BIOVIA

3DEXPERIENCE®

FROM SURFACE CHARGES TO DRUG DESIGN & DEVELOPMENT

Datasheet

DASSAULT SYSTEMES

SOLVENT SCREENING

New APIs are often available only in small amounts and computational pre-screening over a large database of solvents and mixtures can save valuable time and substance. Solubility predictions for pure compounds and mixtures are key applications for COSMOtherm and COSMOquick. They allow for the optimization of solvents and solvent mixtures for extraction or downstream processing in a virtually unlimited range of organic compounds.

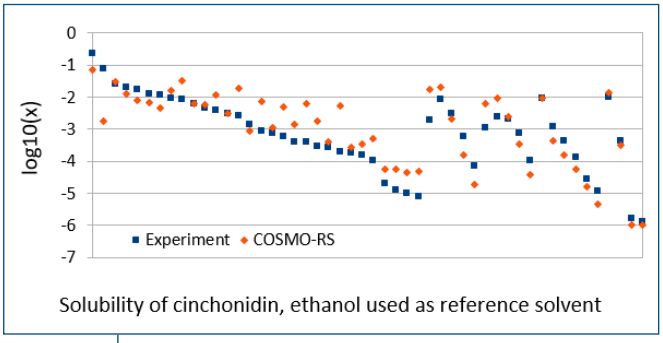


Figure 1: Solubility of cinchonidine, ethanol used as reference solvent

Applications

- Solubility & solubility screening
- Partitioning behavior
- Cocrystal screening
- Predicting free energy of solvation & reaction chemistry
- ADME property estimation

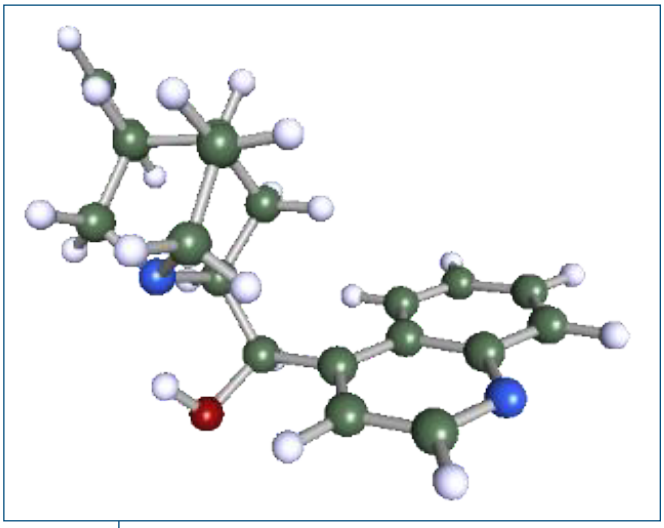


Figure 2: Software: COSMO*therm*, COSMO*conf*, TURBOMOLE

- Providing QSPR descriptors and predictions
- Crystal morphology prediction
- Providing 3D-QSAR descriptors

COCRYSTAL SCREENING

Cocrystals are becoming more and more important in the pharmaceutical industry due to their potential to improve the properties of conventional drugs, in particular, to improve their bio-availability.

COSMOquick and COSMOtherm use the excess enthalpy of an undercooled melt of an API and a coformer to assess their propensity for co-crystallization. This serves as an accurate means to screen quickly many potential coformers.

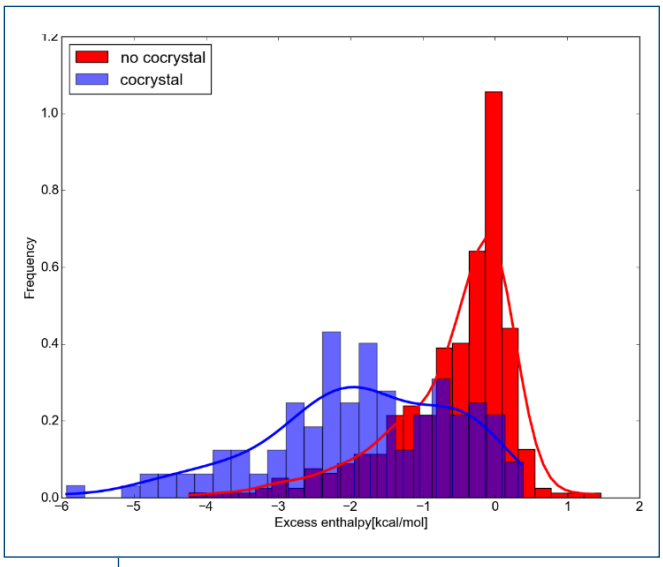


Figure 3: Software: COSMO*quick*

PROPERTIES IN SOLUTION

COSMOtherm is the universal tool for predictive property alculation of liquids, and combines quantum chemistry and thermodynamics in a unique fashion. It calculates the chemical potential of molecules in pure or mixed liquid at variable temperature. This is the key for the prediction of a multitude of properties, including free energy of solvation, solubility and partitioning. In contrast to several other available methods COSMOtherm is able to predict properties as function of concentration and temperature by applying thermodynamically consistent equations.

Predictable Properties

- Solubility of liquids, solids and gases
- Free energy of solvation, Henry's law constant and vapor pressure
- Two-phase partitioning (e.g. LogP), liquid extraction and activity coefficients
- pK_a, chemical reaction equilibria in different solvents
- Conformer relevance in different mixtures
- Phase behavior: liquid-liquid, liquid-vapor and liquid-solid equilibria
- Energy of transfer to a flat liquid-liquid interface
- Interfacial tension, adsorption and environmental properties
- Bio-membrane and micelle partitioning

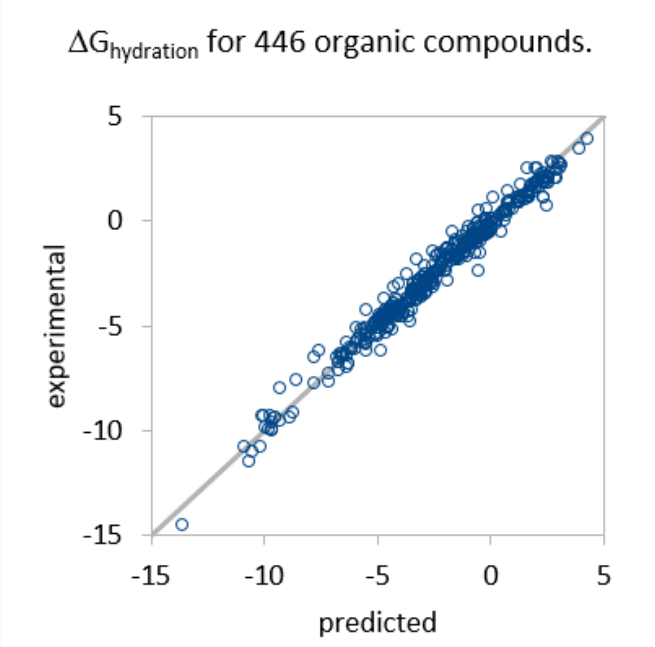


Figure 4: $\Delta G_{hydration}$ for 446 organic compounds

SKIN PENETRATION MODEL

BIOVIA COSMOplex can simulate the self-assembly of biomembranes consisting of different membrane components, e.g. phospholipids, ceramides, cholesterol etc. It can even include small molecules such as penetration enhancers or potentially toxic molecules. The example below shows the predicted permeation of UV-filter molecules through skin, where COSMOplex was used to generate the bio-membranes and BIOVIA COSMOplex and BIOVIA COSMOtherm were used for diffusion constants, free energies and partitioning coefficients, which are all required for the used skin permeation model.

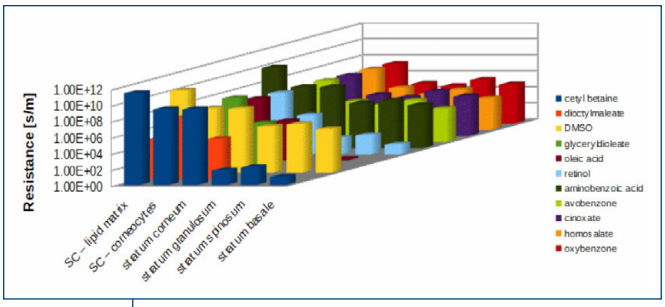


Figure 5: Skin compartment

CRYSTAL MORPHOLOGY PREDICTION

By integrating COSMO-RS and Materials Studio, scientists can accurately predict how solvent choice affects crystal shape. Utilizing these predictions in formulation and pre-formulation stages directly impacts key properties: dissolution rate (kinetic solubility), filtration rate (especially crucial for needle-shaped crystals with prolonged solvent retention potentially clogging filters), powder flow (addressing stickiness concerns), and compressibility.

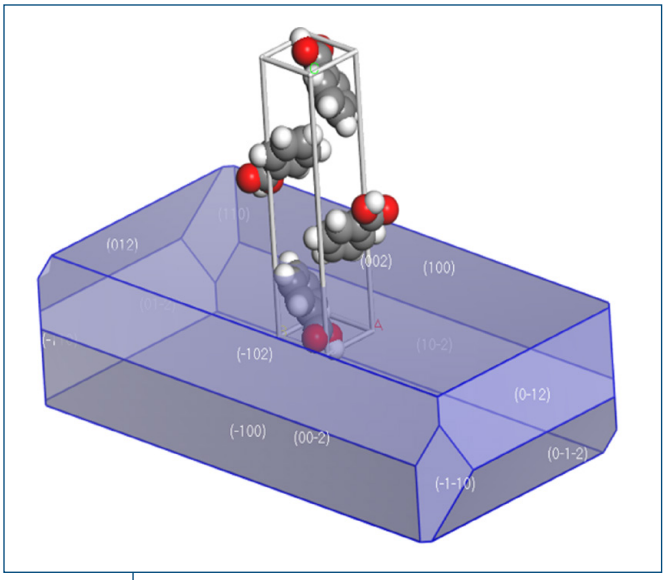
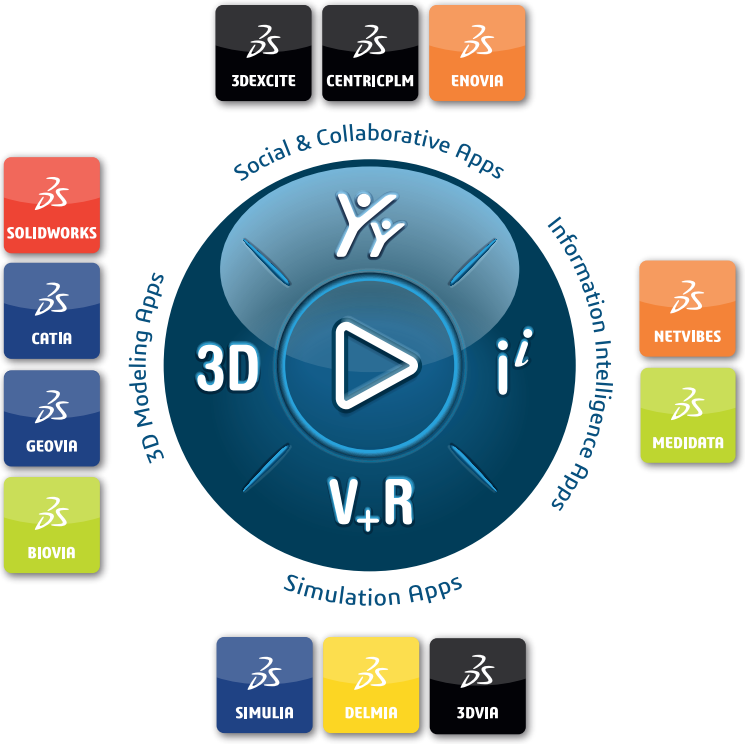


Figure 6: Illustration of an API crystal shape



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