Subject: Re: 'Search ChEMBL Database' function
Posted by thomas on Tue, 28 Aug 2018 19:10:51 GMT
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Thank you very much for the hint. I wasn't aware of the problem, which was caused by a recent server
update that now uses 64-bit descriptors rather than 32 bit ones in order to accelerate the search. Unfortunately this wasn't consistently done and the pre-screening of candidates for the substructure search
didn't work because it expected the wrong type of descriptors.
I updated the server and the problem disappeared. There is still a more cosmetic problem. Large result sets
as dopamine as substructure (which retrieves 207'075 rows) are retrieved, but cause an error when retrieving
retrieving the respective assay descriptions (about 30'000). The error message is inconclusive. After closing
the error dialog DataWarrior opens a window with the 207075 results nonetheless.

Whether I can remove the remaining problem with another server update or whether is comes with the next DataWarrior
update I still need to find out.

Thanks again and best wishes,

Thomas