Subject: datawarrior descriptor literature refs
Posted by Maxwell on Mon, 18 Dec 2023 13:44:09 GMT
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Hi warriors.

Can anyone point me at literature references that discuss the Datawarrior descriptors (FragFp, SkelSpheres etc) and perhaps even discusses comparison with other popular descriptors?

Thanks

Subject: Re: datawarrior descriptor literature refs
Posted by nbehrnd on Mon, 18 Dec 2023 15:02:02 GMT
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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