Subject: TPSA
Posted by sansun on Mon, 03 Aug 2020 11:13:30 GMT
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I found disagreement between TPSA values calculated from DW and RDKit although both seem to follow same methodology by Peter Ertl et al. in J. Med. Chem. 43, 3714-3717 (2000).

In some case the difference is quite large e.g. 87 vs 252

However, Spearman correlation is > 0.9 for my data set (N > 20000).