
Subject: Re: Importing compounds with assay data from Pubchem into Datawarrior
Posted by [nbehrnd](#) on Mon, 26 Jul 2021 19:55:23 GMT

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Dear Jon,

there was indeed an problem to access and subsequently keep a local copy of the .csv files. By now, yhe support by PubChem was able to correct the underlying error. The downloaded file contains a (late) column labelled «cmpdname»

Open the file in a text editor to copy all content into the working memory of the computer. In DataWarrior, paste these information via Edit -> Paste Special -> New From Data With Header Row. Establish the structures via Chemistry -> Add Structures From Name which opens a new interface. To guide DW's action, select the column of interest, «cmpdname».

Norwid

File Attachments

- 1) [name2structure.png](#), downloaded 914 times
 - 2) [Data_From_Clipboard.dwar](#), downloaded 1624 times
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