Subject: Confirming Sali values generated in Datawarrior / Machine learning and multiple descriptors in DW
Posted by Jo W on Wed, 22 Sep 2021 23:06:20 GMT
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The question relates to Sali plots - DW generated Sali values compared to those using the Sali equation in the scientific literature. I assume I must be doing something wrong but cannot figure out what to do (see attached).

The other is a question on using multiple descriptors for machine learning predictions in DW (see attached).
Many thanks in advance

File Attachments

1) Question on Sali plot calculations in Datawarrior.docx, downloaded 669 times