Subject: nasty functions not activated in 4.4.4
Posted by dataviz on Sun, 05 Feb 2017 13:16:40 GMT
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Hello
it looks in version 4.4.4 that the search for nasty functions is not activated. The message seen in the column is: initialization error
many thanks

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).

Subject: Re: nasty functions not activated in 4.4.4
Posted by thomas on Tue, 21 Mar 2017 19:43:19 GMT
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Dear dataviz and arofab,

sorry, I notized your first message to late for version 4.5.1. In today's update 4.5.2 this issue is fixed.

Thanks for reporting,

Thomas