Subject: Re: conformer generation sometimes skips isomer generation
Posted by thomas on Thu, 08 Jun 2023 12:13:56 GMT
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Dear Norwid,

the conformation generator does not change any stereo centers. If an input structure contains a racemic stereo center (or an unknown one), then created conformers are allowed to contain any stereo parity at that atom. If an input conformation,
however, has a defined absolute stereo configuration, then all conformers should have this configuration.

Your 10mol.dwar file only contains molecules with given absolute configurations. Thus, all conformers have the same configuration. Random_Molecules.dwar contains exclusively unknown stereo centers. Thus, generated conformers contains all possible stereo isomers.

Part of the reason is that random molecules in the current dev version seem to get unknown stereo configurations, while 5.5.0 generates molecules with absolute configurations. Currently, I don't know why, but I will go back to the old behaviour.

Does this explain it?

Best wishes,

Thomas