Peter Kollman

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On May 25, 2001, Peter Kollman lost his battle with cancer, and the fields of computational chemistry and computational biochemistry lost a prominent leader. His fight was mercifully brief: one day he was giving lectures on quantum chemistry and playing basketball and the next he was diagnosed with incurable metastatic cancer of unknown origin.

Peter was absolutely devoted to science. His enthusiasm was contagious and he was an inspiring group leader. He had a very curious mind and always wanted to reach down to the molecular level and figure out how things worked. Peter was unusual because he was such a nice person, and without a trace of ego. He succeeded in his field through his high standards and tenacious pursuit of knowledge, not by attacking others. In this regard, he was a rare and wonderful role model who helped set the tone of scientific meetings and debate. In human terms, this characteristic may well be his greatest legacy.

Peter also leaves behind an impressive scientific legacy. He began his academic career in 1962 at Grinnell College, Iowa, going on to obtain his Ph.D. in 1970 with Lee Allen at Princeton. There he developed a love of hydrogen bonds that continued throughout his career. Peter would become ecstatic when confronted with a table of hydrogen bond statistics, mentally translating numbers into a molecular structure. He spent 1970–1971 as a NATO fellow at Cambridge with David Buckingham. In 1971, he joined the faculty at the University of California, San Francisco, bringing his rigorous quantum mechanical training on small molecules to the macromolecular world of proteins and nucleic acids.

From 1981–1997, Peter was the 11th most highly cited chemist in the world according to the Institute for Scientific Information. Peter's almost 500 publications involve nearly 350 different collaborators, a clear testament to his enthusiasm and desire to share his love of science. He is probably best known for the molecular

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simulation package AMBER (Assisted Model Building with Energy Refinement). Peter's goal in developing this software was not only to use it for his own research but also to create a tool that would give everyone the ability to perform calculations of chemicals and biomolecules. In this he was successful: AMBER is used by hundreds of academic and industrial groups worldwide and is the most widely used and cited package for macromolecular simulation.

Peter's scientific achievements are many, spanning ~35 years. One of his earliest contributions involved the spectroscopic properties of small water clusters. Two of his most recent achievements also involved water, this time in the presence of biological macromolecules: in 1995 he simulated the A to B transition of DNA in aqueous solution and in 1998 he carried out the longest (1 μs) molecular dynamics simulation of a small protein in water to date. These applications were always complemented by careful computational chemistry on molecular components, such as his 1990 method to derive atomic charges using semi-empirical methods and his 1995 study of non-additive effects in cation–π electron cloud interactions, an area of particular importance for protein–drug interactions.

One of Peter's most important contributions was his work in the area of free energy perturbation calculations. In 1987, he was the first to apply this technique to macromolecules and he spent years improving the technique making it widely useful. Peter was extremely excited by this work because it linked simulations with experiment, or as he put it, it made them 'full partners'. Such was his philosophy: he sought to bring disparate approaches, fields, and even people together. We have all suffered a great loss due to his unsuccessful battle with cancer.

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