Subject: Re: Comparing Structure Files
Posted by nbehrnd on Tue, 08 Mar 2022 22:06:30 GMT
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Dear Olivier,

after accepting the disclaimer on the download page[1], an additional text box is visible with links for either an installation in Linux and Mac,[2] or for the Windows operating system.[3] These archives contain only the .jar of ongoing development of DataWarrior you substitute in an already existing installation.

So far, DataWarrior's identification of similar/identical molecules in two sets of molecules worked best for me be when starting with two .dwar containing only the structures of either set without any further computed data. Then, there was no ambiguity in selecting the column in question when running an instance with one set and reaching out for the other set to compare with by Chemistry -> Find Similar Compounds In File. It is dissimilar to a copy-paste of structures of one .dwar into an other .dwar; in parlance of DataWarrior append data (without header).

Norwid

[1] https://openmolecules.org/datawarrior/download.html
[2] https://openmolecules.org/datawarrior/dw550x.zip
[3] https://openmolecules.org/datawarrior/dw550win.zip