Mini How-To prepare input files for a first R.E.D. Server Development/PyRED job

An extended documentation is available @:
http://q4md-forcefieldtools.org/REDServer-Development/Documentation/
An extended tutorial is available @:
http://q4md-forcefieldtools.org/Tutorial/Tutorial-4.php
A demonstration is available @:
http://q4md-forcefieldtools.org/REDServer-Development/RED-Server-demo1.php
Frequently asked questions are available @:
http://q4md-forcefieldtools.org/REDServer-Development/faq.php

Prepare PDB input file(s) for the *$n* input molecule(s)

Strictly follow the PDB file format

See http://www.wwpdb.org/documentation/file-format-content/format33/sect9.html
& http://q4md-forcefieldtools.org/REDServer-Development/Documentation/readme.txt

Generate correct name and extension for each PDB input file

`Mol_red$n.pdb` *$n* integer (1, …) = molecule number, which is incremented

Generate correct geometry(ies) for each input molecule

Avoid close contacts and bumps between atoms in your input geometry(ies)
This will save a lot of cpu time!
Rigorously control/define the conformation(s) you wish to use

Add the hydrogen atoms to your molecule

Check the total charge and spin multiplicity of each molecule

- The total charge can be defined in the PDB input file
  it depends on the hydrogen atoms and on the pH
- The spin multiplicity of an organic molecule likely equals one

Define specific options in the “Project.config” and “Sytem.config” input files

The “Project.config” & “Sytem.config” files are generally not needed for a first PyRED job
PyRED default options allow directly generating a force field for the input molecule(s)

- if the spin multiplicity of each molecule equals one
- if the total charge of each molecule equals zero or is defined in the PDB input file

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

Keywords required for generating molecular fragments, correcting atom types or modifying chemical equivalencing (among others) can be provided in a second job using the '`Re_Fit`' mode:

Read http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo1.pdf

Define missing/mandatory force field parameters in the “frcmod.user” input file

The “frcmod.user” file is not needed for a first PyRED job

It can be provided in a second job using the '`Re_Fit`' mode:

Read http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo1.pdf

Create an archive file to submit these input files to R.E.D. Server Development/PyRED

Read http://q4md-forcefieldtools.org/REDServer-Development/Documentation/Create-archive.php

Do you need help? → http://q4md-forcefieldtools.org/REDServer-Development/faq.php#5

Last update of this Mini HowTo: August 24th, 2022.