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
View Forum Message <> Reply to Message

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 molceules and I try to specificall look for amines while filtering out alpha and beta aminoacids. In the structure filter search I tried exluding -R(N,O,S) and =O as this would indicate a carboxylgroup or carboxyl derivatives.
The problem is that it still shows aminoacids 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
View Forum Message <> Reply to Message

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 (for Linux and Mac).

File Attachments

1) Screenshot from 2019-10-28 21-48-37.png, downloaded 697 times