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Electronic Supplementary Information

Light-controlled switchable complexation by a non-photoresponsive hydrogen-bonded amide macrocycle†

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Contents

1. General methods

All chemicals were obtained from commercial supplier, which were used directly in the subsequent reactions without further purification and were used as received. All reactions were conducted with oven-dried glassware under atmosphere or nitrogen. Solvents were dried and distilled following usual protocols. Column chromatography was carried out using silica gel (300-400 mesh). Solvents for extraction and chromatography were reagent grade. $CDCl_3$, CD_3CN and CD_3OD were from Cambridge Isotope Laboratories (CIL).

Analytical NMR spectra were recorded on Bruker AVANCE AV II-400 MHz, at a constant temperature of 298 K. Chemical shifts are reported in δ values in ppm using tetramethylsilane (TMS) or residual solvent as internal standard. HRESI mass spectra were recorded on a Bruker Daltonics MicroTOF-Q II. UV-vis spectra were measured by SHIMADZU UV-2450.

2. ^{1}H NMR spectra of the compounds

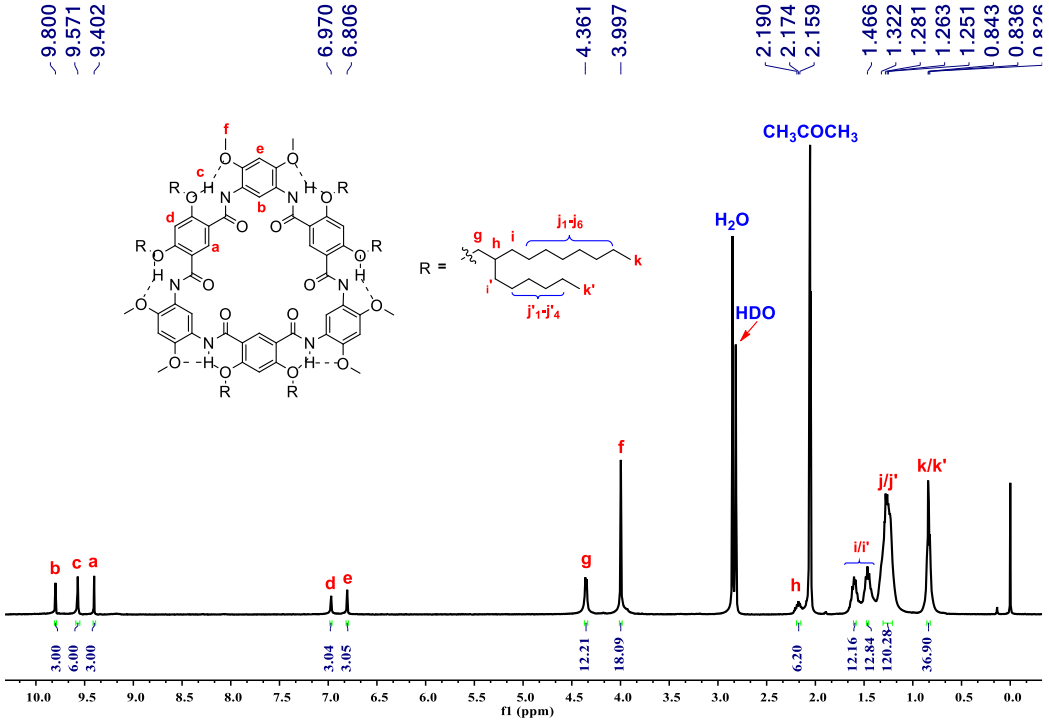

Figure S1. ^{1}H NMR spectrum (400 MHz, CD_3COCD_3, 298 K) of compound **1**

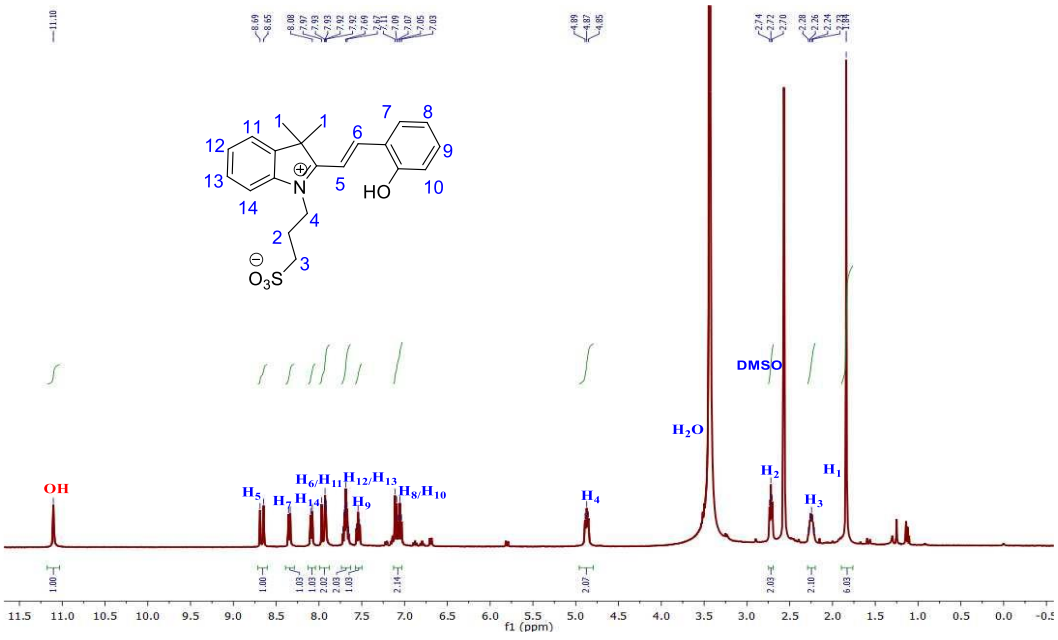

Figure S2. ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **1-MEH**.

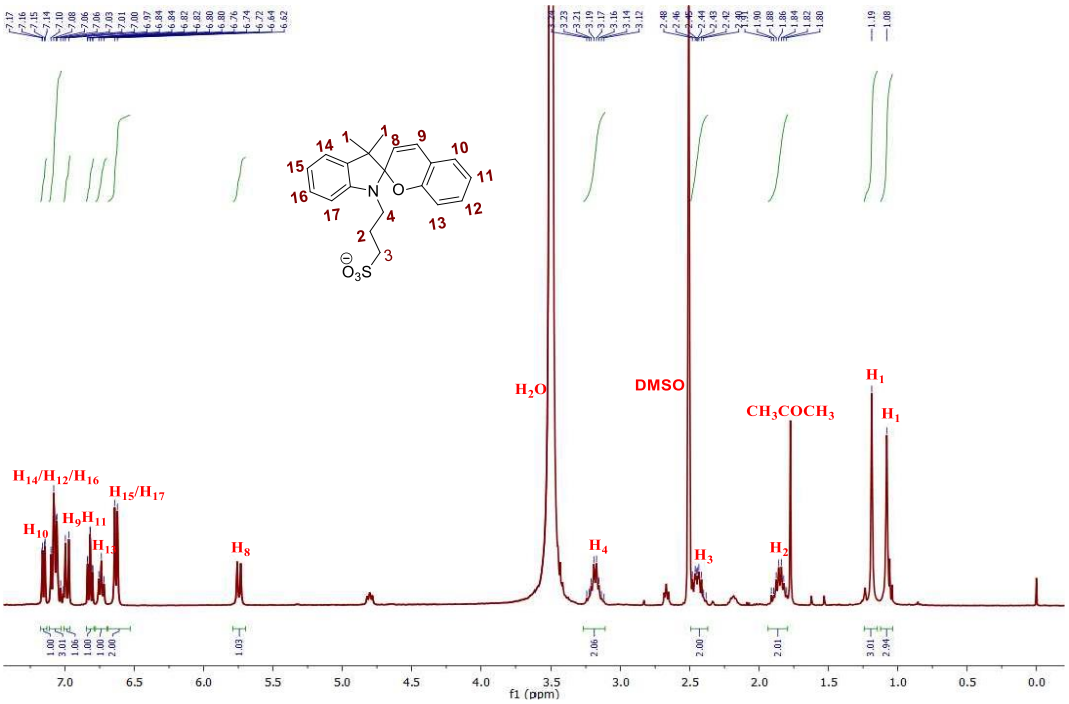

Figure S3. ^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K) of **1-SP**.

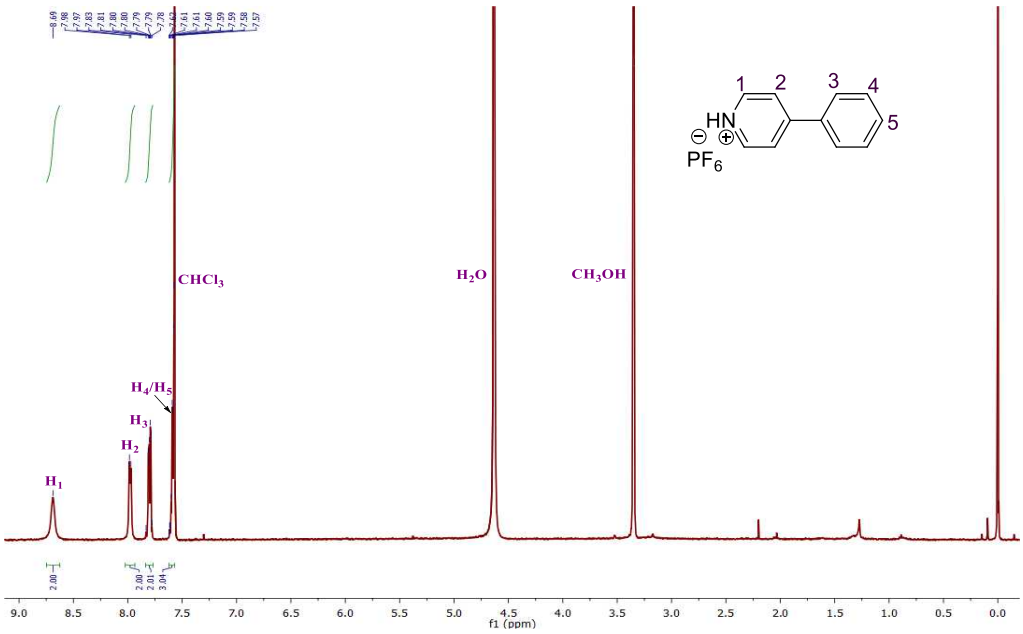

Figure S4. ^{1}H NMR spectrum (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of **2a**.

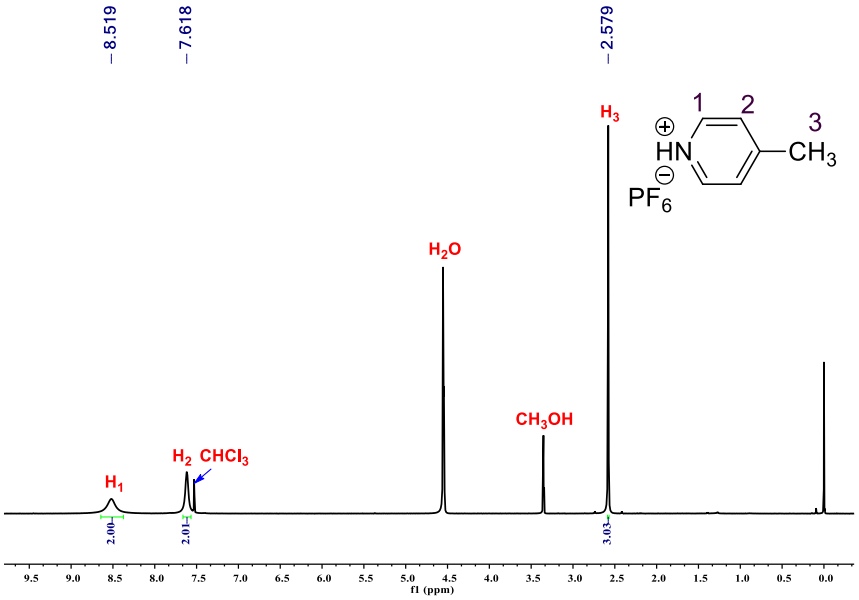

Figure S5. ^{1}H NMR spectrum (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of **2b**.

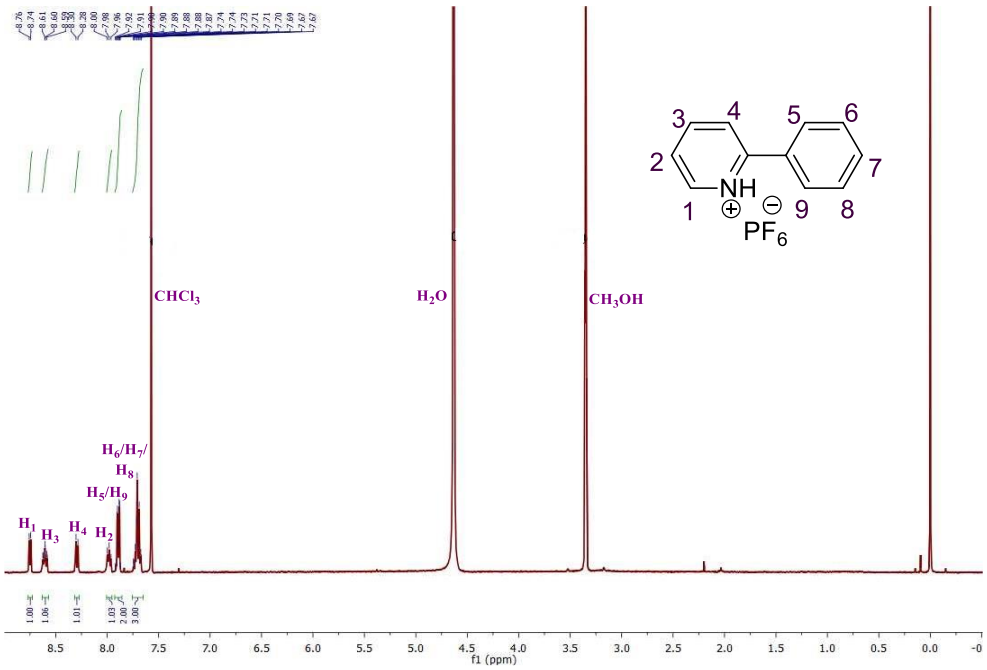

Figure S6. ^{1}H NMR spectrum (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of **2c**.

3. Binding constants of 1 ⊃ 2a -2c by UV-vis titration

To determine the association constants (Ka) corresponding to the reactions between macrocycle **1** and guests **2a-2c, UV**-vis titration experiments were performed in $CHCl_3/CH_3CN$ (1:1, v/v, 298 K) solutions at a constant concentration of **1** (50 μM) and varying concentrations of guests **2a-2c**. For each titration, at least 20 data points were collected. One wavelength (365 nm) was selected after

monitoring absorption at different wavelengths. Association constants were obtained by a global fitting analysis to a 1:1 binding model using the website http://app.supramolecular.org/bindfit/

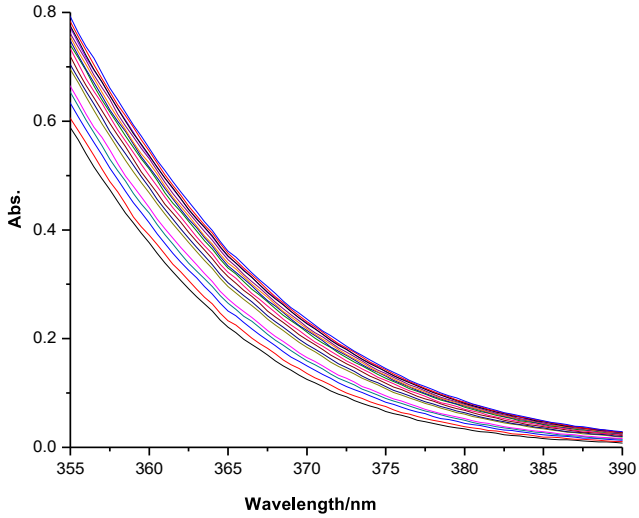

Figure S7. Stacked UV-vis spectra of **1** (50 μM**)** titrated with **2a** from 0 equiv to 1.5 equiv in $CHCl_3/CH_3CN$ (1:1, v/v, 298 K).

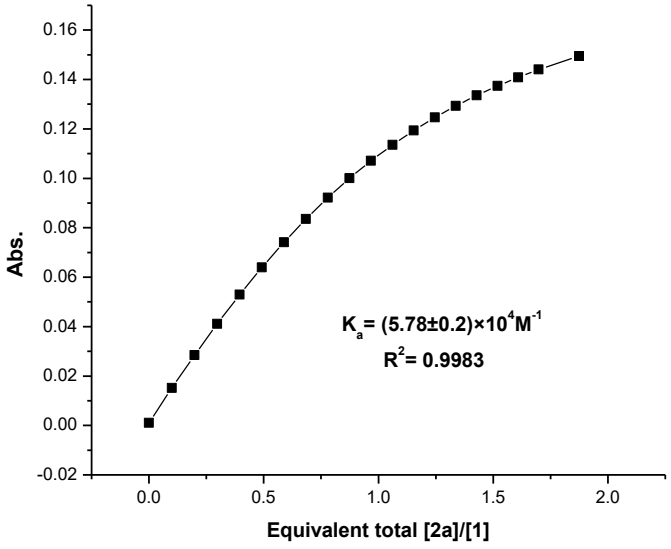

Figure S8. Determination of the binding constant of **1** (50 μM) and **2a** in $CHCl_3/CH_3CN$ (1/1, v/v, 298 K).

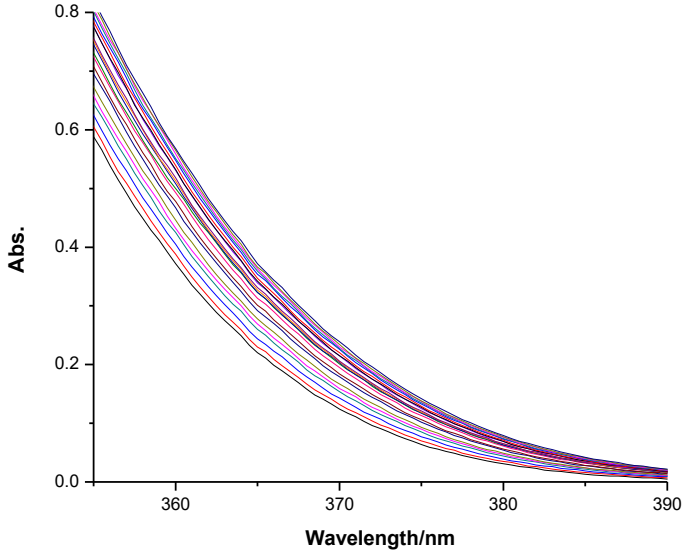

Figure S9. Stacked UV-vis spectra of **1** (50 μM**)** titrated with **2b** from 0 equiv to 1.5 equiv in $CHCl_3/CH_3CN$ (1:1, v/v, 298 K).

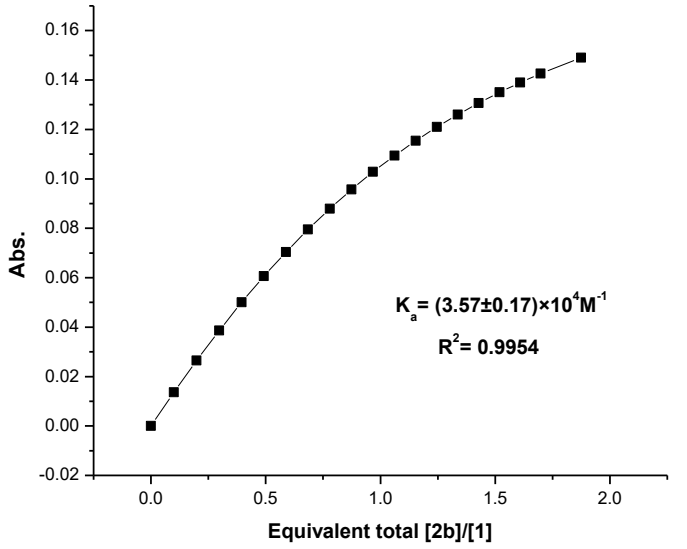

Figure S10. Determination of the binding constant of **1** (50 μM) and **2b** in $CHCl_3/CH_3CN$ (1/1, v/v, 298 K).

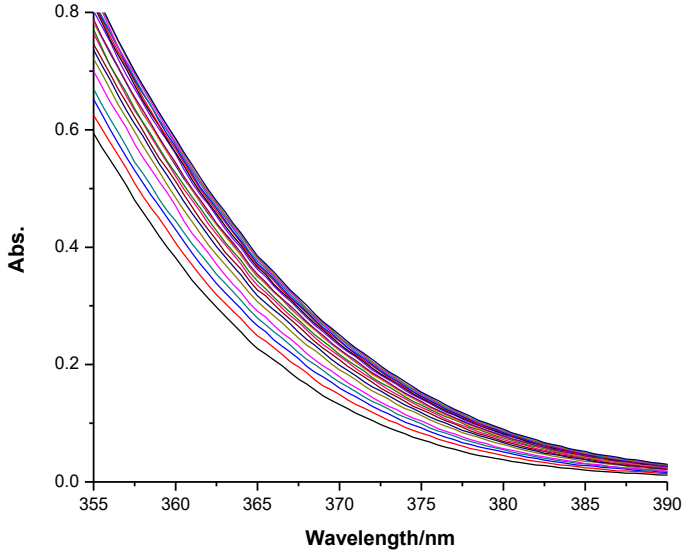

Figure S11. Stacked UV-vis spectra of **1** (50 μM**)** titrated with **2c** from 0 equiv to 1.5 equiv. in $CHCl_3/CH_3CN$ (1:1, v/v, 298 K).

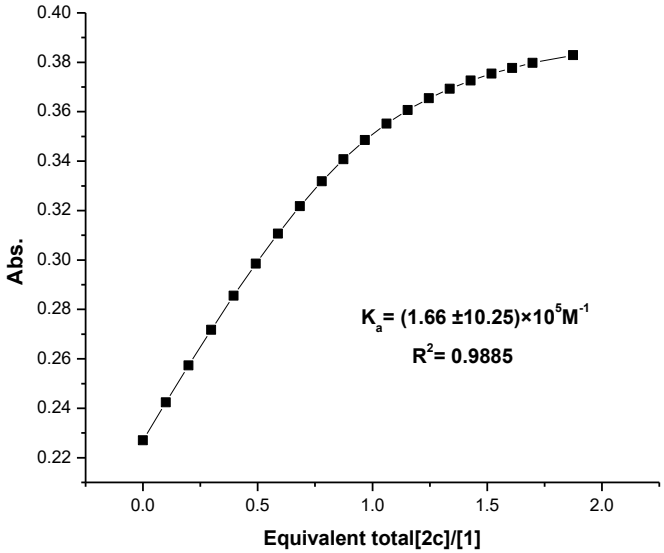

Figure S12. Determination of the binding constant of **1** (50 μM) and **2c** in $CHCl_3/CH_3CN$ (1/1, v/v, 298 K).

4. Interaction study of photoacid on host 1 and neutral form of guest 2a

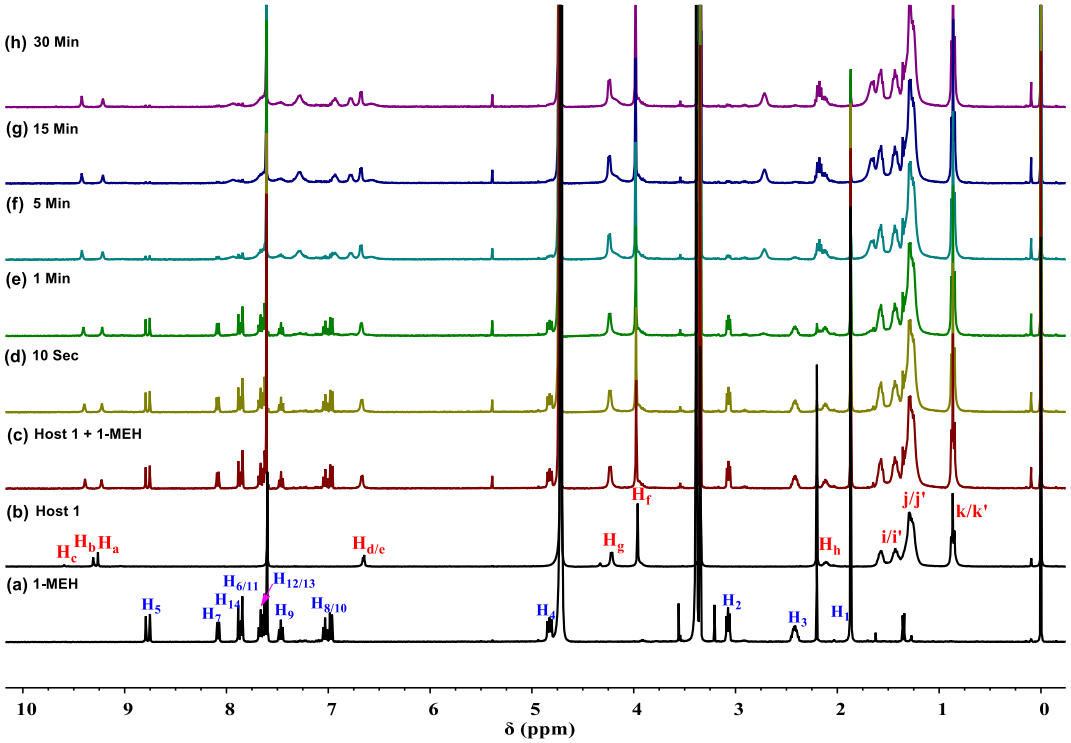

Figure S13 ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) **1-MEH**, (b) host **1** (c) host **1** + photoacid without irradiation, (d) sample b after 10 sec irradiation, (e) 1 min, (f) 5 min, (g) 15 min and (h) 30 min.

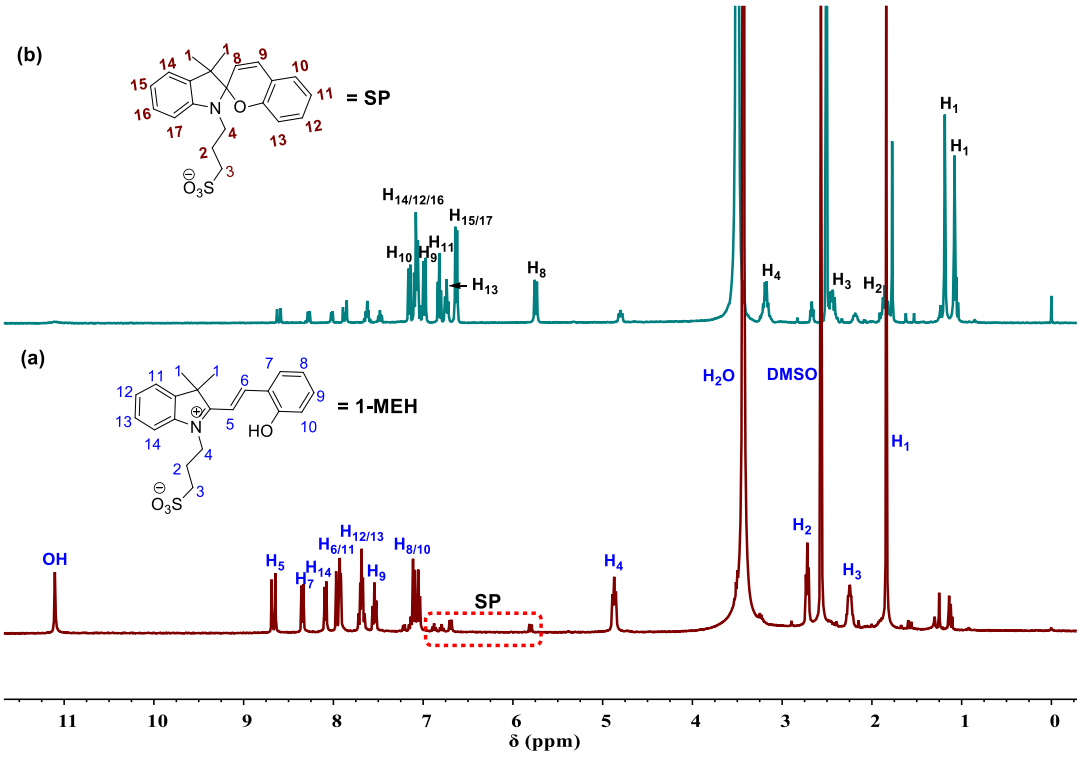

Figure. S14 Stacked ^{1}H NMR spectra (400 MHz, DMSO-d_6, 298 K) of (a) **1-MEH** and (b) **SP.**

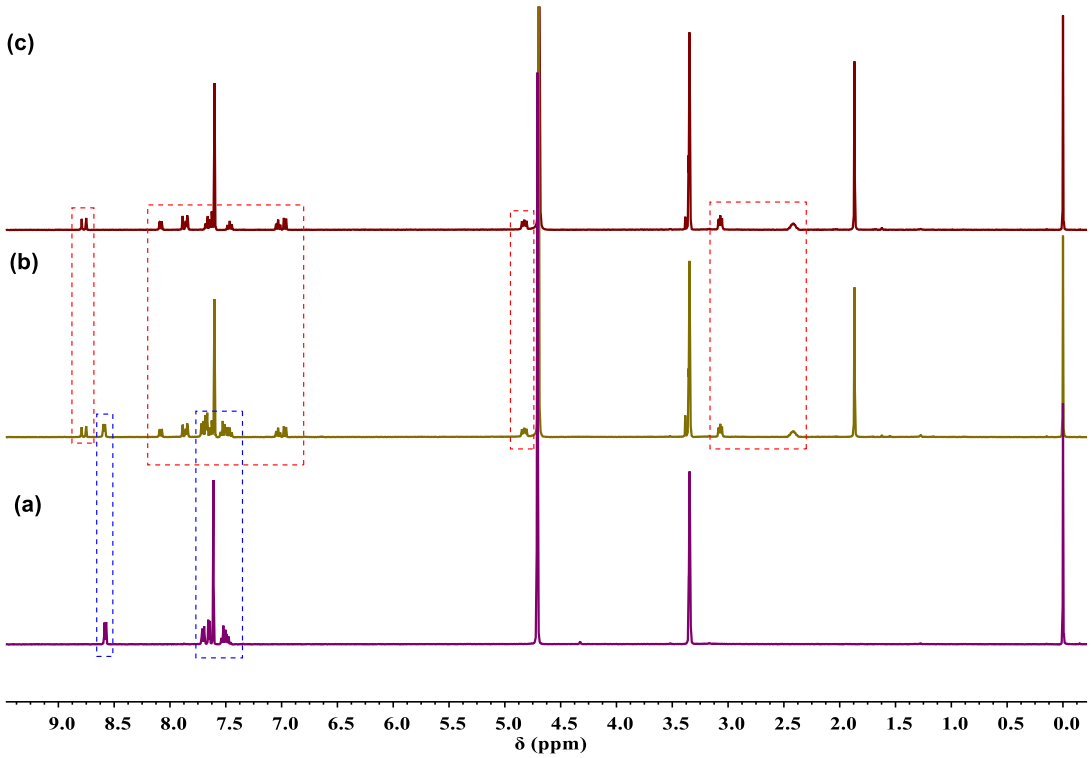

Figure S15 ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) 4-phenylpyridine, (b) 4-phenylpyridine with photoacid, and (c) photoacid.

5. ^{1}H NMR studies on the complexation between 1 ⊃ 2a-2c

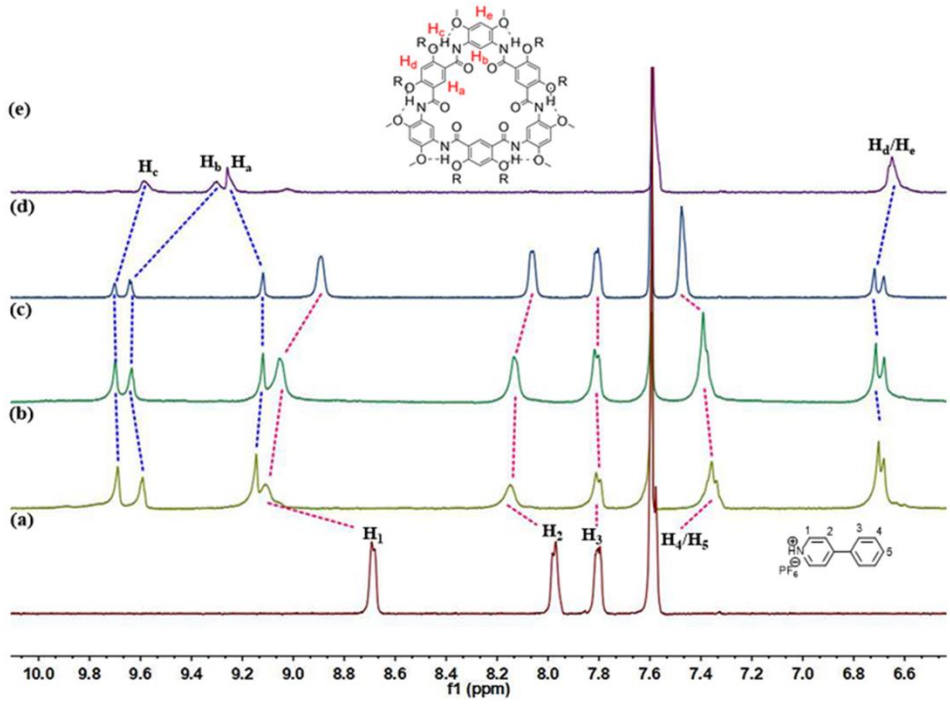

Figure S16. Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) free guest **2a**, (b) host **1** with 0.5 equiv guest **2a**, (c) host **1** with 1 equiv of guest **2a,** (d) 0.5 equiv host **1** with 1 equiv of guest **2a** and (e) free host **1**.$[\mathbf{1}]_0 = [\mathbf{2a}]_0$ = 3.0 mM.

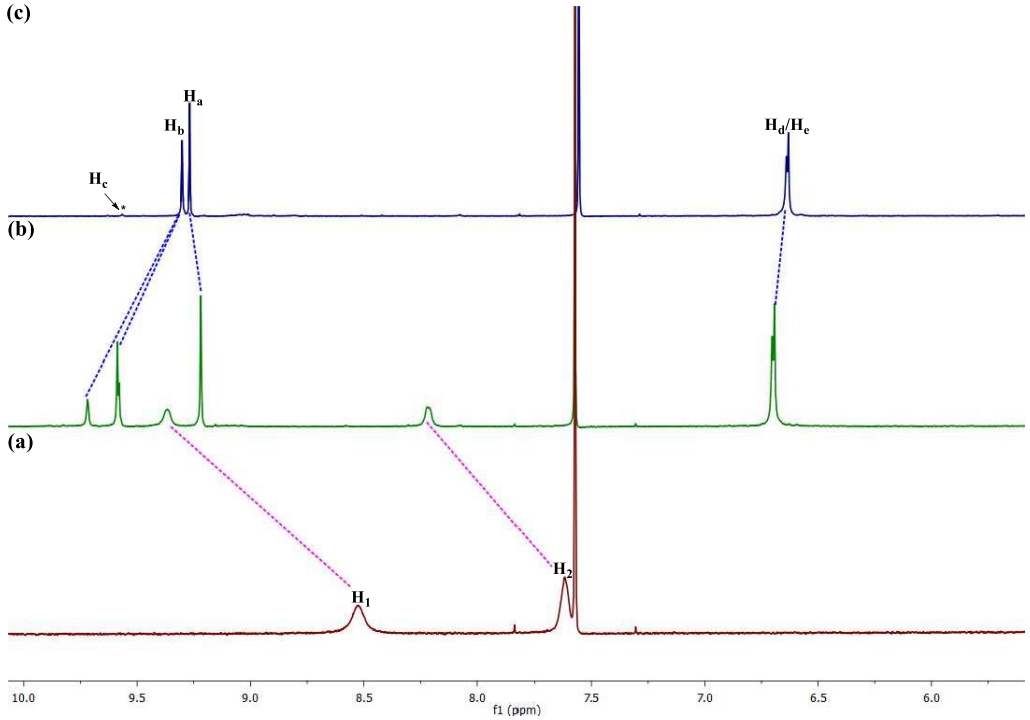

Figure S17. Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) free guest **2b**, (b) host **1** with 1.0 equiv guest **2b** and (c) free host **1**.$[\mathbf{1}]_0 = [\mathbf{2b}]_0$ = 3.0 mM.

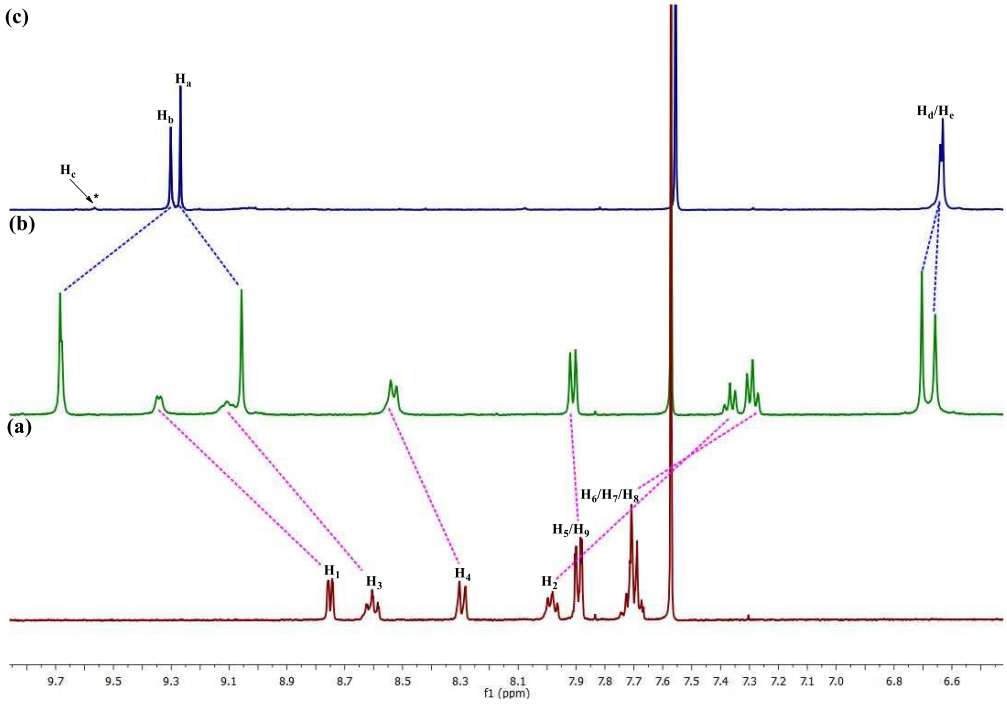

Figure S18. Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) free guest **2c**, (b) host **1** with 1.0 equiv guest **2c** and (c) free host **1**.$[\mathbf{1}]_0 = [\mathbf{2c}]_0$ = 3.0 mM.

6. 2D ROESY for H-G interactions

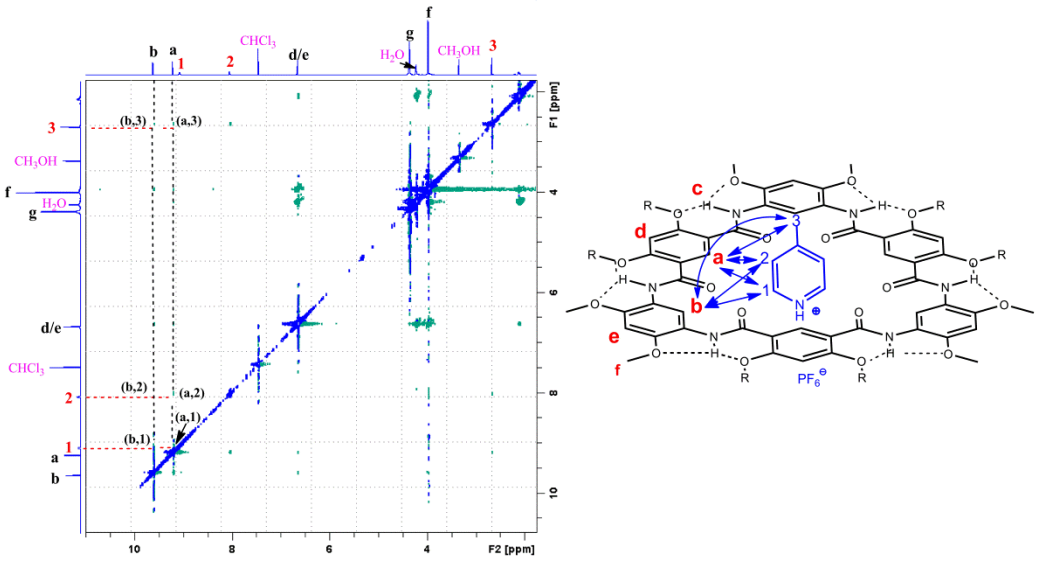

Figure S19. Expanded 2D ^{1}H-^{1}H ROESY NMR spectrum of **1** ⊃ **2b** in $CDCl_3/CD_3OD$ (1:1, v/v, 298 K 600 MHz, 10 mM, mixing time: 0.4 s).

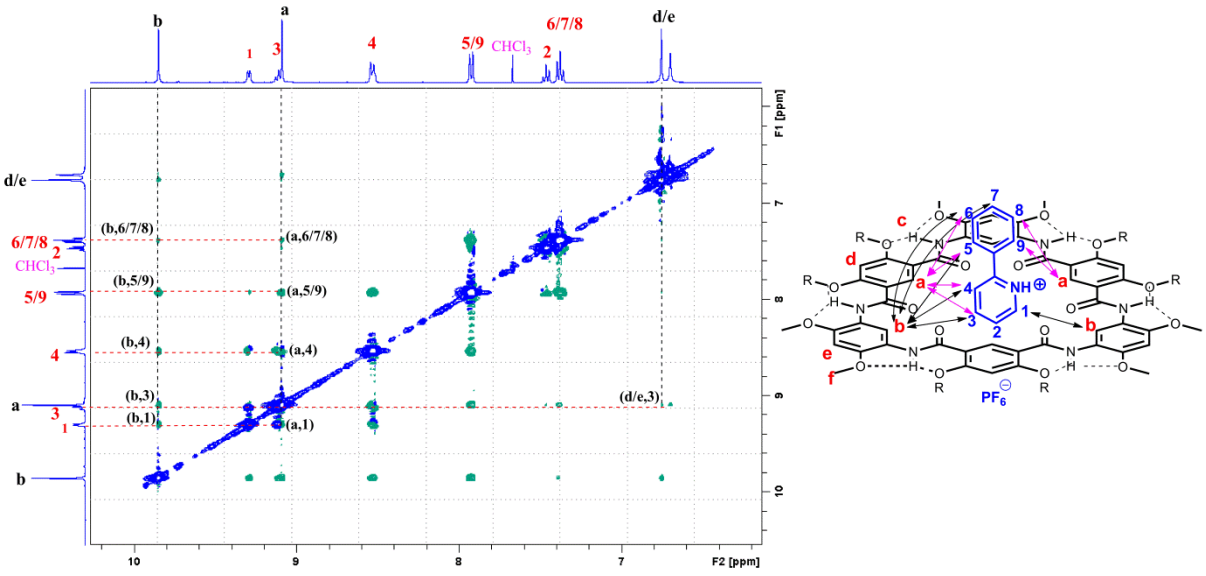

Figure S20. Expanded 2D ^{1}H-^{1} HROESY NMR spectrum of **1** ⊃ **2c** in $CDCl_3/CD_3OD$ (1/1, v/v, 298 K , 600 MHz, 10 mM, mixing time: 0.4 s).

7. Determination of stoichiometry of 1 ⊃ 2a-2c by job plot

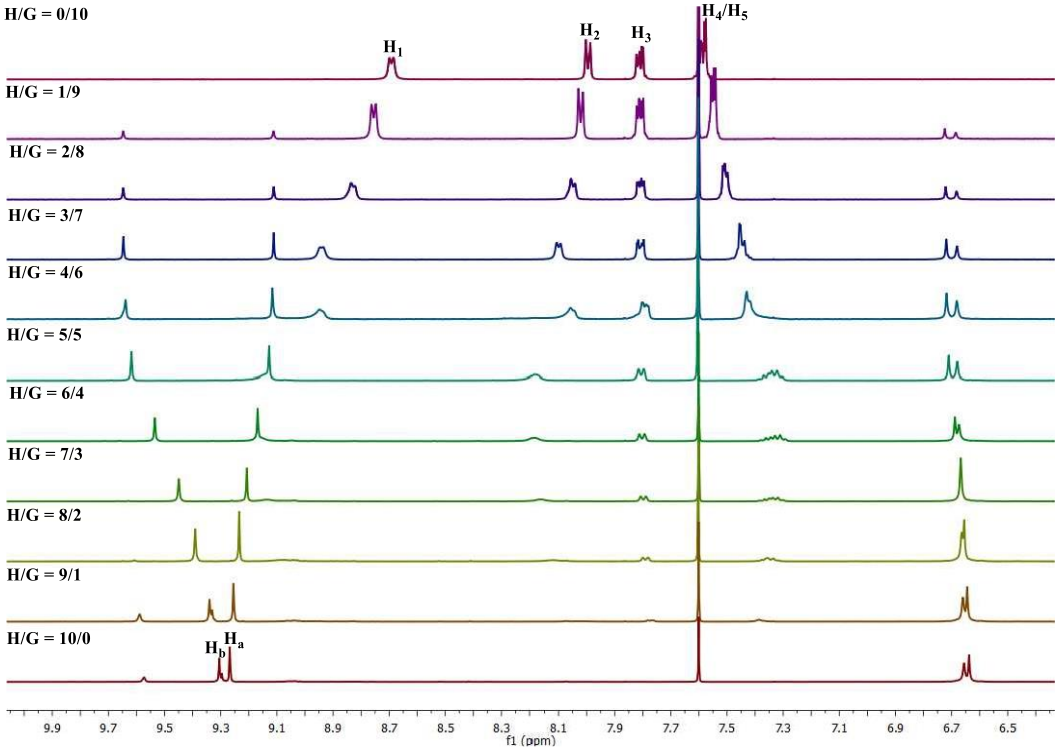

Figure S21. Partial stacked ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of **1** ⊃ **2a** in the presence of the different ratio of **1** and **2a** at a fixed total concentration 1.0 mM.

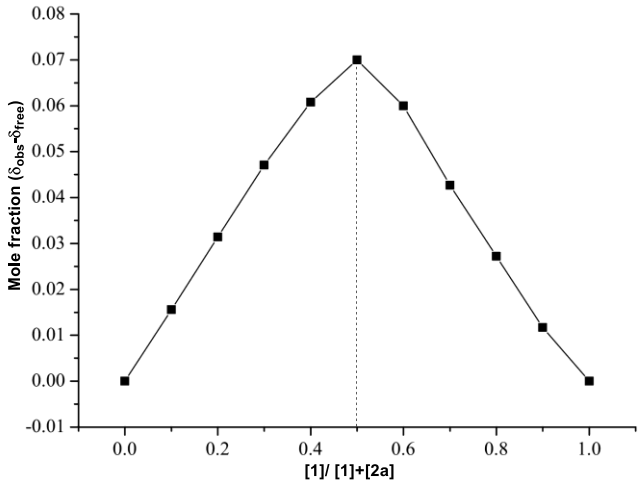

Figure S22. Job plot for the determination of stoichiometry in the complex formed by **1** and **2a** from ^{1}H NMR measurements in $CDCl_3/CD_3OD$ (1:1, v/v, 298 K).

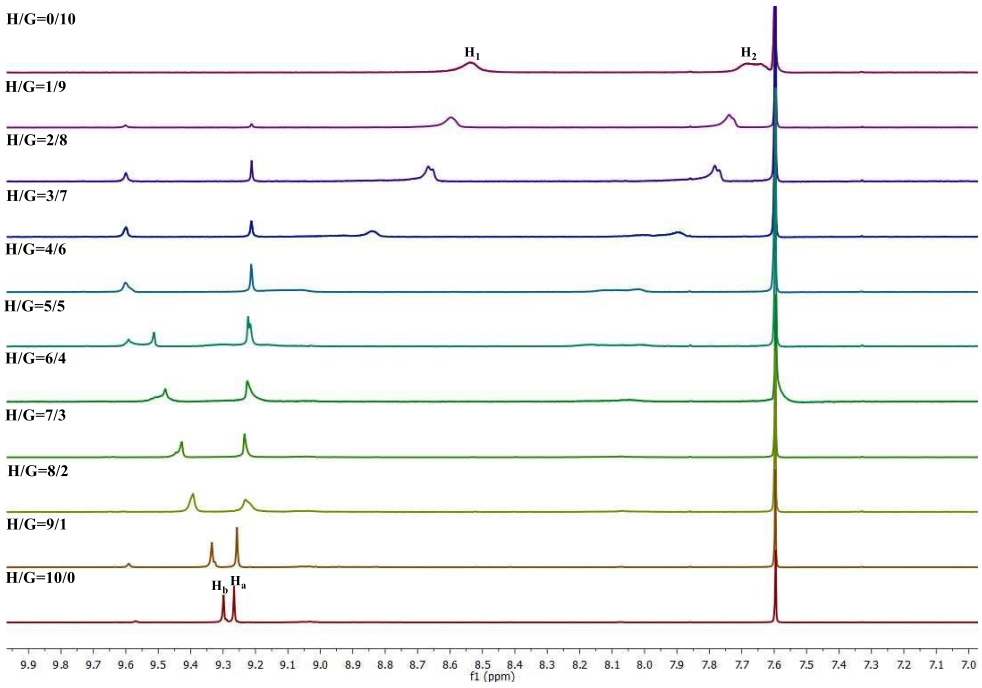

Figure S23. Partial stacked ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1/1, v/v 298 K,) of **1** ⊃ **2b** in the presence of the different ratio of **1** and **2b** at a fixed total concentration 1.0 mM.

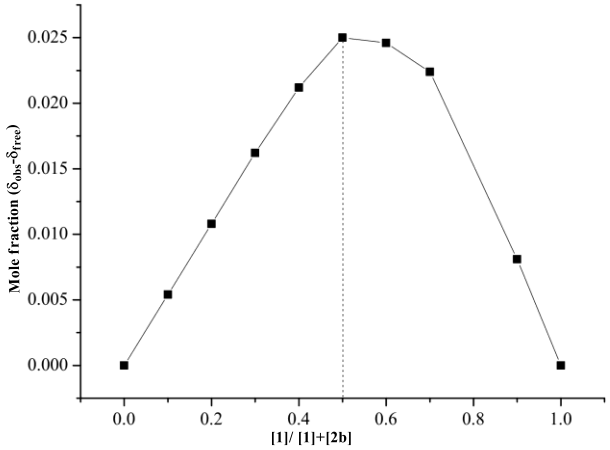

Figure S24. Job plot for the determination of stoichiometry in the complex formed by **1** and **2b** from ^{1}H NMR measurements in $CDCl_3/CD_3OD$ (1:1, v/v, 298 K).

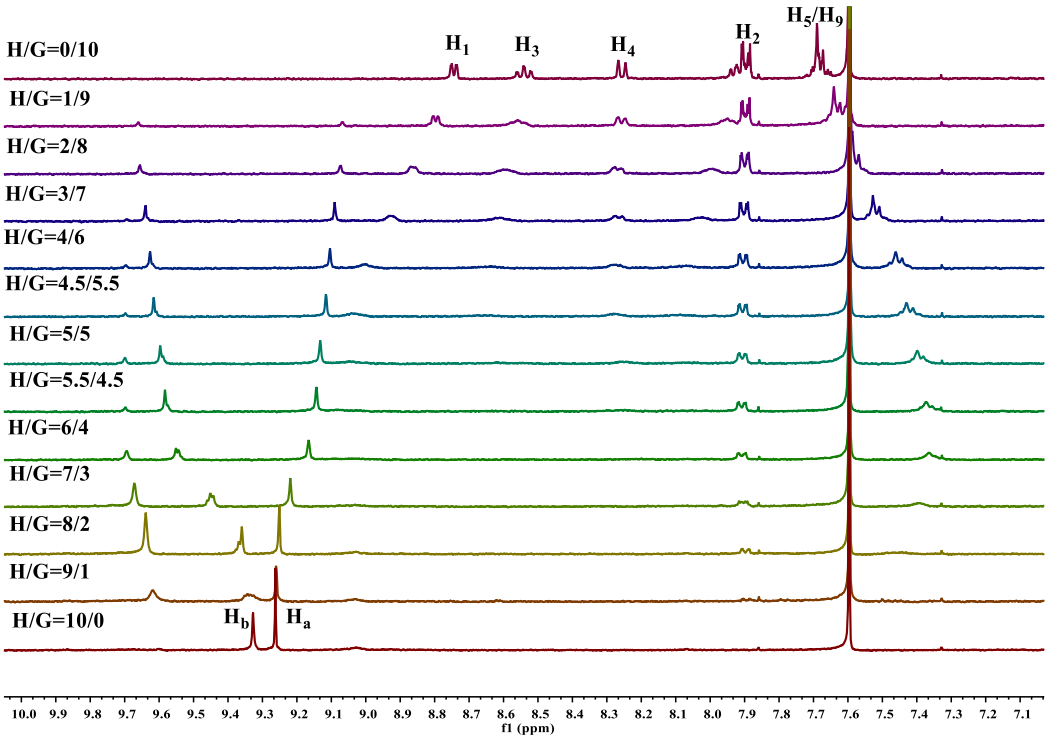

Figure S25. Partial stacked ^{1}H NMR spectra (400 MHz, $CDCl_3$: CD_3OD, 1/1, v/v, 298 K,) of **1** ⊃ **2c** in the presence of the different ratio of **1** and **2c** at a fixed total concentration 1.0 mM.

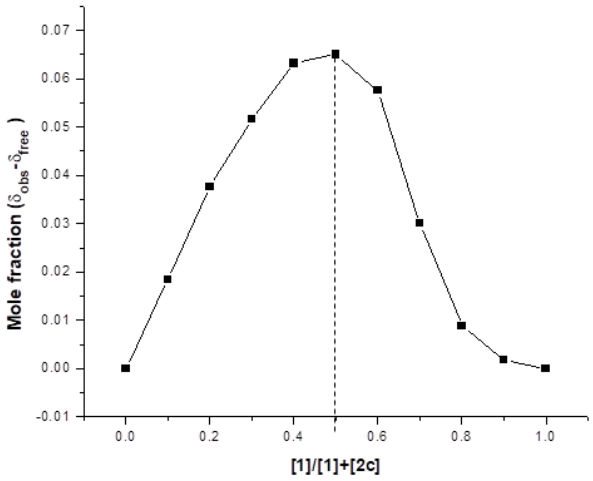

Figure S26. Job plot for the determination of stoichiometry in the complex formed by **1** and **2c** from ^{1}H NMR measurements in $CDCl_3$/CD_3OD (1:1, v/v, 298 K).

8. HRESI-MS spectra of the complexes 1 ⊃ 2a-2c

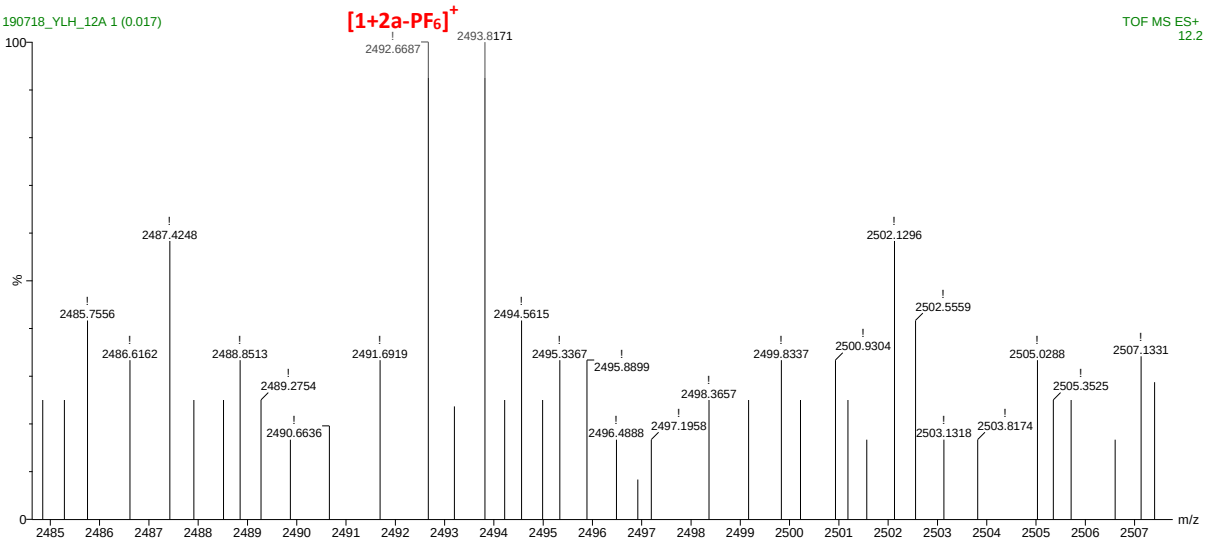

Figure S27. Partial HRESI MS spectrum of complex **1⊃2a.**

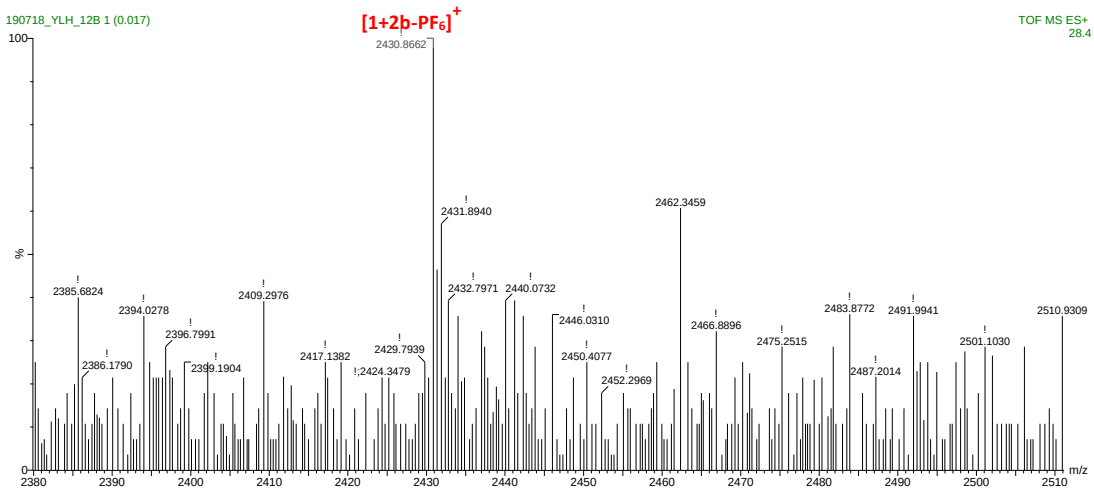

Figure S28. Partial HRESI MS spectrum of complex **1 ⊃ 2b.**

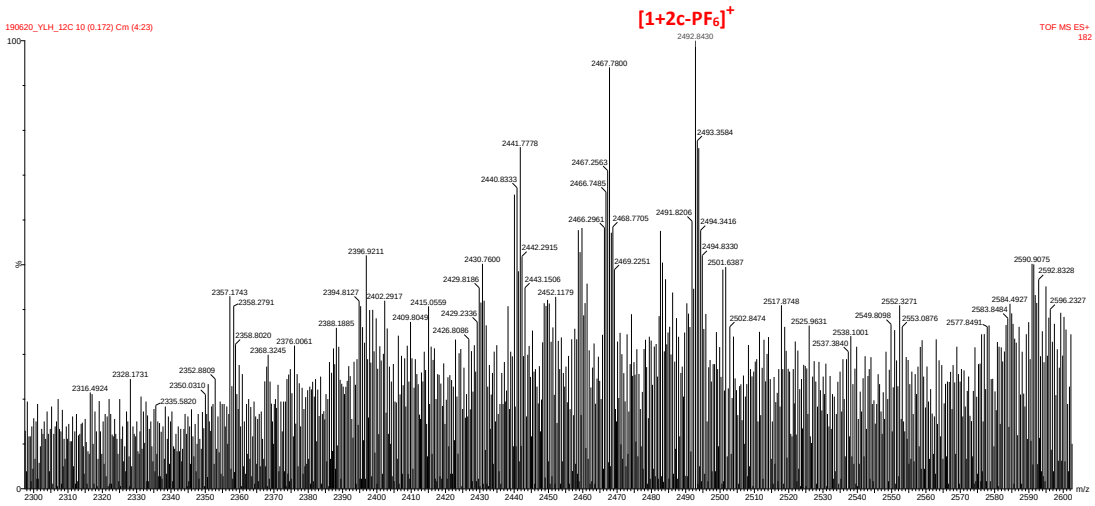

Figure S29. Partial HRESI MS spectrum of complex **1 ⊃ 2c.**

9. Acid-base controlled binding and release process of 2a in the complex

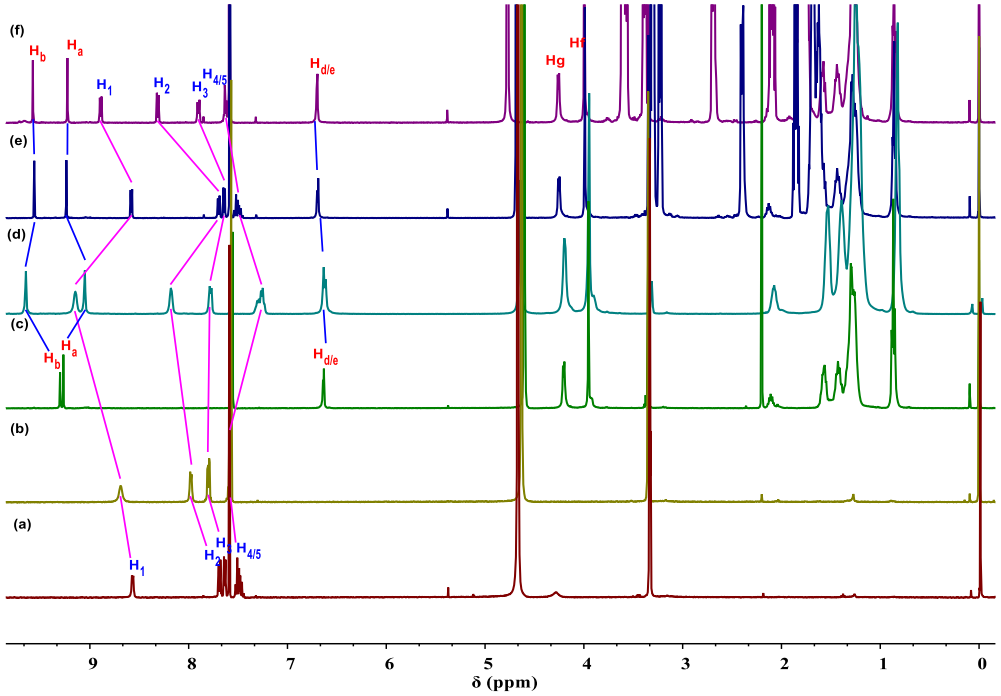

Figure. S30. ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) 4-phenylpyridine, (b) guest **2a**, (c) host **1**, (d) guest **2a** + host **1** (1.0 equiv), (e) solution of d 1.5 equiv of DBU added and (f) solution of e 1.5 equiv of TFA added. [H]0 = 3.0 mM.

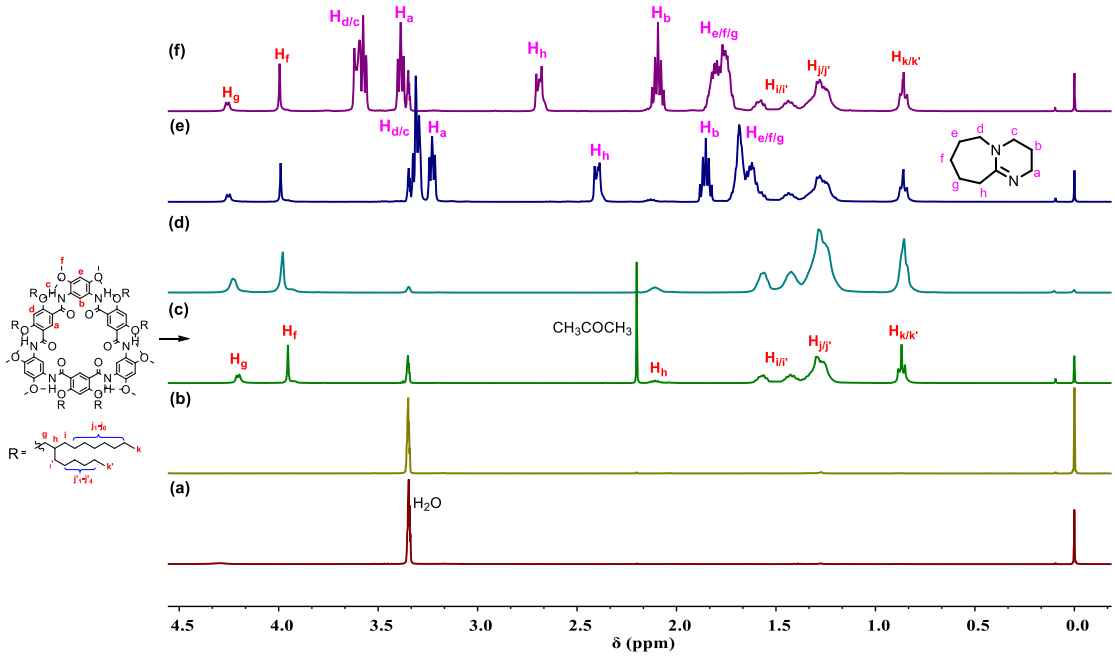

Figure. 31. ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) 4-phenylpyridine, (b) guest **2a**, (c) host **1**, (d) guest **2a** + host **1** (1.0 equiv), (e) solution of d 1.5 equiv of DBU added and (f) solution of e 1.5 equiv of TFA added. [H]0 = 3.0 mM.

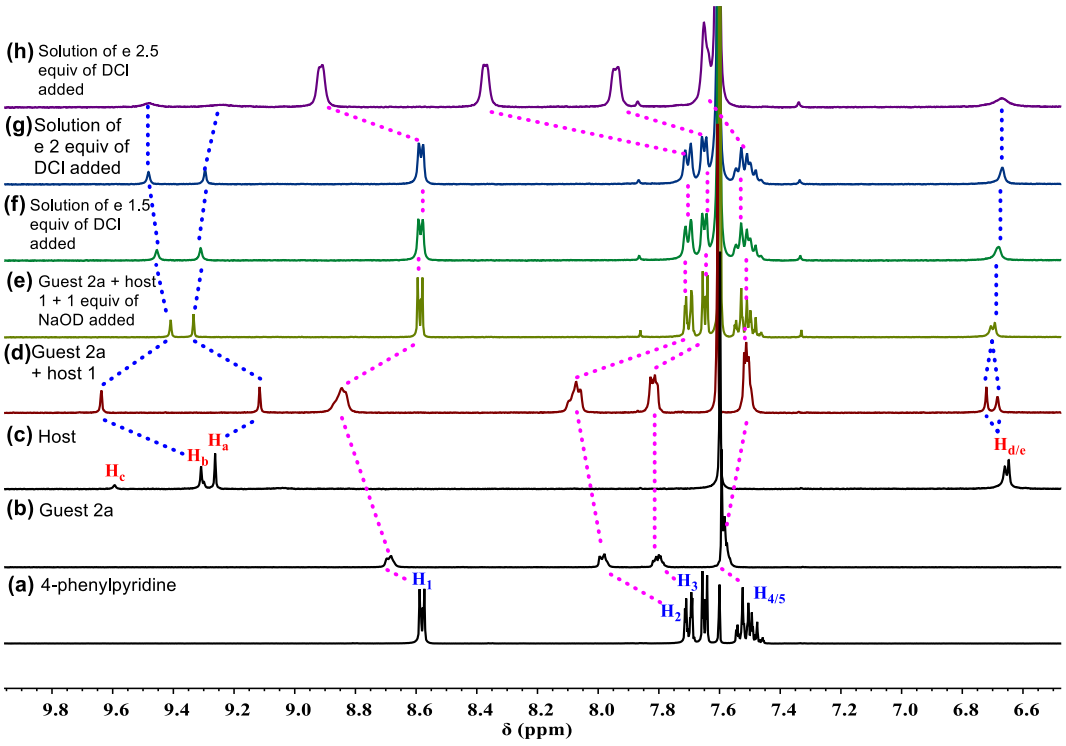

Figure. S32 ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, v/v, 298 K) of (a) 4-phenylpyridine, (b) guest **2a**, (c) host **1**, (d) guest **2a** + host **1** (1.0 equiv), (e) solution of d 1 equiv of NaOD added (f) solution of e 1.5 equiv of DCl added, (g) solution of e 2 equiv of DCl added, (h) solution of e 2.5 equiv of DCl added. [H]0 = 3.0 mM.

10.Photoacid controlled binding and release process of 2b and 2c in the complexes

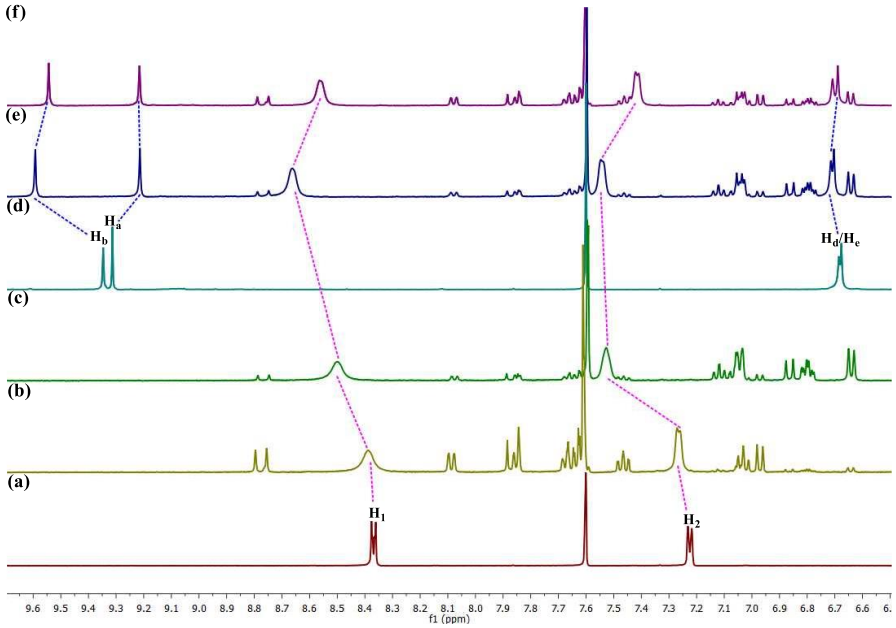

Figure S33. Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1/1, v/v, 298 K) of (a) 4-methylpyridine, (b) 4-methylpyridine + **1-MEH** (1.2 equiv) before light irradiation, (c) solution of b irradiated for 5 min with 420 nm light, (d) host macrocycle **1,** (e) solution of c 1.0 equiv of **1** added and (f) solution of e placed under dark conditions for 120 min. $[H]_0 = [G1]_0 = 3.0$ mM.

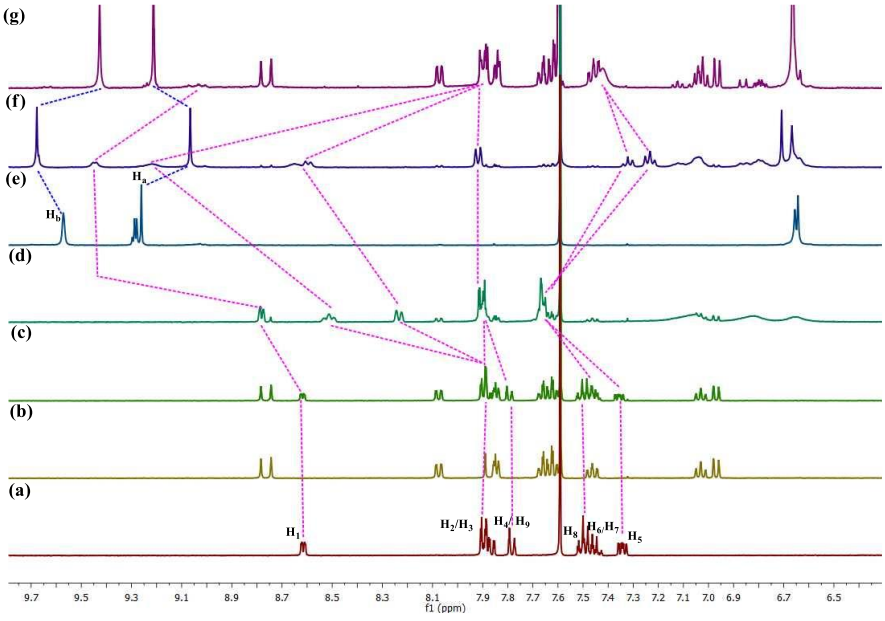

Figure S34. Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1/1, v/v, 298 K) of (a) 2-phenylpyridine, (b) **1-MEH**, (c) 2-phenylpyridine + **1-MEH** (1.2 equiv) before light irradiation, (d) solution of c irradiated for 5 min

with 420 nm light, (e) host macrocycle **1,** (f) solution of d 1.0 equiv of **1** added and (g) solution of f placed under dark conditions for 120 min. $[H]_0 = [G1]_0 = 3.0$ mM

11. ^{1}H NMR studies on the complexation between 1 and dibenzylamine

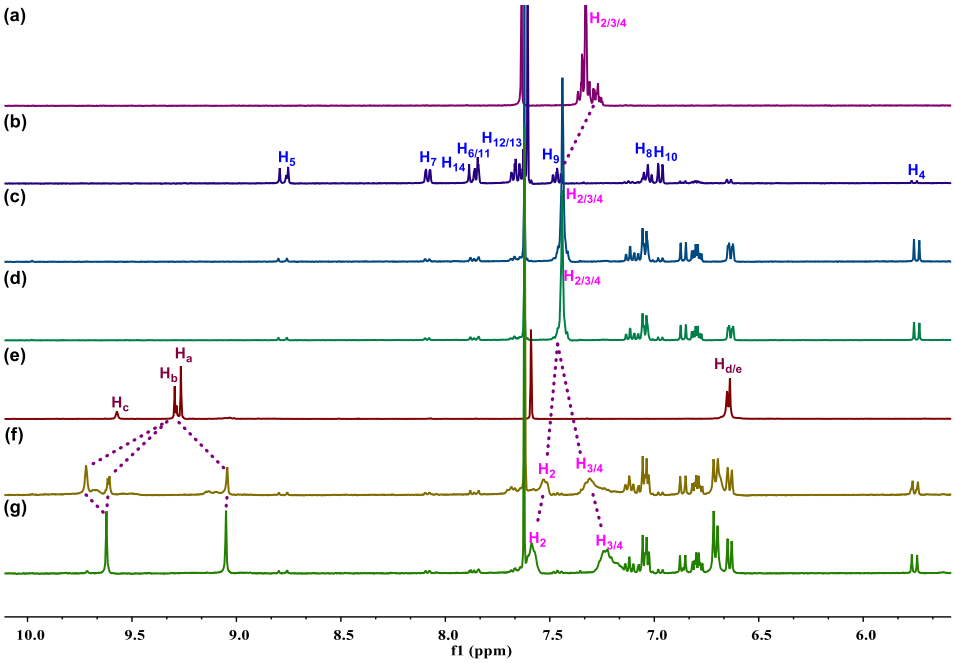

Figure S35. Partial ^{1}H NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1/1, v/v, 298 K) of (a) dibenzylamine, (b) **1-MEH** before irradiation, (c) dibenzyl amine + **1-MEH** before irradiation, (d) dibenzyl amine + **1-MEH** after irradiation, (e) host macrocyle **1**, (f) solution of d 1.0 equiv of **1** added and (g) solution of f placed under dark conditions for 150 min. [H]0 = [G1]0= 3.0 mM

12. ^{1}H NMR study on H-D exchange of the amide proton H_c of 1 with deuterated methanol

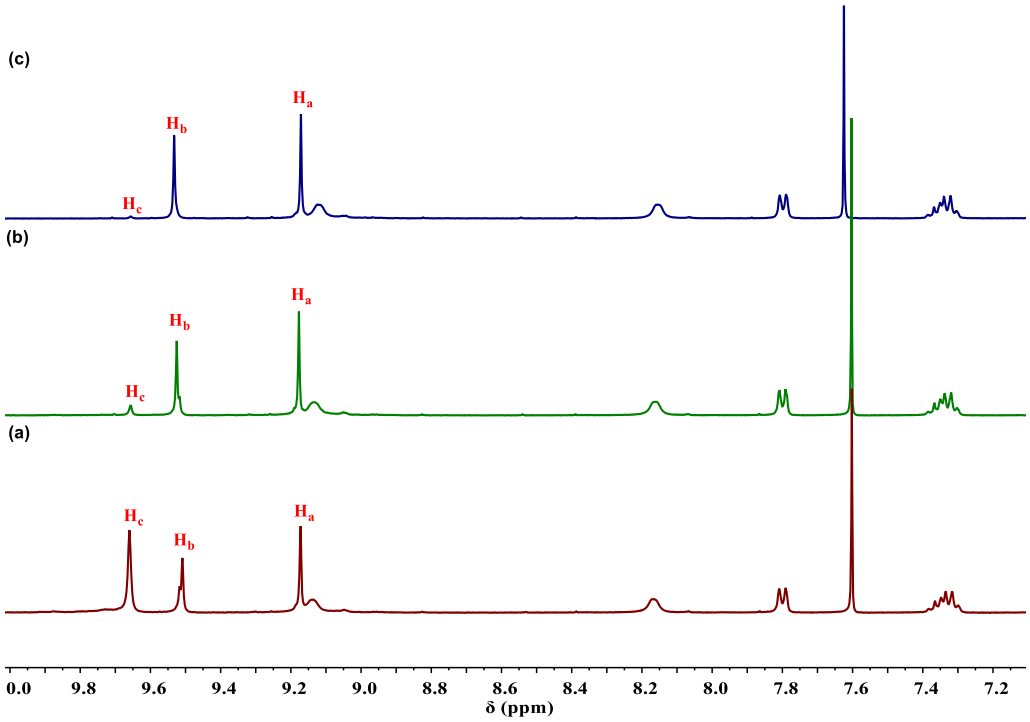

Figure S36. ^{1}H-NMR spectra (400 MHz, $CDCl_3/CD_3OD$, 1:1, V/V, 298 K) of complex **1** ⊃ **2a** (a) immediately after adding mixed solvent, (b) 10 min and (c) 30 min.

13. Molecular modelling of 1 ⊃ 2b and 1 ⊃ 2c

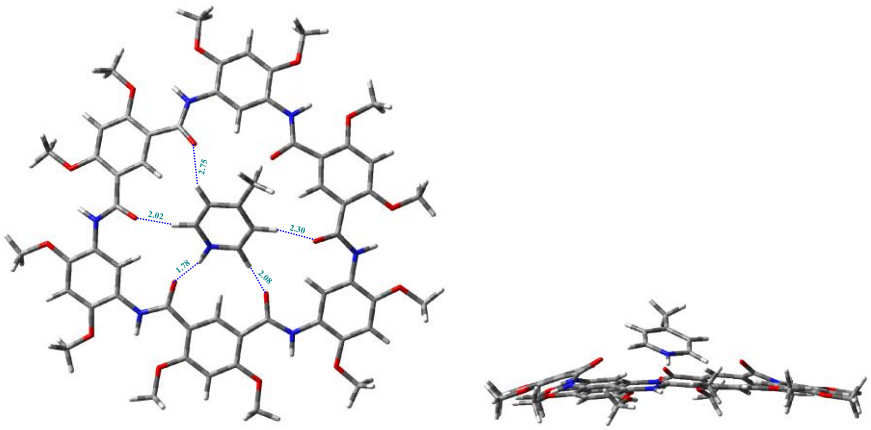

Figure S37. Top (left), Side (right) and view of optimized geometry of **1** ⊃ **2b** at the RB3PW91/6-31G (d,p) level: (perpendicular conformation) The blue dashed lines indicate intermolecular H-bonds. All side chains are replaced by methyl groups for simplicity (gray = C, white = H, red = O, and blue = N).

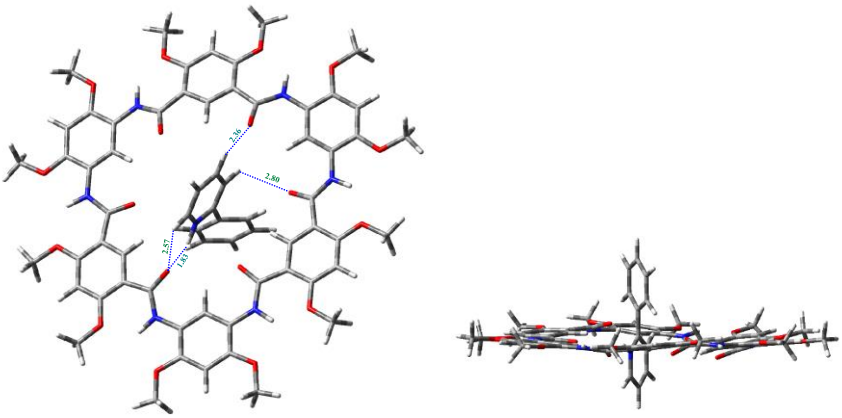

Figure S38. Top (left), Side (right) and view of optimized geometry of **1⊃2c** at the RB3PW91/6-31G(d,p) level: (perpendicular conformation) The blue dashed lines indicate intermolecular H-bonds. All side chains are replaced by methyl groups for simplicity (gray = C, white = H, red = O, and blue = N).

1 ⊃ 2a DFT Original data

		Coordinates (Angstroms)		
Center number	Symbol	X	Y	Z
1	C	5.549141	3.465723	-0.22323
2	C	4.210844	3.841979	-0.07471
3	C	3.789129	5.140772	-0.36887
4	C	4.738969	6.087533	-0.80113
5	C	6.081586	5.725932	-0.94073
6	C	6.488237	4.419007	-0.65808
7	H	3.491044	3.123474	0.274985
8	H	6.804588	6.455481	-1.27592
9	O	4.243771	7.336086	-1.08161
10	O	7.776003	3.962837	-0.79467
11	C	5.141095	8.331196	-1.54953
12	H	5.611522	8.037169	-2.49617
13	H	4.542215	9.22847	-1.71067
14	H	5.92092	8.548603	-0.80931

15	C	8.768909	4.867487	-1.25335
16	H	9.701627	4.302976	-1.28777
17	H	8.538537	5.24438	-2.25772
18	H	8.887938	5.714529	-0.56665
19	N	6.005929	2.138684	-0.05047
20	C	5.302337	1.106531	0.494833
21	H	6.933925	1.940366	-0.40345
22	O	4.226691	1.265599	1.079267
23	C	5.812178	-0.29537	0.283335
24	C	7.122231	-0.71694	-0.02098
25	C	4.837461	-1.28319	0.38393
26	C	7.402228	-2.08078	-0.18255
27	C	5.057349	-2.64798	0.210024
28	H	3.829654	-0.95952	0.588073
29	C	6.38682	-3.04019	-0.07329
30	H	8.412182	-2.39629	-0.39732
31	O	8.070492	0.2518	-0.13795
32	C	9.423461	-0.10924	-0.40757
33	H	9.827683	-0.74534	0.387388
34	H	9.514866	-0.61854	-1.37358
35	H	9.977831	0.828343	-0.43736
36	O	6.627158	-4.37166	-0.23202
37	C	7.945668	-4.83313	-0.51709
38	H	7.865855	-5.91711	-0.5927
39	H	8.311875	-4.42679	-1.46635
40	H	8.63806	-4.57401	0.291106
41	C	3.827518	-3.51019	0.314998

42	O	2.747428	-2.99973	0.657716
43	N	3.941444	-4.82443	-0.01193
44	H	4.872628	-5.15937	-0.23232
45	N	2.43718	5.542401	-0.34545
46	C	1.373389	4.833547	0.146013
47	H	2.237936	6.438346	-0.77302
48	O	1.500062	3.804013	0.813761
49	C	-0.00844	5.302674	-0.23073
50	C	-0.40405	6.59545	-0.63201
51	C	-0.99824	4.321565	-0.18147
52	C	-1.745	6.862192	-0.93233
53	C	-2.34239	4.534769	-0.48901
54	H	-0.70881	3.319369	0.103753
55	C	-2.70859	5.846779	-0.86106
56	H	-2.03981	7.859369	-1.22293
57	O	0.568227	7.550907	-0.69884
58	C	0.226261	8.882728	-1.06968
59	H	-0.1915	8.92125	-2.08232
60	H	-0.48474	9.320897	-0.36038
61	H	1.15896	9.445801	-1.04009
62	O	-4.02253	6.077629	-1.148
63	C	-4.44853	7.374515	-1.5522
64	H	-3.95328	7.684742	-2.47915
65	H	-5.52112	7.29013	-1.72582
66	H	-4.26424	8.117185	-0.76767
67	C	-3.21255	3.30079	-0.39502
68	O	-2.688	2.218028	-0.13272

69	N	-4.55744	3.450013	-0.60761
70	H	-4.89063	4.378699	-0.83426
71	C	-5.53439	2.434504	-0.62222
72	C	-6.85153	2.817071	-0.95369
73	C	-5.27188	1.089485	-0.34936
74	C	-7.86881	1.863689	-1.02596
75	C	-6.28441	0.127404	-0.41528
76	H	-4.27052	0.79806	-0.08663
77	C	-7.58824	0.519067	-0.76409
78	H	-8.87243	2.164065	-1.28969
79	C	2.916236	-5.79245	-0.11316
80	C	1.555564	-5.50529	0.016312
81	C	3.314842	-7.11131	-0.40737
82	C	0.585825	-6.49905	-0.14743
83	H	1.247948	-4.50461	0.252765
84	C	2.356079	-8.11379	-0.57184
85	C	0.997331	-7.81286	-0.44614
86	H	2.665226	-9.12328	-0.80021
87	O	4.667309	-7.31242	-0.52328
88	O	-0.01174	-8.72654	-0.60857
89	C	5.135481	-8.61971	-0.8204
90	H	4.849818	-9.33504	-0.03968
91	H	4.761372	-8.97054	-1.79012
92	H	6.22331	-8.55108	-0.86051
93	C	0.331003	-10.0721	-0.90613
94	H	-0.61167	-10.6154	-0.98113
95	H	0.868468	-10.1495	-1.8594

96	H	0.938741	-10.5168	-0.10875
97	N	-0.80293	-6.25549	-0.0882
98	C	-1.40973	-5.10216	0.319711
99	H	-1.40041	-7.01406	-0.39402
100	O	-0.77386	-4.15753	0.799165
101	C	-2.89478	-4.96025	0.117612
102	C	-3.81719	-5.92303	-0.34675
103	C	-3.39347	-3.68191	0.366227
104	C	-5.15824	-5.57462	-0.55712
105	C	-4.70738	-3.28204	0.144428
106	H	-2.70531	-2.93628	0.733805
107	C	-5.60112	-4.26382	-0.33351
108	H	-5.85568	-6.3215	-0.90586
109	O	-3.34697	-7.18289	-0.57335
110	O	-6.88919	-3.87772	-0.55286
111	C	-4.23104	-8.19993	-1.03715
112	H	-5.03665	-8.38194	-0.31745
113	H	-4.65663	-7.94276	-2.01356
114	H	-3.62136	-9.09811	-1.13277
115	C	-7.8454	-4.82619	-1.01882
116	H	-7.56238	-5.2305	-1.99732
117	H	-7.97133	-5.64481	-0.30171
118	H	-8.78292	-4.27826	-1.11
119	N	-6.04064	-1.25364	-0.24276
120	C	-4.96118	-1.81274	0.379432
121	H	-6.73555	-1.88177	-0.62654
122	O	-4.1509	-1.15531	1.036493

123	O	-7.03548	4.156775	-1.19549
124	O	-8.51318	-0.49306	-0.84287
125	C	-8.33876	4.613241	-1.51984
126	H	-8.7046	4.161127	-2.45028
127	H	-9.05104	4.405155	-0.71176
128	H	-8.25852	5.692747	-1.65537
129	C	-9.84276	-0.16448	-1.2131
130	H	-10.303	0.522438	-0.49194
131	H	-9.88532	0.281519	-2.21492
132	H	-10.3987	-1.10308	-1.21442
133	C	-3.81774	2.534107	4.05794
134	C	-3.43381	3.87238	4.160425
135	C	-2.17328	4.267195	3.708489
136	C	-1.29451	3.330576	3.17151
137	C	-1.66697	1.97713	3.071833
138	C	-2.9457	1.594555	3.515861
139	C	-0.72475	0.972771	2.537545
140	C	-1.17257	-0.25386	2.002661
141	C	-0.26315	-1.2009	1.576408
142	N	1.06294	-0.94749	1.642159
143	C	1.54066	0.22787	2.105091
144	C	0.667617	1.192635	2.561294
145	H	-4.79792	2.21926	4.402163
146	H	-4.11497	4.603718	4.585464
147	H	-1.87435	5.309316	3.768032
148	H	-0.33714	3.659728	2.781578
149	H	-3.26041	0.559178	3.448402

150	H	-2.22705	-0.47174	1.881681
151	H	-0.54483	-2.17288	1.185776
152	H	1.722678	-1.67081	1.313035
153	H	2.613164	0.378596	2.068378
154	H	1.086909	2.11996	2.925318

1 ⊃ 2b DFT Original data

		Coordinates (Angstroms)		
Center number	Symbol	X	Y	Z
1	C	-5.71621	3.000844	-0.27668
2	C	-5.47463	1.635394	-0.11613
3	C	-6.5116	0.702063	-0.14253
4	C	-7.82874	1.148483	-0.34985
5	C	-8.08847	2.515444	-0.50433
6	C	-7.04151	3.440354	-0.4634
7	H	-4.46724	1.295784	0.030069
8	H	-9.10207	2.856907	-0.65657
9	O	-8.78635	0.16903	-0.40307
10	O	-7.20208	4.797131	-0.59685
11	C	-10.1349	0.551462	-0.62678
12	H	-10.2559	1.05867	-1.59224
13	H	-10.7152	-0.37209	-0.63142
14	H	-10.5056	1.203293	0.17395
15	C	-8.51184	5.308452	-0.79263
16	H	-8.40613	6.390914	-0.87594

17	H	-8.96105	4.919719	-1.71482
18	H	-9.16591	5.074624	0.056435
19	N	-4.69675	3.981729	-0.26059
20	C	-3.35646	3.746815	-0.20981
21	H	-5.00506	4.944921	-0.31353
22	O	-2.87856	2.605778	-0.18036
23	C	-2.40359	4.914866	-0.17284
24	C	-2.68141	6.297977	-0.14181
25	C	-1.0627	4.543902	-0.13529
26	C	-1.63158	7.226642	-0.07641
27	C	0.011811	5.422948	-0.04416
28	H	-0.85211	3.487162	-0.1889
29	C	-0.29668	6.801971	-0.03029
30	H	-1.85432	8.282922	-0.05679
31	O	-3.98926	6.671153	-0.18025
32	C	-4.33711	8.053809	-0.14318
33	H	-3.98708	8.525136	0.781688
34	H	-3.93125	8.587344	-1.00971
35	H	-5.42576	8.083768	-0.17592
36	O	0.748945	7.671285	0.034477
37	C	0.506092	9.075767	0.085453
38	H	1.489355	9.541012	0.148858
39	H	-0.00551	9.423299	-0.81894
40	H	-0.08096	9.342457	0.970885

41	C	1.357664	4.762346	0.051669
42	O	1.41825	3.543423	0.295364
43	N	2.465975	5.513922	-0.17291
44	H	2.324113	6.504418	-0.334
45	N	-6.27399	-0.68691	-0.05178
46	C	-5.14881	-1.27328	0.465965
47	H	-7.00576	-1.29754	-0.39242
48	O	-4.28185	-0.63441	1.066302
49	C	-4.93185	-2.74058	0.198705
50	C	-5.88183	-3.70581	-0.19616
51	C	-3.61097	-3.16684	0.325581
52	C	-5.48896	-5.03018	-0.42785
53	C	-3.1679	-4.46675	0.082332
54	H	-2.86758	-2.43596	0.611358
55	C	-4.14668	-5.41161	-0.29646
56	H	-6.22677	-5.76436	-0.71496
57	O	-7.17441	-3.29069	-0.3281
58	C	-8.18332	-4.2231	-0.70563
59	H	-7.98349	-4.64869	-1.69559
60	H	-8.27414	-5.02809	0.032033
61	H	-9.11294	-3.65511	-0.7364
62	O	-3.73057	-6.69029	-0.52296
63	C	-4.66953	-7.68807	-0.91199
64	H	-5.14869	-7.43429	-1.86426

65	H	-4.09181	-8.60455	-1.02988
66	H	-5.4335	-7.83644	-0.14066
67	C	-1.67691	-4.65757	0.229312
68	O	-0.9894	-3.7091	0.619608
69	N	-1.14378	-5.86952	-0.10363
70	H	-1.78821	-6.60103	-0.37811
71	C	0.223698	-6.21598	-0.15428
72	C	0.522187	-7.55045	-0.49786
73	C	1.275241	-5.31994	0.07016
74	C	1.848116	-7.96776	-0.62503
75	C	2.607458	-5.72735	-0.059
76	H	1.055239	-4.30308	0.3449
77	C	2.888982	-7.06079	-0.41192
78	H	2.069103	-8.99063	-0.89326
79	C	3.810173	5.077405	-0.23182
80	C	4.204676	3.749783	-0.06109
81	C	4.789339	6.050875	-0.51383
82	C	5.54458	3.369514	-0.16304
83	H	3.461923	3.007395	0.158647
84	C	6.131442	5.681702	-0.63303
85	C	6.512169	4.346093	-0.46195
86	H	6.877512	6.429782	-0.85816
87	O	4.324112	7.332638	-0.66351
88	O	7.797735	3.888804	-0.58112

89	C	5.252275	8.359221	-0.9831
90	H	6.004743	8.47974	-0.19423
91	H	5.754404	8.16314	-1.9383
92	H	4.670974	9.278249	-1.06682
93	C	8.823129	4.818804	-0.89833
94	H	9.749506	4.244886	-0.94139
95	H	8.648402	5.295381	-1.87096
96	H	8.916509	5.591988	-0.12594
97	N	5.963483	2.025556	-0.05666
98	C	5.256443	1.012933	0.532017
99	H	6.877835	1.802915	-0.43027
100	O	4.217096	1.218707	1.16491
101	C	5.721418	-0.4009	0.317232
102	C	6.979808	-0.84104	-0.14417
103	C	4.757319	-1.37976	0.561261
104	C	7.223712	-2.20671	-0.33372
105	C	4.942196	-2.7448	0.353711
106	H	3.785023	-1.06122	0.909035
107	C	6.215709	-3.15223	-0.10042
108	H	8.195799	-2.53453	-0.67002
109	O	7.925386	0.112957	-0.3836
110	O	6.413494	-4.48708	-0.29262
111	C	9.221278	-0.27171	-0.83484
112	H	9.720944	-0.91358	-0.10105

113	H	9.171031	-0.78405	-1.80228
114	H	9.782634	0.655939	-0.94467
115	C	7.676903	-4.96227	-0.74834
116	H	7.925666	-4.55193	-1.7336
117	H	8.471739	-4.71994	-0.03431
118	H	7.574175	-6.04469	-0.82133
119	N	3.708263	-4.85287	0.061782
120	C	3.710357	-3.5911	0.590559
121	H	4.588894	-5.20997	-0.28739
122	O	2.742541	-3.10128	1.174012
123	O	-0.56353	-8.36791	-0.69937
124	O	4.220501	-7.37279	-0.54096
125	C	-0.33456	-9.7238	-1.04836
126	H	0.204015	-9.80997	-2.00043
127	H	0.225457	-10.2514	-0.26636
128	H	-1.31918	-10.1819	-1.152
129	C	4.571212	-8.69333	-0.92286
130	H	4.227711	-9.43	-0.18606
131	H	4.16388	-8.95034	-1.90884
132	H	5.660915	-8.71771	-0.9679
133	C	-0.28132	-1.08825	2.826895
134	C	1.353374	0.511258	2.045581
135	C	-0.94142	0.895724	1.615961
136	C	-1.28141	-0.27707	2.263869

137	H	1.863861	-1.29189	3.054862
138	H	2.36469	0.873902	1.897178
139	H	0.615187	2.148363	1.061606
140	H	-1.67017	1.543687	1.138161
141	H	-2.32805	-0.56113	2.29186
142	N	0.355872	1.26587	1.535742
143	C	1.053155	-0.67311	2.689853
144	C	-0.61935	-2.37893	3.509186
145	H	0.129588	-2.64277	4.259696
146	H	-1.6038	-2.33341	3.981909
147	H	-0.64332	-3.16969	2.749862

1 ⊃ 2c DFT Original data

		Coordinates (Angstroms)		
Center number	Symbol	X	Y	Z
1	C	1	C	6.4114
2	C	2	C	5.3305
3	C	3	C	5.5113
4	C	4	C	6.819
5	C	5	C	7.9123
6	C	6	C	7.7133
7	H	7	H	4.336
8	H	8	H	8.9143
9	O	9	O	6.9193
10	O	10	O	8.7218

11	C	11	C	8.2124
12	H	12	H	8.819
13	H	13	H	8.0594
14	H	14	H	8.7419
15	C	15	C	10.0581
16	H	16	H	10.6844
17	H	17	H	10.3574
18	H	18	H	10.1977
19	N	19	N	6.2595
20	C	20	C	5.1317
21	H	21	H	7.0697
22	O	22	O	4.1362
23	C	23	C	5.0782
24	C	24	C	6.1278
25	C	25	C	3.8084
26	C	26	C	5.8747
27	C	27	C	3.5031
28	H	28	H	2.9913
29	C	29	C	4.5763
30	H	30	H	6.6879
31	O	31	O	7.3755
32	C	32	C	8.4756
33	H	33	H	8.3271
34	H	34	H	8.6397
35	H	35	H	9.3441

36	O	36	O	4.2943
37	C	37	C	5.3365
38	H	38	H	4.8574
39	H	39	H	6.097
40	H	40	H	5.8055
41	C	41	C	2.0328
42	O	42	O	1.2623
43	N	43	N	1.6157
44	H	44	H	2.3284
45	N	45	N	4.4376
46	C	46	C	3.1233
47	H	47	H	4.681
48	O	48	O	2.7424
49	C	49	C	2.0936
50	C	50	C	2.2892
51	C	51	C	0.7795
52	C	52	C	1.1902
53	C	53	C	-0.3431
54	H	54	H	0.6158
55	C	55	C	-0.1157
56	H	56	H	1.3515
57	O	57	O	3.5731
58	C	58	C	3.8352
59	H	59	H	3.4871
60	H	60	H	3.3692

61	H	61	H	4.9183
62	O	62	O	-1.2076
63	C	63	C	-1.0411
64	H	64	H	-0.4472
65	H	65	H	-2.0463
66	H	66	H	-0.5724
67	C	67	C	-1.647
68	O	68	O	-1.6103
69	N	69	N	-2.8181
70	H	70	H	-2.7489
71	C	71	C	-4.1249
72	C	72	C	-5.2112
73	C	73	C	-4.3885
74	C	74	C	-6.5227
75	C	75	C	-5.6919
76	H	76	H	-3.5601
77	C	77	C	-6.769
78	H	78	H	-7.3513
79	C	79	C	0.2807
80	C	80	C	-0.8218
81	C	81	C	0.0667
82	C	82	C	-2.1242
83	H	83	H	-0.6617
84	C	84	C	-1.2316
85	C	85	C	-2.3254

86	H	86	H	-1.3899
87	O	87	O	1.1992
88	O	88	O	-3.635
89	C	89	C	1.0555
90	H	90	H	0.5729
91	H	91	H	0.4811
92	H	92	H	2.0654
93	C	93	C	-3.9097
94	H	94	H	-4.9955
95	H	95	H	-3.5409
96	H	96	H	-3.4717
97	N	97	N	-3.2741
98	C	98	C	-3.29
99	H	99	H	-4.1647
100	O	100	O	-2.2663
101	C	101	C	-4.6156
102	C	102	C	-5.9272
103	C	103	C	-4.4863
104	C	104	C	-7.0221
105	C	105	C	-5.5348
106	H	106	H	-3.4847
107	C	107	C	-6.8344
108	H	108	H	-8.0215
109	O	109	O	-6.0632
110	O	110	O	-7.8652

111	C	111	C	-7.3589
112	H	112	H	-7.8412
113	H	113	H	-7.9967
114	H	114	H	-7.1983
115	C	115	C	-9.2038
116	H	116	H	-9.4867
117	H	117	H	-9.336
118	H	118	H	-9.8315
119	N	119	N	-5.9863
120	C	120	C	-5.0967
121	H	121	H	-6.9549
122	O	122	O	-3.9049
123	O	123	O	-4.8806
124	O	124	O	-8.0189
125	C	125	C	-5.9253
126	H	126	H	-6.5778
127	H	127	H	-6.5282
128	H	128	H	-5.4394
129	C	129	C	-9.1495
130	H	130	H	-9.141
131	H	131	H	-9.2045
132	H	132	H	-10.0239
133	C	133	C	-1.4795
134	C	134	C	-0.6622
135	C	135	C	0.3428

136	C	136	C	0.5313
137	C	137	C	-0.3058
138	C	138	C	-1.3078
139	C	139	C	-0.1085
140	C	140	C	-1.1453
141	C	141	C	1.23
142	C	142	C	1.1389
143	H	143	H	-2.2427
144	H	144	H	-0.8011
145	H	145	H	0.9815
146	H	146	H	1.3009
147	H	147	H	-1.896
148	H	148	H	-2.1367
149	H	149	H	-2.1029
150	H	150	H	0.1123
151	H	151	H	2.2124
152	H	152	H	2.0358
153	C	153	C	0.0717
154	N	154	N	-1.198