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

1. The Toy example consist in 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 Superpose
@ 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	# Topological file for the full trajectory without WAT,ions…but with all the LIGANDS
OneLig.NoWat.2ohk_Sol_vdw2301_ZeroB.top	# Topological file for the full trajectory without WAT,ions…but with ONLY ONE LIGAND
RMS_first.dat	
RMSD_FIRST_NoWat_alone.nc	# The full trajectory (without WAT, ions..) but with ALL the LIGAND
gen_one_traj.out	# General Info about the process