Subject: uncaught exception - diverse set
Posted by sp13 on Tue, 23 Apr 2019 13:06:52 GMT
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Hi Thomas,

When I try to pick a diverse set of compounds based on FragFp I get the following error:
"uncaught exception J cannot be cast to ["
The rest of the message is cut off.

Notably, I only get this error when using Datawarrior 5.0.0. I uninstalled the latest version and re-installed 4.7.3 and do not have a problem.

Windows 10

Subject: Re: uncaught exception - diverse set
Posted by thomas on Thu, 25 Apr 2019 07:48:41 GMT
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Hi sp13,

thank you for reporting this. For version 5.0.0 I had updated the fingerprint descriptors from int to long (32 to 64 bit integers), which was not done properly in the code of the diversity selection, which till now I was not aware of. I have fixed the issue and provide update files under the usual links: You may download updated exe/jar files for Windows and OSX&Linux under these links: openmolecules.org/datawarrior/dw500win.zip and dw500x.zip, respectively. Just unpack the respective zip file for your OS and move the files it contains into your installation folder, where they should replace the original files.

Thomas