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Optimizing Proteins and Ligands for Computerized Drug Discovery

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Abstract

The reliability of physics-based in-silico studies of protein-ligand complexes highly depends on the quality of available structures and force-field parameters. Both these subjects have been largely addressed by both experimental and computational scientists from industry and academia. Yet, tasks like obtaining an initial structure with the correct protonation states and hydrogen-bond network or accurate force-field parameters for a given ligand can still be out of reach for the non-experts in those particular fields. Here we showcase two software tools that aim at bridging this gap: *proteinPrepare* [1,2] and *parameterize*. We show how these softwares can be easily used by the community and how we are integrating these tools within a wider computational pipeline for drug discovery.

Stefan Doerr, Toni Giorgino, Gerard Martínez-Rosell, João M. Damas, and Gianni De Fabritiis. High-Throughput Automated Preparation and Simulation of Membrane Proteins with HTMD. Journal of Chemical Theory and Computation 2017 13 (9), 4003-4011. DOI: 10.1021/acs.jctc.7b00480

Gerard Martínez-Rosell, Toni Giorgino, and Gianni De Fabritiis. PlayMolecule ProteinPrepare: A Web Application for Protein Preparation for Molecular Dynamics Simulations. Journal of Chemical Information and Modeling 2017 57 (7), 1511-1516. DOI: 10.1021/acs.jcim.7b00190

Keywords

MD simulations, drug discovery, force-fields, protein preparation