
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 678 times
