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Erratum

Erratum to the paper: In vitro membrane binding and protein binding (IAM MB/PB technology) to estimate *in vivo* distribution: applications in early drug discovery

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The authors of the original paper published with the same title [1] apologize for the error in the plot on Figure 5.

The correct plot, statistics and explanation in Figure 5 on page 25 using the published data in the Appendix Table A1 and A2 by equation 3 are shown below.

"In turn, the volume of distribution of marketed drugs could be modeled by the difference in the membrane and the protein binding of compounds as described by Equation 3 and shown in Figure 5 for the investigated compounds. There are only 40 compounds that have been included in the training set, the majority of the compounds were not included in the original model. That explains that the statistics are slightly worse (r^2 = 0.76; root mean square error = 0.33 in the original model, while here the r^2 = 0.65 and root mean square error = 0.40). "

It is considered as an excellent prediction of the *in vivo* behaviour of the compounds using only two measured biomimetic properties, namely the IAM membrane binding and the HSA protein binding (see the original paper for details).

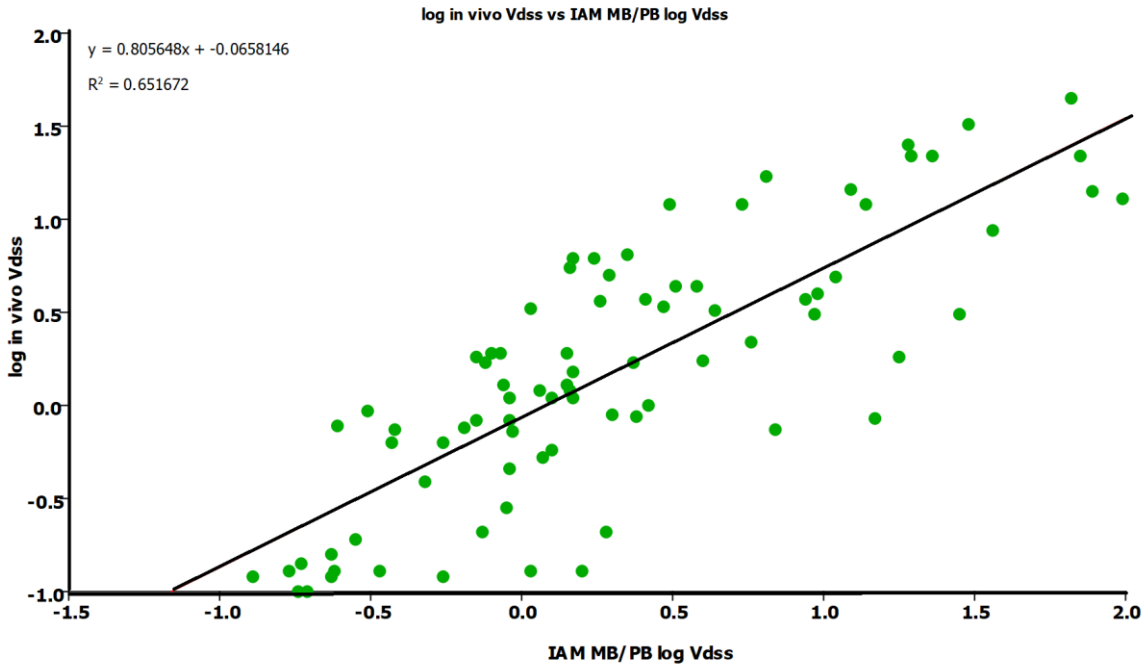

Figure 5. The observed in vivo log *V*dss vs the estimated *V*dss by the IAM MB/PB Technology® using Equation 3.

References

[1] K. Valko, S. Teague, C. Pudgeon. In vitro membrane binding and protein binding (IAM MB/PB technology) to estimate in vivo distribution: applications in early drug discovery. *ADMET & DMPK* **5**(**1**) (2017) 14-38. https://dx.doi.org/10.5599/admet.5.1.373