

SIMCA 15

Multivariate Data Analysis Solution

SMILES converter for visualization of molecular structures

9 June 2020

Introduction

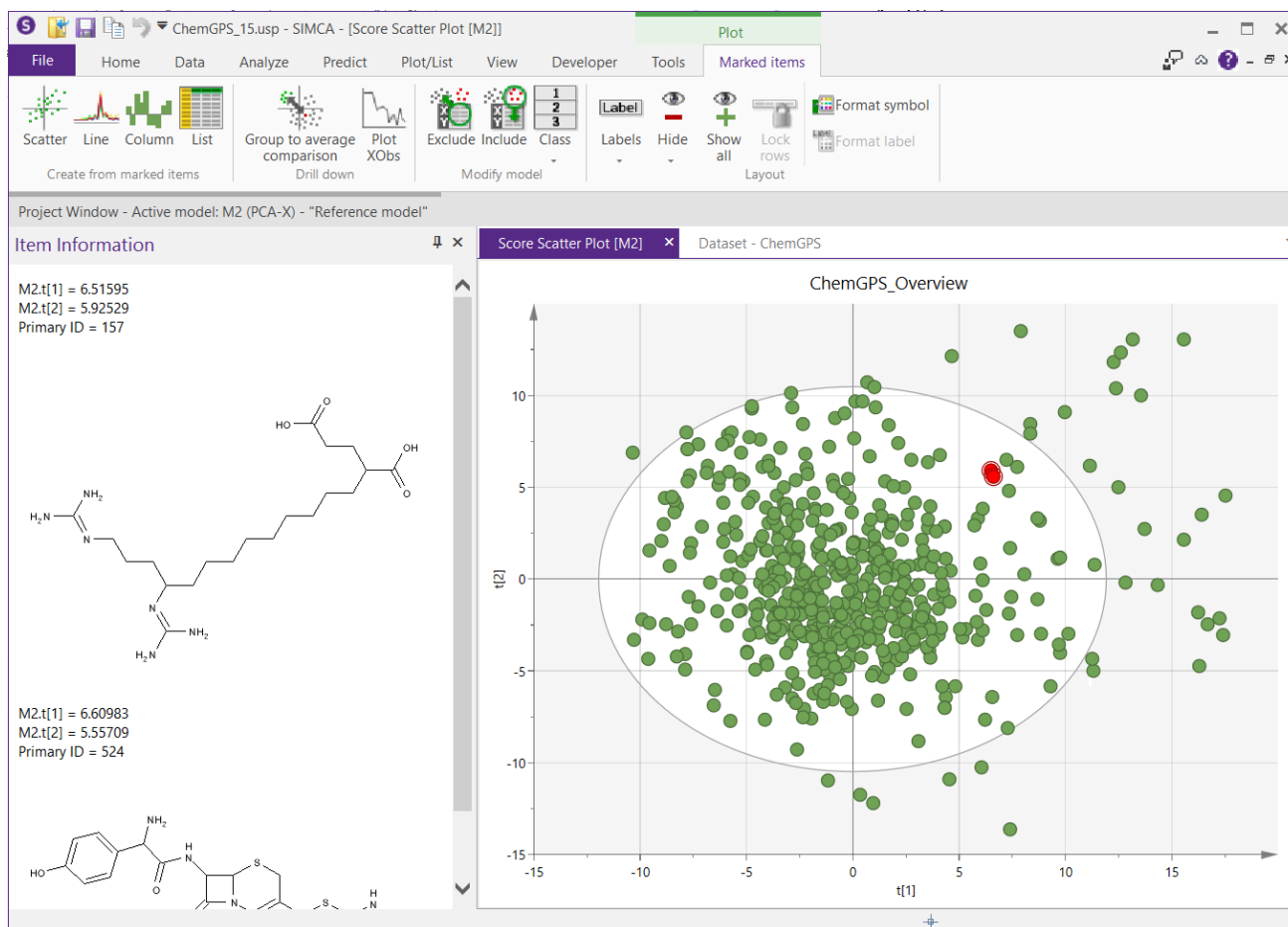
SIMCA has an extensive history of being used for QSAR and QSPR investigations. To facilitate interpretation a SMILES converter is offered for SIMCA which allows visualization of molecular structure inside SIMCA Item information pane.

The structural depiction is based on licensed technology from OpenEye Scientific Software. Customers who already have access to OpenEye's OGHAM software can re-use their license in combination with the SIMCA add-in provided by Sartorius Data Analytics.

Displaying molecular structures in Item Information view

To display molecular structures there must be a SecondaryID in the SIMCA project containing SMILES strings. The Secondary ID must also be specifically named "SMILES" to be recognized as containing SMILES strings.

Activate the Item Information from the Show group of the View ribbon. Open an observation related plot or list and select one or more observations. The Item Information pane will display the molecular structure for the selected observations, i.e. substances.



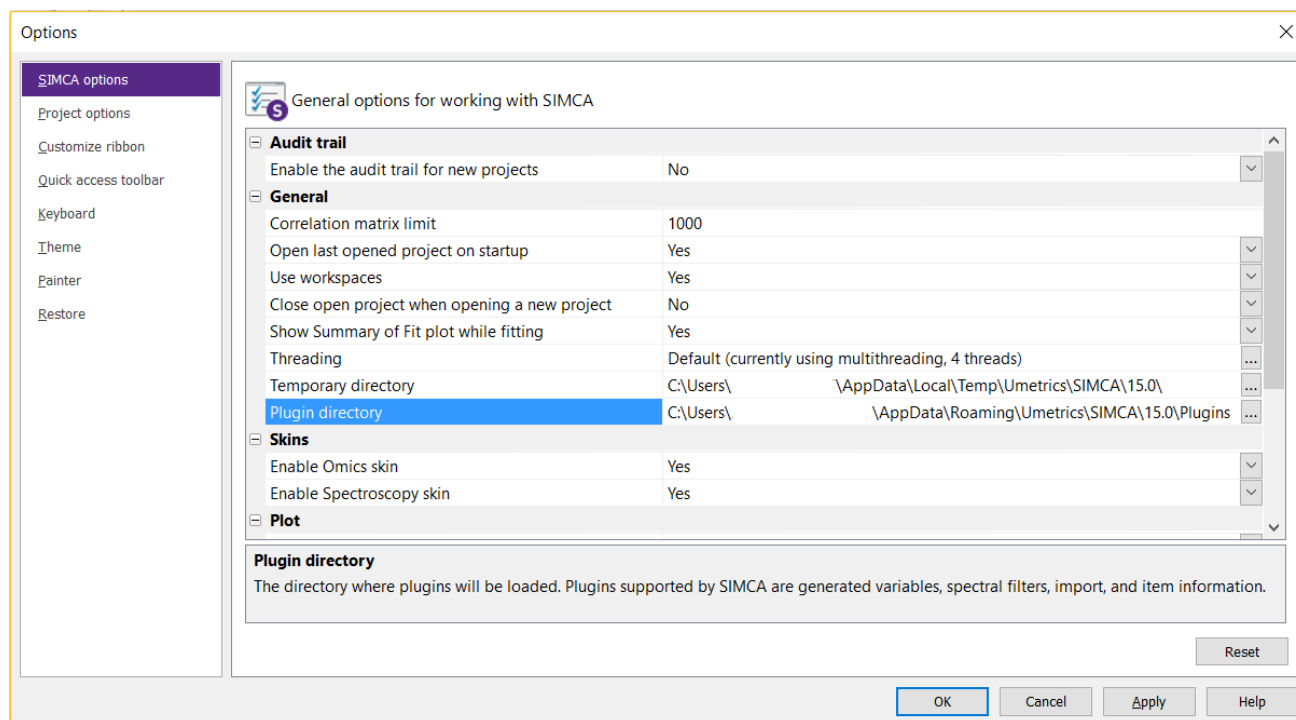
Access the plugin

Contact local sales representative for information on how to access the plugin.

There are two versions available, one for users who already have OpenEye's OGHAM software and another for customers not using the mentioned software.

Installation of plugin

The plugin dll should be copied to SIMCA plugin directory. To locate the plugin directory open **File | Options**. If you were running SIMCA during this process, restart SIMCA after the dll has been copied to plugin directory.



OpenEye's OGHAM software

If you already use OpenEye's OGHAM software an environment variable pointing to the OGHAM license must be specified. The variable must be called OE_LICENSE and it must contain the full path, including file name, to the OGHAM license file.

In Windows 10 you do this in **Control panel | System | Advanced system settings | Environment variables**. Click on New in the upper part of the dialog and write OE_LICENSE in the Variable Name field and the path to the OGHAM license file, including file name, in the Variable Value field and click OK. If you have done it right, it will look like something similar to the picture below.