

## ***Electronic Supplementary Information for***

### ***Coumarin-Based Chiral Fluorescence Sensor Incorporating Thiourea unit for Highly Enantioselective Recognition of N-Boc-protected Proline***

Zhitao Xing,<sup>a</sup> Yong Fu,<sup>a</sup> Jiecong Zhou,<sup>a</sup> Chengjian Zhu<sup>\*a,b</sup> and Yixiang Cheng<sup>\*a</sup>

<sup>a</sup> State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093 China E-mail: cjzhu@nju.edu.cn

<sup>b</sup> State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China

Fax: (+86)-25-8331-7761; Tel: (+86)-25-8359-4886;

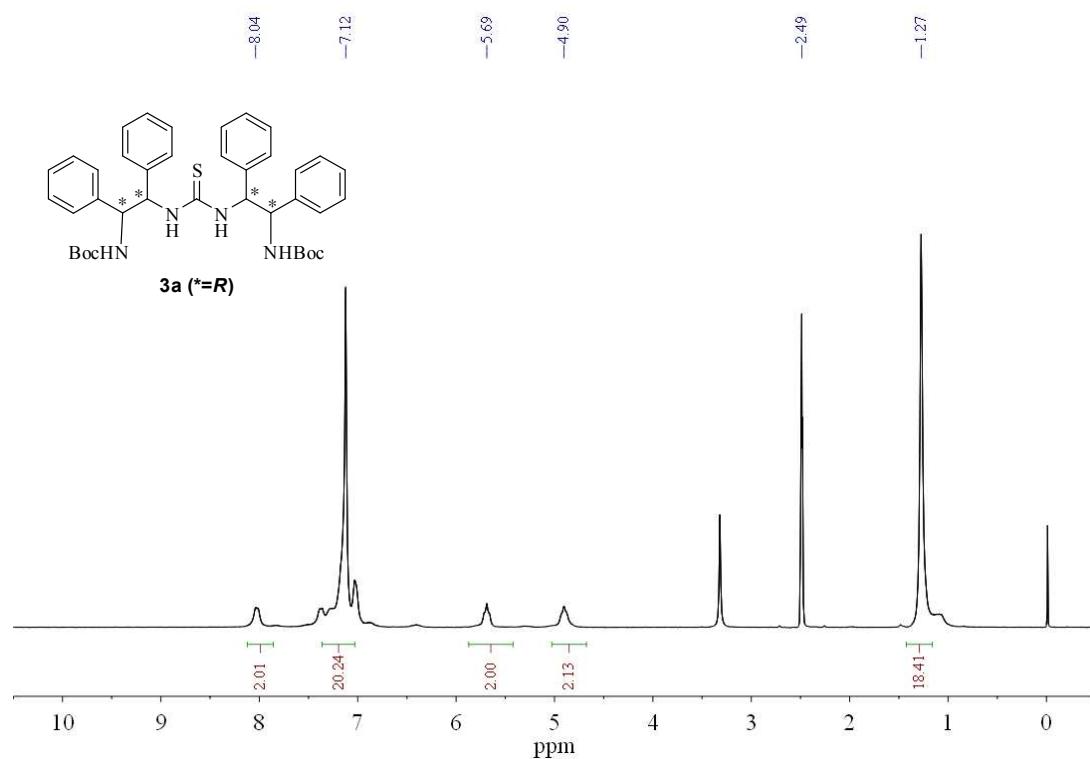
E-mail: cjzhu@nju.edu.cn;

## **Contents:**

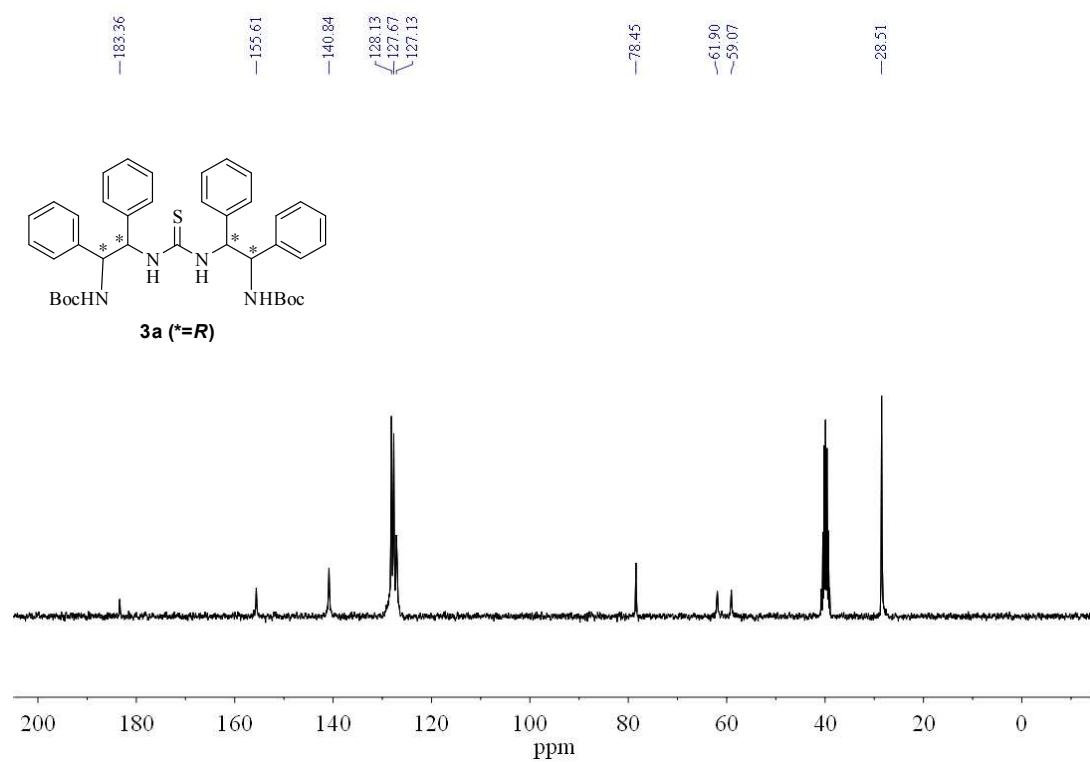
SI 1. <sup>1</sup> H NMR, and <sup>13</sup> C NMR Spectra	Page S2-S5
SI 2. Spectra Data	Page S6-S10

## SI 1. $^1\text{H}$ NMR, and $^{13}\text{C}$ NMR Spectra

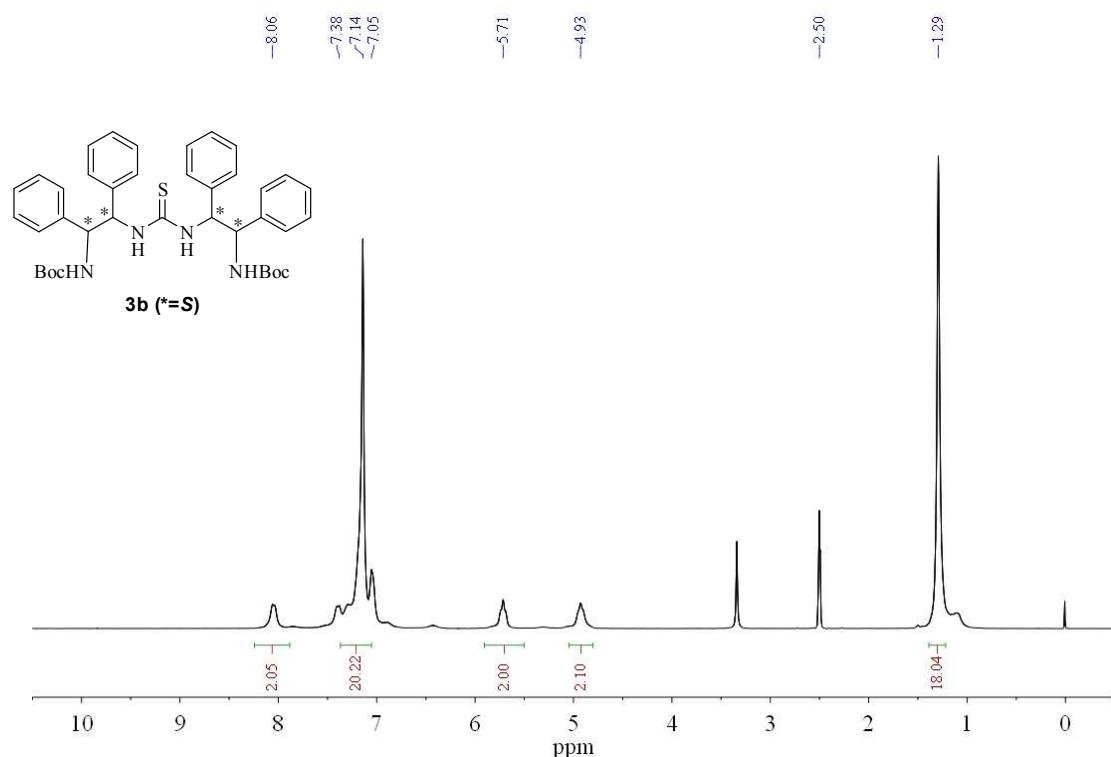
$^1\text{H-NMR}$  Spectra of **3a** (300MHz, DMSO- $d_6$ )



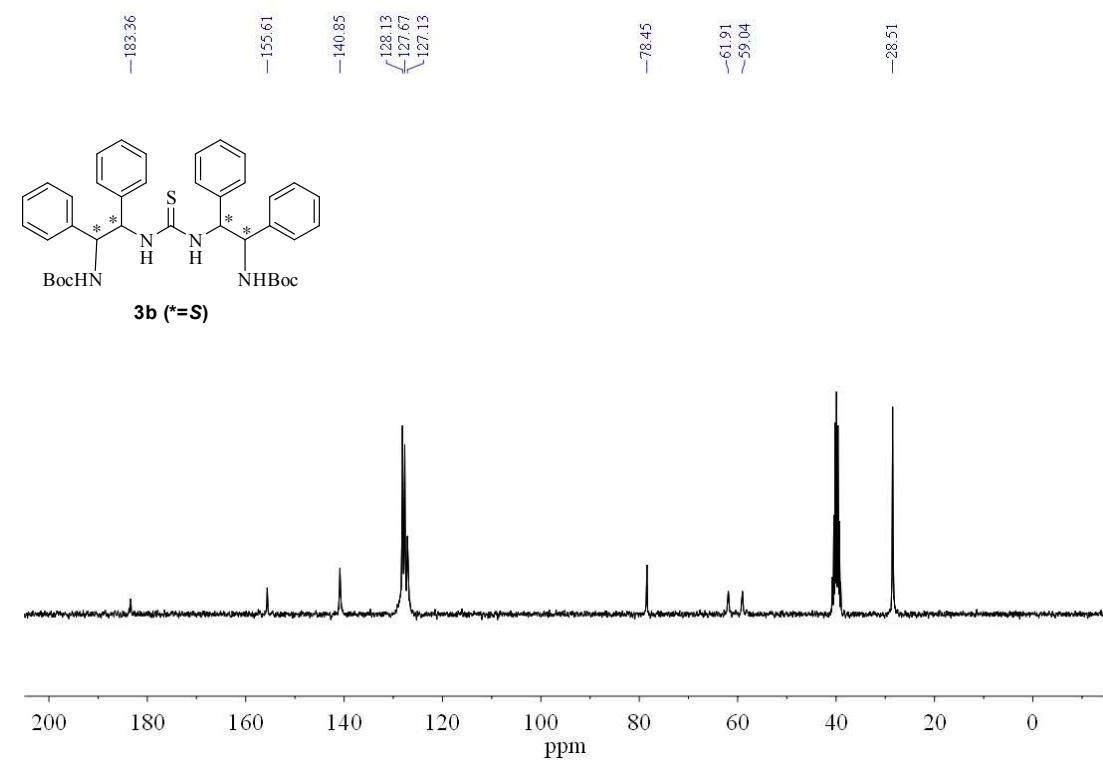
$^{13}\text{C-NMR}$  Spectra of **3a** (75MHz, DMSO- $d_6$ )



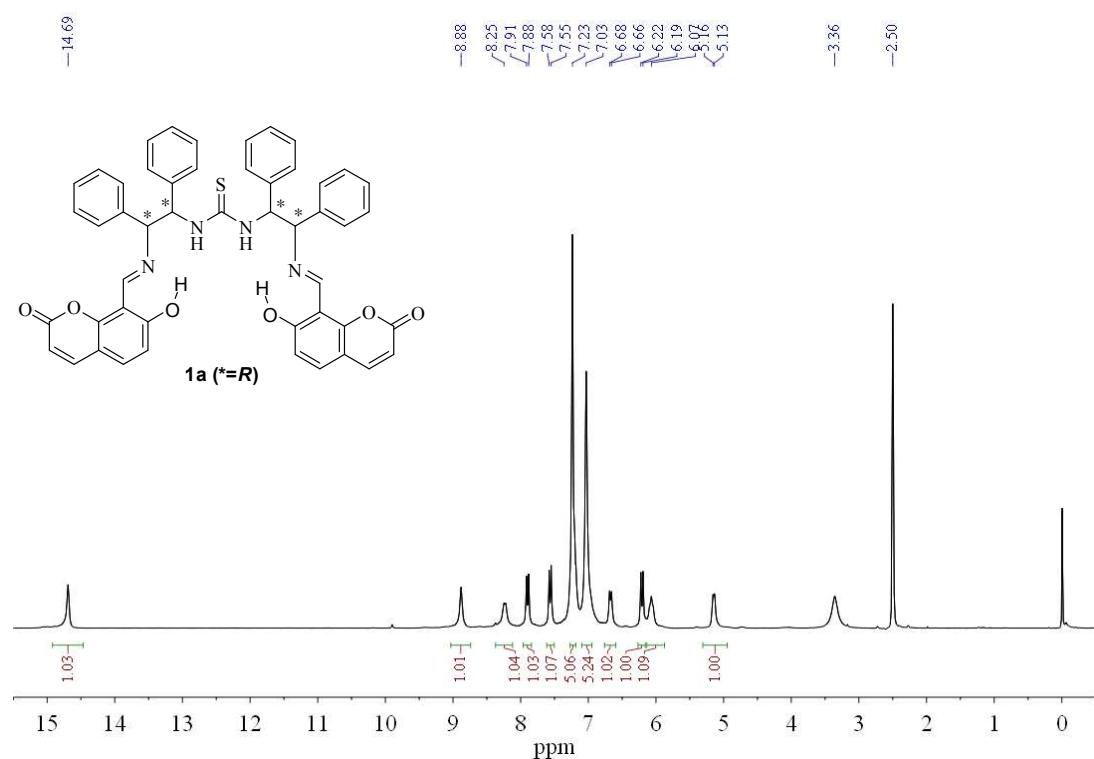
<sup>1</sup>H-NMR Spectra of **3b** (300MHz, DMSO-d<sub>6</sub>)



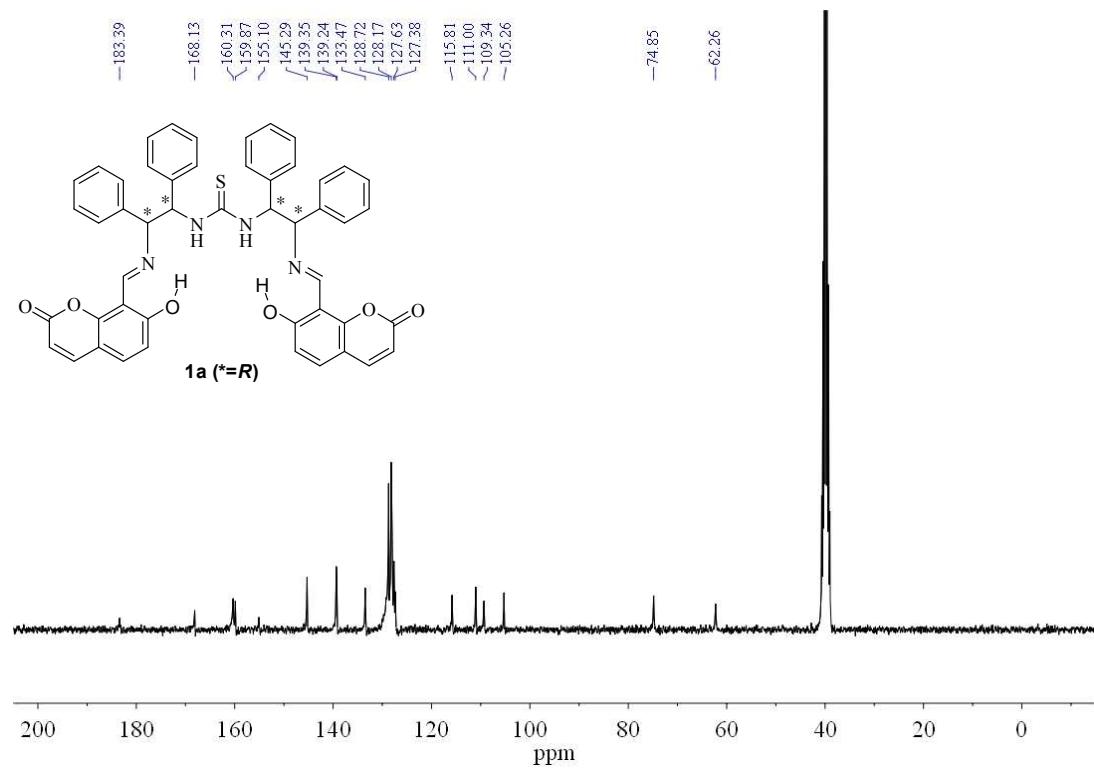
<sup>13</sup>C-NMR Spectra of **3b** (75MHz, DMSO-d<sub>6</sub>)



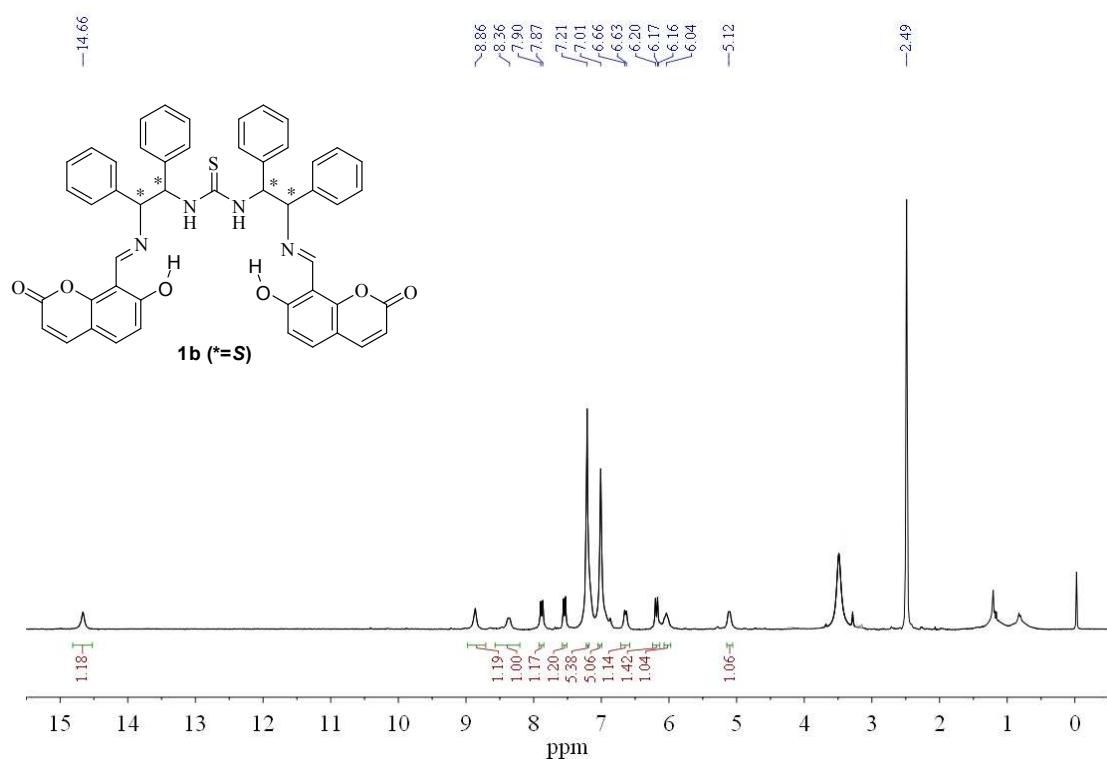
<sup>1</sup>H-NMR Spectra of **1a** (300MHz, DMSO-d<sub>6</sub>)



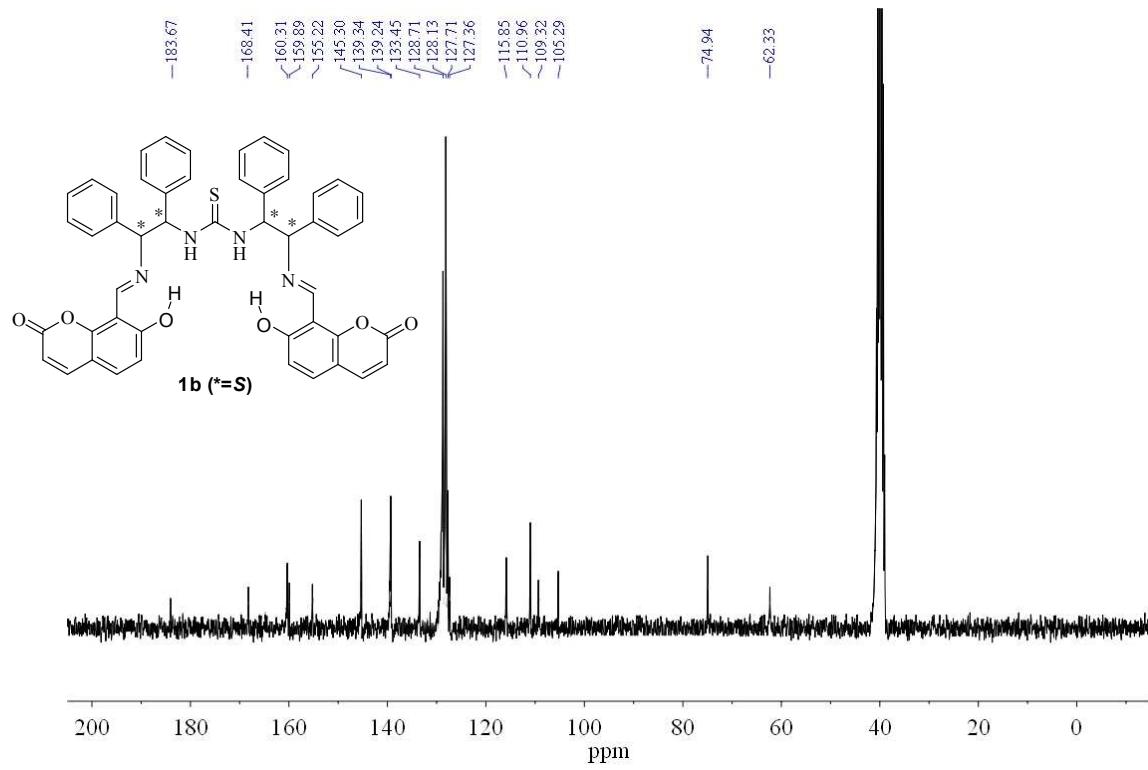
<sup>13</sup>C-NMR Spectra of **1a** (75MHz, DMSO-d<sub>6</sub>)



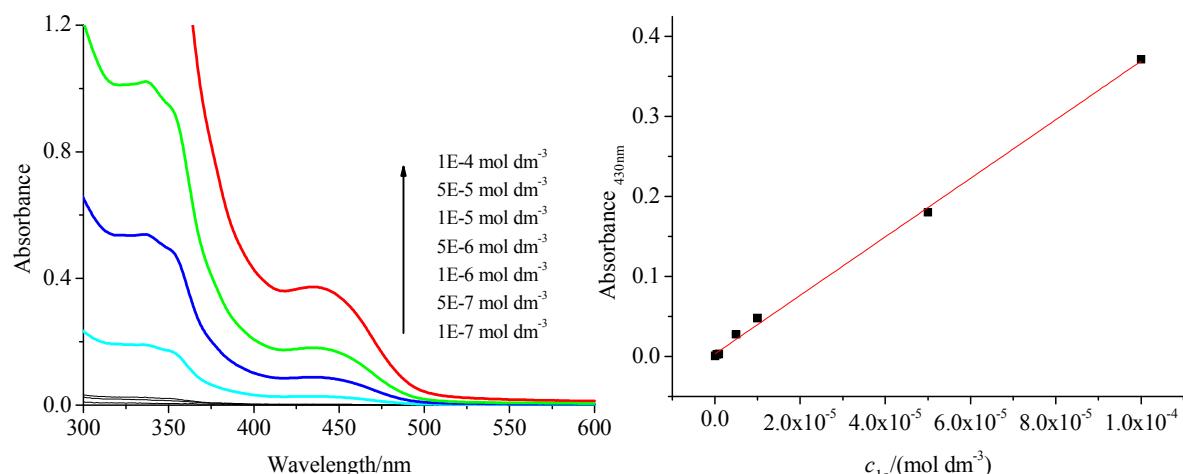
*<sup>1</sup>H-NMR Spectra of 1b (300MHz, DMSO-d<sub>6</sub>)*



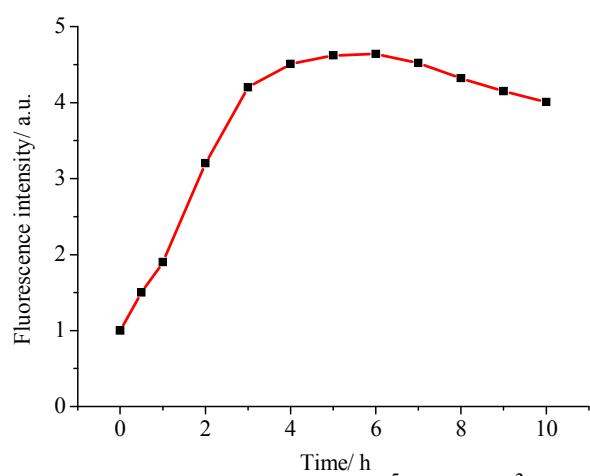
*<sup>13</sup>C-NMR Spectra of **1b** (75MHz, DMSO-d<sub>6</sub>)*



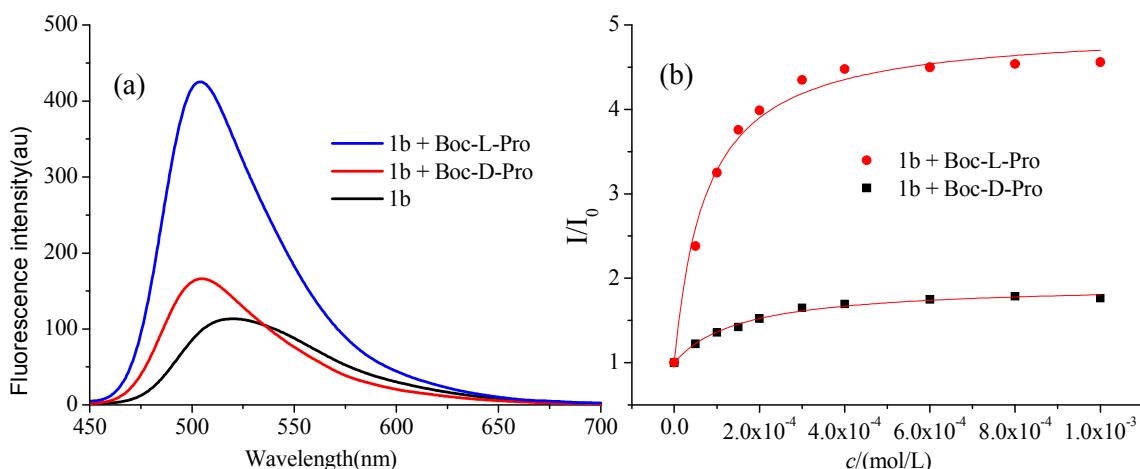
## SI 2. Spectra Data



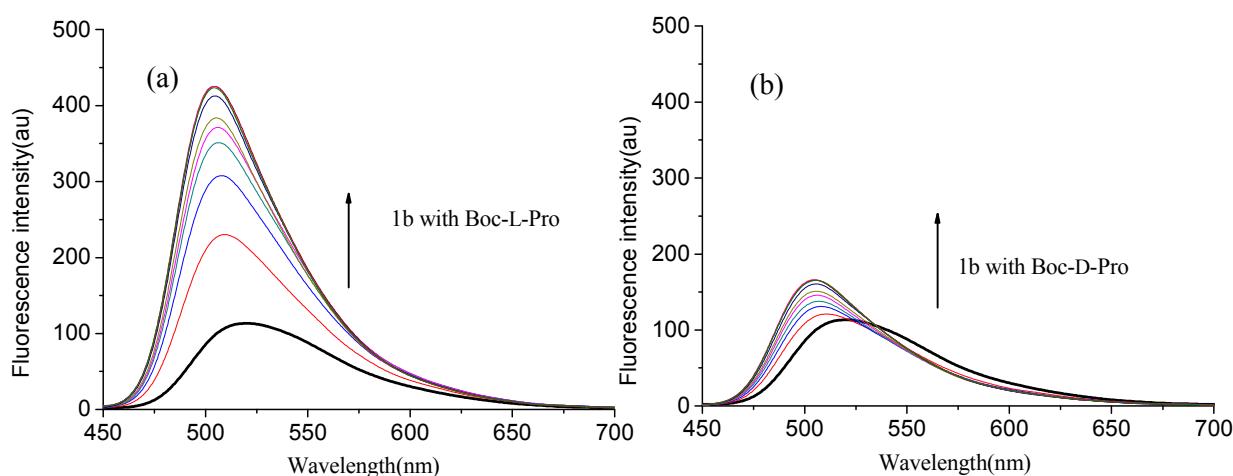
**Figure S1.** Concentration effect on the UV-Vis spectra of **1a** in toluene



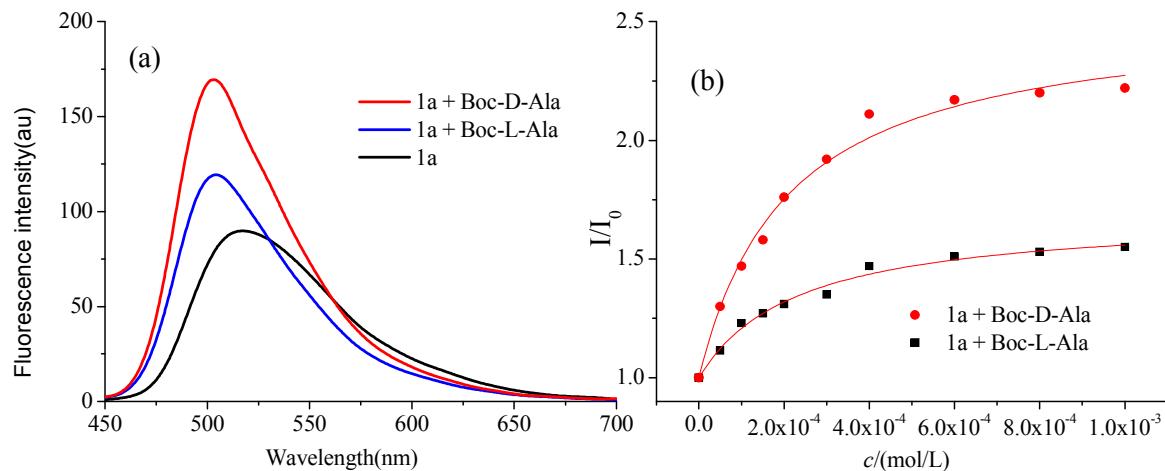
**Figure S2.** Kinetic study of sensor **1a** ( $1.0 \times 10^{-5}$  mol dm<sup>-3</sup>) with Boc-D-Pro ( $1.0 \times 10^{-3}$  mol dm<sup>-3</sup>) in toluene  $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm.



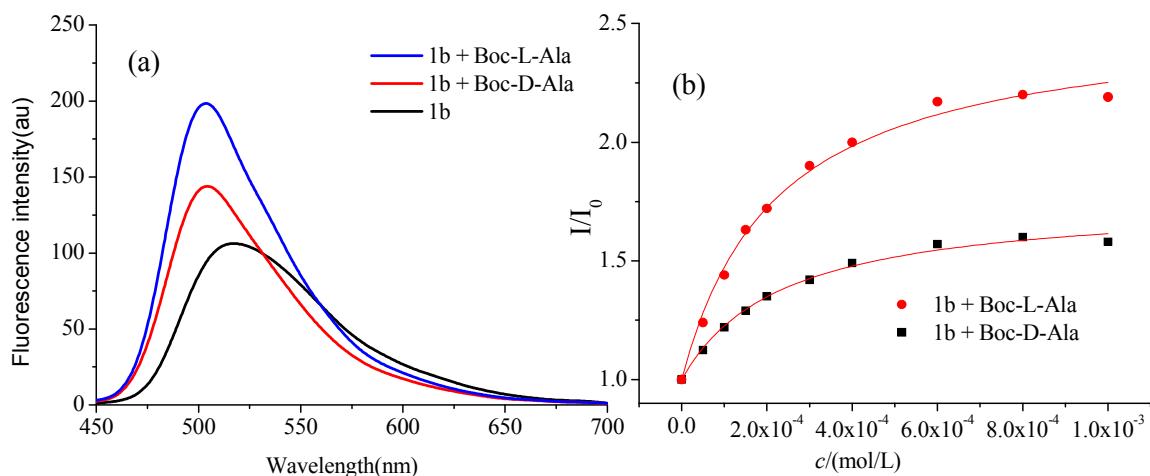
**Figure S3.** **a)** Fluorescence spectra of **1b** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(*D* or *L*)-Pro ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and **b)** the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1b** with Boc-(*D* or *L*)-Pro ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).



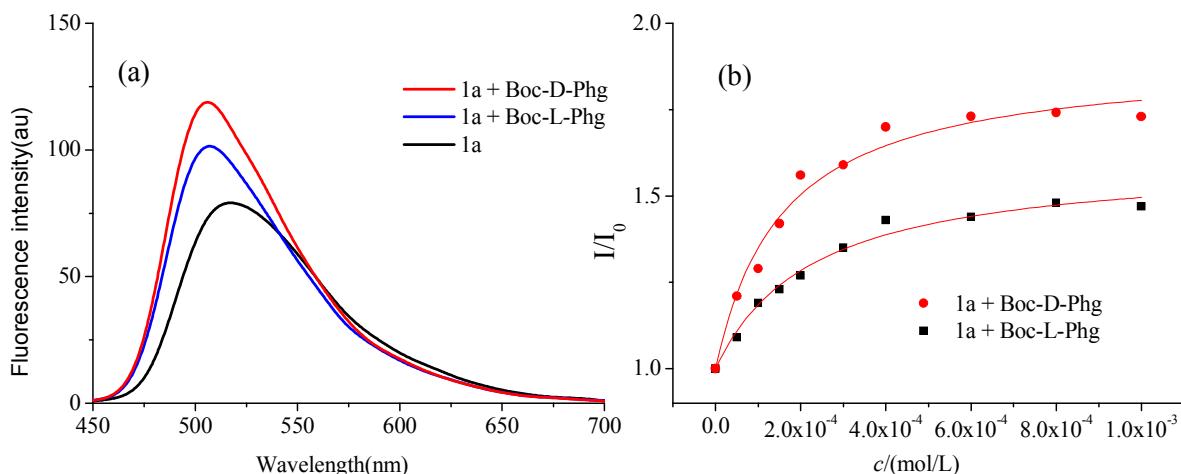
**Figure S4.** Fluorescence spectra of **1b** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene solution) with **a)** Boc-*L*-Pro and **b)** Boc-*D*-Pro; Concentrations of Boc-(*L* or *D*)-Pro are from  $5.0 \times 10^{-5}$  mol dm $^{-3}$  to  $1.0 \times 10^{-3}$  mol dm $^{-3}$  ( $\lambda_{\text{ex}} = 430$  nm).



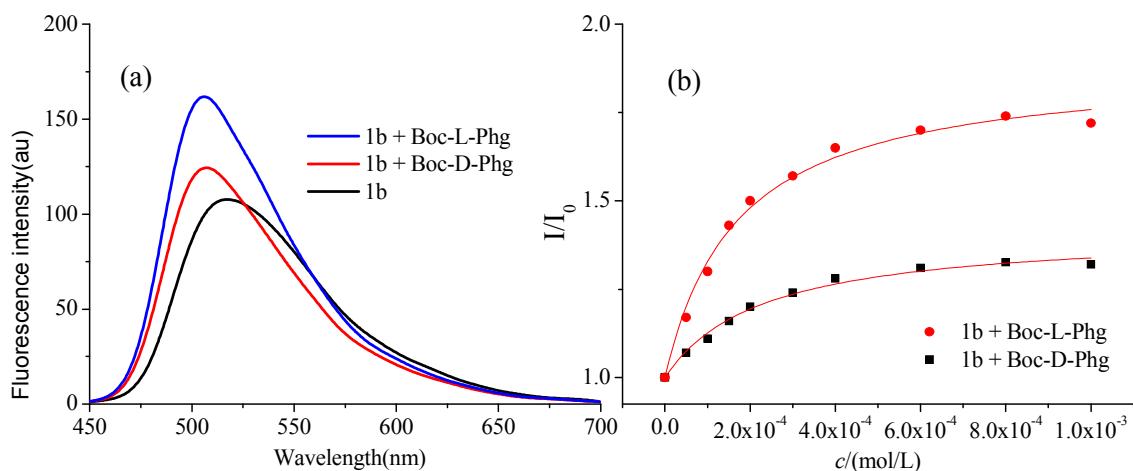
**Figure S5.** a) Fluorescence spectra of **1a** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(D or L)-Ala ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and b) the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1a** with Boc-(D or L)-Ala ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).



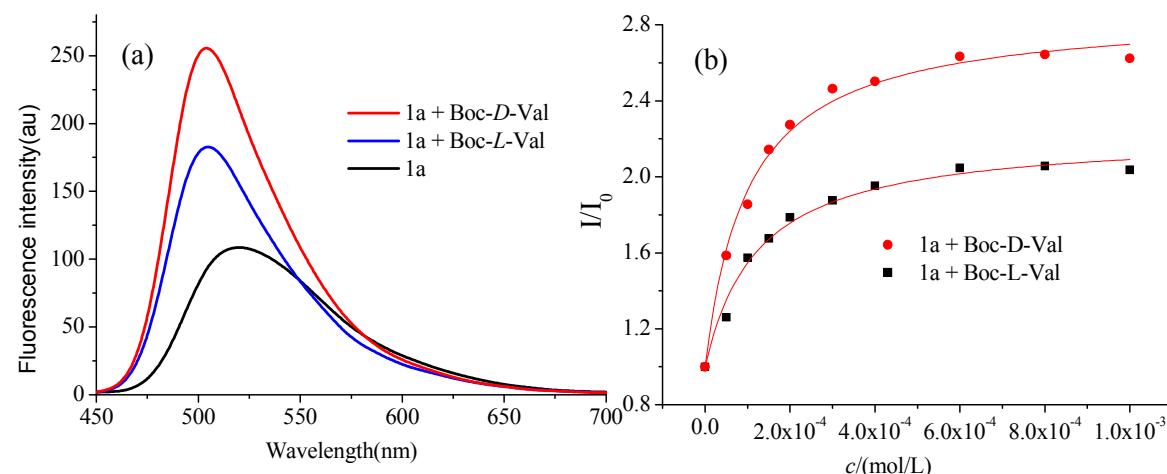
**Figure S6.** a) Fluorescence spectra of **1b** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(D or L)-Ala ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and b) the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1b** with Boc-(D or L)-Ala ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).



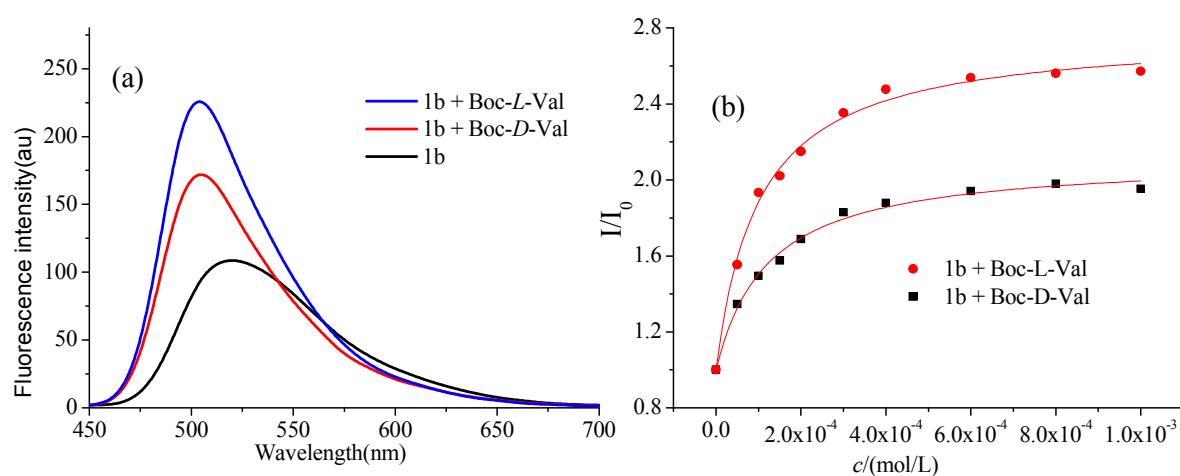
**Figure S7.** **a)** Fluorescence spectra of **1a** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(*D* or *L*)-Phg ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and **b)** the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1a** with Boc-(*D* or *L*)-Phg ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).



**Figure S8.** **a)** Fluorescence spectra of **1b** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(*D* or *L*)-Phg ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and **b)** the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1b** with Boc-(*D* or *L*)-Phg ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).



**Figure S9.** **a)** Fluorescence spectra of **1a** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(D or L)-Val ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and **b)** the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1a** with Boc-(D or L)-Val ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).



**Figure S10.** **a)** Fluorescence spectra of **1b** ( $1.0 \times 10^{-5}$  mol dm $^{-3}$  in toluene) with Boc-(D or L)-Val ( $1.0 \times 10^{-3}$  mol dm $^{-3}$ ) and **b)** the plots of ( $I/I_0$ ) versus the concentration of acids during the titration of **1b** with Boc-(D or L)-Val ( $\lambda_{\text{ex}} = 430$  nm,  $\lambda_{\text{em}} = 502$  nm).