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 (for Linux and Mac).

File Attachments

1) Screenshot from 2019-10-28 21-48-37.png, downloaded 1401 times

