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Subject: Re: Why is clustering limited up to 10000 molecules?

Posted by [thomas](#) on Thu, 03 Mar 2016 20:49:57 GMT

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Dear Nikita, the current DataWarrior version is limited to 10.000 compounds. For 100.000 compounds the current algorithm would need 20GB of memory and many hours to finish. The only way to do it would be to patch the datawarrior.jar file (OSX or Linux only) or to change the source code and to recompile.

Regards, Thomas

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