

"Computational alchemist" J. Andrew McCammon joins UCSD as first holder of Joseph E. Mayer Chair in Theoretical Chemistry

November 3, 1994

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"COMPUTATIONAL ALCHEMIST" JOINS UCSD AS FIRST HOLDER OF JOSEPH E. MAYER CHAIR IN THEORETICAL CHEMISTRY

J. Andrew McCammon, a leading authority in the rational design of pharmaceuticals, will become the first holder of the Joseph E. Mayer Chair of Theoretical Chemistry at the University of California, San Diego.

McCammon will join the UCSD chemistry and biochemistry department, and the department of pharmacology at the UCSD School of Medicine, effective January 1. He comes to UCSD from the University of Houston where he was the M.D. Anderson Professor of Chemistry and director of the Institute for Molecular Design.

Several other researchers from his lab will join him at UCSD, including two senior scientists, four postdoctoral researchers and two graduate students.

McCammon said it was an honor to be named the Mayer Chair, "particularly since my official field is statistical mechanics, and Joseph Mayer was one of the great pioneers in this field."

UCSD Chancellor Richard C. Atkinson added: "This appointment is a direct reflection of the high regard held for Dr. McCammon by the UCSD academic community."

While at the University of Houston, McCammon invented what has become popularly known as "computational alchemy"--a method for predicting how molecules recognize and bind to one another. With this method, researchers use a computer model of a drug-receptor complex to change atoms from one kind into another. From these two alternatives, researchers can then calculate the relative binding strengths of the two drug-receptor complexes.

The method, for example, is being used to predict how a change or mutation in the common cold virus can weaken a drug's ability to bind with the viruses and combat them. Mutations such as these can lead to drug-resistant strains of pathogens.

Computer modeling methods developed by McCammon and others in his lab could help in redesigning drugs to restore their effectiveness in fighting such resistant strains. Among other things, McCammon's lab is attempting to design drugs to shut down the enzymes that help the AIDS virus break down a victim's immune system.

"At UCSD, we hope to increase our understanding of how complex molecules behave, based on theories of how their constituent atoms interact with one another," said McCammon.

"With time, this understanding should yield useful tools for designing pharmaceuticals, enzymes and antibodies for application in medicine, industry and agriculture."

McCammon cited several reasons for coming to UCSD, including the reputation of its faculty, a colony of young biotechnology and drug companies nearby, and the San Diego Supercomputer Center located on the UCSD campus.

"UCSD is long recognized as a leader in interdisciplinary work linking life sciences and physical sciences, which is what our group tries to do," McCammon said.

He noted that during the summer of 1964 he worked as a high school student at UCSD's Scripps Institution of Oceanography.

"I've wanted to be at UCSD ever since then, but it just took a while to happen," he said.

Much of McCammon's research involves the solution of computationally intense equations that can only be solved by supercomputers and then translated into visual images resembling motion pictures. In essence, McCammon uses the computer to simulate the activities and motions of molecules as they obey fundamental laws of physics.

"We try to mimic the behavior of atoms and molecules in the computer," he said. "We essentially make a mathematical model of a molecule."

Born in Lafayette, Indiana in 1947, McCammon received his B.A. in chemistry from Pomona College (where he was a "Times Scholar in Science" sponsored by the Los Angeles Times) and his M.A. and Ph.D. in physics and chemical physics from Harvard University.

While at Harvard, he worked with John Deutch on biological applications of statistical mechanics and hydrodynamics. Deutch currently serves as U.S. Deputy Secretary of Defense. From 1976-78, while an NSF and NIH research fellow at Harvard, McCammon collaborated with Martin Karplus in developing computer simulation approaches to protein dynamics.

He joined the University of Houston in 1978 where he was named to the Anderson Chair in 1981.

McCammon has received numerous awards and honors. In 1987, he garnered the first annual George H. Hitchings Award for Innovative Methods in Drug Design from the Burroughs Wellcome Fund. The award recognized McCammon's achievements in developing new theoretical methods for computer-aided design of drugs.

He also has received the Camille and Henry Dreyfus Teacher-Scholar Award (1982-87), the NIH Research Career Development Award (1980-85), an Alfred P. Sloan Research Fellowship (1980-84), and a Woodrow Wilson Fellowship (1969).

His professional organizations include the American Physical Society, the American Association for the Advancement of Science, American Chemical Society, Biophysical Society, Texas Mycological Society and Protein Society.

McCammon coauthored with S.C. Harvey the "Dynamics of Proteins and Nucleic Acids," published by Cambridge University Press.

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