Use of the General Amber Force Field, and generation of an OPLS or Glycam 2006 type force field

Tutorial by:
F. Wang,(1) J.-P. Becker, (1) P. Cieplak,(2) and F.-Y. Dupradeau(1)

(1) Université de Picardie - Jules Verne, Amiens
(2) Sanford-Burnham Institute for Medical Research, La Jolla, CA

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The quantum mechanics (QM) Gaussian, GAMESS or Firefly program is selected during the input submission procedure using the web interface: one can use the public account or a private account:
See http://q4md-forcefieldtools.org/REDServer-Development/faq.php#3

Input molecules of PyRED are provided in the PDB file format:
See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/readme.txt

APPROACH COMPATIBLE WITH GAFF [1]

1- Define specific keywords in the Project.config file:

See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/Project.config
The user has to define the total charge and spin multiplicity of the molecules involved in force field generation if they are different from zero and one, respectively. She/he can also define bond(s), angle(s) and/or dihedral(s), which can be constrained during geometry optimization. Charge constraints can be requested during the charge fitting step to lead to molecular fragments as well, etc...

Then, the user has to provide the atom types for the molecules provided as input files. In this case the dictionary of atom types developed in PyRED is not used, and the GAFF atom types (lower case) provided in the `MOLECULE1-ATMTYPE` keyword are read:

```
# For instance for methanol
MOLECULE1-ATMTYPE      = c3 h1 h1 h1 oh ho
```

2- Define specific keywords in the System.config file (optional):

See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/System.config

Select the *charge model* (optional):

```
# RESP-A1 is the default; so this keyword is not really needed...
CHR_TYP        = RESP-A1
```

3- Use the gaff.dat file as a frcmod.user file:

The gaff.dat force field parameter file has to be provided as a *frcmod.user* file:

```
cp $AMBERHOME/dat/leap/parm/gaff.dat frcmod.user
```

APPROACH COMPATIBLE WITH THE OPLS FORCE FIELD [2]

1- Define specific keywords in the Project.config file:

The user has to provide the OPLS atom types for the molecules provided as input files in the `MOLECULE1-ATMTYPE` keyword.

2- Define specific keywords in the System.config file:

Select the charge model: [2]

```
# RESP-O1 is required for OPLS
CHR_TYP        = RESP-O1
```

3- Define specific force field parameters in the frcmod.user file:

OPLS force field parameters have to be provided in the *frcmod.user* file.

APPROACH COMPATIBLE WITH THE GLYCAM 2006 FORCE FIELD [3]

A similar approach can be followed if one is interested in working with the Glycam 2006 force field:

- Define the atom types one wishes to use in the *Project.config* file,
- Select the `RESP-C2` charge model in the *System.config* file,
- `cp $AMBERHOME/dat/leap/parm/GLYCAM_06h(*).dat frcmod.user`

(*) whatever version of the Glycam force field.

4- Create an archive file to upload the different PyRED inputs (for the GAFF, OPLS or GLYCAM 2006 force field)

See http://q4md-forcefieldtools.org/REDServer-Development/popup/poparchive.php

```
tar -zcvf Archive.tgz Mol_red*.pdb Project.config System.config frcmod.user
```


[1] J. Wang, R. M. Wolf, J. W. Caldwell; P. A. Kollman, D. A. Case, *J. Comput. Chem.* 2004, 25, 1157.
[2] R. H. Henchman, J. W. Essex, *J. Comp. Chem.* 1999, 20, 483.
[3] K. N. Kirschner, A. B. Yongye, S. M. Tschampel, J. Gonzalez-Outeirino, C. R. Daniels, B. Lachele Foley, R. J. Woods, *J. Comput. Chem.* 2008, 29, 622.

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