**Input Data for**: **fdMD_ReactiveTraj.py**

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

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|---|---|---|
| -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 Plot [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 amission). |
| -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).