Modification of the file: **fdMD_MMGBSA_Analize.py** for the TEST (Toy) example:

This program creates a picture of DeltaG vs time for each of the reactive trajectories.

A) First, we need to modify the script:
fdMD_MMGBSA_Analize.py

The User **MUST** have this structure**:**

```
snaps_by_one = 1     # Number of snapshot by nano second
ns_ave       = 10    # Number of ns for the average
prefix       ='lig_' # Prefix
```

B) Second, run the program:
python3 fdMD_MMGBSA_Analize.py

B) Once the calculations finished, we will have the "pictures" directory with the plots of the Binding Free Energy vs time.

lig_405.png

and also a file : ave_gbpb.res with the average values of DeltaG along the trajectory for each ns_ave interval