J. Andrew McCammon is an Investigator of the Howard Hughes Medical Institute and of the NSF Center for Theoretical Biological Physics at UCSD. He holds the Joseph E. Mayer Chair of Theoretical Chemistry at UCSD, and is a Professor of Pharmacology at the UCSD School of Medicine. He was born in Lafayette, Indiana in 1947. Professor McCammon received his B.A. from Pomona College, and his Ph.D. in chemical physics from Harvard University, where he worked with John Deutch on biological applications of statistical mechanics and hydrodynamics. In 1976-78 he was a research fellow at Harvard, where he developed the computer simulation approach to protein dynamics in collaboration with Martin Karplus. He joined the faculty of the University of Houston as Assistant Professor of Chemistry in 1978, and was promoted to Full Professor and appointed to the M.D. Anderson Chair in 1981. He moved to his faculty positions at UCSD in 1995.

Professor McCammon has developed novel theoretical methods for accurately predicting and interpreting molecular recognition, the rates of diffusion-controlled 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, enzymes, receptors, 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 about 500 publications on a variety of subjects in theoretical chemistry and theoretical biochemistry. About 50 of his former students now have tenured or tenure-track positions at leading universities or research institutes. As a consultant to industry, 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 development of a new class of potential antiviral drugs by Merck & Co.; these compounds entered clinical trials in 2005.

Professor McCammon has served on advisory boards for the National Academy of Sciences, the National Science Foundation, the National Institutes of Health, and other agencies. He received the first George Herbert Hitchings Award for Innovative Methods in Drug Design from the Burroughs Wellcome Fund in 1987. In 1991, he was the Centennial Lecturer at the University of Chicago. In 1995, he received the Smithsonian Institution’s Information Technology Leadership Award for Breakthrough Computational Science, sponsored by Cray Research. In 2002, he received the UCSD Chancellor’s Associates Award for Research. His other awards include an Alfred P. Sloan Fellowship, a Research Career Development Award from the National Institutes of Health, and a Camille and Henry Dreyfus Teacher-Scholar Award. 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.

Monday, October 6, 4pm

HIV/AIDS, Bird Flu and Other Nasty Beasties: Saving Lives Through Computer-Aided Drug Discovery

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.

Tuesday, October 7, 4pm

Rate Processes in Biophysics: From the Molecule to the Cell

This lecture will provide an overview of theoretical and computational methods for predicting the rates of diffusion-controlled reactions. The initial focus will be on enzyme-catalyzed reactions, including the effects of electrostatic steering in guiding substrates to active sites. Methods for dealing with supramolecular and subcellular systems will then be considered. Examples will include molecules and cells involved in neurotransmission.

Wednesday, October 8, 4pm

Enhanced Sampling: Atomistic and Coarse-grained

This lecture will describe a number of methods that are being used to greatly speed the sampling of molecular configurations for structural, thermodynamic and kinetic studies. The accelerated molecular dynamics simulation methods have proven to be very helpful in assessing the range of conformational fluctuations in atomistic models of proteins on the millisecond timescale, and in rapidly calculating free energies. Coarse-grained models, together with Brownian dynamics simulation, allow assessment of kinetic properties of complex systems, such as enzymes subject to crowding by other macromolecules.