
Subject: Re: Search for "any atom" in structure editor
Posted by [rkp@23](#) on Fri, 28 Apr 2023 19:37:36 GMT
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I am new to Datawarrior and I have a similar question.

I am trying to understand the difference between a molecule and a query.
I am trying to search ChemBL database using the feature "similar structures to"
While doing that , I tried to draw using the structure editor, a query molecule, with any R group attached to a halide.

In the first try, it allows me to change the atom properties. But if I want to further do any changes, selecting lasso tool and double clicking it, select the entire molecule and not a particular atom.

I am trying to understand how to define a molecule as a molecule with a query feature as opposed to just a molecule.

is there a way to define a structure as a query in DataWarrior?
I could not find a clear explanation of this in the documentation, except that in the Lasso tool section, its written that if not a query, the entire molecule will be selected and no "Atom Properties" dialog will open.

Please help!
