
Subject: Exclude function in the structure filter does not work with 2 exclude groups
Posted by [Xavien](#) on Sun, 27 Oct 2019 23:53:49 GMT

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Hello forum,

I am not sure if I should post this in the bug reports or just in the functionality subforum but I have the following problem.

I have a database of around 1800 molecules and I try to specifically look for amines while filtering out alpha and beta amino acids. In the structure filter search I tried excluding -R(N,O,S) and =O as this would indicate a carboxyl group or carboxyl derivatives.

The problem is that it still shows amino acids after I used the filter with the exclude groups. I suspect it has to do with trying to use two exclude groups as there is no problem if I want to exclude a single group.

Subject: Re: Exclude function in the structure filter does not work with 2 exclude groups

Posted by [thomas](#) on Mon, 28 Oct 2019 21:03:49 GMT

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Good question. The exclude group logic was indeed not very intuitive in version 5.0.0. If atoms of two independent groups were marked as exclude group (e.g. as in the image below), then they were still considered as one group. Thus, an initial substructure match was refused only, if all exclude atoms were found extending the match of the non-exclude atoms.

Recently the handling was updated, such that if at least one of multiple disconnected exclude groups is found, then the substructure match is not considered a match anymore. In the example below the nitrogen atom is considered a match only, if it is neither part of an alpha-, nor a beta-amino-acid-derivative.

An official update is due around the end of the year, but beta-updates are available now: openmolecules.org/datawarrior/dw500win.zip (for Windows) and [dw500x.zip](http://openmolecules.org/datawarrior/dw500x.zip) (for Linux and Mac).

File Attachments

1) [Screenshot from 2019-10-28 21-48-37.png](#), downloaded 805 times
