

## Chemometrics-coupled chiral recognition using D- $\pi$ -A typed cyanostilbenes

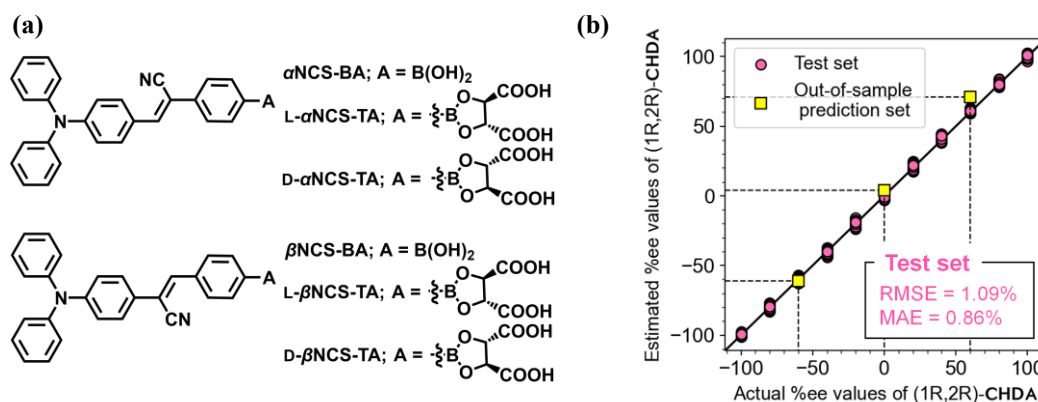
(<sup>1</sup>Graduate School of Urban Environmental Sciences, Tokyo Metropolitan University)

○Kaede Kawaguchi,<sup>1</sup> Ayana Moro,<sup>1</sup> Yuji Kubo,<sup>1</sup>

**Keywords:** Chemometrics; Chiral Recognition; Aggregation-Induced Emission; Boronic acid; Cyanostilbenes

Detection of chirality is analytically significant because the enantio-purity of products is essential for various applications in the pharmaceutical, agrochemical, and food industry. Fluorescence sensing for chirality is a highly sensitive, facile, and cost-effective method for determining enantiomer purity. However, the synthesis of well-designed host molecules is often tedious. We focused on the boronate ensembles with aggregation-induced emission (AIE) units because enantio-dependent aggregation modes endow the systems with chiral sensing capability.

Two types of boronic acid-appended D- $\pi$ -A cyanostilbenes were synthesized to produce chiral boronate ensembles *via* dehydration with tartaric acid (Fig. 1a). The aggregation-induced high sensitivity and positional effect of the CN group on the emission properties resulted in fingerprint-like emission responses for several chiral diamines. These responses were suitable for chiral recognition and calibration using linear discriminant analysis (LDA) or artificial neural network (ANN). Remarkably, the enantiomer pairs of chiral diamines were discriminated in 100% of accuracy by LDA. Furthermore, data processing with an ANN allowed for the accurate determination and prediction of enantiomer excess (% ee) for *trans*-1,2-cyclohexanediamines (**CHDAs**) with a mean absolute error of 0.86 % (Fig. 1b).<sup>1)</sup>



**Fig. 1** (a) Chemical structures of boronic acid-appended cyanostilbenes and analogs. (b) Parity plots of ANN predicted and experimental % ee values of (1R, 2R)-CHDA.

1) K. Kawaguchi, A. Moro, S. Kojima, Y. Kubo, *Chem. Commun.*, **2021**, 57, 12952–12955.