Using ASGARD to automatically analyze GROMACS Molecular Dynamics simulations in different study cases

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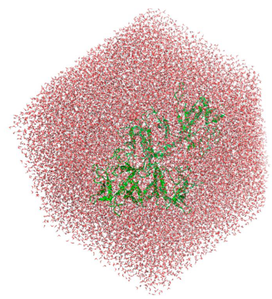
INTRODUCTION

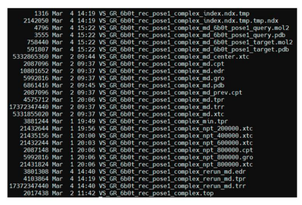
Protein-Ligand

GROMACS FAST. FLEXIBLE. FREE.



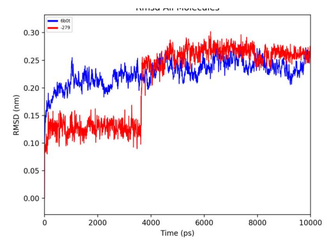
Molecular Dynamics Simulation

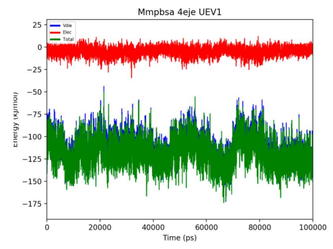
GROMACS FAST. FLEXIBLE. FREE.



Results

?

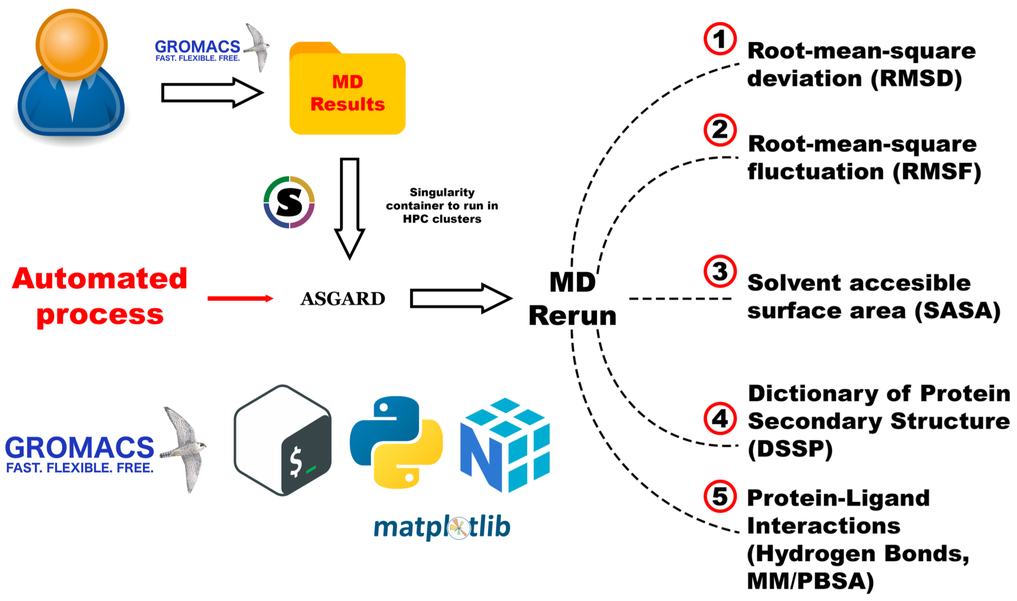




Analysis

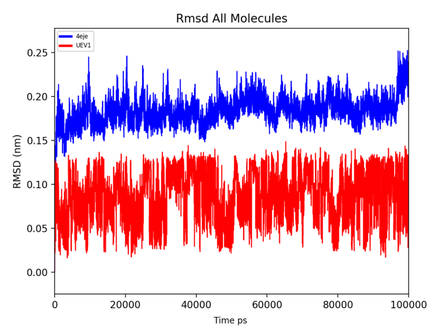
Automated Scripts for Gromacs to Analyze and Run Dynamics (ASGARD) allows to generate an PDF analysis report with one single command from Molecular Dynamics simulation files obtained by GROMACS!

METHODOGY



RESULTS

1



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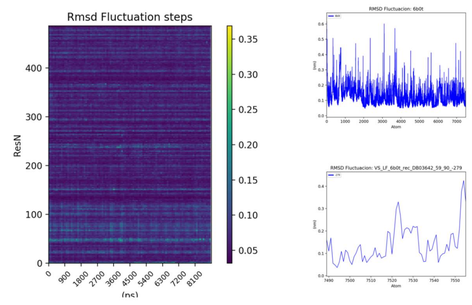

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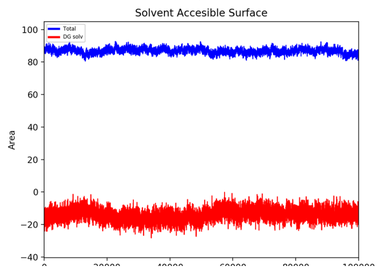

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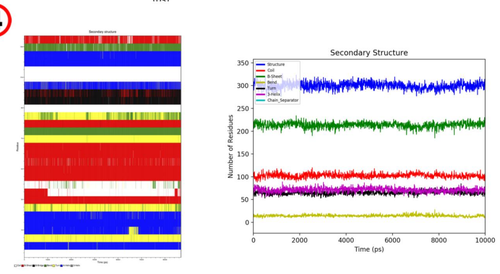

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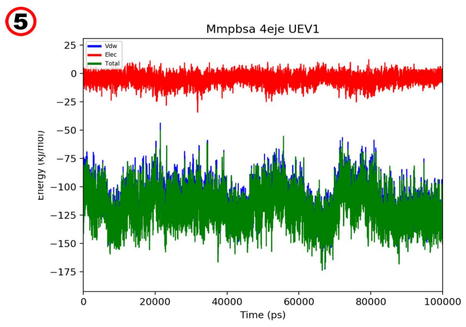
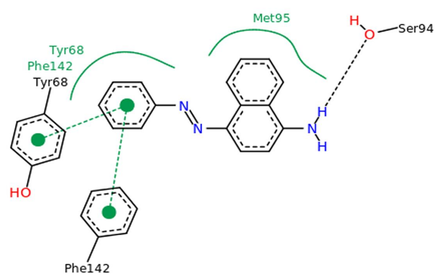


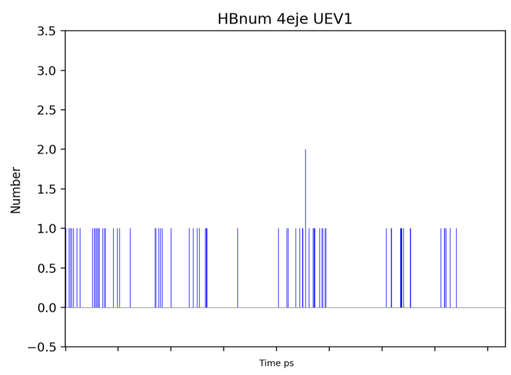
Molecular Mechanics with Poisson–Boltzmann surface area solvation (MM/PBSA)

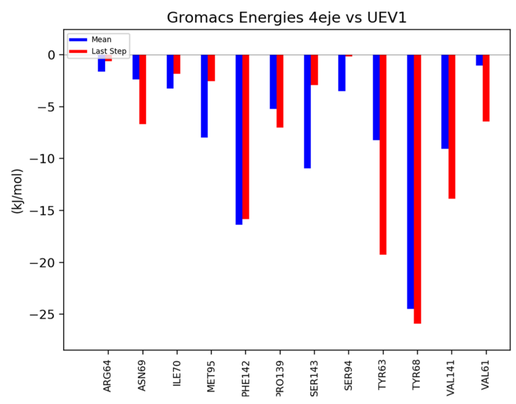
Ligand-Protein residues graphic 2D view through PoseView



5

Hydrogen Bonds formation during simulation





Protein-Ligand Interaction Energies for each residues

CONCLUSIONS

1- Tool to analyze the generated trajectories by GROMACS Molecular Dynamics simulations
2- Open-source analysis tool for an open-source MD package
3- Fully automated process to generate analysis results and its corresponding report
4- ASGARD was testing in different contexts: lysozyme as free protein, lysozyme-2-propylphenol protein-ligand complex and SARS-CoV2 Main protein-Paxlovid®

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NLHPC National Laboratory for High Performance Computing Chile

Available on GitHub

Take a look the repository

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[3] Rodríguez-Martínez, A.; Nelen, J.; Carmena-Bargueño, M.; Martínez-Cortés, C.; Luque, I.; Pérez-Sánchez, H. ASGARD. A Simple and Automatic GROMACS Tool to Analyze Molecular Dynamic Simulations. ChemRxiv February 14, 2023

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