
Subject: Re: How to add the "Structure of smile similarity" score to the column
Posted by [thomas](#) on Mon, 30 Jan 2023 09:30:22 GMT

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Dear Shane,

You can do that, but not with a simple mouse click:

-move the mouse over the selected reference structure (or marker representing it), right mouse click and choose

'Copy->Structure of SMILES As->ID-Code'

-In the main menu choose 'Data->Add Calculated Values'. As formula use:

`chemsim(SkelSpheres_of_StructureofSMILES,"ffmPP@CN@aQTfVUyWeVeijZjjjZ@@ ")`

(instead of ffmPP... use your copied idcode!)

Thomas
