

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\_gbp.res** with the average values of DeltaG along the trajectory for each **ns\_ave** interval