Subject: Re: Search for "any atom" in structure editor
Posted by thomas on Sat, 29 Apr 2023 11:50:14 GMT
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DataWarrior distinguishes molecules from substructure queries:

Molecules are considered atom-complete except for plain hydrogen atoms, which typically are not drawn. Any open valences of a molecule are implicitly considered to be filled by hydrogen atoms. Molecule atoms or bonds cannot carry query features. The structure editor, when editing queries for similar or exact molecule search, is in 'molecule mode'. Therefore, you cannot add query features and implicit hydrogens are shown on hetero atoms.

Substructure queries are atom-incomplete, which means that open atom valences are NOT considered to be filled by hydrogen atoms. They allow query features on atoms and bonds that narrow or broaden the meaning of the drawn atom/bond, e.g. require it to be in an aromatic ring, or allow an atom to be either N,O,S or a bond to be either single or double. In addition, one can define attachment groups, which are not allowed at a particular position ('exclude groups').

Details are explained in the "Help->Chemical Structures->The Structure Filter"; scoll down to 'Substructure Search'...