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Subject: Re: Filter out nasty functions

Posted by [nbehrnd](#) on Mon, 29 May 2023 16:56:48 GMT

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Dear Julio,

I do not know the parameters to set up the evolutionary library you used -- motives may be similar to approved drugs, or natural products, or molecules derived from a different "seed library". Nor how the internally generated molecules eventually were filtered to be retained in the library; criteria may be sensitive to molecular patterns, scalar properties like molecular weight, or a combination. Second, your script seems to be stuck in the rut once the first set of molecules was saved. Because there are only the two levels of "safe molecules", and "harmful molecules" by only one remaining filter, the manual intervention after DW's computation to save either one sub set may be considered "still acceptable" (cf. the silent attached). (The small test set of natural product-like compounds, more than half were not considered "safe" either.)

The DataWarrior macro/script should be portable and work equally well regardless of the operating system in which DataWarrior is working. It was not previously tested in Windows because (for a couple of years) DW no longer is satisfied with a 32bit, but requires a 64bit system.

Norwid

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File Attachments

1) [record.mp4](#), downloaded 481 times

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