Subject: Find similars using Flexophore
Posted by sansun on Sat, 16 Jul 2022 06:36:41 GMT
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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 322 times

Subject: Re: Find similars using Flexophore
Posted by nbehrnd on Sat, 16 Jul 2022 07:16:35 GMT
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Dear Sansun,

in a first step, update the development version of DW again; typically, there are about two updates per month). The most reliable approach is to completely de-install DW; then run the installer (compiled by April 2021, ca 152 MB) followed by the update package (the latest I'm aware of was published by July 13th 2022, ca 28 MB). Does the problem still occur? Do you refer to the Windows version, or the one for Mac/Linux (and then, do you use DW in Mac, or Linux)?

If the problem still is seen, attach a .dwar leading to the roadblock. If the .dwar is larger than 2048kB, the limit for attachements per question here, archive it as a .zip and upload the zip instead. If the file still is too big, divide your data set into two and check which one is problematic. Though you likely have to apply this bisection multiple times until the (zipped) .dwar file passes the limit for the upload, it reduces the set of structures /potentially/ causing the road block. (This approach of simplification assumes that there is only one «special» molecule in your data.)

With regards,

Norwid

Subject: Re: Find similars using Flexophore
Posted by sansun on Sat, 16 Jul 2022 11:02:17 GMT
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Thanks Norwid

I have updated the developmental version and I am still having same problem.

I was wondering if absolute stereochemistry needs to be defined for using flexophore? My file has many molecules with undefined stereochemistry.

I'll try other suggestions too.

Thanks
SS