Subject: Re: conformer generation sometimes skips isomer generation
Posted by nbehrnd on Fri, 09 Jun 2023 10:14:44 GMT
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Dear Thomas,

I do agree with the reasoning to impose a constraint on the conformer generation; to retain stereochemistry assigned as either (R/S), (E/Z), (P/M) in the data submitted in the new set of conformers. Equally, I'm comfortable with the current approach «if ambiguous / a mixture / a racemate, skip this very entry, continue with the next one» your prompt update by 2023-06-08 implements.

After some test runs, I would like to suggest an approach which skips only the entry in the submitted .dwar file which is ambiguous. This is because the submission of `Random_Molecules.dwar` now yields an empty set altogether; there however are some entries DW's internal sketcher recognizes as «this enantiomer». An other which is skipped has no structural CIP relevant motif. With `10mol.dwar` only with entries of an absolute configuration, there is no variation of stereochemistry among the conformers suggested; still, some IDs of the original data set do not appear again among the results. The later observation contrasts with my present anticipation.

For the most recent test run, the previously used instance of DW was removed by `sudo bash ./uninstall.sh`, coherent to the program's documentation. Then, on top of a pristine installation of DW, the update packaged by 2023-06-08 was applied.

With regards,

Norwid

File Attachments

1) 2023-06-09_notes_dw.zip, downloaded 403 times