FORECASTER Platform Tutorial

Sites of Metabolism using IMPACTS

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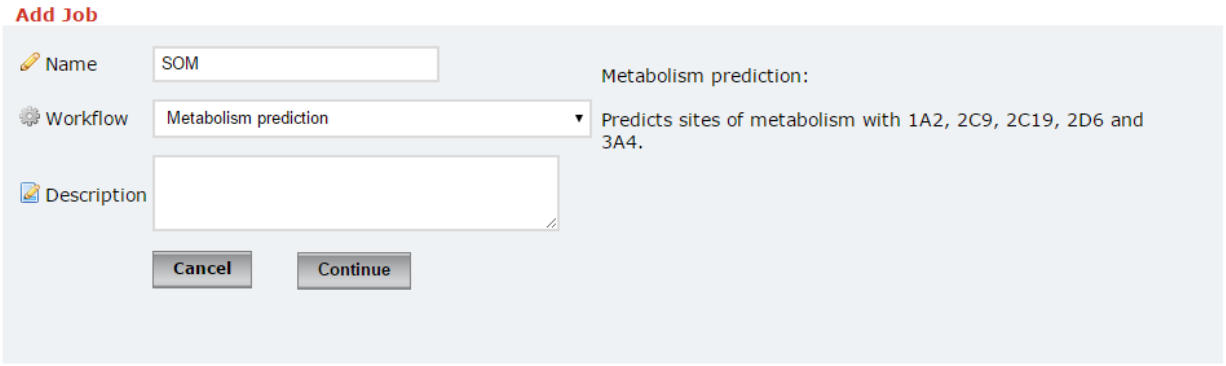
Metabolism prediction

From a single molecule drawn in 2D, we will predict the two possible sites of metabolism from the CYP 450.

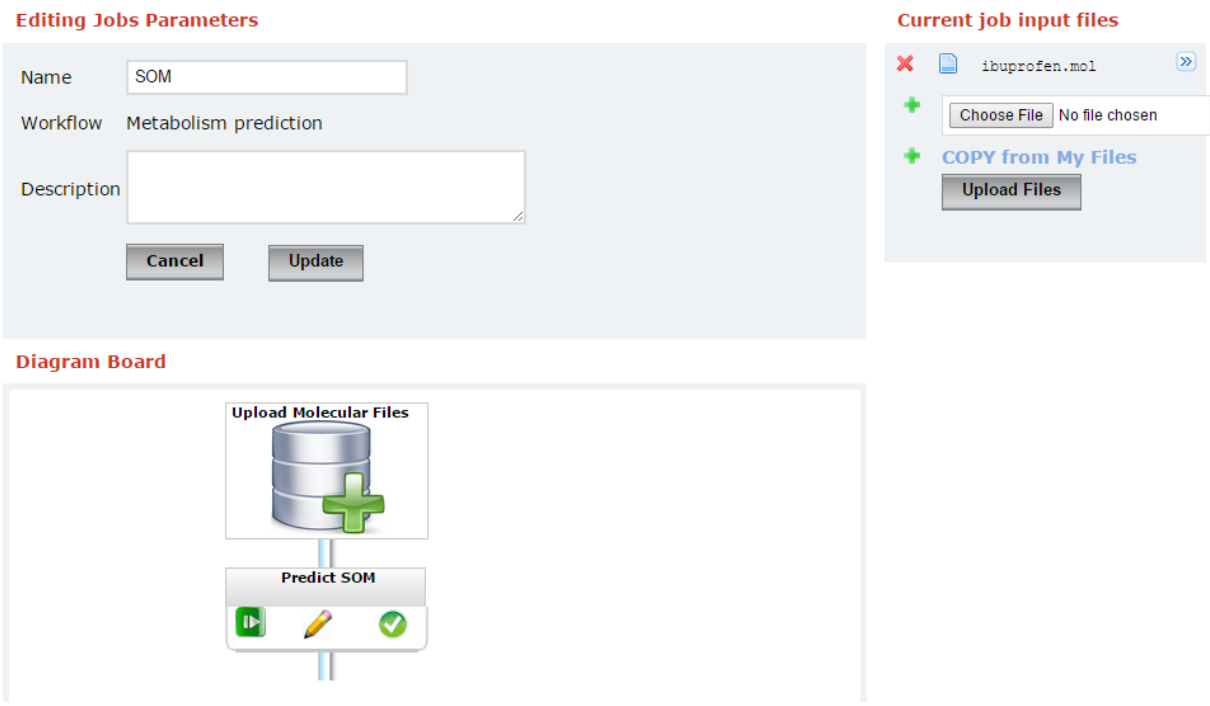
Add a new job from the job manager.



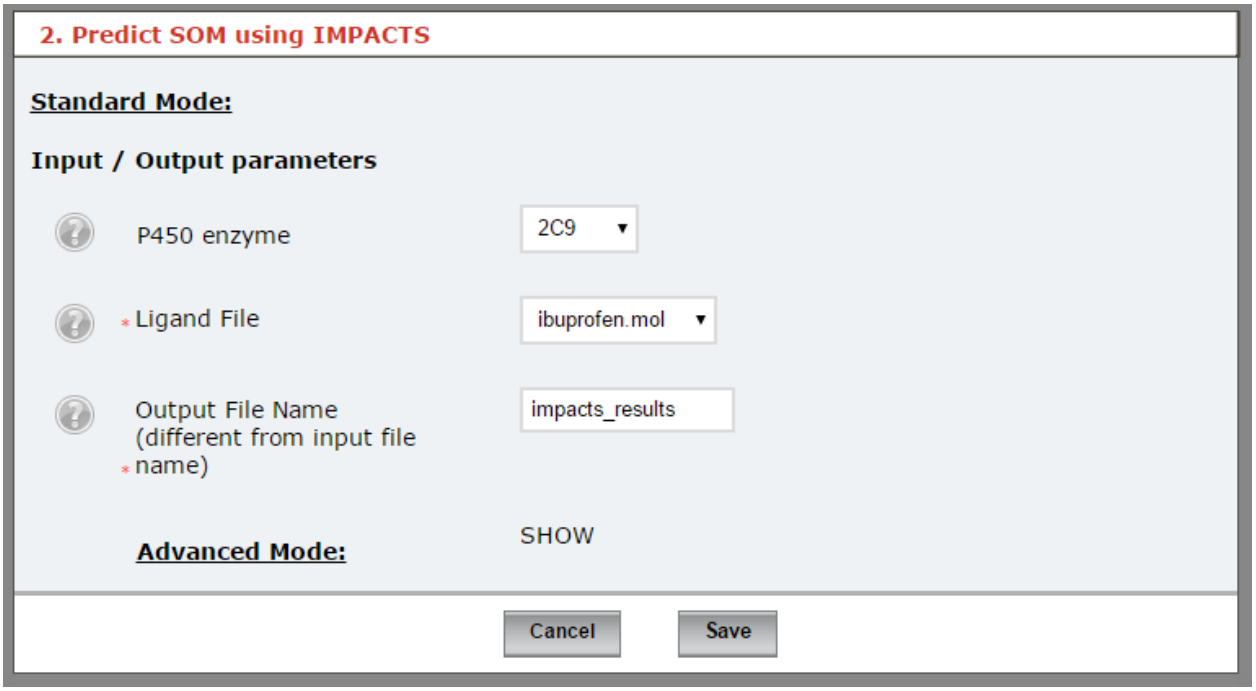
The required file can be downloaded here: http://molecularforecaster.com/files/ibuprofen.zip

We will use the ibuprofen molecule (file ibuprofen.mol). The file can be uploaded via the "Upload Molecular Files" icon or directly from the "Current job input files" section on the right side of the page.

Alternatively, the molecule can be drawn directly using the 2D sketcher.



Clicking on the pen in the middle on the "Predict SOM" box will open the following box:



The IMPACTS program will generate two structure files. The file impacts_results_Metabolites3D.sdf contains the 3D conformation of the oxidized molecule in complex with the heme's iron. The file impacts_results_Metabolites2D.sdf contains 2D structures of the 2 possible metabolites.