GoSilico™ Chromatography Modeling Software

DATA FORMATS

GoSilico™ Chromatography Modeling Software enables the computer-based development of preparative liquid chromatographic downstream processes. This software is licensed on a rental basis. GoSilico™ Chromatography Modeling Software stores data in an open and documented format which gives you access to existing modeling data even after the licensing contract is terminated.

Modeling parameters

All parameters used for simulating a chromatographic experiment in GoSilico™ Chromatography Modeling Software are stored in an encrypted so called .dspx file, which is accessible when opening it in the software with an active license. Apart from the .dspx file, you can also export all data to an XML-based text file, which can be read and edited with any text editor.

We recommend using the Notepad++ free source code editor due to its source code highlighting. This can be downloaded from https://notepad-plus-plus.org/.

The .dspx and exported .xml files contain information about:

- The type of model selected for the respective simulation (column, pore, isotherm model).
- The parameters for the numerical simulation and algorithms (space discretization, time stepping, external algorithms).
- The simulated column and process (geometries, flow rates).
- The simulated protein and salt species including the preset or optimized isotherm parameters.
- If applicable for the respective modeling case, information about the process optimization, parameter estimation, and parameter sampling settings (objective functions).

Exported modeling results

The modeling results generated with GoSilico™ Chromatography Modeling Software are also exported in other widely used data formats.

The GoSilico™ Chromatography Modeling Software result table contains the intermediate and results of the process optimization, parameter estimation, and parameter sampling module. The result table can be exported in Microsoft® Excel® XLS format.

Plots of the corresponding chromatograms can be exported as figures in JPEG, PNG, PS, EPS, SVG and TIFF format.

The simulated intra column concentrations can be exported in the MATLAB™ format MAT or the VTK™ data format.

Reading MAT files require a MATLAB™ license (MathWorks™). Reading .vtk files requires an open source, multiplatform data analysis and visualization application that can be downloaded from https://www.paraview.org/.