
Subject: nasty functions not activated in 4.4.4
Posted by [dataviz](#) on Sun, 05 Feb 2017 13:16:40 GMT
[View Forum Message](#) <> [Reply to Message](#)

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

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

Dear dataviz and arofab,

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

Thanks for reporting,

Thomas
