
Subject: Re: Filter out nasty functions

Posted by [juliocoll](#) on Thu, 01 Jun 2023 07:40:00 GMT

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dear Norwick,

I am only using either drugs or natural products for the evolutionary libraries (EL). The criteria were only: docking scores (x4 relative weight), molecular weights between 400-500g/mol (x2) and $\log P < 3$ (x1). I am evolving different parents and pdb complexes from several biological systems: coronavirus, monkey-vaccinia, rodenticides, new antibiotics, collagen hsp, and other. That's all.

Thanks for the movie. GOOD IDEA!!!.

I will try to incorporate that method to the macro11 to avoid the need for the actual *.sdf manual elimination!

Just one more question:

Is it possible to save in a variable the number of rows at the bottom of the tables (Visible:... and Total:...)?

I am manually using those row numbers to easily differentiate *.dwar and *.sdf files from different experiments. It will be great to automatically save those number in the file name.

I would like also to automatically incorporate into the variable a short label for each experiment.

I need the EL *.sdf files to convert them to *.pdbqt for AutoDockVina for consensus with docking-scores in nM affinities.....

When getting a large number of different files it is confusing for me to keep track of all those files to avoid mistakes even using different directories. I usually have a lot of those!!!

Thank you for your attention!

sincerely

julio

Any ideas?