

Supplementary Information

Figure S1. Comparison between experimental (horizontal axis) and predicted (vertical axis) pK values for (a) and (b) scramble tests, and (c) additional set of test compounds. Points represent training (black) and test (red) compounds. Cross-validation and prediction coefficients are given as q₂ and p₂, respectively.

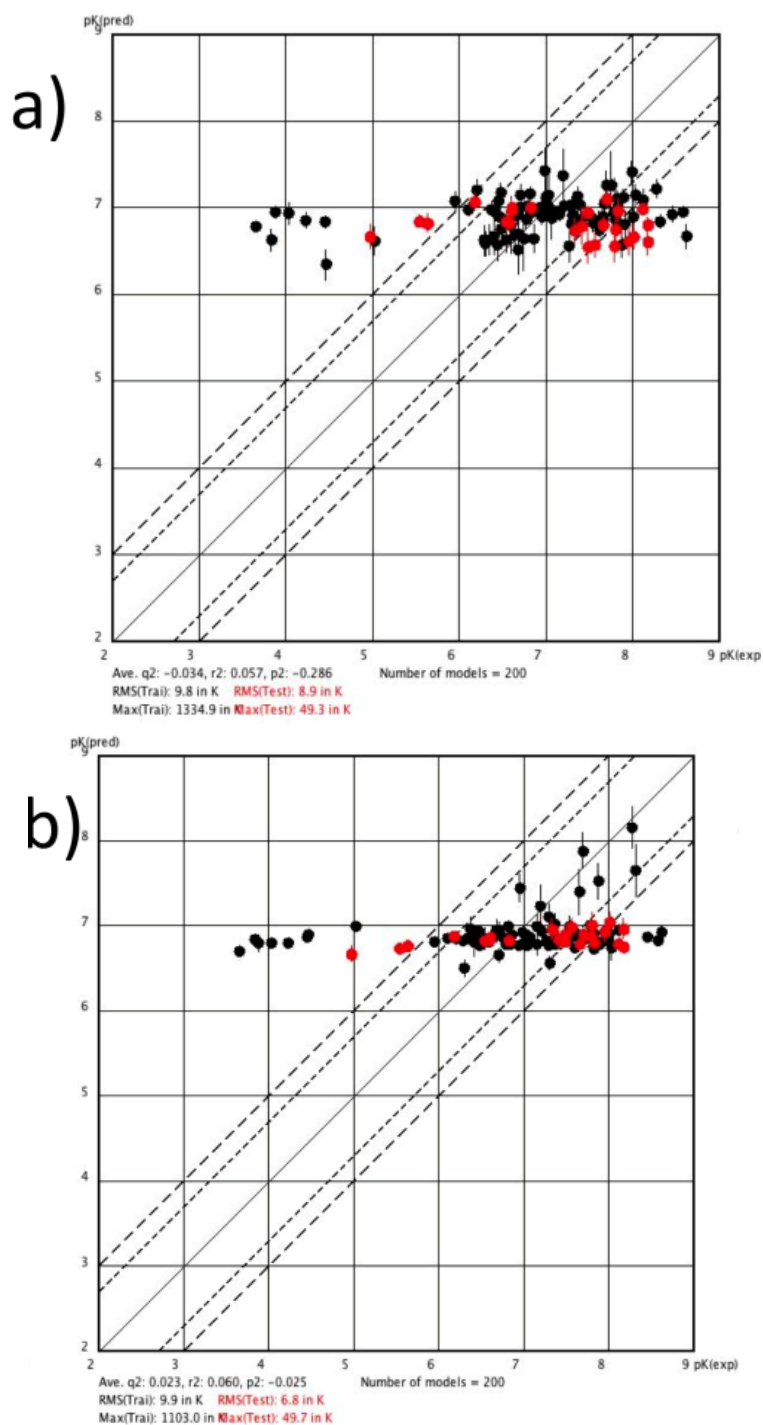
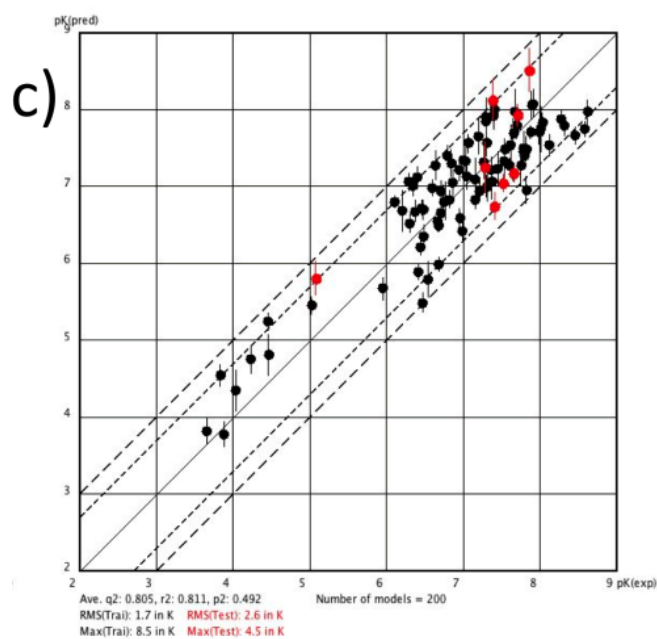


Figure S1. *Cont.*

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