Subject: Re: nasty functions not activated in 4.4.4
Posted by arofab on Fri, 17 Mar 2017 09:09:02 GMT

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Hello,
I can confirm that "Nasty Functions" compound properties processing also fails in newest 4.5.1 version.
It stopped working since 4.4.4 version (in version 4.4.3 it worked).

Looking at the source code, the error seems to be related to the "twice activated DB" function. By commenting out the corresponding line in com.actelion.research.chem.NastyFunctionDetector class, the calculation succeeds (obviously excluding "twice activated DB" detection).