Subject: compare datatets
Posted by david.l on Fri, 19 Aug 2016 13:00:05 GMT
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Dear users,
I would like to compare at least two datasets in order to visualize their chemical space (3D or 2D) according to descriptors used to display it. Is this possible in Datawarrior?
Best regards
David

Subject: Re: compare datatets
Posted by thomas on Sat, 20 Aug 2016 23:01:51 GMT
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With the Append File function you may combine two or more files into one.
You can configure this such that a new column contains the name of the original datasets.

Then you may run a PCA, create a SOM or (which I would prefer) do a similarity analysis (best with the SkeletonSpheres descriptor, which should create before starting the analysis).
In any case you get a 2D- or 3D-view (the latter in the PCA case) where you may color markers by dataset name. This way you visualize how the original datasets cluster in the combined chemical
space.

Hope this helps,

Thomas