Electronic Supplementary Information

Accurate chiral pattern recognition for amines from just a single chemosensor

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CONTENTS

1. General

Materials

3-Formyl-2,2'-dihydroxy-1,1'-naphthalenes ((R)-**2**) was synthesized according to a previous method.[1] Sodium hydride, *N,N*-dimethylformamide, ethyl acetate, hexane, ammonium chloride, sodium sulfate, zinc(II) acetate dehydrate, and MeOH were purchased from Kanto Chemical Co. Inc. (1R,2R)-(−)-1,2-cyclohexanediamine ((1R,2R)-CHDA), (1S,2S)-(+)-1,2-cyclohexanediamine ((1S,2S)-CHDA), (1R,2R)-(+)-1,2-diphenylethylenediamine ((1R,2R)-DPDA), (1S,2S)-(−)-1,2-diphenylethylenediamine ((1S,2S)-DPDA), (1S,2R)-(−)-1-amino-2-indanol ((1S,2R)-AID), (1R,2S)-(+)-1-amino-2-indanol ((1R,2S)-AID), (1S,2R)-(+)-2-amino-1,2-diphenylethanol ((1S,2R)-ADPE), (1R,2S)-(−)-2-amino-1,2-diphenylethanol ((1R,2S)-ADPE)), (R)-leucinol, (S)-leucinol, and 2-(chloromethyl)pyridine hydrochloride were purchased from Tokyo Chemical Industry Co., Ltd.

Measurements

NMR spectra were taken by a Bruker Avance 500 MHz NMR spectrophotometer (^{1}H: 500 MHz, ^{13}C: 126 MHz), In ^{1}H and ^{13}C NMR measurements, chemical shifts (δ) were reported downfield from the initial standard Me$_3$Si. Mass spectrometry (MS) was performed by a Shimadzu LCMS-2020 with methanol as an eluent in an electrospray

ionization (ESI). Elemental analyses were performed on an Exeter Analytical, Inc. CE-440F Elemental Analyzer. UV−vis spectra were measured by a Shimadzu UV-2600 spectrophotometer within the wavelength range from 300 nm to 500 nm. The CD spectra were recorded by a JASCO J-820 spectropolarimeter within the wavelength range from 300 nm and 500 nm. Fluorescence spectra were measured by a HITACHI F-7100 spectrophotometer. The solutions of (R)-**1** with Zn^{2+} was excited at 365 nm. Fluorescence spectra were recorded within the wavelength range from 390 nm and 700 nm at a scan rate of 240 nm/min under ambient room conditions at 25 °C. The band passes of both excitation and emission were set to 10 nm. Titration of chiral amines was performed in MeOH. The titration isotherms were constructed from changes in the fluorescence maximum at 490 nm for the complexes. The absolute emission quantum yields were measured using a Hamamatsu Photonics Quantaurus-QY, C11347-01. The fluorescence lifetimes of the fluorophores were recorded on a fluorescence lifetime spectrometer (Hamamatsu Photonics Quantaurus-Tau, C11367-01). A quartz cuvette (Hamamatsu Photonics A10095-02, 10 mm × 10 mm) was used for the optical measurements.

Preparation of the mixture of (R)-1, amines, and Zn(OAc)₂

(R)-**1** in MeOH (8.0 mM) and $Zn(OAc)_2$ in MeOH (8.0 mM) were mixed at a volume ratio of 1 to 1 in a 200 μL microtube. 100 μL of the resulting mixture (*i.e.* sensor stock

solution) was incubated at 400 rpm at 25 °C for 1 h by a Thermo-Shaker TS-100. Next,

solutions of target chiral amines (4.0 mM) were prepared in MeOH. 50 μL of the amine

solution (4.0 mM) and 50 μL of the sensor solution (4.0 mM) were mixed and incubated

at 400 rpm at 25 °C for 24 h. The final concentration was 2.0 mM for each of (R)-**1,**

Zn(OAc)$_2$ and the chiral amines. The solution was diluted and subsequently analyzed by

UV-vis (10 times dilution) and fluorescence measurements (200 times dilution).

Array experiments

The array experiments for qualitative and quantitative analyses were performed in 384-

well microplates. The solutions containing (R)-**1** (10 μM), Zn(OAc)$_2$ (10 μM), and chiral

amines were injected into the microplates with the contact-free dispenser. Each

experiment was repeated for 24 times. Each micro-well received 100 μL of the solution

which contained the (R)-**1** and Zn(OAc)$_2$, and a mixture of chiral amimes. Fluorescence

spectra were measured by a Biotek SYNERGY H1 microplate reader within the

wavelength range from 400 nm to 680 nm. The resulting spectra data were applied to the

Student's t-test to exclude 4 outlier data-points from the 24 repetitions. The coefficient of

variability among the data within the class of 20 repetitions was lower than 12%. The

obtained data for the qualitative assay by a linear discriminant analysis (LDA) was carried

out without any further pretreatment. In ANN-BP regression procedure, % ee analysis of CHDA was performed in CHDA solutions with different % ee values (0, 10, 20, 30, 40, 50, 60, 70, 80, 86, 96, and 100%ee). ANN-BP algorithm was trained using 10 types of (1R,2R)-CHDA sample with 20 replications for each % ee value (totally 200 samples for training dataset). Prediction dataset also included 2 samples with 10 repetitions (totally 20 samples for prediction dataset). The training datasets were only preprocessed by autoscaling. The optimal number of the neurons was found to be 3, and venetian blinds with 10 splits was utilized for cross validation process. The calculation software SYSTAT13 was purchased from HULINKS. The artificial neural network (ANN) analysis was performed using PLS Toolbox 8.7 (Eigenvector Research, Inc., Manson, WA USA 98831; http://www.eigenvector.com) under MATLAB 2018a (MATLAB 9.4, The Mathworks Inc., Natick).

2. Synthesis of (*R*)-2-hydroxy-2'-(2-pyridylmethyloxy)-3-formyl-1,1'-binaphthalene ((*R*)-1)
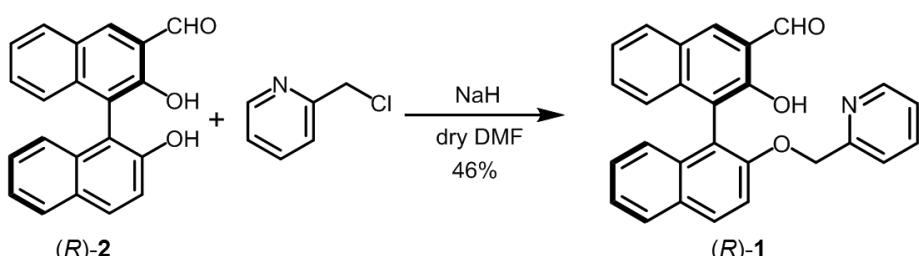
Compound (*R*)-2[1] (2.00 g, 6.37 mmol) and NaH (0.637 g, 15.9 mmol) were dissolved in dry DMF (40 mL) under a N_2 condition and the resultant solution was stirred for 30 min at room temperature. To the solution was added a solution of 2-(chloromethyl)pyridine hydrochloride (1.25 g, 7.63 mmol) in dry DMF (20 mL) at room temperature. The mixture was stirred for 3 hours in the range of room temperature to 40 °C. After addition of *sat*. NH_4Cl aqueous solution, the target was extracted using AcOEt：hexane＝3：1 (v/v). The organic phase was dried with Na_2SO_4 and evaporated. The residue was chromatographed on silica gel (Wakogel C-300) using an eluent AcOEt：hexane＝1：2 (v/v) to give (*R*)-1 (0.496 g) as a yellow solid. Because 1.18 g of (*R*)-2 was also isolated from the chromatography, the production yield based on recovered starting material was determined to be 46% yield.

^{1}H NMR (500 MHz, CDCl₃): *δ* (ppm) 10.50 (s, 1H), 10.22 (s, 1H), 8.46–8.47 (s, 1H), 8.34 (m, 1H), 7.99–8.01 (m, 2H), 7.95 (d, 1H, *J* = 9.10 Hz), 7.87 (d, 1H, *J* = 8.20 Hz),

7.43 (d, 1H, J = 9.10 Hz), 7.33–7.42 (m, 4H), 7.27–7.29 (m, 2H), 7.18–7.22 (m, 2H), 7.07 (dd, 1H, J = 7.18 and 5.13 Hz), 6.90 (d, 1H, J = 7.85 Hz), 5.27 (d, 1H, J = 14.3 Hz), 5.22 (d, 1H, J = 14.4 Hz); ^{13}C NMR (126 MHz, CDCl$_3$): δ (ppm) 196.7, 157.6, 153.8, 153.5, 148.8, 137.9, 137.7, 136.6, 133.7, 130.3, 130.2, 129.8, 129.5, 128.2, 127.6, 126.8, 125.4, 124.9, 124.3, 124.0, 122.3, 122.2, 120.8, 118.6, 117.9, 114.9, 71.4; FAB-MS$^+$: *m/z* 406 [M+H]$^+$; Elemental analysis calcd (%) for C$_{27}$H$_{19}$NO$_3$ 0.1H$_2$O: C 79.63, H 4.75, N 3.44 ; found: C 79.51, H 4.69, N 3.34.
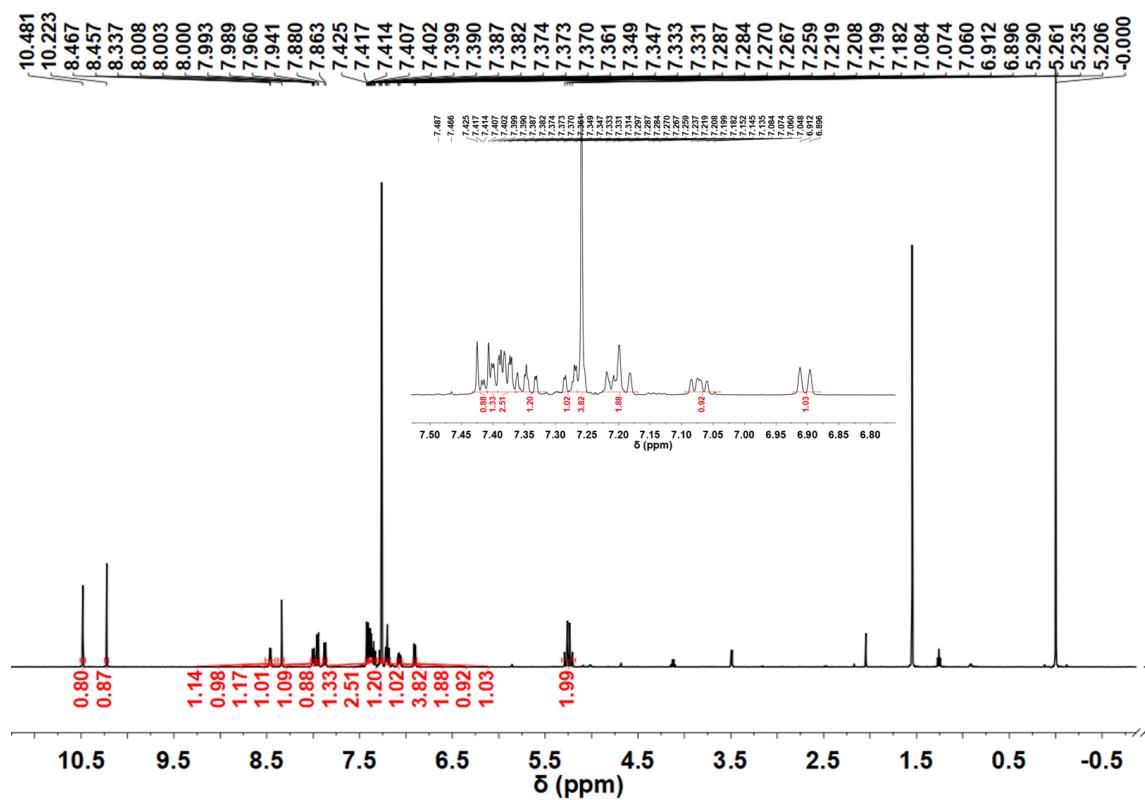
Fig. S1 ^{1}H NMR spectrum of (*R*)-**1** (500 MHz, CDCl$_3$).
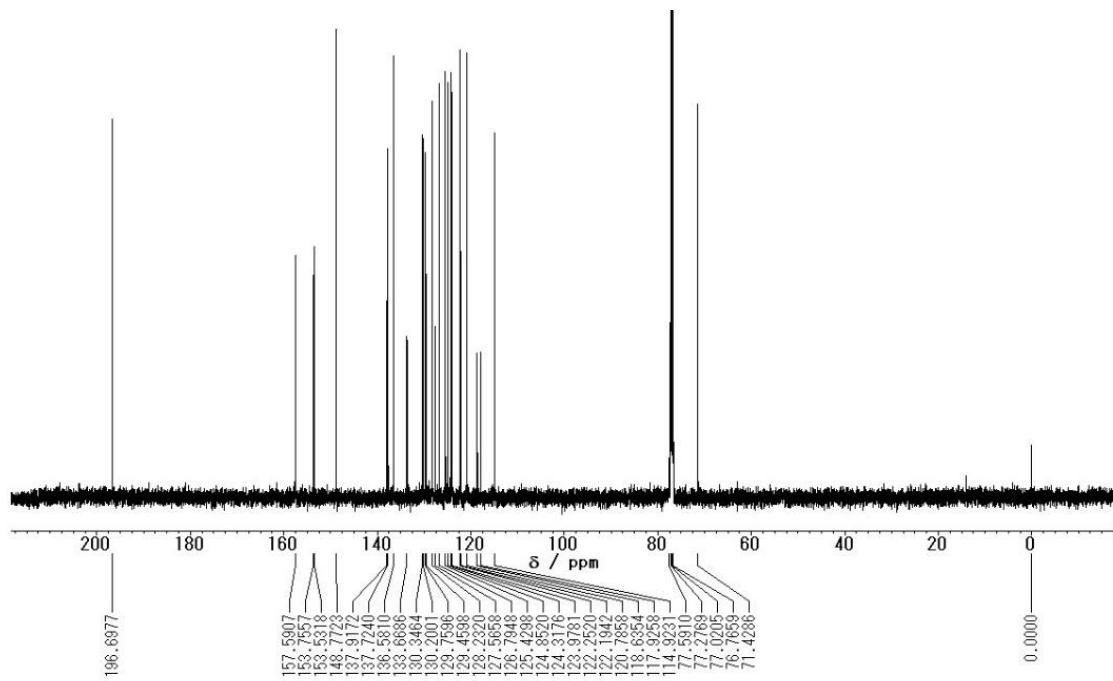
Fig. S2 ^{13}C NMR spectrum of (*R*)-**1** (126 MHz, CDCl$_3$).

3. X-ray Structural Analysis

The data were collected on a Rigaku XtaLAB P200 diffractometer using a graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) at 93 K. Data reduction was performed using CrysAlis[Pro].[2] The structure was solved by direct methods using SHELXS-2013[3] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/1[4] The hydrogen atoms on carbon were calculated in ideal positions. The isotropic displacement parameters of hydrogen atoms were set to 1.2 x Ueq (1.5 x Ueq for hydroxy hydrogen atoms) of the attached atom. (The function, $\sum w(|Fo|^2 - |Fc|^2)^2$, was minimized, where w = $1/[(\sigma2(Fo))^2 + (0.0537*P)^2 + (0.1283*P)]$ and P = $(|Fo|^2 + 2|Fc|^2)/3$. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the *International Tables for X-ray Crystallography*.[5] All figures were generated using Mercury from CCDC.
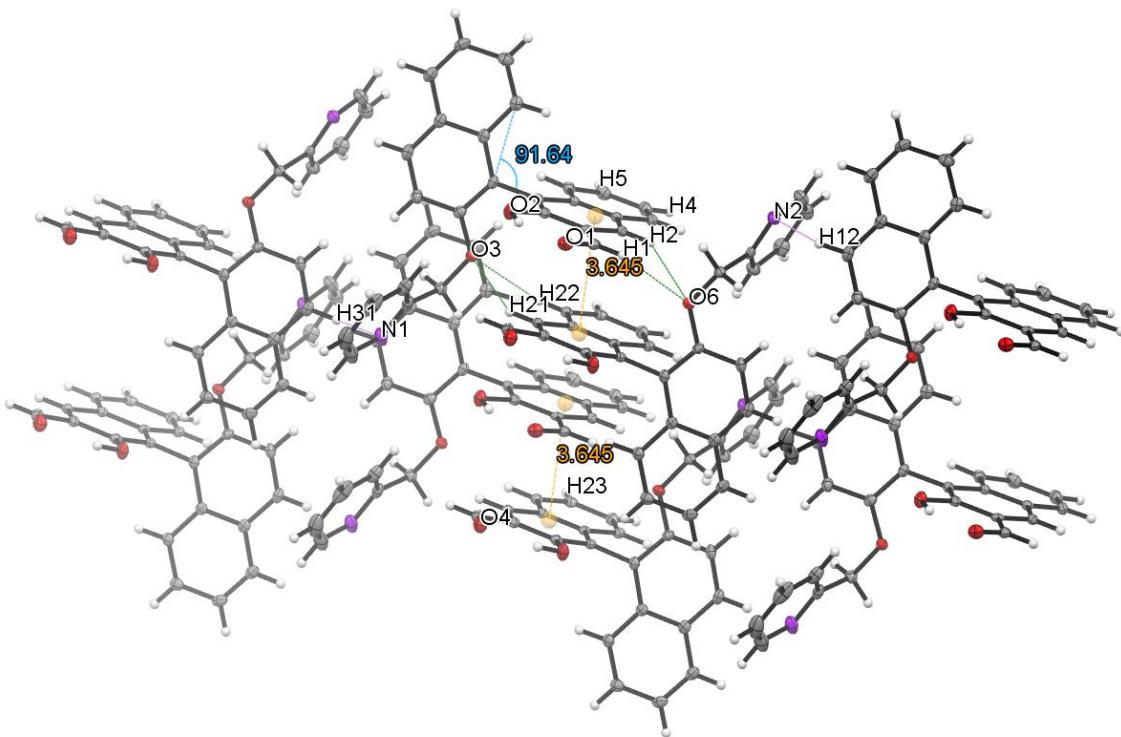
Fig. S3 The X-ray diffraction packing structure of (*R*)-**1**. Thermal ellipsoids are scaled to the 50% probability level. The carbon atoms are shown in dark grey, the nitrogen atoms in purple, the oxygen atoms in red (CCDC 1976941).

The single crystal structure of (*R*)-**1** was assigned the triclinic of crystal system with *P*-1 of space group. The ideal face-to-face π-stacking[6] (*i.e.* [centroid$_{naphthalene}$···centroid$_{naphthalene}$ distance (Å): 3.645] for π$_{naphthalene}$—π$_{naphthalene}$ stack) was also observed in the packing structure. The inner O3 and O6 of the ether units showed two intermolecular hydrogen bonds (*i.e.* [O$_{ether}$···H distances (Å): O3···H21 2.518, O3···H22 2.550, O6···H1 2.563, O6···H2 2.630] for O$_{ether}$—H forces). In addition, the N$_{pyridine}$s exhibited hydrogen bonds with H$_{naphtalene}$ at the outer packing layer in Fig. S3 (*i.e.* [N$_{pyridine}$···H distances (Å): N1···H31 2.500, N2···H12 2.564] for N$_{pyridine}$—H strength). It was found that multi O—H intermolecular hydrogen bonds contributed to

two dimensional expansion of naphthalene units (*i.e.* [$O_{alcohol}\cdots H$ distances (Å): O1$\cdots$

H4 2.563, O4$\cdots$H23 2.465] for $O_{alcohol}$—H strength and [$O_{aldehyde}\cdots H$ distance (Å):

O2$\cdots$H14 2.660] for $O_{aldehyde}$—H strength).

Table S1 Crystallographic data and structure refinement for (*R*)-**1**.

Empirical formula	C27 H19 N O3
Formula weight	405.43
Temperature	93 K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	a = 7.1378(2) Å alpha = 88.9786(16)deg.
	b = 9.8466(2) Å beta = 79.0044(17)deg.
	c = 14.7942(3) Å gamma = 74.6213(19)deg
Volume	983.56(4) Å
Z, Calculated density	2, 1.369 g/m^3
Absorption coefficient	0.089 mm^{-1}
F(000)	424
Crystal size	0.06 x 0.10 x 0.22 mm
Theta range for data collection	2.81 to 28.82 deg
Limiting indices	-9<=h<=7, -12<=k<=12, -19<=l<=19
Reflections collected / unique	15510 / 7323 [R(int) = 0.0205]
Completeness to theta =	25.24 99.9 %
Absorption correction	MULTI-SCAN
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7323 / 3 / 567
Goodness of fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0904
R indices (all data)	R1 = 0.0368, wR2 = 0.0923
Largest diff. peak and hole	0.30 and -0.23 e. Å^{-3}

4. ^{1}H NMR Titration
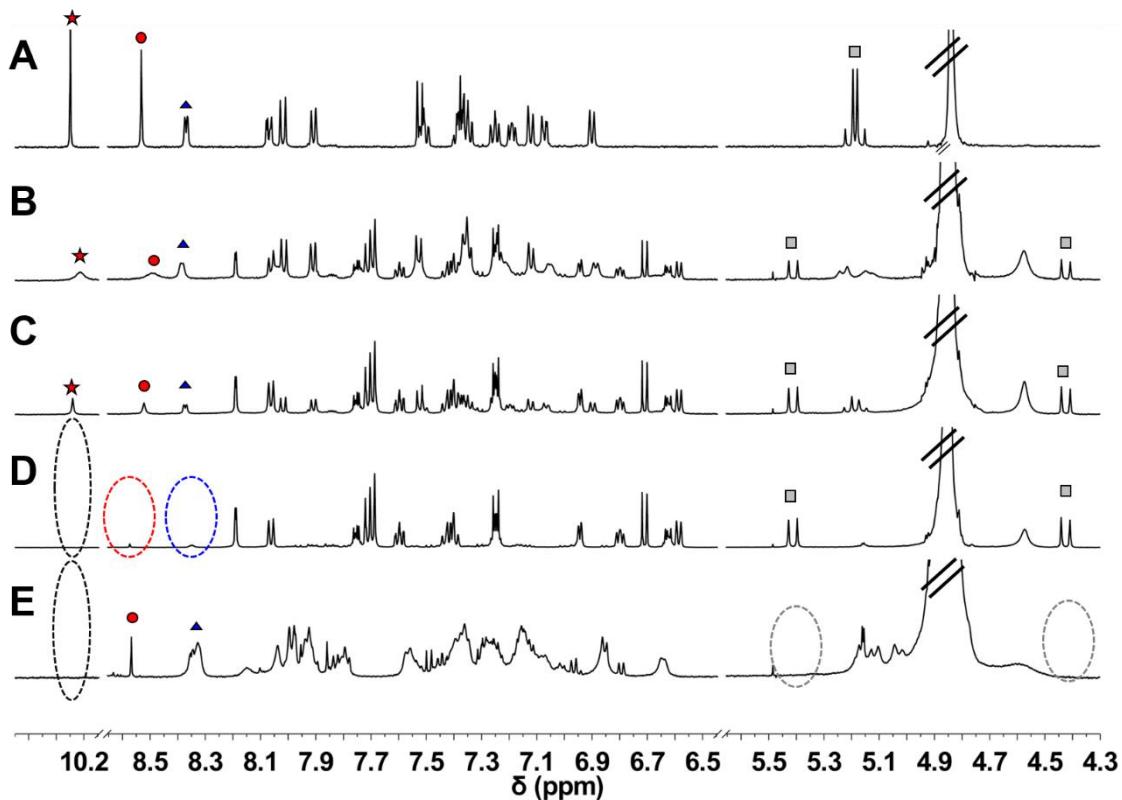
Fig. S4 ^{1}H NMR spectra (500 MHz, MeOD) of (A) (*R*)-**1**, and the mixture of (*R*)-**1** and (B) 0.75 mM, (C) 1.5 mM, (D) 3 mM, and (E) 9 mM of (1*R*,2*R*)-CHDA in the presence of Zn(OAc)$_2$. [(*R*)-**1**] = 3.0 mM, [Zn(OAc)$_2$] = 3.0 mM. The mixture of (*R*)-**1** and (1*R*,2*R*)-CHDA in the presence of Zn(OAc)$_2$ was incubated at 25 °C for 24 h.

5. Time Dependent Fluorescence Spectra
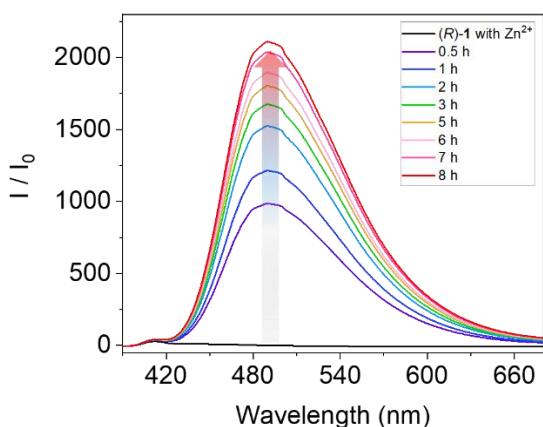
Fig. S5 Time-dependent fluorescence spectral changes of a mixture of (*R*)-**1** upon and (1*R*,2*R*)-CHDA in the presence of Zn(OAc)$_2$ in MeOH at 25 °C. [(*R*)-**1**] = [Zn(OAc)$_2$] = [(1*R*,2*R*)-CHDA] = 10 μM. λ_{ex} = 365 nm. The mixture was incubated for 8 h.

6. Examples of Fluorescence Titrations
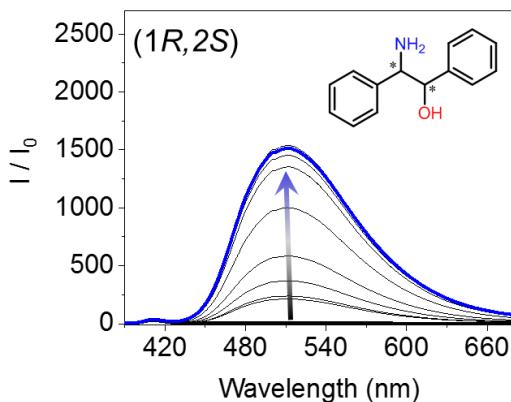
Fig. S6 Fluorescence spectra of (R)-**1** with Zn(OAc)$_2$ upon the addition of (1R,2S)-ADPE in MeOH at 25 °C. [(R)-**1**] = [Zn(OAc)$_2$] = 10 µM, [(1R,2S)-ADPE] = 0–30 µM. λ_{ex} = 365 nm.
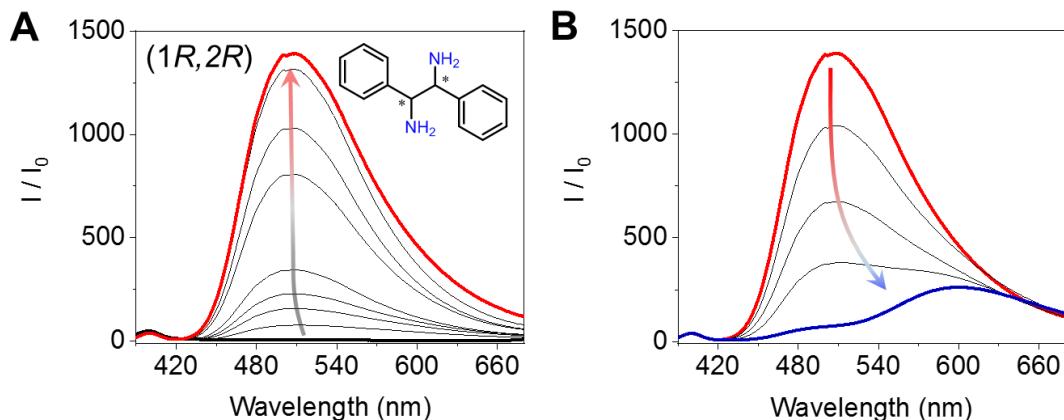
Fig. S7 Fluorescence spectra of (R)-**1** with Zn(OAc)$_2$ upon the addition of (1R,2R)-DPDA in MeOH at 25 °C. [(R)-**1**] = [Zn(OAc)$_2$] = 10 µM, [(1R,2R)-DPDA] = (A) 0–12.5 µM and (B) 12.5–30 µM. λ_{ex} = 365 nm.
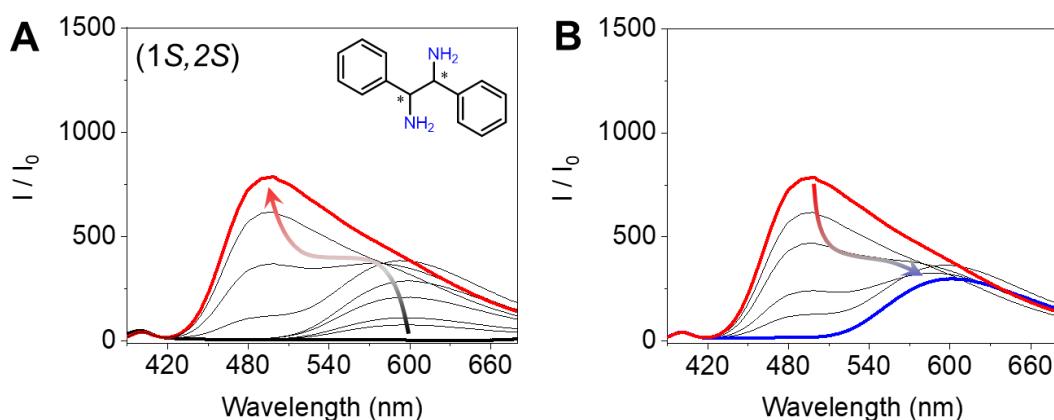
Fig. S8 Fluorescence spectra of (R)-**1** with Zn(OAc)$_2$ upon the addition of (1S,2S)-DPDA in MeOH at 25 °C. [(R)-**1**] = [Zn(OAc)$_2$] = 10 µM, [(1S,2S)-DPDA] = (A) 0–10 µM and (B) 10–30 µM. λ_{ex} = 365 nm.
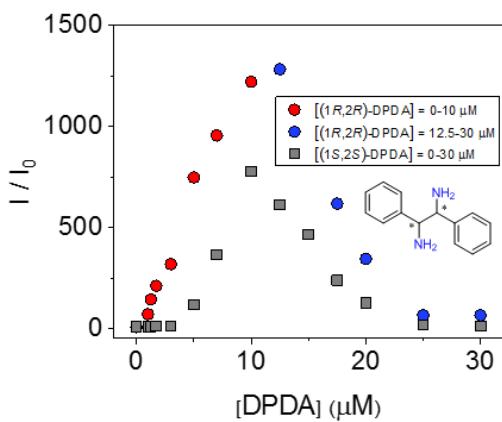
Fig. S9 Titration isotherms for DPDA. The isotherms were obtained by collecting the intensities at the maximum emission wavelength (λ_{em}= 490 nm) at various concentrations of DPDA.
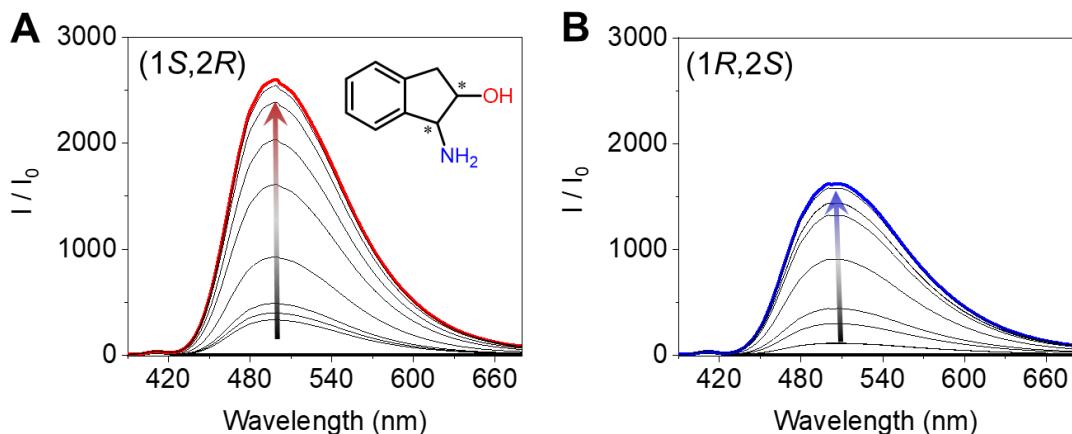
Fig. S10 Fluorescence spectra of (*R*)-**1** with $Zn(OAc)_2$ upon the addition of (A) (1*S*,2*R*)-AID and (B) (1*R*,2*S*)-AID in MeOH at 25 °C. [(*R*)-**1**] = [$Zn(OAc)_2$] = 10 μM, [AID] = 0–30 μM. λ_{ex} = 365 nm.
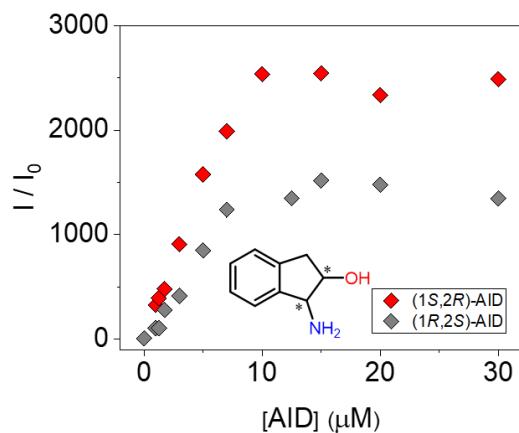
Fig. S11 Titration isotherms for AID. The titration isotherms were obtained by collecting the intensities at the maximum emission wavelength (λ_{em}= 490 nm) at various concentrations of AID.
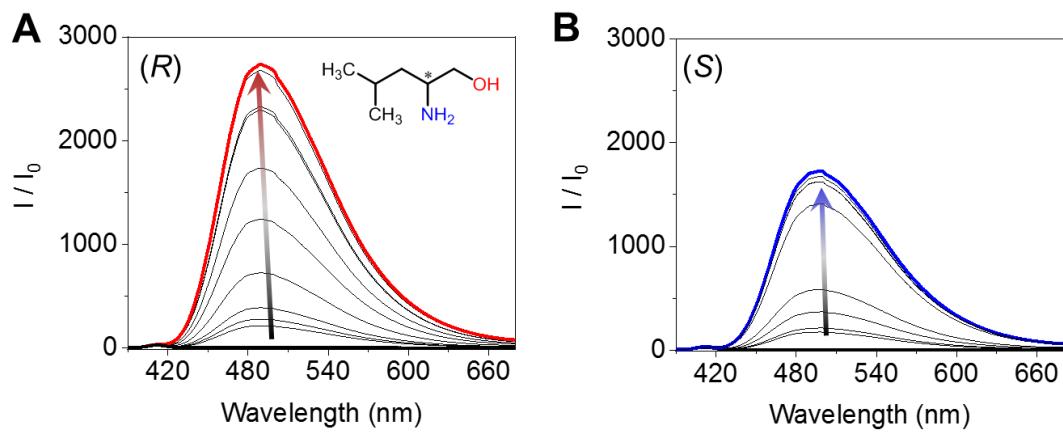
Fig. S12 Fluorescence spectra of (*R*)-**1** with $Zn(OAc)_2$ upon the addition of (A) (*R*)-leucinol and (B) (*S*)-leucinol in MeOH at 25 °C. [(*R*)-**1**] = [$Zn(OAc)_2$] = 10 μM, [leucinol] = 0–30 μM. λ_{ex} = 365 nm.
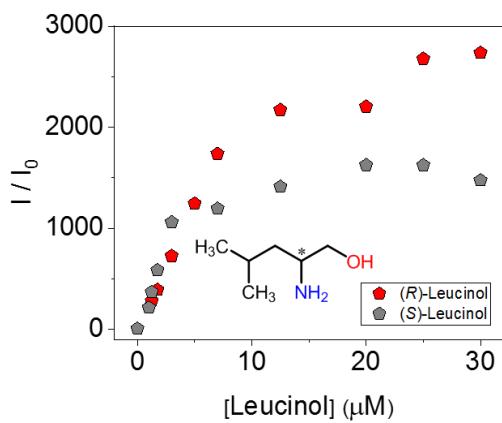
Fig. S13 Titration isotherms for leucinol. The isotherms were obtained by collecting the intensities at the maximum emission wavelength (λ_{em}= 490 nm) at various concentrations of leucinol.

7. Examples of CD and UV-vis titrations
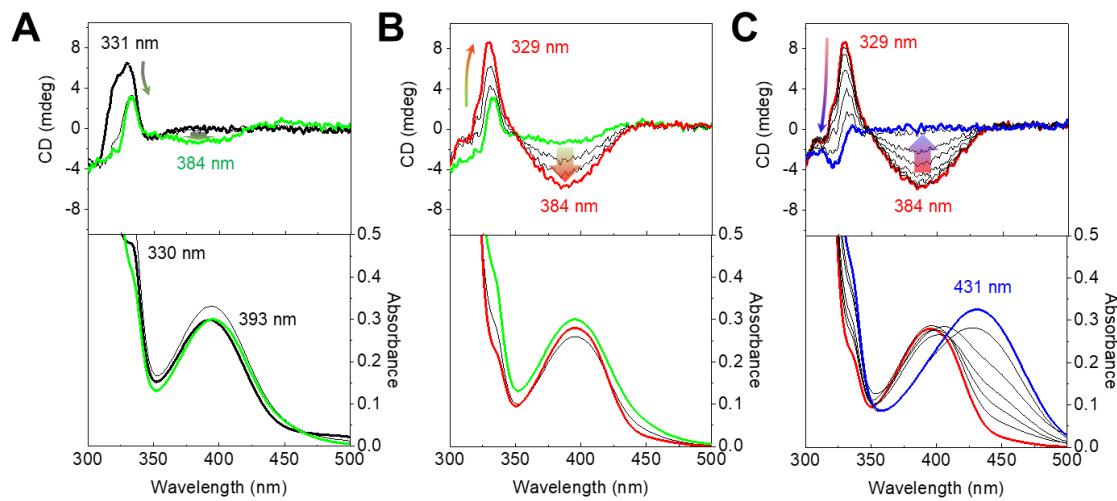
Fig. S14 CD and UV-vis spectra of (*R*)-**1** with Zn(OAc)$_2$ upon the addition of (1*R*,2*R*)-CHDA in MeOH at 25 °C. [(*R*)-**1**] = [Zn(OAc)$_2$] = 200 μM, [(1*R*,2*R*)-CHDA] = (A) 0—60 μM, (B) 60—200 μM, and (C) 200—600 μM. The mixture of (*R*)-**1** and (1*R*,2*R*)-CHDA with Zn(OAc)$_2$ was incubated at 25 °C for 24 h.
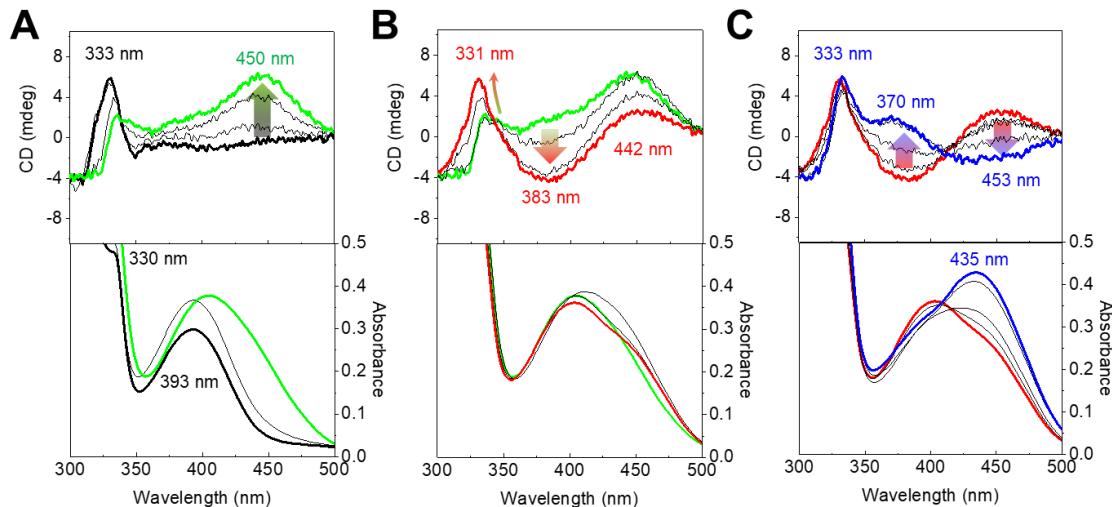
Fig. S15 CD and UV-vis spectra of (*R*)-**1** with Zn(OAc)$_2$ upon the addition of (1*S*,2*S*)-CHDA in MeOH at 25 °C. [(*R*)-**1**] = [Zn(OAc)$_2$] = 200 μM, [(1*S*,2*S*)-CHDA] = (A) 0—100 μM, (B) 100—300 μM, and (C) 300—600 μM. The mixture of (*R*)-**1** and (1*S*,2*S*)-CHDA with Zn(OAc)$_2$ was incubated at 25 °C for 24 h.
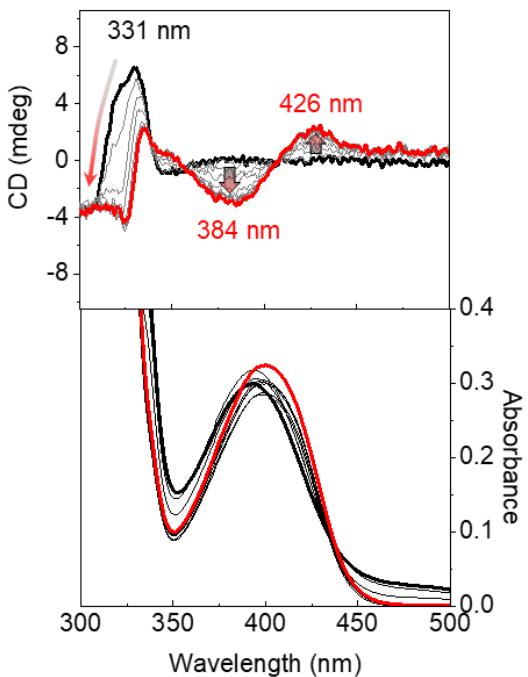
Fig. S16 CD and UV-vis spectra of (*R*)-**1** with Zn(OAc)$_2$ upon the addition of (1*S*,2*R*)-ADPE in MeOH at 25 °C. [(*R*)-**1**] = [Zn(OAc)$_2$] = 200 μM, and [(1*S*,2*R*)-ADPE] = 0—600 μM. The mixture of (*R*)-**1** and (1*S*,2*R*)-ADPE with Zn(OAc)$_2$ was incubated at 25 °C for 24 h.

8. Emission Quantum yield and Emission Lifetime

Table S2 The emission quantum yield (*Φ*) and emission lifetime (*τ*) of (*R*)-**1** and CHDA complexes in the presence of Zn(OAc)$_2$.

Target amine	*Φ* (%)	τ_1 (ns)	τ_2 (ns)
(1*R*,2*R*)-CHDA	20.0	9.6	
(1*S*,2*S*)-CHDA	7.0	2.0	4.4

[(*R*)-**1**] = [Zn(OAc)$_2$] = [CHDA] = 10 μM. λ_{ex} = 365 nm. The mixture of (*R*)-**1**, CHDA, and Zn(OAc)$_2$ was incubated at 25 °C for 24 h.

Table S3 The emission quantum yield (*Φ*) and emission lifetime (*τ*) of (*R*)-**1** and ADPE complexes in the presence of Zn(OAc)$_2$.

Target amine	*Φ* (%)	*τ* (ns)
(1*S*,2*R*)-ADPE	14.0	14.1
(1*R*,2*S*)- ADPE	6.3	12.0

[(*R*)-**1**] = [Zn(OAc)$_2$] = [ADPE] = 10 μM. λ_{ex} = 365 nm. The mixture of (*R*)-**1**, ADPE, and Zn(OAc)$_2$ was incubated at 25 °C for 24 h.

9. ESI MS Analysis
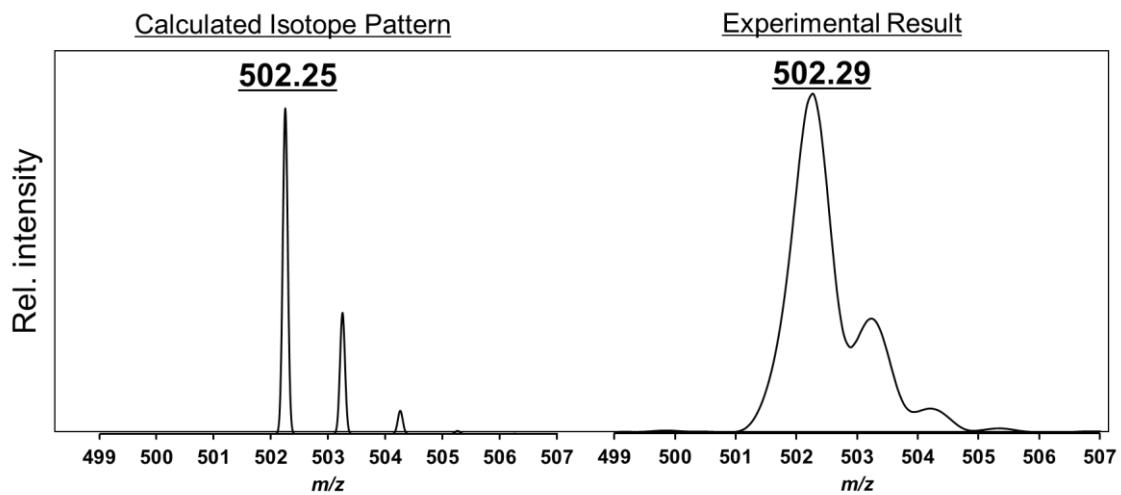
Fig. S17 ESI mass spectra (positive) of the mixture of (*R*)-**1**, (1*R*,2*R*)-CHDA, and Zn(OAc)$_2$ in MeOH. Calculated isotope pattern for C$_{33}$H$_{32}$N$_3$O$_2^+$.
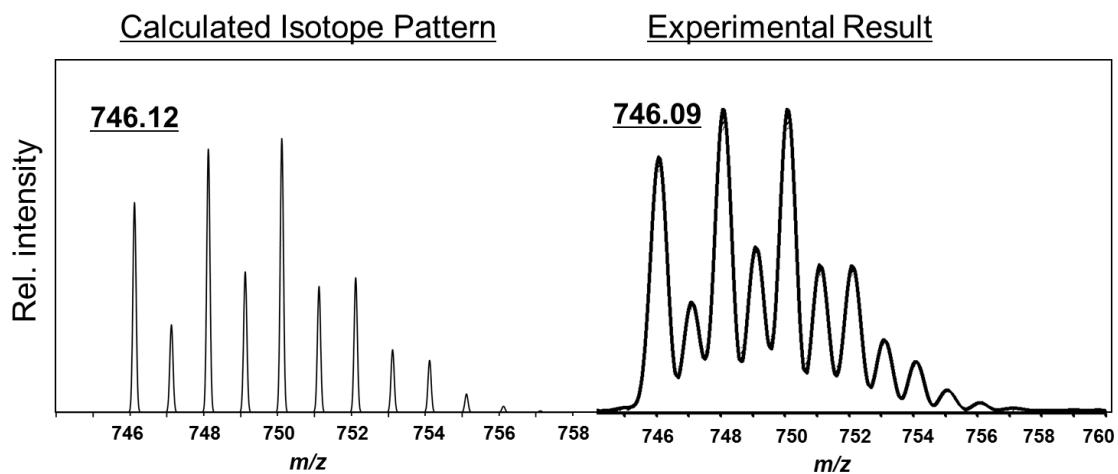
Fig. S18 ESI mass spectra (positive) of the mixture of (*R*)-**1**, (1*R*,2*R*)-CHDA, and Zn(OAc)$_2$ in MeOH. Calculated isotope pattern for C$_{37}$H$_{36}$N$_3$O$_6$Zn$_2^+$.

10. Linear Discriminant Analysis (LDA)
Qualitative assay
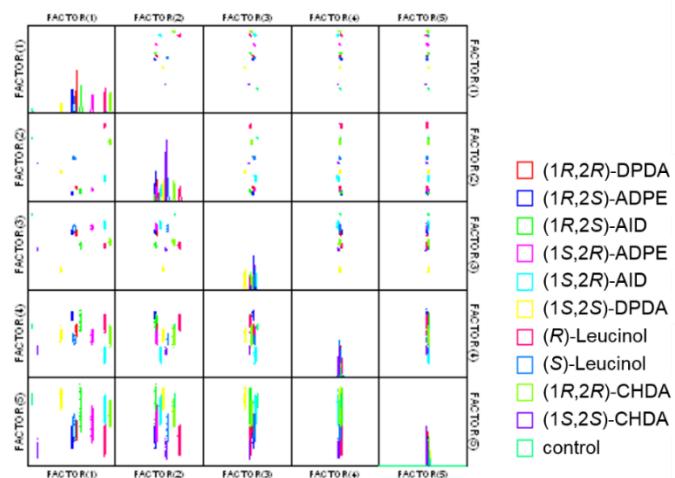
Fig. S19 The canonical score plot of qualitative assay for chiral amines.

Table S4 The jackknifed classification matrix of qualitative assay.

Jackknifed Classification Matrix

	(1R,2R)-DPDA	(1R,2S)-ADPE	(1R,2S)-AID	(1S,2R)-ADPE	(1S,2R)-AID	(1S,2S)-DPDA	(R)-Leucinol	(S)-Leucinol	(1R,2R)-CHDA	(1S,2S)-CHDA	control	%correct
(1R,2R)-DPDA	20	0	0	0	0	0	0	0	0	0	0	100
(1R,2S)-ADPE	0	20	0	0	0	0	0	0	0	0	0	100
(1R,2S)-AID	0	0	20	0	0	0	0	0	0	0	0	100
(1S,2R)-ADPE	0	0	0	20	0	0	0	0	0	0	0	100
(1S,2R)-AID	0	0	0	0	20	0	0	0	0	0	0	100
(1S,2S)-DPDA	0	0	0	0	0	20	0	0	0	0	0	100
(R)-Leucinol	0	0	0	0	0	0	20	0	0	0	0	100
(S)-Leucinol	0	0	0	0	0	0	0	20	0	0	0	100
(1R,2R)-CHDA	0	0	0	0	0	0	0	0	20	0	0	100
(1S,2S)-CHDA	0	0	0	0	0	0	0	0	0	20	0	100
control	0	0	0	0	0	0	0	0	0	0	20	100
%correct	20	20	20	20	20	20	20	20	20	20	20	100

Semi-quantitative assay for the concentrations of CHDA
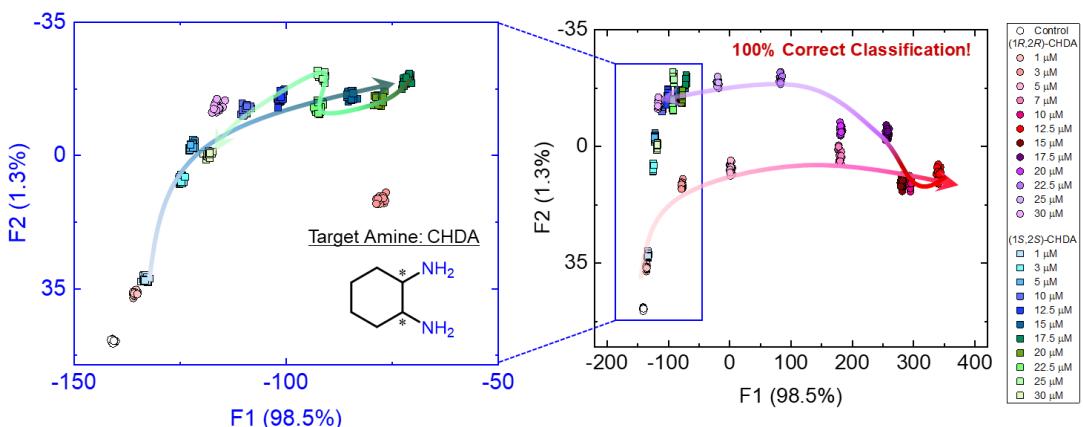
Fig. S20 LDA results of the semi-quantitative assay for CHDA (circle: (1R,2R)-CHDA, square: (1S,2S)-CHDA). Twenty repetitions were conducted for each target.
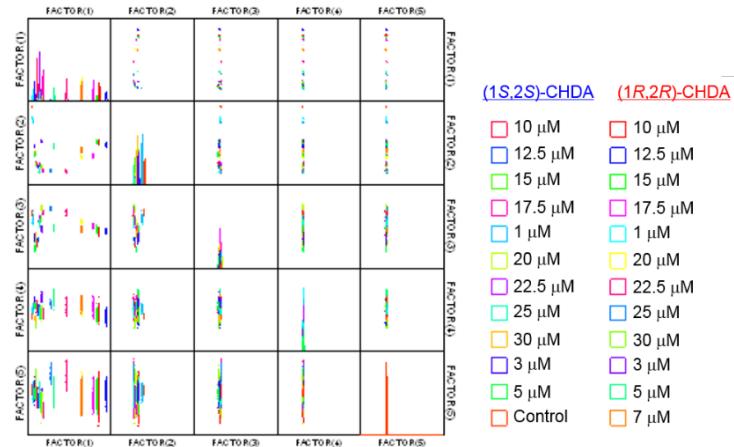
Fig. S21 The canonical score plot of semi-quantitative assay for CHDA.

Table S5 The jackknifed classification matrix of semi-quantitative assay.

Jackknifed Classification Matrix

	10 μM	12.5 μM	15 μM	17.5 μM	1 μM	20 μM	22.5 μM	25 μM	30 μM	3 μM	5 μM	7 μM	10 μM	12.5 μM	15 μM	17.5 μM	1 μM	20 μM	22.5 μM	25 μM	30 μM	3 μM	5 μM	control	%correct
10 μM	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
12.5 μM	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
15 μM	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
17.5 μM	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
1 μM	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
20 μM	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
22.5 μM	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
25 μM	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
30 μM	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
3 μM	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
5 μM	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	0	100
7 μM	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	0	100
10 μM	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	0	100
12.5 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	0	100
15 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	0	100
17.5 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	0	100
1 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	0	0	100
22.5 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	0	100
25 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	0	100
30 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	0	100
3 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	0	100
5 μM	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	0	100
control	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	20	100
%correct	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	100
Total	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	20	100

(1*S*,2*S*)-CHDA (blue)   (1*R*,2*R*)-CHDA (red)

(1*S*,2*S*)-CHDA (blue)	(1*R*,2*R*)-CHDA (red)
0 μM	0 μM
1 μM	1 μM
3 μM	3 μM
5 μM	5 μM
10 μM	7 μM
12.5 μM	10 μM
15 μM	12.5 μM
17.5 μM	15 μM
20 μM	17.5 μM
22.5 μM	20 μM
25 μM	22.5 μM
30 μM	25 μM
	30 μM

Semi-quantitative assay for the determination of % ee
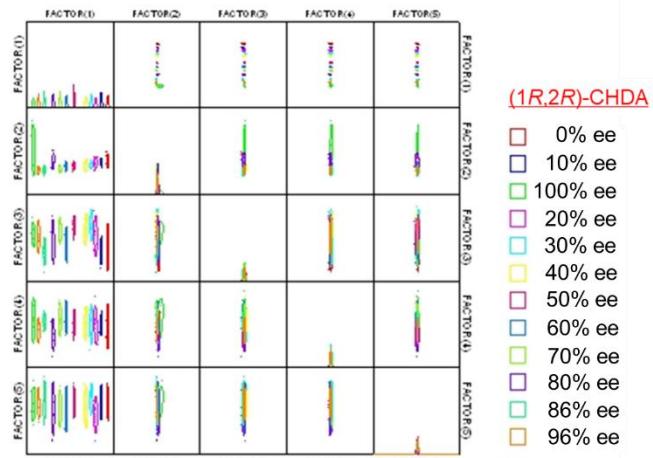
Fig. S22 The canonical score plot of % ee determination in (1*R*,2*R*)-CHDA.

Table S6 The jackknifed classification matrix of % ee determination in (1*R*,2*R*)-CHDA

Jackknifed Classification Matrix

	0% ee	10% ee	100% ee	20% ee	30% ee	40% ee	50% ee	60% ee	70% ee	80% ee	86% ee	96% ee	%correct
0% ee	20	0	0	0	0	0	0	0	0	0	0	0	100
10% ee	0	20	0	0	0	0	0	0	0	0	0	0	100
100% ee	0	0	20	0	0	0	0	0	0	0	0	0	100
20% ee	0	0	0	19	1	0	0	0	0	0	0	0	95
30% ee	0	0	0	0	20	0	0	0	0	0	0	0	100
40% ee	0	0	0	0	0	20	0	0	0	0	0	0	100
50% ee	0	0	0	0	0	0	20	0	0	0	0	0	100
60% ee	0	0	0	0	0	0	0	20	0	0	0	0	100
70% ee	0	0	0	0	0	0	0	0	20	0	0	0	100
80% ee	0	0	0	0	0	0	0	0	0	20	0	0	100
86% ee	0	0	0	0	0	0	0	0	0	0	20	0	100
96% ee	0	0	0	0	0	0	0	0	0	0	0	20	100
Total	20	20	20	19	21	20	20	20	20	20	20	20	100

11. Input / Output Datasets of the % ee determination in (1*R*,2*R*)-CHDA

Table S7 Input calibation dataset of the % ee determination in (1*R*,2*R*)-CHDA

% ee in (1*R*,2*R*)-CHDA	Fluorescence intensities									
	400 nm	410 nm	420 nm	430 nm	440 nm	450 nm	460 nm	470 nm	480 nm	490 nm
100% ee	812	1253	1456	2735	6321	13753	19022	23246	26781	26727
100% ee	913	2769	1297	2414	6135	12284	18545	23615	25992	25861
100% ee	925	1343	1509	2553	5831	12159	19186	23874	25477	26968
100% ee	910	1262	1301	2599	8132	11972	18649	22998	26742	26700
100% ee	1778	1267	1482	2488	8421	11698	18614	23263	26082	26315
100% ee	905	1261	1376	2697	6167	11928	18650	23435	25386	26104
100% ee	945	1240	1407	2588	5938	12006	18900	22766	25371	26999
100% ee	990	1234	1310	2696	6145	11995	20073	22962	26277	26320
100% ee	2500	1284	1409	2526	5902	11890	19809	23614	26371	27479
100% ee	912	1305	3253	2588	5965	12142	20973	24744	25801	25994
100% ee	903	5034	1281	2634	6024	11961	19068	24293	25621	26141
100% ee	812	1170	1401	2590	5977	12474	18667	22868	26688	26617
100% ee	899	1367	1432	2456	5919	11844	19094	22916	25790	27147
100% ee	835	1274	3871	2538	5913	12052	18789	23796	26223	26369
100% ee	1547	3367	1275	4962	6105	14043	19355	23172	26099	26077
100% ee	895	1200	1289	2671	6170	12326	18382	22959	25328	26702
100% ee	893	1187	1402	4529	6254	12252	18420	23793	25397	27350
100% ee	843	1198	1447	2586	6192	12298	19221	24060	26306	26737
100% ee	932	1276	1446	2557	5904	12104	19004	23561	25552	27002
100% ee	2580	4986	1399	2679	6083	11751	18595	22967	26389	26719
96% ee	896	1206	1462	2405	5628	11865	18552	21973	25278	25914
96% ee	805	1230	1162	2460	5816	11435	18522	22898	25674	24906
96% ee	806	1182	1234	2463	5823	11252	17932	22963	24967	25924
96% ee	801	1144	1281	2438	5702	11705	18380	22494	25026	26070
96% ee	893	1125	1271	2348	5918	11778	18196	22736	25325	26026
96% ee	805	1304	1264	2376	5730	11813	18256	22626	25657	26357
96% ee	828	1177	1371	2630	5590	11801	18309	22009	25242	26003

96% ee	866	1302	1218	2375	5782	11704	18411	22395	25480	24704
96% ee	833	1176	1256	2398	5854	11266	17819	22957	24928	25468
96% ee	929	1156	1236	2406	5824	11669	18631	22982	25027	25728
96% ee	840	1151	1316	2601	5818	11683	18260	22760	25599	24966
96% ee	825	1168	1337	2469	5675	11744	17592	22524	24947	25275
96% ee	846	1117	1291	2421	5745	11539	18381	22794	24469	25632
96% ee	898	1134	1267	2416	5791	11724	18420	22187	25574	25500
96% ee	796	1141	1304	2434	5768	11478	18418	22292	25373	26084
96% ee	800	1197	1329	2370	5718	11548	18601	22620	25469	25344
96% ee	820	1142	1203	2359	5877	11628	18311	22700	24480	25551
96% ee	837	1277	1274	2422	5984	11769	17755	22978	25107	25536
96% ee	900	1186	1226	2454	5931	11606	18453	22227	24379	25925
96% ee	830	1194	1242	2536	5603	11783	17963	22641	24756	26379
86% ee	789	1167	1265	2377	5529	10996	17856	21575	24496	24969
86% ee	840	1154	1202	2310	5791	10988	17402	21433	24817	25081
86% ee	775	1157	1412	2292	5459	11179	16356	21526	23834	24620
86% ee	843	1182	1295	2329	5475	11312	17377	22025	24081	24296
86% ee	813	1170	1225	2361	5411	11242	17499	21476	24119	24533
86% ee	816	1149	1224	2393	5632	11273	17604	21465	23129	24731
86% ee	817	1179	1245	2275	5528	11393	17578	20907	24585	24061
86% ee	823	1160	1235	2555	5237	11140	17674	21708	24210	23591
86% ee	826	1173	1287	2362	5723	11296	17407	21870	24279	24498
86% ee	830	1169	1447	2263	5508	11135	17393	21791	24189	24741
86% ee	844	1131	1295	2302	5194	11082	17514	21527	23806	24766
86% ee	823	1148	1284	2255	5536	10506	17672	21732	24332	24751
86% ee	827	1150	1267	2347	5560	11183	17046	21704	24276	24946
86% ee	800	1136	1266	2355	5599	11112	17310	21031	23398	24375
86% ee	908	1348	1249	2287	5485	10684	17620	21883	23820	24620
86% ee	799	1361	1226	2394	5636	11130	17368	21459	23999	24110
86% ee	953	1131	1256	2290	5511	11119	17807	20537	24201	24711
86% ee	816	1202	1242	2513	5595	11041	16958	22029	23583	24728
86% ee	825	1192	1296	2296	5491	10936	17533	21546	24440	24845
86% ee	789	1217	1235	2183	5431	11283	16958	20924	24225	24741
80% ee	1176	1158	1585	2191	5568	10258	16324	20764	22728	22183
80% ee	834	1148	1227	2303	5305	10027	16744	20643	22950	21913

80% ee	764	1113	1479	2495	5312	10544	16469	20579	21763	22711
80% ee	807	1119	1231	2265	5300	10080	16051	20162	22103	22286
80% ee	1059	1512	1587	2239	5227	10104	16828	19599	21446	22078
80% ee	797	1534	1215	2419	5480	10513	16534	19367	22311	22452
80% ee	792	1502	1200	2441	5378	10808	16798	20281	22930	22213
80% ee	835	1653	1251	2163	5306	10365	17054	20162	23251	23405
80% ee	1059	1433	1500	2230	5276	10386	16493	20667	21661	23904
80% ee	803	1193	1248	2195	5243	10636	16538	20643	22929	23016
80% ee	802	1168	1157	2425	5438	11073	15968	20721	21738	22600
80% ee	783	1147	1144	2280	5102	10813	15786	20161	21711	23536
80% ee	832	1152	1196	2237	5621	10717	17183	20024	22089	23358
80% ee	983	1371	1276	2778	5168	10534	15614	19786	22773	23700
80% ee	806	1101	1176	2648	5785	10587	15932	20777	22017	23232
80% ee	1060	1154	1219	2211	5274	10920	16450	19480	22396	22627
80% ee	837	1178	1589	2262	5587	10442	16955	19805	21724	23313
80% ee	813	1101	1201	2629	5265	10698	15897	19460	23375	23123
80% ee	990	1159	1526	2259	5244	10315	16590	20001	22955	22363
80% ee	833	1579	1202	2226	5158	10467	16158	19429	23186	23810
70% ee	822	1175	1153	2168	5096	9735	15496	19239	21387	21157
70% ee	826	1152	1242	2177	5012	9897	15529	18806	20933	22162
70% ee	783	1151	1255	2136	4841	9704	15822	19012	21881	22089
70% ee	796	1166	1260	2152	4854	10109	15505	19117	21305	21817
70% ee	827	1132	1239	2128	4882	9959	15694	19306	21602	22275
70% ee	758	1142	1205	2173	4922	9934	15244	19249	21359	21667
70% ee	786	1103	1144	2108	5057	9641	15414	19013	21340	22200
70% ee	782	1137	1181	2116	4961	10067	15499	19651	21130	22262
70% ee	760	1157	1142	2175	4899	9935	15839	19640	21456	22033
70% ee	822	1130	1206	2070	4957	9868	15574	19127	21657	22240
70% ee	787	1122	1196	2118	4895	10063	15803	19299	21668	21949
70% ee	807	1122	1190	2140	4883	9820	15535	19542	21374	21682
70% ee	805	1125	1144	2134	4959	9790	15420	18789	21179	21857
70% ee	801	1133	1213	2068	4982	9960	15458	19556	20917	21984
70% ee	843	1159	1176	2124	5049	10012	15771	19119	21914	21115
70% ee	806	1108	1170	2198	5014	9883	15106	19195	21429	21859
70% ee	831	1087	1231	2146	4986	10035	15288	19419	21329	22132

70% ee	813	1140	1187	2115	4952	10008	15807	19481	21319	21301
70% ee	820	1145	1189	2107	4947	9998	15843	19139	21346	21721
70% ee	809	1136	1184	2137	5049	10061	15569	19273	21617	22186
60% ee	797	1237	1200	2061	4656	9196	14091	17870	20394	19807
60% ee	822	1179	1190	2071	4821	9522	14832	18602	20138	20622
60% ee	820	1138	1325	2065	4712	9305	14595	18735	19838	20578
60% ee	790	1153	1153	2075	4617	9203	14698	18029	20678	20473
60% ee	818	1172	1171	2256	4764	9702	14559	18690	19980	21362
60% ee	823	1157	1185	2052	4609	9682	14579	18175	20811	20565
60% ee	818	1178	1263	2050	4826	9030	15055	18276	20365	20534
60% ee	836	1174	1179	2249	4812	9377	15213	18056	20094	20891
60% ee	929	1117	1213	2122	4748	9490	15065	18037	20973	20716
60% ee	809	1156	1201	1984	4810	9196	14491	17980	20322	20402
60% ee	831	1116	1178	2112	4744	9499	14917	17609	19529	19977
60% ee	791	1127	1145	2041	4834	9506	14591	17541	20014	19848
60% ee	823	1247	1165	2007	4875	9667	14160	18129	20470	20943
60% ee	846	1326	1186	1999	5035	9229	15020	18499	19574	20179
60% ee	833	1434	1180	2078	4727	9650	14563	17700	19780	21207
60% ee	813	1198	1159	2040	4707	9416	14250	17689	19841	20138
60% ee	838	1123	1208	2004	4631	9413	14918	18038	19792	21505
60% ee	959	1133	1182	2117	4748	9441	15030	18130	19956	21082
60% ee	830	1123	1252	2115	4857	9196	14558	17608	19833	20518
60% ee	914	1349	1402	2035	4669	9656	14128	18719	20564	20229
50% ee	878	1151	1252	1879	4484	8825	13899	16754	19260	19249
50% ee	835	1200	1165	2011	4386	8645	14018	16719	18723	19471
50% ee	823	1149	1146	1940	4335	8745	13893	17266	19223	19246
50% ee	843	1129	1156	1942	4423	8914	14009	16897	18374	19628
50% ee	845	1144	1203	1987	4510	8682	13806	17313	18715	19323
50% ee	855	1108	1157	1933	4499	8936	13742	16540	18942	19568
50% ee	881	1145	1158	1999	4425	9016	13932	16826	18577	19564
50% ee	811	1134	1219	2015	4507	8705	13776	16418	19190	19300
50% ee	881	1147	1247	2024	4535	8972	13865	17152	19249	19318
50% ee	822	1170	1190	1955	4529	8951	13564	16800	18989	18806
50% ee	846	1189	1216	2042	4439	8963	14025	17295	19001	19675
50% ee	823	1177	1193	2048	4532	9007	13650	17260	18798	18863

50% ee	814	1156	1153	2029	4547	9032	13994	17167	18456	19190
50% ee	835	1102	1209	1921	4468	8841	14004	17242	18958	19089
50% ee	883	1133	1133	1896	4335	8837	13708	16815	19156	19712
50% ee	857	1182	1131	1975	4473	8622	13612	17093	19305	19547
50% ee	864	1199	1175	2009	4413	8863	13369	16987	19270	19618
50% ee	804	1159	1192	1978	4524	8866	13692	16960	18615	19243
50% ee	844	1105	1249	1953	4400	8620	13788	16861	18816	19415
50% ee	855	1149	1183	1914	4524	8591	14005	16865	18515	19517
40% ee	866	1211	1114	1735	3844	7711	12487	15575	16465	16938
40% ee	763	1103	1116	1882	4012	7964	12276	15465	16398	16564
40% ee	774	1129	1060	1743	4064	8142	11976	14727	16978	17831
40% ee	783	1093	1108	1848	3984	7838	11792	15033	17460	17651
40% ee	785	1096	1176	1737	4133	8181	11841	15455	17507	16869
40% ee	791	1154	1168	1769	4058	8095	12563	14738	16620	17315
40% ee	787	1116	1114	1904	4208	7636	12291	15360	16080	17318
40% ee	791	1114	1141	1791	4071	7912	12626	15072	16569	16833
40% ee	785	1094	1059	1783	4069	7971	12051	15023	16835	16675
40% ee	792	1148	1132	1759	4042	7689	12502	15194	17202	16724
40% ee	763	1158	1089	1808	3977	8036	12341	14561	17238	17685
40% ee	792	1077	1075	1748	4049	7807	11933	15083	16332	16886
40% ee	765	1070	1106	1864	3961	7586	12452	15113	16306	17647
40% ee	849	1126	1085	1750	4120	8269	12342	14896	16658	16707
40% ee	821	1077	1088	1791	4046	7956	12517	15157	16822	17626
40% ee	797	1202	1097	1808	4282	7812	12108	15435	17360	16933
40% ee	787	1161	1087	1836	3854	7890	12781	15338	16941	17720
40% ee	892	1126	1215	1794	3955	7985	12387	14773	17178	17765
40% ee	813	1116	1219	1742	3924	7700	12275	15673	17188	17167
40% ee	797	1083	1146	1846	3933	8126	12241	14735	16582	17162
30% ee	788	1121	1171	1777	3773	7687	11181	13905	16338	15753
30% ee	791	1170	1157	1771	3866	7611	11359	14430	16321	16888
30% ee	786	1049	1140	1827	3962	7408	12007	14823	16275	16543
30% ee	805	1131	1093	1807	3901	7639	11947	14261	16126	16255
30% ee	852	1123	1039	1794	3776	7254	11500	14453	16124	15730
30% ee	758	1146	1079	1634	3892	7762	11532	14031	15961	16558
30% ee	768	1138	1045	1687	3928	7378	11756	14313	15565	16066

30% ee	773	1079	1152	1778	3857	7398	12061	14809	15968	16318
30% ee	835	1112	1136	1644	3691	7647	11562	13905	15626	16878
30% ee	857	1114	1115	1721	3927	7404	11598	14101	15864	15990
30% ee	870	1203	1088	1683	3667	7272	11742	13920	15433	15709
30% ee	822	1095	1162	1741	3801	7352	11681	14518	15394	16245
30% ee	803	1102	1148	1719	3663	7648	11248	14676	16023	16078
30% ee	846	1085	1133	1709	3895	7281	12001	14506	15459	16787
30% ee	800	1061	1090	1714	3999	7607	11688	14584	15411	16278
30% ee	802	1064	1146	1731	3828	7530	12027	14042	15709	15771
30% ee	841	1117	1083	1700	3869	7457	11894	13970	16287	15916
30% ee	768	1131	1047	1737	3784	7606	11352	14803	15298	16592
30% ee	794	1118	1056	1808	3714	7708	11763	14408	15881	16254
30% ee	801	1087	1082	1697	3752	7518	11391	14761	15754	16237
20% ee	891	1117	1139	1621	3543	7126	11157	13731	15355	15159
20% ee	815	1174	1140	1729	3814	7389	11387	14177	15416	16066
20% ee	841	1148	1196	1734	3497	6909	10904	14088	15079	14707
20% ee	856	1228	1111	1705	3786	7364	11303	13787	15517	15314
20% ee	827	1114	1149	1708	3671	7118	11452	12771	14132	15227
20% ee	813	1175	1042	1736	3674	7108	10944	13853	15369	14934
20% ee	815	1155	1115	1711	3731	7319	11158	12914	15736	16075
20% ee	815	1147	1185	1674	3687	6815	11195	13609	14661	14863
20% ee	835	1161	1081	1656	3493	6911	10442	14036	15878	16106
20% ee	801	1144	1115	1755	3456	7189	10533	13267	14820	15883
20% ee	839	1151	1132	1655	3602	7406	10604	13612	15689	14619
20% ee	831	1103	1131	1733	3645	7073	10926	14266	15299	15820
20% ee	825	1119	1119	1618	3744	7070	10399	13102	15673	14979
20% ee	848	1180	1106	1612	3531	7298	11448	13224	14301	15797
20% ee	845	1132	1106	1684	3717	6890	11507	13032	14969	14640
20% ee	825	1136	1134	1612	3760	7058	10581	13850	14400	16104
20% ee	888	1177	1100	1613	3536	7085	10906	13947	14847	15774
20% ee	853	1108	1169	1722	3689	7174	10788	13338	15365	15603
20% ee	828	1101	1096	1740	3558	6841	11108	12892	14218	15641
20% ee	827	1216	1073	1785	3469	6693	11446	12882	14560	14928
10% ee	826	1117	1064	1557	3425	6418	10270	12138	13776	14155
10% ee	841	1114	1101	1626	3276	6708	10136	12536	13746	14056

10% ee	803	1111	1196	1611	3359	6782	10143	12395	13741	14161
10% ee	817	1165	1093	1609	3378	6435	10506	12140	14141	13755
10% ee	858	1121	1102	1550	3403	6576	9951	12507	14251	14702
10% ee	788	1108	1069	1544	3292	6528	10369	12288	13718	14129
10% ee	785	1082	1077	1548	3559	6445	9975	12565	13977	14298
10% ee	809	1221	1056	1551	3368	6759	10252	12864	13923	14142
10% ee	817	1134	1075	1615	3330	6358	10450	12089	13454	14424
10% ee	778	1142	1138	1648	3432	6622	10331	12612	14291	14021
10% ee	798	1128	1049	1621	3571	6872	10504	12488	14027	13890
10% ee	845	1112	1065	1578	3435	6692	10412	12568	14197	14574
10% ee	843	1116	1086	1604	3492	6417	9973	12883	13739	14339
10% ee	799	1112	1058	1587	3431	6636	10194	12283	13861	14537
10% ee	809	1103	1019	1556	3421	6589	10400	12181	14092	14618
10% ee	811	1108	1095	1610	3449	6689	10255	12794	13623	14401
10% ee	826	1078	1065	1743	3294	6646	10197	12490	14320	13867
10% ee	840	1144	1062	1715	3223	6446	10212	12798	13680	14356
10% ee	803	1121	1078	1613	3411	6861	9866	12594	13883	14650
0% ee	807	1087	1013	1557	3158	6051	9171	11211	13205	13676
0% ee	831	1114	1055	1463	3121	6131	9288	11579	12791	13341
0% ee	766	1108	969	1510	3027	5974	9551	11690	12682	12559
0% ee	788	1146	1063	1494	3203	6023	8925	12120	12934	13364
0% ee	1007	1062	1291	1497	3187	6134	9017	11583	13035	12966
0% ee	778	1024	1111	1438	3349	5755	9585	11198	12328	13454
0% ee	796	1147	1025	1500	3031	5738	9210	11350	12487	12632
0% ee	775	1103	1274	1769	3053	5952	9760	11496	13359	13219
0% ee	818	1326	1083	1570	2989	6404	9766	12008	12630	13762
0% ee	819	1129	1095	1426	3109	6087	9638	11659	13439	13177
0% ee	828	1101	1062	1563	3511	6544	9461	11312	12377	12995
0% ee	845	1349	1064	1442	3257	6115	9968	11339	12875	12804
0% ee	942	1313	1020	1488	3175	6107	9383	11995	12819	13622
0% ee	743	1161	1057	1548	3051	6642	9601	11528	12375	13008
0% ee	798	1125	1051	1772	3200	5833	9346	11307	13315	12842
0% ee	844	1138	1011	1692	3160	6020	9176	11380	12763	12741
0% ee	814	1124	1007	1473	3075	6146	9327	11468	12592	12844
0% ee	843	1076	1049	1488	3290	6367	9732	11947	12477	12998

| 0% ee | 961 | 1117 | 1257 | 1520 | 2969 | 5913 | 9839 | 11702 | 12976 | 13097 |
| 0% ee | 840 | 1068 | 1087 | 1505 | 3129 | 5812 | 9278 | 11259 | 13376 | 13693 |

% ee in (1*R*,2*R*)-CHDA	Fluorescence intensities									
	500 nm	510 nm	520 nm	530 nm	540 nm	550 nm	560 nm	570 nm	580 nm	590 nm
100% ee	24329	22767	18607	15964	12643	9960	7811	6025	4496	3601
100% ee	25214	21837	18808	16043	12658	10318	7740	6275	4673	3681
100% ee	24603	22277	19283	15313	12883	10023	7833	6292	4695	3730
100% ee	25421	22392	19458	15308	13248	10115	7910	6330	4679	3634
100% ee	24596	21709	18683	15302	13044	9956	8215	6139	4776	3825
100% ee	24412	21811	18873	15419	12968	10317	7825	5950	4826	3691
100% ee	24203	22558	18638	15968	12996	9982	8080	5978	4553	3609
100% ee	24334	21742	19127	15398	13243	9981	7965	6222	4692	3565
100% ee	25114	22413	19346	15544	13164	10326	8043	6350	4853	3634
100% ee	24686	22707	19003	15835	13186	10227	8155	6267	4672	3708
100% ee	24997	22442	18855	15858	13010	9963	8084	6008	4791	3577
100% ee	25238	21755	19373	15523	13244	10340	8128	6083	4804	3584
100% ee	25437	21950	19175	15704	12690	9939	7922	6163	4776	3656
100% ee	24508	21935	19631	15769	12775	9971	8016	6070	4749	3682
100% ee	24527	22204	19294	15797	12744	10366	8091	6033	4671	3673
100% ee	24861	21635	19176	15792	12802	9853	7844	6082	4521	3713
100% ee	25769	22103	19526	15437	12837	10190	7959	6040	4565	3771
100% ee	25131	22534	19505	15679	13192	9865	8189	6004	4755	3665
100% ee	25181	22487	18902	15835	13197	10241	8109	6075	4737	3747
100% ee	25345	21809	19052	15443	12830	10164	7728	6239	4580	3685
96% ee	23770	20894	18888	15495	12603	9989	7670	5878	4392	3568
96% ee	23825	21751	19001	15362	12560	9501	7796	5936	4540	3476
96% ee	24107	21826	18792	15548	12256	9925	7636	5927	4500	3579
96% ee	24720	21144	18565	15546	12888	9891	7821	6048	4668	3716
96% ee	24036	21767	18969	14814	12724	9695	7772	6093	4399	3516
96% ee	24199	21457	18732	15626	12923	9966	7512	5740	4760	3642
96% ee	23717	20899	18935	15115	12458	10043	7914	5848	4491	3658
96% ee	23946	21559	18672	15019	12389	10109	7484	6106	4692	3606
96% ee	24233	21379	17985	15118	12845	9754	7615	5998	4692	3685
96% ee	24538	21136	18551	15160	12335	9971	7684	6075	4636	3482

96% ee	24364	21856	18486	15501	12906	9566	7967	5889	4679	3669
96% ee	24479	21129	18675	14690	12821	9871	7551	5815	4462	3592
96% ee	24589	21692	18293	15435	12916	10099	7816	5765	4774	3509
96% ee	24603	21639	17919	15294	12492	9601	7673	6148	4584	3542
96% ee	23247	21894	18705	15060	12500	9716	7978	6080	4568	3677
96% ee	24072	21327	18426	15239	12656	9817	7599	6039	4580	3638
96% ee	24439	21987	18300	14904	12369	9614	7828	5977	4635	3553
96% ee	23728	22017	18732	15389	12583	9929	7762	6225	4675	3667
96% ee	23417	21873	18221	14735	12448	9939	7958	6239	4605	3592
96% ee	23314	21176	18981	15208	12627	9753	7941	6116	4523	3564
86% ee	22501	20257	18012	14865	12341	9576	7585	5801	4597	3553
86% ee	23059	20925	17759	14912	12123	9635	7539	5606	4406	3568
86% ee	23510	20879	17900	14727	12266	9475	7638	5970	4603	3505
86% ee	23173	20554	17855	14685	11975	9686	7605	5946	4556	3527
86% ee	23430	20617	18066	14401	12052	9401	7510	5992	4294	3404
86% ee	23029	20857	17292	14662	12303	9664	7456	5988	4481	3425
86% ee	22923	20667	17891	14683	12138	9744	7518	5970	4579	3508
86% ee	23171	20850	18139	14725	12152	9549	7503	5850	4355	3644
86% ee	22482	20503	17818	14413	11808	9517	7261	5783	4284	3599
86% ee	23619	20680	17732	14834	12340	9314	7531	5822	4467	3511
86% ee	23488	20490	17795	14578	12275	9648	7679	6030	4464	3542
86% ee	23033	20788	17983	14092	11975	9416	7546	5901	4428	3553
86% ee	22970	20010	17976	14570	12184	9658	7440	5998	4373	3371
86% ee	23097	20548	17161	14181	12242	9531	7663	5839	4569	3582
86% ee	23421	20673	17991	14650	12124	9135	7450	5803	4468	3641
86% ee	23235	20003	17817	14627	11655	9738	7382	5692	4371	3550
86% ee	22918	20970	17729	14475	11708	9580	7574	5744	4497	3628
86% ee	22162	20027	17995	14465	12206	9663	7555	5960	4583	3553
86% ee	23133	20715	17829	14811	12157	9525	7558	5804	4499	3536
86% ee	23471	20648	17294	14580	12410	9519	7482	5706	4388	3550
80% ee	20911	20161	16850	13805	11789	9285	6969	5600	4270	3271
80% ee	22511	18629	16287	13822	11014	8467	7181	5512	4393	3239
80% ee	21188	19376	16393	14010	11179	8769	7082	5301	4053	3372
80% ee	22170	19571	15890	14181	11766	8430	6795	5533	4466	3499
80% ee	21785	18506	16646	13478	11818	9113	6722	5925	4320	3244

80% ee	21934	18439	16144	14388	11057	8903	7370	5649	4405	3365
80% ee	22030	20069	16398	13978	11672	9335	7178	5472	4308	3374
80% ee	20844	18870	17053	14184	11585	8591	7151	5360	3964	3168
80% ee	22183	18987	17294	13247	11169	8913	7284	5545	4344	3359
80% ee	20835	19774	15994	14256	11828	9363	7101	5374	4273	3383
80% ee	20822	19363	16792	13942	11538	8877	7228	5586	4161	3213
80% ee	21410	19840	16542	13667	11780	8962	7116	5587	4356	3578
80% ee	22396	18410	16653	13222	10844	8764	7173	5733	4178	3497
80% ee	21579	19332	16435	14149	11237	8793	7384	5461	4494	3304
80% ee	22432	19750	17043	13380	11269	8837	7304	5685	4326	3489
80% ee	21950	18455	16927	13092	11721	9271	7407	5316	4152	3598
80% ee	21355	18940	17223	13674	11619	8921	6887	5544	4316	3359
80% ee	21853	19024	17128	13339	11303	9343	6931	5952	4110	3288
80% ee	20561	19251	17476	14439	11275	9152	7317	5696	4326	3506
80% ee	21140	19679	17485	13655	10977	9327	6674	5588	4152	3320
70% ee	19977	18582	16063	12779	11118	8443	6777	5341	4012	3158
70% ee	20827	18857	15713	13067	10820	8403	6933	5359	4081	3343
70% ee	20930	18448	16016	13130	10532	8216	6701	5448	4221	3219
70% ee	20741	17999	16204	13218	10884	8411	6967	5356	4141	3171
70% ee	20397	18218	16240	13407	11084	8598	6834	5301	4167	3206
70% ee	20271	18628	15853	12981	10860	8627	6794	5170	4110	3199
70% ee	20406	18339	16090	12931	10891	8697	6973	5259	4110	3257
70% ee	20859	18239	15860	12931	10912	8517	6898	5348	4120	3143
70% ee	20416	18576	16101	12989	10594	8607	6595	5327	4064	3293
70% ee	20798	18623	15674	13016	10874	8479	6899	5334	4017	3123
70% ee	20631	18061	15496	13381	10859	8423	6775	5350	4046	3186
70% ee	20792	18707	15781	13305	11027	8798	6676	5407	4112	3088
70% ee	20535	18672	16248	13159	10812	8341	6993	5248	4033	3337
70% ee	20250	18395	15601	13435	10797	8598	6982	5330	4007	3202
70% ee	19810	18543	16176	13086	11120	8654	6722	5363	4186	3209
70% ee	19840	18154	15741	12693	10958	8574	6834	5202	4063	3314
70% ee	20779	18296	15948	13475	10829	8534	6940	5198	4068	3297
70% ee	20636	17910	15633	13168	10761	8331	6805	5448	4038	3218
70% ee	20438	18622	15810	13216	10975	8443	6788	5469	3929	3256
70% ee	20594	18563	16200	13152	10806	8578	6998	5304	4201	3180

60% ee	20217	17068	14779	12483	10184	8400	6650	4958	3893	3271
60% ee	20145	16846	14415	12034	10772	8100	6542	5003	4121	3233
60% ee	19232	16414	15108	11917	10525	7905	6311	4917	3809	3184
60% ee	19734	17420	14857	12673	10426	8079	6831	5005	3904	3200
60% ee	19002	17551	14975	12565	10561	8066	6862	5415	4099	3107
60% ee	18839	16656	14621	12884	10717	8454	6464	5242	4083	3350
60% ee	19612	17465	14872	12759	10447	7941	6313	5153	3931	3377
60% ee	18757	17036	14509	12768	10237	8050	6625	5416	4153	3150
60% ee	19254	17190	15762	12152	10132	8545	6644	5047	3919	3093
60% ee	19431	17925	15535	12348	10328	7835	6354	5288	3870	3312
60% ee	19364	17151	15575	12460	10086	8437	6424	5151	3926	3394
60% ee	19484	17066	14672	12082	10075	8062	6681	5408	4074	3042
60% ee	19392	17874	15020	12225	10182	8213	6431	5249	4162	3033
60% ee	19057	16775	15115	12286	10656	7846	6874	5073	3946	3073
60% ee	18757	17891	14511	12809	10440	8217	6359	5299	4051	3149
60% ee	18874	17229	15401	12149	10335	8298	6528	5002	3859	3248
60% ee	19846	17374	15450	11876	10150	7947	6270	4985	4125	3075
60% ee	18567	16716	14969	12620	10382	7881	6580	5461	3874	3262
60% ee	20146	17313	14490	12998	10105	8294	6750	5064	4015	3196
60% ee	19274	17496	15091	12255	10946	8563	6563	5126	4168	3188
50% ee	18172	16600	14271	11628	9683	7637	6293	4848	3762	3074
50% ee	18563	16139	13793	11888	9582	7823	6215	4759	3804	2925
50% ee	18486	16642	14363	11674	9990	7819	6175	4776	3728	2987
50% ee	18527	16299	13760	11725	9966	7773	6226	4794	3708	3085
50% ee	18175	16327	13974	11610	9547	7765	6222	4906	3709	3017
50% ee	18407	16388	13845	11542	9669	7557	6243	4893	3870	3007
50% ee	18211	16065	13908	11708	9829	7753	6186	4792	3685	3112
50% ee	17948	16604	14442	11779	9808	7868	6361	4932	3724	2995
50% ee	17760	16241	14173	11723	9980	7705	6032	4875	3873	3007
50% ee	18381	16428	13979	11885	9718	7890	6071	4895	3921	3028
50% ee	18396	16555	14337	11756	9682	7608	6071	4821	3819	3089
50% ee	18121	15883	14281	11340	9852	7846	6244	4784	3889	3024
50% ee	18381	16438	13975	11498	9850	7821	6237	4935	3831	3114
50% ee	18001	16559	14568	11308	9885	7566	6369	4938	3828	2950
50% ee	18547	16715	14124	11931	9975	7700	6010	4818	3856	3023

50% ee	18336	15991	14169	11870	9547	7815	6329	4823	3682	3101
50% ee	18076	15995	14061	11810	9934	7529	6312	4954	3859	3116
50% ee	17940	16210	14260	11611	9740	7708	6203	4791	3808	2991
50% ee	17814	16079	14423	11729	9860	7528	6236	4802	3713	3000
50% ee	18358	16333	13988	11567	9809	7676	6268	4921	3746	3040
40% ee	16772	14449	12289	10115	9020	7396	5925	4823	3530	2864
40% ee	16683	14639	13339	10892	8660	6999	5559	4607	3444	2965
40% ee	15738	14154	12954	10314	9121	6640	5946	4385	3624	2765
40% ee	16268	14102	12648	10189	8230	7053	5591	4146	3681	2772
40% ee	15894	14079	13309	10147	8616	6859	5785	4363	3581	2668
40% ee	16359	14771	13143	10068	9181	6776	6048	4555	3468	2603
40% ee	16517	14926	12398	10378	8705	7113	5561	4534	3724	3016
40% ee	15404	14191	12300	9913	8662	7529	5514	4561	3531	2660
40% ee	16814	14556	12726	10024	9089	6555	5812	4344	3427	3027
40% ee	16363	15191	12086	10735	8917	6972	5789	4344	3787	2758
40% ee	15924	14261	12348	10858	8496	6782	5400	4503	3408	2822
40% ee	15847	14406	12581	10763	8471	7167	5266	4835	3361	2781
40% ee	16005	15181	12461	10801	8415	7315	5451	4543	3331	2992
40% ee	16878	14986	12954	10262	9186	7173	5530	4547	3638	2770
40% ee	15586	13872	12353	9926	9003	6935	5571	4404	3330	2752
40% ee	15687	14135	12656	10513	8272	7007	5518	4880	3367	2864
40% ee	15879	13904	12813	10591	9300	6749	5474	4555	3433	2875
40% ee	16470	14910	11909	10905	8797	7313	5914	4599	3577	2944
40% ee	15894	15099	13262	10570	8791	7266	5875	4436	3697	3033
40% ee	15690	14547	12344	10099	8655	6909	6017	4416	3475	2624
30% ee	15001	13776	12195	9795	8223	6840	5511	4491	3412	2715
30% ee	15483	14258	11538	9752	8509	6688	5259	4208	3359	2694
30% ee	15359	13924	12441	9899	8398	6468	5394	4515	3377	2796
30% ee	14837	13843	11747	10194	8582	6706	5580	4182	3495	2815
30% ee	15224	13398	11949	9950	7951	6555	5207	4563	3499	2774
30% ee	15557	13358	11706	9953	8116	6348	5370	4385	3521	2642
30% ee	15249	13521	11727	9672	8477	6879	5558	4300	3483	2659
30% ee	14751	14167	11798	9979	8242	6898	5580	4410	3554	2696
30% ee	14928	13717	11829	10257	8728	6503	5383	4300	3311	2705
30% ee	14844	13476	11753	9722	8418	6596	5259	4313	3283	2776

30% ee	15140	13632	12357	9862	8170	6763	5417	4175	3403	2652
30% ee	15137	13530	12250	10298	8505	6708	5553	4167	3220	2755
30% ee	15249	13227	12164	10295	8418	6525	5453	4276	3381	2864
30% ee	15697	13947	11996	10103	8211	6640	5374	4321	3447	2875
30% ee	15302	13626	12031	10140	8262	6718	5475	4223	3344	2859
30% ee	14876	13373	12332	9616	8325	6492	5423	4299	3536	2681
30% ee	14652	13299	11726	10276	8661	6971	5364	4470	3350	2830
30% ee	15484	14325	12093	9928	8201	6505	5226	4273	3290	2809
30% ee	15754	14329	12255	9592	8568	6892	5562	4162	3384	2699
30% ee	15604	14124	11819	10405	8688	6892	5441	4259	3337	2673
20% ee	14780	13657	11654	10036	8082	6037	5327	4436	3136	2558
20% ee	15266	12727	11751	9290	8503	6393	5134	3960	3540	2536
20% ee	14074	13358	11387	9136	8516	6401	5025	4405	3255	2531
20% ee	14256	13442	12000	9365	8300	6277	5512	4437	3098	2821
20% ee	13989	12351	11341	9281	8018	6839	4984	4219	3296	2702
20% ee	14679	13495	11656	9364	8212	6283	5532	4344	3255	2705
20% ee	13997	13019	10746	8859	8124	6367	5530	4238	3420	2749
20% ee	13602	12988	11164	10016	7869	6556	5483	4490	3204	2624
20% ee	15094	12627	11381	9012	7963	6768	4963	4453	3393	2587
20% ee	14256	13220	11022	9142	8479	6110	5423	4366	3367	2686
20% ee	14870	13438	10819	9712	8341	6542	5221	4056	3484	2755
20% ee	14991	12636	11827	9368	7511	6775	5136	4029	3341	2731
20% ee	13797	12566	11647	8992	7925	6372	5229	4352	3487	2721
20% ee	13552	13387	11024	9690	7747	6609	5180	4484	3472	2751
20% ee	14935	12266	11936	9785	7582	6684	5539	4080	3240	2587
20% ee	14726	13502	11755	10020	7499	6740	4957	4245	3530	2866
20% ee	14369	13802	11695	9911	8345	6529	5396	4098	3448	2503
20% ee	13870	12514	11836	9914	7731	6088	4931	4266	3253	2843
20% ee	14265	12340	10702	9518	7583	6555	4930	4165	3190	2576
20% ee	15094	12968	11135	10061	7880	6046	5217	4225	3527	2872
10% ee	13268	11920	10807	8982	7377	6027	5100	4048	3231	2717
10% ee	13745	12435	10857	8708	7500	5938	5176	3875	3365	2558
10% ee	13752	12506	10608	9094	7593	6083	4814	4013	3321	2653
10% ee	13620	12014	10300	9052	7418	5898	5002	4006	3204	2728
10% ee	13198	11906	10966	8796	7650	6263	4920	4205	3388	2650

10% ee	13826	11828	10402	9011	7738	5957	5185	4132	3189	2756
10% ee	13385	12451	10647	8685	7433	6051	4903	4004	3150	2589
10% ee	13282	12190	10772	9030	7548	5986	4998	4246	3281	2500
10% ee	13697	12549	10486	8788	7606	5986	4910	4111	3209	2661
10% ee	13626	12348	10906	8807	7822	6203	5044	4126	3227	2658
10% ee	13524	12117	10535	8893	7606	6213	5075	3973	3316	2627
10% ee	13662	12155	10455	9103	7389	6067	4953	4107	3160	2558
10% ee	13296	12151	10520	8852	7774	6184	4963	3907	3348	2782
10% ee	13864	12387	10501	8756	7779	6061	4910	4183	3283	2590
10% ee	13497	12132	10587	8656	7761	6163	4965	3924	3185	2707
10% ee	13694	12114	11007	8916	7676	5897	5013	4146	3371	2708
10% ee	13433	12283	10819	8673	7473	6014	5077	4032	3165	2569
10% ee	13460	12070	10568	8988	7539	5939	5105	3960	3194	2566
10% ee	13001	11935	10712	8943	7500	6284	4892	4030	3142	2752
0% ee	12089	11663	10067	7973	6637	5895	4829	3988	3076	2533
0% ee	12429	11281	9434	8653	7220	5517	4949	3675	3148	2570
0% ee	11978	10858	10319	8337	6765	5714	4907	3764	2988	2590
0% ee	12792	11719	10348	8461	7251	5739	4631	3909	2917	2665
0% ee	12236	10738	10156	8244	7367	5951	4578	4052	3370	2599
0% ee	12487	11225	10326	8498	6916	5568	4374	3813	3225	2380
0% ee	12753	10728	9789	7855	7170	5710	4559	3746	3374	2364
0% ee	12617	11510	9574	8651	7400	5361	4979	3772	2965	2359
0% ee	12056	11326	9937	8094	6944	5625	4650	3581	3147	2399
0% ee	12918	11514	9743	8553	6696	5557	4642	3847	3048	2481
0% ee	12523	11185	9360	7994	7054	5893	4577	3813	3068	2685
0% ee	12899	11003	9956	8247	7293	5774	4771	4079	3066	2601
0% ee	11939	10705	9416	7843	7042	5729	4807	3982	2946	2431
0% ee	12161	11119	9979	8246	7278	5887	4779	3876	3108	2600
0% ee	12332	11527	10010	8396	7160	5929	4979	3866	3230	2473
0% ee	12543	11081	10048	7873	6892	5517	4824	3951	3273	2490
0% ee	12938	11396	9812	7794	6672	5654	4670	3868	3225	2690
0% ee	12158	11286	10129	8479	7140	5641	4462	3674	3096	2502
0% ee	12073	11446	9643	8161	6813	5420	4616	3860	3102	2550
0% ee	12643	11126	9487	8553	7210	5924	4561	3541	2915	2405

% ee in (1*R*,2*R*)-CHDA	Fluorescence intensities								
	600 nm	610 nm	620 nm	630 nm	640 nm	650 nm	660 nm	670 nm	680 nm
100% ee	2746	2208	1584	1325	941	661	507	482	393
100% ee	2635	2163	1576	1233	890	712	561	410	403
100% ee	2850	2167	1617	1271	960	717	561	375	295
100% ee	2708	2075	1571	1209	923	674	617	399	457
100% ee	2669	2140	1539	1198	869	700	552	486	304
100% ee	2770	2067	1626	1257	941	670	557	358	329
100% ee	2665	2188	1588	1329	923	710	484	452	351
100% ee	2674	2095	1610	1175	979	677	552	487	316
100% ee	2647	2171	1604	1231	1012	659	558	486	247
100% ee	2687	2149	1536	1297	985	755	565	414	327
100% ee	2717	2172	1607	1266	887	643	574	425	233
100% ee	2729	2195	1570	1216	1001	691	585	374	218
100% ee	2764	2133	1579	1210	898	644	543	401	301
100% ee	2623	2120	1614	1189	938	664	512	458	433
100% ee	2821	2049	1574	1149	860	759	508	408	325
100% ee	2784	2175	1643	1305	900	668	555	378	383
100% ee	2627	2201	1536	1230	949	697	560	344	452
100% ee	2631	2069	1632	1279	941	693	614	310	459
100% ee	2764	2081	1631	1209	946	736	591	389	373
100% ee	2867	2094	1533	1185	915	666	564	524	370
96% ee	2728	2156	1473	1194	911	726	494	473	347
96% ee	2657	2160	1526	1161	970	773	469	383	389
96% ee	2716	2032	1454	1260	957	779	529	518	241
96% ee	2643	2025	1440	1239	881	753	548	448	263
96% ee	2703	2079	1471	1170	931	711	547	373	346
96% ee	2589	2027	1631	1174	921	704	454	361	368
96% ee	2687	2167	1622	1224	988	730	461	541	404
96% ee	2771	2130	1662	1213	888	731	531	349	185
96% ee	2703	2068	1553	1293	976	753	553	310	279
96% ee	2631	2159	1501	1235	960	724	517	421	417
96% ee	2673	2033	1484	1167	924	674	556	342	191
96% ee	2756	2198	1635	1182	947	644	544	355	198

96% ee	2707	2164	1514	1240	947	653	514	349	328
96% ee	2650	2158	1619	1187	900	702	538	501	207
96% ee	2653	2171	1623	1245	913	658	533	466	235
96% ee	2710	2203	1583	1159	939	674	466	370	321
96% ee	2545	2184	1458	1195	889	653	590	379	321
96% ee	2744	2023	1668	1280	933	674	556	412	297
96% ee	2591	2137	1624	1130	917	695	568	486	394
96% ee	2571	2055	1562	1200	945	677	555	508	318
86% ee	2652	2079	1459	1298	904	659	517	389	361
86% ee	2642	2130	1460	1227	867	647	580	440	391
86% ee	2697	2035	1532	1180	894	759	615	522	218
86% ee	2696	2036	1529	1183	961	723	592	359	214
86% ee	2540	2138	1538	1217	974	753	520	485	377
86% ee	2705	2059	1519	1271	895	717	486	467	436
86% ee	2649	2168	1537	1205	917	777	508	332	419
86% ee	2703	2107	1511	1253	911	746	485	454	363
86% ee	2667	2013	1589	1218	976	677	449	382	431
86% ee	2693	2056	1602	1216	919	680	461	394	402
86% ee	2564	2102	1490	1179	932	777	581	423	430
86% ee	2647	2180	1536	1199	961	726	594	409	355
86% ee	2706	2183	1613	1210	936	731	577	460	329
86% ee	2543	2136	1522	1146	959	703	494	387	361
86% ee	2508	2138	1498	1214	938	749	521	436	422
86% ee	2661	2117	1551	1262	906	692	541	476	409
86% ee	2662	2029	1528	1258	962	711	626	295	387
86% ee	2731	2137	1543	1269	943	732	453	501	419
86% ee	2654	2131	1632	1290	873	704	587	419	331
86% ee	2681	2074	1506	1172	966	740	585	501	355
80% ee	2558	2035	1517	1155	958	616	503	408	298
80% ee	2532	2005	1607	1231	928	707	564	387	317
80% ee	2662	2055	1572	1160	982	664	597	378	240
80% ee	2643	1958	1595	1284	904	765	508	501	238
80% ee	2499	2052	1464	1185	981	791	601	472	302
80% ee	2517	2125	1520	1195	843	574	480	399	278
80% ee	2566	2032	1525	1161	842	774	478	367	299

80% ee	2361	1980	1463	1286	977	594	500	417	204
80% ee	2564	2065	1412	1149	948	730	548	404	325
80% ee	2312	2137	1511	1161	949	695	592	416	319
80% ee	2531	1937	1499	1249	908	636	570	416	339
80% ee	2401	2070	1467	1226	914	633	513	430	358
80% ee	2617	2011	1552	1230	854	694	507	383	207
80% ee	2569	1841	1588	1256	944	686	560	440	366
80% ee	2390	1905	1456	1299	919	744	641	416	188
80% ee	2523	1987	1451	1240	930	661	576	465	301
80% ee	2457	1961	1574	1209	900	627	639	422	366
80% ee	2438	2103	1624	1094	850	687	579	471	364
80% ee	2665	2117	1566	1209	942	675	543	395	260
80% ee	2455	2032	1454	1160	916	694	520	477	383
70% ee	2465	1901	1466	1120	823	740	573	450	261
70% ee	2510	2008	1461	1220	880	670	539	378	427
70% ee	2381	1996	1513	1120	795	728	541	430	465
70% ee	2461	1893	1514	1201	923	662	643	433	298
70% ee	2420	1906	1468	1157	844	728	545	384	304
70% ee	2503	1963	1471	1161	935	739	498	416	368
70% ee	2384	1855	1493	1189	895	651	467	445	330
70% ee	2417	1896	1522	1183	847	715	568	353	434
70% ee	2427	2025	1463	1187	816	669	573	406	353
70% ee	2352	1838	1457	1225	927	684	567	453	349
70% ee	2460	1897	1423	1122	866	705	546	367	413
70% ee	2365	1971	1537	1089	878	700	493	380	425
70% ee	2430	1926	1461	1175	804	717	594	358	241
70% ee	2468	1943	1488	1090	947	660	504	360	230
70% ee	2364	1970	1445	1141	888	639	559	423	363
70% ee	2469	2050	1404	1169	816	637	568	465	410
70% ee	2420	1977	1398	1155	894	730	519	465	367
70% ee	2347	1981	1493	1207	934	651	511	339	427
70% ee	2395	2039	1496	1179	815	700	534	337	281
70% ee	2458	1897	1527	1190	925	654	540	350	362
60% ee	2305	1947	1419	1113	942	732	621	382	427
60% ee	2463	1993	1367	1209	869	693	587	350	432

60% ee	2321	1943	1412	1028	925	729	473	408	269
60% ee	2280	1940	1424	1138	816	619	571	460	433
60% ee	2347	1913	1515	1074	824	643	541	476	282
60% ee	2445	1840	1392	1181	890	631	452	354	427
60% ee	2487	1828	1435	1102	839	692	621	425	388
60% ee	2326	1881	1418	1224	786	624	532	438	305
60% ee	2418	1868	1542	1208	884	665	543	447	374
60% ee	2505	2000	1440	1142	885	769	583	517	316
60% ee	2448	1967	1570	1121	858	698	595	472	348
60% ee	2454	1885	1566	1157	861	712	540	472	377
60% ee	2516	1982	1514	1166	821	745	533	445	343
60% ee	2300	2004	1415	1168	869	773	534	414	423
60% ee	2454	1969	1490	1076	932	693	568	507	435
60% ee	2572	1914	1470	1206	893	775	538	418	347
60% ee	2517	1920	1534	1205	860	723	506	434	411
60% ee	2409	1997	1500	1089	806	721	541	407	286
60% ee	2367	2031	1415	1205	806	631	540	511	283
60% ee	2306	1853	1385	1197	846	774	634	433	306
50% ee	2247	1753	1470	1108	849	724	555	387	209
50% ee	2373	1800	1400	1093	906	746	530	425	267
50% ee	2354	1821	1355	1081	870	761	540	451	204
50% ee	2287	1836	1428	1147	860	706	497	478	390
50% ee	2302	1861	1439	1058	895	633	511	471	294
50% ee	2235	1775	1343	1162	799	693	435	422	407
50% ee	2311	1787	1418	1156	866	620	544	324	289
50% ee	2244	1794	1433	1117	877	747	536	454	326
50% ee	2381	1840	1446	1106	787	718	589	421	200
50% ee	2284	1795	1480	1146	798	662	576	364	381
50% ee	2324	1828	1413	1094	843	728	528	474	321
50% ee	2342	1862	1364	1055	824	668	527	432	286
50% ee	2253	1871	1398	1193	821	702	543	510	416
50% ee	2318	1763	1350	1135	831	604	603	466	327
50% ee	2368	1783	1439	1185	844	718	597	461	293
50% ee	2285	1850	1383	1142	803	723	541	529	233
50% ee	2330	1877	1418	1104	867	726	524	356	253

50% ee	2343	1830	1461	1153	892	704	584	428	221
50% ee	2337	1783	1482	1080	822	652	543	368	425
50% ee	2251	1783	1441	1172	875	644	473	365	199
40% ee	2132	1796	1258	1034	786	620	582	403	343
40% ee	2108	1687	1377	1029	828	690	448	394	369
40% ee	2176	1745	1438	1146	747	652	577	509	366
40% ee	2168	1826	1390	1157	859	694	511	417	323
40% ee	2207	1764	1188	1168	864	690	494	299	304
40% ee	2190	1752	1355	1206	855	589	486	426	404
40% ee	2088	1778	1422	1065	791	668	549	413	345
40% ee	2121	1734	1313	1069	816	722	561	405	258
40% ee	2216	1749	1477	976	876	583	630	424	234
40% ee	2240	1704	1252	1073	816	778	529	533	270
40% ee	2201	1838	1424	1090	876	586	496	311	382
40% ee	2280	1745	1205	1130	820	702	631	404	296
40% ee	2273	1872	1457	1037	754	708	494	372	331
40% ee	2072	1740	1342	1124	774	665	646	479	285
40% ee	2153	1591	1321	1108	793	691	609	464	423
40% ee	2108	1794	1324	1088	921	764	462	430	392
40% ee	2331	1672	1320	1211	827	681	561	403	238
40% ee	2125	1791	1457	1110	886	686	648	450	320
40% ee	2119	1837	1413	1089	863	609	611	473	215
40% ee	1964	1826	1397	1112	911	722	560	498	392
30% ee	2048	1672	1341	1145	787	664	455	503	358
30% ee	2184	1762	1354	1031	785	637	547	368	421
30% ee	2206	1738	1334	1059	785	669	557	378	275
30% ee	2172	1665	1253	1088	780	744	530	477	363
30% ee	2218	1648	1341	1084	822	659	575	404	313
30% ee	2195	1770	1283	1166	849	581	490	357	277
30% ee	2064	1667	1301	1124	823	658	554	401	281
30% ee	2072	1739	1308	1075	894	666	456	373	257
30% ee	2163	1651	1240	1000	871	728	474	462	245
30% ee	2133	1778	1347	1105	810	596	486	495	337
30% ee	2174	1723	1335	1051	786	569	490	467	445
30% ee	2021	1652	1408	1085	857	636	470	445	456

30% ee	2021	1632	1374	1135	853	650	577	460	252
30% ee	2224	1784	1293	999	769	681	515	404	387
30% ee	2141	1746	1297	1059	847	705	513	448	418
30% ee	2187	1756	1325	1069	872	700	525	467	379
30% ee	2219	1722	1330	1060	877	646	613	477	279
30% ee	2111	1649	1330	1093	785	698	582	355	288
30% ee	2022	1708	1276	1081	902	604	511	417	235
30% ee	2180	1631	1242	994	875	624	605	479	362
20% ee	1939	1760	1391	1098	786	721	614	433	178
20% ee	2101	1580	1297	1076	853	613	591	405	370
20% ee	2144	1794	1313	1008	899	667	558	376	404
20% ee	2096	1713	1418	1052	859	617	615	381	279
20% ee	2104	1785	1373	1022	802	695	567	432	433
20% ee	1961	1709	1349	1053	825	672	573	517	320
20% ee	1918	1634	1355	1054	837	719	616	530	239
20% ee	2031	1659	1444	1083	786	666	500	548	246
20% ee	2159	1760	1219	1009	812	689	589	426	302
20% ee	2214	1836	1317	1061	843	649	583	449	235
20% ee	2028	1688	1258	1063	901	685	586	503	304
20% ee	2137	1597	1289	974	814	689	577	450	496
20% ee	2116	1693	1362	1134	815	688	506	501	317
20% ee	2120	1652	1455	1130	797	632	529	449	366
20% ee	2185	1708	1412	999	783	690	609	534	273
20% ee	2108	1849	1346	1140	855	720	559	339	351
20% ee	2130	1837	1289	1078	779	730	637	455	296
20% ee	2038	1803	1257	1071	828	733	540	478	448
20% ee	2022	1666	1290	1085	826	616	605	477	246
20% ee	2092	1591	1309	1020	858	673	540	441	183
10% ee	2080	1624	1303	1147	889	658	472	391	355
10% ee	2107	1794	1282	1130	824	677	489	520	313
10% ee	2001	1649	1402	1044	800	692	583	543	398
10% ee	2043	1677	1295	1050	822	686	492	469	336
10% ee	2122	1610	1342	1161	917	701	605	410	375
10% ee	2012	1789	1387	1057	770	653	567	431	352
10% ee	2004	1735	1388	1098	881	640	525	378	325

10% ee	2046	1662	1306	1118	854	706	493	353	338
10% ee	2108	1779	1355	1127	839	708	524	443	413
10% ee	2062	1691	1308	1037	832	671	524	542	278
10% ee	2141	1747	1306	1003	803	717	610	448	319
10% ee	2065	1801	1261	1096	839	692	449	445	406
10% ee	2040	1610	1378	1147	856	695	609	402	287
10% ee	2115	1666	1335	1152	789	738	579	452	266
10% ee	2070	1773	1364	1155	863	705	603	534	448
10% ee	2143	1700	1315	1161	857	633	606	496	309
10% ee	2111	1746	1262	1017	800	738	528	431	363
10% ee	2134	1706	1322	1081	896	694	605	404	368
10% ee	1984	1695	1336	1067	855	675	520	373	360
0% ee	2085	1718	1371	1050	841	690	618	532	426
0% ee	2015	1577	1373	1056	861	711	470	526	473
0% ee	1911	1525	1266	1008	857	717	477	446	234
0% ee	1896	1550	1385	1054	852	702	571	509	257
0% ee	1879	1567	1292	1052	862	649	589	390	282
0% ee	2123	1613	1188	999	898	637	572	480	476
0% ee	1972	1665	1371	1188	965	711	601	440	241
0% ee	1885	1739	1240	997	774	714	555	526	347
0% ee	2134	1761	1379	1084	901	699	525	528	435
0% ee	1979	1662	1250	904	862	558	532	491	385
0% ee	2025	1762	1402	1024	912	676	507	477	443
0% ee	1993	1707	1212	1099	818	655	470	400	359
0% ee	1874	1674	1227	1167	718	679	512	544	355
0% ee	2130	1704	1345	967	764	555	488	495	225
0% ee	1909	1697	1244	1182	781	757	493	410	464
0% ee	2052	1753	1300	1135	848	608	553	454	378
0% ee	1929	1589	1303	1022	803	718	630	435	319
0% ee	1998	1655	1249	1097	910	741	508	463	390
0% ee	1884	1637	1422	1073	815	640	560	377	351
0% ee	2062	1674	1344	1158	719	652	580	469	335

Table S8 Output calibration / prediction datasets of the % ee determination in (1*R*,2*R*)-CHDA

% ee values of (1*R*,2*R*)-CHDA			
Calibration dataset		**Prediction dataset**	
Actual % ee	Predicted % ee	Actual % ee	Predicted % ee
100	100.33	70	65.41
100	98.70	70	66.90
100	99.10	70	66.85
100	100.84	70	69.46
100	100.52	70	68.22
100	98.40	70	66.46
100	97.67	70	67.43
100	100.10	70	67.07
100	101.20	70	67.83
100	100.62	70	67.72
100	100.45	70	66.82
100	100.41	70	67.90
100	99.11	70	65.84
100	99.30	70	69.16
100	102.37	70	68.84
100	98.13	70	64.96
100	101.07	70	67.81
100	99.20	70	68.36
100	98.73	70	67.42
100	99.52	70	69.44
96	94.20	30	29.65
96	94.13	30	30.78
96	94.26	30	33.00
96	95.29	30	32.10
96	94.00	30	28.43
96	96.78	30	30.83
96	95.04	30	30.18
96	95.88	30	32.01
96	94.13	30	29.10
96	94.95	30	28.41

96	96.37	30	26.83
96	96.01	30	29.93
96	95.77	30	29.32
96	96.44	30	31.59
96	95.65	30	32.08
96	95.82	30	30.05
96	94.33	30	31.27
96	95.92	30	29.62
96	94.17	30	31.65
96	95.09	30	30.23
86	88.47		
86	87.47		
86	88.31		
86	90.02		
86	88.35		
86	86.79		
86	87.15		
86	87.22		
86	87.97		
86	89.03		
86	86.14		
86	86.91		
86	88.52		
86	88.06		
86	87.65		
86	86.94		
86	86.35		
86	87.17		
86	88.17		
86	86.85		
80	80.55		
80	77.66		
80	78.92		
80	78.09		
80	78.24		

80	80.52
80	78.90
80	81.32
80	78.70
80	79.56
80	77.36
80	78.55
80	80.33
80	77.94
80	81.13
80	77.83
80	80.45
80	78.87
80	79.78
80	77.38
60	60.20
60	61.26
60	59.14
60	58.81
60	61.23
60	58.81
60	59.68
60	59.57
60	60.55
60	59.52
60	60.63
60	58.27
60	58.92
60	59.96
60	61.01
60	57.08
60	59.76
60	58.92
60	59.39
60	59.47

50	50.25
50	51.22
50	50.83
50	51.90
50	50.93
50	49.87
50	51.14
50	51.65
50	51.03
50	51.53
50	52.40
50	50.69
50	53.44
50	51.26
50	51.77
50	50.13
50	50.50
50	51.58
50	50.27
50	50.18
40	38.27
40	38.92
40	38.29
40	38.56
40	39.08
40	39.83
40	38.87
40	38.08
40	37.16
40	37.96
40	39.39
40	38.91
40	38.38
40	39.91
40	38.77

40	40.51
40	39.69
40	40.87
40	38.75
40	38.85
20	20.93
20	23.70
20	18.72
20	23.80
20	19.56
20	21.33
20	20.57
20	20.41
20	21.26
20	20.43
20	20.43
20	20.92
20	19.30
20	21.13
20	20.94
20	23.88
20	21.09
20	19.53
20	16.34
20	20.15
10	9.62
10	9.37
10	7.77
10	8.73
10	9.30
10	9.45
10	8.94
10	9.99
10	9.22
10	11.33

10	10.27
10	11.17
10	8.67
10	10.36
10	9.42
10	10.20
10	9.04
10	7.78
10	9.69
10	8.91
0	0.70
0	0.17
0	0.06
0	0.66
0	-0.85
0	-0.03
0	-0.91
0	0.64
0	0.51
0	-0.19
0	1.12
0	1.83
0	-0.69
0	2.04
0	2.03
0	-0.12
0	-0.70
0	0.83
0	-1.34
0	0.40

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