Subject: Re: Category Filter logic Posted by nbehrnd on Mon, 04 Sep 2023 19:36:57 GMT View Forum Message <> Reply to Message

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