Supplementary Materials: of

Spectroscopic Study of a Novel Binaphthyl Amine Fluorescent Probe for Chiral Recognition of D/L-Lysine

Figure S1：Fluorescence spectra of (L, R)-1 blank group at a concentration of 2μM, as well as the groups containing 100-fold equivalent amounts of D-Lys and L-Lys.

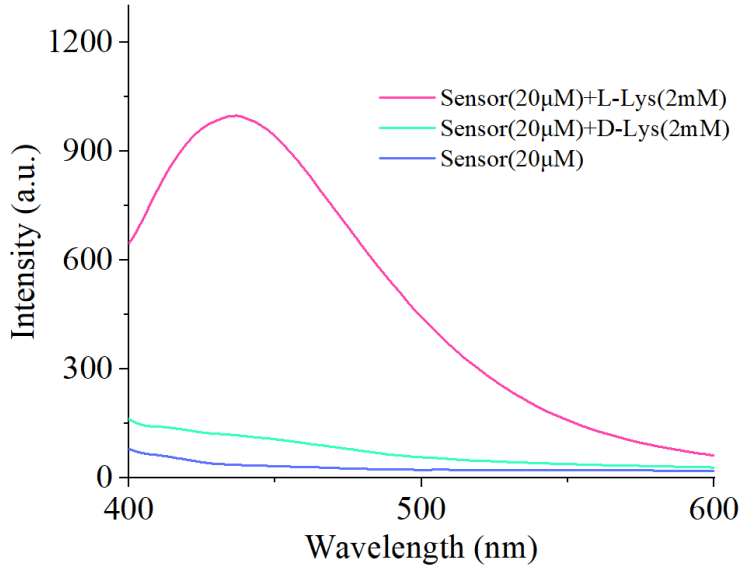


Figure S2：UV absorption spectra under working conditions of (L, R)-1 as well as absorption spectra at the same concentration without adding L-lysine.

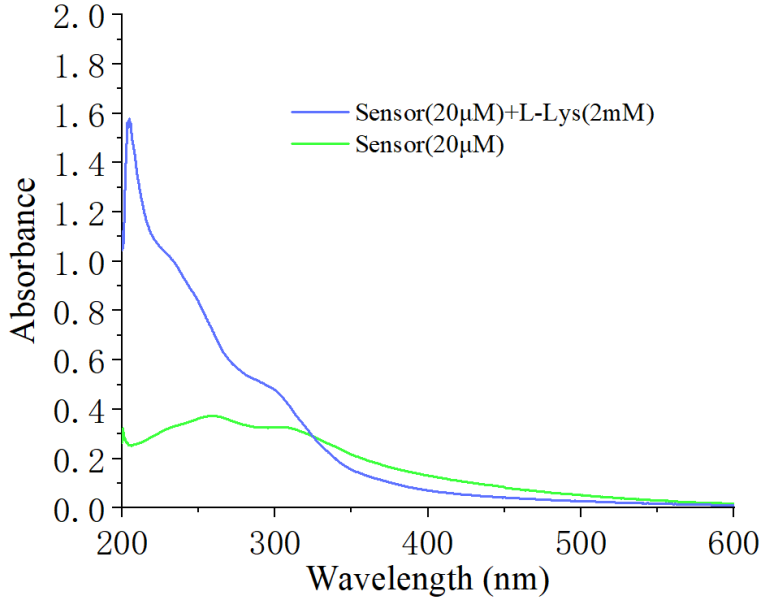


Table S1： The method of calculating the enhancement factor (ef) values through the ratio of I/I_0 and the ef values for three amino acids are presented. The fluorescence intensity of amino acids that do not react with the probe is close to the fluorescence intensity of the probe itself, hence calculating the ef value is meaningless. Notably, the four probes do not recognize D-Trp, making the calculation of the ef value for Trp highly erroneous. Additionally, (L, R)-1 does not recognize D/L-His, thus the highlighted five values are meaningless.

$$ef = \frac{\Delta I_L}{\Delta I_D} = \frac{I_L - I_0}{I_D - I_0} = \frac{\frac{I_L - I_0}{I_0}}{\frac{I_D - I_0}{I_0}} = \frac{\frac{I_L}{I_0} - 1}{\frac{I_D}{I_0} - 1}$$

	(D, R)-1	(D, S)-1	(L, R)-1	(L, S)-1
Lys	9.97	9.12	15.29	10.43
His	3.03	2.66	0.15	2.82
Trp	14.45	24.18	24.77	4.97

Figure S3： At room temperature, in PBS buffer (1% V/V EtOH) with a pH of 3-9, the fluorescent response of (D/L, R/S)-1 (0.02 mM) upon recognizing 100 equivalents of D-Lys is observed. The probe still does not recognize D-Lys after changing the pH.

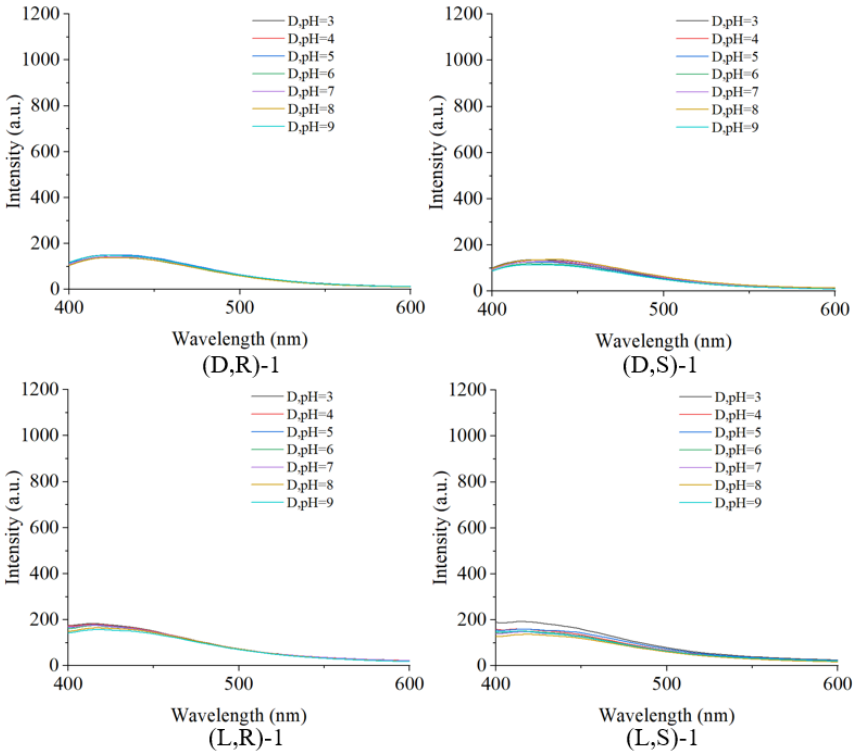


Figure S4：In PBS buffer (pH=7.4, 1% V/V EtOH), the fluorescence response of (D/L, R/S)-1 (0.02 mM) to the concentration gradient recognition of 1 to 50 equivalents of D-Lys is observed. After changing the concentration, the probe still does not recognize D-Lys.

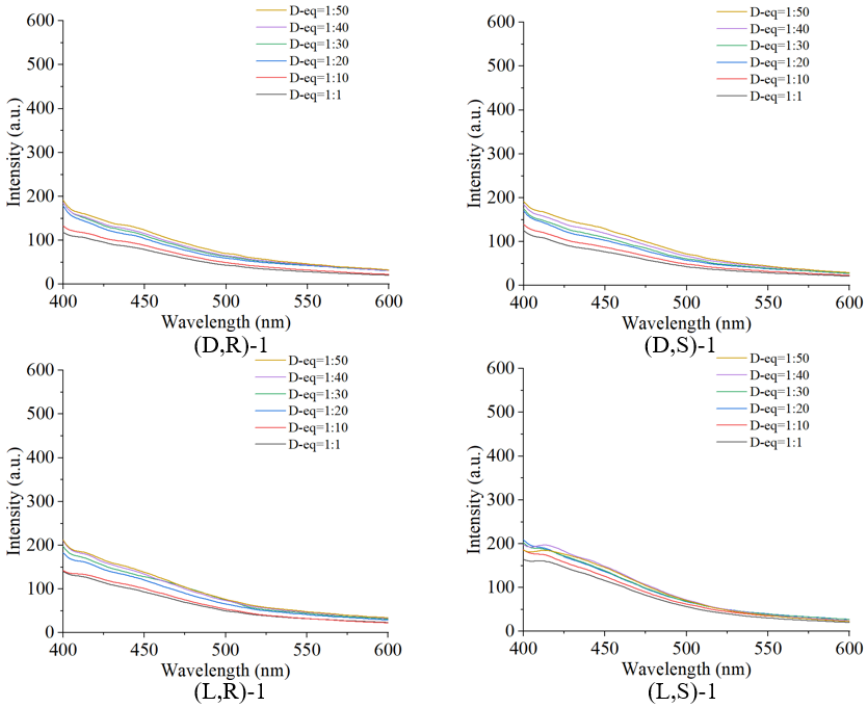


Figure S5：In PBS buffer (pH 7.4, 1% V/V EtOH), upon the addition of 2 equivalents of metal ions Co^{2+}, Fe^{2+}, Fe^{3+}, Mn^{2+}, Pd^{2+}, Ru^{3+}, Zn^{2+}, Sn^{2+}, Ca^{2+} to (D/L, R/S)-1 (0.02 mM), the fluorescence response when recognizing 100 equivalents of D-Lys is observed. Even after the addition of metal ions, the probe still does not recognize D-Lys.

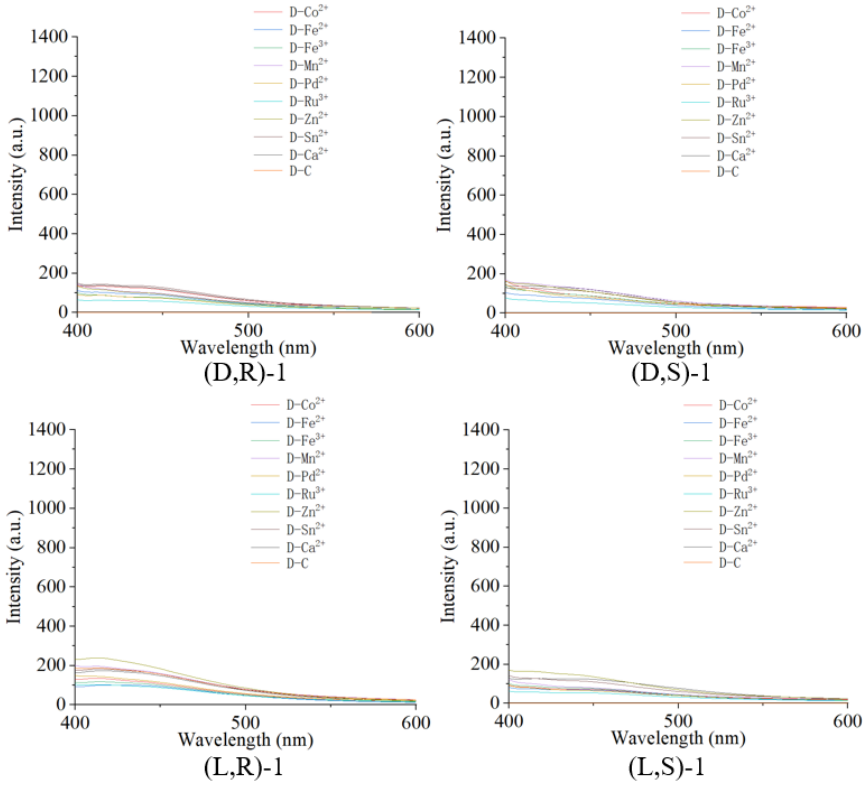


Figure S6：(a) UV absorption spectra of sulfate quinine at concentrations of 2μM, 2μM, 6μM, 8μM, and 10μM. Solvent: 1N H_2SO_4.（b）Absorbance intensity plot at 329 nm. The adjusted R-squared of the linear fitting equation is 0.990.

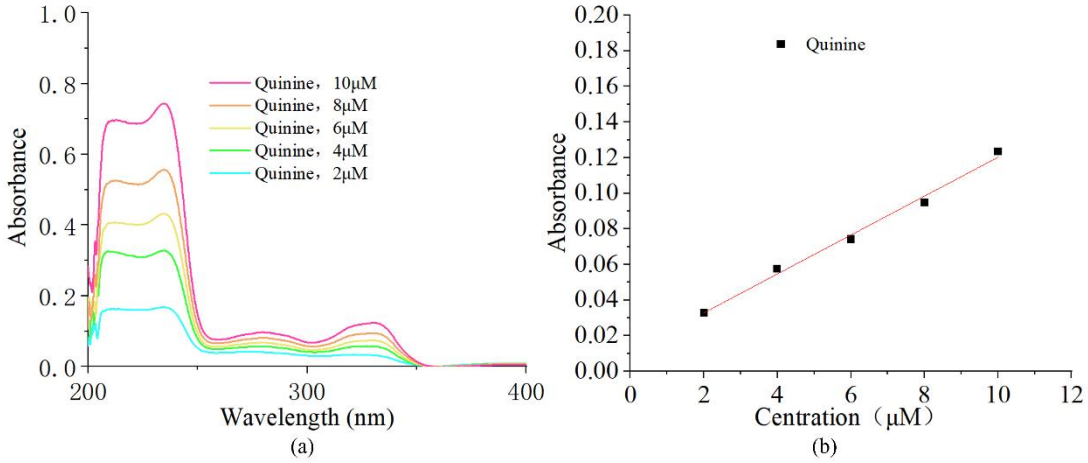


Figure S7：(a) UV absorption spectra of (L, R)-1 at concentrations of 2μM, 2μM, 6μM, 8μM, and 10μM. The concentration of L-lysine in each sample is 100 times that of the probe. Solvent: 1% EtOH (v/v) in PBS, pH=7.4.（b）Absorbance intensity plot at 329 nm. The adjusted R-squared of the linear fitting equation is 0.981.

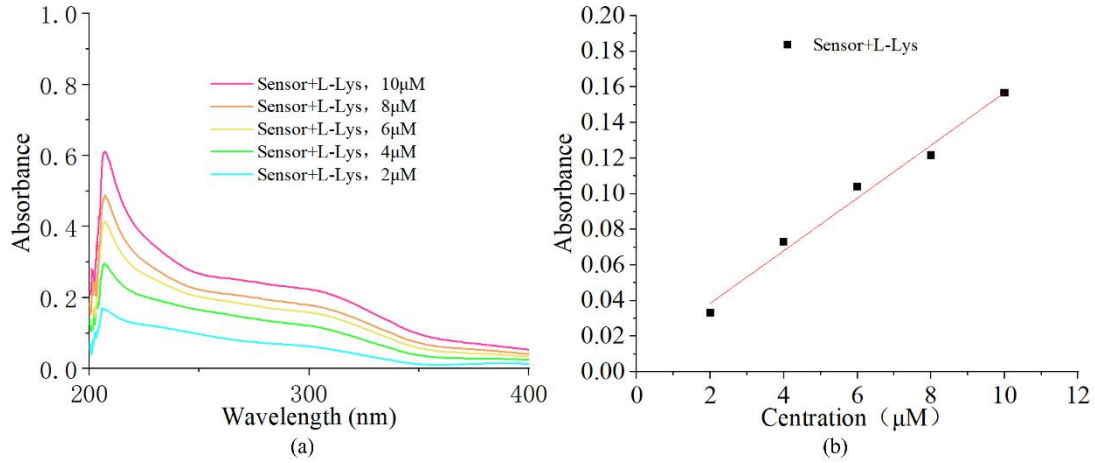


Figure S8：The fluorescence spectrum of quinine sulfate excited at 329 nm.

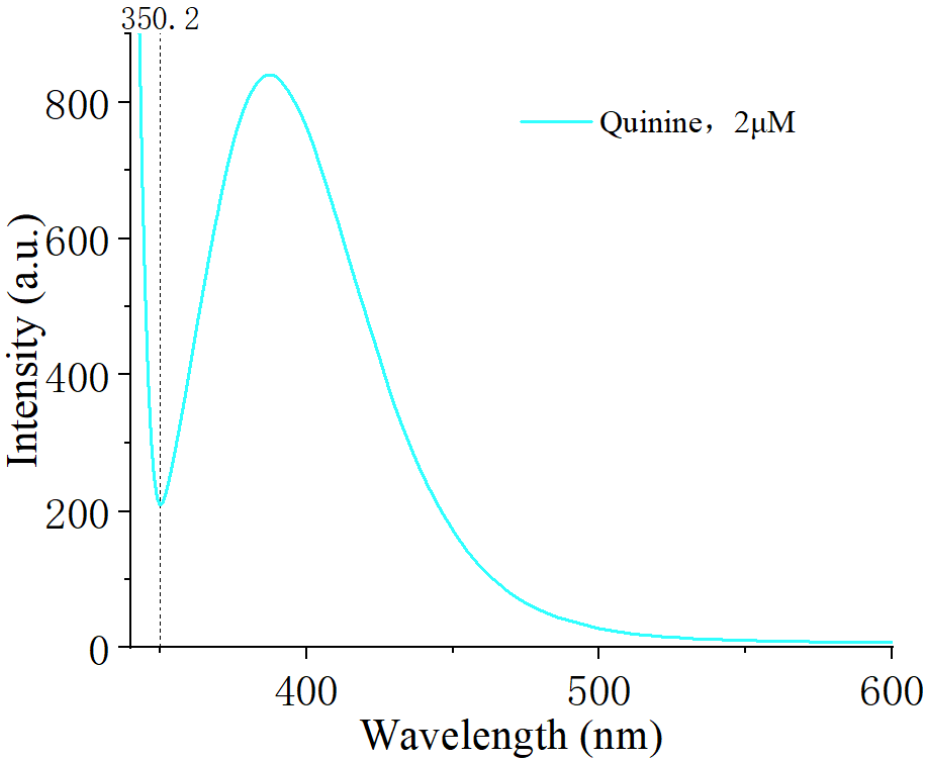


Figure S9：^{1}H NMR spectra of R/S-1.（400M DMSO）

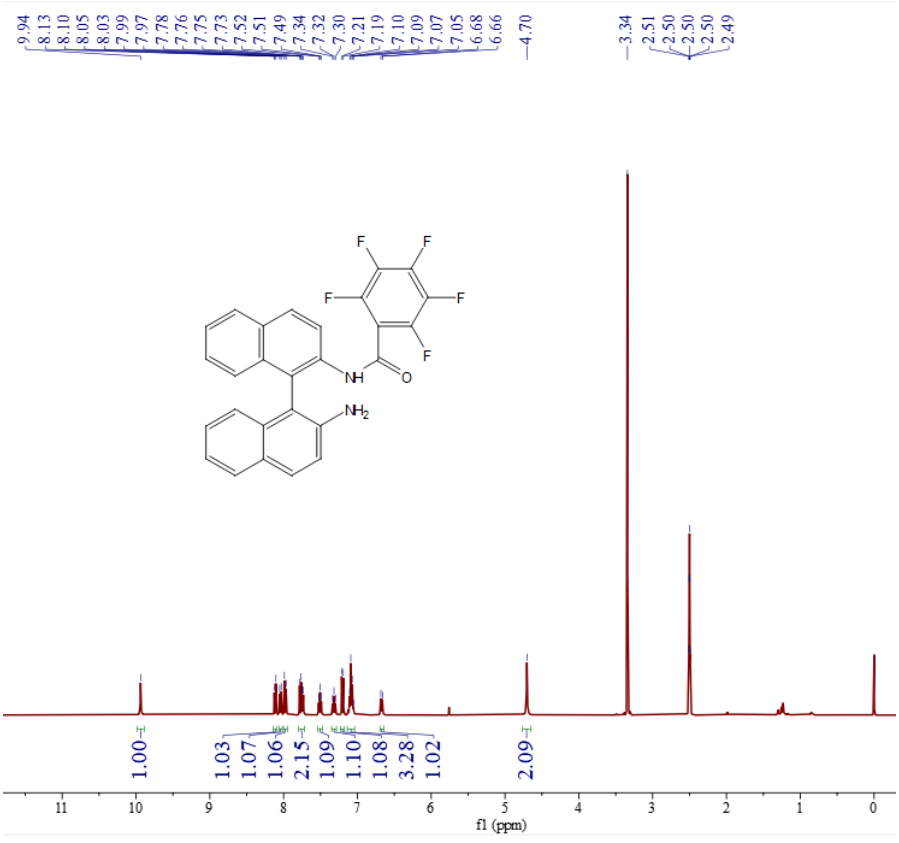
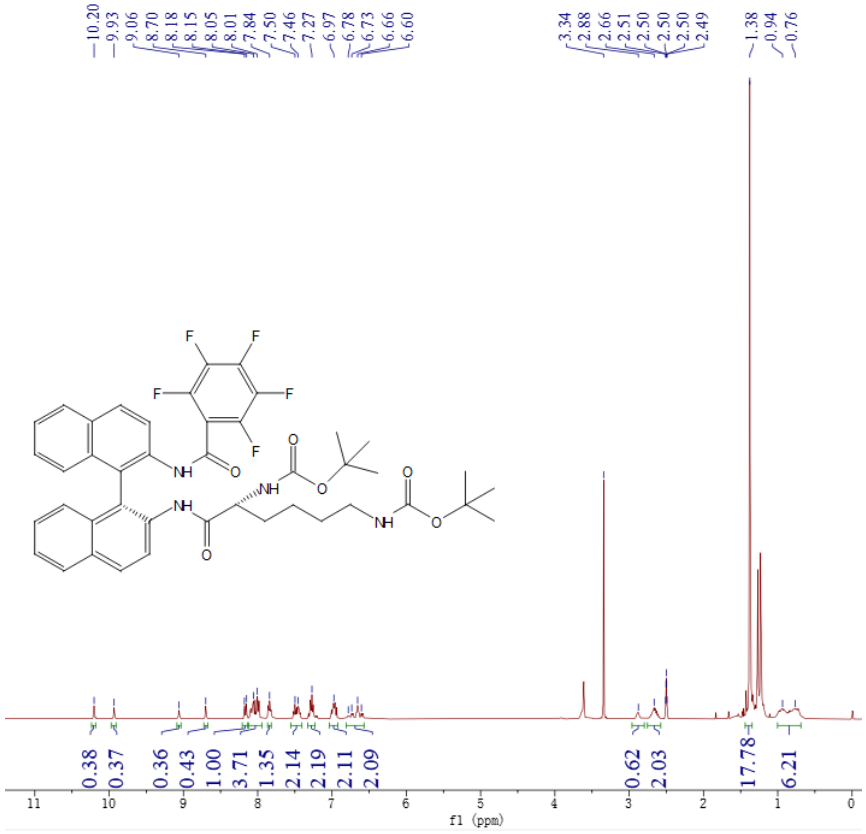
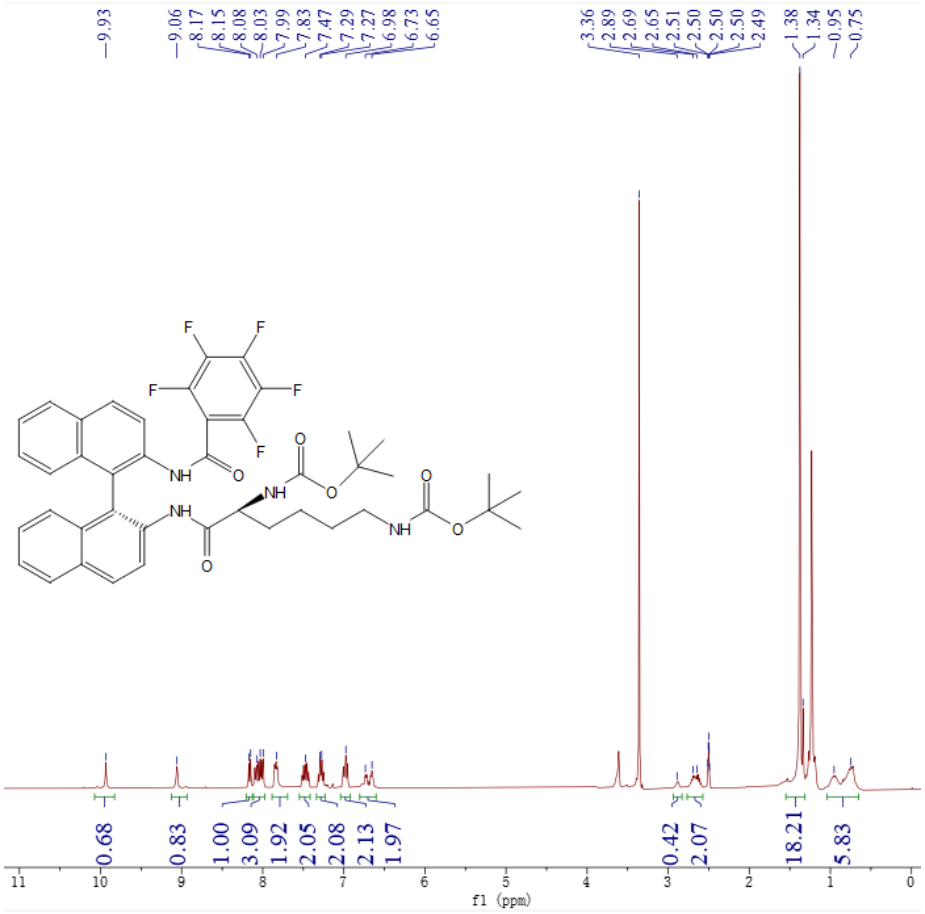


Figure S10：^{1}H NMR spectra of (D/L，R/S)-1.（400M DMSO）




9.93
9.06
8.17
8.15
8.08
8.03
7.99
7.83
7.47
7.29
7.27
6.98
6.73
6.65
3.36
2.89
2.69
2.65
2.51
2.50
2.50
2.50
2.49
1.38
1.34
0.95
0.75
F
F
F
F
F
NH
O
NH
O
O
O
NH
O
NH
O
0.68
0.83
1.00
3.09
1.92
2.05
2.08
2.13
1.97
0.42
2.07
18.21
5.83
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

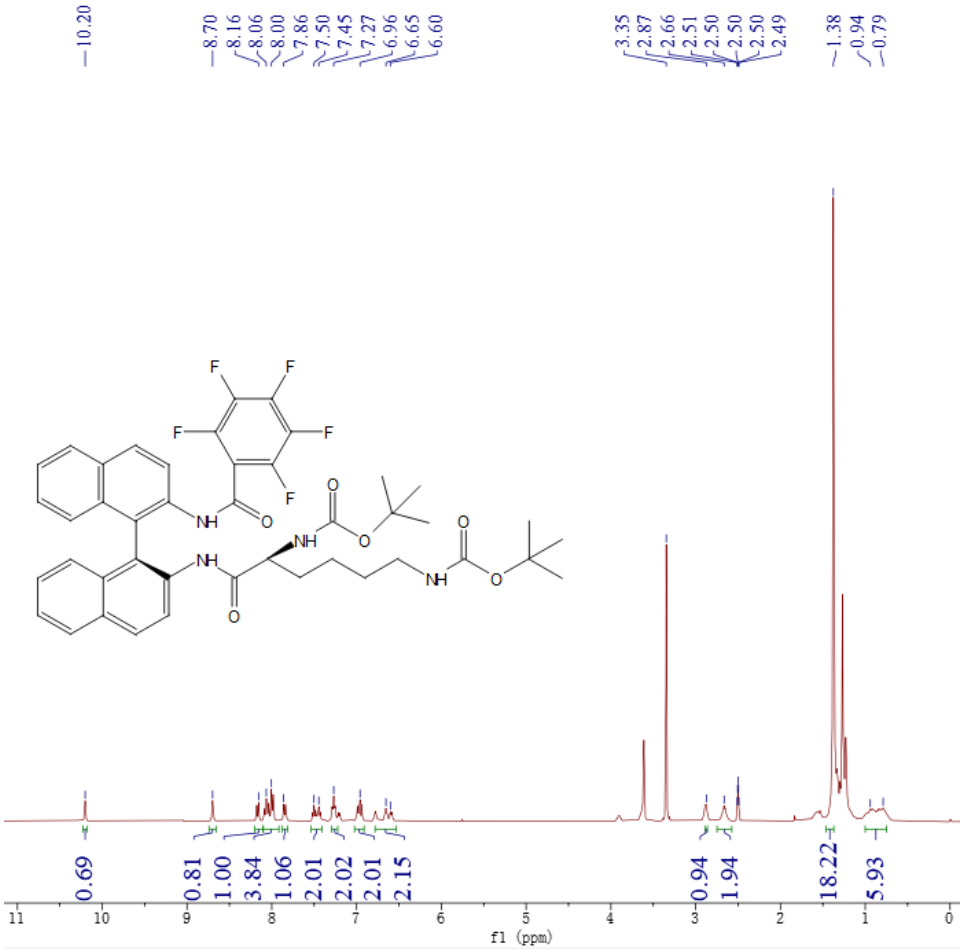
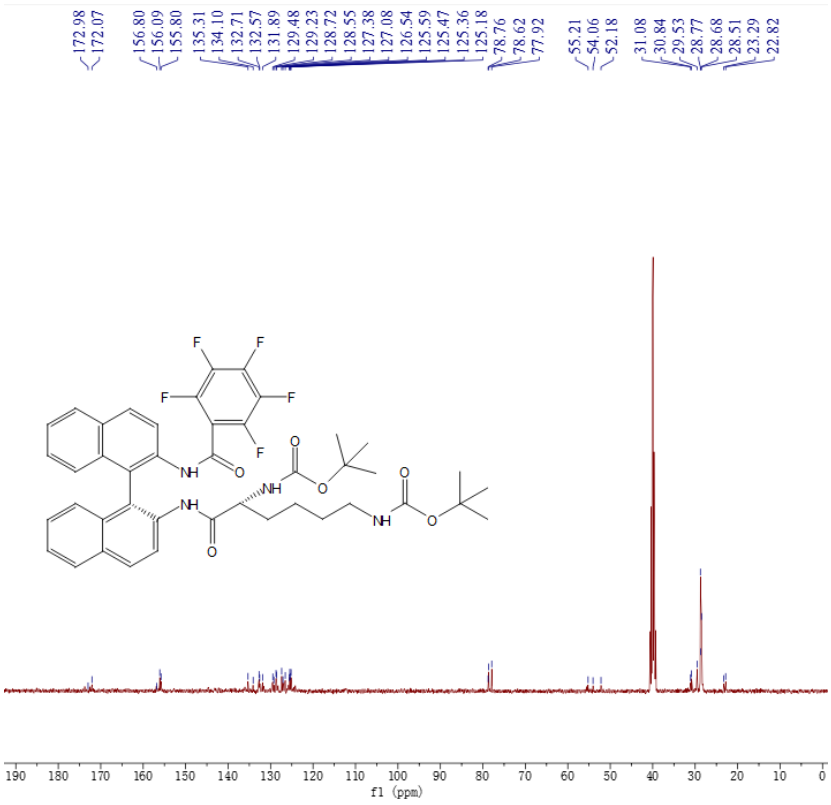
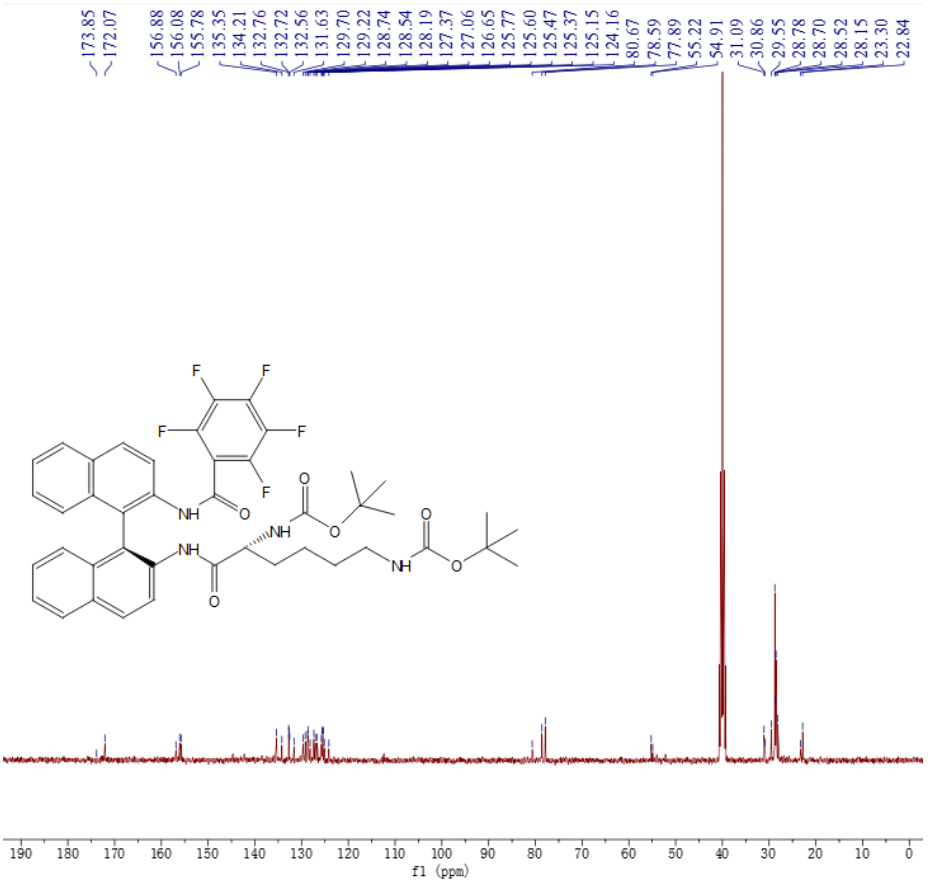
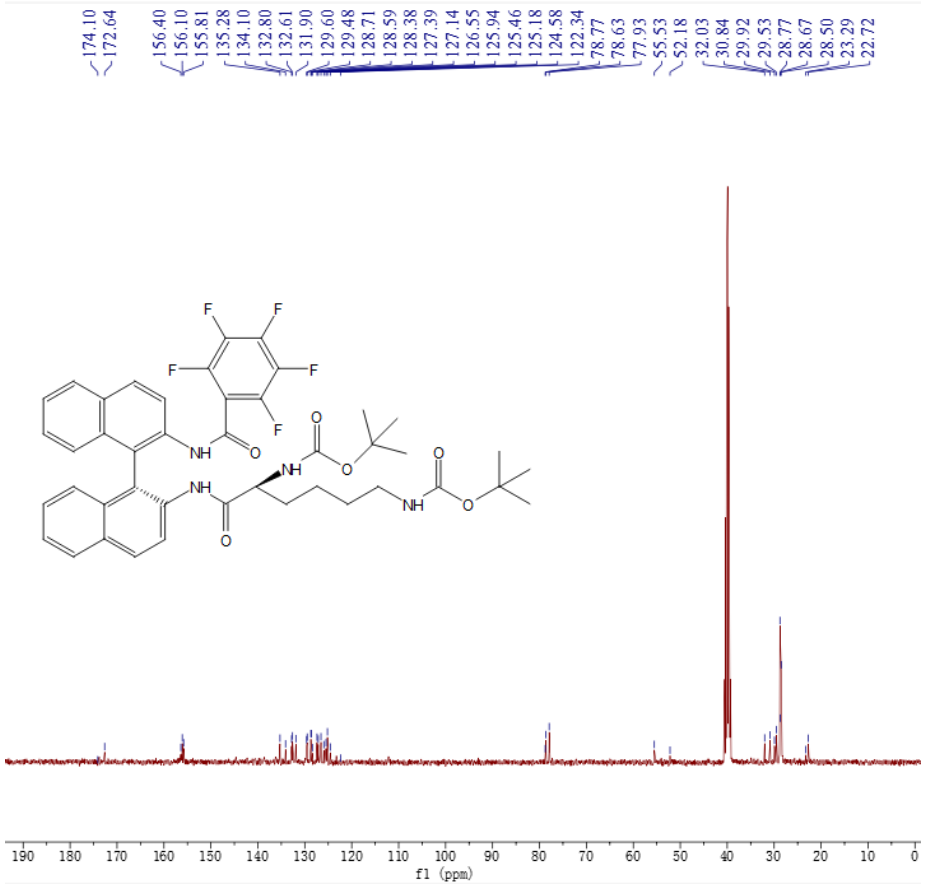


Figure S11：^{13}C NMR spectra of (D/L，R/S)-1.（400M DMSO）




173.85
172.07
156.88
156.08
155.78
135.35
134.21
132.76
132.72
132.56
131.63
129.70
129.22
128.74
128.54
128.19
127.37
127.06
126.65
125.77
125.60
125.47
125.37
125.15
124.16
80.67
78.59
77.89
55.22
54.91
31.09
30.86
29.55
28.78
28.70
28.52
28.15
23.30
22.84
F
F
F
F
F
O
NH
O
O
NH
NH
O
O
NH
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


174.10
172.64
156.40
156.10
155.81
135.28
134.10
132.80
132.61
131.90
129.60
129.48
128.71
128.59
128.38
127.39
127.14
126.55
125.94
125.46
125.18
124.58
122.34
78.77
78.63
77.93
55.53
52.18
32.03
30.84
29.92
29.53
28.77
28.67
28.50
23.29
22.72
F
F
F
F
F
O
NH
O
O
NH
NH
O
O
NH
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

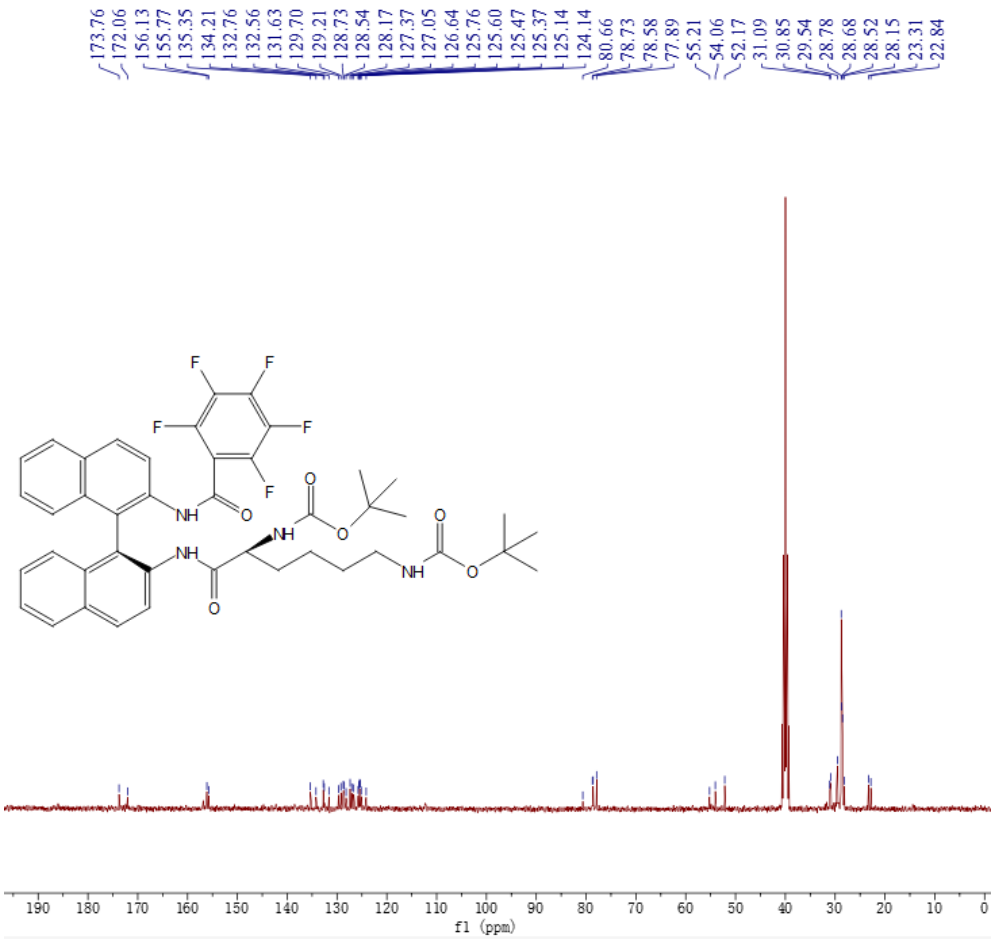
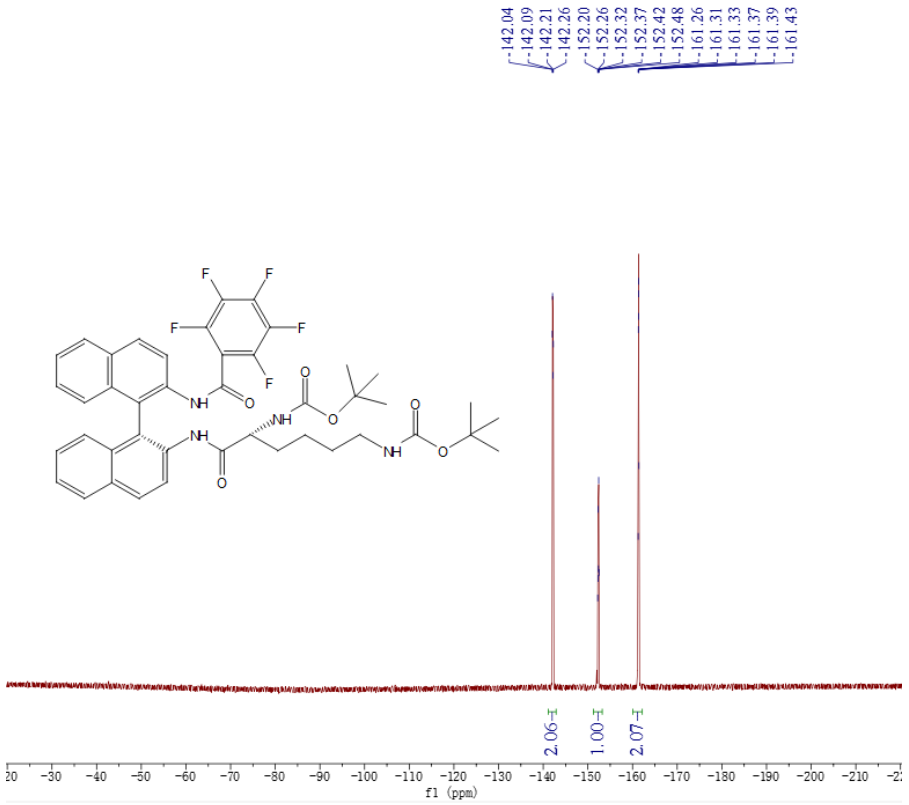


Figure S12：^{19}F NMR spectra of (D/L，R/S)-1.（400M DMSO）

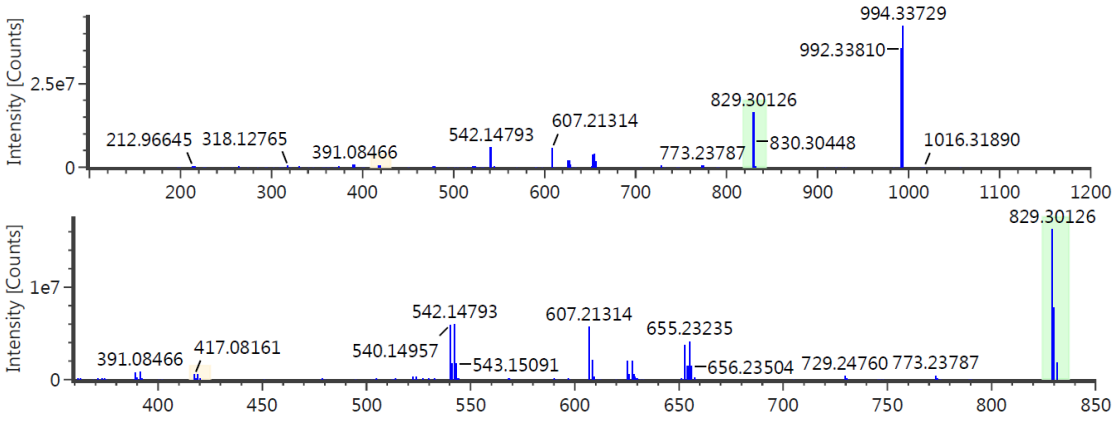



-142.03
-142.05
-142.09
-142.11
-152.35
-152.41
-152.46
-161.30
-161.32
-161.36
-161.38
-161.42
-161.44
2.09
1.00
2.10
f1 (ppm)

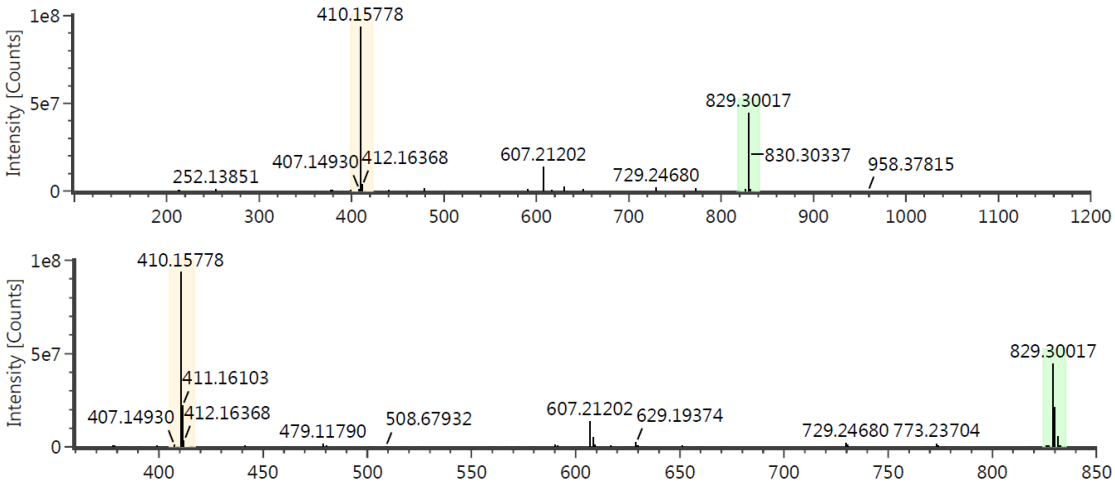

-142.01
-142.04
-142.08
-142.10
-152.37
-152.43
-152.49
-161.33
-161.37
-161.39
-161.43
2.03
1.00
2.02
f1 (ppm)

Figure S13：MS spectra of (D/L，R/S)-1.

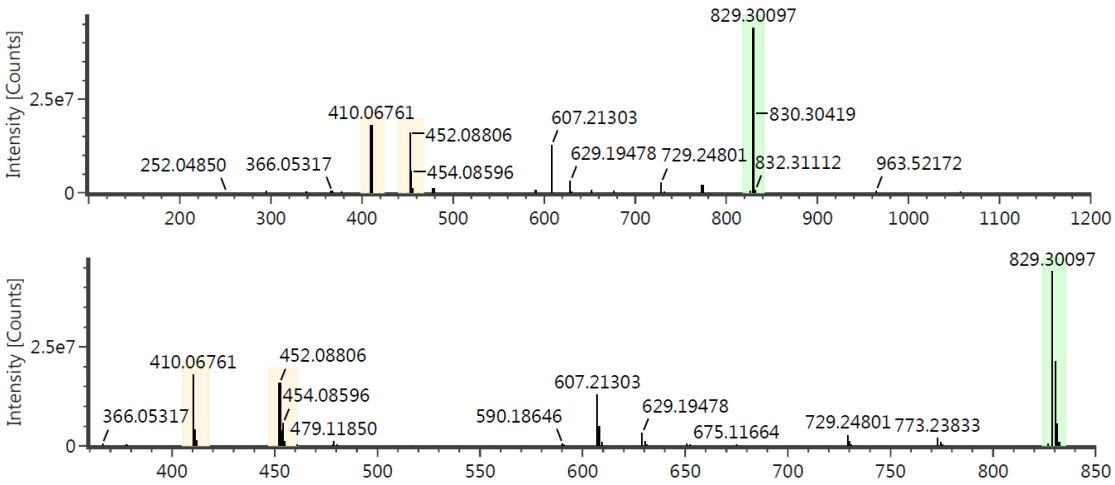
	Formula	Neutral mass	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
(D，R)-1	C43H43F5N4O6	806.31028	829.30126	1.8	2.1	5409572	+Na	Identified



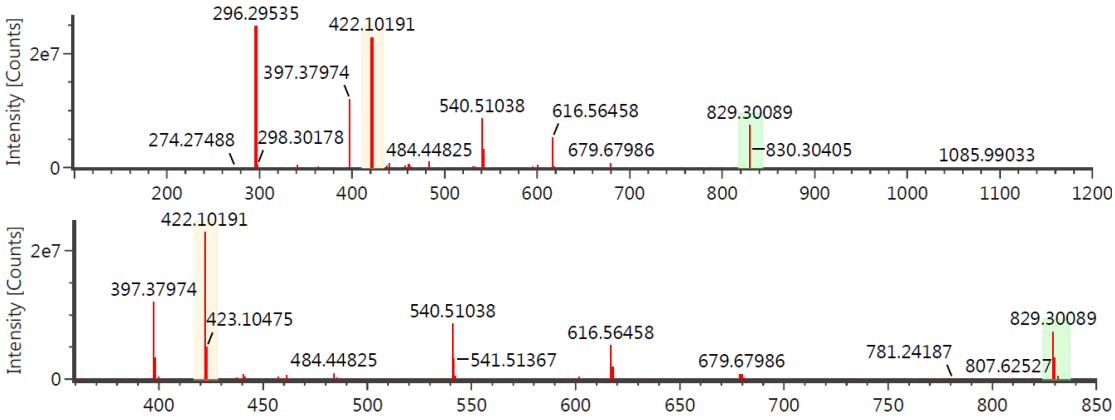
	Formula	Neutral mass	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
(D，S)-1	C43H43F5N4O6	806.31028	829.30017	0.7	0.8	14739752	+Na	Identified



	Formula	Neutral mass	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
(L，R)-1	C43H43F5N4O6	806.31028	829.30097	1.5	1.8	14596839	+Na	Identified



	Formula	Neutral mass	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
(L，S)-1	C43H43F5N4O6	806.31028	829.30089	1.4	1.7	2450287	+Na	Identified



MS Instrument Type: Waters Vion® IMS QTof	
Experiment Settings:	
Experiment type: ESI+	Scan Mode: MS
Capillary voltage: 3.0kv	Low mass: 50m/z
Soure temperature: 120°C	High mass: 2000m/z
Desolvation temperature: 450°C	Scan time: 0.200s
Cone gas: 50L/h	Desolvation gas: 800L/h