

Supplementary Information

Hydroxylated Pillar[5]arene-based Amphiphiles: Synthesis and Characterization

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Single crystal X-ray diffraction data:**Table 1S.** Summary on the nature of the crystals and various crystallographic parameters of **Pilla-1**, and **Pillar-2b**.

Crystal Name	Pillar-1	Pillar-2b
Crystal Dimension/mm	0.25 × 0.20 × 0.06	0.22 × 0.16 × 0.14
Crystal Color, Habit	Colorless, Block	Colorless, Block
Formula	C ₁₀₉ H ₉₈ Cl ₄ O ₁₀	C ₁₀₉ H ₁₁₄ Cl ₂ O ₁₀
Crystal system	Monoclinic	Monoclinic
Space group(no.)	P 21/n (14)	P 21/c (14)
T/K	150	150
a/Å	20.5360(5)	19.3435(9)
b/Å	21.5224(5)	25.2081(11)
c/Å	20.9960(15)	20.5824(14)
α	90	90
β	109.550(8)	110.810(8)
γ	90	90
V/ Å ³	8744.9(8)	9381.5(10)
Z	4	4
$\mu(\text{CuK}\alpha) / \text{mm}^{-1}$	0.199	0.128
$\rho_{\text{calcd}}/\text{g cm}^{-3}$	1.299	1.172
$\theta_{\text{max}}/\text{deg}$	25.03	27.44
Reflections collected	49964	64186
Unique reflections	15429	21224
R _{int}	0.0422	0.0815
R (I > 2 σ)	0.0753	0.0977
R (all data)	0.1022	0.1948
R _w (all data)	0.2626	0.3362
$\Delta \rho _{\text{max}}/\text{e Å}^{-3}$	1.030	1.201

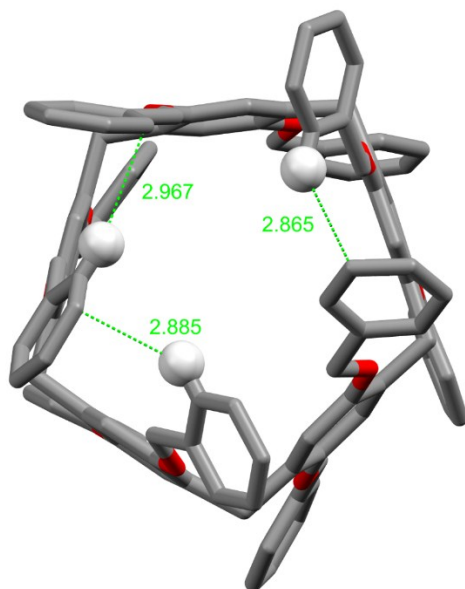


Figure S1. Top view of the extended **Pillar-1** cavity by C-H $\cdots$ π interactions.

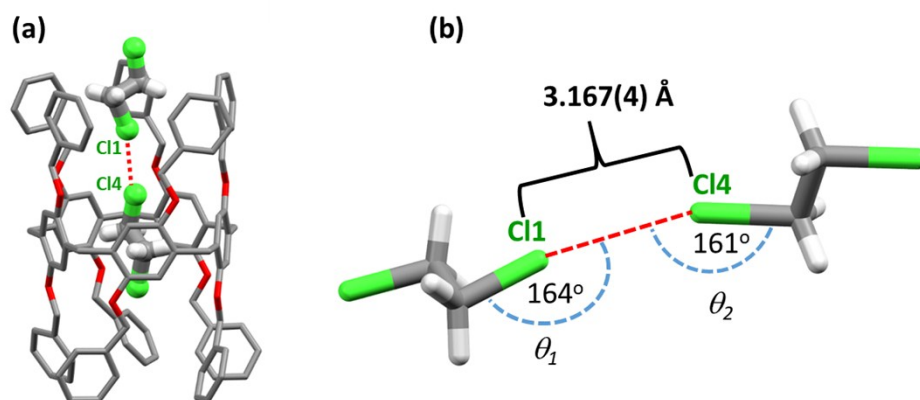


Figure S2. Halogen $\cdots$ halogen (Cl $\cdots$ Cl) interactions. a) side view, b) type-I interactions ($\theta_1 \approx \theta_2$) pillararene removed for clarity.

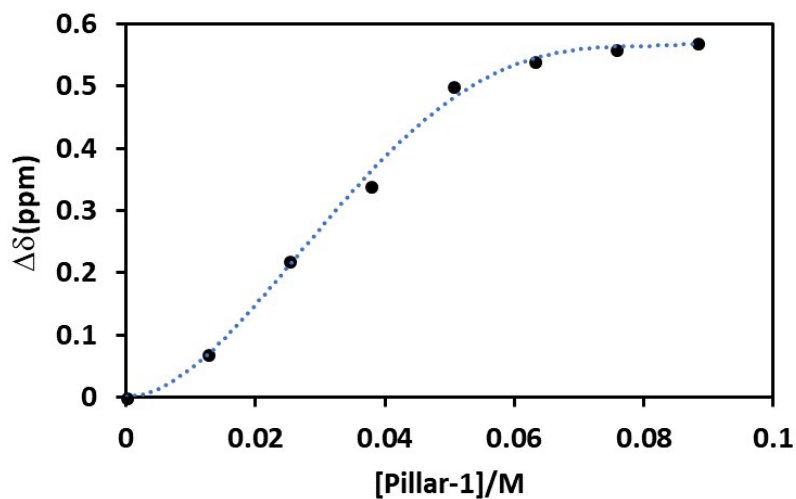


Figure S3. Plot of chemical shift (δ) changes for the guest (OMA) proton of trimethyl region as function of host (Pillar-1) concentration in CDCl_3 at 25 °C.

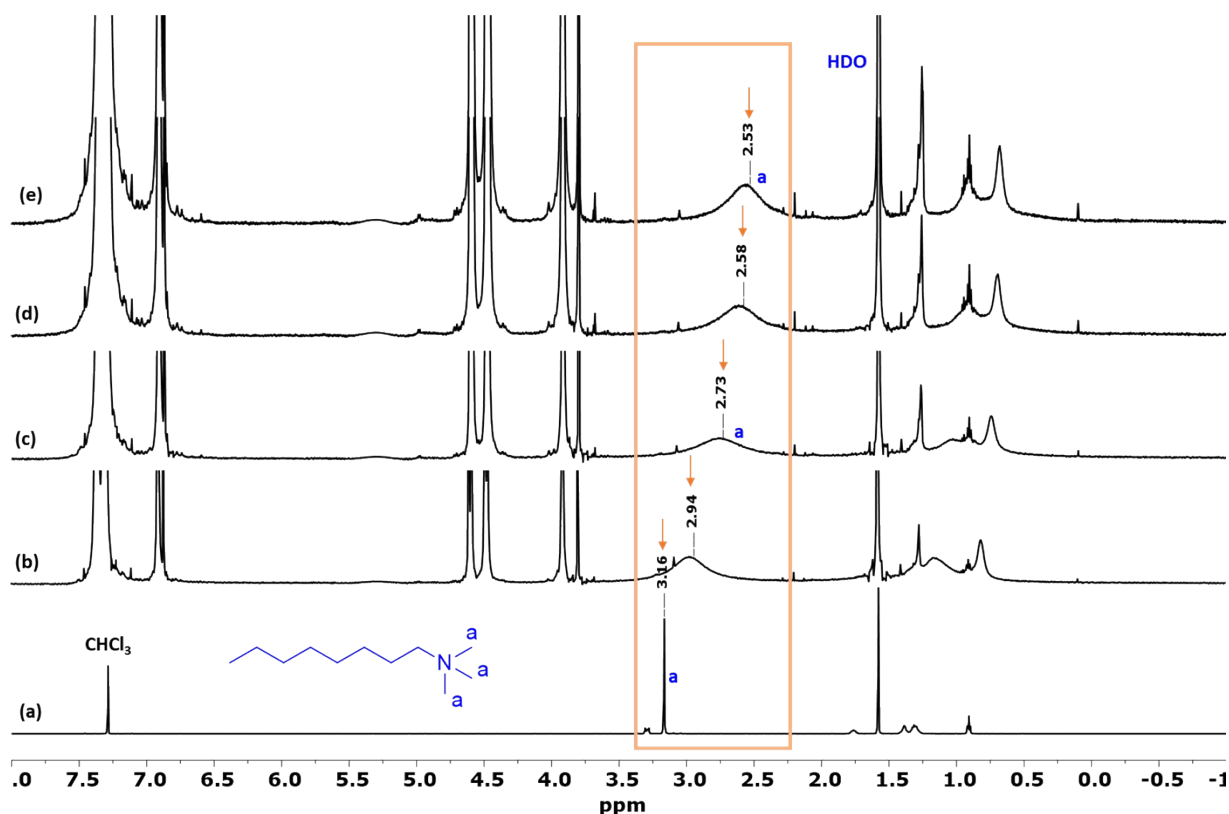


Figure S4. ^1H NMR spectra (600 MHz, chloroform- d , 25 °C) of Pillar-1 and OMA (a); 6.3 mM OMA (b); 2.5 mM Pillar-1 and 6.3 mM OMA (c); 5 mM Pillar-1 and 6.3 mM OMA (d); 7.6 mM Pillar-1 and 6.3 mM OMA (e); 8.8 mM Pillar-1 and 6.3 mM OMA.

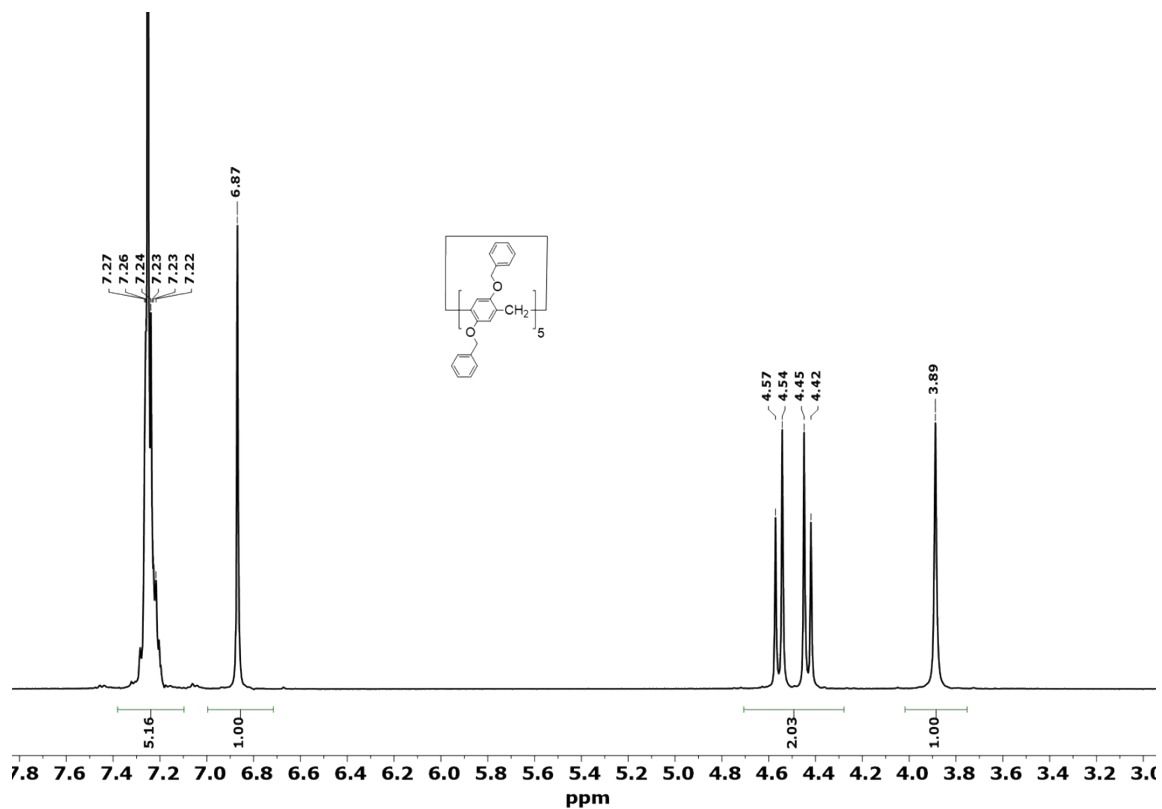


Figure S5. ¹H NMR (600 MHz, CDCl₃) spectrum of Pillar-1.

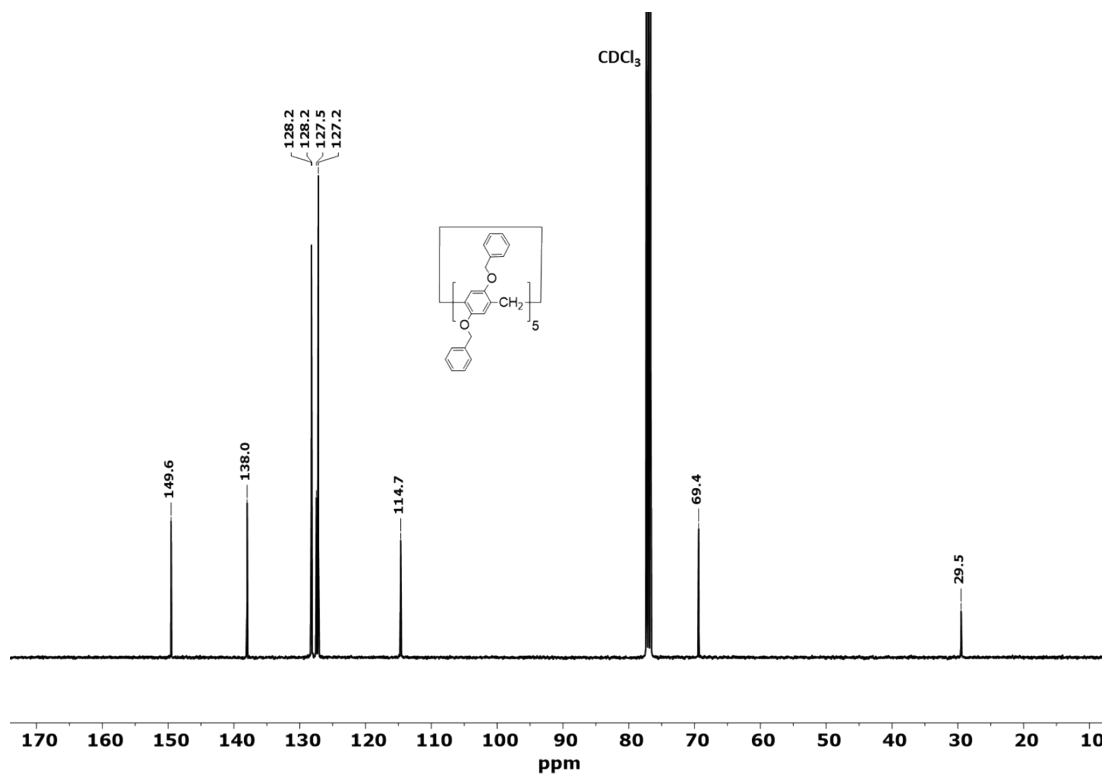


Figure S6. ¹³C NMR (150 MHz, CDCl₃) spectrum of Pillar-1.

^{13}C NMR spectrum of poly(2,2-bis(4-(benzyloxy)phenyl)propane) in CDCl_3 . The spectrum shows peaks from 127.3 to 149.8 ppm. A chemical structure of the polymer is shown with a box highlighting the repeating unit. The structure is: $[-\text{O}-\text{C}_6\text{H}_4-\text{CH}_2-\text{C}_6\text{H}_4-\text{O}-\text{CH}_2-\text{C}_6\text{H}_4-\text{O}-\text{CH}_2-\text{C}_6\text{H}_4-\text{O}-]_n$, where the C_6H_4 groups are 2,2-bis(4-(benzyloxy)phenyl)propane units. The box highlights the repeating unit: $[-\text{O}-\text{C}_6\text{H}_4-\text{CH}_2-\text{C}_6\text{H}_4-\text{O}-\text{CH}_2-\text{C}_6\text{H}_4-\text{O}-\text{CH}_2-\text{C}_6\text{H}_4-\text{O}-]_4$. The peaks are labeled with their chemical shifts: 149.8, 149.8, 138.3, 138.2, 128.8, 128.6, 128.5, 128.5, 128.4, 128.4, 128.3, 127.9, 127.7, 127.6, 127.5, 127.5, 127.4, 127.4, 127.3, 115.0, 114.9, 114.8, 114.7, 70.2, 69.7, 69.6, 69.5, 68.0, 32.0, 31.8, 30.0, 29.8, 29.6, 29.5, 26.5, 22.9, 22.8, 14.3, 14.3.

S6

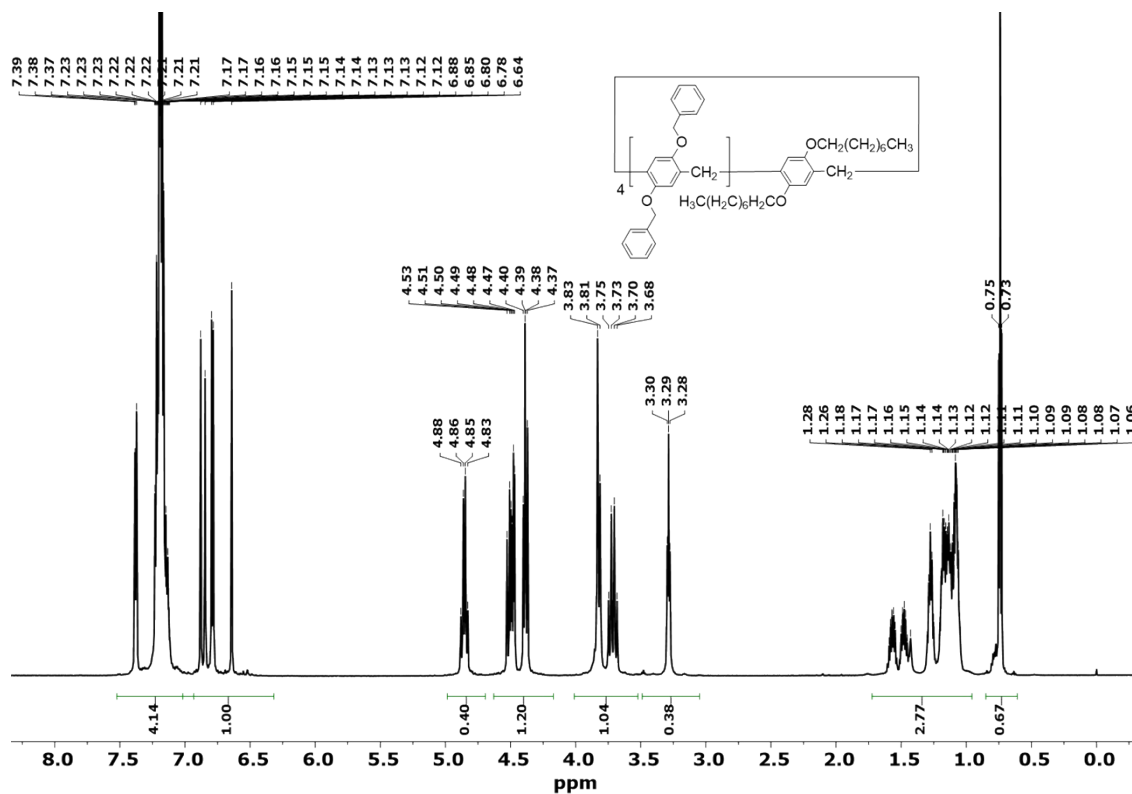


Figure S9. ^1H NMR (600 MHz, CDCl_3) spectrum of **Pillar-2b**.

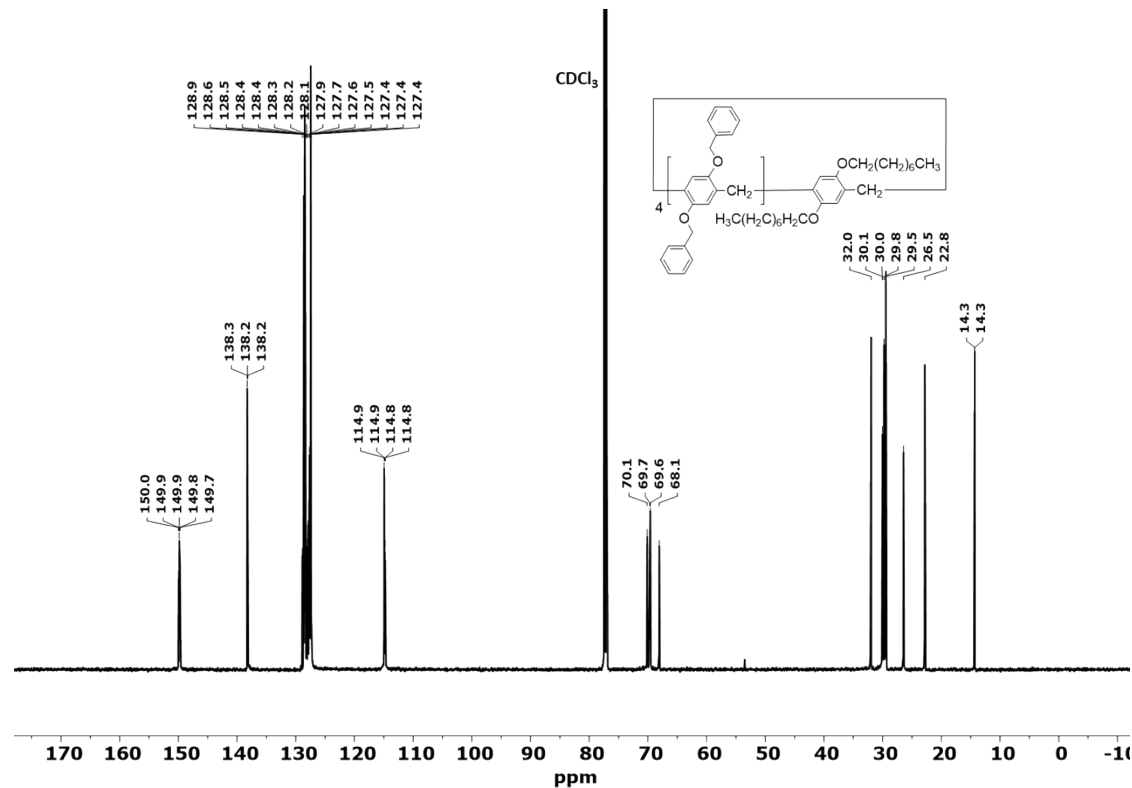
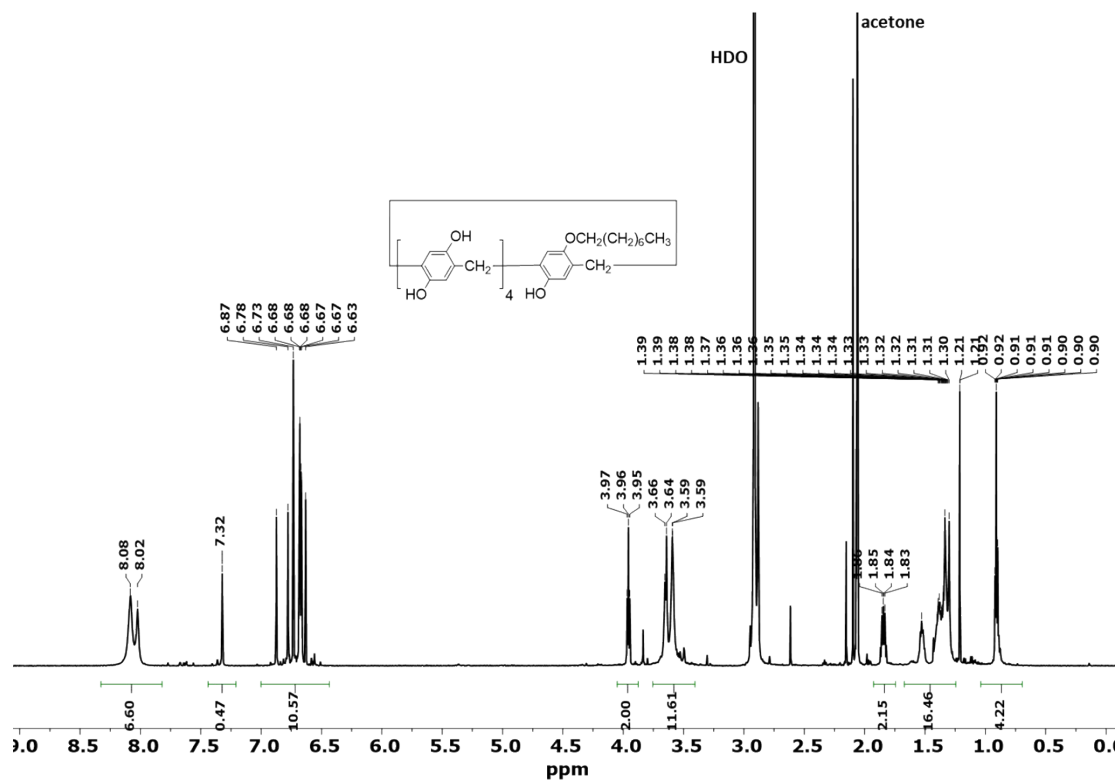
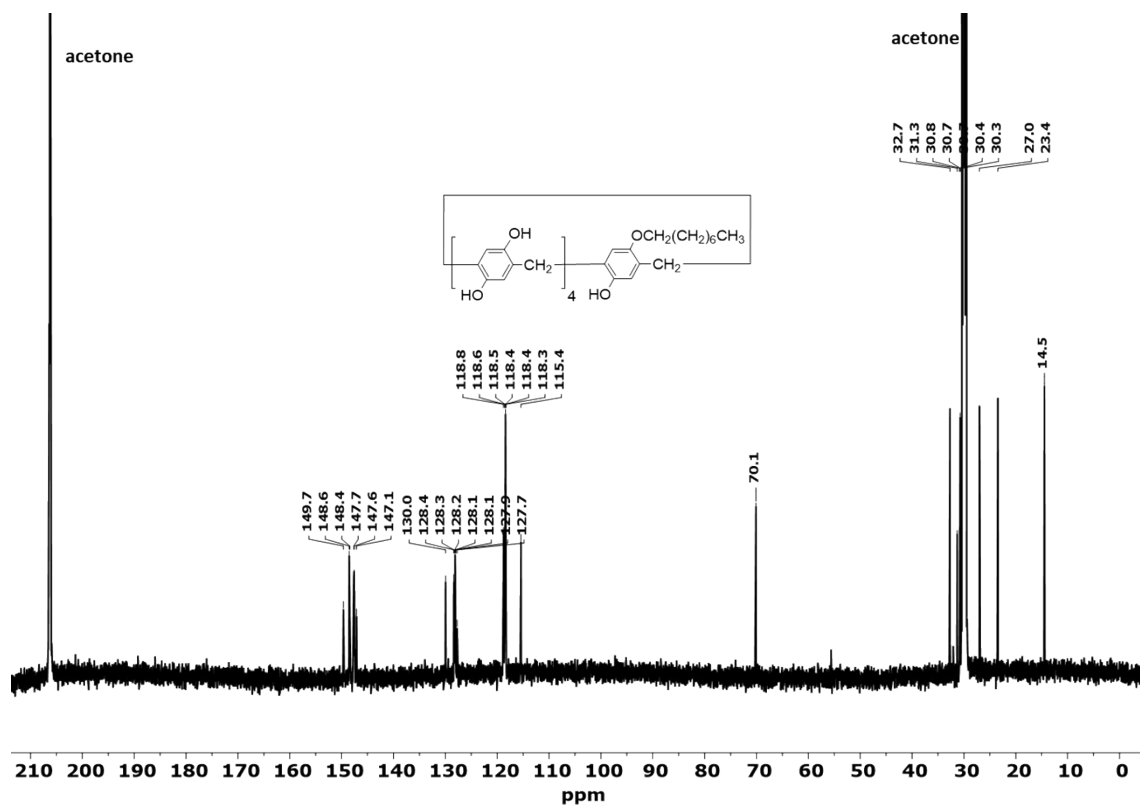
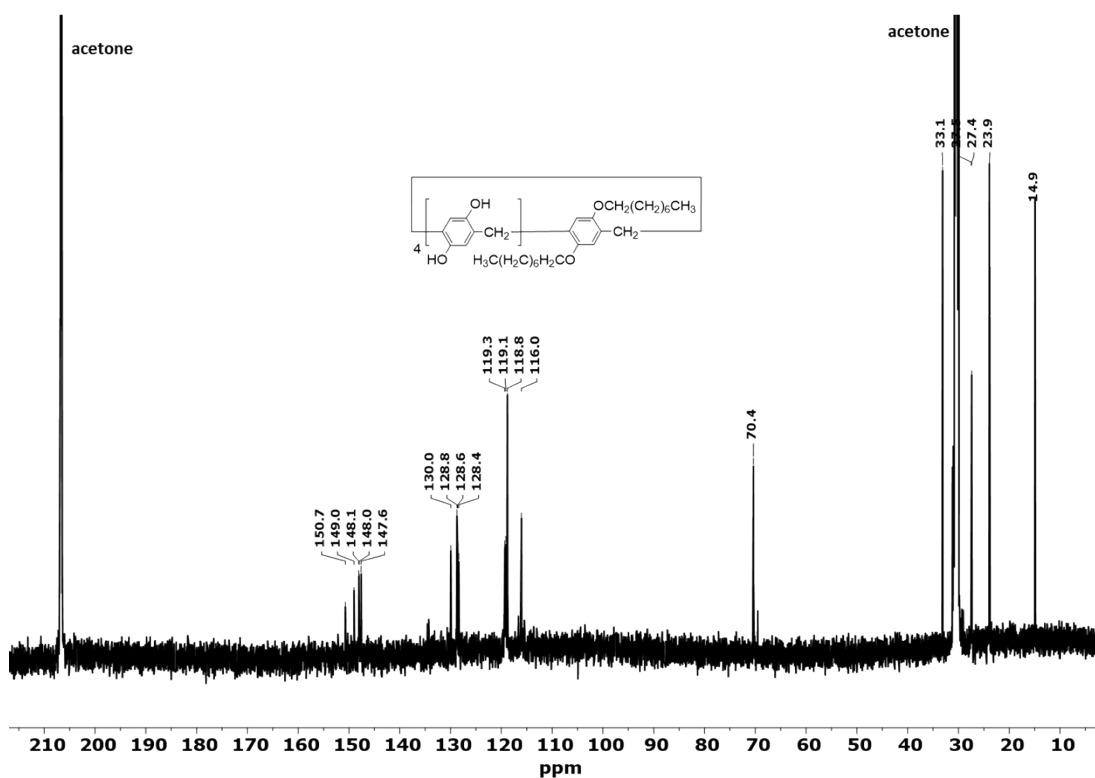
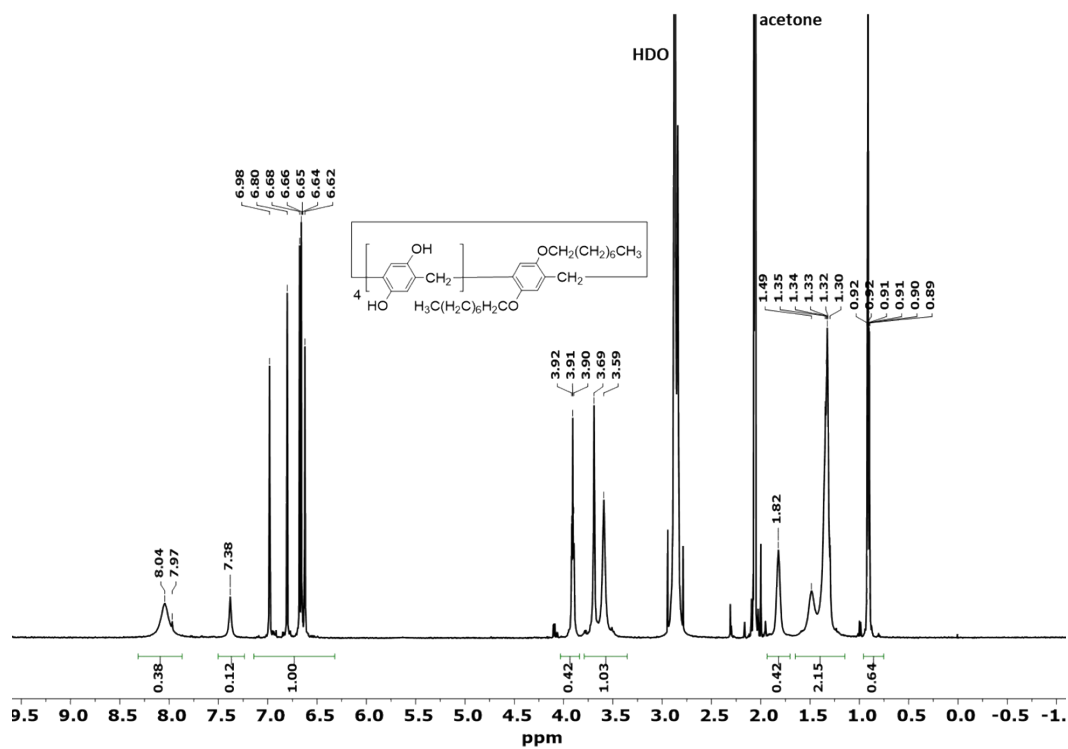


Figure S10. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **Pillar-2b**.

Figure S11. ¹H NMR (600 MHz, Acetone-*d*₆) spectrum of Pillar-3a.Figure S12. ¹³C NMR (150 MHz, Acetone-*d*₆) spectrum of Pillar-3a.



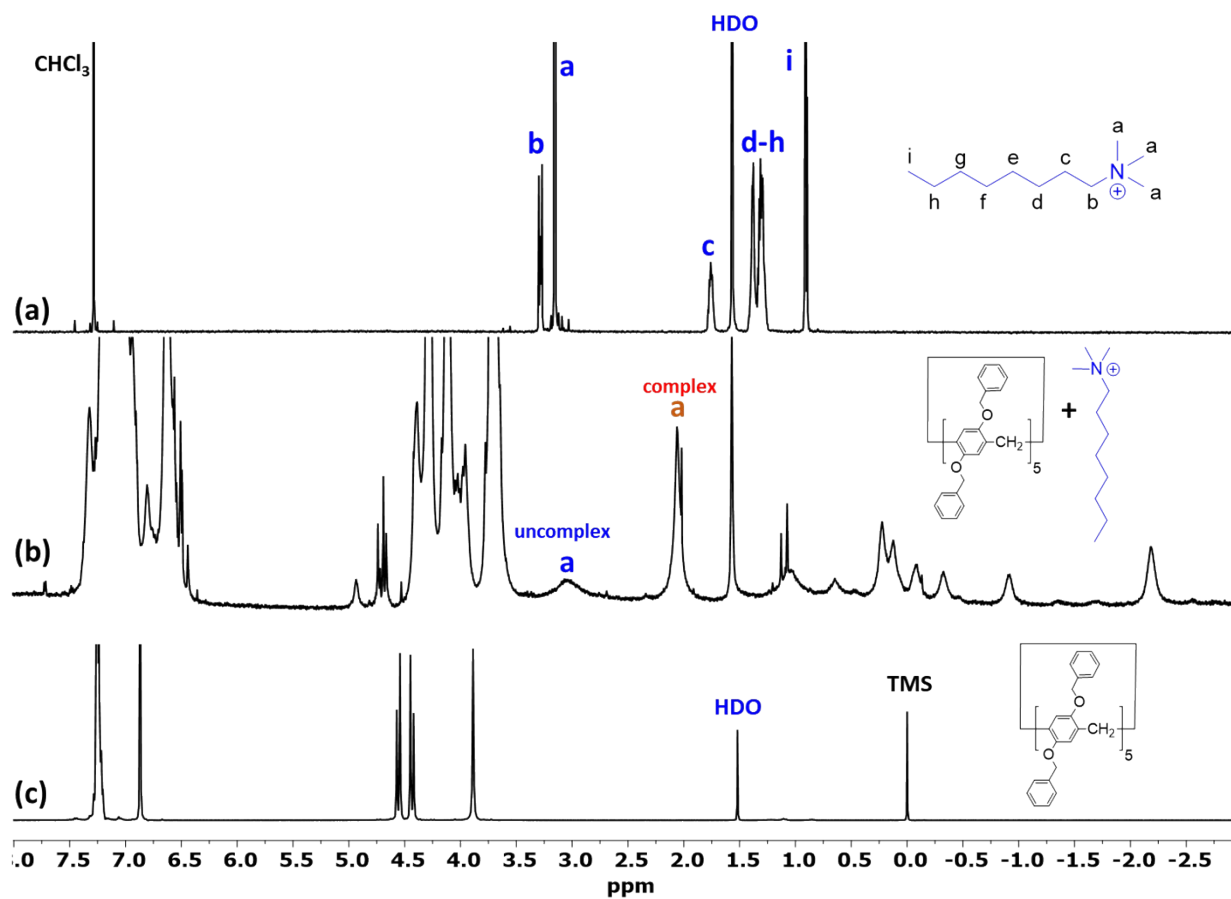


Figure S15. ^1H NMR (600 MHz, CDCl_3 at 233 K) spectra of (a) 0.63 mM **OMA**, (b) 6.3 mM each of **Pillar-1** and **OMA**, and (c) 6.3 mM of **Pillar-1**.