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Subject: Generating evolutionary library

Posted by [sublimeuser](#) on Wed, 17 Jul 2024 09:12:34 GMT

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Hello, everyone!

Would like to ask your advice on the following aspect: my aim is to generate a evolutionary library based on a starting compounds where at the end I will have roughly 1 million resulting compounds.

I want to use different fitness criteria (logP, logS and so on) while possibly protecting a certain portion of the parent compound that is known to be involved in binding.

Any suggestions on how I can convince DW to generate a more or less strict number of compounds using the Build Evolutionary Library functionality?

Many thanks!

sublime

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