

BioBB Workflows – Supplementary Material

Exploring Biomolecular Modeling & Simulations 9-10/04/2025

EuroCC4 & BioExcel training workshop

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Supplementary Material

1) Additional BioBB Jupyter Notebooks:

- GROMACS / AMBER Protein MD Setup
- AMBER Protein-ligand MD Setup
- Protein-ligand Docking
- Mutation Free energy calculations (lite)

2) Command-line interface (CLI) BioBB Workflows:

- GROMACS / AMBER Protein-ligand MD Setup
- Mutation Free energy calculations (complete)

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GROMACS Protein MD Setup

 **GROMACS PROTEIN MD SETUP** 2024.1



This tutorial aims to illustrate the process of setting up a simulation system containing a protein, step by step, using the BioExcel Building Blocks library (biobb). The particular example used is the Lysozyme protein (PDB code 1AKI).

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gmx **md** **protein**

(*) **MyBinder** provides a **free**, online version of **Jupyter Lab**. Take into account that the provided **resources** are **finite** and, in some occasions, it can take a long time to load or to execute your notebooks. **Please be patient** and don't try to execute several notebooks at the same time.

- **Protein: Lysozyme (1AKI)**
- **GROMACS MD Setup (Min + NVT eq + NPT eq + unrestrained short MD)**

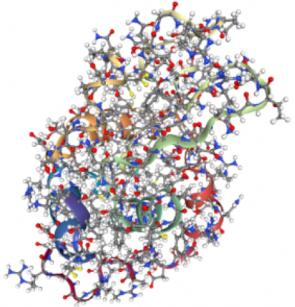


- `git clone https://github.com/bioexcel/biobb_wf_md_setup.git`
- Deploy notebook: `biobb_wf_md_setup/notebooks/biobb_wf_md_setup.ipynb`

AMBER Protein MD Setup

AMBER PROTEIN MD SETUP

2024.1



This tutorial aims to illustrate the process of setting up a simulation system containing a protein, step by step, using the BioExcel Building Blocks library (biobb) wrapping the AmberTools utility from the AMBER package. The particular example used is the Lysozyme protein (PDB code 1AKI).

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- **Protein: Lysozyme (1AKI)**
- **AMBER MD Setup (Min + Heat + NVT eq + NPT eq + unrestrained short MD)**



- `git clone https://github.com/bioexcel/biobb_wf_amber.git`
- Deploy notebook: `biobb_wf_amber_md_setup/notebooks/mdsetup/biobb_amber_setup_notebook.ipynb`

AMBER Protein-ligand Complex MD Setup

AMBER PROTEIN-LIGAND COMPLEX MD SETUP

2024.1



This tutorial aims to illustrate the process of setting up a simulation system containing a protein in complex with a ligand, step by step, using the BioExcel Building Blocks library (biobb) wrapping the AmberTools utility from the AMBER package. The particular example used is the T4 lysozyme protein (PDB code 3HTB) with two residue modifications L99A/M102Q complexed with the small ligand 2-propylphenol (3-letter code JZ4).

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- **Complex: T4 Lysozyme (3HTB) + 2-propylphenol (JZ4)**
- **Ligand parameterization**
- **AMBER MD Setup (Min + Heat + NVT eq + NPT eq + unrestrained short MD)**



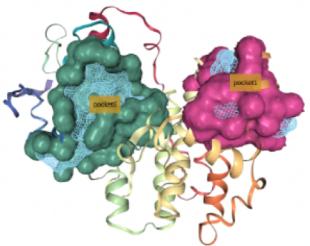
- `git clone https://github.com/bioexcel/biobb_wf_amber.git`
- Deploy notebook: `biobb_wf_amber_md_setup/notebooks/mdsetup/biobb_amber_complex_setup_notebook.ipynb`

Protein-ligand Docking

PROTEIN-LIGAND DOCKING (FPOCKET)

2024.1

This tutorial aims to illustrate the process of protein-ligand docking, step by step, using the BioExcel Building Blocks library (biobb). The particular example used is the Mitogen-activated protein kinase 14 (p38- α) protein (PDB code 3HEC), a well-known Protein Kinase enzyme, in complex with the FDA-approved Imatinib, (PDB Ligand code STI, DrugBank Ligand Code DB00619), a small molecule kinase inhibitor used to treat certain types of cancer.



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docking ligand protein

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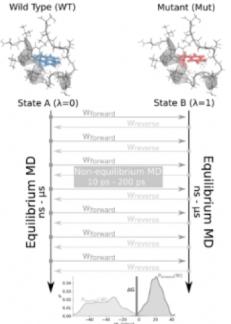
- **Protein: Mitogen-activated protein kinase 14 (p38 α) (3HEC)**
- **Ligand: FDA-approved imatinib (STI)**
- **Finding pockets (fpocket) + Docking (AutoDock Vina)**



- `git clone https://github.com/bioexcel/biobb_wf_virtual-screening.git`
- Deploy notebook: `biobb_wf_virtual-screening/notebooks/fpocket/wf_vs_fpocket.ipynb`

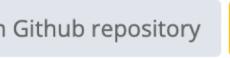
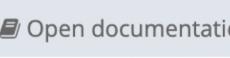
Mutation Free Energy Calculations

 MUTATION FREE ENERGY CALCULATIONS 2024.1



This tutorial aims to illustrate how to compute a fast-growth mutation free energy calculation, step by step, using the BioExcel Building Blocks library (biobb). The particular example used is the Staphylococcal nuclease protein (PDB code 1STN), a small, minimal protein, appropriate for a short tutorial.

free_energy **gmx** **md**

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- **Protein: Staphylococcal nuclease (1STN)**
- **Fast Growth mutation free energy calculation (PMX + GROMACS)**



- `git clone https://github.com/bioexcel/biobb_wf_pmx_tutorial.git`
- Deploy notebook: `biobb_wf_pmx_tutorial/notebooks/biobb_wf_pmx_tutorial.ipynb`

BioBB Demonstration Workflows (ALL)

<https://mmb.irbbarcelona.org/biobb/workflows>

- *MD setup (Protein / DNA) (AMBER / GROMACS)*
- *Ligand parameterization*
- *Protein-Ligand Docking*
- *Free energy calculations*
- *DNA helical parameters*
- *Conformational Ensemble generation*
- *Molecular Interaction Potentials*
- *Structure Checking*

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GROMACS Protein-Ligand MD Setup

GROMACS PROTEIN-LIGAND COMPLEX MD SETUP

2024.1



This tutorial aims to illustrate the process of setting up a simulation system containing a protein in complex with a ligand, step by step, using the BioExcel Building Blocks library (biobb). The particular example used is the T4 lysozyme L99A/M102Q protein (PDB code 3HTB), in complex with the 2-propylphenol small molecule (3-letter Code JZ4).

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- **Complex: T4 Lysozyme (3HTB) with 2-propylphenol (JZ4)**
- **Ligand parameterization (ACPyte)**
- **GROMACS MD Setup (Min + NVT eq + NPT eq + unrestrained short MD)**



- `cp -r /arf/home/egitim/BioBB/biobb_workflows/biobb_wf_protein-complex_md_setup .`
- `cd biobb_wf_protein-complex_md_setup/python`
- `sbatch launch.sh`

GROMACS Protein-Ligand MD Setup - Output

```
(biobb_env) [egitim213@arf-ui1 python]$ ls -lrth biobb_wf_protein-complex_md_setup
total 12K
-rw-r--r--. 1 egitim213 egitim213 0 Apr  9 09:33 log.err
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step0_reduce_remove_hydrogens
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step2_extract_molecule
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step00_cat_pdb
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step4_fix_side_chain
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step5_pdb2gmx
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step9_make_ndx
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step10_genrestr
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step11_gmx_trjconv_str_protein
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step12_gmx_trjconv_str_ligand
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step13_cat_pdb_hydrogens
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step14_append_ligand
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step15_editconf
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step16_solvate
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step17_grompp_genion
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step18_genion
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step19_grompp_min
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step20_mdrun_min
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step21_gmx_energy_min
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step22_make_ndx
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:33 step23_grompp_nvt
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:36 step24_mdrun_nvt
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:36 step25_gmx_energy_nvt
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:36 step26_grompp_npt
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:38 step27_mdrun_npt
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:38 step28_gmx_energy_npt
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:39 step29_grompp_md
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step30_mdrun_md
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step34_gmx_image
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step34b_gmx_image2
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step35_gmx_trjconv_str
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step31_rmsd_first
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step32_rmsd_exp
-rw-r--r--. 1 egitim213 egitim213 11K Apr  9 09:53 log.out
drwxr-xr-x. 1 egitim213 egitim213 0 Apr  9 09:53 step33_gmx_rgryr
```

AMBER Protein-Ligand MD Setup

AMBER PROTEIN-LIGAND COMPLEX MD SETUP

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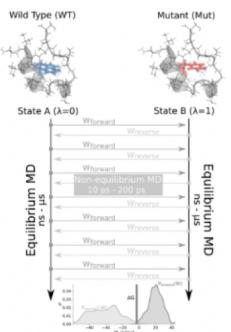


- `cp -r /arf/home/egitim/BioBB/biobb_workflows/biobb_wf_amber_md_setup_lig .`
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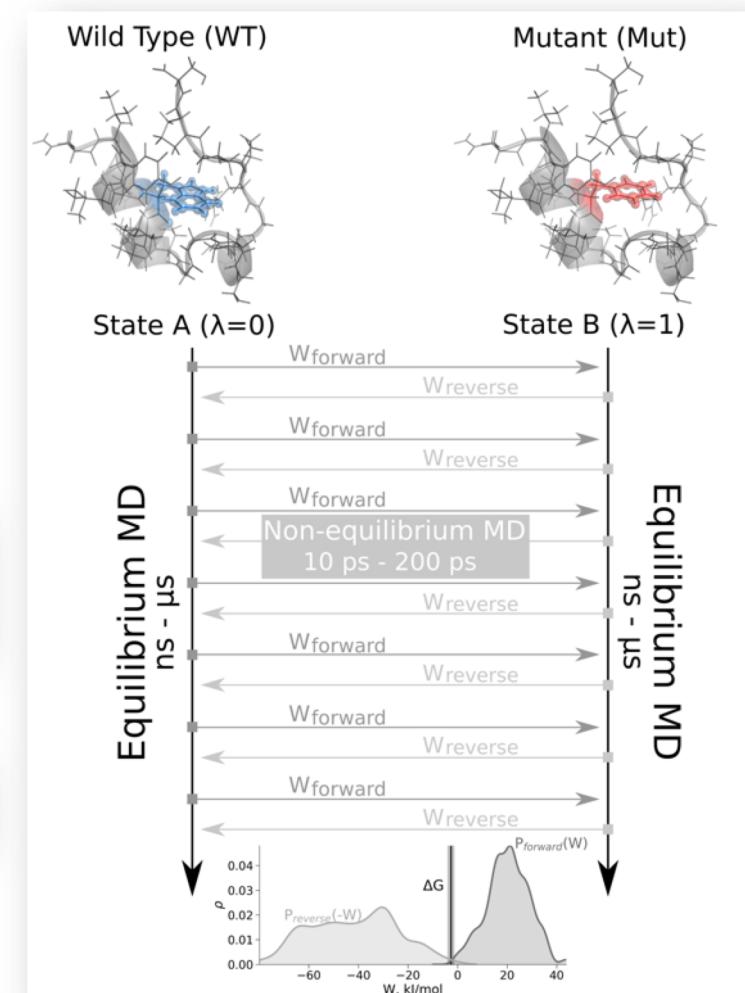
Mutation Free Energy Calculations - Output

```
[biobb_env] [egitim213@arf-ui1 biobb_wf_pmx_tutorial_1]$ ls  
log.err  log.out  stateA  stateB  step11_pmx_analyse
```

```
(biobb_env) [egitim213@arf-uit1 biobb_wf_pmx_tutorial_1]$ ls stateA
frame0  frame11  frame14  frame17  frame2  frame22  frame3  frame6  frame9
frame1  frame12  frame15  frame18  frame20 frame23  frame4  frame7  step0_trjconv
frame10 frame13  frame16  frame19  frame21 frame24  frame5  frame8
```

```
(biobb_env) [egitim213@arf-ui1 biobb_wf_pmx_tutorial_1]$ ls stateA/frame0
step10_gmx_mdrun  step2_gmx_pdb2gmx  step4_gmx_makendx  step8_gmx_mdrun
step1_pmx_mutate  step3_pmx_gentop   step7_gmx_grompp  step9_gmx_grompp
```

```
(biobb_env) [egitim213@arf-ui1 biobb_wf_pmx_tutorial_1]$ ls step11_pmx_analyse/  
pmx.plots.png pmx.txt step11_pmx_analyse_log.err step11_pmx_analyse_log.out
```



Acknowledgments



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IN BIOMEDICINE



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**Barcelona
Supercomputing
Center**

Centro Nacional de Supercomputación



Pau Andrio



Josep Ll. Gelpí



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