

Design, Development and Applications of the MEAD Suite for Macromolecular Electrostatics

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MEAD (Macroscopic Electrostatics with Atomic Detail) is an Object oriented software suite for linear Poisson--Boltzmann modeling of electrostatic effects in macromolecules. MEAD is free software: it has been distributed under the GNU General Public License since its appearance in 1992. Applications include pKa prediction, MM/PBSA analysis, and hybrid calculations with quantum mechanical treatment of active sites. The core of MEAD is an object-oriented C++ library whose classes correspond to the entities of the electrostatic theory and the macromolecule: electrostatic potentials, dielectric and electrolyte environments, charge distributions and sets of atoms. We have recently streamlined and documented the library to facilitate modification by the user community. Improvements to the methods include a robust solvent-accessible-volume definition in terms Delaunay triangulations. A Python interface, developed using SWIG, closely follows MEAD's own object oriented design and enables rapid development of higher-level programs or prototypes. We have also developed PyAmber, a Python library for manipulating Amber molecular mechanics models. A stand-alone MM/PBSA application in both Python and C++ has been developed.