Subject: Re: Similarity analysis using "find similar compounds..." - slow analysis of libraries

Posted by SM2020 on Tue, 02 Mar 2021 22:40:17 GMT

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Hi Thomas - FYI, 120K vs 234K was sitting at ~1hr using an 8 core/16 thread setup (skelspheres) using the newest dev version. A definite speed improvement.

Thanks again.