Subject: Re: Filter out nasty functions

Posted by nbehrnd on Tue, 13 Jun 2023 19:33:02 GMT

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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 circonflexe, 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 461 times
- 2) NastyFunctionDetector.java, downloaded 467 times