
Subject: Re: Generating evolutionary library
Posted by [thomas](#) on Mon, 22 Jul 2024 14:45:04 GMT
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1 million compounds is a lot. If you run 1000 generations, let 20 compounds every generation, and do that 50 times (50 runs) then you will get about one million compounds, provided that your criteria are not very strict and allow that many different compounds in related generations.

Typically, with strict criteria, e.g. docking, 3D-superpositioning, or a chemical similarity, you should reach reasonably optimized compounds with much less compounds. If you aim for diverse, druglike compounds, creating random compounds may be the better solution...
