Subject: Re: Chemistry in 3D
Posted by nbehrnd on Tue, 22 Mar 2022 12:57:17 GMT
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Dear Christophe,

the conformer generator's aim is the provision e.g., of starting geometries for (in silico) docking experiments and considers only the isolated, single molecule in question. Once the molecule experiences interactions with neighbouring molecules e.g., intermolecular hydrogen bonds may render these predicted energetic minima more shallow/more deep. Then, some conformations might be not longer favourable, and others are locked-in; both render a reliable prediction more demanding. (One reason for prediction contests like the ones by CCDC,[1] or CASP.[2])

The number of conformers per molecule one want to query equally depends on the number of bonds which are conformational flexible. In this perspective, the default of up to 16 is (an empiric) suggestion. DataWarrior neither is the only program to offer this functionality,[3] nor do the force fields provided aim to compete in accuracy and precision with higher level(s) of theory/specialized programs.

Because I have no working experience with the shape alignment and docking you refer to, my suggest were to screen the 500+ citations on ACS's landing page for the the primary publication about DataWarrior,[4] or/and collect advice by others.

Norwid

[1] Reilly et al. Acta Cryst. 2016, B72, 439-459; doi 10.1107/S2052520616007447
[2] https://en.wikipedia.org/wiki/AlphaFold
[3] Ebejer, J. P. et al. J. Chem. Inf. Model. 2012, 52, 1146-1158; doi 10.1021/ci2004658
[4] Sander T. et al. J. Chem. Inf. Model. 2015, 55, 460-473; doi 10.1021/ci500588j