Subject: Re: Drug Likeness vs Drug Score
Posted by ELFritzen on Tue, 02 Feb 2021 15:57:10 GMT
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Thanks for the reply. I'm trying to figure out exactly how Datawarrior calculates the Druglikeness and what factors are considered. The calculated value obtained is just a number to me. I'm not sure what the number means and how I might use it to determine the probability of finding a good drug lead. Are bigger numbers better? I can't figure that out. The article you provided is very informative, and it does point to a Web-based calculator which assesses the druglikeness of any molecule submitted, but I can't fine an overall druglikeness number like I see calculated in Datawarrior.

Ed