Supporting Information – S2

Calculating the Partition Coefficients of Organic Solvents in Octanol/Water and Octanol/Air

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This document (Supporting Information – S2) provides additional information for the publication "Calculating the Partition Coefficients of Organic Solvents in Octanol/Water and Octanol/Air".

In the first section, we report the Evaluation Metrics: MAD, MSE, RMSE, MAPE given by the displayed below formulas for the observed and calculated value.

In the second section of the S2 document the presented plots are for the cases where the predicted versus experimental data for the Octanol/Water and Octanol/Air partition coefficients are with the specific points deviated from the linearity before the application of 4-sigma rule test for the outliers. The deviated points are marked.

Section one: Evaluation Metrics formulas

$$\mathrm{MAD} = \frac{\sum_{t=1}^{n} |A_t - F_t|}{n}$$

MAD is the sum of absolute differences between the actual value and the forecast divided by the number of observations.

$$\mathrm{MSE} = \frac{\sum_{t=1}^{n} (A_t - F_t)^2}{n}$$

Mean square error (MSE) is probably the most commonly used error metric. It penalizes larger errors because squaring larger numbers has a greater impact than squaring smaller numbers. The MSE is the sum of the squared errors divided by the number of observations.

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{t=1}^{n} (A_t - F_t)^2}{n}}$$

RMSE: the root mean square error (RMSE) is the square root of the MSE.

$$\mathrm{MAPE} = \frac{\sum_{t=1}^{n} \left| \frac{A_t - F_t}{A_t} \right|}{n} \times 100$$

Mean Absolute Percentage Error (MAPE) is the average of absolute errors divided by actual observation values.

Section two: Figure S1; Figure S2; Figure S3

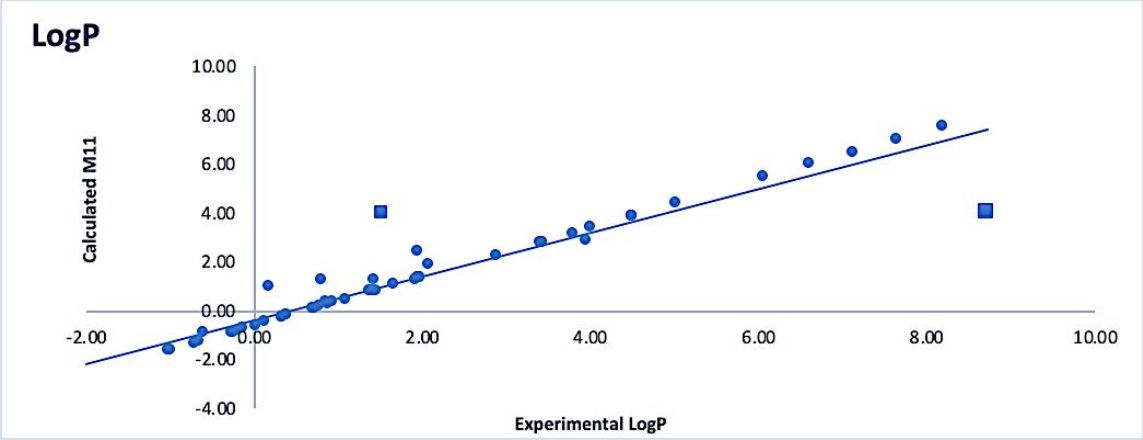

Figure S1. Comparison of the calculated LogP to the experimental values.

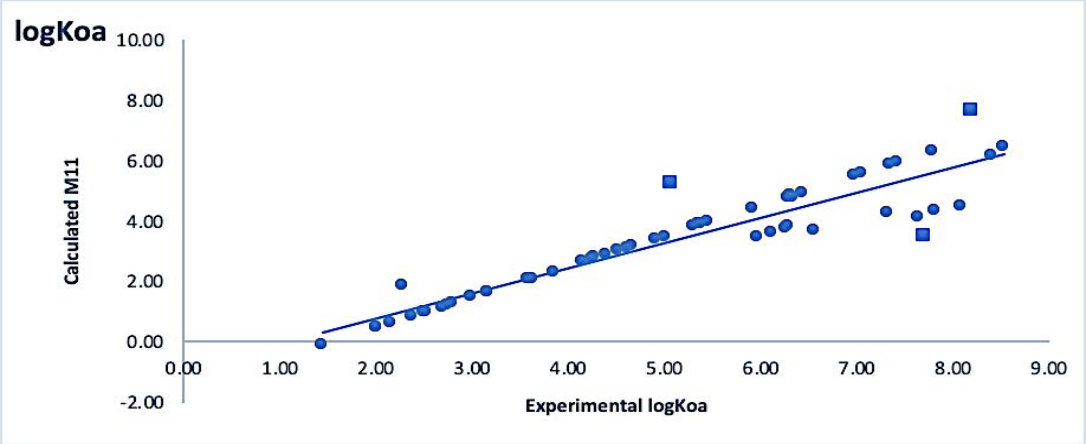

Figure S2. Comparison of the calculated logKoa to the experimental values.

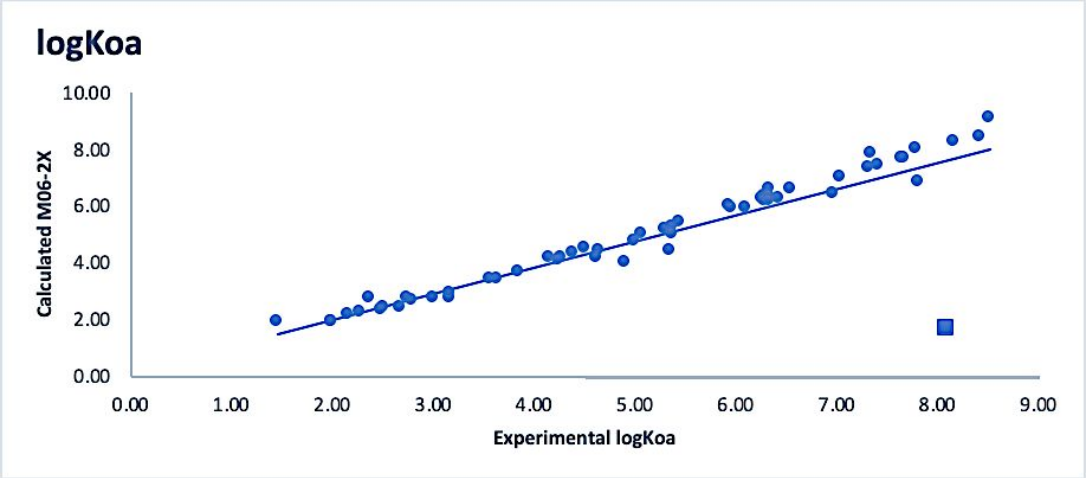

Figure S3. Comparison of the calculated logKoa to the experimental values.