Supporting Information for:

Nonplanar Macrocycle Consisting of Four Pyridine and Phenol Units Connected with Acetylene Bonds Displaying Preferential Binding to Maltoside over Monosaccharides

Yuki Ohishi, Naoto Yamamoto, Hajime Abe*, Masahiko Inouye*

Graduate School of Pharmaceutical Sciences, University of Toyama

Toyama, Toyama 930-0194, Japan

inouye@pha.u-toyama.ac.jp, inouye@pha.u-toyama.ac.jp

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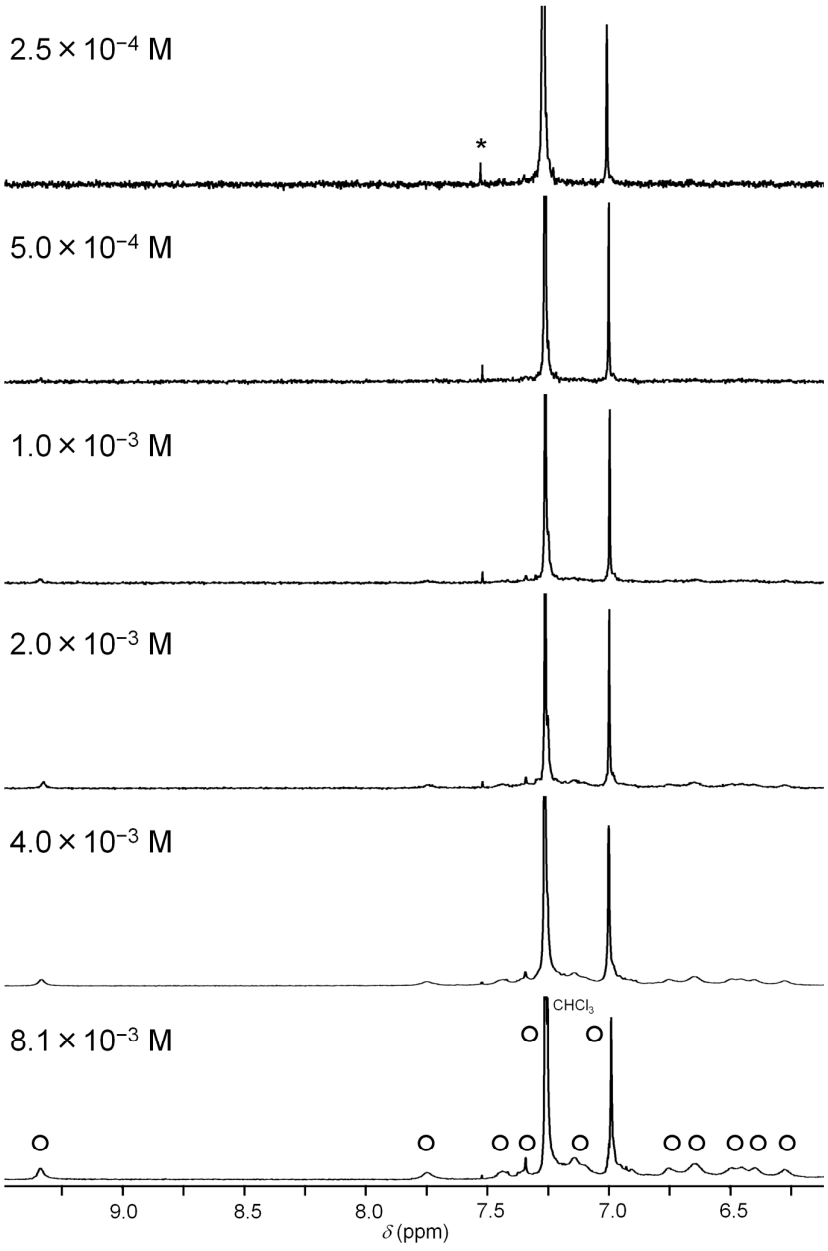


Figure S1. ^{1}H NMR spectra of **2** (2.5×10^{-4} to 8.1×10^{-3} M). Signals marked with circles and asterisks were attributed to the aromatic protons of **2** and $^{13}CHCl_3$, respectively. Conditions: $CDCl_3$, 25 °C, 400 MHz.

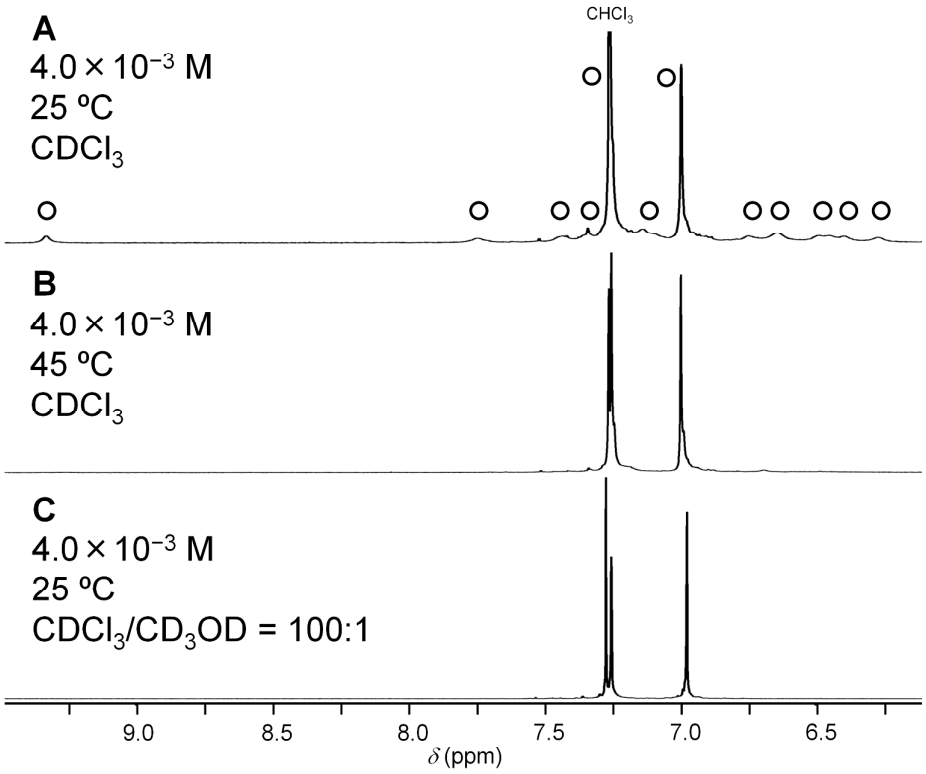


Figure S2. ^{1}H NMR spectra of **2** (4.0×10^{-3} M). A) 25 °C in $CDCl_3$, B) 45 °C in $CDCl_3$, C) 25 °C in $CDCl_3/CD_3OD$ (100:1). Signals marked with circles were attributed to the aromatic protons of **2**. Conditions: 400 MHz.

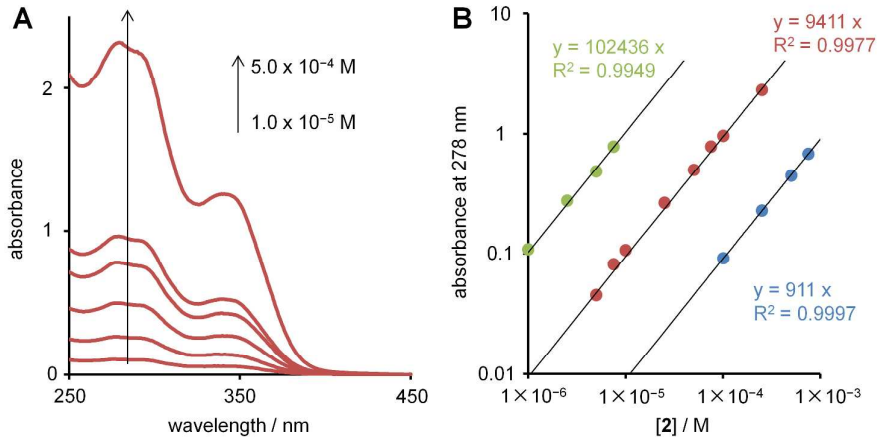


Figure S3. A) Concentration dependence of a UV spectrum of **2** in DCE. Conditions: [**2**] = 1.0×10^{-5} to 5.0×10^{-4} M, DCE, 25 °C, path length = 1 mm. B) Concentration dependence of absorbance of **2** at 278 nm in DCE. Conditions: [**2**] = 1.0×10^{-6} to 5.0×10^{-4} M, DCE, 25 °C, path length = 10 mm (green circles), 1 mm (red circles), and 0.1 mm (blue circles).

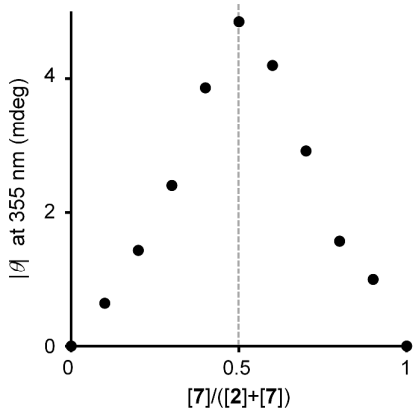


Figure S4. Job's plot of ellipticity at 355 nm for mixtures of **2** and **7** keeping the total concentration [**2**] + [**7**] = 1.5×10^{-5} M. Conditions: DCE, 25 °C, path length = 10 mm.

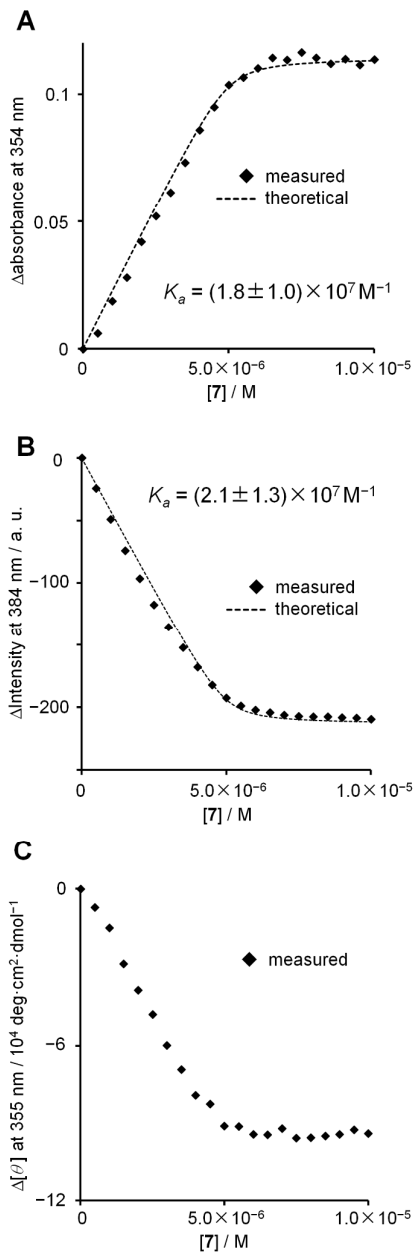


Figure S5. Results of titration experiment of **2** with **7**. A) Titration curve of absorbance at 354 nm. B) Titration curve of fluorescence intensity at 384 nm. C) Titration curve of molar ellipticity at 355 nm. The broken lines are fitted curves assuming 1:1 binding. Conditions: [**2**] = 5.0×10^{-6} M, [**7**] = 0 to 1.0×10^{-5} M, DCE, 25 °C, path length = 10 mm, λ_{ex} = 300 nm.

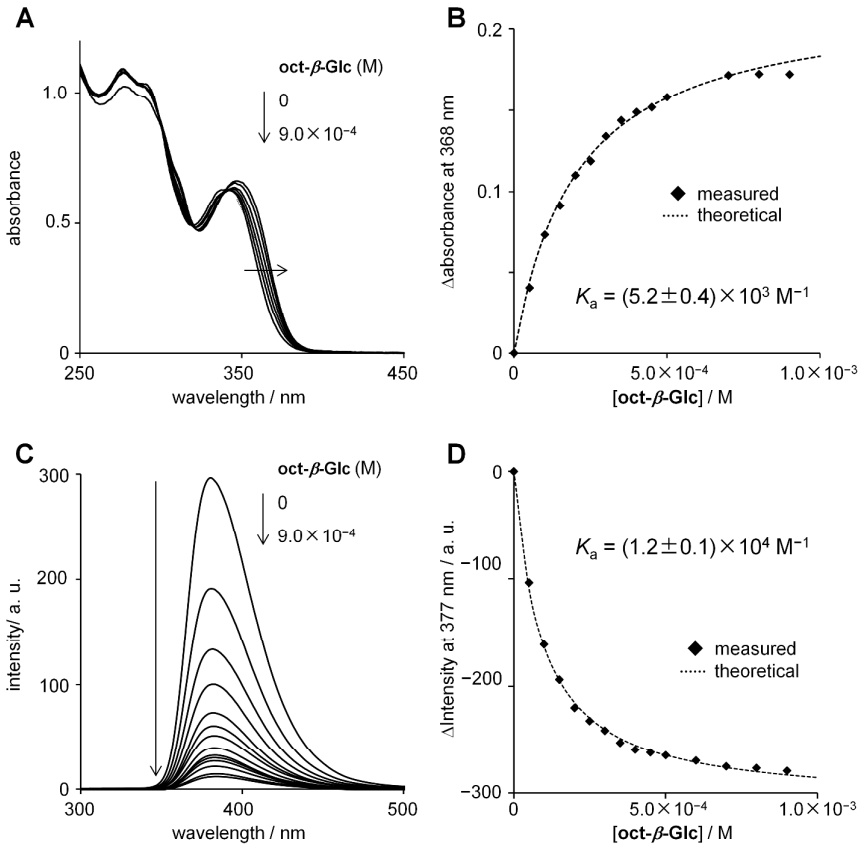


Figure S6. Results of titration experiment of **2** with **oct-*β*-Glc**. A) Change of UV/Vis spectrum of **2**. B) Titration curve of absorbance at 368 nm. C) Change of fluorescence spectrum of **2**. D) Titration curve of fluorescence intensity at 377 nm. The dotted line is a fitted curve assuming 1:1 binding. Conditions: **2** (1.0×10^{-5} M), **oct-*β*-Glc** (0 to 9.0×10^{-4} M), DCE, 25 °C, path length = 10 mm.

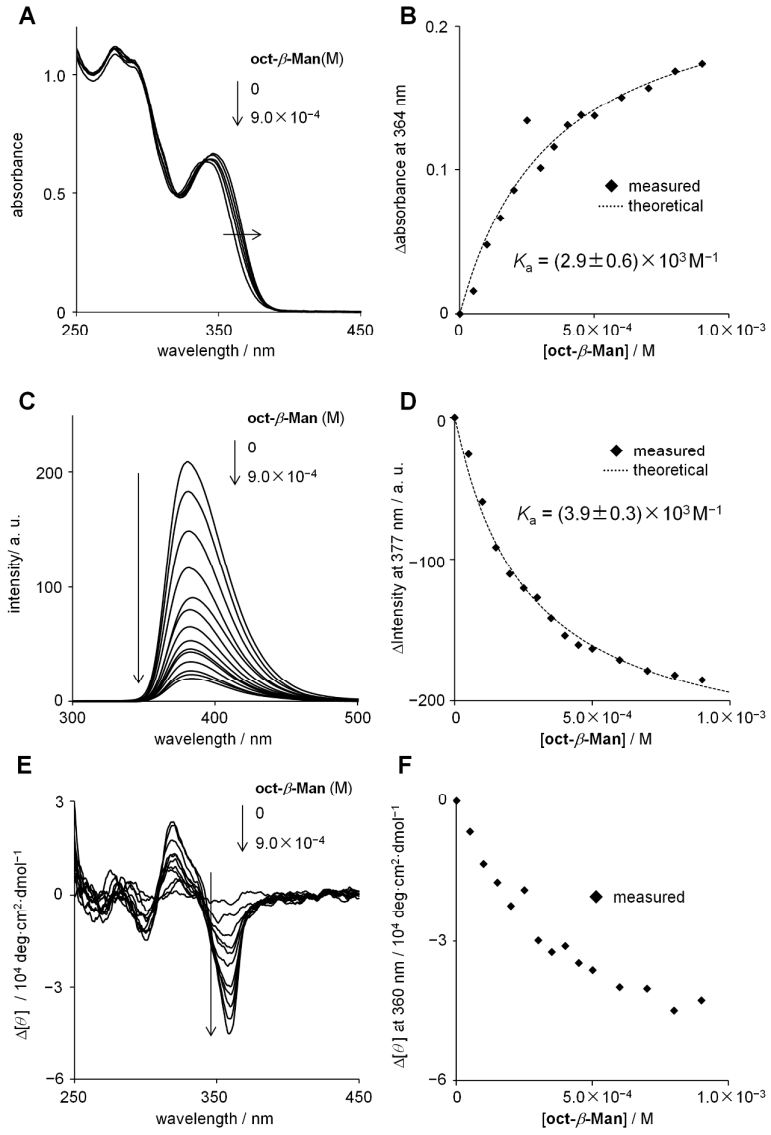


Figure S7. Results of titration experiment of **2** with **oct-*β*-Man**. A) Change of UV/Vis spectrum of **2**. B) Titration curve of absorbance at 364 nm. C) Change of fluorescence spectrum of **2**. D) Titration curve of fluorescence intensity at 377 nm. E) Titration curve of ellipticity at 360 nm. F) Titration curve of molar ellipticity at 360 nm. The dotted line is a fitted curve assuming 1:1 binding. Conditions: **2** (1.0×10^{-5} M), **oct-*β*-Man** (0 to 9.0×10^{-4} M), DCE, 25 °C, path length = 10 mm.

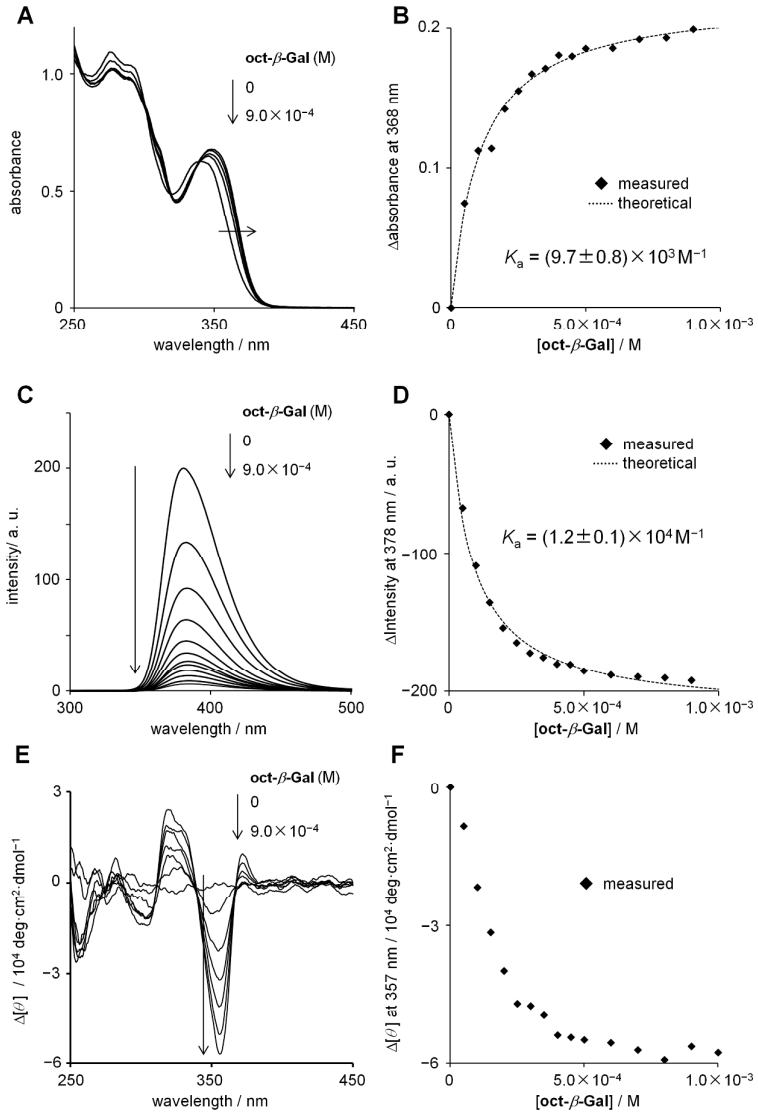


Figure S8. Results of titration experiment of **2** with **oct-β-Gal**. A) Change of UV/Vis spectrum of **2**. B) Titration curve of absorbance at 368 nm. C) Change of fluorescence spectrum of **2**. D) Titration curve of fluorescence intensity at 378 nm. E) Change of CD spectrum of **2**. F) Titration curve of molar ellipticity at 357 nm. The dotted line is a fitted curve assuming 1:1 binding. Conditions: **2** (1.0×10^{-5} M), **oct-β-Gal** (0 to 9.0×10^{-4} M), DCE, 25 °C, path length = 10 mm.

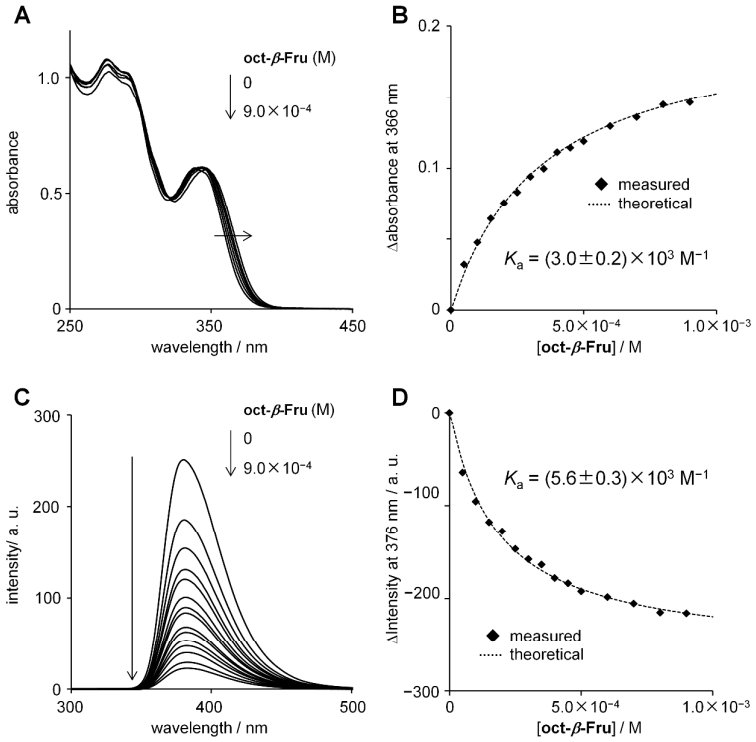


Figure S9. Results of titration experiment of **2** with **oct-*β*-Fru**. A) Change of UV/Vis spectrum of **2**. B) Titration curve of absorbance at 366 nm. C) Change of fluorescence spectrum of **2**. D) Titration curve of fluorescence intensity at 376 nm. The dotted line is a fitted curve assuming 1:1 binding. Conditions: **2** (1.0×10^{-8} M), **oct-*β*-Fru** (0 to 9.0×10^{-4} M), DCE, 25 °C, path length = 10 mm.

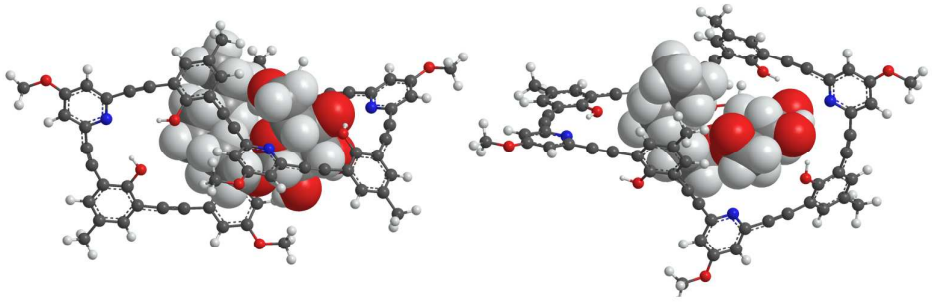


Figure S10. A complex between model of **2** and **oct-*β*-Glc** proposed by Monte Carlo simulation. The model is an analogue of **2** whose side alkyl chains are shortened to methyl groups. Conditions: OPLS2005, under $CHCl_3$.

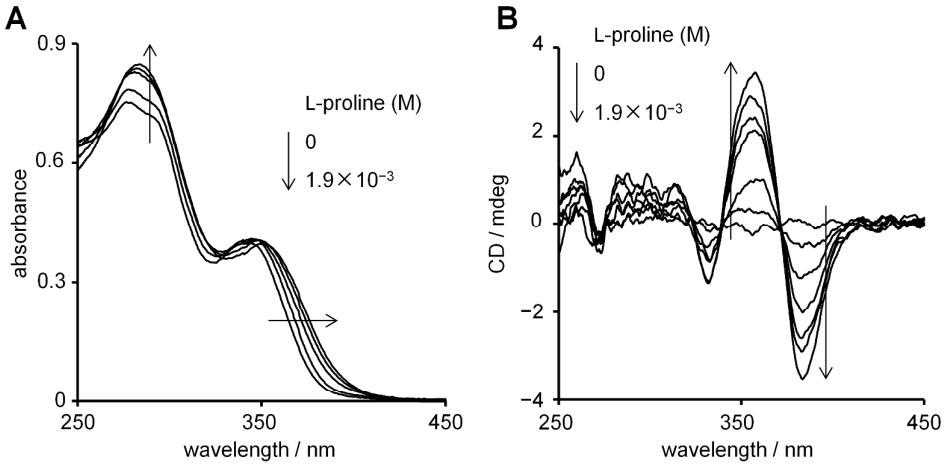


Figure S11. Change of A) UV/Vis and B) CD spectrum of **2** during the addition of L-proline. Conditions: **2** (1.0×10^{-5} M), L-proline (0 to 1.9×10^{-3} M), DCE, 25 °C, path length = 10 mm.

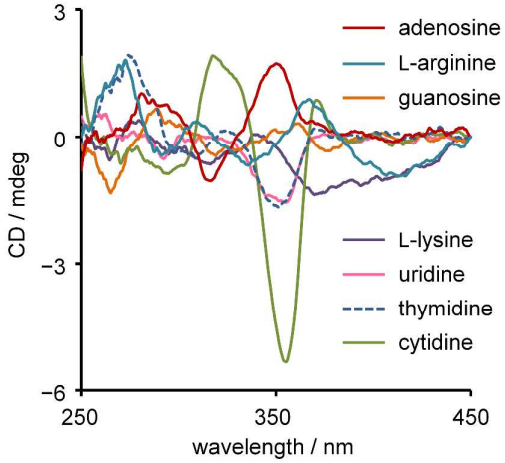


Figure S12. CD spectra of the filtrate after solid–liquid extraction of various kinds of native saccharides and nucleosides with **2**. The samples were prepared by the procedure described in the main text. L-Arginine (5.7×10^{-5} mol), L-lysine (6.8×10^{-5} mol), adenosine (3.7×10^{-5} mol), guanosine (3.5×10^{-5} mol), cytidine (4.1×10^{-5} mol), uridine (4.1×10^{-5} mol), and thymidine (4.1×10^{-5} mol). CD measurement conditions: DCE, 25 °C, path length = 10 mm.

2. Fitting methods for association constants

1,2-Dichloroethane (DCE) solutions of **2** were titrated with a DCE solutions of guest glycosides, and the observed absorbance or fluorescence intensity was plotted versus the concentration of the glycosides. The formal binding constants were obtained by iterative curve-fitting measurements based on the equation.

Equation:

$$A_{\mathrm{obs}}-A_0=\frac{A_{11}-A_0}{2K_{11}[\mathbf{2}]_0}\left[1+K_{11}[\mathbf{2}]_0+K_{11}[\mathrm{G}]_0-\left\{(1+K_{11}[\mathbf{2}]_0+K_{11}[\mathrm{G}]_0)^2-4{K_{11}}^2[\mathbf{2}]_0[\mathrm{G}]_0\right\}^{1/2}\right]$$

K_{11}: the 1:1 binding constant of **2** with glycosides

A_{obs}: the observed absorbance or fluorescence intensity

A_0: absorbance or fluorescence intensity of **2** before addition of glycosides

A_{11}: absorbance or fluorescence intensity of 1:1 host-guest complex (at the saturation point)

$[\mathbf{2}]_0$: the total concentration of **2**

$[\mathrm{G}]_0$: the total concentration of guest glycoside

3. Calculated energies and geometric coordinates

macrocycle **2** and β-D-maltose

E = −290.936 kJ/mol

Atom	X	Y	Z
1 C1	1.8703	-4.1818	0.1356
2 C2	2.5961	-4.8014	-0.8863
3 C3	2.1459	-5.9912	-1.4578
4 C4	0.9511	-6.5590	-1.0156
5 C5	0.2090	-5.9518	0.0014
6 C6	0.6672	-4.7561	0.5927
7 H7	3.5270	-4.3668	-1.2279
8 H8	0.5997	-7.4774	-1.4670
9 C9	2.4220	-2.9598	0.7145
10 C10	2.9392	-1.9612	1.1910
11 C11	5.0698	1.2950	2.7524
12 C12	3.6903	1.4550	2.5459
13 C13	2.9617	0.3834	2.0301
14 C14	3.6261	-0.8060	1.7401
15 C15	5.6539	0.0695	2.4346
16 H16	5.6831	2.0882	3.1468
17 H17	1.9013	0.4816	1.8580
18 C18	-1.0417	-6.5825	0.4100
19 C19	7.0726	-0.1793	2.6221
20 C20	8.2512	-0.4622	2.7756
21 C21	-2.1082	-7.0446	0.7848
22 C22	-5.8013	-8.1923	2.4034
23 C23	-5.4395	-8.7331	1.1587
24 C24	-4.2119	-8.3725	0.602
25 C25	-3.3888	-7.4924	1.3013
26 C26	-4.9147	-7.3192	3.0321
27 H27	-6.7374	-8.4315	2.8801
28 H28	-3.9150	-8.7678	-0.3563
29 C29	12.3077	-1.6200	3.3819
30 C30	11.9998	-0.3606	2.8624
31 C31	10.6645	-0.0001	2.6663

32	C32	9.6330	-0.8899	2.9813
33	C33	9.9404	-2.1630	3.4995
34	C34	11.2893	-2.5221	3.6998
35	H35	13.3412	-1.8994	3.5359
36	H36	10.4288	0.9784	2.2698
37	C37	-5.2019	-6.7093	4.3175
38	C38	-5.3167	-6.1599	5.4023
39	C39	-5.3533	-4.2800	9.2208
40	C40	-4.1282	-4.4795	8.5776
41	C41	-4.0919	-5.0735	7.2981
42	C42	-5.2995	-5.4938	6.7020
43	C43	-6.5147	-5.2871	7.3609
44	C44	-6.5469	-4.6740	8.6143
45	H45	-5.3793	-3.8264	10.2028
46	H46	-7.4392	-5.6075	6.8994
47	C47	11.6397	-3.8391	4.2232
48	C48	11.6902	-4.9784	4.6598
49	C49	10.8633	-8.8195	6.1157
50	C50	9.9016	-7.8212	5.9617
51	C51	11.4756	-6.3200	5.1687
52	C52	12.5003	-7.2557	5.2901
53	C53	12.1941	-8.5291	5.7716
54	H54	10.5693	-9.7837	6.4954
55	H55	13.5130	-7.0077	5.0149
56	C56	-2.9080	-4.1018	9.2845
57	C57	-1.8306	-3.8954	9.8222
58	C58	2.1334	-3.7240	11.1809
59	C59	1.6894	-4.5931	10.1857
60	C60	-0.4759	-3.7850	10.3347
61	C61	-0.1199	-2.8841	11.3356
62	C62	1.2064	-2.8474	11.7685
63	H63	3.1691	-3.7453	11.4780
64	H64	-0.8514	-2.2235	11.7736
65	C65	2.5690	-5.5452	9.5330
66	C66	3.2411	-6.3847	8.9539
67	C67	5.2821	-9.4636	6.8428

68 C68	5.9491	-8.2582	7.0794
69 C69	5.2953	-7.2142	7.7659
70 C70	3.9825	-7.4182	8.2368
71 C71	3.3353	-8.6338	7.9975
72 C72	3.9752	-9.6528	7.2924
73 H73	5.7823	-10.2623	6.3113
74 H74	2.3248	-8.7854	8.3540
75 C75	7.3327	-8.1421	6.6289
76 C76	8.5060	-8.0283	6.3082
77 N77	4.9523	-0.9750	1.9401
78 N78	-3.7204	-6.9723	2.5028
79 N79	0.4097	-4.6276	9.754
80 N80	10.1912	-6.5875	5.4971
81 O81	-2.8926	-5.2506	6.6287
82 H82	-2.1360	-4.8015	7.0473
83 O83	5.9181	-5.9972	7.9596
84 H84	6.4510	-5.7278	7.1915
85 O85	-0.0445	-4.1571	1.6149
86 H86	-0.6658	-4.7568	2.0568
87 O87	8.9321	-3.0545	3.8129
88 H88	8.2042	-3.0339	3.1702
89 C89	13.1112	0.6162	2.5216
90 H90	13.3397	1.2424	3.3846
91 H91	14.0234	0.0939	2.2295
92 H92	12.8272	1.2676	1.6940
93 C93	3.2600	-10.9656	7.0286
94 H94	3.4709	-11.6771	7.8276
95 H95	2.1795	-10.8261	6.9734
96 H96	3.5817	-11.4077	6.0846
97 O97	13.2422	-9.4193	5.8733
98 C98	12.9916	-10.7354	6.3574
99 H99	13.9252	-11.2981	6.3699
100 H100	12.6041	-10.7217	7.3774
101 H101	12.2933	-11.2742	5.7149
102 O102	1.5074	-1.9378	12.7599
103 C103	2.8454	-1.8532	13.2422

104 H104	2.9015	-1.0870	14.0156
105 H105	3.1722	-2.7937	13.6889
106 H106	3.5414	-1.5708	12.4505
107 C107	-7.8715	-4.4576	9.3243
108 H108	-8.6849	-4.3129	8.6119
109 H109	-8.1122	-5.3219	9.9443
110 H110	-7.8382	-3.5767	9.9670
111 O111	-6.2167	-9.6057	0.4269
112 C112	-7.4828	-10.0078	0.9417
113 H113	-7.9564	-10.6927	0.2381
114 H114	-7.3818	-10.5335	1.8926
115 H115	-8.1530	-9.1564	1.0712
116 C116	2.9497	-6.6605	-2.5580
117 H117	4.0128	-6.4320	-2.467
118 H118	2.8436	-7.7456	-2.5216
119 H119	2.6103	-6.3169	-3.5357
120 O120	2.9852	2.6085	2.8166
121 C121	3.6763	3.7396	3.3387
122 H122	2.9690	4.5554	3.4894
123 H123	4.1340	3.5207	4.3048
124 H124	4.4441	4.0951	2.6496
125 C125	2.8924	-6.0648	4.9451
126 C126	2.1030	-7.3347	4.5745
127 C127	0.8209	-6.9638	3.7969
128 C128	-0.0003	-5.9114	4.5678
129 C129	0.9163	-4.7167	4.9498
130 H130	3.7103	-6.2696	5.6397
131 H131	1.8127	-7.8116	5.5133
132 H132	1.1216	-6.5329	2.8395
133 H133	-0.3695	-6.3794	5.4834
134 H134	1.2534	-4.2250	4.0341
135 O135	2.0758	-5.1779	5.6729
136 O136	3.3371	-5.4498	3.7709
137 O137	2.8682	-8.2867	3.8506
138 H138	2.2398	-8.9871	3.6240
139 O139	0.0360	-8.1143	3.4919

140 H140	-0.8033	-7.7843	3.1381
141 O141	-1.1518	-5.5230	3.8196
142 H142	-1.9036	-5.4469	4.4290
143 H143	0.9118	-2.8442	6.0545
144 H144	-0.5563	-3.1423	5.1678
145 C145	0.2047	-3.6287	5.7804
146 O146	-0.4178	-4.1516	6.9424
147 H147	0.2640	-4.3860	7.5936
148 C148	4.7292	-5.5188	3.4442
149 C149	4.7931	-5.9468	1.9635
150 H150	5.2496	-6.2755	4.0375
151 H151	4.0143	-5.4054	1.4269
152 C152	5.3760	-4.1245	3.6795
153 H153	4.6622	-3.3647	3.3549
154 C154	6.4806	-4.1257	1.5699
155 H155	5.7001	-3.4476	1.2082
156 C156	6.1460	-5.6018	1.3098
157 H157	6.9220	-6.2057	1.7898
158 O158	6.5944	-3.9308	2.9447
159 C159	5.7019	-3.8579	5.1657
160 H160	6.0235	-2.8218	5.2869
161 H161	4.8053	-3.9711	5.7779
162 O162	6.7259	-4.7251	5.6490
163 H163	7.5364	-4.5432	5.1436
164 O164	7.6895	-3.8813	0.9807
165 H165	7.6959	-4.4162	0.1764
166 O166	6.1368	-5.9400	-0.0725
167 H167	5.7559	-6.8290	-0.1059
168 O168	4.5103	-7.3342	1.8037
169 H169	3.8748	-7.5936	2.4999

macrocycle **2** and **oct-*β*-Glc**

E = −386.233 kJ/mol

Atom	X	Y	Z
1 C1	2.3963	-3.1779	3.5257
2 C2	3.5801	-2.4480	3.6608
3 C3	4.1312	-2.2185	4.9234
4 C4	3.4889	-2.7155	6.0594
5 C5	2.3061	-3.4511	5.9418
6 C6	1.7580	-3.6989	4.6680
7 H7	4.0628	-2.0411	2.7822
8 H8	3.9085	-2.5209	7.0374
9 C9	1.8243	-3.3487	2.1928
10 C10	1.2325	-3.4984	1.1350
11 C11	-1.1159	-3.9251	-2.3084
12 C12	-1.3785	-4.7706	-1.2315
13 C13	-0.5934	-4.6495	-0.0759
14 C14	0.4205	-3.6927	-0.0528
15 C15	-0.0825	-2.9954	-2.2025
16 H16	-1.7125	-3.9902	-3.2044
17 H17	-0.7573	-5.2639	0.7947
18 C18	1.6521	-3.9299	7.1566
19 C19	0.2175	-2.0660	-3.2787
20 C20	0.4803	-1.2270	-4.1275
21 C21	1.0000	-4.3256	8.1107
22 C22	-1.7691	-5.5957	10.9941
23 C23	-0.4046	-5.7008	11.3123
24 C24	0.5391	-5.2842	10.3719
25 C25	0.0953	-4.7782	9.1524
26 C26	-2.1222	-5.0775	9.7494
27 H27	-2.5415	-5.9016	11.6800
28 H28	1.5925	-5.3569	10.5922
29 C29	1.4908	1.8524	-6.8984
30 C30	1.3261	0.5346	-7.3310
31 C31	0.9941	-0.4614	-6.4090
32 C32	0.8172	-0.1506	-5.0571
33 C33	0.9752	1.1794	-4.6195

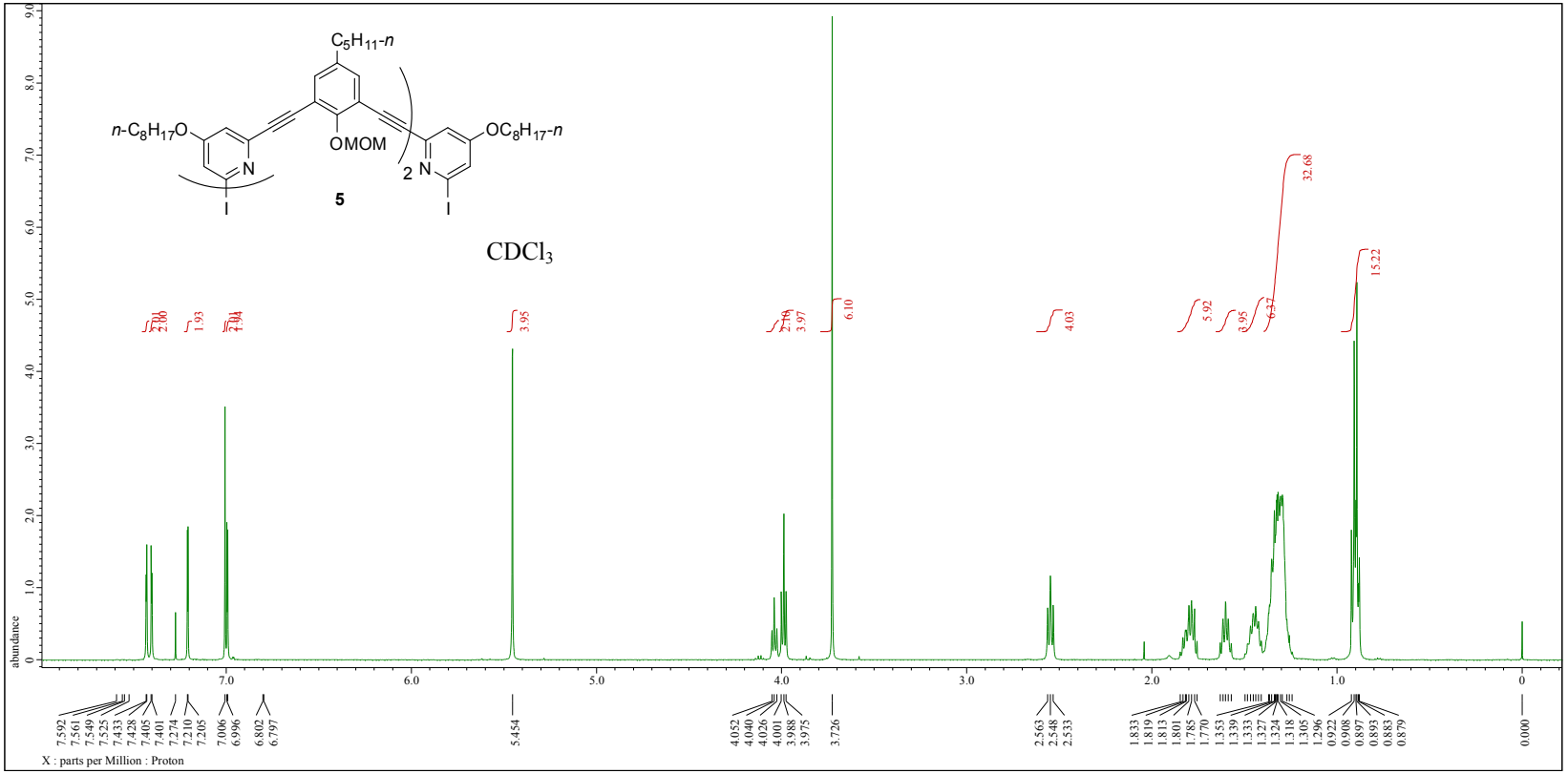
34	C34	1.3181	2.1801	-5.5513
35	H35	1.7551	2.6216	-7.6116
36	H36	0.8760	-1.4829	-6.7449
37	C37	-3.5013	-4.9237	9.3213
38	C38	-4.5916	-4.7278	8.8062
39	C39	-8.0146	-4.0244	6.3769
40	C40	-7.0602	-3.0126	6.5133
41	C41	-5.9542	-3.2002	7.3658
42	C42	-5.7870	-4.4369	8.0201
43	C43	-6.7510	-5.4384	7.8721
44	C44	-7.8708	-5.2317	7.0637
45	H45	-8.8642	-3.8788	5.7233
46	H46	-6.6237	-6.3879	8.3748
47	C47	1.5000	3.5629	-5.1193
48	C48	1.6006	4.6301	-4.5344
49	C49	1.7071	7.7221	-1.7129
50	C50	1.2798	6.4259	-1.4321
51	C51	1.6539	5.7517	-3.6149
52	C52	2.0969	7.0199	-3.9858
53	C53	2.1230	8.0298	-3.0094
54	H54	1.7187	8.4808	-0.9463
55	H55	2.4101	7.1974	-5.0013
56	C56	-7.2016	-1.7994	5.7111
57	C57	-7.1862	-0.7786	5.0399
58	C58	-6.7279	2.7550	2.8305
59	C59	-5.6799	2.1354	3.5106
60	C60	-7.0707	0.4424	4.2617
61	C61	-8.1709	0.9974	3.6114
62	C62	-8.0028	2.1723	2.8810
63	H63	-6.5380	3.6638	2.2834
64	H64	-9.1420	0.5319	3.6686
65	C65	-4.3406	2.6989	3.4955
66	C66	-3.2252	3.1960	3.4509
67	C67	0.6792	4.8934	3.2923
68	C68	-0.1301	4.9571	2.1548
69	C69	-1.4259	4.4031	2.1806

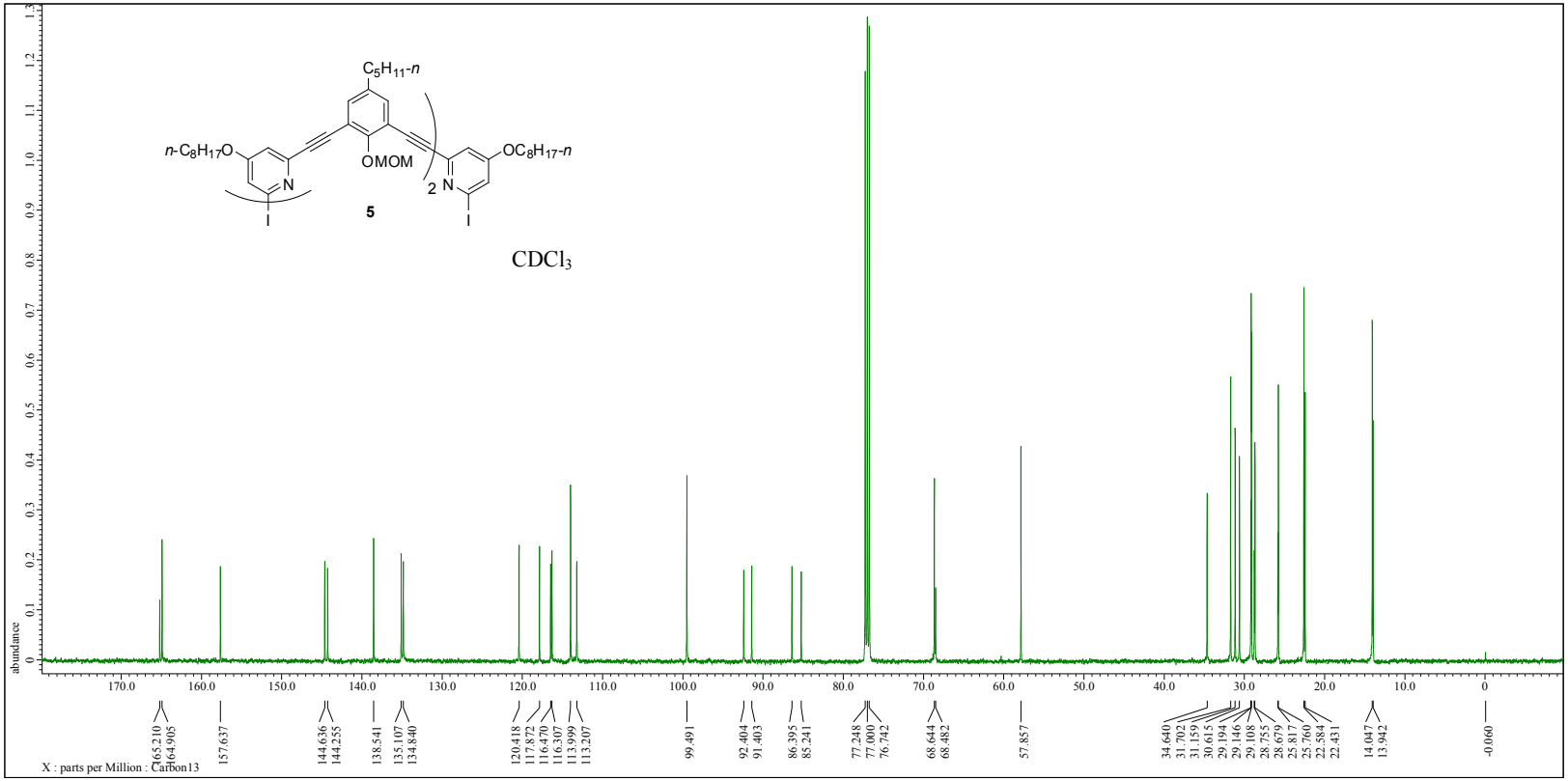
70 C70	-1.8952	3.7936	3.3617
71 C71	-1.0703	3.7400	4.4890
72 C72	0.2155	4.2816	4.4573
73 H73	1.6779	5.3086	3.2694
74 H74	-1.4221	3.2627	5.3942
75 C75	0.4112	5.5781	0.9482
76 C76	0.8243	6.0189	-0.1137
77 N77	0.6889	-2.8745	-1.0962
78 N78	-1.2135	-4.6697	8.8347
79 N79	-5.8324	0.9907	4.2176
80 N80	1.2466	5.4464	-2.3624
81 O81	-5.0413	-2.1788	7.5394
82 H82	-4.1445	-2.4733	7.7669
83 O83	-2.2133	4.4525	1.0470
84 H84	-1.7141	4.8400	0.3219
85 O85	0.6017	-4.4420	4.5340
86 H86	0.1144	-4.5615	5.3602
87 O87	0.7991	1.5114	-3.2889
88 H88	0.9537	2.4511	-3.1464
89 C89	1.5204	0.1825	-8.7952
90 H90	0.8825	-0.6519	-9.0901
91 H91	1.2776	1.0258	-9.4431
92 H92	2.5572	-0.1006	-8.9798
93 C93	1.1061	4.1977	5.6836
94 H94	0.9523	5.0664	6.3242
95 H95	0.8885	3.3007	6.2661
96 H96	2.1603	4.1578	5.4064
97 O97	2.5360	9.3260	-3.2336
98 C98	2.9729	9.7011	-4.5367
99 H99	3.2598	10.7528	-4.5313
100 H100	3.8456	9.1255	-4.8495
101 H101	2.1797	9.5820	-5.2766
102 O102	-9.1227	2.6785	2.2558
103 C103	-9.0111	3.8782	1.4955
104 H104	-9.9850	4.1302	1.0755
105 H105	-8.6944	4.7190	2.1148

106 H106	-8.3153	3.7635	0.6627
107 C107	-8.9093	-6.3278	6.9043
108 H108	-8.6482	-6.9750	6.0663
109 H109	-9.8999	-5.9114	6.7166
110 H110	-8.9773	-6.9442	7.8018
111 O111	0.0867	-6.1931	12.5027
112 C112	-0.8271	-6.6324	13.5035
113 H113	-0.2689	-6.9852	14.3709
114 H114	-1.4759	-5.8219	13.8396
115 H115	-1.4419	-7.4620	13.1506
116 C116	5.4067	-1.4080	5.0653
117 H117	5.9914	-1.4147	4.1444
118 H118	5.1674	-0.3717	5.3064
119 H119	6.0389	-1.8064	5.8599
120 O120	-2.4136	-5.6688	-1.3840
121 C121	-2.6856	-6.5997	-0.3398
122 H122	-3.5100	-7.2467	-0.6401
123 H123	-1.8251	-7.2393	-0.1361
124 H124	-2.9842	-6.0972	0.5813
125 O136	-2.3290	-2.4533	7.3228
126 C148	-2.1070	-2.2589	5.9288
127 C149	-2.6406	-3.4627	5.1225
128 H150	-1.0252	-2.1944	5.7906
129 H151	-3.7038	-3.5776	5.3464
130 C152	-2.7487	-0.9515	5.3855
131 H153	-3.8226	-0.9754	5.5836
132 C154	-3.1428	-1.8714	3.2294
133 H155	-4.2201	-1.8255	3.4280
134 C156	-2.4977	-3.2141	3.6027
135 H157	-1.4389	-3.1327	3.3401
136 O158	-2.5335	-0.8431	3.9663
137 C159	-2.2028	0.3294	6.0475
138 H160	-2.8392	1.1721	5.7738
139 H161	-2.2358	0.2557	7.1355
140 O162	-0.8776	0.5919	5.6160
141 H163	-0.8859	0.4868	4.6545

142 O164	-2.9261	-1.6978	1.8591
143 O166	-3.0508	-4.2681	2.8271
144 H167	-3.0385	-3.9368	1.9201
145 O168	-2.0328	-4.6914	5.5039
146 H169	-2.3210	-5.3381	4.8456
147 HO13	-1.8927	-3.2887	7.5755
148 H148	-4.1365	0.0159	1.8667
149 H149	-3.7149	-0.6328	0.3044
150 C150	-3.3214	-0.4440	1.3037
151 C151	-2.1185	0.5102	1.2048
152 H152	-1.7992	0.7695	2.2128
153 H153	-2.4439	1.4458	0.7487
154 C154	-0.9283	-0.0708	0.4135
155 H155	-0.5825	-0.9871	0.8937
156 H156	-1.2662	-0.3788	-0.5776
157 C157	0.2579	0.9001	0.2433
158 H158	1.0304	0.4031	-0.3474
159 H159	-0.0657	1.7493	-0.3608
160 C160	0.8817	1.4294	1.5522
161 H161	1.6699	2.1360	1.2905
162 H162	0.1418	2.0098	2.1010
163 C163	1.4552	0.3366	2.4748
164 H164	0.6588	-0.3608	2.7400
165 H165	2.1958	-0.2543	1.9338
166 C166	2.0645	0.8840	3.7793
167 H167	1.3397	1.5211	4.2871
168 H168	2.2463	0.0509	4.4599
169 C169	3.3780	1.6552	3.5802
170 H170	3.7930	1.9673	4.5389
171 H171	4.1265	1.0391	3.0808
172 H172	3.2290	2.5541	2.9818

4. ^{1}H NMR and ^{13}C NMR Spectra of New Compounds




C5H11-n
n-C8H17O
OMOM
OC8H17-n
N
N
2
I
I
5
CDCl3
abundance
X : parts per Million : Carbon13
165.210
164.905
157.637
144.636
144.255
138.541
135.107
134.840
120.418
117.872
116.470
116.307
113.999
113.207
99.491
92.404
91.403
86.395
85.241
77.248
77.000
76.742
68.644
68.482
57.857
34.640
31.702
31.159
30.615
29.194
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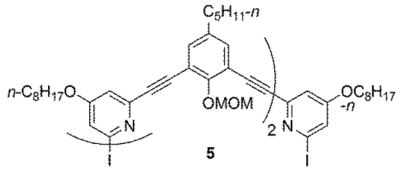
25.817
25.760
22.584
22.431
14.047
13.942
-0.060



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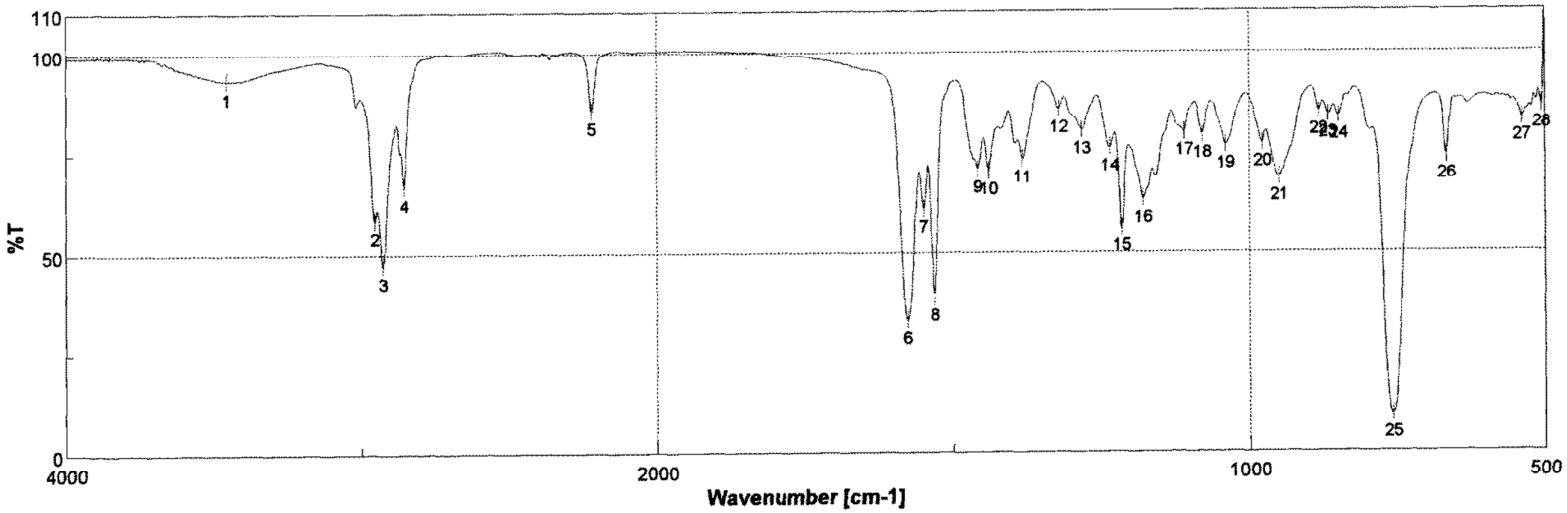

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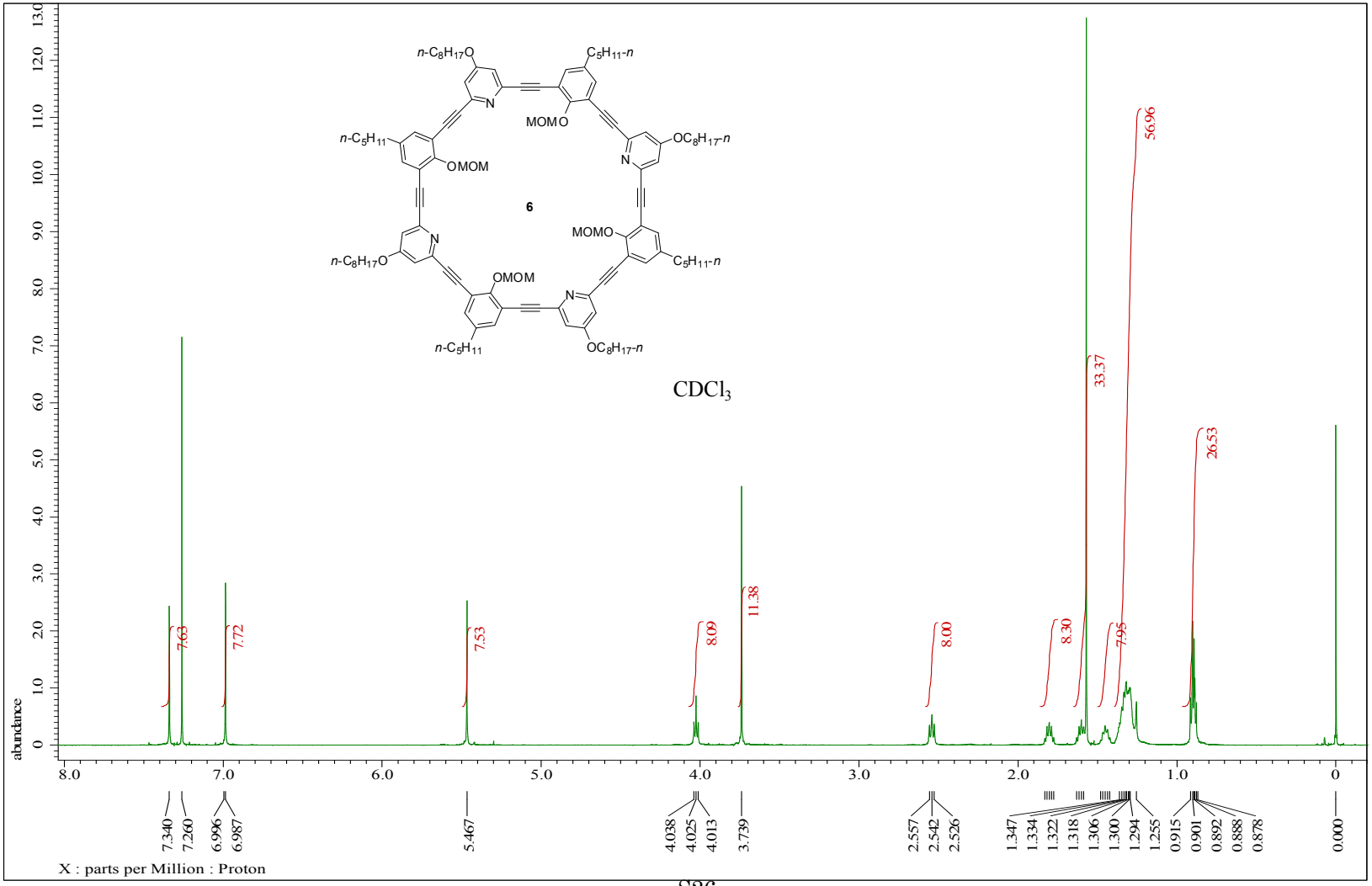
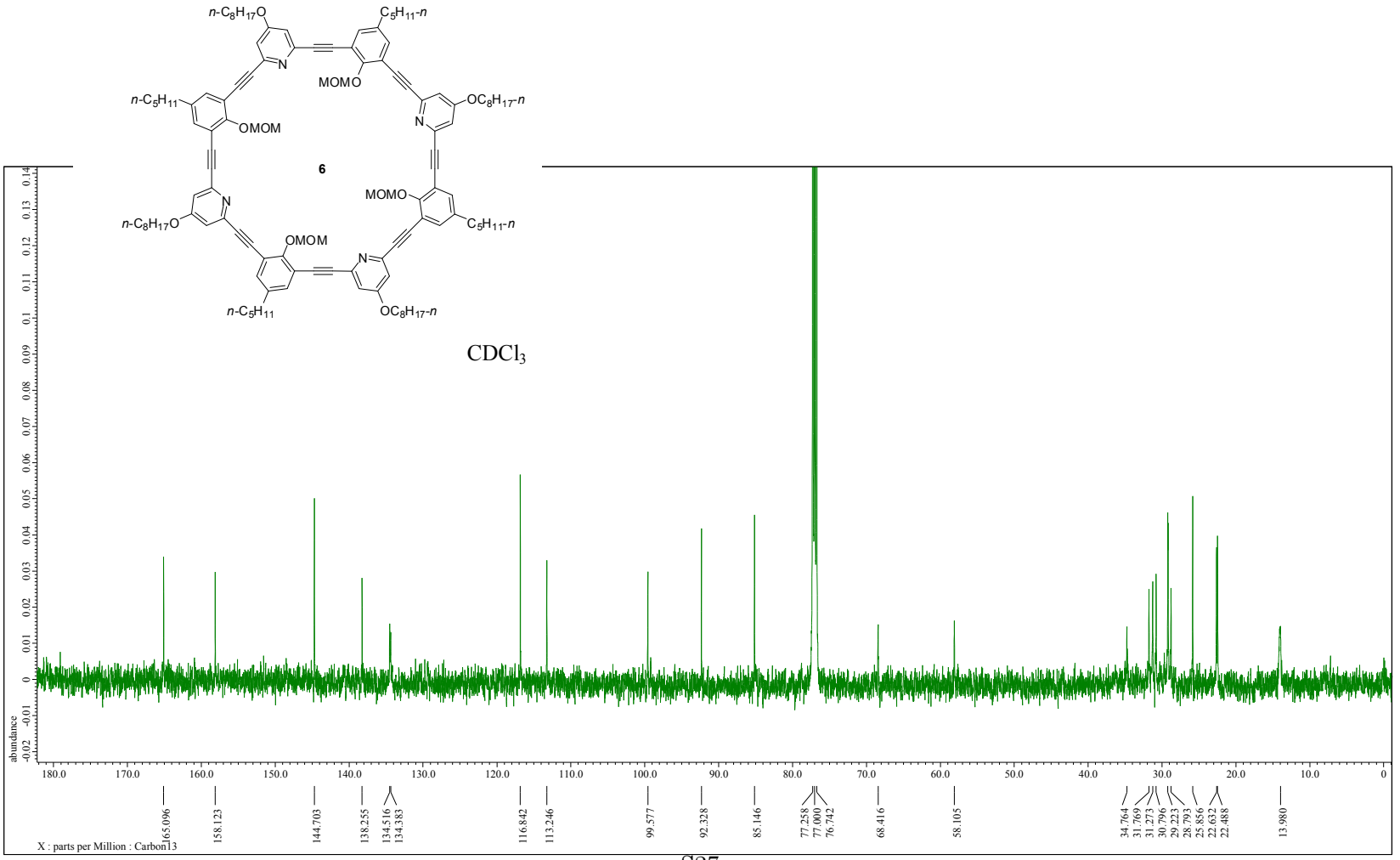
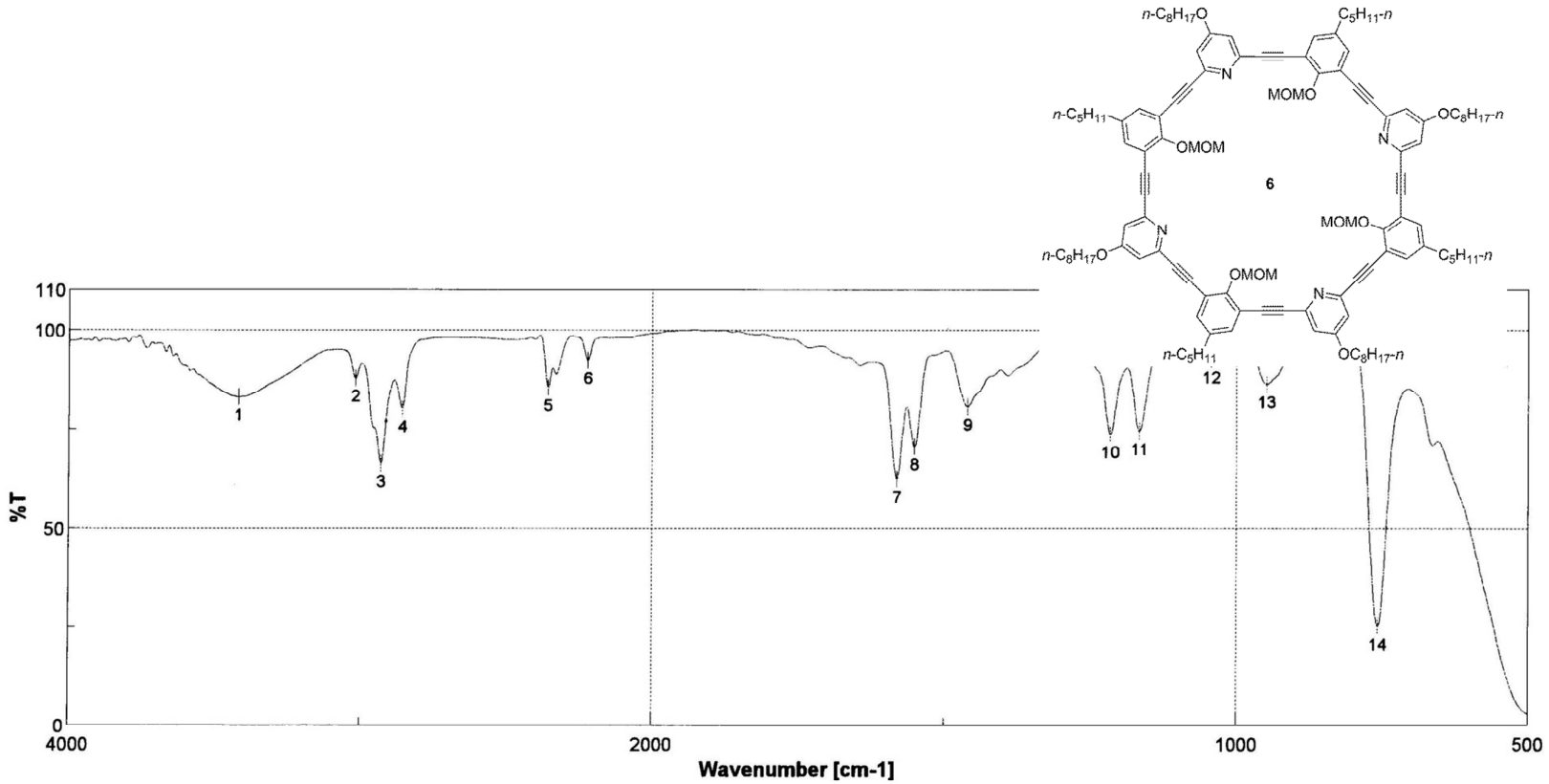
1	3456	93.59	2	2955	58.46	3	2929	47.30	4	2857	66.98	5	2220	85.82
6	1577	33.42	7	1550	61.16	8	1531	38.97	9	1457	70.94	10	1439	70.49
11	1383	73.50	12	1321	85.83	13	1282	80.51	14	1235	76.22	15	1215	56.10
16	1179	63.28	17	1109	80.00	18	1079	79.45	19	1039	76.75	20	979	77.25
21	950	68.74	22	882	85.23	23	866	84.29	24	849	83.91	25	758	9.33
26	667	74.00	27	539	83.26	28	506	86.45						


n-C8H17O
C5H11-n
MOMO
n-C5H11
OMOM
OC8H17-n
6
CDCl3
abundance
X : parts per Million : Proton


n-C8H17O
C5H11-n
MOMO
n-C5H11
OMOM
OC8H17-n
6
MOMO
n-C8H17O
C5H11-n
OMOM
n-C5H11
OC8H17-n
CDCl3
abundance
X : parts per Million : Carbon13
165.096
158.123
144.703
138.255
134.516
134.383
116.842
113.246
99.577
92.328
85.146
77.258
77.000
76.742
68.416
58.105
34.764
31.769
31.273
30.796
29.223
28.793
25.856
22.632
22.488
13.980



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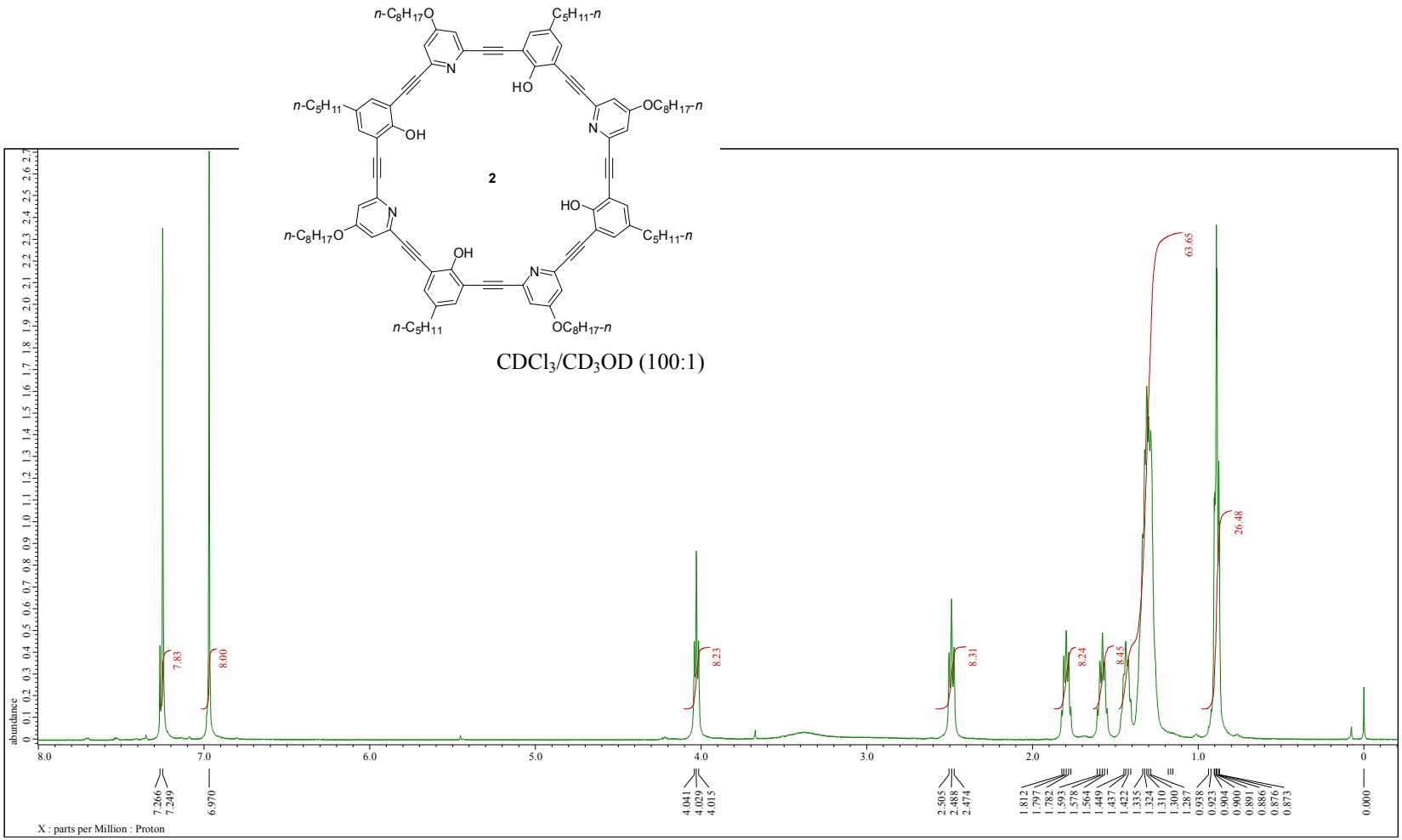
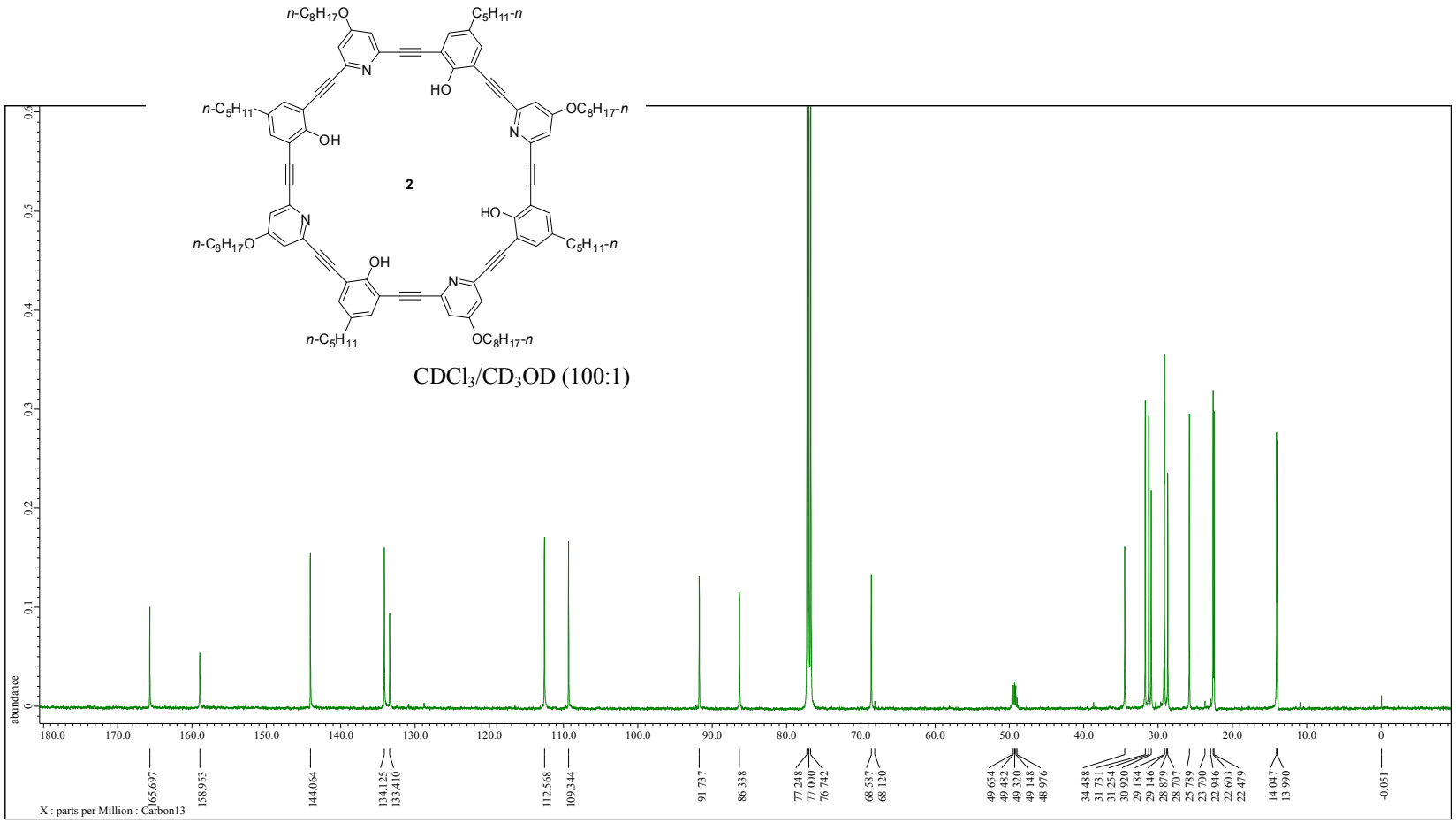
1	3415	83.05	2	3017	87.84	3	2928	66.39	4	2858	80.21	5	2358	85.47
6	2221	92.39	7	1581	62.42	8	1550	70.61	9	1459	80.67	10	1215	73.75
11	1166	74.47	12	1043	92.59	13	949	86.34	14	758	25.14			


n-C8H17O
C5H11-n
n-C5H11
OC8H17-n
HO
OH
N
2
n-C8H17O
C5H11-n
OH
n-C5H11
OC8H17-n
CDCl3/CD3OD (100:1)
abundance
7.83
8.00
8.23
8.31
8.24
8.45
63.65
26.48
7.266
7.249
6.970
4.041
4.029
4.015
2.505
2.488
2.474
1.812
1.797
1.782
1.593
1.578
1.564
1.449
1.437
1.422
1.335
1.324
1.310
1.300
1.287
0.938
0.923
0.904
0.900
0.891
0.886
0.876
0.873
0.000
X : parts per Million : Proton


n-C8H17O
C5H11-n
HO
n-C5H11
OH
OC8H17-n
2
HO
n-C8H17O
C5H11-n
OH
n-C5H11
OC8H17-n
CDCl3/CD3OD (100:1)
abundance
X : parts per Million : Carbon13
165.697
158.953
144.064
134.125
133.410
112.568
109.344
91.737
86.338
77.248
77.000
76.742
68.587
68.120
49.654
49.482
49.320
49.148
48.976
34.488
31.731
31.254
30.920
29.184
29.146
28.879
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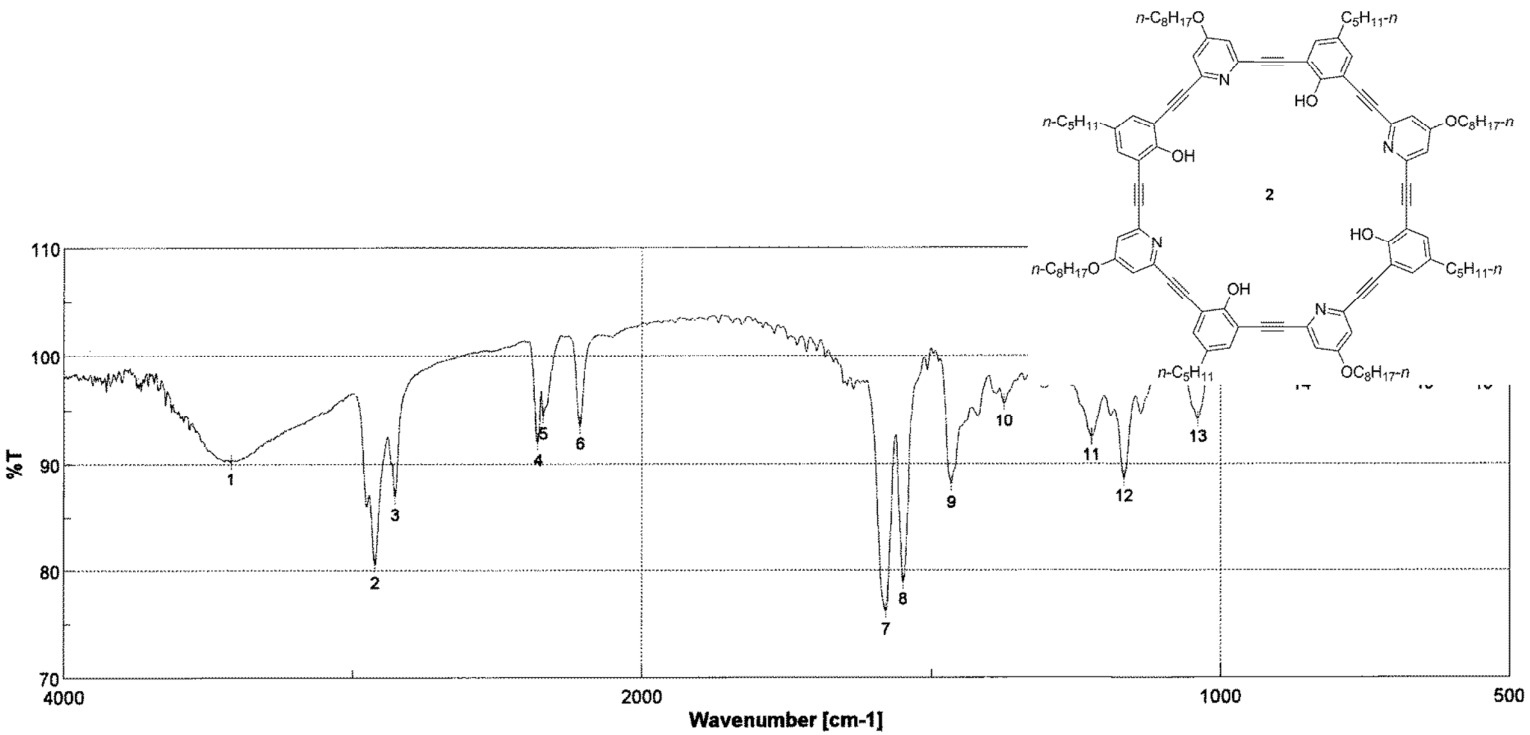
25.789
23.700
22.946
22.603
22.479
14.047
13.990
-0.051



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3420	90.22	2	2926	80.53	3	2855	86.89	4	2360	92.00	5	2342	94.45
6	2214	93.51	7	1579	76.14	8	1550	78.93	9	1466	88.03	10	1375	95.62
11	1224	92.49	12	1167	88.62	13	1038	94.17	14	859	99.03	15	647	99.05
16	546	99.03												