Below is a breakdown of inputs for the paper:

“Pathway Specific Unbinding Free Energy Profiles of Ritonavir Dissociation From HIV-1 Protease”

Jupyter notebook used for milestoning can be found on our group github page. A link has been provided in the “Notes” section of our Zenodo page. We have detailed the method to construct PMF in the “Methods” section of the paper.

MD files for Pathway’s A, B, and C can be found in our group google drive. A link has been provided in the “Notes” section of our Zenodo page.

Each pathway has its own folder containing the parameter (.prmtop) file as well as two coordinate (.dcd) files.

The .dcd files are as follows:

rit_seed##_diss_nowat_unwrap.dcd

> This is the dissociation trajectory of ritonavir used for PCA and RMSD analysis

Repre_meta_1RepPerMS.dcd

> This is one representative frame per milestone. This trajectory was used for correlation analysis.