Subject: How to add the "Structure of smile similarity" score to the colume
Posted by Shane on Mon, 30 Jan 2023 03:14:31 GMT
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Dear DW forum,

I've tried a similarity analysis by the SkelSpheres descriptor.
I could get the different data columns (such as Neighbor Count, Neighbor Cluster No, Neighbor Cluster Size, and Neighbor Similarity SkelSpheres 80%), and Simiarity chart.
In the simiarity chart, choose reference structure, then I can get the "Neighbor Analysis X&Y" and "Structure of smile similarity" of this structure. After that, move the mouse to another structure (no click), can get "Structure of smile similarity" based on reference structure.(Figure 1&2).
So, there is a problem that I cannot find the option about to add "Structure of smile similarity" based on reference structure in the empty column.

Thank you for your help
Shane

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File Attachments
1) Figure 1.png, downloaded 265 times
2) Figure 2.JPG, downloaded 226 times
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Subject: Re: How to add the "Structure of smile similarity" score to the colume
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@aQTfVUyWeVeijZjjjjZ@@ ")
  (instead of ffmPP... use your copied idcode!)

Thomas

Subject: Re: How to add the "Structure of smile similarity" score to the colume
Posted by Shane on Tue, 31 Jan 2023 02:53:15 GMT
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Hi Thomas

Thank you for your help.

I can do it!

Shane