Subject: Re: How to perform general R group searches in DW
Posted by thomas on Tue, 11 Jan 2022 15:41:44 GMT
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DataWarrior uses an atom table derived from MDL's original when defining the Molfile format. This table contains R, R1 till R16, A, the amino acids, e.g. 'Ala' and a few others as pseudo atoms. Therefore, you can use these labels, but there is no logic behind them. If a Chembl molecule would contain an R as pseudo atom, you could find it with a substructure search.

You could use the following substructure definintion to exclusively find alkyl alcohols:

This is a C-O with the carbon defined to have no pi electrons and the oxygen set to have no further non-H neighbour. Then there are to exclude groups:

1) The '!C' is an ANY atom except carbon. This prevents any matches to molecules with non-carbon atoms in addiction to the required OH.

2) A C=C double bond to prevent double bonds anywhere. Actually this is not quite correct. Better would a carbon atom with 'at least one pi-electron' as exclude group.

Two R-groups at an otherwise specified molecules could be done analogously.

File Attachments

1) t.png, downloaded 1548 times

