Subject: Re: Generating derivatives of parent structure
Posted by thomas on Fri, 08 Dec 2023 23:42:10 GMT
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You could also use the "Build Evolutionary Library..." functionality. This creates new molecules from a starting generation by random small modifications. You can also define parts of the molecule that shall not be modifed by just selecting it. I tried that with your molecule and selected all but 4 ring positions. This causes random modifications at all selected atoms, which includes ring cleavages.

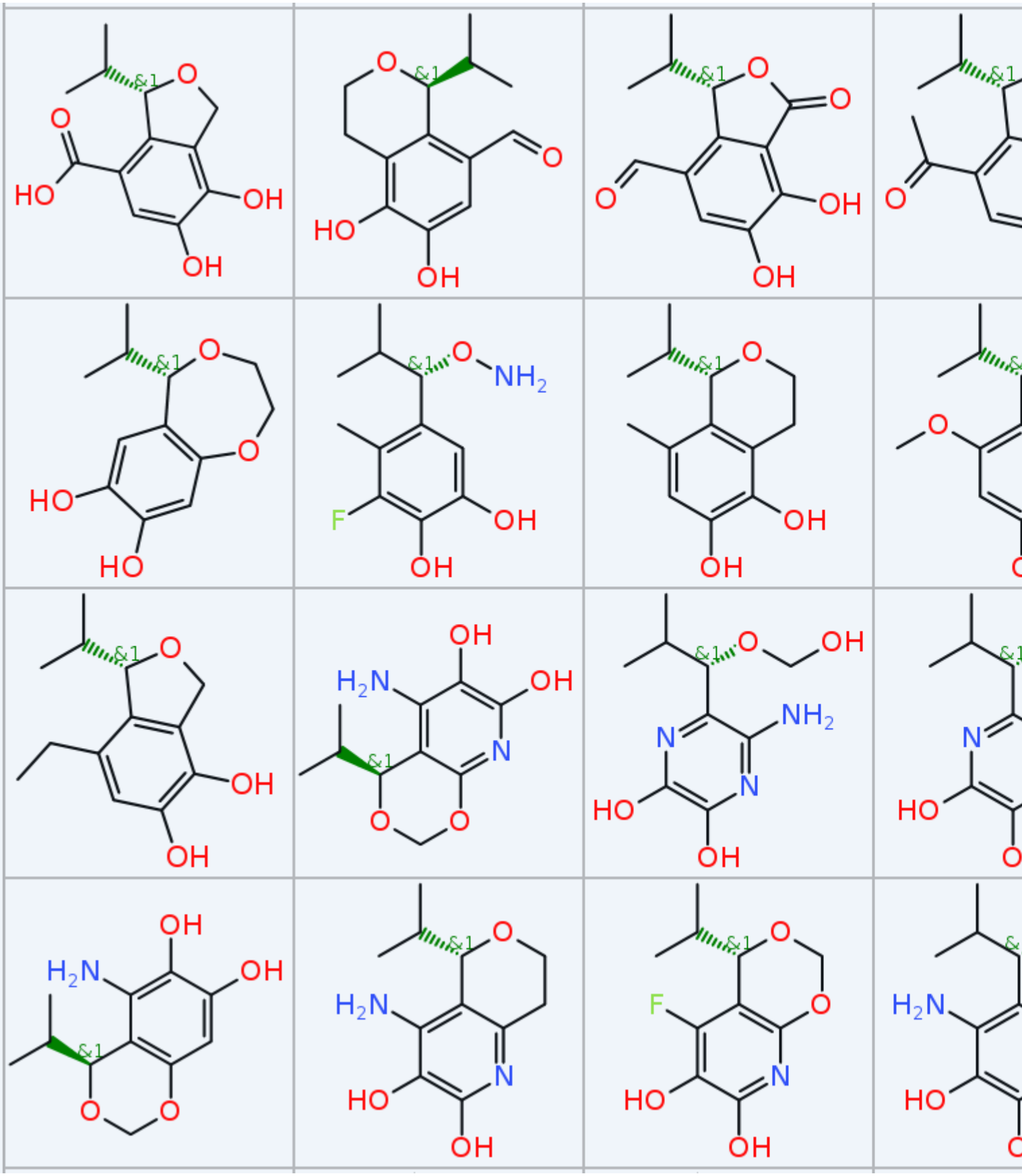
Then you are supposed to add fitness criteria, which are used to value the quality of created structures. Those structures, that match your criteria best will be kept and form at the same time the parent generation for the next round of random changes. I just defined a simple criterion: the molecular weight shall be not higher than 240. Otherwise I just use default options for everything else. The settings look like this:

In less than one second DataWarrior created 267 different molecules in 15 generations that all contain the selected (red) part of your defined starting structure, with lots of variations regarding substitution, ring size, partially open ring structures and molecular weights always below 240. The picture shows a small subset.

Of course, you can be more specific with fitness criteria, e.g. use chemical similarities, pharmacophore similaries or even a docking score...

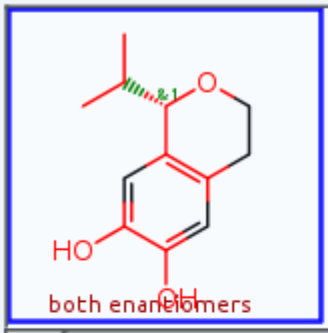
File Attachments

1) temp2.png, downloaded 1274 times



2) temp1.png, downloaded 1396 times

Root generation compounds: Default



(Select sub-structures to protect

automatic Cycle

128 Compounds per cycle

8 Compounds survive a cycle

Fitness Criteria

Prefer 'Molecular weight' >= and <= 240