# Tutorial gmx_qk

## gmx_qk

Good day and welcome to the **gmx_qk**!!. This is a **Zenity**, **Python**, **gromacs** and **g_mmpbsa** dependent bash program. It is designed for beginners to the gromacs who would like to simulate the Protein-Ligand Complex. **Gmx_qk** is a fully automated program that works well with Gromacs versions 5.0 and 2021.4.

Informative and question widgets are supported by Zenity (GUI).

https://github.com/harry-maan.


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## About


**About: gmx_qk 1.0.0**

The tool gmx_qk is a **Zenity**, **Python**, **Gromacs and g_mmpbsa** dependent bash program. It is designed for beginners to the gromacs who would like to simulate the **Protein/Protein-Ligand complex.Abridged with MMPBSA calculations). Gmx_qk** is a fully automated program, efficiently works with gromacs version 5.0 and newer one as 2021.4. Informative widgets are supported by Zenity (GUI).

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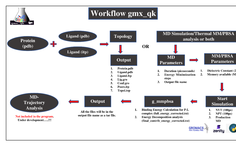
## Workflow

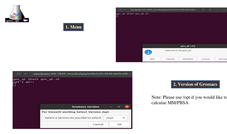



## Installation **gmx_qk**

1. Download the package from
2. Open the terminal and run "bash configure.sh" **gmx_qk** will be appeared in the applications menu.
3. Click on **gmx_qk**


## Step 1: Launching **gmx_qk** in terminal

1. Open the terminal and run "gmx_qk".
2. Select executable gromacs usually gromacs installed in /usr/local/ or /opt




## Step 2: Select Protein or Receptor file, ligand file (.pdb) and ligand parameter file (.itp)

1. This is a zenity supported widget *Please select a receptor file (.pdb)
2. Receptor file can be downloaded from https://www.rcsb.org/
3. Make your receptor file clean using https://charmm-gui.org/ or whatever else you are familiar with the protein preparation tools.
4. Remove all the hetero atoms i.e., ions, ligand, free water or solvent.
5. **Ligand File**: This is also zenity supported widget *Please select a ligand file (.pdb)
6. ligand file can be downloaded from https://pubchem.ncbi.nlm.nih.gov/ as 3D .sdf or copy Canonical SMILES and paste in the http://cartblanche.chem.yale.edu/ligpargen/
7. Download the zipped file from ligpargen sever.
8. Extract .zip file which has name.pdb and name.itp(required for next step)
9. **ligand parameter file**:This is also zenity supported widget *Please select a ligand file (.itp)
10. .itp file generated via http://cartblanche.chem.yale.edu/ligpargen/ in the zipped file.(Downloaded in the last step)


## Step 3: Select a task would you like to perform

a. Generate Topology b) Simulate the P-L complex c) MD & Thermal MMPBSA analysis * d) Protein in water


## Step 4: Protein topology generation check point


## Step 5: Molecular Dynamic simulation and MM/PBSA parameters

1. Use numeric only to define simulation course as picoseconds
2. Do not include any space in the entries
3. Energy minimization nano-steps are recommended as 5000
4. Di-electric constant can be decoded as per requirement (recommended is 2)


## Step 6: Run the simulation

1. Simulation will start as soon as NVT, NPT equilibrations have finished
2. Do not interrupt the simulation using terminal let it be completed.
3. It will initiate the MM/PBSA calculation for each frame of simulation trajectory


## Step 7: Output

1. Untar the output directory
2. There is a log file if the simulation has been intrupted or failed as per gromacs


## Step 8: Thankyou for using **gmx_qk**


## References


1. Kumari R, Kumar R, Open Source Drug Discovery Consortium, Lynn A. g_mmpbsa : A GROMACS tool for high-throughput MM-PBSA calculations. Journal of chemical information and modeling. 2014 Jul 28;54(7):1951-62.
2. Van Der Spoel D, Lindahl E, Hess B, Groenhof G, Mark AE, Berendsen HJ. GROMACS: fast, flexible, and free. Journal of computational chemistry. 2005 Dec;26(16):1701-18
3. Singh H, Raja A, Shekhar N, Chauhan A, Prakash A, Avti P, Medhi B. Computational attributes of protein kinase-C gamma C2-domain & virtual screening for small molecules- elucidation from meta-dynamics simulations & free-energy calculations. *Journal of Biomolecular Structure and Dynamics*. 2022 May 14:1-2. Please feel free to contact me : https://github.com/harry-maan