**Modification of the file**: **fdMD_OneTraj.cmd** for the TEST ( Toy ) example:

1. The Toy example consists of ten files each one containing 20 snapshots that represent 20ns of MD:

**2ohk_1_dyn_50.nc** ( 20 snapshots )
**2ohk_2_dyn_50.nc** ( 20 snapshots )
**2ohk_3_dyn_50.nc** ( 20 snapshots )
**2ohk_4_dyn_50.nc** ( 20 snapshots )
**2ohk_5_dyn_50.nc** ( 20 snapshots )
**2ohk_6_dyn_50.nc** ( 20 snapshots )
**2ohk_7_dyn_50.nc** ( 20 snapshots )
**2ohk_8_dyn_50.nc** ( 20 snapshots )
**2ohk_9_dyn_50.nc** ( 20 snapshots )
**2ohk_10_dyn_50.nc** ( 20 snapshots )

A total of 200 snapshot for 200 ns of MD. Thus, 1 snapshot / ns

2. A topology file:

**2ohk_Sol_vdw2301_ZeroB.top** ( with vdW repulsion between C99 Atoms and Mass Repartitioning )

3. A reference file (the first one from the MD):

**first_lig.pdb**

**A) First, we need to modify the script:**

- **fdMD_OneTraj.cmd**

The User **MUST** have this structure **:**

```
# -----------------------
# -    fdMD_OneTraj    -
# -----------------------
#
# AMBER version and directory
set amber_version = 18
set amber_dir = /home/prog/amber$amber_version
set cpptraj   = $amber_dir/bin/cpptraj
# Number of Protein residues
# Number of Ligands in the simulation
@ num_res_prot = 387
@ num_lig      =  26
# Residues to Superimpose
@ ini_res_sup  =  1
@ ifi_res_sup  = 387
# Refers to the Protein PLUS ONE ligand: Without wat,Na+,Cl-.. but both prepared !!!
# xray can be = yes/no
set xray = 'no'
if ( $xray == 'yes' ) then
  set ref_pdb  = "Name_Of_XRay_PDB.pdb"
else
```

```
  set ref_pdb  = "first_lig.pdb"
endif
set dir_traj    = .
set top_name    = "2ohk_Sol_vdw2301_ZeroB.top"
set top_file    = $dir_traj/$top_name
set prefix_traj  = "2ohk"
@ ini_traj = 1
@ end_traj = 10
@ ini_read   =   1
set end_read = last
@ inc_read   =   1
set last_pdb = 'yes'
if ( $last_pdb == 'yes' ) then
  @ num_snaps_total  = 200
  echo " Number of Snapshots    : " $num_snaps_total
endif
```

**A) Second, we need to run the script:**

./ **fdMD_OneTraj.cmd**

**Then, the output will be a new script :**

**inptrj_one_lig**

**C) Run the new script:**

**./inptrj_one_lig**

**Then, you will have many file ( one for each ligand ) :**

| | |
|---|---|
| lig_388.nc | # The full trajectory for the first ligand: RESNUM 388). |
| lig_388_c99.pdb | # Same as before but for the position of the C99 atoms. |
| lig_388_LAST.pdb | # The Last snapshot for the RESNUM ligand. |

**and some general files:**

| | |
|---|---|
| NoWat.2ohk_Sol_vdw2301_ZeroB.top | # Topology file for the full trajectory without WAT,ions…but with all the LIGANDS |
| OneLig.NoWat.2ohk_Sol_vdw2301_ZeroB.top | # Topology file for the full trajectory without WAT,ions…and with ONLY ONE LIGAND |
| RMS_first.dat | |
| RMSD_FIRST_NoWat_alone.nc | # The full trajectory ( without WAT, ions..) but with ALL the LIGANDS |
| gen_one_traj.out | # General Info about the process |