Subject: Confidentiality of compound structures Posted by mhf2021 on Tue, 16 Feb 2021 13:12:39 GMT

View Forum Message <> Reply to Message

hello,

can we use datawarrior with non public domain compound structure?

Are the structures sent to an external server to run calculations, such as similarity or molecular properties.

or does everything run locally on my machine.

Thanks

With best regards,

MH

Subject: Re: Confidentiality of compound structures Posted by thomas on Tue, 16 Feb 2021 17:04:41 GMT

View Forum Message <> Reply to Message

You are save to use DataWarrior for almost any purpose without the risk of being tracked. Except for Database queries (COD, ChEMBL, Enamine, ChemSpace, Google, and name-to-structure conversions)

nothing is sent to any server. All calculations are done locally.

Currently, searches on COD, ChEMBL, Enamine, and name-to-structure run on my own servers are are not tracked, either.

Thomas

Subject: Re: Confidentiality of compound structures Posted by nbehrnd on Tue, 16 Feb 2021 17:41:45 GMT

View Forum Message <> Reply to Message

In addition to the above, it is possible to search in and work with the snapshots of the databases COD, Drugbank, and about US patents off-line. The corresponding files may be obtained from http://openmolecules.org/datawarrior/datafiles.html

Norwid