QMe HOW-TO:

Installation

- Tested on Ubuntu, PyMOL version 1.7.x.
- Download QMe.zip from repository (github.com/QMePyMOL/QMe-PyMOL-Plugin)
- In PyMOL select Plugin -> Plugin Manager -> Install New Plugin -> Choose file -> Select QMe.zip -> Ok

Usage

Warnings:

- ❖ If PDB file has more than 9999 residues, it's necessary to use "QMe PDB loader" to load it into PyMOL since it doesn't natively support such files. Upper limit is 99999 residues. In PDB files from AMBER residue numbers go up to 9999 and then start repeating from 1.
- ❖ Saving such files after loading them into PyMOL will result in malformed PDB file. Use QMe option to save created PDB file or use saved session in PyMOL.
- ❖ Order of residues, as well as order of atoms within residues may be changed compared to input PDB file.

1) Load PDB file with QMe PDB loader (Plugin -> QMe PDB loader)
2) After loading PDB file make named selections for QM region, center atom and optionally link-atoms.
   E.g. Use command: "select YourSelectionName, (resi 19+20+21 and sidechain) or resi 22-26"
   to select sidechains of residues 19,20,21 and all residues from 22 to 26. Alternatively use manual selection.
   Note that:
   - Selections can't be name "sele". Rename them using "set_name OldName, NewName" command before using QMe plugin.
   - Center selection should preferably have only one atom from QM region since outer radius will be calculated based on distance from each atom in this selection.
   - For more selection examples check PyMOL documentation.
3) Run QMe plugin (Plugin -> QMe) and specify:
   - Center Selection – selection with atom from which distances will be calculated
   - Outer Radius - distance from Center Selection up to which waters won't be removed.
   - Optimization Radius – distance from Center Selection up to which residues will have optimization flag set to 0, residues beyond this radius are frozen (flag -1)
   - Link-Atoms Selection – selection containing link-atoms. Setting it to "Default" will result in setting every atom directly connected to QM selection as link-atom.
   - QM Region Selection – selection for QM region.
   - IN Files Directory – directory containing IN files with information about non-standard residue types from PDB file. Unless IN files are provided non-standard residues will have type "XX".
   - Save Directory - directory where ATQ file will be saved. File is named "out.atq" and may be overwritten.
   - Save PDB file – select to save PDB file containing atoms from "QMe" object.
4) Click "Convert".
5) Plugin saves ATQ file in specified directory (optionally PDB file) and creates additional PyMOL object named "QMe" containing all atoms from protein and waters up to Outer Radius from Center. It contains all atoms from "*_Outer" selection and it represents atoms from newly created ATQ and PDB files. There is number of selection on "QMe" object:
   - QMe_QM – QM region atoms
   - QMe_Center – Center atoms
   - QMe_Opt – All not-frozen atoms.
   - QMe_LA – Link-atoms