
Subject: Find similars

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

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

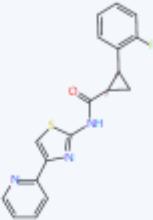
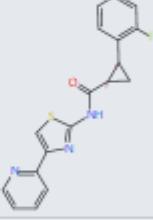
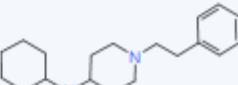
I am trying to find 'similar' molecules in a file. I am selecting another datawarrior file in the dialogue box.

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 787 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)
