Subject: non-toxic Build Evolutionary Library
Posted by juliocoll on Wed, 28 Jun 2023 08:18:45 GMT
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dear Thomas,

I wonder if a check by non-toxic criteria could be included into the "build evolutionary library" right after each new molecule is being generated and before selection to be included in the final table.

That would increase the numbers of useful molecules at the final table and avoid waste of resources like memory during the evolutionary proccesses.

The possibility was raised because in one extreme case, I generated ~6000 BEL molecules, but only ~200 (~3 %) were non-toxic. As examined, most of the toxic BEL contained a "tertiary immoniun" nasty function (see part of the file attached)

Thank you for your attention, sincerely
julio

File Attachments

1) 2427v2Evolutionary_Library.dwar, downloaded 740 times