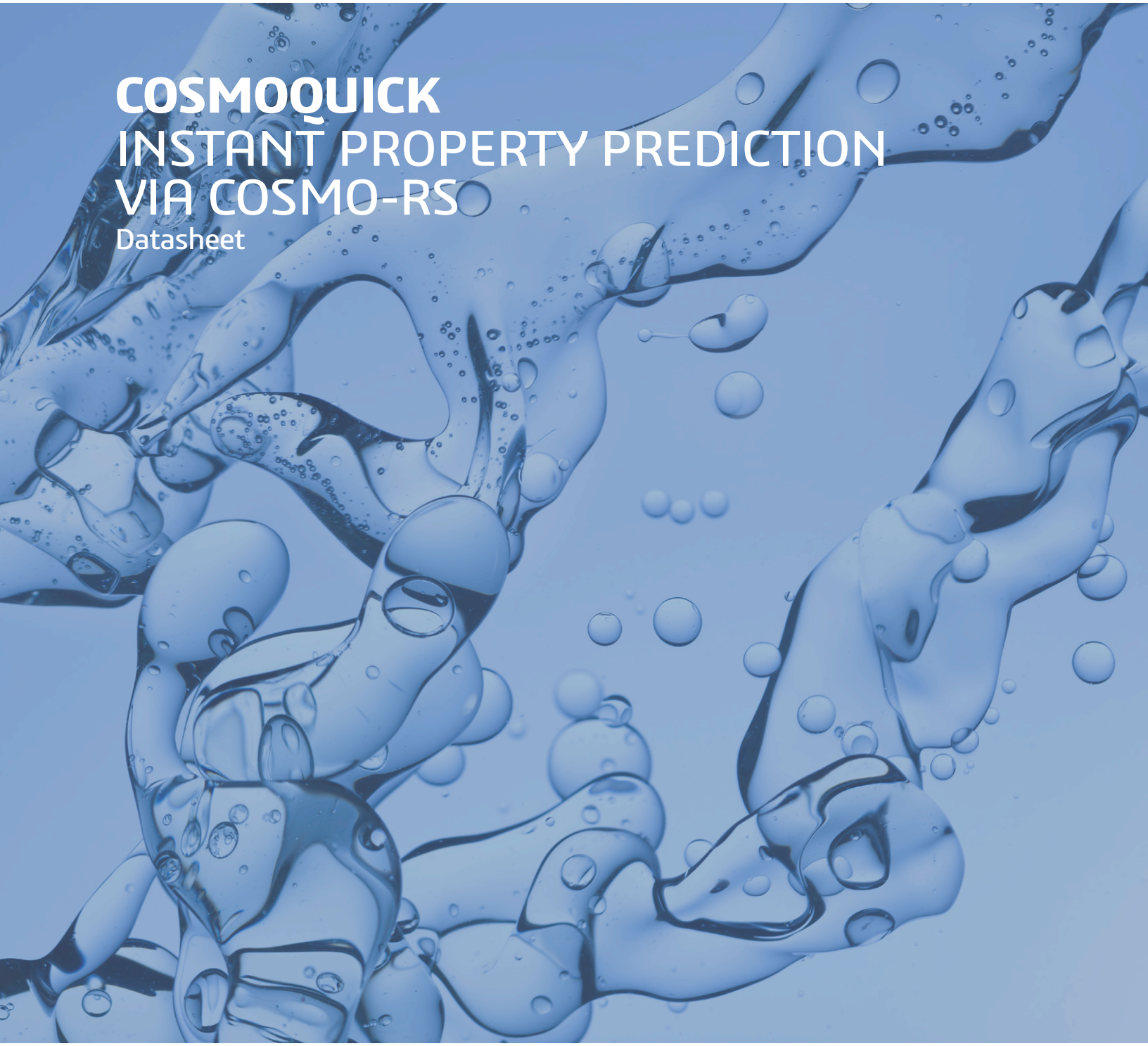
BIOVIA

3DEXPERIENCE®

COSMOQUICK
INSTANT PROPERTY PREDICTION VIA COSMO-RS
Datasheet



DASSAULT SYSTEMES

FAST & EFFICIENT

COSMOquick is a powerful toolbox removing the need for costly computations. It enables you to predict COSMO-RS based physico-chemical properties within a few clicks.

HOW IT WORKS

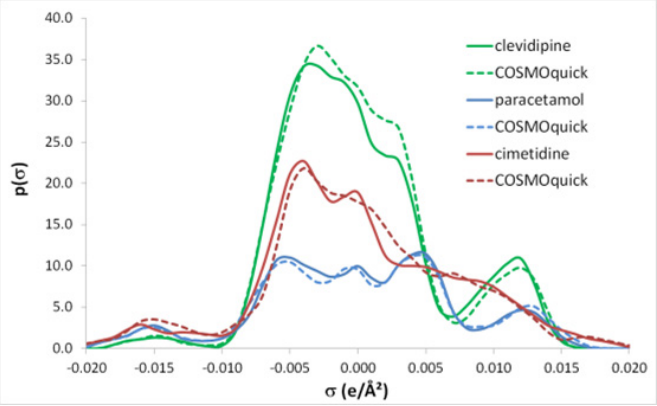
In contrast to the conventional COSMO-RS approach it is not necessary to carry out a quantum chemical calculation. Instead COSMOquick uses a library of about 200.000 molecules pre-computed by quantum-chemistry to generate σ-profiles within a fraction of a second.

YOUR BENEFIT

- Quickly check novel ideas avoiding costly computations
- Speed up your experiments
- Identify new solvents, solvent mixtures, cocrystal coformers or other excipients.

Application areas

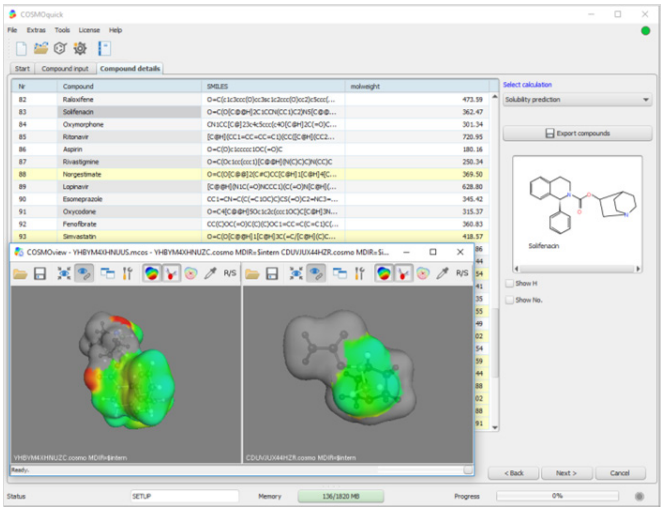
- Drug development
- General chemistry
- QSPR & ADME properties
- High throughput screening
- Formulation/polymers



KEY FEATURES

COSMOquick provides not only an efficient graphical user interface, but also many convenient features such as: Input via SMILES, SD file or 2D editor, easy processing of large list of molecules and much more:

- No quantum chemistry required
- Solubility prediction
- Cocrystal / solvate screening
- pKa prediction
- COSMO-RS based descriptor generation
- QSPR model building & deployment
- Reverse σ-profile fitting
- Partition coefficients
- Henry's law & gas solubility prediction
- Hansen parameter estimation via COSMO-RS
- 3D structure generation / SMARTS analysis

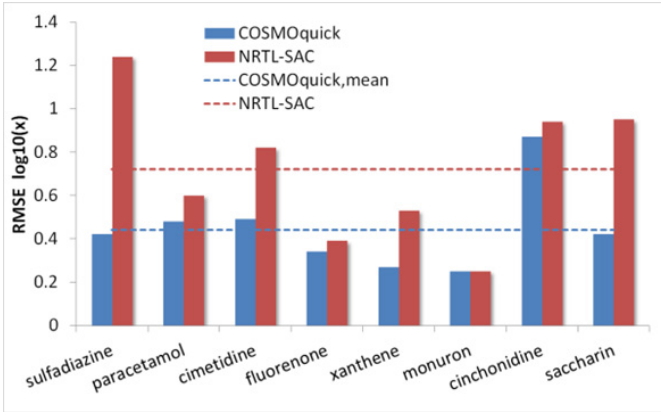


The underlying COSMOquick database can be easily extended to improve prediction accuracy. Currently no conformational effects are taken into account and support for ionic compounds is limited.

SOLUBILITY PREDICTION & SOLVENT SCREENING

COSMO*quick* contains a novel, highly efficient and accurate solubility prediction algorithm. A few experimental reference values (usual measured solubilities) can be used to refine the results for the solubility of a solute in any new solvent.

Fast solvent screenings allow identification of suitable solvents or solvent mixtures for a new active.



Use COSMOquick to

- Screen large libraries for the optimal solvent or solvent mixture
- Optimize mixtures for 2 solutes, e.g. API & coformer
- Identify the σ-profile of solutes of unknown structure or composition

As a rather new option COSMOquick uses experimental data for 'reverse engineering' the σ-profile of ill-defined species

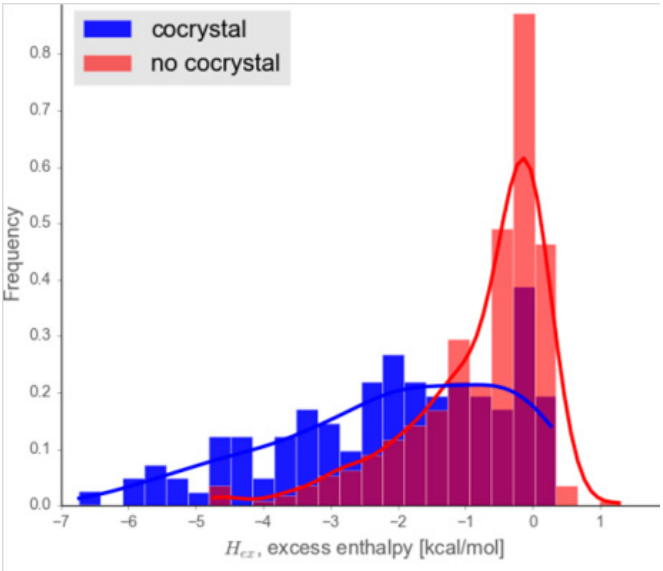
(e.g. macromolecules, mixtures, residues). This can be useful if experimental data is available but no concrete structure can be associated with a compound. Reverse engineered σ-profiles can be used subsequently for any available COSMO-RS property prediction.

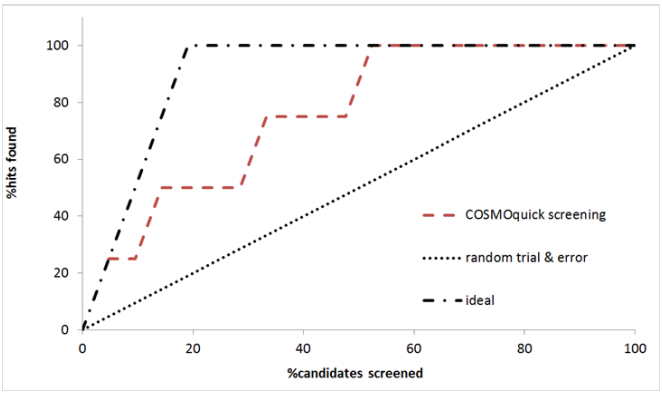
COCRYSTAL & SOLVATE SCREENING

Cocrystals are becoming more and more important in the pharmaceutical industry due to their potential to improve the properties of conventional drugs. COSMOquick uses the excess enthalpy of an undercooled melt of a drug and a coformer (Hex) to assess their propensity for co-crystallization.

It has been shown that this serves as an accurate means to efficiently screen many potential coformers.

This approach can also be applied for solvate screening and results can be further improved taking into account experimental data.





COSMOquick strengths

- Efficiently generates predictions for many molecules within minutes
- Easy to use – no 3D structure necessary
- Takes into account all relevant intermolecular interactions
- Based on the well-established COSMORS theory

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