Subject: Re: Bypass "Maximum number of open filters reached." message on file open?
Posted by nbehrnd on Tue, 28 Nov 2023 21:51:54 GMT
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Hello Andrew,

out of curiosity: if you open the large .sdf file, aside from the structure as a criterion about which DW provides a filter, the additional criteria DW exports into a .sdf follow the pattern of

```
>  <criterion>
entry
```

as e.g. for

```
>  <Smiles>
CCc(cc1)c([C@H](CCl)C(NC(COCC)=O)=O)cc1C(O)=O

>  <Total Molweight>
341.79

>  <H-Acceptors>
6

>  <H-Donors>
2
```

Assuming every entry in your large .sdf file has the same number of these additional property tags -- how many are assigned to the individual model entry vs how many are actually (still) displayed (e.g. as filter) by DW's attempt to read the file? Perhaps there is a «critical threshold» in the number of properties one might better know while processing larger .sdf with DW.

On the other hand, the large .sdf file (with annotated properties) in hand could be rewritten as .sdf to contain only the structures e.g., by openbabel with a command in pattern of

obabel -isdf annotated.sdf -osdf -xm > plain_structures.sdf

to yield an undisturbed, pristine view in DW. This approach works best if the structures explicitly describe unique stereochemistry, i.e. double bonds either in (E), or (Z) and stereogenic centres either (R), (S), (P), or (M) configuration. (In contrast to the sketcher in DW where one can draw a molecule with crossed double bonds, or stereogenic centres with `&` and `or` about e.g. racemates and diastereomeric mixtures as extended stereochemistry.)

With regards,

Norwid