medical sciences forum

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Abstract

YAMACS: A Python Based Tool Kit for GROMACS †

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† Presented at the 8th International Electronic Conference on Medicinal Chemistry, 1–30 November 2022; Available online: https://ecmc2022.sciforum.net/.

Abstract: Molecular dynamics (MD) is a powerful tool used to study the evolution of molecular systems and predict their properties from the inherent interactions. GROMACS is a famous tool for MD and developed as open-source software. GROMACS is run from the command line with user-provided configuration files. However, the absence of a graphical user interface (GUI) of GROMACS and proper protocol to develop the input files (Ex: itp files, topology files, etc.) prevent the researcher from visualizing the MD trajectory in a real-time manner as well as addressing the structural problem. This issue was addressed by developing a graphical user interface of GROMACS as plugins for the YASARA molecular graphics suite, called YAMACS. YAMACS is an open-source project and is available on GitHub. The tool can perform MD simulations for protein, protein–ligand complexes, membrane–protein complexes, membrane–protein complexes, and small molecule systems. Easily YAMACS automatizes several steps of input file preparation and allows visualizing the MD trajectory in real-time. At this conference, I will present the application of YAMACS to simulate the complex sphingomyelin/POPC embedded in a membrane of POPC. I will also introduce a collaborative platform to create an open community of users and developers, extend the functionalities of YAMACS, and improve the quality of computational drug design studies.

Keywords: molecular dynamics; GROMACS; YAMACS; YASARA

Citation: Sarkar, A.; Sessa, L.; Di Biasi, L.; Piotto, S. YAMACS: A Python Based Tool Kit for GROMACS. *Med. Sci. Forum* **2022**, *14*, 98. https://doi.org/10.3390/ECMC2022-13433

Academic Editor: Alfredo Berzal-Herranz

Published: 1 November 2022

Supplementary Materials: The following are available online at https://www.mdpi.com/article/10.3390/ECMC2022-13433/s1.

Author Contributions: Conceptualization, S.P. and A.S.; methodology, A.S. and L.S.; validation, L.S. and L.D.B.; investigation, A.S.; writing—review and editing, A.S.; All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by POR CAMPANIA FESR 2014/2020 project MIND: Molecules Inhibiting Neurological Diseases, CUP B31B19001540007.

Data Availability Statement: Available online: https://sciforum.net/paper/view/13433.

Conflicts of Interest: The authors declare no conflict of interest.