Subject: Re: Exporting a descriptor as a Textfile
Posted by thomas on Thu, 02 Jun 2022 07:46:22 GMT
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Hi Christoph,

if you use Java, you could use this line to decode the SkeletonSpheres descriptor into a byte array, which contains 1024 count values:

byte[] counts = new DescriptorHandlerSkeletonSpheres().decode(encodedSkeletonSph eres);

Then you could loop over the counts array and write numbers where ever you want. The only dependency would be OpenChemLib, which you can find on GitHub.

Likewise you can decode the OrgFunctions descriptor with

int[][] pairs = new DescriptorHandlerFunctionalGroups().decode();

Here you get an array of arrays with length of 2. Every one of these small arrays contains a functional group ID and an associated count value. Thus, this is not a simple matrix and making use of it will probably need the some knowledge of the groups, i.e. the similarity tree. You may study the FunctionalGroupClassifier to understand which groups have which ID and how the tree is organized.

By the way, UMAP support in DataWarrior is planned.

Thomas