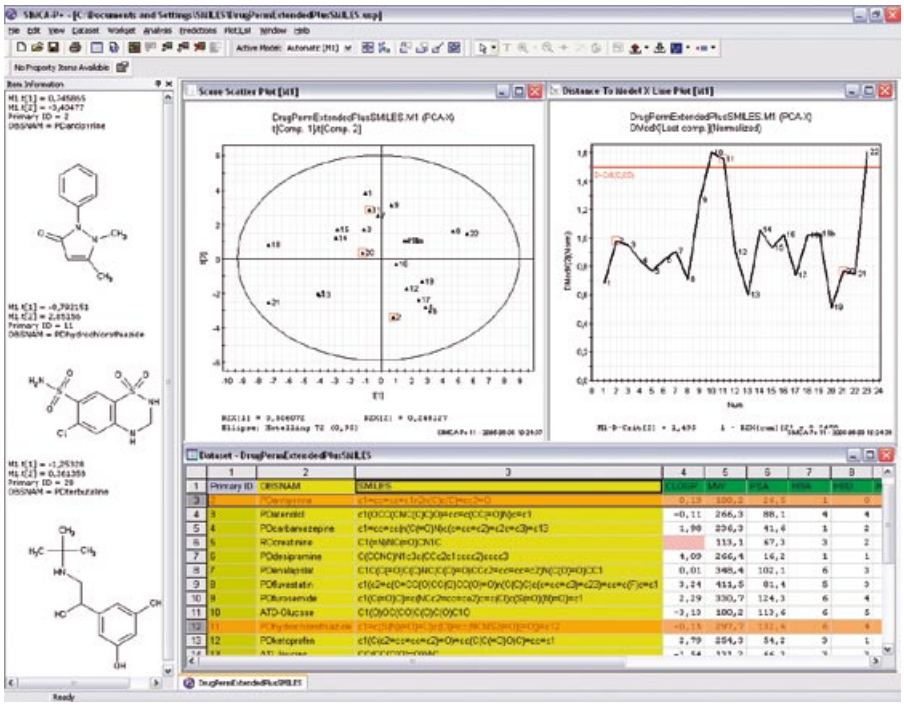
Molecular Structure Display in SIMCA-P



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.

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

By providing SMILES codes as a secondary ID when importing the data, SIMCA-P can automatically visualise chemical structures in parallel with the on-going analysis. Just click on any output and the associated molecule will automatically appear. SIMCA-P will display SMILES relating to both objects (molecules) and variables (chemical fragments description). Because plots and lists are linked in SIMCA-P, the selection made in one plot is also shown in all other plots as well as in the data set, making interpretation even easier.

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.

OpenEye Scientific Software

The structural depiction is available as an add-in based on licensed technology from OpenEye Scientific Software Inc. For more information about OpenEye, please visit www.openeye.com

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