Input Data for: **fdMD_OneTraj.cmd**

The User **MUST** modify the variables in RED in the **fdMD_OneTraj.cmd file :**

```
# AMBER  directory

set amber_version = 18
set amber_dir = /home/prog/amber$amber_version

@ num_res_prot = 387    # Number of  protein residues.
@ num_lig     =  26          # Number of Ligands in the simulation.

# The program will superimpose ALL the snapshots of the MD to the FIRST snapshot using the
Alpha
# Carbons ( CA ) of the  Protein  and the residues [ini_res_sup  , ifi_res_sup  ]

@ ini_res_sup  =   1       # Initial protein residue to superimpose
@ ifi_res_sup   =  387     # Final   protein residue to superimpose

#  The USER can use a X-Ray structure as reference to superimpose the full trajectory.
# However, this X-Ray file MUST contain ONLY the protein and ONE ligand.
# ( No  wat,Na+,Cl- …) and MUST be well prepared (like done for the MD system).
# set ref_pdb   : is the name of the file containing the X-Ray structure ( a PDB file ) .
# This file MUST be in the working directory.

set xray = 'no'

if ( $xray == 'yes' ) then
  set ref_pdb  = "Name_Of_XRay_PDB.pdb"
endif

#  Directory where the trajectory is stored, which MUST be referred to the Working Directory
set dir_traj    =  .     #  .  it means: Trajectories are in the working directory

#  set top_name    : Name of the topology file. MUST be the file used in the MD
# ( with wat, ligands.. ) and modified to include the vdW repulsion.  Must be located in the
# same directory where there is the trajectory

set top_name     = "Name_Of_TopFile.top"

set top_file     = $dir_traj/$top_name

# Trajectory files MUST have an specific name :   $prefix_traj'_'$count_traj'_dyn.nc'
# For example :  2ohk_1_dyn.nc, 2ohk_2_dyn.nc  ……
# Then  set prefix_traj  must be set to  2hok
```

```
set prefix_traj = "Prefix_Traj"


# It is supposed that there exist different files to describe the full trajectory:
# From ini_traj to end_traj .

@ ini_traj   =  1
@ end_traj = 10

# It is possible to skip snapshots from the full trajectory as used in the trajin command.

@ ini_read    =   1
set end_read = last
@ inc_read    =   1

# In order to obtain a pdb file containing the last snapshots it is necessary to specify how many
# TOTAL snapshots we have.

set last_pdb = 'yes'
@ num_snaps_total  = 200
```

OUTPUT : This program will generate a file named : **inptrj_one_lig** that MUST be executed (first do: chmod u+x inptrj_one_lig) to generate the desired information.

Then, we will have some new files:

```
lig_NUMLIG.nc                 # Have the full trajectory for only ONE  ligand ( NUMLIG).
lig_NUMLIG_c99.pdb            # Same as before but for  the position of the C99 atoms.
lig_NUMLIG_LAST.pdb           # The Last snapshot for the NUMLIG ligand.
```

were NUMLIG is the residue number of each ligand.
Also, we will have two new topology files. One for the system without WAT (NoWat.) and another without WAT and with only ONE ligand (OneLig.NoWat.).