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Artifact or reality? Force field issues in the simulation proteins and nucleic acids¹

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Access to ever-increasing computational power is providing the means to critically evaluate the performance of atomistic force fields of biomolecules. With greater sampling, and more detailed comparisons to experiment, limitations and artifacts in the applied simulation protocols and force fields can be discovered and ultimately overcome. Additionally, we are able to more carefully validate and assess the performance of the simulations in comparison with experiment. In this talk, we will outline our experiences in large-scale simulations of protein and nucleic acid systems in the context of the AMBER biomolecular simulation program. Issues related to salt and dihedral parameters will be highlighted in applications ranging from ligand-induced remodeling of dihydrofolate reductase and cytochrome P450 2B4 protein structures to large-scale decoy sets and NMR comparisons of various RNA structures.

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