Supplementary Information

Proximally *meso-meso* Linked Calix[4]pyrroles: Synthesis and Anion Binding Properties

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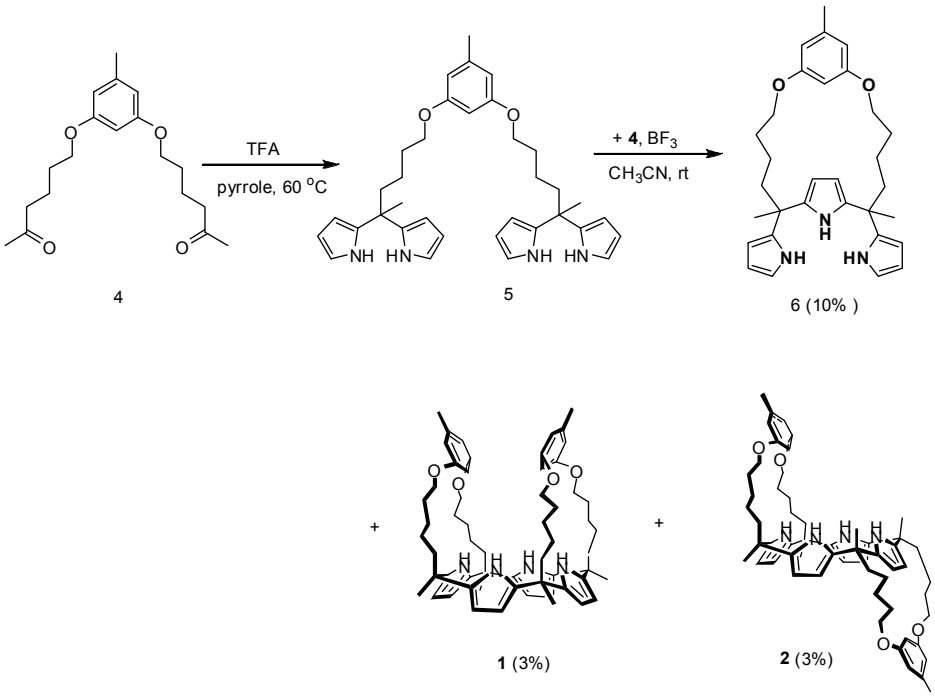
Synthetic schemes:



Experimental Section

General

^{1}H NMR spectra were recorded on a 400 and 300 MHz Bruker NMR spectrometer using TMS as the internal standard. Chemical shifts are reported in parts per million (ppm). When peak multiplicities are given, the following abbreviations are used: s, singlet; brs, broad singlet; d, doublet; t, triplet; m, multiplet. ^{13}C NMR spectra were proton decoupled and recorded on a 100 MHz Bruker spectrometer using TMS as the internal standard. Fluorescence spectra were recorded using LS-55B (Perkin Elmer) model spectrometer. Pyrrole was distilled at atmospheric pressure from CaH_2. All other chemicals and solvents were purchased from commercial sources and were used as such, unless otherwise mentioned. Column chromatography was performed over silica gel (Merck, 230-400 mesh). All titrations (UV-vis and fluorescence) were performed using HPLC grade CH_3CN purchased from Aldrich. Compound **4** and **5** were synthesized using our previously reported procedure.[8b]

Synthetic procedures

Doubly ether strapped calix[4]pyrrole (1) and (2)

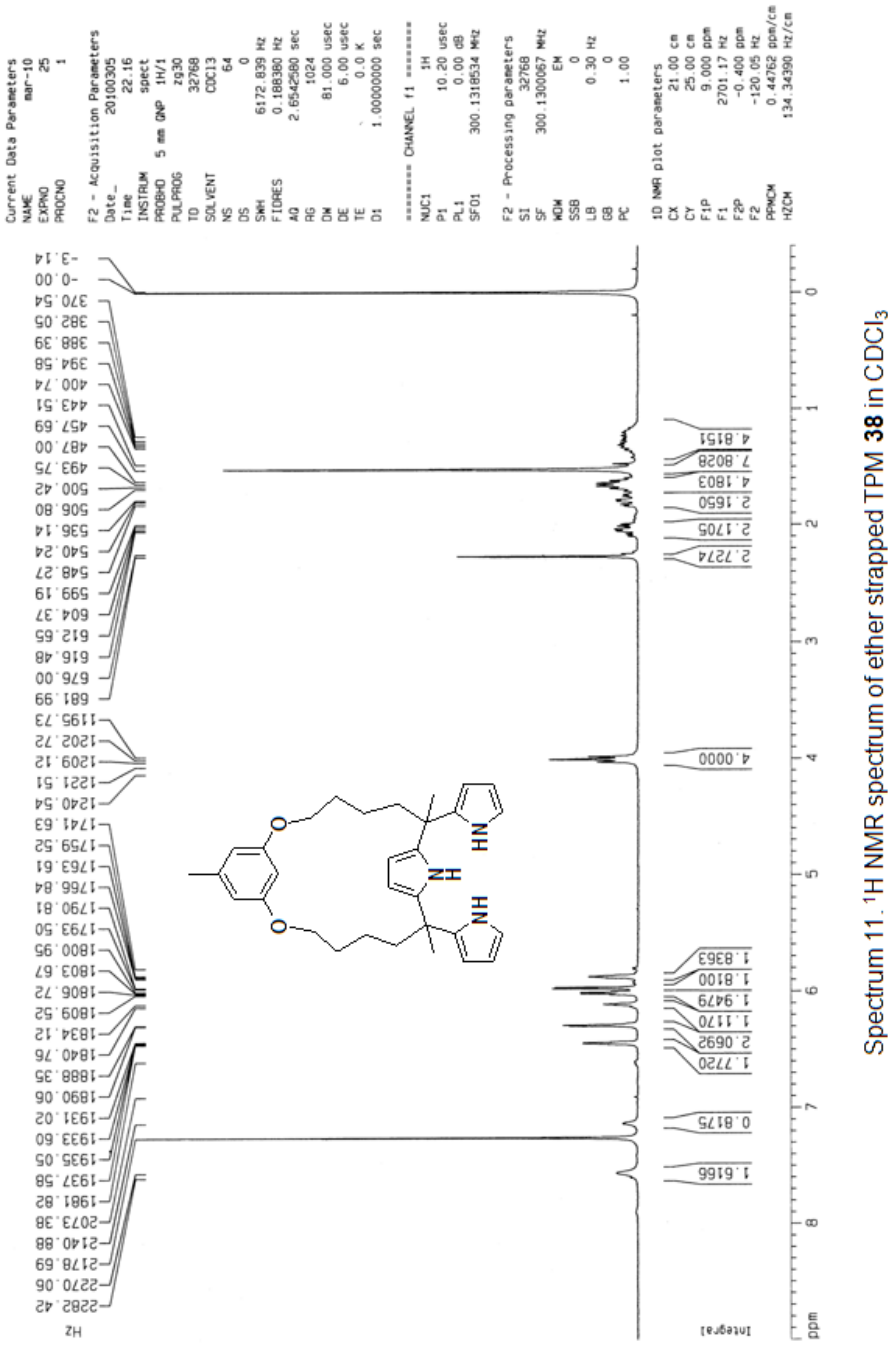
To the mixture of **5** (0.5 g, 0.9 mmol) and **4** (0.5 g, 0.9 mmol) in CH_3CN (150 mL) was added $BF_3.OEt_2$ (0.017 mL. 0.14 mmol). The whole mixture was stirred for 12 hr at room temperature and combined with aqueous NaOH (0.1 N, 30 mL). Then, the mixture was extracted with CH_2Cl_2 (50 mL × 3) and the organic layer was dried over anhydrous Na_2SO_4. Solvent was then removed in vacuo and the rmaining brown solid was purified by column chromatography on silica gel ($CHCl_3$/ EtOAc = 20/1). The three compounds **1**, **2** and **6** were cleanly separated and each fraction was recrystalized from ethyl acetate/acetonitrile.

Compound 1: Yield 0.025 g (3%); mp 151 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.67 (br s, 2H, NH), 7.08 (br s, 2H, NH), 6.30 (d, J = 1.73 Hz, 4H, Ar-H), 5.96 (s, 2H, Ar-H), 5.83-5.80 (m, 8H, pyrrole-H), 4.26-4.20 (m, 4H, CH_2), 4.10-4.03 (m, 4H, CH_2), 2.27 (s, 6H, CH_3), 2.02-1.94 (m, 4H, CH_2), 1.79-1.70 (m, 4H, CH_2), 1.64-1.58 (m, 8H, CH_2), 1.55 (s, 12H, CH_3), 1.35-1.28 (m, 8H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 140.7, 138.5, 137.5, 107.7, 104.2, 102.9, 68.1, 53.4, 41.1, 38.7, 27.1, 23.9, 21.9, 21.8; UV-Vis. λ_{max} (ε x 10^3), 241 (1.40), 275 (0.44), 282 (0.41); IR (cm^{-1}, neat) 3427, 3105, 2934, 2867, 1589; MALDI-TOF MS calcd. for $C_{54}H_{70}N_4O_4$ exact mass 837.14, found 837.52 (M^+), 839.52 ($M+2H^+$).

Compound 2: Yield 0.023 g (3%); %); mp 240 ^oC (decomp); ^1H NMR (400 MHz, $CDCl_3$) δ 6.99 (br s, 2H, NH), 6.82 (br s, 2H, NH), 6.28 (d, J = 1.57 Hz, 4H, Ar-H), 6.00 (s, 2H, Ar-H) 5.87-5.83 (m, 8H, pyrrole-H), 4.02-3.91 (m, 8H, CH_2), 2.23 (s, 6H, CH_3), 1.99-1.91 (m, 4H, CH_2), 1.77-1.60 (m, 12H, CH_2), 1.49 (s, 12H, CH_3), 1.36-1.25 (m, 4H, CH_2), 1.01-0.980 (m, 4H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 140.7, 138.5, 136.4, 109.7, 104.7, 102.7, 94.2, 67.0, 40.2, 38.7, 28.4, 25.3, 21.5, 20.0; UV-Vis. λ_{max} (ε x 10^3), 242 (1.40), 275 (0.34), 282 (0.31); IR (cm^{-1}, neat) 3438, 3377, 2937, 2866, 1590; MALDI-TOF MS calcd. for $C_{54}H_{70}N_4O_4$ exact mass 837.14, found 837.59 (M^+), 869.57 ($M+Na^+$).

Compound 6: Yield 0.059 g (10%); ^1H NMR (300 MHz, $CDCl_3$) δ 7.56 (br s, 2H, NH), 7.13 (br s, 1H, NH), 6.46-6.43 (m, 2H, pyrrole-H), 6.30-6.29 (m, 2H, Ar-H) 6.13-6.11 (m, 1H, Ar-H), 6.03-6.00 (m, 2H, pyrrole-H), 5.97 (d, J = 2.69 Hz, 2H, pyrrole-H), 5.89-5.86 (m, 2H, pyrrole-H), 4.01 (t, J = 6.70 Hz, 4H, CH_2), 2.27 (s, 3H, CH_3), 2.08-2.00 (m, 2H, CH_2), 1.83-1.74 (m, 2H, CH_2), 1.71-1.62 (m, 4H, CH_2), 1.52 (s, 6H, CH_3), 1.34-1.21 (m, 4H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 140.7, 138.4, 136.7, 116.6, 108.8, 107.9, 104.7, 104.0, 97.1, 67.3, 41.0, 39.3, 28.5, 25.9, 21.7, 21.1; UV-Vis. λ_{max} (ε x 10^3), 242 (1.1), 275 (0.26), 282 (0.25); MALDI-TOF MS calcd. for $C_{31}H_{39}N_3O_2$ exact mass 485.66, found 486.33 ($M+H^+$), 508.32 ($M+Na^+$).

Figure S1 300 MHz ^{1}H NMR spectrum of compound **6** in $CDCl_3$.



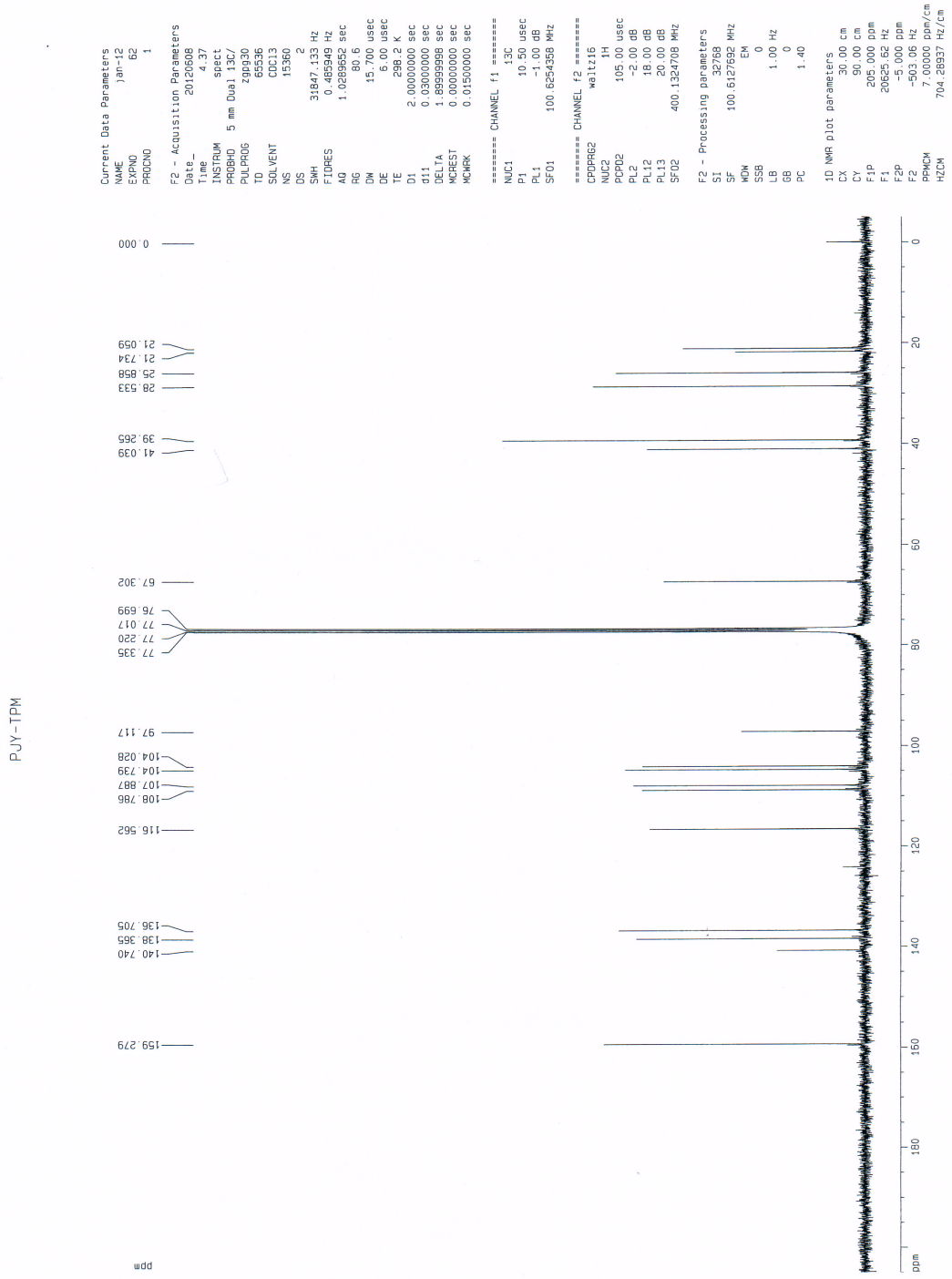

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Figure S2. MALDI-TOF spectrum of compound **6**.

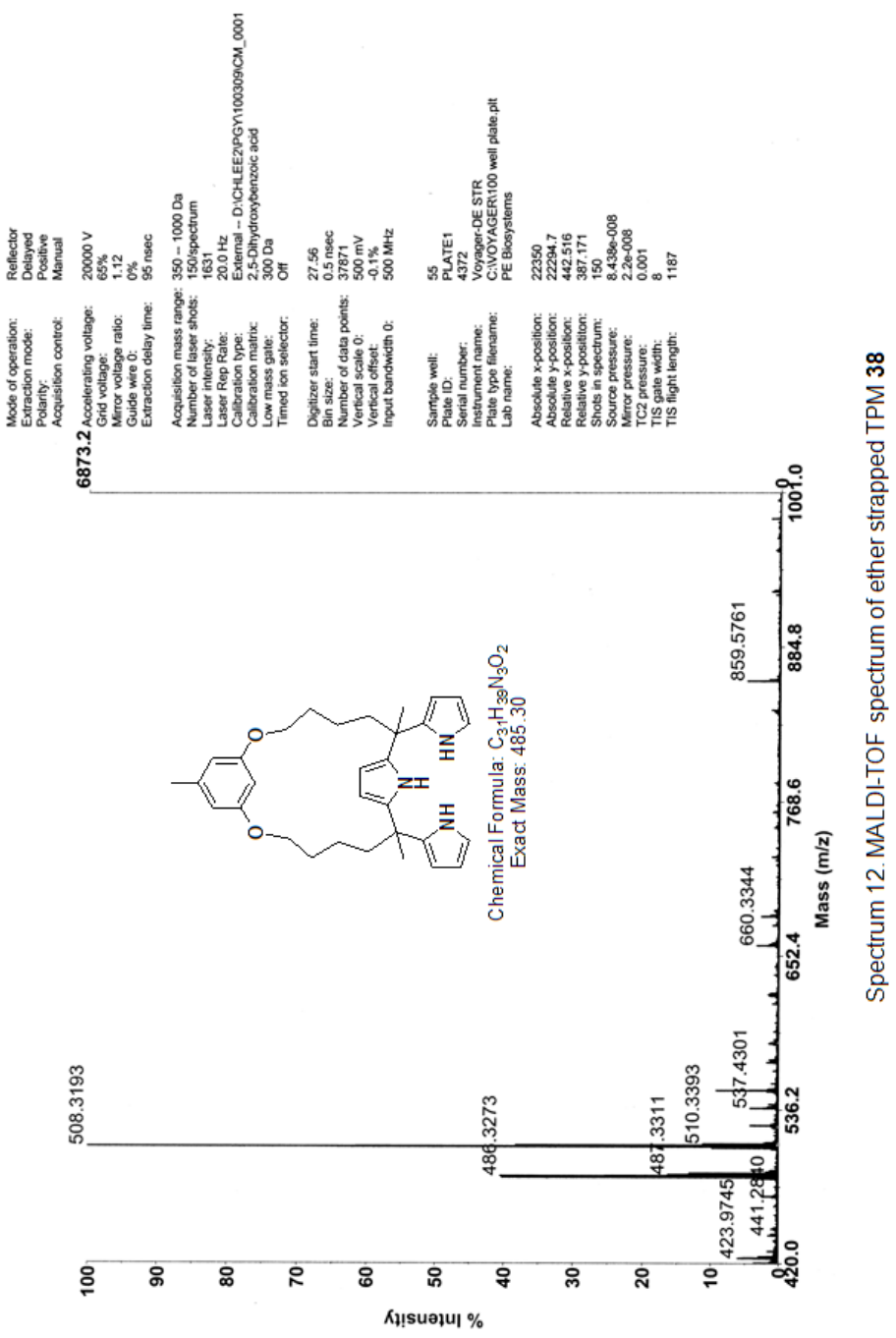


Figure S3. 300 MHz ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

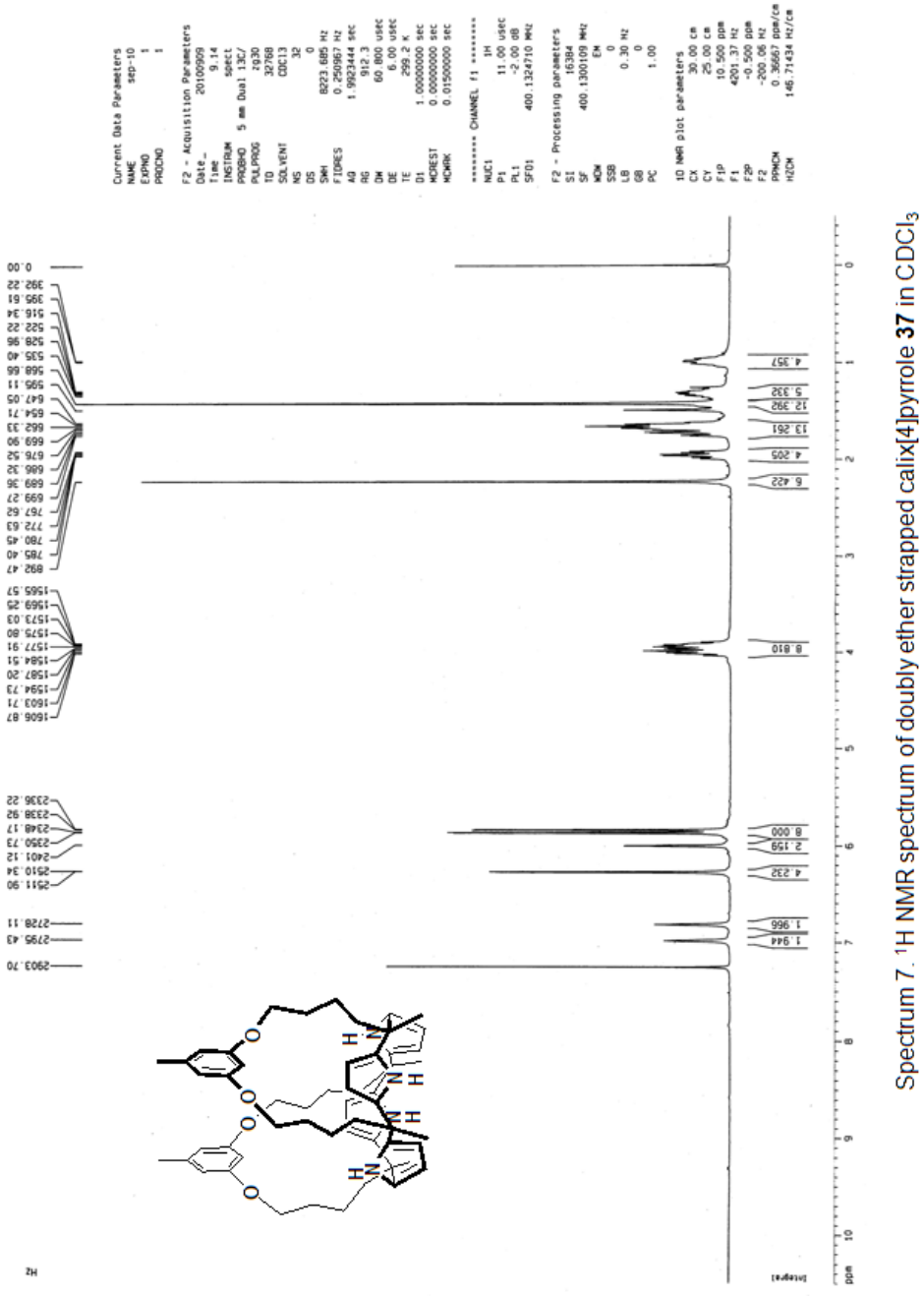


Figure S4. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

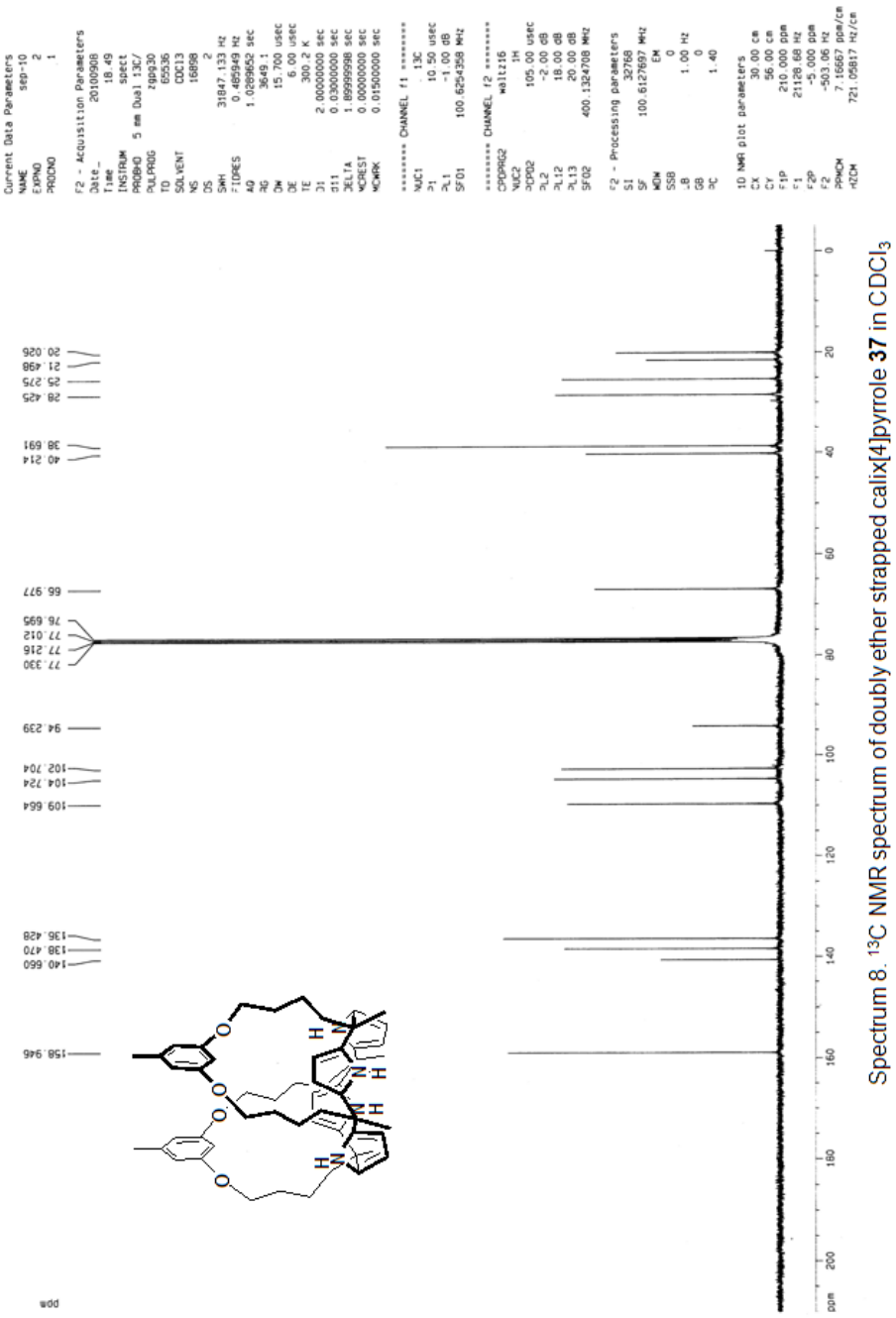
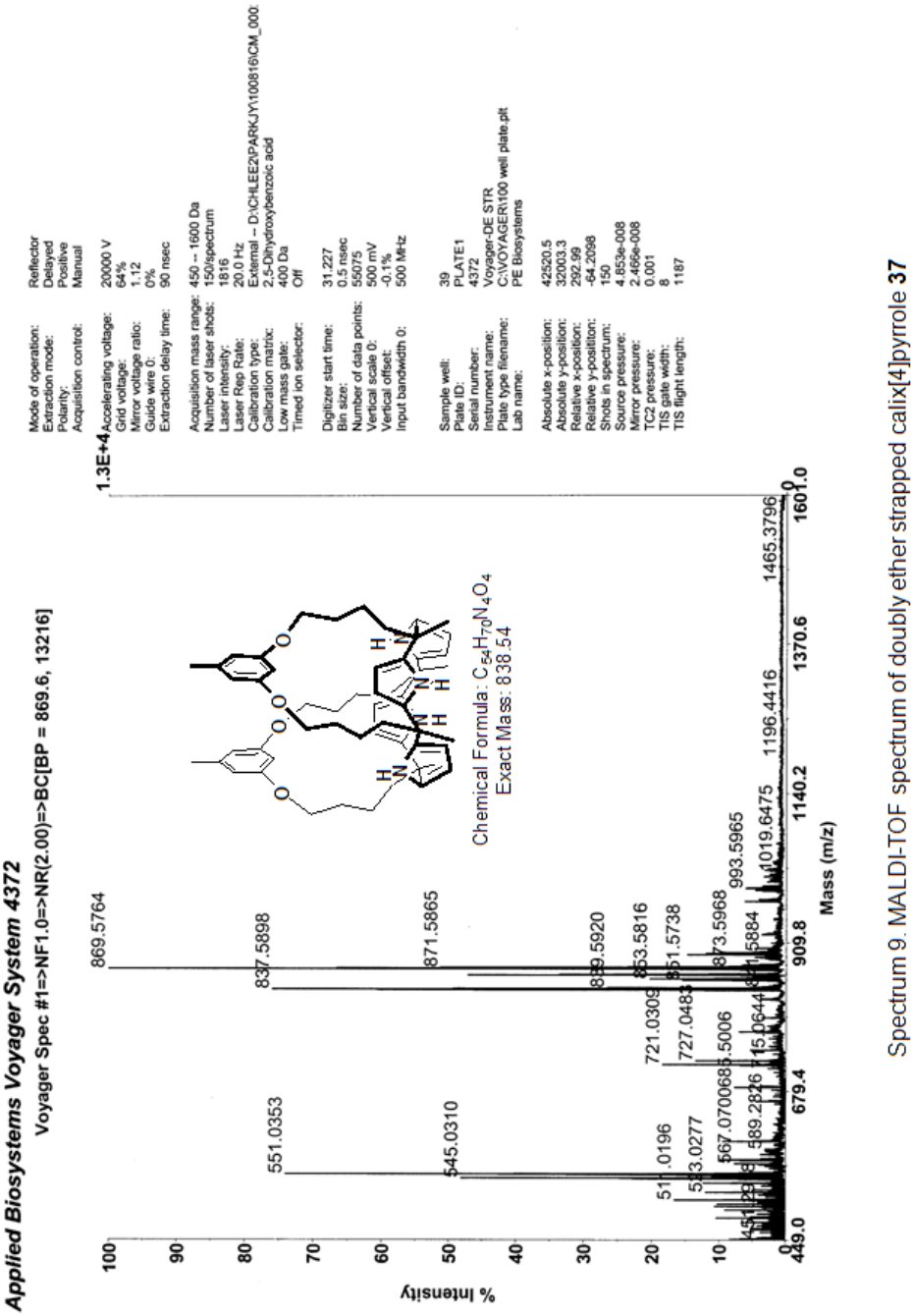


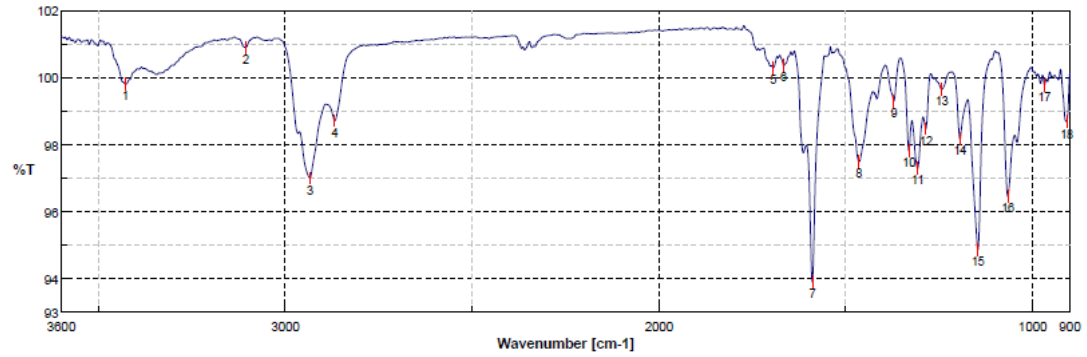
Figure S5. MALDI-TOF mass spectrum of compound **1**.



Spectrum 9. MALDI-TOF spectrum of doubly ether strapped calix[4]pyrrole **37**

Figure S6. IR spectra of compound 1 (a) and 2 (b).

(a)



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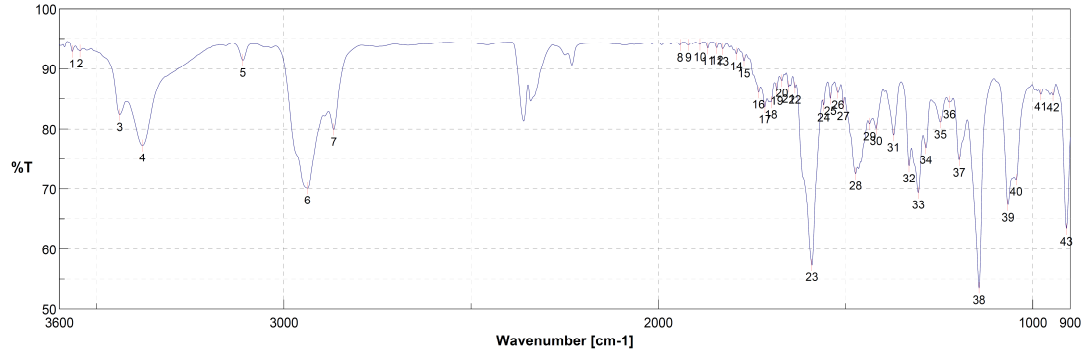
(b)



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11	1867.72	93.4009	12	1843.61	93.4681	13	1828.19	93.2917	14	1791.55	92.4586	15	1771.3	91.308
16	1732.73	86.1169	17	1715.37	83.6405	18	1698.98	84.4458	19	1683.55	86.7182	20	1670.05	88.038
21	1652.7	87.0611	22	1635.34	86.9044	23	1590.02	57.3752	24	1558.2	83.9431	25	1540.85	85.0397
26	1520.6	86.041	27	1506.13	84.1709	28	1473.35	72.5934	29	1435.74	80.8464	30	1418.39	80.062
31	1372.1	79.0078	32	1330.64	73.8342	33	1305.57	69.3516	34	1285.32	76.879	35	1246.75	81.1543
36	1222.65	84.4589	37	1196.61	74.8246	38	1143.58	53.4786	39	1066.44	67.268	40	1044.26	71.5776
41	978.697	85.7569	42	945.913	85.6051	43	910.236	63.3258						

Figure S7. UV-vis absorption spectra of compound **1** (dash) and **2** (line) in $CHCl_3$. [1] = [2] = 4.0×10^{-4} M.

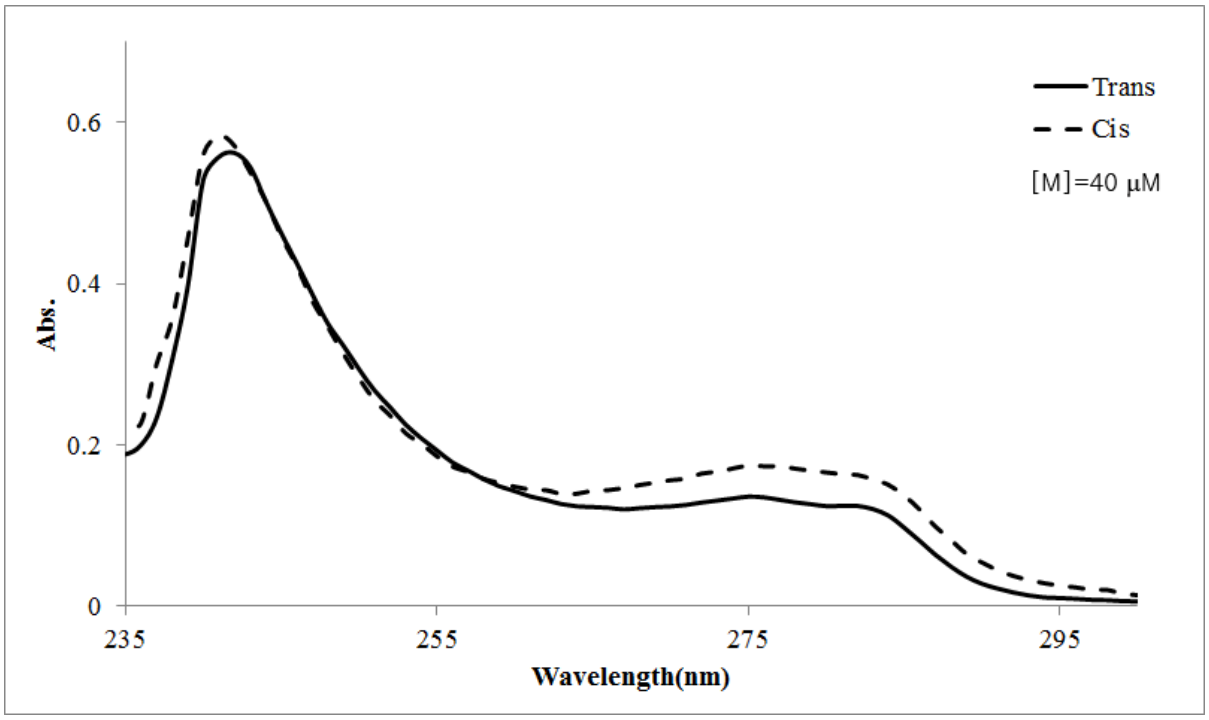


Figure S8. 300 MHz ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

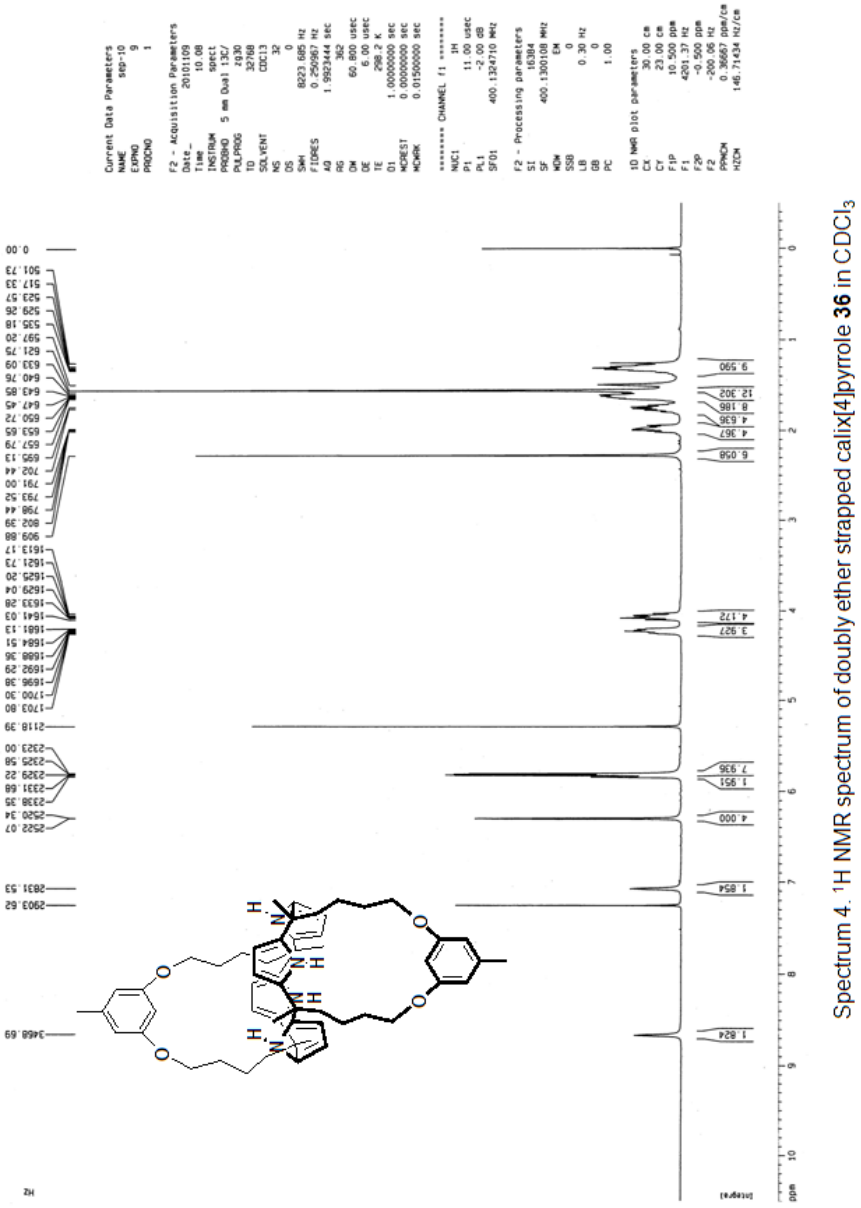


Figure S9. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

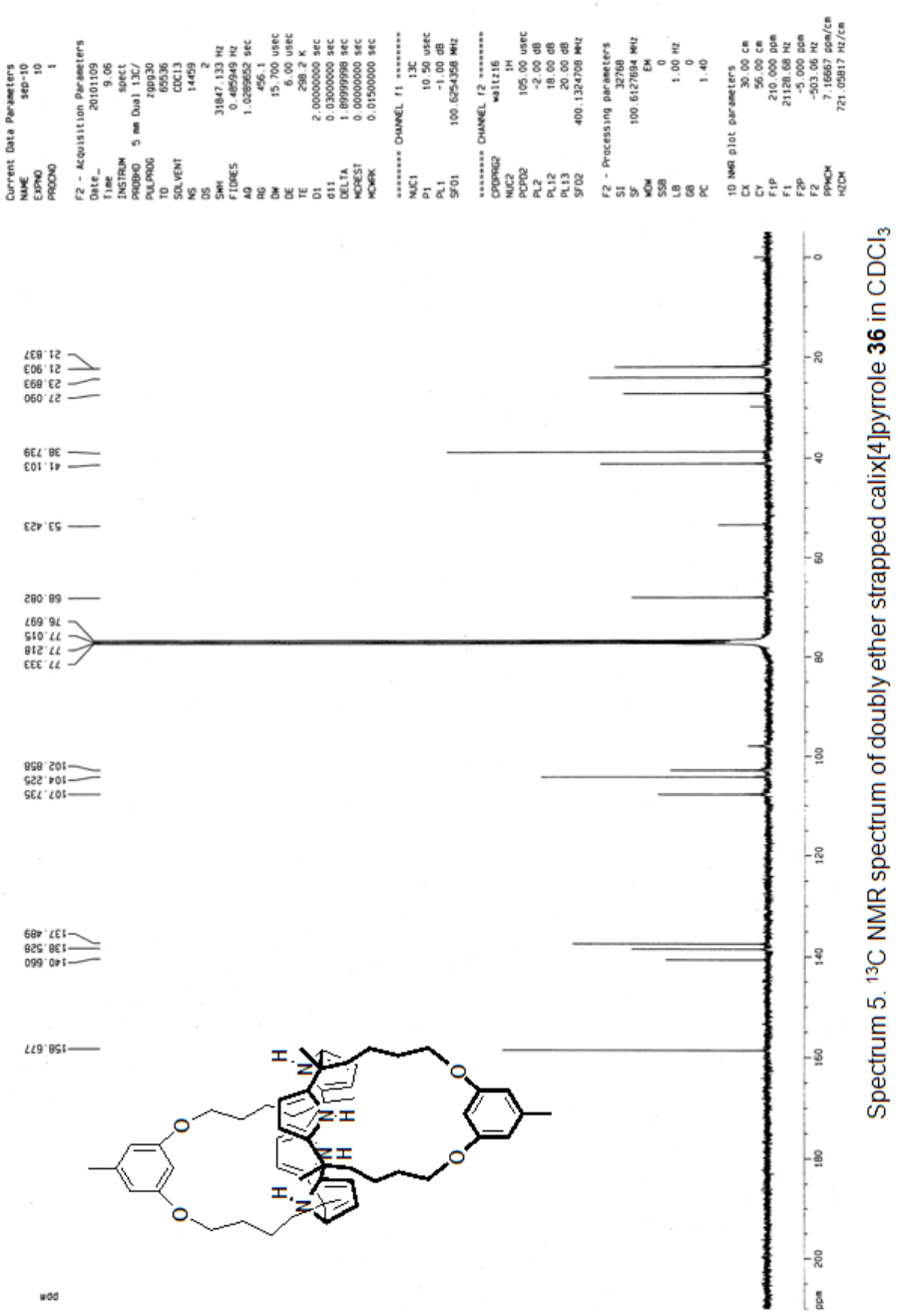
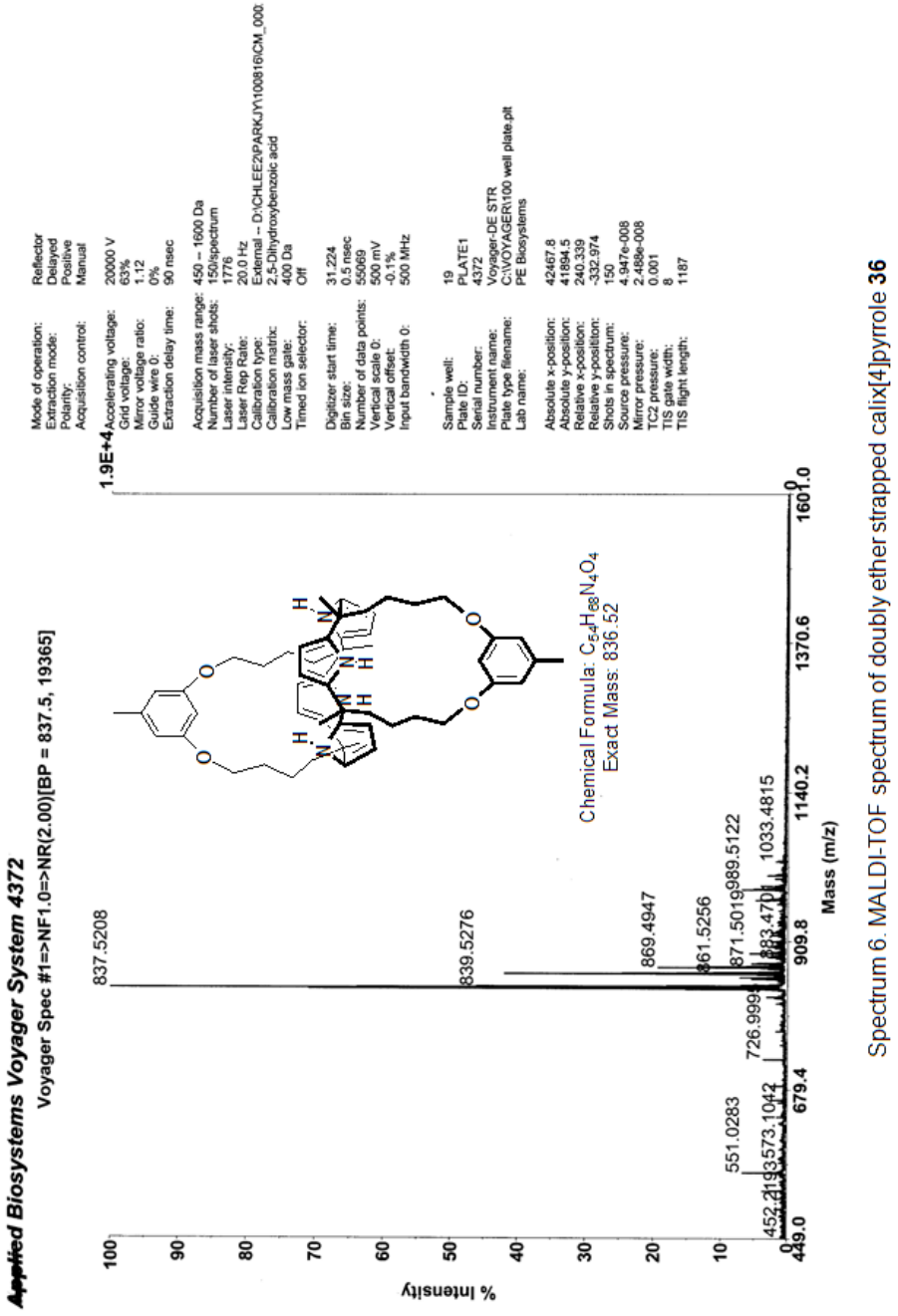


Figure S10. MALDI-TOF mass spectrum of compound **2** in $CDCl_3$.



Spectrum 6. MALDI-TOF spectrum of doubly ether strapped calix[4]pyrrole **36**

Figure S11. HETCO spectrum of compound **1** in $CDCl_3$.

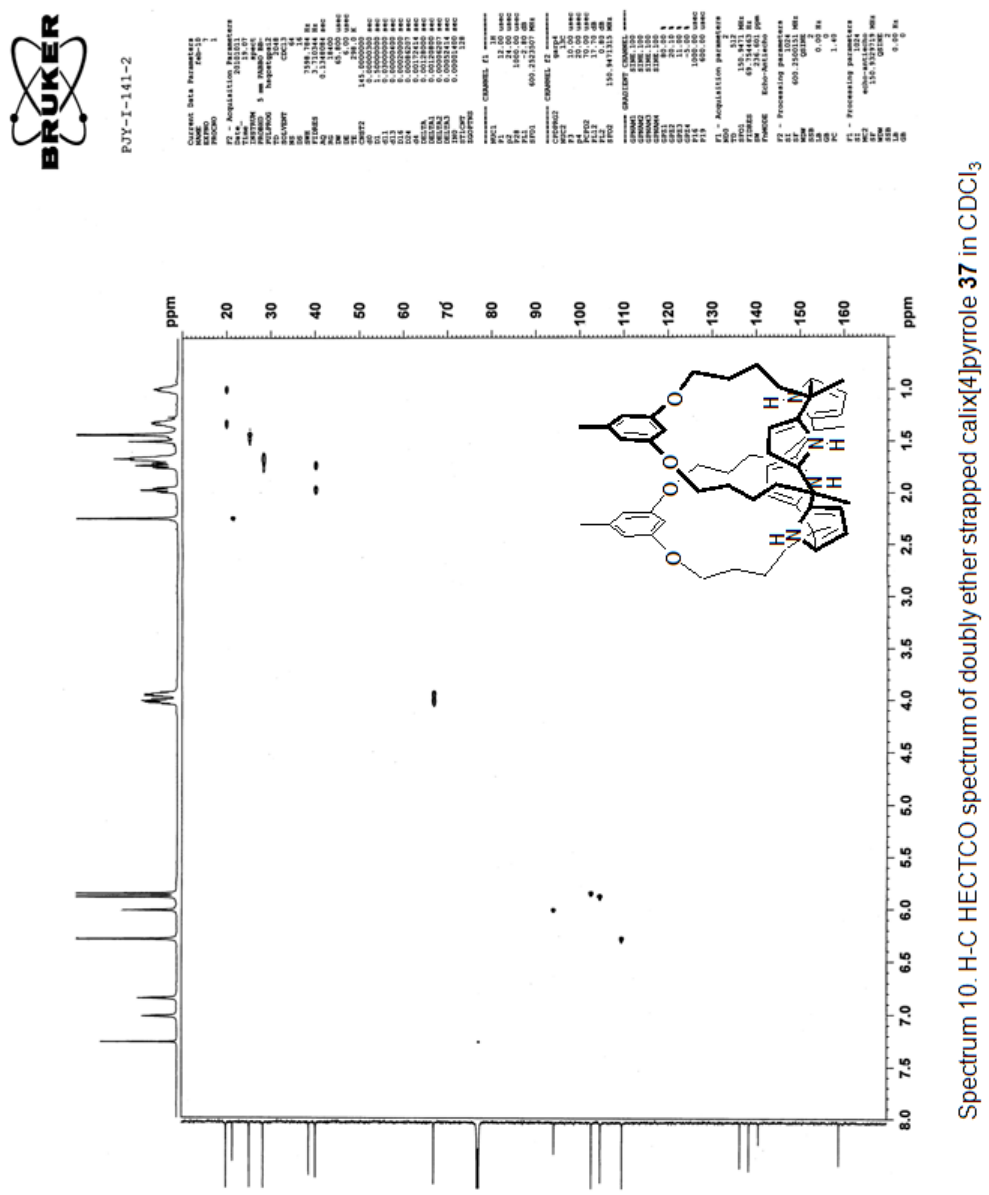


Figure S12. ^{1}H NMR spectral changes of receptor **2** upon addition of fluoride anion (as its tetrabutyl ammonium salt) in $CDCl_3$.

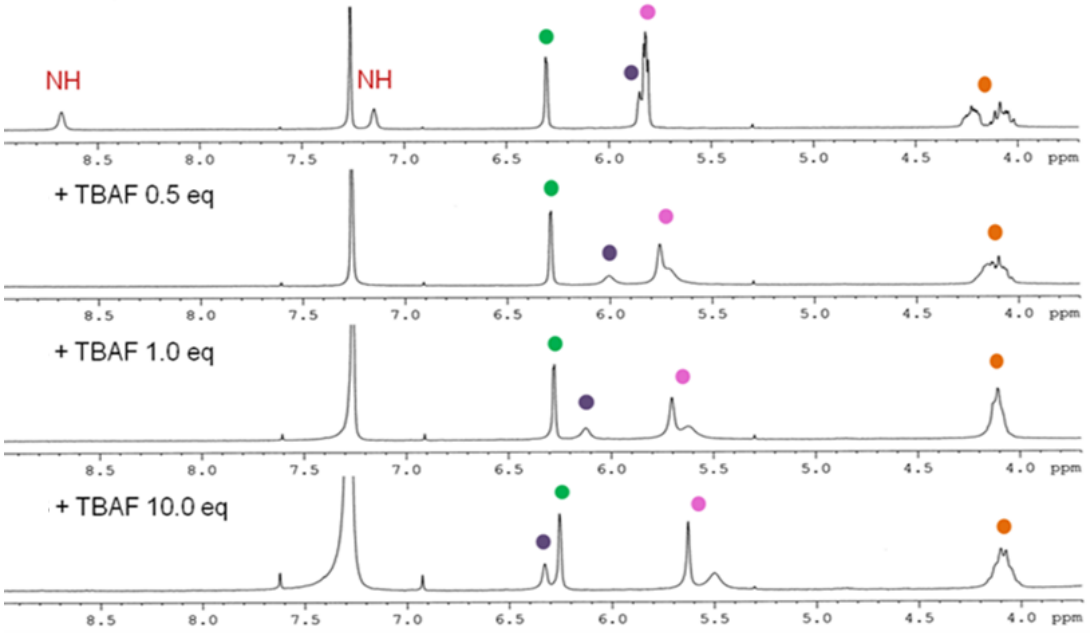


Figure S13. Changes in the ^{1}H NMR spectra of receptor **1** following the addition of fluoride anions (as its tetrabutyl ammonium salt) in $CDCl_3$.

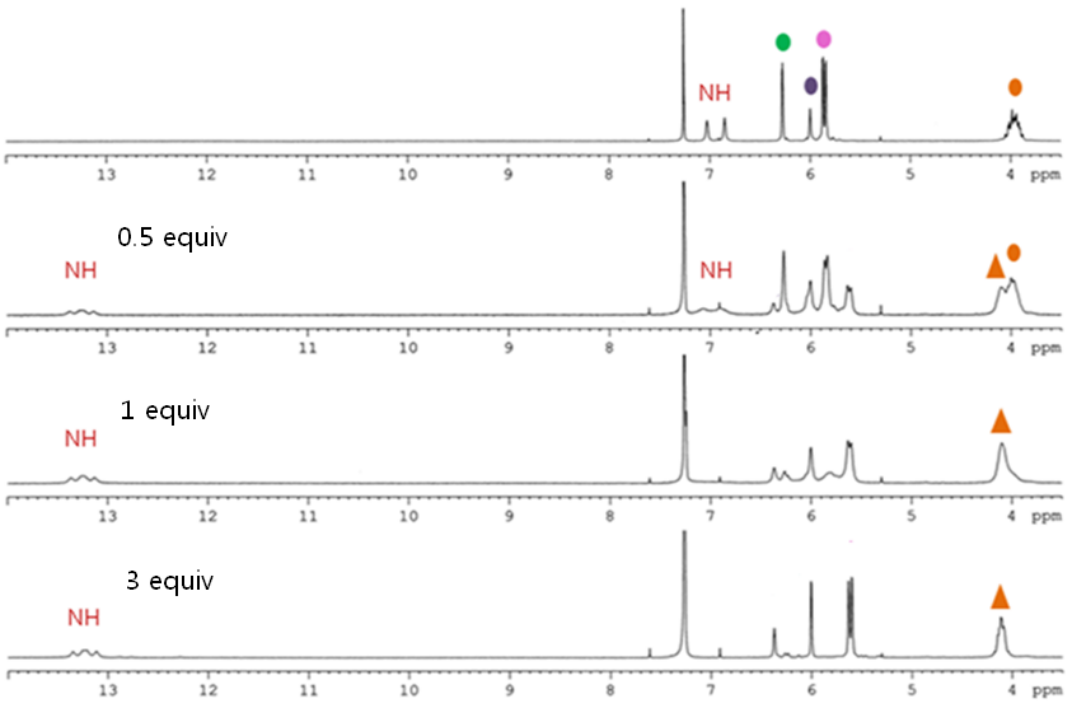


Figure S14. ^{1}H NMR spectral changes of receptor **2** upon addition of chloride anion (as its tetrabutyl ammonium salt) in $CDCl_3$.

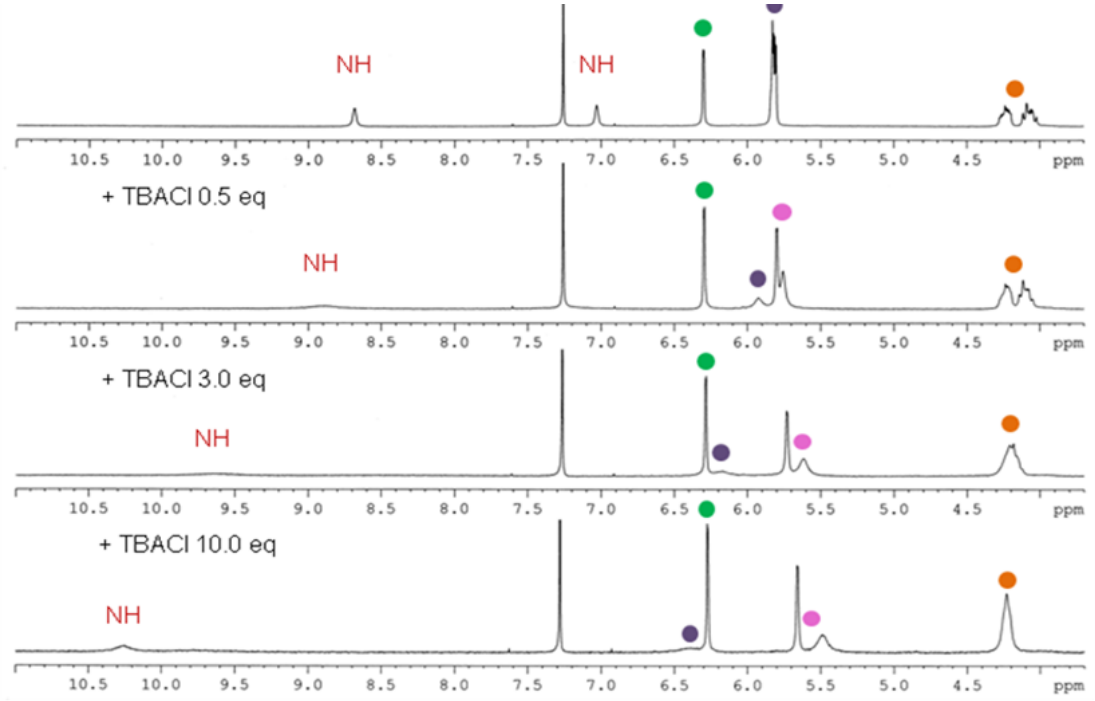
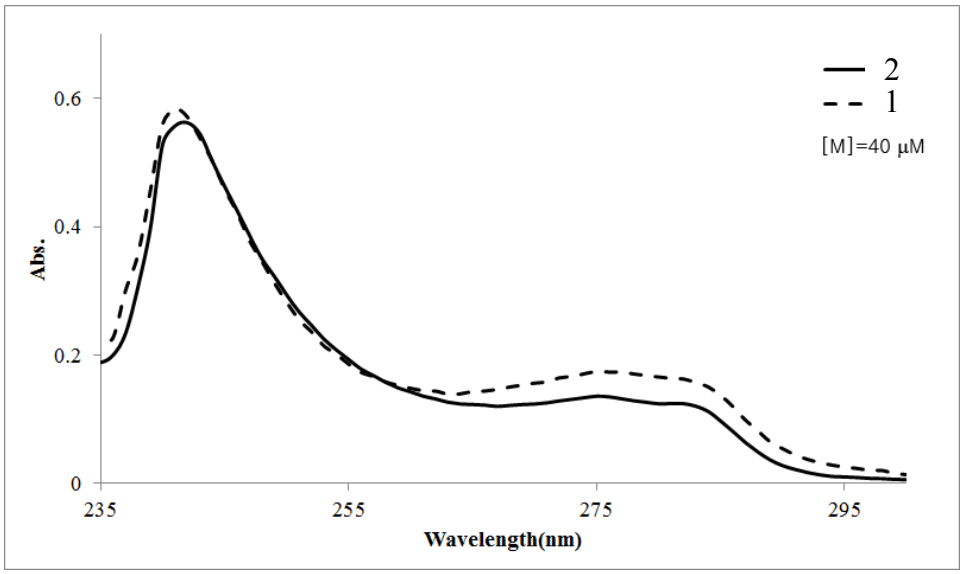
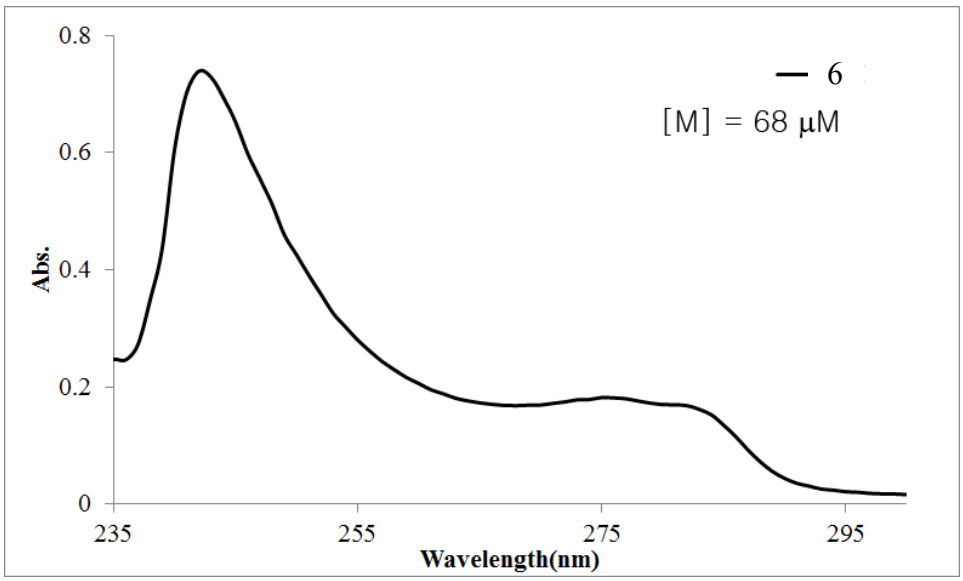


Table 1. Melting Points and UV-vis absorption data of compound **1**, **2** and **6**.

compound	**2**	**1**	**6**
m.p	240 °C	151 °C	206 °C
Molar absorptivity	242 nm = 1.40 x 10^4 275 nm = 3.40 x 10^3 282 nm = 3.12 x 10^3	241 nm = 1.46 X 10^4 275 nm = 4.37 x 10^3 282 nm = 4.08 x 10^3	242 nm = 1.08 x 10^4 275 nm = 2.65 x 10^3 282 nm = 2.45 x 10^3

Figure S15. UV-vis absorption spectra of of compound **1**, **2** and **6**.





ITC Titration Data

Microcalorimetric titrations were performed using an isothermal titration calorimeter (ITC). The ORIGIN software provided by Microcal Inc. was used to calculate the binding constant (*Ka*). The solventsCH_2Cl_2, were purchased from Daejung respectively. The curve shows the fit of the experimental data to a 1:1 binding mode.

Table 2. Calculated association constants and thermodynamic parameters for receptors **1** and **2** with various anions (as their tetrabutyl ammonium salt) in acetonitrile at 25°C. [**1**] = 0.05 mM and [**2**] = 0.05 mM.

	1				**2**			
	ΔG	*ΔH*	*ΔS*	*Ka*	*ΔG*	*ΔH*	*ΔS*	*Ka*
Cl^-	-7.39	-8.35	-3.22	2.62×10^5	-5.95	-9.89	-13.2	2.31×10^4
Br-	-5.16	-15.3	-34.0	5.74×10^3	-4.21	-10.5	-21.1	1.14×10^3
I-	-3.81	-7.33	-11.8	6.10×10^2	-3.17	-19.81	-55.8	2.06×10^2
AcO^-	-6.71	-8.59	-6.28	8.34×10^4	-5.89	-7.37	-4.95	2.09×10^4

Figure S16. ITC titration curves produced from the titration of 1 and 2 with chloride anion (as its tetrabutylammonium salt) in acetonitrile at 25 ºC. [1] =[2] = 0.5 mM, [TBACl] = 13.1 mM.

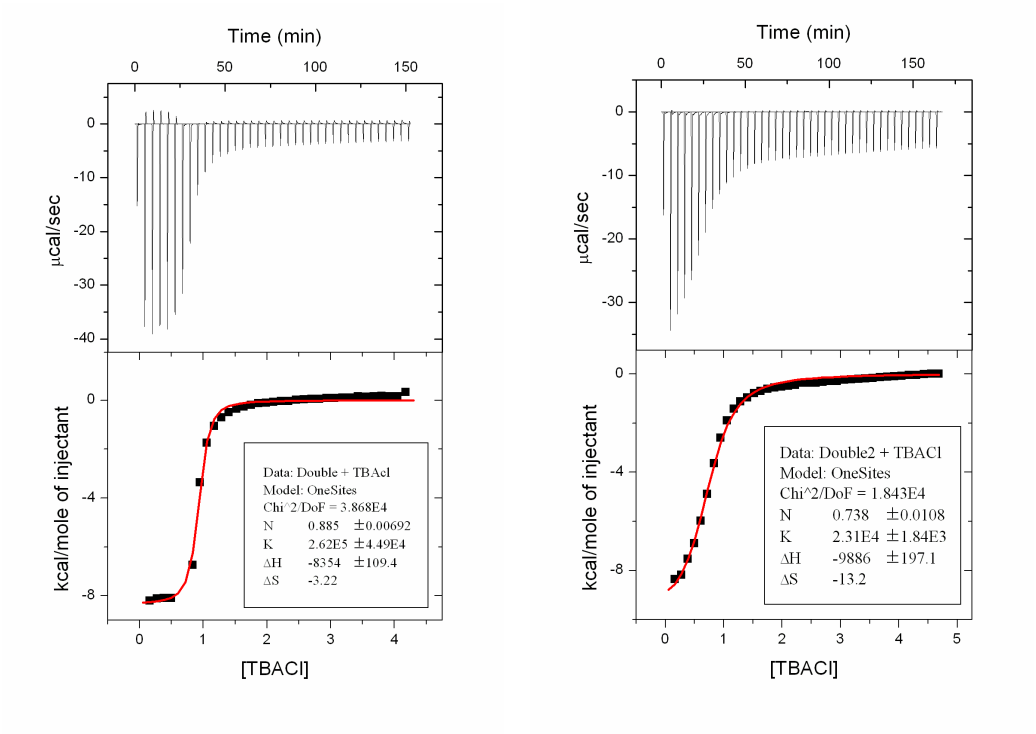


Figure S17. ITC titration curves produced from the titration of 1 and 2 with bromide anion (as its tetrabutylammonium salt) in acetonitrile at 25 ºC. [1] =[2] = 0.5 mM, [TBACl] = 13.1 mM.

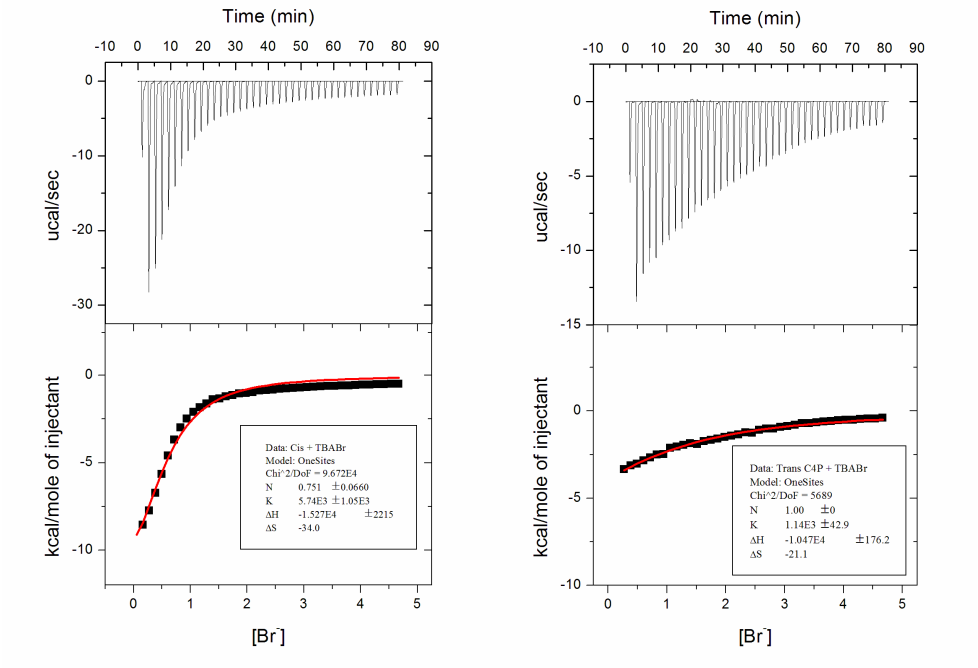


Figure S18. ITC titration curves produced from the titration of 1 and 2 with iodide anion (as its tetrabutylammonium salt) in acetonitrile at 25 ºC. [1] =[2] = 0.5 mM, [TBACl] = 13.1 mM.

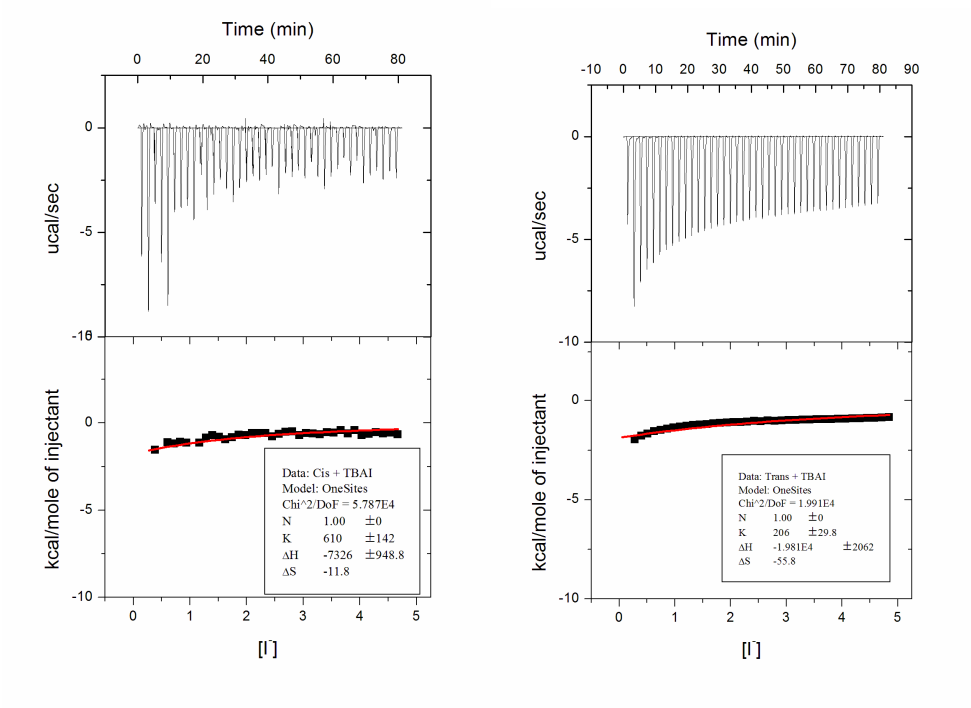
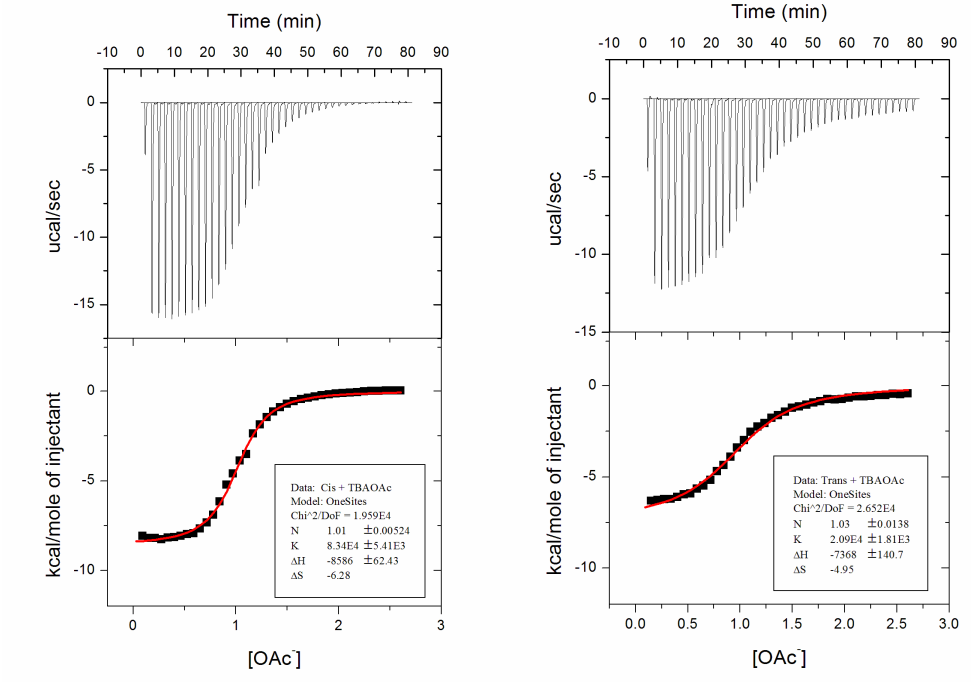


Figure S19. ITC titration curves produced from the titration of 1 and 2 with acetate anion (as its tetrabutylammonium salt) in acetonitrile at 25 ºC. [1] =[2] = 0.5 mM, [TBACl] = 13.1 mM.



Single Crystal data

Table 1. Crystal data and structure refinement for compound **1**.

Identification code	01211chl	
Empirical formula	C55 H68 N4 O5	
Formula weight	865.13	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Orthorhombic	
Space group	P ccn	
Unit cell dimensions	a = 34.4374(8) Å	α= 90°.
	b = 10.2869(2) Å	β= 90°.
	c = 13.5539(3) Å	γ = 90°.
Volume	4801.52(18) $Å^3$	
Z	4	
Density (calculated)	1.197 Mg/m^3	
Absorption coefficient	0.600 mm^{-1}	
F(000)	1864	
Crystal size	0.10 x 0.10 x 0.05 mm^3	
Theta range for data collection	5.14 to 68.24°.	
Index ranges	-41<=h<=41, -11<=k<=11, -16<=l<=16	
Reflections collected	47801	
Independent reflections	4347 [R(int) = 0.0676]	
Completeness to theta = 68.24°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9706 and 0.9424	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4347 / 0 / 299	
Goodness-of-fit on F^2	1.102	
Final R indices [I>2sigma(I)]	R1 = 0.0642, wR2 = 0.1634	
R indices (all data)	R1 = 0.1136, wR2 = 0.2029	
Largest diff. peak and hole	0.286 and -0.257 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4936(1)	3305(2)	5295(2)	67(1)
O(2)	5564(1)	-763(2)	6137(2)	68(1)
N(2)	7326(1)	4667(2)	3498(2)	68(1)
N(1)	6834(1)	1849(2)	3689(2)	64(1)
C(22)	7599(1)	5288(3)	4078(2)	66(1)
C(16)	6607(1)	4167(3)	3439(2)	62(1)
C(1)	4700(1)	1973(3)	6562(2)	65(1)
C(12)	5184(1)	3463(3)	4444(2)	66(1)
C(23)	6966(1)	4681(3)	3942(2)	63(1)
C(13)	5586(1)	3923(3)	4710(2)	61(1)
C(2)	5280(1)	165(3)	6246(2)	63(1)
C(18)	6654(1)	2771(3)	3112(2)	61(1)
C(14)	6271(1)	4255(3)	4200(2)	64(1)
C(19)	6823(1)	632(3)	3249(2)	62(1)
C(15)	5876(1)	3784(3)	3868(2)	65(1)
C(3)	4706(1)	842(3)	7120(2)	67(1)
C(4)	5000(1)	-60(3)	6959(2)	66(1)
C(26)	7017(1)	-1659(3)	2949(2)	72(1)
C(8)	5835(1)	-571(3)	5342(2)	65(1)
C(27)	6994(1)	-545(3)	3720(2)	65(1)
C(20)	6626(1)	805(3)	2379(2)	65(1)
C(9)	6075(1)	-1776(3)	5212(2)	67(1)
C(10)	6356(1)	-1614(3)	4336(2)	66(1)
C(24)	7013(1)	5329(3)	4820(2)	71(1)
C(21)	6521(1)	2130(3)	2296(2)	67(1)
C(5)	4975(1)	2185(3)	5836(2)	63(1)
C(25)	7405(1)	5713(3)	4908(2)	71(1)
C(17)	6515(1)	5017(3)	2537(2)	71(1)
C(28)	6740(1)	-993(3)	4613(2)	66(1)
C(6)	4391(1)	583(4)	7861(2)	79(1)
C(7)	5269(1)	1278(3)	5673(2)	63(1)
O(3)	7500	2500	1969(4)	126(3)
C(31)	7500	2500	1048(7)	122(2)
O(4)	7500	2500	189(11)	114(7)

Table 3. Bond lengths [Å] and angles [°] for compound **1**.

O(1)-C(5)	1.372(3)
O(1)-C(12)	1.444(3)
O(2)-C(2)	1.374(3)
O(2)-C(8)	1.441(3)
N(2)-C(23)	1.376(3)
N(2)-C(22)	1.382(4)
N(2)-H(1)	0.8800
N(1)-C(18)	1.377(4)
N(1)-C(19)	1.387(4)
N(1)-H(2)	0.8800
C(22)-C(25)	1.379(4)
C(22)-C(27)#1	1.507(4)
C(16)-C(23)	1.507(4)
C(16)-C(18)	1.511(4)
C(16)-C(17)	1.537(4)
C(16)-C(14)	1.553(4)
C(1)-C(5)	1.384(4)
C(1)-C(3)	1.387(4)
C(1)-H(3)	0.9500
C(12)-C(13)	1.506(4)
C(12)-H(10)	0.9900
C(12)-H(11)	0.9900
C(23)-C(24)	1.374(4)
C(13)-C(15)	1.523(4)
C(13)-H(12)	0.9900
C(13)-H(13)	0.9900
C(2)-C(7)	1.384(4)
C(2)-C(4)	1.385(4)
C(18)-C(21)	1.367(4)
C(14)-C(15)	1.514(4)
C(14)-H(14)	0.9900
C(14)-H(15)	0.9900
C(19)-C(20)	1.373(4)
C(19)-C(27)	1.490(4)
C(15)-H(16)	0.9900
C(15)-H(17)	0.9900
C(3)-C(4)	1.391(4)

C(3)-C(6)	1.503(4)
C(4)-H(4)	0.9500
C(26)-C(27)	1.552(4)
C(26)-H(18)	0.9800
C(26)-H(19)	0.9800
C(26)-H(20)	0.9800
C(8)-C(9)	1.501(4)
C(8)-H(21)	0.9900
C(8)-H(22)	0.9900
C(27)-C(22)#1	1.507(4)
C(27)-C(28)	1.563(4)
C(20)-C(21)	1.415(4)
C(20)-H(5)	0.9500
C(9)-C(10)	1.542(4)
C(9)-H(23)	0.9900
C(9)-H(24)	0.9900
C(10)-C(28)	1.517(4)
C(10)-H(25)	0.9900
C(10)-H(26)	0.9900
C(24)-C(25)	1.411(4)
C(24)-H(6)	0.9500
C(21)-H(7)	0.9500
C(5)-C(7)	1.394(4)
C(25)-H(8)	0.9500
C(17)-H(27)	0.9800
C(17)-H(28)	0.9800
C(17)-H(29)	0.9800
C(28)-H(30)	0.9900
C(28)-H(31)	0.9900
C(6)-H(32)	0.9800
C(6)-H(33)	0.9800
C(6)-H(34)	0.9800
C(7)-H(9)	0.9500
O(3)-C(31)	1.249(8)
C(31)-O(4)	1.164(13)

C(5)-O(1)-C(12)	117.6(2)
C(2)-O(2)-C(8)	116.5(2)
C(23)-N(2)-C(22)	110.9(3)

C(23)-N(2)-H(1)	124.5
C(22)-N(2)-H(1)	124.5
C(18)-N(1)-C(19)	111.4(3)
C(18)-N(1)-H(2)	124.3
C(19)-N(1)-H(2)	124.3
C(25)-C(22)-N(2)	106.4(3)
C(25)-C(22)-C(27)#1	131.1(3)
N(2)-C(22)-C(27)#1	122.0(3)
C(23)-C(16)-C(18)	112.2(2)
C(23)-C(16)-C(17)	109.3(2)
C(18)-C(16)-C(17)	109.3(2)
C(23)-C(16)-C(14)	106.9(2)
C(18)-C(16)-C(14)	109.2(2)
C(17)-C(16)-C(14)	109.9(2)
C(5)-C(1)-C(3)	120.7(3)
C(5)-C(1)-H(3)	119.7
C(3)-C(1)-H(3)	119.7
O(1)-C(12)-C(13)	112.8(2)
O(1)-C(12)-H(10)	109.0
C(13)-C(12)-H(10)	109.0
O(1)-C(12)-H(11)	109.0
C(13)-C(12)-H(11)	109.0
H(10)-C(12)-H(11)	107.8
C(24)-C(23)-N(2)	106.2(3)
C(24)-C(23)-C(16)	131.1(3)
N(2)-C(23)-C(16)	122.4(3)
C(12)-C(13)-C(15)	113.2(2)
C(12)-C(13)-H(12)	108.9
C(15)-C(13)-H(12)	108.9
C(12)-C(13)-H(13)	108.9
C(15)-C(13)-H(13)	108.9
H(12)-C(13)-H(13)	107.8
O(2)-C(2)-C(7)	122.3(3)
O(2)-C(2)-C(4)	117.0(3)
C(7)-C(2)-C(4)	120.7(3)
C(21)-C(18)-N(1)	106.2(3)
C(21)-C(18)-C(16)	131.2(3)
N(1)-C(18)-C(16)	122.4(3)
C(15)-C(14)-C(16)	117.1(2)

C(15)-C(14)-H(14)	108.0
C(16)-C(14)-H(14)	108.0
C(15)-C(14)-H(15)	108.0
C(16)-C(14)-H(15)	108.0
H(14)-C(14)-H(15)	107.3
C(20)-C(19)-N(1)	105.4(3)
C(20)-C(19)-C(27)	132.0(3)
N(1)-C(19)-C(27)	122.6(3)
C(14)-C(15)-C(13)	109.7(2)
C(14)-C(15)-H(16)	109.7
C(13)-C(15)-H(16)	109.7
C(14)-C(15)-H(17)	109.7
C(13)-C(15)-H(17)	109.7
H(16)-C(15)-H(17)	108.2
C(1)-C(3)-C(4)	119.0(3)
C(1)-C(3)-C(6)	120.2(3)
C(4)-C(3)-C(6)	120.8(3)
C(2)-C(4)-C(3)	120.3(3)
C(2)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(27)-C(26)-H(18)	109.5
C(27)-C(26)-H(19)	109.5
H(18)-C(26)-H(19)	109.5
C(27)-C(26)-H(20)	109.5
H(18)-C(26)-H(20)	109.5
H(19)-C(26)-H(20)	109.5
O(2)-C(8)-C(9)	109.3(2)
O(2)-C(8)-H(21)	109.8
C(9)-C(8)-H(21)	109.8
O(2)-C(8)-H(22)	109.8
C(9)-C(8)-H(22)	109.8
H(21)-C(8)-H(22)	108.3
C(19)-C(27)-C(22)#1	111.3(2)
C(19)-C(27)-C(26)	109.4(3)
C(22)#1-C(27)-C(26)	107.4(2)
C(19)-C(27)-C(28)	110.5(3)
C(22)#1-C(27)-C(28)	108.8(2)
C(26)-C(27)-C(28)	109.4(2)
C(19)-C(20)-C(21)	108.6(3)

C(19)-C(20)-H(5)	125.7
C(21)-C(20)-H(5)	125.7
C(8)-C(9)-C(10)	110.3(2)
C(8)-C(9)-H(23)	109.6
C(10)-C(9)-H(23)	109.6
C(8)-C(9)-H(24)	109.6
C(10)-C(9)-H(24)	109.6
H(23)-C(9)-H(24)	108.1
C(28)-C(10)-C(9)	113.7(3)
C(28)-C(10)-H(25)	108.8
C(9)-C(10)-H(25)	108.8
C(28)-C(10)-H(26)	108.8
C(9)-C(10)-H(26)	108.8
H(25)-C(10)-H(26)	107.7
C(23)-C(24)-C(25)	108.7(3)
C(23)-C(24)-H(6)	125.6
C(25)-C(24)-H(6)	125.6
C(18)-C(21)-C(20)	108.4(3)
C(18)-C(21)-H(7)	125.8
C(20)-C(21)-H(7)	125.8
O(1)-C(5)-C(1)	116.4(3)
O(1)-C(5)-C(7)	123.3(3)
C(1)-C(5)-C(7)	120.3(3)
C(22)-C(25)-C(24)	107.7(3)
C(22)-C(25)-H(8)	126.1
C(24)-C(25)-H(8)	126.1
C(16)-C(17)-H(27)	109.5
C(16)-C(17)-H(28)	109.5
H(27)-C(17)-H(28)	109.5
C(16)-C(17)-H(29)	109.5
H(27)-C(17)-H(29)	109.5
H(28)-C(17)-H(29)	109.5
C(10)-C(28)-C(27)	114.9(2)
C(10)-C(28)-H(30)	108.6
C(27)-C(28)-H(30)	108.6
C(10)-C(28)-H(31)	108.6
C(27)-C(28)-H(31)	108.6
H(30)-C(28)-H(31)	107.5
C(3)-C(6)-H(32)	109.5

C(3)-C(6)-H(33)	109.5
H(32)-C(6)-H(33)	109.5
C(3)-C(6)-H(34)	109.5
H(32)-C(6)-H(34)	109.5
H(33)-C(6)-H(34)	109.5
C(2)-C(7)-C(5)	119.0(3)
C(2)-C(7)-H(9)	120.5
C(5)-C(7)-H(9)	120.5
O(4)-C(31)-O(3)	180.000(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+1/2,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	59(1)	57(1)	83(1)	6(1)	7(1)	1(1)
O(2)	68(1)	60(1)	78(1)	5(1)	6(1)	5(1)
N(2)	57(2)	70(2)	78(2)	-11(1)	2(1)	-9(1)
N(1)	62(2)	61(2)	69(2)	-1(1)	-4(1)	-4(1)
C(22)	57(2)	60(2)	80(2)	-6(2)	1(2)	-10(2)
C(16)	56(2)	57(2)	73(2)	0(2)	0(1)	-2(1)
C(1)	53(2)	65(2)	76(2)	-3(2)	2(1)	-1(1)
C(12)	61(2)	63(2)	75(2)	4(2)	6(2)	1(2)
C(23)	52(2)	63(2)	74(2)	-2(2)	4(1)	-5(1)
C(13)	54(2)	55(2)	75(2)	-2(1)	3(1)	2(1)
C(2)	62(2)	56(2)	71(2)	0(2)	-2(2)	0(2)
C(18)	53(2)	55(2)	75(2)	0(2)	1(1)	-3(1)
C(14)	58(2)	56(2)	78(2)	-5(2)	3(2)	-3(1)
C(19)	61(2)	53(2)	73(2)	1(2)	2(2)	-5(1)
C(15)	58(2)	62(2)	75(2)	-3(2)	2(2)	-3(1)
C(3)	59(2)	71(2)	69(2)	-1(2)	-2(2)	-7(2)
C(4)	64(2)	65(2)	68(2)	5(2)	-3(2)	-6(2)
C(26)	67(2)	64(2)	83(2)	-6(2)	4(2)	-5(2)
C(8)	66(2)	59(2)	71(2)	4(2)	5(2)	-2(2)
C(27)	56(2)	61(2)	77(2)	1(2)	-2(2)	-6(1)
C(20)	69(2)	59(2)	68(2)	-3(2)	1(2)	-2(2)
C(9)	60(2)	60(2)	81(2)	0(2)	1(2)	-6(2)
C(10)	60(2)	57(2)	80(2)	1(2)	3(2)	-7(1)
C(24)	59(2)	75(2)	80(2)	-5(2)	8(2)	-9(2)
C(21)	63(2)	69(2)	70(2)	-3(2)	-4(2)	1(2)
C(5)	59(2)	55(2)	76(2)	2(2)	-1(2)	-7(2)
C(25)	65(2)	74(2)	74(2)	-7(2)	-1(2)	-14(2)
C(17)	70(2)	64(2)	78(2)	4(2)	3(2)	-6(2)
C(28)	60(2)	60(2)	78(2)	6(2)	0(2)	-6(1)
C(6)	63(2)	97(3)	77(2)	12(2)	4(2)	-6(2)
C(7)	57(2)	59(2)	73(2)	-2(2)	3(2)	-1(2)
O(3)	157(5)	152(6)	70(4)	0	0	71(4)
C(31)	136(6)	143(6)	85(5)	0	0	-1(5)
O(4)	140(13)	140(14)	62(10)	0	0	52(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **1**.

	x	y	z	U(eq)
H(1)	7375	4310	2921	82
H(2)	6943	2011	4264	77
H(3)	4505	2608	6680	77
H(10)	5064	4098	3988	79
H(11)	5204	2622	4093	79
H(12)	5680	3419	5284	73
H(13)	5572	4848	4909	73
H(14)	6347	3750	4791	77
H(15)	6246	5175	4406	77
H(16)	5892	2862	3664	78
H(17)	5787	4301	3294	78
H(4)	5009	-835	7340	79
H(18)	6757	-1830	2684	107
H(19)	7118	-2446	3266	107
H(20)	7191	-1402	2411	107
H(21)	6006	178	5491	78
H(22)	5692	-379	4724	78
H(5)	6569	145	1910	78
H(23)	5902	-2530	5093	80
H(24)	6225	-1946	5822	80
H(25)	6407	-2480	4044	79
H(26)	6229	-1075	3824	79
H(6)	6814	5492	5290	85
H(7)	6382	2510	1764	81
H(8)	7515	6181	5443	85
H(27)	6476	5918	2749	106
H(28)	6278	4697	2217	106
H(29)	6731	4978	2069	106
H(30)	6892	-1623	5009	79
H(31)	6687	-229	5037	79
H(32)	4370	1324	8312	119
H(33)	4454	-202	8237	119
H(34)	4143	459	7517	119

H(9)	5459	1421	5177	76

Table 6. Torsion angles [°] for compound **1**.

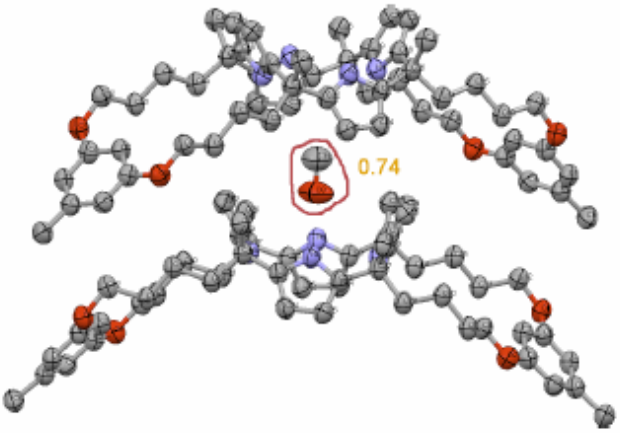
C(23)-N(2)-C(22)-C(25)	-0.4(4)
C(23)-N(2)-C(22)-C(27)#1	-173.1(3)
C(5)-O(1)-C(12)-C(13)	-80.6(3)
C(22)-N(2)-C(23)-C(24)	0.2(4)
C(22)-N(2)-C(23)-C(16)	175.0(3)
C(18)-C(16)-C(23)-C(24)	-130.6(4)
C(17)-C(16)-C(23)-C(24)	108.0(4)
C(14)-C(16)-C(23)-C(24)	-10.9(4)
C(18)-C(16)-C(23)-N(2)	56.0(4)
C(17)-C(16)-C(23)-N(2)	-65.3(4)
C(14)-C(16)-C(23)-N(2)	175.8(3)
O(1)-C(12)-C(13)-C(15)	166.1(2)
C(8)-O(2)-C(2)-C(7)	-4.6(4)
C(8)-O(2)-C(2)-C(4)	175.1(2)
C(19)-N(1)-C(18)-C(21)	0.9(3)
C(19)-N(1)-C(18)-C(16)	177.0(3)
C(23)-C(16)-C(18)-C(21)	-143.8(3)
C(17)-C(16)-C(18)-C(21)	-22.3(4)
C(14)-C(16)-C(18)-C(21)	97.9(4)
C(23)-C(16)-C(18)-N(1)	41.2(4)
C(17)-C(16)-C(18)-N(1)	162.7(3)
C(14)-C(16)-C(18)-N(1)	-77.1(3)
C(23)-C(16)-C(14)-C(15)	-179.7(3)
C(18)-C(16)-C(14)-C(15)	-58.0(3)
C(17)-C(16)-C(14)-C(15)	61.8(3)
C(18)-N(1)-C(19)-C(20)	-0.8(3)
C(18)-N(1)-C(19)-C(27)	-179.5(3)
C(16)-C(14)-C(15)-C(13)	179.1(2)
C(12)-C(13)-C(15)-C(14)	-179.5(3)
C(5)-C(1)-C(3)-C(4)	1.9(4)
C(5)-C(1)-C(3)-C(6)	-176.0(3)
O(2)-C(2)-C(4)-C(3)	179.3(3)
C(7)-C(2)-C(4)-C(3)	-1.0(4)
C(1)-C(3)-C(4)-C(2)	-0.6(4)
C(6)-C(3)-C(4)-C(2)	177.4(3)
C(2)-O(2)-C(8)-C(9)	-169.7(2)
C(20)-C(19)-C(27)-C(22)#1	133.0(3)

N(1)-C(19)-C(27)-C(22)#1	-48.8(4)
C(20)-C(19)-C(27)-C(26)	14.5(4)
N(1)-C(19)-C(27)-C(26)	-167.3(3)
C(20)-C(19)-C(27)-C(28)	-106.0(4)
N(1)-C(19)-C(27)-C(28)	72.3(3)
N(1)-C(19)-C(20)-C(21)	0.4(3)
C(27)-C(19)-C(20)-C(21)	178.9(3)
O(2)-C(8)-C(9)-C(10)	177.6(2)
C(8)-C(9)-C(10)-C(28)	87.6(3)
N(2)-C(23)-C(24)-C(25)	0.1(4)
C(16)-C(23)-C(24)-C(25)	-174.1(3)
N(1)-C(18)-C(21)-C(20)	-0.6(3)
C(16)-C(18)-C(21)-C(20)	-176.2(3)
C(19)-C(20)-C(21)-C(18)	0.1(3)
C(12)-O(1)-C(5)-C(1)	-171.4(2)
C(12)-O(1)-C(5)-C(7)	7.7(4)
C(3)-C(1)-C(5)-O(1)	177.3(3)
C(3)-C(1)-C(5)-C(7)	-1.8(4)
N(2)-C(22)-C(25)-C(24)	0.4(4)
C(27)#1-C(22)-C(25)-C(24)	172.2(3)
C(23)-C(24)-C(25)-C(22)	-0.3(4)
C(9)-C(10)-C(28)-C(27)	-167.5(3)
C(19)-C(27)-C(28)-C(10)	72.5(3)
C(22)#1-C(27)-C(28)-C(10)	-165.0(3)
C(26)-C(27)-C(28)-C(10)	-48.0(3)
O(2)-C(2)-C(7)-C(5)	-179.1(3)
C(4)-C(2)-C(7)-C(5)	1.2(4)
O(1)-C(5)-C(7)-C(2)	-178.8(3)
C(1)-C(5)-C(7)-C(2)	0.2(4)

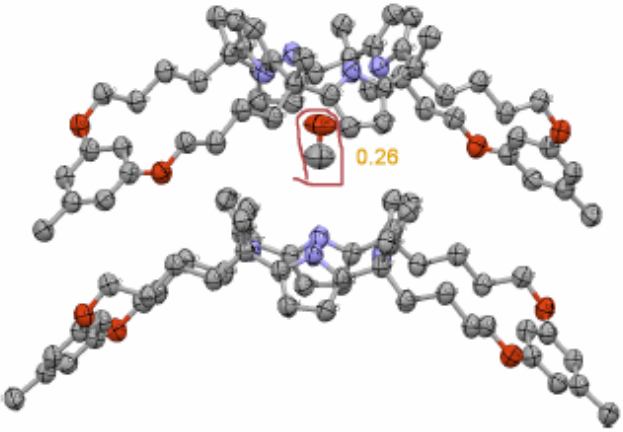
Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+1/2,z

PART 1 (methanol oxygen is hydrogen-bonded with two N(2)-H.)



PART 2 (methanol oxygen is hydrogen-bonded with two N(1)-H.)



Total View (PART 1 + PART 2)

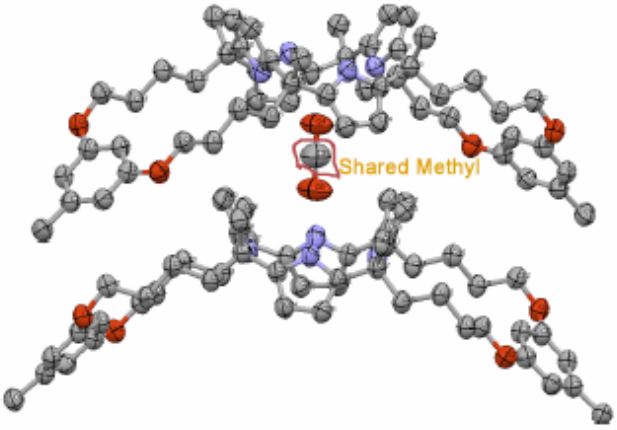


Table 1. Crystal data and structure refinement for compound **2**.

Identification code	01130chl
Empirical formula	C56 H72 Cl3 N4 O5
Formula weight	987.53
Temperature	93(2) K
Wavelength	1.54187 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 11.7904(6) Å a= 72.935(3)°.
	b = 12.5321(6) Å b= 78.389(3)°.
	c = 19.6483(10) Å g = 68.038(3)°.
Volume	2560.2(2) Å3
Z	2
Density (calculated)	1.281 Mg/m3
Absorption coefficient	2.032 mm-1
F(000)	1054
Crystal size	0.20 x 0.20 x 0.05 mm3
Theta range for data collection	3.92 to 60.00°.
Index ranges	-13<=h<=12, -14<=k<=14, -21<=l<=22
Reflections collected	21173
Independent reflections	7406 [R(int) = 0.1997]
Completeness to theta = 60.00°	97.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9052 and 0.6867
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	7406 / 1 / 621
Goodness-of-fit on F2	0.894
Final R indices [I>2sigma(I)]	R1 = 0.1251, wR2 = 0.2857
R indices (all data)	R1 = 0.2272, wR2 = 0.3635
Largest diff. peak and hole	0.333 and -0.352 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	-2428(3)	-155(2)	5519(2)	104(1)
Cl(2)	-4853(3)	1241(3)	5087(2)	125(1)
O(1)	3331(6)	5519(5)	-2895(3)	80(2)
O(2)	-349(6)	1906(5)	2713(3)	77(2)
O(3)	2653(6)	3570(5)	2562(3)	75(2)
O(4)	311(6)	3701(5)	-2814(4)	84(2)
C(1)	1817(9)	4579(7)	-2794(5)	72(3)
N(1)	4414(7)	1906(6)	1592(4)	71(2)
C(2)	183(9)	2359(8)	3060(5)	72(3)
N(2)	1345(7)	162(6)	1680(4)	76(2)
N(3)	2240(8)	2334(6)	504(4)	80(2)
C(3)	1146(9)	2731(8)	2674(5)	74(3)
C(4)	1705(9)	3229(7)	2995(6)	69(3)
C(5)	627(9)	2623(8)	-1573(5)	75(3)
C(6)	2721(10)	4995(8)	-3173(6)	80(3)
N(4)	3721(8)	-453(7)	2658(4)	84(2)
C(7)	3301(9)	4599(8)	-863(5)	83(3)
C(8)	2471(10)	3308(8)	598(5)	75(3)
C(9)	3708(9)	3408(7)	446(5)	71(3)
C(10)	2204(10)	-1505(8)	2752(5)	80(3)
C(11)	823(8)	1503(7)	-273(5)	74(3)
C(12)	1224(8)	344(8)	970(5)	72(3)
C(13)	1212(9)	-764(8)	3236(5)	79(3)
C(14)	5195(9)	2174(8)	3022(5)	81(3)
C(15)	1637(10)	4053(8)	-3831(5)	87(3)
C(16)	42(10)	3030(9)	4867(5)	92(3)
C(17)	419(10)	2934(8)	4089(6)	84(3)
C(18)	-185(9)	2432(8)	3779(5)	80(3)
C(19)	4509(9)	-2388(9)	2993(5)	86(3)
C(20)	4631(10)	2363(8)	861(6)	75(3)
C(21)	3447(10)	-1496(9)	2802(5)	79(3)
C(22)	-117(9)	3684(8)	-2075(5)	81(3)
C(23)	571(9)	1539(8)	541(5)	74(3)
C(24)	210(8)	2663(8)	-808(5)	78(3)

C(25)	3304(9)	4076(8)	2845(5)	83(3)
C(26)	3650(9)	4525(7)	678(5)	84(3)
C(27)	3688(9)	4497(8)	-1647(5)	83(3)
C(28)	2990(10)	5614(8)	-2168(5)	93(3)
C(29)	3108(10)	4936(8)	-3880(5)	80(3)
C(30)	6807(8)	-303(8)	2790(5)	86(3)
C(31)	5453(10)	954(9)	1828(6)	84(3)
C(32)	-813(9)	1877(8)	775(5)	87(3)
C(33)	2233(10)	-2823(7)	3011(5)	90(3)
C(34)	1353(10)	4043(8)	789(5)	76(3)
C(35)	431(9)	3514(8)	811(5)	76(3)
C(36)	4892(10)	-669(9)	2740(5)	83(3)
C(37)	5450(10)	282(8)	2617(5)	79(3)
C(38)	6330(9)	830(8)	1258(6)	78(3)
C(39)	1264(10)	4111(8)	-3138(6)	81(3)
C(40)	-1007(10)	294(9)	3578(5)	90(3)
C(41)	1337(9)	3329(8)	3697(6)	77(3)
C(42)	2117(9)	-1607(9)	1445(5)	82(3)
C(43)	5803(10)	1691(9)	652(6)	87(3)
C(44)	2993(10)	4445(9)	-4986(5)	100(3)
C(45)	1026(9)	2455(8)	635(5)	71(3)
C(46)	4259(9)	3207(9)	3328(5)	86(3)
C(47)	2575(10)	4464(8)	-4221(6)	82(3)
C(48)	4740(9)	1145(8)	3105(5)	81(3)
C(49)	-114(9)	-677(8)	3226(5)	83(3)
C(50)	-3653(10)	1191(9)	5502(6)	103(4)
C(51)	5456(10)	-1890(8)	2952(5)	85(3)
C(52)	1903(9)	-1039(8)	1975(6)	81(3)
C(53)	4130(10)	3553(8)	-356(5)	89(3)
C(54)	1717(8)	-729(8)	816(5)	75(3)
C(55)	-1383(10)	1530(8)	3061(5)	91(3)
Cl(3)	-3125(3)	2410(2)	4976(2)	116(1)
C(56)	5428(17)	562(17)	-933(7)	158(6)
O(6)	4298(14)	751(15)	-450(14)	450(20)

Table 3. Bond lengths [Å] and angles [°] for compound **2**.

Cl(1)-C(50)	1.759(10)
Cl(2)-C(50)	1.743(11)
O(1)-C(6)	1.403(11)
O(1)-C(28)	1.431(10)
O(2)-C(2)	1.359(10)
O(2)-C(55)	1.443(10)
O(3)-C(4)	1.385(10)
O(3)-C(25)	1.429(10)
O(4)-C(39)	1.372(11)
O(4)-C(22)	1.436(10)
C(1)-C(6)	1.353(13)
C(1)-C(39)	1.386(12)
C(1)-H(1)	0.9500
N(1)-C(20)	1.391(11)
N(1)-C(31)	1.397(11)
N(1)-H(65)	0.8800
C(2)-C(3)	1.387(12)
C(2)-C(18)	1.412(12)
N(2)-C(12)	1.373(10)
N(2)-C(52)	1.392(11)
N(2)-H(66)	0.8800
N(3)-C(45)	1.360(11)
N(3)-C(8)	1.413(10)
N(3)-H(67)	0.8800
C(3)-C(4)	1.389(12)
C(3)-H(2)	0.9500
C(4)-C(41)	1.387(12)
C(5)-C(22)	1.488(11)
C(5)-C(24)	1.495(11)
C(5)-H(3)	0.9900
C(5)-H(4)	0.9900
C(6)-C(29)	1.386(12)
N(4)-C(36)	1.338(11)
N(4)-C(21)	1.398(11)
N(4)-H(68)	0.8800
C(7)-C(53)	1.528(12)
C(7)-C(27)	1.545(12)

C(7)-H(5)	0.9900
C(7)-H(6)	0.9900
C(8)-C(34)	1.351(12)
C(8)-C(9)	1.473(12)
C(9)-C(20)	1.494(12)
C(9)-C(53)	1.532(12)
C(9)-C(26)	1.569(11)
C(10)-C(21)	1.492(13)
C(10)-C(52)	1.528(13)
C(10)-C(13)	1.548(12)
C(10)-C(33)	1.569(11)
C(11)-C(24)	1.537(11)
C(11)-C(23)	1.579(12)
C(11)-H(7)	0.9900
C(11)-H(8)	0.9900
C(12)-C(54)	1.350(11)
C(12)-C(23)	1.485(12)
C(13)-C(49)	1.531(12)
C(13)-H(9)	0.9900
C(13)-H(10)	0.9900
C(14)-C(48)	1.528(12)
C(14)-C(46)	1.543(12)
C(14)-H(11)	0.9900
C(14)-H(12)	0.9900
C(15)-C(39)	1.359(12)
C(15)-C(47)	1.388(13)
C(15)-H(13)	0.9500
C(16)-C(17)	1.532(12)
C(16)-H(14)	0.9800
C(16)-H(15)	0.9800
C(16)-H(16)	0.9800
C(17)-C(41)	1.360(12)
C(17)-C(18)	1.418(12)
C(18)-H(17)	0.9500
C(19)-C(21)	1.362(13)
C(19)-C(51)	1.448(13)
C(19)-H(18)	0.9500
C(20)-C(43)	1.375(13)
C(22)-H(19)	0.9900

C(22)-H(20)	0.9900
C(23)-C(45)	1.505(12)
C(23)-C(32)	1.532(12)
C(24)-H(21)	0.9900
C(24)-H(22)	0.9900
C(25)-C(46)	1.504(12)
C(25)-H(23)	0.9900
C(25)-H(24)	0.9900
C(26)-H(25)	0.9800
C(26)-H(26)	0.9800
C(26)-H(27)	0.9800
C(27)-C(28)	1.524(12)
C(27)-H(28)	0.9900
C(27)-H(29)	0.9900
C(28)-H(30)	0.9900
C(28)-H(31)	0.9900
C(29)-C(47)	1.370(12)
C(29)-H(32)	0.9500
C(30)-C(37)	1.551(12)
C(30)-H(33)	0.9800
C(30)-H(34)	0.9800
C(30)-H(35)	0.9800
C(31)-C(38)	1.365(12)
C(31)-C(37)	1.533(13)
C(32)-H(36)	0.9800
C(32)-H(37)	0.9800
C(32)-H(38)	0.9800
C(33)-H(39)	0.9800
C(33)-H(40)	0.9800
C(33)-H(41)	0.9800
C(34)-C(35)	1.458(12)
C(34)-H(42)	0.9500
C(35)-C(45)	1.360(11)
C(35)-H(43)	0.9500
C(36)-C(51)	1.391(12)
C(36)-C(37)	1.505(12)
C(37)-C(48)	1.549(12)
C(38)-C(43)	1.418(12)
C(38)-H(44)	0.9500

C(40)-C(49)	1.520(12)
C(40)-C(55)	1.540(13)
C(40)-H(45)	0.9900
C(40)-H(46)	0.9900
C(41)-H(47)	0.9500
C(42)-C(52)	1.359(12)
C(42)-C(54)	1.417(12)
C(42)-H(48)	0.9500
C(43)-H(49)	0.9500
C(44)-C(47)	1.489(12)
C(44)-H(50)	0.9800
C(44)-H(51)	0.9800
C(44)-H(52)	0.9800
C(46)-H(53)	0.9900
C(46)-H(54)	0.9900
C(48)-H(55)	0.9900
C(48)-H(56)	0.9900
C(49)-H(57)	0.9900
C(49)-H(58)	0.9900
C(50)-Cl(3)	1.821(11)
C(51)-H(59)	0.9500
C(53)-H(60)	0.9900
C(53)-H(61)	0.9900
C(54)-H(62)	0.9500
C(55)-H(63)	0.9900
C(55)-H(64)	0.9900
C(56)-O(6)	1.456(10)
C(56)-H(69)	0.9800
C(56)-H(70)	0.9800
C(56)-H(71)	0.9800
O(6)-H(72)	0.8400

C(6)-O(1)-C(28)	118.5(8)
C(2)-O(2)-C(55)	120.6(8)
C(4)-O(3)-C(25)	118.7(7)
C(39)-O(4)-C(22)	120.2(8)
C(6)-C(1)-C(39)	118.1(10)
C(6)-C(1)-H(1)	121.0
C(39)-C(1)-H(1)	121.0

C(20)-N(1)-C(31)	109.1(8)
C(20)-N(1)-H(65)	125.4
C(31)-N(1)-H(65)	125.4
O(2)-C(2)-C(3)	116.4(9)
O(2)-C(2)-C(18)	123.0(9)
C(3)-C(2)-C(18)	120.6(10)
C(12)-N(2)-C(52)	110.1(8)
C(12)-N(2)-H(66)	125.0
C(52)-N(2)-H(66)	125.0
C(45)-N(3)-C(8)	112.4(8)
C(45)-N(3)-H(67)	123.8
C(8)-N(3)-H(67)	123.8
C(2)-C(3)-C(4)	118.9(10)
C(2)-C(3)-H(2)	120.5
C(4)-C(3)-H(2)	120.5
O(3)-C(4)-C(41)	124.8(9)
O(3)-C(4)-C(3)	114.1(9)
C(41)-C(4)-C(3)	121.1(9)
C(22)-C(5)-C(24)	112.2(8)
C(22)-C(5)-H(3)	109.2
C(24)-C(5)-H(3)	109.2
C(22)-C(5)-H(4)	109.2
C(24)-C(5)-H(4)	109.2
H(3)-C(5)-H(4)	107.9
C(1)-C(6)-C(29)	121.4(11)
C(1)-C(6)-O(1)	123.7(10)
C(29)-C(6)-O(1)	114.9(10)
C(36)-N(4)-C(21)	112.2(9)
C(36)-N(4)-H(68)	123.9
C(21)-N(4)-H(68)	123.9
C(53)-C(7)-C(27)	111.1(8)
C(53)-C(7)-H(5)	109.4
C(27)-C(7)-H(5)	109.4
C(53)-C(7)-H(6)	109.4
C(27)-C(7)-H(6)	109.4
H(5)-C(7)-H(6)	108.0
C(34)-C(8)-N(3)	104.7(9)
C(34)-C(8)-C(9)	132.9(9)
N(3)-C(8)-C(9)	122.2(9)

C(8)-C(9)-C(20) 112.3(8)
C(8)-C(9)-C(53) 110.1(8)
C(20)-C(9)-C(53) 109.5(8)
C(8)-C(9)-C(26) 108.5(8)
C(20)-C(9)-C(26) 107.0(8)
C(53)-C(9)-C(26) 109.4(7)
C(21)-C(10)-C(52) 110.3(8)
C(21)-C(10)-C(13) 110.7(8)
C(52)-C(10)-C(13) 110.7(8)
C(21)-C(10)-C(33) 107.9(9)
C(52)-C(10)-C(33) 108.1(7)
C(13)-C(10)-C(33) 109.0(8)
C(24)-C(11)-C(23) 116.2(7)
C(24)-C(11)-H(7) 108.2
C(23)-C(11)-H(7) 108.2
C(24)-C(11)-H(8) 108.2
C(23)-C(11)-H(8) 108.2
H(7)-C(11)-H(8) 107.4
C(54)-C(12)-N(2) 106.6(8)
C(54)-C(12)-C(23) 132.2(9)
N(2)-C(12)-C(23) 121.1(8)
C(49)-C(13)-C(10) 116.3(8)
C(49)-C(13)-H(9) 108.2
C(10)-C(13)-H(9) 108.2
C(49)-C(13)-H(10) 108.2
C(10)-C(13)-H(10) 108.2
H(9)-C(13)-H(10) 107.4
C(48)-C(14)-C(46) 114.4(8)
C(48)-C(14)-H(11) 108.7
C(46)-C(14)-H(11) 108.7
C(48)-C(14)-H(12) 108.7
C(46)-C(14)-H(12) 108.7
H(11)-C(14)-H(12) 107.6
C(39)-C(15)-C(47) 121.6(11)
C(39)-C(15)-H(13) 119.2
C(47)-C(15)-H(13) 119.2
C(17)-C(16)-H(14) 109.5
C(17)-C(16)-H(15) 109.5
H(14)-C(16)-H(15) 109.5

C(17)-C(16)-H(16) 109.5
H(14)-C(16)-H(16) 109.5
H(15)-C(16)-H(16) 109.5
C(41)-C(17)-C(18) 120.2(10)
C(41)-C(17)-C(16) 119.8(10)
C(18)-C(17)-C(16) 120.0(10)
C(2)-C(18)-C(17) 118.5(10)
C(2)-C(18)-H(17) 120.7
C(17)-C(18)-H(17) 120.7
C(21)-C(19)-C(51) 109.4(9)
C(21)-C(19)-H(18) 125.3
C(51)-C(19)-H(18) 125.3
C(43)-C(20)-N(1) 106.5(9)
C(43)-C(20)-C(9) 130.9(10)
N(1)-C(20)-C(9) 122.6(9)
C(19)-C(21)-N(4) 105.1(9)
C(19)-C(21)-C(10) 131.8(10)
N(4)-C(21)-C(10) 123.0(9)
O(4)-C(22)-C(5) 113.3(8)
O(4)-C(22)-H(19) 108.9
C(5)-C(22)-H(19) 108.9
O(4)-C(22)-H(20) 108.9
C(5)-C(22)-H(20) 108.9
H(19)-C(22)-H(20) 107.7
C(12)-C(23)-C(45) 110.9(8)
C(12)-C(23)-C(32) 109.8(8)
C(45)-C(23)-C(32) 109.1(8)
C(12)-C(23)-C(11) 108.3(8)
C(45)-C(23)-C(11) 109.0(7)
C(32)-C(23)-C(11) 109.7(8)
C(5)-C(24)-C(11) 113.6(7)
C(5)-C(24)-H(21) 108.8
C(11)-C(24)-H(21) 108.8
C(5)-C(24)-H(22) 108.8
C(11)-C(24)-H(22) 108.8
H(21)-C(24)-H(22) 107.7
O(3)-C(25)-C(46) 115.6(7)
O(3)-C(25)-H(23) 108.4
C(46)-C(25)-H(23) 108.4

O(3)-C(25)-H(24) 108.4
C(46)-C(25)-H(24) 108.4
H(23)-C(25)-H(24) 107.4
C(9)-C(26)-H(25) 109.5
C(9)-C(26)-H(26) 109.5
H(25)-C(26)-H(26) 109.5
C(9)-C(26)-H(27) 109.5
H(25)-C(26)-H(27) 109.5
H(26)-C(26)-H(27) 109.5
C(28)-C(27)-C(7) 111.6(8)
C(28)-C(27)-H(28) 109.3
C(7)-C(27)-H(28) 109.3
C(28)-C(27)-H(29) 109.3
C(7)-C(27)-H(29) 109.3
H(28)-C(27)-H(29) 108.0
O(1)-C(28)-C(27) 111.9(8)
O(1)-C(28)-H(30) 109.2
C(27)-C(28)-H(30) 109.2
O(1)-C(28)-H(31) 109.2
C(27)-C(28)-H(31) 109.2
H(30)-C(28)-H(31) 107.9
C(47)-C(29)-C(6) 120.9(11)
C(47)-C(29)-H(32) 119.5
C(6)-C(29)-H(32) 119.5
C(37)-C(30)-H(33) 109.5
C(37)-C(30)-H(34) 109.5
H(33)-C(30)-H(34) 109.5
C(37)-C(30)-H(35) 109.5
H(33)-C(30)-H(35) 109.5
H(34)-C(30)-H(35) 109.5
C(38)-C(31)-N(1) 108.1(9)
C(38)-C(31)-C(37) 132.2(10)
N(1)-C(31)-C(37) 119.7(10)
C(23)-C(32)-H(36) 109.5
C(23)-C(32)-H(37) 109.5
H(36)-C(32)-H(37) 109.5
C(23)-C(32)-H(38) 109.5
H(36)-C(32)-H(38) 109.5
H(37)-C(32)-H(38) 109.5

C(10)-C(33)-H(39) 109.5
C(10)-C(33)-H(40) 109.5
H(39)-C(33)-H(40) 109.5
C(10)-C(33)-H(41) 109.5
H(39)-C(33)-H(41) 109.5
H(40)-C(33)-H(41) 109.5
C(8)-C(34)-C(35) 108.8(8)
C(8)-C(34)-H(42) 125.6
C(35)-C(34)-H(42) 125.6
C(45)-C(35)-C(34) 107.6(8)
C(45)-C(35)-H(43) 126.2
C(34)-C(35)-H(43) 126.2
N(4)-C(36)-C(51) 107.9(9)
N(4)-C(36)-C(37) 124.0(9)
C(51)-C(36)-C(37) 128.1(10)
C(36)-C(37)-C(31) 109.8(8)
C(36)-C(37)-C(48) 110.7(8)
C(31)-C(37)-C(48) 110.6(8)
C(36)-C(37)-C(30) 109.2(8)
C(31)-C(37)-C(30) 107.5(8)
C(48)-C(37)-C(30) 108.9(8)
C(31)-C(38)-C(43) 107.1(9)
C(31)-C(38)-H(44) 126.5
C(43)-C(38)-H(44) 126.5
C(15)-C(39)-O(4) 116.2(10)
C(15)-C(39)-C(1) 120.8(10)
O(4)-C(39)-C(1) 123.1(10)
C(49)-C(40)-C(55) 113.8(8)
C(49)-C(40)-H(45) 108.8
C(55)-C(40)-H(45) 108.8
C(49)-C(40)-H(46) 108.8
C(55)-C(40)-H(46) 108.8
H(45)-C(40)-H(46) 107.7
C(17)-C(41)-C(4) 120.5(10)
C(17)-C(41)-H(47) 119.7
C(4)-C(41)-H(47) 119.7
C(52)-C(42)-C(54) 107.3(9)
C(52)-C(42)-H(48) 126.3
C(54)-C(42)-H(48) 126.3

C(20)-C(43)-C(38) 109.2(9)
C(20)-C(43)-H(49) 125.4
C(38)-C(43)-H(49) 125.4
C(47)-C(44)-H(50) 109.5
C(47)-C(44)-H(51) 109.5
H(50)-C(44)-H(51) 109.5
C(47)-C(44)-H(52) 109.5
H(50)-C(44)-H(52) 109.5
H(51)-C(44)-H(52) 109.5
C(35)-C(45)-N(3) 106.4(8)
C(35)-C(45)-C(23) 132.2(9)
N(3)-C(45)-C(23) 121.2(8)
C(25)-C(46)-C(14) 115.3(8)
C(25)-C(46)-H(53) 108.4
C(14)-C(46)-H(53) 108.4
C(25)-C(46)-H(54) 108.4
C(14)-C(46)-H(54) 108.4
H(53)-C(46)-H(54) 107.5
C(29)-C(47)-C(15) 117.2(11)
C(29)-C(47)-C(44) 119.3(10)
C(15)-C(47)-C(44) 123.5(11)
C(14)-C(48)-C(37) 116.2(8)
C(14)-C(48)-H(55) 108.2
C(37)-C(48)-H(55) 108.2
C(14)-C(48)-H(56) 108.2
C(37)-C(48)-H(56) 108.2
H(55)-C(48)-H(56) 107.4
C(40)-C(49)-C(13) 110.4(8)
C(40)-C(49)-H(57) 109.6
C(13)-C(49)-H(57) 109.6
C(40)-C(49)-H(58) 109.6
C(13)-C(49)-H(58) 109.6
H(57)-C(49)-H(58) 108.1
Cl(2)-C(50)-Cl(1) 110.8(6)
Cl(2)-C(50)-Cl(3) 107.0(6)
Cl(1)-C(50)-Cl(3) 109.1(6)
C(36)-C(51)-C(19) 105.4(9)
C(36)-C(51)-H(59) 127.3
C(19)-C(51)-H(59) 127.3

C(42)-C(52)-N(2) 106.8(9)
C(42)-C(52)-C(10) 131.3(9)
N(2)-C(52)-C(10) 121.9(9)
C(7)-C(53)-C(9) 116.6(8)
C(7)-C(53)-H(60) 108.1
C(9)-C(53)-H(60) 108.1
C(7)-C(53)-H(61) 108.1
C(9)-C(53)-H(61) 108.1
H(60)-C(53)-H(61) 107.3
C(12)-C(54)-C(42) 109.2(9)
C(12)-C(54)-H(62) 125.4
C(42)-C(54)-H(62) 125.4
O(2)-C(55)-C(40) 113.1(8)
O(2)-C(55)-H(63) 109.0
C(40)-C(55)-H(63) 109.0
O(2)-C(55)-H(64) 109.0
C(40)-C(55)-H(64) 109.0
H(63)-C(55)-H(64) 107.8
O(6)-C(56)-H(69) 109.5
O(6)-C(56)-H(70) 109.5
H(69)-C(56)-H(70) 109.5
O(6)-C(56)-H(71) 109.5
H(69)-C(56)-H(71) 109.5
H(70)-C(56)-H(71) 109.5
C(56)-O(6)-H(72) 109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for compound **2**. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	108(2)	89(2)	108(2)	-23(2)	-13(2)	-25(2)
Cl(2)	142(3)	112(2)	137(3)	-10(2)	-55(2)	-53(2)
O(1)	86(5)	90(4)	70(4)	-19(3)	-11(4)	-34(4)
O(2)	66(5)	93(4)	85(4)	-23(3)	-17(4)	-36(4)
O(3)	77(5)	69(4)	85(4)	-17(3)	-16(4)	-27(3)
O(4)	86(5)	82(4)	86(5)	-14(3)	-14(4)	-34(4)
C(1)	78(8)	63(5)	80(7)	-24(5)	-10(6)	-23(5)
N(1)	58(5)	77(5)	85(6)	-33(4)	3(4)	-27(4)
C(2)	72(7)	72(6)	74(7)	-11(5)	-26(6)	-21(5)
N(2)	80(6)	71(5)	76(6)	-27(4)	-12(4)	-15(4)
N(3)	84(7)	69(5)	98(6)	-36(4)	-11(5)	-23(4)
C(3)	68(7)	81(6)	79(7)	-23(5)	-7(5)	-28(5)
C(4)	65(7)	57(5)	87(7)	-18(5)	-6(6)	-21(5)
C(5)	71(7)	80(6)	80(7)	-21(5)	-13(5)	-29(5)
C(6)	83(8)	64(6)	92(8)	-19(5)	-25(7)	-15(5)
N(4)	74(6)	75(5)	106(6)	-17(4)	-12(5)	-32(4)
C(7)	74(7)	81(6)	90(8)	-16(5)	1(6)	-28(5)
C(8)	78(8)	71(6)	91(7)	-28(5)	-17(6)	-32(6)
C(9)	68(7)	69(6)	85(7)	-22(5)	-15(6)	-25(5)
C(10)	91(8)	72(6)	86(7)	-19(5)	-14(6)	-34(6)
C(11)	66(7)	63(5)	92(7)	-27(5)	-13(5)	-12(5)
C(12)	60(6)	66(6)	85(7)	-13(5)	-20(5)	-13(5)
C(13)	76(7)	85(6)	81(7)	-15(5)	-12(6)	-34(6)
C(14)	78(7)	80(6)	92(7)	-21(5)	-12(6)	-31(6)
C(15)	113(10)	89(7)	63(7)	-18(5)	-3(6)	-41(7)
C(16)	105(9)	104(7)	72(7)	-24(5)	5(6)	-44(7)
C(17)	77(8)	80(6)	92(8)	-21(5)	-22(6)	-16(6)
C(18)	80(8)	78(6)	91(8)	-14(5)	-26(6)	-35(5)
C(19)	68(7)	92(7)	107(8)	-31(6)	-23(6)	-27(6)
C(20)	71(7)	71(6)	93(8)	-29(6)	-13(6)	-25(5)
C(21)	65(7)	87(7)	97(7)	-22(5)	-26(6)	-31(6)
C(22)	78(7)	96(7)	75(7)	-13(5)	-15(6)	-35(6)
C(23)	53(6)	91(7)	76(7)	-22(5)	-4(5)	-22(5)
C(24)	65(7)	80(6)	84(7)	-16(5)	-8(5)	-21(5)

C(25)	84(8)	79(6)	93(7)	-25(5)	-8(6)	-33(6)
C(26)	92(8)	75(6)	95(7)	-24(5)	-23(6)	-29(6)
C(27)	68(7)	90(7)	100(8)	-26(6)	-2(6)	-36(6)
C(28)	120(10)	74(6)	90(8)	-16(6)	-21(7)	-35(6)
C(29)	83(8)	82(7)	73(7)	-15(5)	-12(6)	-26(6)
C(30)	64(7)	90(7)	113(8)	-33(6)	-17(6)	-24(5)
C(31)	62(7)	85(7)	110(9)	-39(6)	-11(6)	-17(6)
C(32)	77(8)	86(7)	104(8)	-37(6)	1(6)	-28(6)
C(33)	116(9)	56(5)	113(8)	-17(5)	-32(7)	-39(5)
C(34)	82(8)	61(5)	87(7)	-28(5)	-11(6)	-18(5)
C(35)	58(7)	84(7)	81(7)	-23(5)	-7(5)	-14(5)
C(36)	57(7)	99(8)	101(8)	-21(6)	-16(6)	-33(6)
C(37)	80(8)	78(6)	89(7)	-20(5)	-12(6)	-36(6)
C(38)	51(6)	89(7)	98(8)	-39(6)	5(6)	-20(5)
C(39)	74(8)	67(6)	98(8)	-19(6)	-11(6)	-19(5)
C(40)	84(8)	125(9)	84(7)	-4(6)	-24(6)	-67(7)
C(41)	67(7)	77(6)	90(8)	-24(5)	-4(6)	-27(5)
C(42)	88(8)	76(6)	93(8)	-18(6)	-32(6)	-30(5)
C(43)	81(8)	94(7)	86(8)	-10(6)	-19(6)	-34(6)
C(44)	110(9)	98(7)	88(8)	-42(6)	0(7)	-23(7)
C(45)	47(6)	80(6)	93(7)	-36(5)	-8(5)	-16(5)
C(46)	68(7)	91(7)	109(8)	-25(6)	-15(6)	-35(6)
C(47)	84(8)	70(6)	83(8)	-18(5)	-12(6)	-13(5)
C(48)	83(8)	76(6)	87(7)	-37(5)	1(6)	-24(5)
C(49)	71(7)	83(7)	95(7)	-23(6)	5(6)	-34(6)
C(50)	76(8)	87(7)	152(10)	-35(7)	-29(7)	-20(6)
C(51)	75(8)	75(6)	99(8)	-22(5)	-25(6)	-9(5)
C(52)	85(8)	72(6)	97(8)	-22(6)	-18(6)	-32(5)
C(53)	92(8)	81(6)	94(8)	-21(6)	-7(6)	-29(6)
C(54)	56(6)	83(6)	83(7)	-25(5)	-5(5)	-16(5)
C(55)	101(9)	86(7)	100(8)	-25(6)	-16(6)	-44(6)
Cl(3)	115(3)	98(2)	130(3)	-21(2)	0(2)	-44(2)
C(56)	138(14)	242(19)	149(12)	-58(12)	1(12)	-125(15)
O(6)	177(15)	238(18)	1050(70)		-350(30)	-190(20) 7(13)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for compound **2**.

	x	y	z	U(eq)
H(1)	1568	4607	-2307	87
H(65)	3730	2174	1863	85
H(66)	1105	723	1914	91
H(67)	2817	1719	375	96
H(2)	1419	2646	2198	89
H(3)	1500	2572	-1677	90
H(4)	567	1902	-1652	90
H(68)	3185	262	2529	100
H(5)	3348	5347	-818	100
H(6)	2438	4621	-727	100
H(7)	1723	1261	-408	89
H(8)	544	880	-326	89
H(9)	1426	-1107	3735	95
H(10)	1249	50	3092	95
H(11)	5414	2482	2507	97
H(12)	5953	1869	3264	97
H(13)	1248	3723	-4054	104
H(14)	673	2435	5167	138
H(15)	-745	2895	5034	138
H(16)	-42	3823	4899	138
H(17)	-824	2150	4050	95
H(18)	4613	-3209	3130	103
H(19)	-981	3707	-1988	98
H(20)	-99	4406	-1973	98
H(21)	-692	2844	-726	93
H(22)	388	3316	-713	93
H(23)	2700	4641	3114	99
H(24)	3712	4535	2439	99
H(25)	3009	5223	443	126
H(26)	4446	4649	538	126
H(27)	3460	4399	1198	126
H(28)	4581	4357	-1760	100
H(29)	3529	3809	-1706	100

H(30)	2096	5761	-2050	112
H(31)	3159	6300	-2114	112
H(32)	3751	5228	-4131	96
H(33)	6831	-632	3307	129
H(34)	7216	294	2632	129
H(35)	7232	-939	2540	129
H(36)	-1089	1223	790	131
H(37)	-1254	2589	432	131
H(38)	-980	2035	1251	131
H(39)	2910	-3312	2736	135
H(40)	1453	-2862	2938	135
H(41)	2354	-3117	3520	135
H(42)	1193	4784	893	91
H(43)	-430	3849	928	92
H(44)	7141	271	1266	94
H(45)	-626	326	3973	108
H(46)	-1756	87	3789	108
H(47)	1730	3676	3905	93
H(48)	2469	-2437	1489	99
H(49)	6197	1788	177	104
H(50)	3771	4605	-5122	150
H(51)	2371	5054	-5287	150
H(52)	3113	3665	-5054	150
H(53)	3833	2873	3782	103
H(54)	4714	3643	3444	103
H(55)	3866	1479	3011	97
H(56)	4774	684	3609	97
H(57)	-289	-503	2725	99
H(58)	-224	-1445	3484	99
H(59)	6286	-2309	3050	102
H(60)	4956	3630	-442	107
H(61)	4220	2816	-484	107
H(62)	1786	-873	359	90
H(63)	-1837	1520	2691	109
H(64)	-1947	2114	3330	109
H(69)	5707	1242	-1031	237
H(70)	5275	475	-1383	237
H(71)	6062	-159	-711	237
H(72)	3818	504	-574	668

Table 6. Torsion angles [°] for compound **2**.

C(55)-O(2)-C(2)-C(3)	-178.0(8)
C(55)-O(2)-C(2)-C(18)	3.5(12)
O(2)-C(2)-C(3)-C(4)	178.4(7)
C(18)-C(2)-C(3)-C(4)	-3.1(13)
C(25)-O(3)-C(4)-C(41)	-0.7(12)
C(25)-O(3)-C(4)-C(3)	-179.0(7)
C(2)-C(3)-C(4)-O(3)	-179.9(7)
C(2)-C(3)-C(4)-C(41)	1.8(13)
C(39)-C(1)-C(6)-C(29)	-1.3(14)
C(39)-C(1)-C(6)-O(1)	178.2(8)
C(28)-O(1)-C(6)-C(1)	0.5(13)
C(28)-O(1)-C(6)-C(29)	-180.0(8)
C(45)-N(3)-C(8)-C(34)	-0.3(11)
C(45)-N(3)-C(8)-C(9)	-176.4(8)
C(34)-C(8)-C(9)-C(20)	128.5(12)
N(3)-C(8)-C(9)-C(20)	-56.6(12)
C(34)-C(8)-C(9)-C(53)	-109.1(12)
N(3)-C(8)-C(9)-C(53)	65.7(11)
C(34)-C(8)-C(9)-C(26)	10.5(15)
N(3)-C(8)-C(9)-C(26)	-174.6(8)
C(52)-N(2)-C(12)-C(54)	-0.9(10)
C(52)-N(2)-C(12)-C(23)	175.3(8)
C(21)-C(10)-C(13)-C(49)	178.9(8)
C(52)-C(10)-C(13)-C(49)	56.2(11)
C(33)-C(10)-C(13)-C(49)	-62.5(11)
O(2)-C(2)-C(18)-C(17)	-179.2(8)
C(3)-C(2)-C(18)-C(17)	2.4(13)
C(41)-C(17)-C(18)-C(2)	-0.3(13)
C(16)-C(17)-C(18)-C(2)	179.9(8)
C(31)-N(1)-C(20)-C(43)	-0.1(10)
C(31)-N(1)-C(20)-C(9)	-178.6(8)
C(8)-C(9)-C(20)-C(43)	134.3(11)
C(53)-C(9)-C(20)-C(43)	11.6(14)
C(26)-C(9)-C(20)-C(43)	-106.9(12)
C(8)-C(9)-C(20)-N(1)	-47.6(12)
C(53)-C(9)-C(20)-N(1)	-170.3(8)
C(26)-C(9)-C(20)-N(1)	71.3(11)

C(51)-C(19)-C(21)-N(4)	-1.1(11)
C(51)-C(19)-C(21)-C(10)	-179.9(10)
C(36)-N(4)-C(21)-C(19)	1.0(12)
C(36)-N(4)-C(21)-C(10)	179.9(9)
C(52)-C(10)-C(21)-C(19)	-114.8(12)
C(13)-C(10)-C(21)-C(19)	122.3(12)
C(33)-C(10)-C(21)-C(19)	3.1(16)
C(52)-C(10)-C(21)-N(4)	66.6(12)
C(13)-C(10)-C(21)-N(4)	-56.3(12)
C(33)-C(10)-C(21)-N(4)	-175.5(8)
C(39)-O(4)-C(22)-C(5)	-83.0(10)
C(24)-C(5)-C(22)-O(4)	176.6(7)
C(54)-C(12)-C(23)-C(45)	-135.8(10)
N(2)-C(12)-C(23)-C(45)	49.1(12)
C(54)-C(12)-C(23)-C(32)	103.6(12)
N(2)-C(12)-C(23)-C(32)	-71.5(11)
C(54)-C(12)-C(23)-C(11)	-16.2(14)
N(2)-C(12)-C(23)-C(11)	168.7(8)
C(24)-C(11)-C(23)-C(12)	179.4(8)
C(24)-C(11)-C(23)-C(45)	-59.8(10)
C(24)-C(11)-C(23)-C(32)	59.6(10)
C(22)-C(5)-C(24)-C(11)	171.3(8)
C(23)-C(11)-C(24)-C(5)	171.6(8)
C(4)-O(3)-C(25)-C(46)	79.1(10)
C(53)-C(7)-C(27)-C(28)	-171.9(8)
C(6)-O(1)-C(28)-C(27)	86.3(10)
C(7)-C(27)-C(28)-O(1)	-179.2(8)
C(1)-C(6)-C(29)-C(47)	0.6(14)
O(1)-C(6)-C(29)-C(47)	-178.9(8)
C(20)-N(1)-C(31)-C(38)	1.6(10)
C(20)-N(1)-C(31)-C(37)	-179.5(8)
N(3)-C(8)-C(34)-C(35)	-0.1(10)
C(9)-C(8)-C(34)-C(35)	175.4(9)
C(8)-C(34)-C(35)-C(45)	0.5(10)
C(21)-N(4)-C(36)-C(51)	-0.4(12)
C(21)-N(4)-C(36)-C(37)	179.6(9)
N(4)-C(36)-C(37)-C(31)	-64.2(13)
C(51)-C(36)-C(37)-C(31)	115.8(12)
N(4)-C(36)-C(37)-C(48)	58.2(13)

C(51)-C(36)-C(37)-C(48)	-121.8(12)
N(4)-C(36)-C(37)-C(30)	178.1(9)
C(51)-C(36)-C(37)-C(30)	-1.9(15)
C(38)-C(31)-C(37)-C(36)	-95.7(13)
N(1)-C(31)-C(37)-C(36)	85.8(11)
C(38)-C(31)-C(37)-C(48)	141.8(10)
N(1)-C(31)-C(37)-C(48)	-36.7(12)
C(38)-C(31)-C(37)-C(30)	23.0(14)
N(1)-C(31)-C(37)-C(30)	-155.5(8)
N(1)-C(31)-C(38)-C(43)	-2.5(10)
C(37)-C(31)-C(38)-C(43)	178.9(10)
C(47)-C(15)-C(39)-O(4)	178.6(8)
C(47)-C(15)-C(39)-C(1)	-0.4(15)
C(22)-O(4)-C(39)-C(15)	177.6(8)
C(22)-O(4)-C(39)-C(1)	-3.4(12)
C(6)-C(1)-C(39)-C(15)	1.2(14)
C(6)-C(1)-C(39)-O(4)	-177.8(8)
C(18)-C(17)-C(41)-C(4)	-1.0(14)
C(16)-C(17)-C(41)-C(4)	178.8(8)
O(3)-C(4)-C(41)-C(17)	-177.9(8)
C(3)-C(4)-C(41)-C(17)	0.3(14)
N(1)-C(20)-C(43)-C(38)	-1.4(11)
C(9)-C(20)-C(43)-C(38)	176.9(9)
C(31)-C(38)-C(43)-C(20)	2.5(11)
C(34)-C(35)-C(45)-N(3)	-0.6(10)
C(34)-C(35)-C(45)-C(23)	-177.4(10)
C(8)-N(3)-C(45)-C(35)	0.6(11)
C(8)-N(3)-C(45)-C(23)	177.8(8)
C(12)-C(23)-C(45)-C(35)	-128.3(11)
C(32)-C(23)-C(45)-C(35)	-7.3(14)
C(11)-C(23)-C(45)-C(35)	112.5(11)
C(12)-C(23)-C(45)-N(3)	55.3(12)
C(32)-C(23)-C(45)-N(3)	176.3(8)
C(11)-C(23)-C(45)-N(3)	-63.9(11)
O(3)-C(25)-C(46)-C(14)	51.6(11)
C(48)-C(14)-C(46)-C(25)	-82.3(11)
C(6)-C(29)-C(47)-C(15)	0.1(14)
C(6)-C(29)-C(47)-C(44)	178.4(9)
C(39)-C(15)-C(47)-C(29)	-0.3(14)

C(39)-C(15)-C(47)-C(44)	-178.4(9)
C(46)-C(14)-C(48)-C(37)	162.0(8)
C(36)-C(37)-C(48)-C(14)	-178.7(9)
C(31)-C(37)-C(48)-C(14)	-56.7(11)
C(30)-C(37)-C(48)-C(14)	61.2(11)
C(55)-C(40)-C(49)-C(13)	87.3(10)
C(10)-C(13)-C(49)-C(40)	-166.6(8)
N(4)-C(36)-C(51)-C(19)	-0.3(11)
C(37)-C(36)-C(51)-C(19)	179.7(10)
C(21)-C(19)-C(51)-C(36)	0.9(12)
C(54)-C(42)-C(52)-N(2)	1.8(11)
C(54)-C(42)-C(52)-C(10)	-176.1(10)
C(12)-N(2)-C(52)-C(42)	-0.6(11)
C(12)-N(2)-C(52)-C(10)	177.5(9)
C(21)-C(10)-C(52)-C(42)	89.6(13)
C(13)-C(10)-C(52)-C(42)	-147.4(11)
C(33)-C(10)-C(52)-C(42)	-28.1(16)
C(21)-C(10)-C(52)-N(2)	-88.0(11)
C(13)-C(10)-C(52)-N(2)	34.9(12)
C(33)-C(10)-C(52)-N(2)	154.2(9)
C(27)-C(7)-C(53)-C(9)	-168.5(7)
C(8)-C(9)-C(53)-C(7)	57.1(11)
C(20)-C(9)-C(53)-C(7)	-179.0(8)
C(26)-C(9)-C(53)-C(7)	-62.0(11)
N(2)-C(12)-C(54)-C(42)	2.0(10)
C(23)-C(12)-C(54)-C(42)	-173.6(10)
C(52)-C(42)-C(54)-C(12)	-2.5(11)
C(2)-O(2)-C(55)-C(40)	-80.0(10)
C(49)-C(40)-C(55)-O(2)	-57.4(11)

Symmetry transformations used to generate equivalent atoms: