Supporting Information.

Tweezer-Type Ratiometric Chemosensor for Ureas and Uronium Salts

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Content

Theoretical calculations.

Calculated geometries were optimized by the Gaussian 03 package at the DFT level of theory by using the B3LYP functional and the 3-21g(**) basis set.

1,10-Phenanthroline-*N*-oxide (1). To a solution of 1,10-phenanthroline monohydrate (4.87 g, 24.57 mmol) in acetic acid (30 mL) was added 30% H_2O_2 (3.2 mL). The temperature was carefully maintained at 70 ^oC for 3 h, after which an additional portion of H_2O_2 (3.2 mL) was added and the heating was continued for an additional 3 h. After cooling to rt, a third portion of H_2O_2 (2 mL) was added and the reaction mixture was stirred for 10 h. Then, the solution was concentrated under vacuum to a total volume of approximately 10 mL, which was followed by addition of water (35 mL) and re-concentration back to a volume of 10 ml. To the resulting dark-brown oil a solid K_2CO_3 (50.0 g) was added and the mixture was extracted (Soxhlet apparatus) by $CHCl_3$ (500 mL) for 3 h. To the $CHCl_3$ solution a charcoal and $MgSO_4$ were added. Subsequently, solids were filtered of and the solvent was removed to afford **1** as a greenish powder (3.43 g, 71%). M.p 170-175 ^oC (lit. 180-181 ^oC). ^1H NMR (400 MHz, $CDCl_3$) δ: 9.31 (dd, J = 1.8, 4.3 Hz, 1H), 8.73 (dd, J = 1.2, 6.3 Hz, 1H), 8.23 (dd, J = 1.8, 8.0Hz, 1H), 7.80 (d, J = 8.8 Hz, 1H), 7.74 (d, J = 8.9 Hz, 1H), 7.74 (d, J = 8.0, 1.0 Hz, 1H), 7.66 (dd, J = 4.4, 8.1 Hz, 1H,), 7.45 (dd, J = 6.3, 8.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.0, 142.7, 140.8, 138.5, 135.8, 133.3, 129.02, 128.89, 126.5, 124.26, 123.12, 122.8. IR (KBr): 3410, 1627, 1600, 1432, 1413, 1256, 1204, 1069 cm^{-1}. MS (CI+): m/z 197.1 (MH^+). λ_{max} (MeOH): 241, 268, 325 nm.

2-Chloro-1,10-phenanthroline (2). To a mixture of **1** (495 mg, 2.52 mmol) and NaCl (3.0 g, 51.0 mmol) in DMF (9.0 mL), a neat $POCl_3$ (0.7 ml, 7.53 mmol) was added by syringe at 0 ºC. Then, the reaction mixture was heated to 100 ºC for 6 h. After cooling to rt, water (20 mL) was added and the mixture was basified with aqueous ammonia and saturated with NaCl. Solids were filtered and solution was extracted with $CHCl_3$ (3 × 15 mL). The combined extracts were washed with brine (3 × 15 mL), dried over $MgSO_4$ and evaporated. The crude residue was purified by column chromatography (SiO_2; 3:2, EtOAc/hexanes; R_f = 0.3) to afford **2** as a yellow solid (279 mg, 52%). M.p. 129-130 ºC (lit. 129-130 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.22 (dd, *J* = 1.4, 4.1 Hz, 1H), 8.25 (dd, *J* = 1.7, 8.1 Hz, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.77 (d, *J* = 8.8 Hz, 1H), 7.65 (dd, *J* = 4.3, 8.1 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (125 MHz, CDCl3) δ: 151.5, 150.8, 146.1, 145.1, 138.6, 136.0, 129.0, 127.25, 126.91, 125.69, 124.3, 123.4. IR (KBr): 3464, 3049, 2358, 1580, 1491, 1402, 1124, 1072, 841, 728, 615 cm^{-1}. MS (EI+): m/z 214.1 (M^+). λ_{max}(MeOH): 227, 268 nm.

2-Amino-1,10-phenanthroline (3). A mixture of **2** (1.75 g, 8.15 mmol), acetamide (9.63 g, 163.0 mmol) and K_2CO_3 (7.9 g, 57.0 mmol) was heated to 200 ºC and stirred for 1.5 h. After cooling to rt, water (50 mL) was added and resulting mixture was extracted with CH_2Cl_2 (4 × 80 mL). The combined organic extracts were washed with brine (3 × 40 ml), dried over $MgSO_4$ and evaporated. The crude residue was purified by flash chromatography (SiO_2; 3:7:90, NH_4OH (25%)/MeOH/EtOAc; R_f = 0.3) to afford **3** as a yellow powder (886 mg, 56% yield). M.p. 200-203 ºC (lit. 204-206 ºC). ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.09 (dd, *J* = 1.7, 4.3 Hz, 1H), 8.15 (dd, *J* = 1.7, 8.1 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.51 (dd, *J* = 4.3, 8.1 Hz, 1H), 7.51 (d, *J* = 8.6 Hz, 1H), 6.90 (d, *J* = 8.6 Hz, 1H), 5.23 (br s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 157.8, 149.5, 145.85, 145.22, 138.0, 135.8, 129.3, 126.4, 122.88, 122.34, 121.89, 111.8. IR (KBr): 3482, 3199, 2923, 1658, 1464, 1394, 844 cm^{-1}. MS (EI+): m/z 195.1 (M^+), λ_{max}($CHCl_3$): 241, 286 nm.

2,5,8,11-Tetraoxatridecan-13-yl 4-methylbenzenesulfonate. To a solution of tetraethylene-glycol monomethyl ether (10.0 g, 48.02 mmol) and pyridine (84 mL) in CH_2Cl_2 (170 mL) solid *p*-toluenesulfonyl chloride (22.0 g, 115.39 mmol) was added portion-wise at -20 ºC under inert atmosphere and the resulting reaction mixture was stirred for 10 h. Then, the reaction mixture was allowed to warm up to rt and water (200 mL) was added. with and the aqueous layer was extracted with CH_2Cl_2 (3 × 150 mL). The combined organic layers were dried over $MgSO_4$ and evaporated. The crude product was purified by flash chromatography (SiO_2; step gradient from 1:1, EtOAc/hexanes to EtOAc; R_f = 0.3 in EtOAc) to afford 2,5,8,11-tetraoxatridecan-13-yl-4-methylbenzenesulfonate as a colorless oil (15.3 g, 88 %). ^{1}HNMR (200 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.4Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 4.16 (m, 2H), 3.59 (m, 14H), 3.36 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 144.7, 132.9, 129.7, 127.9, 71.8, 70.61, 70.48, 70.44, 70.40, 69.17, 68.58, 58.9, 21.5. IR (CH_2Cl_2): 2887, 1726, 1599, 1545, 1359, 1276, 1246, 1179, 1100, 1018, 924 cm^{-1}. MS (CI+): m/z 363.2 (MH^+), λ_{max}($CHCl_3$): 225 nm.

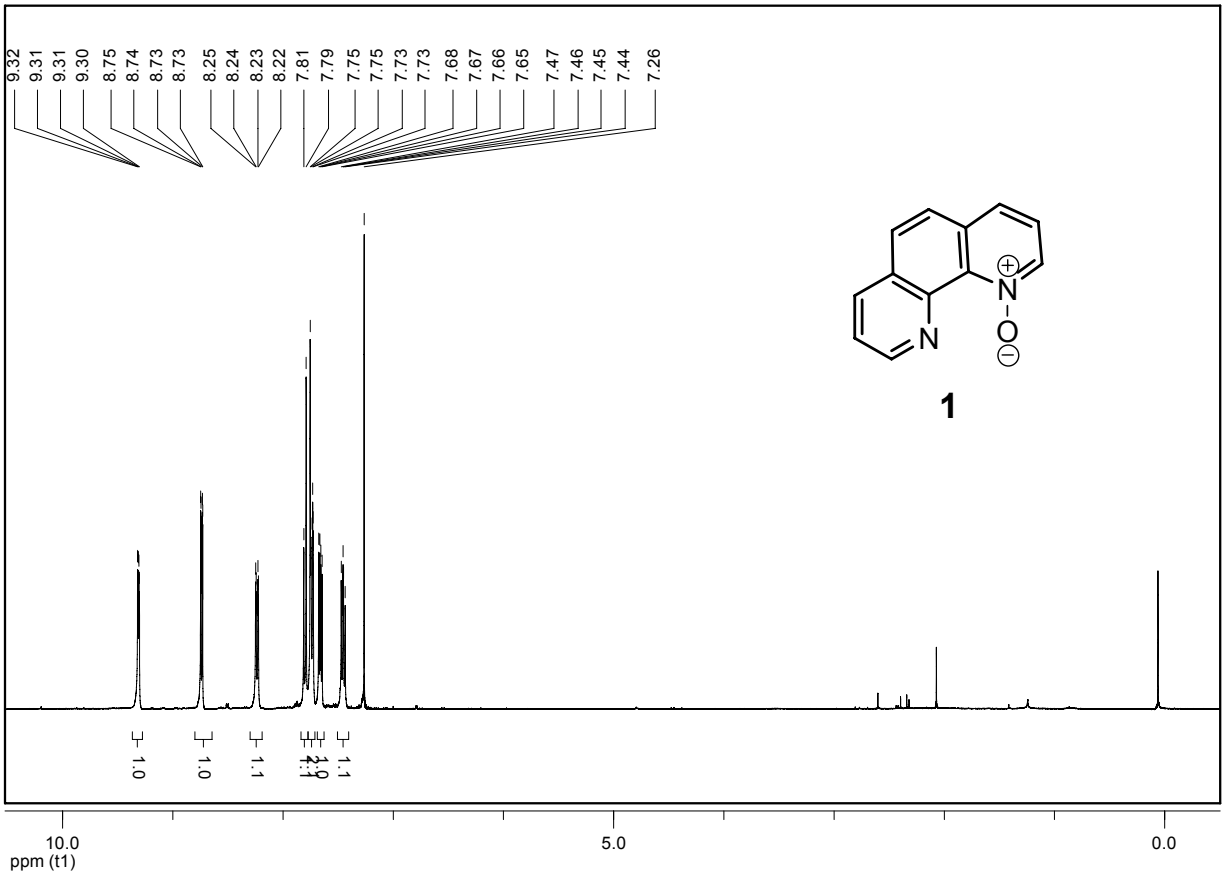


Figure S(1): ^{1}H NMR of compound **1** in $CDCl_3$ at 400 MHZ.

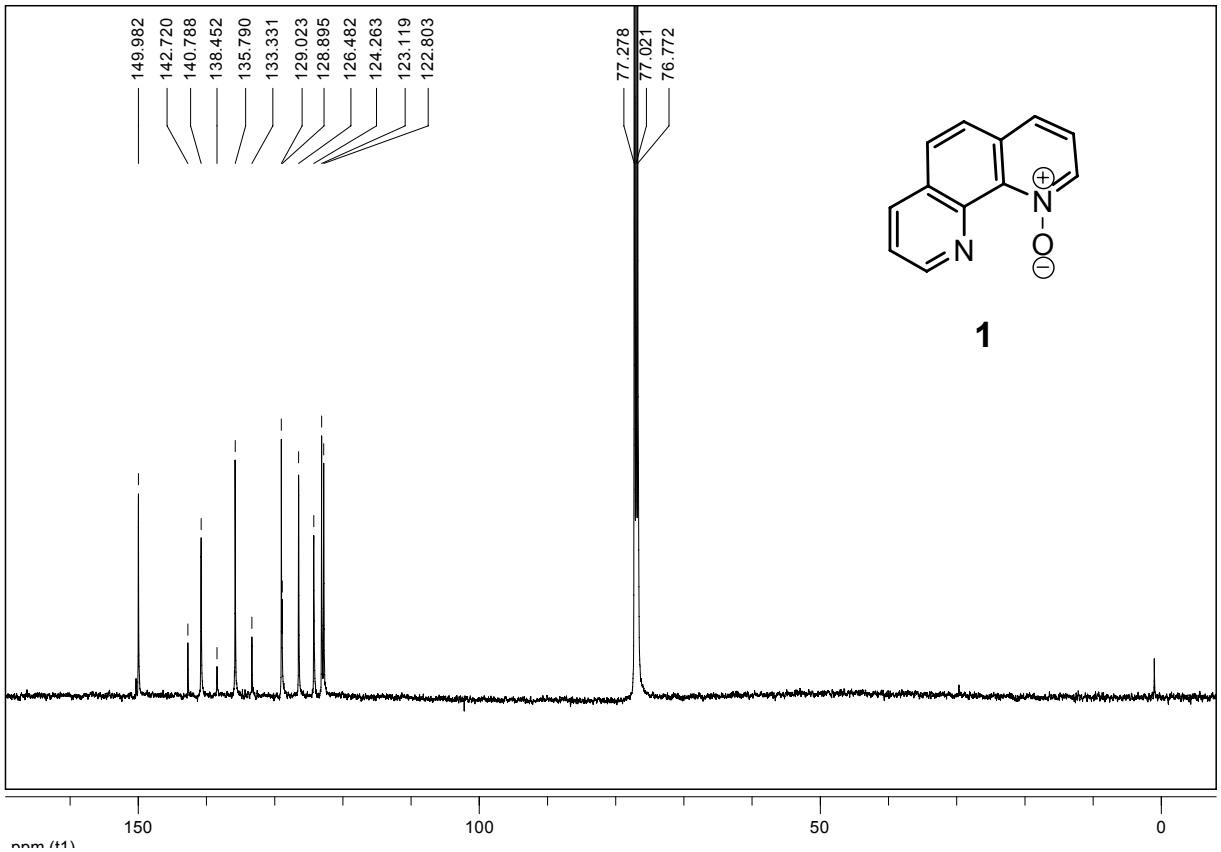


Figure S(2): ^{13}C NMR of compound **1** in $CDCl_3$ at 100 MHZ.

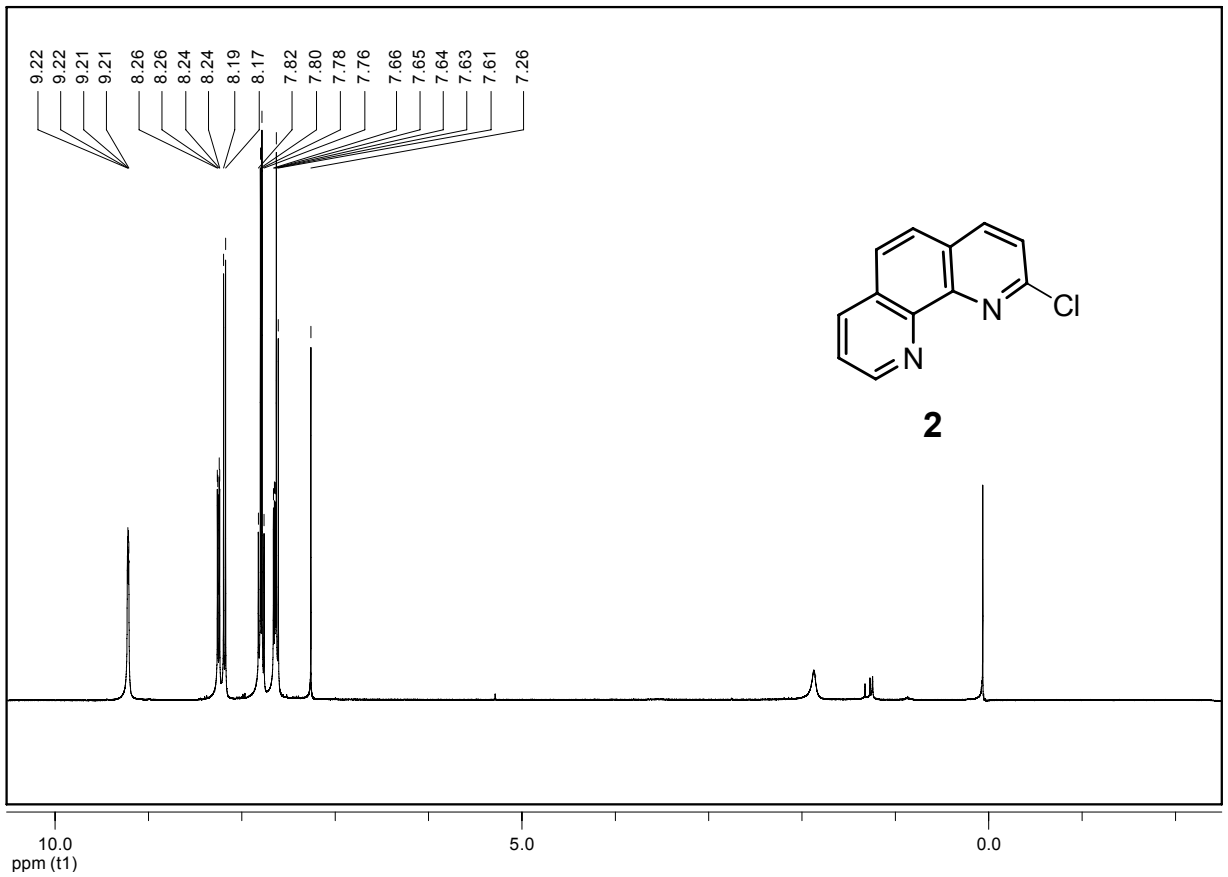


Figure S(3): ^{1}H NMR of compound **2** in $CDCl_3$ at 400 MHZ.

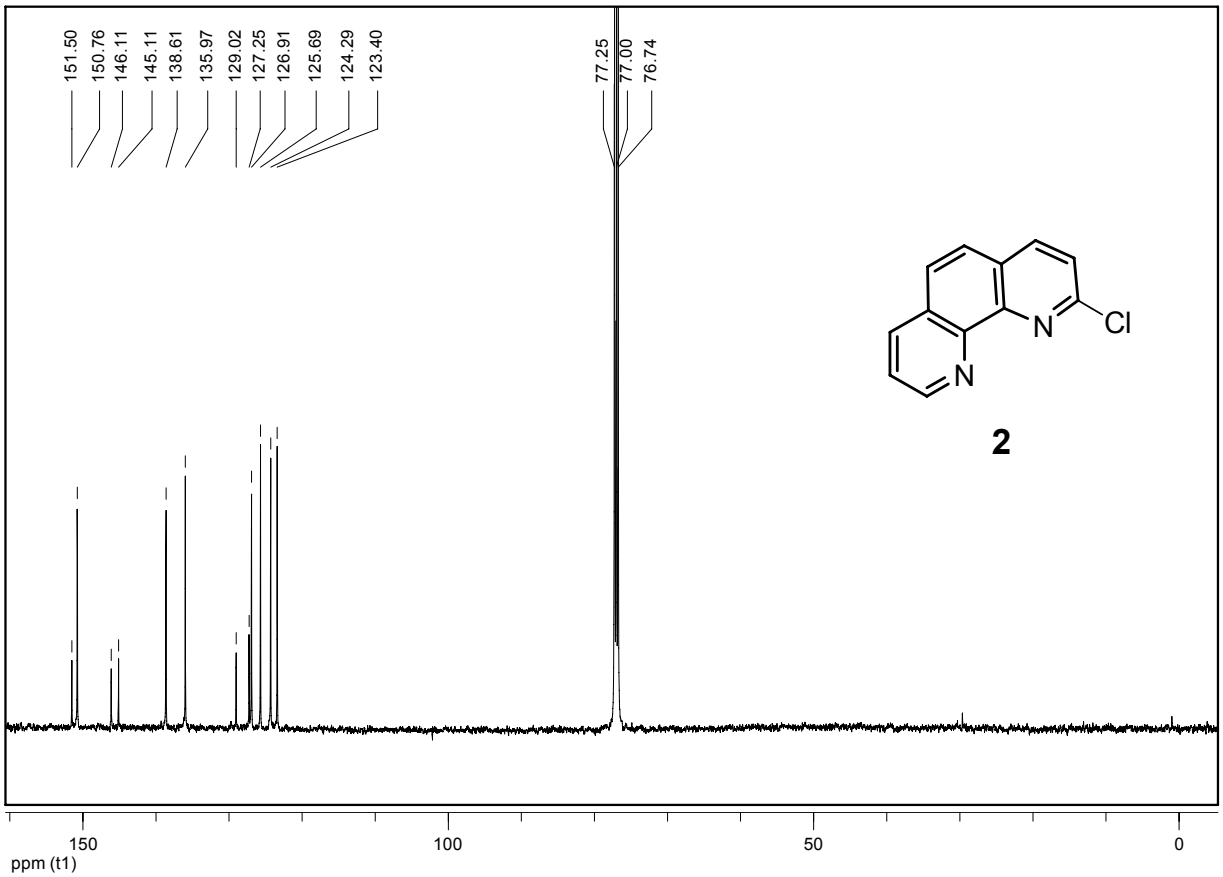


Figure S(4): ^{13}C NMR of compound **2** in $CDCl_3$ at 125 MHZ.

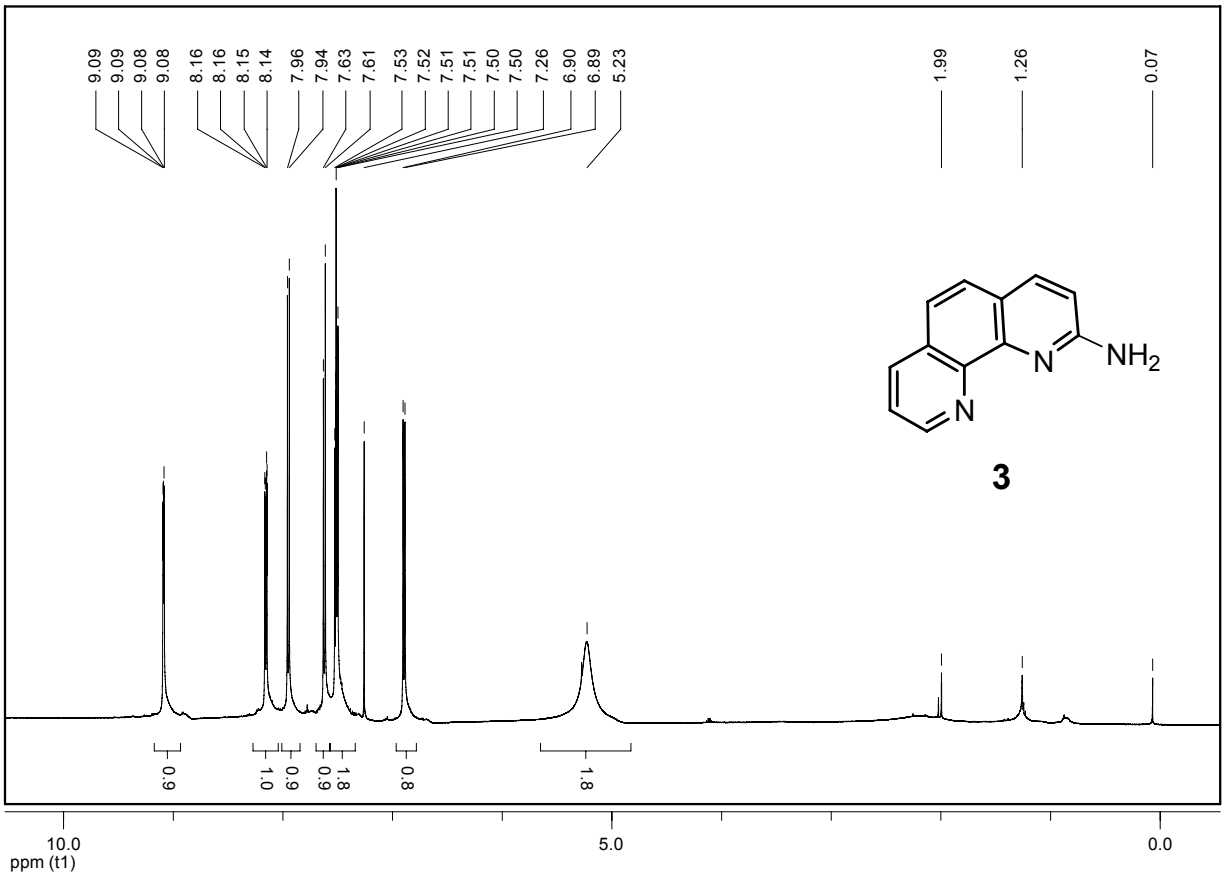


Figure S(5): ^{1}H NMR of compound **3** in $CDCl_3$ at 500 MHZ.

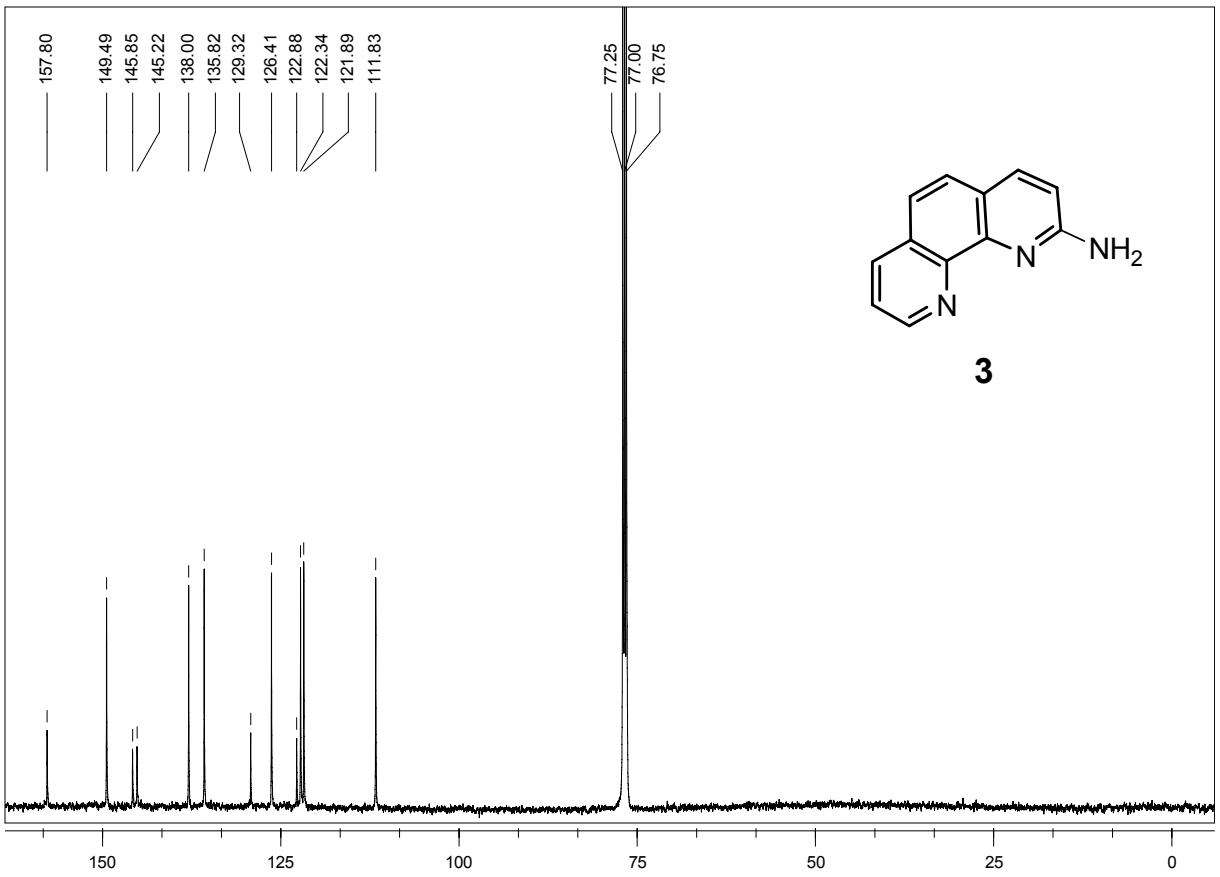


Figure S(6): ^{13}C NMR of compound **3** in $CDCl_3$ at 125 MHZ.

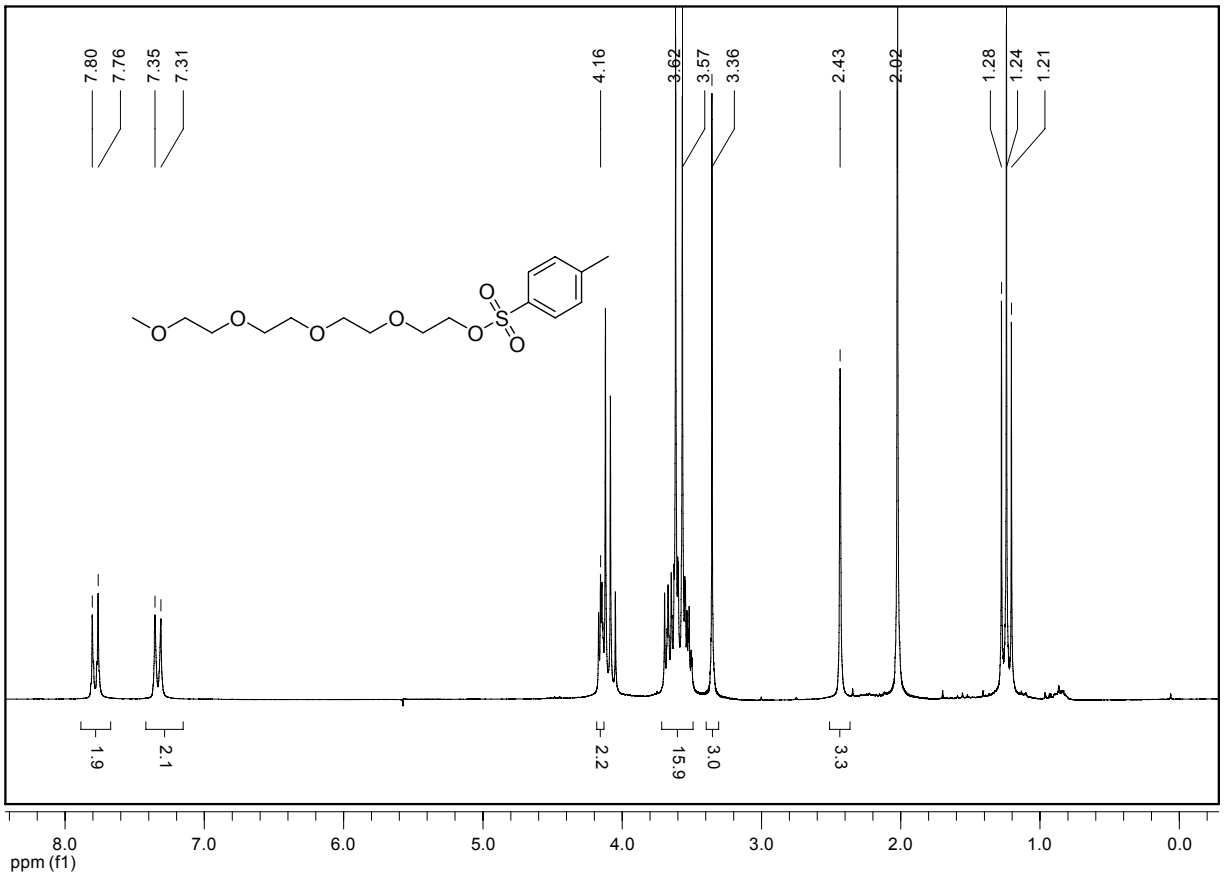


Figure S(7): ^{1}H NMR of 2,5,8,11-tetraoxatridecan-13-yl 4-methylbenzenesulfonate in $CDCl_3$ at 200 MHZ.

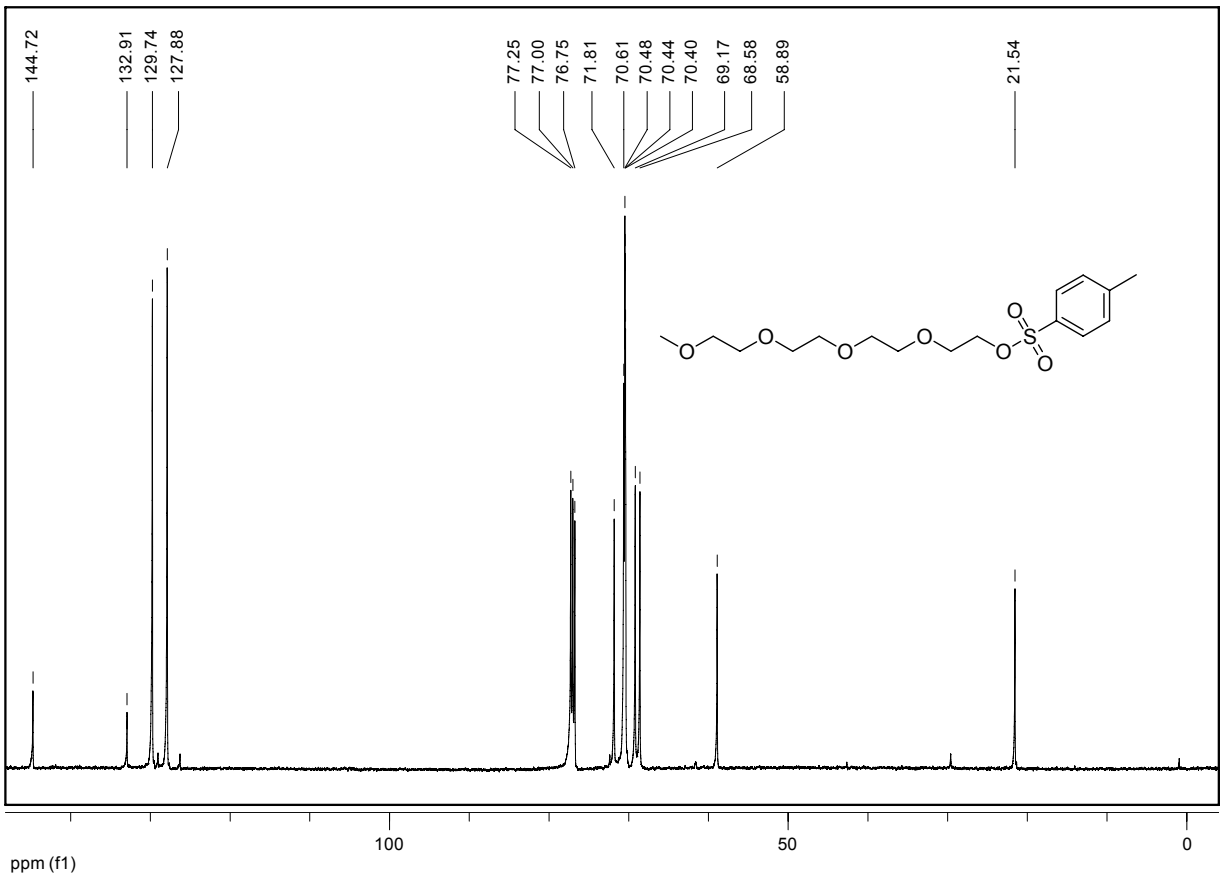


Figure S(8): ^{13}C NMR of 2,5,8,11-tetraoxatridecan-13-yl 4-methylbenzenesulfonate in $CDCl_3$ at 125 MHZ.

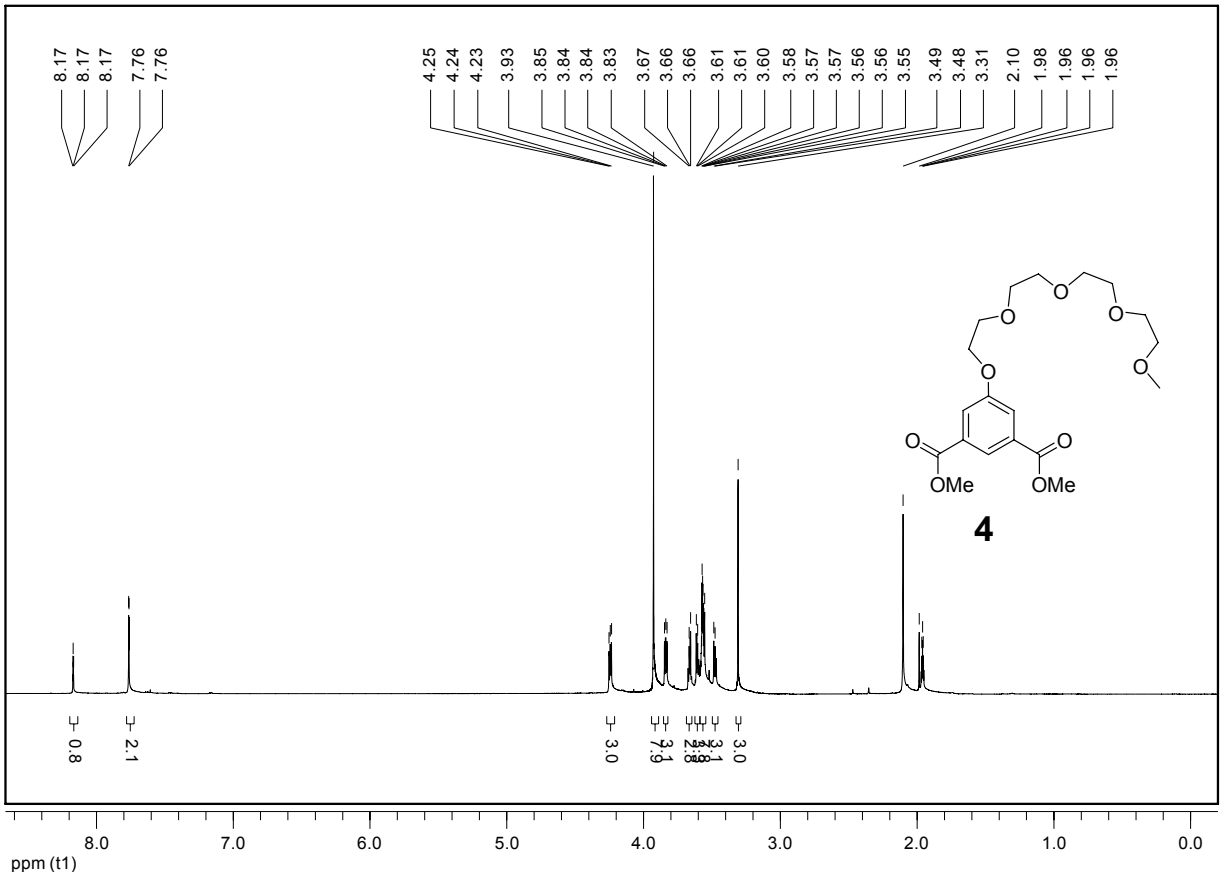


Figure S(9): ^{1}H NMR of compound **4** in CD_3CN at 500 MHZ.

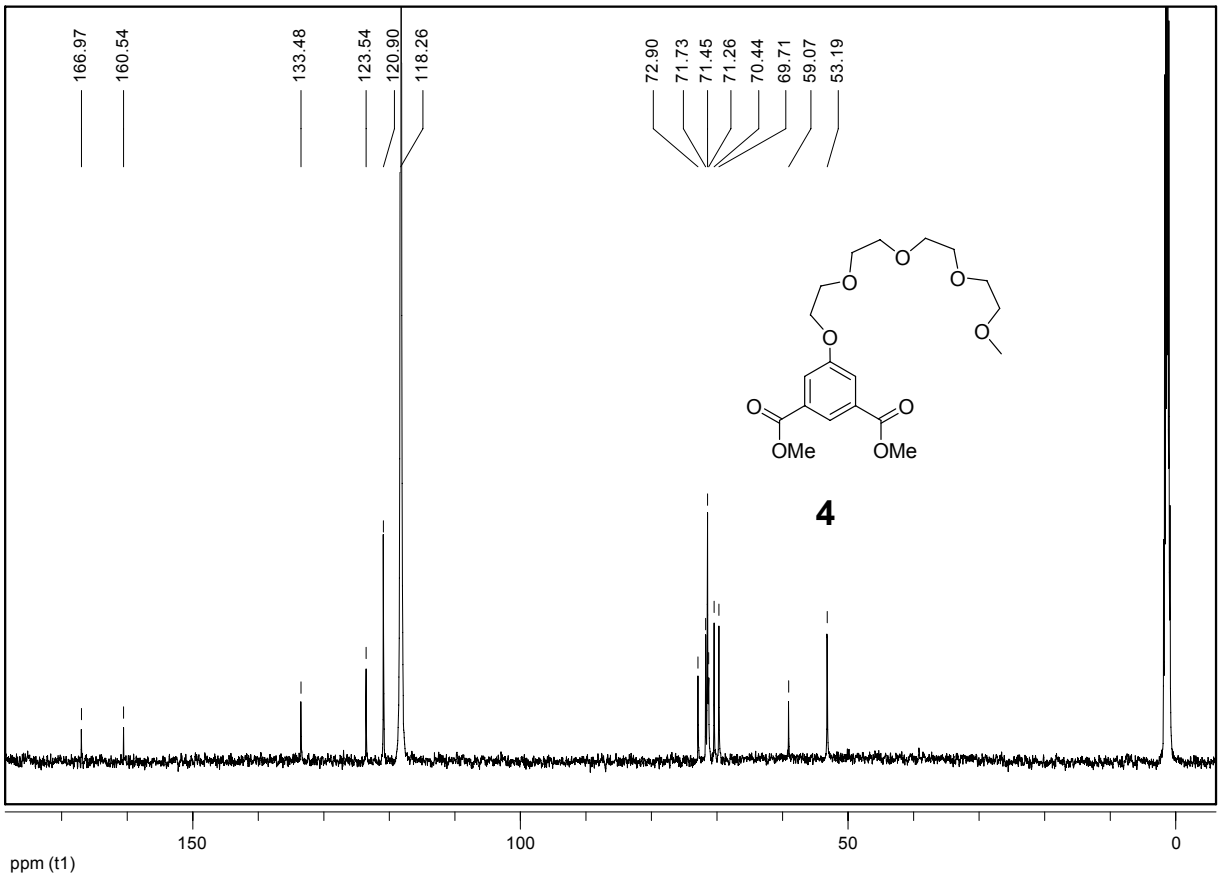


Figure S(10): ^{13}C NMR of compound **4** in CD_3CN at 125 MHZ.

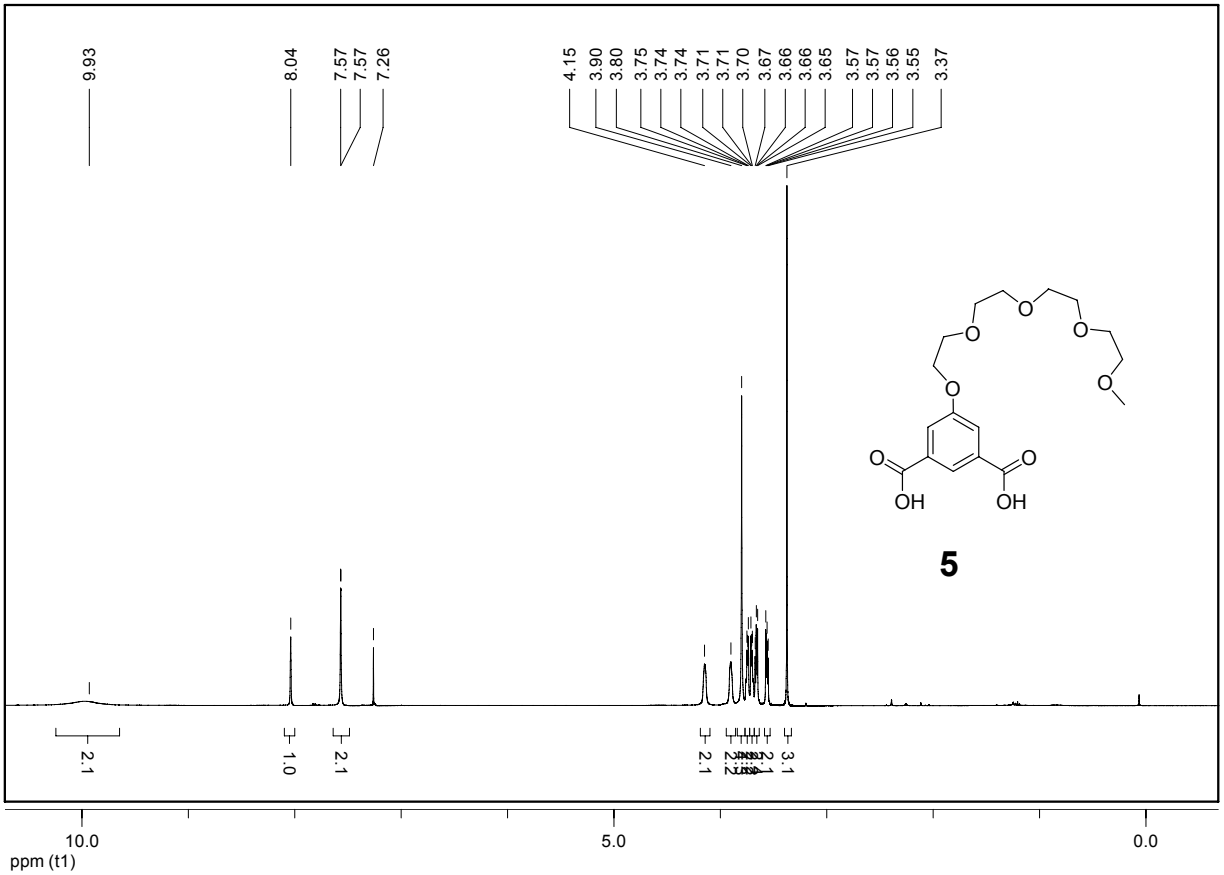


Figure S(11): ^{1}H NMR of compound **5** in $CDCl_3$ at 400 MHZ.

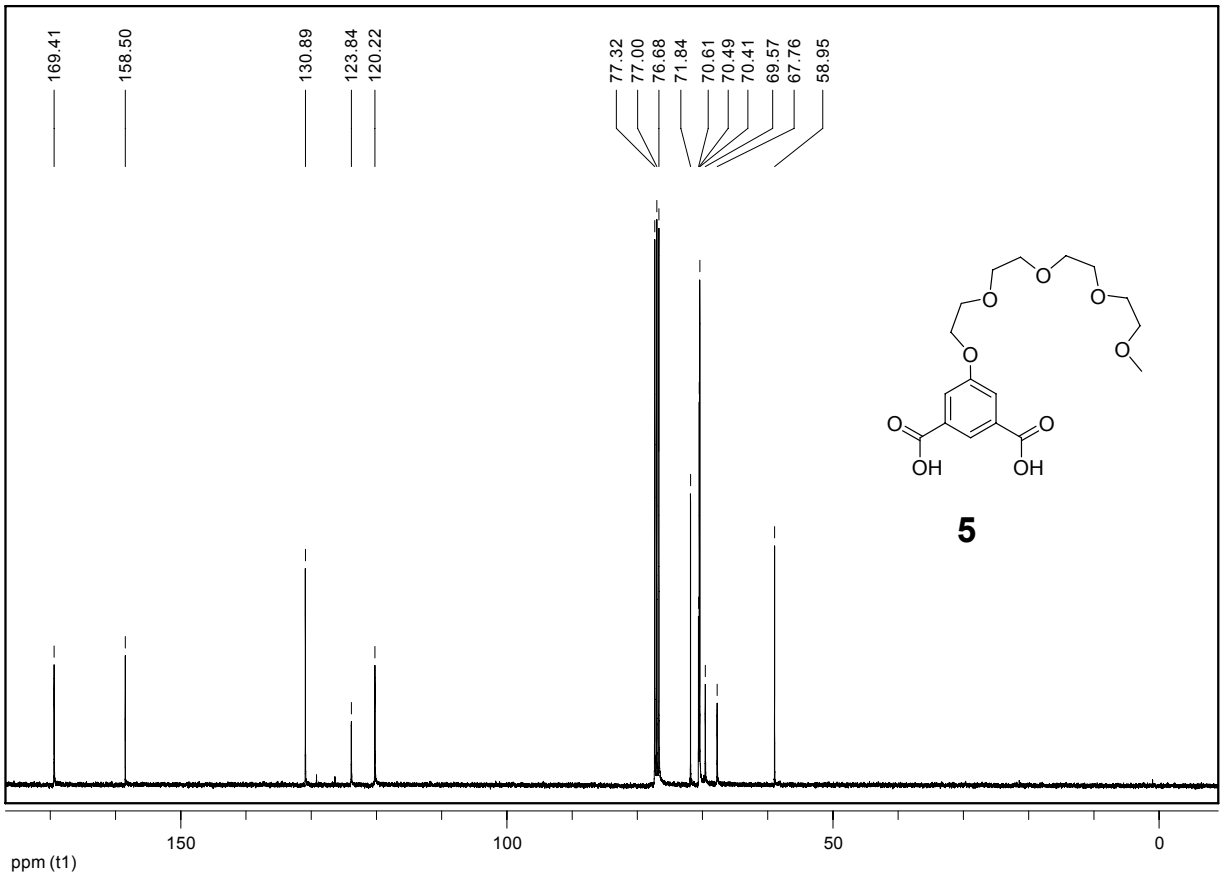


Figure S(12): ^{13}C NMR of compound **5** in $CDCl_3$ at 100 MHZ.

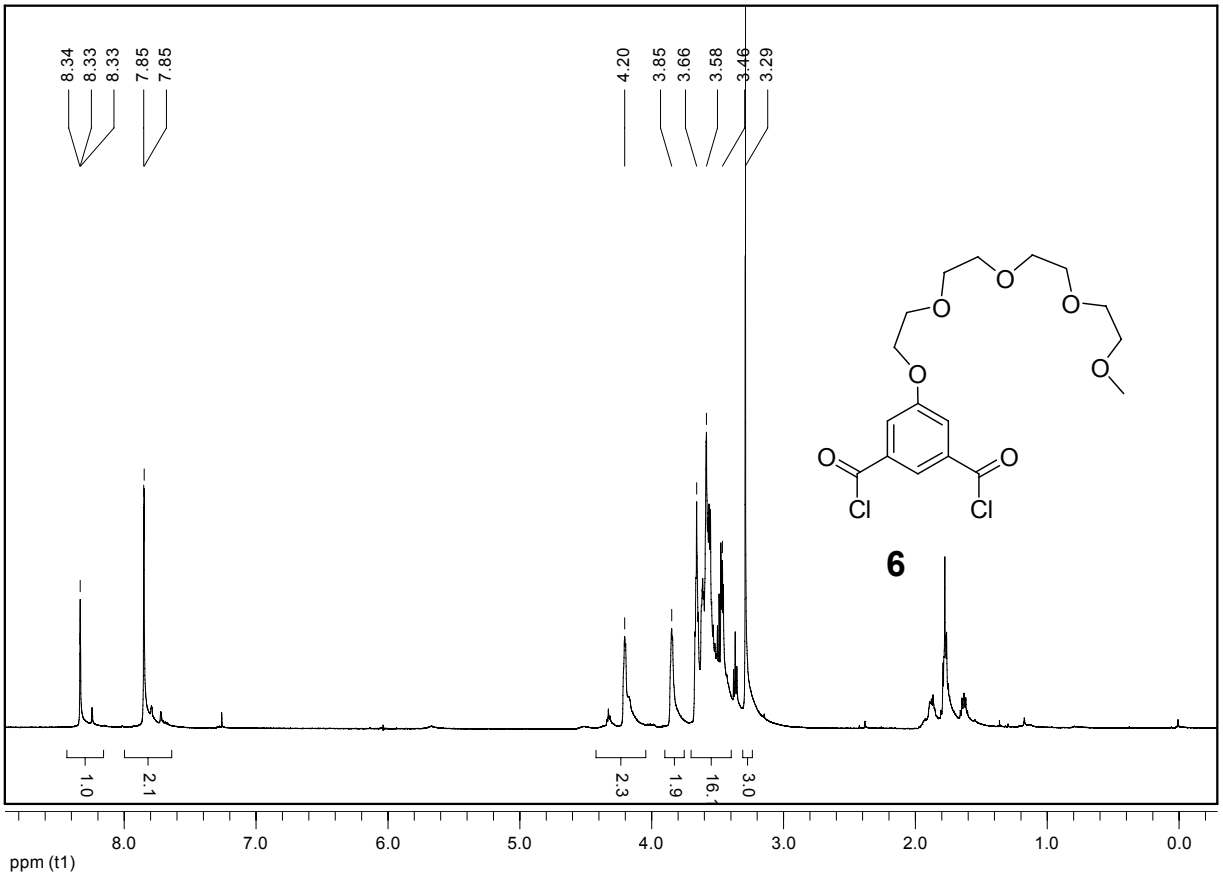


Figure S(13): ^{1}H NMR of compound **6** in $CDCl_3$ at 500 MHZ.

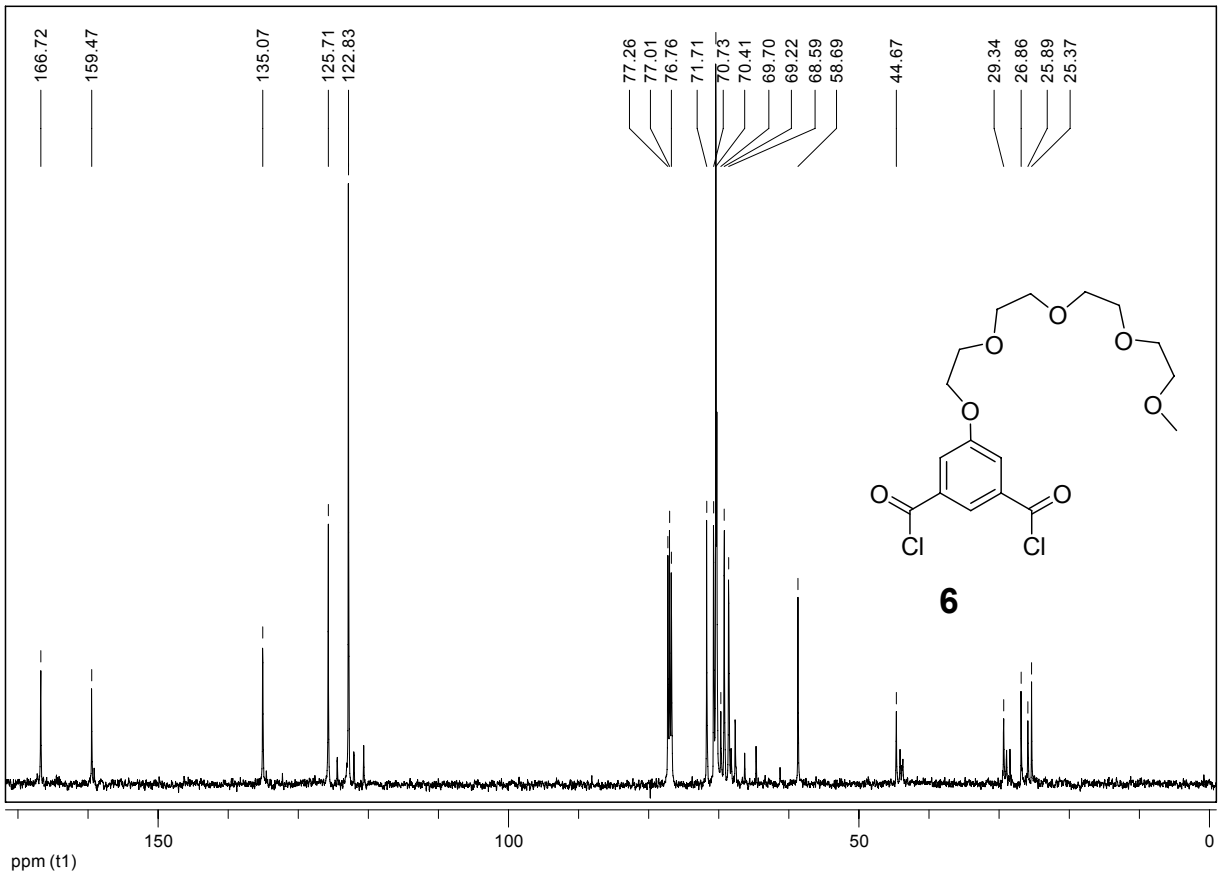


Figure S(14): ^{13}C NMR of compound **6** in $CDCl_3$ at 125 MHZ.

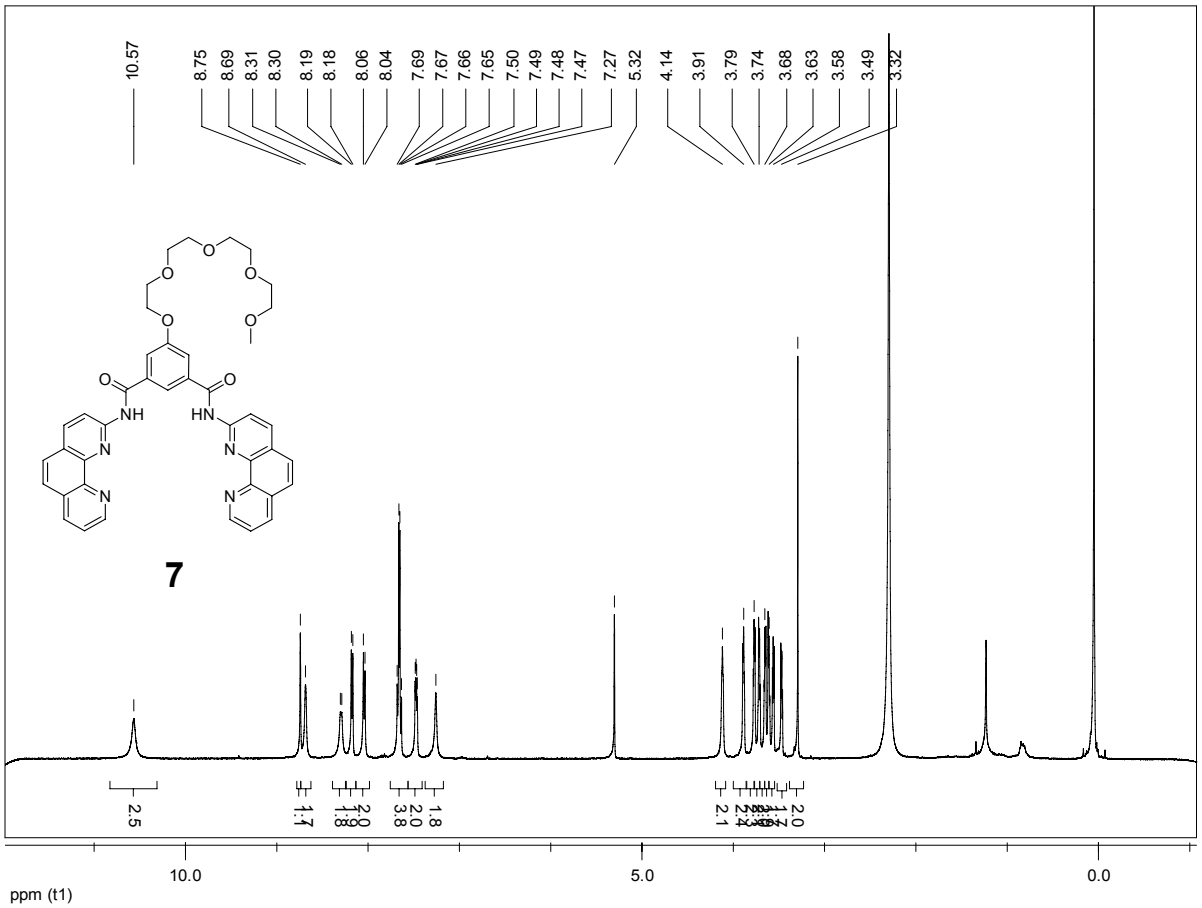


Figure S(15): ^{1}H NMR of compound **7** in CD_2Cl_2 at 500 MHZ.

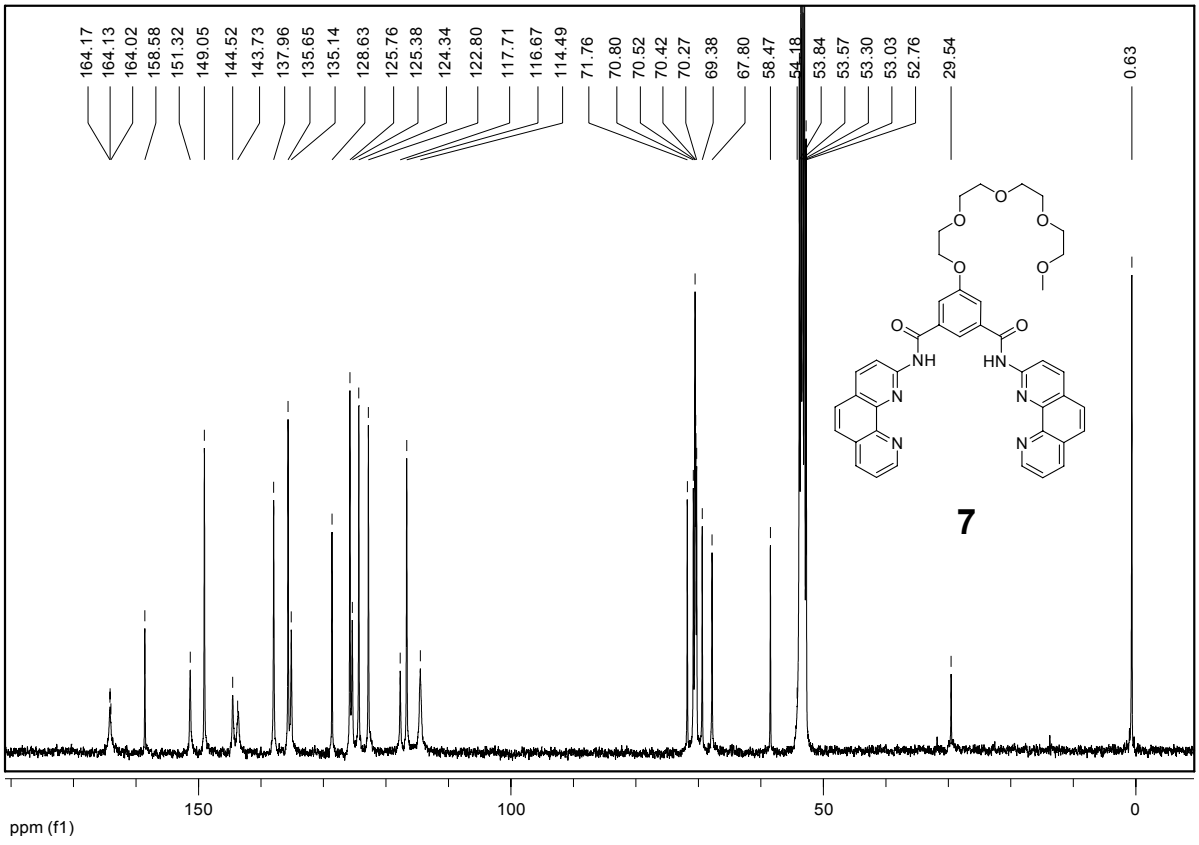


Figure S(16): ^{13}C NMR of compound **7** in CD_2Cl_2 at 100 MHZ.

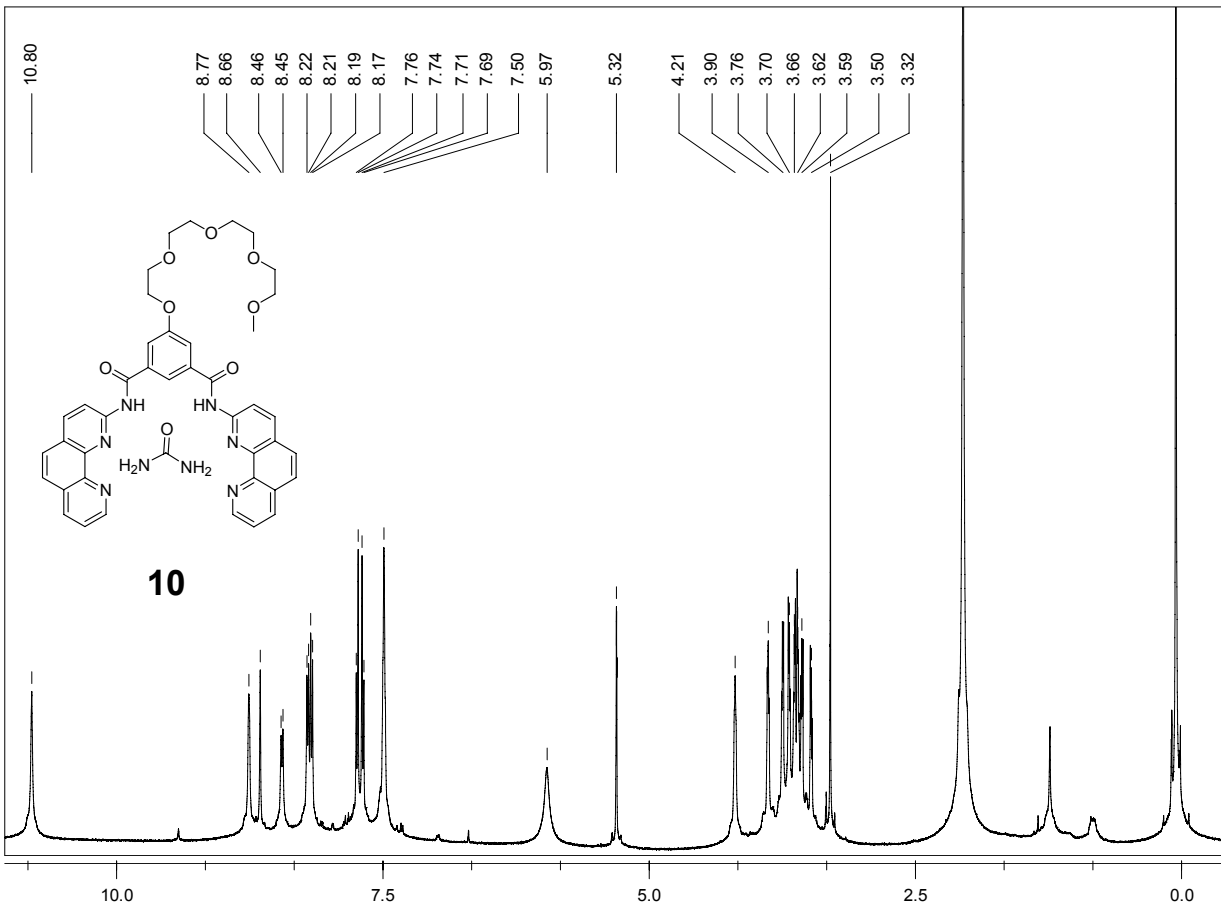


Figure S(17): ^{1}H NMR of compound **7** complex with urea in CD_2Cl_2 at 500 MHZ.

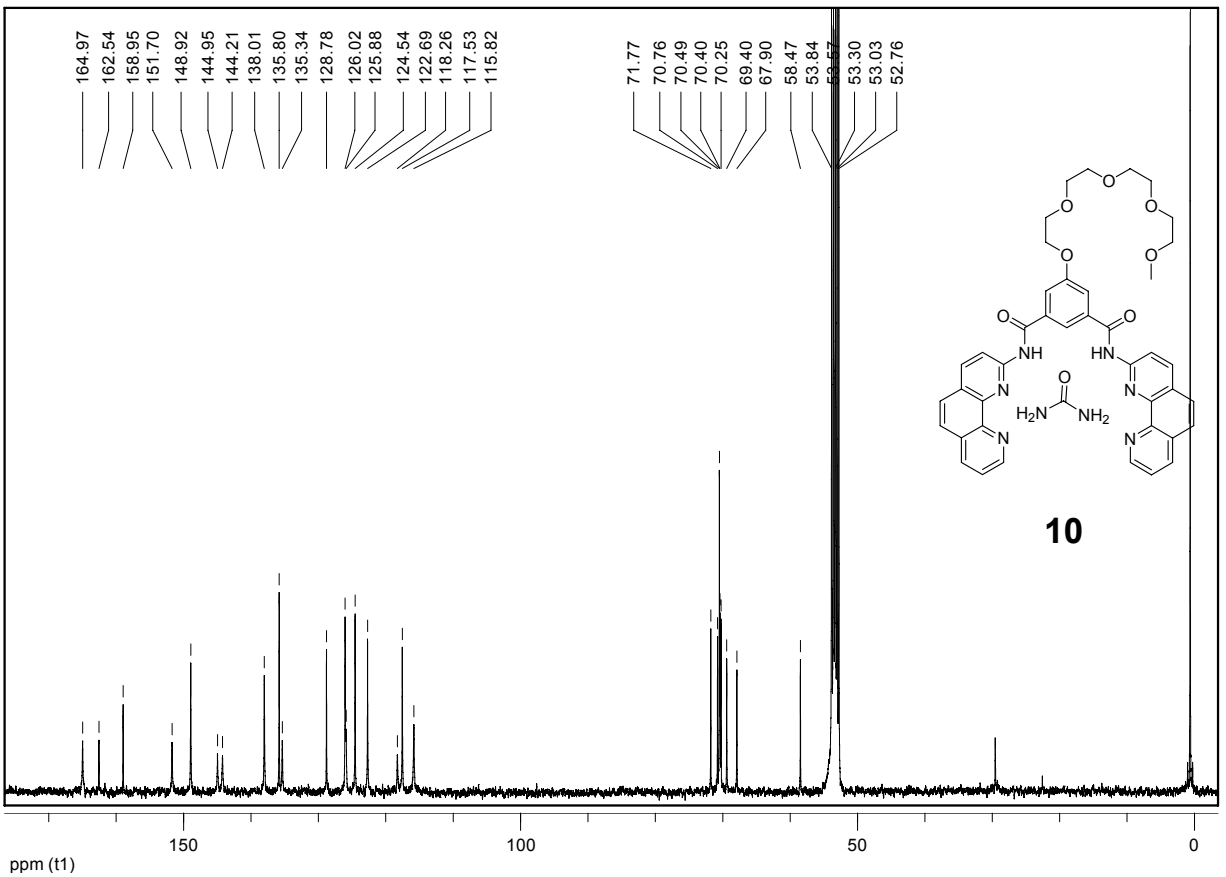


Figure S(18): ^{13}C NMR of host **7** complex with urea in CD_2Cl_2 at 100 MHZ.

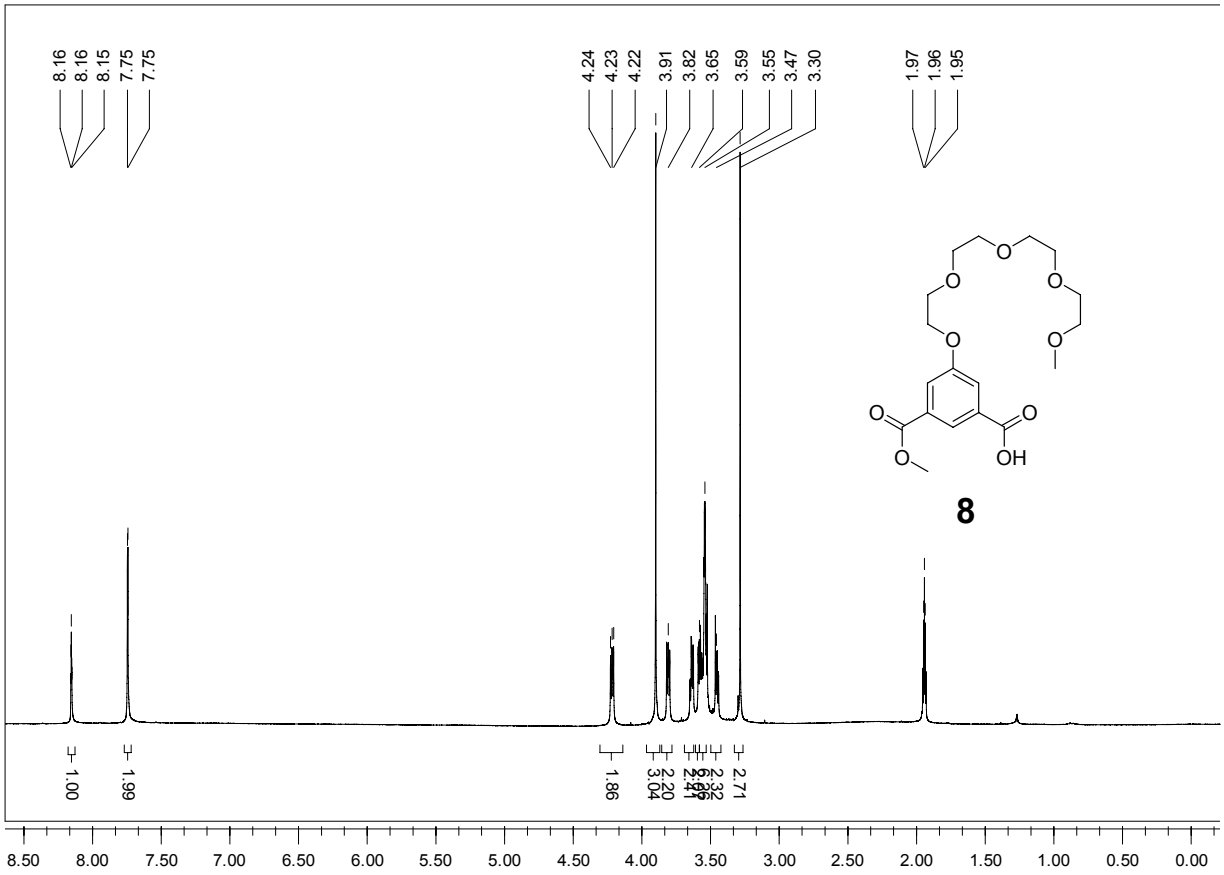


Figure S(19): ^{1}H NMR of compound **8** in CD_3CN at 400 MHZ.

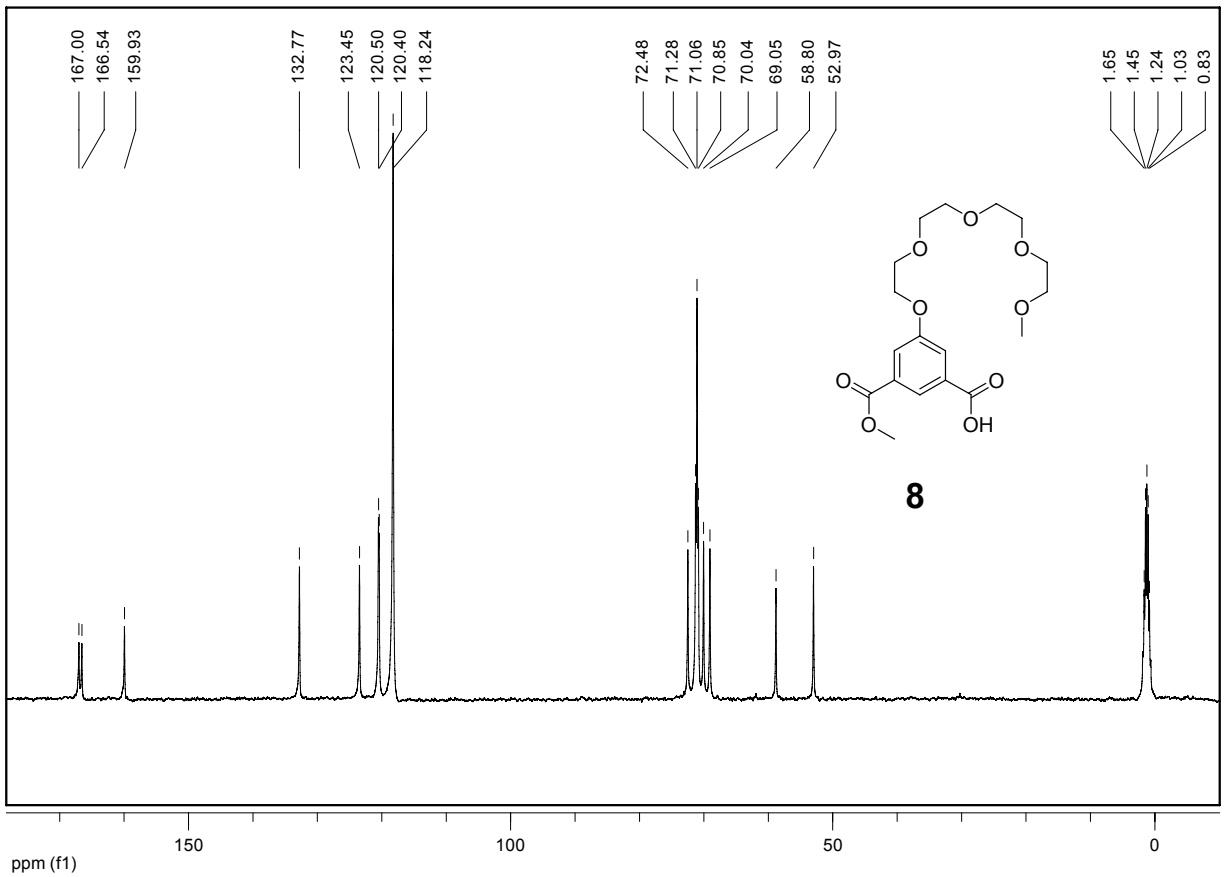


Figure S(20): ^{13}C NMR of compound **8** in CD_3CN at 100 MHZ.

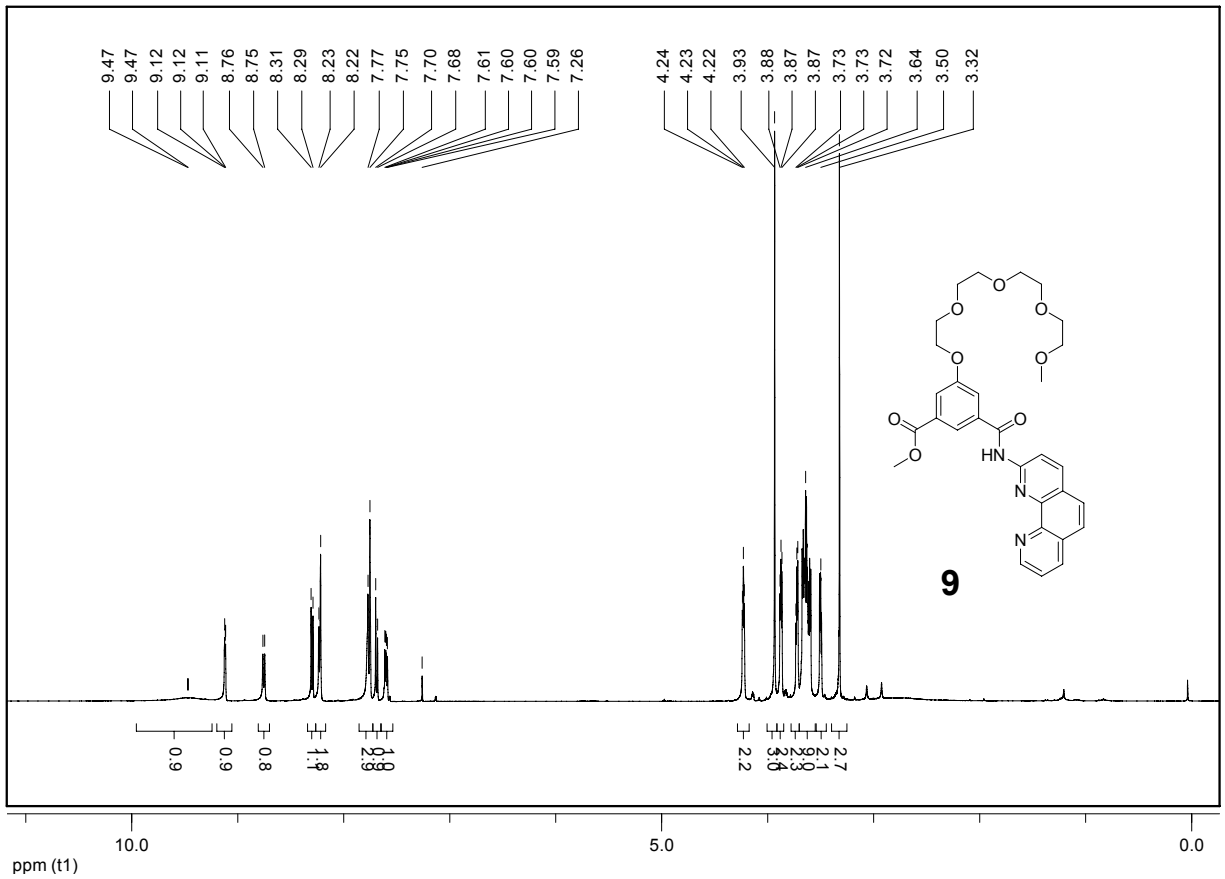


Figure S(21): ^{1}H NMR of compound **9** in $CDCl_3$ at 500 MHZ.

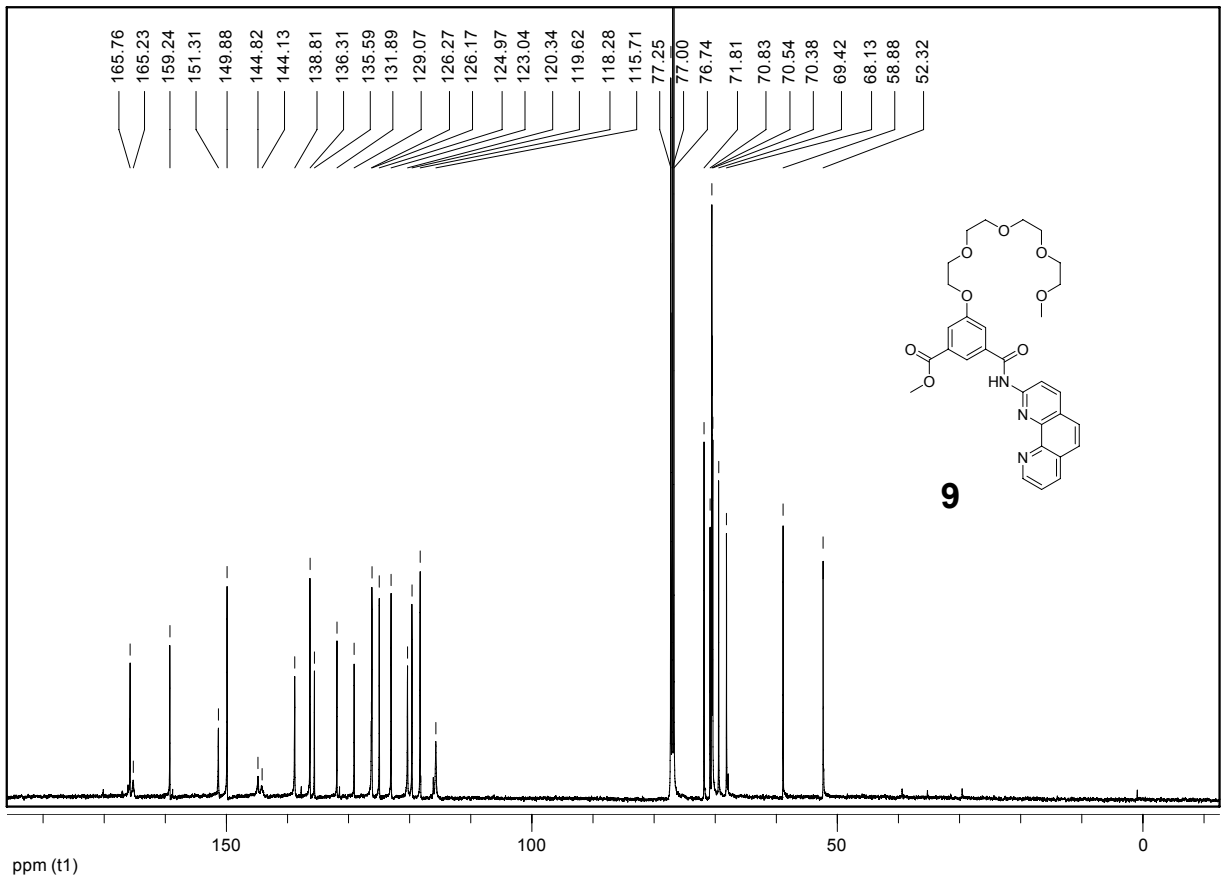


Figure S(22): ^{13}C NMR of compound **9** in $CDCl_3$ at 125 MHZ.

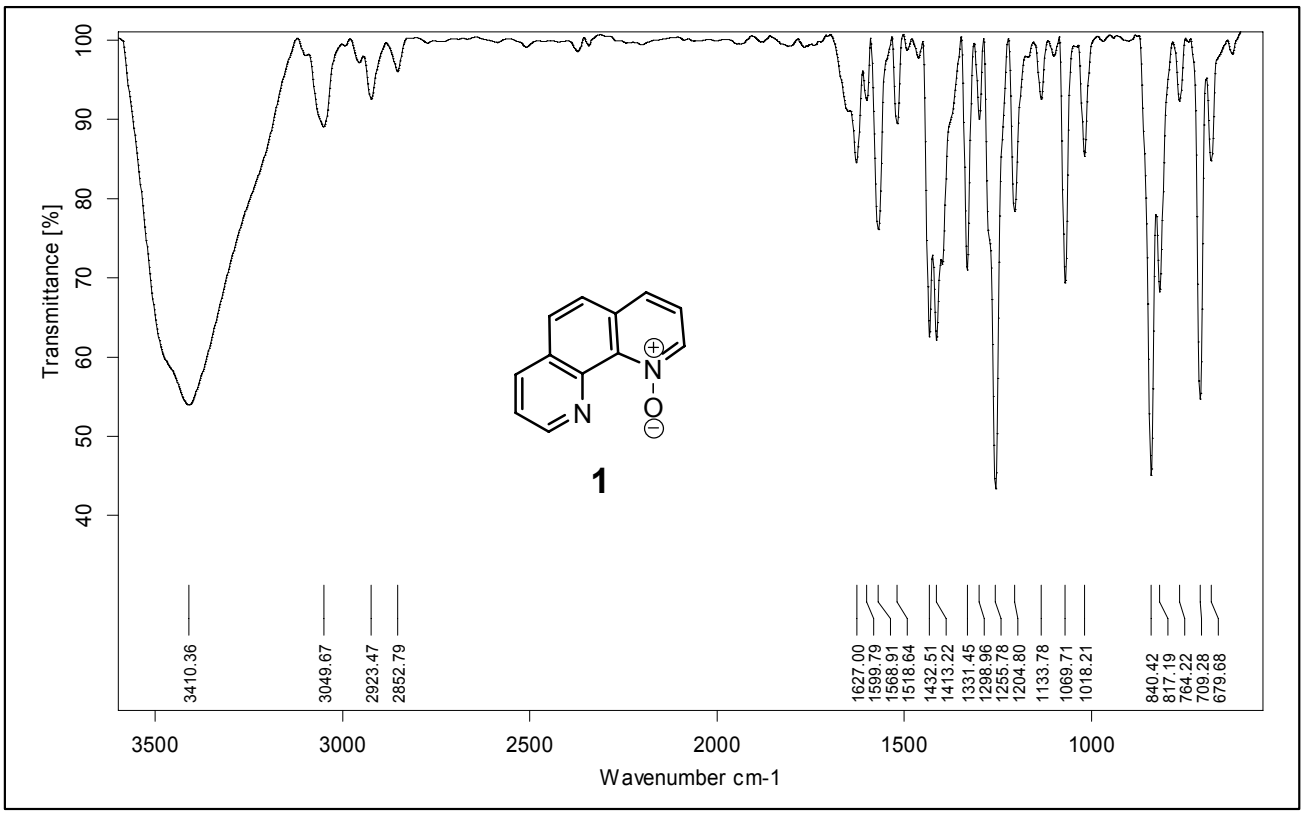


Figure S(23): IR Spectrum of compound **1** IN KBr.

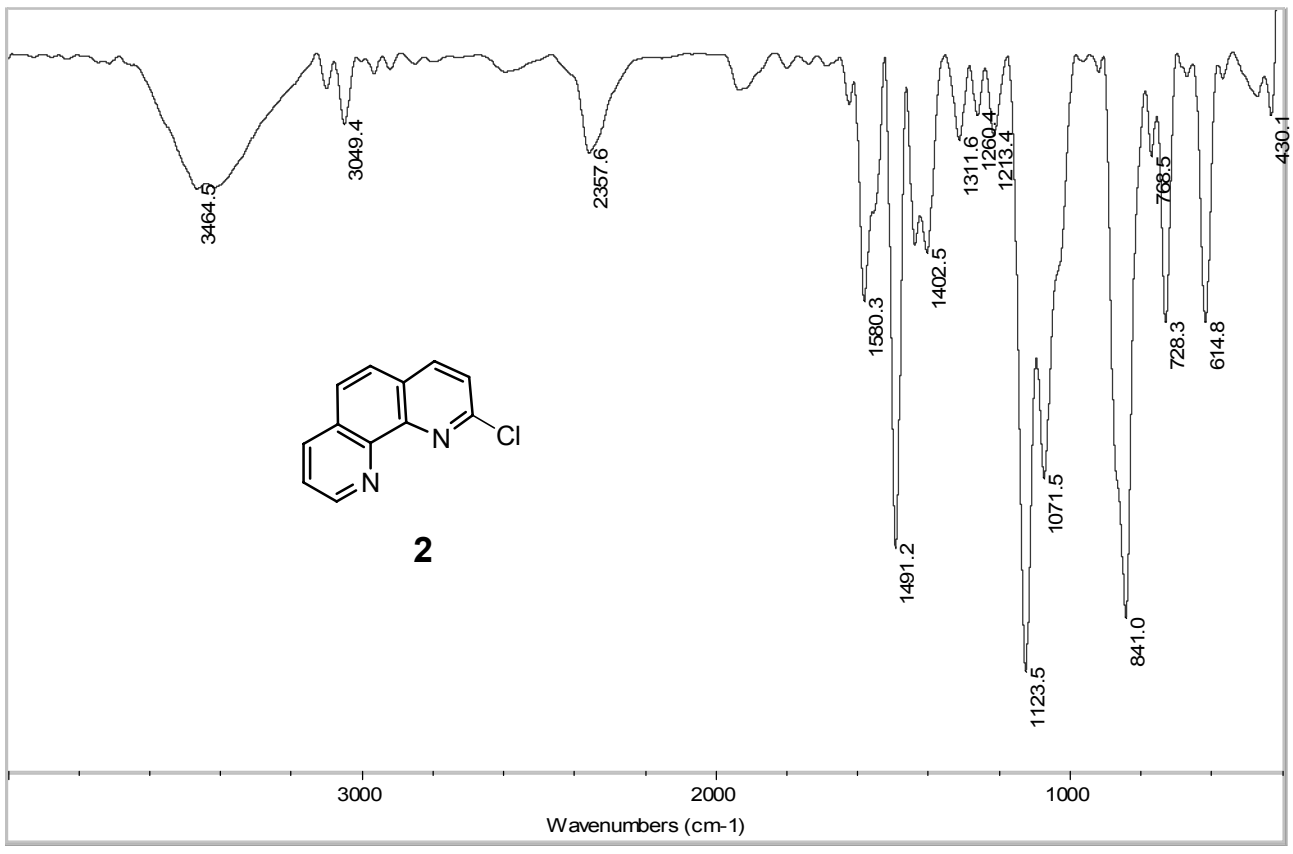


Figure S(24): IR Spectrum of compound **2** IN KBr

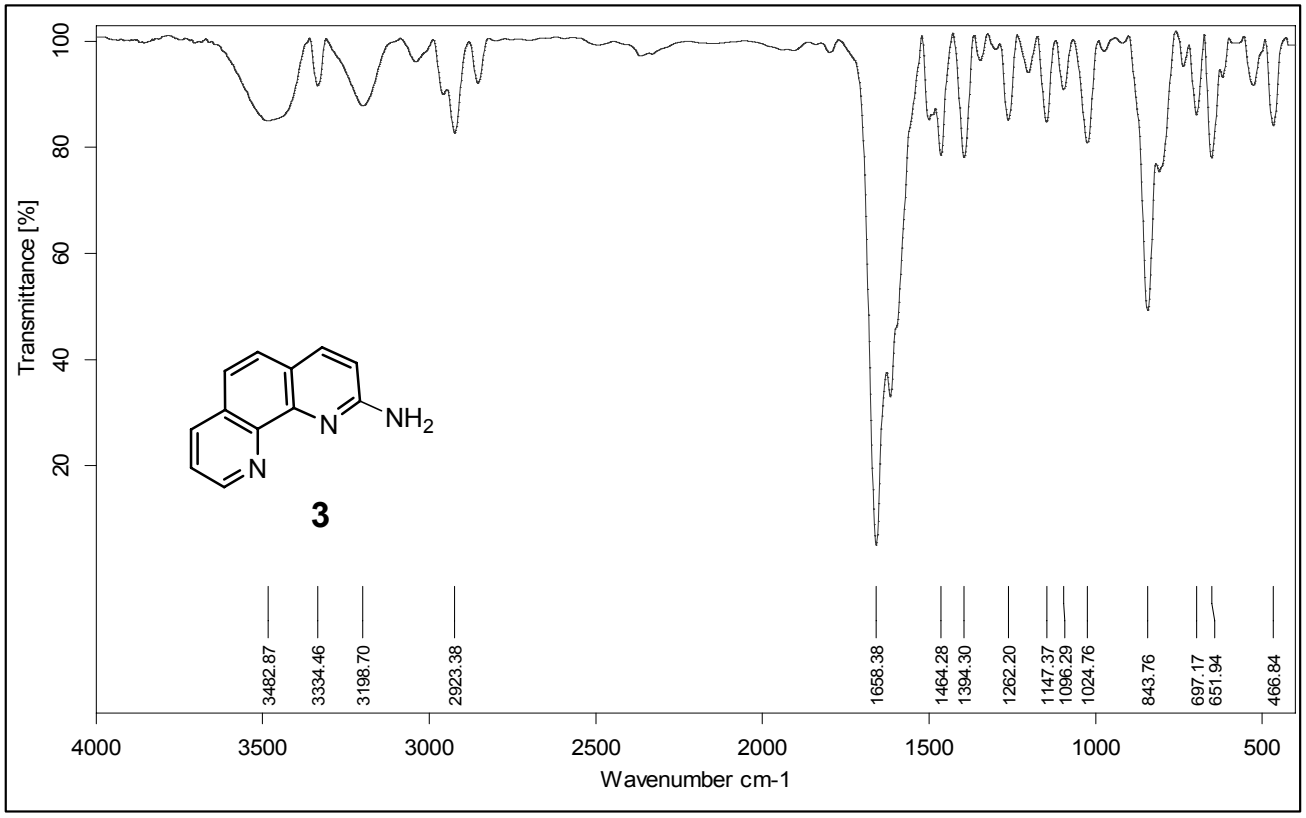


Figure S(25): IR Spectrum of compound **3** IN KBr

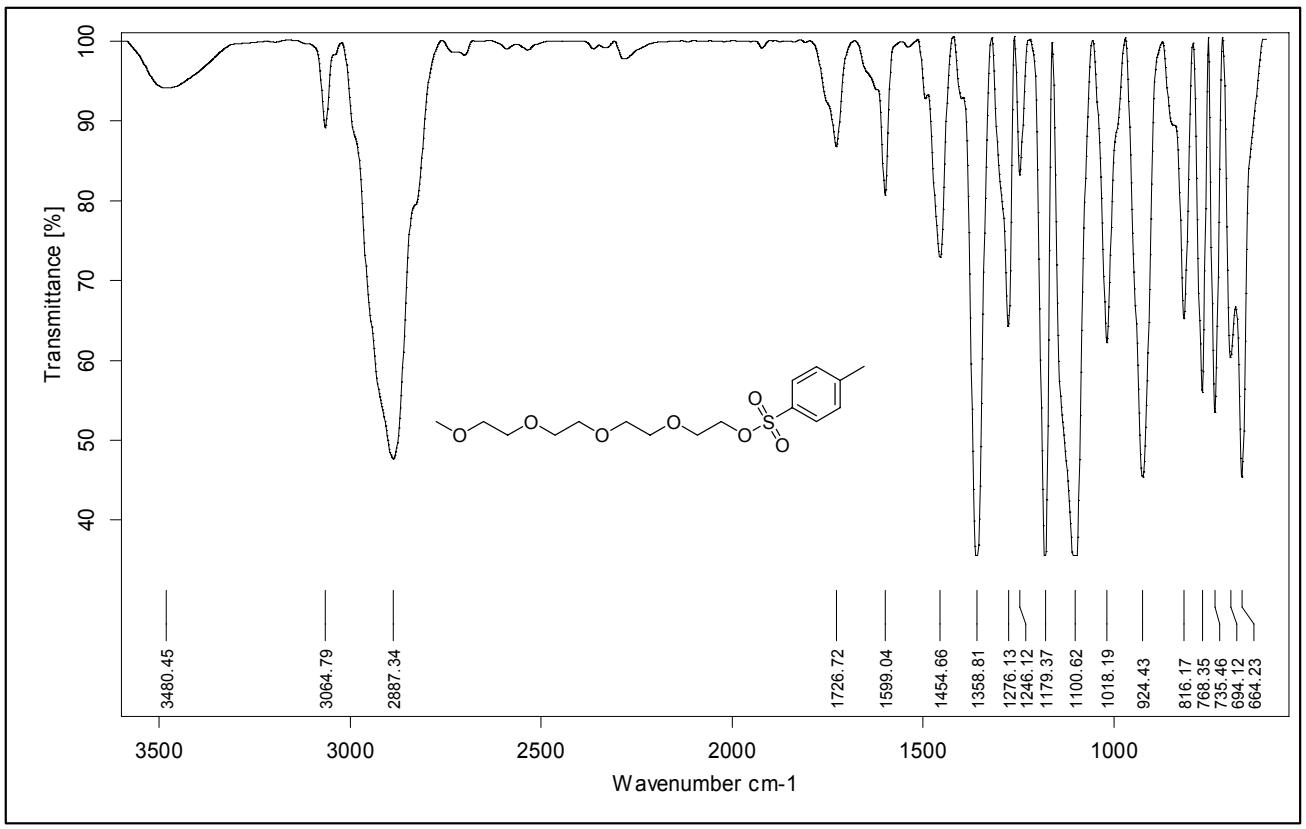


Figure S(26): IR Spectrum of compound 2,5,8,11-tetraoxatridecan-13-yl 4-methylbenzenesulfonate in CH_2Cl_2

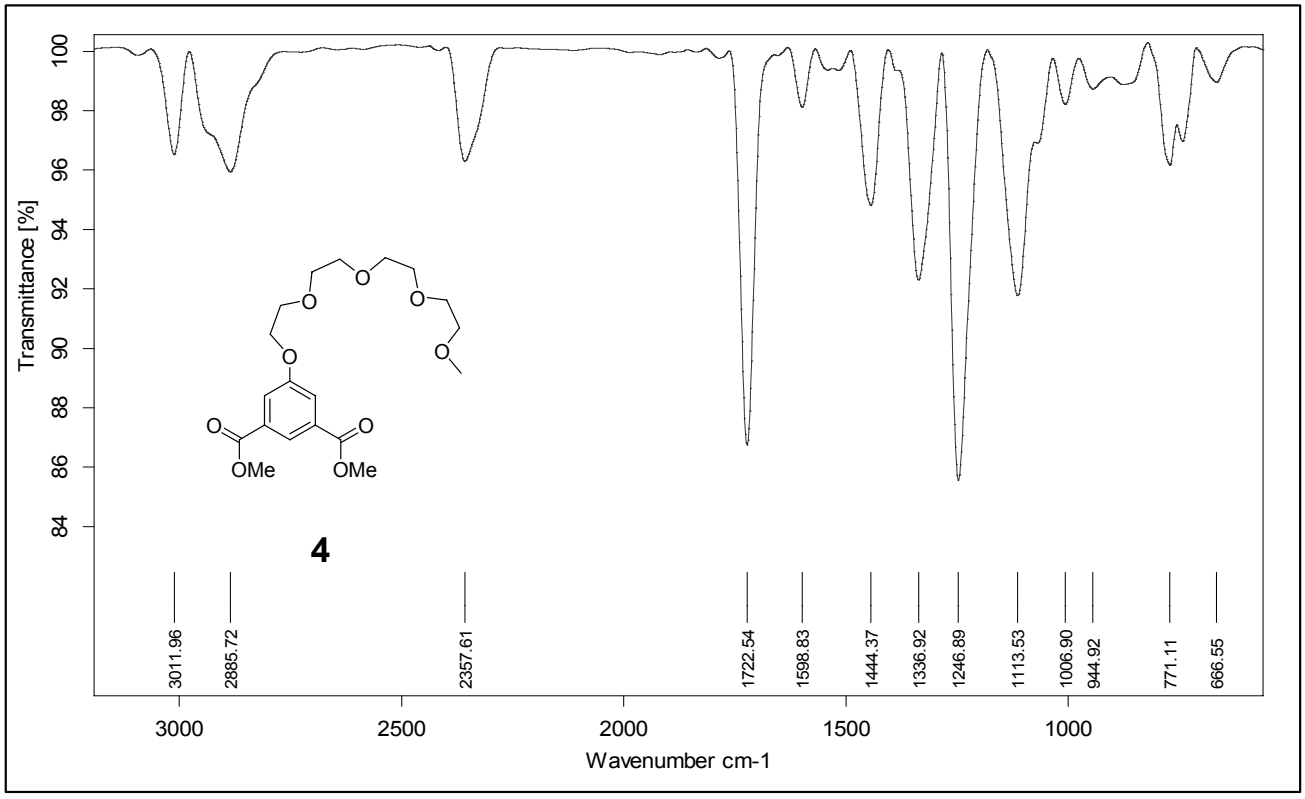


Figure S(27): IR Spectrum of compound **4** IN CH_2Cl_2

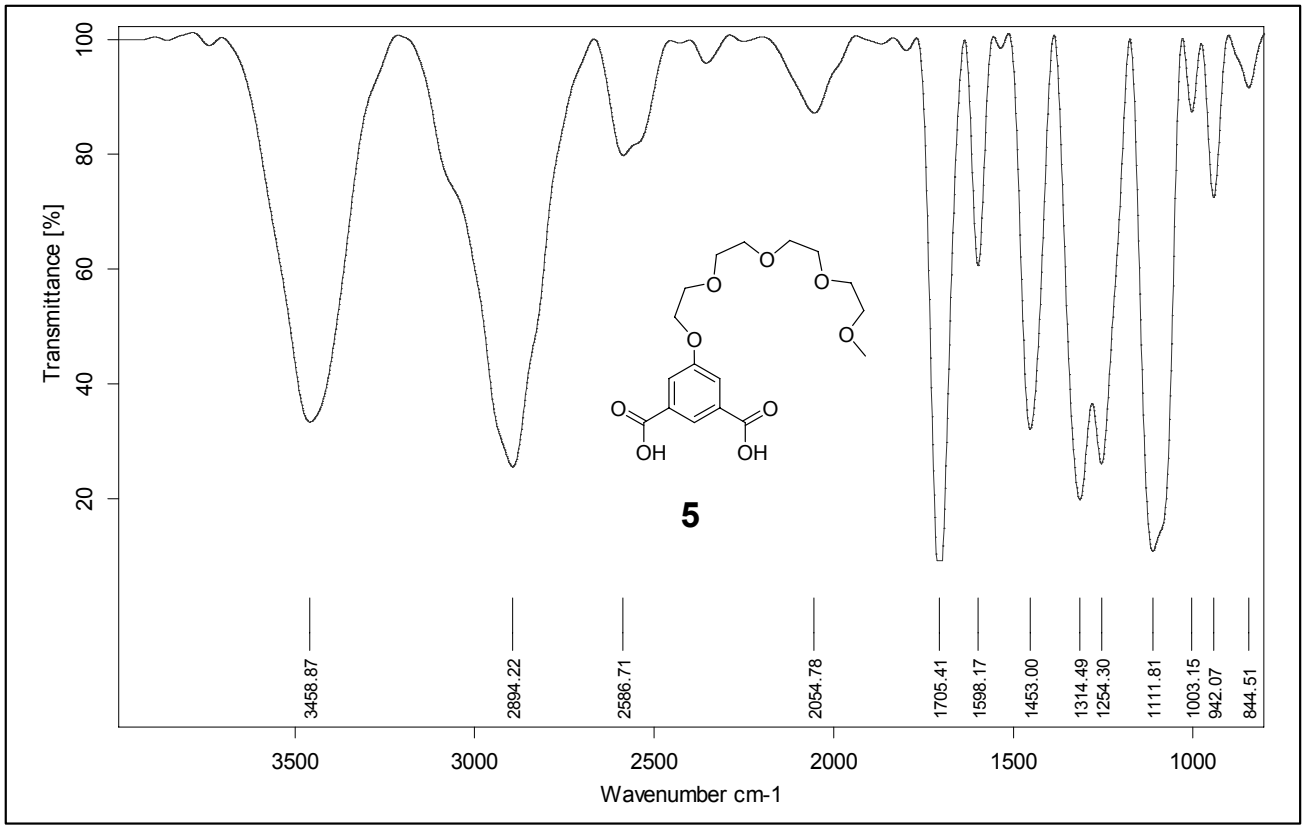


Figure S(28): IR Spectrum of compound **5** IN KBr.

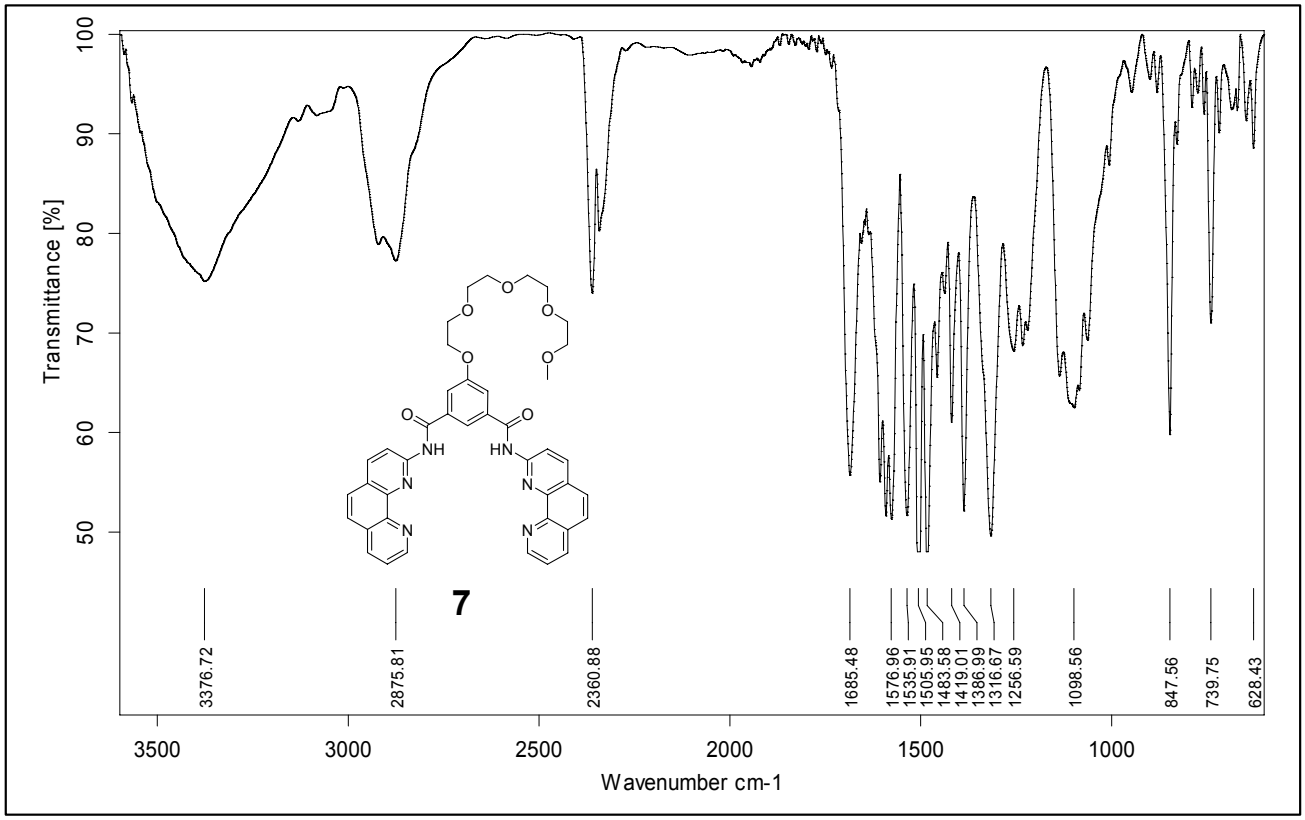


Figure S(29): IR Spectrum of compound **7** in KBr.

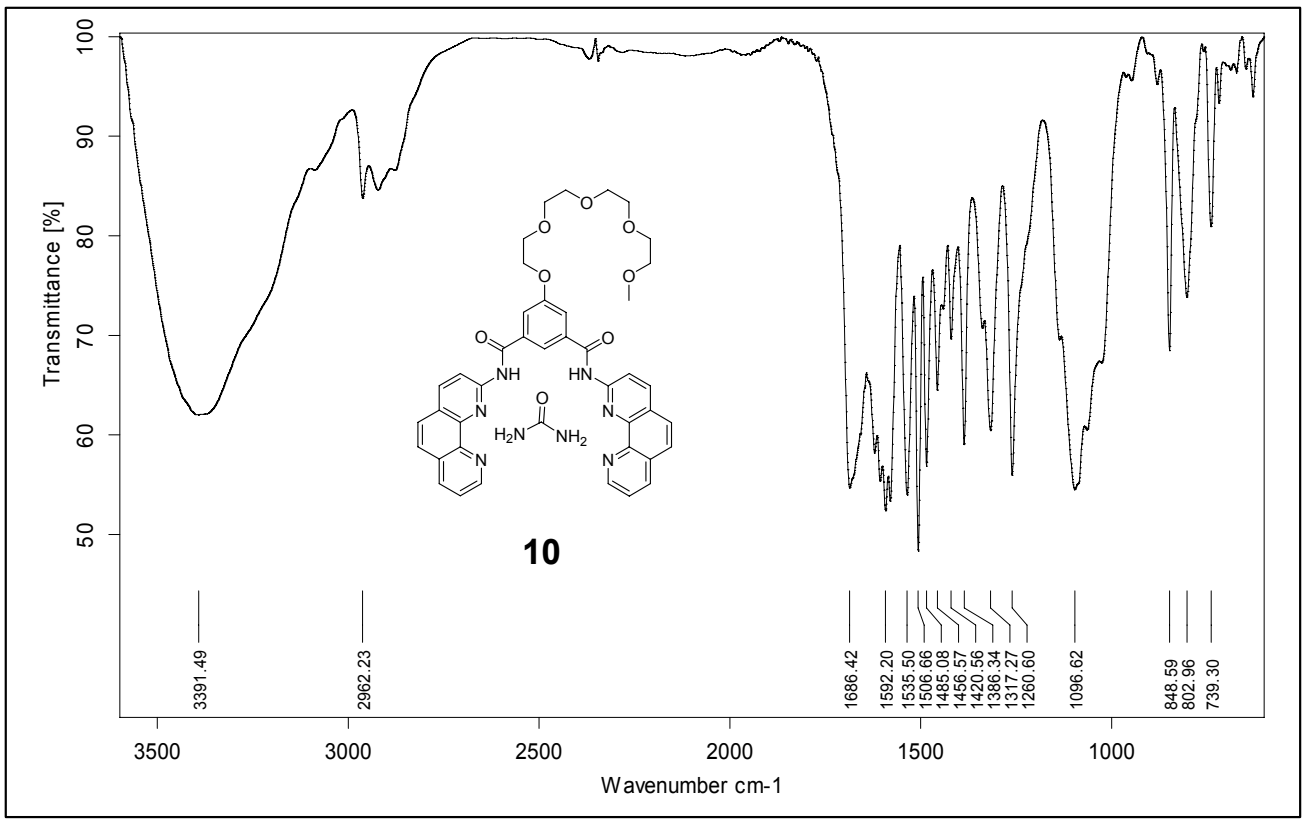


Figure S(30): IR Spectrum of complex **10** in KBr.

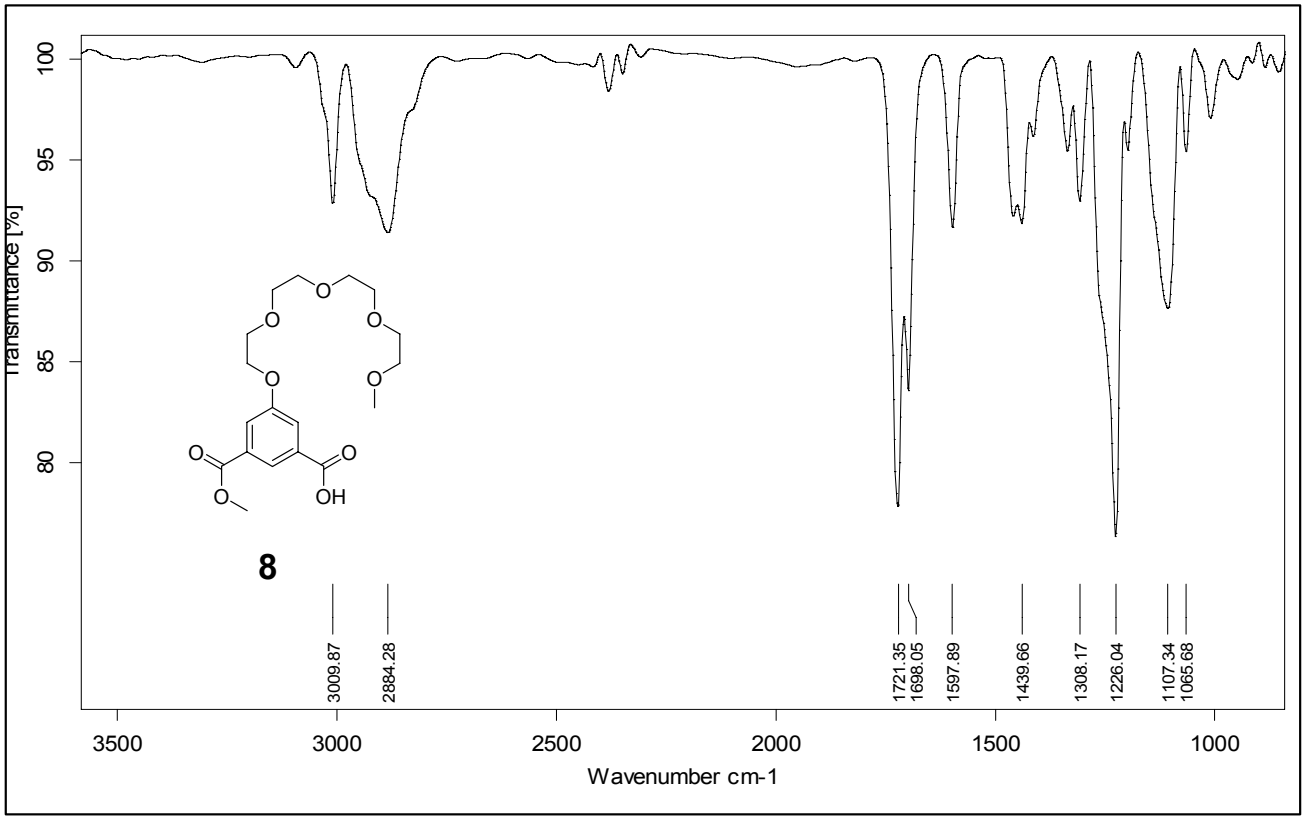


Figure S(31): IR Spectrum of compound **8** IN CH_2Cl_2

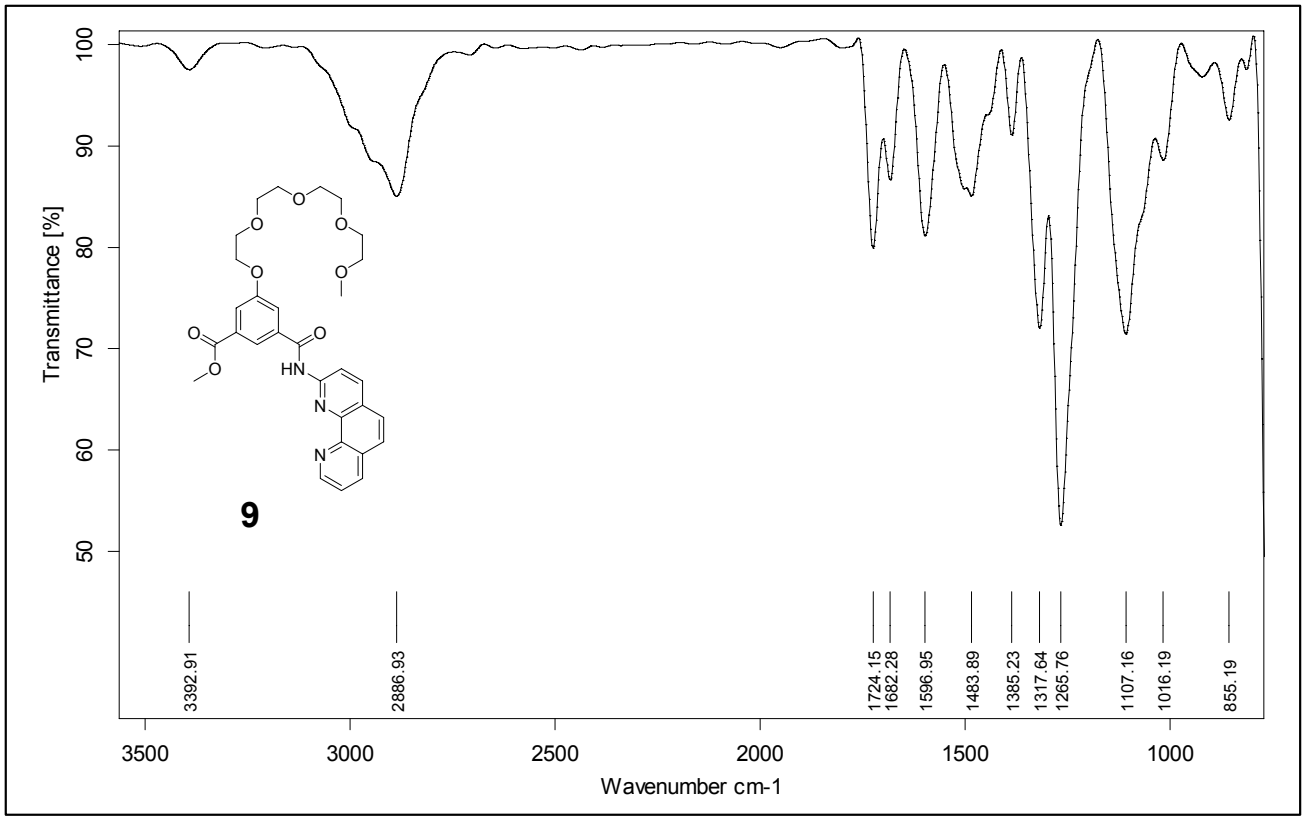


Figure S(32): IR Spectrum of compound **9** IN CH_2Cl_2

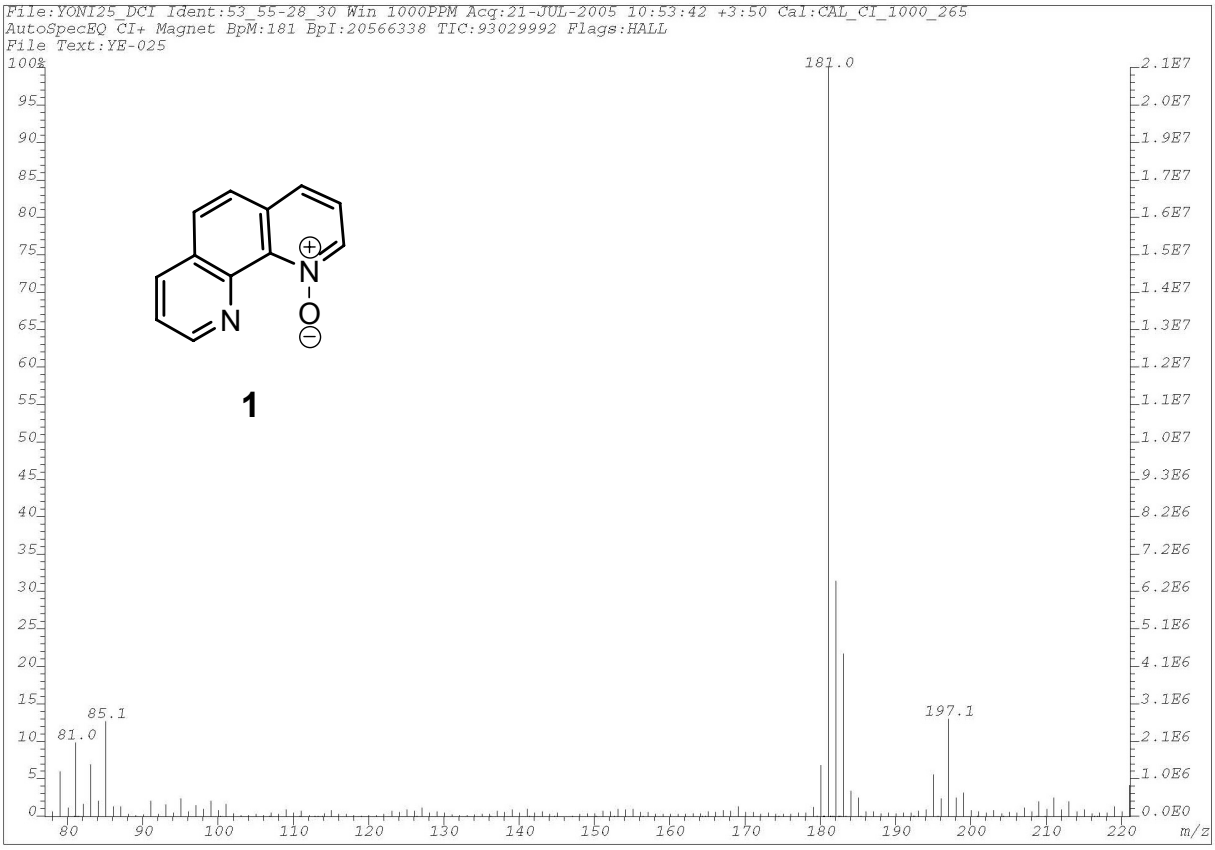


Figure S(33): CI-MS Spectrum of compound **1**.

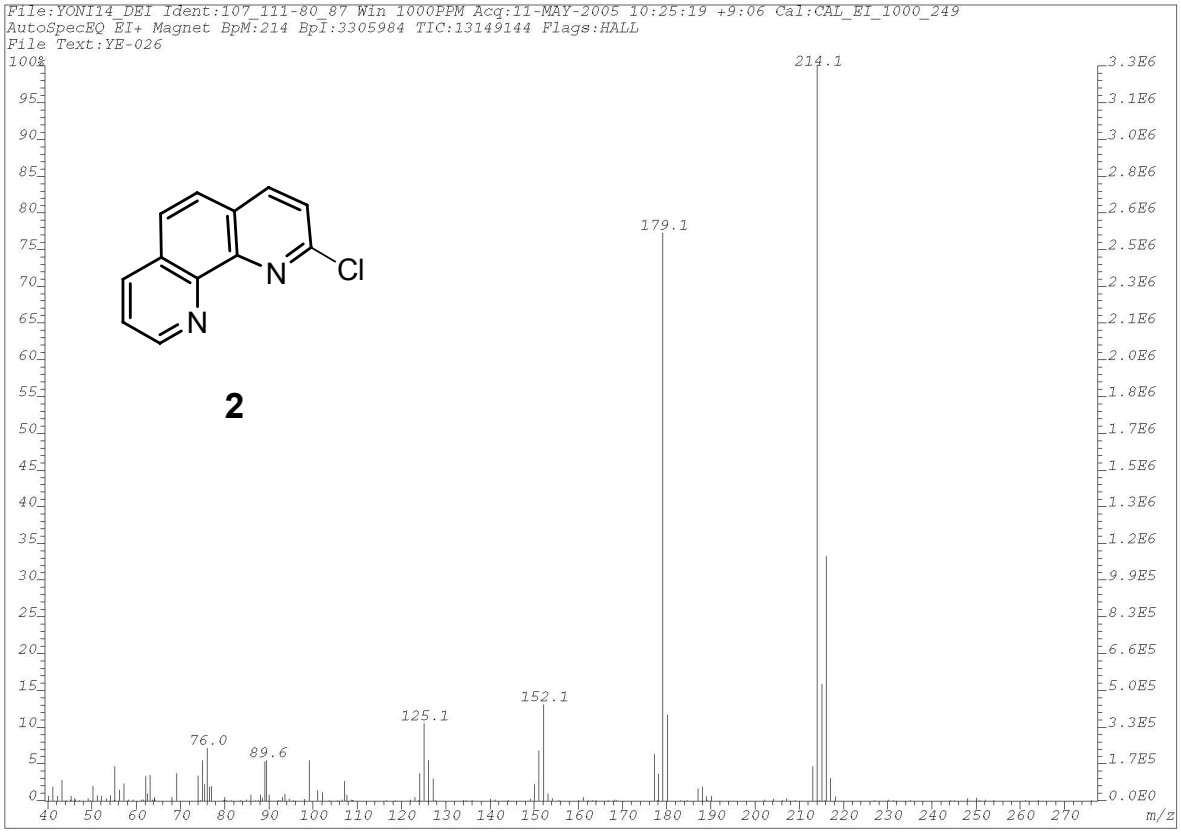


Figure S(34): EI-MS Spectrum of compound **2**.

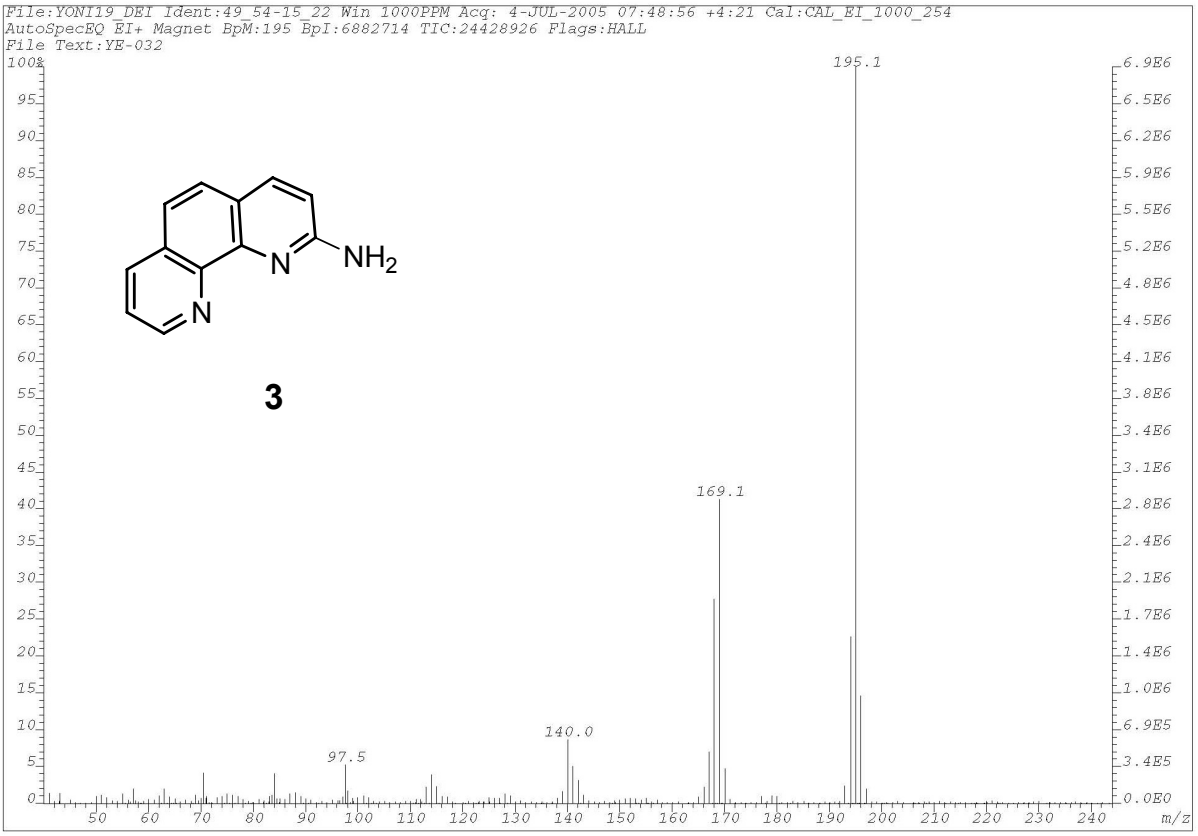


Figure S(35): EI-MS Spectrum of compound **3** .

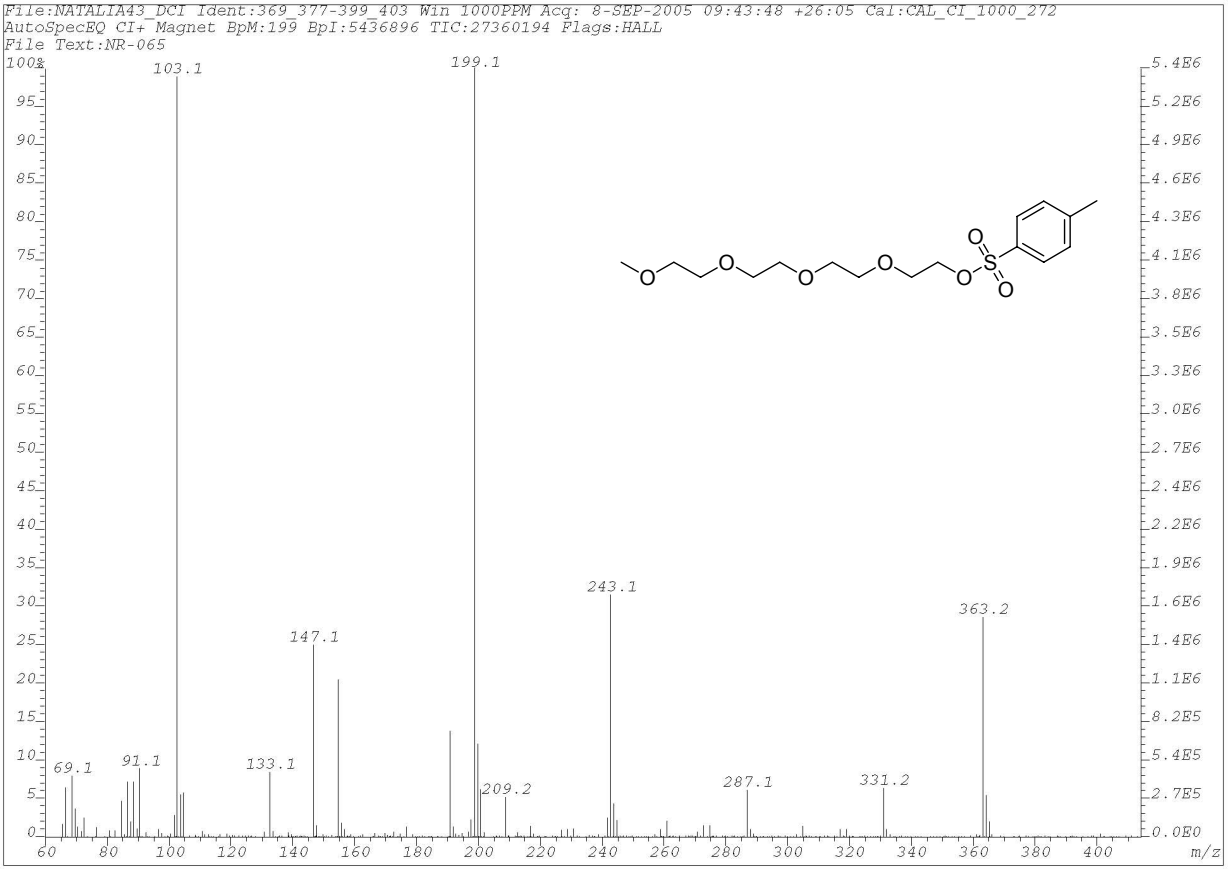


Figure S(36): CI-MS Spectrum of 2,5,8,11-tetraoxatridecan-13-yl-4-methylbenzenesulfonate.

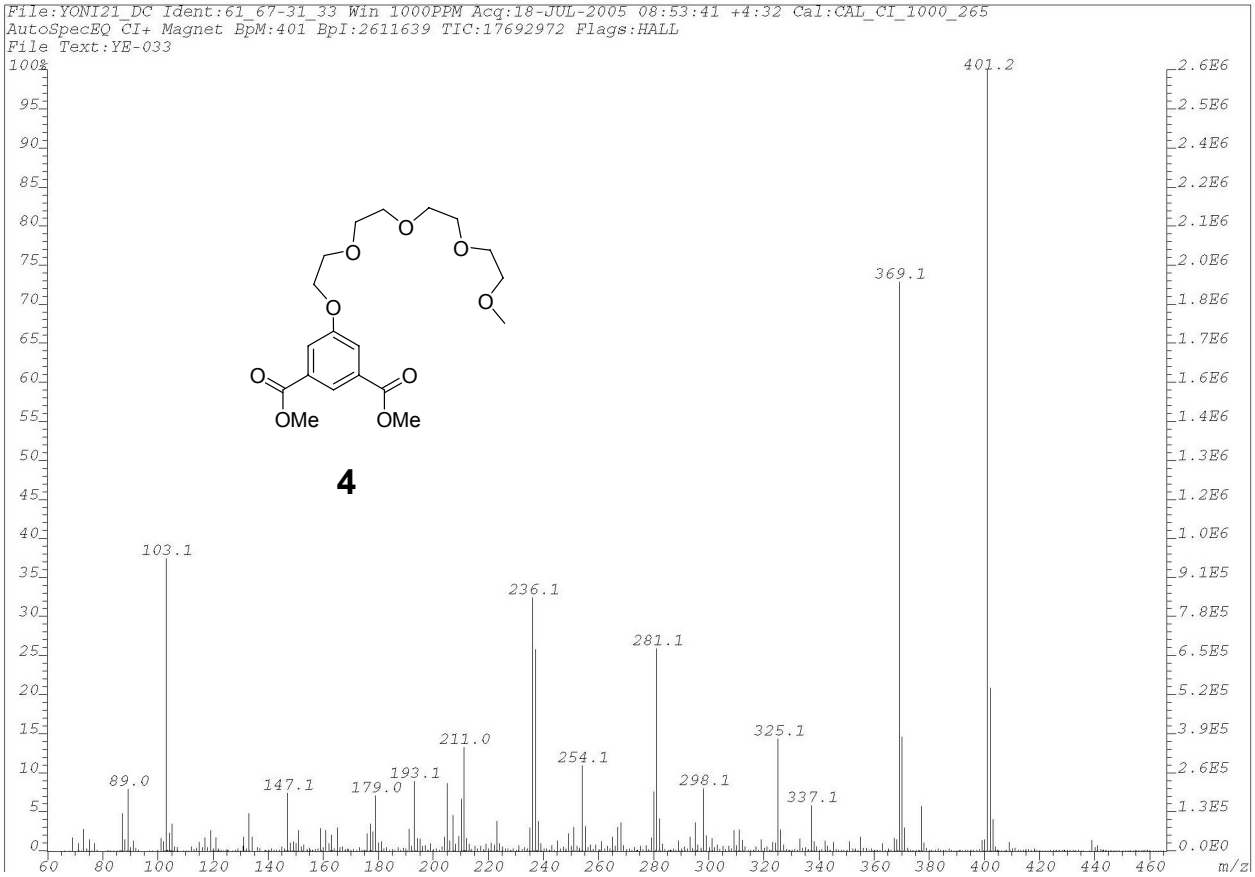


Figure S(37): CI-MS Spectrum of compound **4**.

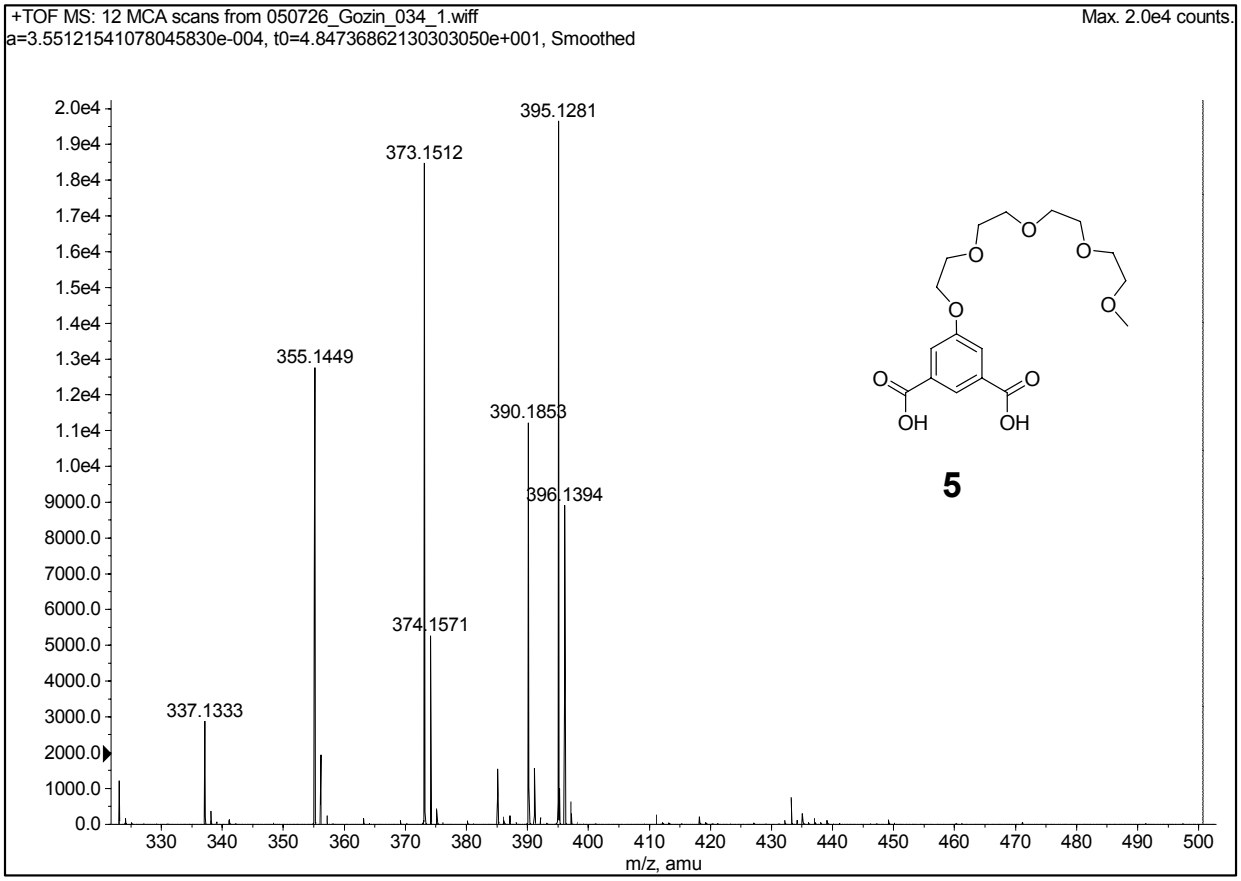


Figure S(38): MALDI-TOF HRMS Spectrum of compound **5**.

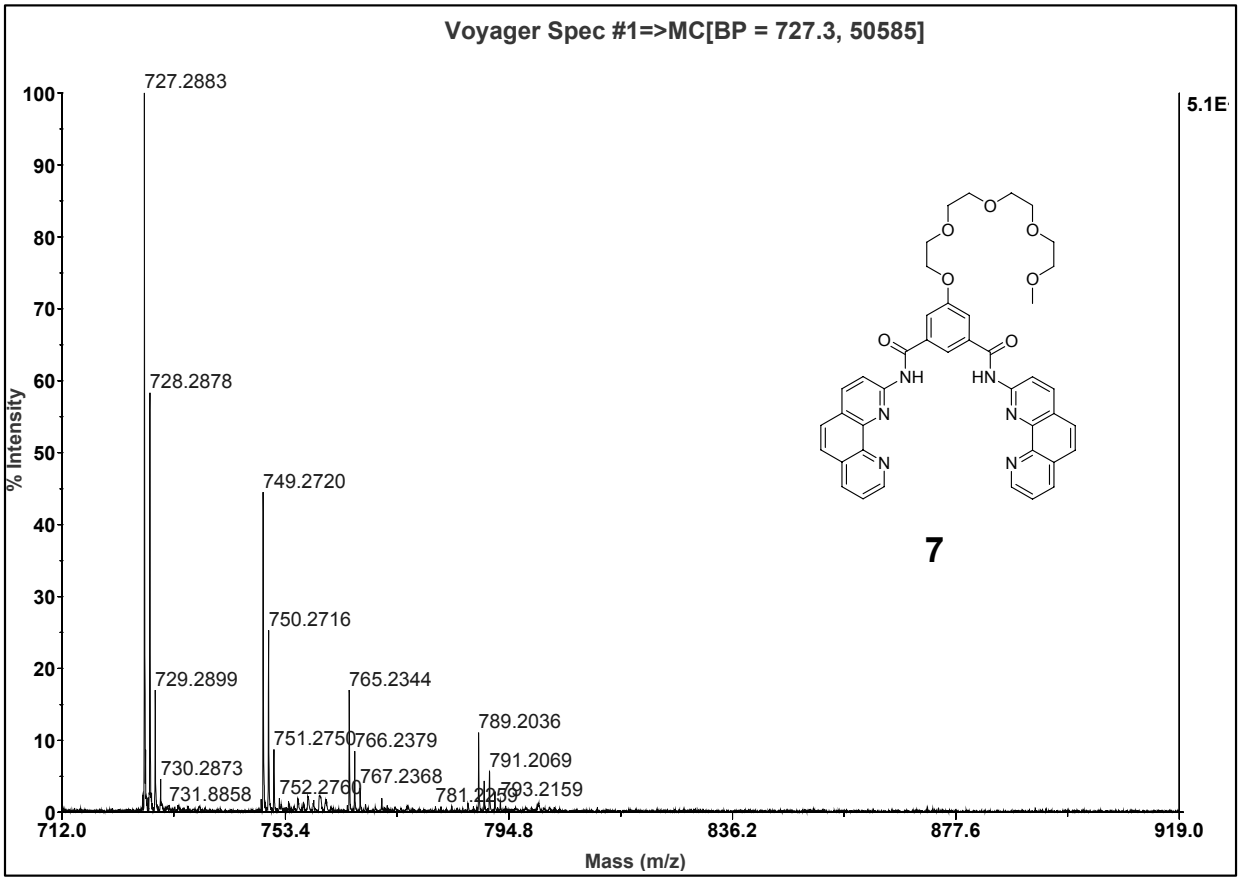


Figure S(39): MALDI-TOF HRMS Spectrum of compound **7**.

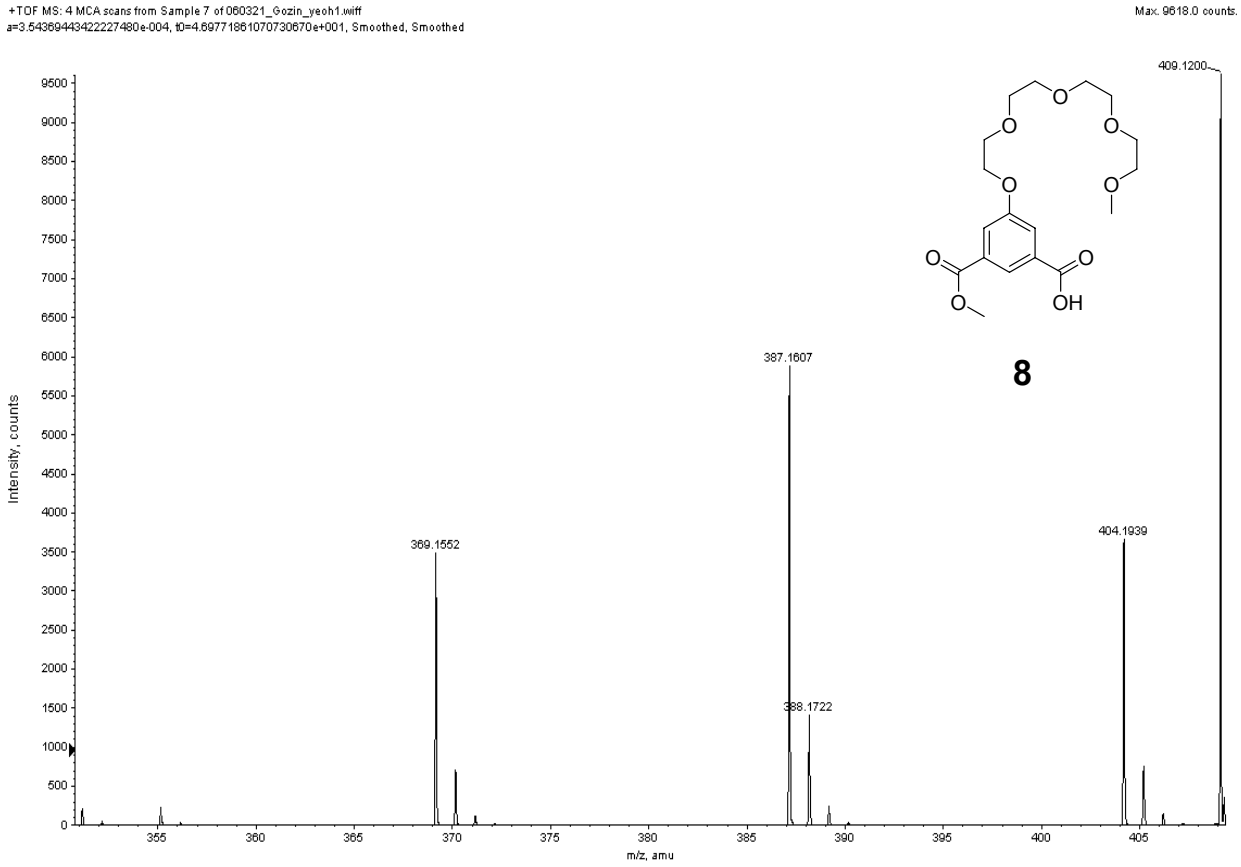


Figure S(40): MALDI-TOF HRMS Spectrum of compound **8**.

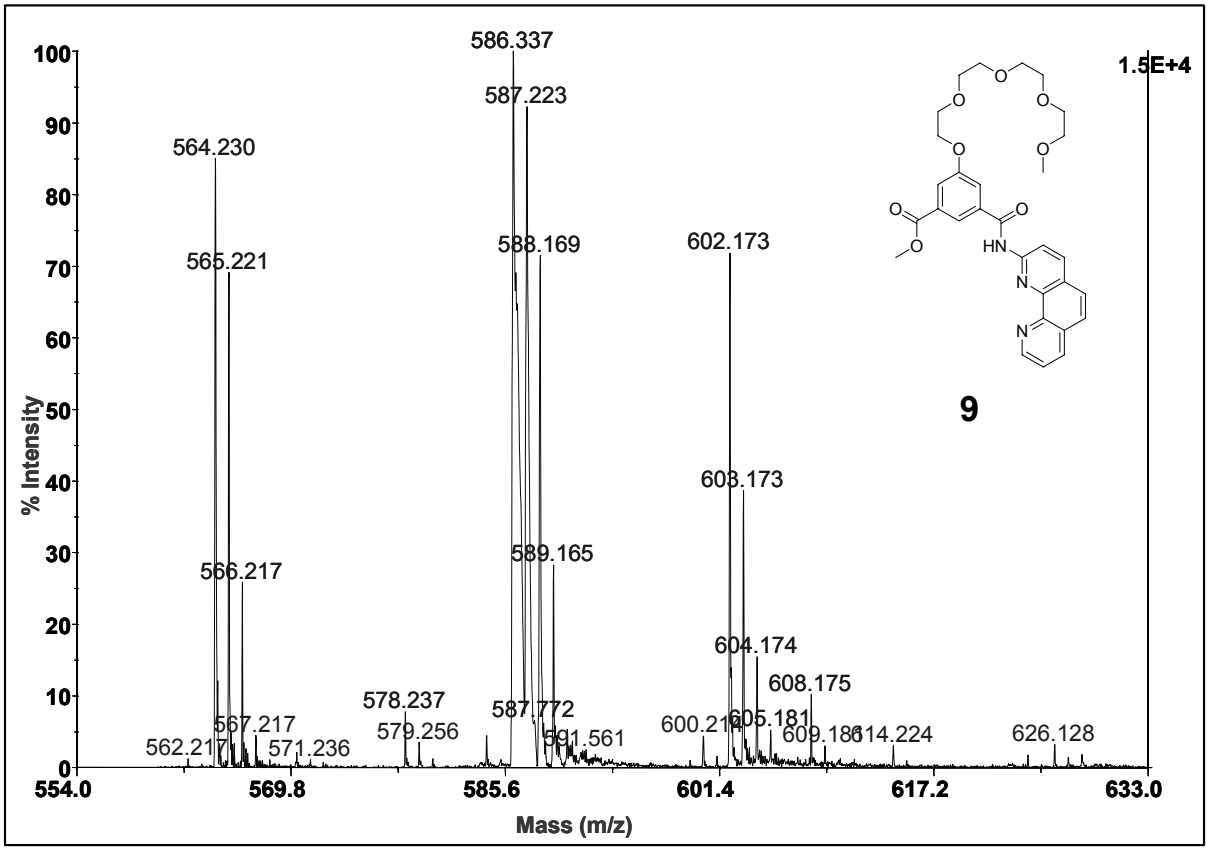


Figure S(41): MALDI-TOF HRMS Spectrum of compound **9.**

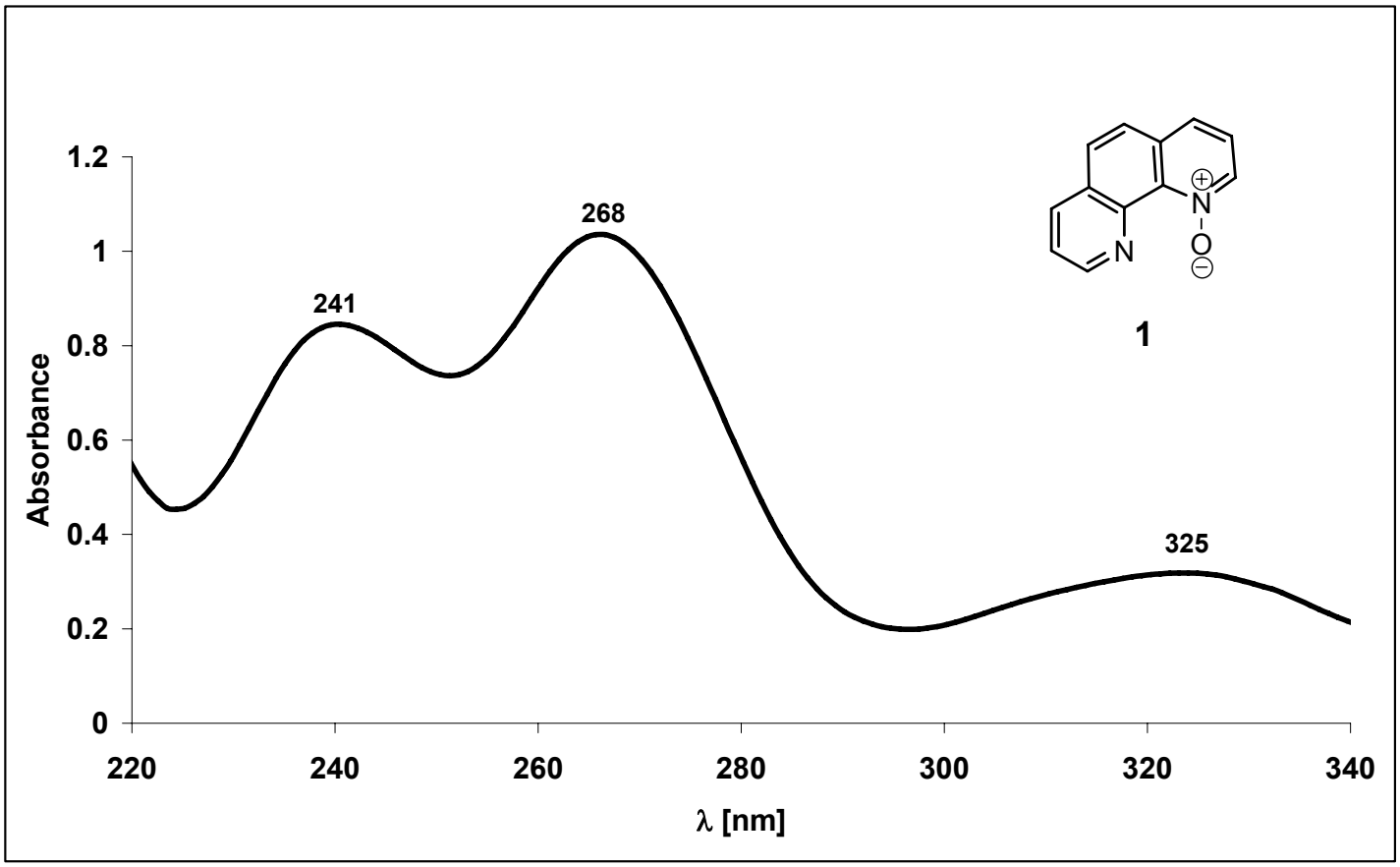


Figure S(42): UV-Vis Spectrum of compound **1** IN MeOH.

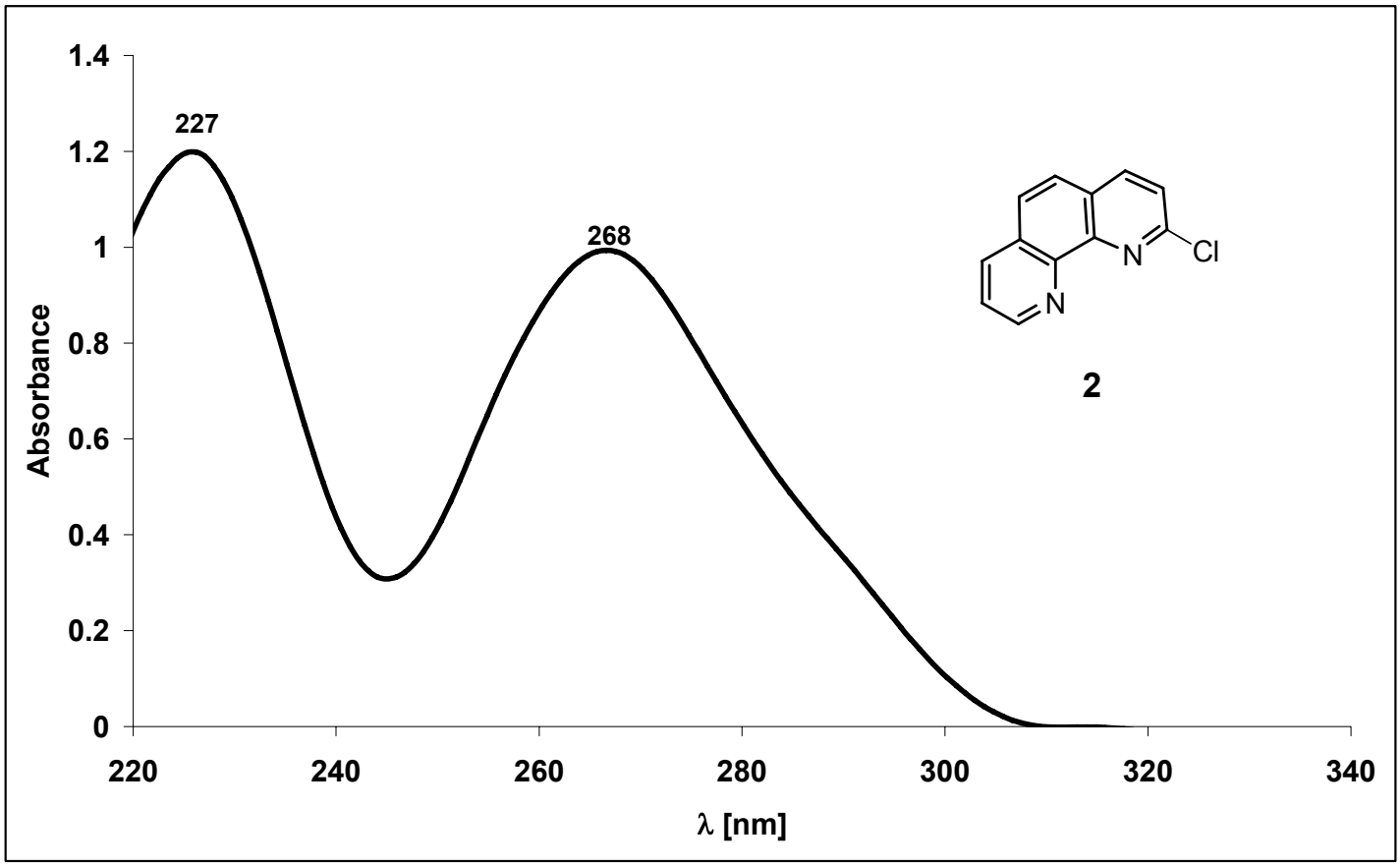


Figure S(43): UV-Vis Spectrum of compound **2** IN MeOH.

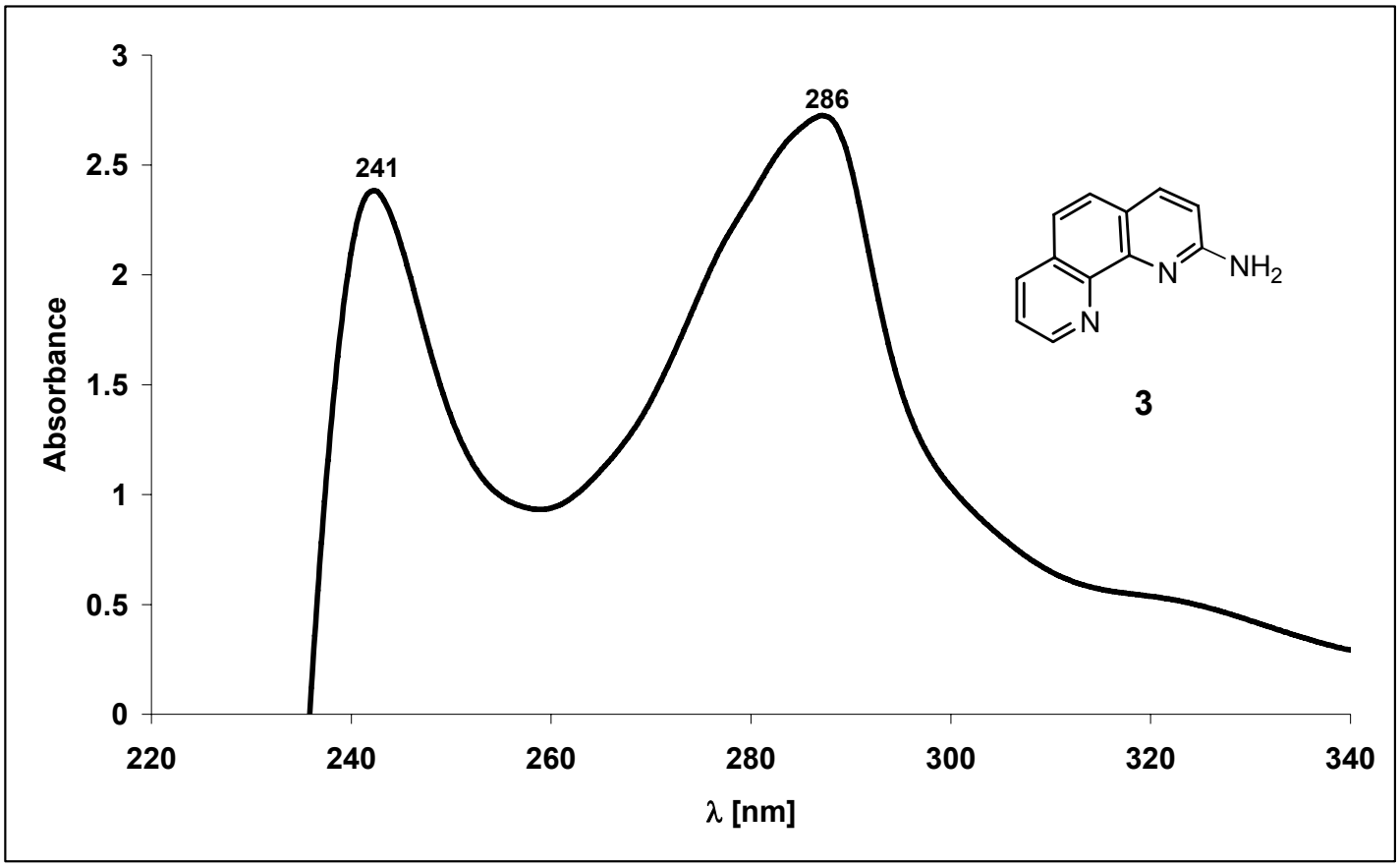


Figure S(44): UV-Vis Spectrum of compound **3** IN $CHCl_3$.

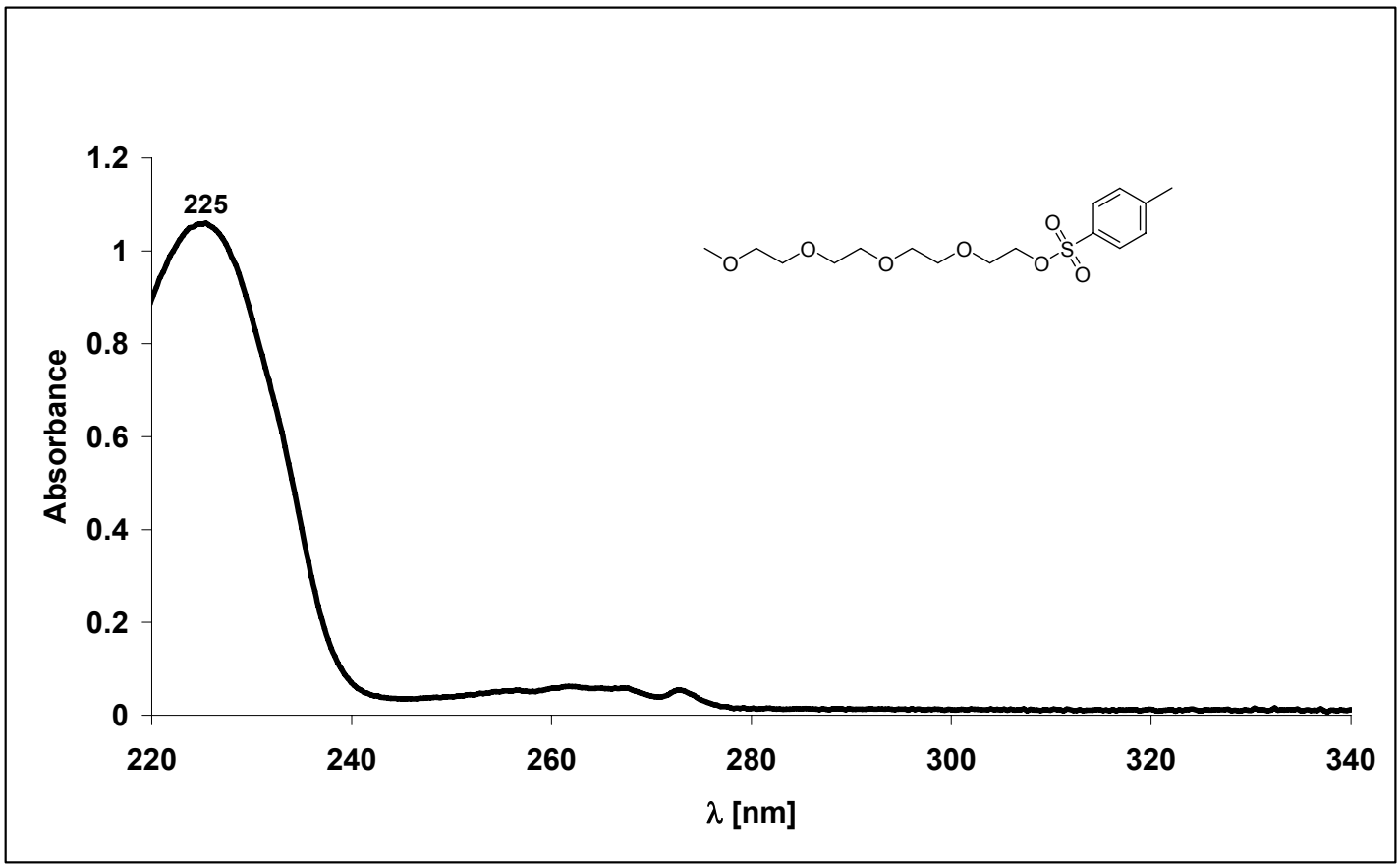


Figure S(45): UV-Vis Spectrum of compound 2,5,8,11-Tetraoxatridecan-13-yl-4-methylbenzenesulfonate IN CH_3CN.

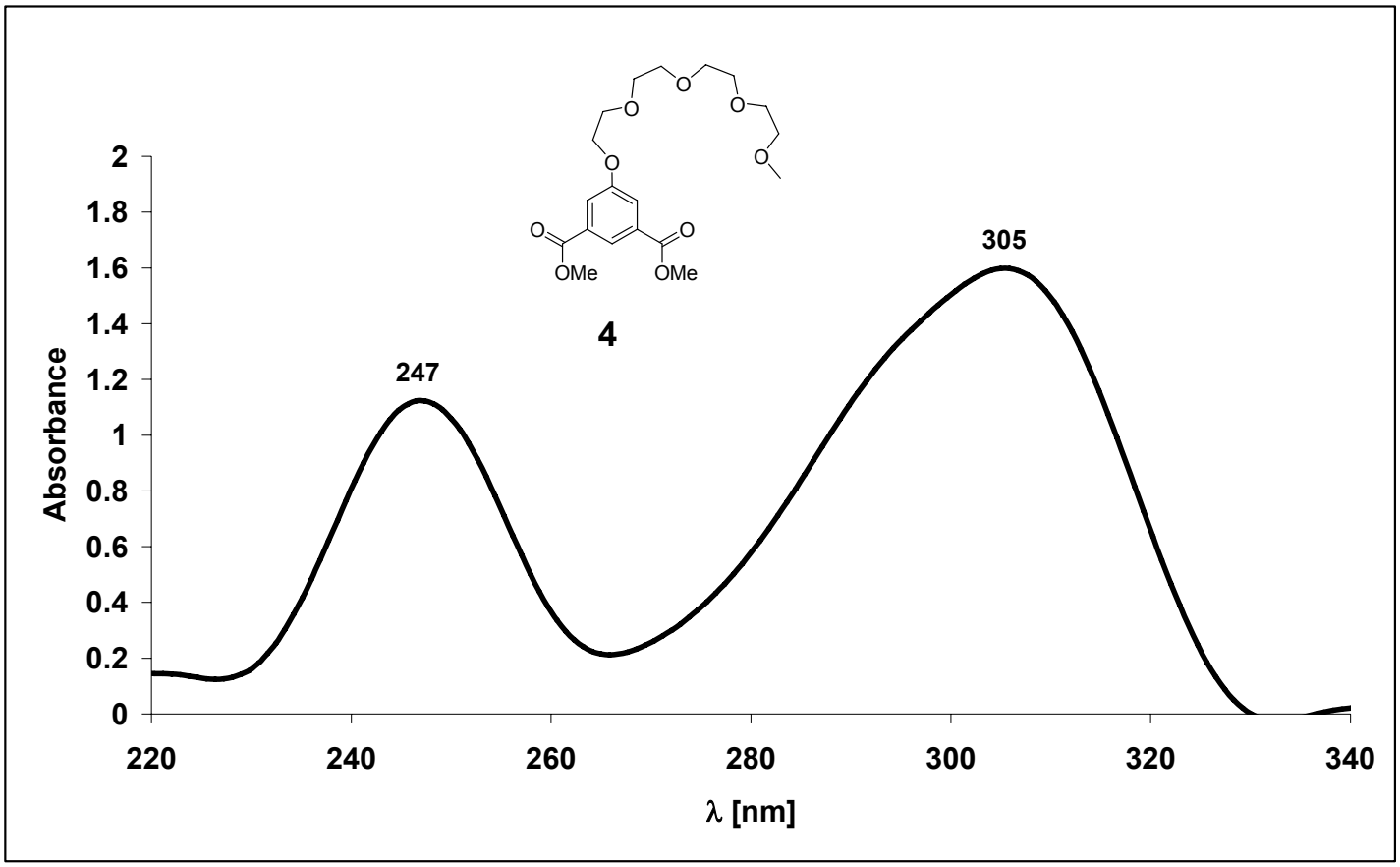


Figure S(46): UV-Vis Spectrum of compound **4** IN $CHCl_3$.

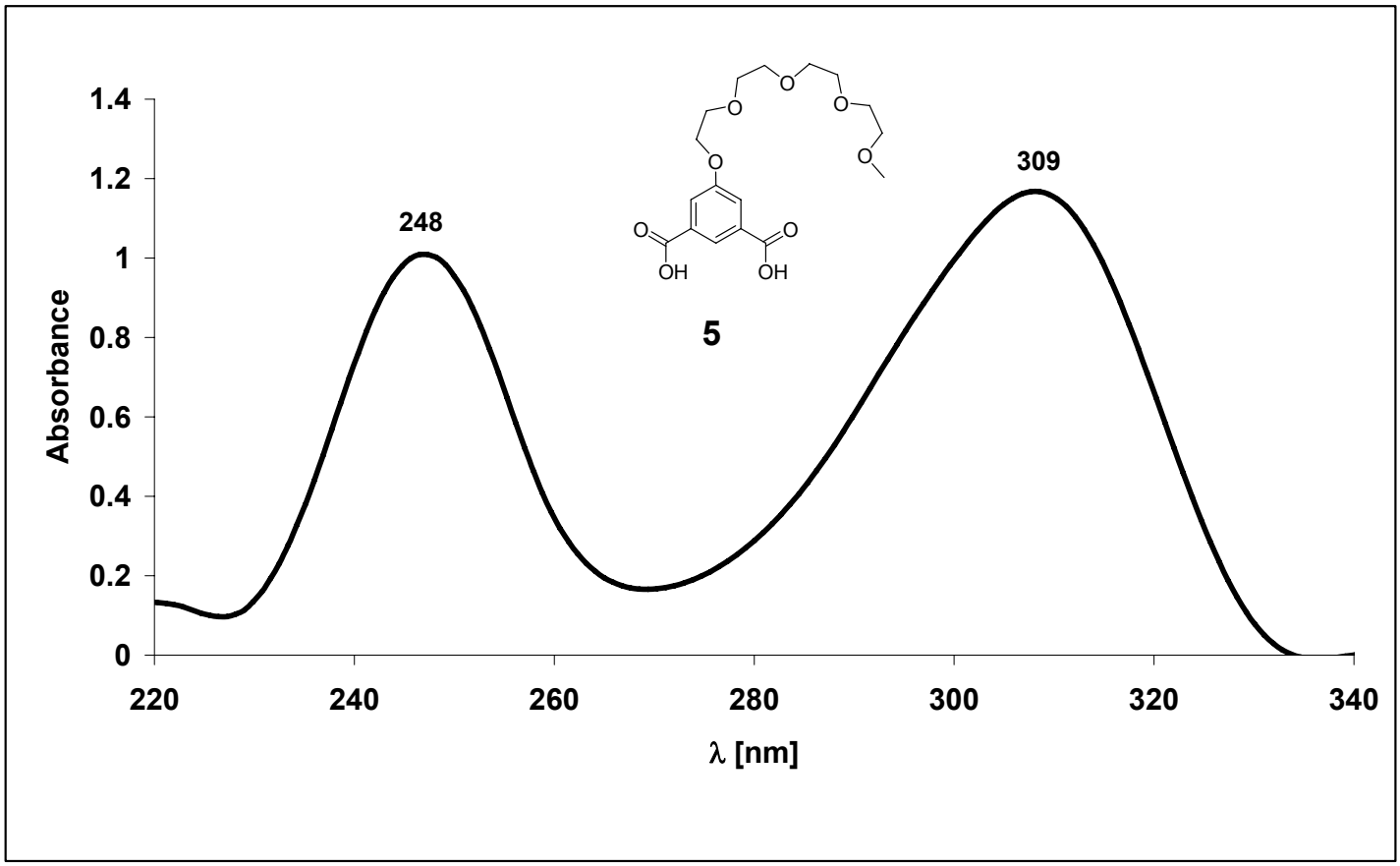


Figure S(47): UV-Vis Spectrum of compound **5** IN $CHCl_3$.

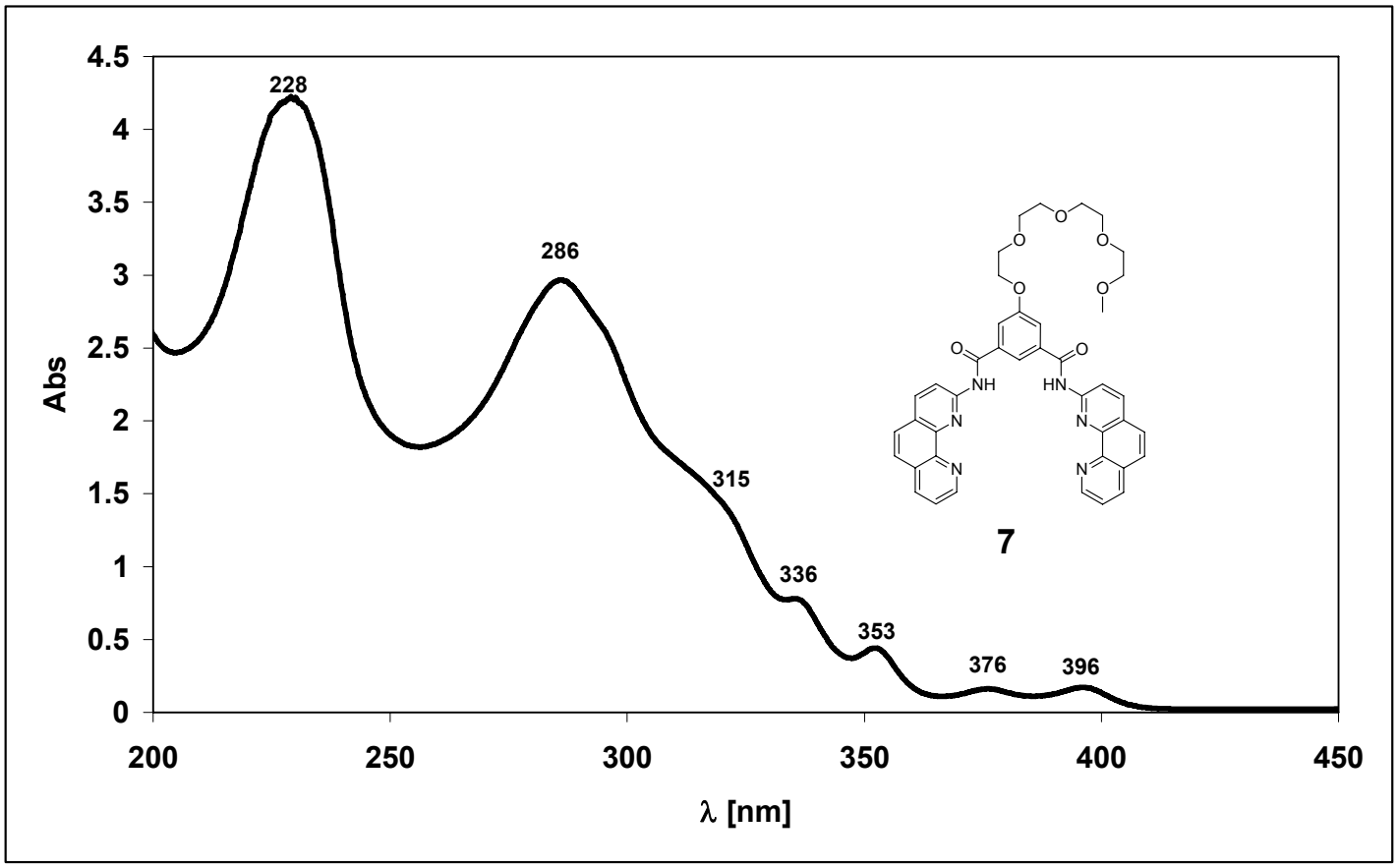


Figure S(48): UV-Vis Spectrum of compound **7** IN CH_3CN.

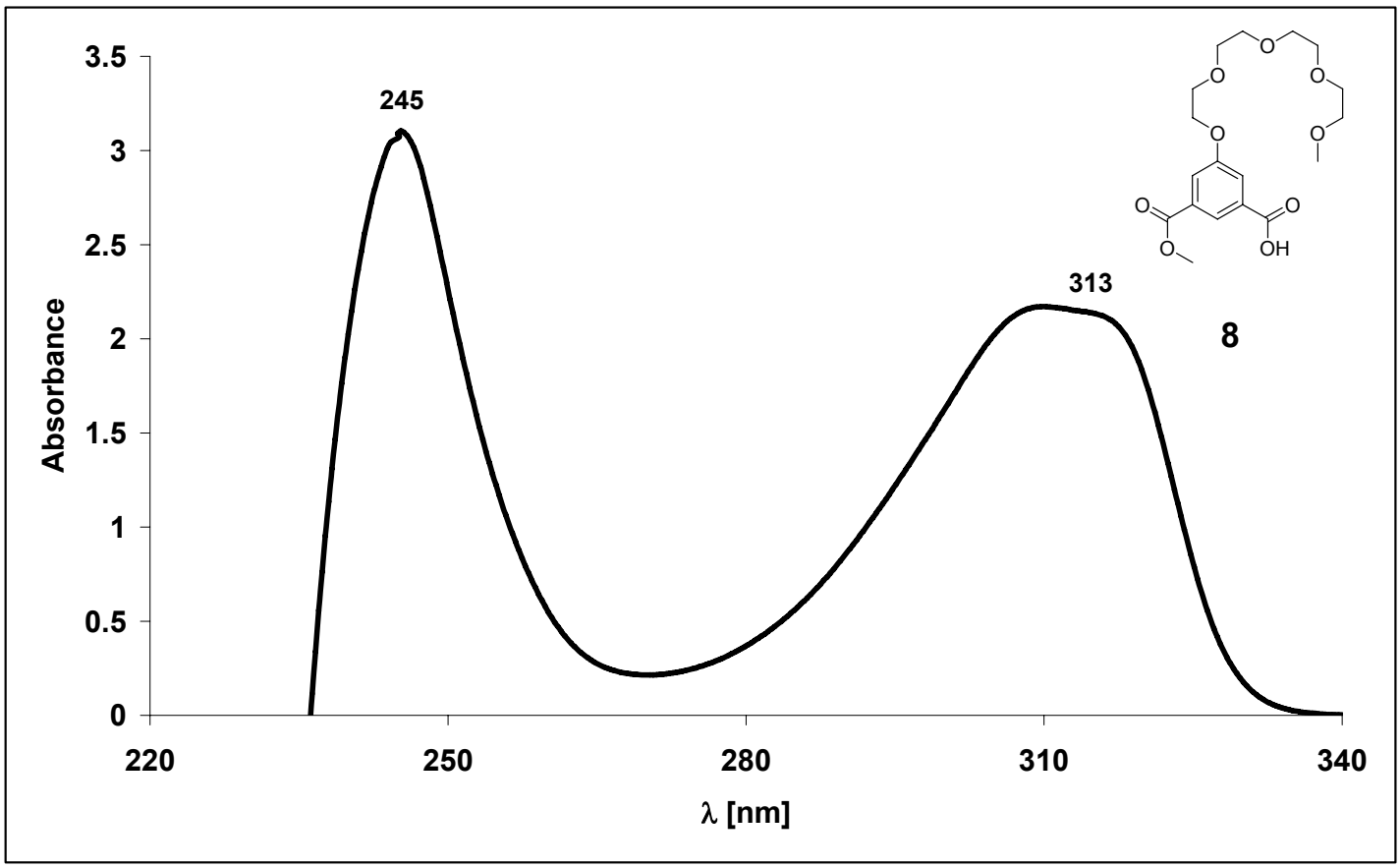


Figure S(49): UV-Vis Spectrum of compound **8** IN CH_3CN.

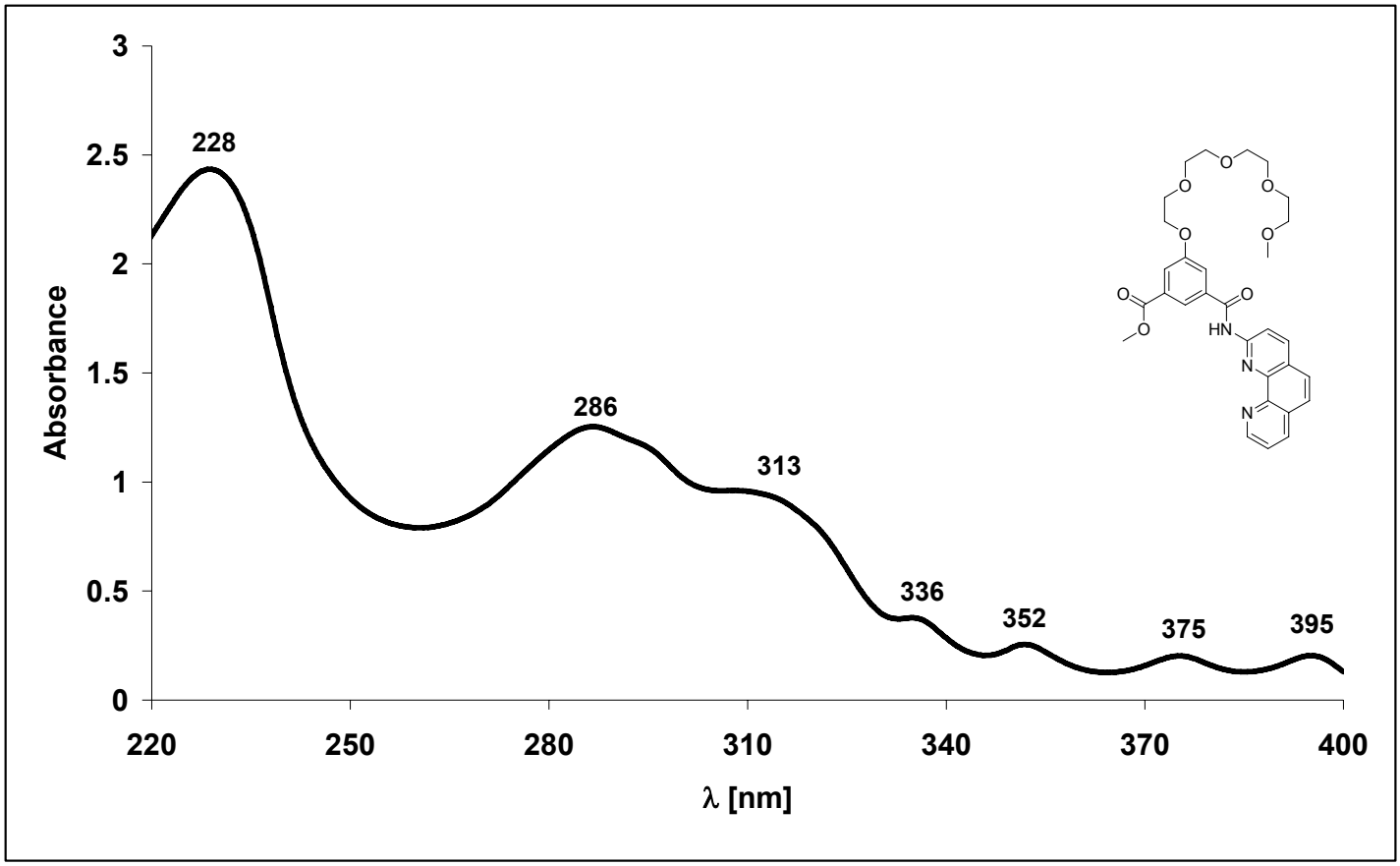


Figure S(50): UV-Vis Spectrum of compound **9** IN CH_3CN.

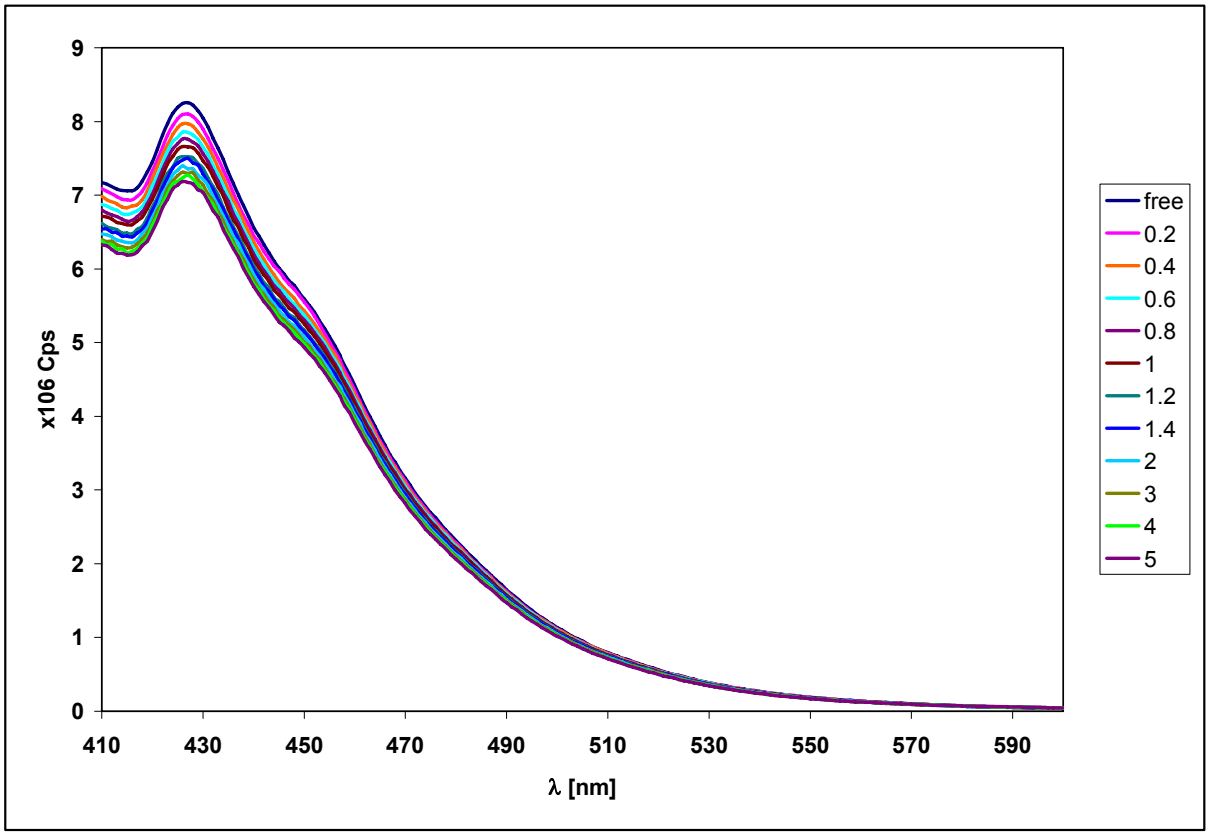


Figure S(51): Spectral changes observed during fluorescence titration of host **7** (at 5.22 × 10^{-5} M) with **Thiourea**.

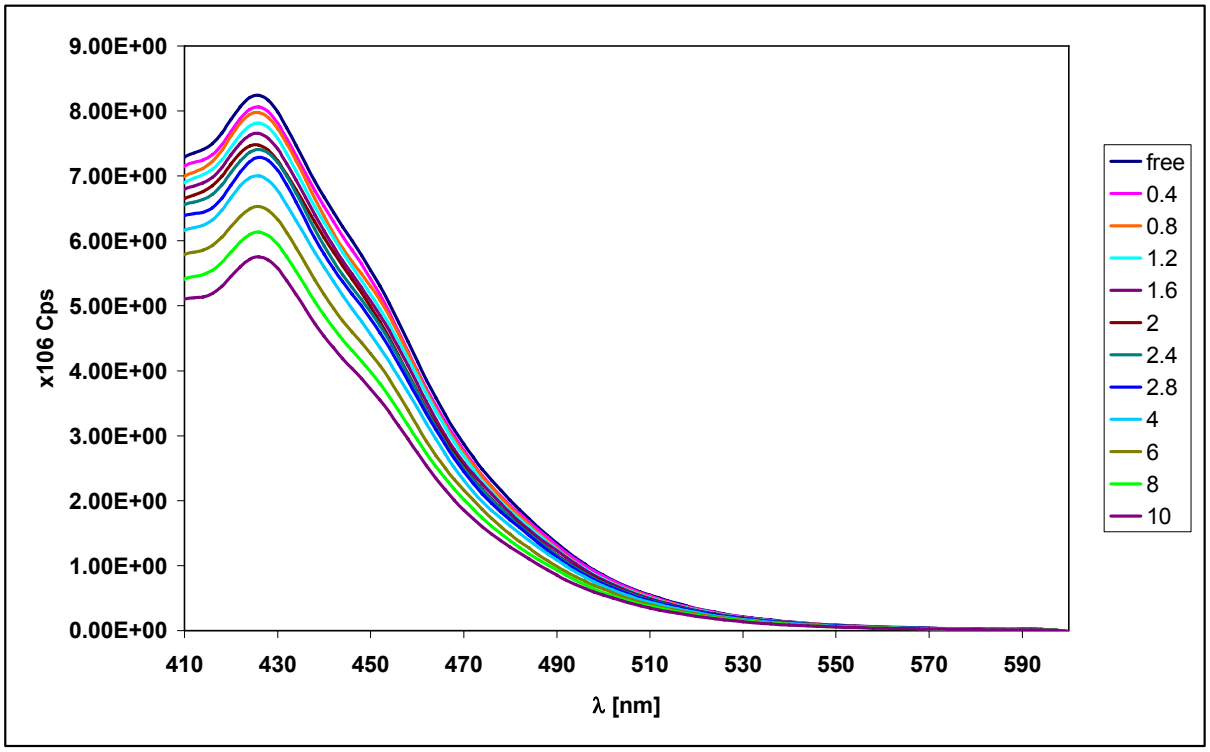


Figure S(52): Spectral changes observed during fluorescence titration of host **7** (at 5.22 × 10^{-5} M) with **2-imidazolidone.**

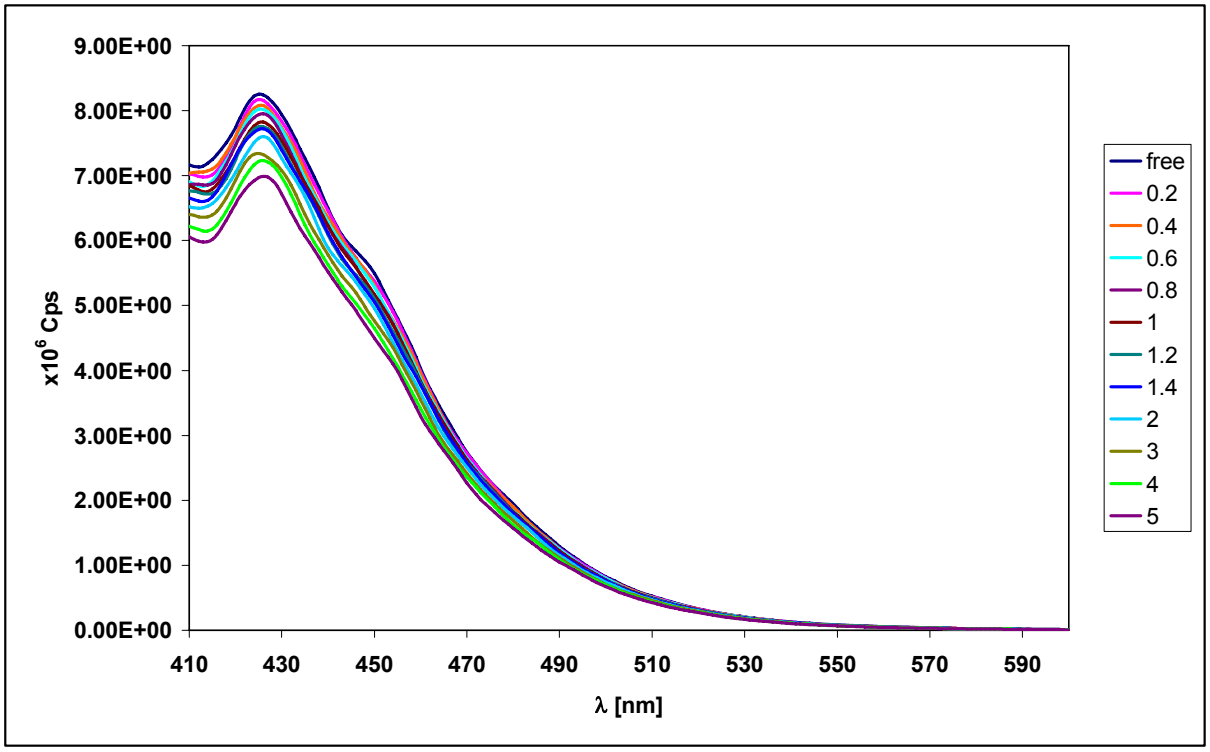


Figure S(53): Spectral changes observed during fluorescence titration of host **7** (at 5.22 × 10^{-5} M) with **tetrahydropyrimidin-2(*1H*)-one.**

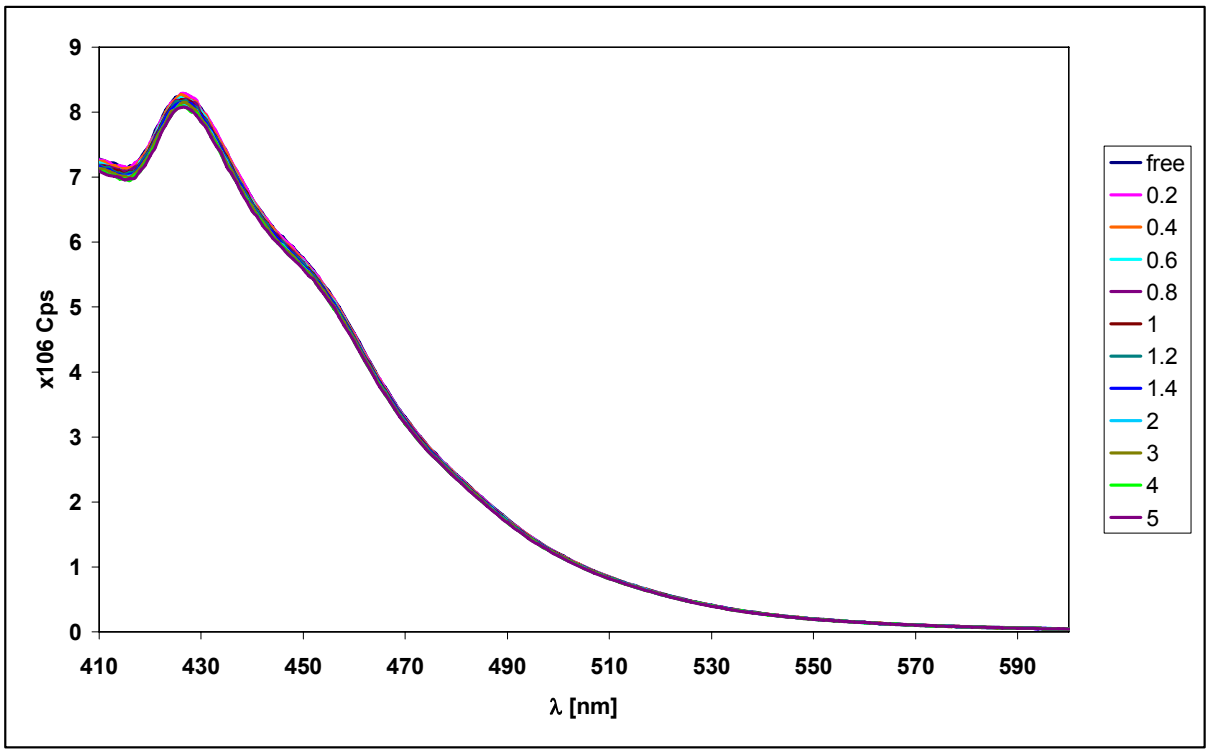


Figure S(54): Spectral changes observed during fluorescence titration of host **7** (at 5.22 × 10^{-5} M) with **1,3-dimethylurea.**

Figure S(54): Binding profiles associated with spectral changes observed during fluorescence titrations of various urea guests with host **7** (at 5.22×10^{-5} M).

Figure S(54A): Host **7** with 2-imidazolidone.

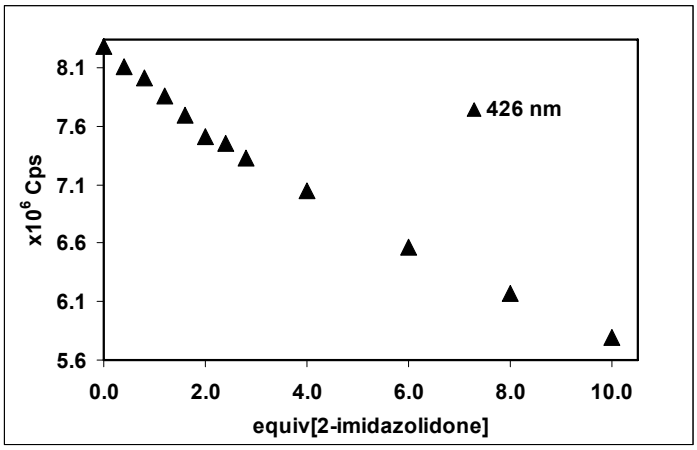


Fig S(54B): Host **7** with thiourea.

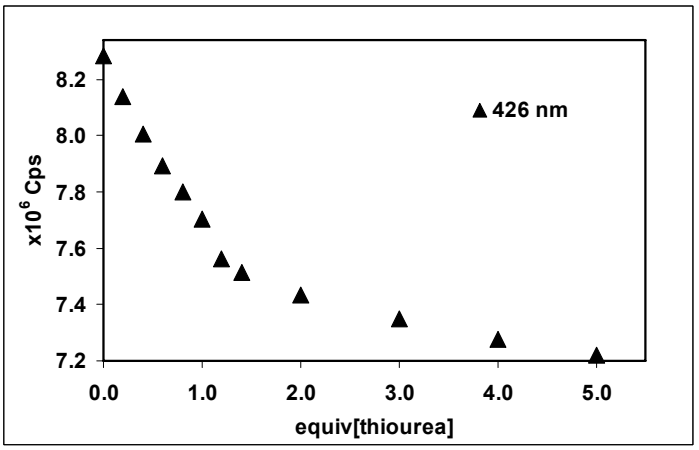
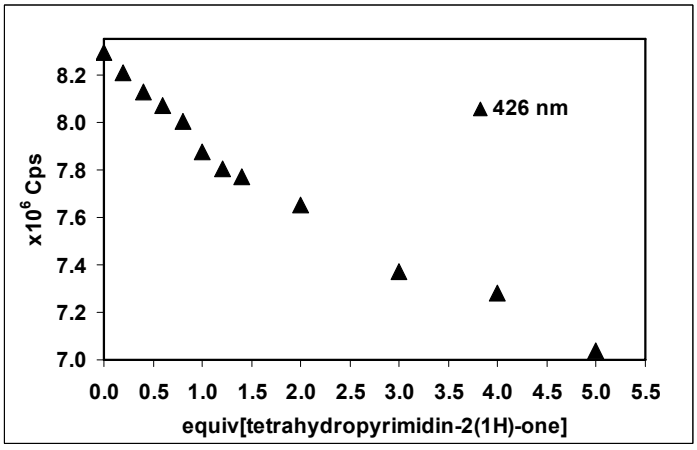


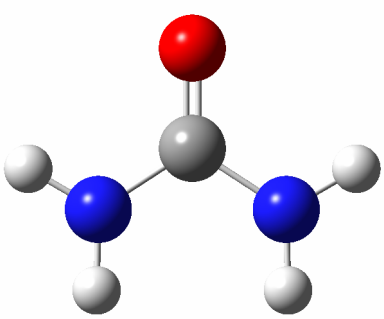
Fig S(54C): Host **7** with tetrahydropyrimidin-2(*1H*)-one.



DFT Calculations at the DFT B3LYP/ 3-21g level:**

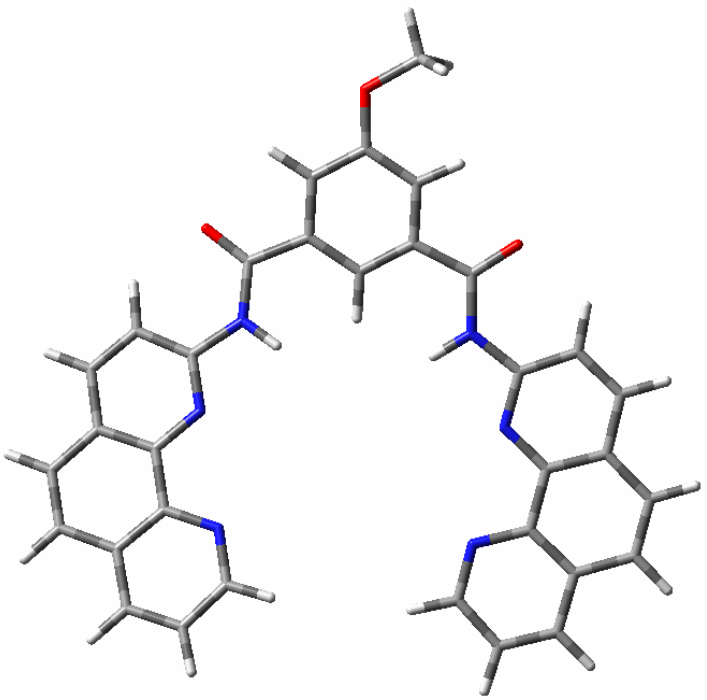
Urea: E= -224.043343459

1	C1	0.0000	0.1459	-0.0001 C
2	O2	0.0000	1.3850	0.0000 O
3	N3	1.1620	-0.6088	-0.0001 N
4	H4	2.0283	-0.1064	0.0001 H
5	H5	1.1832	-1.6100	0.0005 H
6	N6	-1.1620	-0.6088	0.0001 N
7	H7	-2.0283	-0.1064	0.0001 H
8	H8	-1.1832	-1.6100	-0.0004 H



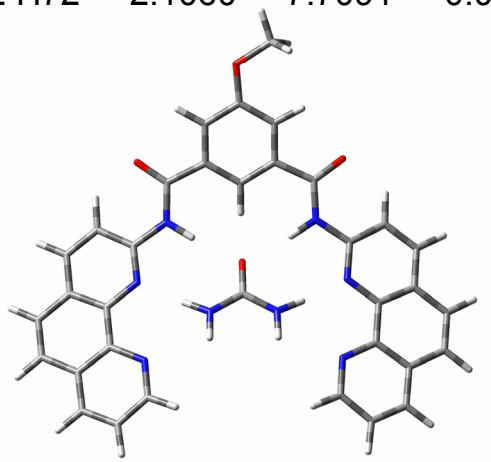
Chemosensor 7: E= -1815.06660222

1 O1	0.4049	7.0561	0.2587 O
2 C2	1.6978	7.7306	0.3875 C
3 C3	1.5398	4.8808	0.1862 C
4 C4	1.4312	3.4889	0.0748 C
5 C5	0.1781	2.8854	-0.0526 C
6 C6	-0.9701	3.6935	-0.0624 C
7 C7	-0.8567	5.0779	0.0309 C
8 C8	0.3995	5.6807	0.1633 C
9 C9	2.7498	2.7663	0.0914 C
10 C10	-2.3745	3.1797	-0.2074 C
11 O11	-3.3190	3.9549	-0.4513 O
12 C12	4.9294	-4.1517	-0.1897 C
13 C13	4.4983	-5.4975	-0.2637 C
14 C14	3.1463	-5.7805	-0.3096 C
15 C15	2.2312	-4.7063	-0.2808 C
16 N16	2.6035	-3.4277	-0.2107 N
17 C17	3.9310	-3.1379	-0.1651 C
18 C18	4.3456	-1.7487	-0.0890 C
19 C19	5.7343	-1.4467	-0.0429 C
20 C20	6.7077	-2.4991	-0.0709 C
21 C21	6.3215	-3.8039	-0.1413 C
22 N22	3.4039	-0.7776	-0.0643 N
23 C23	3.7833	0.4969	0.0060 C
24 C24	5.1389	0.9055	0.0586 C
25 C25	6.1011	-0.0810	0.0324 C
26 C26	-5.5715	-3.3282	0.1736 C
27 C27	-5.3692	-4.7013	0.4498 C
28 C28	-4.1116	-5.1484	0.8081 C
29 C29	-3.0600	-4.2105	0.8873 C
30 N30	-3.2158	-2.9108	0.6329 N
31 C31	-4.4487	-2.4601	0.2792 C
32 C32	-4.6276	-1.0466	0.0004 C
33 C33	-5.9184	-0.5750	-0.3638 C
34 C34	-7.0234	-1.4839	-0.4579 C
35 C35	-6.8579	-2.8117	-0.2003 C
36 N36	-3.5646	-0.2150	0.0932 N
37 C37	-3.7277	1.0820	-0.1607 C
38 C38	-4.9718	1.6558	-0.5229 C
39 C39	-6.0562	0.8109	-0.6218 C
40 N40	-2.5402	1.8217	-0.0362 N
41 H41	1.4582	8.7891	0.4437 H
42 H42	2.2206	7.4194	1.2949 H
43 H43	2.5372	5.2801	0.2782 H
44 H44	0.0881	1.8175	-0.1863 H
45 H45	-1.7495	5.6819	-0.0041 H
46 H46	5.2342	-6.2898	-0.2838 H
47 H47	2.7884	-6.7979	-0.3670 H
48 H48	1.1674	-4.9016	-0.3177 H
49 H49	7.7557	-2.2342	-0.0344 H
50 H50	7.0549	-4.5984	-0.1623 H
51 H51	5.3611	1.9563	0.1181 H
52 H52	7.1489	0.1846	0.0704 H
53 H53	-6.2038	-5.3855	0.3775 H
54 H54	-3.9282	-6.1904	1.0256 H
55 H55	-2.0664	-4.5354	1.1678 H
56 H56	-7.9917	-1.0920	-0.7385 H
57 H57	-7.6908	-3.4978	-0.2717 H
58 H58	-5.0218	2.7163	-0.6971 H
59 H59	-7.0253	1.2047	-0.8965 H
60 H60	-1.7748	1.2368	0.2602 H
61 O61	3.8203	3.4035	0.1683 O
62 N62	2.7009	1.3929	0.0216 N
63 H63	1.8228	0.9000	-0.0182 H
64 H64	2.3346	7.5393	-0.4793 H



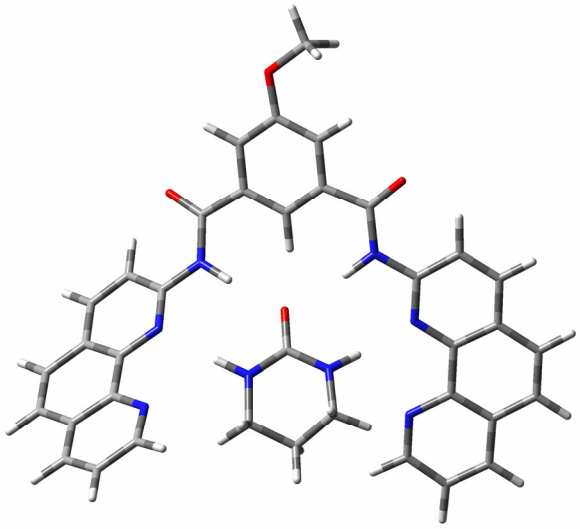
Complex 10: E= -2039.18990330

1	O1	0.2301	7.0699	0.6652 O
2	C2	1.5049	7.7674	0.8185 C
3	C3	1.4330	4.9617	0.2696 C
4	C4	1.3552	3.5895	-0.0072 C
5	C5	0.1238	2.9670	-0.1882 C
6	C6	-1.0440	3.7192	-0.0249 C
7	C7	-0.9759	5.0840	0.2498 C
8	C8	0.2663	5.7127	0.3955 C
9	C9	2.6686	2.8843	-0.1151 C
10	C10	-2.4204	3.1499	-0.1569 C
11	O11	-3.3991	3.9153	-0.2708 O
12	C12	5.5258	-3.8181	-0.2431 C
13	C13	5.3137	-5.2022	-0.0393 C
14	C14	4.0752	-5.6554	0.3699 C
15	C15	3.0552	-4.7068	0.5801 C
16	N16	3.2218	-3.3958	0.3997 N
17	C17	4.4313	-2.9320	-0.0152 C
18	C18	4.6202	-1.5048	-0.2346 C
19	C19	5.9054	-1.0583	-0.6414 C
20	C20	6.9805	-1.9802	-0.8494 C
21	C21	6.8004	-3.3165	-0.6632 C
22	N22	3.5844	-0.6400	-0.0510 N
23	C23	3.7682	0.6739	-0.2559 C
24	C24	5.0373	1.2020	-0.6341 C
25	C25	6.0805	0.3331	-0.8269 C
26	C26	-5.9594	-3.2211	-0.1785 C
27	C27	-5.9052	-4.6105	0.0833 C
28	C28	-4.7367	-5.1775	0.5517 C
29	C29	-3.6263	-4.3363	0.7604 C
30	N30	-3.6431	-3.0235	0.5247 N
31	C31	-4.7823	-2.4485	0.0531 C
32	C32	-4.8106	-1.0183	-0.2218 C
33	C33	-6.0296	-0.4540	-0.6832 C
34	C34	-7.1904	-1.2640	-0.8954 C
35	C35	-7.1599	-2.6038	-0.6583 C
36	N36	-3.6945	-0.2602	-0.0352 N
37	C37	-3.7338	1.0584	-0.2852 C
38	C38	-4.9300	1.7028	-0.7173 C
39	C39	-6.0523	0.9409	-0.9168 C
40	N40	-2.5336	1.7598	-0.1147 N
41	H41	1.2389	8.8025	1.0181 H
42	H42	2.0835	7.3667	1.6547 H
43	H43	2.4182	5.3879	0.3697 H
44	H44	0.0707	1.9290	-0.4572 H
45	H45	-1.8863	5.6538	0.3462 H
46	H46	6.1301	-5.8909	-0.2084 H
47	H47	3.8841	-6.7060	0.5305 H
48	H48	2.0764	-5.0353	0.9056 H
49	H49	7.9390	-1.5883	-1.1616 H
50	H50	7.6080	-4.0169	-0.8244 H
51	H51	5.1340	2.2669	-0.7363 H
52	H52	7.0503	0.7097	-1.1224 H
53	H53	-6.7867	-5.2133	-0.0879 H
54	H54	-4.6662	-6.2349	0.7588 H
55	H55	-2.6997	-4.7548	1.1322 H
56	H56	-8.0921	-0.7846	-1.2515 H
57	H57	-8.0328	-3.2204	-0.8216 H
58	H58	-4.9132	2.7683	-0.8523 H
59	H59	-6.9687	1.4061	-1.2537 H
60	H60	-1.7032	1.1844	0.0871 H
61	O61	3.7222	3.5512	-0.1916 O
62	N62	2.6421	1.4909	-0.0941 N
63	H63	1.7541	0.9995	0.0861 H
64	C64	-0.0804	-0.9429	0.8397 C
65	O65	-0.0186	0.2188	0.2914 O
66	N66	1.0483	-1.6268	1.1373 N
67	H67	1.0238	-2.5789	1.4464 H
68	H68	1.9407	-1.3259	0.7457 H
69	N69	-1.2747	-1.4923	1.1576 N
70	H70	-1.3565	-2.4411	1.4666 H
71	H71	-2.1337	-1.0917	0.7806 H
72	H72	2.1060	7.7091	-0.0924 H



Complex of 7 with tetrahydropyrimidin-2(*1H*)-one : E= -2155.28805069

1	O1	0.1496	7.1335	0.5420 O
2	C2	1.3218	7.8451	1.0462 C
3	C3	1.4147	5.0250	0.5740 C
4	C4	1.4245	3.6474	0.3126 C
5	C5	0.2931	3.0074	-0.1848 C
6	C6	-0.8687	3.7561	-0.3909 C
7	C7	-0.8810	5.1298	-0.1607 C
8	C8	0.2631	5.7704	0.3315 C
9	C9	2.7256	2.9576	0.5575 C
10	C10	-2.1490	3.1608	-0.8806 C
11	O11	-3.0337	3.8912	-1.3699 O
12	C12	5.7284	-3.4901	-0.9165 C
13	C13	5.5000	-4.8174	-1.3509 C
14	C14	4.2064	-5.2828	-1.4868 C
15	C15	3.1441	-4.4134	-1.1664 C
16	N16	3.3252	-3.1585	-0.7472 N
17	C17	4.5924	-2.6783	-0.6323 C
18	C18	4.7937	-1.2958	-0.2311 C
19	C19	6.1255	-0.8182	-0.1155 C
20	C20	7.2419	-1.6755	-0.3790 C
21	C21	7.0548	-2.9662	-0.7714 C
22	N22	3.7187	-0.4934	-0.0098 N
23	C23	3.9074	0.8006	0.2856 C
24	C24	5.2107	1.3510	0.4557 C
25	C25	6.2972	0.5361	0.2574 C
26	C26	-6.4550	-2.5002	0.2043 C
27	C27	-6.7639	-3.5714	1.0748 C
28	C28	-5.8669	-3.9365	2.0595 C
29	C29	-4.6493	-3.2338	2.1474 C
30	N30	-4.3186	-2.2294	1.3314 N
31	C31	-5.2026	-1.8389	0.3744 C
32	C32	-4.8879	-0.6926	-0.4639 C
33	C33	-5.8634	-0.2699	-1.4061 C
34	C34	-7.0900	-0.9884	-1.5768 C
35	C35	-7.3790	-2.0703	-0.8030 C
36	N36	-3.7136	-0.0251	-0.2895 N
37	C37	-3.5022	1.1125	-0.9673 C
38	C38	-4.4414	1.6192	-1.9110 C
39	C39	-5.5938	0.9109	-2.1370 C
40	N40	-2.3069	1.7900	-0.6922 N
41	H41	1.0084	8.8828	1.1299 H
42	H42	1.6272	7.4713	2.0269 H
43	H43	2.3276	5.4600	0.9477 H
44	H44	0.3030	1.9588	-0.4208 H
45	H45	-1.7768	5.6964	-0.3596 H
46	H46	6.3462	-5.4522	-1.5757 H
47	H47	4.0029	-6.2882	-1.8242 H
48	H48	2.1212	-4.7556	-1.2470 H
49	H49	8.2382	-1.2690	-0.2701 H
50	H50	7.8954	-3.6119	-0.9845 H
51	H51	5.2915	2.3868	0.7303 H
52	H52	7.2973	0.9303	0.3767 H
53	H53	-7.7084	-4.0862	0.9631 H
54	H54	-6.0816	-4.7409	2.7473 H
55	H55	-3.9203	-3.5083	2.8976 H
56	H56	-7.7888	-0.6395	-2.3249 H
57	H57	-8.3104	-2.6071	-0.9184 H
58	H58	-4.2357	2.5588	-2.3888 H
59	H59	-6.3157	1.2635	-2.8609 H
60	H60	-1.5665	1.2234	-0.2551 H
61	O61	3.7324	3.6208	0.8828 O
62	N62	2.7472	1.5761	0.3762 N
63	H63	1.8680	1.0615	0.2632 H
64	H64	2.1656	7.7684	0.3559 H
65	O65	-0.0103	0.1880	0.1331 O
66	C66	-0.0472	-0.9888	0.6454 C
67	N67	1.1090	-1.6472	0.9294 N
68	N68	-1.2275	-1.6045	0.9204 N
69	C69	1.1295	-2.9584	1.5970 C
70	H70	1.9681	-1.3195	0.4874 H
71	C71	-1.3497	-3.0084	1.3692 C
72	H72	-2.0937	-1.1043	0.7309 H
73	C73	-0.0573	-3.7908	1.0780 C
74	H74	2.0797	-3.4248	1.3539 H
75	H75	1.0519	-2.8477	2.6839 H
76	H76	-1.5534	-3.0432	2.4447 H
77	H77	-2.2001	-3.4508	0.8570 H
78	H78	0.0600	-3.9329	0.0024 H
79	H79	-0.0999	-4.7656	1.5666 H



Complex of 7 with imidazolidin-2-one: E= -2116.17706174

1	O1	-0.0148	7.1310	0.3054 O
2	C2	1.1726	7.8653	0.7366 C
3	C3	1.2546	5.0272	0.3937 C
4	C4	1.2636	3.6390	0.1918 C
5	C5	0.1190	2.9779	-0.2441 C
6	C6	-1.0561	3.7127	-0.4317 C
7	C7	-1.0658	5.0955	-0.2610 C
8	C8	0.0946	5.7596	0.1541 C
9	C9	2.5735	2.9699	0.4721 C
10	C10	-2.3644	3.0966	-0.8133 C
11	O11	-3.2818	3.8100	-1.2660 O
12	C12	5.9439	-3.3796	-0.5717 C
13	C13	5.8470	-4.6898	-1.0959 C
14	C14	4.6257	-5.1676	-1.5285 C
15	C15	3.5008	-4.3277	-1.4135 C
16	N16	3.5550	-3.0907	-0.9140 N
17	C17	4.7542	-2.5961	-0.5052 C
18	C18	4.8333	-1.2286	-0.0151 C
19	C19	6.1052	-0.7366	0.3814 C
20	C20	7.2711	-1.5660	0.3291 C
21	C21	7.1984	-2.8444	-0.1320 C
22	N22	3.7141	-0.4545	0.0198 N
23	C23	3.8131	0.8301	0.3962 C
24	C24	5.0525	1.3988	0.8113 C
25	C25	6.1741	0.6090	0.8089 C
26	C26	-6.2379	-2.8818	0.5157 C
27	C27	-6.3149	-4.0819	1.2608 C
28	C28	-5.2206	-4.5112	1.9863 C
29	C29	-4.0436	-3.7379	1.9437 C
30	N30	-3.9345	-2.6070	1.2425 N
31	C31	-5.0101	-2.1584	0.5418 C
32	C32	-4.9153	-0.8967	-0.1741 C
33	C33	-6.0612	-0.4391	-0.8765 C
34	C34	-7.2670	-1.2112	-0.9055 C
35	C35	-7.3575	-2.3920	-0.2334 C
36	N36	-3.7614	-0.1787	-0.1232 N
37	C37	-3.7086	1.0248	-0.7123 C
38	C38	-4.8151	1.5598	-1.4340 C
39	C39	-5.9666	0.8178	-1.5183 C
40	N40	-2.5080	1.7322	-0.5631 N
41	H41	0.8610	8.9060	0.7809 H
42	H42	1.5103	7.5384	1.7234 H
43	H43	2.1749	5.4781	0.7282 H
44	H44	0.1296	1.9215	-0.4411 H
45	H45	-1.9731	5.6496	-0.4413 H
46	H46	6.7373	-5.3008	-1.1570 H
47	H47	4.5232	-6.1596	-1.9424 H
48	H48	2.5300	-4.6804	-1.7329 H
49	H49	8.2136	-1.1471	0.6548 H
50	H50	8.0781	-3.4707	-0.1837 H
51	H51	5.0637	2.4335	1.0992 H
52	H52	7.1242	1.0169	1.1261 H
53	H53	-7.2371	-4.6468	1.2578 H
54	H54	-5.2542	-5.4175	2.5725 H
55	H55	-3.1678	-4.0559	2.4926 H
56	H56	-8.1092	-0.8269	-1.4649 H
57	H57	-8.2703	-2.9714	-0.2435 H
58	H58	-4.7190	2.5408	-1.8608 H
59	H59	-6.8175	1.1995	-2.0659 H
60	H60	-1.7323	1.1938	-0.1634 H
61	O61	3.5568	3.6693	0.7984 O
62	N62	2.6319	1.5847	0.3419 N
63	H63	1.7712	1.0436	0.2003 H
64	C64	-0.0648	-1.0903	0.2137 C
65	O65	-0.0144	0.1790	0.1406 O
66	N66	1.0153	-1.9259	0.1876 N
67	H67	1.9529	-1.6204	-0.0584 H
68	N68	-1.2045	-1.8277	0.3383 N
69	H69	-2.1302	-1.4315	0.4700 H
70	C70	-0.8940	-3.2488	0.5824 C
71	H71	-0.9577	-3.4883	1.6481 H
72	H72	-1.5559	-3.9102	0.0282 H
73	C73	0.5867	-3.3346	0.0885 C
74	H74	0.6234	-3.6826	-0.9477 H
75	H75	1.1944	-3.9902	0.7077 H
76	H76	1.9934	7.7551	0.0235 H