Monte Carlo simulation and thermodynamic integration applied to protein charge transfer

Jan Kaiser, Mike Castellano, David Gnandt, Thorsten Koslowski

Institut für Physikalische Chemie, Universität Freiburg

We introduce a combination of Monte Carlo simulation and thermodynamic integration methods to address a model problem in free energy computations, electron transfer in proteins [1]. The feasibility of this approach is tested using the ferredoxin protein from *Clostridium acidurici*. The results are compared to numerical solutions of the Poisson-Boltzmann equation and data from recent molecular dynamics simulations on charge transfer in a protein complex, the NrfHA nitrite reductase of *Desulfovibrio vulgaris* [2]. Despite the conceptual and computational simplicity of the Monte Carlo approach, the data agree well with those obtained by other methods. A link to experiments is established *via* the cytochrome subunit of the bacterial photoreaction centre of *Rhodopseudomonas viridis*.

[1] J. Kaiser, M. Castellano, D. Gnandt, T. Koslowski, J. Comp. Chem., in press, doi: 10.1002/jcc.26155

[2] G. Gnandt, S. Na, T. Koslowski, Biophys. Chem., **2018**, 241, 1-7