Subject: search for conformers, empty column «minimization error»
Posted by nbehrnd on Thu, 17 Mar 2022 20:13:14 GMT

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Dear Thomas,

using DataWarrior to generate conformers (chemistry -> generate conformers), I notice the presence of a fifth column to report «minimization errors». So far, I did not met a run with a run where one of the entries were marked by a categorical warning, or a real number against a reference value (if the later, what would be the critical threshold). The chapter «Chemistry in 3D» of the help doesn't provide additional documentation about this. So, what is the anticipated user scenario where this assists the user?

The observation refers to DW 5.5.0 for Linux/Mac including the development updates by 2022-03-14.

Thank you,

Norwid

(Exporting these results as a text file typically yields /two/ tabulators prior to the anticipated line feed, which once was unexpected for an AWK script down the road; one for the empty column, one for the general format of the record lines.)

File Attachments
1) 3molecules_conformers.dwar, downloaded 128 times
2) 3molecules_conformers.txt, downloaded 164 times
3) 3molecules_conformers.png, downloaded 130 times