Subject: Re: Forcing column headers on import, using regression
Posted by thomas on Tue, 09 Aug 2016 11:36:22 GMT
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Sorry for the delay. I see the point and added two menu options to enforce pasting with and without a header row. The 'Paste' macro task now also has these options.

To your second point: I had built in a PLS regression only temporarily and just for the purpose of calculating atom type based contributions for polar and non-polar surface prediction, but I didn't invest the time to build an UI, test, and document it to open it for general model building. If there is sufficient interest, I may add it after the upcoming DataWarrior update.

Kind regards,

Thomas