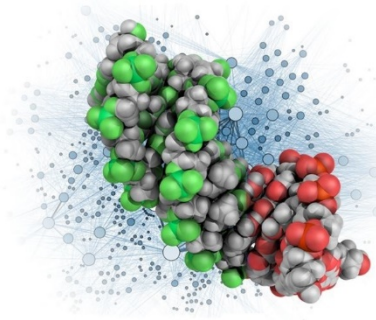

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QwikMD – easy and fast molecular dynamics simulations with VMD and NAMD

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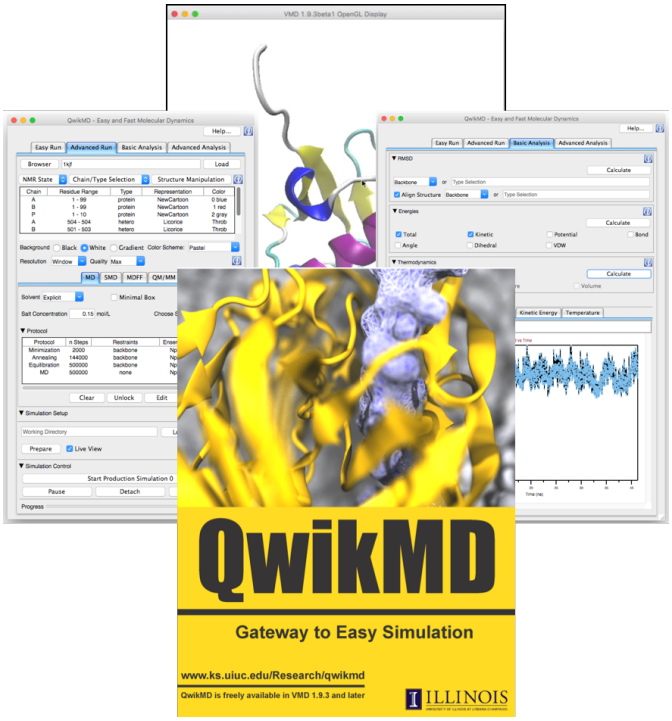
Graphical Abstract *(mandatory)*



Abstract. *(mandatory)*

"Everything that living things do can be understood in terms of jigglings and wigglings of atoms." Richard Feynman's remarks in the early 1960's summarize what is today widely accepted, namely, that biological processes can be described by the dynamics of biomolecules. Molecular dynamics (MD) simulation, in this regard, is the main methodology employed in structural biology to explore the dynamical behavior of macromolecules at a microscopic level. Aided by MD, researchers have been able, for instance, to resolve atomic structures of multi-protein complexes from cryo-EM densities, thus unveiling the atomistic details of enzymatic mechanisms and characterize the binding of small molecules to proteins. To achieve all this, the capabilities of MD packages are constantly evolving, providing a multitude of complex

	simulation and analysis techniques, e.g., enhanced sampling and free energy calculations. Although applicable to a wide variety of research problems, a broader usage of MD is hindered by a steep initial learning curve imposed by nearly every MD software. To reduce this initial barrier and make the methodology more accessible to the general community of biomolecular researchers, we developed an intuitive tool named QwikMD (1), which assists the users in the preparation, execution, and analysis of biomolecular MD simulations. Among many other features, QwikMD automatically checks the initial structure for structural inconsistencies, facilitates structure manipulations such as point mutations and partial deletions, simplifies the protein insertion in lipid membranes and enables the visualization and analysis of MD simulations on the fly. The user-friendly graphical interface of QwiKMD allows the preparation of MD simulations in a point-and-click fashion, offering the user multiple MD protocols, such as unbiased MD simulations, Steered MD, MD Flexible Fitting (MDFF), and, most recently, hybrid QM/MM simulations. The latter exploits the recently developed VMD and NAMD interface to common quantum mechanics software packages. QwikMD facilitates performing MD simulations for nearly any user, novice or expert. While assisting the user, QwikMD ensures reproducibility of the results by recording all parameters and steps into two log files, one in a script-like format and another in a "methods section" format. QwikMD also serves as a learning tool, providing the theoretical background of the different MD protocols and options in many "info buttons".

References *(mandatory)*

1. J. V Ribeiro *et al.*, QwikMD — Integrative Molecular Dynamics Toolkit for Novices and Experts. *Sci. Rep.* **6**, 26536 (2016).