Subject: Re: Exporting a descriptor as a Textfile
Posted by Christophe on Tue, 24 May 2022 13:24:35 GMT
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Hi Norwid,

Thank you

It looks you managed to convert the structure DW column into one of the finger print managed by open babel.

I am not sure this procedure captures the native information of the skelspheres descriptor. It generated a FP2 (by default) FP descriptor.

I know how to generate a lot of different FP from structures. For example PaDEL (free java program, http://www.yapcwsoft.com/dd/padeldescriptor) does a very good job. It provides a matrix (.csv file) with structures (in rows) and bits (binary or count, depending on the FP you select) (in columns).

If you know how bits (or series of bits) are organized you can try to trace the source that causes the differences in distribution by multidimension reduction methods in R for example.

with DW, when I apply a similarity (or activity cliff) with Skelspheres and/or OrgFunctions, I have data sets that cluterize very well but it is quite challenging then to relate the resulting clusters to the distributional differences in term of structure (SkelSpheres) or functionalization (Orgfunctions). If these two descriptors are different from the one I used so far such as ExtFP, MACCSFP .... may be I could gain more information. But I need the "matrix formalism" into a text file.
Christophe