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,

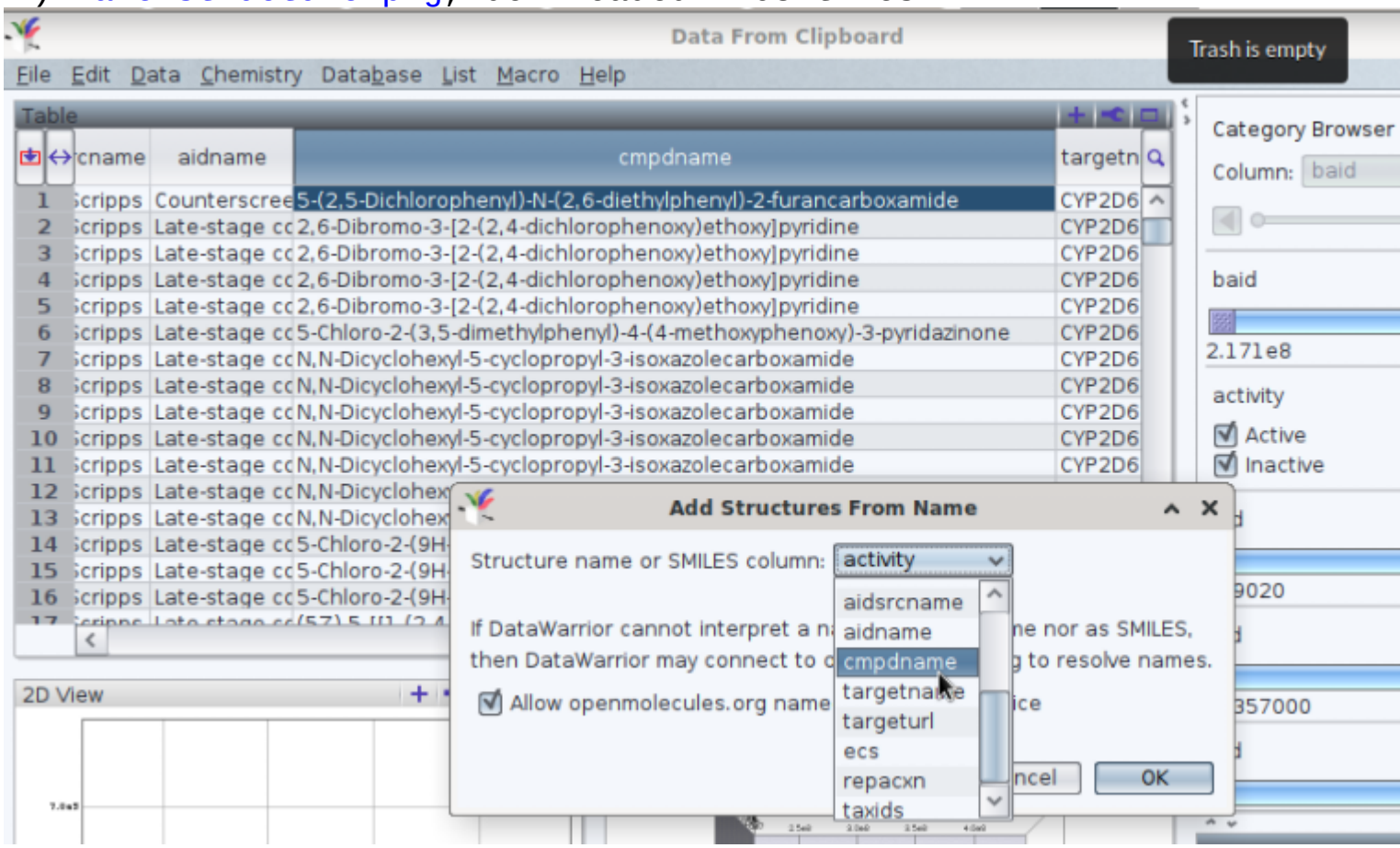
there was indeed an problem to access and subsequently keep a local copy of the .csv files. By now, yhe support by PubChem was able to correct the underlying error. The downloaded file contains a (late) column labelled «cmpdname»

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 2108 times



2) Data_From_Clipboard.dwar, downloaded 2090 times