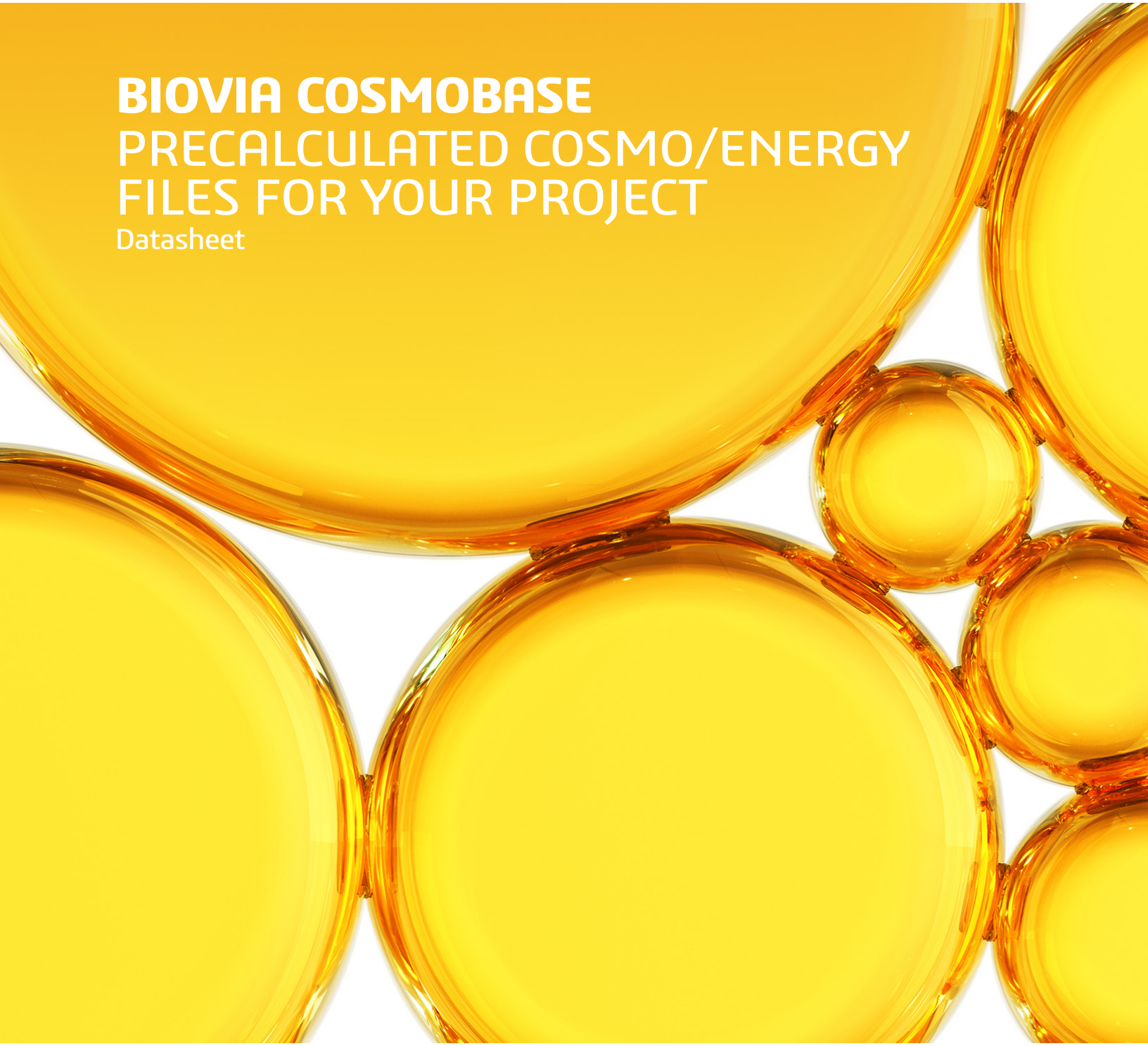
BIOVIA

3DEXPERIENCE®

BIOVIA COSMOBASE
PRECALCULATED COSMO/ENERGY FILES FOR YOUR PROJECT

Datasheet



DASSAULT SYSTEMES

WHAT IS BIOVIA COSMOBASE?

BIOVIA COSMObase is a high quality collections of precalculated compound information needed for COSMO-RS calculations. The data is available for all parametrizations supported by BIOVIA COSMOtherm. Each compound is represented by a set of COSMO (s-surface information) and energy (gas phase energy) files. Additional files contain physical compound data are provided for a subset of compounds.

Your benefit

- Skip the time consuming quantum chemical calculation of the COSMO & energy file generation and focus on your BIOVIA COSMOtherm project
- Benefit from BIOVIA's expertise and use the COSMO-RS optimized conformer sets of the database
- Use the physical compound data

Application Areas

All BIOVIA COSMOtherm / COSMO-RS calculations

COMPOUND CLASSES

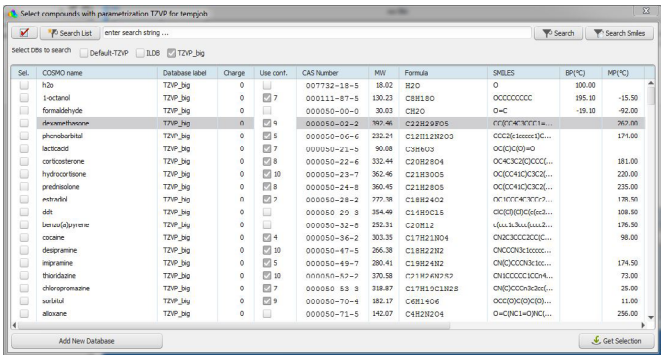
The BIOVIA COSMObase includes almost all common solvents, ranging from small molecules to large and complex substances, covering substance classes with all kinds of functional groups (e.g. hydrocarbons, alcohols, ethers, carbonyls, acids, esters, amines, amides, nitro compounds, heterocycles, halogenated compounds, and many more).

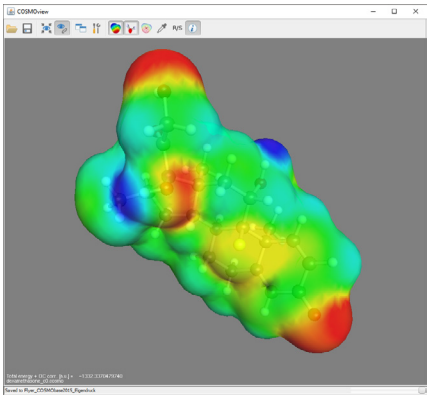
BIOVIA COSMOthermX GUI

Add the databases to your BIOVIA COSMOthermX settings and use the compounds for your research

KEY FEATURES

- The database includes > 10200 different compounds
- Different conformations are taken into account whenever needed
- Data on gas phase and COSMO level
- Over 4200 melting points and 3600 boiling points are included in the physical data
- Compounds can be searched by CAS registry numbers (CAS numbers are available for over 7800 compounds)





BIOVIA COSMObaseIL & BIOVIA COSMObaseFF

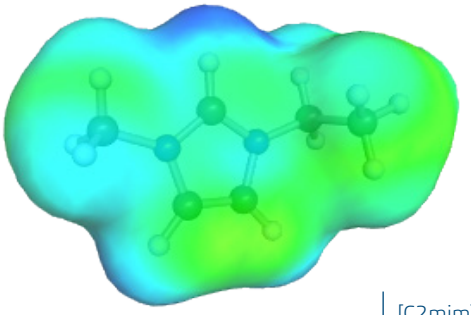
Besides the BIOVIA COSMObase, which is a universal data set designed for a broad application spectrum, we offer two special purpose databases.

Ionic Liquids: BIOVIA COSMObaseIL

BIOVIA COSMObaseIL is a collection of typical ionic liquid anions and cations. The current database contains 372 cations and 98 anions that can be independently combined to form a huge set of potential ionic liquids. This is especially interesting for ionic liquid screening purposes. The BIOVIA COSMOthermX GUI offers special ionic liquids screening options.

Flavors & Fragrances: BIOVIA COSMObaseFF

As a special purpose database the BIOVIA COSMObaseFF contains over 2000 flavors and fragrances. The BIOVIA COSMObaseFF is the ideal add-on for consumer goods or fragrance companies.



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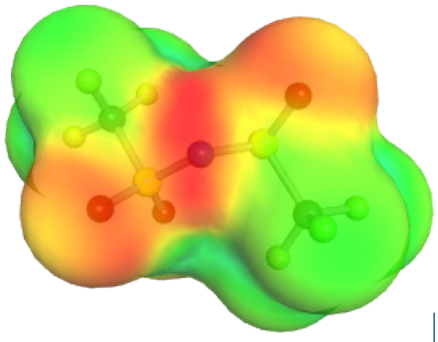

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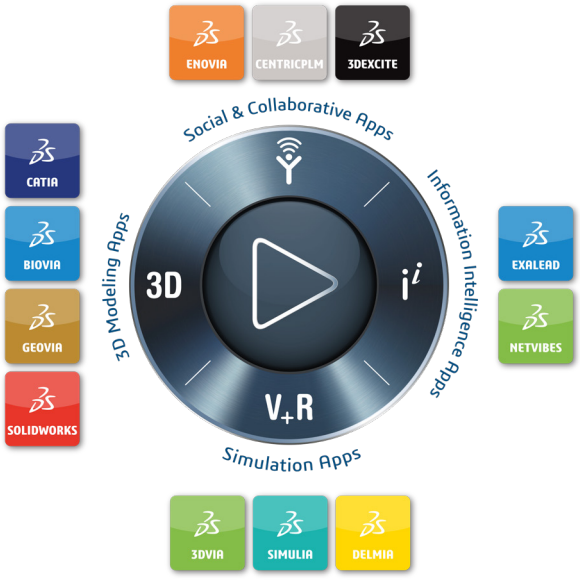

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