Subject: Retrieve Data from SQL database
Posted by alienke on Mon, 15 Jul 2019 14:27:10 GMT

Hi Thomas,

first and foremost: compliments for including a SQL interface. Connection with MySQL works perfect. How can I access MS SQL Server. I tried various connection strings and always get the same error message.

Do I need special drivers?
Do I need to use a sideway?

Best wishes

Achim

Subject: Re: Retrieve Data from SQL database
Posted by thomas on Tue, 23 Jul 2019 15:13:26 GMT

Hi Achim,

the current and official DataWarrior 5.0.0 does not support SQL-Server nor PostgreSQL. However, I have built support for both database engines into the current development version, which you may download as zip-file containing 4 files, which you need to replace in the official installation. The links are for Windows: openmolecules.org/datawarrior/dw500win.zip and for Linux/Mac: openmolecules.org/datawarrior/dw500x.zip

Since I don't have access to a SQL-Server not a PostgreSQL database, I could not test it and would be grateful, if anybody you would let me know, whether it works.

There are some other bug fixes and new functionality coming with that version, e.g. the generation of random molecules or predicting missing values from chemical structures using machine learning approaches. This functionality is not described in the manual, but is rather straight forward.

Enjoy, Thomas

Subject: Re: Retrieve Data from SQL database
Posted by will on Wed, 14 Aug 2019 18:54:41 GMT

Thanks so much for this. Like the original poster, I had the same question. I followed your instructions and it worked nicely. I was then going to make a macro to pull from a database but I

noticed that it showed up as an unknown task and the macro editor did not have an entry for grabbing data from a SQL database. Is this true?

Thanks!

Subject: Re: Retrieve Data from SQL database
Posted by thomas on Fri, 23 Aug 2019 22:11:33 GMT
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Sorry for that. I have overlooked something. This should now be fixed in the dw500 update files.