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YAMACS: a graphical interface for GROMACS

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pharmaceuticals MDPI

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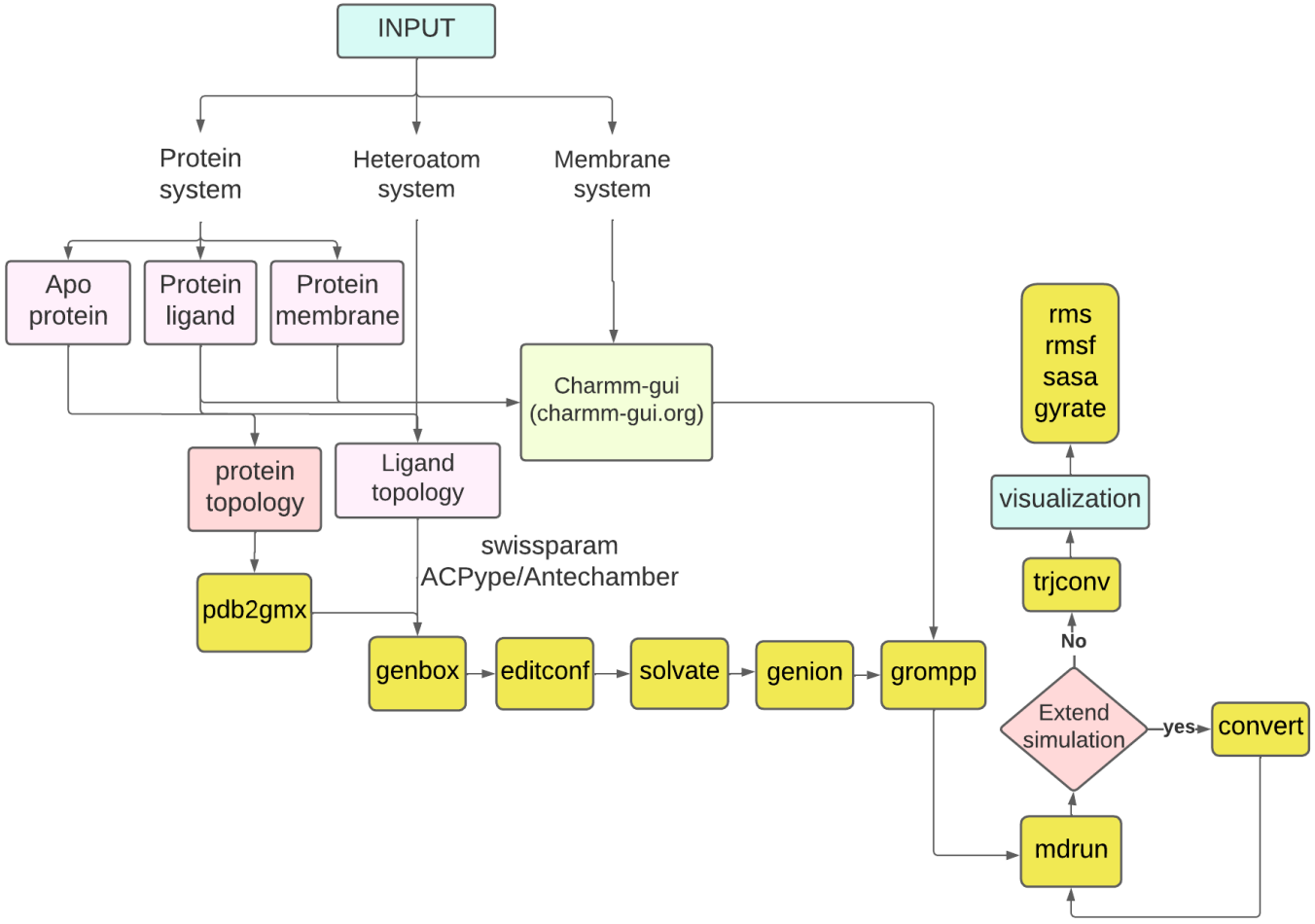
YAMACS: a graphical interface for GROMACS

Graphical Abstract



Abstract:

Molecular dynamics (MD) is a powerful tool used to study the evolution of molecular systems and predict their properties. GROMACS is a famous MD tool that runs 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** prevent the researcher from visualizing the MD trajectory in a real-time manner and addressing the structural problem. This issue was addressed by developing **YAMACS: a graphical user interface of GROMACS for the YASARA molecular graphics suite**. YAMACS automatizes several steps of input file preparation and **allows visualizing MD trajectory in real time**. In addition, a collaborative platform is created on the Git-hub page **to build 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

Introduction

- GROMACS is a renowned, freely available tool to perform the MD simulation. However, the absence of a graphical user interface (GUI) can distract the researcher from addressing the chemical or biological problem from GROMACS.

- YAMACS[1] is the Python-based YASARA Plugin suit is developed to perform the MD simulation by using GROMACS through the GUI of the YASARA molecular viewer. In addition, the suite allows the interactive display of MD simulations, a feature absent in GROMACS.

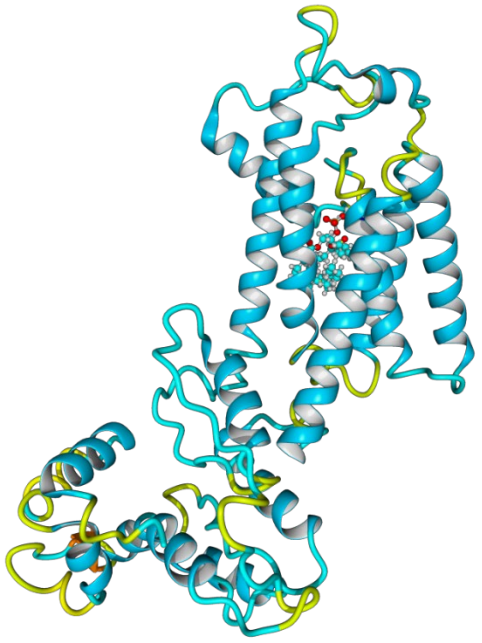


Figure 1: SMS1/POPC complex structure[2]

For more information, please visit the page:
https://academic.oup.com/bioinformatics/article/38/19/4645/6673904

1. Sarkar A. et al. YAMACS: a graphical interface for GROMACS. *Bioinformatics*. 2022 Oct 1;38(19):4645-6.
2. Sessa L. et al. (2021) Hydroxylated fatty acids: the role of the sphingomyelin synthase and the origin of selectivity. *Membranes*, 11, 787.

Discussion

Preparing the simulation environment may still be complex, and users may encounter errors to resolve.

Developers and experts can modify the plugins by a fork from the Git-Hub page (https://github.com/YAMACS-SML/YAMACS). However, many versions of YAMACS would confuse the users to get access.

A Git-hub community is therefore essential to invite all the users and experts under the same roof for discussion. Currently the platform is the YAMACS Git-hub discussion page (https://github.com/YAMACS-SML/YAMACS/discussions). The platform is divided into two major categories:

- Users
- Developers

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- ❑ Users
- ❑ Developers

Discussion

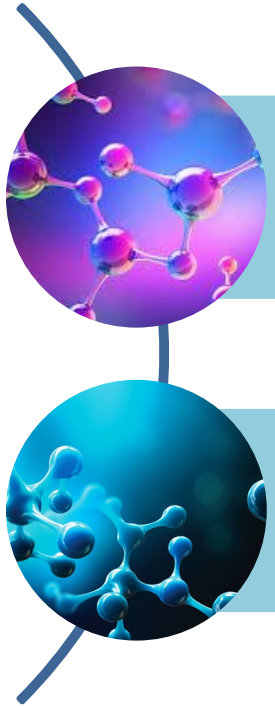
Users

- ❑Notify a bug or error of YAMACS plugins.
- ❑Contribute with plugins.

Developers

- ❑Notify a bug or error.
- ❑Contribute with plugins and check the existing plugins.
- ❑Authorize the new plugins.
- ❑Authorize the experts.

Conclusion



YAMACS provides a graphical interface to GROMACS and has been designed with maximum ease of use. The tool can automatize several steps of MD simulation and helps the user to perform the MD with less complication.

A global community of all YAMACS users and developers is created on the Git-hub discussion page to monitor and improve the quality of the YAMACS. That will increase the applicability of YAMACS MD simulation to the researchers and motivate them to develop new drugs through computational drug design studies.

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