'Twisted' isophthalamide analogues

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DMSO solutions containing 1.0 mM receptor in the absence or presence of 10.0 mM tetrabutylammonium anion salts are shown in Figure 2. Compounds **1** and **2** undergo a light yellow to dark red colour change upon addition of fluoride anions, however, no significant colour change was observed upon addition of the other anions studied. Compound **3**, shows a colour change from yellow to red with fluoride but also colour changes to orange with dihydrogen phosphate and benzoate, presumably reflecting the enhanced interaction with the oxo-anions by the more acidic receptor.

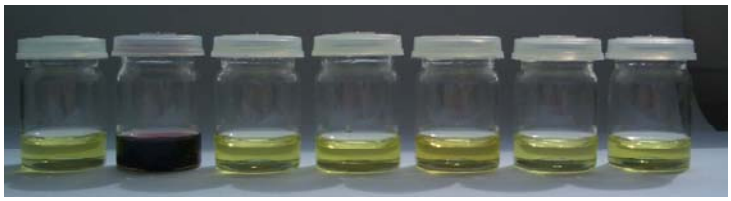


Figure S1 Compound **1** in DMSO in the absence of anions (far left) and presence of anions (10 equiv.) From second left to right – fluoride, chloride, bromide, dihydrogen phosphate, benzoate, hydrogen sulfate (added as tetrabutylammonium salts).

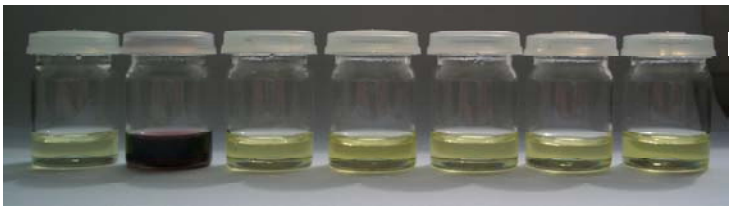


Figure S2 Compound **2** in DMSO in the absence of anions (far left) and presence of anions (10 equiv.) From second left to right – fluoride, chloride, bromide, dihydrogen phosphate, benzoate, hydrogen sulfate (added as tetrabutylammonium salts).

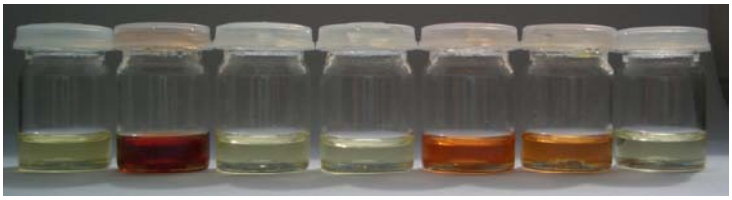


Figure S3 Compound **3** in DMSO in the absence of anions (far left) and presence of anions (10 equiv.) From second left to right – fluoride, chloride, bromide, dihydrogen phosphate, benzoate, hydrogen sulfate (added as tetrabutylammonium salts).

Figure 4 Comparison of compounds **1** (top row), **2** (middle row) and **3** (bottom row) in DMSO (1.0 mM) in the absence of anions (far left) and presence of anions (10 equiv.) From second left to right – fluoride, chloride, bromide, dihydrogen phosphate, benzoate, hydrogen sulfate (added as tetrabutylammonium salts).

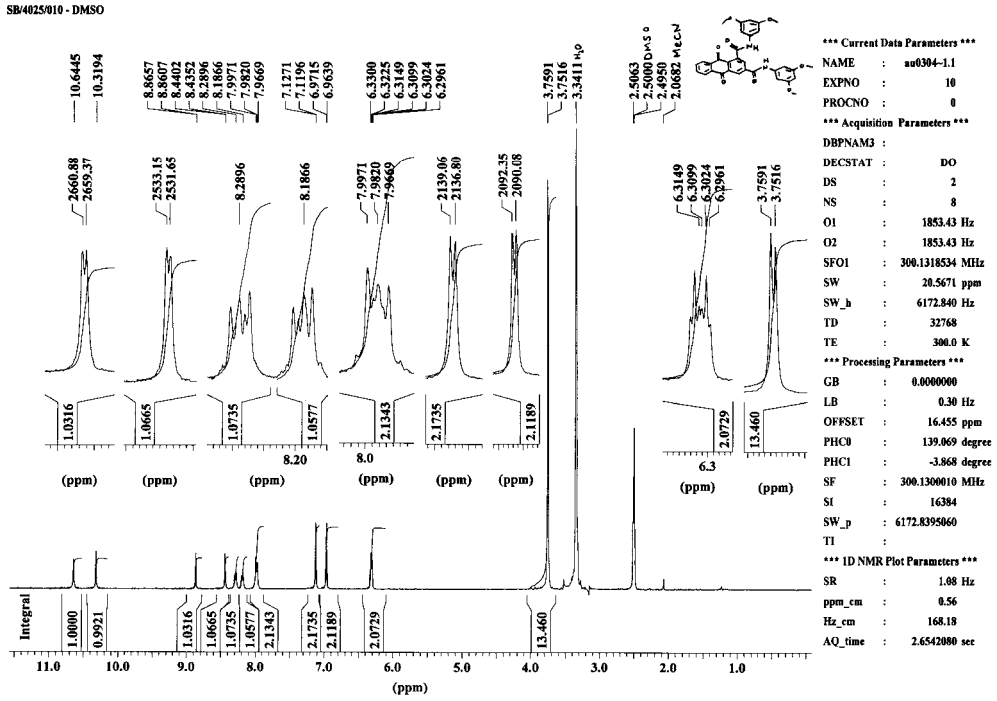


Figure S5 The ^{1}H NMR spectrum of compound **1** in DMSO-d_6

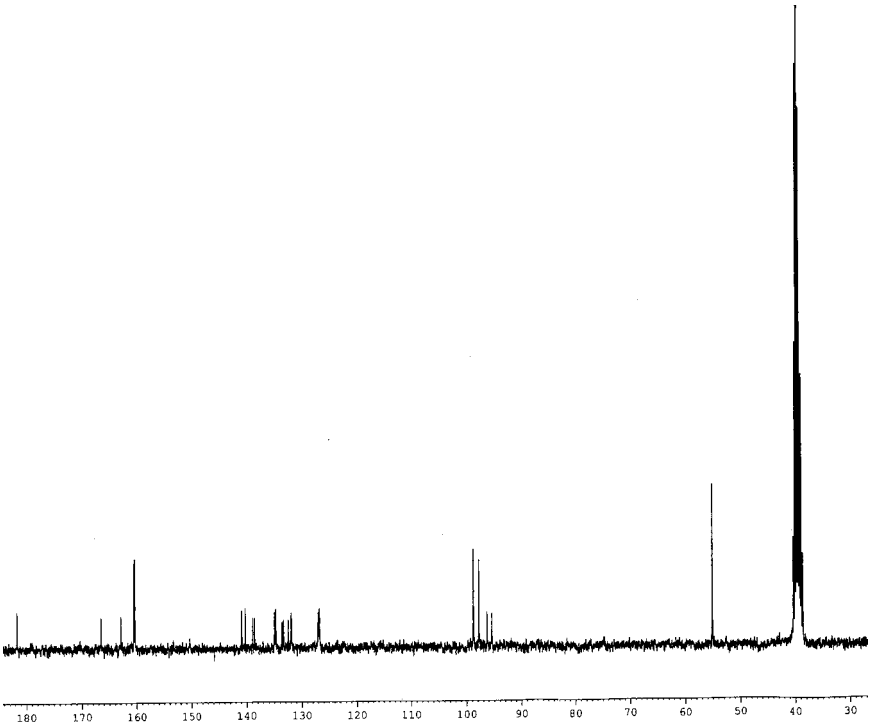


Figure S6 The ^{13}C NMR spectrum of compound **1** in DMSO-d_6

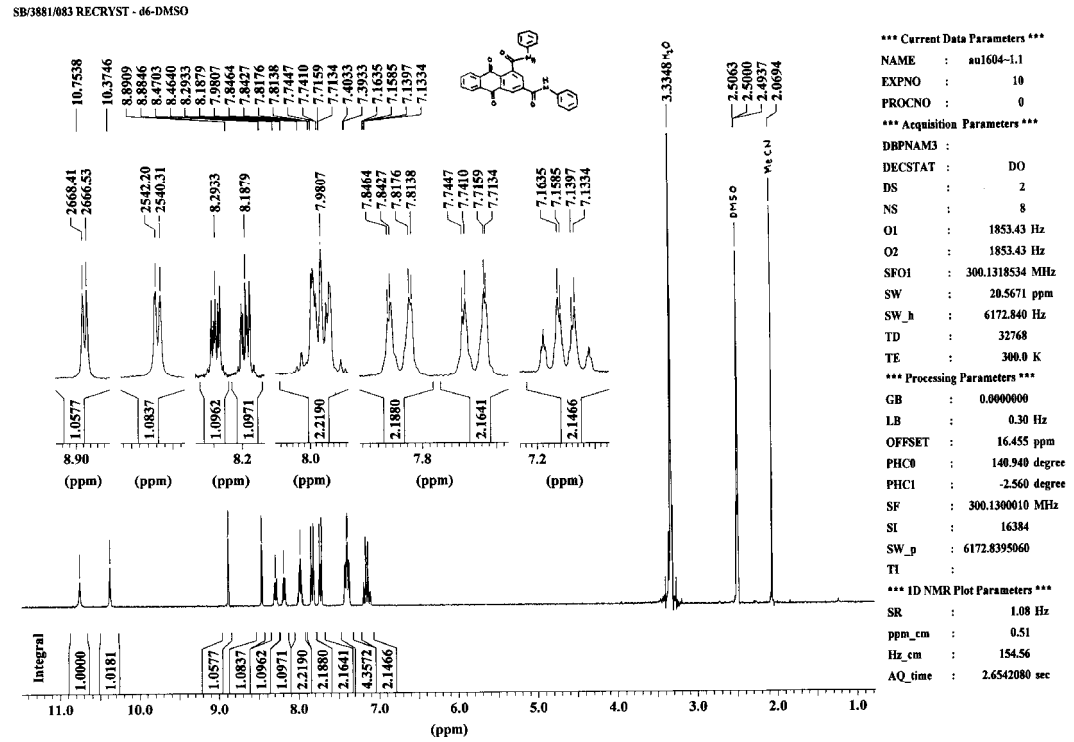


Figure S7 The ^{1}H NMR spectrum of compound **2** in DMSO-d_6

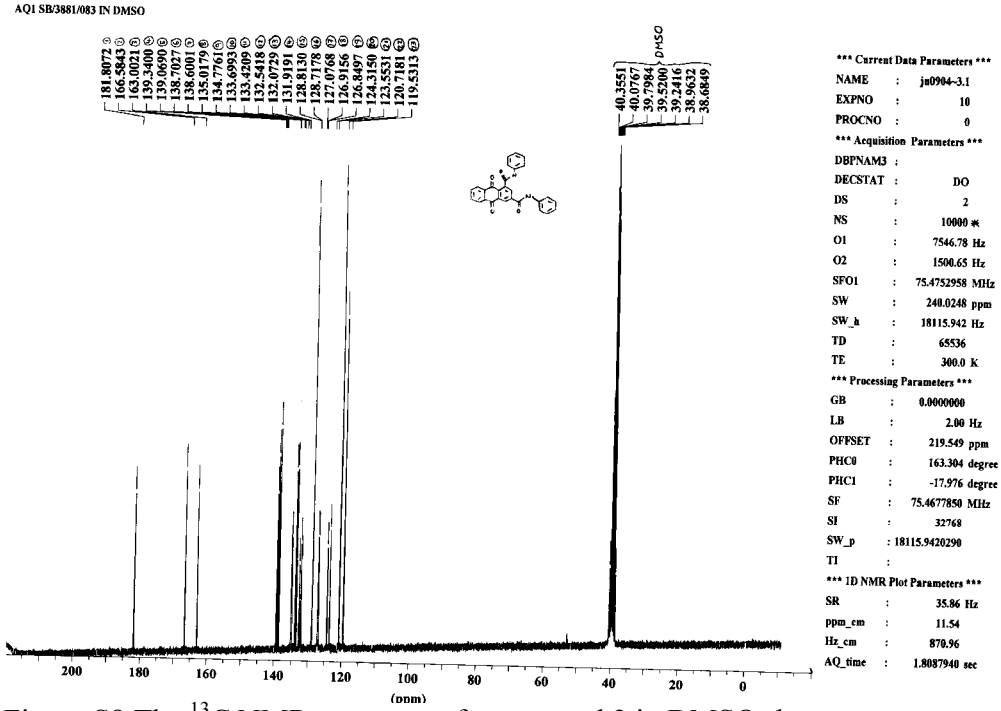


Figure S8 The ^{13}C NMR spectrum of compound **2** in DMSO-d$_6$

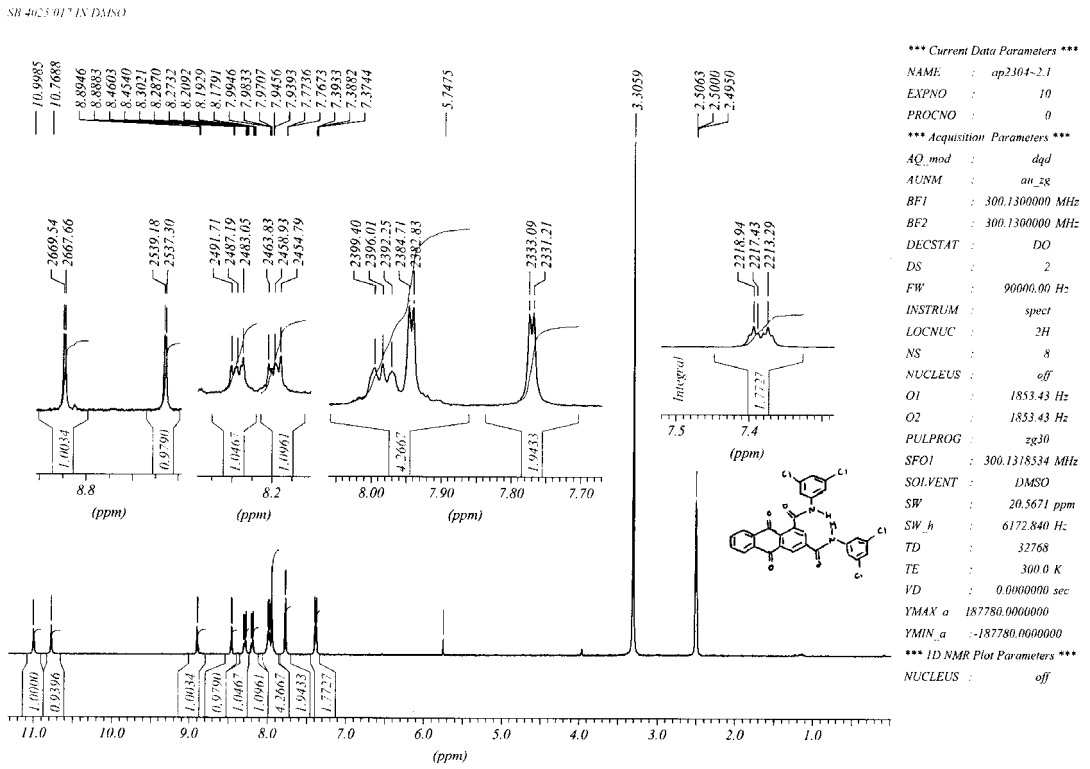


Figure S9 The ^{1}H NMR spectrum of compound **3** in DMSO-d$_6$

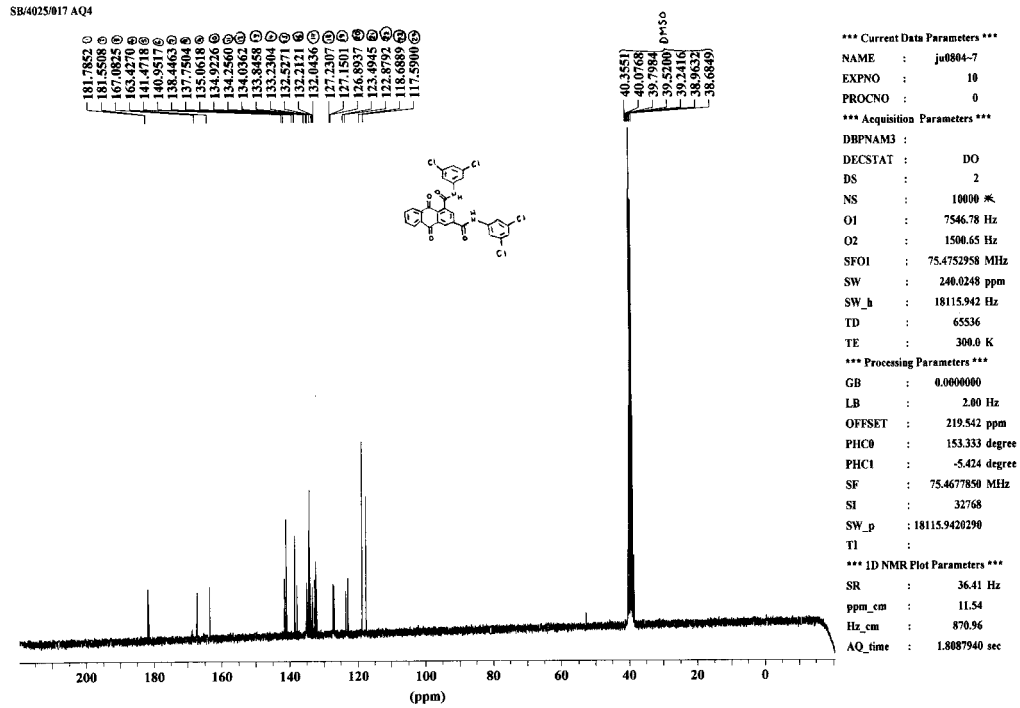


Figure S10 The ^{13}C NMR spectrum of compound **3** in DMSO-d_6

_N_1,_N_3-bis(3,5-dimethoxyphenyl)-9,10-anthraquinone-1,3-dicarboxamide. 1

3,5-Dimethoxyaniline (1.90 g, 12.2 mmol), triethylamine (1.29 g, 12.8 mmol), DMAP (0.013 g, 0.1 mmol) and dichloromethane (80 mL) were placed in a 250 mL round bottomed flask and allowed to stir under N_2 for 30 minutes. After a slow addition of anthraquinone-1,3-dicarbonyl chloride (2.02 g, 6.1 mol) the reaction was left stirring under N_2 overnight. The product was removed via filtration of reaction mixture and subsequently washed with both dichloromethane and water. The solvent was removed *in vacuo* to leave a pale yellow powder 1.23 g (35.6 %). ^1H NMR DMSO-d_6 (300 MHz): δ (ppm) 10.64 (s, 1H, N*H*), 10.31 (s, 1H, N*H*), 8.86 (d, 1H, J = 1.5 Hz, ar C*H*), 8.44 (d, 1H, J = 1.5 Hz, ar C*H*), 8.29 (m, 1H, ar C*H*), 8.19 (m, 1H, ar C*H*), 7.98 (m, 2H, ar C*H*), 7.13 (d, 2H, J = 2.2 Hz, *o*-aniline C*H*), 6.96 (d, 2H, J = 2.2 Hz, o-aniline C*H*), 6.31 (m, 2H, overlapping *p*-aniline ar C*H*), 3.76 (s, 6H, CH_3), 3.75 (s, 6H, CH_3). ^{13}C NMR DMSO-d_6 (75 MHz): δ (ppm) 181.7, 166.6, 163.0, 160.6, 160.4, 140.9, 140.3, 138.9, 138.6, 134.9, 134.8, 133.7, 133.4, 132.5, 132.0, 131.9, 127.1, 126.9, 126.8, 98.8, 97.8, 96.3, 96.5, 55.2, 55.1. LRMS (ES-): 601.2 $(M+Cl)^-$, 1167.5 $(2M+Cl)^-$. HRMS (ES-) $(M+Cl)^-$ Calculated Mass: 601.1383. Observed Mass: 601.1365 (Δ = 2.9ppm) (ES+) $(M+H)^+$ Calculated Mass: 567.1762. Observed Mass: 567.1758 (Δ = 0.6ppm). Melting Point (° C) Above 250.

***N*1,*N*3-diphenyl-9,10-anthraquinone-1,3-dicarboxamide. 2**

Aniline (1.005 g, 10.8 mmol), triethylamine (1.205 g, 11.9 mmol), DMAP (0.008 g, 0.07 mmol) and dichloromethane (30 mL) were placed in a 100 mL round bottomed flask and allowed to stir under N_2 for 30 minutes. After a slow addition of anthraquinone-1,3-diacarbonyl chloride (1.7830 g, 5.4 mol) the reaction was left stirring under N_2 overnight. The product was removed via filtration of the reaction mixture and subsequently washed with both dichloromethane and water. The solvent removed *in vacuo* to leave a pale yellow powder 1.0355 g (42.9 %). ^{1}H NMR DMSO-d_6 (300 MHz): δ (ppm) 10.75 (s, 1H, N*H*), 10.36 (s, 1H, N*H*), 8.89 (d, 1H, J = 1.9 Hz, ar C*H*), 8.47 (d, 1H, J = 1.9 Hz, ar C*H*), 8.29 (m, 1H ar C*H*), 8.19 (m, 1H, ar C*H*), 7.98 (m, 2H, ar C*H*), 7.82 (dd, 2 H, J = 8.7 & 1.1 Hz, *o*-aniline C*H*), 7.72 (d, 2H, J = 8.7 & 1.1 Hz, *o*-aniline C*H*), 7.40 (m, 4H, *m*-aniline C*H*), 7.14 (m, 2H, *p*-aniline C*H*). ^{13}C NMR DMSO-d_6 (75 MHz): δ (ppm) 181.8, 166.6, 163.0, 139.3, 139.1, 138.7, 138.6, 135.0, 134.8, 133.7, 133.4, 132.5, 132.1, 131.9, 128.8, 128.7, 127.1, 126.9, 126.9, 124.3, 123.6, 120.7, 119.5. LRMS (ES+) 447.1 $(M+H)^+$, 893.3 $(2M+H)^+$. HRMS (ES-) $(M+Cl)^-$ Calculated Mass: 481.0960. Observed Mass: 481.0949 (Δ = 2.4ppm). (ES+) $(M+H)^+$ Calculated Mass; 447.1339. Observed Mass : 447.1336 (Δ = 0.8ppm). Melting Point (° C) Above 250.

_N_1,_N_3-bis(3,5-dichlorophenyl)-9,10-anthraquinone-1,3-dicarboxamide 3.

3,5-Dichloroaniline (1.92 g, 11.6 mmol), triethylamine (1.29 g, 12.8 mmol), DMAP (0.01 g, 0.08 mmol) and dichloromethane (80 mL) were placed in a 250 mL round bottomed flask and allowed to stir under N_2 for 30 minutes. After a slow addition of anthraquinone-1,3-dicarbonyl chloride (1.94 g, 5.8 mol) the reaction was left to stir under N_2 overnight. The product was removed via filtration of reaction mixture and subsequently washed with both dichloromethane and water. The solvent was removed *in vacuo* to leave a pale yellow powder 0.21 g (6.3 %). ^{1}H NMR DMSO-d_6 (300 MHz): δ (ppm) 10.99 (s, 1H, N*H*), 10.77 (s, 1H, N*H*), 8.89 (d, 1H, J = 1.5 Hz, ar C*H*), 8.45 (d, 1H, J = 1.5 Hz, C*H*), 8.28 (m, 1H, ar C*H*), 8.19 (m, 1H, ar C*H*), 7.98 (m, 2H, ar C*H*), 7.93 (d, 2H, J = 1.9 Hz, *o*-aniline ar C*H*), 7.76 (d, 2H, J = 1.9 Hz, *o*-aniline ar C*H*), 7.38 (m, 2H, overlapping *p*-aniline ar C*H*). ^{13}C NMR DMSO-d_6 (75 MHz): δ (ppm) 181.8, 181.6, 167.1, 163.4, 141.5, 141.0, 138.5, 137.8, 135.1, 134.9, 134.3, 134.0, 133.5, 133.2, 132.5, 132.2, 132.0, 127.2, 127.2, 126.9, 123.5, 122.9, 118.7, 117.6. LRMS (ES-) 618.9 $(M+Cl)^-$, 699.0 $(M+2MeCN+Cl)^-$, 1202.5 $(2M+Cl)^-$. HRMS (ES-) $(M+Cl)^-$ Calculated Mass: 616.9402. Observed Mass: 616.9395 (Δ = 1.1ppm). Melting Point (° C) Above 250.

_N_1-(3,5-dimethoxyphenyl)-_N_3-(3-methoxy-5-methoxy)phenyl)isophthalamide 4.

3,5-Dimethoxyaniline (0.83g, 5.4mmol) was dissolved in dry dichloromethane (25 ml) under N_2. To this was added isophthaloyl dichloride (0.51 g, 2.5 mmol), DMAP (few mg), and triethylamine (0.75 g, 7.4 mmol), and the mixture stirred for 3 days. Solvent was removed *in vacuo* and compound was purified via recrystalliation from hot acetonitrile yielding needle like white crystals 0.42g (39 %). ^{1}H NMR DMSO-d_6 (300 MHz): 10.35 (s, 2H, N*H*), 8.49 (s, 1H, ar C*H*), 8.13 (d, 2H, ar C*H*), 7.69 (t, 1H, ar C*H*), 7.10 (s, 4H, ar C*H*), 6.28 (m, 2H, ar C*H*), 3.74 (s, 15H, CH_3). ^{13}C NMR DMSO-d_6 (75 MHz): 165.1, 160.4, 140.7, 135.1, 130.7, 128.6, 126.9, 98.5, 95.8, 55.1. LRMS (ES^-) 471.0 $(M + Cl)^-$, 907.4 $(2M + Cl)^-$. HRMS (ES^+): 437.1705 (M^-, Δ = 0.6ppm). Melting Point (° C) 242.

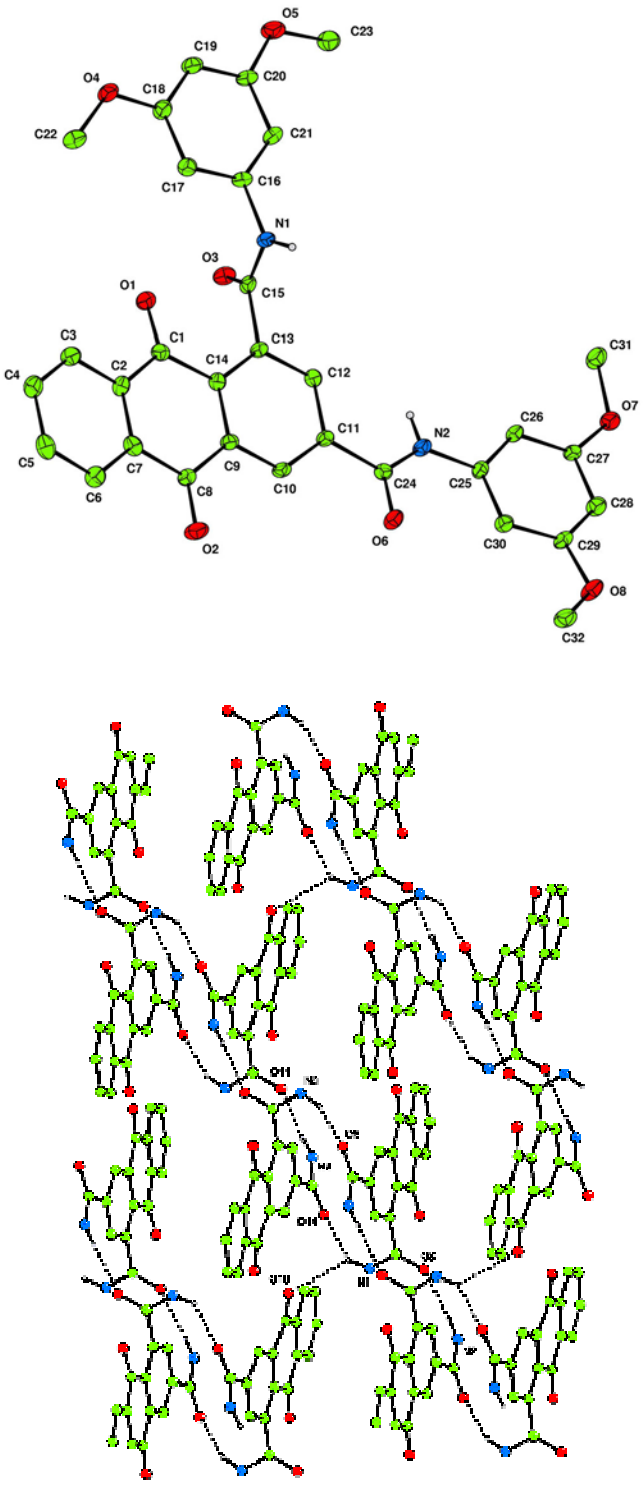


Figure S11 ORTEP plot of compound **1** (top) and packing diagram showing hydrogen bonding in the crystal (bottom).

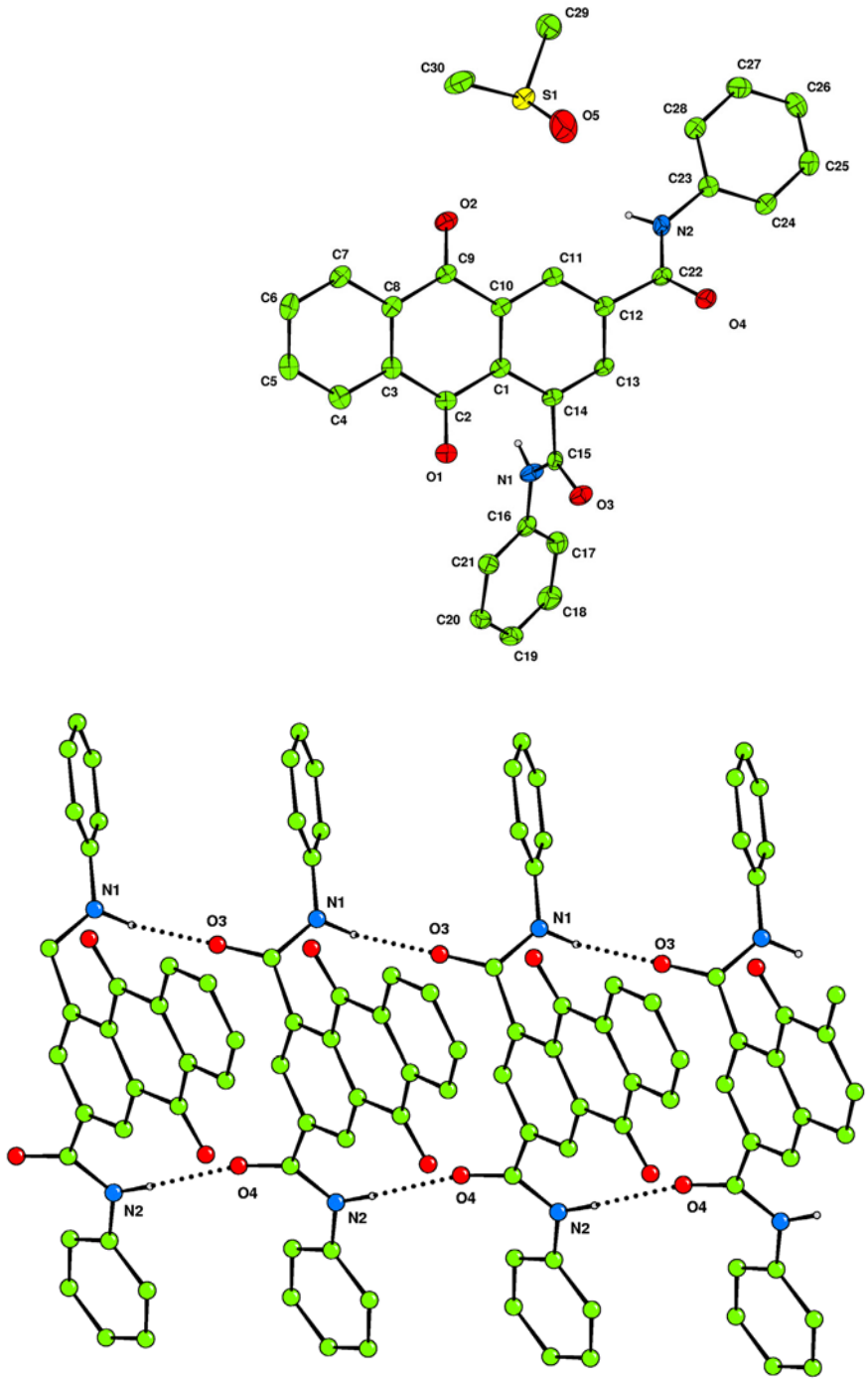


Figure S12 ORTEP plot of compound **2** (top) and packing diagram showing hydrogen bonding in the crystal (bottom).

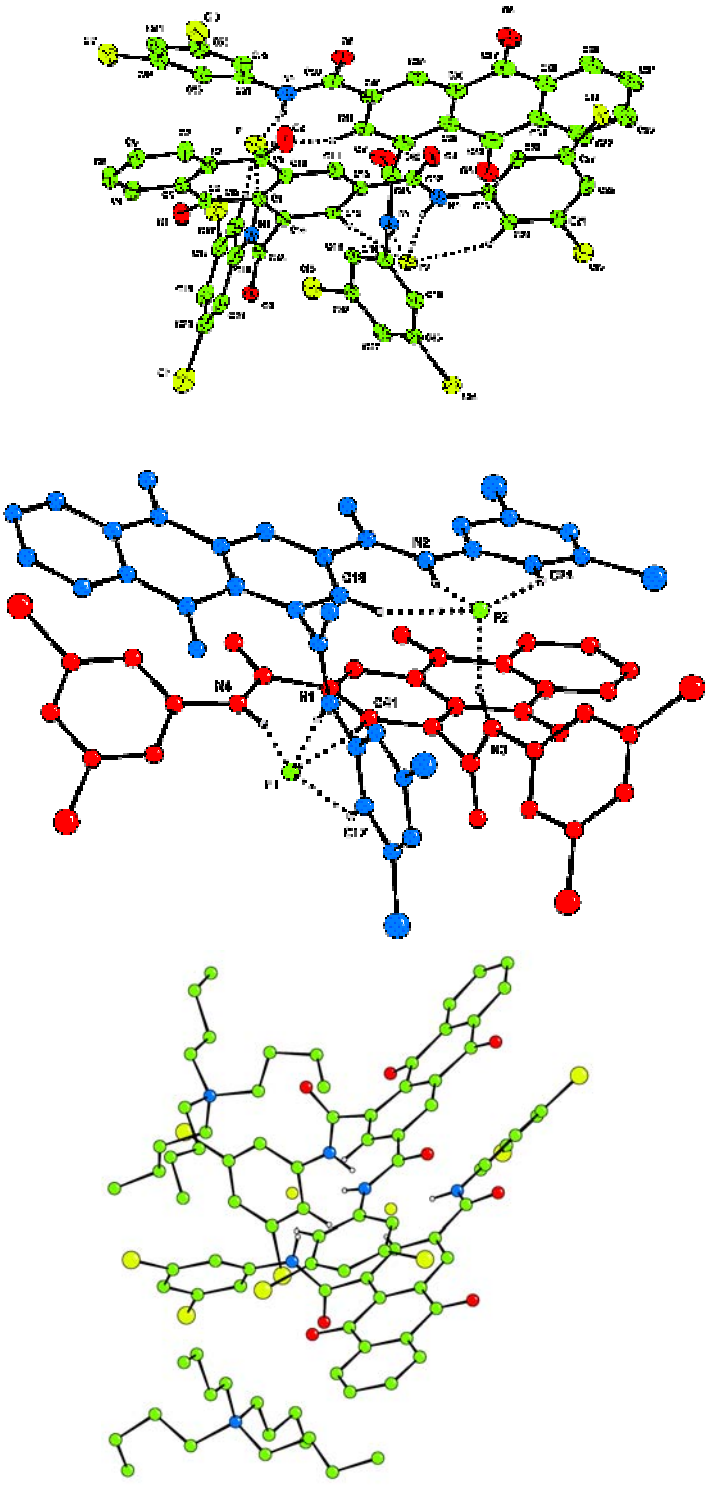


Figure S13 ORTEP plot of the tetrabutylammonium complex of compound **3** (counter cations, various hydrogen atoms and disorder omitted for clarity) (top), figure showing the two receptors in red and blue (centre) and the complex including counter cation (bottom).

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
N1–H1···F1	0.88	1.73	2.577(7)	160.2
N2–H2···F2	0.88	1.77	2.615(6)	159.2
N3–H3···F2	0.88	1.73	2.574(6)	159.5
N4–H4A···F1	0.88	1.74	2.594(7)	162.0
Possible C–H···F hydrogen bonds				
C24–H24···F2	0.95	2.32	3.061(7)	134.8
C13–H13···F2	0.95	2.17	3.062(9)	156.0
C17–H17···F1	0.95	2.14	2.789(8)	134.1
C41–H41···F1	0.95	2.12	3.034(8)	161.1

Table S1 Hydrogen bonds [Å and °] in the fluoride complex of **3**.

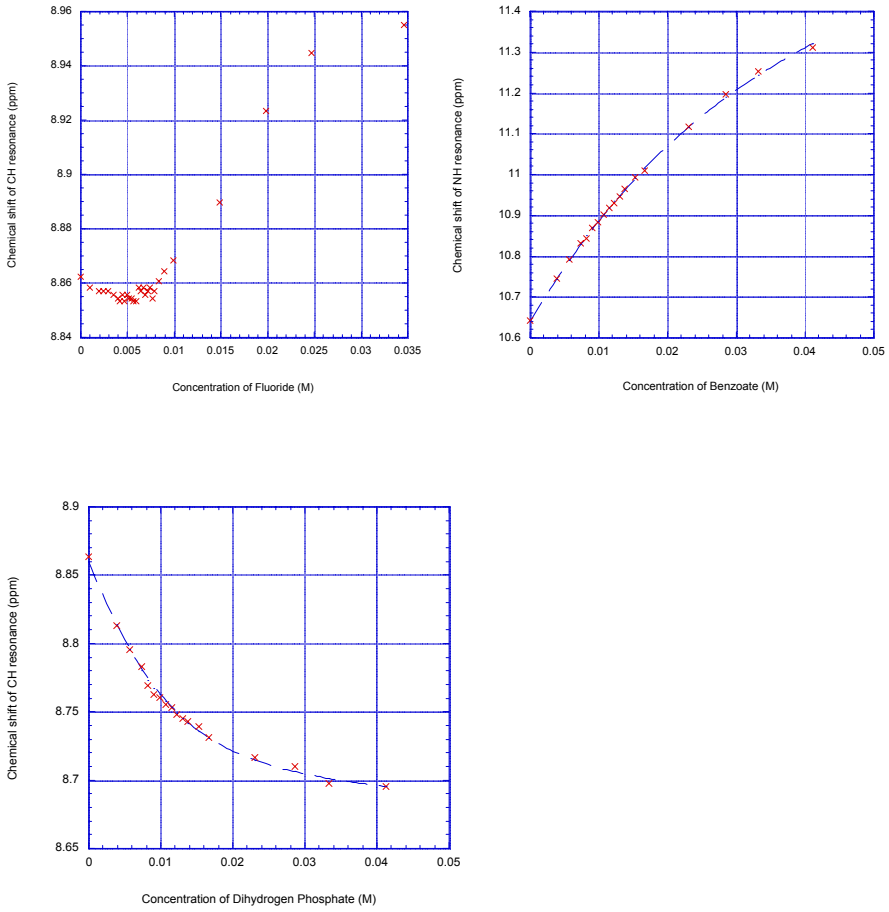
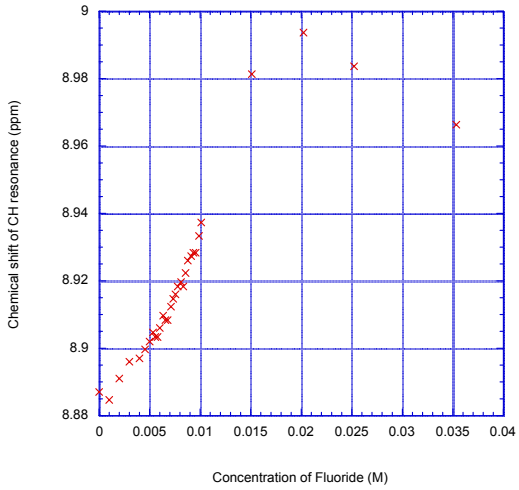
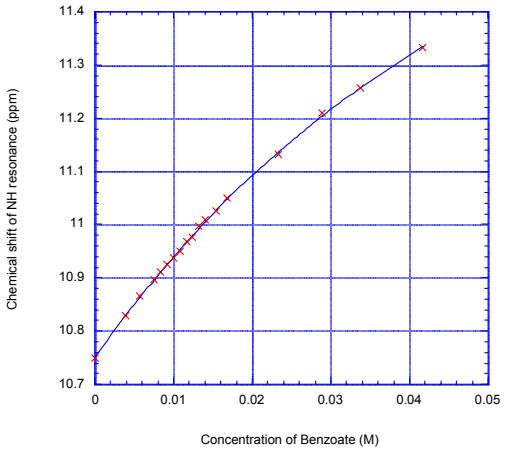


Figure S14 ^{1}H NMR titration curves of compound **1** with anions





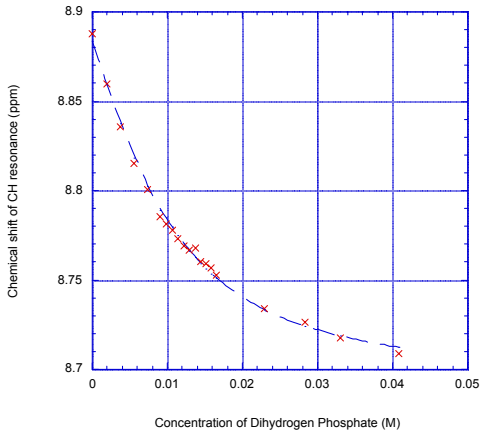


Figure S15 ^{1}H NMR titration curves of compound **2** with anions

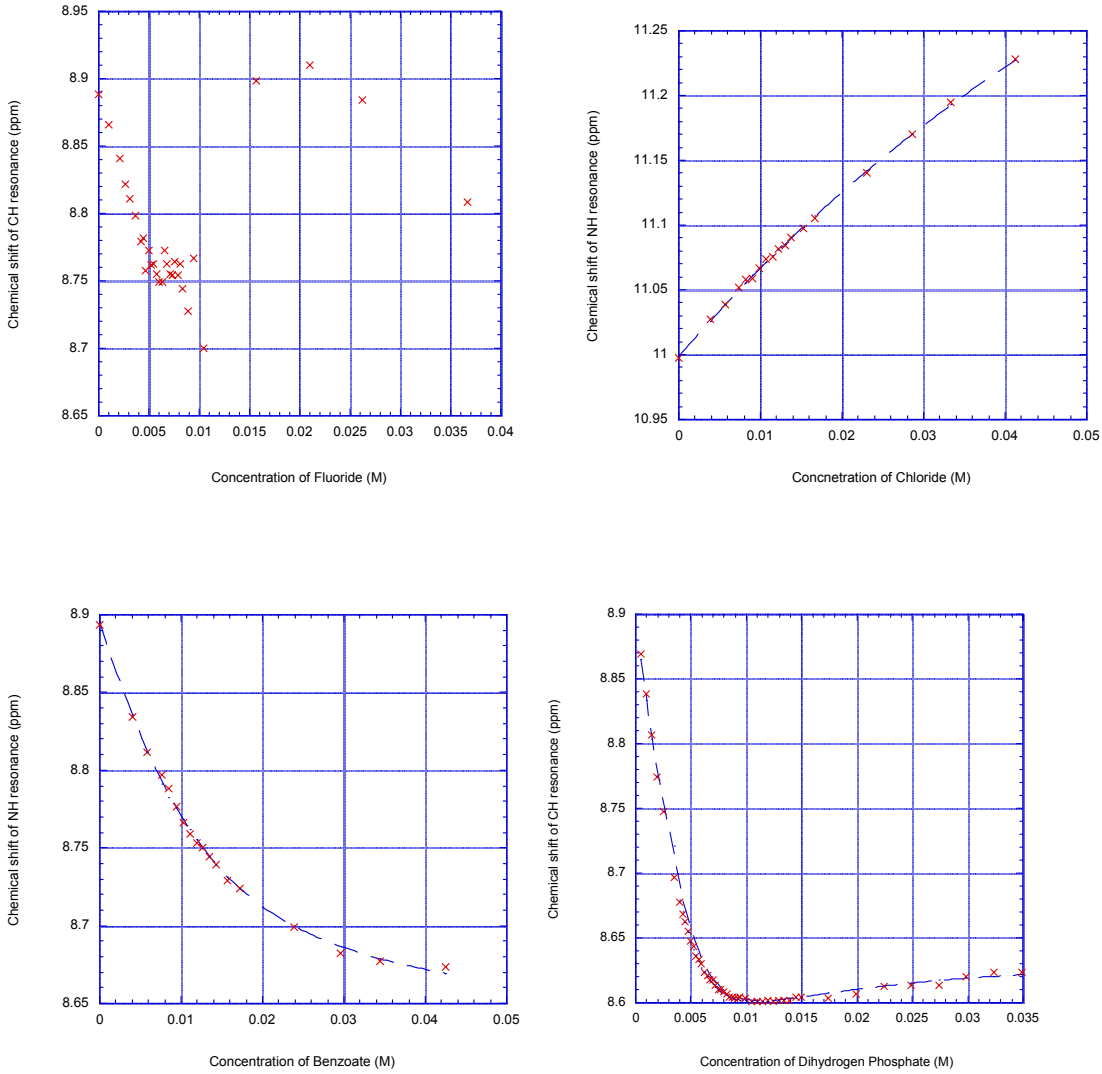


Figure S16 ^{1}H NMR titration curves of compound **3** with anions

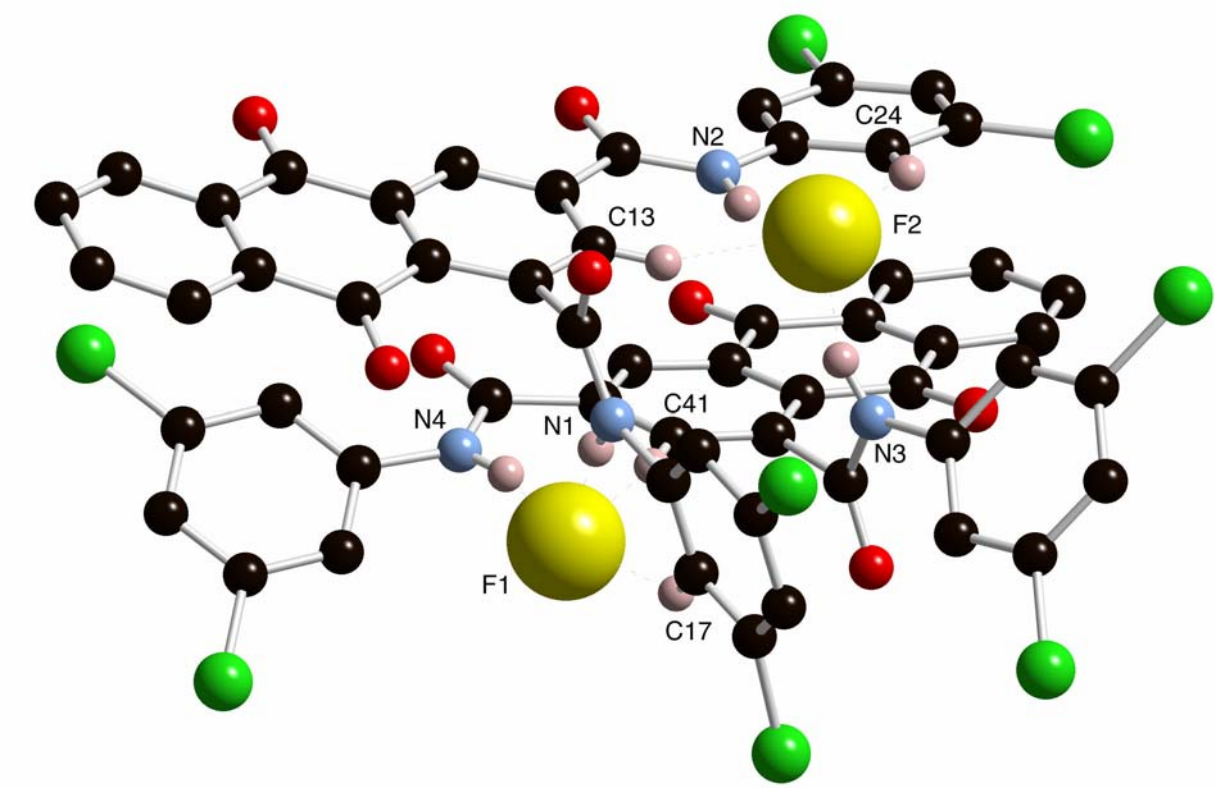


Figure S17 Version of Figure 2 (fluoride complex of **3**) from the communication with atom colours corresponding to elements.