

Supplementary material for the article:

Predicting the Bioconcentration Factor in Fish from Molecular Structures

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Figure S1 A - ROC curve for the LDA model calculated for the training set

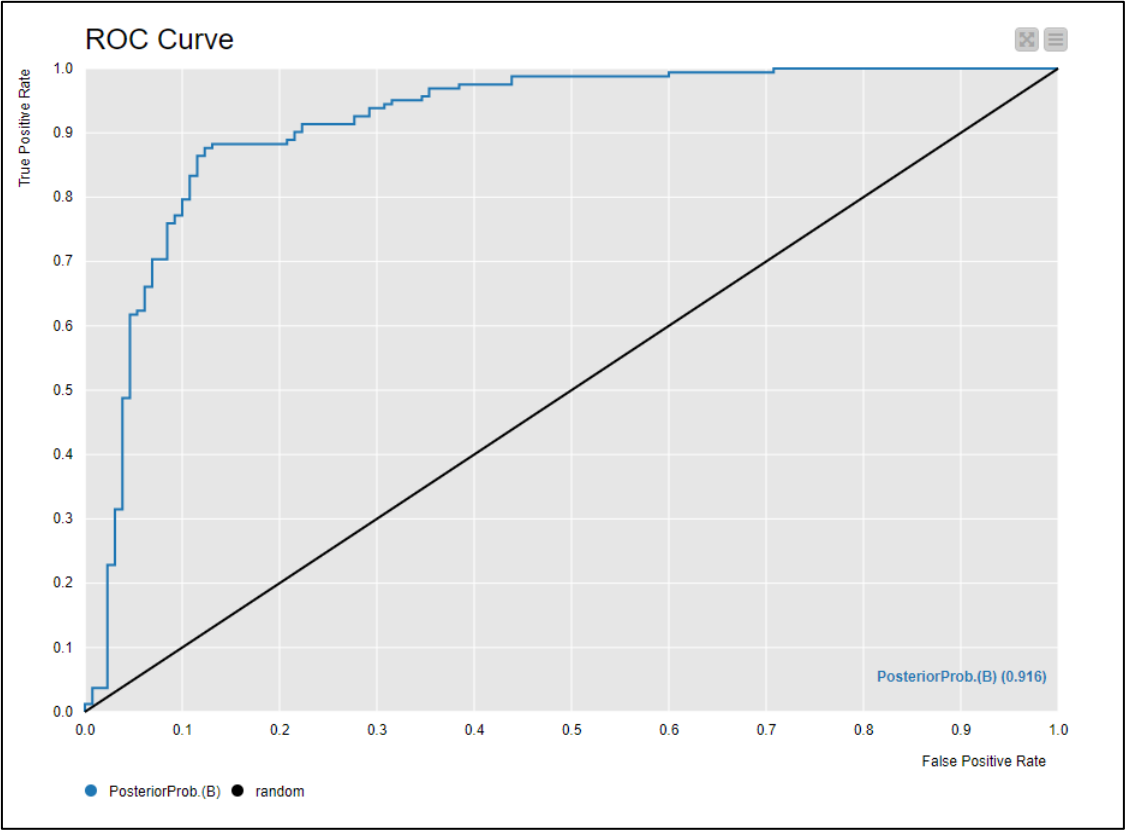


Figure S1 B – ROC curve for the LDA model calculated for the prediction set

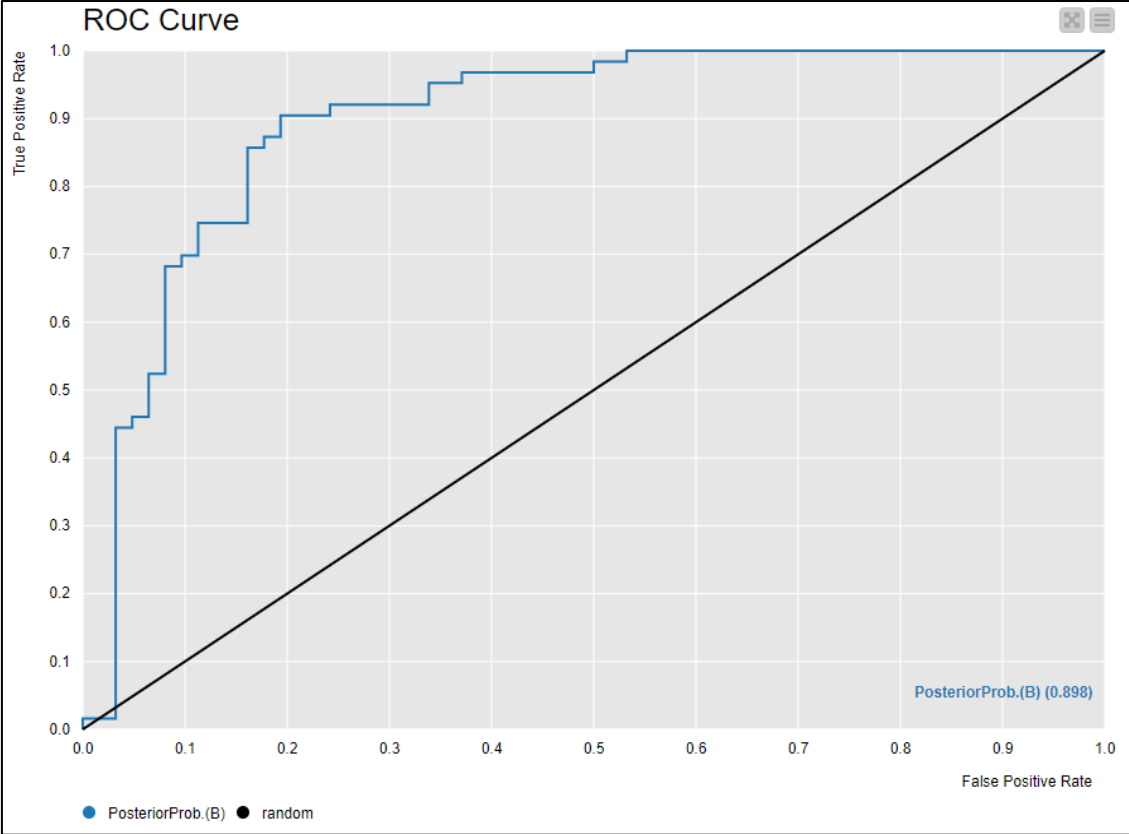


Figure S1 C - ROC curve for the LDA model calculated for the 5-folds cross validation

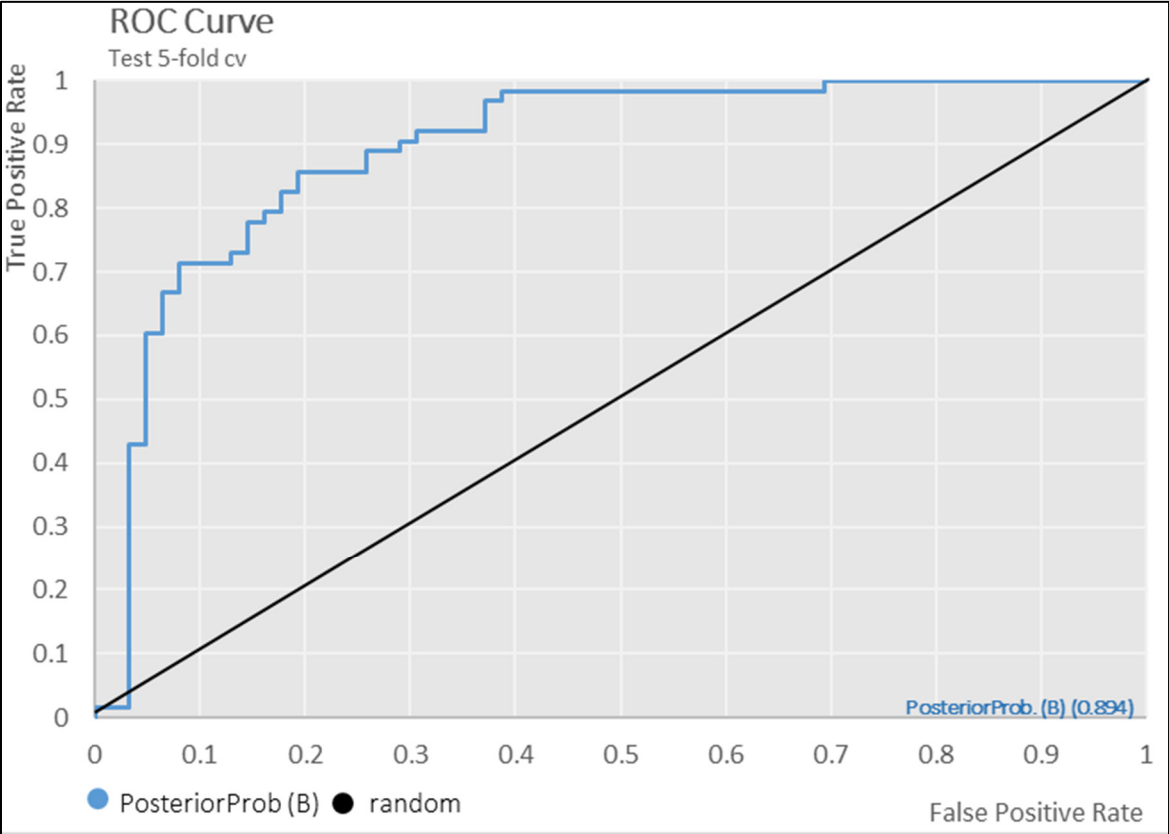


Figure S2 A - ROC curve for the ANN model calculated for the training set

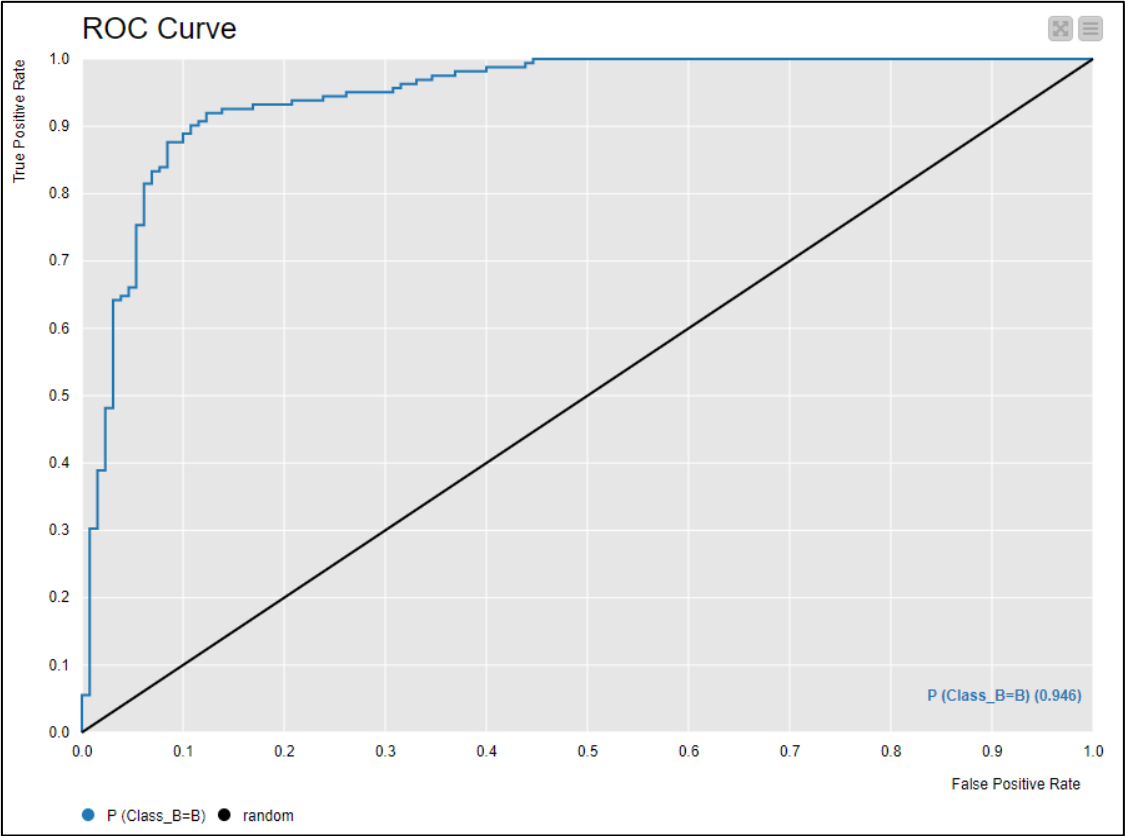


Figure S2 B – ROC curve for the LDA model calculated for the prediction set

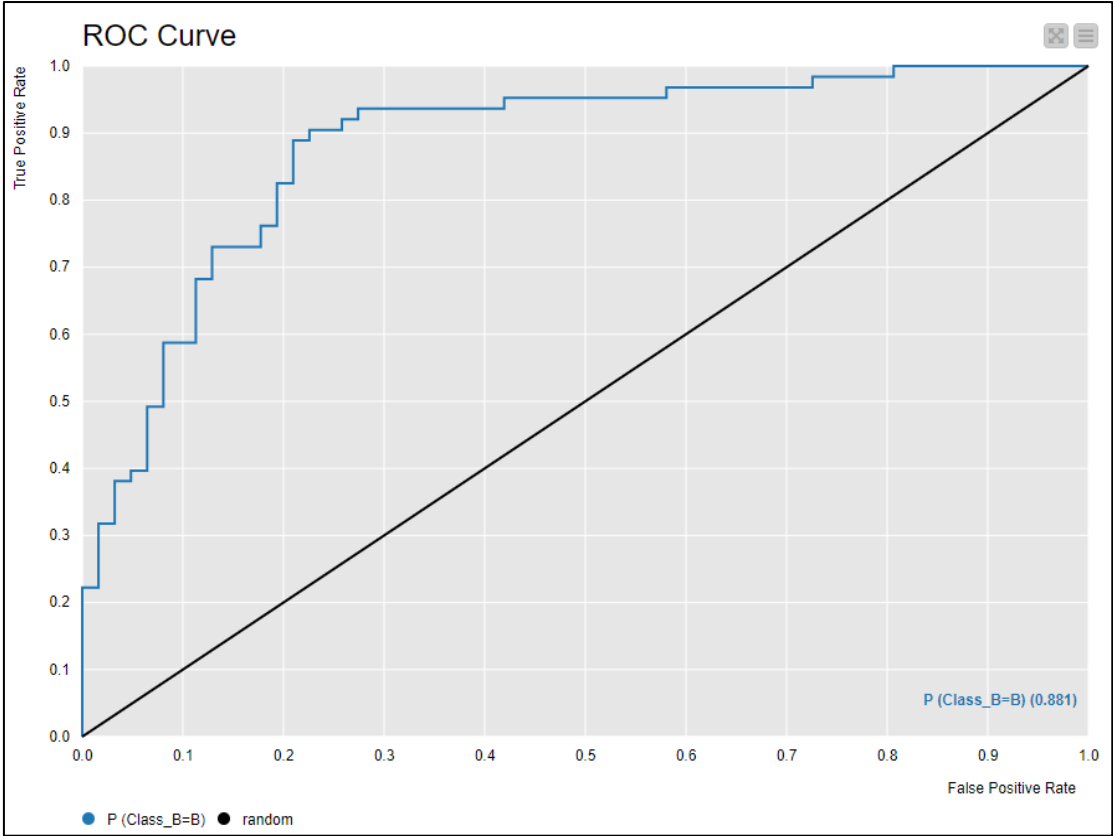


Figure S2 C - ROC curve for the LDA model calculated for the 5-folds cross validation

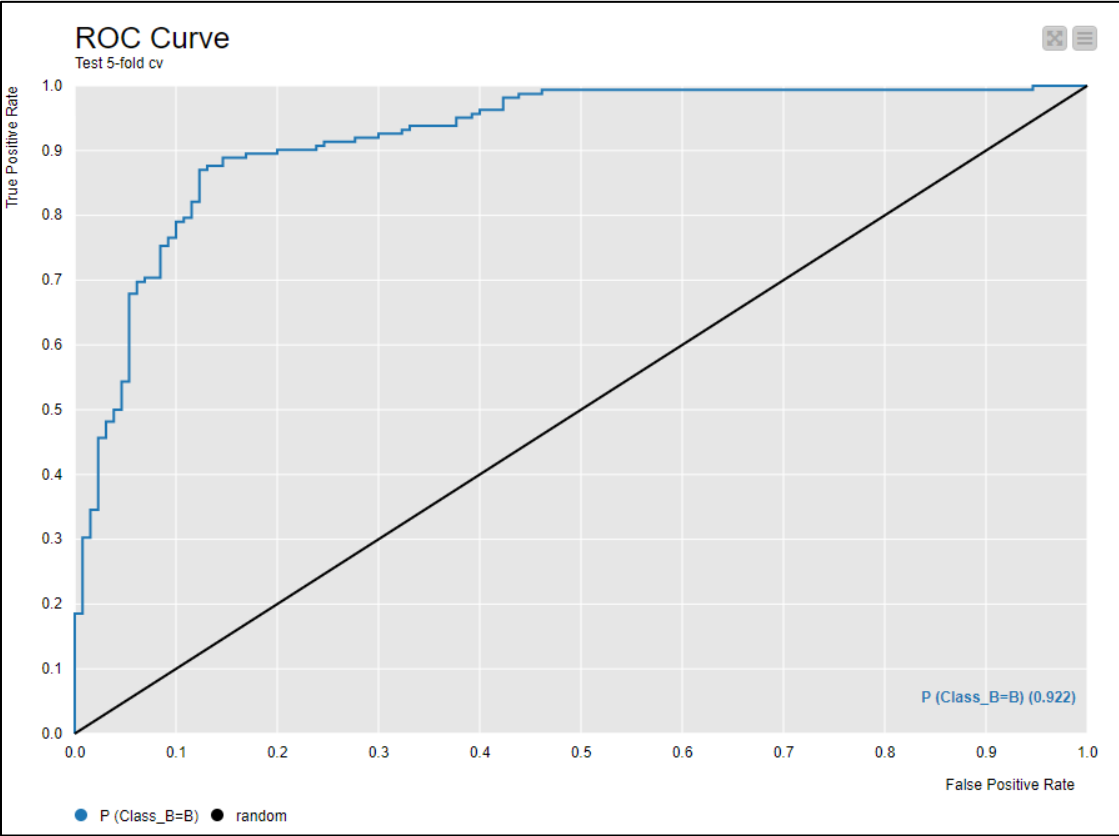


Figure S3. Box plots comparing the experimental range in the external prediction set composed of notB compounds and the distribution of the common errors in prediction among LDA and ANN models

