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Using side-chain models derived from atomic resolution X-ray crystallography to develop force fields which can predict global energy minimum geometries

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Prediction of low energy conformers in a protein is a challenging computational problem because the energy depends on a large number of intermolecular interactions. Each conformer will experience a very different set of interactions and the energies of these must be determined accurately to find a minimum. The energies depend on the accuracy of the geometry and the competence of the mathematical modeling of potential energy. To learn how to compute these energies, we are exploring energy functions using a large set of models of amino acids models with diverse contact shells. The models are derived from atomic resolution protein crystallography and are extremely accurate. The initial test set consists of models of amino acids plus neighboring residues. Conformers are generated using a modified allegrow. These are tested using energy minimization using an empirical geometry optimization force field and additional energy terms. Preliminary results show that results for polar side-chains depend on the solvation state. Published methods for adding explicit solvent and creating optimum hydrogen bonding networks to each conformational model are being tested.

Biography

Regine S. Bohacek is founder and owner of Boston Denovo.com and has published extensively in the field of computational chemistry with a particular interest in de novo methods and structure based design

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