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Coarse-grained molecular models for high-throughput and multi-scale functional investigations

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In this contribution we discuss the development, implementation, and the subsequent application of *in silico*, coarse-grained molecular models. The proposed approach allows for bridging a methodological gap between sequence-based bioinformatics and molecular dynamics simulations: molecular interactions can be modeled based on physio-chemical model in a highly parallelizable and high-throughput-ready fashion.

We demonstrate the broad applicability of such an approach by discussing the assembly of the bacterial ribosome [1] and potential points of interference by antibiotica, HIV protease [2] and its evolutionary dynamics en route to drug resistance [3]. These methodologies were further applied to a signaling cascade in leukemia [4,5] and can be used for design by e.g. global optimization techniques [6]. In addition we show recent results on further computational improvements and additional observations from a physicist's/chemist's point of view.

References

1. Hamacher K, Trylska J, McCammon JA: **Dependency Map of Proteins in the Small Ribosomal Subunit.** *PLoS Comput Biol* 2006, **2:**e10.
2. Hamacher K, McCammon JA: **Computing the Amino Acid Specificity of Fluctuations in Biomolecular Systems.** *J Chem Theo Comp* 2006, **2:**873.
3. Hamacher K: *Gene* 2007. submitted
4. Hamacher K, Hübsch A, McCammon JA: **A minimal model for stabilization of biomolecules by hydrocarbon cross-linking.** *J Chem Phys* 2006, **124:**164907-164914.
5. Hamacher K: **Information Theoretical Measures to Analyze Trajectories in Rational Molecular Design.** *J Comp Chem* 2007, **28:**2576-2580.
6. Hamacher K: **Adaptation in Stochastic Tunneling Global Optimization of Complex Potential Energy Landscapes.** *Europhys Lett* 2006, **74:**944-950.
7. Hamacher K: **Energy landscape paving as a perfect optimization approach under detrended fluctuation analysis.** *Physica A* 2007, **378:**307-314.