Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

Simultaneous determination of concentration and enantiomeric excess of amino acids with a coumarin-derived achiral probe

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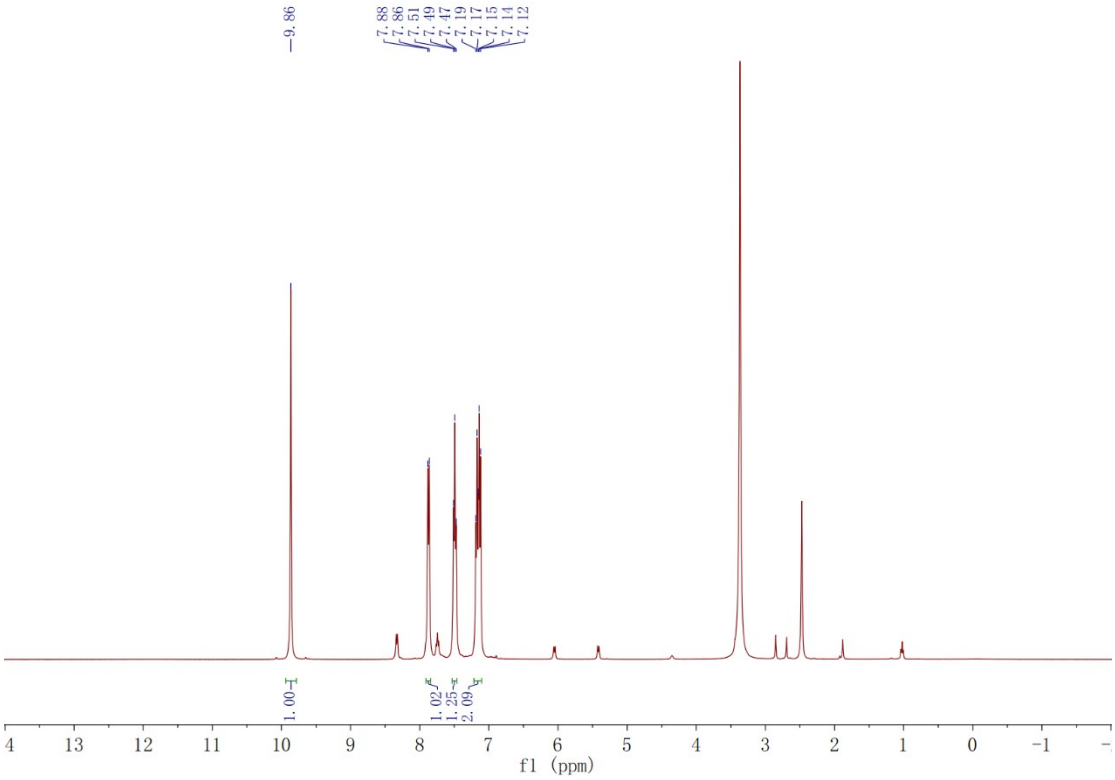


Fig. S1. [1]H NMR Spectrum of probe **1** in DMSO-d_6.

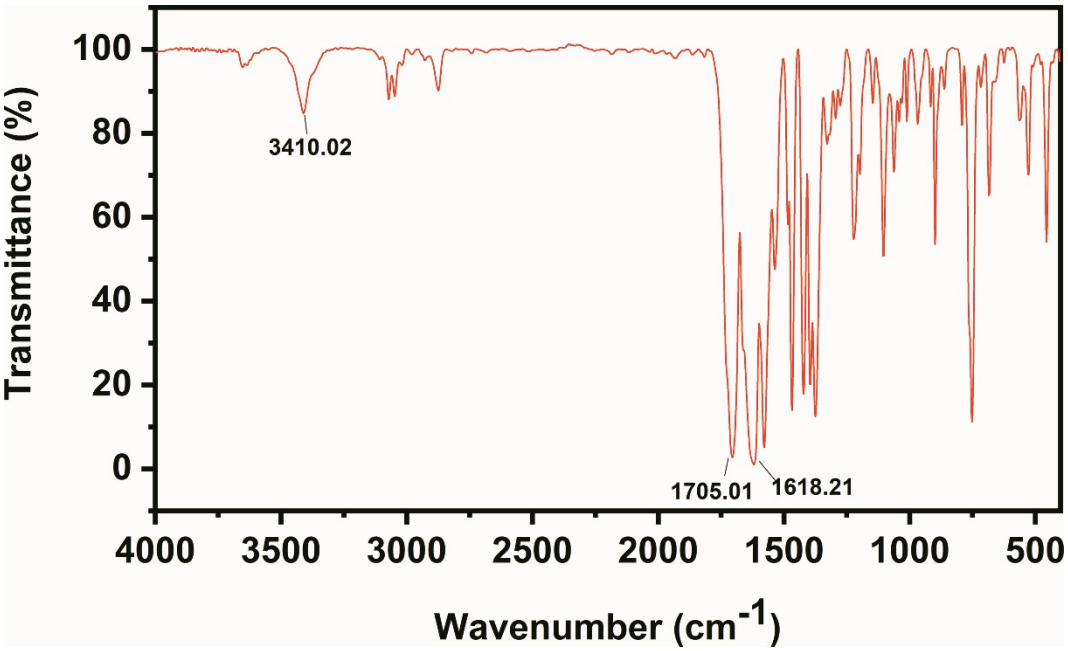


Fig. S2. IR spectrum of probe **1**.

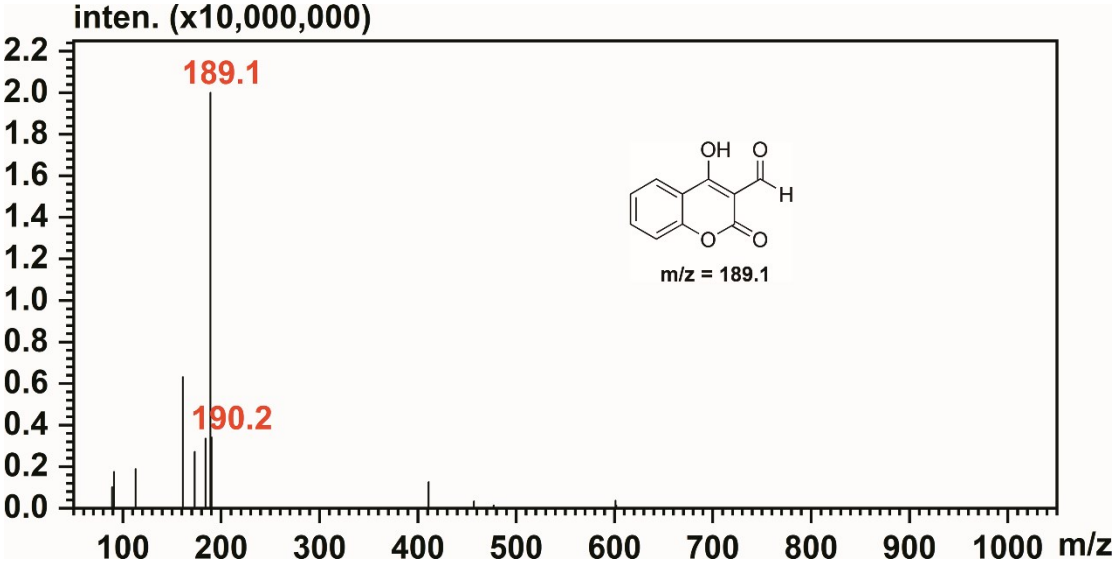


Fig. S3. ESI-MS spectrum of probe **1** (negative ion mode).

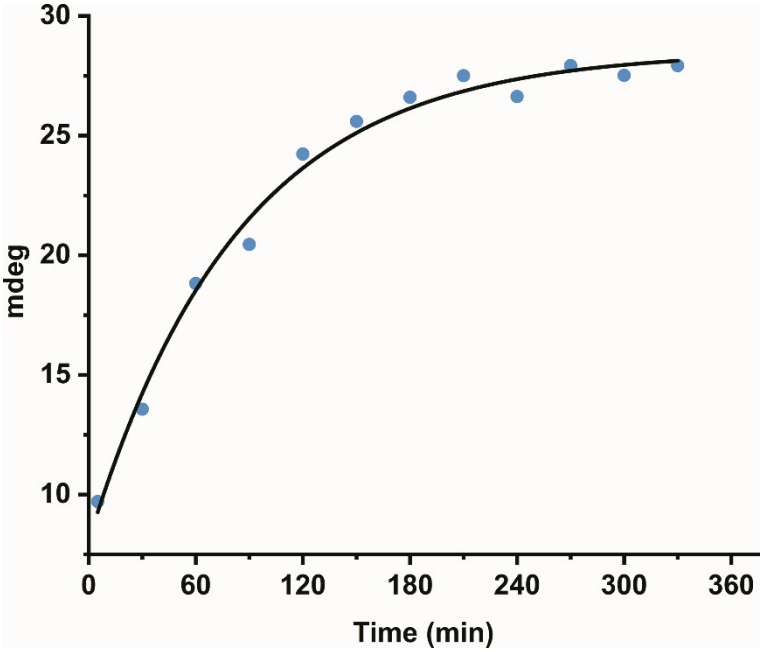


Fig. S4. CD analysis of the reaction between D-Phe and probe **1**. (CD signals were collected at 318 nm)

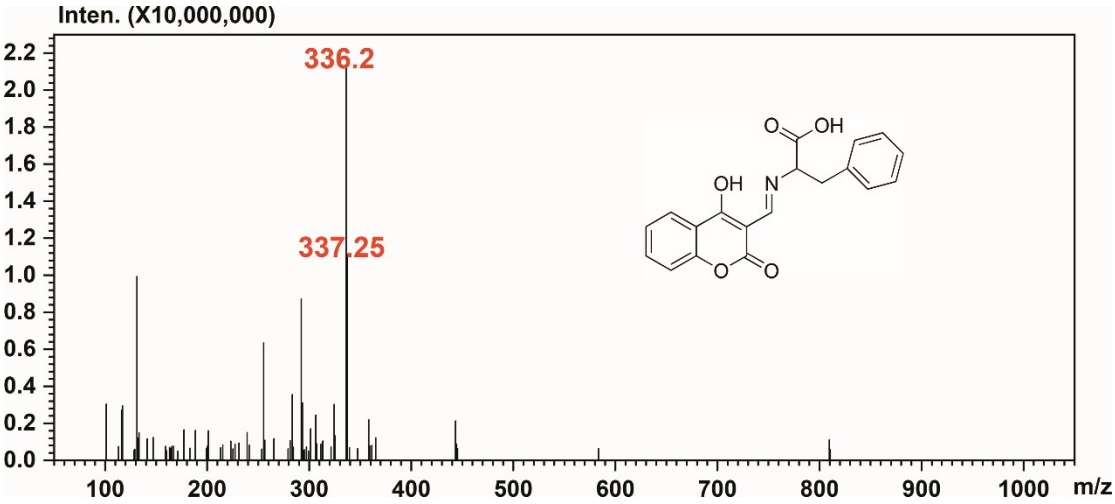


Fig. S5. ESI-MS spectrum of the reaction between L-Phe (5.0 mM) and probe **1** (5.0 mM) (negative ion mode).

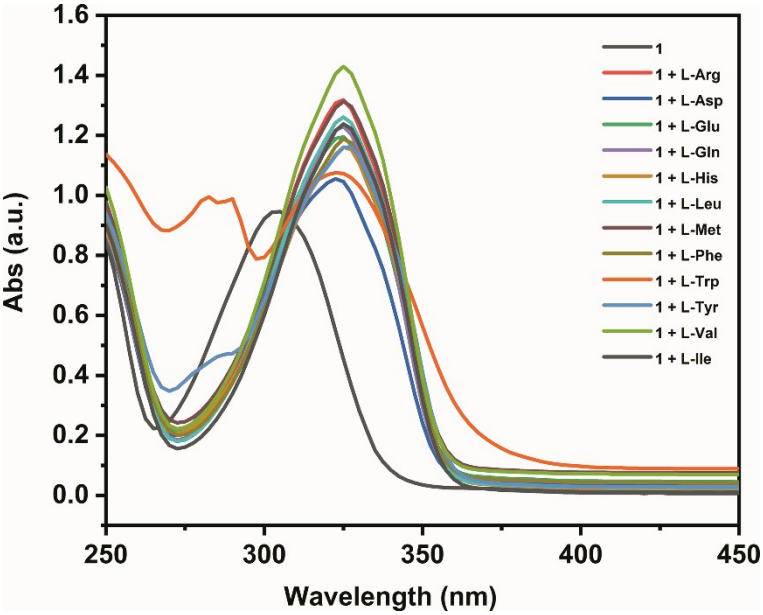


Fig. S6. UV-vis spectra obtained from probe **1** with amino acids.

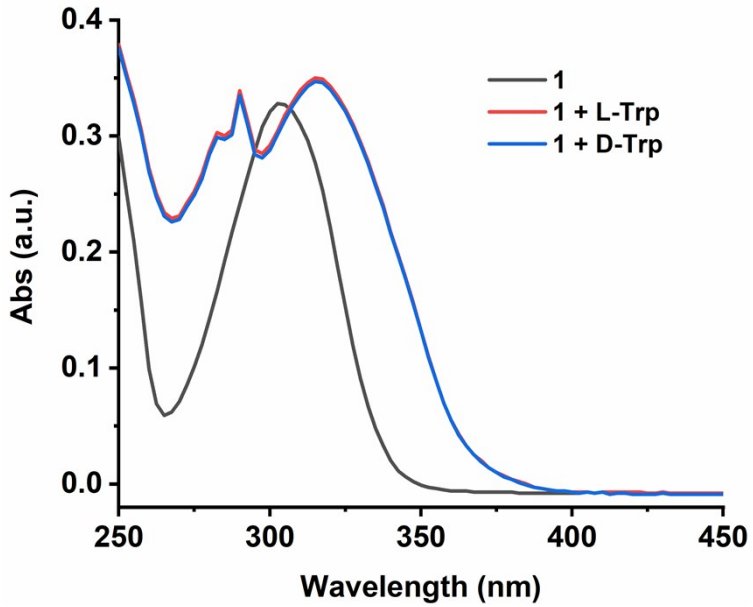


Fig. S7. UV-vis spectra obtained from probe **1** with L-Trp (red), D-Trp (blue) and probe **1** (black). (UV-vis measurements were taken at 50 μM after diluting with methanol)

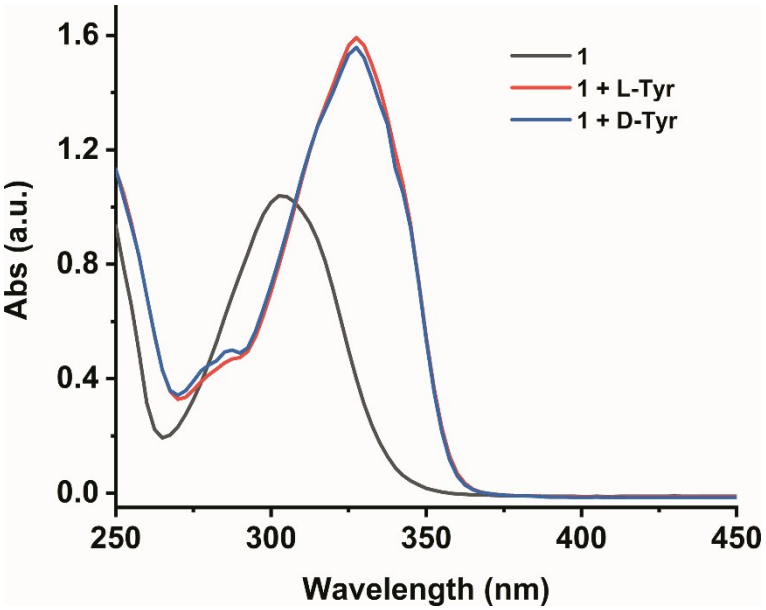


Fig. S8. UV-vis spectra obtained from probe **1** with L-Tyr (red), D-Tyr (blue) and probe **1** (black). (UV-vis measurements were taken at 125 μM after diluting with methanol)

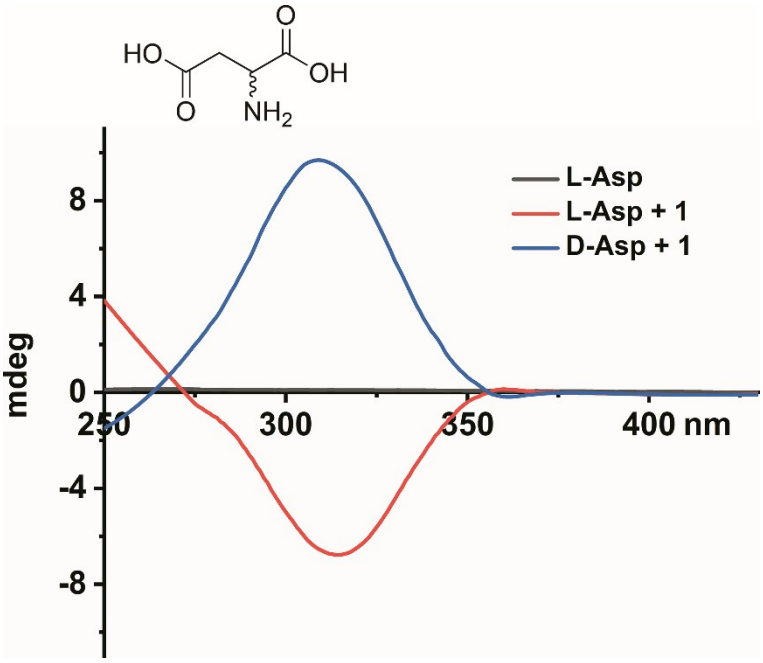


Fig. S9. CD spectra obtained from probe **1** with L-Asp (red), D-Asp(blue) and L-Asp(black). (CD measurements were taken at 250 μM after diluting with methanol)

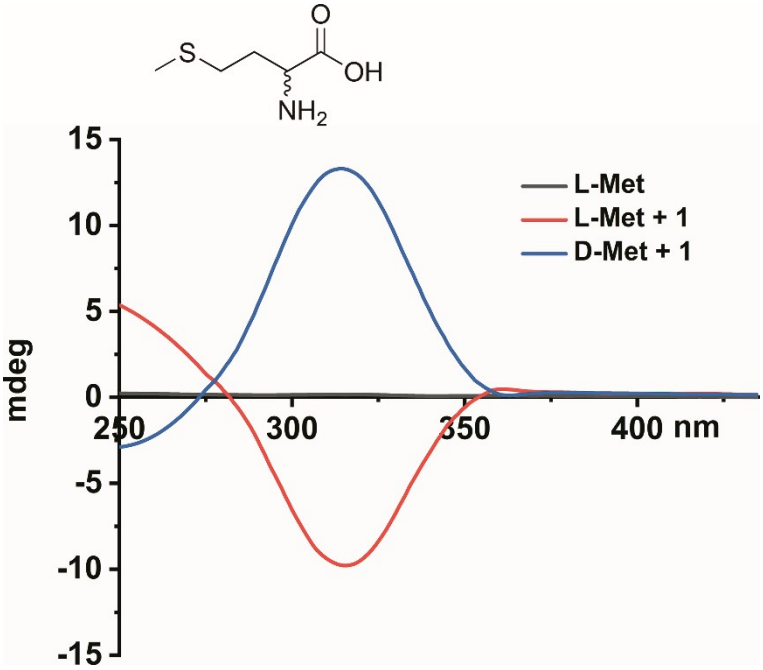


Fig. S10. CD spectra obtained from probe **1** with L-Met (red), D-Met(blue) and L-Met (black). (CD measurements were taken at 250 μM after diluting with methanol)

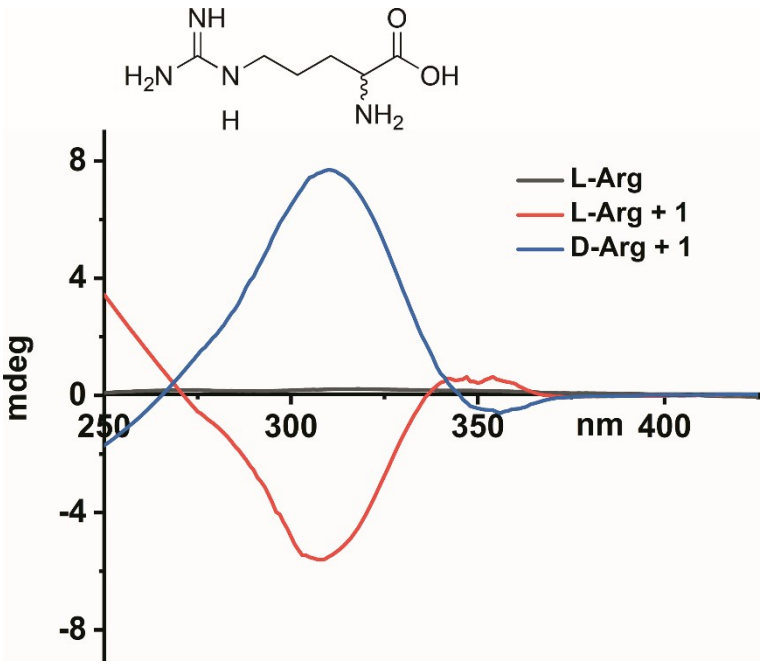


Fig.S11. CD spectra obtained from probe **1** with L-Arg (red), D-Arg (blue) and L-Arg (black). (CD measurements were taken at 250 μM after diluting with methanol)

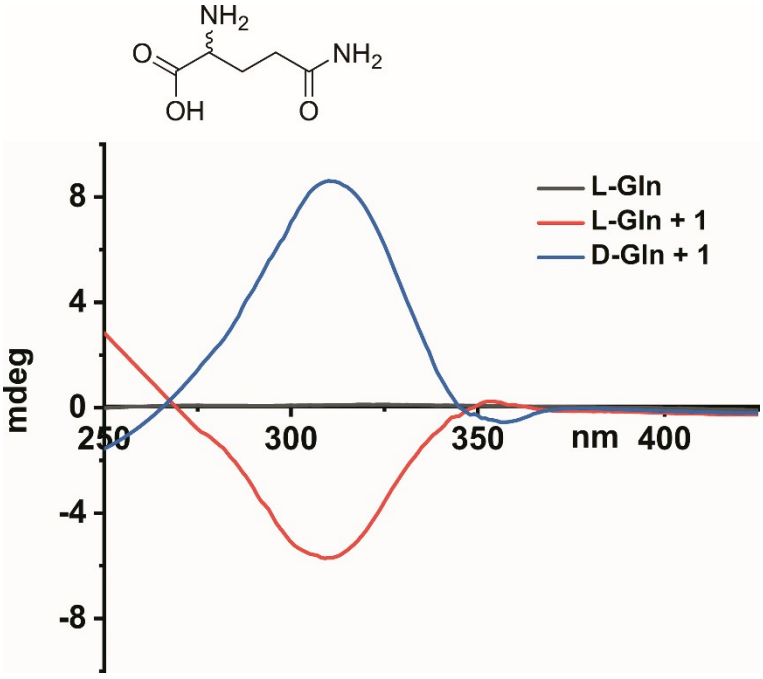


Fig. S12. CD spectra obtained from probe **1** with L-Gln (red), D-Gln (blue) and L-Gln (black). (CD measurements were taken at 250 μM after diluting with methanol)

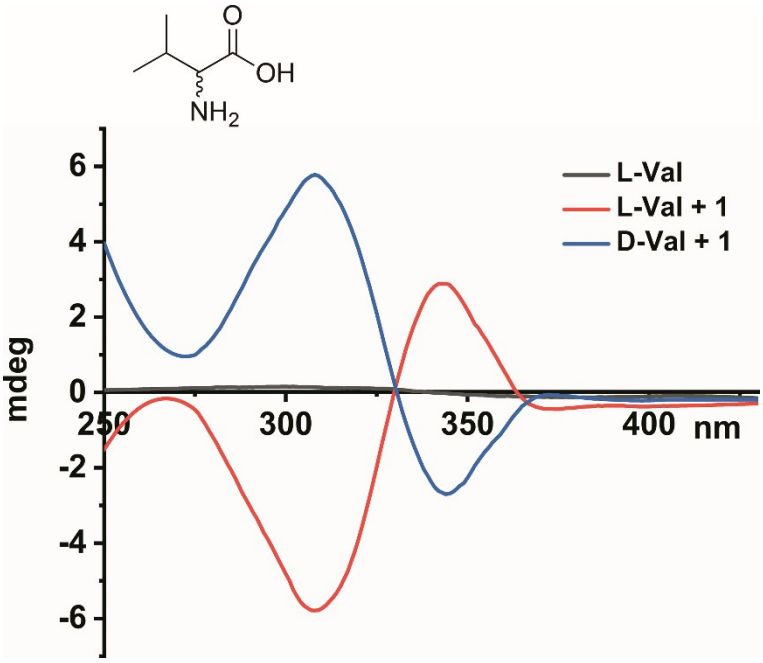


Fig. S13. CD spectra obtained from probe **1** with L-Val (red), D-Val(blue) and L-Val (black). (CD measurements were taken at 250 μM after diluting with methanol)

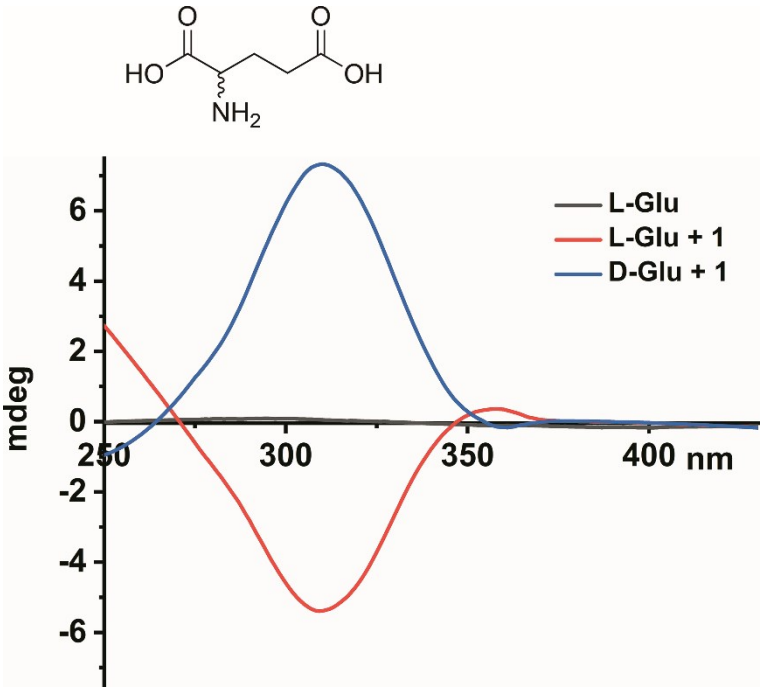


Fig. S14. CD spectra obtained from probe **1** with L-Glu (red), D-Glu (blue) and L-Glu (black). (CD measurements were taken at 250 μM after diluting with methanol)

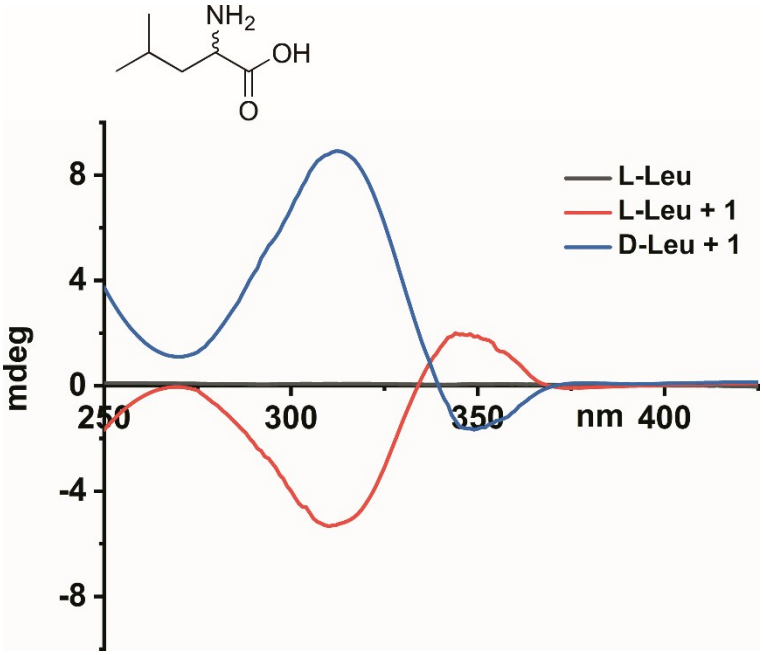


Fig. S15. CD spectra obtained from probe **1** with L-Leu (red), D-Leu (blue) and L-Leu (black). (CD measurements were taken at 250 μM after diluting with methanol)

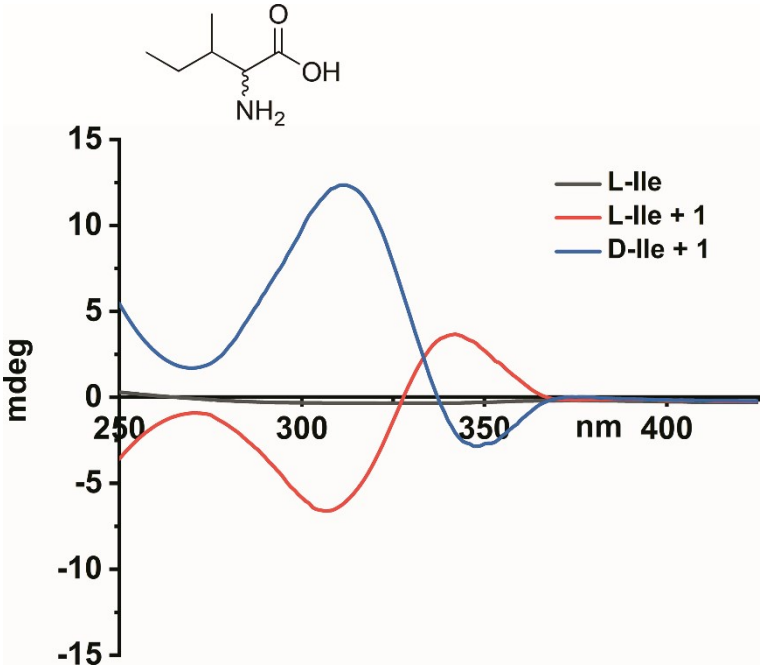


Fig. S16. CD spectra obtained from probe **1** with L-Ile(red), D-Ile (blue) and L-Ile(black). (CD measurements were taken at 250 μM after diluting with methanol)

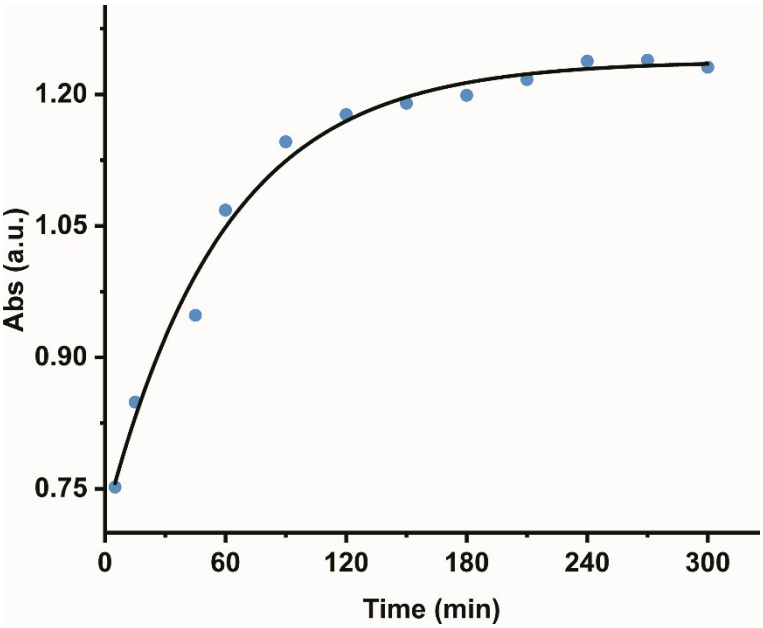


Fig. S17. UV-vis analysis of the reaction between L-Arg and probe **1**. (UV-vis signals were collected at 325 nm)

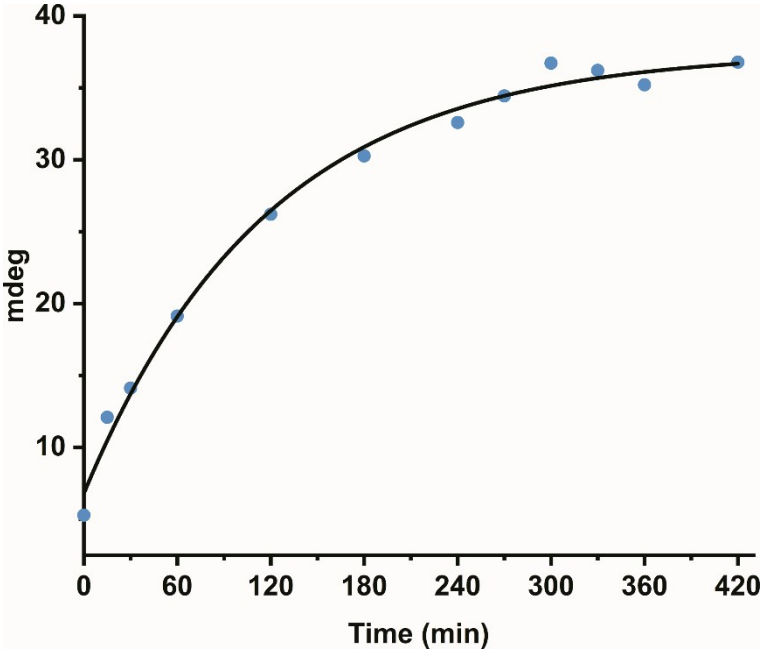


Fig. S18. CD analysis of the reaction between D-Trp and probe **1**. (CD signals were collected at 336 nm)

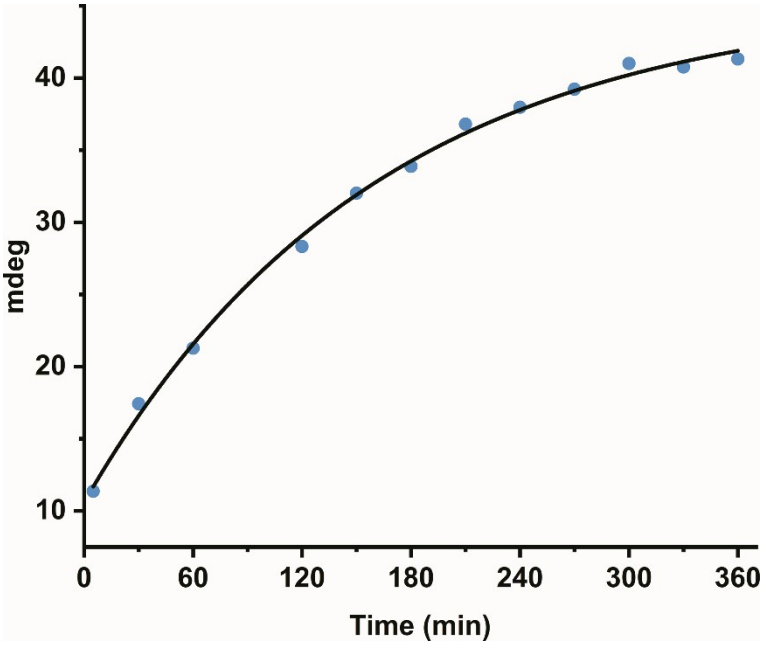


Fig. S19. CD analysis of the reaction between D-Tyr and probe **1**. (CD signals were collected at 323 nm)

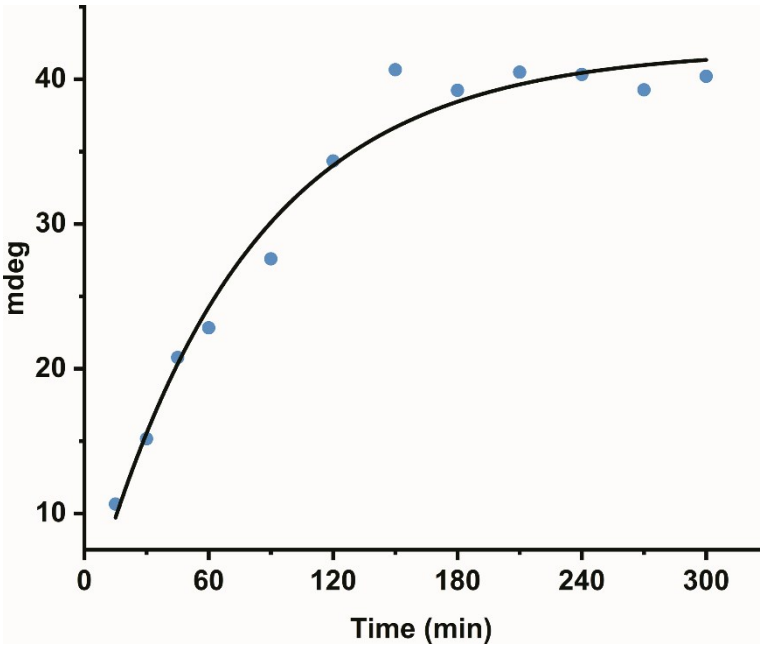


Fig. S20. CD analysis of the reaction between D-Tyr and probe **1** at 45℃. (CD signals were collected at 323 nm)

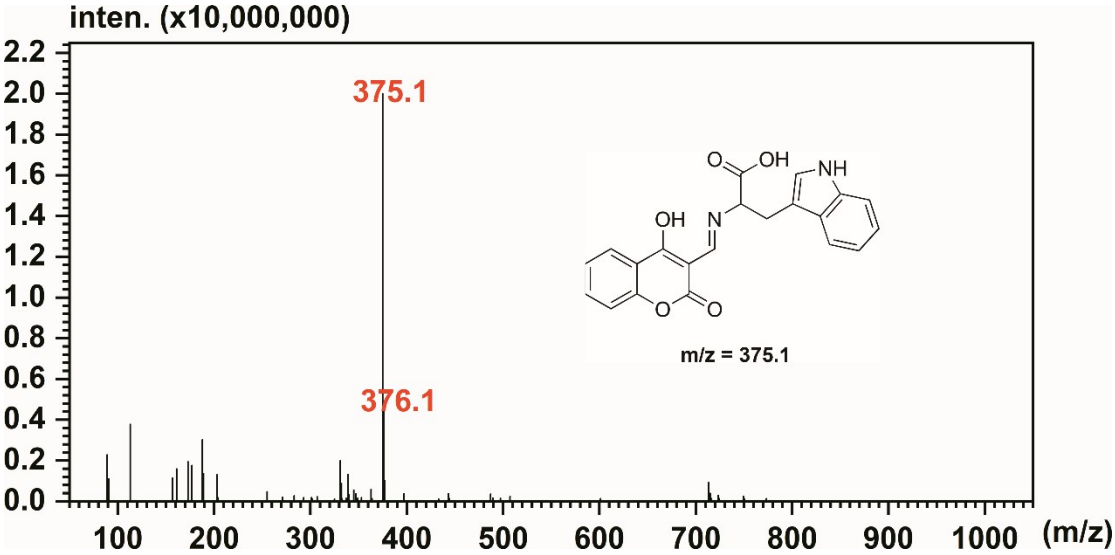


Fig. S21. ESI-MS spectrum of the reaction between L-Trp (5.0 mM) and probe **1** (5.0 mM) (negative ion mode).

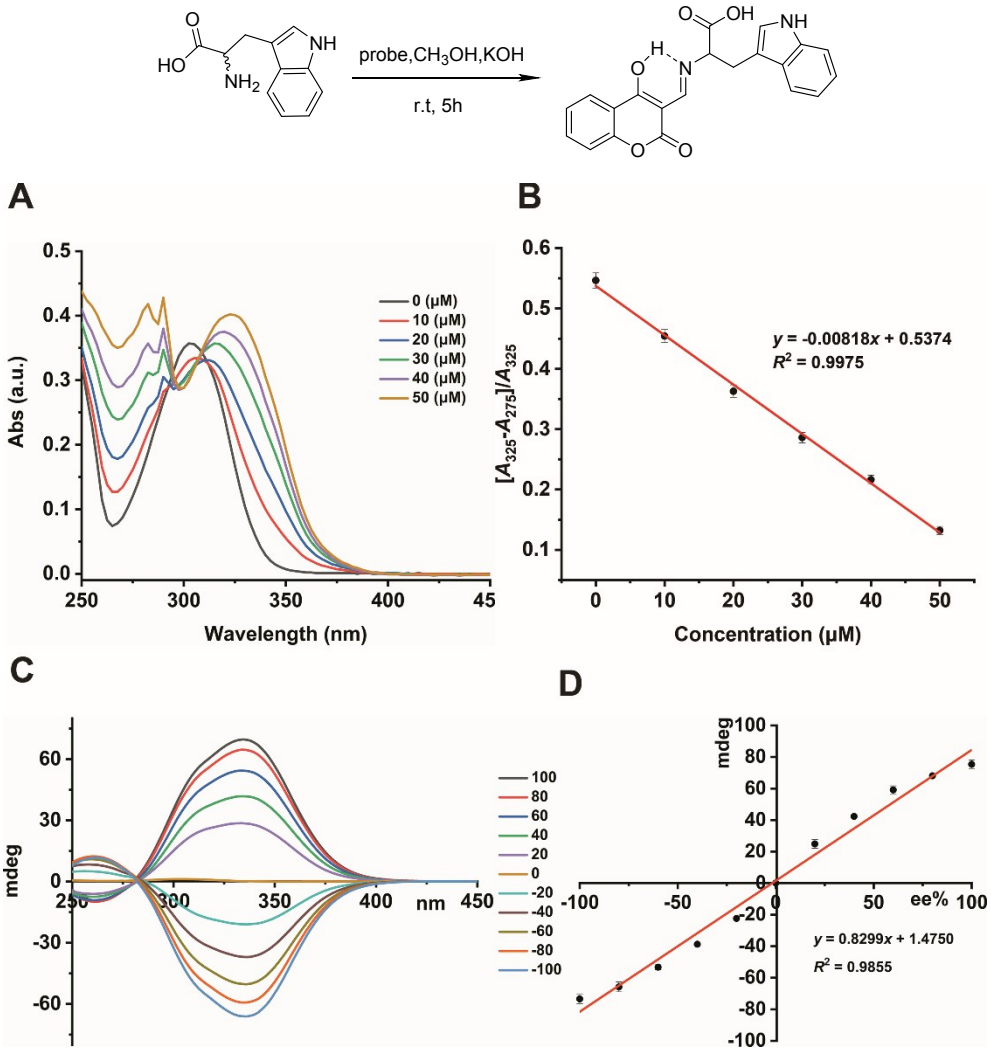


Fig. S22. Chiroptical sensing of Trp. (A) UV-vis response of **1** to varying amounts of Trp. (B)

linear correlation between absorbance and concentration of Trp. (C) CD response of **1** to nonracemic sample of Trp, and (D) linear correlation between the induced CD signal at 336 nm and the sample *ee*.

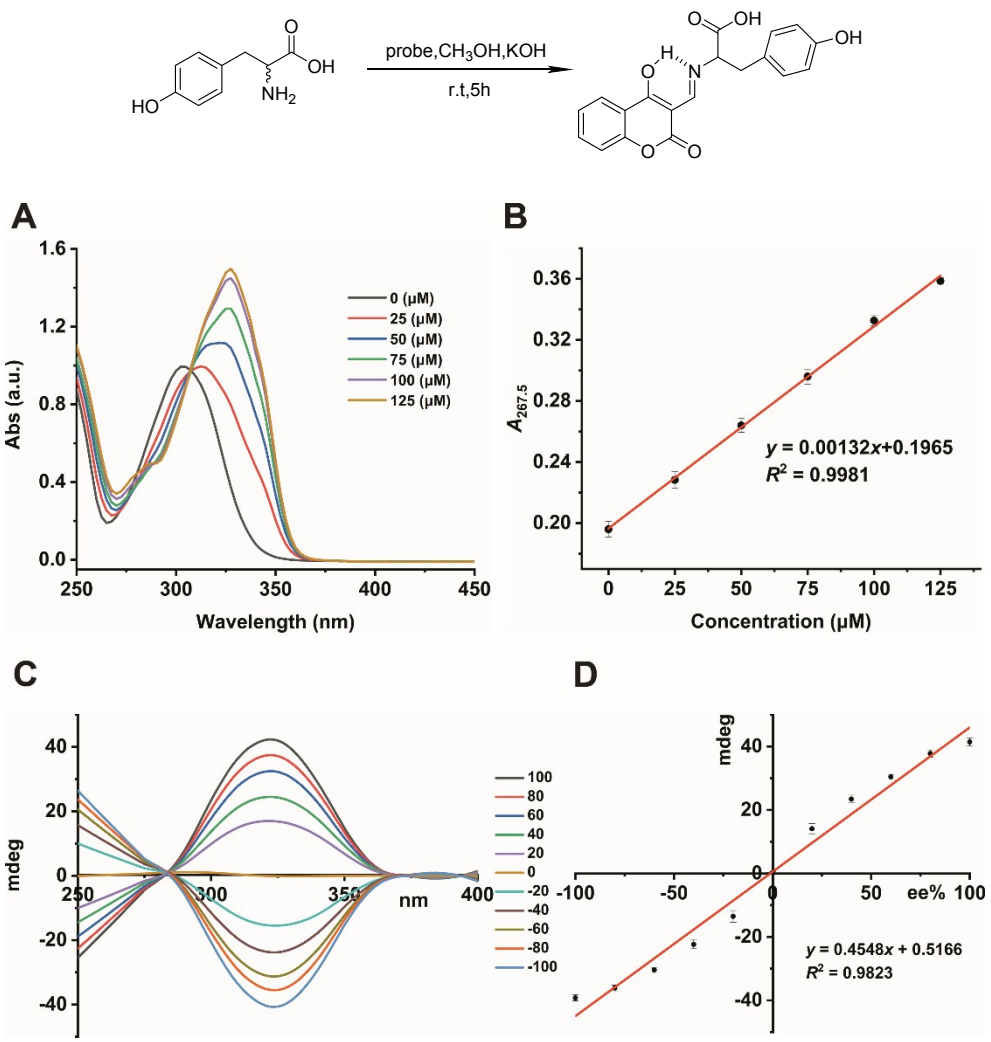


Fig. S23. Chiroptical sensing of Tyr. (A) UV-vis response of **1** to varying amounts of Tyr. (B) linear correlation between absorbance and concentration of Tyr. (C) CD response of **1** to nonracemic sample of Tyr, and (D) linear correlation between the induced CD signal at 323 nm and the sample *ee*.

Tab. S1. The detection limits of 12 amino acids.

Amino acids	Detection limit (μM)	Amino acids	Detection limit (μM)
Phe	0.11	Gln	0.42
Trp	0.31	Glu	0.43
Tyr	1.02	Ile	0.46
His	0.46	Leu	0.37
Asp	0.48	Met	0.44
Arg	0.35	Val	0.37

Tab. S2. The detection limits of amino acids in this work compared with other methods.

Amino acids	Detection limit (μM)	Ref.
Trp	0.33	45
	2.1	46
	27 (L-Trp), 44 (D-Trp)	47
	0.31	this work
Tyr		
	33	48
	10.3	49
	1.02	this work
His	67.5	50
	11	51
	0.46	this work
Arg	1.29 (L-Arg), 0.023 (D-Arg)	52
	0.35	this work

Tab. S3. Concentration of phenylalanine determined by UV responses of probe **1**.

Actual Concentration (μM)	Calculated Concentration (μM)
33.1	37.8±0.27
61.3	62.0±1.19
86.3	90.5±1.34
116.9	120.9±0.85

Tab. S4. Concentration, *ee* and absolute configuration of samples of Trp determined by the combined UV and CD responses of probe **1**.

	Sample composition			Sensing results		
Entry	**Abs.config.**	**Conc. (μM)**	**% ee**	**Abs.config.**	**Conc. (μM)**	**% ee**
1	L	30.0	-16.6	L	29.1±0.67	-14.9±1.24
2	D	50.0	30.0	D	50.6±0.89	26.5±0.25
3	L	14.0	-28.6	L	13.00±0.91	-22.8±0.43
4	D	37.5	33.3	D	38.57±0.38	31.2±0.67
5	L	23.5	-70.2	L	21.28±0.84	-72.6±0.44
6	D	30.0	50.0	D	30.31±0.14	46.6±0.26

Tab. S5. Concentration, *ee* and absolute configuration of samples of Tyr determined by the combined UV and CD responses of probe **1**.

	Sample composition			Sensing results		
Entry	**Abs.config.**	**Conc. (μM)**	**% ee**	**Abs.config.**	**Conc. (μM)**	**% ee**
1	D	100.0	25.0	D	103.4±2.47	23.0±1.39
2	L	56.2	-33.3	L	53.3±1.14	-27.4±0.17
3	D	68.8	45.4	D	72.7±1.37	40.6±0.37
4	L	62.5	-52.0	L	65.0±1.29	-59.9±2.43
5	D	87.5	28.6	D	80.9±0.94	25.0±0.57
6	L	50.0	-40.0	L	55.1±1.78	-35.9±0.74

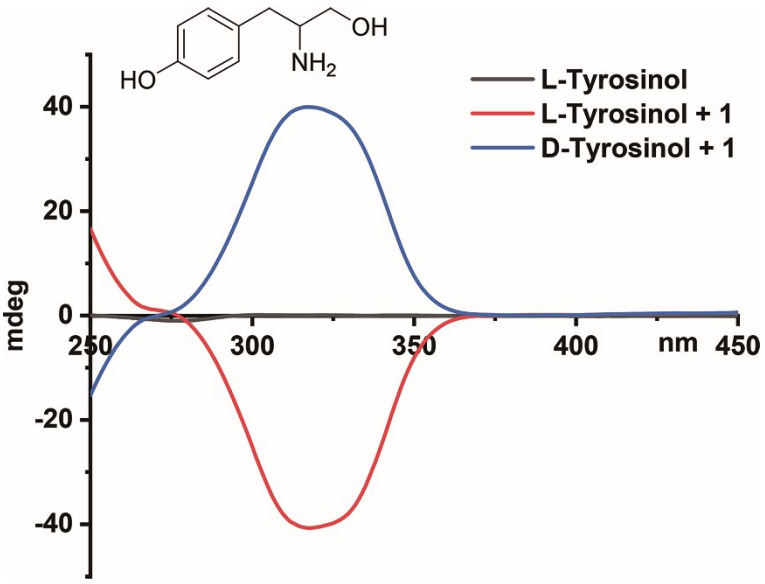


Fig. S24. CD spectra obtained from probe 1 with L- tyrosinol (red), D- tyrosinol (blue) and L-tyrosinol (black). (CD measurements were taken at 250 μM after diluting with methanol)

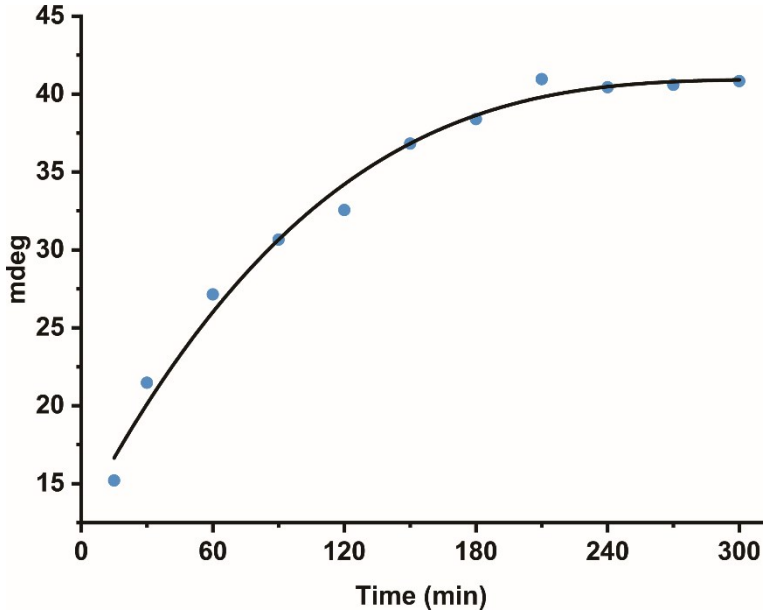
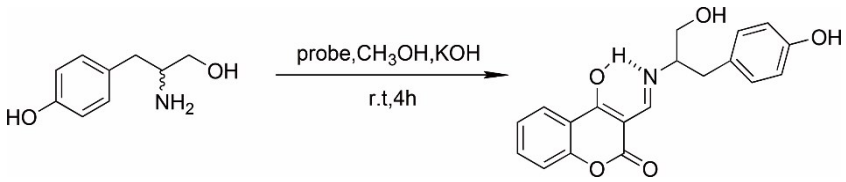


Fig. S25. CD analysis of the reaction between D- tyrosinol and probe 1. (CD signals were collected at 320 nm)



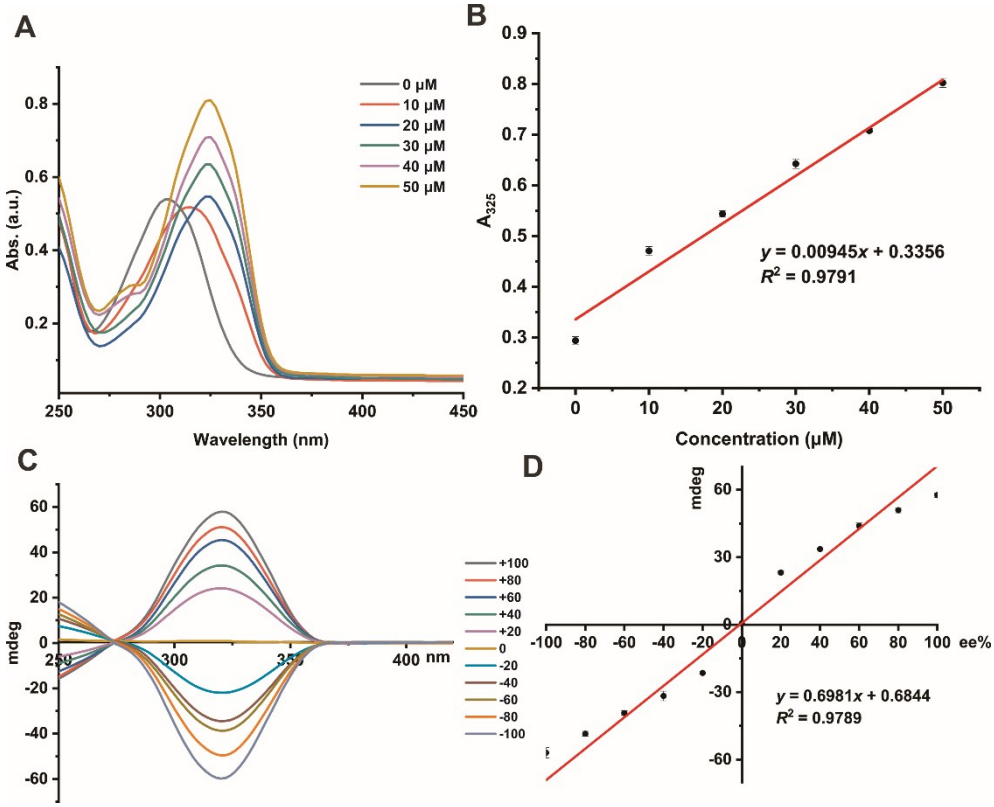


Fig. S26. Chiroptical sensing of tyrosinol. (A) UV-vis response of 1 to varying amounts of tyrosinol. (B) linear correlation between absorbance and concentration of tyrosinol. (C) CD response of 1 to nonracemic sample of tyrosinol, and (D) linear correlation between the induced CD signal at 320 nm and the sample *ee*.

Tab. S6. Concentration, *ee* and absolute configuration of samples of tyrosinol determined by the combined UV-vis and CD responses of probe 1.

	Sample composition			**Sensing results**		
Entry	**Abs.config.**	**Conc. (μM)**	**% ee**	**Abs.config.**	**Conc. (μM)**	**% ee**
1	L	14.0	-28.6	L	13.1±0.23	-28.1±1.17
2	D	50.0	33.3	D	48.0±0.60	35.6±0.83
3	L	23.5	-40.0	L	21.3±0.26	-41.6±0.61
4	D	30.0	50.0	D	28.9±0.73	54.8±0.40
5	L	40.0	-50.0	L	41.0±0.82	-52.0±0.82
6	D	35.0	16.6	D	34.9±0.18	14.4±0.93