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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

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