Subject: Re: non-toxic Build Evolutionary Library
Posted by juliocoll on Sun, 08 Oct 2023 20:50:27 GMT
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In case any of you would be interested in finding more about possible docking applications for the Build Evolutionary Library, BEL of recent versions of Data Warrior,

BEL co-evolution criteria was comparatively applied as a preliminary attempt to improve putative control predictions of coagulation, antibiotics, cancer, diabetes, or fibrosis.

The report, included 9 protein targets (Vkorc1, FtsZ, Sglt1, Vegfr, Nkcc1, Hsp47, Sglt2, P2x3r, LolEC) ,their corresponding reference ligands (parents) and their corresponding dwar and pdb data files.
It can be found at:

https://chemrxiv.org/engage/chemrxiv/article-details/6512b16 2ade1178b2424c325

More fine-tunings still being cooked.....