Subject: Find & Replace or alternative for stereoisomers
Posted by Paul on Mon, 29 Aug 2022 17:55:59 GMT
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Hello All

I would like to invert the configuration of all asymmetric carbon atoms (sp3) in a data set.

I have made many attempts using Find & Replace, but only succeed when exact carbon skeletons are supplied.

For example, I can convert 3,3,4(S)-trimethylhexane to 3,3,4(R)-trimethylhexane, but I cannot convert all structures with that common sub-structure to the inverted configuration for higher alkanes.

It seemed to me that the Query Feature Dialog would be appropriate for this use. The dialog is accessible (using the "q" key on hovering on an atom/bond) in the Find This structure editor window. However, the query feature only produces the "unknown" response in the replace with structure editor window.

Ultimately, I would like to generate a specific molecular representation for every stereoisomer, for each substance with 1 or more asymmetric carbon atoms in a data set.

So far, I have accomplished this by using smiles with @/@@ notation in Excel spreadsheets (this approach is somewhat doable in DataWarrior for simple cases, but much easier in Excel with more than 1 asymmetric C-atom. The method quickly goes from clunky to prohibitive as molecular complexity/number of asymmetric C-atoms increases.

Is this something for DataWarrior is suited?

I've attached a DWAR for C9H20 compounds with no racemates, should anyone want to use it for an example.

Thanks,

Paul

File Attachments

1) C9H20_no-racemates.dwar, downloaded 190 times