Subject: Re: Calculating similarity to one query compound
Posted by rkp@23 on Mon, 01 May 2023 13:48:16 GMT
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I have a question about ID-Code.
Are ID-code and SMARTS inter-convertible?
For example, if I want to convert SMARTS string to an ID-code or vice-versa, are there any method within DataWarrior that can do that?

I am asking specifically for macros and editing them outside DataWarrior.
I want to provide reaction SMARTS as SMARTS string in the macro specification , as well as reactant 0 and 1 as SMILES/SMARTS, but I see that Macros are written out with ID-codes rather than SMARTS string.

My goal is to prepare a macro outside DataWarrior: provide required reaction SMARTS, reactants for combinatorial library generation , as a SMARTS/SMILES string, may be using shell variable or python. I would like to get a Macro document, with those SMARTS string converted to ID-code, which DataWaarrior can now work on.

Has anybody tried this before?
Let me know