M winmostar tutorial

Gromacs Protein

V11.3.1

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About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult <u>Beginner's Guide</u>.
- For those who wish to explore the details of each feature, please refer to <u>Winmostar User Manual.</u>
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
 - <u>Winmostar Introductory Training Session</u>: This guide only introduces the operation methods of the Basic Tutorial.
 - <u>Winmostar Basic Training Session</u>: We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
 - <u>Individual Training Session</u>: You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult <u>Frequently asked questions</u>.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using <u>Contact page</u>. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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Overview

• This tutorial explains how to prepare a Gromacs input from the PDB file of chicken eggwhite lysozyme, enabling molecular dynamics simulations.



Note :

- Crystal water from the XRD-derived PDB file should be removed, and missing hydrogen atoms must be added.
- The system size, such as the number of solvent molecules, can significantly affect protein behavior.
- The required number of equilibration steps may vary depending on molecular species and initial density.
- Calculation results are also strongly influenced by the chosen force field and interaction methods.

Operating Environment Settings

- To use this feature, it is necessary to set up Cygwin.
- <u>https://winmostar.com/en/installation/</u> Set up Cygwin by following the configuration steps outlined in the installation instructions.



• By default, it is installed directly under C:, but you can install it in a location of your choice by changing the 'Program Path' > 'Cygwin' in Winmostar Preference.



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Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**. This manual focuses on operations in Project Mode.



For basic operations, please refer to Gromacs Basics tutorial.

- A. Click File | New Project, enter 'protein' in Project name, and click Save.
- B. Click File | Import | Sample File | 1aki.pdb.
 - If you wish to load a different file at this stage, use File | Import File instead.
- C. In Import File dialog, click Discard and import.



- A. Click Select | Select by Molecular Species, click on the row for Comp2 O 78, and then click Close.
- B. Click discrete Competence Comp



A. Click Edit | Add Hydrogens | Using pdb2gmx… and then Execute.

- Even if the PDB file already includes hydrogen atoms, this step may still be necessary to ensure proper force field assignment based on residue information later.



- A. Click **Solvate/Build Cell**.
- B. Click Add Displayed Molecule, enter '1', and click OK.
- C. Click Add Water, enter '3000', and click OK.
- D. Enter '0.9' in **Set Density** and click **Build** and when asked '...you want to continue?' click **Yes**.



A. Click **MD | Generate Ions** and **Yes** when the warning message appears.B. Click **Execute**.

| 🚳 Generate lons | | _ | | × | Marked Order Marked Atom: Length= 28.66 |
|---------------------------|---------------------|-------------|---------|--------|---|
| Commands for Cygwin: | | | | | |
| echo "SOL" gmx genion - | s %OUTPUTNAME%.tmp. | tpr -o %OUT | PUTNAME | 5% | |
| Hide Detail | E | xecute | | | |
| Neutral | True | | | \sim | |
| Concentration [mol/L] | 0.15 | | | | |
| Cations | NA | | | | |
| Number of Cations | 0 | | | | |
| Anions | CL | | | | |
| Number of Anions | 0 | | | | |
| | | | | | ľ. |



B. Execution of Calculation (Energy minimization with protein position restraints)

- A. Select **Gromacs** from **Solver**, and open **Markflow Setup**).
- B. Click **No** when the message of '... Do you want to assign charges now?' appears.
- C. Click **OK** in the window of **Assigned force field parameters**. Click **OK** as each message appears in order. 'NOTE:...' and 'Assigned force field parameters.' are displayed.
- D. In the Gromacs Workflow Setup window, click the '-' button for # of Jobs twice.
 This energy minimization step may not converge, but it will not adversely affect the subsequent NVT simulation. Due to current Winmostar specifications, if the minimization fails to converge, the workflow will be interrupted. Therefore, only the energy minimization is executed at this stage. If the workflow is interrupted, the simulation can be resumed later from work1 without any issues.
- E. Change **Precision** to **Low**, then click **Details**.

| 🚾 Gromacs Workflow Setup | | | | — | | × | |
|---------------------------------------|-----------------|--------|------------------|------------|-----------|-----|--|
| Preset Fluid/Amorphous NPT Equilibrat | ion ~ (mod | ified) | # of Jo | bs: + | 1 | | |
| | | | Enable scan o | alculation | Confi | g | |
| 1st job | | | | | | | |
| Ensemble Minimize ~ | Temperature [K] | 300. | Pressure [atm] | 1. | | | |
| Simulation time [ps] 10. | # of snapshots | 50 | Initial velocity | From par | rent | | |
| Free boudnary condition | Precision | Low | De | tails | \langle | | |
| | | | | | | | |
| Reset Import 🔽 | Export | | 0 | ĸ | Can | cel | |

B. Execution of Calculation (Energy minimization with protein position restraints)

- A. Switch to the Advanced tab, check -DPOSRES, and click OK.
- B. Click OK, then make appropriate settings in Job Setting window and click Run.

| 🚾 Gromacs Keyword Set | up | | - 🗆 | × |
|-----------------------|------------|---------------------------|---------------------|--------|
| | | | | |
| Preset | ~ | | | |
| Basic Advanced | n Other | Automatic Options | | |
| Boundary Condition | | Constraints | | |
| pbc | xyz 🗸 | constraints | hbonds | \sim |
| Energy Minimization | | constraint-algorithm | LINCS | \sim |
| emtol [KJ/mol/nm] | 100.0 | continuation | no | \sim |
| emstep [nm] | 0.01 | lincs-order | 4 | |
| Run Control | | lincs-iter | 1 | |
| comm-mode | Linear V | shake-tol | 1e-5 | |
| nstcomm | 50 | Misc. | | |
| Temperature/Pressur | e Coupling | print-nose-hoover-chain-v | variables yes | \sim |
| nh-chain-length | 10 | define | | |
| nsttcouple | -1 | | -DPOSRES | |
| nstpcouple | -1 | | | |
| refcoord-scaling | no 🗸 | Extend simulation from | full-precision traj | ectory |
| | | | | |
| Reset Import | Export | ОК | | Run |
| | | | | |

C. Execution of Calculation (Equilibration with protein position restraints)

- A. After the status of work1_GMX_MIN in Working Folders changes to ABORT, open (Workflow Setup).
 - Even if the job ends with ABORT, continuation is possible if the final structure has been output.
- B. If prompted with 'Do you want to continue from previous run?', click **Yes**.

C. Click **OK** in **Select working folder**. Click **Yes** when the message of '...Do you want to ignore and continue?' appears.

| ✤ Project | | |
|---------------------------|--------|----------|
| Working Folders (protein) | 0 | ptions 🔻 |
| Name | Status | Prof |
| ⊙ work1_GMX_MIN | ABORT | Loca |
| | | |
| | | |
| | | |
| | | |
| | | |

| Name | Status | Profile | Output Location | Description |
|---------------|--------|-----------|-----------------|-------------|
| work1_GMX_MIN | ABORT | Local Job | Local | |
| | | | | |
| | | | | |
| | | | | |
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C. Execution of Calculation (Equilibration with protein position restraints)

- A. Reset the **Preset** to **Fluid/Amorphous NPT Equilibration**.
- B. Click the '-' button at the top right of the **1st job** row.
- C. Set the **Precision** of both the **1st** and **2nd jobs** to **Low**.
- D. Click **Details** for the **1st job**, check **-DPOSRES**, and click **OK**.
- E. Click **Details** for the **2nd job**, check **-DPOSRES**, and click **OK**.
- F. Click OK, then make appropriate settings in Job Setting window and click Run.

| | | 🞯 Gromacs Workflow Setup | | | – 🗆 X |
|---|--------------------------------|--------------------------------------|-----------------|------------------|--------------------------------|
| | | Preset Fluid/Amorphous NPT Equilibra | ation v (mod | lified) | # of Jobs: + 2 - |
| | | Coninue from work1_GMX_MIN | | | Enable scan calculation Config |
| | | 1st job | | | + - |
| 🞯 Gromacs Workflow Setup | – 🗆 × | Ensemble NVT \sim | Temperature [K] | 300. | Pressure [atm] |
| Preset Fluid/Amorphous NPT Equilibration | # of Jobs: + 3 - | Simulation time [ps] 10 | # of snapshots | 50 | Initial velocity Random |
| Coninue from work1_GMX_MIN | Enable scan calculation Config | Free boudnary | Precision | Low \checkmark | Details (modifi |
| 1st job Ensemble Minimize V Temperature [K] 300. | Pressure [atm] | 2nd job | | | + |
| Simulation time [ps] 10. # of snapshots 50 | Initial velocity From parent | Ensemble NPT ~ | Temperature [K] | 300. | Pressure [atm] |
| Tracision Madian | Deteile | Simulation time [ps] 50 | # of snapshots | 50 | Initial velocity From parent |
| | | Free boudnary | Precision | Low \checkmark | Details (modifie |
| | | | | | |
| | | Reset Import 🔽 | Export | 6 | OK Cancel |

D. Execution of Calculation (Equilibration)

- A. Once the status of work3_GMX_NPT changes to END, click Morkflow Setup) again.
- B. If prompted with 'Do you want to continue from previous run?', click Yes.
- C. Select work3_GMX_NPT and click **OK**.
- D. Reset the **Preset** to **Fluid/Amorphous NPT Equilibration**.
- E. Set the Precision of the 1st , 2nd and 3rd jobs to Low.
- F. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

| | | Gromacs worknow setup | |
|---------------------------|-----------|--|-------------------------------------|
| | | Preset Fluid/Amorphous NPT Equilibration \checkmark (modified) | # of Jobs: + 3 |
| M Project | | Coninue from work3_GMX_NPT | Enable scan calculation Confi |
| V Hoject | | 1st job | |
| Working Folders (protein) | Options ▼ | Ensemble Minimize V Temperature [K] 300. | Pressure [atm] 1. |
| Name | Status | Simulation time [ps] 10. # of snapshots 50 | Initial velocity From parent ~ |
| | | Free boudnary condition Precision Low | ∨ Details |
| work1_GMX_MIN | ABORT | | |
| ⊙ └ work2_GMX_NVT | END | 2nd job | |
| work3 GMX NPT | END | Ensemble NVT V Temperature [K] 300. | Pressure [atm] 1. |
| | | Simulation time [ps] 10. # of snapshots 50 | Initial velocity Random ~ |
| | | Free boudnary condition Precision Low | ∨ Details |
| | | 3rd job | |
| | | Ensemble NPT V Temperature [K] 300. | Pressure [atm] 1. |
| < | > | Simulation time [ps] 50 # of snapshots 50 | Initial velocity From parent \sim |
| | | Free boudnary condition Precision Low | ∨ Details… |
| | | | |
| | | Reset Import 🔻 Export | OK Can |

Comment Manufallow Control

E. Execution of Calculation (Main Calculation)

- A. Once **the status** of work6_GMX_NPT changes to **END**, click **(Workflow Setup)** again.
- B. If prompted with 'Do you want to continue from previous run?', click Yes.
- C. Select work6_GMX_NPT and click **OK**.
- D. Change Preset to Fluid/Amorphous NPT Production.
- E. Adjust **Precision** and **Simulation time** as needed. In this tutorial, set **Precision** to **Low**.
- F. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

| | | | Gromacs Workflow Setup – L X |
|----|-------------------------|-----------|--|
| ≽ | Project | | Preset Fluid/Amorphous NPT Production \checkmark (modified) # of Jobs: + 1 |
| Wo | rking Folders (protein) | Options ▼ | Coninue from work6_GMX_NPT Enable scan calculation Config |
| | Name | Status | 1st job |
| | work1_GMX_MIN | ABORT | Example December M 200 December [ster] |
| | work2_GMX_NVT | END | Ensemble NPT V Temperature [K] 300. Pressure [atm] |
| | work3_GMX_NPT | END | Simulation time [ps] 50 # of snapshots 250 Initial velocity From parent ~ |
| O | work4_6MX_MIN | END | |
| | work5_GMX_NVT | END | Low V Details |
| | work6_GMX_NPT | END | |
| | | | Reset Import 🔻 Export OK 📐 Cancel |

F. Analysis of Results

This section explains how to confirm that the protein is properly restrained.

- A. In the **Working Folders**, click the job you want to check (e.g., work3_GMX_NPT), then select **Root Mean Square Deviation** from the **Action** menu.
- B. Select '5: Main Chain' in the Target Group and click Draw.



Finally

• For detailed information on each feature, please refer to Winmostar User Manual.





Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending <u>Winmostar Introductory Training Session</u>, <u>Winmostar Basic Training Session</u>, or <u>Individual Training Session</u>. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult <u>Frequently asked questions</u>.
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