Supporting Information

A Rapid and Sensitive Method for Chiroptical Sensing of α-Amino Acids via Click-like Labeling with o-Phthalaldehyde and p-Toluenethiol

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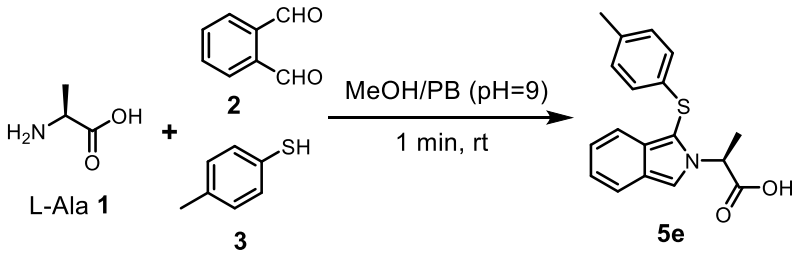
Content

1. Reagents and Instrument

Unless otherwise noted, chemicals and solvents were purchased from Sigma Aldrich, *J&K* Chemical, or Energy Chemical and were used without further purification.

UPLC-MS analyses were performed with a Dionex UltiMate 3000 connected to a thermo scientific MSQ PLUS mass spectrometer using a Thermo Scientific C18 (1.9 μm, 2.1 × 100 mm) analytical column. Flash chromatography columns were packed with 300–400 C18 packing material with MeOH and H_2O as eluents. ^1H and ^{13}C NMR data were recorded using a Varian Mercury (500MHz) spectrometer with TMS as an internal standard. HRMS data were collected on a Thermo Exactive plus Orbitrap mass spectrometer. ECD spectra were recorded on a Jasco J-815 spectrometer. The emission and excitation spectra as well as quantum yields were measured on a FS5 spectrometer with an integrating sphere (Edinburgh Instruments, UK).

2. Synthetic procedures and structural elucidation

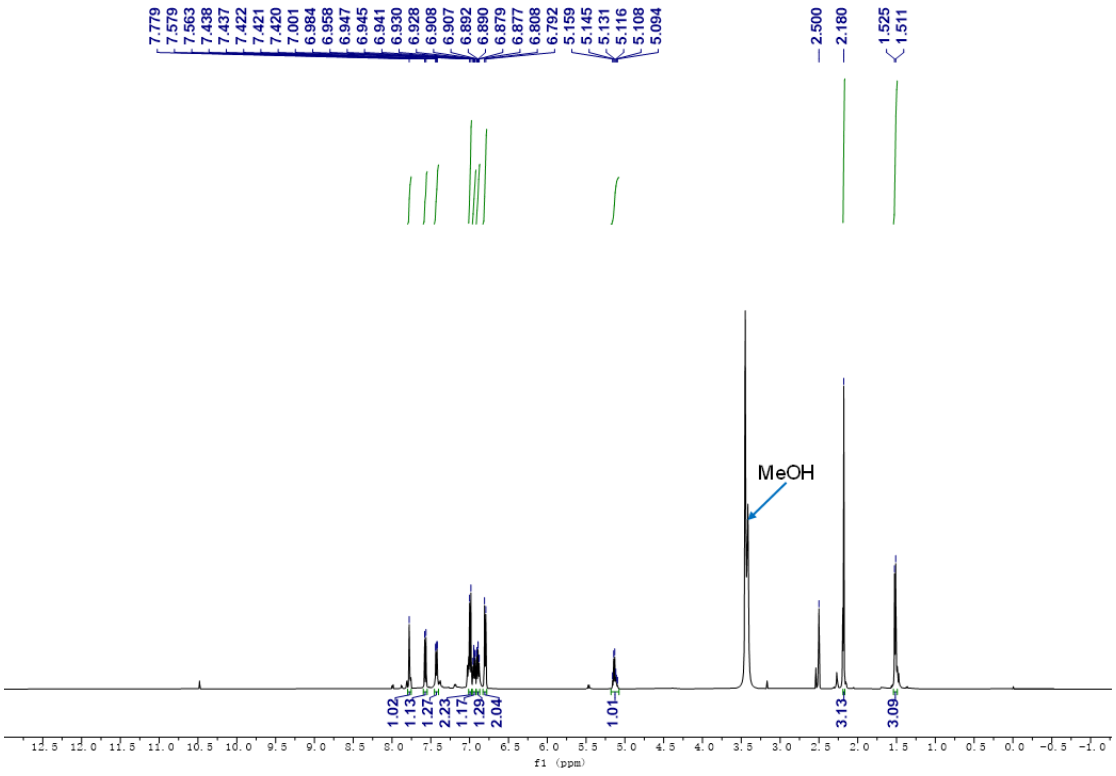


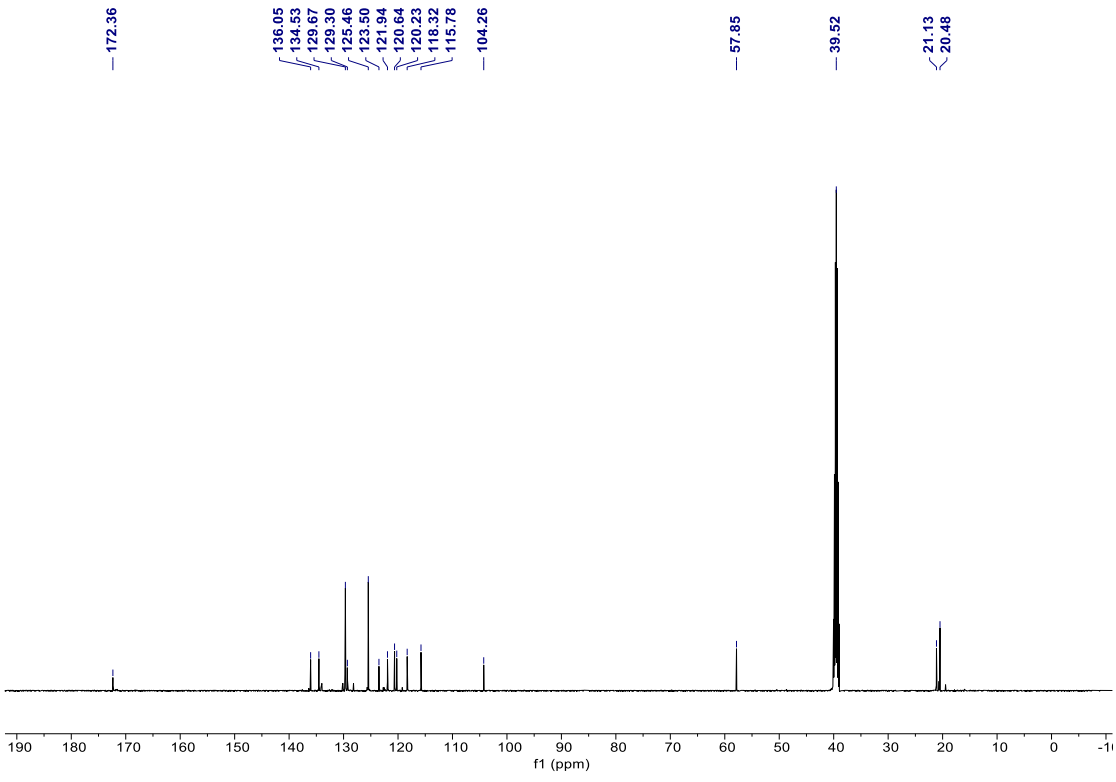
To a solution of L-Ala (**1**) in MeOH-phosphate buffer (PB) (1 : 2, pH = 9), p-toluenethiol (**3e**, 1.2 equiv) and o-phthaladehyde (**2**, 1 equiv) were added at room temperature without avoiding light and air. Being shaken for 1 min, the reaction mixture was directly purified by flash column chromatography packed with 300–400 C18 packing material (methanol-water 20 : 80 with 0.5% HCOOH as eluents) to afford **5e** as freeze-dried white powder (300 mg, 97%). (Freeze drying takes a relatively long time to remove the H_2O, during which a tiny amount of **5e** occurred decomposes.)

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 7.79 (s, 1H), 7.58 (d, *J* = 8.5 Hz, 1H), 7.42 (d, *J* = 8.5 Hz 1H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.96–6.93 (m, 1H), 6.91–6.88 (m, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 5.09-5.16 (m, 1H), 2.18 (s, 3H), 1.52 (d, *J* = 7.5 Hz, 3H).

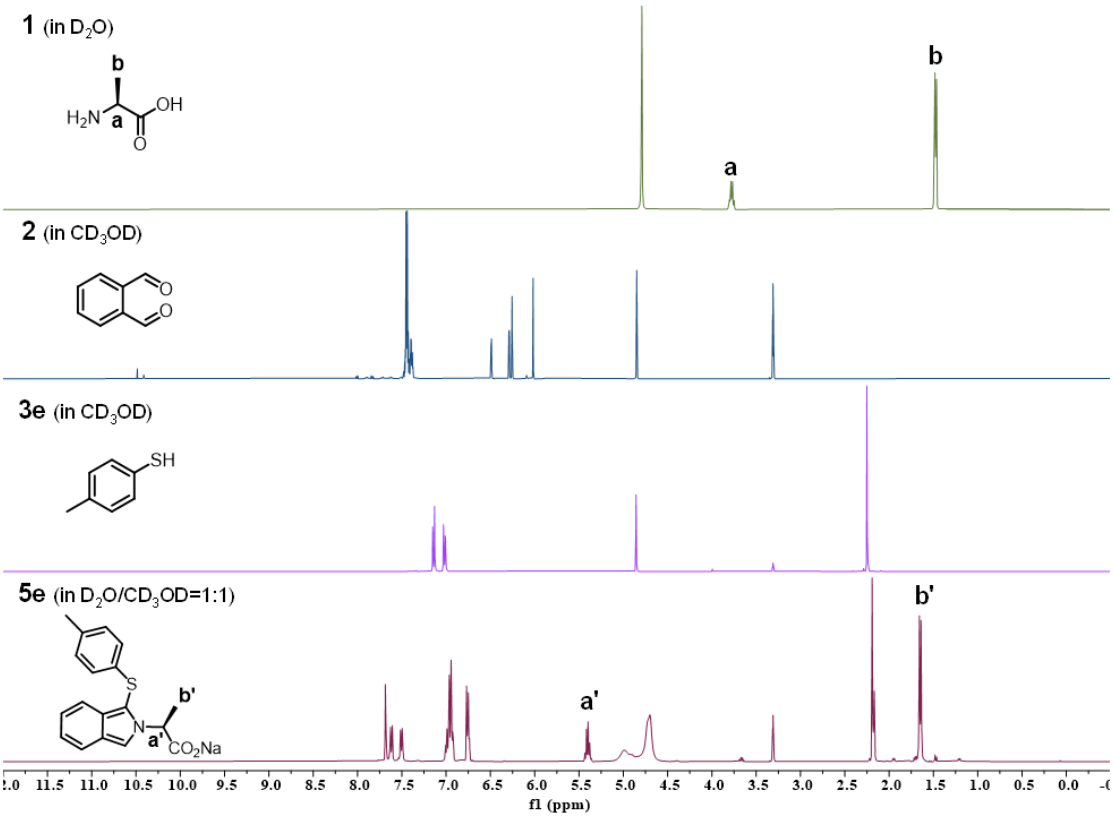
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 172.36, 136.05, 134.53, 129.67, 129.30, 125.46,

123.50,121.94, 120.64,120.23 118.32, 115.78, 104.26, 57.85, 21.13, 20.48.





^{1}H NMR analysis of the three-component reaction

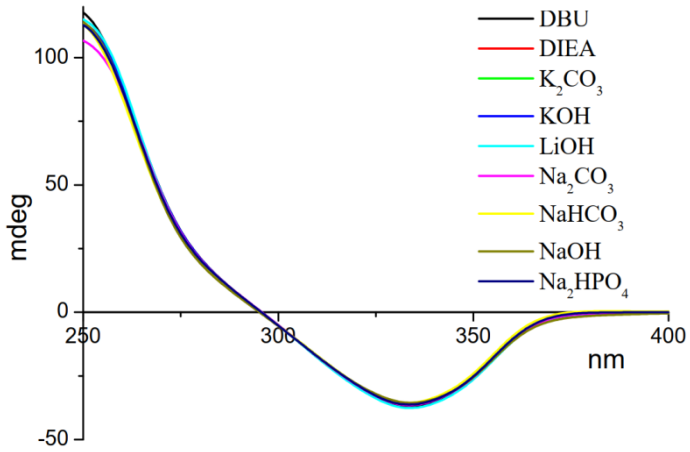


Supplementary Figure 1. 1 (1.0 equiv), **2** (1.0 equiv), **3e** (1.2 equiv) and NaOH (1.1 equiv) were mixed in 3 mL D_2O/CD_3OD (1:1) at 10.0 mM for 1 min, after which 500 uL reaction solution was taken out for ^{1}H NMR test.

3. Optimization of sensing procedure

Base optimization

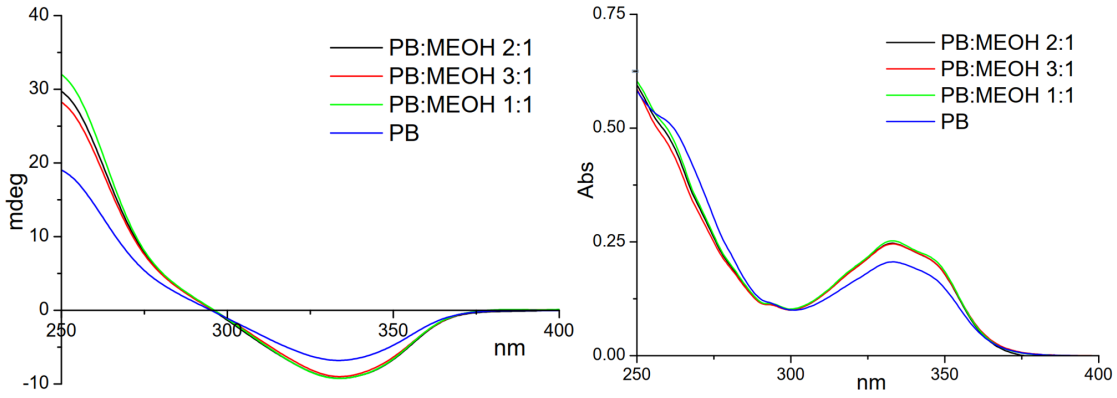
Comparison of CD signals of L-Ala using different bases at 2 mM, diluted to 1 mM for test with a pathlength of 1 mm.



Supplementary Figure 2. After screening of bases, it was found that bases had negligible influence for the sensing procedure.

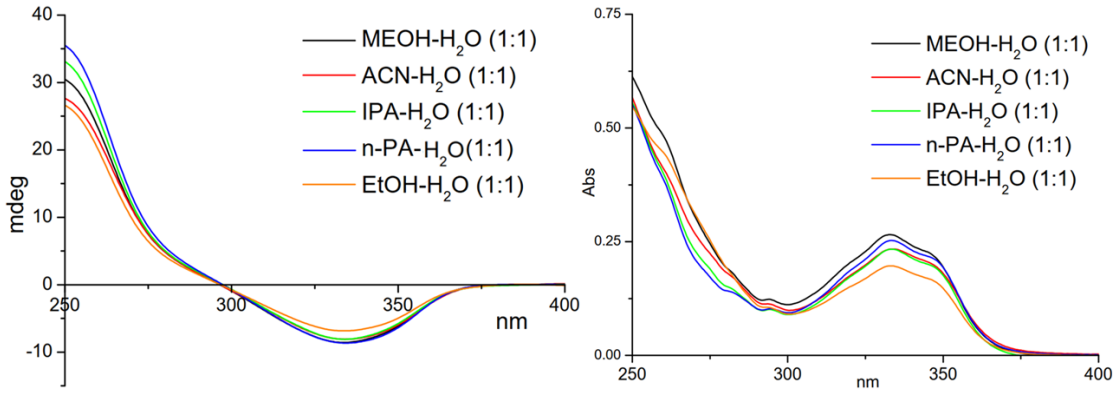
Solvent optimization

Comparison of CD and UV signals of L-Ala in MeOH/PB at 2 mM, diluted to 0.285 mM for test.



Supplementary Figure 3. Mixed solvents gave the better results in CD and UV signals, so we chose PB:MeOH=(1-3) :1 (v/v) as the optimal solvent. Because the isoindole products formed by different amino acids may differ in solubility, the ratio of PB and MeOH was adjusted to guarantee the three-component reaction to proceed well.

Comparison of CD and UV signals of L-Ala in different mixed solvents at 2 mM, diluted to 0.285 mM for test.

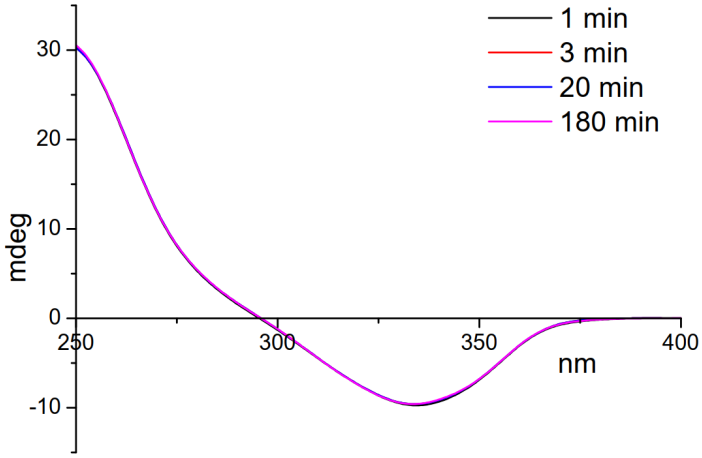


Supplementary Figure 4. ACN= acetonitrile; IPA= isopropanol; n-PA= n-propanol

As shown in Figure 4, the UV and CD spectra of **5e** were only slightly influenced by the reaction solvents. Among these assays, it was found that both H_2O/MeOH and PB/MeOH could give nearly identical results. Aqueous MeOH medium is relatively favorable because of its better solubilizing ability.

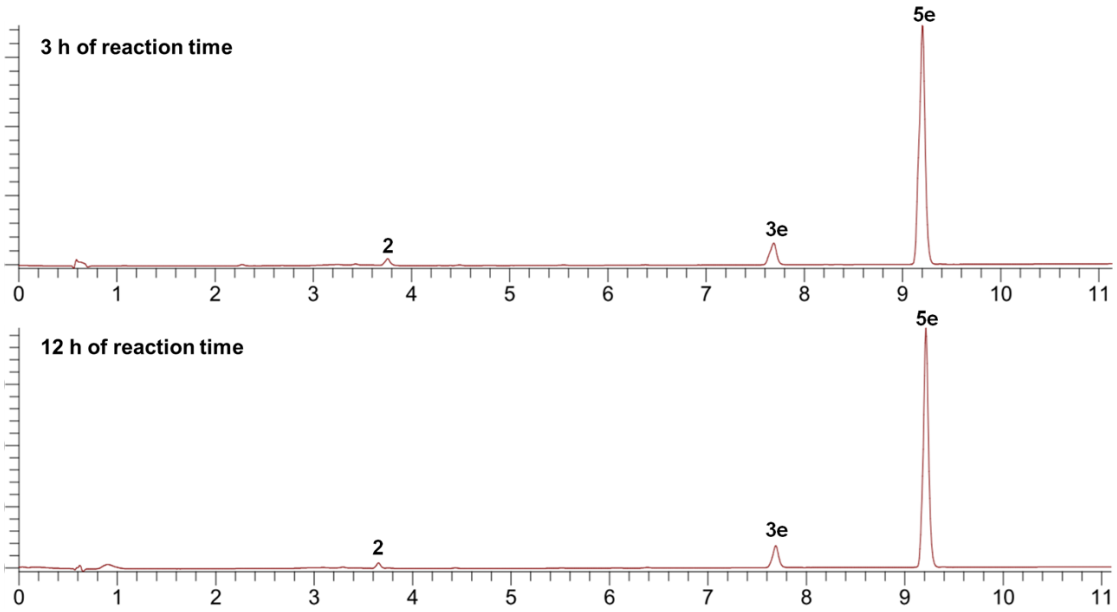
4. Stability test

CD spectra of L-Ala reacting with **2** and **3e** over time



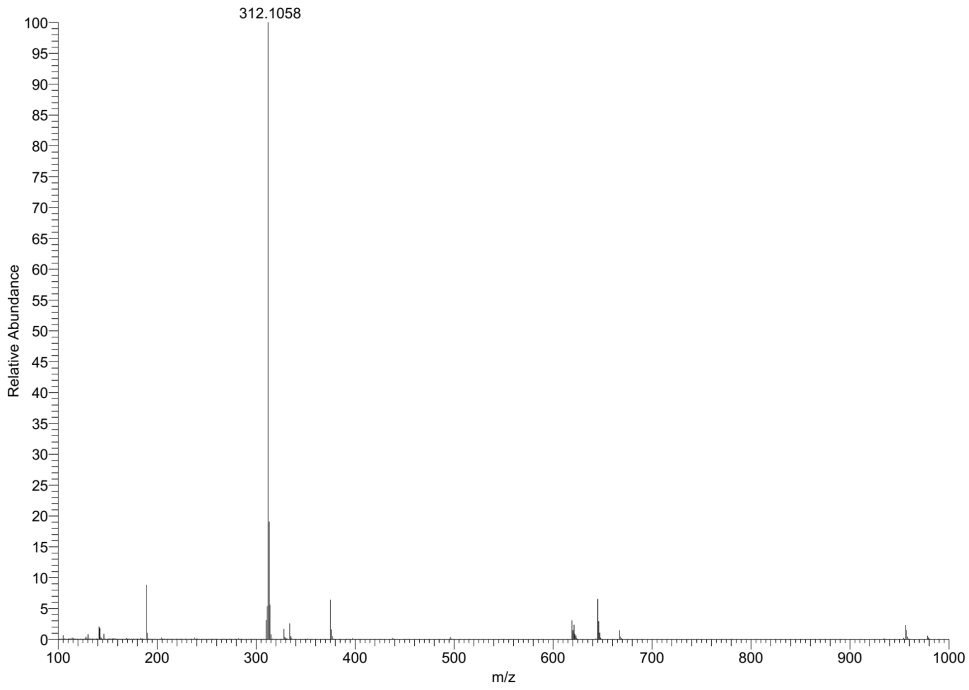
Supplementary Figure 5. The reaction was performed in MeOH/PB (1:2) at 2 mM, diluted to 0.285 mM for CD test.

UPLC traces of L-Ala reacting with **2** and **3e** over time



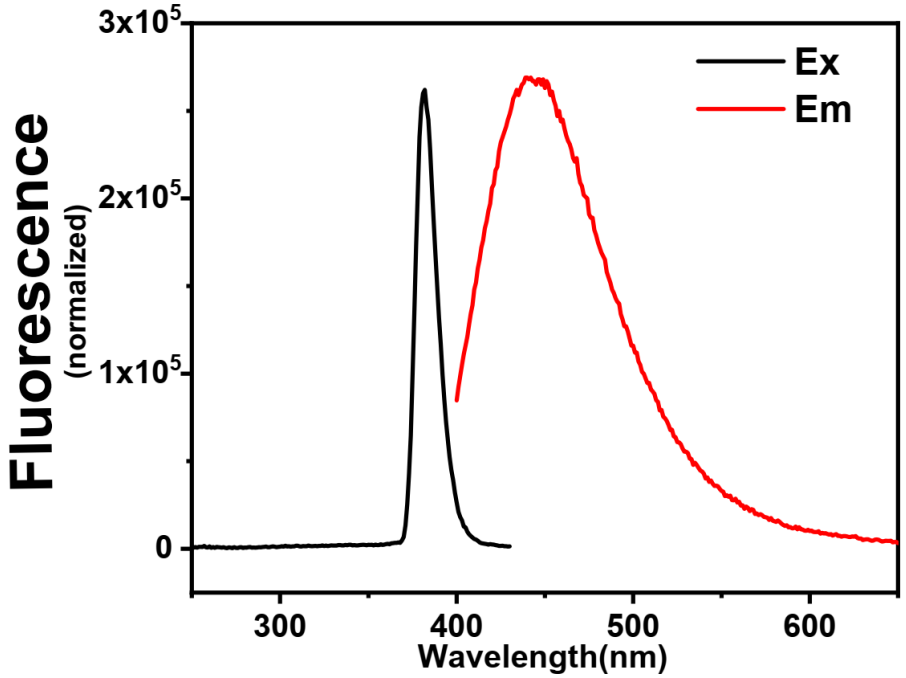
Supplementary Figure 6. All the reactions were carried out at 5.0 mM. t_{5e}=9.21 min, λ = 220 nm. LC-MS analysis showed that product **5e** was stable over a period of 12 hours.

HRMS of **5e**



HRMS: Calcd for $C_{18}H_{18}NO_2S$ $[M+H]^+$:312.1053; found: 312.1058

5. Fluorescence spectra of 5e



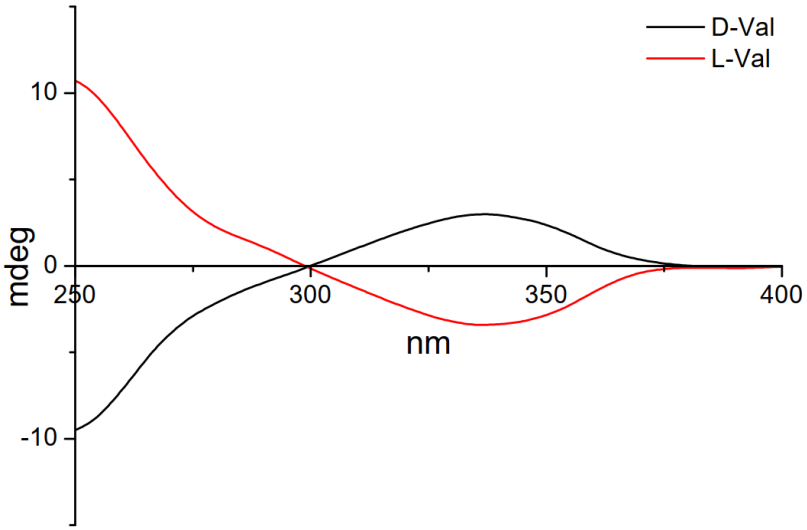
Ex=382 nm, Em=450 nm; The fluorescence quantum yield of **5e** in degassed aqueous solution (MeOH/buffer=1:2) is 8.3%

6. Chiroptical sensing of various analytes

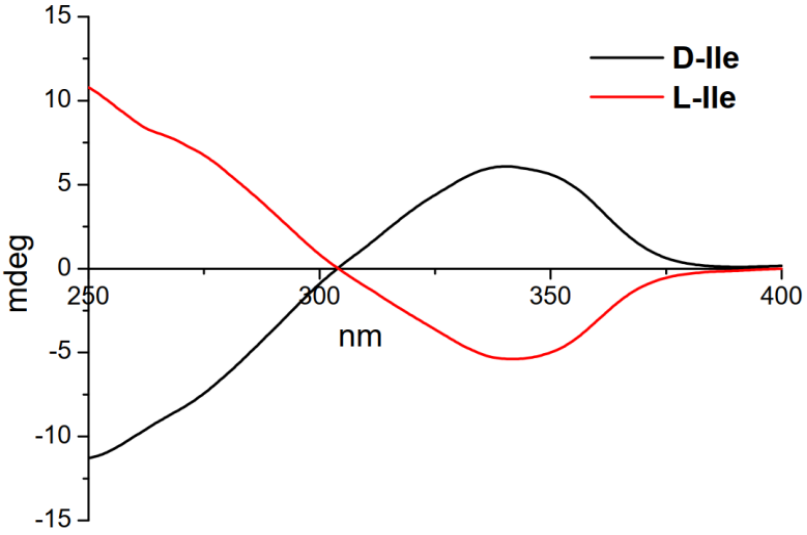
All CD spectra were measured on a JASCO J-815 automatic spectrometer (Tokyo, Japan). The mixture solvent of methanol and PB or water was used as a blank and automatically subtracted from the samples during scanning. Data were recorded from 250 to 400 nm with a scan speed of 100 nm/min and data pitch of 0.5 nm, a bandwidth of 1 nm, a response of 1 s. The reaction mixture was diluted to suitable concentration for the test. The pathlength was 1 mm and 10 mm, for high concentration (80 - 2000 μM) and low concentration (5- 400 μM), respectively. The measurements were repeated twice. OPA and p-Toluenethiol were dissolved in methanol as stock solution and were used without avoiding light and air for sensing procedure.

Due to chiroptical sensing of various AAs at relatively high concentration (> 500 μM), for assaying we used the standard condition: mixing AAs (1.0 equiv), **2** (1 equiv) and **3e** (1.2 equiv) at r.t. for 1 min. For AAs at relatively low concentration (< 500 μM), the reaction time was 3 min, and **2** and **3e** were excess to promote the reaction.

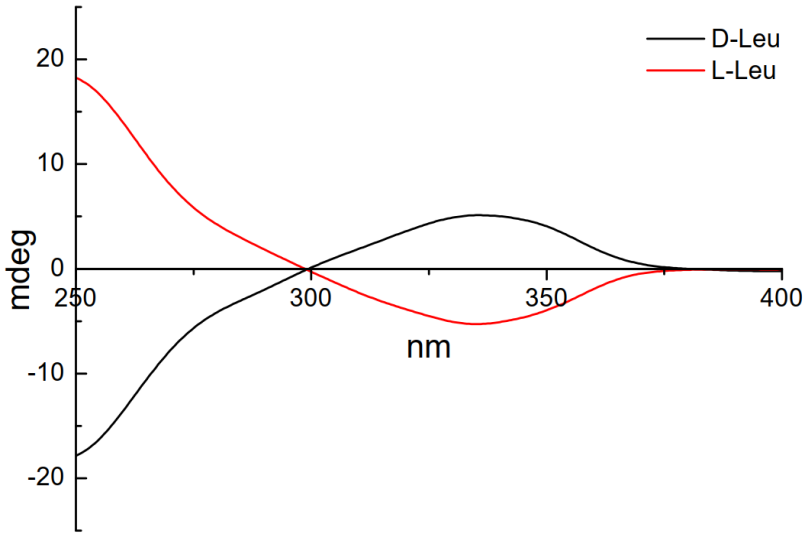
6.1 Successful analytes



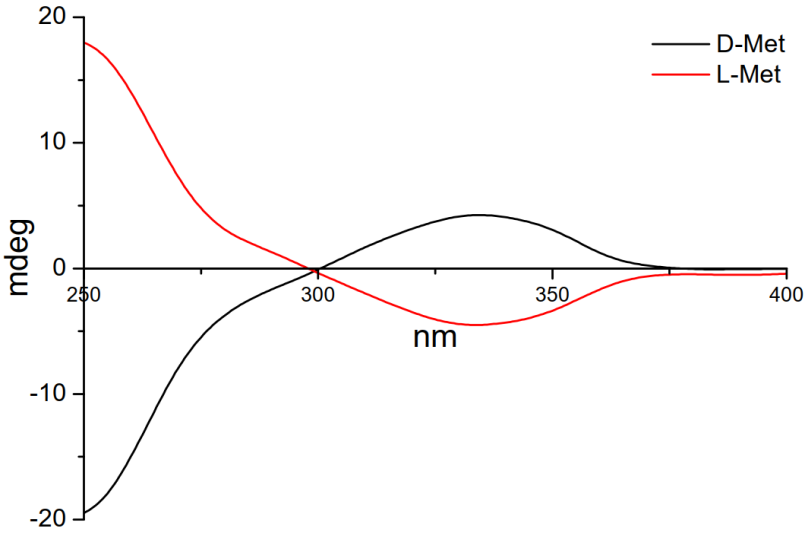
All CD spectra of **6e** were obtained at 0.33 mM



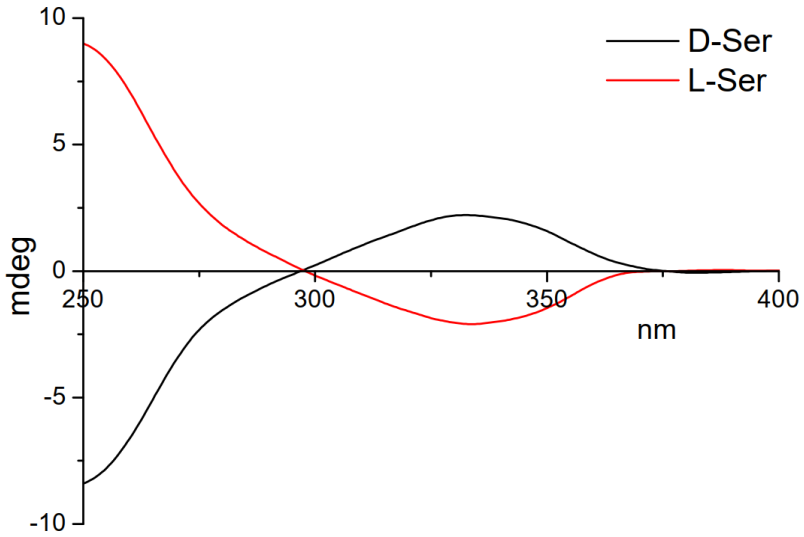
All CD spectra of **7e** were obtained at 0.33 mM.



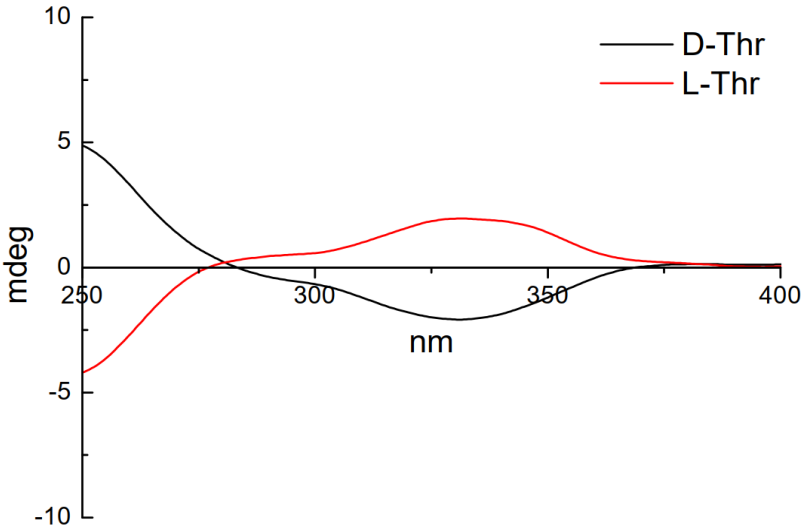
All CD spectra of **8e** were obtained at 0.33 mM.



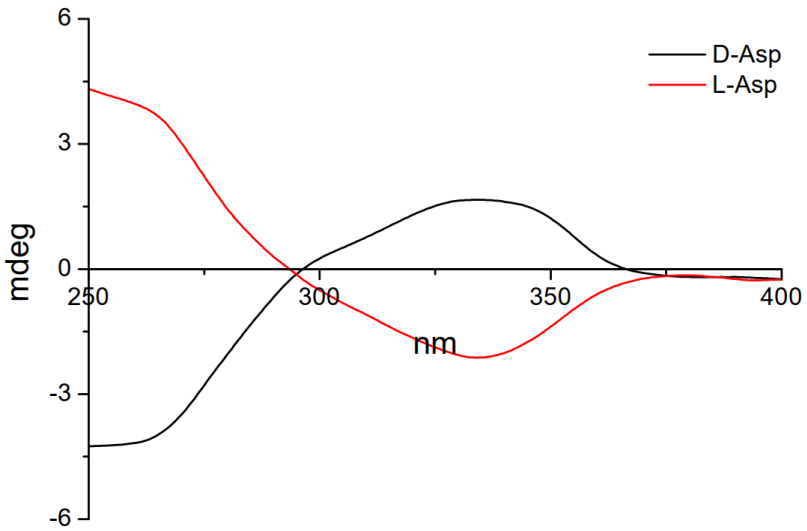
All CD spectra of **9e** were obtained at 0.33 mM.



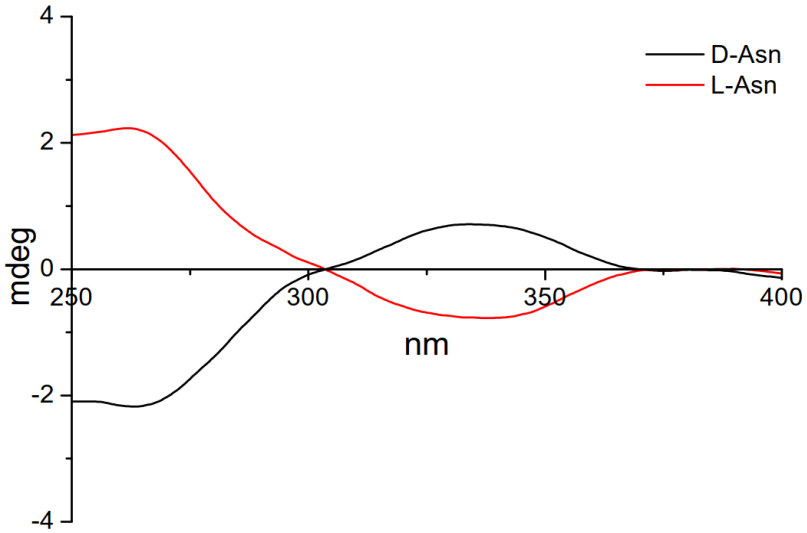
All CD spectra of **10e** were obtained at 0.33 mM.



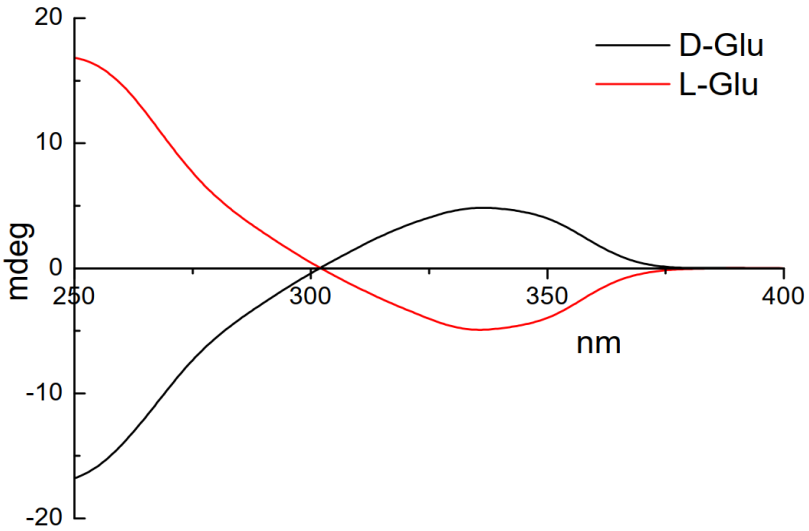
All CD spectra of **11e** were obtained at 0.33 mM



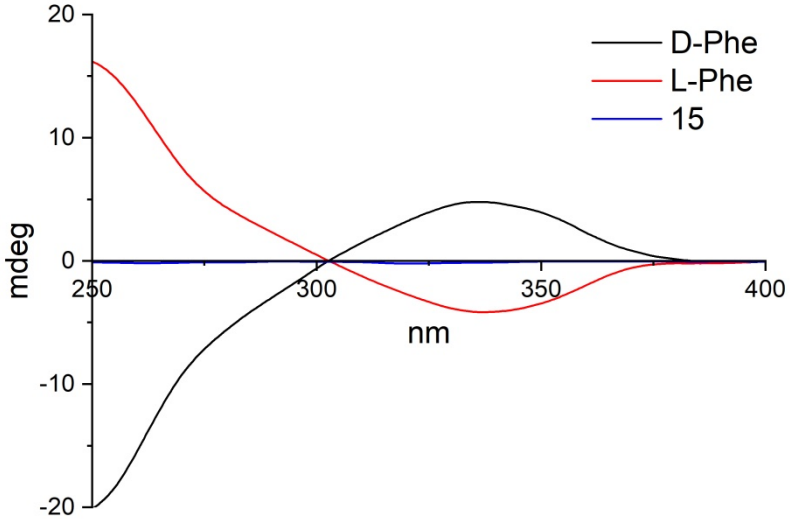
All CD spectra of **12e** were obtained at 0.33 mM.



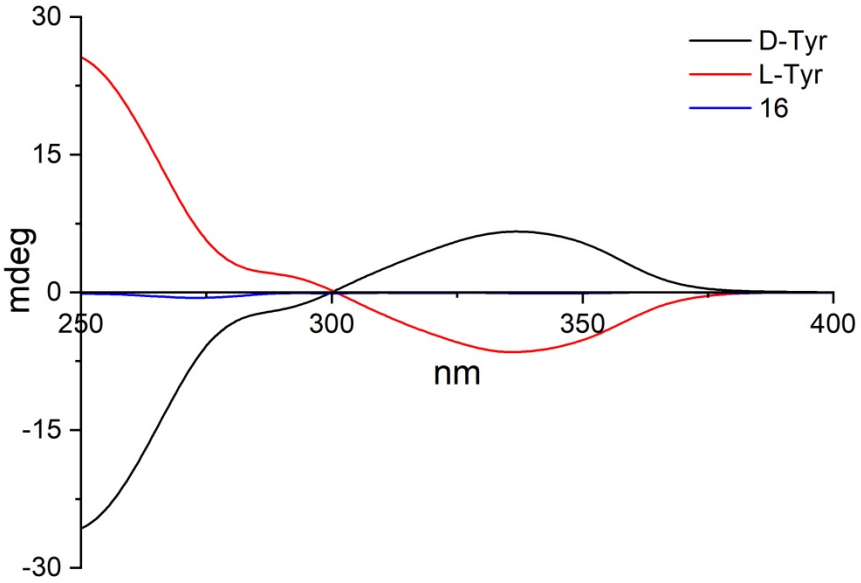
All CD spectra of **13e** were obtained at 0.33 mM.



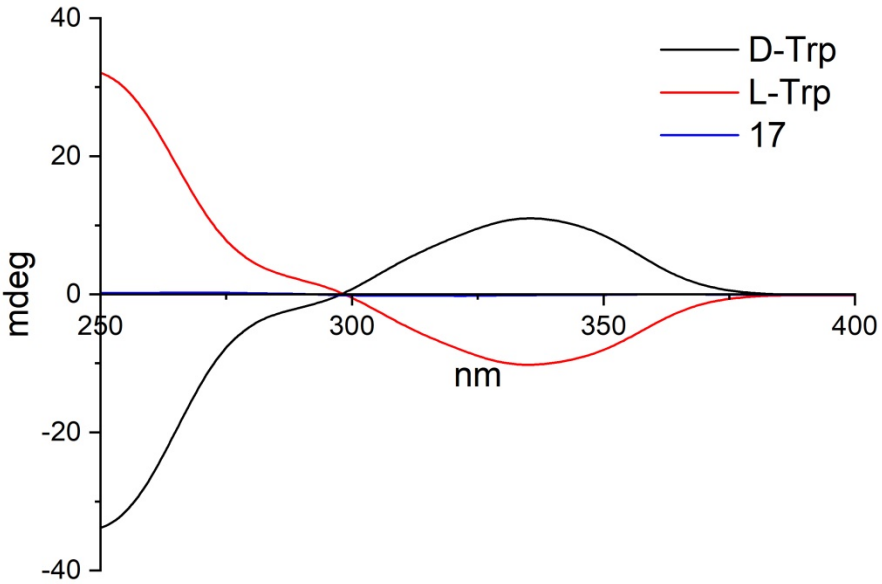
All CD spectra of **14e** were obtained at 0.33 mM.



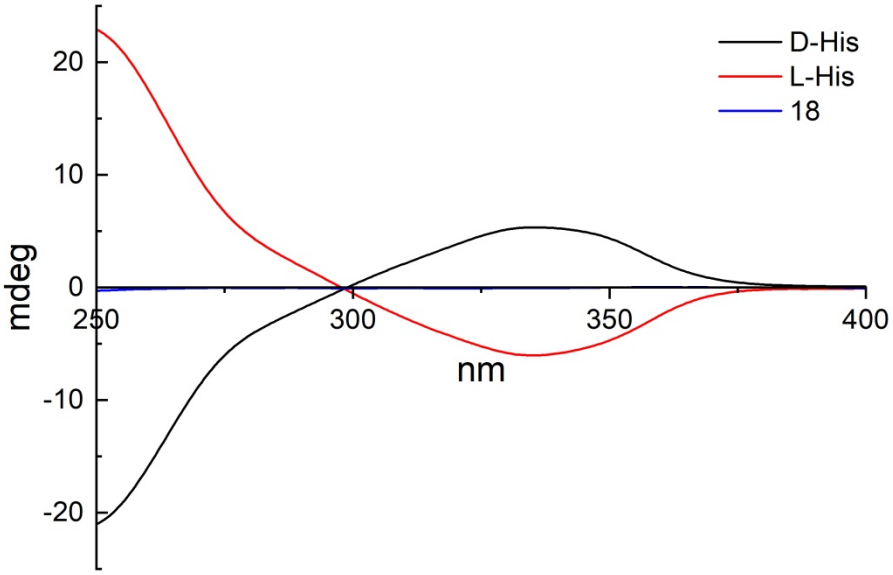
All CD spectra of **15e** were obtained at 0.33 mM.



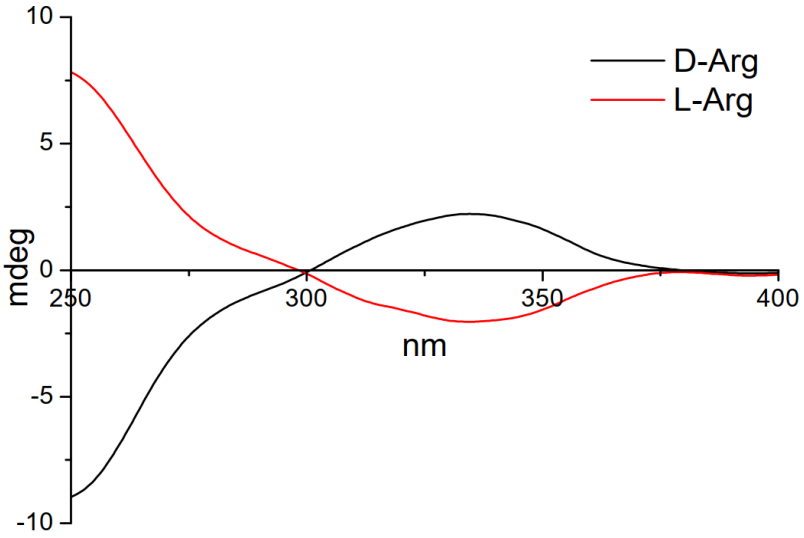
All CD spectra of **16e** were obtained at 0.33 mM.



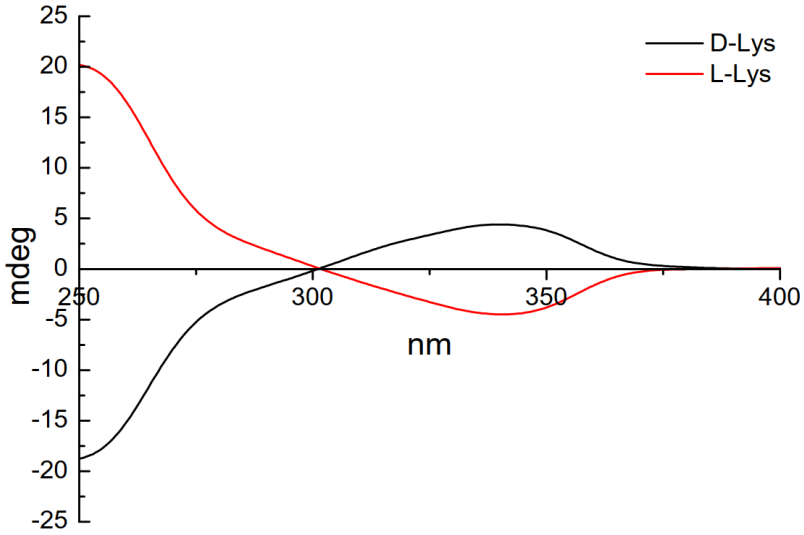
All CD spectra of **17e** were obtained at 0.33 mM.



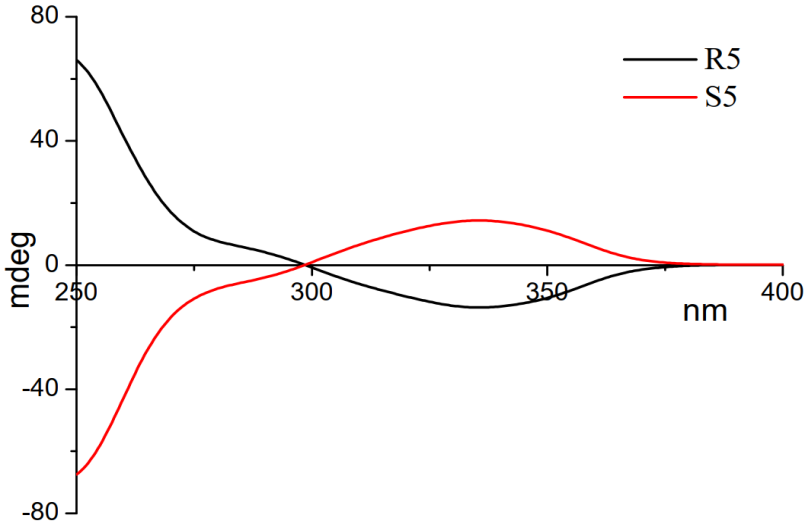
All CD spectra of **18e** were obtained at 0.33 mM.



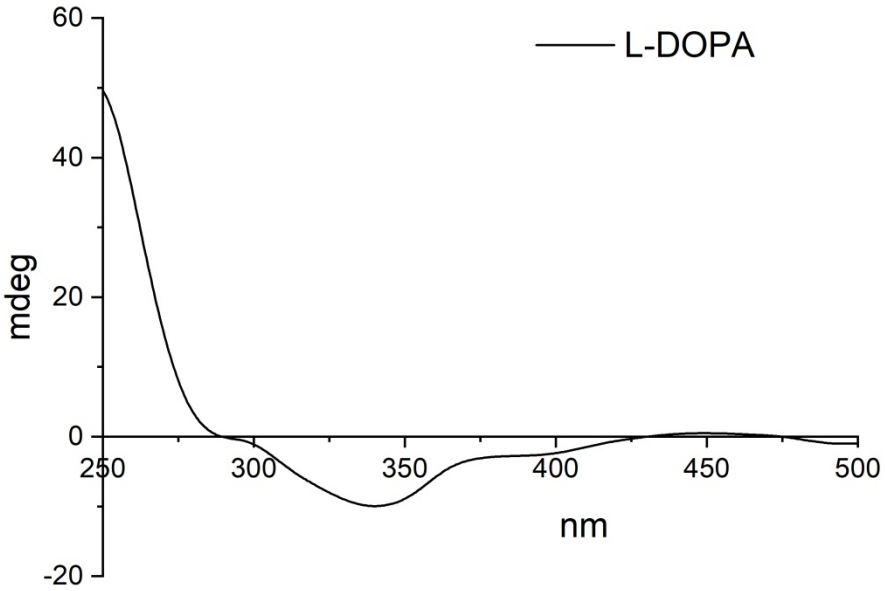
All CD spectra of **19e** were obtained at 0.33 mM.



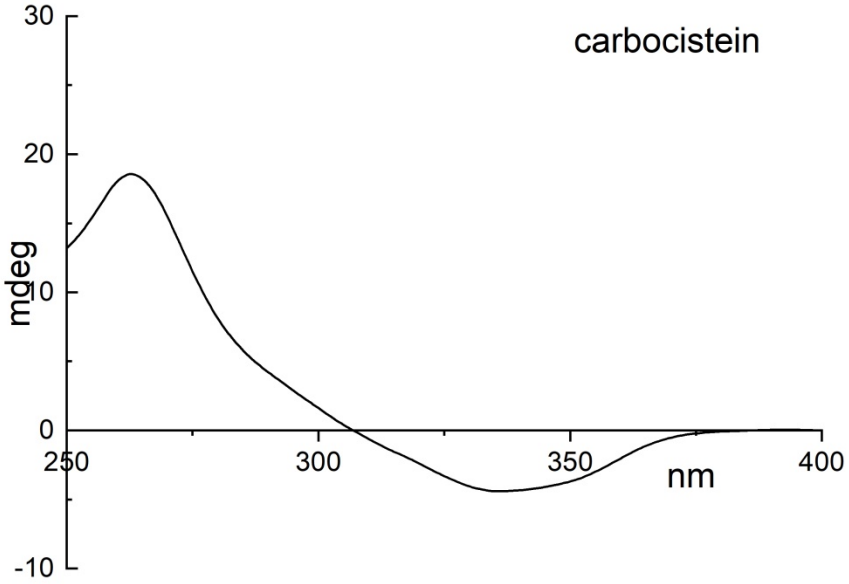
All CD spectra of **20e** were obtained at 0.33 mM (MeOH:PB=2:1).



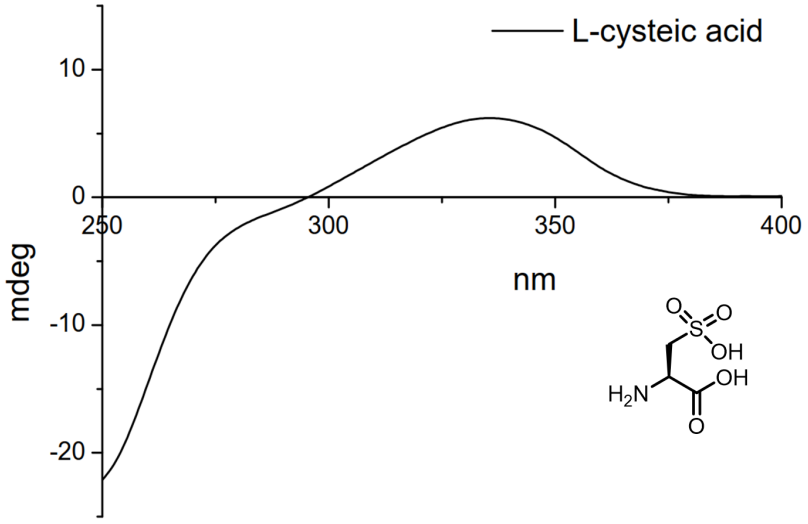
All CD spectra of **21e** were obtained at 1.33 mM.



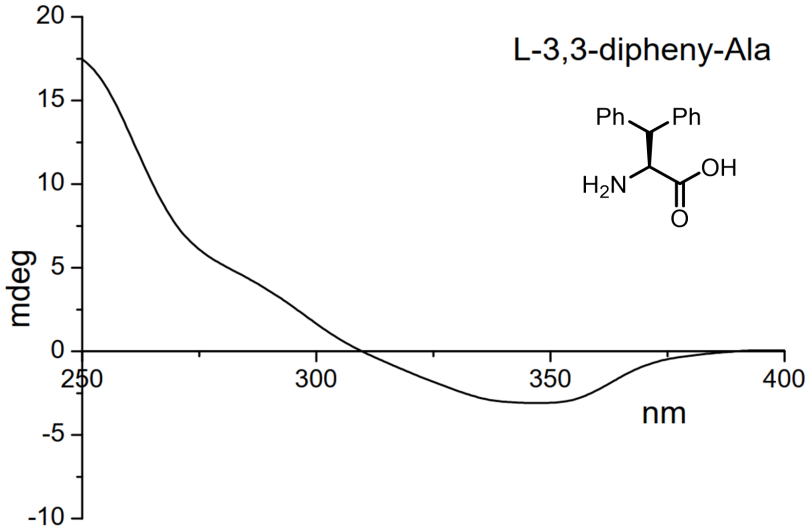
CD spectra of sensing **22e** was obtained at 0.33 mM



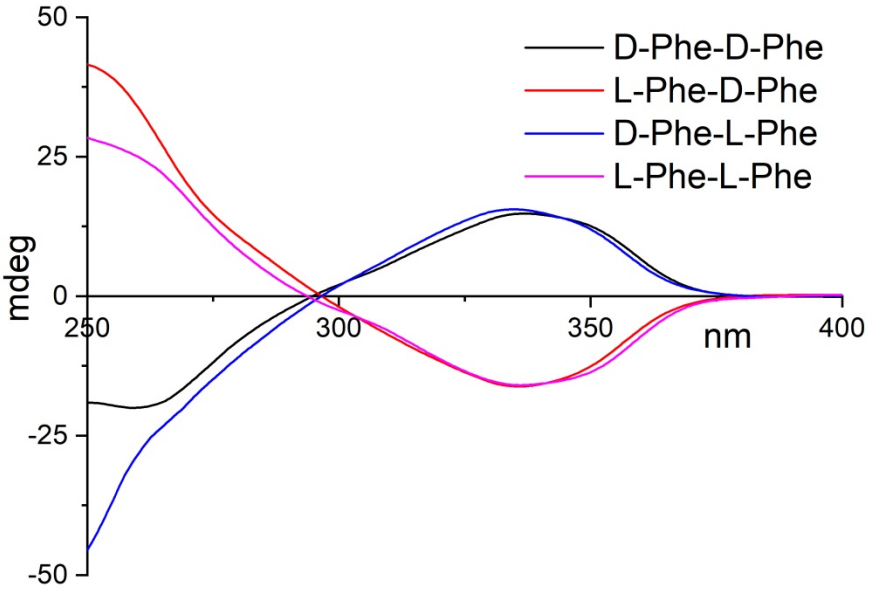
CD spectra of sensing **23e** was obtained at 0.33 mM



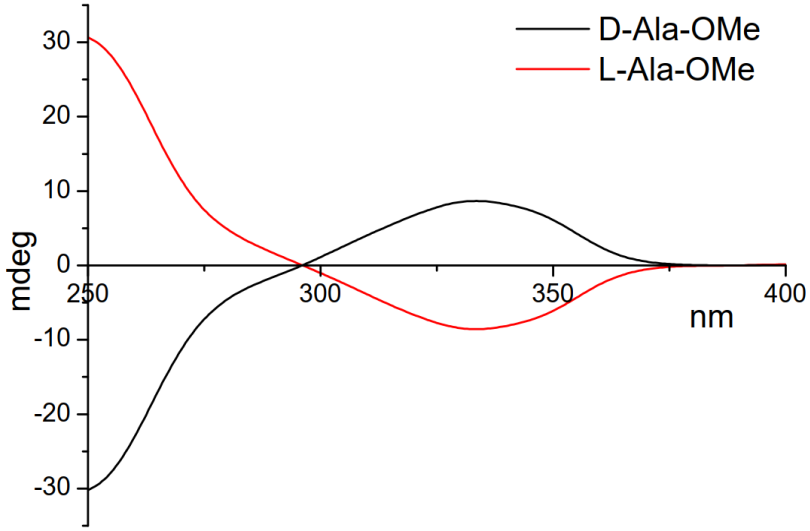
CD spectra of **24e** was obtained at 0.33 mM (one enantiomer shown).



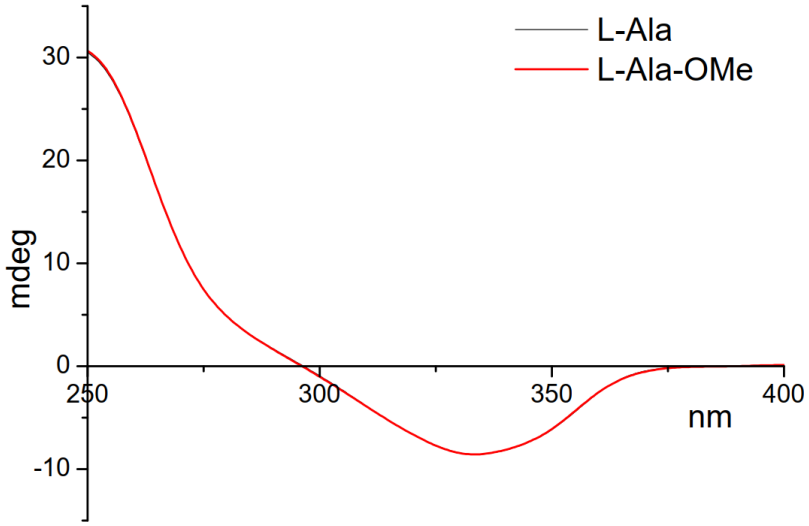
CD spectra of **25e** was obtained at 0.33 mM (one enantiomer shown).



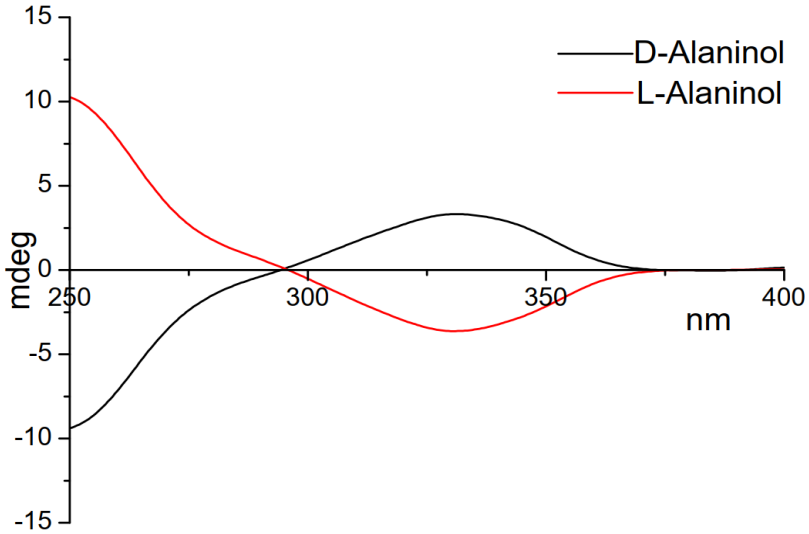
All CD spectra of **26e** were obtained at 0.33 mM.



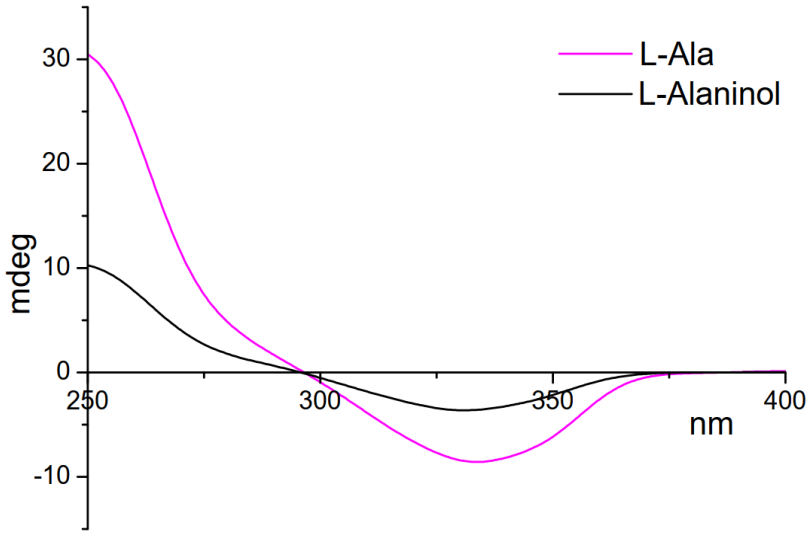
All CD spectra of **27e** were obtained at 0.285 mM (MeOH : H_2O=3:1, a small amount of PB was used to dissolve Ala-OMe).



Comparison of CD signals of L-Ala and **27** (L-Ala-OMe) at 0.285 mM (MeOH : H_2O=3:1) and **27e** gave the same signal compared with L-Ala at 335 nm.

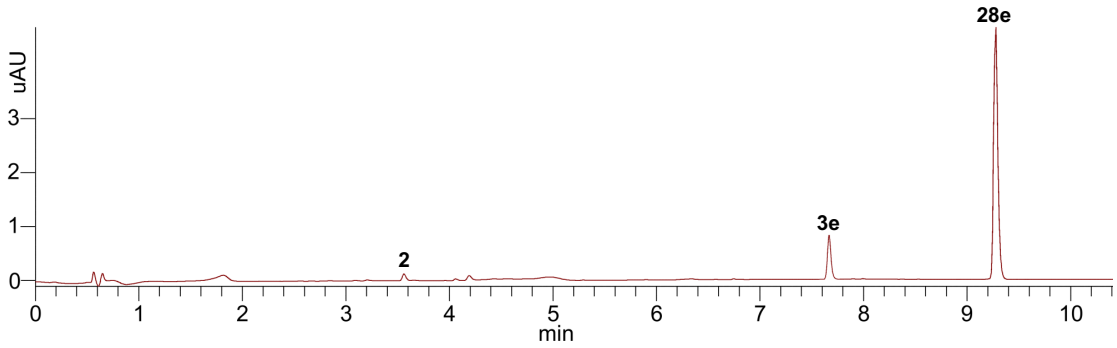


All CD spectra of **28e** were obtained at 0.285 mM (MeOH : H_2O=3:1, without base)



Comparison of CD signals of L-Ala and **28** (L-Alaninol) at 0.285 mM and **28e** gave weaker CD signal (~40%) compared with L-Ala at 335 nm, which indicated the importance of the carboxylate group.

UPLC-HRMS analysis of the reaction of 28e

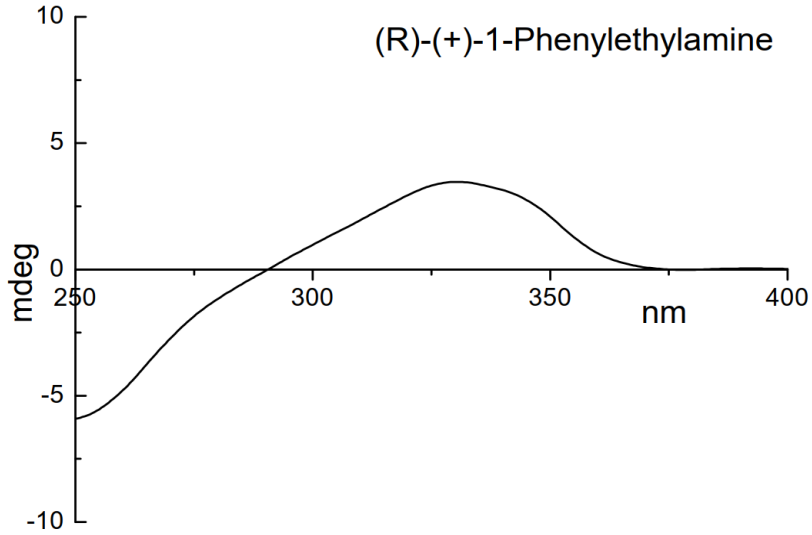


Supplementary Figure 7. UPLC trace of the reaction of L-Alaninol at 1 min using MeOH/H_2O (3:1) as solvent (without adding base)

Note: This reaction also proceeded quickly, cleanly and completely monitored by LC-MS, which indicated that the weaker CD signal of alaninol compared with Ala was due to the lack of carboxylate group.

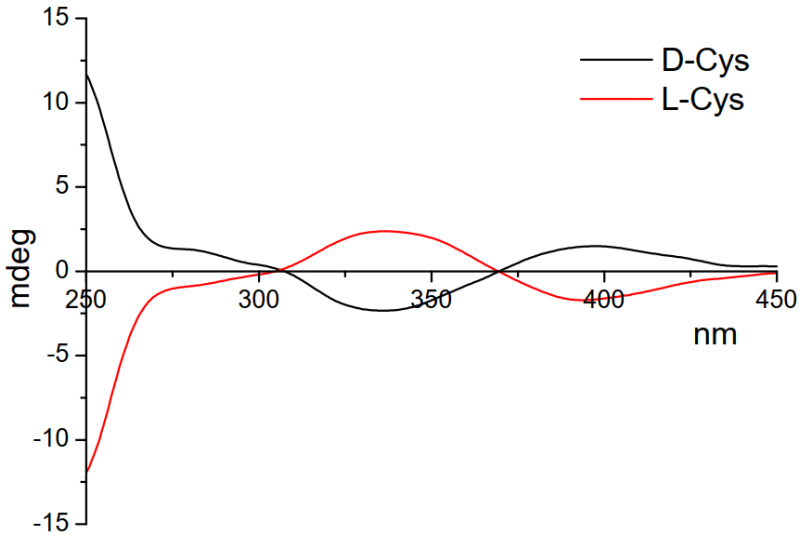
HRMS of 28e

HRMS: Calcd for $C_{18}H_{20}NOS$ $[M+H]^+$: 298.1260; found: 298.1270

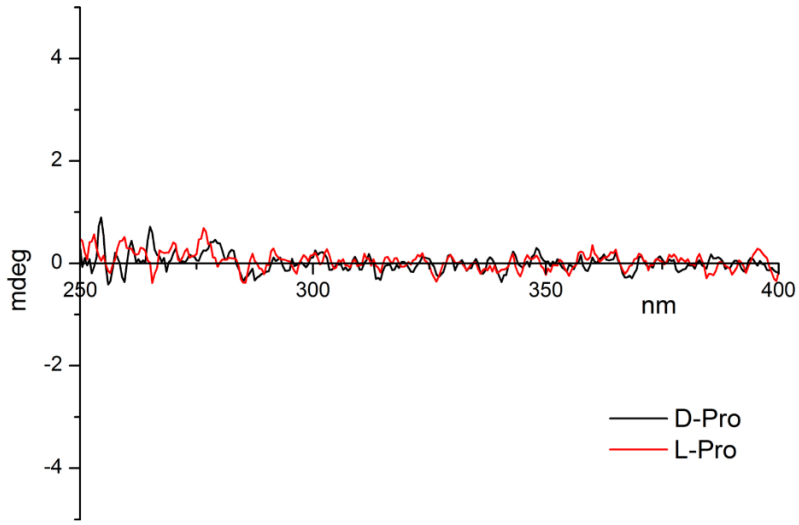


CD spectra of **29e** was obtained at 0.33 mM (one enantiomer shown).

6.2 Problematic analytes



All CD spectra of **30e** were obtained at 0.5 mM

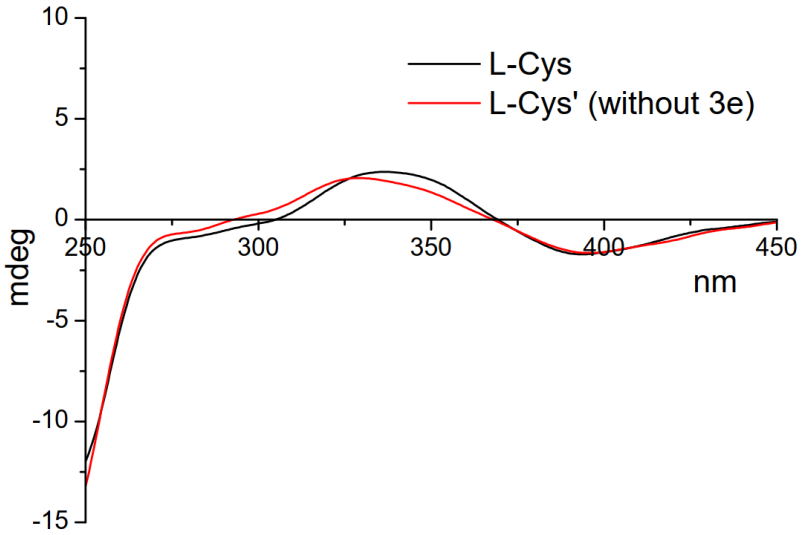


All CD spectra of **31e** was obtained at 1.33 mM

Chiroptical sensing of Pro cannot display any CD signals because its secondary amino group cannot form the corresponding isoindole product.

6.3 Elucidation of unusual products

Comparison of the influence of **3e** for CD signals of L-Cys.

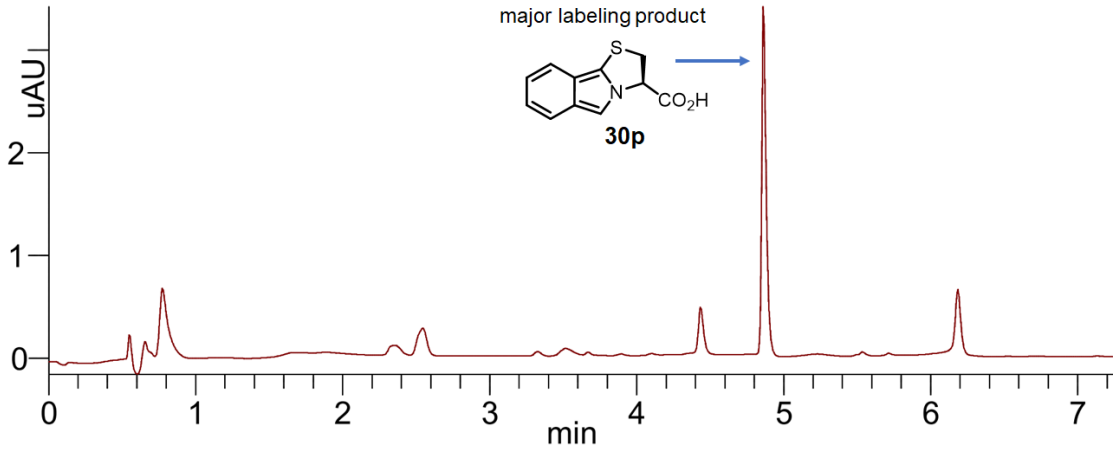


All CD spectra of **30** were obtained at 0.33 mM.

The CD signals show that 3e has small influence for the chiroptical sensing of L-Cys.

Therefore, 3e may not take part in the actual reaction and we reason that the CD signals ought to be induced by the reaction of oPA and L-Cys.

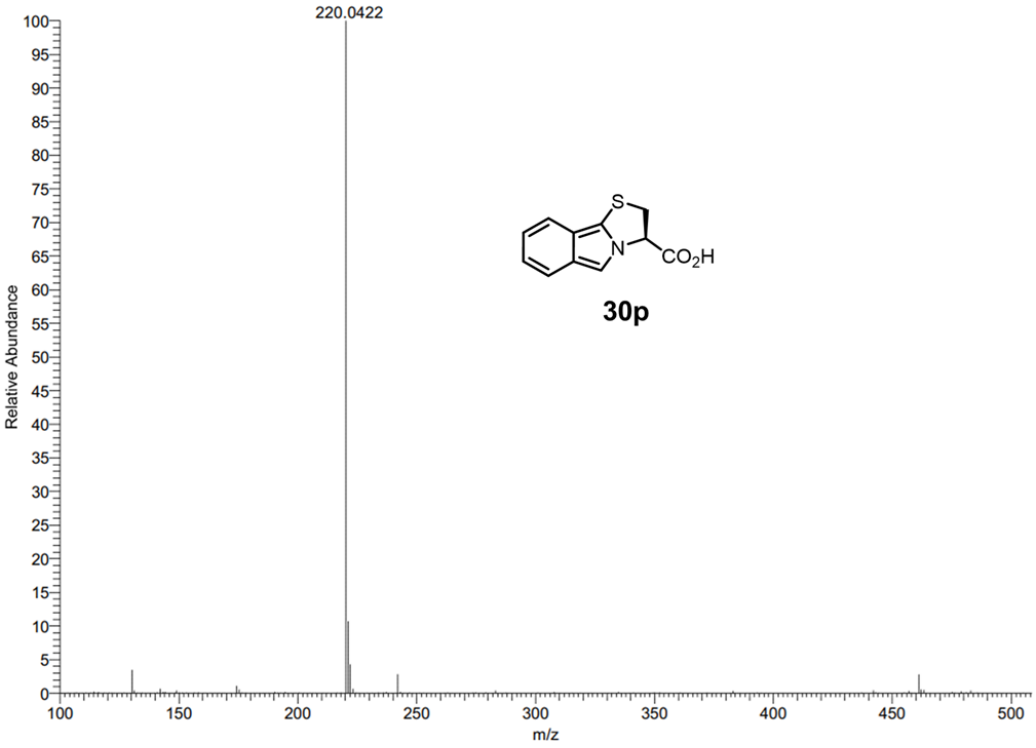
UPLC-HRMS analysis of the reaction of Cys



Supplementary Figure 8. UPLC trace of the reaction of Cys at 1 min using the standard condition (without 3e).

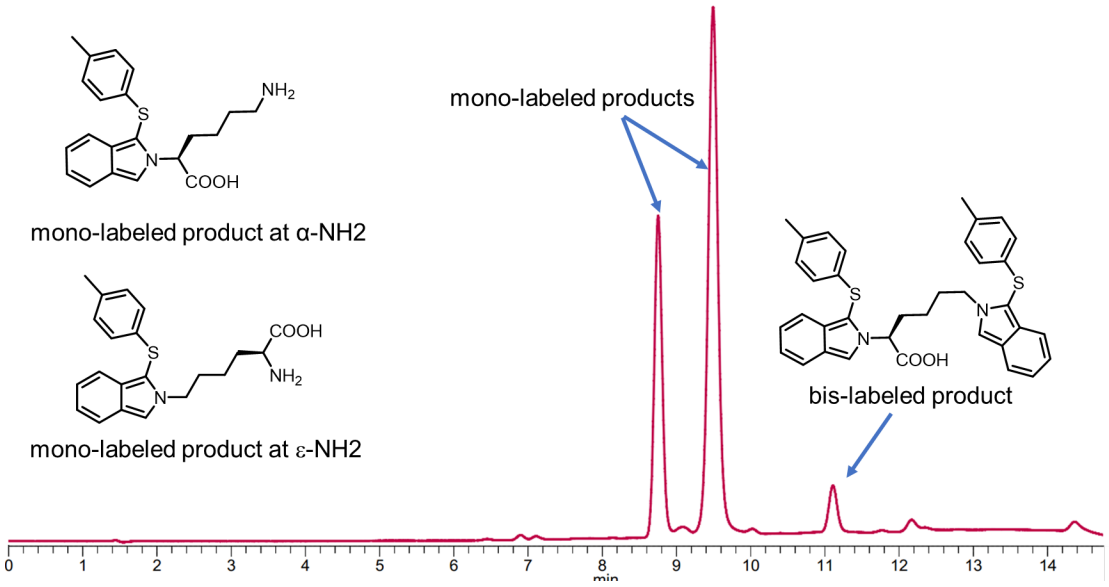
Note: Due to the stronger nucleophilicity of SH side chain, the reaction of Cys preferred to forming tricyclic isoindole product. It is worth mentioning that the reaction system is not clean on the LC-MS spectrum and the tricyclic isoindole product 30p wasn't stable as the time went on (decomposed within 10 min).

Therefore, we couldn't separate this product and its proposed structure was only elucidated by HRMS and the disparate UV (see Figure 2B) and CD signals.



HRMS: Calcd for $C_{11}H_{10}NO_2S$ $[M+H^+]$:220.0427; found: 220.0422

UPLC-HRMS analysis of the reaction of Lys (20)

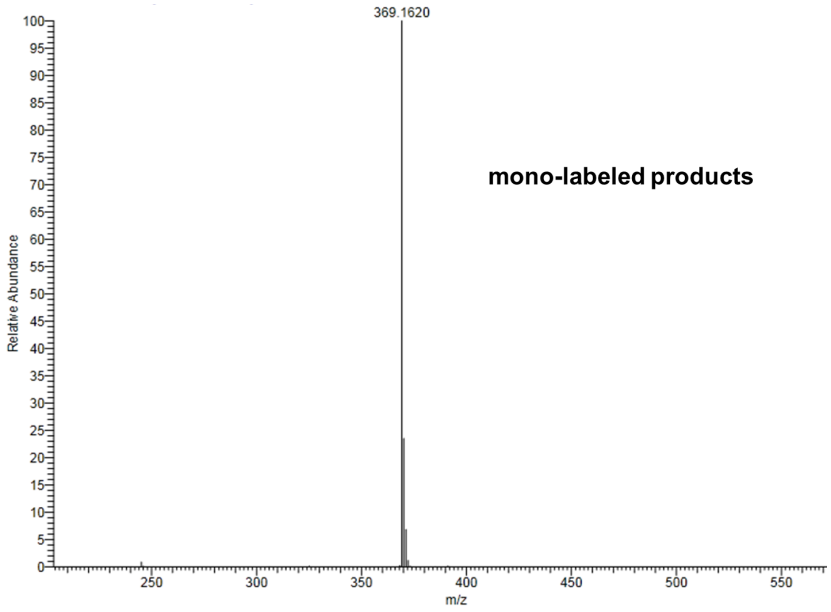


Supplementary Figure 9. UPLC trace of the reaction of Lys at 1 min using the standard condition.

Note: Due to the nucleophilicity of ε-NH_2 at side chain, the reaction of Lys produced a mixture of mono- and bis-labeled products which were determined by

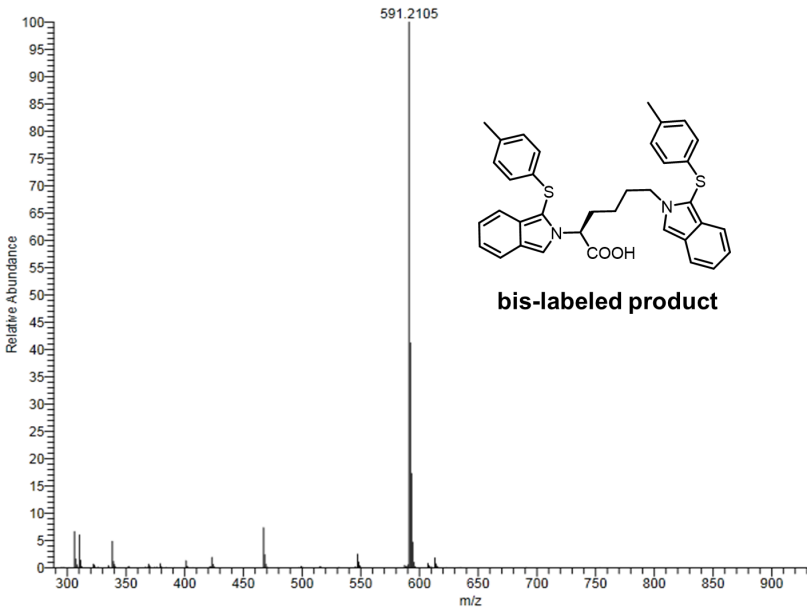
HRMS. We reasoned that the isoindole structure forming at the ε-amino terminal will not have Cotton effect when compared with α-amino position. So mono-labeled product at ε-NH_2 made negligible impact on CD signals which was buttressed by its linear relationship between g-factor and ee (see Figure 3B). But the bis-labeled product actually had a slight influence on its UV absorption of Lys vs concentration.

HRMS of mono-labeled products



HRMS: Calcd for $C_{21}H_{25}N_2O_2S$ [$M+H^+$]:369.1631; found: 369.1620

HRMS of bis-labeled product

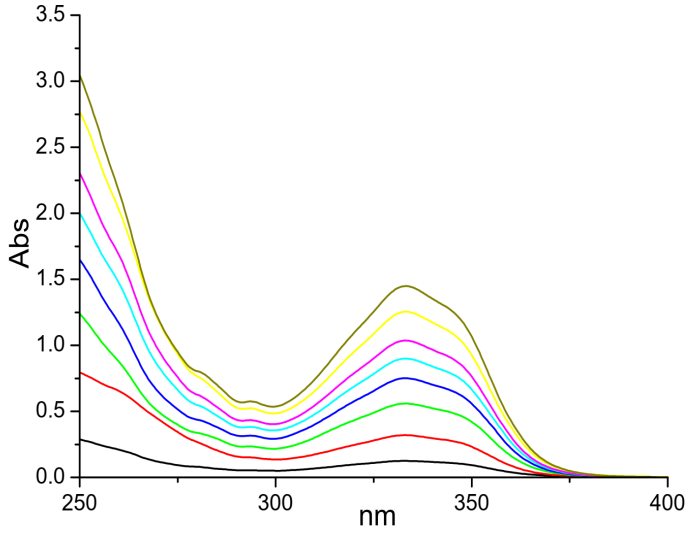


HRMS: Calcd for $C_{36}H_{35}N_2O_2S_2$ [M+H$^+$]:591.2134; found:591.2105

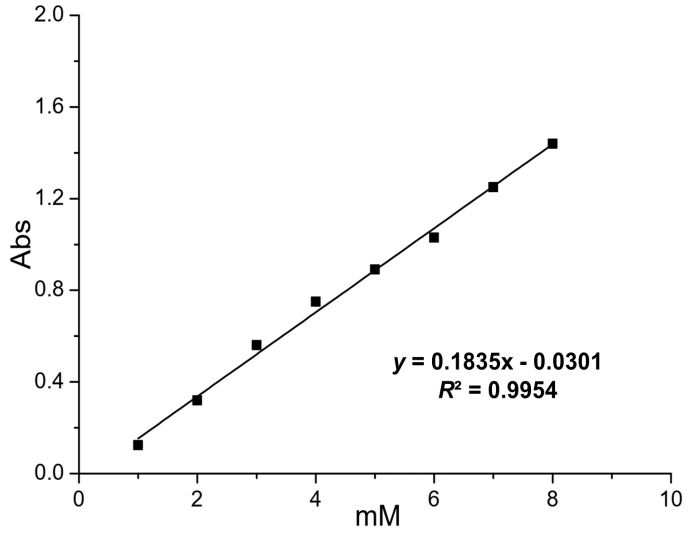
7. Test of typical amino acids

7.1 Ala

UV absorption of Ala at **1-8 mM** (six times dilution to **0.167-1.33 mM** for test).

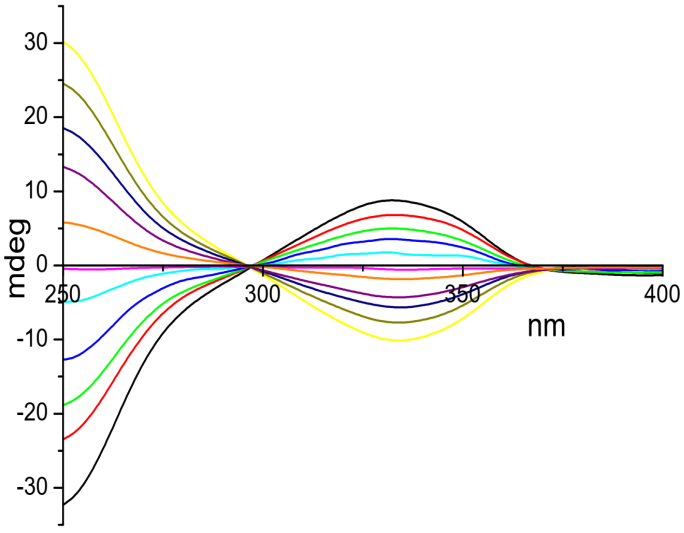


Linear relationship between UV absorption at **335 nm** and the concentration of **Ala**

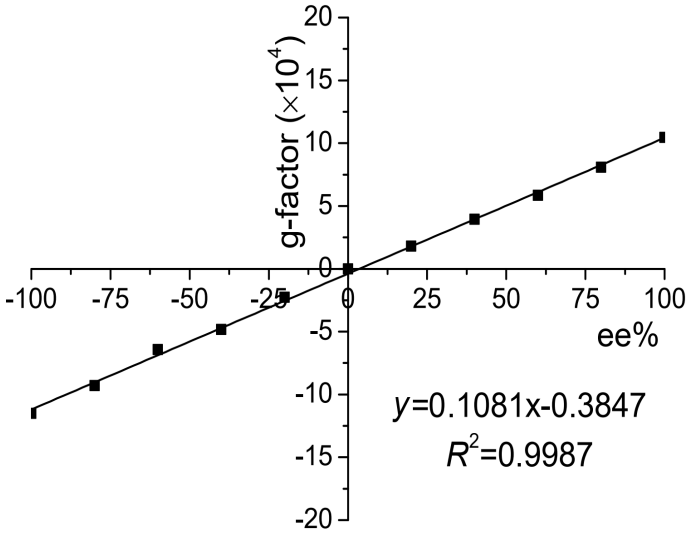


Chiroptical sensing of **Ala** at varying ee's.

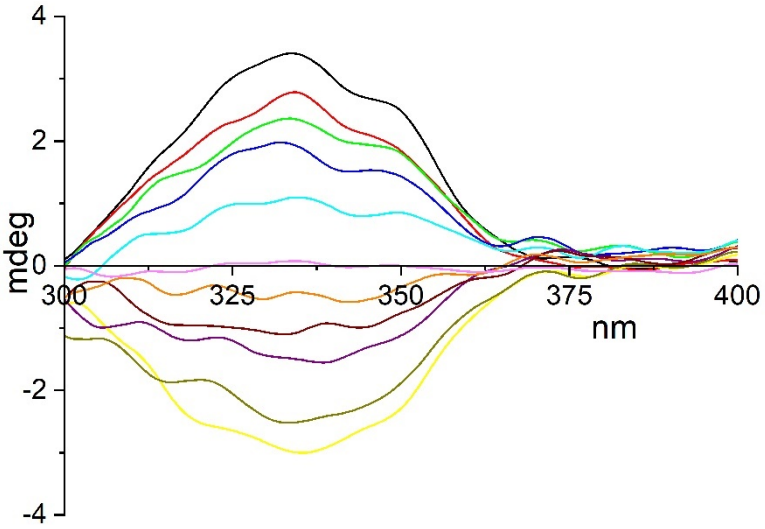
1) All CD spectra of **Ala** samples were obtained at **2 mM** (four times dilution to 0.5 mM for test).



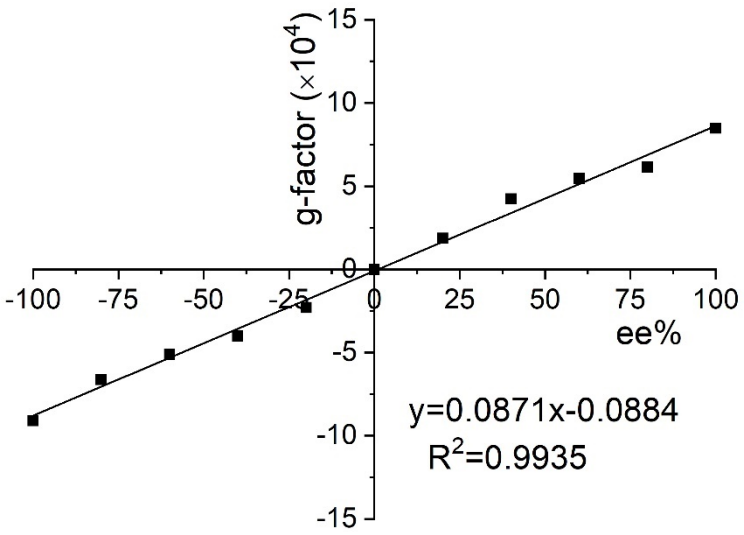
Linear relationship between g-factor and ee of **Ala** samples measured at **335 nm**



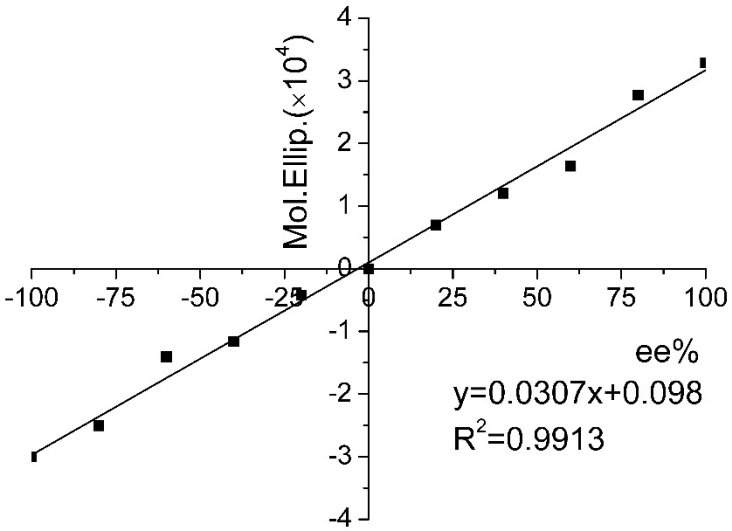
2) All CD spectra of **Ala** samples were obtained at **10 μM**.



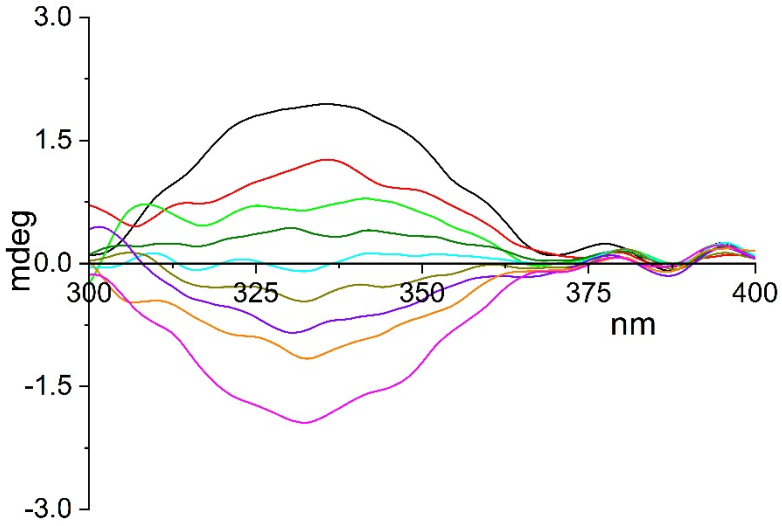
Linear relationship between g-factor and ee of **Ala** samples measured at **335 nm** (10 μM)



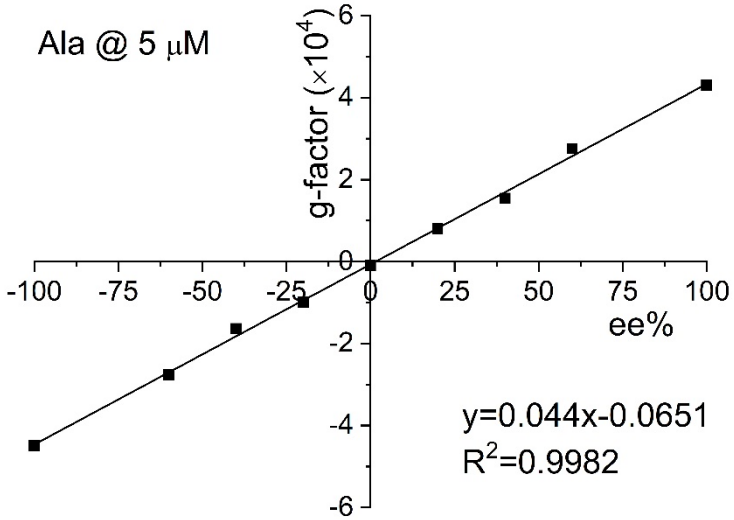
Linear relationship between molar ellipticity and ee of **Ala** samples measured at **335 nm** (10 μM)



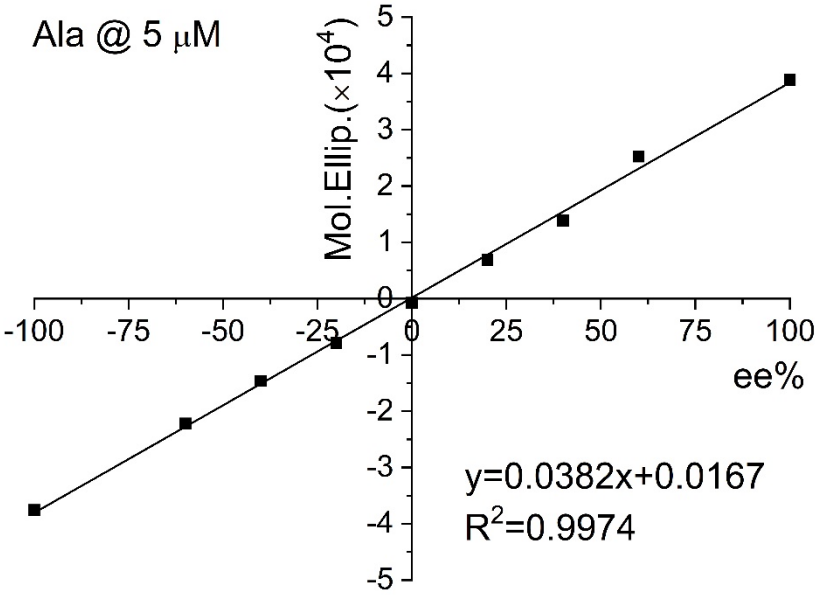
3) All CD spectra of **Ala** samples were obtained at **5 μM**.



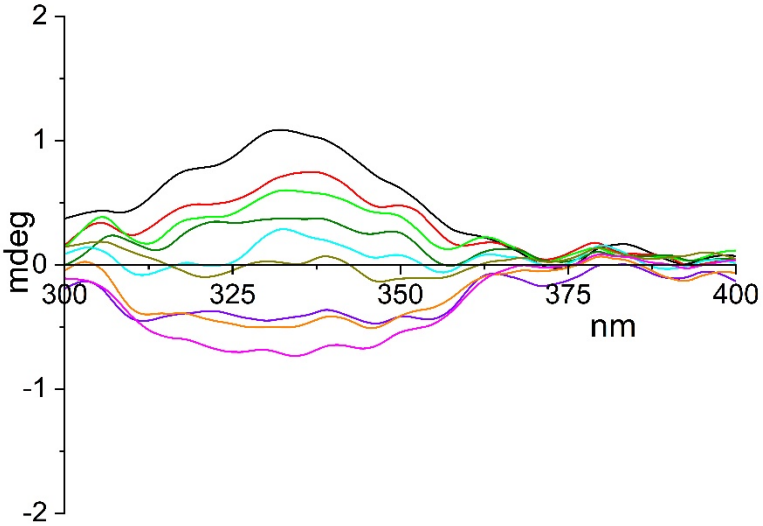
Linear relationship between g-factor and ee of **Ala** samples measured at **335 nm** (5 μM)



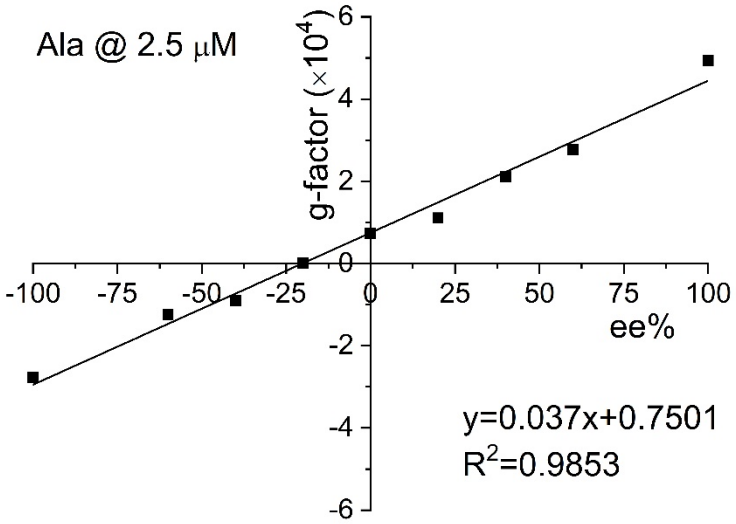
Linear relationship between molar ellipticity and ee of **Ala** samples measured at **335 nm** (5 μM)



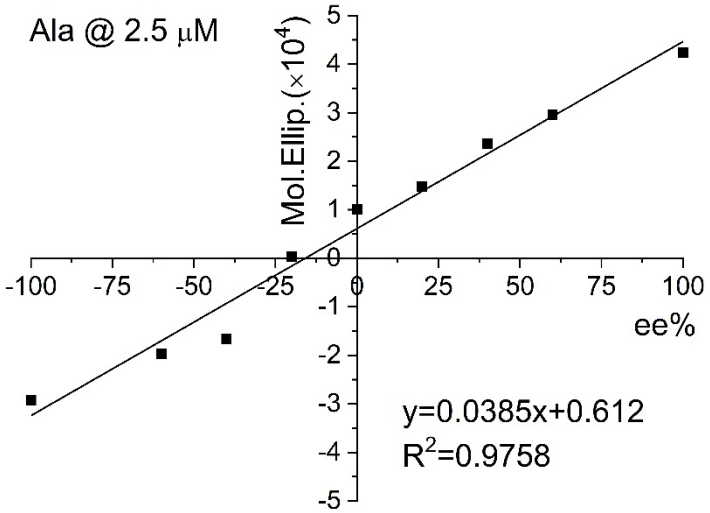
4) All CD spectra of **Ala** samples were obtained at 2.5 μM.



Linear relationship between g-factor and ee of **Ala** samples measured at **335 nm** (2.5 μM)

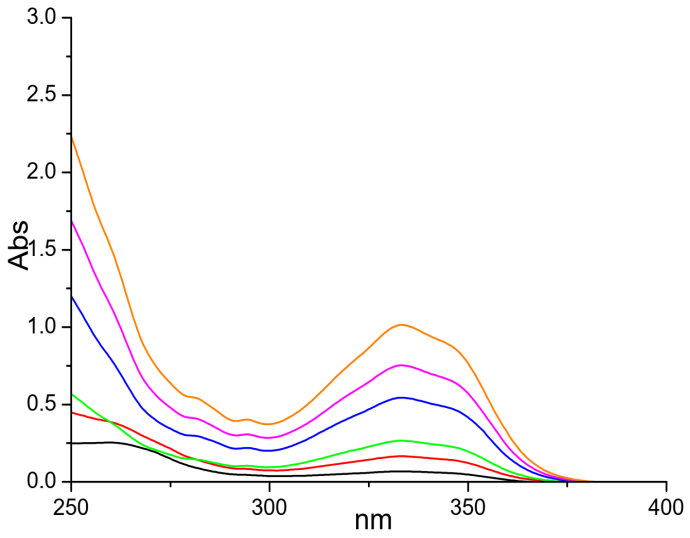


Linear relationship between molar ellipticity and ee of **Ala** samples measured at **335 nm** (2.5 μM)

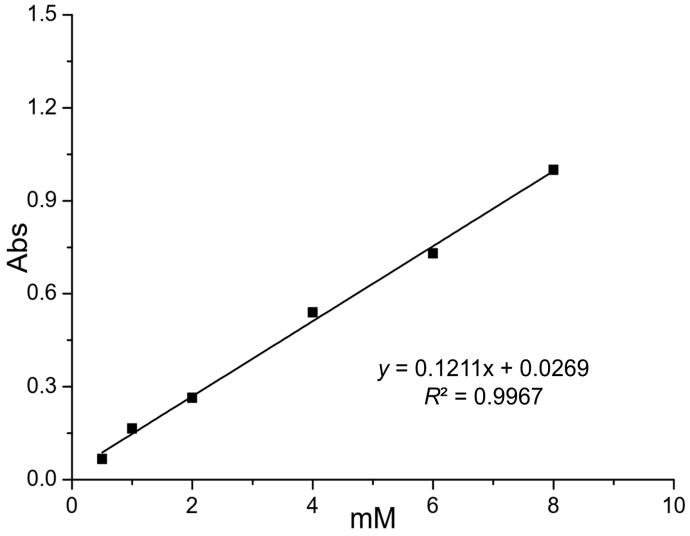


7.2 Glu

UV absorption of **Glu** at **<u>0.5-8 mM</u>** (six times dilution to **0.083-1.33 mM** for test).

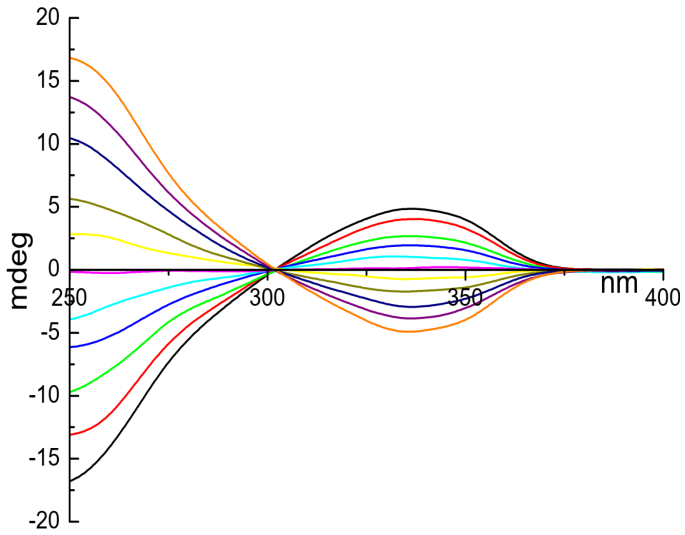


Linear relationship between UV absorption at **335 nm** and the concentration of **Glu**



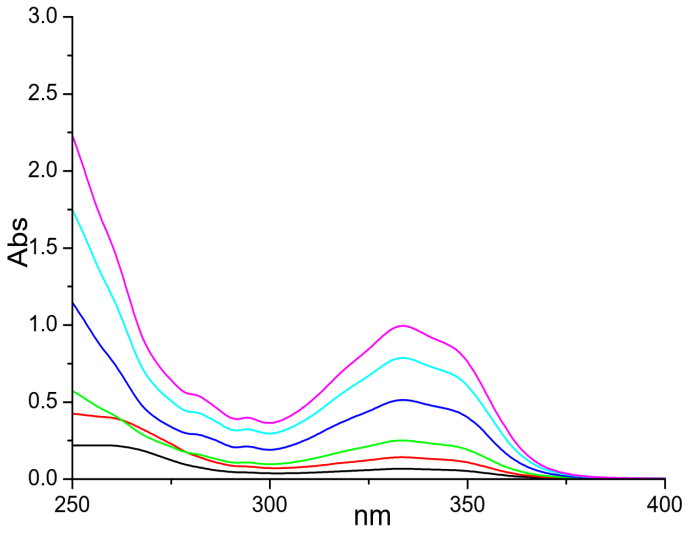
Chiroptical sensing of **Glu** at varying ee's.

All CD spectra of were obtained at **2 mM** (three times dilution to **0.67 mM** for test).



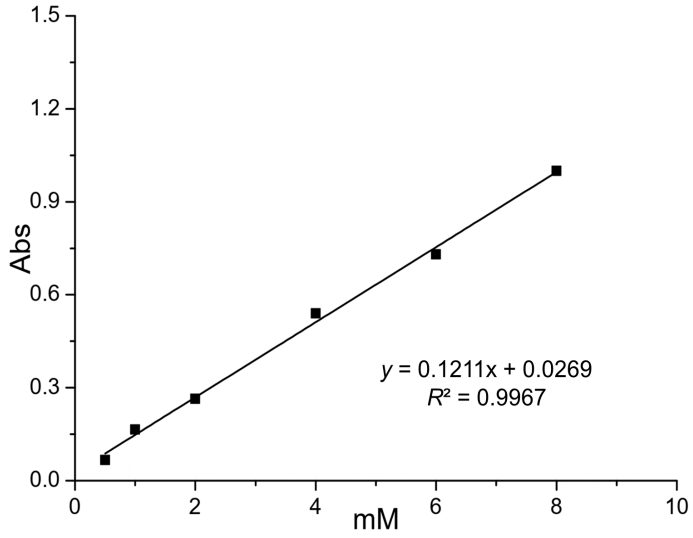
Linear relationship between g-factor and ee of **Glu** samples measured at **335 nm** has shown in Figure 3B

UV absorption of **Leu** at **<u>0.5-8 mM</u>** (six times dilution to **0.083-1.33 mM** for test).



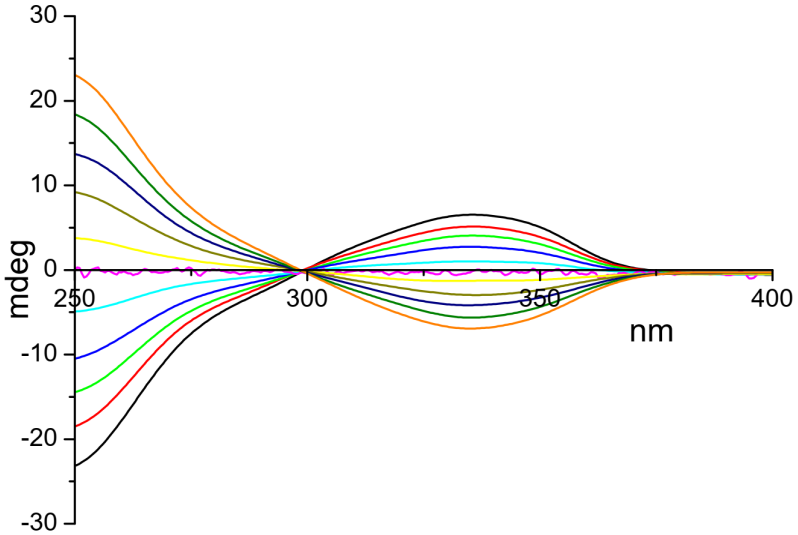
7.3 Leu

Linear relationship between UV absorption at **335 nm** and the concentration of **Leu**



Chiroptical sensing of **Leu** at varying ee's.

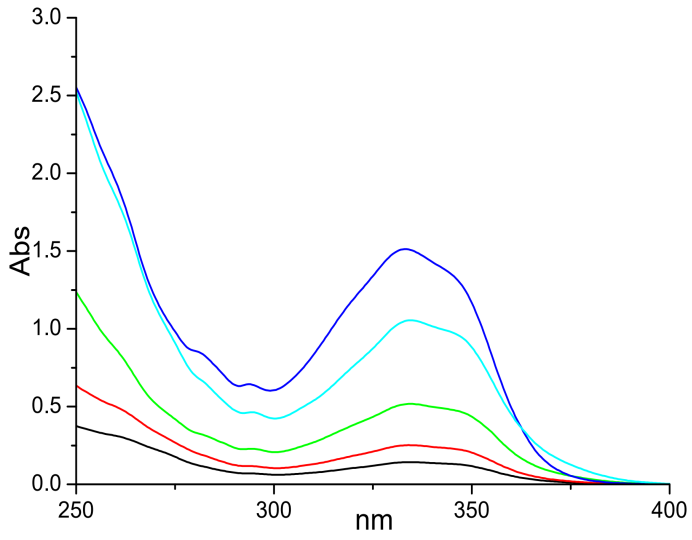
All CD spectra of were obtained at **2 mM** (four times dilution to **0.50 mM** for test).



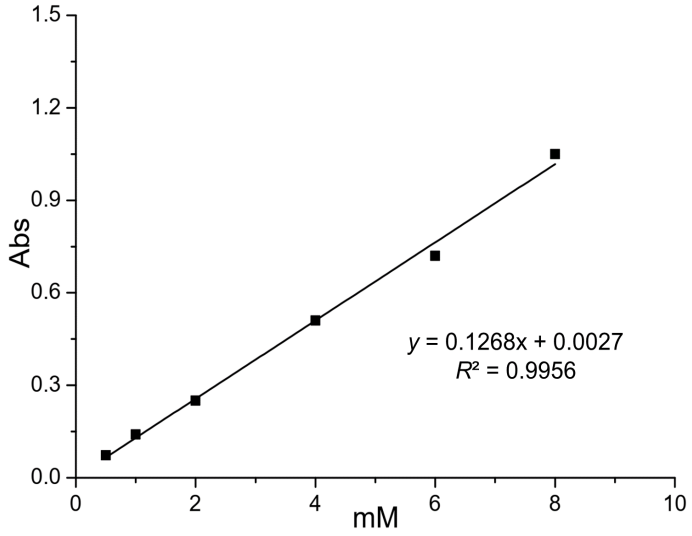
Linear relationship between g-factor and ee of **Leu** samples measured at **335 nm** has shown in Figure 3B

7.4 His

UV absorption of **His** at **0.5-8 mM** (six times dilution to **0.083-1.33 mM** for test).

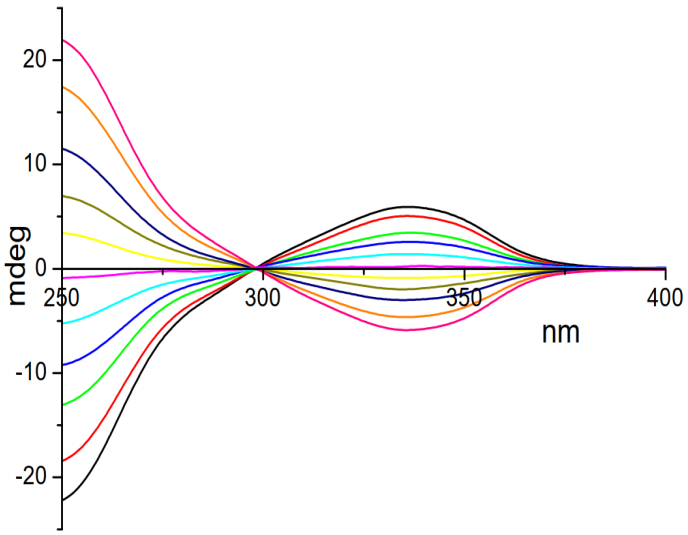


Linear relationship between UV absorption at **335 nm** and the concentration of **His**



Chiroptical sensing of **His** at varying ee's.

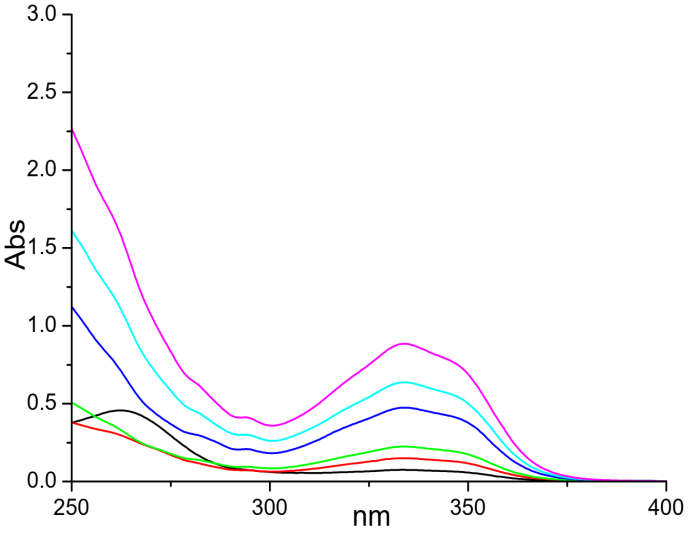
All CD spectra of were obtained at **2 mM** (six times dilution to **0.33 mM** for test).



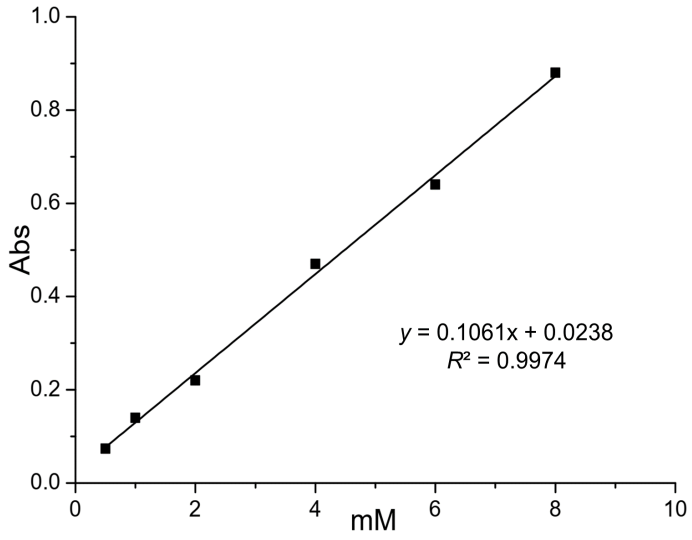
Linear relationship between g-factor and ee of **His** samples measured at **335 nm** has shown in Figure 3B

7.5 Thr

UV absorption of **Thr** at **0.5-8 mM** (six times dilution to **0.083-1.33 mM** for test).

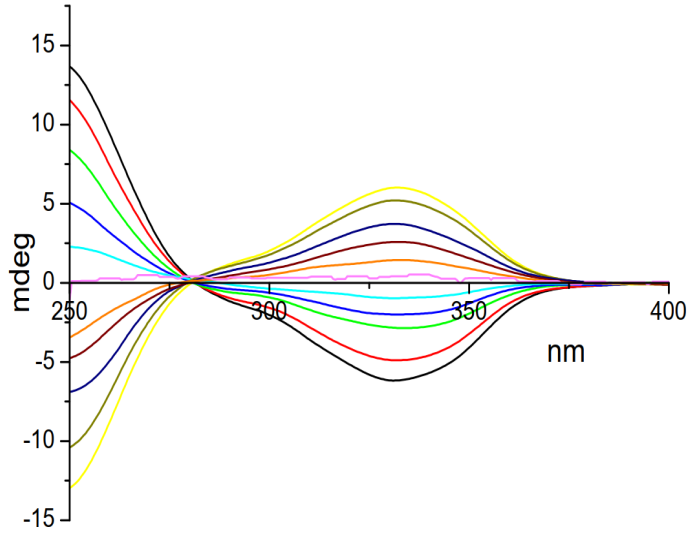


Linear relationship between UV absorption at **335 nm** and the concentration of **Thr**



Chiroptical sensing of **Thr** at varying ee's.

All CD spectra of were obtained at **2 mM** (two times dilution to **1 mM** for test).



Linear relationship between g-factor and ee of **Thr** samples measured at **335 nm** has shown in Figure 3B

Chiroptical sensing of Glu and Thr samples at varied concentration and ee.

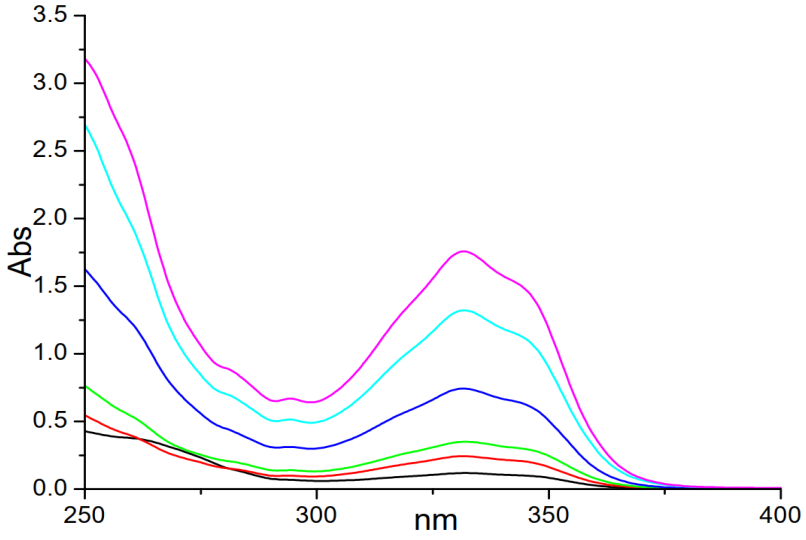
	SAMPLE			**SENSING**		
entry	Conf.	Conc.	ee %	Conf.	Conc.	ee %
1	Glu-D	3.00 mM	3.6	D	2.96 mM	3.5
2	Glu-D	6.50 mM	15.0	D	6.51 mM	16.0

3	Glu-L	5.00 mM	-55.0	L	5.21 mM	-57.6
4	Thr-D	1.60 mM	-55.0	D	1.66 mM	-58.7
5	Thr-L	3.50 mM	2.8	L	3.54 mM	2.7
6	Thr-D	4.50 mM	-30.0	D	4.52 mM	-29.8

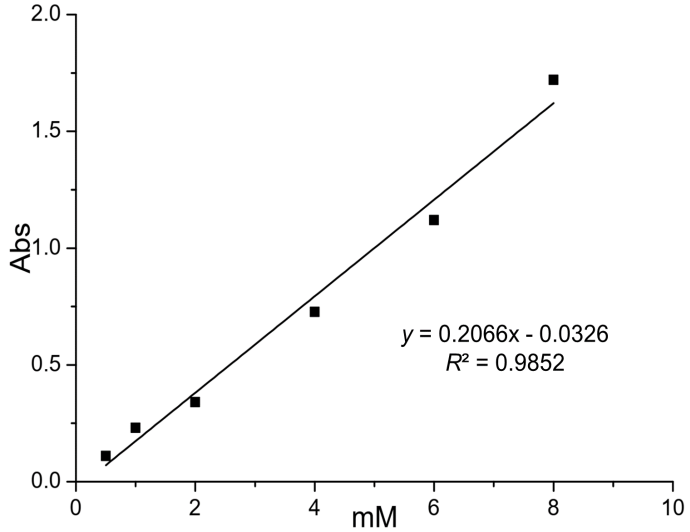
7.6 Lys

UV absorption of **Lys** at **<u>0.5-8 mM</u>** (six times dilution to **0.083-1.33 mM** for test).

MeOH/PB=2:1 as solvent

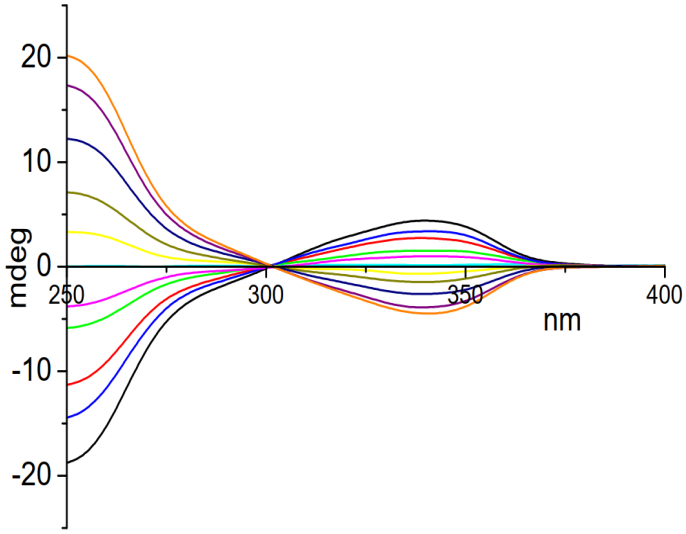


Linear relationship between UV absorption at **335 nm** and the concentration of **Lys**



Chiroptical sensing of **Lys** at varying ee's.

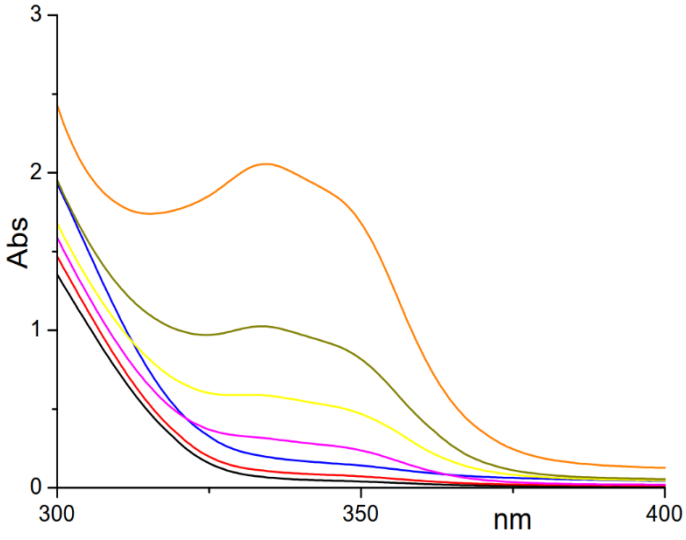
All CD spectra of were obtained at **2 mM** (six times dilution to **0.33 mM** for test). MeOH/PB=2:1 as solvent



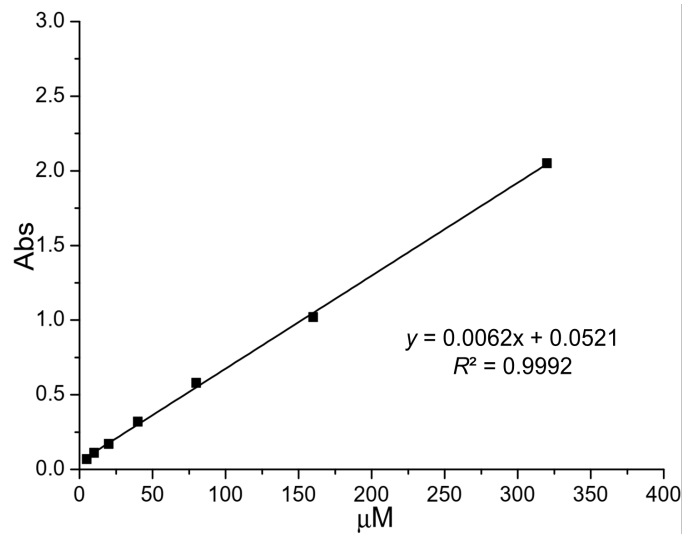
Linear relationship between g-factor and ee of **Lys** samples measured at **335 nm** has shown in Figure 3B

7.7 Trp

UV absorption of **Trp** at **<u>5-320 μM</u>** without dilution for test

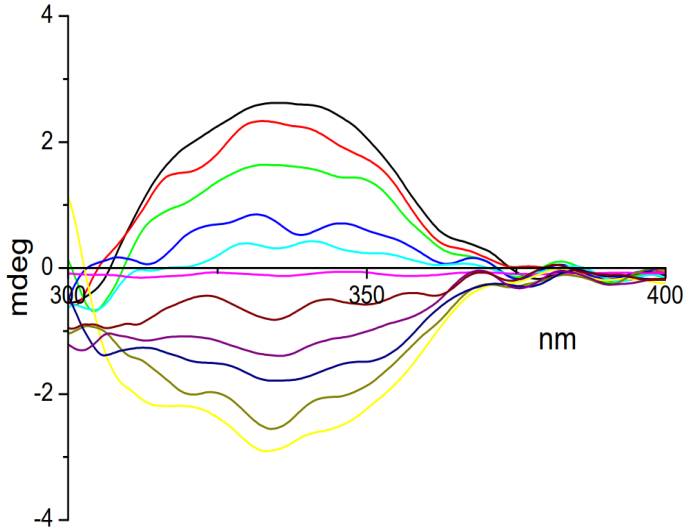


Linear relationship between UV absorption at **335 nm** and the concentration of **Trp**

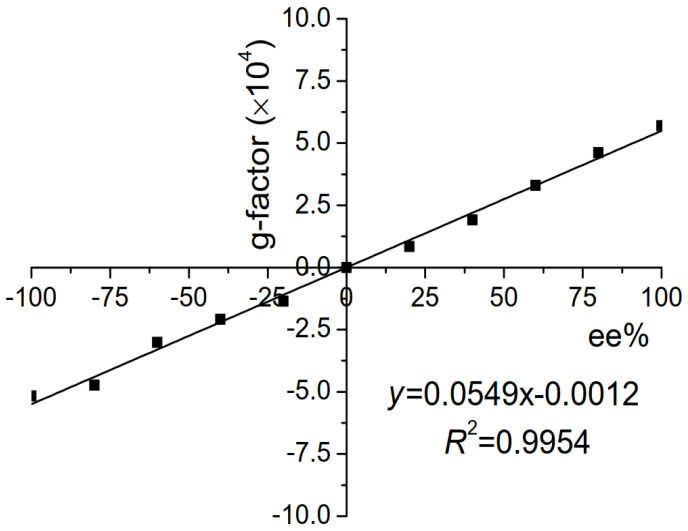


Chiroptical sensing of **Trp** at varying ee's.

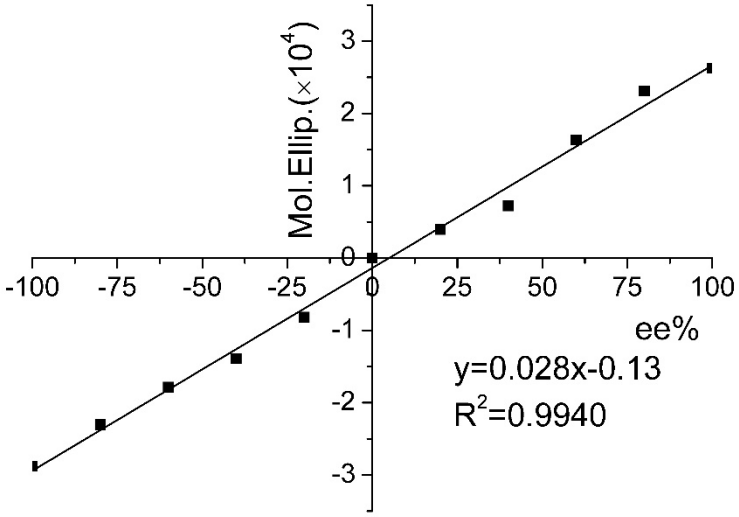
1) All CD spectra of **Trp** samples were obtained at **10 μM** without dilution for test



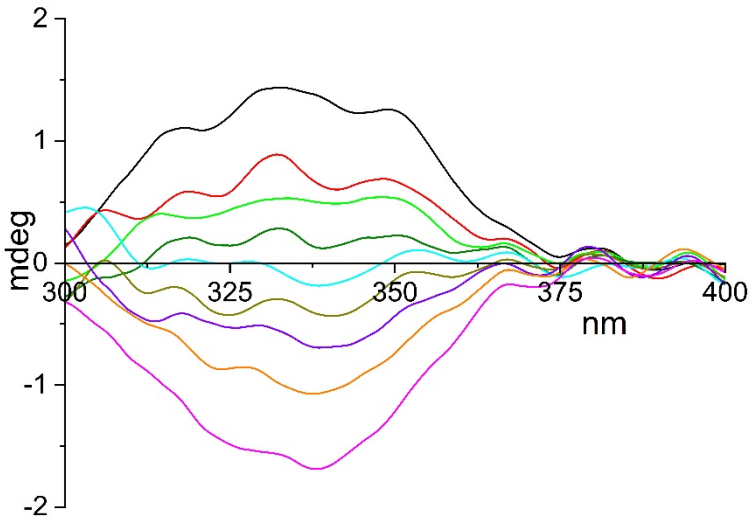
Linear relationship between g-factor and ee of **Trp** samples measured at **335 nm** (10μM)



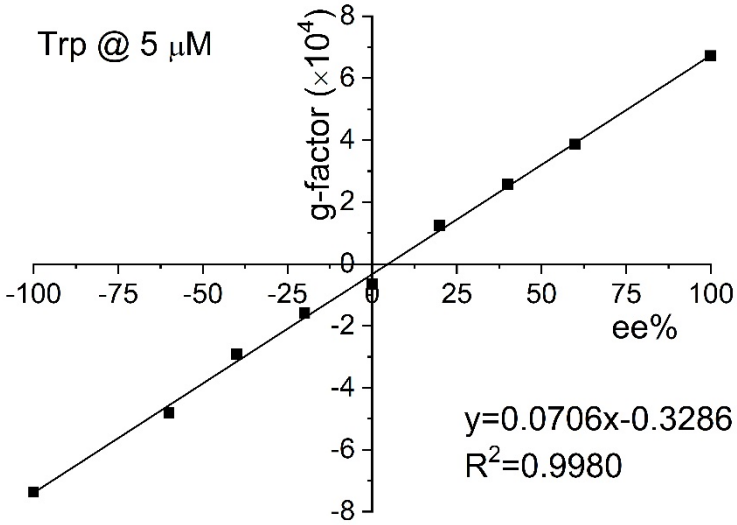
Linear relationship between molar ellipticity and ee of **Trp** samples measured at **335 nm** (10μM)



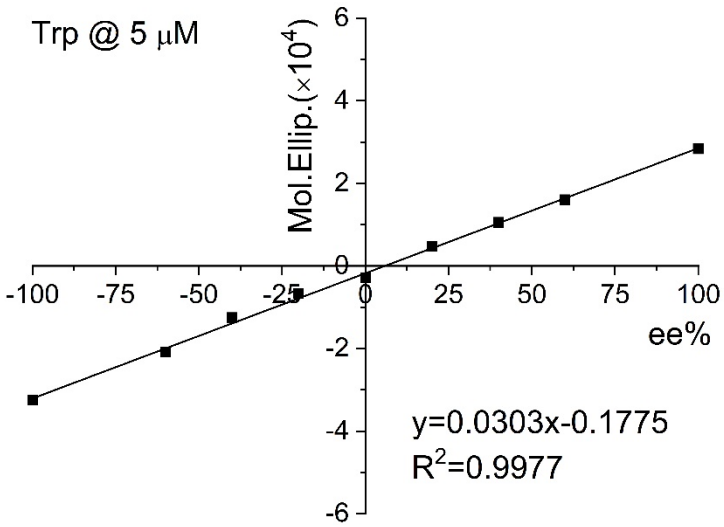
2) All CD spectra of **Trp** samples were obtained at **5 μM**.



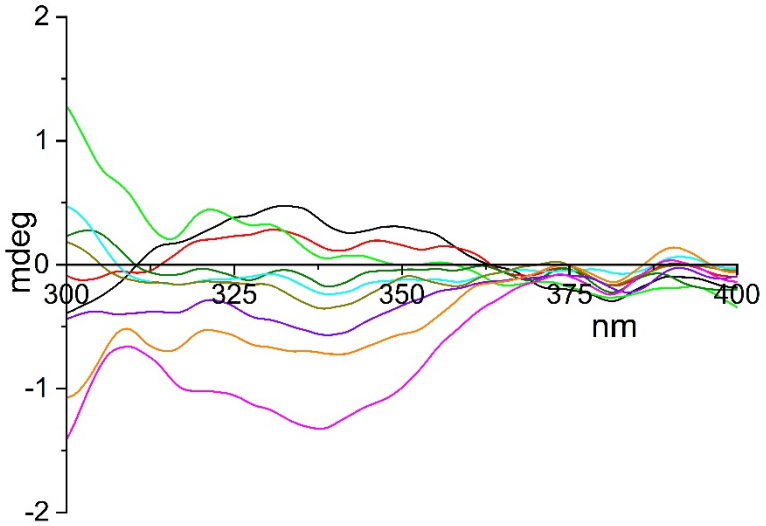
Linear relationship between g-factor and ee of **Trp** samples measured at **335 nm** (5 μM)



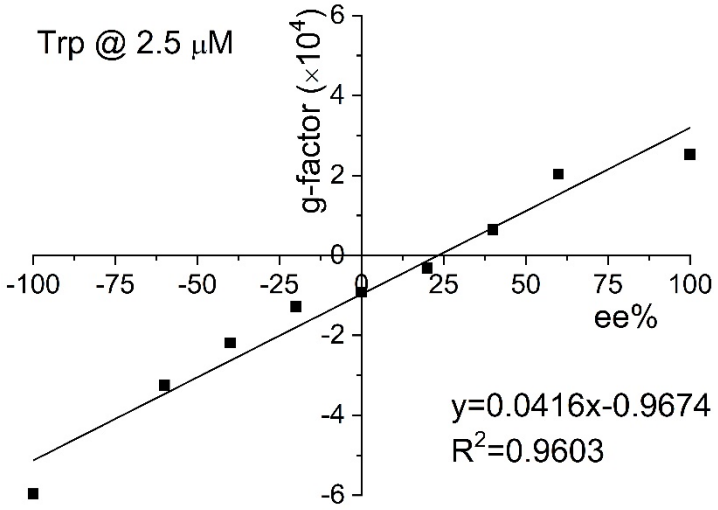
Linear relationship between molar ellipticity and ee of **Trp** samples measured at **335 nm** (5 μM)



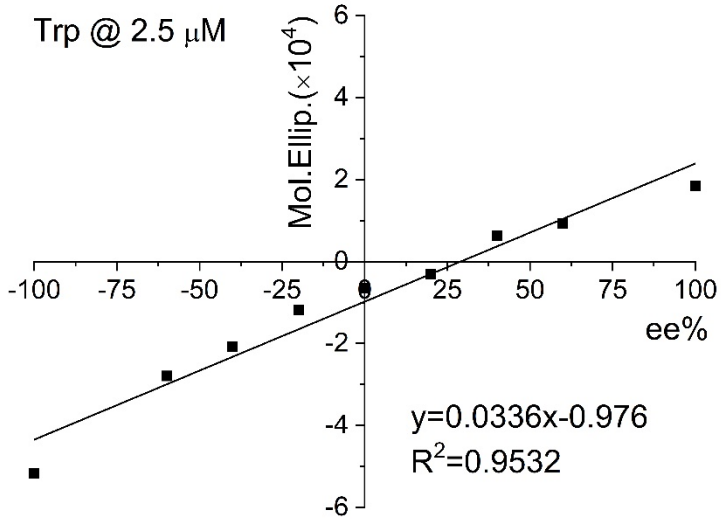
3) All CD spectra of **Trp** samples were obtained at **2.5 μM**.



Linear relationship between g-factor and ee of **Trp** samples measured at **335 nm** (2.5 μM)



Linear relationship between molar ellipticity and ee of **Trp** samples measured at **335 nm** (2.5 μM)

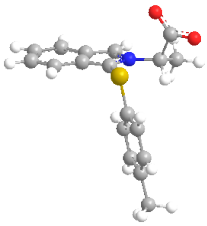
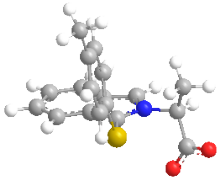
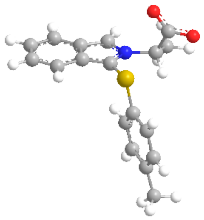
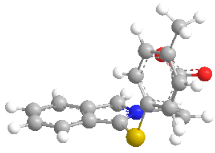


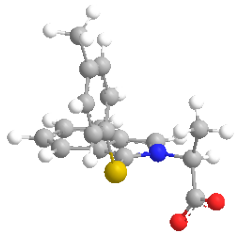
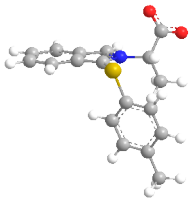
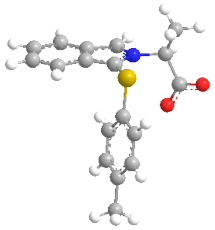
8. DFT calculations for stereochemical analysis

Preliminary conformational search of (*S*)-**5e** was performed in the MMFF94 molecular mechanics force field via the MOE software package.[1] Twelve conformers were identified within an energy window of 6 kcal/mol, and were further optimized using density functional theory (DFT) and M06-2X hybrid functional at the 6-311+G(d,p) basis set level. These conformers degenerated to seven real minima of potential energy surface and no vibrational imaginary frequencies were found. Boltzmann populations of all conformers were calculated according to their relative free energies (ΔG) from

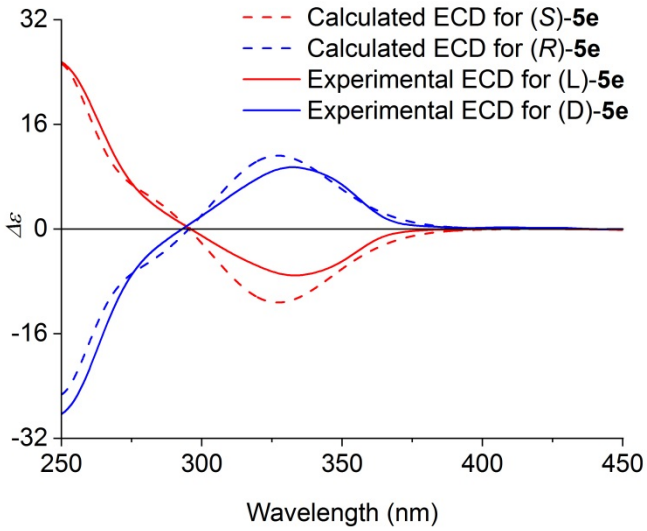
the M06-2X/6-311+G(d,p) approach. Solvent effects were considered by adopting polarizable continuum model (PCM) and the solvation model based on density (SMD) for water. One hundred lowest electronic transitions were obtained for all the conformers using B3LYP/6-311+G(d,p) approach. The overall ECD spectra were then generated at the bandwidth of 0.3 eV according to the Boltzmann weighting of each conformer using SpecDis1.71 software.[2] All quantum computations were carried out by using Gaussian 16 program package.[3]

Table S1. Main conformers of (*S*)-**5e** in water and their Boltzmann distribution

Entry	Conformers	ΔG (kcal/mol)[a]	P (%)[a]	ΔG (kcal/mol) [b]	P (%)[b]
5eC1		0.00	49.19	0.00	30.29
5eC2		0.49	21.69	0.72	8.94
5eC3		0.71	14.82	0.23	20.42
5eC4		1.06	8.19	0.60	11.08

5eC5		1.49	3.97	0.96	6.01
5eC6		2.07	1.50	0.16	23.07
5eC7		2.56	0.65	3.03	0.18

a) using the SMD/water/B3LYP/6-311+G(d,p)//M06-2X/6-311+G(d,p) approach; b) using the PCM/water/B3LYP/6-311+G(d,p)//M06-2X/6-311+G(d,p) approach.



Supplementary Figure 10. Comparison of experimental and calculated ECD spectra of **5e**.

1) Cartesian coordinates of conformer **5eC1**

C	3.14849300	3.06991100	0.76816900
H	3.34338400	3.97975600	1.32446800
C	4.00166500	2.74249900	−0.33316900
H	4.81865500	3.41148500	−0.57733100

C	3.80241400	1.60996700	-1.07523000
H	4.44948300	1.36643000	-1.91072800
C	2.72340800	0.75206400	-0.72898900
C	1.87331100	1.07906600	0.38077300
C	2.10211700	2.26507500	1.12907200
H	1.45938400	2.51883700	1.96514000
C	2.24385800	-0.44210700	-1.27017600
H	2.59720400	-1.01400700	-2.11236300
N	1.16506700	-0.82957800	-0.54684500
C	0.91591000	0.06694900	0.46956900
S	-0.35052900	-0.14371800	1.64782300
C	-1.81714300	0.37183200	0.74971100
C	-1.76184700	1.16964000	-0.38960400
H	-0.80531200	1.50112300	-0.77917200
C	-2.94236000	1.54548300	-1.02553200
H	-2.88992400	2.16767100	-1.91318900
C	-4.18912100	1.14631400	-0.54175400
C	-4.22325000	0.35381400	0.60886300
H	-5.18012000	0.03088800	1.00647700
C	-3.05358500	-0.03913100	1.24886200
H	-3.10384000	-0.66564800	2.13328000
C	-5.46050500	1.53403900	-1.24805000
H	-6.24851200	1.77569500	-0.53235100
H	-5.82272700	0.71048800	-1.87007800
H	-5.30089100	2.39685600	-1.89618400
C	0.40620300	-2.06910900	-0.72430900
H	-0.65193700	-1.81335600	-0.65130700
C	0.67247800	-2.71843800	-2.07703000
H	0.47735300	-2.01896900	-2.89152100
H	0.00335700	-3.57209100	-2.18505900
H	1.70141700	-3.07634500	-2.15119700
C	0.73269100	-3.08639600	0.39477700
O	1.85197100	-3.01764800	0.94986600
O	-0.15727200	-3.94499100	0.61115200

2) Cartesian coordinates of conformer **5eC2**

C	1.92824000	3.57810000	-0.90213800
H	1.71777100	4.47198700	-1.47819100
C	2.93613900	3.63517700	0.11122300
H	3.46112300	4.56952000	0.27274500
C	3.24341700	2.53999900	0.87314100
H	4.00653900	2.58926400	1.64206200
C	2.53462400	1.33084100	0.64034000

C	1.53034800	1.27423400	-0.38290100
C	1.23050300	2.42741900	-1.15470800
H	0.46544200	2.38909600	-1.92308700
C	2.58219100	0.06369000	1.22544100
H	3.19907700	-0.32854700	2.01922900
N	1.66277400	-0.72042900	0.61335800
C	1.00358100	-0.02027700	-0.37083700
S	-0.23129800	-0.69869600	-1.39670200
C	-1.75012500	-0.11576100	-0.64092700
C	-1.79168400	0.57305000	0.56863200
H	-0.87615500	0.79198600	1.10697600
C	-3.01711100	0.98594700	1.08508800
H	-3.03776600	1.52667100	2.02596200
C	-4.21577600	0.72152000	0.42074900
C	-4.15268800	0.03099400	-0.79217700
H	-5.06853500	-0.18173500	-1.33420600
C	-2.93727200	-0.38553400	-1.32299500
H	-2.91512200	-0.91537100	-2.26984200
C	-5.53704900	1.14446400	1.00490200
H	-5.93978300	0.36136400	1.65396400
H	-6.27094500	1.33255900	0.21957300
H	-5.42865700	2.04860000	1.60616300
C	1.41395800	-2.11493900	0.99262100
H	2.22571100	-2.36964500	1.67972300
C	0.08709100	-2.26876800	1.72377800
H	0.02527600	-3.26769300	2.15489700
H	-0.76162400	-2.13084300	1.05230900
H	0.02320200	-1.53879100	2.53333100
C	1.60136400	-3.07268100	-0.21265300
O	2.45842500	-2.75628800	-1.07027300
O	0.92873700	-4.13010300	-0.19314300

3) Cartesian coordinates of conformer **5eC3**

C	3.07324300	-3.13363600	-0.75792100
H	3.24235200	-4.05261700	-1.30756700
C	3.94450600	-2.81490200	0.33154700
H	4.74909900	-3.49936200	0.57387500
C	3.77758200	-1.67132300	1.06462700
H	4.43832100	-1.43406400	1.89115500
C	2.71438900	-0.79324200	0.72072400
C	1.84584600	-1.11185700	-0.37677300
C	2.04086500	-2.30953100	-1.11581200
H	1.38439200	-2.55662300	-1.94311500

C	2.26878000	0.41803300	1.25347900
H	2.64567200	0.99160500	2.08428700
N	1.19319600	0.82362900	0.53625800
C	0.91210700	-0.07775000	-0.46763600
S	-0.35957700	0.14979600	-1.63597400
C	-1.83030900	-0.34845200	-0.73532900
C	-3.06411900	-0.06082800	-1.32013400
H	-3.11042100	0.45402100	-2.27419800
C	-4.23887100	-0.43530800	-0.67822100
H	-5.19264900	-0.21035400	-1.14466900
C	-4.21432000	-1.08954000	0.55622800
C	-2.97025700	-1.36827900	1.12402100
H	-2.92341000	-1.88291800	2.07841600
C	-1.78397800	-1.00718300	0.49039300
H	-0.83065100	-1.24472700	0.94958300
C	-5.49143500	-1.45698100	1.26316000
H	-6.27942600	-1.70059600	0.54860600
H	-5.84678300	-0.62288900	1.87526700
H	-5.34145200	-2.31232700	1.92373400
C	0.46096200	2.07965000	0.71205700
H	-0.60250700	1.84401000	0.64908900
C	0.75144800	2.73067000	2.05885800
H	0.10367500	3.60073400	2.16611200
H	1.78912200	3.06398500	2.12425500
H	0.54498600	2.04063700	2.87862000
C	0.79776000	3.08304200	-0.41656100
O	-0.07900400	3.95478800	-0.63345300
O	1.91217200	2.99069100	-0.97803700

4) Cartesian coordinates of conformer **5eC4**

C	-4.12746300	2.19959500	-0.35424900
H	-4.58484700	3.18239700	-0.34476100
C	-4.79666100	1.13665800	-1.04144300
H	-5.74189300	1.34447100	-1.52940800
C	-4.26525100	-0.12286700	-1.09233200
H	-4.77438600	-0.92516900	-1.61497700
C	-3.02210500	-0.36343000	-0.44511300
C	-2.35244900	0.70428800	0.24431400
C	-2.93281200	2.00154400	0.28253100
H	-2.43114600	2.81157100	0.80076900
C	-2.21915300	-1.49524100	-0.31688300
H	-2.34405700	-2.48663600	-0.72099800
N	-1.13224700	-1.16373100	0.42470100

C	-1.17274200	0.17354300	0.76927700
S	-0.02545200	0.95324600	1.82921200
C	1.45527700	1.02451900	0.81710900
C	2.68763100	0.85323100	1.44354400
H	2.73557600	0.66399500	2.51056900
C	3.85830800	0.90854400	0.69296300
H	4.81445200	0.77179100	1.18756300
C	3.82127200	1.11268500	-0.68749100
C	2.57492100	1.29040100	-1.29543800
H	2.52394800	1.45887000	-2.36645500
C	1.39924600	1.25810000	-0.55503300
H	0.44064800	1.39372600	-1.04497100
C	5.08343100	1.10905200	-1.50688800
H	5.94767300	1.38004600	-0.89872900
H	5.01026800	1.80597400	-2.34357700
H	5.26634200	0.11342000	-1.92169100
C	0.02670000	-2.03116800	0.63769500
H	0.53194100	-1.66734600	1.53189100
C	-0.37933200	-3.48768600	0.84552100
H	0.50567900	-4.05868900	1.12798600
H	-0.78870900	-3.92424400	-0.06726100
H	-1.11825900	-3.57151000	1.64409500
C	1.02562100	-1.95261200	-0.54634200
O	0.57377500	-1.70918700	-1.68727400
O	2.22036400	-2.20499000	-0.25532700

5) Cartesian coordinates of conformer **5eC5**

C	-1.87812800	-3.59678200	-0.90460700
H	-1.65477000	-4.48774500	-1.48033000
C	-2.88809400	-3.66697100	0.10586300
H	-3.40170500	-4.60791600	0.26560600
C	-3.21121900	-2.57608800	0.86738500
H	-3.97580200	-2.63526800	1.63415100
C	-2.51734000	-1.35788700	0.63678900
C	-1.51098400	-1.28817700	-0.38363700
C	-1.19418500	-2.43730600	-1.15474000
H	-0.42750400	-2.38901600	-1.92093600
C	-2.58347600	-0.09138900	1.22140800
H	-3.20786200	0.29292400	2.01321800
N	-1.67279100	0.70469800	0.61168700
C	-1.00164000	0.01324000	-0.37042000
S	0.22765800	0.70800700	-1.39218800
C	1.75015500	0.13716400	-0.63473700

C	2.93621600	0.41339700	-1.31803700
H	2.91023700	0.94286300	-2.26500700
C	4.15387700	0.01087900	-0.78421400
H	5.06907200	0.23403100	-1.32343200
C	4.22179200	-0.67577800	0.43177700
C	3.02644700	-0.93948000	1.10038100
H	3.05168700	-1.46520300	2.04947600
C	1.79705800	-0.54005500	0.58014700
H	0.88393500	-0.75569300	1.12389800
C	5.54475200	-1.13383700	0.98475600
H	5.88305300	-2.04066900	0.47529000
H	5.46788300	-1.35758600	2.04966900
H	6.31389800	-0.37211800	0.84319800
C	-1.44416700	2.10270000	0.99053300
H	-2.26088000	2.34662300	1.67566600
C	-0.12117700	2.27578300	1.72457800
H	0.73090000	2.14875100	1.05522100
H	-0.04910500	1.54779600	2.53521600
H	-0.07431800	3.27603300	2.15445200
C	-1.64209600	3.05709500	-0.21555100
O	-2.48721100	2.72540800	-1.07916400
O	-0.99009600	4.12736000	-0.19061100

6) Cartesian coordinates of conformer **5eC6**

C	-3.49581300	-2.92019200	0.14470900
H	-3.83941400	-3.89788600	0.46269400
C	-4.19410500	-2.25623000	-0.91408000
H	-5.04871700	-2.74813900	-1.36404700
C	-3.80244600	-1.02505000	-1.36380200
H	-4.33286500	-0.52783200	-2.16838300
C	-2.67673300	-0.40445700	-0.75527500
C	-1.98448600	-1.06780600	0.31601900
C	-2.41300700	-2.34920100	0.75608800
H	-1.88784500	-2.85683400	1.55804200
C	-2.01716900	0.80325100	-0.97547500
H	-2.20524600	1.59477000	-1.68586400
N	-0.99398000	0.89295800	-0.08901300
C	-0.93928900	-0.22807700	0.70783000
S	0.25470800	-0.47586300	1.95969600
C	1.72620800	-0.72387900	0.95745400
C	2.86947400	0.01727000	1.23641400
H	2.86802800	0.73693400	2.04784200
C	4.01199400	-0.15363500	0.45580900

H	4.89887700	0.43171700	0.67515400
C	4.02714300	-1.04862800	-0.61330200
C	2.86404600	-1.78054200	-0.88146400
H	2.85500500	-2.48011800	-1.71129500
C	1.72464700	-1.63070200	-0.10288700
H	0.82994800	-2.20318400	-0.32532300
C	5.26216400	-1.24331300	-1.45045100
H	5.96669600	-0.42321100	-1.30728600
H	5.01006300	-1.30791600	-2.51065100
H	5.76784600	-2.17359100	-1.17630400
C	-0.05325800	2.01691700	-0.06706100
H	0.53337200	1.90942300	0.84860800
C	0.87226800	1.96979000	-1.27404800
H	0.31166200	2.12209900	-2.19898300
H	1.37845500	1.00227400	-1.32133600
H	1.62585300	2.75304000	-1.19192500
C	-0.82845000	3.35070400	0.10198700
O	-1.75926200	3.35432100	0.94306200
O	-0.43677600	4.32995900	-0.57228300

7) Cartesian coordinates of conformer **5eC7**

C	-3.44175800	-2.67939700	0.57469700
H	-3.65060200	-3.63570300	1.04063200
C	-4.28886300	-2.23328400	-0.48840600
H	-5.11544100	-2.86301800	-0.79643700
C	-4.07158400	-1.03693400	-1.11664200
H	-4.71377400	-0.70330100	-1.92427500
C	-2.97951700	-0.23435300	-0.68940100
C	-2.13435400	-0.68054400	0.38067000
C	-2.38165300	-1.93024400	1.00914800
H	-1.73990900	-2.27567000	1.81288700
C	-2.48095600	1.00135500	-1.10448500
H	-2.81939300	1.68039100	-1.87188700
N	-1.39967400	1.30112800	-0.34634200
C	-1.15249900	0.29805500	0.56777100
S	0.14097500	0.32411400	1.74072800
C	1.51065300	-0.44394300	0.86973000
C	2.79245000	0.03300900	1.12574200
H	2.93874000	0.86608700	1.80494500
C	3.88847000	-0.55374300	0.49563900
H	4.88457400	-0.17487600	0.69997600
C	3.72492000	-1.60501800	-0.40567500
C	2.42760300	-2.07030100	-0.64783300

H	2.27830400	-2.89265200	-1.34045700
C	1.32762600	-1.50633000	-0.01446700
H	0.33082500	-1.88326200	-0.21624700
C	4.90215700	-2.21389900	-1.11908800
H	5.83908100	-1.94885500	-0.62749000
H	4.95183200	-1.85895000	-2.15234000
H	4.82021500	-3.30223200	-1.15050800
C	-0.65738000	2.56107300	-0.47919400
H	-1.06152900	3.02774200	-1.38144900
C	-0.90636200	3.48797200	0.70097300
H	-0.47030300	4.46483800	0.49080700
H	-0.46163400	3.10160800	1.61794000
H	-1.98060700	3.61488500	0.84972000
C	0.83583500	2.29727300	-0.81002300
O	1.06617800	1.41667100	-1.67189000
O	1.68669700	3.02642400	-0.25036100

Reference:

[1] MOE2009.10, Chemical Computing Group Inc.

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