Subject: Re: Out of memory Posted by thomas on Mon, 17 Mar 2025 19:52:18 GMT

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25'000 Molecules is a rather small file. I am astonished. Do you have hundreds of columns? I just ran a UMAP from SkelSpheres (the largest of the vector descriptors) with 250'000 molecules, which also worked fine with just a few GB of -Xmx.

Which version and which OS do you use? On all platforms except Windows you can increase the -Xmx setting easily.