Subject: Problemin exporting structures as SMILES generated from evolutionary library into excel
Posted by Jo W on Sun, 18 Jul 2021 08:44:11 GMT
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The generation of new compounds from the Evolutionary library feature is amazing.
What I would like to do is compare some of the generated molecules with "known" compounds in databases that are NOT linked to Datwarrior to see how many compounds this process generates that have been synthesised before.

In general, I would also like to export structures located in Datawarrior to CSV files as SMILES.

However I can't figure out how to do this despite looking at the manual and forum posts.

A previous forum post in 2016 had a few answers on how to do this but they didnt work
[see message #160 - I cant post the link apparently this is because this is my first post]

The advisor suggests to select "ALL" and "copy" from a table of structures (in my case generated from the evolutionary library built into Datwarrior) and paste directly into Excel.

However, when I do that, the ID for compounds and associated data IS pasted with formatting which is useful. However, I want to be able to export the SMILES as well, so how do you do that.

Does Datawarrior have built in converter to convert ID structures into SMILES and then copy and paste into excel?

Or even better can you just add a SMILES column so that as the evolutionary library structures that are created, the SMILES column is automatically populated and ready for export via cut and paste into excel?

Many thanks in advance
Jon

Subject: Re: Problemin exporting structures as SMILES generated from evolutionary library into excel
Posted by thomas on Mon, 19 Jul 2021 07:53:10 GMT
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You can generate a column containing SMILES from the 'Chemistry' menu with 'From Chemical Structure->Add SMILES Code...'.
Then Copy/Paste or 'Save Special->Text File...' will include the SMILES column.

Thomas