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

File Attachments
1) Figure 1.png, downloaded 87 times
2) Figure 2.JPG, downloaded 82 times

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