Subject: Stereochemical questions
Posted by don on Mon, 07 Nov 2022 16:16:32 GMT
View Forum Message <> Reply to Message

Hi all,
I'm a newb to DataWarrior and have a couple of questions about identifying enantiomers from a compound set.

1) How do I filter a dataset so that the only compounds displayed are single stereoisomers of absolute configuration (filtering out both racemic compounds and compounds with no stereochemistry)?

2) Is there a way one can use DataWarrior to filter a set of compounds so that the only compounds displayed are single enantiomers AND their corresponding enantiomers? In other words, the search would only identify pairs of enantiomers (not single enantiomers, not racemic compounds, not compounds without stereochemistry).

Thanks in advance for your help.
don