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Is it possible to improve considerably the accuracy of docking programs?

Protein-ligand binding free energy calculation is one of the key problems for molecular modeling in the computer-aided structural based drug design. Only with accuracy better than 1 kcal/mol of the protein-ligand binding free energy calculations it is possible to perform the rational inhibitor optimization on the basis of computer modeling. However such high accuracy has not been reached yet for a randomly selected target protein by any docking programs. It is not surprising because this accuracy depends on many interrelated factors in a complicated manner. Those factors are: the force field describing inter- and intra-molecular interactions, the water model, the target protein and ligand models, method and approximations of the free energy calculation, algorithms of calculations and computing resources concentrated on solving the docking problem for one protein-ligand pair, etc. The results of binding energy calculations within the multi-well approximation (protein-ligand and free ligand low energy local minima spectra are taken into account when the binding energy is calculated) will be presented for a set of protein-ligand complexes using MMFF94 force field, quantum-chemical method PM7 and implicit water models. Comparison of calculated and experimental energies is presented. The roles of the ligand strain energy, the de-solvation energy and the ligand vibrations are discussed. The broad discussion of the subject is invited.

Biography

Vladimir Sulimov has completed his from Lomonosov Moscow State University in 1979 and he received the degree Doctor of Sciences in Physics and Mathematics in 1997 from Prokhorov General Physics Institute. He is the Head of the Lab at Research Computer Center of Lomonosov Moscow State University. He has published more than 220 papers in reputed journals with 40 years of theoretical research. His recent research activities are molecular modeling in structural-based drug design, development of docking programs and their application for new inhibitors design. He is Founder and CEO of private Russian research company Dimonta, Ltd.

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