

## Research report

2013

### Overview

#### PI

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

#### Research fields

Quantum Biochemistry

Citizen Cyber Science

### Publications

#### Articles / published (peer reviewed)

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.