Subject: Re: Filter out nasty functions Posted by juliocoll on Sat, 27 May 2023 19:11:40 GMT View Forum Message <> Reply to Message

dear Norwid,

I tested an hybrid macro between my 1 and your suitable_compounds_color. It was successful on a ~12000.dwar compound file from an Evolutionary Library (EL) !!!!!. :)

With your "skip entry" filter, it would be impossible to retain any of those nasty rows for further analysis. In the EL example tested only ~3800 compounds were retained !!! 80

I am working under windows 10-64, which may be one of the reasons the macros did not exchange well. I relied mainly on recording macros to design mine. Nevertheless, I attached the final 11.dwam just in case you wanted to take a look or it may interest to others in the forum.

Thank you for the information on the nasties. My DW windows code says that there are 20 nasty compounds but I could not find their names......

File Attachments
1) 11.dwam, downloaded 103 times