
Subject: Re: Filter out nasty functions

Posted by [juliocoll](#) on Fri, 09 Jun 2023 05:58:59 GMT

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dear Thomas,

THANK YOU fo your last proposal!

Unfortunately, it has failed in a couple of files with ~6000 rows.

Norwid proposal, filtering those rows previously labeled to be skip, works beautifully (see my last 111.darm version).

Still the problem of automatically label the numerous EL files remains.

I handled about 200 dwar and sdf files from EL with thousands of non-toxic children each. The actual file labeling as "Evolutionary-library.dwar" is insufficient. The manual labeling is prone to errors.

If possible I suggested to automatically use the number of rows that EL shows in its Tables (visible and total). I am using that manually. It resulted almost unique given the variations from experiment to experiment. I failed to incorporate any variable to the *ask* command on the filtering macros.

you can check what I mean by looking into my last publication which makes extensive use of EL for generating diverse libraries:

https://chemrxiv.org/engage/chemrxiv/article-details/6479b8c_fbe16ad5c57577cce

Can you help me?

sincerely

julio
