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)

Subject: Re: Video tutorial on using Datawarrior to undertake QSAR predictions
Posted by nbehrnd on Thu, 17 Mar 2022 21:53:31 GMT
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Dear Jon,

there are at least two recordings of tutorials by Isabelle Giraud mirrored on youtube.[1,2] Thanks to both her and a special interests group in the Royal Chemical Society, this knowledge is disseminated further.

Norwid

[1] https://www.youtube.com/watch?v=mQCf9GakQW0
[2] https://www.youtube.com/watch?v=Is2hLqqSFvM

Subject: Re: Video tutorial on using Datawarrior to undertake QSAR predictions
Posted by Jo W on Sat, 26 Mar 2022 17:59:12 GMT
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Dear Norwid and Thomas
Thanks and yes I am aware of those videos, however, they don't cover from start to finish a QSAR or biological prediction in Datawarrior (DW). Could this be arranged by colleagues at DW along the lines suggested in my original post above?

Subject: Re: Video tutorial on using Datawarrior to undertake QSAR predictions
Posted by sansun on Mon, 04 Apr 2022 07:00:03 GMT
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Dear Jon

I don't think there is a direct way to perform QSAR in DW.
Although you can calcuate various properties (e.g. clogp, PSA, etc.) that can be used as independent variables for QSAR model development in other specialized programs.