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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 antibiotics, 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.

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