BIOVIA

3DEXPERIENCE®

SOLVATION CHEMISTRY COMPONENT COLLECTION

Datasheet

The Solvation Chemistry Component Collection is a compilation of property calculators, readers, utilities, COSMObase access components, and example protocols.

It complements the standard capabilities of the BIOVIA Pipeline Pilot by the COSMO-RS method for the prediction of liquid phase properties, the use of TURBOMOLE[1®] for quantum chemical calculations, and a conformer generator, which allows for the generation of the most relevant conformers for COSMO-RS.

With this collection, you can create your own protocols for a wide range of application.

DASSAULT SYSTEMES

CALCULATORS

The BIOVIA Solvation Chemistry collection offers calculators for the following applications:

COSMOtherm

The collection contains three COSMOtherm components that use the COSMO-RS method to predict a wide range of properties.

You can calculate properties for pure liquids, such as density, boiling point, flash point, partition coefficients, as well as mixture properties, such as vapor-liquid equilibria, liquid-liquid equilibria, solubilities, vapor pressures, activity coefficients, etc.

The integration of COSMOtherm in a workflow environment boosts the screening potential of the COSMO-RS method. You can screen the properties of a large set of solutes, solvents or solvent mixtures, for example the solubility of a drug in a vast set of solvents.

COSMOconf

The COSMOconf component is a conformer generation tool. You can use pre-defined standard procedures that allow for the generation of the most relevant conformers for COSMO-RS or employ your own procedure.

COSMOperm

This component predicts the permeability of a solute through biomembranes. You can choose from a set of pre-defined membrane systems or use your own membrane.

COSMOplex

This component provides the COSMOplex extension of the COSMO-RS method. You can use it to calculate properties for inhomogeneous systems, e.g., interfacial tensions or critical micelle concentrations, or to create new biomembrane systems.

COSMOquick

The COSMOquick fragmentation technology can be used as a fast shortcut for COSMO-RS calculations. The component can also be used to apply pre-defined QSPR models or to compute unique chemical descriptors.

TURBOMOLE[1]

The collection offers a component that you can use to perform quantum chemical calculations with the TURBOMOLE[1]® program package.

COSMO DATABASES

You can integrate COSMO databases for the use in Pipeline pilot. This works for the BIOVIA COSMObase as well as for your own custom COSMO file databases. A special component is available for the compound data access.

READERS AND UTILITIES

The Solvation Chemistry Component Collection offers a couple of readers and utilities. You can use the COSMO file reader and the TURBOMOLE[1]® coord file reader to access this specific file formats. The preconditioner can help you to ensure that the relevant properties needed for the other components are set properly.

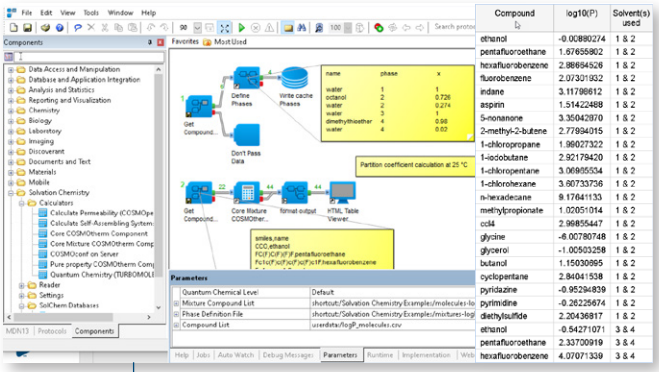

Figure 1: Pipeline Pilot Professional Client Calculation

REFERENCES

1. TURBOMOLE, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, 2007-2021

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