Subject: Re: Bug in how stereochemistry is reported
Posted by tryckmans@ridgelinediscov on Mon, 24 Jul 2023 12:01:44 GMT
View Forum Message <> Reply to Message

Hello Thomas,
I have an issue similar to the one above. When generating a sdf file using ChemDoodle, when I open the sdf in Datawarrior the wrong stereoisomer is created. I notice the SDF does not contain a chiral flag as described above (the 5th character on line 4 is "0", not "1".) When contacted, ChemDoodle answered me this
"While I cannot help with DataWarrior, they are likely handling the SDF file in un-inverted y-axis coordinates. In 2D computer applications, the y-axis is inverted, so the reading application needs to take this into account when loading the SDF file if it contains a 2D drawing. Every chemical drawing application inverts the y-axis in this way."

many thanks for your comments!

The SMILE gives the correct (S) configuration:
N[C@@H](CC(=CC=C1)C=C1)C(O)=O

SD file below:
Molecule Name
  ChemDodl07242313512D 0   0.00000   0.00000   0
[Insert Comment Here]
  0 0 0   0 0   999 V3000
M V30 BEGIN CTAB
M V30 COUNTS 12 12 0 0 0
M V30 BEGIN ATOM
M V30 1 N 0.8511 1.0249 -1.0000 0
M V30 2 C 0.8803 0.0253 -1.0000 0
M V30 3 C 1.7604 -0.4492 1.0000 0
M V30 4 C 0.0292 -0.4997 -1.0000 0
M V30 5 O 2.6115 0.0759 1.0000 0
M V30 6 O 1.7896 -1.4489 1.0000 0
M V30 7 C -0.8511 -0.0252 -1.0000 0
M V30 8 C -0.8803 0.9744 -1.0000 0
M V30 9 C -1.7022 -0.5503 -1.0000 0
M V30 10 C -1.7604 1.4489 -1.0000 0
M V30 11 C -2.5823 -0.0758 -1.0000 0
M V30 12 C -2.6115 0.9238 -1.0000 0
M V30 END ATOM
M V30 BEGIN BOND
M V30 1 1 1 2
M V30 2 1 2 4
M V30 3 1 4 7
M V30 4 1 7 8
M V30 5 2 7 9
M V30 6 1 9 11
M V30 7 2 11 12

M V30 8 1 12 10
M V30 9 2 10 8
M V30 10 1 2 3 CFG=3
M V30 11 1 3 6
M V30 12 2 3 5
M V30 END BOND
M V30 BEGIN COLLECTION
M V30 MDLV30/STEABS ATOMS=(1 2)
M V30 END COLLECTION
M V30 END CTAB
M END
> <DATE>
24-07-2023

$$$$