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