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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

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