- Electronic Supplementary Information -

Tuning the Polarity and Surface Activity of Hydroxythiazoles – Extending Applicability of Highly Fluorescent Self-Assembling Chromophores to Supra-Molecular Photonic Structures

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Table of Contents

Synthetic Procedures

Methyl 2-(5-phenyl-2-(pyridin-2-yl)thiazol-4-yloxy)acetate (2a)

General procedure for the synthesis of the ethers **2a-c**, **9a-c**:

A solution of **1** (1.31 g, 5.2 mmol) and methyl bromoacetate (0.54 mL, 6.7 mmol, 1.1 eq.) in acetone (70 mL) was treated with K_2CO_3 (1.07 g, 7.7 mmol, 1.5 eq.) and then heated to reflux. The mixture was stirred at that temperature until all starting material had been used up as indicated by TLC (silica, heptane/EtOAc 1:1). Acetone was then removed under reduced pressure until only 10 mL were left. The resulting suspension was treated with H_2O (50 mL) and extracted with DCM (3 * 50 mL). The combined organic extracts were washed with saturated NaCl solution and dried over $MgSO_4$. The solvent was removed *in vacuo* and the crude product was recrystallized from methanol/chloroform. The product was obtained as light yellow crystalline solid (1.48 g, 4.5 mmol, 88%). Mp: 143 °C. ^{1}H-NMR (200 MHz, $CDCl_3$): δ 3.79 (s, 3H), 5.07 (s, 2H), 7.17-7.32 (m, 2H), 7.32-7.48 (m, 3H), 7.66-7.88 (m, 3H), 8.01 (d, J = 7.9 Hz, 1H), 8.56 (d, J = 4.2 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 52.12, 66.42, 115.11, 118.93, 124.24, 127.08, 127.18, 128.74, 131.17, 136.89, 149.42, 151.01, 157.44, 160.54, 169.77. MS EI m/z: 326 ($M^{\bullet+}$, 92 %), 255 ($M^{\bullet+}$ - $C_{10}H_9N_2O_3$, 100 %), 77 ($M^{\bullet+}$ - $C_{11}H_9N_2O_3S$, 77 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 349.061120000 (calc. 349.062284620 for $C_{17}H_{14}N_2O_3SNa$). UV/Vis (THF): λ_{max} (log ε): 270 (4.06), 372 (4.32). Fluorescence (THF): λ_{max} (λ_{exc}): 440 nm (372 nm). Φ_{Em} = 85% relative to quinine sulfate.

4-(3-Chloropropoxy)-5-phenyl-2-(pyridin-2-yl)thiazole (2b)

2b was prepared according to the general procedure given for **2a**. The starting material **1** (1.315 g, 5.2 mmol) was alkylated with 1-bromo-3-chloropropane (0.56 mL, 5.7 mmol, 1.1 eq). After workup, the crude product was purified by column chromatography (silica, EtOAc/heptane 1:2) to yield the ether as a yellow solid (1.614 g, 4.9 mmol, 94%). Mp: 56 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 2.33 (p, J = 6.2 Hz, 2H), 3.78 (t, J = 6.4 Hz, 2H), 4.69 (t, J = 5.9 Hz, 2H), 7.22-7.33 (m, 2H), 7.40 (t, J = 7.7 Hz, 2H), 7.76-7.79 (m, 3H), 8.12 (d, J = 7.9 Hz, 1H), 8.60 (d, J = 4.8 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 32.62, 41.69, 67.04, 114.84, 118.98, 124.18, 126.87, 126.93, 128.74, 131.60, 136.90, 149.45, 151.19, 158.45, 160.65. MS EI *m/z*: 330 ($M^{\bullet+}$, 100 %), 254 ($M^{\bullet+}$ - C_3H_5Cl, 33 %), 121 ($M^{\bullet+}$ - $C_{10}H_{10}ClN_2O$, 52 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 353.050700000 (calc. 353.049133451 for $C_{17}H_{15}ClN_2OSNa$). UV/Vis (THF): λ_{max} (log ε): 373 (4.36). Fluorescence (THF): λ_{max} (λ_{exc}): 444 nm (373 nm). Φ_{Em} = 81% relative to quinine sulfate.

4-Methoxy-5-phenyl-2-(pyridin-2-yl)thiazole (2c)

2c was prepared according to the general procedure given for **2a**. The starting material **1** (891 mg, 3.5 mmol) was alkylated with CH_3I (0.24 mL, 3.9 mmol, 1.1 eq.). After workup, the crude product was purified by column chromatography (silica, EtOAc/heptane 1:2) to yield the ether as a pale yellow solid (858 mg, 3.2 mmol, 91%). Mp: 68 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 4.19 (s, 1H), 7.22-7.31 (m, 2H), 7.39 (t, J = 7.7 Hz, 2H), 7.75-7.81 (m, 3H), 8.13 (d, J = 7.9 Hz, 1H), 8.60 (d, J = 4.8 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 57.60, 114.32, 118.96, 124.09, 126.77, 126.94, 128.69, 131.68, 136.87, 149.43, 151.29, 159.73, 160.42. MS EI *m/z*: 268 ($M^{\bullet+}$, 100 %), 121 ($M^{\bullet+}$ - $C_8H_7N_2O$, 18 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 291.056640000 (calc. 291.056805360 for $C_{15}H_{12}N_2OSNa$). UV/Vis (THF): λ_{max} (log ε): 374

(4.43). Fluorescence (THF): λ_{max} (λ_{exc}): 444 nm (374 nm). Φ_{Em} = 75% relative to quinine sulfate.

Methyl 2-(5-phenyl-2-(pyrazin-2-yl)thiazol-4-yloxy)acetate (9a)

9a was prepared according to the general procedure given for **2a**. The starting material **8** (764 mg, 3.0 mmol) was alkylated with methyl bromoacetate (0.31 mL, 3.3 mmol, 1.1 eq). After workup, the crude product was recrystallized from methanol/chloroform. (silica, EtOAc/heptane 1:2). The product was obtained as a yellow crystalline solid (833 mg, 2.5 mmol, 85%). Mp: 162 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 3.82 (s, 3H), 5.10 (s, 2H), 7.26-7.32 (m, 1H), 7.38-7.44 (m, 2H), 7.83 (d, J = 7.8 Hz, 2H), 8.51-8.56 (m, 2H), 9.26 (s, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 52.18, 66.41, 116.65, 127.32, 127.51, 128.82, 130.69, 140.86, 143.82, 144.70, 146.49, 157.52, 157.88, 169.53. MS EI *m/z*: 327 ($M^{\bullet+}$, 98 %), 296 ($M^{\bullet+}$ - CH_3O, 6 %), 268 ($M^{\bullet+}$ - $C_2H_3O_2$, 12 %), 121 ($M^{\bullet+}$ - $C_9H_8N_3O_3$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 350.058600000 (calc. 350.057533590 for $C_{16}H_{13}N_3O_3SNa$). UV/Vis (THF): λ_{max} (log ε): 274 (4.01), 385 (4.36). Fluorescence (THF): λ_{max} (λ_{exc}): 455 nm (385 nm). Φ_{Em} = 76% relative to quinine sulfate.

4-(3-Chloropropoxy)-5-phenyl-2-(pyrazin-2-yl)thiazole (9b)

9b was prepared according to the general procedure given for **2a**. The starting material **8** (2.10 g, 8.2 mmol) was alkylated with 1-bromo-3-chloropropane (0.89 mL, 9.0 mmol, 1.1 eq). After workup, the crude product was purified by column chromatography (silica, EtOAc/heptane 1:2) to yield the ether as a yellow solid (2.61 g, 7.9 mmol, 94%). Mp: 87 °C. ^{1}H-NMR (200 MHz, $CDCl_3$): δ 2.32 (p, J = 6.2 Hz, 2H), 3.76 (t, J = 6.4 Hz, 2H), 4.68 (t, J = 5.9 Hz, 2H), 7.2-7.29 (m, 1H), 7.35-7.42 (m, 2H), 7.75 (d, J = 8.0 Hz, 2H), 8.49-8.55 (m, 2H), 9.32 (d, J = 1.3 Hz, 1H). ^{13}C-NMR (50 MHz, $CDCl_3$): δ 32.50, 41.58, 67.22, 116.14, 127.05, 127.29, 128.82, 131.12, 140.92, 143.84, 144.62, 146.65, 157.57, 159.15. MS EI *m/z*: 331 ($M^{\bullet+}$, 27 %), 255 ($M^{\bullet+}$ - C_3H_5Cl, 13 %), 121 ($M^{\bullet+}$ - $C_9H_9ClN_3O$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 354.044800000 (calc. 354.044382421 for $C_{16}H_{14}ClN_3OSNa$). UV/Vis (THF): λ_{max} (log ε): 276 (3.92), 387 (4.33). Fluorescence (THF): λ_{max} (λ_{exc}): 472 nm (387 nm). Φ_{Em} = 74% relative to quinine sulfate.

4-Methoxy-5-phenyl-2-(pyrazin-2-yl)thiazole (9c)

9c was prepared according to the general procedure given for **2a**. The starting material **8** (525 mg, 2.1 mmol) was alkylated with CH_3I (0.14 mL, 2.3 mmol, 1.1 eq.). After workup, the crude product was purified by column chromatography (silica, EtOAc/heptane 1:2) to yield the ether as a yellow solid (500 mg, 1.9 mmol, 90%). Mp: 130 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 4.21 (s, 3H), 7.27 (t, J = 7.3 Hz, 1H), 7.40(t, J = 7.6 Hz, 2H), 7.72-7.83 (m, 2H), 8.54 (d, J = 6.6 Hz, 2H), 9.36 (s, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 57.76, 115.66, 127.06, 127.18, 128.76, 131.21, 140.92, 143.83, 144.51, 1466.78, 157.34, 160.15. MS EI *m/z*: 269 ($M^{\bullet+}$, 100 %), 121 ($M^{\bullet+}$ - $C_7H_6N_3O$, 20 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 292.051920000 (calc. 292.052054330 for $C_{14}H_{11}N_3OSNa$). UV/Vis (THF): λ_{max} (log ε): 277 (3.89), 387 (4.34). Fluorescence (THF): λ_{max} (λ_{exc}): 471 nm (387 nm). Φ_{Em} = 72% relative to quinine sulfate.

Methyl 2-((5-(4-(chlorosulfonyl)phenyl)-2-(pyridin-2-yl)thiazol-4-yl)oxy)acetate (3a)
General procedure for the synthesis of the sulfchlorides **3a-c**, **10a-c**:
5 mL chlorosulfonic acid were cooled to 0 °C. 508 mg (1.6 mmol) **2a** were then added portionwise over a period of 15 minutes. The mixture is allowed to warm up to room temperature and stirred for one hour. The reaction mixture is then added dropwise to 300 mL of ice water. After extraction of the aqueous phase with chloroform (3 * 30 mL), the organic phase is washed with saturated NaCl solution and dried ober $MgSO_4$. The solvent was removed under reduced pressure and the crude product was purified by column chromatography (silica, heptane/EtOAc 1:1) to afford the desired product as a yellow solid (553 mg, 1.3 mmol, 84 %). ^{1}H-NMR (250 MHz, DMSO-d_6): δ 3.71 (s, 3H), 5.16 (s, 2H), 7-55-7.53 (m, 1H), 7.65 (d, J = 8.3 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H), 7.96 (d, J = 3.7 Hz, 2H), 8.61 (d, J = 4.7 Hz, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 52.36, 66.76, 113.72, 119.09, 125.76, 126.52, 126.60, 131.12, 138.40, 147.28, 150.04, 150.17, 158.05, 161.04, 169.78. MS EI *m/z*: 424 ($M^{\bullet+}$, 100 %), 325 ($M^{\bullet+}$ - ClO_2S, 30 %), 219 ($M^{\bullet+}$ - $C_{10}H_8N_2O_3$, 100 %), 120 ($M^{\bullet+}$ - $C_{10}H_9ClN_2O_5S$, 93 %).

4-(4-(3-Chloropropoxy)-2-(pyridin-2-yl)thiazol-5-yl)benzenesulfonyl chloride (3b)
3b was prepared according to the general procedure given for **3a**. **2b** (573 mg, 1.7 mmol) was treated with chlorosulfonic acid. After workup, the yellow solid was used without further purification (674 mg, 91%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 2.39 (p, J = 6.1 Hz, 2H), 3.79 (t, J = 6.3 Hz, 2H), 4.79 (t, J = 6.0 Hz, 2H), 7.36-7.40 (m, 1H), 7.84 (td, ^3J = 7.8 Hz, ^4J = 1.6 Hz), 7.98 (d, J = 8.9 Hz, 2H), 8.04 (d, J = 8.9 Hz, 2H), 8.16 (d, J = 7.9 Hz, 1H), 8.63 (d, J = 4.2 Hz, 1H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 32.37, 41.45, 67.60, 111.65, 119.65, 125.10, 126.91, 127.63, 137.18, 139.17, 141.00, 149.65, 150.43, 160.93, 164.01. MS EI *m/z*: 428 ($M^{\bullet+}$, 83 %), 393 ($M^{\bullet+}$ - Cl, 7 %), 352 ($M^{\bullet+}$ - C_3H_5Cl, 36 %), 329 ($M^{\bullet+}$ - ClO_2S, 15 %), 219 ($M^{\bullet+}$ - $C_{10}H_{10}ClN_2O$, 42 %), 120 ($M^{\bullet+}$ - $C_{10}H_{10}ClN_2O_3S$, 100 %).

4-(4-Methoxy-2-(pyridin-2-yl)thiazol-5-yl)benzenesulfonyl chloride (3c)
3c was prepared according to the general procedure given for **3a**. **2c** (573 mg, 1.7 mmol) was treated with chlorosulfonic acid. After workup, the crude product purified by column chromatography (silica, heptane/EtOAc 2:1) to afford the desired product as a yellow solid (674 mg, 88%). ^{1}H-NMR (300 MHz, $CDCl_3$): δ 4.27 (s, 3H), 7.35-7.39 (m, 1H), 7.83 (td, ^3J = 7.8 Hz, ^4J = 1.6 Hz, 1H), 7.96-8.04 (m, 4H), 8.16 (d, J = 7.9 Hz, 1H), 8.63 (d, J = 4.8 Hz, 1H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 57.98, 111.21, 119.41, 125.01, 126.90, 127.55, 137.13, 139.28, 140.84, 149.64, 150.53, 161.91, 163.83. MS EI *m/z*: 366 ($M^{\bullet+}$, 100 %), 331 ($M^{\bullet+}$ - Cl, 6 %), 267 ($M^{\bullet+}$ - SO_2Cl, 44 %), 219 ($M^{\bullet+}$ - $C_8H_7N_2O$, 64 %), 120 ($M^{\bullet+}$ - $C_8H_7ClN_2O_3S$, 53 %).

Methyl 2-((5-(4-(chlorosulfonyl)phenyl)-2-(pyrazin-2-yl)thiazol-4-yl)oxy)acetate (10a)
10a was prepared according to the general procedure given for **3a**. **9a** (594 mg, 1.8 mmol) was treated with chlorosulfonic acid. After workup, the crude product purified by column chromatography (silica, chloroform/EtOAc 7:1) to afford the desired product as a yellow solid (641 mg, 83%). ^{1}H-NMR (250 MHz, DMSO-d_6): δ 3.71 (s, 3H), 5.19 (s, 2H), 7.66 (d, J = 8.3 Hz, 2H), 7.77 (d, J = 8.2 Hz, 2H), 8.68-8.72 (m, 2H), 9.15 (s, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 52.40, 66.80, 114.95, 126.65, 126.71, 130.78, 140.38, 145.05, 145.64, 146.27, 147.47, 158.27, 158.42, 169.70. MS EI *m/z*: 425 ($M^{\bullet+}$, 100 %), 390 ($M^{\bullet+}$ - Cl, 12 %), 326 ($M^{\bullet+}$

- ClO_2S, 38 %), 253 ($M^{•+}$ - $C_3H_5ClO_4S$, 32 %), 219 ($M^{•+}$ - $C_9H_8N_3O_3$, 100 %), 120 ($M^{•+}$ - $C_9H_8ClN_3O_5S$, 100 %).

4-(4-(3-Chloropropoxy)-2-(pyrazin-2-yl)thiazol-5-yl)benzene-1-sulfonyl chloride (10b)
10b was prepared according to the general procedure given for **3a**. **9b** (800 mg, 2.4 mmol) was treated with chlorosulfonic acid. After workup, the crude product purified by column chromatography (silica, chloroform/EtOAc 10:1) to afford the desired product as a yellow solid (530 mg, 51%). ^{1}H-NMR (250 MHz, DMSO-d_6): δ 2.27 (p, J = 6.2 Hz, 2H), 3.82 (t, J = 6.4 Hz, 2H), 6.42 (t, J = 6.1 Hz, 2H), 7.86 (q, J = 8.4 Hz, 4H), 8.69 (dd, J = 7.4 Hz, 1.8 Hz, 2H), 9.25 (s, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 32.32, 42.55, 67.94, 115.03, 126.58, 126.67, 131.03, 140.46, 145.00, 145.81, 146.16, 147.37, 158.47, 159.38. MS EI *m/z*: 429 ($M^{•+}$, 84 %), 394 ($M^{•+}$ - Cl, 8 %), 353 ($M^{•+}$ - C_3H_5Cl, 100 %), 219 ($M^{•+}$ - $C_9H_9ClN_3O$, 33 %), 120 ($M^{•+}$ - $C_9H_9Cl_2N_3O_3S$, 52 %), 106 ($M^{•+}$ - $C_{11}H_9Cl_2O_3S_2$, 56 %).

4-(4-Methoxy-2-(pyrazin-2-yl)thiazol-5-yl)benzenesulfonyl chloride (10c)
10c was prepared according to the general procedure given for **3a**. **9c** (328 mg, 1.2 mmol) was treated with chlorosulfonic acid. After workup, the crude product purified by column chromatography (silica, heptane/EtOAc 2:1) to afford the desired product as a yellow solid (380 mg, 85%). ^{1}H-NMR (250 MHz, $CDCl_3$): δ 4.16 (s, 3H), 7.66 (d, J = 8.5 Hz, 2H), 7.72 (d, J = 8.5 Hz, 2H), 8.67-8.72 (m, 2H), 8.26 (d, J = 1.3 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 58.38, 114.49, 126.51, 126.66, 131.16, 140.44, 145.03, 145.84, 146.14, 147.20, 158.32, 160.30. MS EI *m/z*: 367 ($M^{•+}$, 95 %), 332 ($M^{•+}$ - Cl, 4 %), 268 ($M^{•+}$ - $C_7H_6N_3O$, 25 %), 219 ($M^{•+}$ - $C_7H_6N_3O$, 50 %), 120 ($M^{•+}$ - $C_7H_6ClN_3O_3S$, 100 %).

Methyl 2-((5-(4-(*N*,*N*-diethylsulfamoyl)phenyl)-2-(pyridin-2-yl)thiazol-4-yl)oxy)acetate (4a)
General procedure for the synthesis of the sulfonamides **4a-c**, **5a-c**, **11a-c**, **12a-c**:
3a (350 mg, 0.8 mmol) was dissolved in CH_2Cl_2 (20 mL). Diethylamine (0.10 mL, 0.9 mmol, 1.1 eq) and triethylamine (0.23 mL, 1.5 mmol, 2 eq) were added with syringes. The resulting mixture was stirred at room temperature for 2 hours and EtOAc (30 mL) was added. The resulting solution was then treated with H_2O and extracted with EtOAc (2*30 mL). The combined organic extracts was washed with saturated NH_4Cl solution and saturated NaCl solution, dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude product was purified by column chromatography (silica, heptane/EtOAc 1:1) to afford the desired product as a yellow solid (336 mg, 0.73 mmol, 89 %). Mp: 127 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 1.15 (t, J = 7.1 Hz, 6H), 3.25 (q, J = 7.1 Hz, 4H), 3.82 (s, 3H), 5.13 (s, 2H), 7,32 (ddd, ^3J = 7.5 Hz, 4.9 Hz, ^4J = 1.1 Hz, 1H), 7.79-7.83 (m, 3H), 7.94 (d, J = 8.6 Hz, 2H), 8.03 (d, J = 7.9 Hz, 1H), 8.59 (d, J = 4.3 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 14.23, 42.11, 52.23, 66.44, 113.12, 119.15, 124.75, 127.08, 127.49, 135.38, 137.01, 137.96, 149.54, 150.56, 158.62, 162.45, 169.42. MS EI *m/z*: 461 ($M^{•+}$, 88 %), 389 ($M^{•+}$ - $C_3H_4O_2$, 13 %), 325 ($M^{•+}$ - $C_4H_{10}NO_2S$, 100 %), 120 ($M^{•+}$ - $C_{14}H_{19}N_3O_5S$, 59 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 484.097860000 (calc. 484.097685791 for $C_{21}H_{23}N_3O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 284 (4.06), 374 (4.46). Fluorescence (THF): λ_{max} (λ_{exc}): 443 (374 nm). Φ_{Em} = 83% relative to quinine sulfate.

4-(4-(3-Chloropropoxy)-2-(pyridin-2-yl)thiazol-5-yl)-*N*,*N*-diethylbenzenesulfonamide (4b)

4b was prepared according to the general procedure given for **4a**. **3b** (320 mg, 0.75 mmol) was treated with diethylamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, heptane/EtOAc 2:1) to afford the desired product as a yellow solid (306 mg, 0.66 mmol, 88%). Mp: 145 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 1.16 (t, J = 7.1 H, 6H), 2.35 (p, J = 6.2 Hz, 2H), 3.27 (q, J = 7.1 Hz, 4H), 3.77 (t, J = 6.4 Hz, 2H), 4.73 (t, J = 6.0 Hz, 2H), 7.33 (ddd, ^3J = 7.5 Hz, 4.8 Hz, ^4J = 1.o Hz, 1H), 7.75-7.91 (m, 5H), 8.13 (d, J = 7.9 Hz, 1H), 8.60 (d, J = 4.5 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 14.22, 32.46, 41.52, 42.11, 67.32, 112.65, 119.22, 124.69, 126.76, 127.50, 135.83, 137.02, 137.72, 149.55, 150.74, 159.95, 162.53. MS EI *m/z*: 465 ($M^{\bullet+}$, 98 %), 393 ($M^{\bullet+}$ - $C_4H_{10}N$, 11 %), 329 ($M^{\bullet+}$ - $C_4H_{10}NO_2S$, 82 %), 256 ($M^{\bullet+}$ - $C_{10}H_{10}ClN_2O$, 42 %), 253 ($M^{\bullet+}$ - $C_7H_{15}ClNO_2S$, 55 %), 120 ($M^{\bullet+}$ - $C_{14}H_{20}N_3O_3S$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 488.084180000 (calc. 488.084534621 for $C_{21}H_{24}ClN_3O_3S_2Na$). UV/Vis (THF): λ_{max} (log ε): 377 (4.42). Fluorescence (THF): λ_{max} (λ_{exc}): 447 nm (377 nm). Φ_{Em} = 81% relative to quinine sulfate.

***N*,*N*-Diethyl-4-(4-methoxy-2-(pyridin-2-yl)thiazol-5-yl)benzenesulfonamide (4c)**

4c was prepared according to the general procedure given for **4a**. **3c** (280 mg, 0.76 mmol) was treated with diethylamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, heptane/EtOAc 2:1) to afford the desired product as a yellow solid (248 mg, 0.61 mmol, 80%). Mp: 135 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ 1.16 (t, J = 7.1 Hz, 6H), 3.26 (q, J = 7.1 Hz, 4H), 4.23 (s, 3H), 7.31-7.36 (m, 1H), 7.79-7.81 (m, 3H), 7.90 (d, J = 8.6 Hz, 2H), 8.15 (d, J = 7.9 Hz, 1H), 8.61 (d, J = 4.7 Hz, 1H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ 14.24, 42.11, 57.80, 112.14, 119.22, 124.65, 126.75, 127.46, 135.96, 137.04, 137.48, 149.56, 150.82, 160.95, 162.31. MS EI *m/z*: 403 ($M^{\bullet+}$, 100 %), 331 ($M^{\bullet+}$ - $C_4H_{10}N$, 18 %), 267 ($M^{\bullet+}$ - $C_4H_{10}NO_2S$, 76 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 426.091250000 (calc. 426.092206531 for $C_{19}H_{21}N_3O_3S_2Na$). UV/Vis (THF): λ_{max} (log ε): 378 (4.48). Fluorescence (THF): λ_{max} (λ_{exc}): 447 nm (378 nm). Φ_{Em} = 80% relative to quinine sulfate.

Methyl 2-((5-(4-(*N*,*N*-bis(2-hydroxyethyl)sulfamoyl)phenyl)-2-(pyridin-2-yl)thiazol-4-yl)oxy)acetate (5a)

5a was prepared according to the general procedure given for **4a**. **3a** (553 mg, 1.3 mmol) was treated with diethanolamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, chloroform/methanol 10:1) to afford the desired product as a yellow solid (534 mg, 1.1 mmol, 83%). Mp: 129 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 3.30 (t, J = 4.6 Hz, 4H), 3.71 (s, 2H), 3.81 (s, 3H), 3.88 (t, J = 4.6 Hz, 4H), 5.13 (s, 2H), 7.32 (dd, J = 6.6 Hz, 4.9 Hz, 1H), 7.72-7.87 (m, 3H), 7.95-8.01 (m, 3H), 8.59 (d, J = 4.3 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 52.27, 53.00, 62.26, 66.45, 112.87, 119.21, 124.84, 127.25, 127.76, 135.73, 136.05, 137.06, 149.55, 150.47, 158.78, 162.72, 169.41. MS EI *m/z*: 493 ($M^{\bullet+}$, 16 %),462 ($M^{\bullet+}$ - CH_3O, 39 %), 389 ($M^{\bullet+}$ - $C_4H_{10}NO_2$, 8 %), 325 ($M^{\bullet+}$ - $C_4H_{10}NO_4S$, 100 %), 120 ($M^{\bullet+}$ - $C_{14}H_{19}N_3O_7S$, 81 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 516.088450000 (calc. 516.087514991 for $C_{21}H_{23}N_3O_7S_2Na$). UV/Vis (THF): λ_{max} (log ε): 373

(4.32). Fluorescence (THF): λ_{max} (λ_{exc}): 443 nm (373 nm). Φ_{Em} = 78% relative to quinine sulfate.

4-(4-(3-Chloropropoxy)-2-(pyridin-2-yl)thiazol-5-yl)-*N*,*N*-bis(2-hydroxyethyl)benzenesulfonamide (5b)

5b was prepared according to the general procedure given for **4a**. **3b** (329 mg, 0.77 mmol) was treated with diethanolamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, chloroform/methanol 6:1) to afford the desired product as a yellow solid (308 mg, 0.62 mmol, 81%). Mp: 129 °C. ^{1}H-NMR (300 MHz, DMSO-d_6): δ 2.30 (p, *J* = 6.2 Hz, 2H), 3.19 (t, *J* = 6.3 Hz, 4H), 3.53 (q, *J* = 6.1 Hz, 4H), 3.86 (t, *J* = 6.4 Hz, 2H), 4.66 (t, *J* = 6.1 Hz, 2H), 4.85 (t, *J* = 5.4 Hz, 2H), 7.48-7.55 (m, 1H), 7.84 (d, *J* = 8.6 Hz, 2H), 7.90-8.03 (m, 3H), 8.09 (d, *J* = 7.9 Hz, 1H), 8.63 (d, *J* = 4.3 Hz, 1H). ^{13}C-NMR (75 MHz, DMSO-d_6): δ 32.34, 42.61, 51.56, 60.37, 68.04, 112.20, 119.35, 126.03, 127.24, 128.15, 135.59, 137.17, 138.34, 150.04, 150.32, 160.15, 162.96. MS EI *m/z*: 497 ($M^{\bullet+}$, 12 %), 466 ($M^{\bullet+}$ - CH_3O, 32 %), 393 ($M^{\bullet+}$ - $C_4H_{10}NO_2$, 7 %), 329 ($M^{\bullet+}$ - $C_4H_{10}NO_4S$, 100 %), 120 ($M^{\bullet+}$ - $C_{14}H_{20}ClN_3O_5S$, 59 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 520.074860000 (calc. 520.074363821 for $C_{21}H_{24}ClN_3O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 377 (4.46). Fluorescence (THF): λ_{max} (λ_{exc}): 447 nm (377 nm). Φ_{Em} = 77% relative to quinine sulfate.

***N*,*N*-Bis(2-hydroxyethyl)-4-(4-methoxy-2-(pyridin-2-yl)thiazol-5-yl)benzenesulfonamide (5c)**

5c was prepared according to the general procedure given for **4a**. **3c** (256 mg, 0.70 mmol) was treated with diethanolamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, chloroform/methanol 10:1) to afford the desired product as a yellow solid (234 mg, 0.54 mmol, 77%). Mp: 135 °C. ^{1}H-NMR (400 MHz, DMSO-d_6): δ 3.19 (t, *J* = 6.3 Hz, 4H), 3.53 (dd, *J* = 11.8 Hz, 6.1 Hz), 4H), 4.18 (s, 3H), 4.83 (t, *J* = 5.4 Hz, 2H), 7.52 (ddd, ^3J = 7.5 Hz, 4.5 Hz, ^4J = 1.0 Hz), 7.83 (d, *J* = 8.6 Hz, 2H), 7.94 (d, *J* = 8.6 Hz, 2H), 7.99 (td, ^3J = 7.7 Hz, ^4J = 1.6 Hz, 1H), 8.10 (d, *J* = 7.9 Hz, 1H), 8.64 (d, *J* = 4.3 Hz, 1H). ^{13}C-NMR (100 MHz, DMSO-d_6): δ 51.52, 58.38, 60.36, 111.81, 119.33, 125.99, 127.23, 128.08, 135.62, 137.21, 138.32, 150.09, 150.32, 160.98, 162.87. MS ESI *m/z*: 458.1 ($[M+Na]^+$, 100%). HRMS (ESI [+], $CHCl_3$ + MeOH): 458.083040000 (calc. 458.082035731 for $C_{19}H_{21}N_3O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 377 (4.36). Fluorescence (THF): λ_{max} (λ_{exc}): 448 nm (377 nm). Φ_{Em} = 79% relative to quinine sulfate.

Methyl 2-((5-(4-(*N*,*N*-diethylsulfamoyl)phenyl)-2-(pyrazin-2-yl)thiazol-4-yl)oxy)acetate (11a)

11a was prepared according to the general procedure given for **4a**. **10a** (260 mg, 0.61 mmol) was treated with diethylamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, chloroform/EtOAc 7:1) to afford the desired product as a yellow solid (260 mg, 0.56 mmol, 92%). Mp: 150 °C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 1.16 (t, *J* = 7.1 Hz, 6H), 3.27 (q, *J* = 7.1 Hz, 4H), 3.84 (s, 3H), 5.15 (s, 2H), 7.83 (d, *J* = 8.6 Hz, 2H), 7.95 (d, *J* = 8.6 Hz, 2H), 8.53-8.57 (m, 1H), 8.60 (d, *J* = 2.5 Hz, 1H), 9.27 (s, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ 14.24, 42.12, 52.32, 66.49, 114.46, 127.31, 127.55, 134.86, 138.50, 140.96, 143.97, 145.27, 146.07, 158.99, 159.44, 169.24. MS EI *m/z*: 462

($M^{•+}$, 91 %), 390 ($M^{•+}$ - $C_4H_{10}N$, 33 %), 326 ($M^{•+}$ - $C_4H_{10}NO_2S$, 94 %), 256 ($M^{•+}$ - $C_9H_8N_3O_3$, 16 %), 253 ($M^{•+}$ - $C_7H_{15}NO_4S$, 37 %), 120 ($M^{•+}$ - $C_{13}H_{18}N_4O_5S$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 485.093640000 (calc. 485.092934761 for $C_{20}H_{22}N_4O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 286 (4.05), 385 (4.44). Fluorescence (THF): λ_{max} (λ_{exc}): 454 nm (385 nm). Φ_{Em} = 79% relative to quinine sulfate.

4-(4-(3-Chloropropoxy)-2-(pyrazin-2-yl)thiazol-5-yl)-*N*,*N*-diethylbenzenesulfonamide (11b)

11b was prepared according to the general procedure given for **4a**. **10b** (189 mg, 0.44 mmol) was treated with diethylamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, chloroform) to afford the desired product as a yellow solid (62 mg, 0.13 mmol, 30%). Mp: 154 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 1.16 (t, *J* = 7.1 Hz, 6H), 2.36 (p, *J* = 6.1 Hz, 2H), 3.27 (q, *J* = 7.1 Hz, 4H), 3.77 (t, *J* = 6.3 Hz, 2H), 4.75 (t, *J* = 6.0 Hz, 2H), 7.82 (d, *J* = 8.6 Hz, 2H), 7.88 (d, *J* = 8.7 Hz, 2H), 8.55 (s, 1H), 8.60 (s, 1H), 9.36 (s, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 14.21, 32.37, 41.41, 42.10, 67.57, 113.92, 126.96, 127.55, 135.29, 138.27, 141.01, 143.96, 145.16, 146.25, 159.48, 160.29. MS EI *m/z*: 466 ($M^{•+}$, 68 %), 330 ($M^{•+}$ - $C_5H_2N_3S$, 74 %), 254 ($M^{•+}$ - $C_{10}H_{14}NO_2S$, 36 %), 120 ($M^{•+}$ - $C_{13}H_{19}ClN_4O_3S$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 489.078560000 (calc. 489.079783591 for $C_{20}H_{23}ClN_4O_3S_2Na$). UV/Vis (THF): λ_{max} (log ε): 286 (4.05), 389 (4.44). Fluorescence (THF): λ_{max} (λ_{exc}): 470 nm (389 nm). Φ_{Em} = 73% relative to quinine sulfate.

***N*,*N*-Diethyl-4-(4-methoxy-2-(pyrazin-2-yl)thiazol-5-yl)benzenesulfonamide (11c)**

11c was prepared according to the general procedure given for **4a**. **10c** (271 mg, 0.74 mmol) was treated with diethylamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, heptane/EtOAc 1:1) to afford the desired product as a yellow solid (267 mg, 0.66 mmol, 90%). Mp: 166 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 1.15 (t, *J* = 7.1 Hz, 6H), 3.26 (q, *J* = 7.1 Hz, 4H), 4.24 (s, 3H), 7.80 (d, *J* = 8.6 Hz, 2H), 7.89 (d, *J* = 8.5 Hz, 2H), 8.52-8.61 (m, 2H), 9.36 (d, *J* = 1.3 Hz, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 14.20, 42.07, 57.97, 113.43, 126.94, 127.48, 135.39, 138.06, 141.03, 143.93, 145.10, 146.31, 159.24, 161.26. MS EI *m/z*: 404 ($M^{•+}$, 70 %), 332 ($M^{•+}$ - $C_4H_{10}N$, 25 %), 268 ($M^{•+}$ - $C_4H_{10}NO_2S$, 88 %), 148 ($M^{•+}$ - $C_{11}H_{14}NO_2S$, 45 %), 120 ($M^{•+}$ - $C_{11}H_{16}N_4O_3S$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 427.086470000 (calc. 427.087455500 for $C_{18}H_{20}N_4O_3S_2Na$). UV/Vis (THF): λ_{max} (log ε): 289 (4.06), 390 (4.45). Fluorescence (THF): λ_{max} (λ_{exc}): 470 nm (390 nm). Φ_{Em} = 75% relative to quinine sulfate.

Methyl 2-((5-(4-(*N*,*N*-bis(2-hydroxyethyl)sulfamoyl)phenyl)-2-(pyrazin-2-yl)thiazol-4-yl)oxy)acetate (12a)

12a was prepared according to the general procedure given for **4a**. **10a** (614 mg, 1.4 mmol) was treated with diethanolamine and triethylamine in CH_2Cl_2. After workup, the crude product recrystallized from chloroform to afford the desired product as a yellow crystalline solid (305 mg, 0.62 mmol, 43%). Mp: 172 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ 3.19 (t, *J* = 6.2 Hz, 4H), 3.52 (q, *J* = 6.1 Hz, 4H), 3.73 (s, 3H), 4.82 (t, *J* = 5.4 Hz, 2H), 5.24 (s, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 8.01 (d, *J* = 8.5 Hz, 2H), 8.69-8.77 (m, 2H), 9.19 (d, *J* = 1.2 Hz, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 51.47, 42.48, 60.32, 67.02, 113.53, 127.65, 128.11, 134.79, 137.93, 140.58, 145.12, 145.39, 146.69, 159.38, 159.92. MS ESI (pos.) *m/z*: 517.0 ($[M+Na]^+$, 100%). UV/Vis (THF): λ_{max} (log ε): 286 (4.00), 385 (4.36). HRMS (ESI [+], $CHCl_3$ + MeOH): 517.082460000 (calc. 517.082763961 for $C_{20}H_{22}N_4O_7S_2Na$). Fluorescence (THF): λ_{max} (λ_{exc}): 453 nm (385 nm). Φ_{Em} = 77% relative to quinine sulfate.

4-(4-(3-Chloropropoxy)-2-(pyrazin-2-yl)thiazol-5-yl)-*N,N*-bis(2-hydroxyethyl)benzenesulfonamide (12b)

12b was prepared according to the general procedure given for **4a**. **10b** (321 mg, 0.75 mmol) was treated with diethanolamine and triethylamine in CH_2Cl_2. After workup, the crude product was purified by column chromatography (silica, chloroform/methanol 15:1) to afford the desired product as a yellow solid (308 mg, 0.62 mmol, 83%). Mp: 155 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ 2.30 (p, J = 6.3 Hz, 2H), 3.18 (t, J = 6.2 Hz, 4H), 3.52 (q, J = 6.0 Hz, 4H), 3.85 (t, J = 6.4 Hz, 2H), 4.67 (t, J = 6.1 Hz, 2H), 4.82 (t, J = 5.4 Hz, 2H), 7.83 (d, J = 8.5 Hz, 2H), 7.94 (d, J = 8.5 Hz, 2H), 8.69 (d, J = 1.4 Hz, 1H), 8.74 (d, J = 2.3 Hz, 1H), 9.27 (s, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 32.31, 42.57, 51.54, 60.35, 68.26, 113.35, 127.40, 128.15, 135.13, 137.56, 140.63, 145.06, 145.54, 146.56, 160.04, 160.40. MS EI *m/z*: 498 ($M^{\bullet+}$, 9 %), 467 ($M^{\bullet+}$ - CH_3O, 57 %), 330 ($M^{\bullet+}$ - $C_7H_{17}ClO_2S$, 100 %), 120 ($M^{\bullet+}$ - $C_{13}H_{19}ClN_4O_5S$, 61 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 521.070860000 (calc. 521.069612791 for $C_{20}H_{23}ClN_4O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 286 (4.03), 389 (4.41). Fluorescence (THF): λ_{max} (λ_{exc}): 470 nm (389 nm). Φ_{Em} = 76% relative to quinine sulfate.

233. *N,N*-Bis(2-hydroxyethyl)-4-(4-methoxy-2-(pyrazin-2-yl)thiazol-5-yl)benzenesulfonamide (12c)

12c was prepared according to the general procedure given for **4a**. **10c** (1.36 g, 3.7 mmol) was treated with diethanolamine and triethylamine in CH_2Cl_2. Since the product was insoluble in EtOAc, instead of adding water, the solvent was removed under reduced pressure and the crude product was taken up in EtOAc, heated to reflux and filtered while still hot. It was then washed with H_2O and dried *in vacuo* to afford the desired product as a yellow solid (1.05 g, 2.4 mmol, 65 %). Mp: 171 °C. ^{1}H-NMR (250 MHz, $CDCl_3$): δ 3.18 (t, J = 6.3 Hz, 4H), 3.62 (q, J = 6.1 Hz, 4H), 4.19 (s, 3H), 4.82 (t, J = 5.4 Hz, 2H), 7.82 (d, J = 8.5 Hz, 2H), 7.93 (d, J = 8.6 Hz, 2H), 8.69 (d, J = 1.4 Hz, 1H), 8.74 (d, J = 2.4 Hz, 1H), 9.27 (s, 1H). ^{13}C-NMR (63 MHz, $CDCl_3$): δ 51.49, 58.55, 60.33, 112.96, 127.40, 128.08, 135.15, 137.57, 140.60, 145.06, 145.57, 146.53, 159.93, 161.23. MS EI *m/z*: 436 ($M^{\bullet+}$, 11 %), 405 ($M^{\bullet+}$ - CH_3O, 38 %), 332 ($M^{\bullet+}$ - $C_4H_{10}NO_2$, 13 %), 268 ($M^{\bullet+}$ - $C_6H_6N_3OS$, 100 %), 120 ($M^{\bullet+}$ - $C_{11}H_{16}N_4O_5S$, 43 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 459.077900000 (calc. 459.077284701 for $C_{18}H_{20}N_4O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 286 (4.06), 389 (4.45). Fluorescence (THF): λ_{max} (λ_{exc}): 470 nm (389 nm). Φ_{Em} = 75% relative to quinine sulfate.

2-((5-(4-(*N,N*-Diethylsulfamoyl)phenyl)-2-(pyridin-2-yl)thiazol-4-yl)oxy)acetic acid (6)

General procedure for the preparation of carboxylic acids **6**, **7**, **13** and **14**:

4a (215 mg, 0.47 mmol) and KOH (105 mg, 1.9 mmol, 4 eq) were suspended in 40 mL EtOH. After stirring at room temperature for 2 hours, H_2O is added until the mixture became clear (20 mL). The solution was filtered through a glas frit to remove any undissolved material and the filtrate was treated with dilute HCl until the product precipitated (pH ~ 5). After about one hour, the product was filtered off, washed with water and dried *in vacuo* to afford carboxylic acid **6** as a yellow solid (197 mg, 0.44 mmol, 95%). Mp: 190 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ 1.04 (t, J = 7.1 Hz, 6H), 3.17 (q, J = 7.1 Hz, 4H), 3.36 (s, 1H), 5.10 (s, 2H), 7.48-7.53 (m, 1H), 7.82 (d, J = 8.5 Hz, 2H), 7.94-8.02 (m, 4H), 8.63 (d, J = 4.7 Hz, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 14.61, 42.34, 66.78, 112.00, 119.25, 126.06, 127.44, 127.88, 135.30, 137.97, 138.34, 149.91, 150.34, 159.39, 12.63, 170.52. MS EI *m/z*: 447 ($M^{\bullet+}$, 37 %), 402 ($M^{\bullet+}$ - CHO_2, 14 %), 375 ($M^{\bullet+}$ - $C_4H_{10}N$, 17 %), 311 ($M^{\bullet+}$ - $C_4H_{10}NO_2S$, 100 %), 266 ($M^{\bullet+}$ - $C_5H_{11}NO_4S$, 12 %), 252 ($M^{\bullet+}$ - $C_6H_{13}NO_4S$, 31 %), 120 ($M^{\bullet+}$ - $C_{13}H_{17}N_3O_5S$, 90 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 470.082880000 (calc. 470.082035731 for $C_{20}H_{21}N_3O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 283 (3.93), 378 (4.31). Fluorescence (THF): λ_{max} (λ_{exc}): 446 nm (378 nm). Φ_{Em} = 75% relative to quinine sulfate.

2-((5-(4-(*N*,*N*-Bis(2-hydroxyethyl)sulfamoyl)phenyl)-2-(11yridine-2-yl)thiazol-4-yl)oxy)acetic acid (7)

7 was prepared from **5a**, according to the general procedure given for **6**. **5a** (425 mg, 0.86 mmol) gave 7 as a yellow-orange solid (400 mg, 0.83 mmol, 97%). Mp: 159 °C. ^{1}H-NMR (400 MHz, DMSO-d_6): δ 3.20 (t, J = 6.3 Hz, 4H), 3.53 (t, J = 6.0 Hz, 4H), 4.83 (s, 2H), 5.12 (s, 2H), 7.46-7.57 (m, 1H), 7.85 (d, J = 8.6 Hz, 2H), 7.95-8.07 (m, 4H), 8.64 (d, J = 4.6 Hz, 1H), 13.12 (s, 1H). ^{13}C-NMR (100 MHz, DMSO-d_6): δ 51.51, 60.35, 66.80, 112.03, 119.28, 126.08, 127.43, 128.08, 135.41, 137.44, 138.37, 149.94, 150.37, 159.43, 162-68, 170.56. MS EI *m/z*: 479 ($M^{\bullet+}$, 9 %), 448 ($M^{\bullet+}$ - CH_3O, 44 %), 375 ($M^{\bullet+}$ - $C_4H_{10}NO_2$, 10 %), 311 ($M^{\bullet+}$ - $C_4H_{10}NO_4S$, 100 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 502.070810000 (calc. 502.071864931 for $C_{20}H_{21}N_3O_7S_2Na$). UV/Vis (THF): λ_{max} (log ε): 377 (4.38). Fluorescence (THF): λ_{max} (λ_{exc}): 446 nm (377 nm). Φ_{Em} = 71% relative to quinine sulfate.

2-(5-(4-(*N*,*N*-Diethylsulfamoyl)phenyl)-2-(pyrazin-2-yl)thiazol-4-yloxy)acetic acid (13)

13 was prepared from **11a**, according to the general procedure given for **6**. After acidifiying the aqueous phase, it was extracted with EtOAc (3*20 mL). The combined organic extracts were washed with H_2O and saturated NaCl solution and dried over $MgSO_4$. The solvent was removed under reduced pressure.**11a** (946 mg, 2.0 mmol) gave **13** as a yellow solid (892 mg, 2.0 mmol, 97%). Mp: 210 °C. ^{1}H-NMR (250 MHz, DMSO-d_6): δ 1.05 (t, J = 7.1 Hz, 6H), 3.17 (q, J = 7.1 Hz, 4H), 5.13 (s, 2H), 7.83 (d, J = 8.5 Hz, 2H), 8.00 (d, J = 8.5 Hz, 2H), 8.70 (d, J = 1.4 Hz, 1H), 8.74 (d, J = 2.4 Hz, 1H), 9.20 (s, 1H), 13.17 (s, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 14.63, 42.36, 66.99, 113.25, 127.64, 127.91, 134.86, 138.33, 140.54, 145.12, 145.44, 146.63, 159.71, 170.48. MS EI *m/z*: 448 ($M^{\bullet+}$, 39 %), 376 ($M^{\bullet+}$ - $C_4H_{10}N$, 22 %), 312 ($M^{\bullet+}$ - $C_4H_{10}NO_2S$, 100 %), 120 ($M^{\bullet+}$ - $C_{12}H_{16}lN_4O_5S$, 59 %). HRMS (ESI [+], $CHCl_3$ + MeOH): 471.077770000 (calc. 417.077284701 for $C_{19}H_{20}N_4O_5S_2Na$). UV/Vis (THF): λ_{max} (log ε): 286 (4.03), 391 (4.39). Fluorescence (THF): λ_{max} (λ_{exc}): 468 nm (391 nm). Φ_{Em} = 67% relative to quinine sulfate.

2-((5-(4-(*N*,*N*-Bis(2-hydroxyethyl)sulfamoyl)phenyl)-2-(pyrazin-2-yl)thiazol-4-yl)oxy)acetic acid (14)

14 was prepared from **12a**, according to the general procedure given for **6**. Instead of acidifying the aqueous phase after filtration, it was extracted with EtOAc (3*20 mL) to remove any starting material. The aqueous phase was then acidified to precipitate the product. After one hour, it was filtered off, washed with water and dried *in vacuo*. **12a** (263 mg, 0.53 mmol) gave **14** as a yellow solid (214 mg, 0.45 mmol, 84%). Mp: 223 °C. ^{1}H-NMR (250

MHz, DMSO-d_6): δ 3.19 (t, J = 6.3 Hz, 4H), 3.52 (t, J = 6.2 Hz, 4H), 4.82 (s, 2H), 5.14 (s, 2H), 7.85 (d, J = 8.6 Hz, 2H), 8.01 (d, J = 8.6 Hz, 2H), 8.67-8.72 (m, 1H), 8.75 (d, J = 2.5 Hz, 1H), 9.21 (d, J = 1.4 Hz, 1H), 13.13 (s, 1H). ^{13}C-NMR (63 MHz, DMSO-d_6): δ 51.49, 60.33, 66.97, 113.28, 127.61, 128.09, 134.95, 137.81, 140.56, 145.13, 145.45, 146.64, 159.71, 159.76, 170.47. MS ESI (neg.) *m/z*: 479.2 ([M-H]$^-$, 100%). HRMS (ESI [+], $CHCl_3$ + MeOH): 503.066190000 (calc. 503.067113901 for $C_{10}H_{20}N_4O_7S_2Na$). UV/Vis (THF): λ_{max} (log ε): 286 (3.98), 389 (4.33). Fluorescence (THF): λ_{max} (λ_{exc}): 467 nm (389 nm). Φ_{Em} = 67% relative to quinine sulfate.

Additional crystal structure graphics for 4c

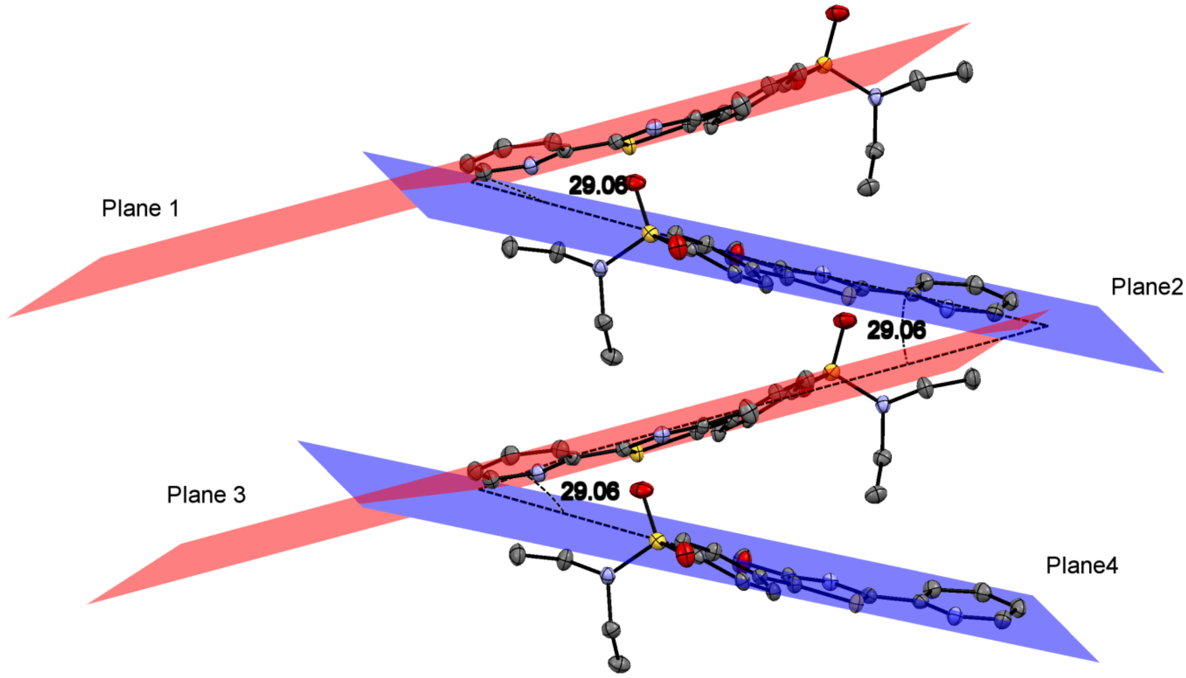

Figure S1: ORTEP-plot of **4c** (50% probability ellipsoids) with angles between different planes. Hydrogen atoms were omitted for clarity. Planes were created from the mean of all atoms of the respective molecules, excluding the sulfonamide moieties.

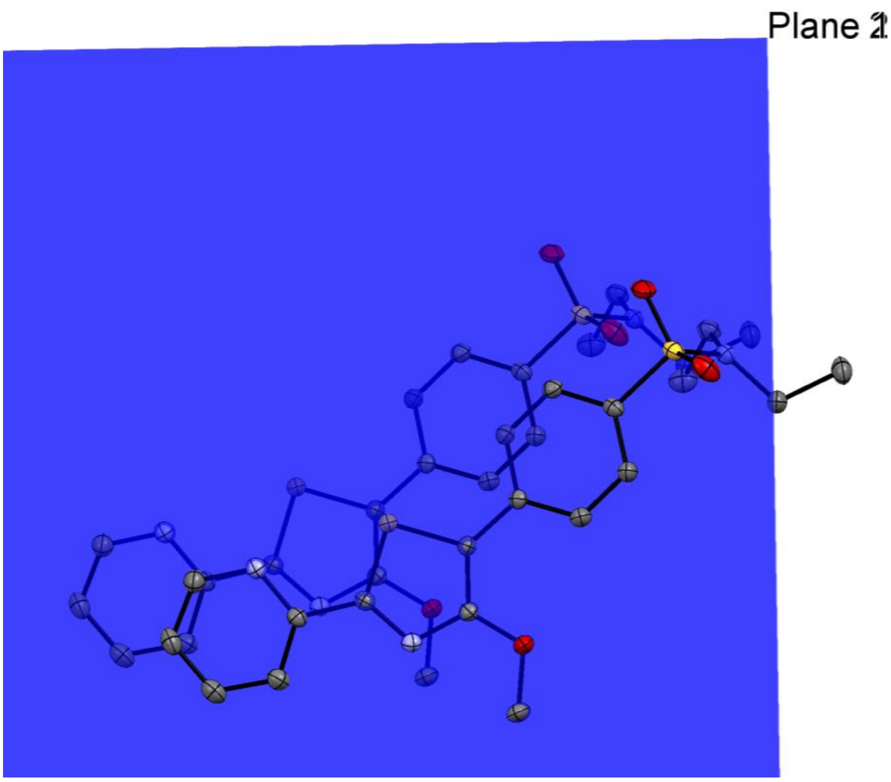

Figure S2: ORTEP-plot of 2 closest parallelly arranged molecules of **4c** (50% probability ellipsoids) with planes created from the mean of all atoms of the respective molecules, excluding the sulfonamide moieties. Planes were arranged to perfectly cover each other in order to identify atoms that are located on top of each other.

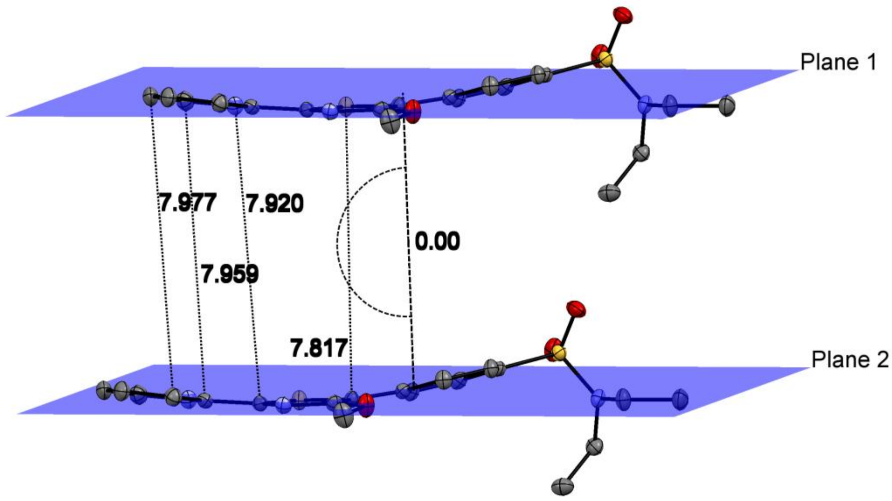

Figure S3: ORTEP-plot of 2 closest parallelly arranged molecules of **4c** (50% probability ellipsoids) with planes created from the mean of all atoms of the respective molecules, excluding the sulfonamide moieties. The angle between the two planes and distances between atoms that are located on top of each other (see Figure S2) were calculated.

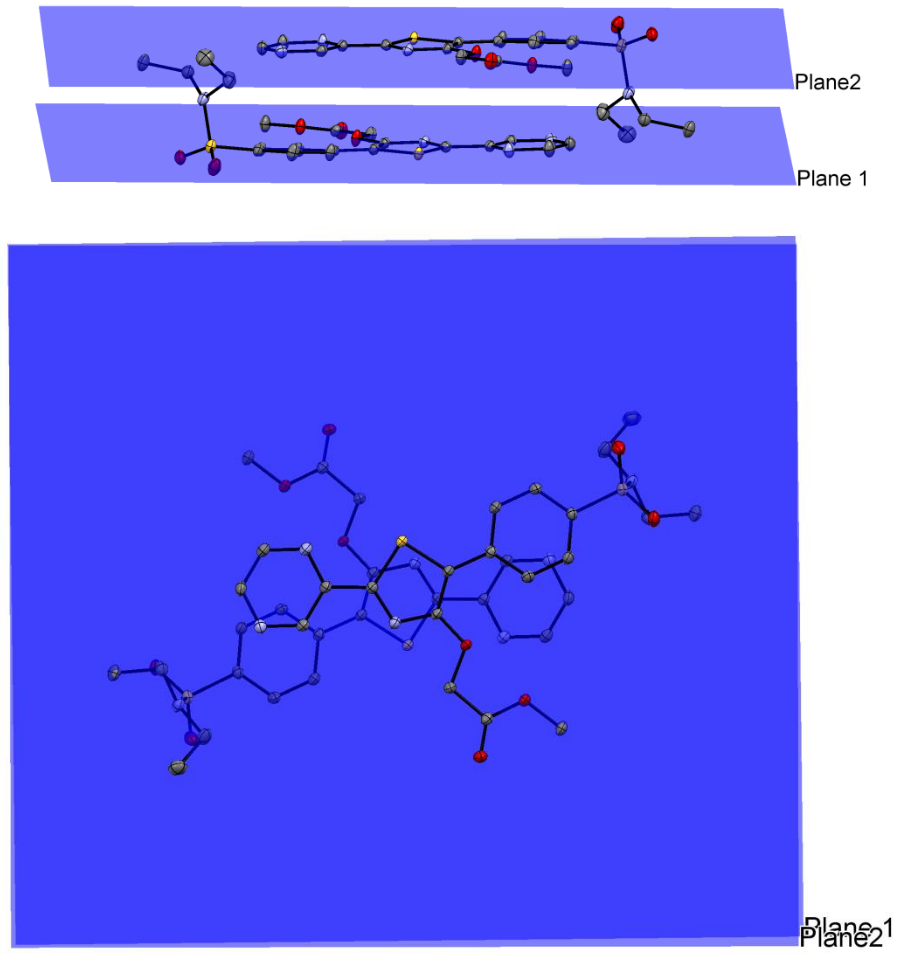

Figure S4: ORTEP-plot of 2 parallelly arranged molecules of **11a** (50% probability ellipsoids) with planes created from the mean of all atoms of the respective molecules, excluding the sulfonamide moieties.

UV/Vis and fluorescence spectra

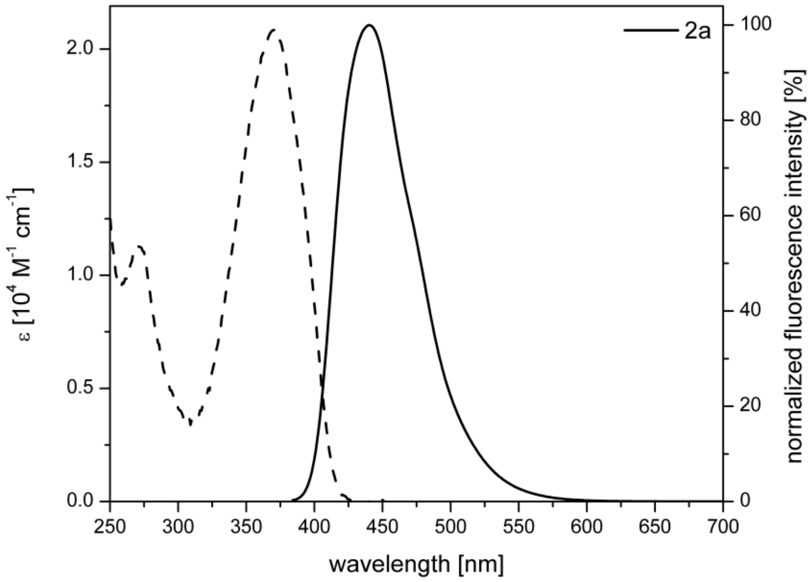

Figure S5: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **2a**, $2*10^{-6}$ M in THF.

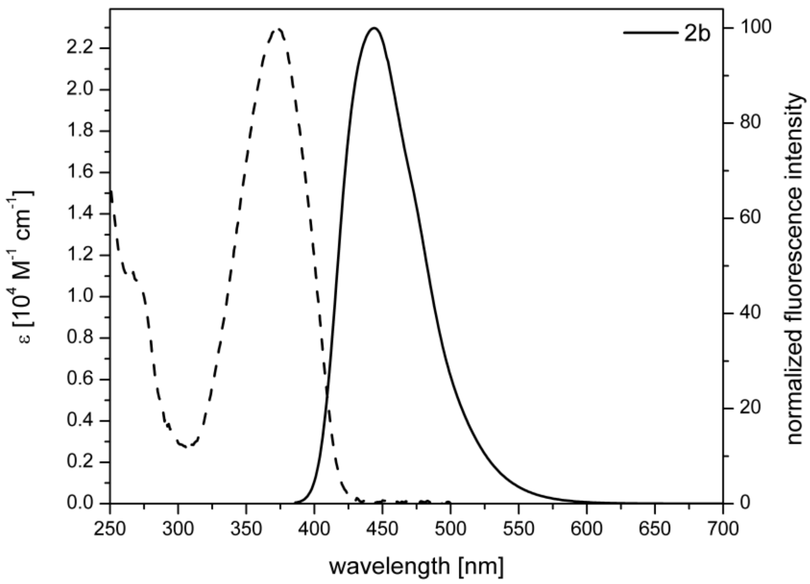

Figure S6: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **2b**, $2*10^{-6}$ M in THF.

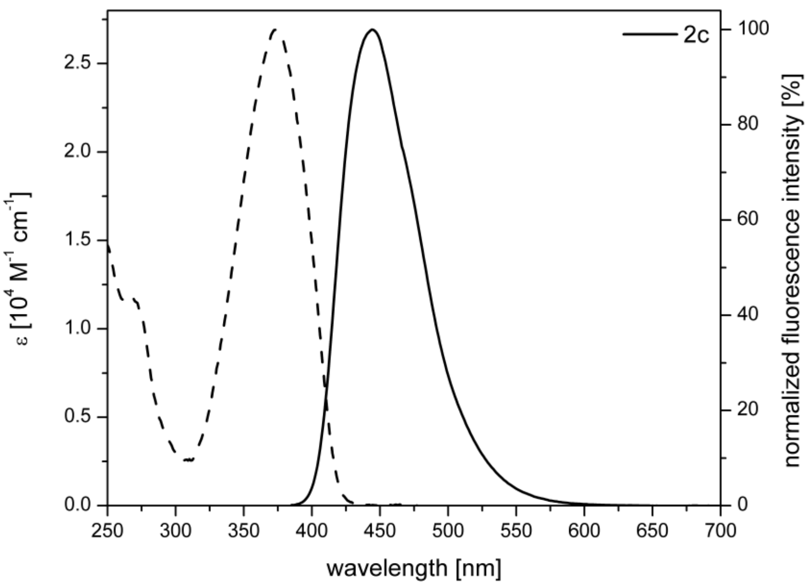

Figure S7: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **2c**, $2{\times}10^{-6}$ M in THF.

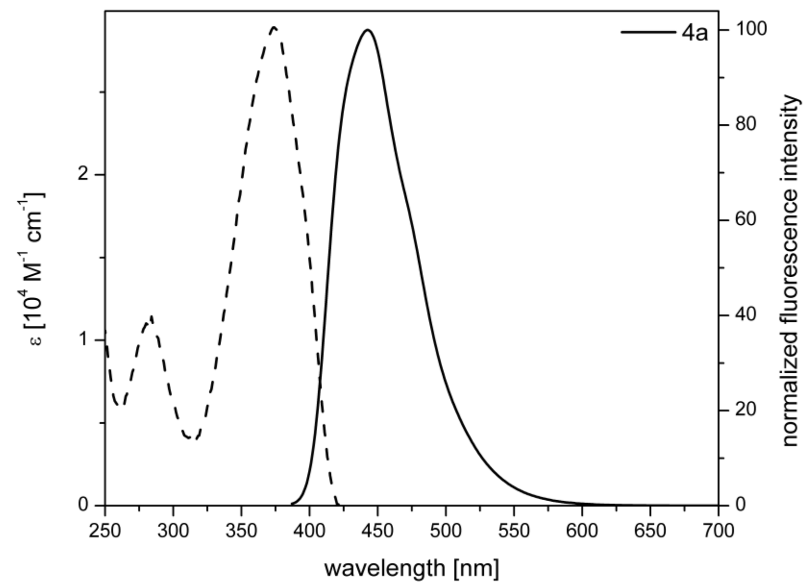

Figure S8: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **4a**, $2{\times}10^{-6}$ M in THF.

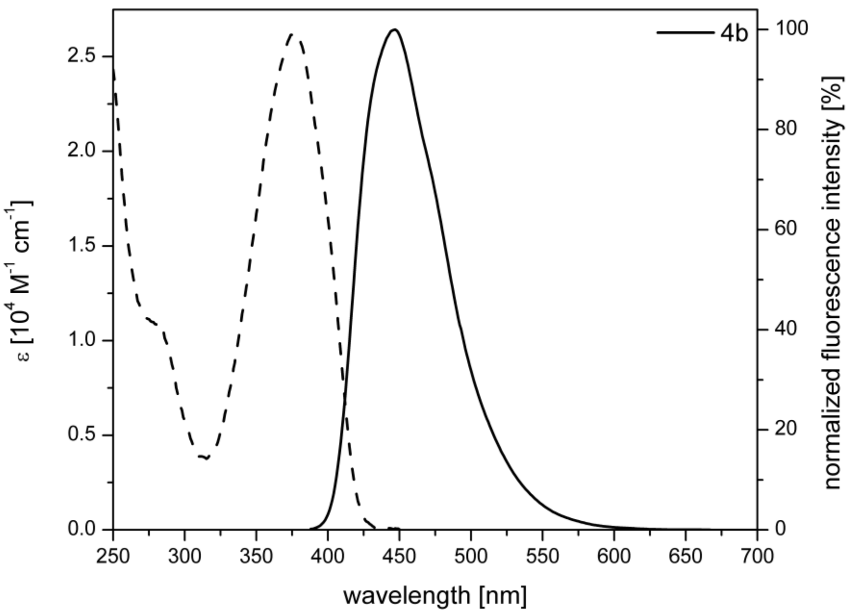

Figure S9: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **4b**, 2×10^{-6} M in THF.

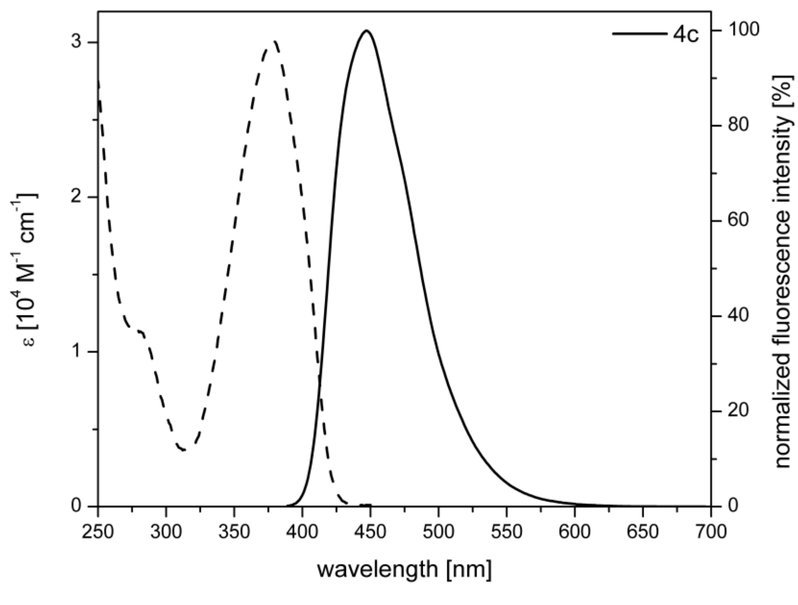

Figure S10: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **4c**, 2×10^{-6} M in THF.

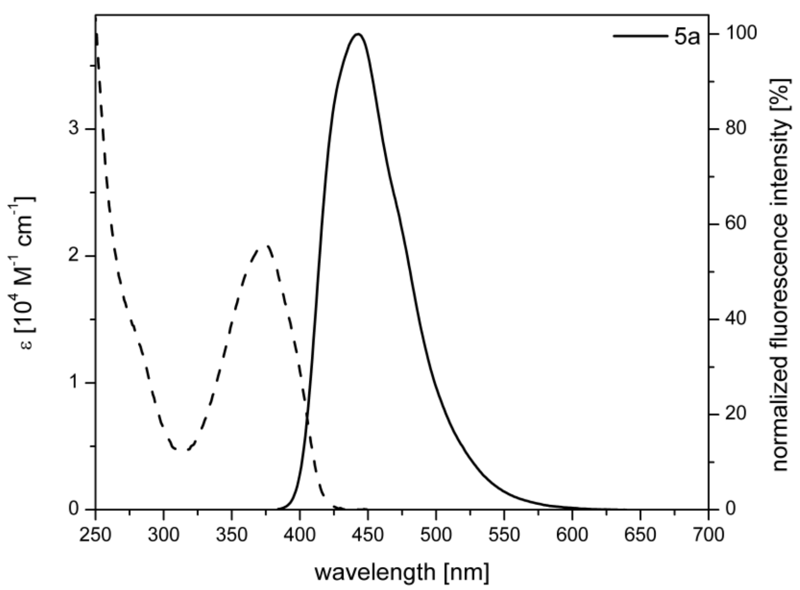

Figure S11: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **5a**, 2×10^{-6} M in THF.

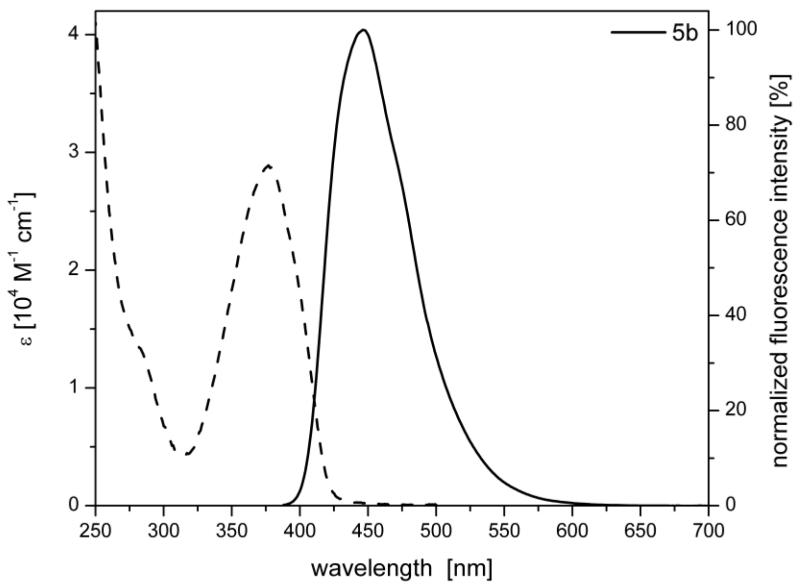

Figure S12: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **5b**, 2×10^{-6} M in THF.

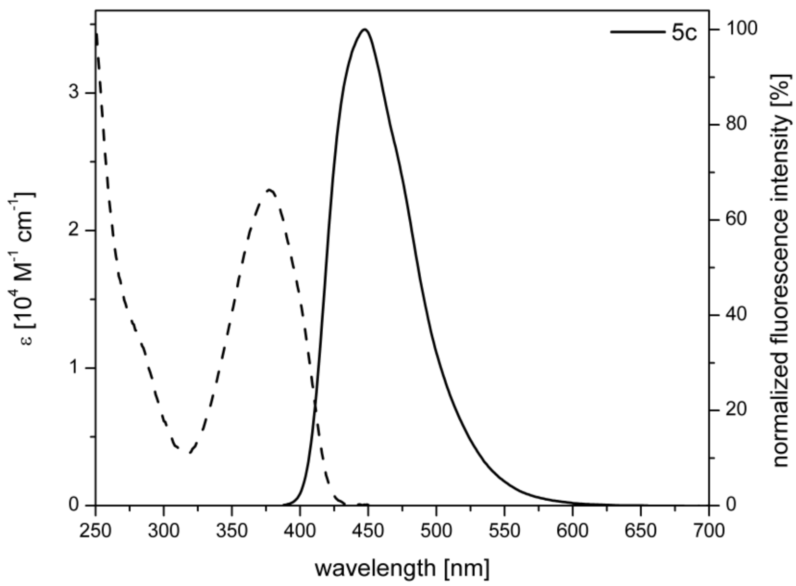

Figure S13: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **5c**, $2{\times}10^{-6}$ M in THF.

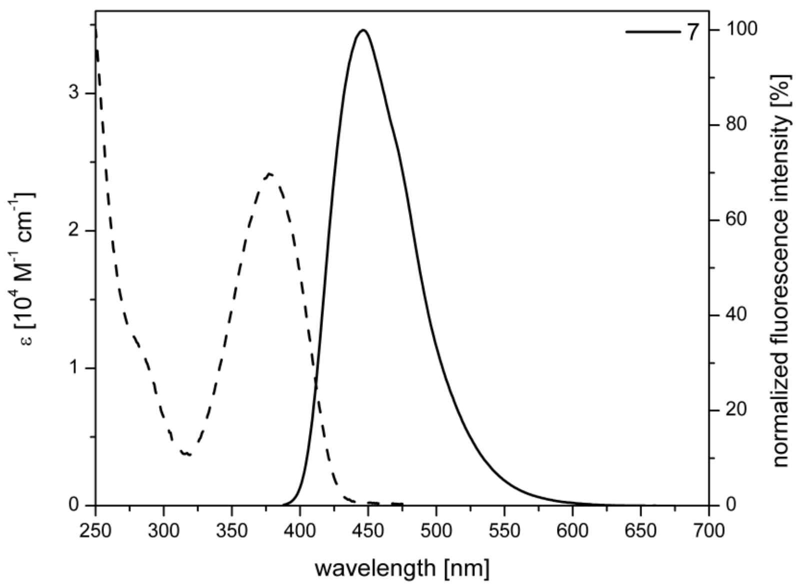

Figure S14: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **7**, $2{\times}10^{-6}$ M in THF.

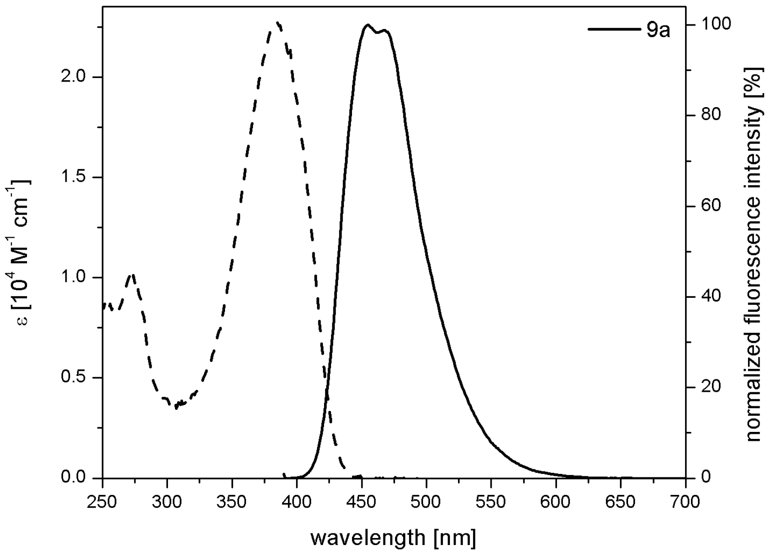

Figure S15: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **9a**, 2×10^{-6} M in THF.

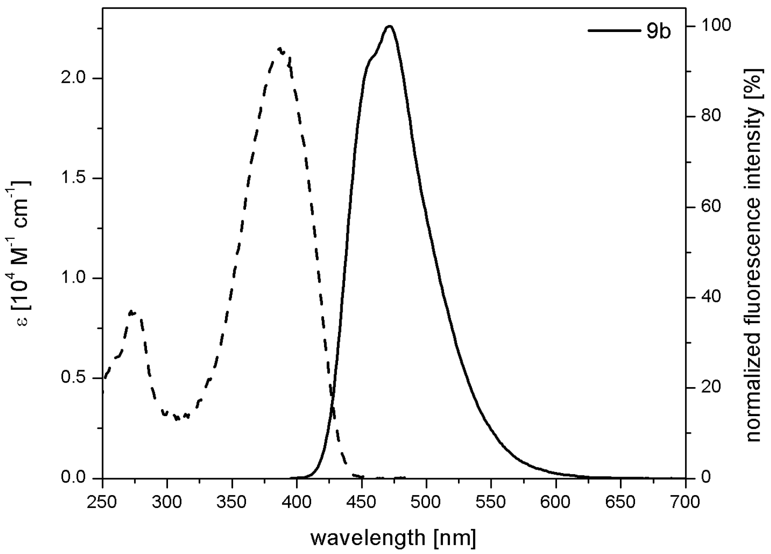

Figure S16: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **9b**, 2×10^{-6} M in THF.

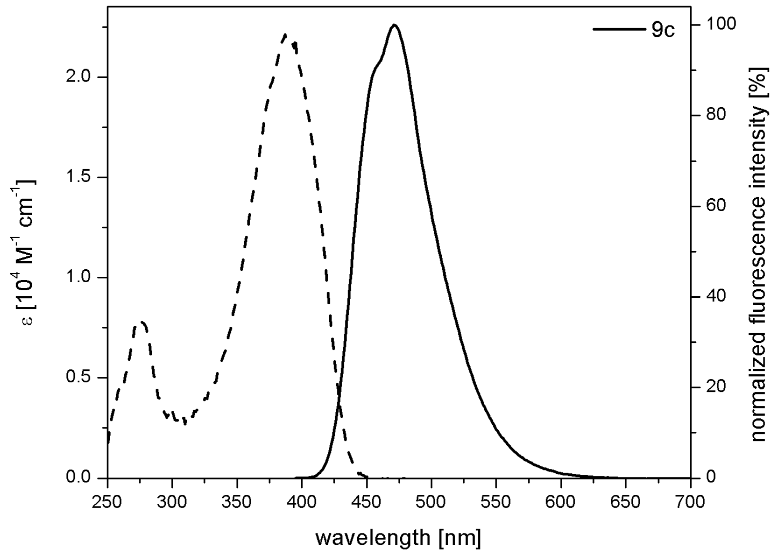

Figure S17: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **9c**, 2×10^{-6} M in THF.

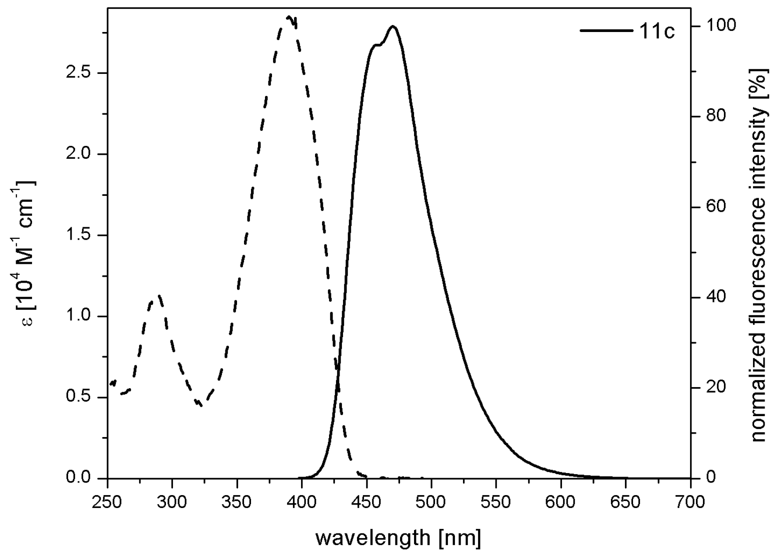

Figure S18: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **11c**, 2×10^{-6} M in THF.

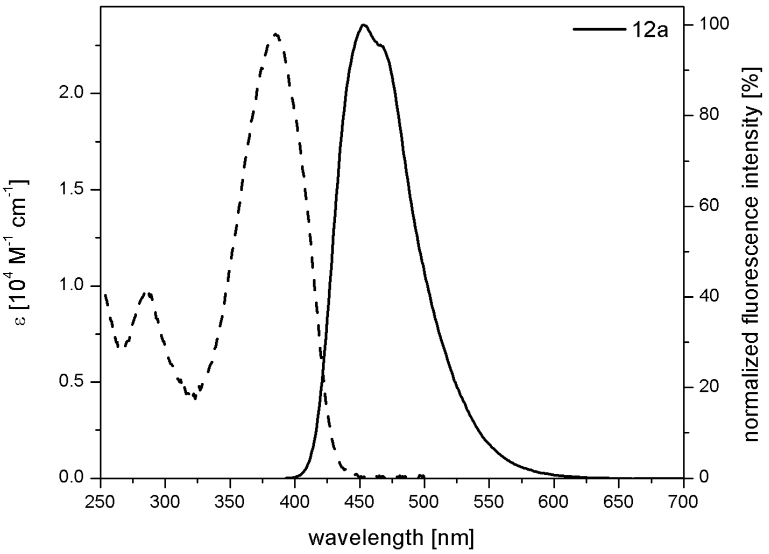

Figure S19: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of 1**2a**, 2×10^{-6} M in THF.

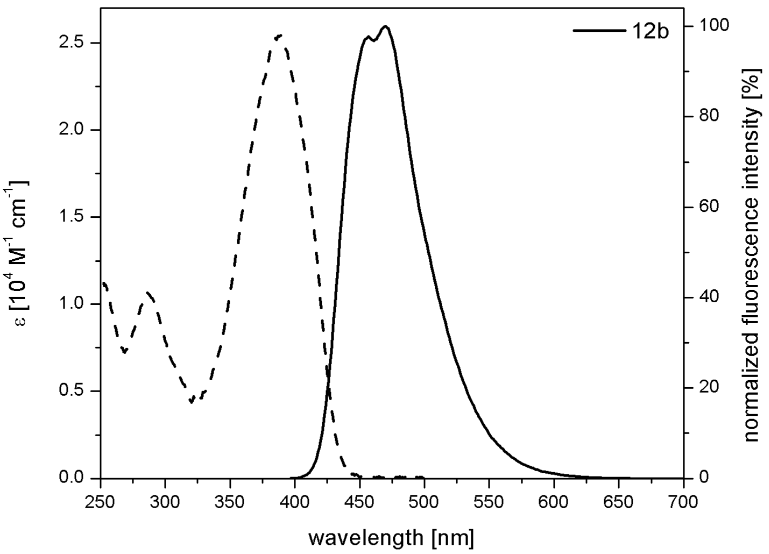

Figure S20: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of1 **12b**, 2×10^{-6} M in THF.

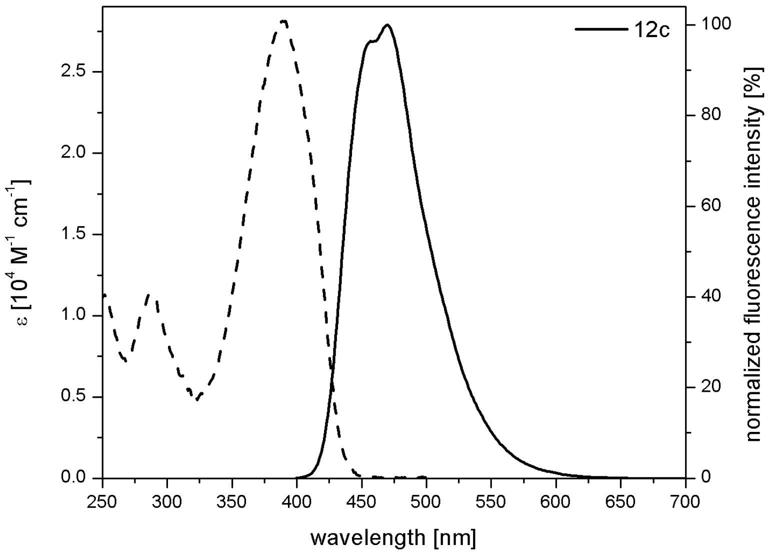

Figure S21: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **12c**, $2{\times}10^{-6}$ M in THF.

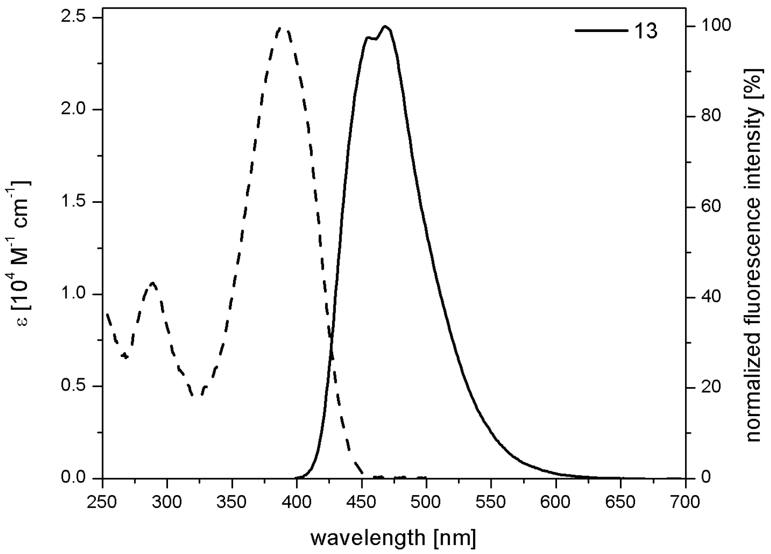

Figure S22: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **13**, $2{\times}10^{-6}$ M in THF.

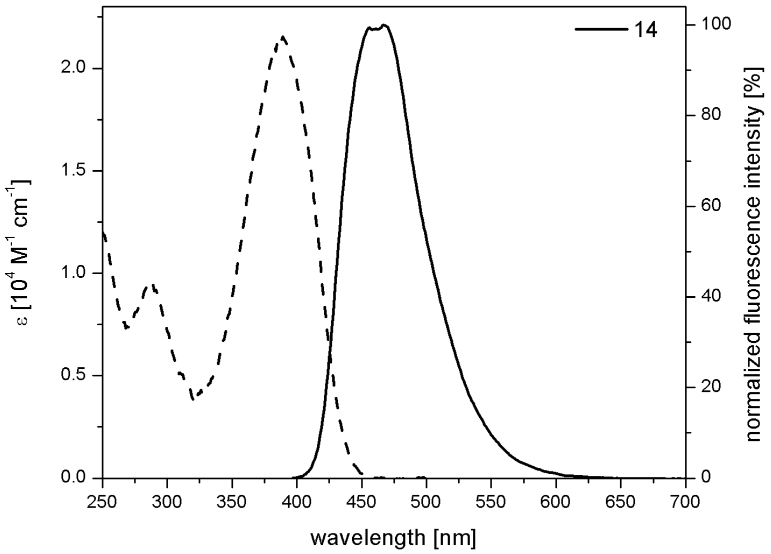

Figure S23: UV/Vis absorption (dashed) and fluorescence emission (solid) spectra of **14**, 2×10^{-6} M in THF.

XYZ data for 4a-c, 5a-c, 6, 7, 11a-c, 12a-c, 13 and 14

4a

0 1

C	0.60940900	0.43479300	1.91715500
C	0.40437000	1.63988200	2.55764000
N	0.19296500	1.60141200	3.89697200
C	0.22778400	0.37034800	4.33604100
S	0.52302900	-0.81885100	3.12312100
C	0.86549400	0.15050100	0.50470700
O	0.40716900	2.81719000	1.90280600
C	0.03776500	-0.01202000	5.74192100
C	-0.19472900	0.95315700	6.72175800
C	-0.36478900	0.53033700	8.03321400
C	-0.29738600	-0.82877900	8.31784200
C	-0.06101800	-1.71403300	7.26919200
N	0.10381200	-1.32241200	6.00725000
C	0.98945200	1.18286500	-0.44249700
C	1.24460900	0.89521200	-1.77551200
C	1.37724600	-0.42802500	-2.18762300
C	1.26148200	-1.46785000	-1.26905100
C	1.00860600	-1.17505100	0.06174200
S	1.66086500	-0.79244400	-3.90790200
O	2.16364400	-2.16466400	-3.98225400
N	0.20005800	-0.78587100	-4.68799200
O	2.44765400	0.30905400	-4.46445100
C	-0.68792100	-1.94066500	-4.44393200
C	-0.45080300	0.51544700	-4.91452000
C	-1.19199300	0.54735500	-6.24381900
C	-0.65474700	-2.95654500	-5.57642800
C	0.19684400	3.99154100	2.66162500
H	-0.23762500	2.00032800	6.44898200
H	-0.54711300	1.25266400	8.82180900
H	-0.42396700	-1.20173100	9.32768100
H	-0.00169100	-2.78324700	7.45213100
H	0.89423900	2.21511000	-0.13428000
H	1.36013400	1.70451000	-2.48738200
H	1.38986000	-2.49510400	-1.58909600
H	0.92888100	-1.99874100	0.76304700
H	-0.41971400	-2.42523800	-3.50100700
H	-1.69786500	-1.54339100	-4.30867300
H	-1.14050100	0.73348900	-4.08761100
H	0.32638700	1.27942000	-4.91697500
H	-0.50459500	0.36266600	-7.07307000
H	-1.99075900	-0.19791700	-6.28414500
H	-0.94275500	-2.49632800	-6.52487100
H	0.34918200	-3.37185700	-5.68459800
H	-0.77442700	3.97115800	3.16470500
H	0.96952500	4.11421000	3.42626100
H	-1.34931100	-3.77537400	-5.36496700
H	-1.64874000	1.53119100	-6.38182100
C	0.24332800	5.16331800	1.70740300
O	0.41832100	5.09657100	0.51309300
O	0.05990300	6.29804500	2.38265000
C	0.07593500	7.51359500	1.61327100
H	-0.08529500	8.31386600	2.33172500

H	-0.72219200	7.49706600	0.87012700
H	1.04016000	7.63007100	1.11711500

4b

0 1

C	0.58803500	0.51238100	1.90330300
C	0.47534900	1.69630500	2.60596500
N	0.24364200	1.59619000	3.94061000
C	0.16506300	0.34436400	4.30787700
S	0.37171000	-0.79620600	3.03146900
C	0.84746900	0.28148300	0.48243600
O	0.59090700	2.90407300	2.02491600
C	-0.08233200	-0.09951300	5.68683400
C	-0.25191800	0.82450100	6.71804100
C	-0.48287800	0.34399500	8.00000900
C	-0.53641600	-1.02986800	8.20603700
C	-0.35478200	-1.87086000	7.11115800
N	-0.13218600	-1.42364300	5.87679800
C	0.75248100	1.32176700	-0.45797300
C	0.99516200	1.08897100	-1.80374200
C	1.33634700	-0.19039900	-2.23456600
C	1.44448600	-1.23694600	-1.32238900
C	1.20347500	-0.99688900	0.02134400
S	1.59280900	-0.49851800	-3.97001800
O	2.34466900	-1.74889900	-4.08143200
N	0.11676500	-0.77561400	-4.66903400
O	2.12114200	0.73202000	-4.56047400
C	-0.51814800	-2.07763300	-4.37977300
C	-0.78261500	0.37665700	-4.84683600
C	-1.59402900	0.26190500	-6.12963500
C	-0.33885000	-3.08086600	-5.50946600
C	0.55085800	4.06099300	2.87197600
H	-0.20171000	1.88525700	6.50587100
H	-0.61923800	1.03335400	8.82653400
H	-0.71431400	-1.44739800	9.19038400
H	-0.38952000	-2.94991700	7.23225500
H	0.49190800	2.31859900	-0.13063900
H	0.93392300	1.90674900	-2.51258000
H	1.74031000	-2.22391800	-1.65809700
H	1.31158300	-1.81912500	0.72055200
H	-0.11960800	-2.48961300	-3.44832900
H	-1.57862100	-1.88181500	-4.19878200
H	-1.45045600	0.46295500	-3.97872000
H	-0.16587000	1.27421200	-4.88971500
H	-0.93438600	0.20554500	-6.99903400
H	-2.23992400	-0.62011200	-6.12760700
H	-0.75380800	-2.69661700	-6.44457200
H	0.72117000	-3.29275000	-5.66256700
H	-0.40897000	4.09355100	3.39562200
H	1.34674700	3.98874900	3.61934100
C	0.73807900	5.26704300	1.96856300
H	-0.06297200	5.29173100	1.22417400
H	1.68789600	5.17630200	1.43402600
C	0.72513900	6.54862200	2.78192100
H	1.53958500	6.58070900	3.50542000
H	-0.22144300	6.69315900	3.30246700

Cl	0.94007200	7.99412100	1.71790300
H	-0.84952700	-4.01694300	-5.26348100
H	-2.23468000	1.14177500	-6.23438300

4c

0 1

C	0.42886300	0.54871600	1.84427000
C	0.07584300	1.71171100	2.50335700
N	-0.12121700	1.61949200	3.84403500
C	0.06890900	0.39583900	4.26108200
S	0.50425300	-0.72755200	3.02798100
C	0.71272200	0.31573700	0.42898000
O	-0.07157300	2.89123400	1.87718200
C	-0.06791500	-0.03064300	5.66075300
C	-0.41974500	0.88155800	6.65583600
C	-0.53271300	0.42035800	7.96042500
C	-0.29303200	-0.92354200	8.22398600
C	0.05229200	-1.75494000	7.16167400
N	0.16439400	-1.32598200	5.90599500
C	0.57517000	1.33801600	-0.52681400
C	0.84941800	1.10284400	-1.86611900
C	1.26539600	-0.16046200	-2.27766900
C	1.41626200	-1.18883500	-1.35082300
C	1.14299500	-0.94691600	-0.01400900
S	1.56683800	-0.47215500	-4.00462700
O	2.39004200	-1.67871300	-4.09140700
N	0.12052700	-0.83924100	-4.72571500
O	2.03432800	0.78044600	-4.60033600
C	-0.43845100	-2.17768800	-4.44576100
C	-0.84502200	0.25727800	-4.90868000
C	-1.64573200	0.09301900	-6.19282700
C	-0.21585900	-3.15643700	-5.58953100
C	-0.41354200	4.02971600	2.67506500
H	-0.59591300	1.91873700	6.39900100
H	-0.80400600	1.10146700	8.76006900
H	-0.36977500	-1.32519100	9.22783000
H	0.24721600	-2.81071600	7.32785600
H	0.25852200	2.32345900	-0.21580000
H	0.75678000	1.90905100	-2.58476100
H	1.76733300	-2.16315400	-1.66975600
H	1.27977600	-1.75785400	0.69327500
H	-0.00525200	-2.57819200	-3.52519600
H	-1.50633300	-2.04463200	-4.25053900
H	-1.51899900	0.30616900	-4.04232700
H	-0.28215900	1.18954300	-4.95224200
H	-2.33271600	0.93655800	-6.30270600
H	-0.98190800	0.06884200	-7.06053400
H	-2.24313600	-0.82244500	-6.18839300
H	-0.67150400	-4.12199900	-5.34935200
H	-0.66137000	-2.78593500	-6.51602400
H	0.85237800	-3.30878800	-5.75672600
H	-0.47152500	4.86240000	1.97621900
H	-1.37647500	3.88066800	3.16743900
H	0.35561200	4.21905200	3.42636600

5a

c 0 1

C	0.61020700	0.49684600	1.88269500
C	0.41587000	1.69045100	2.54775100
N	0.20489500	1.62579300	3.88608400
C	0.22484100	0.38526100	4.29876900
S	0.50576300	-0.78146500	3.06096300
C	0.86372500	0.23984500	0.46490400
O	0.43144000	2.88102200	1.91802100
C	0.02672200	-0.02497500	5.69568400
C	-0.19905400	0.92130200	6.69528200
C	-0.37938700	0.47204200	7.99656500
C	-0.32863200	-0.89359400	8.25179400
C	-0.09748800	-1.75851000	7.18513300
N	0.07735400	-1.34142200	5.93276700
C	0.82869800	1.27441500	-0.48698700
C	1.06666500	1.01262800	-1.82843800
C	1.34450400	-0.28732400	-2.24176600
C	1.39725000	-1.32805300	-1.31772200
C	1.15888900	-1.06013000	0.02053800
S	1.59426800	-0.62868800	-3.96906100
O	2.31629500	-1.89663800	-4.06702000
N	0.10400200	-0.89446000	-4.65770700
O	2.13380400	0.58078700	-4.58829900
C	-0.54140300	-2.18327100	-4.37016400
C	-0.77235800	0.26475300	-4.85558400
C	-1.42127500	0.22258900	-6.23038100
C	-0.30306600	-3.19450800	-5.47992300
C	0.26031800	4.04276100	2.70600100
H	-0.22957800	1.97453400	6.44515500
H	-0.55712500	1.17911900	8.79989500
H	-0.46409400	-1.28693300	9.25271300
H	-0.05100800	-2.83204600	7.34499400
H	0.62100100	2.28920400	-0.17643300
H	1.05333500	1.82456800	-2.54633500
H	1.64528300	-2.33287600	-1.63870500
H	1.21668000	-1.88075300	0.72745700
H	-0.19219000	-2.59858700	-3.42047300
H	-1.61433400	-2.00389600	-4.26132100
H	-1.54665000	0.29752100	-4.07929800
H	-0.17710300	1.17511900	-4.78630800
H	-0.64232900	0.25586200	-7.00086200
H	-1.99784900	-0.70197100	-6.35877200
H	-0.64258000	-2.78286000	-6.43834300
H	0.76655900	-3.41320100	-5.55256700
H	-0.69507100	4.02441500	3.23856900
H	1.05800900	4.13981000	3.44827900
C	0.29046200	5.23313100	1.77440200
O	0.40071600	5.18776500	0.57149500
O	0.17104200	6.35738300	2.48100500
C	0.17278000	7.58784200	1.73552000
H	0.06800500	8.37647100	2.47694700
H	-0.66399600	7.60327800	1.03613200
H	1.11143000	7.69411700	1.19044500
O	-2.27499100	1.35611900	-6.30868000
H	-2.69597600	1.37888000	-7.17610100
O	-1.04550000	-4.35890600	-5.13583800
H	-0.84242500	-5.06303000	-5.76267500

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C	0.60883400	0.49040800	1.91391400
C	0.46646600	1.67765900	2.60634400
N	0.25885700	1.58430200	3.94528500
C	0.22886700	0.33455500	4.32659500
S	0.45487800	-0.81238100	3.05952400
C	0.85380100	0.25287100	0.49199600
O	0.53050900	2.88206900	2.01158500
C	0.01837800	-0.10205900	5.71397900
C	-0.16741300	0.82721600	6.73758300
C	-0.36180700	0.35355100	8.02813900
C	-0.36427600	-1.01890500	8.24976500
C	-0.17023600	-1.86552600	7.16132800
N	0.01771200	-1.42487700	5.91892200
C	0.75985400	1.29058600	-0.45176700
C	0.99161100	1.05175000	-1.79817900
C	1.32022800	-0.23185800	-2.22586800
C	1.42792100	-1.27675200	-1.31136400
C	1.19753600	-1.02992500	0.03255000
S	1.56635900	-0.54679000	-3.95857300
O	2.32853500	-1.78920900	-4.07577500
N	0.08005100	-0.85372600	-4.63856600
O	2.06108400	0.68625200	-4.56888400
C	-0.52137200	-2.16484000	-4.35589000
C	-0.83470000	0.27837600	-4.81826100
C	-1.49911900	0.22488300	-6.18525000
C	-0.25837700	-3.15962000	-5.47494300
C	0.44709300	4.04725800	2.84431700
H	-0.15742400	1.88659400	6.51318600
H	-0.50947700	1.04708900	8.84920000
H	-0.51248700	-1.43117500	9.24122100
H	-0.16558900	-2.94369200	7.29460300
H	0.50897100	2.29040800	-0.12676700
H	0.93265500	1.86770400	-2.50924900
H	1.71433200	-2.26735100	-1.64456500
H	1.30314100	-1.85136500	0.73293800
H	-0.15233100	-2.57527200	-3.41149500
H	-1.59870800	-2.02103900	-4.23831200
H	-1.60017600	0.28219900	-4.03254500
H	-0.26705700	1.20630800	-4.75060700
H	-0.73127600	0.28601900	-6.96508100
H	-2.04975100	-0.71549700	-6.31239500
H	-0.61655400	-2.75128700	-6.42798300
H	0.81713600	-3.34403000	-5.55572600
H	-0.50581700	4.04124800	3.38140200
H	1.25607300	4.02285200	3.58057800
O	-2.38695100	1.33308800	-6.24548800
H	-2.81945900	1.34871200	-7.10739700
O	-0.96188200	-4.34932400	-5.13585100
H	-0.74140600	-5.04140800	-5.77016200
C	0.56433300	5.24767100	1.92163000
H	-0.25131700	5.22740300	1.19319600
H	1.50659500	5.18996900	1.36937200
C	0.51267000	6.53928900	2.71732000
H	1.34029000	6.61768600	3.42207100

H	-0.42788300	6.65048800	3.25655600
Cl	0.64105400	7.97666300	1.62858000

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C	0.41618800	0.51263500	1.85905300
C	-0.06722900	1.64408600	2.48992300
N	-0.22850700	1.57174100	3.83661500
C	0.12295500	0.39617600	4.28624500
S	0.67650900	-0.70311100	3.07928900
C	0.69376700	0.26892700	0.44473700
O	-0.37436500	2.77311900	1.83019000
C	0.06878700	0.00129800	5.70074900
C	-0.37603500	0.89240100	6.67744500
C	-0.40295800	0.46154500	7.99705500
C	0.01141700	-0.83207600	8.29304700
C	0.43807800	-1.64604700	7.24685100
N	0.46880800	-1.24587000	5.97720800
C	0.58984400	1.29464000	-0.51179700
C	0.86199800	1.05138500	-1.84973500
C	1.24300900	-0.22422600	-2.25765500
C	1.36167600	-1.25674100	-1.33052400
C	1.08843900	-1.00632200	0.00449700
S	1.54064800	-0.54600100	-3.98057100
O	2.33578800	-1.77006000	-4.06910600
N	0.08005100	-0.89508900	-4.69573000
O	2.02013700	0.69417300	-4.58895400
C	-0.49614700	-2.21780600	-4.41437400
C	-0.85677900	0.21267100	-4.90924100
C	-1.49029800	0.12623800	-6.28920600
C	-0.18277500	-3.21536900	-5.51789600
C	-0.88470800	3.87232200	2.59240800
H	-0.68805100	1.89037500	6.39552300
H	-0.74262600	1.12742600	8.78328900
H	0.00681500	-1.20847300	9.30951700
H	0.76914000	-2.66291500	7.43826600
H	0.30214900	2.28928000	-0.20194500
H	0.79708500	1.85986100	-2.56881400
H	1.68368900	-2.24168400	-1.64755900
H	1.18926400	-1.82275500	0.71138000
H	-0.13850700	-2.61100000	-3.45832200
H	-1.57908200	-2.09964600	-4.32224500
H	-1.63909600	0.20863300	-4.14022800
H	-0.31184300	1.15411700	-4.84164300
H	-0.70762300	0.19501800	-7.05351400
H	-2.01636300	-0.82821200	-6.41529800
H	-0.52914300	-2.82483000	-6.48273100
H	0.89875700	-3.37243400	-5.57215900
H	-1.06104000	4.66571300	1.86819800
H	-1.81813200	3.59783900	3.08774900
H	-0.15628200	4.19556300	3.33849100
O	-2.40201400	1.21246100	-6.38340500
H	-2.81785400	1.20477100	-7.25357600
O	-0.86331300	-4.41980400	-5.18411300
H	-0.60853700	-5.11203800	-5.80526200

6

0 1

C	0.55671100	0.51150300	1.87411900
C	0.31065400	1.69582000	2.53770600
N	0.09390500	1.62389200	3.87451000
C	0.16070500	0.38541000	4.28843300
S	0.49596900	-0.76932800	3.05281100
C	0.82944600	0.26317000	0.45782600
O	0.28099300	2.88759300	1.90794700
C	-0.02934100	-0.03188200	5.68432800
C	-0.29421900	0.90540800	6.68278500
C	-0.46458000	0.44966200	7.98315200
C	-0.36557100	-0.91328700	8.23863200
C	-0.09774400	-1.76904600	7.17317000
N	0.06801200	-1.34566500	5.92166600
C	0.78001100	1.29826300	-0.49277400
C	1.03829700	1.04436600	-1.83208700
C	1.35022500	-0.24764900	-2.24614200
C	1.41544400	-1.28796800	-1.32302300
C	1.15816500	-1.02848100	0.01385200
S	1.62333100	-0.57916000	-3.97484500
O	2.32866300	-1.85816800	-4.06417000
N	0.14893000	-0.80541900	-4.69535500
O	2.20818500	0.62510800	-4.56596300
C	-0.54104800	-2.07851600	-4.40383000
C	-0.70127100	0.37961700	-4.89867000
C	-1.49466100	0.28567900	-6.19444700
C	-0.38783100	-3.09782600	-5.52299800
C	0.06018300	4.03818100	2.69719400
H	-0.36148900	1.95693900	6.43268500
H	-0.67168600	1.14969100	8.78560800
H	-0.49153500	-1.31142900	9.23888800
H	-0.01294000	-2.84019200	7.33329000
H	0.54537900	2.30732100	-0.18281800
H	1.01331100	1.85769400	-2.54819200
H	1.68749000	-2.28628700	-1.64483800
H	1.22682200	-1.84940600	0.71955300
H	-0.17045700	-2.49803900	-3.46428400
H	-1.59504700	-1.83917000	-4.23763700
H	-1.37986000	0.50010900	-4.04309200
H	-0.04907600	1.25190600	-4.93818700
H	-0.82330100	0.19470300	-7.05191000
H	-2.17624800	-0.56907900	-6.19611500
H	-0.77293100	-2.70438600	-6.46701400
H	0.66443800	-3.35510500	-5.65921900
H	-0.89681700	3.98426300	3.22499100
H	0.84873100	4.16779500	3.44460500
H	-0.94070200	-4.00970200	-5.27726900
H	-2.09692900	1.18994500	-6.31766300
C	0.04863600	5.22975100	1.77103800
O	0.17060400	5.20018500	0.57053900
O	-0.12411600	6.35577400	2.47553900
H	-0.13399400	7.11057200	1.86307000

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0 1

C	0.55790900	0.50413500	1.89453300
C	0.28663000	1.68285100	2.55865600
N	0.09342800	1.60871200	3.89882600
C	0.20546700	0.37427200	4.31516500
S	0.55664700	-0.77387000	3.07803000
C	0.81562400	0.26005600	0.47505100
O	0.21194000	2.87096900	1.92657900
C	0.05065700	-0.04356400	5.71525700
C	-0.23113700	0.88836900	6.71406600
C	-0.36626000	0.43256400	8.01854600
C	-0.21688700	-0.92511800	8.27750300
C	0.06397600	-1.77576700	7.21127000
N	0.19635000	-1.35225500	5.95586200
C	0.73729400	1.29425400	-0.47470200
C	0.98409800	1.04517600	-1.81691000
C	1.31288200	-0.24177900	-2.23357600
C	1.40681600	-1.28181500	-1.31221100
C	1.16028500	-1.02636500	0.02707900
S	1.57677700	-0.56815300	-3.96181400
O	2.33335700	-1.81548400	-4.06294400
N	0.09625500	-0.87131300	-4.65575300
O	2.08509800	0.65824500	-4.57413600
C	-0.51562200	-2.17702000	-4.37082900
C	-0.80987000	0.26461900	-4.85450300
C	-1.45803400	0.20425600	-6.22903300
C	-0.24678200	-3.18069700	-5.48051000
C	-0.03910100	4.01608200	2.71503100
H	-0.33825600	1.93589400	6.46109000
H	-0.58516900	1.12848700	8.82143800
H	-0.31412400	-1.32310000	9.28101900
H	0.18776000	-2.84270100	7.37405700
H	0.48920600	2.29929700	-0.16230400
H	0.93804500	1.85801300	-2.53244400
H	1.69231400	-2.27565000	-1.63630100
H	1.24974600	-1.84630300	0.73146000
H	-0.15856700	-2.58331300	-3.42007500
H	-1.59326100	-2.02629400	-4.26529300
H	-1.58459600	0.27846500	-4.07805100
H	-0.23787600	1.18984300	-4.78660400
H	-0.68053000	0.25637900	-6.99991500
H	-2.01111900	-0.73470800	-6.35613900
H	-0.59292900	-2.77683800	-6.43987700
H	0.82847400	-3.37148800	-5.54900700
H	-0.99500000	3.93775900	3.24168400
H	0.74500000	4.16626900	3.46319100
C	-0.07902600	5.20625500	1.78795500
O	0.05800500	5.18006700	0.58909000
O	-0.29518600	6.32647400	2.48975100
O	-2.34029300	1.31563600	-6.30831100
H	-2.76141200	1.32706600	-7.17588900
O	-0.96028200	-4.36427400	-5.14077000
H	-0.73645300	-5.06207500	-5.76759000
H	-0.32040700	7.08049100	1.87675800

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C	0.87959300	0.14034900	0.50476400
C	1.01203800	-1.18538800	0.05984200
C	1.00944800	1.17386100	-0.43987100
C	1.26051200	-1.47749700	-1.27190200
H	0.92664400	-2.01008500	0.75933700
C	0.62773000	0.42455800	1.91852000
C	1.26010500	0.88671800	-1.77398200
H	0.92224200	2.20620100	-0.12965800
C	1.38209300	-0.43661900	-2.18843800
H	1.38066700	-2.50502000	-1.59418100
C	0.41875300	1.63024200	2.55897200
S	0.55192200	-0.82879400	3.12280200
H	1.38040600	1.69636200	-2.48461900
S	1.65939800	-0.80025800	-3.91059600
N	0.21165200	1.59020200	3.89821200
O	0.41367200	2.80568800	1.90330400
C	0.25421800	0.35864300	4.33541500
N	0.19673300	-0.78447000	-4.68583300
O	2.15460500	-2.17497300	-3.98733000
O	2.45074700	0.29806100	-4.46653200
C	0.19611200	3.98029200	2.66093300
C	0.06871200	-0.01690600	5.73976900
C	-0.44813800	0.52046400	-4.90908600
C	-0.69596300	-1.93628200	-4.44496400
C	0.23395100	5.15042800	1.70419900
H	0.96886200	4.10875900	3.42444900
H	-0.77469000	3.95361500	3.16458300
C	-0.16540500	0.94748200	6.72513500
N	0.13304900	-1.31712700	6.03875700
C	-1.19028800	0.55911700	-6.23765700
H	0.33265400	1.28075800	-4.91036700
H	-1.13611100	0.73970800	-4.08108700
C	-0.67084000	-2.94676800	-5.58248700
H	-0.42714000	-2.42681900	-3.50534600
H	-1.70357100	-1.53479900	-4.30478000
O	0.04608400	6.28514000	2.37748800
O	0.40633100	5.08134500	0.50965600
N	-0.33426000	0.61082200	8.00079900
H	-0.21410100	1.99920100	6.46551700
C	-0.03568000	-1.64966700	7.31404700
H	-1.99347200	-0.18134800	-6.27872400
H	-1.64140400	1.54587100	-6.37327000
H	-0.50472100	0.37212100	-7.06789600
H	-0.95936100	-2.48070200	-6.52788200
H	-1.36871100	-3.76326100	-5.37292100
H	0.33073600	-3.36641800	-5.69557600
C	0.05317800	7.49942200	1.60575200
C	-0.26926200	-0.68819200	8.29515400
H	0.01507400	-2.70400800	7.56698200
H	1.01507100	7.61976800	1.10603400
H	-0.74754700	7.47728700	0.86556500
H	-0.10961500	8.30009500	2.32336900
H	-0.40533300	-0.97474900	9.33304100

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C	0.58506600	0.50153400	1.90051400
C	0.47722700	1.68342000	2.60922100
N	0.24867800	1.57596500	3.94308800
C	0.16773100	0.32165100	4.30176200
S	0.36747700	-0.81209400	3.01947400
C	0.84245600	0.27789400	0.47754400
O	0.59531600	2.89220000	2.03352200
C	-0.07599700	-0.12060200	5.67778300
C	-0.23904100	0.79927600	6.71865500
C	-0.51659900	-0.91231300	8.18306500
C	-0.35521900	-1.82947900	7.14675600
N	-0.13509100	-1.43693800	5.89650300
C	0.72154600	1.31875500	-0.45861600
C	0.96294000	1.09444600	-1.80611300
C	1.32775100	-0.17677500	-2.24138900
C	1.46089800	-1.22361200	-1.33306600
C	1.22184100	-0.99187100	0.01260200
S	1.58481900	-0.47479300	-3.97929000
O	2.35499900	-1.71330200	-4.09580000
N	0.11166100	-0.77113900	-4.67492800
O	2.09360900	0.76576700	-4.56551100
C	-0.50324600	-2.08351900	-4.38923500
C	-0.80466600	0.36804000	-4.85071300
C	-1.61467500	0.24323300	-6.13345900
C	-0.30957800	-3.08081900	-5.52181200
C	0.56194400	4.04596900	2.88638100
H	-0.18865400	1.86478800	6.52391100
H	-0.69502900	-1.24776600	9.19966200
H	-0.40490100	-2.89747500	7.33429700
H	0.44222800	2.30920300	-0.12720700
H	0.88223700	1.91272900	-2.51238100
H	1.77503300	-2.20336500	-1.67320600
H	1.35121700	-1.81302300	0.70950800
H	-0.09805600	-2.49189700	-3.45903700
H	-1.56643800	-1.90412700	-4.20724700
H	-1.47335900	0.44291200	-3.98221900
H	-0.20128700	1.27467300	-4.89235300
H	-0.95446500	0.19794400	-7.00306400
H	-2.24739400	-0.64827300	-6.13258000
H	-0.73139200	-2.70047400	-6.45543600
H	0.75337200	-3.27617800	-5.67656000
H	-0.39650700	4.07914100	3.41243800
H	1.35964100	3.96660200	3.63104200
C	0.75135400	5.25517300	1.98791200
H	-0.05077400	5.28533400	1.24488700
H	1.70011500	5.16396900	1.45160700
C	0.74318200	6.53338000	2.80676200
H	1.55840200	6.56000600	3.52960000
H	-0.20243200	6.67862400	3.32884400
Cl	0.96150000	7.98215700	1.74816500
H	-0.80570800	-4.02519200	-5.27779600
H	-2.26827200	1.11369400	-6.23670100
N	-0.45867400	0.40272000	7.96907700

11c

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C	0.43650800	0.53505600	1.84423600
C	0.07616300	1.69493500	2.50705700
N	-0.11880700	1.59627600	3.84686600
C	0.08050500	0.37188100	4.25775000
S	0.52226600	-0.74392600	3.02160600
C	0.71911800	0.30769100	0.42714600
O	-0.07910900	2.87406200	1.88455500
C	-0.05513100	-0.05229300	5.65417000
C	-0.41766100	0.85430200	6.65566900
C	-0.30686100	-0.80864100	8.19613300
C	0.05441300	-1.71247900	7.19930900
N	0.18045300	-1.33766100	5.93066800
C	0.56994800	1.33171300	-0.52452800
C	0.84199800	1.10242300	-1.86541200
C	1.26690300	-0.15629300	-2.28132200
C	1.42943900	-1.18604100	-1.35815800
C	1.15855500	-0.95005400	-0.01977700
S	1.56583300	-0.46106000	-4.01066900
O	2.39516900	-1.66290300	-4.10206200
N	0.11979000	-0.83334100	-4.72830400
O	2.02538000	0.79602400	-4.60267900
C	-0.43204200	-2.17528300	-4.45077000
C	-0.85104700	0.25879400	-4.90986100
C	-1.65167500	0.09190400	-6.19373100
C	-0.20684300	-3.15019300	-5.59730400
C	-0.43091400	4.00815800	2.68555400
H	-0.60544800	1.89451500	6.41385400
H	-0.40582600	-1.12950100	9.22816900
H	0.24401500	-2.75520500	7.43392400
H	0.24598000	2.31355700	-0.20981700
H	0.74058200	1.90983900	-2.58146800
H	1.78755800	-2.15638200	-1.68122300
H	1.30448800	-1.76193500	0.68464200
H	0.00490500	-2.57586100	-3.53199100
H	-1.50017900	-2.04780500	-4.25320000
H	-1.52477800	0.30352600	-4.04311400
H	-0.29264400	1.19374500	-4.95285000
H	-2.34226300	0.93259900	-6.30267800
H	-0.98816700	0.07115400	-7.06175700
H	-2.24518900	-0.82607300	-6.18956600
H	-0.65714000	-4.11854600	-5.35834200
H	-0.65618600	-2.77985800	-6.52198800
H	0.86178000	-3.29678600	-5.76707600
H	-0.49459700	4.84197400	1.98875100
H	-1.39317600	3.84969900	3.17617800
H	0.33624100	4.20092000	3.43793000
N	-0.54310500	0.47547200	7.92438100

12a

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C	0.62057600	0.48844400	1.87983100
C	0.42711300	1.68114400	2.54896000
N	0.21890700	1.61097400	3.88675400
C	0.24004500	0.36827200	4.29299400
S	0.51838600	-0.79360200	3.05142300
C	0.87156400	0.23591000	0.46022900

O	0.44128900	2.87211600	1.92259900
C	0.04430800	-0.03923500	5.68707100
C	-0.18074600	0.90361600	6.69507700
C	-0.31209300	-0.76870600	8.22382100
C	-0.08826200	-1.70881500	7.21996900
N	0.08992400	-1.34719600	5.95394500
C	0.82223900	1.27224900	-0.48858200
C	1.05696900	1.01527700	-1.83164300
C	1.34524200	-0.28114600	-2.24833900
C	1.41235900	-1.32327600	-1.32696600
C	1.17769300	-1.06020100	0.01293200
S	1.59070500	-0.61697000	-3.97804300
O	2.32081600	-1.87976200	-4.08070400
N	0.09952800	-0.89096000	-4.66025500
O	2.11984000	0.59763500	-4.59583400
C	-0.53617600	-2.18467900	-4.37292000
C	-0.78511100	0.26274100	-4.85396100
C	-1.43966700	0.21726100	-6.22600200
C	-0.29526900	-3.19221300	-5.48550400
C	0.27170500	4.03286100	2.71349900
H	-0.21482600	1.96195100	6.46135500
H	-0.45556900	-1.07895700	9.25386700
H	-0.05312800	-2.76970100	7.44683400
H	0.60624200	2.28438400	-0.17508200
H	1.03280800	1.82843600	-2.54784300
H	1.66871900	-2.32490300	-1.65131300
H	1.24759900	-1.88154900	0.71796600
H	-0.18064800	-2.59941800	-3.42531300
H	-1.60981900	-2.01254000	-4.25971500
H	-1.55627900	0.29004800	-4.07437600
H	-0.19535600	1.17681800	-4.78673000
H	-0.66430900	0.25589300	-6.99983200
H	-2.01108900	-0.71074300	-6.35251000
H	-0.64111500	-2.78102800	-6.44183600
H	0.77550300	-3.40369000	-5.56261100
H	-0.68166800	4.01194900	3.24949500
H	1.07246100	4.12927100	3.45249200
C	0.29657900	5.22421000	1.78285800
O	0.40024000	5.17916100	0.57935300
O	0.18068300	6.34735100	2.49104300
C	0.17737300	7.57878600	1.74690400
H	0.07610200	8.36635900	2.48990000
H	-0.66331600	7.59422800	1.05225600
H	1.11297100	7.68624600	1.19686900
O	-2.30068800	1.34550400	-6.29963500
H	-2.72464000	1.36711300	-7.16564800
O	-1.02867900	-4.36204900	-5.14068500
H	-0.82503700	-5.06305500	-5.77083400
N	-0.35844500	0.53792100	7.96151700

12b

0 1

C	0.61692000	0.47669500	1.91266700
C	0.47468700	1.66258400	2.60946600
N	0.27143000	1.56315900	3.94794800
C	0.24485400	0.31122900	4.32261400

S	0.46846800	-0.83012600	3.05148600
C	0.85854700	0.24441500	0.48870100
O	0.53529800	2.86764600	2.01837100
C	0.04030900	-0.12288600	5.70761300
C	-0.14373600	0.80281100	6.73967800
C	-0.32917200	-0.89988900	8.22875100
C	-0.14698900	-1.82293900	7.20107100
N	0.03779000	-1.43769400	5.94291900
C	0.74833200	1.28360500	-0.45113000
C	0.97737900	1.05076900	-1.79914900
C	1.31878500	-0.22793900	-2.23102000
C	1.44207000	-1.27405600	-1.32010200
C	1.21480500	-1.03321400	0.02550400
S	1.56287500	-0.53564200	-3.96605600
O	2.33169300	-1.77333000	-4.08795000
N	0.07673600	-0.84825700	-4.64260400
O	2.04962600	0.70223800	-4.57257000
C	-0.51801400	-2.16262400	-4.36063700
C	-0.84329900	0.27977200	-4.82137500
C	-1.50916100	0.22340700	-6.18756000
C	-0.25199600	-3.15498800	-5.48112600
C	0.45181500	4.03105200	2.85489400
H	-0.13949900	1.86694100	6.53136600
H	-0.47815800	-1.22941800	9.25200500
H	-0.15081800	-2.88961500	7.40212500
H	0.48718700	2.27962000	-0.12252300
H	0.90625200	1.86785400	-2.50777300
H	1.73826100	-2.26034900	-1.65741500
H	1.33328900	-1.85513100	0.72332800
H	-0.14554400	-2.57230700	-3.41722500
H	-1.59580000	-2.02396400	-4.24114000
H	-1.60789000	0.28006300	-4.03480200
H	-0.27965700	1.21017500	-4.75436800
H	-0.74266600	0.28839300	-6.96839800
H	-2.05555100	-0.71949900	-6.31425800
H	-0.61440900	-2.74786600	-6.43306100
H	0.82433100	-3.33352100	-5.56436700
H	-0.49953700	4.02086900	3.39458900
H	1.26330600	4.00588800	3.58829600
O	-2.40222500	1.32743400	-6.24610800
H	-2.83531300	1.34198300	-7.10775100
O	-0.94833100	-4.34867000	-5.14136800
H	-0.72823200	-5.03808200	-5.77872600
C	0.56350300	5.23377600	1.93471300
H	-0.25436500	5.21326600	1.20880000
H	1.50422600	5.17946500	1.37953400
C	0.51128900	6.52361200	2.73340500
H	1.34075200	6.60243600	3.43590100
H	-0.42793300	6.63169900	3.27553800
Cl	0.63344500	7.96298700	1.64677400
N	-0.32778400	0.41358000	7.99814500

12c

0 1

C	0.42774900	0.57507400	1.83707900
C	0.13261100	1.73686300	2.52720800

N	-0.05566700	1.61829600	3.86632300
C	0.08107900	0.37563700	4.24769000
S	0.45244800	-0.73383100	2.98267100
C	0.69001200	0.36922000	0.41311400
O	0.03726400	2.93512300	1.92996800
C	-0.07093700	-0.07338900	5.63468000
C	-0.38155700	0.82710400	6.65888900
C	-0.35568100	-0.87582000	8.15896200
C	-0.04600200	-1.77355800	7.13953300
N	0.09667700	-1.37568700	5.87972400
C	0.41242400	1.37101300	-0.53270700
C	0.65602000	1.16209000	-1.88206700
C	1.18138400	-0.05448900	-2.30905700
C	1.47587400	-1.06017100	-1.39165300
C	1.23151700	-0.84360300	-0.04489600
S	1.44423000	-0.33817400	-4.04534500
O	2.40318400	-1.43471500	-4.17171600
N	0.01885800	-0.89751900	-4.69376700
O	1.71181400	0.95616900	-4.67027600
C	-0.34181600	-2.29235100	-4.40147800
C	-1.07954400	0.06060600	-4.85562400
C	-1.75240000	-0.11072300	-6.20858400
C	0.05239600	-3.22651900	-5.53429400
C	-0.21337100	4.07415900	2.76116100
H	-0.51445400	1.88129000	6.44255400
H	-0.46918000	-1.21555700	9.18343000
H	0.08801200	-2.83027000	7.34848100
H	0.00769600	2.31905500	-0.20705100
H	0.45239000	1.95137100	-2.59643700
H	1.91640700	-1.99257600	-1.72458100
H	1.48345300	-1.63023100	0.65814500
H	0.12393400	-2.63525700	-3.47335700
H	-1.42332600	-2.33525700	-4.24736100
H	-1.81936400	-0.06399500	-4.05524000
H	-0.67790400	1.07223500	-4.79862700
H	-1.02419300	0.08239100	-7.00480000
H	-2.13171800	-1.13340700	-6.32499300
H	-0.40788800	-2.89252500	-6.47233100
H	1.13992300	-3.21508300	-5.65478000
H	-0.23771000	4.92449800	2.08209100
H	-1.17052600	3.97252200	3.27611600
H	0.58555200	4.19836700	3.49488100
O	-2.82204800	0.82420400	-6.24798100
H	-3.27654400	0.75288700	-7.09565600
O	-0.41329500	-4.52210000	-5.17431600
H	-0.09957600	-5.16454100	-5.82149500
N	-0.52331200	0.42527600	7.91879400

13

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C	0.56716000	0.50232500	1.87218600
C	0.32041800	1.68502900	2.54064100
N	0.10553500	1.60645300	3.87664700
C	0.17433400	0.36556100	4.28320300
S	0.50913100	-0.78310900	3.04320100
C	0.83775700	0.25961500	0.45398300

O	0.28865100	2.87756300	1.91510600
C	-0.01580600	-0.05027000	5.67554600
C	-0.28157400	0.88271600	6.68279300
C	-0.36599800	-0.79528500	8.20862400
C	-0.10056100	-1.72550400	7.20568200
N	0.07450000	-1.35612600	5.94145100
C	0.77380200	1.29679700	-0.49297000
C	1.02882000	1.04862700	-1.83409500
C	1.35159900	-0.23919700	-2.25230200
C	1.43158000	-1.28120700	-1.33236200
C	1.17781700	-1.02752300	0.00629400
S	1.62029500	-0.56414200	-3.98362100
O	2.33631300	-1.83668400	-4.07815800
N	0.14482700	-0.80115700	-4.69720200
O	2.19217500	0.64681100	-4.57338300
C	-0.53275300	-2.08127000	-4.40719500
C	-0.71624500	0.37687700	-4.89591500
C	-1.51289600	0.27816000	-6.18929900
C	-0.37398100	-3.09603600	-5.52969700
C	0.06734800	4.02651000	2.70773300
H	-0.35095400	1.93954900	6.45010200
H	-0.50686700	-1.11183000	9.23711000
H	-0.02915400	-2.78472100	7.43180300
H	0.53054900	2.30270400	-0.17949300
H	0.99264800	1.86337200	-2.54806700
H	1.71237100	-2.27581800	-1.65804500
H	1.25866300	-1.84940900	0.70963800
H	-0.15551100	-2.50001200	-3.46993400
H	-1.58827200	-1.85165900	-4.23711600
H	-1.39307000	0.48989100	-4.03794800
H	-0.07169800	1.25480200	-4.93597000
H	-0.84349900	0.19430100	-7.04900100
H	-2.18711500	-0.58241900	-6.19015600
H	-0.76585800	-2.70358000	-6.47131100
H	0.68012300	-3.34332400	-5.67011700
H	-0.88743300	3.96818400	3.23899200
H	0.85886400	4.15683000	3.45180400
H	-0.91769800	-4.01355600	-5.28460400
H	-2.12325500	1.17742600	-6.30912200
C	0.04805700	5.21901400	1.78274400
O	0.16232800	5.18973100	0.58150700
O	-0.12215800	6.34370000	2.48927100
H	-0.13787200	7.09938400	1.87797500
N	-0.45639100	0.50924100	7.94734700

14

0 1

C	0.57380600	0.49181300	1.89377600
C	0.29645900	1.66847200	2.56126000
N	0.10603400	1.58870000	3.90080800
C	0.22653300	0.35308600	4.31146100
S	0.58250500	-0.78898200	3.07149300
C	0.82930900	0.25241800	0.47252000
O	0.21385400	2.85605100	1.93185400
C	0.07414300	-0.06205900	5.70867800
C	-0.21727300	0.86495700	6.71428800

C	-0.20737200	-0.80543900	8.25064300
C	0.08336600	-1.72973300	7.24919800
N	0.22424600	-1.36115300	5.98050000
C	0.74071400	1.28871000	-0.47358900
C	0.98418400	1.04430700	-1.81738700
C	1.31937600	-0.23951100	-2.23802500
C	1.42384400	-1.28124800	-1.31988100
C	1.18094400	-1.03056200	0.02097800
S	1.57819300	-0.56051400	-3.96872500
O	2.33792500	-1.80535500	-4.07484700
N	0.09593100	-0.86574600	-4.65687700
O	2.08099000	0.66905400	-4.57885000
C	-0.51209500	-2.17325000	-4.37172200
C	-0.81318100	0.26839700	-4.85272400
C	-1.46552100	0.20711400	-6.22525500
C	-0.24482600	-3.17511100	-5.48343300
C	-0.04400600	3.99927600	2.72195800
H	-0.33579400	1.91628100	6.47655700
H	-0.31966800	-1.12129300	9.28284900
H	0.20344800	-2.78346100	7.48029100
H	0.48721800	2.29138400	-0.15796800
H	0.93025800	1.85853700	-2.53075200
H	1.71446700	-2.27233000	-1.64773900
H	1.27872600	-1.85176400	0.72281700
H	-0.15105300	-2.57987800	-3.42259900
H	-1.58967400	-2.02490500	-4.26242800
H	-1.58552400	0.28030100	-4.07389000
H	-0.24288600	1.19477300	-4.78636100
H	-0.69057600	0.26108400	-6.99857400
H	-2.01717200	-0.73288100	-6.35095100
H	-0.59533100	-2.77109000	-6.44112700
H	0.83059700	-3.36344200	-5.55600600
H	-0.99839200	3.91330700	3.25008400
H	0.74079600	4.15427300	3.46831600
C	-0.09442200	5.18895500	1.79461300
O	0.03847100	5.16216200	0.59532700
O	-0.31486900	6.30768200	2.49674500
O	-2.35018600	1.31675400	-6.30109900
H	-2.77338300	1.32845600	-7.16766900
O	-0.95446000	-4.36053900	-5.14217800
H	-0.73262900	-5.05682600	-5.77139800
H	-0.34731100	7.06167400	1.88402700
N	-0.35767500	0.49230500	7.98337200

Additional LB-Isotherms

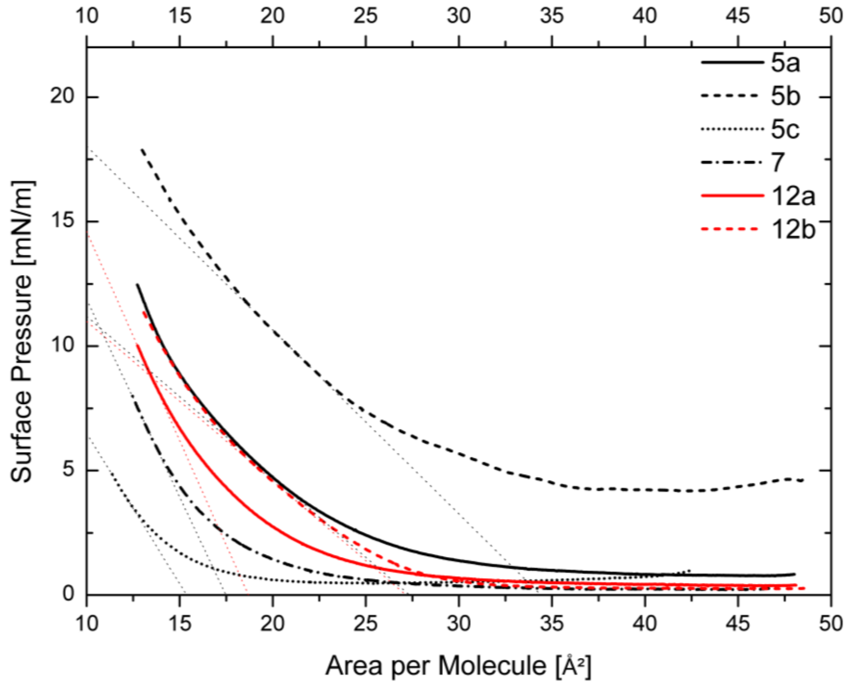


Figure S24: LB-isotherms of **5a-c**, **7** and **11a,b**, recorded with a constant barrier speed of 5 mm/min. For the measurement a volume of 50µL was spread on the trough. Linear regions oft he isotherms were fitted.

Table S1: Intercepts, slopes and R^2 of the linear fits of the linear regions of the LB isotherms.

entry	Intercept	Slope	R^2
4a	33.95361	-0.68471	0.99935
4b	131.6928	-1.66538	0.99736
4c	44.04455	-1.04634	0.99951
5a	17.6523	-0.6453	0.99908
5b	25.4158	-0.7385	0.99963
5c	18.5776	-1.2070	0.99841
7	27.7370	-1-5861	0.9986
11a	27.15814	-0.42522	0.99927
11b	155.3652	-2.79578	0.99836
11c	129.5949	-3.19589	0.99917
12a	31.4011	-1.6794	0.9993
12b	17.3941	-0.6404	0.9995

Technical Details of Generation of Potential Distribution on van-der-Walls Surfaces

Distributions of the electrostatic potential on a van-der-Walls surface due to the electron cloud as well as the nuclear charges can readily be visualized using Gaussian09 and GaussView by post-processing results from single-point calculations. However, we decided to use our own implementation based on Python and various modules [1, 2], the Computational Geometry Algorithms Library (CGAL) [3], the Simplified Wrapper and Interface Generator (SWIG) [4] and a self-written interface. We decided in favor of our own implementation mainly due to the high level of control this offers over all data structures, allowing for further post-processing, and the possibility to use input data from arbitrary sources. These include, among others, Gaussian CUBE-files, APBS Data Explorer “DX” files and force field calculations, the latter of which are especially useful for quick estimates because of the low computational effort involved in force field computations compared to complex quantum chemistry. Furthermore, potential distributions over arbitrary surfaces at arbitrary degrees of discretization can be drawn and computed thanks to the many different surface reconstruction algorithms and refinement techniques included in the CGAL such as skin-surface [5] and convex-hull generation [6]. It may be notable that these surfaces are not sampled on a grid but rather discretizations of the exact surfaces.

Figure S25 shows a direct comparison between the aforementioned plots obtained using both, the MMFF94 force field and DFT at the CAM-B3LYP 6-31+g(d,p) level of theory. The force field approach, as it is limited to charges centred at the nuclear positions, clearly shows some deviations from the data obtained from DFT. These are most prominent for the pyrazinyl moieties. However, given the highly different nature of both approaches, the results agree reasonably well.

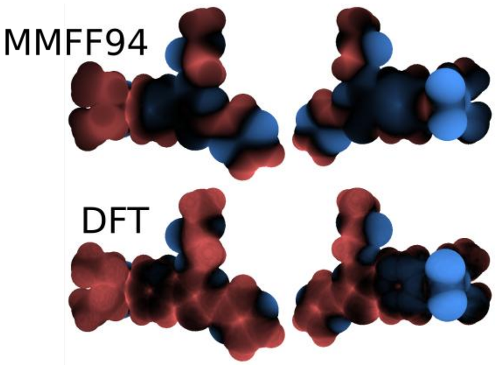


Figure S25: Plots of the electrostatic potential on the van-der-Waals surface of molecule **11a** obtained using the MMFF94 force field by portioning partial charges for each atom (top) or using DFT at the CAM-B3LYP 6-31+g(d,p) level of theory by interpolation of the electrostatic potential on a grid as obtained from the DFT calculations (bottom). Interpolation of the DFT data has been performed by means of simple inverse distance weighting of the potential data. The circular visual artefacts visible in the bottom two figures result from the sparse potential grid being of cubic structure whereas the plotted surface is rather “round”.

In our implementation, Python is mainly used to “glue-together” the various external libraries. As a first step, geometry data is read in using Openbabel because it supports a multitude of different chemical file formats (at least 130 as of June 2015) and has built-in support for different force fields which can be used to partition charges. As a second step, if so desired, external charge distribution data from e.g. Gaussian09 is read in instead of partitioning partial charges using the force field.

Next, we need to generate the surface on which the potential distribution shall be visualized. This process will be explained for the generation of a skin surface as an example. Van-der-Waals radii and nuclear coordinates, i.e., the properties defining the surface, are read from the openbabel data structures and transformed into simple Python lists. We used SWIG to generate a well-defined interface that transforms these lists into C++ std::vector containers. The wrapper function these containers are passed to wraps all CGAL data structures and functions that generate the skin surface and returns a list of vertices in the form of std::vector containers that can easily be transformed back to Python lists. Before returning, the surface can be manipulated as desired, including an arbitrary number of refinements to reduce or increase the mean facet size.

As a last step before visualization, the electrostatic potential at each discretization point is computed as a sum over potential contributions from point charges which are either partial charges at the nuclear positions or by interpolation of the electrostatic potential on a grid as obtained from DFT calculations. Finally, the resulting meshed surface can be visualized using OpenGL with shaders being applied to obtain linear color gradients between adjacent vertices.

In the future, the here described approach might be used to automatically estimate a molecule's most likely orientation at an interface by assuming that polar and non-polar moieties favor being in a polar and non-polar solvent, respectively.

^{1}H NMR spectra

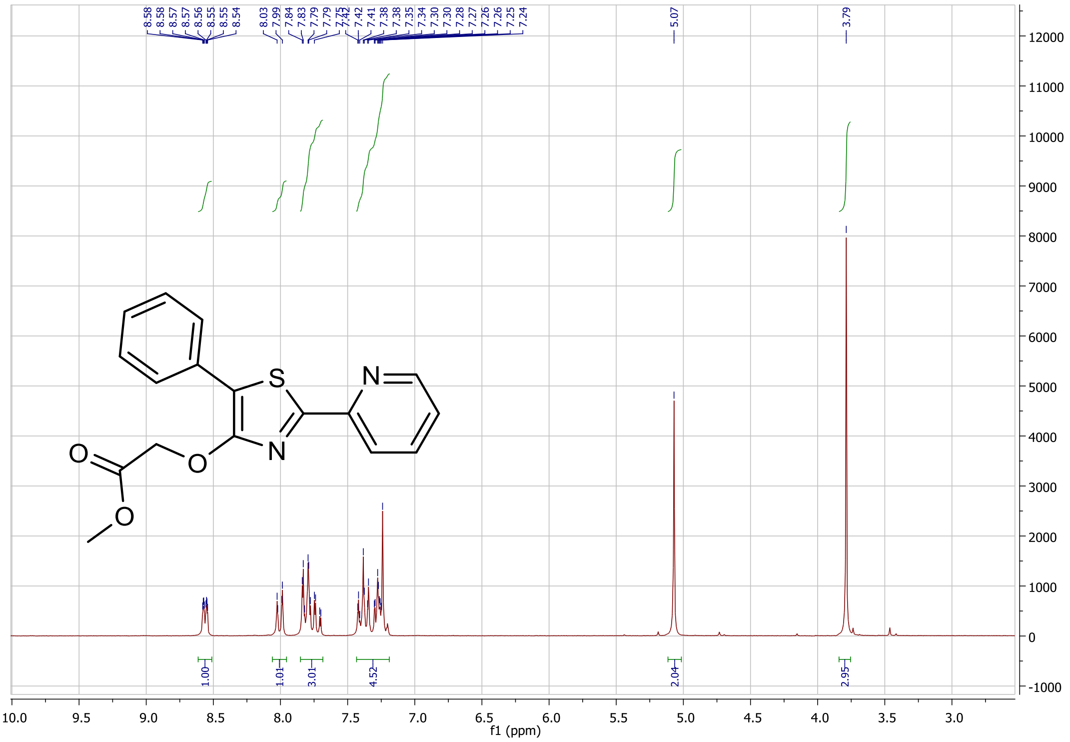


Figure S26: ^{1}H NMR spectrum of **2a** (200 MHz, $CDCl_3$).

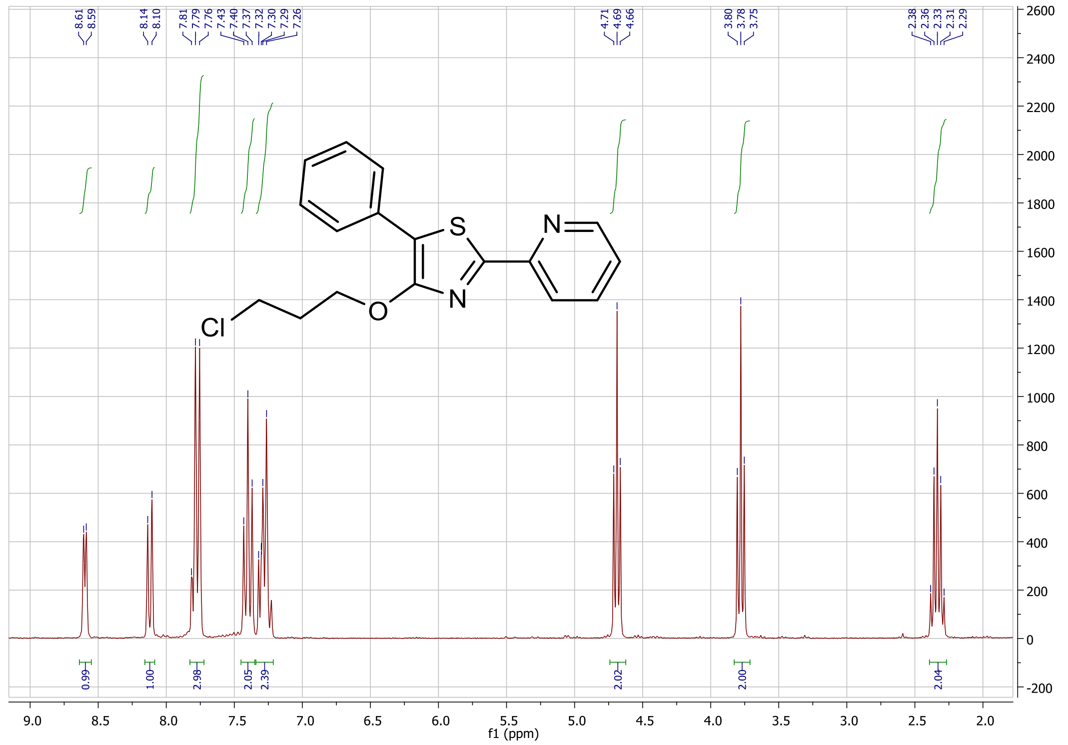


Figure S27: ^{1}H NMR spectrum of **2b** (250 MHz, $CDCl_3$).

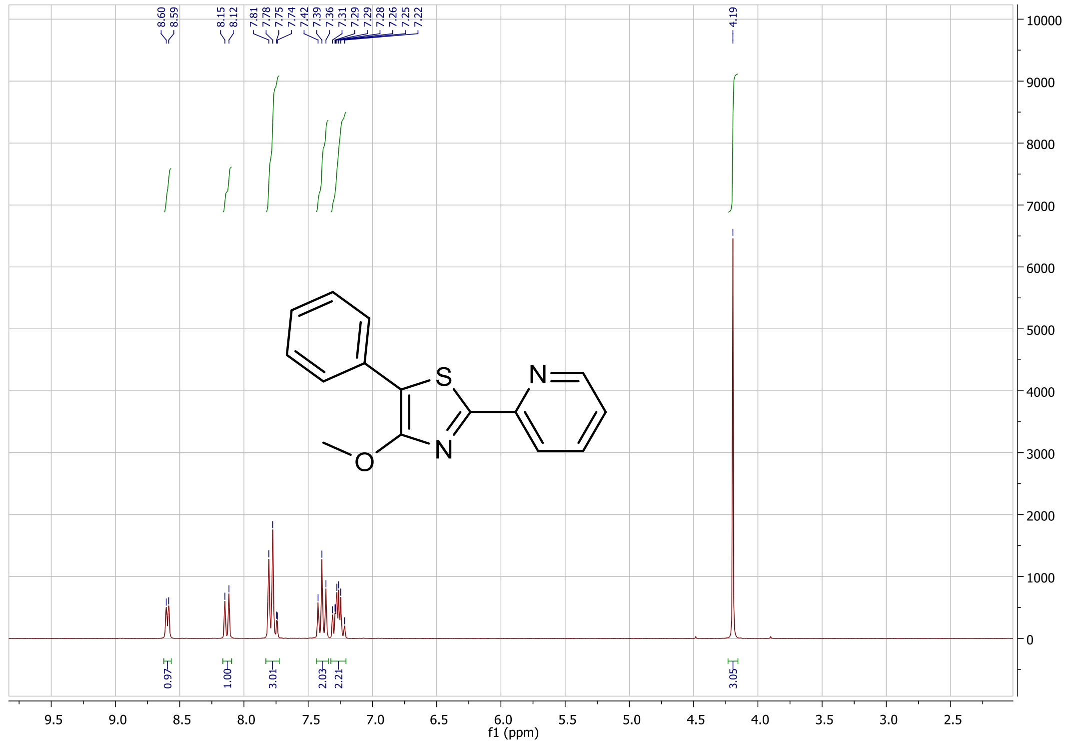
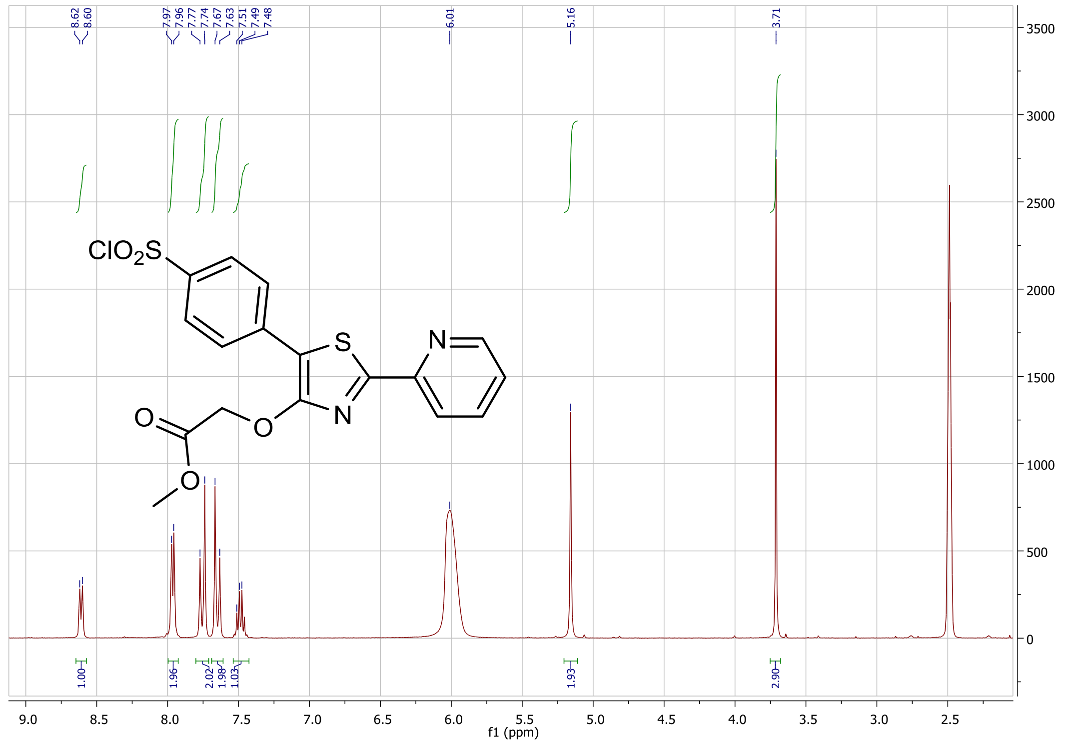


Figure S28: [1]H NMR spectrum of **2c** (250 MHz, $CDCl_3$).



FigureS 29: 1H NMR spectrum of **3a** (250 MHz, DMSO-d_6)

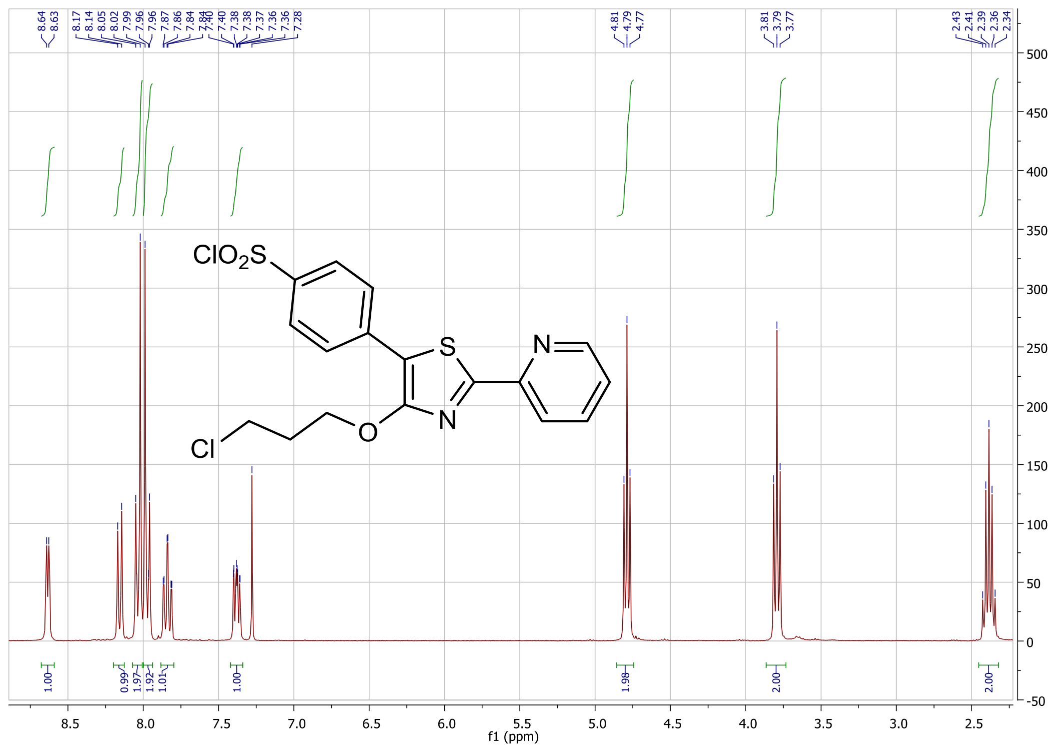


Figure S30: ^{1}H NMR spectrum of **3b** (300 MHz, $CDCl_3$).

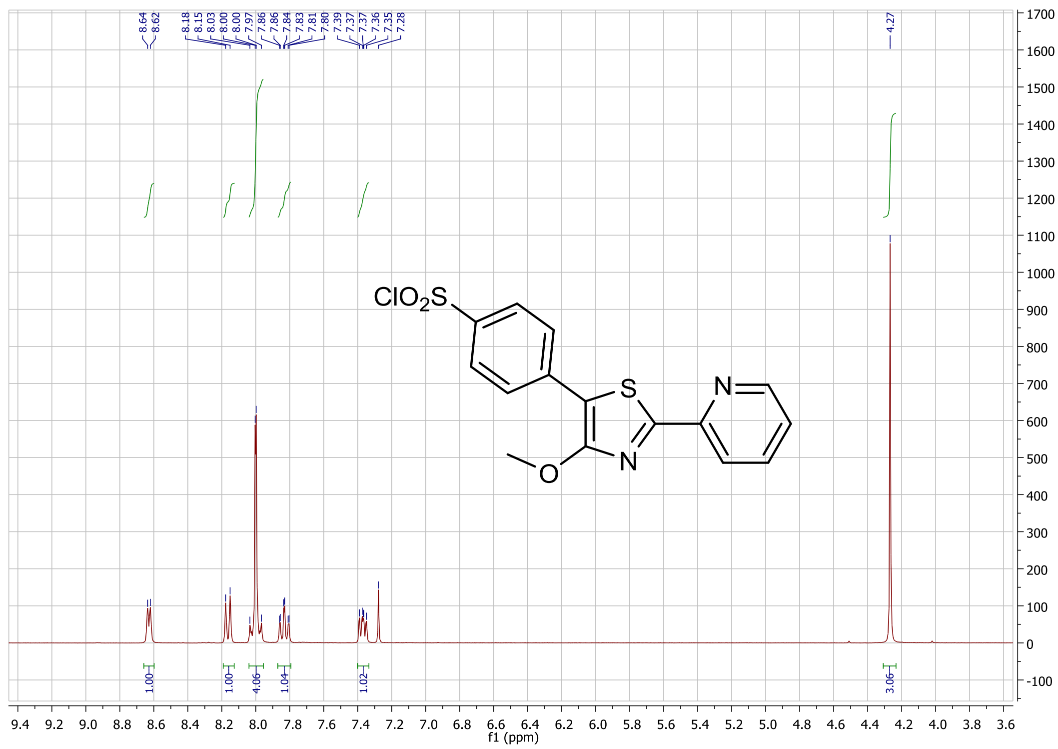


Figure S31: ^{1}H NMR spectrum of **3c** (300 MHz, $CDCl_3$).

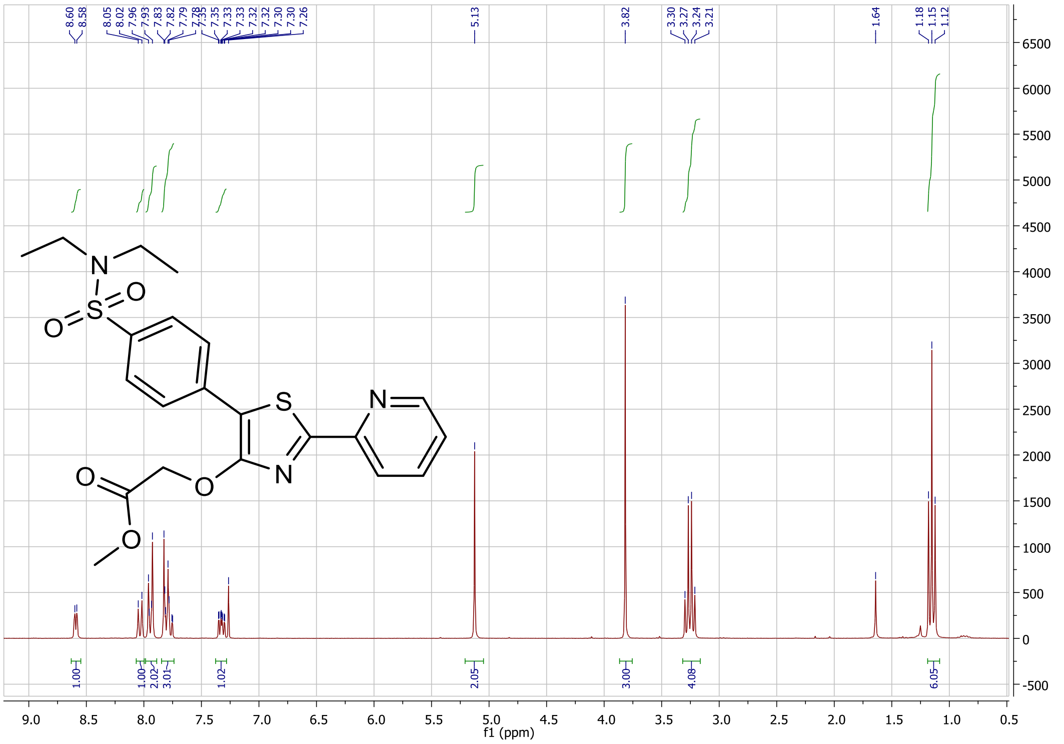


Figure S32: ^{1}H NMR spectrum of **4a** (250 MHz, $CDCl_3$).

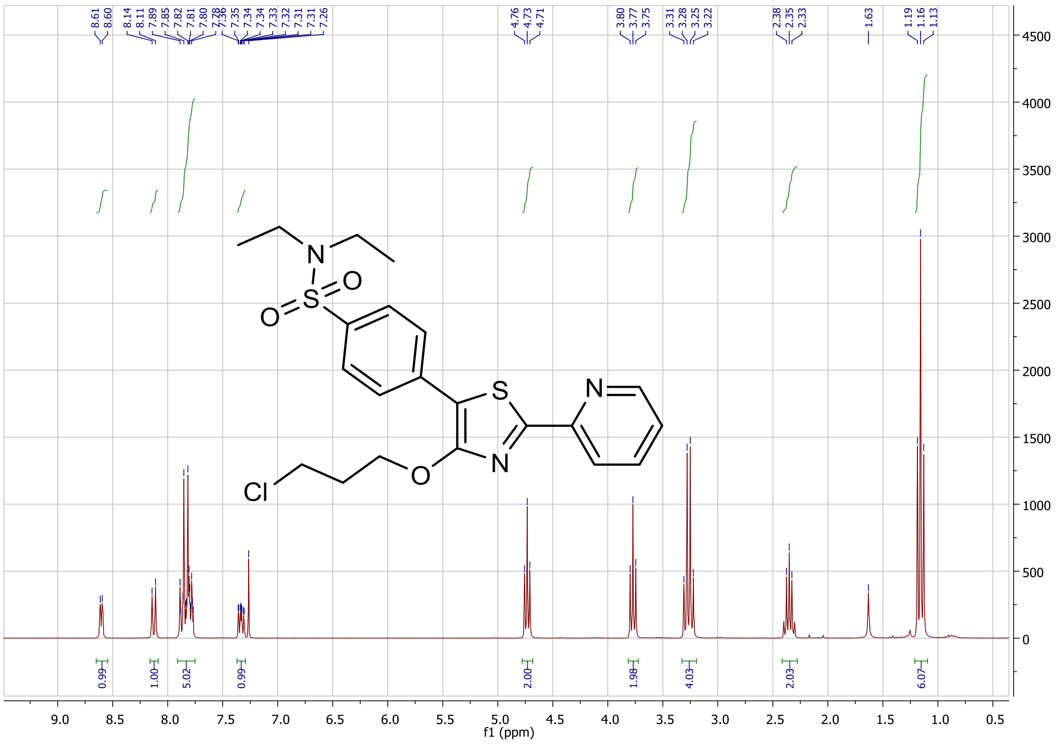


Figure S33: ^{1}H NMR spectrum of **4b** (250 MHz, $CDCl_3$).

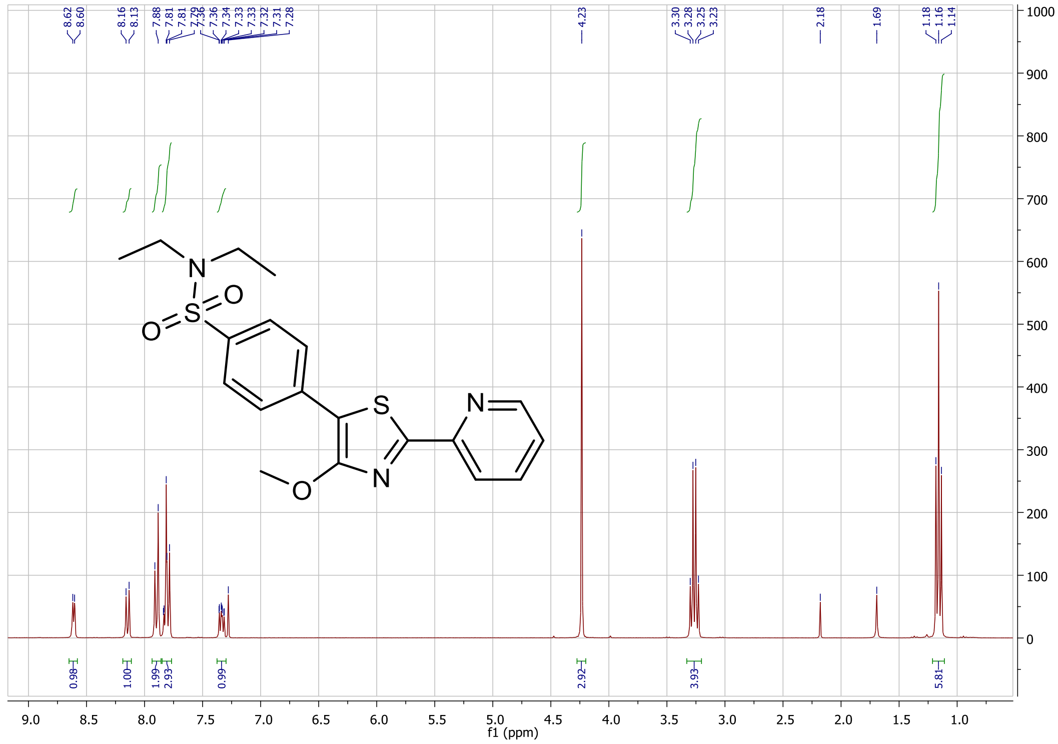


Figure S34: ^{1}H NMR spectrum of **4c** (300 MHz, $CDCl_3$).

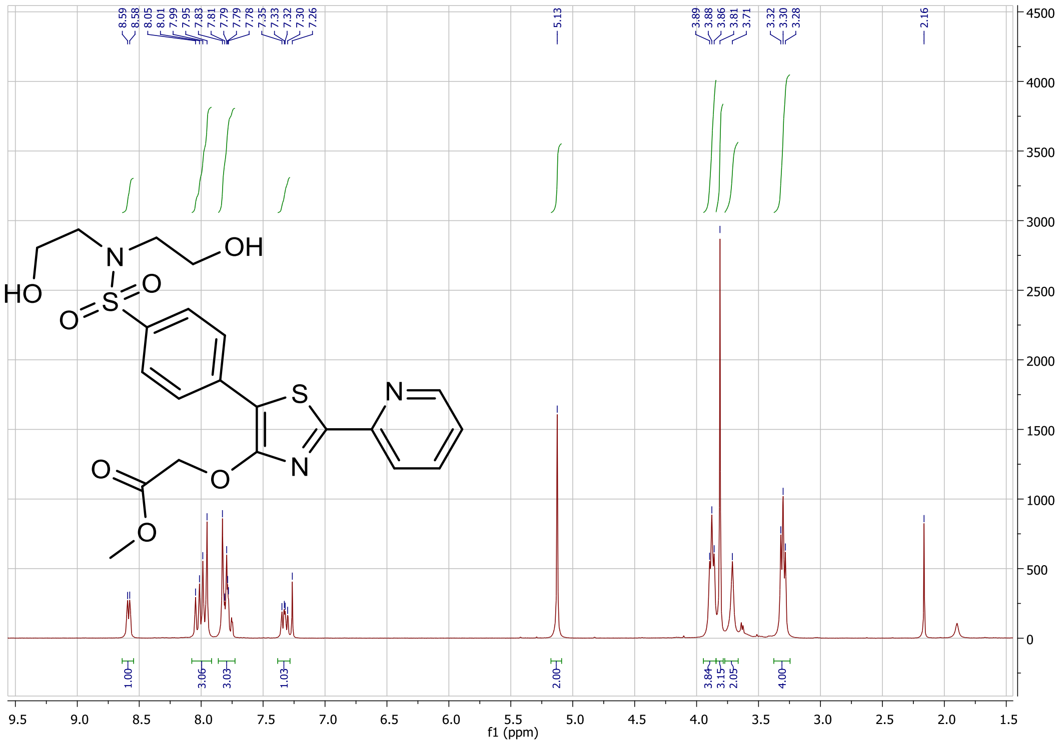


Figure S35: ^{1}H NMR spectrum of **5a** (250 MHz, $CDCl_3$).

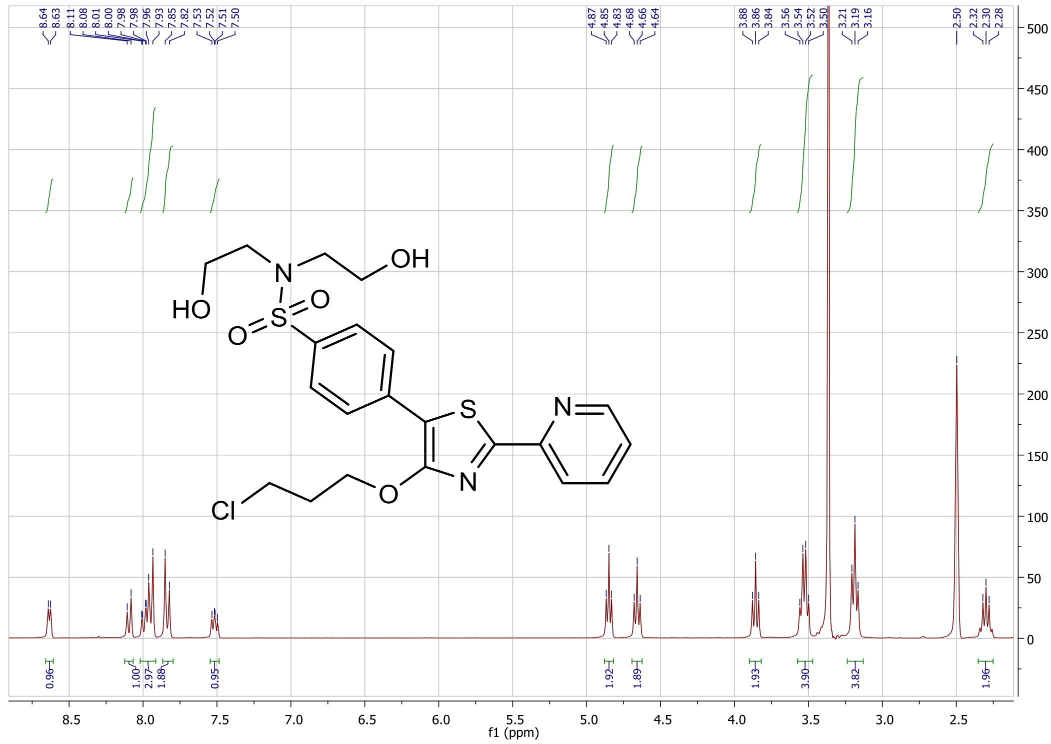


Figure S36: ^{1}H NMR spectrum of **5b** (300 MHz, DMSO-d_6).

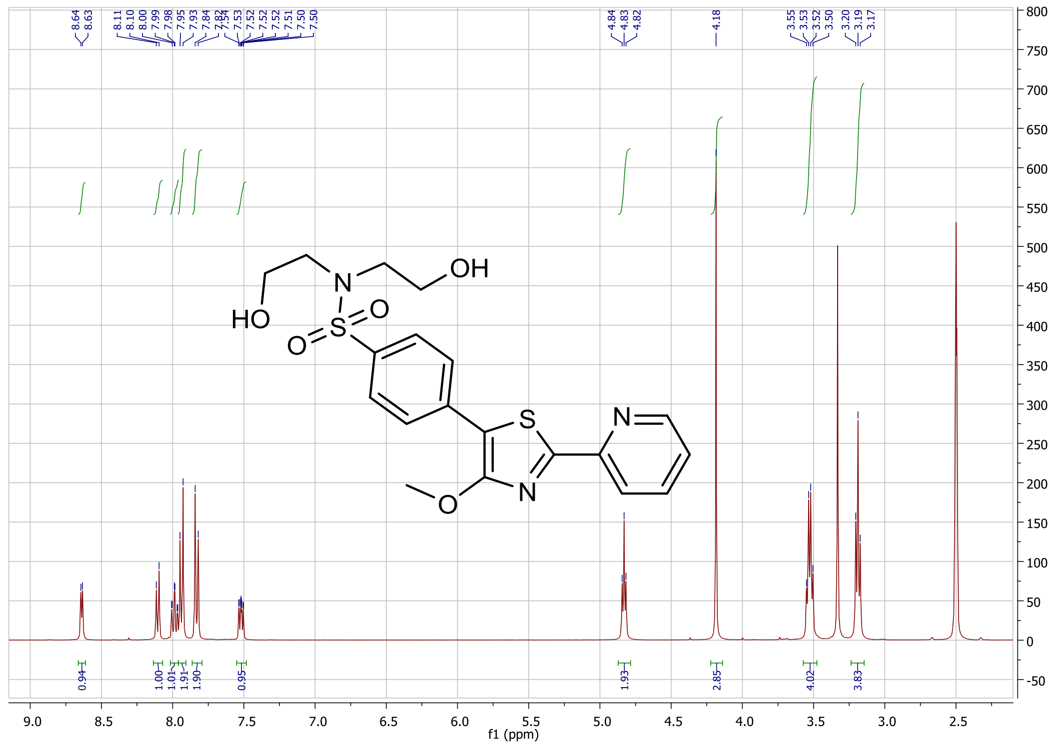


Figure S37: ^{1}H NMR spectrum of **5c** (400 MHz, DMSO-d_6).

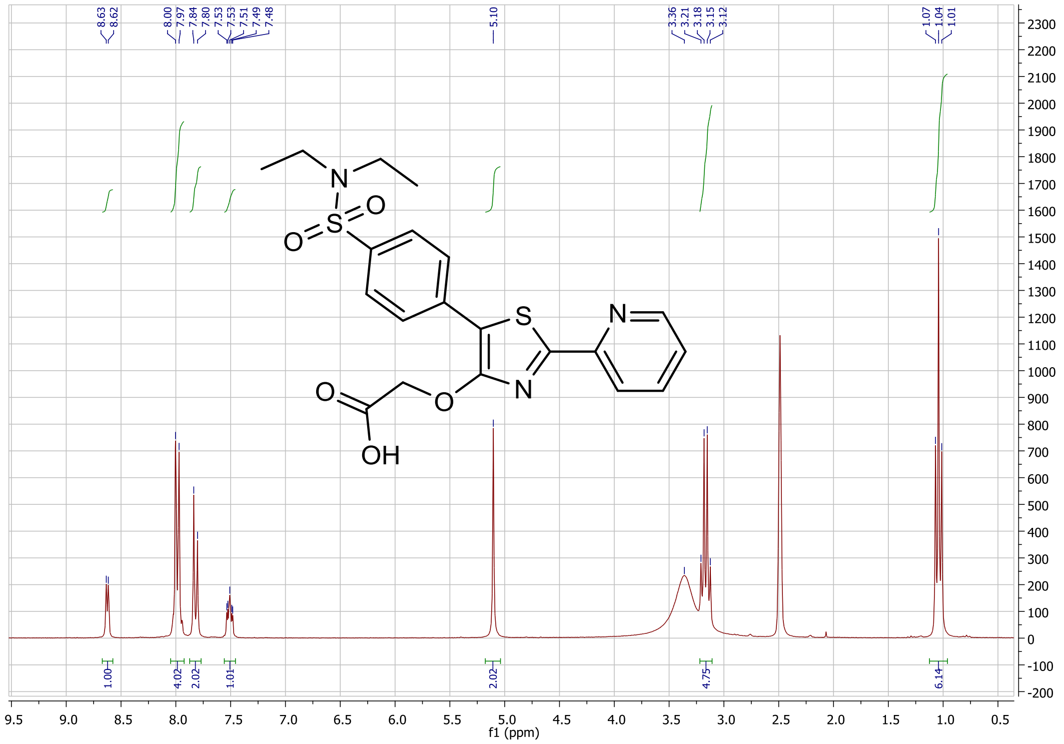


Figure S38: ^{1}H NMR spectrum of **6** (250 MHz, DMSO-d_6).

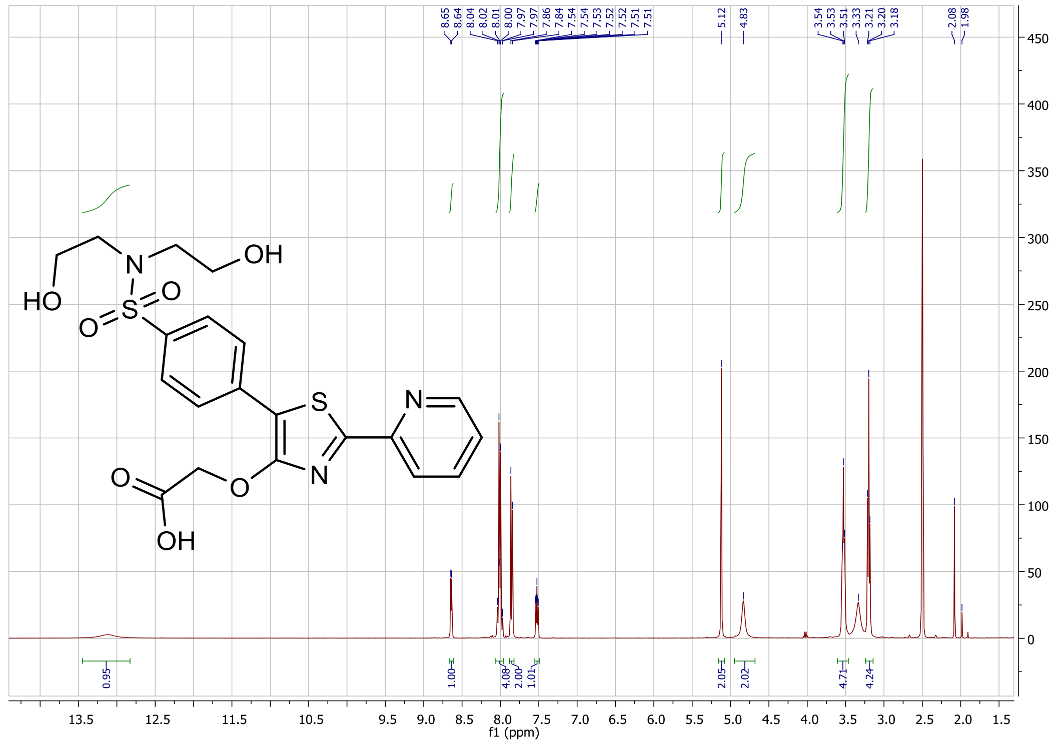


Figure S39: ^{1}H NMR spectrum of **7** (400 MHz, DMSO-d_6).

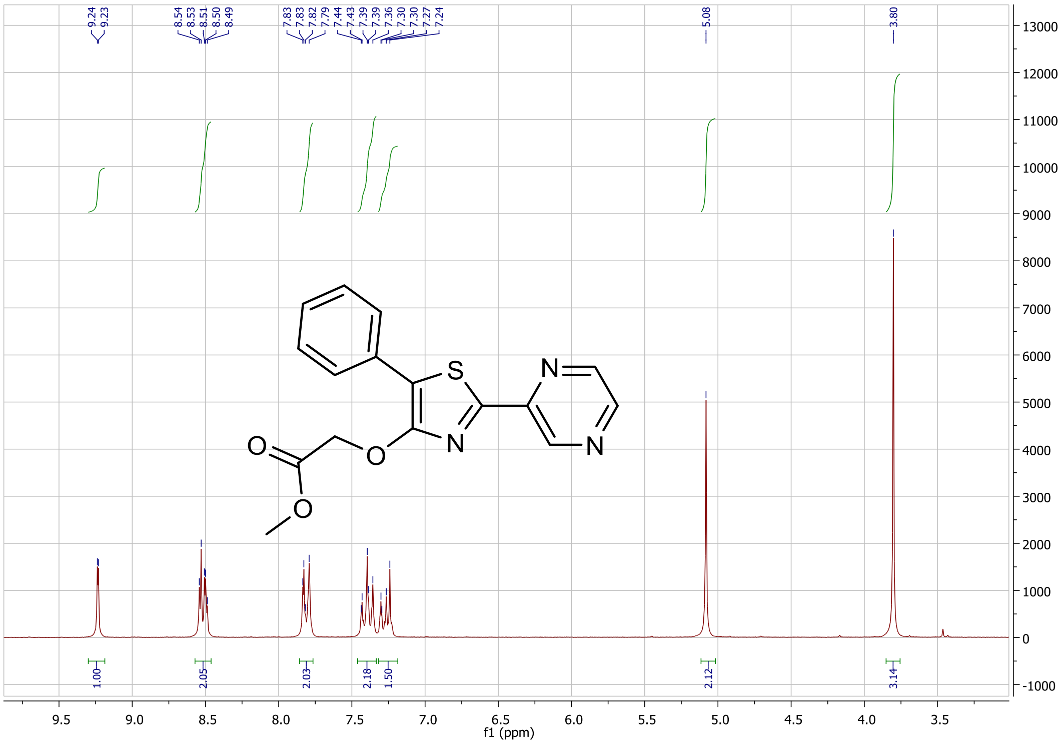


Figure S40: ^{1}H NMR spectrum of **9a** (250 MHz, $CDCl_3$).

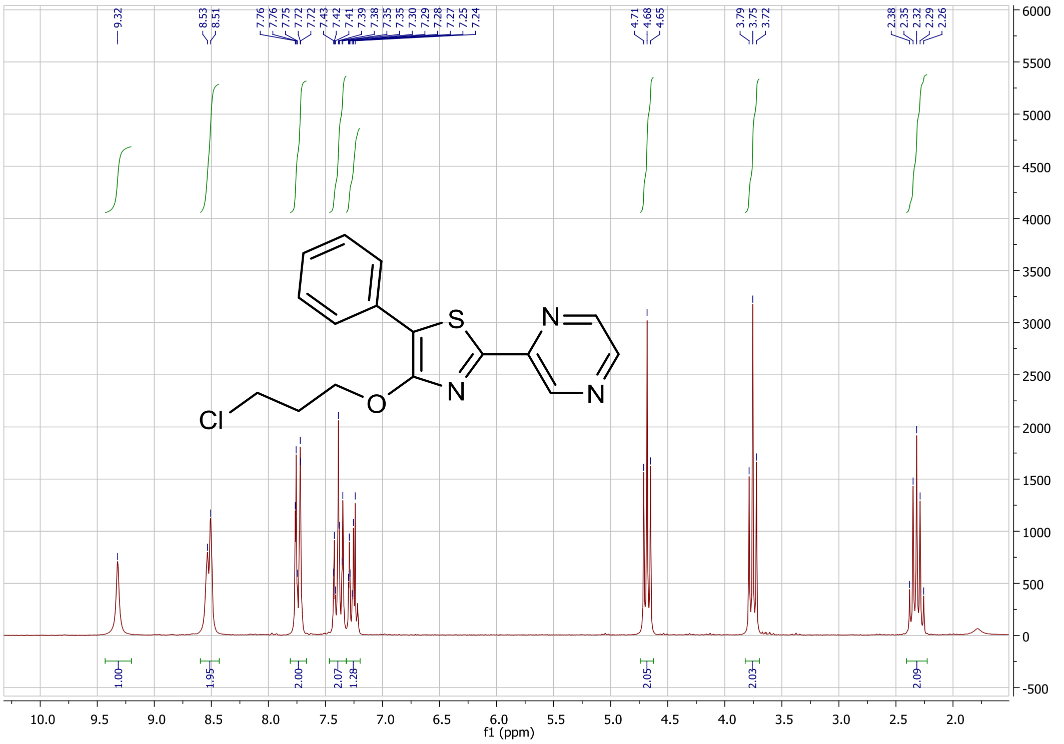


Figure S41: ^{1}H NMR spectrum of **9b** (200 MHz, $CDCl_3$).

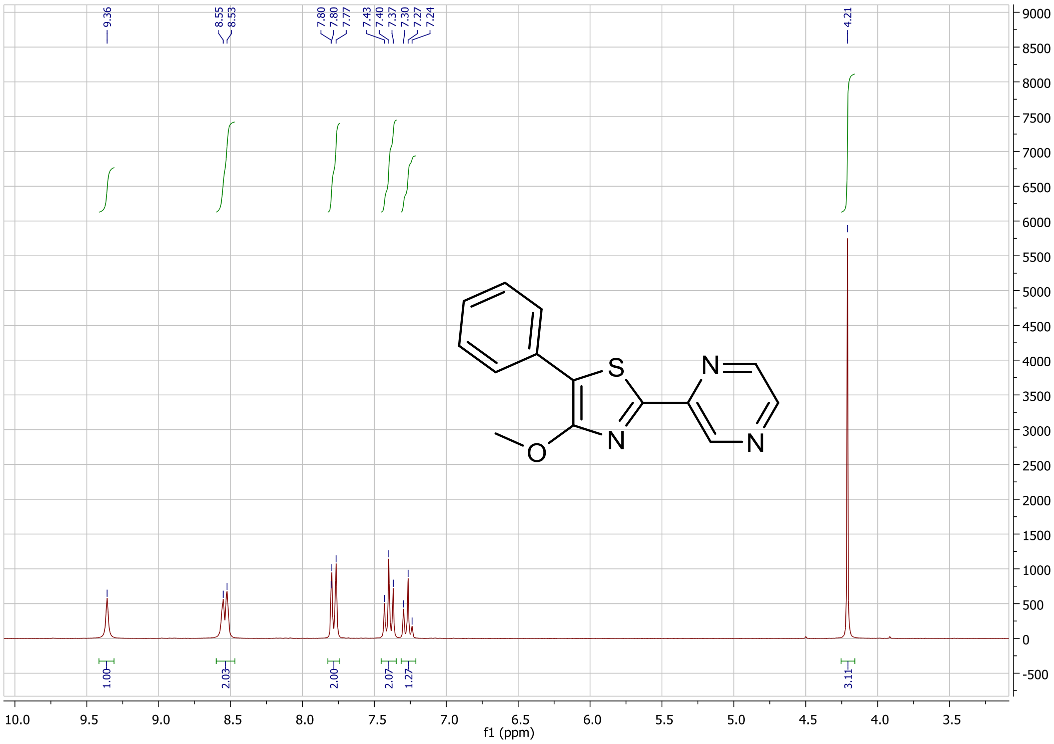


Figure S42: ^{1}H NMR spectrum of **9c** (250 MHz, $CDCl_3$).

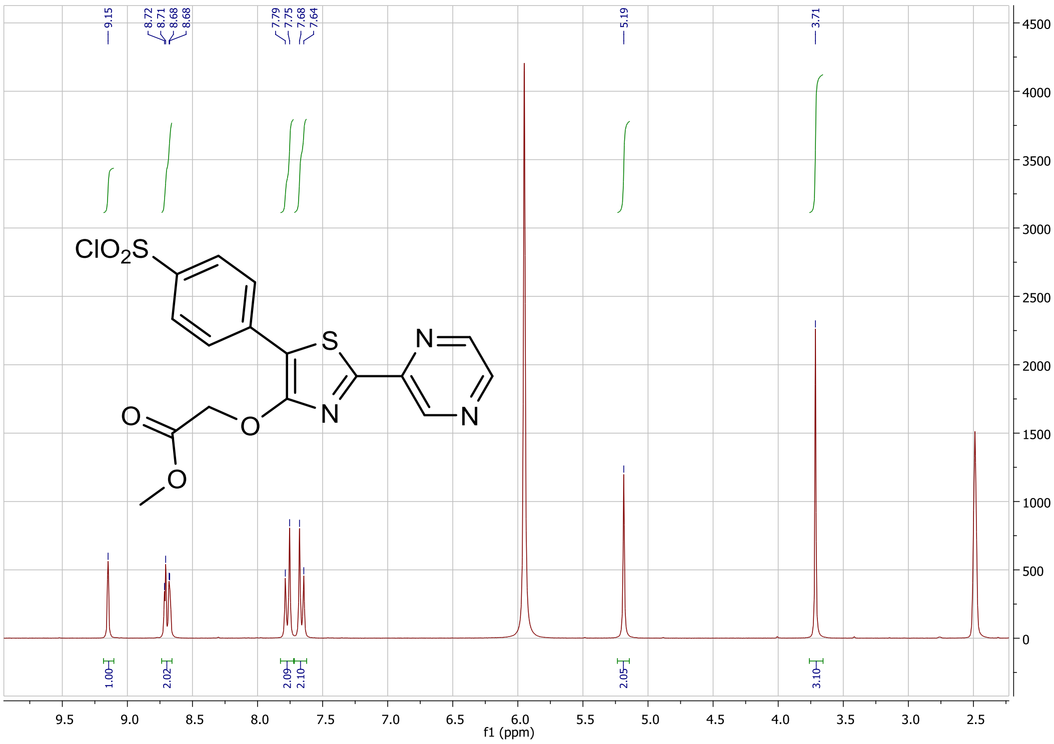


Figure S43: ^{1}H NMR spectrum of **10a** (250 MHz, DMSO-d_6).

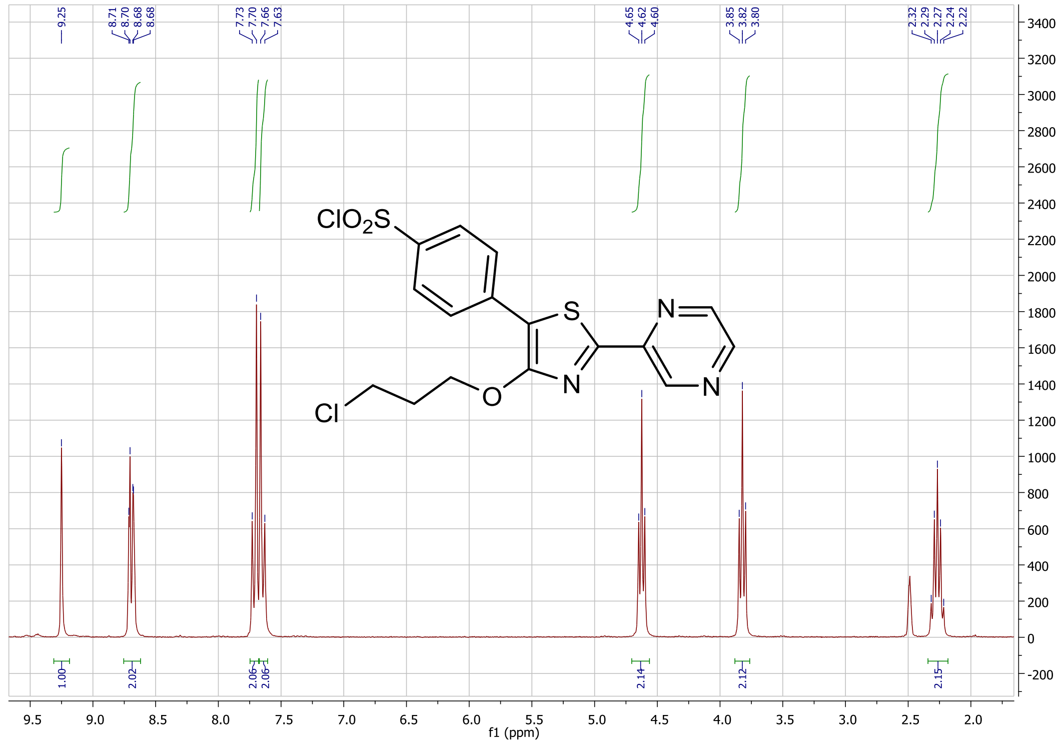


Figure S44: ^{1}H NMR spectrum of **10b** (250 MHz, DMSO-d_6).

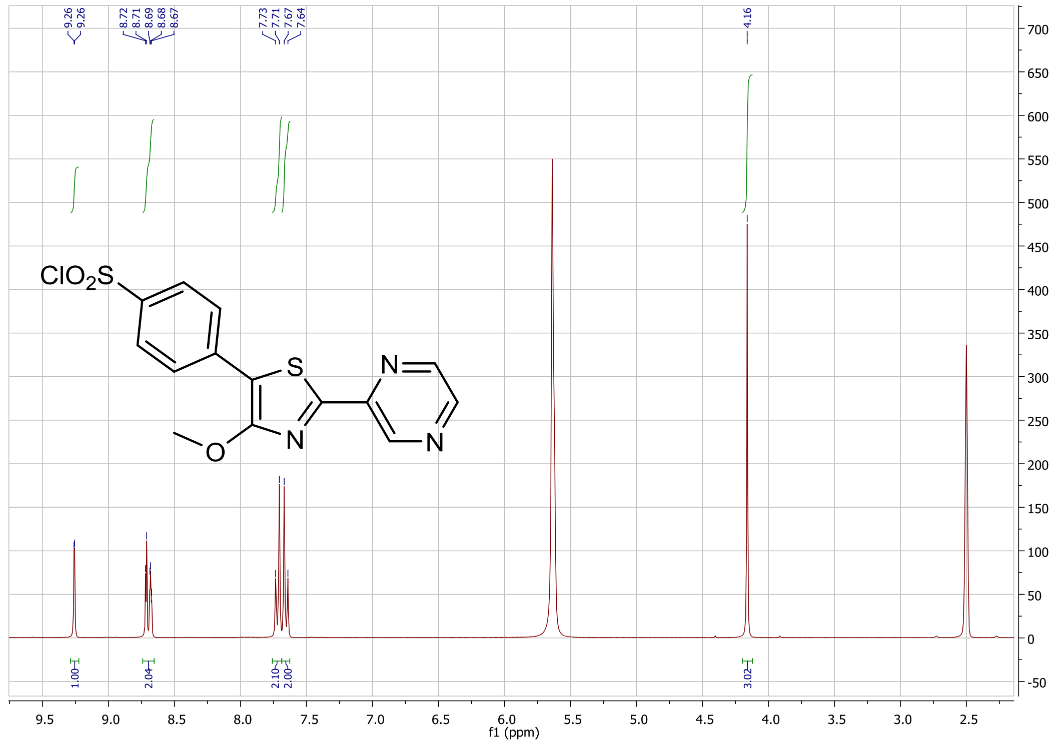


Figure S45: ^{1}H NMR spectrum of **10c** (250 MHz, $CDCl_3$).

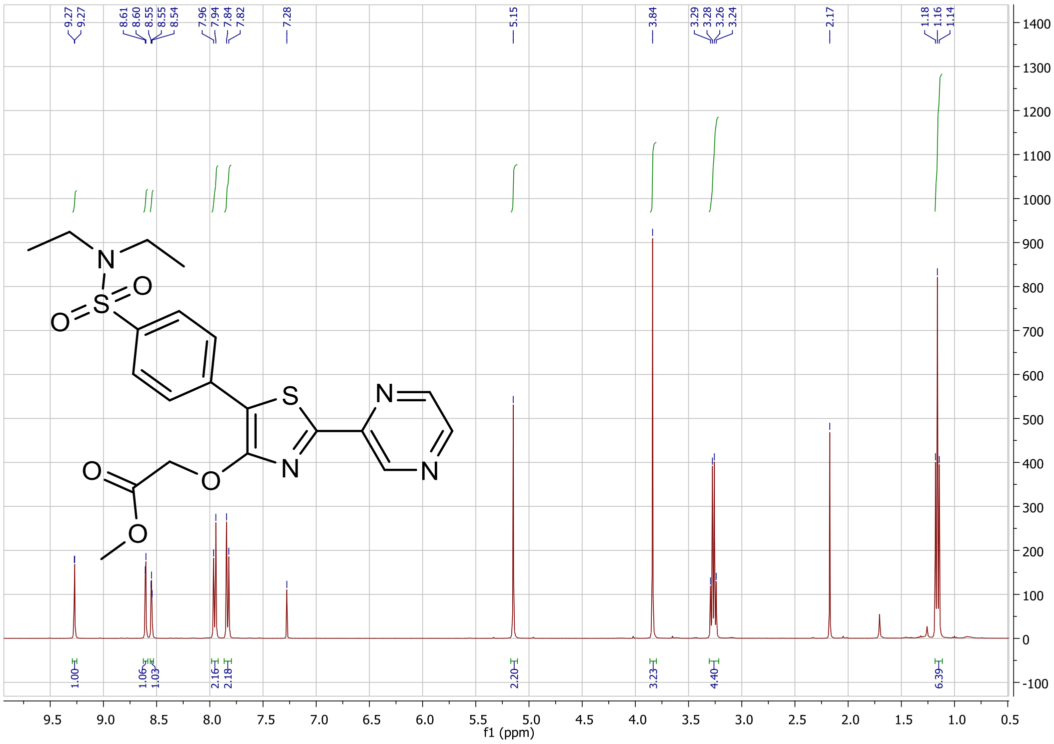


Figure S46: ^{1}H NMR spectrum of **11a** (400 MHz, $CDCl_3$).

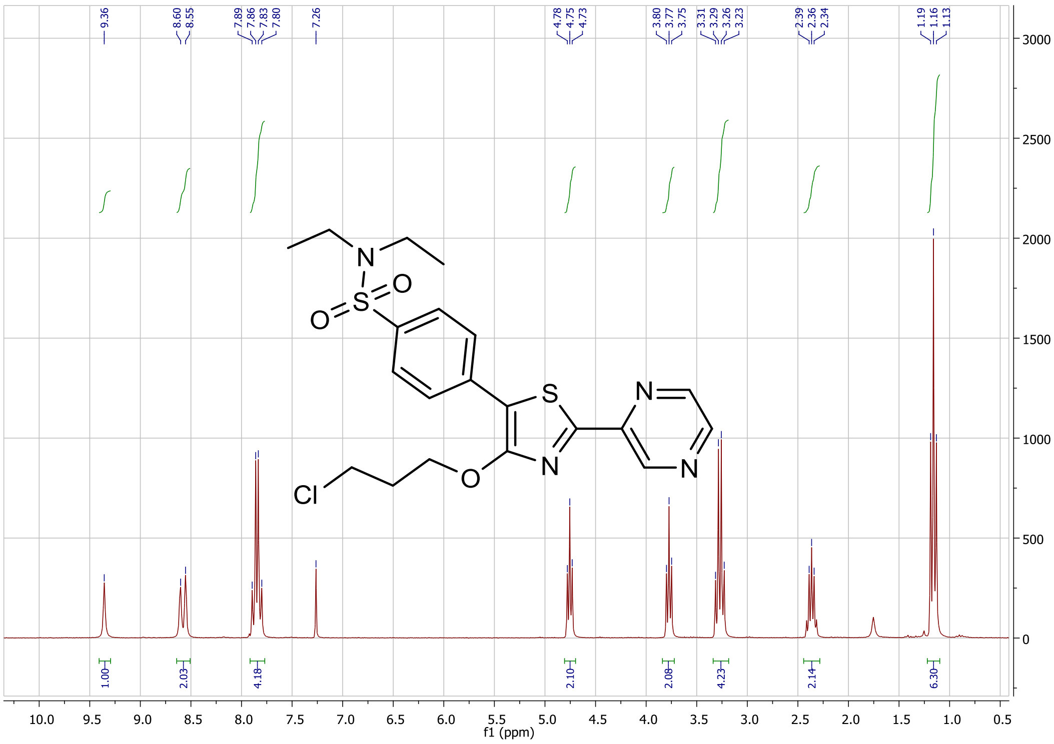


Figure S47: ^{1}H NMR spectrum of **11b** (250 MHz, $CDCl_3$).

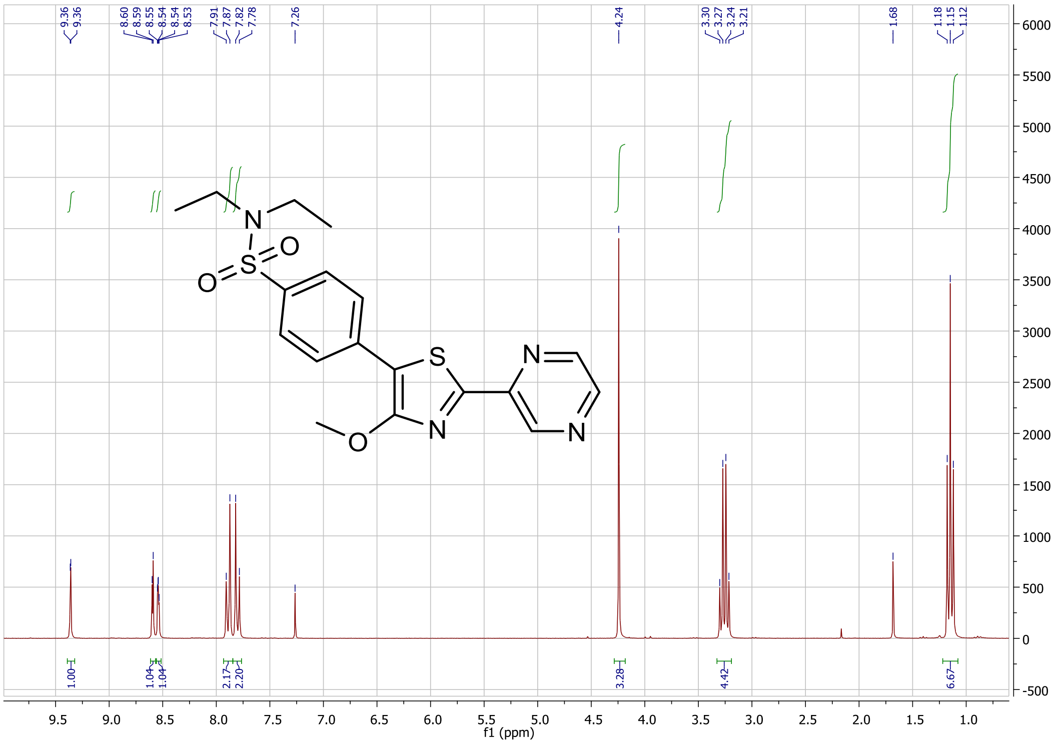


Figure S48: ^{1}H NMR spectrum of **11c** (250 MHz, $CDCl_3$).

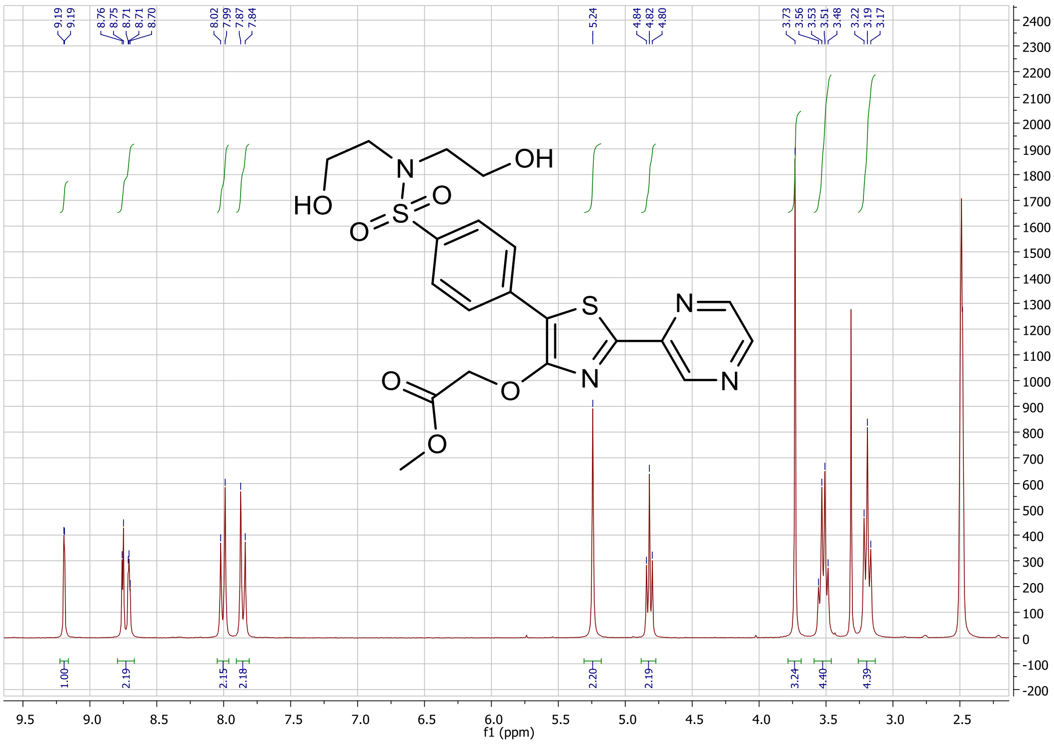


Figure S49: ^{1}H NMR spectrum of **12a** (250 MHz, DMSO-d_6).

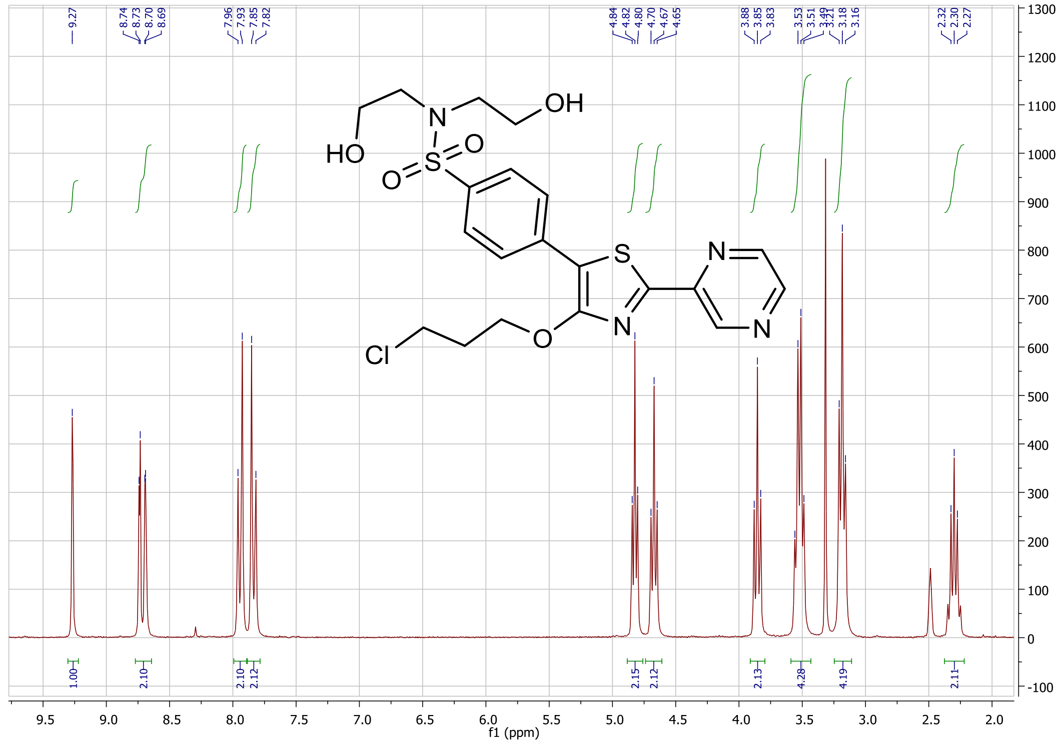


Figure S50: ^{1}H NMR spectrum of **12b** (250 MHz, DMSO-d_6).

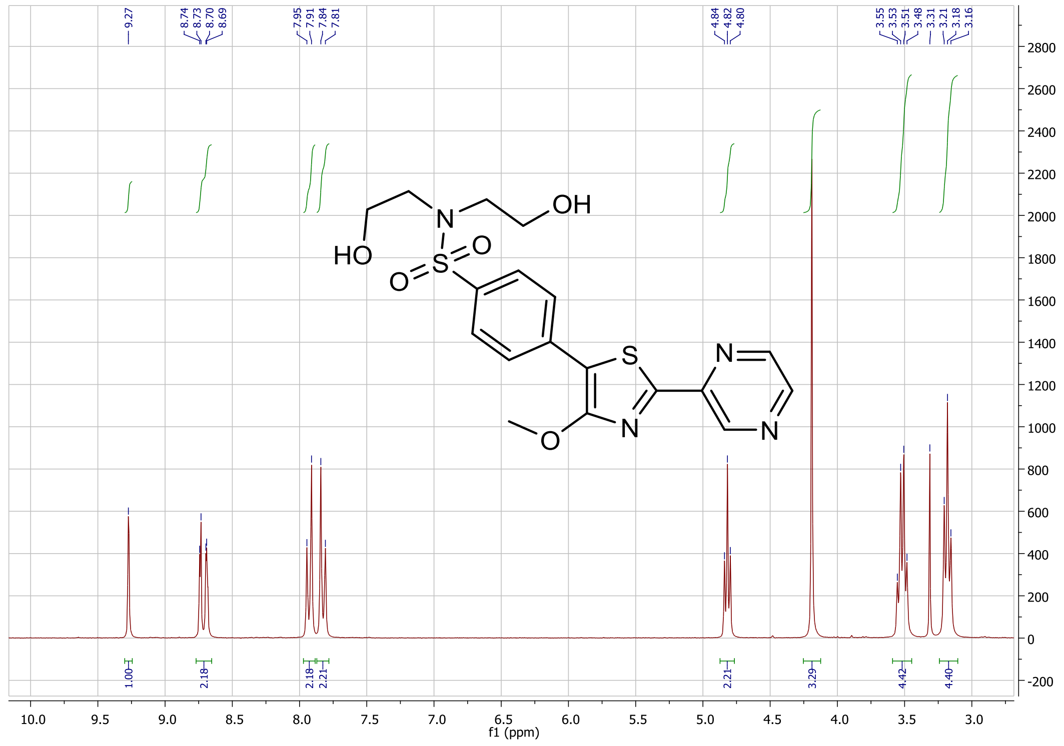


Figure S51: ^{1}H NMR spectrum of **12c** (250 MHz, $CDCl_3$).

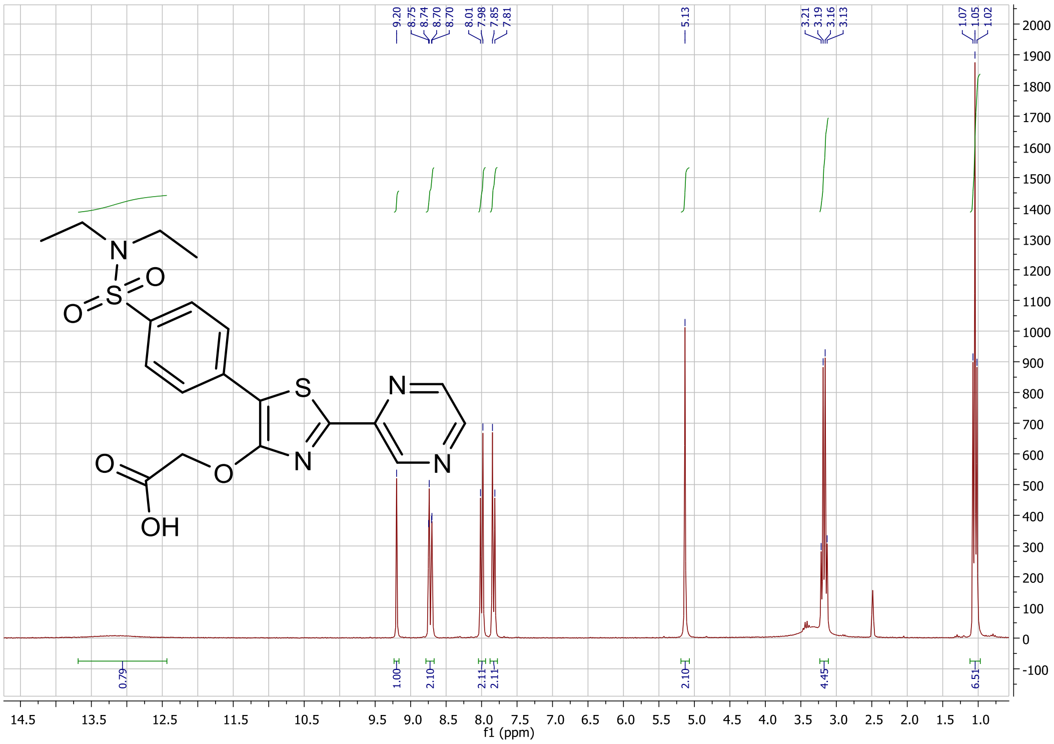


Figure S52: ^{1}H NMR spectrum of **13** (250 MHz, DMSO-d_6).

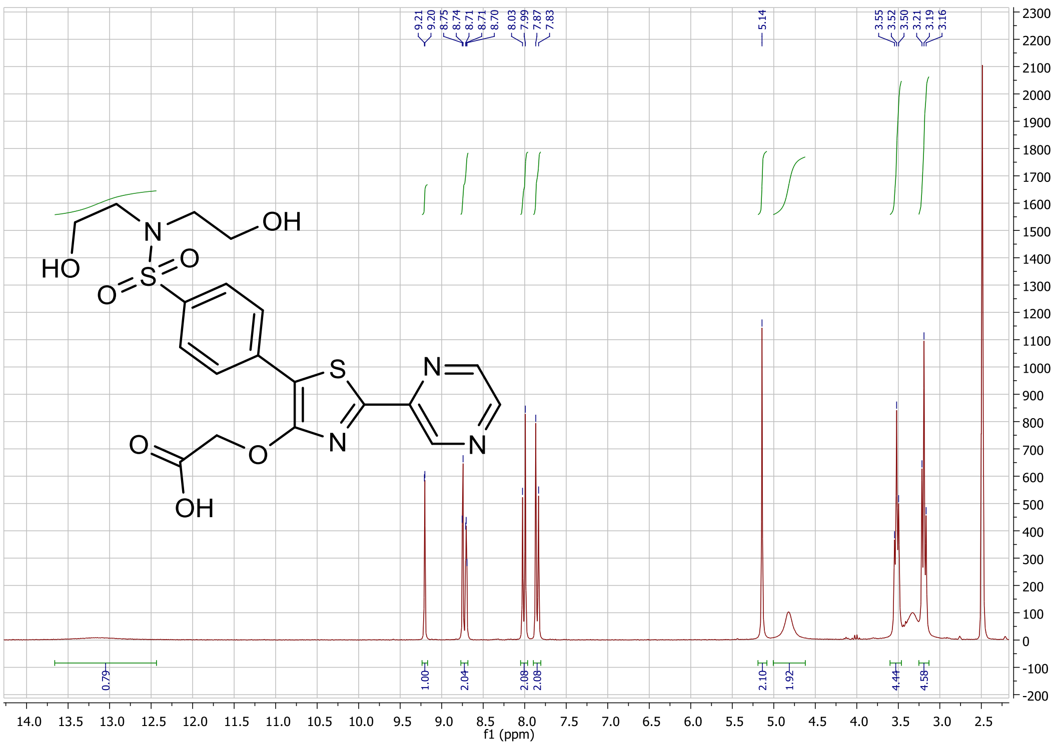


Figure S53: ^{1}H NMR spectrum of **14** (250 MHz, DMSO-d_6).

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