Sensing anions on surfaces: tethering triazolium based anion receptors to polymer resins

Supporting Information

Synthetic Procedures

Synthesis of zinc 5-[3-(prop-2-yn-1-yloxy)phenyl]10,15,20-tris-[p-tolyl]porphyrin (5). Under argon, zinc 5-[m-hydroxyphenyl]10,15,20-tris-[p-tolyl]porphyrin 4 (500 mg, 0.68 mmol) was dissolved in dry dimethylformamide (15 mL). To this anhydrous potassium carbonate (470 mg, 3.4 mmol) and propargyl bromide (380 μ L, 3.4 mmol) were added and the mixture was then heated to 80 °C overnight. The mixture was then diluted with DCM (100 mL) and washed with water (30 mL). The organic layer was separated and the solvent evaporated *in vacuo* to give the crude product, which was subsequently purified by silica gel chromatography (eluent: 80% DCM / 20% Hexane) to give the product as a purple solid (504 mg, 96 %). mp > 300 °C; m/z (ESI-MS) [M + H]⁺ 773.2291 C₅₀H₃₇N₄OZn (calc. 773.2259); ¹H NMR (400 MHz, CDCl₃) δ 8.99 (8H, m, β -*H*), 8.12 (6H, m, Ar-*H*), 7.89(1H, m, Ar-*H*), 7.67 (1H, m, Ar-*H*), 7.58 (6H, m, Ar-*H*), 7.43 (1H, m, Ar-*H*), 4.89 (2H, d, J = 2.4 Hz, CH₂), 2.73 (9H, s, CH₃), 2.60 (1H, s, CH); ¹³C NMR (100MHz, CDCl₃) δ 155.8, 150.4, 150.3, 150.3, 150.0, 144.2, 139.8, 137.1, 134.4, 132.1, 132.0, 131.9, 131.8, 128.5, 127.4, 127.3, 121.2, 121.1, 120.2, 114.4, 78.6, 75.8, 56.0, 21.6.

Synthesis of 1-(4-butoxyphenyl)-4-(pyren-1-yl)-1H-1,2,3-triazole (6a). Under argon, 1-ethynylpyrene (260 mg, 1.15 mmol) and 4-butoxyphenylazide (240 mg, 1.26 mmol) were dissolved in dry dichloromethane (50 mL). To this mixture $Cu(MeCN)_4PF_6$ (33 mg, 0.09 mmol), TBTA (10 mg, 0.02 mmol) and diisopropylethylamine (280 mg, 2.17 mmol) were added and the reaction left to stir for 24 hours. The solution was then washed with 2M ammonium chloride solution (20 mL), dried over Na_2SO_4 and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a yellow solid (334 mg, 70 %). mp 164-166 °C; m/z (ESI-MS) [M + H]⁺ 418.1924 $C_{28}H_{24}N_{3}O$ (calc. 418.1919); ¹H NMR (400 MHz, acetone-d₆) δ 9.04 (1H s, -NC*H*), 8.47-8.23 (8H, m, Ar*H*), 8.11 (1H, t, J = 8.1 Hz, Ar*H*), 8.00 (2H, d, J = 8.0 Hz, Ar*H*), 7.21 (2H, d, J = 7.2 Hz, Ar*H*), 4.13 (2H, t, J = 6.4 Hz, -OC*H*₂), 1.86-1.79 (2H, m, -OCH₂C*H*₂), 1.59-1.50 (2H, m, -OCH₂CH₂C*H*₂), 1.00 (3H, t, J = 7.3 Hz, C*H*₃); ¹³C NMR (100 MHz, CDCI3) δ 159.5, 147.9, 131.4, 130.9, 130.3, 128.6, 128.2, 127.9, 127.4, 127.2, 126.1, 125.4, 125.2, 125.0, 124.9, 124.8, 124.7, 122.1, 121.0, 115.3, 68.1, 31.2, 19.2, 13.9.

Synthesis of 4-(anthracen-9-yl)-1-(4-butoxyphenyl)-1H-1,2,3-triazole (6b). Under argon, 9-ethynylanthracene (100 mg, 0.50 mmol) and 4-butoxyphenylazide (95 mg, 0.50 mmol) were dissolved in dry dichloromethane (25 mL). To this mixture Cu(MeCN)₄PF₆ (40 mg, 0.11 mmol), TBTA (15 mg, 0.03 mmol) and diisopropylethylamine (130 mg, 1.0 mmol) were added and the reaction left to stir for 24 hours. The solution was then washed with 2M ammonium chloride solution (10 mL), dried over Na₂SO₄ and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: 20% hexane / 80% DCM) to give the product as a yellow solid (148 mg, 76 %). mp 106-108 °C; m/z (ESI-MS) [M + H]⁺ 394.1929 C₂₆H₂₄N₃O (calc. 394.1919); ¹H NMR (400 MHz, CDCl3) δ 8.57 (1H, s, -NCH), 8.15 (1H, s, ArH), 8.06 (2H, d, J = 8.2 Hz, ArH), 7.94 (2H, d, J = 8.6 Hz, ArH), 7.81 (2H, d, J = 9.0 Hz, ArH), 7.47 (4H, m, ArH), 7.08 (2H, d, J = 9.0 Hz, ArH), 4.06 (2H, t, J =

6.4 Hz, OCH₂), 1.84 (2H, m, OCH₂CH₂), 1.56 (2H, m, OCH₂CH₂CH₂), 1.03 (3H, t, J = 7.2 Hz, CH₃); 13C NMR (100 MHz, CDCl3) δ 159.5, 144.5, 131.3, 130.3, 128.5, 128.4, 126.2, 125.3, 124.2, 122.8, 122.1, 115.4, 68.2, 31.2, 19.2, 13.9.

Synthesis of zinc 5-[3-((1-(4-butoxyphenyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl] 10,15,20-tris-[p-tolyl]porphyrin (6c). Under argon, alkyne porphyrin 5 (400 mg, 0.52 mmol) and 4-butyoxyphenylazide (99 mg, 0.52 mmol) were dissolved in dry DCM (50 mL). To this mixture Cu(MeCN)₄PF₆ (39 mg, 0.10 mmol), TBTA (20 mg, 0.04 mmol) and diisopropylethylamine (134 mg, 1.0 mmol) were added and the reaction left to stir for 24 hours. The solution was then washed with 2M ammonium chloride solution (20 mL), dried over Na₂SO₄ and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a purple solid (495 mg, 98 %). mp 202-204 °C; m/z (ESI-MS) $[M + H]^+$ 964.3312 C₆₀H₅₀N₇O₂Zn (calc. 964.3317); ¹H NMR (400 MHz, DMSO-d₆) δ 8.84 (1H, s, -NCH), 8.78 (8H, m, βH) 8.03 (6H, m, ArH), 7.86 (1H, s, ArH), 7.76 (3H, m, ArH), 7.67 (1H, m, ArH), 7.55 (6H, m, ArH), 7.50 (1H, m, ArH), 7.05 (2H, m, ArH), 5.42 $(2H, s, ArCH_2O)$, 3.98 $(2H, t, J = 6.7 Hz, OCH_2)$, 2.63 $(9H, s, ArCH_3)$, 1.70 (2H, m, OCH₂CH₂), 1.43 (2H, m, OCH₂CH₂CH₂), 0.93 (3H, t, J = 7.4 Hz, CH₃); 13 C NMR (100 MHz, DMSO-d₆) δ 159.2, 156.6, 149.9, 149.8, 149.6, 144.7, 140.3, 137.0, 134.5, 132.0, 130.3, 127.6, 123.2, 122.1, 121.5, 120.8, 120.7, 120.1, 115.7, 68.0, 55.4, 31.1, 21.5, 19.2, 14.1.

Synthesis of 1-(4-butoxyphenyl)-3-methyl-4-(pyren-1-yl)-1H-1,2,3-triazol-3-ium tetrafluoroborate (7a). To a solution of the pyrene triazole 6a (163 mg, 0.39 mmol) in dry DCM (20 mL) was added trimethyloxonium tetrafluoroborate (87 mg, 0.59 mmol). The reaction was allowed to stir for 24 hours after which 15 drops of methanol were added and the solvent removed *in vacuo*. The crude product was then purified by silica gel chromatography (eluent: 10% MeOH/DCM) to give the pure product as a cream solid (177 mg, 87 %). mp 104-106 °C; m/z (ESI-MS) $[M - BF_4^-]^+$ 432.2079 $C_{29}H_{26}N_3O$ (calc. 432.2076); ¹H NMR (400 MHz, CDCl3) δ 8.88 (1H, s, -NCH), 8.23 (1H d, J = 7.4 Hz, ArH), 8.19-8.10 (5H m, ArH), 8.04 (1H, m, ArH), 7.95 (1H, d, J = 9.0 Hz, ArH), 7.90 (2H, d, J = 9.0 Hz, ArH), 7.72 (1H, d, J = 9.0 Hz, ArH), 6.95 (2H, d, J = 9.0 Hz, ArH), 4.06 (3H, s, -NCH₃), 3.92 (2H, t, J = 6.7 Hz, $-OCH_2$), 1.80-1.73 (2H, m, $-OCH_2CH_2$), 1.56-1.47 (2H, m, $-OCH_2CH_2CH_2$), 1.00 (3H, t, J = 7.4 Hz, CH₃); ¹³C NMR (100 MHz, CDCl3) δ 161.7, 143.2, 133.7, 130.8, 130.3, 130.3, 129.8, 128.5, 127.7, 127.0, 126.9, 126.8, 126.6, 125.0, 124.2, 123.8, 123.4, 122.0, 115.7, 114.2, 68.3, 38.4, 31.1, 19.2, 13.8; ¹⁹F NMR (376 MHz, CDCl₃) δ -153.0.

Synthesis of 4-(anthracen-9-yl)-1-(4-butoxyphenyl)-3-methyl-1H-1,2,3-triazol-3-ium tetrafluoroborate (7b). To a solution of the anthracene triazole 6b (100 mg, 0.25 mmol) in dry DCM (10 mL) was added trimethyloxonium tetrafluoroborate (38 mg, 0.38 mmol). The reaction was allowed to stir for 24 hours after which 15 drops of methanol were added and the solvent removed *in vacuo*. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a yellow solid (110 mg, 87 %). mp 184-186 °C; m/z (ESI-MS) $[M - BF_4^-]^+$ 408.2087 C₂₇H₂₆N₃O (calc. 408.2076); ¹H NMR (400 MHz, Acetone-d₆) δ 9.68 (1H, s, -NCH), 9.06 (1H, s, ArH), 8.32 (2H, m, ArH), 8.17 (2H, m, ArH), 7.95 (2H, m, ArH), 7.67 (4H, m, ArH), 7.33 (2H, m, ArH), 4.20 (3H, s, -NCH₃), 4.18 (2H, t, J = 6.3, OCH₂), 1.83 (2H, m, OCH₂CH₂), 1.54 (2H, m, OCH₂CH₂CH₂), 0.99 (3H, t, J = 7.4 Hz, CH₃); ¹³C NMR (100 MHz, CDCl3) δ 161.8, 140.6, 132.5, 131.5, 131.1, 129.6, 129.2, 128.6, 128.5,

126.2, 124.3, 123.6, 115.8, 113.9, 68.3, 38.0, 31.0, 18.9, 13.2; $^{19}\mathrm{F}$ NMR (376 MHz, CDCl₃) δ -153.2.

zinc 5-[3-((1-(4-butoxyphenyl)-3-methyl-1H-1,2,3-triazol-3-ium-4-**Synthesis** of yl)methoxy)phenyl] 10,15,20-tris-[p-tolyl]porphyrin tetrafluoroborate (7c). To a solution of porphyrin triazole 6c (100 mg, 0.10 mmol) in dry DCM (20 mL) was added trimethyloxonium tetrafluoroborate (25 mg, 0.17 mmol). The reaction was allowed to stir for 6 hours after which 15 drops of methanol were added. The reaction mixture was then washed with water (10 mL x 5), dried over Na₂SO₄ and filtered. To the crude solution excess $Zn(BF_4)_2$ in methanol was added and stirred for one hour, followed by washing with water (10 mL x 5), drying over Na₂SO₄ and evaporation of solvent. The crude product was then purified by a short silica column (eluent: 10 % MeOH/ 90% DCM) to give the product as a purple solid (98 mg, 90 %). mp 290-292 °C; m/z (ESI-MS) $[M - BF_4]^+$ 978.3464 $C_{61}H_{52}N_7O_2Zn$ (calc. 978.3474); ¹H NMR (400 MHz, Acetone-d₆) δ 9.33 (1H, s, -NCH), 8.87 (8H, m, β H), 8.08 (6H, m, ArH), 7.97 (1H, s, ArH), 7.91 (1H, m, ArH), 7.82 (2H, m, ArH), 7.74 (1H, m, ArH), 7.59 (6H, m, ArH), 7.54 (1H, m, ArH), 7.13 (2H, m, ArH), 5.77 (2H, s, OCH₂), 4.54 (3H, s, NCH₃), 4.08 (2H, t, J = 6.7 Hz, OCH₂), 2.68 (9H, s, ArCH₃), 1.80 (2H, m, OCH₂CH₂), 1.52 (2H, m, OCH₂CH₂CH₂), 0.98 (3H, t, J = 7.4 Hz); ¹³C NMR (100 MHz, Acetone-d₆) δ 161.7, 155.7, 150.2, 150.1, 150.0, 149.6, 145.1, 140.9, 140.3, 137.0, 134.3, 134.2, 131.6, 131.5, 131.2, 128.8, 127.8, 127.7, 127.7, 127.2, 123.2, 121.0, 120.9, 120.6, 119.4, 115.7, 114.3, 68.2, 58.7, 38.5, 30.9, 20.6, 18.9, 13.2; ¹⁹F NMR (376 MHz, Acetone-d₆) δ -151.7.

Tosyl functionalised Tentagel resins (HL/LL-9). Under argon Tentagel-OH beads (103 mg, 0.24 mmol/g OH loading), tosyl chloride (103 mg, 0.54 mmol) and a catalytic amount of 4-dimethylaminopyridine were added to the reaction vessel and suspended in dry DCM (3 mL). To this mixture Et_3N (100 µL) was added and the reaction was left for one week with occasional stirring. After this time the beads were filtered and washed sequentially with DCM and hexane several times (5 x 5 mL each), followed by a final wash with acetone (5 mL), water (5 mL) and acetone (5 mL). The resulting off white beads were allowed to air dry.

Azide functionalised Tentagel resins (HL/LL-10). The tosyl functionalised Tentagel beads HL/LL-9 were suspended in dry DMF (3 mL) and sodium azide (351 mg, 5.4 mmol) was then added. The reaction was left for one week with occasional stirring, before the beads were filtered, washed with water (10 x 5 mL), acetone (5 mL) and sequential rinsing with DCM and hexane (5 x 5 mL each). The off white beads were then allowed to air dry.

Pyrene triazole functionalsed tentegel resins (HL/LL-11a). To a round bottomed flask containing azide functionalised TentaGel resin **HL/LL-10** (82 mg) suspended in dry DCM (3 mL) was added 1-ethynylpyrene (150 mg, 0.66 mmol), Cu(MeCN)₄PF₆ (20 mg, 0.05 mmol), TBTA (15 mg, 0.025 mmol) and DIPEA (170 mg, 1.32 mmol). The reaction mixture was left under Argon for one week with occasional gentle stirring. The TentaGel resins were then filtered from the reaction mixture and the resulting beads were washed thoroughly with dichloromethane and hexane (5 x 5 mL sequentially), followed by acetone (5 mL), water (5 mL), acetone (5 mL) and dichloromethane (5 mL). The pale yellow beads were then allowed to air dry. ¹H HR MAS NMR (400 MHz, CDCl₃) δ 8.78 (s, NC*H*), 7.98-8.34 (m, Ar*H*), 7.81 (d, J = 7.8 Hz, Ar*H*), 7.34 (m, Ar*H*).

Anthracene triazole functionaled tentegel resins (HL/LL-11b). To a round bottomed flask under argon containing azide functionalised TentaGel resin 10 (81 mg), 9-ethynylanthracene (134 mg, 0.66 mmol), Cu(MeCN)₄PF₆ (20 mg, 0.05 mmol), and TBTA (15 mg, 0.025 mmol) DCM (3 mL) and DIPEA (170 mg, 1.32 mmol) were added. The reaction was left for one week with occasional gentle stirring. The TentaGel resins were then filtered from the reaction mixture and the resulting beads were washed thoroughly with dichloromethane and hexane (5 x 5 mL sequentially), followed by acetone (5 mL), water (5 mL), acetone (5 mL) and dichloromethane (5 mL). The orange beads were allowed to air dry. ¹H HR MAS NMR (400 MHz, CDCl₃) δ 8.55 (s, NC*H*), 8.07 (m, Ar*H*), 7.85 (m, Ar*H*), 7.30-7.51 (m, Ar*H*).

Porphyrin triazole functionalised tentagel resins (HL/LL-11c). To a round bottomed flask under argon containing azide functionalised TentaGel resin **10** (84 mg), porphyrin alkyne **5** (300 mg, 0.39 mmol), Cu(MeCN)₄PF₆ (16 mg, 0.04 mmol), and TBTA (12 mg, 0.02 mmol) DCM (3 mL) and DIPEA (104 mg, 0.80 mmol) were added. The reaction was left for one week with occasional gentle stirring. The TentaGel resins were then filtered from the reaction mixture and the resulting beads were washed thoroughly with dichloromethane and hexane (5 x 5 mL sequentially), followed by acetone (5 mL), water (5 mL), acetone (5 mL) and dichloromethane (5 mL). The purple beads were allowed to air dry. ¹H HR MAS NMR (400 MHz, CDCl₃) δ 8.85 (m, β H), 8.75 (s, NCH), 8.02 (m, ArH), 7.72 (m, ArH), 7.46 (m, ArH), 7.25 (m, ArH), 2.64 (s, ArCH₃).

Synthesis of 4-(3-azidophenyl)-2-methylbut-3-yn-2-ol (13). 4-(3-aminophenyl)-2methylbut-3-yn-2-ol (730 mg, 4.17 mmol) was dissolved in a solution of water (20 mL) and conc. HCl (20 mL). The reaction mixture was then cooled in an ice bath to 0 °C and a solution of sodium nitrite (343 mg, 5.0 mmol) in water (5 mL) was added dropwise. The reaction was stirred at room temperature for 1 hour before being cooled again to 0 °C. A solution of sodium azide (541 mg, 8.34 mmol) in water (5 mL) was added dropwise, and the reaction stirred for a further 3 hours at room temperature. After this time the crude product was extracted with CHCl₃ (3 x 15 mL). The combined organic layers were then washed with brine (15 mL x 2), dried over Na₂SO₄, filtered and solvent evaporated to give the product as a brown oil (713 mg, 85 %). m/z (ESI-MS) $[2M + H]^+$ 403.1871 C₂₂H₂₃N₆O₂ (calc. 403.1882); ¹H NMR (400 MHz, CDCl₃) δ 7.27 (1H, m, ArH), 7.18 (1H, m, ArH), 7.08 (1H, m, ArH), 6.96 (1H, m, ArH), 2.02 (1H, br s, OH), 1.62 (6H, s, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ 140.2, 129.7, 128.2, 124.4, 121.9, 119.1, 94.7, 81.1, 65.6, 31.4.

Synthesis of 2-methyl-4-(3-(4-(pyren-1-yl)-1H-1,2,3-triazol-1-yl)phenyl)but-3-yn-2-ol (14a). Under argon, 1-ethynylpyrene (700 mg, 3.1 mmol) and azide 13 (683 mg, 3.4 mmol) were dissolved in dry DCM (50 mL). To this mixture Cu(MeCN)₄PF₆ (225 mg, 0.6 mmol), DIPEA (800 mg, 6.2 mmol) and TBTA (50 mg, 0.1 mmol) were added and the reaction was left to stir for four days. The solution was then diluted with DCM (50 mL) and washed with 2M NH₄Cl solution (3 x 25 mL), dried over Na₂SO₄, filtered and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a yellow solid (950 mg, 68%). mp 214-216 °C; m/z (ESI-MS) [M + H]⁺ 428.1745 C₂₉H₂₂N₃O (calc. 428.1763); ¹H NMR (400 MHz, Acetone-d₆) δ 9.24 (1H, s, NC*H*), 9.04 (1H, d, J = 9.4 Hz, Ar*H*), 8.48 (1H, d, J = 7.6 Hz, Ar*H*), 8.38 (1H, d, J = 8.2 Hz, Ar*H*), 8.33 (2H, d, J = 7.6 Hz, Ar*H*), 8.27 (1H, d, J = 9.4 Hz, Ar*H*), 8.22 (2H, s, Ar*H*), 8.11 (3H, m, Ar*H*), 7.67 (1H, m, Ar*H*), 7.56 (1H, d, J = 7.6 Hz, Ar*H*), 4.59 (1H, s, O*H*), 1.59 (6H, s, C*H*₃); ¹³C NMR (100 MHz, Acetone-d₆) δ 147.9, 137.5, 131.5, 131.4, 131.4, 131.0, 130.2, 128.4, 128.1, 127.9,

127.4, 127.3, 126.4, 125.6, 125.3, 125.3, 125.2, 125.0, 125.0, 124.6, 122.8, 122.0, 120.0, 96.9, 79.6, 64.3, 31.0.

Synthesis of 4-(3-(4-(anthracen-9-yl)-1H-1,2,3-triazol-1-yl)phenyl)-2-methylbut-3-yn-2-ol (14b). Under argon, 9-ethynylanthracene (450 mg, 2.2 mmol) and azide 13 (493 mg, 2.5 mmol) were dissolved in dry DCM (50 mL). To this mixture was added Cu(MeCN)₄PF₆ (162 mg, 0.44 mmol), DIPEA (574 mg, 4.4 mmol) and TBTA (20 mg, 0.04 mmol) and the reaction was left to stir for four days. The solution was then diluted with DCM (50 mL) and washed with 2M NH₄Cl solution (3 x 25 mL), dried over Na₂SO₄, filtered and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a yellow solid (217 mg, 23%). mp 100-102 °C; m/z (ESI-MS) [M + H]⁺ 404.1754 C₂₇H₂₂N₃O (calc. 404.1763); ¹H NMR (400 MHz, Acetone-d₆) δ 8.97 (1H, s, NC*H*), 8.71 (1H, s, Ar*H*), 8.13 (4H, m, Ar*H*), 7.98 (2H, m, Ar*H*), 7.66 (1H, m, Ar*H*), 7.51 (5H, m, Ar*H*), 4.62 (1H, s, O*H*), 1.59 (6H, s, C*H*₃); ¹³C NMR (100 MHz, Acetone-d₆) δ 144.2, 137.6, 131.5, 131.3, 131.2, 130.1, 128.5, 128.3, 126.2, 162.1, 125.4, 125.1, 124.8, 123.8, 122.9, 120.0, 96.9, 79.7, 64.3, 31.1.

Synthesis of zinc 5-[3-((1-(3-(3-hydroxy-3-methylbut-1-yn-1-yl)phenyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl] 10,15,20-tris-[p-tolyl]porphyrin (14c). Under argon, alkvne porphyrin 5 (200 mg, 0.26 mmol) and azide 13 (53 mg, 0.26 mmol) were dissolved in dry DCM (50 mL). To this mixture was added Cu(MeCN)₄PF₆ (40 mg, 0.10 mmol), TBTA (20 mg, 0.04 mmol) and diisopropylethylamine (67 mg, 0.52 mmol) and the reaction was left to stir for 24 hours. The solution was then washed with 2M ammonium chloride solution, dried over Na_2SO_4 and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a purple solid (208 mg, 82 %). mp 224-226 °C; m/z (ESI-MS) $[M + H]^+$ 974.3242 C₆₁H₄₈N₇O₂Zn (calc. 974.3161); ¹H NMR (400 MHz, DMSO-d₆) δ 9.11 (1H, s, -NCH), 8.77 (8H, m, βH), 8.02 (6H, m, ArH), 7.97 (1H, s, ArH), 7.93 (1H, m, ArH), 7.87 (1H, s, ArH), 7.78 (1H, m, ArH), 7.68 (1H, m, ArH), 7.53 (9H, m, ArH), 5.56 (1H, s, OH), 5.44 (2H, s, O-CH₂), 2.63 (9H, m, ArCH₃), 1.48 (6H, s, CH₃); ¹³C NMR (100 MHz, DMSO-d₆) δ 155.6, 149.9, 149.8, 149.8, 149.6, 144.7, 144.6, 140.3, 137.2, 137.0, 134.5, 132.0, 132.0, 131.9, 131.8, 130.8, 128.2, 127.7, 124.7, 123.5, 122.7, 121.6, 120.9, 120.7, 120.3, 120.1, 114.6, 98.0, 79.8, 64.1, 61.9, 31.9, 21.5.

Synthesis of 1-(3-ethynylphenyl)-4-(pyren-1-yl)-1H-1,2,3-triazole (15a). To a solution of 14a (950 mg, 2.2 mmol) in toluene (125 mL) was added potassium hydroxide (250 mg, 4.4 mmol). The reaction was then heated to 120 °C and stirred for 30 mins. The mixture was allowed to cool and was then filtered, followed by washing with water (50 mL x 3), drying over Na₂SO₄, filtration and evaporation of solvent. The crude product was then purified by silica gel column (eluent: 20% hexane / 80% DCM) to give the product as a yellow solid (754 mg, 92%). mp 188-190 °C; m/z (ESI-MS) [M + H]⁺ 370.1339 C₂₆H₁₆N₃ (calc. 370.1344); ¹H NMR (400 MHz, CDCl3) δ 8.75 (1H, d, J = 9.4 Hz, Ar*H*), 8.41 (1H, s, NC*H*), 8.01-8.37 (9H, m, Ar*H*), 7.96 (1H, d, J = 8.2 Hz, Ar*H*), 7.60 (2H, m, Ar*H*), 3.24 (1H, s, C≡C*H*); ¹³C NMR (100 MHz, CDCl3) δ 148.4, 137.1, 132.4, 131.6, 131.4, 130.9, 130.0, 128.7, 128.4, 128.1, 127.4, 127.2, 126.2, 125.6, 125.3, 125.1, 124.9, 124.7, 124.6, 124.5, 124.1, 123.9, 121.0, 120.7, 82.1, 79.2.

Synthesis of 4-(anthracen-9-yl)-1-(3-ethynylphenyl)-1H-1,2,3-triazole (15b). To a solution of 14b (200 mg, 0.5 mmol) in toluene (50 mL) was added potassium hydroxide (56 mg, 1.0

mmol). The reaction was then heated to 120 °C and stirred for 30 mins. The mixture was allowed to cool and was then filtered, followed by washing with water (20 mL x 3), drying over Na₂SO₄, filtration and evaporation of solvent. The crude product was then purified by silica gel chromatography (eluent: DCM) to give the product as a yellow solid (154 mg, 89%). mp 176-178 °C; m/z (ESI-MS) [M + H]⁺ 346.1335 C₂₄H₁₆N₃ (calc. 346.1344); ¹H NMR (400 MHz, CDCl3) δ 8.59 (1H, s, NCH), 8.26 (1H, s, ArH), 8.06 (3H, m, ArH), 7.97 (1H, m, ArH), 7.90 (2H, m, ArH), 7.59 (2H, m, ArH), 7.47 (4H, m, ArH), 3.22 (1H, s, C=CH); ¹³C NMR (100 MHz, CDCl3) δ 144.9, 137.0, 132.3, 131.3, 130.0, 128.7, 128.6, 126.3, 125.8, 125.3, 124.0, 123.8, 123.7, 122.6, 120.7, 82.1, 79.2.

Synthesis of zinc 5-[3-((1-(3-ethynylphenyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl] 10,15,20-tris-[p-tolyl]porphyrin (15c). Porphyrin 14c (500 mg, 0.51 mmol) dissolved in toluene (125 mL) and KOH (56 mg, 1.0 mmol) added. The mixture was heated to 120 °C for 30 minutes and then cooled and filtered. Solvent removed by vaccum and crude product purified by silica gel chromatography (eluent: DCM) to give the product as a purple solid (354 mg, 75 %). mp decomp. >230 °C; m/z (ESI-MS) [M + H]⁺ 916.2710 C₅₈H₄₂N₇OZn (calc. 916.2742); ¹H NMR (400 MHz, DMSO-d₆) δ 9.09 (1H, s, NCH), 8.77 (8H, m, βH), 8.02 (8H, m, ArH), 7.86 (1H, s, ArH), 7.77 (1H, m, ArH), 7.68 (1H, m, ArH), 7.55 (9H, m, ArH), 5.44 (2H, s, OCH₂), 4.38 (1H, s, C≡CH), 2.63 (9H, m, ArCH₃); ¹³C NMR (100 MHz, DMSO-d₆) δ 156.6, 149.9, 149.8, 149.8, 149.6, 144.7, 144.6, 140.3, 140.3, 137.2, 137.0, 134.5, 132.3, 132.0, 132.0, 131.9, 130.9, 128.2, 127.7, 123.8, 123.5, 123.3, 121.6, 121.0, 120.9, 120.7, 120.1, 114.6, 82.9, 82.7, 61.9, 21.5.

Synthesis of 1-(3-ethynylphenyl)-3-methyl-4-(pyren-1-yl)-1H-1,2,3-triazol-3-ium tetrafluoroborate (16a). To a solution of pyrene triazole 15a (725 mg, 2.0 mmol) dissolved in DCM (25 ml) was added Me₃OBF₄ (2.96 g, 20 mmol). The reaction was allowed to stir overnight followed by the addition of 15 drops of methanol. The reaction mixture was then washed with water (10 mL x 3), dried over Na₂SO₄, filtered and the solvent evaporated. The crude product was then precipitated from CHCl₃ to give the product as a pale yellow powder (560 mg, 63%). mp 230-232 °C; m/z (ESI-MS) [M – BF₄]⁺ 384.1504 C₂₇H₁₈N₃ (calc. 384.1501); ¹H NMR (400 MHz, DMSO-d₆) δ 10.07 (1H, s, NCH), 8.60 (1H, d, J = 7.8 Hz, ArH), 8.50 (2H, d, J = 7.8 Hz, ArH), 8.44 (2H, m, ArH), 8.36 (3H, m, ArH), 8.25 (3H, m, ArH), 7.88 (2H, m, ArH), 4.58 (1H, s, C≡CH), 4.29 (3H, s, NCH₃); ¹³C NMR (100 MHz, DMSO-d₆) δ 142.2, 135.7, 135.2, 133.7, 131.5, 131.1, 130.6, 130.4, 130.3, 129.9, 129.0, 127.7, 127.6, 127.3, 127.1, 125.5, 125.1, 124.2, 124.2, 124.0, 123.7, 122.5, 116.0, 84.0, 82.0, 79.6; ¹⁹F NMR (376 MHz, DMSO-d₆) δ -148.3.

Synthesis of 4-(anthracen-9-yl)-1-(3-ethynylphenyl)-3-methyl-1H-1,2,3-triazol-3-ium tetrafluoroborate (16b). To a solution of anthracene triazole 15b (130 mg, 0.38 mmol) dissolved in DCM (25 ml) was added Me₃OBF₄ (84 mg, 0.57 mmol). The reaction was allowed to stir overnight followed by the addition of 15 drops of methanol. The reaction mixture was then washed with water (10 mL x 3), dried over Na₂SO₄, filtered and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: 5% MeOH / 95% DCM) to give the product as a yellow solid (140 mg, 83%). mp 139-141 °C; m/z (ESI-MS) [M – BF₄]⁺ 360.1508 C₂₅H₁₈N₃ (calc. 360.1495); ¹H NMR (400 MHz, Acetone-d₆) δ 9.83 (1H, s, NCH), 9.07 (1H, s, ArH), 8.38 (1H, s, ArH), 8.32 (3H, m, ArH), 7.98 (2H, m, ArH), 7.68 (4H, m, ArH), 4.24 (3H, s, NCH₃), 4.02 (1H, s, C=CH); ¹³C NMR (100 MHz, Acetone-d₆) δ 140.9, 135.9, 135.0, 132.6, 131.5, 131.1, 130.9,

130.3, 129.2, 128.7, 126.2, 125.4, 124.4, 124.3, 122.7, 113.7, 81.3, 81.2, 38.3; $^{19}\mathrm{F}$ NMR (376 MHz, Acetone-d₆) δ -153.2

of 5-[3-((1-(3-ethynylphenyl)-3-methyl-1H-1,2,3-triazol-3-ium-4-Synthesis zinc yl)methoxy)phenyl] 10,15,20-tris-[p-tolyl]porphyrin tetrafluoroborate (16c). To a solution of porphyrin 15c (300 mg, 0.33 mmol) dissolved in DCM (50 mL) was added Me_3OBF_4 (72 mg, 0.49 mmol). The reaction was allowed to stir overnight after which 15 drops of methanol were added. The reaction mixture was then washed with water (10 mL x 5) and dried over Na_2SO_4 and filtered. To the solution excess $Zn(BF_4)_2$ dissolved in methanol was added and stirred for one hour, followed by washing with water (10 mL x 5) drying over Na₂SO₄ and removal of solvent to give the product as a purple solid (270 mg, 81%). mp > 300 °C; m/z (ESI-MS) $[M - BF_4^-]^+$ 930.2915 C₅₉H₄₄N₇OZn (calc. 930.2899); ¹H NMR (400 MHz, CDCl₃) δ 9.84 (1H, s, NCH), 8.79 (8H, m, βH), 8.23 (1H, s, ArH), 8.03 (8H, m, ArH), 7.90 (1H, m, ArH), 7.81 (2H, m, ArH), 7.73 (1H, m, ArH), 7.59 (7H, m, ArH), 5.77 (2H, s, OCH₂), 4.52 (1H, s, C=CH), 4.45 (3H, s, NCH₃), 2.65 (9H, m, ArCH₃); ¹³C NMR (100 MHz, CDCl₃) δ 155.8, 149.9, 149.9, 149.8, 149.5, 145.0, 141.4, 140.3, 137.1, 135.4, 135.2, 134.5, 134.5, 132.1, 132.0, 131.9, 131.3, 128.7, 128.2, 127.7, 125.0, 124.1, 122.4, 121.3, 121.0, 120.8, 119.7, 115.0, 83.9, 81.9, 57.4, 21.5; ¹⁹F NMR (376 MHz, DMSO-d₆) δ -148.3.

Synthesis of 1-(3-(1-(4-butoxyphenyl)-1H-1,2,3-triazol-4-yl)phenyl)-3-methyl-4-(pyren-1yl)-1H-1,2,3-triazol-3-ium tetrafluoroborate (17a). Under argon, pyrene triazolium 16a (100 mg, 0.21 mmol) and 4-butoxyphenylazide (44 mg, 0.23 mmol) were dissolved in dry acetone (10 mL). To this mixture was added Cu(MeCN)₄BF₄ (13 mg, 0.042 mmol), TBTA (22 mg, 0.042 mmol) and DIPEA (54 mg, 0.42 mmol) and the reaction left to stir overnight. The reaction mixture was then diluted with DCM (100 mL) and washed with water (25 mL x 5), dried over Na_2SO_4 , filtered and the solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: 10% MeOH / 90% DCM) to give the product as a yellow solid (104 mg, 75%). mp 214-216 °C; m/z (ESI-MS) [M - BF₄]⁺ 575.2546 $C_{37}H_{31}N_6O$ (calc. 575.2559); ¹H NMR (400 MHz, CDCl₃) δ 9.97 (1H, s, NCH), 9.17 (1H, s, NCH), 8.85 (1H, s, ArH), 8.59 (1H, d, J = 8.2 Hz, ArH), 8.34-8.54 (7H, m, ArH), 8.21-8.31 (3H, m, Ar*H*), 7.96 (1H, t, J = 8.0 Hz, Ar*H*), 7.88 (2H, d, J = 9.0 Hz, Ar*H*), 7.18 (2H, d, J = 9.0 Hz, ArH), 4.55 (3H, s, NCH₃), 4.12 (2H, t, J = 6.4 Hz, OCH₂), 1.81 (2H, m, OCH₂CH₂), 1.53 (2H, m, OCH₂CH₂CH₂), 0.99 (3H, t, J = 7.2 Hz, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ 159.4, 145.8, 142.3, 136.2, 133.7, 133.1, 131.8, 131.1, 130.6, 130.4, 130.3, 130.2, 129.8, 129.1, 128.7, 127.6, 127.3, 127.1, 125.5, 124.2, 122.2, 121.4, 118.3, 116.2, 115.9, 68.1, 39.2, 31.1, 19.2, 14.2; ¹⁹F NMR (376 MHz, DMSO-d₆) δ -148.3.

Synthesis of 4-(anthracen-9-yl)-1-(3-(1-(4-butoxyphenyl)-1H-1,2,3-triazol-4-yl)phenyl)-3methyl-1H-1,2,3-triazol-3-ium tetrafluoroborate (17b). Under argon, anthracene triazolium 16b (110 mg, 0.25 mmol) and 4-butoxyphenylazide (52 mg, 0.27 mmol) were dissolved in dry acetone (10 mL). To this mixture was added Cu(MeCN)₄BF₄ (16 mg, 0.05 mmol), TBTA (27 mg, 0.05 mmol) and DIPEA (64 mg, 0.49 mmol) and the reaction left to stir overnight. The reaction mixture was then diluted with DCM (100 mL) and washed with water (25 mL x 5), dried over Na₂SO₄, filtered and solvent evaporated. The crude product was then purified by silica gel chromatography (eluent: 10% MeOH / 90% DCM) to give the product as a yellow solid (51 mg, 32%). mp 152-154 °C; m/z (ESI-MS) [M – BF₄]⁺ 551.2559 C₃₅H₃₁N₆O (calc. 551.2559); ¹H NMR (400 MHz, CDCl₃) δ 9.14 (1H, s, NCH), 8.56 (1H, s, NCH), 8.48 (1H, s, ArH), 8.29 (1H, s, ArH), 8.22 (1H, d, J = 7.8 Hz, ArH), 7.94 (2H, d, J = 8.6 Hz, ArH), 7.85 (1H, m, Ar*H*), 7.62 (2H, d, J = 9.0 Hz, Ar*H*), 7.53 (5H, m, Ar*H*), 7.37 (2H, m, Ar*H*), 6.90 (2H, d, J = 9.0 Hz, Ar*H*), 3.94 (2H, t, J = 6.4 Hz, OC*H*₂), 3.89 (3H, s, NC*H*₃), 1.77 (2H, m, OCH₂C*H*₂), 1.49 (2H, m, OCH₂CH₂C*H*₂), 0.98 (3H, t, J = 7.4 Hz, C*H*₃); ¹³C NMR (100 MHz, CDCl₃) δ 159.1, 145.4, 141.3, 135.3, 133.2, 132.6, 131.0, 130.6, 130.6, 130.0, 129.2, 129.0, 128.9, 128.6, 126.0, 123.3, 121.2, 120.6, 119.5, 119.0, 115.1, 112.1, 68.0, 38.3, 31.2, 19.2, 13.8; ¹⁹F NMR (376 MHz, CDCl₃) δ -151.3.

Synthesis of zinc 5-[3-((1-(3-(1-(4-butoxyphenyl)-1H-1,2,3-triazol-4-yl)phenyl)-3-methyl-1H-1,2,3-triazol-3-ium-4-yl)methoxy)phenyl 10,15,20-tris-[p-tolyl] porphyrin tetrafluoroborate (17c). Under argon, porphyrin 16c (245 mg, 0.24 mmol) and 4butoxyphenylazide (51 mg, 0.27 mmol) were dissolved in dry DCM (25 mL). To this mixture was added Cu(MeCN)₄BF₄ (15 mg, 0.048 mmol), TBTA (20 mg, 0.04 mmol) and DIPEA (62 mg, 0.48 mmol) and the reaction was left to stir overnight. The crude mixture was then washed with water (5 x 10 mL), dried, filtered and the solvent evaporated. The crude product was recrystallised by diffusion (DCM/hexane) to give the product as a purple solid (98 mg, 34%). mp 232-234 °C; m/z (ESI-MS) $[M - BF_4^-]^+$ 1121.3955 $C_{69}H_{57}N_{10}O_2Zn$ (calc. 1121.3957); ¹H NMR (400 MHz, DMSO-d₆) δ 9.89 (1H, s, NCH), 9.38 (1H, s, NCH), 8.80 (8H, m, βH), 8.62 (1H, s, ArH), 8.22 (1H, m, ArH), 8.02 (8H, m, ArH), 7.90 (1H, m, ArH), 7.81 (4H, m, ArH), 7.63 (1H, m, ArH), 7.56 (6H, m, ArH), 7.14 (2H, m, ArH), 5.79 (2H, s, OCH₂), 4.49 (3H, s, NCH₃), 4.02 (2H, t, J = 5.5Hz, OCH₂), 2.64 (9H, s, ArCH₃), 1.71 (2H, m, OCH_2CH_2), 1.44 (2H, m, $OCH_2CH_2CH_2$), 0.93 (3H, t, J = 7.4 Hz, CH_3); ¹³C NMR (100 MHz, DMSO-d₆) δ 159.4, 155.9, 149.9, 149.8, 149.8, 149.5, 145.8, 145.0, 141.4, 140.2, 137.1, 137.0, 135.9, 134.5, 134.4, 133.0, 132.1, 131.9, 131.6, 130.1, 129.1, 128..6, 128.3, 127.7, 122.2, 121.3, 121.0, 120.8, 119.7, 118.2, 115.9, 115.0, 68.1, 59.5, 39.3, 31.1, 21.5, 19.2, 14.2; ¹⁹F NMR (376 MHz, DMSO- d_6) δ -148.3

Pyrene triazolium functionalised tentegel resins (18a). To a round bottomed flask under argon containing azide functionalised TentaGel resin **LL-10** (100 mg) suspended in dry acetone (15 mL) was added pyrene alkyne **16a** (200 mg, 0.42 mmol), TBTA (22 mg, 0.04 mmol), Cu(MeCN)₄BF₄ (26 mg, 0.08 mmol) and DIPEA (108 mg, 0.84 mmol). The reaction was left for two days with occasional gentle stirring. The TentaGel resins were then filtered from the reaction mixture and the resulting beads were washed thoroughly with acetone (5 x 5 mL), dichloromethane and hexane (5 x 5 mL sequentially), followed by acetone (5 mL), water (5 mL), acetone (5 mL) and dichloromethane (5 mL). The pale yellow beads were then allowed to air dry. ¹H HR MAS NMR (400 MHz, CD₃CN) δ 9.61 (s, NC*H*), 8.71 (s, NC*H*), 8.63 (s, Ar*H*), 7.98 (m, Ar*H*), 7.79 (m, Ar*H*).

Anthracene triazolium functionalised tentagel resins (18b). To a round bottomed flask under argon containing azide functionalised TentaGel resin LL-10 (100 mg) suspended in dry acetone (15 mL) was added anthracene alkyne 16b (150 mg, 0.33 mmol), TBTA (18 mg, 0.03 mmol), Cu(MeCN)₄BF₄ (21 mg, 0.07 mmol) and DIPEA (86 mg, 0.66 mmol). The reaction was left for two days with occasional gentle stirring. The TentaGel resins were then filtered from the reaction mixture and the resulting beads were washed thoroughly with acetone (5 x 5 mL), dichloromethane and hexane (5 x 5 mL sequentially), followed by acetone (5 mL), water (5 mL), acetone (5 mL) and dichloromethane (5 mL). The pale yellow beads were then allowed to air dry. ¹H HR MAS NMR (400 MHz, Acetone-d₆) δ 10.00 (s, NC*H*), 9.11 (s, NC*H*), 8.87 (s, Ar*H*), 8.72 (s, Ar*H*), 8.36 (m, Ar*H*), 8.29 (d, J = 8.2 Hz, Ar*H*), 8.05 (d, J = 8.2 Hz, Ar*H*), 7.95 (t, J = 8.2 Hz, Ar*H*), 7.74 (m, Ar*H*).

Porphyrin triazolium functionalised tentagel resins (18c). To a round bottomed flask under argon containing azide functionalised TentaGel resin **LL-10** (100 mg) suspended in dry DCM (15 mL) was added porphyrin alkyne **16c** (400 mg, 0.39 mmol), TBTA (20 mg, 0.04 mmol), Cu(MeCN)₄BF₄ (25 mg, 0.08 mmol) and DIPEA (100 mg, 0.84 mmol). The reaction was left for two days with occasional gentle stirring. The TentaGel resins were then filtered from the reaction mixture and the resulting beads were washed thoroughly with dichloromethane and hexane (5 x 5 mL sequentially), followed by acetone (5 mL), water (5 mL), acetone (5 mL) and dichloromethane (5 mL). The purple beads were then allowed to air dry. ¹H HR MAS NMR (400 MHz, DMSO-d₆) δ 9.92 (br-s, NC*H*), 8.75 (m, β *H*), 8.54 (br-s, Ar*H*), 8.37 (s, Ar*H*), 7.37-8.15 (m, Ar*H*).



Anion Binding Studies and Compound Characterisation

Figure S1 – Change in the chemical shift of triazolium proton c on addition of anions to a 2mM solution of triazolium receptors **7a-c**; a) pyrene receptor **7a** in acetone- d_6 , b) anthracene receptor **7b** in CDCl₃, and c) porphyrin receptor **7c** in 1%MeOD/CDCl₃. Symbols represent experimental data points; continuous lines represent calculated curves; anions are shown by colour: chloride (green), bromide (red), iodide (purple) and acetate (blue). All anions were added as their TBA salts.



Figure S2: IR spectra of TentaGel-OH beads LL-8 (blue), azide functionalised TentaGel beads LL-10 (red) and triazole functionalised beads LL-11a (green).



Figure S3: 32 loop CPMG ¹H HR MAS NMR spectrum in CDCl₃ of a) pyrene triazole **HL-11a**; b) pyrene triazole **LL-11a**; c) anthracene triazole **HL-11b**; d) anthracene triazole **LL-11b**.



Figure S4: Change in the chemical shift of triazolium proton a on addition of anions to a 2mM solution of triazolium **17b** in CDCl₃ at 293 K. Symbols represent experimental data points; continuous lines represent calculated curves; anions are shown by colour: chloride (green), bromide (red), iodide (purple) and acetate (blue). All anions were added as their TBA salts



Figure S5: a) ¹H NMR spectrum of pyrene triazolium sensor **17a** in CD₃CN; and b) 32 loop CPMG ¹H HR MAS NMR spectrum of pyrene triazolium functionalized resins **18a** in CD₃CN.



Figure S6: a) ¹H NMR spectrum of porphyrin triazolium sensor **17c** in DMSO-d₆; and b) 32 loop CPMG ¹H HR MAS NMR spectrum of porphyrin triazolium functionalized resins **18c** in DMSO-d₆.

	7b	17b	18b
	(Acetone-d ₆)	(CDCl ₃)	(Acetone-d ₆)
	($\Delta\delta$ for proton	($\Delta\delta$ for proton	($\Delta\delta$ for proton
	c)	c)	c)
Cl-	1.232	2.183	1.396
Br⁻	0.488	1.821	0.637
I-	0.082	1.208	0.158
AcO-	1.419	2.642	1.317

Table S1: Change in chemical shift of triazolium proton c upon addition of various anions to anthracene triazolium receptor 7b and anthracene triazolium functionalized resins 18b.



Figure S7: Fluorescence spectra in CHCl₃ when excited at 340 nm of: 0.5 μ M pyrene triazole **6a** (blue), 0.5 μ M pyrene triazolium **7a** (red), 0.5 μ M pyrene triazolium 1**7a** (green).



Figure S8: Fluorescence spectra in CHCl₃ when excited at 255 nm of: 0.5 μ M anthracene triazole **6b** (blue), 0.5 μ M anthracene triazolium **7b** (red), and 0.5 μ M anthracene triazolium 1**7b** (green).



Figure S9: UV absorbance spectra in CH_2Cl_2 of porphyrin triazolium 17c showing changes upon the addition of TBA chloride.

Selected NMR data for target anion receptors



Figure S10: ¹H (top) and ¹³C (bottom) NMR spectra for compound 7a NMR in CDCl₃.



Figure S11: ¹H (top) and ¹³C (bottom) NMR spectra for compound 7b NMR in Acetone-*d*₆.



Figure S12: ¹H (top) and ¹³C (bottom) NMR spectra for compound 7c NMR in Acetone-d₆.



Figure S13: ¹H (top) and ¹³C (bottom) NMR spectra for compound 17a NMR in DMSO-d₆.



Figure S14: ¹H (top) and ¹³C (bottom) NMR spectra for compound **17b** NMR in CDCl₃. (Small impurities noted in final spectrum, less than 5 %. Further purification hampered due to solubility and stability issues)



Figure S15: ¹H (top) and ¹³C (bottom) NMR spectra for compound 17c NMR in DMSO-*d*₆.