Subject: Re: Category Filter logic
Posted by nbehrnd on Mon, 04 Sep 2023 19:36:57 GMT
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Dear Javier,

the program's internal documentation, chapter «working with data» briefly describes
`chemsim(descriptor, idcode)` and `chemsim(descriptor1, descriptor2)` as if one could run build a
new column of computed (Boolean) values line of
`chemsim(PP3DMM2_of_Structure,"gFx@@eJf`@@@")` «check if column
PP3DMM2_of_Structure contains the 3D motif of pyridine. I'm not aware if there either is a
sketcher/converter to yield the DW's (2D) idcodes other than by access of a .dwar file with a text
editor, or if/how e.g., a SMILES/SMARTS string could serve for a (sub) structure search.
(Possibly, «descriptor» refers to the ones via Chemistry -> From Chemical Structure ->
Calculate Descriptor.) Once identified, an extension to logical .and. and .or. would a next
consequent step.

Norwid