Hello Thomas,

my understanding of DataWarrior's manual is that the program internally stores
the molecules in a format capable to discern and (if selecting .sdf v3000)
export of double bonds including those without explicit assignment of (E)/(Z)
configuration. As anticipated, the SMILES strings

C/C=C/C
C/C=C\C
CC=CC

yield three different representations of but-2-ene.

For a small test set (cf. double_bond.dwar and the screen photos in the .zip
archive attached), I aimed to use the features of extended stereochemisty as a
criterion to retain a sub set (Chemisty -> From Chemical Structure -> Add
Substructure Count), including the unassigned double bond visualized as a
crossed double bond. So far, the attempts failed.

As anticipated, the search pattern of (cis)-butene, retained both (cis)-butene
and cyclohexene and withdrew the oxime. However -- contrasting to anticipation
-- (trans)-butene and the unassigned butene equally were retained. Does the
search for, e.g. crossed double bonds, require a particular instruction?

Version info: DataWarrior 5.5.0 for Linux in Debian 12/bookworm (branch
testing), including the update as «development version» as fetched on Sunday,
2021-11-28.

Norwid

File Attachments
1) double_bonds.dwar, downloaded 501 times
2) double_bond_documentation.zip, downloaded 510 times