Subject: Stereochemistry of double bonds
Posted by luecking70 on Wed, 17 Jun 2020 10:51:28 GMT
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Dear all,

is it possible to define the stereochemistry of double bonds in substructure searches, e.g.when filtering results from an HTS ?

Best

Subject: Re: Stereochemistry of double bonds
Posted by thomas on Sat, 20 Jun 2020 10:58:06 GMT
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in principal this can be done in the substructure editor: with the lasso tool double click a double bond. The bond query feature dialog opens, which lets you select 'Match stereo configuration'. However, it seems that the stereo match is not applied for double bonds, which are part of a small ring (7 or less members). I will look into that...

Thomas

Subject: Re: Stereochemistry of double bonds
Posted by thomas on Sun, 21 Jun 2020 12:17:18 GMT
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Double bond configuration matching in substructure searches now also works, if the double bond is found as part of a small ring. The current development version includes this change.