Zhaomin Liu et al., Med chem 2016, 6:10(Suppl)
http://dx.doi.org/10.4172/2161-0444.C1.027

Evaluating small molecules potential energy through the long standing chemical principles

Zhaomin Liu and **Nicolas Moitessier**
McGill University, Canada

Molecular mechanics (MM)-based methods evaluate relative potential energies of given molecules and various conformations by summing the bonding and non-bonding interactions described by a set of functions and parameters. These parameters are often derived from computational and/or experimental data for large training sets of small molecules. Modeling systems with molecules structurally close to those of the training set is expected to provide accurate results. However, structurally different molecules including some potential drug candidates may not be parameterized properly. One way to address this issue is to continuously develop parameters covering more diverse molecules. Alternatively, we could study the origins of the conformational behaviors of molecules and seek for rules to derive parameters. Chemical principles such as steric clashes, hyperconjugation, inductive and resonance effects are applied qualitatively to rationalize experimental observations over decades. We proposed to develop predictive methods through those long standing principles. We will present our efforts to understand and quantify chemical principles and then develop rules to derive MM parameters. Personalized parameters are generated on-the-fly from atomic properties.

Biography

Zhaomin Liu has obtained his MSc in Chemistry at Southern Illinois University Edwardsville focusing on protein modeling and structure-based studies of G-protein coupled receptors. He continued his studies at McGill University for his PhD with Prof. Nicolas Moitessier and his current research is on drug design and software refinement targeting nucleic acids and on molecular mechanics development, deriving molecular mechanics terms from fundamental principles.

zhaomin.liu@mail.mcgill.ca

Notes: