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).