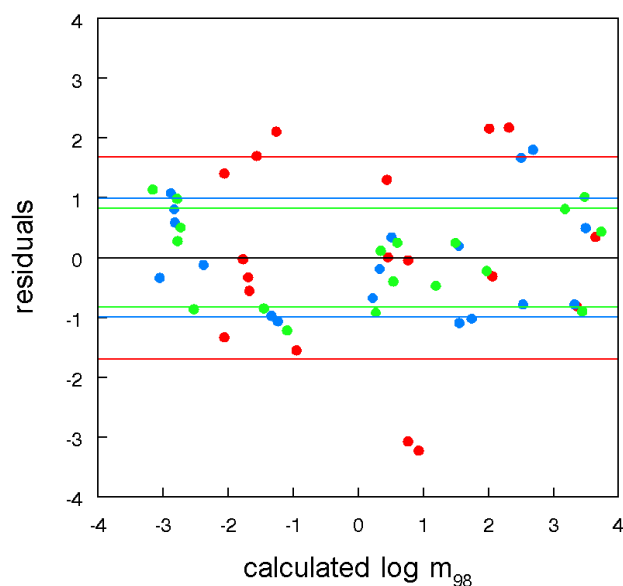


Supporting Information for:

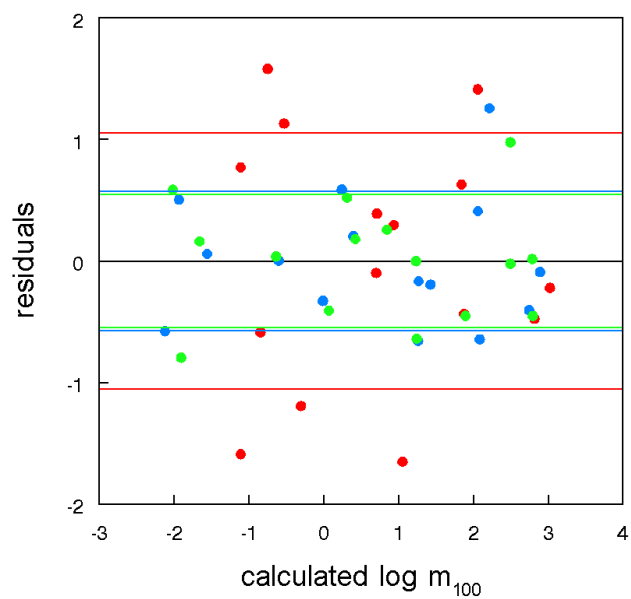
Correlations of Nitrenium Ion Selectivities with Quantitative Mutagenicity
and Carcinogenicity of the Corresponding Amines

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Plot of residuals vs. calculated value of $\log m_{98}$ for single variable regression against $\log S$ (●), multiple variable regression against $\log S$ and I_{rings} (●), and multiple variable regression against $\log S$, I_{rings} , and Clog P (●). The color-coded horizontal lines are the square roots of the mean square error (RMSE) for the three cases.



Plot of residuals vs. calculated value of $\log m_{100}$ for single variable regression against $\log S$ (●), multiple variable regression against $\log S$ and I_{rings} (●), and multiple variable regression against $\log S$, I_{rings} , and $\text{Clog } P$ (●). The color-coded horizontal lines are the square roots of the mean square error (RMSE) for the three cases.