Subject: Re: How to perform general R group searches in DW
Posted by nbehrnd on Tue, 11 Jan 2022 06:06:19 GMT
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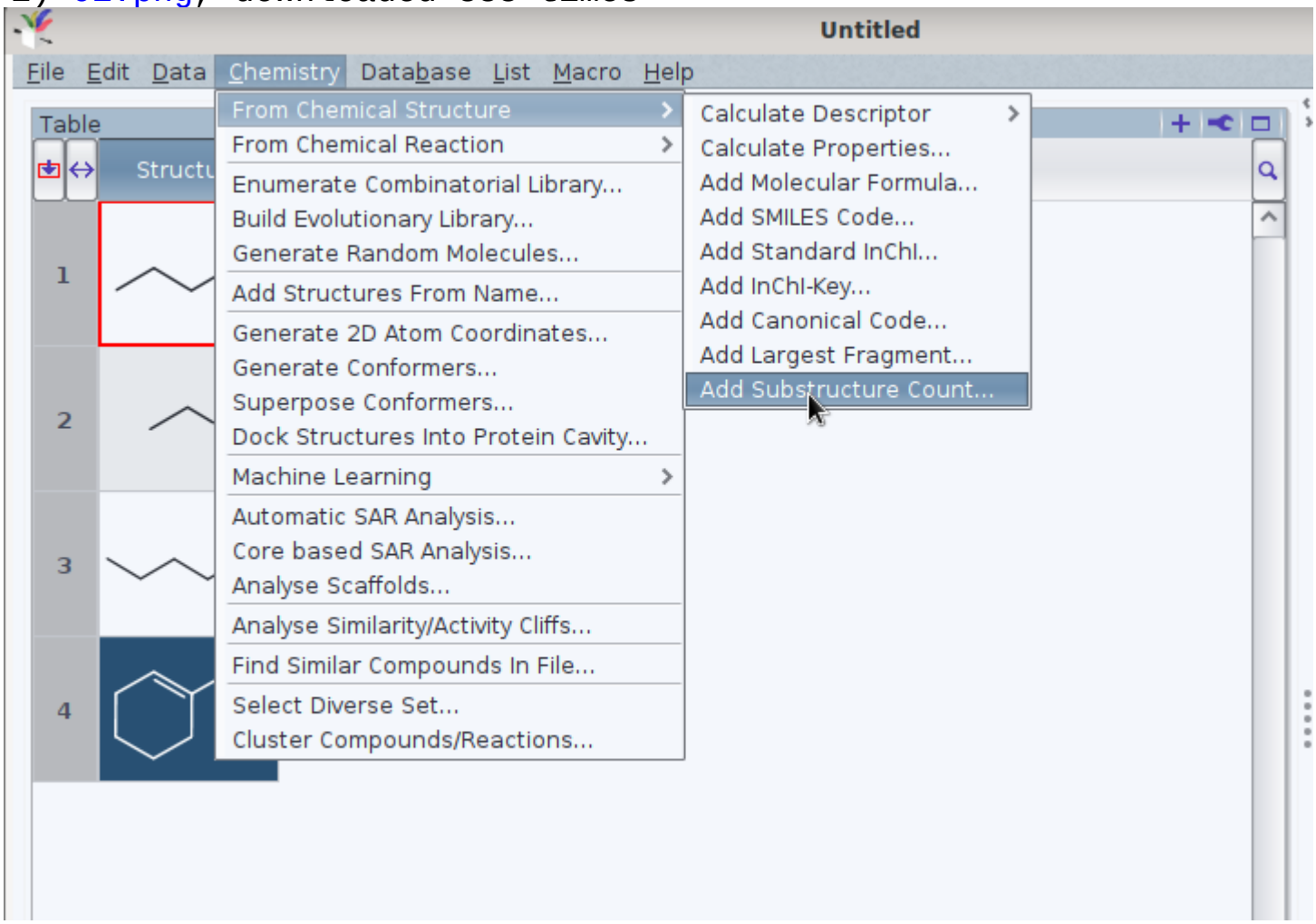
Dear JonW,

at least the nightly-builds version of DW contains a function to define a substructure query. Follow Chemistry -> From Chemical Structure -> Add Substructure Count to open a new instance of the sketcher, and decide in favour/against the criterion of overlapping substructure matches. In the matrix view, you obtain a new column with the number of occurrences of the pattern; at the right hand side, there will be a new slide ruler to filter the display. By substructure, one may define queries permitting more than one atom type on one site, too:

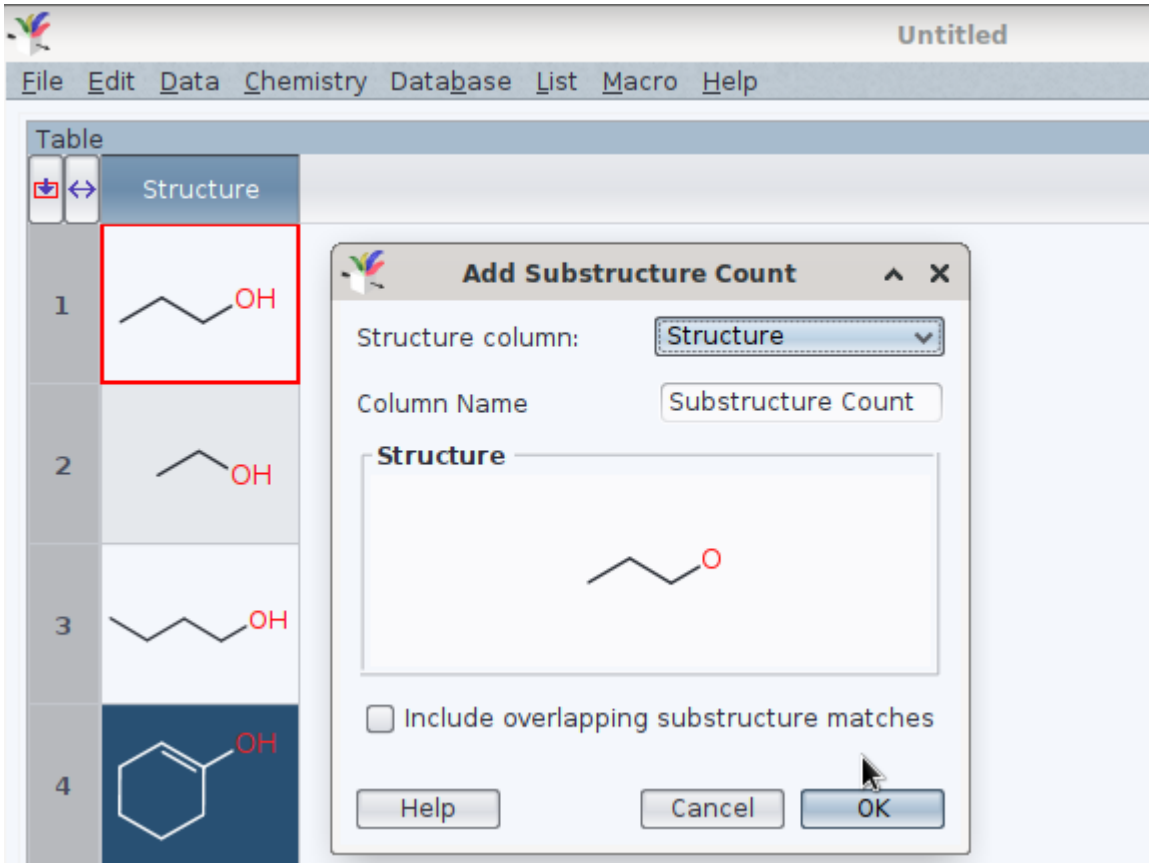
Norwid

File Attachments

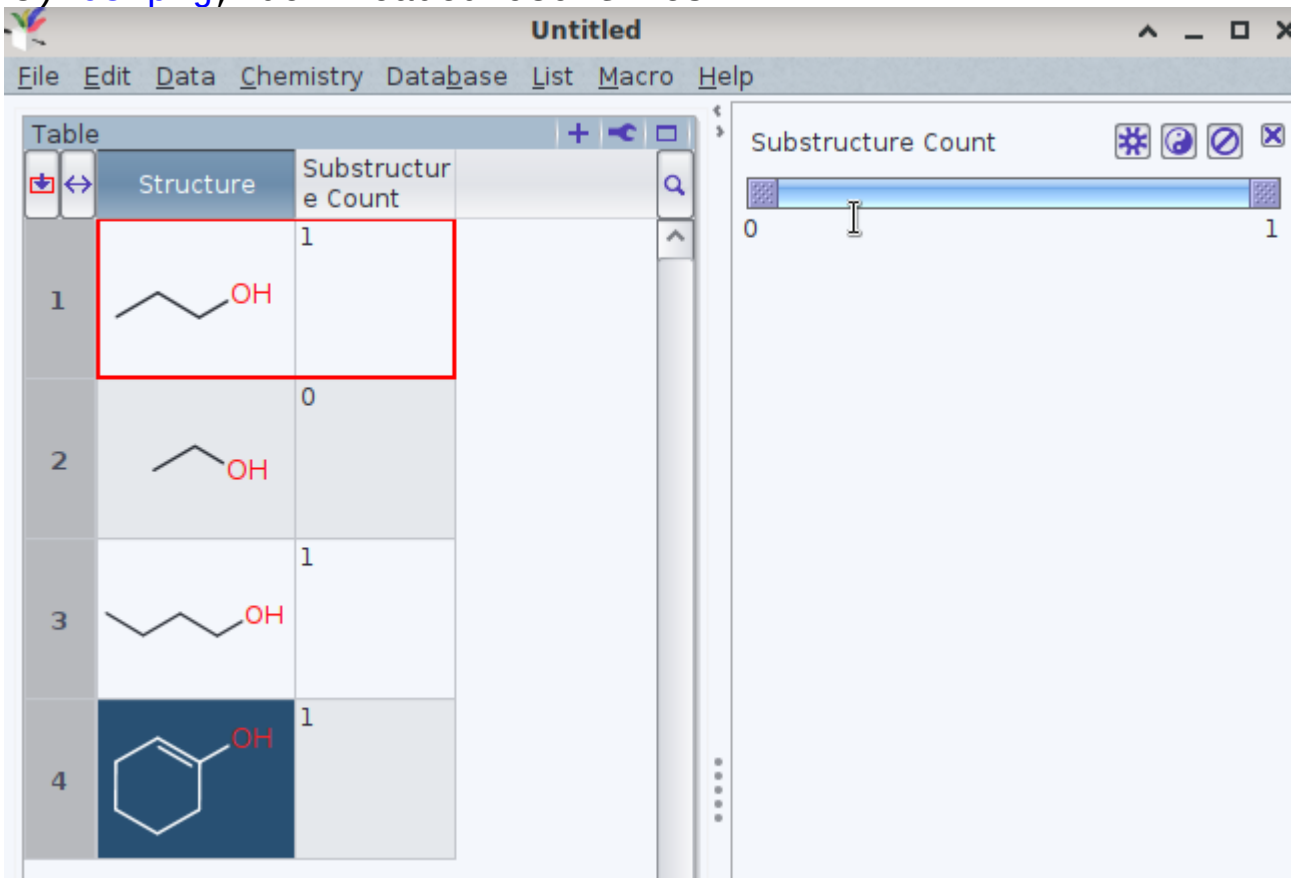
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4) 04.png, downloaded 1717 times

