Subject: conformer generation misses some entries
Posted by nbehrnd on Tue, 04 Jul 2023 21:13:04 GMT
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Dear Thomas,

running the generation of conformers departing from a small DW generated library of molecules, the current nightly update (packaged by 2023-06-08, Linux version) appears to omit entries for which there are less than 16 possible stereoisomers. With pristine installations with the installer to Linux/Mac in hand, it was possible to narrow the change in functionality provided by the updates happened somewhere between the update packaged by 2023-05-18 (still working the anticipated way) and 2023-06-08 (now yielding gaps).

The attached .zip archive includes the submitted test data and collected results in an instance of Linux Debian 13/trixie (testing).

With regards,
Norwid

File Attachments

1) 2023-07-03_dw_conformer_test.zip, downloaded 559 times