1. Surface area for some configurations is missing.

WARNING: Missing PBNONPOL for PB in 0 -> Taken from -1
WARNING: Missing ELRAELE for PB in 0 -> Taken from -1
WARNING: Missing EPB for PB in 0 -> Taken from -1
WARNING: Missing PBNONPOL for PB in 1 -> Taken from 0
WARNING: Missing ELRAELE for PB in 1 -> Taken from 0
WARNING: Missing EPB for PB in 1 -> Taken from 0
WARNING: Missing PBNONPOL for PB in 2 -> Taken from 1
WARNING: Missing ELRAELE for PB in 2 -> Taken from 1
WARNING: Missing EPB for PB in 2 -> Taken from 1
WARNING: Missing PBNONPOL for PB in 3 -> Taken from 2
WARNING: Missing ELRAELE for PB in 3 -> Taken from 2
WARNING: Missing EPB for PB in 3 -> Taken from 2
WARNING: Missing PBNONPOL for PB in 4 -> Taken from 3
WARNING: Missing ELRAELE for PB in 4 -> Taken from 3
WARNING: Missing EPB for PB in 4 -> Taken from 3

We must check three mm/pbsa output files. In these files, we can find:

1

BOND = 37.5339 ANGLE = 90.7117 DIHED = 107.6899
VDWAALS = -32.7338 EEL = -339.8294 EGB = -397.5131
1-4 VDW = 35.0731 1-4 EEL = 301.8880 RESTRAINT = 0.0000
corrected reaction field energy: -668.991774
surface area = 1728.747
ECAVITY = 1728.747

EDISPER = 0.0000

The last three lines will be missing. We must use other softwares to calculate the surface area for some configurations. In amber9 and amber10, they use Molsurf to calculate the surface area.

For GB/SA, we don't have this problem.

MM

GB

MS

1

BOND = 1285.9137 ANGLE = 3260.6397 DIHED = 3965.5584

VDWAALS = -3400.2218 EEL = -29552.5792 EGB = -4639.2235

1-4 VDW = 1440.5764 1-4 EEL = 15465.2572 RESTRAINT = 0.0000

surface area = 18381.715

2. Missing bondi radii of Br and F for surface area calculation

The error information:

Generate PQR

No radius found for BR

No radius found for F

You must add Bondi radii for Br and F in mm_pbsa_calceneent.pm.

This implementation uses bondi radii

```
# Parameters: $pdb,$pqr,$r_mol
my $pdb = shift;
my $pqr = shift;
my $r_mol = shift;

# Bondi radii + 1.4A and probe radius of 0.0A yields SAS
# Bondi radii + 0.0A and probe radius of 1.4A yields molecular surface
# Bondi radii + 0.0A and probe radius of 0.0A yields vdW surface
my %exp_rad = (
                "N"    => 1.550 + 1.400,
                "H"    => 1.200 + 1.400,
                "C"    => 1.700 + 1.400,
                "O"    => 1.500 + 1.400,
                "P"    => 1.800 + 1.400,
                "S"    => 1.800 + 1.400,
                "FE"   => 1.300 + 1.400,
                "Na+"  => 1.200 + 1.400,
                "Cl-"  => 1.700 + 1.400,
                "MG"   => 1.180 + 1.400,
                 "F"    => 1.470 + 1.400,
```

If your ligands contain I atom, we can't use LCPO method to calculate the surface area for GB/SA calculation..

3. Fillratio error for the small ligand

   --- error massage –

PB Bomb in setgrd(): focusing grid too large 2

reset fillratio to a larger number 2.000

fillratio can be changed using the pb namelist. To run it via mm_pbsa.pl you need to edit the mm_pbsa_createinput.pm routine in mm_pbsa_createinput.pm, just to add fillratio = 4.0 (or whatever) to the namelist.

4. *In the output file, mmpbsa.out, we always find some warnings:*

Reading d3hvpMD_com.all.out
WARNING: Missing GB for GB in 21 -> Taken from 20
WARNING: Missing SURF for MS in 34 -> Taken from 33
WARNING: Missing SURF for MS in 58 -> Taken from 57
Reading d3hvpMD_rec.all.out
Checking CALC
WARNING: Missing SURF for MS in 58 -> Taken from 57
Reading d3hvpMD_lig.all.out
Checking CALC
WARNING: Missing SURF for MS in 58 -> Taken from 57
WARNING: Missing SURF for MS in 62 -> Taken from 61
WARNING: Missing SURF for MS in 70 -> Taken from 69

It means that e.g. no surface area was found/calculated for the complex snapshot 34. To get an idea as to what might have gone wrong here, comment the line "unlink $mol;" in the subroutine calc_ms in mm_pbsa.pl ..

Similarly, you may want to comment the other "unlink ..." lines in the calc_... routines in mm_pbsa.pl. Have a look in the xxx_{com,rec,lig}.all.out files and the output files after commenting the "unlink ..." lines.

5. Delphi calculation, pbsa=1

When we try to do a MM/PBSA calculations with AMBER using the option PB=1 but at the end of the calculations we have PBCAL=0, what it means that this energy term hasn't been calculated.

mm_pbsa has been tested on delphi II. We need to comment the line "unlink $delphiout;" in mm_pbsa_calceneent.pl which will give us the delphi output file. Then we can find which errors have happened.