Subject: Filter out nasty functions
Posted by juliocoll on Sat, 13 May 2023 08:51:33 GMT
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dear Thomas
I am trying to design a filter for large tables of docked chemicals that, among other things, would automatically select for all toxic to eliminate them from the final table.

The partial macro looks like this:

<task name="calculateCompoundProperties">
propertyList=mutagenic tumorigenic reproEffective irritant nasty
structureColumn=Structure
</task>
<task name="changeCategoryFilter">
column=Mutagenic
settings=high low
duplicate=1
</task>
<task name="changeCategoryFilter">
column=Tumorigenic
settings=high low
duplicate=1
</task>
<task name="changeCategoryFilter">
column=Reproductive Effective
settings=high low
duplicate=1
</task>
<task name="changeCategoryFilter">
column=Irritant
settings=high low
duplicate=1
</task>
<task name="changeCategoryFilter">
column=Nasty Functions
settings=<multiple categories>
duplicate=1
</task>

The macro works well except for the nasty.
Despite using the <multiple categories>, the chemicals with "simultaneous nasties" per molecule were not removed.
For instance, the
Nc1c([C@@H](CC(C2=CNC(Nc3ccccc3)=CC2=O)=O)C(C(O[C@@H]2[C@@H]3CCCC2)=O)=C3O)cccc1 molecule predicted a double "nasty" like "polar activated DB; twice activated DB" but it was not removed among other 5434 molecules.

They may be not too many, but it would be better to remove any of those possible cases.
should those names be included at the settings?
That could be an enormous number of dual or perhaps nth number of possibilities!! 8o

Is there any other alternative code solution?

thanks for your attention
julio