

0_Concatenating_trajecories

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[1]: import os
import glob
import numpy as np
import mdtraj as md
import itertools
```

1 Simulation data set

In this notebook we take the simulation data of FAT10 from the KonDATA repository and concatenate it into one trajectory with a fixed ordering for analysis.

The protein consists of 165 residues (Sequence: MAPNASCLCVHVRSEEWDLMTFDAN-PYDSVKKIKEHVRSKTKVPVQDQVLLLGSKILKPRRSLSSYGIDKEKTIHLTLKVVKPSDEELPLFLVESGD

It has two terminal flexible tails and two ubiquitin-like domains (N-terminal domain ND and C-terminal domain CD) connected by a flexible linker (KPSDE).

The simulations were generated by simulating 2 different ion concentrations (no added NaCl and 150 mM NaCl) and 25 different starting conformations (25 different relative angles between the two domains (Phi of Asp85) for 200 ns (2001 frames) in triplicate.

The concatenated trajectory consists of 300150 simulation frames of the ubiquitin-like protein FAT10.

In this notebook, we concatenate the 150 (3x2x25) individual simulations of FAT10 into one trajectory in the following order: - Replicate 1 - No NaCl, Phi(Asp85) 1-25 - 150 mM NaCl, Phi(Asp85) 1-25 - Replicate 2 - No NaCl, Phi(Asp85) 1-25 - 150 mM NaCl, Phi(Asp85) 1-25 - Replicate 3 - No NaCl, Phi(Asp85) 1-25 - 150 mM NaCl, Phi(Asp85) 1-25

It is then saved as an .xtc trajectory

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[2]: data_directory = "../FAT10_simulation_data"
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[3]: topology = os.path.join(data_directory, "FAT10_ASP85_Phi_01_I", "topol_prot.
    ↪pdb")
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[4]: traj_list = []
for replica in ["I", "II", "III"]:
    traj_list.append(sorted(glob.glob(os.path.join(data_directory,
    ↪f"FAT10_ASP85_Phi_??_{replica}", "traj_no_water_dt_100.xtc"))))
```

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traj_list.append(sorted(glob.glob(os.path.join(data_directory,
↪f"FAT10_ASP85_Phi_??_NaCl_{replica}", "traj_no_water_dt_100.xtc"))))

flat_traj_list = list(itertools.chain.from_iterable(traj_list))
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[5]: full_trajectory = md.load(flat_traj_list,
                                top = topology)
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[ ]: full_trajectory.save_xtc("./FAT10_123_traj_center_dt100.xtc")
```