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AtomicChargeCalculator: interactive web-based calculation of atomic charges in large biomolecular complexes and drug-like molecules

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Abstract

Background: Partial atomic charges are a well-established concept, useful in understanding and modeling the chemical behavior of molecules, from simple compounds, to large biomolecular complexes with many reactive sites.

Results: This paper introduces AtomicChargeCalculator (ACC), a web-based application for the calculation and analysis of atomic charges which respond to changes in molecular conformation and chemical environment. ACC relies on an empirical method to rapidly compute atomic charges with accuracy comparable to quantum mechanical approaches. Due to its efficient implementation, ACC can handle any type of molecular system, regardless of size and chemical complexity, from drug-like molecules to biomacromolecular complexes with hundreds of thousands of atoms. ACC writes out atomic charges into common molecular structure files, and offers interactive facilities for statistical analysis and comparison of the results, in both tabular and graphical form.

Conclusions: Due to high customizability and speed, easy streamlining and the unified platform for calculation and analysis, ACC caters to all fields of life sciences, from drug design to nanocarriers. ACC is freely available via the Internet at http://ncbr.muni.cz/ACC.

Keywords: Conformationally dependent atomic charges, Biomacromolecules , Drug-like molecules, Paracetamol, Benzoic acids, Protegrin, Proteasome, Allostery, Chemical reactivity

Background

Partial atomic charges are real numbers meant to quantify the uneven distribution of electron density in the molecule, and have been used for decades in theoretical and applied chemistry in order to understand the chemical behavior of molecules. Atomic charges are extensively used in many molecular modeling and chemoinformatics applications. With respect to biomacromolecules, charges can elucidate electrostatic effects critical for long range molecular recognition phenomena, protein folding, dynamics and allostery, directed adduction of substrates and egression of products in enzymes, ligand binding and complex formation for proteins and nucleic acids, etc. [1–3]. With respect to drug-like molecules, atomic charges provide information related to reactivity and can be used in the prediction of various pharmacological, toxicological or environmental properties [4, 5].

Although, in principle, it is possible to estimate atomic charges based on experimental measurements (e.g., [6, 7]), such calculations are impractical. Most commonly, atomic charges are estimated based on theoretical approaches. Quantum mechanical (QM) approaches first solve the Schrödinger equation [8] and calculate the electron density using a combination of theory level and basis set. They then partition the obtained molecular

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