Research report

Computational Biochemistry (2011-2016)

Overview

PI

Jun.-Prof. Dr. M. Korth, Institute for Theoretical Chemistry, Ulm University, Germany

Research fields

Quantum Biochemistry

Publications

Articles / published (peer reviewed)

N. D. Yilmazer, **M. Korth**, Prospects of applying enhanced semi-empirical QM methods for virtual drug design, *Curr. Med. Chem.* **2016,** *23,* 2101. (Invited review.)

N. D. Yilmazer, **M. Korth**, Recent progress in treating Protein-Ligand interactions with quantum-mechanical methods, *Int. J. Mol. Sci.* **2016,** *17,* 742. (Invited review.)

N. D. Yilmazer, **M. Korth**, Enhanced semiempirical quantum-mechanical methods for biomolecular interactions, *Comp. Struct. Biotech. J.* **2015,** *13,* 169. (Invited mini-review.)

N. D. Yilmazer, P. Heitel, T. Schwabe, **M. Korth**, Benchmark of electronic structure methods for protein-ligand interactions based on highlevel reference data, *J. Theor. Comput. Chem.* **2015,** *14,* 1540001.

J. C. Kromann, A. Christensen, C. Steinmann, **M. Korth**, J. H. Jensen, A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+, *PeerJ* **2014,** *2,* e449.

N. D. Yilmazer, **M. Korth**, Comparison of Molecular Mechanics, Semi-Empirical Quantum Mechanical, and Density Functional Theory Methods for Scoring Protein-Ligand Interactions, *J. Phys. Chem. B* **2013,** *117,* 8075. (Computational chemistry highlight November 2013.)

M. Korth, A quantum chemical view of enthalpy-entropy compensation, *Med. Chem. Commun.* **2013,** *4,* 1025.

M. Korth, Error estimates for (semi-)empirical dispersion terms and large biomacromolecules, *Org. Biomol. Chem.* **2013,** *11,* 6515.

M. Korth, Empirical Hydrogen-Bond Potential Functions – An Old Hat Reconditioned, *Chem. Phys. Chem.* **2011,** *12,* 3131–3142. (Invited mini-review, including original research.)