Subject: Re: Drug Likeness vs Drug Score
Posted by nbehrnd on Mon, 01 Feb 2021 17:37:35 GMT
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The manual's page

http://www.openmolecules.org/properties/properties.html

reads like a druglikeness is computed in first place, subsequently used to compute a drug score.

Lipinski's rule of five properties is one, but not the sole approach to define druglikeness. An implementation other than DataWarrior computing the later and others may be SwissADME (https://doi.org/10.1038/srep42717, open access).