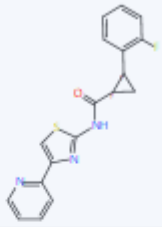
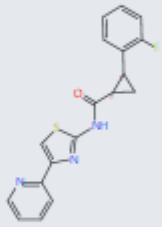
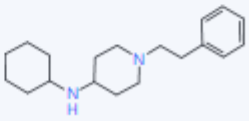
Subject: Find similars
Posted by sansun on Mon, 21 Mar 2022 12:36:40 GMT
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I am trying to find 'similar' molecules in a file. I am selecting another datawarrior file in the dialogue box.
As usual it creates additional coloumns highest similarity and 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 1430 times

Matches [75%; SkelSpheres] 2	Highest Similarity [SkelSpheres] 2	Most Similar Structure 2	Reference
0			
0			
0			Antimicrob. Agents Chemother. 54 (9), 3597-3604 (2010)

Subject: Re: Find similars
Posted by nbehrnd on Tue, 22 Mar 2022 11:45:51 GMT
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Dear Sansun,

to ease replication of your observation, consider to complement your post with minimal data e.g., a .dwar file prior and after the critical step. If these are still larger than the limit of 2048 kB, archive them as a .zip.

Norwid

Subject: Re: Find similars
Posted by thomas on Sat, 02 Apr 2022 14:47:11 GMT
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Dear Sansun,

I checked with thousands of structures and various files, but could not reproduce the effect. Do you use the newest dev version (patch files downloadable from a link in the small print after clicking 'Read and understood...'). As Norvid pinted out, I would be grateful for two very small sample files to reproduce the problem.

Thanks in advance,

Thomas

Subject: Re: Find similars
Posted by sansun on Fri, 15 Jul 2022 07:34:46 GMT
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Hi
Sorry, I couldn't reply earlier.

The problem was solved by exporting the file in SDF format and then opening again in DW.

I don't know how but it got sorted out.

SS