Subject: Re: Search for "any atom" in structure editor
Posted by thomas on Wed, 13 Jul 2022 20:30:35 GMT
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The key is to use the lasso tool. If you edit a substructure (as opposed to a molecule, which does not support query features), then you can select the lasso tool and double click an atom (or one of multiple selected atoms) to open the atom query feature dialog. Here you define your example cases as follows:
- "any atom": first checkbox in the dialog is 'Any atomic number'
- "either carbon or nitrogen": type 'N,C' in the 'Allowed Atoms' field
- "not a carbon": select 'Any atomic number' and type 'C' in 'Excluded Atoms' field

This works in all places that allow you to edit substructures, e.g. reaction in combinatorial enumeration, 2D-coordinate generation, etc.