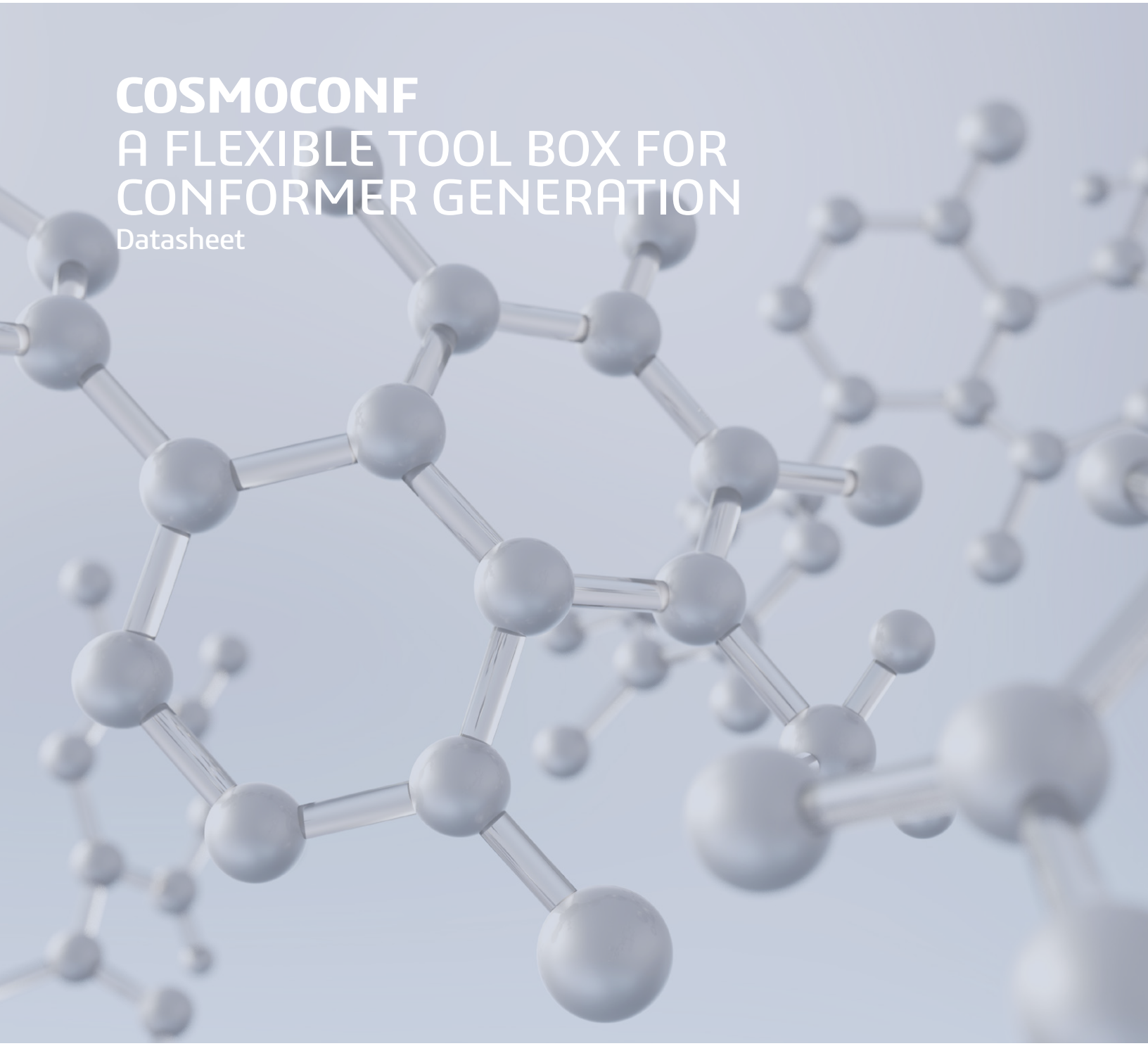
BIOVIA

3DEXPERIENCE®

COSMOCONF
A FLEXIBLE TOOL BOX FOR CONFORMER GENERATION
Datasheet



DASSAULT SYSTEMES

CONFORMERS, WHY BOTHER?

Conformers have different energies/structures and the results of a calculation depend on the used conformer ensemble

FIND A SUITABLE SET OF CONFORMERS

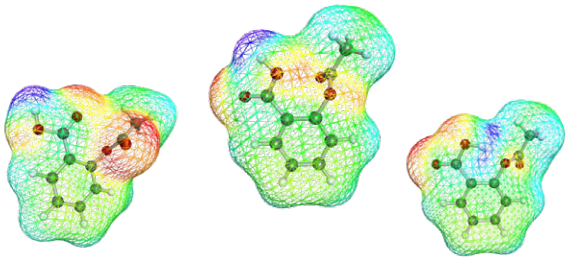
COSMOconf is a flexible tool box for conformer generation. It enables you to use pre-defined procedures that are optimized for the generation of the most relevant conformers for COSMO-RS

YOUR BENEFIT

- Pre-defined procedures can easily be used by unexperienced users
- Full flexibility for expert users
- Build up your own COSMO bases

APPLICATION AREAS

- COSMO & energy file creation
- Quantum Chemistry



A COSMOTHERM CONFORMER EXAMPLE

The choice of a conformer set used in a COSMOtherm calculation can affect the results substantially.

Conformational equilibrium in pure DME and a DME/water mixture (xDME= 2%) at 25°C

DME	$w_{(liquid\ DME)}$ [%]		$w_{(2\%\ in\ H2O)}$ [%]	
	exp.	BP-TZVP	exp.	BP-TZVP
tgt	37	42.2	78	62.2
tgg'	36	24.7	14	5.6
ttt	16	13.0	1	2.5
tgg	8	10.8	6	24.0
ttg	3	5.8	0	1.9
ggg'		1.9		1.3
ggg		0.8		1.8
gtg'		0.5		0.3
gtg		0.2		0.1

Table 1: Exp. data taken from reference [2]. Parameterization: C30_1401

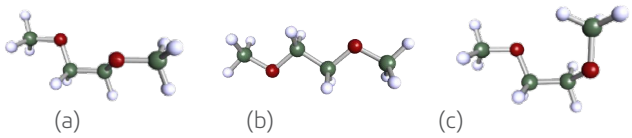
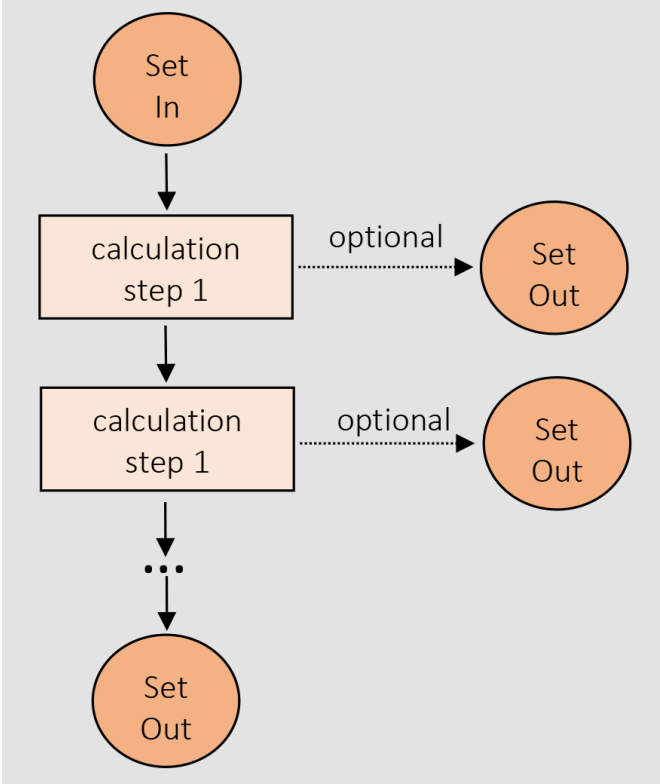


Figure 1: (a) DME **tgt**, (b) DME **ttt**, (c) DME **tgg'**

THE COSMOCONF TOOL BOX

A COSMOconf procedures can be defined by a sequence of unit operations



QM calculations

Opt. & single points: AM1, PM3, DFT (BP with SV(P)...TZVPD)

Conformer generation

COSMOfrag + MOPAC7 (AM1), constraint opt.

Genetic algorithm with MMFF94 force field (BALLOON [1])

Clustering

geodis/geocheck: local structural similarity

SMS: sigma profile similarity

EVNN: energy and nuclear repulsion

MU: chemical potential in different solvents

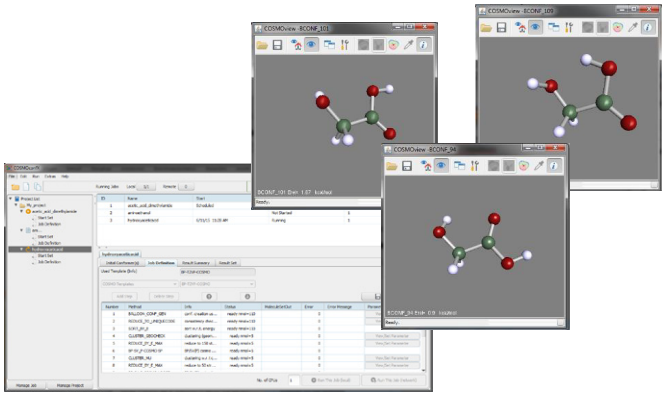
Data sorting, reduction & adding , etc...

Get a free Demo Version

http://www.cosmologic.de/products/cosmoconf.html

THE GRAPHICAL USER INTERFACE

The COSMOconfX GUI is available for Windows, Linux & Mac.



COSMOCONF STRENGTHS

- Accuracy and robustness due to use of density functional theory calculations
- Automatic conformer selection by relevance to the chemical potential (μ-clustering) in diverse solvents
- User-defined conformational search schemes for full flexibility
- Command line version available for automated batch processing
- Works on local and remote (Linux) machines

REFERENCES

1. M. J. Vainio, M. S. Johnson , J. Chem. Inf. Model., 2007, 47 (6), 2462−2474. http://users.abo.fi/mivainio/balloon/
2. R. Wada, K. Fujimoto, M. Kato, J. Phys. Chem. B 2014, 118, 12223−12231.

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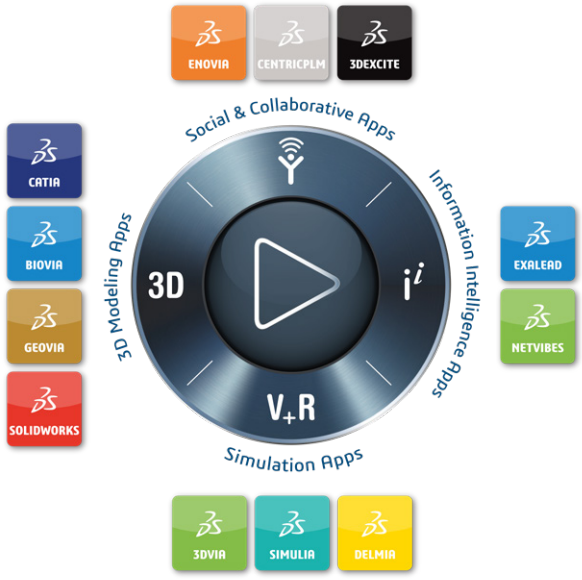

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