
Subject: Re: Filter out nasty functions

Posted by [nbehrnd](#) on Tue, 13 Jun 2023 19:33:02 GMT

[View Forum Message](#) <> [Reply to Message](#)

Dear Julio,

postscript to what DW considers a nasty (organic) function: DW builds on openchemlib,[1] a relevant part of it is `NastyFunctionDetector.java`. [2] With varying success one can recover a structure scheme (encoded in the idcode [A-Z, a-z, @, tilde, accent grave and circumflexe, backslash; no numbers] which is enclosed in double quotes) by copy-paste into DataWarrior's sketcher. Because sometimes the recovery failed (e.g., entry oxirane/aziridine), I enclose both the file in question, as well as the .dwar retaining the original description about this set of 50 motifs.

Sincerely,

Norwid

[1] <https://github.com/Actelion/openchemlib>

[2] <https://github.com/Actelion/openchemlib/blob/master/src/main/java/com/actelion/research/chem/NastyFunctionDetector.java>

File Attachments

1) [nasty.dwar](#), downloaded 241 times

2) [NastyFunctionDetector.java](#), downloaded 266 times
