Obituary

Peter A. Kollman, 1945–2001

Peter A. Kollman passed away on May 25, 2001, at the age of 56, shortly after being diagnosed with cancer. While his death leaves an empty space in the computational chemistry community, it also gives us the occasion to celebrate the now-completed opus of his life. From the standpoint of the fashionable "scientific statistics," his contribution was prodigious: over his 31-year career he was an author on more than 400 journal articles (more than one per month, on average), and more than 50 reviews and chapters, and he was the 11th most-cited chemist between 1981 and 1997. Over most of this time he was a Professor of Chemistry and Pharmaceutical Chemistry at the University of California at San Francisco, starting in 1971 and becoming full professor in 1980. Prior to this, he was a postdoctoral fellow with David Buckingham (Cambridge), following his Ph.D. with Leland Allen (Princeton). At UCSF, his early work using quantum chemistry to examine hydrogen bonding slowly evolved toward molecular mechanics methods, leading to the development in his laboratory of the AMBER suite of programs in 1981 and an associated general force field in 1984. He continued the development of the program, refusing to concede exclusive rights for its development commercially so he could ensure its availability to the academic community. He has since welcomed the efforts of many collaborators, especially the major involvement of David Case at Scripps, in developing the program. It is today one of the most widely used academic packages for biomolecular simulation, applied in over 1000 academic and industrial laboratories.

He maintained up to his death a strong effort in force field development as a main focus of his research, refining his "simple but general" two-body additive model, still widely used today, and then pressing forward beyond the two-body approximation into polarizable force fields. His sense of the importance of electrostatics led to his championing the use of atomic charges fit from a quantum-mechanically-derived electrostatic potential, and the incorporation and use of Ewald sums, to capture critical long-range effects. He had an uncanny ability to discern which experimental data and which chemical interactions were the most important to account for; this allowed his force fields to maintain surprising accuracy and generality given the simplicity of his approach in both functional form and parameterization. This, together with his insistence on generality of overall approach (e.g. for atomic charge fitting), enabled his group to tackle with equal facility a wide spectrum of applied problems involving proteins, nucleic acids, and small molecules. Another major turning point in his research came with the incorporation of free-energy calculations into AMBER in 1987. Recognizing the importance to the biological community of calculating relative free energies of binding, Peter's research group began a sustained effort in this area, applying slow-growth perturbation and the more rigorous free-energy perturbation methods, using windows or thermodynamic integration, to a diverse variety of protein, nucleic acid, and small-molecule problems. Recently, he had been extending approximate free-energy methods to include enhanced sampling and continuum dielectric methods (the latter again to improve the treatment of long-range electrostatics), culminating in the MM-PBSA method.

While he will certainly be remembered for his excellent science and breadth of knowledge, for those who knew him personally his legacy will be as much associated with his strength of character and *joie de vivre*. He fearlessly tackled a wide spectrum of biological problems, many of them daunting in their complexity. Often challenged on the validity of applying his then-current methodologies to a particularly challenging problem, Peter was always very open with a careful and knowledgeable assessment of the limitations of the methods, but never failed in his optimism that these problems could nevertheless be modeled in a meaningful way. He was widely acknowledged by students, post-docs, and faculty alike as being universally encouraging to those with whom he was in any kind of supervising or mentoring capacity. Going over your project with him one-on-one, after the fast-paced scientific discussion examining issues in the project and making suggestions, he would inevitably conclude by reiterating the progress made (no matter how small), and "cheer-lead" you on to more. In group meetings, on occasions when a presentation by a post-doc or student exposed to the group a potentially embarrassing shortcoming in their approach, Peter would always give grace. His face would adopt a studied, slightly puzzled expression and he would say something like, "I don't quite understand why you did [description of shortcoming]; why don't you take another look at [references] and maybe talk to [group expert on issue] later"; then he would change the topic. Experienced group members came to recognize this form; everyone appreciated it (especially the person up front). With successes, Peter was always generous in his recognition and praise of those involved, both in public and in private. A gregarious man, his booming voice and ready laughter attracted a crowd at any kind of professional or social meeting. His positive approach has had a lasting impact on those who passed through his laboratory and serves for many as a model of scientific interaction. Even as we miss him deeply, we can rejoice at his rich life and count ourselves lucky to have had him with us.

Christopher I. Bayly
Merck Frosst Canada & Co.

Former postdoctoral fellow with Peter Kollman at UCSF

Editorial note: At the time of his death, Peter Kollman was a member of the *Biophysical Journal* Editorial Board. With his passing the *Journal* has lost a counselor whose wisdom and energy will be sorely missed.