
Subject: Re: Filter out nasty functions

Posted by [juliocoll](#) on Wed, 17 May 2023 15:54:24 GMT

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dear nbehrnd,

Thank you for your attention and my apologies for the irregularities you mention of my previous communication. I am trying to improve it here.

I am doing intense DataWarrior Build Evolutionary Library during the last 2-3 months with several different systems and cavities. I manage to make libraries of a few thousand children molecules per every experiment with 3 runs each. However, I also found that 8.8 to 66 % of the children generated were classified as toxic by DW chemical properties depending on the runs, parent, etc.

Therefore I designed macro 1 to save the results in dwar and sdf formats, before and after elimination of the toxic-children molecules automatically (I enclose the 1.dwam file)

I first found out the children with the smiles I sent you with the 2 nasties without being eliminated by macro 1. However, after sending the topic to the forum, I realized that other nasties were also not being eliminated !!!!!.

I reproduced those failures and select some of the toxic rows and other healthy for you from experiments B10 (~3500 rows) and B13 (~5400 rows) in the files selected-15B10... and selected-24B13... Evolutionary_Library.dwar Both of them came from DataWarrior Build Evolutionary Libraries after being "detoxicated" with macro 1.

The particular smiles that I sent you in the previous communication, corresponds to ID879 of the experiment B10. I visually confirmed that it was the same smiles that I sent you before (I hope).

Thank you for your help !
sincerely Julio

File Attachments

- 1) [1.dwam](#), downloaded 553 times
 - 2) [selected-15B10Evolutionary_Library.879sentbefore.dwar](#), downloaded 595 times
 - 3) [selected-24B13Evolutionary_Library.dwar](#), downloaded 578 times
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