Subject: Re: Calculating similarity to one query compound
Posted by thomas on Sat, 25 Apr 2015 06:34:21 GMT
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Hi Paul,

you are right, the chemsim() function should do it. ID-Codes are DataWarrior's internal canonical structure representations. They contain all stereo features and in case of query fragments they also contain query features.

What you need to do is to copy the idcode of a compound into the clipboard (in DataWarrior: right mouse click->Copy As->ID-Code), then open the 'Add Calculated Values...' dialog, type the formula 'chemsim(,"")', move the cursor after the opening bracket, select the descriptor from the popup (e.g. FragFp_of_Structure) and click 'Add Variable', move the cursor between the double quotes and paste in the idcode. Click OK. This should do it.

ID-Codes are a little cryptic, but they are more compact than SMILES and don't have the aromaticity issues and stereo issues of SMILES and they support MDL's concept of enhanced stereo representation, which was introduced with the molfile version 3.

Kind regards,

Thomas