Subject: Substructure search and stereochemistry
Posted by Andrew0 on Tue, 09 May 2017 14:42:13 GMT
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Hi Thomas,

I recently ran into an issue while performing substructure searches using DataWarrior's filtering tools. If you search for a specific enantiomer, the result will return both the stereochemistry you were looking for AND its enantiomer, assuming one exists in the file.

It's possible that this is a user error as well and there is some search parameter I am missing. For your convenience, I have attached a very simple file with only three molecules. If you paste one of the chiral molecules into the search box, it does filter out benzene, but not the other chiral molecule.

One other note - I'm not sure how difficult it is, but it would be great if you supported https on your website!

Thank you so much for your continued work on this tool!

Best regards,
Andrew

File Attachments
1) enantiomers.dwar, downloaded 1097 times

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

Subject: Re: Substructure search and stereochemistry
Posted by Andrew0 on Wed, 03 Jan 2018 20:27:22 GMT
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Thomas,

Thanks for the explanation of stereo searching - that was a subtlety that I hadn't run into before.

Cheers,
Andrew
