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Subject: .SDF exporting conventions

Posted by [cwt43361](#) on Wed, 20 Nov 2024 18:01:50 GMT

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Upon exporting data from data warrior using save special --> .SDF option, I noticed the following issue:

If my data has 'Compound ID' or 'Structure ID' or 'ID' or 'Name' or 'Structure Name', it seems as though upon export to .SDF it looks like the option to specify the Compound Name Column never includes these labels but rather just SMILES and other descriptors calculated within Data Warrior.

The issue I'm having is that if I use the <automatic> option it will create an additional column called 'structure no'. When I'm attempting to use this file downstream in another program where I need to have the column specifically named 'Name' or 'ID', the renaming or adding of column that data warrior is doing upon export is creating issues.

Is there a specific wording that data warrior requires for the compound name column for the program to recognize? For example, I have noticed how I include by biological activity in data sets can affect whether data warrior can interpret this as biological data (such as relative activity at 10uM).

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Subject: Re: .SDF exporting conventions

Posted by [thomas](#) on Wed, 20 Nov 2024 21:55:53 GMT

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I checked the source code. The rule is that all alphanumerical columns qualify as 'Name column' unless one or more cells contain more than one identifier (separated by "; " or in two separate lines).

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Subject: Re: .SDF exporting conventions

Posted by [cwt43361](#) on Wed, 20 Nov 2024 22:22:56 GMT

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God bless you! I looked at the compound library (from my college) and there is a single compound in ~30K compounds that has a semi-colon in the name! You're a legend, a hero!

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