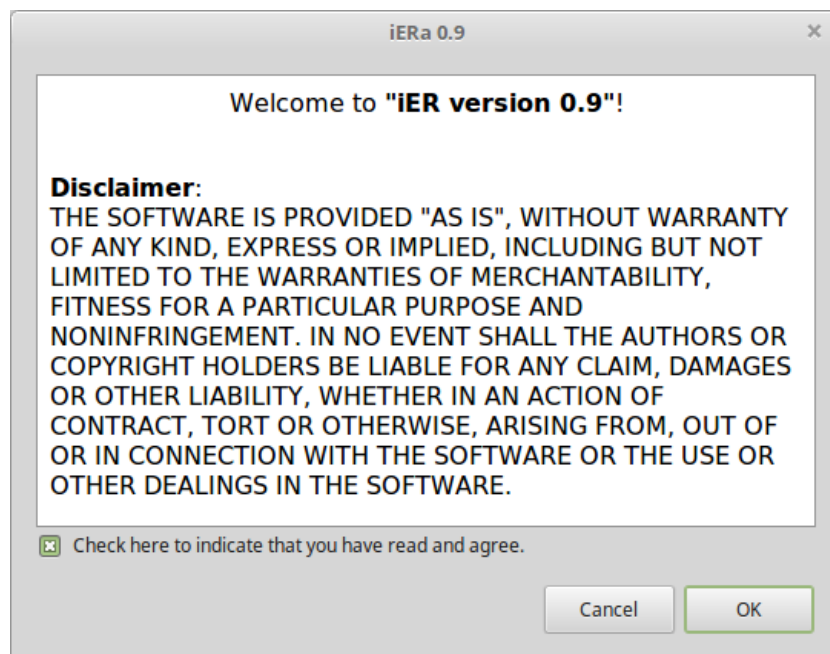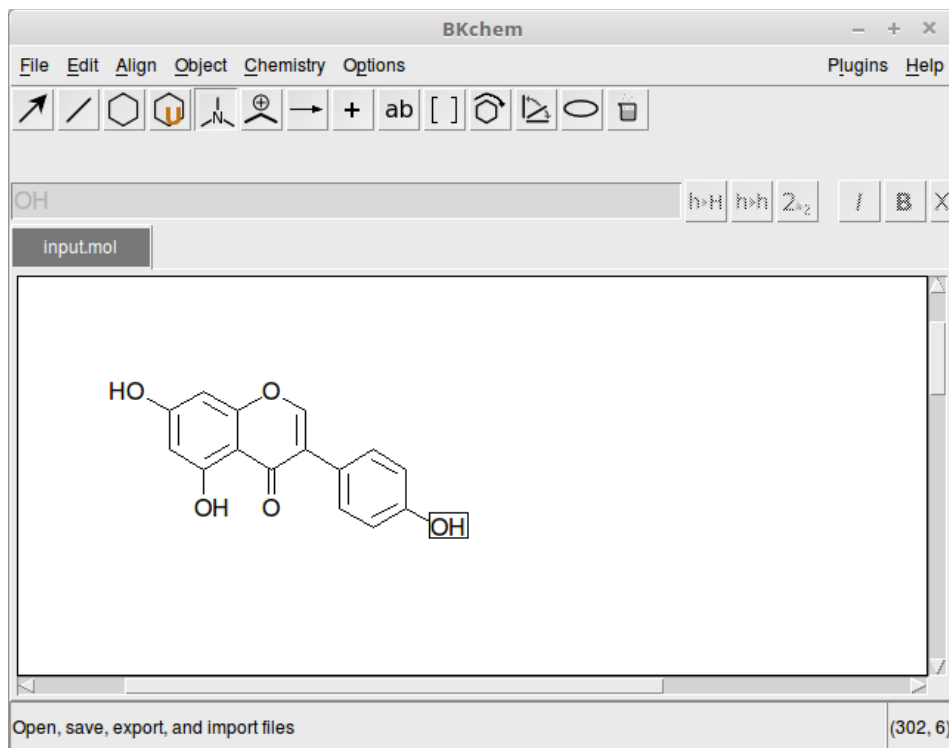Tutorial "iERa 0.9" - In silico test of genistein as ligand for Eralpha
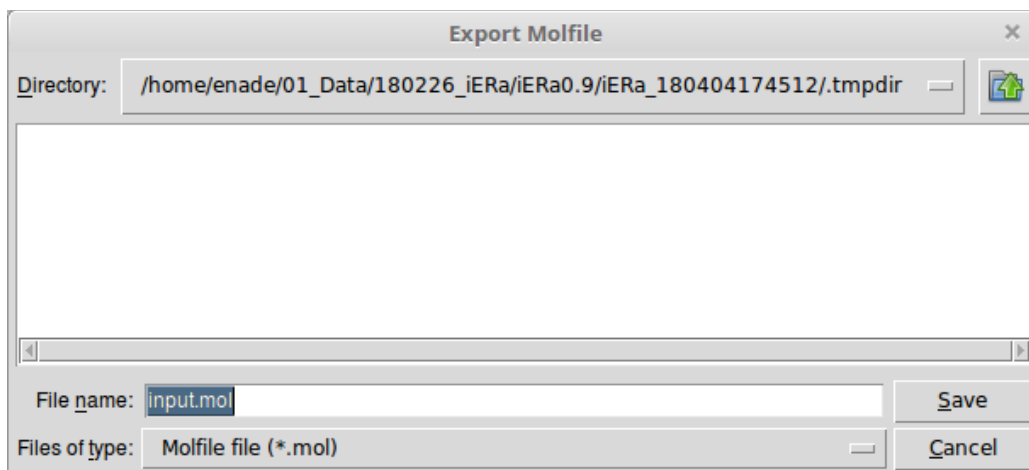
1. After being unzipped and all dependencies were installed, open directory "iERa0.9".

2. Click to run the file "run.sh".
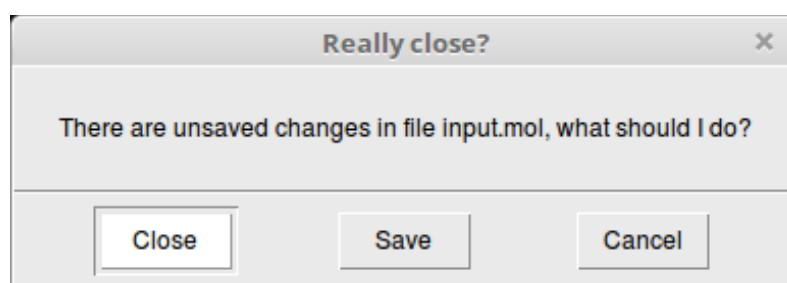
3. Click "Check here to indicate …" and click "OK".

4. Build the test structure (in this case genistein) in the pop-up BKChem window.
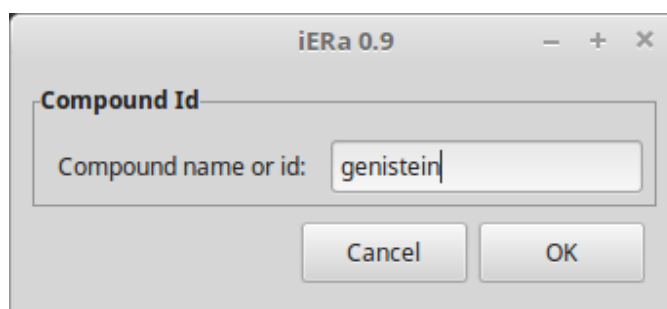
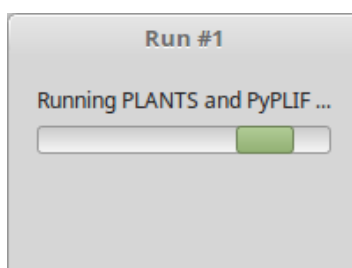5. Export the file as "input.mol": Click "File > Export > Molfile" and then click "Save"

6. Close the BKChem window by clicking "x" in the top-right corner, and click "Close"

7. Give the identity of the compound. In this case "genistein". And then click "OK"

8. And then wait for this application performing the in silico test.

9. There are two outputs of the applications, i.e. the following report and a directory started with "iERa_". Please contact your local computational chemistry expert to explore more the output directory.
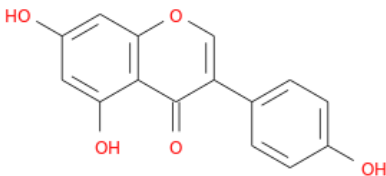

iERa 0.9

The tested compound was predicted as an ERalpha **potent** ligand.
References:
[1] Istyastono EP et al., 2017, Asian J. Pharm. Clin. Res., 10(12).
[2] Mysinger MM et al., 2012, J. Med. Chem. 55(14).
[3] Manuscript submitted to Indonesian Journal of Chemistry.

The 2D structure of tested compound was:

genistein

Cancel   OK