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Subject: Re: Macro for evolutionary library (EL) in Datwarrior (DW)

Posted by [nbehrnd](#) on Sat, 27 Aug 2022 15:20:41 GMT

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Dear Jon,

thanks to Thomas' new update of DW for Mac/Linux (packaged 2022-08-27 15:02), I generated a new (tiny) set of random molecules (file Random\_Molecules.dwar) used to record a toy macro (1to1.dwam) to loop over the first three entries of the molecule library, to pick one molecule at a time as 1st generation molecule of the evolutionary library. For now, only a computationally affordable criterion of fitness was set (molecular weight .lt. 400 g/mol).

When I let this macro work\*, it generates three individual evolutionary libraries. Instead of a set of multiple molecules, there is only one molecule as seed for this new collection.

Does this matches better your intent mentioned by August 9th? If this were the case, one could now reflect about further work along this direction; 1) about an approach which doesn't stop after the third cycle. And 2) instead of the current pick of seed molecules by structure to address the input by row number in Random\_Molecules.dwar.

Norwid

\*) DW 5.5.0 with the afternoon update 2022-08-27 15:02 in Linux Debian 12/bookworm. Both Random\_Molecules.dwar as well as the macro 1to1.dwam were in the same folder (Desktop) during the test run. The path for the new data deposits (here three lines), e.g.

```
fileName=/home/norwid/Desktop/Evolutionary_Library_01.dwar
```

in 1to1.dwam requires an update to your environment accessible.

### File Attachments

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- 1) [Random\\_Molecules.dwar](#), downloaded 244 times
  - 2) [1to1.dwam](#), downloaded 251 times
  - 3) [Evolutionary\\_Library\\_01.dwar](#), downloaded 222 times
  - 4) [Evolutionary\\_Library\\_02.dwar](#), downloaded 246 times
  - 5) [Evolutionary\\_Library\\_03.dwar](#), downloaded 223 times
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