Subject: Category Filters for Structures/Substructures
Posted by tschrader on Mon, 14 Jan 2019 20:42:25 GMT
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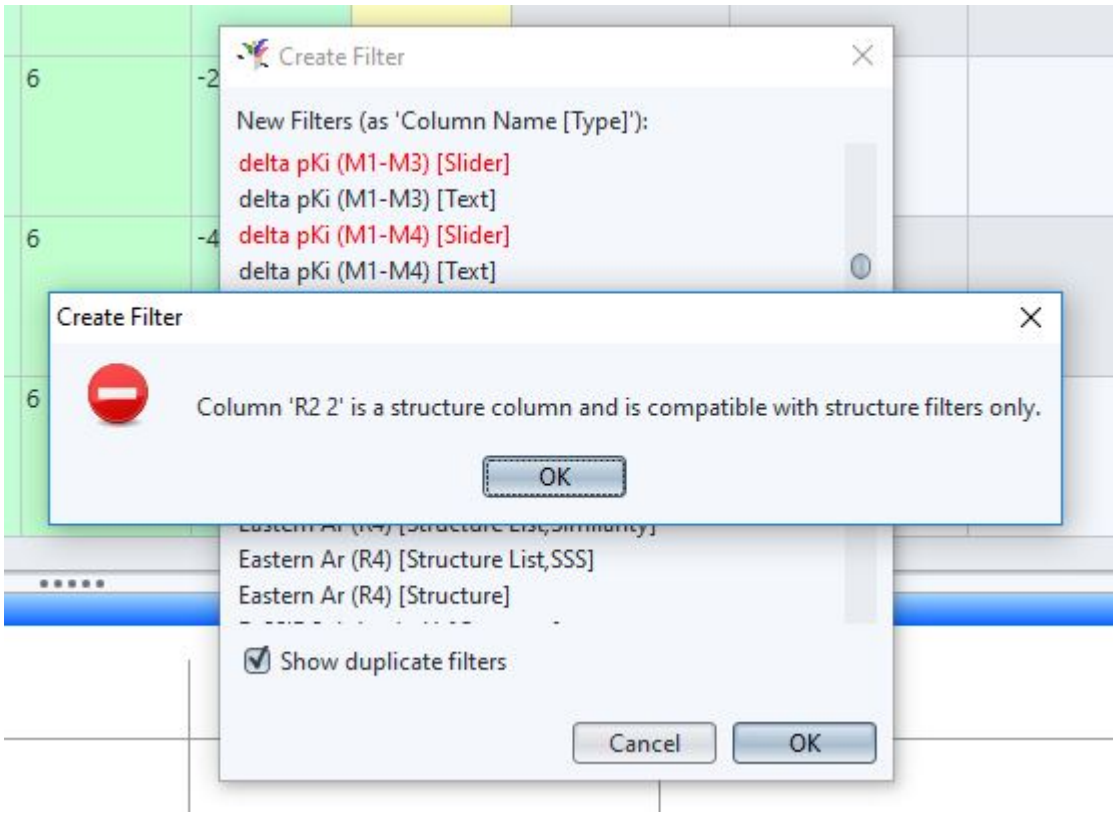
Hello,

I noticed that with the new version of DW (5.0.0) that I am now unable to create category filters from columns that contain structures. This is an extremely useful feature for SAR analysis. Can we regain this functionality please?

Thank you

File Attachments

1) Error message for structure category filter.JPG, downloaded 1767 times



Subject: Re: Category Filters for Structures/Substructures
Posted by thomas on Wed, 16 Jan 2019 22:38:59 GMT
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I will check this and release a fix quickly, Thomas

Subject: Re: Category Filters for Structures/Substructures
Posted by thomas on Thu, 17 Jan 2019 19:13:27 GMT
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Until there will be a full new version upgrade, I publish frequent intermediate DataWarrior builds with fixes of known bugs, which can be downloaded from this website. These are just the DataWarrior.exe file for Windows and the datawarrior.jar file for Linux and MacOS. To update, just replace these files. The links to these files are: openmolecules.org/datawarrior/dw500win.zip and openmolecules.org/datawarrior/dw500x.zip, respectively.

The current files include fixes for this structure-category-filter bug and some other small issues. It also contains a new column filter hiding columns instantly based on column names.

Thomas

Subject: Re: Category Filters for Structures/Substructures
Posted by tschrader on Tue, 22 Jan 2019 23:30:15 GMT
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Thank you so much Thomas. The fix works great. Truly appreicate it 8

Subject: Re: Category Filters for Structures/Substructures
Posted by alfred on Mon, 28 Jan 2019 15:47:56 GMT
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Hi Thomas

thanks for the update. I may have missed something but how does the column filter work? It sounds like a handy tool to show / hide columns with a filter but I don't see it in the New Filter list.

Best
Alfred

Subject: Re: Category Filters for Structures/Substructures
Posted by thomas on Tue, 12 Feb 2019 18:04:03 GMT
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Hi Alfred, the column filter is just a small text field, which opens when clicking the new magnification glass icon in the table view. If you type a few letters into the text field, then all columns disappear, whose column names don't contain the typed letters in that order.

Thomas

Subject: Re: Category Filters for Structures/Substructures
Posted by alfred on Fri, 15 Feb 2019 08:29:37 GMT
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Hi Thomas

thank you for your explanation and sorry for my misunderstanding. Actually, would it be possible to create a "real" filter (like the category filters) to show/hide columns? It would be much more friendly than hiding the columns one by one, and help working with large tables. With the new magnifying glass, tou can only keep columns sharing the same name (partly at least).

Alfred

Subject: Re: Category Filters for Structures/Substructures
Posted by tschrader on Tue, 05 Mar 2019 21:31:42 GMT
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Hello again,

I noticed that some category filters no longer become available after a certain number of categories are reached. Is there a way to remedy this?

Please let me know. Thanks.

Subject: Re: Category Filters for Structures/Substructures
Posted by thomas on Thu, 07 Mar 2019 15:39:06 GMT
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Hi Alfred,

1st question: a dialog to show/hide multiple columns at once is on the (very large) list of new features, but not available yet.

2nd question: It seemed to me that a category filter beyond a certain number of categories would not be practical anymore. Thus, there are maximum category counts for different purposes, e.g. to decide whether a category filter still makes sense. These numbers are hard-coded into the program and cannot be changed from outside.

Thomas