

The Input Data for: **fdMD\_ReactiveTraj.py**

Is defined in the file : **run\_fdMD\_ReactiveTraj**

```
./fdMD_ReactiveTraj.py      \  
    -pocket      False      \  
    -xray        False      \  
    -fil_prot    first_lig.pdb \  
    -dis_min     5           \  
    -prefix_filpdb _c99      \  
    -name_atom   C99         \  
    -num_plots   2           \  
    -dis_plots   5,25        \  
    -snaps_byone 1           \  
    -num_ns_anal 20          \  
    -percent_anal 10         \  
> Info_fdMD_ReactiveTraj
```