Subject: Bypass "Maximum number of open filters reached." message on file open?
Posted by Andrew0 on Tue, 28 Nov 2023 20:21:49 GMT
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When opening a .sdf, it seems that DataWarrior tries to create a filter for every column. I am running a macro that opens a file and applies a template with the filters I want. However, my original .sdf has grown large enough that I now receive the message "Maximum number of open filters reached" whenever I open the file.

Is there any way, either as an option on file open (something like "do not create filters") or as part of a macro (disable/ignore/accept warning messages) to suppress this message and proceed with the macro?

Thank you!
Andrew

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

Subject: Re: Bypass "Maximum number of open filters reached." message on file open?
Posted by Andrew0 on Wed, 29 Nov 2023 15:07:07 GMT
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Hi Norwid,

Thanks for your reply. It looks like the .sdf has 87 property tags, and DataWarrior hits its limit at 64 filters. Ultimately I do not want all these filters present - after importing the file, the macro applies a DataWarrior template that reduces to ~7 filters that users actually need.

I also appreciate your thoughts on removing the annotated properties for a clean DataWarrior intake. Unfortunately, the application I'm working on requires all the fields to remain intact (or otherwise to be re-associated with the structures after import into DataWarrior).

Thanks,
Andrew

Subject: Re: Bypass "Maximum number of open filters reached." message on file open?
Posted by nbehrnd on Thu, 30 Nov 2023 22:44:11 GMT
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Dear Andrew,

intrigued by your report, I revisited the the issue and can replicate your observation of a «critical threshold» of annotated properties DW processes as filter. Starting from a DW generated library of random molecules saved as .dwar, as soon as the 70th column was added DW issued a warning no additional filter could be displayed. At this point, the user can amend the array by additional columns (in the test attached in the .zip archive, I stopped with 79 columns [count includes the column about the molecule's structure]). During these incremental steps beyond the threshold, DW faithfully continues to work -- no additional nagging, still functional export to .dwar, .sdf (v3000), and .txt.

You introduced the idea to skip the automatic/default creation of filters. With the bits and bolts the macro editor provides, I wrote two DW macros attached below. Based on the assumption that criteria in early columns of DW's array might be of later interest for you, one only mutes the filters to be toggled on/off as usual. The second one removes the filters, but retains the columns in DW's array which complements the functionality of the other. As checked (cf. zip archive), neither one of the approaches bypasses DW's warning if there are too many criteria. If deemed necessary, DW issues this note only once per .dwar/.sdf read and you can carry with the work ahead.

With best regards,

Norwid

File Attachments

1) 2023-11-30_silent_read.zip, downloaded 552 times
2) mute_filters.dwam, downloaded 640 times
3) remove_all_filters.dwam, downloaded 577 times

Subject: Re: Bypass "Maximum number of open filters reached." message on file open?
Posted by Andrew0 on Thu, 07 Dec 2023 21:21:48 GMT
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Thanks Norwid. It sounds like there isn't an option to bypass or suppress the message altogether. As you said, since it only happens once, it isn't a big issue.

Subject: Re: Bypass "Maximum number of open filters reached." message on file open?
Posted by thomas on Tue, 12 Dec 2023 10:35:21 GMT
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In the next dev update the 'Open File' macro task will have options to prevent default filters and default views for non-dwar files.

Subject: Re: Bypass "Maximum number of open filters reached." message on file open?
Posted by Andrew0 on Fri, 05 Jan 2024 21:16:51 GMT
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Many thanks, Thomas!