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

Posted by [nbehrnd](#) on Tue, 09 Aug 2022 20:06:12 GMT

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Dear Jon,

when generating an evolutionary library, DataWarrior offers (at least) twice to use a set of molecules from a .sdf or a .dwar as reference; in the screen photo below, they are marked by (A) and (B).

Should your question be understood in lines of «instead of molecules of an (of one) EL to be similar enough to a set of e.g., 20 molecules defined in box A, you would rather generate 20 EL where each of these reference molecules is a unique seed for an individual EL (more like an iteration)»?

Anyway, a .dwar and macro .dwam to represent a minimal working example (even if it currently stops after the first molecule of reference) to complement your question would be welcomed.

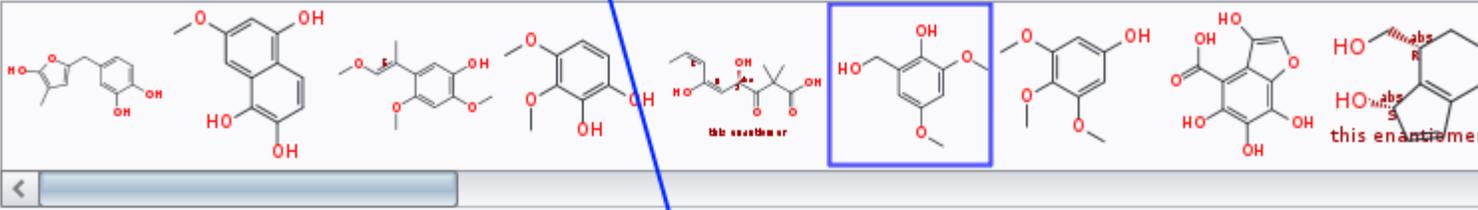
Norwid

File Attachments

1) [2022-08-09_clarifying_question.png](#), downloaded 1482 times

Build Evolutionary Library

1st generation: **Random structures** (Selected sub-structures are kept untouched)



automatic Generations Create compounds like **Natural products**

128 Compounds per generation

8 Compounds survive a generation Total run count: 1

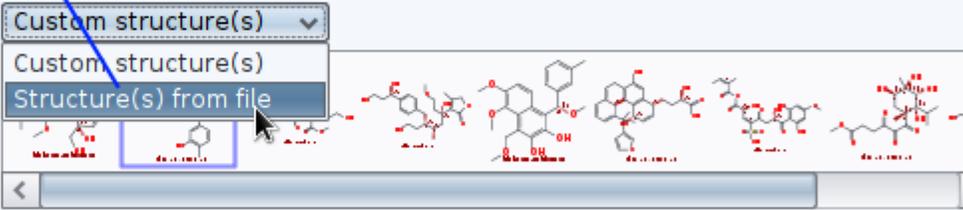
Fitness Criteria **Add Criterion ->** **Structural (dis)similarity**

Create molecules similar to any **Custom structure(s)**

Descriptor used: **SkelSpheres**

Weight: 1.0 0.25 1.0 4.0

Custom structure(s)
Custom structure(s)
Structure(s) from file



Help Cancel OK