Electronic Supplementary Information

Anion-modulated, highly sensitive supramolecular fluorescence chemosensor for C_{70}

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Experimental

General: ^{1}H NMR, ^{13}CNMR spectra (300 or 400 MHz) were recorded using TMS as the internal standard. Fluorescence titration studies were carried out at 298 K. Toluene/acetonitrile (5%) solutions of the receptor or substrate were titrated by adding known quantities of a concentrated solution of the corresponding substrate or receptor. The data were fitted to a 1:1 receptor-to-substrate binding profile according to the method of Oster[1] using the changes in the emission. Job plots were obtained using emission spectra that spectra were recorded on a Perkin Elmer LS-55B at 298 K. All reagents were obtained from Aldrich or TCI used as received unless noted otherwise.

X-ray Crystallography: The X-ray diffraction data were collected on a Bruker SMART APEX diffractometer equipped with a monochromater in the Mo Kα (λ = 0.71073 Å) incident beam. A crystal was mounted on a glass fiber. The CCD data were integrated and scaled using the Bruker-SAINT software package, and the structure was solved and refined using SHEXTL V6.12.[2] All hydrogen atoms were placed in the calculated positions. The crystallographic data are listed in Table 1. Tables of positional and thermal parameters, bond lengths and angles, and torsion angles are located in tables 2 through 6.

References

1. *Binding Constants: The Measurement of Molecular Complex Stability.* Connors, A. K.
Wiley: New York, 1987.
2. Bruker, SHELXTL/PC. Version 6.12 for Windows XP. 2001, Bruker AXS Inc., Madison, Wisconsin, USA.

1, 3-Bis(2-(hydroxy)propan-2-yl)pyrene(1)

1,3-Acetylpyrene (0.572 g, 0.002 mole) was dissolved in dry THF (30 mL) under N_2 atmosphere, then CH_3MgBr (3.3 mL, 0.04 mole) was added dropwise over a period of 5 min at 0 ^oC. The whole mixture was stirred for 12 h at 0 ^oC. Then, the reaction was quenched by adding aqueous saturated $NaHCO_3$ (20 mL). The mixture was extracted with ethyl acetate and the organic layer was dried (Na_2SO_4) and solvent was removed in vacuo. The purification by silica gel column chromatography (CH_2Cl_2/EtOAc = 19/1) yielded **4** (0.430 g, 67 %) as yellow solid. ^{1}H NMR ($CDCl_3$) δ 9.07 (d, 2H, *J* = 9.52 Hz), 8.36 (s, 1H), 8.16 (d, 2H, *J* = 7.58 Hz), 8.06 (d, 2H, *J* = 9.52Hz), 7.99 (t, 1H, *J* = 7.58 Hz), 2.17(s, 2H), 2.02 (s, 12H) ; ^{13}C NMR($CDCl_3$) δ 140.63, 131.06, 128.60, 127.77, 126.91, 126.50, 126.34, 125.74, 125.54, 120.94, 75.17, 32.64; FAB-MS Calcd for $C_{22}H_{22}O_2$ 318.162, Found 318.1622(M), 319.1612(M + 1),

1, 3-Bis(2-(1*H*-pyrrol-2-yl)propan-2-yl)pyrene (2)

Compound **3** (0.5 g, 1.57 × 10^{-3} mole) and pyrrole (11 mL, 0.157 mole) were dissolved in CH_2Cl_2 (10 mL) with stirring, then BF_3•OEt_2 (276 μL, 2.20 × 10^{-4} mole) were added. The whole mixture was stirred for 15 min at 25 ^oC. Then, aqueous NaOH (30 mL, 1N) was added to the solution. The mixture was extracted with CH_2Cl_2 (20 mL X 3) and the organic layer was dried (Na_2SO_4). The solvent and excess pyrroles were removed in vacuo. The purification by silica gel column chromatography (CH_2Cl_2/Hexanes = 7/3) yielded **5** (0.430 g, 74 %) ; ^{1}H NMR ($CDCl_3$) δ 8.53 (s, 1H), 8.03 (d, 2H, *J* = 9.50 Hz), 8.02 (d, 2H, *J* = 7.52 Hz), 7.89 (t, 1H, *J* = 7.59 Hz), 7.78 (d, 2H, *J* = 9.52 Hz), 7.49 (br s, 2H), 6.50-6.46 (m, 2H), 6.32-6.31(m, 2H), 6.25-6.23 (q, 2H, *J* = 4.55 Hz), 2.05 (s, 12H) ; ^{13}C NMR ($CDCl_3$) δ 142.68, 140.38, 130.88, 129.21, 127.71, 127.01, 126.42, 125.51, 125.39, 125.27, 123.31, 116.68, 108.56, 103.04, 58.89, 41.09, 32.42, 18.81 ; FAB-MS Calcd for $C_{30}H_{28}N_2$ 416.2252, Found 416.2252(M), 417.2287(M + 1)

Calix[1]pyreno[3]pyrrole (**3**)

Compound **2** (0.1 g, 2.4 × 10^{-4} mole), pyrrole (16.6 μL, 2.4 × 10^{-4} mole) and acetone (37 μL, 4.8 × 10^{-4} mole) was dissolved in CH_2Cl_2 (20 mL) with stirring, then TFA (20 μL, 2.5 × 10^{-4} mole) was added. The whole mixture was stirred for 24 hr at 25 ^oC. Then, triethyl amine (300 μL) and water (20 mL) were added to the solution. The mixture was then extracted with CH_2Cl_2 (10 mL x 3). The organic layer was dried (Na_2SO_4) and solvent was removed in vacuo. The purification by silica gel column chromatography (CH_2Cl_2/Hexanes = 1/1) yielded **1** (0.012 g, 5.0 × 10^{-4} mole, 9%) ; ^{1}H NMR (CD_3CN) δ 8.61 (br s, 1H), 8.47 (d, 2H, *J* = 9.47 Hz), 8.14 (d, 2H, *J* = 7.61 Hz,), 7.97 (t, 1H, *J* = 7.57 Hz), 7.93 (d, 2H, *J* = 9.54 Hz), 7.74(s, 1H), 7.00 (br s, 2H), 6.20 (t, 2H, *J* = 3.13 Hz), 5.94 (t, 2H, *J* = 3.01 Hz), 5.52 (d, 2H, *J* = 2.84 Hz), 1.88 (s, 12H), 1.44 (s, 12H; ^{13}C NMR (CD_3CN) δ 140.78, 139.35, 139.33, 137. 08, 130. 17, 127.07, 126. 42, 126.03, 125.57, 125.02, 124.99, 124.62, 124.55, 103.85, 102.65, 101.08, 40.56, 35.06, 29.78, 28.79 ; MALDI-TOF Calcd for $C_{40}H_{41}N_3$ 563.33, Found 563.29(M), 576.30 (M + Na^+), 588.33 (M + K^+)

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

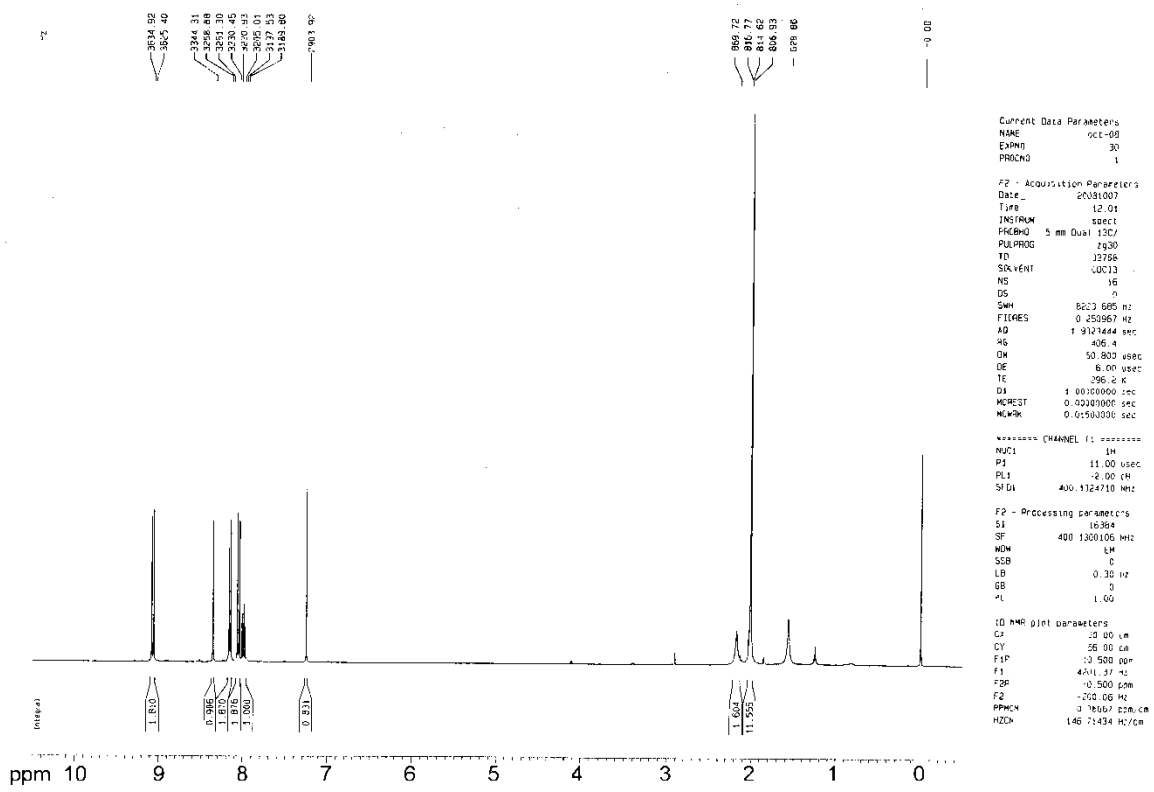


Figure 2. ^{13}C NMR spectrum of compound **1** in $CDCl_3$

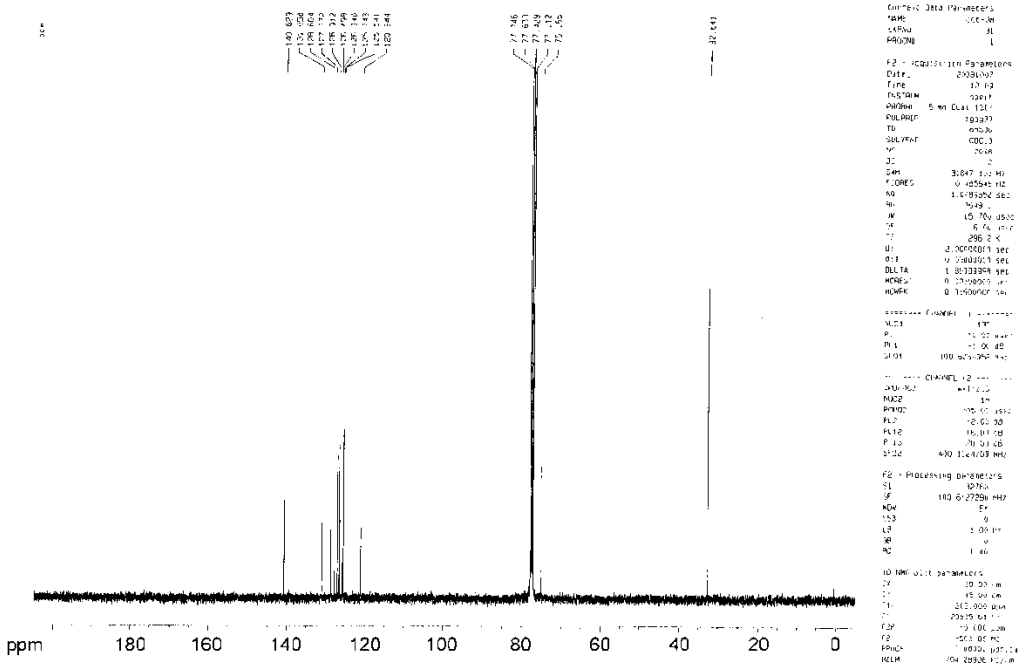


Figure 3. FAB-MS spectrum of compound **1**

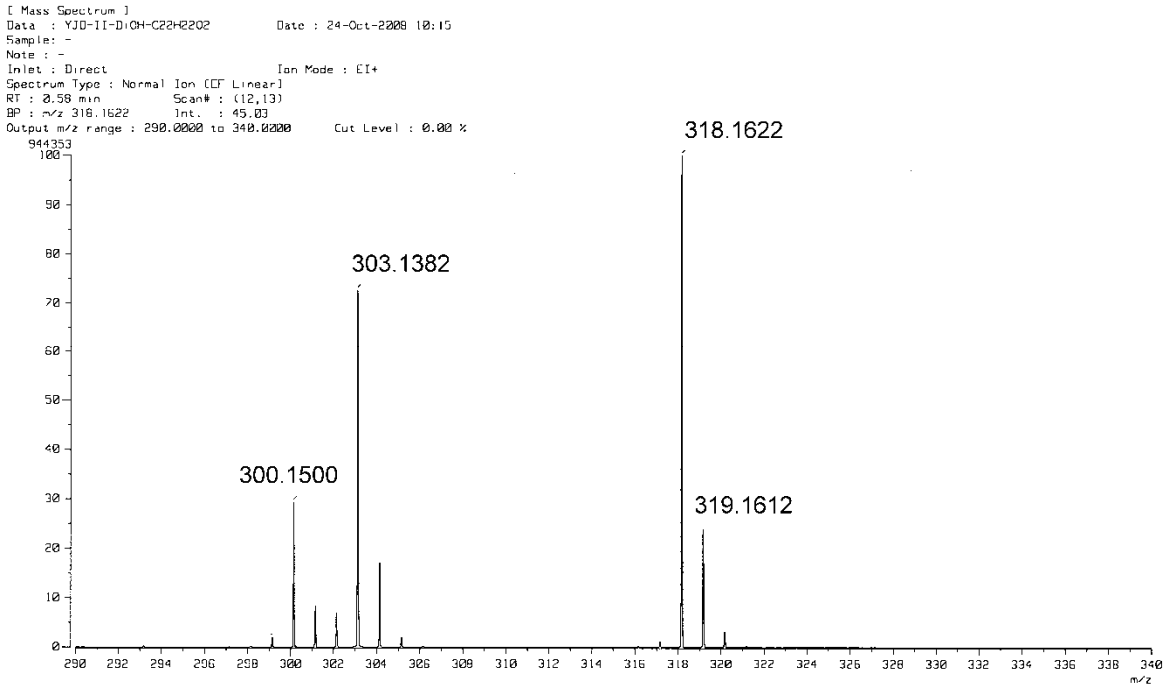


Figure 4. ^{1}H NMR spectrum of compound **2** in $CDCl_3$

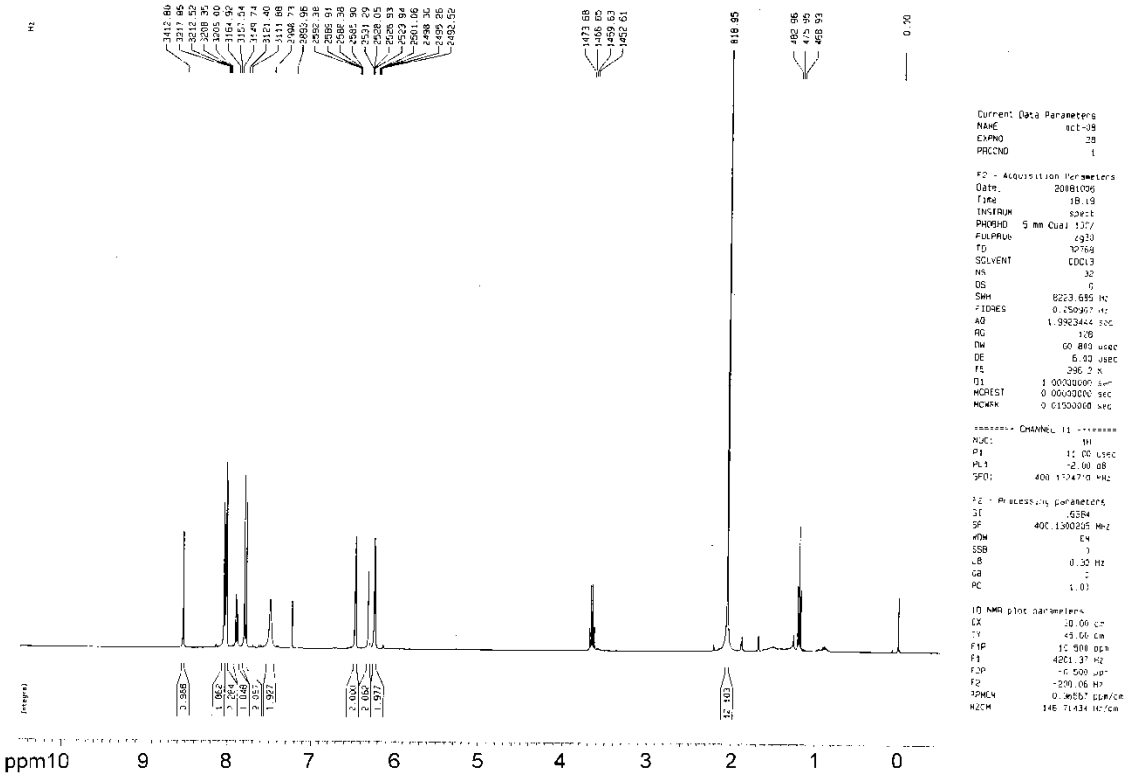


Figure 5. ^{13}C NMR spectrum of compound **2** in $CDCl_3$

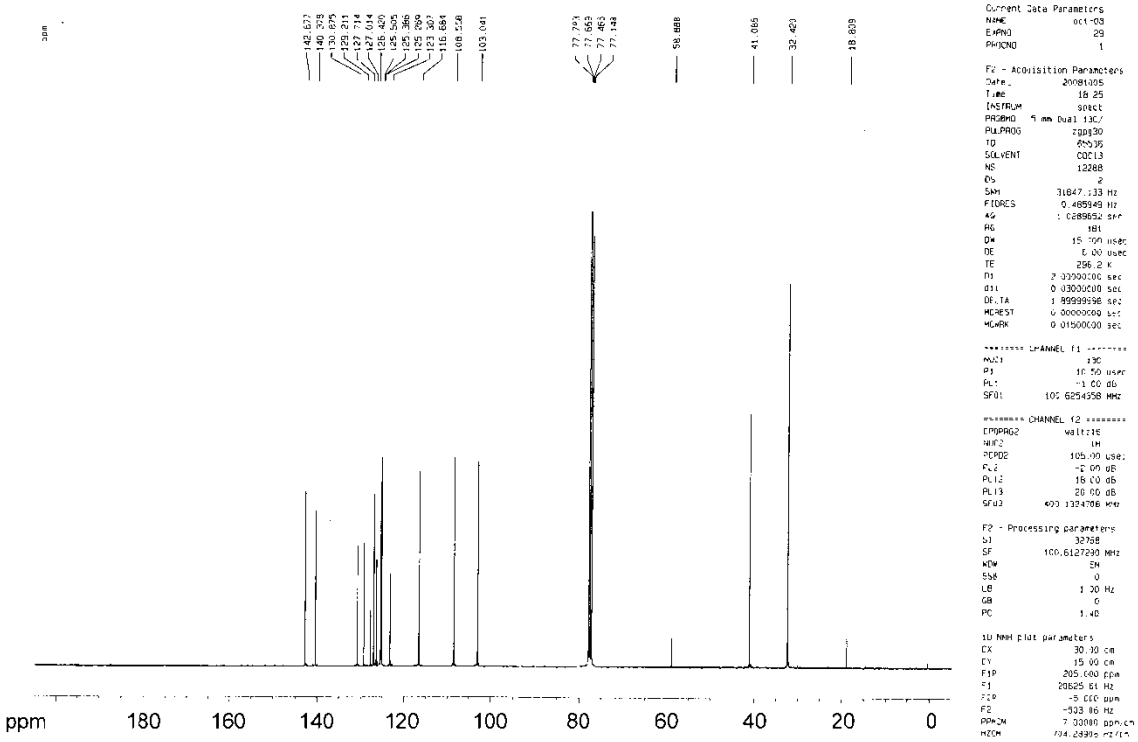


Figure 6. FAB- MS spectrum of compound **2**

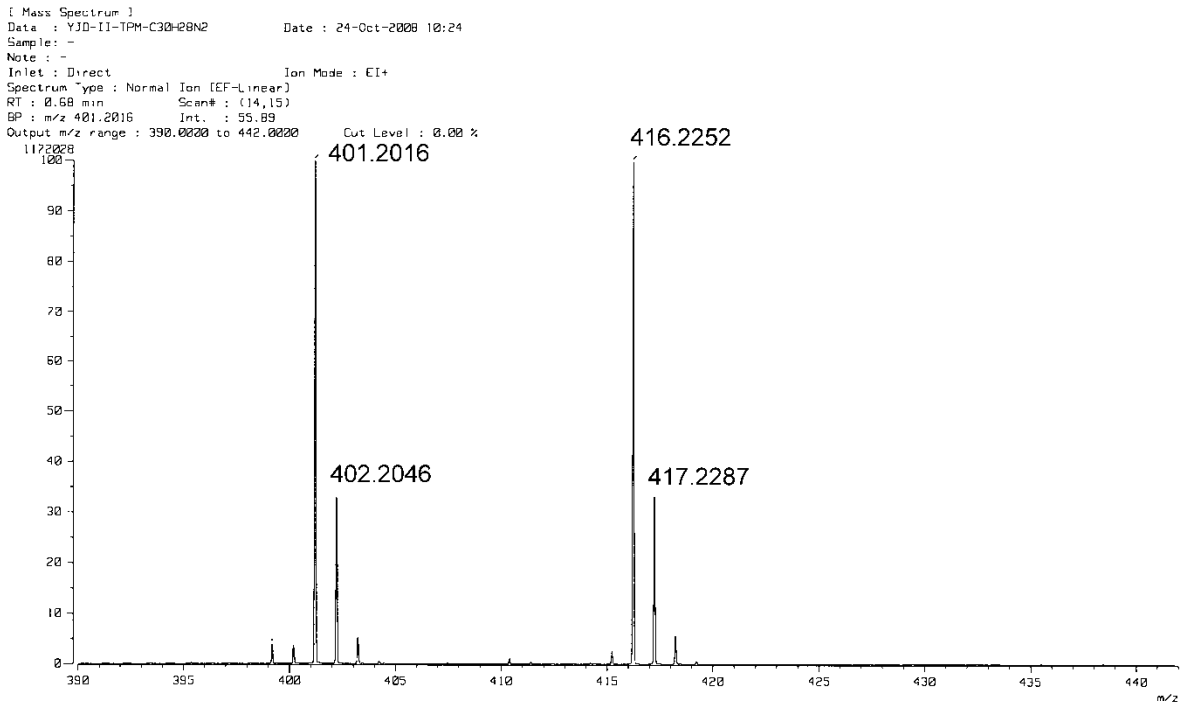


Figure 7. ^{1}H NMR spectrum of receptor **3** in CD_3CN

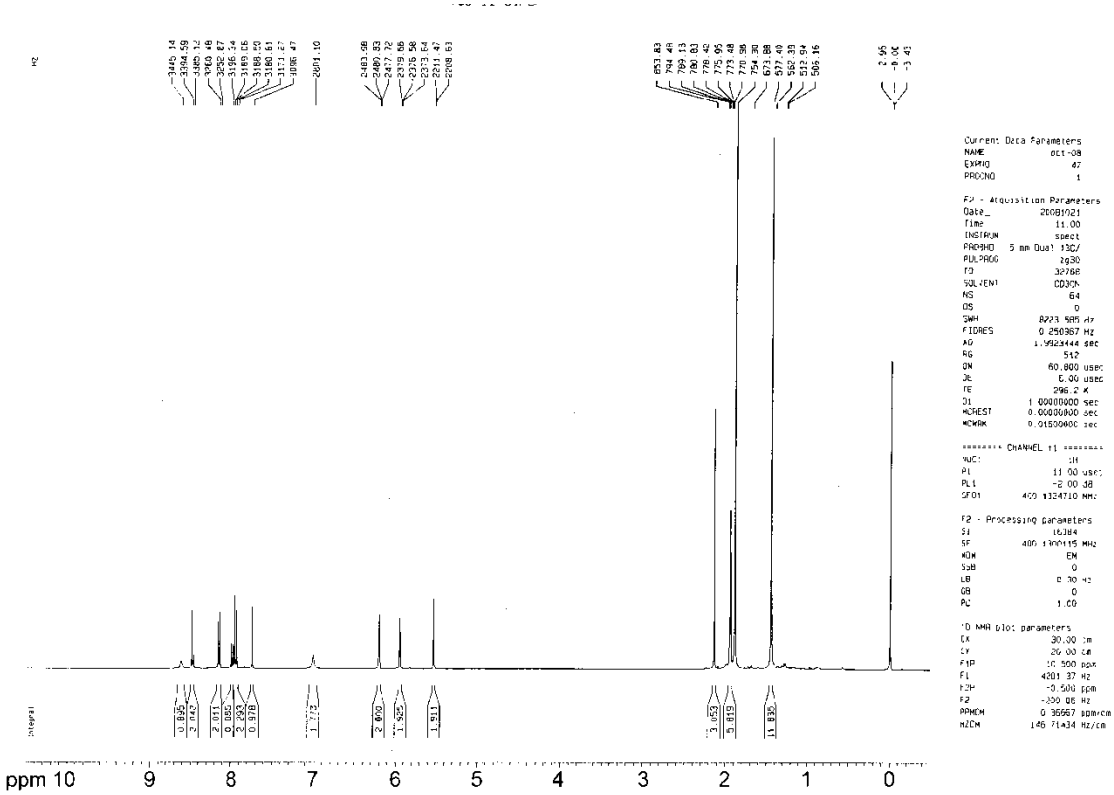


Figure 8. ^{13}C NMR spectrum of c receptor **3** in CD_3CN

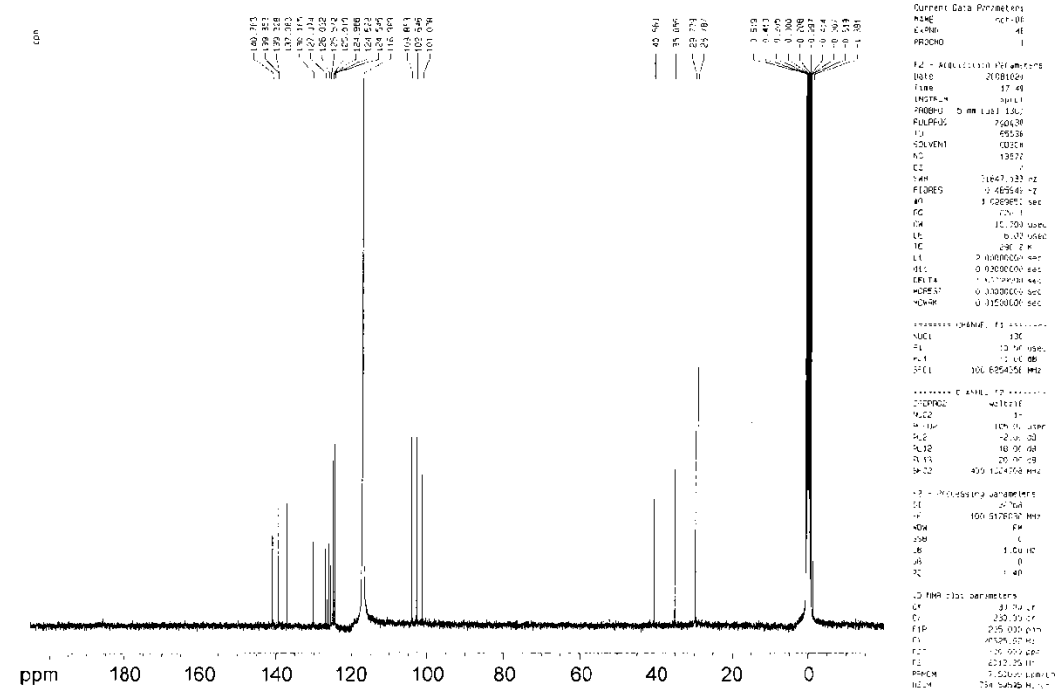


Figure 9. MALDI-TOF MS spectrum of receptor **3**

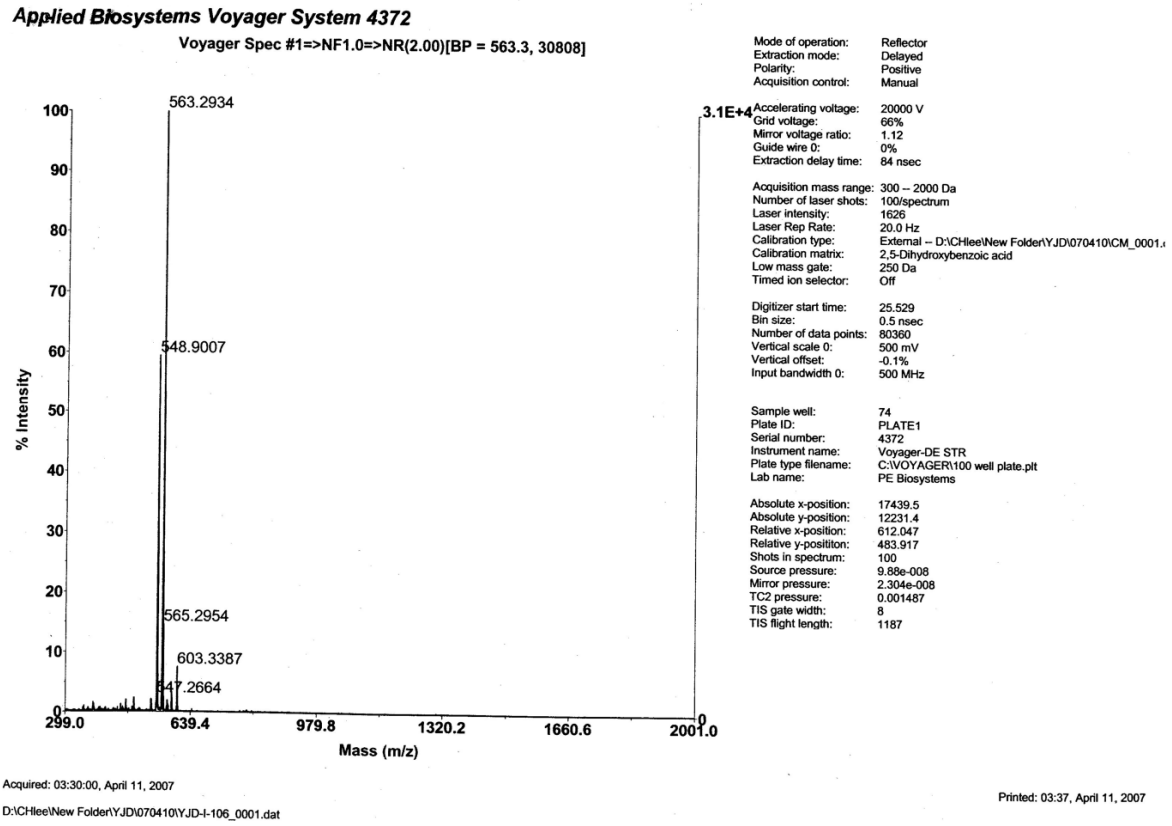


Figure 10. ^{1}H NMR titation of receptor **3** (3.0 mM) with tetrabutlyammonium fluoride in toluene-d_8/CD_3CN (5%).

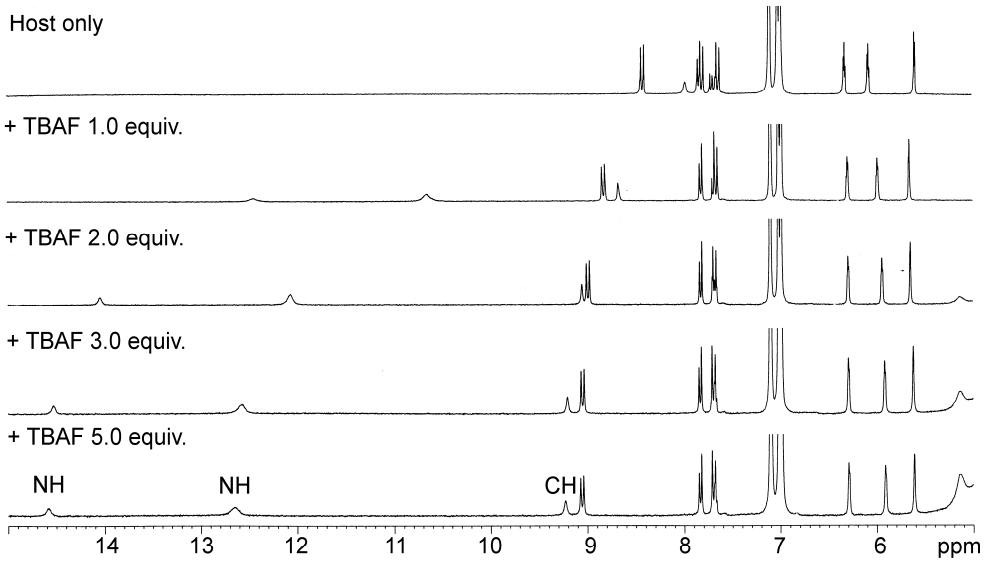
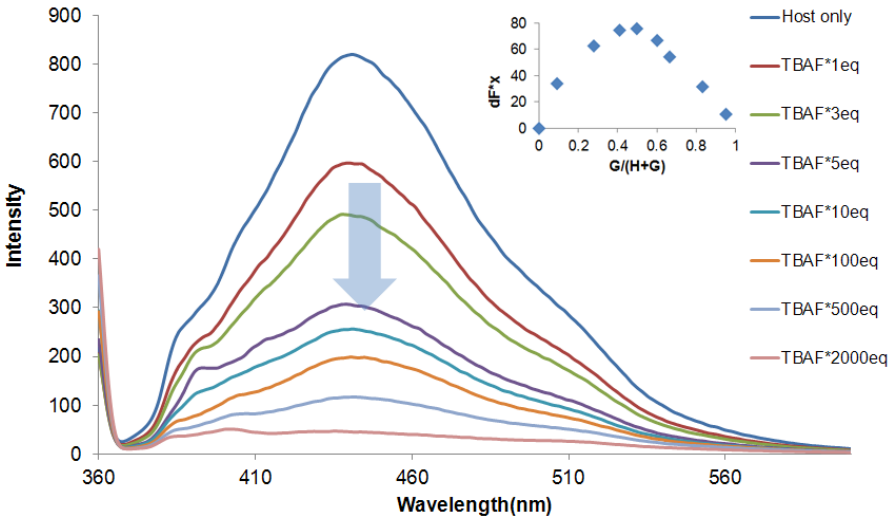


Figure 11. Fluorescence spectral changes of receptor **3** (7.13 x 10^{-6} M) upon addition of TBAF in toluene /CH_3CN (5%). (λ_{ex} = 357 nm).



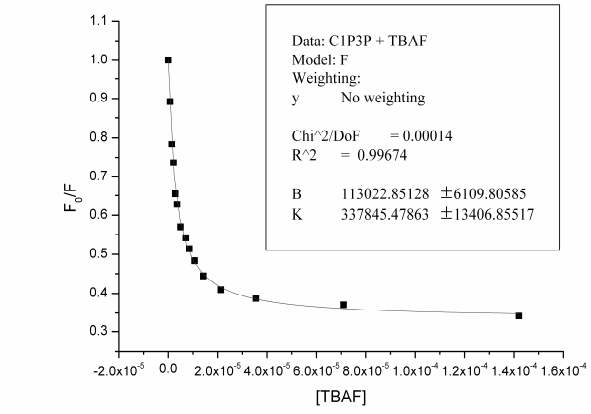
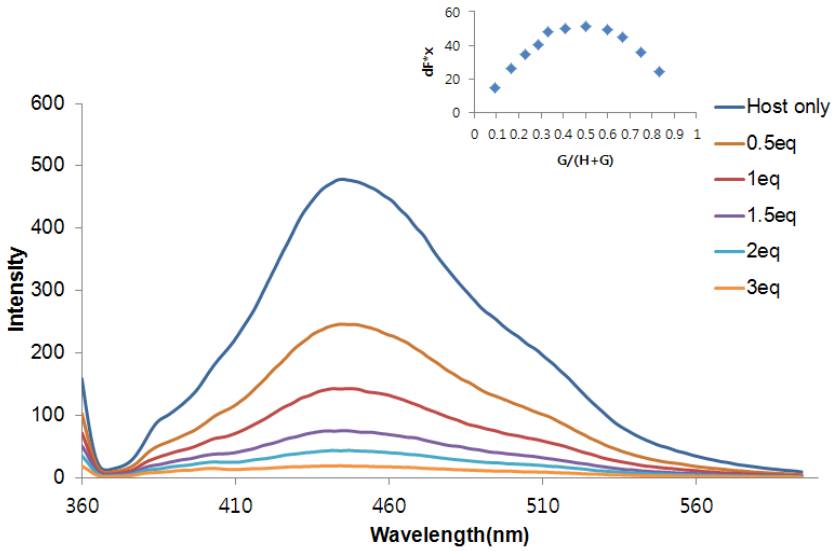


Figure 12. Fluorescence spectral changes of receptor **3** (7.13 x 10^{-6} M) upon addition of C_{60} in toluene /CH_3CN (5%). (λ_{ex} = 357 nm).



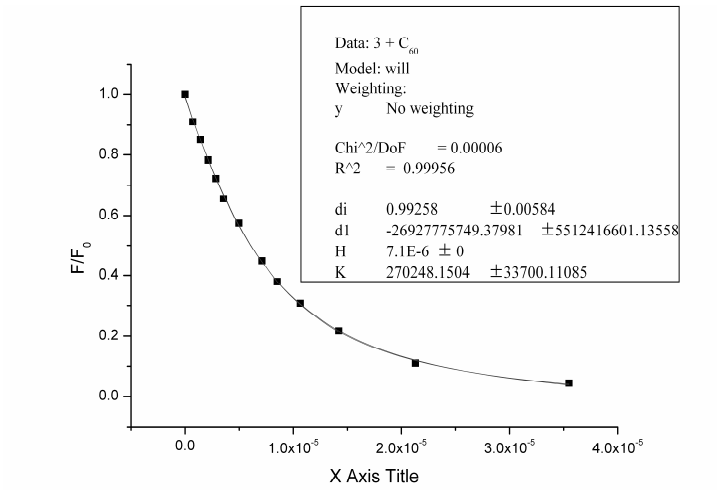
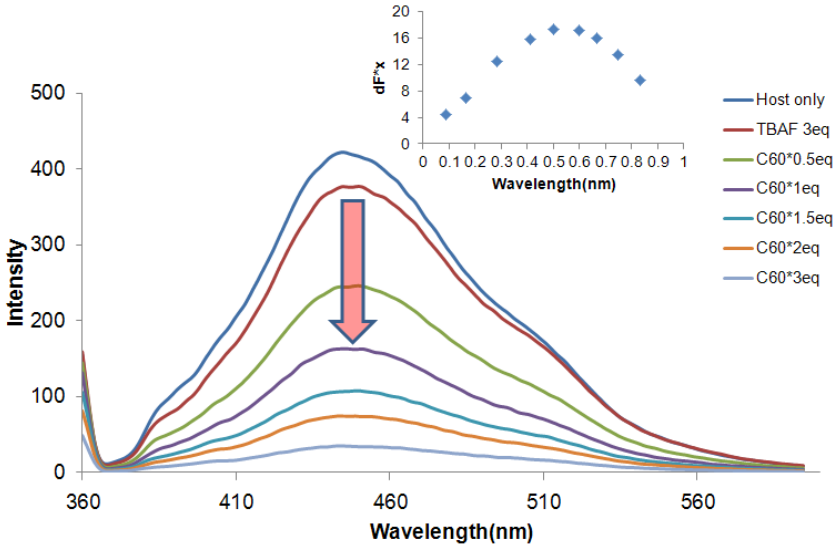


Figure 13. Fluorescence spectral changes of receptor **3** (7.13 x 10^{-6} M) upon addition of TBAF (3eq) and C_{60} in toluene /CH_3CN (5%). (λ_{ex} = 357 nm).



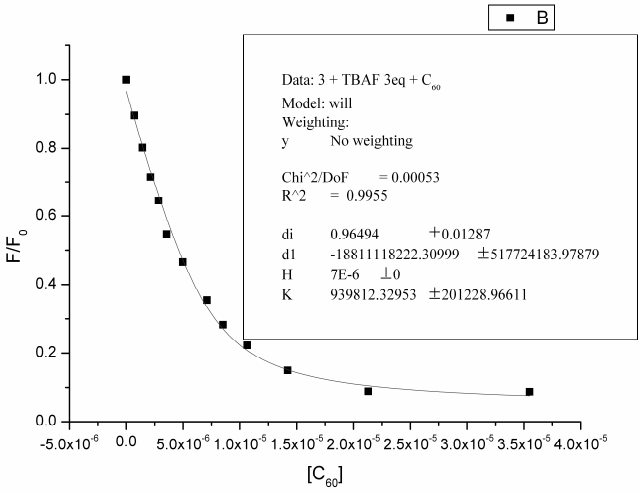
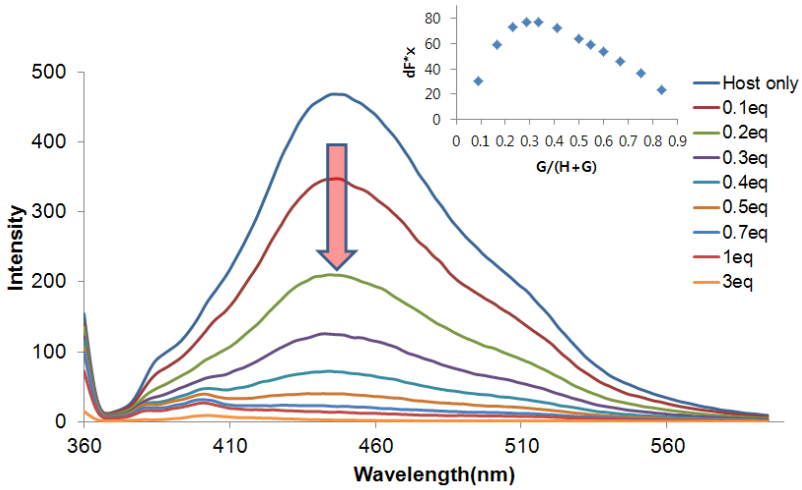


Figure 14. Fluorescence spectral changes of receptor **3** (7.13 x 10^{-6} M) upon addition of C_{70} in toluene /CH_3CN (5%). (λ_{ex} = 357 nm).



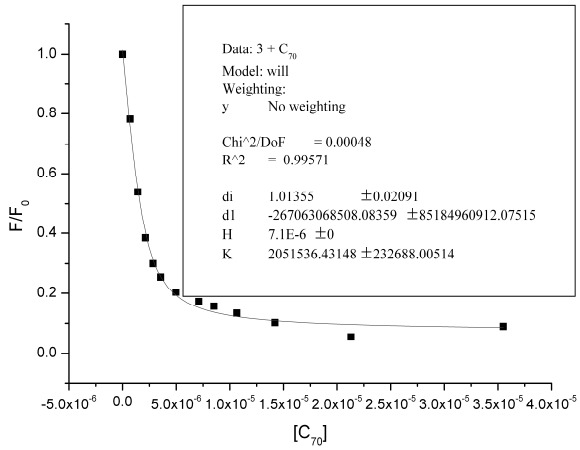
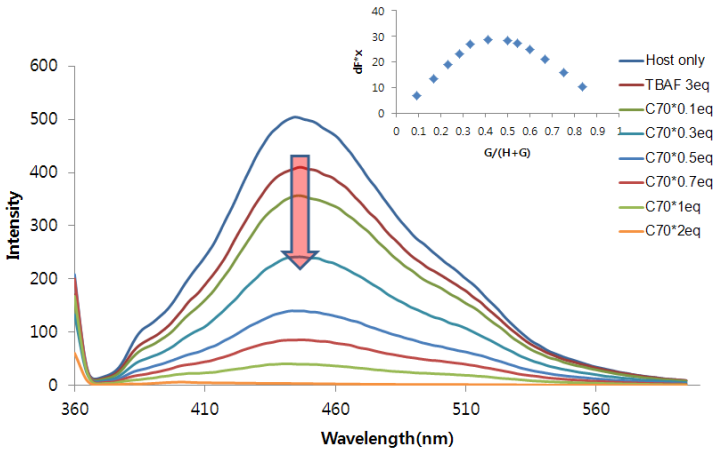


Figure 15. Fluorescence spectral changes of receptor **3** (7.13 x 10^{-6} M) upon addition of TBAF (3eq) and C_{70} in toluene /CH_3CN (5%). (λ_{ex} = 357nm)



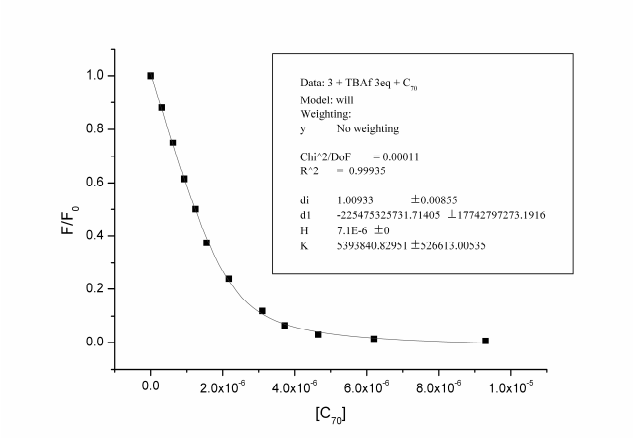


Figure 16. Standard calibration curve for detection of C_{60} with receptor **3**. [**3**] = 7.13 μM.

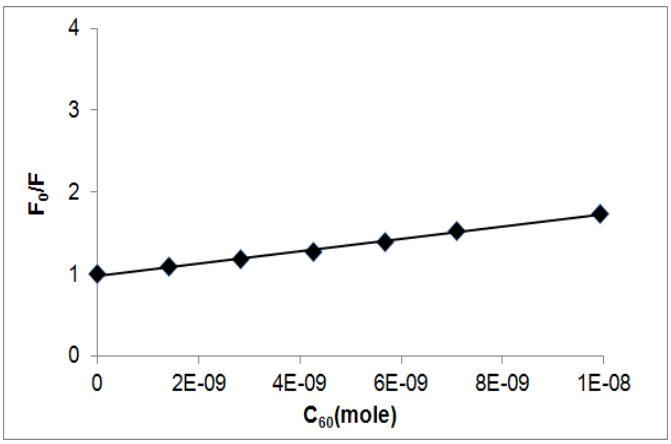


Figure 17. Standard calibration curve for detection of C_{70} with receptor **3**. [**3**] = 7.13 μM.

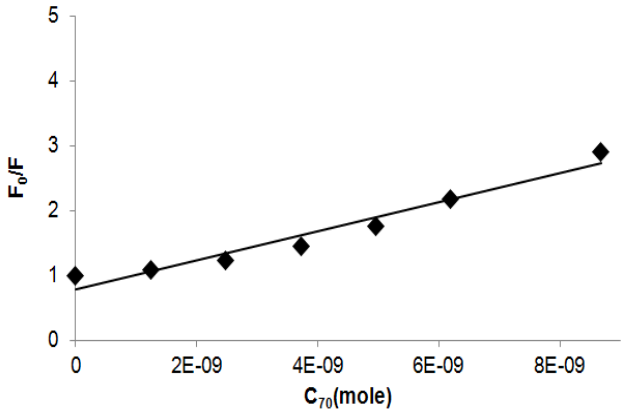


Figure 18. tep view of receptor **3** showing the atom labeling. Displacement ellipsoids are scaled to the 50% probability level.

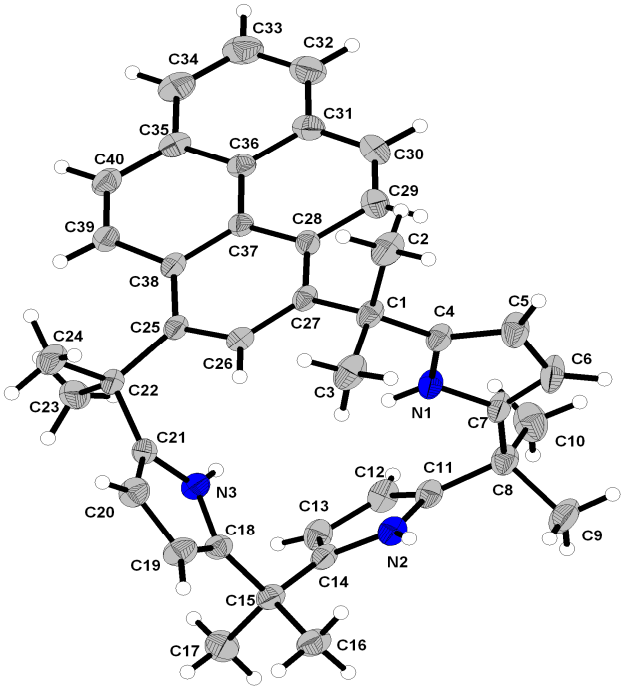


Figure 19. View of receptor **3** showing the dimer formation. Displacement ellipsoids are scaled to the 50% probability level.

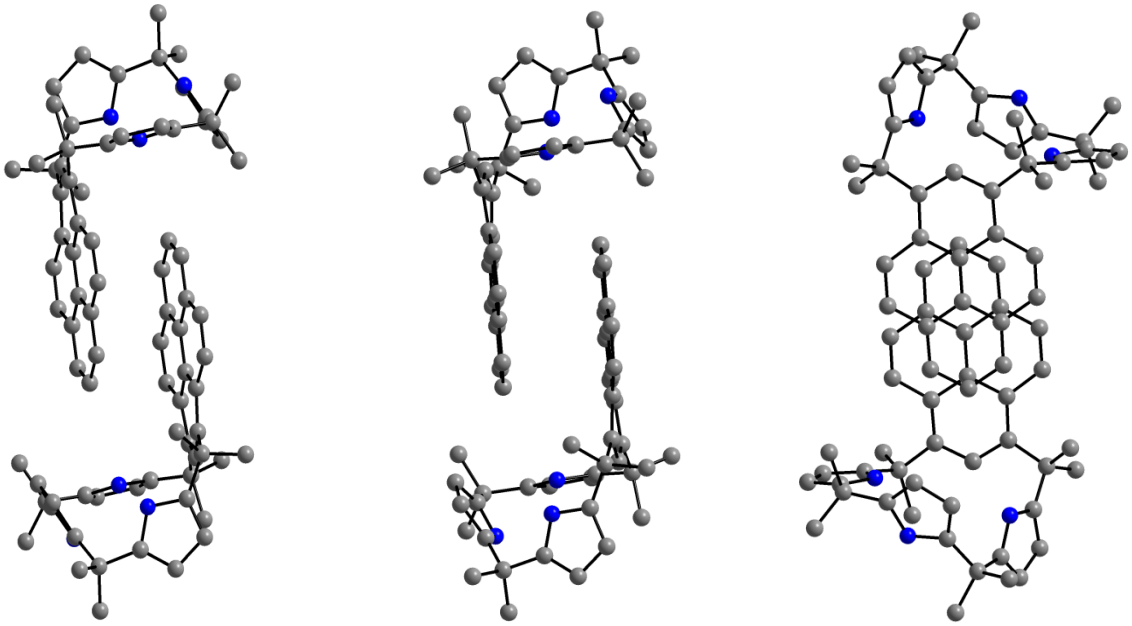


Table 1. Crystal data and structure refinement for receptor **3**

Empirical formula	C40 H41 N3	
Formula weight	563.76	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.0878(11) Å	□= 90.00°
	b = 32.621(4) Å	□= 109.273(2)°
	c = 10.2902(11) Å	□ = 90.00°
Volume	3196.5(6) $Å^3$	
Z	4	
Density (calculated)	1.171 Mg/m^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	1208	
Crystal size	0.15 x 0.08 x 0.08 mm^3	
Theta range for data collection	2.19 to 26.0016.	
Index ranges	$-12 \leq h \leq 12$, $-33 \leq k \leq 40$, $-11 \leq l \leq 12$	
Reflections collected	17811	
Independent reflections	6284 [R(int) = 0.0550]	
Completeness to theta = 26.00	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6284 / 0 / 408	
Goodness-of-fit on F^2	0.676	
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0648	
R indices (all data)	R1 = 0.0895, wR2 = 0.0692	
Largest diff. peak and hole	0.108 and -0.169 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	9479(2)	1324(1)	2115(2)	45(1)
C(2)	10666(2)	1195(1)	1565(2)	67(1)
C(3)	9554(2)	1794(1)	2252(2)	64(1)
C(4)	9708(2)	1157(1)	3539(2)	45(1)
C(5)	10855(2)	1031(1)	4584(2)	66(1)
C(6)	10450(2)	974(1)	5766(2)	68(1)
C(7)	9064(2)	1061(1)	5425(2)	48(1)
C(8)	8060(2)	1048(1)	6239(2)	51(1)
C(9)	8756(2)	1249(1)	7658(2)	80(1)
C(10)	7726(2)	599(1)	6458(2)	77(1)
C(11)	6722(2)	1270(1)	5477(2)	45(1)
C(12)	5367(2)	1144(1)	4981(2)	55(1)
C(13)	4527(2)	1483(1)	4343(2)	54(1)
C(14)	5371(2)	1815(1)	4445(2)	42(1)
C(15)	5048(2)	2242(1)	3889(2)	44(1)
C(16)	6052(2)	2553(1)	4844(2)	60(1)
C(17)	3532(2)	2354(1)	3800(2)	67(1)
C(18)	5165(2)	2268(1)	2462(2)	42(1)
C(19)	5456(2)	2582(1)	1731(2)	55(1)
C(20)	5300(2)	2438(1)	391(2)	53(1)
C(21)	4908(2)	2038(1)	309(2)	41(1)
C(22)	4589(2)	1720(1)	-825(2)	43(1)
C(23)	3077(2)	1568(1)	-1025(2)	65(1)
C(24)	4641(2)	1929(1)	-2149(2)	71(1)
C(25)	5688(2)	1373(1)	-417(1)	38(1)
C(26)	6983(2)	1463(1)	555(1)	41(1)
C(27)	8047(2)	1179(1)	1122(1)	39(1)
C(28)	7755(2)	764(1)	752(2)	40(1)
C(29)	8662(2)	433(1)	1422(2)	55(1)
C(30)	8391(2)	45(1)	998(2)	64(1)
C(31)	7200(2)	-65(1)	-130(2)	52(1)
C(32)	6929(2)	-465(1)	-585(2)	68(1)
C(33)	5758(2)	-565(1)	-1675(2)	72(1)
C(34)	4819(2)	-264(1)	-2335(2)	65(1)
C(35)	5038(2)	141(1)	-1908(2)	47(1)
C(36)	6247(2)	250(1)	-787(2)	42(1)

C(37)	6498(2)	663(1)	-333(2)	38(1)
C(38)	5491(2)	974(1)	-969(2)	38(1)
C(39)	4330(2)	852(1)	-2156(2)	47(1)
C(40)	4116(2)	463(1)	-2596(2)	51(1)
N(1)	8631(2)	1171(1)	4064(1)	48(1)
N(2)	6712(2)	1679(1)	5138(1)	48(1)
N(3)	4817(1)	1939(1)	1578(1)	44(1)

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

C(1)-C(4)	1.509(2)
C(1)-C(3)	1.538(2)
C(1)-C(27)	1.5430(18)
C(1)-C(2)	1.543(2)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-C(5)	1.3576(18)
C(4)-N(1)	1.3642(18)
C(5)-C(6)	1.417(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.3541(19)
C(6)-H(6)	0.9300
C(7)-N(1)	1.3708(18)
C(7)-C(8)	1.513(2)
C(8)-C(11)	1.504(2)
C(8)-C(10)	1.535(2)
C(8)-C(9)	1.543(2)
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(12)	1.355(2)
C(11)-N(2)	1.377(2)
C(12)-C(13)	1.414(2)
C(12)-H(12)	0.9300
C(13)-C(14)	1.361(2)
C(13)-H(13)	0.9300
C(14)-N(2)	1.3783(19)
C(14)-C(15)	1.502(2)
C(15)-C(18)	1.513(2)
C(15)-C(16)	1.5376(19)
C(15)-C(17)	1.5460(19)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600

C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(19)	1.358(2)
C(18)-N(3)	1.3757(19)
C(19)-C(20)	1.416(2)
C(19)-H(19)	0.9300
C(20)-C(21)	1.358(2)
C(20)-H(20)	0.9300
C(21)-N(3)	1.3766(18)
C(21)-C(22)	1.513(2)
C(22)-C(24)	1.5404(19)
C(22)-C(25)	1.544(2)
C(22)-C(23)	1.5513(19)
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.3894(17)
C(25)-C(38)	1.407(2)
C(26)-C(27)	1.3921(19)
C(26)-H(26)	0.9300
C(27)-C(28)	1.409(2)
C(28)-C(37)	1.4248(18)
C(28)-C(29)	1.437(2)
C(29)-C(30)	1.338(2)
C(29)-H(29)	0.9300
C(30)-C(31)	1.414(2)
C(30)-H(30)	0.9300
C(31)-C(32)	1.384(2)
C(31)-C(36)	1.416(2)
C(32)-C(33)	1.373(2)
C(32)-H(32)	0.9300
C(33)-C(34)	1.380(2)
C(33)-H(33)	0.9300
C(34)-C(35)	1.387(2)
C(34)-H(34)	0.9300
C(35)-C(36)	1.4186(19)
C(35)-C(40)	1.426(2)

C(36)-C(37)	1.422(2)
C(37)-C(38)	1.4321(19)
C(38)-C(39)	1.4414(18)
C(39)-C(40)	1.341(2)
C(39)-H(39)	0.9300
C(40)-H(40)	0.9300
N(1)-H(1N)	0.860(14)
N(2)-H(2N)	0.848(15)
N(3)-H(3N)	0.885(15)

C(4)-C(1)-C(3)	106.53(13)
C(4)-C(1)-C(27)	109.95(13)
C(3)-C(1)-C(27)	111.99(13)
C(4)-C(1)-C(2)	111.63(13)
C(3)-C(1)-C(2)	106.64(14)
C(27)-C(1)-C(2)	110.04(12)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(5)-C(4)-N(1)	106.23(14)
C(5)-C(4)-C(1)	134.09(15)
N(1)-C(4)-C(1)	119.04(14)
C(4)-C(5)-C(6)	107.85(15)
C(4)-C(5)-H(5)	126.1
C(6)-C(5)-H(5)	126.1
C(7)-C(6)-C(5)	108.46(14)
C(7)-C(6)-H(6)	125.8
C(5)-C(6)-H(6)	125.8
C(6)-C(7)-N(1)	105.84(15)
C(6)-C(7)-C(8)	132.35(16)
N(1)-C(7)-C(8)	121.81(14)
C(11)-C(8)-C(7)	110.32(14)
C(11)-C(8)-C(10)	109.48(14)

C(7)-C(8)-C(10)	109.17(15)
C(11)-C(8)-C(9)	109.77(15)
C(7)-C(8)-C(9)	109.43(13)
C(10)-C(8)-C(9)	108.64(14)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-N(2)	105.99(16)
C(12)-C(11)-C(8)	132.10(18)
N(2)-C(11)-C(8)	121.91(16)
C(11)-C(12)-C(13)	108.31(17)
C(11)-C(12)-H(12)	125.8
C(13)-C(12)-H(12)	125.8
C(14)-C(13)-C(12)	108.79(16)
C(14)-C(13)-H(13)	125.6
C(12)-C(13)-H(13)	125.6
C(13)-C(14)-N(2)	105.38(17)
C(13)-C(14)-C(15)	131.21(16)
N(2)-C(14)-C(15)	123.30(15)
C(14)-C(15)-C(18)	110.22(14)
C(14)-C(15)-C(16)	110.78(13)
C(18)-C(15)-C(16)	109.73(14)
C(14)-C(15)-C(17)	109.13(14)
C(18)-C(15)-C(17)	108.77(13)
C(16)-C(15)-C(17)	108.16(14)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5

H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-N(3)	106.05(14)
C(19)-C(18)-C(15)	132.81(17)
N(3)-C(18)-C(15)	120.87(16)
C(18)-C(19)-C(20)	108.29(15)
C(18)-C(19)-H(19)	125.9
C(20)-C(19)-H(19)	125.9
C(21)-C(20)-C(19)	108.43(15)
C(21)-C(20)-H(20)	125.8
C(19)-C(20)-H(20)	125.8
C(20)-C(21)-N(3)	105.95(15)
C(20)-C(21)-C(22)	133.52(16)
N(3)-C(21)-C(22)	120.52(16)
C(21)-C(22)-C(24)	108.57(14)
C(21)-C(22)-C(25)	110.01(13)
C(24)-C(22)-C(25)	109.53(13)
C(21)-C(22)-C(23)	105.71(13)
C(24)-C(22)-C(23)	110.07(13)
C(25)-C(22)-C(23)	112.81(14)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(38)	117.41(14)
C(26)-C(25)-C(22)	117.40(15)
C(38)-C(25)-C(22)	125.18(14)
C(25)-C(26)-C(27)	124.93(15)
C(25)-C(26)-H(26)	117.5
C(27)-C(26)-H(26)	117.5
C(26)-C(27)-C(28)	117.51(14)
C(26)-C(27)-C(1)	119.77(16)

C(28)-C(27)-C(1)	122.73(15)
C(27)-C(28)-C(37)	119.17(15)
C(27)-C(28)-C(29)	123.29(15)
C(37)-C(28)-C(29)	117.54(16)
C(30)-C(29)-C(28)	121.75(17)
C(30)-C(29)-H(29)	119.1
C(28)-C(29)-H(29)	119.1
C(29)-C(30)-C(31)	122.33(17)
C(29)-C(30)-H(30)	118.8
C(31)-C(30)-H(30)	118.8
C(32)-C(31)-C(30)	122.46(19)
C(32)-C(31)-C(36)	119.66(18)
C(30)-C(31)-C(36)	117.86(18)
C(33)-C(32)-C(31)	121.44(19)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(32)-C(33)-C(34)	119.9(2)
C(32)-C(33)-H(33)	120.1
C(34)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	120.81(19)
C(33)-C(34)-H(34)	119.6
C(35)-C(34)-H(34)	119.6
C(34)-C(35)-C(36)	119.93(18)
C(34)-C(35)-C(40)	122.26(18)
C(36)-C(35)-C(40)	117.75(17)
C(31)-C(36)-C(35)	118.30(17)
C(31)-C(36)-C(37)	120.71(16)
C(35)-C(36)-C(37)	121.00(16)
C(36)-C(37)-C(28)	119.60(15)
C(36)-C(37)-C(38)	119.93(15)
C(28)-C(37)-C(38)	120.47(16)
C(25)-C(38)-C(37)	119.08(14)
C(25)-C(38)-C(39)	124.35(15)
C(37)-C(38)-C(39)	116.57(15)
C(40)-C(39)-C(38)	122.86(16)
C(40)-C(39)-H(39)	118.6
C(38)-C(39)-H(39)	118.6
C(39)-C(40)-C(35)	121.52(16)
C(39)-C(40)-H(40)	119.2
C(35)-C(40)-H(40)	119.2
C(4)-N(1)-C(7)	111.61(14)
C(4)-N(1)-H(1N)	127.6(11)

C(7)-N(1)-H(1N)	120.8(11)
C(11)-N(2)-C(14)	111.53(15)
C(11)-N(2)-H(2N)	125.7(12)
C(14)-N(2)-H(2N)	122.7(12)
C(18)-N(3)-C(21)	111.27(15)
C(18)-N(3)-H(3N)	122.3(10)
C(21)-N(3)-H(3N)	126.0(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for receptor **3** 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}
C(1)	32(1)	68(1)	34(1)	-6(1)	9(1)	-10(1)
C(2)	39(1)	117(2)	49(1)	-8(1)	18(1)	-7(1)
C(3)	55(1)	79(2)	52(1)	-7(1)	9(1)	-28(1)
C(4)	30(1)	70(1)	35(1)	-1(1)	11(1)	-4(1)
C(5)	35(1)	113(2)	48(1)	12(1)	12(1)	6(1)
C(6)	43(1)	113(2)	39(1)	16(1)	2(1)	4(1)
C(7)	40(1)	70(1)	30(1)	6(1)	7(1)	1(1)
C(8)	52(1)	65(2)	37(1)	8(1)	15(1)	0(1)
C(9)	71(1)	131(2)	34(1)	-4(1)	14(1)	11(1)
C(10)	73(1)	87(2)	77(1)	32(1)	31(1)	9(1)
C(11)	48(1)	56(1)	34(1)	6(1)	17(1)	-4(1)
C(12)	53(1)	62(2)	49(1)	3(1)	14(1)	-14(1)
C(13)	40(1)	67(2)	49(1)	-2(1)	6(1)	-9(1)
C(14)	35(1)	59(1)	32(1)	-6(1)	11(1)	-4(1)
C(15)	39(1)	55(1)	40(1)	-8(1)	14(1)	-3(1)
C(16)	64(1)	61(1)	53(1)	-17(1)	19(1)	-6(1)
C(17)	50(1)	87(2)	67(1)	-1(1)	24(1)	10(1)
C(18)	42(1)	43(1)	40(1)	-7(1)	12(1)	-4(1)
C(19)	68(1)	45(1)	52(1)	-9(1)	21(1)	-14(1)
C(20)	66(1)	48(1)	46(1)	6(1)	21(1)	-4(1)
C(21)	47(1)	41(1)	34(1)	6(1)	13(1)	5(1)
C(22)	48(1)	45(1)	31(1)	0(1)	5(1)	5(1)
C(23)	44(1)	72(2)	67(1)	-18(1)	2(1)	11(1)
C(24)	108(2)	65(2)	38(1)	7(1)	20(1)	15(1)
C(25)	40(1)	45(1)	28(1)	1(1)	10(1)	-1(1)
C(26)	44(1)	44(1)	34(1)	-4(1)	13(1)	-5(1)
C(27)	34(1)	56(1)	29(1)	-2(1)	12(1)	-4(1)
C(28)	33(1)	52(1)	34(1)	2(1)	12(1)	4(1)
C(29)	43(1)	62(2)	54(1)	-1(1)	8(1)	7(1)
C(30)	56(1)	63(2)	68(1)	5(1)	14(1)	19(1)
C(31)	57(1)	49(2)	55(1)	-4(1)	26(1)	4(1)
C(32)	80(2)	55(2)	73(2)	-2(1)	32(1)	10(1)
C(33)	102(2)	46(2)	76(2)	-11(1)	38(1)	-4(1)
C(34)	77(2)	61(2)	59(1)	-15(1)	24(1)	-14(1)
C(35)	52(1)	49(1)	44(1)	-10(1)	20(1)	-10(1)

C(36)	46(1)	46(1)	38(1)	-2(1)	20(1)	1(1)
C(37)	35(1)	47(1)	33(1)	-2(1)	12(1)	3(1)
C(38)	36(1)	49(1)	29(1)	-3(1)	10(1)	-5(1)
C(39)	43(1)	56(1)	38(1)	-5(1)	9(1)	3(1)
C(40)	46(1)	63(2)	40(1)	-13(1)	8(1)	-7(1)
N(1)	34(1)	76(1)	33(1)	5(1)	10(1)	3(1)
N(2)	38(1)	63(1)	44(1)	-1(1)	14(1)	-9(1)
N(3)	56(1)	37(1)	39(1)	1(1)	16(1)	-5(1)

Table 5. Hydrogen coordinates (Å x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for receptor **3**

	x	y	z	U(eq)
H(2A)	11553	1283	2195	101
H(2B)	10516	1318	681	101
H(2C)	10666	902	1475	101
H(3A)	8869	1887	2648	96
H(3B)	9366	1915	1359	96
H(3C)	10475	1873	2836	96
H(5)	11749	990	4534	79
H(6)	11036	891	6629	81
H(9A)	8999	1527	7535	119
H(9B)	9589	1099	8155	119
H(9C)	8113	1245	8168	119
H(10A)	7070	589	6953	116
H(10B)	8575	460	6977	116
H(10C)	7325	467	5581	116
H(12)	5045	881	5050	66
H(13)	3558	1478	3922	64
H(16A)	6993	2502	4857	90
H(16B)	6010	2526	5759	90
H(16C)	5778	2826	4513	90
H(17A)	3320	2628	3446	100
H(17B)	3446	2339	4701	100
H(17C)	2886	2165	3197	100
H(19)	5713	2846	2055	66
H(20)	5442	2591	-314	63
H(23A)	3099	1377	-311	98
H(23B)	2701	1437	-1906	98
H(23C)	2496	1798	-983	98
H(24A)	3951	2144	-2407	107
H(24B)	4448	1731	-2876	107
H(24C)	5558	2044	-1989	107
H(26)	7152	1733	848	49
H(29)	9459	490	2170	66
H(30)	9008	-160	1461	77
H(32)	7553	-671	-143	81
H(33)	5599	-836	-1969	87
H(34)	4029	-332	-3075	78
H(39)	3701	1052	-2637	56

H(40)	3349	401	-3369	61
H(1N)	7779(16)	1247(5)	3649(16)	77(7)
H(2N)	7424(16)	1834(5)	5342(16)	67(7)
H(3N)	4657(15)	1692(5)	1850(15)	63(6)

Table 6. Torsion angles [°] for receptor **3**

C(3)-C(1)-C(4)-C(5)	-92.2(2)
C(27)-C(1)-C(4)-C(5)	146.2(2)
C(2)-C(1)-C(4)-C(5)	23.8(3)
C(3)-C(1)-C(4)-N(1)	77.13(18)
C(27)-C(1)-C(4)-N(1)	-44.4(2)
C(2)-C(1)-C(4)-N(1)	-166.84(15)
N(1)-C(4)-C(5)-C(6)	-0.7(2)
C(1)-C(4)-C(5)-C(6)	169.59(19)
C(4)-C(5)-C(6)-C(7)	0.6(2)
C(5)-C(6)-C(7)-N(1)	-0.3(2)
C(5)-C(6)-C(7)-C(8)	178.67(18)
C(6)-C(7)-C(8)-C(11)	166.4(2)
N(1)-C(7)-C(8)-C(11)	-14.8(2)
C(6)-C(7)-C(8)-C(10)	-73.2(2)
N(1)-C(7)-C(8)-C(10)	105.56(18)
C(6)-C(7)-C(8)-C(9)	45.5(3)
N(1)-C(7)-C(8)-C(9)	-135.66(16)
C(7)-C(8)-C(11)-C(12)	119.68(19)
C(10)-C(8)-C(11)-C(12)	-0.5(2)
C(9)-C(8)-C(11)-C(12)	-119.6(2)
C(7)-C(8)-C(11)-N(2)	-59.8(2)
C(10)-C(8)-C(11)-N(2)	-179.91(14)
C(9)-C(8)-C(11)-N(2)	60.92(19)
N(2)-C(11)-C(12)-C(13)	-0.35(19)
C(8)-C(11)-C(12)-C(13)	-179.85(16)
C(11)-C(12)-C(13)-C(14)	0.2(2)
C(12)-C(13)-C(14)-N(2)	0.11(19)
C(12)-C(13)-C(14)-C(15)	176.35(15)
C(13)-C(14)-C(15)-C(18)	-89.1(2)
N(2)-C(14)-C(15)-C(18)	86.56(17)
C(13)-C(14)-C(15)-C(16)	149.27(17)
N(2)-C(14)-C(15)-C(16)	-35.1(2)
C(13)-C(14)-C(15)-C(17)	30.3(2)
N(2)-C(14)-C(15)-C(17)	-154.05(14)

C(14)-C(15)-C(18)-C(19)	-153.62(18)
C(16)-C(15)-C(18)-C(19)	-31.4(2)
C(17)-C(15)-C(18)-C(19)	86.8(2)
C(14)-C(15)-C(18)-N(3)	33.2(2)
C(16)-C(15)-C(18)-N(3)	155.47(15)
C(17)-C(15)-C(18)-N(3)	-86.40(18)
N(3)-C(18)-C(19)-C(20)	-0.83(19)
C(15)-C(18)-C(19)-C(20)	-174.73(16)
C(18)-C(19)-C(20)-C(21)	0.3(2)
C(19)-C(20)-C(21)-N(3)	0.33(18)
C(19)-C(20)-C(21)-C(22)	-179.82(16)
C(20)-C(21)-C(22)-C(24)	-5.1(2)
N(3)-C(21)-C(22)-C(24)	174.71(13)
C(20)-C(21)-C(22)-C(25)	114.7(2)
N(3)-C(21)-C(22)-C(25)	-65.44(18)
C(20)-C(21)-C(22)-C(23)	-123.19(19)
N(3)-C(21)-C(22)-C(23)	56.64(18)
C(21)-C(22)-C(25)-C(26)	-23.07(19)
C(24)-C(22)-C(25)-C(26)	96.19(16)
C(23)-C(22)-C(25)-C(26)	-140.84(14)
C(21)-C(22)-C(25)-C(38)	158.14(14)
C(24)-C(22)-C(25)-C(38)	-82.60(19)
C(23)-C(22)-C(25)-C(38)	40.4(2)
C(38)-C(25)-C(26)-C(27)	-6.7(2)
C(22)-C(25)-C(26)-C(27)	174.38(14)
C(25)-C(26)-C(27)-C(28)	-4.4(2)
C(25)-C(26)-C(27)-C(1)	175.55(13)
C(4)-C(1)-C(27)-C(26)	113.76(16)
C(3)-C(1)-C(27)-C(26)	-4.47(19)
C(2)-C(1)-C(27)-C(26)	-122.89(16)
C(4)-C(1)-C(27)-C(28)	-66.30(19)
C(3)-C(1)-C(27)-C(28)	175.48(14)
C(2)-C(1)-C(27)-C(28)	57.06(19)
C(26)-C(27)-C(28)-C(37)	10.0(2)
C(1)-C(27)-C(28)-C(37)	-169.96(13)
C(26)-C(27)-C(28)-C(29)	-169.61(14)
C(1)-C(27)-C(28)-C(29)	10.4(2)
C(27)-C(28)-C(29)-C(30)	-176.46(16)
C(37)-C(28)-C(29)-C(30)	3.9(2)
C(28)-C(29)-C(30)-C(31)	-0.1(3)
C(29)-C(30)-C(31)-C(32)	178.92(17)
C(29)-C(30)-C(31)-C(36)	-2.4(3)

C(30)-C(31)-C(32)-C(33)	179.41(17)
C(36)-C(31)-C(32)-C(33)	0.7(3)
C(31)-C(32)-C(33)-C(34)	-0.4(3)
C(32)-C(33)-C(34)-C(35)	-0.2(3)
C(33)-C(34)-C(35)-C(36)	0.6(3)
C(33)-C(34)-C(35)-C(40)	177.69(17)
C(32)-C(31)-C(36)-C(35)	-0.4(2)
C(30)-C(31)-C(36)-C(35)	-179.13(14)
C(32)-C(31)-C(36)-C(37)	179.64(15)
C(30)-C(31)-C(36)-C(37)	0.9(2)
C(34)-C(35)-C(36)-C(31)	-0.2(2)
C(40)-C(35)-C(36)-C(31)	-177.50(14)
C(34)-C(35)-C(36)-C(37)	179.72(15)
C(40)-C(35)-C(36)-C(37)	2.5(2)
C(31)-C(36)-C(37)-C(28)	2.9(2)
C(35)-C(36)-C(37)-C(28)	-177.02(13)
C(31)-C(36)-C(37)-C(38)	-177.16(14)
C(35)-C(36)-C(37)-C(38)	2.9(2)
C(27)-C(28)-C(37)-C(36)	175.12(14)
C(29)-C(28)-C(37)-C(36)	-5.3(2)
C(27)-C(28)-C(37)-C(38)	-4.8(2)
C(29)-C(28)-C(37)-C(38)	174.85(14)
C(26)-C(25)-C(38)-C(37)	11.9(2)
C(22)-C(25)-C(38)-C(37)	-169.31(14)
C(26)-C(25)-C(38)-C(39)	-167.89(13)
C(22)-C(25)-C(38)-C(39)	10.9(2)
C(36)-C(37)-C(38)-C(25)	173.64(14)
C(28)-C(37)-C(38)-C(25)	-6.5(2)
C(36)-C(37)-C(38)-C(39)	-6.6(2)
C(28)-C(37)-C(38)-C(39)	173.34(13)
C(25)-C(38)-C(39)-C(40)	-174.95(15)
C(37)-C(38)-C(39)-C(40)	5.3(2)
C(38)-C(39)-C(40)-C(35)	0.0(2)
C(34)-C(35)-C(40)-C(39)	178.84(16)
C(36)-C(35)-C(40)-C(39)	-4.0(2)
C(5)-C(4)-N(1)-C(7)	0.6(2)
C(1)-C(4)-N(1)-C(7)	-171.48(15)
C(6)-C(7)-N(1)-C(4)	-0.2(2)
C(8)-C(7)-N(1)-C(4)	-179.27(16)
C(12)-C(11)-N(2)-C(14)	0.44(18)
C(8)-C(11)-N(2)-C(14)	180.00(14)
C(13)-C(14)-N(2)-C(11)	-0.34(18)

C(15)-C(14)-N(2)-C(11)	-176.95(14)
C(19)-C(18)-N(3)-C(21)	1.07(18)
C(15)-C(18)-N(3)-C(21)	175.86(13)
C(20)-C(21)-N(3)-C(18)	-0.87(18)
C(22)-C(21)-N(3)-C(18)	179.25(13)

Symmetry transformations used to generate equivalent atoms: