Subject: Similarity Search
Posted by Rishi on Mon, 28 Oct 2024 13:55:40 GMT
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Hi,

I want to conduct a similarity search for one compound against ~60K compounds within the same set. I'm only really interested in the similarity between the one specific compound against the 60K set, and not the similarity between all other compounds within the set.

When I run a search such as the FragFP similarity search the estimated time is >50 hours. I assume this is because it's calculating similarity between all compounds with the 60K set.

Is there a way of just conducting the search on the one compound against the set to reduce calculation times of similarity based positions?

Many thanks!