
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.



Add Job

The 'Add Job' form is displayed with the following fields and options:

- Name:** SOM
- Workflow:** Metabolism prediction (dropdown menu)
- Description:** (empty text area)
- Metabolism prediction:** Predicts sites of metabolism with 1A2, 2C9, 2C19, 2D6 and 3A4.
- Buttons:** Cancel and Continue

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.

Editing Jobs Parameters

Name:

Workflow: Metabolism prediction

Description:

Current job input files

No file chosen

[COPY from My Files](#)

Diagram Board

The diagram board shows a workflow starting with a box labeled 'Upload Molecular Files' containing a database icon and a green plus sign. A vertical line connects this to a box labeled 'Predict SOM' which contains a play button, a pencil icon, and a checkmark.

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

2. Predict SOM using IMPACTS

Standard Mode:

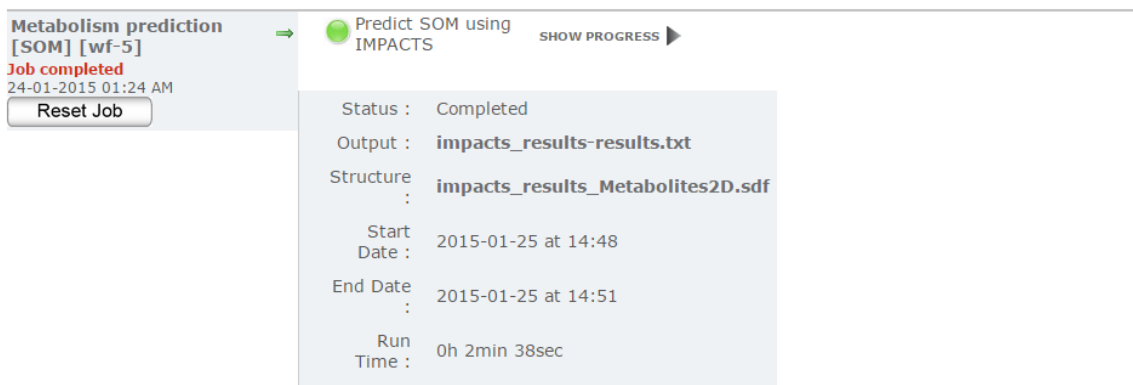
Input / Output parameters

<input type="button" value="?"/>	P450 enzyme	<input type="text" value="2C9"/>
<input type="button" value="?"/>	* Ligand File	<input type="text" value="ibuprofen.mol"/>
<input type="button" value="?"/>	Output File Name (different from input file * name)	<input type="text" value="impacts_results"/>

Advanced Mode:

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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.



The screenshot shows a job completion notification for a metabolism prediction task. The notification is titled "Metabolism prediction [SOM] [wf-5]" and indicates that the job is "Job completed" on "24-01-2015 01:24 AM". A "Reset Job" button is visible. The job details are as follows:

Status :	Completed
Output :	impacts_results-results.txt
Structure :	impacts_results_Metabolites2D.sdf
Start Date :	2015-01-25 at 14:48
End Date :	2015-01-25 at 14:51
Run Time :	0h 2min 38sec