Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supporting Information for

Chiral discrimination of 2-heptlyaminium salt by planar-chiral monohydroxy-functionalized pillar[5]arene

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Single crystal X-ray diffraction data.

Table S1. Summary on the nature of the crystals and various crystallographic parameters under two different data collection conditions.

Crystal Sample	**PCM_Mo**	**PCM_Cu**
Instrument Used	Rigaku Rapid II	Bruker X8 prospector
Crystal Dimension/mm	0.22 X 0.14 X 0.11	0.21 X 0.12 X 0.09
Crystal Color, Habit	Colorless, block	Colorless, block
Formula weight	$C_{116}H_{162}BrF_3O_{12}$	$C_{116}H_{162}BrF_3O_{12}$
Crystal system	monoclinic	monoclinic
Space group	P 21	P 21
T/K	150	150
a/Å	15.0627(8)	15.1538(3)
b//Å	13.3599(7)	13.5668(3)
c/Å	27.1554(19)	27.2737(5)
α	90	90
β	94.396(7)	92.794(2)
γ	90	90
V/ Å^3	5448.6(6)	5600.5(2)
Z	2	2
μ / mm^{-1}	0.440	0.981
ρ_{calcd}/g cm^{-3}	1.149	1.118
θ_{max}/deg	25.670	66.560
Reflections collected	31279	43635
Unique reflections	20079	17977
R_{int}	0.0324	0.0452
R (I > 2σ)	0.1101	0.1071
R (all data)	0.1679	0.1467
R_w(all data)	0.3380	0.3259
flack χ parameter	0.036(15)	0.04(4)
$\lvert\Delta\rho\rvert_{max}$e Å^{-3}	1.042	0.547

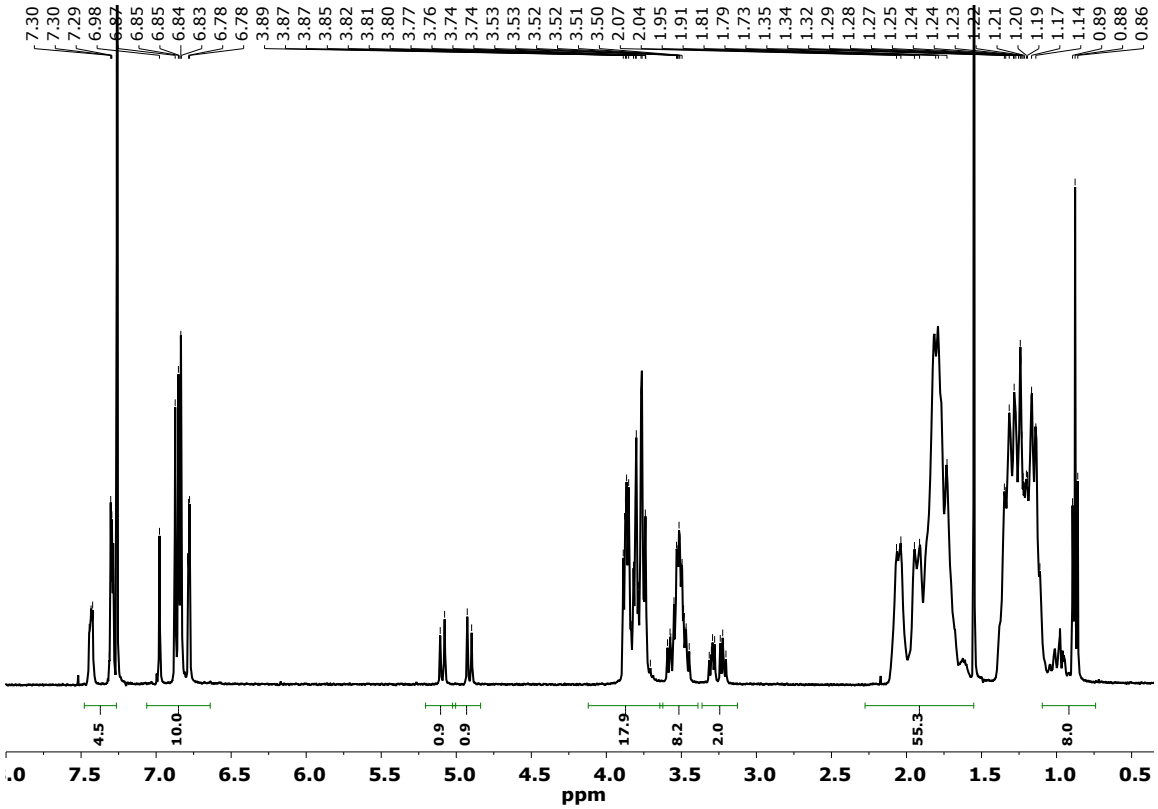

Figure S1. ^{1}HNMR (400 MHz, $CDCl_3$) spectrum of **Pillar-1**.

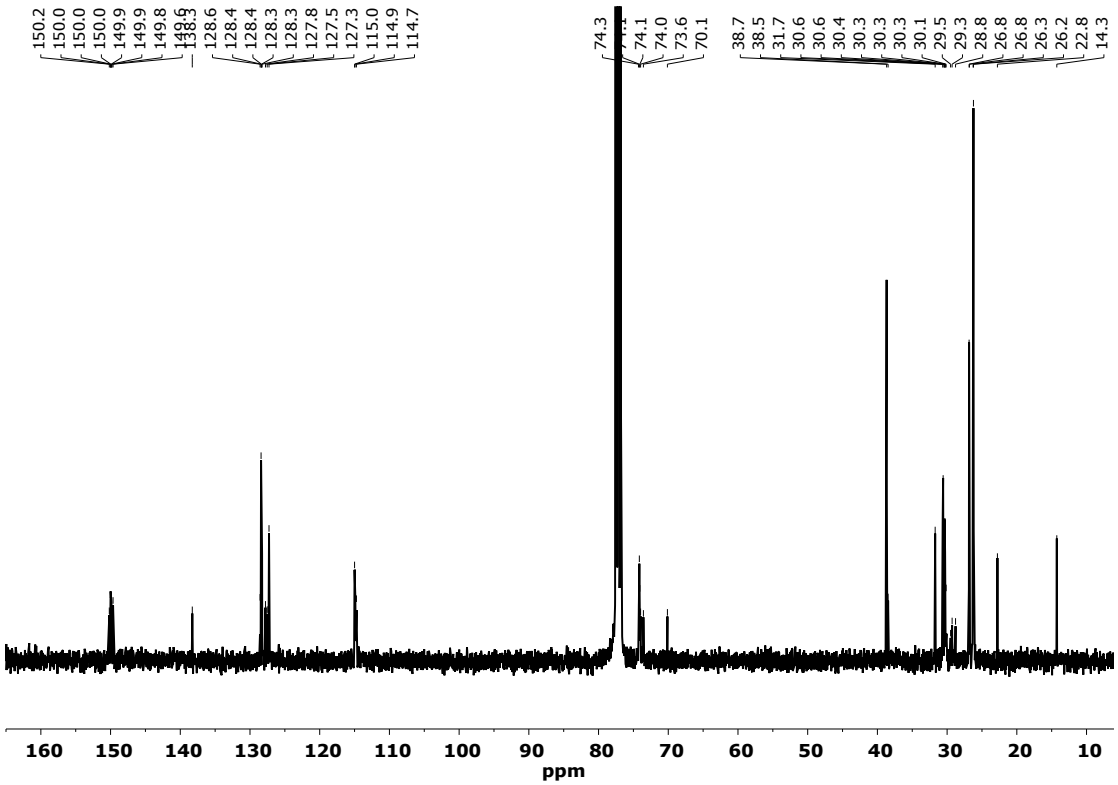

Figure S2. ^{13}CNMR (100 MHz, $CDCl_3$) spectrum of **Pillar-1**.

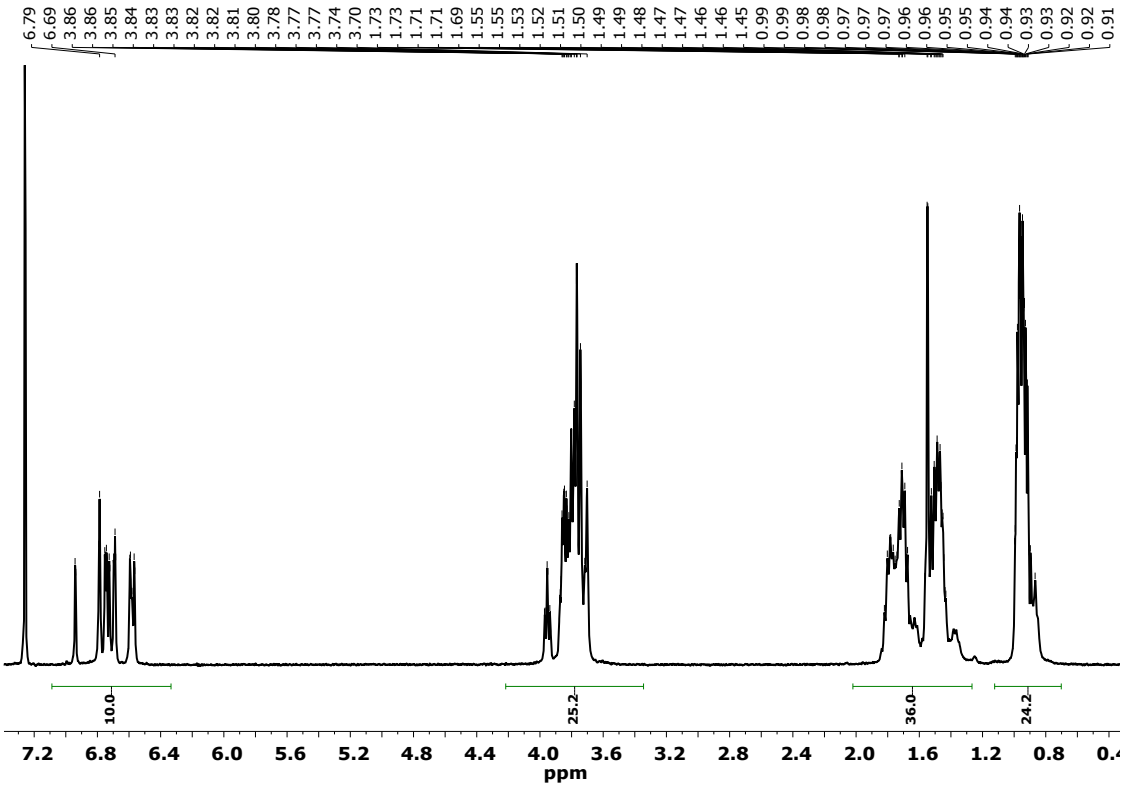

Figure S3. ^{1}HNMR (400 MHz, $CDCl_3$) spectrum of **Pillar-2**.

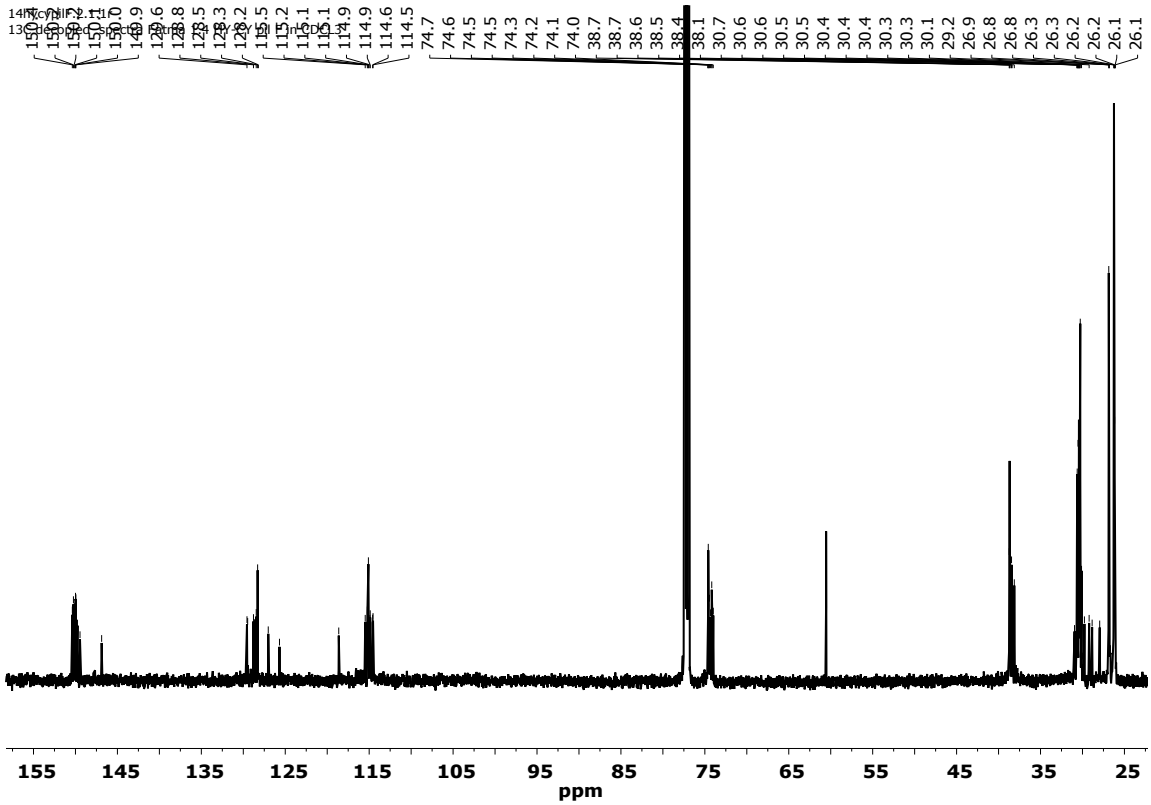

Figure S4. ^{13}CNMR (150 MHz, $CDCl_3$) spectrum of **Pillar-2**.

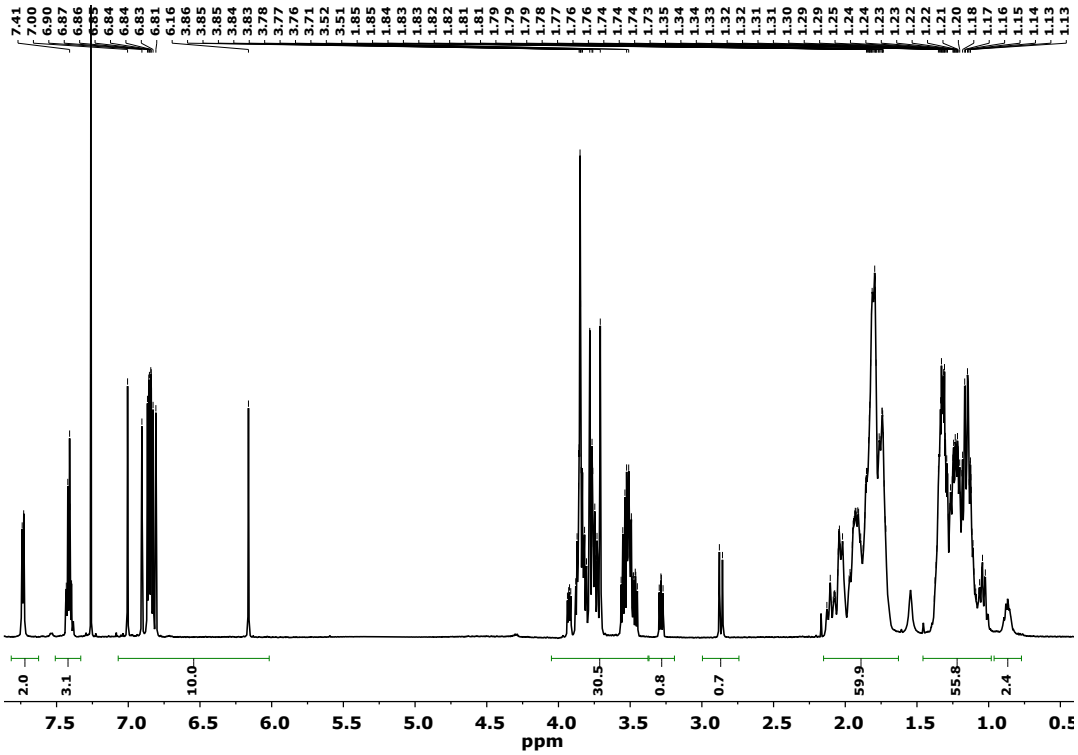

Figure S5. ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of **Pillar-3a**.

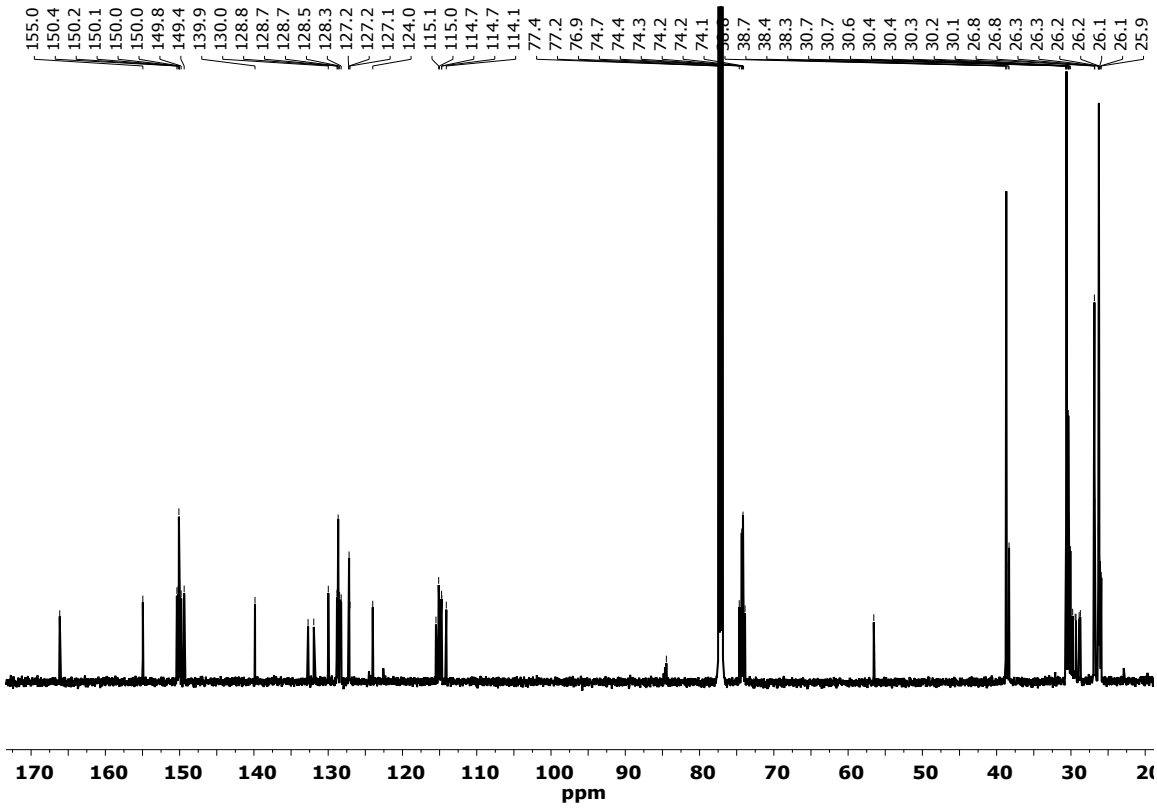

Figure S6. ^{13}CNMR (150 MHz, $CDCl_3$) spectrum of **Pillar-3a**.

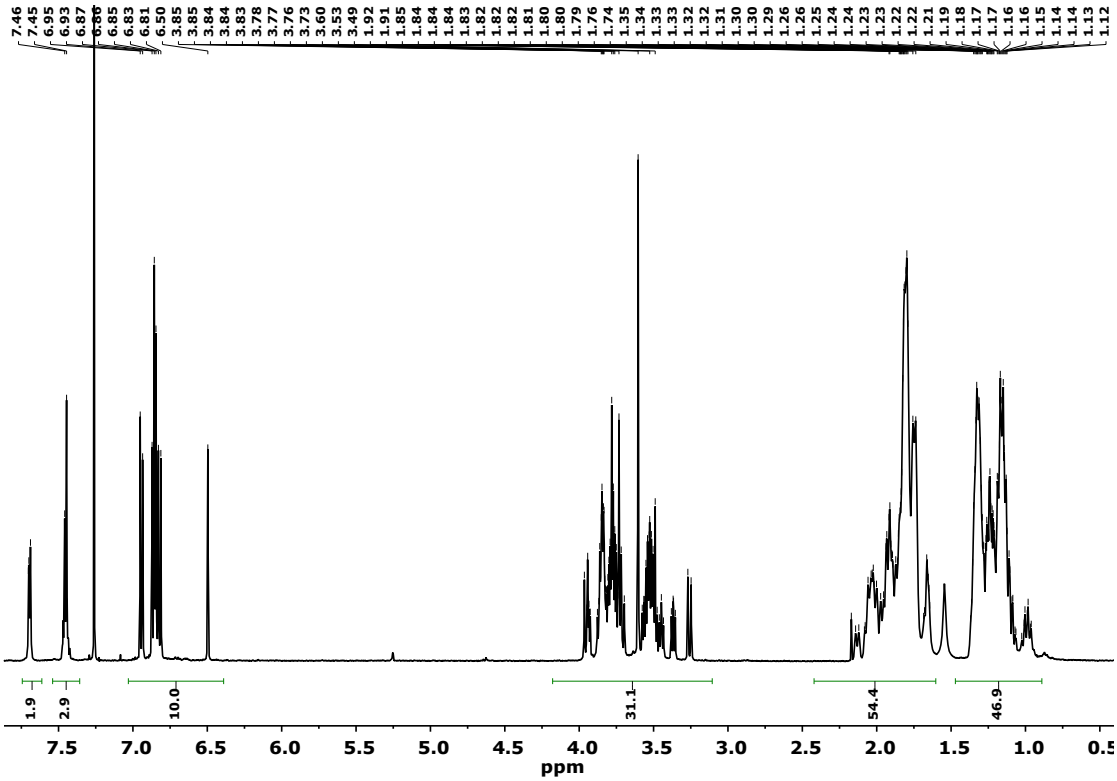

Figure S7. ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of **Pillar-3b**.

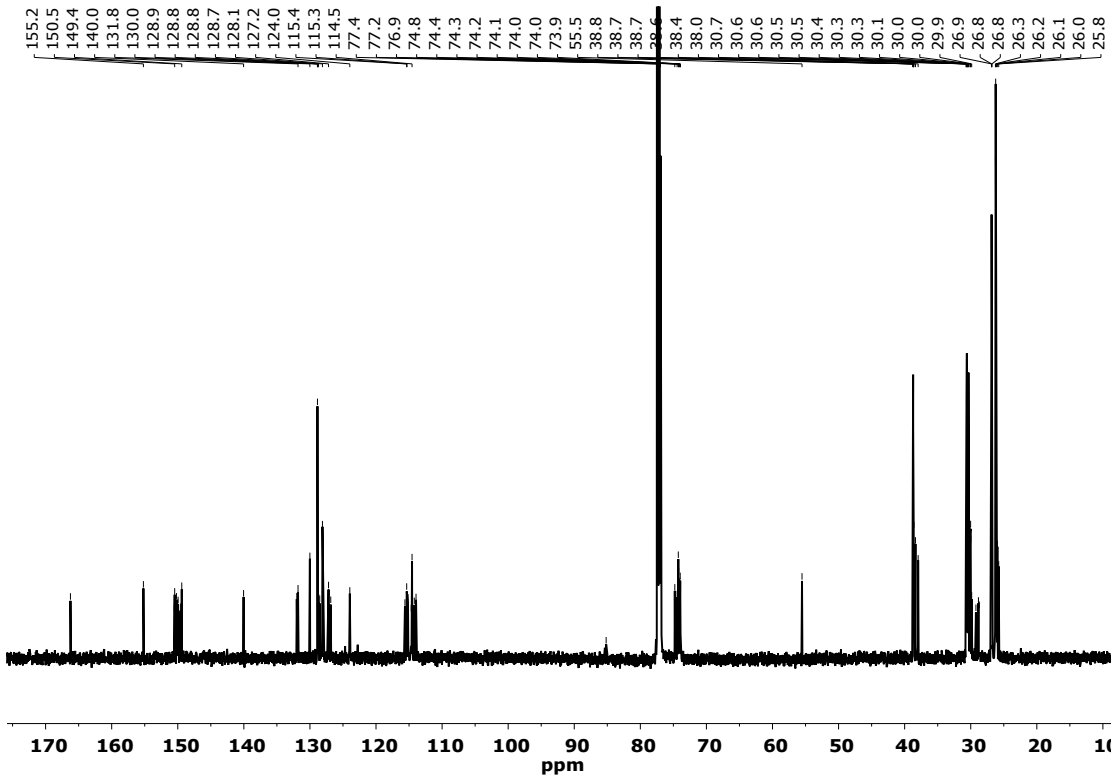

Figure S8. ^{13}CNMR (150 MHz, $CDCl_3$) spectrum of **Pillar-3b**.

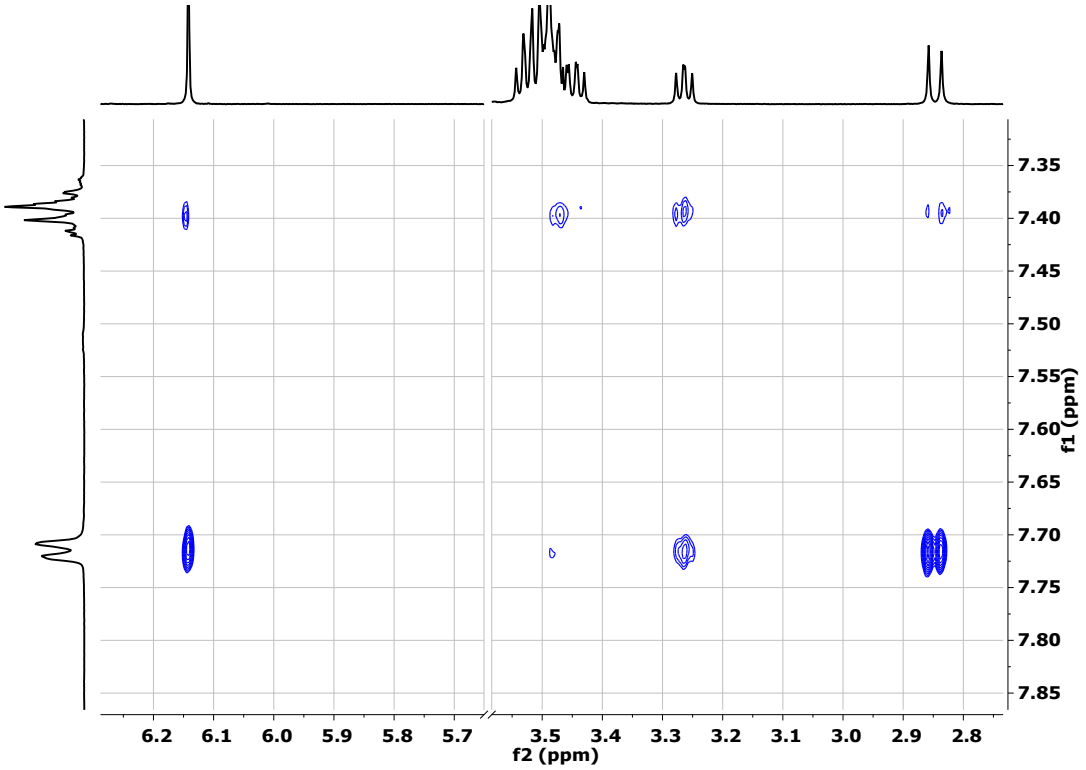

Figure S9. Expanded of 2D ROSEY spectrum (600 MHz, $CDCl_3$, 25 °C) of **Pillar-3a**.

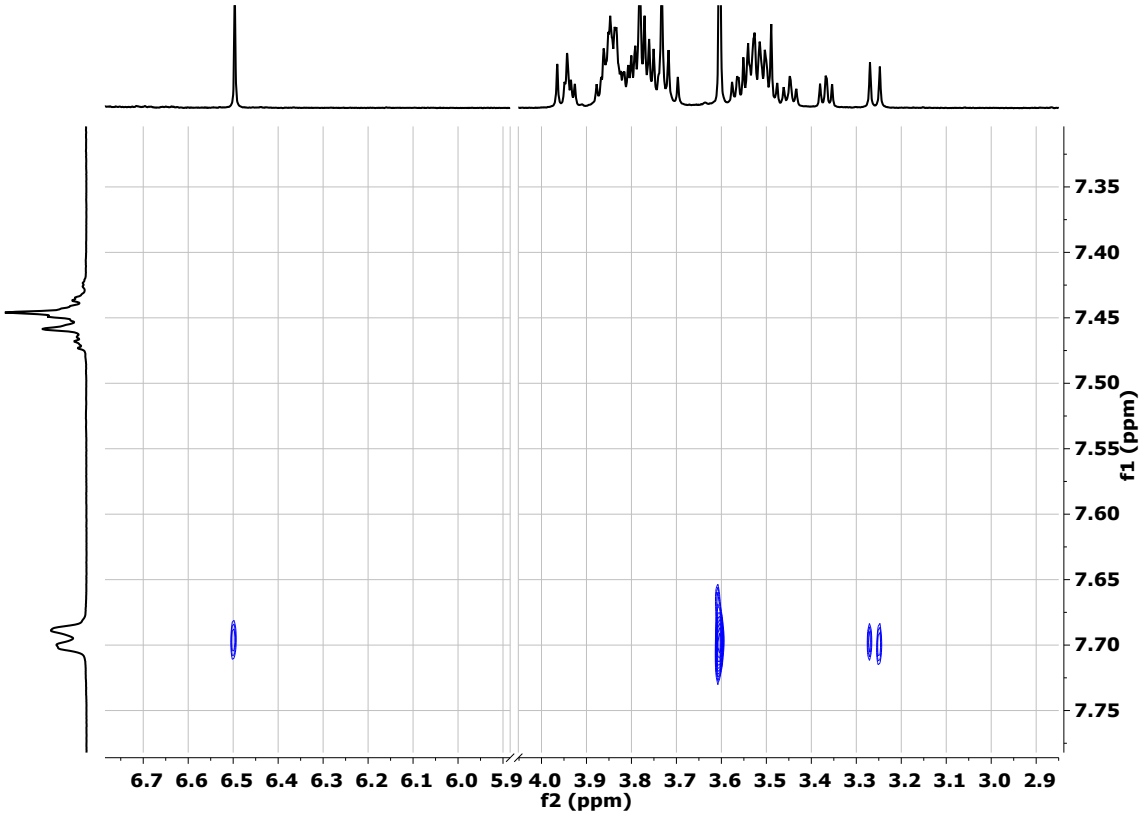

Figure S10. Expanded of 2D ROSEY spectrum (600 MHz, $CDCl_3$, 25 °C) of **Pillar-3a**.

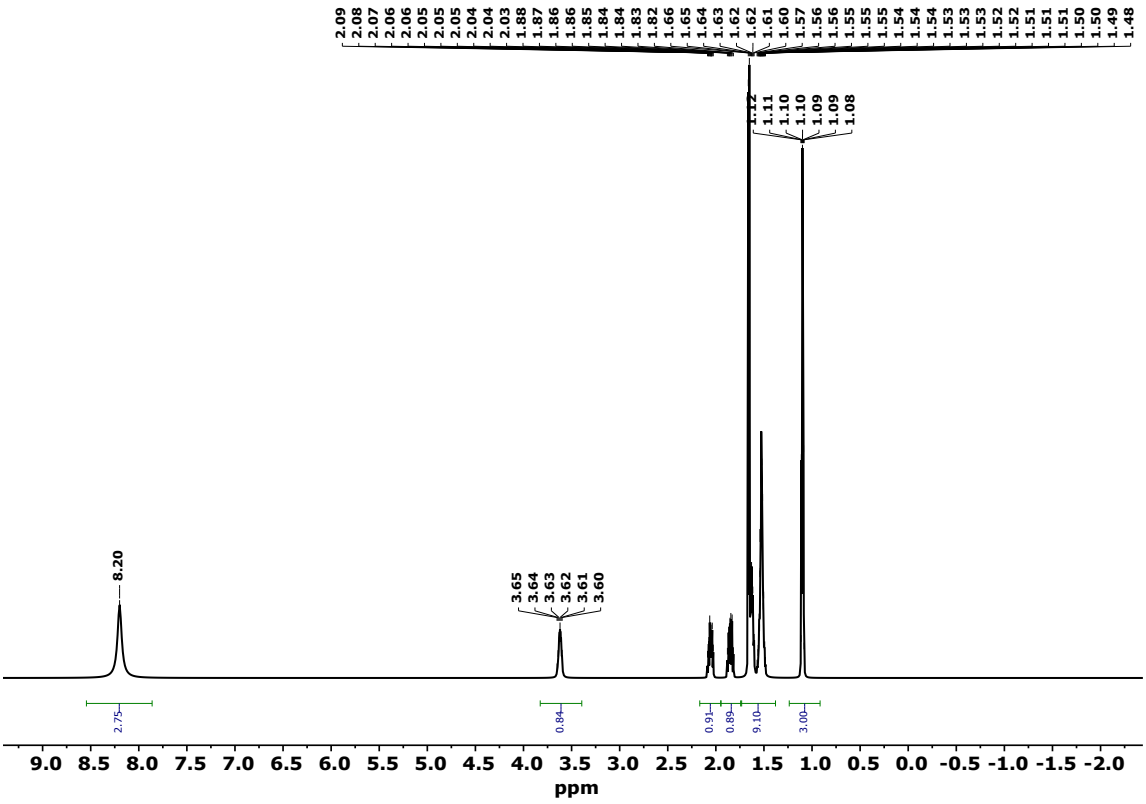

Figure S11. ^{1}HNMR (600 MHz, $CDCl_3$) spectrum of **G2**.

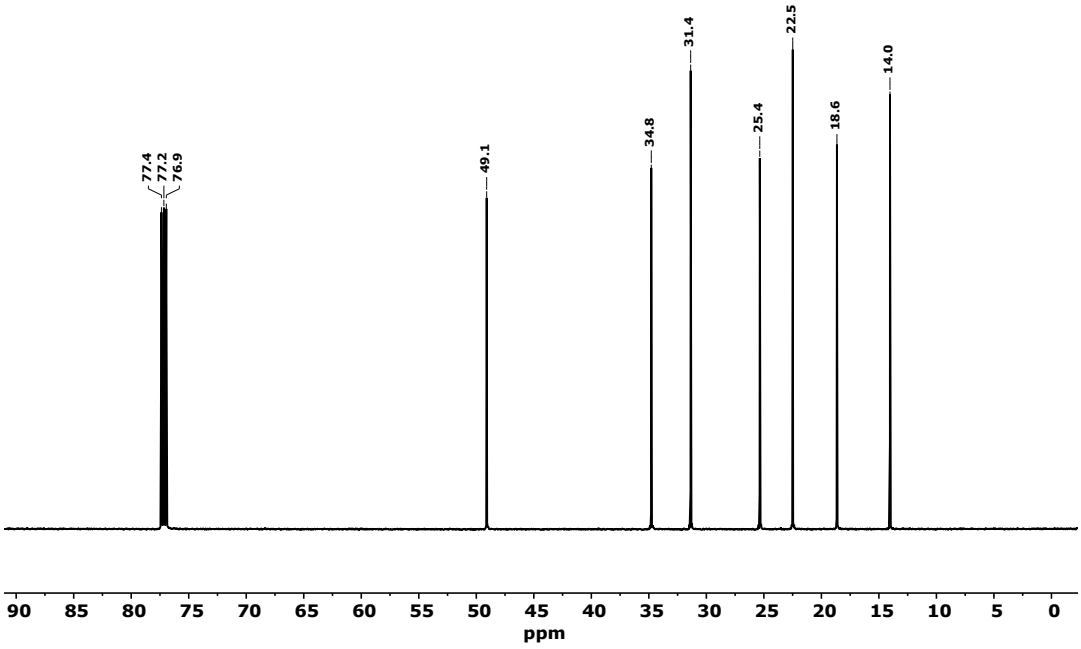

Figure S12. ^{13}CNMR (150 MHz, $CDCl_3$) spectrum of **G2**.

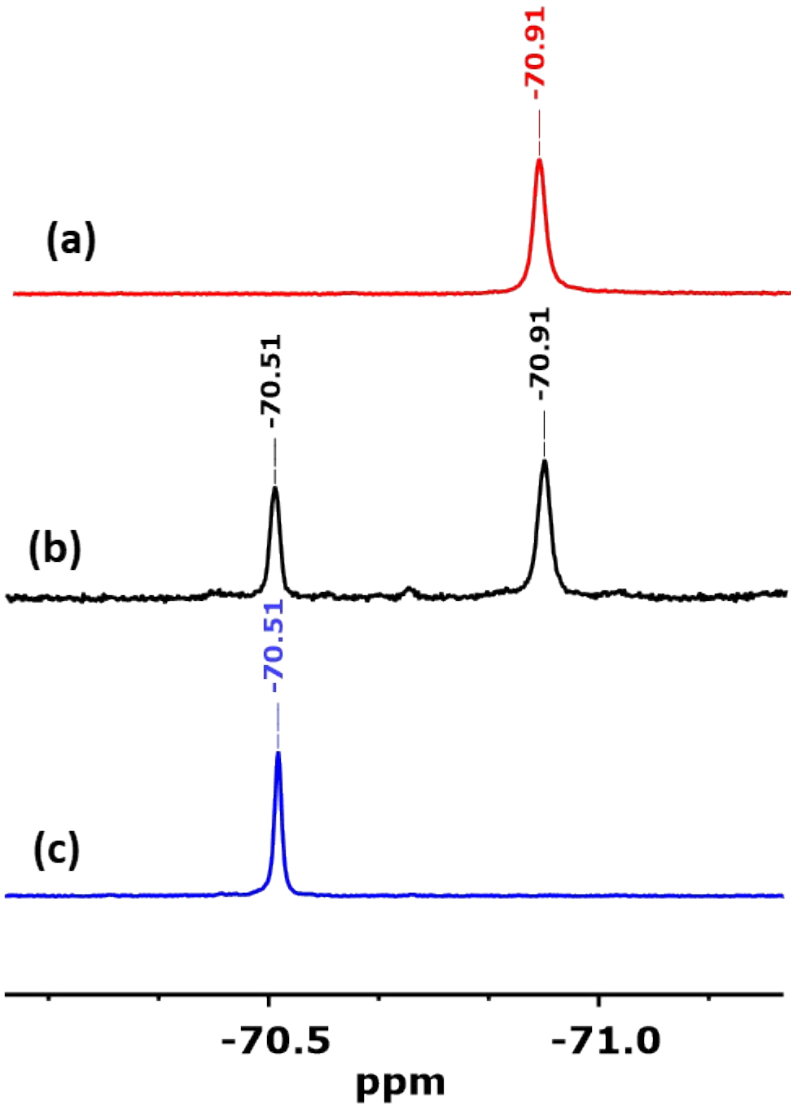

Figure S13. ^{19}F NMR spectra ($CDCl_3$, 376 MHz) of MTPA derivative hydoxy-functionalized pillar[5]arenes before and after separation by column chromatography. (a) First fraction **Pillar-3b**. (b) reaction mixture. (c) Second fraction **Pillar-3b**.

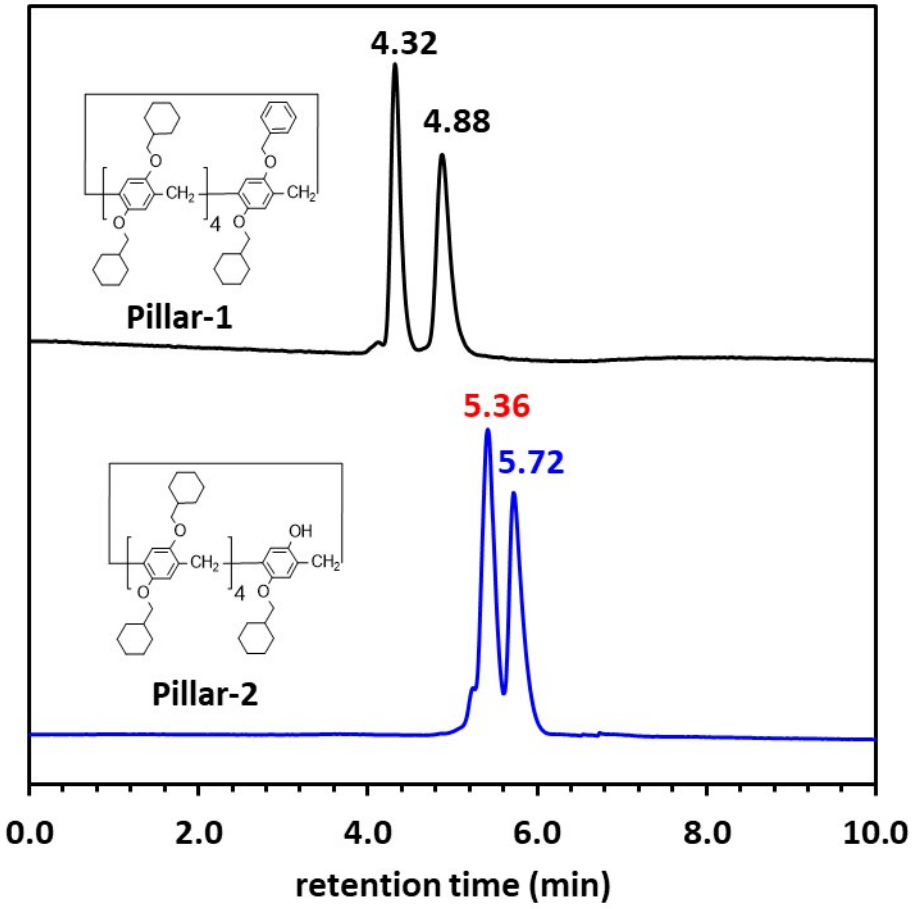

Figure S14. Chiral HPLC traces of racemic **Pillar-1** and **Pillar-2**. Hexane/isopropanol =95/5 (vol%) was used as eluent.

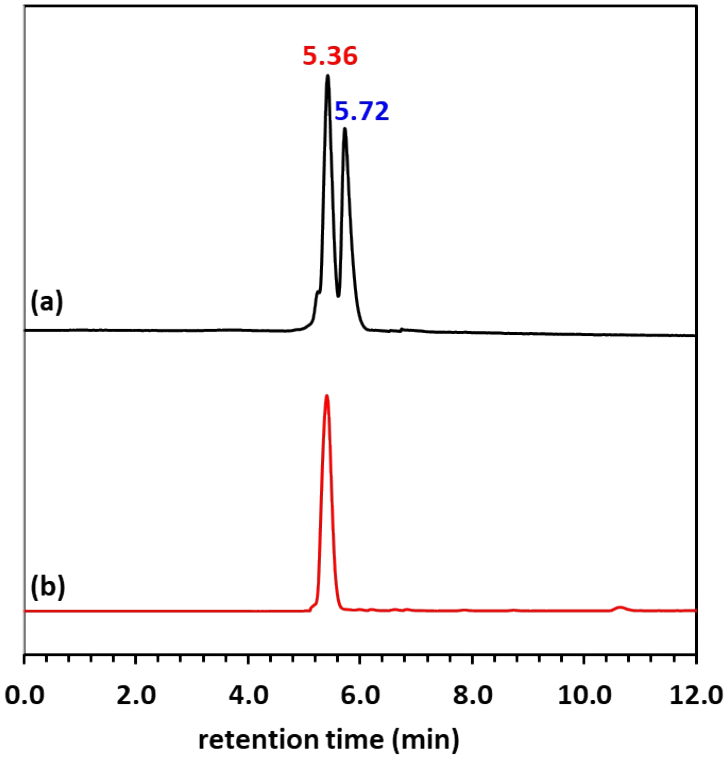

Figure S15. Chiral HPLC traces (a) racemic **Pillar-2** and (b) after the removal of MTPA group of the first fraction (**Pillar-2a**). Hexane/isopropanol =95/5 (vol%) was used as eluent.

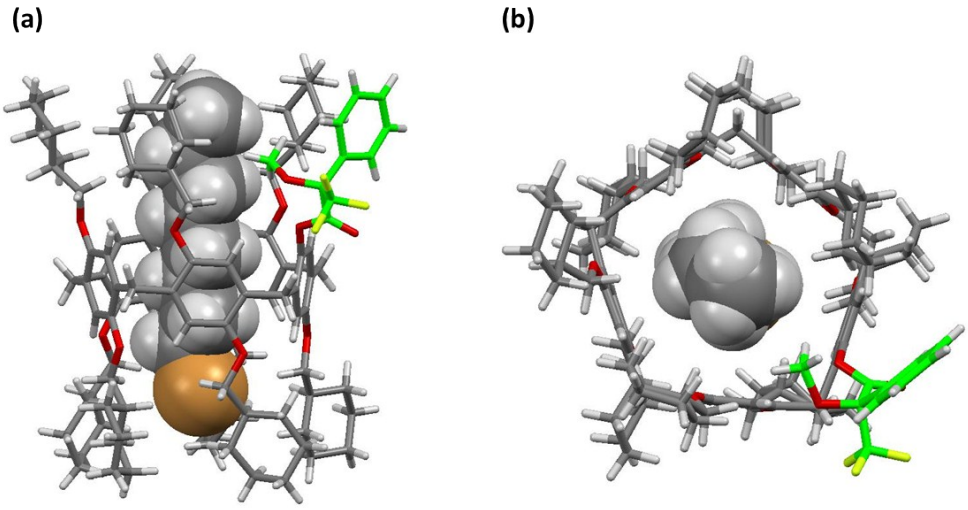

Figure S16. Inclusion complex molecular structure of Pillar-3b ⊃ 1-bromooctane molecules determined by single-crystal X-ray diffraction: (a) side view, (b) top view.

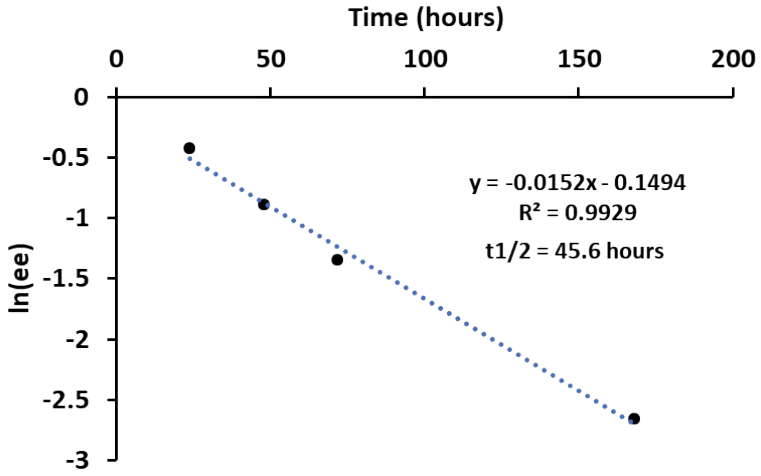

Figure S17. The Plot of ln(e/e) versus time (hours) at 313 K for compound Pillar-2a.

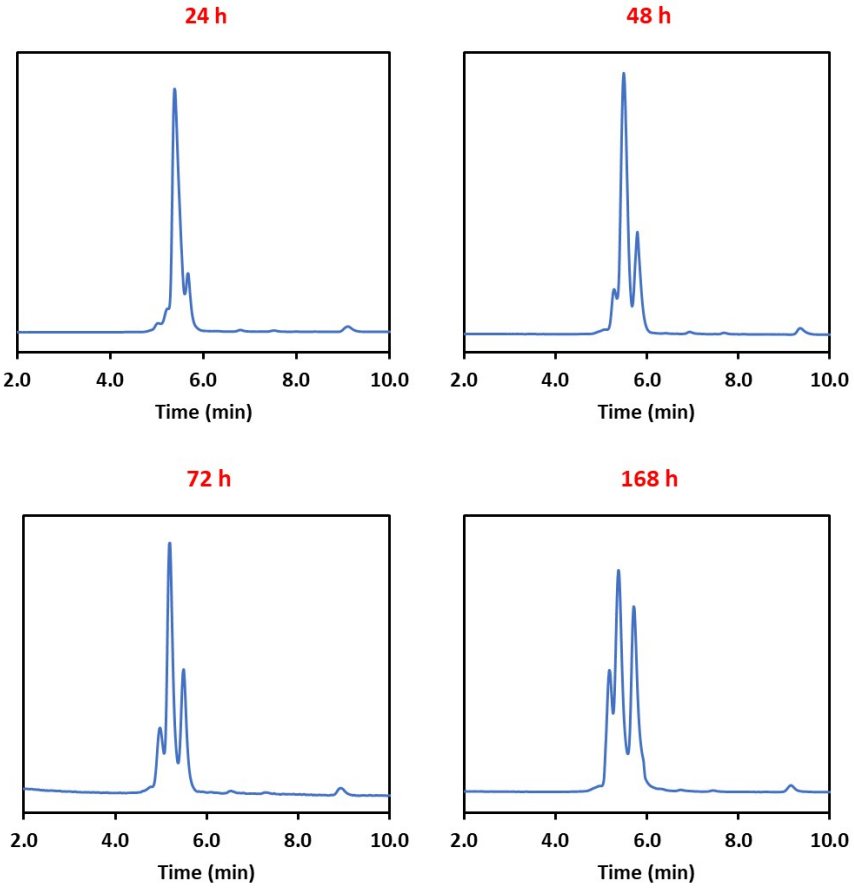

Figure S18. Chiral HPLC chromatograms as function of time for compound Pillar-2a at 313 K.

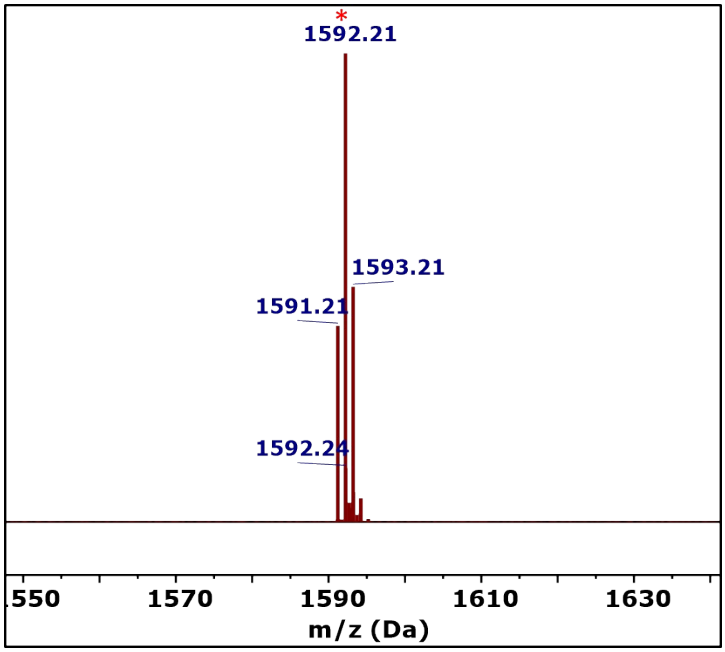

Figure S19. ES-MS spectrum of Inclusion of the complex [Pillar-2a ⊃ G2-Br]$^{+}$.

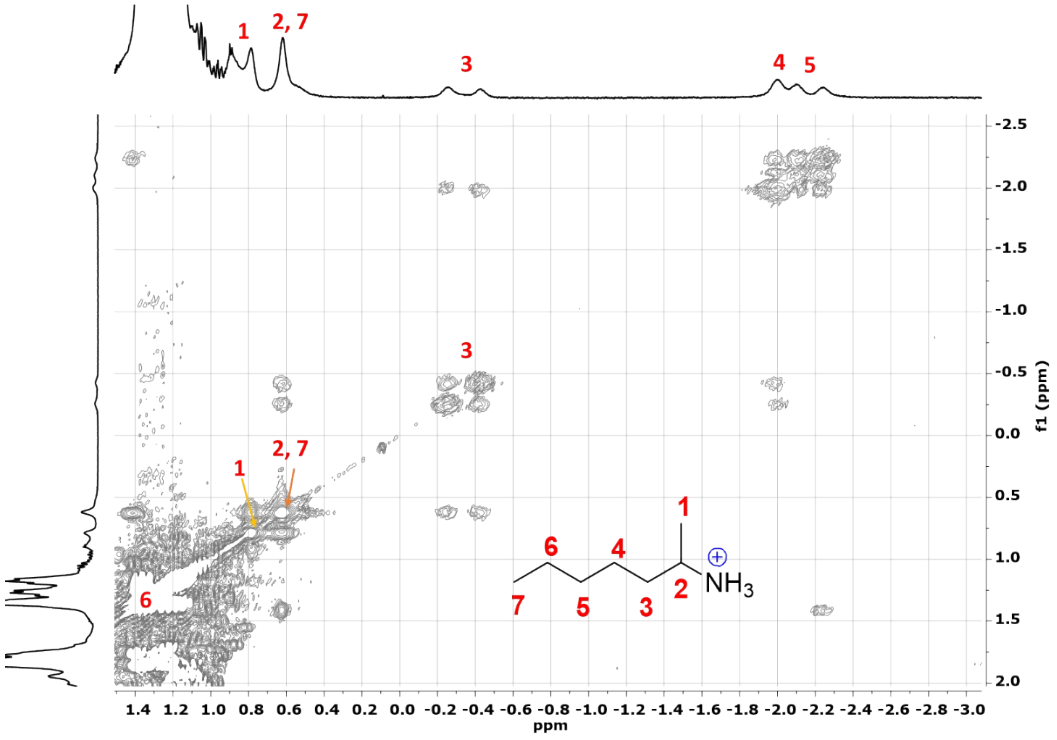

Figure S20. Partial COSY spectrum (600 MHz, $CDCl_3$) of the Inclusion complex [Pillar-2a ⊃ G2].

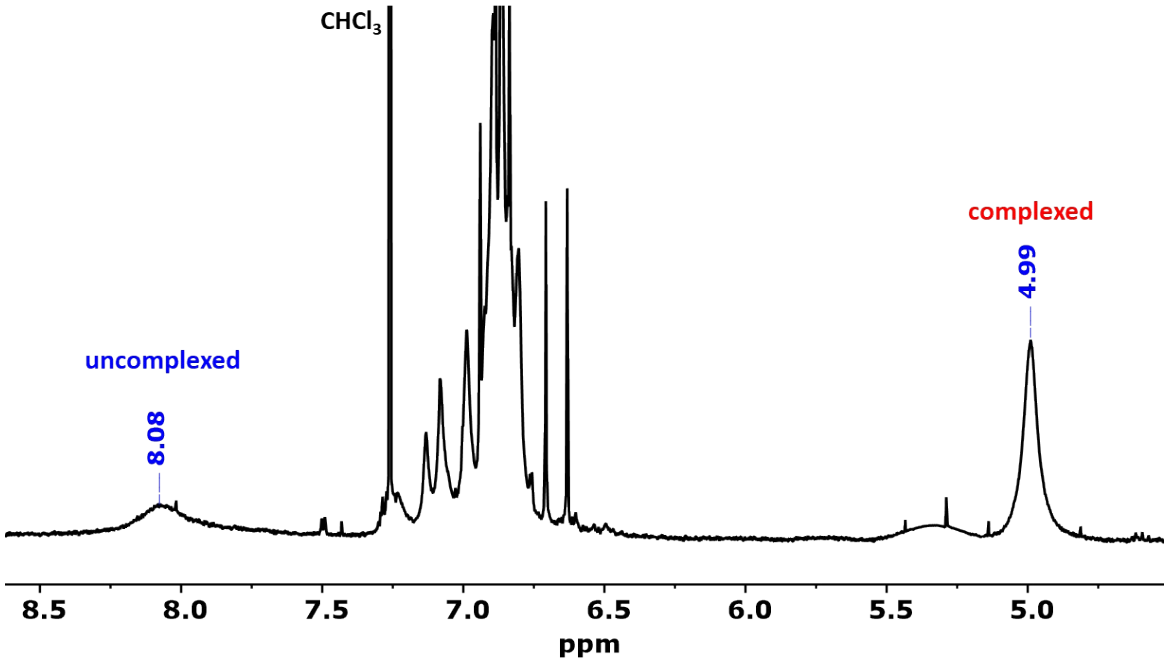

Figure S21. Partial ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the Inclusion complex [Pillar-2b ⊃ G2].

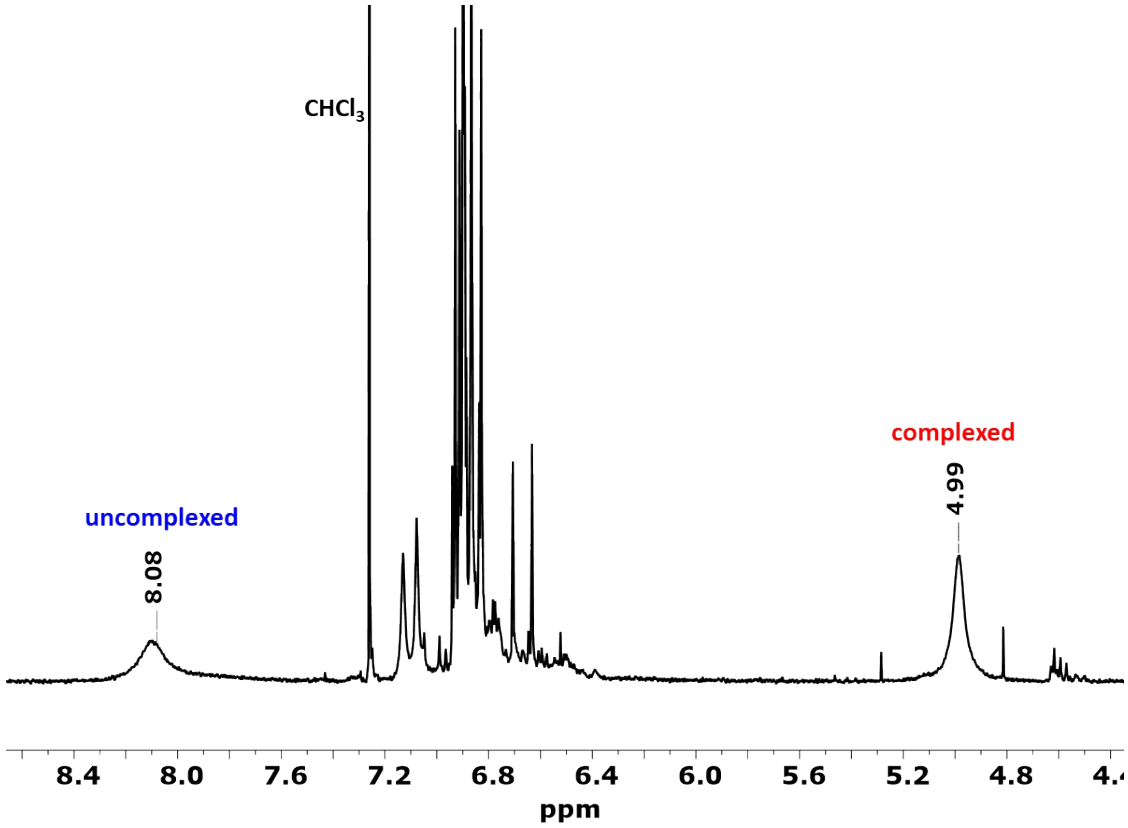

Figure S22. Partial ^{1}H NMR spectrum (600 MHz, $CDCl_3$, 298 K) of the Inclusion complex [Pillar-2a ⊃ G2].

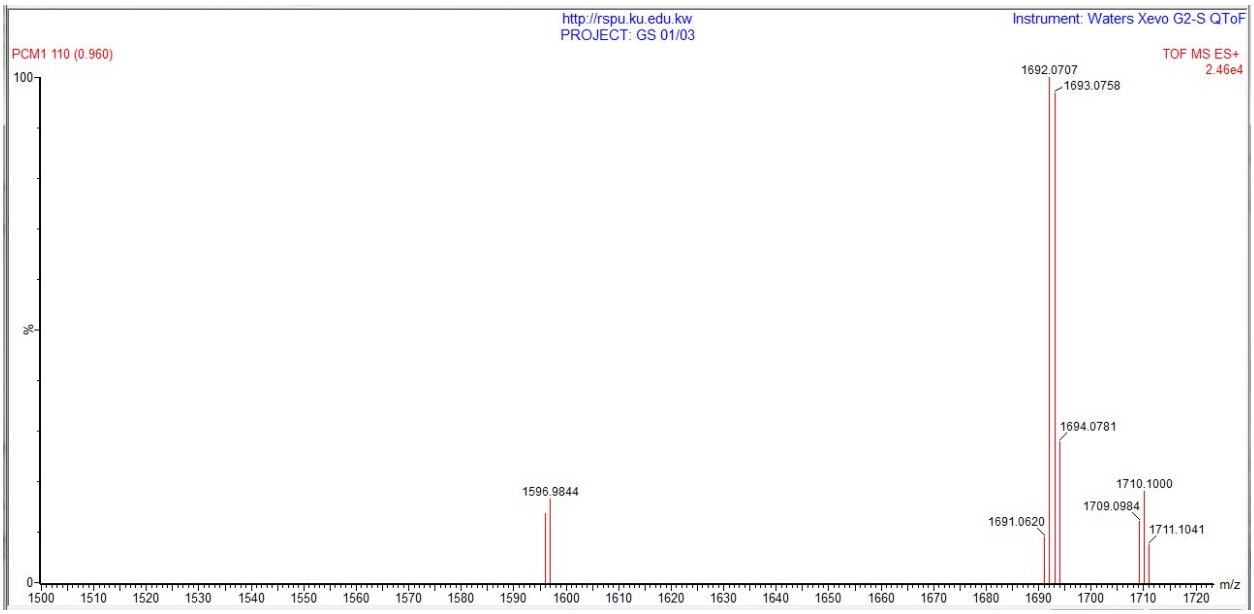

Figure S23. High resolution mass spectrum of **Pillar-3a**.

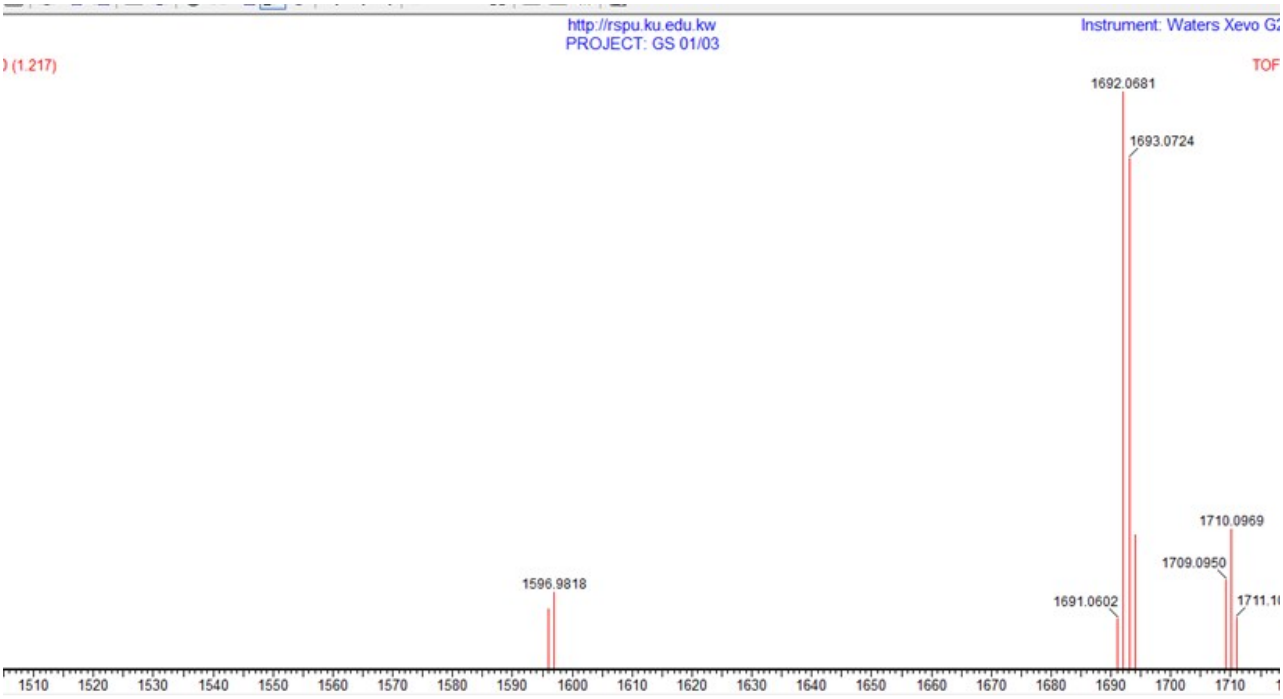

Figure S24. High resolution mass spectrum of **Pillar-3b**.