QSARINS-Chem

Standalone Version

How To…

QSAR Research Unit in Environmental Chemistry and Ecotoxicology
Department of Theoretical and Applied Sciences (DiSTA)
University of Insubria

Authors

Nicola Chirico (Research Fellow)
Alessandro Sangion (Research Fellow)
Paola Gramatica (Senior Professor)
Ester Papa (Associate Professor)

QSAR Research Unit in Environmental Chemistry and Ecotoxicology
Department of Theoretical and Applied Sciences (DiSTA)
University of Insubria, Varese, Italy
http://dunant.dista.uninsubria.it/qsar/

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We would also appreciate citations to the website: http://dunant.dista.uninsubria.it/qsar/

Limitations of Liability and Disclaimer of Warranty

HOW TO…

Enter user's descriptors for model predictions

To enter manually the descriptors of the molecules (and optionally their experimental endpoints) in the "User descriptors" sub-tab of the "Models" tab, click on the cell, enter the data and press enter to confirm.
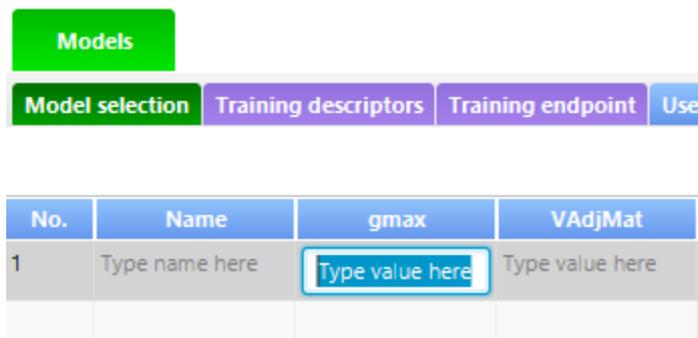
If the value inserted is problematic, the cell will turn red and a warning will be displayed in the "Status" column. Placing the mouse pointer upon the red cell for few seconds a tool tip reporting the issue will be displayed, as shown in the example below.
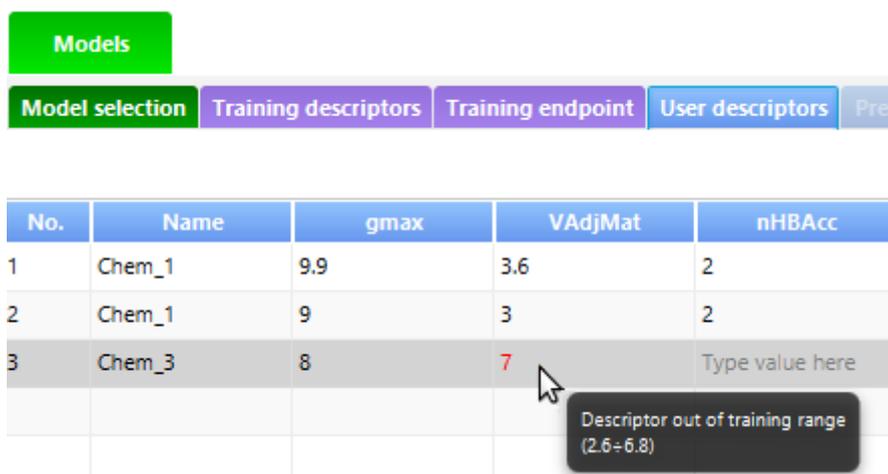
It is possible to calculate the descriptors by means of the PaDEL Descriptor software (bundled with this software), and automatically import them. To accomplish this task, you have to right-click on the table and select "Import and calculate descriptors…" form the drop-down menu.
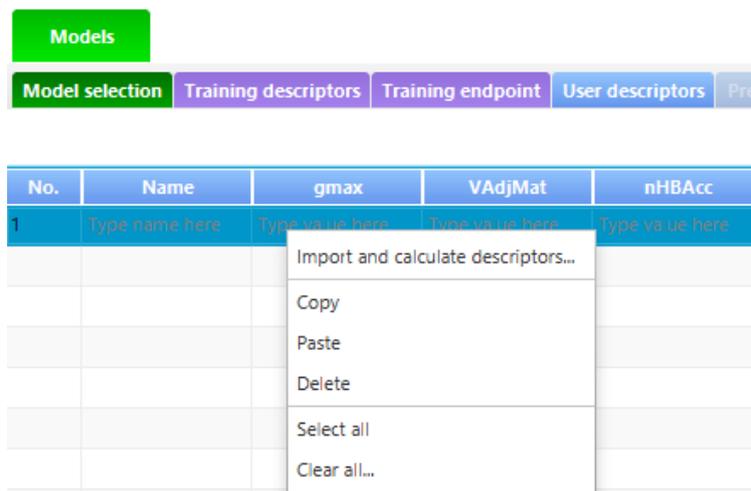
You will be asked for the folder containing the molecules structures files for descriptors calculation, then the PaDEL Descriptor software is automatically executed (you know that is executing because the splash screen will appear during the descriptor's calculation).

Once calculation is completed, the descriptors values will be imported automatically. Issues with molecular descriptors, if any, will be highlighted as "Warning" in the "Status" column.

Cells can be edited manually, if needed.

If data are pasted from an external source (e.g. from Excel), or a new folder is selected for additional descriptor calculation with PaDEL Descriptor, they will be automatically added below the last row (data are never overwritten).

Once data are entered either by the user or by automatic descriptors calculation, press "Apply model" to calculate model predictions. This will enable the "Predictions" and "Graphs" sub-tabs, where the model's predictions can be analyzed by the user.

Multiple rows selection

Multiple table rows can be selected in various ways. If you need to select consequent rows of a table, select the first row then, holding the "shift key" button on your keyboard, click on the final row.

Alternatively, still holding the "shift key", move the final row selection by means of the "up/down cursor keys" of your keyboard.

You can select singularly multiple non-consequent rows holding the "ctrl" key and selecting the row with the mouse cursor. Clicking on the same row will cyclically select and deselect it.

Rearrange table columns

The order of the columns can be changed manually dragging the header of the column with the mouse cursor.

Resize table columns

Table columns can be resized moving the mouse cursor between the two columns headers. The mouse pointer will change as a "double arrow" indicating the possible resize direction, as shown below, then resize follows while holding and moving the left mouse key.

Select a model

To select a model click on the "Models" main tab and select the "Model selection" sub-tab. Then click on the drop-down list to choose the model, as shown in the figure below.
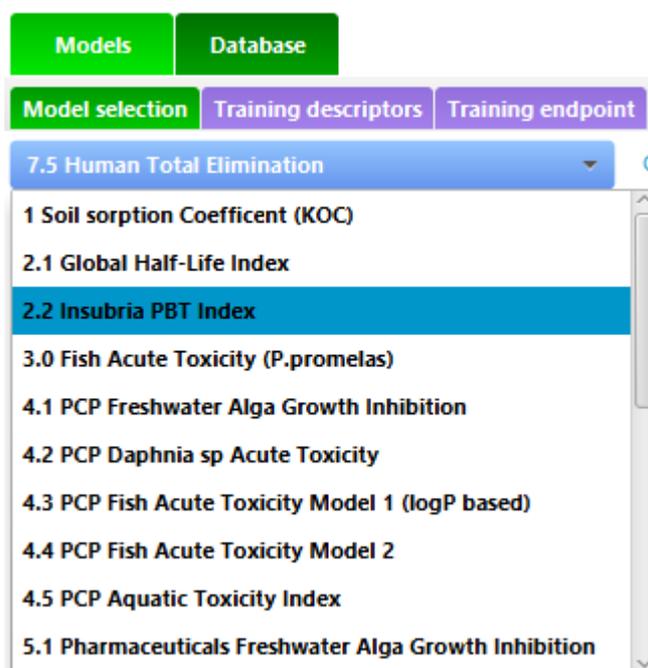
Select tabs on limited screen resolution

Depending on the screen resolution, it is possible that some tabs cannot be shown. In this case an arrow is displayed to the right of the screen. Clicking on the arrow a drop-down menu will appear allowing for selection of all tabs, as shown below.
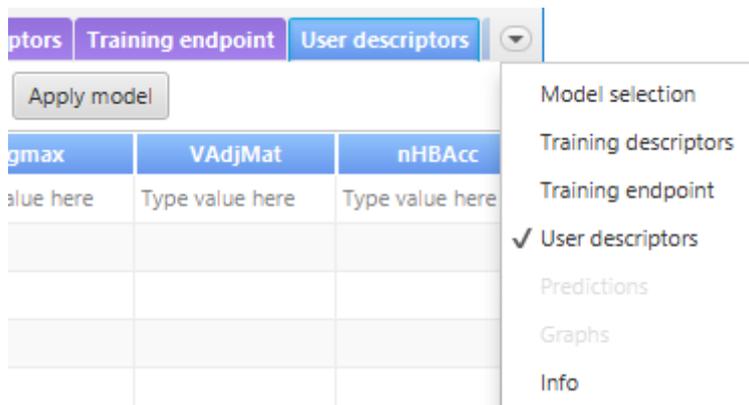
Show model's training descriptors or training endpoint

To show the model's training descriptors or the training endpoint, click on the corresponding sub-tabs of the "Models" tab.

Sort table columns

To sort a column click cyclically on the column header. An arrow on the right of the column's name will appear indicating the sorting order (up arrow means ascending, down arrow means descending).

Experimental endpoint▲
7.3
7.4
8.1

Experimental endpoint▼
12
12
12

Visualize predictions and statistics of the applied models

To visualize the model's prediction click on the "Prediction" sub-tab. As in the "User descriptors" sub-tab, problematic entries will be displayed in red. Placing the mouse pointer on these values a tool-tip explaining the reason of the problem will be displayed.

Visualize model's predictions graphically

To visualize the model's predictions graphically you need first to select the sub-tab "Graphs" and then to press the "Calculate graphs" button.

To resize the graphs, move the mouse pointer upon the vertical or horizontal border separating the graphs. The mouse pointer will change as a "double arrow" indicating the possible resize direction, as shown below.

Holding the left mouse button and moving the mouse according to the suggested directions will resize the graphs.

Graph points are supported by tool-tips. Leaving the mouse pointer upon one graphic point will pop up the corresponding informative tool-tip, as shown in the figure below.
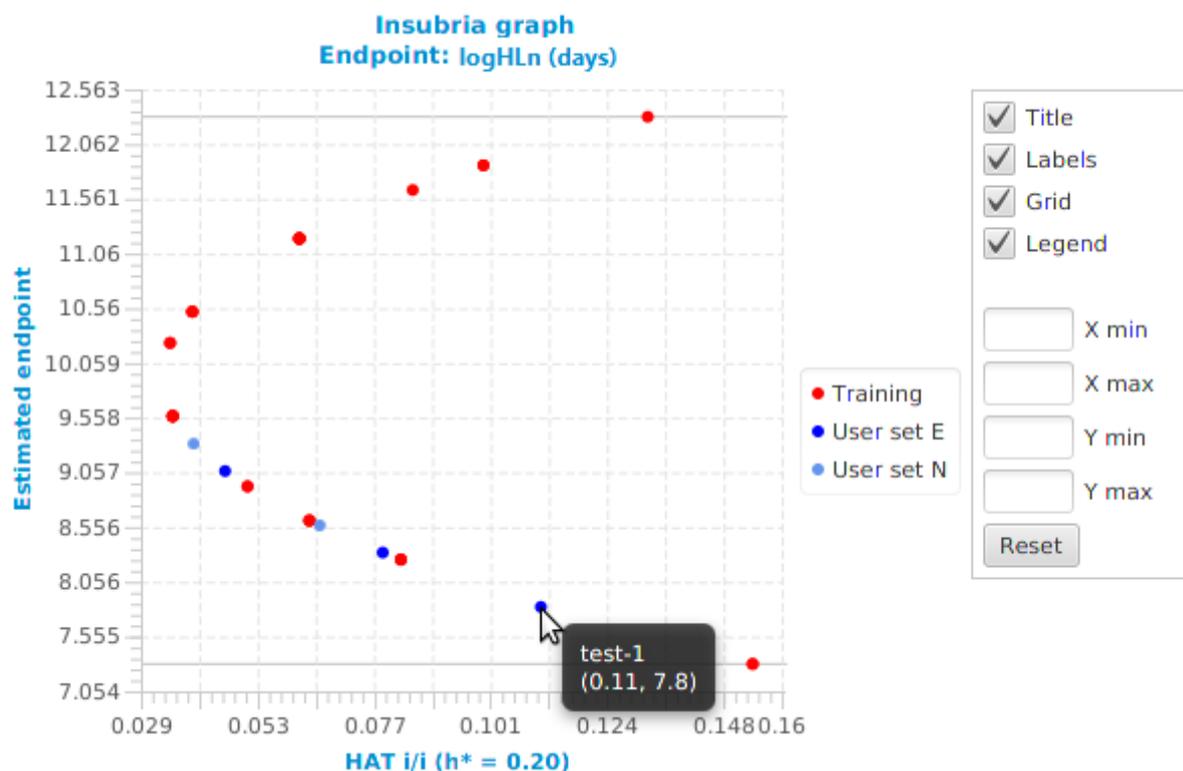
Data points are colored according to the dataset they belong to. Red is for the training set, blue for the user (prediction) set (Note: in the Insubria graph, as shown above, the color of the user set is further differentiated when the experimental endpoint value is provided for some, but not all, molecules. In this case, molecules with the experimental endpoint -"User set E"- are blue colored, while the one without the experimental endpoint -"User set N"- are colored as light blue).

It is also possible to customize the layout of the graphs. As shown in the figure above, the title, labels, grid and legend can be switched on and off and the range of the graph axes can be manually changed. Pressing the "Reset" button will reset the ranges to default.