Subject: Re: Video tutorial on using Datawarrior to undertake QSAR predictions
Posted by sansun on Mon, 04 Apr 2022 07:00:03 GMT
View Forum Message <> Reply to Message

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.