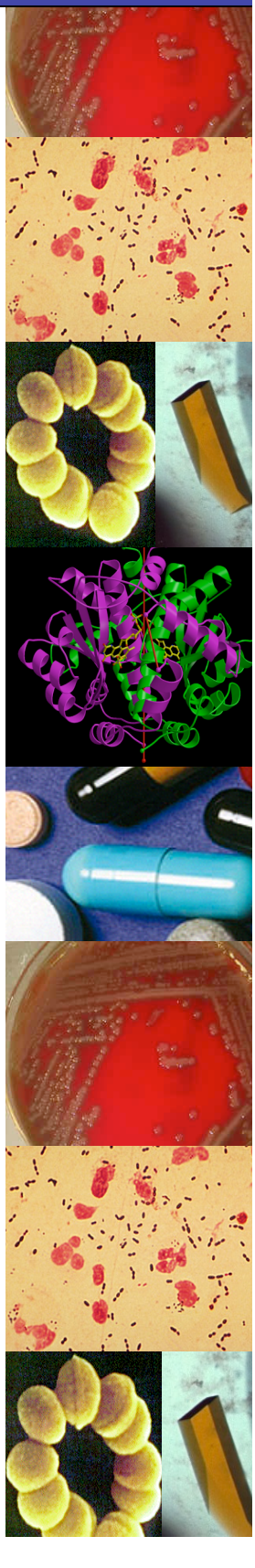
Webster Centre for Molecular Research in Infectious Diseases Mini-Symposium Room 228 Biochemistry Department

UNIVERSITY of OTAGO
Te Whare Wānanga o Otāgo

"Protein dynamics, structure-aided drug design and theoretical protein chemistry"

Wednesday 5 December 2007

9.15 am – 9.30 am	**Welcome, Introductory Comments** (Kurt Krause)
9.30 am	**Dr Joel Tyndall** **Lecturer, School of Pharmacy** **University of Otago** Crystal Structures of Highly Constrained Substrate and Hydrolysis Products Bound to HIV-1 Protease. Implications for Catalytic Mechanism and Drug Design.
10.00 am	**Professor Terry Lybrand** **Department of Chemistry** **Vanderbilt University** Molecular simulation of cyclooxygenase-inhibitor complexes: Insights into inhibitor binding and selectivity
10.30 am	Break
10.45 am	"Keynote Speaker" **Professor J. Andrew McCammon** University of California at San Diego Integrated Computational Biology: From the Molecule to the Cell.
11.30 am	**Professor Michael Gilson** **Centre for Advanced Research in Biotechnology** **University of Maryland Biotechnology Institute** Entropy, affinity and the design of targeted molecules
12.15 pm	**Roundtable "Future of Computational Biology in Protein Research and Drug Design"** **Conclusion**
1.00 pm	**Lunch**



RSVP : **to Teena Joyce (teena.joyce@stonebow.otago.ac.nz) by Monday 3 December 2007**

Webster Centre for Molecular Research in Infectious Diseases Mini-Symposium

UNIVERSITY of OTAGO
Te Whare Wānanga o Otāgo

Professor Michael Gilson
CARB Fellow and Professor
Center for Advanced Research in Biotechnology
University of Maryland Biotechnology Institute
A.B. Bioengineering, Harvard College, 1981.
Ph.D. Biochemistry and Molecular Biophysics 1988. Columbia University, New York, NY.
M.D. 1989. Columbia University College of Physicians and Surgeons, New York, NY
Medicine Residency 1989-1991. Stanford University, Palo Alto, CA.
Howard Hughes Physician Postdoctoral Fellowship, 1991-1994. With Prof. J. A. McCammon, Department of Chemistry, University of Houston, Houston, TX.
CARB Fellow, NIST Research Chemist & Adjunct Assistant Professor, University of Maryland Biotechnology Institute, Rockville, MD, 1994- 1999.
CARB Fellow and Associate Professor, University of Maryland Biotechnology Institute, Rockville, MD, 2000 - 2001.
Founder and Chief Scientific Officer, VeraChem LLC, Gaithersburg, MD, 2000 – 2007.
CARB Fellow and Professor, University of Maryland Biotechnology Institute, Rockville, MD, 2001 - present.

Professor Terry P. Lybrand
Vanderbilt University
Professor of Chemistry, College of Arts & Science
Professor of Pharmacology, School of Medicine
Prof. Lybrand obtained his Ph.D. in pharmaceutical chemistry at the University of California, San Francisco, in 1984 with the late Prof. Peter A. Kollman (Dr. Lybrand was Prof. Kollman's first graduate student at UCSF). He then pursued postdoctoral studies with Prof. J.A. McCammon at the University of Houston from 1985 until 1987. He next moved to the University of Minnesota, where he was a Senior Fellow at the Minnesota Supercomputer Institute for three years. In 1990, he moved to the University of Washington in Seattle as an assistant professor in the Department of Bioengineering, where he remained for over 10 years. In late 2000, he moved to Vanderbilt University as a founding faculty member of the new Center for Structural Biology. His research involves detailed computational and molecular modeling studies of protein-ligand interactions and enzyme reaction mechanisms. His research group also develops software for molecular modeling and molecular graphics applications.

Professor J. Andrew McCammon
Investigator, Howard Hughes Medical Institute
Investigator, NSF Center for Theoretical Biological Physics
Joseph E. Mayer Professor of Theoretical Chemistry
Distinguished Professor of Pharmacology
University of California at San Diego
J. Andrew McCammon is the Joseph E. Mayer Chair Professor of Theoretical Chemistry and Distinguished Professor of Pharmacology at UCSD, and is an Investigator of the Howard Hughes Medical Institute. He received his B.A. from Pomona College, and his Ph.D. in chemical physics from Harvard University, where he worked with John Deutch. In 1976-78, he developed the computer simulation approach to protein dynamics in Martin Karplus's lab at Harvard. He joined the University of Houston as Assistant Professor of Chemistry in 1978, and became the M.D. Anderson Chair Professor of Chemistry in 1981. He moved to UCSD in 1995. Professor McCammon has invented theoretical methods for accurately predicting and interpreting molecular recognition, the rates of reactions, and other properties of chemical systems. In addition to their fundamental interest, these methods play a growing role in the design of new drugs and other materials. Professor McCammon is the author with Stephen Harvey of "Dynamics of Proteins and Nucleic Acids" (Cambridge University Press), and is the author or co-author of more than 500 publications in theoretical chemistry and biochemistry. About 50 of his former students have tenured or tenure-track positions at leading universities or research institutes. In the 1980's, Professor McCammon guided the establishment of the computer-aided drug discovery program of Agouron Pharmaceuticals (now Pfizer Global Research and Development, La Jolla Laboratories), and contributed to the development of the widely prescribed HIV-1 protease inhibitor, Viracept. The McCammon group's studies of HIV-1 integrase flexibility contributed to the discovery of the first in a new class of antiviral drugs by Merck & Co., named Isentress (raltegravir) and approved by the US FDA in 2007. Professor McCammon received the first George Herbert Hitchings Award for Innovative Methods in Drug Design from the Burroughs Wellcome Fund in 1987. In 1995, he received the Smithsonian Institution's Information Technology Leadership Award for Breakthrough Computational Science, sponsored by Cray Research. He is the recipient of the American Chemical Society's 2008 national award for computational chemistry. He is a Fellow of the American Academy of Arts and Sciences, the American Association for the Advancement of Science, the American Physical Society, and the Biophysical Society.

Dr. Joel Tyndall
Senior Lecturer
Scool of Pharmacy
University of Otago
Dr Joel Tyndall is a Senior Lecturer in the School of Pharmacy at the University of Otago. His work is in the area of computational biology, pharmacophore analysis, structure-aided drug design and structural biology. He graduated from Monash University in 1994 with a BSc (Hons) and a PhD from the University of Queensland in 2000. Distinctions include winning an Anglo-Australian Postdoctoral Fellowship in 2000, an APA scholarship in 1996, a Centre for Drug Design and Development Scholarship in 1996 and a Faculty Scholar Award from Monash in 1994.