Subject: Stereochemistry incorrectly reported for InChI
Posted by AngelS on Fri, 04 Jul 2025 02:51:17 GMT
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I want to believe this is not an evil feature but a glitch.

When pasting SMILES from clipboard or opening a csv file with SMILES, e.g.:
CC(N)C1=CC=CC=C1

DW interprets the structure automatically as either a wedged or hashed bond around the chiral carbon. Upon further detail in the structure (double click), it indicates "both enantiomers", and the carbon has a "&1" label.

When using the Chemistry menu to create the Standard InChI string, it assumes a given stereochemistry, matching the initial wedged or hashed bond:
InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3/t7-/m0/s1

This InChI translates to this SMILES:
C[C@@](N)([H])C1=CC=CC=C1

However, when creating the SMILES string in DW (Chemistry menu), it is generated as racemic, confirming the lack of stereochemistry:
CC(c1ccccc1)N

This behaviour is not observed when the molecule has 2 or more chiral centers.

The expected InChI string should be:
InChI=1S/C8H11N/c1-7(9)8-5-3-2-4-6-8/h2-7H,9H2,1H3

I found an old reference from 2019 in this forum with a similar issue, which was apparently known and fixed by a patch, but nothing else newer.
My version of DW is v.06.04.02