

Supporting Information

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1. Experimental Section

Materials:

All reagents and solvents were chemically pure (CP) grade or analytical reagent (AR) and were used as received unless otherwise indicated general. ¹H NMR and ¹³C NMR spectra were measured on a Bruker AV 500 spectrometer at 303K from sample solution in CDCl₃ for sensor **5** or DMSO-d₆ for sensors **4** and **6**. Infrared spectra were recorded on a Bruker TENSOR 27 spectrometer. Absorption spectra were recorded on a Shimadzu UV-2550 PC spectrophotometer. Mass spectra were measured on a Waters Q-TOF micro spectrometer. Fluorescence emission spectra were collected on a Perkin Elmer LS 55 Fluorescence Spectrometer. The fluorescence spectra for the AIE effect were measured after the addition of water and leaving the mixture to stand for 3h at 298K. To measure changes in the fluorescence intensity in the presence of chiral guests, all mixtures of sensors **4-6** and chiral guests **7-14** were left to stand 2h at 298K before measuring their fluorescence spectra. Absorption spectra were measured in THF/ H₂O (1/ 1.6) after the mixture stand for 1h. Optical rotations were measured at 25 °C on an Anton Paar MCP 500 polarimeter using a sodium lamp as the light source (589 nm).

Job plot measurements

Sensor **4** and chiral guests such as *L* and *D*-tartaric acid were prepared with concentration of 2×10⁻⁵ M in mixed solvent THF/ H₂O (1/ 1.6). 2.0, 1.8, 1.6, 1.4, 1.2, 1.0, 0.8, 0.6, 0.4, 0.2 and 0 ml of the chiral sensor solution were transferred to the tubes. 0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8 and 2.0 ml of analyte solutions were added to the each sensor solution separately. Each tube will have the total volume of 2 ml.

Titration measurements

Sensor **4** and tartaric acid were dissolved in the mixed solvent of THF/ H₂O (V/V 1/ 1.6) to obtain the sample solutions. 0, 0.2, 0.4, 0.5, 0.8, 1, 1.2, 1.4, 1.5, 1.8 and 2eq of analyte solutions were added to the 1mL sensor solution separately, then added the mixed solvent of THF/ H₂O (V/V 1/ 1.6) to the total volume of 2 ml. The concentration of compound **4** was kept 2×10⁻⁵ M.

¹H NMR titration experiments

The solvents of THF-D₈ and D₂O are expensive, so the ¹H NMR titration experiments were carried out in DMSO-d₆. In order to assess the chiral recognition properties between receptor **4** and chiral tartaric acid at a much broader concentration range in DMSO-d₆. The concentration of receptor **4** was a constant (2×10⁻⁵ mol/L) in DMSO-d₆, the concentration of guests range from 0eq to 1.8eq.

2. Spectrum of compound

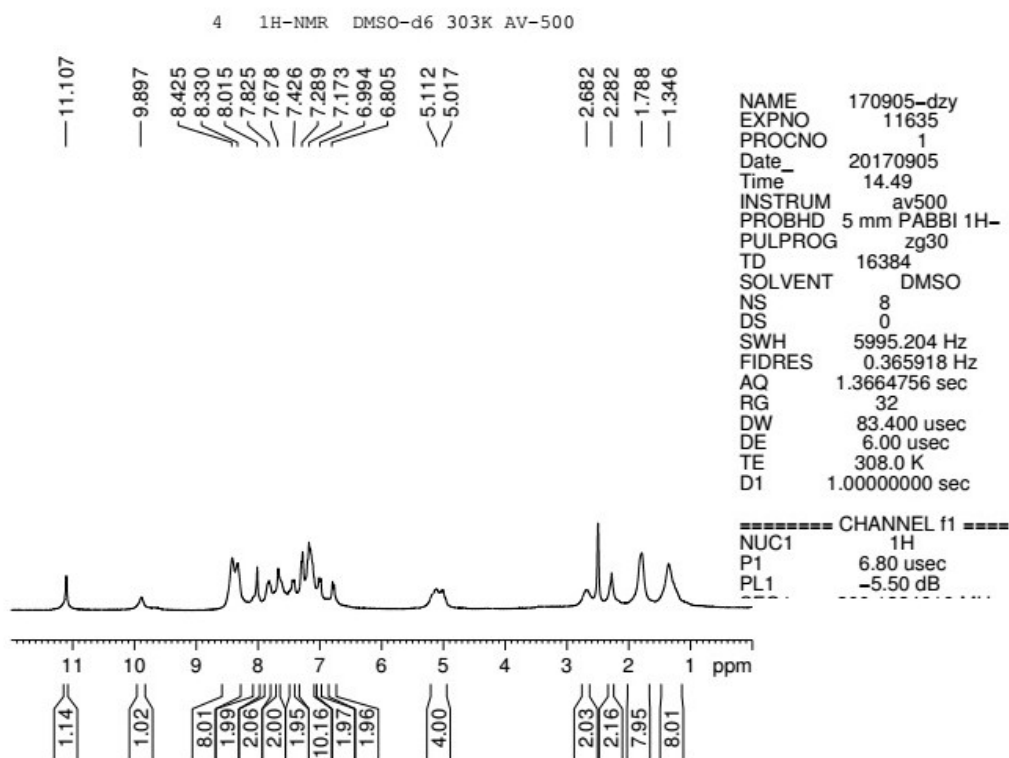


Figure S 1. ^1H NMR spectrum of **4** in DMSO- d_6 .

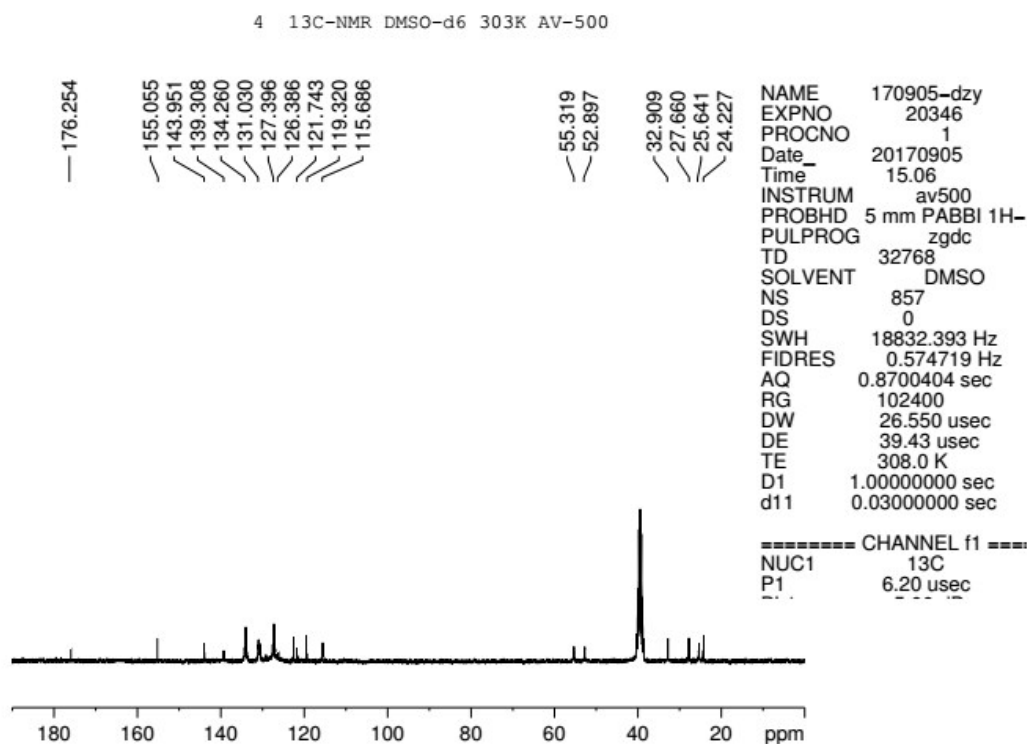
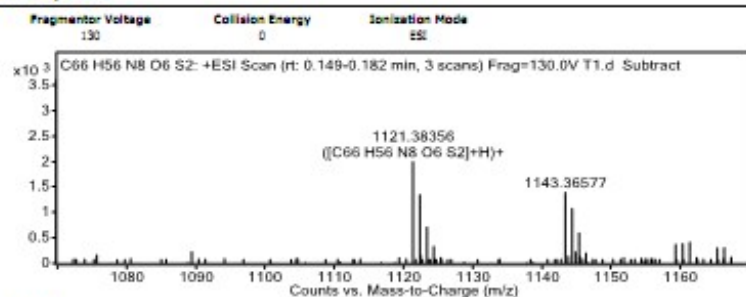


Figure S 2. ^{13}C NMR spectrum of **4** in DMSO- d_6 .

Qualitative Analysis Report

Data Filename	T1.d	Sample Name	T1
Sample Type	Sample	Position	Vial 22
Instrument Name	Instrument 1	User Name	
Acq Method	method-POST.m	Acquired Time	9/22/2017 7:56:35 PM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	5200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6157)

User Spectra



Peak List

m/z	z	Abund
88.07662		6514.77
102.12874	1	591576.69
102.22632		90470.11
103.13133	1	54176.66
116.10718		4582.5
196.1341	1	90710.5
196.2676		8088.01
197.13706	1	15263.25
515.24667	1	7147.34
764.57259	1	5049.85

Formula Calculator Element Limits

Element	Min	Max
C	56	76
H	46	66
N	6	10
O	4	8
S	2	2

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Calculated Mz
C66 H56 N8 O6 S2	TRUE	1120.3766	1120.3764	+0.06	C66 H57 N8 O6 S2	1121.3837
C61 H56 N10 O8 S2	FALSE	1120.3766	1120.3724	+3.75	C61 H57 N10 O8 S2	1121.37968
C71 H56 N6 O4 S2	FALSE	1120.3764	1120.3804	-3.63	C71 H57 N6 O4 S2	1121.38772

*** End Of Report ***

Figure S 3. HRMS spectrum of 4

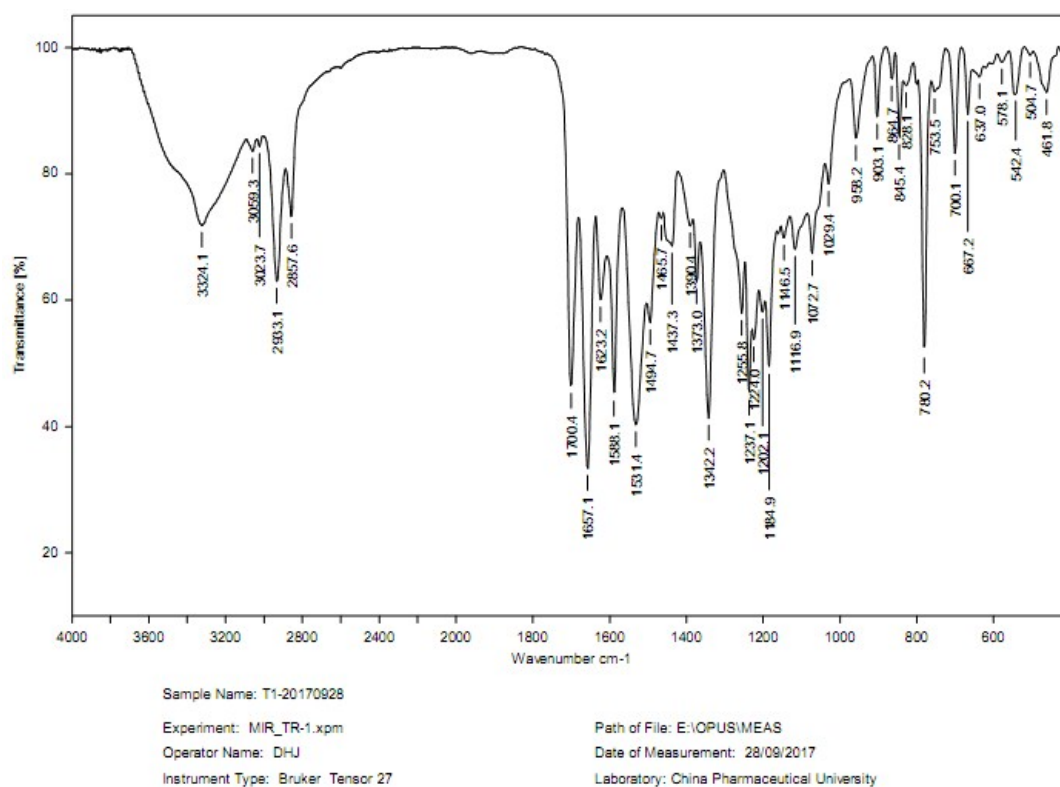


Figure S 4. IR spectrum of 4

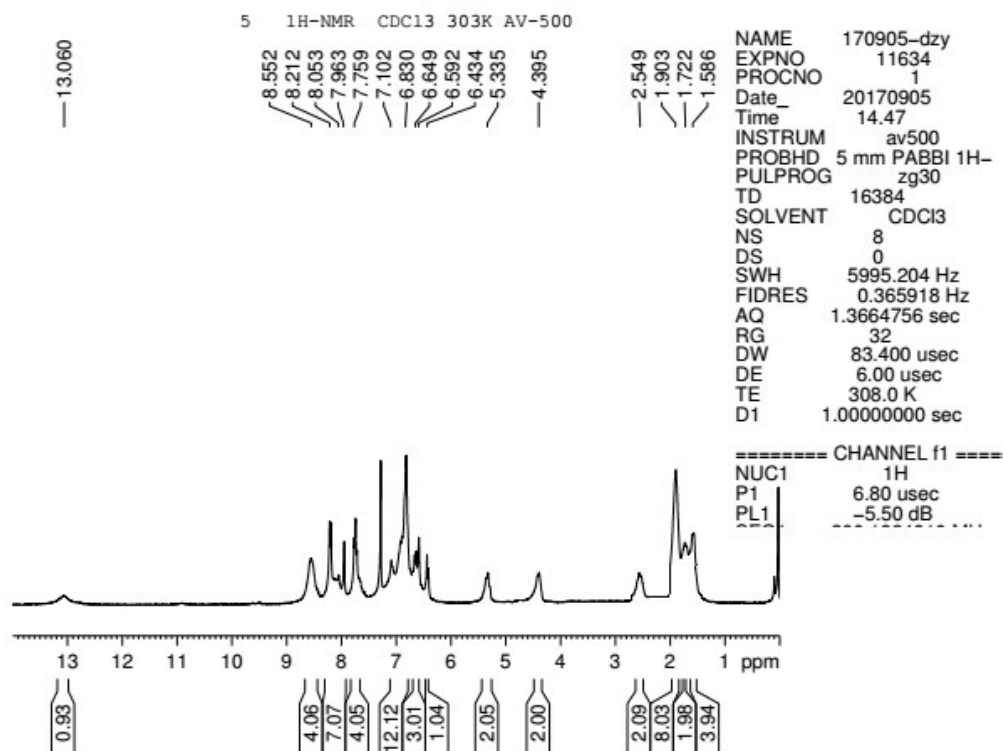


Figure S 5. ¹H NMR spectrum of 5 in CDCl₃

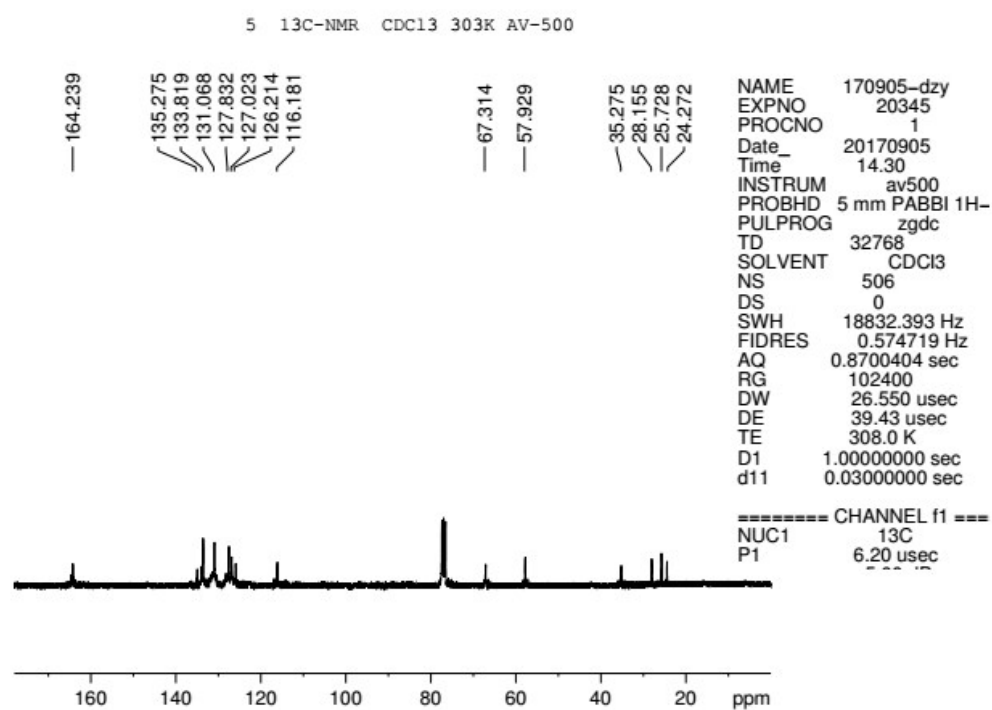


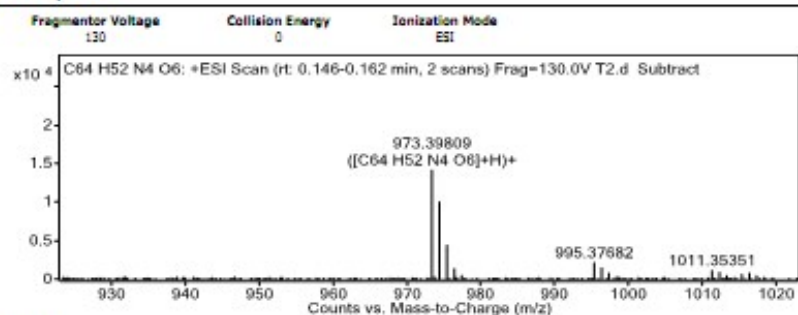
Figure S 6. ¹³C NMR spectrum of **5** in CDCl₃

Qualitative Analysis Report

Data Filename	T2.d	Sample Name	T2
Sample Type	Sample	Position	Vial 23
Instrument Name	Instrument 1	User Name	
Acq Method	method-POS.Lm	Acquired Time	9/22/2017 7:59:09 PM
IRM Calibration Status	Success	DA Method	1.m
Comment			

Sample Group	Info.		
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF 8.06.01 (B6157)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
102.1487		16006.77		
168.10322		2917.75		
196.13481	1	51451.5		
196.26824		22577.39		
295.14585		8093.16		
487.2052	2	5362.61		
487.70599	2	3630.49		
973.39809	1	14148.44	C64 H52 N4 O6	(M+H)+
974.40156	1	10034.72	C64 H52 N4 O6	(M+H)+
975.40475	1	4416.25	C64 H52 N4 O6	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	54	74
H	42	52
N	2	6
O	4	8

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Calculated Mz
C69 H52 N2 O4	FALSE	972.3912	972.3927	1.57	C69 H53 N2 O4	973.39998
C64 H52 N4 O6	TRUE	972.3912	972.3887	-2.63	C64 H53 N4 O6	973.39596

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Figure S 7. HRMS spectrum of 5

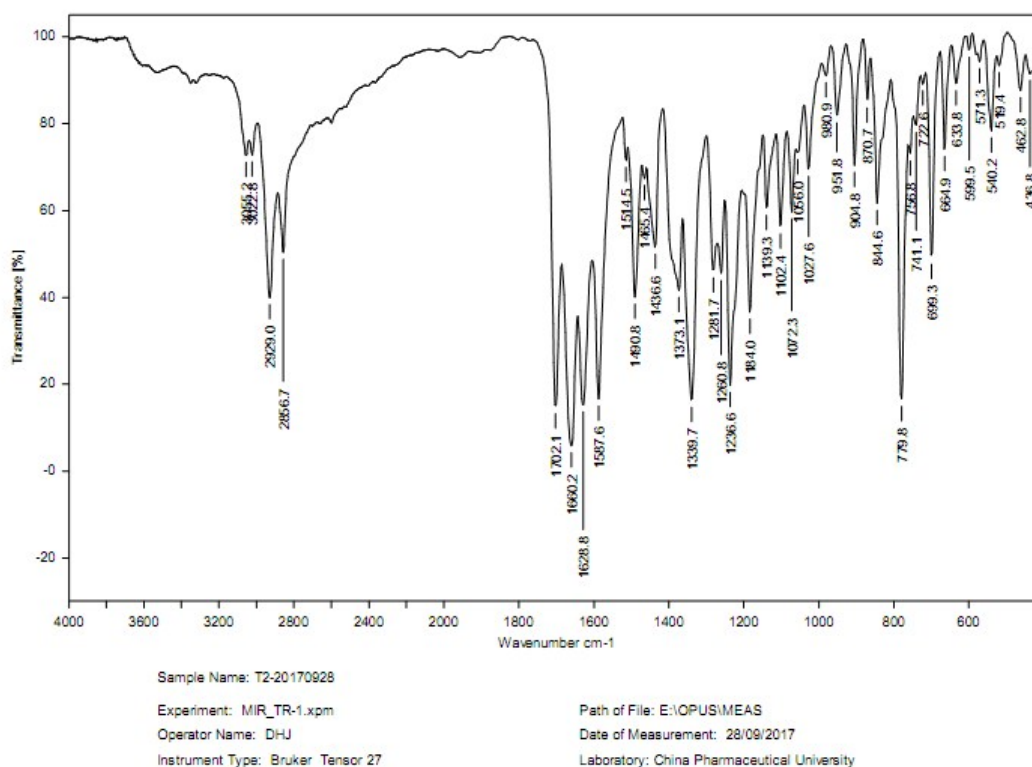


Figure S 8. IR spectrum of 5

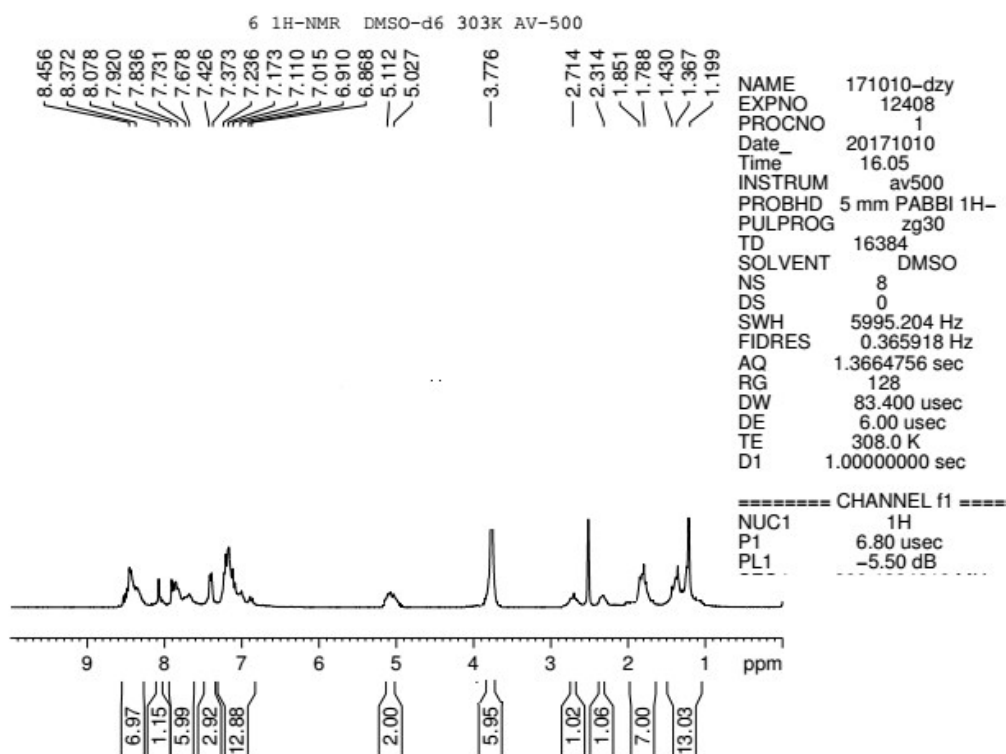


Figure S 9. ¹H NMR spectrum of 6 in DMSO-d₆

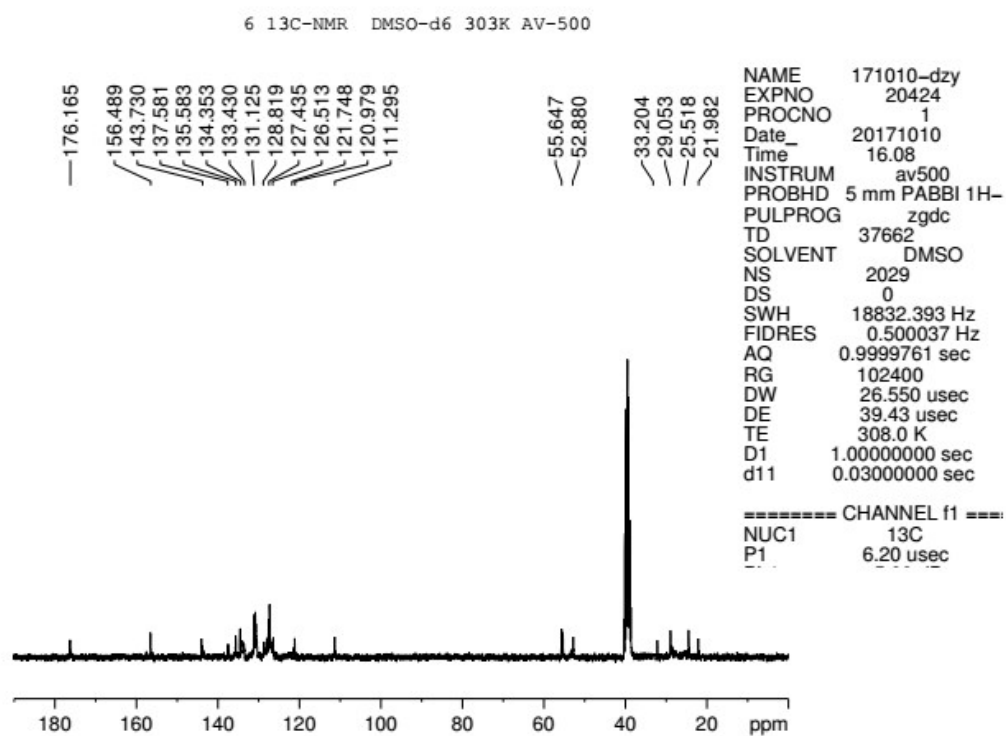


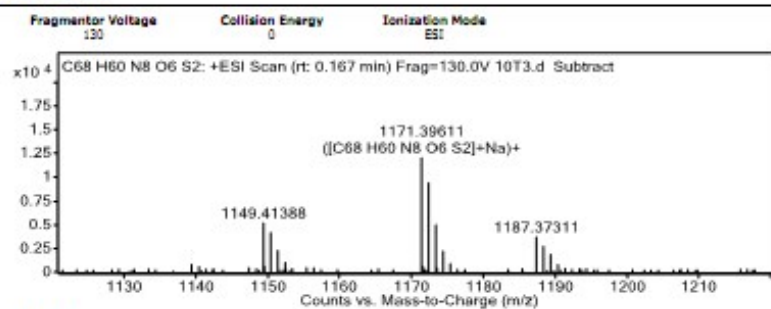
Figure S 10. ¹³C NMR spectrum of **6** in DMSO-d₆

Qualitative Analysis Report

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Sample Type	Sample	Position	Vial 1
Instrument Name	Instrument 1	User Name	
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IRM Calibration Status	Success	DA Method	1.m
Comment			

Sample Group	LC 1	Info.	6200 series TOF/6500 series
Stream Name		Acquisition SW	Q-TOF B.06.01 (B6157)
		Version	

User Spectra



Peak List

m/z	z	Abund
229.14835	1	29655.17
353.15343	1	46075.87
409.17061	1	88770.41
423.18585	1	24673.76
450.19504	1	51280.79
453.34377	1	42407.67
475.32534	1	46952.38
579.51067	1	30720.24
701.49442	1	63549.86
702.49745	1	25237.92

Formula Calculator Element Limits

Element	Min	Max
C	58	78
H	50	70
N	7	9
O	5	7
S	2	2

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Calculated Mz
C68 H60 N8 O6 S2	TRUE	1148.4069	1148.4077	0.76	C68 H60 N8 Na O6 S2	1171.39694

--- End Of Report ---

Figure S 11. HRMS spectrum of sensor 6

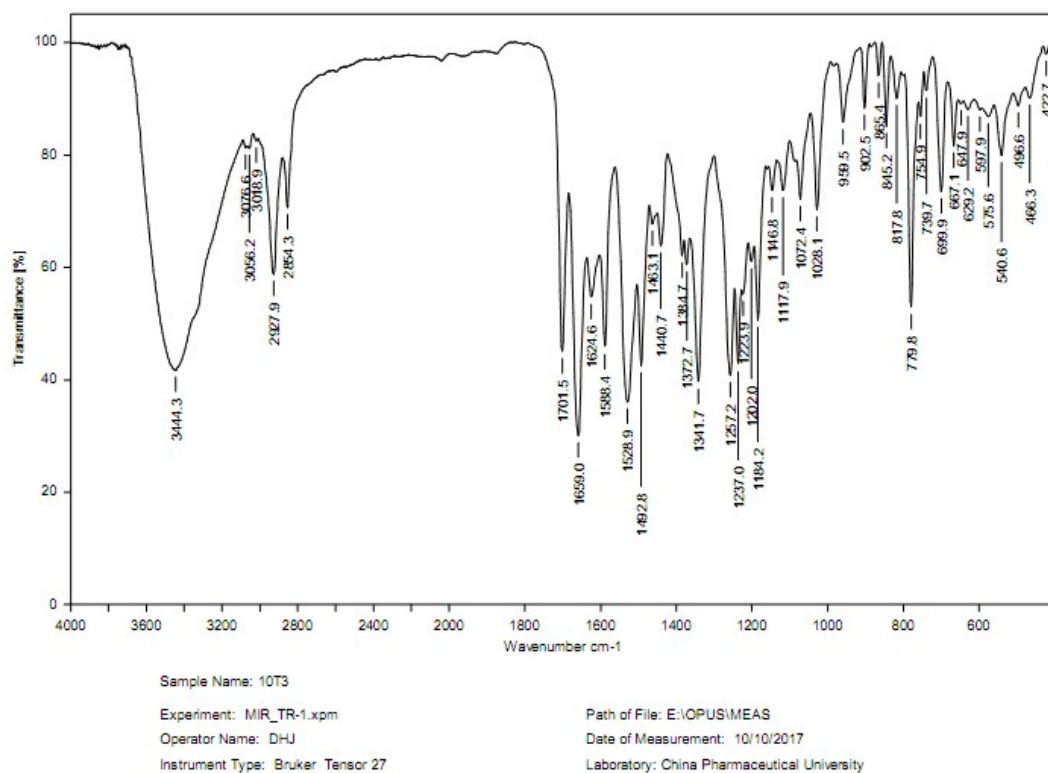
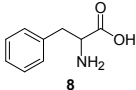
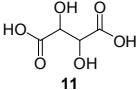
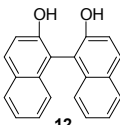


Figure S 12. IR spectrum of compound **6**

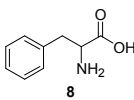
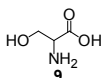
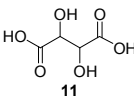
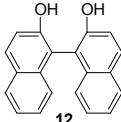
S Table1 Fluorescence intensity ratio and state of the mixture of enantiomer of analytes with **5** in mixed solvents.

Entry	Analytes	I_1 / I_2^a	State ^b	Solvent ^c
1		1.23(L/D)	Sus / Sol	4.2×10^{-4} M in THF /H ₂ O (1:1.4)
2		1.38 (L/D)	Sus / Sol	3.8×10^{-4} M in THF /H ₂ O (1:1.6)
3		1.14(L/D)	Sus / Sol	4×10^{-4} M in THF /H ₂ O (1:1.5)
4		1.17 (L/D)	Sus / Sol	4.2×10^{-4} M in THF /H ₂ O (1:1.4)
5		1.15(D/L)	Sus / Sol	4.2×10^{-4} M in THF /H ₂ O (1:1.4)
6		1.05 (R/S)	Sus / Sol	3.7×10^{-4} M in THF /H ₂ O (1:1.7)
7		1.56(S,S/ R,R)	Sus / Sol	3.9×10^{-4} M in THF /H ₂ O (1:1.6)

8		1.17 (S/R)	Sus / Sol	4×10^{-4} (1:1.5)	M in THF /H ₂ O
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^a $I_1 / I_2 = (I_1^+ - I_0) / (I_2^+ - I_0)$; (I_1^+ , I_2^+ were enantioselective fluorescent intensity values);
^bEnantiomer 1 / enantiomer 2. Abbreviations: Sus, suspension; Sol, solution; ^cVolume ratio of solvents. [5] = [analyte].

S Table2 Fluorescence intensity ratio and state of the mixture of enantiomer of analytes with 6 in mixed solvents.

Entry	Analytes	I_1 / I_2^a	State ^b	Solvent ^c
1		4.78(L/D)	Sus / Sol	4.2×10^{-4} (1:1.4)
2		1.79 (L/D)	Sus / Sol	3.8×10^{-4} M in THF /H ₂ O (1:1.6)
3		2.86(L/D)	Sus / Sol	4×10^{-4} (1:1.5)
4		1.88 (L/D)	Sus / Sol	4.2×10^{-4} (1:1.4)
5		3.79(D/L)	Sus / Sol	4.2×10^{-4} (1:1.4)
6		2.22 (R/S)	Sus / Sol	3.7×10^{-4} (1:1.7)
7		5.83(S,S/ R,R)	Sus / Sol	3.9×10^{-4} (1:1.6)
8		1.68 (S/R)	Sus / Sol	4×10^{-4} (1:1.5)

^a $I_1 / I_2 = (I_1^+ - I_0) / (I_2^+ - I_0)$; (I_1^+ , I_2^+ were enantioselective fluorescent intensity values);
^bEnantiomer 1 / enantiomer 2. Abbreviations: Sus, suspension; Sol, solution; ^cVolume ratio of solvents. [6] = [analyte].

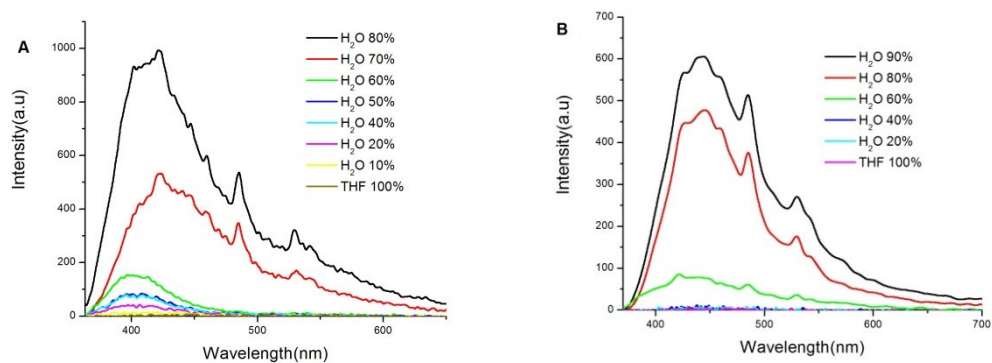


Figure S 13. Change of the fluorescence for sensors in THF with added water. Conditions: λ_{ex} 340 nm, ex / em slits 10/ 5 nm. (A: compound **5** in the mixed solvents; the concentration of **5** is 2×10^{-4} M; B: compound **6** in the mixed solvents; the concentration of **6** is 2×10^{-4} M.)

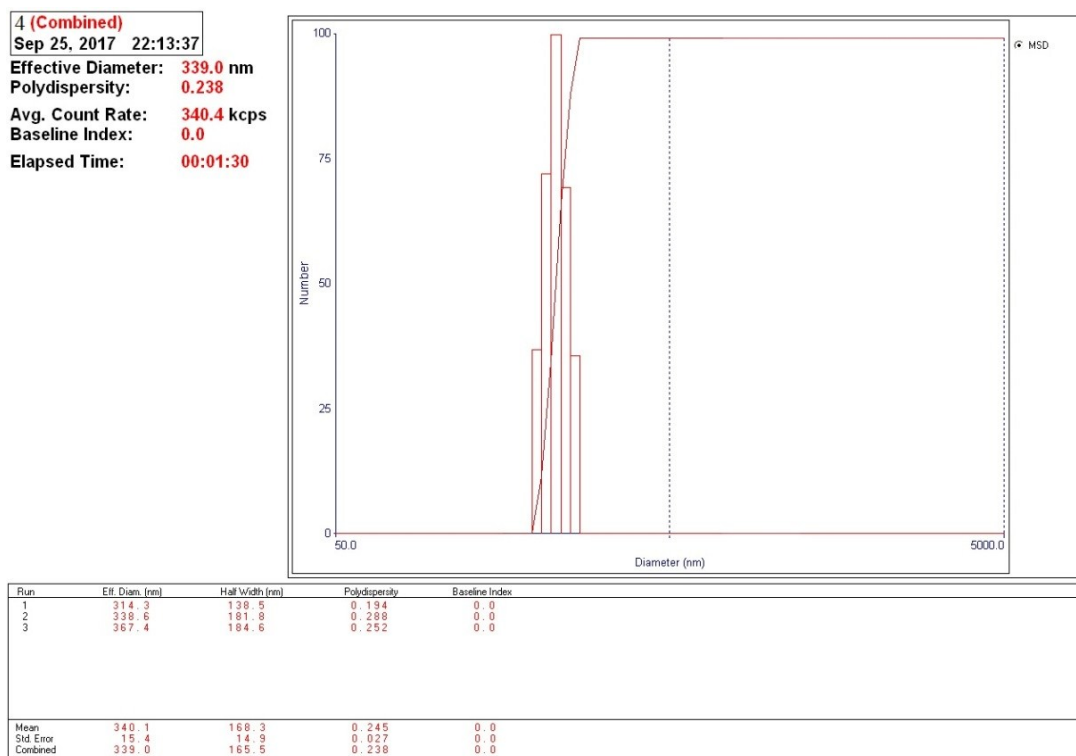


Figure S 14. Dynamic light scattering (DLS) diagrams of solution of sensor **4** in water/ THF (9/1) at room temperature (2×10^{-4} M).

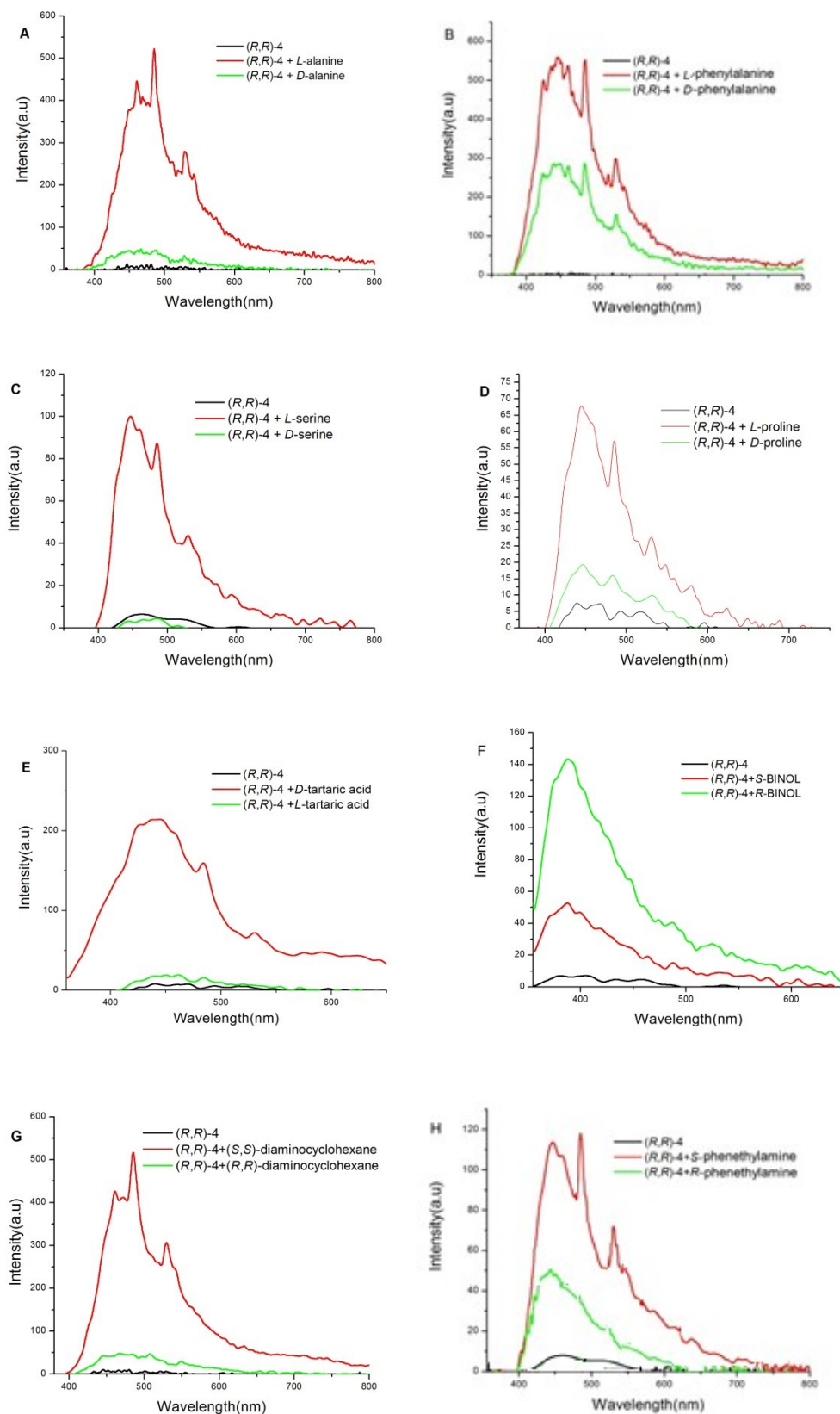


Figure S 15. The fluorescence spectrum for the mixture of guests and sensor **4** in solvents; Conditions: λ_{ex} 340 nm, ex / em slits 10/ 5 nm. A) 4.17×10^{-4} M in THF /H₂O (1:1.4); B) 3.85×10^{-4} M in THF /H₂O (1:1.6); C) 4×10^{-4} M in THF /H₂O (1:1.5); D) 4.17×10^{-4} M in THF /H₂O (1:1.4); E) 4.17×10^{-4} M in THF /H₂O (1:1.4); F) 3.7×10^{-4} M in THF /H₂O (1:1.7); G) 4.17×10^{-4} M in THF /H₂O

(1:1.4); H) 4×10^{-4} M in THF / H₂O (1:1.5).

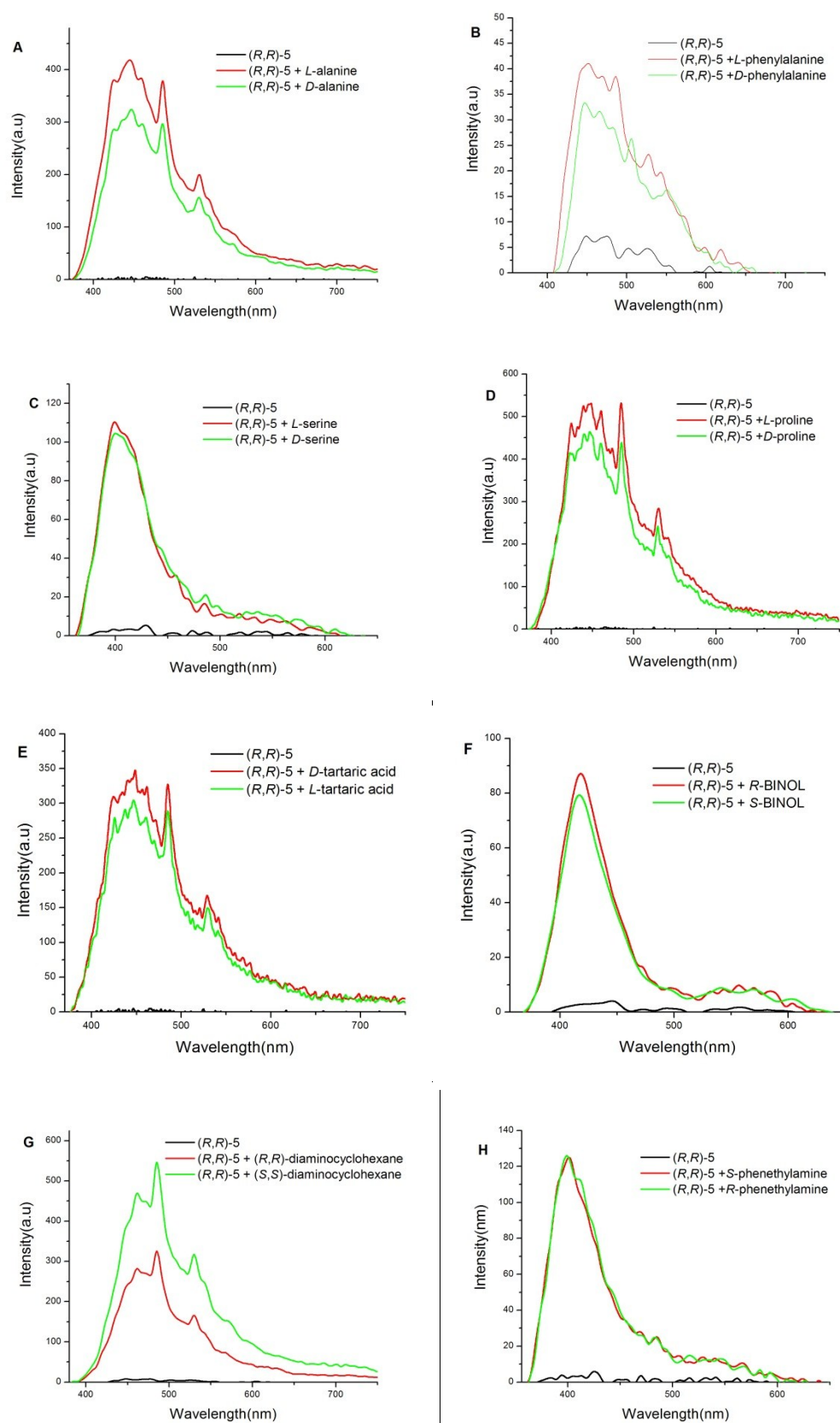


Figure S 16. The fluorescence spectra of the mixture of enantiomers and sensor **5** in solvents; Conditions: λ_{ex} 340 nm, ex / em

slits 10/ 5 nm. A) 4.17×10^{-4} M in THF /H₂O (1:1.4); B) 3.85×10^{-4} M in THF /H₂O (1:1.6); C) 4×10^{-4} M in THF /H₂O (1:1.5); D) 4.17×10^{-4} M in THF /H₂O (1:1.4); E) 4.17×10^{-4} M in THF /H₂O (1:1.4); F) 3.7×10^{-4} M in THF /H₂O (1:1.7); G) 4.17×10^{-4} M in THF /H₂O (1:1.4); H) 4×10^{-4} M in THF / H₂O (1:1.5).

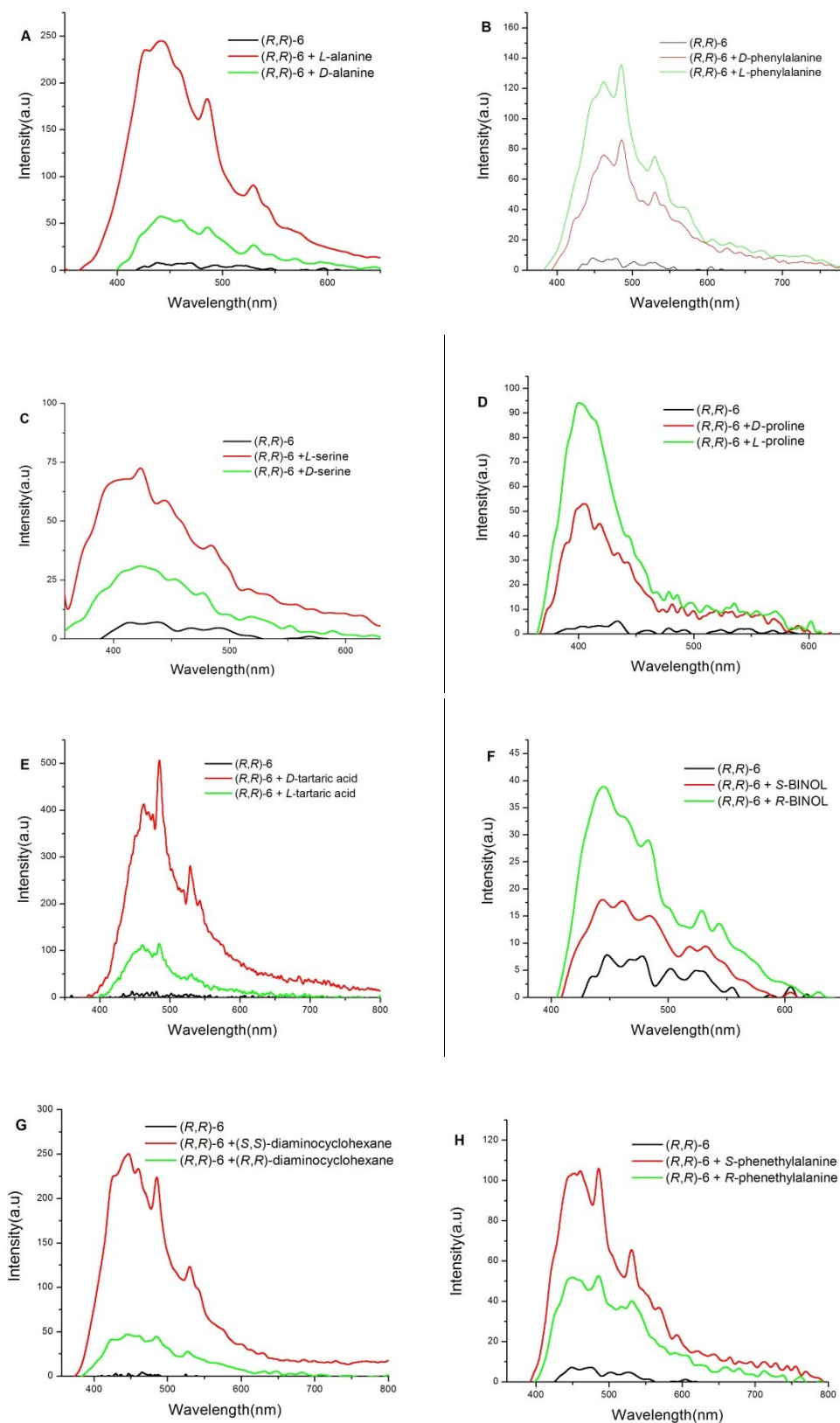


Figure S 17. The fluorescence spectra of the mixture for enantiomers and sensor **6** in solvents; Conditions: λ_{ex} 340 nm, ex / em slits 10/ 5 nm. A) 4.17×10^{-4} M in THF /H₂O (1:1.4); B) 3.85×10^{-4} M in THF /H₂O (1:1.6); C) 4×10^{-4} M in THF /H₂O (1:1.5); D) 4.17×10^{-4} M in THF /H₂O (1:1.4); E) 4.17×10^{-4} M in THF /H₂O (1:1.4); F) 3.7×10^{-4} M in THF /H₂O (1:1.7); G) 4.17×10^{-4} M in THF /H₂O (1:1.4); H) 4×10^{-4} M in THF / H₂O (1:1.5).

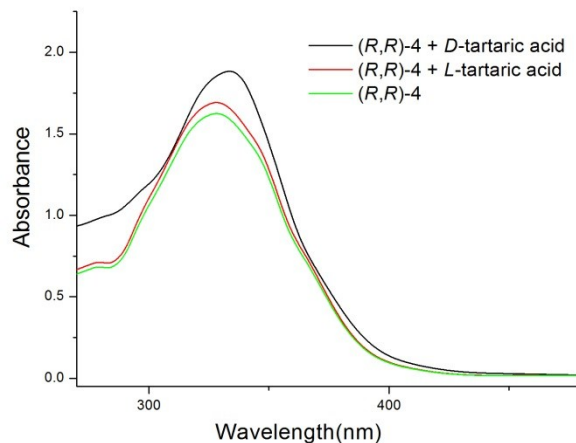


Figure S 18 The UV-vis spectra for the mixture of sensor **4** with *D* and *L* tartaric acid in THF/ H₂O (1/1.6) (2×10^{-5} M). The vertical axis is Absorbance; the horizontal axis is Wavelength (nm).

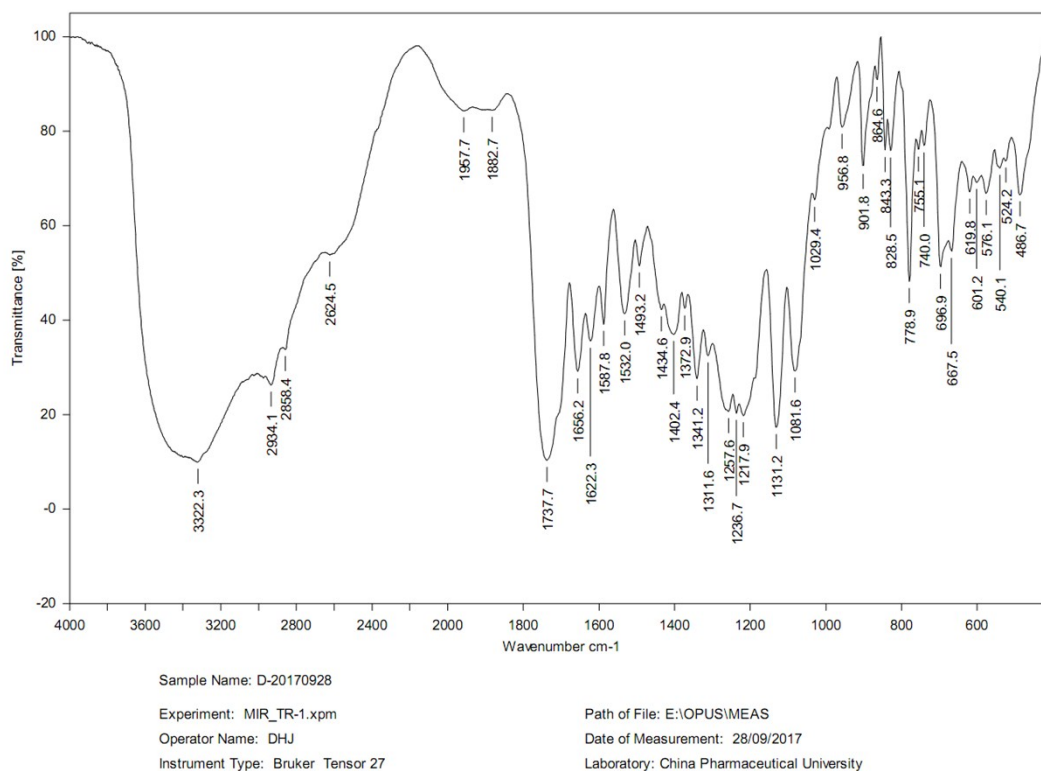


Figure S 19. IR spectra for the complex of sensor **4** and *D*-tartaric acid

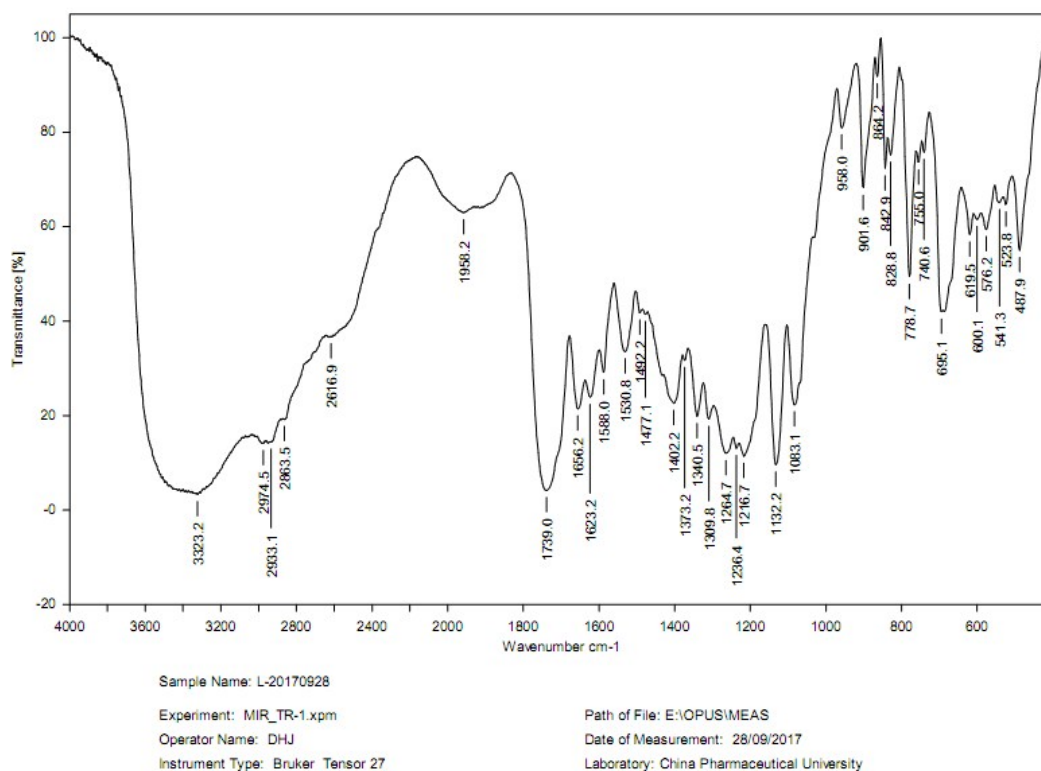


Figure S 20. IR spectra for the complex of sensor **4** and *L*-tartaric acid

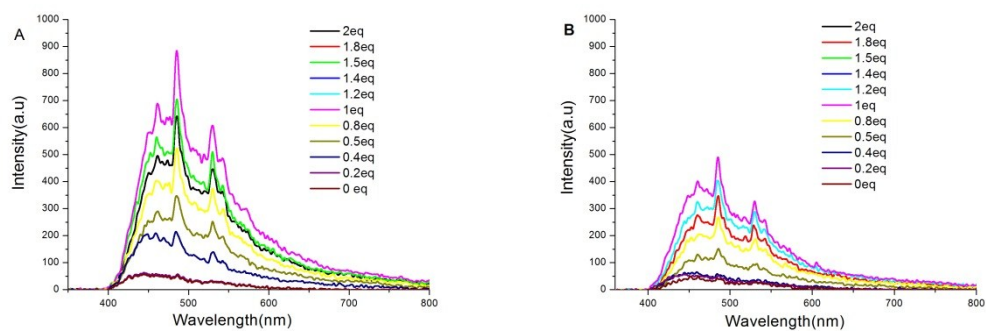
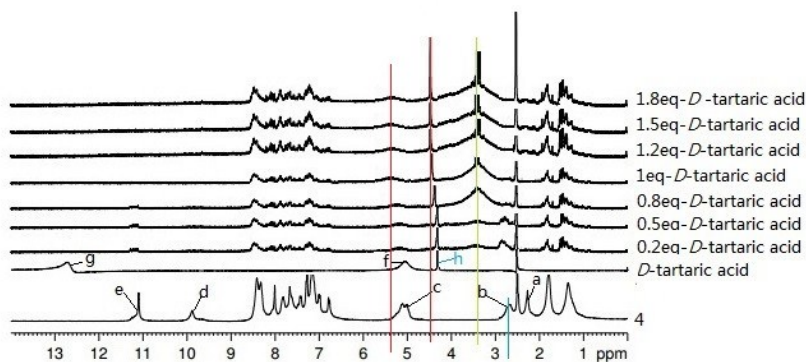


Figure S 21. Fluorescence spectra of titration experiment for sensor **4** and tartaric acid. The molar ratios between sensor **4** and tartaric acid ranging from 1: 0 to 1: 2 in mixed solvent of THF and water (volume ratio of THF: water is 1/1.6; the concentration of sensor **4** is 2×10^{-5} M). (A: Fluorescence spectra of **4** and *D*-tartaric acid; B: Fluorescence spectra of **4** and *L*-tartaric acid.)

A



B

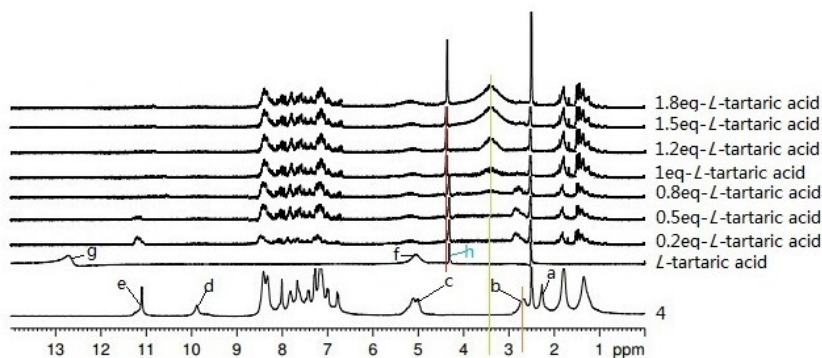
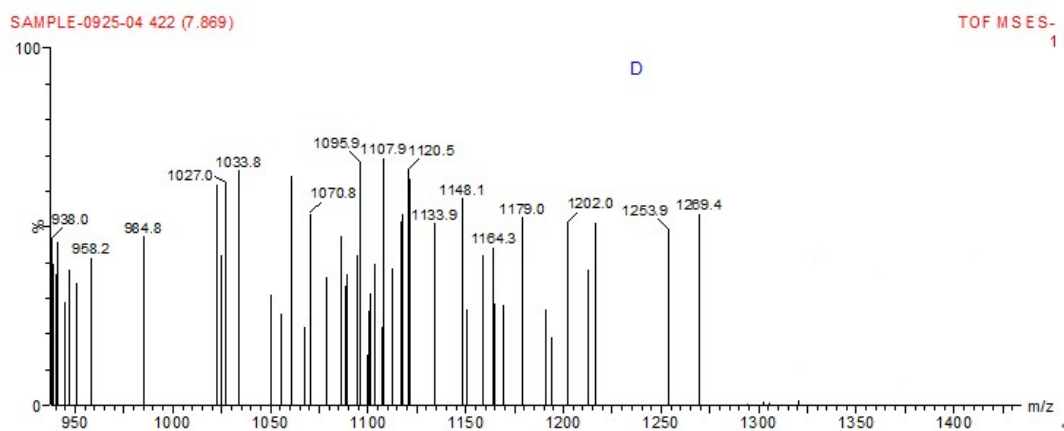


Figure S 22. Changes in the ^1H NMR spectra of (R,R) -4 with increasing tartaric acid in $\text{DMSO}-d_6$, $[(R,R)$ -4] = 2×10^{-5} M; the number over the spectrum is the molar ratio of tartaric acid to (R,R) -4.



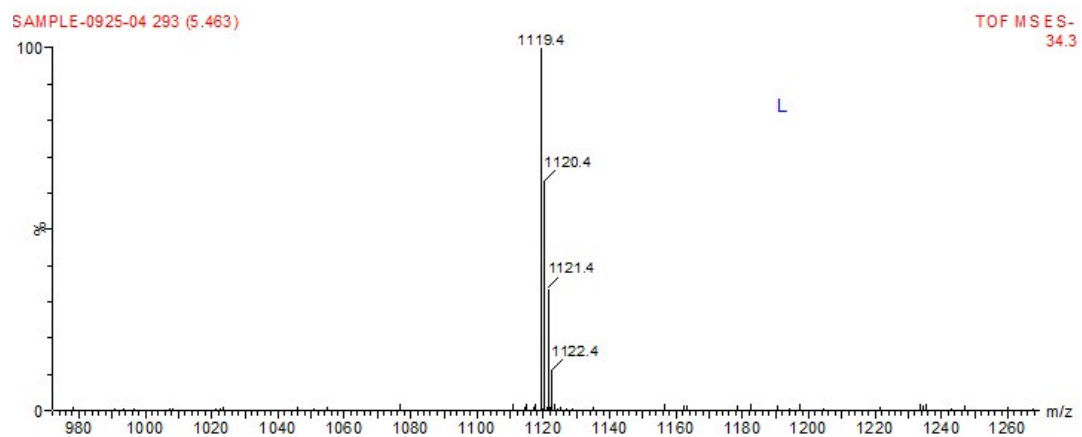


Figure S 23. The electrospray ionization mass spectrometry (ESI-MS) spectra of sensor **4** and tartaric acid (the complex ratio is 1:1)