Subject: Re: Substructure search and stereochemistry
Posted by thomas on Sat, 27 May 2017 13:46:41 GMT
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Hi Andrew,

the default for substructure searches with stereo centers is to match all configurations. In order to find one enantiomer only, you need to set the query feature 'match stereo center' for the those stereo centers you intend to match. For that you select the lasso tool in the editor and double click a stereo center. The query feature dialg opens and lets you define query features.

For stereo center matching DataWarrior works as originally suggested by MDL, when they explained their concept of 'Enhanced Stereo Representation': an absolute configuration in the query matches only that configuration. An racemic configuration in the query matches racemic, but also both absolute configurations. That means a less specific query also matches more specific configurations in searched molecules.

Concerning HTTPS: I is since some time on my agenda, but it is a matter of priorities. DataWarrior downloads are already HTTPS, because they use dropbox. For me this was the most important point.

Best wishes, Thomas