MURPA Seminar 18 August 2011 at 9am: Nasty Beasties: Computer-aided Drug Discovery for Infectious Diseases.

Venue: Room 135, Building 26 Monash Clayton

Presenter: Prof J. Andy McCammon, Joseph E. Mayer Chair Professor of Theoretical Chemistry and Distinguished Professor of Pharmacology at UCSD,

ABSTRACT: This lecture will provide a general introduction to some of the ways that modern theoretical and computational chemistry are contributing to the discovery of new pharmaceuticals, with special emphasis on drugs for infectious diseases. The basic sciences and computing technologies involved have advanced to the point that physics-based simulations of drug targets are now yielding truly valuable suggestions for new compounds.

Additional information and graphics can be found at http://mccammon.ucsd.edu/

BIO: 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. 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, 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 650 publications in theoretical chemistry and biochemistry. More than 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 (nelfinavir). 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 Computers in Chemical and Pharmaceutical Research. 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. He is a Member of the US National Academy of Sciences.