Subject: Automatic Calculation of Properties
Posted by ELFritzen on Wed, 22 Jan 2020 19:20:26 GMT
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I was wondering if Datawarrior could automatically calculate molecular properties for new compounds appended to a Datawarrior file from an SD file? I have a Datawarrior File containing a number of calculated properties. As I append new compounds, the columns for these calculated properties are not populated. If I calculate properties after the compounds are appended, Datawarrior creates a whole new set of columns for the calculated properties. The only way I can think of to avoid all the additional columns is to open an SD file in Datawarrior, calculate the molecular properties and then append the new Datawarrior File to my master Datawarrior file. I was just wondering if there was a simpler way.
Thanks.

Ed Fritzen

Subject: Re: Automatic Calculation of Properties
Posted by thomas on Mon, 10 Feb 2020 21:15:21 GMT
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This seems to be a frequent question. The problem of such an automatic property completion (and for consistency reasons calculated value completion) is that calculated values depend on other columns values. If there a multiple columns with calculated values, the order of calculation becomes important. This would be rather complex to track, especially since users may delete or change columns in between.

There is another solution that seems much simpler to me: You may create a macro that removes the calculated/property columns first and then freshly calculates them again. To do so:
- open file with the property columns
- start recording a new macro
- delete all property columns
- calculate all desired properties
- stop macro recording
- save the file. It now contains the macro, which can be started any time from the Macro menu.

Thomas

Subject: Re: Automatic Calculation of Properties
Posted by ELFritzen on Tue, 11 Feb 2020 21:42:40 GMT
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Thank you for the reply, Thomas. I'll give the macro a try.

Ed