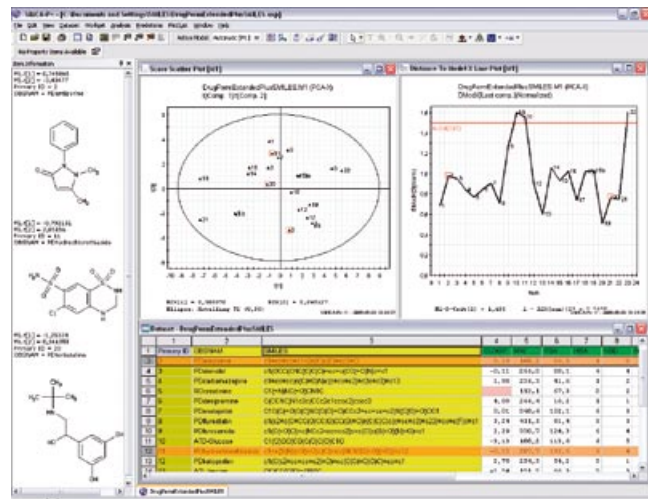


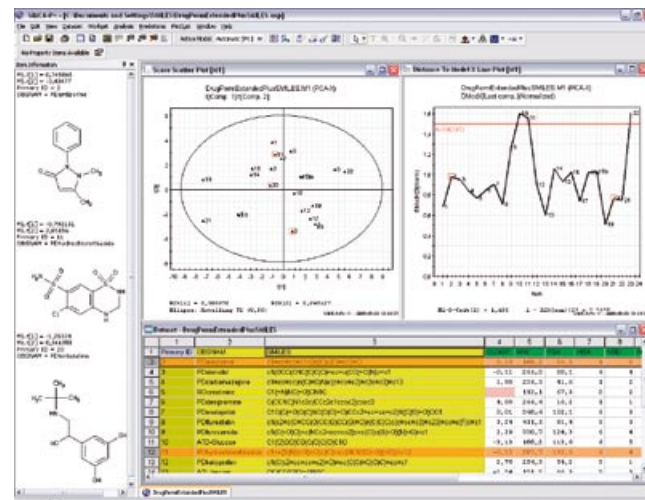
To view molecular structures from SMILES codes in SIMCA-P/P+ you must have a secondary id in the dataset, called SMILES, and SMILES codes as the observation or variable ID. The structures will then be displayed in the Item Information window when observations/variables are marked in a plot or list.



The selected compounds (2, 11, 20) in the upper score plot are shown as molecular structures in the left window. They are also automatically highlighted in the DModX chart (upper right) as well as in the data set list below.

SIMCA-P SMILES Converter 1.0

Installation Instructions



In QSAR and ADME/Tox modelling, the connection between the analysis results and chemical structure is of vital importance. The SMILES plug-in makes this a simple task in SIMCA-P.

The structural depiction is based on licensed technology from OpenEye. Customers who already have access to Openeye's OGHAM software can re-use their license in combination with the SIMCA-P add-in.



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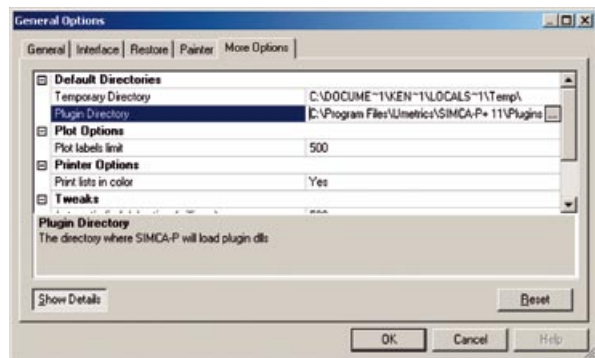
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IID 2027 2005

Installing the SIMCA-P SMILES converter plug-in

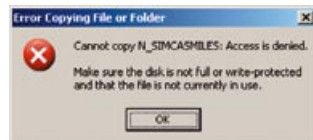
1. Locate the SIMCA-P/P+ plug-in directory.

It can be found in SIMCA-P/P+ under **View | General Options** in the **More Options** tab. Note that you may need to create the directory if it does not exist, or change to an existing directory.



2. Insert the CD and locate the **zlib1.dll** and the *smiles plug-in dll*. The plug-in dll is called either **L_SIMCASMILES.dll** or **N_SIMCASMILES.dll** depending on your license.
3. Copy the **smiles plug-in dll** and the **zlib1.dll** to the SIMCA-P/P+ plug-in directory on your hard disk.

Note that you must have write privileges to the plug-in directory. If you don't, you will get a message similar to:



In that case you must contact your IT department for assistance.

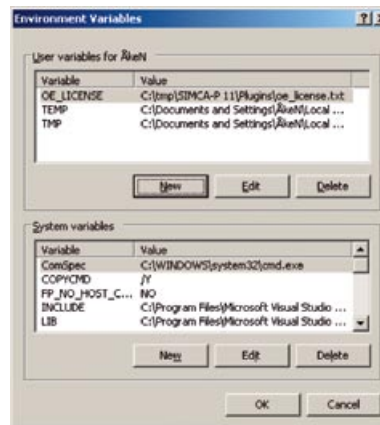
4. If you have a previous license for OGHAM software from OpenEye Scientific Software Inc., please *continue on next page*.

If you were running SIMCA-P/P+ while installing the plug-in, you must restart SIMCA-P/P+ to complete the installation.

For customer with access to OGHAM software from OpenEye

If you have access to OGHAM software from OpenEye Scientific Software Inc., (having received the L_SIMCASMILES.dll), you must also add an environment variable that points to the OGHAM license file. The variable must be called **OE_LICENSE** and it must contain the full path, including file name, to the Ogham license file. In Windows XP you do it this way:

5. Open the **Control Panel**
Open **System**
Select the **Advanced** tab
Click on **Environment Variables**
Click on **New** in the upper part of the dialog and write **OE_LICENSE** in the *Variable Name* field and the path in the *Variable Value* field
Click **OK**.
If you have done it right, you will look at something similar to the picture below.



For older Windows versions, the procedure might be slightly different. If you have problems adding the environment variable or you don't know the location of the Ogham license file, please contact your IT department for assistance.

6. If you were running SIMCA-P/P+ while installing the plug-in, you must restart SIMCA-P/P+ to complete the installation.