Subject: thresholds and weights of toxicity risk
Posted by nbehrnd on Tue, 22 Aug 2023 15:45:36 GMT
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Dear Thomas,

the generation of evolutionary libraries can be restrained by fitness criterion «toxicity risk». Based on some preliminary tests, I have difficulties to comprehend the thresholds available. Departing from «nasty functions» as one of DW's calculated properties, one could assume DW counts functional groups. The suggested default is 2, an integer. Then, choosing a toxicity risk less or equal to zero would render the restraint a constraint.

Interestingly, however, DataWarrior equally permits to enter an upper threshold as a real/floating number (a negative one like `-1.23` does not hinder DW to work either).

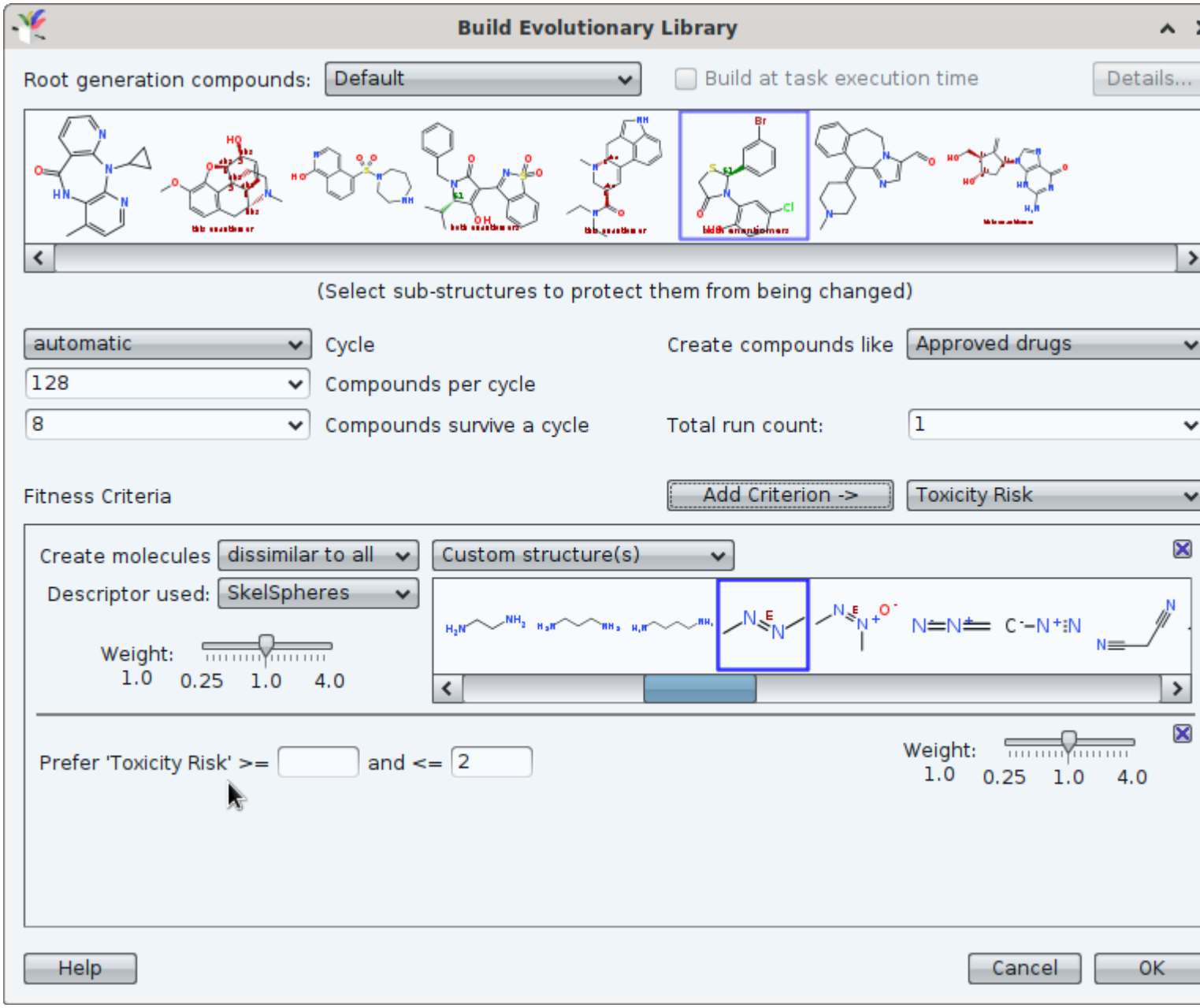
Can you please share some insight how to engage well these thresholds? Do the weights act on a linear penalty scale to provide the fitness criterion greater influence on the overall fitness of the molecules suggested? (DW's internal documentation (via F1) includes the string «toxicity» only once.)

Best regards,

Norwid

File Attachments

1) toxicity_risk.png, downloaded 425 times


Build Evolutionary Library
Root generation compounds:
Default
Build at task execution time
Details...
(Select sub-structures to protect them from being changed)
automatic
Cycle
Create compounds like
Approved drugs
128
Compounds per cycle
8
Compounds survive a cycle
Total run count:
1
Fitness Criteria
Add Criterion ->
Toxicity Risk
Create molecules
dissimilar to all
Custom structure(s)
Descriptor used:
SkelSpheres
Weight:
1.0
0.25
1.0
4.0
Prefer 'Toxicity Risk' >=
and <=
2
Weight:
1.0
0.25
1.0
4.0
Help
Cancel
OK