Subject: Re: non-toxic Build Evolutionary Library
Posted by juliocoll on Wed, 23 Aug 2023 07:52:42 GMT
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Dear Thomas
Thanks to Norwith B.

, a few days ago I detected a "prefer toxic risk" criteria added to the build evolutionary library:
THANKS A LOT!!!

I am experimenting now with a coouple of models using simultaneous docking score, mol weight,logP, and presence or absence of toxic risk criteria with different thresholds and weights.

I will comment the results on due time to the forum

Cheers
Julio