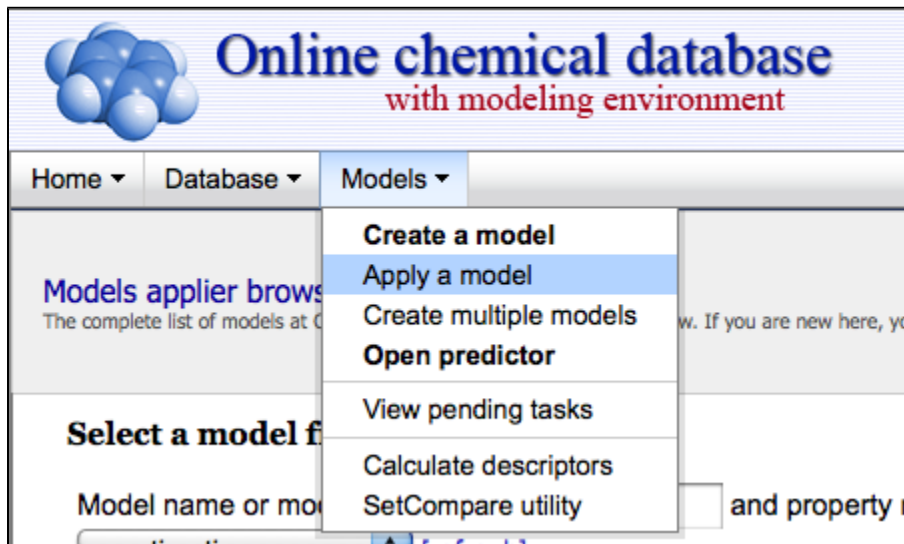


# Using model browser

The model browser is a browser that gives you access to all models available to you. These include public models and your private models. You can open the Model browser by selecting the "Model > Apply a model" menu item.



The browser provides traditional filter elements to find the model by public name or identifier, filter models for a specific property only, or to limit the list to public or private models only.

**Models applier browser**  
The complete list of models at OCHEM available for you is displayed below. If you are new here, you can also switch to a simplified OCHEM predictor

**Select a model from the list**

Model name or model ID:  and property name:  or by article id:  Models visibility:  Order by:  [refresh]

1 - 15 of 50  items on page  of 4 > >>

		delta_density_LibSVM_[ChemaxonDescriptors] (compounds out) , published by xenol	predicts delta_density using Ajmani_delta_train (3857) validated by Ajmani_delta_test (672)	LibSVM	2012-11-22
		BP (compounds out) , published by xenol	predicts Mix_BP using bp_train (3239) validated by bp_test_mix_out (631)	LibSVM	2012-11-22
		delta_density_LibSVM_[InductiveDescriptors] (compounds out) , published by xenol	predicts delta_density using Ajmani_delta_train (3857) validated by Ajmani_delta_test (672)	LibSVM	2012-11-22
		delta_density_LibSVM_[Dragon (blocks: 1-20)] (compounds out) , published by xenol	predicts delta_density using Ajmani_delta_train (3857) validated by Ajmani_delta_test (672)	LibSVM	2012-11-22
		BP (mixtures out) , published by xenol	predicts Mix_BP using bp_train (3239) validated by bp_test_mix_out (631)	LibSVM	2012-11-22
		k-Medoid logBCF, DRAGON , published by stefan	predicts BCF using k-Medoid_logBCF (238)	MLRA	2012-09-14
		PLS-Optimal -logIGC50 , published by stefan	predicts Boiling Point using k-Medoid_BoilingPoint (1198)	PLS	2012-09-13
		PLS-Optimal logLC50 , published by stefan	predicts Lethal Concentrations using PLS-Optimal logLC50 (535)	PLS	2012-09-13

The items of the browser represent models. From this view you can easily jump to model training and test sets by clicking the appropriate links. Clicking on the model name or the model profile icon ( ) leads you to the detailed model profile (see Model profile).

The export icon ( ) leads to the export dialog, where you can export model statistics for training and test sets, descriptors for individual molecules and even linear equation for linear models.

To apply multiple models using the model browser select the desired models by clicking the appropriate checkboxes

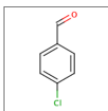
on the right of every model item. OCHEM featured models have a golden star (★) next to their name. If you would only like to apply OCHEM featured models, you can also use the simplified [OCHEM Predictor](#). Click "Next>>" button when you are satisfied with your selection of models to proceed to molecule set selection screen.

Apply the model

### Provide the compound(s) to predict

Please provide compounds for which you want to predict the target property  
Several options are available:

- ☐ Upload compounds from a file  
(SDF/MOL2/SMILES/Excel sheet)
- ☐ Provide a Name/CAS-RN/SMILES
- ☒ Draw Molecule  
(click on depiction to the right to draw)
- ☐ Choose a previously prepared set:
- ☐ Select molecules by a tag:



### Additional options

Prediction scenario:

☐ Disable prediction cache

You can identify the target molecules by:

- 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

Click "Next>>" to proceed to the prediction process. Once all the selected models were applied to the molecules, you are redirected to the predictions browser.

### OCHEM predictor - results

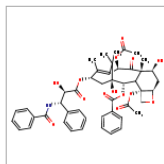
Here you can browse the predictions for your compounds and export them in a variety of formats

 [Export results in a file \(Excel, CSV or SDF\)](#)

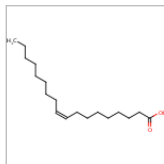
Sorting

1 - 15 of 37

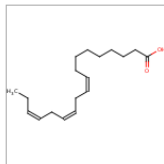
items on page  of 3 >>



Boiling Point (PLS-Optimal -log<sub>10</sub>GC50) = 1089.79 °C  
Lethal Concentrations (PLS-Optimal log<sub>10</sub>LC50) = -6.41 log(mol/L)  
LogKoc (PLS-Optimal logKOC) = 1.91 Log unit



Boiling Point (PLS-Optimal -log<sub>10</sub>GC50) = 393.9 °C  
Lethal Concentrations (PLS-Optimal log<sub>10</sub>LC50) = -6.42 log(mol/L)  
LogKoc (PLS-Optimal logKOC) = 4.65 Log unit



Boiling Point (PLS-Optimal -log<sub>10</sub>GC50) = 287.79 °C  
Lethal Concentrations (PLS-Optimal log<sub>10</sub>LC50) = -6.42 log(mol/L)  
LogKoc (PLS-Optimal logKOC) = 4.36 Log unit

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).