Subject: Re: datawarrior descriptor literature refs
Posted by nbehrnd on Mon, 18 Dec 2023 15:02:02 GMT
View Forum Message <> Reply to Message

Hello Maxwell,

I suggest to start the literature search from two points of departure: the seminal paper about DataWarrior (2015JChemInfModel460, https://doi.org/10.1021/ci500588j) as well as the review-like «Limits of Prediction for Machine Learning in Drug Discovery» by Modest von Korff and Thomas (2022FrontPharmacol, https://doi.org/10.3389/fphar.2022.832120, open access).

Norwid