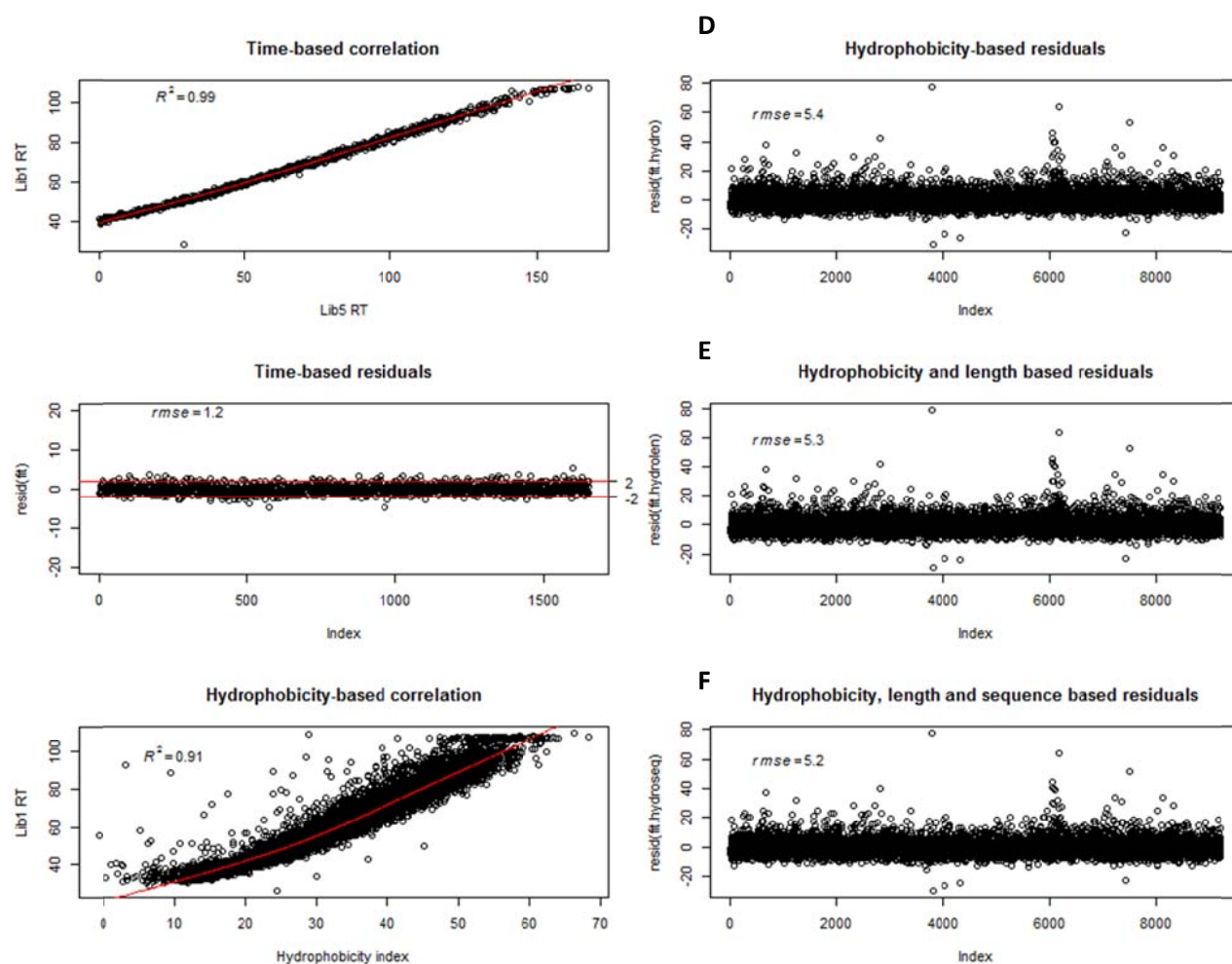


Supplemental Figure

Comparison of time-based and hydrophobicity-based retention time prediction. A) Time-based correlation between the observed retention time of common peptides in Lib1 and Lib5. $R^2=0.99$. B) Prediction residuals of time-based method using the observed retention time of common peptides in Lib1 and Lib5. Root Mean Square Error (RMSE)=1.2 minutes. C) The correlation between peptide hydrophobicity index calculated using SSRCalc and the observed retention time of Lib1. $R^2=0.91$. D). Prediction residuals of hydrophobicity-based method using the observed retention time of common peptides in Lib1. Root Mean Square Error (RMSE)=5.4 minutes. E) Prediction residuals of hydrophobicity and peptide length based method using the observed retention time of common peptides in Lib1. Root Mean Square Error (RMSE)=5.3 minutes. F) Prediction residuals of hydrophobicity, peptide length and sequence based method using the observed retention time of common peptides in Lib1. Root Mean Square Error (RMSE)=5.2 minutes.



Boxplots of prediction errors for the time based, hydrophobicity based, hydrophobicity and peptide length based, hydrophobicity, peptide length and peptide sequence based methods over five-fold experiments.

