Supporting information

Retip: retention time prediction for compound annotation in untargeted metabolomics

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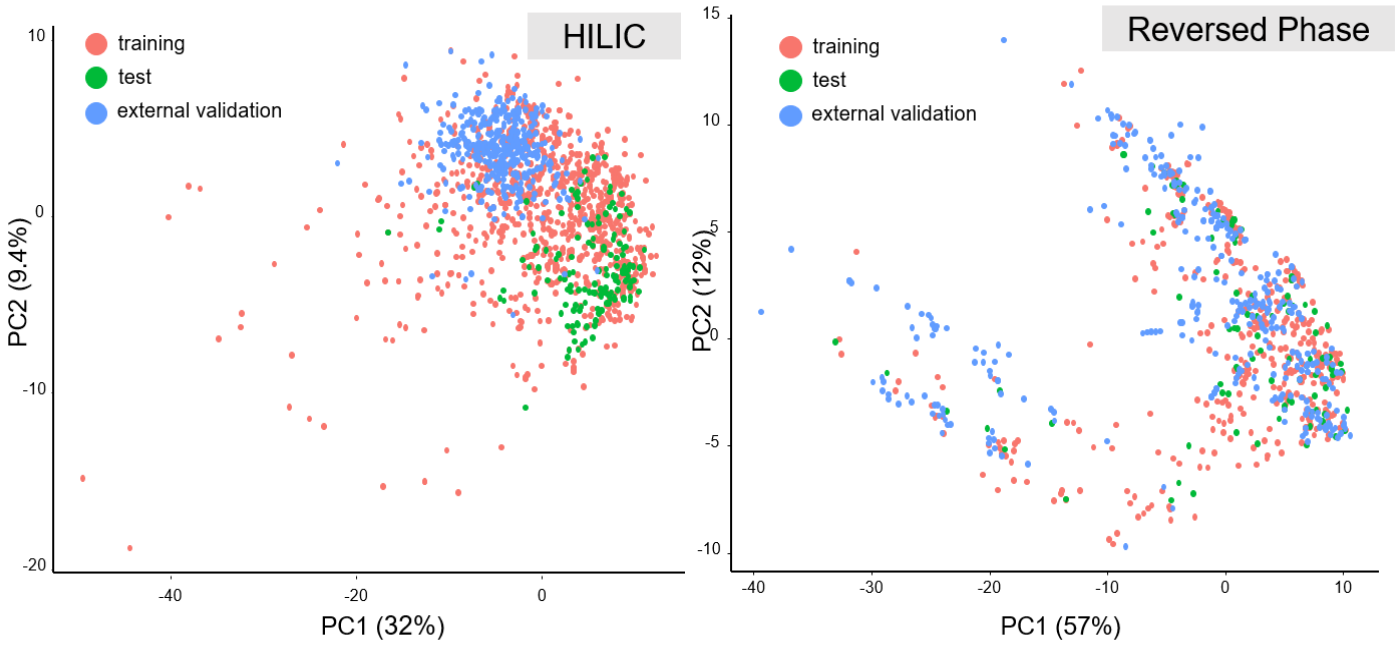
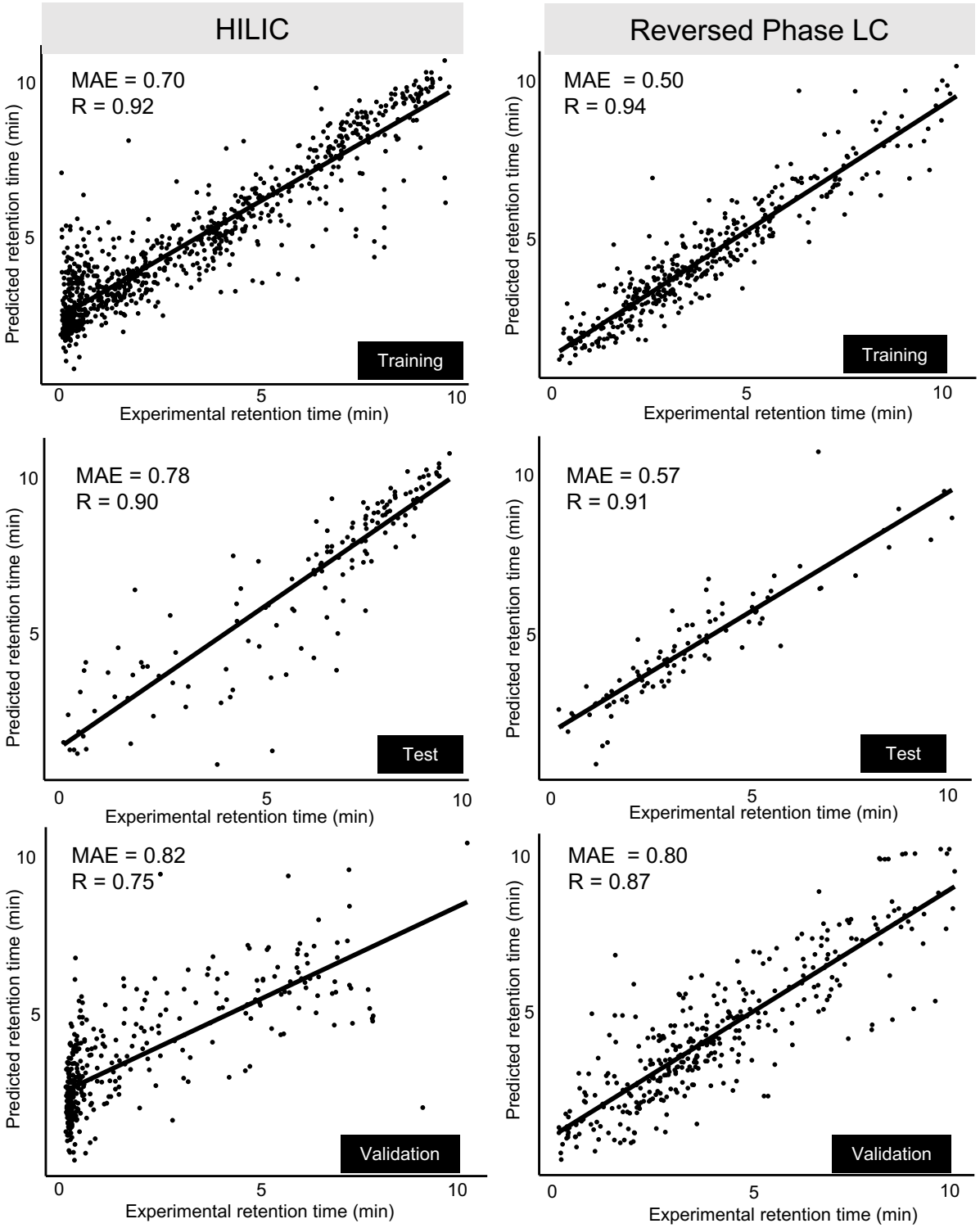


Supporting Figure S1. Predicting LC-retention times on HILIC- and Reversed-phase LC methods. Principal Component Analyses (PCA) on 2D-chemical descriptors to show chemical diversity in training and validation sets. 147 descriptors for HILIC and 142 descriptors for RP were used. Data were centered and auto-scaled.



Supporting Figure S2. Visualizing prediction errors for Keras machine learning for HILIC- and reversed-phase LC methods. MAE is mean absolute error, R is correlation coefficient for experimental versus predicted retention times. Keras method details are given in the main manuscript. Data from Supporting Tables S1-S6.