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 View Forum Message <> Reply to Message

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**