Subject: Find similars

Posted by sansun on Mon, 21 Mar 2022 12:36:40 GMT

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I am trying to find 'similar' molecules in a file. I am selecting another datawarrior file in the dialogue box.

As usual it creates additional coloumns highest similarity and most similar structures. However, in certain cases it is showing similarity value but not the structure and vice versa. See attached snapshot.

I am using the latest official release.

File Attachments

1) Capture.PNG, downloaded 734 times