Subject: Re: non-toxic Build Evolutionary Library
Posted by juliocoll on Mon, 28 Aug 2023 10:25:36 GMT
View Forum Message <> Reply to Message

PRELIMINARY REMARKS
- The toxicity risk added by Thomas to work during EL is a new important feature that allows ~2-fold increase in the number of molecules explored for best docking during 3 consecutive runs, taking only 6-24h per pair to complete with one appropriated high-RAM computer.

- The resulting children still required a macro filter at the end of the runs to fine tune the elimination of toxicities "surviving" the preferenced toxicity risk criteria

- Any further improvements in the toxicity risk will most probably be reflected on further yield improvements in non-toxic children

To best understand the EL selective process for fitnes, some questions still remain since it is unclear how weight calculations decide which raw children may be included into the fitting children list. For instance:

- Are the final toxicity risks altered by the rest of the criteria weights?.
- Do each of the weight criteria act independently?.
- Are toxicity, nasty functions and risks applied as filters to all molecules in the same cycle or one by one after been generated?.
- Would a mathematical formulation help to clarify these possibilities?.
- Is there any room for further improvement?

Thanks Thomas for your patience!!