Subject: Video tutorial on using Datawarrior to undertake QSAR predictions
Posted by Jo W on Thu, 17 Mar 2022 21:31:12 GMT
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Can Isabelle or someone else at DW conduct a workshop (and upload it on to youtube) on a complete prediction e.g., going from start to finish, from an initial lead compound, undertaking similarity searches and obtaining pIC50 values from chEMBL, and then using the built-in machine learning predictors and/or using the linear regression in the 2D scatter plot section of DW to show how predictive modeling can be undertaken to predict the biological activity of say similar compounds generated from the evolutionary library in DW.

Can any of the experienced users of DW create or contribute/ upload short videos on this or similar topics that we can all use for inspiration?

DW is so good, it should be built into windows 11 (or equivalent on Apple) 8)