
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 isotope, an abnormal valence and/or a radical state. when drawing a structure in the structure 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
