Subject: Feature query - molecular fingerprints and library diversity
Posted by SM2020 on Mon, 15 Jun 2020 15:06:12 GMT
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Hi,
Is there a way in Datawarrior (using any defined molecular fingerprint/descriptor) to...

1) derive the total number of fingerprints used to describe/make-up a compound library

2) tabulate the number of times a fingerprint is applied to a given structure within the library (i.e. proportional abundance)?

Came across an interesting way of describing/comparing library diversity in the literature (DOI: 10.3390/molecules24152838) but have no idea how to practically implement. Any suggestions/help appreciated.

Many thanks