Subject: Suggest: select within cluster by property
Posted by DrCJM on Fri, 29 May 2020 02:06:26 GMT
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Something I'd find really useful, that I can't see how to do at present, is to select compounds after clustering by a particular property. The "representative" compound in a cluster is identified, I assume, as the most "central" compound in the cluster, which is fine. But sometimes I want to select the most active compound in the cluster, or the smallest MW in the cluster etc. etc.

If that's already possible, advice on how would be great!

Otherwise, a method of saying "Select from each cluster by value of property X" is something I'd use a lot.

Cheers,

Craig.