Subject: Why is clustering limited up to 10000 molecules?
Posted by Nastasia on Wed, 22 Jul 2015 14:37:15 GMT

I am trying to cluster my molecules, but the number of my molecules is far beyond 10000, actually it's about 50000. However, there are some duplicate molecules, which may be joined, but when I do that I loose my different descriptors important for each case, as they are just merged into some multiple group. Is it possible to increase the size for clusters?