Subject: conformer generation sometimes skips isomer generation
Posted by nbehrnd on Wed, 07 Jun 2023 14:15:49 GMT
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Dear Thomas,

is there a toggle in the program, or perhaps a critical motif in an input structure which prevents DW from altering stereo chemical information while creating conformers?

On re-visit of an old set of random molecules (10mol.dwar, generated by DW, cf. in the attached .zip archive enclosed) which can feature configurations described by R/S, E/Z, P/M, or a combination of them, I noticed the entry `Stereo Isomer` remains equal to `1`. With a newer set of random molecules (Random_Molecules.dwar, equally generated by DW), the anticipated change between the configurations and entries of `Stereo Isomer` different / in addition to the one equal to `1` however take place. The parameters to generate the conformers retain the suggestions, and aim to be the same in both runs.

Both observations refer to DW 5.5.0 for Linux in Linux Debian 12/bookworm including the updates as fetched by yesterday 2023-06-06 / stamped by 2023-05-18. As to document the observations in further detail, the .zip archive attached includes both input and output as provided by DW.

With regards,

Norwid

File Attachments

1) 2023-06-07_conformer_generation.zip, downloaded 532 times