
Subject: Find similars

Posted by [sansun](#) on Mon, 21 Mar 2022 12:36:40 GMT

[View Forum Message](#) <> [Reply to Message](#)

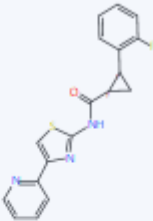
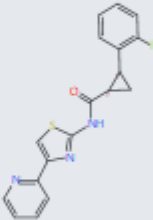
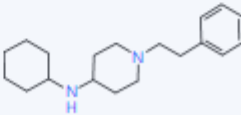
I am trying to find 'similar' molecules in a file. I am selecting another datawarrior file in the dialogue box.

As usual it creates additional columns 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 1073 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

[View Forum Message](#) <> [Reply to Message](#)

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

[View Forum Message](#) <> [Reply to Message](#)

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 Norwid pined 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

[View Forum Message](#) <> [Reply to Message](#)

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
