16. Saehuan, C., Rojanarata, T., Wiyakrutta, S., **McLeish, M. J.**, and Meevootisom, V. (2007) Isolation and characterization of a benzoylformate decarboxylase and a NAD⁺/NADP⁺-dependent benzaldehyde dehydrogenase involved in D-phenylglycine metabolism in *Pseudomonas stutzeri* ST-201, *Biochimica et Biophysica Acta* 1770, 1585-1592.
 17. Gee, C. L., Drinkwater, N., Tyndall, J. D. A., Grunewald, G. L., Qian Wu, Q., **McLeish, M. J.**, and Martin, J. L. (2007) Enzyme adaptation to inhibitor binding: a cryptic binding site in phenylethanolamine *N*-methyltransferase, *Journal of Medicinal Chemistry* 50, 4845-4853.
 18. Bera, A. K., Polovnikova, L. S., Roestamadji, J., Widlanski, T. S., Kenyon, G. L., **McLeish, M. J.**, and Hasson, M. S. (2007) Mechanism-based inactivation of benzoylformate decarboxylase, a thiamin diphosphate-dependent enzyme, *Journal of the American Chemical Society* 129, 4120-4121.
 19. Janzen, E., Müller, M., Kolter-Jung, D., Kneen, M. M., **McLeish, M. J.**, and Pohl, M. (2006) Characterization of benzaldehyde lyase from *Pseudomonas fluorescens* - a versatile enzyme for asymmetric C-C-bond formation, *Bioorganic Chemistry* 34, 345-361.
 20. Yep, A., Kenyon, G. L., and **McLeish, M. J.** (2006) Determinants of substrate specificity in KdcA, a thiamin diphosphate-dependent decarboxylase, *Bioorganic Chemistry* 34, 325-336.
 21. Wang, P.-F., Flynn, A. J., Naor, M. M., Jensen, J. H., Cui, G., Merz Jr., K. M., Kenyon, G. L., and **McLeish, M. J.** (2006) Exploring the role of the active site cysteine in human muscle creatine kinase, *Biochemistry* 45, 11464-11472.
 22. Wang, P.-F., Kenyon, G. L., and **McLeish, M. J.** (2006) Heterogeneity of *Escherichia coli*-expressed human muscle creatine kinase, *IUBMB Life* 58, 421-428.
 23. Andricopulo, A. D., Akoachere, M. B., Krogh, R., Nickel, C., McLeish, M. J., Kenyon, G. L., Arscott, L. D., Williams, C. H. J., Davioud-Charvet, E., and Becker, K. (2006) Specific inhibitors of *Plasmodium falciparum* thioredoxin reductase as potential antimalarial agents, *Bioorganic and Medicinal Chemistry Letters* 16, 2283-2292.
 24. Gee, C. L., Tyndall, J. D. A., Grunewald, G. L., Wu, Q., **McLeish, M. J.**, and Martin, J. L. (2005) Binding mode of methyl acceptor substrates to the adrenaline-synthesizing enzyme phenylethanolamine *N*-methyltransferase: implications for catalysis, *Biochemistry* 44, 16875-16885.
 25. Kneen, M. M., Pogosheva, I. D., Kenyon, G. L., and **McLeish, M. J.** (2005) Exploring the active site of benzaldehyde lyase by modeling and mutagenesis, *Biochimica et Biophysica Acta - Proteins and Proteomics* 1753, 263-271.

26. Wu, Q., Gee, C. L., Lin, F., Tyndall, J. D., Martin, J. L., Grunewald, G. L., and **McLeish, M. J.** (2005) Structural, mutagenic and kinetic analysis of the binding of substrates and inhibitors of human phenylethanolamine *N*-methyltransferase, *Journal of Medicinal Chemistry* 48, 7243-7252.
27. Siegert, P., **McLeish, M. J.**, Baumann, M., Kneen, M. M., Kenyon, G. L., and Pohl, M. (2005) Exchanging the substrate specificities of pyruvate decarboxylase from *Zymomonas mobilis* and benzoylformate decarboxylase from *Pseudomonas putida*, *Protein Engineering, Design and Selection* 18, 345-357.
28. Wang, P.-F., Flynn, A. D., **McLeish, M. J.**, and Kenyon, G. L. (2005) Loop movement and catalysis in creatine kinase, *IUBMB Life* 57, 355-362.
29. **McLeish, M. J.**, and Kenyon, G. L. (2005) Relating structure to mechanism in creatine kinase, *Critical Reviews in Biochemistry and Molecular Biology* 40, 1-20.
30. Gee, C. L., Nourse, A., A-Yen Hsin, A.-Y., Wu, Q., Tyndall, J. D., Grunewald, G. L., **McLeish, M. J.**, and Martin, J. L. (2005) Disulfide-linked dimers of human adrenaline synthesizing enzyme PNMT are catalytically active, *Biochimica et Biophysica Acta - Proteins and Proteomics* 1750, 82-92.
31. Wu, Q., Criscione, K. R., Grunewald Gary, L., and **McLeish, M. J.** (2004) Phenylethanolamine *N*-methyltransferase: re-evaluation of kinetic data, *Bioorganic and Medicinal Chemistry Letters* 14, 4217-4220.
32. Romero, F. A., Vodonick, S. M., Criscione, K. R., **McLeish, M. J.**, and Grunewald, G. L. (2004) Inhibitors of phenylethanolamine *N*-methyltransferase that are predicted to penetrate the blood-brain barrier: Design, synthesis and evaluation of 3-fluoromethyl-7-(*N*-substituted-aminosulfonyl)-1,2,3,4-tetrahydroisoquinolines that possess low affinity towards the α_2 -adrenoceptor, *Journal of Medicinal Chemistry* 47, 4483-4493.
33. Novak, W. R. P., Wang, P.-F., **McLeish, M. J.**, Kenyon, G. L., and Babbitt, P. C. (2004) Isoleucine 69 and Valine 325 form a specificity pocket in human muscle creatine kinase, *Biochemistry* 43, 13766-13774.
34. McMillan, F. M., Archbold, J., **McLeish, M. J.**, Caine, J. M., Criscione, K. R., Grunewald, G. L., and Martin, J. L. (2004) Molecular recognition of sub-micromolar inhibitors by the epinephrine-synthesising enzyme phenylethanolamine *N*-methyltransferase, *Journal of Medicinal Chemistry* 47, 37-44.
35. Gopalakrishna, K. N., Stewart, B. H., Kneen, M. M., Andricopulo, A. D., Kenyon, G. L., and **McLeish, M. J.** (2004) Mandelamide hydrolase from *Pseudomonas putida*: Characterization of a new member of the amidase signature family, *Biochemistry* 43, 7725-7735.
36. Polovnikova, E. S., **McLeish, M. J.**, Sergienko, E. A., Burgner, J. T., Anderson, N. L., Bera, A. K., Jordan, F., Kenyon, G. L., and Hasson, M. S. (2003) Structural and kinetic analysis of catalysis by a thiamin diphosphate-dependent enzyme, benzoylformate decarboxylase, *Biochemistry* 42, 1820-1830.
37. **McLeish, M. J.**, Kneen, M. M., Gopalakrishna, K. N., Koo, C. W., Babbitt, P. C., Gerlt, J. A., and Kenyon, G. L. (2003) Identification and characterization of a mandelamide hydrolase and an NAD(P)⁺-dependent benzaldehyde dehydrogenase from *Pseudomonas putida* ATCC 12633, *Journal of Bacteriology* 185, 2451-2456.
38. Davioud-Charvet, E., **McLeish, M. J.**, Veine, D. M., Giegel, D., Arscott, L. D., Andricopulo, A. D., Becker, K., Müller, S., Schirmer, R. H., Williams Jr., C. H., and Kenyon, G. L. (2003) Mechanism-based inactivation of thioredoxin reductase by Mannich bases. Implication for cytotoxicity, *Biochemistry* 42, 13319-13330.
39. Wang, P.-F., Novak, W. R. P., Cantwell, J. S., Babbitt, P. C., **McLeish, M. J.**, and Kenyon, G. L. (2002) Expression of *Torpedo californica* creatine kinase in *Escherichia coli* and purification from inclusion bodies, *Protein Expression and Purification* 26, 89-95.
40. Lahiri, S. D., Wang, P. F., Babbitt, P. C., **McLeish, M. J.**, Kenyon, G. L., and Allen, K. N. (2002) The 2.1 Å structure of *Torpedo californica* creatine kinase complexed with the ADP-Mg²⁺/NO₃⁻/creatine transition-state analogue complex, *Biochemistry* 41, 13861-13867.
41. Begun, J., **McLeish, M. J.**, Caine, J. M., Palant, E., Grunewald, G. L., and Martin, J. L. (2002) Crystallization of PNMT, the adrenaline-synthesizing enzyme, is critically dependent on a high protein concentration, *Acta Crystallographica D* 58, 314-315.
42. Wang, P.-F., **McLeish, M. J.**, Kneen, M. M., Lee, G., and Kenyon, G. L. (2001) An unusually low *pK_a* for Cys282 in the active site of human muscle creatine kinase, *Biochemistry* 40, 11698-11705.
43. Martin, J. L., Begun, J., **McLeish, M. J.**, Caine, J. M., and Grunewald, G. L. (2001) Getting the adrenaline going: crystal structure of the adrenaline-synthesizing enzyme PNMT, *Structure* 9, 977-985.

44. Grunewald, G. L., **McLeish, M. J.**, and Criscione, K. R. (2001) Phenylethanolamine *N*-methyltransferase kinetics: bovine *versus* recombinant human enzyme, *Bioorganic and Medicinal Chemistry Letters* 11, 1579-1582.
45. Cantwell, J. S., Novak, W. R., Wang, P. F., **McLeish, M. J.**, Kenyon, G. L., and Babbitt, P. C. (2001) Mutagenesis of two acidic active site residues in human muscle creatine kinase: implications for the catalytic mechanism, *Biochemistry* 40, 3056-3061.
46. Sergienko, E. A., Wang, J., Polovnikova, L., Hasson, M. S., **McLeish, M. J.**, Kenyon, G. L., and Jordan, F. (2000) Spectroscopic detection of transient thiamin diphosphate-bound intermediates on benzoylformate decarboxylase, *Biochemistry* 39, 13862-13869.
47. Najbar, L. V., Craik, D. J., Wade, J. D., and **McLeish, M. J.** (2000) Identification of initiation sites for T4 lysozyme folding using CD and NMR spectroscopy of peptide fragments, *Biochemistry* 39, 5911-5920.
48. Montserret, R., **McLeish, M. J.**, Bockmann, A., Geourjon, C., and Penin, F. (2000) Involvement of electrostatic interactions in the mechanism of peptide folding induced by sodium dodecyl sulfate binding, *Biochemistry* 39, 8362-8373.
49. Lazoura, E., **McLeish, M. J.**, and Aguilar, M. I. (2000) Studies on the conformational properties of CP-10(42-55), the hinge region of CP-10, using circular dichroism and RP-HPLC, *Journal of Peptide Research* 55, 411-418.
50. Chen, L. H., White, C. B., Babbitt, P. C., **McLeish, M. J.**, and Kenyon, G. L. (2000) A comparative study of human muscle and brain creatine kinases expressed in *Escherichia coli*, *Journal of Protein Chemistry* 19, 59-66.
51. Montserret, R., Aubert-Foucher, E., **McLeish, M. J.**, Hill, J. M., Ficheux, D., Jaquinod, M., van der Rest, M., Deleage, G., and Penin, F. (1999) Structural analysis of the heparin-binding site of the NC1 domain of collagen XIV by CD and NMR, *Biochemistry* 38, 6479-6488.
52. Hasson, M. S., Muscate, A., **McLeish, M. J.**, Polovnikova, L. S., Gerlt, J. A., Kenyon, G. L., Petsko, G. A., and Ringe, D. (1998) The crystal structure of benzoylformate decarboxylase at 1.6 Å resolution: diversity of catalytic residues in thiamin diphosphate-dependent enzymes, *Biochemistry* 37, 9918-9930.
53. Najbar, L. V., Craik, D. J., Wade, J. D., Salvatore, D., and **McLeish, M. J.** (1997) Conformational analysis of LYS(11-36), a peptide derived from the β -sheet region of T4 lysozyme, in TFE and SDS, *Biochemistry* 36, 11525-11533.
54. Nguyen, K. T., Stephens, D. P., **McLeish, M. J.**, Crankshaw, D. P., and Morgan, D. J. (1996) Pharmacokinetics of thiopental and pentobarbital enantiomers after intravenous administration of racemic thiopental, *Anesthesia and Analgesia* 83, 552-558.
55. Jones, D. J., Nguyen, K. T., **McLeish, M. J.**, Crankshaw, D. P., and Morgan, D. J. (1996) Determination of (*R*)-(+)- and (*S*)-(-)-isomers of thiopentone in plasma by chiral high-performance liquid chromatography, *Journal of Chromatography. B, Biomedical Applications* 675, 174-179.
56. Caine, J. M., Macreadie, I. G., Grunewald, G. L., and **McLeish, M. J.** (1996) Recombinant human phenylethanolamine *N*-methyltransferase: overproduction in *Escherichia coli*, purification, and characterization, *Protein Expression and Purification* 8, 160-166.
57. Wade, J. D., Perich, J. W., **McLeish, M. J.**, Otvos, L., Jr., and Tregear, G. W. (1995) Synthesis and conformational analysis of an *O*-phosphotyrosine-containing α -helical peptide, *Letters in Peptide Science* 2, 71-76.
58. Najbar, L. V., Craik, D. J., Wade, J. D., Lin, F., and **McLeish, M. J.** (1995) CD and NMR determination of the solution structure of a peptide corresponding to T4 lysozyme residues 38-51, *Biochimica Biophysica Acta* 1250, 163-170.
59. Wilson, J. C., Nielsen, K. J., **McLeish, M. J.**, and Craik, D. J. (1994) A determination of the solution conformation of the nonmammalian tachykinin eledoisin by NMR and CD spectroscopy, *Biochemistry* 33, 6802-6811.
60. **McLeish, M. J.**, Nielsen, K. J., Najbar, L. V., Wade, J. D., Lin, F., Doughty, M. B., and Craik, D. J. (1994) Conformation of a peptide corresponding to T4 lysozyme residues 59-81 by NMR and CD spectroscopy, *Biochemistry* 33, 11174-11183.
61. Mackay, M. F., **McLeish, M. J.**, and Campbell, M. (1994) Two nitrogen-containing analogues of chorismic acid, *Acta Crystallographica C* 50, 1734-1737.

62. **McLeish, M. J.**, Nielsen, K. J., Wade, J. D., and Craik, D. J. (1993) A peptide corresponding to the N-terminal 13 residues of T4 lysozyme forms an α -helix, *FEBS Letters* 315, 323-328.
63. Campbell, M., and **McLeish, M. J.** (1993) Improved synthesis of a precursor to 4-amino-4-deoxy-chorismic acid using an iminophosphorane as a base-labile protecting group, *Journal of Chemical Research*, 148-149.
64. Campbell, M., **McLeish, M. J.**, Lynch, D. E., Smith, G., Byriel, K. A., and Kennard, C. H. L. (1992) The preparation and crystal structure of 2-phenoxypropenoic acid, *Australian Journal of Chemistry* 45, 2061-2066.
65. **McLeish, M. J.**, and Caine, J. M. (1991) Chemical modification of PABA synthase, *Biochemistry International* 24, 1033-1042.
66. Mackay, M. F., Campbell, M., and **McLeish, M. J.** (1991) The crystal structure of dimethyl (1 α ,2 α ,5 β ,6 α) β -hexahydroazirino[2,1-*b*]benzoxazole-1 α ,5(1*H*)-dicarboxylate, *Australian Journal of Chemistry* 44, 1145-1149.
67. Morgan, D. J., Szutu, M., Mihaly, G. W., **McLeish, M. J.**, and Kumar, K. (1990) Stereoselective elimination of clomiphene isomers by the isolated perfused rat liver, *Journal of Biopharmaceutical Sciences* 1, 33-46.
68. **McLeish, M. J.**, and Huang, J. L. (1990) A comparison of the alkaloid levels in the nuts of *Areca catechu* Linn., *Science in New Guinea* 16, 55-60.
69. Szutu, M., Morgan, D. J., **McLeish, M.**, Phillipou, G., Blackman, G. L., Cox, L. W., and Dollman, W. (1989) Pharmacokinetics of intravenous clomiphene isomers, *British Journal of Clinical Pharmacology* 27, 639-640.
70. **McLeish, M. J.**, Julin, D. A., and Kirsch, J. F. (1989) Aspartate aminotransferase catalyzed oxygen exchange with solvent from oxygen-18-enriched α -ketoglutarate: evidence for slow exchange of enzyme-bound water, *Biochemistry* 28, 3821-3825.
71. Huang, J. L., and **McLeish, M. J.** (1989) High-performance liquid chromatographic determination of the alkaloids in betel nut, *Journal of Chromatography* 475, 447-450.
72. **McLeish, M. J.**, Wookey, P. J., and Mortimer, K. G. (1988) The cloning and over-expression of PABA synthase in *E. coli*, *Biochemistry International* 16, 727-735.
73. Sitaram, B. R., Lockett, L., **McLeish, M.**, Hayasaka, Y., Blackman, G. L., and McLeod, W. R. (1987) Gas chromatographic-mass spectroscopic characterisation of the psychotomimetic indolealkylamines and their *in vivo* metabolites, *Journal of Chromatography* 422, 13-23.
74. Broxton, T. J., and **McLeish, M. J.** (1983) Studies of the carbanionic and free radical mechanisms of dediazonation of substituted 2-chlorobenzenediazonium salts, *Journal of Organic Chemistry* 48, 191-195.
75. Broxton, T. J., and **McLeish, M. J.** (1983) General acid and intramolecular electrostatic catalysis in the ionization of methyl (*E*)-2-organyl-5-nitrophenylazo ethers in alcoholic solvents, *Australian Journal of Chemistry* 36, 55-66.
76. Broxton, T. J., and **McLeish, M. J.** (1983) Further evidence for the mechanism of dediazonation in basic alcoholic solution, *Australian Journal of Chemistry* 36, 1031-1035.
77. Broxton, T. J., and **McLeish, M. J.** (1982) A comparison of the available methods for the measurement of the rate of ionization of (*Z*)-arylazo alkyl ethers in alcoholic solvents, *Australian Journal of Chemistry* 35, 319-329.
78. Broxton, T. J., and **McLeish, M. J.** (1982) Kinetic studies of the decomposition of *Z* ethers derived from some substituted 2-nitrobenzenediazonium salts, *Journal of Organic Chemistry* 47, 3673-3679.

Chapters in edited books

1. **McLeish, M. J.** (1992). Thiopental sodium. In *Analytical Profiles of Drug Substances and Excipients*, Vol. 21, pp. 535-72. Academic Press, New York.
2. **McLeish, M. J.**, Capuano, B. & Lloyd, E. J. (1993). Clozapine. In *Analytical Profiles of Drug Substances and Excipients*, Vol. 22, pp. 145-84. Academic Press, New York.
3. **McLeish, M. J.** (1998). Clomiphene citrate. In *Analytical Profiles of Drug Substances and Excipients*, Vol. 25, pp. 85-120. Academic Press, New York.
4. **McLeish, M. J.** & Kenyon, G. L. (2001). Creatine kinase, Human. In *Wiley Encyclopedia of Molecular Medicine*, Vol. 2, pp. 934-935. Wiley and Sons, New York.

5. **McLeish, M. J.** (2001). Phenylethanolamine *N*-methyltransferase. In *Wiley Encyclopedia of Molecular Medicine*, Vol. 4, pp. 2536-2539. Wiley and Sons, New York.
6. Davioud-Charvet, E., **McLeish, M. J.**, Veine, D., Giegel, D., Andricopulo, A. D., Becker, K., Muller, S., Schirmer, R. H., Williams, C. H. & Kenyon, G. L. (2002). Mechanism-based inactivation of thioredoxin reductase from *Plasmodium falciparum* by Mannich Bases. Implications for drug design. In *Flavins and Flavoproteins 2002* (Chapman, S. K., Perham, R. N. & N.S., S., eds.), pp. 845-851. Agency for Scientific Publications, Berlin.
7. **McLeish, M. J.** & Kenyon, G. L. (2003). Approaches to the rational design of enzyme inhibitors. In *Burger's Medicinal Chemistry* 6th edit., Vol. 1, Drug Discovery, pp. 715-779. Wiley and Sons, New York.
8. **McLeish, M. J.**, Kenyon, G. L., Polovnikova, E. S., Bera, A. S., Anderson, N. L. & Hasson, M. S. (2004). Benzoylformate decarboxylase: Lessons in enzymology. In *Thiamin: Catalytic mechanisms and role in normal and disease states* (Jordan, F. & Patel, M. S., eds.), pp. 131-141. Marcel Dekker Inc., New York.
9. Siegert, P., Pohl, M., Kneen, M. M., Pogozheva, I. D., Kenyon, G. L. & **McLeish, M. J.** (2004). Exploring the substrate specificity of benzoylformate decarboxylase, pyruvate decarboxylase and benzaldehyde lyase. In *Thiamin: Catalytic mechanisms and role in normal and disease states* (Jordan, F. & Patel, M. S., eds.), pp. 275-290. Marcel Dekker Inc., New York.
10. Andricopulo, A. D., Akoachere, M. B., Krogh, R., Nickel, C., **McLeish, M. J.**, Davioud-Charvet, E., Kenyon, G. L., Arscott, L. D., Williams, J., C. H. & Becker, K. (2005). Specific Inhibitors of *Plasmodium falciparum* thioredoxin reductase. In *Flavins and Flavoproteins 2005* (Nishino, T., Miura, R., Tanokura, M. & Fukui, K., eds.). ARchiTect Inc., Tokyo.
11. **McLeish, M. J.** & Kenyon, G. L. (2006). Using site-directed mutagenesis to elucidate structure and mechanism in creatine kinase. In *Creatine Kinase* (Vial, C., ed.), pp. 27-68. Nova Science, New York.

PRESENTATIONS

In excess of 100 poster presentations have been made at national and international conferences. Further details are available on request.

INVITED LECTURES:

2010: Institute of Technical Biochemistry/Institute of Microbiology, University of Stuttgart, Germany; Institute of Technical Biocatalysis, Hamburg University of Technology, Germany. **2009:** Chemistry Department, Wesleyan University, Middletown, CT, College of Pharmacy and Health Sciences, Butler University, Indianapolis, IN **2008:** 7th International Conference on Mechanisms and Physiology of Thiamine, Wittenberg, Germany. **2007:** Microbiology Department, Mahidol University, Thailand; Biochemistry Department, Indiana University School of Medicine, Indianapolis, IN; Department of Chemistry & Chemical Biology, Indiana University-Purdue University, Indianapolis, IN; College of Pharmacy, Texas A&M Health Science Center, Kingsville, TX; Peking University Health Science Center, Beijing, China; Shenyang Pharmaceutical University, Shenyang, China; Enzyme Engineering Conference, Dalian, China; Department of Chemistry and Biochemistry, Florida International University, Miami, FL; School of Pharmacy, Duquesne University, Pittsburgh, PA; **2006:** Institut für Pharmazeutische Wissenschaften, Albert-Ludwigs-Universität Freiburg, Germany; Interdisciplinary Research Center, Justus-Liebig University Giessen, Germany; Victorian College of Pharmacy, Monash University, Australia; **2005:** Institut de Biologie et Chimie des Proteins - CNRS Lyon, France; Biochemistry Department, Université Claude Bernard Lyon 1, Villeurbanne, France; Department of Chemistry, University of Iowa, Iowa City, IA; **2004:** 2nd Brazilian Symposium on Medicinal Chemistry, Rio de Janeiro, Brazil; Instituto de Física, Universidade de São Carlos, São Carlos, Brazil; Faculdade de Ciências Farmacêuticas, São Paulo State University, Araraquara, Brazil; Interdepartmental Program in Medicinal Chemistry, University of Michigan, MI; **2003:** Department of Medicinal Chemistry, University of Kansas, Lawrence KS; Protein Engineering Network of Centres of Excellence, University of Toronto, Toronto, Canada; Department of Biochemistry, University of Mississippi Medicine Center, Jackson, MS; **2002:** International Conference on Thiamin, Its Biochemistry and Structural Biology, Newark, NJ; **2001:** Department of Biochemistry, Wayne State University, Michigan, MI; **2000:** Interdepartmental Program in Medicinal Chemistry, University of Michigan, MI; **1999:** Biophysics Research Division, University of Michigan, MI; **1997:** Department of Medicinal Chemistry, University of Utah, Salt Lake City, UT; Department of Medicinal Chemistry, University of Kansas, Lawrence KS; **1996:** Howard Florey Institute, University of Melbourne, Parkville, Australia; Institut de Biologie et Chimie des Proteins - CNRS Lyon, France; **1995:** CSIRO Division of Animal Health, Parkville, Australia; **1995:** Institut de Biologie et Chimie des Proteins - CNRS Lyon, France; Department of Pharmacy, University of Papua New Guinea; **1994:** Biochemistry Department, Monash University, Clayton, Australia; RACI Analytical Chemistry Group, Melbourne, Australia; Medicinal Chemistry Department, University of Kansas, Lawrence, KS; **1992:** Chemistry Department, University of Papua New Guinea; **1991:** RACI 9th Conference on Medicinal & Agricultural Chemistry, Kyneton, Australia; **1990:** University of Tübingen, Germany; Rhone-Poulenc Co, Lyon, France; Institute For Biochemistry, Karl-Marx-University, Leipzig, East Germany; **1986:** Chemistry Department, La Trobe University, Bundoora, Australia; School of Pharmacy, University of Georgia, Athens, GA; Medicinal Chemistry Department, University of Kansas, Lawrence, KS; **1985:** Science Faculty, University of Papua New Guinea; Biochemistry Department, University of Melbourne, Parkville Australia

TEACHING ACTIVITIES

TEACHING IN UNDERGRADUATE/GRADUATE PROGRAMS

Department of Chemistry & Chemical Biology, IUPUI

Developed a new medicinal chemistry concentration at the undergraduate level. Approved courses are:

C488: The practice of medicinal chemistry

C489: Introduction to medicinal and agricultural chemistry

Currently teaching

C496 Special Topics: The practice of medicinal chemistry

C496 Special Topics: Introduction to medicinal and agricultural chemistry

Awards:

Obtained Student Technology Fund support (\$6200) to purchase “Molecular Conceptor”, a computer-aided instruction course for self-paced learning of the drug discovery process.

College of Pharmacy, University of Michigan

Taught the physiochemical properties and drug action, and drugs affecting the peripheral nervous system as components of MC410 “Principles of Medicinal Chemistry”.

Taught part of MC532, a course which takes a mechanistic organic chemistry/biochemistry approach to medicinal chemistry. My section of the course introduces the concept of enzymes as drug targets, and emphasizes the rational design of inhibitors of enzyme action.

Mentored students in Pharm.D. investigations projects.

Project Advisor for Brian DeSmet, 2002-2003 Merck Research Scholar Awardee.

Victorian College of Pharmacy, Monash University, Australia

Taught B.Pharm. courses in kinetics and thermodynamics; stereochemistry; spectroscopy; aromatic chemistry; reactions of pharmaceutical importance; receptor structure and function; chemistry of enzymes, enzyme inhibitors as drugs; anti-infective agents; steroids; peptides and proteins as drugs.

College of Pharmacy, University of Kansas

As a Visiting Professor, taught part of a medicinal chemistry course on neuroeffector agents.

SUPERVISION OF GRADUATE STUDENTS

Lockett, L.	M.Pharm.	1985	“Study of the metabolism of the psychomimetic indolealkylamines”
Szutu, M.	M.Pharm.	1988	“Pharmacokinetics and metabolism of clomiphene isomers”
Sheen, M.	M.Pharm.	1988	“Design, synthesis and testing of PABA synthase inhibitors”
Huang, J.L.	M.Pharm.	1990	“An HPLC assay for <i>Areca</i> alkaloids”
Najbar, L.V.	Ph.D.	1996	“Nucleation sites for the folding of T4 lysozyme”
Nguyen, K.	M.Pharm.	1997	“Pharmacokinetics of thiopentone isomers”(joint advisor with D.J. Morgan)
Campbell, M.	Ph.D.	1997	“PABA synthase: from putative intermediate to potential inhibitor”
Caine, J.M.	Ph.D.	1999	“Cloning, expression and characterization of human phenylethanolamine <i>n</i> -methyltransferase”
Lazoura, E.	Ph.D.	1999	“Hydrophobic stabilization of peptides to study protein folding” (joint advisor with M-I Aguilar)
Andrews, F.	Ph.D.	2008	Structure-function studies on benzoylformate decarboxylase

MEMBER OF THESIS COMMITTEE

Thomas, C.E.	Ph.D.	2004	“A comparison of the active sites of eukaryotic and bacterial tRNA-guanine transglycosylases” (University of Michigan)
Chakraborty, S.	Ph.D.	2006	“Characterization of enzyme-bound intermediates on thiamin diphosphate-dependent enzymes” (Rutgers University)
Saehuan, C.	Ph.D.	2007	“Characterization of a benzoylformate decarboxylase and a NAD ⁺ /NADP ⁺ -dependent benzaldehyde dehydrogenase from <i>Pseudomonas stutzeri</i> ST-201” (Mahidol University, Thailand)
Zahniser, M.P.D.	Ph.D.	2010	“On the structure of benzaldehyde dehydrogenase from <i>Pseudomonas putida</i> ” (Brandeis University)

SUPERVISION OF VISITING STUDENTS

Iding, H.	1997	Institut für Enzymtechnologie, Jülich, Germany	UCSF
Siegert, P.	2000	Institut für Enzymtechnologie, Jülich, Germany	Michigan
Shivraj, P.	2005	Austin College, Sherman, Texas	Michigan
Saehuan, C.	2006-7	Mahidol University, Thailand	Michigan
Drinkwater, N.	2008	University of Queensland, Australia	IUPUI

SUPERVISION OF POSTDOCTORAL RESEARCH FELLOWS

Potter, J.J.	1986-1988	VCP/Monash University
Mortimer, K.	1986-1988	VCP/Monash University
Kneen, M.M.	1998-2010	University of Michigan, IUPUI
Wang, P.F.	1999-2008	University of Michigan
Alzeer, J.	1999-2000	University of Michigan
Zhang, L.	1999-2001	University of Michigan
Andricopulo, A	1999-2002	University of Michigan
Zha, C.	2000-2001	University of Michigan
Gopalakrishna, G.	2000-2002	University of Michigan
Krogh, R.	2001-2002	University of Michigan
Davioud-Charvet, E.	2001-2002	University of Michigan
Wu, Q.	2002-2006	University of Michigan
Anisimov, R.	2005-2006	University of Michigan
Yeung, C.	2005-2007	University of Michigan
Yep, A.	2005-2008	University of Michigan
Chakraborty, S.	2008	University of Michigan, IUPUI
Stan, R.	2010-	IUPUI
Waghmare, J.	2010-	IUPUI
Prasad, S.	2010-	IUPUI

1/10/2011

ROBERT EARL MINTO

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402 N. Blackford St., Rm. 326G
Indiana University-Purdue University Indianapolis
Indianapolis, IN 46202-3274

(317) 274-6869 (office)
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CITIZENSHIP: Canadian, U.S. Permanent Resident

EDUCATION AND TRAINING

*Associate Professor, Indiana University
Purdue University - Indianapolis (IUPUI)*

Dept. of Chemistry and Chemical Biology (2005-present)
Director of Graduate Admissions (2006-present)
(2008-present)

*Director, IUPUI Signature Center for Membrane
Biosciences*

*Assistant Professor,
Miami University, Oxford, OH*

Dept. of Chemistry and Biochemistry (1997-2005)

*Postdoctoral Fellow,
The Johns Hopkins University, Baltimore, MD*

Dept. of Chemistry (1994-97)

University of California, Berkeley, CA

Ph.D. in Chemistry (Organic) (1989-94), GPA 3.92

University of Waterloo, Waterloo, Ontario, Canada

Co-op Honours B.Sc. in Applied Chemistry, Degree-by-
Thesis Option (1984-89), GPA 3.9

HONORS AND AWARDS

AC Pratt (RE Minto research supervisor), 2010 Chancellor's Award for Undergraduate Research

Highlighted in *J. Proteome Res. (J. Am. Chem. Soc., 2004, 126, 9504-9505)*

Outstanding Professor Nominee, Miami University Student Foundation (2003)

Full Member, Sigma Xi (2003-)

NSERC 1967 Postgraduate Scholarship (1989-93)

Regents' Scholarship, University of California, Berkeley (1989-90)

Valedictorian, Faculty of Science, University of Waterloo (1989)

NSERC (Canada) Industrial Student Research Award, Polysar Limited (1987); Merck Frosst Canada (1988)

RESEARCH AND WORK EXPERIENCE

Independent Research Career: IUPUI, Indianapolis, IN (2005-present) and Miami University, Oxford, OH (1997-2005)

- Studying the biosynthesis of polyacetylenic natural products in plants and fungi using biochemical and molecular biological techniques; isolation and synthesis of polyacetylenic natural products from plants and fungi
- Isolated desaturases from fungi; synthesized and performed biophysical studies on transmembrane domains from plant diverged microsomal desaturases and other membrane-bound proteins
- Synthesized radiolabeled and stable-isotope probes for fatty acid and tannin metabolic studies
- Mentor for 2 post-doctoral, 4 M.S., 2 Ph.D. and 2-5 undergraduate students; active in several collaborations

Postdoctoral Research: Dept. of Chemistry, The Johns Hopkins Univ., with Professor Craig A. Townsend. (1994-97)

- Investigated the aflatoxin B₁ pathway using biochemical and molecular biological techniques, including DNA cloning, sequencing, native enzyme isolation, and genetic transformations in *Aspergillus*.

Doctoral Research: Dept. of Chemistry, Univ. of California, Berkeley, CA with Prof. Robert G. Bergman. (1989-94)

- Synthesized macrocyclic enediyne analogs of the calicheamicin aglycon and studied the physical organic chemistry of 1,4-didehydrobenzene formation.

Undergraduate Research: Dept. of Chemistry, Univ. of Waterloo, Waterloo, Ontario, Canada. (1984-89)

- Examined the mechanism for addition of organopentafluorosilicates to α,β -unsaturated carbonyl systems and other electrophiles over two academic years with Professors Arthur J. Carty and John F. Honek.

Merck Frosst Canada, Kirkland, Quebec, Canada (1988)

Radiation Research Laboratories, University of Notre Dame, South Bend, IN (1988)

Polysar Corporation, Elastomer Research Division, Sarnia, Ontario, Canada (1987)

TEACHING/SUPERVISORY EXPERIENCE (details below)***Indiana University Purdue University – Indianapolis, Indianapolis, IN, (2005–present)***

Lecturing experience for undergraduate organic chemistry lecture and graduate-level organic spectroscopy courses
 Supervised the research of 2 postdoctoral, 2 Ph.D. and 2 M.S graduate, and 12 B.S./B.A. undergraduate students.
 Thesis reader for M.S. and Ph.D. committees. Director for Graduate Admissions (2006-present).

Miami University, Oxford, OH (1997–2005)

Extensive lecturing experience for undergraduate organic chemistry lecture and lab courses, biochemistry lab, graduate/senior undergraduate level organic spectroscopy and graduate courses in "Organic Principles and Theory", "Secondary Metabolism" and "Organometallic Chemistry". Organized organic and biological chemistry graduate seminar courses. Supervised the research of 6 M.S/Ph.D. graduate and 17 B.S./B.A. undergraduate students. Thesis reader for numerous M.S. and Ph.D. committees.

The Johns Hopkins University, Baltimore, MD (1996)

Lecturer for a segment of an introductory organic chemistry course.

University of California, Berkeley, CA (1989–91)

Teaching assistant for undergraduate general and introductory organic chemistry.

University of Waterloo, Waterloo, Ontario, Canada (1987–88)

Teaching assistant for an analytical chemistry course and senior organic chemistry and biochemistry laboratories.

PEER-REVIEWED PUBLICATIONS

20 in peer-reviewed journals plus >5 published abstracts (see attached list)
 (4 additional manuscripts in preparation)

BOOK SECTIONS

1 chapter in Comprehensive Natural Products Chemistry (see attached list)

PATENTS

Nicolau, K.C.; Sorensen, E.; Hwang, C.-K.; Discordia, R.; Bergman, R.G.; Minto, R.E. "Ten-membered ring enediyne diols and enediyne diones having DNA cleaving properties", *U. S. Patent*, 5,183,942 (1993).
 Nicolau, K.C.; Sorensen, E.; Hwang, C.-K.; Discordia, R.; Bergman, R.G.; Minto, R.E. Open chain enediyne dihydroperoxides having DNA cleaving properties. *U.S. Patent*, 5,288,761 (1994).

CONFERENCE PRESENTATIONS

47 posters and oral presentations (see attached list)

FUNDED EXTERNAL GRANTS

1. "Collaborative Research: Biosynthesis of Alkamides – Experimental Modeling of a Modular Secondary Metabolic Pathway", National Science Foundation – MCB 0919938, Minto (PI); B Nicolau, Iowa State Univ. (Co-PI) (08/01/09-07/31/12), \$655,912 (IUPUI).
2. "MRI: Acquisition of a High Resolution LC-MS/MS System", National Science Foundation – DBI 0821661, Minto (PI) (08/01/08-07/31/11), \$479,500.
3. "Anti-Atherosclerotic Effect of Ganodermanotriol", Methodist Research Institute, Minto (co-investigator); D Sliva, PI; Postdoctoral Fellow, SJ P'Pool (07/01/07-06/31/08), \$48,500.
4. "Acquisition of a 500 MHz NMR Spectrometer", National Science Foundation – CHE 0619254, Minto (co-PI) (08/01/06-07/31/09), \$516,500.
5. "Desaturases and Acetylenases from Basidiomycete Fungi", NIH 7 R15 GM06493-02, Minto (PI) (08/04-07/08), \$213,000.
6. "Ohio NMR Consortium, Phase II" OBoR/Hayes Investment Fund, Minto (co-PI) (08/02-07/04), \$480,000.
7. "Probes for Desaturase Enzymes Involved in Antitumor Agent Production", American Cancer Society, Ohio Division, Minto (PI) (07/01-12/03), \$19,100.
8. "Acquisition of a 400 MHz Solid-State NMR Spectrometer", National Science Foundation, Major Research Instrumentation – CHE 0116333, Chemistry, Minto (co-PI) (02/01), \$705,479.

9. "Fungal Fatty Acid Desaturating Enzymes for Oil Seed Modification", Ohio Plant Biotechnology Consortium, Minto (PI) (06/00-05/02), \$10,000.
10. "Fungal Fatty Acid Desaturating Enzymes for Oil Seed Modification", Ohio Plant Biotechnology Consortium, Minto (PI), (06/00-05/01), \$2,009.
11. "Circular Dichroism Spectrometer for Protein/Peptide Structure/Function Studies" NSF, Instrumentation & Instrument Development/Multi-User Instrumentation - DBI 0070169, Minto (co-PI), (06/00-05/01), \$51,415.
12. "A proposal to Establish a State-of-the-Art Ohio Mass Spectrometry Consortium", Hayes Investment Fund. Minto (Co-PI) (01/98), \$218,000.

FUNDED MAJOR INTERNAL GRANTS

1. "Acquisition of Mass Spec Instrumentation Upgrades for the Mass Spectrometry Facility Housed in the Department of Chemistry and Chemical Biology (CCB)", IUPUI, Minto (PI) (09-10), \$96,795.
2. "IUPUI Signature Center for Membrane Biosciences", Office of the Vice Chancellor for Research, IUPUI, Minto (PI) (02/01/08-01/31/11), \$300,000.

PROFESSIONAL AND DEPARTMENTAL SERVICE

Manuscript reviewer for *Afr. J. Plant Sci.*, *Appl. Environ. Microbiol.*, *Appl. Microbiol. Biotech.*, *Chem. Phys. Lipids*, *Int. J. Plant Biol.*, *J. Exp. Biol.*, *J. Food Agric. Chem.*, *J. Lab. Comp. Radiopharm.*, *J. Phytopath.*, *Synthesis*, *Tetrahedron Lett.*

Ad hoc reviewer for National Science Foundation, Research Corporation, Petroleum Research Fund, Baker Fund (Ohio Univ. 04). Ad hoc reviewer (08-present) and review panelist, Research Support Funds Grants, IUPUI (06,10)

Provided expert opinion for 2 patent applications (08-09)

Faculty Advisor for Student Affiliate of the Center for Membrane Biosciences (09-present)

Executive Committee (05-07); Graduate Recruiting Committee (member 05-06; chair, 06-present)

Chair, Honors and Awards Committee (00-04); Member (98-05)

Member of Library Committee (97-04) and Equipment Committee (97-99)

Faculty Advisor for Gamma Theta Phi Chemistry Honorary (99-02)

PROFESSIONAL MEMBERSHIP

American Chemical Society and Canadian Society for Chemistry (Biological and Organic Chem. Sections, continuing)

American Society for Microbiology

Indiana Academy of Sciences

PEER-REVIEWED RESEARCH PUBLICATIONS

(undergraduate marked by †, corresponding author marked by asterisk)

1. BJ Blacklock, BE Scheffler, MR Shepard, N Jayasuriya[†], **RE Minto^{*}** "Functional diversity in fungal fatty acid synthesis. The first acetylenase from the Pacific golden chanterelle, *Cantharellus formosus*", *J. Biol. Chem.* **2010**, *285*(37), 28442-28449. published online 7/6/2010.
2. **Minto, R.E.^{*}**; Blacklock, B.J.; Younus, H.; Pratt, A.†. "Atypical biosynthetic properties of a delta-12/v+3 desaturase from the model Basidiomycete, *Phanerochaete chrysosporium*", *Appl. Environ. Microbiol.* **2009**, *75*, 1156-1164. (published ahead of print Dec. 2008)
3. **Minto, R.E.^{*}**, Blacklock, B.J. "Biosynthesis and Function of Polyacetylenes and Allied Natural Products", *Prog. Lipid Res.*, **2008**, *47*, 233-306. DOI 10.1016/j.plipres.2008.02.002.
4. Ramamoorthy, V., Cahoon, E.B., Li, J., Thokala, M., **Minto, R.E.**, Shah, D.M.* "Glucosylceramide synthase is essential for alfalfa defensin-mediated growth inhibition but not for pathogenicity of *Fusarium graminearum*", *Mol. Microbiol.* **2007**, *66*, 771-786.
5. Cai, K., Hagerman, A.E., **Minto, R.E.**, Bennick, A.* "Decreased polyphenol transport across cultured intestinal cells by a salivary proline-rich protein", *Biochem. Pharmacol.*, **2006**, *71*, 1570-1580.
6. Karp, E.S., Gibbons, W.J., Jr., Cellar, N.†, **Minto, R.E.**, Lorigan, G.A.* "Solid-state NMR Studies of a Diverged Microsomal Amino-Proximate Δ^{12} Desaturase Peptide Reveal Causes of Stability in Bilayer: Tyrosine Anchoring and Arginine Snorkeling", *Biophys. J.*, **2006**, *90*, 1249-1259 (Biophys. J. BioFAST: December 2, 2005. doi:10.1529/biophysj.105.067884).

7. Minto, R.E.; Adhikari, P.R. and Lorigan, G.A.* "A ^2H Solid-state NMR Spectroscopic Investigation of Biomimetic Bicelles Containing Cholesterol and Polyunsaturated Phosphatidylcholine", *Chem. Phys. Lipids*, **2004**, *132*, 55-64.
8. Lorigan, G.A.*; Dave, P.C.; Tiburu, E.K.; Damodaran, K.; Abu-Baker, S.; Karp, E.S.†; Gibbons, W.J. and Minto, R.E. "Solid-State NMR Spectroscopic Studies of an Integral Membrane Protein Inserted into Aligned Phospholipid Bilayer Nanotube Arrays", *J. Am. Chem. Soc.*, **2004**, *126*, 9504-9505.
9. Hancock, M.T.; Minto, R.E.* and Pinhas, A.R.* "The Conversion of an Aziridine Plus a Phenyl-substituted Amine Oxide or Aminoether to a Benzodiazepine Derivative", *Tetrahedron Lett.*, **2003**, *44*, 8357-8360.
10. Tiburu, E.K.; Dave, P.C.; Vanlerberghe, J.F.†; Cardon, T.B.; Minto, R.E. and Lorigan, G.A.* "An Improved Synthetic and Purification Procedure for the Hydrophobic Segment of the Transmembrane Peptide Phospholamban", *Anal. Biochem.* **2003**, *318*, 146-151.
11. Cahoon, E.B.; Schnurr, J.; Huffman, E.A. and Minto, R.E.* "Fungal Responsive Fatty Acid Acetylenases Occur Widely in Evolutionarily Distant Plant Families", *Plant J.*, **2003**, *34*, 671-83.
12. Chen, Y.; Hagerman, A.E. and Minto, R.E.* "Preparation of 1,2,3,4,6-Penta-O-Galloyl-[U- ^{14}C]Glucopyranose" *J. Lab. Comp. Radiopharm.*, **2003**, *46*, 99-105.
13. Minto, R.E.*; Gibbons, W.J., Jr.; Cardon, T.B. and Lorigan, G.A. "Synthesis and conformational studies of a transmembrane domain from a diverged microsomal Δ^{12} -desaturase", *Anal Biochem.*, **2002**, *308*, 134-140.
14. Zhu, L. and Minto, R.E.* "Improved Syntheses of Methyl (14E)- and (14Z)-Dehydrocrepenynate: Key Intermediates In Plant and Fungal Polyacetylene Biosynthesis", *Tetrahedron Lett.*, **2001**, *42*, 3803-3805.
15. Lorigan, G.A.*; Minto, R.E. and Zhang, W. "Teaching the Fundamentals of Pulsed NMR Spectroscopy in an Undergraduate Physical Chemistry Laboratory", *J. Chem. Ed.*, **2001**, *78*, 956-958.
16. Minto, R.E. and Townsend, C.A.* "Enzymology and Molecular Biology of Aflatoxin Biosynthesis", *Chem. Rev.*, **1997**, *97*, 2537-2556.
17. Silva, J.C.; Minto, R.E.; Barry, C.E. III; Holland, K.A. and Townsend, C.A.* "Isolation and characterization of the versicolorin B synthase gene from *Aspergillus parasiticus*: Evidence for partial gene clustering of the aflatoxin B₁ biosynthetic genes", *J. Biol. Chem.*, **1996**, *271*, 13600-13608.
18. Nicolau, K.C.; Sorensen, E.J.; Discordia, R.; Hwang, C.-K.; Minto, R.E.; Bharucha, K.N. and Bergman, R.G.* "Ten-membered ring enediynes with remarkable chemical and biological profiles", *Angew. Chem. Int. Ed. Engl.* **1992**, *31*, 1044-1046.
19. Bharucha, K.N.; Marsh, R.M.; Minto, R.E. and Bergman, R.G.* "Double cycloaromatization of (Z,Z)-deca-3,7-diene-1,5,9-triyn: Evidence for the intermediacy and diradical character of 2,6-didehydronaphthalene", *J. Am. Chem. Soc.* **1992**, *114*, 3120-3122.
20. Minto, R.E.† and Das, P.K.* "Laser flash photolysis study of photodehydroxylation phenomena of 9-phenylxanthen-9-ol and photobehavior of related intermediates. Enhanced electrophilicity of 9-phenylxanthenium cation singlet", *J. Am. Chem. Soc.* **1989**, *111*, 8858-8872.
21. Minto, R.E.†; Samanta, A. and Das, P.K.* "Time-resolved nanosecond and picosecond absorption studies of excited-state properties of 1-thiobenzoylnaphthalene", *Can. J. Chem.* **1989**, *67*, 967-972.

OTHER MANUSCRIPTS

1. EM Kennedy, SJ P'Pool, D Sliva, RE Minto* "Total synthesis of the *Ganoderma* triterpene ganodermanontriol and its stereoisomeric triols", *J. Nat. Prod.* **2010** submitted 1/2011).
2. Zhu, L.; Grande, R.D.; Merves, M.E. and Minto, R.E.* "Synthesis of Regioselectively Deuterated Linoleic Acids", **2010** (in preparation for *Org. Lett.*).
3. Shepard, M. R.; Furr, N.; Minto, R. E.* "Multiple Enantioselective Routes to Falcarindiol", **2010** (in preparation for *Tetrahedron Lett.*).

4. Younus, H.; Pratt, A.; Jenkins, J.; Minto, R. E.* "Revealing the catalytic potential of *Phanerochaete chrysosporium* desaturase: characterization of mutants and the identification of key functional residues", 2010 (in preparation for *J. Biol. Chem.*)

BOOK CHAPTERS

1. Townsend, C.A. and Minto, R.E. "Biosynthesis of Aflatoxins", in "Comprehensive Natural Products Chemistry", eds. Barton, D. H. R., Nakanishi, K. and Meth-Cohn, O., Vol. 1., Ch. 17, Pergamon, Oxford, 1999; p. 443-471.

CONFERENCE PRESENTATIONS/INVITED TALKS

(presenter underscored, undergraduate/high school authors marked by asterisk)

1. "Functional Diversity within the Delta 12-Desaturases of Basidiomycetes", R.E. Minto, H. Younus, A.C. Pratt*, B.J. Blacklock, M.R. Shepard, G.A. Birch, and J. Jenkins*. Plant Lipid Biomaterials Symposium, International Symposium on Plant Lipids 2010, Cairns, Australia, (07/12/10) - Selected Oral.
2. "Modulation of Temozolomide-Mediated DNA Damage in Glioblastoma Multiforme by the HDM2 antagonist, Nutlin3", H. Wang, S. Cai, B.J. Bailey, A.L. Sinn, J.M. Silver, R.E. Minto, T.M. Georgiadis, E.C. Long, J.N. Sarkaria, L.D. Mayo, and K.E. Pollok, American Association for Cancer Research 101st Annual Meeting 2010, Washington, DC, (04/17-04/21/10).
3. "Development of a Constraint-Based Method for Membrane Protein Structure Determination", Undergraduate Research Conference, A.C. Pratt* and R.E. Minto, 24th National Conference on Undergraduate Research, Missoula, MT, (04/15-04/17/2010) - Selected Poster.
4. "Lipid Natural Products: Diversity through Small Changes", R.E. Minto, Andrews University, Department of Chemistry, Berrien Springs, MI (01/21/2010)- Invited Talk.
5. "The Grease You Eat: Mass Spectrometric Analysis of the Lipid Content in Food", S.T. Maitland*, M.R. Shepard, R.E. Minto, Indiana CTSI Scientific Poster Session, Indianapolis, IN (09/16/2009) - Poster, 1st prize in high school poster category.
6. "Cloning and Functional Characterization of *Dictyostelium discoideum* Fatty Acid Elongase Genes", B.J. Blacklock, S. Frazier, S. Hernandez-Buquer, A. Grotenhuis, R.E. Minto, G. Birch, Dicty 2009 International Dictyostelium Conference, Estes Park, CO (08/23-08/28/2009) - Poster.
7. "A Comparison of Approaches to the Synthesis of Falcariindiol", M.R. Shepard, Jr., N.A. Furr, R.E. Minto. National Meeting of the American Chemical Society, Washington, DC (08/19/2009) - Poster.
8. "Preparation and Characterization of Reversibly Photochromic Polydiacetylenes", N.A. Furr, R.E. Minto, M. Akers*, National Meeting of the American Chemical Society, Washington, DC (08/16/2009) - Poster.
9. "Synthesis of Ganoderma Lanostane Terpenoids with $\Delta 7,9(11)$ Cores", E.M. Kennedy, S.J. P'Pool, D. Sliva, R.E. Minto, National Meeting of the American Chemical Society, Washington, DC (08/17-08/19/2009)- Poster, additionally selected for Sci-mix session.
10. "Functional Diversity In The Enzymes Of Fungal Fatty Acid Biosynthesis", H. Younus, A.C. Pratt*, B.J. Blacklock, R.E. Minto, National Meeting of the American Chemical Society, Washington, DC (August 19, 2009) - Poster.
11. "Development of a Constraint-Based Method for Membrane Protein Structure Determination", Undergraduate Research Conference, A.C. Pratt* and R.E. Minto, Summer Undergraduate Research Poster Session, IUPUI, Indianapolis, IN (07/22/2009) -Poster.
12. "The Grease You Eat: Mass Spectrometric Analysis of the Lipid Content in Food", S.T. Maitland*, M.R. Shepard, Jr., R.E. Minto, 2009 Project SEED Poster Session, Indianapolis, IN (07/20/2009) - Poster.
13. "Lipid Natural Products: Diversity through Small Changes", R.E. Minto, Purdue University, Department of Biochemistry, West Lafayette, IN (11/19/2009) - Invited Talk.
14. "The Activity of 46 Mutants of the $\Delta 12$ Desaturase from the Fungus *Phanerochaete chrysosporium*", H. Younus, A.C. Pratt*, J. Jenkins* and R.E. Minto, Department of Chemistry and Chemical Biology Poster Presentations, IUPUI (12/03/2008) - Poster. Awarded 1st prize in the student competition.
15. "Cloning Acetylenic Fatty Acid Biosynthesis Genes from a Basidiomycete", B.J. Blacklock, B.E. Scheffer, R.E. Minto, 2008 Banff Conference on Plant Metabolism, 2008, Banff, Alberta, Canada (07/20/2008-08/03/2008) - Poster.

16. "Cloning and Expression of Acetylenic Fatty Acid Biosynthesis Genes from a Basidiomycete", B.J. Blacklock, B.E. Scheffer and R.E. Minto, Gordon Research Conference: Enzymes, Coenzymes, and Metabolic Pathways, 2008, University of New England, Maine, USA (07/13/2008-07/18/2008) - Poster.
17. "Identification of Novel Lipids from a Desaturase Mutant", J. Jenkins, H. Younus, A.C. Pratt* and R.E. Minto, 2008 Committee on Institutional Cooperation (CIC) Summer Research Opportunities Program 22nd Annual Conference held at Michigan State University, East Lansing, MI (07/16/2008-07/18/2008) - Poster.
18. "A Comparison of Approaches to the Synthesis of Falcariindiol", M.R. Shepard, N.A. Furr and R.E. Minto, 39th Central Regional Meeting of the American Chemical Society, Columbus, OH (June 10-14, 2008) - Poster.
19. "Preparation and Characterization of Reversibly Photochromic Polydiacetylenes", N.A. Furr, R.E. Minto, M. Akers*, 39th Central Regional Meeting of the American Chemical Society, Columbus, OH (June 10-14, 2008) - Poster.
20. "Isotopic Labeling of Acetylenic Fatty Acids", K. R. Gordon and R. E. Minto*, 7th Annual Kentuckiana Undergraduate Research Symposium, Louisville, KY (3/31/2007) - Poster.
21. "Isotopic Labeling of Acetylenic Fatty Acids for Mechanistic Studies of Desaturases", K. R. Gordon and R. E. Minto*, 8th Annual Indiana Local ACS Poster Section, Indianapolis, IN (10/11/2007) - Poster.
22. "Acetylenic Fatty Acid Biosynthesis - Cloning and Expression of the First Genes from a Basidiomycete", R.E. Minto, B.J. Blacklock, B.E. Scheffler and N.N. Jayasuriya, 7th Annual Indiana Section American Chemical Society Poster Session (10/10/06) - Poster.
23. "Cloning and Expression of Acetylenic Fatty Acid Biosynthesis Genes from a Basidiomycete", B.J. Blacklock, B.E. Scheffler, and R.E. Minto, International Symposium on Plant Lipids (07/16-07/21/06) - Selected oral presentation.
24. "Acetylenic Fatty Acid Biosynthesis - Cloning and Expression of the First Genes from a Basidiomycete", R.E. Minto, B.J. Blacklock, B.E. Scheffler and N.N. Jayasuriya, 232nd National Meeting of the American Chemical Society (9/10-09/14/06) - Poster.
25. "Fungal Responsive Fatty Acid Acetylenases Occur Widely in Evolutionarily Distant Plant Families", E.B. Cahoon; J.A. Schnurr; E.A. Huffman and R.E. Minto, Plant Biology 2003: Meeting of the American Society of Plant Biologists, Honolulu, HI (07/25/03-07/30/03) - Poster.
26. "Isolation of a FAD2 Desaturase Homolog from a Basidiomycete", R.E. Minto, 2003 Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, Fallen Leaf Lake, CA (06/04/03-06/08/03) - Poster.
27. "Fungal Responsive Fatty Acid Acetylenases Occur Widely in Evolutionarily Distant Plant Families", R.E. Minto; J.A. Schnurr; E.A. Huffman and E.B. Cahoon, 2003 Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, Fallen Leaf Lake, CA (06/04/03-06/08/03) - Poster.
28. "Progress toward the Synthesis of *Fistulina hepatica* Natural Products", D.M. Schwoppe; G.V. Givan and R.E. Minto, 2003 National Meeting of the American Chemical Society, New Orleans, LA (3/23/03-3/28/03) - Poster.
29. "Dimethyl Disulfide Addition to 1,4-Enynes: A New Route to 2,5-Dialkylthiophenes", G.V. Givan; L. Zhu, R.A. Taylor and R.E. Minto, 2003 National Meeting of the American Chemical Society, New Orleans, LA (3/23/03-3/28/03) - Poster.
30. "Preparation and NMR Spectroscopic Characterization of Polyunsaturated Lipid Bilayer Discs", M.B. Mikolaj; P.R. Adhikari; R.E. Minto and G.A. Lorigan, 2003 National Meeting of the American Chemical Society, New Orleans, LA (3/23/03-3/28/03) - Poster
31. "Synthesis of Regioselectively Deuterated Linoleic Acids", L. Zhu and R.E. Minto 2003 National Meeting of the American Chemical Society, New Orleans, LA (3/23/03-3/28/03) - Oral Presentation.
32. "Dimethyl Disulfide Addition To 1,4-Enynes: A New Route To 2,5-Dialkylthiophenes", G.V. Givan; L. Zhu and R.E. Minto, 1st Annual Ohio Valley Organic Chemistry Symposium, Oxford, OH (12/13/02-12/14/02) - Poster.
33. "New Chemical Methods For Studying Polymeric Polyphenolics (Tannins)", A.E. Hagerman; L. Niemeyer; R. Forkner; Y. Chen; R.E. Minto and G. Ansong, 19th Annual Meeting of the International Society for Chemical Ecology, Hamburg, Germany, (08/02) - Poster.
34. "Overexpression, Purification And Cleavage Of Ubiquitin-Tagged Hydrophobic Proteins", B.M. Hardesty, J. Esposito, K. Peterson, A. Schloemer and R.E. Minto, 34th Central Regional Meeting of the American Chemical Society, Ypsilanti, MI (6/26/02-6/29/02) - Poster.

35. "Conformational And Dynamic Studies Of The Amino-Proximate Transmembrane Peptide From CREP-1, A Diverged Microsomal Delta-12 Desaturase", W.J. Gibbons Jr., R.E. Minto, N. Cellar and G.A. Lorigan, 34th Central Regional Meeting of the American Chemical Society, Ypsilanti, MI (6/26/02-6/29/02) - Poster.
36. "Dimethyl Disulfide Addition To 1,4-Enynes: A New Route To 2,5-Dialkylthiophenes", G.V. Givan, L. Zhu and R.E. Minto, 34th Central Regional Meeting of the American Chemical Society, Ypsilanti, MI (6/26/02-6/29/02) - Poster.
37. "Preparation and Secondary Structure Characterization of the Crepis Acetylenase Transmembrane Domain B", P. Adhikari, G.A. Lorigan and R.E. Minto, 34th Central Regional Meeting of the American Chemical Society, Ypsilanti, MI (6/26/02-6/29/02) - Poster.
38. "Expression and Structural Studies of Transmembrane Domains of a Diverged *FAD2* Desaturase", R.E. Minto, W.J. Gibbons, Jr., B.M. Hardesty, A.E. Schoemer, J.P. Esposito and G.A. Lorigan, 2001 Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, South Lake Tahoe, CA (6/6/01-6/10/01) - Oral presentation.
39. "Probing Polyacetylene Biosynthesis in Basidiomycete Fungi", R.E. Minto, L. Zhu and E. A. Huffman, 33rd Great Lakes/Central Regional American Chemical Society Meeting, Grand Rapids, MI (6/11/01-6/13/01) - Oral presentation.
40. "NMR Spectroscopic Studies of the Membrane-Bound Protein CREP-1", G.A. Lorigan, W.J. Gibbons, Jr. and R.E. Minto, Cincinnati Meeting of the American Chemical Society, Covington, KY (5/16/00-5/18/00) - Poster.
41. "Isolation and Characterization of Secondary Metabolites from *Fistulina hepatica*", E.A. Huffman and R.E. Minto, Cincinnati Meeting of the American Chemical Society, Covington KY (5/16/00-5/18/00) - Poster.
42. "Plant and Fungal Alkyne Biosynthesis", R.E. Minto, E.A. Huffman and L. Zhu, Cincinnati Meeting of the American Chemical Society, Covington, KY (5/16/00-5/18/00) - Oral presentation.
43. "Syntheses of Methyl 14-(*E*)- and 14-(*Z*)-Dehydrocrepenynate", L. Zhu and R.E. Minto, Cincinnati Meeting of the American Chemical Society Covington, KY, (5/16/00-5/18/00) - Poster.
44. "Acetylene Biosynthesis in *Fistulina hepatica*", R.E. Minto, E. Huffman, R.D. Grande, M. Gunn, J.P. Fritz and L. Zhu, 1999 Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, South Lake Tahoe, CA (5/31/99-6/4/99) - Poster.
45. "Studies toward the Mechanism of Alkyne Biosynthesis", R.E. Minto, J.P. Fritz, M.E. Gunn and C. Venkataramani, 81st Canadian Society for Chemistry Conference, Whistler, BC, Canada (5/31/99-6/4/99) - Poster.
46. "Cures and Toxins: Approaches to Fungal Secondary Metabolism", R.E. Minto, 9th Annual Student Research Conference, Western Illinois University, Macomb, IL (4/3/98-4/4/98) - Oral presentation.
47. "10-Membered Ring Ene-dienes: Synthesis and Reactivity of Novel Ring Conformations" R.E. Minto, with R.G. Bergman, Chemical Institute of Canada Meeting, Edmonton, Alberta, Canada (5/31/92- 6/4/92) - Oral presentation.
48. "10-Membered Ring Ene-dienes: Synthesis and Reactivity of Novel Ring Conformations" R.E. Minto, with R.G. Bergman, American Chemical Society Meeting, San Francisco, CA (4/5/92-4/10/92) - Oral presentation.
49. "Mechanistic Studies on the Interaction of Alkylpentafluorosilicates with Various Acceptors" R.E. Minto, with J.F. Honek, Chemical Institute of Canada/3rd Chemical Congress of North America, Toronto, Ontario, Canada (8/88) - Poster.

CONFERENCE ORGANIZATION

- "Membrane Biosciences in Pathogenesis Symposium", Center for Membrane Biosciences, IUPUI (11/06/2009).
 "Bio-organic Chemistry Symposium", Cincinnati Meeting of the American Chemical Society, (05/2000).

TEACHING ASSIGNMENTS

IUPUI

- CHEM C341 - Organic Chemistry (3 credits) Fall 05, 84 students; Fall 07, 115; Spring 08, 100; Fall 08, 138; Fall 09, 121; Spring 10, 121
- CHEM 696 - Analytical Spectroscopy (3 credits) Spring 06, 22 students
- CHEM 696 - Organic Spectroscopy (3 credits) Spring 07, 4 students; Spring 09, 19

Miami University

- CHM 251 - Organic Chemistry for Chemistry Majors (3 credits)
- CHM 241/242 - Organic Chemistry (3 credits + 3 credits)
- CHM 231 - Fundamentals of Organic Chemistry (4 credits)
- CHM 245 - Organic Chemistry Laboratory
- CHM 438 - Biochemistry Laboratory
- CHM 426/526 - Spectroscopic Identification of Structure
- CHM 641 - Organic Principles and Theory
- CHM 740.H - Secondary Metabolism
- CHM 740.O - Organometallic Chemistry
- CHM 720 - Graduate Seminar in Organic and Biochemistry
- CHM 725 - Graduate Seminar in Biological Chemistry

CURRICULUM VITAE

NAME

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EDUCATION

PhD	1978	University of Virginia Charlottesville, Virginia Biophysics (Physics)
BS	1972	Louisiana State University New Orleans, Louisiana Cum Laude in Physics

EXPERIENCE

1989-Present	Associate Professor of Chemistry
1985-1989	Assistant Professor of Chemistry Department of Chemistry Indiana University–Purdue University Indianapolis Indianapolis, Indiana 46202-3274
1982-1985	Research Assistant Professor of Medicine and Biochemistry Department of Medicine University of Texas Health Science Center at San Antonio San Antonio, Texas 78284
1978-1981	Postdoctoral Fellow Department of Biochemistry University of Texas Health Science Center at San Antonio San Antonio, Texas 78284
1972-1978	Teaching and Research Assistantships Department of Physics University of Virginia Charlottesville, Virginia 22901

1968-1972 Computer Operator, Programmer and Lab Instructor
Computer Research Center
Louisiana State University
New Orleans, Louisiana 70122

AWARDS, HONORS, AND SPECIAL TRAINING AND CONFERENCES

Phi Beta Kappa, Sigma Pi Sigma, Phi Eta Sigma, awarded scholarship at Louisiana State University, fellowship at the University of Virginia, and support to attend physiology course at Woods Hole, Massachusetts (1975). Received support to attend Synchrotron Radiation in Biology Series at the Institute for Structural and Functional Studies, Philadelphia, Pennsylvania (1985), as well as for several trips to Stanford Synchrotron Radiation Laboratory and AT&T Laboratories to acquire and analyze EXAFS data. Also received support to attend symposium "Nitric Oxide in Health and Disease" at Rutgers, New Jersey (1993). Attended "Metals in Biology" Gordon Research Conferences (early 1980s) and the "Origin of Life" Gordon Conference (2006).

PROFESSIONAL SOCIETIES

Biophysical Society
American Chemical Society
American Society of Biochemistry and Molecular Biology

COURSE PARTICIPATION AND CURRICULUM DESIGN

Taught computer science laboratories at Louisiana State University, New Orleans; physics recitation sessions for engineers at University of Virginia; magnetic resonance section of physical biochemistry at the University of Texas Health Science Center at San Antonio (graduate); and biophysical chemistry (graduate), biospectroscopy (graduate), physical chemistry (BS), physical chemistry with biochemical emphasis (BA), physical chemistry laboratory, freshman (general) chemistry, introductory (nonmajor) chemistry, chemistry recitation sessions, the two semester sequence of capstone in chemistry, and spectroscopy/fluorescence section of physical biochemistry (Department of Biochemistry, Medical School, graduate) at Indiana University-Purdue University at Indianapolis.

Introduced a graduate level biospectroscopy course covering both the theoretical and practical use of spectroscopy to probe the structure and function of biological systems. Upgraded the BA physical chemistry course integrating additional mathematics, physics and biochemistry. Developed an approach to nonmajor introductory chemistry by which current news articles were used to show students the tremendous importance of chemistry (science) to their lives, to motivate them to learn, and to teach them cost-benefit analysis. Supervised (with others) freshman chemistry course, recitations and laboratories (approximately 500 students/fall). Designed curriculum and assembled overall laboratory equipment requirements for a proposed Biochemistry and Molecular Biology program in Chemistry and Biology, which was later revisited and implemented. Also coordinated curricular review and modification through the Educational Policies Committee for the Department of Chemistry at Indiana University-Purdue University.

COMMITTEE MEMBERSHIP

Curriculum Committee (University), School of Science Steering Committee, SELB (new science and engineering building) Committee, Educational Policies Committee, Teaching and Learning Committee, Academic Support Task Force – Enrollment Management Group, NSF Mathematics Initiative: Mathematics and Undergraduate Education (Steering Committee and later Executive Committee), Council of Schools of Liberal Arts and Sciences, Associate Dean for Research Search (School of Science), Center for Earth and Environmental Affairs, Faculty Search (in Departments of Chemistry, Biology and Geology), General Chemistry, Graduate, Curriculum, Executive, Physical Chemistry, Biological Chemistry. Also was a member of the School of Science and University Research Committees and American Chemical Society Education Committee.

GRADUATE STUDENT AND POSTDOCTORAL PROPOSALS

Inspired authorship and submission of research proposals by students to Federal Agencies.

GRADUATE STUDENTS SUPERVISED

1. Steup, M. (MS, August 1988) Thesis title: Preparation and characterization of myoglobin reconstituted with selected hemes. Position at graduation: Research Associate, The University of Arizona, Department of Pharmacology and Toxicology, Tucson, Arizona.
2. Ponsler, D. (MS, December 1989) Thesis title: The effects of metals on Na^+/K^+ -ATPase activity and on the intrinsic fluorescence of biomembranes. Position at graduation: Research Associate, Department of Biochemical Toxicology, Eli Lilly and Company, Indianapolis, Indiana.
3. Carfagna, M. (PhD, August 1990) Thesis title: Relationship between drug-induced perturbations of Na^+/K^+ -ATPase activity and synaptic plasma membrane structure. Position at graduation: Postdoctoral Fellow, Chemical Industry Institute of Toxicology, Research Triangle Park, North Carolina.
4. Park, J. (MS, August 1991, co-chair) Thesis title: Studies of novel polymeric bioseparation methods. Position at graduation: Research Associate, DuPont, Wilmington, Delaware.
5. Mattison, K. (PhD, August, 1999, co-chair) Thesis title: Structure, mobility, and enzyme activity in protein-polyelectrolyte complexes.

GRADUATE STUDENT THESIS COMMITTEE MEMBER

Served as a committee member on approximately 30 MS and PhD committee starting in 1986 both within the Chemistry Department (in the areas of physical, biochemical, analytical, inorganic, and theoretical) and outside the department (pharmacology and biology).

RESEARCH INTERESTS AND EXPERIENCE

Molecular basis of neurodegenerative diseases such as Alzheimers, Parkinsons, etc: involvement of metal ions and protein conformational change in both the processes of aggregation and free radical damage leading to cell death.

Structure-function relationships in metalloproteins: heme and metal coordination, structural determinants of ligand/inhibitor binding and substrate catalysis, cooperativity, stability/denaturation, protein-protein and protein-polymer complexation and aggregation, and thermodynamics relating to these processes.

Interaction of drugs and small molecules with proteins and biomembranes: structure-activity relationships, determinants of drug/inhibitor binding, membrane surface versus interior perturbation, modulation of conformation and activity of enzymes, and drug metabolism and disposition.

Spectroscopic techniques used to characterize and quantitate above: optical difference, fluorescence, electron paramagnetic resonance, resonance Raman, EXAFS, and other spectroscopies.

SPECIALIZED RESEARCH TECHNIQUES - EXAFS AND COMPUTATIONAL

Performed EXAFS studies of Biological Systems. Member of Eastern Regional Consortium/Participating Research Team (Metalloenzymes, Proteins, and Models - EXAFS and X-ray Absorption Edge studies at Stanford Synchrotron Radiation Laboratory and Brookhaven National Laboratories) with the Institute for Structural and Functional Studies (1980-1987). Had hands on experience in data acquisition and analysis at SSRL, Institute for Structural and Functional Studies, and ATT Laboratories.

Performed Semiempirical and DFT calculations of metal-drug complexes using Gaussian and Spartan to characterize ligand/inhibitor to metal binding parameters, as well as Molecular Modeling with QUANTA and CHARMM.

REFEREE

Referees articles for the *Journal of Biological Chemistry*, *Biochemistry*, *Biophysical Journal*, *Journal of Pharmacology and Experimental Therapeutics*, *Archives of Biochemistry and Biophysics*, *Journal of Inorganic Biochemistry*, and *Hepatology*, as well as proposals for the National Science Foundation, Office of Naval Research, and other funding organizations.

PUBLICATIONS

1. Muhoberac, B.B. and Wharton, D.C. (1980) EPR study of heme NO complexes of ascorbic acid-reduced *Pseudomonas* cytochrome oxidase and corresponding model complexes. *J. Biol. Chem.* **255**, 8437-8442.
2. Muhoberac, B.B. and Brill, A.S. (1980) Associations of alcohols with heme proteins: Optical analysis and thermodynamic models. *Biochemistry* **19**, 5157-5167.
3. Muhoberac, B.B., Babcock, L.M., Harrington, P.C., Wilkins, R.G. and Wharton, D.C. (1980) EPR spectroscopy of semi-methemerythrin. *Biochim. Biophys. Acta* **626**, 337-345.
4. Harrington, P.C., Muhoberac, B.B., Wharton, D.C. and Wilkins, R.G. (1981) Some redox properties of myohemerythrin from retractor muscle of *Themiste zostericola*.

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12. Muhoberac, B.B. (1984) Correlations among parameters that describe low-spin ferric heme complexes. *Arch. Biochem. Biophys.* **233**, 682-697.
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25. Ehrig, T., Muhoberac, B.B., Hurley, T.D. and Bosron, W.F. (1992) The effects of alkaline pH and ternary complex formation of tryptophane fluorescence quenching in human $\beta_1\beta_1$ and horse EE alcohol dehydrogenase. *FEBS Letters* **300**, 283-285.
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27. Ehrig, T., Muhoberac, B.B., Brems, D. and Bosron, W.F. (1993) Monomers of human $\beta_1\beta_2$ alcohol dehydrogenase exhibit activity that differs from the dimer. *J. Biol. Chem.* **268**, 11721-11726.
28. Carfagna, M.A. and Muhoberac, B.B. (1993) Interaction of tricyclic drug analogs with synaptic plasma membranes: structure-mechanism relationships in inhibition of neuronal Na⁺/K⁺-ATPase activity. *Molec. Pharmacol.* **44**, 129-141.
29. Xia, J., Dubin, P.L., Morishima, Y., Sato, J. and Muhoberac, B.B. (1995) Quasi-elastic light scattering, electrophoresis, and fluorescence studies of lysozyme-poly(2 acrylamido-methylpropylsulfate) complex. *Biopolymers* **35**, 411-418.
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31. Carfagna, M.A., Ponsler, G.D. and Muhoberac, B.B. (1996) Inhibition of ATPase activity in rat synaptic plasma membranes by simultaneous exposure to metals. *Chemico-Biological Interactions* **100**, 53-65.
32. Xia, J., Mattison, K., Romano, V., Dubin, P. and Muhoberac, B.B. (1997) Complexation of trypsin and alcohol dehydrogenase with Poly(diallyldimethylammonium Chloride). *Biopolymers* **41**, 359-365.
33. Gao, J.Y., Dubin, P.L. and Muhoberac, B.B. (1997) Measurement of the binding of proteins to polyelectrolytes by frontal analysis continuous capillary electrophoresis. *Analytical Chemistry* **69**, 2945-2951.
34. Gao, J.Y., Dubin, P.L. and Muhoberac, B.B. (1998) Capillary electrophoresis and dynamic light scattering studies of structure and binding characteristics of protein-polyelectrolyte complexes. *J. Phys. Chem. B* **102**, 5529-5535.
35. Nurok, D., Kleye, R.M., Muhoberac, B.B., Frost, M.C., Hajdu, P., Robertson, D.H., Kamat, S.V. and Russell, A.J. (1999) Study of enzyme catalyzed reactions in organic solvents using multiple linear regression. *J. Molecular Catalysis B: Enzymatic* **7**, 273-282.
36. Xia, J.L., Dubin, P.L., Kokufuta, E., Havel, H. and Muhoberac, B.B. (1999) Light scattering, circular dichroism, and ligand binding studies of ferrihemoglobin-polyelectrolyte complexes. *Biopolymers* **50**, 153-161.
37. Baraibar, M.A., Barbeito, A.G., Muhoberac, B.B., and Vidal, R. (2008) Iron-mediated aggregation and a localized structural change characterize Ferritin from a mutant light chain polypeptide that causes neurodegeneration. *Journal of Biological Chemistry* **283**, 31679 - 31689.
38. Baraibar, M.A., Muhoberac, B.B., Garringer, H.J., Hurley, T.D., and Vidal, R. (2010) Unraveling of the E-helices and disruption of 4-fold pores are associated with iron mishandling in a mutant ferritin causing neurodegeneration. *Journal of Biological Chemistry* **285**, 1950 - 1956.
39. Muhoberac, B.B., Baraibar, M.A., and Vidal, R. (In Press, 2011) Iron loading-induced aggregation and reduction of iron incorporation in heteropolymeric ferritin containing a mutant light chain that causes neurodegeneration. *Biochim. Biophys. Acta - Molecular Basis of Disease*.

PATENTS/DISCLOSURES/DESCRIPTIONS

1. Dubin, P.L., Muhoberac, B.B. and Xia, J. (1992) Polyelectrolyte-protein coacervates as enzyme micro reactors.
2. Dubin, P.L., Muhoberac, B.B. and Xia, J. (1993) Enzyme compositions and use thereof.
3. Dubin, P.L., Muhoberac, B.B. and Xia, J. (1994) Polyelectrolyte-protein coacervate as enzyme micro reactors that improve stability and recovery of proteins.

4. Dubin, P.L., Muhoberac, B.B. and Xia, J. (1998) Enzyme-polyelectrolyte coacervate complex and method of use. U.S. Patent Number 5,834,271.

ABSTRACTS

1. Powers, L., Ching, Y., Angiolillo, P., Barlow, C., Chance, B., Yang, E. and Muhoberac, B. (1980) EXAFS Studies on authentic states of cytochrome oxidase. *Fed. Proc.* **39**, 2401.
2. Berger, H., Muhoberac, B.B. and Wharton, D.C. (1980) Reaction of *Pseudomonas* cytochrome oxidase with nitrite. *Fed. Proc.* **39**, 2406.
3. Muhoberac, B.B. and Wharton, D.C. (1980) EPR study of *Pseudomonas* cytochrome oxidase and corresponding model compounds. *Fed. Proc.* **39**, 2407.
4. Chance, B., Barlow, C., Smith, J., Leigh, J., Angiolillo, P., D'Ambrosio, C., Blumberg, W., Peisach, J., Powers, L., Ching, Y. and Muhoberac, B. (1980) SSRL Activity Report 80/01, VII-69.
5. Muhoberac, B.B. and Wharton, D.C. (1981) Spectral studies of the interaction of fluoride with *Pseudomonas* cytochrome oxidase (nitrite reductase). *Fed. Proc.* **40**, 2010.
6. Muhoberac, B.B. and Wharton, D.C. (1981) The interaction of heme \underline{d}_1 with some anionic ligands. *Fed. Proc.* **41**, 5469.
7. Horowitz, P., Muhoberac, B.B., Falksen, K. and Wharton, D.C. (1981) Proteolytic activation of *Pseudomonas* cytochrome oxidase. *Fed. Proc.* **41**, 5485.
8. Chance, B., Barlow, C., Angiolillo, P., D'Ambrosio, C., Blumberg, W., Peisach, J., Powers, L., Ching, Y. and Muhoberac, B. (1981) SSRL Activity Report 81/02, VII-44.
9. Muhoberac, B.B., Wharton, D.C., Falksen, K. and Horowitz, P.M. (1982) Controlled subtilisin digestion of *Pseudomonas* cytochrome oxidase in the absence and presence of the inhibitor KCN. *Biophys. J.* **37**, 374a.
10. Powers, L., Ching, Y., Chance, B. and Muhoberac, B. (1982) Cytochrome oxidase: structure and mechanisms, redox states, oxygen intermediates, pulsed and copper-depleted forms - A synchrotron x-ray study. *Biophys. J.* **37**, 403a.
11. Ching, Y., Ondrias, M.R., Rousseau, D.L. and Muhoberac, B.B. (1982) Resonance raman spectra of heme \underline{c} and heme \underline{d}_1 in *Pseudomonas* cytochrome oxidase. *Biophys. J.* **37**, 374a.
12. Muhoberac, B.B. (1982) EPR study of the interaction of NaF and KCN with the heme \underline{d}_1 moiety(ies) of *Pseudomonas* cytochrome oxidase. Gordon Research Conference (Metals in Biology).
13. Muhoberac, B.B., Hanew, T., Halter, S. and Schenker, S. (1983) Model for cytochrome P-450 dysfunction in drug metabolism. *Gastroenterology* **84**, 1386.
14. Muhoberac, B.B. (1983) Correlations among parameters describing low spin ferric heme

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15. Muhoberac, B.B., Tucker, M.P., Wharton, D.C. and Caughey, W.S. (1985) Infrared evidence for multiple types of carbon monoxide binding to *Pseudomonas* cytochrome oxidase. *Fed. Proc.* **44**, 7996.
 16. Steup, M.B. and Muhoberac, B.B. (1987) An apomyoglobin-heme d₁ complex as a model for the catalytic center of *Pseudomonas* cytochrome oxidase. *Biophys. J.* **51**, 298a.
 17. Carfagna, M.A. and Muhoberac, B.B. (1988) Synergistic effect of ethanol and amitriptyline on Na, K-ATPase activity of synaptic plasma membranes. *The Toxicologist* **8**, 147.
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 19. Carfagna, M.A. and Muhoberac, B.B. (1988) Effects of amitriptyline and ethanol on synaptic plasma membrane structure. *The Pharmacologist* **30**, A119.
 20. Carfagna, M.A., Ponsler, D.G. and Muhoberac, B.B. (1988) Investigation of the mechanism of synaptic plasma membrane perturbation by psychotropic drugs using the fluorescence probe ANS. *Biophys. J.* **55**, 137a.
 21. Carfagna, M.A., Ponsler, G.D. and Muhoberac, B.B. (1989) Simultaneous exposure to metals synergistically inhibits Na⁺/K⁺-ATPase activity in synaptic plasma membranes. *The Toxicologist* **9**, 137.
 22. Muhoberac, B.B., Larsen, R.W., Nunez, D.J., Morgan, W.T. and Ondrias, M.R. (1990) Resonance Raman Studies of the interaction of mesoheme and copper with histidine-rich glycoprotein. *Biophys. J.* **57**, 229a.
 23. Carfagna, M.A. and Muhoberac, B.B. (1990) Mechanism of Na⁺/K⁺ ATPase inhibition by tricyclic drug analogs. *The Toxicologist* **10**, 104.
 24. Carfagna, M.A. and Muhoberac, B.B. (1990) A relationship between amphiphilic drug structure and mechanism of Na⁺/K⁺-ATPase inhibition. *FASEB Journal* **4**, 3514.
 25. Ehrig, T., Muhoberac, B.B., Hurley, T.D. and Bosron, W.F. (1992) Tryptophan fluorescence quenching by alkaline pH and ternary complex formation in human β_1 and horse alcohol dehydrogenases. *FASEB Journal* **6**, 358.
 26. Ehrig, T., Sedarous, S.S., Muhoberac, B.B., Hurley, T.D., Brown, W.F. and Prendergast, F.G. (1993) Fluorescence spectroscopy of wildtype and a W314F mutant of human alcohol dehydrogenase. *Biophys. J.* **66**, 166a.
 27. Baraibar, M.A., Barbeito, A.G., Muhoberac, B.B., Ghetti B., and Vidal, R. (2007) Structural and functional characterization of ferritin light chain mutant (FTL498-499InsTC) associated with a neurodegenerative disorder. Society for Neuroscience, National Meeting, Program/Poster 491.19/BB7.

28. Sen, S.E. and Muhoberac, B.B. (2008) Undergraduate Student Involvement in Multidisciplinary Research Through the "Independent Project Experience" in Capstone in Chemistry Courses. Council on Undergraduate Research, National Conference, June 21-24, 2008, Saint Joseph, MN.
29. Baraibar, M.A., Barbeito, A.G., Muhoberac, B.B., Hurley, T.D., and Vidal, R. (2008) Crystal structure and Functional Analysis of the Ferritin Mutant FTL-498-499InsTC Associated With Hereditary Ferritinopathy. Society for Neuroscience, National Meeting, Nov 15-19, 2008, Washington DC.

GRANTS AWARDED (ONLY DIRECT COSTS LISTED)

1. Spectroscopic studies of *Pseudomonas* cytochrome oxidase, B.B. Muhoberac, \$6,000 (Institutional, UTHSC), December 1982 - May 1984.
2. Joint interaction of ethanol and drugs with biomembranes, B.B. Muhoberac, \$112,500 (NIAAA), September 1984 - August 1987.
3. Structural studies of the catalytic center(s) of *Pseudomonas* cytochrome oxidase, B.B. Muhoberac, 21 shifts at SSRL (EXAFS at Stanford Synchrotron Radiation Laboratory), January 1982 - June 1986.
4. Binding of Cu⁺² to cross-linked vinylpyridine resins, P.L. Dubin and B.B. Muhoberac, \$4,187 (Reilly Industries), January 1986 - June 1987.
5. Biochemical and biophysical studies of the cytoplasmic membrane of the pathogenic fungus, *Candida albicans*, M. Bard, M. Kemple, N.D. Lees and B.B. Muhoberac, \$4,000 (Institutional, IUPUI), January 1987 - December 1987.
6. Combined effects of ethanol and drugs on biomembranes, M.A. Carfagna (Sponsor B.B. Muhoberac), \$21,052 (NIAAA predoctoral fellowship), July 1988 - July 1990.
7. The use of NMR and ESR spectroscopy to examine the structure of alcohol dehydrogenase (ADH) and its complexes with substrates and inhibitors, W.F. Bosron, B.D. Nageswara Rao and B.B. Muhoberac, \$75,954 (NIAAA, as part of the Alcohol Research Center with Indiana University Medical School), September 1988 - September 1990.
8. NMR spectroscopic studies of the catalytic site of *Pseudomonas* cytochrome oxidase (nitrite reductase), B.B. Muhoberac and B.D. Nageswara Rao, \$4,000 (Institutional, IUPUI), January 1989 - December 1989.
9. Affinity-labeled quaternized poly(4-vinylpyridine) for selective coacervation of proteins, P.L. Dubin and B.B. Muhoberac, \$12,525 (Reilly Industries), September 1989 - September 1990.
10. Structural and functional properties of plasma membranes isolated from ethanol-

- preferring and nonpreferring rats, B.B. Muhoberac, \$77,998 (NIAAA, as part of the Alcohol Research Center with Indiana University Medical School), 1990-1992.
11. Studies of complexation of proteins with polyelectrolytes (travel grant), B.B. Muhoberac with several others (E. Kokututa, PI) \$40,000 (Japanese Ministry of Education), 1992-1994.
 12. Correlations between drug-induced changes in biomembrane structure and function, B.B. Muhoberac \$1,900 (BRSB), July 1991 - March 1993.
 13. Nitric oxide synthase purification and enzymological characterization, B.B. Muhoberac \$17,000 (Bristol Myers Squibb Pharmaceuticals), Summer 1993.
 14. Summer Faculty Fellowship: Stanford-Ames Aeronautics and Space Research Program, B.B. Muhoberac \$12,154 (NASA), Summer 1993.
 15. Acquisition of Instruments for the Molecular Spectroscopy Laboratory, B.B. Muhoberac with several others \$100,000 (Research Investment Fund, Institutional, IUPUI), 1994.
 16. Rapid Kinetic Experiments for the Advanced Chemistry Laboratories, N.E. Breen and B.B. Muhoberac, \$42,748 (NSF-Instrumentation), June 1997 - May 1999.
 17. Structure and function of ACC oxidase, B.B. Muhoberac, Sabbatical leave at Purdue University, West Lafayette, IN, Fall 1997.

Christoph A. Naumann

Professional Preparation

University Leipzig	Physics	Diplom	1990
Technical University Munich	Physics	Ph.D.	1995
MPI for Polymer Research Mainz	Biophysics	Postdoc	1996
Stanford University	Chemical Engineering	Postdoc	1996-1999

Appointments

Associate Professor, IUPUI, Department of Chemistry	2005-present
Assistant Professor of Chemistry, Department of Chemistry	1999-2005
Adjunct Professor, IUPUI, Biomedical Engineering	1999-present

Representative publications:

1. Garg, S., Tang, J. X., Ruehe, J., Naumann, C. A. (2009) "Actin-induced perturbation of PS lipid-cholesterol interaction: A possible mechanism of cytoskeleton-based regulation of membrane organization. *J. Struct. Biol.* **168**, 11-20.
2. Murcia, M. J., Minner, D. E., Mustata, G.-M., Ritchie, K., Naumann, C. A. (2008) "Design of quantum dot-conjugated lipids for long-term high-speed tracking experiments on cell surfaces" *J. Am. Chem. Soc.* **130**, 15054-15062.
3. Deverall, M. A., Garg, S., Luedtke, K., Jordan, R., Ruehe, J., Naumann, C. A. (2008) "Transbilayer coupling of obstructed lipid diffusion in polymer-tethered phospholipid bilayers" *Soft Matter* **4**, 1899-1908.
4. Murcia, M. J., Shaw, D. L., Long, E. C., Naumann, C. A. (2008) "Fluorescence correlation spectroscopy of CdSe/ZnS quantum dot optical bioimaging probes with ultra-thin biocompatible coatings" *Opt. Comm.* **281**, 1771-1780.
5. Deverall, M. A., Gindl, E., Sinner, E.-K., Besir, H., Ruehe, J., Saxton, M. J., Naumann, C. A. (2005) "Membrane lateral mobility obstructed by polymer-tethered lipids studied at the single molecule level." *Biophys. J.* **88**, 1875-1886.
6. Luedtke, K., Jordan, R., Furr, N., Garg, S., Forsythe, K., Naumann, C. A. (2008) "Two-dimensional center-of-mass diffusion of lipid tethered poly(2-methyl-2-oxazoline) at the air-water interface" *Langmuir* **24**, 5580-5584.
7. Garg, S., Ruehe, J., Luedtke, K., Jordan, R., Naumann, C. A. (2007) "Domain registration in raft-mimicking lipid mixtures studied using polymer-tethered lipid bilayers." *Biophys. J.* **92**, 1263-1270.
8. Murcia, M. J., Shaw, D. L., Woodruff, H., Naumann, C. A., Young, B., Long, E. (2006) "Facile sonochemical synthesis of highly luminescent ZnS-shelled CdSe quantum dots." *Chem. Mater.* **18**, 2219-2225.
9. Luedtke, K., Jordan, R., Hommes, Nuyken, O., Naumann, C. A. (2005) "Lipopolymers from new 2-substituted-2-oxazolines for artificial cell membrane constructs." *Macromol. Biosci.* **5**, 384-393.
10. Foreman, M. B., Coffman, J. P., Murcia, M. J., Cesana, S., Jordan, R., Smith, G. S.,

Naumann, C. A. (2003) "Gelation of amphiphilic lipopolymers at the air-water interface: 2D analogue to the 3D gelation of colloidal systems with grafted polymer chains?" *Langmuir* **19**, 326-332.

Selected Awards & Honors

DAAD Research Fellow (2007)

Postdoctoral fellowship of the Deutsche Forschungsgemeinschaft (1996-1998)

Synergistic Activities

- (i) Design of new classes in the Department of Chemistry and Chemical Biology on Biomaterials Science and Biomimetics Chemistry
- (ii) Supervision of undergraduate research projects: LaTeca Glass, John Fields, Daniel Minner, Nathan Furr, Michelle Jordan, Charis Manuputi, Isaac Warren, Emily Lugo-Ruiz (list of students supervised during last 4 years)
- (iii) Co-Director, IUPUI-Nanoscale Imaging Center.
- (iv) Member of Steering Committee, Medical Biophysics Program, Biomolecular Imaging.
- (v) Member, Leadership team, Integrated Nanosystems Development Institute
- (vi) ACS SEED Summer High School Outreach Program
- (vii) *Reviewer for:* PNAS, Biophys. J., Langmuir, Journal Physical Chemistry, JACS, Biomacromolecules, ChemPhysChem, Biomaterials, European Biophysical Journal, Biochimica et Biophysica Acta, Interface, Journal of Non-Crystalline Solids, European Journal of Biochemistry, Proteins, Small, Journal Structural Biology

Collaborators & Other Affiliations

(1) J. Tang, Department of Physics, Brown University. (2) K. Ritchie, Department of Physics, Purdue University, West Lafayette. (3) W. Yu, Department of Physiology, Northwestern University, (4) E. Long, Department of Chemistry and Chemical Biology, IUPUI. (5) J. Elmendorf, Department of Cellular & Integrative Physiology, IUPUI. (6) R. Siddiqui, Clarian Health, Methodist Research Institute. (7) R. Jordan, Department of Chemistry, Technical University Dresden. (8) J. Ruehe, Institute for Microsystem Technique, University of Freiburg. (9) J. Kaes, Department of Physics, University of Leipzig. (10) W. Goldmann, Center for Medical Physics and Technology, University Erlangen. (11) H. Nakshatri, IUSM, IUPUI.

Thesis Advisees

John Coffman (M. S., 2003)

Wei-min Liao (M.S., 2004)

Miranda Deverall (Ph.D. 2005)

Mert Hektanir (M.S., 2006)

Mike Murcia (Ph.D., 2006)

Sumit Garg (Ph.D., 2008)

Ann Kimble-Hill (Ph.D., 2008)

Danny Minner (Ph.D., current)

Amanda Siegel (Ph.D., current)

Yu-Hung Lin (Ph.D., current)

DAVID NUROK

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PERSONAL

Date of Birth: November 1, 1938
Marital Status: Married, two children
Citizenship: USA

EDUCATION

1958 B.Sc., University of Cape Town, Majoring in Chemistry and Physics
1959 B.Sc. (Honors), University of Cape Town in Chemistry
1966 Ph.D., University of Cape Town, "Separation of Diastereomers by Gas-Liquid Chromatography"

PROFESSIONAL CAREER

1960-62 Predoctoral Associate, Weizmann Institute of Science, Rehovot, Israel
1962-66 Doctoral Candidate, University of Cape Town
1967-70 Research Officer, Research Department, AE and CI, P.O. North Rand, South Africa
1970-76 Senior Research Officer, Sugar Milling Research Institute, University of Natal, South Africa
1977-78 Research Associate/Visiting Assistant Professor, University of Houston, Houston, Texas 77004
1978-2003 Associate Professor of Analytical Chemistry, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana 46202
1987 Visiting Scientist, Weizmann Institute of Science, Rehovot, Israel.
2004 - Associate Professor Emeritus

RESEARCH INTERESTS

My major interest is in developing Planar Electrochromatography (PEC). Electroosmotic flow is used to drive the mobile phase in this technique, and this results in separations that are more efficient and rapid than is possible with other forms of Thin Layer Chromatography. Our group published the first modern report on PEC in 1998, and recently developed Pressurized PEC (PPEC), which is performed at very high pressure. This results in separations that are over 20 times faster as compared to conventional Thin Layer Chromatography, and chromatographic efficiency that is competitive with that of High Performance Liquid Chromatography. Multiple samples can be separated simultaneously with separation time per sample measured in seconds.

TEACHING INTERESTS

My teaching interests were in the areas of general and analytical chemistry. I found the interaction with students in the classroom most rewarding, and enjoyed the challenge of explaining difficult material. I have experience teaching all sizes of classes, including those having only four or five students, and those having over 100 students.

Courses Taught

C106 Principles of Chemistry II
C224 Quantitative Analysis
C310 Analytical Chemistry
C342 Organic Chemistry II

C410 Instrumental Methods of Analysis
525 Intermediate Analytical Chemistry
621 Advanced Analytical Chemistry
629 Chromatographic Method of Analysis□

SERVICE

School of Science

Deans Administration Advisory Committee 1981-1982
School of Science Research Committee 1984-1986
Nominations and Awards Committee 1990-1991
Academic Appeals Committee 1991-1997, 2000 - 2003

Department of Chemistry

Department Executive Committee 1981-1983, 1988-1989
Search Committee for Chairman of Chemistry 1980
Executive Committee 1982-1983, 1989-1990
Chair, Graduate Policies Committee 1984-1986
Chair, Analytical Chemistry Search Committee 1986
Chair, Building Planning for Chemistry 1987
Organizer of Open House for Prospective Graduate Students 1988-1992, 1998-1999.
Curriculum Committee 1991-1996
Chair, Instrument Committee 1997-1998
Graduate Advisor 2000- 2003
Chair, Analytical Division 2002 - 2003

Editorial Board

Member Advisory Board of the *Journal of Planar Chromatography* 1988-
Member Advisory Board of *Acta Chromatographica* 2003 -

International Scientific Committee for Following Conferences

Planar Chromatography 2001
Planar Chromatography 2002
Planar Chromatography 2003
Planar Chromatography 2004

Consultant to

Oral Health Institute, School of Dentistry, 1986
Epstein & Frisch, Attorneys at Law 1997-1998

SOCIETY MEMBERSHIP

American Chemical Society
Analytical Chemistry Division
Chromatography Division

REVIEWING

Papers Reviewed for:

Analytical Chemistry
Journal of Chromatography
Journal of Planar Chromatography
Journal of Separation Science
Journal of High Resolution Chromatography
Analytica Chimica Acta
LC.GC. *The Magazine of Separation Science*

Proposals Reviewed for:

National Research Council
Petroleum Research Fund
National Science Foundation

THESIS STUDENTS DIRECTED

Patricia D. Cunningham	(1981)	“Studies in Modern Thin Layer Chromatography”
Rose M. Becker	(1982)	“Optimization Techniques in Thin Layer Chromatography”
Ronald E. Tecklenburg, Jr.	(1983)	“Optimization Methods in Thin Layer Chromatography”
Eric K. Johnson	(1984)	“Computer Aided Studies of Optimization in Thin Layer Chromatography”
James E. Steinbrunner	(1985)	“Evaluation of Computer Aided Optimization Methods for Two-Dimensional Thin layer Chromatography”
Edda A. Guerrero	(1986)	“Studies in Continuous Development Thin Layer Chromatography”
Kenneth J. Ruterbories	(1987)	“Computer Aided Studies in Planar Chromatography”
Ziyad A. Rajabi	(1987)	“Computer Aided Optimization of Thin Layer Chromatography Methods”
Christopher E. Uhegbu	(1988)	“Reproducibility and Correlation Studies in Planar Chromatography”
Sohrab Habibi-Goudarzi	(1989)	“Optimization Methods in Two-Dimensional Planar Chromatography”
Lisa A. Julian	(1989)	“A Study of a New Solvent Strength Parameter for Planar Chromatography”

Donald S. Risley	(1989)	“Computer Aided Studies of Solvent Optimization in Planar Chromatography”
Mary Jo Wenning	(1990)	“Optimization of Experimental Variables for Planar Chromatography, with Emphasis on Temperature”
Kirk D. Knotts	(1992)	“Approaches to Optimizing Separation in Thin Layer Chromatography”
Megan C. Frost	(1999)	“Improving the Performance of Planar Chromatography”
James M. Koers	(2002)	“Studies in Planar Electrochromatography”
Allyson L. Novotny	(2009)	“Studies in Pressurized Planar Electrochromatography”
Scott D. Woodward	(2010)	“Improving the Performance of Pressurized Planar Electrochromatography”

PATENTS

U.S. Patent 6,303,029 B1. Arrangement and Method for Performing Chromatography, D. Nurok and M.C. Frost. Issued October 2001.

U.S. Patent No. 6,610,202 Arrangement and Method for Performing Chromatography, D. Nurok and M.C. Frost, Issued 2003.

U.S. Patent No. 7,279,105 Arrangement and Method for Performing Chromatography. D. Nurok and M.C. Frost, Issued October 2007.

U.S. Patent No. 7,736,517 Method and Apparatus for Performing Planar Electrochromatography at Elevated Pressure, D. Nurok, J.M.Koers, R. E. Santini, R. W. Replogle, and G. L. Hawkins. Issued 2010.

Method and System for Separating Analytes. D. Nurok, A.L. Novotny, T. Stachowiak, F. Svec. Filed 2007. 0059442 A1 Pending

PUBLICATIONS

1. E. Gil-Av and D. Nurok, “The Separation of Diastereomers by Gas-Liquid Chromatography,” *Proc. Chem. Soc.*, 146, 1962.
2. E. Gil-Av, R. Charles-Sigler, G. Fischer and D. Nurok, “Resolution of Optical Isomers by Gas-Liquid Partition Chromatography,” *J. Gas Chromatog.*, **4**, 51, 1966.
3. E. Gil-Av and D. Nurok, “Resolution of Optical Isomers by Gas Chromatography of Diastereoisomers,” *Advances in Chromatography*, Giddings and Keller, eds., Marcel Dekker, Inc., New York, **10**, 99, 1974.
4. D. Nurok, G.L. Taylor and A.M. Stephen, “Separation of Diastereoisomers by Gas-Liquid Chromatography: Esters of 2,3-Butanediol,” *J. Chem. Soc.*, **B3**, 291, 1968.

5. A.W. MacGillivray and D. Nurok, "Comparison of Three Methods for the Determination of Water in Final Molasses," *Proc. S. Afr. Sugar Tech. Assoc.*, **47**, 39, 1973.
6. D. Nurok, "The Separation of Kestose Isomers by Gas Chromatography," *Int. Sugar J.*, **76**, 305, 1974.
7. D. Nurok and T.J. Reardon, "Quantitative Determination of Sugars in Factory Products by Gas Chromatography Using Open Tubular Columns," *Proc. S. Afr. Sugar Tech. Assoc.*, **49**, 99, 1975.
8. M. Kort, M. Matic, P. Mellet and D. Nurok, "Analysis of Final Molasses for Sucrose and Pol," *Proc. S. Afr. Sugar Tech. Assoc.*, **49**, 99, 1975.
9. D. Nurok, "The Preparation of Trimethylsilyl Ethers of the Kestose Isomers in Aqueous Solution," *J. Chromatogr. Sci.*, **14**, 305, 1976.
10. D. Nurok and T.J. Reardon, "The Rapid Gas Chromatographic Determination of Sucrose as Its TMS Ether on an Open Tubular Column," *Carbohydr. Res.*, **56**, 165, 1977.
11. D. Nurok and T.J. Reardon, "Operating Conditions for the Determination of Sucrose by Capillary Gas Chromatography," *Anal. Chem.*, **50**, 855, 1978.
12. D. Nurok and A. Zlatkis, "The Separation of Malto-Oligosaccharides by High-Performance Thin-Layer Chromatography," *Carbohydrate Res.*, **65**, 265, 1978.
13. D. Nurok and A. Zlatkis, "The Separation of Malto-Oligosaccharides by High-Performance Thin-Layer Chromatography at Moderate Temperature," *J. Chromatogr.*, **142**, 449, 1977.
14. D. Nurok, J.W. Anderson and A. Zlatkis, "Profiles of Sulfur Containing Compounds Obtained from Arabica and Robusta Coffees by Capillary Column Chromatography," *Chromatographia*, **11**, 188, 1978.
15. M. Martinez, D. Nurok and A. Zlatkis, "A Two Phase Sample Preparation and Concentration Technique for Sugar Derivatives," *Anal. Chem.*, **50**, 1226, 1978.
16. K.Y. Lee, D. Nurok and A. Zlatkis, "Simultaneous Determination of Antiarrhythmia Drugs by High Performance Thin-Layer Chromatography," *J. Chromatogr.*, **158**, 403, 1978.
17. K.Y. Lee, D. Nurok and A. Zlatkis, "A Combined Headspace and Extraction Technique for Profile Analysis by Capillary Gas Chromatography," *J. Chromatogr.*, **158**, 377, 1978.
18. F. Hsu, D. Nurok and A. Zlatkis, "The Determination of Sucrose in Molasses by High Performance Thin-Layer Chromatography," *J. Chromatogr.*, **158**, 411, 1978.
19. K.Y. Lee, D. Nurok and A. Zlatkis, "The Determination of Glucose, Fructose and Sucrose in Molasses by High Performance Thin-Layer Chromatography," *J. Chromatogr.*, **174**, 187, 1979.
20. D. Nurok and A. Zlatkis, "The Separation of Malto-Oligosaccharides by High Performance Thin-Layer Chromatography Using Multiple Developments," *Carbohydrate Res.*, **81**, 167, 1980.

21. M. Martinez, D. Nurok, A. Zlatkis, D. McQuittay and J. Evans, "The Use of Chromatographic Profiles for the Identification of Yeast Genera," *J. High Res. Chromatogr.*, **3**, 528, 1980.
22. D. Nurok, "Controlled Migration Thin-Layer Chromatography," *Anal. Chem.*, **53**, 714, 1981.
23. D. Nurok and M.J. Richard, "Prediction of Optimum Solvent Composition for Thin-Layer and Liquid Chromatography," *Anal. Chem.*, **53**, 563, 1981.
24. D. Nurok, "Modern Liquid Chromatography," *Intern. Sugar J.*, **84**, 99, 1982.
25. D. Nurok, R.M. Becker, M.J. Richard, P.D. Cunningham, W.B. Gorman and C.L. Bush, "Optimization of Binary Solvents in Thin-Layer Chromatography," *J. High. Res. Chromatogr.*, **5**, 373-376, 1982.
26. D. Nurok, R.M. Becker, K.A. Sassic, "Time Optimization in Thin-Layer Chromatography," *Anal. Chem.*, **54**, 1955-1959, 1982.
27. R.E. Tecklenburg, Jr., R.M. Becker, E.K. Johnson and D. Nurok, "Time Optimized Thin-Layer Chromatography in a Chamber with Fixed Plate Lengths," *Anal. Chem.*, **55**, 2196, 1983.
28. R.E. Tecklenburg, Jr., B.L. Maidak and D. Nurok, "Separation of Steroid Mixtures by Time Optimized Thin-Layer Chromatography," *J. High Res. Chromatogr.*, **6**, 627-628, 1983.
29. D. Nurok, R.E. Tecklenburg, Jr. and B.L. Maidak, "The Separation of Complex Mixtures by Parallel Development Thin-Layer Chromatography," *Anal. Chem.*, **56**, 293-297, 1984.
30. R.E. Tecklenburg, Jr., G.H. Fricke and D. Nurok, "Overlapping Resolution Maps as an Aid in Parallel Development Thin-Layer Chromatography," *J. Chromatogr.*, **290**, 75-81, 1984.
31. R.E. Tecklenburg, Jr. and D. Nurok, "Correlations in Continuous Development Thin-Layer Chromatography," *Chromatographia*, **18**, 249-252, 1984.
32. E.K. Johnson and D. Nurok, "Computer Simulation as an Aid to Optimizing Continuous Development Two-Dimensional Thin-Layer Chromatography," *J. Chromatogr.*, **302**, 135-147, 1984.
33. J.E. Steinbrunner, E.K. Johnson, S. Habibi-Goudarzi and D. Nurok, "The Computer-Aided Evaluation of Continuous Development Two-Dimensional Thin-Layer Chromatography," in *Planar Chromatography*, R.E. Kaiser, ed., Heuthig, Heidelberg, Vol. 1, 239-255, 1986.
34. E.K. Johnson, M.J. Wenning, R.E. Tecklenburg, Jr. and D. Nurok, "Analysis Time in Conventional and Continuous Development Thin-Layer Chromatography," *J. High Res. Chromatogr.*, **9**, 285-288, 1986.

35. D. Nurok, S. Habibi-Goudarzi and R. Kleyle, "Statistical Approach to Solvent Selection as Applied to Two-Dimensional Thin-Layer Chromatography," *Anal. Chem.*, **59**, 2424-2428, 1987.
36. K.J. Ruterbories and D. Nurok, "Thin-Layer Chromatographic Separation of Diastereomeric Amino Acid Derivatives Prepared Using Marfey's Reagent," *Anal. Chem.*, **59**, 2735-2736, 1987.
37. J.E. Steinbrunner, D.J. Malik and D. Nurok, "Contour Diagrams for the Presentation of Separation Quality in Two-Dimensional Thin-Layer Chromatography," *J. High Res. Chromatogr. and Chromatogr. Comm.*, **10**, 560-563, 1987.
38. D. Nurok, "Computer-Aided Optimization of Separation in Planar Chromatography," feature article, *LC.GC Magazine*, **6**, 310-322, 1988.
39. S. Habibi-Goudarzi, K.J. Ruterbories, J.E. Steinbrunner and D. Nurok, "A Computer-Aided Survey of Systems for Separating Steroids by Two-Dimensional Thin Layer Chromatography," *J. Planar Chromatogr.*, **1**, 161-167, 1988.
40. D. Nurok, "Strategies for Optimizing the Mobile Phase in Planar Chromatography," *Chemical Reviews*, **89**, 363-375, 1989.
41. D.S. Risley, S. Habibi-Goudarzi, R. Kleyle and D. Nurok, "Correlations Between the Ranking of One- and Two-Dimensional Solvent Systems for Planar Chromatography," *J. Planar Chromatogr.*, **3**, 216-221, 1990.
42. D. Nurok, L.A. Julian and C.E. Uhegbu, "A Parameter for Predicting Retention in Planar Chromatography," *Anal. Chem.*, **63**, 1524-1529, 1991.
43. A.D. Kossoy, D.S. Risley, R.M. Kleyle and D. Nurok, "Novel Computational Method for the Determination of Partition Coefficients by Planar Chromatography," *Anal. Chem.*, **64**, 1345-1349, 1992.
44. C.E. Uhegbu, M.L. Kearns, K.D. Knotts, L.A. Julian, M.L. Klein and D. Nurok, "Relationship Between \hat{R}_f and a Solvent Strength Parameter," *J. Planar Chromatogr.*, **5**, 259-262, 1992.
45. D. Nurok, K.D. Knotts, M.L. Kearns, K.J. Ruterbories, C.E. Uhegbu and P.C. Alberti "A Quantitative Study of Thin Layer Chromatographic Separation in a Series of Mobile Phases," *J. Planar Chromatogr.*, **5**, 350-358, 1992.
46. K.D. Knotts, M.L. Kearns, L.A. Julian, K.B. Lipkowitz and D. Nurok, "The Relationship Between Separation Quality and Certain Properties of the Mobile Phase," *J. Planar Chromatogr.*, **6**, 105-111, 1993.
47. D. Nurok, R.M. Kleyle, K.B. Lipkowitz, S.S. Myers and M.L. Kearns, "Dependence of Retention and Separation Quality in Planar Chromatography on Certain Properties of the Mobile Phase," *Anal. Chem.*, **65**, 3701-3707, 1993.
48. D. Nurok, R.M. Kleyle, P. Hajdu, B. Ellsworth, S.S. Myers, T.M. Brogan, K.B. Lipkowitz and R.C. Glen, "Solvent Dependent Regression Equations for the Prediction of Retention in Planar Chromatography," *Anal. Chem.*, **67**, 4423-4430, 1995.

49. R.M. Kleyle, D. Nurok, A.D. Kossoy and S.C. Burris, "Novel Computational Methods for the Determination of Partition Coefficients by Planar Chromatography," *J. Chromatogr.*, **749**, 211-217, 1996.
50. A.K. Chaudhary, S.V. Kamat, E.J. Beckman, A.J. Russell, D. Nurok, R.M. Kleyle and P. Hajdu, "Control of Subtilisin Substrate Specificity By Solvent Engineering in Organic Solvents and Supercritical Fluoroform," *J. Am. Chem. Soc.*, **118**, 12891-12901, 1996.
51. D. Nurok, R.M. Kleyle, C.L. McCain, D.S. Risley and K.J. Ruterbories, "Statistical Method for Quantifying Mobile Phase Selectivity in One- and Two-Dimensional Overpressured Layer Chromatography," *Anal. Chem.*, **69**, 1398-1405, 1997.
52. M.C. Frost, T. Lahr, R.M. Kleyle and D. Nurok, "Empirical Equation for the Accurate Prediction of Retention in Planar Chromatography," *J. Chromatogr.*, **788**, 207-211, 1997.
53. D. Nurok, M.C. Frost, C.L. Pritchard, and D.M. Chenoweth, "The Performance of Planar Chromatography Using Electroosmotic Flow," *J. Planar Chromatogr.*, **11**, 244-246, 1998.
54. D. Nurok, R.R. Sorrell, C.L. McCain, M.C. Frost, P. Hajdu, T.C. Powell, T. Lahr and R.M. Kleyle, "The Prediction of Retention by the Polar and Non-Polar Surface Areas of Single Solvents Used as Mobile Phases," *J. Planar Chromatogr.*, **12**, 42-45, 1999.
55. D. Nurok, R.M. Kleyle, M.C. Frost, P. Hajdu, D.H. Robertson, B.B. Muhoberac, A.J. Russell and S.V. Kamat, "Study of Enzyme Catalyzed Reactions in Organic Solvents Using Multiple Linear Regression," *J. Mol. Catal. B. Enzymatic*, **7**, 273-282, 1999.
56. D. Nurok, "Forced Flow Techniques in Planar Chromatography," *Anal. Chem* **72**, 634A-641A, 2000.
57. D. Nurok, M.C. Frost and D. Chenoweth, "Separation Using Planar Chromatography with Electroosmotic Flow," *J. Chromatography A*, **903**, 211-217, 2000.
58. D. Nurok, J. M. Koers, D. A. Nyman and W. Liao, "Variables that Affect Performance in Planar Electrochromatography with Electroosmotic Flow," *J. Planar Chromatogr.*, **14**, 409-414, 2001.
59. D. Nurok, J. M. Koers, M. A. Carmichael, W. Liao and T.H. Dzido, "The Performance of Planar Electrochromatography in a Horizontal Chamber," *J. Planar Chromatogr.* **15**, 320-323, 2002.
60. D. Nurok, J. M. Koers, and M. A. Carmichael , "The Role of Buffer Concentration and Applied Voltage in Obtaining a Good Separation in Planar Electrochromatography" *J. Chromatography A* **983**, 247 – 253, 2003.
61. D. Nurok, J. M. Koers, A. L. Novotny, M. A. Carmichael, J. J. Kosiba, R. E. Santini, G. L. Hawkins, and R. W. Replogle, "Apparatus and Initial Results for Pressurized Planar Electrochromatography" *Analytical Chem.* **76**, 1690 – 1695, 2004.
62. D. Nurok, "Planar Electrochromatography" *J. Chromatogr. A*, **1044**, 83 – 96, 2004.

63. A. L. Novotny, D. Nurok, R. W. Replogle, G. L. Hawkins, and R. E. Santini, "Results with an Improved Apparatus for Pressurized Planar Electrochromatography" *Analytical Chem.* **78**, 2823 – 2831, 2006.
64. D. J. Janecki, A. L. Novotny, S. D. Woodward, J. M. Wiseman, and D. Nurok, "A Preliminary Study of the Coupling of Desorption Electrospray Ionization – Mass Spectrometry with Pressurized Planar Electrochromatography", *J. Planar Chromatogr.* **21**, 11 - 14, 2008.
65. S. D. Woodward, I. Urbanova, D. Nurok and F. Svec, "Separation of Peptides and Oligonucleotides Using a Monolithic Polymer Layer and Pressurized Planar Electrophoresis and Electrochromatography", *Analytical Chem.* **82**, 3445 – 3448, 2010.

INVITED REVIEWS

1. D. Nurok, "Modern Liquid Chromatography," *Intern. Sugar J.*, **84**, 99 (1982). (see publication number 24).
2. D. Nurok, "Computer-Aided Optimization of Separation in Planar Chromatography," feature article, *LC.GC Magazine*, **6**, 310 (1988). (see publication number 38).
3. D. Nurok, "Strategies for Optimizing the Mobile Phase in Planar Chromatography," *Chemical Reviews*, **89**, 363 (1989). (see publication number 40).
4. D. Nurok, "Forced Flow Techniques in Planar Chromatography," *Anal. Chem.* **72**, 634A-641A (2000). (See publication number 56).
5. D. Nurok, "Planar Electrochromatography" *J. Chromatogr. A*, **1044**, 83 – 96, 2004. (See publication number 62).

LECTURE SESSIONS CHAIRED OR CO-CHAIRLED AT:

International Symposium on Advances in Chromatography, Las Vegas, 1982.
 International Symposium on Advances in Chromatography, Houston, 1983.
 International Symposium of Chromatography, Taipei, Taiwan, 1986.
 10th International Symposium on Instrumental Planar Chromatography, Visegrad, Hungary, 1998.
 Planar Chromatography 2001, Lillafured, Hungary, 2001.
 Planar Chromatography 2002, Heviz, Hungary, 2002.
 26th Annual Symposium on the Separation of Organic Compounds, **co-chaired opening session**, Szczyrk, Poland, 2002.
 4th Slovenian Symposium on Separation Techniques, Novo Mesto, Slovenia, 2002.
 Planar Chromatography Today 2002, Novo Mesto, Slovenia, 2002.
 Planar Chromatography 2003, **co-chaired opening session**, Budapest, Hungary, 2003.

PRESENTATIONS AT NATIONAL/INTERNATIONAL MEETINGS

1. D. Nurok, M. Richard and P. Cunningham, "An Approach to the Prediction of Optimum Solvent Composition in Liquid Chromatography," Expochem., Houston, TX, September 1981.

2. D. Nurok and R.M. Becker, "Optimization of Binary Solvents in Thin-Layer Chromatography," 17th International Symposium on Advances in Chromatography, Las Vegas, NV, April 1982.
3. D. Nurok, R.M. Becker, and R.E. Tecklenburg, Jr., "Time Optimization in Thin-Layer Chromatography," 3rd Biennial Symposium Advances in Thin-Layer Chromatography, Parsippany, NJ, December 1982.
4. D. Nurok, "Time Optimization in Thin-Layer Chromatography" presented at Workshop in Thin-Layer Chromatography, Pittsburgh Conference in Atlantic City, NJ, March 1983.
5. D. Nurok, R.E. Tecklenburg, Jr., E.K. Johnson, M.J. Wenning, and B.C. Maidak, "Optimization of Continuous Development Thin-Layer Chromatography," 20th Anniversary International Symposium on Advances in Chromatography, Amsterdam, The Netherlands, October 1983.
6. D. Nurok, E.K. Johnson, and M. Kennedy, "The Separation of Complex Mixtures by Thin-Layer Chromatography," 20th International Symposium on Advances in Chromatography, New York, April 1984.
7. D. Nurok, "Aspects of Computer-Aided Optimization in Thin Layer Chromatography," Pittsburgh Conference, New Orleans, LA, February 1985.
8. D. Nurok, "Computer-Aided Optimization of Two-Dimensional Thin Layer Chromatography," Pittsburgh Conference, Atlantic City, NJ, March 1986.
9. D. Nurok, "The Optimization of Two-Dimensional Thin-Layer Chromatography," International Symposium on Chromatography, Taiwan, April 1986. **(Airfare and all expenses paid by organizers of symposium).**
10. D. Nurok, "A Statistical Approach to Solvent Selection in Two-Dimensional Thin Layer Chromatography," 22nd International Symposium on Advances in Chromatography, Houston, TX, September 1986.
11. D. Nurok, "Optimization of the Mobile Phase in Planar Chromatography," Pittsburgh Conference, Atlanta, GA, March 1989. **(All expenses paid by organizers of symposium).**
12. D. Nurok, "A Statistical Approach to Solvent Selection in Planar Chromatography," 6th International Symposium on Instrumental Planar Chromatography, Interlaken, Switzerland, April 1991.
13. D. Nurok, R. Kleyale and D. Risley, "Determination of Solvent Selectivity by a Statistical Method," National Symposium on Planar Chromatography, Somerset, NJ, September 1991.
14. D. Nurok, R. Kleyale, K. Lipkowitz, S. Myers and M. Kearns, "The Dependence of Separation Quality on Certain Properties of the Mobile Phase," 7th International Symposium on Instrumental Planar Chromatography, Brighton, U.K., March 1993.

15. "Prediction of Retention in Planar Chromatography," 10th International Symposium on Instrumental Planar Chromatography, Visegrad, Hungary, 1998 (**All expenses, except airfare, paid by organizers of symposium**).
16. D. Nurok, J. M. Koers, D. A. Nyman and W. Liao, "Variables that Affect Performance in Planar Electrochromatography" Planar Chromatography 2001, Lillafured, Hungary, June 2001.
17. D. Nurok, J. M. Koers, M. A. Carmichael, W. Liao and T.H. Dzido, "Planar Electrochromatography: A New Technique with Promise", Planar Chromatography 2002, Heviz, Hungary, 2002. (**This was the opening plenary lecture**).
18. D. Nurok, J. M. Koers, M. A. Carmichael, W. Liao and T.H. Dzido, 26th Annual Symposium on the Separation of Organic Compounds, Szczyrk, Poland, 2002. (**Plenary lecture, all expenses, except airfare paid by organizers of the symposium**)
19. D. Nurok,, "An Overview of Planar Electrochromatography" 4th Slovenian Symposium on Separation Techniques, Novo Mesto, Slovenia. October 2002.
20. D. Nurok, J. M. Koers, M. A. Carmichael, "Experimental Variables that Influence Separation in Planar Electrochromatography" Planar Chromatography Today 2002, Novo Mesto, Slovenia. October 2002. (**Airfare and all expenses paid by organizers of the two back-to-back symposia, 19 and 20**).
21. D. Nurok, J. M. Koers, A. L. Novotny, M. A. Carmichael, and J. J. Kosiba, "Performance of Planar Electrochromatography at Elevated Pressure", Planar Chromatography 2003, Budapest, Hungary, 2003.
22. D. Nurok, A. L. Novotny, R. E. Santini R. W. Replogle, and G. L. Hawkins, "Pressurized Planar Electrochromatography: A New Tool for Proteomics? " Annual Meeting of the American Electrophoresis Society, San Francisco, 2006.

SEMINARS

1. "Modern Thin-Layer Chromatography," Dow Chemical Company, Indianapolis, IN, August 1981.
2. D. Nurok, "Optimization in Thin-Layer Chromatography," Midwestern Universities Analytical Chemists Congress, West Lafayette, IN, October 1981.
3. "Time and Solvent Optimization in Thin-Layer Chromatography," University of Houston, Houston, TX, November 1982.
4. "Some Approaches to Optimization in Chromatography," Varian Non-Commercial Chromatography Symposium, Indianapolis, IN, April 1984.
5. "Time and Solvent Optimization in Thin-Layer Chromatography," Department of Chemistry, Weizmann Institute of Science, Israel, August 1984.
6. "Time and Solvent Optimization in Thin-Layer Chromatography," Merrell Dow Research Institute, Indianapolis, IN, October 1984.

7. "Optimization Strategies in Thin-Layer Chromatography," Rose-Hulman Institute of Technology, Terre Haute, IN, October 1984.
8. "Time and Solvent Optimization in Thin-Layer Chromatography," Analytical Division, Chemistry Department, Purdue University, West Lafayette, IN, April 1985.
9. "Time and Solvent Optimization in Thin Layer Chromatography," Ball State University, Muncie, IN, January 1986.
10. "Time and Solvent Optimization in Thin Layer Chromatography," Indiana University-Purdue University at Fort Wayne, IN, April 1986.
11. "Time and Solvent Optimization in Thin Layer Chromatography," Eli Lilly and Company, December 1986.
12. "Solvent Optimization in Planar Chromatography," Department of Organic Chemistry, Weizmann Institute of Science, Israel, May 1987.
13. "Optimization in Planar Chromatography," Chemistry Department, DePauw University, October 1987.
14. "Planar Electrochromatography", Pfizer Pharmaceutical, Groton, CT, November 2000.
15. "Pressurized Planar Electrochromatography", MUACC conference, Indianapolis, IN, October 2003.

SHORT COURSES

One lecture at a short course on Planar Chromatography at Pittsburgh Conference, 1983.

Three lectures at a short course, *Methods in Scientific Examination of Works of Art: Thin Layer Chromatography*, at the Getty Conservation Institute, Marina del Rey, CA, February 1994.

PRESENTATIONS BY PREVIOUS GRADUATE STUDENT

Oral presentations

Novotny, A.L.; Replogle, R.W.; Santini, R.E.; Nurok, D. An Improved Apparatus for PPEC. Presented at Chromatographic Methods of Investigating Organic Compounds, Katowice, Poland, June 2005.

Novotny, A.L.; Replogle, R.W.; Santini, R.E.; Nurok, D. Apparatus and Results for Pressurized Planar Electrochromatography. Presented at Eli Lilly and Company, Indianapolis, IN, June 2005.

Posters

Novotny, A.L.; Nurok, D.; Hawkins, G.L.; Replogle, R.L.; Santini, R.E.
Initial Results for Pressurized Planar Electrochromatography with Temperature Control. Presented at Planar Chromatography 2004, Visegrád, Hungary, May 2004

Novotny, A. L.; Kosiba, J. J.; Rontu, N.; Nurok, D. Pressurized Planar Electrochromatography: A Separation Technique with Potential. Presented at the 36th Central Regional Meeting of the American Chemical Society, Indianapolis, IN, June 2004.

EXTERNALLY FUNDED GRANTS

“The Performance of Thin-Layer Chromatography at Elevated Temperature,” The Research bgCorporation, \$5,500, funded November 1979.

Society for Analytical Chemistry of Pittsburgh, starter grant, \$3,500, funded May 1982.

“A Study of Quantitation and Optimization in Thin-Layer Chromatography,” Dow Chemical Company, \$5,500, funded May 1983.

“A Study of Quantitation and Optimization in Thin-Layer Chromatography,” Dow Chemical Company, \$10,000, funded March 1984.

“A Study of Optimization in Thin-Layer Chromatography,” Dow Chemical Company, \$10,000, funded May 1985.

“Studies in Planar Chromatography,” Dow Chemical Company, \$10,000, funded February 1986.

Purchase of ‘Chrompres 25’ Overpressured Layer Chromatography equipment contributed to equally by Eli Lilly and Company and Lilly Industrial Coatings. \$4,500, funded in 1987.

“A Study of a New Solvent Strength Parameter for Planar Chromatography,” Research Corporation, \$23,350, funded November 1989.

“A Study of the Mobile Phase in Liquid Chromatography,” Dow Chemical Company, \$5,850, funded August 1993.

“A Study of the Mobile Phase in Liquid Chromatography,” Dow Chemical Company, \$5,000, funded August 1994.

“A Study of the Mobile Phase in Liquid Chromatography,” Dow Chemical Company, \$6,000, funded February 1995.

“Construction and Use of Apparatus for Planar Electrochromatography”, Pfizer Inc., \$39,284, funded December 2001.

“Grant to Fund the Research of a Graduate Student”, Eli Lilly and Company, \$30,000, funded June 2005.

“Studies in Pressurized Planar Electrochromatography”, PerkinElmer Life and Analytical Sciences, \$59,600, funded August 1, 2006.

Internal Funding Since 1994

“The Dependence of Separation in Liquid Chromatography on the Properties of the Mobile Phase,” Faculty Development Grant, \$3,000, Funded, 1994.

“The Use of Multiple Linear Regression to Study the Mobile Phase in Liquid Chromatography,” Faculty Development Grant, \$3,000, Funded, 1996.

“The Use of Electroosmotic Flow in Planar Chromatography”, Faculty Development Grant, \$3,000, Funded, 1998.

“IUPUI Honors Program Research Fellow” \$2,000, Funded 2000.

“IUPUI Honors Program Research Fellow” \$2,000, Funded 2001.

“IUPUI Honors Program Research Fellow” \$2,000, Funded 2003.

“IUPUI Honors Program Research Fellow” \$2,000, Funded 2009.

Collaborations 1995 - present

Robert M. Kleyle, IUPUI.

Alan J. Russell, University of Pittsburgh.

Aaron D. Kossoy, Eli Lilly & Co.

Robert C. Glen, Tripos Inc.

Donald S. Risley (ex-graduate student), Eli Lilly & Co.

Kenneth J. Ruterbories (ex-graduate student), Eli Lilly & Co.

Tadeusz H. Dzido, Medical Academy, Lublin, Poland.

Robert E. Santini, Amy Facility for Chemical Instrumentation, Purdue University, West Lafayette.

Wayne Patton, Director of Biochemistry, PerkinElmer Life and Analytical Sciences.

Frantisel Svec, Lawrence Berkeley National Laboratory

Viktor Krchnak, Department of Chemistry, Notre Dame University.

Research with Undergraduates

Dana Awad

Talha Allam

Melissa Bode

Neal Bowlen

James Brink

Tracy Broad

Terry Brogan

Chris Bush

Karinna Campbell

Matthew Carmichael

David Chenoweth

Jenny Fong

Karla Glaser

William Gorman

Elizabeth Hanson

Michael Hood

Michelle Kearns

Margaret Klein

Justin Kosiba

Tom Lahr

Misti Langmaack

Rebecca Leapman

Wei-min Liao

Charlotte McCain

Robert Muller

Mark Nielson

Jennifer Phan

Joseph Platt

Derrick Plahn

Mike Robertson

Daniel Robinson

Nabilah Rontu

Tehseen Shaikh

Scott Sharp

Robert Tharp

Greg Thoman

Scott Foster
Megan Frost
Elizabeth Gamble

Marie McGillem
Jessica Miller
Abigail Mills
Jordan Mossler

Bryan Turner
Joe Turpin
Sara Williams

Research with Non-Thesis Masters Students

Mike Richard
Brett Farrell
Karin Sassie
Bonnie Maidak
Dave Robbins
Dan Nyman

Pam Alberti
Ed Harris
Steve Myers
Brenda Ellsworth
Joel Calvin
Jeff Bender

Charles Held
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CURRICULUM VITAE
(See Final Page for Summary)

January 2011

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PERSONAL

Born: July 8, 1946, Iowa Falls, Iowa.
Married: Wife: Kitty; Children: Patrick (34), Michael (31), Kathleen (24).

EDUCATION

B.S. 1968, Chemistry (Honors and High Distinction), University of Iowa, Ph.D. 1973,
Organic Chemistry, Yale University, K.B. Wiberg, Advisor.
Thesis: Synthesis and Study of Strained Medium-Ring Compounds.
Postdoc. 1973-75, Université Catholique de Louvain, Louvain-la-Neuve, Belgium, L. Ghosez, Advisor. Research in
Cycloaddition Reactions and the Synthetic Design of a Novel Approach to the Prostanoids.

PROFESSIONAL EXPERIENCE

E. I. du Pont de Nemours and Company
Summers 1966, 1967: Summer Technical Employee, Chicago, IL.
Summer, 1968: Resident Research Chemist, Experimental Station, Wilmington, DE.
Indiana University–Purdue University at Indianapolis (IUPUI)
Assistant Professor of Chemistry, 1975 - 1979.
Associate Professor of Chemistry with tenure, 1979 - 1984.
Professor of Chemistry, 1984 - present.
Chancellor's Professor, 2007 - present.
Imperial College of Science and Technology, London, England
Visiting Professor of Chemistry, July - December 1985.

AWARDS AND HONORS

- Loren T. Jones Award for Outstanding Teaching, Purdue University School of Science at Indianapolis, May 1981.
- Research Award, Purdue University School of Science at Indianapolis, 1983.
- NCU Fellowship for Research in Japan, September-October 1992.
- 1995 Chancellor's Award for Excellence in Teaching, 1995. This award, the highest campus honor given for teaching at IUPUI, is given annually to a single faculty member in the university.
- 1996 President's Award for Distinguished Teaching, 1996. One of five awardees for the Indiana University System (eight campuses).
- Election to FACET (Faculty Colloquium on Excellence in Teaching), 1998. One of seven faculty for IUPUI.
- Closing Plenary Lecture, European Peptide Symposium, France, 2000.
- Lecturer, Wageningen Symposium on Diversity in Organic Chemistry, Netherlands, 2002.
- Teaching Award, School of Science, IUPUI, May 2006.
- Chancellors Professor, May 2007.

PRESS RELEASES

- "The Synthesis of Amino Acid Derivatives by Phase-Transfer Catalysis," *Chemical & Engineering News*, September 17, 1979, page 24.
- "The Stereoselective Synthesis of α -Amino Acids by Phase-Transfer Catalysis," *Chemical & Engineering News*, April 10, 1989, pages 25-27.
- "Solid-Phase Unnatural Peptide Synthesis," *Chemical & Engineering News*, July 8, 1996, page 32.
- "The Enantioselective Synthesis of α -Amino Acid Derivatives via Organoboranes," *Chemical & Engineering News*, August 12, 2002, page 30.

EDITORIAL WORK

- "Annual Reports in Organic Synthesis," (with L.G. Wade, Jr.), Academic Press, NY, 1978-1985. (My responsibility: annual preparation of 200-250 pages of camera-ready copy from abstracting 50 primary journals for carbon-carbon bond-forming reactions).
- "Current Awareness Profile in Phase-Transfer Reactions," Chemical Information Center, Bloomington, IN 1981-1985.
- " α -Amino Acid Synthesis," *Tetrahedron*, Symposium-in-Print, (Issue 17) M.J. O'Donnell, Invited Guest Editor, Pergamon, London, 1988.

SOCIETIES

American Chemical Society
 Program Chairman, Indianapolis Section, 1979-1980
 Visiting Associate, National ACS Committee on Professional Training, 1989-1991
 The Chemical Society (London)
 The Belgian Chemical Society
 Phi Lambda Upsilon National Chemistry Honorary Fraternity
 Phi Eta Sigma Honorary Fraternity

REVIEWING

Papers Reviewed for:

Accounts of Chemical Research	Synthesis
Journal of the American Chemical Society	Tetrahedron
Journal of Organic Chemistry	Tetrahedron Asymmetry
Journal of Combinatorial Chemistry	Tetrahedron Letters
Organic Letters	Industrial & Engineering Chemistry Research
Proc. Nat. Acad. Sci. (USA)	Journal of Molecular Catalysis
SYNLETT	

Proposals Reviewed for:

National Science Foundation	Petroleum Research Fund (Types AC and B)
National Institutes of Health	Research Corporation

RESEARCH INTERESTS

Synthetic organic chemistry, new synthetic methods in amino acid, peptide and peptidomimetic chemistry, the application of phase-transfer reactions to synthesis, asymmetric synthesis using catalytic enantioselective phase-transfer reactions and organometallic catalysis, combinatorial chemistry, solid-phase synthesis.

PUBLICATIONS

Journal Articles

- M.J. O'Donnell, J.M. Boniece and S.E. Earp, "The Synthesis of Amino Acids by Phase-Transfer Reactions," *Tetrahedron Lett.*, 2641 (1978).
- M.J. O'Donnell and T.M. Eckrich, "The Synthesis of Amino Acid Derivatives by Catalytic Phase-Transfer Alkylations," *Tetrahedron Lett.*, 4625 (1978).
- K.B. Wiberg and M.J. O'Donnell, "Preparation and Diels-Alder Reactions of the [n](1,4)Naphthalenophanes. Isolation of a Paddlane Derivative Containing the Tricyclo[14.2.2.2^{1,6}]Docosane Ring System," *J. Amer. Chem. Soc.*, **101**, 6660 (1979).
- P. Michel, M.J. O'Donnell, R. Biname, A.M. Hesbain-Frisque, L. Ghosez, J.P. Declercq, G. Germain, E. Arte and M. VanMeerssche, "Vicinal Alkylation of Olefins. Regio- and Stereoselective Addition of [C_m + C_n] Units of Cyclopentadiene," *Tetrahedron Lett.*, **21**, 2577 (1980).
- M.J. O'Donnell and R.L. Polt, "A Mild and Efficient Route to Schiff Base Derivatives of Amino Acids," *J. Org. Chem.*, **47**, 2663 (1982).
- L. Ghosez, J.P. Antoine, E. Deffense, M. Navarro, V. Libert, M.J. O'Donnell, W.A. Bruder, K. Willey and K. Wojciechowski, "Synthesis of Amino Acids. Alkylation of Aldimine and Ketimine Derivatives of Glycine Ethyl Ester

- under Various Phase-Transfer Conditions," *Tetrahedron Lett.*, **23**, 4255 (1982).
12. M.J. O'Donnell, B. LeClef, D.B. Rusterholz, L. Ghosez, J.P. Antoine, M. Navarro, " α -Methyl Amino Acids by Catalytic Phase-Transfer Alkylations," *Tetrahedron Lett.*, **23**, 4259 (1982).
 15. M.J. O'Donnell, W.A. Bruder, T.M. Eckrich, D.F. Shullenberger and G.S. Staten, "Simple Syntheses of the Amino Acids: 1-Aminocyclopropane-1-Carboxylic Acid, Cycloleucine and 2,6-Diaminopimelic Acid," *Synthesis*, 127 (1984).
 16. M.J. O'Donnell, K. Wojciechowski, L. Ghosez, M. Navarro, F. Sainte and J.P. Antoine, "Alkylation of Protected Amino Acid Derivatives in the Presence of Potassium Carbonate," *Synthesis*, 313 (1984).
 17. M.J. O'Donnell, W.A. Bruder, B.W. Daugherty, D. Liu and K. Wojciechowski, "Nitrogen Alkylation of Schiff Bases and Amidines as a Route to N-Alkyl Amino Acids," *Tetrahedron Lett.*, **25**, 3651 (1984).
 19. M.J. O'Donnell, W.D. Bennett and R.L. Polt, "Preparation of an Electrophilic Glycine Cation Equivalent and Its Reaction with Heteroatom Nucleophiles," *Tetrahedron Lett.*, **26**, 695 (1985).
 20. M.J. O'Donnell and J.B. Falmagne, "The Synthesis of Amino Acids by Reaction of an Electrophilic Glycine Cation Equivalent with Carbon Nucleophiles," *Tetrahedron Lett.*, **26**, 699 (1985).
 21. M.J. O'Donnell, C. Barney and J.R. McCarthy, "A Convenient Synthesis of erythro- and threo-3-Fluorophenylalanine from a Protected Glycine Synthone," *Tetrahedron Lett.*, **26**, 3067 (1985).
 22. M.J. O'Donnell and J.B. Falmagne, "The Synthesis of Amino Acids via Organoboranes," *Chem. Commun.*, 1168 (1985).
 25. J.R. McCarthy, C.L. Barney, M.J. O'Donnell and J.C. Huffman, "New Pathway for the Reaction of Difluorocarbene with Imines," *Chem. Commun.*, 469 (1987).
 27. M.J. O'Donnell and W.D. Bennett, "The Synthesis of Amino Acids by Reaction of an Electrophilic Glycine Cation Equivalent with Neutral Carbon Nucleophiles," *Tetrahedron*, **44**, 5389 (1988).
 28. M.J. O'Donnell, W.D. Bennett, W.A. Bruder, W.N. Jacobsen, K. Knuth, B. LeClef, R.L. Polt, F.G. Bordwell, S.R. Mrozack and T.R. Cripe, "Acidities of Glycine Schiff Bases and Alkylation of their Conjugate Bases," *J. Am. Chem. Soc.*, **110**, 8520 (1988).
 29. M.J. O'Donnell and D.B. Rusterholz, "Synthesis of α -Methylhistidine by Catalytic Phase-Transfer Alkylations," *Synth. Commun.*, **19**, 1157 (1989).
 30. M.J. O'Donnell, W.D. Bennett and S. Wu, "The Stereoselective Synthesis of α -Amino Acids by Phase Transfer Catalysis," *J. Am. Chem. Soc.*, **111**, 2353 (1989) [Press release: *Chemical & Engineering News*, April 10, 1989, p. 25-27]
 31. M.J. O'Donnell, W.D. Bennett, W.N. Jacobsen, Y.-a. Ma and J.C. Huffman, "Selective Monophenylation of an Active Methylene Compound," *Tetrahedron Lett.*, **30**, 3909 (1989).
 32. M.J. O'Donnell, W.D. Bennett, W.N. Jacobsen and Y.-a. Ma, "Phenylation of Amino Acid Derivatives: A New Route to α -Phenyl α -Substituted Amino Acids," *Tetrahedron Lett.*, **30**, 3913 (1989).
 33. M.J. O'Donnell, A. Arasappan, W.J. Hornback and J.C. Huffman, "Preparation and Wittig Reactions of an α -Keto Amino Acid Derivative," *Tetrahedron Lett.*, **31**, 157 (1990).
 34. M.J. O'Donnell, X. Yang and M. Li, "2-Aza- π -Allylpalladium Complexes for the Synthesis of β -Carboxyaspartic Acid (ASA) Derivatives," *Tetrahedron Lett.*, **31**, 5135 (1990).
 35. K.B. Lipkowitz, M.W. Cavanaugh, B. Baker and M.J. O'Donnell, "Theoretical Studies in Molecular Recognition: Asymmetric Induction of Benzophenone Imine Ester Enolates by the Benzylcinchoninium Ion," *J. Org. Chem.*, **56**, 5181 (1991).
 36. M.J. O'Donnell, G.K. Cook and D.B. Rusterholz, "Oxygen Alkylation of Schiff Base Derivatives of Amino Acids," *Synthesis*, 989 (1991).
 37. M.J. O'Donnell and S. Wu, "A Catalytic Enantioselective Synthesis of α -Methyl Amino Acid Derivatives by Phase-Transfer Catalysis," *Tetrahedron: Asymmetry*, **3**, 591 (1992).

39. M.J. O'Donnell, T.P. Burkholder, V.V. Khau, R.W. Roeske and Z. Tian, "Selective Alkylation of Protected Peptide Derivatives by Phase-Transfer Catalysis," *Pol. J. Chem.*, **68**, 2477 (1994).
40. M.J. O'Donnell, S. Wu and J.C. Huffman, "A New Active Catalyst Species for Enantioselective Alkylation by Phase-Transfer Catalysis," *Tetrahedron*, **50**, 4507 (1994).
41. M.J. O'Donnell, L.K. Lawley, P.R. Pushpavanam, A. Burger, F.G. Bordwell and X.-M. Zhang, "Preparation of an α -Aminophosphonate Cation Equivalent and its Reaction with Organoboranes," *Tetrahedron Lett.*, **35**, 6421 (1994).
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43. M.J. O'Donnell, C. Zhou, A. Mi, N. Chen, J.A. Kyle and P.G. Andersson, "Palladium-Catalyzed Reaction of a Malonate Anion with a Glycine Cation Equivalent: Bis-Phosphine Ligands and in situ Catalyst Formation," *Tetrahedron Lett.*, **36**, 4205 (1995).
52. M.J. O'Donnell, C. Zhou and N. Chen, "Preparation of Optically Active β -Carboxyaspatic Acid Derivatives via Pd(0)-Catalyzed Asymmetric Substitution of Schiff Base Acetates," *Tetrahedron: Asymmetry*, **7**, 621 (1996).
53. M.J. O'Donnell, C. Zhou and W.L. Scott, "Solid-Phase Unnatural Peptide Synthesis (UPS)," *J. Am. Chem. Soc.*, **118**, 6070 (1996) [Press release: *Chemical & Engineering News*, July 8, 1996, p. 32].
57. W.L. Scott, C. Zhou, Z. Fang and M.J. O'Donnell, "The Solid-Phase Synthesis of α,α -Disubstituted Unnatural Amino Acids and Peptides (di-UPS)," *Tetrahedron Lett.*, **38**, 3695 (1997).
58. M.J. O'Donnell, N. Chen, C. Zhou, A. Murray, C.P. Kubiak, F. Yang and G.G. Stanley, "Efficient Catalytic Enantioselective Reaction of a Glycine Cation Equivalent with Malonate Anions via Palladium Catalysis," *J. Org. Chem.*, **62**, 3962 (1997).
59. M.J. O'Donnell, Z. Fang, X. Ma and J.C. Huffman, "New Methodology for the Synthesis of α,α -Dialkylamino Acids using the 'Self-Regeneration of Stereocenters' Method: α -Ethyl- α -Phenylglycine," *Heterocycles*, Invited Paper in Memory of Professor S. Yamada, **46**, 617 (1997).
60. M.J. O'Donnell, C.W. Lugar, R.S. Pottorf, C. Zhou, W.L. Scott and C.L. Cwi, "Solid-Phase Synthesis of Unnatural Amino Acids using Unactivated Alkyl Halides," *Tetrahedron Lett.*, **38**, 7163 (1997).
61. D.L. Griffith, M.J. O'Donnell, R.S. Pottorf, W.L. Scott and J.A. Porco, Jr., "Tandem UPS: Sequential Mono- and Dialkylation of Resin-Bound Glycine via Automated Synthesis," *Tetrahedron Lett.*, **38**, 8821 (1997).
62. E. Dominguez, M.J. O'Donnell and W.L. Scott, "Solid-Phase Synthesis of Substituted Glutamic Acid Derivatives via Michael Addition Reactions," *Tetrahedron Lett.*, **39**, 2167 (1998).
63. M.J. O'Donnell, F. Delgado, C. Hostettler and R. Schwesinger, "An Efficient Homogeneous Catalytic Enantioselective Synthesis of α -Amino Acid Derivatives," *Tetrahedron Lett.*, **39**, 8775 (1998).
64. M.J. O'Donnell, F. Delgado, M.D. Drew, R.S. Pottorf, C. Zhou and W.L. Scott, "Solid-Phase Synthesis of Unnatural α -Amino Acid Derivatives Using a Resin-Bound Glycine Cation Equivalent," *Tetrahedron Lett.*, **40**, 5831 (1999).
65. M.J. O'Donnell, F. Delgado and R.S. Pottorf, "Enantioselective Solid-Phase Synthesis of α -Amino-Acid Derivatives," *Tetrahedron*, **55**, 6347 (1999).
66. M.J. O'Donnell, M.D. Drew, R.S. Pottorf, and W.L. Scott, "UPS on Weinreb Resin: A Facile Solid-Phase Route to Aldehyde and Ketone Derivatives of "Unnatural" Amino Acids and Peptides," *J. Comb. Chem.*, **2**, 172 (2000).
68. W.L. Scott, F. Delgado, K. Lobb, R. Pottorf, M.J. O'Donnell, "Solid-Phase Synthesis of Amino Amides and Peptide Amides with Unnatural Side Chains," *Tetrahedron Lett.* **42**, 2073 (2001).
70. M.J. O'Donnell and F. Delgado, "Enantiomeric Enrichment of α -Amino Acid Derivatives: Recrystallization of N-Fmoc α -Amino Acid t-Butyl Esters," *Tetrahedron*, **57**, 6641 (2001).
72. M.J. O'Donnell, F. Delgado, E. Dominguez, J. de Blas and W.L. Scott, "Enantioselective Solution- and Solid-Phase Synthesis of Glutamic Acid Derivatives via Michael Addition Reactions," *Tetrahedron: Asymmetry* **12**, 821 (2001).

73. W.L. Scott, M.J. O'Donnell and J. Alsina, "A Solid-Phase Synthetic Route to Unnatural Amino Acids with Diverse Side Chain Substitutions," *J. Org. Chem.*, **67**, 2960 (2002).
74. M.J. O'Donnell, M.D. Drew, J.T. Cooper, F. Delgado and C. Zhou, "The Enantioselective Synthesis of α -Amino Acid Derivatives via Organoboranes," *J. Am. Chem. Soc.*, **124**, 9348 (2002) [Press release: *Chemical & Engineering News*, August 12, 2002, p. 30].
75. M.J. O'Donnell, J.T. Cooper and M. Mader, "Acyclic Stereoselective Boron Alkylation Reactions for the Asymmetric Synthesis of β -Substituted α -Amino Acid Derivatives," *J. Am. Chem. Soc.*, **125**, 2370 (2003).
76. W.L. Scott, J. Alsina and M.J. O'Donnell, "The Manual and Automated Solid-Phase Synthesis of α -Substituted Prolines and Homologues," *J. Comb. Chem.*, **5**, 684 (2003).
77. M.J. O'Donnell, J. Alsina and W.L. Scott, "Solid-Phase Synthesis and Utilization of Side-Chain Reactive Unnatural Amino Acids," *Tetrahedron Lett.*, **44**, 8403 (2003).
79. W.L. Scott, J. Alsina, J. H. Kennedy and M. J. O'Donnell, "Solid-Phase Synthesis of Constrained Terminal and Internal Lactam Peptidomimetics," *Org. Lett.* **6**, 1629 (2004).
80. J. Alsina, W.L. Scott and M.J. O'Donnell, "Solid-Phase Synthesis of α -Substituted Proline Hydantoins and Analogs," *Tetrahedron Lett.* **46**, 3131 (2005).
81. P.V. Ramachandran, S. Madhi, L. Bland-Berry, M.V.R. Reddy and M. J. O'Donnell, "Catalytic Enantioselective Synthesis of Glutamic Acid Derivatives via Tandem Conjugate Addition-Elimination of Activated Allylic Acetates under Chiral PTC Conditions," *J. Am. Chem. Soc.*, **127**, 13450 (2005).
82. P.V. Ramachandran, S. Madhi, M.J. O'Donnell, "Regioselective Hydroboration-Oxidation and -Amination of Fluoro-Substituted Styrenes," *J. Fluorine Chem.* **127**, 1252 (2006).
84. M.J. O'Donnell, J.D. Keeton, V.V. Khau and J.C. Bollinger, "The Regioselective α -Alkylation of the Benzophenone Imine of Glycinamide, Alaninamide and Related Derivatives," *Can. J. Chem.* **84**, 1301 (2006).
85. P.V. Ramachandran, S. Madhi, M.J. O'Donnell, "Synthesis of Fluorinated Glutamic Acid Derivatives via Vinylalumination," *J. Fluorine Chem.* **128**, 78 (2007).
86. W.L. Scott, J.G. Martynow, J.C. Huffman, M.J. O'Donnell, "The Solid-Phase Synthesis of Multiple Classes of Peptidomimetics from Versatile Resin-Bound Aldehyde Intermediates," *J. Am. Chem. Soc.* **129**, 7077 (2007).
87. W. L. Scott, M. J. O'Donnell, "Distributed Drug Discovery, Part 1: Linking Academics and Combinatorial Chemistry to Find Drugs for Developing World Diseases," *J. Comb. Chem.* **11**, 3 (2009).
88. W. L. Scott, J. Alsina, C. O. Audu, J. L. Dage, E. Babaev, L. Cook, L. A. Goodwin, J. G. Martynow, D. Matosiuk, M. Royo, J. G. Smith, A. T. Strong, K. Wickizer, E. M. Woerly, Z. Zhou, M. J. O'Donnell, "Distributed Drug Discovery, Part 2: Global Rehearsal of Alkylating Agents for the Synthesis of Resin-Bound Unnatural Amino Acids and Virtual D³ Catalog Construction," *J. Comb. Chem.* **11**, 14 (2009).
89. W. L. Scott, C. O. Audu, J. L. Dage, L. A. Goodwin, J. G. Martynow, L. K. Platt, J. G. Smith, A. T. Strong, K. Wickizer, E. M. Woerly, M. J. O'Donnell, "Distributed Drug Discovery, Part 3: Using D³ Methodology to Synthesize Analogs of an Anti-Melanoma Compound," *J. Comb. Chem.* **11**, 34 (2009).
90. J. E. Green, D. M. Bender, S. Jackson, M. J. O'Donnell, J. R. McCarthy, "Mitsunobu Approach to the Synthesis of Optically Active α,α -Disubstituted Amino Acids," *Org. Lett.* **11**, 807 (2009).
91. W. L. Scott, Z. Zhou, J. G. Martynow, M. J. O'Donnell, "Solid-Phase Synthesis of Amino- and Carboxyl-Functionalized Unnatural α -Amino Acids," *Org. Lett.* **11**, 3558 (2009).
92. W. L. Scott, Z. Zhou, P. Zajdel, M. Pawlowski, M. J. O'Donnell, "Solid-Phase Synthetic Route to Multiple Derivatives of a Fundamental Peptide Unit," *Molecules*, **15**, 4961 (2010).

Reviews

1. L. Ghosez and M.J. O'Donnell, "Pericyclic Reactions of Cumulenes," in "Pericyclic Reactions," Vol. 2, A.P. Marchand and R. Lehr, Eds., Academic Press, NY, pp. 79-140, 1977.
38. M.J. O'Donnell, "Asymmetric Phase-Transfer Reactions," in *Catalytic Asymmetric Synthesis*, I. Ojima, Ed., Verlag Chemie, New York, 1993, Chap. 8.
45. M.J. O'Donnell, "Benzophenone Imine," in *Encyclopedia of Reagents for Organic Synthesis*, L.A. Paquette, Editor-in-Chief, John Wiley & Sons, New York, 1996, Vol. 1, p. 293.
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50. M.J. O'Donnell, "Ethyl N-(Diphenylmethylene)-2-acetoxglycinate," in *Encyclopedia of Reagents for Organic Synthesis*, L.A. Paquette, Editor-in-Chief, John Wiley & Sons, New York, 1996, Vol. 4, p. 2234.
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69. M.J. O'Donnell, "The Preparation of Optically Active α -Amino Acids from the Benzophenone Imines of Glycine Derivatives," *Aldrichimica Acta*, **34**, 3 (2001).
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Books

5. "Annual Reports in Organic Synthesis - 1978," L.G. Wade, Jr. and M.J. O'Donnell, Eds., Academic Press, NY, 1979 (for a book review of this volume, see: *J. Amer. Chem. Soc.*, **102**, 3664 (1980)).
7. "Annual Reports in Organic Synthesis - 1979," L.G. Wade, Jr. and M.J. O'Donnell, Eds., Academic Press, NY, 1980 (for a book review of this volume, see: *J. Amer. Chem. Soc.*, **103**, 1911 (1980)).
8. "Annual Reports in Organic Synthesis - 1980," L.G. Wade, Jr. and M.J. O'Donnell, Eds., Academic Press, NY, 1981 (for a book review of this volume, see: *J. Amer. Chem. Soc.*, **104**, 4737 (1982)).
10. "Annual Reports in Organic Synthesis - 1981," L.G. Wade, Jr. and M.J. O'Donnell, Eds., Academic Press, NY, 1982 (for a book review of this volume, see: *J. Amer. Chem. Soc.*, **105**, 5183 (1982)).
14. "Annual Reports in Organic Synthesis - 1982," L.G. Wade, Jr. and M.J. O'Donnell, Eds., Academic Press, NY, 1983.
18. "Annual Reports in Organic Synthesis - 1983," M.J. O'Donnell and L. Weiss, Eds. Academic Press, NY, 1984.

23. "Annual Reports in Organic Synthesis - 1984," M.J. O'Donnell and L. Weiss, Eds. Academic Press, NY, 1985.
24. "Annual Reports in Organic Synthesis - 1985," M.J. O'Donnell and E.F.V. Scriven, Eds., Academic Press, NY, 1986.

Symposium-in-Print

26. " α -Amino Acid Synthesis," *Tetrahedron*, Symposium-in-Print, (Issue 17) M.J. O'Donnell, Ed., Pergamon Press, London, 1988.

Proceedings

13. M.J. O'Donnell, W. Bruder, K. Wojciechowski, L. Ghosez, M. Navarro, F. Sainte and J.P. Antoine, "The Synthesis of Amino Acids Using Phase-Transfer Catalyzed Alkylations with Potassium Carbonate as Base," *Peptides: Structure and Function, Proc. 8th Amer. Pept. Symp.*, 151 (1983).
71. M.J. O'Donnell and W.L. Scott, "Unnatural Amino Acid and Peptide Synthesis" in *Peptides 2000*. Martinez J, Fehrentz J-A, Eds., EDK: Paris, 2001, 31.

Patents

44. M.J. O'Donnell, S. Wu, I. Esikova and A. Mi, "Catalytic Enantioselective Synthesis of α -Amino Acid Derivatives by Phase-Transfer Catalysis," U.S. Patent Number 5,554,753, September 10, 1996.
83. G.K. Mulholland, M.J. O'Donnell, F.T. Chin and F. Delgado, "Nucleophilic Approach for Preparing Radiolabeled Imaging Agents and Associated Compounds," U.S. Patent 7,115,766, 2006.

Abstracts

- F.T. Chin, G.K. Mulholland and M.J. O'Donnell, "Nucleophilic Approaches to Fluorine-18 Labeled Fluorophenol." Book of Abstracts, 216th ACS National Meeting, Boston, August 23-27, 1998, MEDI-352 (*Chem. Abstr.* 1998:529837).
- P. Romanovskis, D. Mendel, M.J. O'Donnell, W.L. Scott, A.F. Spatola and C. Zhou, "Unnatural Peptide Synthesis (UPS): A Positional Scan Study." *Peptides: Frontiers of Peptide Science, Proceedings of the 15th American Peptide Symposium*, Nashville, June 14-19, 1997, 319-320 (*Chem. Abstr.* 1999:396545).
- M.J. O'Donnell and J.T. Cooper, "Stereoselective Synthesis of β -branched α -Amino Acids." Abstracts of Papers, 222nd ACS National Meeting, Chicago, August 26-30, 2001, ORGN-196 (*Chem. Abstr.* 2001:640559).
- K.M. Diaz, X. Deng, M.J. O'Donnell, W.L. Scott and E.C. Long, "Synthesis of Amino-Pyrimidine- and Amino-Pyridine-containing Ni(II)-Metallopeptides and Their Potential Interactions with DNA." Abstracts, 36th Central Regional ACS Meeting, Indianapolis, June 2-4, 2004, GEN-197 (*Chem. Abstr.* 2004:435049).
- Scott, W.L. and M.J. O'Donnell, "Utilizing Educational Laboratories for Distributed Drug Discovery." Abstracts, 36th Central Regional ACS Meeting, Indianapolis, June 2-4, 2004, INV-031 (*Chem. Abstr.* 2004:435230).
- M.J. O'Donnell, "Schiff Base Esters: Versatile Starting Materials for the Synthesis of Amino Acids." Abstracts, 36th Central Regional ACS Meeting, Indianapolis, June 2-4, 2004, INV-092 (*Chem. Abstr.* 2004:435275).

GRANTS

- "The Alkylation of Some Nitrogen-Containing Compounds,"
Eli Lilly and Company, Research Grant, 1977-1978.
- "The Alkylation of Schiff Bases,"
American Chemical Society, Petroleum Research Fund Type B Grant, 1977-1979.
- "The Synthesis of Amino Acids by Phase-Transfer Reactions,"
Research Corporation, Cottrell Research Grant, 1978-1979.
- "The Synthesis of Amino Acids by Phase-Transfer Reactions," (with L. Ghosez),
North Atlantic Treaty Organization (NATO), Research Grant, 1978-1982.
- "Amino Acid Synthons,"
American Chemical Society, Petroleum Research Fund Type B Grant, 1979-1981.

"Schiff Base Synthons in Amino Acid Chemistry,"

National Institutes of Health, Research Grant (RO1-GM28193), 1980-1984.

"Purchase of NMR and IR Equipment for Undergraduate Teaching and Research,"

Co-PI's: P.W. Rabideau and M.J. O'Donnell, Eli Lilly (25%), Merrell-Dow (25%) and University (50%), 1982.

"The Synthesis of Amino Acids by Phase-Transfer Alkylations,"

(with L. Ghosez), North Atlantic Treaty Organization (NATO), Research Grant, 1983-1987.

"Schiff Base Synthons in Amino Acid Chemistry,"

National Institutes of Health, Research Grant (RO1-GM28193), 1985-1989.

"HPLC Fluorescence Detector,"

National Institutes of Health, Small Instrumentation Program, 1987.

"Purchase of a Superconducting NMR,"

National Science Foundation, Chemical Instrumentation Program, 1988. P.W. Rabideau, PI (Project Directors: W. Fife, M.J. O'Donnell, and F. Schultz).

"Preparation of Key Intermediates for the Synthesis of β -Lactam Antibiotics,"

Eli Lilly and Company, 1990-1993.

"Schiff Base Synthons in Amino Acid Chemistry,"

National Institutes of Health, Research Grant (RO1-GM28193), 1991-1995.

"Research Agreement with SIPSY S.A.,"

SIPSY S.A., France, 1994-1995.

"Lilly Visiting Fellow Award," (postdoctoral support, one year), Eli Lilly and Company, 1996.

"Schiff Base Synthons in Amino Acid Chemistry," National Institutes of Health, Research Grant (RO1-GM28193), 1997-2000.

"Stereodefined Olefin Synthesis via Tandem Pd-Catalysis," National Institutes of Health, Research Grant R15 GM/OD55904, 1997-2000. *This grant was originally obtained by Professor Michael Organ, who left the university. I was approved as the new PI on this grant, which was used for the Ph.D. project of Jeremy Cooper.*

"Development of Targeted Libraries by Unnatural Peptide Synthesis," (postdoctoral support, two years), Eli Lilly and Company, 2000-2002.

"Schiff Base Synthons in Amino Acid Chemistry," National Institutes of Health, Research Grant (RO1-GM28193), 2004-2009.

"Distributed Discovery in Undergraduate Organic Chemistry: Combined Solid-Phase Synthesis of Amino Acid Derivatives," (with W.L. Scott), Dreyfus Foundation, 2004-2008.

THESES SUPERVISED

1. T.P. Burkholder, "Alkylation of Imine Anions Derived from Primary Amines and Dipeptides by Phase-Transfer Methods," Master's Degree, IUPUI, August 1982.
2. K.A. Willey, "An HPLC Study of the Phase-Transfer Catalyzed Alkylations of Schiff Base Derivatives of Amino Esters," Master's Degree, IUPUI, August 1982.
3. F. Victor, "Studies into the t-Alkylation of α -Amino Acids by New and Direct Routes," Master's Degree, IUPUI, May 1983.
4. B.W. Daugherty, "New Synthetic Routes to N-Methyl Amino Acids," Master's Degree, IUPUI, August 1983.
5. G.K. Cook, "Transesterification of Schiff Base Protected α -Amino Acid and Dipeptide Esters," Master's Degree, IUPUI, February 1984.
6. C.L. Barney, "Preparation of β -Fluorinated- α -Amino Acids by Alkylation and Subsequent Deprotection of a Glycine Synthron," Master's Degree, IUPUI, December 1984.
7. D.F. Schullenberger, "Preparation of Schiff-Base-Protected Amides and Peptide Derivatives from the Corresponding

- Tetrabutylammonium Salts," Master's Degree, IUPUI, August 1985.
8. W.D. Bennett, "The Preparation and Use of Amino Acid Schiff Base Cation Synthons," Ph.D. Degree, Indiana University (course work completed in Bloomington, research completed in Indianapolis), August 1986.
 9. W.N. Jacobsen, "Phenylation of Protected Amino Acid Derivatives as a New Route to α -Phenylsubstituted Amino Acids," Master's Degree, IUPUI, December 1986.
 10. T.B. Nguyen, "Novel Approach to Vinyl Glycine Synthesis," Master's Degree, IUPUI, December 1986.
 11. L. Bhagavatula, "2-Azaallenium Cation Derivatives in Amino Acid Synthesis," Master's Degree, IUPUI, August 1987.
 12. K.B. Sippy, "A Novel Synthesis of 3,3,3-Trifluoroalanine," Master's Degree, IUPUI, August 1987.
 13. Todd Grote, "New Preparations of *erythro* β -Hydroxy- α -Amino Acids," Master's Degree, IUPUI, December 1988.
 14. Vien Van Khau, "Selective Alkylation of Protected Schiff Base Dipeptide Derivatives by Catalytic Phase Transfer Alkylations," Master's Degree, IUPUI, December 1988.
 15. Xiaobei Yang, "Synthesis of β -Carboxyaspartic Acid *via* Palladium Catalyzed Reactions," Master's Degree, IUPUI, August 1989.
 16. Ashok Arasappan, "Synthesis of α , β -Dehydroamino Acid Derivatives via C_{α} - C_{β} Bond Formation, Master's Degree, IUPUI, August 1989.
 17. Min Li, "Synthesis of β,γ -Unsaturated α -Amino Acids via Zr-catalyzed Carbometalation and Pd-Catalyzed Coupling Reactions," Master's Degree, IUPUI, December 1990.
 18. Nancy J. Snyder, "A Study of the Synthesis of 3,3-Difluoroamino Acids," Master's Degree, IUPUI, May 1991.
 19. Ying Qiao, "Synthesis of α,β -Dehydroamino Acid Derivatives via Palladium Catalyzed Coupling Reactions of Organotin Reagents with Organic Halides," Master's Degree, IUPUI, December 1991.
 20. Pradeep Pushpavanam, "Synthesis of 1-Aminoalkylphosphonates via Organoborane Reactions," Master's Degree, IUPUI, May 1992.
 21. Linda K. Lawley, "The Synthesis of α -Aminophosphonic Acid Derivatives via an Electrophilic of α -Aminophosphonate," Master's Degree, IUPUI, May 1992.
 22. Shengde Wu, "Catalytic Enantioselective Synthesis of α -Amino Acids and α,α -Dialkyl Amino Acids by Phase-Transfer Catalysis," Ph.D. Degree, Purdue University, August 1992.
 23. Theresa Nahreini, "The Catalytic, Enantioselective Synthesis of α -Amino-Acid Derivatives by Phase-Transfer Catalysis: A Kinetic Study," Master's Degree, IUPUI, May 1993.
 24. Jeffrey A. Kyle, "Stereocontrolled Synthesis of Novel 2,3-Diaminosuccinic Acid Derivatives via Oxidative Coupling Reactions and Palladium Catalyzed Coupling Reactions," Master's Degree, IUPUI, August 1994.
 25. Xiaojun Ma, "Stereoselective Synthesis of α -Alkyl- α -Aryl Amino Acids via Oxazolidin-5-one Intermediates," Master's Degree, IUPUI, December 1995.
 26. Ning Chen, "Catalytic Asymmetric Synthesis of β -Carboxyaspartic Acid Derivatives Using Chiral Palladium Phosphine Complexes," Master's Degree, IUPUI, August 1996.
 27. Charles W. Lugar, III, "Solution and Solid Phase Studies of Amino Acid Derivatives," Master's Degree, IUPUI, May 1997.
 28. Michael Robertson, "Stereoselective Solid-Phase Synthesis of Unnatural Peptides," Master's Degree, IUPUI, May 2000.
 29. Frederick T. Chin, "Novel Approach to the Synthesis of 6-[F-18]-Fluoro-(Meta)-Tyrosine and Related [F-18]-Fluorocatecholamines," Ph.D. Degree, Purdue University, December 2000.
 30. Jeremy T. Cooper, "The Stereoselective Synthesis of β -Branched α -Amino Acid Derivatives via Organoboranes," Ph.D. Degree, Purdue University, December 2001.
 31. Jeremy Keeton, "The Regioselective Alkylation of the Benzophenone Imine of Alaninamide Derivatives and a Regioselective Palladium-Catalyzed Cross-Coupling in the Total Synthesis of Papulacandin D," Master's Degree, IUPUI, November 2002.

32. Jonathan Green, Mitsunobu Approach to the Synthesis of Optically Active α,α -Disubstituted Amino Acids, Master's Degree, IUPUI, August 2005.
33. Eli A. Stoddard, The Preparation of Optically Active Stable Isotope Labeled α -Amino Acids and Their Utility in the Synthesis of Other Molecules, Master's Degree, IUPUI, December, 2007.
34. Lindsey Fischer, Solid-Phase Synthesis of N-Carboxyalkyl Unnatural Amino Acids," Master's Degree, IUPUI, August, 2010.

PAPERS PRESENTED

"The Practical Synthetic Design of Natural Products," The Scientific Society of Belgium, Louvain-la-Neuve, Belgium, March 29, 1974.

"Vicinal Carbofunctionalization of Olefins," First International IUPAC Congress on Organic Synthesis, Louvain-la-Neuve, Belgium, August 29, 1974 (Press release: *Chem. Eng. News*, September 16, 1974, page 15).

"A New Method of Carbon Chain Lengthening," The Chemical Society (London), Leicester, England, September 24, 1974.

"Synthetic Routes to the Paddlanes," International Symposium on the Chemistry of Strained Rings, Binghamton, NY, May 27, 1977.

"The Synthesis of Amino Acids by Phase-Transfer Alkylations," 174th National ACS Meeting, Chicago, IL, August 31, 1977. Abstract: ORGN 123.

"Amino Acid Synthesis by Phase-Transfer Alkylations of Schiff Base," Symposium on the 10th Anniversary of Phase-Transfer Catalysis, 1977 Central Regional ACS Meeting, Charleston, W.Va., October 13, 1977. Abstract: ORGN 11.

"The Synthesis of Some Cyclic Amino Acids by Phase-Transfer Reactions," 175th National ACS Meeting, Anaheim, CA, March 16, 1978. Abstract: ORGN 180.

"The Synthesis of Amino Acids by Phase-Transfer Reactions," Joint Central-Great Lakes Regional ACS Meeting, Indianapolis, IN, May 25, 1978. Abstract: ORGN 54.

"The Synthesis of Amino Acids by Phase-Transfer Reactions," EUCHEM Conference on Phase-Transfer Catalysis, Gargnano, Italy, June 5, 1978. Abstract: ORGN 4.

"The Synthesis of Amino Acids by Phase-Transfer Reactions," Western Regional ACS Meeting, San Francisco, CA, September 28, 1978. Abstract: ORGN 115.

"The Synthesis of Amino Acids by Phase-Transfer Reactions," Indiana Academy of Science, Anderson, Indiana, November 3, 1978. Abstract: *Proceedings of the Indiana Academy of Sciences*, **88**, 129 (1979).

"The Synthesis of Amino Acid Derivatives by Phase-Transfer Alkylations," 178th National ACS Meeting, Washington, DC, September 12, 1979. Abstract: ORGN 125 (Press Release: *Chem. Eng. News*, September 17, 1979, page 24).

"The Acidities of C-H Protons in Imines," 181st National ACS Meeting, Atlanta, GA, March 31, 1981. Abstract: ORGN 91.

" α -Methyl Amino Acid Derivatives by Catalytic Phase-Transfer Alkylations: α -Methyl-p-Tyrosine, -m-Tyrosine and -DOPA," 183rd National ACS Meeting, Las Vegas, NV, April 1, 1982. Abstract: ORGN 198.

- * "New Methods in Amino Acid Synthesis," EUCHEM Conference on Methods in Organic Synthesis, Louvain-la-Neuve, Belgium, July 6, 1982.

"Nitrogen Alkylation of Schiff Bases and Amidines as a Route to N-Alkyl Amino Acids," 185th National ACS Meeting, Seattle, WA, March 25, 1983. Abstract: ORGN 257.

"The Synthesis of Amino Acids Using Phase-Transfer Catalyzed Alkylations with Potassium Carbonate as Base," 8th American Peptide Symposium, Tucson, AZ, May 24, 1983.

- * "The Stereoselective Synthesis of α -Amino Acids by Phase Transfer Catalysis," Eighth Biennial Marvel Symposium on Organic Synthesis, Tucson, AZ, March 13, 1989.

"Preparation and Wittig Reactions of α -Keto Amino Acid Derivatives," 198th National ACS Meeting, Miami Beach, Florida, September 13, 1989. Abstract: ORGN 185.

"2-Aza- π -Allyl Palladium Complexes for the Synthesis of β -Carboxyaspatic Acid (ASA) Derivatives," International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 19, 1989. Abstract: ORGN 273.

* "Enantioselective Synthesis of α -Amino Acids by Phase-Transfer Catalysis," International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 21, 1989. Abstract: ORGN 613.

* "The Enantioselective Synthesis of α -Amino Acids by Phase Transfer Catalysis," 201st ACS National Meeting, Atlanta, Georgia, April 15, 1991, ORGN 132.

"Synthesis of β,γ -Unsaturated Amino Acid Derivatives by Carbometalation-Palladium Catalyzed Coupling of 2-Aza- π -Allylpalladium Complexes," 201st ACS National Meeting, Atlanta, Georgia, April 18, 1991, ORGN 286.

"Catalytic Enantioselective Synthesis of α -Methyl Amino Acid Derivatives by Phase-Transfer Catalysis," 203rd ACS National Meeting, San Francisco, California, April 6, 1992, ORGN 96.

* "The Catalytic Enantioselective Synthesis of α -Amino Acids by Phase-Transfer Catalysis," 24th ACS Central Regional Meeting, Cincinnati, Ohio, May 28, 1992, BIOL 137.

* "The Catalytic Enantioselective Synthesis of α -Amino Acids by Phase-Transfer Catalysis," Symposium on Optically Active Compounds, The Pharmaceutical Society of Japan, Tokyo, Japan, October 1, 1992.

"Selectivity in Amino Acid Synthesis: `Why Not Just Let Nature Do Its Thing?'" Faculty Spotlight Lecture, IUPUI, February 17, 1995.

* "Amino Acid and Peptide Synthesis using Phase-Transfer Catalysis and Other Mild Base Systems," Pacifichem '95 Congress, Honolulu, Hawaii, December 21, 1995, ORGN 1128.

* "Solid-Phase Unnatural Peptide Synthesis (UPS)," (Joint presentation with Dr. W.L. Scott of Lilly), First Lake Tahoe Symposium on Molecular Diversity in Drug Discovery, Tahoe City, California, November 6, 1996.

* "UPS: Unnatural Amino Acid and Peptide Synthesis," 1997 International Phase-Transfer Catalysis Conference, Nagoya, Japan, September 26, 1997, Abstract I-9.

* "Unnatural Amino Acid and Peptide Synthesis," 32nd Central Regional ACS Meeting, Covington, KY, May 18, 2000, ORGN 407.

* "Unnatural Amino Acid and Peptide Synthesis" (Closing Plenary Lecture), European Peptide Symposium, Montpellier, France, September 10-15, 2000.

* "Unnatural Amino Acid and Peptide Synthesis," Wageningen Symposium on Diversity in Organic Chemistry, Wageningen, Netherlands, April 25-26, 2002.

* "The Stereoselective Synthesis of α -Amino Acids via Organoboranes," Gordon Research Conference on Organic Reactions & Processes, Roger Williams University, July 21-26, 2002.

* "Schiff Base Esters: Versatile Starting Materials for the Synthesis of Amino Acids," 36th Central ACS Meeting; Symposium: "At the Frontiers of Organic Synthesis and New Methodologies," Indianapolis, IN, June 2, 2004.

* "Distributed Discovery in the Undergraduate Organic Lab: Combinatorial Solid-Phase Synthesis of Amino Acid Derivatives," 18th Biennial Conference on Chemical Education (BCCE); Symposium: "Combinatorial Chemistry in the Undergraduate Curriculum," Ames, Iowa, July 21, 2004.

- Invited Plenary Lecture

INVITED SEMINARS**Academic**

University of Aachen, GERMANY
 University of Aarhus, DENMARK
 University of Alcalá, SPAIN
 Autònoma University (Barcelona), SPAIN
 University of Akron
 Ball State University
 Bowling Green University
 Brandeis University
 Brigham Young University
 Brown University
 California Institute of Technology
 CNRS, Gif-sur-Yvette (Paris), FRANCE
 University of California, Berkeley
 University of California, Irvine
 Chinese Academy of Sciences, Chengdu, CHINA
 Chinese Academy of Sciences, Shanghai, CHINA
 Columbia University
 University Complutense, Madrid, SPAIN
 University of Durham, ENGLAND
 University of East Anglia, ENGLAND
 Eastern Illinois University
 Ecole Polytechnique, Paris, FRANCE
 University of Edinburgh, SCOTLAND
 University of Freiburg, GERMANY
 Harvard University
 IECB, Bordeaux, FRANCE
 University of Illinois
 University of Illinois (Chicago)
 Illinois Institute of Technology
 Imperial College (London), ENGLAND
 University of Karlsruhe, GERMANY
 Kyoto University, JAPAN
 Leicester University, ENGLAND
 University of Louvain, BELGIUM

University of Louisville
 Ludwig-Maximilians University, Munich, GERMANY)
 Marshall University
 Massachusetts Institute of Technology
 University of Newcastle-upon-Tyne, ENGLAND
 Nagoya City University, JAPAN
 University of Nebraska
 Northwestern University
 Notre Dame University
 University of Nottingham, ENGLAND
 University of Oklahoma
 Osaka University, JAPAN
 Oxford University, ENGLAND
 University of Pisa, ITALY
 University of P. and M. Curie, Paris, FRANCE
 Polish Academy of Sciences, Warsaw, POLAND
 University of Rouen, FRANCE
 Salford University, ENGLAND
 University of California, Santa Cruz
 Scripps Institute (La Jolla)
 Stanford University
 University of Sussex, ENGLAND
 University of Toledo
 Technical University of Clausthal, GERMANY
 Teikyo University, JAPAN
 Tsinghua University, CHINA
 UMIST, Manchester, ENGLAND
 University College (London), ENGLAND
 Valparaíso University
 Wabash College
 Wright State University
 Yale University
 Youngstown State University

Industrial

Beecham Pharmaceuticals, ENGLAND
 Burroughs Wellcome
 Continental Pharma, BELGIUM
 Dow Chemical USA
 DSM Fine Chemicals, NETHERLANDS
 Eli Lilly & Company
 Eli Lilly & Company, ENGLAND
 Eli Lilly & Company, GERMANY
 Eli Lilly & Company, SPAIN
 Glaxo Pharmaceuticals, ENGLAND
 ICI Pharmaceuticals, ENGLAND
 Le Petit S.P.A. (Dow Chemical), ITALY

Merrell Dow Pharmaceuticals
 Monsanto
 Northwest Textile Institute, CHINA
 Novartis Pharmaceuticals
 Pfizer, ENGLAND
 Pfizer, JAPAN
 Rhone Poulenc Rorer
 R.W. Johnson Pharmaceuticals
 Sandoz Pharmaceuticals
 Sankyo, JAPAN
 Standard Oil of California
 Tanabe, JAPAN111

TEACHING

Awards

- Loren T. Jones Award for Outstanding Teaching, Purdue School of Science at Indianapolis, May, 1981.
- 1995 Chancellor's Award for Excellence in Teaching, April 1995. This award, the highest campus honor given for teaching at IUPUI, is given annually to a single faculty member in the university.
- 1996 President's Award for Distinguished Teaching, March, 1996. One of five awardees for the entire Indiana University System (eight campuses).
- Election to FACET (Faculty Colloquium on Excellence in Teaching), 1998. One of seven faculty for IUPUI.
- Teaching Award, School of Science, IUPUI, May 2006.

Courses Taught

<u>Course</u>	<u>Times Taught</u>	<u>Evaluations*</u>
C110 - The Chemistry of Life (one semester organic + biochem.)	35	4.44 (93%)
C341 - Organic Chemistry 1 (Lecture)	5	4.03 (65%)
C342 - Organic Chemistry 2 (Lecture)	7	4.56 (96%)
C651 - Advanced Organic Chemistry (physical organic & spectroscopy)	2	4.53 (98%)
C652 - Synthetic Organic Chemistry	15	4.53 (95%)

* Student evaluations. Score (out of 5.00) and average percentile rank in School of Science on global score.

Summary of Current Educational Research

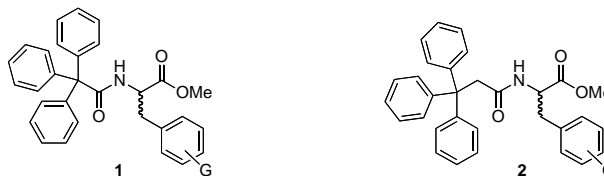
Distributed Drug Discovery for Undergraduates:
Second Semester Organic Chemistry Laboratory (C344) and Undergraduate Research (C409)

An outgrowth of my research collaboration with Professor Bill Scott over the past ten years has been our recent efforts in implementing a research-based experience, termed "Distributed Drug Discovery," in the second semester organic chemistry laboratory (C344) and for our undergraduate research students (C409). In this collaborative program IUPUI undergraduates (C344 & C409) as well as students at other institutions (currently Spain, Poland and Russia) prepare and analyze amino acid-based potential drug candidates using solid-phase combinatorial synthesis. While all students make a known control compound, they each can make up to 5 new compounds. We recognized that these new compounds, with appropriate purification and characterization, could be submitted to the NIH in response to their Molecular Libraries Small Molecule Repository initiative (see: NOT-RM-06-017 and <http://pubchem.ncbi.nlm.nih.gov/>). Accordingly, contact was made with appropriate representatives from NIH, a Material Transfer agreement was established between IU and NIH and we are in the process of submitting our first series of compounds. After IUPUI successfully pioneers this process, we anticipate that other participating schools will also become a source of compounds for the NIH Small Molecule Repository.

The research-based fall 2005 and spring 2006 C344 laboratories are illustrative of our Distributed Drug Discovery program. In fall 2005 our undergraduates prepared a series of biologically interesting targets. The two parent compounds (**1** and **2**, G = H) were

reported as leads from a melanoma screen by the Hergenrother group at Illinois earlier in 2005. Our 19 C344 students made a total of 38 new compounds (**1** and **2**, G = o, m, or p-substituent) in addition to the two parents. Control **1** (G=H) was purified, and analyzed (TLC, GC/MS, NMR) by the C344 students and the duplicates of the 38 new compounds were purified and analyzed by our undergraduate research students (C409). Samples of all 40 compounds were then delivered to Professor Hergenrother's laboratory at Illinois where they are undergoing biological testing in the melanoma screen.

C344 Undergraduate Laboratory (Fall 2005): Pro-Apoptotic Agents for Late Stage Melanoma



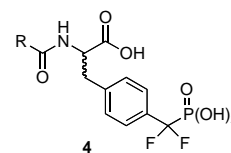
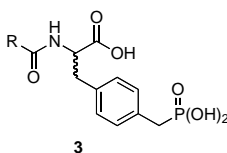
Reference:
"Synthesis and Identification of Small Molecules that Potentially Induce Apoptosis in Melanoma Cells through G1 Cell Cycle Arrest"
Paul Hergenrother et al (Department of Chemistry and Biochemistry, University of Illinois)
J. Am. Chem. Soc. **2005**, *127*, 8686-8696.

In spring 2006 our 60 C344 students, in four lab sections, prepared, isolated and analyzed 80 new compounds based on the two generic unnatural amino acid derivative structures shown (**3** and **4**, R= variable group), which are potential Protein Tyrosine Phosphatase (PTP) inhibitors. These compounds have been tested for biological activity in collaboration with Professor Zhong-Yin Zhang at the IU School of Medicine at IUPUI. We are currently following up on several leads resulting from these initial screens.

The undergraduates involved in these research-based educational laboratories have been excited about preparing compounds with the potential to fulfill humanitarian needs. In addition to conducting a four-step synthetic sequence on a 50 μ mol scale they learn the principles of both solid-phase and combinatorial chemistry. They are asked to analyze their data and present it in a clear and logical fashion.

The first three papers in the Distributed Drug Discovery program were published as the first three papers of 2009 in the *Journal of Combinatorial Chemistry* (publications #87, #88 and #89 on page 5). These were preceded by a special editorial describing our program (A. W. Czarnik, "Editorial." *J. Comb. Chem.* **2009**, *11*, 1-2). Additionally, a virtual catalog of >48,000 *N*-acylated amino acids and their methyl esters was generated from this research and is available free of charge by registering for a read-download account with Collaborative Drug Discovery (CDD) at <https://www.collaborativedrug.com/register/iupui-d3>.

C344 Undergraduate Laboratory (Spring 2006): Protein Tyrosine Phosphatase (PTP) Inhibitor Project



Reference:
"Small Molecule Approach to Studying Protein Tyrosine Phosphatase"
Zhong-Yin Zhang et al (IU School of Medicine, IUPUI)
Methods **2005**, *35*, 9-21.

SERVICE

Departmental

Departmental Executive Committee: 1979, 1980, 1983, 1984, 1989, 1992, 1993, 1997, 2000-2003, 2008-2010
Chair, Search and Screen Committee for Organic Chemistry Faculty: 2008
Chair, Organic Laboratory Renovation Committee: 2008
Graduate Coordinator and Advisor, Chemistry Department: 1984-1987, 2005-Present
Chair, Undergraduate Committee: 2008
Search and Screen Committee for Chairman of Chemistry: 1980, 1990, 2000, 2002
Chair, Search and Screen Committee for Chairperson for Chemistry: 1990, 2000, 2002
Departmental Curriculum Committee: 2003, 2004, 2007
Departmental Seminar Chairman: 1975-1978, 1981, 1992, 2000
Graduate Industrial Co-op Director: 1987-1990

School

School Steering Committee. 2008-Present
School Unit (P & T) Committee: 1986, 1987, 1988, 1989, 1993, 1997, 1998, 2000, 2001, 2002, 2009, 2010
Chair, School Promotions and Tenure Committee: 1993
Search and Screen Committee for Dean of the School of Science: 1987, 1988
School Research Committee: 1980-1983

University

University Ethics Committee: 1991-2008
University Fellowship Committee: 2001-2003
University Promotions and Tenure Committee: 1986, 1989
Search and Screen Committee for Vice-Chancellor for Research and Graduate Education: 1997-1998
Purdue, West Lafayette Graduate Council: 1987-1990
University Library Committee: 1978-1980
University Teaching Awards Committee: 1996, 1997

RESEARCH STUDENTS/POSTDOCTORALS/COLLABORATORS: 1975-PRESENTUndergraduates

Chris Audu	Steven Henry	Judith Smith
Cornelius Audu	Vincent Herring	Andrew Strong
James Boniece	Yasir Issa	Barbara Thompson
Nancy Bollinger	Patrick Kelly	Valerie Walker
William Bruder	Keith Knuth	Tim Weisel
Steve Brown	Anna Makosza	Kirk Wickizer
Rebekah Criscimagna	Barbara McDaniel	Thomas Wilson
Eric Crockett	Laura Platt	Mark Winter
Samuel Earp	Robin Polt	Robert Winton
Thomas Eckrich	Peter Sempstrott	Eric Woerly
Courtney Gloss	Ila Sharma	
Noreen Halligan	Patsy Shirley	

Thesis Masters

Ashok Arasapan
Charlotte Barney
Lakshmi Bhagavatula
Timothy Burkholder
Ning Chen
Gwen Cook
Byron Daugherty
Lindsey Fischer
Jonathan Green
Todd Grote
William Jacobsen
Jeremy Keeton
Vien Van Khau
Jeffrey Kyle
Linda Lawley
Min Li
Charles Lugar
Xiaojun Ma
Theresa Nahreini
Toan Nguyen
Pradeep Pushpavanam
Ying Qiao
Michael Robertson
Daniel Shullenberger
Kevin Sippy
Nancy Snyder
Eli Stoddard
Franz Victor
Kathleen Willey
Xiaobei Yang

Current Position

Ph.D.-Purdue; Postdoctoral-Duke; Schering-Plough, NJ
Marion Merrell Dow, Cincinnati
Abbott Laboratories, Chicago
Ph.D.-Purdue; Marion Merrell Dow; Lilly
IDUN Pharmaceuticals, California
Lilly
Lilly
Dow AgroSciences
Lilly
Lilly
Lilly
Lilly
Lilly
Lilly
University of Texas, Medical Center
Procter & Gamble Pharmaceuticals, Cincinnati
Lilly
Novartis, New Jersey
SUNY, Stony Brook, Pharmacology
Ph.D.-Yale
Schering-Plough, New Jersey
Novartis, New Jersey
Lilly
Ph.D.-IUPUI Biochem., Assoc. Prof.-St. Francis College
Abbott Laboratories, Chicago
Lilly
Lilly
Lilly
University Connecticut Medical Center
CIBA-GEIGY, New Jersey

Ph.D.

William Bennett	Advanced Chem Tech, Louisville
Fred Chin	Head, Radiochem Imaging Program, Stanford University
Jeremy Cooper	Wake Forest University, Visiting Professor
Shengde Wu	Procter & Gamble Pharmaceuticals, Cincinnati

Postdoctoral Associates/Visiting Scientists

Dr. Jordi Alsina	Lilly
Dr. Francisca Delgado	University of Alcala, Spain
Dr. Mark Drew	Rhone-Poulenc Rorer, Pennsylvania
Dr. Jamal Eddine	Assoc. Prof., Hassan University, Morocco
Dr. Irena Esikova	Cygnus Corp., San Francisco
Dr. Jean-Bernard Falmagne	Continental Pharma, Belgium

Zhiqiang Fang
 Dr. Vidyadhar Jadhav
 Dr. Sateesh Madhi
 Dr. Anatoliy Khusid
 Dr. Brigitte LeClef
 DeShan Liu
 You-an Ma
 Dr. Jacek Martinow
 Aiqiao Mi
 Dr. Rick Pottorf
 Dr. Jan Prejzner
 Dr. David Rusterholz
 Jack Samaritoni
 Dr. Massoud Stephan
 Dr. Krzysztof Wojciechowski
 Dr. Changyou Zhou
 Dr. Ziniu Zhou

Collaborators (≥ one publication)

Prof. Pher G. Andersson
 Dr. Alain Burger
 Prof. Frederick G. Bordwell
 Dr. Esteban Dominguez
 Dr. John C. Huffman
 Prof. Léon Ghosez
 Dr. Joseph H. Kennedy
 Prof. Clifford P. Kubiak
 Prof. Kenneth B. Lipkowitz
 Prof. Keith Mulholland
 Dr. Mary Mader
 Dr. James R. McCarthy
 Dr. John A. Porco, Jr.
 Prof. P.V. Ramachandran
 Prof. Roger W. Roeske
 Dr. Reinhard Schwesinger
 Dr., Prof. William L. Scott
 Prof. Arno F. Spatola
 Prof. George G. Stanley

Chicago
 D&O Pharmachem, Mumbai, India
 Purdue/IUPUI
 Russian Academy of Science, Moscow
 Medgenix Pharma, Belgium
 Assoc. Prof., Peking University, China
 Technical University, Xian, China
 Rib-X, New Haven, CT
 Prof., Chinese Academy of Science, Chengdu, China
 Provid Research, New Jersey
 Assoc. Prof., Polish Academy of Science, Warsaw
 Prof. & Chairman, University Wisconsin, River Falls
 IUPUI
 Postdoctoral, Japan
 Assoc. Prof., Tech. University, Warsaw, Poland
 Merck, New Jersey
 Purdue University

Uppsala Universtiy, Sweden
 Université Louis Pasteur, France
 Northwestern University
 Lilly, Spain
 Indiana University
 Université Catholique de Louvain, Belgium
 Lilly
 Purdue University, U. Cal., San Diego (Chair)
 IUPUI (Chemistry), North Dakota State (Chair), Howard University
 IUPUI (Radiology)
 Lilly
 Marion Merrell Dow, Lilly, IUPUI
 Argonaut Technologies
 Purdue University
 IUPUI (Biochemistry)
 University of Freiburg, Germany
 Lilly, IUPUI (Chemistry)
 University of Louisville
 Louisiana State University

Martin J. O'Donnell - Summary

Education

B.S., Chemistry, University of Iowa, 1968.
Ph.D., Organic Chemistry, Yale, 1973 (K. B. Wiberg).
Postdoctoral, UCL, Belgium, 1973-1975 (L. Ghosez).

Appointments

1975-1979 Assistant Professor, IUPUI.
1979-1984 Associate Professor, IUPUI.
1984- Professor, IUPUI.
2007- Chancellor's Professor

Research Interests and Honors

Organic Synthesis, Solid-Phase Reactions, Combinatorial Chemistry, Amino Acid and Peptide Synthesis, Phase-Transfer Reactions, Organometallic Chemistry.

Fall 1985 Visiting Professor, Imperial Coll. (London).
1992 NCU Fellowship for Research in Japan.
2000 Closing Plenary Lecture, 26th European Peptide Symposium, France.
2002 Wageningen Lecturer, Netherlands.

Research Students and Postdoctorals since 1975

34 Undergraduate Research Students.
30 Master's Theses.
4 Ph.D. Theses.
23 Postdoctorals.

Selected Major Publications

3. O'Donnell MJ, Eckrich, TM. The synthesis of amino acids by catalytic phase-transfer alkylations," *Tetrahedron Lett* 1978;4625.
30. O'Donnell MJ, Bennett WD, Wu S The stereoselective synthesis of α -amino acids by phase transfer catalysis," *J Am Chem Soc* 1989; 111:2353.
53. O'Donnell MJ, Zhou C, Scott, WL. Solid-phase unnatural peptide synthesis (UPS). *J Am Chem Soc* 1996;118:6070.
75. O'Donnell MJ, Cooper JT, Mader MM. Acyclic stereoselective boron alkylation reactions for the asymmetric synthesis of β -substituted α -amino acids. *J Am Chem Soc* 2003;125:2370-1.
86. Scott WL, Martynow JG, Huffman JC, O'Donnell MJ, The Solid-Phase Synthesis of Multiple Classes of Peptidomimetics from Versatile Resin-Bound Aldehyde Intermediates, *J Am Chem Soc* 2007;129:7077.
87. Scott WL, O'Donnell MJ. Distributed drug discovery, Part 1: Linking academics and combinatorial chemistry to find drugs for developing world diseases. *J Comb Chem* 2009;11:3.

Invited Reviews/Chapters

38. "Asymmetric Phase-Transfer Reactions," *Catalytic Asymmetric Synthesis*, 1992, I. Ojima, Ed., VCH.
67. "Asymmetric Phase-Transfer Reactions, 2nd Ed." *Catalytic Asymmetric Synthesis*, 2000, I. Ojima, Ed.
69. "The Preparation of Optically Active α -Amino Acids from the Benzophenone Imines of Glycine Derivatives," *Aldrichimica Acta* 2001;34,3.
78. "The Enantioselective Synthesis of α -Amino Acids

by Phase-Transfer Catalysis with Achiral Schiff Base Esters," *Acc Chem Res* 2004;37:506.

Editorial Work

- Coeditor, "Annual Reports in Organic Synthesis," 8 years (1978-1985), Academic Press.
- Invited Guest Editor, " α -Amino Acid Synthesis," *Tetrahedron*, Symposium-in-Print, 1988, Issue 17.

Citations/Applications by Others

- 2,297 unique citations of O'Donnell publications in 172 different journals, Web of Science.
- h-index = 21.
- 1,247 publications & 497 patents for 3,084 unique compounds with benzophenone imine activating group (O'Donnell's Schiff Bases), SciFinder Scholar.

Funding

NIH (RO1-GM28193) 1980-2008; Research Corporation; Petroleum Research Fund; Dreyfus Foundation; NATO; Eli Lilly & Co.

Other

- 106 Invited Academic/Industrial/Meeting Presentations in 14 Different Countries.
- Organized Symposium: "Phase-Transfer Catalysis," Pacificchem '95 Congress, Hawaii, 1995.
- Patents:
 - O'Donnell MJ, Wu S, Esikova I, Mi A. Catalytic Enantioselective Synthesis of α -Amino Acid Derivatives by Phase-Transfer Catalysis. US Patent 5,554,753, 1996.
 - Mulholland GK, O'Donnell MJ, Chin FT, Delgado F. Nucleophilic Approach for Preparing Radiolabeled Imaging Agents and Associated Compounds. US Patent 7,115,766, 2006.

Major Teaching Responsibilities and Honors

Chem C110 The Chemistry of Life.
Chem C342 Organic Chemistry 2.
Chem C696 Organic Synthesis.
1995 Chancellor's Award for Teaching at IUPUI (highest campus award for teaching).
1996 President's Award for Distinguished Teaching (1/5 awardees for IU System).
2006 School of Science Teaching Award, IUPUI.

Major Departmental/School/University Service

Department Executive Committee, 13 years.
Chair, Search & Screen, 5 times (chair, 3x)
School Promotion and Tenure Committee, 12 years.
Search & Screen Committee for Dean of the School of Science (1987)
University Ethics Committee, 15 years.
Search & Screen for Vice-Chancellor for Research & Graduate Education (1998).
Fellowship Committee, 4 years.
Teaching Awards Committee, 2 years.
Purdue Graduate Council, 3 years.

CURRICULUM VITAE

Kyungsoo Oh, Assistant Professor
Department of Chemistry & Chemical Biology
Indiana University Purdue University Indianapolis
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Indianapolis, IN 46202
Tel. (317)-278-7531
Fax. (317)-274-4701
Email: ohk@iupui.edu

EDUCATION

D.Phil. Chemistry, 2002
University of Sussex, U.K.

B.Sc. Chemistry, 1999
University of London, U.K.

APPOINTMENTS

2005-Present Assistant Professor, Department of Chemistry & Chemical
Biology, Indiana University Purdue University Indianapolis

2002-2005 Postdoctoral Fellow, Department of Chemistry, University of
Pennsylvania (with Professor Jeffrey D. Winkler)

RESEARCH INTERESTS

1. Synthetic Utility of Cyclic Beta-Keto Thioethers
 - Development of Tandem Intramolecular Michael Reactions of Vinyl Sulfoxide and Sulfone
 - Investigation of the Binding Mode of Biotin Analogs and the Role of the Sulfur Atom of Biotin
2. Asymmetric Oxidations using Chiral Tertiary Amine *N*-Oxides
 - Asymmetric Epoxidation of α,β -Unsaturated Carbonyl Compounds
 - Asymmetric Sulfoxidation of Sulfides
 - Asymmetric α -Hydroxylation of Ketones
3. Catalytic Asymmetric Reactions: Complete Reversal of Enantioselectivity Using a Single Chiral Source
 - [3+2] Cycloaddition of Azomethine Ylides
 - Enantio- and Diastereoselective Henry Reactions
 - Mannich Reactions
4. Use of Niobium-Alkyne Complexes as Precursors for 1,3-Dienes

- Tandem Diels-Alder Reactions using 1,3-Dienes Generated from Niobium-Alkyne Complexes

HONORS AND AWARDS

1999	Bader Prize (University of Sussex) Draper Prize (University of London) College Candidate for Neil Anott Competition (University of London, Second overall)
1998	Constance Maynard Prize (University of London)
1997	C.M. French Prize (University of London)
1996	Undergraduate Overseas Scholarship (University of London)

PROFESSIONAL ACTIVITIES

Search Committee Member of the School of Science for Associate Dean for Research and Graduate Education (Spring/2008)

Coordinator, Departmental Seminar Series (Fall/2007-present)

Member, Center for Environmental Health-IUPUI (Fall/2007-present)

Member, Center for Sensor and Ubiquitous Networking-IUPUI (Fall/2007-present)

Member, American Chemical Society

Proposal Reviewer for National Science Foundation (NSF)

Manuscript Reviewer for *Chemical Reviews*, *Organic Letters*, *Journal of Organic Chemistry* (ACS), *Dalton Trans* (RSC), *Tetrahedron Letters*, *Tetrahedron* (Elsevier), *Advanced Synthesis & Catalysis* (Wiley-VCH), *Synlett* (Thieme), *Current Organic Synthesis* (Bantham Publishing)

Judge, Intel International Science and Engineering Fair (2006)

PUBLICATIONS

RESEARCH ARTICLES

a) Research at IUPUI

1. Kim, H. Y.; Kim, S.[#]; **Oh, K.** "Orthogonal Enantioselectivity Approaches Using Homogeneous and Heterogeneous Catalyst Systems: Friedel-Craft Alkylation of Indole." *Angew. Chem. Int. Ed.* **2010**, *49*, in press. ([#] Denotes Undergraduate Researcher)
2. **Oh, K.**; J.-Y. Li.; Ryu, J. "Brucine *N*-Oxide Catalyzed Morita-Baylis-Hillman Reaction: A Mechanistic Implication of Dual Catalyst System with Proline." *Org. Biomol. Chem.* **2010**, *8*, 3015-3024.
3. Kim, H. Y.; **Oh, K.** "Brucine-Derived Amino Alcohol-Catalyzed Asymmetric Henry Reaction: An Orthogonal Enantioselectivity Approach." *Org. Lett.* **2009**, *11*, 5682-5685.
4. Kim, H. Y.; Shih, H. -J.[#]; Knabe, W. E.; **Oh, K.** "Reversal of Enantioselectivity between the Copper(I)- and Silver(I)-Catalyzed 1,3-Dipolar Cycloadditions Using a Brucine-Derived Amino Alcohol Ligand." *Angew. Chem. Int. Ed.* **2009**, *48*, 7420-7423. ([#] Denotes Undergraduate Researcher)-Highlighted in *Synfacts* (**2009**, *12*, 1381) and chosen as the Editors' Choice in *ChemInform* (Number 01/2010-01-117).
5. **Oh, K.**; Knabe, W. E. "Lewis Acid-Promoted Electron Transfer Deoxygenation of Epoxides, Sulfoxides, and Amine *N*-Oxides: The Role of Low-Valent Niobium Complexes from NbCl₅ and Zn." *Tetrahedron* **2009**, *69*, 2966-2974.
6. **Oh, K.**; Ryu, J. "Chiral Tertiary Amine *N*-Oxides in Asymmetric Epoxidation of α,β -Unsaturated Ketones." *Tetrahedron Lett.* **2008**, *49*, 1935-1938.
7. **Oh, K.**; Kim, H.; Cardelli, F.[#]; Bwititi, T.[#]; Martynow, A. M.[#] "Synthesis of Cyclic Thioethers through Tandem C(sp³)-S and C(sp²)-S Bond Formations from α,β' -Dichloro Vinyl Ketones." *J. Org. Chem.* **2008**, *73*, 2432-2434. ([#] Denotes Undergraduate Researchers)
8. **Oh, K.** "A Rapid Synthesis of the Biotin Core through a Tandem Michael Reaction." *Org. Lett.* **2007**, *9*, 2973-2975.
9. **Oh, K.** "An Efficient Epimerization of Biotin Sulfone Derivatives to 2-*epi*-Biotin Analogs." *Tetrahedron Lett.* **2007**, *48*, 3685-3688.

REVIEWS

10. **Oh, K.** 4-Ethylhexahydro-4-methyl-(4*S*,9*aS*)-pyrrolo[1,2-*d*][1,4]thiazepin-5(4*H*)-one. in *The Electronic Encyclopedia of Reagents for Organic Synthesis*. Crich, D. Ed. John Wiley & Sons Ltd.: Sussex, 2007.
11. **Oh, K.** Copper (I) Chloride. in *The Electronic Encyclopedia of Reagents for Organic Synthesis*. Crich, D. Ed. John Wiley & Sons Ltd.: Sussex, 2006.
12. **Oh, K.** *N,N*-Diethyl-1,3,2-benzodioxaborol-2-amine in *The Electronic Encyclopedia of Reagents for Organic Synthesis*. Crich, D. Ed. John Wiley & Sons Ltd.: Sussex, 2006.

b) Work Prior to IUPUI

13. Winkler, J. D.; **Oh, K.** "A One-Step Synthesis of 2,3-Dihydro-4*H*-pyran-4-ones from 3-Ethoxy α,β -Unsaturated Lactones." *Org. Lett.* **2005**, 7, 2421-2423.
14. Winkler, J. D.; **Oh, K.**; Asselin, S. M. "Synthesis of Highly Functionalized Furanones via Aldol Reaction of 3-Silyloxyfurans." *Org. Lett.* **2005**, 7, 387-389.
15. **Oh, K.**; Cheshire, D.; Parsons, P. J. "Studies Towards the Synthesis of Rapamycin: Regiocontrol in the Addition of Carbanions to Enantiomerically Pure Epoxides and the Formation of a Highly Substituted Tetrahydrofuran." *Synlett* **2005**, 1630-1632.
16. **Oh, K.**; Parsons, P. J.; Cheshire, D. "An Efficient Stereoselective Synthesis of Substituted 1,3-Dienes." *Synlett* **2004**, 2771-2775.
17. **Oh, K.** "A Synthetic Approach Towards Rapamycin: Synthesis of the C10-C27 Fragment." (Ph.D. Dissertation, University of Sussex, 2002)

PRESENTATIONS/ WORKSHOP (EXTERNAL)

a) From IUPUI

1. Oh, K. "Orthogonal Enantioselectivity Approaches In Catalysis." Gordon Research Conferences (Organometallic Chemistry), Salve Regina University, Newport, RI, July 11-16, 2010.
2. Oh, K. "Reversal of Enantioselectivity in the Cu(I)- and Ag(I)-Catalyzed Reactions with Brucine-Derived Amino Alcohol Ligand." Gordon Research Conferences (Organometallic Chemistry), Salve Regina University, Newport, Rhode Island, July 12-17, 2009.
3. Kim, H. Y.; Shih, H. -J.; Knabe, W. E.; Oh, K. "A New Approach to Reversal of Enantioselectivity." 41st National Organic Chemistry Symposium, University of Colorado, Boulder, Colorado, June 7-11, 2009.
4. Shih, H.-J.; Oh, K. "Catalytic Asymmetric 1,3-Dipolar Cycloaddition of Azomethine Ylides." 2008 CIC-SROP Conference, University of Michigan, MI, July 2008.
5. Oh, K.; Martynow, A.; Kim, H. "Synthesis of Biotin and Its Analogs." The 2007 Lilly Undergraduate Research Fellowship Day, Indianapolis, Aug 7th 2007.
6. Oh, K.; Labuda, J. "Intramolecular [2+2] Cycloaddition Approaches toward Multi-substituted Tetrahydrofurans." *Abstract of Papers of the American Chemical Society*, 233rd National Meeting: 293-ORGN Part 2, Chicago, IL, Mar 25 2007.

7. Oh, K.; Knabe, E. "Reductive Deoxygenation of Epoxides by Niobium." *Abstract of Papers of the American Chemical Society*, 233rd National Meeting: 293-ORGN Part 2, Chicago, IL, Mar 25 2007.

8. Oh, K.; Bwititi, T. "A Step-Wise Hetero-Diels-Alder Reaction of α,β' -Dichloro Vinyl Ketones with Carbonyl Compounds." 2006 Annual Committee on Institutional Cooperation, UIUC, IL, July, 2006.

9. Invited Participant, Mentoring Workshop Program, NIH/NIGMS, Washington, DC, May 12-14 2006.

b) Prior to IUPUI

10. Oh, K.; Winkler, J. D. "Synthetic Application of Furan-3-one and Thiophen-3-one." *Abstract of Papers of the American Chemical Society*, 228th National Meeting: 293-ORGN Part 2, Philadelphia, PA, AUG 22 2004.

11. Oh, K. "A Synthetic Approach Towards Rapamycin: Synthesis of the C10-C27 Fragment." *AstraZeneca Symposium*, Warwick University, Warwick, U.K., SEP 2002

12. Parsons, P.; Cheshire, D.; Oh, K. "Synthetic Studies towards Rapamycin: C10-C27 Fragment synthesis by Silicon-Mediated Fragmentation." *Abstract of Papers of the American Chemical Society*, 224th National Meeting: 776-ORGN Part 2, Boston, MA, AUG 18 2002.

FUNDED RESEARCH PROPOSAL

"Acquisition of a 500-MHz NMR Spectrometer", National Science Foundation (NSF), Senior Personnel, July 2006.

"Synthesis and Biological Evaluation of Vitamin H Analogs", Indiana University, Research Support Funds Grant (RSFG), 9/1/2006-8/31/2007, \$30,000.

"Small-Molecule Inhibition of Interactions of the Urokinase Receptor (co-PI, PI-Meroueh)." National Institutes of Health, 4/1/2009-3/30/2014, \$64,000 per year (direct cost to KOH).

PENDING RESEARCH PROPOSAL

"Asymmetric Synthesis by Modified *Strychnos* Alkaloids." National Science Foundation (NSF), 2/1/2010-1/31/2013, \$618,945.

“Preparation of Transition Metal Incorporated Silica and Zeolite Materials.” American Chemical Society-Petroleum Research Fund (ND) (PI: K. Oh), \$ 100,000; 9/1/2011-8/31/2013.

INVITED LECTURES

“Orthogonal Enantioselectivity Approaches in Catalysis.” Purdue University, August 31, 2010.

“Orthogonal Enantioselectivity Approaches in Catalysis.” University of Cincinnati, May 27, 2010.

“Asymmetric Catalysis by Modified *Strychnos* Alkaloids.” University of Kansas, Oct 9, 2009.

“Reversal of Enantioselectivity Using Chiral Amino Alcohol Ligands with Multiple Metal Binding Modes.” 41st Central Regional Meeting of the American Chemical Society (CERMACS), Cleveland, Ohio, May 21, 2009.

“Tandem Cycloaddition Reactions in Natural Product Synthesis.” Indiana State University, Jan 16, 2007.

RESEARCH SCHOLARS/STUDENTS

Current Members

Post-Doctoral Associate (Oct/08-present)—Kim, Hun Young (Ph.D. University of Pennsylvania)

Research Project: Asymmetric 1,3-Dipolar Cycloaddition Reactions Using *Strychnos* Alkaloids.

Research Associate (Jan/2008-present)-- Knabe, Eric (M.S. IUPUI)

Research Project: Synthesis of Anti-Cancer Molecules (Collaboration with Professor Meroueh at IUMS).

Graduate Student (Aug/2009-present)--Li, Jian-Yuan (M.S. National Chung Hsing University, Taiwan)

Research Project: Synthetic Modification of *Strychnos* Alkaloids.

Undergraduate Researcher (Dec/2008-present)--Kim, Sungkyung (Junior at IUPUI - 2009 Dean's Scholar, 2009 UROP Fellow, and the Lilly Undergraduate Fellow).

Research Project: Synthetic Modification of *Strychnos* Alkaloids.

Past Members

Research Associate (Sep/2006-Aug/2007)--Kim, Hyunjung, (M.S. Yonsei University, South Korea)-Now in South Korea
Research Project: Synthesis of Sulfur Heterocycles using $\text{NaSH} \cdot x\text{H}_2\text{O}$.

Research Associate (Sep/2006-July/2007)-- Ryu, Jinhyang (M.S. Hanyang University, South Korea)- Now in South Korea
Research Project: Asymmetric Epoxidation of Electron-Deficient Olefins using Chiral Tertiary Amine Oxides.

M.S. (Sep/2005-Dec/2007)--Knabe, Eric (B.S. IUPUI, IN)
Thesis Title: Catalytic Deoxygenation of Epoxides Mediated by Niobium (III).
Now Research Associate at IUPUI

M.S. (Sep/2005-Dec/2007)--Labuda, Joe (B.S., Illinois State University, IL)
Thesis Title: Intramolecular [2+2] Cycloaddition Approaches Toward Multi-Substituted Tetrahydrofurans.
Now Organic Laboratory Coordinator at Benedictine University, IL

Undergraduate Researcher (June/2008-Dec/2008)—Shih, Hui-Ju (2008 Summer Research Opportunity Program Fellow and 2008 Undergraduate Research Opportunity Program Fellow)
Research Project: Asymmetric 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides.

Undergraduate Researcher (May/2007-July/2008)-- Kennedy, Erin
Research Project: Three Components Mannich Reaction in Aqueous Media.
Now Graduate Student at Dept. Chem & Chem. Biology (Professor R. Minto)

Undergraduate Researcher (May/2006-May/2008)-- Cardelli, Francesco
Research Project: Synthesis of Cyclic Thioethers.
Now at IU Medical School (M.D.)/Research Assistant at IUMS (Professor K. Takagi)

Undergraduate Researcher (May/2005-May/2007)--Bwititi, Tamayi (Summer Research Opportunity Program (SROP) and Undergraduate Research Opportunity Program (UROP)-Winner of 2006/2007)
Research Project: A Mukaiyama Aldol Approach to Hetero Diels-Alder Reaction.
Now at IU Medical School (M.D.)

Undergraduate Researcher (Sep/2005-Aug/2007)--Martynow, Anna (Honors Program and Undergraduate Research Opportunity Program (UROP)-Winner of 2006, Eli Lilly Summer Research Fellowship-Winner of 2007)-Now Graduate Student at Ball State University.

TEACHING

Chem 341 Organic Chemistry I
Chem 409 Chemical Research
Chem 696 Special Topics: Organometallics

Jingzhi Pu

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Indiana University-Purdue University Indianapolis
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Indianapolis, IN 46202
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Fax: (317) 274-4701
Email: jpu@iupui.edu
Webpage: <http://www.chem.iupui.edu/Faculty/Pu/>

Education

2004 University of Minnesota, Twin Cities – Minneapolis, MN

- Ph. D. in Chemistry

1999 Peking University – Beijing, P. R. China

- B. S. in Chemistry

Teaching and Research Experience

- Assistant Professor: Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis (2010-present)
- Research Associate: Department of Chemistry and Chemical Biology, Harvard University (2005-2010), advisor: Martin Karplus
- Research Associate: Department of Chemistry, University of Minnesota – Twin Cities (2004-2005), advisor: Jiali Gao
- Research Assistant: Department of Chemistry, University of Minnesota – Twin Cities (2001-2004), advisor: Donald G. Truhlar
- Teaching Assistant: Department of Chemistry, University of Minnesota – Twin Cities (1999-2001), Physical Chemistry and General Chemistry

Publications

1. “Test of Variational Transition State Theory with Multidimensional Tunneling Contributions Against an Accurate Full-Dimensional Rate Constant Calculation for a Six-Atom system,” **Pu, J.**; Corchado, J. C.; Truhlar, D. G. *J. Chem. Phys.* **2001**, *115*, 6266.
2. “Parametrized Direct Dynamics Study of Rate Constants of H with CH₄ from 250 to 2400 K,” **Pu, J.**; Truhlar, D. G. *J. Chem. Phys.* **2002**, *116*, 1468.
3. “Validity of Variational Transition State Theory with Multi-dimensional Tunneling Contributions against Accurate Quantum Mechanical Dynamics for H + CH₄ → CH₃ + H₂ in an Extended Temperature Interval,” **Pu, J.**; Truhlar, D. G. *J. Chem. Phys.* **2002**, *117*, 1479.
4. “Tests of Potential Energy Surfaces for H + CH₄ → CH₃ + H₂: Deuterium and Muonium Kinetic Isotope Effects for the Forward and Reverse Reaction,” **Pu, J.**; Truhlar, D. G. *J. Chem. Phys.* **2002**, *117*, 10675.
5. “Lateral Confinement of Image Electron Wavefunction by an Interfacial Dipole

- Lattice,” G. Dutton, **Pu, J.**; Truhlar, D. G.; Zhu, X. -Y. *J. Chem. Phys.* **2003**, *118*, 4337.
6. “Generalized Hybrid Orbital (GHO) Method for Combining Ab Initio Hartree-Fock Wave Functions with Molecular Mechanics,” **Pu, J.**; Gao, J.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 632-650.
7. “Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights,” Dybala-Defratyka, A.; Paneth, P.; **Pu, J.**; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 2475-2468.
8. “Tests of Second-Generation Density Functionals for Thermochemical Kinetics,” Zhao, Y.; **Pu, J.**; Lynch, B. J. Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2004**, *6*, 673-676.
9. “Efficient Molecular Mechanics for Chemical Reactions: Multiconfiguration Molecular Mechanics using Partial Electronic Structure Hessians,” Lin, H.; **Pu, J.**; Albu, T. V.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 4112-4124.
10. “Combining Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) with Molecular Mechanics by the Generalized Hybrid Orbital (GHO) Method,” **Pu, J.**; Gao, J.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 5454-5463.
11. “Use of Block Hessian for the Optimization of Molecular Geometries,” **Pu, J.**; Truhlar, D. G. *J. Chem. Theor. Comput.* **2005**, *1*, 54-60.
12. “Benchmark Calculations of Reaction Energies, Barrier Heights, and Transition State Geometries for Hydrogen Abstraction from Methanol by a Hydrogen Atom,” **Pu, J.**; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 773-778.
13. “Temperature Dependence of Carbon-13 Kinetic Isotope Effects of Importance to Global Climate Change,” Lin, H.; Zhao, Y.; Ellingson, B. A.; **Pu, J.**; Truhlar, D. G. *J. Am. Chem. Soc.* **2005**, *127*, 2830-2831.
14. “Small Temperature Dependence of the Kinetic Isotope Effect for the Hydride Transfer Reaction Catalyzed by *Escherichia coli* Dihydrofolate Reductase,” **Pu, J.**; Gao, J.; Truhlar, D. G. *J. Phys. Chem. B* **2005**, *109*, 8551-8556.
15. “Generalized Hybrid Orbital Method for Combined Quantum Mechanical and Molecular Mechanical Calculations Based on Density Functional Theory and Hybrid Density Functional Theory,” **Pu, J.**; Gao, J.; Truhlar, D. G. *ChemPhysChem* **2005**, *6*, 1853-1865.
16. “Nonperfect Synchronization of Reaction Center Rehybridization in the Transition State of the Hydride Transfer Catalyzed by Dihydrofolate Reductase,” **Pu, J.**; Ma, S.; Garcia-Viloca, M.; Gao, J.; Truhlar, D. G.; Kohen, A. *J. Am. Chem. Soc.* **2005**, *127*, 14879-14886.

17. "Finding Saddle Points by Using the Nudged Elastic Band Method: An Implementation for Application to Gas-Phase Systems," Gonzalez-Garcia, N.; **Pu, J.**; Gonzalez-Lafont, A.; Lluch, J. M.; Truhlar, D. G. *J. Chem. Theor. Comput.* **2006**, 2, 895.
18. "Hydride Transfer Reaction Catalyzed by Hyperthermophilic Dihydrofolate Reductase is Dominated by Quantum Mechanical Tunneling and is Promoted by Both Inter- and Intramonomeric Correlated Motions," Pang, J.; **Pu, J.**; Gao, J.; Truhlar, D. G.; Allemann, R. K. *J. Am. Chem. Soc.* **2006**, 128, 8015-8023.
19. "Multidimensional Tunneling, Recrossing, and Transmission Coefficient for Enzymatic Reactions," **Pu, J.**; Gao, J.; Truhlar, D. G. *Chem. Rev.* **2006**, 106, 3140-3169.
20. "Mechanism and Free Energies of Enzymatic Reactions," Gao, J.; Ma, S.; Major, D. T.; Nam, K.; **Pu, J.**; Truhlar, D. G. *Chem. Rev.* **2006**, 106, 3188-3209.
21. "Multi-coefficient Gaussian-3 Calculation of the Rate Constant for the OH + CH₄ Reaction and its ¹²C/¹³C Kinetic Isotope Effect with Emphasis on the Effects of Coordinate System and Tensional Treatment," Ellingson, B. A.; **Pu, J.**; Lin, H.; Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2007**, 111, 11706-11717.
22. "Development of a Polarizable Intermolecular Potential Function for Liquid Amides and Alkanes," Xie, W.; **Pu, J.**; MacKerell, Jr. A. D.; Gao, J. *J. Chem. Theor. Comput.* **2007**, 3, 1878-1889.
23. "How Subunits Coupling Produces the Rotary Motion in F₁-ATPase," **Pu, J.**; Karplus, M. *Proc. Natl. Acad. Sci. USA* **2008**, 105, 1192-1197 (track II, direction submission); selected by *Faculty of 1000 Biology*:
<http://www.f1000biology.com/article/id/1102040/evaluation>
24. "CHARMM: The Biomolecular Simulation Program," Brooks, B. R.; Brooks III, C. L.; MacKerell, Jr., A. D.; Nilsson, L.; Petrella, R. J.; Roux, B.; Won, Y.; Archontis, G.; Bartels, C.; Boresch, S.; Caflisch, A.; Caves, L.; Cui, Q.; Dinner, A. R.; Feig, M.; Fischer, S.; Gao, J.; Hodoscek, M.; Im, W.; Kuczera, K.; Lazaridis, T.; Ma, J.; Ovchinnikov, V.; Paci, E.; Pastor, R. W.; Post, C. B.; **Pu, J.**; Schaefer, M.; Tidor, B.; Venable, R. M.; Woodcock, H. L.; Wu, X.; Yang, W.; York, D. M.; Karplus, M. *J. Comput. Chem.* **2009**, 30, 1545-1614.
25. "A Coupled Polarization-Matrix Inversion and Iteration Approach for Accelerating the Dipole Convergence in a Polarizable Potential Function," Xie, W.; **Pu, J.**; Gao, J. *J. Phys. Chem. A* **2009**, 113, 2109-2116.
26. "How Biomolecular Motors Work: Synergy between Single Molecule Experiments and Single Molecule Simulations," Karplus, M.; **Pu, J.**, in *Springer Series in Chemical Physics* **2010**, 96 (*Single Molecule Spectroscopy in Chemistry, Physics, and Biology*), pp. 271-285.

Presentation and Posters

“Parametrized Direct Dynamics Study: Reaction of H with CH₄ from 250 to 2400 K, and KIEs involving Mu atom,” **Pu, J.**; Truhlar, D. G. *Midwest Theoretical Chemistry Conference*, Minneapolis, MN, 2001.

“Application of Variational Transition State Theory with Multidimensional Tunneling Contribution (VTST/MT) to Calculate Deuterium and Muonium Kinetic Isotope Effects for the Reaction of H with CH₄,” **Pu, J.**; Truhlar, D. G. *XIIth International Workshop: Quantum Atomic and Molecular Tunneling in Solid (QAMTS)*, Gainesville, FL, 2002.

“Ensemble-Averaged Variational Transition State Theory with Multidimensional Tunneling,” Truhlar, D. G.; Gao, J.; Garcia-Viloca, M.; Poulsen, T.; **Pu, J.**; Alhambra C.; Corchado, J. C.; Sanchez, M. L. *223rd American Chemical Society National Meeting*, Orlando, FL, 2002.

“Carbon-13 Kinetic Isotope Effects of Importance to Atmospheric Science and Their Temperature Dependence,” Lin H.; Zhao, Y.; Ellingson, B. A.; **Pu, J.**; Truhlar, D. G. *228th American Chemical Society National Meeting*, Philadelphia, PA, 2004.

“Generalized Hybrid Orbital (GHO) Method for Combined Quantum Mechanical Molecular Mechanical Calculations based on DFT and Hybrid DFT,” **Pu, J.**; Gao, J.; Truhlar, D. G. *Computational Chemical Dynamics: from Gas-Phase to Condensed-Phase Systems*, Minneapolis, MN, 2004.

“Using Statistical Mechanics with Quantum Mechanics for Enzyme and Nanoparticles,” Truhlar, D. G.; Bhatt, D.; Dybala-Defratyka, A.; Gao, J.; Garcia-Viloca, M.; Li, Z. H.; Paneth, P.; **Pu, J.**; Siepmann, J. I. *234th American Chemical Society National Meeting*, Boston, MA, 2007.

“Plastic Network Model and Its Application to F₁-ATPase,” **Pu, J.** *CHARMM Developers Meeting*, Baltimore, MD, 2007 (talk).

“How Subunit Coupling Produces the Rotary Motion in F₁-ATPase: Insights from Simulation,” **Pu, J.**; Karplus, M. *Biophysical Society 52nd Annual Meeting*, Long Beach, CA, 2008 (talk).

“How Subunit Coupling Produces γ -Subunit Rotation in F₁-ATPase: Insights from Simulation,” **Pu, J.**; Karplus, M. *235th American Chemical Society National Meeting*, New Orleans, LA, 2008.

“Combining Constrained QM with MM to Study Electron Transfer” **Pu, J.** *CHARMM Developers Meeting*, Boston, MA 2008 (talk).

“Mechanical and Chemomechanical Coupling in F₁-ATPase,” **Pu, J.**; Karplus, M. *236th American Chemical Society National Meeting*, Philadelphia, PA, 2008 (talk).

“Multiscale Simulations of F₁-ATPase,” **Pu, J.**; Karplus, M. *240th American Chemical Society National Meeting*, Boston, MA, 2010 (talk).

Synergistic Proposal Effort

“The dynamics and pathologies of molecular motors”, computational resource grant (MCB070062), NSF TeraGrid in 2007, awarded 360,000 CPU hours.

“Molecular simulations of conformational dynamics and its role in motor proteins, structure-function relationship, binding thermodynamics, signal transduction, DNA replication error correction, and catalysis in biological systems”, proposal for allocation of high performance computing resources at National Energy Research Scientific Computing Center (NERSC) in 2007, awarded 1,500,000 CPU hours.

“Simulating biological processes of interest to biofuels, including chemomechanical coupling in ATP regulated molecular motors, fidelity in DNA replications, structure-function relationships, free energies and dynamical coupling in signal transduction”, proposal for allocation of high performance computing resources at National Energy Research Scientific Computing Center (NERSC) in 2008, awarded 3,000,000 CPU hours.

“Molecular simulations of biological processes coupled to biofuel production: from ATP regulated molecular motors, to DNA repair enzymes, to signal transduction proteins and enzyme catalysis in the glycolytic pathway”, proposal for allocation of high performance computing resources at National Energy Research Scientific Computing Center (NERSC) in 2009, awarded 1,400,000 CPU hours.

Computational Chemistry Software Development

CGPLUS (co-author), CHARMM (developer),
GAMESSPLUS (co-author), MOPAC5.010mn (co-author),
MULTILEVEL (co-author), MULTILEVELRATE (co-author),
POLYRATE (co-author)

Awards and Honors

- John Overend Award for Excellent Graduate Research in Physical Chemistry, University of Minnesota, 2003.
- Lester C. and Joan M. Krough Fellowship, awarded by Department of Chemistry, University of Minnesota, 2002.
- HUIKAI Scholarship, First Prize, Peking University, 1998.

Professional Memberships

- American Chemical Society
- Biophysical Society
- Sigma Xi Scientific Research Society

Professional Activities

- IEEE Computer Society/American Institute of Physics CiSE Portal, Chemistry Portal Committee, 2000-2002.
- Organizing chair, *The 42nd Meeting of the American Chemical Society Central Region*, Indianapolis, IN, 2011.

Rajesh Sardar, Ph.D.

Assistant Professor
Department of Chemistry and Chemical
Biology
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LD 326, Indianapolis, IN 46202

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PROFESSIONAL APPOINTMENTS

Assistant Professor

Department of Chemistry and Chemical Biology, *Indiana University-Purdue University Indianapolis*, Indianapolis, IN, August 2010-Current

Post Doctoral Research Fellow

Department of Chemistry, *University of North Carolina*, Chapel Hill, NC, 08/2008 – 07/2010

Research advisor: Dr. Royce W. Murray

Faculty Intern

Department of Chemistry, *University of Utah*, Salt Lake City, UT, 02/2006 - 08/2008

Research advisor: Dr. Jennifer S. Shumaker-Parry

Graduate Research Assistant

Department of Chemistry, *The City University of New York*, College of Staten Island, NY, 08/2001- 12/2005

Undergraduate Research Assistant

Indian Association for the Cultivation of Science (IACS), Summer 2000

Research supervisor: Dr. Deb S. Roy

EDUCATION

Graduate

The Graduate Center, The City University of New York, New York, 08/2001 - 01/2006

Ph.D. in Chemistry, May 2006

Dissertation: Hydrosiloxanes: Efficient agents for controlled generation and nucleation of noble metal nanoparticles.

Research advisor: Dr. Bhanu P. S. Chauhan

Indian Institute of Technology, Kharagpur, India, 08/1999 - 06/2001

M. Sc. in Chemistry, June 2001

M. Sc Thesis: Development of a sensor switch using conducting polymers

Research advisor: Dr. Panchanan Pramanik

Undergraduate

The University of Calcutta, Calcutta, India, 07/1996 - 06/1999

B. Sc. In Chemistry, June 1999

AWARDS

University Fellowship from CUNY Graduate Center, 2002

Science Fellowship from CUNY Graduate Center, 2003

Jagadis Bose national science talent search award (JBNSTS), 1997

PUBLICATIONS (* signifies undergraduate research student)

Peer Review Publications

1. pH effects on the polymer-based synthesis of gold and silver nanoparticles. *Bjorge, N. S.; **Sardar, R.**; *Pecchia-Bekkum, C.; Shumaker-Parry, J. S. Manuscript under preparation.
2. Electrochemistry and contact angles of electrolyte droplets on films of fully-ferrocenated gold nanoparticles. *Zaino, L. S.;[#] **Sardar, R.**,[#] Murray, R. W. Manuscript under preparation. ([#]equal contribution)
3. Controlled growth of redox labeled highly ionic Au nanoparticles film. Beasley, C. A.; **Sardar, R.**; *Gadient, J.; *Barnes, N. M.; Murray, R. W. Manuscript under preparation.
4. Synthesis of soft ligand stabilized gold nanoparticles and tunable two dimensional assembly. Shem, P. M.;[#] **Sardar, R.**,[#] Shumaker-Parry, J. S. Submitted to J. Phys. Chem. C. ([#]equal contribution)
5. Spectroscopic and microscopic investigation of gold nanoparticle formation: Ligand and temperature effects on rate and particle size. **Sardar, R.**; Shumaker-Parry, J. S. J. Am. Chem. Soc. Revision requested.
6. Persistent multilayer electrode adsorption of poly-cationic Au nanoparticles. Beasley, C. A.; **Sardar, R.**; *Barnes, N. M.; Murray, R. W. *J. Phys. Chem. C.* **2010**, *114*, 18384.
7. Single-step generation of fluorophore-encapsulated gold nanoparticle core-shell materials. **Sardar, R.**; Shem, P. M.; *Pecchia-Bekkum, C.; *Bjorge, N. S; Shumaker-Parry, J. S. *Nanotechnology* 2010, 21, 345603. **Cover Highlights, Vol. 21, No. 34 August 2010.**

8. Interfacial Ion transfers between a monolayer phase of cationic Au nanoparticles and contacting organic solvent. **Sardar, R.**; Beasley, C. A.; Murray, R. W. *J. Am. Chem. Soc.* **2010**, *132*, 2058.
9. One-Step Synthesis of Phosphine-Stabilized Gold Nanoparticles Using the Mild Reducing Agent 9-BBN. Shem, P. M.; **Sardar, R.**; Shumaker-Parry, J. S. *Langmuir* **2009**, *25*, 13279. **Most-read paper (no. 13), November-December, 2009.**
10. Gold nanoparticles: Past, present, and future. **Sardar, R.**; Funston, A. M.; Mulvaney, P.; Murray, R. W. *Langmuir (Perspective)* **2009**, *25*, 13840. **Most-read paper (no. 3), in last 12 months, 2009-2010.**
11. Electrospray ionization mass spectrometry of intrinsically cationized nanoparticles, $[\text{Au}_{144/146}\{\text{SC}_{11}\text{H}_{22}\text{N}(\text{CH}_2\text{CH}_3)_3\}_x\{\text{S}(\text{CH}_2)_5\text{CH}_3\}_y]^+$. Fields-Zinna, C. A.; **Sardar, R.**; Beasley, C. A.; Murray, R. W. *J. Am. Chem. Soc.* **2009**, *131*, 16266.
12. Ferrocenated Au nanoparticle monolayer adsorption on self-assembled monolayer coated electrodes. **Sardar, R.**; Beasley, C. A.; Murray, R. W. *Anal. Chem.* **2009**, *81*, 6960.
13. 9-BBN induced synthesis of nearly monodisperse ω -functionalized alkylthiol stabilized nanoparticles. **Sardar, R.**; Shumaker-Parry, J. S. *Chem. Mater.* **2009**, *21*, 1167-1169.
14. pH-controlled assemblies of polymeric amine-stabilized gold nanoparticles. **Sardar, R.**; Bjorge, N. S; Shumaker-Parry, J. S. *Macromolecules* **2008**, *41*, 4347.
15. Asymmetrically functionalized gold nanoparticles organized in one-dimensional chains. **Sardar, R.**; Shumaker-Parry, J. S. *Nano Lett.* **2008**, *8*, 731.
16. Polymer induced synthesis of stable gold and silver nanoparticles and subsequent ligand exchange in water. **Sardar, R.**; Park, J.-W.; Shumaker-Parry, J. S. *Langmuir* **2007**, *23*, 11883. **Most-accessed paper (no. 15), October-December, 2007.**
17. Versatile solid phase synthesis of gold nanoparticle dimers using an asymmetric functionalization approach. **Sardar, R.**; Heap, T. B; Shumaker-Parry, J. S. *J. Am. Chem. Soc.* **2007**, *129*, 5356.
18. Nanoengineering of metallic solution through silicon constructs (review article). Chauhan, B. P. S.; **Sardar, R.**; Latif, U. Chauhan, M.; Lamoreaux, W. L. *Acta. Chim. Slov.* **2005**, *52*, 361. **Cover Highlights, Vol. 52, No. 4 December 2005.**
19. Self-assembled stable silver nanoclusters and nanonecklaces formation: Polymethylhydrosiloxane mediated one-pot route to organosols. Chauhan, B. P. S.; **Sardar, R.** *Macromolecules* **2004**, *37*, 5136 **Cover Highlights, Vol. 38, No. 1 January 11, 2005.**

20. Synthesis, stabilization and applications of nanoscopic siloxane-metal particle conjugates. Chauhan, B. P. S.; Rathore, J. S.; **Sardar, R.**; Tewari, P.; Latif, U. *J. Organometal. Chem.* **2003**, 686, 24.

Proceedings and abstracts

20. Combinatorial approach to functional noble metal nanoparticles. Chauhan, B. P. S.; **Sardar, R.** *Polymeric Materials* **2004**, 90, 719.
21. Multishaped nanoframes of silver in acetonitrile. Chauhan, B. P. S.; Tewari, P.; **Sardar, R.**; *Sharma, P. *Polymer Preprint* **2003**, 44, 256.

PATENTS APPLICATIONS

1. Asymmetrically functionalized gold nanoparticles organized in one-dimensional chains. Shumaker-Parry, J. S.; **Sardar, R.** U.S. Pat. Appl. Publ. 2009/221764 A1.
2. Asymmetrically Functionalized Nanoparticles. Shumaker-Parry, J. S.; **Sardar, R.** U.S. Pat. Appl. Publ. 2009/256116 A1.
3. Method of Synthesizing Metal Nanoparticles Using 9-borabicyclo [3.3.1] Nonane (9-BBN) as a Reducing Agent. Shumaker-Parry, J. S.; **Sardar, R.** Shem, P. M. U.S.. Pat. Appl. Publ. 2010/227189 A1.

INVITED RESEARCH PRESENTATION

Invited presentations at Conferences/Meetings

1. Using surface functionalization to control nanoparticle assembly. Sardar, R.; Shumaker-Parry, J. S. Joint 63rd Northwest and 21st Rocky Mountain Regional Meeting (NORM/RMRM) of the ACS, Park City, Utah. 2008.

Invited seminars at universities

1. Indiana University Purdue University Indianapolis, September 2010
2. Ohio State University, January 2010

CONTRIBUTED CONFERENCE PRESENTATIONS/ABSTRACTS

1. Monolayer protected cluster (MPC) adsorption on an electrode surface: What influences film formation? Sardar, R.; Beasley, C. A.; Murray, R. W. 238th ACS

National Meeting, Washington, DC. 2009.

2. Synthesis of positively charged quaternary-ammonium thiolate monolayer protected clusters (MPCs): Applications in fluorescence and redox sensing. Sardar, R.; Beasley, C. A.; Murray, R. W. 238th ACS National Meeting, Washington, DC. 2009.
3. Facile synthetic approach to phosphine stabilized gold nanoparticles. Shem, P. M.; Sardar, R.; Shumaker-Parry, J. S. 237th ACS National Meeting, Salt Lake City, Utah. 2009.
4. Fluorophore-gold nanoparticle conjugates formed using a pyrene-based fluorophore in a dual role as reducing and stabilizing agent in a single step aqueous phase synthesis. *Pecchia-Bekkum, C.; Sardar, R.; *Bjorge, N. S.; Shumaker-Parry, J. S. 237th ACS National Meeting, Salt Lake City, Utah. 2009, poster presentation.
5. Polymer-induced single step synthesis and stabilization of noble metal nanoparticles in water. Sardar, R.; Park, J-W.; Shumaker-Parry. 2007 AIChE Annual Meeting. Salt Lake City, Utah. 2007.
6. Different assemblies of asymmetrically functionalized gold nanoparticles. Sardar, R.; *Heap, T. B.; Shumaker-Parry, J. S. 54th AVS Conference at Seattle, Washington. 2007.
7. First synthesis of monosiloxane induced formation of self-assembled monolayers of silver nanoparticles. Chauhan, B. P. S.; Sardar, R.; *Sharma, P. 38th Silicon Symposium at University of Colorado, Boulder. 2005, poster presentation.
8. Role of polyhydrosiloxane and counter anions in the self-assembly of silver nanoclusters. Chauhan, B. P. S.; Sardar, R.; *Chueng, V. 38th Silicon Symposium at University of Colorado, Boulder. 2005, poster presentation.
9. Polymethylhydrosiloxane directed synthesis of self-assembled nanosized silver necklaces. Chauhan, B. P. S.; Sardar, R.; *Sharma, P. 37th Silicon Symposium at University of Pennsylvania. 2004, poster presentation.
10. Silicon thiol mediated self-assembly of silver nanoparticles. Sardar, R.; Chauhan, B. P. S. 3rd International Symposium in Silicon Containing Polymers, RPI. 2003, poster presentation.
11. Silicon Symposium in Akron, OH. 2003. Silicon polymers as manipulating agents for metallic nanoarchitectures. Tewari, P.; Sardar, R.; *Sharma, P.; Chauhan, B. P. S. 2003, poster presentation.
12. Chauhan, B. P. S.; Sardar, R.; Tewari, P.; *Sharma, P. 36th Silicon Symposium in Akron, OH. 2003, poster presentation.

SERVICE/PROFESSIONAL ACTIVITIES

University of Utah ACCESS program

I worked with Dr. Jennifer S. Shumaker-Parry in Summer 2006-2007 in teaching the ACCESS students transmission electron microscopic (TEM) technique and helped them to analyze their sample. ACCESS is a scholarship program sponsored by the college of science to integrate women into science, mathematic, and engineering careers.

Journal Reviews

Analytical Chemistry, Journal of the American Chemical Society, Langmuir, Journal of Physical Chemistry C, and Nano Letters.

PENDING PROPOSAL

Project title: PRF: Polyhydrosiloxane containing vinylpyridine or bipyridine metal complexes: implementation for charge storage devices

RESEARCH GROUP

Current Post Doctoral Research Associate

Dr. Karthik Ramasamy

Current Graduate Student

1. Gayatri Joshi, October 2010-present

Current Undergraduate Students

1. John Newton, August 2010-present
2. Nathanael Dennis, September 2010-present
3. Phillip McClory, October 2010-present

TEACHING

Fall 2010

C310 Analytical Chemistry
C311 Analytical Chemistry Laboratory

Summer 2006 and 2007

The Department of Chemistry, University of Utah
General Chemistry II, CHEM 1220

Jay A. Siegel, Ph.D.

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School of Science
402 N. Blackford St.
Indianapolis, IN 46202
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317-274-6883 (w)

317-274-4701 (fax)

PRESENT POSITION: Chair – Department of Chemistry and Chemical Biology and Director of Forensic and Investigative Sciences Program, School of Science, IUPUI

EDUCATION: B.S. Chemistry, George Washington University, 1968
M.S. Chemistry, George Washington University, 1970
Ph.D. Chemistry, George Washington University, 1975

EXPERIENCE:

2008-present	Chair – Department of Chemistry and Chemical Biology, Indiana University, Purdue University Indianapolis
2004-present	Professor and Director, Forensic and Investigative Sciences Program, Indiana University, Purdue University Indianapolis
2003-2004	Adjunct Professor, Michigan State University College of Law
1980-2005	Professor of Forensic Science and Director of the Forensic Science Program (1980-2004), School of Criminal Justice, Michigan State University, East Lansing, MI. Coordinator of graduate programs in forensic science.
1977-80	Associate Professor of Chemistry, Metropolitan State College, Denver, CO.
1977-present	Consultant in forensic science. Testified a total of more 200 times as an expert witness in 12 states, federal and military courts.
1975-77	Forensic Analytical Chemist - Virginia Bureau of Forensic Sciences. Analyzed controlled substances and trace evidence. Testified in court over 100 times as expert witness
1970-75	Graduate Teaching Assistant - George Washington University

1968-69 Analytical Chemist, Byron Motion Pictures. In charge of all
chemicals in motion picture processing lab

PROFESSIONAL AFFILIATIONS

American Academy of Forensic Sciences (Fellow). Chairman of Education Committee of Criminalistics Section, 1986-1996. Chair of poster sessions for 1996 national meeting, Nashville, TN. Named Distinguished Fellow – February, 2009

President of Council of Forensic Science Educators, 1992-93

American Chemical Society

Southwestern Association of Forensic Sciences (Distinguished Member) 1977-1995

Midwestern Association of Forensic Scientists

The Forensic Science Society (England)

Member, Editorial Board, Journal of Forensic Sciences 1980-2007

Forensic Science Education Accreditation Commission 2003-2008

International Association for Identification

PUBLICATIONS

Journal Articles

Siegel, J.A. and Perros, T.P., Preparation and Thermal Decomposition of Tetra-n-propylammonium Hexafluoroplatinate (IV), *Zeitschrift für Naturforschung*, Band 266, Heft, 6, 53, (1971).

Siegel, J.A. and Rowley, D.R., Reactions of Coordinated Complexes I: The Reaction of Bis(acetylacetonato) Nickel II with Carbon Disulfide, *Inorganica Chimica Acta*, 9,19 (1974).

Siegel, J.A. and Cormier, R.L., Thin Layer Chromatography of Analgesics, *J. Chem. Ed.* 56,180 (1979).

Siegel, J.A., The Chemist as Technical Expert, *Lawyer's Medical Journal*, 9, 4, 495 (1980).

Siegel, J.A., Lateef, B. and Smith, T., Introduction of Forensic Science: A Model Curriculum, in the Curriculum and Course Development Project, H. Abidinsky, Project Leader, Academy of Criminal Justice Sciences, 1982.

Siegel, J.A. and Baldwin, R., Death Investigation and the Role of the Criminal Investigator, *Peace Officer*, Winter, 1983.

Siegel, J.A. and Weisz, S.C., The Analysis of Metronidazole in Human Serum: An Unusual Overdose Case, J. Forensic Sci., 29, 2 (1984).

Siegel and Weisz, S.C., The Effects of the New Michigan Drunk Driving Laws on Hospital Laboratories, The Michigan Department of Public Health Newsletter, January, 1983.

Siegel, J.A. *et al*, Fluorescence of Petroleum Products I: Three Dimensional Fluorescence Plots of Motor Oils and Lubricants, J. Forensic Sci., 30, 3, 741 (1985).

Siegel, J.A., Solving Crimes with 3-D Fluorescence Spectroscopy, Analytical Chem., 57, 934A (1985).

Siegel, J.A. and Horowitz, R., Patterns of Injury in Motor Vehicle Accidents, J. Forensic Sci., 32, 1, 45 (1987).

Siegel, J.A. *et al*, Fluorescence of Petroleum Products II: The Analysis of Gasolines by Three-Dimensional Fluorescence, J. Forensic Sci., 32, 1, 78 (1987).

Siegel, J.A., The Appropriate Educational Background for Entry Level Forensic Scientists: A Survey of Practitioners, J. Forensic Sci., 33, 4, 1065 (1988).

Siegel, J.A. and Fenzan, G., Fluorescence of Petroleum Products III: Three Dimensional Fluorescence or Petrolatum Products, J. Forensic Sci., 33, 6, 1405 (1988).

Siegel, J.A. and Cheng, N.Z., Fluorescence of Petroleum Products IV: Three Dimensional Fluorescence and Capillary Gas Chromatography of Midrange Petroleum Products, J. Forensic Sci., 34, 5, 1128 (1989).

Siegel, J.A. and DeGaetano, D., Survey of U.S. Forensic Science Laboratories to Determine the Status of Gunshot Residue Analysis, J. Forensic Sci., 35, 5, 1087 (1990).

Siegel, J.A., DeGaetano, D. and Klomperans, K., Comparison of Three Sampling Methods of Gunshot Residue Analysis by SEM-EDX, J. Forensic Sci., 37, 1, 281, 1992.

Siegel, J.Horvath, F., and Gardner, K., Range of Fire Estimates from Shotgun Pellet Patterns: The Effect of Shell and Barrel Temperature, J. Forensic Sci., 38,3, 585, 1993.

Siegel, J.A., Crime and Science: Extending the Frontiers, Criminal Justice Reviews 18(1), 78, 1993.

Siegel, J.A. and Sheff, L., Fluorescence of Petroleum Products V: Three Dimensional Fluorescence and Capillary Gas Chromatography of Evaporated Gasoline Samples, J. Forensic Sci., 41(4), 225, 1994.

Siegel, J.A. and Midkiff, C., Worldwide Graduate and Undergraduate Forensic Science Education Programs, J. Forensic Science, 34,1, 103, 1994.

Siegel, J.A., Forensic Applications of Fluorescence Spectroscopy, Forensic Science Review, Dec. 1995

Siegel, J.A., Forensic Sciences at Michigan State University, MSU Alumni Magazine, Dec. 1994.

Siegel, J.A., Review of Scientific Evidence, 2nd Ed., by Gianelli, P., in Journal of Criminal Justice, 1995.

Siegel, J.A. Evidential Value of Textile Fiber - Transfer and Persistence, Forensic Science Review, 9:81; 1997

Siegel, J.A. Collection and Chain of Evidence, In Encyclopedia of Forensic Science, Academic Press Limited, London, August, 2000 , 426-8.

Siegel, J.A., Grim, D., Allison, J., Evaluation of Desorption/Ionization Mass Spectrometric Methods in the Forensic Applications of the Analysis of Inks on Paper, J. Forensic Sci, July, 2002, Vol. 46, No. 6, 1411-20.

Siegel, J.A., Grim, D., Allison, J., Evaluation of Laser Desorption Mass Spectrometry and UV Accelerated Aging of Dyes on Paper as Tools for the Evaluation of a Questioned Document, J. Forensic Sci, July, 2002, Vol. 47, No. 3, 476-84.

Siegel, J.A., Grim, D., Allison, J., Does Ink Age Inside of a Pen Cartridge?, J. Forensic Sci, July 2002, Vol. 47, No. 4, 1294-7.

Siegel, J.A. Dunn, J., Allison, J., Photodegradation and Laser Desorption Mass spectrometry for the Characterization of Dyes Used in Red Pen Inks, J. Forensic Sci, May 2003, Vol 48, No. 3, 393-98.

Siegel, J.A., Esslinger, K.J., Stallworth, S., Using STR Analysis to Detect Human DNA from Exploded Pipe Bomb Devices, J. Forensic Sci, May 2004, Vol. 49, No. 3, 693-6.

Siegel, J.A., Barnes, A.T., Nolan, J.A. and Kuk, R.A., Comparison of gasolines using gas chromatography-mass spectrometry and target ion response, September, 2004, J. Forensic Sci., Vol. 49, No. 5, 1049-55.

J. A. Siegel, P. L. Szymanski and C. Bommarito " Laser Ablation in Forensic Science" in: *Laboratory News* 2004, 28, 13-14.

Siegel, J.A., Accreditation of Undergraduate and Graduate Forensic Science Education Programs. Forensic Magazine, Winter, 2004, Vol. 1, No. 3, pp. 23-26

Method, P. Siegel, J and Londino, G., Comparison of Blood and Duplicate Breath Testing for Ethanol in Indiana, J. Alcohol Testing Alliance, April, 2006, Vol. 5, No. 1 , pp. 9-13.

Siegel, J.A., McNorton, S. and Guy, Analysis of Automobile Body Fillers and Putties, J. Forensic Science, January 2008, Vol. 53, No. 1, 13-23.

Books

Editor in Chief, Encyclopedia of Forensic Science, Academic Press Limited, London, August, 2000

Editor of Series: Forensic Drug Handbooks: Liang, R., Hallucinogens: A Forensic Drug Handbook, Academic Press, Boston, MA, April, 2003.

Editor of Series: Forensic Drug Handbooks: Smith, F., Ed., Handbook of Forensic Drug Analysis, Elsevier/Academic Press, Boston, MA, January, 2005.

Houck, M. and Siegel, J. "Fundamentals of Forensic Science", Elsevier, 2006

Siegel, J., "Forensic Science: The Basics", Taylor and Francis, 2006

Siegel, J., "Forensic Science: A Beginner's Guide, One World Press, May 2009.

Book Chapters

Siegel, J.A., Forensic Identification of Controlled Substances, in Forensic Science Handbook, Vol. II, R. Saferstein, Ed., Prentice-Hall, Englewood Cliffs, N.J., 1987.

Siegel, J.A., Three Dimensional Fluorescence in Forensic Chemistry, in Analytical Methods in Forensic Science, R. Liu, Ed. Ellis Horwood, London, 1991.

Siegel, J.A., Science and Law in the Courtroom: Two Ships Passing in the Night, Focus on Law Studies, American Bar Association, 1995

Siegel, J.A., Analysis of Textile Fibers, in Forensic Science, by Cyril Wecht, 1996.

Siegel, J.A. History and Development Expert Testimony, in More Chemistry and Crime, American Chemical Society, Washington, D.C., 1997.

Siegel, J.A. Forensic Chemistry, in Macmillan Encyclopedia of Chemistry, Macmillan Company, New York, 1997

Siegel, J.A. and Houck, M.M., Analysis of Textile Fibers, in Forensic Science, by Cyril Wecht, 2002

Siegel, J.A., Forensic Identification of Illicit Drugs, in Forensic Science Handbook, Vol. II, 2nd Ed., R. Saferstein, Ed., Prentice-Hall, Englewood Cliffs, N.J., 2004

Siegel, J.A., Szymanski, Patino, L, Bommarito, C. Laser Ablation in Forensic Science, Laboratory News, November, 2004, 13-14.

Siegel, J.A. and Houck, M.M., Analysis of Textile Fibers, in Forensic Science, by Cyril Wecht, 2006

PAPERS PRESENTED

American Chemical Society, Middle Atlantic Regional Meeting, January 1973. "The Reaction of Bis(acetylacetonato) Nickel II: with Carbon disulfide."

American Academy of Forensic Sciences. February 1983. "The Analysis of Metronidazole in Human Serum." "Three -Dimensional Fluorescence of Petroleum Products."

American Academy of Forensic Sciences. February 1983. "The Use of Physical Evidence by Prosecutors." (With Frank Horvath).

American Academy of Forensic Sciences. February 1984. "Three -Dimensional Fluorescence of Gasolines." "The Analysis of Human Seminal Fluid for Spermine and Sperminidine."

Midwestern Association of Forensic Scientists. October 1985. "Fluorescence of Petroleum Products." "Roundtable on Forensic Science Education."

American Academy of Forensic Sciences. February 1986. "Three-Dimensional Fluorescence of Motor Oils."

Joint Meeting of Regional Forensic Science Associations. Lexington, KY. October 1986. "The Analysis of Lubricants Used in Sexual Assault Crimes by Three -Dimensional Fluorescence." Paper won award as best paper by a new forensic scientist. (Gerianne Fenzan).

American Academy of Forensic Sciences. February 1987. "Three Dimensional Fluorescence of Petroleum Products." "The Need for a Masters Program in Forensic Sciences-Survey of the Crime Lab Directors."

American Academy of Forensic Sciences. February 1989. "Three Dimensional Fluorescence Spectroscopy and Capillary Gas Chromatography of Midrange Hydrocarbons."

American Academy of Forensic Sciences. February 1990. "Survey of Crime Lab Directors on Analysis of Gunshot Residues by SEM-EDX." (With D. DeGaetano).

American Academy of Forensic Sciences. February 1991. "Comparison of Three Methods of Analysis of Gunshot Residues by SEM-EDX." (With D. DeGaetano).

American Academy of Forensic Sciences, February 1994. "Forensic Science in the Adversary System."

American Academy of Forensic Sciences. February 1997. "Use of Scientific Evidence by Prosecutors", New York.

American Academy of Forensic Sciences. February 1999. "Transfer and Persistence of Fibers - A Mass Transfer Study". (With Max Houck)

American Academy of Forensic Sciences. February 2000. "Analysis of Inks using HPLC and FTIR".

American Academy of Forensic Sciences, Feb. 2002, D. Grim and J. Siegel, "Analysis of Inks by Laser Desorption Mass Spectrometry"

American Academy of Forensic Sciences, Feb. 2003

C. Stark and J. Siegel, "Analysis of Lipsticks by ATR/FTIR"

S. Walbridge and J. Siegel, "Transfer and Persistence of Fibers"

K. Esslinger and J. Siegel, "Recovery of DNA from Exploded Pipe Bombs"

American Chemical Society, Midwest Regional Meeting, Indianapolis, IN, June, 2004

J. Siegel, "Analysis of Ink Dyes by Laser Desorption"

J. Siegel, "Accreditation of University Forensic Science Programs"

American Academy of Forensic Sciences, Feb. 2005

G. Nutter, S. McNorton and J. Siegel, Analysis of Automobile Body Fillers.

J. Siegel, FEPAC Accreditation of Forensic Science Programs – Poster

Midwestern Association of Forensic Scientists, May, 2006

J. Siegel, Use of statistics in analysis of DNA

J. Siegel, Color analysis in microspectrophotometry

American Academy of Forensic Sciences, Feb. 2006

J. Siegel, G. Londino, J. Allison, Analysis of Pigmented Inks: Concept Paper

J. Siegel, Kristen Jaumann, Analysis of Cosmetic Glitter

J. Siegel, Forensic Science Education Resources

American Academy of Forensic Sciences, Feb. 2007

J. Siegel, "Forensic Science Education" in Workshop on New Developments in Forensic Science

J. Siegel, "Teaching Ethics to Forensic Science Students" in Workshop on Ethics in Forensic Science.

American Academy of Forensic Sciences, Feb. 2008

J. Siegel, BAJ Fisher, "Pattern Evidence", Panel and Roundtable

Michigan Science Teachers' Association, March, 2008

J. Siegel, K. Mirakovits, Presenter, Murder, Madness, Mayhem

National Science Teachers' Association, April, 2008

J. Siegel, K. Mirakovits, Teaching forensic science in high school

J. Siegel, K. Mirakovits, Presenter, Murder, Madness, Mayhem

American Academy of Forensic Sciences, Feb. 2009

Barrett, J., Goodpaster, J., Siegel, J. "Analysis of Red Hair Dyes by Microspectrophotometry"

Goodpaster, J., Rivas, L., Siegel, J. "Analysis of Pigmented Inks by Pyrolysis GC-MS"

J. Siegel, BAJ Fisher, "Individualization of Evidence, Panel and Roundtable

OTHER PRESENTATIONS

Denver District Attorneys Association. May 1976. "The Analysis of Fire Residues."

The Denver District Attorneys Association. May 1980. "The Investigation of Arson."

Michigan Judicial Institute. 1981 -84. Seventeen presentations on Forensic Science, physical evidence and Michigan Drunk Driving Laws. Programs given to judges, court reporters and court personnel.

Michigan Associations of Academically Talented Children. 1982 -87. Four presentations to Michigan chapters on forensic science.

National Association of Court Reporters. March 1983. "The Analysis of Scientific Evidence."

Michigan Court Stenographers Assoc. June 1983. "The Analysis of Controlled Substances."

Southwestern Association of Forensic Sciences. November 1979. "The Preparation of d-Pseudococaine from 1 - Cocaine."

Federation of Analytical Chemistry and Spectroscopy Societies. Sept. 1980. "Comparison of Criminalistics Curricula at U.S. Colleges and Universities."

Midwest Association of Criminal Justice Educators. October 1980. "The Future of Forensic Science in the Criminal Justice System."

Southwestern Association of Forensic Sciences. November 1980. "The Cocaine Isomers Defense."

Southwest Association of Forensic Sciences. November 1981. "Forensic Science Internship Programs."

The Michigan Association of Laboratory Technologists. November 1985. "The Effects of the New Michigan Drunk Driving Laws on Clinical Laboratories."

South-Central Michigan Laboratorians Association. January 1985. "The Practice of Forensic Science in the Laboratory."

American Society of Crime Lab Directors. September 1985. "Forensic Science Education Today."

International Association of Forensic Sciences. August 1987. Chair and participant of panel of forensic science education.

American Academy of Forensic Sciences. February 1988. Chair of panel on Arson Analysis.

Midwest Criminal Justice Association. October 1990. Chair and presenter on panel on "Future of Forensic Sciences."

Presentations on "Drugs in the Workplace" since 1987.

- Brotherhood of Electrical Workers of Michigan

- Michigan Firefighters Association (4 presentations)

- International Association of Firefighters

- Capitol Area Substance Abuse Commission

- Industrial Relations Research Association Kalamazoo Area Substance Abuse Commission

- Michigan Employment Relations Commission

- MSU School of Labor and Industrial Relations Alumni Assoc.

- Michigan Association of Fire Chiefs

Great Lakes Chemistry Conference, March 1992. Keynote speaker. "Careers in Forensic Chemistry."

Gordon Research Conference, August 1993. Invited speaker. "Applications of Analytical Chemistry to Forensic Science."

Visiting Scientist, Dow Chemical Corp., Midland MI, October, 1993.

Alma College Career Fair, March 1994. Invited speaker. "Forensic Science Careers."

"Incorporating Forensic Science into High School and College Science Courses", Mid - Michigan Section, American Chemical Society meeting, Ann Arbor, MI, May 1994.

"Investigation of Violent Death", Oakland County, MI Bar Association Youth Law Day. Invited speaker. March 1995-2003.

"Update in Forensic Science", SCH, Inc. Executive Management seminar, East Lansing, MI. April 1994.

"Analysis of DNA Evidence", East Lansing, MI chapter of Kiwanis Club, June 1994.

Keynote speaker, Southwest Michigan Chapter, American Chemical Society, Kalamazoo, MI. Sept 1994.

"The Analysis of Petroleum Products by Three Dimensional Fluorescence Spectroscopy", International Forensic Science Conference, Taipei, Taiwan, ROC. November 1994.

"Forensic Science Education in the 1990s", Department of Chemistry and Biochemistry, University of Windsor, Windsor, Ontario, Canada. March 1995.

"Analysis of DNA Evidence in Court", Michigan Clinical Laboratory Association, East Lansing, MI. April 1995.

"Forensic Chemistry", Central Indiana Society for Applied Spectroscopy. Feb 1996.

"Careers in Forensic Chemistry", Central Michigan University, invited speaker. March 1996.

"The Status of Forensic Science in the US", New South Wales, AU Forensic Science Society, Sydney, AU. May 1996.

"Scientific Evidence Issues", Michigan Defense Attorneys Association, Traverse City, MI. Sept 1996.

"Admissibility of Scientific Evidence - Where are we now?" invited plenary speaker, Midwest Association of Forensic Sciences, October 1996

"Update in Forensic Science", SCH, Inc. Executive Management seminar, December, 1996. Lansing, MI.

"Forensic Chemistry", invited speaker at Department of Chemistry, Ohio Wesleyan University, Delaware, Ohio, March, 1997

"Forensic Science Update and Case Preparation", invited speaker by SEAK, Inc., Cape Cod, MA, June 1997.

"Investigation of Violent Death", Ohio Continuing Legal Education Inc., Columbus, OH, Dec. 1997, 1999, 2001, 2003, 2005, 2007.

"The Status of Forensic Science in the US", New South Wales, AU Forensic Science Society, Sydney, AU, March, 1998

"Forensic Science Research Issues", New South Wales Drug Laboratory, Sydney, AU, April, 1998

A series of 5 seminars on scientific evidence, presented to the Department of Chemistry, Physics and Earth Science, Flinders University, Adelaide, AU, May and June, 2000

A series of 2 seminars on scientific evidence, presented to the staff of the South Australia Crime Lab, Adelaide, AU, June, 2000

"Update on Forensic Science". Michigan Defense Attorneys Association, Traverse City, MI, Oct. 2000.

Guest lecturer, Okemos High School, May 7, 2002, Forensic Science

Pike High School, Indianapolis, IN – Careers in Forensic Science, November, 2004

University High School, Indianapolis, IN – Careers in Forensic Science, February, 2005

Moderator and Organizer – CSI Effect Panel for IUPUI Alumni Association, Indianapolis, April 10, 2007

Forensic Science Update, Indiana University Alumni Association, Sanibel Island, January 10-11, 2007

Invited speaker – Texas A&M Department of Anthropology, College Station, TX, Update on forensic science, Sept. 28, 2007

Invited speaker – Indiana Public Defender's Association, Daubert Defenses in Pattern Evidence, January, 29, 2009

Invited speaker – John Marshall College of Law, Cleveland, OH, National Academy of Sciences report on the Needs of Forensic Science, March 19, 2009

Invited panelist – Arizona State University, Sandra Day O'Connor College of Law, Tempe, AZ. National Academy of Sciences report on the Needs of Forensic Science, March 30, 2009

Invited panelist – National Institute of Justice Applied Technologies Conference, Kansas City, MO, National Academy of Sciences report on the Needs of Forensic Science, April 17, 2009

Invited speaker – Arizona State Judges Conference, Scottsdale, AZ, National Academy of Sciences report on the Needs of Forensic Science, June 19, 2009

MAJOR INTERNATIONAL ACTIVITIES

Visiting Professor – The Criminal Police College of China, May-June 1993

Chief Delegate – International Conference on Forensic Science, Taiwan, PRC, June, 1994

Visiting Professor – The University of Technology, Sydney, Australia, January - July, 1998

Visiting Professor – Flinders University, Adelaide, Australia, May-June, 2001

Member, Board of Visitors – Deakin University, Geelong, Australia, 2003-present

Invited Presenter – International Conference on Forensic Science, San Salvador, El Salvador, May 2006.

GRANTS

National Science Foundation. Grants for Scientific Education. 1980. Development of a course in forensic science for nonscience majors. \$300. Associate investigator.

National Science Foundation. Science Faculty Development Grant. 1981 -83. Research in forensic serology and toxicology. \$53,000. Principal investigator.

Michigan State University. All-University Research Initiation Grants. 1981-82. Use of physical evidence by prosecutors. \$7500. Co-principal investigator with Frank Horvath.

Office of Criminal Justice, State of Michigan. Grants for scientific equipment for the MSU forensic science laboratory. 1982-83. \$95,000. Principal investigator.

Michigan State Police, Office of Highway Safety Planning. 1984. Study of patterns of injury in motor vehicle fatalities. \$5000. Principal investigator.

Perkin-Elmer Corporation. Corporate Donation Program. 1986.
Spectrofluorimeter to support forensic chemistry research. \$37,000.

Midwest Association of Forensic Scientists. Research Grant program. 1988. Analysis of Midrange Hydrocarbons by Three-Dimensional Fluorescence. \$2200. Principal investigator.

Michigan State University. All-University Research Initiation Grants. 1988-89. Study of gunshot residues by SEM-EDX. \$2600. Co-Principal investigator.

USAID - Office of Democratic Initiatives. 1989-90. Education project for El Salvadorian students for training in forensic science. \$68,000. Principal investigator.

Michigan State University. IT-CDG grant program. 1990-91. Adding high technology to forensic science education. \$1000 plus 100 hours of video production time.
Hewlett-Packard Corp. Corporate donation program. 1992. Gas -chromatograph/mass spectrometer, \$62,000. Joint with the department of chemistry.

Michigan State University, All-University Research Initiation Grants. Use of Scientific Evidence by Prosecutors. 1995. \$7500.

Nicolet Corp. University donation program. 1992. Data station and IR source for FTIR. \$21,000.

Michigan State Police. Evaluation of Drunk Driving Training Programs. 1996. \$41,000

Michigan State University. All-University Outreach Grant program. Forensic Science as problem-solving tool for high schoolteachers. 1996. \$7500.

National Institute of Justice. Analysis of Inks using Laser Desorption Mass Spectrometry, \$240,000. Co-PI. 2001-2004.

Analysis of Pigmented Inks. National Institute of Justice. \$271,000. Principle Investigator. 2006-2008.

Analysis of Automobile Paint Clear Coats. Midwest Forensic Science Center. \$50,000. Principle Investigator. 2007-2008

AWARDS AND HONORS

Outstanding Graduate Assistant. George Washington University, Department of Chemistry. 1974.

American Chemical Society Congressional Fellow. 1988-89

Distinguished Member, Southwestern Association of Forensic Sciences.

Chief US Delegate to International Forensic Science Conference, Taipei, Taiwan, ROC, November, 1994

Visiting Professor, Criminal Police College of China. 1993.

Visiting Professor - Department of Chemistry, Materials and Forensic Science, University of Technology, Sydney, Australia. January to June, 1998

Visiting Professor - School of Chemistry, Physics and Earth Science, Flinders University, Adelaide, AU, May-June, 2000

Member, External Advisory Committee. Deakin University Forensic Science Course, Geelong, Victoria, Australia, 2003-present

Paul Kirk Award winner. Criminalistics Section, American Academy of Forensic Sciences, Feb. 22, 2005.

Member, Committee to Study the Needs of Forensic Science, National Academy of Sciences, 2006-2008.

Member, Committee on the Research Programs of the National Institute of Justice, National Academy of Sciences, 2007-2009.

Distinguished Fellow, American Academy of Forensic Sciences, February, 2009

Distinguished Alumni Scholar Award, George Washington University, April 30, 2009

CONSULTING

Denver Police Department. 1979-80. Casework, internships, personnel.

Denver Districts Attorneys Office. 1979 -80. Casework and scientific evidence.

Colorado Bureau of Investigation. 1979 -80. Analytical techniques, internships and personnel.

Denver Public Defenders Office. 1979 -80. Casework and scientific evidence. Wisconsin State Police. 1987. Casework.

Michigan State Police. 1987-present. Casework, internships, personnel. U.S. Bureau of Alcohol, Tobacco and Firearms. 1989. Casework.

Cameron Parish, Louisiana Sheriffs Department. 1989. Casework.

Over 100 cases with numerous law firms, insurance companies, and traffic accident reconstructors. 1977-present. Analysis of evidence, testimony, depositions, drug testing protocols. Testified as expert witness in over 200 cases in 12 states, Federal and Military courts.

University of Wisconsin at Milwaukee. Invited consultant on starting a forensic science program. March, 1997.

Consultant in Forensic Chemistry, Speckin Forensic Laboratories. 1996 -present.

Analysis of illicit drugs for Hamilton, Boone and Hendricks Counties, Indiana. Pilot program of Governor's Office. January 2006-present.

SHORT COURSES AND SEMINARS TAUGHT

Denver Poisonlabs seminar on forensic toxicology. 1977.

University of Denver Law Center. Continuing Legal Education Division. Course in Forensic Science for Attorneys. 1979.

Michigan Judicial Institute. Approximately 30 short courses and seminars to judges and court personnel on various forensic science topics. 1981 -93.

Michigan State University, Lifelong Education Programs. Approximately 20 programs in Criminal Justice and Forensic Science to Criminal Justice professionals. 1980 -present. Visiting Lecturer, Criminal Police College of China, Shenyang, PRC, July 1992.

Michigan Judicial Institute, Judges Seminar in Scientific Evidence, Troy, MI., May, 1993.

American Bar Association. Continuing Education Program for Appellate Court Judges, Workshop on Admissibility of Scientific Evidence. Sun Valley, ID, July, 1994.

Five State Judges Association. Continuing Education Seminar for Judges. Workshop on Admissibility of Scientific Evidence. Rapid City, SD, July, 1995.

American Bar Association. Continuing Education Program for Appellate Court Judges, Workshop on Admissibility of Scientific Evidence. Jackson Hole, WY, July, 1996.

Michigan State University, High school teachers enrichment program. 5 hour short course in teaching forensic science in high school. March, 1997.

SHORT COURSES AND SEMINARS TAKEN

Drug Enforcement Administration course in forensic drug analysis. 1977. McCrone Institute course in forensic microscopy. 1980.

FBI International Conference in Forensic Toxicology. 1984.

DNA typing by Polymerase Chain Reaction, 1994.

McCrone Institute course on building materials analysis, Chicago, IL, October 16, 17, 2000

One day course on analysis of Inks, US Department of Internal Revenue, Chicago, IL, October 18, 2000

Paint analysis, Midwest Association of Forensic Scientists, Lansing, MI, May 5 -9, 2003

MAJOR MEDIA APPEARANCES

Expert witness for the defense, State of Florida v. William Kennedy Smith, December, 1993, nationally televised

"Eye to Eye with Connie Chung", Sept. 1994, Use of DNA evidence in court and role of financial resources in ability to offer defense in criminal justice system

"ABC Evening News", April, 1995. Tagging Explosives

"Science Friday-Talk of the Nation", National Public Radio, Forensic Science, April, 1996.

"CBS Early Morning", October 2002, DC Sniper attacks

"CBS Early Morning", October 2002, The forensic science program at MSU

"Inside Indiana Business", August, 2004, The forensic science program at IUPUI

"Inside Indiana Business", July, 2007, The forensic science program at IUPUI

CURRICULUM VITAE

Pratibha Varma-Nelson

Professor of Chemistry, Department of Chemistry and Chemical Biology

Executive Director, Center for Teaching and Learning

Indiana University Purdue University, Indianapolis

UL 1125, 755 West Michigan Street

Indianapolis, IN 46202

317-278-3425 (voice)

317-278-0241 (fax)

pvn@iupui.edu

EDUCATION

Ph.D., Organic Chemistry, 1978, University of Illinois at Chicago, Thesis, "Protein Ancestors: Heteropolypeptides from Hydrogen Cyanide and Water". Advisor: Clifford Matthews

M.S., Chemistry, 1974, University of Illinois at Chicago

B.Sc., First Class, Chemistry, 1970, Poona University, India

PROFESSIONAL EXPERIENCE

Professor of Chemistry, Department of Chemistry and Chemical Biology and Executive Director, Center for Teaching and Learning at Indiana University Purdue University Indianapolis (IUPUI), 2008-present

Senior Faculty of University College, IUPUI, 2010-present

Program Director (IPA), Division of Undergraduate Education at the National Science Foundation, August 2006-August 2008

Professor of Chemistry and Department Chair, July 1, 2002 – August 2008, Northeastern Illinois University, Chicago

Professor of Chemistry, 1992-2002, Saint Xavier University, Chicago

Associate Professor of Chemistry, with tenure, 1986-1992, Saint Xavier University, Chicago

Associate Professor of Chemistry, without tenure, 1984-1986, Saint Xavier University, Chicago

Assistant Professor of Chemistry, 1979-1984, Saint Xavier University, Chicago

Post Doctoral Fellow, 1977-1979, "Characterization of Anhydro-Chymotrypsin", Department of Biochemistry and Biophysics, Stritch School of Medicine, Loyola University, Maywood, IL

Teaching Assistant, 1972-1977, Chemistry Department, University of Illinois at Chicago

Research Associate, Hines VA Hospital, 1989-1990, sabbatical leave. Developed Immunoassays for Gentamicin and AZT

Research Associate, Summer 1984, Department of Biochemistry and Biophysics, Stritch School of Medicine, Loyola University, Maywood, IL

ADMINISTRATIVE EXPERIENCE

Program Director (rotator), August 2006-August 2008 in the Division of Undergraduate Education (DUE), The National Science Foundation, Arlington, VA. I was assigned to the following programs: Scholarships in Science, Technology, Engineering and Mathematics (S-STEM, Co-Lead), Course Curriculum and Laboratory Improvement (CCLI), STEM Talent

Expansion Program (STEP), International Programs and National Science Digital Library (2006-2007).

As Program Director I was responsible for :

- reviewing, funding, post-award management, and evaluation of the programs
- participating in the design and implementation of the proposal review and evaluation process
- selection of qualified individuals for review panels
- management and monitoring of ongoing grants, to ensure fulfillment of commitments to NSF
- recommending new or revised policies and plans in scientific, fiscal, and administrative matters to improve the activities and management of the Program
- participation in outreach activities on behalf of DUE such as offering workshops on proposal writing, seminars and webinars for reviewers
- addressing concerns, questions of prospective principal investigators
- contributing to the management of the Division of Undergraduate Education by participating in weekly Program Director meetings as well interviews and selection of new Program Directors and other professional staff

Chair, Department of Chemistry, Earth Sciences and Physics, July 1, 2002 – 2006, NEIU.

The department consists of 22 full time faculty, several adjunct faculty, two secretaries and three laboratory managers and awards BS degrees in Chemistry, Earth Science and Physics and MS degrees in Chemistry and Earth Science. Responsibilities include oversight of all the degree programs, personnel management and evaluation, outreach, fund raising and advising.

Co-Chair, Science Department, Saint Xavier University, 1992-1995

Responsibilities included management of departmental budget, faculty recruitment and evaluations, staff recruitment, and public relations. The department consisted of six full time biologists, five full time chemists, one physicist, a laboratory coordinator, two secretaries and several adjunct faculty.

GRANTS

In each of the following cases I contributed to the research design, writing of the grants, implementation, evaluation, dissemination, site visits, annual reports as well as visits by the National Visiting Committee. These grants were all peer reviewed and funded by the National Science Foundation.

PI, NSF, CCLI Type I Special Project “The Role of Centers for Teaching and Learning in Improvement of Undergraduate Engineering Education” **\$98,000**, Pratibha Varma-Nelson, Co-PI Terri Tarr. 2010-2011

PI NSF, CCLI Type I “Development of cPLTL, Co-PIs Randy Newbrough, Lorie Shuck, Tom Janke, Lin Zhu. **\$200,000**, 2010-2013

IUPUI Multidisciplinary Undergraduate Research Institute (MURI), Cyber Peer-Led Team learning (cPLTL), **\$13,100** Varma-Nelson, P., Janke, T. and Newbrough, R., Summer 2009. Three students were hosted by CTL

Co-PI, Center for Authentic Practice in Education (CASPiE), Aug 2004-2006, first NSF funded Undergraduate Research Center (URC). I am responsible for directing the development and course implementation of CASPiE activities at NEIU. I am the primary expert and coordinator of all Peer-Led Team Learning (PLTL) related activities in the consortium, including development of workshop units, training of faculty and peer leaders. I also assist in overall management of the project. See <http://www.purdue.edu/dp/caspie/partners.html>. [Currently on leave from being PI due to conflict of interest issues while at NSF]

Grant details

Weaver G., F. Lytle, P. Varma-Nelson, D. Wink and R. Morris, "Center for Authentic Science Practice in Education (CASPiE)." 2004-2009. Total value \$ 2.9 million. NSF, CHE- 0418902 **NEIU Share \$ 320,000.**

Co-PI, "PLTL National Dissemination: Building a National Network". 2002-2006
Director of the Midwest Regional PLTL Center and the Workshop Projects Associate (WPA) Grant Program. Also director for the Chautauqua Faculty Development Program on PLTL. See: <http://www.pltl.org>. Working with the PI in determining the overall direction of the national project.

Grant Details

Gosser D., P. Varma-Nelson, V. Strozac and M. Gaines, Peer Led Team Learning (PLTL) National Dissemination: Building a National Network. Supplement Proposal: Evaluation of the WPA Program, NSF-DUE 0231349, DUE 0231349 **NEIU Share: \$ 89,000. 2002-2005.**

Gosser D., P. Varma-Nelson, V. Strozac and M. Gaines, "PLTL National Dissemination: Building a National Network". 2002-2005, NSF, DUE 0231349. **NEIU share \$ 340,000.**

Management Team, Multi-Initiative Dissemination (MID) Project, 2000-2004, <http://www.cchem.berkeley.edu/~midp/>. Responsibilities included coordinating the PLTL workshops and working closely with other members and PI in determining the overall direction of the project. Other members of the project were representatives of the other three Systemic Change Initiatives to change teaching of undergraduate chemistry, also funded by NSF, in the CCLI Program.

Grant Details

Lewis E. PI, Senior Faculty E. Peace, Russell, A and P. Varma-Nelson, "Strategies to Promote Active Learning in Chemistry: Multi-Initiative Dissemination (MID) Project." 2000-2004, NSF, DUE-0196527 Total amount \$ 1, 000,000 awarded to coalition of 4 systemic change initiatives. Lead Institution University of California, Berkeley.

Varma-Nelson P. and R. Iasillo, "Peer-Led Team Learning Workshops at Mother McAuley High School". From The Agatha O'Brien Ministry Fund, \$20,000. July 2002 -June 2003.

Co-PI, Workshop Project: Peer-Led Team-Learning (PLTL) National Dissemination Project. 1999-2002. Director of the Workshop Projects Associate (WPA) Grant Program and the Chautauqua Faculty Development Program on PLTL. Working with the PI in determining the overall direction of the national project and securing additional funding for the project.

Grant Details

Gosser, D. et.al, NSF-DUE –99722457 1999-2002, **SXU Share \$ 500,150**. Subcontracts from Research Foundation of City University of New York (CUNY) on behalf of City College.
Subcontract no. 40257-00-01D, 2001-2002, \$ 170,000.
Subcontract no. 40257-00-01-D, 2000-2001, \$ 165,150.
Subcontract no. 402570001-D, 1999-2000, \$ 165,000.

Management Team of “Workshop Chemistry Project” 1996-2000, a Systemic Change Initiative in teaching of undergraduate chemistry. Responsible for implementing peer-led workshops at SXU in organic chemistry and chemistry for health professionals as well as planning the national dissemination activities for the project and assisting with preparing for the annual National Visiting Committee meetings.

Grant Details

Gosser, D. M. Weiner and S. Radel, NSF-DUE-9455920, 1995-2000, **SXU share \$ 41,517**. Subcontracts from Research Foundation of City University of New York (CUNY) on behalf of City College
Subcontract no. 40906-E, 1998-1999, \$ 13,743.
Subcontract no. 40906-E, 1997-1998, \$ 23,774.
Subcontract no. 40906-E, 1996-1997, in the amount of \$ 4000.
In addition during 1995-1996 support for travel to conferences and meetings and summer salary were received in the amount of \$ 9,597, received directly from CUNY Research Foundation

Varma-Nelson, P. \$ 1500 from the Eli Lilly Foundation (Center for Educational Practice) to develop the course “Environmental Concerns: Cultural Perspectives” offered Fall, 1996

Several small Projects Grants from SXU

Workshop Project Associate (WPA) Grants (1999-2005)

In 1999, and 2002 NSF awarded the PLTL consortium two National Dissemination grants to expand the PLTL model into other science disciplines. The centerpiece of these awards was the Workshop Project Associate (WPA) grant program that provided funds to assist faculty from across the country in implementing and evaluating a PLTL course on their campus.

I was the director of the WPA Grants program initially in chemistry and eventually all disciplines. We made awards to faculty in chemistry, biology, physics and math. We processed 101 proposals and have awarded and administered 92 grants. The amount awarded was \$491,866 and the amount that was matched by the institutions receiving the awards was \$544,443. The type of institutions receiving the awards included 18 two-year colleges, 42 four-year institutions and 10 research universities. The recipients of these awards were from chemistry, biology, physics, mathematics and computer science. The names and institutions of the recipients can be found on the PLTL web site (www.pltl.org).

INTERNATIONAL ACTIVITIES

Atilim University, Turkey

Invited to present Workshops on Effective Teaching and Learning in a University, October 18-22, 2010. Co-presenter Stacy Morrone, School of Education, Indiana University. Hosted by Provost Hasan Akay.

Singapore Roundtable Discussion

Pedagogies of Engagement in Science; A comparison of PBL, POGIL and PLTL, round table discussion (75 minutes), June 11 2009. Republic Polytechnic Institute, conference “What are we learning about Learning?” 2nd International PBL conference, Singapore –Peer reviewed.

PKAL Delegate to China

I was a member of the Project Kaleidoscope (PKAL) delegation invited to the People’s Republic of China June 30-July 15, 2005. My host was Dr. Nie, Assoc. Chair, Chemistry Department at Huazhong University of Science and Technology (HUST), Wuhan. The delegation was composed of six US educators representing chemistry, biology, earth science and physics. I represented the Peer-Led Team Learning (PLTL) national project. I spent two weeks at HUST demonstrating the implementation of the PLTL model into a sophomore organic chemistry class consisting of 65 students and 11 peer leaders. The demonstration included training peer leaders and teaching an organic chemistry class using the PLTL model. Nine faculty members from HUST Chemistry Department participated. In addition to teaching, the delegation was there to plan for a larger meeting to be held at Wuhan University in November 1-7, 2005, which I attended with a larger (11members) PKAL delegation and was a speaker in a Seminar on Sino-US Undergraduate STEM Education Reform.”

ACS Delegate to Cuba

In December 1998 I was one of an eight-member delegation of American Chemical Society selected to participate in the III International Congress of the Cuban Chemical Society. Co-sponsored by International Union of Pure and Applied Chemistry (IUPAC) in Havana. My presentation was on December 2, 1998 on Workshop Chemistry: Peer Led Team Learning. See report in January 11, 1999, Volume 77, Number 2, CENEAR 77 2 pp. 8-13 ISSN 0009-2347 <http://pubs.acs.org/hotartcl/cenear/990111/7702newfocus.html>

HONORS

PEARS 2009 Prestigious External Award Recognition (PEAR) recipient in honor of having been given the James Flack Norris Award for Outstanding Achievement in Chemistry Teaching by the American Chemical Society, April 17, 2009

2008 James Flack Norris Award for outstanding achievement in the teaching of chemistry. Co-recipients of the 2008 award were Jack Kampmeier, University of Rochester, and David K. Gosser, City College of New York.

Nominated for the first Bernard J. Brommel Distinguished Research Professor Award at NEIU in 2006.

Nominated for US Professor of the Year Program by Dean of College of Arts and Sciences at NEIU, 2004, Carnegie Foundation for the Advancement of Teaching, Council for the Advancement and Support of Education and in 1998 by Provost of SXU

Teacher /Scholar Award recipient, SXU, School of Arts and Sciences, 2002

Sigma Xi Honor Society

Recognized by SXU for "Excellence in Scholarship," May, 1999 and April, 2001, May 2002

PUBLICATIONS: ARTICLES

Gosser, D.K.; Kampmeier, J.A.; Varma-Nelson's. Peer-Led Team Learning: 2008 James Flack Norris Award Address. *Journal of Chemical Education*, 87, Vol 4, April 2010, 374-380.

Invited

Eberlein, T., Kampmeier, J., Minderhout, V., Moog, R., Platt, T., Varma-Nelson, P. and White, H., (2008), "Pedagogies of Engagement : A Comparison of PBL, POGIL and PLTL" in preparation for *Biochemistry and Molecular Biology Education*, 36, 4, 262-273 **Invited**

Gafney, L and Varma-Nelson P. (2007), "Evaluating Peer-Led Team Learning: A Study of Long-Term Effects on Former Workshop Leaders." *Journal of Chemical Education*, 84, 535-539.

Varma-Nelson, P. (2006) "Peer-Led Team Learning" in *Metropolitan Universities Journal: "STEM Innovation and Dissemination: Improving Teaching and Learning in Science, Technology, Engineering and Mathematics,"* 17, 19-29. **Invited**

Weaver, G., D. Wink, P. Varma-Nelson, F. Lytle, R. Morris, W. Fornes, C. Russell, and W. J. Boone. 2006. "Developing a New Model to Provide First and Second-Year Undergraduates with Chemistry Research Experience: Early Findings of the Center for Authentic Science Practice in Education (CASPiE)." *The Chemical Educator*, 11, 1-5.

Weaver, G. C., Varma-Nelson, P., Wink, D., Morris, R., Lytle, F. "Experiencing Research in a First or Second Year Science Course - Preliminary Results and Reflections on the Goals and Progress of the Center for Authentic Science Practice in Education (CASPiE)." (2005). *The Chemical Educator*, 11, 125-129.

Varma-Nelson, P. *The peer-led team learning workshop model*, Project Kaleidoscope Volume IV: *What Works, What Matters, What Lasts*. Retrieved May 21, 2007, from Approaches to Assessing 21st Century Pedagogies Web site:

<http://www.pkal.org/documents/Vol4PeerLedTeamWorkshop.cfm>. **Invited**

Gafney, L. and Varma-Nelson, P., *What Happens Next? A Follow-up Study of Workshop Leaders at St. Xavier University* Progressions, Volume 3, Issue 2, Winter 2002, p.1.

Invited

Varma-Nelson, P. 2000. Peer-Led Team Learning Symposium Report, 16th Biennial Conference on Chemical Education. In *CHED Newsletter*.

Gosser, D., V. Roth, L. Gafney, J. Kampmeier, V. Strozak, P. Varma-Nelson, S. Radcliff, and M. Weiner. 1996. Workshop Chemistry: Overcoming Barriers to Student Success. *The Chemical Educator* 1(1), <http://link.springer-ny.com/link/service/journals/00897/index.htm> **Invited**

Varma-Nelson, P., J. E. Nelson and T. Kloempkin. 1992. A particle concentration immunoassay for AZT. In *Proceedings of the PCFIA Users Symposium*. IDDEX, Portland, MA. **Invited**

Nelson, J.E., P. Varma-Nelson and T. Kloempkin. 1992. A graphic grade scaling method. *Journal of Chemical Education*. 6, 462-3.

Varma-Nelson, P., J.E. Nelson and S.M. Belknap. 1991. A particle concentration fluorescence immunoassay for gentamicin. *Therapeutic Drug Monitoring* 13 (3): 260-2.

Schultz, R.M., P. Varma-Nelson, R. Ortiz, K. A. Koslowski, A. T. Orawski, P. Ragast, A. Frankfater. 1989. "Active and inactive forms of the transition-state analog protease inhibitor leupeptin: Explanation of the observed slow binding of leupeptin to cathepsin B and papain." *Journal of Biological Chemistry* 264 (3): 1497-1507.

Schultz, R.M., P. Varma-Nelson, J. Peters and W. Treadway. 1979. "Effect of essential catalytic residue modifications on conformation and binding affinity in α -chymotrypsin." *Journal of Biological Chemistry* 254: 12411.

Matthews, C., J. Nelson, P. Varma and R. Minard. 1978. "Deuterolysis of amino acid precursors in chemical evolution studies." H. Noda (Ed). *Origin of Life* 123-8. Center for Academic Publications, Japan. **Invited**

Matthews, C., J. Nelson, P. Varma-Nelson, R. Minard. 1977. "Deuterolysis of amino acid precursors: Evidence for hydrogen cyanide polymers as protein ancestors." *Science* 198: 622-625.

Minard, R., W. Yang, P. Varma-Nelson, J. Nelson and C. Matthews. 1975. "Heteropolypeptides from poly- α -cyanoglycine and hydrogen cyanide: A model for the origin of proteins." *Science* 190: 387-389.

PUBLICATIONS: BOOKS AND MANUALS

"Vision and Change for Biology Education" commissioned by the American Association for Advancement of Science Submitted for review.

Varma-Nelson, P., Bentley, A., Weaver G and Wink, D., *Peer-Led Team Learning for Undergraduate Research*, in preparation.

Gafney, L., and Varma-Nelson, P. (2008), *Peer-led Team Learning: Evaluation, Dissemination, and Institutionalization of a College-level Educational Initiative* (Innovations in Science Education and Technology), Dordrecht, The Netherlands: Springer-Verlag.

Kampmeier, J., Varma-Nelson P., Wamser ,C. and Wedegaertner, D. 2006. Second Edition, *Peer-Led Team Learning: Organic Chemistry*. Prentice Hall, Upper Saddle River, NJ.

Varma-Nelson, P., and Dreyfuss, AE. (2001). *The Peer-Led Team Learning Dissemination Manual*. URL: <http://www.pltl.org/>; under Dissemination Materials.

Varma-Nelson, P. and M.S. Cracolice. 2001. *Peer-Led Team Learning: General, Organic, and Biochemistry*. Prentice Hall, Upper Saddle River, NJ.

Kampmeier, J.A., P. Varma-Nelson and D.K. Wedegaertner. 2001. *Peer-Led Team Learning: Organic Chemistry*. Prentice Hall, Upper Saddle River, NJ.

Gosser, D.K., M.S. Cracolice, J.A. Kampmeier, V. Roth, V. Strozak, and P. Varma-Nelson. 2001. *Peer-Led Team Learning: A Guidebook*. Prentice Hall, Upper Saddle River, NJ.

Varma-Nelson, P. and R. Van Lanen. 1993, 2001. *Laboratory Manual: Small Scale Organic Chemistry and Biochemistry Experiments*. Saint Xavier University, Chicago, IL.

PUBLICATIONS: CHAPTERS IN BOOKS

Kampmeier, J. A., Varma-Nelson, P. (2009) *Peer-Led Team Learning; Organic Chemistry*. In Pienta, N.; Cooper, M.M.; Greenbowe, T. (Eds.), *Chemists' Guide to Effective Teaching*, Vol.2. Chapter 9, 122-145, Upper Saddle River, NJ: Prentice Hall **Invited**

Varma-Nelson, P. and Gosser, D. (2005) Dissemination of Peer-Led Team Learning (PLTL) and Formation of a National Network Embracing a Common Pedagogy. In M. Ouellet (Ed.), *Teaching Inclusively: Diversity and Faculty Development*. (pp. 503-518). Stillwater, OK: New Forums Press. **Invited**

Varma-Nelson, P., Cracolice, M., and Gosser, D., January 2005. "Peer-Led Team Learning: A Student-Faculty Partnership for Transforming the Learning Environment". *Invention and Impact: Building Excellence in Undergraduate Science, Technology, Engineering and Mathematics (STEM) Education*, Proceedings of an April 2004 Conference Co-sponsored by the National Science Foundation (NSF) Division of Undergraduate Education (DUE) and the American Association for the Advancement of Science (AAAS) Directorate for Education and Human Resources Programs (EHR)-Retrieved May 21, 2007
http://www.aaas.org/publications/books_reports/CCLI/ **Invited**

Varma-Nelson, P. and Coppola, B., 2005, "Team Learning." In Cooper, M.M., Greenbowe, T., Pienta, N. (Eds). *"The Chemists' Guide to Effective Teaching"*, Vol.1 Chapter 13,155-169, Prentice Hall Publishing. Upper Saddle River, NJ. **Invited**

Sarquis, J.L., L.J. Dixon, D.K. Gosser, J.A. Kampmeier, V. Roth, V.S. Strozak and P. Varma-Nelson. 2001. The Workshop Project: Peer-Led Team Learning in Chemistry. In *Student-Assisted Teaching: A Guide to Faculty Student Teamwork*, eds. J.E. Miller, J.E. Groccia, and M.S. Miller, Chapter 23, 150 -155. Anker Publishing Company, Bolton, MA. **Invited**

Kampmeier, J.A. and P. Varma-Nelson. 2001. Institutionalizing The Workshops. In *Peer-Led Team Learning: A Guidebook*. Chapter 5. Prentice Hall, Upper Saddle River, NJ. **Invited**

INVITED PRESENTATIONS

Varma-Nelson, P., Opening Keynote, Chemical Education Section, “Development of Peer-Led Team Learning: Lessons Learned and New Directions” June 16, 2010, CERMACS, Dayton Ohio.

Varma-Nelson, P., Keynote “Evaluation, Dissemination, and Institutionalization of a College Level Initiative” at Appalachian Colleges Association Annual Summit, October 16, 2009, Abingdon, VA

Varma-Nelson, P., Opening Keynote “History, Lessons Learned and New Directions” at Morehouse College national PLTL Conference, “Expanding Peer Led Team Learning in the Sciences and Mathematics”, November 13, 2009, Atlanta, Georgia

Varma-Nelson, P., “Peer-Led Team Learning”, Committee on Minority Affairs-American Chemical Society, 237th National Meeting, March 23, 2009 Salt Lake City, Utah

Gosser, D. K., Kampmeier J.A., and Varma-Nelson, P., “Peer-Led Team Learning” Northeastern Section of the American Chemical Society, James Flack Norris Award Presentation 2008, November 8, 2009, Brandeis University, MA

Varma-Nelson, P., Midwest “Peer Leaders: Future Noyce Scholars?”, Plenary Talk April 4, 2009, Midwest Noyce Conference, at IUPUI

Varma-Nelson, P., “Bringing the Research Model of Teaching to the Classroom”, Homi Bhabha Center for Science Education, November 21, 2007, Mumbai, India.

Varma-Nelson, P., “Peer-Led Team Learning”, Historically Black Colleges and Universities Undergraduate Program, 2007 National Research Conference, sponsored by NSF and AAAS, October 2, 2007, Washington DC.

Varma-Nelson, P., S Hixson, E. Lewis, H. Richtol, National Science Foundation, Division of Undergraduate Programs, American Chemical Society, 234th National Meeting, August 20, 2007, Boston.

Varma-Nelson, P., "CASPiE: The Center for Authentic Science Practice in Education", 2007 Middle Atlantic Discovery Chemistry Project (MADCP) Meeting, Keynote Speaker at the dinner, June 3, Washington College, MD.

Watford, B., D. McBride and P. Varma-Nelson, National Science Foundation's Scholarships in Science, Technology, Engineering, and Mathematics (S-STEM) Program, Orientation, Review Panel Meeting, April 4, 2007, Washington DC.

Varma-Nelson, P., E. Lewis, H. Richtol, and S Hixson, 14 September 2006 San Francisco NSF Division of Undergraduate Programs, American Chemical Society, 232nd National Meeting, September 14, 2006 San Francisco, CA USA

Varma-Nelson, P and D. Malik “Peer-Led Team Learning and other 21st Century Pedagogies: Transforming the Learning Environment”, plenary talk, Nov.4, 2005, Wuhan University, People’s Republic of China.

Varma-Nelson, P. Peer-Led Team Learning, Department Seminar, October 14, 2005. University of Oregon, Eugene, OR.

Varma-Nelson, P., and A. Bennett Golomb, Peer-Led Team Learning, Workshop. October 18th, 2005, Northeastern Illinois University, Center for Teaching and Learning, Chicago, IL.

Varma-Nelson P., American Education System, July 13, 2005, Huazhong University of Science and Technology, Wuhan, China.

Varma-Nelson, P., Dissemination of Peer-led Team Learning (PLTL): Formation of a National Network Embracing a Common Pedagogy June 30, 2005, at Gordon Research Conference on Chemistry Education Research & Practice, Connecticut College, New London, CT

Varma-Nelson, P., Peer-Led Team Learning February 19, 2005. Invention and Impact: Building Excellence in Undergraduate STEM Education Symposium, American Association for the Advancement of Science (AAAS) Meeting, Washington DC. Organized by NSF

Weaver, G, F. Lytle, D. Lehman and P. Varma-Nelson, NSF Workshop on Implementation of Undergraduate Research Centers, September 17, 2004 National Science Foundation, Arlington, VA

Varma-Nelson, P. and B.P. Coppola, Team Learning, July 18, 2004. 18th Bicentennial Conference on Chemical Education, Iowa State University, Ames, IA.

Varma-Nelson, P. and I.J. Leal, PLTL: A Student-Faculty Partnership. June 28, 2004. Institutional Research and Academic Career Development Award (IRACDA) Retreat. Emory University, Atlanta, GA.

Varma-Nelson, P. Evaluation of PLTL: Multi-dimensional and Collaborative. June 2, 2004, 36th Central Regional Meeting, Indiana University Purdue University Indianapolis, IN.

Varma-Nelson, P. May 3, 2004. PLTL: A Student-Faculty Partnership for Transforming the Learning Environment. Chicago Symposium Series “Excellence in Teaching Mathematics and Science: Research and Practice”. University of Illinois, Chicago.

Varma-Nelson, P. and M.S. Cracolice, Student Leaders: I.J. Leal and A. Santorro April 16, 2004. Peer-Led Team Learning: A Versatile Student-Centered Curriculum Strategy. "Invention and Impact" Co-sponsored by the National Science Foundation (NSF) Division of Undergraduate Education (DUE) and the American Association for the Advancement of Science (AAAS) Directorate for Education and Human Resources Programs (EHR)

Varma-Nelson, P. and Student Presenter: I.J. Leal. October 4, 2003. "Peer-Led Team Learning: A Student-Faculty Partnership for Educational Change", Chemistry Department, Notre Dame University, Indiana.

Varma-Nelson, Pratibha "Peer Led Team Learning; Overview of the Project", Northwestern University Searle Center for Teaching Excellence, June 13, 2003.

Varma-Nelson, P. and J.A. Kampmeier, February 7-8, 2003. "Peer-Led Team Learning. Workshop Project", Emory University, Atlanta, GA.

Varma-Nelson, P. and Christopher Bauer, October 27-28, 2002, "Workshop Project: Peer-Led Team Learning", University of New Hampshire, and NH.

Varma-Nelson, P., August 2, 2002, "History of Peer-Led Team Learning," keynote address, Fourth PLTL Leadership meeting, University of Montana, Missoula.

Varma-Nelson, P. October 12, 2001. "Peer-Led Team Learning in Physical Sciences, Physics and Chemistry Department," The University of Maine, Orono, ME.

Varma-Nelson, P. July 13, 2001 National Conference on Peer-Led Team Learning, Dissemination, "Who's Listening?" Goucher College, Towson, Maryland

Varma-Nelson, P. May 3, 2001. "Peer-Led Team Learning," North Carolina State University, Raleigh, NC.

Varma-Nelson, P. April 21, 2001, "New Developments for Peer-Led Team Learning, Presented to the ChemConnections Annual Consortium Meeting," McAlester College St. Paul, MN.

Varma-Nelson, P. Feb 3-4, 2001, WPA program report, MID project overview and PLTL National Dissemination Project. National Visiting Committee Meeting, New York.

Moore, J., B. Spencer, A. Stacy and P. Varma-Nelson, January 10, 2001, "Lessons Learned about Curricular Transformation from the NSF Chemistry Initiatives," Innovations in College Chemistry Teaching, Gordon Research Conference, Ventura, CA

Varma-Nelson, P., J.A. Kampmeier and D.K. Wedegaertner. August 1, 2000. "The Organic Workshop Project: Peer-Led Team Learning," Symposium: Spectrum of Active Learning Methods Currently in Use in the Introductory Organic Classroom. 16th Biennial Conference On Chemical Education, University of Michigan, Ann Arbor, MI.

Varma-Nelson, P. April 28-30, 2000. "Workshop Project: Peer-Led Team Learning Overview," Miami Conference on Active Learning in Science Courses, University of Miami, Coral Gables, FL.

Varma-Nelson, P. December 8th, 1999, "Workshop Project: Peer-Led Team Learning. Chemistry Department, Purdue University, Lafayette, IN.

Varma-Nelson, P. August 7-11, 1999. National Dissemination Project on Peer-Led Team Learning. Presented dissemination strategies and led general session WPA program. Big Sky Conference: First Rocky Mountain Conference on Peer-Led Team Learning University of Montana, Missoula, MT.

Kampmeier, J.A. and P. Varma-Nelson. August 7-11, 1999. Breakout session on Organic/Biochemistry Dissemination. Big Sky Conference: First Rocky Mountain Conference on Peer-Led Team Learning University of Montana, Missoula, MT.

Varma-Nelson, P. February 5, 1998. Future Plans for Dissemination of the Workshop Chemistry Project. National Visiting Committee, City College New York.

Varma-Nelson, P. February 20, 1997. Dissemination Activities of the Workshop Chemistry Project. National Visiting Committee, New York City Technical College.

Varma-Nelson, P. August 7, 1996. Workshops in Chemistry for the Allied Health Fields. Workshop Chemistry: Peer Led Team Learning in Chemistry, 14th Biennial Conference in Chemical Education (BCCE), Clemson University, South Carolina.

Varma-Nelson, P. February 8, 1996. Workshops at Saint Xavier University: Progress Report. Workshop Chemistry Project National Visiting Committee, City College of New York (CCNY).

OTHER PRESENTATIONS

Runshe Dunlap, D., Varma-Nelson, P., Tarr, T., "Welcoming Faculty by Meeting Their Specific Disciplinary Needs"; Professional and Organizational and Development (POD) Network; Houston, TX; October 31, 2009

Varma-Nelson, P. "High teaching loads, limited resources, and not enough hours in the day: How can I do it all?" 231st ACS National Meeting in Atlanta, GA, March 29, 2006.

"CASPiE: A program to include research as part of the mainstream first and second year laboratory curriculum." Weaver, G. C., Boone, W. J., Russell, C. B., Wink, D. J., Lytle, F. E., Varma-Nelson, P., Morris, R. J., and Bentley, A. K. (2006). 231st ACS National Meeting, Atlanta, GA.

Varma-Nelson, P., T.R. Weaver and R. Gilman "Chemistry Capstone Seminar with Green Theme" 229th ACS National Meeting in San Diego, March 15, 2005

Varma-Nelson, P. and L. Gafney, "What Happens Next? A Follow-Up Study of PLTL Workshop Leaders," 229th ACS National Meeting in San Diego, March 15, 2005

Varma-Nelson, P., Peer-Led Team Learning (PLTL) in a course for Allied Health Professionals, ACS National Meeting in San Diego, March 15, 2005

Varma-Nelson, P., "PLTL: A student-faculty partnership for transforming the learning environment", 229th ACS National Meeting in San Diego, March 14, 2005

Varma-Nelson, P. and L. Gafney, "What Happens Next? A Follow-Up Study of Workshop Leaders," October 23, 2004. The International Society for the Scholarship of Teaching and Learning (IS-SOTL) Inaugural Meeting. Bloomington, IN.

Varma-Nelson, P. and L. Gafney. Evaluation of Dissemination of Peer-Led Team Learning (PLTL) and Formation of a National Network: Embracing Common Pedagogy. October 23, 2004. The International Society for the Scholarship of Teaching and Learning (IS-SOTL) Inaugural Meeting. Bloomington, IN.

Varma-Nelson, P. and R. Gilman, March 31, 2004, "Ethics in a Chemistry Seminar Course", ACS Meeting, Anaheim, CA.

"The Center for Authentic Science Practice in Education (CASPiE): Applying Disciplinary Research in the Undergraduate Laboratory." Weaver, G. C., Varma-Nelson, P., Lytle, F. E., Boone, W., Wink, D., and Morris, R. (2004). International Society for the Scholarship of Teaching and Learning.

Varma-Nelson, Pratibha, Ingrid Leal and Yoriela Marciano, June 2, 2003, Peer-Led Team Learning, Great Lakes Regional ACS Meeting, Loyola University, Chicago, IL.

Varma-Nelson, Pratibha, March 24, 2003, PLTL: Promoting change through communication at all levels of the education enterprise (abstract). American Chemical Society, National Meeting, New Orleans, LA.

Varma-Nelson, P. and L. Gafney, July 31, 2002, Impact of Being a Peer-Leader on Students at St. Xavier University, Chicago, 17th Biennial Conference on Chemical Education, Western Washington University, Bellingham, WA

Gafney, L. and P. Varma-Nelson, July 31, 2002, Role of the WPA Program in Curricular Reform, 17th Biennial Conference on Chemical Education, Western Washington University, Bellingham, WA

Varma-Nelson, P. August 26-30, 2001. National Dissemination of Peer-Led Team Learning: Its Design, Implementation, Documentation, and Evaluation. Symposium Chair. ACS 222nd National Meeting, Chicago, IL.

Kampmeier, J.A., P. Varma-Nelson and D.K. Wedegaertner. October 25-28, 2000. Teaching Organic Chemistry in the New Century. ACS 221st National Meeting San Diego, CA.

Wedegaertner, D.K., P. Varma-Nelson and J. A. Kampmeier. March 21-25, 1999. The Organic Workshop Project: Peer-Led Team Learning. ACS 217th National Meeting Anaheim, CA.

Varma-Nelson, P. and J. McNellis. February, 1998. The Scholarship of Teaching. Spring Faculty Study Day, Saint Xavier University, Chicago, IL.

Varma-Nelson, P. Sept 9, 1997. Workshop Chemistry: Peer Led Team Learning. Presented as part of Systemic Reform in Chemical Education Symposium, ACS 214th National Meeting, Las Vegas, NV.

Varma-Nelson, P. June 25, 1997 Workshop Chemistry Peer-Led Team Learning. Student presenter: Carole Munch. The Second Annual Illinois Scientific Literacy Network Conference Illinois Math and Science Academy, Aurora, IL.

Varma-Nelson, P. and D. Gosser. Aug 25, 1996. Developing a Workshop Curriculum: Scholarship or Teaching. Scholarship of Teaching Chemistry symposium, ACS 212th National Meeting, Orlando, FL.

POSTERS

Mauser, Sours, Zhu and Varma-Nelson, "Cyber PLTL (cPLTL): Development, implementation, and initial findings" 239th National ACS National; San Francisco, CA; March 21, 2010 Poster

Weaver, G. C., Varma-Nelson, P., Wink, D., Lytle, F., and Morris, R. "The Center for Authentic Science Practice in Education (CASPiE): An Experiment in Undergraduate Research." (2005). Poster presented Gordon Research Conference on Chemistry Education Research and Practice, New London, CT.

Varma-Nelson, P. and L. Gafney, April 7–11, 2002. Poster: Evaluation of the WPA Program in Curricular Reform. ACS American Chemical Society National Meeting Orlando, FL.

Varma-Nelson, P. and D.K. Gosser, March 26-27, 2000. Peer-Led Team learning: National Dissemination by the Workshop Project. ACS 219th American Chemical Society National Meeting San Francisco, CA.

Varma-Nelson, P., J.A. Kampmeier, and D.K. Wedegaertner. June 22, 1999. Organic Chemistry Workshop: Assessment and Materials. Innovations in College Chemistry Teaching. Gordon Research Conference, Conneticut College, New London, CT.

Varma-Nelson, P. and V. Strozac, September 20-25, 1998. Workshop Chemistry Project: Peer Led Team Learning at the "New Developments and Visualization in Science and Chemistry Education" Gordon Research Conference, Queens College, Oxford, England.

Van Lanen, R. and P. Varma-Nelson. Oct 18, 1996. Peer Led Team Learning in Organic Chemistry, Illinois State Academy of Science, 89th Annual Meeting, Illinois Wesleyan University, Bloomington, IL.

Varma-Nelson, P. and R. Van Lanen, June 30 - July 5, 1996, "Workshop Chemistry at a Small Liberal Arts Institution," Innovations in College Chemistry Teaching. Gordon Research conference, Plymouth State College, Plymouth, NH.

Varma-Nelson, P. and R. Van Lanen, June 1-3, 1992, "Small Scale Laboratory Experiments for a One-Semester Organic Chemistry - Biochemistry Course." ACS 25th Great Lakes Meeting, Milwaukee, WI.

INVITED WORKSHOPS

Varma-Nelson and Pelaez, Proposal Writing Workshop; Assessment Institute, IUPUI, Indianapolis; October 25, 2009

Varma-Nelson, P., Murphree S.S., and Lang, C., "Peer-Led Team Learning : Bringing the research model (of teaching) to the classroom", Physics Teachers Education Coalition March 2009 meeting, Pittsburgh. Presented a workshop on PLTL

Hamilton, S., and Varma-Nelson, P., "Going for the Gold", October 2008, Assessment Institute, Indianapolis

Varma-Nelson, P., Peer-Led Team Learning, June 15, 2007, at the 11th Annual Science, Technology, Engineering and Mathematics (STEM) Education Scholars Program, Sponsored by the Center for Integration of Research, Teaching and Learning (CIRTL), at Howard University, Washington, DC.

Varma-Nelson, P., Writing Effective NSF Proposals, June 5, 2007, Middle Atlantic Discovery Chemistry Project (MADCP) annual meeting, Washington College, MD

Varma-Nelson, P. and E. Lewis, Writing Effective NSF Proposals, March 29, 2007, Northeastern Illinois University, Center for Teaching and Learning, Chicago, IL.

Varma-Nelson, P. and A. Bennett Golomb, Peer-Led Team Learning December 1-2, 2005. Morehouse College, Atlanta, GA

Varma-Nelson, P., I.J. Leal and several workshop leaders from UW Madison, Peer-Led Team Learning Workshop, May 16-17, 2005. United Tribes Technical College, Bismarck, North Dakota.

Varma-Nelson, P., S. Horowitz and I. Leal, Peer-Led Team Learning, April 2-3, 2005. Computer Science Department, for Wisconsin Emerging Scholars-CS consortium, University of Madison-Wisconsin, Madison, WI. Consortium headed by UW Madison and supported by NSF includes UW Milwaukee, Purdue University, Loyola of Baltimore, Georgia Tech, Beloit College, Duke University and Rutgers University

Varma-Nelson, P., Student Presenters: M.G. Belanger, J. Kinsella, I.J. Leal, J. Mahoney, and Z. Rouse. Peer-Led Team Learning Workshop. March 4-5, 2005, CASPiE Consortium, at University of Illinois at Chicago.

Varma-Nelson, P. Student Leaders: M. Alonso, C. Budziak, I.J. Leal, J. Mahoney and E. Straky. May 3, 2004. PLTL: A Student-Faculty Partnership for Transforming the Learning Environment. Chicago Symposium Series "Excellence in Teaching Mathematics and Science: Research and Practice". University of Illinois, Chicago-breakout session.

Varma-Nelson, P. and J. Sarquis, Student Presenters C. Budziak, and I.J. Leal. January 23-25, 2004. Multi-Initiative Dissemination (MID) Project workshop. Louisiana State University, Baton Rouge, LA.

Varma-Nelson, P. and Fraiman, A. Student Leaders: I. J. Leal, Y. Marcano, and L. Thottappilly. Workshop on PLTL as part of MID project, March 7-8, 2003 Northeastern Illinois University, Chicago

Varma-Nelson, P. and Bauer, C., Workshop on PLTL as part of MID project, September 27-28, 2002 University of New Hampshire, NH.

Varma-Nelson, P. and R. Blake, April 26-27, 2002. Peer-Led Team Learning: The Workshop Model. University of Arizona. MID Workshop.

Varma-Nelson, P. and M. Cracolice, February 22-23, 2002. Peer-Led Team Learning: The Workshop Model. University of S. Florida.

Varma-Nelson, P. and Cracolice, M. July 22-25, 2001. Workshop: Science for All: Beginning Chemistry. Project Kaleidoscope, Snowbird, UT. Peer Leader: Richard James (BYU).

Varma-Nelson, P. and R. Blake. Peer Leaders: Yvonne O'Connel (SXU) and Natalie Leach (IUPUI). February 22-25, 2001. Peer-Led Team Learning: The Workshop Model. (MID) Florida Atlantic University Workshop, Boca Raton, FL.

Varma-Nelson, P. and J.A. Kampmeier. May 3, 2000. Workshop Project: Peer-Led Team Learning. Cayey University, Cayey, Puerto Rico.

Varma-Nelson, P. and J.A. Kampmeier. May 4, 2000. Workshop Project: Peer-Led Team Learning. Arecibo University, Arecibo, Puerto Rico.

Varma-Nelson, P. and Mark Cracolice. Peer Leaders: Cyrena Bowers, Carson Robertson, Matthew Sexton, University of North Colorado. October 9, 1999. Undergraduate Chemistry Curriculum Reform: Workshop Chemistry. University of Northern Colorado, Greeley, CO.

Varma-Nelson, P., V. Strozak and P. Anderseon-Meyer. Peer Leaders: Beth Beringer, Gaby Gracia, Jamie Jett, Vasso Melachrinidis, and Phdra Ranjbar. Sept. 24-25, 1999. Workshop at 2YC3 regional meeting of the community colleges, South Suburban College, IL

Varma-Nelson, P. and V. Strozak. Peer Leaders: Derek Haverson, Jamie Jett, Vasso Melachrinidis, Keith Schrunck, Angel Whittington, Jason Wray. July 8-11, 1999. NSF Workshop on Chemistry Curriculum Reform, Iowa General Chemistry Network (IGCN) Summer Conference, Iowa State, Ames IA.

Varma-Nelson, P. Peer Leaders from SXU: Patrick McCullough, Jamie Jett, Angel Whittington and Vasso Melachrinidis. May 10, 1999. The Workshop Model: Peer-Led Team Learning. Workshop. Presented in a breakout session at the third symposium in a series titled Excellence in Teaching Undergraduate Science and Mathematics: National and Chicago Perspectives, University of Illinois at Chicago, Chicago, IL.

Varma-Nelson, P., D. K. Gosser, J. Kampmeier. March 12, 1999. Workshop Chemistry: Peer Led Team Learning, Morehouse College, Atlanta, GA.

Varma-Nelson, P., A. Diegelman, and V. Roth. January 7-8, 1999. TA Training Retreat: Adapting Workshop Chemistry to UCLA. UCLA, Los Angeles, CA.

Varma-Nelson, P., Peer Leaders from University of Kentucky: C. Bradley, M. Grant, J. Hackett, K. Hong, A. Poe, and L. Watson. November 23, 1998. Workshop Chemistry: Peer Led Team Learning. University of Kentucky, Lexington, KY.

Gosser, D.K., V.S. Strozak, P. Varma-Nelson. November 6-8, 1998. Workshop Chemistry: Peer Led Team Learning. Presented at Project Kaleidoscope Workshop, Special Opportunities and Challenges: Science and Mathematics at the Urban and Commuter Institution, California State University-Fullerton, Fullerton, CA.

Varma-Nelson, P. and D.K. Gosser. June 15-16, 1998. Workshop Chemistry Project: Peer-Led Team Learning. Middle Atlantic Discovery Chemistry Project (MADCP), Franklin and Marshall College, Lancaster, PA.

Varma-Nelson, P., M. Walter, P. Anderson-Meyer. Peer Leaders: V. Melachrinidis, C. Munch, D. Patitucci, and F. Suhail. November 3, 1997. Undergraduate Chemistry Curriculum Reform. Discussion and demonstration of Workshop Chemistry following an ACS teleconference, Oakton Community College, Skokie, IL.

Varma-Nelson, P. and J. Kampmeier. Peer Leaders: A. Johanek and R. Zhang. Aug 8 -9, 1997. The Organic Workshop Project: Peer Led Team Learning. Middle Atlantic Discovery Chemistry Project (MADCP) Meeting, Hope College, Frederick MD.

Varma-Nelson, P. and D. Gosser. Peer Leaders: C. Boeschel, R. Zhang, and J. Daniel. V. Strozak coordinating. July 21, 1997. Peer-Led Team Learning. Presented as part of the Improving the Teaching/Learning Process in General Chemistry, Stony Brook, NY,

Gosser, D.K. and P. Varma-Nelson. Peer Leaders: Jewel Daniel (CCNY), D. Patitucci, C. Munch, A. Johanek, C. Boeschel, and S. Semlow of SXU. May 10-11, 1997. Workshop Chemistry presented at Day 2 to Day-40 Workshop Symposium in Chemical Education, University of Michigan, Ann Arbor, MI.

Varma-Nelson, P. and V. Strozak. Peer Leaders: D. Patitucci, M. Boyle, C. Boeschel, S. Semlow, and S. Pellegrini. January 31 - February 1, 1997. A Peer Led Team Learning Model for Teaching Chemistry and A Student's Perspective on Workshop Chemistry. Presented as part of

Revitalizing General Chemistry at the Community College, PKAL and Project Kaleidoscope, Oakton, Des Plaines, IL.

OTHER WORKSHOPS

Varma-Nelson, P. "Effective Teaching and Learning for Chemistry Instructors. Peer-Led Team Learning: A Faculty-student Partnership." July 18, 2004. 18th BCCE Meeting at the University of Iowa-Ames, IA.

Varma-Nelson, P. and J. Kampmeier. July 29, 2002, Peer-Led Team Learning. 17th Biennial Conference on Chemical Education, Western Washington University, Bellingham, WA

Varma-Nelson, P. and M. Cracolice. August 12, 1998. Workshop Chemistry Project: Peer-Led Team Learning. 15th Biennial Conference on Chemical Education (BCCE), University of Waterloo, Waterloo, Ontario, Canada

CHAUTAUQUA FACULTY DEVELOPMENT PROGRAM NSF SHORT COURSES FOR COLLEGE TEACHERS

<http://www.engrng.pitt.edu/~chautauq/>

Each of these workshops had approximately 25 participants. All workshops had student who had served as peer leaders as co-presenters.

Varma-Nelson, P., (Director) and Donald Wink, June 20-21, 2005, Peer-Led Team Learning: The Workshop Model, University of Illinois Chicago, Chicago, IL.

Varma-Nelson, P., (Director), Mark Cracolice, May 24-26, 2004, Peer-Led Team Learning: The Workshop Model, California State-Fullerton, Fullerton, CA.,

Varma-Nelson, P., (Director), and Mark Cracolice, May 19-21, 2003, Peer-Led Team Learning: The Workshop Model, NASA/Jet Propulsion Laboratory, Pasadena, CA.,

Varma-Nelson, P. (Director), and M. Cracolice. May 20-22, 2002. Chautauqua Course: 49, Peer-Led Team Learning: The Workshop Model. Pasadena, CA.

Varma-Nelson, P., (Director), and M. Cracolice. May 21-23, 2001. Course: 53, Peer-Led Team Learning: The Workshop Model. Pasadena, CA.

Varma-Nelson, P., (Director), D.K. Gosser and V. Strozak. June 15-17, 2000. Course: 51, Peer-Led Team Learning: The Workshop Model. Philadelphia, PA.

Varma-Nelson, P., (Director), M. Cracolice, R. Narode and J. Kampmeier. May 18-20, 2000. Course: 51, Peer-Led Team Learning: The Workshop Model. Pasadena, CA.

Varma-Nelson, P., ((Director), D. Gosser, J. Kampmeier, V. Roth and V. Strozak. June 10-12, 1999. Course: 40, Workshop Chemistry Project: Peer-Led Team Learning. Philadelphia, PA.

Varma-Nelson, P., (Director), D. Gosser, J. Kampmeier, V. Roth. June 11-13, 1998. Course: 30, Workshop Chemistry Project: Peer-Led Team Learning. Philadelphia, PA.

CHAired SYMPOSIA

Varma-Nelson P., Chair, “DUE: Supporting Undergraduate Education at NSF” symposium, Sunday, 25 March 2007, 233th, ACS National Meeting, Chicago, IL.

Varma-Nelson P., Chair, Research in Chemical Education session, Organic Chemistry Wednesday Afternoon, March 16, 2005, 229th, ACS National Meeting, San Diego

Varma-Nelson P., Chair, August 26-30, 2001. NSF Initiatives: Winding Down or Just Getting Started.

National Dissemination of Peer-Led Team Learning. ACS National Meeting, Chicago, IL.

Varma-Nelson P., Chair, “From the Big Bang to the Space Age”, Visualization in Science Education. August 5-10, 2001, Gordon Research Conference on Science Education and Visualization, Mount Holyoke College, South Hadley, MA.

Varma-Nelson P., Chair, July 31 & August 2, 2000, Peer-Led Team Learning. 16th Biennial Conference on Chemical Education, Ann Arbor, MI.

SERVICE

National

Advisory Board, DePaul University STEP Project, 2008-2012

Advisory Board member, 2007-2010, Chemical and Engineering News, a weekly news magazine for professionals in the chemical sciences.

Editorial Board member, Journal of Science Education and Technology, 2006-present

Mentor to a Preparing Future Faculty (PFF) Fellow from Northwestern University Department of Chemistry 2005-present

Reviewer: Science, The Journal of Chemical Education, The Chemical Educator, Journal of Women and Minorities in Science and Engineering and Journal of Science Education and Technology, National Science Foundation, CCLI program (1995-2006), Undergraduate Research Centers in the Chemistry Division.

Member, 2006-present, New Member Committee, Division of Chemical Education, American Chemical Society.

Founding Chair, 2002-2006, New Member Committee, Division of Chemical Education, American Chemical Society.

Member, 2002-present, Long Range Planning Committee, Division of CHED, American Chemical Society.

Advisory Board Member, 2003-2006, Process Oriented Guided Inquiry Learning (POGIL) National Dissemination Project.

Member, August 5-10, 2001, U.S. Program Advisory Board, Gordon Research Conference on Science Education and Visualization held at Mount Holyoke College, CT.

Member, 2000–2003, Committee on Chemical Education Research, Division of Chemical Education (CHED), American Chemical Society.

Member, 1999-2002, International Activities Committee, Division of CHED, American Chemical Society.

National Visiting Committee Member, 1996-2000. NSF funded, Molecular Science Project, UCLA, Chemistry

Saint Xavier University Committees

Faculty Task Force on Scholarship of Teaching, 1997-98

Chair, Faculty Affairs, 1997-98, member and contract negotiator 1994-98,

Search for Vice-President of Academic Affairs, 1995

Faculty Senate, 1991-94

Faculty Promotion and Tenure, 1988-91

Admissions, 1984-85

Academic Policies, 1983-84

University By-Laws, 1980-83

Board of Trustees By-Laws, 1981-83

Other Saint Xavier University Responsibilities

Advisor, 1990- 2001, pre-pharmacy students

Faculty advisor, 1984-1991, ACS student chapter

OTHER PROFESSIONAL ACTIVITIES

Varma-Nelson, P., Chair Faculty Development Track, Assessment Institute; Westin, Indianapolis, IN; October, 2009 and October, 2010

Session Facilitator: Varma-Nelson P., White H., and Withers M.,” “Student – centered learning (how students learn and appropriate pedagogy)” at the “Transforming Undergraduate Education in Biology: Mobilizing the Community for Change.” Invitation only, conference held in Washington, DC on July 15-17, 2009. Organized by the American Association for Advancement of Science

Facilitator: Varma-Nelson P., STEP PI meeting “Gathering and Analyzing Data” March 12, 2009, and “Leveraging your STEP Project” March 13, 2009 Washington DC, Organized by NSF.

Chaired and hosted the Peer-Led Team Learning National Leadership Conference, October 8-10, 2004 at Downers Grove Illinois and Northeastern Illinois University, Chicago.

Varma-Nelson, P. and Student Presenter: I. J. Leal. October 29, 2003. "Peer-Led Team Learning." on Radio Talk Show, Vantage Point 101.9 WTMX-FM.

Hosted the Multi-Initiative Dissemination (MID) Workshop, March 7-8, 2003, Northeastern Illinois University, Chicago.

Varma-Nelson, P. September 24-25, 2001. Hosted and coordinated with Center for Educational Practice (CEP) at Saint Xavier University, Dr. Brian P. Coppola's Visit and Presentation on "Future Roles and Responsibilities of Faculty". Dr. Coppola is Professor of Chemistry at the University of Michigan, Ann Arbor, MI.

Varma-Nelson, P. 1995-1999. Project Partner: Workshop Chemistry Project, A National Science Foundation (NSF) Systemic Reform of Undergraduate Chemistry Curriculum Initiative.

Varma-Nelson, P. March 30-31, 1998. Hosted and coordinated with Committee for Educational Practice (CEP), at Saint Xavier University "The Power Of Mentoring: Suggestions, Road Maps, and Not Doing That Again", Dr. Billy Joe Evans Visit and Presentation. Dr. Evans is Professor of Chemistry, Michigan University, Ann Arbor, MI.

Attended, January 4-8, 1998. Innovations in College Chemistry Teaching, and Implementing Workshop Chemistry. Gordon Research Conference, Ventura, CA.

Varma-Nelson, P. August 20-21, 1997. Hosted and coordinated along with Committee for Educational Practice (CEP), Saint Xavier University, Dr. Charles Glassick's Visit and Presentation "Scholarship Assessed" on Faculty Study Day. Dr. Glassick is Senior Associate of the Carnegie Foundation for the Advancement of Teaching. SXU, Chicago, IL.

Varma-Nelson, P. May 18-19, 1997. Hosted a meeting of the Workshop Chemistry Project subgroup to assisted faculty members from four institutions (American University, Washington DC., Clark-Atlanta, Atlanta Georgia, University of Kentucky, and University of Montana) to write and develop an Adapt/Adopt proposal to be submitted to NSF. Holiday Inn, Countryside, IL.

Varma-Nelson, P., D.K. Gosser and J.A. Kampmeier. Peer Leaders: G. Amarasinghe, C. Cherian, D. Johnson, D. Patitucci, S. Pellegrini, T. Rosenow. Coordinators: Varma-Nelson, P., P. Anderson-Meyer, and R. Van Lanen. April 27, 1996. Faculty Development Workshop: Workshop Chemistry: A Peer Led Team Learning Model for Teaching Chemistry at Saint Xavier University. The Chemistry Division of the Associated Colleges of the Chicago Area (ACCA) is a consortium of 14 private liberal arts colleges.

COURSES TAUGHT

At Northeastern Illinois University

Chemistry Capstone Seminar, Chem 391

(new course that I designed and implemented, included 3 parts, Responsible Conduct for Scientists, Research Projects in Green Chemistry and lectures by experts in the field of chemistry)

Senior Seminar, Chem 390

Chemistry of Biological Molecules, Chem 348 (I redesigned the existing course to meet the ACS accreditation requirements)

Undergraduate research

At Saint Xavier University

Organic Chemistry, 251-252

Organic Chemistry Laboratory, 251L-252L

Biochemistry, 301

Principles of Inorganic Chemistry, 107

Principles of Organic/Biochemistry, 108 (completely reorganized the course)

Toxic Substances in the Environment, 104 and 304 (new courses that I designed and implemented)

Environmental Science, 103 (new courses that I designed and implemented for non-science majors)

Senior Seminar, 355 (part of a team that redesigned the course)

Independent Study, 354

PARTICIPATION IN WORKSHOPS

The National Academies “The Dragon and the Elephant: Understanding the Development of Innovation Capacity in China and India” held at National Academies headquarters, Washington DC, September 24-25, 2007.

The National Academies, Workshop on “Research Evidence related to Future Skill Demands” held at The Keck Center of the National Academies. Washington, DC May 31-June 1, 2007.

The National Academies, “Understanding Interventions That Encourage Minorities to Pursue Research Careers: Major Questions and Appropriate Methods”, held at AAAS, Washington DC, May 3-4, 2007.

PROPOSALS SUBMITTED BUT NOT FUNDED

Bruce M, F. Amar and P. Varma-Nelson , “Leader Training: Overcoming a Critical Roadblock to Sustainable Adoption of PLTL,” Submitted to June 2004, NSF, CCLI-EMD Program.

Varma-Nelson P., L Sanders and D. Rutschman, “Enhancing Recruitment and Retention of STEM Majors Through University-Community College Partnerships”. \$ 500,000 5 years. NSF, STEP, Program.

Cracolice M., V. Strozac, Varma-Nelson P., and Gaines M., “Development of Formal Thinking Skills in High School Biology and Chemistry,” Submitted August 26, 2002, NSF, IMD Program.

Varma-Nelson P., L Sanders and D. Rutschman, "Increasing Retention and Recruitment Through Implementation of Peer-Led Team Learning", June 3, 2002. NSF, Submitted to NSF, STEP Program.

Gosser D., P. Varma-Nelson, V. Strozac and M. Gaines, "PLTL National Dissemination: Expanding the Leadership". June 6, 2001 submitted to NSF CCLI-ND Program.

MEMBERSHIPS

American Association for Advancement of Science

American Chemical Society

Midwest Association of Chemistry Teachers at Liberal Arts Colleges (1979-2002)

Associated Colleges of the Chicago Area (1979-2002)

Research Faculty

BRENDA J. BLACKLOCK

Department of Chemistry and Chemical Biology
420 North Blackford Street
Science Building, LD326J
Indianapolis, IN 46202-3274

Phone: (317) 278-8181
FAX: (317) 274-4701
E-mail: bblacklo@iupui.edu

EDUCATION AND TRAINING

University of Alberta, Edmonton, AB (1989-94)

Ph.D. in Biochemistry

University of Waterloo, Waterloo, ON (1984-89)

Honours B.Sc. in Biochemistry, Co-operative Program

APPOINTMENTS

Department of Chemistry and Chemical Biology, IUPUI (2005-present)

Research Assistant Professor (2007-present), Assistant Research Scientist (2005-2007)

Conducting independent research into fatty acid elongation and sphingolipid metabolism and function.

Mentoring graduate and undergraduate research students.

Teaching Biological Chemistry (C484/533) and Biological Chemistry Laboratory (C486).

Served as faculty advisor for Chemistry majors. Active in outreach activities linking area undergraduate and high school students with local scientists. Appointed to the School of Science Awards and Nominations Committee.

Department of Chemistry and Biochemistry, Miami University, Oxford, OH (1997-2005)

Research Scholar (2004-2005), Research Associate (1997-2002), Adjunct Assistant Professor (from 2000),

As a Research Scholar, collaborated with Professor R. E. Minto examining novel fatty acid desaturases in fungi.

As a Research Associate with Professor J. G. Jaworski (1997-2002) and independently (2002-2004) studied fatty acid elongation in plants.

Supervised a B.S. level technician and NSF-REU, Hughes Summer Scholars and Miami Undergraduate students.

Research Advisor for Miami Undergraduate Honors Dissertation.

Taught as a Visiting Instructor or Visiting Assistant Professor: College Chemistry II, College Chemistry II Laboratory, Fundamentals of Organic Chemistry Laboratory, Chemistry in Modern Society Laboratory, Outlines of Biochemistry Laboratory.

Department of Biological Chemistry, School of Medicine, The Johns Hopkins University, Baltimore, MD (1994-1997)

Post-doctoral fellowship with Professor P. N. Devreotes examining G protein-coupled signal transduction.

Department of Biochemistry, School of Medicine, University of Alberta, Edmonton, AB (1989-1994)

Graduate research with Professor R. O. Ryan investigating the mechanism of action and structure/function of the insect lipid transfer particle.

Department of Biology, University of Waterloo, Waterloo, ON (1988-89)

Studied inositol trisphosphate signaling in insect hemocytes with Professor R. G. H. Downer.

Merck Frosst Canada Inc., Pointe Claire, PQ (1987-88)

Examined leukotriene production upon anaphylaxis in rat and translocation of 5-lipoxygenase in macrophages.

Labatt Brewing Company, London, ON (1985-86) and **National Research Council, Ottawa, ON** (1985)

Characterized the fermentation properties and genetics of yeast strains with glucoamylase activity.

FUNDING

"URM: A Multi-year Immersion in Interdisciplinary Research in Biological Signaling at IUPUI" S.K. Randall, PI; **B.J. Blacklock**, co-PI, NSF, \$943,000 (2010-2015)

"High Value Lipids from Non-fermentable Feedstocks for a Biorenewable Economy" **B.J. Blacklock**, PI; M.G. Goebel, M. Bard, R.E. Minto, and S.K. Randall, co-PIs, IUPUI Center for Membrane Biosciences Seed Grant, \$90,000 (2010-2011)

"Acquisition of Mass Spec Instrumentation and Upgrades for the Mass Spectrometry Facility Housed in the Department of Chemistry and Chemical Biology" **B.J. Blacklock**, senior personnel; R.E. Minto, PI, IUPUI School of Science Core Instrumentation Grant, \$96,795 (2009-2010)

- "Acquisition of Confocal Microscopy Instrumentation in the IUPUI School of Science" **B.J. Blacklock**, senior personnel; C.A. Naumann, PI, IUPUI School of Science Core Instrumentation Grant, \$220,000 (2009-2010)
- "Proof of Concept Testing for the Efficacy of Rosiglitazone in Inhibiting Kidney and Liver Cyst Growth in an Animal Model of Autosomal Dominant Polycystic Kidney Disease" **B.J. Blacklock**, V.H. Gattone, and R.L. Bacallao, co-investigators/collaborators; B. Blazer-Yost, PI, CTSI Preclinical Project Development Grant, \$37,417 (2009-2010)
- "Collaborative Development of Methods for Lipidomics and Proteomics in the Center for Membrane Biosciences" **B.J. Blacklock**, PI; R.E. Minto and S.K. Randall, coPIs, IUPUI Center for Membrane Biosciences Seed Grant, \$35,000 (2009-2010)
- "Identification of Lipid Components Responsible for Fluid Secretion in Human Autosomal Dominant Polycystic Kidney Disease (ADPKD) Cyst Fluid" **B.J. Blacklock** and J.C. Haydon, coPI's; B. Blazer-Yost, PI, IUPUI Center for Membrane Biosciences Seed Grant, \$35,000, (2009-2010)
- "MRI: Acquisition of a High Resolution LC-MS/MS System" **B.J. Blacklock**, senior personnel; R.E. Minto, PI, NSF, \$479,590 (2008-2011)
- "Functional Characterization of a 3-Ketoacyl-CoA Synthase from *Dictyostelium discoideum*" A.M.N. Grotenhuis student; **B.J. Blacklock**, research mentor, IUPUI Undergraduate Research Opportunities Program, \$1,000. (2008)
- "Fatty Acid Elongation in *Dictyostelium discoideum*" **B.J. Blacklock**, IUPUI Research Support Funds Grant, \$30,000 (2007-2009)
- "MRI: Acquisition of a 500 MHz NMR Spectrometer: **B.J. Blacklock**, senior personnel; R.E. Minto, PI, NSF, \$516,500 (2006-2009)
- "Very Long Chain Fatty Acid Elongases" **B.J. Blacklock**, PI, Cargill Inc., \$74,592 (2002-2003)
- "Fatty Acid Elongation" J.G. Jaworski and **B.J. Blacklock**, coPI's, Cargill Inc., \$324,528 (2000-2002)

PUBLICATIONS AND PATENTS (* indicates undergraduate author)

- Blacklock, B.J.**, Scheffler, B.E., Shepard, M.R., Jayasuriya, N., Minto, R.E. Functional diversity in fungal fatty acid synthesis. The first acetylenase from the Pacific Golden Chanterelle, *Cantharellus formosus*. (2010) *J. Biol. Chem.*, **285**, 28442-28449.
- Minto, R.E., **Blacklock, B.J.**, Younus, H., Pratt*, A. Atypical biosynthetic properties of a $\Delta^{12}/v+3$ desaturase from the model Basidiomycete, *Phanerochaete chrysosporium*. (2009) *Appl. Environ. Microbiol.* **75**, 1156-1164.
- Blacklock, B.J.**, Kelley*, D., and Patel*, S. A fatty acid elongase ELO with novel activity from *Dictyostelium discoideum*. (2008) *Biochem. Biophys. Res. Comm.* **374**, 226-230.
- Minto, R.E. and **Blacklock, B.J.** Biosynthesis and function of polyacetylenes and allied natural products. (2008) *Prog. Lipid Res.* **47**, 233-306.
- Blacklock, B. J.** and Jaworski, J. G. Substrate specificity of Arabidopsis 3-ketoacyl-CoA synthases. (2006) *Biochem. Biophys. Res. Comm.* **346**, 583-590.
- Moon, H., Chowrira, G., Rowland, O., **Blacklock, B.**, Smith, M. A., and Kunst, L. (2004) A root-specific condensing enzyme from *Lesquerella fendleri* that elongates very-long-chain saturated fatty acids. *Plant Mol. Biol.* **56**, 917-927.
- Blacklock, B. J.** and Jaworski, J. G. (2002) Studies into factors contributing to substrate specificity of membrane-bound 3-ketoacyl CoA synthases. *Eur. J. Biochem.* **269**, 4789-4798.
- Jaworski, J.G. and **Blacklock, B.J.** Fatty Acid Elongase 3-Ketoacyl CoA Synthase Polypeptides. US patent 6, 713, 664, World patents.
- Parent, C. A., **Blacklock, B. J.**, Froehlich*, W. M., Murphy, D. B., and Devreotes, P. N. (1998) G protein signaling events are activated at the leading edge of chemotactic cells. *Cell* **95**, 81-91.
- Blacklock, B. J.** and Ryan, R. O. (1995) Structural studies of *Manduca sexta* lipid transfer particle with apoprotein-specific antibodies. *J. Lipid Res.* **36**, 108-116.
- Blacklock, B. J.** and Ryan, R. O. (1994) Hemolymph lipid transport. *Insect Biochem. Molec. Biol.* **24**, 855-873.
- Blacklock, B. J.** and Ryan, R. O. (1993) Structure and function of *Manduca sexta* hemolymph lipid transfer particle. In *Insect Lipids: Chemistry, Biochemistry and Biology*. D. W. Stanley-Samuels and D. R. Nelson, eds. (Lincoln, Nebraska: University of Nebraska Press), pp. 25-43.
- Singh, T. K. A., **Blacklock, B. J.**, Wientzek, M., and Ryan, R. O. (1992) A turbidimetric assay of facilitated lipid transfer. *Anal. Biochem.* **256**, 137-141.

Blacklock, B. J., Smillie*, M., and Ryan, R. O. (1992) Insect lipid transfer particle can facilitate net vectorial lipid transfer via a carrier-mediated mechanism. *J. Biol. Chem.* **267**, 14533-14537.

Foster, A., Letts, G., Charleson, S., Fitzsimmons, B., **Blacklock, B.**, and Rokach, J. (1988) The *in vivo* production of peptide leukotrienes after pulmonary anaphylaxis in the rat. *J. Immunol.* **141**, 3544-3555.

PRESENTATIONS

Hernandez-Buquer, S. and **Blacklock, B.J.** "Characterization of the Fatty Acid Elongase Condensing Enzyme, EloA" IUPUI Department of Chemistry and Chemical Biology Annual Departmental Poster Session 2010, poster

Birch, G.L., Minto, R.E. and Blacklock, B.J. "Progress Toward A Lipodomic Profile Of *Dictyostelium discoideum*" IUPUI Department of Chemistry and Chemical Biology Annual Departmental Poster Session 2010, poster

Blacklock, B.J., Birch, G.L., Hernandez-Buquer, S., and Grotenhuis, A. "Molecular and *in vivo* Characterization of Fatty Acid Elongation in the Cellular Slime Mould, *Dictyostelium discoideum*" 19th International Symposium on Plant Lipids, 2010, Cairns, Australia, oral presentation

Minto, R.E., Younus, H., Pratt, A.C., **Blacklock, B.J.**, Shepard, M.R., Birch, G.L., and Jenkins, J. "Functional Diversity within the Δ^{12} -Desaturases of Basidiomycetes" 19th International Symposium on Plant Lipids, 2010, Cairns, Australia, oral presentation

Hernandez-Buquer, S. and **Blacklock, B.J.** "Site-directed Mutagenesis of the Fatty Acid Elongase Condensing Enzyme, EloA" IUPUI Research Day 2010, poster

Birch, G.L., Minto, R.E. and Blacklock, B.J. "Progress Toward A Lipodomic Profile Of *Dictyostelium discoideum*" IUPUI Research Day 2010, poster

Hernandez-Buquer, S. and **Blacklock, B.J.** "Site-directed Mutagenesis of the Fatty Acid Elongase Condensing Enzyme, EloA" Butler Undergraduate Research Conference 2010, oral presentation

Birch, G.L., Minto, R.E., and **Blacklock, B.J.** "The Preparation of Unusual Fatty Acids for Lipidomic Studies" IUPUI Department of Chemistry and Chemical Biology Annual Departmental Poster Session 2009, poster

Haydon, J.C., Bacallao, R.L., Gattone, V.H., Lai, X., Witzmann, F.A., **Blacklock, B.J.**, and Blazer-Yost, B.L. "Studies to Determine the Components of Cyst Fluid Responsible for Cyst Growth in Polycystic Kidney Disease" IUPUI Department of Chemistry and Chemical Biology Annual Departmental Poster Session 2009, poster

Hernandez-Buquer*, S., and **Blacklock, B.J.** "Site-directed Mutagenesis of a Fatty Acid Elongase Condensing Enzyme, EloA" IUPUI Department of Chemistry and Chemical Biology Annual Departmental Poster Session 2009, poster

Younus, H., Pratt*, A.C., **Blacklock, B.J.**, and Minto, R.E. "Functional Diversity in the Enzymes of Fungal Fatty Acid Biosynthesis" IUPUI Department of Chemistry and Chemical Biology Annual Departmental Poster Session 2009, poster

Blacklock, B.J., Frazier*, S., Hernandez-Buquer*, S., Grotenhuis*, A., Minto, R.E., and Birch, G. "Cloning and Functional Characterization of *Dictyostelium discoideum* Fatty Acid Elongase Genes" Annual International Dictyostelium Conference 2009, Estes Park, CO, poster

Younus, H., Pratt*, A.C., **Blacklock, B.J.**, and Minto, R.E. "Functional Diversity in the Enzymes of Fungal Fatty Acid Biosynthesis" American Chemical Society Fall 2009 National Meeting, Washington, DC, poster

Hernandez-Buquer*, S., and **Blacklock, B.J.** "Site-directed Mutagenesis of a Fatty Acid Elongase Condensing Enzyme, EloA" 2009 CIC-SROP Poster Symposium, 2009, Ann Arbor, MI, poster

Haydon, J.C., Bacallao, R.L., Gattone, V.H., Lai, X., Witzmann, F.A., **Blacklock, B.J.**, and Blazer-Yost, B.L. "Studies to determine the components of cyst fluid responsible for cyst growth in polycystic kidney disease" 44th Annual Lake Cumberland Biological Transport Group Meeting, 2009, Jamestown, KY, oral presentation

Hernandez-Buquer*, S., and **Blacklock, B.J.** "Site-directed Mutagenesis of a Fatty Acid Elongase Condensing Enzyme, EloA" 2009 CRL Summer Research Programs Student Poster Symposium, 2009, Indianapolis, IN, poster

Frazier*, S. and **Blacklock, B.J.** "Characterization of the *Dictyostelium discoideum* Lipidome" 2009 CRL Summer Research Programs Student Poster Symposium, 2009, Indianapolis, IN, poster

Haydon, J.C., Bacallao, R.L., Gattone, V.H., Lai, X., Witzmann, F.A., **Blacklock, B.J.**, and Blazer-Yost, B.L. "Studies to Determine the Components of Cyst Fluid Responsible for Cyst Growth in Polycystic Kidney Disease" IUPUI Research Day, Spring 2009, Indianapolis, IN, poster

- Blacklock, B.J.**, Patel*, S., Kelley*, D., and Grotenhuis*, A. "*Dictyostelium discoideum* has Plant-like Fatty Acid Elongation Pathways" IUPUI Department of Chemistry and Chemical Biology Departmental Seminar, Fall 2008, poster
- Blacklock, B.J.**, Patel*, S., Kelley*, D., and Grotenhuis*, A. "*Dictyostelium discoideum* has Plant-like Fatty Acid Elongation Pathways" 2008 Banff Conference on Plant Metabolism, 2008, poster
- Blacklock, B.J.**, Scheffer, B.E., Minto, R.E., "Cloning Acetylenic Fatty Acid Biosynthesis Genes from a Basidiomycete" 2008 Banff Conference on Plant Metabolism, 2008, poster
- Blacklock, B.J.**, Scheffer, B.E., Minto, R.E., "Cloning and Expression of Acetylenic Fatty Acid Biosynthesis Genes from a Basidiomycete" Gordon Research Conference: Enzymes, Coenzymes, and Metabolic Pathways, 2008, poster
- Grotenhuis*, A.M.N. and **Blacklock, B.J.** "Functional Characterization of a 3-Ketoacyl-CoA Synthase from *Dictyostelium discoideum*" Butler University Undergraduate Research Conference, 2008, oral presentation
- Grotenhuis*, A.M.N. and **Blacklock, B.J.** "Functional Characterization of a 3-Ketoacyl-CoA Synthase from *Dictyostelium discoideum*" IUPUI UROP Research Symposium, 2008, poster
- Blacklock, B.J.** "Fatty Acid Elongation in Plants and a Cellular Slime Mold" Department of Chemistry, Butler University, 2008, invited talk
- Blacklock, B.J.** Patel*, S., Kelley* D., and Grotenhuis*, A. "Cloning and Functional Characterization of *Dictyostelium discoideum* Fatty Acid Elongases" IUPUI Department of Chemistry and Chemical Biology Departmental Seminar, Fall 2007, poster
- Minto, R.E., **Blacklock, B.J.**, and Scheffler, B.E. "Cloning and Expression of Acetylenic Fatty Acid Biosynthesis Genes from a Basidiomycete", 17th Annual International Symposium on Plant Lipids, East Lansing, MI, 2006, invited talk
- Minto, R.E., **Blacklock, B.J.**, Scheffler, B.E., and Jayasuriya*, N.N. "Acetylenic Fatty Acid Biosynthesis - Cloning And Expression Of The First Genes From a Basidiomycete", 232nd National American Chemical Society Meeting, San Francisco, CA, 2006, poster
- Minto, R.E., **Blacklock, B.J.**, Scheffler, B.E., and Jayasuriya*, N.N. "Acetylenic Fatty Acid Biosynthesis - Cloning And Expression Of The First Genes From a Basidiomycete", 7th Annual Indiana Local Section American Chemical Society Poster Session, Richmond, IN, 2006, poster
- Blacklock, B.J.** "Fatty Acid Elongation in *Dictyostelium discoideum*", Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis Departmental Poster Session, 2006. poster
- Blacklock, B.J.** "Fatty Acid Elongation in *Dictyostelium discoideum*", International Dictyostelium Conference 2006, Santa Fe, New Mexico, 2006. poster
- Blacklock, B.J.** "Fatty Acid Elongation in *Dictyostelium discoideum*", 17th Annual International Plant Lipid Symposium, East Lansing, Michigan, 2006. poster
- Blacklock, B.J.** "Fatty Acid Elongation in Plants and *Dictyostelium discoideum*", Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis Departmental Poster Session, 2005. poster
- Blacklock, B.J.** "Fatty Acid Elongation in Plants: 3-Ketoacyl-CoA Synthases", Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis Departmental Seminar, 2005. invited speaker
- Blacklock, B.J.** and Jaworski, J.G. "Arabidopsis 3-Ketoacyl-CoA Synthases", Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, 2003. poster
- Blacklock, B.J.** "Fatty Acid Elongation in Plants: 3-Ketoacyl-CoA Synthases", Department of Chemistry and Physical Sciences, College of Mount St. Joseph, Cincinnati, OH 2003. invited speaker
- Blacklock, B.J.** and Jaworski, J.G. "Substrate Specificity of 3-Ketoacyl-CoA Synthases", Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, 2001. poster
- Blacklock, B.J.** and Jaworski, J.G. "The Use of Chimeric Enzymes to Identify Regions Involved in Substrate Specificity of Plant Fatty Acid Elongase 3-Ketoacyl-CoA Synthases", 11th International Conference on Arabidopsis Research, 2000. poster
- Blacklock, B.J.** and Jaworski, J.G. "Structural Studies of Plant Fatty Acid Elongases by Domain Swapping", Biochemistry and Molecular Biology of Plant Fatty Acids and Glycerolipids Symposium, 1999. poster
- Blacklock, B.J.** "Regulation of G Protein-Mediated Activation of Adenylyl Cyclase in *Dictyostelium discoideum*", Earlham College, Richmond, IN, 1998. and Department of Microbiology, Miami University, Oxford, OH, 1999. invited speaker
- Blacklock, B.J.** and Ryan, R.O. "The Use of Apoprotein-Specific Antibodies in Structure/Function Studies of *Manduca sexta* Lipid Transfer Particle", American Society for Biochemistry and Molecular Biology Conference, 1993. poster

Blacklock, B.J. and Ryan, R.O. "Mechanistic Studies on *Manduca sexta* Lipid Transfer Particle", Canadian Lipoprotein Conference, 1992. poster

Blacklock, B.J. and Ryan, R.O. "Lipid Transfer Particle Facilitates Diacylglycerol Transfer via a Carrier-Mediated Mechanism", Entomological Society of America Annual Meeting, 1991. talk, received President's Prize, First Prize Award

Résumé

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Research Interests and Key Word Summary:

Computational chemistry, including chemometrics, computer-aided drug design (CADD), computer-aided molecular design (CAMD), molecular databases, molecular mechanics, molecular modeling, molecular simulations, quantitative structure-activity relationships (QSAR), quantum chemistry, rationalization of bioactivity, structure-property relationships.

Education:

1959-63: The Pennsylvania State University, University Park, Pennsylvania. Dean's List. Chemistry major. B.S. in chemistry with distinction awarded June 1963.

1963-67: Harvard University, Cambridge, Massachusetts. Ph.D. in chemistry, March 1968. Research with Professor William N. Lipscomb (Nobel Laureate in Chemistry, 1976) on ab initio and semiempirical quantum chemistry of biological and inorganic compounds of phosphorus. Ph.D. thesis entitled "Molecular Orbitals for ATP and Phosphorus Compounds". Awarded NIH Predoctoral Fellowship, 1964-67.

Employment:

1967-68: Postdoctoral Research Associate, Department of Chemistry, Cornell University, Ithaca, New York, with Professor Roald Hoffmann (Nobel Laureate in Chemistry, 1981) on quantum chemistry of phosphate esters and phosphonium ylides and application of the orbital symmetry rules to these molecules. Awarded NIH Postdoctoral Fellowship, 1967-68.

1968-74: Senior Physical Chemist, Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, Indiana.

1975-89: Research Scientist, Lilly Research Laboratories.

1990-93: Senior Research Scientist, Lilly Research Laboratories.

Recent Professional Activities:

1994-present: Research Professor of Chemistry, Purdue School of Science, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana.

Founder and member of the Executive Steering Committee, Gordon Research Conferences on Computational Chemistry, 1986-present.

Co-founder and co-editor with Professor K. B. Lipkowitz of book series, *Reviews in Computational Chemistry*, 1990-2002.

Editorial Board, *Structural Chemistry*, 1991-present.

Editorial Board, *Journal of Medicinal Chemistry* 1992-1997.

Editor of the *Journal of Molecular Graphics and Modelling* (a publication of the Computers in Chemistry Division of the American Chemical Society and the Molecular Graphics and Modelling Society), 1998-2001.

Editorial Advisory Board, *Modern Drug Discovery* (American Chemical Society). 1998-2004.

Co-inventor on 6 patents.

American Chemical Society Canvassing Committee for the ACS Award for Computers in Chemical and Pharmaceutical Research, 1996-1999.

Referee for over 60 scientific journals and funding agencies.

Evaluator on faculty promotion committees at many universities and institutes.

Recent Publications in Refereed Journals:

64. Chiral Recognition of the Angiotensin II (AT₁) Receptor by a Highly Potent Phenoxyproline Octanoamide. M. I. Steinberg, A. D. Palkowitz, K. J. Thrasher, J. K. Reel, K. M. Zimmerman, C. A. Whitesitt, R. L. Simon, K. L. Hauser, S. L. Lifer, W. Pfeifer, K. Takeuchi, S. A. Wiest, V. Vasudevan, K. G. Bemis, J. B. Deeter, C. J. Barnett, T. M. Wilson, W. S. Marshall, and D. B. Boyd, *Bioorg. Med. Chem. Lett.*, 4, 51-56 (1994). (Invited paper for symposium-in-print on angiotensin II antagonists.)

65. Structural Evolution and Pharmacology of a Novel Series of Triacid Angiotensin II Receptor Antagonists. A. D. Palkowitz, M. I. Steinberg, K. J. Thrasher, J. K. Reel, K. L. Hauser, K. M. Zimmerman, S. A. Wiest, C. A. Whitesitt, R. L. Simon, W. Pfeifer, S. L. Lifer, D. B. Boyd, C. J. Barnett, T. M. Wilson, J. B. Deeter, K. Takeuchi, R. E. Riley, W. D. Miller, and W. S. Marshall, *J. Med. Chem.*, 37, 4508-4521 (1994).
66. Synthesis and Pharmacological Evaluation of a Novel Series of 5-Aryl Benzimidazole Angiotensin II Receptor Antagonists. A. D. Palkowitz, M. I. Steinberg, K. M. Zimmerman, K. J. Thrasher, K. L. Hauser, and D. B. Boyd, *Bioorg. Med. Chem. Lett.*, 5, 1015-1020 (1995).
67. Molecular Orbital Study of the Structure and Interactions of Ylidene Rhodanines. R. J. Loncharich, J. S. Nissen, and D. B. Boyd, *Struct. Chem.*, 7, 37-49 (1996).
68. Stochastic Approach to Force Field Evaluations: Conformational Analysis of Raloxifene, a Potential New Therapeutic Agent for Post-menopausal Osteoporosis. D. B. Boyd and R. D. Coner, *J. Mol. Struct.: THEOCHEM*, 368, 7-15 (1996).
69. Inhibition of Human Immunodeficiency Virus Type 1 Reverse Transcriptase by Degradation Products of Ceftazidime. S. W. Baertschi, A. S. Cantrell, M. T. Kuhfeld, L. J. Lorenz, D. B. Boyd, and S. R. Jaskunas, *Antiviral Chem. Chemother.*, 8, 353-362 (1997).
70. Evidence that There Is a Future for Semiempirical Calculations. D. B. Boyd, *J. Mol. Struct.: THEOCHEM*, 401, 219-225 (1997).
71. On the Rhodanines and Their Presence in Biologically Active Ligands. D. B. Boyd, *J. Mol. Struct.: THEOCHEM*, 401, 227-334 (1997).
72. Arylpiperazines with Serotonin-3 Antagonist Activity: A Comparative Molecular Field Analysis. A. Morreale, E. Gálvez-Ruano, I. Iriepa-Canalda, and D. B. Boyd, *J. Med. Chem.*, 41 (12), 2029-2039 (1998).
73. Superimposition-Based Protocol as a Tool for Determining Bioactive Conformations. I. Application to Ligands of the Glycinergic Receptor (GlyR). E. Gálvez-Ruano, I. Iriepa-Canalda, A. Morreale, and D. B. Boyd, *J. Mol. Graphics Modell.*, 19 (3-4), 331-337 (color plates 391-395) (2001).
74. Superimposition-Based Protocol as a Tool for Determining Bioactive Conformations. II. Application to the GABA_A Receptor. E. Gálvez-Ruano, I. Iriepa-Canalda, A. Morreale, and D. B. Boyd, *J. Mol. Graphics Modell.*, 20 (2), 183-197 (2001).
75. Synthesis, Conformational Analysis, and Biological Activity of New Analogues of Thiazole-4-carboxamide Adenine Dinucleotide (TAD) as IMP Dehydrogenase Inhibitors. P. Franchetti, L. Cappellacci, M. Pasqualini, R. Petrelli, V. Jayaprakasan, H. N. Jayaram, D. B. Boyd, M. D. Jain, and M. Grifantini, *Bioorg. Med. Chem.*, 13, 2045-2053 (2005).

76. Evaluation of Computational Chemistry Methods: Crystallographic and Cheminformatics Analysis of Aminothiazole Methoximes. T. Ercanli and D. B. Boyd, *J. Chem. Inf. Mod.*, 45, (3, May-Jun), 591-601 (2005).
77. Exploration of the Conformational Space of a Polymeric Material that Inhibits Human Immunodeficiency Virus. T. Ercanli and D. B. Boyd, *J. Chem. Inf. Mod.*, 46 (3, May-June), 1321-1333 (2006).

Recent Contributions to Books:

21. A Perspective of Modern Methods in Computer-Aided Drug Design. L. M. Balbes, S. W. Mascarella, and D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1994, Vol. 5, Chapter 7, pp. 337-379.
22. Compendium of Software for Molecular Modeling. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1994, Vol. 5, Appendix, pp. 381-428.
23. Molecular Modeling and Quantitative Structure-Activity Relationship Studies in Pursuit of Highly Potent Substituted Octanoamide Angiotensin II Receptor Antagonists. D. B. Boyd, A. D. Palkowitz, K. J. Thrasher, K. L. Hauser, C. A. Whitesitt, J. K. Reel, R. L. Simon, W. Pfeifer, S. L. Lifer, K. Takeuchi, V. Vasudevan, A. D. Kossoy, J. B. Deeter, M. I. Steinberg, K. M. Zimmerman, S. A. Wiest, and W. S. Marshall, in *Computer-Aided Molecular Design: Applications in Agrochemicals, Materials, and Pharmaceuticals*, C. H. Reynolds, M. K. Holloway, and H. K. Cox, Eds., ACS Symp. Series 589, American Chemical Society, Washington, DC, 1995, Chapter 2, pp. 14-35.
24. Computer-Aided Molecular Design. D. B. Boyd, in *Encyclopedia of Computer Science and Technology*, A. Kent and J. G. Williams, Eds., Marcel Dekker, New York, 1995, Vol. 33 (Supplement 18), Chapter 2, pp. 41-71.
25. Preface (on Changes Affecting the Job Market for Computational Chemists). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1995, Vol. 6, pp. v-ix.
26. Molecular Modeling Software in Use: Publication Trends. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1995, Vol. 6, pp. 317-354.
27. Compendium of Software for Molecular Modeling. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1995, Vol. 6, Appendix 2, pp. 383-437.
28. Preface (on Trends in the Job Market for Computational Chemists). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1995, Vol. 7, pp. v-xi.

29. Compendium of Software for Molecular Modeling. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1995, Vol. 7, Appendix, pp. 303-380.
30. Introduction to the CD-ROM Version. *Proceedings of the First Electronic Computational Chemistry Conference (ECCC)*, November 7- December 2, 1994, S. M. Bachrach, D. B. Boyd, S. K. Gray, W. L. Hase, and H. S. Rzepa, Eds., ARInternet Corporation, Landover, MD, 1995.
31. A Tool for Negotiating through Structure-Activity Relationship Space: The Hypersurface Iterative Projection Method. D. B. Boyd, in *Proceedings of the First Electronic Computational Chemistry Conference (ECCC)*, November 7- December 2, 1994, S. M. Bachrach, D. B. Boyd, S. K. Gray, W. L. Hase, and H. S. Rzepa, Eds., ARInternet Corporation, Landover, MD, Paper 19, 1995. Posted by S. M. Bachrach, with permission, on the World Wide Web in the *Internet Journal of Chemistry*, <http://www.ijc.com/articles/1999v2/119/>, January 1999.
32. Preface (on the Prevalence of Computational Chemistry Papers in Some Journals). *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1996, Vol. 8, pp. v-ix.
33. Preface (on the Geographical Distribution of Computational Chemistry Around the World). *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 1996, Vol. 9, pp. v-xxii.
34. Preface (on Retrospection and the Convergence of Computational Chemistry Journals). *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, printed in 1996, copyright date 1997, Vol. 10, pp. v-xi.
35. Computer-Aided Molecular Design. D. B. Boyd, in *Encyclopedia of Library and Information Science*, A. Kent, Ed., Marcel Dekker, New York, 1997, Vol. 59, Suppl. 22, Chapter 3, pp. 54-84.
36. Preface (on Computer Aided Ligand Design). *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 1997, Vol. 11, pp. v-x.
37. Compendium of Software and Internet Tools for Computational Chemistry. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 1997, Vol. 11, Appendix, pp. 373-399.
38. Drug Design. D. B. Boyd, in *Encyclopedia of Computational Chemistry*, P. v. R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. Kollman, and H. F. Schaefer III, Eds., John Wiley & Sons, Chichester, 1998, Vol. 1, pp. 795-804.
39. Progress in Rational Design of Therapeutically Interesting Compounds. D. B. Boyd, in *Rational Molecular Design in Drug Research*, Proceedings of the Alfred Benzon Symposium No. 42, T. Liljefors, F. S. Jørgensen, and P. Krosgaard-Larsen, Eds., Munksgaard, Copenhagen, 1998, pp. 15-23.
40. Molecular Modeling - Industrial Relevance and Applications. D. B. Boyd, in *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH, Weinheim, 1998, 6th Edition on CD-ROM.

41. Preface (on the Improved Job Market for Computational Chemists). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 1998, Vol. 12, pp. v-xiii.
42. Is Rational Design Good for Anything? D. B. Boyd, in *Rational Drug Design: Novel Methodology and Practical Applications*, A. L. Parrill and M. R. Reddy, Eds., ACS Symp. Series 719, American Chemical Society, Washington, DC, 1999, Chapter 22, pp. 346-356.
43. Preface (on Well-Known Persons in Computational Chemistry). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 1999, Vol. 13, pp. v-xvii.
44. Beta-Lactam Antibacterial Agents: Computational Chemistry Investigations. D. B. Boyd, in *The Amide Linkage: Structural Significance in Chemistry, Biochemistry, and Materials Science*, A. Greenberg, C. M. Breneman, and J. F. Liebman, Eds., John Wiley & Sons, New York, 2000, Chapter 11, pp. 337-375.
45. Preface (on Important Scientific Equations). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, printed in 1999, copyright date 2000, Vol. 14, pp. v-viii.
46. History of the Gordon Research Conferences on Computational Chemistry. D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, printed in 1999, copyright date 2000, Vol. 14, pp. 399-439.
47. Preface (A Tribute to the Halcyon Days of QCPE and a Commentary on Information Resources for Chemists). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2000, Vol. 15, pp. v-xxxv.
48. Preface (on the Pharmaceutical Industry Being the Largest Employer of Computational Chemists). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2000, Vol. 16, pp. v-xxiii.
49. Preface (on Caveats for Using the CAlus Database and a Tribute to Deceased Computational Chemists). K. B. Lipkowitz and D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2001, Vol. 17, pp. v-xxviii.
50. Books Published on the Topics of Computational Chemistry. K. B. Lipkowitz and D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2001, Vol. 17, pp. 255-357.
51. Preface (on Eternal Change). D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2002, Vol. 18, pp. v-ix.
52. Epilogue and Dedication. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2002, Vol. 18, pp. xi-xii.

53. Examination of the Employment Environment for Computational Chemistry. D. B. Boyd and K. B. Lipkowitz, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., Wiley-VCH, New York, 2002, Vol. 18, Appendix, pp. 293-319.
54. Particle Swarm Optimization and Neural Network Application for QSAR. Z. Wang, G. L. Durst, R. C. Eberhart, D. B. Boyd, and Z. Ben Miled, *HiCOMP 2004* (Proceedings of Third IEEE International Workshop on High Performance Computational Biology, Santa Fe, New Mexico, April 26, 2004), online at <http://www.hicomb.org/proceedings.html> (2004).
55. The Power of Computational Chemistry to Leverage Stress Testing of Pharmaceuticals, D. B. Boyd, in *Understanding Drug Degradation*, S. W. Baertschi, Ed., Taylor & Francis, London, U.K., 2005, Ch. 12, pp. 355-418.
56. History of Computers in Pharmaceutical Research and Development: A Narrative. D. B. Boyd and M. M. Marsh, in *Computer Applications in Pharmaceutical Research and Development*, S. Ekins, Ed., Wiley, New York, 2006, pp. 1-50.
57. Molecular Modeling - Industrial Relevance and Applications. D. B. Boyd, in *Ullmann's Encyclopedia of Industrial Chemistry*, 7th edition, Wiley-VCH, Weinheim, 2006.
58. How Computational Chemistry Became Important in the Pharmaceutical Industry. D. B. Boyd, in *Reviews in Computational Chemistry*, K. B. Lipkowitz and T. Cundari, Eds., Wiley-VCH, Hoboken, NJ, 2007, Vol. 23, pp. 401-451.
59. Molecular Modeling. D. B. Boyd, in *Ullmann's Modeling and Simulation*, Wiley-VCH, Weinheim, 2007, Chapter 3, pp. 307-322.

Miscellaneous Recent Publications:

69. Molecular Modeling and QSAR Studies in Pursuit of Highly Potent Substituted Octanoamide Angiotensin II Receptor Antagonists. D. B. Boyd, A. D. Palkowitz, K. J. Thrasher, K. L. Hauser, C. A. Whitesitt, J. K. Reel, R. L. Simon, W. Pfeifer, S. L. Lifer, K. Takeuchi, V. Vasudevan, J. B. Deeter, M. I. Steinberg, K. M. Zimmerman, S. A. Wiest, and W. S. Marshall. Abstracts of the 207th National Meeting of the American Chemical Society, 1994, San Diego, California, March 13-18, COMP 92.
70. Synthesis and Modification of Novel Benzimidazole and Indole Angiotensin II Receptor Antagonists. J. K. Reel, R. L. Simon, W. Pfeifer, C. A. Whitesitt, S. L. Lifer, M. I. Steinberg, A. D. Palkowitz, K. J. Thrasher, K. L. Hauser, K. M. Zimmerman, K. Takeuchi, S. A. Wiest, D. B. Boyd, and W. S. Marshall. Abstracts of the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 206.
71. Synthesis and In Vitro Evaluation of a Novel Series of Benzimidazole Alkyl Amides as Potent Nonpeptide Angiotensin II (AT₁) Receptor Antagonists. K. J.

- Thrasher, A. D. Palkowitz, J. K. Reel, K. L. Hauser, C. A. Whitesitt, M. I. Steinberg, K. M. Zimmerman, R. L. Simon, W. Pfeifer, D. B. Boyd, S. L. Lifer, S. A. Wiest, and W. S. Marshall. Abstracts of the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 207.
72. Synthesis and Evaluation of a Novel Series of Proline Octanoamide Angiotensin II (AT₁) Receptor Antagonists. W. Pfeifer, C. A. Whitesitt, R. L. Simon, K. L. Hauser, S. L. Lifer, S. A. Wiest, V. Vasudevan, J. K. Reel, A. D. Palkowitz, K. J. Thrasher, K. M. Zimmerman, M. I. Steinberg, D. B. Boyd, and W. S. Marshall. Abstracts of the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 204.
73. Synthesis and Evaluation of Proline Octanoamide Angiotensin II (AT₁) Receptor Antagonists Related to LY301875. R. L. Simon, C. A. Whitesitt, K. M. Zimmerman, M. I. Steinberg, V. Vasudevan, S. A. Wiest, S. L. Lifer, W. Pfeifer, J. K. Reel, A. D. Palkowitz, K. J. Thrasher, K. L. Hauser, D. B. Boyd, and W. S. Marshall. Abstracts of the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 203.
74. Pharmacology of a Series of Novel Proline Octanoamide Angiotensin II (AT₁) Receptor Antagonists. K. M. Zimmerman, M. I. Steinberg, S. A. Wiest, A. D. Palkowitz, K. J. Thrasher, J. K. Reel, C. A. Whitesitt, R. L. Simon, W. Pfeifer, D. B. Boyd, K. L. Hauser, S. L. Lifer, and W. S. Marshall. Abstracts of the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 209.
75. Synthesis and In Vitro Evaluation of Novel Indole, Indazole, Benzimidazole Angiotensin II Receptor Antagonists. J. K. Reel, A. D. Palkowitz, R. L. Simon, K. J. Thrasher, M. I. Steinberg, K. M. Zimmerman, C. A. Whitesitt, S. A. Wiest, W. Pfeifer, K. L. Hauser, D. B. Boyd, S. L. Lifer, and W. S. Marshall. Poster paper for the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 206.
76. Synthesis and In Vitro Evaluation of a Novel Benzimidazole Octanoamide Derivatives as Potent Nonpeptide Angiotensin II (AT₁) Receptor Antagonists. K. J. Thrasher, A. D. Palkowitz, M. I. Steinberg, K. M. Zimmerman, K. L. Hauser, J. K. Reel, C. A. Whitesitt, S. A. Wiest, R. L. Simon, W. Pfeifer, D. B. Boyd, S. L. Lifer, V. Vasudevan, and W. S. Marshall. Poster paper for the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 207.
77. Synthesis and In Vitro Evaluation of Imidazole Derived Phenoxyproline Octanoamides as Angiotensin II (AT₁) Receptor Antagonists. Part 1. A. D. Palkowitz, K. J. Thrasher, J. K. Reel, M. I. Steinberg, K. M. Zimmerman, C. A. Whitesitt, S. A. Wiest, R. L. Simon, W. Pfeifer, K. L. Hauser, D. B. Boyd, S. L. Lifer, and W. S. Marshall. Poster paper for the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 204.

78. Synthesis and In Vitro Evaluation of Imidazole Derived Phenoxypoline Octanoamides as Angiotensin II (AT₁) Receptor Antagonists. Part 2. R. L. Simon, A. D. Palkowitz, M. I. Steinberg, K. M. Zimmerman, K. J. Thrasher, J. K. Reel, C. A. Whitesitt, S. A. Wiest, W. Pfeifer, K. L. Hauser, D. B. Boyd, S. L. Lifer, V. Vasudevan, and W. S. Marshall. Poster paper for the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 203.
79. Pharmacology of a Series of Novel Proline Octanoamide Angiotensin II (AT₁) Receptor Antagonists. K. M. Zimmerman, M. I. Steinberg, S. A. Wiest, A. D. Palkowitz, K. J. Thrasher, J. K. Reel, C. A. Whitesitt, R. L. Simon, W. Pfeifer, D. B. Boyd, K. L. Hauser, S. L. Lifer, and W. S. Marshall. Poster paper for the 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994, MEDI 209.
80. Homology Modeling and Refinement of Proteins that Recognize Beta-Lactam Antibacterial Agents. Jiaan Yang, Valentine J. Klimkowski, and Donald B. Boyd. Abstracts of the Fourth International Conference on Chemical Synthesis of Antibiotics and Related Microbial Products, Nashville, Indiana, September 11-16, 1994.
81. Homology Modeling and Refinement of Proteins that Recognize Beta-Lactam Antibacterial Agents. Jiaan Yang, Valentine J. Klimkowski, and Donald B. Boyd. Abstracts of the Chemistry Department Open House, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana., October 15, 1994.
82. A Tool for Negotiating through Structure-Activity Relationship Space: The Hypersurface Iterative Projection Method. Donald B. Boyd. Abstracts of and poster paper in the First Electronic Conference on Computational Chemistry (ECCC-1), the Internet, November 7-18, 1994.
83. Is Attendee a Word?, (letter to the editor). Don Boyd, International Union of Crystallography Newsletter, 3 (1), 2 (1995).
84. Molecular Modeling. (letter to the editor) Donald B. Boyd and Kenny B. Lipkowitz, Chemical & Engineering News, 73 (27), July 3, 1995, p. 2.
85. Experimental and Computational QSAR Studies of Octanoamides that Antagonize the Vasoconstrictive Effect Induced by Angiotensin II. Aaron D. Kossoy, D. B. Boyd, and Stuart C. Burris. Poster paper for the Gordon Research Conference on Quantitative Structure-Activity Relationships, Tilton, New Hampshire, August 6-11, 1995.
86. Stochastic Approach to Force Field Evaluations: Conformational Analysis of Raloxifene, a Potential New Therapeutic Agent for Post-Menopausal Osteoporosis. Donald B. Boyd and Robert D. Coner. Abstracts of the Second Electronic Conference on Computational Chemistry, the Internet, November 1-November 30, 1995.
87. Chair's Notebook and Guidelines for the Gordon Research Conference on Computational Chemistry. Donald B. Boyd, October 2, 1995.

88. On the Rhodanines. D. B. Boyd, Richard J. Loncharich, and Jeffrey S. Nissen. Abstracts of the 211th American Chemical Society National Meeting, March 24-28, 1996, New Orleans, Louisiana, COMP 128.
89. Semiempirical and Ab Initio Calculations on the Ylidene 2-Thioxo-Thiazolidin-4-one Moiety Found in Biologically Active Compounds. D. B. Boyd, R. J. Loncharich, and J. S. Nissen. Abstracts of the 29th Midwest Theoretical Chemistry Conference, May 30-June 1, 1996, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana.
90. A Survey of a Chemical Abstracts Service Database Shows the Growing Impact of Computational Chemistry. D. B. Boyd. Abstracts of the 29th Midwest Theoretical Chemistry Conference, May 30-June 1, 1996, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana. (A report of this paper appeared in the Fall 1996 newsletter of Gaussian, Inc., Gaussian NEWS.)
91. Progress in Rational Design of Therapeutically Interesting Compounds. D. B. Boyd. Abstracts of the Alfred Benzon Symposium No. 42 on Rational Molecular Design in Drug Research, Royal Danish Academy of Sciences and Letters, Copenhagen, Denmark, June 8-12, 1997.
92. Is Rational Design Good for Anything? D. B. Boyd. Abstracts of the 213th American Chemical Society National Meeting, September 7-11, 1997, Las Vegas, Nevada, COMP 055.
93. H. Van de Waterbeemd, R. E. Carter, G. Grassy, H. Kubinyi, Y. C. Martin, M. S. Tute, and P. Willett, *Pure & Appl. Chem.*, 69 (5), 1137-1152 (1997). Glossary of Terms Used in Computational Drug Design. D. B. Boyd is listed among 14 reviewers for the International Union of Pure and Applied Chemistry (IUPAC), Medicinal Chemistry Section, Working Party on Glossary of Terms Used in Computational Drug Design.
94. Book Review of "Online Searching: A Scientist's Perspective. A Guide for the Chemical and Life Sciences", by Damon D. Ridley (University of Sydney), Wiley, New York, 1996. D. B. Boyd, *J. Am. Chem. Soc.*, 120 (1), 240-241 (1998).
95. Early History of the Gordon Research Conference on Computational Chemistry. (based on the "Chair's Notebook and Guidelines", October 2, 1995), Gordon Research Conference on Computational Chemistry Home Page on the World Wide Web, <http://chem.iupui.edu/rcc/grccc.html>, January 1998.
96. Innovation and the Rational Design of Drugs. D. B. Boyd, *CHEMTECH*, 28 (5), 19-23 (1998). (Feature article in the May issue.)
97. Arylpiperazines with Serotonin-3 Antagonist Activity: A Comparative Molecular Field Analysis. A. Morreale, E. Gálvez-Ruano, I. Iriepa-Canalda, and D. B. Boyd. Poster paper for the 15th International Symposium on Medicinal Chemistry, Edinburgh, Scotland, September 6-10, 1998.
98. CoMFA Study of Arylpiperazines Exhibiting Serotonin-3 Antagonism. A. Morreale, E. Gálvez-Ruano, I. Iriepa-Canalda, and D. B. Boyd. Poster paper for the Fifth Electronic Computational Chemistry Conference (ECCC-5), the Internet, November 2-30, 1998.

99. Rational Drug Design: Controlling the Size of the Haystack. D. B. Boyd, *Modern Drug Discovery*, November/December, 1998, pp. 41-48.
100. Journal of Molecular Graphics and Modelling Becomes Publication of COMP. D. B. Boyd, an announcement with the ACS Computers in Chemistry Division mailing with COMP election ballots, February 1999.
101. History. (letter to the editor) D. B. Boyd, *Today's Chemist at Work*, 8 (5), May 1999, p. 71.
102. Reinvention of the Journal of Molecular Graphics and Modelling: Defining a Discipline. (editorial) R. E. Hubbard and D. B. Boyd, *Journal of Molecular Graphics and Modelling*, 16 (3), 113-114 (1998).
103. The Division's Own Journal. D. B. Boyd, *ACS Computers in Chemistry Division COMP Newsletter, Abstracts Booklet*, 218th ACS National Meeting, August 22-26, 1999.
104. Book Review of "Molecular Modeling of Nucleic Acids", Neocles B. Leontis and John SantaLucia, Jr., Eds., ACS Symposium Series 682, American Chemical Society, Washington, DC, 1998. D. B. Boyd, *J. Med. Chem.*, 42 (15), 3009 (1999).
105. Reinvention of the Journal of Molecular Graphics and Modelling: News and Views. (editorial) R. E. Hubbard and D. B. Boyd, *Journal of Molecular Graphics and Modelling*, 16 (4/5/6), 177 (1998).
106. Quantum Chemistry Program Exchange, QCPE: End of an Era or a New Chapter? D. B. Boyd, *J. Mol. Graphics Mod.*, 17 (1), 62-64 (1999).
107. Book Review of "Molecular Modeling on the PC", Matthew F. Schlecht, Wiley-VCH, New York, 1998. D. B. Boyd, *J. Mol. Graphics Mod.*, 17 (1), 70-71 (1999).
108. Chair's Guidebook for the Gordon Research Conference on Computational Chemistry. Donald B. Boyd, November 1, 1999.
109. Book Review of "Advances in Quantitative Structure-Property Relationships", Marvin Charton and Barbara I. Charton, Eds., JAI Press, Stamford, Connecticut, 1999. D. B. Boyd, *J. Mol. Graphics Mod.*, 17 (3-4, appeared March 2000), 231-234 (1999).
110. The Division's Own Journal. D. B. Boyd, *ACS Computers in Chemistry Division COMP Newsletter, COMP Newsletter and Abstracts Booklet*, 220th National Meeting of the American Chemical Society, August 20-24, 2000, Washington, DC, pp 2-3.
111. Introduction and Foreword to the Special Issue on Molecular Modeling of Carbohydrates. D. B. Boyd and J. R. Grigera, *J. Mol. Graphics Modell.*, 18 (2), 93-94 (2000).
112. A Thank You to Those Who Have Refereed Papers for the Journal. D. B. Boyd and R. E. Hubbard, *J. Mol. Graphics Modell.*, 18 (3), 233-234 (2000).
113. Introduction and Foreword to the Special Issue on Combinatorial Library Design. D. B. Boyd, D. K. Agrafiotis, and E. J. Martin. *J. Mol. Graphics Modell.*, 18 (4/5), 317-319 (2000).

114. Book Review of "Chemical Applications of Molecular Modelling", Jonathan M. Goodman, Royal Society of Chemistry, Cambridge, 1998. D. B. Boyd, *J. Mol. Graphics Modell.*, 18 (4/5), 545-546 (2000).
115. Meeting Report on the 2000 Gordon Research Conference on Computational Chemistry, D. B. Boyd, posted on the Gordon Research Conference on Computational Chemistry Home Page, December 2000.
116. Emerging Technologies Symposium, D. B. Boyd, *J. Mol. Graphics Modell.*, 18 (6), 618-620 (2000).
117. ISI Rankings of Chemistry Journals, D. B. Boyd, *J. Mol. Graphics Modell.*, 18 (6), 620 (2000).
118. A Letter to the Community of Computational Chemists about Gordon Research Conferences on Computational Chemistry, T. R. Stouch, B. R. Brooks, W. C. Swope, J. D. Madura, K. N. Houk, J. McKelvey, W. L. Jorgensen, P. A. Kollman, K. B. Lipkowitz, and D. B. Boyd. Posted on the Gordon Research Conference on Computational Chemistry Home Page, December 2000.
119. The Division's Own Journal: JMGM Makes Significant Progress Since Affiliating with COMP, COMP Newsletter, Spring 2001, 221st National Meeting of the American Chemical Society, San Diego, CA, April 1-5, 2001, pp. 3-4.
120. Invitation to Participate in the Symposium on Emerging Computational Technologies at the 125th Anniversary of the ACS, Chicago, Illinois, August 2001. Announcement in Calls for Papers in Chicago, Chemical & Engineering News, February 12, 2001, p. 49. Prepared for the American Chemical Society's Computers in Chemistry website and for the COMP Newsletter, Spring 2001, 221st National Meeting of the American Chemical Society, San Diego, CA, April 1-5, 2001, p. 6. Meeting report on the Chicago symposium for the website of the ACS's Division of Computers in Chemistry, October 2001.
121. Introduction and Foreword to the Special Issue on Commemorating the Thirtieth Anniversary of Eiji Osawa's C60 Paper. D. B. Boyd and Z. Slanina, *J. Mol. Graphics Modell.*, 19 (2), 181-104 (2001). (Editorial).
122. Introduction and Foreword to the Special Issue on Computational Drug Design and Informatics. D. B. Boyd and D. A. Winkler, *J. Mol. Graphics Modell.*, 19 (5), 403-404 (2001). (Editorial).
123. Introduction and Foreword to the Special Issue on Computational Protein Flexibility and Folding. D. B. Boyd, L. A. Kuhn, and M. F. Thorpe, *J. Mol. Graphics Modell.*, 19 (1), 1-2 (2001). (Editorial).
124. Book Review of "Evolutionary Algorithms in Molecular Design", David E. Clark, Ed., Wiley-VCH, Weinheim, 2000. F. Barbosa and D. B. Boyd, *J. Am. Chem. Soc.*, 123 (22), 5384 (2001).
125. Prediction of the Oral Bioavailability of Compounds: A Computational Study. F. Barbosa and D. B. Boyd, Abstract for the Gordon Research Conference on Quantitative Structure-Activity Relationships, Tilton, New Hampshire, August 5-10, 2001.

126. Oral Human Bioavailability: A Computational Study. F. Barbosa and D. Boyd, Poster paper presented at the Gordon Research Conference on Quantitative Structure-Activity Relationships, Tilton, New Hampshire, August 5-10, 2001.
127. A New Beginning for the Journal. D. B. Boyd, *J. Mol. Graphics Modell.*, 19 (6), 479-480 (2001). (Editorial).
128. A Letter to the Community of Computational Chemists: The Gordon Research Conferences on Computational Chemistry, T. R. Stouch, B. R. Brooks, W. C. Swope, J. D. Madura, K. N. Houk, J. McKelvey, W. L. Jorgensen, K. B. Lipkowitz, and D. B. Boyd, *J. Mol. Graphics Modell.*, 19 (6), 617 (2001).
129. Introduction and Foreword to the Special Issue Commemorating the 25th Anniversary of Molecular Connectivity as a Structure Description System. D. B. Boyd, L. H. Hall, and L. B. Kier, *J. Mol. Graphics Modell.*, 20 (1), 1-3 (2001). (Editorial).
130. Introduction and Foreword to the Special Section on the ACS COMP Symposium on QSAR in vivo. D. B. Boyd and R. D. Clark, *J. Mol. Graphics Modell.*, 20 (4), 257-258 (2002). (Editorial).
131. Invitation to Participate in the Symposium on Emerging Technologies in Computational Chemistry at the 224th National Meeting of the American Chemical Society, Boston, Massachusetts, August 18-22, 2002. Announcement for the website of the ACS's Division of Computers in Chemistry, October 2001. A meeting report on the symposium and photographs were published on the website of the ACS's Division of Computers in Chemistry, September 2002.
132. Announcement for the Symposium on Emerging Technologies in Computational Chemistry at the 226th National Meeting of the American Chemical Society, New York City, September 2003, written for the website of the ACS's Division of Computers in Chemistry, September 2002.
133. Meeting Report on the 2002 Gordon Research Conference on Computational Chemistry, D. B. Boyd, posted on the Gordon Research Conference on Computational Chemistry Home Page, October 2002, updated November 2002.
134. The Eyes Have It. (letter to the editor) D. B. Boyd, *Modern Drug Discovery*, March 2003, p. 8. .
135. Book Review of "Bioinformatics - From Genomes to Drugs", Thomas A. Lengauer, Ed., Wiley-VCH, Weinheim, 2002. D. B. Boyd, *J. Med. Chem.*, 46 (11), 2258-2259 (2003).
136. Chair's Guidebook for the Gordon Research Conference on Computational Chemistry. D. B. Boyd, November 2003.
137. Crystallographic and Computational Chemistry Analysis of Aminothiazole Methoximes, T. Ercanli and D. B. Boyd. Abstract for the 36th Central Regional Meeting of the American Chemical Society, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana, June 2-4, 2004.
138. Evaluation of Quantum and Molecular Mechanics Methods, T. Ercanli and D. B. Boyd. Abstract 8-A for the Fifth Annual Local Section American Chemical

- Society Poster Session, DePauw University, Greencastle, Indiana, October 11, 2004.
139. Conformational Analysis of New Inhibitors of Human Inosine Monophosphate Dehydrogenase, M. D. Jain and D. B. Boyd. Abstract 14-A for the Fifth Annual Local Section American Chemical Society Poster Session, DePauw University, Greencastle, Indiana, October 11, 2004.
 140. Book Review of "Computational Medicinal Chemistry for Drug Discovery", Patrick Bultinck, Hans De Winter, Wilfried Langenaeker, and Jan P. Tollenaere, Eds., Marcel Dekker, New York, 2004. D. B. Boyd, *J. Med. Chem.*, 47 (25), 6433 (2004).
 141. How to Find the Best Computational Chemistry Method Using Cheminformatics, T. Ercanli and D. B. Boyd. Abstracts of the National Meeting of the American Chemical Society, San Diego, California, March 13-17, 2005, CINF 62.
 142. Chair's Guidebook for the Gordon Research Conference on Computational Chemistry. D. B. Boyd, January 10, 2006. [21 pages, twenty year anniversary edition, sent to Dr. Wilfred F. van Gunsteren (ETH) and Dr. Jed W. Pitera (IBM).]
 143. Reviews in Computational Chemistry website. D. B. Boyd, February 2006. [updated and expanded; over 40 files and over 200 printed pages].
 144. Gordon Research Conference on Computational Chemistry website. D. B. Boyd, March 2006. [updated and expanded; over 30 files and over 30 printed pages].
 145. Exploration of the Molecular Shape of a Polymer with Bioactivity Against HIV-1, Karolina A. Kill and Donald B. Boyd. Abstracts of the 8th Annual Indiana Local Section American Chemical Society Poster Session, Lilly Corporate Center, Eli Lilly and Company, Indianapolis, Indiana, October 11, 2007, Abst. 32.
 146. Chair's Guidebook for the Gordon Research Conference on Computational Chemistry. D. B. Boyd, January 17, 2008. [24 pages, sent to Dr. Jed W. Pitera (IBM, Calif.) and Prof. Dr. Walter Thiel (Max-Planck-Institut für Kohlenforschung, Germany)].
 147. Molecular Shape and Charge Distribution of a Polymer That Inhibits HIV-1 Reverse Transcriptase Activities, K. A. Kill and D. B. Boyd. Abstracts of the 9th Annual Indiana Local Section American Chemical Society Poster Session, Ball State University, Muncie, Indiana, October 16, 2008.
 148. Molecular Shape and Charge Distribution of a Polymer That Inhibits HIV-1 Reverse Transcriptase Activities, K. A. Kill and D. B. Boyd. Abstracts of the Departmental Poster Session, Department of Chemistry and Chemical Biology, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana, December 3, 2008.
 149. Book Review of "Pathway Analysis for Drug Discovery. Computational Infrastructure and Applications", Anton Yuryev, Ed., Wiley, Hoboken, NJ, 2008. D. B. Boyd, *J. Med. Chem.*, 52 (7), 2161-2162 (2009).

Recent Presentations:

55. University of Kentucky, College of Pharmacy, Division of Medicinal Chemistry and Pharmaceutics Seminar, Lexington, Kentucky, January 25, 1994. Invited lecture on "Computer-Aided Drug Design Applications."
56. Purdue University, School of Pharmacy, Department of Industrial and Physical Pharmacy Seminar, West Lafayette, Indiana, January 27, 1994. Invited lecture on "Computer-Aided Drug Design Applications."
57. Wright State University, Department of Chemistry Seminar, Dayton, Ohio, February 4, 1994. Invited lecture on "Computer-Aided Drug Design Applications."
58. Marion Merrell Dow Research Institute, Marion Merrell Dow Inc., Cincinnati, Ohio, February 24, 1994. "Computer-Aided Drug Design Applications."
59. Symposium on the Chemist and Chemistry in the Health Care Industry, 71st National Meeting of the American Institute of Chemists, Indianapolis, Indiana, March 4, 1994. Invited lecture on "Computer-Aided Drug Design in Pharmaceutical Research."
60. Symposium on Applications of Computer-Aided Molecular Design: Agrochemicals, Materials, and Pharmaceuticals, 207th National Meeting of the American Chemical Society, San Diego, California, March 13-18, 1994. Invited lecture on "Molecular Modeling and QSAR Studies in Pursuit of Highly Potent Phenoxyproline Octanoamide Angiotensin II (AT₁) Receptor Antagonists."
61. Fifth Gordon Research Conference on Computational Chemistry, New Hampton, New Hampshire, July 3-8, 1994. Invited short talk on "Trends in the Tools for Computer-Aided Drug Design."
62. Fourth International Conference on Chemical Synthesis of Antibiotics and Related Microbial Products, Nashville, Indiana, September 11-16, 1994. Jiaan Yang, Valentine J. Klimkowski, and Donald B. Boyd, poster presentation on "Homology Modeling and Refinement of Proteins that Recognize Beta-Lactam Antibacterial Agents."
63. Chemistry Department Open House, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana., October 15, 1994. Jiaan Yang, Valentine J. Klimkowski, and Donald B. Boyd, poster presentation on "Homology Modeling and Refinement of Proteins that Recognize Beta-Lactam Antibacterial Agents."
64. First Electronic Conference on Computational Chemistry, the Internet, November 7-December 2, 1994. Hypertext poster presentation via World-Wide-Web on "A Tool for Negotiating through Structure-Activity Relationship Space: The Hypersurface Iterative Projection Method."
65. Second Electronic Conference on Computational Chemistry, the Internet, November 1-November 30, 1995. Donald B. Boyd and Robert D. Coner, hypertext poster presentation via World-Wide-Web on "Stochastic Approach to

- Force Field Evaluations: Conformational Analysis of Raloxifene, a Potential New Therapeutic Agent for Post-menopausal Osteoporosis."
66. Symposium on Semi-Empirical Methods: Is There a Future?, 211th American Chemical Society National Meeting, March 24-28, 1996, New Orleans, Louisiana. Invited lecture on "On the Rhodanines."
 67. Akzo Nobel Chemicals Inc., Dobbs Ferry, New York, May 10, 1996. Invited lecture on "Overview of Computer-Aided Molecular Design and Quantitative Structure-Activity Relationships."
 68. Sixth Gordon Research Conference on Computational Chemistry, New Hampton, New Hampshire, June 30-July 5, 1996. Donald B. Boyd and Greg Pearl, poster presentation on "Peptidomimetic Angiotensin II Receptor Antagonists."
 69. The Alfred Benzon Symposium No. 42 on Rational Molecular Design in Drug Research, Royal Danish Academy of Sciences and Letters, Copenhagen, Denmark, June 8-12, 1997. Invited lecture on "Progress in Rational Design of Therapeutically Interesting Compounds".
 70. Symposium on Rational Drug Design, 213th American Chemical Society National Meeting, Las Vegas, Nevada, September 7-11, 1997. Invited lecture on "Is Rational Design Good for Anything?".
 71. 1997 Executive Bioinformatics Science Seminar, Johnson & Johnson Corporate Headquarters, New Brunswick, New Jersey, November 10, 1997. Invited lecture on "Molecular Modeling".
 72. Universidad de Alcalá de Henares, Madrid, Spain, Departamento de Química Orgánica "Conference" (seminar), September 23, 1998. Invited lecture on "Drug Discovery by Computer-Aided Rational Design".
 73. National Institute on Alcohol Abuse and Alcoholism (NIAAA) Workshop on Preclinical Medications Development, National Institutes of Health (NIH), Bethesda, Maryland, November 16-17, 1998. Invited lecture on "Drug Discovery by Molecular Modeling and Rational Design".
 74. Pharmaceutical Engineering Seminar Series, College of Engineering and College of Pharmacy, University of Michigan (teleconferenced to Parke-Davis/Warner-Lambert, Pharmacia and Upjohn, Searle, and Monsanto), Ann Arbor, Michigan, January 13, 2000. Invited lecture on "Has the Drug Discovery Process Been Aided by Computational Chemistry and Rational Design?"
 75. Ninth Gordon Research Conference on Computational Chemistry, New London, New Hampshire, June 30-July 5, 2002. Opening session remarks on the scope and mission of the conference series.
 76. Ninth Gordon Research Conference on Computational Chemistry, New London, New Hampshire, June 30-July 5, 2002. D. B. Boyd, poster presentation on "Trends in the Job Market for Computational Chemists".
 77. 10th Gordon Research Conference on Computational Chemistry, Holderness School, Plymouth, New Hampshire, July 4-9, 2004. T. Ercanli and D. B. Boyd,

- poster presentation on Cluster Analysis for Evaluating Computational Chemistry Methods.
78. Department of Chemistry Poster Session, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana, October 6, 2004. T. Ercanli and D. B. Boyd, poster presentation on A Cheminformatics Approach to Computational Chemistry.
 79. Department of Chemistry Poster Session, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana, October 6, 2004. M. D. Jain and D. B. Boyd, poster presentation on Molecular Modeling of Thiazole-4-carboxamide Adenine Dinucleotides with Antitumor Activity.
 80. Fifth Annual Local Section American Chemical Society Poster Session, DePauw University, Greencastle, Indiana, October 11, 2004. T. Ercanli and D. B. Boyd, poster presentation on Evaluation of Quantum and Molecular Mechanics Methods.
 81. Fifth Annual Local Section American Chemical Society Poster Session, DePauw University, Greencastle, Indiana, October 11, 2004. M. D. Jain and D. B. Boyd, poster presentation on Conformational Analysis of New Inhibitors of Human Inosine Monophosphate Dehydrogenase.
 82. 229th National Meeting of the American Chemical Society, San Diego, California, March 13-17, 2005, Sci-Mix, CINF 62. T. Ercanli and D. B. Boyd, invited poster presentation on How to Find the Best Computational Chemistry Method Using Cheminformatics.
 83. Special Workshop on Theoretical & Computational Bridges from Molecular Quantum Behavior to Biological Simulation, University Place Hotel and Conference Center, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana, September 30-October 1, 2005. T. Ercanli and D. B. Boyd, invited poster presentation on Cluster Analysis for Comparison of Quantum Mechanical and Force Field Methods.
 84. 232nd National Meeting of the American Chemical Society, San Francisco, California, September 10-14, 2006, COMP 258. Nidhi and D. B. Boyd, poster presentation on How to Find the Best Computational Chemistry Method Using Cheminformatics.
 85. 11th Gordon Research Conference on Computational Chemistry, Les Diablerets, Switzerland, October 8-13, 2006. Nidhi and D. B. Boyd, poster presentation on Conformational Analysis of a Bioactive Polymer Using a Monte Carlo Method.
 86. IUPUI School of Informatics Course I572, Computational Chemistry & Molecular Modeling, March 27, 2007. D. B. Boyd, invited lecture on Historical Perspective on Computing in the Pharmaceutical Industry.
 87. 8th Annual Indiana Local Section American Chemical Society Poster Session, Lilly Corporate Center, Eli Lilly and Company, Indianapolis, Indiana, October 11, 2007. K. A. Kill and D. B. Boyd, poster presentation on Exploration of the Molecular Shape of a Polymer with Bioactivity against HIV-1.

88. Indiana University Undergraduate Research Conference, Indiana University Southeast, New Albany, Indiana, November 30, 2007. K. A. Kill and D. B. Boyd, poster presentation on Molecular Modeling Analysis of a Polymer that Can Inhibit HIV-1 Reverse Transcriptase Activities.
89. Capstone Poster Session, Department of Chemistry and Chemical Biology, IUPUI, Indianapolis, December 3, 2007. A. C. Smith and D. Boyd, Molecular Mechanics Investigation of the Secondary Structure of the ATMO Polymer Capable of Inhibiting Human Immunodeficiency Virus Reverse Transcriptase.
90. 12th Gordon Research Conference on Computational Chemistry, Mount Holyoke College, South Hadley, Massachusetts, July 27-August 1, 2008. K. A. Kill and D. B. Boyd, poster presentation on Shape and Charge Distribution of a Polymer that Inhibits HIV-1 Reverse Transcriptase Activities.
91. 12th Gordon Research Conference on Computational Chemistry, Mount Holyoke College, South Hadley, Massachusetts, July 27-August 1, 2008. D. B. Boyd, poster presentation on Current Trends in the Job Market for Computational Chemists.
92. 9th Annual Indiana Local Section American Chemical Society Poster Session, Ball State University, Muncie, Indiana, October 16, 2008. K. A. Kill and D. B. Boyd, poster presentation on Molecular Shape and Charge Distribution of a Polymer That Inhibits HIV-1 Reverse Transcriptase Activities.
93. Departmental Poster Session, Department of Chemistry and Chemical Biology, Indiana University-Purdue University at Indianapolis, Indianapolis, Indiana, December 3, 2008. K. A. Kill and D. B. Boyd, poster presentation on Molecular Shape and Charge Distribution of a Polymer That Inhibits HIV-1 Reverse Transcriptase Activities.

Partial List of Seminars Arranged for the IUPUI Department of Chemistry:

Dr. Steven W. Baertschi (Lilly) February 21, 1996
Dr. Gary Wiggins (Indiana University) September 11, 1996
Dr. Herbert Kirst (Lilly) October 30, 1996
Prof. Eric Glendening (Indiana State University) January 22, 1997
Dr. James J. P. Stewart (Fujitsu) February 26, 1997
Dr. David A. Demeter (R. W. Johnson Research Institute) March 26, 1997
Dr. Shashi Rao (Searle) November 5, 1997
Dr. V. Joseph Klimkowski (Lilly) November 12, 1997
Dr. Mike Wiley (Lilly) March 4, 1998
Dr. Allen Kline (Lilly) November 18, 1998
Dr. Robert E. Babine (Lilly) March 31, 1999
Dr. David Spellmeyer (CombiChem) October 20, 1999
Dr. William Wheeler (Lilly) February 16, 2000
Dr. Daniel Robertson (Lilly) March 12, 2003
Prof. Sean Mooney (School of Informatics, IUPUI) April 6, 2005

Dr. Kumiko Takeuchi (Lilly) November 29, 2006

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EDUCATION

- 1990-1993 Postdoctoral Research at Columbia University, and Columbia University
College of Physicians & Surgeons, New York, New York
- 1989 Chemistry, Ph.D. University of California, Los Angeles
- 1983 Chemistry, B.S. Indiana University, Bloomington, Indiana

EXPERIENCE

- 2008-Present IUPUI, Indianapolis, Indiana
Director of Synthesis, Chemical Synthesis & Organic Drug
Lead Development Core
Assistant Research Professor, Dept. Chemistry & Chemical Biology
- custom synthesis; medicinal chemistry
- 2006-2007 Barnes & Thornburg LLP, Technical Analyst Intellectual Property
Indianapolis, Indiana
- patent prosecution and litigation support
- 2005-2006 Indiana University School of Medicine, Indianapolis, Indiana
Visiting Associate Professor, Dept. Chemistry & Chemical Biology
- organic chemistry methodology
- 2003-2005 Semafore Pharmaceuticals, Inc., Indianapolis, Indiana
Principal Research Scientist
- oncology research; synthesis of PTEN and PI3 kinase inhibitors
- 2002-2003 Indiana University School of Medicine, Indianapolis, Indiana
Visiting Associate Professor, Dept. Biochemistry & Mol. Biology
- organic chemistry methodology
 - oncology research; synthesis of apurinic endonuclease 1 (APE1) inhibitors
- 2001-2002 3-Dimensional Pharmaceuticals, Inc., Cranbury, New Jersey
Principal Research Scientist
- oncology research; synthesis of kinase inhibitors (individual compounds and small focused libraries) in the hit-to-lead group
- 1998-2001 Provid Research, Piscataway, New Jersey
Research Scientist II
- oncology research; synthesis of angiogenesis inhibitors
 - arthritis research; synthesis of TNF- α peptides inhibitors
- 1993-1998 R.W. Johnson Pharmaceutical Research Institute, Raritan, New Jersey
- 1995-1998 Senior Scientist, Drug Discovery
- 1993-1995 Scientist, Medicinal Chemistry
- reproductive medicine research, synthesis of nonsteroidal contraceptives

Patent Applications, Publications, & Presentations

- 3 issued US patents
- 8 patent applications: c-fms kinase inhibitors
- 2 patent application: PTEN inhibitors
- 9 publications in peer reviewed journals
- 6 posters & presentations at national scientific meetings

Issued Patents

1. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T.M. *C-Fms Kinase Inhibitors* US 7,790,724; **Issued: Sept. 7, 2010.**
2. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T.M. *C-Fms Kinase Inhibitors* US 7,429,603; **Issued: Sept. 30, 2008.**
3. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. *C-Fms Kinase Inhibitors* US 7,427,683; **Issued: Sept. 23, 2008.**

Patent Applications

1. Garlich, J. R.; Durden, D. L.; Georgiadis, T. M.; Su, J.; Peng, X.; Smith, T. C. *Pten Inhibitors*. U.S. Pat. Appl. Publ. (2007) US 20070203098 A1.
2. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. *C-Fms Kinase Inhibitors*. PCT Int. Appl. (2006) PCT/US2006/014886. Publ. No. WO/2007/123516.
3. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. *C-Fms Kinase Inhibitors* U.S. Pat. Appl. Publ. (2006) US 20060258666 A1.
4. Garlich, J. R.; Durden, D. L.; Georgiadis, T. M.; Su, J.; Peng, X.; Smith, T. C. *Preparation of (Heteroaryl) Amides and Hydrazides as Inhibitors of Phosphatase Located on Chromosome 10 (PTEN)*. PCT Int. Appl. (2005) PCT/US2005/011626. Publ. No. WO/2005/097119.
5. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. M. *C-Fms Kinase Inhibitors*. U.S. Pat. Appl. Publ. (2005), US 20050131022 A1.
6. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. M. *Inhibitor of C-Fms Kinase*. PCT Int. Appl. (2005) PCT/US2005/038307. Publ. No. WO/2006/047479.
7. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. M. *Inhibitor of C-Fms Kinase*. PCT Int. Appl. (2005) PCT/US2005/038340. Publ. No. WO/2006/047503.
8. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. *Inhibitors of C-FMS Kinase*. U.S. Pat. Appl. Publ. (2005), US 2005113566 A1.
9. Player, M. R.; Baindur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. M. *C-Fms Kinase Inhibitors*. U.S. Pat. Appl. Publ. (2005) US 2005004112 A1.

10. Player, M. R.; Baidur, N.; Brandt, B. M.; Chadha, N.; Patch, R. J.; Asgari, D.; Georgiadis, T. M. *C-Fms Kinase Inhibitors*. PCT Int. Appl. (2004) PCT/US2004/012729. Publ. No. WO/2004/096795.

Publications

1. Patch, R. J.; Brandt, Benjamin M.; Asgari, D.; Baidur, N.; Chadha, N. K.; Georgiadis, T.; Cheung, W. S.; Petrounia, I. P.; Donatelli, R. R.; Chaikin, M. A.; Player, M. R. Potent 2'-aminoanilide inhibitors of cFMS as potential anti-inflammatory agents. *Bioorg. Med. Chem. Lett.* (2007), 17(22), 6070-6074.
2. Georgiadis, T. M.; Baidur, N.; Player, M. R. Solid-Phase Synthesis of an Oxalic Acid Amide Library. *J. Comb. Chem.* **6**(2), 224-229, (2004).
3. Yoon, S. S., Georgiadis, T. M., and Still, W. C. Conformational Flexibility and Binding Selectivity in a Synthetic Receptor for Peptides. *Tetrahedron Lett.* **34**, 6697-6670 (1993).
4. Landry, D. W., Zhao, K., Yang, G. X.-Q., Glickman, M., and Georgiadis, T. M. Antibody-Catalyzed Degradation of Cocaine. *Science* **259**, 1899-1901 (1993).
5. Georgiadis, M. P., Albizati, K., and Georgiadis, T. M. Oxidative Rearrangement of 2-Furyl Carbinols and Methodologies for Preparing 6-Hydroxy-2H-pyran-3(6H)-ones. A Review. *Org. Prep. Proced. Int.* **24**, 95-118 (1992).
6. Constantinou-Kokotou, V., Couladouros, E. A., Georgiadis, M. P., Kokotos, G. C., and Georgiadis, T. M. Products from furans. 11. Total synthesis of 4-(D-alanyl amino)-2-amino-2,3,4-trideoxy-DL-threo-pentose (3-deoxy-DL-prumycin) *Carbohydr. Res.* **222**, 163-172 (1991).
7. Georgiadis, T. M., Georgiadis, M. M., and Diederich, F. Synthesis and Complexation Properties of a Water-Soluble Optically Active Cyclophane Incorporating a 4-Naphthyl-1,2,3,4 tetrahydroisoquinoline Unit as a Chiral Spacer. *J. Org. Chem.* **56**, 3362-3369 (1991).
8. Castro, P. P., Georgiadis, T. M., and Diederich, F. Chiral Recognition in Clefts and Cyclophane Cavities Shaped by the 1,1'-Binaphthyl Major Groove. *J. Org. Chem.* **54**, 5835-5838 (1989).
9. Rubin, Y., Dick, K., Diederich, F., and Georgiadis, T. M. Chiral Recognition in Aqueous Solution. Concept and Search for Water-Soluble Hosts with Apolar Binding Sites. *J. Org. Chem.* **51**, 3270-3278 (1986).

Posters & Presentations

1. Wang H.; Cai, S., Bailey, B.J., Sinn, A.L., Minto, R.E., Georgiadis, T.M., Long, E.C., Sarkaria, J.N., Mayo, L.D., and Pollok, K.E. *Modulation of temozolomide-mediated DNA damage in glioblastoma multiforme by the HDM2 antagonist, nutlin3* [abstract]. In: Proceedings of the 101st Annual Meeting of the American Association for Cancer Research; 2010 Apr 17-21; Washington, DC. Philadelphia (PA): AACR; 2010. p#. Abstract nr 5373.
2. Garlich, J.R., Patterson, M., Smith, T.C., Suhr, R.G., Georgiadis, T. M. *Novel Purification Techniques and Solid Phase Synthesis of Macrocyclic Ligands*. Presented at the 36th Central Regional Meeting, American Chemical Society, Indianapolis, IN,

Abstract #33, June2-4 **2004**.

3. Georgiadis, T. M., Baindur, N., and Player, M. *Solid Phase Synthesis of an Oxalic Acid Amide Library*. Presented at the 224th ACS National Meeting, Boston, MA, ORGN-159, August 18-22, **2002**.
4. Zhang, M., Georgiadis, T. M., May, W. P., Self, C. R., Cook, C. M., Olson, G. L., Taylor, J., and Baum, J. *Conformational Studies Of A Cyclic Peptide Derived From The p55 TNF Receptor*. Presented at the 16th American Peptide Symposium, "Peptides for the New Millennium", Minneapolis, MN, Abstract # P397, June 26-July 1, **1999**.
5. Georgiadis, T. M., Jacobs, J., Cornelius, L. A. M., and Combs, D. W. *The Use Of Inverse-Electron-Demand Intermolecular Diels-Alder Cyclizations To Form 1-(Arylsulphonyl)-3-Aryl-1,4,5,6-tetrahydropyridazines*. Presented at the 12th Biennial Carl S. Marvel Symposium, "Frontiers in Biological Chemistry", Tucson, AZ, Abstract #30, March 19-21, **1997**.
6. Georgiadis, T. M., Castro, P. P., and Diederich, F. *Chiral Recognition of Naproxen Derivatives in Aqueous Solutions*. Presented at the 198th American Chemical Society, National Meeting, Miami, FL, ORGN-198, Sept. **1989**.
7. Diederich, F., Dharanipragada, R., and Georgiadis, T. M. *Novel Optically Active Hosts for Chiral Recognition Complexes in Aqueous Solutions*. Presented at the 194th American Chemical Society, National Meeting, New Orleans, LA, ORGN-79, Sept. **1987**.

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Doctor of Philosophy

Department of Pharmaceutical Science, The University of Melbourne, 1988-1991

Dissertation title: ^{31}P and ^{19}F Nuclear Magnetic Resonance Studies of Myocardial Metabolism*Undergraduate*

Bachelor of Agricultural Science

The University of Melbourne, 1979-1982

Employment History

<i>Research Assistant Professor</i>	Department of Chemistry and Chemical Biology, Indiana University-Purdue University, Indianapolis, USA	current
<i>Research Investigator</i>	College of Pharmacy, University of Michigan, Ann Arbor, USA	2004-2008
<i>Senior Research Fellow</i>	College of Pharmacy, University of Michigan Ann Arbor, USA	2002 -2004
<i>Research Fellow</i>	College of Pharmacy, University of Michigan, Ann Arbor, USA	1998-2002
<i>Research Fellow</i>	Department of Medicine, The University of Melbourne, Austin and Repatriation Medical Centre, Heidelberg, Australia	1998
<i>Post-Doctoral Fellow</i>	Cell and Membrane Biophysics Laboratory, Cardiovascular Research Institute, University of California, San Francisco, USA	1996-1997
<i>Research Officer</i> (<i>Post-Doctoral Fellow</i>)	Department of Physiology, The University of Melbourne, Parkville, Australia	1992-1996
<i>Teaching Assistant/NMR</i> <i>Service Operator (part-time)</i>	School of Pharmaceutical Chemistry, Victorian College of Pharmacy, Parkville, Australia	1988-1992
<i>Technical Assistant</i>	School of Pharmaceutical Chemistry, Victorian College of Pharmacy, Parkville, Australia	1984-1988

Summary of Research Experience

College of Pharmacy, University of Michigan

- amplification, construction of plasmid vectors for protein expression in *E. coli*, and site-directed mutagenesis of the *Pseudomonas putida* ATCC 12633 mandelate pathway enzymes; mandelamide hydrolase (MAH), benzoylformate decarboxylase (BFD), benzaldehyde dehydrogenase (BADH), mandelate racemase (MR) and mandelate dehydrogenase (MDH).
- amplification, construction of plasmid vectors for protein expression in *E. coli*, and site-directed mutagenesis of benzaldehyde lyase (BAL) from *Pseudomonas fluorescens* and pyruvate decarboxylase (PDC) from *Zymomonas mobilis* and *Saccharomyces cerevisiae*.
- amplification and construction of plasmid vectors for protein expression in *E. coli* of phenylpyruvate decarboxylase (PPDC) from *S. cerevisiae* and a branched-chain 2-keto-acid decarboxylase (KdcA) from *Lactococcus lactis*.
- site-directed mutagenesis and construction of plasmid vectors for protein expression in *E. coli* of human phenylethanolamine-*N*-methyl transferase (PNMT) and human muscle creatine kinase (HMCK)
- overexpression and purification, by various methods, of native and 6xHis-tagged proteins, and mutants, of MAH, BFD, PDC, BAL, PPDC, HMCK.
- enzyme kinetics assays, both direct and coupled, of MAH, BFD, PDC, BAL, PPDC, and HMCK.
- characterisation of wild-type enzymes and/or mutants of MAH, BFD, PDC, BAL, PPDC and HMCK.
- amplification and construction of plasmid vectors for expression in *E. coli* of the gene product of *mdlX*, a putative regulatory protein of the *P. putida* mandelate pathway.
- identification of genes for a second putative regulatory protein (*mdlR*) and a putative porin for the *P. putida* mandelate pathway.
- amplification and construction of plasmid vectors for expression in *E. coli* of the gene product of *mdlR*.
- disruption of various genes in the *P. putida* ATCC 12633 chromosomal mandelate pathway, and subsequent experiments to determine the effect of disruptions on *P. putida* growth rates

Department of Medicine, Austin and Repatriation Medical Centre

- characterisation of the role of the insulin-like growth factor (IGF) / IGF binding-protein (IGFBP) system in the regulation of proliferation and differentiation in the rhabdomyosarcoma cell lines, RD and Rh30
- proliferation, adhesion and agar cloning assays in rhabdomyosarcoma cells
- confocal fluorescence microscopy of IGF and IGFBP-6 immunolocalisation in rhabdomyosarcoma cell lines and other cell lines transfected to express components of the IGF/IGFBP6 system

Summary of Research Experience (continued)

Cardiovascular Research Institute, University of California, San Francisco

- investigation of phase contrast microscopy for measurement of water permeability in cultured cell monolayers
- testing and validation of phase contrast method in epithelial cell types naturally expressing molecular water channels (aquaporins) and in fibroblasts transfected to express aquaporins
- comparison of empirical data with predictions drawn from optics theory
- investigation of water permeability in human tracheal epithelial cells (from normal and cystic fibrosis patients) grown on porous supports
- study of pH-dependency of the absorbance and fluorescence spectra of various *Aequorea victoria* green fluorescent proteins (GFP)
- investigation of the use of GFP as a targetable intracellular pH probe in various cellular locations (mitochondria, endoplasmic reticulum, Golgi, cytosol)
- examination of the likely mechanisms for pH-dependency of fluorescence characteristics in different GFPs

Department of Physiology, The University of Melbourne

- investigation of the effects of peptide hormones proposed to regulate the function of the renal proximal tubule (including angiotensin II, endothelin, atrial natriuretic factor)
- studies of microdissected isolated perfused rat proximal tubules using low light level fluorescence imaging
- studies of isolated rat proximal tubules using laser scanning confocal microscopy
- development of suitable imaging systems and modification of microscopes for fluorescence studies of isolated perfused renal tubules and cultured renal cells
- imaging of fluorescent probes of intracellular composition (e.g. pH, Ca^{2+})
- preparation and use of fluorescently-labelled peptide hormones to localise hormone binding sites on proximal tubules and renomedullary interstitial cells
- confocal microscopy of the *in situ* morphology of renomedullary interstitial cells in isolated rat renal papillae

School of Pharmaceutical Chemistry, Victorian College of Pharmacy (post-graduate studies)

- ^{31}P nuclear magnetic resonance (NMR) spectroscopy studies of post-ischaemic recovery of high-energy phosphates in the isolated perfused rat heart model
 - application of various pharmacological interventions to the heart before and immediately after an ischaemic event to examine mechanisms for maximising post-ischaemic recovery (dihydropyridine Ca^{2+} channel blockers, xanthine oxidase inhibitors, cardioprotective solutions)
 - ^{19}F NMR studies of Ca^{2+} accumulation in the heart using the fluorinated intracellular Ca^{2+} probe, 5,5'-FBAPTA (analogous to fluorescent Ca^{2+} probes)
 - studies of hearts from normotensive rats, hypertensive rats, Mg^{2+} -depleted rats
-

Publications

1. Adam, WR, DJ Craik, JG Hall, MM Kneen & RM Wellard. 1988. Problems in the assessment of magnesium depletion in the rat by *in vivo* ^{31}P NMR. *Magn. Reson. Med.* 7:300-310.
2. Adam, WR, DJ Craik, MM Kneen & RM Wellard. 1989. Effect of magnesium depletion and potassium depletion and chlorothiazide on intracellular pH in the rat, studied by ^{31}P NMR. *Clin. Exp. Pharmacol. Physiol.* 16:33-40.
3. Craik, DJ, KA Higgins, MM Kneen, SLA Munro & KJ Waterman. 1991. Determining the conformation of a ligand bound to an enzyme; application of NMR spectroscopy in drug design. *J. Chem. Ed.* 68:258-261.
4. Hasin, Y, MM Kneen, DJ Craik & WG Nayler. 1992. Relationship between ATP resynthesis and calcium accumulation in the reperfused rat heart. *Clin. Exp. Pharmacol. Physiol.* 19:79-87.
5. Farinas, J, M Kneen, M Moore & AS Verkman. 1997. Plasma membrane water permeability of cultured cells and epithelia measured by light microscopy with spatial filtering. *J. Gen. Physiol.* 110:283-296.
6. Kneen, M, J Farinas, Y Li & AS Verkman. 1998. Green fluorescent protein as a non-invasive intracellular pH indicator. *Biophys. J.* 74:1591-1599.
7. Kneen, MM, DG Harkin, LL Walker, D Alcorn & PJ Harris. 1999. Imaging of renal medullary interstitial cells *in situ* by confocal fluorescence microscopy. *Anat. Embryol.* 200:117-121.
8. Gallicchio, MA, M Kneen, C Hall, AM Scott & LA Bach. 2001. Over-expression of insulin-like growth factor binding protein-6 inhibits rhabdomyosarcoma growth *in vivo*. *Int. J. Cancer*, 94: 645-51.
9. Wang, P-F, MJ McLeish, MM Kneen, G Lee & GL Kenyon. 2001. An unusually low pK_a for Cys282 in the active site of human muscle creatine kinase. *Biochemistry* 40: 11698-11705.
10. McLeish, MJ, MM Kneen, KN Gopalakrishna, CW Koo, PC Babbitt, JA Gerlt & GL Kenyon. 2003. Identification and characterization of a mandelamide hydrolase and an NAD(P) $^{+}$ -dependent benzaldehyde dehydrogenase from *Pseudomonas putida* ATCC 12633. *J. Bacteriol.* 185: 2451-6.
11. Siegert, P, M Pohl, MM Kneen, ID Pogozheva, GL Kenyon & MJ McLeish. 2003. Exploring the substrate specificity of benzoylformate decarboxylase, pyruvate decarboxylase and benzaldehyde lyase. in *Thiamin: Catalytic mechanisms and role in normal and disease states*, Marcel Dekker Inc., New York.
12. Gopalakrishna, KN, BH Stewart, MM Kneen, AD Andricopulo, GL Kenyon & MJ McLeish. 2004. Mandelamide hydrolase from *Pseudomonas putida*: Characterization of a new member of the amidase signature family. *Biochemistry* 43: 7725-35.
13. Siegert, P, MJ McLeish, M Baumann, H Iding, MM Kneen, GL Kenyon & M Pohl. 2005. Exchanging the substrate specificities of pyruvate decarboxylase from *Zymomonas mobilis* and benzoylformate decarboxylase from *Pseudomonas putida*. *Protein Eng. Des. Sel.* 18:345-357.
14. Kneen, MM, ID Pogozheva, GL Kenyon & MJ McLeish. 2005. Exploring the active site of benzaldehyde lyase by modeling and mutagenesis. *Biochim. Biophys. Acta.* 1753:263-271.

Publications (continued)

15. Janzen, E, M Muller, D Kolter-Jung, MM Kneen & MJ McLeish. 2006. Characterization of benzaldehyde lyase from *Pseudomonas fluorescens*: A versatile enzyme for asymmetric C-C-bond formation. *Bioorg. Chem.* 34:345-61.
 16. Chakraborty, S, N Nemeria, GS Brandt, MM Kneen, A Yep, MJ McLeish, GL Kenyon, G Petsko, D Ringe & F Jordan. 2009. Detection and time-course of formation of all thiamin diphosphate-bound covalent intermediates derived from a chromophoric substrate analogue on benzoylformate decarboxylase. *Biochemistry* 48:981-994.
 17. Brandt, GS, MM Kneen, S Chakraborty, AT Baykal, N Nemeria, A Yep, DI Ruby, G Petsko, GL Kenyon, MJ McLeish, F Jordan, & D Ringe. 2009. Snapshot of a reaction intermediate: analysis of benzoylformate decarboxylase in complex with a benzoylphosphonate inhibitor. *Biochemistry* 48:3247-3257.
 18. Brandt GS, MM Kneen, GA Petsko, D Ringe & MJ McLeish. 2010. Active-site engineering of benzaldehyde lyase shows that a point mutation can confer both new reactivity and susceptibility to mechanism-based inhibition. *J. Am. Chem. Soc.* 132:438-439.
 19. Kneen MM, R Stan, A Yep, RP Tyler, C Saehuan & MJ McLeish. 2010. Characterization of a phenylpyruvate decarboxylase from *Saccharomyces cerevisiae*. *FEBS J.* submitted for publication.
-

Invited Seminars

Fluorescence imaging studies of peptide hormone regulation of proximal tubular transport. Department of Physiology, The University of Melbourne, August 1994.

Hormonal regulation of fluid absorption in renal proximal tubule. Zentrum der Physiologie, Klinikum der Johann Wolfgang Goethe-Universität, Frankfurt, Germany, June 1995.

Hormonal regulation of proximal tubular reabsorption. Physiologisches Institut der Albert Ludwigs Universität, Freiburg, Germany, June 1995.

Green fluorescent protein and spatial filters; new methods of measuring intracellular pH and water permeability. Department of Physiology, The University of Melbourne, March 1998.

Green fluorescent protein as a non invasive intracellular pH indicator. Department of Medicine, Austin and Repatriation Medical Centre, April 1998.

Communications

1. Hall, JG, DJ Craik & MM Kneen. NMR studies of specific binding of thyroid hormones to plasma proteins. *RACI Division of Medicinal and Agricultural Chemistry 4th National Conference*, Lorne, Australia, 1985.
2. Kneen, MM, DJ Craik, JG Hall & WG Nayler. Phosphorus-31 NMR studies of myocardial ischaemia in the isolated rat heart. *RACI Division of Medicinal and Agricultural Chemistry 5th National Conference*, Adelaide, Australia, 1986.
3. Panagiotopoulos, S, WG Nayler, MM Kneen & DJ Craik. The effect of anipamil on calcium gain in the ischaemic rat heart. *10th International Congress of Pharmacology*, Sydney, Australia, 1987.
4. Hasin, Y, MM Kneen, DJ Craik & WG Nayler. ATP resynthesis in the reperfused rat heart. *6th Australian NMR Meeting*, Thredbo, Australia, 1988.
5. Craik, DJ & MM Kneen. 1989. Applications of NMR in pharmacy. *Chemistry in Australia*. 56:30-32.
6. Kneen, MM, WG Nayler & DJ Craik. Cytosolic calcium in the stunned heart. *International Society for Heart Research, Australian and New Zealand Section Meeting*, Melbourne, Australia, 1990.
7. Kneen, MM, WG Nayler & DJ Craik. Measurement of intracellular free calcium in perfused rat hearts using ^{19}F NMR spectroscopy. *7th Australian NMR Meeting*, Brisbane, Australia, 1990.
8. Kneen, MM, WG Nayler & DJ Craik. Cytosolic calcium in the perfused rat heart: A ^{19}F NMR study. *Australian Society for Medical Research, 29th National Scientific Conference*, Lorne, Australia, 1990.
9. Kneen, MM & PJ Harris. Fluorescence studies of peptide hormone binding and intracellular ionic composition. *Studies in Honour of Karl Julius Ullrich - An Australian Symposium*, Bowral, Australia, 1994.
10. Kneen, MM & PJ Harris. 1995. Fluorescence imaging studies of peptide hormone regulation of proximal tubular transport. *Proc. Aust. Physiol. Pharmacol. Soc.* 26:13P.
11. Kneen, MM & PJ Harris. 1996. Visualisation of angiotensin II binding in rat proximal tubules by fluorescence imaging. *Proc. Aust. Physiol. Pharmacol. Soc.* 28:54P.
12. Farinas, J, M Kneen, M Moore & AS Verkman. 1997. Plasma membrane water permeability of cultured cells and epithelia measured by light microscopy with spatial filtering, *J. Am. Soc. Nephrol.* 8:A0078.
13. Kneen, MM, JA Marinaro, & LA Bach. 1998. Intracellular localisation of human insulin-like growth factor binding protein 6 (IGFBP-6) using confocal microscopy. *Austin Research Week*, Austin & Repatriation Medical Centre, Heidelberg, Australia, 1998.
14. McLeish MJ, P-F Wang, MM Kneen MM & GL Kenyon. Cysteine 282 mutants of human cytosolic creatine kinases. *American Chemical Society Spring 2000 Meeting*, San Francisco, USA, 2000.
15. McLeish MJ, P-F Wang, MM Kneen MM & GL Kenyon. Mutagenesis of the reactive cysteine residue of human cytosolic creatine kinases. *American Society for Biochemistry and Molecular Biology*, Boston, USA, 2000.

Communications (continued)

16. Gallicchio MA, M Kneen & LA Bach. IGFBP-6 inhibits rhabdomyosarcoma proliferation *in vitro*. 4th International Workshop on IGFBPs, Terrigal, Australia, 2000.
17. McLeish MJ, P-F Wang, MM Kneen, G Lee & GL Kenyon. Mutagenesis of the "essential" cysteine of human muscle creatine kinase. 17th Enzyme Mechanisms Conference, Marco Island, USA, 2001.
18. McLeish, MJ, ID Pogosheva, MM Kneen, GL Kenyon, L Polovnikova & MS Hasson. Exploring the active site of benzaldehyde lyase: Modeling and mutagenesis, 4th European Symposium of the Protein Society, Paris, France, 2001.
19. McLeish MJ, ID Pogosheva, MM Kneen, GL Kenyon, L Polovnikova & MS Hasson. Exploring the active site of benzaldehyde lyase by modeling and mutagenesis. Gordon Conference on Enzymes, Coenzymes and Metabolic Pathways, Meriden, USA, 2001.
20. Gopalakrishna KN, B Hill Stewart, MJ McLeish, MM Kneen & GL Kenyon. Expression and characterization of a mandelamide hydrolase from *P. putida*. American Society for Biochemistry and Molecular Biology, New Orleans, USA, 2002.
21. McLeish, MJ, KN Gopalakrishna, MM Kneen, B Hill Stewart, AD Andricopulo & GL Kenyon. Mandelamide hydrolase; A new component of the mandelate pathway of *P. putida*. Gordon Conference on Enzymes, Coenzymes and Metabolic Pathways, Meriden, USA, 2002.
22. Kneen, MM, MJ McLeish & GL Kenyon. Identification of mandelate pathway regulatory elements in *Pseudomonas putida* ATCC 12633. Experimental Biology 2005, San Diego, USA, 2005.
23. Kenyon, GL, MM Kneen & MJ McLeish. Mandelate pathway regulation in *Pseudomonas putida* ATCC 12633. 30th FEBS Congress - 9th IUBMB Conference, Budapest, Hungary, 2005.
24. Chakraborty S, AT Baykal, N Nemeria, LZ Zhou, MM Kneen, GL Kenyon, MJ McLeish & F Jordan. Mechanism based inhibition of benzoylformate decarboxylase by methyl benzoylphosphonate. 230th ACS National Meeting, Washington, DC, USA, 2005.
25. Yep A, MM Kneen, GL Kenyon & MJ McLeish. Structural basis of substrate specificity in thiamin diphosphate-dependent decarboxylases. . Experimental Biology 2006, San Francisco, USA, 2006.

Competitive Grant Awards

Australian Research Council, *The roles of O-glycosylation of insulin-like growth factor binding protein-6*, Large Research Grant, ~A\$180,000, L Bach, M Kneen & G Neumann, 2000-2002.

National Health and Medical Research Council of Australia, *Mechanisms of peptide hormone action in renal proximal tubule*, Medical Research Project Grant, ~ A\$180,000, PJ Harris & MM Kneen, 1995-1997.

Teaching and Supervision

Laboratory Demonstrator (Teaching Assistant) in Chemistry for 1st year Pharmacy students and 3rd year Pharmacy students (NMR spectroscopy) at the Victorian College of Pharmacy. Supervision of Laboratory Assistants and Summer School Students in the School of Pharmaceutical Chemistry, Victorian College of Pharmacy.

Laboratory Demonstrator (Teaching Assistant) in renal Physiology for 3rd year Physiology students, supervision of 3rd year major student projects in Physiology, informal supervision of B.Sc. Honours and Ph.D. students in renal physiology, examination of B.Sc. Honours theses in Physiology, supervision of Australian Kidney Foundation Summer Scholars in the Department of Physiology, The University of Melbourne.

Supervision of American Heart Association Summer Internship student at UCSF.

Supervision of UROP and Pharm. D. Research Project students, at the College of Pharmacy, University of Michigan.

Supervision of students (undergraduate and graduate) as well as visiting fellows at IUPUI.

Referees

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EDUCATION

B.S. Degree, Arizona State University, 1965
Ph.D. Degree, University of Utah, 1969, under the direction of Professor Roland K. Robins

PROFESSIONAL EXPERIENCE

2009 - present	<u>Research Professor of Chemistry</u> , Indiana University Purdue University Indianapolis
2002 - 2009	<u>Distinguished Research Fellow</u> , Eli Lilly and Company, Indianapolis
1999 - 2001	<u>Research Advisor</u> , Eli Lilly and Company, Indianapolis
1994 - 1999	<u>Senior Director</u> , Medicinal Chemistry, Neurocrine Biosciences, San Diego
1990 - 1993	<u>Director</u> , Discovery Chemistry, Marion Merrell Dow, Inc., Cincinnati
1985 - 1990	<u>Associate Scientist and Group Leader</u> , Chemical Sciences, Merrell Dow Pharmaceuticals, Indianapolis and Cincinnati.
1980 - 1985	<u>Research Associate</u> , Medicinal Chemistry, Group Leader Cardiovascular Research, Merrell Dow Pharmaceuticals, Indianapolis
1981	<u>Visiting Scientist</u> , Medical University of South Carolina, Department of Pharmacology.
1979 - 1986	<u>Adjunct Associate Professor of Chemistry</u> , Indiana University Purdue University Indianapolis.
1976 - 1980	<u>Research Specialist II</u> , The Dow Chemical Company - Pharmaceutical Division, Midland and Indianapolis, Project Director for Antidepressant Chemistry Program.

1973 - 1976	<u>Research Specialist I</u> , The Dow Chemical Company - Pharmaceutical Division, Midland, Principal Investigator, National Cancer Institute Contract for Synthesis of Rifamycins.
1970 - 1973	<u>Research Chemist</u> , The Dow Chemical Company - Pharmaceutical Division, Midland and Indianapolis.
1968 - 1970	<u>Research Chemist</u> , Corporate Special Assignments, Dow Chemical Co.

PROFESSIONAL ORGANIZATIONS

- American Chemical Society, Divisions of Organic Chemistry, Medicinal Chemistry, and Fluorine Chemistry.

ACADEMIC AWARDS

- Ph.D. degree granted with distinction.
- NSF Undergraduate Summer Research Recipient, 1964.

RECENT COMMITTEES, CONFERENCES

- Chair, Symposium "Fluorine in Drug Design", American Chemical Society Meeting, Division of Medicinal Chemistry, Chicago, August 21, 1995.
- Member Long Range Planning Committee, Division of Medicinal Chemistry, American Chemical Society, 1994 - 1996.
- Chair, Medicinal Chemistry Gordon Conference 1998.
- Councilor, Division of Medicinal Chemistry, American Chemical Society, 1998 - 2000.
- Co-Chair, Symposium "Chemokine Antagonists as Anti-inflammatory and Antiviral Agents, American Chemical Society Meeting, San Francisco, March 30, 2000.
- Symposium Organizer "Growth Hormone Secretagogues", American Chemical Society Meeting, Division of Medicinal Chemistry, Chicago, August 22, 2001.
- Program Chair, The 29th National Medicinal Chemistry Symposium, University of Wisconsin – Madison, June 27 – July 1, 2004.
- Chair of the Long Range Planning Committee and Vice Chair of the Division of Medicinal Chemistry, American Chemical Society, 2006.
- Program Chair, Division of the Medicinal Chemistry, American Chemical Society, 2007-2008.
- Chair, Division of the Medicinal Chemistry, American Chemical Society, 2009.
- Past Chair, Division of the Medicinal Chemistry, American Chemical Society, 2010.

EDITORIAL BOARD

- Journal of Medicinal Chemistry, 2001 -2005

PUBLICATIONS

1. The Preparation of 2',3'-Dideoxyadenosine, 2',5'-Dideoxyadenosine and 2',3',5'-Trideoxyadenosine from 2'-Deoxyadenosine. Robins, M. J.; McCarthy, J. R.; Robins, R. K. *Biochemistry* **1966**, 5, 224-231.
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3. The Chemical Transformation of Uridine to an α -L-Lyxose Nucleoside *via* a 4'-Unsaturated Intermediate. Robins, M. L.; McCarthy, J. R.; Robins, R. K. *J. Heterocycl. Chem.* **1967**, 4, 313-314.
4. The Synthesis of Unsaturated Adenine Nucleosides Related to Angustmycin A. McCarthy, J. R.; Robins, M. J.; Robins, R. K. *Chem. Commun.* **1967**, 536-537.
5. The Role of the 5'-Hydroxyl Group of Adenosine in Determining Substrate Specificity for Adenosine Deaminase. Bloch, A.; Robins, M. J.; McCarthy, J. R. *J. Med. Chem.* **1967**, 10, 908-912.
6. The Synthesis of Angustmycin A (Decoyinine) and Related Unsaturated Nucleosides. McCarthy, J. R.; Robins, R. K.; Robins, M. J. *J. Am. Chem. Soc.* **1968**, 90, 4993-4999.
7. The Synthesis of Certain Unsaturated and Deoxynucleosides of Biological Interest. McCarthy, J. R. Ph.D. Thesis, University of Utah, 1969. *Diss. Abstr. B* **1969**, 29, 4595.
8. A 1,3-Bromine Migration. The Deamination of 3-Bromo-2,2-bis-(bromo-methyl)propylamine. Reineke, C. E.; McCarthy, J. R. *J. Am. Chem. Soc.* **1970**, 92, 6376-6378.
9. The Transformation of Formycin and Tubercidin into 2'- and 3'-Deoxynucleosides. Robins, M. J.; McCarthy, J. R.; Jones, R. A.; Mengel, R. *Can. J. Chem.* **1973**, 51, 1313-1321.
10. Preparation of Some Novel Rifamycins by a Facile Intramolecular Dehydration. Moore, J. L.; McCarthy, J. R. *Tetrahedron Lett.* **1976**, 4541-4544.
11. 3-N-Substituted Aminomethyl Derivatives of Rifamycin SV. McCarthy, J. R.; Moore, J. L.; Wysong, D. V.; Aldrich, C. D. *J. Med. Chem.* **1977**, 20, 1272-1276.
12. A Convenient New Method for Converting Aromatic Methyl Ethers to Phenols with Sodium Cyanide - Dimethyl Sulfoxide. McCarthy, J. R.; Moore, J. L.; Cregge, R. J. *Tetrahedron Lett.* **1978**, 5183-5186.
13. The Synthesis of ^{13}C -Labelled N,N'-Dimethyl-2-naphthalene-ethanimidamide Monohydrochloride, a Potential Psychotherapeutic Agent. Goralski, C. T.; McCarthy, J. R.; Linowski, J. W.; Nyguast, R. H.; Putzig, C. L. *J. Labelled Compd. Radiopharm.* **1981**, 18, 1047-1053.

14. Effects of a Pyridine Derivative Thromboxane Synthetase Inhibitor and its Inactive Isomer in Endotoxic Shock in the Rat. Anderegg, K.; Anzeveno, P.; Cook, J. A.; Halushka, P. V.; McCarthy, J. R.; Wagner, E.; Wise, W. C. *Br. J. Pharmacol.* **1983**, 78, 725-732.
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16. The Chloromethylation of 1-Bromo-2-Methoxynaphthalene. A Revised Structure for the Product. McCarthy, J. R.; Huffman, J. C. *J. Org. Chem.* **1984**, 49, 4995-4997.
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18. DAST in Organic Synthesis. II. The Transformation of Sulfoxides to α -Fluorothioethers, McCarthy, J. R.; Peet, N. P.; LeTourneau, M. E.; Inbasekaran, M. *J. Am. Chem. Soc.* **1985**, 107, 735-737.
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56. Stereospecific Method to (*E*)- and (*Z*)-Terminal Fluoroolefins and its Application to the Synthesis of 2'-deoxy-2'-fluoromethylenenucleosides as Inhibitors of Ribonucleoside Diphosphate Reductase. McCarthy, J. R.; Matthews, D. P.; Stermerick, D. M.; Huber, E. W.; Bey, P.; Lippert, B. J.; Snyder, R. D.; Sunkara, P. S. *J. Am. Chem. Soc.* **1991**, *113*, 7439-7440.
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52. Bueno Melendo, Ana Belen; Chen, Shu-Hui; Erickson, Jon Andrer; Gonzalez-Garcia, Maria Rosario; Guo, Deqi; Marcos Liorrente, Alicia; McCarthy, James Ray; Shepherd, Timothy Alan; Sheehan, Scott Martin; Yip, Yvonne Yee Mai. Preparation of amides as BACE inhibitors for treating Alzheimer's. 212 pp. WO2005108391.
53. Durham, Timothy Barrett; Hahn, Patric James; Kohn, Todd Jonantha; McCarthy, James Ray; Broughton, Howard Barff; Dally, Robert Dean; Gonzalez-Garcia, Maria Rosario; Henry, Kenneth James; Shepherd, Timothy Alan; Erickson, Jon Andre; Bueno Melendo, Ana Belen. Preparation of acylated 2-amino-1-(morpholino-3-yl)ethanols and derivatives as BACE inhibitors for treating Alzheimer's. 223 pp. WO 2006034093.
54. Bender, David Michael; McCarthy, James Ray. Cyclopropanecarboxylate esters of acyclovir. 14 pp. WO 2006127217.
55. US patent 7,176,224. Ardecky, Robert J.; Brooks, Dawn A.; Godfrey, Alexander G.; Jones, Sarah B. Mantlo, Nathan B.; McCarthy, James R.; Michellys, Pierre-Yves; Rito, Christopher J.; Tyhonas, John S.; Winneroski, Leonard L.; Xu, Yanping. Preparation of 3-[(oxazolylalkoxy)phenyl]-2-phenoxypropionic acid derivatives as PPAR agonists for treatment of diabetes mellitus and related conditions. February 13, 2007.
56. US patent 7,745,438 B2. Broughton, Howard B.; Dally, Robert D.; Durham, Timothy B.; Gonzalez-Garcia, Maria Rosario; Hahn, Patric J.; Henry, Jr., Kenneth J.; Kohn, Todd J.; McCarthy, James R.; Shepherd, Timothy A.; Erickson, Jon A.; Bueno Melendo, Ana Belen. 3-(2-Acylamino-1-hydroxyethyl)morpholine Derivatives and their use as BACE Inhibitors. June 29, 2010.

INVITED PRESENTATIONS AND ABSTRACTS

ACS National Meeting, Chicago, 1970. Abstract 101, Organic Division. A 1, 3-Bromine Migration in the Deamination of 3-Bromo-2,2-Bis(bromomethyl)propylamine.

University of Utah, Department of Medicinal Chemistry, 1975.

Medical University of South Carolina, Department of Pharmacology, 1980.

Medicinal Chemistry ACS Symposium, University of Arizona, 1984.

University of Chicago, Department of Chemistry, 1985.

ACS National Meeting, Miami Beach, 1985. Abstract 251, Organic Division. DAST in Organic Synthesis. The Transformation of Sulfoxides to α -Fluorothioethers.

ACS National Meeting, Anaheim, 1986. Abstract 60, Medicinal Chemistry Division. Poster Session: Novel Time-Dependent Inhibitors of Dopamine β -Hydroxylase.

Ohio State University, College of Pharmacy, March 8, 1988. New Approaches to the Synthesis of Antihypertensive Agents.

University of Iowa, Department of Chemistry, May 3, 1988. Novel Mechanism-Based Inhibitors of Dopamine β -Hydroxylase.

Medicinal Chemistry Gordon Conference, August 1, 1988. Novel Competitive Inhibitors of Dopamine β -Hydroxylase.

Heterocyclic Compounds Gordon Conference, July 14, 1989. Invited Lecture: New Approaches to the Synthesis of Vinyl Fluorides and Their Applications to Heterocyclic Compounds.

McCarthy, J.R.; Jarvi, E.T.; Mehdi, S. Medicinal Chemistry Gordon Conference, July 29, 1989. Poster Session: 4',5'-Unsaturated 5'-Halogenated Nucleosides: Mechanism-Based and Competitive Inhibitors of S-Adenosyl-L-Homocysteine Hydrolase.

University of Wisconsin, Department of Chemistry, October 12, 1989. New Methods for the Introduction of Fluorine into Organic Molecules and Their Application to the Design of Enzyme Inhibitors.

McCarthy, J.R.; Matthews, D.P.; Edwards, M.L.; Stermerick, D.M.; Jarvi, E.T. ISCHIA Advanced School of Organic and Bioorganic Chemistry, Ischia, Italy, September 25, 1990. Poster Session: Stereospecific Synthesis of Vinyl Fluorides and Application of the Method to the Synthesis of a New Class of Enzyme Inhibitors.

Medicinal Chemistry Gordon Conference, August 9, 1991. Invited Lecture: Stereospecific Method to (E) and (Z) Terminal Fluoro Olefins and its Application to the Synthesis of 2'-deoxy-2'-fluoromethylene Nucleosides as Inhibitors of Ribonucleoside Diphosphate Reductase.

Indiana University Purdue University at Indianapolis, Department of Chemistry, August 28, 1991. New Methods for the Synthesis of Fluoro Olefins.

University of Cincinnati, Department of Chemistry, February 28, 1992. Application of New Methods to the Synthesis of Monofluoro and Difluoro Olefins in the Design of Enzyme Inhibitors.

McCarthy, J.R.; Wolos, J.A. American Chemical Society National Meeting, Division of Organic Chemistry, Washington, D.C., August, 1992. Invited lecture, Abstract 371. The Design and Synthesis of Inhibitors of S-Adenosyl-L-Homocysteine Hydrolase.

Tenth International Roundtable: Nucleosides, Nucleotides and Their Biological Evaluation. September 17, 1992. New Methods for the Synthesis of Fluorinated Nucleosides and Their Biological Activity. Opening lecture of conference.

The Sixteenth Gulf Coast Chemistry Conference. September 16, 1993. New Methods for the Synthesis of Fluoro Olefins. Opening lecture of conference.

The University of California, Santa Barbara, Department of Chemistry, October 14, 1994. New Synthetic Methods to Fluoroolefins and Their Application in Drug Design.

McCarthy, J.R. American Chemical Society Twelfth Winter Fluorine Conference. St. Petersburg, Florida, January 23, 1995. Invited Lecture. Abstract 28. New Methods for the Synthesis of Fluoro Olefins.

McCarthy, J.R. American Chemical Society National Meeting, Division of Medicinal Chemistry, Chicago, Illinois, August 21, 1995. Abstract 111. Design, Synthesis and Antitumor Activity of MDL 101,731.

The University of Arizona, Department of Chemistry, January 23, 1997. Rapid Microscale Synthesis: A New Tool for the Medicinal Chemist.

McCarthy, J.R.; Xie, Y.F.; Erickson, P.E.; Webb, T.R.; Grigoriadis, D.E.; De Souza, E.B.; Whitten, J.P. American Chemical Society National Meeting, Division of Organic Chemistry, San Francisco, April 16, 1997. Invited lecture. Abstract 381. Rapid Microscale Synthesis: A New Tool for the Medicinal Chemist.

University of California, San Diego, Department of Chemistry, February 8, 1999. Application of New Synthetic Methods to Fluoroolefins for the Synthesis of a Phase II Clinical Candidate.

International Conference on Fluorine Chemistry '99 Tokyo, Yokohama, Japan. May 10, 1999. New Methods for the Synthesis of Fluoro Olefins. Invited lecture.

McCarthy, J.R. American Chemical Society National Meeting, Division of Fluorine Chemistry, San Francisco, March 26, 2000. Invited tutorial. Abstract 11. Fluorine in Drug Discovery: Utility of Fluorine in Biologically Active Molecules.

McCarthy, J.R. American Association of Pharmaceutical Scientists Annual Meeting, Indianapolis, Monday, October 30, 2000. Invited lecture. The Design and Synthesis of Corticotropin Releasing Factor (CRF) Receptor Antagonists for Clinical Development

Indiana University Purdue University at Indianapolis, Department of Chemistry, March 23, 2001. Some Lessons in Drug Discovery from the Element Fluorine.

University of Minnesota, Department of Medicinal Chemistry, April 17, 2001. Application of New Synthetic Methods to Fluoroolefins for the Design of a Ribonucleotide Reductase Inhibitor in Phase II Clinical Trials

American Chemical Society National Meeting, Division of Medicinal Chemistry, San Diego, April 2, 2001. PPAR α,γ Co-agonists for the Treatment of Type 2 Diabetes and Cardiovascular Risk Factors". Invited lecture that was presented by Dawn Brooks.

National Organic Symposium, Bloomington, Indiana, June 10, 2003. Fundamentals of Drug Discovery: Strategies and Tactics in Medicinal Chemistry. Part II. Invited minicourse taught with Paul Ornstein.

International Proteolysis Society, Nagoya, Japan. November 13, 2003. Design and SAR of BACE Inhibitors. Invited lecture.

McCarthy, J.R. 230th American Chemical Society National Meeting, Division of Medicinal Chemistry, Washington DC, August 30, 2005. Invited lecture. Abstract 241. The Design and Synthesis of BACE Inhibitors: The Importance of Conformation for Optimizing Potency.

McCarthy, J.R. Frontiers in Drug Discovery Symposium, Albany Molecular, October 7, 2005. The Design and Synthesis of BACE Inhibitors: The Importance of Conformation for Optimizing Potency.

McCarthy, J.R. International Conference on Alzheimer's Disease (ICAD) 2006, Madrid, Spain, July 16, 2006. The Design and Synthesis of an Efficacious BACE Inhibitor.

Medicinal Chemistry Gordon Conference, August 8, 2006. Invited Lecture: Alzheimer's Disease: A Critical Unmet Medical Need.

McCarthy, J.R. Professor Morris J. Robins Symposium, Brigham Young University, April 28, 2007, Peptides to small organic molecules: The design and synthesis of efficacious BACE1 inhibitors.

McCarthy, J.R. Department of Pharmaceutical Sciences, Wayne State University, October 10, 2007, Peptides to small organic molecules: The design and synthesis of efficacious BACE1 inhibitors.

McCarthy, J.R. Methods and Principles in Medicinal Chemistry. Joint Workshop of the Medicinal Chemistry Division Brazilian Chemical Society and American Chemical Society, May 26, 2008. 31st Brazilian Chemical Society Meeting, Águas de São Pedro – SP, Brazil. Fluorine in Drug Design

McCarthy, J.R. May 26 - 28, 2008. 31st Brazilian Chemical Society Meeting, Águas de São Pedro – SP, Brazil. Fundamentals of Drug Discovery Part 1 & Part 2 Minicourse.

McCarthy, J.R. ISCMC Conference, Shanghai, China, July 28-July 31, 2008, Co-sponsored by the Medicinal Chemistry Division, American Chemical Society. Strategies and Issues in the Design of Nucleoside Prodrugs.

McCarthy, J.R. ISCMC Conference, KaoHsiung, Taiwan, February 1-5, 2010, Co-sponsored by the Medicinal Chemistry Division, American Chemical Society. Important events in the evolution of the pharmaceutical industry and drug design.

McCarthy, J.R. 239th American Chemical Society National Meeting, Division of Medicinal Chemistry, San Francisco, March 24, 2010. . Strategies and Issues in the Design of Nucleoside Prodrugs. Invited lecture at the prodrug symposium.

MASTER OF SCIENCE THESIS CO-DIRECTION

"Preparation of β -Fluorinated- α -Amino Acids by Alkylation and Subsequent Deprotection of a Glycine Synthon" by Charlotte L. Barney (co-research advisor with Professor. Martin J. O'Donnell), 1984.

"Stereospecific Synthesis of Chiral α -Methyl- α -Amino Acids" by Jonathan Green (co-research advisor with Professor Martin J. O'Donnell), 2008.

TEACHING RESPONSIBILITIES

Organic Chemistry Lab, Spring 1979, Fall 1979
Graduate Organic Synthesis, Spring 1979
Organic Chemistry, Summer 1979, Summer 1980, Summer 1981
Graduate Medicinal Chemistry, Spring 1983, Spring 1985
Undergraduate Medicinal Chemistry, Spring 2010

REFeree ARTICLES ON A REGULAR BASIS

Journal of Medicinal Chemistry
Journal of Organic Chemistry
Organic Letters

CLINICAL CANDIDATES

1. Napactadine, an antidepressant which demonstrated efficacy in man.

A New Bicyclic Antidepressant Agent. Synthesis and Activity of Napactadine and Related Compounds. McCarthy, J. R.; Wright, D. L.; Schuster, A. J.; Abdullah, A. J.; Shea, P. J.; Eyster, R. *J. Med. Chem.* **1985**, 28, 1721-1727.

J.R. McCarthy, U.S. Patent 3,903,163.

2. Tipentosin, an antihypertensive agent designed as an α_1 blocker and DA₁ agonist which demonstrated antihypertensive activity in man.

6,7-Dihydro-5-(((cis-2-hydroxy-trans-3-phenoxy-cyclopentyl)amino)methyl)-2-methylbenzo[b]thiophen-4(5H)-one, a Novel Alpha-1 Adrenergic Receptor Antagonist and Renal Vasodilator. McCarthy, J. R.; Zimmerman, M. B.; Trepanier, D. L.; LeTourneau, M.

E.; Wiedeman, P. E.; Whitten, J. P.; Broersma, R. J.; Shea, P. J. *J. Med. Chem.* **1985**, *28*, 1142-1145.

M.E. LeTourneau, J.R. McCarthy, D.L. Trepanier, U.S. Patent 4,868,315.

Clinical investigator, J.D. Wallin, M.D., Protocol No. 19,744A-2-I-2.

3. MDL 43,925, a dopamine β -hydroxylase inhibitor approved as a clinical candidate.

1-(Thienylethyl)imidazol-2(3H)-thiones As Potent Competitive Inhibitors of Dopamine β -Hydroxylase. McCarthy, J. R.; Matthews, D. P.; Broersma, R. J.; McDermott, R. D.; Kasther, P. R.; Hornsperger, J. M.; Demeter, D. A.; Weintraub, H. J. R.; Whitten, J. P. *J. Med. Chem.* **1990**, *33*, 1866-1873.

D.P. Matthews, J.R. McCarthy, J.P. Whitten, R.J. Broersma, U.S. Patent 5,057,613.

4. Tezacitabine, a mechanism-based inhibitor of ribonucleotide reductase with broad spectrum antitumor activity currently in Phase II clinical trials.

Stereospecific Method to (*E*)- and (*Z*)-Terminal Fluoroolefins and its Application to the Synthesis of 2'-deoxy-2'-fluoromethylenenucleosides as Inhibitors of Ribonucleoside Diphosphate Reductase. McCarthy, J. R.; Matthews, D. P.; Stemerick, D. M.; Huber, E. W.; Bey, P.; Lippert, B. J.; Snyder, R. D.; Sunkara, P. S. *J. Am. Chem. Soc.* **1991**, *113*, 7439-7440.

U.S. Patent 5,378,693. J.R. McCarthy, M.L. Edwards, D.P. Mathews. 2'-Halomethylene Cytidine, Uridine and Guanosine Compounds and Their Pharmaceutical Compositions. Jan. 3, 1995.

5. MDL 28,842, a mechanism-based inhibitor of S-adenosyl-L-homocysteine hydrolase with immunosuppressant activity. Demonstrated potent antiarthritic activity and prevention of transplant rejection in animal models.

4',5'-Unsaturated-5-Fluoro Adenosine Nucleosides: Potent Mechanism-Based Inhibitors of S-Adenosyl-L-homocysteine Hydrolase and Anti-Retroviral Agents. McCarthy, J. R.; Jarvi, E. T.; Matthews, D. P.; Edwards, M. L.; Prakash, N. J.; Bowlin, T. L.; Mehdi, S.; Sunkara, P. S.; Bey, P. *J. Am. Chem. Soc.* **1989**, *111*, 1127-1128.

E.T. Jarvi, J.R. McCarthy, N.J. Prakash, U.S. Patent 4,997,925.

6. NBI 30755, a potent and selective corticotropin-releasing factor₁ receptor antagonist that demonstrated efficacy in Phase II clinical trials for the treatment of anxiety and depression. E. Chen, Chen; Wilcoxon, Keith M.; Huang, Charles Q.; Haddach, Mustapha; McCarthy, James R. Preparation of Pyrazolo[4.3-b]pyrimidines as corticotrophin releasing factor antagonists. 41 pp. WO 9945007 A1.
7. NBI 34041, a tricyclic CRF receptor antagonist that is more potent than NBI 30755 and lacks some of the potential side effects of NBI 30755.

Haddach, Mustapha; Nelson, Jodie; Dyck, Brian P.; Guo, Zhiqiang; Huang, Charles Q.; McCarthy, James R. Preparation of tricyclic compounds as CRF receptor antagonists. 123 pp. WO 0027846 A2.

8. LY 510929, designed and synthesized as a PPAR α/γ dual agonist. One of the most potent dual agonists reported. First human dose in 2001. Targeted for type 2 diabetics with syndrome X.

US patent 6,930,120. Brooks, Dawn A.; Godfrey, Alexander, G. Jones, Sarah B.; McCarthy, James R.; Rito, Christopher J.; Winneroski, Leonard, L.; Xu, Yanping. Oxazolyl-Arylpropionic acid derivatives and their use as PPAR agonists. August 16, 2005.

The Design and Synthesis of 2-Methyl-2-{4-[2-(5-methyl-2-aryloxazol-4-yl)ethoxy]phenoxy}propionic acids: A New Class of Dual PPAR α/γ Agonists. Brooks, D. A.; Etgen, G. J.; Rito, C. J.; Shuker, A. J.; Dominianni, S. J.; Warshawsky, A. M.; Ardecky, R.; Paterniti, J. R.; Tyhonas, J.; Montrose-Rafizadeh, C.; Winneroski, L. L.; Faul, M. M.; McCarthy, J. R. *J. Med. Chem.* **2001**, *44*, 2061-2064.

Conversion of Human-Selective PPAR α Agonists to Human/Mouse Dual Agonists: A Molecular Modeling Analysis. M. Wang, L. L. Winneroski, R. J. Ardecky, R. E. Babine, D. A. Brooks, G. J. Etgen, D. R. Hutchison, R. F. Kauffman, A. Kunkel, D. E. Mais, C. Montrose-Rafizadeh, K. M. Ogilvie, B. A. Oldham, M. K. Peters, C. J. Rito, D. K. Rungta, A. E. Tripp, S. B. Wilson, Y. Xu, R. W. Zink, J. R. McCarthy. *Bioorg. Med. Chem. Lett.*, **2004**, *14*, 6113-6116.

9. Prodrug currently in clinical trials. Selected as one of top seven most promising clinical entities by Lilly for the next decade.

McCarthy, J.R. ISCMC Conference, Shanghai, China, July 28-July 31, 2008
Co-sponsored by the Medicinal Chemistry Division, American Chemical Society.
Strategies and Issues in the Design of Nucleoside Prodrugs.

Synthesis, Crystallization, and Biological Evaluation of an Orally Active Prodrug of Gemcitabine. Bender, D. M.; Bao, J.; Dantzig, A. H.; Diserod, W. D.; Law, K. L.; Magnus, N. A.; Peterson, J. A.; Perkins, E. J.; Pu, Y. J.; Reutzel-Edens, S. M.; Remick, D. M.; Starling, J. J.; Stephenson, G. A.; Vaid, R. K.; Zhang, D.; McCarthy, J. R. *J. Med. Chem.* **2009**, *52*, 6958-6961.

William L. Scott
Research Professor, Department of Chemistry & Chemical Biology
Indiana University Purdue University Indianapolis, Indianapolis, IN 46202

Education

Williams College	B.A., 1967
UCLA	Ph.D., 1972
Rockefeller University	NIH Postdoctoral Fellow, 1972-74
Caltech	NIH Postdoctoral Fellow, 1974

Appointments

Research Professor, IUPUI, Dept. Chemistry and Chem. Biology	2002-present
Research Scientist, Eli Lilly and Co.	1980-2001
Senior Scientist, Eli Lilly and Co.	1974-1979
Chemistry Lecturer, IUPUI Department of Chemistry	1993-2001
Adjunct Professor of Chemistry, Butler University	1978-2001

Selected Publications

1. Scott, W. L.; Zhou, Z.; Martynow, J. G.; O'Donnell, M. J. Solid-Phase Synthesis of Amino- and Carboxyl-Functionalized Unnatural α -Amino Acid Amides. *Org Lett.*, **2009**, *11*, 3558-3561.
2. Scott, W. L.; O'Donnell, M. J. Distributed Drug Discovery, Part 1: Linking Academics and Combinatorial Chemistry to Find Drugs for Developing World Diseases. *J. Comb. Chem.* **2009**, *11*, 3-13.
3. Scott, W. L.; Alsina, J.; Audu, C. O.; Dage, J. L.; Babaev, E.; Cook, L.; Goodwin, L. A.; Martynow, J. G.; Matosiuk, D.; Royo, M.; Smith, J. G.; Strong, A. T.; Wickizer, K.; Woerly, E. M.; Zhou, Z.; O'Donnell, M. J. Distributed Drug Discovery, Part 2: Global Rehearsal of Alkylating Agents for the Synthesis of Resin-Bound Unnatural Amino Acids and Virtual D³ Catalog Construction. *J. Comb. Chem.* **2009**, *11*, 14-33.
4. Scott, W. L.; Audu, C. O.; Dage, J. L.; Goodwin, L. A.; Martynow, J. G.; Platt, L. K.; Smith, J. G.; Strong, A. T.; Wickizer, K.; Woerly, E. M.; O'Donnell, M. J. Distributed Drug Discovery, Part 3: Using D³ Methodology to Synthesize Analogs of an Anti-Melanoma Compound. *J. Comb. Chem.* **2009**, *11*, 34-43.
5. Scott WL, Martynow JG, Huffman JC, O'Donnell MJ. "The solid-phase synthesis of multiple classes of peptidomimetics from versatile resin-bound aldehyde intermediates". *J Am Chem Soc* **2007**; *129*: 7077-88.
6. O'Donnell MJ, Alsina J., Scott WL. Solid-phase synthesis and utilization of side-chain reactive unnatural amino acids. *Tetrahedron Lett* **2003**; *44*:8403-6.
7. Scott WL, Alsina J, O'Donnell MJ. The manual and solid-phase synthesis of α -substituted prolines and homologues. *J Comb Chem* **2003**; *5*:684-2.
8. Scott WL, O'Donnell MJ, Alsina J. A solid-phase synthetic route to unnatural amino acids with diverse side chain substitutions. *J Org Chem* **2002**; *67*:2960-9.
9. Scott WL, Zhou C, Fang Z, O'Donnell MJ. The solid phase synthesis of α,α -disubstituted unnatural amino acids and peptides (di-UPS), *Tetrahedron Lett.* **1997**; *38*:3695-8.

10. O'Donnell MJ, Zhou C, Scott, WL. Solid-phase unnatural peptide synthesis (UPS). *J Am Chem Soc* **1996**;118:6070-1 (see Chemical & Engineering News, July 8, 1996, page 32 for a press release).

Synergistic Activities

1. Developed a concept termed "Distributed Drug Discovery" that enables chemistry students across the world (IUPUI, Barcelona, Moscow and Lublin, Poland) to learn basic skills in organic synthesis while making new molecules as potential drug leads for neglected diseases. Has given multiple seminars and workshops, nationally and internationally, on solid-phase combinatorial chemistry and how it relates to this project.
2. Invented and arranged manufacture of simple, inexpensive equipment to allow students to carry out synthetic component of Distributed Drug Discovery. Provided equipment for student labs at IUPUI, and collaborators in Barcelona, Moscow, Lublin and Krakow.
3. Developed on-going partnership with Eli Lilly and Company to obtain high volume access to LC/MS analysis of molecules synthesized by students in undergrad labs.
4. Dr. Scott teaches two graduate courses: a) Solid-Phase Synthesis and Combinatorial Chemistry and, b) Drug Discovery and Action.
5. He chaired an NIH Study Section reviewing proposals for NIGMS Pilot Libraries, June 2005.

He is a co-PI with Professor Martin J. O'Donnell on RO1 GM28193-12 2/1/04-1/31/08 NIH-NIGMS. Schiff Base Synthons in Amino Acid Chemistry. "Various Schiff base derivatives of α -amino acids and peptides will be used as starting materials for the preparation of unnatural amino acids and peptides by both solution- and solid-phase chemistry."

National and International Collaborators

- (1) Prof. Fernando Albericia, University of Barcelona, Barcelona, Spain
- (2) Prof. Evgenii Babaev, Moscow State University, Moscow, Russia
- (3) Prof. Dariusz Matosiuk, Department of Synthesis and Chemical Technology of Pharmaceutical Substances Faculty of Pharmacy, Medical University Lublin, Poland
- (4) Prof. Martin J. O'Donnell, Department of Chemistry and Chemical Biology, IUPUI
- (5) Prof. Pawel Zajdel and Maciej Pawlowski, Jagiellonian University, Krakow, Poland
- (6) Prof. Jerremey Willis, Department of Chemistry, Morehouse College, Atlanta
- (7) Prof. Kathy Stickney, University of Indianapolis, Indianapolis, Indiana

Graduate Advisor

Professor David A. Evans, Harvard University

Postdoctoral Advisees in Last Five Years

Dr. Ziniu Zho (2006-present)

Dr. Jacek Martynow (2005-2006) (Now at Rib-X Pharmaceuticals, Inc)

CURRICULUM VITAE

MILLIE M. GEORGIADIS, PH. D.

**DEPARTMENT OF BIOCHEMISTRY AND MOLECULAR BIOLOGY
INDIANA UNIVERSITY SCHOOL OF MEDICINE**

EDUCATION:

1984 B.S. Biochemistry with honors, Indiana University, Bloomington, IN
1990 Ph.D. Biochemistry, University of California, Los Angeles
1990-1993 NIH Postdoctoral Fellow, Columbia University, New York, NY

ACADEMIC APPOINTMENTS:

1994-2002 Assistant Professor, Waksman Institute and Department of Chemistry
 Rutgers, The State University of New Jersey, Piscataway, NJ
2002-present Associate Professor with tenure, Department of Biochemistry and
 Molecular Biology, Indiana University School of Medicine, Indianapolis,
 IN
2004- present Secondary Faculty appointment, Department of Chemistry and Chemical
 Biology, Indiana University Purdue University at Indianapolis,
 Indianapolis, IN

HOSPITAL APPOINTMENTS:

Not applicable

OTHER APPOINTMENTS AND PROFESSIONAL CONSULTANTSHIPS:

2002- present Member, Center for Structural Biology
2002- present Member, IU Simon Cancer Center
2002-2004 Adjunct Faculty Appointment, Center for Computational Biology and
 Bioinformatics
2002- present Member, Graduate Program, Department of Biochemistry and Molecular
 Biology
2005-present Medical Sciences Training Program, Mentor

PROFESSIONAL AFFILIATIONS:

1990-present Member American Crystallographic Association

HONORS AND AWARDS:

1980-1984 National Merit Scholarship, Indiana University
1982 Norton Mavor Latin Award, Indiana University
1982 Phi Beta Kappa, Indiana University
1984 American Chemical Society Senior Award, Indiana University
1990-1993 NIH National Research Service Award (postdoctoral research fellowship)
1995 Sidhu Award for contributions to the field of diffraction
2001 Margaret Oakley Dayhoff Award from the Biophysical Society

2007 Trustee Teaching Award, Indiana University
 "In recognition of teaching excellence in medical education"

Graduate Students:

Dona Ho (PhD- 2002)
 Debanu Das (PhD-2003)

Current Position

Postdoctoral Fellow, Hongkong
 Senior Scientist, Joint Center for Structural Genomics

Sherwin Montano (PhD- 2003)

Postdoctoral Fellow, U Chicago

Robert Crowther (PhD- 2004)

Senior Scientist, Roche Pharmaceutical

LaTeca Glass (MS- 2009)

Scientist, Abbott Laboratories

Sarah Delaplane (MS to be completed)

Postdoctoral Fellows:

Kristie Goodwin (2003-2008)

Current Position

Laboratory Specialist (U Louisville)

Sherwin Montano (2004-2005)

Postdoctoral Fellow (U Chicago)

Rajneesh Gaur (2004-2005)

Consultant business, India

Hongzhen He (2008- present)

Undergraduates Researchers:

Andrew Martin (2006- Biochemistry major IUPUI)

Summer Researchers:

Undergraduates:

Jordan Swenson (2004- Undergraduate Washington University in St. Louis)

Taryn Quattrochi (2005- High School senior, Warren Central High School)

Suraj Adhikary (2006- Undergraduate Hanover College)

High School Teachers:

Linda Monroe, Chemistry Teacher Warren Central High School (Summer 2004, 2005)

Student Dissertation Committees:

<i>Student</i>	<i>Department</i>	<i>Degree Status</i>	
Yaritsabel Roman	Biochemistry & Molecular Biology, 07	MS	Completed
Aditi Bapat	Biochemistry & Molecular Biology, 09	PhD	Completed
Sara Bennett	Biochemistry & Molecular Biology, 10	MS	Completed
LaTeca Glass	Chemistry & Chemical Biology, 09	MS	Completed
Sulochanadevi Baskaran	Biochemistry & Molecular Biology	PhD	In progress
Linden Green	Microbiology & Immunology	PhD	In progress
Bibek Parajuli	Biochemistry & Molecular Biology	PhD	In progress
David Onyango	Pharmacology & Toxicology	PhD	In progress

Faculty Mentoring:

2006- present

Chair, Mentoring Committee for Samy Meroueh, Assistant Professor, Department of Biochemistry and Molecular Biology

2006-present

Member, Mentoring Committee for Karen Polluck, Assistant Professor in Pediatrics

SERVICE ACTIVITIES:

UNIVERSITY COMMITTEE SERVICE:

University Service

- | | |
|--------------|--|
| 2002-2004 | Member, Protein Expression Core Facility Advisory Committee |
| 2002-2004 | Member of the Faculty Search Committee for Computational Biology and Bioinformatics |
| 2005- 2006 | Member of the Faculty Search Committee for Computational Biology and Bioinformatics |
| 2004-2005 | Co-director of the Protein Expression Core Facility |
| 2006-present | Oversight Committee for the Chemical Genomics Core Facility |
| 2006-2007 | Member, Internal review committee for American Cancer Society Institutional Grant Awards, IUSM |
| 2006-present | Member, Faculty Mentoring Committee for Karen Pollock, Assistant Professor in Pediatrics and Wells Center |
| 2006-present | IBMG Admissions Committee for the combined graduate program at IU School of Medicine |
| 2007 | Member, Mary Kay Ash Proposal, Pre-review committee |
| 2007-2008 | Participant - Faculty Development Program, Leading Change in Academic Medicine |
| 2009-2010 | Member of the Faculty Search Committee for Computational Chemistry in the Department of Chemistry and Chemical Biology |

Departmental Service

- | | |
|---------------|--|
| 2002-2004 | Member of the Graduate Admissions Committee for Department of Biochemistry and Molecular Biology |
| 2004-2005 | Member of the Faculty Search Committee for Structural and Chemical Biology in the Department of Biochemistry and Molecular Biology |
| 2006-present | Director of Admissions – represent the department in the combined graduate program |
| 2006- present | Chair, Faculty Mentoring Committee for Samy Meroueh, Assistant Professor, Department of Biochemistry and Molecular Biology |
| 2007-2008 | Chair, Faculty Search Committee for Chemical and Structural Biology in the Department of Biochemistry and Molecular Biology |
| 2007-2008 | Member, Biochemistry Graduate Oversight Committee in the Department of Biochemistry and Molecular Biology |

- 2008-2009 Member, Faculty Search Committee for Structural Biology in the Department of Biochemistry and Molecular Biology
- 2009-2010 Member, Faculty Search Committee in the Department of Biochemistry and Molecular Biology

SERVICE TO THE PROFESSIONAL DISCIPLINE:

- 2003 Ad hoc member of NIH ZRG1 SSS-B, Special Biophysics and Chemistry Study Section, July 14, 2003.
- 2003 Ad hoc member of NIH ZRG1 F0420 Biochemical, Biophysical, and Chemical Science Fellowship Study Section Panel, Nov. 13-14, 2003.
- 2004 Consultant for Semafore Pharmaceuticals
- 2003-2004 Co-organizer of the Biological Division of the American Chemical Society Regional Meeting (CERMACS), July 2-4, 2004.
- 2004 Ad hoc member of NIH VR Study Section, Feb. 24-25, 2004.
- 2004-2008 Member of the NIH VIRA Study Section
- 2007-2009 Molecular Medicine in Action sponsored by IUSM/Wells Center. This is a program for high school students and teachers to introduce state-of-the-art biological research methods. I served as an instructor for the "Visualization of Macromolecules" module for which I developed a computer graphics exercise to allow students to understand the fundamentals of protein structure.
- 2009 Driving Biological Project, Site visit for NIH/NCRR Mass Spectrometry Resource at Washington University, July 23-25, 2009.
- 2009 Ad hoc grant reviewer for NSF
- 2010 Ad hoc grant reviewer for NSF
- 2010 Ad hoc member of an NIH ZRG1 Special Emphasis Panel Study Section, April 1-2, 2010.

PEER REVIEW:

Peer Reviewer for Journal articles submitted to the Journal of Biological Chemistry, Biochemistry, Structure, Journal of the American Chemical Society, Journal of Virology, Virology, Virus, Nucleic Acids Research, and Chemistry and Biology.

Invited Presentations:

2003

"Structural and energetic studies on nucleic acid interactions with Moloney murine leukemia virus reverse transcriptase." Invited seminar, Department of Biological Sciences, Purdue University, LaFayette, IN, March 25, 2003.

2004

“Structural and energetic studies on nucleic acid interactions with Moloney murine leukemia virus reverse transcriptase.” Invited seminar, Department of Chemistry, Indiana University, Bloomington, Indiana, IN, October 15, 2004.

“Structural and energetic studies on nucleic acid interactions with Moloney murine leukemia virus reverse transcriptase.” Invited seminar, Department of Chemistry, Loyola University, Chicago, February 26, 2004,

“A novel host-guest approach to nucleic acid structures: Application to drug-DNA interactions” Department of Chemistry seminar series, Oct. 27, 2004.

2005

“A high-throughput high-resolution pathway to the discovery of specific DNA-drug interactions” Department of Biochemistry and Molecular Biology seminar series, Sept. 12, 2005.

2006

“Structural studies of Ape1 and MMLV RT as a basis for mapping interactions by HDX mass spectrometry” University of Alabama at Birmingham, Biophysical Floor Meeting, March 12, 2006.

2007

“Unfolding Ape1’s redox activity” Center for Computational Biology and Bioinformatics seminar series, March 23, 2007.

“Unfolding Ape1’s redox activity” Department of Microbiology and Immunology seminar series, Feb. 2007.

2008

“From DNA damage induced by bleomycin to Ape1, the enzyme that repairs it: A structural perspective.” Invited seminar, Department of Chemistry, Washington University in St. Louis, St. Louis, MO, October 1, 2008.

“Crystal structures of DNA-bound Co(III)-bleomycins” Invited talk, International Union of Crystallography Meeting, Osaka, Japan, August, 2008.

2009

“Evolution of novel functions in DNA repair proteins.” Invited seminar, Department of Biochemistry and Molecular Biology, Oregon Health&Science University, January 13, 2009.

“The ancient mariner Hsmar1 in humans: From transposition to DNA repair.” Invited seminar, Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, IL, November 18, 2009.

2010

“Crystal structure of an active *Hsmar1* transposase in humans that has evolved into a novel DNA repair protein” Invited presentation, *Annual American Crystallographic Association Meeting*, Chicago, IL, July 24-29, 2010.

VII. GRANTS/FELLOWSHIPS:

Internal Grant Awards:

IUCC Pilot Grant “APE1/ref-1 DNA repair/redox enzyme as a target for cancer therapeutics: Structure-function studies of E3330-APE1 interactions”

Funding period: 3/1/2004-2/28/2005

Award: \$30,000

Role: Co-PI

IUPUI NIH Roadmaps Initiative “Development of a high-throughput, high-resolution new pathway to the discovery of specific drug-DNA interactions” (Long, E. Co-PI)

Funding period: 7/1/2005-6/30/2006

Award: \$60,000

Role: Co-PI.

Collaborative Biomedical Research Grant IUCC/Purdue CC “Structure/function studies on interactions of Ape1/ref-1 DNA repair/redox enzyme with c-Jun and E3330 analogues: Development of novel therapeutics”

Funding period: 12/1/2004-11/30/2005

Award: \$50,000

Role: PI

IUCC EDT ITRAC Grant “Identification of novel APE1 repair inhibitors through HTS and structure-based design” (Kelley, MR- CoPI)

Funding period: 12/1/2006- 11/30/2007

Award: \$20,000

Role: Co-PI

IUCC EDT ITRAC Grant “Identification of novel APE1 repair inhibitors through HTS and structure-based design”

Funding period: 8/10/2007-present

Award: \$42,800

Role: Co-PI

CTSI TRAC1 grant “Exploring inhibition of AP endonuclease activity in *Toxoplasma gondii* in the development of new anti-parasitic agents”

Funding period: 12/1/2008- present

Award: \$25,000 (\$15,400 to Georgiadis/
\$9,600 Chemical Genomics Core Facility)

Role: PI

External Grant Awards:

Completed research awards:

NIH R01 GM055026 “Structural studies of protein-nucleic acid interactions”

Funding period: 2/1/1997-1/31/2006 (no cost extension – 1/31/2007)

Total costs: \$282,000/ year

Role: Principal investigator

NIH R21 AI073091-A1 “APEs as novel drug targets in AIDS opportunist *Toxoplasma*”
(Sullivan, P.I.)

Direct costs: \$125,000 /yr

Funding period: 07/01/07 – 06/30/09

The major goal of this project to treat opportunistic infection of AIDS patients.

Role : Co-Investigator

ACS Postdoctoral Fellowship PF-06-008-01-CDD “Crystallographic studies of the bleomycin-DNA complex” (Goodwin, K.D.)

Funding period: 01/01/2006-12/31/2008

The proposed studies will use a novel host-guest crystallographic method in order to obtain a detailed atomic resolution structure of bleomycin-DNA complexes.

Role: Mentor

Current funding:

NIH R01 CA114571 “Mechanism of redox regulation by Ape1/Ref-1”

Funding Period: 07/01/06 – 05/31/11

Direct costs: \$155,117/year direct costs

The goal of this project is to determine the mechanism of the redox regulation by Ape1 of a number of transcriptional activators including AP-1 and HIF-1 α . An integrated approach to detailing this mechanism includes structural, biophysical, biochemical, cellular, and animal studies.

Role: Principal investigator (3.6 calendar)

NIH R01 CA135380-01A1 “Small-molecule inhibition of the interactions of the urokinase receptor: A target in tumor invasion and metastasis” (Meroueh, S. – PI)

Funding Period: 05/15/09 – 02/28/13

Direct costs: \$166,000/ year

The goal of this project is to optimize the pharmacokinetic properties and potency of three of these compounds to block tumor invasion and metastasis in vivo.

Role: Co-Investigator (0.36 calendar)

NIHT-32 GM077229-01A1 “Indiana Medical Scientist/Engineer Training Program” (Clapp, W. – PI)

Funding Period: 07/01/08 – 06/30/13

Train engaging physician-scientist who are poised to pursue careers as clinical investigators in hypothesis-driven, investigator-initiated research.

Role : Trainer

Corporate Contract with Microbiotix, Inc. “Surface Plasmon Resonance Analyses/DNA Crystallization Analyses” (Long, E.- PI)

Funding period: 02/01/10 – 01/31/11

Total costs: \$24,581

Role: Co-Investigator (no salary support)

VIII. RESEARCH ACTIVITIES:

BIBLIOGRAPHY

A. Peer-Reviewed Manuscripts (42 total, 22 in rank)

* denotes work completed in rank.

- 1) Jenkins, W. T., **Marshall, M. M.**, and Lewin, A. S. (1984) A Chemical Mechanism for the Biosynthesis of ATP Involving Ion-Exchange Reactions. *Arch. Biochem. Biophys.* **232**, 496-504. (Note: Maiden name of Georgiadis, M. M. is Marshall, M. M.)
- 2) Jenkins, W. T. and **Marshall, M. M.** (1984) A Modified Direct Phosphate Assay for Studying ATPases. *Anal. Biochem.* **141**, 155-160.
- 3) Willing, A. H., **Georgiadis, M. M.**, Rees, D. C., and Howard, J. B. (1989) Cross-linking of Nitrogenase Components: Structure and Activity of the Covalent Complex. *J. Biol. Chem.* **264**, 8499-8503.
- 4) Georgiadis, T. M., **Georgiadis, M. M.**, and Diederich, F. (1991) Synthesis and Complexation Properties of a Water-Soluble Optically Active Cyclophane Incorporating a 4-Naphthyl-1,2,3,4 tetrahydroisoquinoline Unit as a Chiral Spacer. *J. Org. Chem.* **56**, 3362-3369.
- 5) **Georgiadis, M. M.**, Komiya, H., Chakrabarti, P., Woo, D., Kornuc, J. J., and Rees, D. C. (1992) Crystallographic Structure of the Nitrogenase Iron Protein from *Azotobacter vinelandii*. *Science* **257**, 1653-1659.

- 6) Rees, D. C., Kim, J., **Georgiadis, M.**, Chan, M. K., Komiyama, H., Woo, D., Chirino, A.J., Schlessman, J., and Hsu, B. T. (1993) Structures and functions of nitrogenase proteins. *Curr. Plant Sci. Biotechnol. Agric.* **17**, 83-88.
- 7) Worhl, B. M., **Georgiadis, M. M.**, Telesnitsky, A., Hendrickson, W. A., and LeGrice S. F. J. (1995) Analysis of translocating murine virus reverse transcriptase and a variant lacking the C-terminal RNaseH domain. *Science* **267**, 96-99.
- 8) **Georgiadis, M. M.**, Jessen, S. M., Ogata, C. M., Telesnitsky, A., Goff, S., and Hendrickson, W. A. (1995) Mechanistic implications from the structure of a catalytic fragment of MMLV reverse transcriptase. *Structure* **3**, 879-892.
- 9) Gao, G., Orlova, M., **Georgiadis, M. M.**, Hendrickson, Wayne A., and Goff, Stephen P. (1997) Conferring RNA polymerase Activity to a DNA polymerase: A single residue in reverse transcriptase controls substrate selection. *Proc. Natl. Acad. Sci. U.S.A.* **94**, 407-411.
- 10) Sun, D., Jessen, S., Liu, C., Liu, X., Najmudin, S., and **Georgiadis, M. M.** (1998) Cloning, expression, and purification of a catalytic fragment of Moloney murine leukemia virus reverse transcriptase: Crystallization of nucleic acid complexes. *Prot. Science* **7**, 1571-1582.
- 11) Najmudin, S., Cote, M. L., Sun, D., Yohannan, S., Montano, S. P., Gu, J., and **Georgiadis, M. M.**, (2000) Crystal structures of an N-terminal fragment from Moloney murine leukemia virus reverse transcriptase complexed with nucleic acid: Functional implications for template-primer binding to the fingers domain. *J. Mol. Biol.* **296**, 613-632.
- 12) Pfeiffer, J. K., **Georgiadis, M. M.**, and Telesnitsky, A. (2000) Structure-based Moloney murine leukemia virus reverse transcriptase mutants with altered intracellular direct repeat deletion frequencies. *J. Virol.* **74**, 9629-9636.
- 13) Emge, T., Agrawal, A., Dalessio, J., Dukovic, G., Inghrim, J., Khurram, J. S., Macaluso, M., Robertson, L., Stiglic, T., Volovik, Y., and **Georgiadis, M. M.** (2000) Alanyltryptophan hydrate, glycytryptophan dihydrate and tryptophylglycine hydrate. *Acta Cryst.* **C56**, e469-e471. *
- 14) Cote, M. L., Yohannan, S., and **Georgiadis, M. M.** (2000) Use of an N-terminal fragment from Moloney murine leukemia virus reverse transcriptase to facilitate crystallization and analysis of pseudo-16-mer DNA molecule containing G-A mispairs. *Acta Cryst.* **D56**, 1120-1131.
- 15) Gu, J., Villanueva, R. A., Snyder-Smith, C., Roth, M. J., and **Georgiadis, M. M.** (2001) Substitution of Asp 114 or Arg 116 in the fingers domain of Moloney murine leukemia virus reverse transcriptase affects interactions with the template-primer resulting in decreased processivity. *J. Mol. Biol.* **305**, 341-359.
- 16) Cote, M. L. and **Georgiadis, M. M.** (2001) Crystal structure of pseudo-16-mer DNA with stacked guanines and two G-A mispairs complexed with the N-terminal fragment of Moloney murine leukemia virus reverse transcriptase. *Acta Cryst.* **D57**, 1238-1250.

- 17) Coburn, G. A., Wiegand, H. L., Kang, Y., Ho, D. N., **Georgiadis, M. M.**, and Cullen, B. R. (2001) Using viral species variation to define a protein:RNA interaction surface. *Genes & Devel.* **15**, 1194-1205.
- 18) Das, D. and **Georgiadis, M. M.** (2001) A directed approach to improving the solubility of Moloney murine leukemia virus reverse transcriptase. *Prot. Science* **10**, 1936-1941.
- 19) Ho, D. N., Coburn, G. A., Kang, Y., Cullen, B. R., and **Georgiadis, M. M.** (2002) The crystal structure and mutational analysis of a novel RNA-binding domain found in the human Tap nuclear mRNA export factor. *Proc. Natl. Acad. Sci. U.S.A* **99**, 1888-1893.
- 20) Montano, S. P., Pierce, M., Coté, M. L., Vershon, A. K., and **Georgiadis, M. M.** (2002) Crystallographic studies of a novel DNA-binding domain from the yeast transcriptional activator Ndt80. *Acta Cryst.* **D58**, 2127-2130.
- 21) Montano, S. P., Coté, M. L., Fingerman, I., Pierce, M., Vershon, A. K., and **Georgiadis, M. M.** (2002) The crystal structure of a novel DNA-binding domain from Ndt80, a transcriptional activator required for meiosis in yeast. *Proc. Natl. Acad. Sci. U.S.A* **99**, 14501-14046.
- 22) Pierce, M., Benjamin, K. R., Montano, S. P., **Georgiadis, M. M.**, Winter, E., and Vershon, A. K. (2003) Sum1 and Ndt80 proteins compete for binding to MSE sequences that control meiotic gene expression. *Mol. Cell Biol.* **23**, 4824-4825.
- 23) Coté, M. L., Pflomm, M. and **Georgiadis, M. M.** (2003) Staying straight with A-tracts: A DNA analogue of the HIV-1 polypurine tract. *J. Mol. Biol.* **330**, 57-74.
- 24) Villanueva, R. A., Rivera, C., Jonsson, C. B., **Georgiadis, M. M.**, and Roth, M. J. (2003) Differential multimerization of Moloney murine leukemia virus integrase purified under non-denaturing conditions. *Virology*, **316**, 146-160.
- 25) Fingerman, I., Sutphen, K., Montano, S. P., **Georgiadis, M. M.**, and Vershon, A. K. (2004) Characterization of critical interactions between Ndt80 and MSE-DNA defining a novel family of Ig-fold transcription factors. *Nucl. Acids Res.* **25**, 2947-2956.
- 26) Crowther, R. L., Remeta, D. P., Minetti, C., Das, D., Montano, S. P., and **Georgiadis, M. M.** (2004) Structural and energetic characterization of nucleic acid binding to the fingers domain of Moloney murine leukemia virus reverse transcriptase. *Proteins* **57**, 15-26.
- 27) Das, D. and **Georgiadis, M. M.** (2004) The crystal structure of the monomeric reverse transcriptase from Moloney murine leukemia virus, *Structure* **12**, 819-829.
- 28) Crowther, R. L. and **Georgiadis, M. M.** (2005) The crystal structure of 5-keto-4-deoxyuronate isomerase from *Eschericia coli*. *Proteins* **61**, 680-684.
- 29) Goodwin, K. D., Long, E. C., and **Georgiadis, M. M.** (2005) A host-guest approach for determining DNA-drug interactions: An example using netropsin. *Nucleic Acids Res.* **33**, 4106-4116.

- 30) Goodwin, K. D., Lewis, M. A., Tanious, F. A., Tidwell, R. R., Wilson, W. D., **Georgiadis, M. M.**[#], and Long, E. C.[#]. (2006) A high-throughput, high-resolution strategy for the study of site selective DNA binding agents: Analysis of a "highly-twisted" benzimidazole diamidine. *JACS* **128**, 7846-7854. (# co-corresponding authors).
- 31) Montano, S. P., Coté, M. L., Roth, M. J., and **Georgiadis, M. M.** (2006) Crystal structures of oligonucleotides including the integrase processing site of the Moloney murine leukemia virus. *Nucleic Acids Res.* **34**, 5353-60.
- 32) Haag Breese, E., Uversky, V. N., **Georgiadis, M. M.**, Harrington, M. A. (2006) The disordered amino-terminus of SIMPL interacts with members of the 70-kDa heat-shock protein family. *DNA Cell Biol.* **25**, 704-14.
- 33) Luo, Y., Kwon, H.J., Montano, S., **Georgiadis, M.**, Goebel, M.G. and Harrington, M.A. (2007) Phosphorylation of SIMPL modulates RelA-associated NF-kappaB-dependent transcription *Am J Physiol Cell Physiol*, **292**, C1013-1023.
- 34) Tanious, F., Laine, W., Peixoto, P., Bailly, C., Goodwin, K. D., Lewis, M.; Long, E. C., **Georgiadis, M. M.**, Tidwell, R., Wilson, D. W. (2007) Unusually strong binding to the DNA minor groove by a highly twisted benzimidazole-diphenylether: Induced fit and bound water. *Biochemistry* **46**, 6944-6956.
- 35) Roman, Y. Oshige, M. Lee, Y.J., Goodwin, K. **Georgiadis, M.M.**, Hromas, R.A., and Lee, S.H. (2007) Biochemical Characterization of a SET and Transposase Fusion Protein, Metnase: Its DNA binding and DNA Cleavage Activity. *Biochemistry* **46**, 11369-11376.
- 36) Goodwin, K. D, Lewis, M. A., Long, E. C., and **Georgiadis, M. M.** (2008) The crystal structure of DNA-bound Co(III)-bleomycin B₂: Insights on intercalation and minor groove binding, *Proc. Natl. Acad. Sci. U.S.A* **105**, 5052-5056.
- 37) **Georgiadis, M. M.**[#] Luo, M., Gaur, R.K., Delaplane, S., Li, X., and Kelley, M. R. (2008) Evolution of the redox function in mammalian apurinic/aprimidinic endonuclease. *Mutat Res* **643**, 54-63. ([#] corresponding author)
- 38) Luo M, Delaplane S, Jiang A, Reed A, He Y, Fishel M, Nyland RL 2nd, Borch RF, Qiao X, **Georgiadis MM**, Kelley MR (2008) Role of the multifunctional DNA repair and redox signaling protein Ape1/Ref-1 in cancer and endothelial cells: small-molecule inhibition of the redox function of Ape1, *Antioxid Redox Signal* **10**, 1853-1867.
- 39) Glass, L.S., Nguyen, B., Goodwin, K.D., Dardonville, C., Wilson, W.D., Long, E.C. and **Georgiadis, M.M.** (2009) Crystal Structure of a Trypanocidal 4,4'-Bis(imidazolylamino)diphenylamine Bound to DNA. *Biochemistry* **48**, 5943-5952.
- 40) Long, E.C.[#], **Georgiadis, M.M.**, Goodwin, K.D., and Lewis, M.A. (2009) "New Approaches to analyzing the site selectivities and crystal structure of DNA targeted metal complexes" in ACS Symposium Series 1012, Bioorganic Chemistry Cellular Systems and Synthetic Models, eds. Long, E.C. and Baldwin, M.J. pp. 63-80. ([#] corresponding author).

- 41) Glass, L., Bapat, A., Kelley, M.R., **Georgiadis, M.M.#**, and Long, E.C.# (2010) Semi-automated high-throughput fluorescent intercalator displacement-based discovery of cytotoxic DNA binding agents from a large compound library. *Bioorg Med Chem Let* 20, 1685-8. (#co-corresponding authors).
- 42) Luo, M., He, H., Kelley, M. R., and **Georgiadis, M. M.** (2010) Redox Regulation of DNA Repair: Implications for Human Health and Cancer Therapeutic Development. *Antioxid Redox Signal* 12, 1247-1269.
- 43) Bapat, A., Glass, L. S., Luo, M., Fishel, M. L., Long, E. C., **Georgiadis, M. M.**, and Kelley, M. R. (2010) Novel small molecule inhibitor of Ape1 endonuclease blocks proliferation and reduces viability of glioblastoma cells. *JPET* 334, 988-998.
- 44) Goodwin, K. D., He, H., Imasaki, T., Lee, S. H., and **Georgiadis, M. M.** (2010) Crystal structure of the human *Hsmar1*-derived transposase in the DNA repair enzyme Metnase. *Biochemistry* 49, 5705-5713.
- 45) Victor J. Anciano Granadillo, Jennifer N. Earley, Sarah C. Shuck, Millie M. Georgiadis , Richard Fitch and John J. Turchi (2010) Small molecule inhibitors of Replication Protein A: Targeting OB-folds. *J. Nucl Acids*, Dec. 6, online.
- 46) Su, D., Delaplane, S., Luo, M., Kelley, M. R., Gross, M. L., and **Georgiadis, M. M.** (2010) Interactions of APE1 with a redox inhibitor: Evidence for an alternate conformation of the enzyme. *Biochemistry*, Dec. 8. Epub ahead of print.
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B. Solicited Book Chapters/Invited Reviews (3)

1. Rees, D. C., Kim, J., **Georgiadis, M. M.**, Komiya, H., Chirino, A. J., Woo, D., Schlessman, J., Chan, M. K., Joshua-Tor, L., Santillan, G., Chakrabarti, P., and Hsu, B. T. (1993) Crystal Structures of the Iron Protein and Molybdenum-Iron Protein of Nitrogenase. In:(eds) Strefel, E. I., Coucouvanis, D., and Newton, W. E., ACS. Symposium on Molybdenum Enzymes, Cofactors and Models, pp. 170-185.
2. **Georgiadis, M. M.**, Chakrabarti, P., and Rees, D. C. (1990) The Crystal Structure of the Nitrogenase Iron Protein from *Azotobacter vinelandii*. In: (eds) Gresshoff,

Roth, Stacey, and Newton, Nitrogen Fixation: Achievements and Objectives, Chapman and Hall, pp. 111-116.

3. Luo, M., He, H., Kelley, M. R., and **Georgiadis, M. M.** (2010) Redox Regulation of DNA Repair: Implications for Human Health and Cancer Therapeutic Development. *Antioxid Redox Signal* 12, 1247-1269.

C. Abstracts from conference presentations (26, only in-rank abstracts included).

1. Debanu Das and **Millie M. Georgiadis** (2003) "Crystal Structure of the Full-length Moloney Murine Leukemia Virus Reverse Transcriptase:DNA Complex" *Annual American Crystallographic Association Meeting*, July 26-31, 2006, Covington, KY.
2. Sherwin Montano, Debanu Das, Kristie Goodwin, and **Millie M. Georgiadis** (2004) "A novel host-guest approach to nucleic acid structures" Abstract, 36th *Central Regional Meeting of the American Chemical Society (CERMACS)*, June 2, 2004.
3. M. A. Lewis, K. D. Goodwin, **M. M. Georgiadis** and E. C. Long (2005) "DNA-Dependent Cu(II)•Xaa-Xaa-His Metal-Peptide Dissociation" *Abstracts*, 12th *International Conference on Bio-Inorganic Chemistry (ICBIC-12)*, July 31-August 5, 2005. Published online at: <http://www.umich.edu/~icbic/ICBIC-12-Abstracts.htm>
4. M. A. Lewis, K. D. Goodwin, **M. M. Georgiadis**, and E. C. Long (2005) "DNA-Dependent Cu(II)•Xaa-Xaa-His Metal-Peptide Dissociation" *Abstracts*, 6th *Annual Indiana Local Section American Chemical Society Poster Session*, 30B, October 10, 2005.
5. K. D. Goodwin, M. A. Lewis, **M. M Georgiadis**, and E. C. Long (2006) "A High-Throughput, High-Resolution Strategy for the Rapid Structural Elucidation of Site-Selective DNA Binding Agents" *IU Cancer Research Day*, May 10, 2006.
6. K. D. Goodwin, M. A. Lewis, **M. M Georgiadis**, and E. C. Long (2006) "A High-Throughput, High-Resolution Strategy for the Structural Elucidation of Site-Selective DNA Binding and Damaging Agents" 8th *Annual Midwest DNA Repair Symposium*, IU School of Medicine, IUPUI, May 20-21, 2006.
7. K. D. Goodwin, M. A. Lewis, E. C. Long, and **M. M. Georgiadis** (2006) "Crystallographic Studies of the Co(III)•Bleomycin-DNA Complex" *American Cancer Society Annual Meeting*, University of Michigan, November 2006.
8. M. A. Lewis, K. D. Goodwin, **M. M. Georgiadis**, and E. C. Long (2006) "High-Throughput, High-Resolution Strategy for the Rapid Structural Elucidation of Site-Selective DNA Binding Agents" *Abstracts of Papers* 232nd National Meeting of the American Chemical Society, San Francisco, CA.; American Chemical Society: Washington, D. C., 2006: BIOL 122, September 9-14, 2006.
9. Kristie D. Goodwin, Masahiko Oshige, Suk-Hee Lee, and **Millie M. Georgiadis** (2006) "Crystallization Studies of Metnase, a SET/Transposase protein" Abstract, *Annual American Crystallographic Association Meeting*, July 22-27, 2006, Honolulu, HI.

10. K. D. Goodwin, M. A. Lewis, E. C. Long and **M. M. Georgiadis** (2007) "A new approach to an old problem: The crystal structure of a DNA-Co(III)•bleomycin-B₂ complex" *Abstracts of Papers, CERMACS 2007*, Central Regional Meeting of the American Chemical Society, Covington, KY, May 20-23.
11. Eric C. Long, **Millie M. Georgiadis**, Kristie D. Goodwin and Mark A. Lewis (2007) "A new approach to analyzing DNA binding agents leading to the crystal structure of a DNA-Co(III)•bleomycin-B₂ complex" *Abstracts of Papers, CERMACS 2007*, Central Regional Meeting of the American Chemical Society, Covington, KY, May 20-23 (invited presentation).
12. K. D. Goodwin, M. A. Lewis, E. C. Long and **M. M. Georgiadis** (2007) "A new approach to an old problem: The crystal structure of a DNA-Co(III)•bleomycin-B₂ complex" *Albany 2007: The 15th Conversation*, State University of New York at Albany, Albany, NY, June 19-23. Abstract published in *Journal of Biomolecular Structure and Dynamics* **2007**, 24 (6), 674.
13. Bapat A., Fishel, ML, **Georgiadis, MM**, and Kelley MR (2007) High Throughput Screen for Inhibitor of Ape1. *MidWest Society for Pediatric Research (MWSPR)*, Abstract, October 18-19, 2007.
14. Bapat A., Fishel, ML, **Georgiadis, MM**, and Kelley MR. (2007) "High Throughput Screen for Inhibitor of Ape1" Abstract, *Indiana University Melvin and Bren Simon Cancer Center-Cancer Research Day 2008*, IUPUI, Indianapolis, IN, May 7.
15. Bapat A., Fishel, ML, **Georgiadis, MM**, and Kelley MR. (2007) "High Throughput Screen for Inhibitor of Ape1" Abstract, *Indiana University Melvin and Bren Simon Cancer Center-Cancer Research Day 2007*, Indiana University School of Medicine, IUPUI, Indianapolis, IN, May 2.
16. Bapat A., Fishel, ML, **Georgiadis, MM**, and Kelley MR. (2007) "High Throughput Screen for Inhibitor of Ape1" Abstract, *2007 Biochemistry & Molecular Biology Research Day*, Indiana University School of Medicine, IUPUI, Indianapolis, IN, September 28.
17. L. S. Glass, **M. M. Georgiadis** and E. C. Long (2008) "High-Throughput Discovery and Analysis of Nucleic Acid Binding Ligands: Towards the Rapid Development of New DNA-Targeted Chemotherapeutics" *Consortium for Urban Education Life and Health Sciences Research Showcase*, IUPUI, Indianapolis, IN, March 18th.
18. L. S. Glass, **M. M. Georgiadis**, and E. C. Long (2008) "High-Throughput Discovery and Analysis of Nucleic Acid Binding Ligands: Towards the Rapid Development of New DNA-Targeted Chemotherapeutics" *Abstract Book-Indiana University Melvin and Bren Simon Cancer Center-Cancer Research Day 2008*, Basic Science, page 10, IUPUI, Indianapolis, IN, May 7.
19. **M. M. Georgiadis**, K. D. Goodwin, M. A. Lewis and E. C. Long (2008) "Crystal Structures of DNA-Bound Co(III)•Bleomycins" [*Acta Cryst.* **2008**, A64, C156] MS.93.4 *Online Abstract Book*, XXI Congress and General Assembly of the International Union of Crystallography (IUCr2008) 23-31 August, Osaka, Japan.

20. LaTeca S. Glass, E. C. Long and **Millie M. Georgiadis** (2008) "High-Throughput, High-Resolution Strategy Approach to the Analysis of DNA Binding Compounds" *2008 Biochemistry & Molecular Biology Research Day* Indiana University School of Medicine, IUPUI, Indianapolis, IN, October 2.
21. LaTeca S. Glass, E. C. Long and **Millie M. Georgiadis** (2008) "High-Throughput, High-Resolution Strategy Approach to the Analysis of DNA Binding Compounds" *NOBCCHE Midwest Regional Conference*, Eli Lilly & Co. Corporate Center, Indianapolis, IN, October 23-25.
22. Bapat A., Fishel, ML, **Georgiadis, MM**, and Kelley MR. (2008) "Inhibition of Ape1s repair activity as a target in cancer" Abstract, *American Association for Cancer Research (AACR) 2008: Mini-symposium, DNA repair and Mutagenesis*, April 11-16, 2008, San Diego, CA.
23. Bapat A., Fishel, ML, **Georgiadis, MM**, and Kelley MR. (2008) "High Throughput Screen for Inhibitor of Ape1" Abstract, *2008 Biochemistry & Molecular Biology Research Day*, Indiana University School of Medicine, IUPUI, Indianapolis, IN, October 2.
24. LaTeca S. Glass, Eric C. Long and **Millie M. Georgiadis** (2009) "Expedited Approaches to the Discovery and Analysis of DNA Binding Ligands" *IUPUI Research Day*, IUPUI, Indianapolis, IN, April 24, 2009.
25. LaTeca S. Glass, Eric C. Long and **Millie M. Georgiadis** (2009) "Expedited Approaches to the Discovery and Analysis of DNA Binding Ligands" Abstract *2009 Indiana University Melvin and Bren Simon Cancer Center Cancer Research Day*, IUPUI, Indianapolis, IN, May 6, 2009.
26. Hongzhen He, Lakshmi Reddy Palam, Ronald C. Wek, **Millie M. Georgiadis** (2009) "Crystal structure of the C-terminal domain of Gcn2 reveals the dimerization mechanism and potential rRNA binding sites" *Annual Biochemistry & Molecular Biology Research Day*, February 19, 2010.

D. Web publications

None

E. Patents, etc.

1. PCT Patent Application, "Therapeutic Methods, APE1 Inhibitors" filed 9/22/2008, publishes May 21, 2009, Kelley, M.R. and Georgiadis, M.M.

INDIANA UNIVERSITY SCHOOL OF MEDICINE

CURRICULUM VITAE

December, 2010

NAME: Merouch, Samy

EDUCATION:

UNDERGRADUATE:	Wayne State University	B.S.	1995
GRADUATE:	Wayne State University	Ph.D.	2001

ACADEMIC APPOINTMENTS:

6/01-9/03	<i>Postdoctoral Associate</i> , Wayne State University School of Medicine, Department of Biochemistry and Molecular Biology
6/03-9/06	<i>Postdoctoral Fellow</i> , University of Notre Dame, Department of Chemistry and Biochemistry
10/06-present	<i>Assistant Professor</i> , Indiana University School of Medicine, Department of Biochemistry and Molecular Biology
10/06-present	<i>Non-Adjunct Assistant Professor</i> , Indiana University Purdue University Indianapolis (IUPUI), Department of Chemistry and Chemical Biology

HOSPITAL APPOINTMENTS: Not applicable.

OTHER APPOINTMENTS AND PROFESSIONAL CONSULTANTSHIPS:

10/06-present	<i>Member</i> , Center for Computational Biology and Bioinformatics
03/08-present	<i>Member</i> , Bren and Mel Simon Cancer Center
10/06-present	<i>Member</i> , Stark Neurosciences Research Institute

LICENSURE AND CERTIFICATION:

10/06	<i>Participant</i> , 'Grant Writing Workshop: write winning grants', Continuing Medical Education, Indiana University School of Medicine
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PROFESSIONAL ORGANIZATIONS:

2001	<i>Member</i> , AAAS
2001	<i>Professional Member</i> , American Chemical Society
2008	<i>Member</i> , American Association for Cancer Research

HONORS AND AWARDS:

1999 Vice-President Graduate Student Award, Wayne State University
2004 Walther Cancer Institute Fellow, University of Notre Dame
2007 Showalter Award
2008 Showalter Award

TEACHING ASSIGNMENTS SINCE APPOINTMENT:

Teaching prior to appointment

95-96 *Teaching Assistant*, Introductory Chemistry laboratory, Department of Chemistry, University of Iowa, 20 hrs/week, >20 students

Spring 1999 *Teaching Assistant*, Physical Chemistry, Department of Chemistry, 1999, 20 hrs/week, >10 students

Teaching since appointment (7/2006)

(A) DIDACTIC COURSES:

Fall 2007 *Lecturer*, Biochemical Basis of Biological Processes G715, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 2 hrs, 35 students

Spring 2008 *Lecturer*, Structural Bioinformatics, School of Informatics I619, 2 hrs, 5 students

Spring 2008 *Lecturer*, Introduction to Structural Biology G749, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 1 hr, 7 students

Spring 2008 *Facilitator*, Concepts in Health and Disease X604, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 16 hrs, 7 students

Spring 2008 *Lecturer*, A Short Course in Bioinformatics for Physicians, Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, 1 hr, 35 students

Fall 2008 *Lecturer*, Biochemical Basis of Biological Processes G715, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 2 hrs, 46 students

Spring 2009 *Lecturer*, Practical Bioinformatics I399, School of Informatics, 2 hrs, 5 students

Spring 2009 *Lecturer*, Bioinformatics, Genomics, Proteomics and Systems Biology, Department of Biochemistry and Molecular Biology B848, 2 hrs, 5 students

- Spring 2009 *Facilitator*, Concepts in Health and Disease X604, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 16 hrs, 7 students
- Spring 2009 *Lecturer*, Structural Bioinformatics, School of Informatics I619, 2 hrs, 9 students
- Spring 2009 *Lecturer*, Introduction to Structural Biology G749, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 2 hrs, 9 students
- Spring 2009 *Lecturer*, Structural and Chemical Biology G807, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 2 hrs, 9 students
- Fall 2009 *Lecturer*, Biochemical Basis of Biological Processes G715, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 2 hrs, 46 students

(B) GRADUATE/PROFESSIONAL STUDENT TRAINING:

- 01/07-01/08 *Mentor and Master's Thesis Committee chair*, Ms. Sara Bennett, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 25 hrs/week
- 01/08-07/08 *Mentor and Master's Thesis Committee chair*, Mr. Sudhir Chowbina, School of Informatics, Indiana University School of Medicine, 25 hrs/week
- 2/08-5/08 *Ph.D Mentor for laboratory rotation*, Ms. Wei-Lun Hsu, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 25 hrs/week
- 10/08-12/08 *Ph.D Mentor for laboratory rotation*, Ms. Jessica Walsh, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine, 25 hrs/week
- 10/06-10/07 *Mentor Undergraduate Thesis*, Mr. Brian O'Callaghan, Department of Chemistry and Chemical Biology, IUPUI, 20 hrs/week
- 10/07-10/08 *Mentor Undergraduate Thesis*, Mr. Jason Kominiak, Department of Chemistry and Chemical Biology, IUPUI, 20 hrs/week
- 06/08-present *Mentor Undergraduate Thesis*, Ms. Meaghan Pilcher, Department of Chemistry and Chemical Biology, IUPUI, 20 hrs/week

06/08-present *Mentor Undergraduate Thesis*, Ms. Agnes Alvarez, Department of Chemistry and Chemical Biology, IUPUI, 20 hrs/week

01/09-present *Mentor Undergraduate Thesis*, Mr. Khuchtumur Bum-Erdene, Department of Chemistry and Chemical Biology, IUPUI, 20 hrs/week

09/09-present *Mentor Graduate Thesis*, Mr. Bo Wang, Department of Chemistry and Chemical Biology, IUPUI, 20 hrs/week

(C) INVITED PRESENTATIONS:

1. Department of Medicinal Chemistry, Purdue University, "Molecular Design of Small Molecules that Target Protein Interactions in Cancer Metastasis", October 14th, 2010.
2. Bioorganic Gordon Research Conference, "Design, Discovery and Develop" Session Chair, June 2010
3. Skaggs College of Pharmacy, University of California San Diego, "Docking the Human Proteome in Search for Cancer Therapeutics", February 24th, 2010
4. Department of Biopharmaceutical Sciences, University of California at San Francisco, "Computational Design of Small Molecules that Modulate Interactions of the Urokinase Receptor", February 18th, 2010
5. Department of Biology and Biochemistry, University of Houston, Computational design of molecules that modulate interactions of uPAR: A target of tumor invasion and metastasis" Jan. 22nd, 2010
6. Department of Pharmaceutical Sciences, Wayne State University, "Computational Design of Small Molecules that Modulate Interactions of the Urokinase Receptor" Jan. 23th, 2010
7. Center for Computational and Systems Biology, Massachusetts Institute of Technology (MIT), "Computational Design of Molecules that Modulate Interactions Critical in Tumor Invasion and Metastasis", Nov. 20th, 2009
8. Gordon Research Conference on Computer-Aided Drug Discovery, Tilton, New Hampshire, "Computational design of small molecules that modulate interactions of the urokinase receptor: A target in tumor invasion and metastasis", July 2009
9. Eli Lilly Inc., "Targeting the human proteome for cancer therapeutics", December 2008
10. Andrews University, Michigan, "Blocking multiple interactions of the urokinase receptor with small molecules", October 2008
11. Experimental and Development Therapeutics Group, Indiana University Simon Cancer Center, "Blocking multiple interactions of the urokinase receptor for anti-cancer therapeutics", August 2008
12. Stark Neurosciences, Indiana University School of Medicine, "Targeting the urokinase receptor with small molecule inhibitors", October 2007
13. Department of Biochemistry and Molecular Biology, Indiana University School of Medicine, Indianapolis, Indiana: "Computational Design of Small Molecules that Target Interactions of the Urokinase Receptor at the Cell Surface", October 2007
14. Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, Indiana: "Computational Design of Small Molecules that Target Protein-Protein Interactions and Inhibit Tumor Cell Proliferation, Migration and Invasion" April 2007

15. Gordon Research Conference on Computer-Aided Drug Discovery, Tilton, New Hampshire: "PDBcal: A Dataset with Isothermal Titration Calorimetry Data and Three-Dimensional Structures for Scoring Function Development in Computational Drug Design", abstract selected for oral presentation, July 2007.
16. Center for Computational Biology and Bioinformatics, Indiana University, Indianapolis, IN: "Molecular Motions in Ligand Binding and Protein Allostery: Implications for Drug Design", April 2007.
17. Department of Physics, IUPUI, "Entropic Effects in Protein Allostery: A Case Study with the Catabolite Activator Protein.", March 2007
18. Bioinformatics Retreat, Bradford Woods, Indiana "Modeling protein-ligand interactions.", February 2007
19. Department of Chemistry and Chemical Biology, IUPUI, "Computer-Assisted Discovery of Matrix Metalloproteinase Inhibitors", October 2006
20. The Center for Genomics and Bioinformatics, Indiana University Bloomington, "Computer-Assisted Discovery of Matrix Metalloproteinase Inhibitors", October 2006
21. Gordon Research Conference on New Antibacterial Discovery, Ventura, California: Three-Dimensional Structure of Cell Wall Peptidoglycan, March 2006
22. Department of Computer Science, University of Notre Dame, Course in Computational Biophysics and Systems Biology (Prof. Jesus Izaguirre): Molecular Docking in the Biomedical Sciences, January 2006
23. Molecular Dynamics Libraries Workshop, University of Notre Dame: Computer-Assisted Discovery and Design of MMP inhibitors and Computing Binding Free Energies, November 2005
24. Drug Design Group, University of Notre Dame: Experimental and Computational Investigations of the Base Flipping Events in the Ribosomal RNA Acyltransfer Site, September 2005
25. Pokagon State Park, Annual Biochemistry Retreat, Angola, Indiana: Interactions of Designer Antibiotics and the Ribosomal RNA Acyltransfer Site, May 2005
26. Walther Cancer Institute Retreat, University of Notre Dame: Computer-Assisted Discovery and Design of Matrix-Metalloproteinase Inhibitors, August 2004

PROFESSIONAL SERVICE:

(1) SERVICE TO THE DISCIPLINE

(a) DEPARTMENTAL:

- 11/09 *Reviewer*, CTSI Core Facility Pilot Grant Review, Indiana University School of Medicine
- 8/08 *Judge*, Peggy Gibson award for best paper by a graduate student, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine
- 8/07 *Judge*, Peggy Gibson award for best paper by a graduate student, Department of Biochemistry & Molecular Biology, Indiana University School of Medicine
- 7/08 *Member*, Faculty search committee, Department of Biochemistry and Molecular Biology

(b) UNIVERSITY:

01/10 *Member*, Faculty search committee, Department of Chemistry and Chemical Biology

UNIVERSITY SERVICE:

(a) NATIONAL AND INTERNATIONAL:

Ad hoc reviewer for Journal of the American Chemical Society, Journal of Molecular Biology, PloS Computational Biology, Wiley Encyclopedia of Chemical Biology, Biophysical Journal, Biopolymers, Chemical Biology and Drug Design, Proteins: Structure, Function and Bioinformatics, Physical Chemistry B, Nucleic Acids Research

SERVICE TO PATIENTS/CLIENTS: Not applicable.

COMMUNITY SERVICE: Not applicable.

OTHER PROFESSIONAL ACTIVITIES:

POSTGRADUATE TRAINING:

2006, 2009 Dr. Shide Liang
2006-present Dr. Liwei Li
2009-present Dr. Xiaodong Peng
2010-present Dr. Hartmut Roehm

GRANTS AND FELLOWSHIPS

GRANTS COMPLETED AND ONGOING:

10/15/09-10/14/10	PI: Meroueh, Research Support Fund Grant, Title: <u>Computational Design of Small Molecule Inhibitors of Ral GTPases to Block Tumor Invasion and Metastasis</u> , Indiana University School of Medicine, \$55,000 direct costs
3/1/09-6/30/13	PI (multi-PI grant; co-PI Thomas Hurley): Meroueh, NIH/NIAAA R21 CA135380-01A1, Title: <u>Targeting ALDH2 for adjuvant treatment of alcohol dependence</u> , \$231,000 total costs
3/1/09-6/30/13	PI: Meroueh, NIH/NCI R01 CA135380-01A1, Title: <u>Small-molecule Inhibition of the Interactions of the Urokinase Receptor</u> , \$166,000 direct costs; 83,000 indirect costs
7/1/09-6/30/11	PI: Meroueh, TeraGrid MCB090165, Title: <u>Biodrugscreen: A portal for customized scoring and ranking of molecules docked to the human proteome</u> . 2,000,000 cpu-hours

5/1/09-4/30/10	co-PI: Meroueh, Indiana University CBR/CTR, Title: <u>Development of a supraphysiological T cell receptors for the immunological treatment of cancer</u> , Indiana University School of Medicine, \$75,000 total costs
7/1/09-6/30/10	PI: Meroueh, Showalter Research Trust, Title: <u>Lead Optimization of Anti-Cancer Agents through Lead Optimization and Chemical Synthesis</u> , Indiana University School of Medicine, \$60,000 total costs (\$50,000 direct, \$10,000 indirect)
6/1/07-5/31/08	PI: Meroueh, Biomedical Research Grant, Title: <u>Inhibition of the Staphylococcus aureus Sortase A Transpeptidase as a Strategy for the Development of Antimicrobial Agents</u> , Indiana University School of Medicine, \$40,000 direct costs
5/1/07-4/30/08	PI: Meroueh, Indiana University Translational Research Collaboration (ITRAC), Title: <u>Targeting the TG2-Fibronectin Interaction for blocking metastatic ovarian cancer</u> , Indiana University School of Medicine, \$23,000 total costs
11/1/07-10/31/08	PI: Meroueh, Research Support Fund Grant, Title: <u>Lead Discovery Guided by Isothermal Titration Calorimetry</u> , Indiana University School of Medicine, \$35,000 total costs
1/1/08-12/31/08	PI: Meroueh, American Cancer Society, Title: <u>Allosteric Regulation of the Interaction between the Urokinase Receptor and Integrin with Small Molecules</u> , Indiana University School of Medicine, \$25,000 direct costs
9/01/08-8/31/09	PI: Meroueh, Indiana University Translational Research Collaboration (ITRAC), Title: <u>Lead Optimization of Small Molecules that Block Multiple Interactions of the Urokinase Receptor</u> , Indiana University School of Medicine, \$54,000 total costs
7/01/08-6/30/09	PI: Meroueh, Grace Showalter Trust, Title: <u>Computer-Guided Design of Small Molecules that Block Tumor Invasion and Metastasis</u> , Indiana University School of Medicine, \$60,000 total costs (\$50,000 direct, \$10,000 indirect)

FUNDING FOR TRAINEES:

3/1/09-2/30/10	PI: Meroueh, Lung Cancer Working Group Postdoctoral Fellowship, Title: <u>Multiple Interactions of the Urokinase Receptor for Discovery of Lung Cancer Therapeutics</u> , Indiana University School of Medicine, \$50,000 total costs (submitted)
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GRANTS PENDING:

10/29/09-11/28/10 PI: Meroueh, BCRF-AACR, Title: Targeted polypharmacology through optimization of promiscuous compounds, Indiana University School of Medicine, \$776,000 total costs

10/29/09-11/28/10 PI: Meroueh, Department of Defense, BC097617 Title: Targeted polypharmacology through optimization of promiscuous compounds, Indiana University School of Medicine, \$776,000 total costs

PRINT AND ELECTRONIC PUBLICATIONS

(I) Teaching: Not applicable.

(II) Research:

*Symbols: *equal authorship; **corresponding author; #work completed at IUSM*

PEER REVIEWED PUBLICATIONS (IN CHRONOLOGICAL ORDER):

1. #Li, L., K. Bumerdene, P.H. Baenziger, J.R. Hemmert, J. Rosen, J. Nellis, M. Pierce, and S.O. Meroueh**, *Biodrugscreen: A Computational Drug Design Resource for Ranking Molecules Docked to the Human Proteome*. Nuc. Acid Res., **2009**. In press (doi: 10.1093/nar/gkp852)
2. #Matute, J.D., A.A. Arias, N.A. Wright, I. Wrobel, C.C. Waterhouse, X.J. Li, C.C. Marchal, N.D. Stull, D.B. Lewis, M. Steele, J.D. Kellner, W. Yu, S.O. Meroueh, W.M. Nauseef, and M.C. Dinanuer, *A new genetic subgroup of chronic granulomatous disease with autosomal recessive mutations in p40 phox and selective defects in neutrophil NADPH oxidase activity*. Blood, **2009**. 114(15): p. 3309-15.19692703
3. #Liang, S., S.O. Meroueh, G. Wang, C. Qiu, and Y. Zhou, *Consensus scoring for enriching near-native structures from protein-protein docking decoys*. Proteins, **2009**. 75(2): p. 397-403.18831053
4. #Liang, S., L. Li, W.L. Hsu, M.N. Pilcher, V. Uversky, Y. Zhou, A.K. Dunker, and S.O. Meroueh**, *Exploring the molecular design of protein interaction sites with molecular dynamics simulations and free energy calculations*. Biochemistry, **2009**. 48(2): p. 399-414.19113835
5. #Li, L., S. Liang, M.M. Pilcher, and S.O. Meroueh**, *Incorporating receptor flexibility in the molecular design of protein interfaces*. Protein Eng Des Sel, **2009**. 22(9): p. 575-86.19643976
6. #Xue, B., L. Li, S.O. Meroueh, V.N. Uversky, and A.K. Dunker, *Analysis of structured and intrinsically disordered regions of transmembrane proteins*. Mol Biosyst, **2009**.19585006

7. Shi, Q., S.O. Meroueh, J.F. Fisher, and S. Mobashery, *Investigation of the mechanism of the cell wall DD-carboxypeptidase reaction of penicillin-binding protein 5 of Escherichia coli by quantum mechanics/molecular mechanics calculations*. J Am Chem Soc, **2008**. 130(29): p. 9293-303.18576637
8. #Li, L. and S.O. Meroueh**, *Receptor-Ligand Interactions in Biological Systems*, in *Encyclopedia for the Life Sciences*. 2008, John Wiley and Sons: London. p. in press.
9. #Li, L., J.J. Dantzer, J. Nowacki, B.J. O'Callaghan, and S.O. Meroueh**, *PDBcal: a comprehensive dataset for receptor-ligand interactions with three-dimensional structures and binding thermodynamics from isothermal titration calorimetry*. Chem Biol Drug Des, **2008**. 71(6): p. 529-32.18482338
10. #Jewell, J.L., E. Oh, S.M. Bennett, S.O. Meroueh, and D.C. Thurmond, *The tyrosine phosphorylation of Munc18c induces a switch in binding specificity from syntaxin 4 to Doc2beta*. J Biol Chem, **2008**. 283(31): p. 21734-46.18541526
11. #Li, L., V.N. Uversky, A.K. Dunker, and S.O. Meroueh**, *A computational investigation of allostery in the catabolite activator protein*. J Am Chem Soc, **2007**. 129(50): p. 15668-76.18041838
12. Rosenblum, G., S. Meroueh, M. Toth, J.F. Fisher, R. Fridman, S. Mobashery, and I. Sagi, *Molecular structures and dynamics of the stepwise activation mechanism of a matrix metalloproteinase zymogen: challenging the cysteine switch dogma*. J Am Chem Soc, **2007**. 129(44): p. 13566-74.17929919
13. Meroueh, S.O. and S. Mobashery, *Conformational transition in the aminoacyl t-RNA site of the bacterial ribosome both in the presence and absence of an aminoglycoside antibiotic*. Chem Biol Drug Des, **2007**. 69(5): p. 291-7.17539821
14. Meroueh, S.O., J.Y. Cha, and S. Mobashery, *Inhibition of Class A beta-Lactamases*, in *Enzyme-Mediated Resistance to Antibiotics: Mechanisms, Dissemination, and Prospects for Inhibition*, R.A. Bonomo, Editor. 2007, ASM Press: Washington D. C.
15. Zhang, W., Q. Shi, S.O. Meroueh, S.B. Vakulenko, and S. Mobashery, *Catalytic mechanism of penicillin-binding protein 5 of Escherichia coli*. Biochemistry, **2007**. 46(35): p. 10113-21.17685588
16. Rekharsky, M., D. Hesek, M. Lee, S.O. Meroueh, Y. Inoue, and S. Mobashery, *Thermodynamics of interactions of vancomycin and synthetic surrogates of bacterial cell wall*. J Am Chem Soc, **2006**. 128(24): p. 7736-7.16771477
17. Rahaman, A., H. Song, A.X. Wang, S.O. Meroueh, and W.L. Hase, *Chemical Dynamics Simulations of Energy Transfer and Unimolecular Decomposition in Collision-Induced Dissociation (CID) and Surface-Induced Dissociation (SID)*, in *Principles of Mass Spectrometry Applied to Biomolecules*, C. Litschitz and J. Laskin, Editors. 2006, Wiley: New York. p. 379-432.

18. Murray, J.B., S.O. Meroueh, R.J. Russell, G. Lentzen, J. Haddad, and S. Mobashery, *Interactions of designer antibiotics and the bacterial ribosomal aminoacyl-tRNA site*. Chem Biol, **2006**. 13(2): p. 129-38.16492561
19. Meroueh, S.O., K.Z. Bencze, D. Heseck, M. Lee, J.F. Fisher, T.L. Stemmler, and S. Mobashery, *Three-dimensional structure of the bacterial cell wall peptidoglycan*. Proc Natl Acad Sci U S A, **2006**. 103(12): p. 4404-9.16537437
20. Heseck, D., M. Toth, S.O. Meroueh, S. Brown, H. Zhao, W. Sakr, R. Fridman, and S. Mobashery, *Design and characterization of a metalloproteinase inhibitor-tethered resin for the detection of active MMPs in biological samples*. Chem Biol, **2006**. 13(4): p. 379-86.16632250
21. Toth, M., P. Osenkowski, D. Heseck, S. Brown, S. Meroueh, W. Sakr, S. Mobashery, and R. Fridman, *Cleavage at the stem region releases an active ectodomain of the membrane type 1 matrix metalloproteinase*. Biochem J, **2005**. 387(Pt 2): p. 497-506.15560752
22. Osenkowski, P., S.O. Meroueh, D. Pavel, S. Mobashery, and R. Fridman, *Mutational and structural analyses of the hinge region of membrane type 1-matrix metalloproteinase and enzyme processing*. J Biol Chem, **2005**. 280(28): p. 26160-8.15901740
23. Meroueh, S.O., J.F. Fisher, H.B. Schlegel, and S. Mobashery, *Ab initio QM/MM study of class A beta-lactamase acylation: dual participation of Glu166 and Lys73 in a concerted base promotion of Ser70*. J Am Chem Soc, **2005**. 127(44): p. 15397-407.16262403
24. Li, J., J.B. Cross, T. Vreven, S.O. Meroueh, S. Mobashery, and H.B. Schlegel, *Lysine carboxylation in proteins: OXA-10 beta-lactamase*. Proteins, **2005**. 61(2): p. 246-57.16121396
25. Lee, M., M.M. Bernardo, S.O. Meroueh, S. Brown, R. Fridman, and S. Mobashery, *Synthesis of chiral 2-(4-phenoxyphenylsulfonylmethyl)thiiranes as selective gelatinase inhibitors*. Org Lett, **2005**. 7(20): p. 4463-5.16178559
26. Ikejiri, M., M.M. Bernardo, S.O. Meroueh, S. Brown, M. Chang, R. Fridman, and S. Mobashery, *Design, synthesis, and evaluation of a mechanism-based inhibitor for gelatinase A*. Journal of Organic Chemistry, **2005**. 70(14): p. 5709-12.15989356
27. Fisher, J.F., S.O. Meroueh, and S. Mobashery, *Bacterial resistance to beta-lactam antibiotics: compelling opportunism, compelling opportunity*. Chem Rev, **2005**. 105(2): p. 395-424.15700950
28. Cross, J.B., T. Vreven, S.O. Meroueh, S. Mobashery, and H.B. Schlegel, *Computational investigation of irreversible inactivation of the zinc-dependent protease carboxypeptidase A*. Journal of Physical Chemistry B, **2005**. 109(10): p. 4761-9.16851559

29. Lim, I.T., S.O. Meroueh, M. Lee, M.J. Heeg, and S. Mobashery, *Strategy in inhibition of cathepsin B, a target in tumor invasion and metastasis*. J Am Chem Soc, **2004**. 126(33): p. 10271-7.15315439
30. Kim, C., J. Haddad, S.B. Vakulenko, S.O. Meroueh, Y. Wu, H. Yan, and S. Mobashery, *Fluorinated aminoglycosides and their mechanistic implication for aminoglycoside 3'-phosphotransferases from Gram-negative bacteria*. Biochemistry, **2004**. 43(9): p. 2373-83.14992574
31. Golemi-Kotra, D., S.O. Meroueh, C. Kim, S.B. Vakulenko, A. Bulychiev, A.J. Stemmler, T.L. Stemmler, and S. Mobashery, *The importance of a critical protonation state and the fate of the catalytic steps in class A beta-lactamases and penicillin-binding proteins*. J Biol Chem, **2004**. 279(33): p. 34665-73.15152012
32. Brown, S., S.O. Meroueh, R. Fridman, and S. Mobashery, *Quest for selectivity in inhibition of matrix metalloproteinases*. Curr Top Med Chem, **2004**. 4(12): p. 1227-38.15320723
33. Birck, C., J.Y. Cha, J. Cross, C. Schulze-Briese, S.O. Meroueh, H.B. Schlegel, S. Mobashery, and J.P. Samama, *X-ray crystal structure of the acylated beta-lactam sensor domain of BlaR1 from Staphylococcus aureus and the mechanism of receptor activation for signal transduction*. Journal of the American Chemical Society, **2004**. 126(43): p. 13945-13947.ISI:000224873600034
34. Wilkinson, A.S., P.K. Bryant, S.O. Meroueh, M.G. Page, S. Mobashery, and C.W. Wharton, *A dynamic structure for the acyl-enzyme species of the antibiotic aztreonam with the Citrobacter freundii beta-lactamase revealed by infrared spectroscopy and molecular dynamics simulations*. Biochemistry, **2003**. 42(7): p. 1950-7.12590581
35. Wang, J.P., S.O. Meroueh, Y.F. Wang, and W.L. Hase, *Efficiency of energy transfer in protonated diglycine and dialanine SID - Effects of collision angle, peptide ion size, and intramolecular potential*. International Journal of Mass Spectrometry, **2003**. 230(1): p. 57-64.ISI:000186009000008
36. Song, K.Y., O. Meroueh, and W.L. Hase, *Dynamics of Cr(CO)(6)(+) collisions with hydrogenated surfaces*. Journal of Chemical Physics, **2003**. 118(6): p. 2893-2902.ISI:000180564800049
37. Rosenblum, G., S.O. Meroueh, O. Kleifeld, S. Brown, S.P. Singson, R. Fridman, S. Mobashery, and I. Sagi, *Structural basis for potent slow binding inhibition of human matrix metalloproteinase-2 (MMP-2)*. J Biol Chem, **2003**. 278(29): p. 27009-15.12679334
38. Meroueh, S.O., G. Minasov, W. Lee, B.K. Shoichet, and S. Mobashery, *Structural aspects for evolution of beta-lactamases from penicillin-binding proteins*. J Am Chem Soc, **2003**. 125(32): p. 9612-8.12904027

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PEER-REVIEWED ABSTRACTS

ABSTRACTS AND SYMPOSIA

- (III) Professional Service: Not applicable.
- (IV) Integration of aspects of faculty work: Not applicable.