Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Supramolecular BODIPY based dimer: synthesis and photophysical characterization

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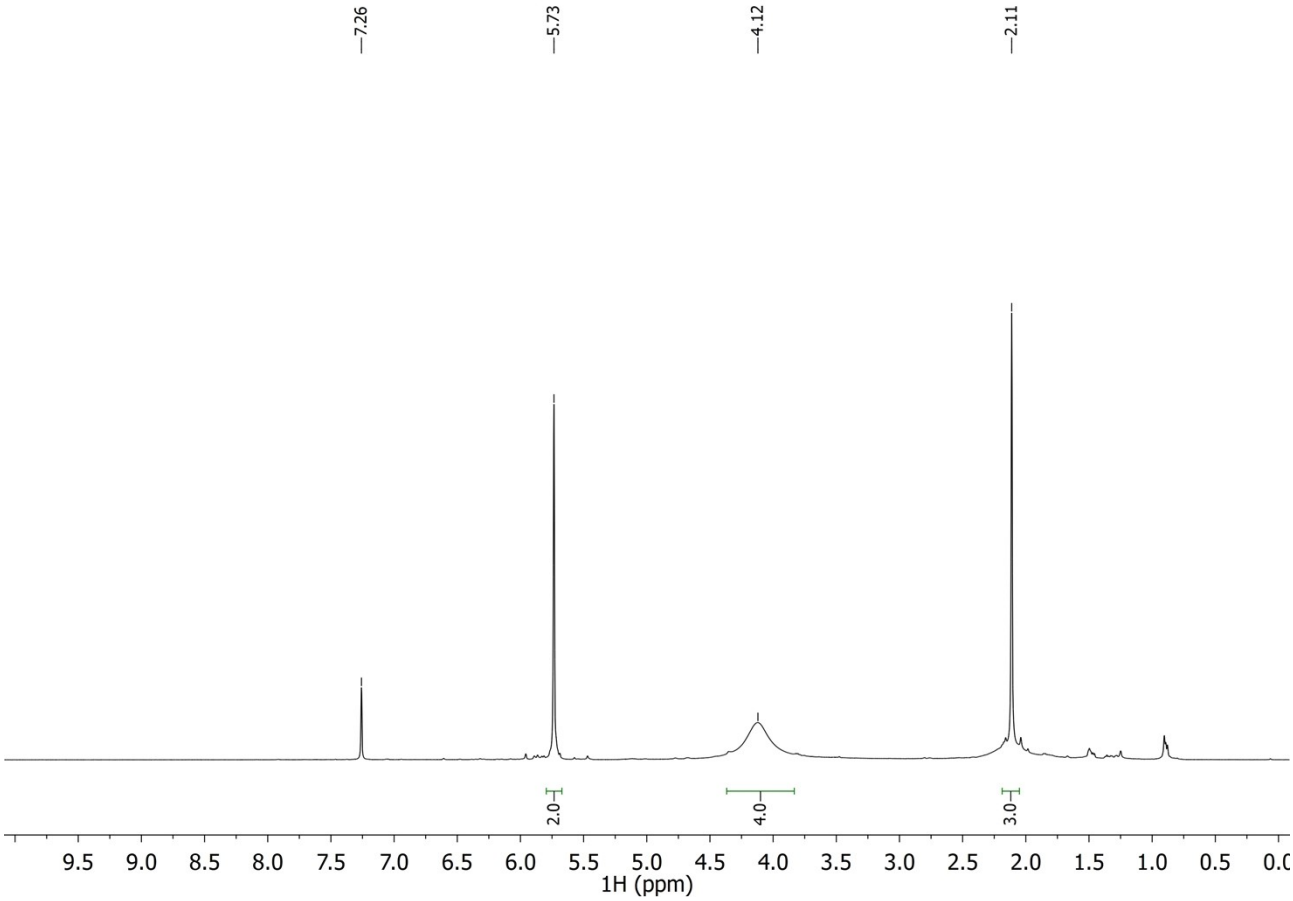

*Figure S1. ^{1}H-NMR (500 MHz, $CDCl_3$) of **5***

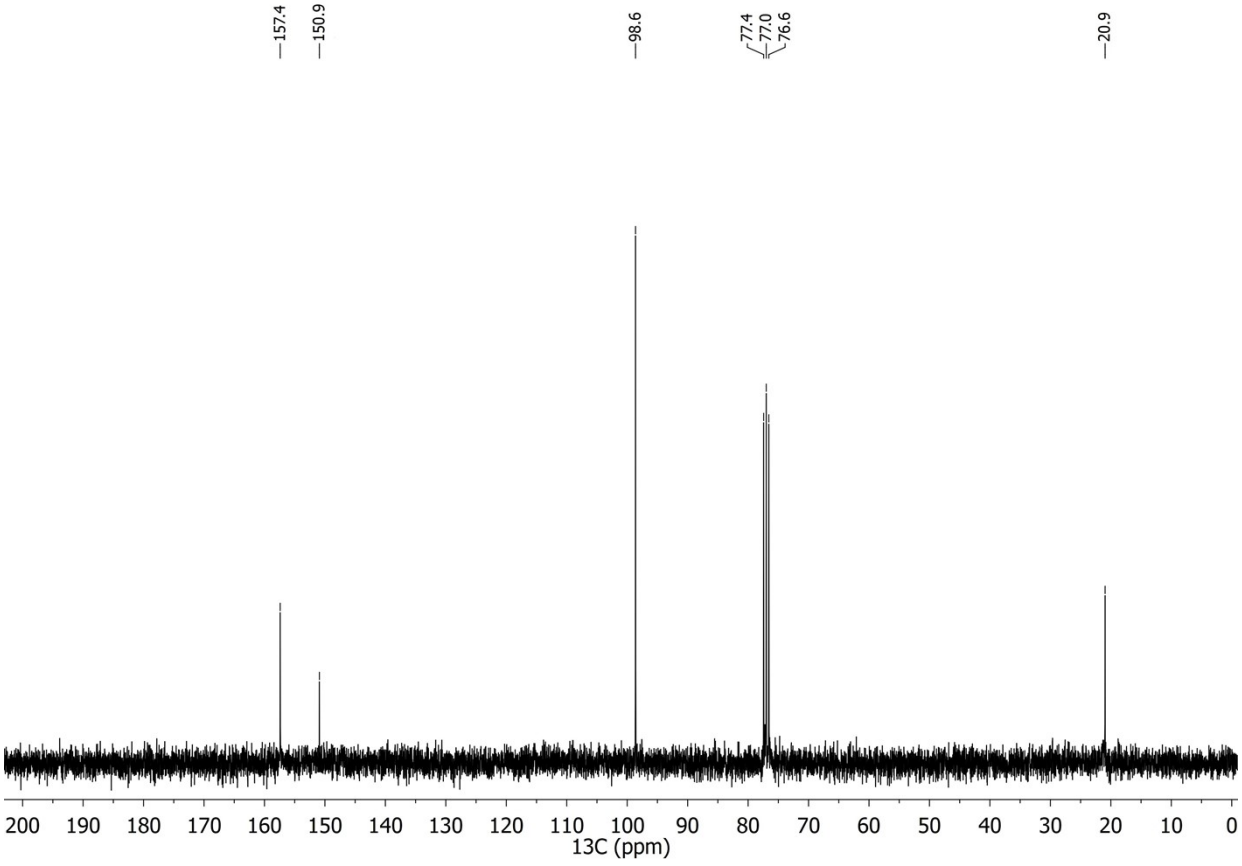

*Figure S2. ^{13}C-NMR (125 MHz, $CDCl_3$) of **5***

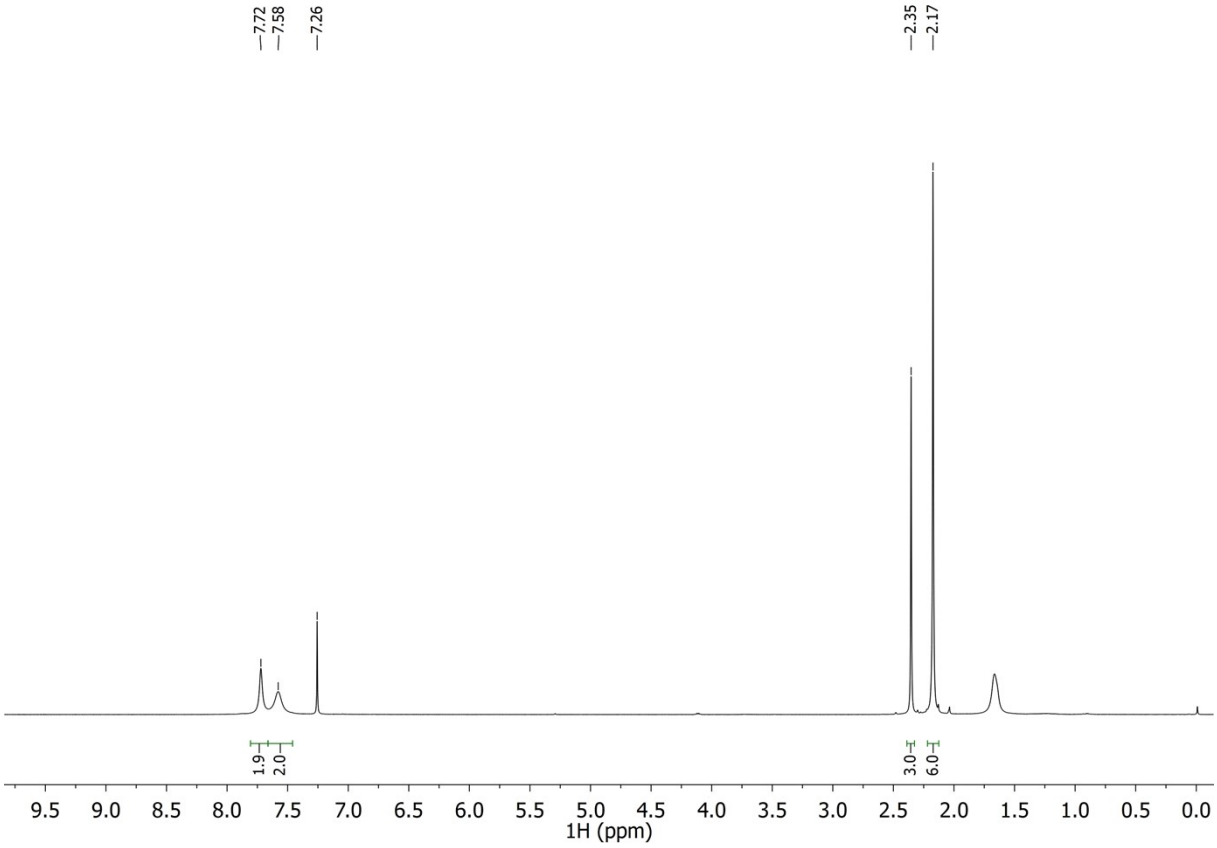

*Figure S3. ^{1}H-NMR (500 MHz, $CDCl_3$) of **6***

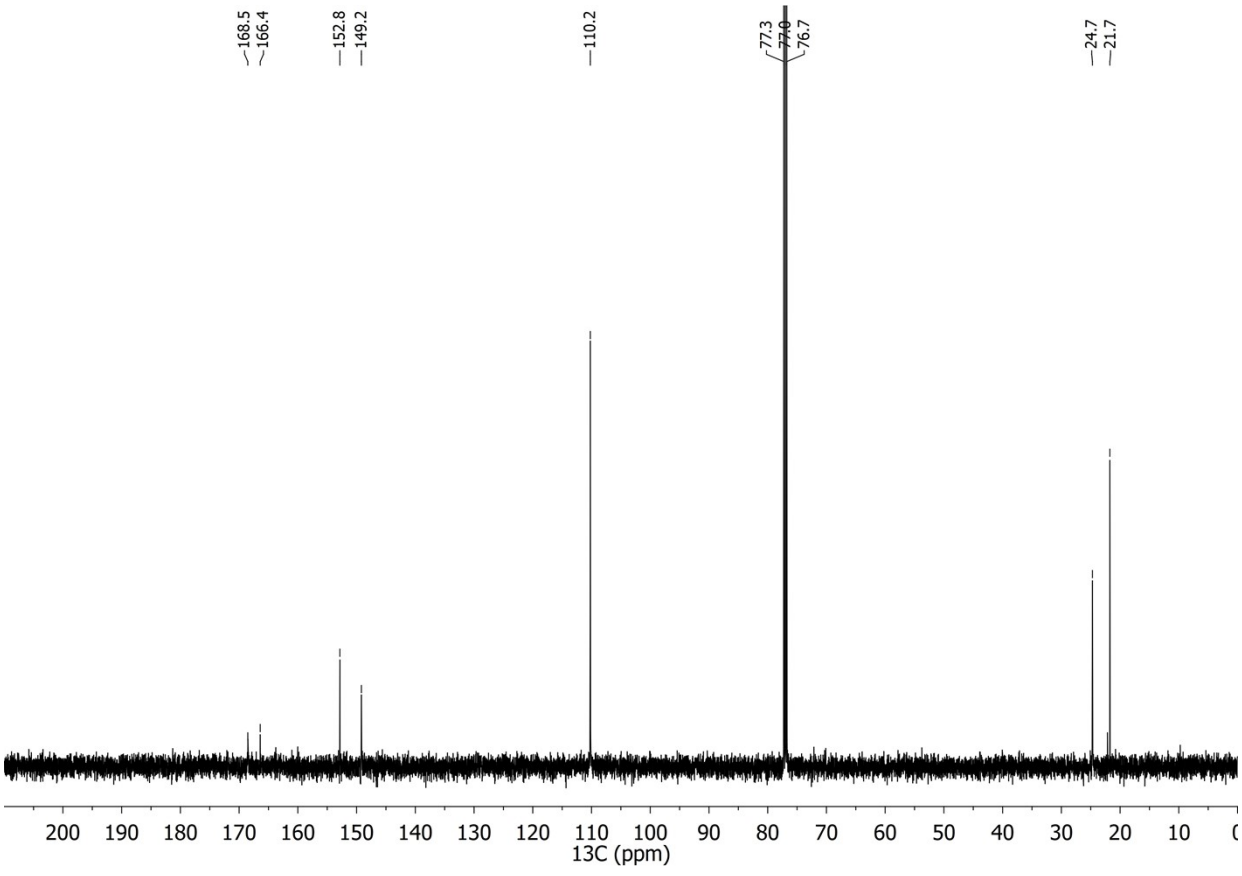

*Figure S4. ^{13}C-NMR (125 MHz, $CDCl_3$) of **6***

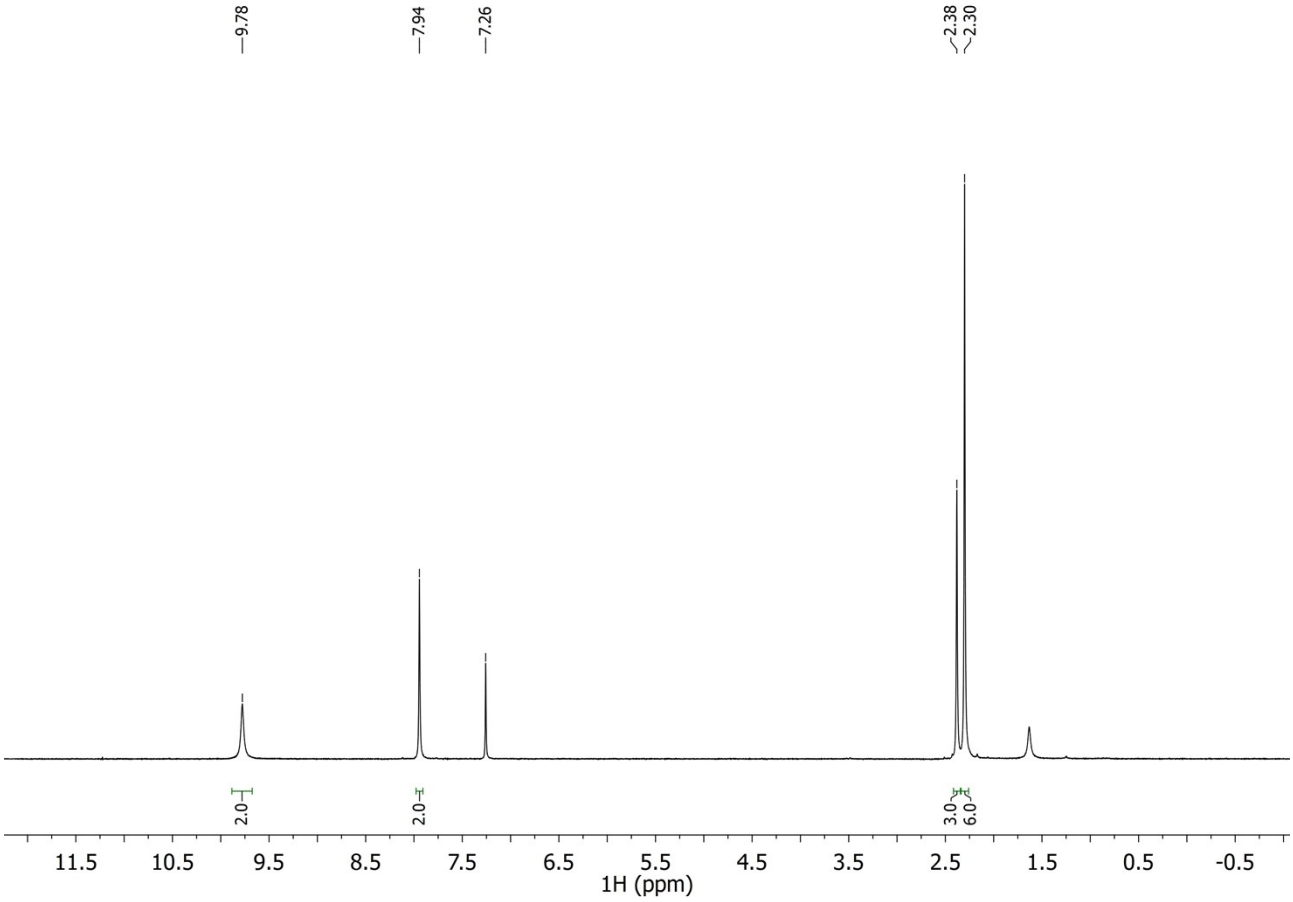

*Figure S5. ^{1}H-NMR (500 MHz, $CDCl_3$) of **7***

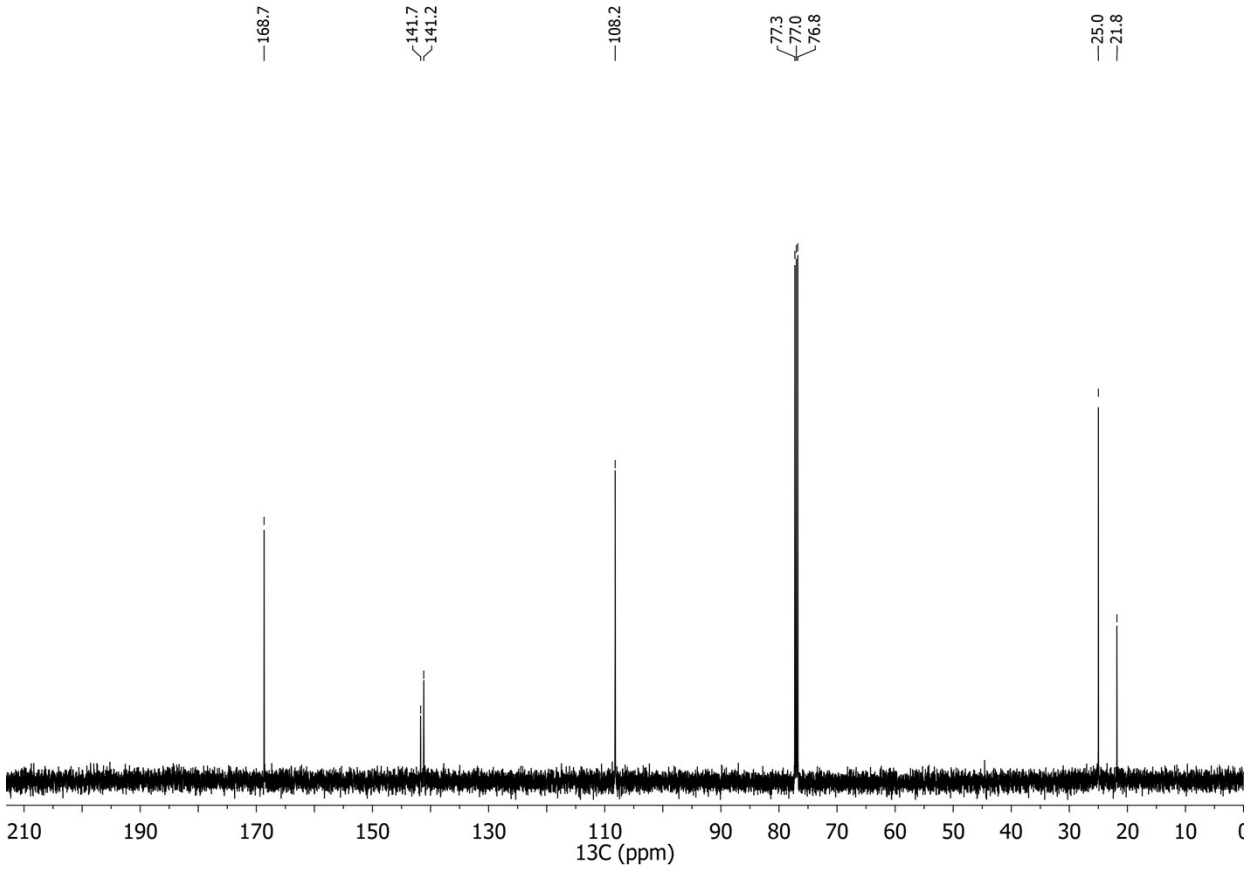

*Figure S6. ^{13}C-NMR (125 MHz, $CDCl_3$) of **7***

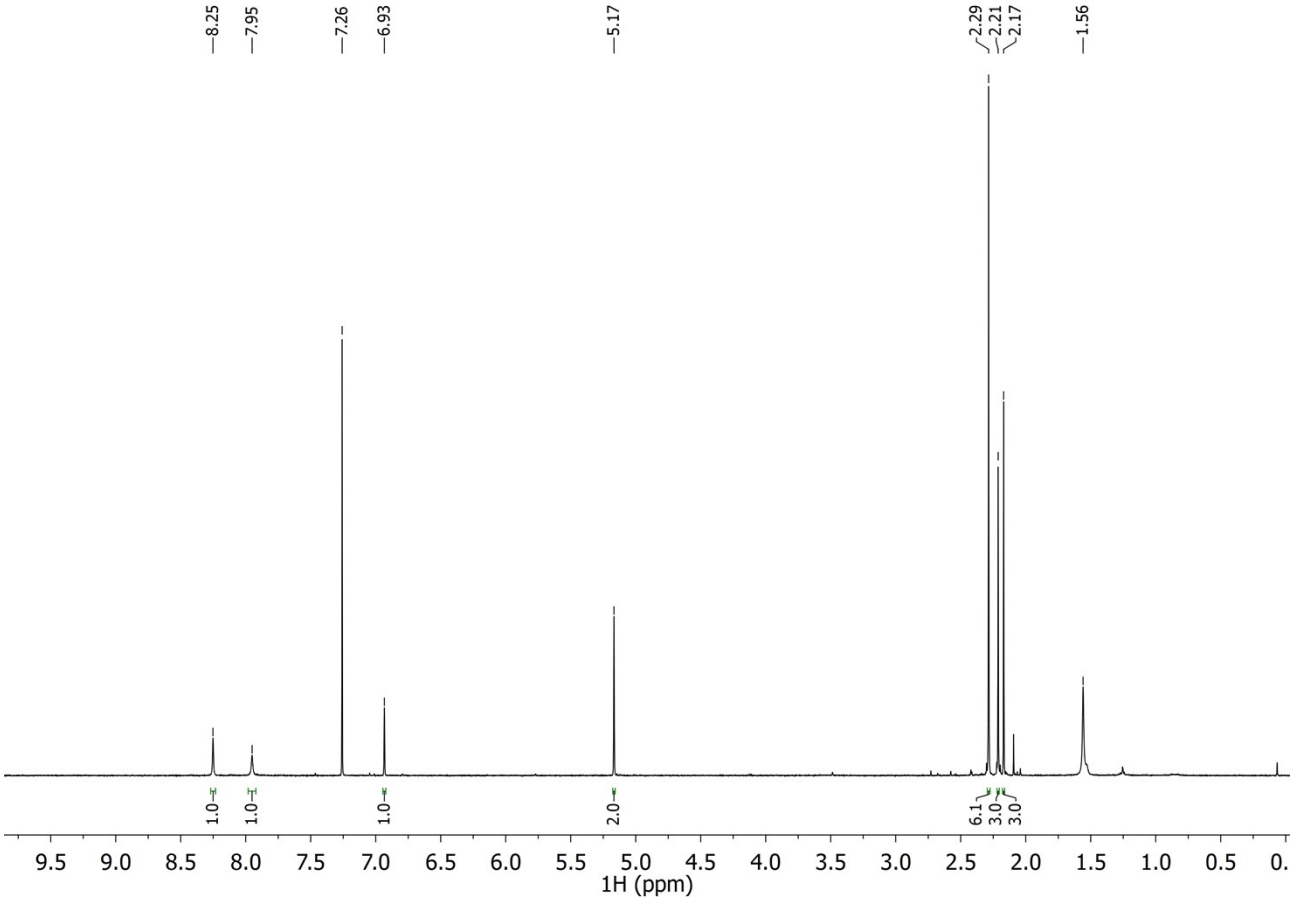

Figure S7. ^{1}H-NMR (500 MHz, $CDCl_3$) of Triacetylated derivative

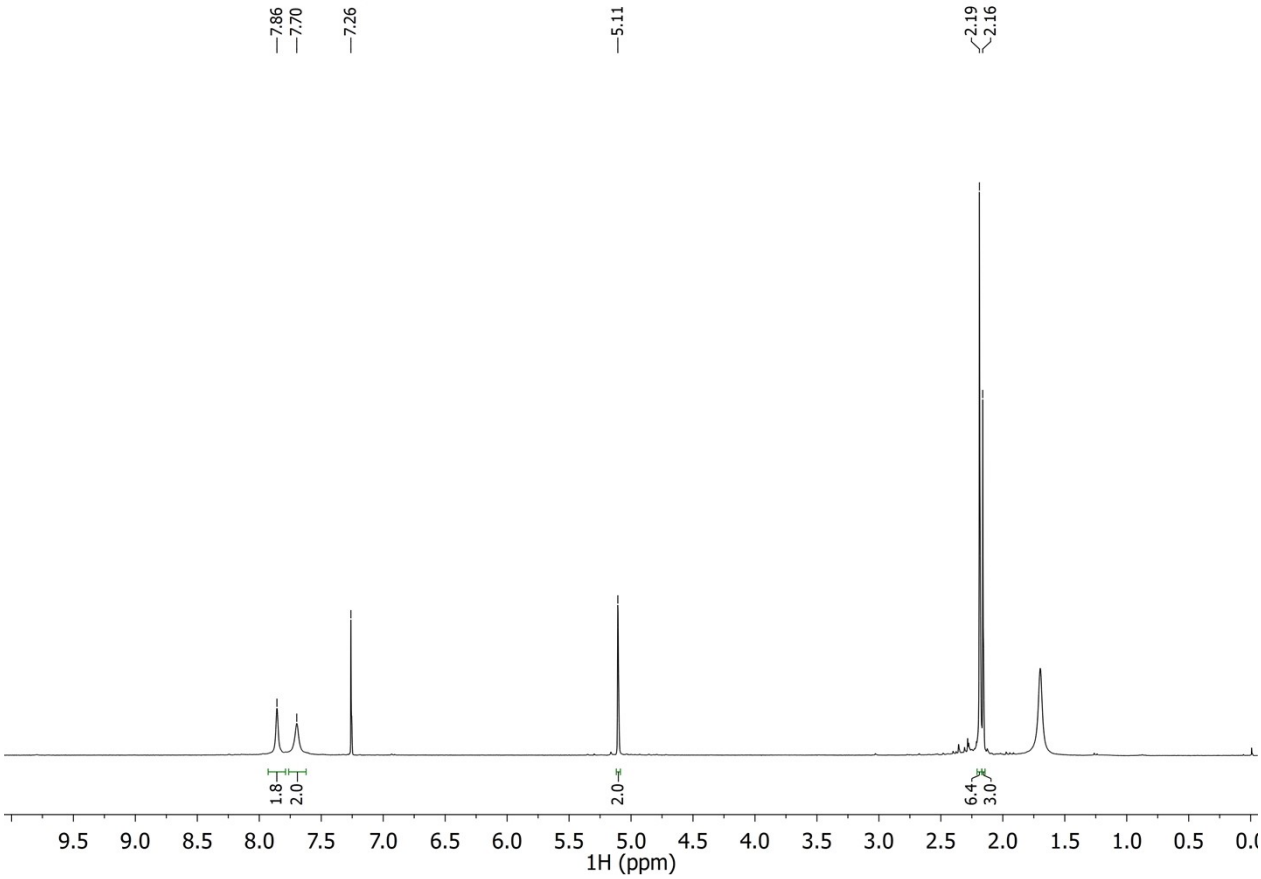

*Figure S8. ^{1}H-NMR (500 MHz, $CDCl_3$) of **8***

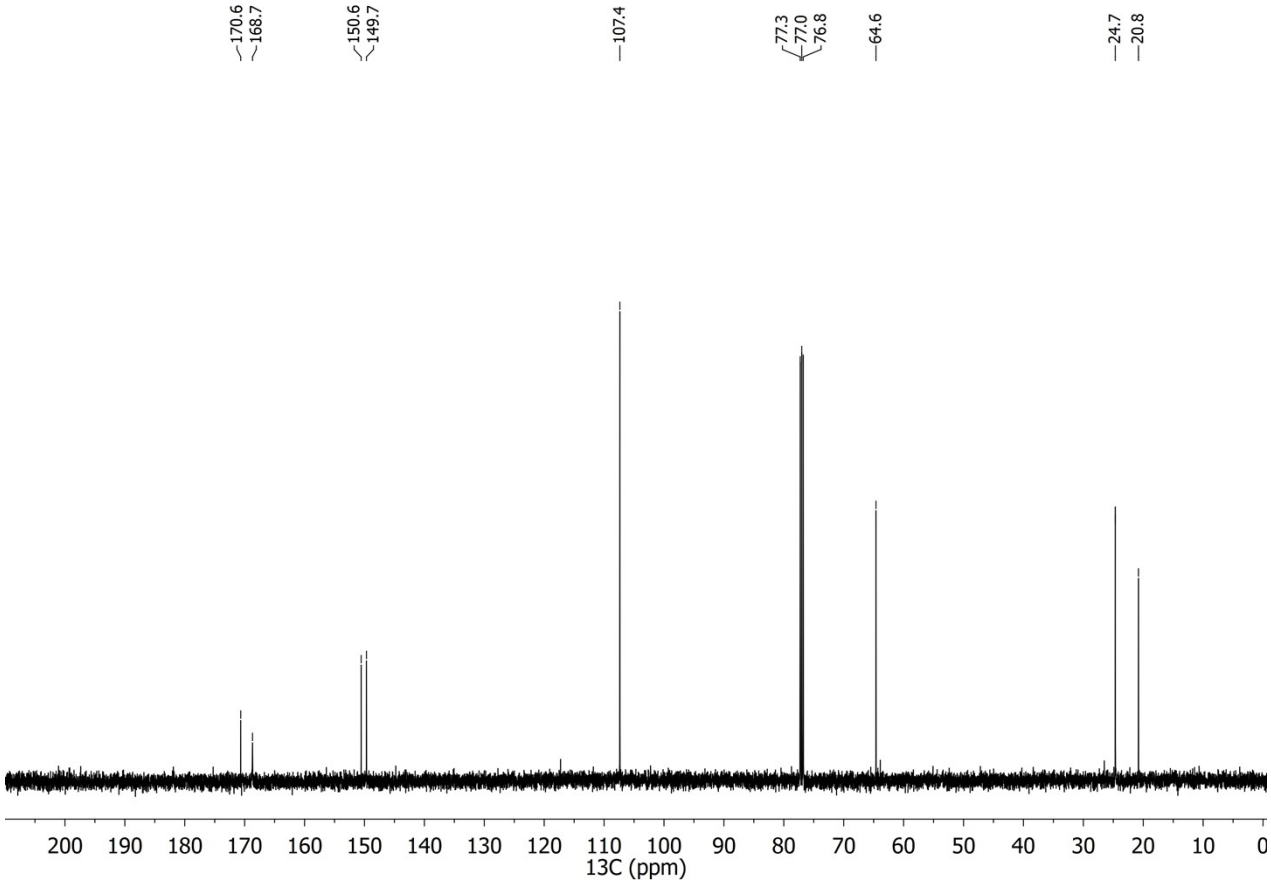

*Figure S9. ^{13}C-NMR (125 MHz, $CDCl_3$) of **8***

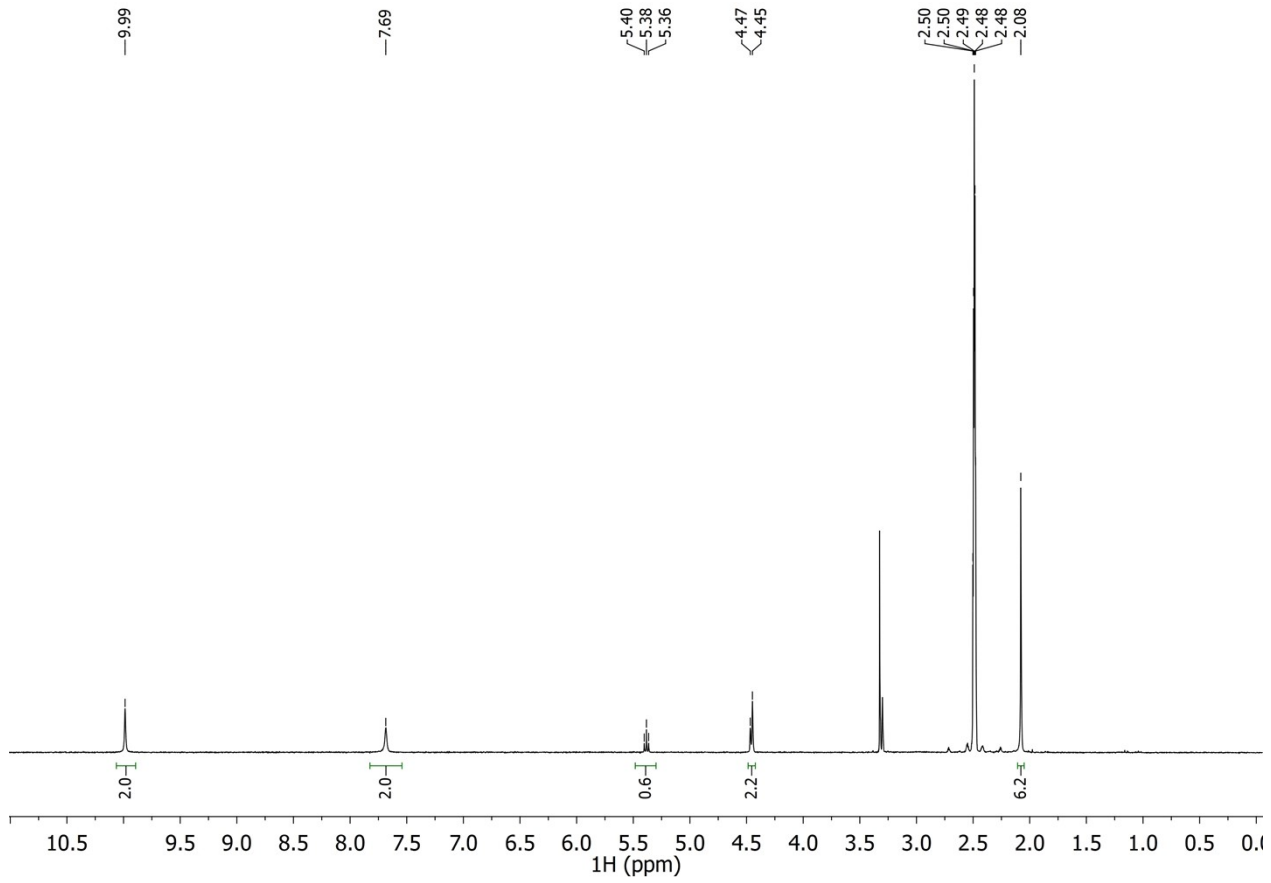

*Figure S10. ^{1}H-NMR (500 MHz, DMSO-d_6) of **9***

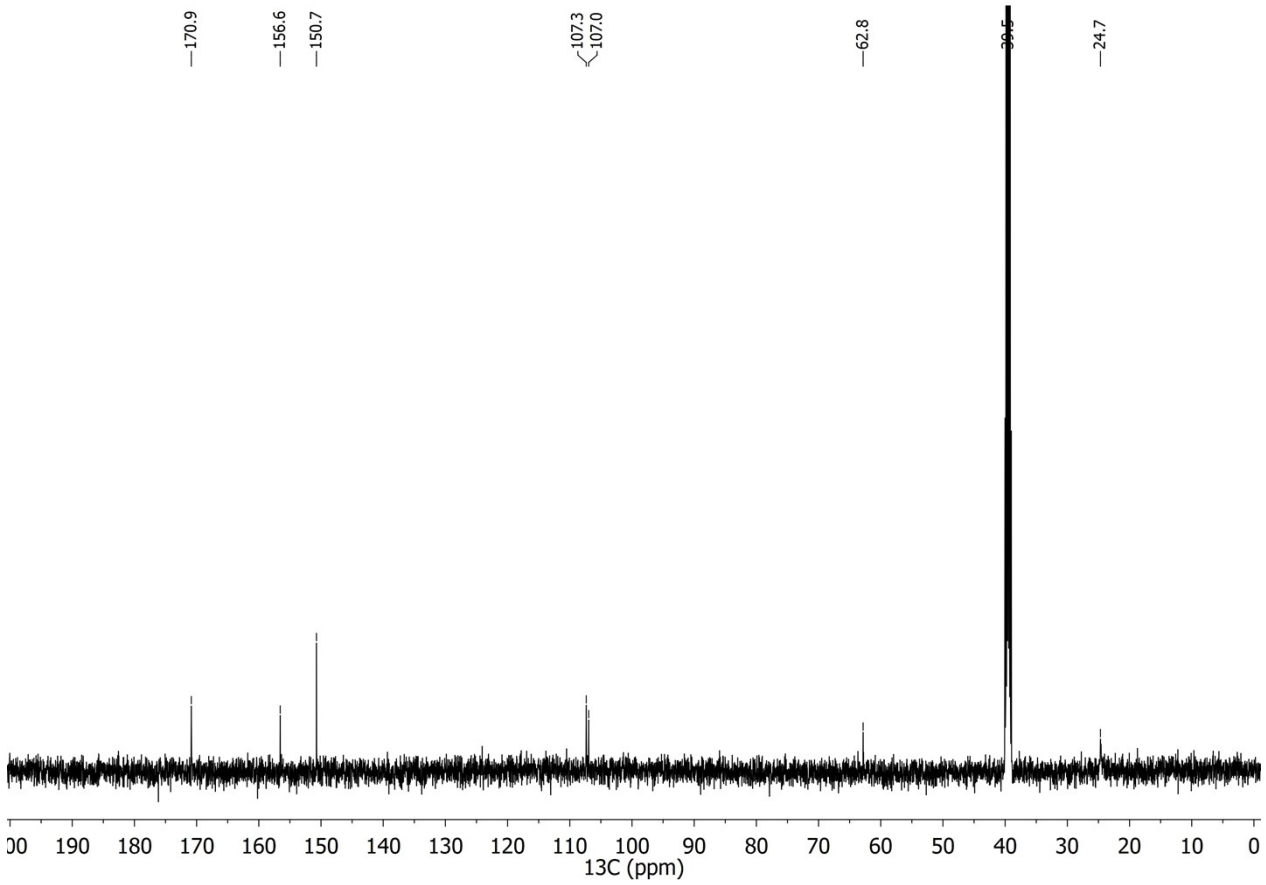

*Figure S11. ^{13}C-NMR (125 MHz, DMSO-d_6) of **9***

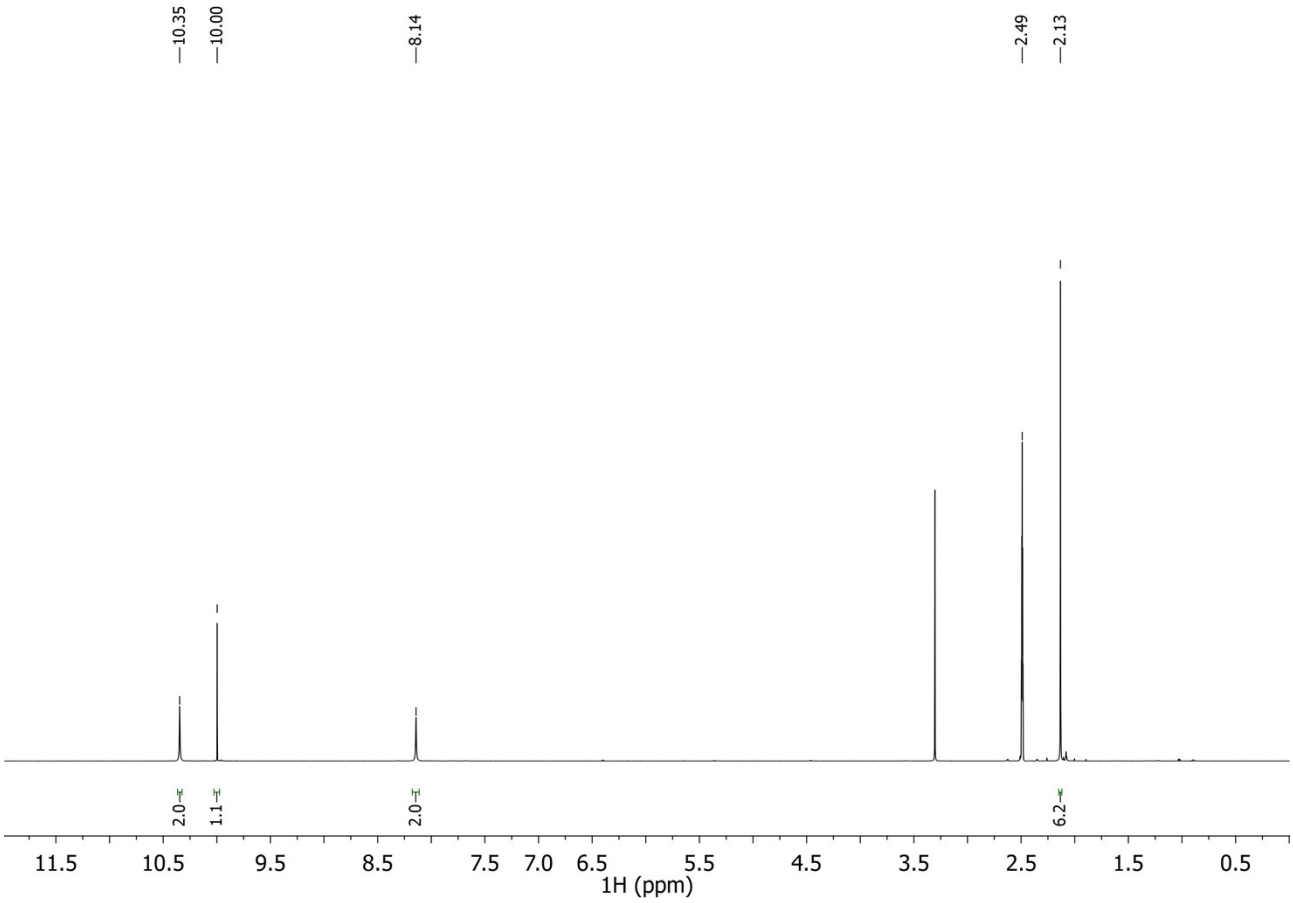

*Figure S12. ^{1}H-NMR (500 MHz, DMSO-d_6) of **10***

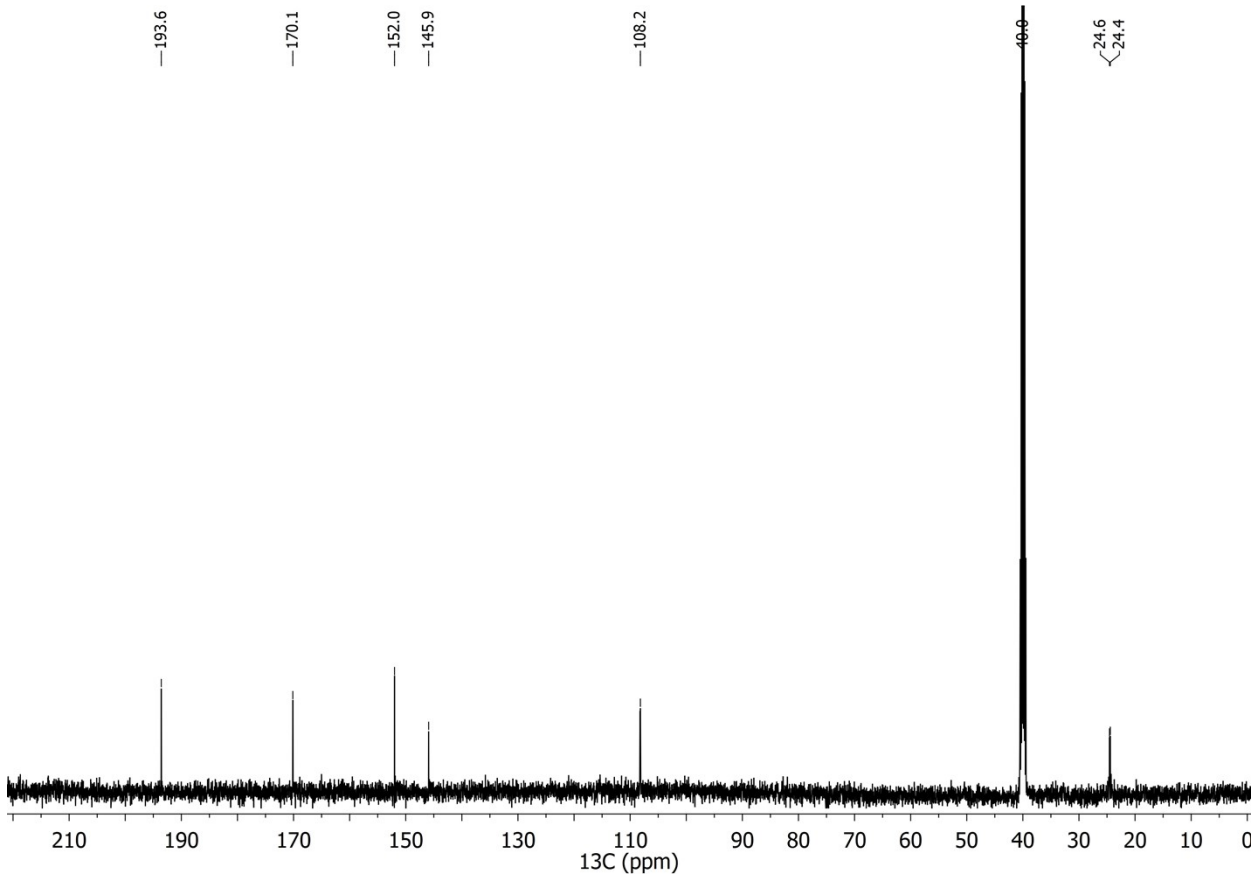

*Figure S13. ^{13}C-NMR (125 MHz, DMSO-d_6) of **10***

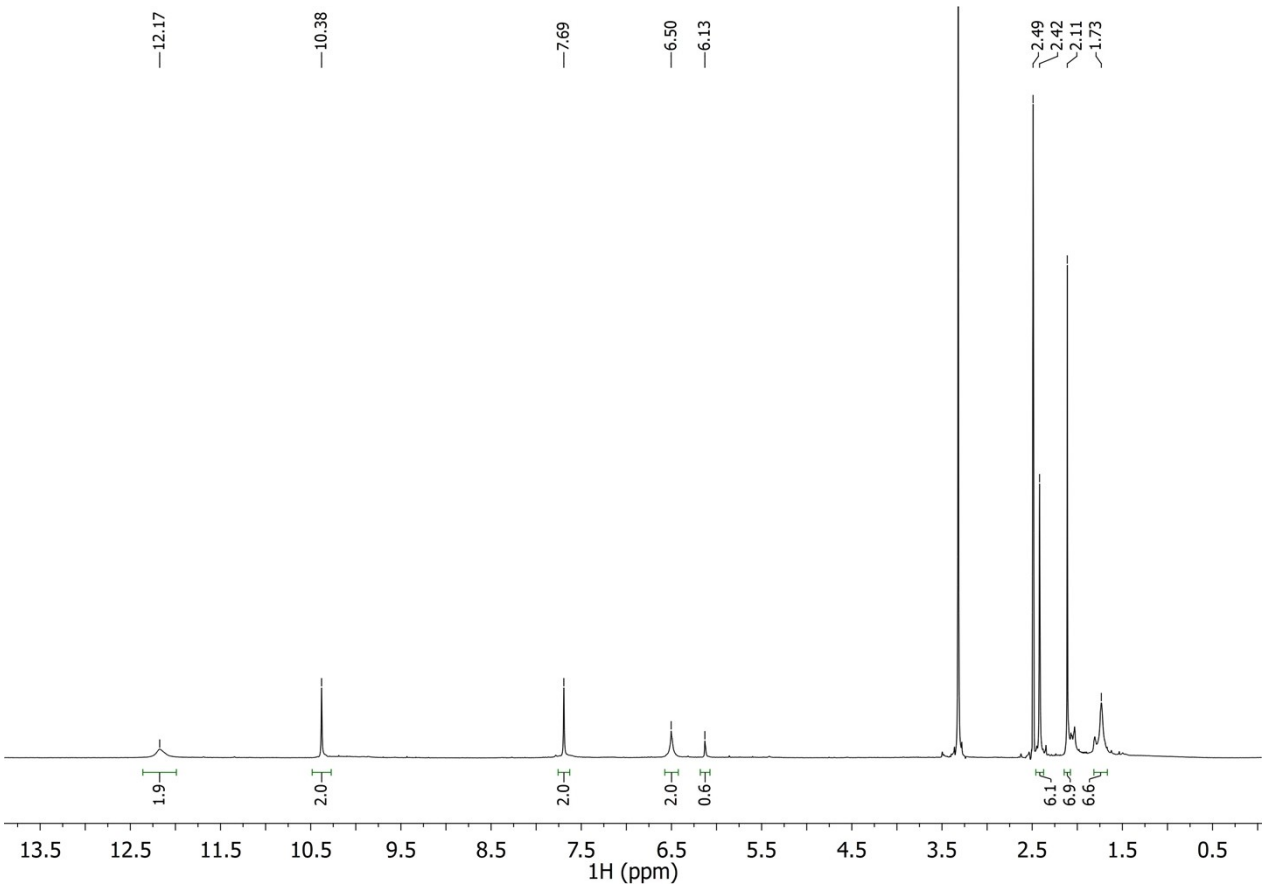

*Figure S14. ^{1}H-NMR (500 MHz, DMSO-d_6) of **11***

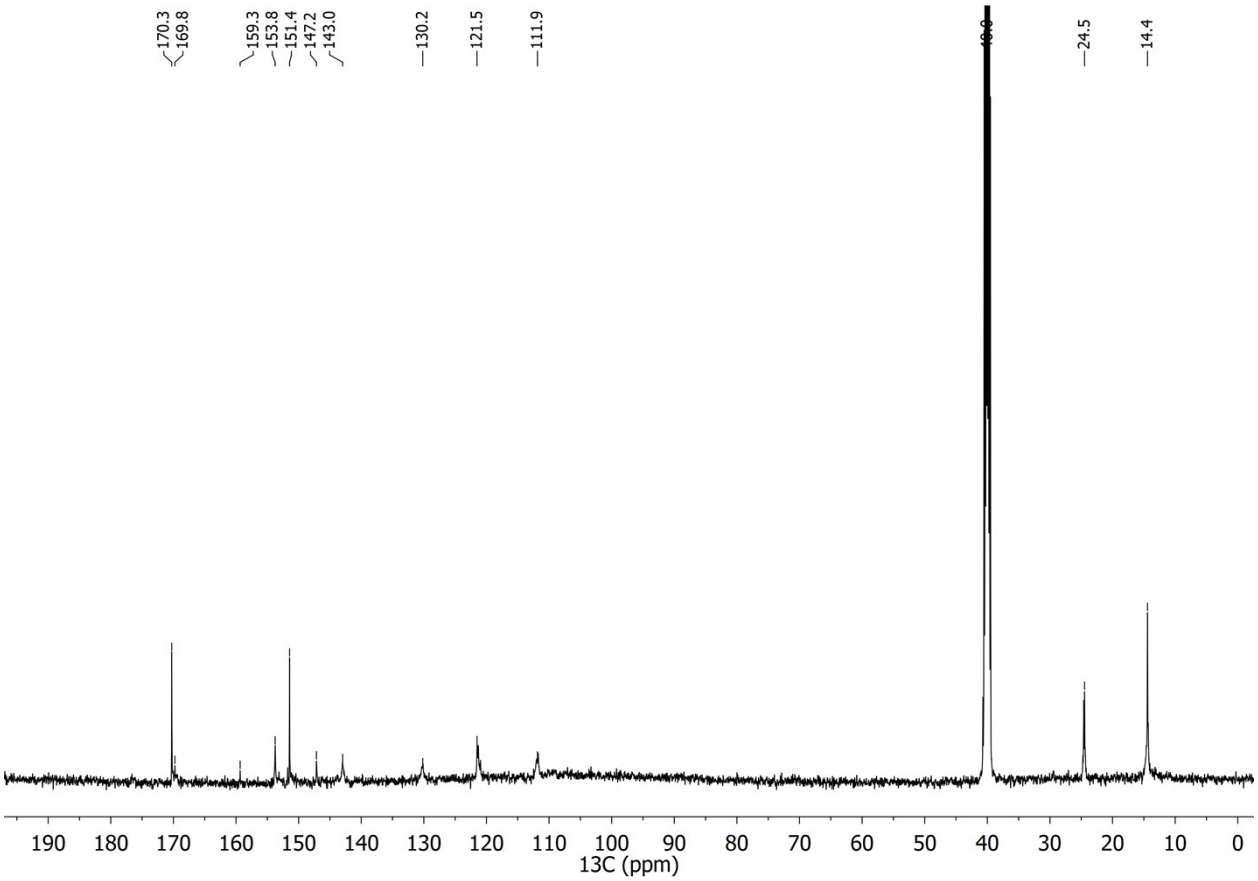

*Figure S15. ^{13}C-NMR (125 MHz, DMSO-d_6) of **11***

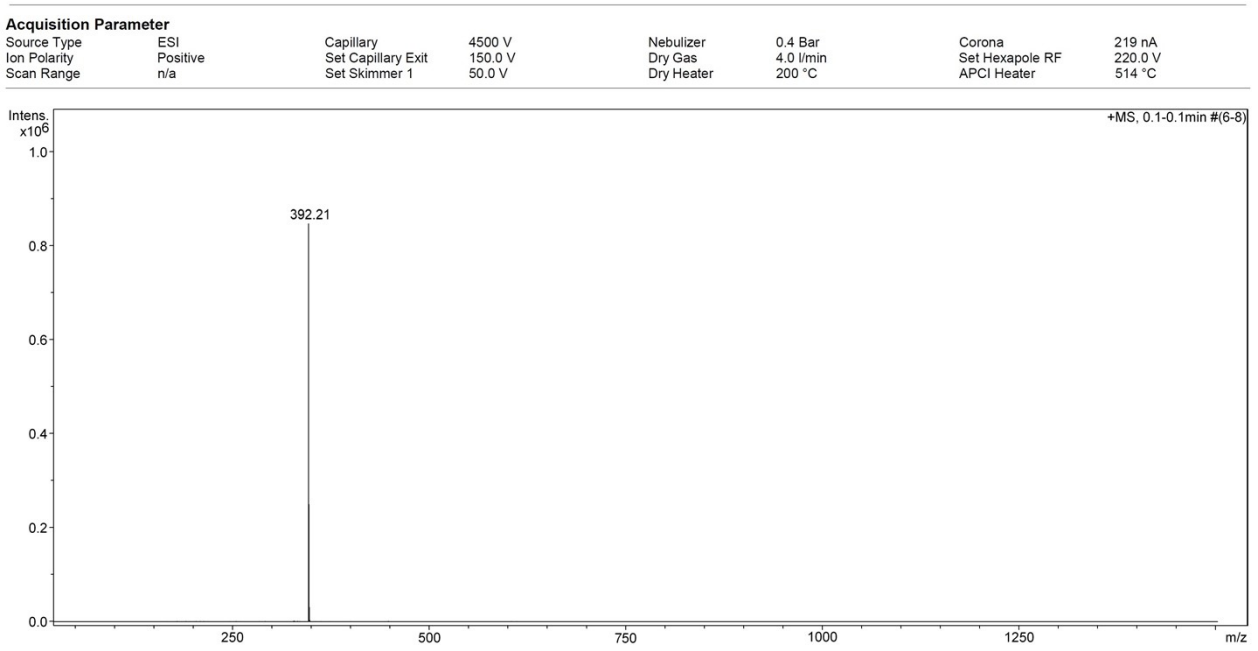

*Figure 16. ESI-MS of **11***

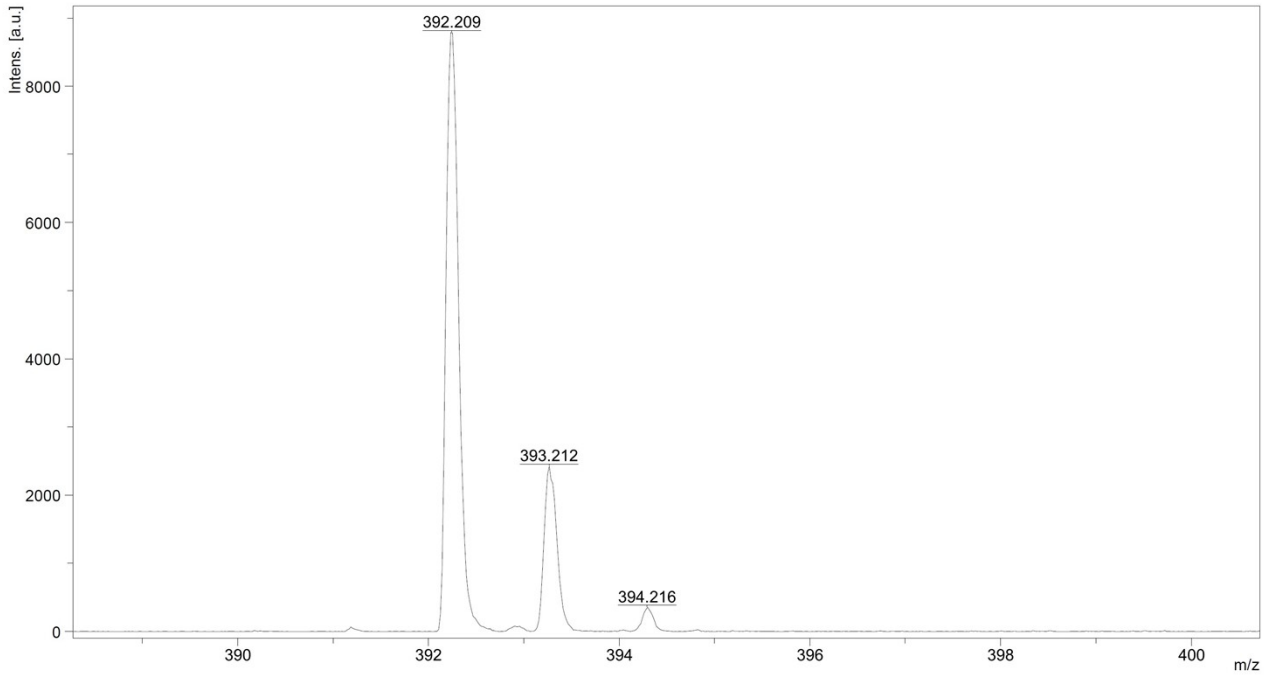

*Figure S17. ESI-MS of **11** zoom*

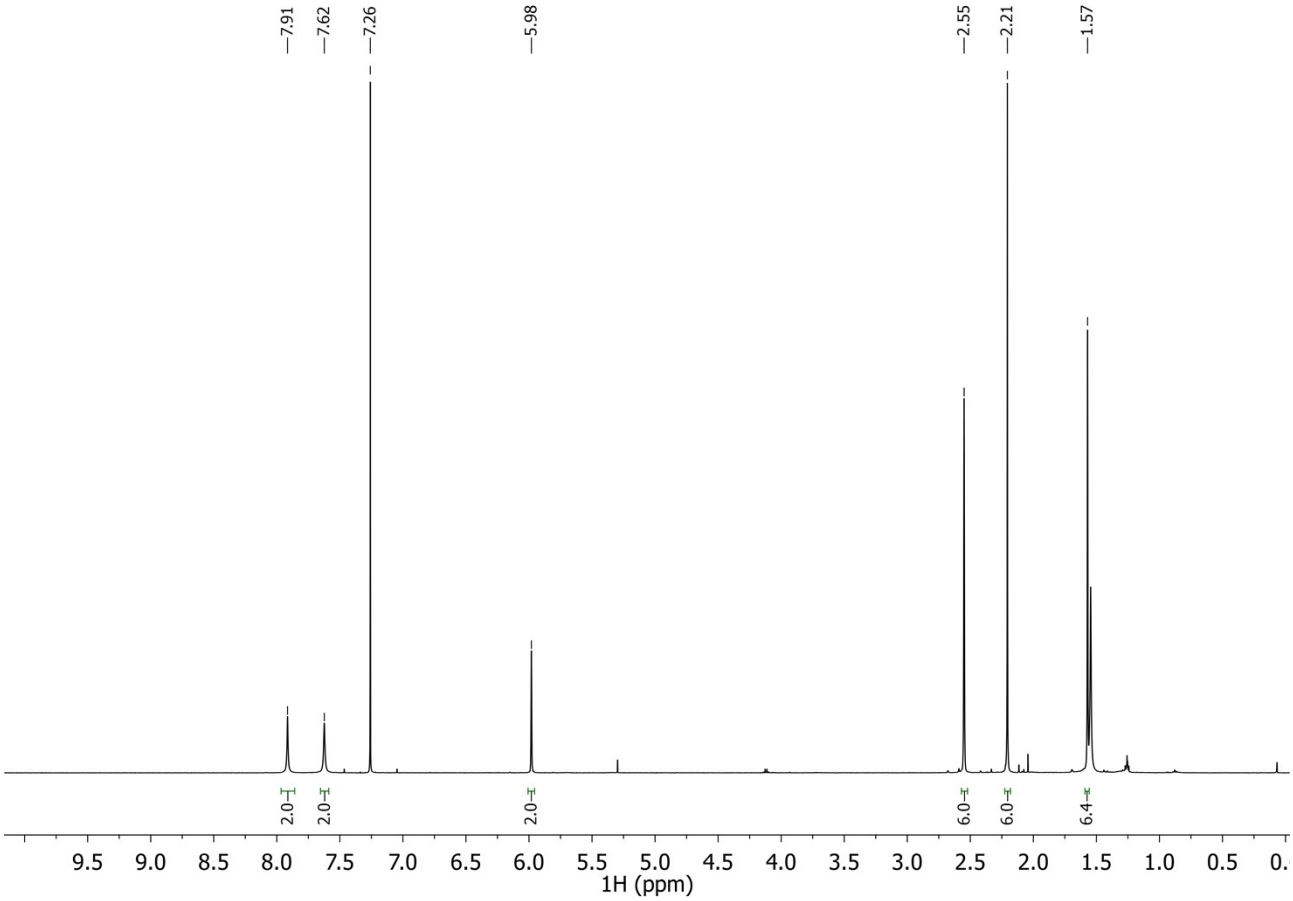

*Figure S18. ^{1}H-NMR (500 MHz, $CDCl_3$) of **12***

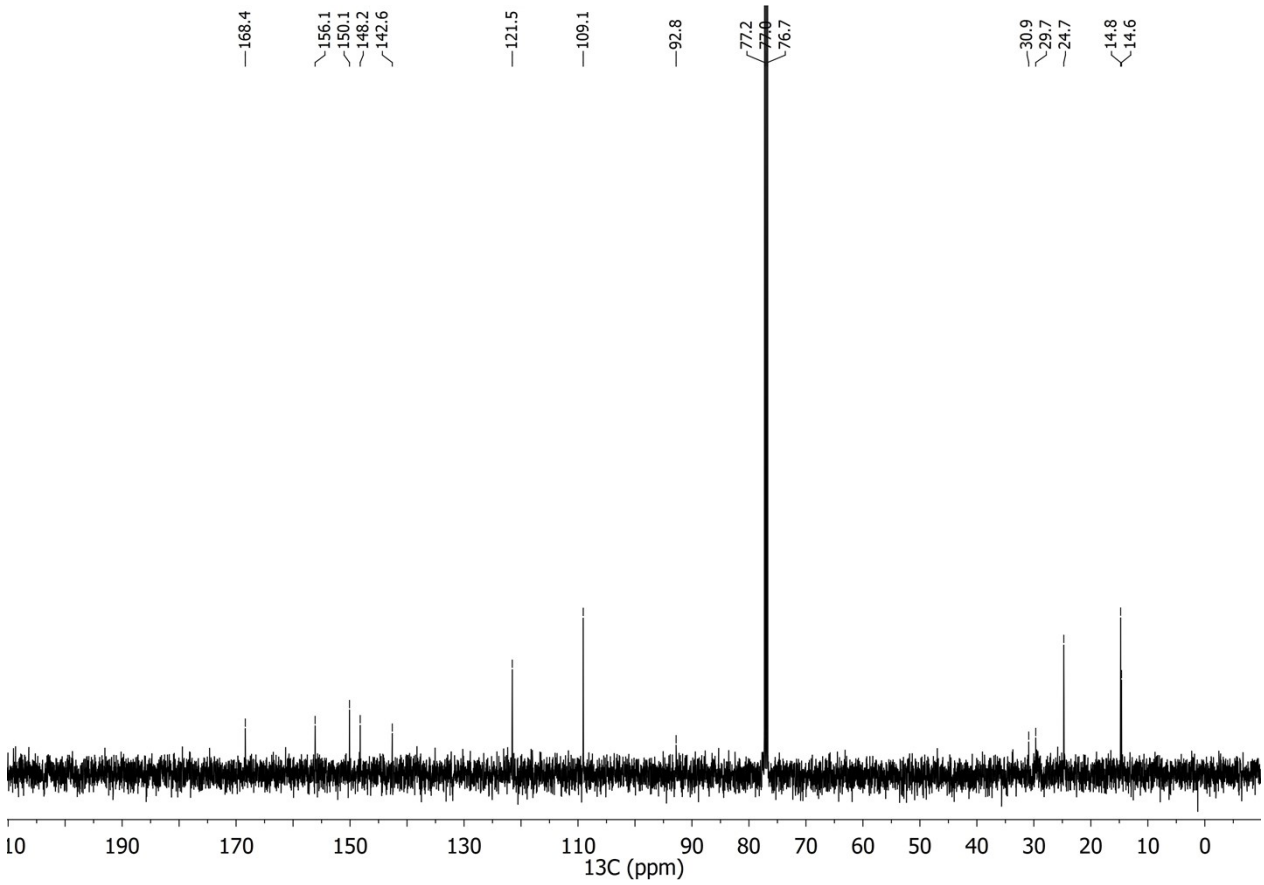

*Figure S19. ^{13}C-NMR (125 MHz, $CDCl_3$) of **12***

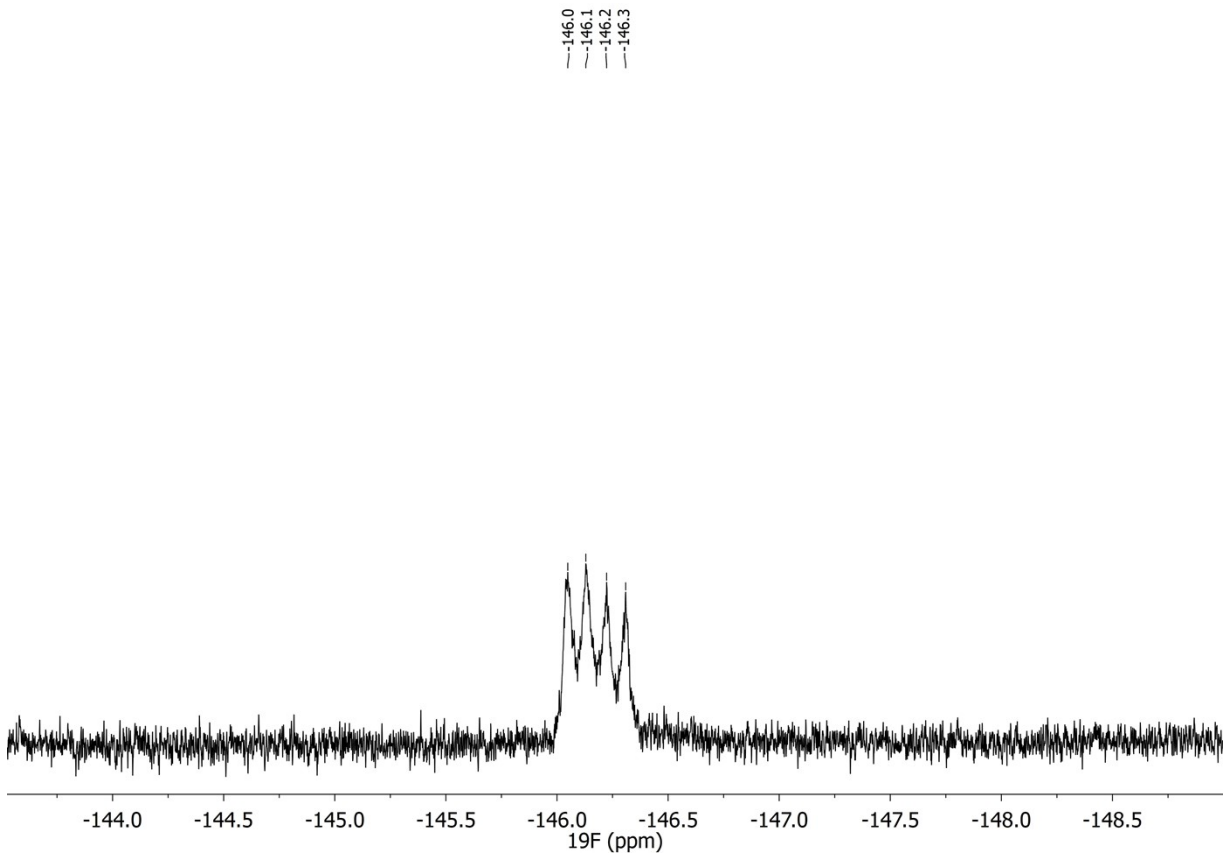

*Figure S20. ^{19}F-NMR (376 MHz, $CDCl_3$) of **12***

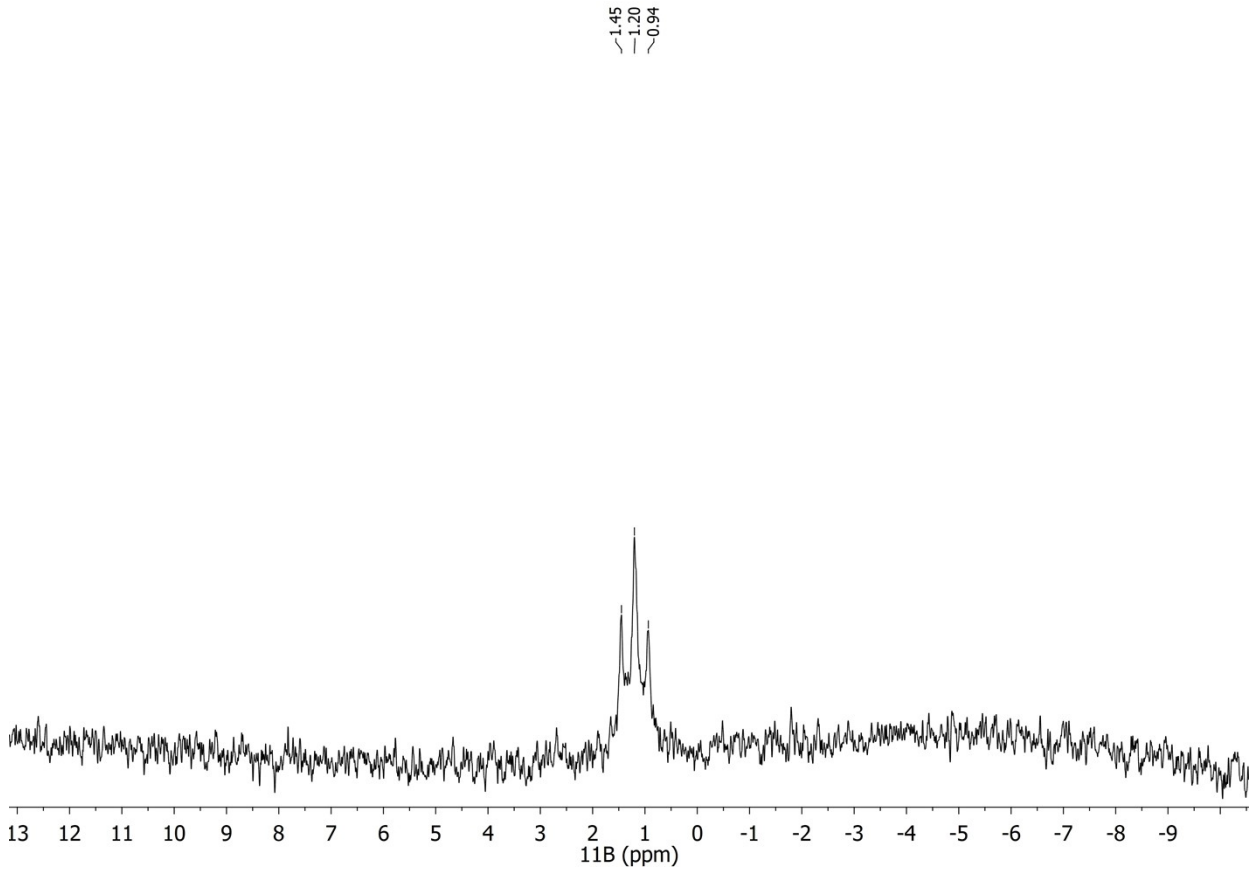

*Figure S21. ^{11}B-NMR (128 MHz, CDCl3) of **12***

Acquisition Parameter

Source Type	ESI	Capillary	4500 V	Nebulizer	0.4 Bar	Corona	214 nA
Ion Polarity	Positive	Set Capillary Exit	150.0 V	Dry Gas	4.0 l/min	Set Hexapole RF	220.0 V
Scan Range	n/a	Set Skimmer 1	50.0 V	Dry Heater	200 °C	APCI Heater	504 °C

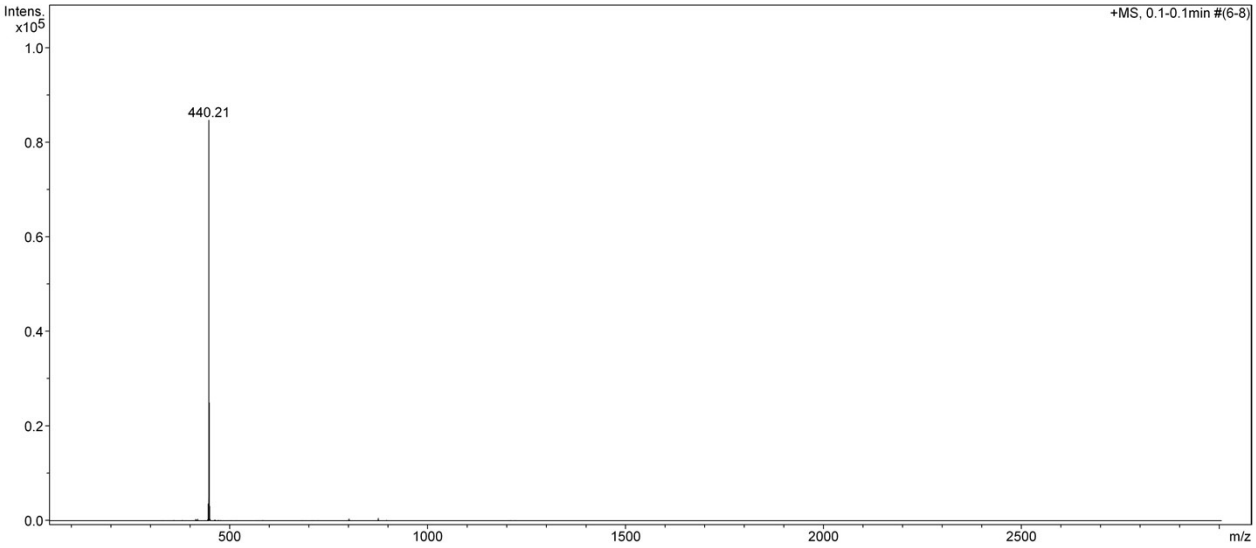

*Figure S22. ESI-MS of **12***

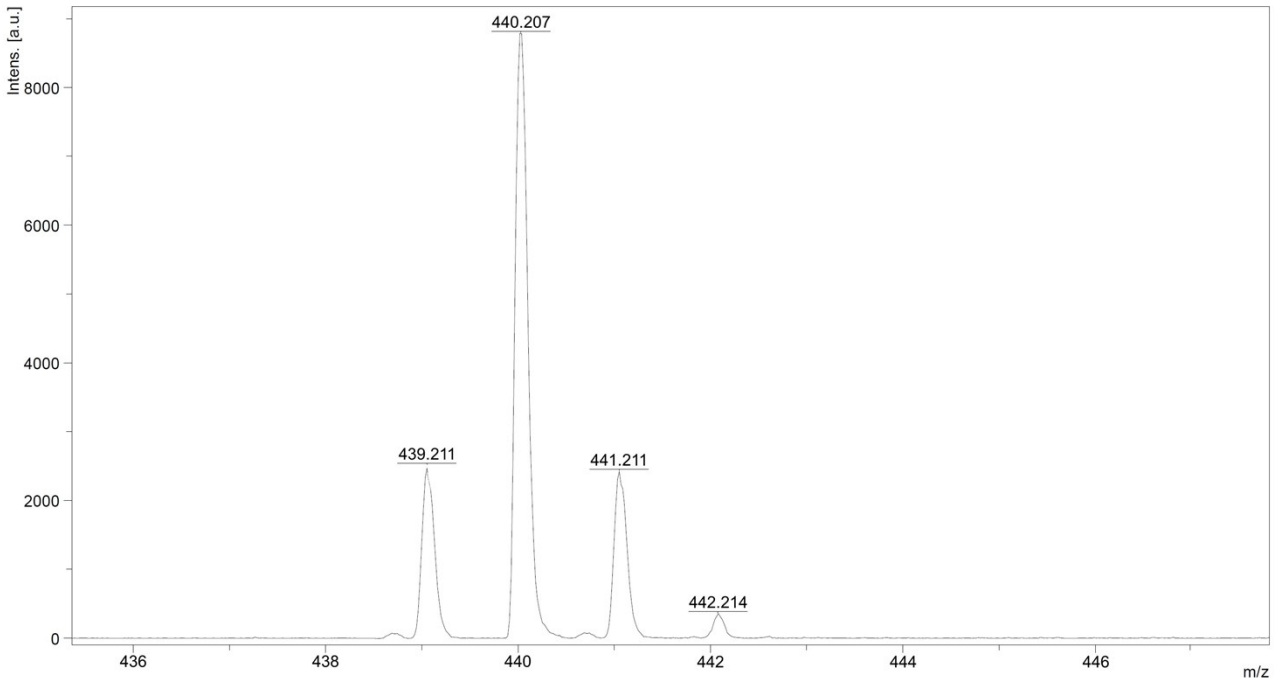

*Figure S23. ESI-MS of **12** zoom*

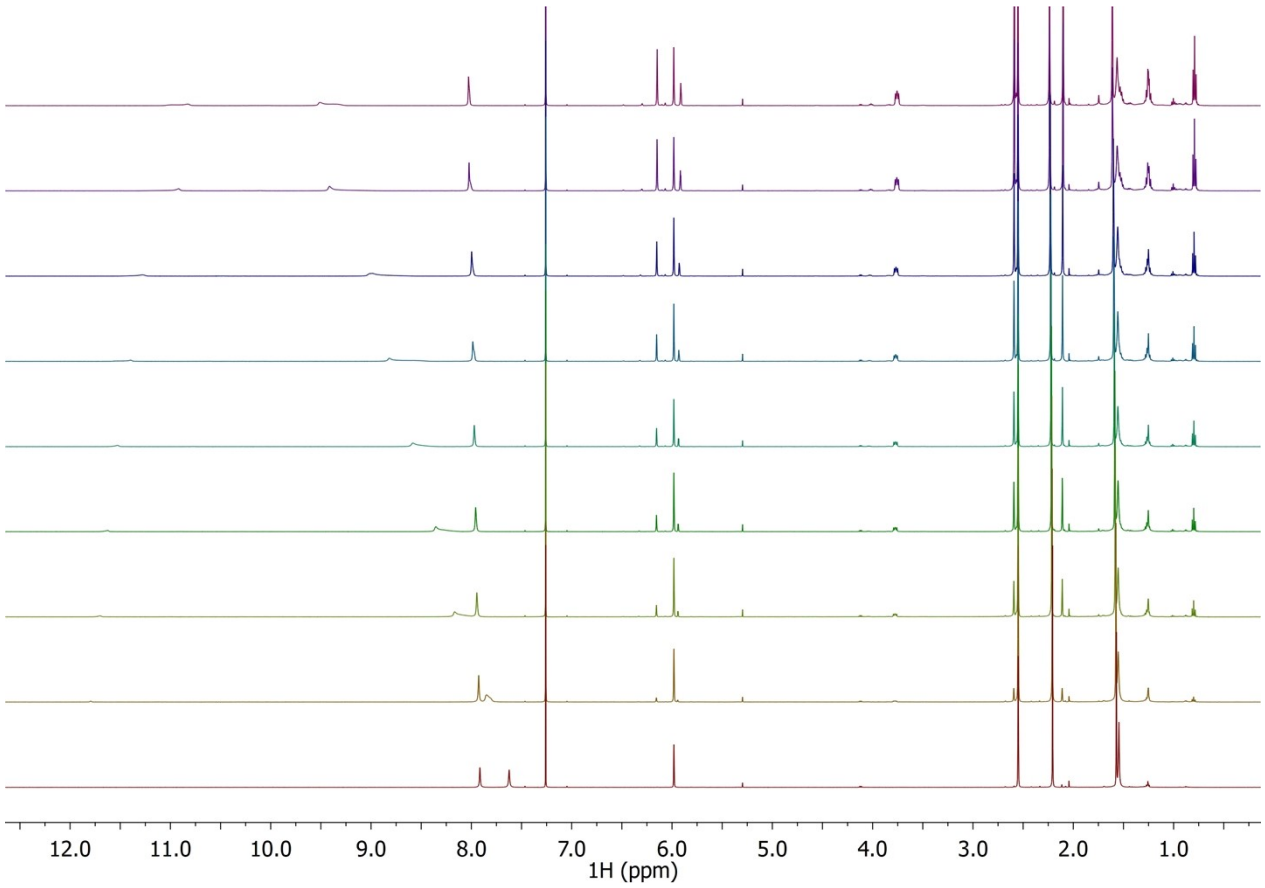

*Figure S24. Superimposed NMR spectra of the titration of **12** (2.0 mg, 5.4 mM) in $CDCl_3$ and gradual additions of 0.25 mg of **13** up to equivalence (2.0 mg 5.4 mM)*

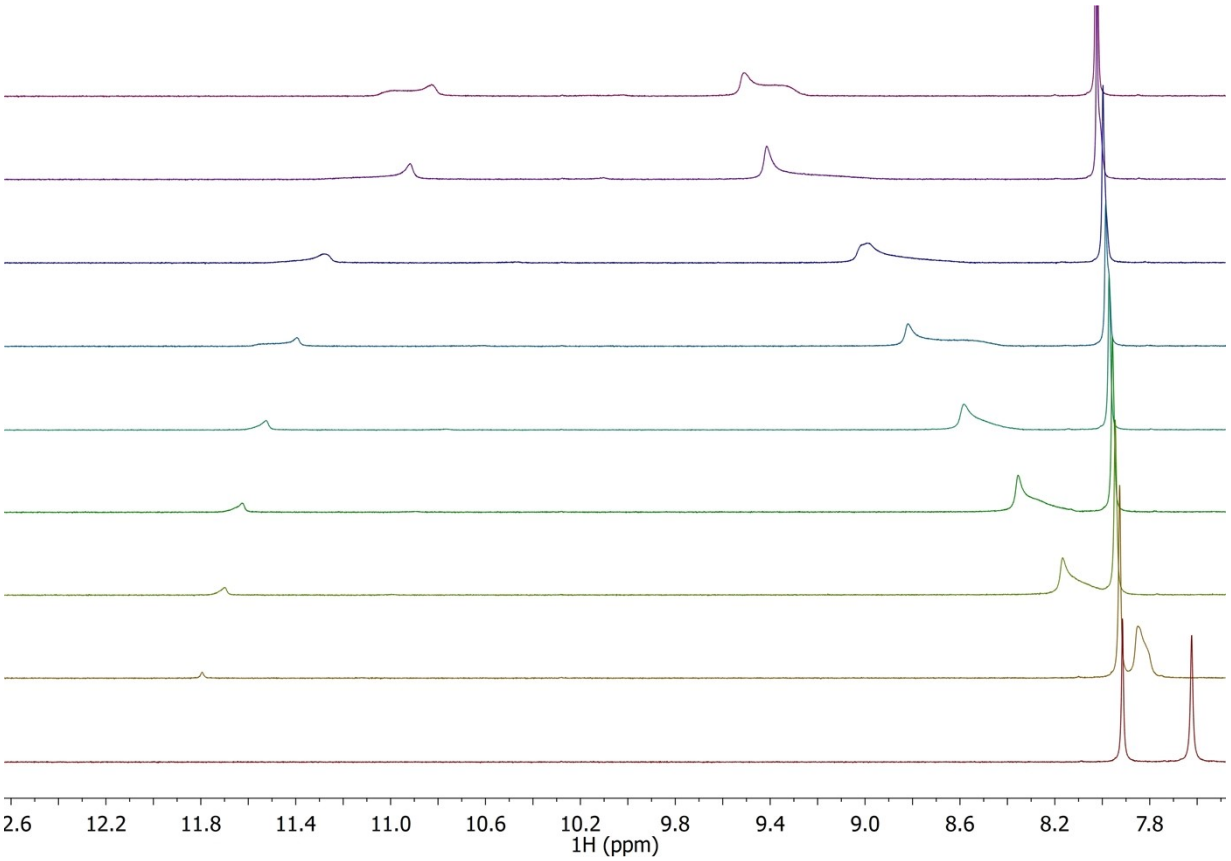

Figure S25. Magnification of the superimposed NMR spectra of Figure S24

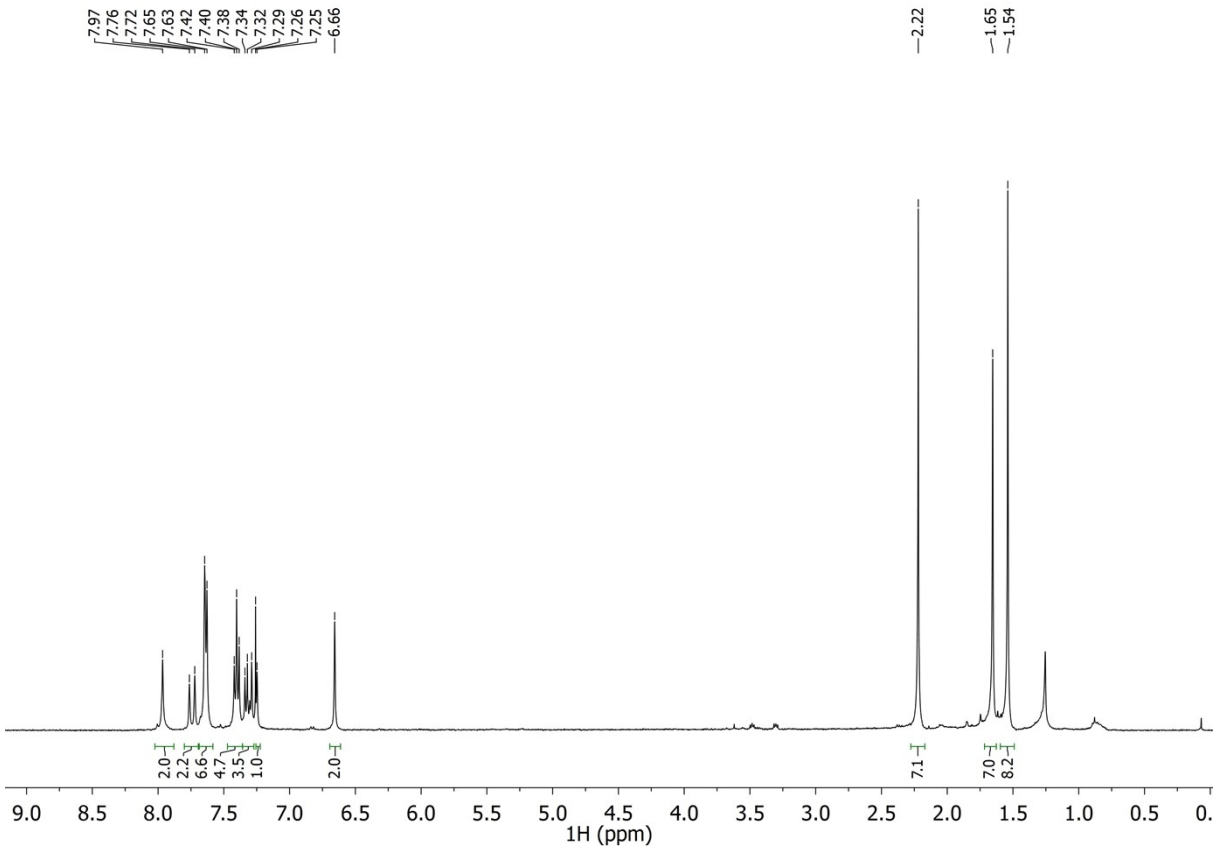

*Figure S26. ^{1}H-NMR (400 MHz, $CDCl_3$) of **1***

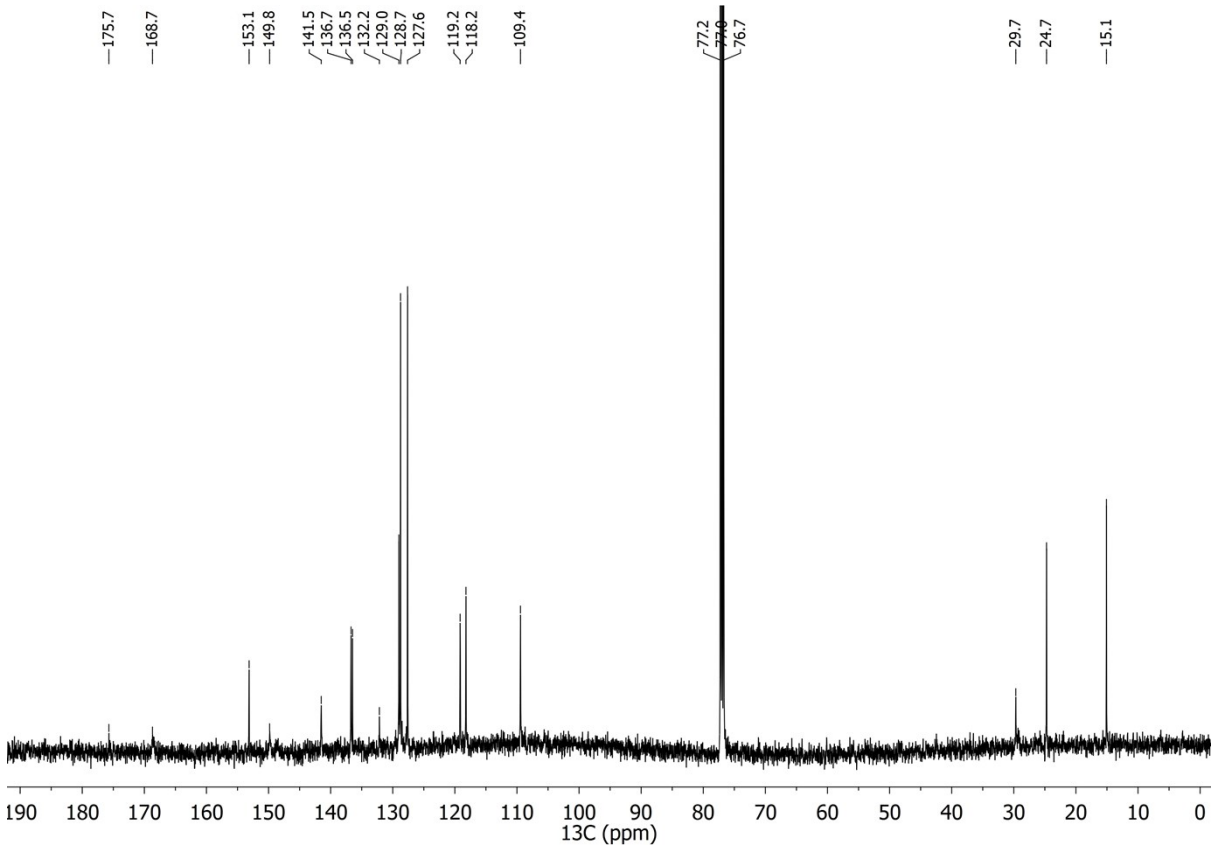

*Figure S27. ^{13}C-NMR (101 MHz, $CDCl_3$) of **1***

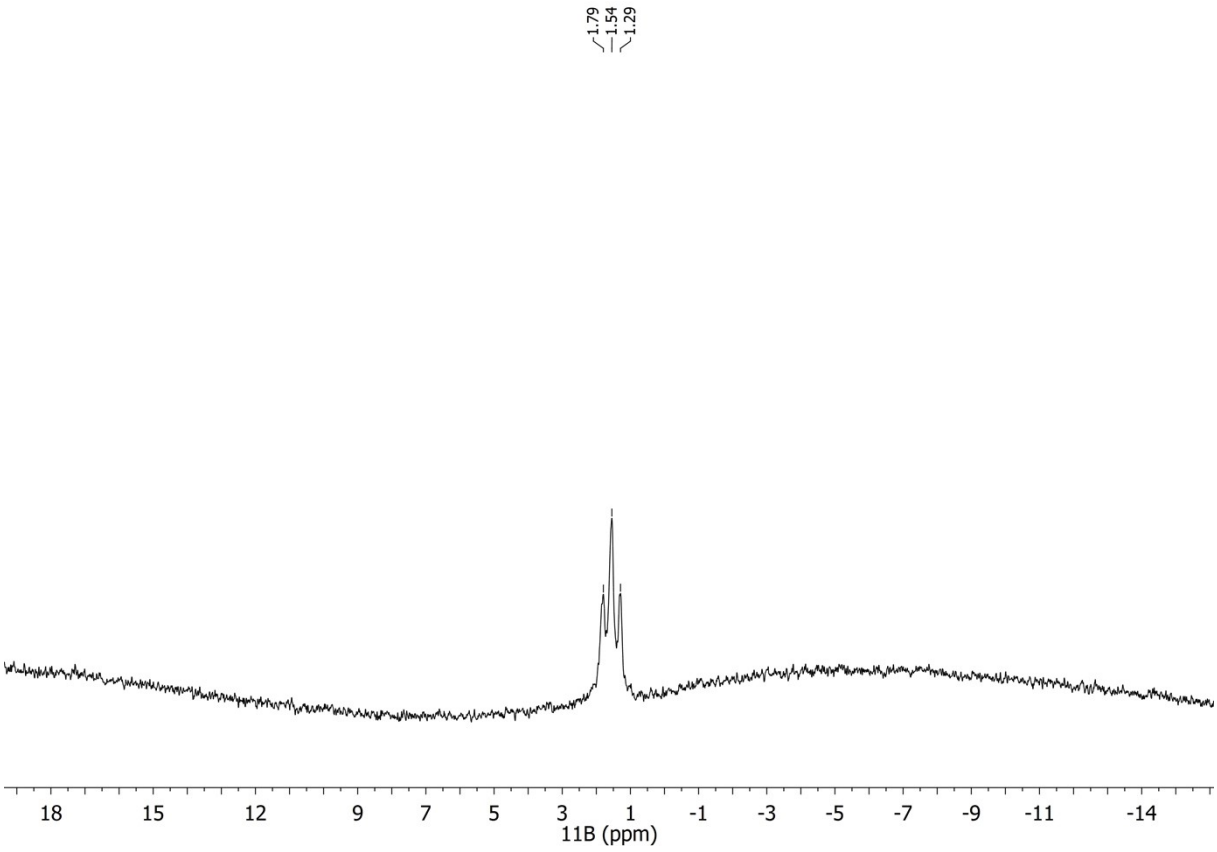

*Figure S28. ^{11}B-NMR (128 MHz, $CDCl_3$) of **1***

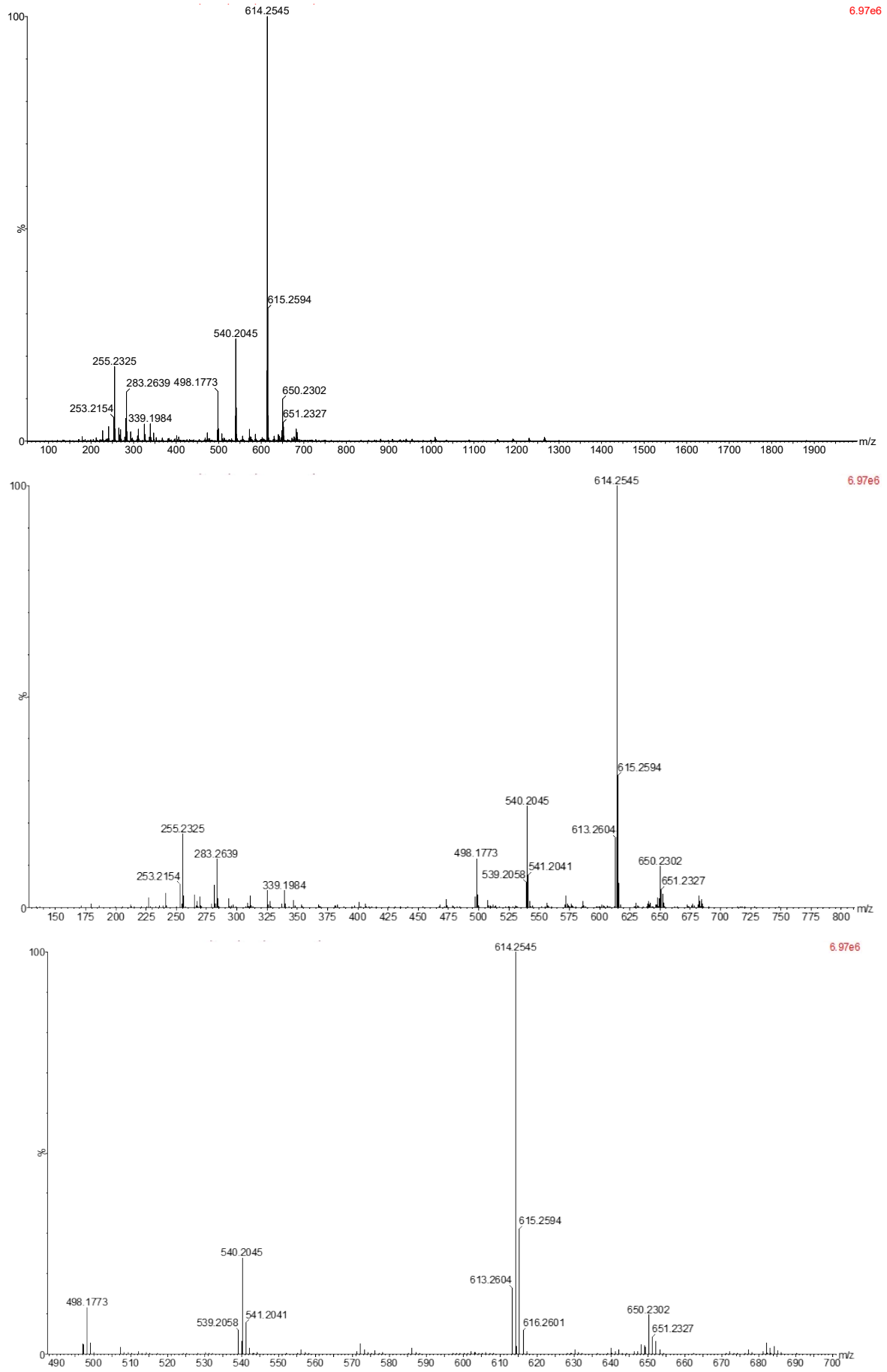

*Figure S29. TOF-Mass spectra of **1***

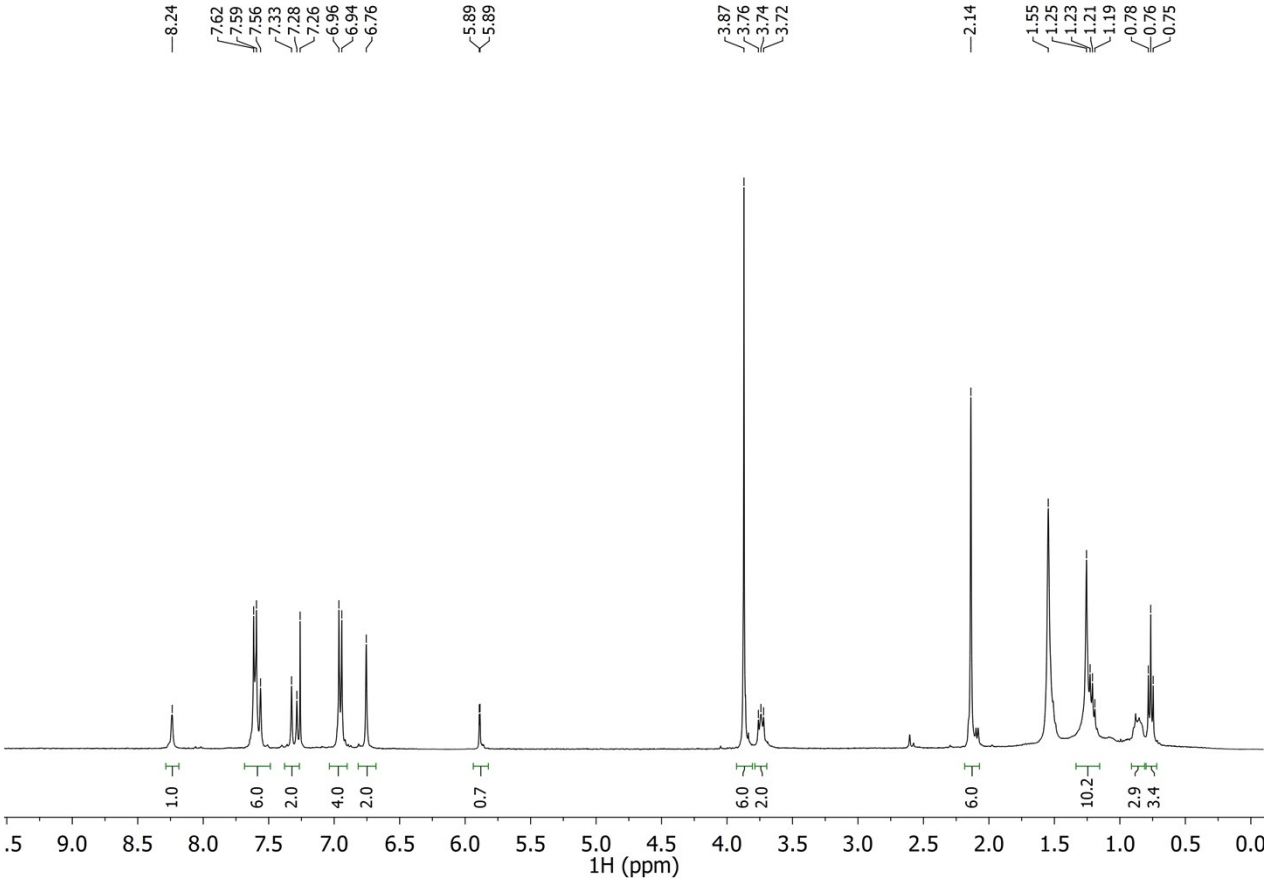

*Figure S30. ^{1}H-NMR (400 MHz, $CDCl_3$) of **2***

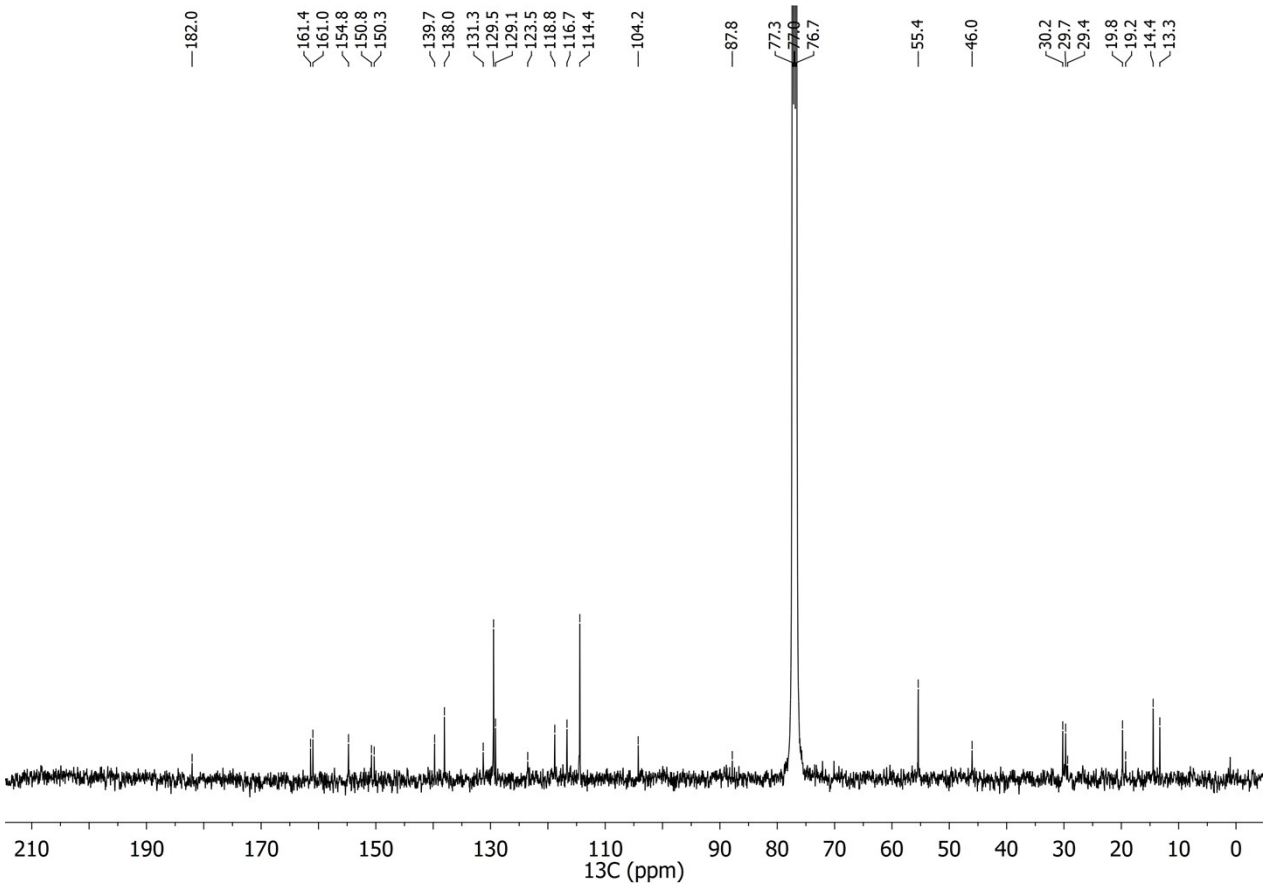

*Figure S31. ^{13}C-NMR (101 MHz, $CDCl_3$) of **2***

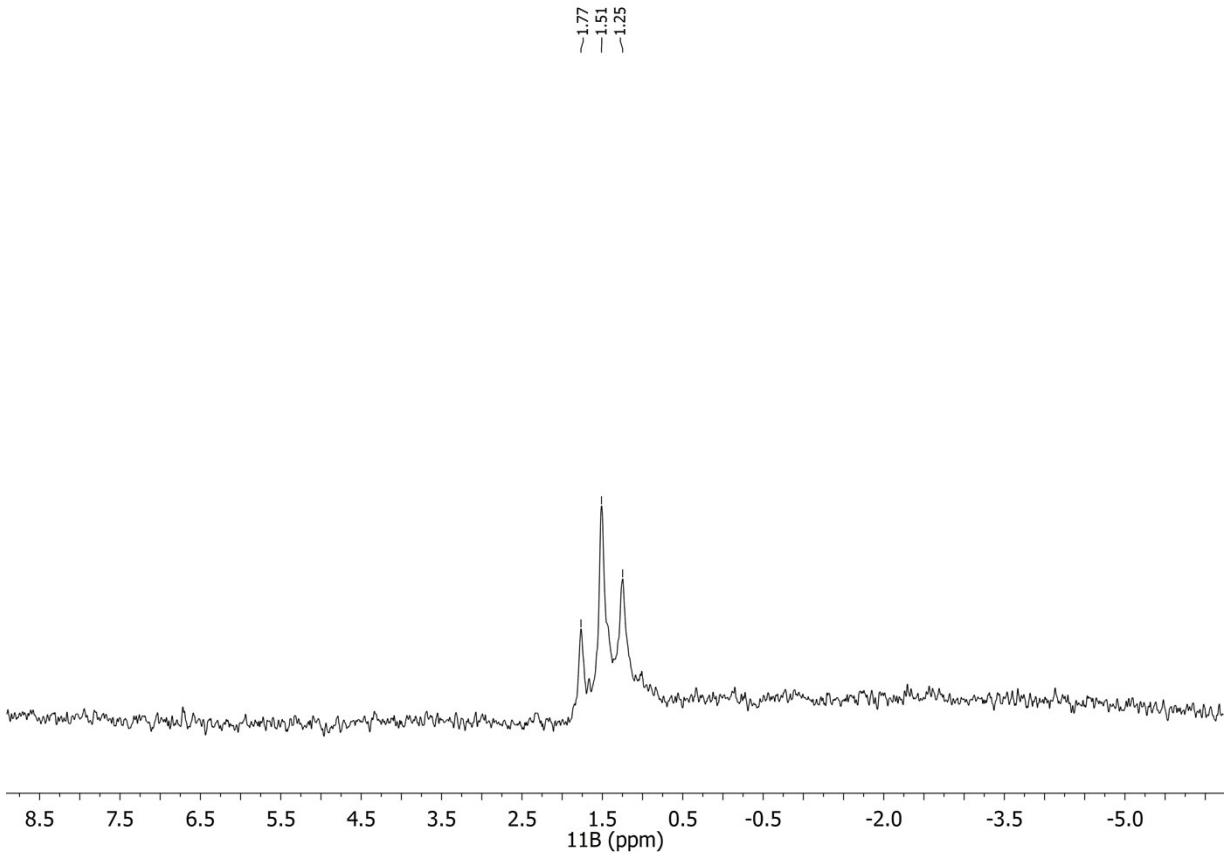

*Figure S32. ^{11}B-NMR (128 MHz, $CDCl_3$) of **2***

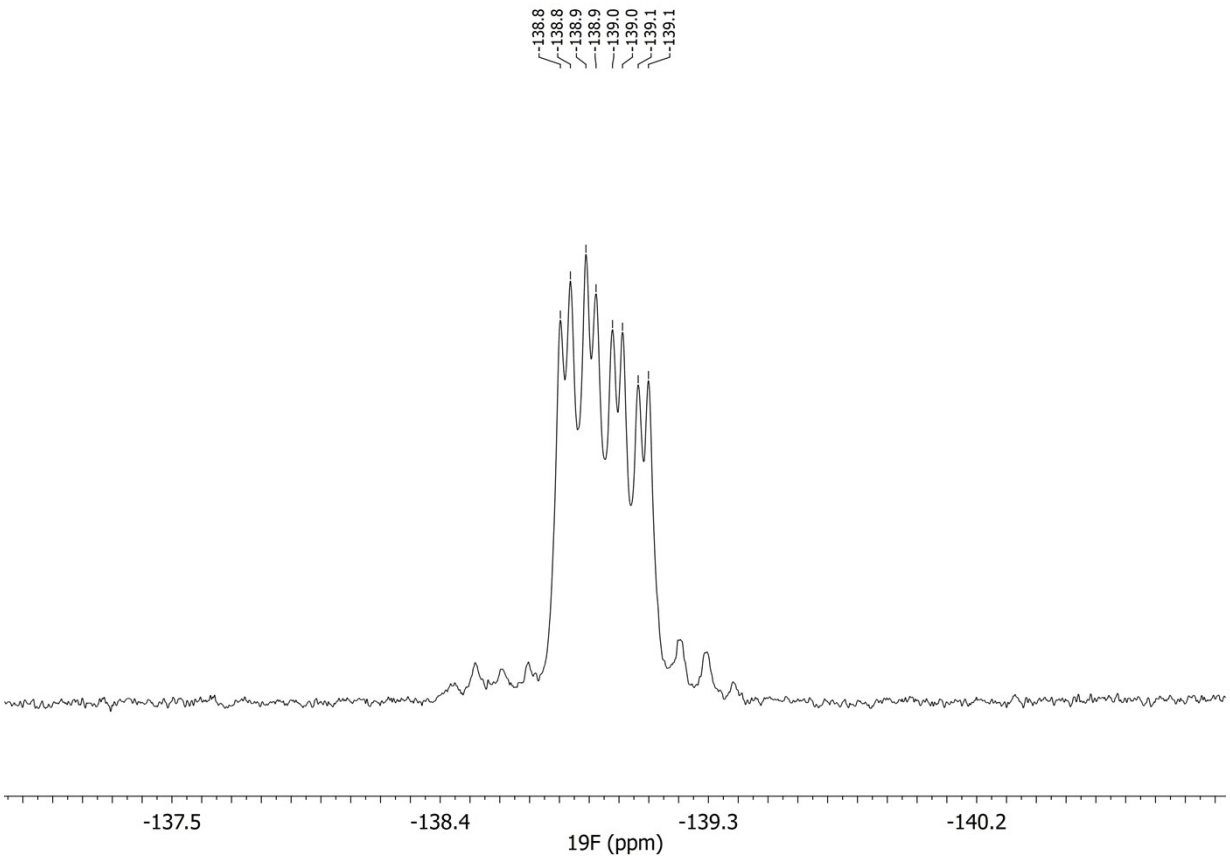

*Figure S33. ^{19}F-NMR (376 MHz, $CDCl_3$) of **2***

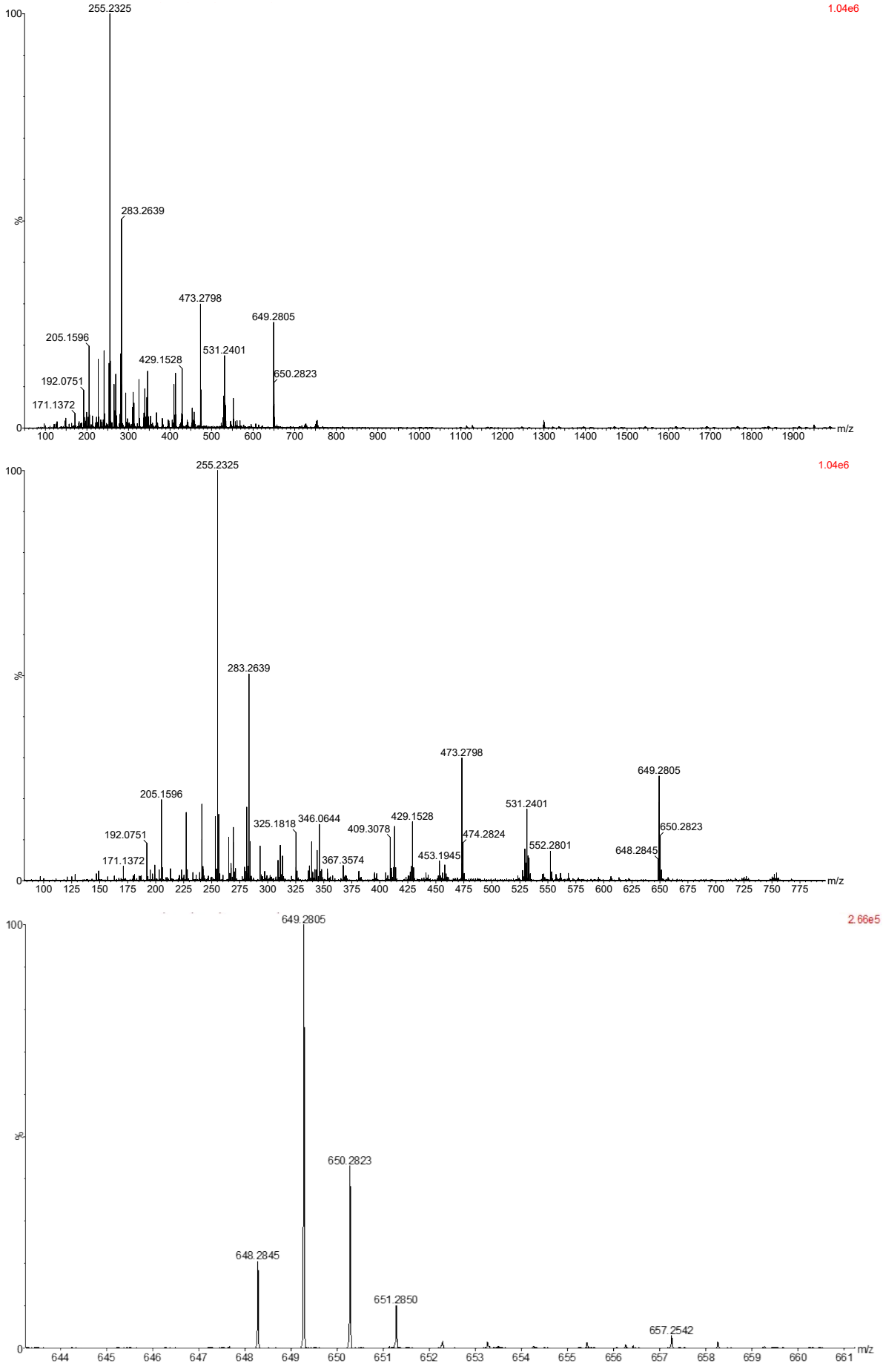

*Figure S34. TOF-Mass spectra of **2***

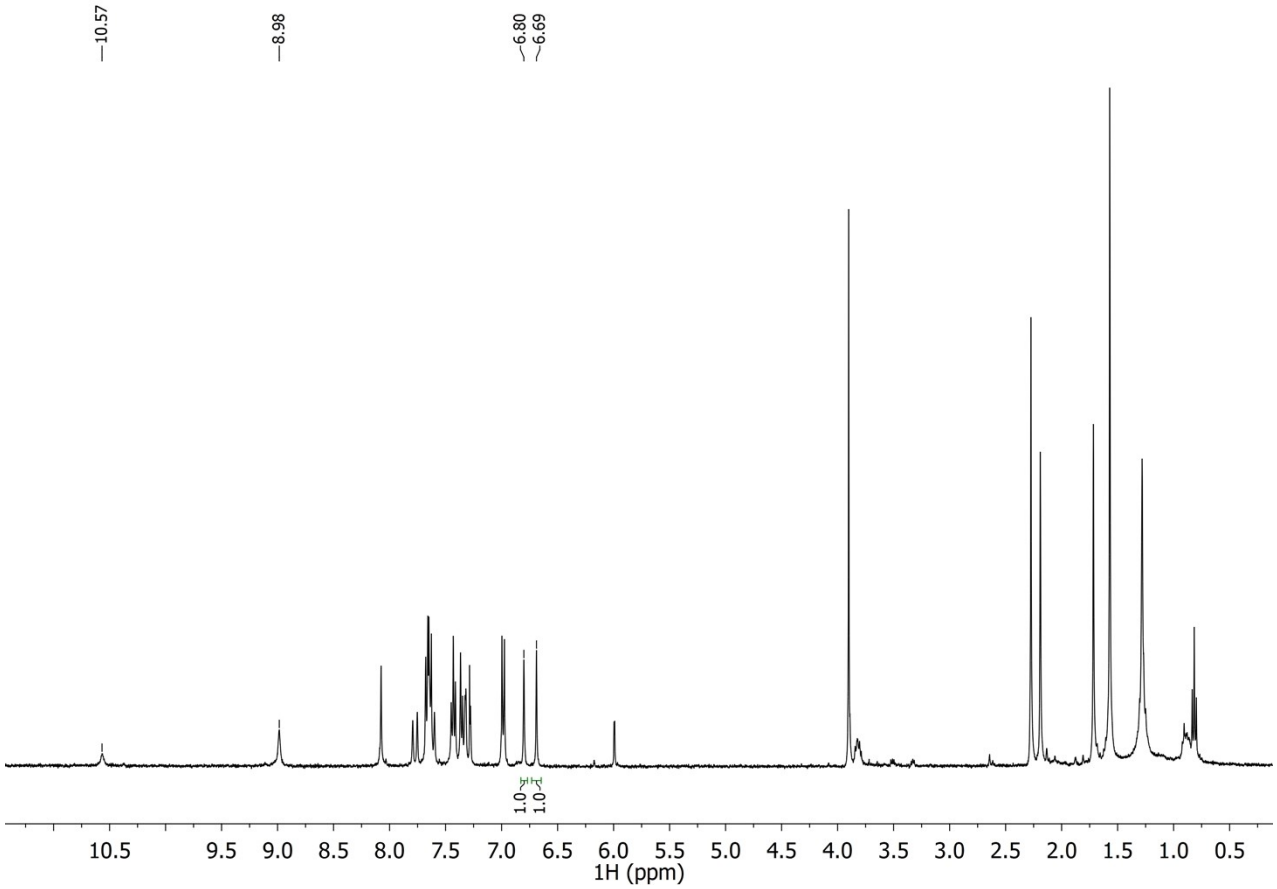

*Figure S35. ^{1}H-NMR (400 MHz, $CDCl_3$) of **3***

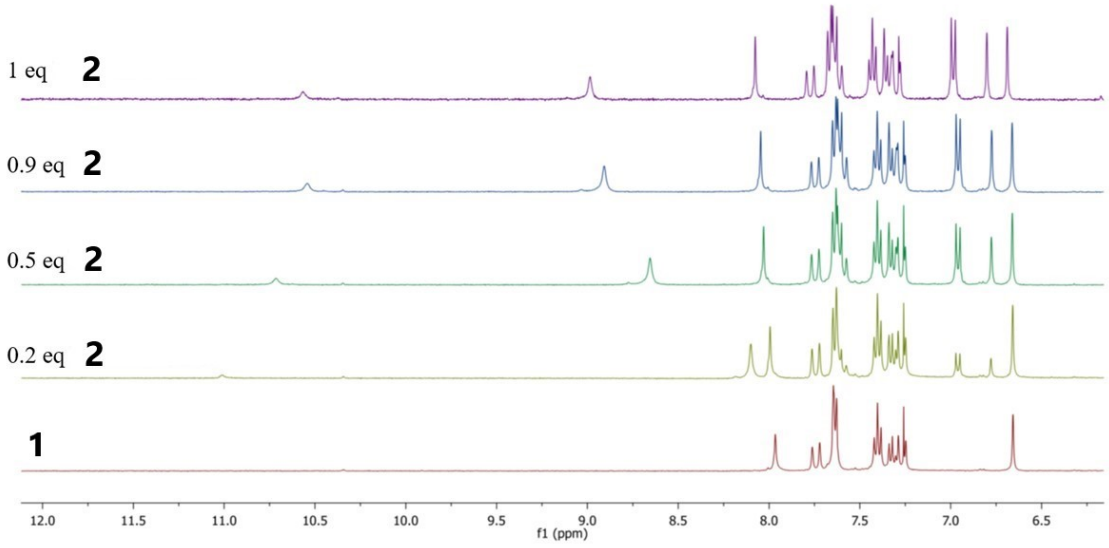

*Figure S36. Magnification of the superimposed ^{1}H-NMR spectra of the titration of **1** (2.0 mg, 5.4 mM) with **2** in $CDCl_3$*

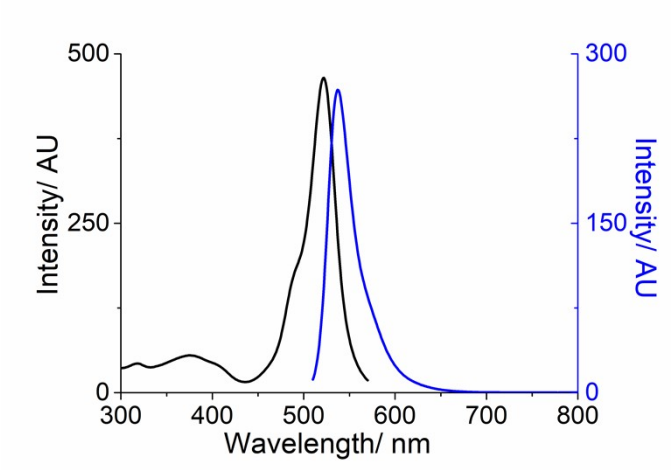

*Figure S37. Excitation and fluorescence spectra of **13** in $CHCl_3$ at λ_{em} 580 nm (dark line) and λ_{ex} 490 nm (blue line), respectively*

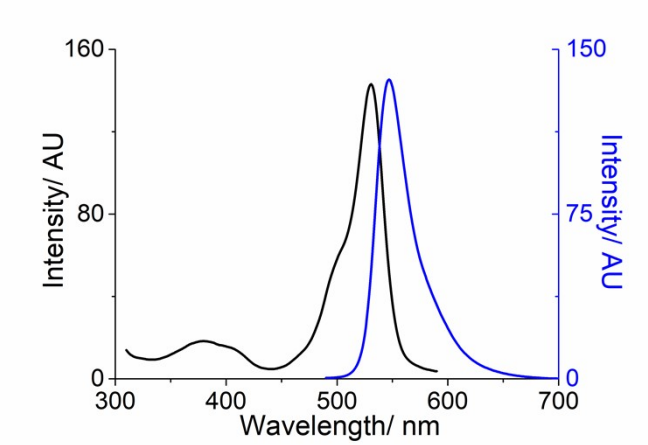

*Figure S38. Excitation and fluorescence spectra of **12** in $CHCl_3$ at λ_{em} 600 nm (dark line) and λ_{ex} 480 nm (blue line), respectively*

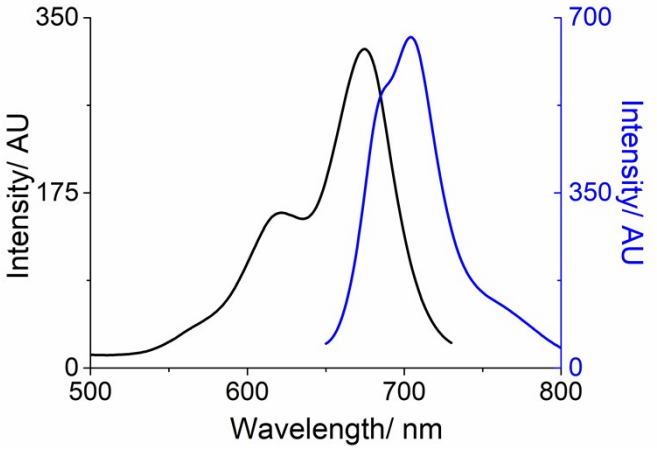

*Figure S39. Excitation and fluorescence spectra of **2** in $CHCl_3$ at λ_{em} 705 nm (dark line) and λ_{ex} 640 nm (blue line), respectively*

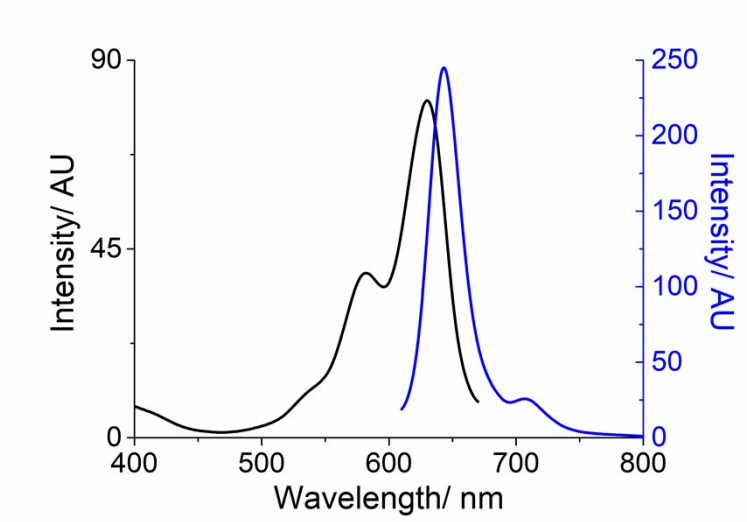

*Figure S40. Excitation and fluorescence spectra of **1** in $CHCl_3$ at λ_{em} 680 nm (dark line) and λ_{ex} 600 nm (blue line), respectively*

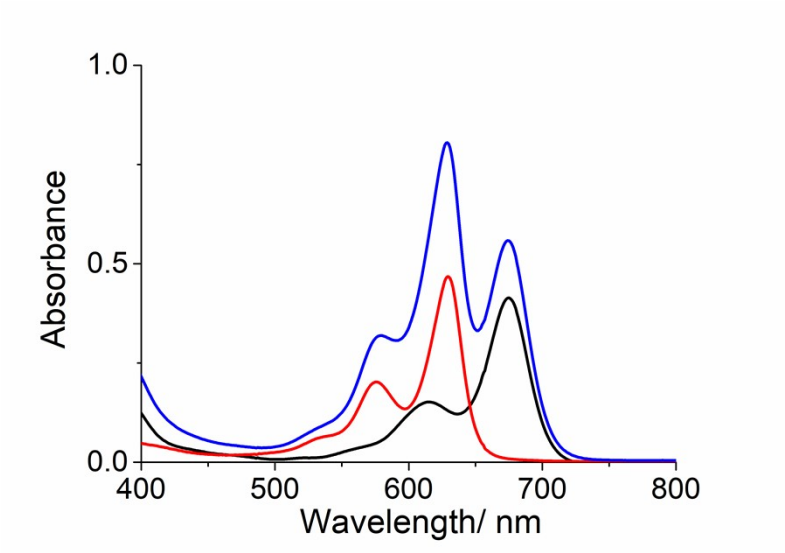

*Figure S41. UV/Vis spectra of **1** (red line), **2** (dark line) and **3** (blue line) in $CHCl_3$*

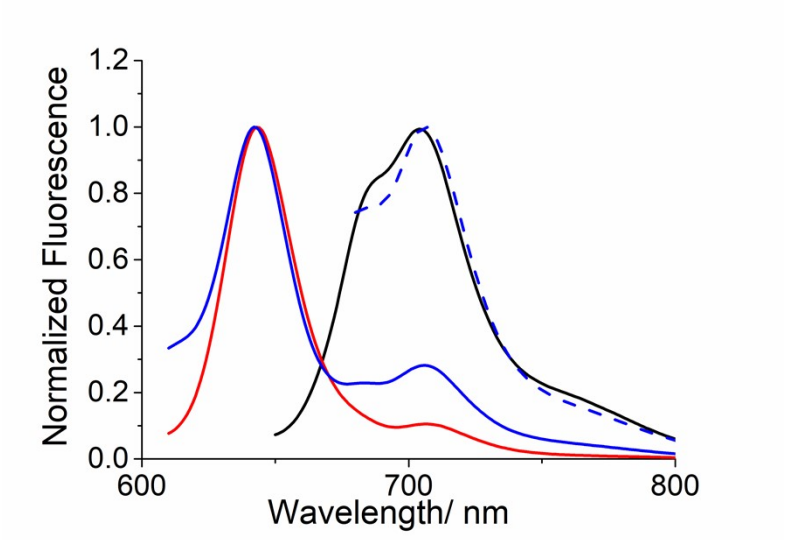

*Figure S42. Fluorescence emission spectra of **1** (red line, λ_{ex} 600 nm), **2** (dark line, λ_{ex} 640 nm) and **3** (blue solid and dotted lines at λ_{ex} 600 and 640 nm, respectively) in $CHCl_3$*

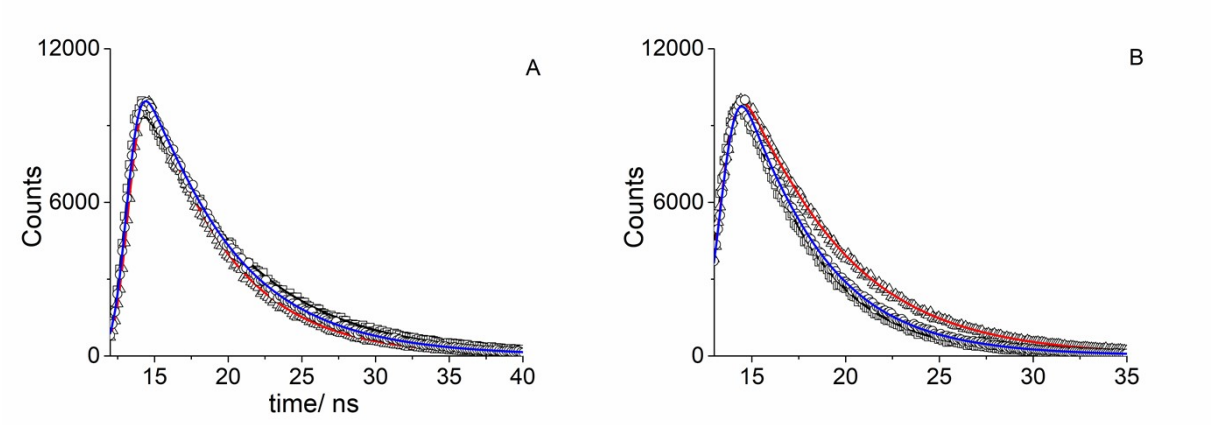

*Figure S43. Fluorescence lifetime decays of (a) **12** (red line, λ_{em} 548 nm), **13** (dark line, λ_{em} 538 nm), **14** (blue line, λ_{em} 550 nm) and (b) of **1** (red line, λ_{em} 644 nm), **2** (dark line, λ_{em} 705 nm) and **3** (blue line, λ_{em} 705 nm) in $CHCl_3$*

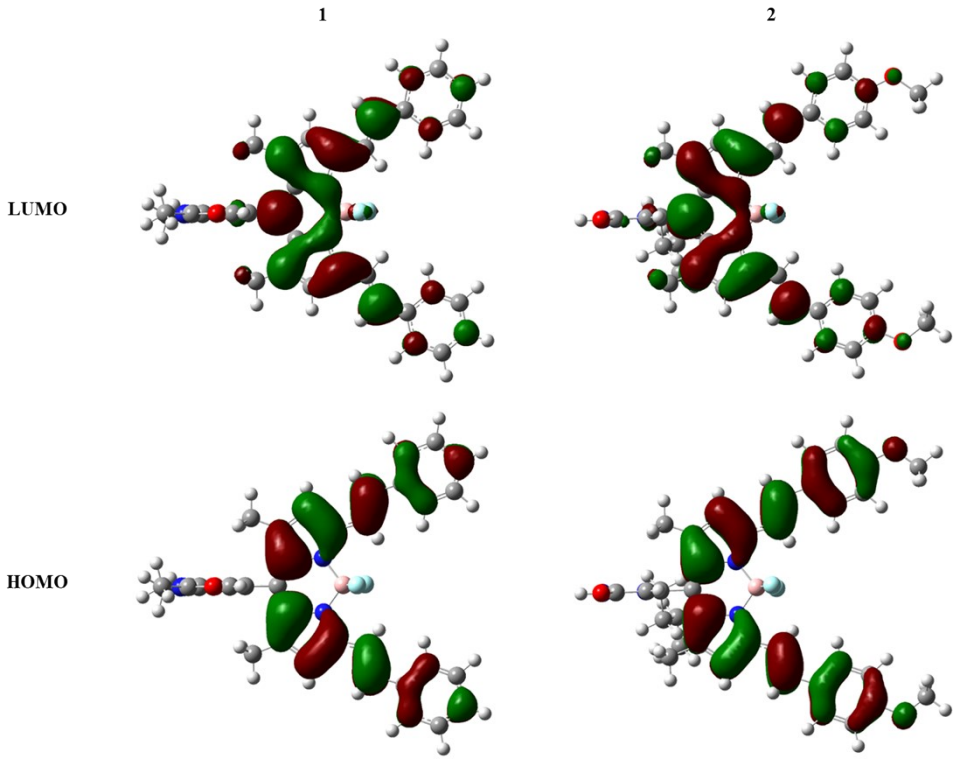

*Figure S44. Computed frontier orbitals related to **1** and **2***

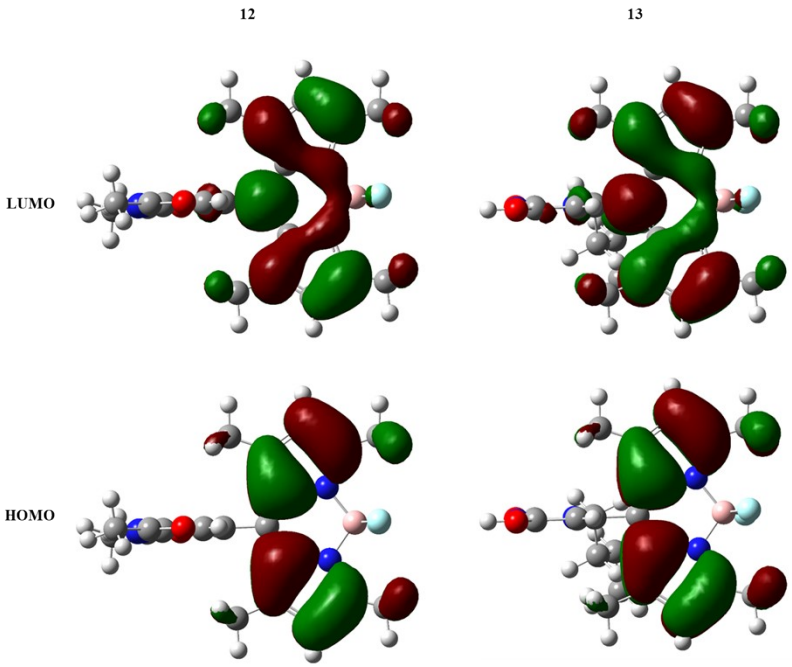

*Figure S45. Computed frontier orbitals related to **12** and **13***

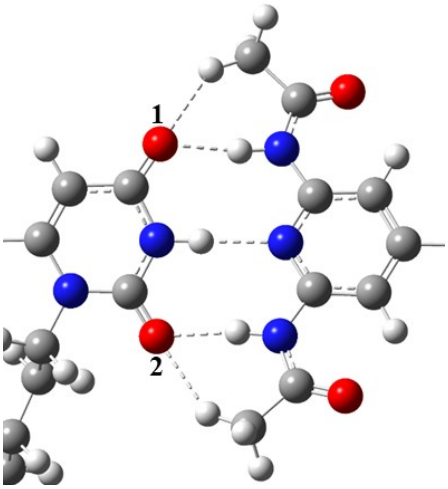

Figure S46. Zoom of interaction region related to DAAP-URA moieties

Chromophores	$\Delta E_{LUMO-HOMO}$ (eV)	$E_{binding}$ (kcal/mol)	C=O_1---H-N (Å)	N-H---N (Å)	C=O_2---H-N (Å)
12	5.17				
13	5.05				
1	4.28*				
2	4.03*				
14	4.68	-12.1	1.907	1.997	1.925
3	4	-12.3	1.908	1.999	1.924

Table S1. Electronic, structural and thermodynamic properties computed at DFT/CAM-B3LYP/6-311++G(d,p) level. To determinate the binding energy (E_b) between two non-covalently bonded chromophores the following formula was used: $E_b = E_{dimer} (E_{URA} + E_{DAAP})$ where E_{dimer} is the energy of the non-covalently bonded complex, E_{URA} and E_{DAAP} are the energies of two independently optimized fragments involved in the hydrogen interactions. (*) The introduction of distyryl arms leads to a thinning of the LUMO-HOMO energetic gap

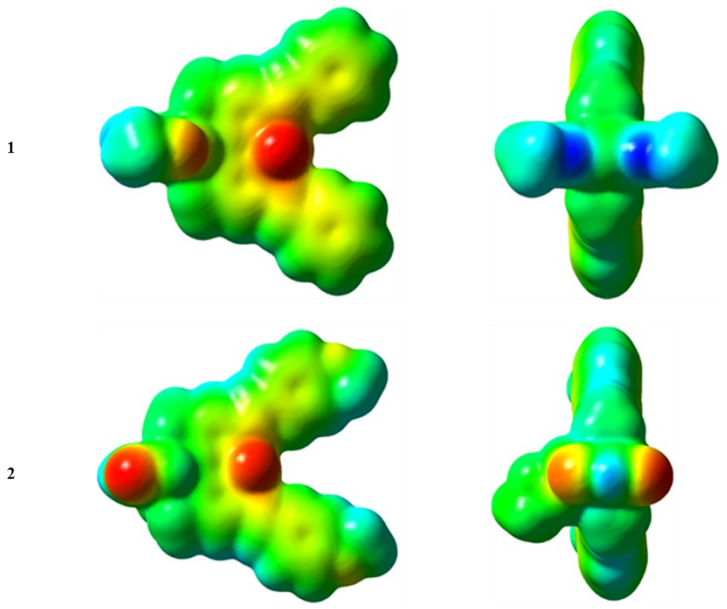

*Figure S47. Different perspective views of the electrostatic potential energy maps of **1** and **2**. the frontal view shows the complementarity of the two chromophores by means of a triple hydrogen bond*

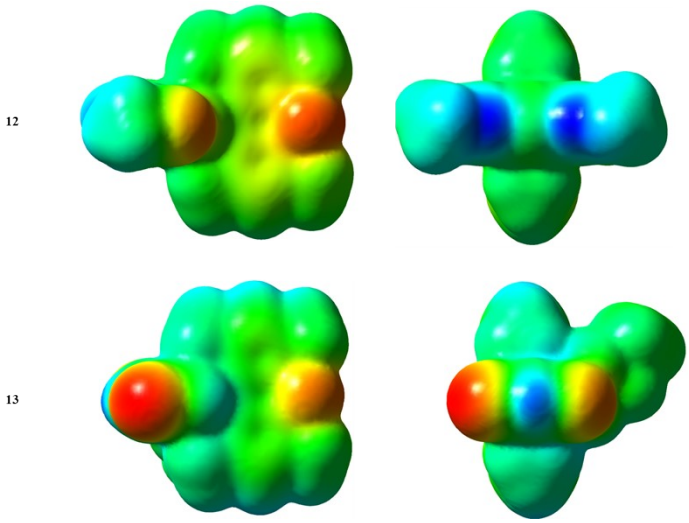

*Figure S48. Different perspective views of the electrostatic potential energy maps of **12** and **13**, the frontal view shows the complementarity of the two chromophores by means of a triple hydrogen bond*

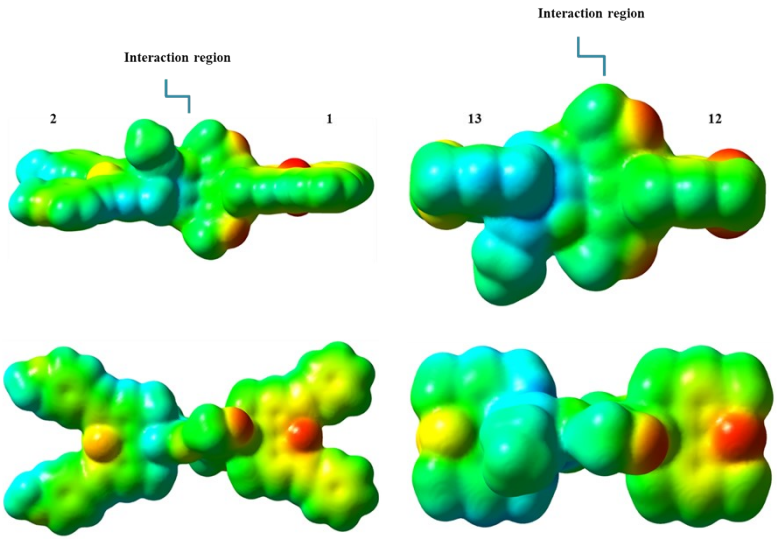

*Figure S49. Different perspective views of the electrostatic potential energy maps of **3** and **14***

Cartesian coordinates:

Tag	Symbol	X	Y	Z
1	C	2.9050530	-1.1459150	0.0063750
2	C	1.5143090	-1.2062450	0.0066300
3	C	0.8294700	0.0001260	0.0001720
4	C	1.5153720	1.2058740	-0.0063690
5	C	2.9060710	1.1442910	-0.0062580
6	N	3.5810090	-0.0011110	0.0000250
7	H	1.0048490	-2.1556780	0.0121970
8	H	1.0067710	2.1557680	-0.0119630
9	N	3.7374990	-2.2696480	0.0149440
10	N	3.7395190	2.2672720	-0.0150070
11	H	4.7197470	-2.0349790	0.0132730
12	C	-0.6611270	0.0005920	0.0001060
13	C	-1.3433690	-0.0006310	1.2162480
14	C	-1.3431500	0.0021470	-1.2161490
15	N	-2.7413020	-0.0011180	1.2400550
16	N	-2.7410710	0.0025050	-1.2402330
17	C	-0.8881890	-0.0005700	2.5664790
18	C	-0.8876870	0.0033940	-2.5662730
19	C	-2.0256010	-0.0012360	3.3552230
20	C	-2.0249360	0.0046490	-3.3552540
21	C	-3.1486010	0.0040870	-2.5159640
22	C	-3.1490950	-0.0015970	2.5157010
23	C	0.5080920	0.0002950	3.0997950
24	C	-4.5824240	-0.0016610	2.9145100
25	C	0.5087110	0.0034970	-3.0992840
26	C	-4.5818530	0.0050800	-2.9150390
27	H	1.0671090	0.8772140	2.7698730
28	H	0.4821760	0.0045080	4.1895620
29	H	1.0654440	-0.8802470	2.7767850
30	H	1.0688490	-0.8721680	-2.7680030
31	H	0.4830430	-0.0022050	-4.1890490
32	H	1.0647940	0.8852740	-2.7773800
33	B	-3.6535250	-0.0010570	-0.0001780
34	H	-2.0556920	0.0056690	-4.4343110
35	H	-2.0565800	-0.0015120	4.4342750
36	F	-4.4782240	1.1384240	0.0015030
37	F	-4.4735250	-1.1441990	-0.0020200
38	C	3.3996930	3.5962460	-0.0112910
39	C	3.3964480	-3.5983030	0.0112770
40	C	4.5713520	4.5440000	0.0271810
41	H	5.5067700	4.0862650	-0.2929780
42	H	4.3477130	5.4011560	-0.6054980
43	H	4.6913850	4.9045150	1.0511720
44	O	2.2487190	3.9904770	-0.0158430
45	C	4.5671510	-4.5472380	-0.0271080
46	H	4.6845950	-4.9106180	-1.0503750
47	H	5.5037120	-4.0896640	0.2899040
48	H	4.3439860	-5.4025330	0.6082830
49	O	2.2451130	-3.9914810	0.0161390
50	H	4.7215550	2.0317030	-0.0135450
51	H	-4.6685070	-0.0105600	3.9999140
52	H	-5.0917670	0.8815620	2.5249800
53	H	-5.0962290	-0.8752660	2.5097330
54	H	-4.6677130	0.0004680	-4.0004870
55	H	-5.0953240	-0.8704130	-2.5138990
56	H	-5.0917030	0.8864420	-2.5220190

12 *SCF ENERGY:* -1501.51788 a.u

Tag	Symbol	X	Y	Z
1	C	-3.2945720	-1.4404160	-1.8566900
2	C	-1.8749780	-1.2395450	-1.6832020
3	C	-1.3984970	-0.6360620	-0.5787830
4	C	-3.6004470	-0.3503030	0.3520440
5	N	-4.0527880	-0.9616620	-0.7946920
6	H	-1.2092690	-1.5815570	-2.4606740
7	C	0.0730120	-0.4395240	-0.4273070
8	C	0.6657150	0.6789530	-1.0053320
9	C	0.8178240	-1.3978910	0.2571790
10	N	2.0433380	0.8800470	-0.8808690
11	N	2.1976910	-1.2399690	0.4022510
12	C	0.1352500	1.7631520	-1.7690770
13	C	0.4483930	-2.6163980	0.8983970
14	C	1.2094560	2.5776100	-2.0712250
15	C	1.6183920	-3.1508760	1.4056060
16	C	2.6778710	-2.2859240	1.0876470
17	C	2.3694710	2.0124810	-1.5149460
18	C	-1.2683400	2.0172180	-2.2163240
19	C	3.7589340	2.5367120	-1.5862760
20	C	-0.9022860	-3.2419970	1.0300420
21	C	4.1173180	-2.4502290	1.4227480
22	H	-1.9866060	1.9630620	-1.3976220
23	H	-1.3362220	3.0129970	-2.6541200
24	H	-1.5801590	1.2951980	-2.9731080
25	H	-1.3510630	-3.4451880	0.0565880
26	H	-0.8184190	-4.1859610	1.5677500
27	H	-1.5946120	-2.6057340	1.5850650
28	B	3.0189810	-0.0485650	-0.1282740
29	H	1.7155460	-4.0758400	1.9533550
30	H	1.1779780	3.4937670	-2.6410300
31	F	3.6177510	0.6421440	0.9393280
32	F	4.0252280	-0.4990360	-0.9958130
33	N	-2.2233260	-0.1877940	0.4359020
34	O	-3.8318220	-1.9669790	-2.8142030
35	H	-5.0570640	-1.0768170	-0.8568360
36	O	-4.3579180	0.0166230	1.2267120
37	C	-1.7204540	0.4603210	1.6644170
38	H	-0.6980390	0.1249190	1.8220950
39	H	-2.3261500	0.0805480	2.4857540
40	C	-1.7902300	1.9813670	1.6246340
41	H	-1.1460840	2.3581920	0.8252050
42	H	-2.8138000	2.2885850	1.3939450
43	C	-1.3581050	2.5935320	2.9543720
44	H	-0.3431140	2.2601750	3.1953490
45	H	-2.0054540	2.2156770	3.7524790
46	C	-1.4036040	4.1175030	2.9379390
47	H	-0.7399860	4.5225300	2.1695160
48	H	-2.4142020	4.4780340	2.7291410
49	H	-1.0932710	4.5331920	3.8986350
50	H	4.4059390	1.8387130	-2.1209510
51	H	3.7718390	3.4960870	-2.1005850
52	H	4.1767180	2.6611150	-0.5859820
53	H	4.4966840	-1.5709840	1.9456840
54	H	4.2574050	-3.3277390	2.0517080
55	H	4.7124640	-2.5677310	0.5149760

13 *SCF ENERGY:* -1409.26190 a.u

Tag	Symbol	X	Y	Z
1	C	-5.0275560	-0.0233790	1.1459800
2	C	-3.6367040	-0.0243590	1.2056370
3	C	-2.9516590	0.0008200	-0.0005480
4	C	-3.6384400	0.0260800	-1.2056050
5	C	-5.0292520	0.0255260	-1.1438140
6	N	-5.7038680	0.0011630	0.0015490

7	H	-3.1270250	-0.0448590	2.1547600
8	H	-3.1302760	0.0461660	-2.1555590
9	N	-5.8596550	-0.0505490	2.2695730
10	N	-5.8629740	0.0530470	-2.2662100
11	H	-6.8420550	-0.0441540	2.0353820
12	C	-1.4608500	0.0005930	-0.0009530
13	C	-0.7775390	-1.2155450	-0.0095660
14	C	-0.7770450	1.2165170	0.0078160
15	N	0.6148300	-1.2425790	-0.0076900
16	N	0.6153410	1.2429240	0.0063100
17	C	-1.2383190	-2.5678040	-0.0224050
18	C	-1.2371970	2.5690010	0.0191030
19	C	-0.1118570	-3.3611040	-0.0273080
20	C	-0.1103590	3.3617990	0.0228370
21	C	1.0255610	2.5258720	0.0148800
22	C	1.0244530	-2.5256940	-0.0174720
23	C	-2.6377010	-3.0934630	-0.0302810
24	C	2.4237420	-2.8913400	-0.0173630
25	C	-2.6362860	3.0954650	0.0262770
26	C	2.4250130	2.8909030	0.0141200
27	H	-3.1960960	-2.7454010	-0.9003360
28	H	-2.6172940	-4.1831080	-0.0533160
29	H	-3.1911730	-2.7828740	0.8570050
30	H	-3.1954060	2.7474670	0.8958830
31	H	-2.6152460	4.1850930	0.0496040
32	H	-3.1894220	2.7854930	-0.8614340
33	B	1.5251180	-0.0000070	-0.0033360
34	H	3.1282940	-2.0708460	-0.0131120
35	H	3.1291870	2.0701050	0.0068330
36	C	2.8565880	4.1595960	0.0220000
37	C	2.8547750	-4.1602390	-0.0198930
38	H	2.1230820	4.9602700	0.0312180
39	H	-0.1000810	4.4403090	0.0316570
40	H	-0.1020610	-4.4396110	-0.0368130
41	H	2.1209540	-4.9606760	-0.0205650
42	C	4.2476570	-4.6098740	-0.0194800
43	C	4.2496300	4.6087380	0.0205990
44	C	5.3373960	-3.7307330	-0.0411150
45	C	4.5068430	-5.9837520	0.0032510
46	C	5.3390060	3.7293880	-0.0093930
47	C	4.5093570	5.9823890	0.0498130
48	C	5.8069190	-6.4680440	0.0063270
49	C	6.6346400	-4.2135990	-0.0382970
50	C	6.6364090	4.2118340	-0.0086530
51	C	5.8095910	6.4662660	0.0506970
52	C	6.8765010	-5.5839630	-0.0142810
53	H	5.1734980	-2.6606950	-0.0616760
54	H	3.6742690	-6.6784690	0.0193710
55	H	5.9838540	-7.5367590	0.0246530
56	H	7.4650080	-3.5178240	-0.0555540
57	C	6.8788030	5.5819810	0.0215590
58	H	3.6770800	6.6772720	0.0725320
59	H	5.9869350	7.5348180	0.0739500
60	H	5.1747090	2.6595140	-0.0347260
61	H	7.4664820	3.5158990	-0.0324090
62	F	2.3464690	0.0061360	-1.1454250
63	F	2.3536430	-0.0065070	1.1331840
64	C	-5.5236380	0.0697460	-3.5954720
65	C	-5.5182670	-0.0707440	3.5982700
66	C	-6.6970690	0.0468730	-4.5417430
67	H	-7.6233670	0.3945740	-4.0853660
68	H	-6.4602100	0.6636440	-5.4067030
69	H	-6.8429860	-0.9785150	-4.8887650
70	O	-4.3731010	0.0797900	-3.9901010
71	C	-6.6900670	-0.0462890	4.5464960

72	H	-6.8316250	0.9786180	4.8967350
73	H	-7.6183920	-0.3893180	4.0907340
74	H	-6.4539970	-0.6663800	5.4093000
75	O	-4.3671280	-0.0832170	3.9910650
76	H	7.8959230	5.9548760	0.0218110
77	H	7.8934980	-5.9571860	-0.0122870
78	H	-6.8450190	0.0485500	-2.0305120

1 *SCF ENERGY:* -2039.62210 a.u

Tag	Symbol	X	Y	Z
1	C	-6.2258080	-0.4719160	-2.0909120
2	C	-4.7917100	-0.3889490	-1.9450430
3	C	-4.2247180	-0.3840850	-0.7242700
4	C	-6.3558150	-0.5551720	0.3858900
5	N	-6.8999080	-0.5475390	-0.8778890
6	H	-4.1880420	-0.3265330	-2.8373760
7	C	-2.7411360	-0.2906320	-0.6004100
8	C	-2.1404850	0.9650890	-0.6153470
9	C	-1.9918500	-1.4623030	-0.5033240
10	N	-0.7570200	1.0790710	-0.4983180
11	N	-0.6057200	-1.4020030	-0.3948550
12	C	-2.6784910	2.2862570	-0.7348820
13	C	-2.3725590	-2.8391850	-0.4897750
14	C	-1.6063750	3.1456400	-0.6796760
15	C	-1.2063850	-3.5614400	-0.3760590
16	C	-0.1216420	-2.6583800	-0.3173490
17	C	-0.4242530	2.3842100	-0.5327040
18	C	-4.0971860	2.7226210	-0.9166310
19	C	0.9402070	2.8391940	-0.4241270
20	C	-3.7383600	-3.4403910	-0.5787520
21	C	1.2883920	-2.9384920	-0.1932900
22	H	-4.7661920	2.2948010	-0.1693750
23	H	-4.1567780	3.8078230	-0.8342090
24	H	-4.4784770	2.4380970	-1.8986980
25	H	-4.2421090	-3.1655420	-1.5064510
26	H	-3.6625310	-4.5268820	-0.5444570
27	H	-4.3782220	-3.1276300	0.2487720
28	B	0.2219740	-0.1031730	-0.3476310
29	H	1.6919440	2.0689790	-0.3196150
30	H	1.9443470	-2.0789040	-0.1749630
31	C	1.7889830	-4.1811200	-0.1065630
32	C	1.2886270	4.1357060	-0.4459320
33	H	1.1008720	-5.0212280	-0.1311750
34	H	-1.1343710	-4.6368980	-0.3404730
35	H	-1.6597060	4.2209410	-0.7429770
36	H	0.5063070	4.8816760	-0.5522710
37	C	2.6365870	4.6817430	-0.3387680
38	C	3.1937440	-4.5530650	0.0195320
39	C	3.7800100	3.8916110	-0.2007370
40	C	2.8106650	6.0726810	-0.3730380
41	C	4.2359140	-3.6251690	0.0777570
42	C	3.5322780	-5.9120580	0.0865610
43	C	4.0605530	6.6469710	-0.2735750
44	C	5.0427670	4.4526270	-0.0998930
45	C	5.5576400	-4.0237190	0.1964110
46	C	4.8427310	-6.3254320	0.2046670
47	C	5.1894310	5.8392620	-0.1355310
48	H	3.6952940	2.8124920	-0.1701970
49	H	1.9419070	6.7127200	-0.4798970
50	H	4.1879710	7.7218180	-0.3002260
51	H	5.9011300	3.8046160	0.0053120
52	C	5.8684750	-5.3818730	0.2604030
53	H	2.7448000	-6.6563470	0.0442930
54	H	5.0971090	-7.3766020	0.2554310

55	H	4.0233310	-2.5644140	0.0306900
56	H	6.3335620	-3.2726620	0.2379140
57	F	0.9117880	-0.0100190	0.8748060
58	F	1.1660800	-0.0871050	-1.3887380
59	N	-4.9711730	-0.4641530	0.4376670
60	O	-6.8405560	-0.4772190	-3.1424520
61	H	-7.9099620	-0.6104810	-0.9151270
62	O	-7.0453690	-0.6396900	1.3817620
63	C	-4.3702520	-0.4878310	1.7867390
64	H	-3.3552990	-0.8661680	1.6910180
65	H	-4.9419760	-1.2093560	2.3686140
66	C	-4.3768040	0.8668940	2.4825590
67	H	-3.7708270	1.5760000	1.9116050
68	H	-5.3989480	1.2539570	2.5076570
69	C	-3.8309330	0.7644460	3.9042270
70	H	-2.8170780	0.3513990	3.8750040
71	H	-4.4384570	0.0532070	4.4733770
72	C	-3.8128500	2.1097360	4.6215450
73	H	-3.1855500	2.8301560	4.0901740
74	H	-4.8190460	2.5312810	4.6910170
75	H	-3.4214160	2.0122300	5.6361210
76	O	6.3767420	6.4833500	-0.0441740
77	O	7.1253170	-5.8723110	0.3764120
78	C	7.5607320	5.7130320	0.1030380
79	C	8.2107370	-4.9584940	0.4340860
80	H	9.1078290	-5.5656530	0.5250180
81	H	8.2693950	-4.3579490	-0.4772040
82	H	8.1273710	-4.3012220	1.3033010
83	H	8.3776280	6.4282630	0.1559790
84	H	7.5348880	5.1223550	1.0222510
85	H	7.7111240	5.0529040	-0.7549020

2 *SCF ENERGY:* -2176.39502 a.u

Tag	Symbol	X	Y	Z
1	C	2.2964470	0.7641580	-0.5347780
2	C	3.6833660	0.8808310	-0.5690110
3	C	4.4276500	-0.1151900	0.0401220
4	C	3.7998870	-1.1829740	0.6579290
5	C	2.4076150	-1.2124930	0.6435860
6	N	1.6707130	-0.2590550	0.0600290
7	H	4.1454950	1.7238840	-1.0538780
8	H	4.3546210	-1.9728910	1.1351440
9	N	1.4467370	1.6949070	-1.1386910
10	N	1.6703090	-2.2277670	1.2577240
11	H	0.4647830	1.4300530	-1.2040840
12	H	0.6694770	-2.0584280	1.3655860
13	C	5.9157920	-0.0364830	0.0305560
14	C	6.5685670	0.6586520	1.0480300
15	C	6.6252740	-0.6598450	-0.9952260
16	N	7.9637780	0.7482550	1.0574020
17	N	8.0218910	-0.6008970	-1.0228880
18	C	6.0826910	1.3603470	2.1888220
19	C	6.2019050	-1.4134220	-2.1279410
20	C	7.2000360	1.8487130	2.8438980
21	C	7.3561730	-1.7828990	-2.7965770
22	C	8.4587540	-1.2717010	-2.0965670
23	C	8.3412720	1.4589520	2.1280070
24	C	4.6761290	1.5700270	2.6489210
25	C	9.7631900	1.7531850	2.4524890
26	C	4.8196550	-1.7739470	-2.5677110
27	C	9.8997140	-1.4189230	-2.4365070
28	H	4.1560820	0.6246890	2.8099170
29	H	4.6785740	2.1213640	3.5893370
30	H	4.0951930	2.1407290	1.9226310
31	H	4.1990270	-0.8903250	-2.7230530

32	H	4.8679370	-2.3251910	-3.5069240
33	H	4.3135620	-2.4011080	-1.8320490
34	B	8.9034640	0.1262680	0.0085390
35	H	7.4121410	-2.3654330	-3.7037100
36	H	7.2057050	2.4313200	3.7526450
37	F	9.7862440	-0.7811960	0.6214700
38	F	9.6631860	1.1297210	-0.6208780
39	C	-1.9200150	-1.2875740	1.0323530
40	C	-3.3588820	-1.2934800	1.0382050
41	C	-4.0429190	-0.4700770	0.2210250
42	C	-2.0273700	0.4467030	-0.6994990
43	N	-1.3558720	-0.3945240	0.1440850
44	H	-3.8716770	-1.9659500	1.7085190
45	C	-5.5346090	-0.4831720	0.2377160
46	C	-6.2019440	0.2845470	1.1871910
47	C	-6.2149480	-1.2869490	-0.6748900
48	N	-7.5993410	0.2892930	1.2193980
49	N	-7.6109510	-1.3166730	-0.6747070
50	C	-5.7404640	1.1419080	2.2335030
51	C	-5.7603400	-2.1684480	-1.6997490
52	C	-6.8738210	1.6329350	2.8509260
53	C	-6.8976070	-2.6985350	-2.2794570
54	C	-8.0211280	-2.1586260	-1.6320680
55	C	-8.0023730	1.0940120	2.2092990
56	C	-4.3439990	1.4670260	2.6570790
57	C	-9.4326830	1.3365990	2.5338620
58	C	-4.3622680	-2.4993730	-2.1115100
59	C	-9.4538940	-2.4419720	-1.9108340
60	H	-3.7265520	1.8232650	1.8316170
61	H	-4.3678500	2.2499030	3.4148600
62	H	-3.8454200	0.5973790	3.0885200
63	H	-3.7902390	-2.9329990	-1.2899260
64	H	-4.3824470	-3.2224090	-2.9263210
65	H	-3.8193880	-1.6201340	-2.4642720
66	B	-8.5200440	-0.4935540	0.2594980
67	H	-6.9306930	-3.4093010	-3.0910700
68	H	-6.9024430	2.3127830	3.6887700
69	F	-9.3045890	0.3986840	-0.4908240
70	F	-9.3670320	-1.3420900	0.9857420
71	N	-3.4079420	0.3973110	-0.6477840
72	O	-1.2015660	-1.9929190	1.7321420
73	H	-0.3242380	-0.3483330	0.1025890
74	O	-1.4303470	1.1982110	-1.4564290
75	C	-4.1323300	1.3017820	-1.5670060
76	H	-5.1082650	0.8627390	-1.7597780
77	H	-3.5759750	1.3022860	-2.5029260
78	C	-4.2726960	2.7225670	-1.0370330
79	H	-4.8594310	2.7139500	-0.1142640
80	H	-3.2825510	3.1164090	-0.7922530
81	C	-4.9493260	3.6320740	-2.0592370
82	H	-5.9289850	3.2185930	-2.3207850
83	H	-4.3603470	3.6391180	-2.9822210
84	C	-5.1181340	5.0588630	-1.5489310
85	H	-5.7316810	5.0828900	-0.6446580
86	H	-4.1509810	5.5074180	-1.3074200
87	H	-5.6014750	5.6912790	-2.2960760
88	C	2.1344600	-3.4296220	1.7339320
89	C	1.7782250	2.9198420	-1.6645110
90	C	1.0833550	-4.3128030	2.3568370
91	H	0.0899420	-3.8704390	2.3583080
92	H	1.0638380	-5.2571320	1.8107290
93	H	1.3874420	-4.5337520	3.3809420
94	O	3.2990900	-3.7813830	1.6653030
95	C	0.6304130	3.6704320	-2.2908660
96	H	-0.3380860	3.2096190	-2.1105230

97	H	0.6371870	4.6906170	-1.9072340
98	H	0.8063330	3.7228860	-3.3671790
99	O	2.9048350	3.3829760	-1.6461380
100	H	-9.5477470	-3.0427390	-2.8138700
101	H	-9.9057500	-2.9859790	-1.0786460
102	H	-10.0168400	-1.5161130	-2.0356000
103	H	-9.5171080	2.0928510	3.3122760
104	H	-9.9795600	1.6689970	1.6502860
105	H	-9.9085160	0.4171070	2.8805060
106	H	10.4282680	-1.9601490	-1.6494930
107	H	10.0091130	-1.9627710	-3.3734360
108	H	10.3771720	-0.4425890	-2.5328130
109	H	10.2418760	2.2962200	1.6357810
110	H	9.8233990	2.3520320	3.3598760
111	H	10.3254430	0.8292160	2.5985890

14 *SCF ENERGY:* -2910.79907 a.u

Tag	Symbol	X	Y	Z
1	C	3.0345700	0.3077350	0.9407210
2	C	4.4249680	0.3040750	1.0135320
3	C	5.1299530	0.0761610	-0.1562300
4	C	4.4603920	-0.1362760	-1.3490390
5	C	3.0680030	-0.1095000	-1.3249260
6	N	2.3693040	0.1062060	-0.2033540
7	H	4.9198860	0.4761570	1.9542250
8	H	4.9835610	-0.3195370	-2.2721390
9	N	2.2218150	0.4988110	2.0615100
10	N	2.2915660	-0.2816440	-2.4734020
11	H	1.2287430	0.3074690	1.9340420
12	H	1.2987330	-0.0602510	-2.3859090
13	C	6.6201100	0.0593080	-0.1308520
14	C	7.2862880	-1.1466430	0.0878110
15	C	7.3206710	1.2494990	-0.3263190
16	N	8.6780260	-1.1888410	0.1174360
17	N	8.7132190	1.2597280	-0.3086050
18	C	6.8062820	-2.4733440	0.3108950
19	C	6.8790690	2.5867630	-0.5657050
20	C	7.9212400	-3.2676270	0.4674580
21	C	8.0166300	3.3551470	-0.6840520
22	C	9.1408000	2.5190730	-0.5224690
23	C	9.0691440	-2.4576650	0.3450360
24	C	5.3998000	-2.9759020	0.3730550
25	C	10.4628190	-2.8338990	0.4344830
26	C	5.4872540	3.1206640	-0.6770730
27	C	10.5450020	2.8628360	-0.5644390
28	H	4.8702760	-2.8100200	-0.5662110
29	H	5.4046010	-4.0470370	0.5755090
30	H	4.8277530	-2.4834910	1.1605970
31	H	4.9212030	2.9664350	0.2426840
32	H	5.5229220	4.1914260	-0.8783250
33	H	4.9326210	2.6411470	-1.4847690
34	B	9.6052760	0.0252330	-0.0790200
35	H	11.1790130	-2.0341560	0.3037700
36	H	11.2376200	2.0448730	-0.4203640
37	C	10.9943100	4.1090750	-0.7664690
38	C	10.8756270	-4.0878960	0.6645440
39	H	10.2723430	4.9087660	-0.9027700
40	H	8.0416430	4.4173180	-0.8697630
41	H	7.9152130	-4.3303400	0.6515110
42	H	10.1307670	-4.8681340	0.7899230
43	C	12.2618460	-4.5459840	0.7696890
44	C	12.3936840	4.5344360	-0.8243890
45	C	13.3636870	-3.6897960	0.6524810
46	C	12.5016540	-5.9043280	0.9990500
47	C	13.4706290	3.6475210	-0.7042100

48	C	12.6728390	5.8919510	-1.0099060
49	C	13.7944760	-6.3958750	1.1072930
50	C	14.6537110	-4.1798610	0.7605430
51	C	14.7747480	4.1073950	-0.7660790
52	C	13.9797880	6.3532620	-1.0715710
53	C	14.8762340	-5.5347040	0.9882750
54	H	13.2148970	-2.6318820	0.4764800
55	H	11.6596700	-6.5813070	1.0927000
56	H	13.9562000	-7.4523460	1.2848190
57	H	15.4936220	-3.5017980	0.6672720
58	C	15.0365000	5.4619240	-0.9496580
59	H	11.8505290	6.5923830	-1.1058310
60	H	14.1720960	7.4097450	-1.2153250
61	H	13.2913110	2.5890610	-0.5633740
62	H	15.5949270	3.4057440	-0.6716170
63	F	10.4489800	-0.1792580	-1.1862300
64	F	10.4126130	0.2112350	1.0580680
65	C	-1.2640960	0.2141290	-1.5068330
66	C	-2.7020680	0.2183810	-1.4715700
67	C	-3.3530340	0.1302230	-0.2953700
68	C	-1.2982490	0.0500000	0.9404060
69	N	-0.6623500	0.1249810	-0.2679610
70	H	-3.2428700	0.2850480	-2.4029710
71	C	-4.8439960	0.1233920	-0.2726340
72	C	-5.5150880	-1.0827200	-0.4521140
73	C	-5.5259260	1.3279420	-0.1066490
74	N	-6.9076440	-1.1144770	-0.4393670
75	N	-6.9172290	1.3502080	-0.0990010
76	C	-5.0501620	-2.4202190	-0.6655380
77	C	-5.0655760	2.6687670	0.0723680
78	C	-6.1727390	-3.2071030	-0.7666190
79	C	-6.1912600	3.4529290	0.1786900
80	C	-7.3297990	2.6228690	0.0707980
81	C	-7.3149970	-2.3851440	-0.6253070
82	C	-3.6508560	-2.9318910	-0.7944630
83	C	-8.7079150	-2.7562360	-0.6578300
84	C	-3.6633680	3.1828660	0.1401460
85	C	-8.7252460	2.9844330	0.1224110
86	H	-3.0169640	-2.6351070	0.0418740
87	H	-3.6645080	-4.0211570	-0.8294320
88	H	-3.1778800	-2.5725280	-1.7097650
89	H	-3.1043180	2.9589860	-0.7693890
90	H	-3.6766090	4.2646840	0.2699220
91	H	-3.1116690	2.7572340	0.9808550
92	B	-7.8232820	0.1121350	-0.2463190
93	H	-9.4189320	-1.9524060	-0.5251300
94	H	-9.4318680	2.1730330	0.0135090
95	C	-9.1529740	4.2460230	0.2904470
96	C	-9.1278300	-4.0188780	-0.8393140
97	H	-8.4131810	5.0348330	0.3917010
98	H	-6.2013950	4.5222660	0.3185870
99	H	-6.1797860	-4.2729910	-0.9309080
100	H	-8.3831710	-4.7991210	-0.9672940
101	C	-10.5080150	-4.4857190	-0.8859920
102	C	-10.5365430	4.7021550	0.3533620
103	C	-11.6131740	-3.6406970	-0.7611580
104	C	-10.7554540	-5.8542590	-1.0657690
105	C	-11.6366000	3.8465310	0.2608260
106	C	-10.7925310	6.0713070	0.5150250
107	C	-12.0390700	-6.3553760	-1.1169420
108	C	-12.9090490	-4.1279680	-0.8106450
109	C	-12.9356200	4.3241600	0.3241680
110	C	-12.0793250	6.5628940	0.5798160
111	C	-13.1288690	-5.4938610	-0.9894720
112	H	-11.4712970	-2.5760700	-0.6233710

113	H	-9.9175630	-6.5351230	-1.1665850
114	H	-12.2235860	-7.4131400	-1.2557520
115	H	-13.7361490	-3.4396680	-0.7104250
116	C	-13.1638890	5.6908610	0.4844390
117	H	-9.9588070	6.7605790	0.5901680
118	H	-12.2701420	7.6213380	0.7042300
119	H	-11.4883140	2.7809880	0.1374470
120	H	-13.7584830	3.6276520	0.2486470
121	F	-8.6165960	-0.0501820	0.9033160
122	F	-8.6750760	0.2602330	-1.3539540
123	N	-2.6798680	0.0459640	0.9096700
124	O	-0.5748410	0.2763720	-2.5194870
125	H	0.3704200	0.1203020	-0.2374270
126	O	-0.6691470	-0.0055280	1.9874280
127	C	-3.3654620	-0.0190300	2.2183870
128	H	-4.3498700	0.4257850	2.0958420
129	H	-2.7957230	0.6120660	2.8986800
130	C	-3.4764540	-1.4306110	2.7788420
131	H	-4.0892810	-2.0431350	2.1116560
132	H	-2.4819580	-1.8829920	2.8191020
133	C	-4.0957850	-1.4259140	4.1740060
134	H	-5.0796690	-0.9469030	4.1332350
135	H	-3.4802570	-0.8121610	4.8398710
136	C	-4.2351800	-2.8285030	4.7552430
137	H	-4.8736620	-3.4533200	4.1254560
138	H	-3.2618200	-3.3196470	4.8345120
139	H	-4.6769330	-2.8007830	5.7532210
140	O	-14.3531300	-6.0674890	-1.0516840
141	O	-14.3919490	6.2557590	0.5576450
142	C	-15.5011800	-5.2398750	-0.9321290
143	C	-15.5347010	5.4174860	0.4663860
144	H	-16.3955240	6.0760420	0.5496990
145	H	-15.5667220	4.8977290	-0.4944900
146	H	-15.5549150	4.6885110	1.2804200
147	H	-16.3577830	-5.9042070	-1.0128310
148	H	-15.5236050	-4.7343480	0.0365410
149	H	-15.5385920	-4.4995620	-1.7351990
150	C	2.7077810	-0.7110220	-3.7100980
151	C	2.6026580	0.9071490	3.3163260
152	C	1.6273030	-0.7610610	-4.7603440
153	H	0.6399460	-0.5114220	-4.3791680
154	H	1.8951280	-0.0638650	-5.5561900
155	H	1.6162260	-1.7621760	-5.1927140
156	O	3.8554910	-1.0313510	-3.9651650
157	C	1.4829770	0.9881420	4.3229170
158	H	0.5038100	0.7754920	3.9003550
159	H	1.6936610	0.2770220	5.1235650
160	H	1.4888560	1.9863660	4.7619120
161	O	3.7490480	1.1867400	3.6194640
162	H	16.0588200	5.8170920	-0.9977170
163	H	15.8876650	-5.9135780	1.0722380

3 *SCF ENERGY:* -4216.03679 a.u