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Supporting Information

A Facile Circular Dichroism Protocol for Rapid Determination of Enantiomeric Excess and Concentration of Chiral Primary Amines

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Supplementary Figure S1

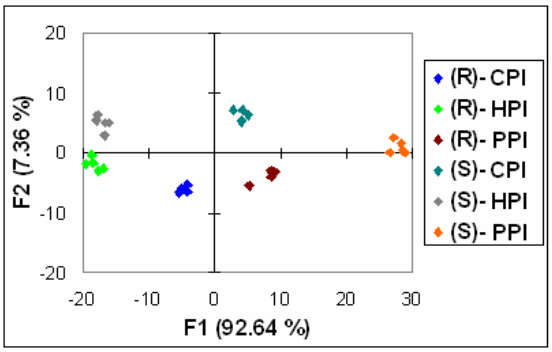
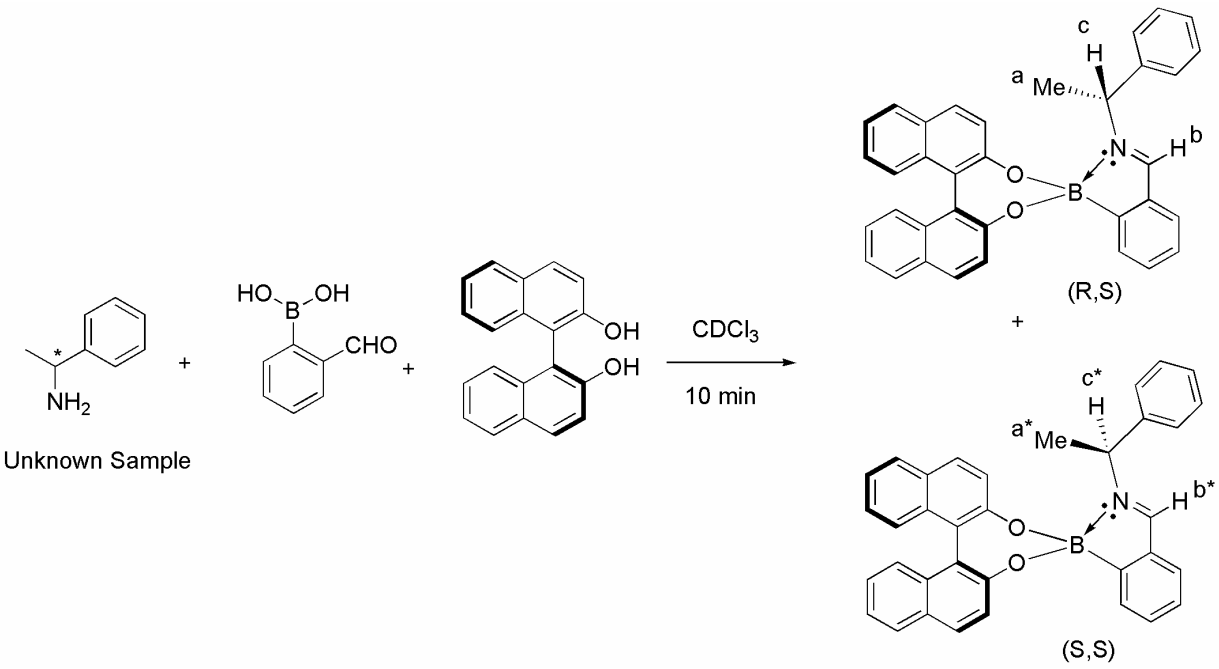


Figure S1. LDA plots obtained with: (*S*)-**1** receptor [0.4 mM].

Methods

^{1}H NMR and ^{13}C NMR was recorded on a Varian Mercury 400 MHz spectrometer. CD measurements were performed on a Jasco J-815 spectropolarimeter and ASU-605 96 well-plate reader. Reagents were used as purchased from various commercial sources. Compounds **1** is a known compound and was prepared according to literature methods.[S1]



Scheme S1. Derivatization reaction employed.

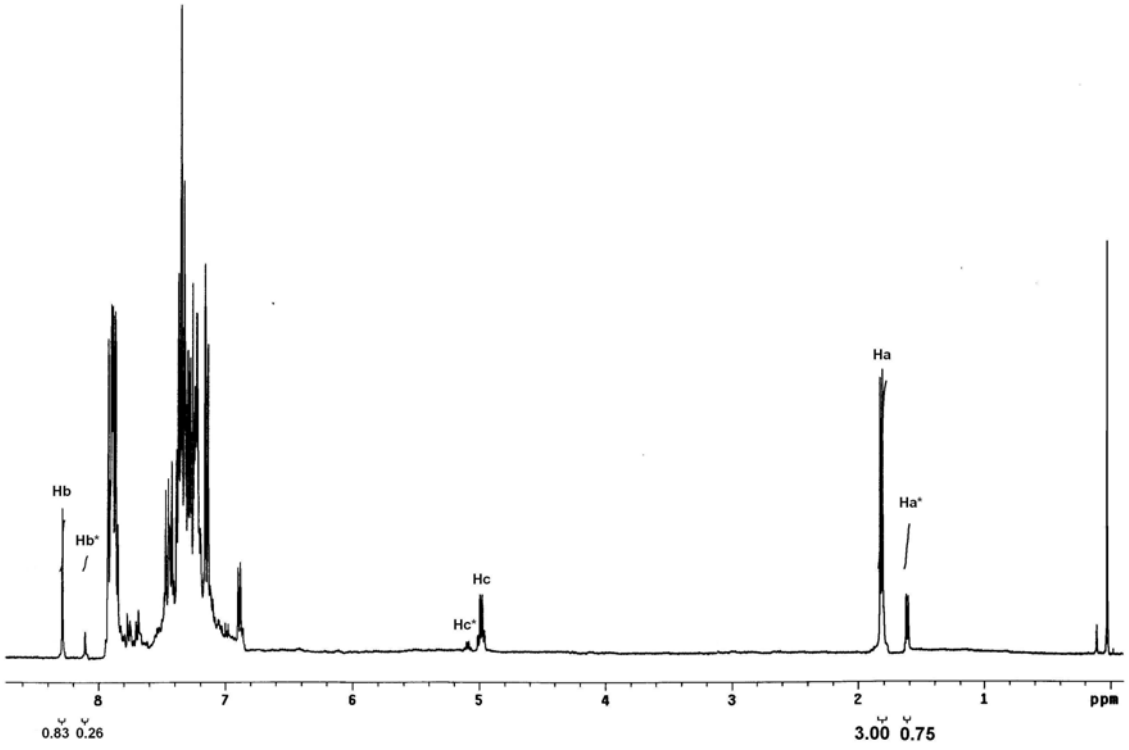


Figure S2. ^{1}H NMR spectrum of the mixture of reaction after derivatization in $CDCl_3$.

Supplementary notes

Linear Discriminant Analysis (LDA): XLSTAT[S1] was the program used to carry out the LDA studies. LDA studies allow for differentiation and classification of the analytes. The generalization error of this classification method is measured using Jackknife analysis. Principle Component Analysis (PCA): XLSTAT[S1] was also used for PCA analysis. PCA allows multivariate data to be represented in lower-dimensional space. The first two principal components are invoked to visualize the objects in two-dimensional space. The first principal component (PC1) is directed along the maximum variance. The second principal component (PC2) is orthogonal to PC1 and carries the second maximum extent of variance.

Artificial Neural Network (ANN): The ANN analyses were carried out employing the program Statistica Neural Networks 8.0.[S2] The training data consists in three *ee* trainings sets at three different $[G]_t$ values (0.2 mM, 0.8 mM and 1.4 mM). The Stadistica Neural Networks program has an embedded intelligent problem solver (IPS) function, which was requested to search for MLP consisting of networks three layers. During learning, output values from the ANN are compared to true values and the coupling weights are adjusted to give the best network. The hidden activation chosen was hyperbolic tangent and the output activation was identity. In the case of the training set data corresponding to **MBA** at 0.2 mM, the ellipticites values at 10, 30 and 50 %R were discarded.

References

S1. From xlstat.com.
S2. StatSoft, Inc.