
Subject: Find similars using Flexophore

Posted by [sansun](#) on Sat, 16 Jul 2022 06:36:41 GMT

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

Hi

I am getting the following error while trying to search similar compounds using the Flexophore descriptor in Datawarrior latest version (updated with the developmental version sometime in Jan).

It indicates a problem with 'atom type'. Several of these messages are popping up which, I am guessing, means a problem with more than one molecule.

How can I identify which molecule is giving the problem?

Also, this error box is quite elongated and doesn't fit the screen even though the actual message in it is limited to above. I had to move it a lot towards my left to see the 'ok' button to close it. However, I found right-clicking on the box also gives the option for closing it.

Thanks

SS

File Attachments

1) [error flexophore.PNG](#), downloaded 1126 times

Message



Uncaught Exception:Base contains Invalid atom type for similarity calculation [(52) (392) (4358*6) (4358*6) (590088,598407,852359) (1313