

---

Subject: Generating evolutionary library

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

[View Forum Message](#) <> [Reply to Message](#)

---

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

---

---

Subject: Re: Generating evolutionary library

Posted by [thomas](#) on Mon, 22 Jul 2024 14:45:04 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

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...

---