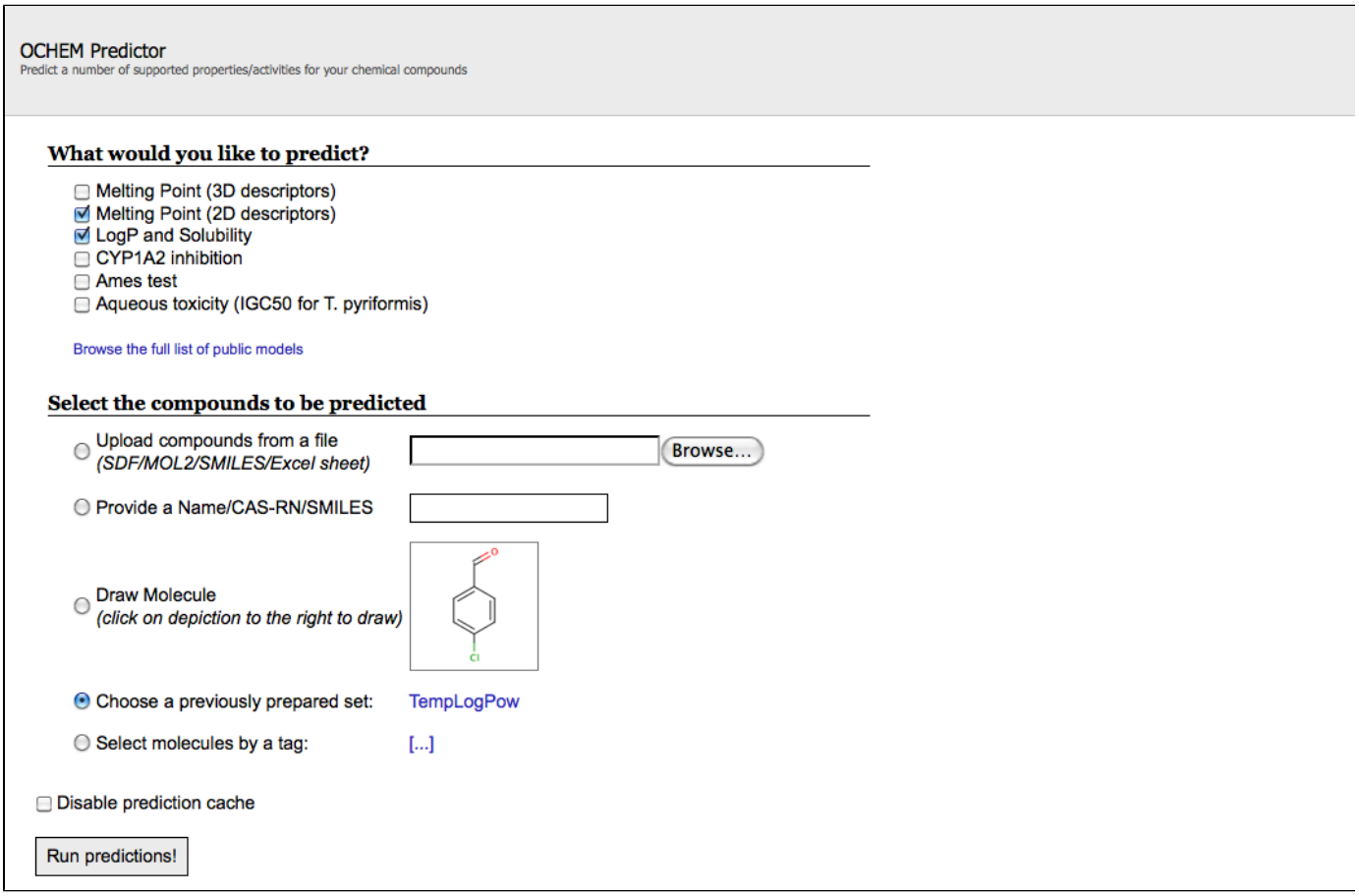
Using OCHEM predictor

The OCHEM Predictor is a simple one-click prediction tool for OCHEM featured models. Currently the models featured by OCHEM:

- Melting Point (3D descriptors)
- Melting Point (2D descrptors)
- LogP and Solubilit
- CYP1A2 inhibition
- Ames test
- Aqueous toxicity (IGC50 for T. pyriformis)

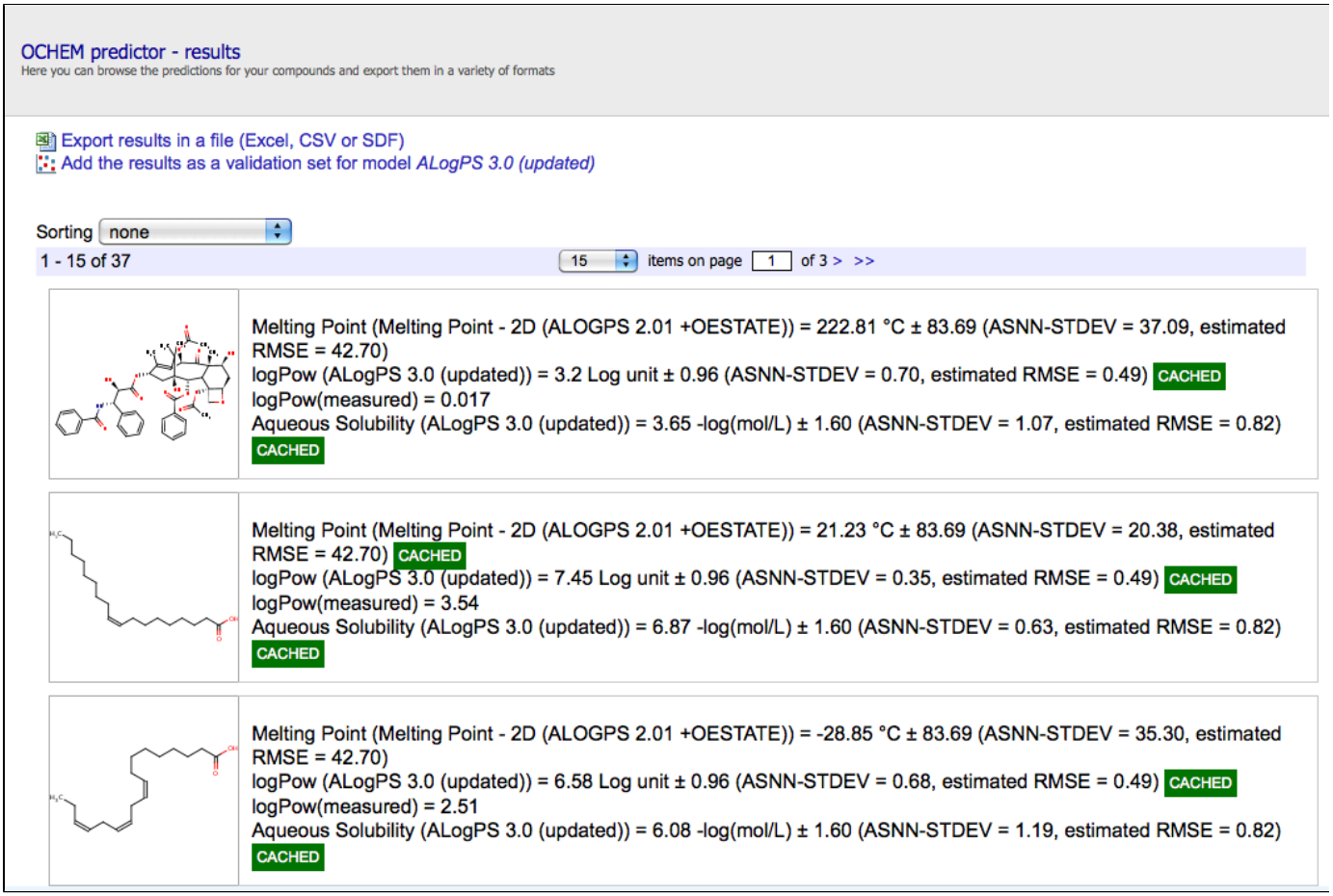
You can reach OCHEM Predictor tool by choosing the "Models > Open Predictor" menu item.



First, select the models you would like to apply in the upper part of the Predictor screen. Then, select the molecules you would like to apply the predictions to. You have the choice between:

- Uploading the SDF file with molecule structures
- Providing a Name, CAS-RN or SMILES. The Name and CAS-RN will be used to search for a molecule structure in PubChem
- Drawing a molecule in sketcher
- Selecting a previously prepared dataset (see Working with datasets for details)
- Selecting all molecules marked by a specific tag

Once you are ready, you can proceed by clicking the "Run predictions!" button. When the prediction process is finished, you are redirected to the predictions browser.



You can either review the prediction values in the predictions browser, or export the predictions in the format of your choice (see Exporting data from OCHEM).