Subject: How to perform general R group searches in DW
Posted by Jo W on Tue, 28 Dec 2021 14:49:52 GMT
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In the Chemical Editor Concepts section of the online manual, the instructions state to use "?" when using specify an unusual/custom atom label, a specific isotop, an abnormal valence and/or a radical state. when drawing a structure in the strcture editor.

However, when I type"R" to specify any group / atom and then do a substructure search in the dataset or via chembl, no structures are returned. So this is obviously the wrong command/label. I have searched the manual and the forums but can't find the answer.

So for example, if you wanted to search for a series of alkane alcohols in a dataset. How do you create:
R-CH2OH as opposed to tediously searching for CH3CH2OH, CH3CH2CH2OH

Also how do you search using two different R groups at the same time within the molecule?
e.g., R1-CH2O-R2
Many thanks