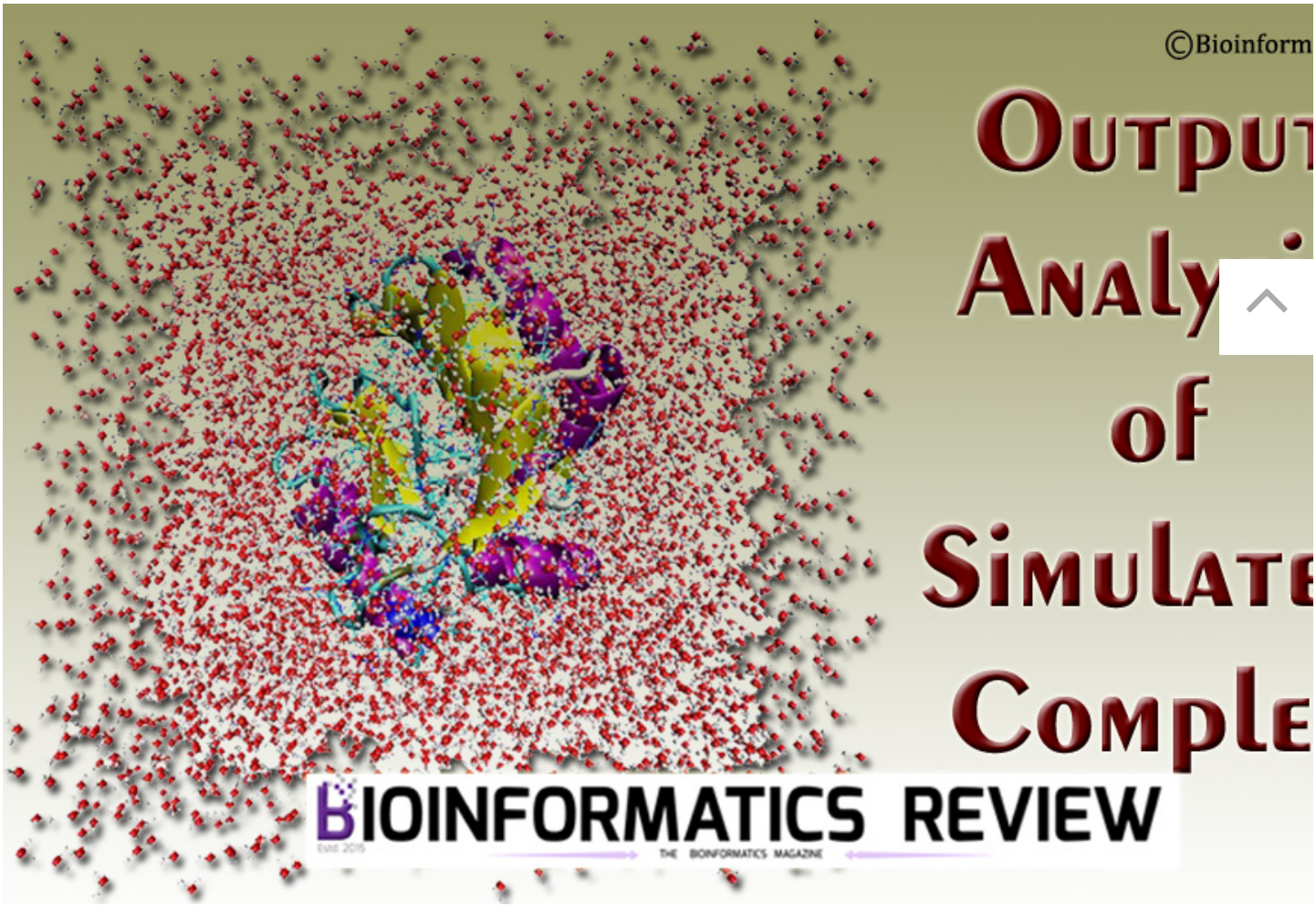
MD SIMULATION

Tutorial: MD simulation output analysis complex using GROMACS

Published **6 months ago** on **December 26, 2020**
By **Dr. Muniba Faiza**



We have provided several tutorials on molecular dynamics (MD) simulation (further reading section). They include installation of simulation software, sim simple protein, and a complex. In this article, we will analyze the GROMACS [1] c simulation of a complex.

We have previously provided a detailed article on GROMACS [1] output ana simulation. Here, we are going to plot some important parameters based o complex simulation can be analyzed.

At first, correct the trajectory because the protein might appear broken or locate of the box. For that, use the *trjconv* module of GROMACS.vTo do this, we need files as input resulted from the final MD run. Open the terminal, and type t command:

```
$ gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc
center
```

When prompted, type "1" for selecting "Protein" as the group to be centered "System". It will generate *md_0_1_noPBC.xtc* as output that will be used for th shown below.

1. RMSD

```
$ gmx rms -s md_0_1.tpr -f md_0_1_noPBC.xtc -o rmsd.xvg -tu n
```

here, `-tu` refers to time units.

When prompted, type "4" for selecting "Backbone" and "0" for "System". It *rmsd.xvg* file that can be plotted using xmgrace software. The RMSD plot for th looks like the one shown in the above-mentioned tutorial.

2. RMSF

```
$ gmx rmsf -f md_0_1_noPBC.xtc -s md_0_1.tpr -o rmsf.xvg
```

When prompted, type "1" for "Protein".

3. Radius of gyration

```
$ gmx gyrate -f md_0_1_noPBC.xtc -s md_0_1.tpr -o gyrate.xvg
```

When prompted, type "1" for protein.

Hydrogen – Acceptor).

```
$ gmx hbond -f md_0_1_noPBC.xtc -s md_0_1.tpr -num -dist
```

here, `-num` calculates the number of hydrogen bonds and `-dist` calculates the ave distance among them.

When prompted, select Protein and Ligand. This will display the status of hydroge between the protein and the ligand. This tells about the stability of hydrogen bon the protein and the ligand.

Protein-ligand interactions

If you want to see whether a hydrogen bond is present between the protein ar during the complete simulation, then find the interaction between the ligand an residues present in the pocket. For example, the binding residue in the pocket is using the gmx distance module, you can find the hydrogen bond distance hydroxyl group of ligand (C1F) and the carbonyl O atom of the receptor (*Ty*

```
$ gmx distance -s md_0_10.tpr -f md_0_10_center.xtc -select 'resna
and name OAB plus resid 150 and name OE1' -oall
```

here, `-oall` represents all distances as a function of time.

These are some basic operations that you can perform to analyze protein-ligand c simulation using GROMACS modules.

References

1. Abraham, M. J., Murtola, T., Schulz, R., Páll, S., Smith, J. C., Hess, B., & Lind GROMACS: High performance molecular simulations through multi-level par laptops to supercomputers. *SoftwareX*, *1*, 19-25.

Further Reading

1. Tutorial: Molecular dynamics (MD) simulation using Gromacs.
2. Tutorial: MD simulation output analysis of protein using GROMACS.

DON'T MISS
How to submit MD simulation job on a cluster server using PBS script?

UP NEXT
Tutorial: MD simulation with mixe solvents using GROMACS

Dr. Muniba Faiza

Dr. Muniba is a Bioinformatician based in New Delhi, India. She has completed her PhD in Bioinforma China University of Technology, Guangzhou, China. She has cutting edge knowledge of bioinformatic algorithms, and drug designing. When she is not reading she is found enjoying with the family. Know Muniba

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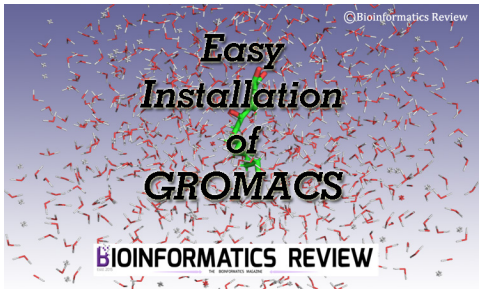
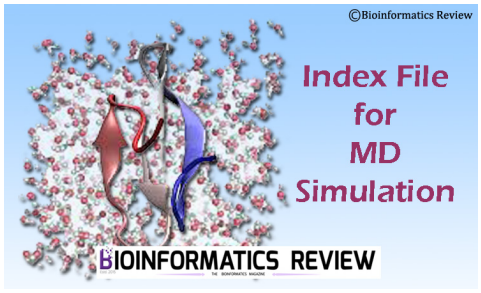
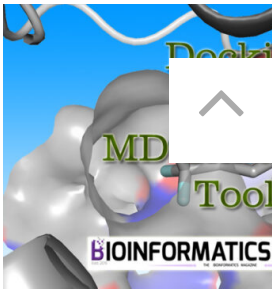


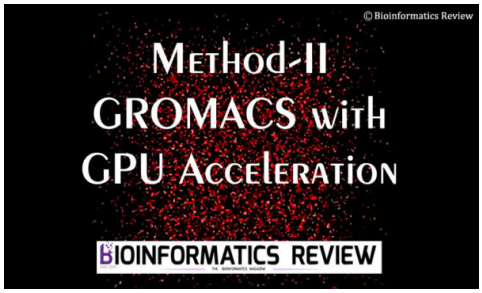
Easy installation of GROMACS on Ubuntu 18.04 & 20.04



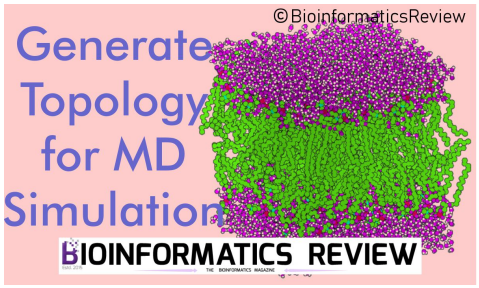
How to create an index file in GROMACS for MD simulation?



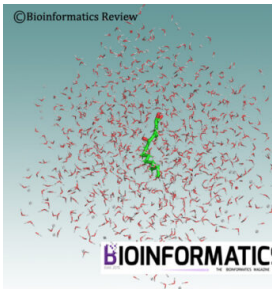
Where to find Docking simulation software?



Method-2: Installing GROMACS on Ubuntu 20.04 with CUDA GPU Support



How to generate topology of small molecules & ligands for MD Simulation?



Tutorial: MD Simulati organic molecules usi

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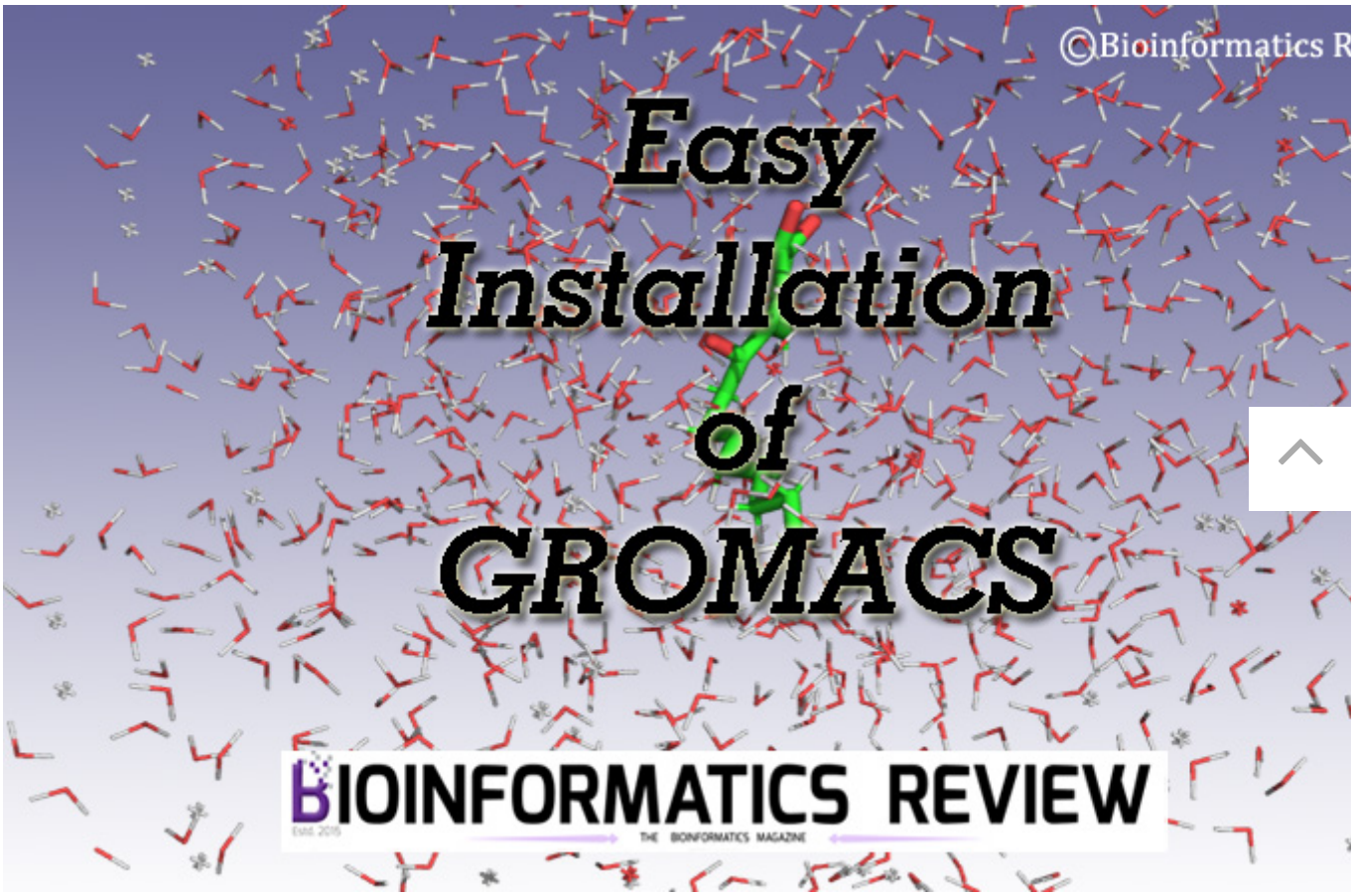
MD SIMULATION

Easy installation of GROMACS on Ubuntu 18.04 & 20.04

Published 3 days ago on June 16, 2021
By **Dr. Muniba Faiza**



We have provided several articles on GROMACS [1] installation on Ubuntu including t
installation method for GROMACS version 5.x.x. In this article, we will provide shell sc
install the latest (2021 series) of GROMACS on Ubuntu 18.04 and 20.04. (more...)

MD SIMULATION

How to create an index file in GROMACS MD simulation?

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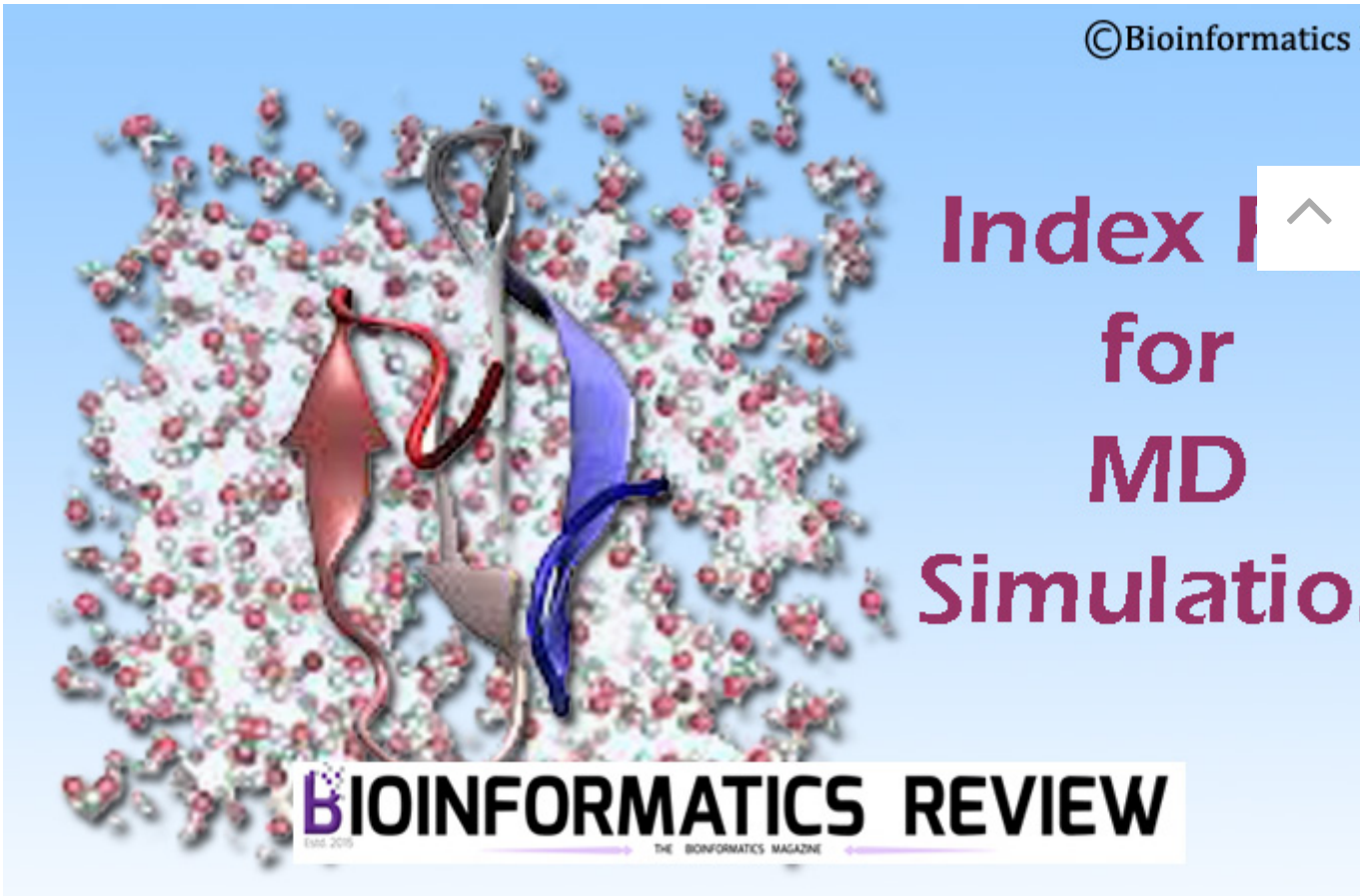
By Dr. Muniba Faiza



MD simulation is a tricky technique if you don't understand what you are doing various parameters and algorithms in GROMACS [1]. That may lead to several errors. article, we are going to create an index file for the protein groups in GROMACS to sol errors. (more...)

CONTINUE READING

MD SIMULATION

How to generate topology of small molecules & ligands for MD Simulation

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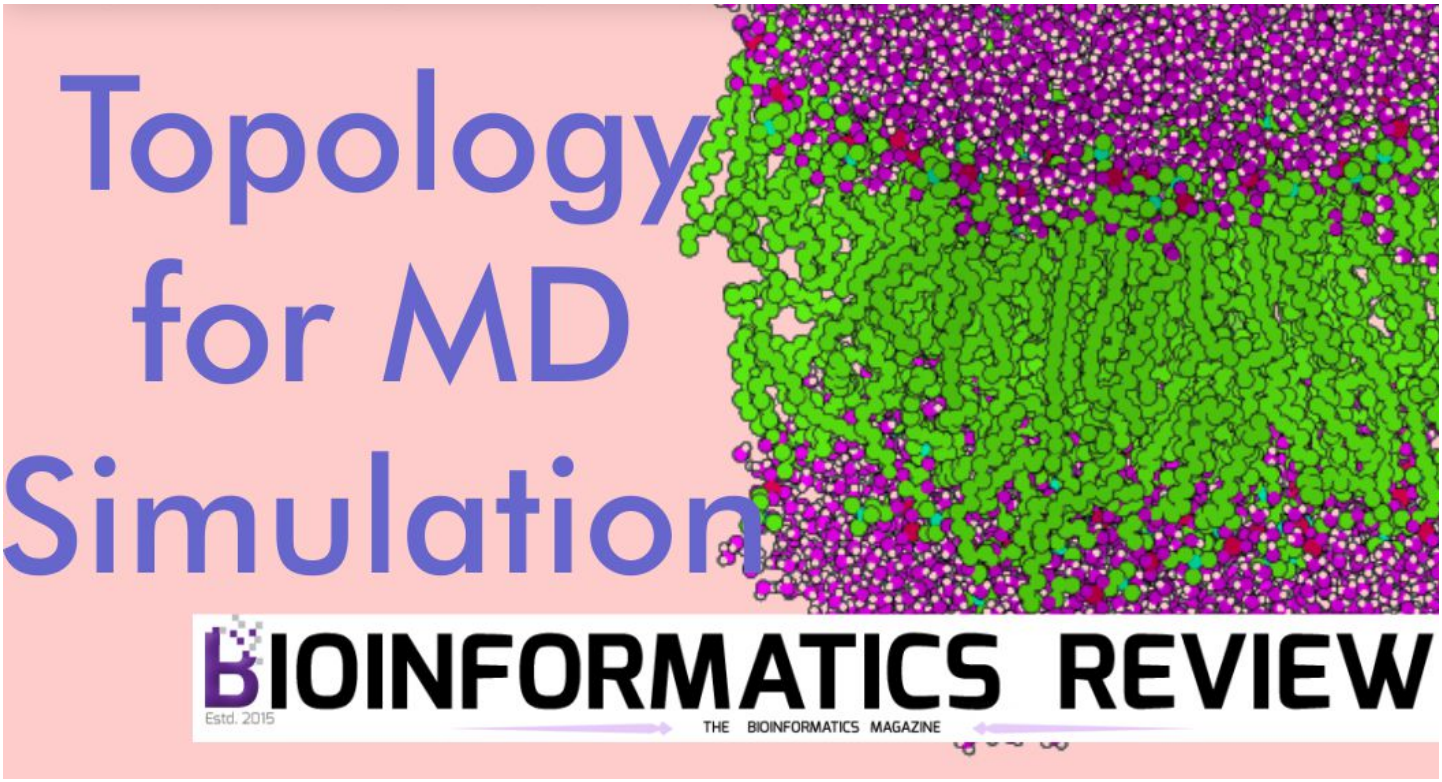
By **Dr. Muniba Faiza**



Generating the topology of small molecules/ligands is an important step dynamics (MD) Simulation. We explained it in previous articles as part of M tutorials. In this article, we will explain how can you generate the topology of ligands simulation of complex or small molecules only. (more...)

CONTINUE READING

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