Subject: Free Wilson Analysis
Posted by amorrison on Fri, 17 Mar 2023 16:44:55 GMT
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Hi Thomas,

I was wondering if you think it would possible to do a Free-Wilson analysis within Datawarrior? Not necessarily a feature you might want to incorporate but if you think it would be achievable and could give me some hints I'd much appreciate it.

I appreciate there are ML models already available in DW, but as a medicinal chemist it's much easier for me to relate to the Free-Wilson models and I've used them successfully in the past. I do have other tools that I can use for this but being able to do it in DW would be marvellous.

Thanks,

Angus