Subject: Re: Why is clustering limited up to 10000 molecules?
Posted by avkitex on Thu, 03 Mar 2016 20:54:28 GMT

Dear, Thomas

I have servers with about 30Gb ram and a lot of time. And I woult like to try doing it.
Can you tell me how to patch and recompile jar file? And what is the best way to run it in console mode? (I have molecules in sdf or mol2 format. I would like to have a clusterisation tree in newick or compatable format.)

Looking forward to hear from you.

Best,
Nikita