

Thomas Terwilliger named as the recipient of the 2013 ACA Ken Trueblood Award



The ACA Trueblood Award recognizes exceptional achievement in computational or chemical crystallography. Thomas C. Terwilliger has made brilliant contributions to the community of crystallographers through his software that permits the nearautomatic determination of molecular structures. His deep understanding of chemical crystallography, statistics, and computer codes has enabled him to produce a

string of programs that have helped to transform the field of macromolecular structure determination.

Among his innovations are the following: *HASSP*: First automated analysis of difference Patterson functions to find heavy-atom sites. *SOLVE*: first Bayesian estimates of heavyatom structure factors from MAD data; analysis of MIR phasing including correlated non-isomorphism; and automated structure solution (finding sites through calculation of an electron density map) for macromolecular structure solution by MIS/MAD/ SAD. *SOLVE*, *PhenixAutoSol wizard*: first systematic set of criteria for automatic assessment of the quality of electron density maps. *RESOLVE*: first rapid and automated procedure for finding non-crystallographic symmetry from heavy-atom sites. *RESOLVE maximum-likelihood density modification:* first Bayesian approach for density modification. *RESOLVE build script:* first procedure capable of map improvement at moderate resolution (2.5-3Å) by iterative model-building, density modification and refinement.

Tom's programs execute with a minimum of required intervention. He has achieved this by incorporating statistical deicision making ("Wizards") into the software. His programs, along with advances in instrumental automation, are one of the major reasons that the structural genomics side of macromolecular crystallography has been able to move ahead. One or more of his programs has been used in many of these structures, as demonstrated by the number of research papers that cite his work.

Ken Trueblood, while brilliant and multitalented, was modest, generous, and devoted to community. He sent out his programs to any scientist who asked and he loved to teach, always making students' needs his first priority. Tom Terwilliger has also been known to put his research aside and help anyone who comes to him for help with one of his programs or some crystallographic problem. He has been dedicated to the dissemination of his work for the benefit of others and has worked in the community to bring about the successes of structural genomics.

Tom has been selected for this award partly because he fits the Trueblood model of generosity and service, but even more because of his brilliant contributions to crystallographic computing.