Subject: Calculating similarity to one query compound
Posted by PaulFinn on Wed, 22 Apr 2015 19:43:42 GMT
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Hi,

I would like to calculate the similarity of the compounds in a table to another compound (either a compound already in the table or one in a SD file) and create a new column with these values. I cannot find a way to do this. The chemsim function maybe should do this in syntax A, but the meaning of idcode in the help text is unclear and I have not been able to get it to work.

Regards,
Paul