Input Data for: **fdMD_ReactiveTraj.py**

To obtain a short help Type : Python3 fdMD_ReactiveTraj.py -h

-pocket	USE_POCKET	Use pocket to define distances (False)
-fil_pocket	FILE_POCKET	File containing the aa of the pocket
-xray	XRAY	Use XRay structure as reference (False)
-fil_prot	PROTEIN_PDB	Reference Protein structure
-dis_min	DIS_LIG_PROT_MIN	Minimum distance Ligand-Prot
-posfix_filpdb	POSFIX_FILREP	Posfix added to pdb files
-name_atom	NAME_ATOMREP	Atom to analyse (C99)
-num_plots	NUM_PLOTS	Num Plots to be done (2)
-dis_plots	DIS_PLOTS	Distances to be plotted [5,25]
-snaps_byone	SNAPS_BY_ONE	Snaps by nanosecond
-num_ns_anal	NUM_NS_ANAL	Num ns to analyse
-percent_anal	PERCENT_ANAL	PerCent out of the limits

-pocket	-A logical variable to allow the program to define a pocket whose geometrical center will be used to calculate the distances to the C99 atoms during the molecular dynamics. (False by omission)
-fil_pocket	-File containing the amino acids defining the pocket. Only one line like the MASK of AMBER.
-xray	-A logical variable to allow the program to use an XRay structure as reference. This file must contain a ligand with one atom named C99 that will be used to calculate the distances to the C99 atoms during the molecular dynamics. (False by omission) . The XRay structure must be in -fil_prot file.
-fil_prot	-Reference Protein structure or XRay structure.
-dis_min	-Minimum distance between C99 and any protein atom to consider a ligand bonded or reactive.
-posfix_filpdb	- A name added at the end of the pdb files generated.
-name_atom	-Name of the atom to be analysed (C99 by omission).
-num_plots	-Number of plots for the distance: C99_last - C99_t , to be done (2 by omission).
-dis_plots	-Maximum distances to be Plot ([5,25] by omission).
-snaps_byone	-Number of Snapshots by nanosecond. To calculate how many snapshots we have in num_ns_anal.
-num_ns_anal	-Number of ns to analyse to study the residence time.
-percent_anal	-% PerCent of snapshots that can be out of the limits during the num_ns_anal ns we analyse.

OUTPUT: This program will generate:

1. A file named **delete_Non_Reactive**. If it is executed, It will delete all the information for the NON-REACTIVE ligands. Thus, it keeps only those ligands having in the last snapshot the ligand near the protein.

2. Files with the generic name: **lig_NUMLIG_disat.csv**, containing a table with distance vs time. Where distance means the distance between the C99 atom at the LAST snapshot and this atom at the different times of the MD.

3. A file named: **Info_fdMD_ReactiveTraj** . This file contains all the information about analysis process for the individual trajectories.

4. A directory: **figures_distances**, containing all the pictures with distance vs time as described before).