Subject: Re: Merge File Issues
Posted by amorrison on Tue, 23 Apr 2024 17:16:01 GMT
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Hi Thomas,
Was not sure how to do this as a macro, so apologies but hopefully you can follow what I am doing. I've attached some files for a small set of compounds from ChEMBL.

Step 1 - Export DataWarrior file CDK2_Dwar.dwar to an sdf file (v3000).
Step 2 - Calculate properties in another program (ACD) and export as a SDF file (CDK2_Export_ACD.sdf)
Step 3 - Open CDK2_Export_ACD.sdf in DataWarrior - Say no to the racemate warning
Step 4 - Merge CDK2_Dwar.dwar in to CDK2_Export_ACD.sdf with Compound_ID as merge key and Structure 'replace with new'

All row filters are then lost and only 3 structures are visible, although the row count is 26. As part of this test I (have just) saved the resulting file and have just reopened it and the structures are now visible although all the row filters are still missing.

Apologies for the long winded explanation but hopefully you get the gist of what I am trying to do.

Best wishes,

Angus

File Attachments

1) CDK2_Dwar.dwar, downloaded 567 times
2) CDK2_Export_ACD.sdf, downloaded 557 times