

## Supporting information

### **High-Efficiency Detection of Primary Amines-Based Chiral Molecules by a Facile Aldimine Condensation Reaction**

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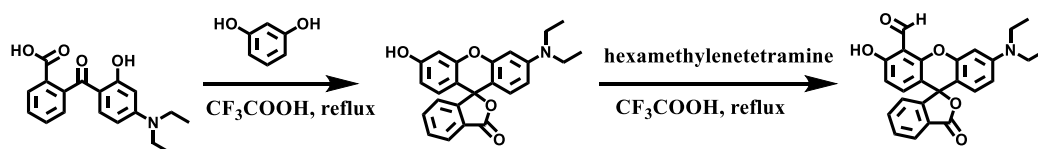
## Table of contents

<b>1. Experimental details.....</b>	<b>3</b>
<b>2. Supplementary Figures.....</b>	<b>6</b>

## 1. Experimental details

### Materials

L-cysteine hydrochloride were bought from Alfa Aesar. D-cysteine hydrochloride was purchased from meryer. D/L-glutamic acid, D/L-Histidine, acetonitrile (ACN) and butylamine were purchased from Aladdin Chemicals. Tetrabutyl ammonium hydroxide (TBAOH) was purchased from Energy Chemicals. (S)-(-)- $\alpha$ -methylbenzylamine (S)-(-)- $\alpha$ -MBA) was bought from Adamas-beta®. Trifluoroacetic acid (CF<sub>3</sub>COOH) was bought from Macklin Chemicals. 6'-(diethylamino)-3'-hydroxy-3-oxo-3H-spiro[isobenzofuran-1,9'-xanthene]-4'-carbaldehyde (R-C) shown in Scheme S1 was synthesized according to the previous work (Adv. Sci. 2022, 9, 2202636) and its <sup>1</sup>H NMR spectrum was shown in Figure S1. Water was purified by a Milli-Q system.



**Scheme S1.** Synthetic route of the molecule R-C.

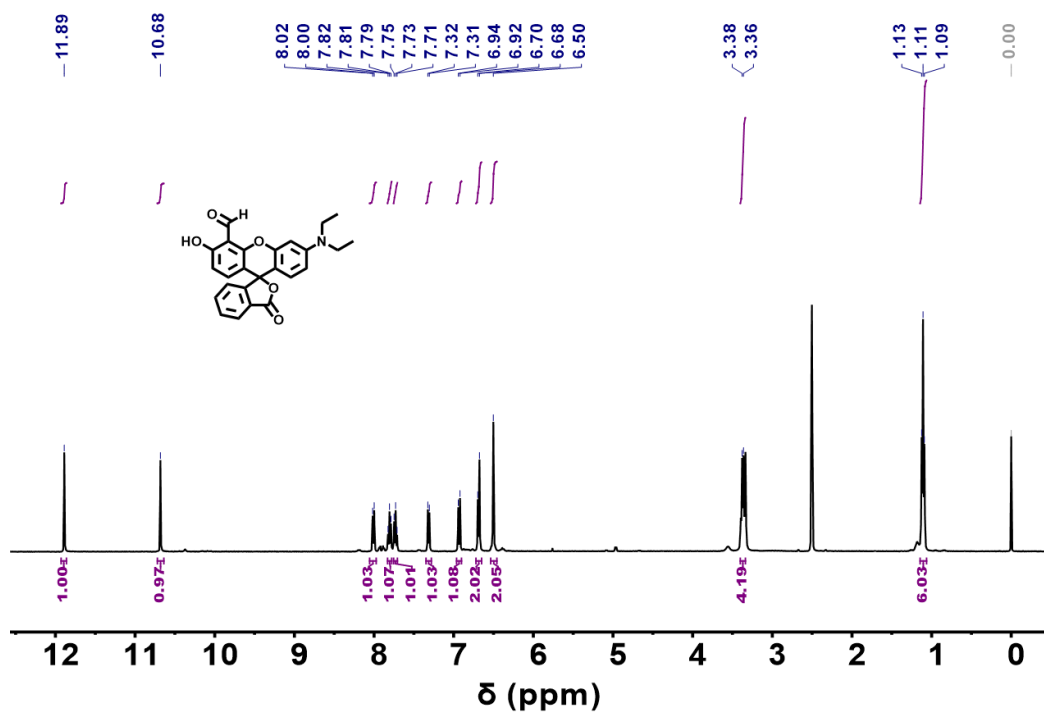
### Instruments and Characterizations

UV-vis absorption spectra were measured on a Shimadzu UV-2550 double-beam spectrophotometer. Circular dichroism (CD) spectra were collected on a Chirascan circular dichroism spectrometer (Applied Photophysics Ltd.), and the measured data were treated with smoothing processing then. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were measured by a Bruker AVANCE NEO 400 M NMR spectrometer. Chemical shift values were given relative to tetramethylsilane (TMS). LC-HRMS analysis was obtained by a Shimadzu LCMS-IT-TOF mass spectrometer.

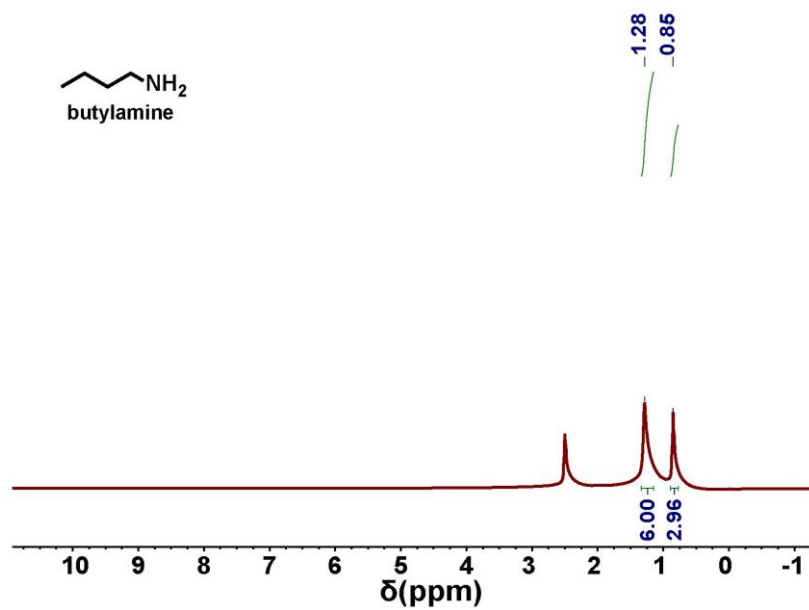
### Detection process for primary amines-based chiral molecules

Firstly, the R-C was dissolved in ACN with a specific concentration. Then, the chiral molecules with primary amines (-NH<sub>2</sub>) was dissolved in water with a specific concentration. After the above two solutions were totally dissolved, they were mixed in a transparent bottle and stirred at 30 °C for 12 hours, so that to react completely. The UV-vis absorption and CD spectra of this reaction product were further measured so that to determine the concentration and configuration of the chiral analyte.

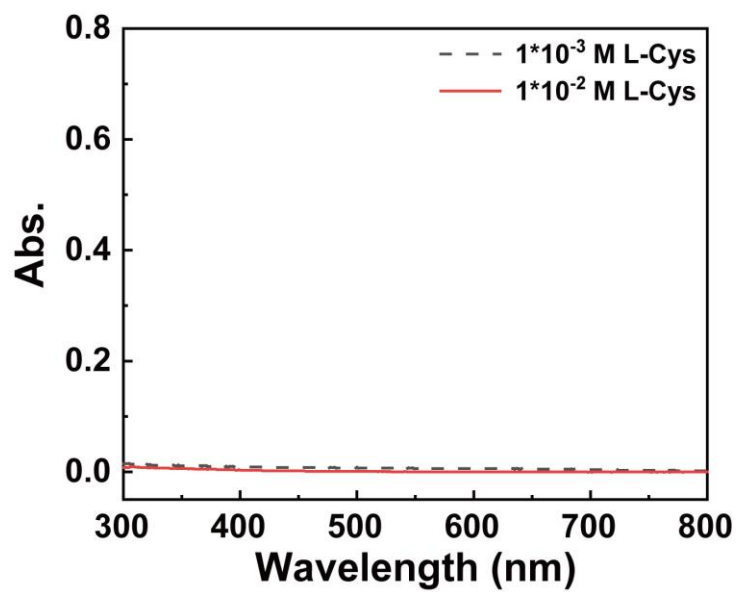
## 2. Supplementary Figures



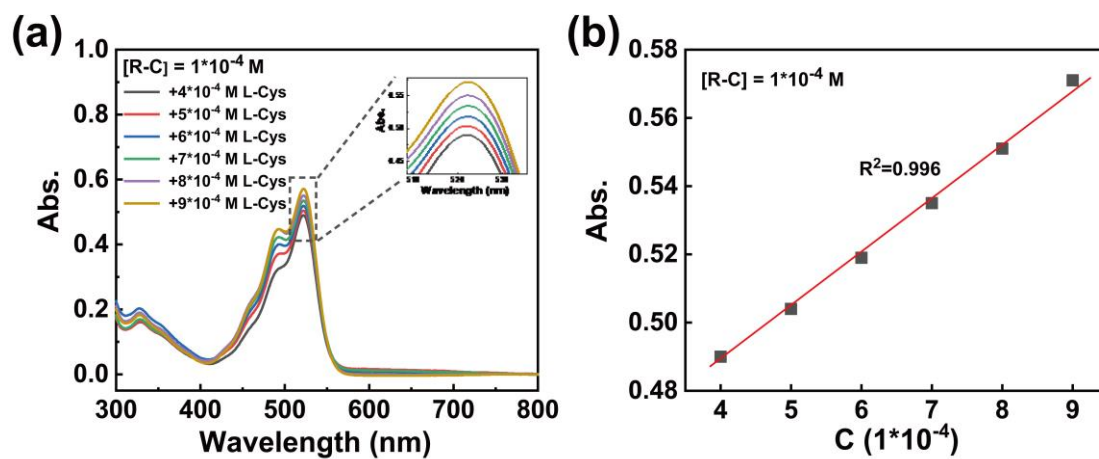
**Figure S1.** <sup>1</sup>H NMR spectrum of R-C in deuterated DMSO recorded at 400 M Hz at room temperature.



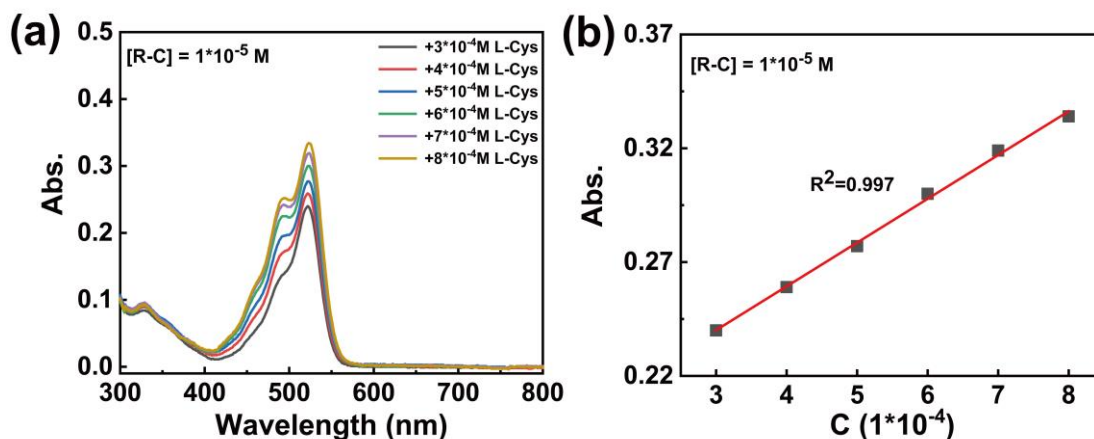
**Figure S2.**  $^1\text{H}$  NMR spectrum of butylamine in deuterated DMSO recorded at 400 MHz at room temperature.



**Figure S3.** UV-vis absorption spectra of the  $1.0 \times 10^{-3}$  M and  $1.0 \times 10^{-3}$  M L-Cys in deionized water, respectively.



**Figure S4.** (a) UV-vis absorption spectra and (b) corresponding absorption values at 522 nm of the mixture of  $1.0 \times 10^{-4}$  M R-C in CH<sub>3</sub>CN and L-Cys in deionized water with various concentrations.



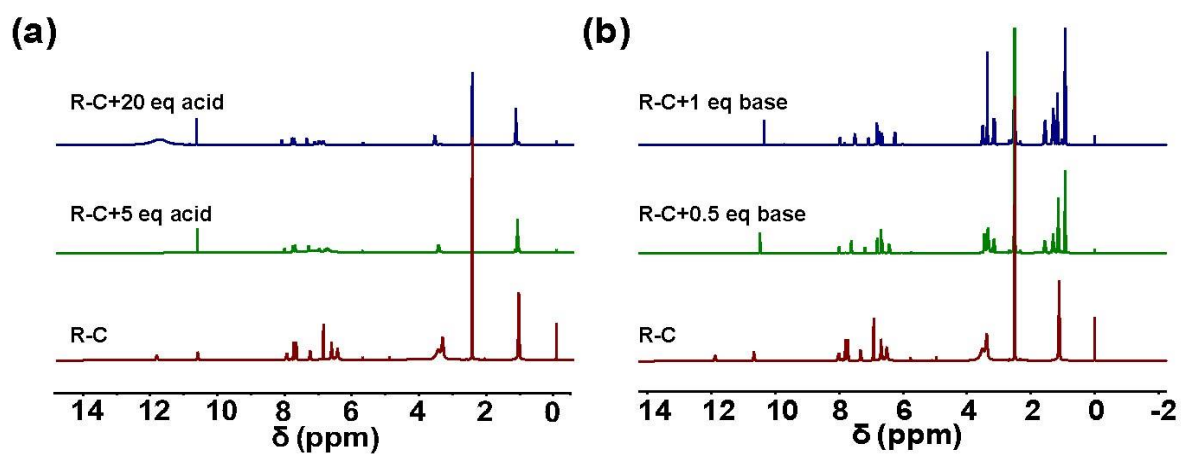
**Figure S5.** (a) UV-vis absorption spectra and (b) corresponding absorption values at 522 nm of the mixture of  $1.0 \times 10^{-5}$  M R-C in  $\text{CH}_3\text{CN}$  and L-Cys in deionized water with various concentrations.

The detailed calculation process of LOQ (limit of quantitation) was shown below:

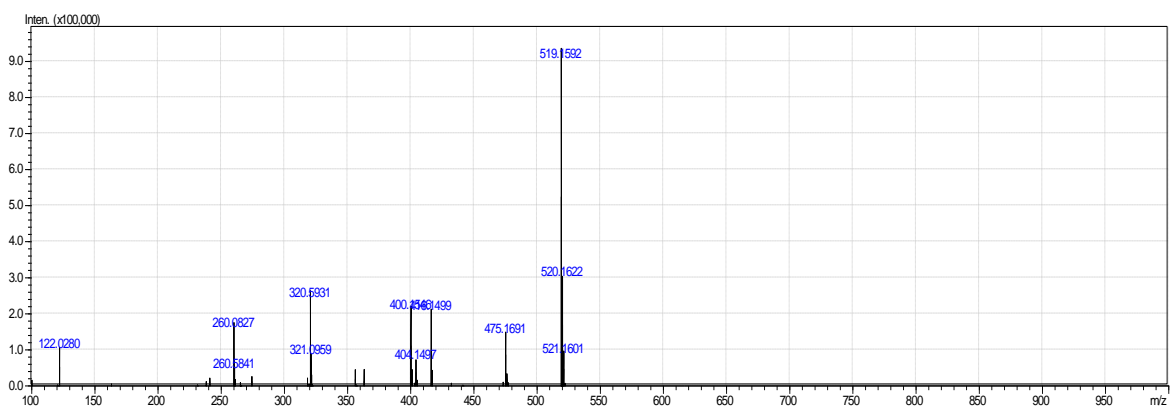
$$\text{LOQ} = 10 \cdot \text{RSD} / k$$

- (1) According to the calibration curve, the  $k$  was  $0.01923 \times 10^4$ ;
- (2) According to the absorption curves of blank samples (measured 11 times), the RSD (relative standard deviation) was 0.0022;
- (3) Thus, the value of LOQ was  $(10 \cdot 0.0022) / (0.01923 \times 10^4) = 1.14 \times 10^{-4}$

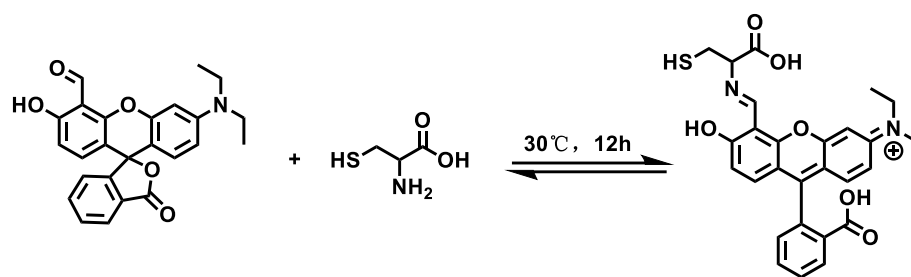




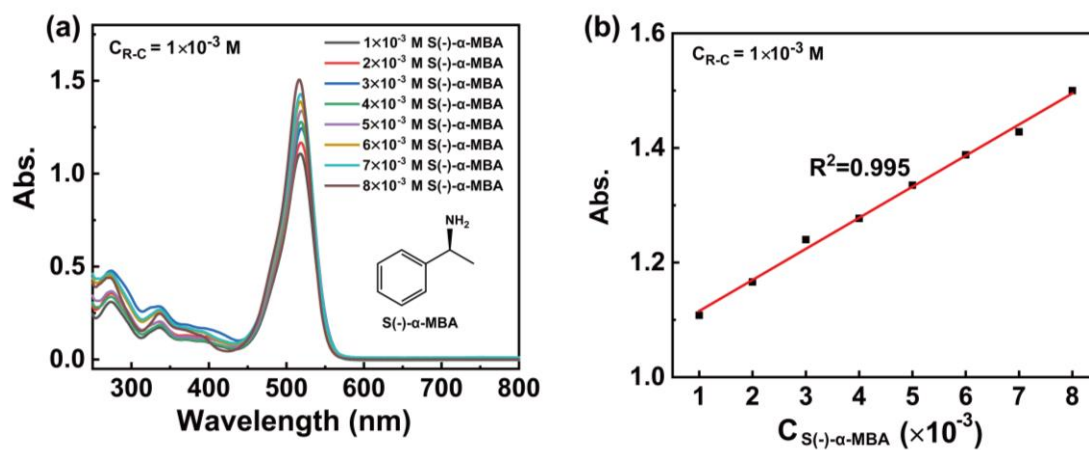
**Figure S6.** (a)  $^1\text{H}$  NMR spectra of R-C and when it was added various eq acid (TFA) in deuterated DMSO, respectively. (b)  $^1\text{H}$  NMR spectra of Rhodol-CHO and when it was added various eq base (TBAOH) in deuterated DMSO, respectively.



**Figure S7.** Mass spectrum of the mixture of R-C and L-Cys at room temperature.



**Figure S8.** Reaction route of R-C and Cys.



**Figure S9.** (a) UV-vis absorption spectra and (b) corresponding absorption values at 518 nm of the mixture of  $1.0 \times 10^{-3}$  M R-C in  $\text{CH}_3\text{CN}$  and S(-)- $\alpha$ -MBA with various concentrations in deionized water.