Supporting Information

N,N′,N″-Tris[(5-methoxy-1*H*-indol-3-yl)ethyl]benzene-1,3,5-tricarboxamide

1 ^{1}H and ^{13}C-NMR spectra of compound **3**.

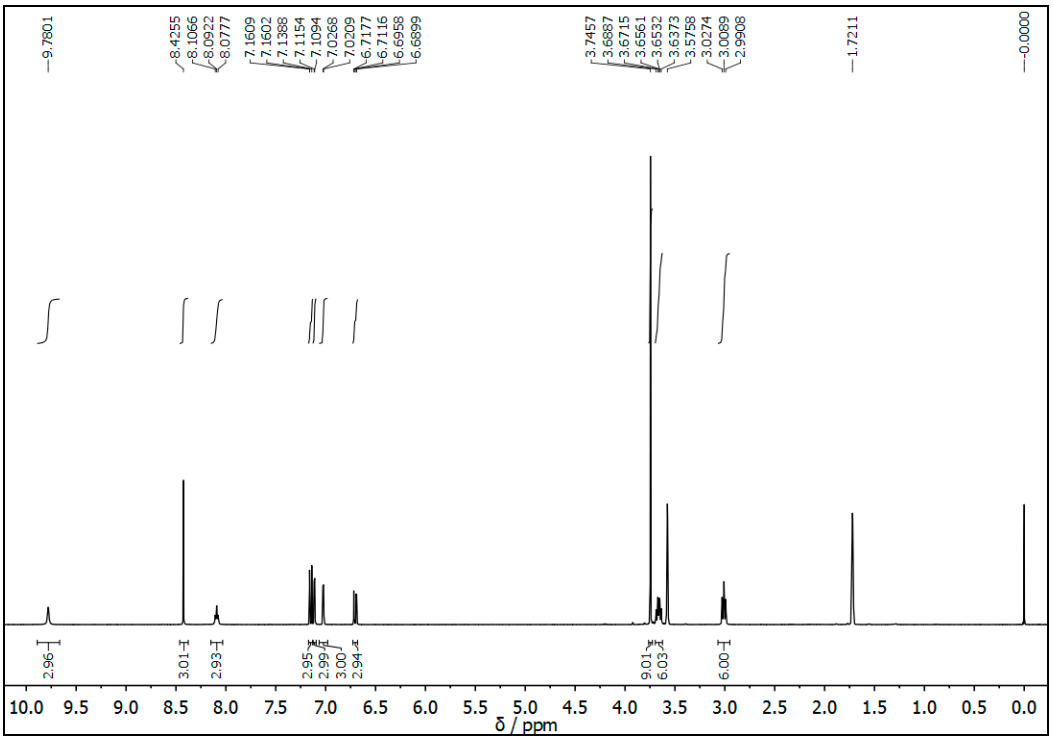

Figure S1. ^{1}H-NMR spectrum of **3** in THF-d_8 (400 MHz).

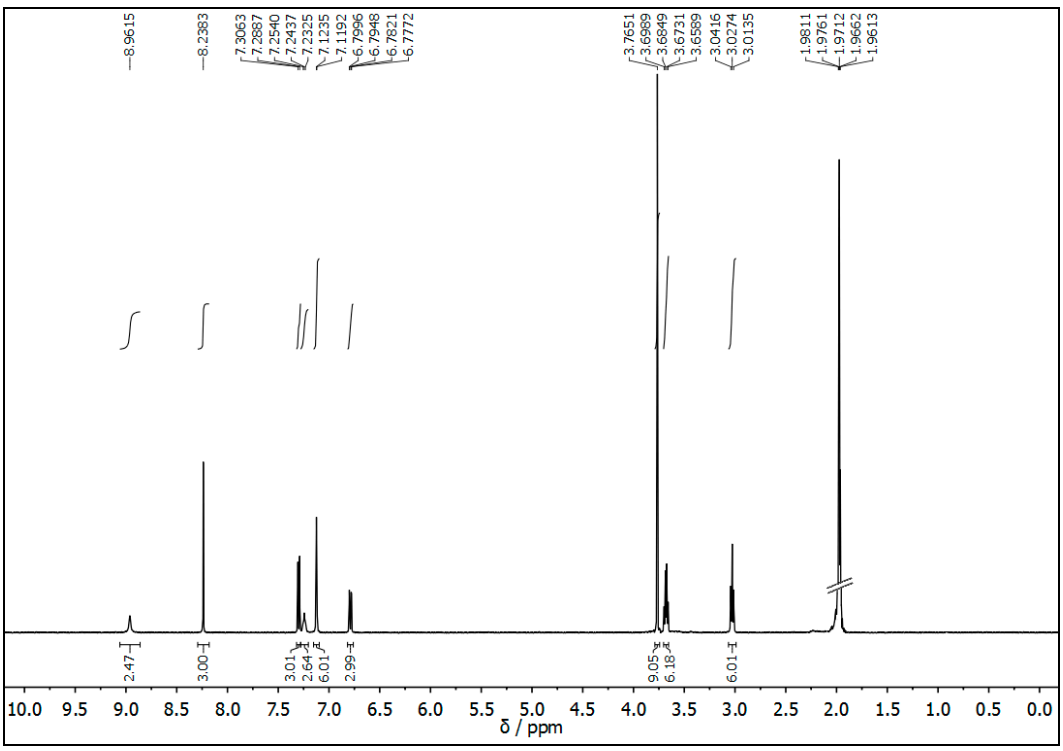

Figure S2. ^{1}H-NMR spectrum of **3** in CD_3CN (500 MHz).

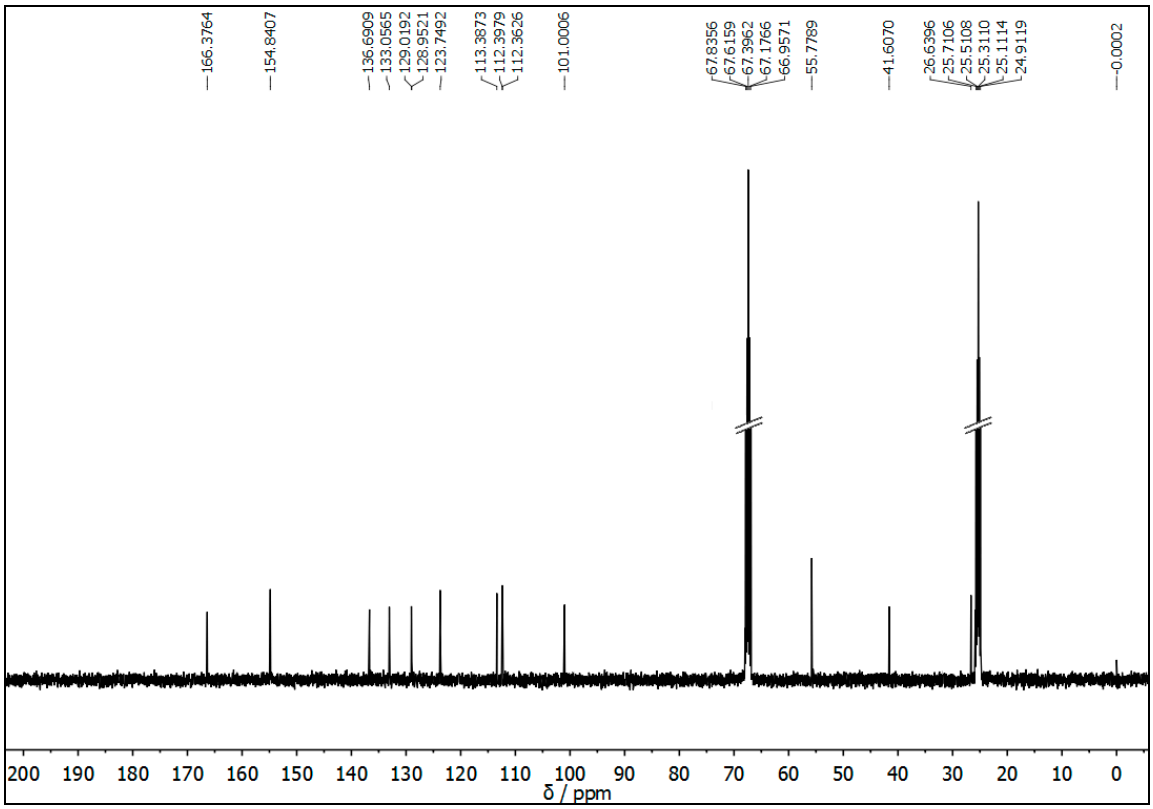

Figure S3. ^{13}C-NMR spectrum of **3** in THF-d_8 (400 MHz).

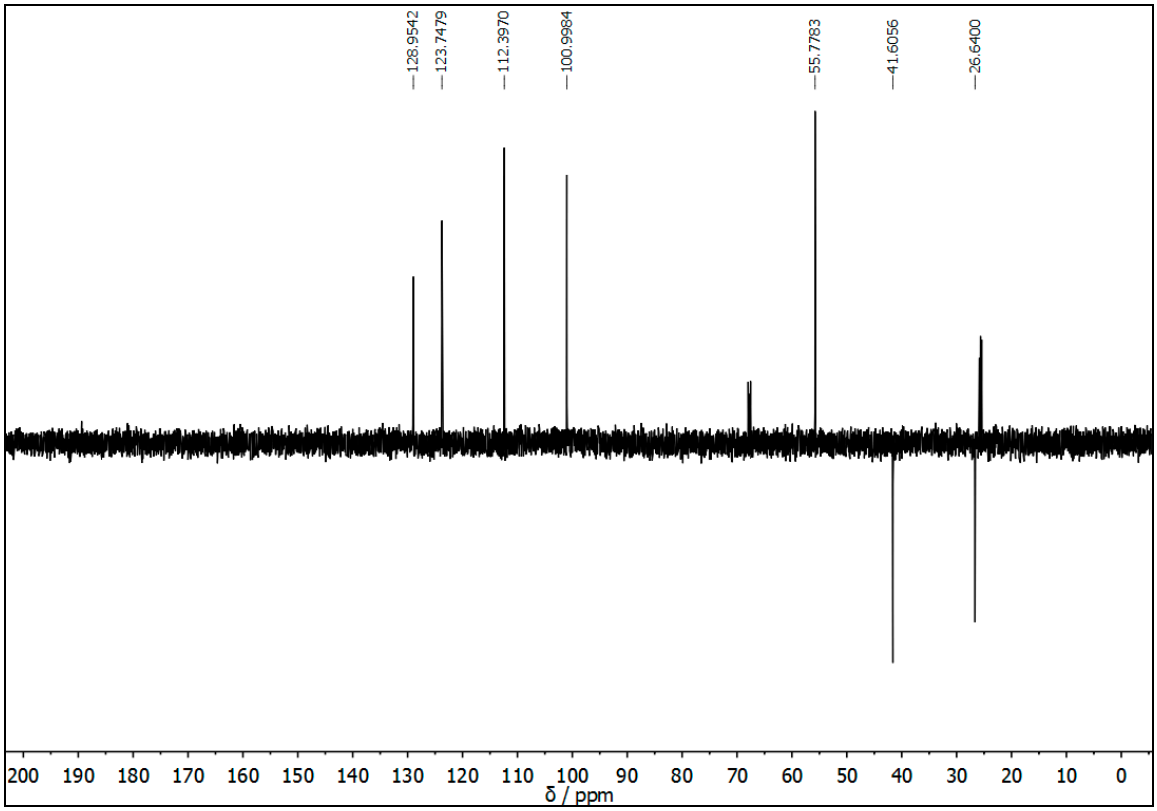

Figure S4. DEPT 135 spectrum of **3** in THF-d_8 (400 MHz).

2 Description of the ^{1}H-NMR titrations

^{1}H-NMR titrations were carried out in CD_3CN at 25 °C (dilution experiments show that compound **3** do not self-aggregate in the used concentration range).

Stock solutions in CD_3CN were prepared for compound **3** and NH_4PF_6. These solutions and the corresponding solvent were combined in a manner so that the concentration of compound **3** was kept constant and that of NH_4PF_6 varied (three titrations were carried out). For each titration 16–20 samples were prepared and the ^{1}H-NMR spectra were recorded (for an example, see Table S1). The titration data were analyzed by non-linear regression analysis, using the program WinEQNMR (see [1]).

Table S1. ^{1}H-NMR titration of compound **3** with NH_4PF_6 in CD_3CN.

	[Receptor] mol/L	[NH_4PF_6] mol/L	Ratio	
			[Receptor]	[NH_4PF_6]
1	0.00100061	0.00000000	1	0.0000
2	0.00100061	0.00010587	1	0.1058
3	0.00100061	0.00021174	1	0.2116
4	0.00100061	0.00031762	1	0.3174
5	0.00100061	0.00042349	1	0.4232
6	0.00100061	0.00052936	1	0.5290
7	0.00100061	0.00063523	1	0.6348
8	0.00100061	0.00074110	1	0.7407
9	0.00100061	0.00084698	1	0.8465
10	0.00100061	0.00105872	1	1.0581
11	0.00100061	0.00127046	1	1.2697
12	0.00100061	0.00148221	1	1.4813
13	0.00100061	0.00190570	1	1.9045
14	0.00100061	0.00211744	1	2.1162
15	0.00100061	0.00232918	1	2.3278
16	0.00100061	0.00254093	1	2.5394
17	0.00100061	0.00296442	1	2.9626
18	0.00100061	0.00338791	1	3.3859
19	0.00100061	0.00423488	1	4.2323

3 Mole ratio plot for the ^{1}H-NMR titration of compound **3** with NH_4PF_6 in CD_3CN.

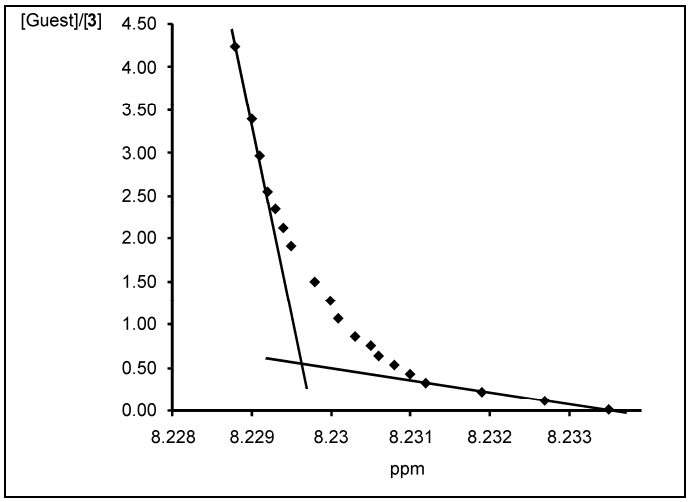

Figure S5. Mole ratio plot: Titration of compound **3** with NH_4PF_6 in CD_3CN; [**3**] = 1 mM (analysis of the complexation-induced upfield shift of the benzene CH of **3**).

Reference

1. Hynes, M.J. EQNMR: A computer program for the calculation of stability constants from nuclear magnetic resonance chemical shift data. *J. Chem. Soc. Dalton Trans.* **1993**, 311–312.