Subject: Uncaught Exception:/ by zero error when using structure view.
Posted by timritchie on Mon, 23 Mar 2020 17:03:05 GMT
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Hello,

I've noticed a lot of uncaught exception errors with the new version, particularly when using the structure view. There is no option but to force close DW and reopen it.

Also on occasion, changing the number of horizontal structure count does not work. It is necessary to set the count to 1, and then change it to the desired value.

Regards,

Tim Ritchie.

Subject: Re: Uncaught Exception:/ by zero error when using structure view.
Posted by thomas on Tue, 24 Mar 2020 15:48:53 GMT
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Hi Tim,

I cannot reproduce this. Possibly, the errors are not related to the view itself, but to the structures displayed. It would be very helpful to get a small file that allows to reproduce the problem.

Best wishes, Thomas

Subject: Re: Uncaught Exception:/ by zero error when using structure view.
Posted by ignjat.filipovic on Thu, 21 May 2020 09:02:39 GMT
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Hello, Thomas

Currently, I am having this problem too.

When I mouse over certain structures this error message pops up. If it would pop up only once, it (probably) wouldn't be a problem but it pops up every time!

Version of DataWarrior is 5.2.1, and I'm using it on Windows 10.

I have noticed and replicated this problem while mousing over (almost) any structure that contains copper in NCI-open database(You can download it from "NCI database Download Page" for witch I will post link in next post).

I would extract problematic data to make it easier for you to troubleshoot but program prevents me

from saving due to this exact error.

Best regards!

Subject: Re: Uncaught Exception:/ by zero error when using structure view.
Posted by thomas on Thu, 21 May 2020 10:19:56 GMT
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Hello Ignjat(?,

thank you for the hint. I have downloaded the NCI database and could reproduce the error with version 5.2.1 on Linux. Luckily, this has already been fixed in the current source code. You may download a patch from openmolecules.org/datawarrior/dw521win.zip. You need to unpack and replace the original files with the files you get from the archive. Linux/Mac users need to download openmolecules.org/datawarrior/dw521x.zip. This version contains fixes and new features, but some are not thoroughly tested or documented. It is updated about weekly and typically the newest patch is better than any one before.

Thomas

Subject: Re: Uncaught Exception:/ by zero error when using structure view.
Posted by ignjat.filipovic on Thu, 21 May 2020 10:56:22 GMT
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Thank you Thomas for your very quick response!

I have downloaded and replaced files, but the error persists!
It wasn't mentioned but it doesn't matter where you mouse over, it happens in both 2d and 3d plot view too.

I am not sure, but at least it feels like it creates less error messages now.
I'll dump here few molecule names from NIC database for witch it interrupts, in case that those might help you:
181100
262139
265309
293938
311999
405713
517954

527325
666270

Thank you once again!
Sincerely, Ignjat F.

Subject: Re: Uncaught Exception:/ by zero error when using structure view.
Posted by zhentg on Mon, 29 Jun 2020 06:52:02 GMT
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Hi Ignjat and Thomas,

I've observed similar "uncaught Exception" with DWv5.2.1 on Win10.
The error occurs mostly after I use "Activity Cliff".
Today I updated the DW executable, and it seems the error did not occur so far.

My JRE is 1.8.0_251-b08, 64bit.

Subject: Re: Uncaught Exception:/ by zero error when using structure view.
Posted by thomas on Thu, 09 Jul 2020 21:32:11 GMT
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Hi Ignjat,

thank you for being persistent. In addition to the issues already fixed, there were unexpected atoms (e.g. 'R') in the dataset with atoms beyond the limits of the periodic table, which caused the problems. Now these are translated into carbons, which at least solves this issue.

Thomas
