**KRE\_DOP: Key Residues Explored in Allostery of *δ* Opioid Receptor Using Elastic Network Model and Complex Network Model Combined with Perturbation Method.**

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The performance process includes three steps: data preparation, data extraction

fcfGNMMD constructed and key residues explored

KRE\_DOP uses the following dependencies:

Matlab 2019

R 4.0.3

VMD

**The process of calculation:**

**Data preparation**

Molecular dynamics (MD) simulation trajectory was available in GPCRmd database, including “10714\_trj\_73.xtc” and “pdb0.pdb”.

The crystal structure of δ Opioid Receptor (DOP) was obtain in RCSB database called“4n6h\_A.pdb”.

**Data extraction**

**Step1:**

Run VMD with“pdb0.pdb” and “10714\_trj\_73.xtc” as input file, then you can obtain “1074trj-cas.dcd”.

Run “mddata\_R.R” and you can obtain Root-mean-square deviation (RMSD) of the trajectory. The MD simulation trajectory began to stabilize in 100-500ns (499-2499 frame).

**Step2:**

Run VMD with“pdb0.pdb” and “10714\_trj\_73.xtc” as input file, then you can obtain “1074trj-cas100-500ns.dcd” and “499CA.pdb”.

**Step3:**

Run ”md\_R.R” and obtain the files called “md\_msf.xlsx, md\_cof.xlsx and md\_cij.csv, respectively.

**fcfGNMMD constructed and key residues explored**

Run “fcfGNMMD.m”, “DPR.m” and “compnetwork.m”.

The output is the value of PCC, the dissipated work, the dynamic correlations upon a site perturbed, degree and Z-score.

**Help**

For any questions, please contact us by [chunhuali@bjut.edu.cn](mailto:chunhuali@bjut.edu.cn).