Haptimol RD Installation and User Guide

To Install

- Before Installing ensure you have an OpenCL compliant GPU and have an OpenCL ready driver installed for your graphics card.
- Double-click on the Installer.msi file included in the Setup folder.
- Go through the instructions on your screen to install it. The default installation folder is C:\Program Files\Haptimol\HaptimolRD.

To launch the software for the first time.

- Go to Start menu -> All Programs -> HaptiMOL
- Click on HaptimolRD from the start menu.

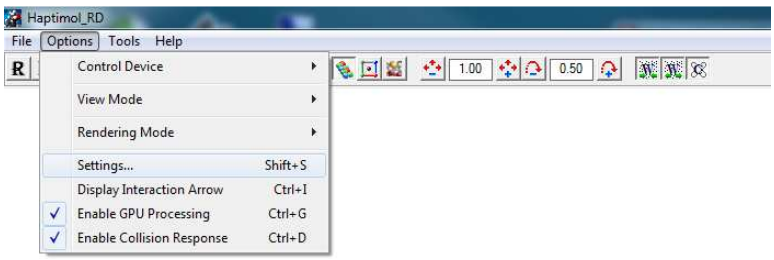
The application should then launch.

On first use you are required to set the file path for some Gromos files.

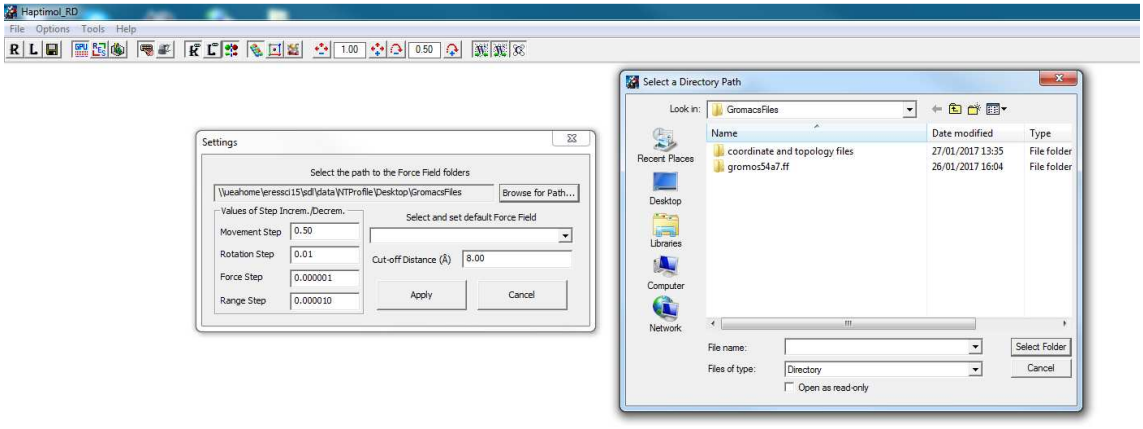
- If you have not already done so please download the supporting gromos force field, protein coordinate and topology files.
  - http://www.haptimol.com/haptimolrd/gromacsfiles.zip
- Extract the zip file to a location on your hard disk.

You now need to set the file path in the software to the location where you just placed the *GromacsFiles* directory.

- Click on Options and Settings as shown in the diagram below.



- Select on *Browse for Path…* from the dialog that appears (as shown below).
- Navigate to the GromacsFiles directory and click on *Select Folder* when you have opened the folder and can see the gromos and coordinate folders as shown in the diagram below.



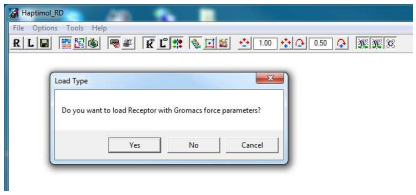
- Click on *Apply* to set this location. This only needs to be done once.

Getting Started

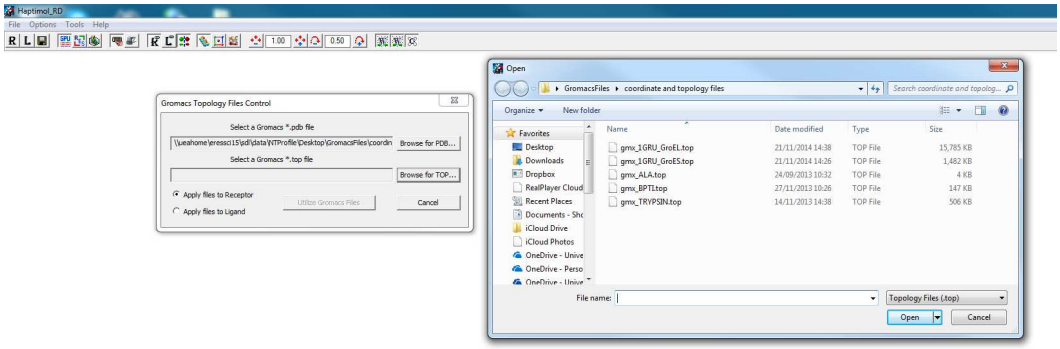
You are now ready to open two molecules one as the ligand and the other as the receptor.

- We suggest starting by loading gmx_ALA.pdb and gmx_ALA.top for the coordinate and topology files for both the receptor and the ligand.

- Click on the “R” in the top-left corner to start the steps for loading the receptor.



- Click *Yes* to include the force field parameters.



- Now you can set the PDB and TOP files in the dialog box as shown above by clicking on the *Browse for* options.

On first use you will need to navigate to the location of the sample coordinate and topology files (which will be where you placed the GromacsFiles directory earlier).

- Click on *Utilize Gromacs Files* to load in the receptor.
- Click on the “L” in the top left of the screen and repeat the above steps to load in the ligand.

Now we are ready to begin using the software.

- To use the haptic device click on the haptic device icon on the taskbar (or press Ctrl + H).
- Press and release the button on the haptic stylus to start moving the ligand and feeling the interaction forces.