Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

Effective enantiomeric identification of aromatic amines by tyrosine-modified pillar[5]arenes chiral NMR solvating agents

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S1. The synthetic route of PCSA.

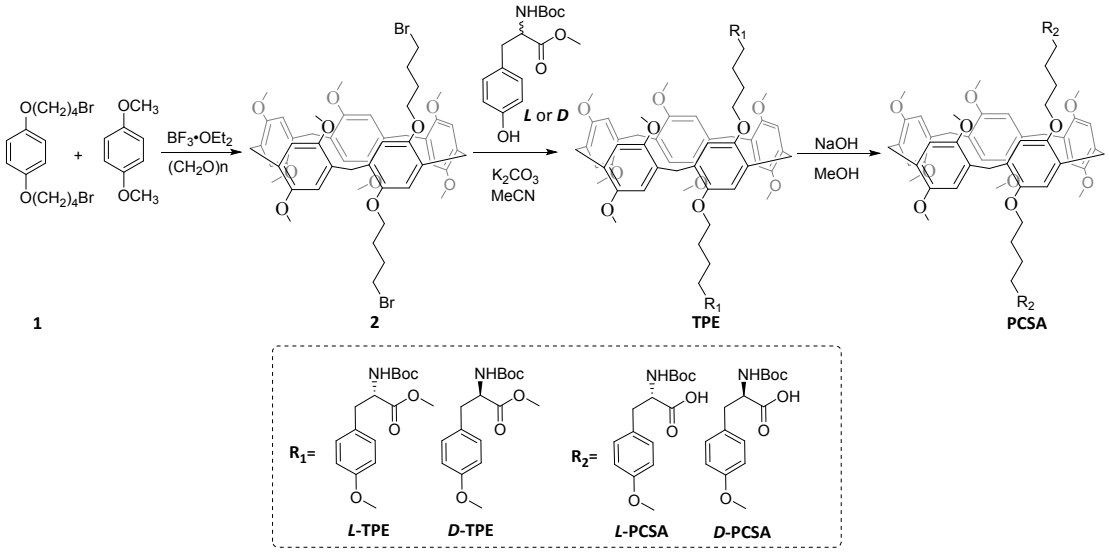


Fig. *S*1 The synthetic route of **PCSAs**.

S2. Experimental Section

2.1. General

The infrared spectra (KBr particle method) were recorded on the Nicolet is50 FT-IR spectrometer (Thermo Scientific Co., Ltd., Madison, WI, USA). ^{1}H NMR, ^{13}C NMR spectra were recorded in $CDCl_3$ solvent on Bruker avance III HD 600 MHz spectrometer (Bruker Ltd., Zurich, Switzerland). The chemical shifts were expressed in ppm (δ) relative to TMS as internal standard. Other reagents were purchased from commercial suppliers and used as received. The mass spectra were recorded on a TSQ Quantum Access MAX HPLC-MS instrument (Thermo Scientific Co., Ltd., Waltham, MA, USA). Melting points were determined on a MP420 automatic melting point apparatus (Hanon Instruments Co., Ltd., Jinan, China), and were not corrected. Other reagents were purchased from commercial suppliers and used as received.

2.2. Compound 2

Compound **1** was synthesized according to the literature[1]. To a solution of Compound **1** (2.00g, 5.26mmol) and 1,4-dimethoxybenzene (2.91g, 21.05mmol) in $ClCH_2CH_2Cl$ (80ml), paraformaldehyde (0.79g, 26.31mmol) was added at 30℃. Boron trifluoride diethyl etherate (7.10mL, 26.31mmol) was then added to the solution and the mixture was stirred at room temperature for 2 h and concentrated by rotary evaporation. The resultant oil was dissolved in CH_2Cl_2 and washed twice with H_2O. The organic layer was dried over anhydrous Na_2SO_4 and evaporated to afford the crude product, which was isolated by flash column chromatography using dichloromethane/petroleum ether (DCM/PE = 1/1, V/V) to give Compound **2** (1.56 g, 29.8%) as a white solid.

2.3. Compound TPE

Compound **2** (600mg, 0.60mmol), *D*- or *L*-type of N-tert-Butoxycarbonyl tyrosine methyl ester (892mg, 3.02mmol), K_2CO_3 (835mg, 6.04mmol) and KI (501mg,3.02mmol) were added to

acetonitrile (25ml) solution to prepare compound **TPE**, which reacted at 75℃ for 12 h. At the end of the reaction, deionized water (100ml) was added and the product was extracted with CH_2Cl_2 (3×40ml). The organic phase was collected and concentrated under reduced pressure. After column chromatography (silica gel, EA/PE= 10/1, V/V), pale yellow oily liquid was obtained. After vacuum distillation, white solid (78.5%) product ***D*-TPE** and ***L*-TPE** was obtained. ***D*-TPE** melting point:71.8-75.1℃; IR (KBr) cm^{-1}: 3437.29 (N-H), 2927.24, 2849.91 (C–H), 1717.92 (C=O), 1612.61 (N-H), 1499.09, 1461.24 (Ar–C=C), 1212.80, 1049.91 (Ar–O, C–O); ^{1}H NMR (600 MHz, Chloroform-d) δ 7.03 (d, J = 8.4 Hz, 4H), 6.83 (d, J = 8.6 Hz, 4H), 6.81 – 6.72 (m, 10H), 4.98 (d, J = 8.0 Hz, 2H), 4.55 (q, J = 5.9 Hz, 2H), 4.09–3.56 (m, 48H), 3.03 (ddt, J = 19.6, 14.0, 5.8 Hz, 4H), 2.10 – 1.87 (m, 8H), 1.43 (s, 18H);^{13}C NMR (151 MHz, Chloroform-d) δ 172.58, 150.98, 150.96, 150.90, 150.86, 150.11, 130.43, 128.47, 128.44, 128.42, 128.33, 128.24, 115.09, 114.62, 114.35, 114.18, 114.11, 68.13, 67.63, 55.96, 55.94, 55.90, 54.69, 52.33, 37.60, 29.85, 29.74, 26.65, 26.48;ESI–MS m/z: $C_{81}H_{100}N_2O_{20}$: 1438.70349 ([M+NH_4^+]).

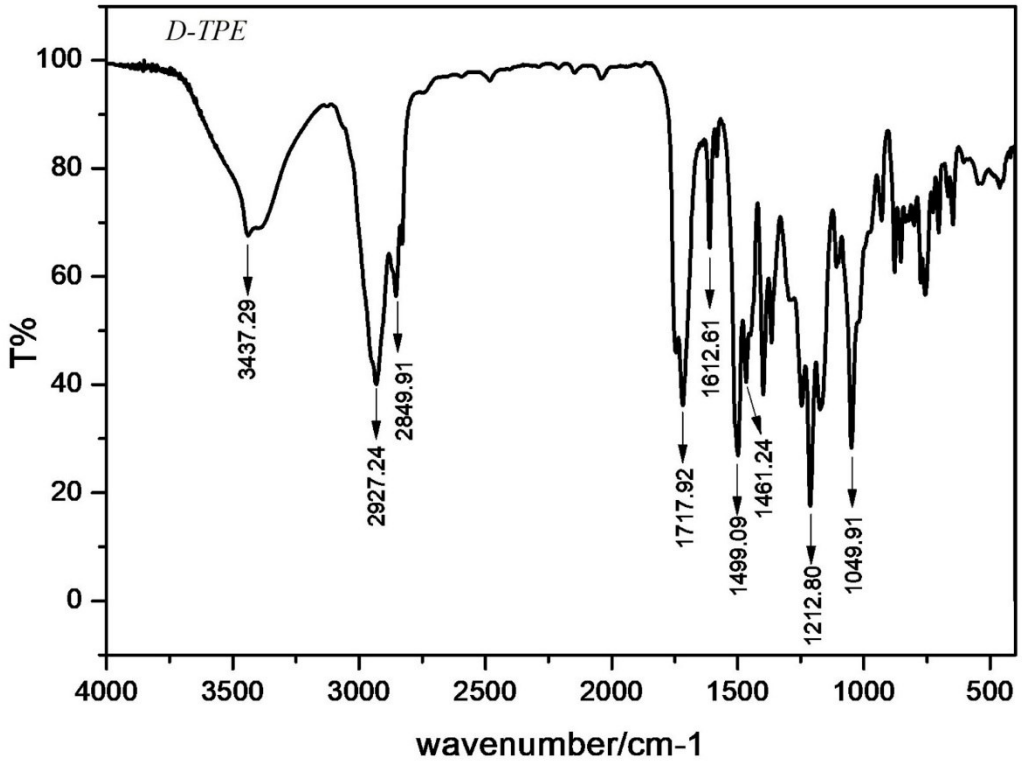


Fig. *S*2. FT-IR spectrum of ***D*-TPE**.

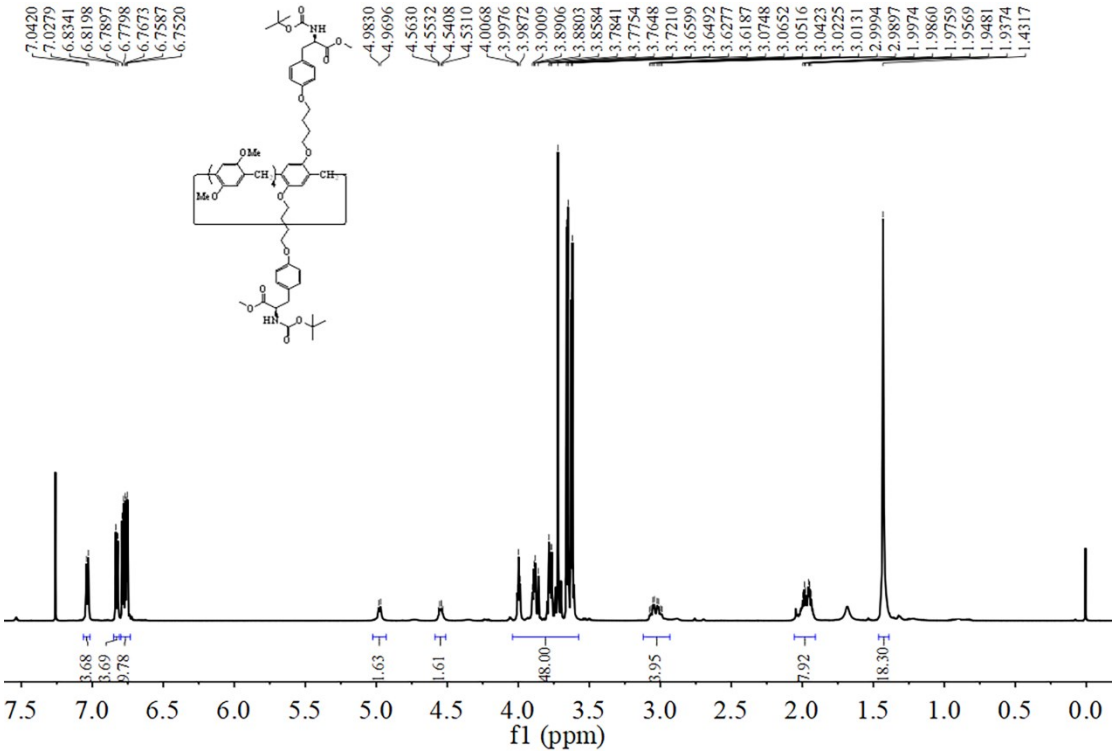


Fig. *S*3. ^{1}H NMR spectrum of ***D*-TPE** in $CDCl_3$.

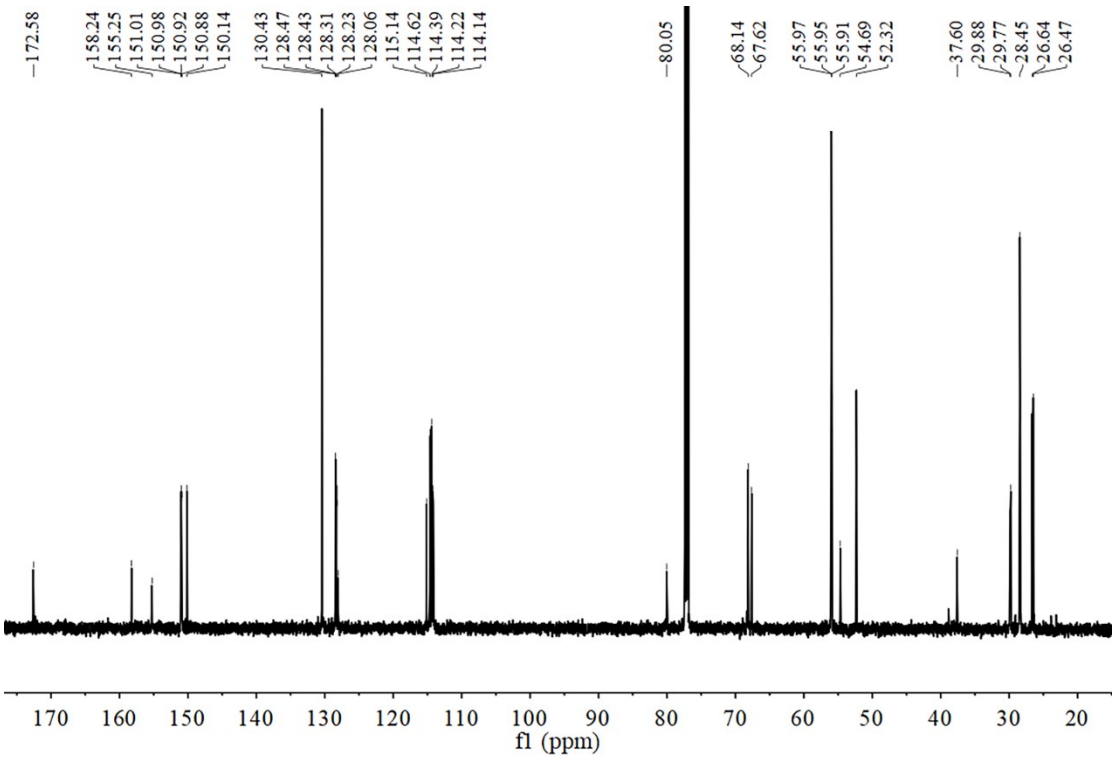


Fig. *S*4. ^{13}C NMR spectrum of ***D*-TPE** in $CDCl_3$.

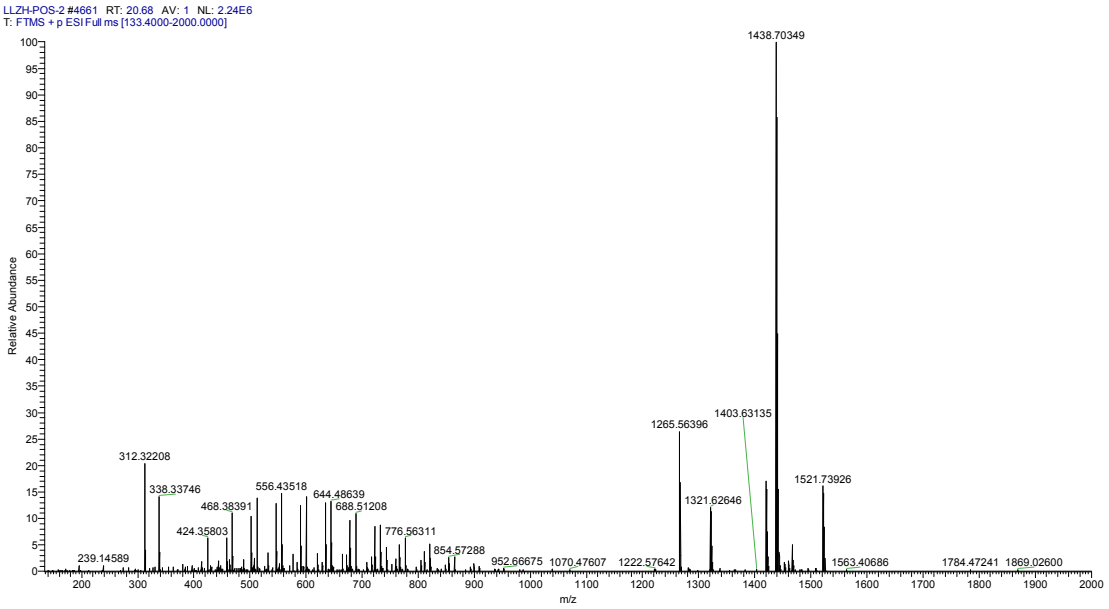


Fig. *S*5. ESI-MS spectrum of ***D*-TPE**.

L-TPE melting point: 71.8-75.2℃; IR (KBr) cm^{-1}: 3434.00 (N-H), 2932.18, 2851.55 (C–H), 1719.56 (C=O), 1609.32(vN-H), 1499.78, 1462.89 (Ar–C=C), 1209.51, 1051.55 (Ar–O, C–O); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.03 (d, J = 8.4 Hz, 4H), 6.83 (d, J = 8.6 Hz, 4H), 6.81 – 6.72 (m, 10H), 4.98 (d, J = 8.0 Hz, 2H), 4.55 (q, J = 5.9 Hz, 2H), 4.09 – 3.56 (m, 48H), 3.03 (ddt, J = 19.6, 14.0, 5.8 Hz, 4H), 2.10 – 1.87 (m, 8H), 1.43 (s, 18H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.58, 150.98, 150.96, 150.90, 150.86, 150.11, 130.43, 128.47, 128.44, 128.42, 128.33, 128.24, 115.09, 114.62, 114.35, 114.18, 114.11, 68.13, 67.63, 55.96, 55.94, 55.90, 54.69, 52.33, 37.60, 29.85, 29.74, 26.65, 26.48； ESI–MS m/z: $C_{81}H_{100}N_2O_{20}$: 1438.70349 ([M+NH_4^+]).

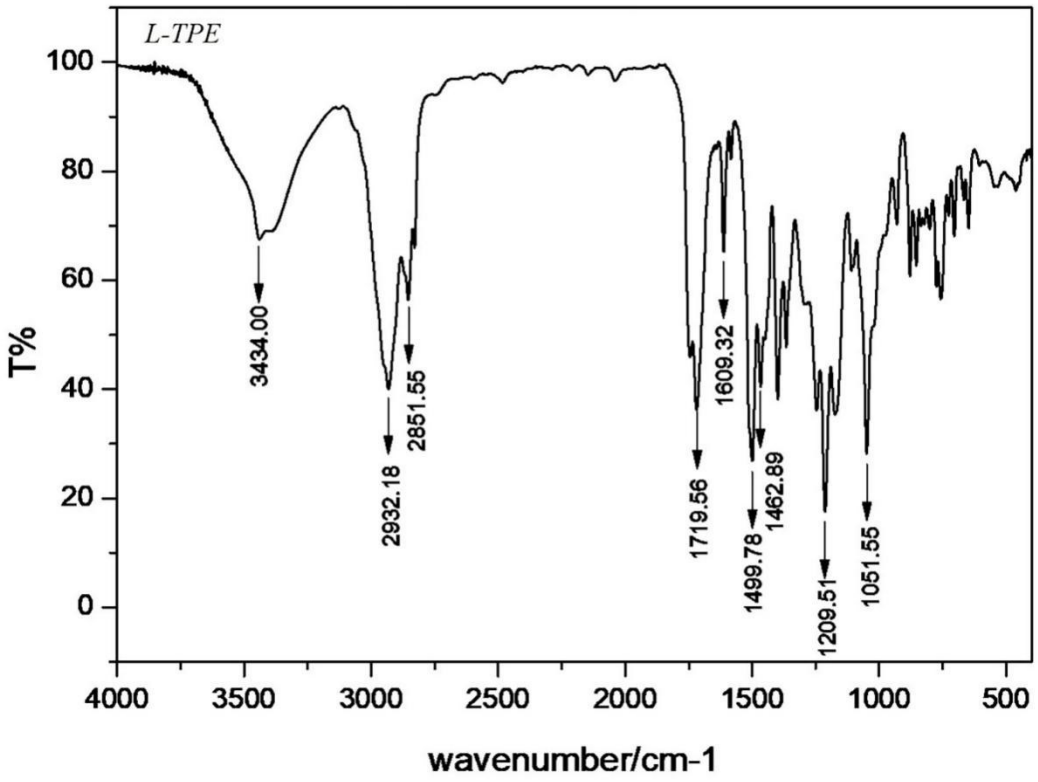


Fig. *S*6. FT-IR spectrum of ***L*-TPE**.

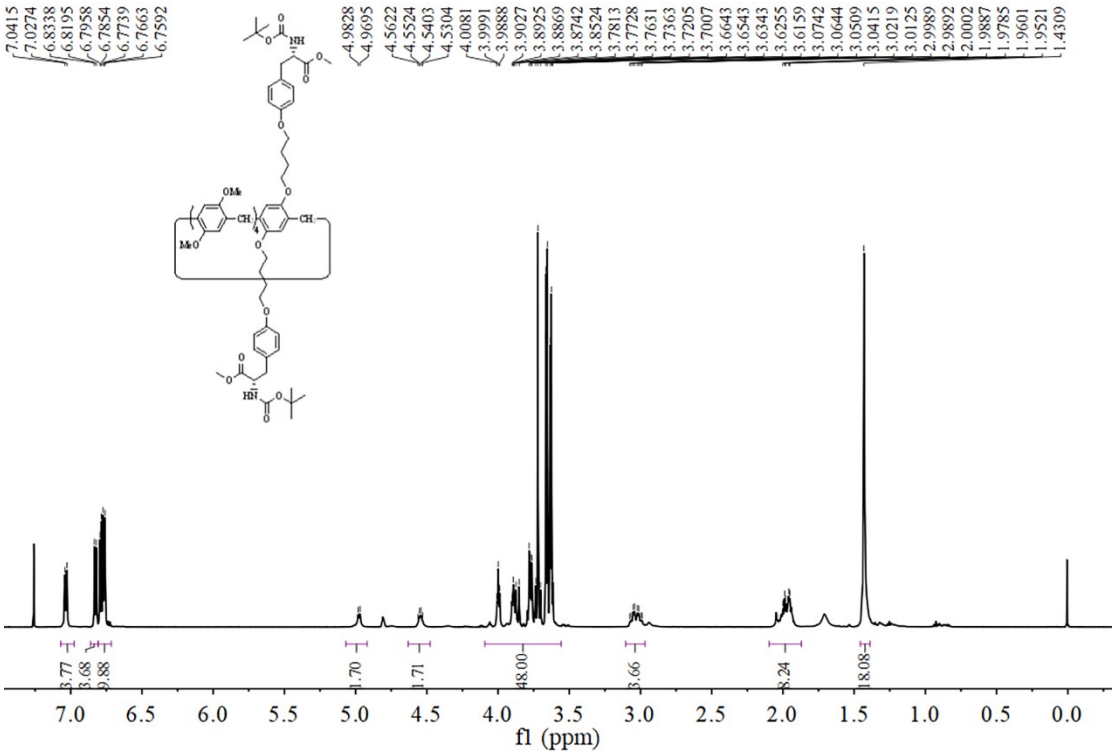


Fig. *S*7 ^{1}H NMR spectrum of ***L*-TPE** in $CDCl_3$.

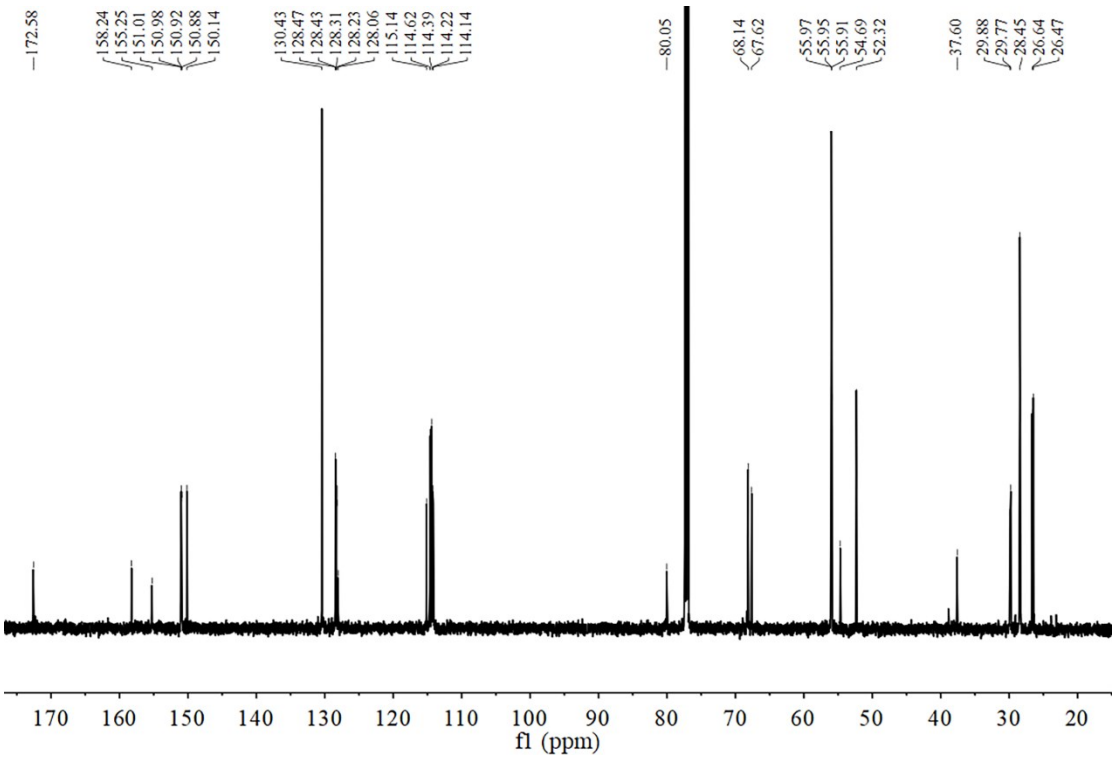


Fig. *S*8. ^{13}C NMR spectrum of ***L*-TPE** in $CDCl_3$.

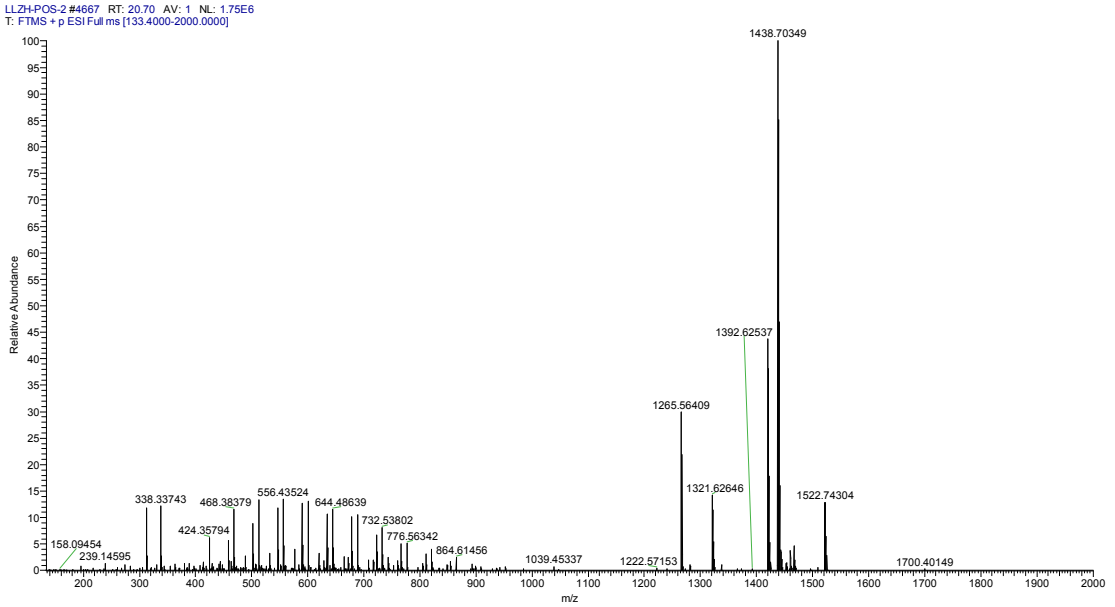


Fig. *S*9 ESI-MS spectrum of ***L*-TPE**.

2.4. Compound PCSA

D or ***L*-TPE** (200mg, 0.14mmol) was dissolved in 25ml methanol, 0.1ml 40% NaOH solution was added, and the reaction time was 5h at 60℃. At the end of the reaction, 50 ml deionized water was added, pH was adjusted to 3, filtration was carried out, filter cake was washed with deionized water, and vacuum dried to obtain ***D*** or ***L*-PCSA** with white solid (80.3/80.5%). ***D*-PCSA** melting point: 97.4-104.8 ℃; IR (KBr) cm^{-1}: 3442.39 (N-H), 2937.41, 2855.16 (C–H),1715.26 (C=O), 1613.28 (N-H), 1499.78, 1463.59 (Ar–C=C), 1210.28, 1047.44 (Ar–O, C–O); ^1H NMR (600 MHz, Chloroform-d) δ 7.07 (d, *J* = 6.6 Hz, 4H,H-j), 6.80 (d, *J* = 8.1 Hz, 4H,H-i), 6.78 – 6.68 (m, 10H,H-a), 4.97 (d, *J* = 6.6 Hz, 2H,H-p), 4.55 (s, 2H,H-g), 4.00 – 3.53 (m, 42H,H-b,c,k,n), 3.08 (s, 4H,H-h), 1.91 (d, *J* = 16.0

Hz, 8H ,H-l,m), 1.43 (s, 18H H-f); ^{13}C NMR (151 MHz, Chloroform-*d*) δ175.50, 158.26, 155.62, 151.03, 151.01, 150.92, 150.09, 130.54, 128.54, 128.48, 128.33, 114.76, 114.51, 114.46, 114.45, 114.31, 114.28, 68.09, 56.06, 56.03, 56.02, 55.95, 29.93, 29.85, 29.81, 28.45, 26.41, 26.22; ESI–MS m/z: $C_{79}H_{96}N_2O_{20}$: 1410.67236([M+NH_3]).

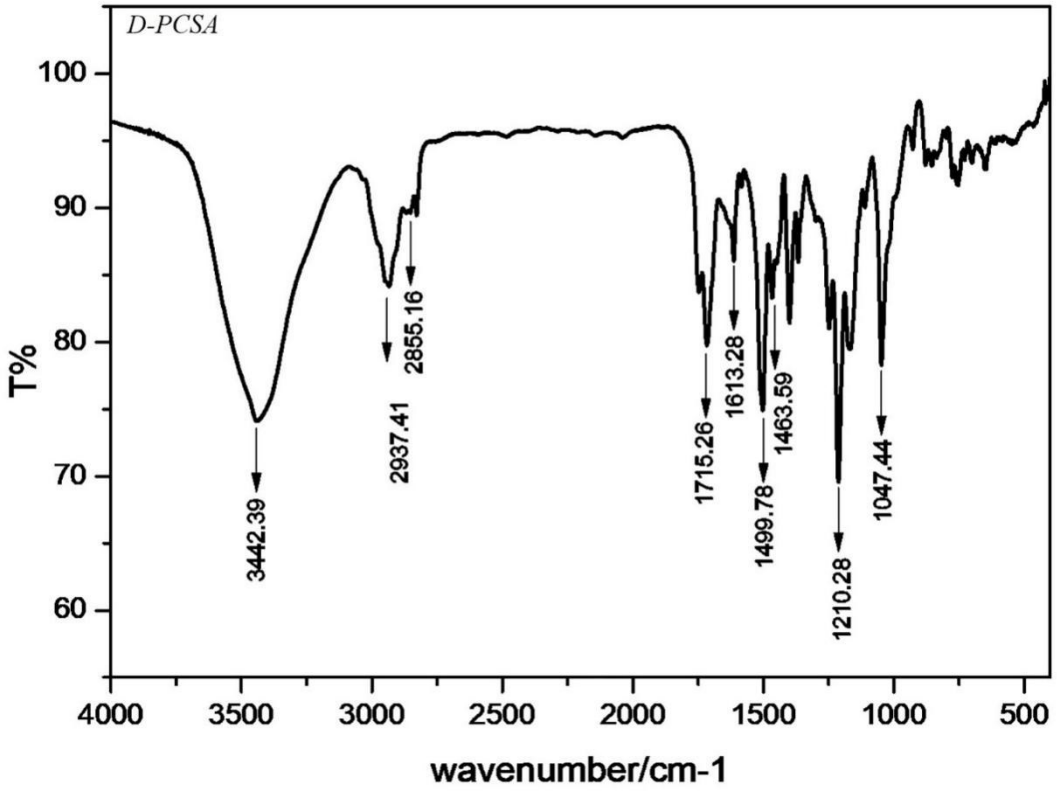


Fig. *S*10 FT-IR spectrum of ***D-PCSA***.

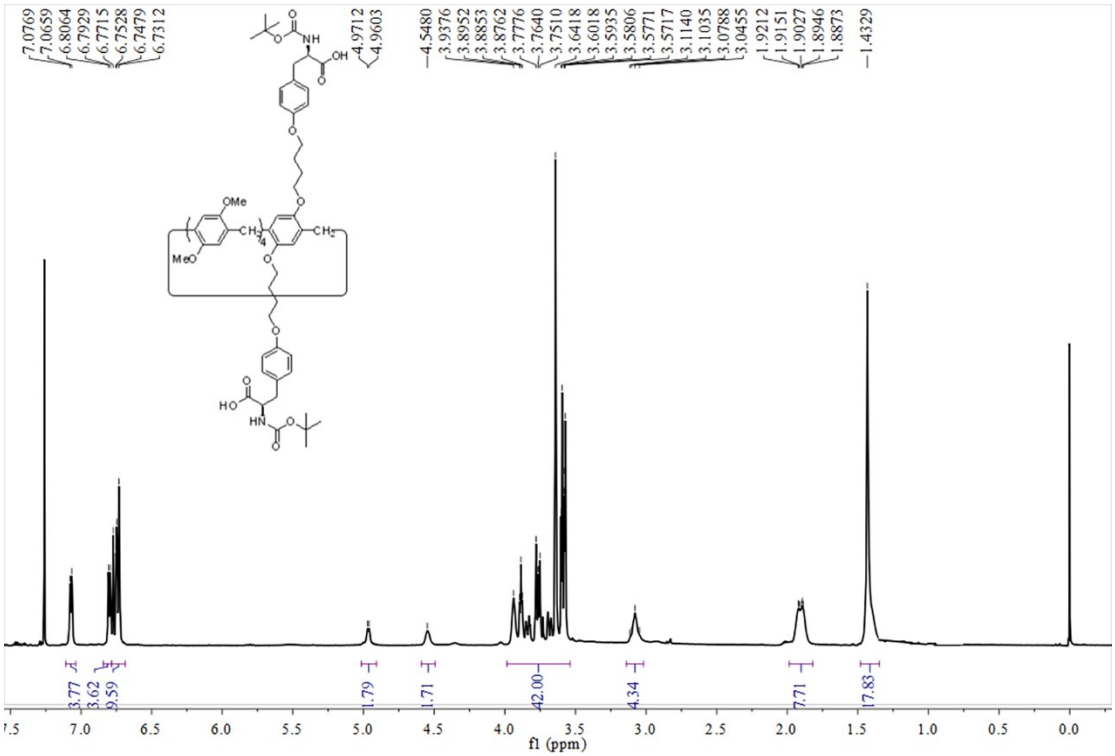


Fig. *S*11 ^{1}H NMR spectrum of ***D-PCSA*** in $CDCl_3$.

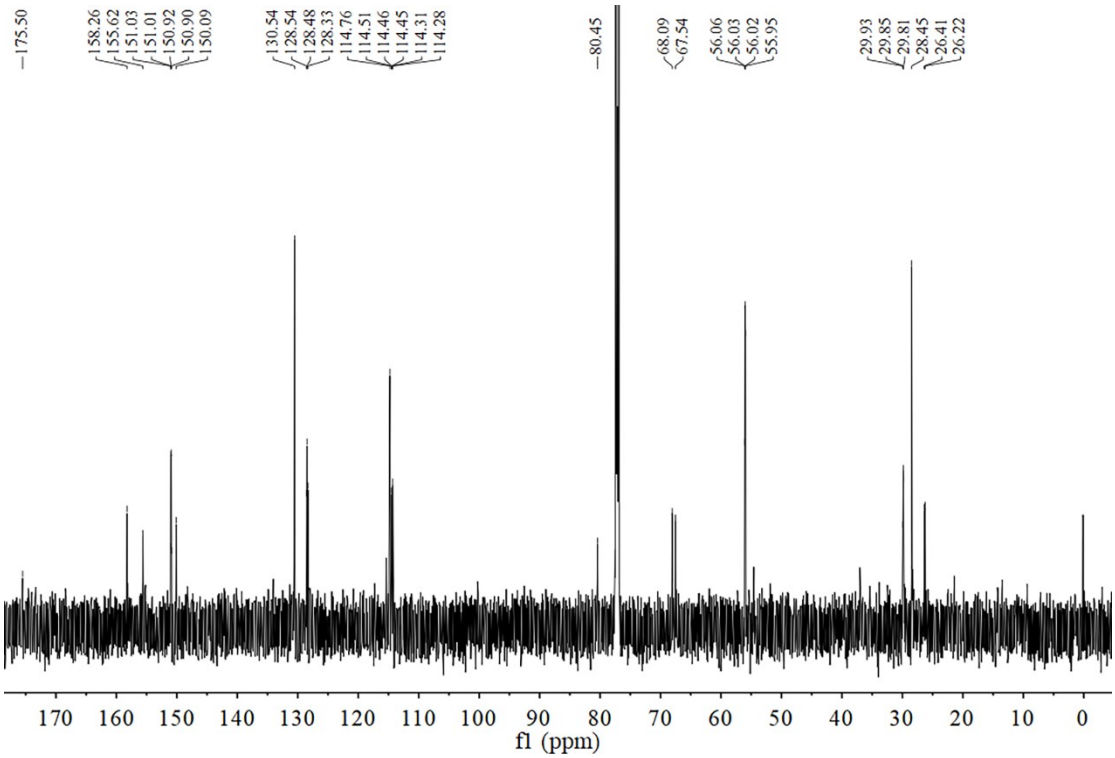


Fig. *S*12 ^{13}C NMR spectrum of ***D-PCSA*** in $CDCl_3$.

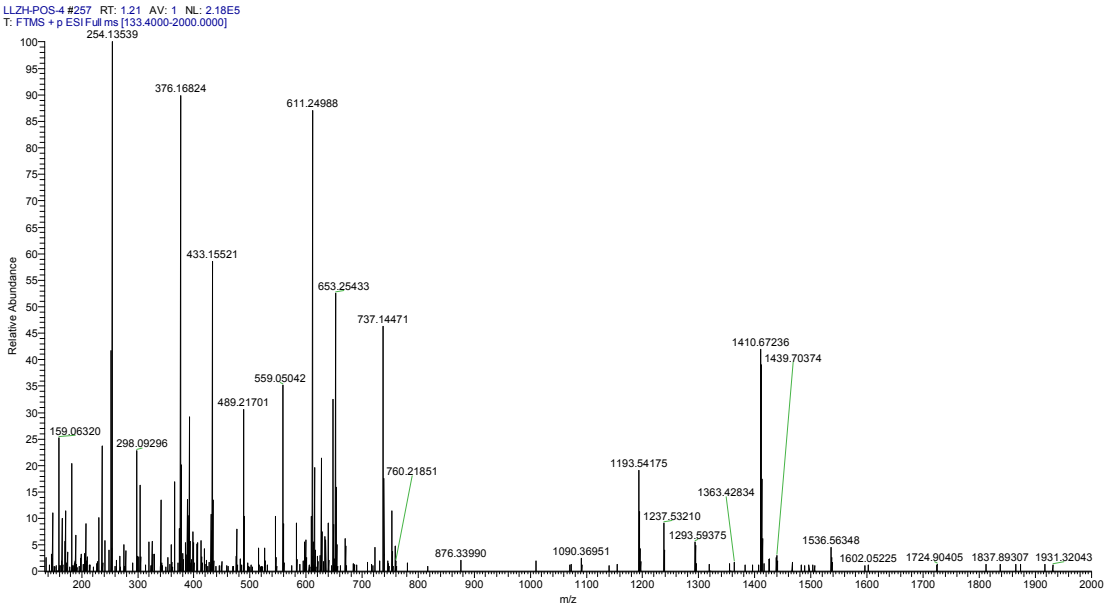


Fig. *S*13 ESI-MS spectrum of ***D-PCSA***.

***L*-PCSA** melting point: 97.9-104.7℃; IR (KBr) cm^{-1}: 3442.39 (N-H),2932.47, 2843.65 (C–H),1715.26 (C=O), 1613.28 (N-H), 1499.78, 1463.59 (Ar–C=C), 1210.28, 1047.44 (Ar–O, C–O); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.07 (d, J = 6.5 Hz, 4H,H-j), 6.79 (d, J = 8.1 Hz, 4H,H-i), 6.78 – 6.67 (m, 10H,H-a), 5.07 – 4.90 (m, 2H, H-p), 4.52 (s, 2H,H-g), 4.00 – 3.51 (m, 42H, H-b,c,k,n), 3.07 (qd, *J* = 15.1, 14.6, 5.3 Hz, 4H, H-h), 1.98 – 1.81 (m, 8H, H-l,m), 1.42 (s, 18H, H-f); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 175.90, 158.23, 151.01, 150.99, 150.91, 150.87, 150.09, 130.53, 128.51, 128.46, 128.32, 128.27, 115.29, 114.72, 114.48, 114.43, 114.28, 114.18, 68.11, 56.04, 56.01, 55.97, 55.95, 29.93, 29.92, 29.80, 28.45, 26.46, 26.29.;ESI–MS m/z: $C_{79}H_{96}N_2O_{20}$:1420.67322 ([M + NH_3]).

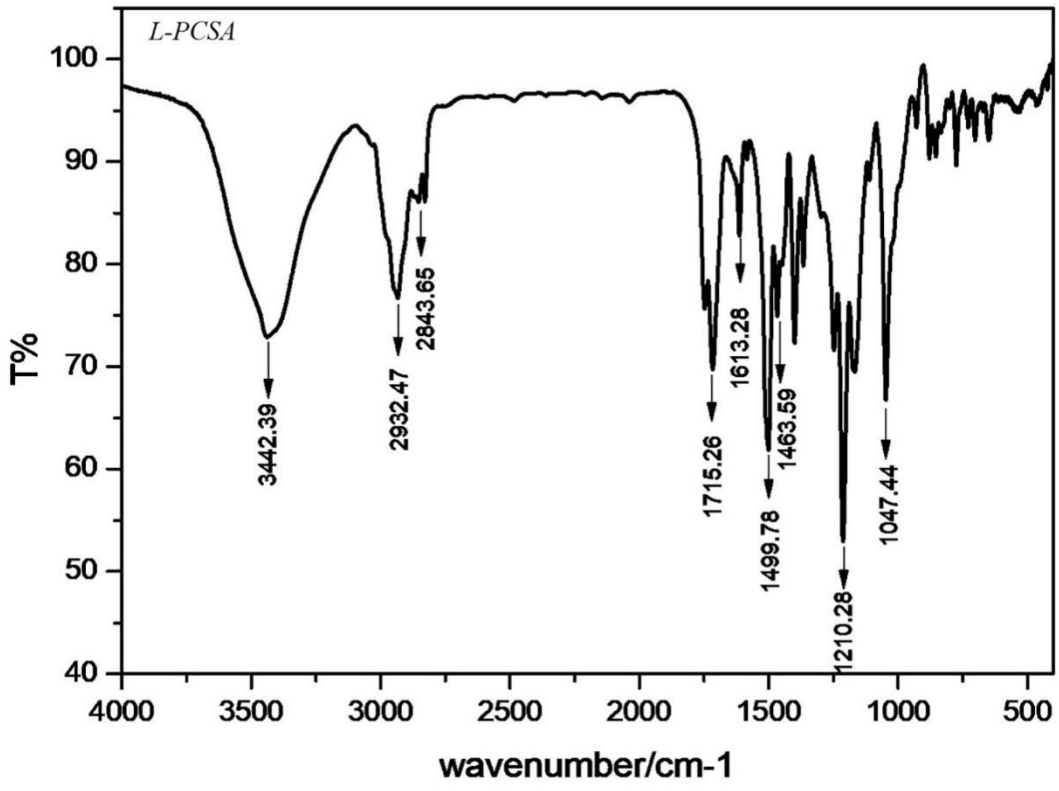


Fig. *S*14 FT-IR spectrum of ***L-PCSA***.

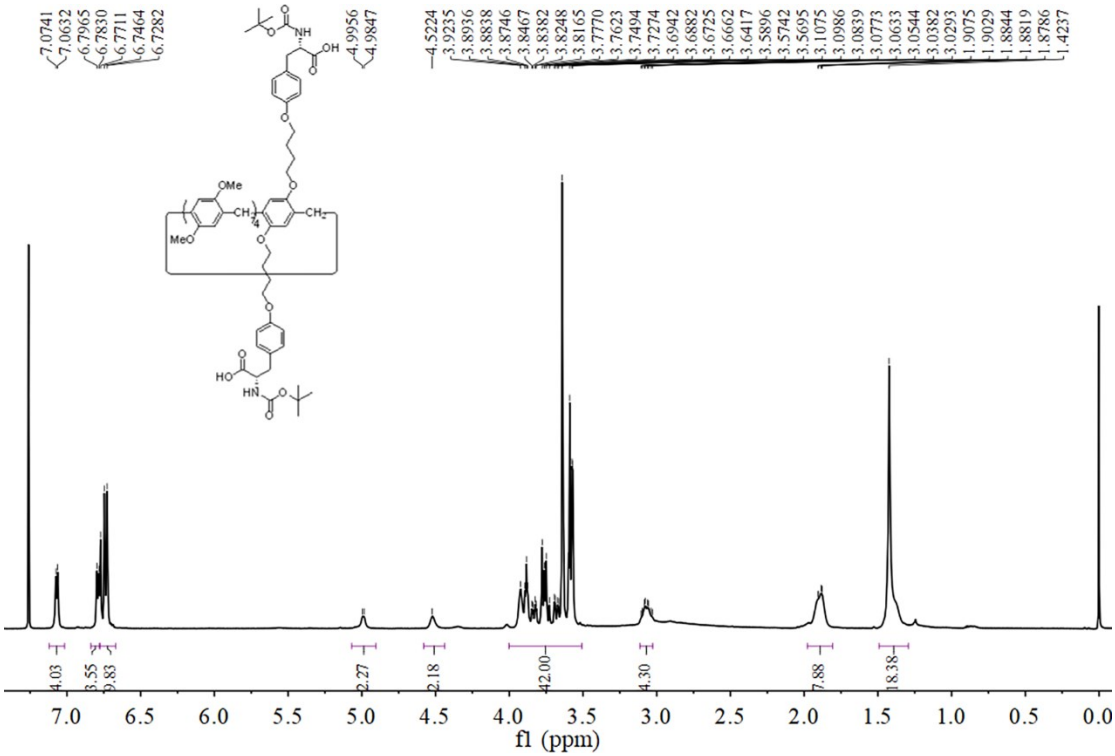


Fig. *S*15 ^{1}H NMR spectrum of ***L-PCSA*** in $CDCl_3$.

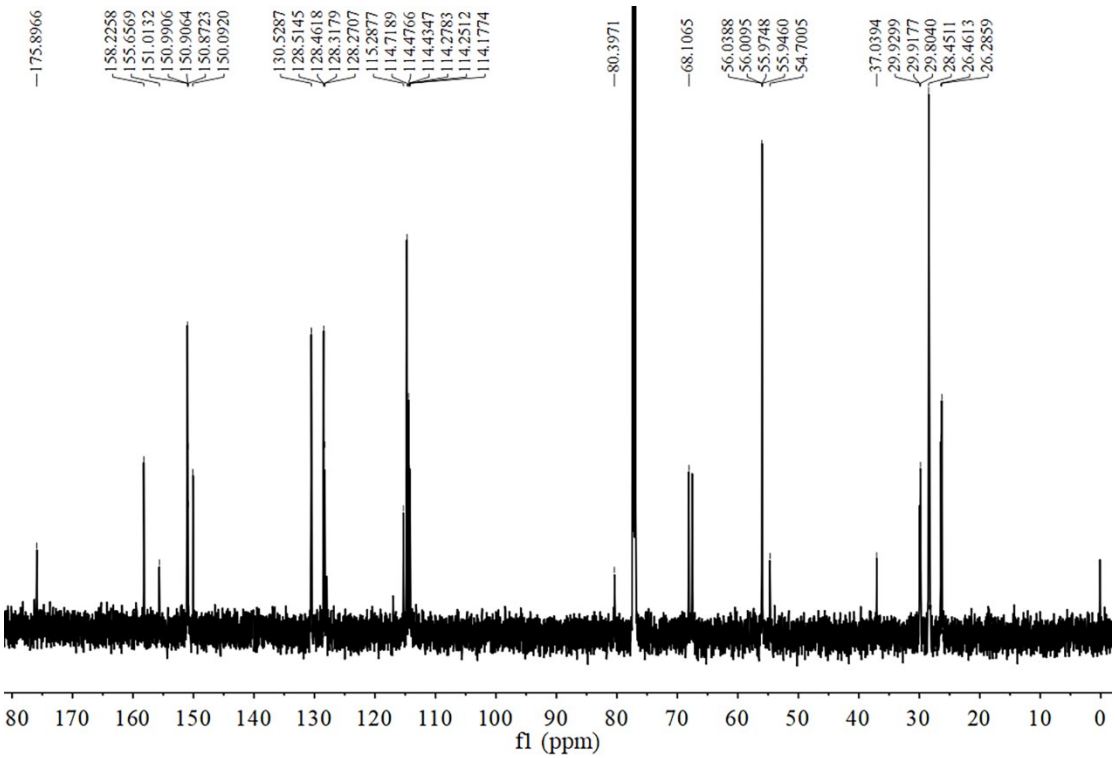


Fig. *S*16 ^{13}C NMR spectrum of ***L*-PCSA** in $CDCl_3$.

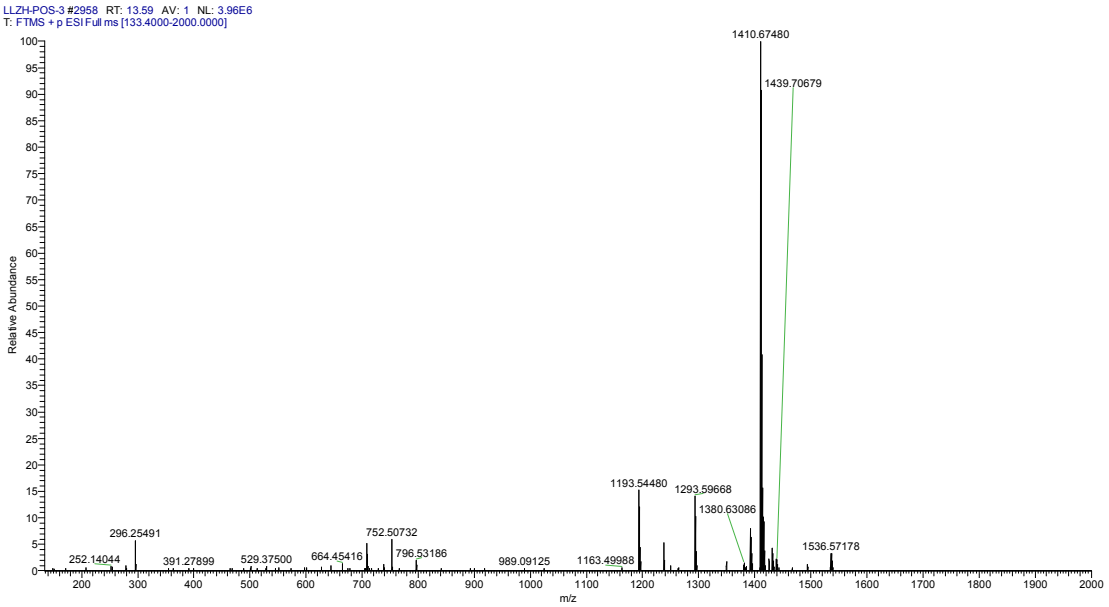


Fig. *S*17 ESI-MS spectrum of ***L*-PCSA**.

*S*3. Host-guest binding behavior of *L*-TPE with G2

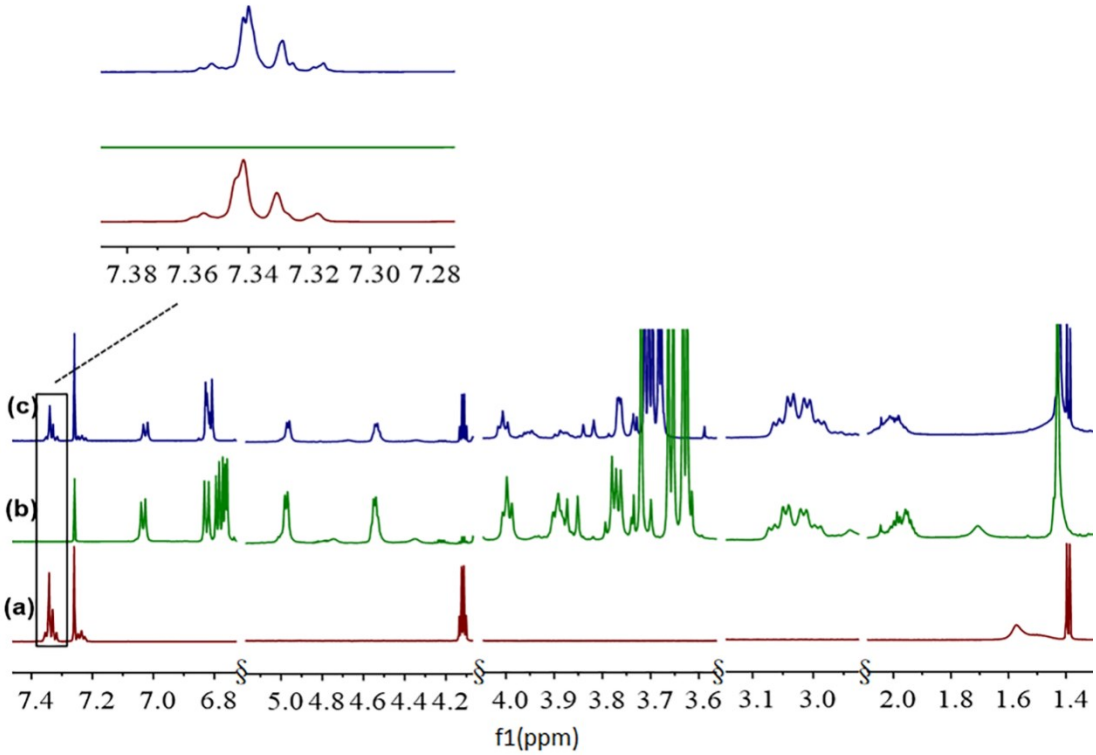


Fig. *S*18 The ^{1}H NMR spectra ($CDCl_3$) of (a) **G2**, (b) ***L*-TPE**, and (c) one equimolar mixture of **G2** and ***L*-TPE** (5.98 mmol/L).

The host-guest property of ***L*-TPE** without COOH group was screened and no nonequivalent chemical shift of any protons in **G2** were observed in ^{1}H NMR analysis, suggesting that the hydrogen bond between the carboxylic acid of ***L*-PCSA** and the amine group of substrate was the main driving force of host-guest interaction.

*S*4 Titration experiment *L*-PCSA and G2.

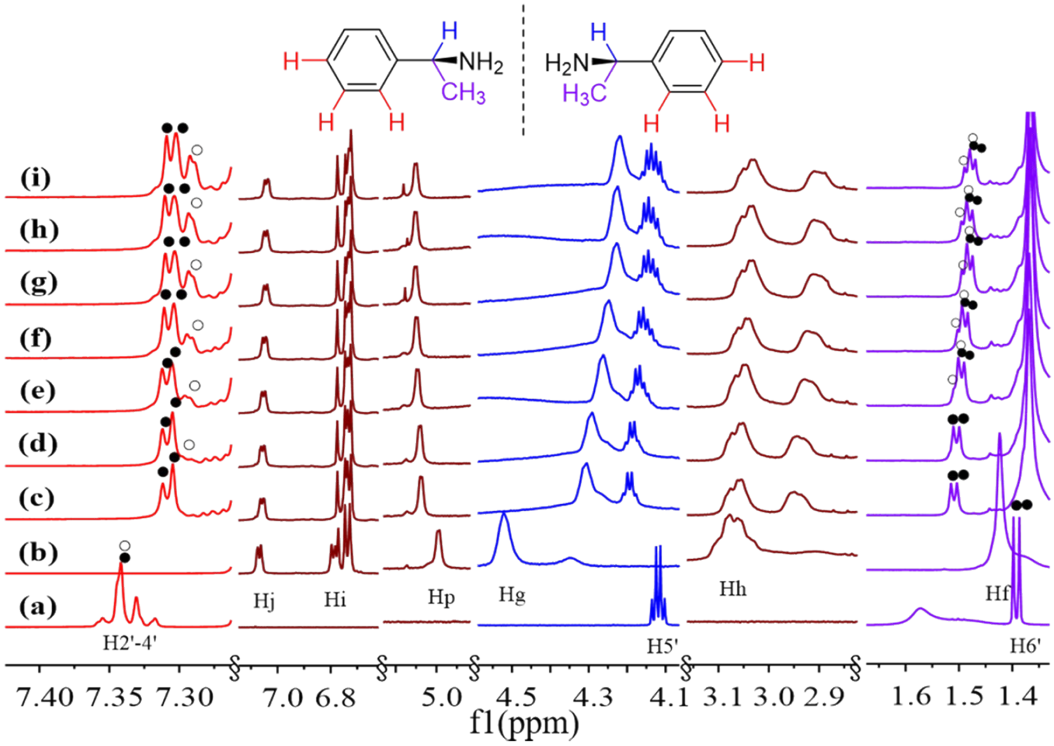


Fig. *S*19 Partial ^{1}H NMR spectra of (a) **G2**, (b) ***L*-PCSA**, and **G2** with various enantiomeric excess in the presence of a ***L*-PCSA** (5.98 mmol/L), (c) ***S*-G2/*R*-G2**=10:0, (d) ***S*-G2/*R*-G2**=10:1, (e) ***S*-G2/*R*-G2**=10:3, (f) ***S*-G2/*R*-G2**=10:5,(g) ***S*-G2/*R*-G2**=10:7, (h) ***S*-G2/*R*-G2**=10:9, (i) ***S*-G2/*R*-G2**=10:10, in $CDCl_3$.

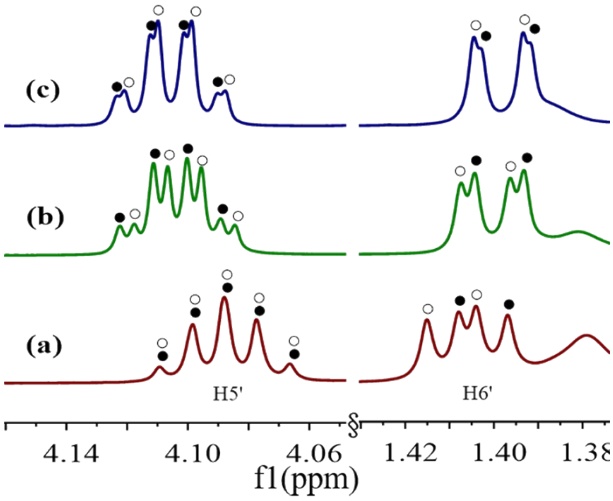


Fig. *S*20 Partial enlarged ^{1}H NMR spectra showing $H^{5'}$ and $H^{6'}$of **G2** with various enantiomeric excess in the presence of a ***L*-PCAS** (5.98 mmol/L) in $CDCl_3$. (a) ***L*-PCAS/*S*-G2/*R*-G2**=1:2.5:2.5, (a) ***L*-PCAS/ *S*-G2/*R*-G2**=1:5:5, and (c) ***L*-PCAS/*S*-G2/*R*-G2**=1:5:7.

*S*5 ^{1}H NMR spectra of *D*-PCSA and Guests

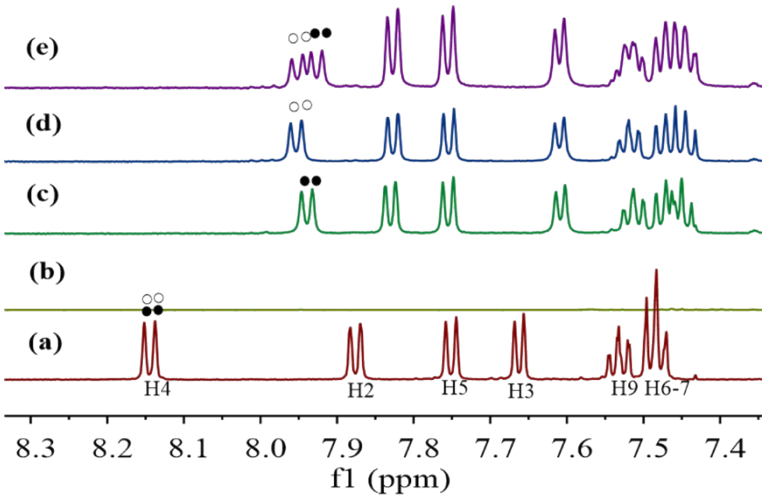


Fig. *S*21 ^{1}H NMR spectra of H^{4} proton of (a) free **(±)-G1**, (b) free ***D*-PCSA**, and the host-guest systems of (c)***S*-G1**, (d) ***R*-G1** and (e) **(±)-G1** (*R*-G1 (○), *S*-G1 (●)) in the presence of ***D*-PCSA** (5.98 mmol/L) at the mole ratio of 1:1.

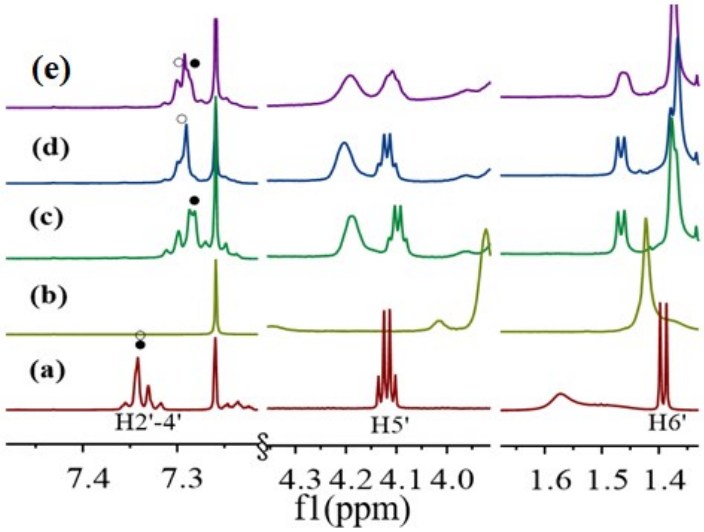


Fig. S22 ^{1}H NMR spectra of H2'-4' protons of (a) free **(±)-G2**, (b) free ***D*-PCSA**, and the host-guest systems of (c)***S*-G2**, (d) ***R*-G2** and (e) **(±)-G2** (*R*-G2 (○), *S*-G2 (●)) in the presence of ***D*-PCSA** (5.98 mmol/L) at the mole ratio of 1:1.

S6 The influence of host and guest interaction on chiral recognition.

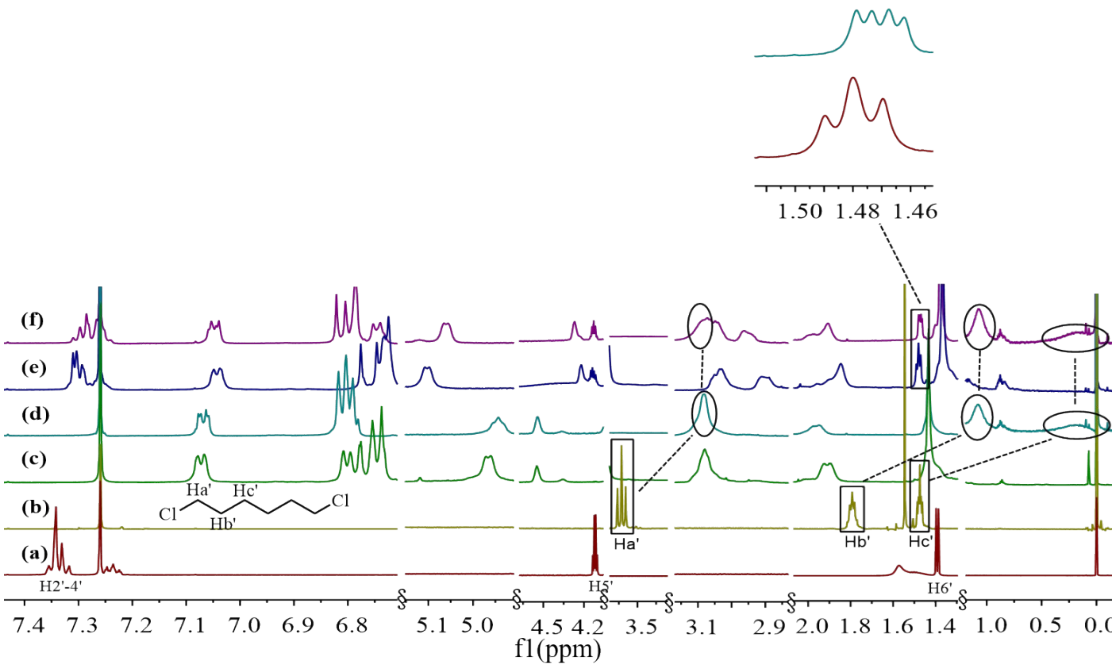


Fig. *S23* The ^{1}H NMR spectra ($CDCl_3$) of (a) **G2** (b) **DCH**, (c) ***L*-PCSA**, (d) ***L*-PCSA@DCH**, (e) ***L*-PCSA@G2** and (f) one equimolar mixture of **DCH** and ***L*-PCSA@G2** (5.98 mmol/L).

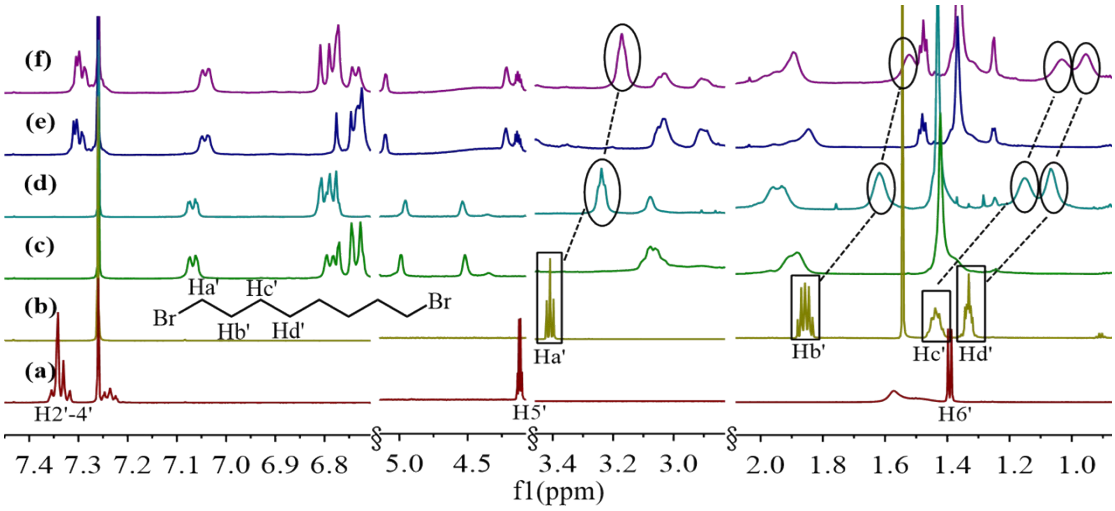


Fig. *S24* The ^{1}H NMR spectra ($CDCl_3$) of (a) **G2**, (b) **DBO**, (c) ***L*-PCSA**, (d) ***L*-PCSA@DBO**, (e) ***L*-PCSA@G2** and (f) one equimolar mixture of DBO and ***L*-PCSA@G2** (5.98 mmol/L).

*S*7 ^{1}H NMR spectroscopy CSA and racemic or chiral α-Phenylethylamine derivatives.

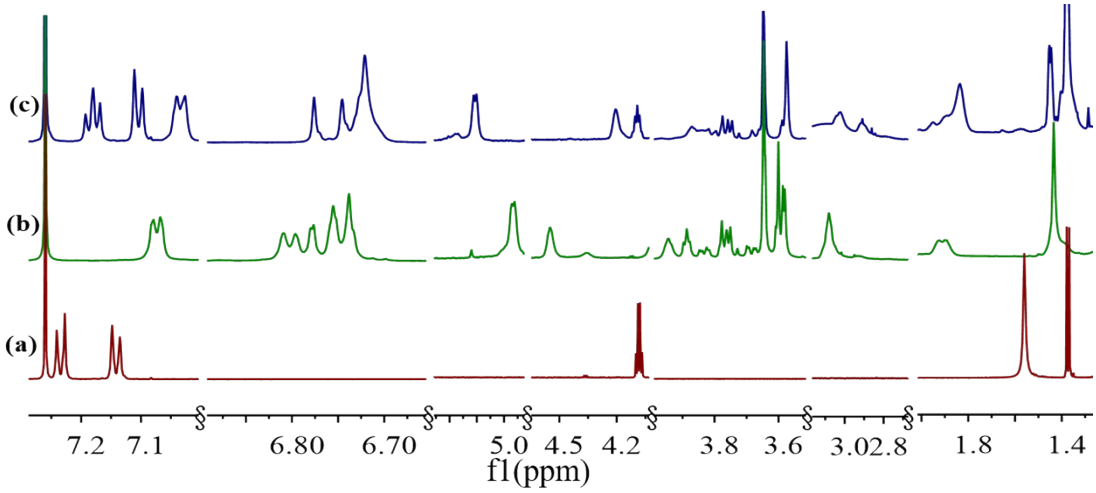


Fig.*S*25 The ^{1}H NMR (600 MHz, $CDCl_3$, 298 k) spectra of (a) **G3**,(b) ***L*-PCSA**, (c) ***L*-PCSA:G3**=1:1.

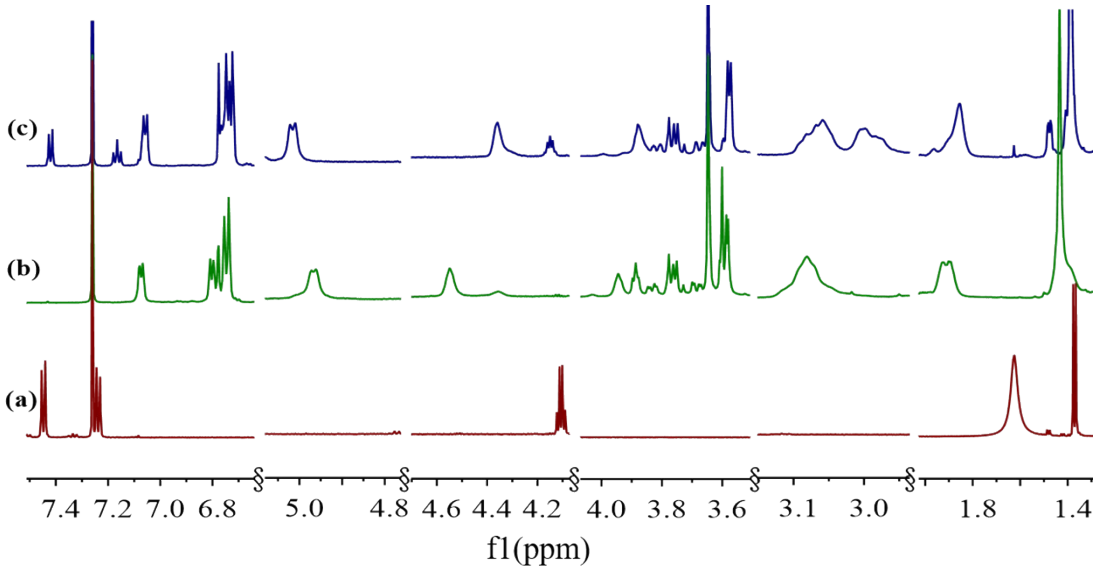


Fig. *S*26 The ^{1}H NMR (600 MHz, $CDCl_3$, 298 k) spectra of (a) **G4**, (b) ***L*-PCSA**, (c) ***L*-PCSA:G4**=1:1

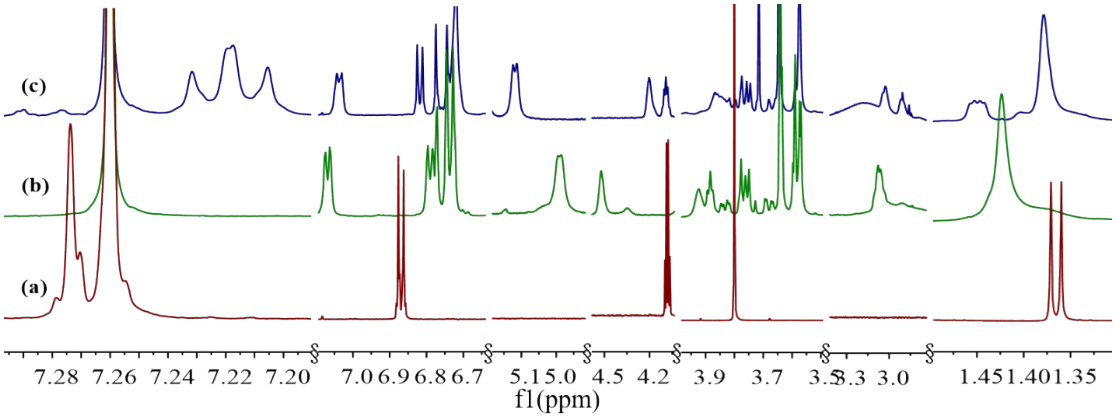


Fig. *S*27 The ^{1}H NMR (600 MHz, $CDCl_3$, 298 k) spectra of (a) **G5**, (b) ***L*-PCSA**, (c) ***L*-PCSA:G5**=1:1

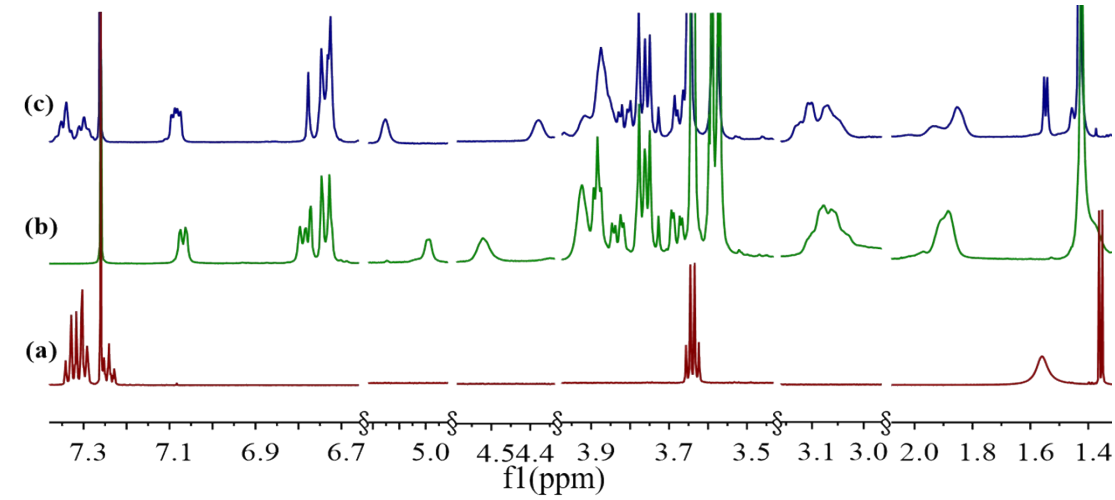


Fig. *S*28 The ^{1}H NMR (600 MHz, $CDCl_3$, 298 k) spectra of (a) **G6**, (b) ***L*-PCSA**, (c) ***L*-PCSA:G6**=1:1.

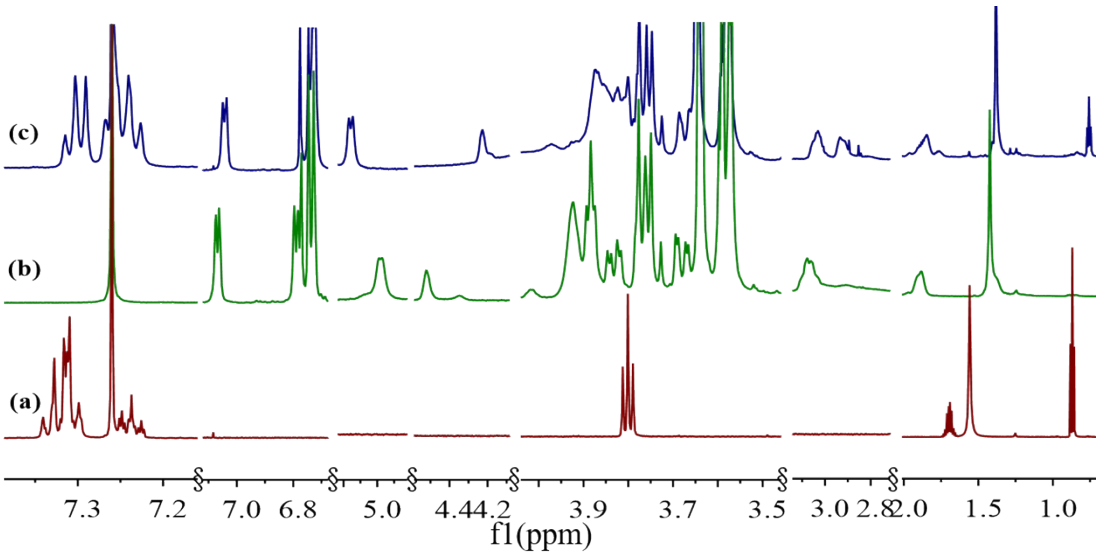
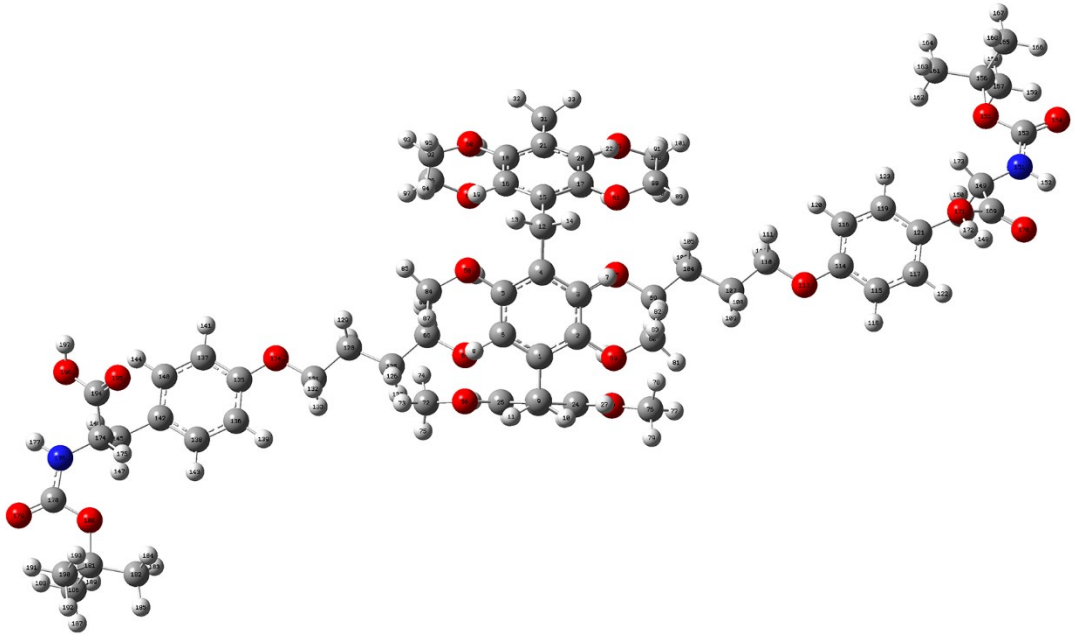


Fig. *S*29: The ^{1}H NMR (600 MHz, CDCl3, 298 k) spectra of (a) **G7**, (b) ***L*-PCSA**, (c) ***L*-PCSA:G7**=1:1.

*S*8 Cartesian Coordinates of Optimized Structures *L*-PCSA, *D*-PCSA and *S*-G2@*L*-PCSA.

_L_-PCSA:



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4	C	-0.602876	6.252675	0.967681
5	C	-1.935222	5.82423	1.08081
6	C	-2.330174	5.031647	2.161886
7	H	1.326414	6.202497	1.863432
8	H	-3.349114	4.675236	2.245658
9	C	-1.863941	3.727065	4.285934
10	H	-1.278881	3.956995	5.179888
11	H	-2.914418	3.923987	4.514214
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13	H	-0.963438	7.681703	-0.590395
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17	C	1.717736	5.814566	-1.451665
18	C	-0.086222	4.861252	-3.35907
19	H	-1.555867	5.999307	-2.253329
20	C	2.147514	4.966861	-2.476122
21	C	1.260292	4.470017	-3.435241

22	H	3.180825	4.649175	-2.536773
23	C	-1.693103	2.253921	3.948094
24	C	-0.496126	1.592093	4.236052
25	C	-2.71259	1.531152	3.307763
26	C	-0.296899	0.254065	3.885205
27	H	0.287887	2.16221	4.718326
28	C	-2.51369	0.193191	2.957455
29	C	-1.309466	-0.463151	3.228026
30	H	-3.283639	-0.365507	2.44042
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33	H	2.781652	3.725428	-4.747234
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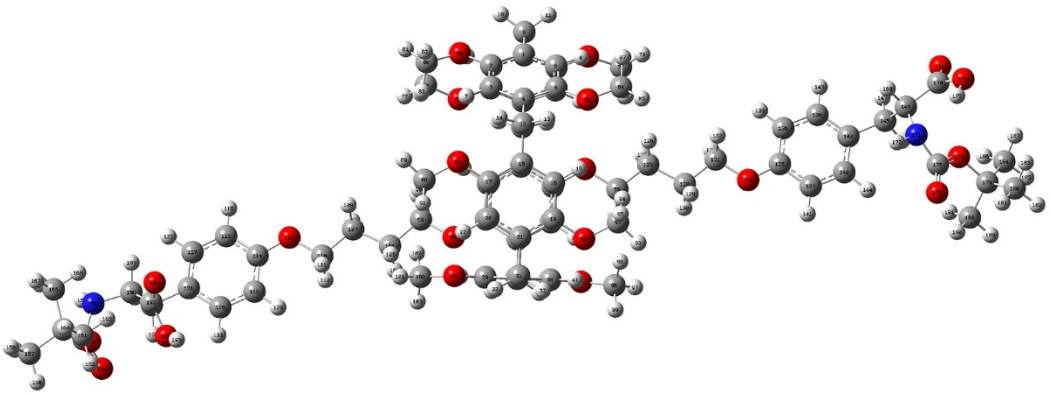

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4	C	-0.602876	6.252675	0.967681
5	C	-1.935222	5.82423	1.08081
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8	H	-3.349114	4.675236	2.245658
9	C	-1.863941	3.727065	4.285934
10	H	-1.278881	3.956995	5.179888
11	H	-2.914418	3.923987	4.514214
12	C	-0.135225	7.067634	-0.228346
13	H	-0.963438	7.681703	-0.590395
14	H	0.665627	7.739786	0.089401
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17	C	1.717736	5.814566	-1.451665
18	C	-0.086222	4.861252	-3.35907
19	H	-1.555867	5.999307	-2.253329
20	C	2.147514	4.966861	-2.476122
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25	C	-2.71259	1.531152	3.307763
26	C	-0.296899	0.254065	3.885205
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33	H	2.781652	3.725428	-4.747234
34	C	-1.096322	-1.902367	2.784195
35	H	-2.054134	-2.427894	2.808238
36	H	-0.424657	-2.399415	3.488641
37	C	1.630346	2.048297	-4.06693
38	C	0.462158	1.319104	-4.306433
39	C	2.678603	1.413771	-3.38124
40	C	0.318621	0.000988	-3.864763
41	H	-0.34465	1.821773	-4.824751
42	C	2.535407	0.095797	-2.939897
43	C	1.359766	-0.626995	-3.162379
44	H	3.327569	-0.393751	-2.387478
45	C	-0.507507	-2.000758	1.385162
46	C	0.877595	-1.989097	1.196635
47	C	-1.330215	-2.069131	0.249236
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49	H	1.501679	-1.923297	2.07888
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65	O	2.804992	-2.017501	-0.307534
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67	H	-3.477172	-1.454601	-1.334029
68	H	-3.280332	-3.210977	-1.175316
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70	H	3.568162	-1.226487	1.456314
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81	H	2.579491	4.773576	4.914461
82	H	2.63189	4.820186	3.131248
83	H	2.127473	6.265788	4.048483
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105	H	5.313419	-1.32773	-0.333772
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108	H	6.074411	-1.456762	2.072174
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116	C	10.374674	-2.686591	0.526325
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118	H	10.082526	-2.74044	3.907827

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125	C	-4.979953	-2.408432	-0.094295
126	H	-5.218309	-1.492884	0.461793
127	H	-5.016406	-3.233826	0.627109
128	C	-6.00565	-2.629444	-1.211765
129	H	-5.969408	-1.803132	-1.932061
130	H	-5.771239	-3.544234	-1.769315
131	C	-7.426135	-2.739531	-0.675188
132	H	-7.705874	-1.827152	-0.128288
133	H	-7.512929	-3.586816	0.020636
134	O	-8.294577	-2.927482	-1.789233
135	C	-9.6378	-3.031851	-1.564834
136	C	-10.240777	-2.995231	-0.302029
137	C	-10.436267	-3.191496	-2.705804
138	C	-11.628275	-3.114398	-0.198034
139	H	-9.647947	-2.880846	0.597402
140	C	-11.81475	-3.306708	-2.581046
141	H	-9.952662	-3.224288	-3.676498
142	C	-12.440364	-3.269632	-1.324979
143	H	-12.083194	-3.089626	0.78949
144	H	-12.419902	-3.430914	-3.475598
145	C	-13.943365	-3.367354	-1.194931
146	H	-14.369496	-3.882904	-2.061869
147	H	-14.214772	-3.947016	-0.306452
148	H	14.504591	-3.456752	2.354039
149	C	14.824111	-1.70554	1.125496
150	H	14.330275	-3.717316	0.618589
151	N	16.245349	-1.919293	0.92393
152	H	16.845303	-1.830678	1.73264
153	C	16.846248	-2.381101	-0.213791
154	O	18.042642	-2.601867	-0.296381
155	O	15.929392	-2.539086	-1.204555
156	C	16.343722	-2.9742	-2.549599
157	C	16.951813	-4.378677	-2.482118
158	H	17.155683	-4.739332	-3.495494
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161	C	15.019214	-2.991684	-3.316527
162	H	14.316226	-3.694592	-2.859438

163	H	14.562303	-1.997756	-3.322514
164	H	15.189124	-3.299978	-4.352254
165	C	17.308927	-1.950961	-3.156621
166	H	18.244791	-1.91938	-2.598837
167	H	17.523923	-2.221068	-4.19551
168	H	16.857806	-0.953661	-3.151636
169	C	14.684911	-0.737042	2.291272
170	O	15.432892	-0.71236	3.246211
171	O	13.617255	0.07173	2.165508
172	H	13.575918	0.605594	2.978043
173	H	14.390792	-1.255029	0.230797
174	C	-14.658191	-1.994229	-1.046785
175	H	-14.277811	-1.479513	-0.165518
176	N	-16.102457	-2.135209	-0.908099
177	H	-16.643806	-2.315401	-1.741514
178	C	-16.783088	-2.369618	0.259861
179	O	-17.978019	-2.610899	0.291144
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181	C	-16.469003	-2.415232	2.699681
182	C	-15.210622	-2.219614	3.548389
183	H	-14.462805	-2.982842	3.313323
184	H	-14.770159	-1.23509	3.366524
185	H	-15.459232	-2.296698	4.610841
186	C	-17.05113	-3.817438	2.903112
187	H	-17.330961	-3.949263	3.953253
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189	H	-16.305128	-4.578684	2.653402
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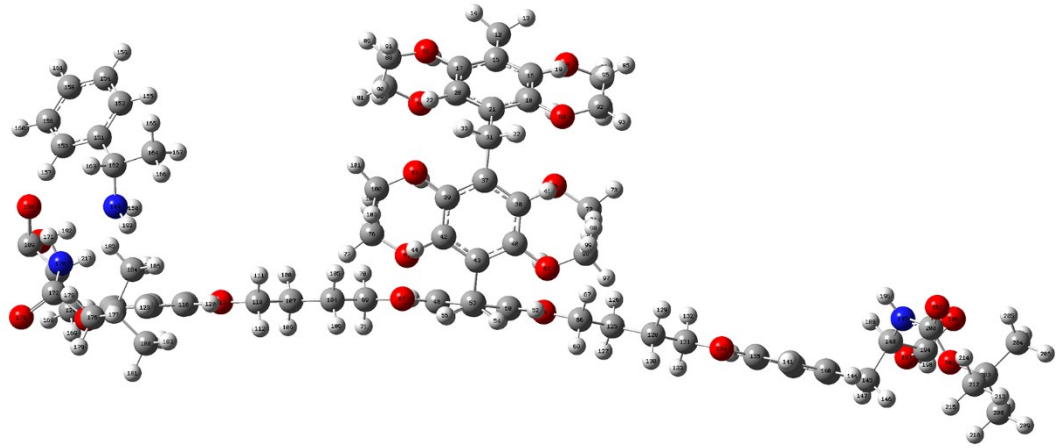
191	H	-18.381505	-1.435537	2.363378
192	H	-17.788409	-1.348542	4.036507
193	H	-17.055977	-0.328183	2.786656
194	C	-14.373137	-1.079225	-2.232186
195	O	-13.703589	-0.075593	-2.209396
196	O	-14.97241	-1.540551	-3.363621
197	H	-14.76087	-0.901562	-4.065172

***S*-G2@*L*-PCSA**



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2	C	-0.38712	5.864167	1.263021
3	C	-0.082641	6.17929	-0.06388
4	C	-1.075288	6.248562	-1.045722
5	C	-2.404861	6.009911	-0.66281
6	C	-2.709768	5.698066	0.66483
7	H	0.940625	6.352178	-0.373009
8	H	-3.728347	5.487606	0.965593
9	C	-2.063977	5.209419	3.068115
10	H	-1.367793	5.692847	3.757989
11	H	-3.069521	5.567961	3.302182
12	C	-0.710742	6.533336	-2.494646
13	H	-1.544365	7.046353	-2.98044
14	H	0.153679	7.201347	-2.520126
15	C	-0.386779	5.26679	-3.271972
16	C	-1.400135	4.547448	-3.912162
17	C	0.923506	4.766339	-3.335407
18	C	-1.135289	3.351646	-4.584914
19	H	-2.408704	4.935871	-3.845828
20	C	1.188908	3.572067	-4.010752
21	C	0.172587	2.84268	-4.634404
22	H	2.191317	3.164233	-4.044045
23	C	-2.007216	3.704557	3.281577
24	C	-0.819992	3.087391	3.685701
25	C	-3.128542	2.893278	3.044854
26	C	-0.729976	1.700755	3.835148
27	H	0.04195	3.72073	3.853699
28	C	-3.038864	1.506966	3.194571
29	C	-1.846145	0.887956	3.579736
30	H	-3.890062	0.870164	2.988958
31	C	0.476359	1.514902	-5.311368

32	H	-0.209895	1.373839	-6.150118
33	H	1.492625	1.544394	-5.712385
34	C	-1.758186	-0.627384	3.678239
35	H	-2.731763	-1.021754	3.979517
36	H	-1.034837	-0.895397	4.452404
37	C	0.347002	0.333374	-4.362291
38	C	-0.874631	-0.329419	-4.213789
39	C	1.434026	-0.098863	-3.585665
40	C	-1.031019	-1.381532	-3.307291
41	H	-1.709603	0.019943	-4.807954
42	C	1.278038	-1.151083	-2.679673
43	C	0.051162	-1.801004	-2.516961
44	H	2.102682	-1.474566	-2.057045
45	C	-1.341653	-1.273866	2.365896
46	C	0.011081	-1.452484	2.061983
47	C	-2.293256	-1.673487	1.413764
48	C	0.422656	-1.994547	0.841387
49	H	0.73584	-1.128928	2.798269
50	C	-1.881679	-2.210191	0.190817
51	C	-0.528363	-2.371092	-0.120725
52	H	-2.605505	-2.491856	-0.563471
53	C	-0.108397	-2.904212	-1.481987
54	H	-0.858271	-3.618336	-1.831422
55	H	0.839928	-3.43779	-1.381217
56	O	-4.284367	3.544513	2.666834
57	O	0.421111	1.051796	4.229324
58	O	-3.353899	6.100755	-1.659762
59	O	0.560103	5.782304	2.26185
60	O	-2.104148	2.609259	-5.226621
61	O	1.894783	5.51377	-2.702189
62	O	-2.217838	-2.060386	-3.127989
63	O	2.625523	0.569498	-3.777531
64	O	-3.618019	-1.502777	1.76037
65	O	1.74683	-2.190349	0.506196
66	C	-4.61739	-2.00743	0.885256
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68	H	-4.443575	-3.074943	0.685474
69	C	2.738141	-1.945383	1.494694
70	H	2.745953	-0.88128	1.773915
71	H	2.518924	-2.524478	2.40368
72	C	-5.454574	2.770807	2.48372
73	H	-6.248913	3.475736	2.23015
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75	H	-5.733119	2.230425	3.398218

76	C	1.547016	1.840535	4.568634
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79	H	1.326189	2.531721	5.392517
80	C	1.90122	6.095192	1.933961
81	H	2.470016	6.003948	2.861424
82	H	2.312464	5.401108	1.189165
83	H	1.998785	7.120176	1.5527
84	C	-4.713855	5.943944	-1.299828
85	H	-5.289659	6.092986	-2.215405
86	H	-4.919314	4.940278	-0.904573
87	H	-5.026093	6.687174	-0.554442
88	C	3.239217	5.084331	-2.808704
89	H	3.838716	5.828516	-2.280616
90	H	3.392956	4.101742	-2.343152
91	H	3.569096	5.034293	-3.854753
92	C	-3.423154	3.122581	-5.258195
93	H	-4.012896	2.409644	-5.837815
94	H	-3.851801	3.210395	-4.251172
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96	C	-3.313241	-1.716297	-3.95657
97	H	-4.126294	-2.390752	-3.68093
98	H	-3.635882	-0.678937	-3.79758
99	H	-3.077883	-1.853699	-5.020065
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101	H	4.591542	0.754984	-3.383926
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103	H	3.999189	-0.924553	-3.285996
104	C	4.086256	-2.35581	0.91617
105	H	4.265012	-1.781664	-0.001874
106	H	4.032524	-3.411185	0.622261
107	C	5.23279	-2.135389	1.909346
108	H	5.294321	-1.077423	2.192303
109	H	5.050245	-2.697676	2.833016
110	C	6.579889	-2.563538	1.34289
111	H	6.807888	-2.005796	0.421791
112	H	6.570147	-3.633797	1.089327
113	O	7.566123	-2.301114	2.334428
114	C	8.868134	-2.63612	2.071545
115	C	9.783451	-2.386656	3.103308
116	C	9.322317	-3.194062	0.870729
117	C	11.129566	-2.693465	2.934226
118	H	9.415701	-1.956983	4.029804
119	C	10.679612	-3.498695	0.722052

120	H	8.636933	-3.404552	0.057886
121	C	11.606305	-3.256981	1.740891
122	H	11.830407	-2.480511	3.736195
123	H	11.026565	-3.942082	-0.206266
124	C	13.084123	-3.588668	1.552502
125	C	-5.969515	-1.806239	1.557554
126	H	-6.100841	-0.737773	1.770676
127	H	-5.956852	-2.321279	2.525889
128	C	-7.128037	-2.318703	0.694531
129	H	-7.149937	-1.791523	-0.267004
130	H	-6.992673	-3.382967	0.467097
131	C	-8.477774	-2.137982	1.375561
132	H	-8.657266	-1.077191	1.605962
133	H	-8.510505	-2.695278	2.323164
134	O	-9.478091	-2.622246	0.48507
135	C	-10.786714	-2.57431	0.878494
136	C	-11.23221	-2.080196	2.109577
137	C	-11.719558	-3.069604	-0.043204
138	C	-12.599264	-2.087676	2.40009
139	H	-10.534192	-1.698366	2.845019
140	C	-13.074368	-3.067568	0.265008
141	H	-11.35807	-3.454138	-0.991287
142	C	-13.544946	-2.575939	1.493559
143	H	-12.931183	-1.706652	3.363229
144	H	-13.781494	-3.461219	-0.46006
145	C	-15.02172	-2.539647	1.815844
146	H	-15.541483	-3.365414	1.319732
147	H	-15.17398	-2.653832	2.893471
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152	C	11.6178	3.766286	0.652855
153	C	13.225447	2.549583	1.968302
154	C	11.909935	4.929491	1.371023
155	H	10.875655	3.812407	-0.136976
156	C	13.516256	3.708068	2.685412
157	H	13.734624	1.622258	2.211585
158	C	12.859374	4.905297	2.389982
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161	H	13.08705	5.808416	2.948995
162	C	11.988876	1.267526	0.173894
163	H	12.935194	0.940653	-0.276837

164	C	10.952825	1.401088	-0.949383
165	H	11.26066	2.13415	-1.702286
166	H	10.832847	0.438108	-1.456209
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168	H	13.560523	-3.60672	2.539641
169	H	13.171831	-4.596477	1.139068
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172	C	14.518605	-4.222264	-1.126462
173	O	15.377293	-4.842807	-0.198019
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175	C	12.879873	-5.300597	-2.639942
176	C	13.911158	-6.004898	-3.537337
177	H	13.466075	-6.245835	-4.507787
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187	H	11.727368	-3.455584	-2.588737
188	H	-15.139059	-0.389008	1.831993
189	C	14.603656	-1.492759	1.314309
190	O	14.950616	-0.571336	0.26511
191	O	13.933189	-0.866743	2.364515
192	H	13.075073	-0.506986	2.006437
193	H	11.3694	-0.64747	0.644598
194	C	-17.1248	-1.099924	2.006299
195	N	-15.68889	-0.974478	-0.045817
196	H	-14.959509	-0.382779	-0.412308
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198	H	-17.757086	-0.829452	3.814524
199	O	-17.924664	-0.11032	1.415622
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201	O	-17.200447	-2.57047	-0.528495
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203	C	-18.181393	-3.251746	-1.392716
204	C	-19.114783	-2.217453	-2.029603
205	H	-18.579003	-1.597266	-2.748423
206	H	-19.933958	-2.729419	-2.544728
207	H	-19.54219	-1.572895	-1.2555

208	C	-18.946017	-4.133577	-0.402428
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210	H	-18.267078	-4.825531	0.104691
211	H	-19.449246	-3.522838	0.35281
212	C	-17.456157	-4.109283	-2.434466
213	H	-18.188009	-4.689334	-3.006179
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215	H	-16.777348	-4.812996	-1.941876
216	C	13.828605	-2.616001	0.676809
217	H	12.94939746	-2.22561781	0.208306

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