

Additional File 4

Comprehensive Benchmarking of Computational Tools for Predicting Toxicokinetic and Physicochemical Properties of Chemicals

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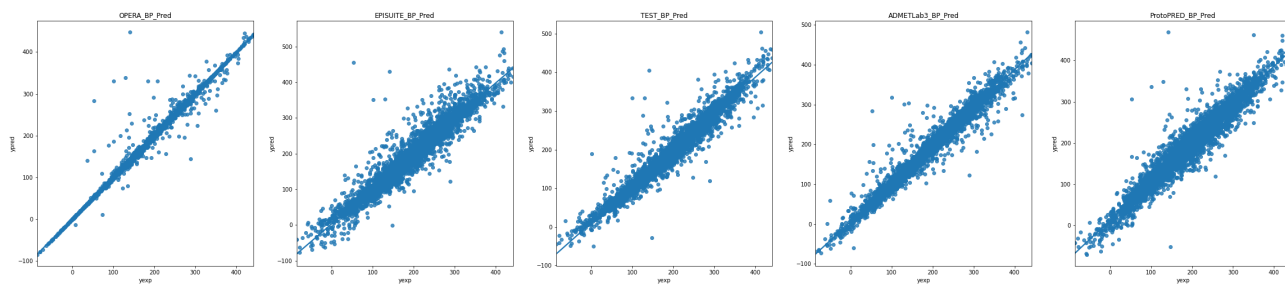


Figure S1: Boiling Point (BP). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

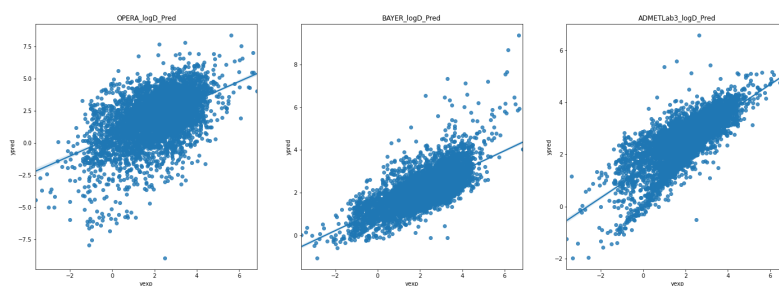


Figure S2: Distribution coefficient (logD). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

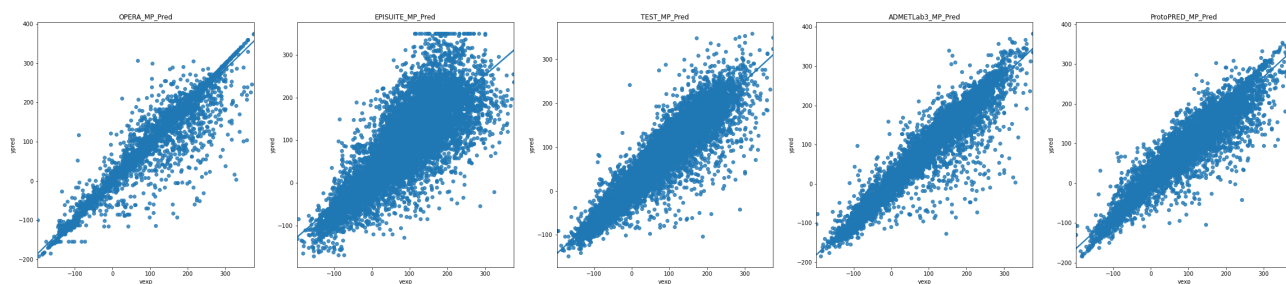


Figure S3: Melting Point (MP). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

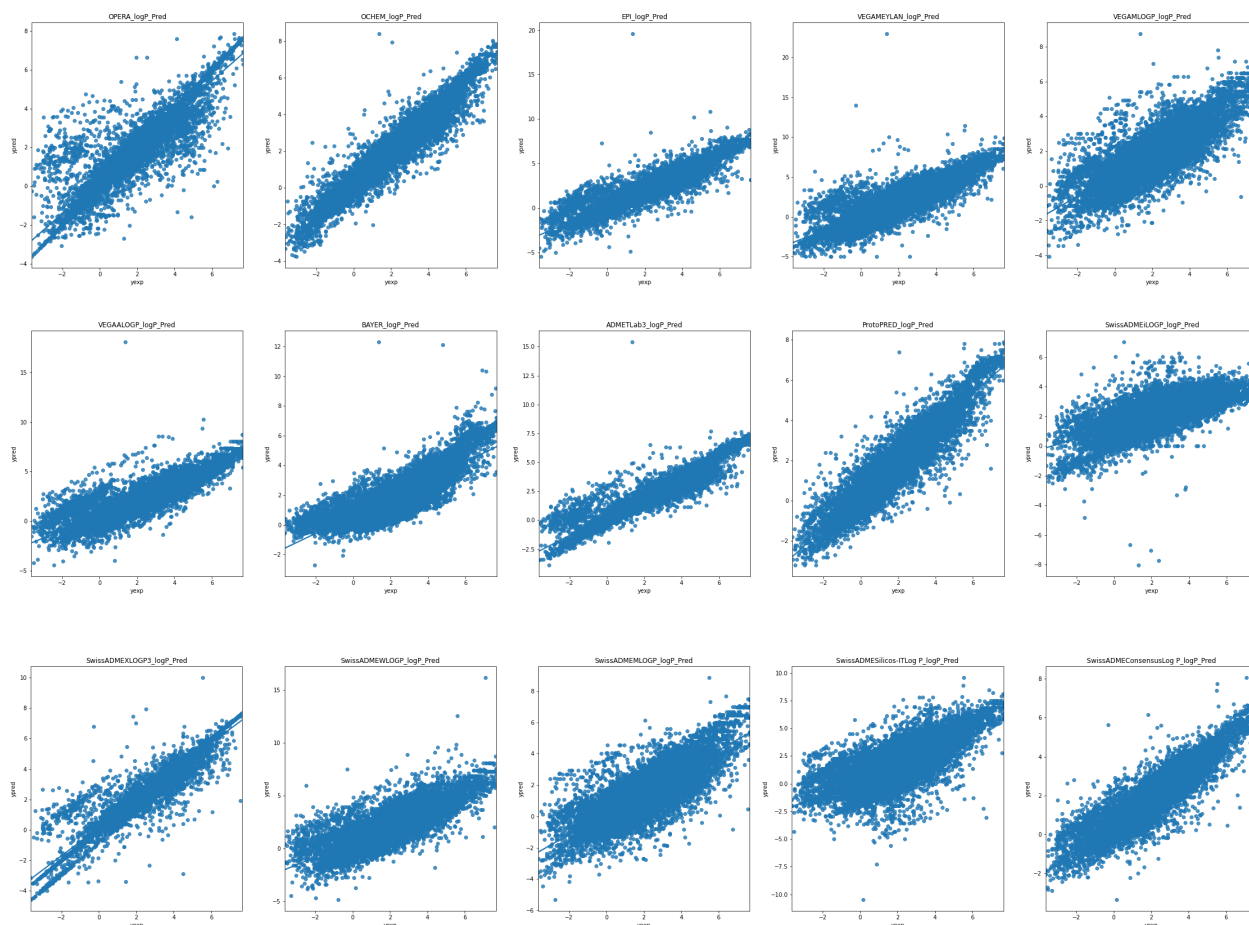


Figure S4: Octanol/water partition coefficient (logP). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

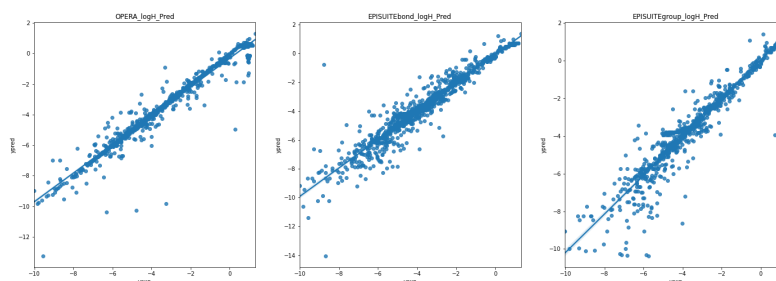


Figure S5: Henry's law constant (logH). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

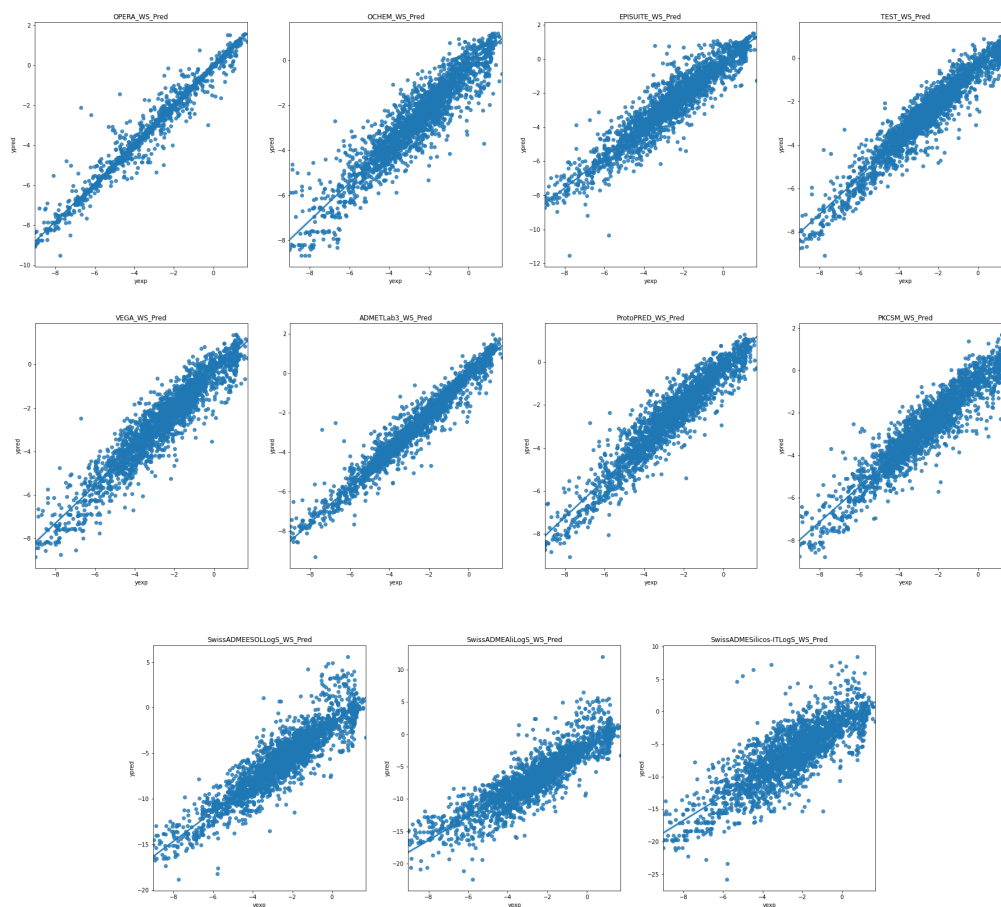


Figure S6: Water Solubility (logWS). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

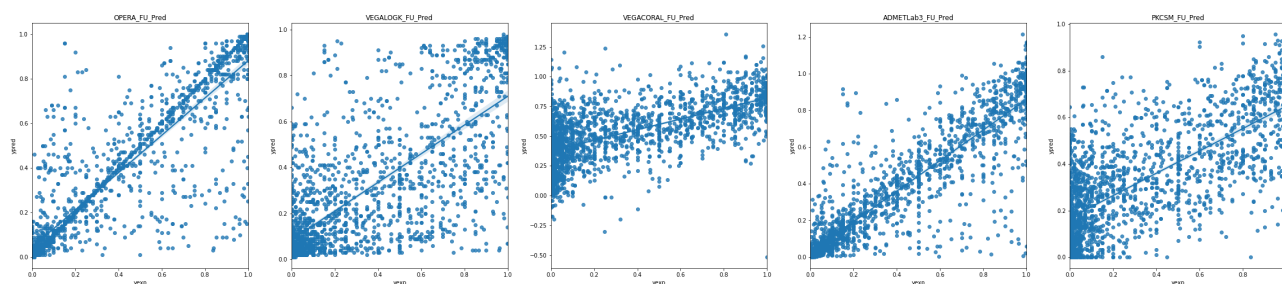


Figure S7: Fraction Unbound (FUB). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

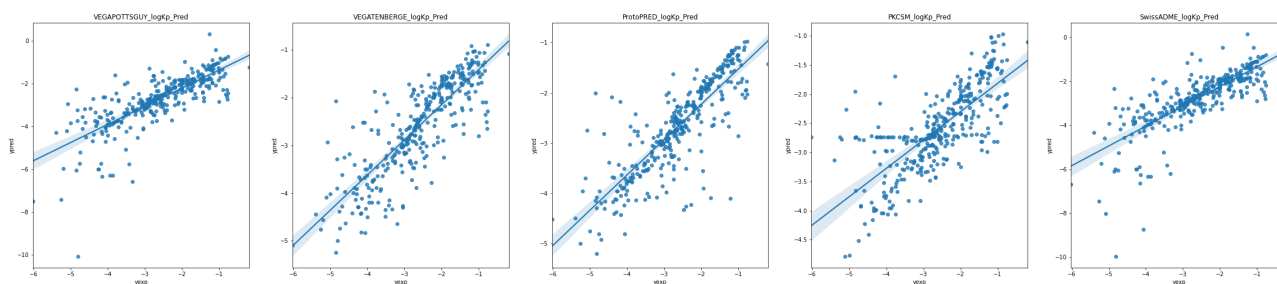


Figure S8: Skin permeation (logKp). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

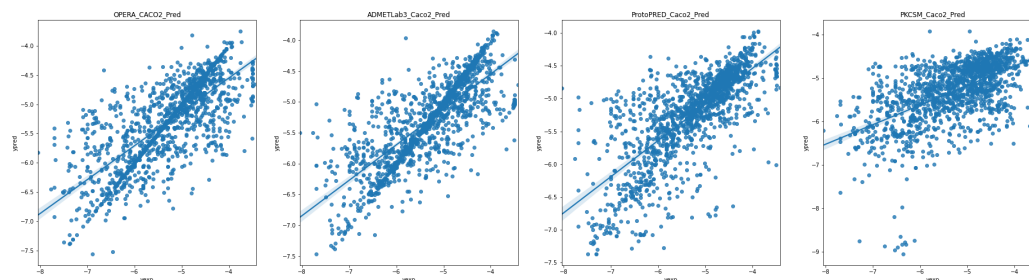


Figure S9: Caco-2 permeability (Caco2). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

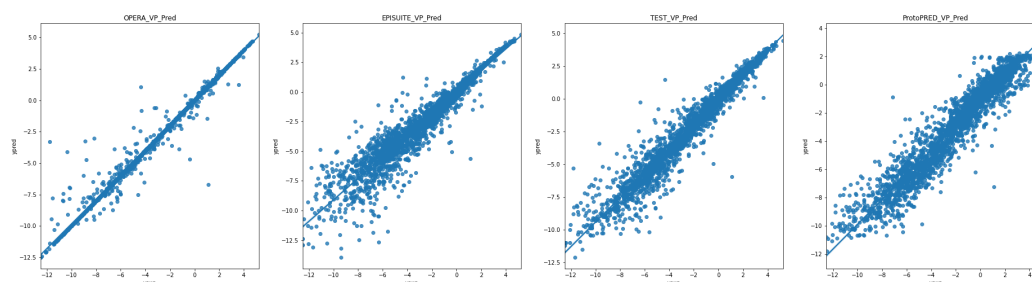


Figure S10: Vapor Pressure (logVP). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

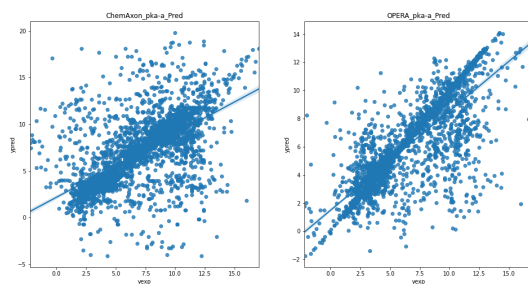


Figure S11: pKa acidic (pka-a). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.

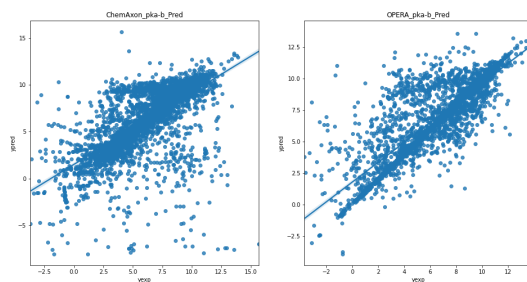


Figure S12: pKa basic (pka-b). Correlation analysis between experimental values (yexp) and predicted values (ypred) by model.