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Protein-ligand low energy minima pose analysis: Docking target functions evaluation with the FLM program

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Choice of the reliable docking target function for the ligand positioning in the protein active site is the important goal of the structural-based computer aided drug design. The target function minima were compared with the experimentally known pose of the ligand in the protein active site. Five target functions were evaluated "as is", i.e. without any fitting parameters on the base of MMFF94 force field, quantum-chemical semiempirical PM7 method and also taking into account several implicit solvent models: PCM, COSMO, Surface GB. Low-energy minima of 16 protein-ligand complexes were found by the original Monte Carlo MPI-based FLM docking program for these target functions examination. The protein is considered as rigid and the ligand is fully flexible, and 105–106 local optimizations were conducted for one protein-ligand complex and 103–104 different minima were chosen into the low energy minima set. About 25 000 CPU*hours per one minima set were consumed during these calculations, overall it was consumed several millions CPU* hours. The importance of solvent accounting for the correct ligand positioning is convincingly demonstrated. Also some improvement of the ligand positioning occurs when MMFF94 force field is substituted by the semiempirical quantum chemical method PM7 with COSMO solvent model.

Biography

Vladimir Sulimov has completed his at the age of 30 years from Lomonosov Moscow State University and he received Doctor of Sciences in Physics and Mathematics degree 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 during more than 40 years of theoretical research in fields of semiconductors, computer modeling, semiconductor devices, fiber optics, non-linear optics, quantum chemistry of solids, and molecular modelling in structural-based drug design.

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