Subject: comparing diversity
Posted by sansun on Fri, 31 Jan 2025 10:05:25 GMT
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I was wondering if it is possible to answer the following using DW.

Out of two libraries of small molecules (A and B), which one is more diverse?

Is it possible to get a single number representing a library's diversity that can be compared?

Thanks
SS

Subject: Re: comparing diversity
Posted by thomas on Thu, 20 Feb 2025 10:19:30 GMT
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I don't see anything obvious. One way might be to calculate the mean or median of all mutual compound similarities. This would require just a few lines of Java-code with OpenChemLib, but DataWarrior doesn't do that.