Subject: Compound selection via check box
Posted by dkchalmers on Thu, 30 Mar 2017 05:00:41 GMT
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Dear Data Warriors,

I frequently want to manually select a subset of compounds from a larger set. It would be really useful to have a manually selectable check-box in the structures and/or table view that could be used to select compounds. The selected subset could then be exported. I know there is the 'list' functionality, but this does not seem to clearly highlight the compounds that have been selected.

Thanks for providing a really useful program.

Cheers

David

Subject: Re: Compound selection via check box
Posted by thomas on Thu, 30 Mar 2017 19:24:29 GMT
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Dear David, I am a bit reluctant about the checkbox for technical reasons and because it would need additional menu items to show and hide and use it for different purposes, while its functionality would overlap with list functionality. What you may do to recognize compounds that are already part a list, you may draw these structure's background in a different color (once you have started a row list: right mouse click on the 'Structure' column title in the Table View -> Set Background Color... -> <List name>).
An alternative is to create a list filter that hides all compounds, which are already part of a list. Then stepwise assign the visible compounds to one or multiple lists untill all interesting compounds are gone or no compound is left.

Currently adding one compound to a list is done using the compound's popup menu. Adding all selected compounds to the list can be done from the list menu. Admittedly, both options are a little cumbersome and I am currently evaluating better options, e.g. Ctrl-Plus and Ctrl-Minus to add the current compound to the first(!) list. Maybe even better would be that a ALT-mouse-click could toggle list membership if the compound background is associated to a list. That would be as easy as a checkbox. What is your opinion?

Best wishes, Thomas

Subject: Re: Compound selection via check box
Posted by dkchalmers on Fri, 31 Mar 2017 01:58:57 GMT
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Hi Thomas,

I guess I am after two things. 1. A quick way to add/remove compounds from list (so a mouse click or simple keystroke would be good here, I only need one list) and 2. visual confirmation that a compound is a member of a list (The set background colour method works well - but it is pretty hard to find!).

Thanks

David
