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

Posted by SM2020 on Thu, 04 Feb 2021 10:11:11 GMT

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Hi Thomas,

Can I ask, did you implement this updated algorithm in your development patch for the DW linux distribution?

I was comparing 2 libraries to each other (120k vs 500k) and on MacOS with development patch, the timing was sitting at ~30hrs whereas linux was sitting at > 170hrs (the linux machine is more hardware capable).

Was just wondering where the time discrepancy is coming from.

Many thanks