Subject: 'Search ChEMBL Database' function
Posted by kerryfowler on Mon, 27 Aug 2018 19:46:59 GMT
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DataWarrior is the tool I've wanted for decades, so thanks to all the developers!

In version 4.7.2 the "Search ChEMBL Database..." function works for

similar structure to (sometimes)
equal structure to
stereo isomers of
tautomers of

but not for "superstructures of" which returns the message "Error in task 'Search ChEMBL Database': Your query did not retrieve any records."

The similarity search sometimes returns an error until the similarity threshold is lowered. For example, similarity search for dopamine as query fails until similarity is decreased from 90% to %89. Substructure query fails for dopamine.