Modification of the file: **fdMD_MMGBSA_Send.cmd** for the TEST (Toy) example:

This script is prepared to be sended to a queue system. Thus, its depends on the computer used.

For the third step we need:

1. A topology file without repulsion:
   2ohk_onelig_norep.top (without vdW repulsion between C99 Atoms)

2. Parameters for the ligand:
   lig.parm & lig.prep

A) First, we need to modify the script:
   fdMD_MMGBSA_Send.cmd

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

```
#!/bin/csh -v
# ......................
# fdMD_MMGBSA_Send.cmd .
# ......................
# top file without repulsion
set nom_top  = 2ohk_onelig_norep.top
#defining the Protein
set ini_res = 1
### ....  Without the ligand.......
set ifi_res = 387
set num_res_prot = @ifi_res
# Number of Ligands in the simulation
@ num_lig     =  26
### ....  Do PB calculations  ?
set pb = 'NO'
set prefix      = '2ohk'
set lig_parm = 'lig.parm'
set lig_prep  = 'lig.prep'
@ startf = 1
@ endf   = 200
@ nfreq  = 1
set indi  = 1.0
set exdi = 80.0

set num_proc  = 8
set AMBERHOME = '/aplic/amber/amber16_ompi'
```

B) Second, we need to send this script to the batch queue using the file:
send_mmpbsa_all
doing: **# were iqtc02.q is the name of the queue.**
qsud -q iqtc02.q **send_mmpbsa_all**

Note that send_mmpbsa_all is a file that must be modified depending on queue system.

Then, the output will be new file :
send_mmpbsa_all

C) Run the new script to send all the calculations to the batch queue:
./ send_mmpbsa_all

D) Once the calculations finished, we will have the MMGBSA results in different directories like:
lig_388
lig_398
lig_405

insight each directory we have two directories:
ffdir : # with the inputs and the output of the MMGBSA
fftop : # with the tops for the ligand, the receptor and the complex

insight the ffdir we will have a file containing the values of the Delta_G (PB) for each snapshot.
DeltaG_BySnaps.csv