Subject: Re: 'Search ChEMBL Database' function
Posted by thomas on Sat, 27 May 2023 16:01:01 GMT
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Assuming that your '[3]' atom list contains Cl,Br,I I could confirm that no rows are returned on the current chembl server with the version 32 database. It also shows a message that your search is not specific enough and would return too many records. If you use the same query, but use iodine instead of all three halogene atoms, then 101'394 rows are returned containing 10'531 distinct structures. Currently, the server limits results to 50'000 distinct structures for sub-structure queries and to 100'000 structures for other structure searches. The idea of the limit is a historic one to make sure that a result download is not taking forever and both, client and server resources are fit to handle the result. For the next server version I will increase these limits by a factor of 2.