Vladimir Potemkin, Med chem (Los Angeles) 2018, Volume 8
DOI: 10.4172/2161-0444-C1-038

Vladimir Potemkin

South Ural State University, Russia

CoMIn to molecular interior-quantum and intermolecular potentials based approaches for rational virtual drug design

A series of grid-based computational technologies for Continual Molecular Interior analysis (CoMIn) is proposed in the presentation. The analysis is fulfilled using a lattice construction analogously to other grid-based methods. The further continual elucidation of molecular structure is performed in two ways: in the terms of intermolecular interactions potentials, e.g. a superposition of Coulomb, Van der Waals interactions and hydrogen bonds. All the potentials are known continual functions and their values can be determined in any point of space; in the terms of quantum functions, e.g. electron density, Laplacian, Hamiltonian, potential energy distribution, the highest occupied, the lowest unoccupied orbitals distribution and their superposition. All the functions can be calculated using a quantum approach at a sufficient level in any point of space. To reduce time of calculations using first principles quantum methods, an original quantum free-orbital approach AlteQ is proposed. Then, the molecules of a dataset can be superimposed in the lattice for the maximal coincidence (or minimal deviations) of the potentials or the quantum functions. The methods and criteria of the superimposition are discussed. Then, a relationship between bioactivity and characteristics of potentials or functions is created. The methods of the relationship construction are discussed. New approaches for rational drug design based on the intermolecular potentials and quantum functions are invented. All the invented methods are present at www.chemosophia.com web page.

Biography

Vladimir Potemkin has completed his PhD at South Ural State University and Postdoctoral studies from Computer Chemistry Center- Erlangen-Nurnberg University, Germany. He is the Head of Laboratory of Computational Modeling of Drugs. He has published more than 80 papers in reputed journals.

potemkinva@susu.ru

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