Subject: Capacity
Posted by laosoriom on Thu, 30 Aug 2018 15:40:21 GMT
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I'm working with Datawarrior and I need to know why I do not load a similarity matrix with a tanimote coefficient for 100 molecules, is there a limit of columns or rows? How can I visualize the results?

Subject: Re: Capacity
Posted by thomas on Thu, 30 Aug 2018 21:35:46 GMT
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I don't understand exactly what you try to perform. The closest thing to calculating a tanimoto similarity matrix is to open one file and then to run 'Find Similar Compounds in File..." from the Chemistry menu. Then select the same file again and check 'Save similar compound pairs to file', then press OK. DataWarrior then writes a new file with all compound pairs of the matrix and their similarity into a new file. The only size limitation is the amount of memory that you give the program. 100x100 should never be a problem. Opening a text file with 100 by 100 entries should also not be a problem. Maybe there is something strange with the file. You may send me a copy of it and I give it a quick check in the debugger...

Thomas