

---

Subject: conformer generation misses some entries  
Posted by [nbehrnd](#) on Tue, 04 Jul 2023 21:13:04 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

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 120 times

---