Subject: Merge File Issues
Posted by amorrison on Wed, 17 Apr 2024 08:39:28 GMT
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Hi,
I recently updated to v6.01.03 and now seem to have an issue with merging data from another file.

The workflow I have is as follows. I have a DataWarrior file that I update with new compounds weekly in DataWarrior I use the advanced stereochemistry flags to indicate chirality. I then export this as an SDF file to calculate properties in another programme, which is then exported as a new SDF file.

As this application does not handle v3000 file format I lose the chiral flags in the structures. When I open the new annotated SDF file (which has the additional compounds) I have been replacing the structures (via merge) with the previously prepared ones in DW with chiral flag annotations. This has worked great until today. Now when I do this all the column filters are lost I can see from the row count they are there but the new compounds I have just added are hidden. Disabling all row filters and resetting all row filters has no effect.

Any help on this one?

Many thanks,

Angus