Supporting Information for

Chemoselective and Enantioselective Fluorescent Recognition of Glutamic and Aspartic Acids

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1. General Data of the Experiments, Synthesis and Characterization of Compounds, and Sample Preparation for Fluorescence Measurement

General data. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. In the optical spectroscopic studies, all the solvents were either HPLC or spectroscopic grade. ^{1}H and ^{13}C NMR spectra were measured on a Bruker AM400 NMR spectrometer. ESI-MS and HRMS spectral data were recorded on a Finnigan LCQDECA and a Bruker Daltonics Bio TOF mass spectrometer, respectively. Fluorescence spectra were obtained using Hitech F-7000 spectro fluorometer at 298 K. UV-Vis absorption spectra were recorded on a Hitachi U1900 spectrometer.

Synthesis and Characterization of (*S*)-2. A mixture of (*S*)-2,2'-dibromomethyl-1,1'-binaphthalene (590 mg, 1.3 mmol) and $NaHCO_3$ (563 mg, 6.7 mmol, 5 equiv) in DMSO (20 mL) was heated at 90 ℃ for 6 h under nitrogen. After the reaction was complete, it was cooled to room temperature, and the mixture was extracted with CH_2Cl_2. The organic extracts were washed with H_2O. The combined organic extracts were dried with Na_2SO_4 and the solvent was removed under reduced pressure. The residue, PCC (867 mg, 4.0 mmol, 3 equiv) and celite (867 mg) were mixed in CH_2Cl_2 (20 mL). After stirred for 3 h at room temperature, the reaction mixture was filtered through celite, and the combined organic extracts were evaporated under reduced pressure. The residue was purified by flash column chromatography on silica gel (eluted with ethyl acetate/petroleum ether, 1:10) to afford (*S*)-**2** as a white solid in 61% yield (246 mg). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.62 (s, 2H), 8.20 (d, J = 8.6 Hz, 2H), 8.13 (d, J = 8.7 Hz, 2H), 8.02 (d, J = 8.2 Hz, 2H), 7.64 (t, J = 7.5 Hz, 2H), 7.37 (t, J = 7.7 Hz, 1H), 7.23 (d, J = 8.5 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 191.1, 139.7, 135.9, 133.4, 133.2, 129.8, 129.4, 128.5, 127.9, 127.3, 122.28. HRMS: m/z calcd. for $C_{22}H_{14}O_2Na$, $M+Na^+$: 333.0981; found: 333.0981. $[\alpha]_D^{25}$ = -2.53 (c = 0.5, $CHCl_3$).

Synthesis and Characterization of (*R*)-2. (*R*)-**2** was prepared in the same way as (*S*)-**2** by starting with (*R*)-BINOL. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.62 (s, 2H), 8.20 (d, J = 8.7 Hz, 2H), 8.13 (d, J = 8.7 Hz, 2H), 8.02 (d, J = 8.2 Hz, 2H), 7.67 – 7.62 (m, 2H), 7.38 (t, J = 7.1 Hz, 2H), 7.23 (d, J = 9.3 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 191.1, 139.7, 135.9, 133.4, 133.2, 129.8, 129.4, 128.5, 127.9, 127.3, 122.3. HRMS: m/z calcd. for $C_{22}H_{14}O_2Na$, $[M+Na]^+$: 333.0981; found: 333.0984. $[\alpha]_D^{25}$ = 2.40 (c = 0.5, $CHCl_3$).

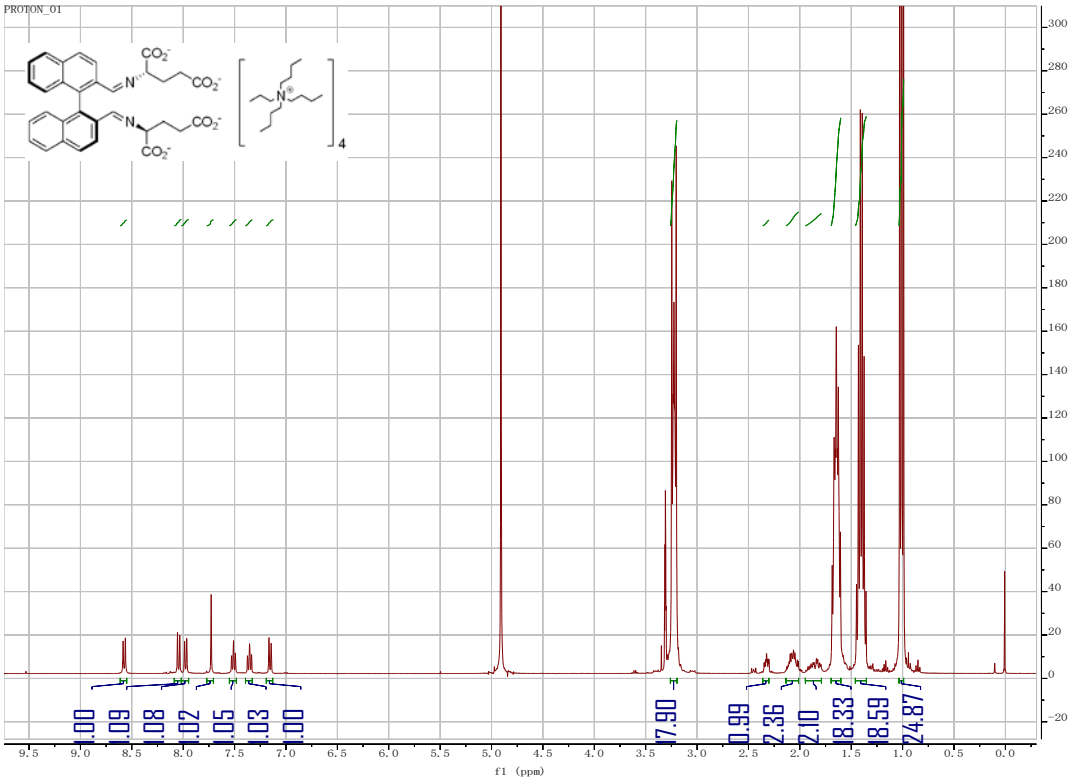
Synthesis and Characterization of (*S*)-3. A mixture of L-Glu (200 mg, 1.36 mmol) and 1 M tetrabutylammonium hydroxide solution (2.72 mL, 2.0 equiv) in MeOH (5 mL) was stirred overnight. Then the solvent was removed under reduced pressure to afford L-Glu-TBA as a white solid. A mixture of L-Glu-TBA (0.203 mg, 0.32 mmol, 2.0 equiv), (*S*)-**2 (**0.050 mg, 0.16 mmol) and activated 4Å molecular sieve in MeOH was stirred at room temperature for 3 d. Then the mixture was filtered, and the solvent of the filtrate was removed under reduced pressure to afford (*S*)-**3** as a light yellow oil in quantitative yield. ^{1}H NMR (400 MHz, CD_3OD) δ 8.57 (d, *J* = 8.7 Hz, 1H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.73 (s, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 8.2 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 1H), 3.20 (s, 18H), 2.32 (s, 1H), 2.08 (s, 2H), 1.83 (s, 2H), 1.64 (s, 18H), 1.41 (s, 19H), 1.02 (s, 24H). $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_3OD) δ 180.8, 178.2,

158.5, 135.9, 134.4, 133.3, 133.2, 128.2, 127.9, 127.1, 126.9, 126.1, 123.8, 78.5, 58.0, 35.5, 32.0, 23.3, 19.2, 12.5. HRMS: m/z calcd. for $C_{32}H_{29}N_2O_8^+$, $[M+5H]^+$: 569.1918; found: 569.1942. m/z calcd. for $C_{32}H_{27}N_2O_8^-$, $[M+3H]^-$: 567.1773; found: 567.1785.

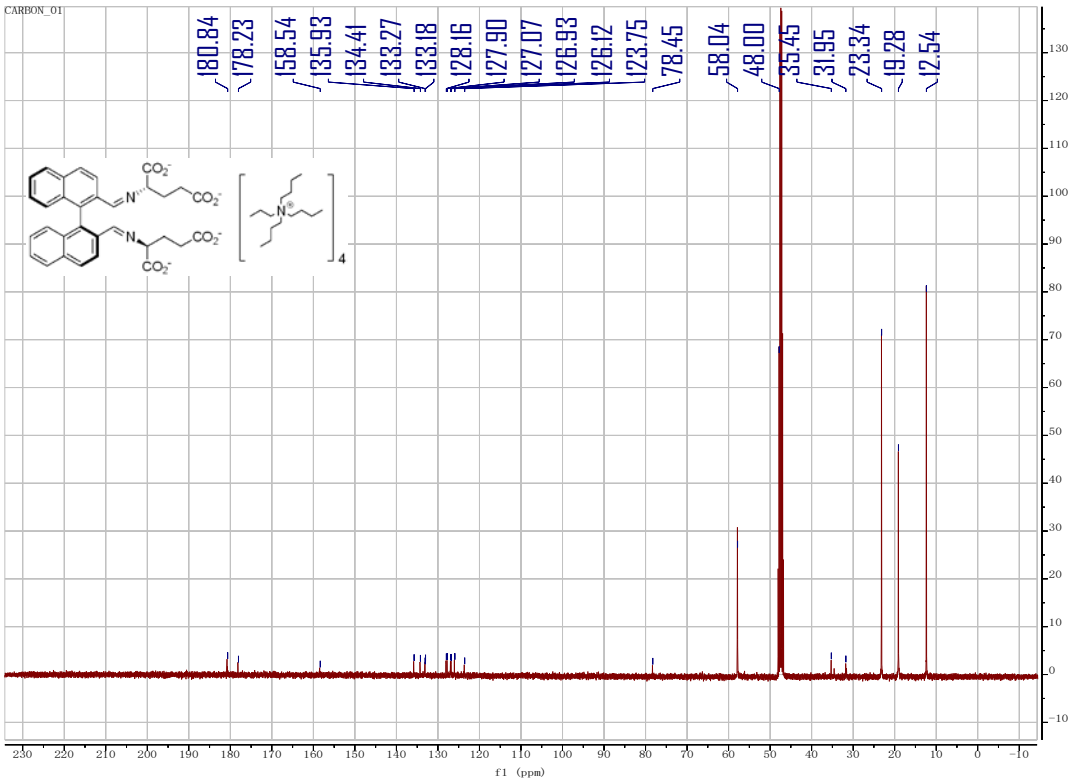
Sample preparation for fluorescence measurement. A stock solution (2.0 mM) of (*S*)-**2** in CH_2Cl_2 was prepared. Stock solutions (10.0 mM) of the TBA salts of amino acids were prepared by mixing amino acids and TBAOH (the equivalent of the carboxylic groups) in methanol in situ. For optical analysis, solutions of (*S*)-**2** (25 μL each) were added to several test tubes. A solution of a TBA salt of an amino acid was added to each test tube. The resulting solution was allowed to stand at 300 K. After 1.5 h, the mixture in each test tube was diluted with methanol to obtain 2.0 × 10^{-5} M solutions of (*S*)-**2** for fluorescence measurements. Fluorescence spectra were recorded within 1 h of the sample preparation.

2. NMR and Mass Spectra of Compounds (*S*)-3, (*R*)-2 and (*S*)-2

^{1}H NMR spectra of (*S*)-**3**

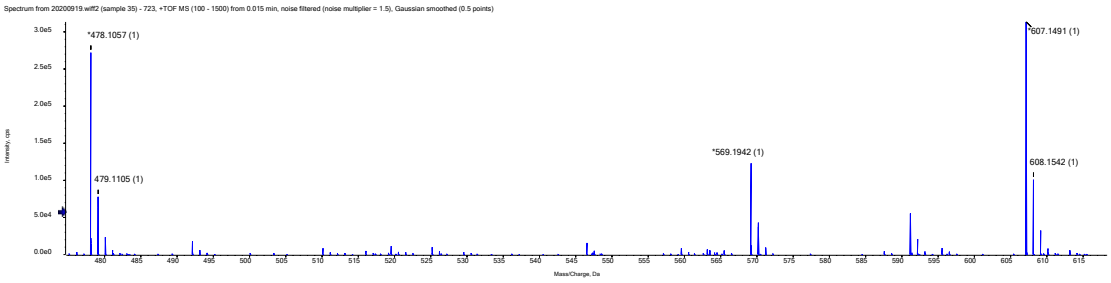


$^{13}C\{^{1}H\}$ NMR spectra of (*S*)-**3**

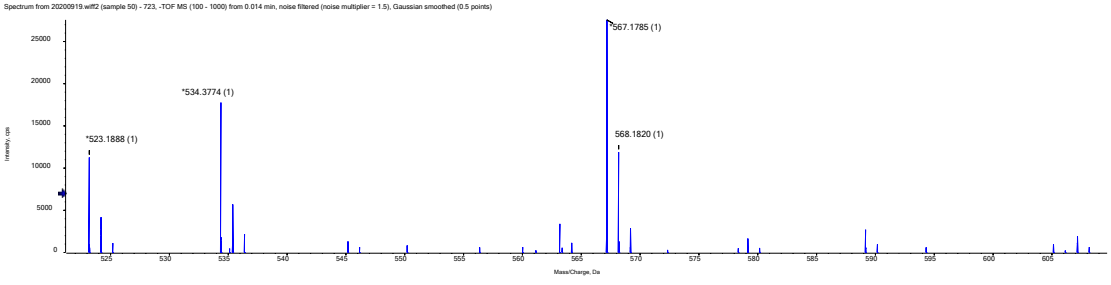


TOF mass spectra of (*S*)-**3**

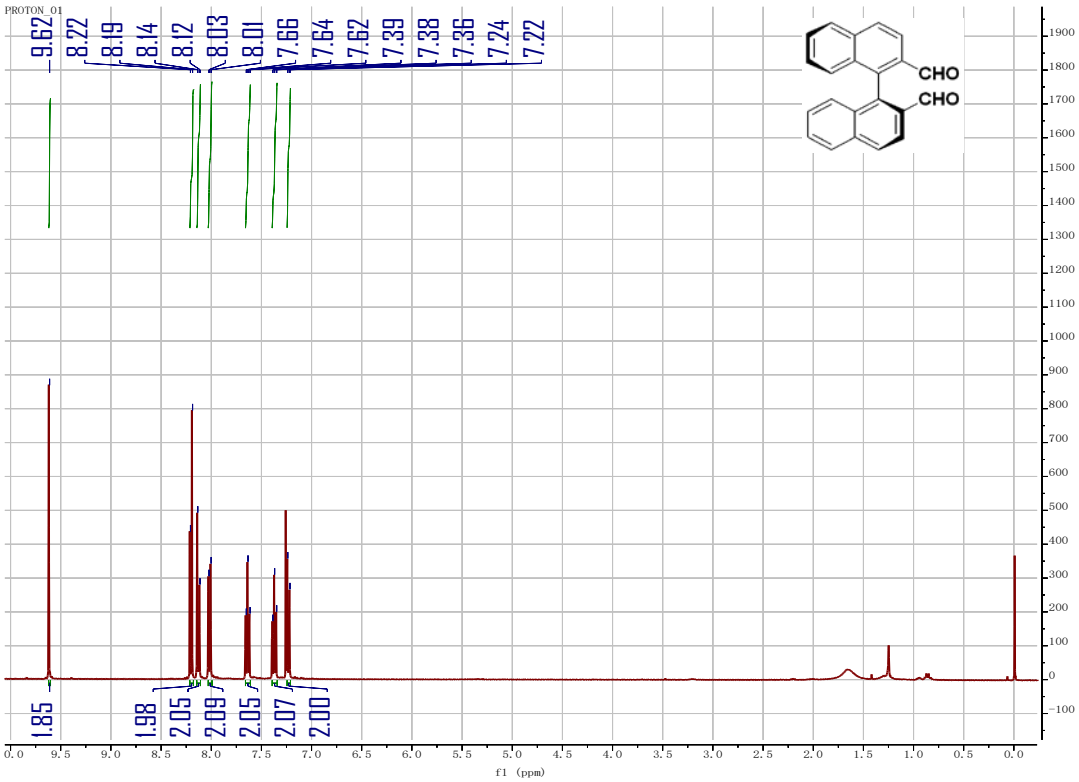
ESI^{+}



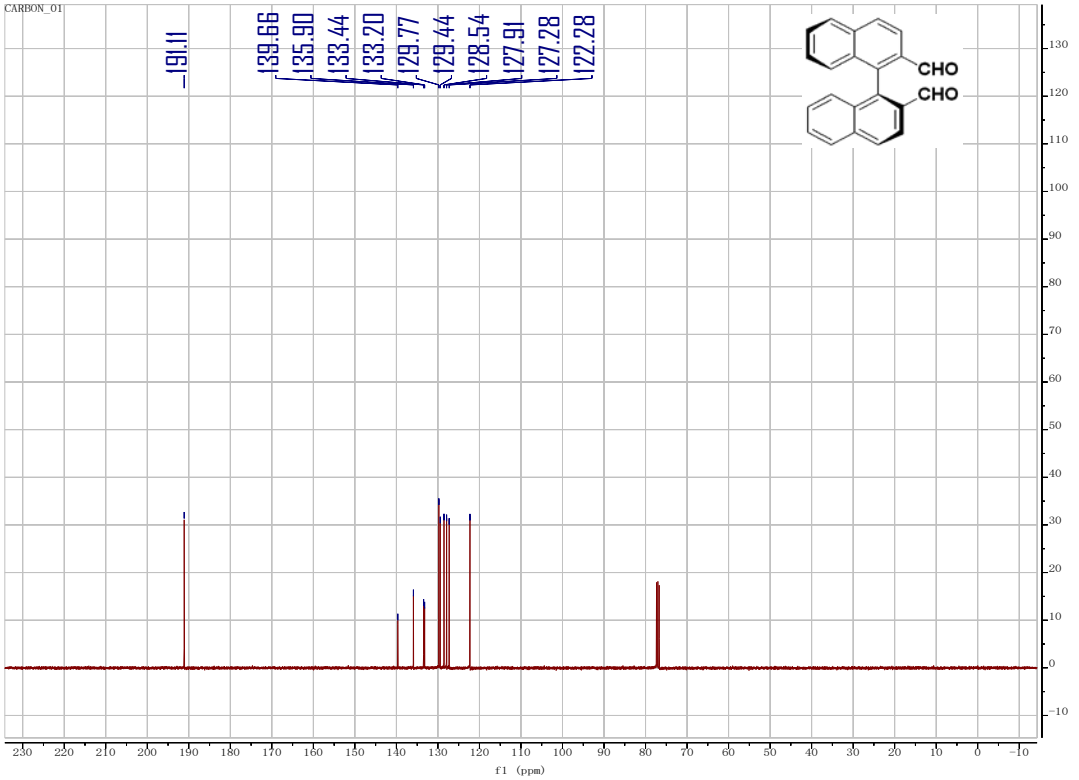
ESI^{-}



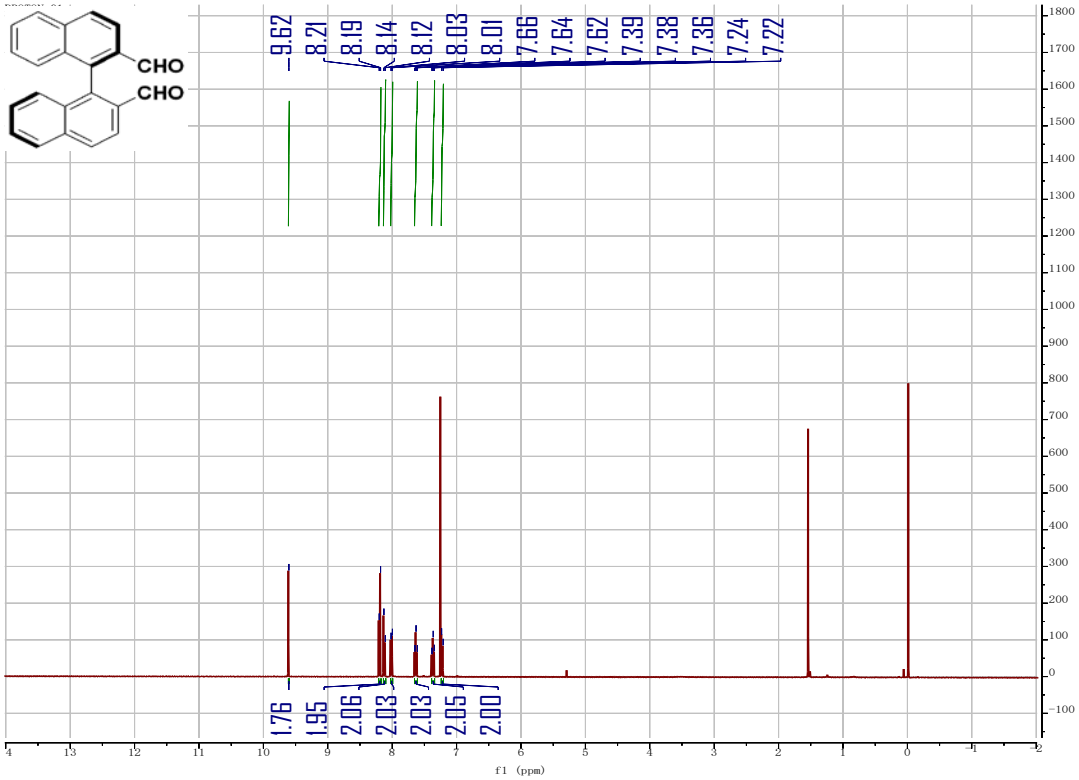
^{1}H NMR spectrum of (*S*)-**2**



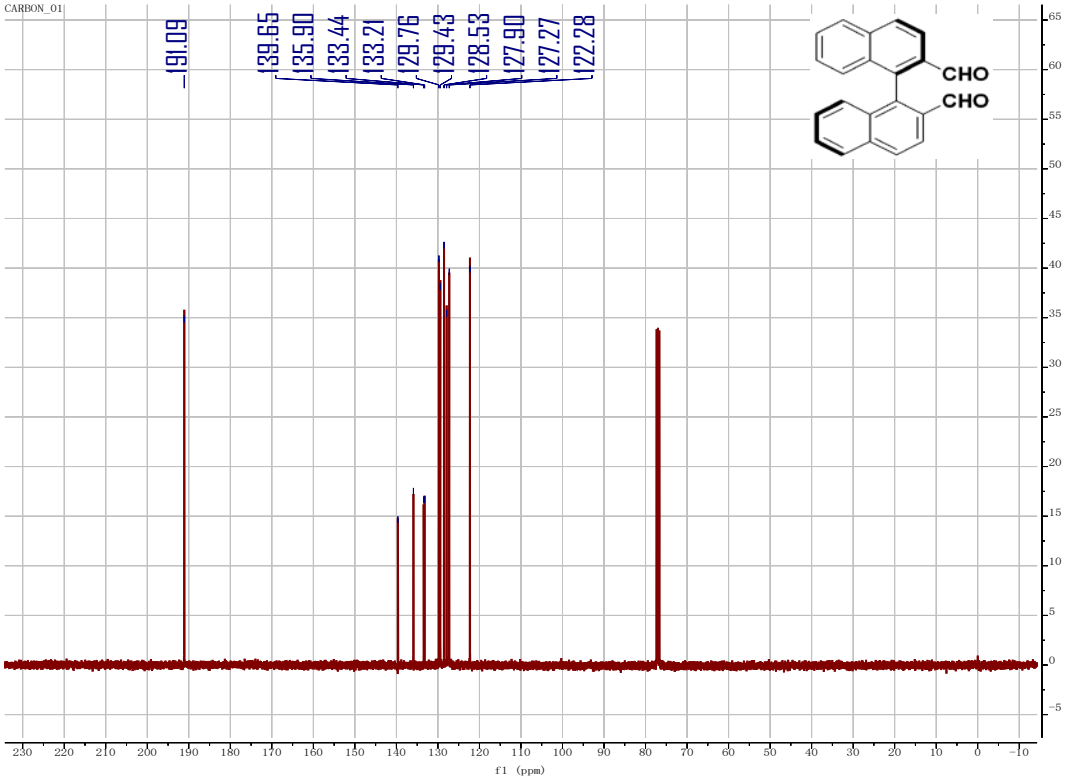
^{13}C{^{1}H} NMR spectrum of (*S*)-**2**



^{1}H NMR spectra of (*R*)-**2**



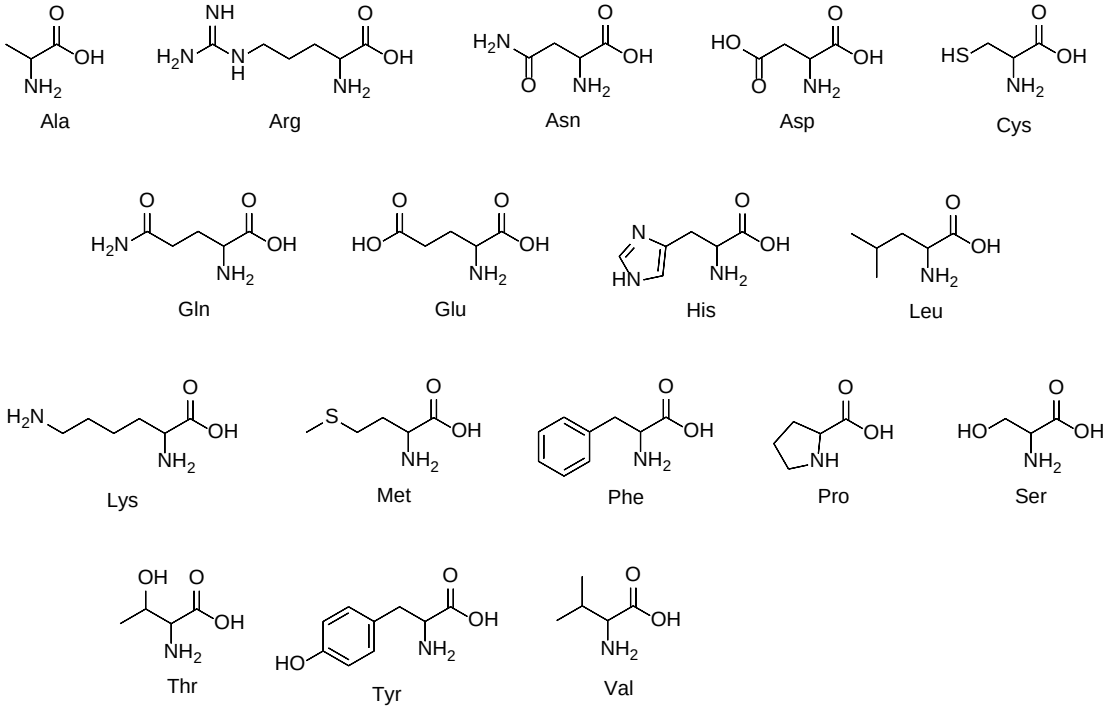
^{13}C{^{1}H} NMR spectra of (*R*)-**2**

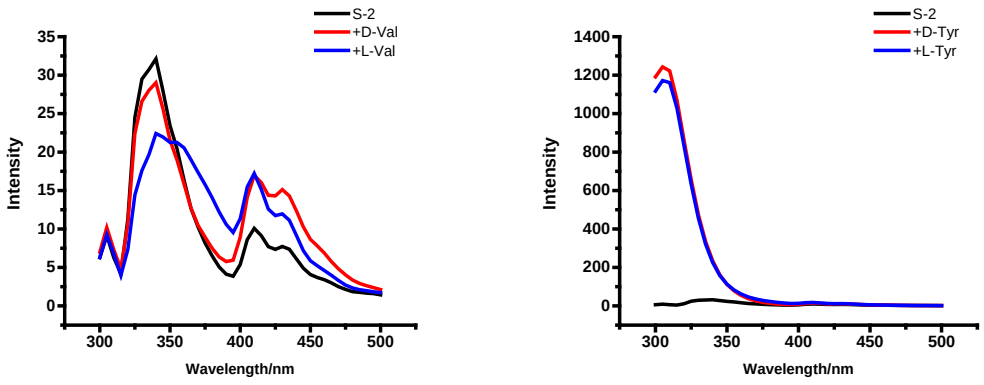


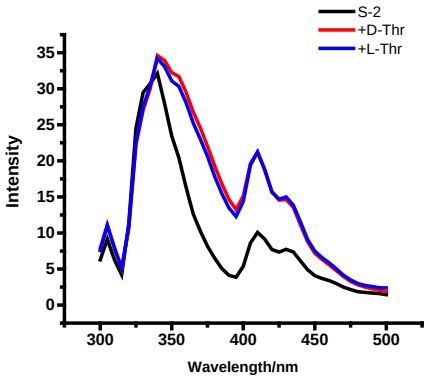
3. Fluorescence Spectra of (S)-2 with Additional 17 Pairs of Amino Acid Enantiomers

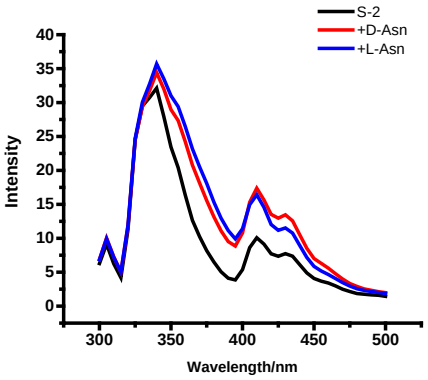
Figure S1. Fluorescence spectra of (*S*)-**2** with additional 17 pairs of amino acid enantiomers. Fluorescence spectra of (*S*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with 17 amino acids (5 equiv. 1.0×10^{-2} M in methanol solution). The mixture was allowed to stand at 300 K for 120 min and each of the solutions was diluted with methanol solution to 2.5 mL and its fluorescent spectrum was obtained. (Solvent: MeOH/ CH_2Cl_2 = 99/1, v/v. λ_{exc} = 280 nm. Slit: 5/5 nm).

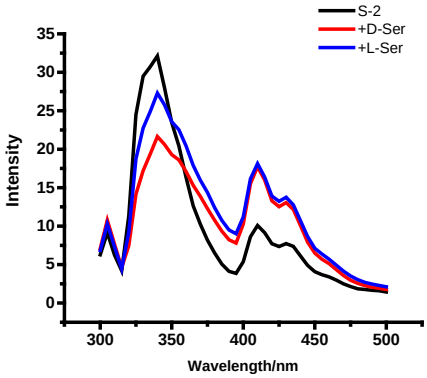
Structures of amino acids studied.

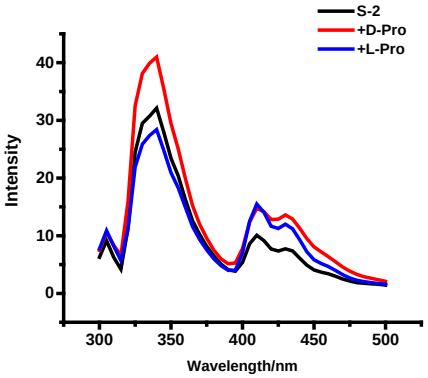


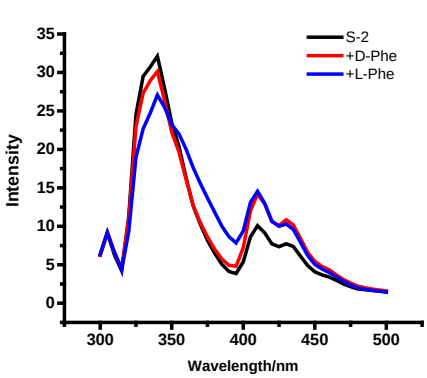


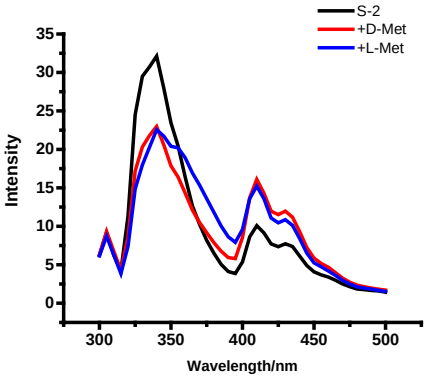

S-2
+D-Thr
+L-Thr
Intensity
Wavelength/nm

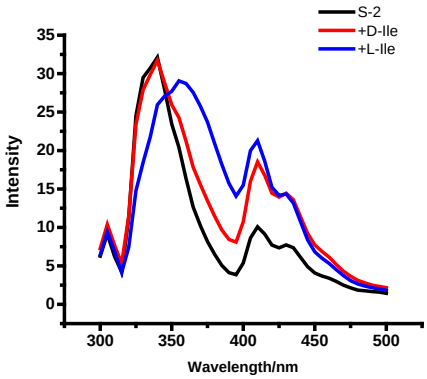

S-2
+D-Asn
+L-Asn
Intensity
Wavelength/nm

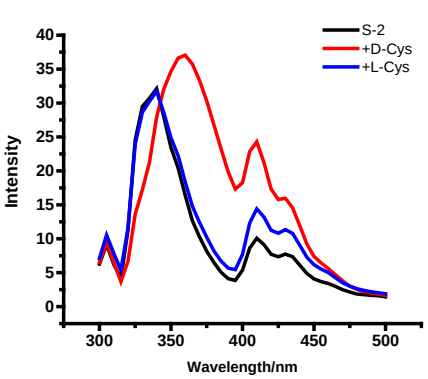

S-2
+D-Ser
+L-Ser
Intensity
Wavelength/nm

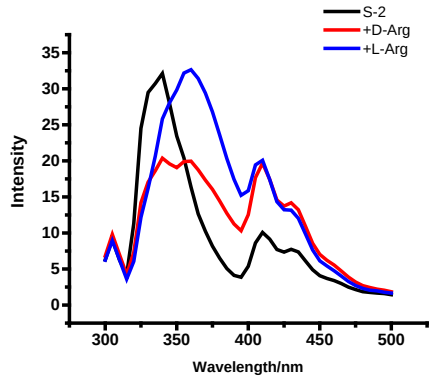

S-2
+D-Pro
+L-Pro
Intensity
Wavelength/nm

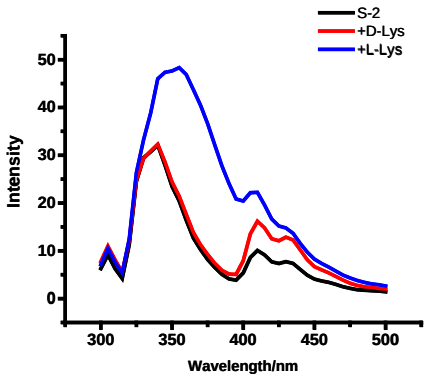

S-2
+D-Phe
+L-Phe
Intensity
Wavelength/nm

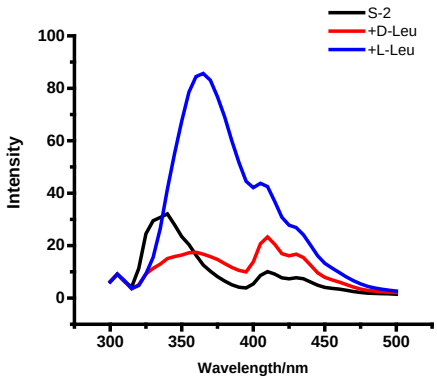

S-2
+D-Met
+L-Met
Intensity
Wavelength/nm

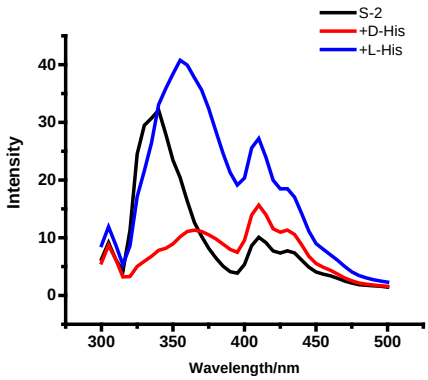

S-2
+D-Ile
+L-Ile
Intensity
Wavelength/nm

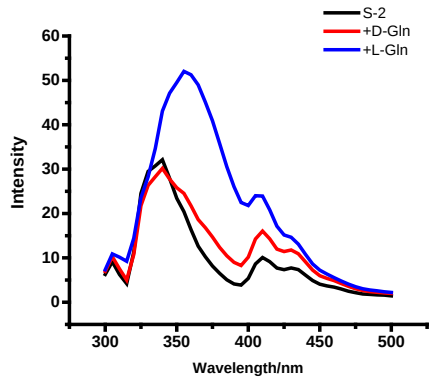

S-2
+D-Cys
+L-Cys
Intensity
Wavelength/nm

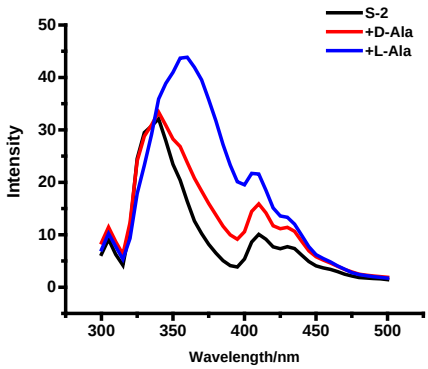

S-2
+D-Arg
+L-Arg
Intensity
Wavelength/nm


S-2
+D-Lys
+L-Lys
Intensity
Wavelength/nm


S-2
+D-Leu
+L-Leu
Intensity
Wavelength/nm


S-2
+D-His
+L-His
Intensity
Wavelength/nm


S-2
+D-Gln
+L-Gln
Intensity
Wavelength/nm


S-2
+D-Ala
+L-Ala
Intensity
Wavelength/nm

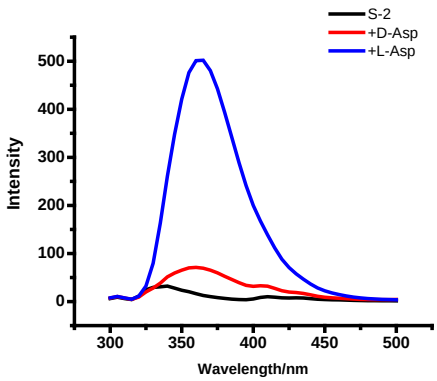

S-2
+D-Asp
+L-Asp
Intensity
Wavelength/nm

Figure S2. (*S*)-**2** (25 μL, 2.0 × 10^{-3} M in CH_2Cl_2) was placed in a 10 mL test tube, to which was added L- or D-Glu (25 μL, 1.0 × 10^{-2} M in methanol). The resulting solutions were allowed to stand at 300 K for 5, 10, 20, 30, 40, 50, 60, 80, 90 and 120 min respectively. Then, each of the solutions was diluted with methanol to 2.5 mL and its fluorescent spectrum was obtained. This figure plots the fluorescent intensities at 365 nm for L-Glu and D-Glu versus the reaction time. (λ_{exc} = 280 nm, slits = 5/5 nm, Reaction at 300 K)

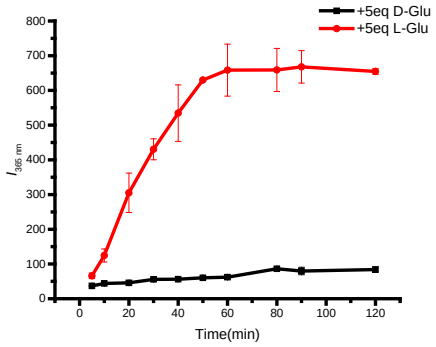
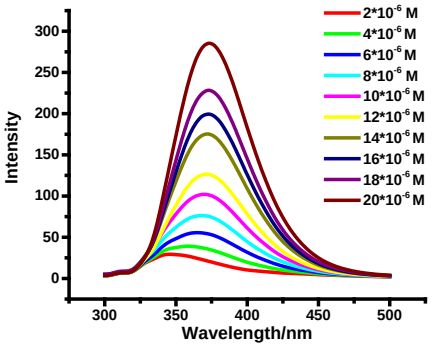
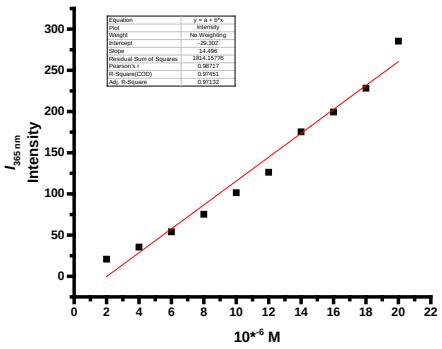


Figure S3. Fluorescence spectra of (*S*)-**2** (25 μL, 2.0 × 10^{-3} M in CH_2Cl_2) with (a) L-Glu (0.1 - 1.0 equiv. 1.0 × 10^{-2} M in methanol). The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol to 2.5 mL and its fluorescence spectrum was obtained. (Solvent: MeOH/CH_2Cl_2 = 99/1, v/v. λ_{exc} = 280 nm. Slit: 5/5 nm). (b) Fluorescence intensity of (*S*)-**2** versus the equivalence of L-Glu at 365 nm.



(a)



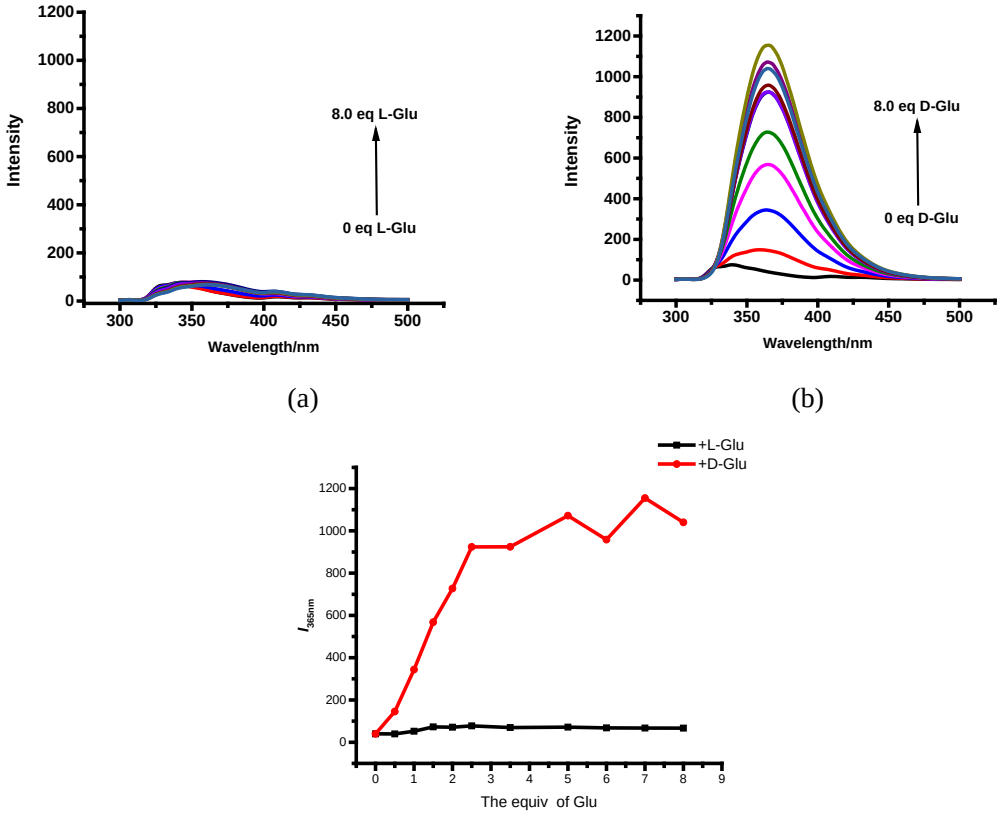
(b)

Standard deviation: 0.23

Limit of detection (LOD)

= （3 × 0.23）/14.496 = 4.76×10^{-8} M

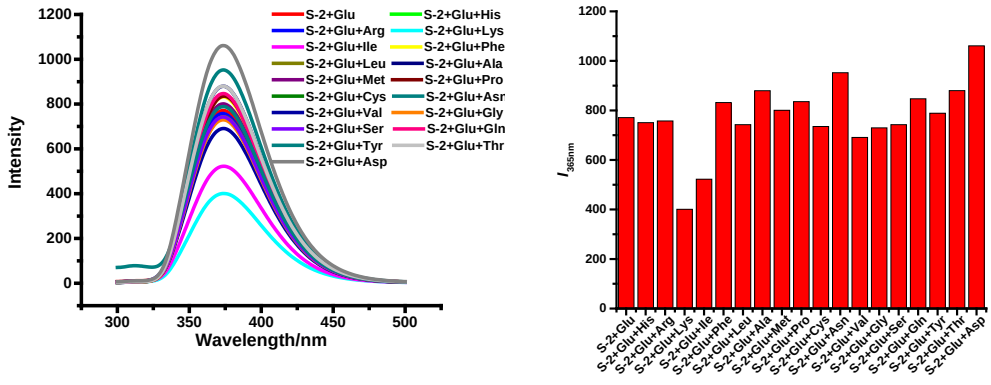
Figure S4. Fluorescence spectra of (*R*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with (a) L-Glu or (b) D-Glu (0.5 - 8.0 equiv. 1.0×10^{-2} M in methanol). The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol to 2.5 mL and its fluorescence spectrum was obtained. (Solvent: $MeOH/CH_2Cl_2$ = 99/1,v/v. λ_{exc} = 280 nm. Slit: 5/5 nm). (c) The fluorescence intensity at 365 nm versus the equivalent of L- and D-Glu.



(a) (b)

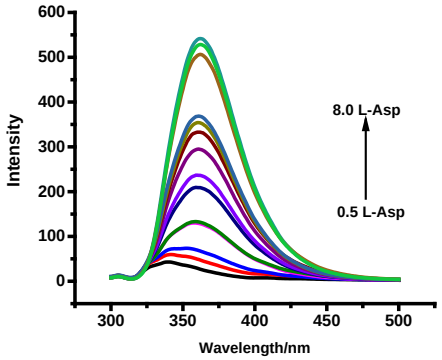
(c)

Figure S5. (a) Fluorescence spectra of (*S*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with L-Glu (4.0 equiv. 1.0×10^{-2} M in methanol) in the presence of various other L-amino acids (1.0 equiv. 1.0×10^{-2} M in methanol). The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol to 2.5 mL before the fluorescence measurement. (Solvent: $MeOH/CH_2Cl_2$ = 99/1, v/v. λ_{exc} = 280 nm. Slit: 5/5 nm). (b) The bar graphs of the fluorescence intensity at 365 nm.

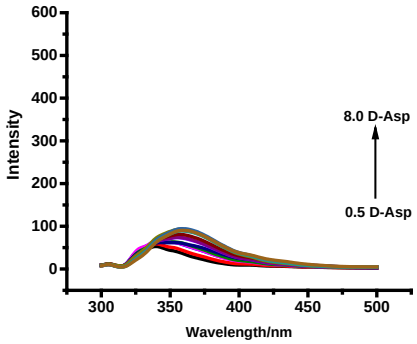


(a) (b)

Figure S6. Fluorescence spectra of (*S*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with (a) L-Asp or (b) D-Asp (0.5-8.0 equiv. 1.0×10^{-2} M in methanol). The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol to 2.5 mL and its fluorescence spectrum was obtained. (c) The fluorescence intensity at 365 nm versus the equivalent of L- and D-Asp. (d) Fluorescence intensity of (*S*)-**2** and (*R*)-**2** at 365 nm versus the ee value of L-Asp (in methanol solution, 5 equiv.) (Error bars from three independent experiments. MeOH/DCM = 99/1,v/v. λ_{exc}=280 nm. Slit: 5/5 nm).



(a)



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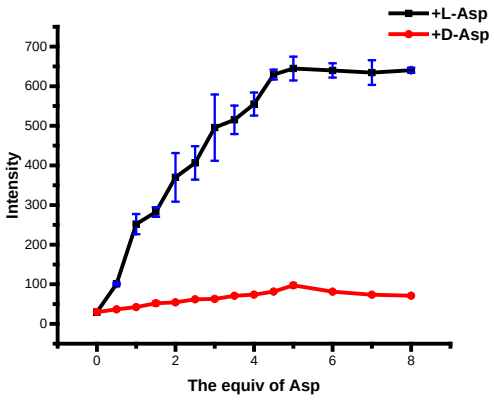
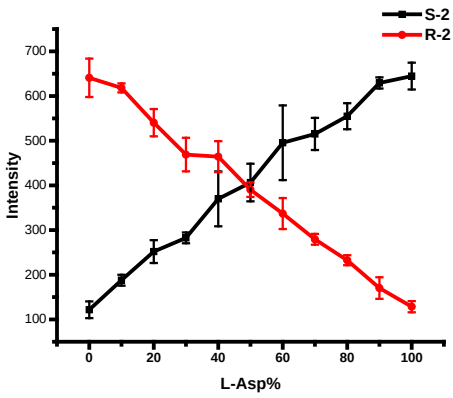


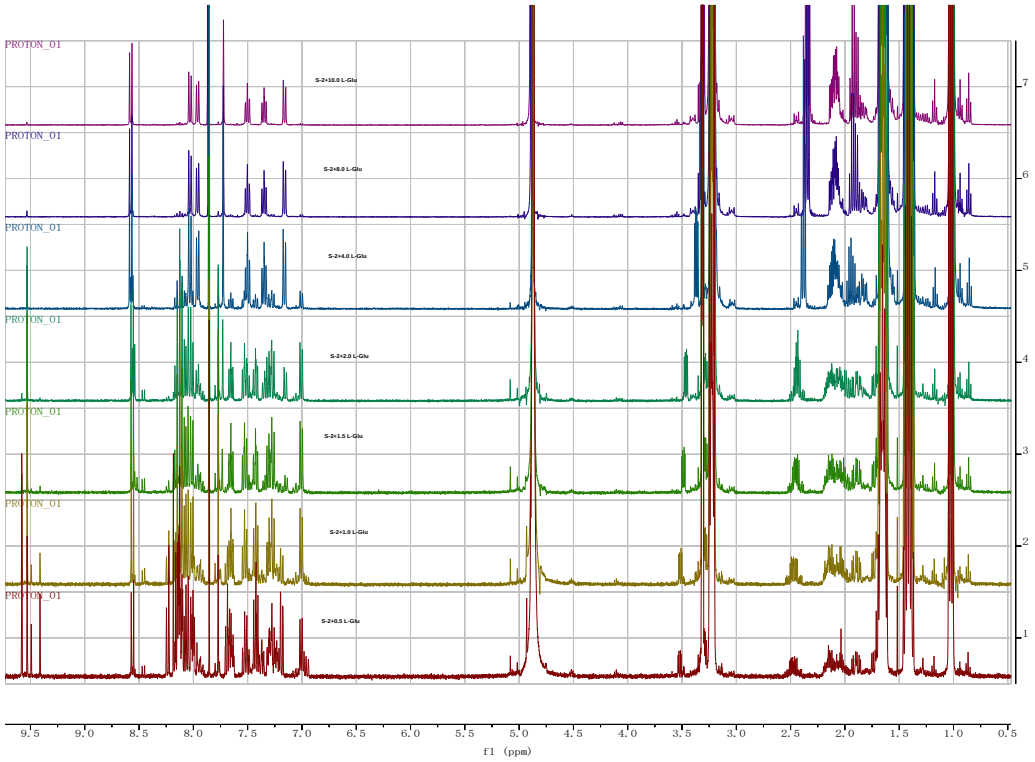
(c)



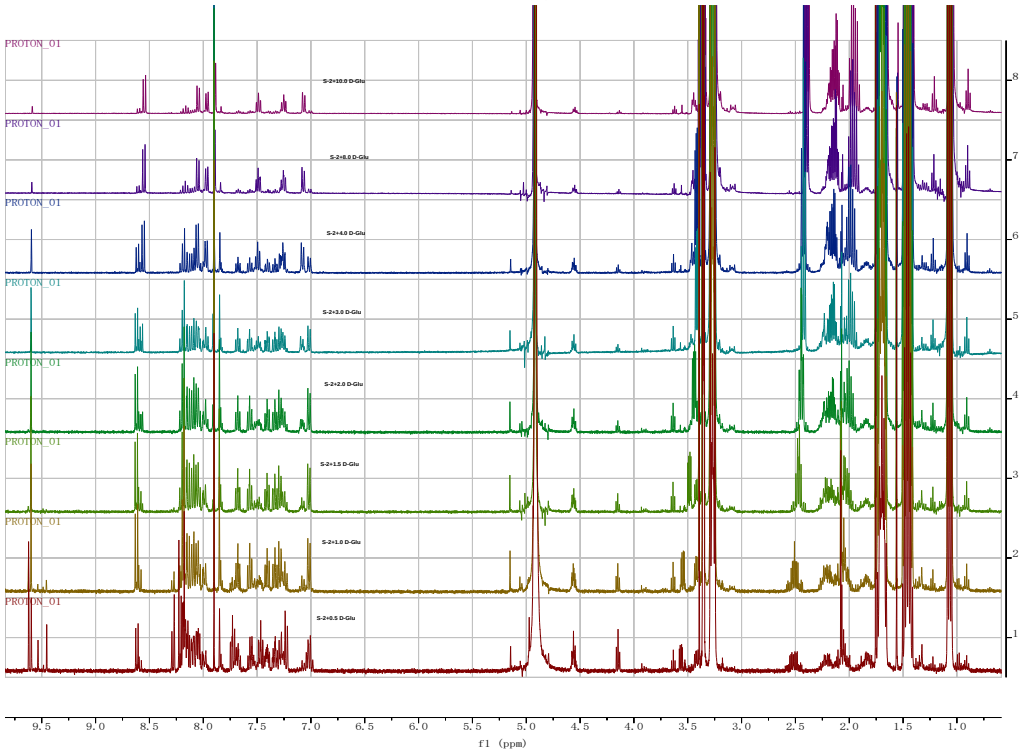
(d)

4. NMR Study for the Reaction of (S)-2 with L- and D-Glu-TBA

Figure S7. ^{1}H NMR spectra of the reaction mixture of (*S*)-**2** (50 μL 5.0 × 10^{-2} M in $CDCl_3$) with (a) L-Glu-TBA (CD_3OD, 0 - 10.0 equiv. 1.0× 10^{-1} M in CD_3OD); (b) D-Glu-TBA (CD_3OD, 0 - 10.0 equiv. 1.0× 10^{-1} M in CD_3OD). Each sample was diluted to 500 μL with CD_3OD ($CDCl_3$/ CD_3OD = 1/9, v/v) and measured after 12 h reaction.

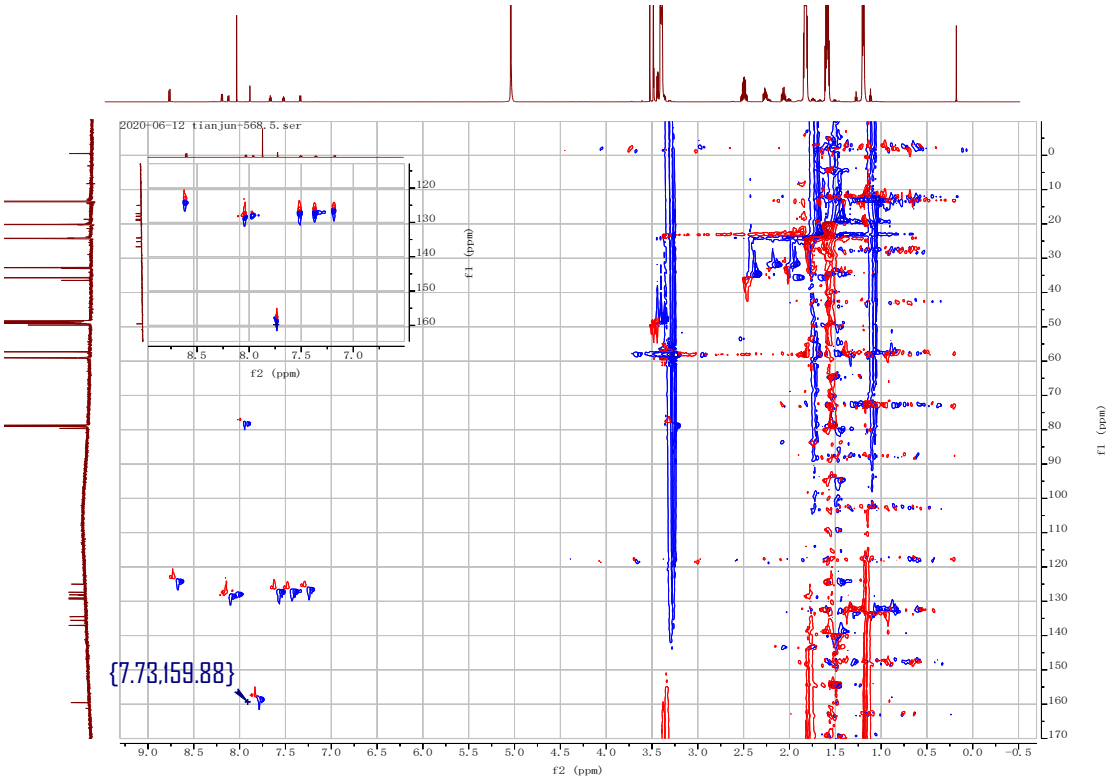


(a)



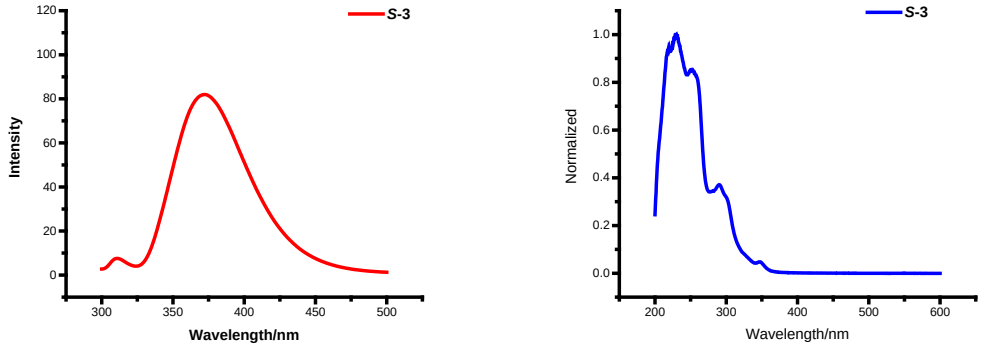
(b)

Figure S8. HSQC spectrum of the reaction mixture of (*S*)-**2** (5 mM) with L-Glu-TBA (10 equiv.) ($CDCl_3$ / CD_3OD = 1/9, v/v).



5. Fluorescence and UV-vis Spectra of (*S*)-3

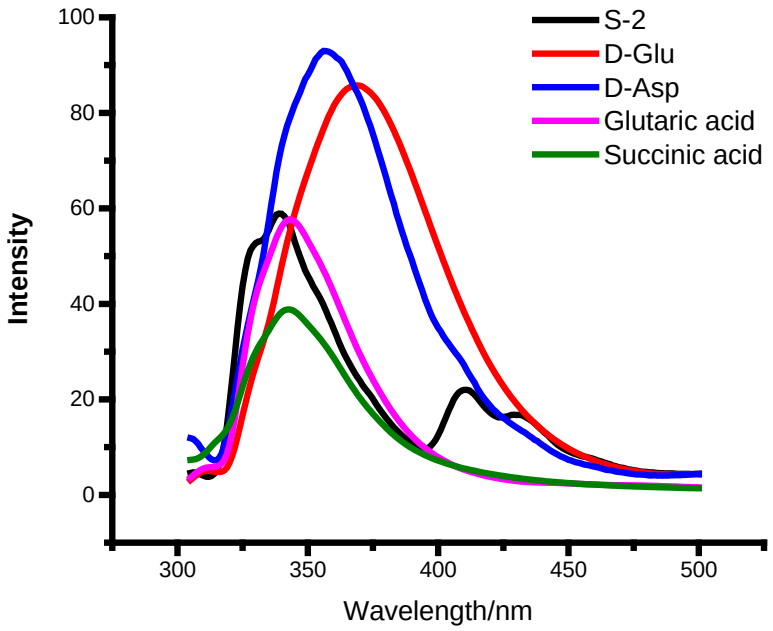
Figure S9. Fluorescence (a) and UV-vis absorption spectra (b) of (*S*)-**3** (2.0×10^{-5} M in 2.5 mL MeOH, λ_{exc} = 280 nm. Slit: 5/5 nm).



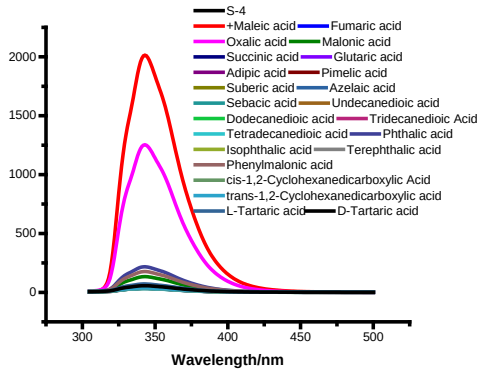
(a) (b)

6. Fluorescence Responses of (*S*)-2 toward Various Dicarboxylic Acids

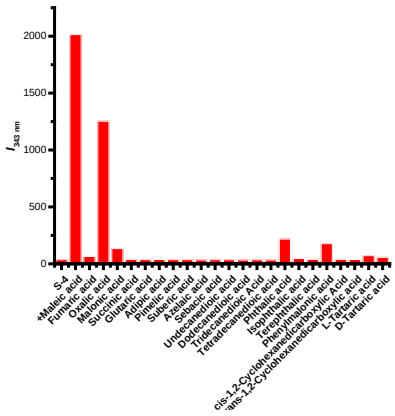
Figure S10. Fluorescence spectra of (*S*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with (a) D-Glu, D-Asp, glutaric acid and succinic acid (5 equiv 1.0×10^{-2} M in methanol solution), (b) 23 dicarboxylic acids (5 equiv, 1.0×10^{-2} M in methanol solution). (c) $\boldsymbol{I}_{343\ nm}$ of the various dicarboxylic acids with (*S*)-**2**. The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol to 2.5 mL to record the fluorescence spectrum (Solvent: MeOH/ CH_2Cl_2 = 99/1, v/v. λ_{exc} = 280 nm. Slit: 5/5 nm).



(a)

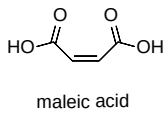


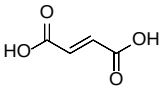
(b)

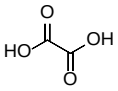


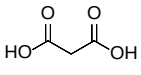
(c)

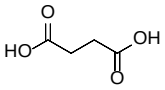
Structures of 23 dicarboxylic acids studied.

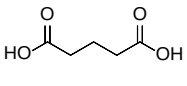

maleic acid

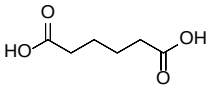

fumaric acid

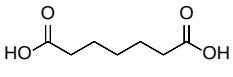

oxalic acid

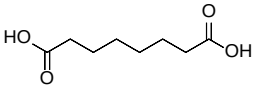

malonic acid

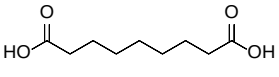

succinic acid

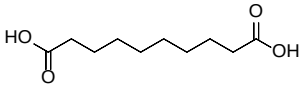

glutaric acid

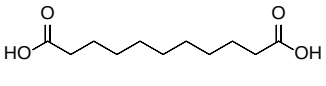

adipic acid

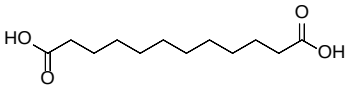

pimelic acid

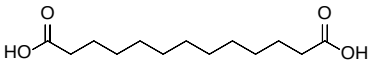

suberic acid

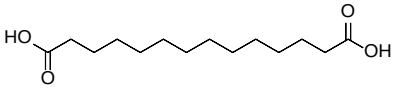

azelaic acid

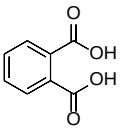

sebacic acid

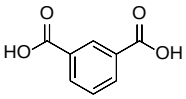

undecanedioic acid

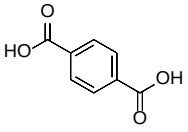

Dodecanedioic acid

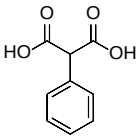

tridecanedioic acid

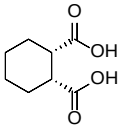

tetradecanedioic acid

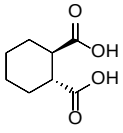

phthalic acid

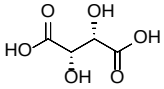

isophthalic acid

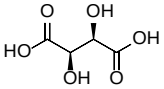

terephthalic acid


phenylmalonic acid


cis-1,2-cyclohexanedicarboxylic acid


trans-1,2-cyclohexanedicarboxylic acid


(2*S*,3*S*)-2,3-dihydroxysuccinic acid


(2*R*,3*R*)-2,3-dihydroxysuccinic acid

7. Study of the Interaction of (*S*)-2 with Maleic Acid and Other Dicarboxylic Acids

Figure S11. Fluorescence spectra of (*S*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with maleic acid (5 equiv, 1.0×10^{-2} M in methanol). The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol solution to 2.5 mL and its fluorescent spectrum was obtained. (MeOH/DCM = 99/1, v/v. λ_{exc} = 280 nm. Slit: 5/5 nm)

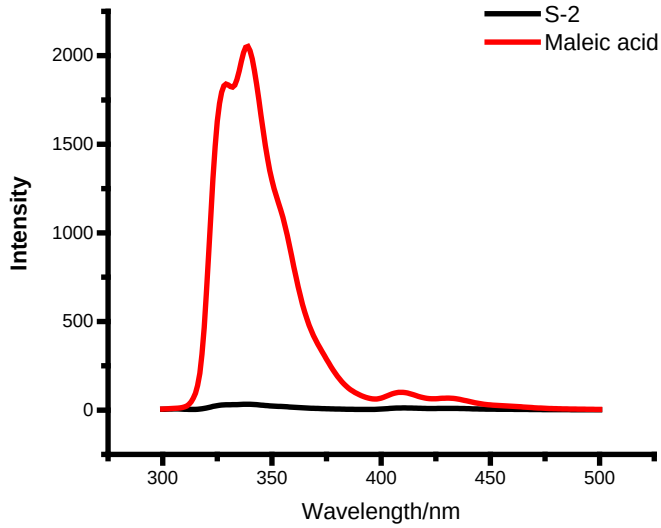
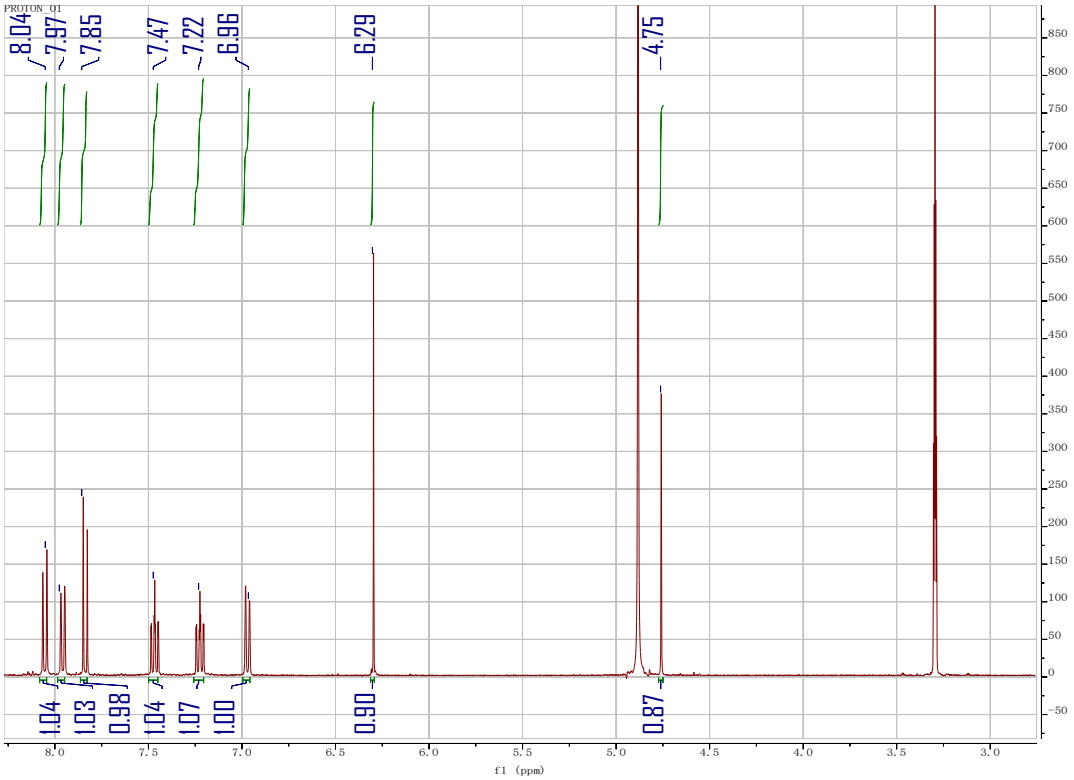
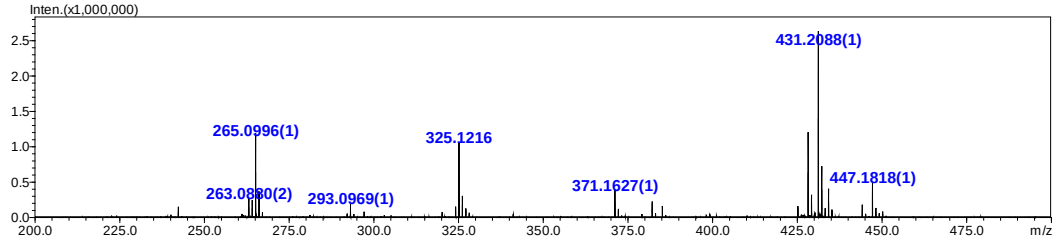


Figure S12. (a) ^{1}H NMR spectrum of the reaction mixture of (*S*)-**2** with maleic acid (5 mM in CD_3OD, 1.0 equiv) at reaction time 2 h.



(b) TOF mass spectra of (*S*)-**2** (5 mM) + Maleic acid (1 equiv).



(c) ^{1}H NMR spectra after (*S*)-**2** was treated with several dicarboxylic acids (5 mM in CD_3OD , 1.0 equiv) at room temperature for 2 h.

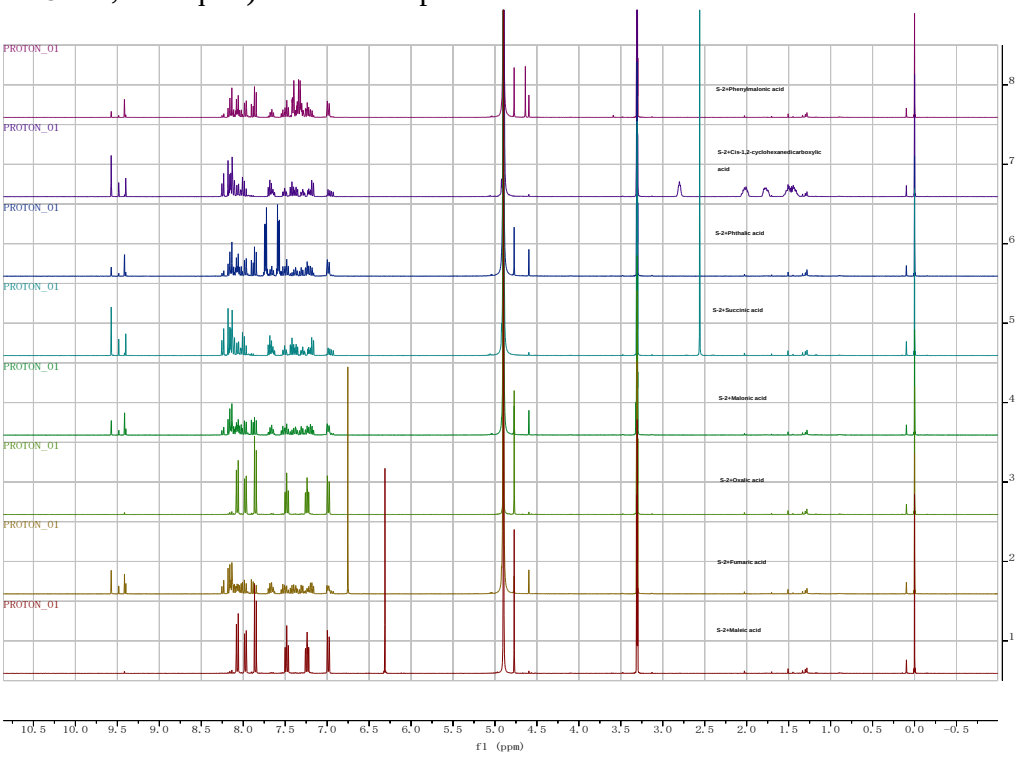
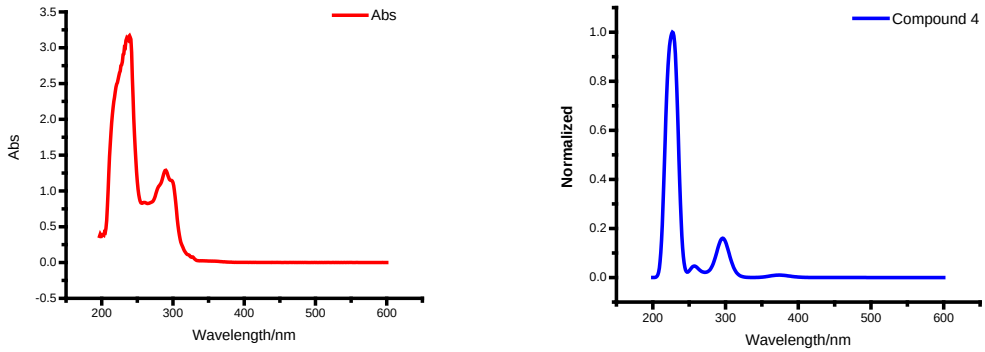


Figure S13. UV-Vis spectra of **4** (2.0×10^{-5} M) in methanol (a) and calculated UV spectrum of **4** (b).



(a) (b)

Figure S14. Three possible diastereomeric products of **4** from the reaction of (*S*)-**2** with maleic acid.

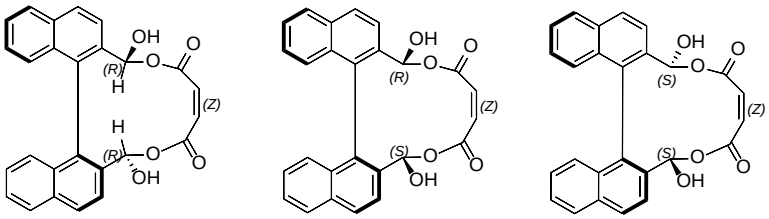
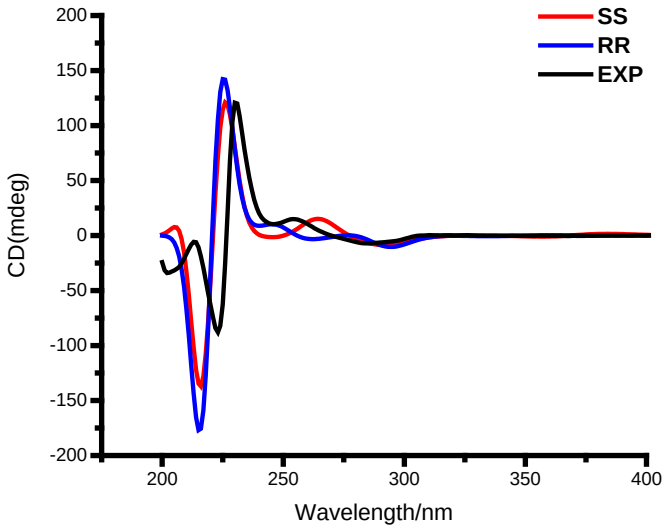


Figure S15. CD spectra of **4** (2.0×10^{-5} M in methanol) and the calculated CD spectra of the SS or RR diastereomers.



ECD Calculation Details

1 ECD Calculation for the **SS** diastereomer

1.1. Methods

Monte Carlo conformational searches were carried out by means of the Spartan's 14 software using Merck Molecular Force Field (MMFF). Total of 2 conformers were generated, and then the conformers were initially optimized at B3LYP/6-31g level in gas. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-31+g (d, p) level for all conformers of compounds **SS**. Rotatory strengths for a total of 30 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.

1.2. Results

Table S1.2.1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **SS**.

Conformers	In MeOH	
	G[a]	*P* (%)[b]
SS.-1	-911566.11008346	99.94
SS.-2	-911561.72755362	0.06

[a]B3LYP/6-31G(d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S1.2.2. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **SS** at B3LYP/6-31G(d,p) level of theory in methanol.

SS-1	Standard Orientation (Ångstroms)				
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	3.028252	3.153374	-2.407191
2.	6.	0.	2.823217	3.115359	-1.008288
3.	6.	0.	1.887903	2.265886	-0.460681
4.	6.	0.	1.106856	1.406722	-1.283047
5.	6.	0.	1.318300	1.447920	-2.700557
6.	6.	0.	2.290300	2.336253	-3.232130
7.	6.	0.	0.125762	0.505180	-0.741411
8.	6.	0.	-0.598074	-0.307202	-1.604212
9.	6.	0.	-0.381381	-0.254024	-3.006226
10.	6.	0.	0.548155	0.600166	-3.539666
11.	6.	0.	-0.113813	0.503450	0.744392
12.	6.	0.	-1.601287	-1.308810	-1.092002
13.	6.	0.	-1.073321	1.424628	1.291630
14.	6.	0.	-1.283832	1.462107	2.709383
15.	6.	0.	-0.534040	0.591209	3.543208
16.	6.	0.	0.375045	-0.281459	3.004459
17.	6.	0.	0.590518	-0.331135	1.602128
18.	6.	0.	-1.833742	2.307087	0.474619
19.	6.	0.	-2.748716	3.175091	1.027506
20.	6.	0.	-2.952894	3.209349	2.426630
21.	6.	0.	-2.234560	2.369925	3.246477
22.	6.	0.	1.569765	-1.353053	1.083694
23.	8.	0.	-2.703733	-1.374138	-1.926721
24.	8.	0.	-0.883896	-2.606195	-1.077566
25.	8.	0.	0.821846	-2.632968	1.061337
26.	8.	0.	2.670295	-1.449604	1.917913
27.	6.	0.	-1.539962	-3.607496	-0.478972
28.	6.	0.	-0.694510	-4.808437	-0.221148
29.	6.	0.	0.580408	-4.824803	0.191426
30.	8.	0.	-2.726240	-3.575859	-0.190727
31.	6.	0.	1.454049	-3.645826	0.456542
32.	8.	0.	2.640771	-3.640540	0.168435
33.	1.	0.	-1.882683	-1.123451	-0.052261
34.	1.	0.	1.855544	-1.168020	0.045093
35.	1.	0.	3.769327	3.827465	-2.826313
36.	1.	0.	3.409359	3.760776	-0.360979

37.	1.	0.	1.742408	2.242291	0.613262
38.	1.	0.	2.440740	2.356997	-4.308244
39.	1.	0.	-0.976577	-0.898757	-3.642670
40.	1.	0.	0.708515	0.638373	-4.613711
41.	1.	0.	-0.693528	0.626600	4.617479
42.	1.	0.	0.954760	-0.944007	3.636883
43.	1.	0.	-1.688769	2.286657	-0.599460
44.	1.	0.	-3.319360	3.838175	0.384218
45.	1.	0.	-3.677828	3.898212	2.849944
46.	1.	0.	-2.384546	2.387610	4.322709
47.	1.	0.	-3.316492	-1.995151	-1.497738
48.	1.	0.	3.268205	-2.082303	1.485071
49.	1.	0.	-1.223227	-5.748101	-0.353377
50.	1.	0.	1.086709	-5.777519	0.317858

SS-2		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	2.961610	3.090457	-2.476400
2.	6.	0.	2.739983	3.116718	-1.079932
3.	6.	0.	1.809191	2.282355	-0.501497
4.	6.	0.	1.046494	1.376830	-1.290305
5.	6.	0.	1.276389	1.352533	-2.704679
6.	6.	0.	2.243872	2.224724	-3.269162
7.	6.	0.	0.067262	0.493037	-0.715774
8.	6.	0.	-0.656066	-0.356231	-1.541642
9.	6.	0.	-0.397384	-0.382596	-2.939258
10.	6.	0.	0.536281	0.444639	-3.506567
11.	6.	0.	-0.140257	0.503866	0.772986
12.	6.	0.	-1.720898	-1.290741	-0.998106
13.	6.	0.	-1.099136	1.405916	1.346857
14.	6.	0.	-1.281789	1.424473	2.768642
15.	6.	0.	-0.505878	0.552248	3.575969
16.	6.	0.	0.406776	-0.300404	3.010358
17.	6.	0.	0.598163	-0.328527	1.604593
18.	6.	0.	-1.884647	2.288189	0.554102
19.	6.	0.	-2.797552	3.140036	1.134117
20.	6.	0.	-2.974971	3.155823	2.537493
21.	6.	0.	-2.232220	2.315413	3.334028
22.	6.	0.	1.595924	-1.316971	1.049051
23.	8.	0.	-2.942839	-1.202341	-1.655036
24.	8.	0.	-1.147710	-2.628752	-1.132769

25.	8.	0.	0.848151	-2.584279	0.877054
26.	8.	0.	2.651479	-1.489061	1.926582
27.	6.	0.	-1.507484	-3.542877	-0.202397
28.	6.	0.	-0.625937	-4.754295	-0.258721
29.	6.	0.	0.691287	-4.770231	-0.017095
30.	8.	0.	-2.427200	-3.435928	0.573539
31.	6.	0.	1.533541	-3.591073	0.311671
32.	8.	0.	2.738686	-3.564238	0.106842
33.	1.	0.	-1.930344	-1.124756	0.056330
34.	1.	0.	1.936497	-1.046992	0.045610
35.	1.	0.	3.699565	3.752839	-2.918806
36.	1.	0.	3.310066	3.800425	-0.458131
37.	1.	0.	1.650265	2.310382	0.570442
38.	1.	0.	2.408189	2.193616	-4.342955
39.	1.	0.	-0.926857	-1.094185	-3.568735
40.	1.	0.	0.727266	0.409311	-4.575571
41.	1.	0.	-0.647430	0.569703	4.653158
42.	1.	0.	1.007191	-0.961680	3.623866
43.	1.	0.	-1.760275	2.279573	-0.522908
44.	1.	0.	-3.388606	3.803547	0.509986
45.	1.	0.	-3.699925	3.831018	2.982189
46.	1.	0.	-2.362606	2.318719	4.412903
47.	1.	0.	-2.786397	-1.174461	-2.608903
48.	1.	0.	3.257374	-2.105922	1.480651
49.	1.	0.	-1.145525	-5.688262	-0.456993
50.	1.	0.	1.247432	-5.700588	-0.076675

2. ECD Calculation for the **RR** diastereomer

2.1. Methods

Monte Carlo conformational searches were carried out by means of the Spartan's 14 software using Merck Molecular Force Field (MMFF). Total of 2 conformers were generated, and then the conformers were initially optimized at B3LYP/6-31g level in gas. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the B3LYP/6-31+g (d, p) level for all conformers of compounds **RR**. Rotatory strengths for a total of 30 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with sigma = 0.3 eV.

2.2. Results

Table S2.2.1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **RR**.

Conformers	In MeOH	
	G^a	P (%)[b]
RR.**-1**	-911556.91643445	96.60
RR.**-2**	-911554.93601289	3.40

[a]B3LYP/6-31G(d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S2.2.2**.** Cartesian coordinates for the low-energy reoptimized MMFF conformers of **RR** at B3LYP/6-31G(d,p) level of theory in methanol.

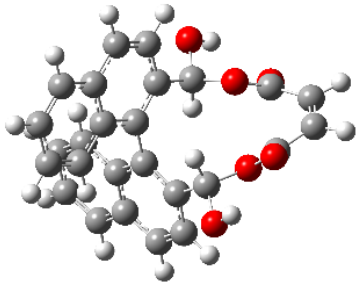
RR-1		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	3.777723	2.773695	-1.472961
2.	6.	0.	3.061718	2.906314	-0.259233
3.	6.	0.	1.973525	2.106928	0.004777
4.	6.	0.	1.531543	1.130737	-0.936137
5.	6.	0.	2.261393	1.002185	-2.164751
6.	6.	0.	3.384874	1.839616	-2.401739
7.	6.	0.	0.389726	0.285361	-0.689098
8.	6.	0.	-0.022086	-0.609068	-1.677309
9.	6.	0.	0.729151	-0.730857	-2.877079
10.	6.	0.	1.837446	0.041459	-3.115091
11.	6.	0.	-0.355312	0.457164	0.611080
12.	6.	0.	-1.281184	-1.476884	-1.615214
13.	6.	0.	-1.411959	1.436894	0.665771
14.	6.	0.	-2.138504	1.634630	1.887155
15.	6.	0.	-1.795521	0.857848	3.020664
16.	6.	0.	-0.765434	-0.045814	2.959260
17.	6.	0.	-0.017971	-0.246123	1.767712
18.	6.	0.	-1.771322	2.232393	-0.461922
19.	6.	0.	-2.778648	3.165951	-0.380561
20.	6.	0.	-3.491943	3.355323	0.827222
21.	6.	0.	-3.177741	2.602871	1.933805
22.	6.	0.	1.155243	-1.219984	1.899759
23.	8.	0.	-2.453801	-0.837759	-1.267193
24.	8.	0.	-1.091270	-2.586446	-0.682431
25.	8.	0.	0.855246	-2.476963	1.216083

26.	8.	0.	2.378345	-0.777775	1.438152
27.	6.	0.	-0.519619	-3.701897	-1.169744
28.	6.	0.	-0.373241	-4.779698	-0.151809
29.	6.	0.	-0.066464	-4.657142	1.145920
30.	8.	0.	-0.189477	-3.862891	-2.329312
31.	6.	0.	0.187785	-3.409214	1.918825
32.	8.	0.	-0.145171	-3.294428	3.083075
33.	1.	0.	-1.447605	-1.914722	-2.599859
34.	1.	0.	1.289987	-1.457054	2.955487
35.	1.	0.	4.636971	3.409078	-1.665053
36.	1.	0.	3.376945	3.643871	0.472536
37.	1.	0.	1.441423	2.212996	0.942627
38.	1.	0.	3.927060	1.726285	-3.336540
39.	1.	0.	0.414283	-1.468375	-3.607829
40.	1.	0.	2.396617	-0.069618	-4.039907
41.	1.	0.	-2.353447	0.993633	3.942928
42.	1.	0.	-0.512707	-0.640892	3.830513
43.	1.	0.	-1.240902	2.091512	-1.396132
44.	1.	0.	-3.031747	3.760897	-1.252814
45.	1.	0.	-4.287108	4.093151	0.874589
46.	1.	0.	-3.718905	2.737009	2.866439
47.	1.	0.	-2.339338	-0.399491	-0.411156
48.	1.	0.	2.296593	-0.518272	0.508660
49.	1.	0.	-0.502900	-5.773218	-0.571568
50.	1.	0.	-0.024271	-5.549214	1.764407

RR-2		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	4.165197	2.561971	-0.488755
2.	6.	0.	3.214636	2.700705	0.550783
3.	6.	0.	2.046922	1.973600	0.535626
4.	6.	0.	1.756501	1.067533	-0.527206
5.	6.	0.	2.724622	0.932942	-1.578181
6.	6.	0.	3.923286	1.694927	-1.527469
7.	6.	0.	0.535667	0.299597	-0.567361
8.	6.	0.	0.297693	-0.525698	-1.666885
9.	6.	0.	1.277588	-0.656750	-2.686804
10.	6.	0.	2.456964	0.042085	-2.645737
11.	6.	0.	-0.448287	0.473688	0.561470
12.	6.	0.	-0.983347	-1.309923	-1.902945
13.	6.	0.	-1.417579	1.531253	0.462369

14.	6.	0.	-2.354811	1.739250	1.525192
15.	6.	0.	-2.308487	0.888147	2.656996
16.	6.	0.	-1.356256	-0.093443	2.748349
17.	6.	0.	-0.398909	-0.301825	1.718161
18.	6.	0.	-1.479722	2.403012	-0.660906
19.	6.	0.	-2.405148	3.419191	-0.724682
20.	6.	0.	-3.330496	3.618273	0.327551
21.	6.	0.	-3.304469	2.791861	1.425731
22.	6.	0.	0.653904	-1.364926	2.030658
23.	8.	0.	-2.097400	-0.529324	-1.643906
24.	8.	0.	-1.075598	-2.480274	-1.032482
25.	8.	0.	0.431776	-2.570895	1.224652
26.	8.	0.	1.974820	-0.999897	1.862415
27.	6.	0.	-0.484643	-3.612662	-1.463920
28.	6.	0.	-0.603645	-4.737980	-0.497661
29.	6.	0.	-0.566995	-4.682797	0.839948
30.	8.	0.	0.055047	-3.743116	-2.546093
31.	6.	0.	-0.421198	-3.482859	1.714696
32.	8.	0.	-0.995742	-3.401743	2.783889
33.	1.	0.	-0.975998	-1.696794	-2.927196
34.	1.	0.	0.546463	-1.663634	3.073662
35.	1.	0.	5.084064	3.139877	-0.460893
36.	1.	0.	3.410633	3.385545	1.370179
37.	1.	0.	1.331516	2.083140	1.341519
38.	1.	0.	4.645650	1.577889	-2.330728
39.	1.	0.	1.080967	-1.341446	-3.505179
40.	1.	0.	3.193220	-0.073752	-3.436082
41.	1.	0.	-3.029024	1.032165	3.457536
42.	1.	0.	-1.326470	-0.742448	3.617460
43.	1.	0.	-0.787591	2.254826	-1.481306
44.	1.	0.	-2.429197	4.072318	-1.592101
45.	1.	0.	-4.057822	4.422282	0.263544
46.	1.	0.	-4.009142	2.932446	2.241168
47.	1.	0.	-2.886606	-1.059131	-1.823830
48.	1.	0.	2.103956	-0.664984	0.963147
49.	1.	0.	-0.684239	-5.705189	-0.985620
50.	1.	0.	-0.691270	-5.601036	1.407227

Figure S16. Density functional calculation for the **SS** diastereomer from the reaction of (*S*)-**2** with maleic acid.



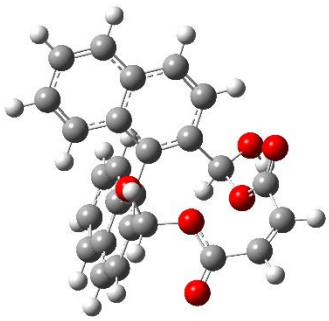
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-311G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1453.340648

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.260374	4.643448	-1.252908
2	6	0	1.828510	3.497846	-1.855721
3	6	0	1.568002	2.242930	-1.358249
4	6	0	0.722570	2.062618	-0.228137
5	6	0	0.156967	3.226802	0.382939
6	6	0	0.443707	4.507990	-0.157027
7	6	0	0.430330	0.766537	0.315718
8	6	0	-0.385883	0.659418	1.436129
9	6	0	-0.922904	1.826876	2.037169
10	6	0	-0.668026	3.070296	1.523901
11	6	0	1.058694	-0.441024	-0.323616
12	6	0	2.287769	-0.952009	0.214505
13	6	0	2.894773	-2.101210	-0.386614
14	6	0	2.272657	-2.701600	-1.510414
15	6	0	1.111010	-2.188198	-2.021352
16	6	0	0.499166	-1.051593	-1.435457
17	6	0	2.937767	-0.356346	1.330825
18	6	0	4.111932	-0.872648	1.826437
19	6	0	4.702977	-2.011862	1.234279
20	6	0	4.106210	-2.609647	0.151057

21	6	0	-0.676604	-0.704459	2.054007
22	6	0	-0.792348	-0.554874	-2.038015
23	8	0	-1.814592	-1.336191	1.341870
24	8	0	-1.864359	-1.310666	-1.357899
25	6	0	-3.109590	-0.896936	-1.589111
26	6	0	-4.127228	-1.462468	-0.656955
27	6	0	-4.095843	-1.482608	0.679783
28	6	0	-3.053164	-0.929800	1.596165
29	8	0	-0.858629	-0.720955	3.425903
30	8	0	-3.368511	-0.184227	2.507064
31	8	0	-3.418539	-0.129728	-2.480488
32	1	0	1.473035	5.626094	-1.657821
33	1	0	2.475384	3.611325	-2.718059
34	1	0	2.009945	1.376429	-1.833010
35	1	0	0.005234	5.380424	0.315227
36	1	0	-1.545511	1.736653	2.916583
37	1	0	-1.089980	3.951903	1.993678
38	1	0	2.733110	-3.572627	-1.963609
39	1	0	0.644131	-2.638429	-2.887322
40	1	0	2.499338	0.517349	1.796185
41	1	0	4.589931	-0.402170	2.677975
42	1	0	5.627566	-2.409184	1.636875
43	1	0	4.553963	-3.481999	-0.312581
44	1	0	0.131103	-1.396153	1.836242
45	1	0	-5.046487	-1.752037	-1.154754
46	1	0	-4.992484	-1.787124	1.209227
47	1	0	-1.691502	-0.263673	3.617787
48	8	0	-0.817974	-0.786683	-3.404539
49	1	0	-1.623834	-0.367253	-3.738428
50	1	0	-0.983051	0.493191	-1.805505

Figure S17. Density functional calculation for the **SR** diastereomer from the reaction of (*S*)-**2** with maleic acid.



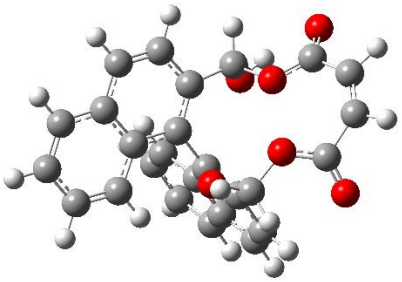
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-311G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1453.335988

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.277523	-3.551931	1.642356
2	6	0	3.272612	-2.191452	2.027578
3	6	0	2.437764	-1.291379	1.409545
4	6	0	1.555903	-1.698188	0.367731
5	6	0	1.570252	-3.076833	-0.020094
6	6	0	2.444066	-3.981500	0.639717
7	6	0	0.669447	-0.776492	-0.289677
8	6	0	-0.144376	-1.239437	-1.317999
9	6	0	-0.114982	-2.610298	-1.685550
10	6	0	0.709845	-3.505309	-1.058765
11	6	0	0.693454	0.657685	0.164748
12	6	0	1.601535	1.573068	-0.466776
13	6	0	1.676137	2.923563	-0.003165
14	6	0	0.853396	3.325644	1.080217
15	6	0	0.016644	2.431921	1.689367
16	6	0	-0.066161	1.086516	1.244063
17	6	0	2.457674	1.182892	-1.531897
18	6	0	3.330998	2.075824	-2.105990
19	6	0	3.391707	3.413698	-1.652676
20	6	0	2.579515	3.825816	-0.624396
21	6	0	-1.099138	-0.381578	-2.128660

22	6	0	-0.916516	0.108257	2.034097
23	8	0	-2.273997	-0.005450	-1.323819
24	8	0	-2.250357	-0.137793	1.454229
25	6	0	-3.131128	0.856301	1.270212
26	6	0	-4.382657	0.376241	0.607076
27	6	0	-4.477985	-0.309774	-0.533936
28	6	0	-3.358351	-0.795108	-1.382100
29	8	0	-0.507842	0.794985	-2.547555
30	8	0	-3.451510	-1.791466	-2.067483
31	8	0	-3.000486	2.003585	1.623386
32	1	0	3.940610	-4.250368	2.139669
33	1	0	3.935059	-1.855781	2.817224
34	1	0	2.449866	-0.254400	1.718420
35	1	0	2.439578	-5.022219	0.334062
36	1	0	-0.770473	-2.947709	-2.479496
37	1	0	0.715786	-4.548202	-1.355696
38	1	0	0.907843	4.351029	1.429998
39	1	0	-0.596154	2.733196	2.525762
40	1	0	2.411555	0.166267	-1.899486
41	1	0	3.975440	1.754886	-2.916602
42	1	0	4.080530	4.109649	-2.117927
43	1	0	2.619859	4.849032	-0.266149
44	1	0	-1.484840	-0.967133	-2.963115
45	1	0	-5.289695	0.686158	1.115405
46	1	0	-5.454910	-0.596259	-0.906232
47	1	0	-1.071897	1.197847	-3.218902
48	8	0	-1.020856	0.527001	3.354212
49	1	0	-1.355214	-0.208370	3.880787
50	1	0	-0.495628	-0.893424	1.968361

Figure S18. Density functional calculation for the RR diastereomer from the reaction of (*S*)-**2** with maleic acid.



Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-311G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1453.332054

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.623650	-2.195812	-1.075235
2	6	0	-4.081323	-1.037297	-1.678957
3	6	0	-2.887435	-0.515269	-1.243625
4	6	0	-2.164845	-1.113813	-0.174168
5	6	0	-2.722583	-2.281773	0.435739
6	6	0	-3.955370	-2.803063	-0.041769
7	6	0	-0.920212	-0.576750	0.304622
8	6	0	-0.297090	-1.185069	1.388453
9	6	0	-0.862248	-2.349984	1.971267
10	6	0	-2.033858	-2.888855	1.512911
11	6	0	-0.415394	0.691446	-0.333440
12	6	0	-0.894503	1.933184	0.213996
13	6	0	-0.498146	3.176557	-0.372760
14	6	0	0.360364	3.160149	-1.497313
15	6	0	0.783641	1.970409	-2.023154
16	6	0	0.398142	0.722549	-1.462383
17	6	0	-1.780028	1.980318	1.327301
18	6	0	-2.238388	3.175780	1.825562
19	6	0	-1.833870	4.400810	1.246024
20	6	0	-0.980734	4.397298	0.171150
21	6	0	0.983200	-0.705729	2.041657

22	6	0	0.924232	-0.488431	-2.217848
23	8	0	2.067695	-0.943193	1.089726
24	8	0	2.073950	-1.096690	-1.514415
25	6	0	3.266531	-0.522877	-1.640731
26	6	0	4.334704	-1.094119	-0.761794
27	6	0	4.365482	-1.208485	0.570982
28	6	0	3.312286	-0.882987	1.568554
29	8	0	0.934820	0.633591	2.403750
30	8	0	-0.024133	-1.483224	-2.337901
31	8	0	3.581723	-0.597045	2.719919
32	8	0	3.531429	0.382035	-2.404680
33	1	0	-5.565122	-2.599049	-1.430448
34	1	0	-4.612109	-0.560249	-2.495081
35	1	0	-2.482408	0.364066	-1.725774
36	1	0	-4.360406	-3.691040	0.431746
37	1	0	-0.349947	-2.814375	2.806491
38	1	0	-2.449930	-3.776369	1.976733
39	1	0	0.666005	4.099185	-1.945564
40	1	0	1.436136	1.965883	-2.887062
41	1	0	-2.092213	1.055582	1.792553
42	1	0	-2.913351	3.181676	2.673968
43	1	0	-2.199957	5.336917	1.652047
44	1	0	-0.664144	5.328735	-0.285958
45	1	0	1.205253	-1.331400	2.907871
46	1	0	1.304068	-0.163867	-3.187526
47	1	0	5.253950	-1.285893	-1.306130
48	1	0	5.300608	-1.492091	1.040843
49	1	0	1.684292	0.789654	2.994569
50	1	0	0.281972	-2.120276	-2.994720

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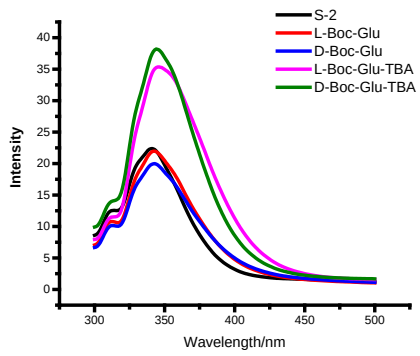
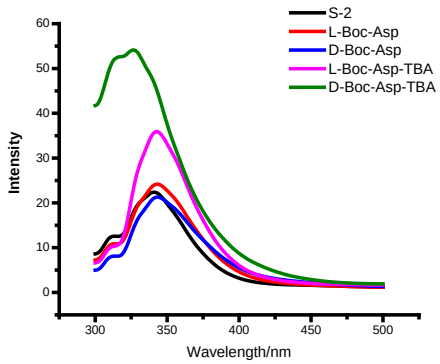
8. Fluorescence Responses of (S)-2 toward L- and D-Boc-Glu, L- and D-Boc-Asp, 4-Aminobutyric Acid, L- and D-Glutamic Acid Dimethyl Esters

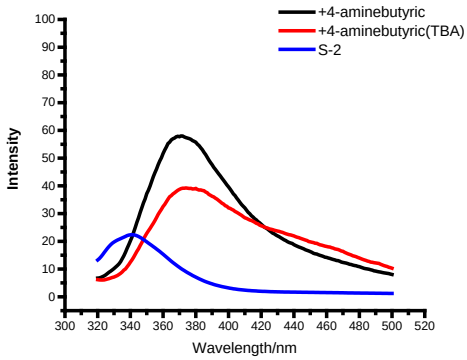
Figure S19. Fluorescence spectra of (*S*)-**2** (25 μL, 2.0×10^{-3} M in CH_2Cl_2) with (a) L/D-Boc-Glu (5 equiv, 1.0×10^{-2} M in methanol), (b) L/D-Boc-Asp(5 equiv, 1.0×10^{-2} M in methanol). (c) 4-amino butyric acid and its TBA salt (5 equiv, 1.0×10^{-2} M in methanol). (d) dimethyl ester of L-Glu (5 equiv, 1.0×10^{-2} M in methanol). The mixture was allowed to stand at 300 K for 90 min and each of the solutions was diluted with methanol to 2.5 mL and its fluorescent spectrum was obtained. (Solvent: MeOH/ CH_2Cl_2 = 99/1, v/v. λ_{exc} = 280 nm. Slit: 5/5 nm).



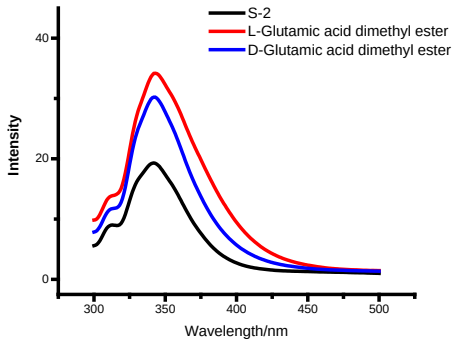
(a)



(b)



(c)



(d)

9. Molecular Modeling Study of the Proposed Intermediate 5

Figure S20. Eight possible diastereomeric structures of the intermediates for the reaction of (*S*)-**2** with L-Glu.

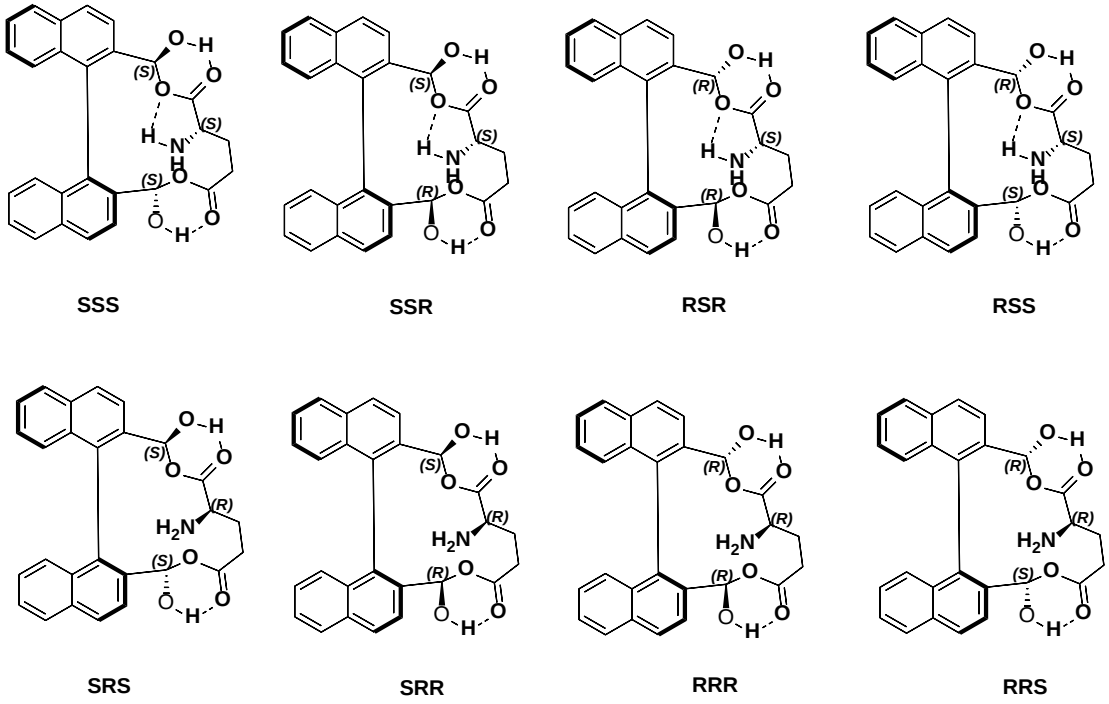
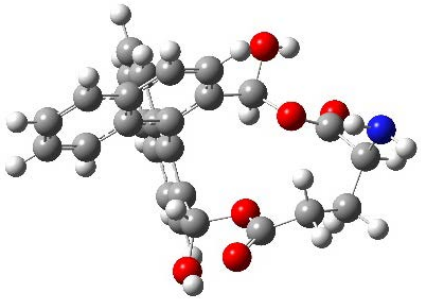


Figure S21. Density functional calculation for the intermediate **SSS** from the reaction of (*S*)-**2** with L-Glu.



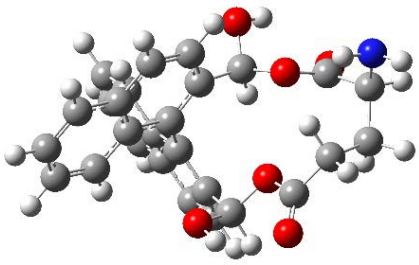
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.915884

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.248050	4.239716	-0.152832
2	6	0	-3.511495	3.160566	0.723993
3	6	0	-2.788608	1.991134	0.632068
4	6	0	-1.761547	1.838688	-0.341348
5	6	0	-1.501096	2.932873	-1.231496
6	6	0	-2.264317	4.124980	-1.109155
7	6	0	-0.985179	0.635061	-0.459174
8	6	0	-0.008642	0.549343	-1.442827
9	6	0	0.233864	1.636525	-2.323449
10	6	0	-0.487945	2.797992	-2.218654
11	6	0	-1.258792	-0.522901	0.461539
12	6	0	-2.166581	-1.553680	0.040832
13	6	0	-2.411197	-2.671519	0.905613
14	6	0	-1.747129	-2.734054	2.158434
15	6	0	-0.888112	-1.736432	2.545902
16	6	0	-0.642479	-0.620972	1.704062
17	6	0	-2.842373	-1.510385	-1.211738
18	6	0	-3.709869	-2.513182	-1.584761
19	6	0	-3.947999	-3.614994	-0.728219
20	6	0	-3.311006	-3.689868	0.489417
21	8	0	1.631003	0.166243	1.597219
22	6	0	2.547482	1.128938	1.808240
23	6	0	3.813536	0.968613	0.997882
24	6	0	0.302560	0.454485	2.186278
25	8	0	2.346022	2.079571	2.551381
26	7	0	5.018175	-0.131075	-1.657728
27	6	0	4.401319	-1.001082	-0.651569
28	6	0	3.018735	-1.408487	-1.143863
29	8	0	2.664446	-2.560117	-1.329276
30	6	0	4.361400	-0.465332	0.809092
31	1	0	-3.824738	5.155782	-0.069196
32	1	0	-4.290756	3.255586	1.474067
33	1	0	-3.000648	1.170568	1.308750
34	1	0	-2.056000	4.947104	-1.788292
35	1	0	1.002146	1.531877	-3.082233
36	1	0	-0.296114	3.628600	-2.891976
37	1	0	-1.931360	-3.584185	2.809226
38	1	0	-0.390660	-1.778410	3.507431
39	1	0	-2.665395	-0.674042	-1.878432
40	1	0	-4.215622	-2.459714	-2.544068
41	1	0	-4.633340	-4.398898	-1.035830

42	1	0	-3.486159	-4.531284	1.154211
43	1	0	4.555412	1.614137	1.470918
44	1	0	3.586863	1.427697	0.027857
45	1	0	4.502892	0.742240	-1.737790
46	1	0	5.961287	0.111028	-1.361179
47	1	0	4.972608	-1.933259	-0.630173
48	1	0	3.806546	-1.176498	1.429694
49	1	0	5.394255	-0.488045	1.170529
50	8	0	2.207950	-0.350996	-1.336021
51	6	0	0.806085	-0.704507	-1.620133
52	8	0	0.687549	-1.175957	-2.923906
53	1	0	1.098070	-2.056168	-2.927491
54	1	0	0.541864	-1.469888	-0.891138
55	8	0	0.373341	0.458884	3.570195
56	1	0	0.914821	1.235646	3.792989
57	1	0	0.028928	1.437515	1.794655

Figure S22. Density functional calculation for the intermediate **SSR** from the reaction of (*S*)-**2** with L-Glu.



Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.911859

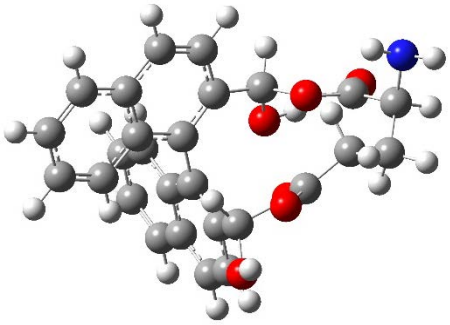
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.281132	4.160763	-0.211419
2	6	0	-3.534196	3.096884	0.687641
3	6	0	-2.775517	1.948231	0.644134

4	6	0	-1.725126	1.796856	-0.303214
5	6	0	-1.476486	2.873632	-1.216405
6	6	0	-2.272194	4.049019	-1.140851
7	6	0	-0.923980	0.606514	-0.381093
8	6	0	0.056148	0.512449	-1.359779
9	6	0	0.294751	1.587004	-2.257211
10	6	0	-0.445725	2.738753	-2.185185
11	6	0	-1.227309	-0.557592	0.525360
12	6	0	-2.193602	-1.523328	0.073829
13	6	0	-2.512671	-2.653759	0.897887
14	6	0	-1.859940	-2.800474	2.146843
15	6	0	-0.937513	-1.871749	2.559262
16	6	0	-0.611321	-0.743151	1.761893
17	6	0	-2.858246	-1.403851	-1.181357
18	6	0	-3.780893	-2.340223	-1.590677
19	6	0	-4.092843	-3.452267	-0.771292
20	6	0	-3.469771	-3.603148	0.445552
21	8	0	1.598720	0.208916	1.501830
22	6	0	2.619155	0.968681	1.945265
23	6	0	3.814551	0.949657	1.021760
24	6	0	0.398132	0.214457	2.356926
25	8	0	2.555349	1.629310	2.972204
26	7	0	5.051325	-0.025419	-1.670368
27	6	0	4.495128	-0.947250	-0.677002
28	6	0	3.114417	-1.401177	-1.131153
29	8	0	2.774597	-2.565771	-1.251551
30	6	0	4.455452	-0.446475	0.796721
31	1	0	-3.885016	5.062007	-0.165149
32	1	0	-4.331789	3.189844	1.418686
33	1	0	-2.971955	1.144547	1.344313
34	1	0	-2.070149	4.858459	-1.837094
35	1	0	1.072974	1.478618	-3.005432
36	1	0	-0.259949	3.558166	-2.873927
37	1	0	-2.097711	-3.656089	2.772191
38	1	0	-0.442242	-1.994170	3.517939
39	1	0	-2.627982	-0.561363	-1.822606
40	1	0	-4.273963	-2.226339	-2.551334
41	1	0	-4.822166	-4.182963	-1.107384
42	1	0	-3.697858	-4.453105	1.082770
43	1	0	4.540188	1.644988	1.445166
44	1	0	3.473425	1.374162	0.071882
45	1	0	4.495544	0.825366	-1.714403
46	1	0	5.988045	0.251627	-1.384360
47	1	0	5.107099	-1.853543	-0.686380

48	1	0	3.958960	-1.207071	1.409444
49	1	0	5.493362	-0.410987	1.141529
50	8	0	-0.127562	1.493224	2.464266
51	1	0	0.529470	1.999772	2.973071
52	1	0	0.737899	-0.157215	3.329221
53	8	0	2.282392	-0.366065	-1.345577
54	6	0	0.871059	-0.741833	-1.528518
55	8	0	0.681976	-1.272434	-2.802277
56	1	0	1.102282	-2.147932	-2.791456
57	1	0	0.656491	-1.476021	-0.752771

Figure S23. Density functional calculation for the intermediate **RSS** from the reaction of (*S*)-**2** with L-Glu.



Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.907212

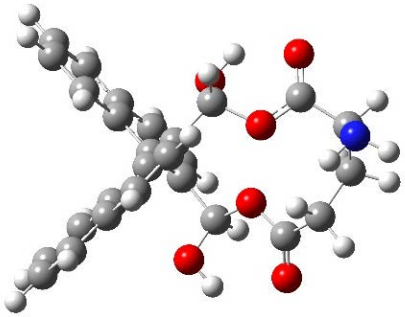
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.089797	4.290235	-0.159220
2	6	0	-3.400614	3.182287	0.664294
3	6	0	-2.706350	1.998761	0.540161
4	6	0	-1.659686	1.853991	-0.415626
5	6	0	-1.353867	2.979489	-1.249582
6	6	0	-2.087303	4.186840	-1.096178
7	6	0	-0.915959	0.626599	-0.558752
8	6	0	0.070116	0.547761	-1.538929
9	6	0	0.353333	1.675212	-2.358620

10	6	0	-0.325428	2.857231	-2.218502
11	6	0	-1.269286	-0.513137	0.359232
12	6	0	-2.263896	-1.464535	-0.050150
13	6	0	-2.611403	-2.542923	0.826835
14	6	0	-1.964831	-2.644242	2.087048
15	6	0	-1.042067	-1.706289	2.474418
16	6	0	-0.700362	-0.623022	1.622108
17	6	0	-2.929917	-1.377057	-1.304021
18	6	0	-3.885931	-2.299295	-1.668379
19	6	0	-4.223889	-3.365600	-0.800380
20	6	0	-3.597247	-3.482646	0.419414
21	8	0	1.614312	0.069610	1.640162
22	6	0	2.545250	1.010567	1.869611
23	6	0	3.830698	0.816293	1.097685
24	6	0	0.266777	0.417082	2.137291
25	8	0	2.343940	1.978602	2.591497
26	7	0	5.208474	-0.127932	-1.511130
27	6	0	4.476815	-1.053386	-0.637015
28	6	0	3.154810	-1.386455	-1.326565
29	8	0	2.949006	-2.432868	-1.925049
30	6	0	4.303676	-0.633790	0.848144
31	1	0	-3.644207	5.217298	-0.050181
32	1	0	-4.195031	3.265542	1.399756
33	1	0	-2.959127	1.159925	1.178088
34	1	0	-1.839934	5.028772	-1.736835
35	1	0	1.129740	1.586588	-3.113161
36	1	0	-0.092177	3.706197	-2.854514
37	1	0	-2.222757	-3.467988	2.746880
38	1	0	-0.571066	-1.765802	3.448454
39	1	0	-2.674237	-0.569536	-1.980816
40	1	0	-4.383154	-2.211004	-2.629750
41	1	0	-4.976888	-4.088172	-1.100381
42	1	0	-3.848482	-4.296663	1.094121
43	1	0	4.590756	1.398753	1.621609
44	1	0	3.654246	1.338059	0.149057
45	1	0	4.760174	0.785396	-1.518380
46	1	0	6.146387	0.012469	-1.141590
47	1	0	5.027358	-1.998175	-0.643347
48	1	0	3.632049	-1.345572	1.337978
49	1	0	5.281939	-0.762348	1.322177
50	8	0	2.247257	-0.408808	-1.206909
51	6	0	0.923431	-0.667996	-1.840788
52	8	0	0.383492	-1.850427	-1.391488
53	1	0	0.983460	-2.545960	-1.716236

54	1	0	1.143534	-0.706374	-2.914506
55	8	0	0.254272	0.450544	3.524741
56	1	0	0.819501	1.206282	3.761022
57	1	0	0.057935	1.402756	1.713628

Figure S24. Density functional calculation for the intermediate **RSR** from the reaction of (*S*)-**2** with L-Glu.



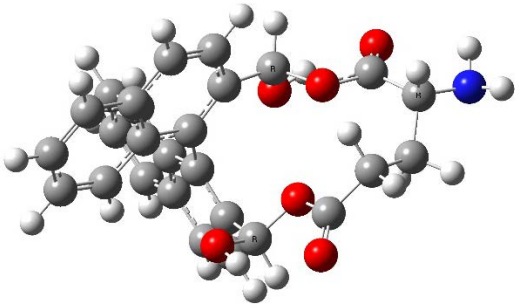
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.903085

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.021733	4.267145	-0.211768
2	6	0	-3.346702	3.181400	0.636119
3	6	0	-2.648145	1.997098	0.558593
4	6	0	-1.586879	1.824105	-0.374774
5	6	0	-1.269277	2.924977	-1.235275
6	6	0	-2.002184	4.138061	-1.126394
7	6	0	-0.850881	0.588037	-0.479942
8	6	0	0.131029	0.474961	-1.459727
9	6	0	0.431881	1.581277	-2.302491
10	6	0	-0.234365	2.772837	-2.193299
11	6	0	-1.263198	-0.547595	0.420994
12	6	0	-2.312994	-1.417604	-0.038396
13	6	0	-2.760762	-2.498178	0.790532
14	6	0	-2.156570	-2.689196	2.058193

15	6	0	-1.169725	-1.837929	2.486215
16	6	0	-0.717735	-0.755041	1.685374
17	6	0	-2.939263	-1.248972	-1.306685
18	6	0	-3.944707	-2.091585	-1.725455
19	6	0	-4.381534	-3.157276	-0.901732
20	6	0	-3.798592	-3.353785	0.328418
21	8	0	1.534517	0.133880	1.507238
22	6	0	2.572423	0.830196	2.005689
23	6	0	3.779757	0.804066	1.097473
24	6	0	0.320851	0.136778	2.332152
25	8	0	2.516301	1.444666	3.061988
26	7	0	5.214384	-0.005218	-1.522569
27	6	0	4.563518	-0.995116	-0.657560
28	6	0	3.244433	-1.407164	-1.307331
29	8	0	3.037427	-2.504892	-1.804524
30	6	0	4.369818	-0.608289	0.835820
31	1	0	-3.578234	5.196652	-0.138487
32	1	0	-4.152979	3.284958	1.356169
33	1	0	-2.902800	1.180561	1.222901
34	1	0	-1.742942	4.961330	-1.786540
35	1	0	1.209945	1.465839	-3.051709
36	1	0	0.009184	3.604037	-2.848826
37	1	0	-2.489072	-3.510096	2.687088
38	1	0	-0.720763	-1.985205	3.464256
39	1	0	-2.614016	-0.441906	-1.952626
40	1	0	-4.406147	-1.939360	-2.696612
41	1	0	-5.174525	-3.815376	-1.243932
42	1	0	-4.123634	-4.167814	0.970697
43	1	0	4.524604	1.461818	1.547022
44	1	0	3.454551	1.265057	0.159939
45	1	0	4.697709	0.871183	-1.509019
46	1	0	6.142140	0.200103	-1.157718
47	1	0	5.177504	-1.899615	-0.681818
48	1	0	3.753479	-1.377475	1.314049
49	1	0	5.353433	-0.668038	1.311692
50	8	0	-0.165002	1.429310	2.492495
51	1	0	0.499938	1.886316	3.036704
52	1	0	0.625109	-0.288761	3.294463
53	8	0	2.331019	-0.432296	-1.243821
54	6	0	0.967450	-0.755204	-1.748785
55	8	0	0.487020	-1.909329	-1.176510
56	1	0	1.069950	-2.620150	-1.498294
57	1	0	1.101145	-0.866276	-2.832101

Figure S25. Density functional calculation for the intermediate **RRR** from the reaction of (*S*)-**2** with D-Glu.



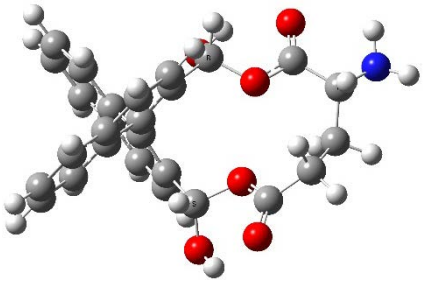
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.905573

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.693365	3.808542	-0.399696
2	6	0	-3.833115	2.732724	0.509511
3	6	0	-2.953060	1.673781	0.484233
4	6	0	-1.884883	1.621844	-0.455889
5	6	0	-1.754327	2.711218	-1.377562
6	6	0	-2.672253	3.795176	-1.321414
7	6	0	-0.961435	0.514975	-0.509565
8	6	0	0.015555	0.504540	-1.500699
9	6	0	0.131554	1.600606	-2.400857
10	6	0	-0.714065	2.676250	-2.341051
11	6	0	-1.172709	-0.615153	0.464581
12	6	0	-2.073447	-1.670238	0.083729
13	6	0	-2.333218	-2.750635	0.989304
14	6	0	-1.694602	-2.756667	2.254588
15	6	0	-0.854747	-1.731071	2.607721
16	6	0	-0.590639	-0.645927	1.729627
17	6	0	-2.731675	-1.688117	-1.179369
18	6	0	-3.591938	-2.706973	-1.522701
19	6	0	-3.842421	-3.772323	-0.624025
20	6	0	-3.223590	-3.790671	0.604105
21	8	0	1.508222	0.524309	1.457957

22	6	0	2.441387	1.402952	1.864187
23	6	0	3.651101	1.425660	0.957665
24	6	0	0.303344	0.441138	2.289224
25	8	0	2.296224	2.124601	2.841637
26	6	0	4.622510	-0.348203	-0.705898
27	6	0	3.368606	-0.905033	-1.375711
28	8	0	3.326682	-1.967263	-1.979255
29	6	0	4.352167	0.055977	0.766070
30	1	0	-4.391877	4.639234	-0.366861
31	1	0	-4.640205	2.744847	1.235979
32	1	0	-3.067379	0.865276	1.195704
33	1	0	-2.552751	4.612467	-2.027502
34	1	0	0.911989	1.570751	-3.155951
35	1	0	-0.610369	3.500799	-3.040555
36	1	0	-1.884859	-3.576403	2.941458
37	1	0	-0.379548	-1.738636	3.584411
38	1	0	-2.547114	-0.883439	-1.881375
39	1	0	-4.081959	-2.695321	-2.491734
40	1	0	-4.521822	-4.570489	-0.907554
41	1	0	-3.406510	-4.601848	1.303658
42	1	0	4.339730	2.165147	1.369784
43	1	0	3.297748	1.805261	-0.006195
44	1	0	3.784863	-0.745664	1.247265
45	1	0	5.324418	0.085762	1.265805
46	8	0	-0.357531	1.662863	2.331875
47	1	0	0.242344	2.259791	2.812983
48	1	0	0.658069	0.152896	3.284958
49	8	0	2.314659	-0.097470	-1.221610
50	6	0	1.024235	-0.598060	-1.755877
51	8	0	0.695497	-1.809761	-1.188933
52	1	0	1.339711	-2.447454	-1.540793
53	1	0	1.191939	-0.695669	-2.834750
54	7	0	5.656517	-1.380919	-0.740786
55	1	0	5.664825	-1.817025	-1.659476
56	1	0	6.565234	-0.943245	-0.611950
57	1	0	4.888055	0.563291	-1.270567

Figure S26. Density functional calculation for the intermediate **RRS** from the reaction of (*S*)-**2** with D-Glu.



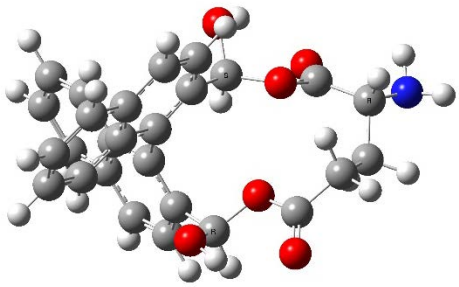
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.910219

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.762602	-3.807545	-0.313415
2	6	0	3.880639	-2.704372	0.565004
3	6	0	3.005063	-1.643976	0.481800
4	6	0	1.960084	-1.624018	-0.486560
5	6	0	1.849174	-2.743799	-1.375138
6	6	0	2.766730	-3.823029	-1.262788
7	6	0	1.028847	-0.527174	-0.587941
8	6	0	0.053825	-0.561578	-1.581867
9	6	0	-0.034338	-1.681079	-2.455239
10	6	0	0.824577	-2.744007	-2.355357
11	6	0	1.178584	0.604613	0.394025
12	6	0	2.009412	1.726592	0.058407
13	6	0	2.166760	2.793790	1.001469
14	6	0	1.499417	2.714848	2.252543
15	6	0	0.738077	1.618512	2.568651
16	6	0	0.586992	0.546351	1.650029
17	6	0	2.696070	1.820749	-1.183865
18	6	0	3.494211	2.904608	-1.475934
19	6	0	3.643588	3.959302	-0.543205
20	6	0	2.991294	3.902618	0.667346
21	8	0	-1.589176	-0.476184	1.600018

22	6	0	-2.374199	-1.559850	1.721799
23	6	0	-3.666209	-1.475648	0.940485
24	6	0	-0.209686	-0.662203	2.082512
25	8	0	-2.039713	-2.550059	2.358412
26	6	0	-4.556997	0.346193	-0.702324
27	6	0	-3.297050	0.855651	-1.398400
28	8	0	-3.262921	1.871261	-2.078768
29	6	0	-4.302135	-0.078989	0.764512
30	1	0	4.458580	-4.637199	-0.235936
31	1	0	4.669534	-2.693476	1.310961
32	1	0	3.110160	-0.807089	1.162089
33	1	0	2.665139	-4.662655	-1.944849
34	1	0	-0.806553	-1.683524	-3.219165
35	1	0	0.738494	-3.589160	-3.032092
36	1	0	1.612956	3.529414	2.962517
37	1	0	0.253133	1.543890	3.534898
38	1	0	2.582521	1.023612	-1.910036
39	1	0	4.011069	2.953567	-2.429721
40	1	0	4.272861	4.810163	-0.786418
41	1	0	3.099512	4.706056	1.391004
42	1	0	-4.359228	-2.174206	1.414270
43	1	0	-3.420136	-1.906134	-0.038019
44	1	0	-3.702863	0.690269	1.256979
45	1	0	-5.277168	-0.074519	1.260005
46	8	0	-2.235546	0.064542	-1.201369
47	6	0	-0.978260	0.515049	-1.853366
48	8	0	-0.614012	1.763900	-1.401369
49	1	0	-1.283810	2.374456	-1.754559
50	1	0	-1.215785	0.530549	-2.922989
51	8	0	-0.189941	-0.794153	3.464912
52	1	0	-0.633223	-1.641246	3.642630
53	1	0	0.143609	-1.572752	1.592420
54	7	0	-5.553218	1.416504	-0.731397
55	1	0	-5.562526	1.839011	-1.656437
56	1	0	-6.474405	1.013094	-0.580584
57	1	0	-4.861301	-0.551778	-1.270979

Figure S27. Density functional calculation for the intermediate **SRR** from the reaction of (*S*)-**2** with D-Glu.



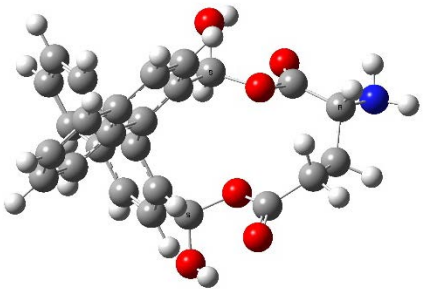
Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.913579

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.916825	3.662309	-0.398464
2	6	0	-3.999954	2.618541	0.554302
3	6	0	-3.071666	1.601065	0.560395
4	6	0	-2.012551	1.566735	-0.388492
5	6	0	-1.935902	2.621725	-1.355839
6	6	0	-2.904239	3.661890	-1.330624
7	6	0	-1.036254	0.512040	-0.414622
8	6	0	-0.058900	0.519025	-1.400085
9	6	0	0.008983	1.572532	-2.350647
10	6	0	-0.898216	2.600011	-2.326321
11	6	0	-1.146974	-0.627695	0.563662
12	6	0	-1.949701	-1.761125	0.189249
13	6	0	-2.084946	-2.868936	1.091292
14	6	0	-1.416056	-2.825522	2.339636
15	6	0	-0.651370	-1.737086	2.678012
16	6	0	-0.508476	-0.628737	1.802671
17	6	0	-2.627208	-1.832956	-1.062766
18	6	0	-3.391729	-2.928235	-1.396881
19	6	0	-3.522990	-4.017063	-0.500988
20	6	0	-2.881465	-3.985196	0.715165
21	8	0	1.527378	0.611165	1.438519

22	6	0	2.429076	1.550382	1.781720
23	6	0	3.612216	1.593912	0.842415
24	6	0	0.346909	0.511528	2.312566
25	8	0	2.275873	2.301015	2.734967
26	6	0	4.556301	-0.284061	-0.729786
27	6	0	3.262703	-0.924383	-1.216486
28	8	0	3.121822	-2.112988	-1.453755
29	6	0	4.395597	0.261520	0.714442
30	1	0	-4.653221	4.460259	-0.390848
31	1	0	-4.800842	2.623214	1.287633
32	1	0	-3.137730	0.813031	1.301522
33	1	0	-2.831223	4.456969	-2.067757
34	1	0	0.791092	1.545628	-3.101993
35	1	0	-0.842533	3.403561	-3.055416
36	1	0	-1.515409	-3.663328	3.023648
37	1	0	-0.141671	-1.714444	3.636683
38	1	0	-2.533844	-1.010106	-1.761695
39	1	0	-3.898642	-2.958651	-2.356601
40	1	0	-4.128866	-4.874292	-0.778189
41	1	0	-2.972297	-4.815302	1.410231
42	1	0	4.261812	2.395705	1.196558
43	1	0	3.217492	1.893995	-0.133471
44	1	0	3.948647	-0.523322	1.331711
45	1	0	5.407515	0.412607	1.100829
46	8	0	2.273291	-0.025778	-1.347323
47	6	0	0.932526	-0.606473	-1.536509
48	8	0	0.829649	-1.172838	-2.804196
49	1	0	1.405621	-1.955829	-2.788191
50	1	0	0.820281	-1.353196	-0.749507
51	7	0	5.610416	-1.295918	-0.733442
52	1	0	5.597343	-1.802897	-1.614880
53	1	0	6.512527	-0.829780	-0.677287
54	1	0	4.750622	0.570727	-1.399578
55	8	0	-0.361830	1.703413	2.333972
56	1	0	0.224169	2.342217	2.776854
57	1	0	0.743420	0.268276	3.304260

Figure S28. Density functional calculation for the intermediate **SRS** from the reaction of (*S*)-**2** with D-Glu.



Calculation Type	FOPT
Calculation Method	RB3LYP
Basis Set	6-31G(d,p)
Charge	0
Spin	Singlet
Solvation	scrf=solvent=methanol
E(RB3LYP)	-1548.917899

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.973816	3.664457	-0.307532
2	6	0	-4.036998	2.596198	0.618518
3	6	0	-3.117422	1.571238	0.568804
4	6	0	-2.084991	1.559220	-0.410713
5	6	0	-2.026980	2.641603	-1.349824
6	6	0	-2.989243	3.683771	-1.269636
7	6	0	-1.109511	0.505790	-0.487452
8	6	0	-0.142681	0.546805	-1.483150
9	6	0	-0.099103	1.622162	-2.410091
10	6	0	-1.010786	2.644276	-2.342866
11	6	0	-1.165478	-0.630090	0.497425
12	6	0	-1.880348	-1.827160	0.153444
13	6	0	-1.920519	-2.915013	1.087568
14	6	0	-1.249923	-2.782416	2.331527
15	6	0	-0.576487	-1.628146	2.644666
16	6	0	-0.535025	-0.541534	1.733601
17	6	0	-2.558773	-1.980260	-1.089040
18	6	0	-3.239002	-3.140205	-1.387627
19	6	0	-3.276417	-4.211438	-0.462712
20	6	0	-2.629987	-4.098558	0.747056
21	8	0	1.566231	0.597916	1.532073
22	6	0	2.312837	1.713498	1.632029

23	6	0	3.574859	1.680683	0.799988
24	6	0	0.218625	0.707451	2.127689
25	8	0	1.967570	2.680222	2.296752
26	6	0	4.481772	-0.245956	-0.727602
27	6	0	3.190389	-0.867775	-1.245222
28	8	0	3.062802	-2.043245	-1.547900
29	6	0	4.315443	0.327216	0.704092
30	1	0	-4.704139	4.466217	-0.256799
31	1	0	-4.817414	2.584722	1.373293
32	1	0	-3.175657	0.757224	1.282823
33	1	0	-2.932898	4.498537	-1.986247
34	1	0	0.669774	1.618093	-3.175196
35	1	0	-0.971178	3.466314	-3.051967
36	1	0	-1.278857	-3.609406	3.035450
37	1	0	-0.073927	-1.523657	3.598888
38	1	0	-2.533868	-1.169036	-1.808039
39	1	0	-3.750464	-3.235501	-2.340650
40	1	0	-3.815249	-5.120454	-0.711998
41	1	0	-2.651744	-4.915149	1.463450
42	1	0	4.224929	2.460583	1.201158
43	1	0	3.265597	2.015676	-0.197264
44	1	0	3.838751	-0.430204	1.331543
45	1	0	5.327774	0.457508	1.097392
46	8	0	2.193838	0.027881	-1.345840
47	6	0	0.871604	-0.556538	-1.640087
48	8	0	0.839208	-1.043067	-2.942566
49	1	0	1.422100	-1.821065	-2.946175
50	1	0	0.732517	-1.351752	-0.906802
51	8	0	0.301064	0.818695	3.507278
52	1	0	0.702226	1.689573	3.668492
53	1	0	-0.219437	1.602663	1.679610
54	7	0	5.515572	-1.278700	-0.702906
55	1	0	5.502173	-1.797722	-1.577215
56	1	0	6.425987	-0.829749	-0.641568
57	1	0	4.706056	0.594574	-1.407320
