Subject: Re: Why is clustering limited up to 10000 molecules?
Posted by thomas on Thu, 30 Mar 2017 18:35:00 GMT

Hi Dataviz,

I have lifted the limit from 10.000 to 100.000 structures, but display a warning above 20.000 compounds. Nevertheless, clustering of significantly more structures than 20.000 will require a Linux or Macintosh computer, where it is easy to increase the memory maximum that DataWarrior is allowed to use. The change will be available with the next update.

Regards, Thomas