Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Functionalized fluorescent terephthalate monomers and their attempted polyester formation

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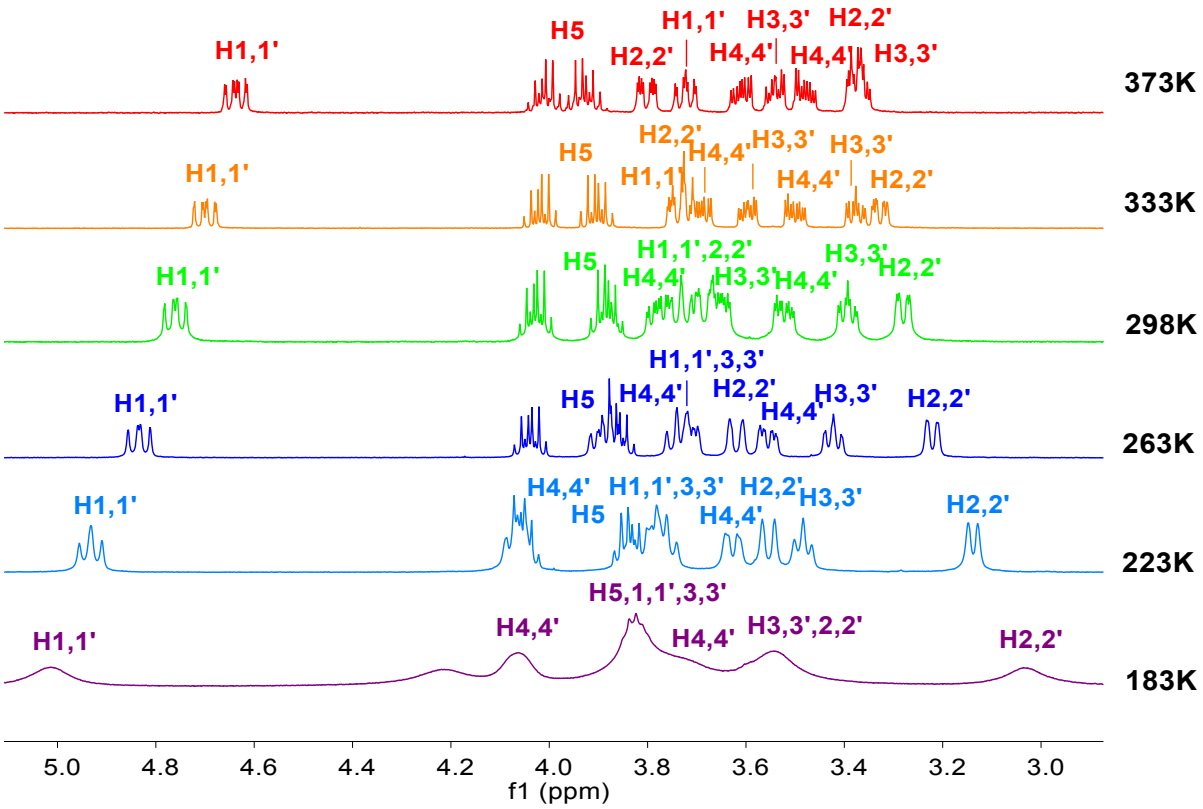
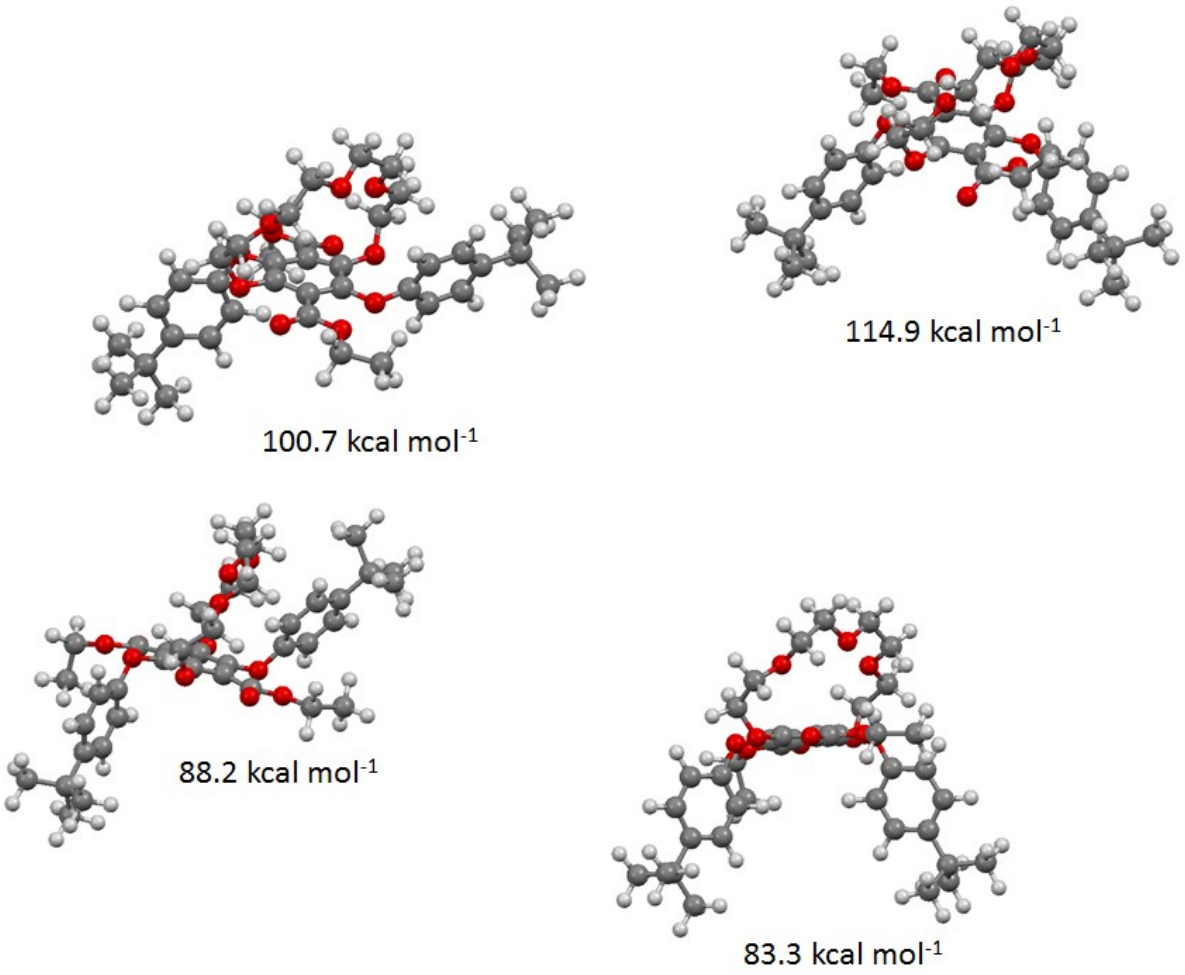
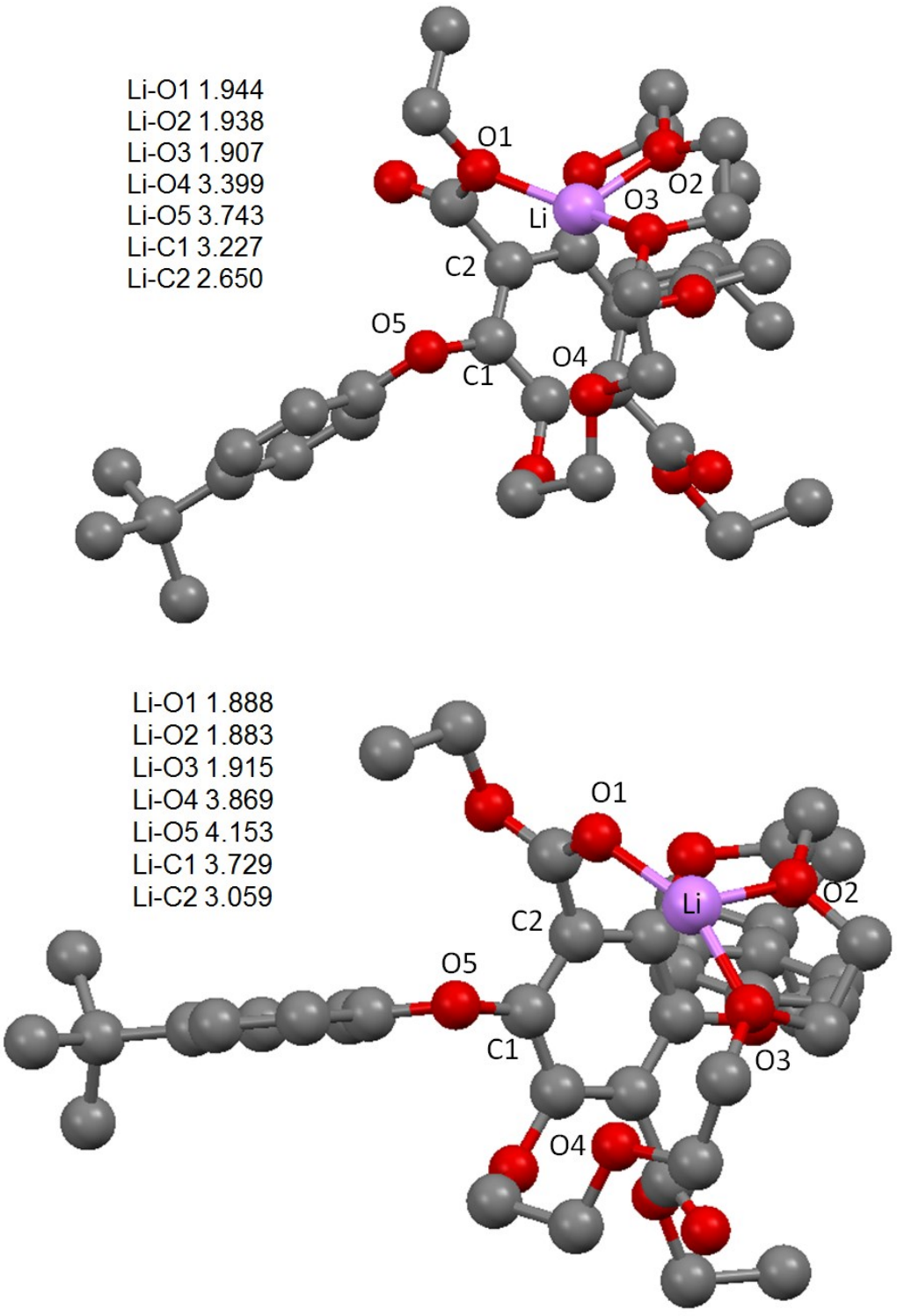


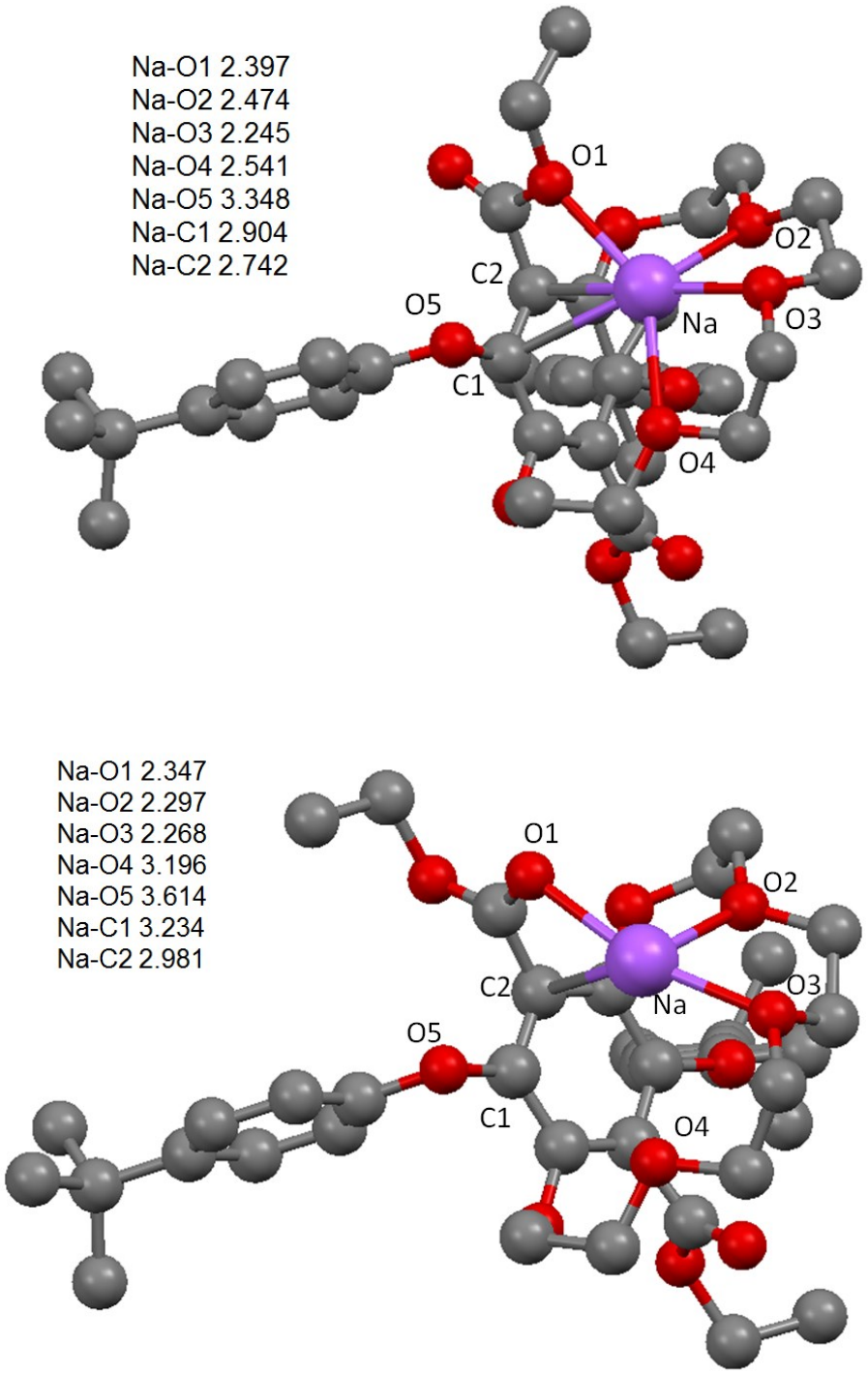
S1. Selected variable temperature ^{1}H NMR spectra of **3** in d^{8}-toluene between 183K and 373K highlighting the methylene proton region.



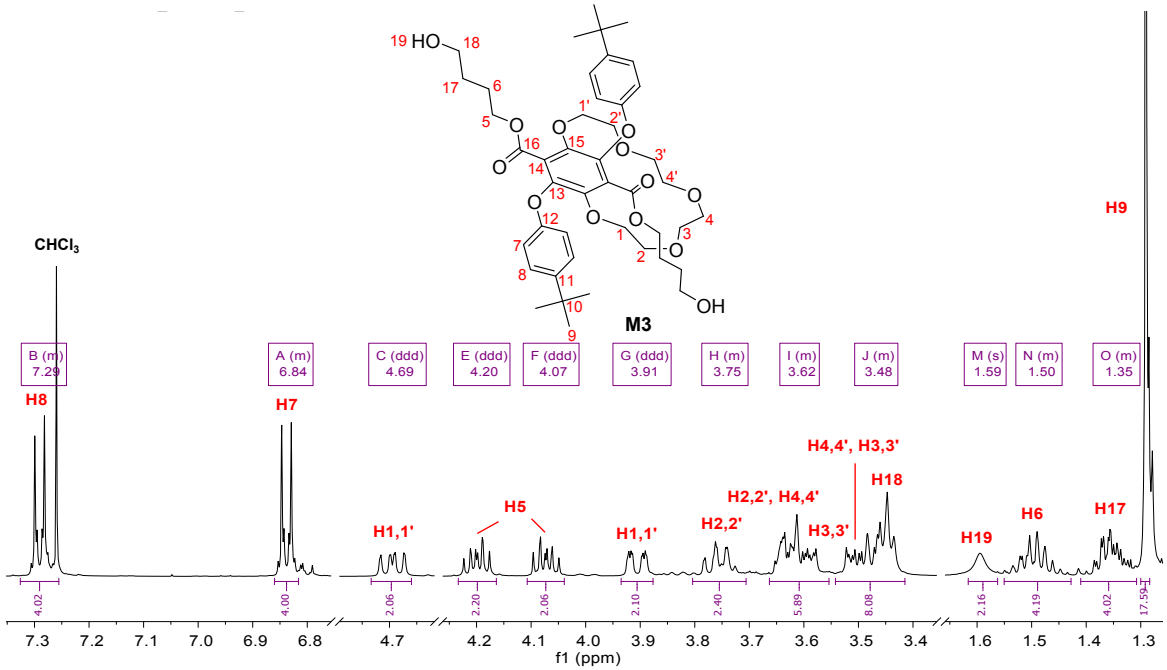
S2. A sample of calculated gas phase conformations and their energies for **3** using molecular dynamics simulations at the MM+ level.



S3. Gaussian calculated energy-minimised gas phase structures for a Li^+ adduct of **3** using B3LYP and a 6-311G basis set. Distances shown as the insert are in Å and hydrogens are omitted for clarity.

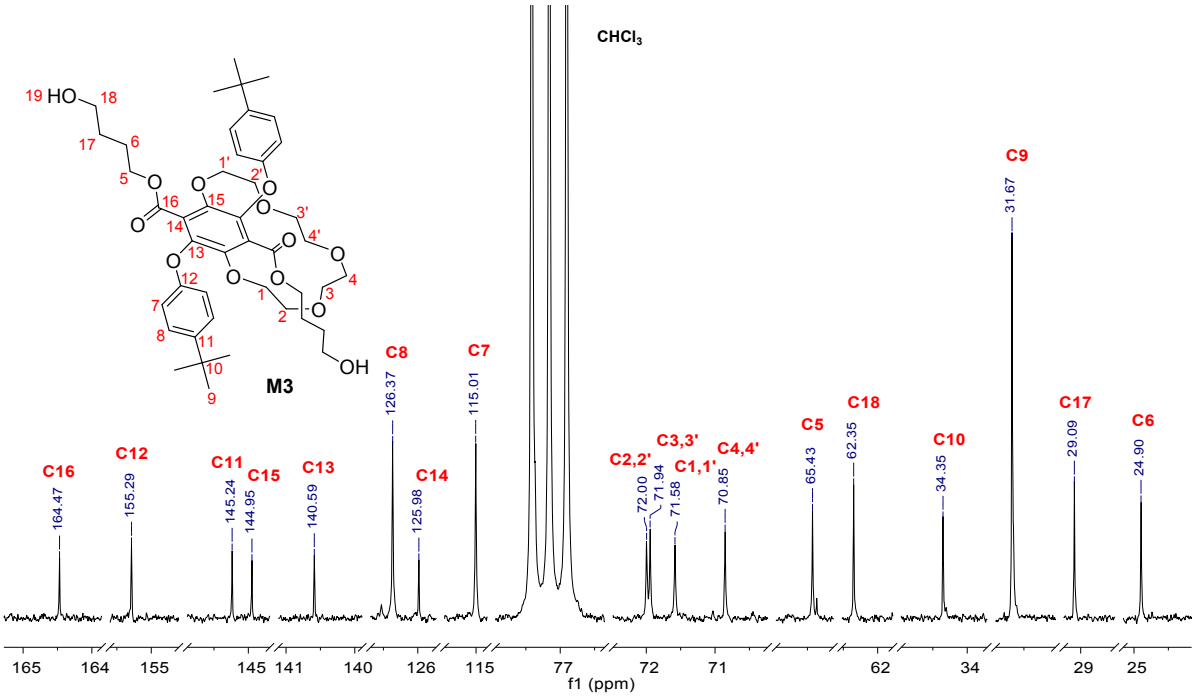


S4. Gaussian calculated energy-minimised gas phase structures for a Na^+ adduct of **3** using B3LYP and a 6-311G basis set. Distances shown as the insert are in Å and hydrogens are omitted for clarity.



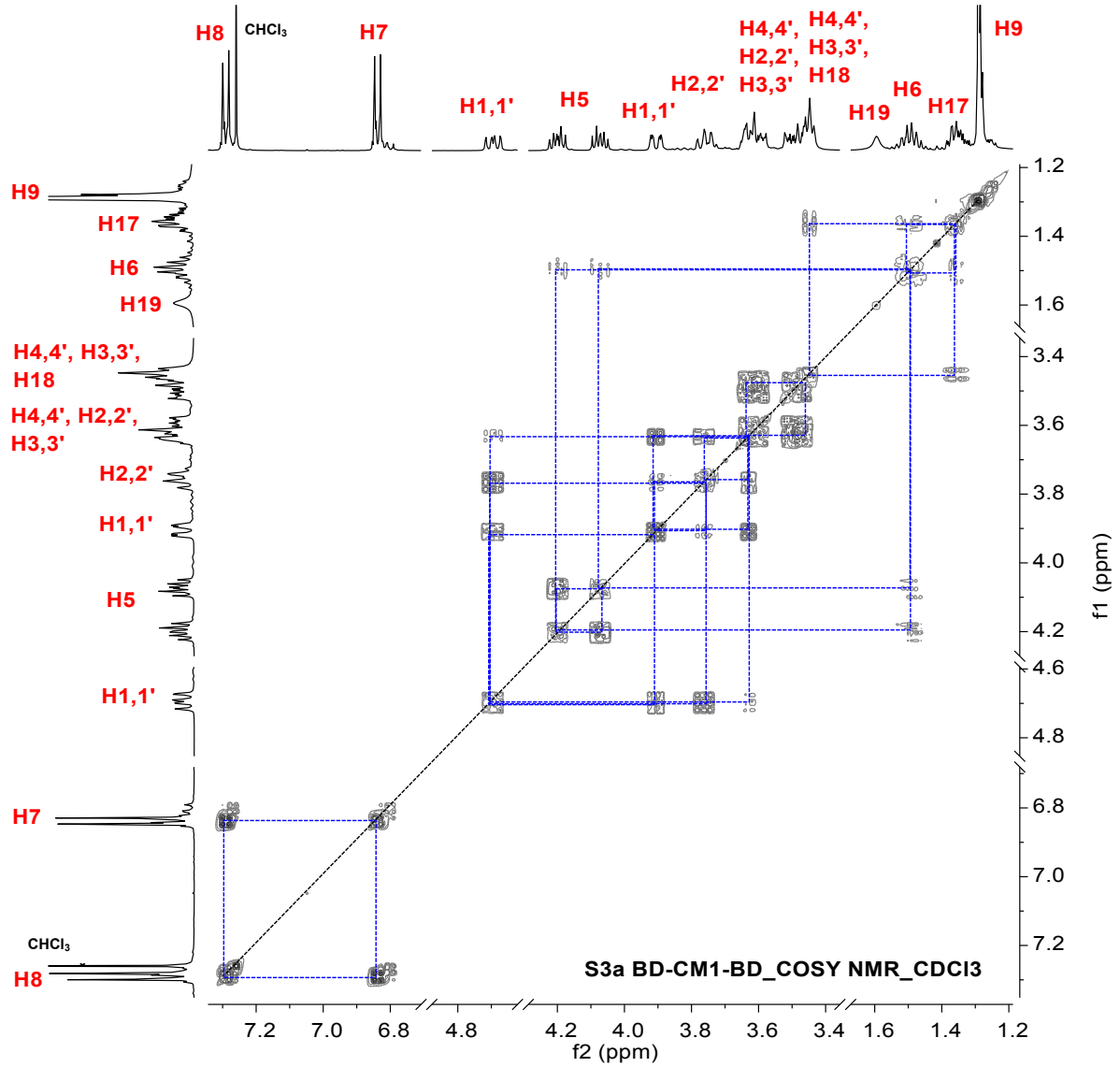
^{1}H NMR (500 MHz, Chloroform - *d*) δ7.33 – 7.26 (m, 4H, H8), 6.86 – 6.82 (m, 4H, H7), 4.69 (ddd, *J*= 13.0, 8.9, 1.3 Hz, 2H, H1, H1'), 4.20 (ddd, *J*= 10.9, 6.8, 5.9 Hz, 2H, H5), 4.07 (ddd, *J*= 10.9, 6.7, 5.9 Hz, 2H, H5), 3.91 (ddd, *J*= 13.0, 3.6, 1.5 Hz, 2H, H1, H1'), 3.80 – 3.71 (m, 2H, H2, H2'), 3.66 – 3.55 (m, 6H, H2, H2', H4, H4', H3, H3'), 3.54 – 3.41 (m, 8H, H4, H4', H3, H3', H18), 1.59 (s, 2H, H19), 1.55 – 1.43 (m, 4H, H6), 1.41 – 1.31 (m, 4H, H17), 1.29 (s, 18H, H9).

S5. ^{1}H NMR (500MHz, $CDCl_3$) spectrum of monomer diol **M3**.

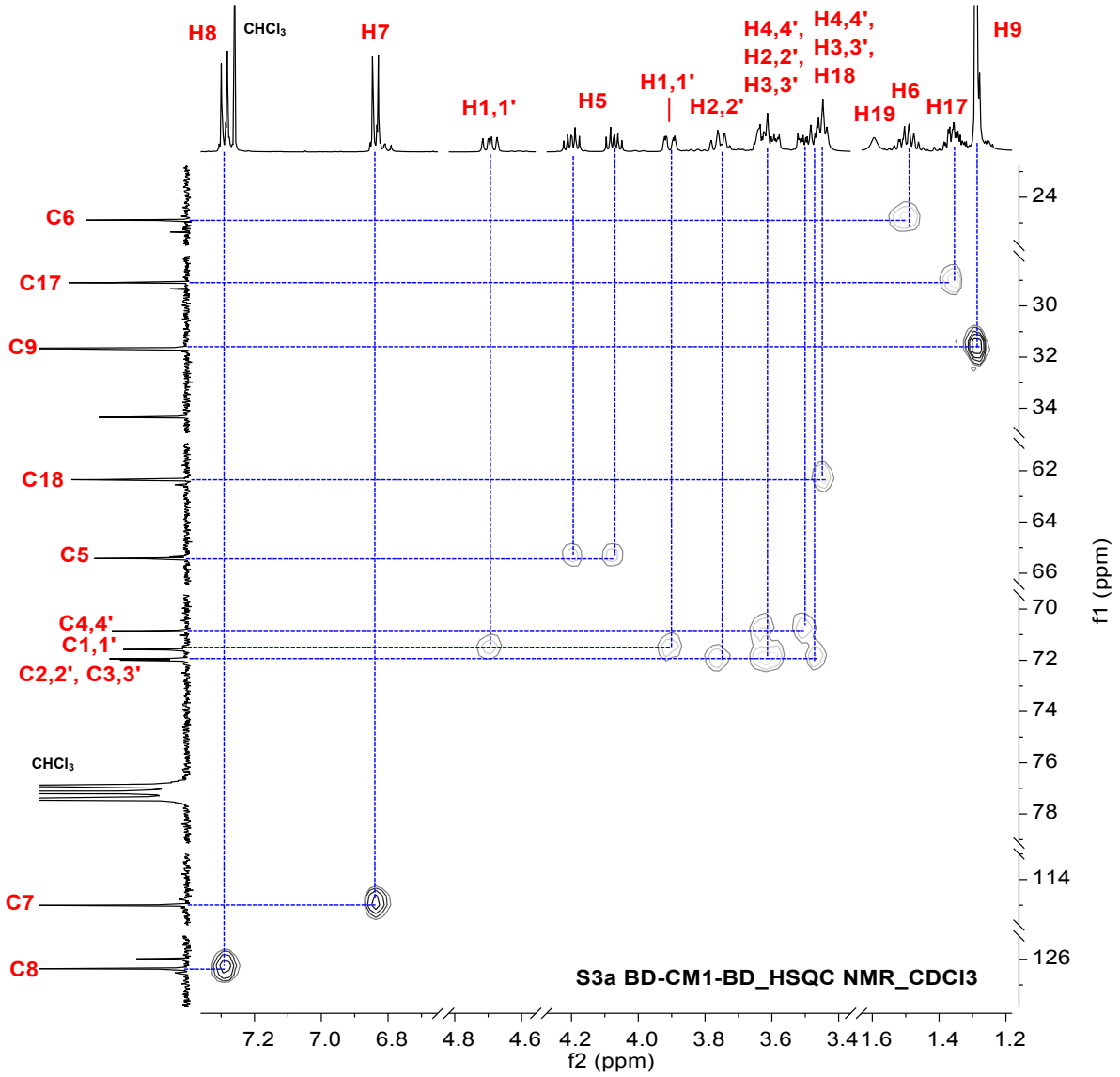


^{13}C NMR (126 MHz, $CDCl_3$) δ164.47 (C16), 155.29 (C12), 145.24 (C11), 144.95 (C15), 140.59 (C13), 126.37 (C8), 125.98 (C14), 115.01 (C7), 72.00 (C2, C2'), 71.94 (C3, C3'), 71.58 (C1, C1'), 70.85 (C4, C4'), 65.43 (C5), 62.35 (C18), 34.35 (C10), 31.67 (C9), 29.09 (C17), 24.90 (C6).

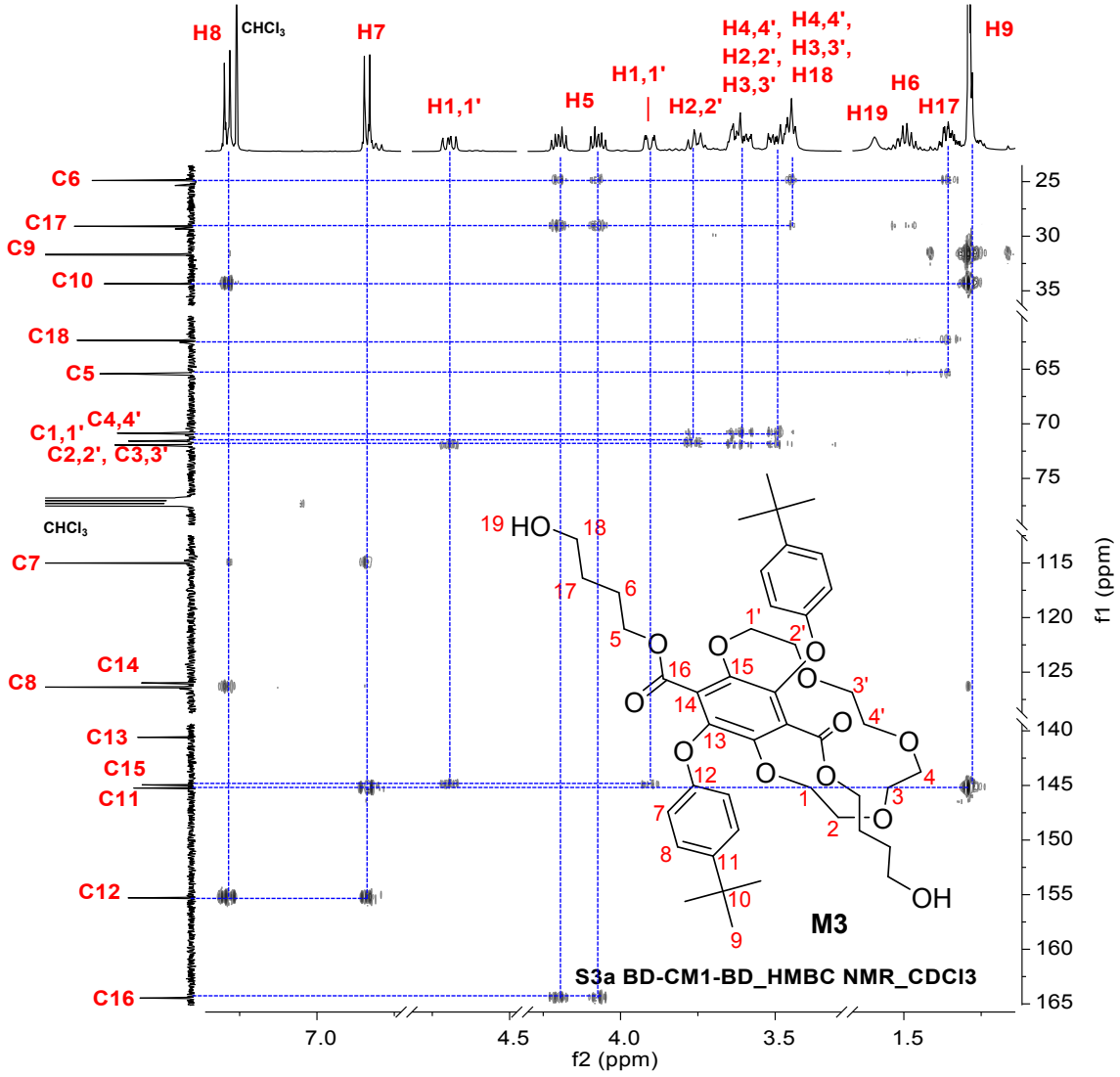
S6. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of monomer diol **M3**.



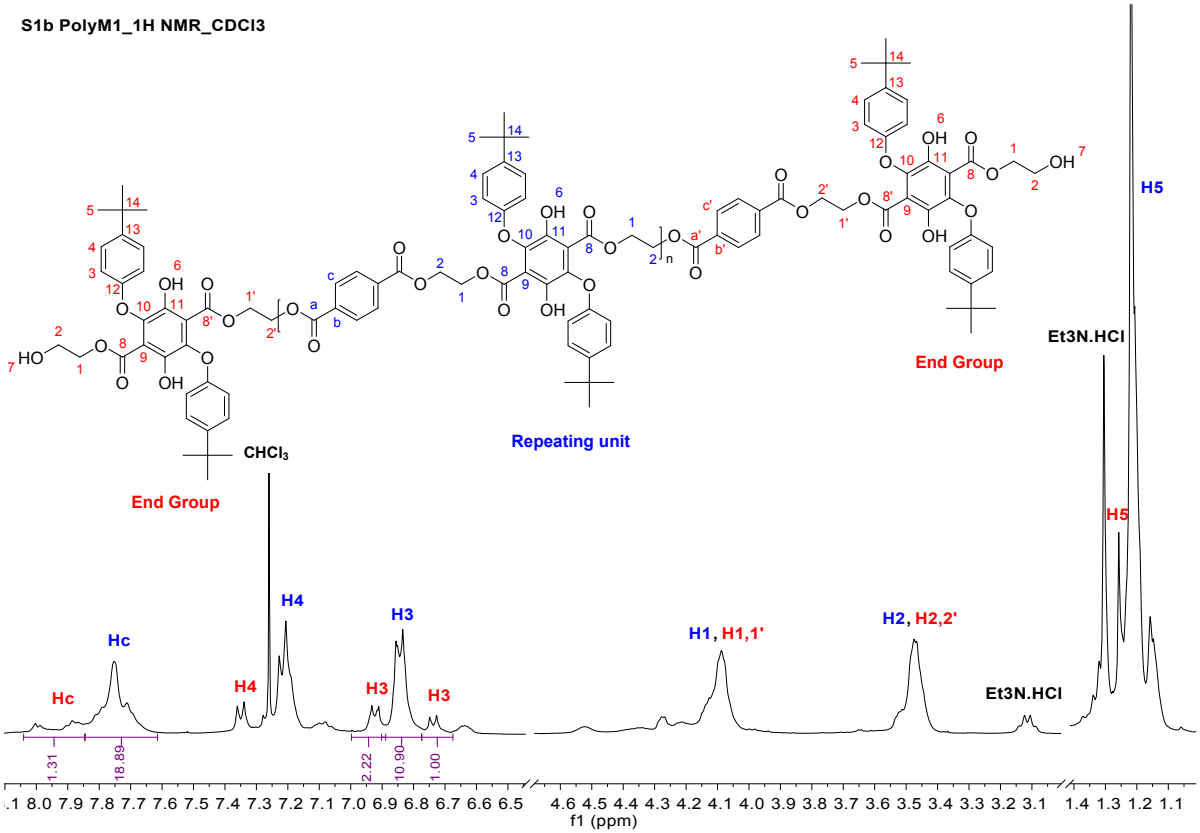
S7. COSY NMR spectrum of monomer diol **M3**.



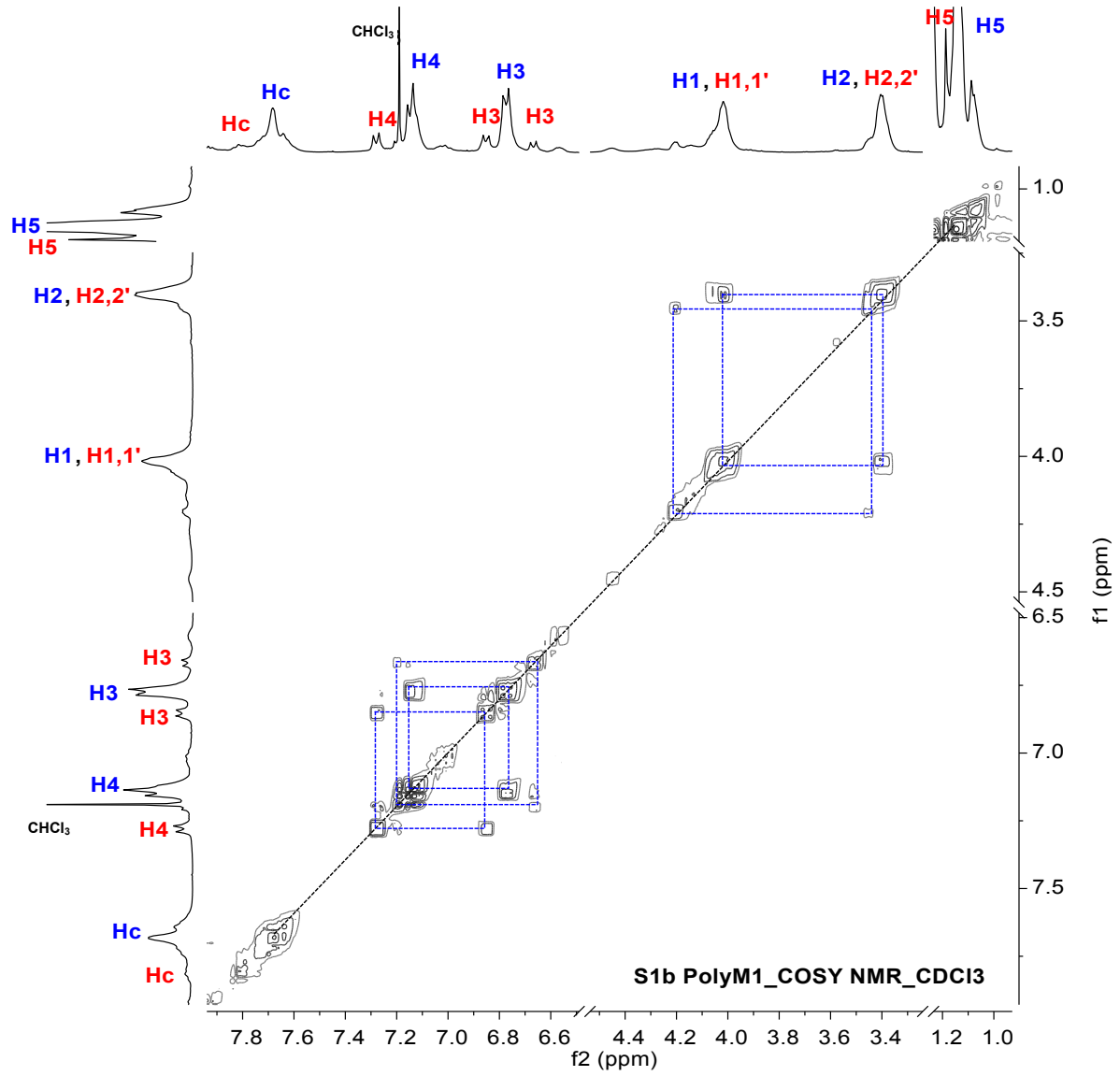
S8. HSQC NMR spectrum of monomer diol **M3**.



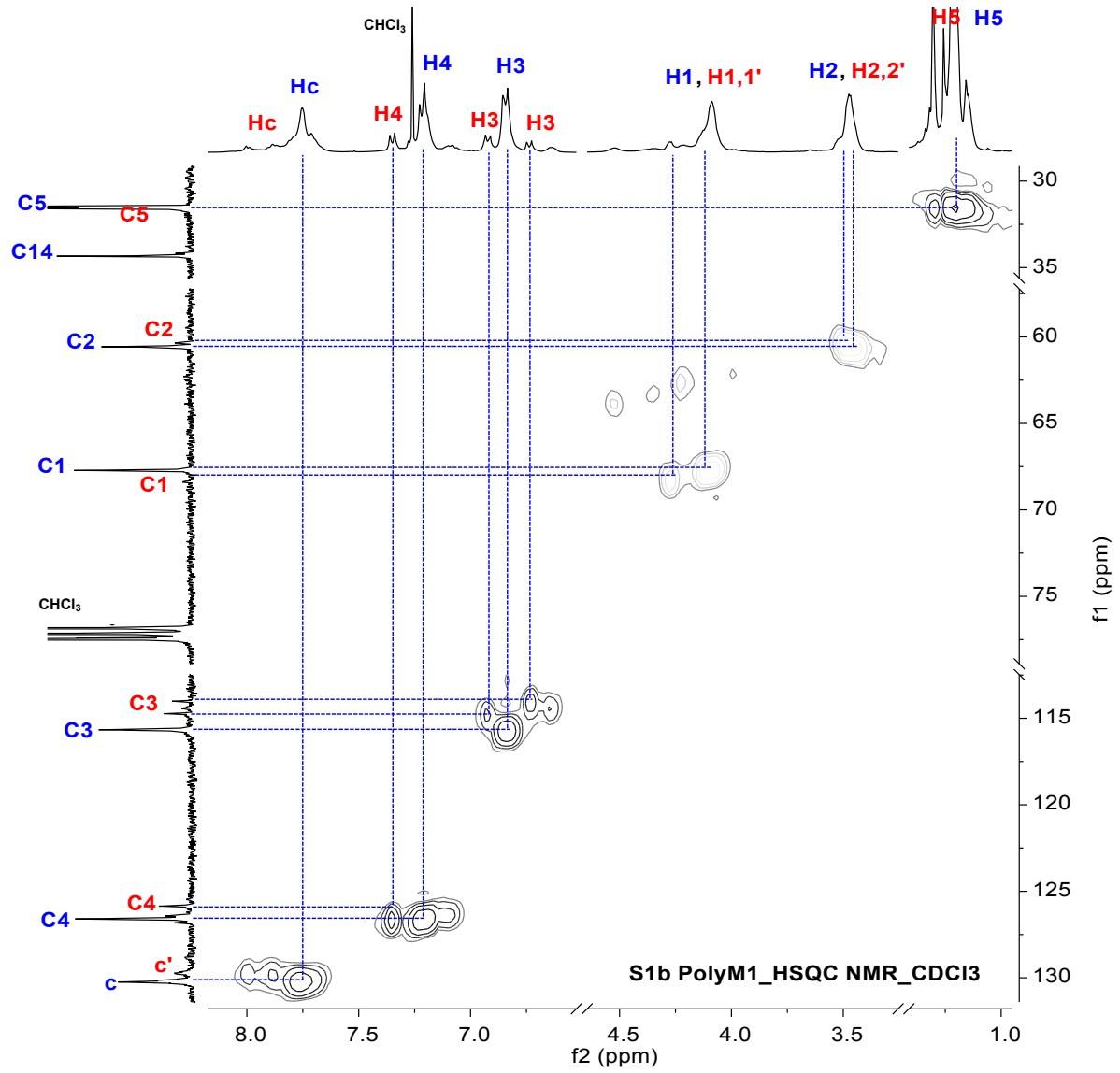
S9. HMBC NMR spectrum of monomer diol **M3**.



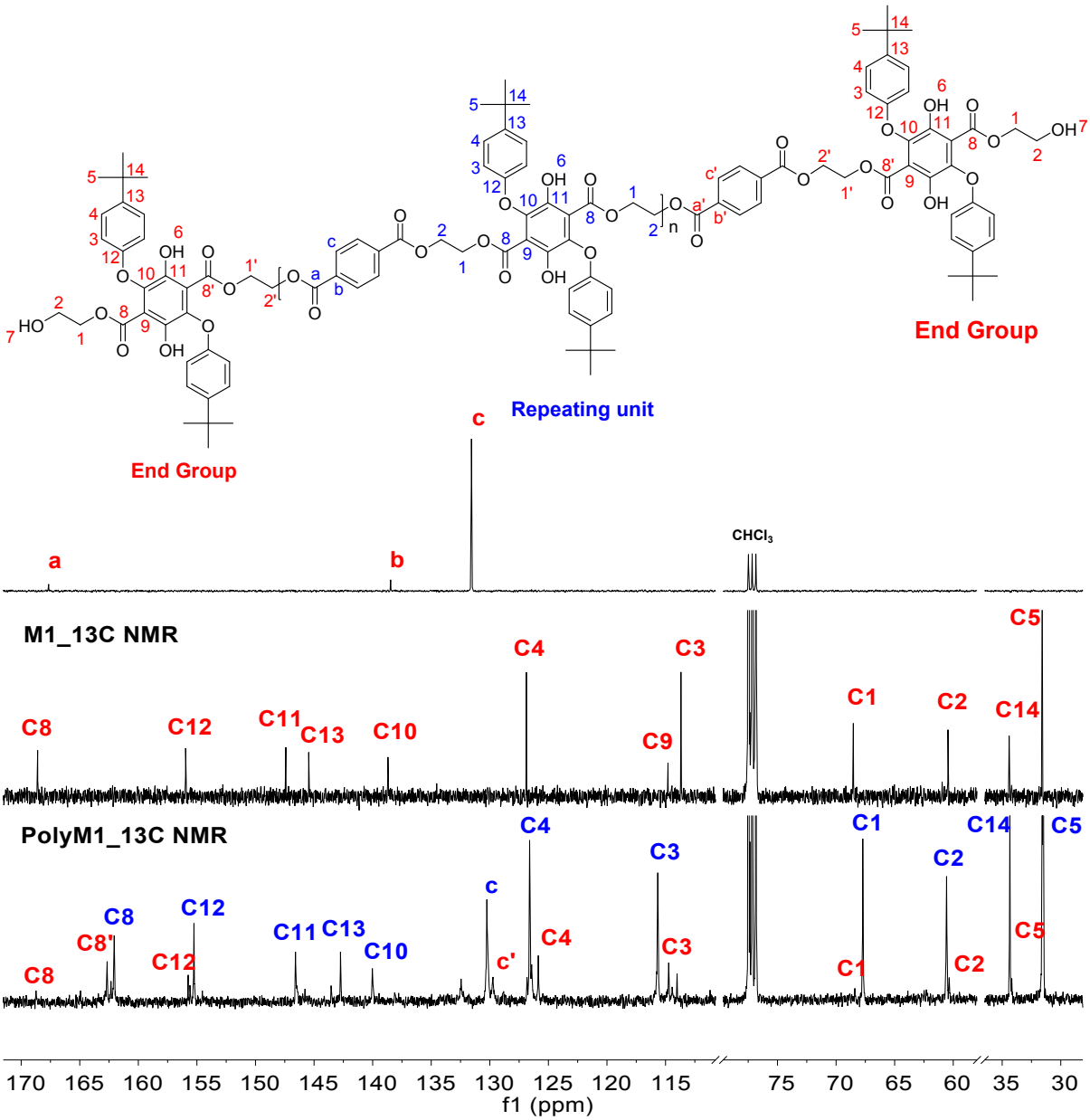
S10. ^{1}H NMR (400MHz, $CDCl_3$) spectrum of **PolyM1**.



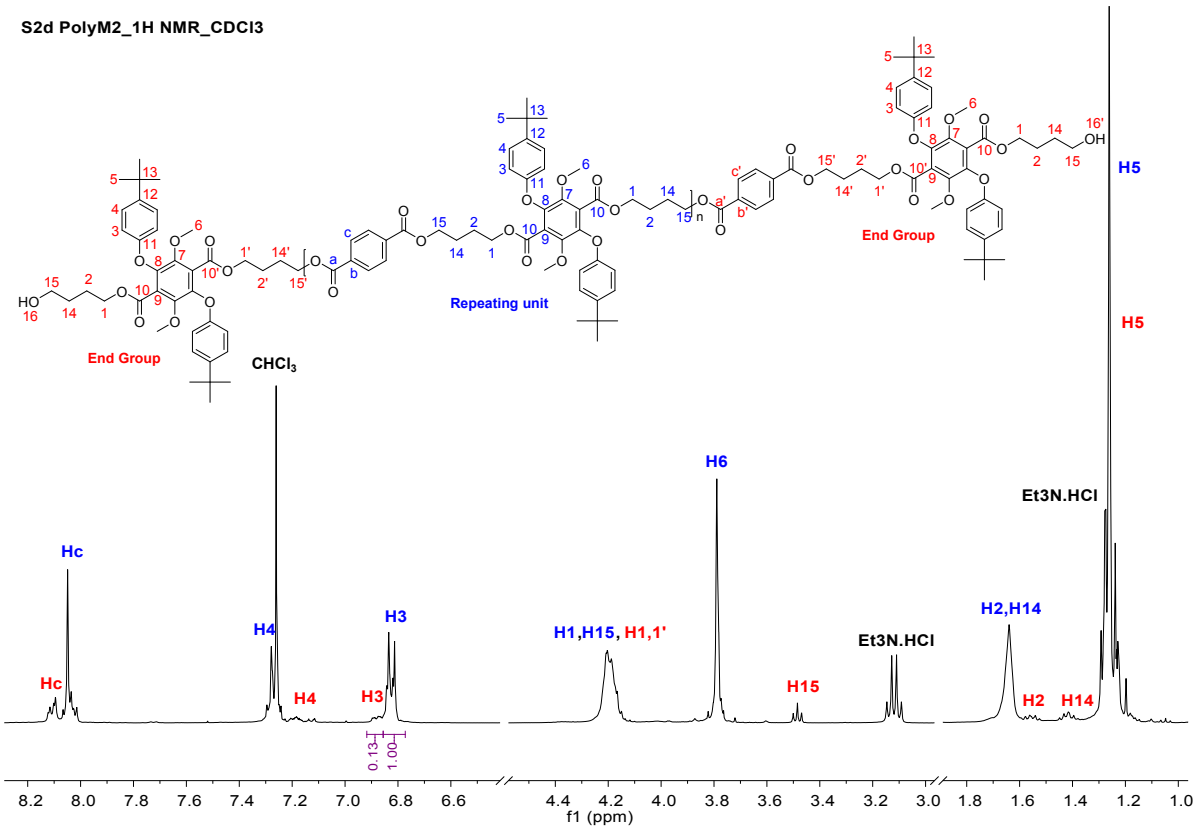
S11. COSY NMR spectrum of **PolyM1**.



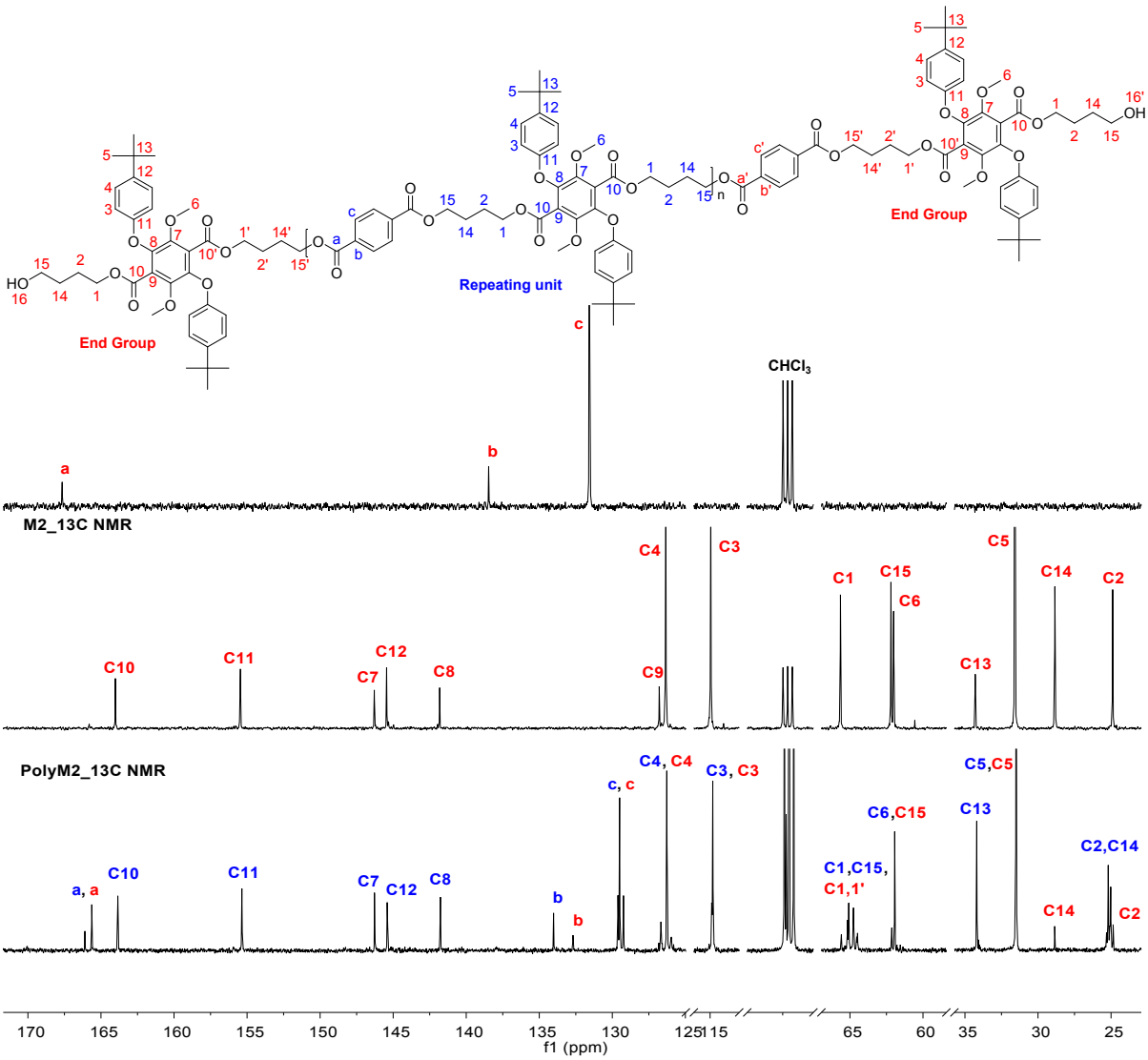
S12. HSQC NMR spectrum of **PolyM1**.



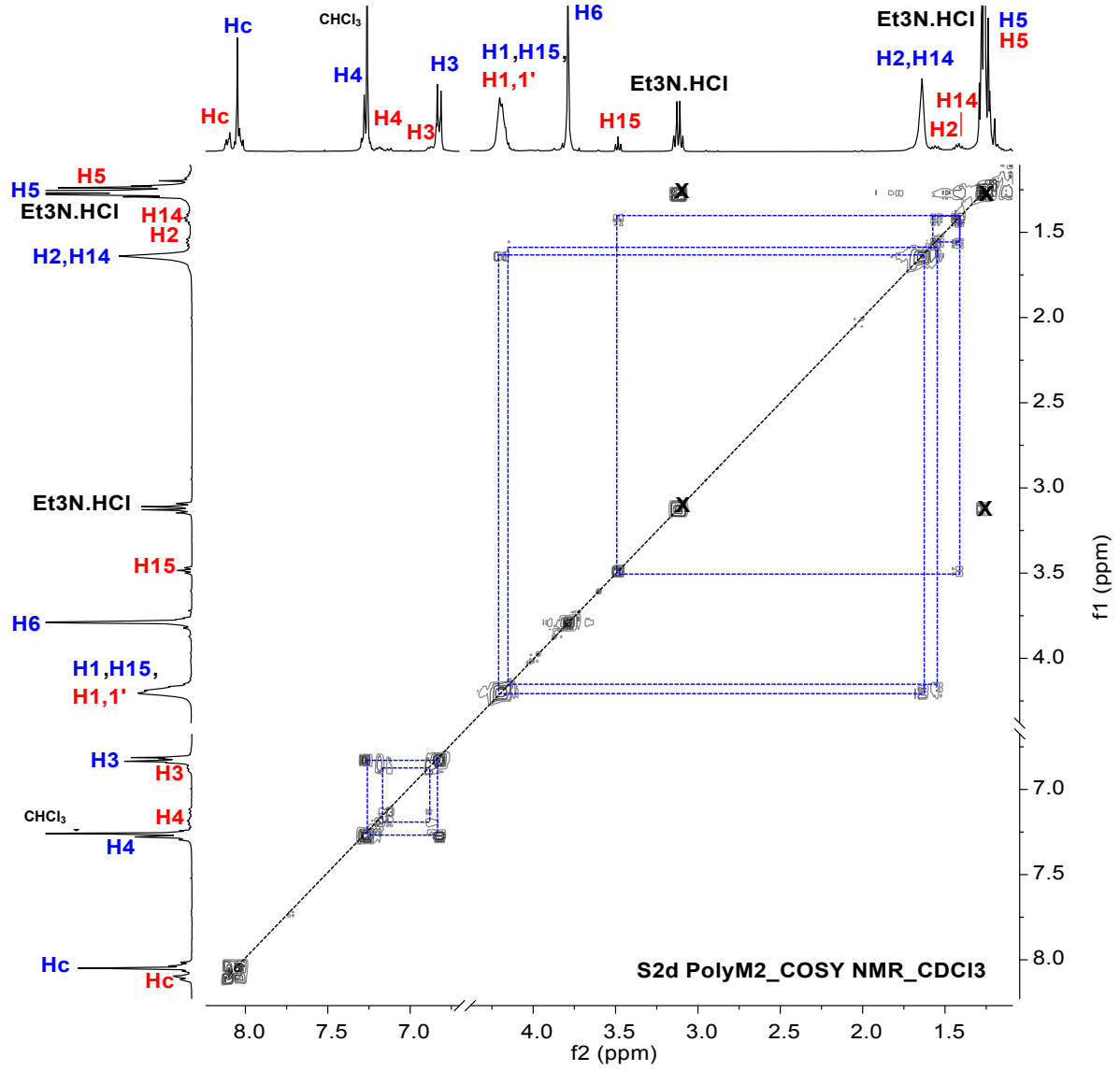
S13. Comparison of ^{13}C NMR spectra (101 MHz, $CDCl_3$) of terephthaloyl chloride (top), **M1** (middle) and **PolyM1** (bottom).



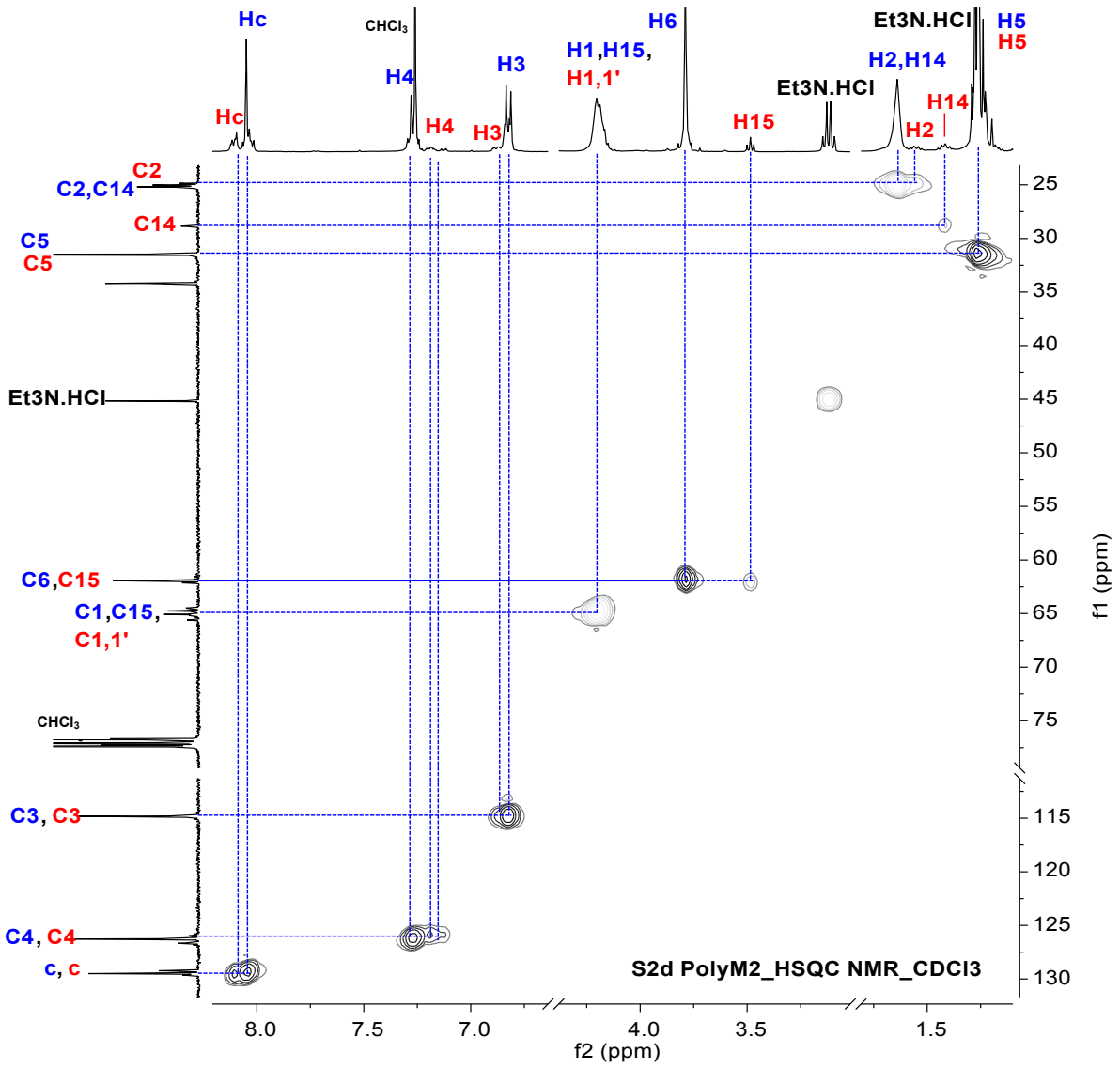
S14. ^{1}H NMR (400MHz, $CDCl_3$) spectrum of **PolyM2**.



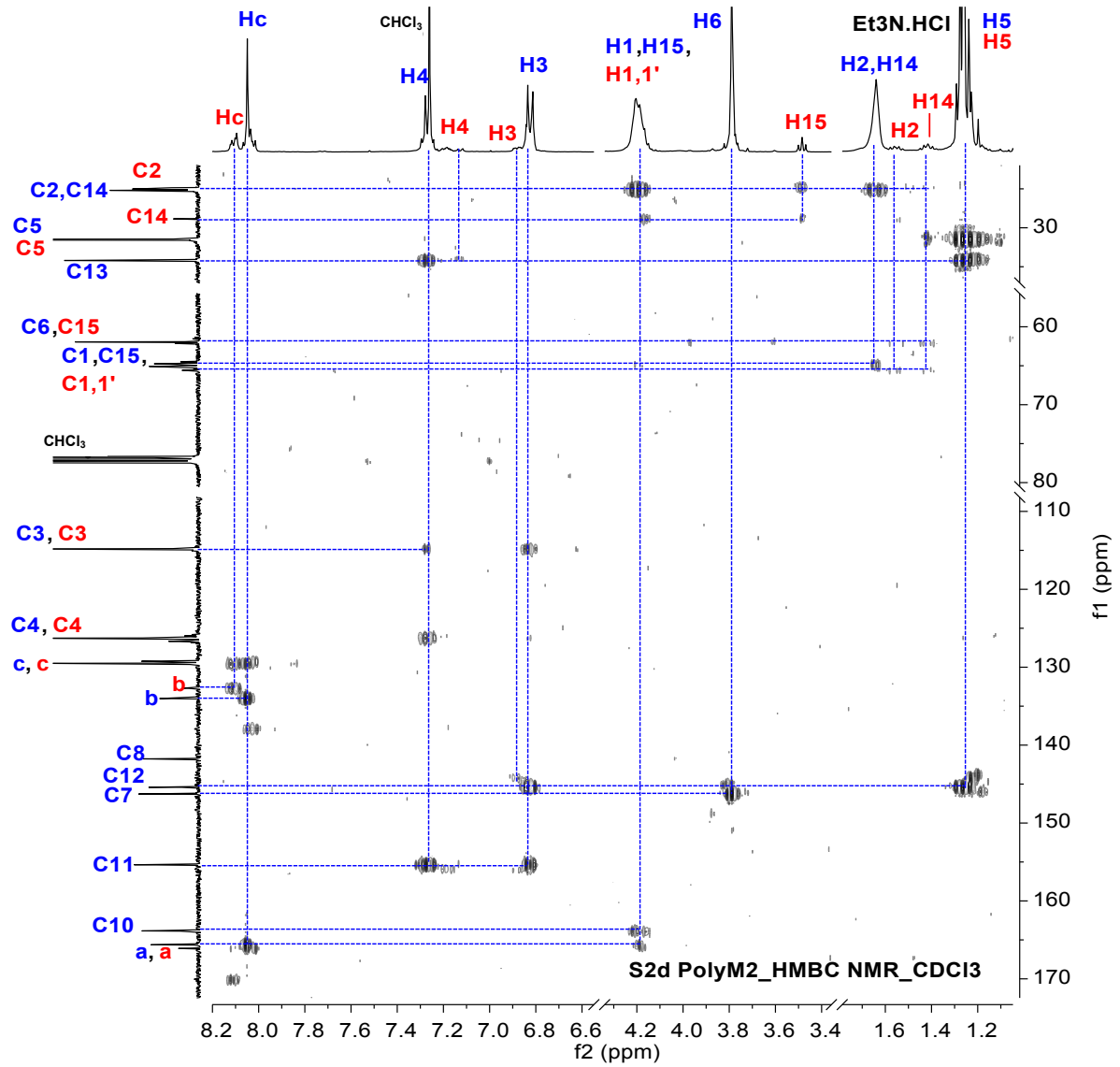
S15. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **PolyM2**.



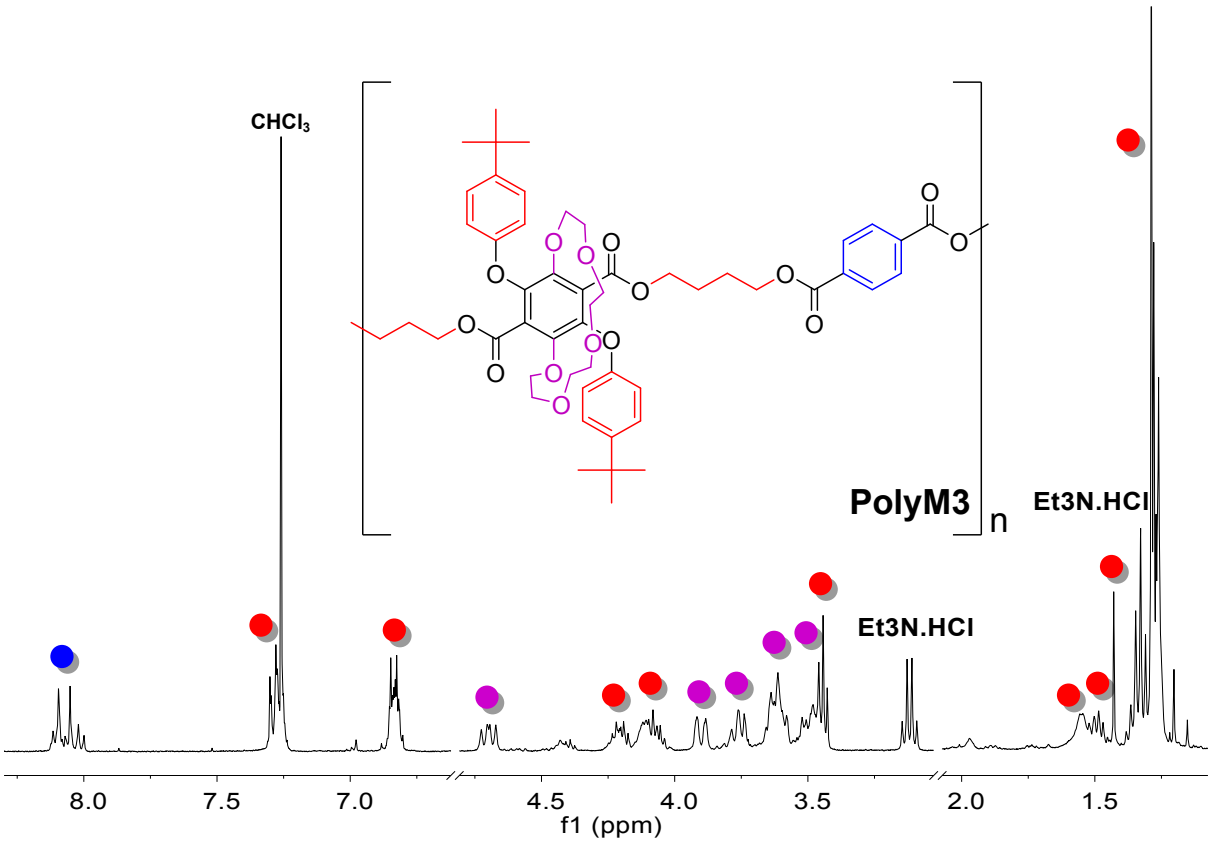
S16. COSY NMR spectrum of **PolyM2**.



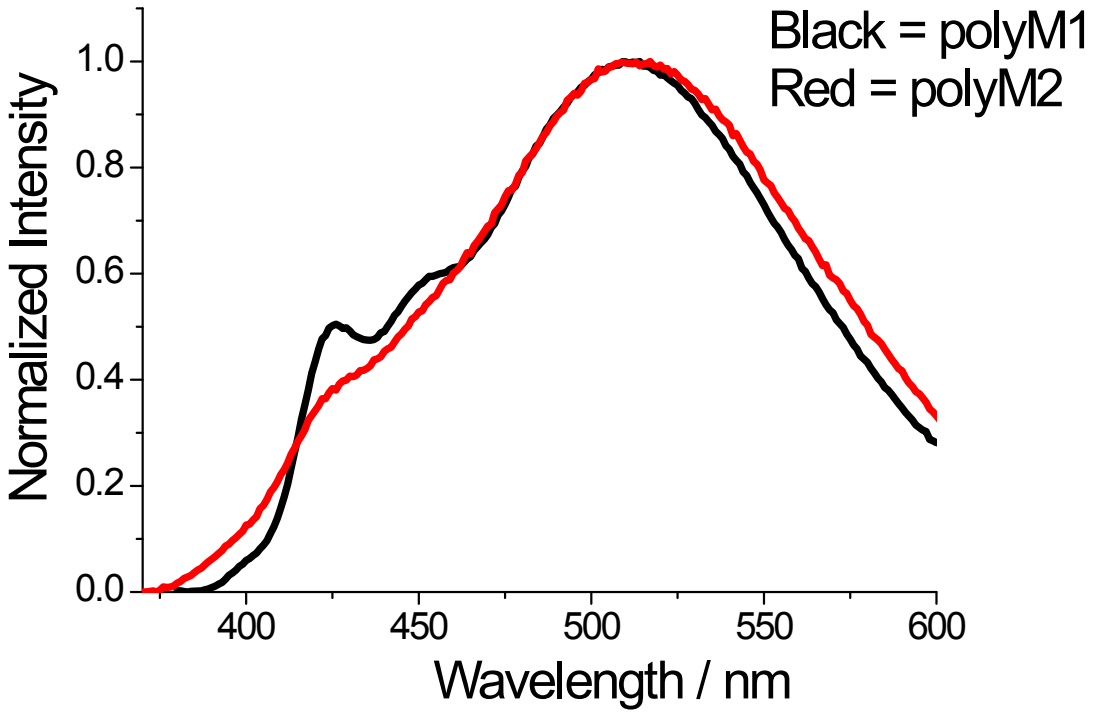
S17. HSQC NMR spectrum of **PolyM2**.



S18. HMBC NMR spectrum of **PolyM2**.

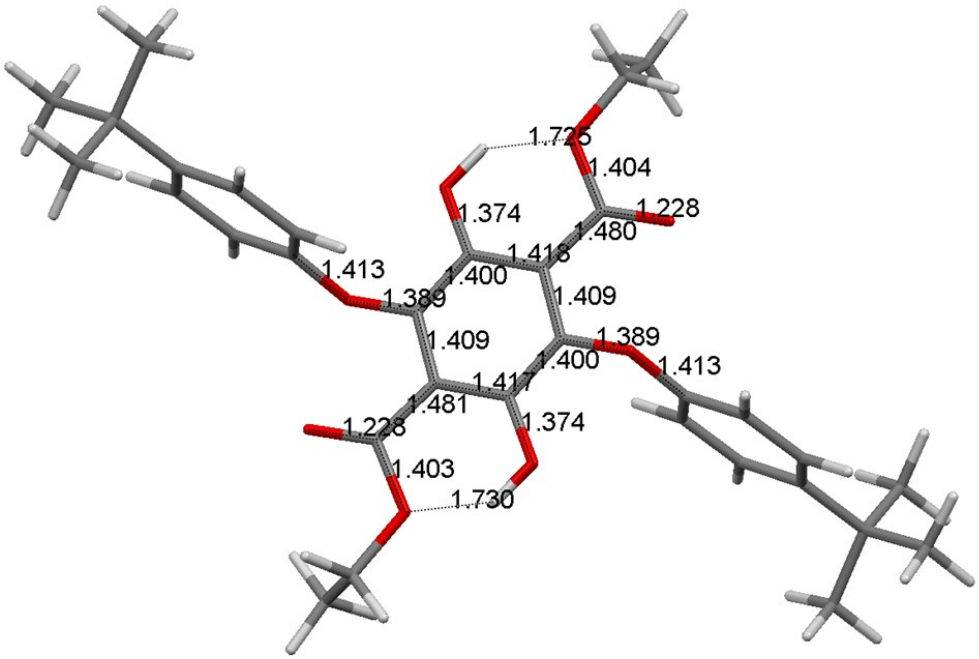


S19. *^{1}H NMR spectrum (400 MHz, $CDCl_3$) of* **PolyM3**.

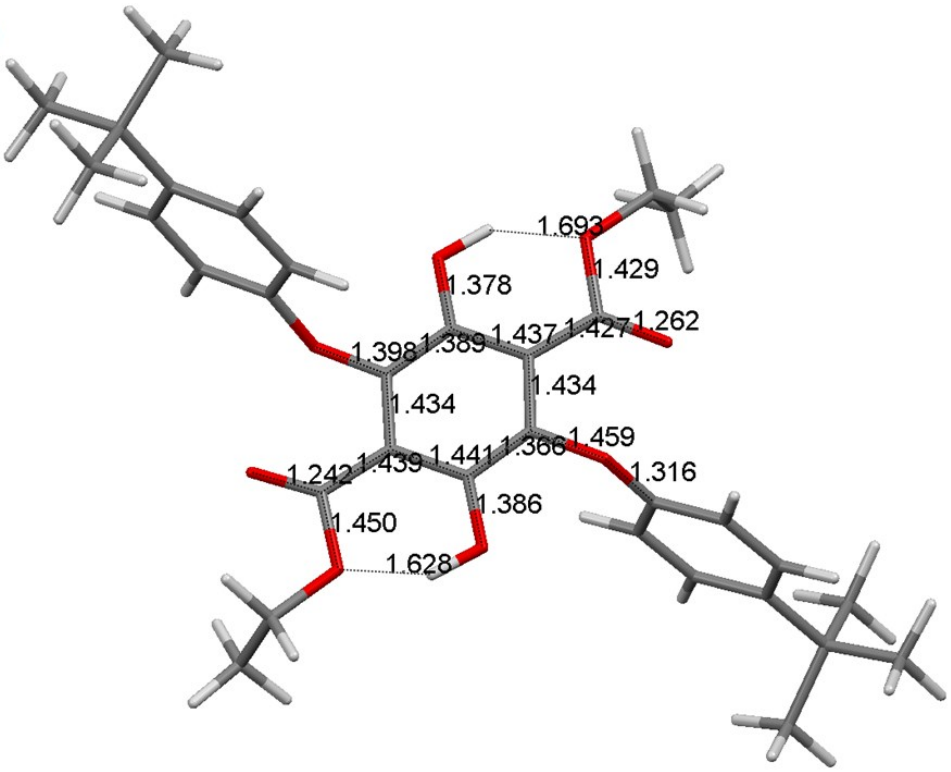


S20. Comparison of the emission spectra for **PolyM1** and **PolyM2** in DCM.

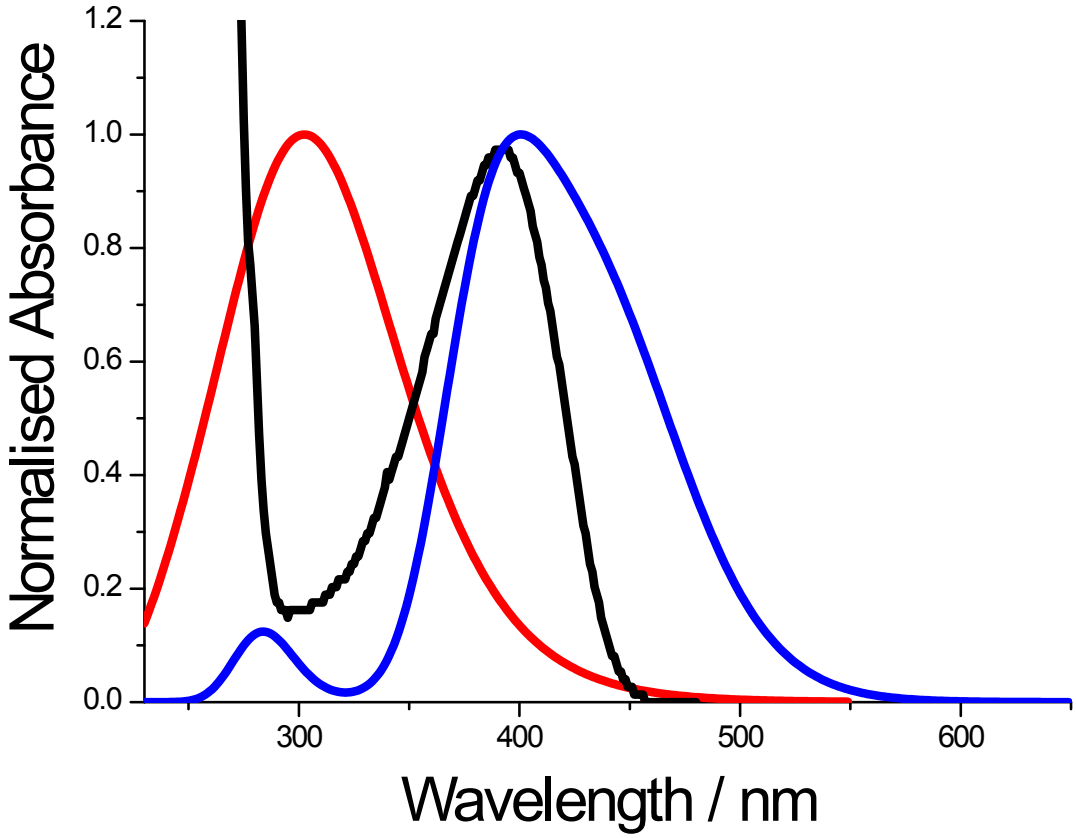
Ground State



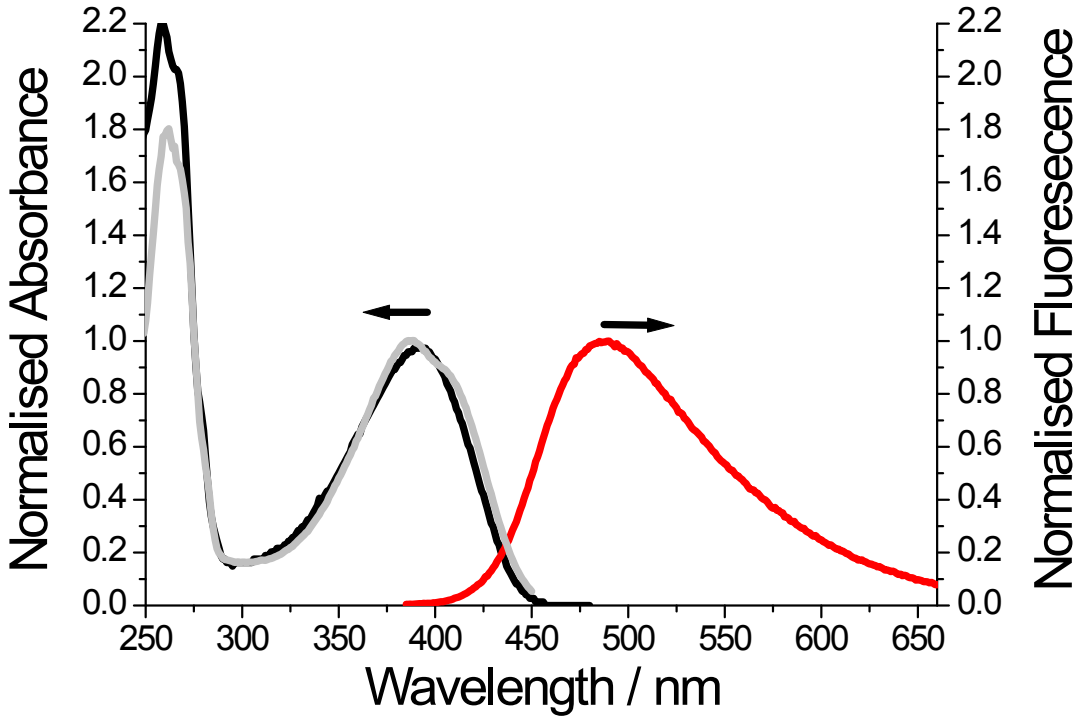
First Singlet State



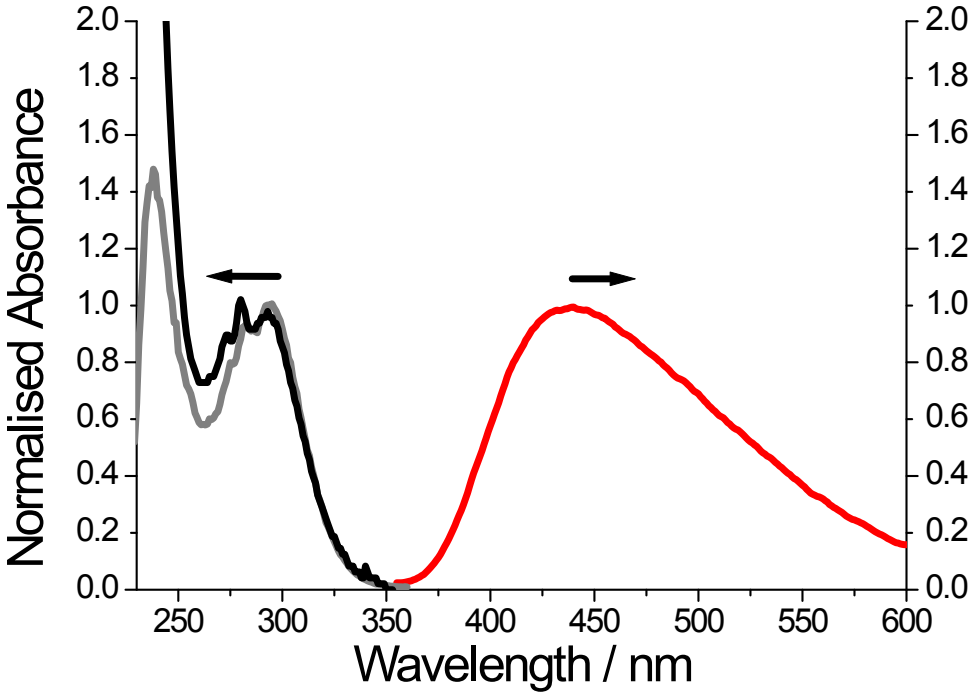
S21. Comparison of the calculated ground state and first-excited singlet state for **1** using Gaussian 09 (B3LYP, 6-311G).



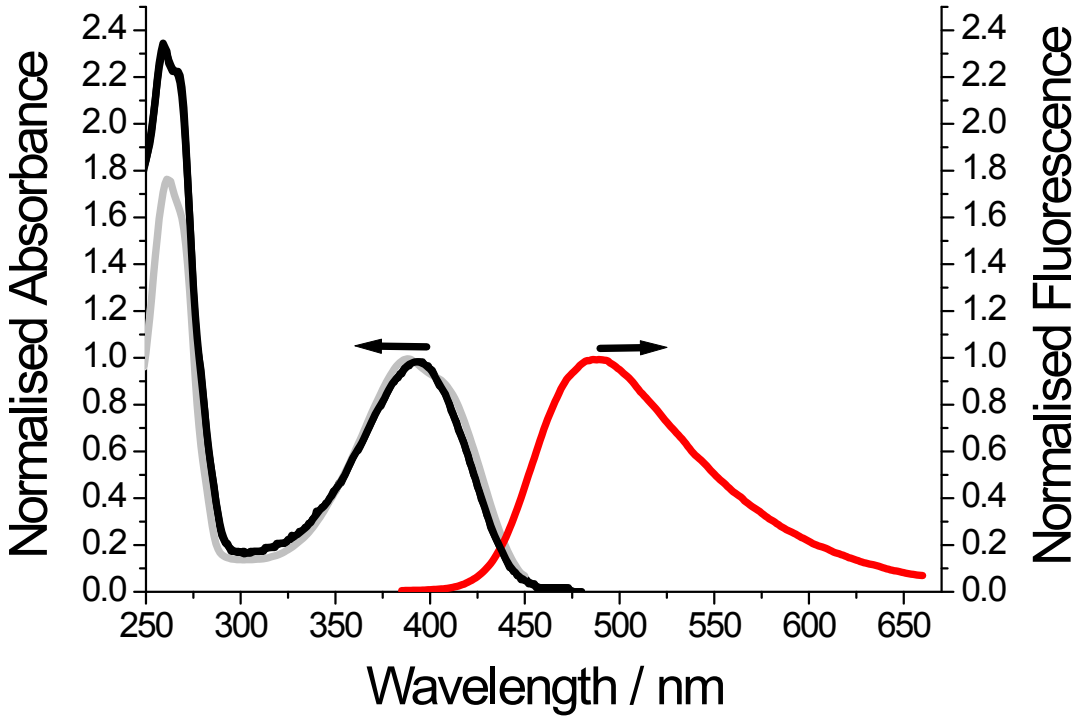
S22. Comparison of TD-DFT calculated absorption spectra for ground-state structure of **1** where the ester groups are twisted out of plane (red), planar (blue) and the actual absorption spectrum (black) in DCM.



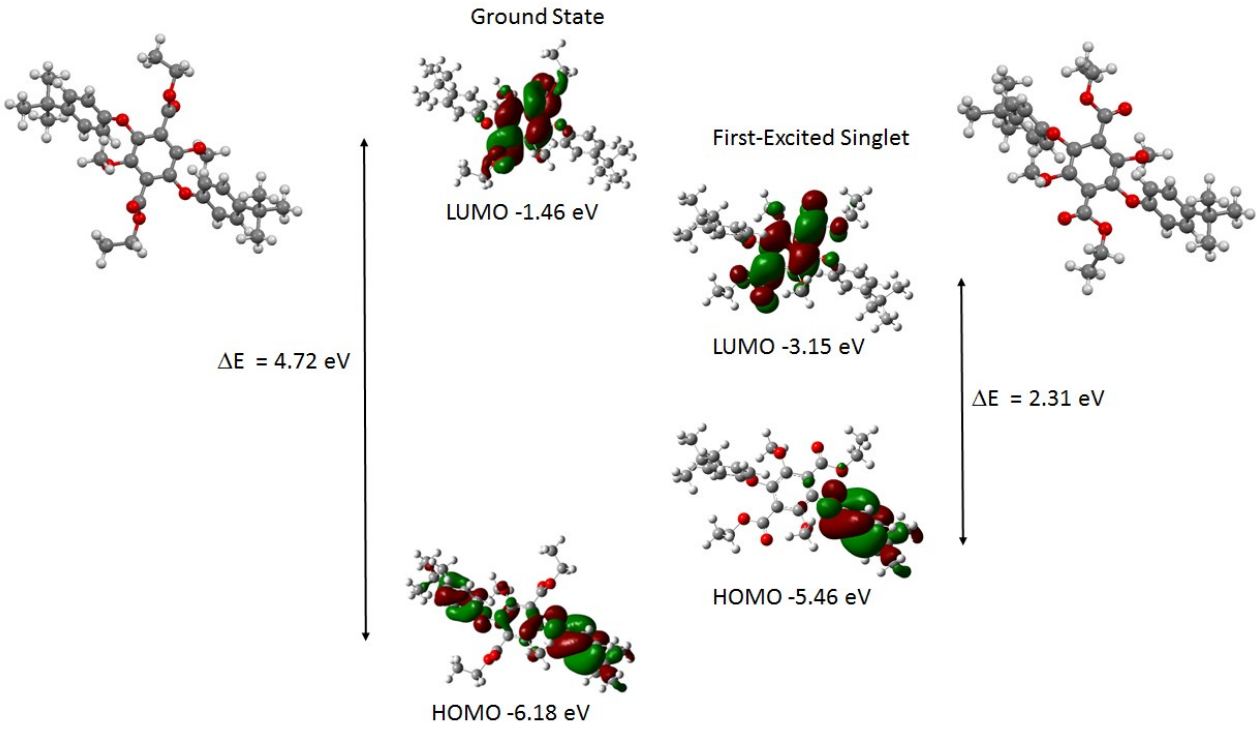
S23. Absorption (black), excitation (grey) and fluorescence (red) spectra of **1** in dilute DCM.



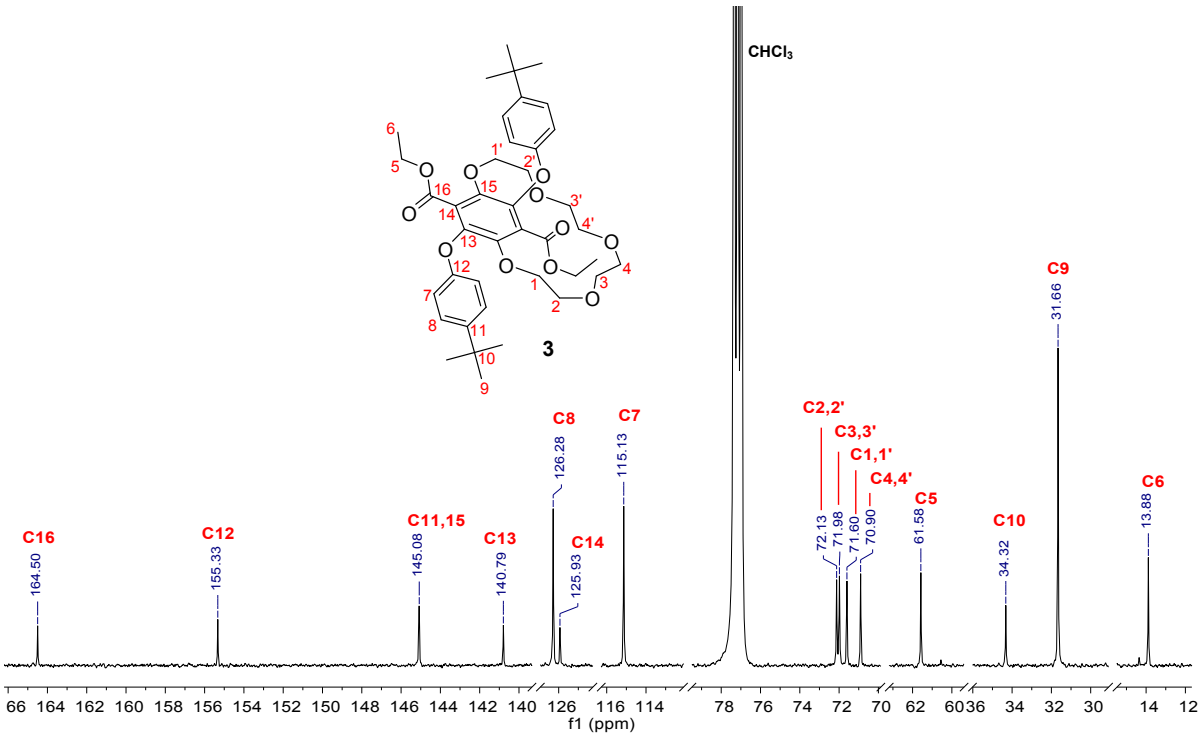
S24. Absorption (black), excitation (grey) and fluorescence (red) spectra of **3** in dilute DCM.



S25. Absorption (black), excitation (grey) and fluorescence (red) spectra of **M1** in dilute DCM.

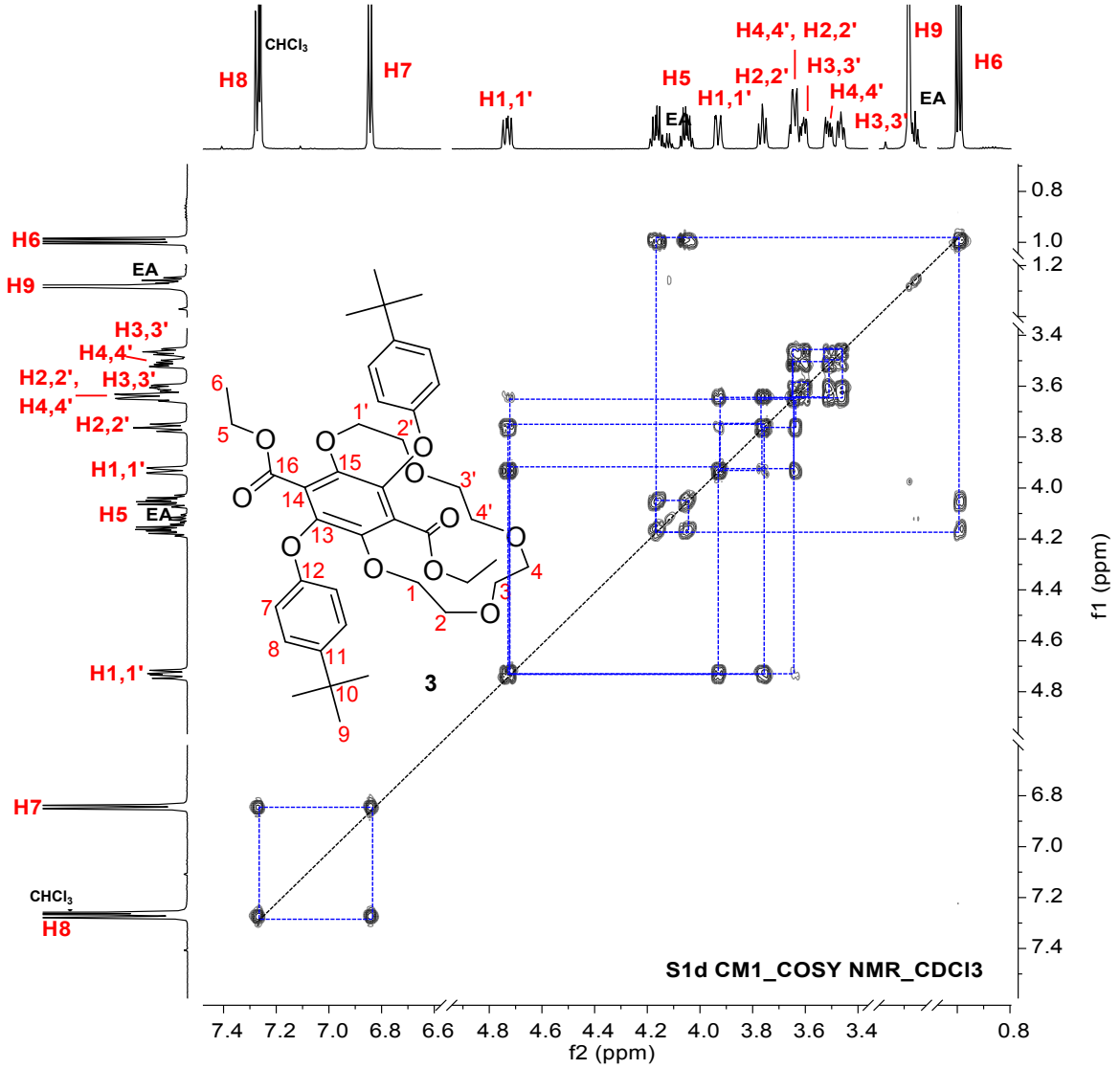


S26. Calculated ground and first-excited state structures for **2** and their corresponding HOMO/LUMO locations. The energy gaps are also shown to help emphasise the effect of alteration in the structure.

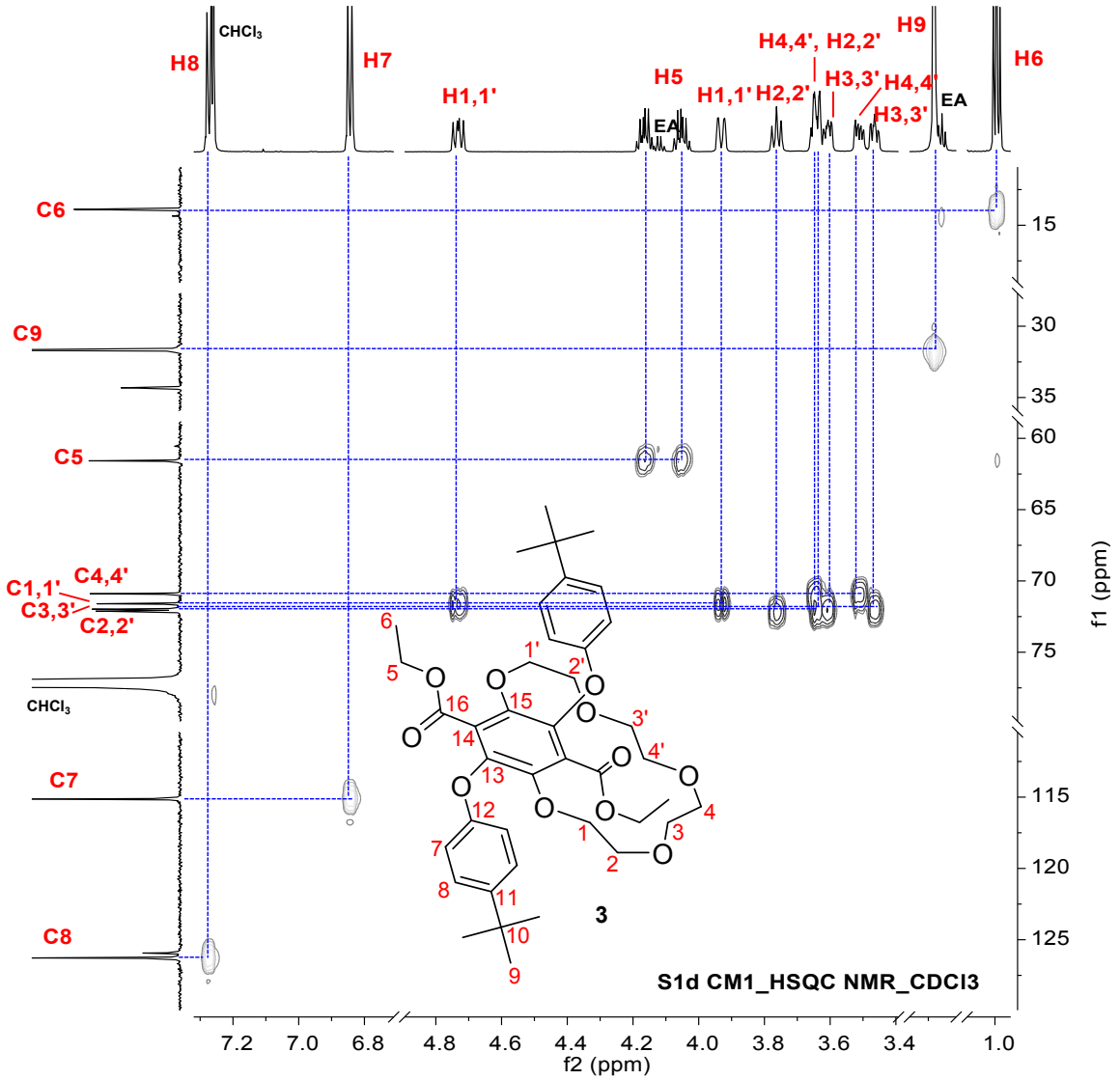


^{13}C NMR (176 MHz, $CDCl_3$) δ164.50 (C16), 155.33 (C12), 145.08 (C11,C15), 140.79 (C13), 126.28 (C8), 125.93 (C14), 115.13 (C7), 72.13 (C2,C2'), 71.98 (C3,C3'), 71.60 (C1,C1'), 70.90 (C4,C4'), 61.58 (C5), 34.32 (C10), 31.66 (C9), 13.88 (C6).

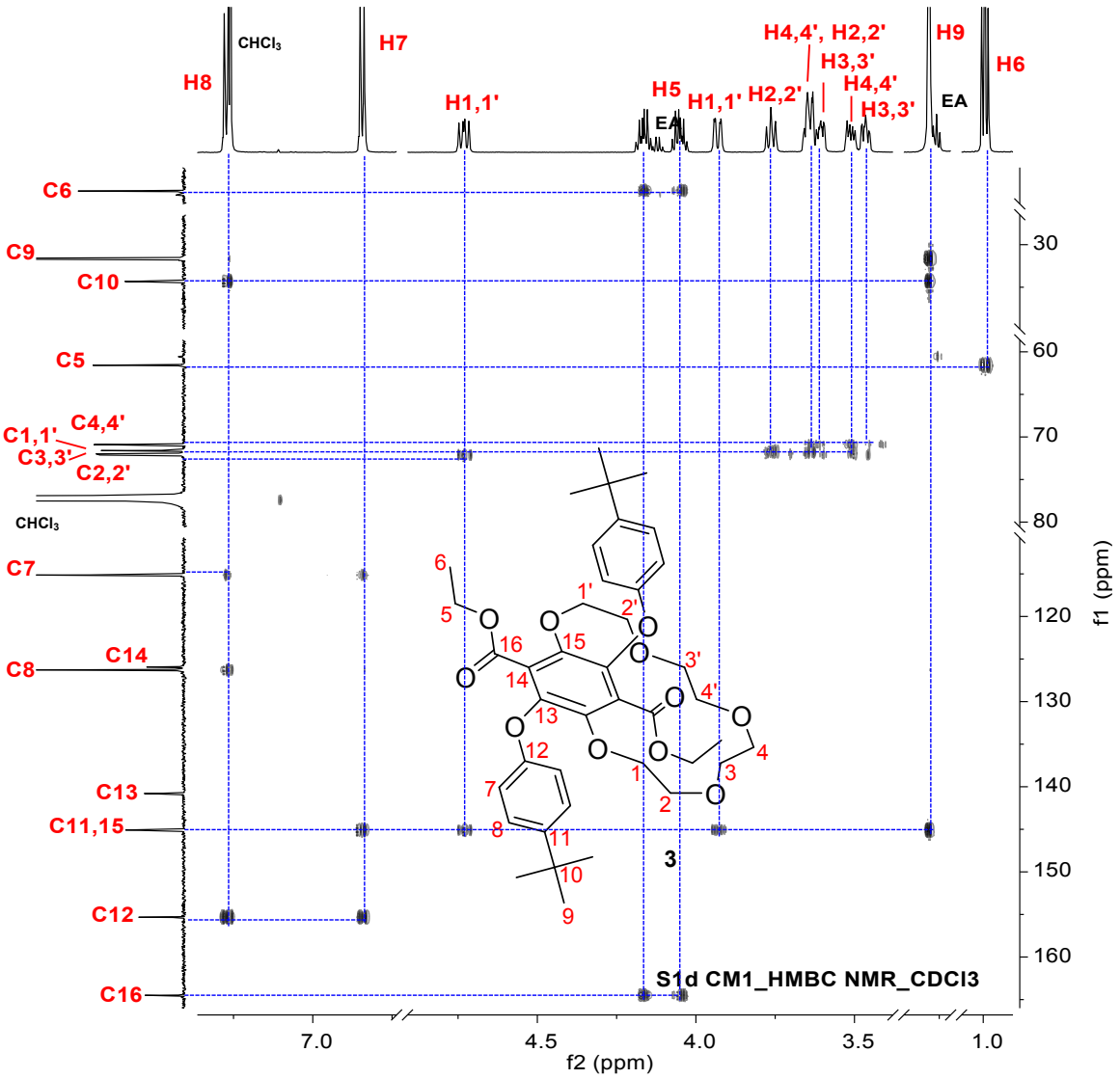
S27. ^{13}C NMR (176 MHz, $CDCl_3$) spectrum of the 1+1 crown ether derivative **3.**



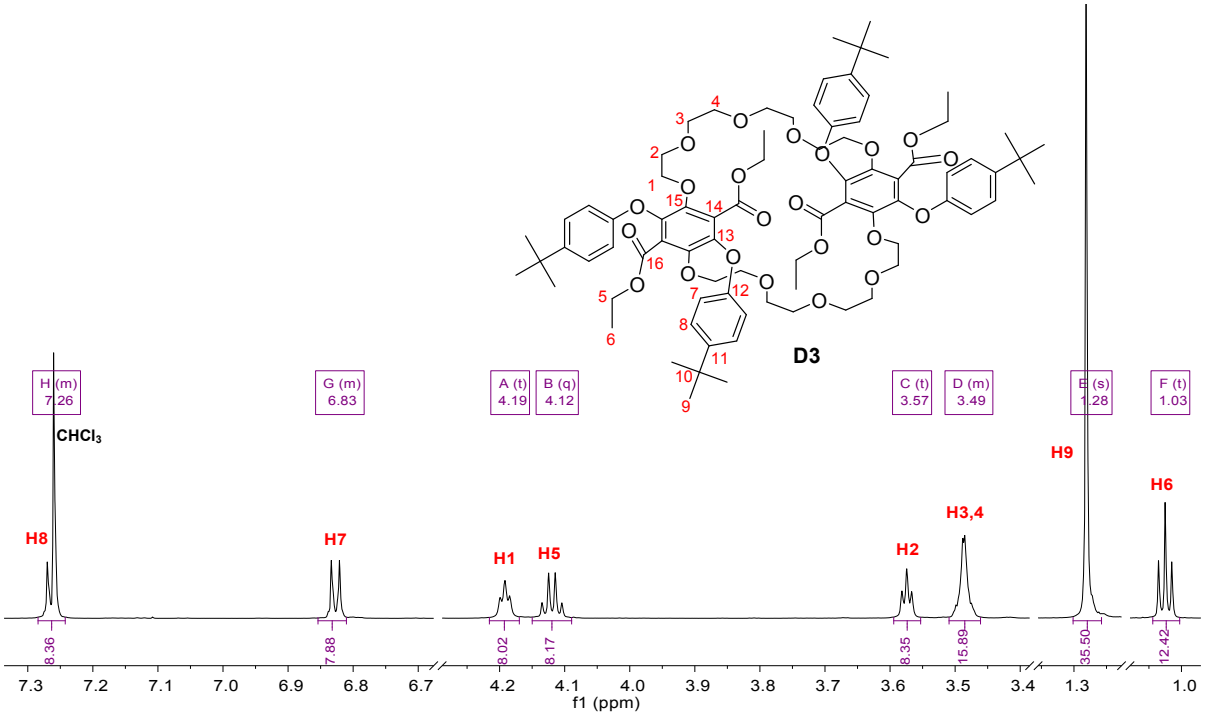
S28. COSY NMR spectrum of the 1+1 crown ether derivative **3.**



S29. HSQC NMR spectrum of the 1+1 crown ether derivative **3.**

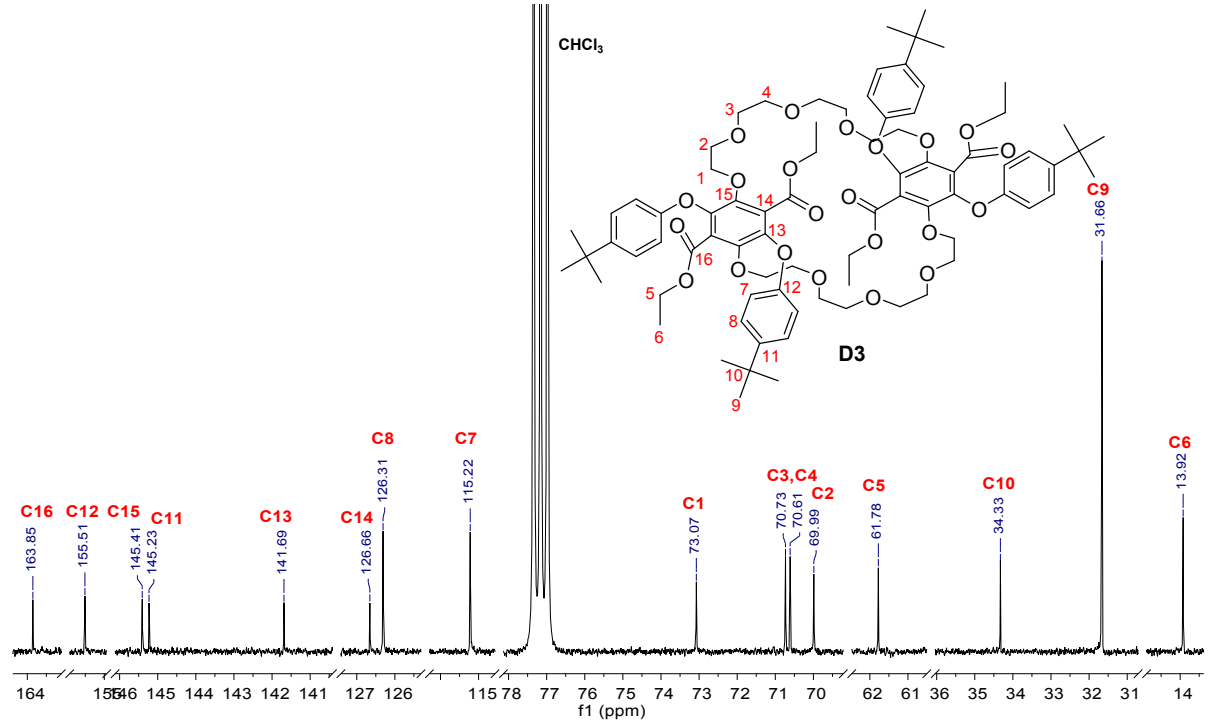


S30. HMBC NMR spectrum of the 1+1 crown ether derivative **3.**



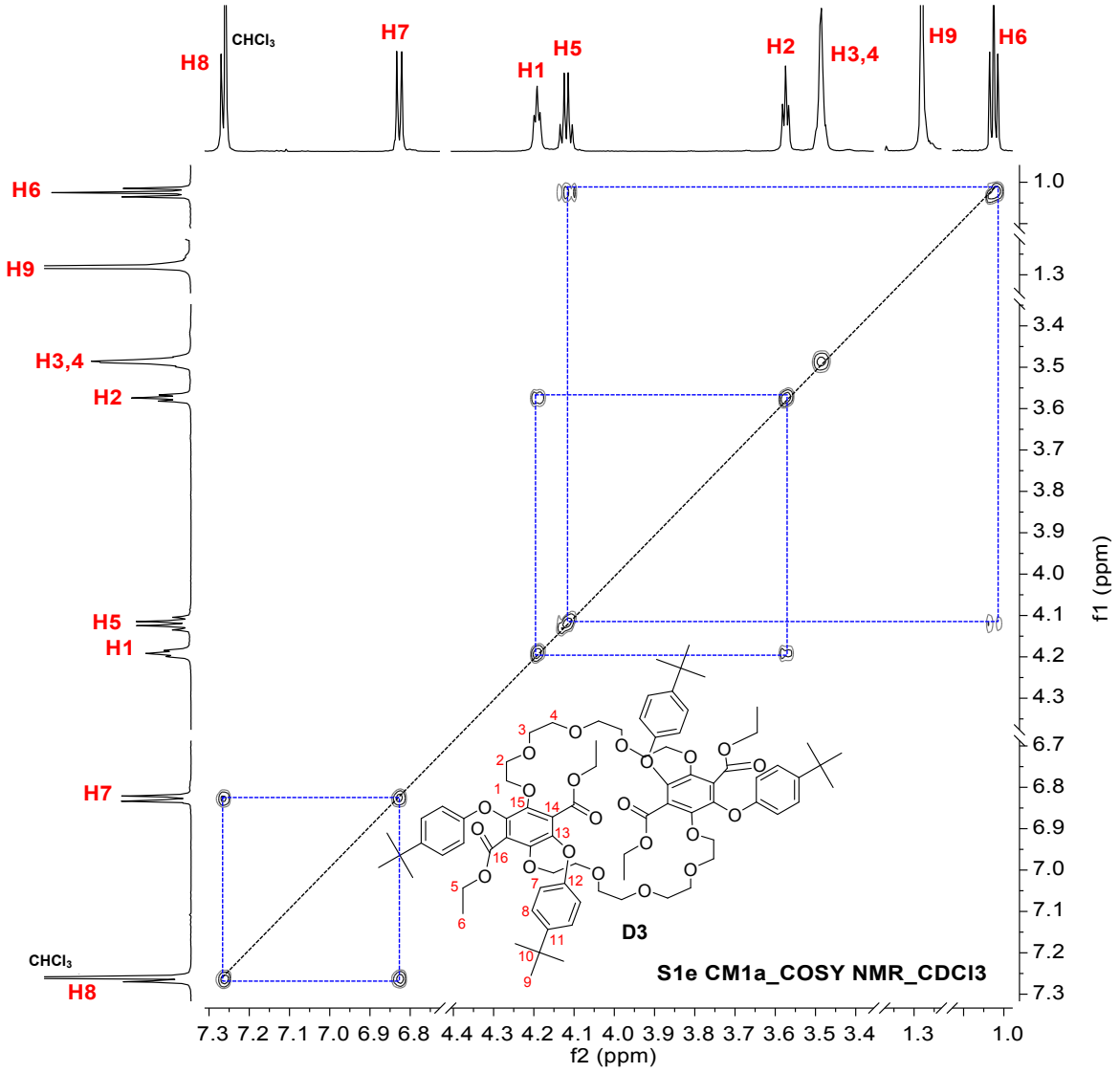
^{1}H NMR (700 MHz, Chloroform - *d*) δ7.28 – 7.24 (m, 8H, H8), 6.85 – 6.81 (m, 8H, H7), 4.19 (t, *J*= 5.4 Hz, 8H, H1), 4.12 (q, *J*= 7.1 Hz, 8H, H5), 3.57 (t, *J*= 5.3 Hz, 8H, H2), 3.51 – 3.46 (m, 16H, H3, H4), 1.28 (s, 36H, H9), 1.03 (t, *J*= 7.1 Hz, 12H, H6).

S31. ^{1}H NMR (700MHz, $CDCl_3$) spectrum of the 2+2 crown ether derivative **D3**.

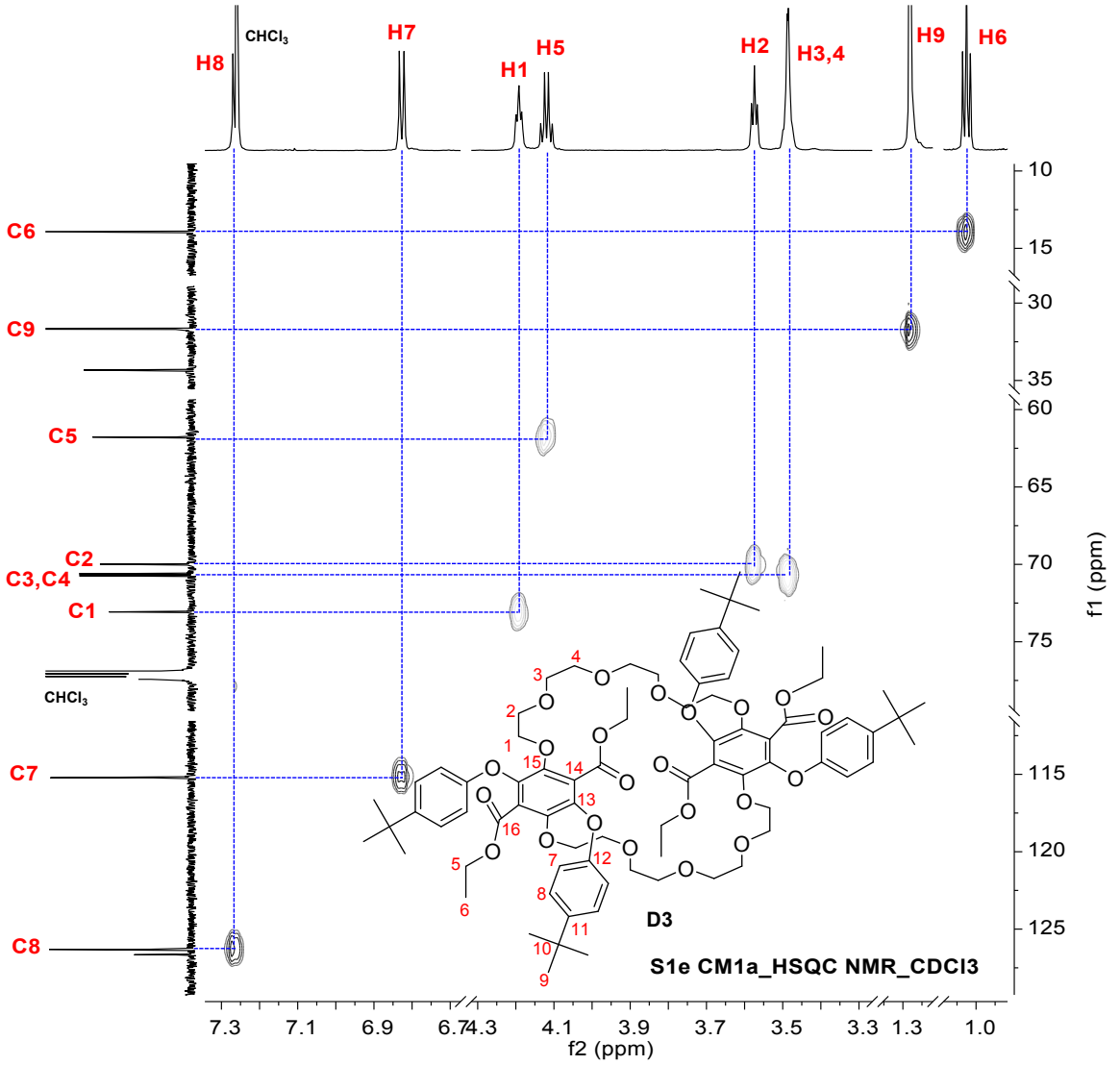


^{13}C NMR (176 MHz, $CDCl_3$) δ163.85 (C16), 155.51 (C12), 145.41 (C15), 145.23 (C11), 141.69 (C13), 126.66 (C14), 126.31 (C8), 115.22 (C7), 73.07 (C1), 70.73, 70.61 (C3,C4), 69.99 (C2), 61.78 (C5), 34.33 (C10), 31.66 (C9), 13.92 (C6).

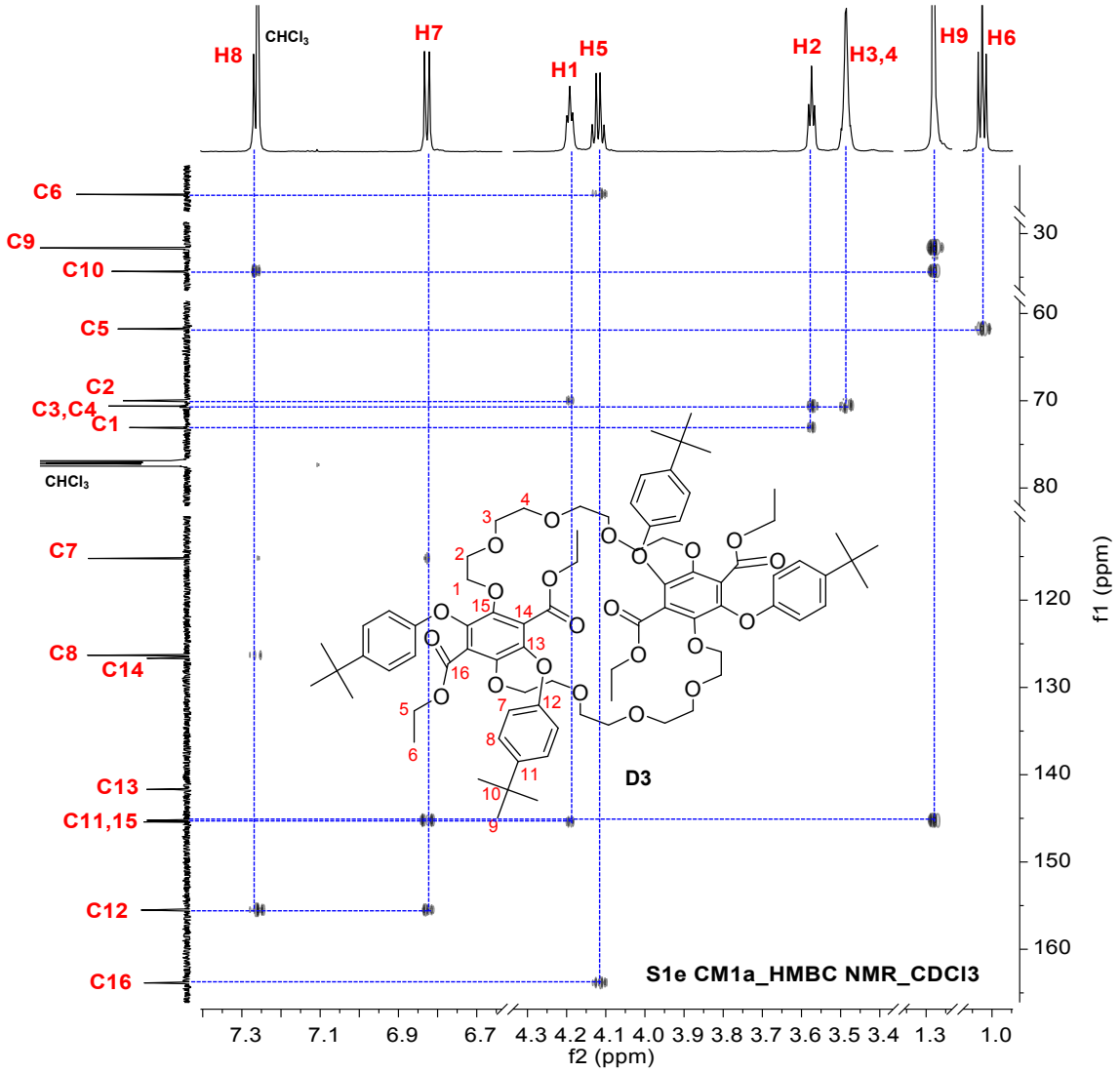
S32. ^{13}C NMR (176 MHz, $CDCl_3$) spectrum of the 2+2 crown ether derivative **D3**.



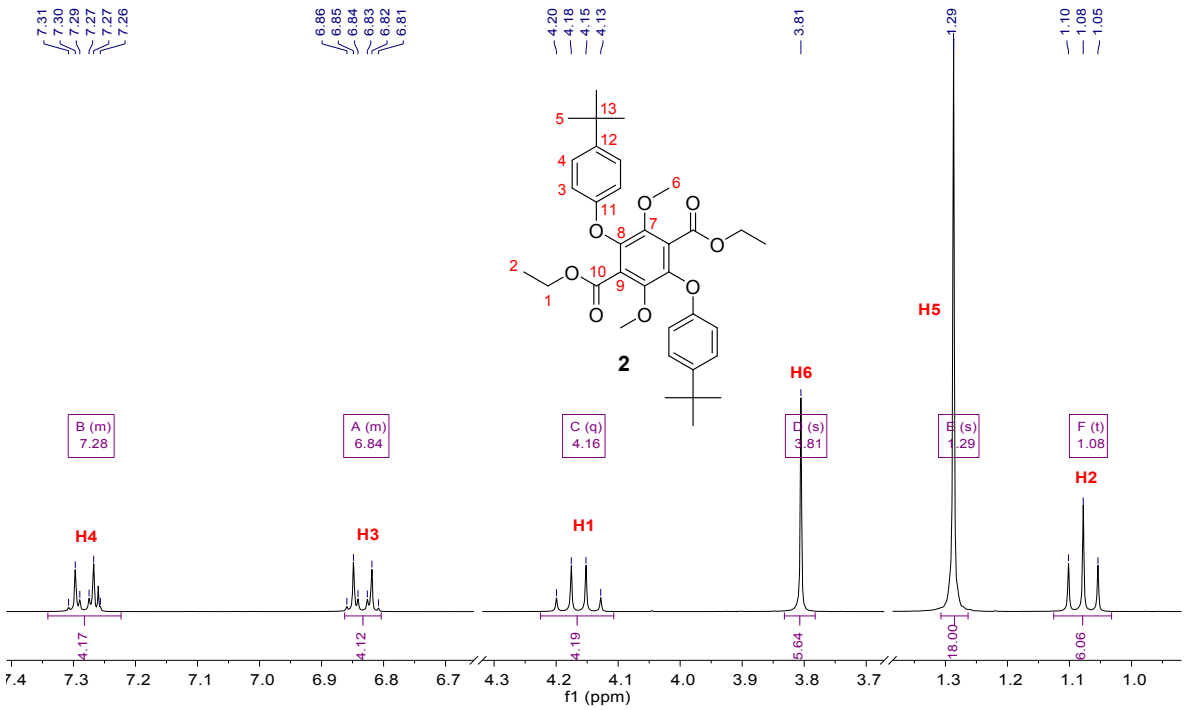
S33. COSY NMR spectrum of the 2+2 crown ether derivative **D3**.



S34. HSQC NMR spectrum of the 2+2 crown ether derivative **D3**.

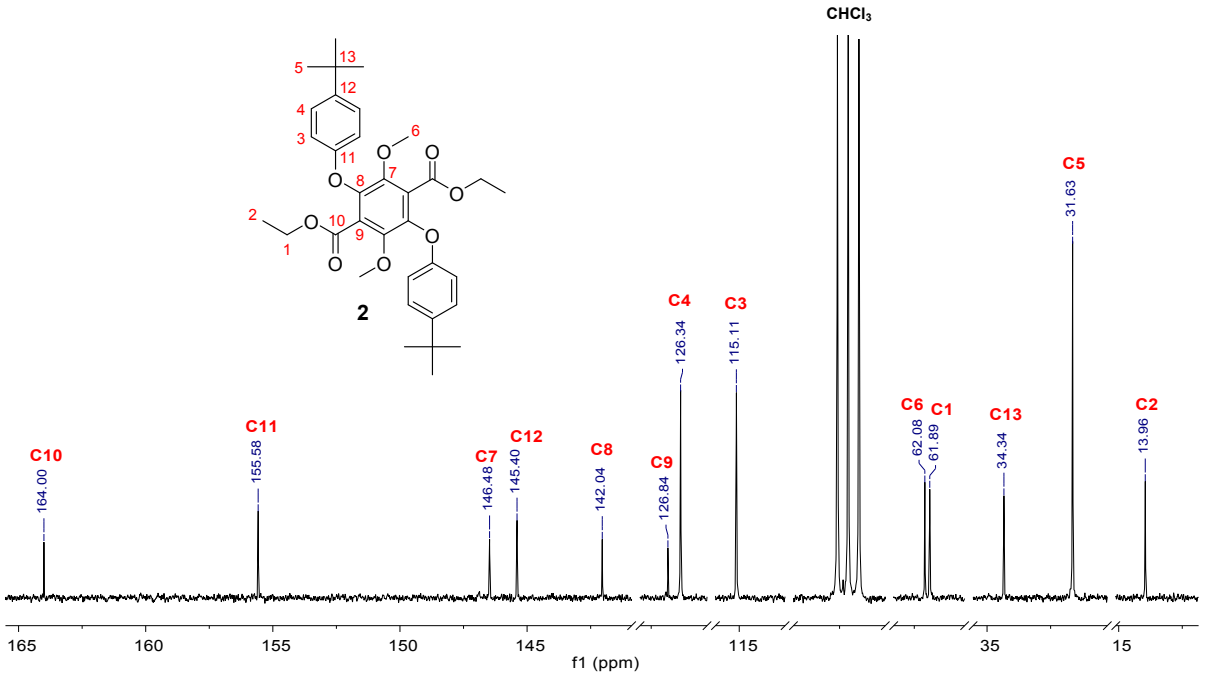


S35. HMBC NMR spectrum of the 2+2 crown ether derivative **D3**.



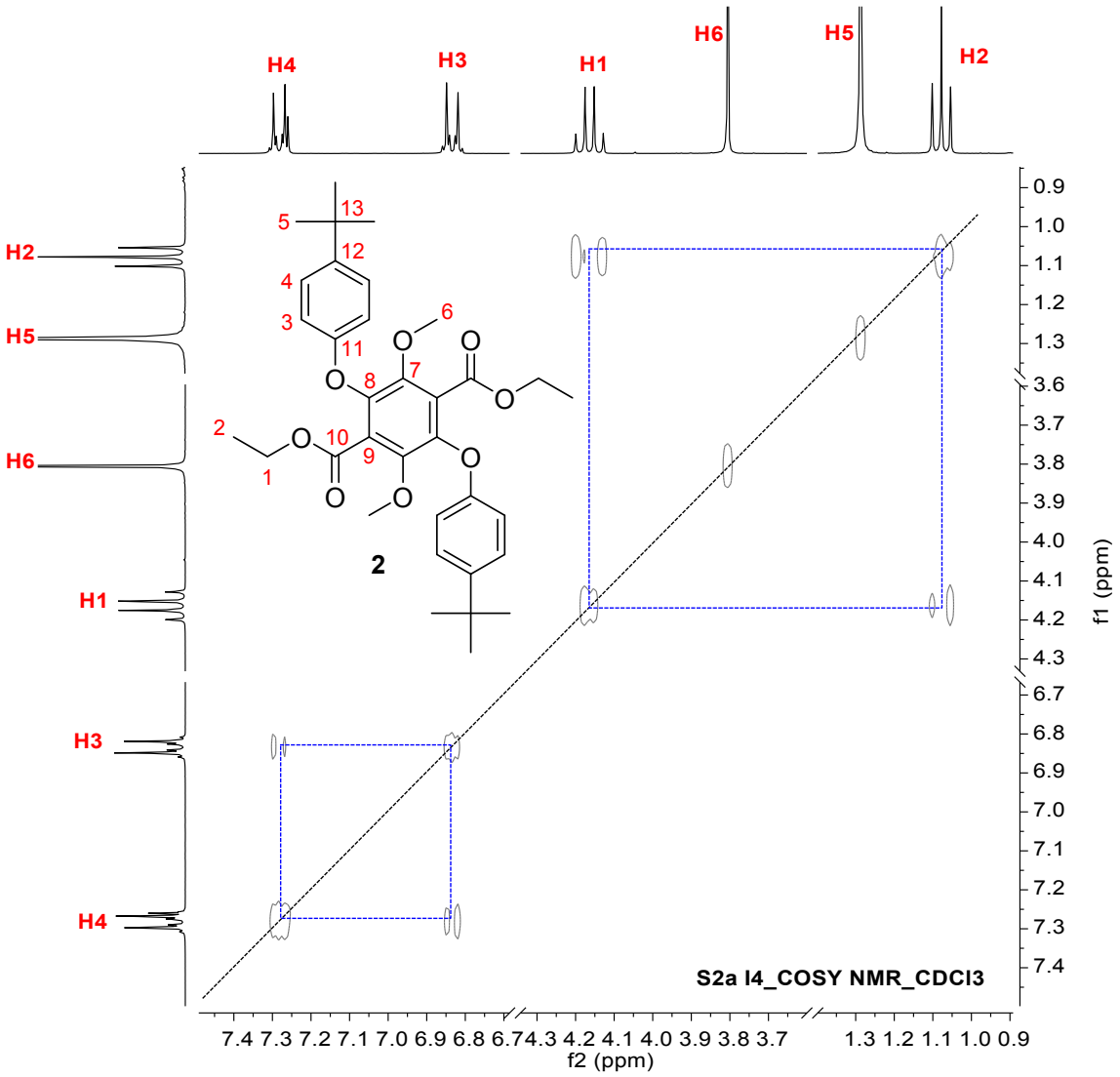
^{1}H NMR (300 MHz, Chloroform - *d*) δ7.34 – 7.22 (m, 4H, H4), 6.86 – 6.80 (m, 4H, H3), 4.16 (q, *J*= 7.1 Hz, 4H, H1), 3.81 (s, 6H, H6), 1.29 (s, 18H, H5), 1.08 (t, *J*= 7.1 Hz, 6H, H2).

S36. ^{1}H NMR (300MHz, $CDCl_3$) spectrum of **2**.

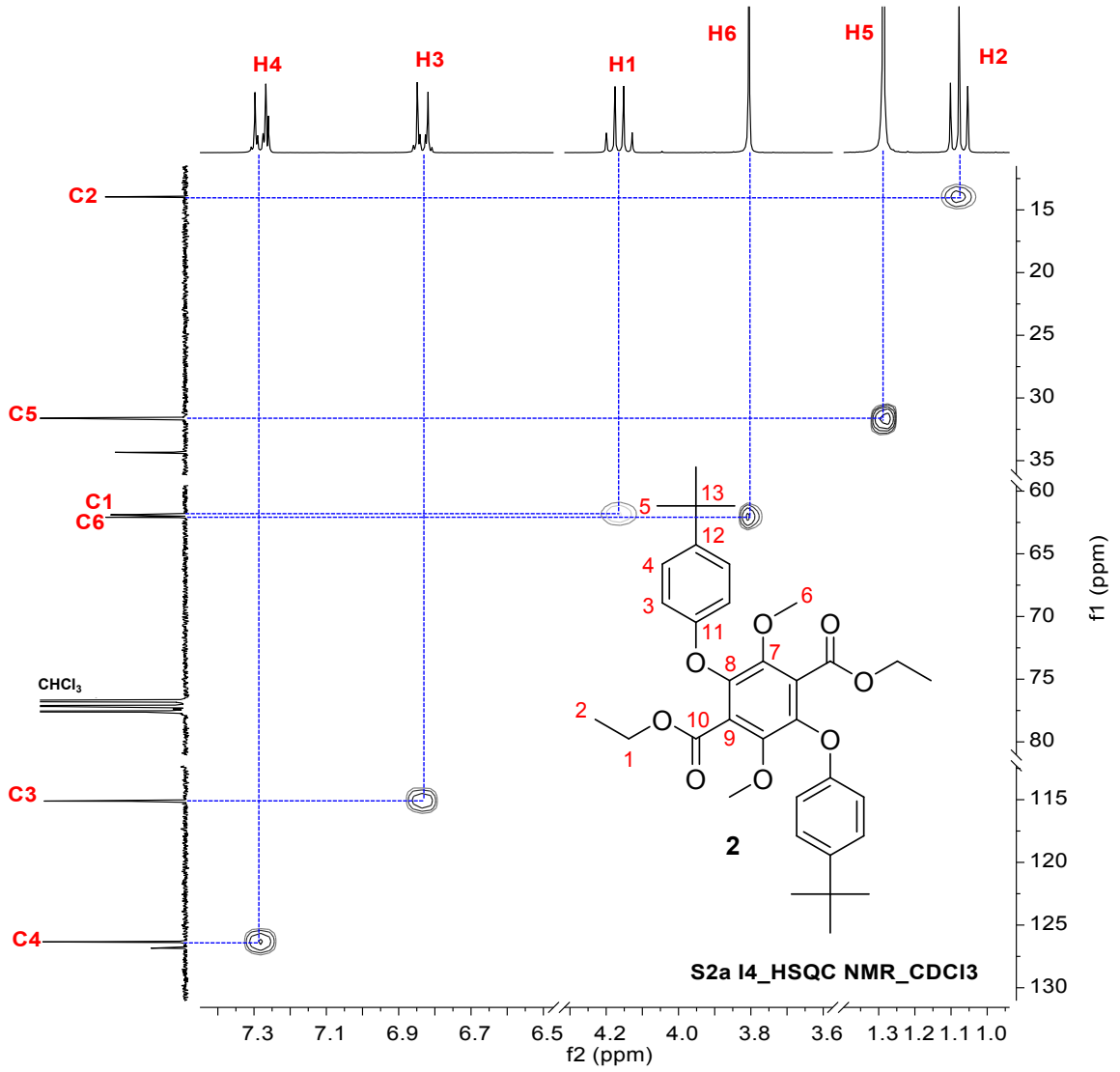


^{13}C NMR (75 MHz, $CDCl_3$) δ164.00 (C10), 155.58 (C11), 146.48 (C7), 145.40 (C12), 142.04 (C8), 126.84 (C9), 126.34 (C4), 115.11 (C3), 62.08 (C6), 61.89 (C1), 34.34 (C13), 31.63 (C5), 13.96 (C2).

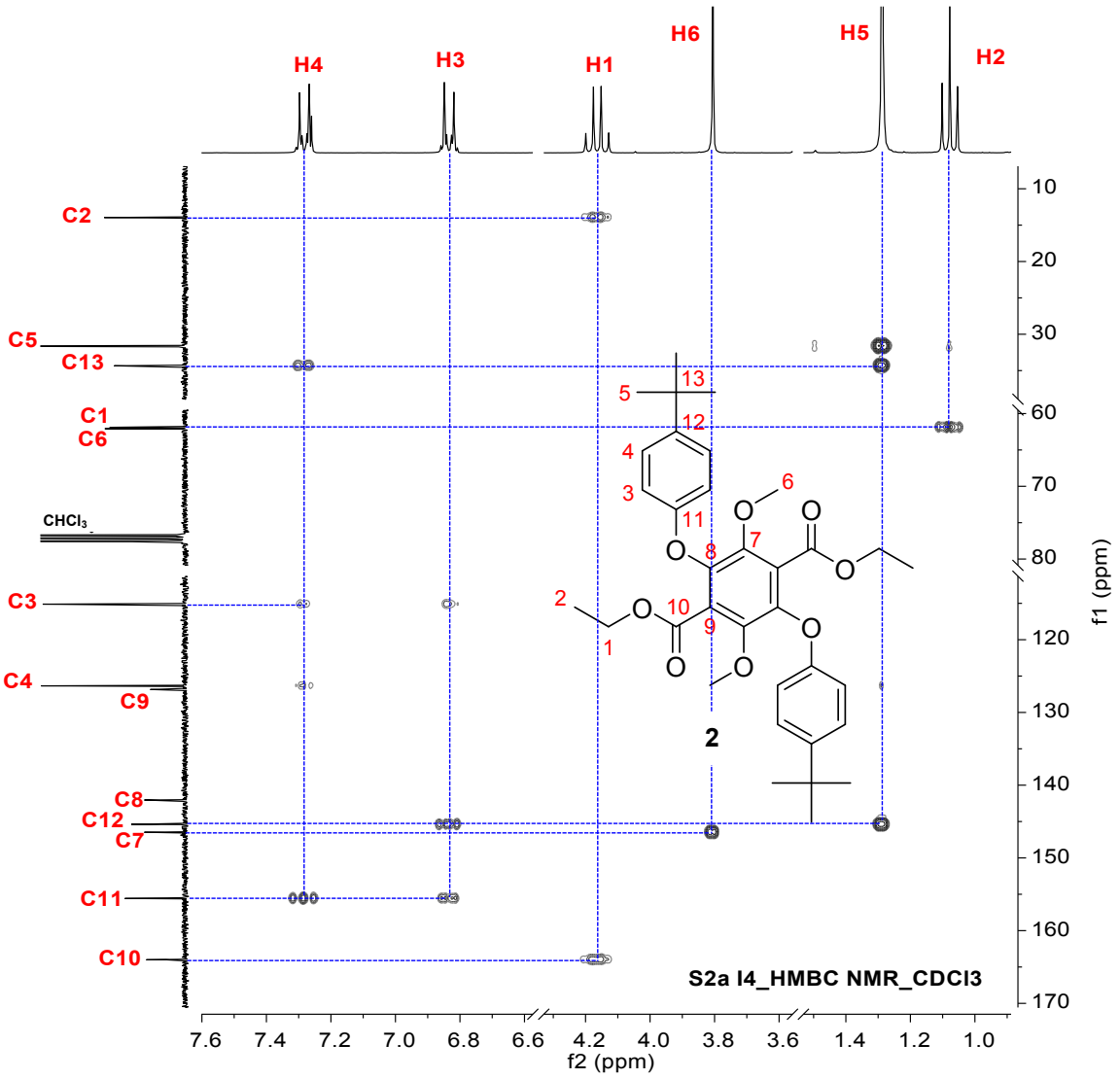
S37. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **2**.



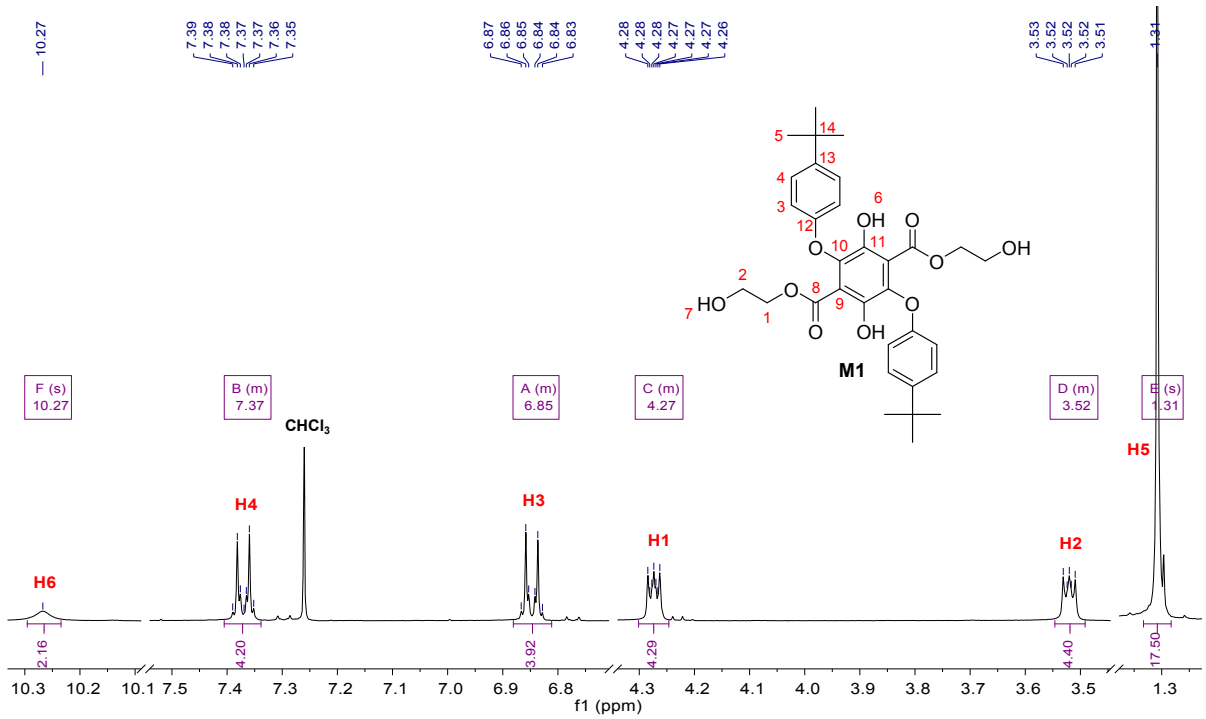
S38. COSY NMR spectrum of **2**.



S39. HSQC NMR spectrum of **2**.

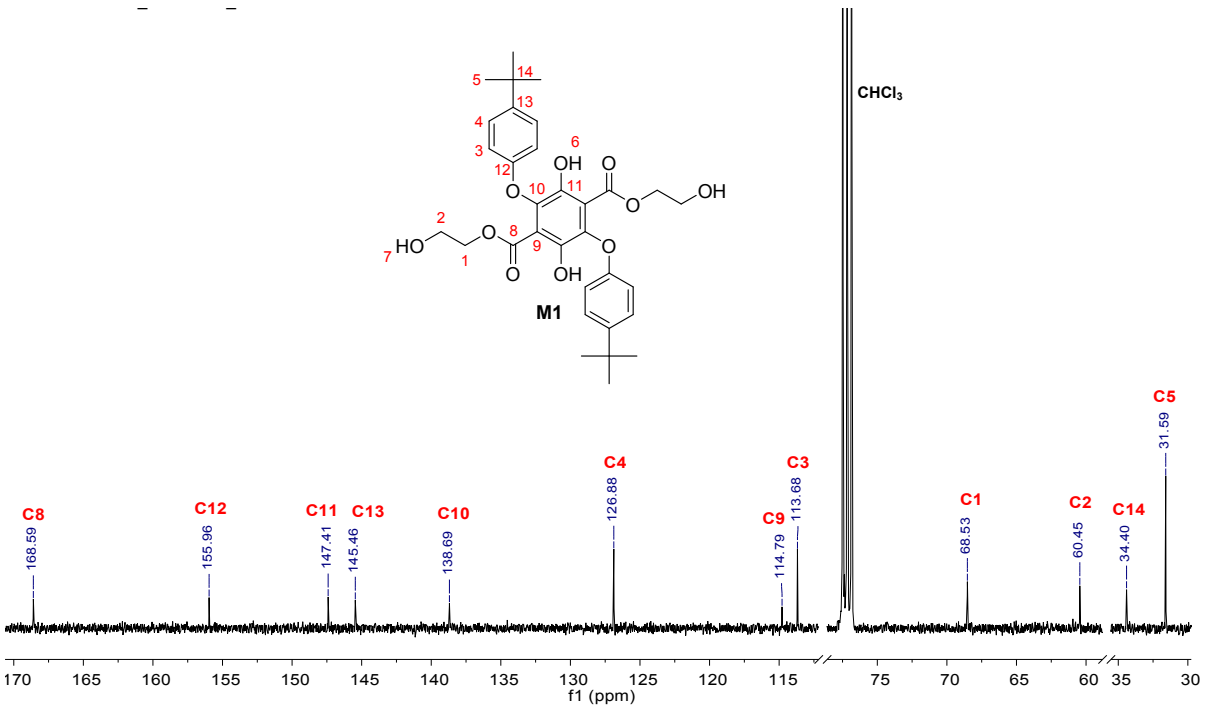


S40. HMBC NMR spectrum of **2**.



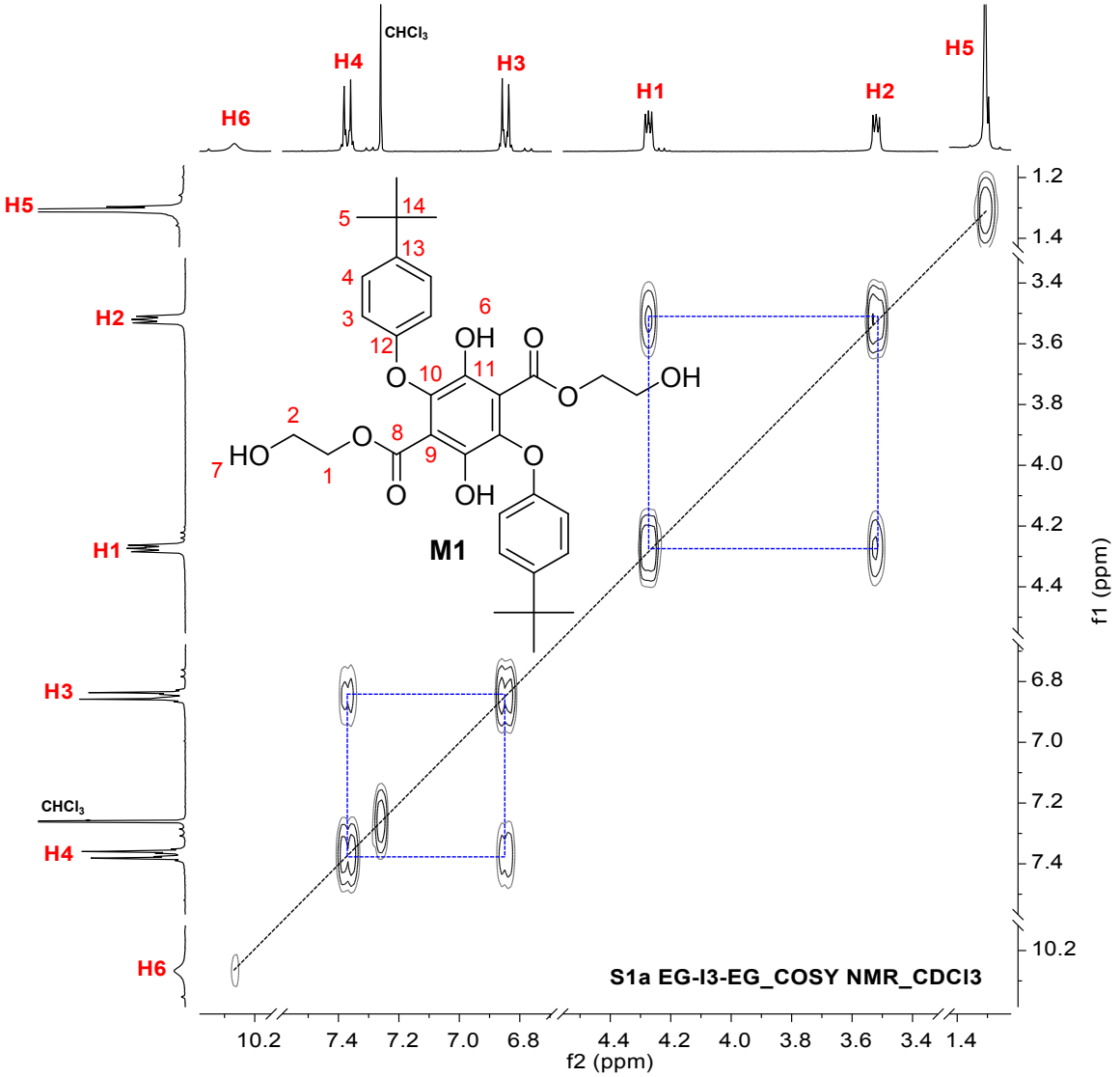
^{1}H NMR (400 MHz, Chloroform - *d*) δ10.27 (s, 2H, H6), 7.41 – 7.34 (m, 4H, H4), 6.88 – 6.81 (m, 4H, H3), 4.30 – 4.25 (m, 4H, H1), 3.55 – 3.49 (m, 4H, H2), 1.31 (s, 18H, H5).

S41. ^{1}H NMR (400MHz, $CDCl_3$) spectrum of monomer diol **M1**.

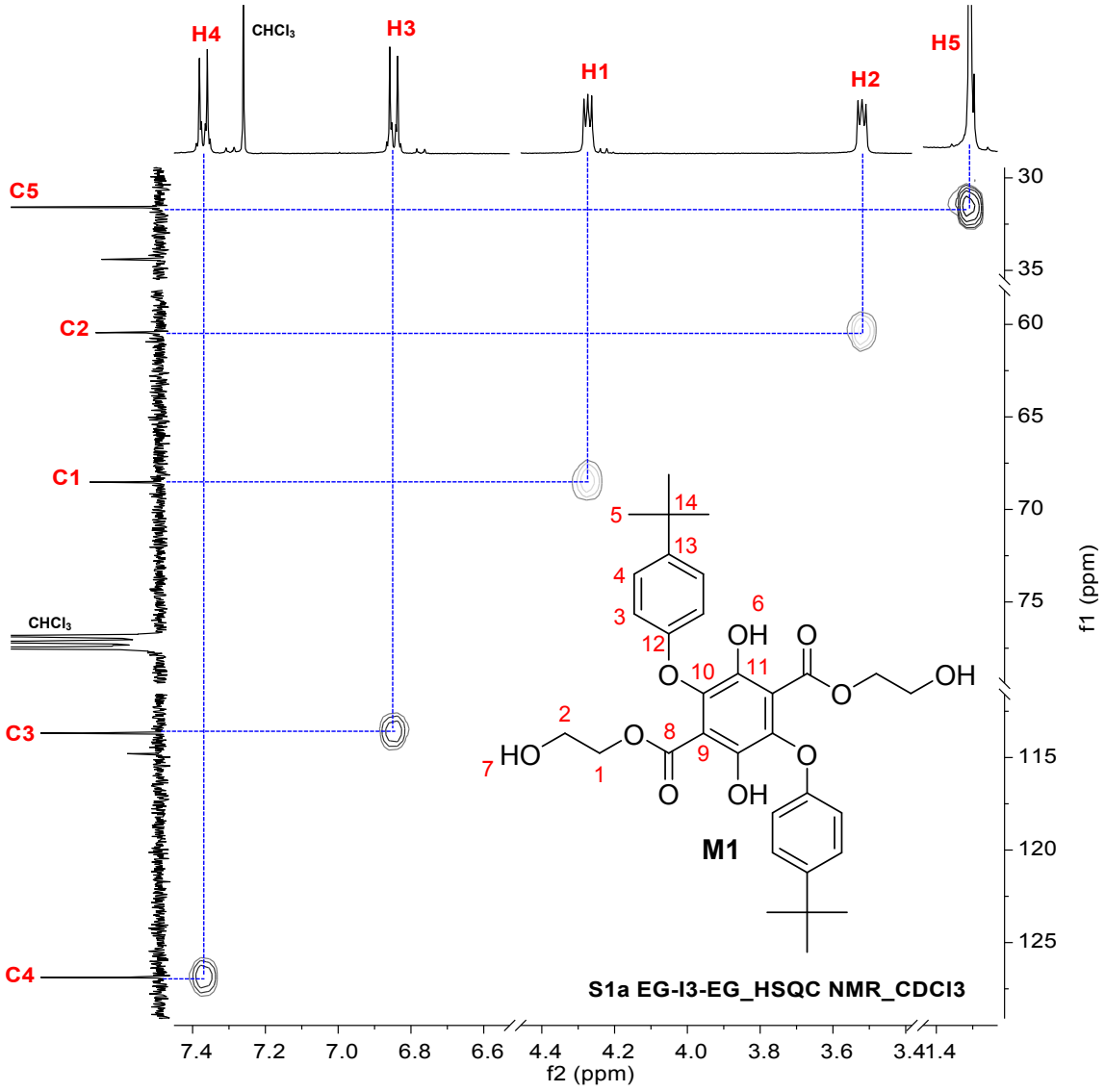


^{13}C NMR (101 MHz, $CDCl_3$) δ168.59 (C8), 155.96 (C12), 147.41 (C11), 145.46 (C13), 138.69 (C10), 126.88 (C4), 114.79 (C9), 113.68 (C3), 68.53 (C1), 60.45 (C2), 34.40 (C14), 31.59 (C5).

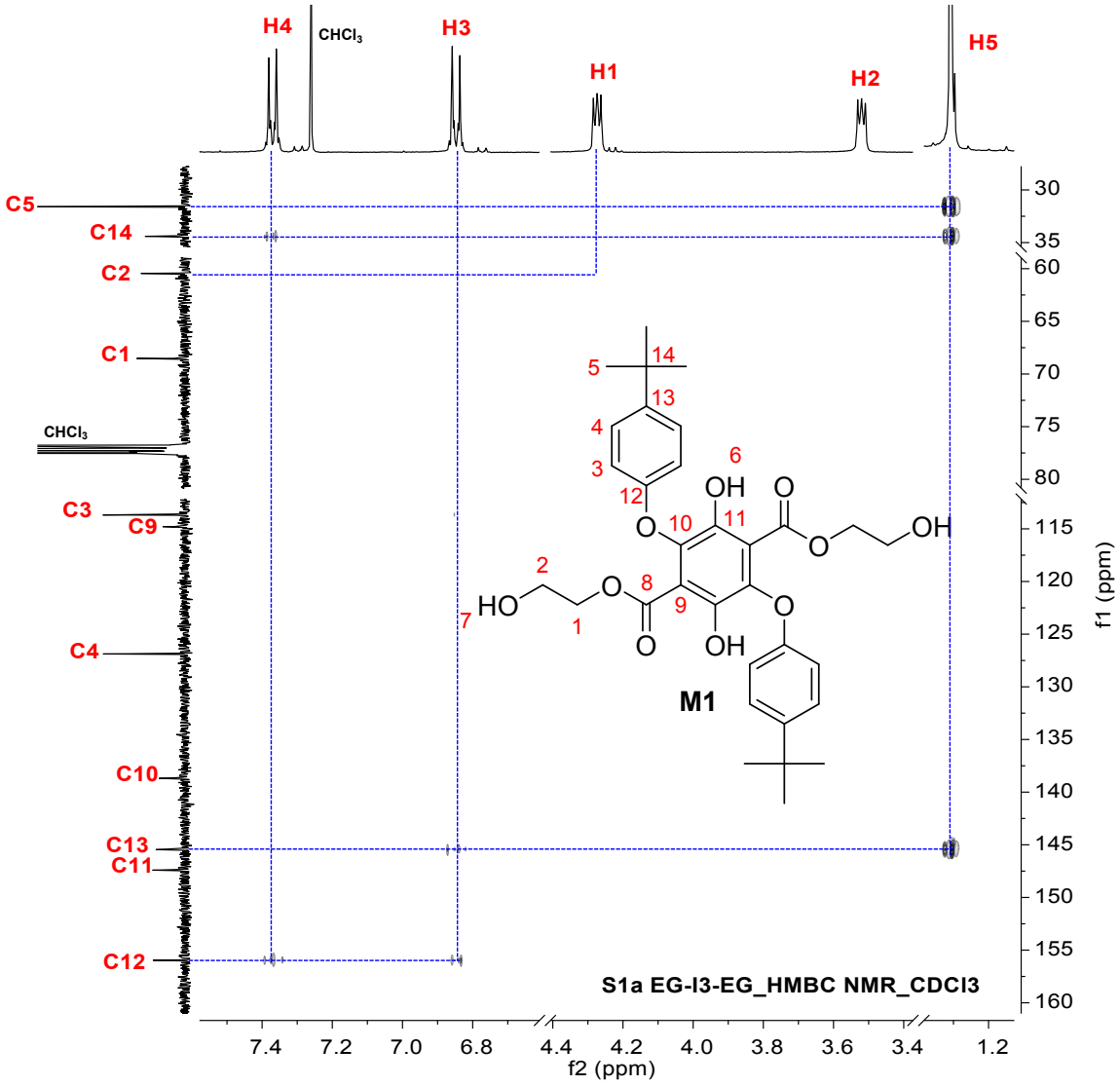
S42. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of monomer diol **M1**.



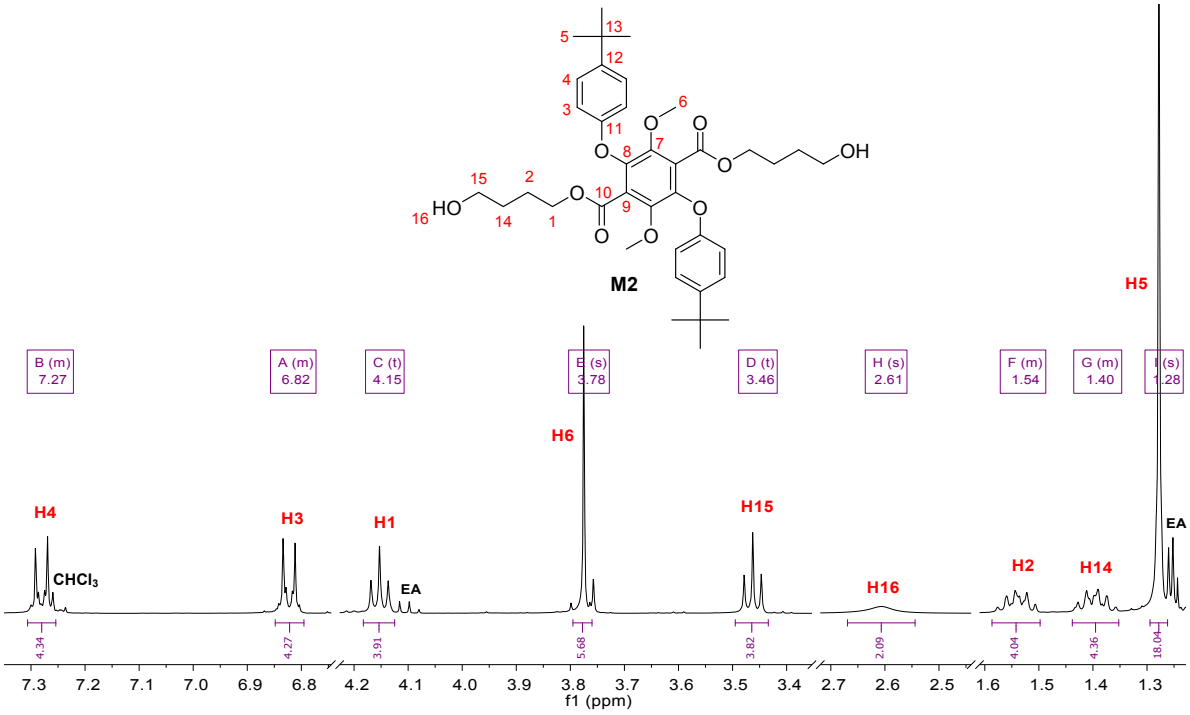
S43. COSY NMR spectrum of monomer diol **M1**.



S44. HSQC NMR spectrum of monomer diol **M1**.

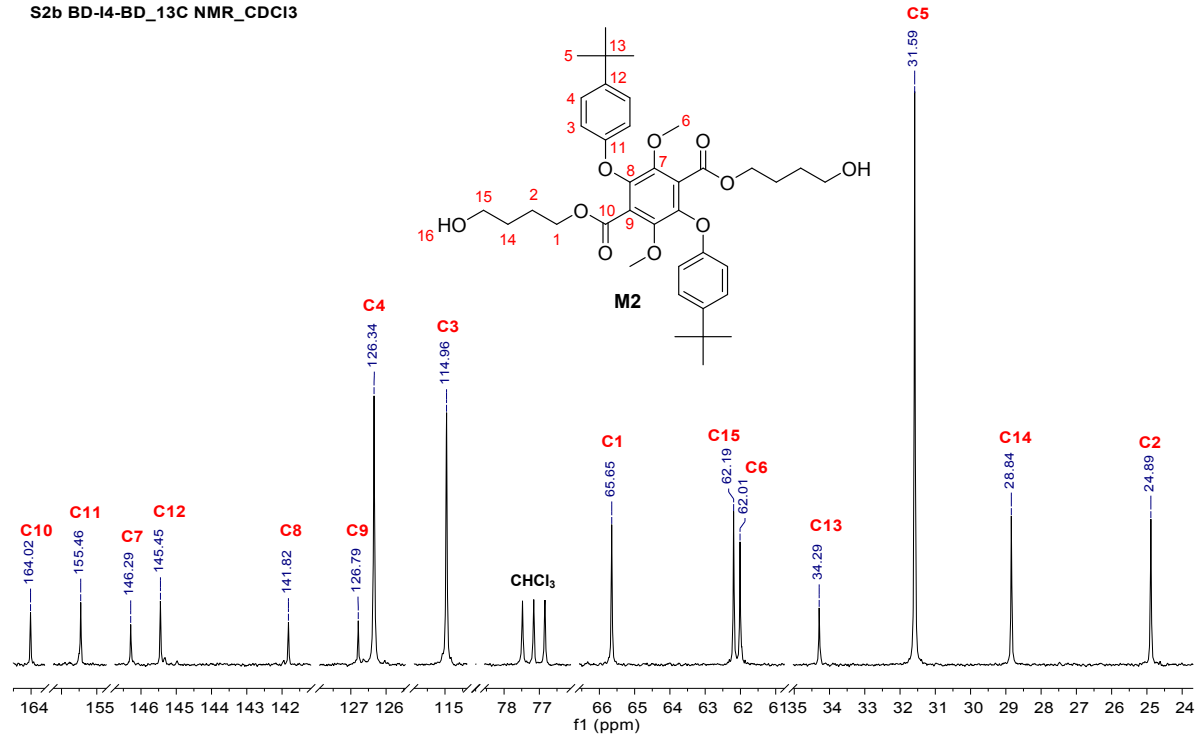


S45. HMBC NMR spectrum of monomer diol **M1**.



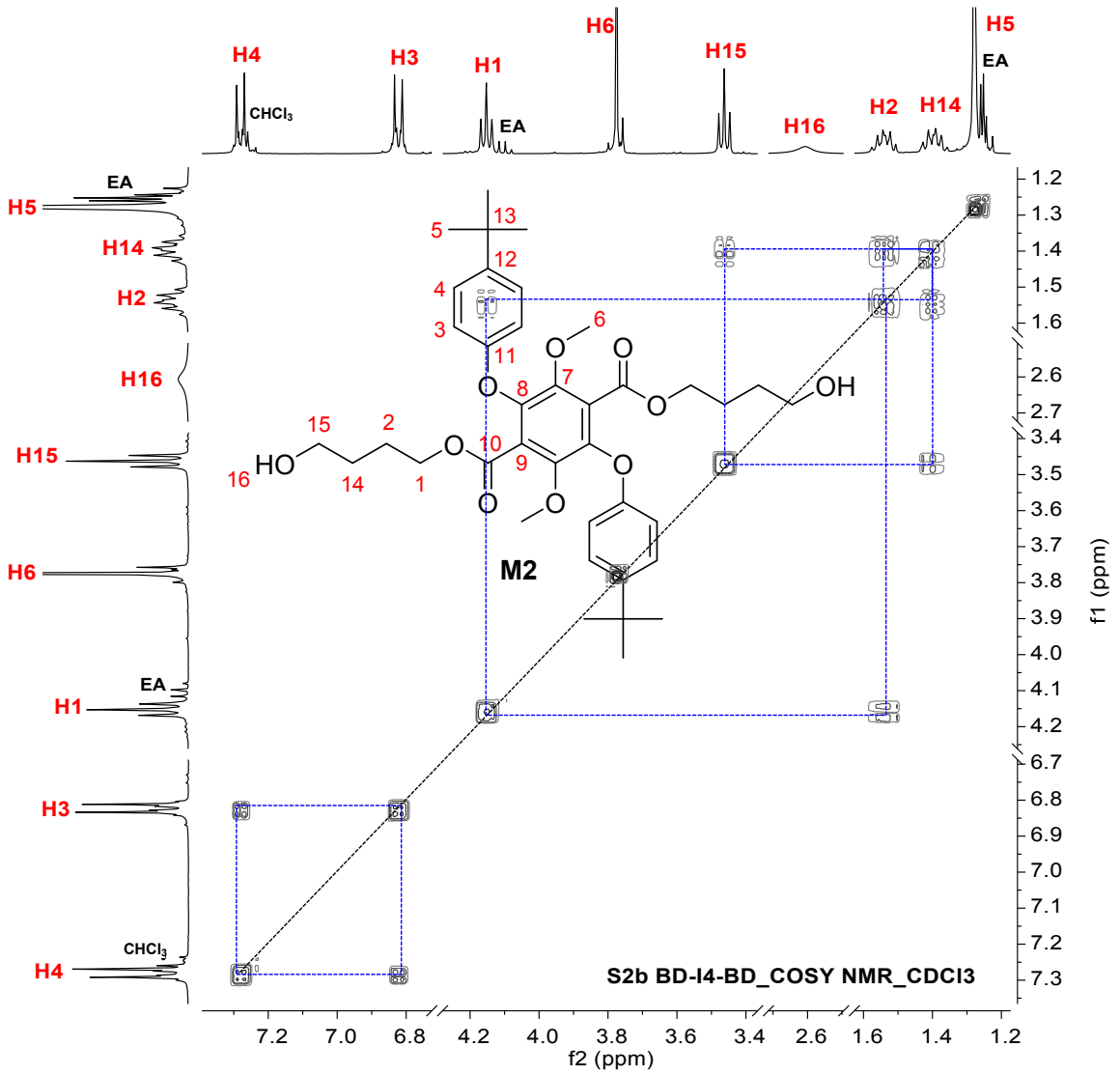
^{1}H NMR (400 MHz, Chloroform - *d*) δ7.31 – 7.25 (m, 4H, H4), 6.85 – 6.80 (m, 4H, H3), 4.15 (t, *J*= 6.4 Hz, 4H, H1), 3.78 (s, 6H, H6), 3.46 (t, *J*= 6.3 Hz, 4H, H15), 2.61 (s, 2H, H16), 1.59 – 1.50 (m, 4H, H2), 1.44 – 1.35 (m, 4H, H14), 1.28 (s, 18H, H5).

S46. ^{1}H NMR (400MHz, $CDCl_3$) spectrum of monomer diol **M2**.

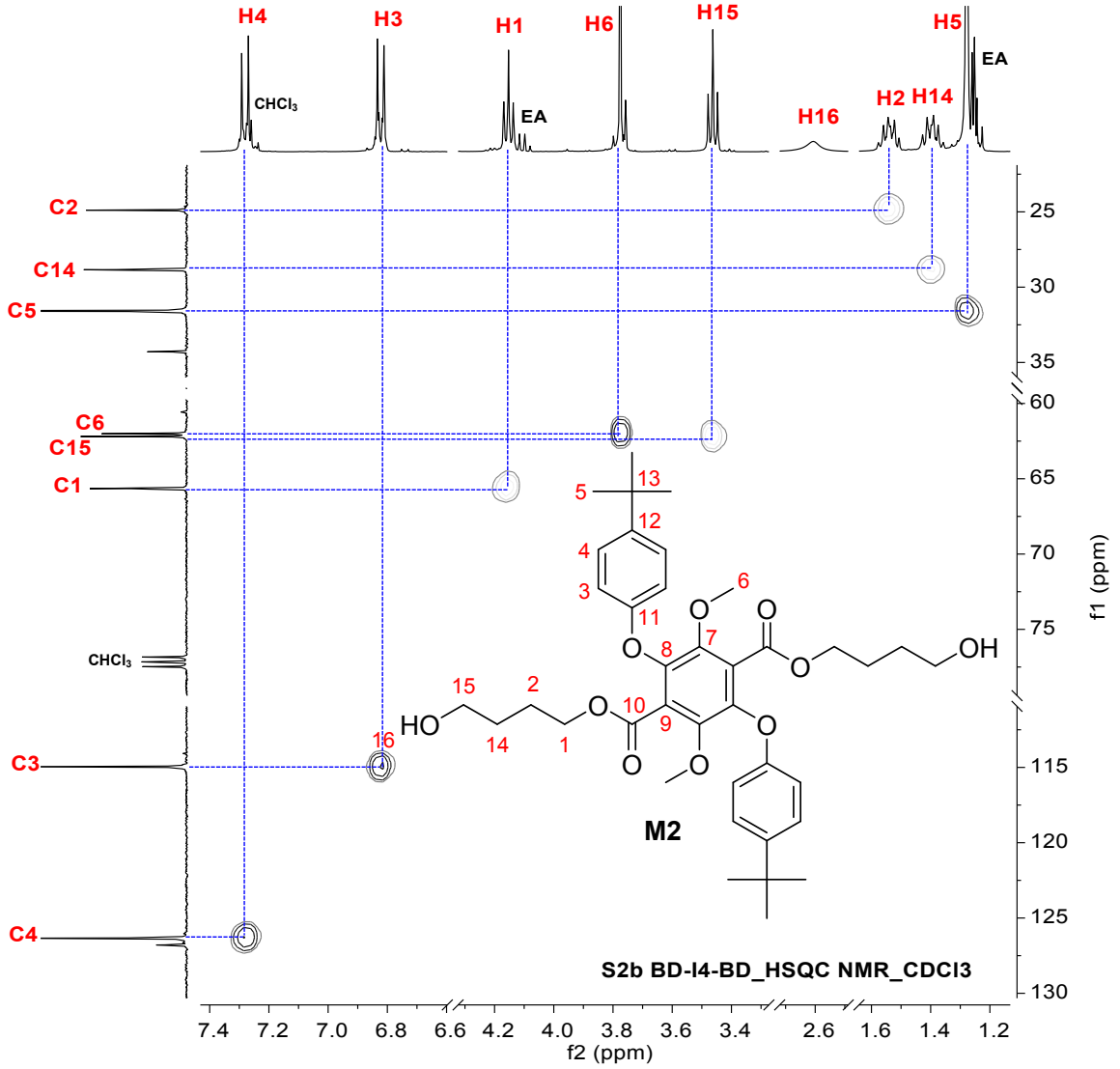


^{13}C NMR (101 MHz, $CDCl_3$) δ164.02 (C10), 155.46 (C11), 146.29 (C7), 145.45 (C12), 141.82 (C8), 126.79 (C9), 126.34 (C4), 114.96 (C3), 65.65 (C1), 62.19 (C15), 62.01 (C6), 34.29 (C13), 31.59 (C5), 28.84 (C14), 24.89 (C2).

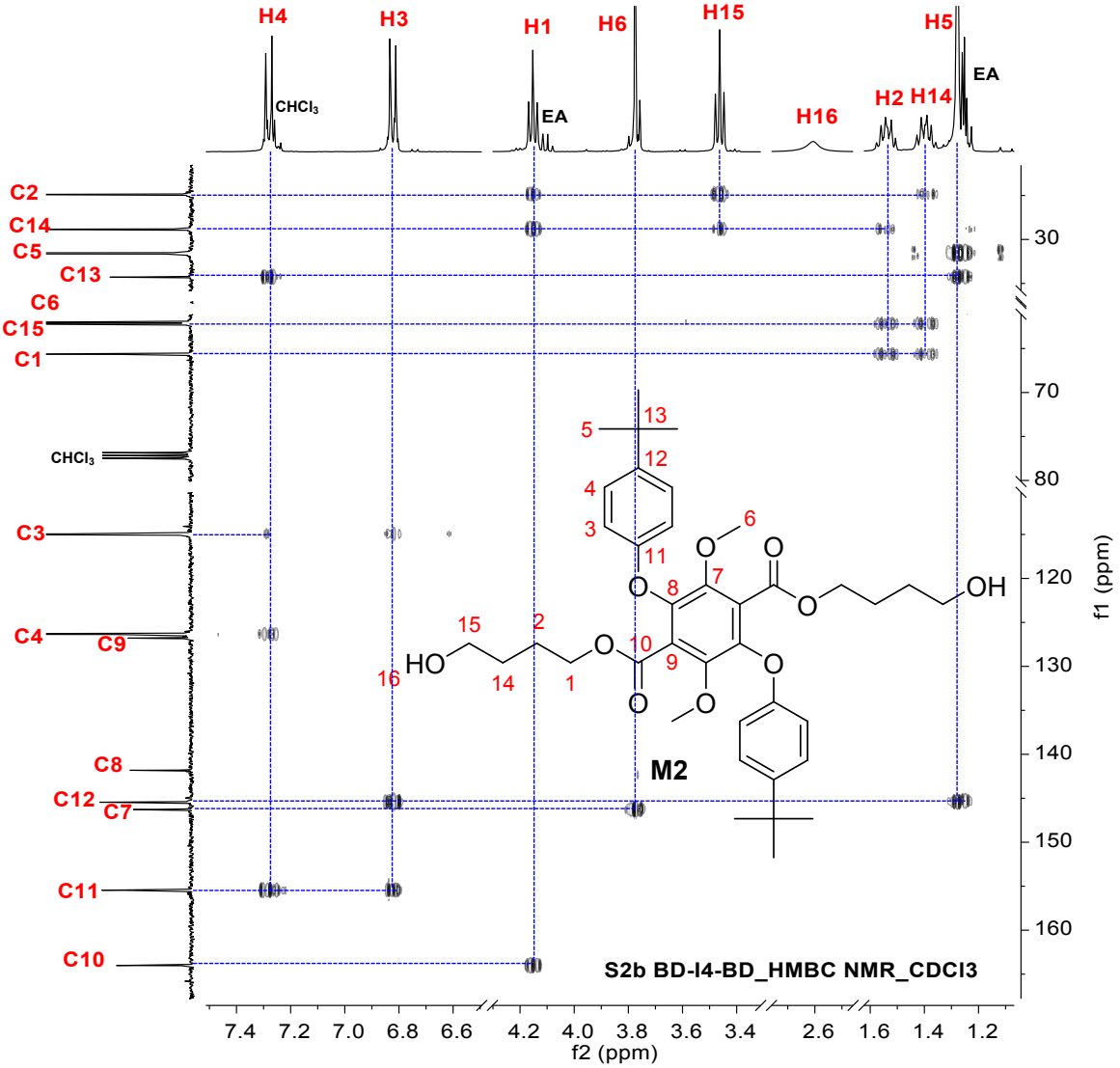
S47. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of monomer diol **M2**.



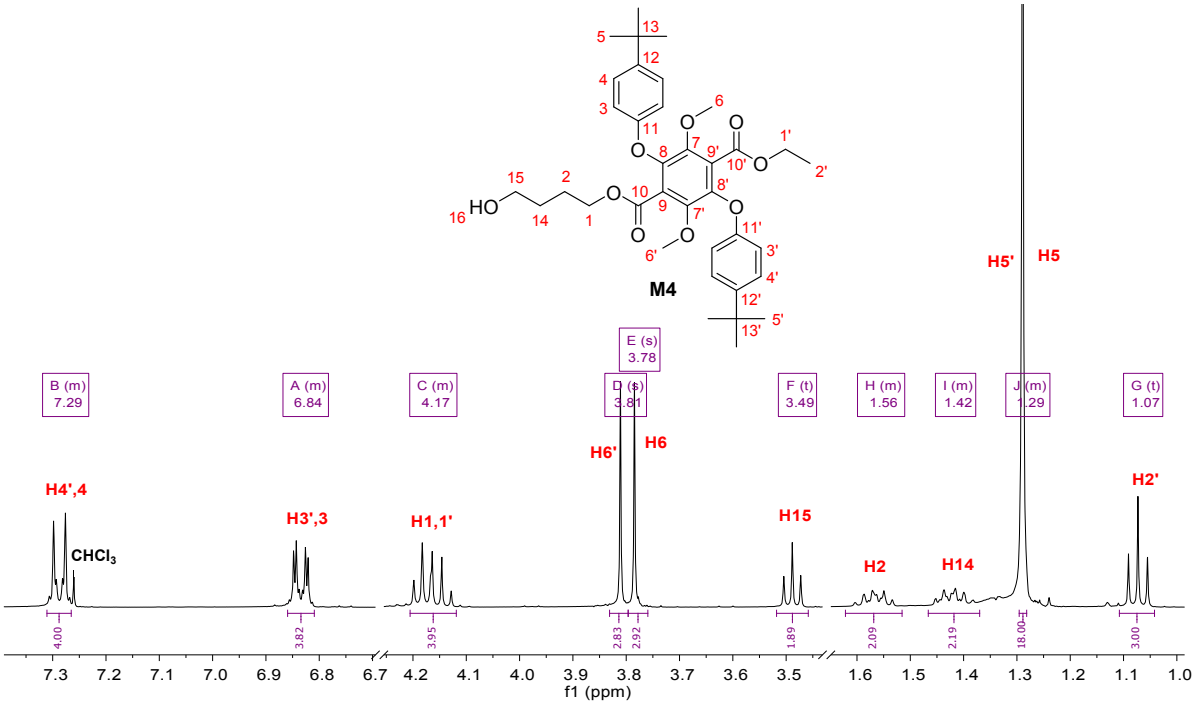
S48. COSY NMR spectrum of monomer diol **M2**.



S49. HSQC NMR spectrum of monomer diol **M2**.

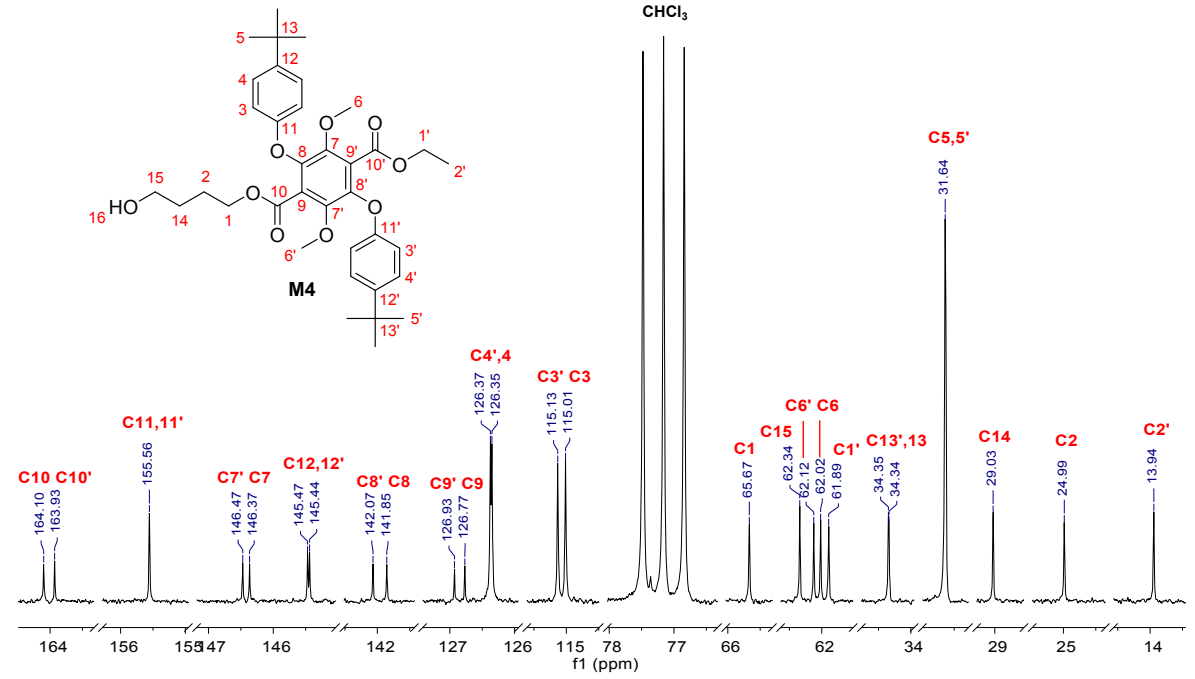


S50. HMBC NMR spectrum of monomer diol **M2**.



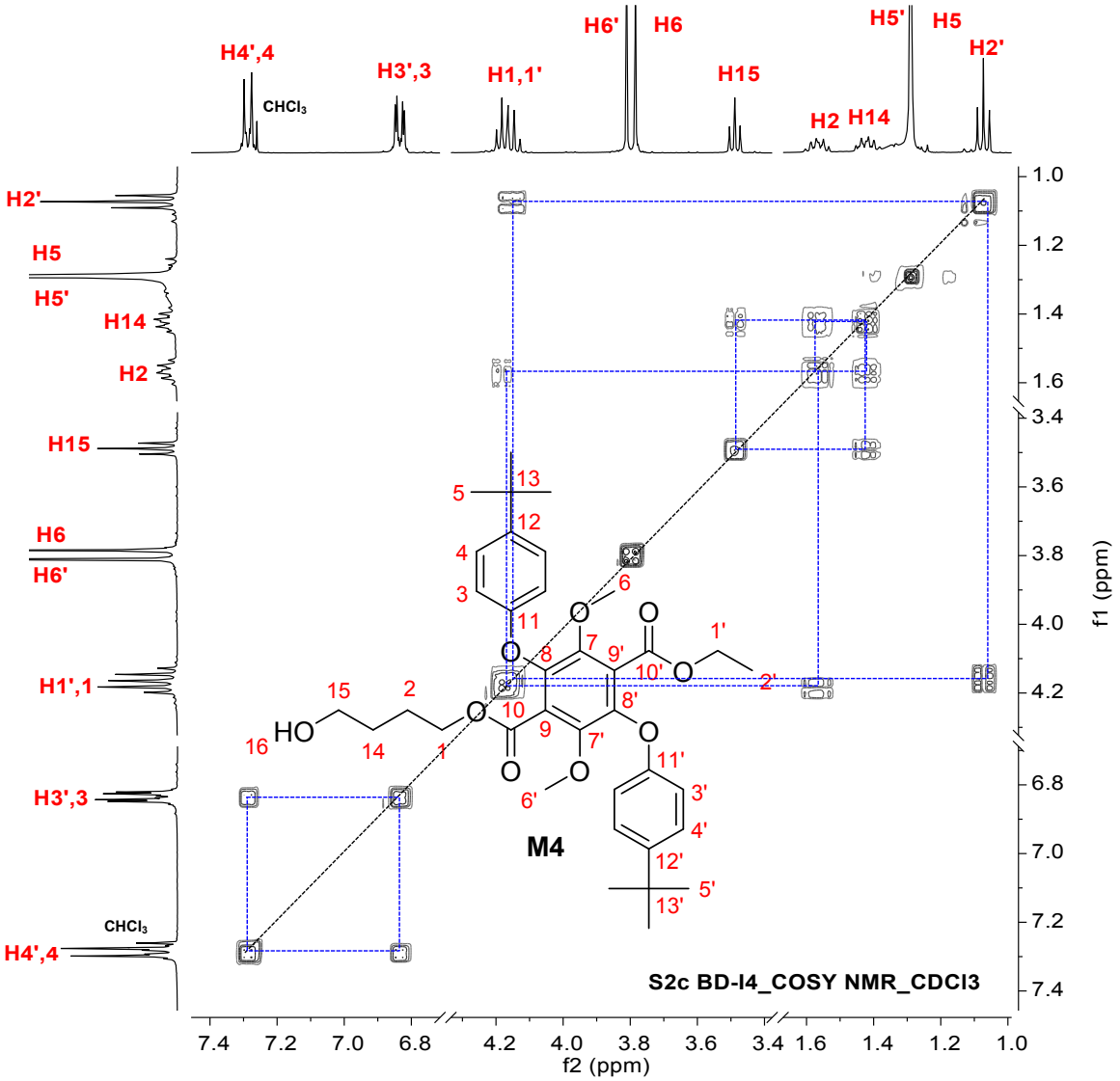
^{1}H NMR (400 MHz, Chloroform - *d*) δ7.31 – 7.27 (m, 4H, H4, H4'), 6.86 – 6.81 (m, 4H, H3', H3), 4.21 – 4.12 (m, 4H, H1, H1'), 3.81 (s, 3H, H6'), 3.78 (s, 3H, H6), 3.49 (t, *J*= 6.3 Hz, 2H, H15), 1.62 – 1.52 (m, 2H, H2), 1.47 – 1.37 (m, 2H, H14), 1.30 – 1.28 (m, 18H, H5', H5), 1.07 (t, *J*= 7.1 Hz, 3H, H2').

S51. ^{1}H NMR (400MHz, $CDCl_3$) spectrum of side product **M4**.

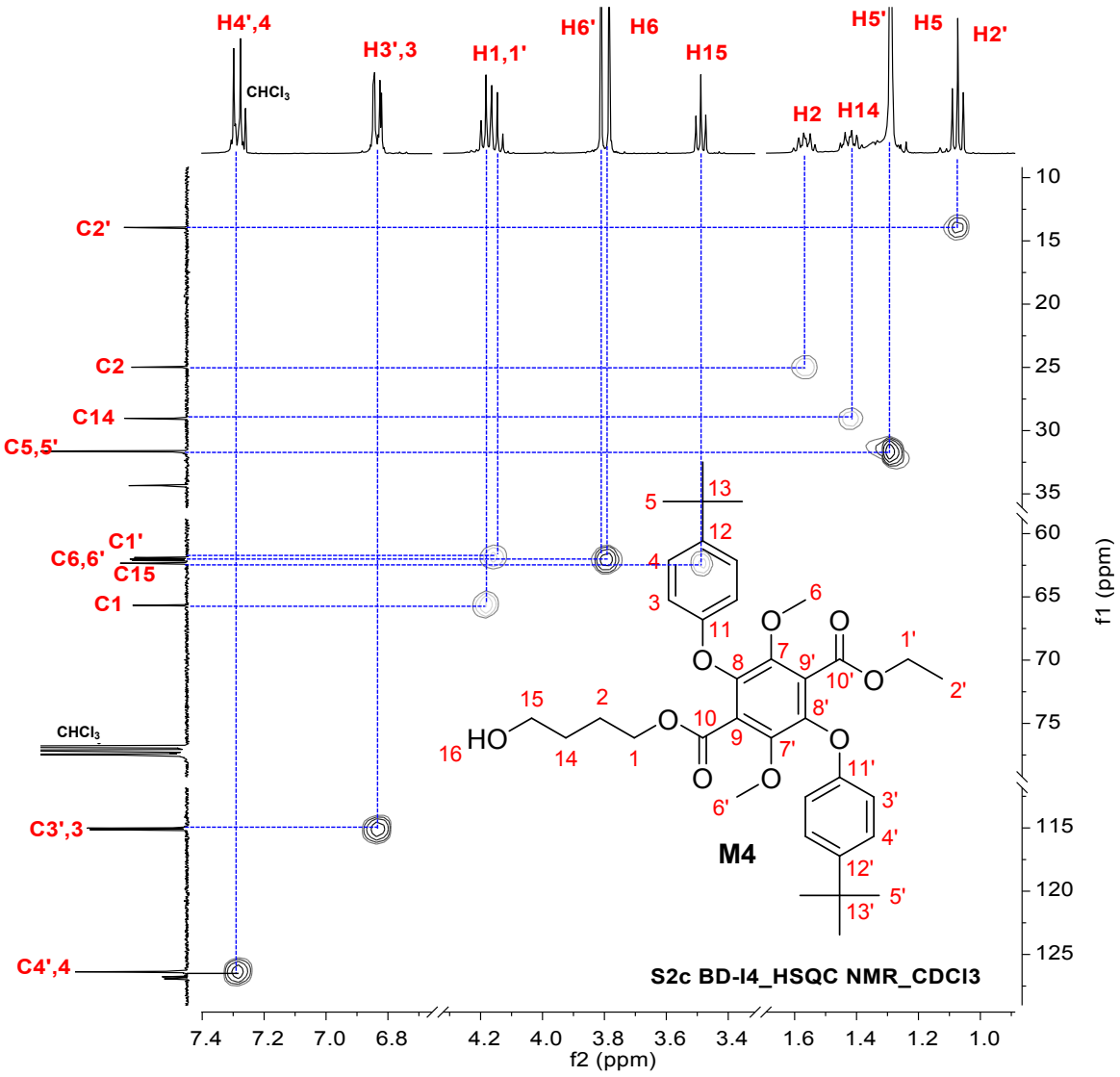


^{13}C NMR (101 MHz, $CDCl_3$) δ164.10 (C10), 163.93 (C10'), 155.56 (C11, C11'), 146.47 (C7'), 146.37 (C7), 145.47, 145.44 (C12, C12'), 142.07 (C8'), 141.85 (C8), 126.93 (C9'), 126.77 (C9), 126.37, 126.35 (C4', C4), 115.13 (C3'), 115.01 (C3), 65.67 (C1), 62.34 (C15), 62.12 (C6'), 62.02 (C6), 61.89 (C1'), 34.35, 34.34 (C13', C13), 31.64 (C5, C5'), 29.03 (C14), 24.99 (C2), 13.94 (C2').

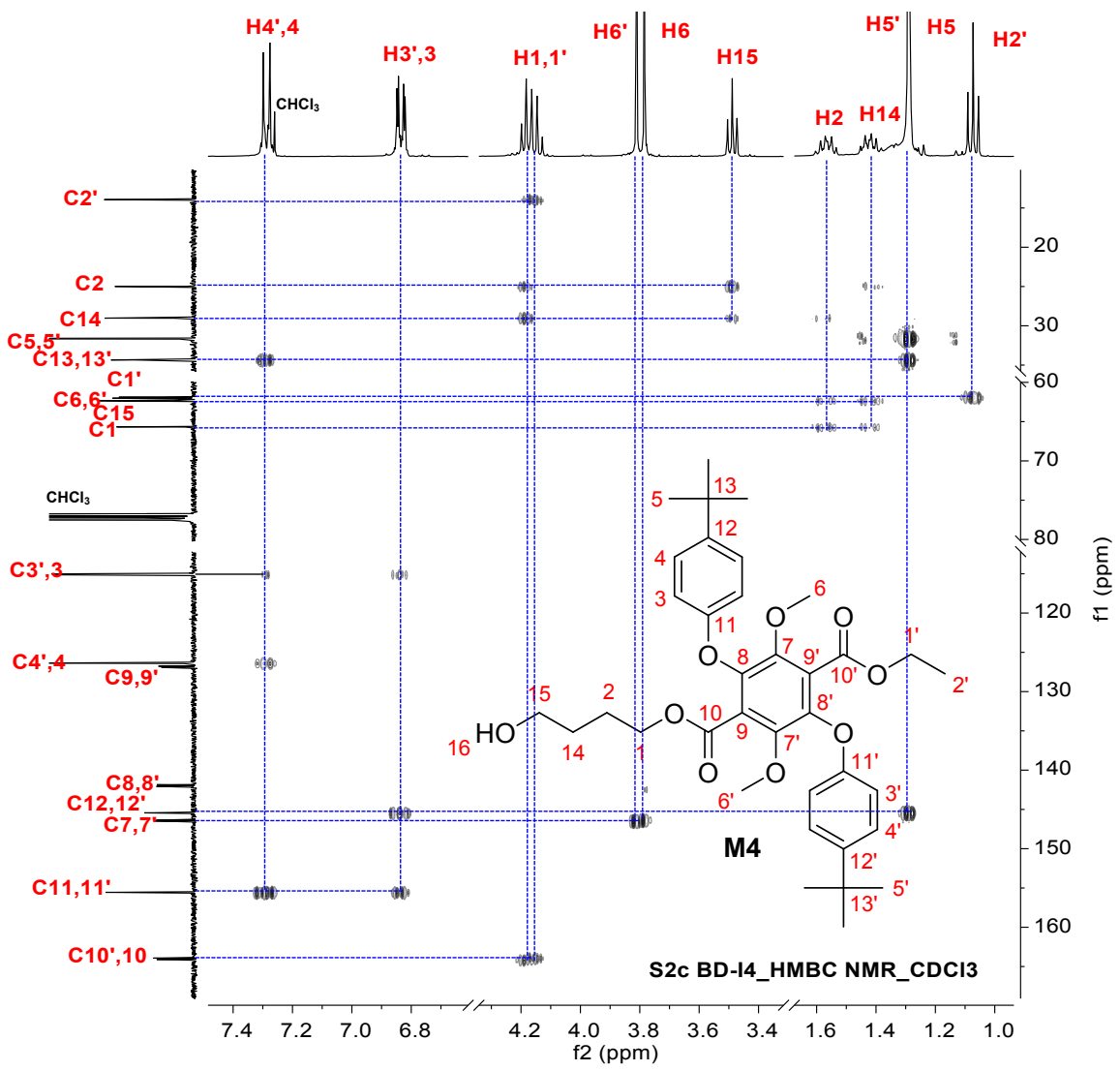
S52. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of side product **M4**.



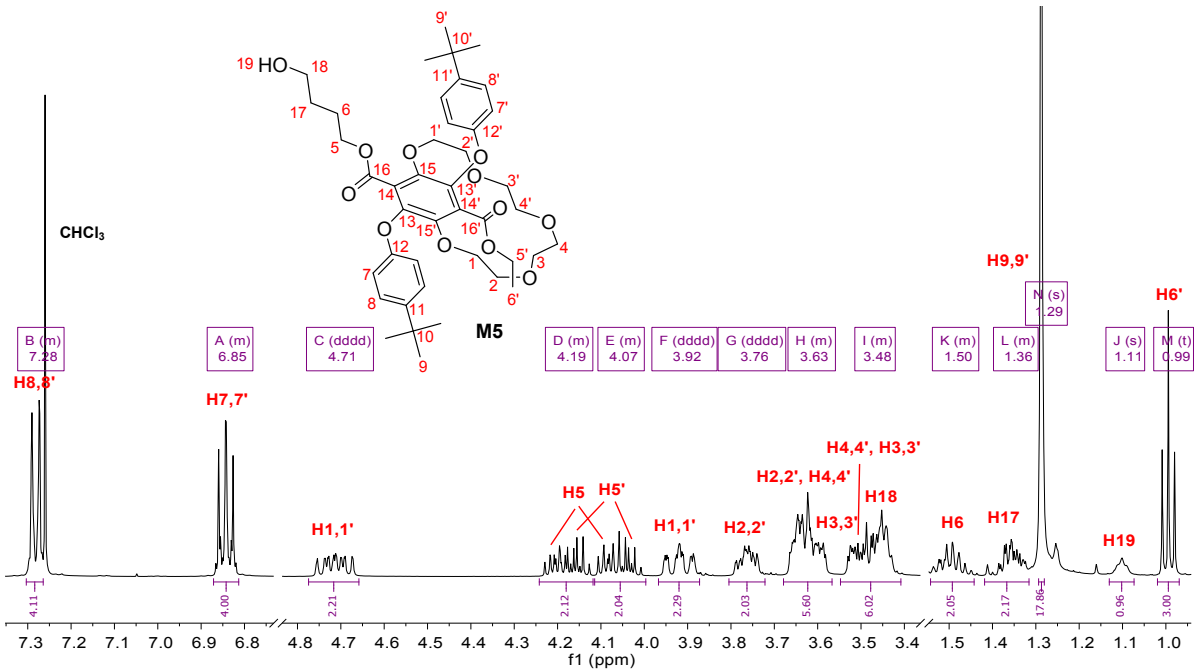
S53. COSY NMR spectrum of side product **M4**.



S54. HSQC NMR spectrum of side product **M4**.

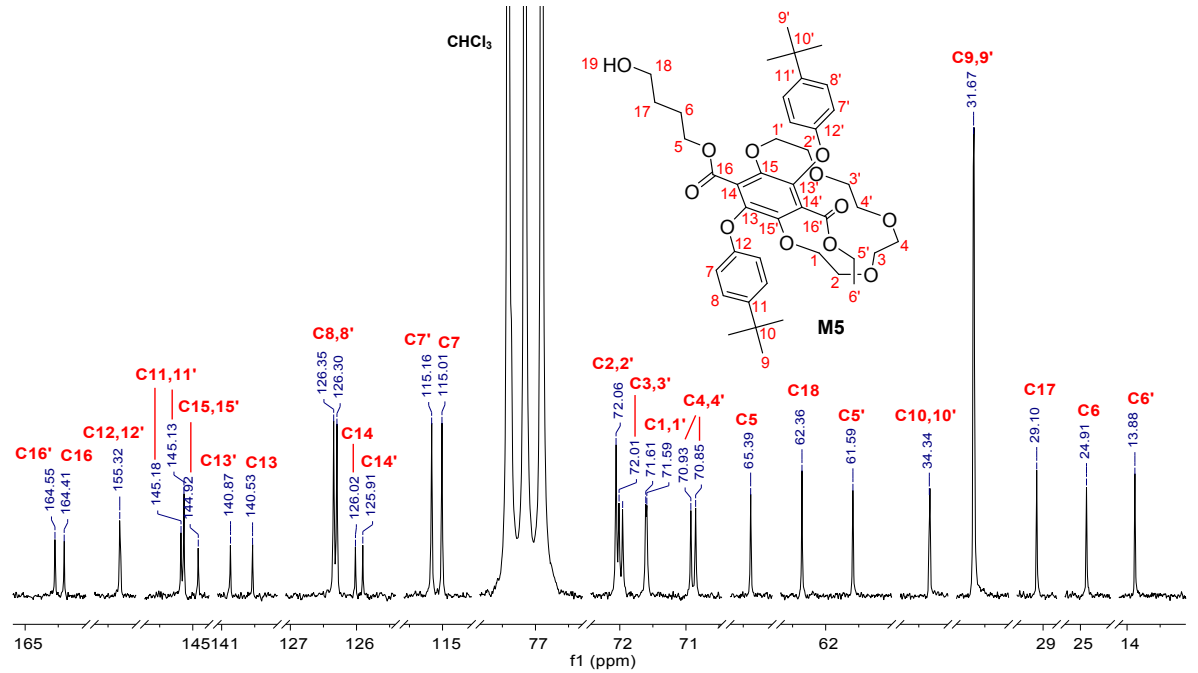


S55. HMBC NMR spectrum of side product **M4**.



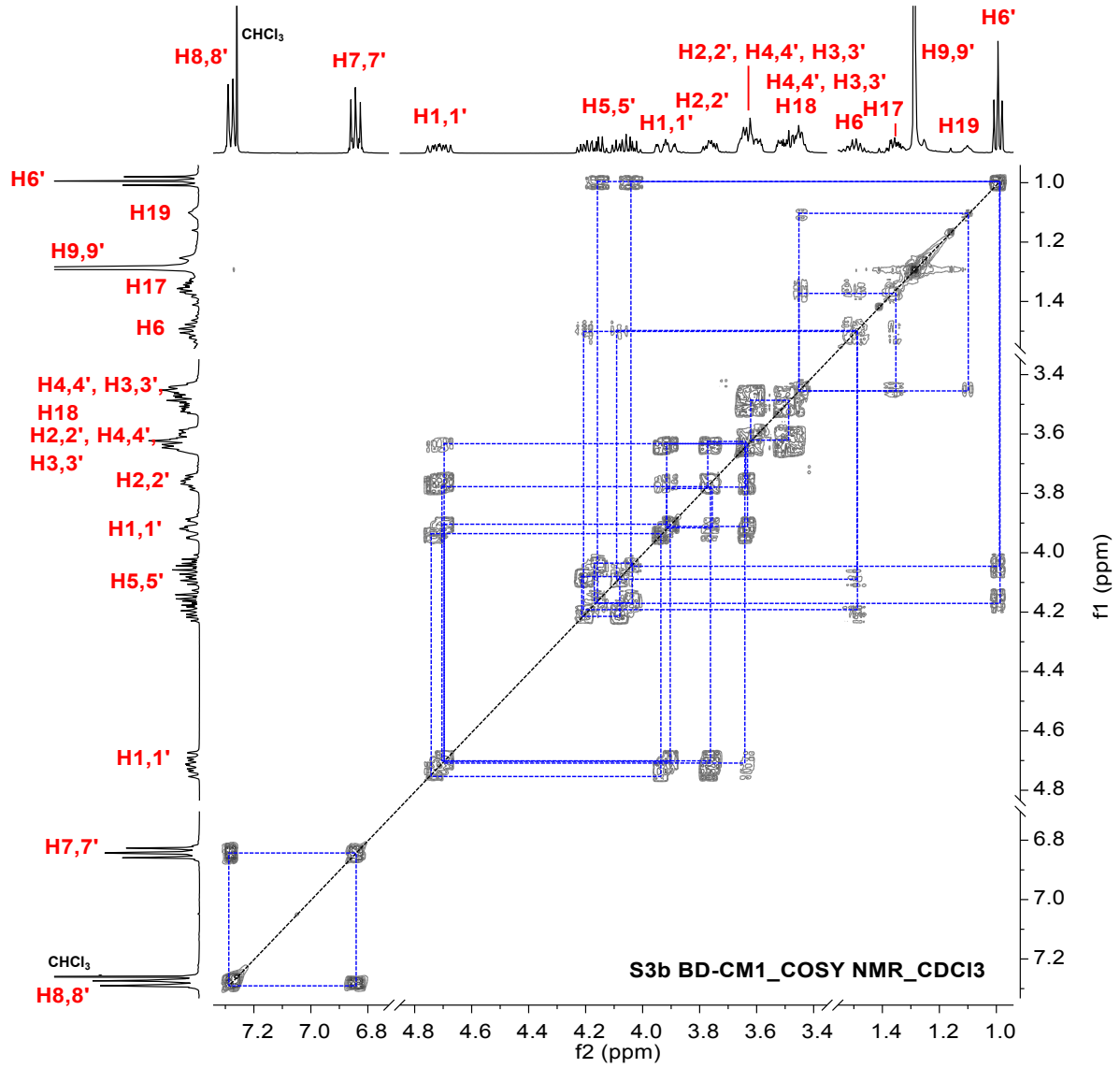
^{1}H NMR (500 MHz, Chloroform - *d*) δ7.30 – 7.26 (m, 4H, H8, H8'), 6.87 – 6.81 (m, 4H, H7, H7'), 4.71 (dddd, *J*= 18.8, 13.0, 9.0, 1.3 Hz, 2H, H1, H1'), 4.24 – 4.12 (m, 2H, H5, H5'), 4.11 – 4.00 (m, 2H, H5, H5'), 3.92 (dddd,*J*= 17.5, 13.0, 3.5, 1.5 Hz, 2H, H1, H1'), 3.76 (dddd, *J*= 10.5, 8.8, 4.8, 1.4 Hz, 2H, H2, H2'), 3.68 – 3.57 (m, 6H, H2, H2', H4, H4', H3, H3'), 3.55 – 3.41 (m, 6H, H4, H4', H3, H3', H18), 1.54 – 1.44 (m, 2H, H6), 1.42 – 1.32 (m, 2H, H17), 1.29 (s, 18H, H9, H9'), 1.11 (s, 1H, H19), 0.99 (t, *J*= 7.1 Hz, 3H, H6').

S56. ^{1}H NMR (500MHz, $CDCl_3$) spectrum of side product **M5**.

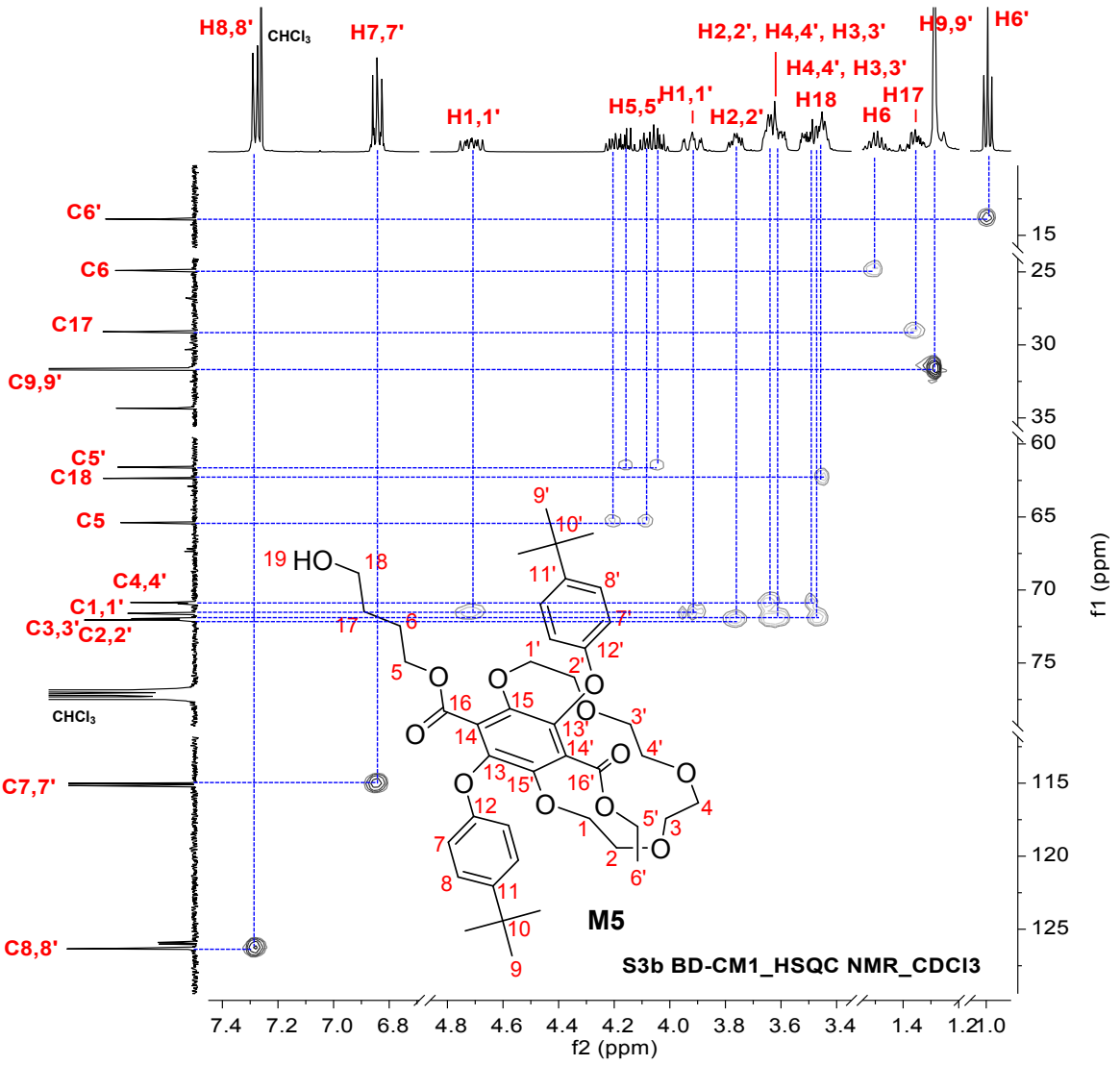


^{13}C NMR (126 MHz, $CDCl_3$) δ164.55 (C16'), 164.41 (C16), 155.32 (C12, C12'), 145.18, 145.13 (C11, C11'), 144.92 (C15, C15'), 140.87 (C13'), 140.53 (C13), 126.35, 126.30 (C8, C8'), 126.02 (C14), 125.91 (C14'), 115.16 (C7'), 115.01 (C7), 72.06 (C2, C2'), 72.01 (C3, C3'), 71.61, 71.59 (C1, C1'), 70.93, 70.85 (C4, C4'), 65.39 (C5), 62.36 (C18), 61.59 (C5'), 34.34 (C10, C10'), 31.67 (C9, C9'), 29.10 (C17), 24.91 (C6), 13.88 (C6').

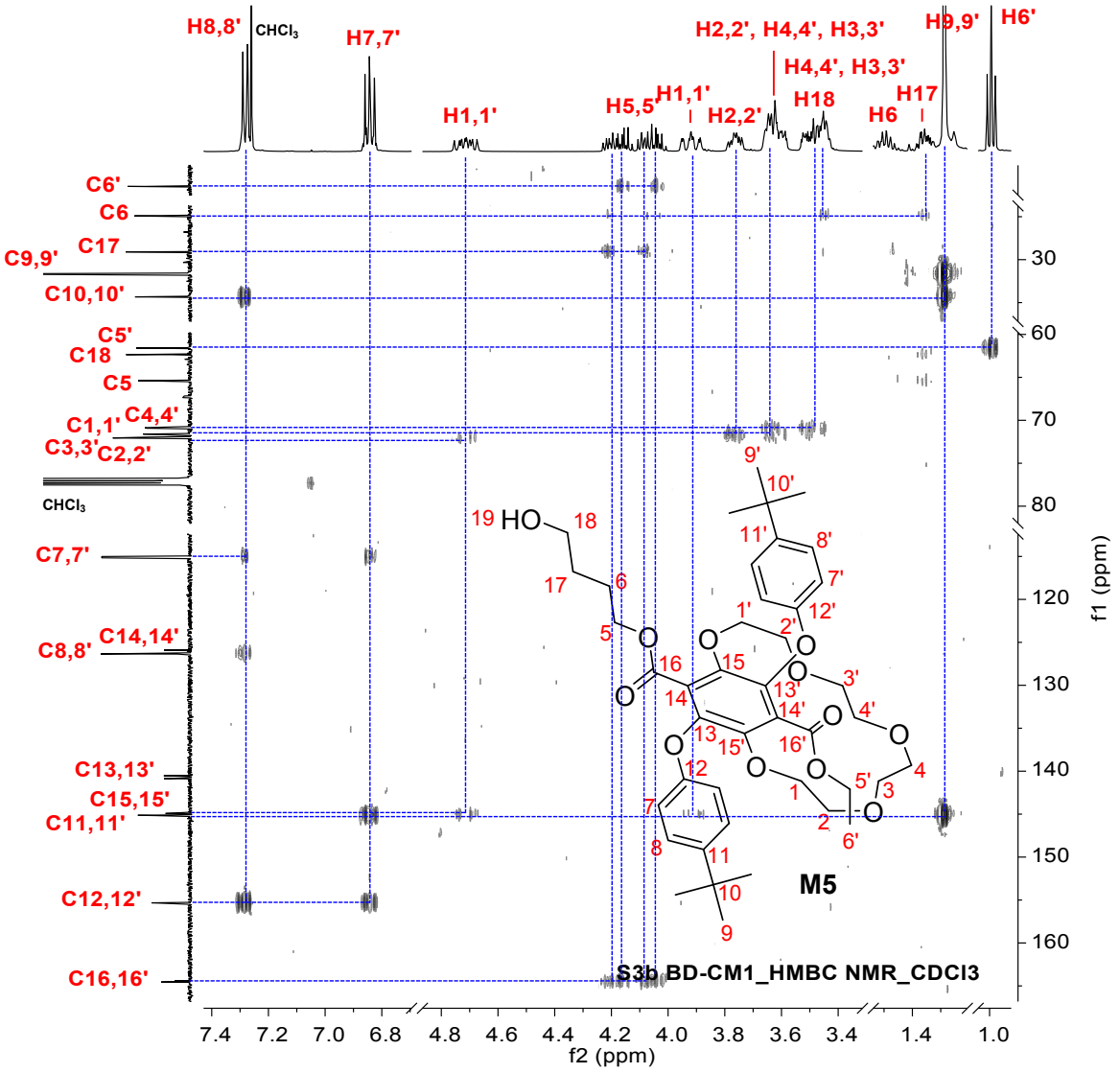
S57. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of side product **M5**.



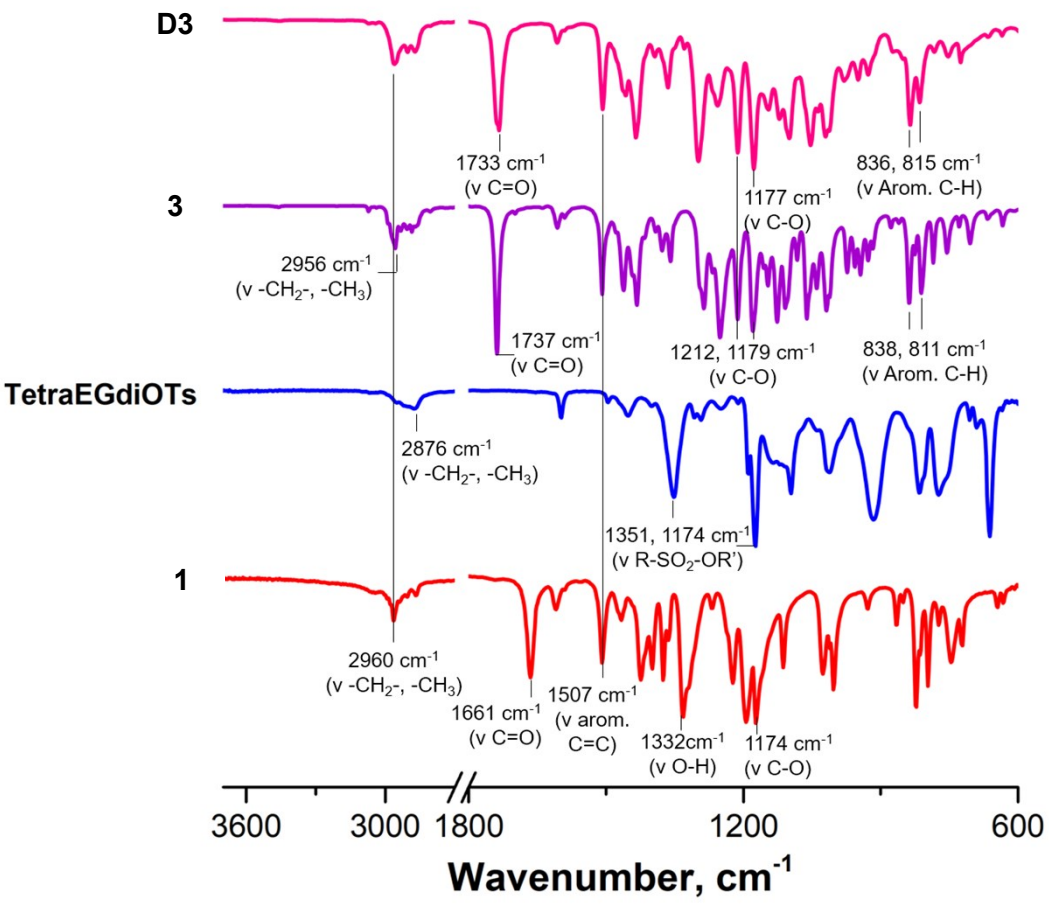
S58. COSY NMR spectrum of side product **M5**.



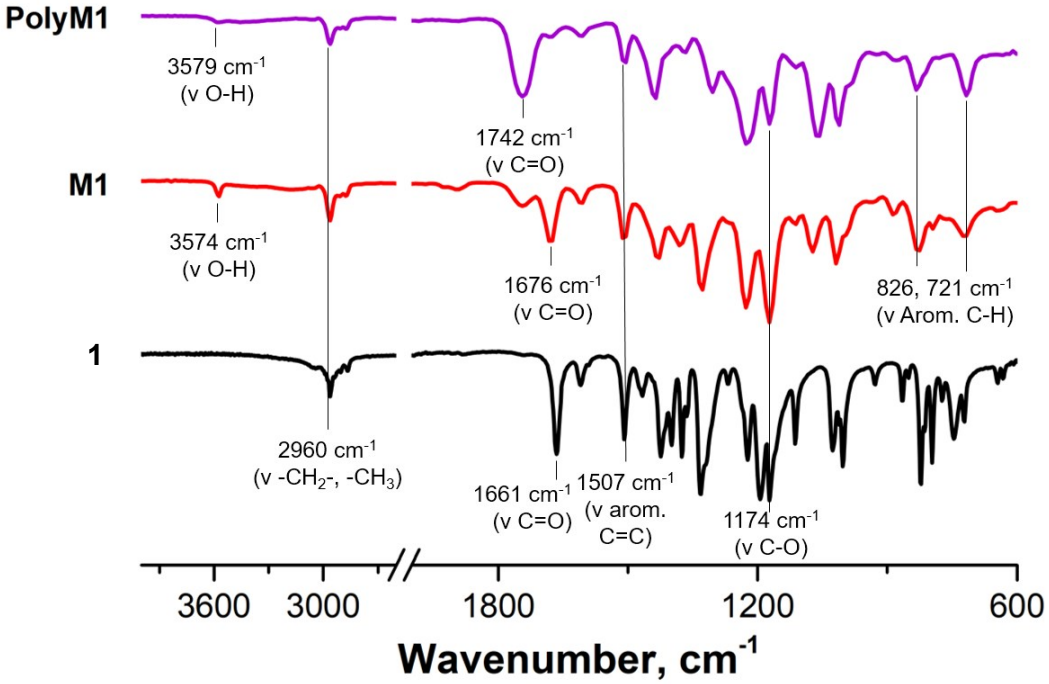
S59. HSQC NMR spectrum of side product **M5**.



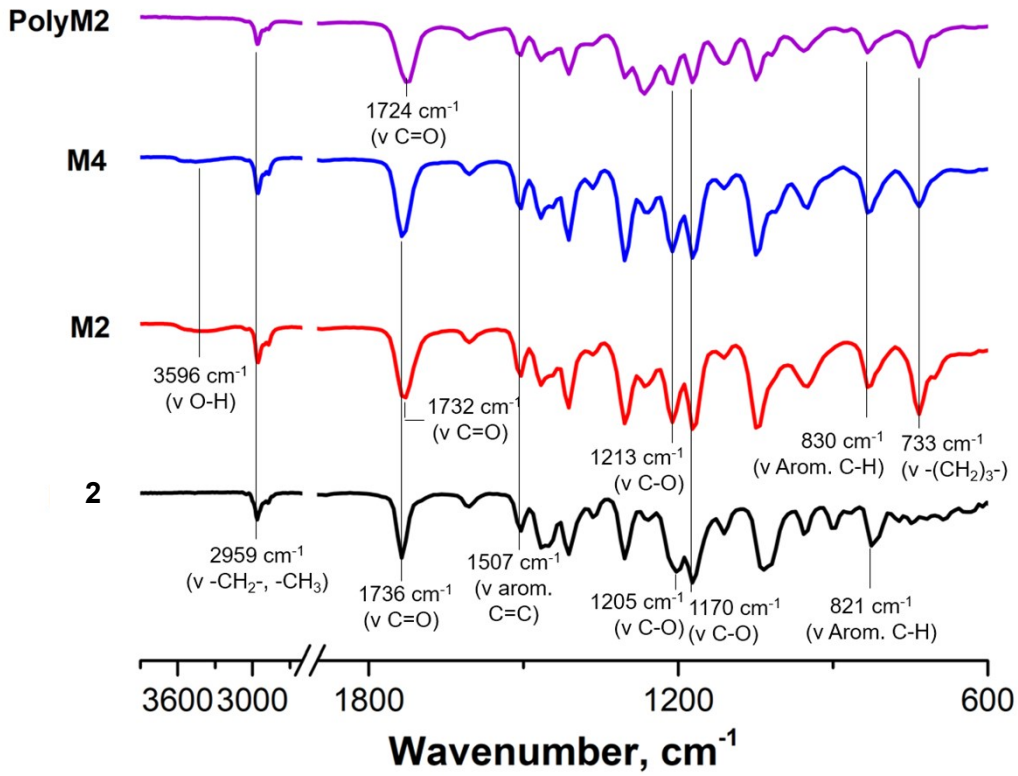
S60. HMBC NMR spectrum of side product **M5**.



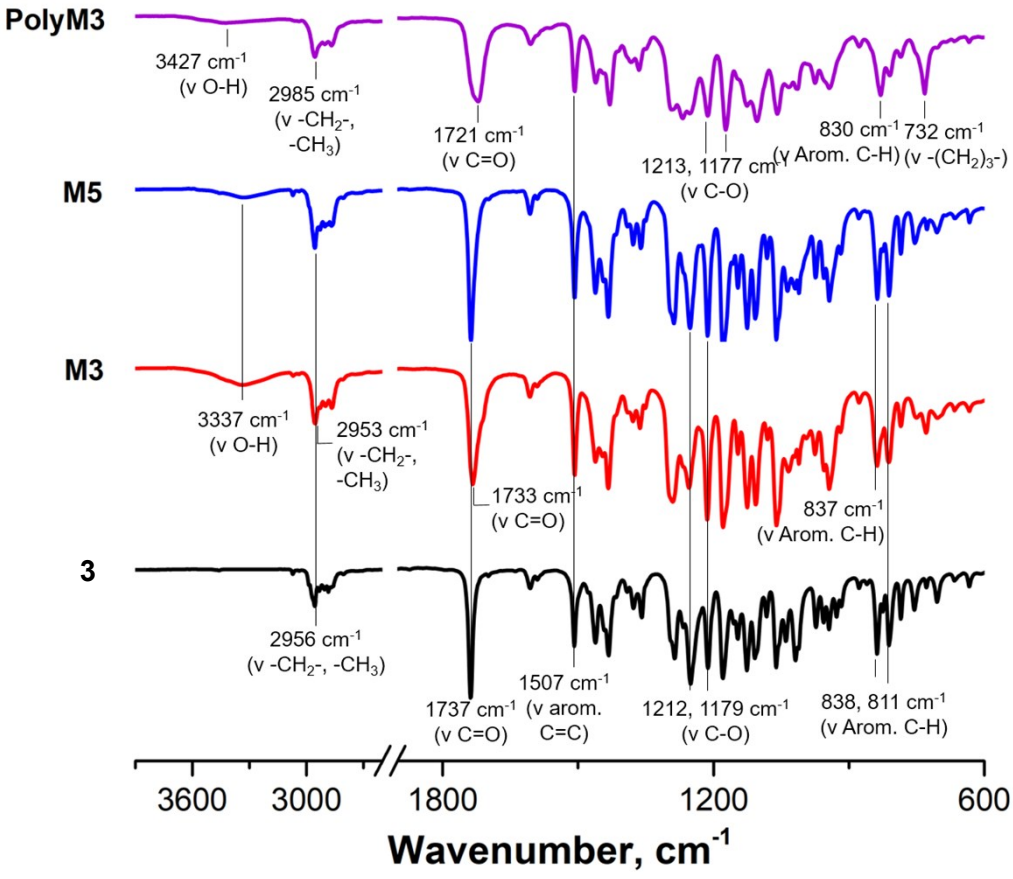
S61. FT-IR spectra of starting materials, compound **3** and **D3**.



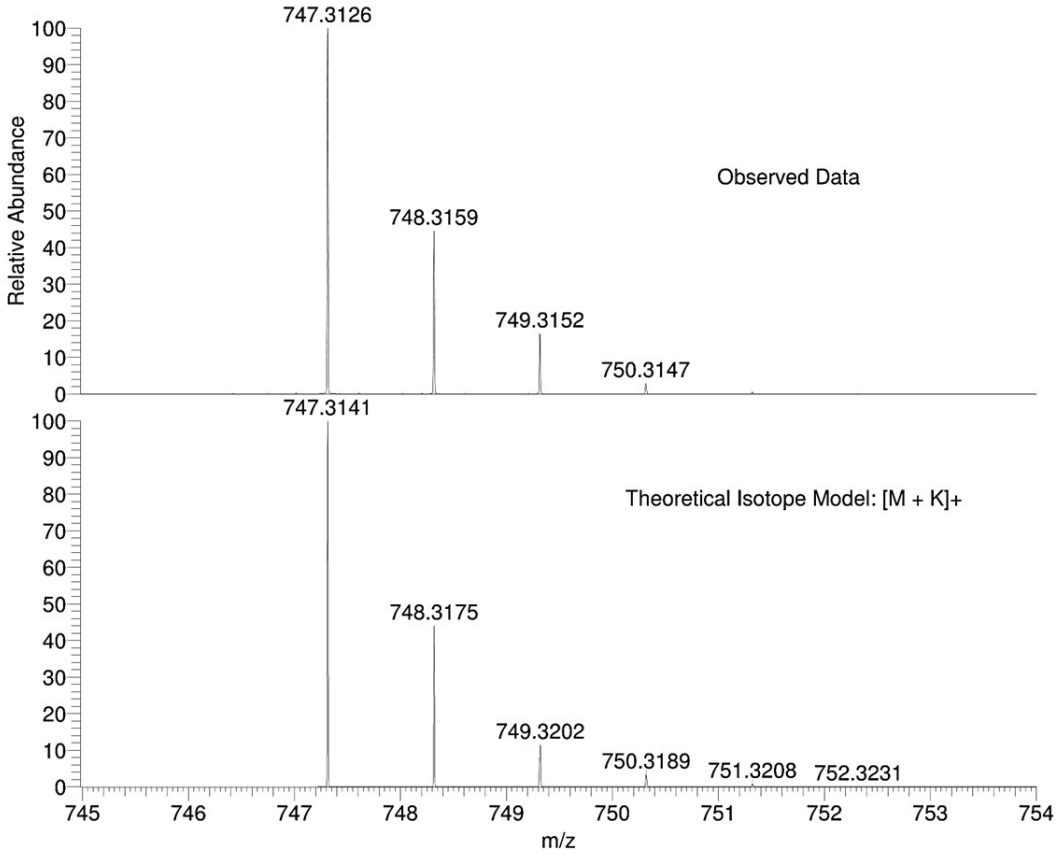
S62. FT-IR spectra of starting materials, compound **M1** and **PolyM1**.

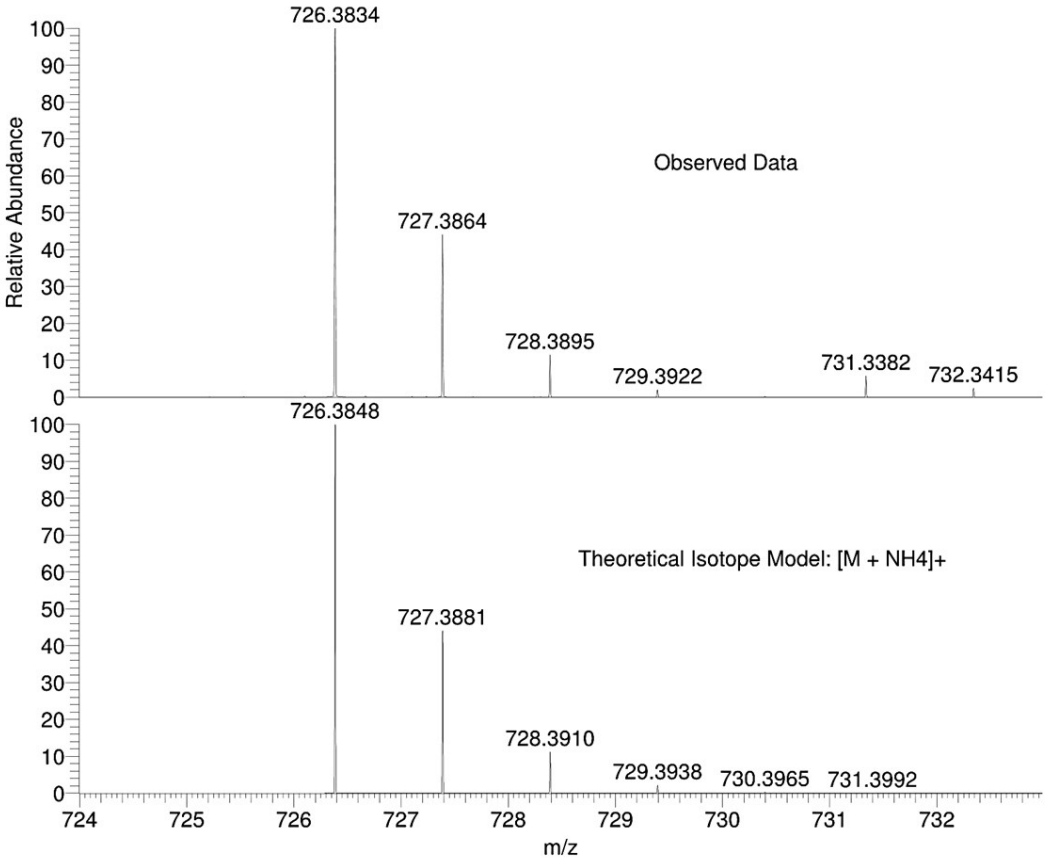


S63. FT-IR spectra of compound **2**, **M2**, **M4** and **PolyM2**.

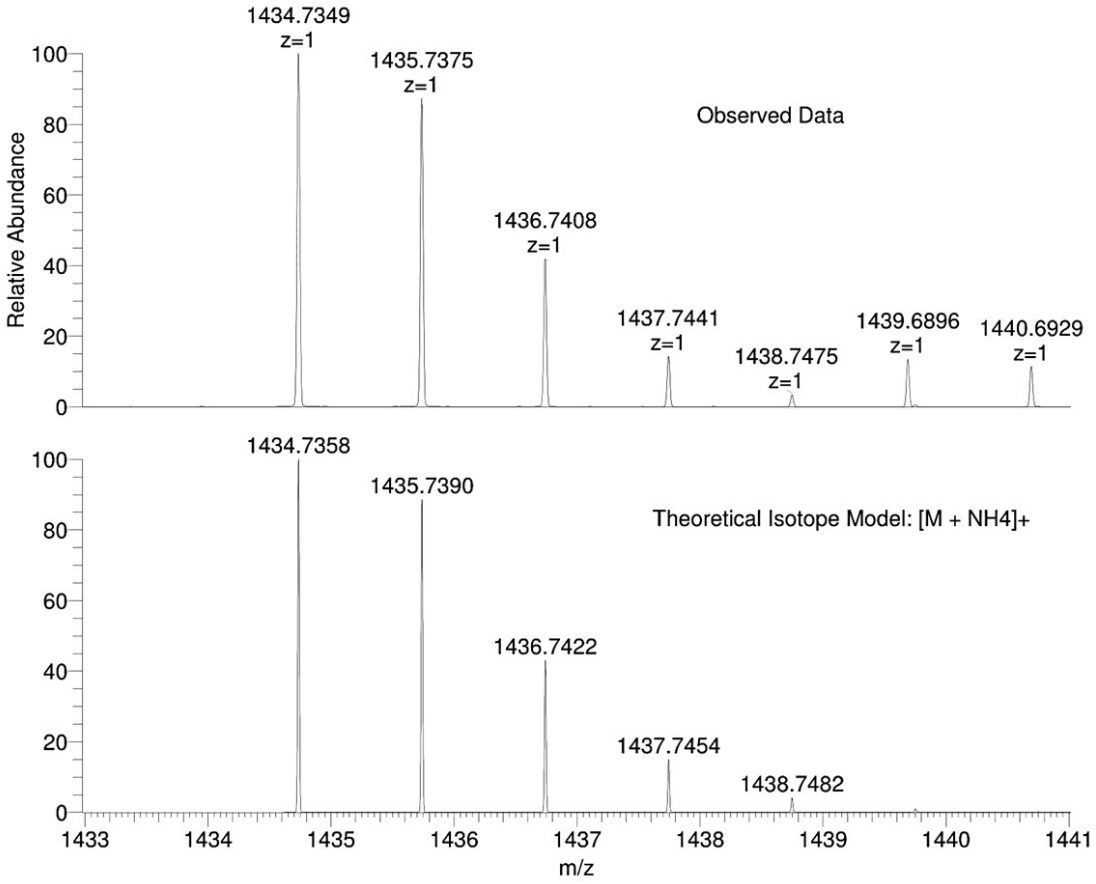


S64. FT-IR spectra of compound **3**, **M3**, **M5** and **PolyM3**.

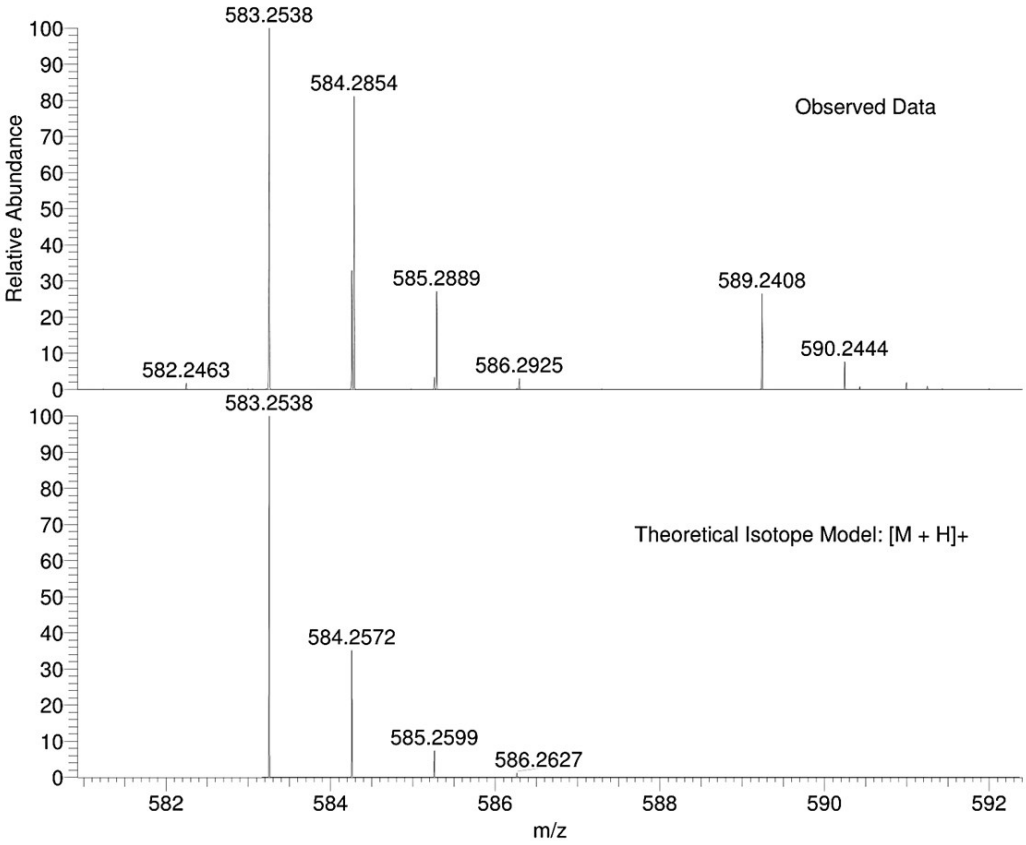


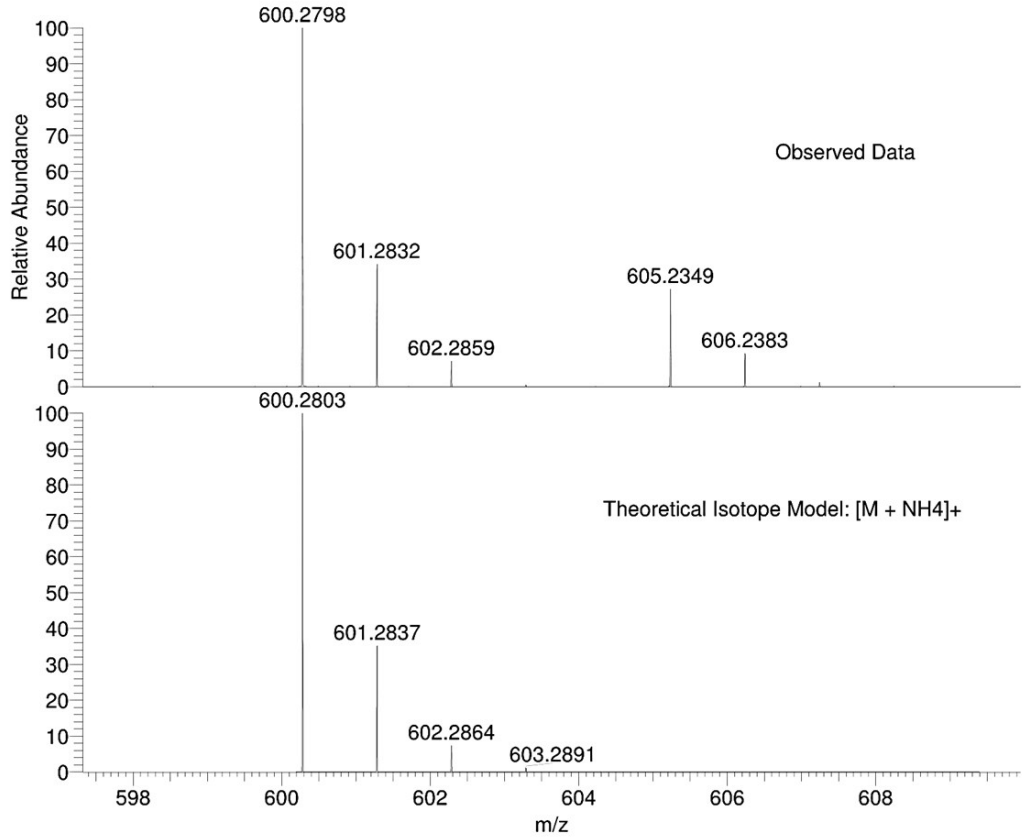


S65. Mass spectra data for the 1+1 crown ether derivative **3** in the presence of K^+ and NH_4^+ ions, respectively.

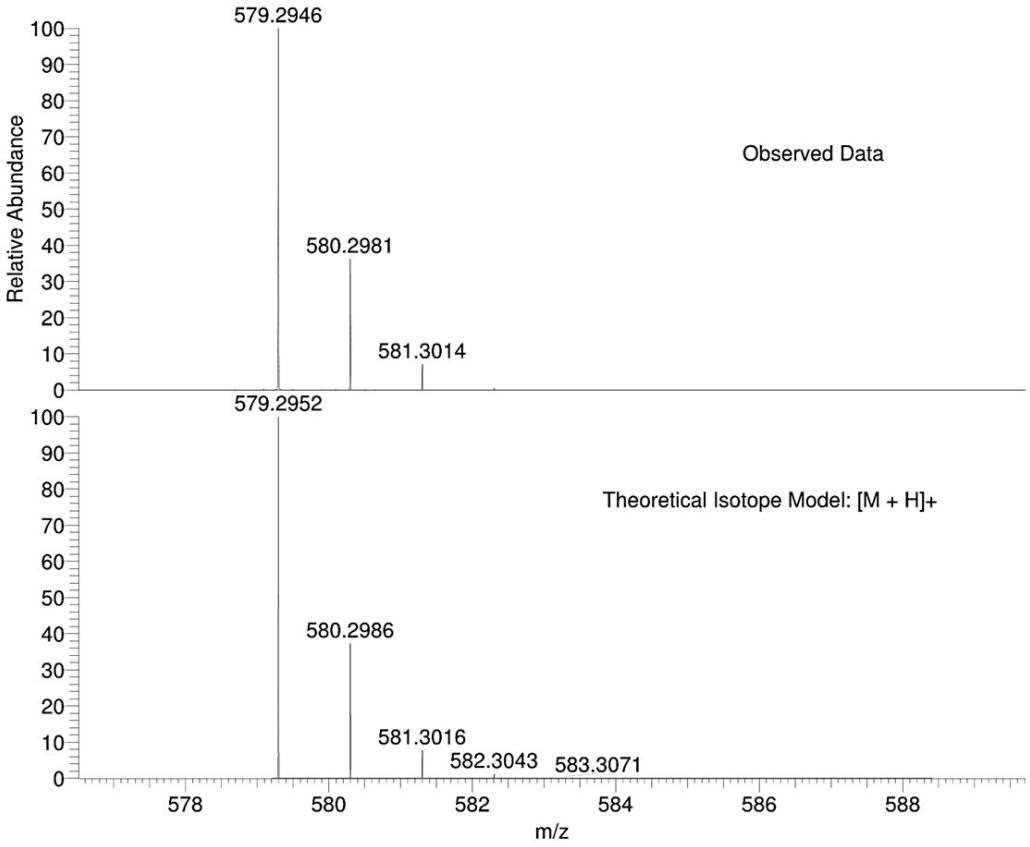


S66. Mass spectra data for the 2+2 crown ether derivative **D3** in the presence of NH_4^+ ions.

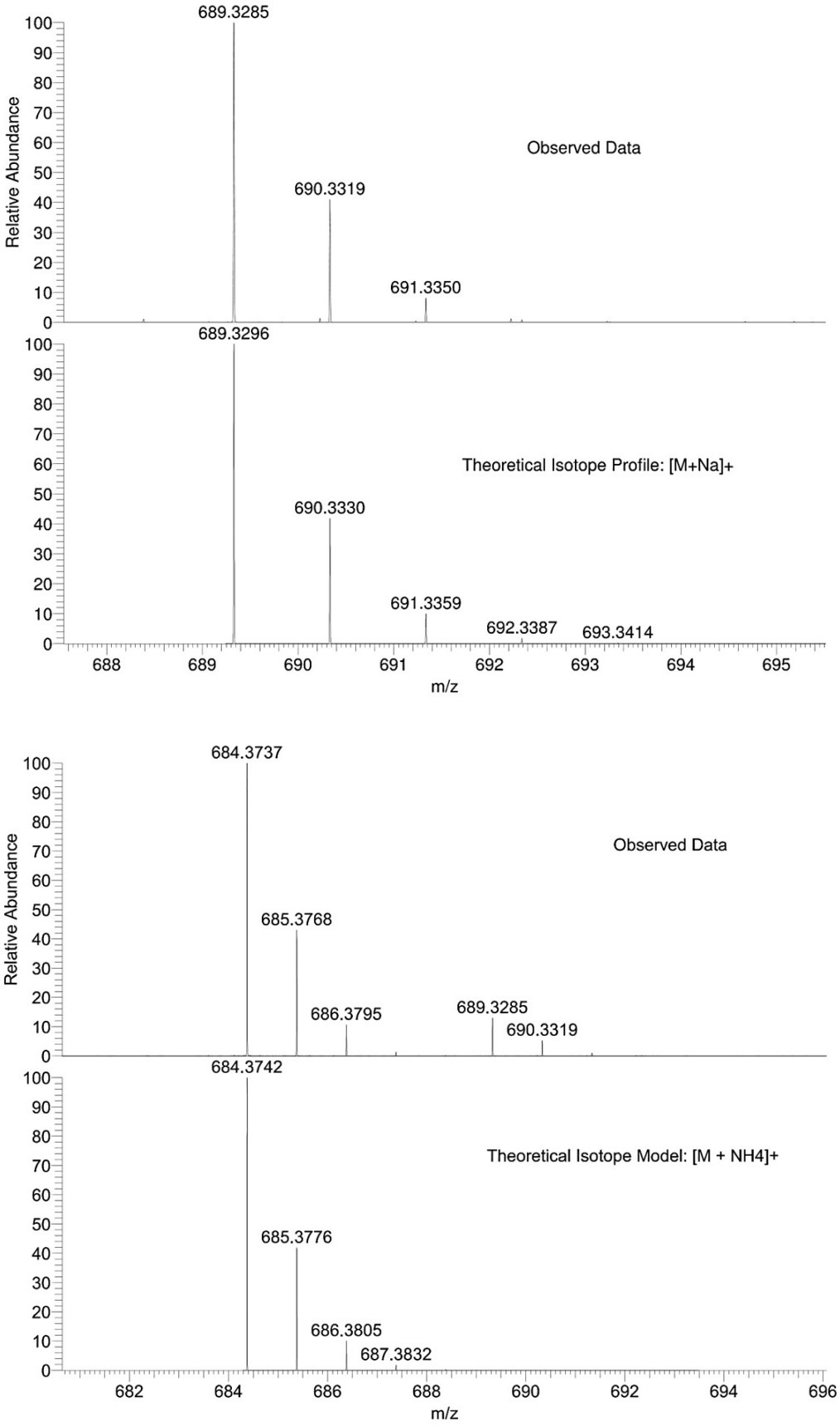




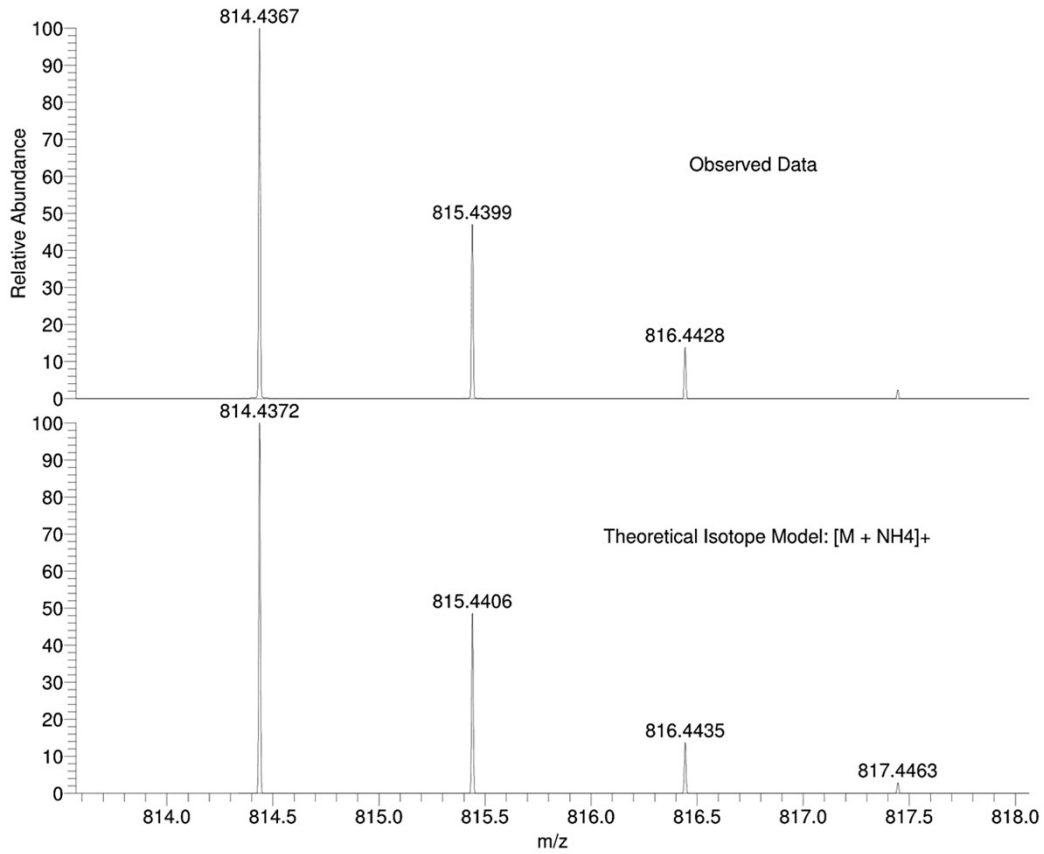
S67. Mass spectra data for monomer diol **M1** in the presence of NH_4^+ ions.



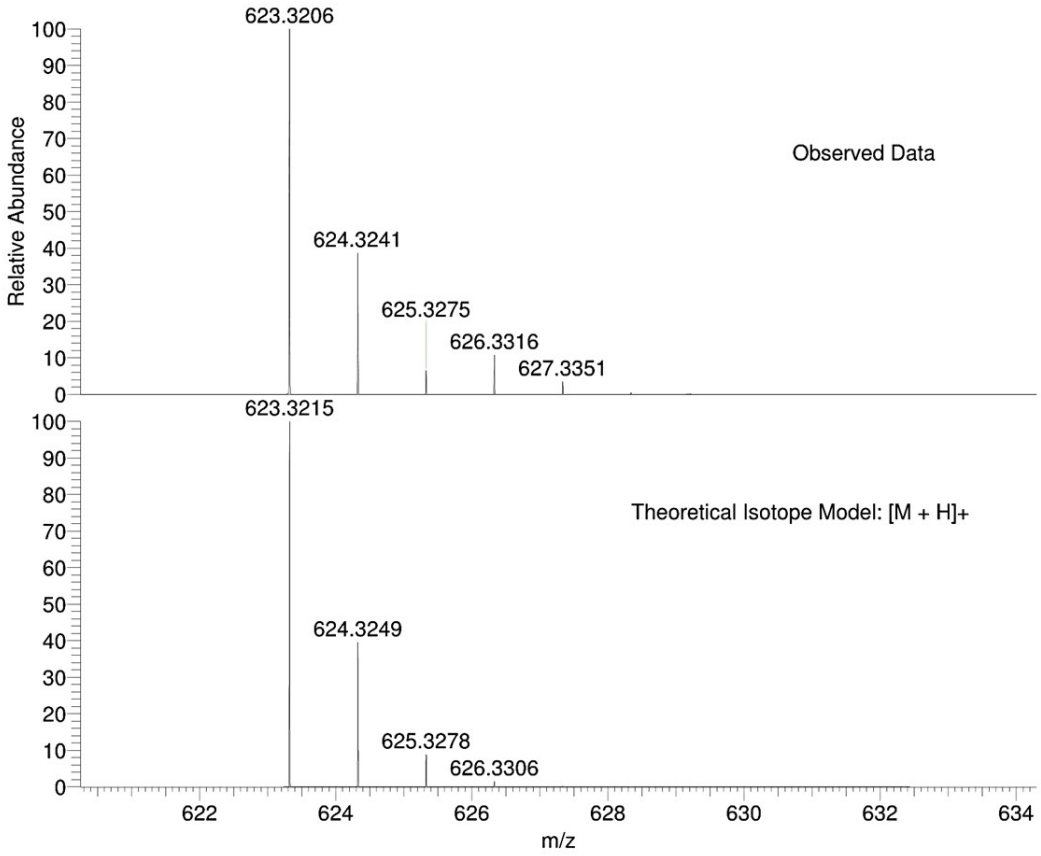
S68. Mass spectra data for **2**.



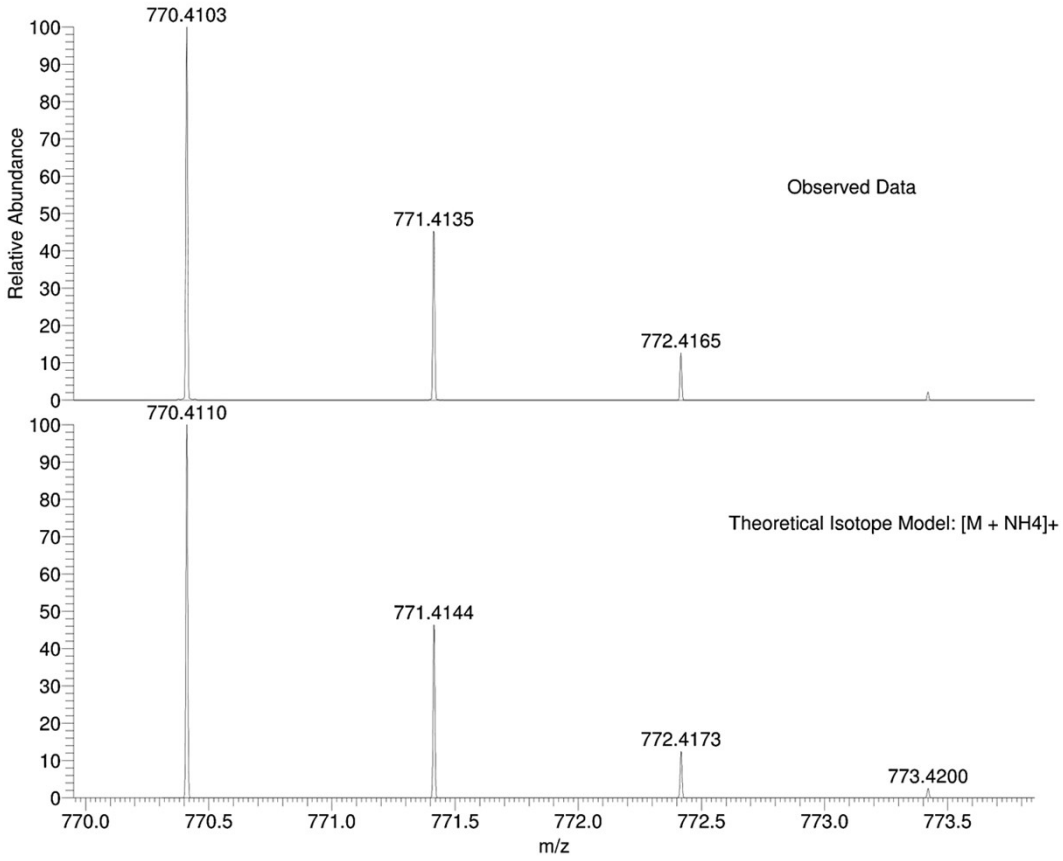
S69. Mass spectra data for monomer diol **M2** in the presence of Na^+ and NH_4^+ ions, respectively.



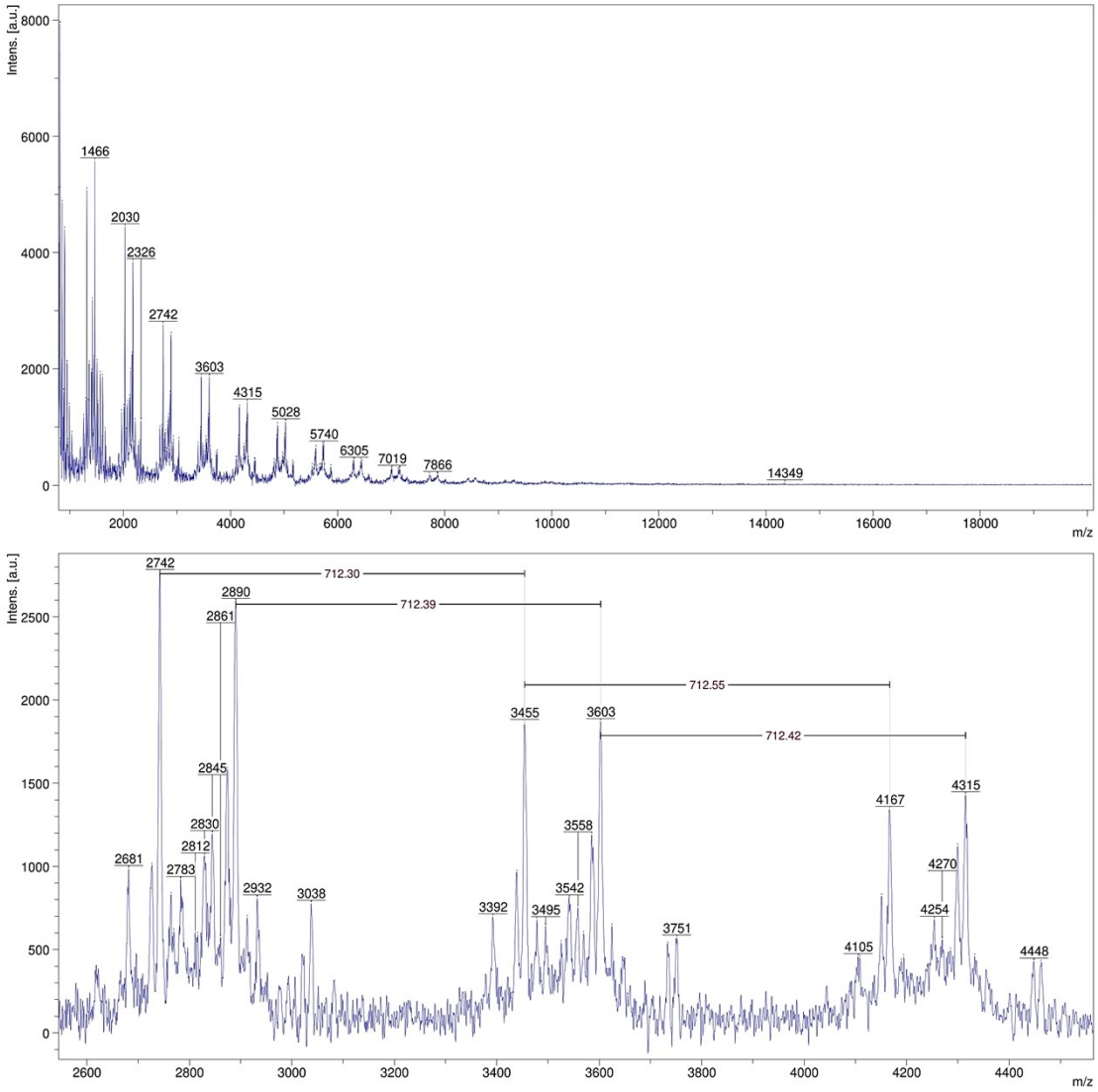
S70. Mass spectra data for monomer diol **M3** in the presence of NH_4^+ ions.



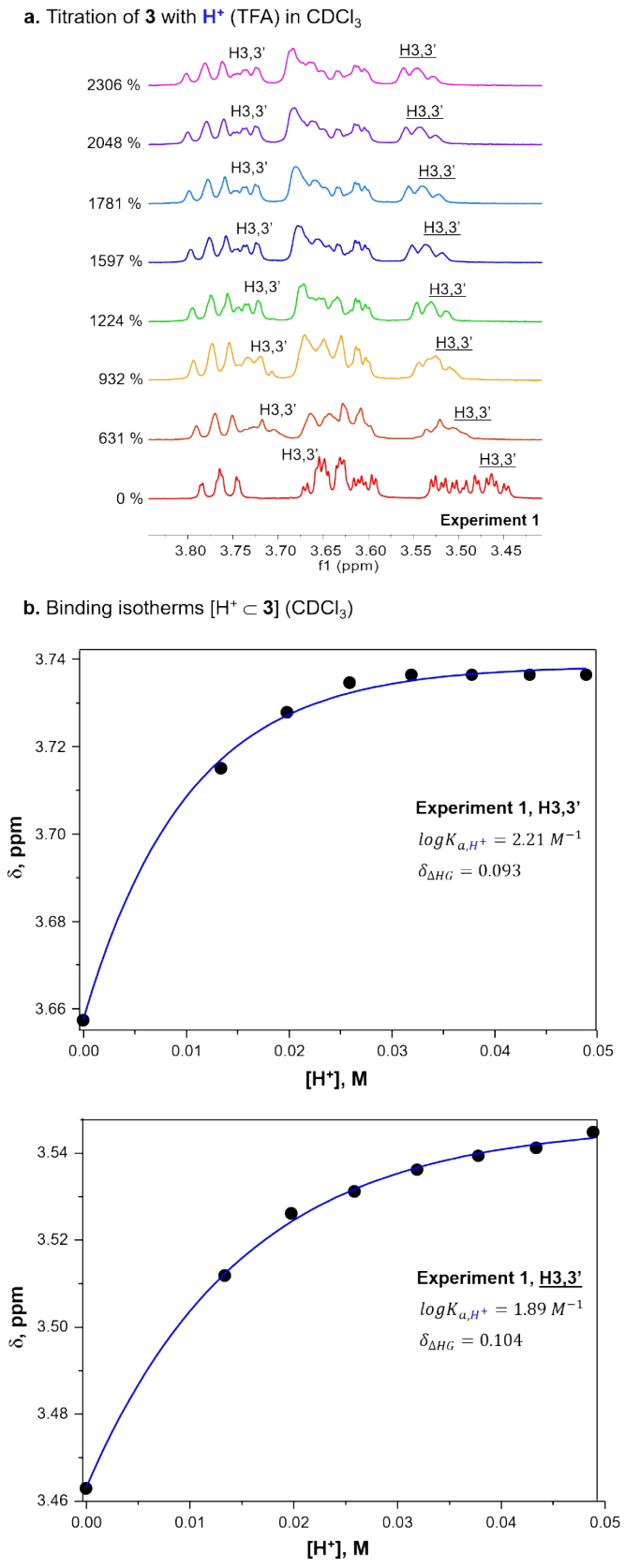
S71. Mass spectra data for side product **M4**.



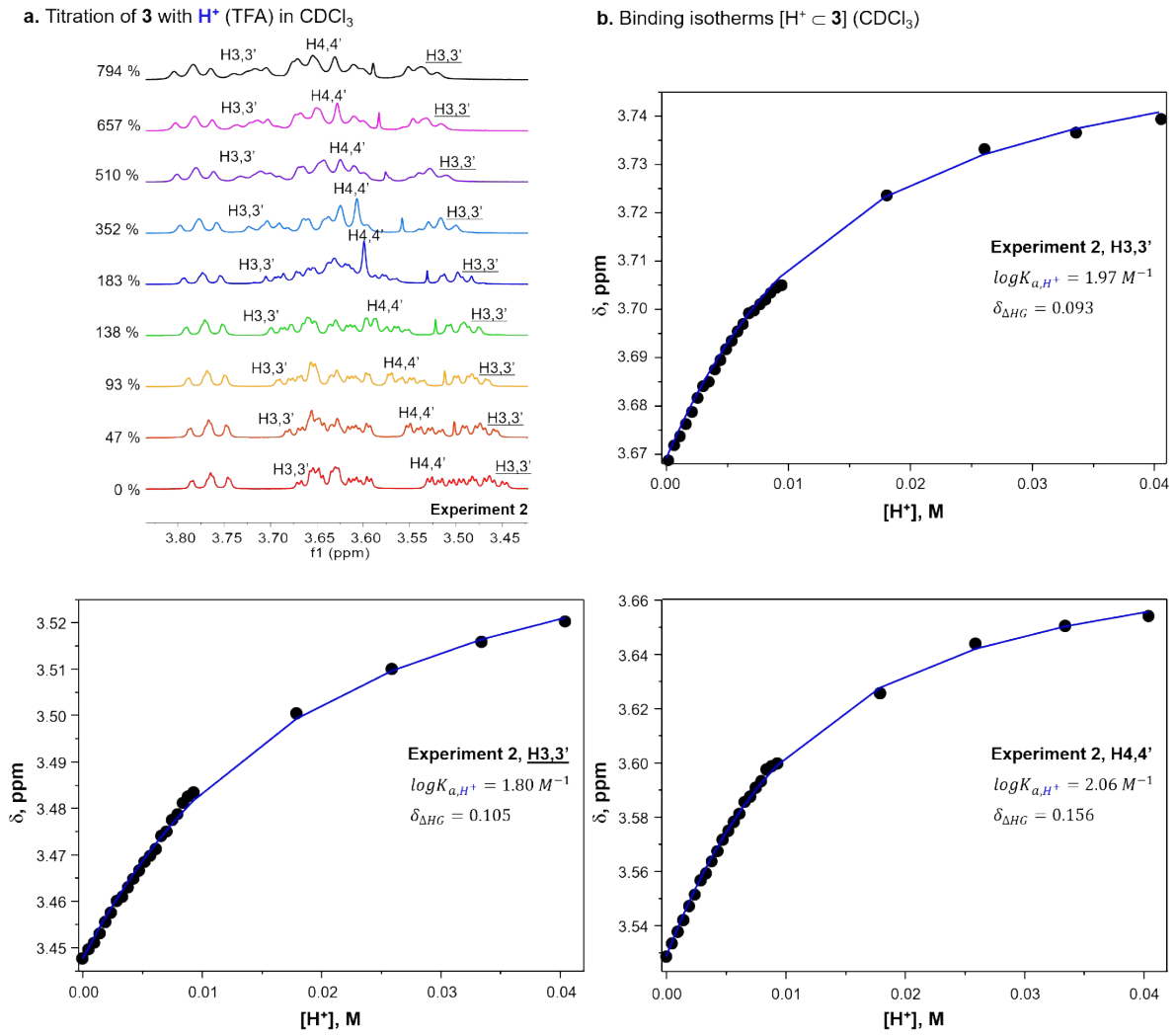
S72. Mass spectra data for side product **M5** in the presence of NH_4^+ ions.



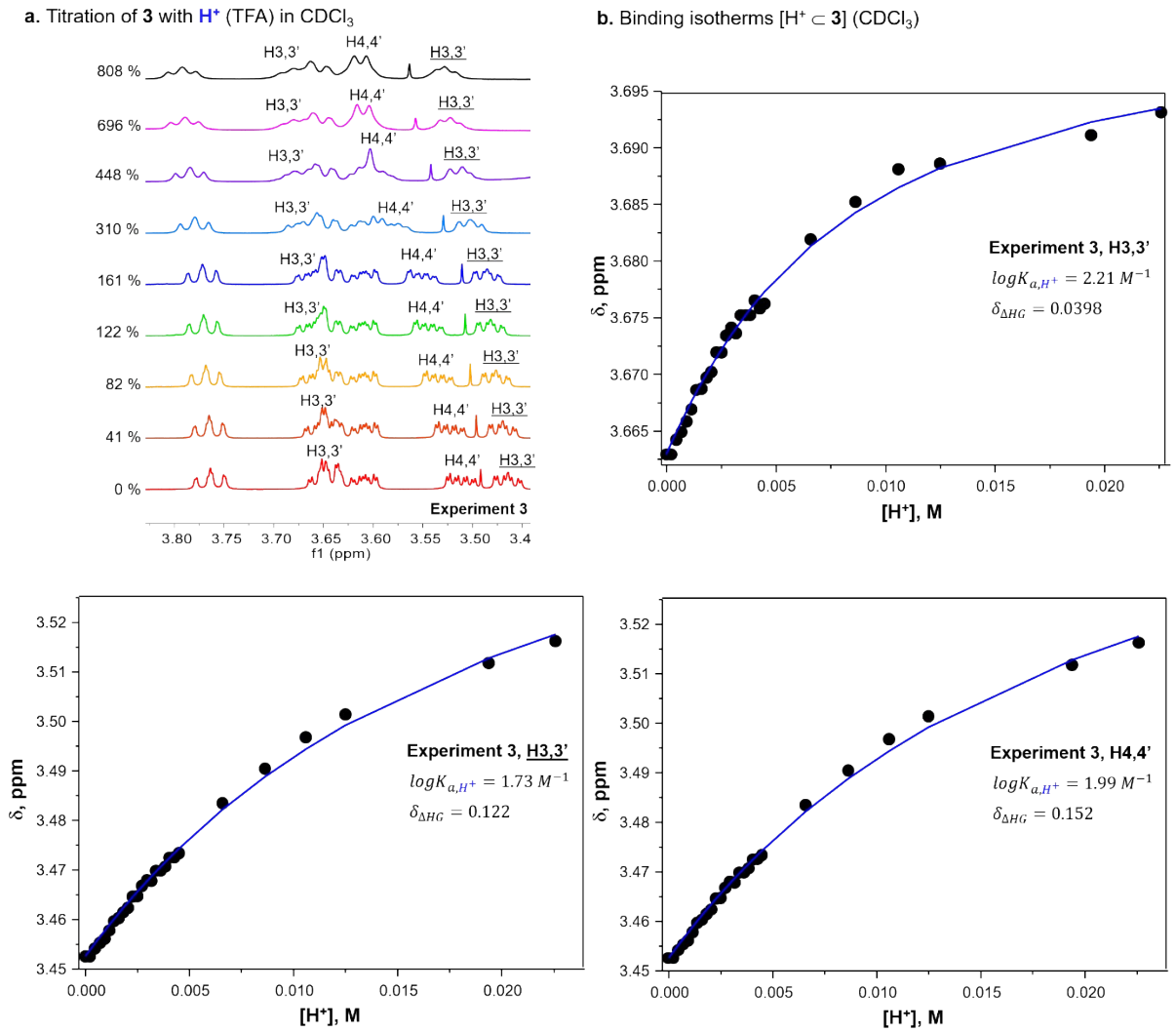
S73. MALDI-TOF data for polymer **PolyM1** in the presence of Na^+ ions.



S74. a) Partial ^{1}H NMR spectra (500 MHz, 298 K, $CDCl_3$) stack plot of **3** (2 mM) titration with TFA from 0 to 2306 mol % and b) Non-linear least-squares fit of the binding isotherms [H+⊂ **3**] based on H3,3' and H3,3', respectively.



S75. a) Partial ^{1}H NMR spectra (500 MHz, 298 K, $CDCl_3$) stack plot of **3** (5 mM) titration with TFA from 0 to 794 mol % and b) Non-linear least-squares fit of the binding isotherms [H+⊂ **3**] based on H3,3', H3,3' and H4,4', respectively.



S76. a) Partial ^{1}H NMR spectra (500 MHz, 298 K, $CDCl_3$) stack plot of **3** (3 mM) titration with TFA from 0 to 808 mol % and b) Non-linear least-squares fit of the binding isotherms [H+⊂ **3**] based on H3,3', H3,3' and H4,4', respectively.

Experiment	Proton	Scientist®[1]		Bindfit[2]	
		log K_a, M^{-1}	ΔG, $kJmol^{-1}$	log K_a, M^{-1}	ΔG, $kJmol^{-1}$
1	**H3,3'**	2.21	-12.6	2.05	-11.7
	H3,3'	1.89	-10.8		
2	**H3,3'**	1.97	-11.3	2.00	-11.4
	H3,3'	1.80	-10.3		
	H4,4'	2.06	-11.8		
3	**H3,3'**	2.21	-12.6	1.94	-11.1
	H3,3'	1.73	-9.9		
	H4,4'	1.99	-11.3		

[1]Micromath Scientist® and [2]Bindfit (http://app.supramolecular.org/bindfit/) are non-linear fitting software used to calculate the binding constant.

S77. Summary of binding constants log K_a and ΔG values determined by ^{1}H NMR titration experiments in $CDCl_3$ using appropriate non-linear fitting software.

Table 1 : Crystal data and structure refinement for M2.

Identification code	acb170005_fa
Empirical formula	$C_{34}H_{40}Cl_6O_{10}$
Formula weight	821.36
Temperature/K	150.0(2)
Crystal system	triclinic
Space group	P-1
a/Å	6.1698(2)
b/Å	8.7425(3)
c/Å	18.2846(4)
α/°	79.864(2)
β/°	83.699(2)
γ/°	80.021(3)
Volume/Å^3	952.98(5)
Z	1
ρ_{calc}g/cm^3	1.431
μ/mm^{-1}	4.571
F(000)	426.0
Crystal size/mm^3	0.34 × 0.08 × 0.06
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.862 to 133.572
Index ranges	$-7 \leq h \leq 7$, $-10 \leq k \leq 10$, $-21 \leq l \leq 21$
Reflections collected	32589
Independent reflections	3384 [R_{int} = 0.0339, R_{sigma} = 0.0141]
Data/restraints/parameters	3384/21/262
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0295, wR_2 = 0.0756
Final R indexes [all data]	R_1 = 0.0346, wR_2 = 0.0790
Largest diff. peak/hole / e Å^{-3}	0.23/-0.21

Table 1B Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for acb170005_fa. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	1077(4)	7227(2)	1966.5(13)	41.2(5)
Cl2	-1754(7)	4813(4)	2366(2)	53.7(5)
Cl3	-1603(4)	6647(4)	887.6(12)	50.5(4)
O1	11351.4(18)	6926.7(11)	5623.6(6)	27.0(2)
O2	7980.4(17)	6231.9(11)	5117.1(6)	30.4(2)
O3	6171.0(16)	7971.9(11)	4259.9(5)	25.0(2)
O4	4506(2)	8112.1(15)	2847.6(6)	37.8(3)
O5	13826.7(15)	9022.2(11)	5724.9(5)	21.1(2)
C1	10622(2)	8421.7(15)	5311.3(7)	20.8(3)
C2	8746(2)	8855.2(16)	4897.0(7)	20.2(3)
C3	11860(2)	9555.2(15)	5400.7(7)	19.4(3)
C4	7580(2)	7570.6(16)	4779.2(7)	22.1(3)
C5	5132(3)	6701.8(18)	4099.1(9)	29.5(3)
C6	3501(3)	7442(2)	3538.9(9)	33.5(4)
C7	13833(2)	8771.4(15)	6495.8(7)	21.1(3)
C8	15848(2)	8106.1(18)	6772.6(8)	28.7(3)
C9	16045(3)	7887.7(19)	7530.7(8)	31.4(3)
C10	14267(2)	8299.2(17)	8036.3(8)	26.9(3)
C11	12272(2)	8948.6(17)	7741.1(8)	26.6(3)
C12	12035(2)	9190.4(17)	6976.7(8)	24.7(3)
C13	14600(3)	8067(2)	8870.0(8)	32.0(4)
C14	15927(3)	9303(2)	9004.9(9)	37.8(4)
C15	15910(4)	6424(2)	9112.5(10)	50.7(5)
C16	12406(3)	8247(3)	9347.2(9)	58.4(6)
C17	-1418(3)	6651(2)	1849.1(10)	38.7(4)
Cl3A	-1726(11)	6412(9)	965(3)	96(2)
Cl2A	-1477(12)	4856(8)	2473(4)	82.3(19)
Cl1A	1147(11)	7182(7)	1919(4)	89(2)

Table 1C Anisotropic Displacement Parameters (Å^2×10^3) for acb170005_fa. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U_{11}+2hka*b*U_{12}+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	41.3(11)	36.2(8)	51.4(8)	-7.1(6)	-22.1(7)	-8.8(7)
Cl2	60.7(9)	36.3(9)	63.3(8)	-0.3(6)	1.4(6)	-17.3(7)
Cl3	53.6(8)	69.8(8)	30.9(5)	-12.1(5)	-14.3(5)	-6.3(7)
O1	30.3(6)	18.9(5)	32.5(6)	0.9(4)	-14.5(4)	-3.0(4)
O2	32.3(6)	22.2(5)	38.1(6)	-0.6(4)	-13.7(5)	-5.3(4)
O3	29.0(5)	25.4(5)	23.3(5)	-2.8(4)	-10.2(4)	-7.4(4)
O4	48.3(7)	40.6(6)	28.4(6)	-4.5(5)	-6.6(5)	-16.7(5)
O5	18.9(5)	26.1(5)	17.7(5)	-2.3(4)	-6.1(4)	-0.7(4)
C1	23.8(7)	20.4(6)	17.1(6)	-1.6(5)	-3.9(5)	-0.9(5)

C2	20.5(7)	23.3(7)	17.2(6)	-3.6(5)	-2.0(5)	-3.2(5)
C3	19.1(7)	23.7(7)	15.0(6)	-2.9(5)	-3.9(5)	-0.7(5)
C4	21.3(7)	23.9(7)	20.9(7)	-4.3(5)	-2.1(5)	-2.4(6)
C5	33.2(8)	28.4(7)	31.3(8)	-4.5(6)	-9.2(6)	-12.5(6)
C6	32.7(9)	42.3(9)	29.0(8)	-2.6(7)	-9.1(6)	-14.5(7)
C7	24.8(7)	21.1(6)	18.1(6)	-1.0(5)	-6.1(5)	-4.9(5)
C8	22.4(8)	39.3(8)	21.8(7)	-2.8(6)	-3.5(6)	0.9(6)
C9	23.0(8)	45.2(9)	24.1(7)	-0.2(6)	-9.1(6)	-1.1(6)
C10	29.4(8)	32.3(8)	20.1(7)	-0.4(6)	-5.5(6)	-9.7(6)
C11	25.0(8)	32.4(8)	22.5(7)	-4.1(6)	-1.0(6)	-5.8(6)
C12	21.0(7)	27.9(7)	24.5(7)	-1.5(6)	-6.1(5)	-2.2(6)
C13	33.4(9)	44.5(9)	20.0(7)	-0.9(6)	-6.2(6)	-12.6(7)
C14	42.9(10)	47.5(10)	27.0(8)	-9.0(7)	-7.6(7)	-12.2(8)
C15	82.1(15)	45.1(10)	26.0(9)	5.4(7)	-21.2(9)	-14(1)
C16	43.8(11)	116.5(19)	19.1(8)	-4.5(10)	0.6(7)	-32.3(12)
C17	41.6(10)	37.3(9)	38.0(9)	-5.6(7)	-5.2(7)	-8.1(7)
Cl3A	109(3)	106(3)	92(3)	-28(2)	-49(2)	-36(2)
Cl2A	76(3)	45(2)	100(4)	13.4(19)	34(2)	10.4(18)
Cl1A	79(4)	96(3)	109(4)	-29(3)	-28(3)	-36(3)

Table 1D Bond Lengths for acb170005_fa.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C17	1.746(3)	C5	C6	1.499(2)
Cl2	C17	1.748(4)	C7	C8	1.387(2)
Cl3	C17	1.775(3)	C7	C12	1.377(2)
O1	C1	1.3516(16)	C8	C9	1.382(2)
O2	C4	1.2211(17)	C9	C10	1.395(2)
O3	C4	1.3188(17)	C10	C11	1.387(2)
O3	C5	1.4607(17)	C10	C13	1.5338(19)
O4	C6	1.421(2)	C11	C12	1.396(2)
O5	C3	1.3803(16)	C13	C14	1.531(2)
O5	C7	1.3882(16)	C13	C15	1.538(3)
C1	C2	1.4129(19)	C13	C16	1.528(2)
C1	C3	1.3927(19)	C17	Cl3A	1.701(6)
C2	C3[1]	1.4021(19)	C17	Cl2A	1.774(7)
C2	C4	1.4912(19)	C17	Cl1A	1.749(6)
C3	C2[1]	1.4021(19)			

[1]2-X,2-Y,1-Z

Table 1E Bond Angles for acb170005_fa.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C4	O3	C5	115.79(11)	C9	C8	C7	119.63(14)
C3	O5	C7	119.57(10)	C8	C9	C10	122.15(14)
O1	C1	C2	123.53(12)	C9	C10	C13	119.80(13)
O1	C1	C3	116.36(12)	C11	C10	C9	116.69(13)
C3	C1	C2	120.10(12)	C11	C10	C13	123.49(14)
C1	C2	C4	117.42(12)	C10	C11	C12	122.23(14)
C3[1]	C2	C1	118.57(12)	C7	C12	C11	119.27(13)
C3[1]	C2	C4	123.97(12)	C10	C13	C15	109.78(13)
O5	C3	C1	116.92(11)	C14	C13	C10	108.83(12)
O5	C3	C2[1]	121.42(12)	C14	C13	C15	108.58(14)
C1	C3	C2[1]	121.31(12)	C16	C13	C10	111.99(13)
O2	C4	O3	122.76(12)	C16	C13	C14	108.45(15)
O2	C4	C2	122.16(12)	C16	C13	C15	109.14(16)
O3	C4	C2	115.00(11)	Cl1	C17	Cl2	113.03(16)
O3	C5	C6	106.47(12)	Cl1	C17	Cl3	109.24(16)
O4	C6	C5	113.15(13)	Cl2	C17	Cl3	110.24(18)
C8	C7	O5	115.43(12)	Cl3A	C17	Cl2A	110.7(3)
C12	C7	O5	124.50(12)	Cl3A	C17	Cl1A	111.7(3)
C12	C7	C8	120.02(13)	Cl1A	C17	Cl2A	105.3(3)

[1]2-X,2-Y,1-Z

Table 1F Hydrogen Bonds for acb170005_fa.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1	H1	O2	0.81(2)	1.84(2)	2.5712(14)	149.7(19)

Table 1G Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for acb170005_fa.

Atom	*x*	*y*	*z*	U(eq)
H1	10480(30)	6390(20)	5542(11)	41
H4	4860(40)	9020(30)	2892(12)	57
H5A	4388	6200	4550	35
H5B	6230	5915	3898	35
H6A	2677	6651	3452	40
H6B	2461	8256	3743	40
H8	17059	7809	6450	34
H9	17408	7452	7710	38
H11	11052	9233	8063	32
H12	10677	9630	6794	30
H14A	17308	9211	8705	57

H14B	16201	9138	9522	57
H14C	15104	10335	8872	57
H15A	15192	5641	8972	76
H15B	15976	6239	9644	76
H15C	17381	6365	8873	76
H16A	11633	9298	9225	88
H16B	12681	8044	9865	88
H16C	11525	7510	9252	88
H17	-2623	7433	2016	46
H17A	-2602	7457	2008	46

Table 1H Atomic Occupancy for acb170005_fa.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
Cl1	0.6372	Cl2	0.6372	Cl3	0.6372
H17	0.6372	H17A	0.3628	Cl3A	0.3628
Cl2A	0.3628	Cl1A	0.3628		

Table 2 : Crystal data and structure refinement for 2.

Identification code	acb160036
Empirical formula	$C_{34}H_{42}O_8$
Formula weight	578.67
Temperature/K	150.0(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	5.9780(3)
b/Å	10.5544(4)
c/Å	25.1034(10)
α/°	90
β/°	92.057(4)
γ/°	90
Volume/Å^3	1582.85(13)
Z	2
ρ_{calc}g/cm^3	1.214
μ/mm^{-1}	0.697
F(000)	620.0
Crystal size/mm^3	0.18 × 0.14 × 0.12
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.048 to 133.792
Index ranges	$-7 \leq h \leq 6$, $-11 \leq k \leq 12$, $-29 \leq l \leq 24$
Reflections collected	14110
Independent reflections	2806 [R_{int} = 0.0384, R_{sigma} = 0.0259]
Data/restraints/parameters	2806/0/195
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0392, wR_2 = 0.0958
Final R indexes [all data]	R_1 = 0.0487, wR_2 = 0.1039
Largest diff. peak/hole / e Å^{-3}	0.29/-0.25

Table 2A Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement

Parameters ($Å^2×10^3$) for acb160036. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	7521.5(17)	4387.5(9)	4133.1(4)	29.7(2)
O2	7300(2)	1769.9(11)	4878.2(6)	57.7(4)
O3	4100.5(19)	1965.4(9)	4395.2(4)	35.5(3)
O4	3049.7(17)	3078.5(9)	5571.6(4)	29.7(2)
C1	6293(2)	4694.5(13)	4565.1(5)	24.8(3)
C2	5341(2)	3740.1(12)	4866.3(5)	25.1(3)
C3	4070(2)	4044.6(12)	5298.6(5)	24.7(3)
C4	9886(3)	4299.5(19)	4257.5(7)	44.2(4)
C5	5731(2)	2377.6(13)	4719.8(5)	28.8(3)
C6	4281(3)	657.8(14)	4206.0(7)	42.3(4)
C7	2102(4)	318.6(19)	3947.3(10)	65.3(6)
C8	3882(2)	2805.7(12)	6085.4(5)	25.0(3)
C9	2542(3)	2057.5(15)	6389.4(6)	35.5(4)
C10	3268(3)	1721.1(15)	6900.4(6)	36.5(4)
C11	5309(2)	2116.0(13)	7122.1(5)	26.8(3)
C12	6616(3)	2855.5(15)	6801.5(6)	33.7(3)
C13	5933(3)	3198.6(15)	6286.3(6)	33.9(3)
C14	6089(3)	1717.8(14)	7688.4(6)	31.4(3)
C15	7351(3)	455.1(15)	7656.7(7)	39.4(4)
C16	4098(3)	1544(2)	8045.7(6)	47.8(5)
C17	7651(3)	2708.8(17)	7946.1(7)	46.3(4)

Table 2B Anisotropic Displacement Parameters ($Å^2×10^3$) for acb160036. The Anisotropic displacement factor exponent takes the form: -$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	31.3(5)	36.7(5)	21.0(5)	-4.8(4)	0.7(4)	-3.1(4)
O2	53.8(8)	33.8(6)	83.4(10)	-8.8(6)	-27.5(7)	9.0(6)
O3	45.3(6)	24.1(5)	36.3(6)	-7.4(4)	-9.3(5)	-0.9(4)
O4	38.3(6)	28.4(5)	22.1(5)	4.2(4)	-4.2(4)	-12.4(4)
C1	27.4(7)	29.3(7)	17.4(6)	-1.3(5)	-3.0(5)	-3.8(5)
C2	28.4(7)	23.9(7)	22.6(6)	-0.7(5)	-5.6(5)	-3.2(5)
C3	29.2(7)	24.3(6)	20.2(6)	2.9(5)	-4.0(5)	-6.3(5)
C4	30.8(8)	63.1(11)	38.8(8)	-11.4(8)	3.6(7)	-7.9(7)
C5	34.1(8)	25.0(7)	27.1(7)	0.5(6)	-1.6(6)	-3.4(6)
C6	62.5(11)	22.4(7)	41.6(9)	-8.1(6)	-4.4(8)	-2.7(7)
C7	70.4(14)	42.9(10)	81.7(15)	-25.1(10)	-9.9(12)	-14(1)
C8	32.1(7)	21.8(6)	21.0(6)	0.1(5)	0.0(5)	-0.8(5)
C9	33.4(8)	43.2(9)	29.6(7)	5.8(6)	-4.3(6)	-15.6(7)
C10	38.1(9)	43.3(9)	28.3(7)	10.0(6)	1.2(6)	-14.6(7)
C11	31.2(7)	25.0(7)	24.2(7)	1.6(5)	1.2(6)	3.4(6)

C12	28.3(8)	41.5(8)	30.9(7)	4.8(6)	-4.0(6)	-6.4(6)
C13	31.7(8)	39.6(8)	30.3(7)	9.7(6)	1.9(6)	-10.6(6)
C14	34.8(8)	32.7(7)	26.4(7)	5.0(6)	-2.2(6)	3.6(6)
C15	43.4(9)	36.9(8)	37.7(8)	7.3(7)	-2.7(7)	6.2(7)
C16	42.8(10)	75.1(13)	25.4(8)	12.6(8)	2.2(7)	10.1(9)
C17	63.0(12)	42.1(9)	32.6(8)	3.5(7)	-15.1(8)	-3.9(8)

Table 2C Bond Lengths for acb160036.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.3704(17)	C6	C7	1.479(3)
O1	C4	1.439(2)	C8	C9	1.375(2)
O2	C5	1.1927(19)	C8	C13	1.373(2)
O3	C5	1.3214(17)	C9	C10	1.386(2)
O3	C6	1.4648(18)	C10	C11	1.387(2)
O4	C3	1.3824(16)	C11	C12	1.383(2)
O4	C8	1.3958(16)	C11	C14	1.5386(19)
C1	C2	1.3931(19)	C12	C13	1.390(2)
C1	C3[1]	1.393(2)	C14	C15	1.535(2)
C2	C3	1.385(2)	C14	C16	1.527(2)
C2	C5	1.505(2)	C14	C17	1.530(2)
C3	C1[1]	1.393(2)			

[1]1-X,1-Y,1-Z

Table 2D Bond Angles for acb160036.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C4	113.18(11)	C9	C8	O4	115.84(12)
C5	O3	C6	116.66(12)	C13	C8	O4	124.12(12)
C3	O4	C8	117.47(10)	C13	C8	C9	120.00(13)
O1	C1	C2	119.97(12)	C8	C9	C10	119.44(14)
O1	C1	C3[1]	120.85(12)	C9	C10	C11	122.43(14)
C3[1]	C1	C2	119.17(13)	C10	C11	C14	121.44(13)
C1	C2	C5	119.25(12)	C12	C11	C10	116.31(13)
C3	C2	C1	120.25(13)	C12	C11	C14	122.23(13)
C3	C2	C5	120.50(12)	C11	C12	C13	122.37(13)
O4	C3	C1[1]	120.51(12)	C8	C13	C12	119.44(13)
O4	C3	C2	118.78(12)	C15	C14	C11	108.80(12)
C2	C3	C1[1]	120.58(12)	C16	C14	C11	111.03(12)
O2	C5	O3	125.62(14)	C16	C14	C15	108.73(13)
O2	C5	C2	124.01(13)	C16	C14	C17	108.10(14)
O3	C5	C2	110.37(12)	C17	C14	C11	111.34(12)
O3	C6	C7	107.25(15)	C17	C14	C15	108.77(13)

[1]1-X,1-Y,1-Z

Table 2E Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters

(Å²×10³) for acb160036.

Atom	*x*	*y*	*z*	U(eq)
H4A	10666	4133	3937	66
H4B	10161	3623	4507	66
H4C	10407	5084	4411	66
H6A	4623	93	4503	51
H6B	5465	589	3953	51
H7A	1733	920	3671	98
H7B	963	330	4207	98
H7C	2195	-514	3796	98
H9	1161	1780	6253	43
H10	2353	1212	7102	44
H12	8001	3133	6935	40
H13	6858	3690	6079	41
H15A	6374	-179	7503	59
H15B	7843	197	8008	59
H15C	8625	558	7439	59
H16A	3223	2307	8045	72
H16B	4630	1361	8403	72
H16C	3188	854	7914	72
H17A	8982	2776	7745	69
H17B	8045	2457	8305	69
H17C	6906	3514	7950	69