

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 the PDB input file(s) for the 'n' input molecule(s) (molecule index; $n > 0$)

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

Mo1_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 generally 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 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>

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