Subject: Re: C=C double bonds/search by extended stereochemistry
Posted by thomas on Tue, 11 Jan 2022 15:12:52 GMT
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Dear Norwid,

sorry for the long delay. I somehow missed your question. As default DataWarrior does not match the stereo configuration of atoms or bonds on the substructure search. You may, however, require for individual atoms or bonds a stereo configuration match. In the editor select the lasso tool and double click an atom or bond. In the dialog that opens, you can select 'Match Stereo Configuration'. Then DataWarrior uses the 'Enhanced Stereo Representation' rules defined by MDL many years ago, e.g. a racemic center in the query matches a racemic, OR, and pure R- or S-center. An explicit R in the query only matches a pure R. For stereo bonds you cannot select 'Match Stereo' for cross bonds, which is in-line with the atom-logic, because an unknown configuration always matches all better specified configurations in the MDL logic. This means you can directly search for E- and Z-bonds, but not for unspecified (cross). You could, however, do that with two individual inverted filters, i.e. excluding E- and excluding Z-.