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Functionalisable acyclic cucurbiturils

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CONTENT

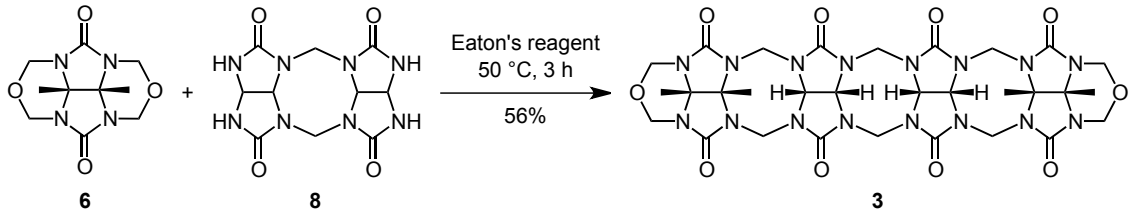
Synthetic Procedures

General details. Analyses were carried out as follows: melting points, Müller SPM-X 300; NMR, Bruker AVANCE III 400 and 600 (peak assignments were confirmed by using H,H-COSY, HMQC, HMBC and ROESY spectra; the stereodescriptors *endo* and *exo* were used according to literature;[1] spectra were referenced to the residual solvent signals (DMSO-d_6: δ^H = 2.50 ppm, δ^C = 39.52 ppm);[2] MALDI TOF-MS, BrukerUltraflex TOF/TOF; ESI MS measurements, these measurements were performed by using a Paul-type quadrupole ion trap instrument (AmaZonETD, Bruker Daltonics), the ion source was set to negative electrospray ionisation mode, scan speed was 8100 (*m/z*) s^{-1} in enhanced resolution scan mode (0.3 FWHM / *m/z*), mass spectra were accumulated for at least two minutes, sample solutions were continuously infused into the ESI chamber by a syringe pump at a flow rate of 120–180 µL min^{-1}, nitrogen was used as drying gas with a flow rate of 3.0 L min^{-1} at 220 °C, the solutions were sprayed at a nebulizer pressure of 900 mbar (13 psi) and the electrospray needle was held at 3.5 kV; elemental analysis, Elementar vario Micro cube; chiral HPLC, Merck-Hitachi LaChrom (interface D-7000, diode array detector L-7455, column oven L-7300, programmable autosampler L-7250, pump L-7100); column, Reprosil Chiral-NR, 250 × 4.6 mm, 8 µm particle size; flow, 1 mL/min; eluent, aqueous: water, organic: acetonitrile; gradient 1: 0–3 min, 10% organic; 3–29 min, linear increase of organic to 60%; 29–36 min, 60% organic; 36–38 min, linear increase to 90% organic; preparative HPLC, Dionex UltiMate 3000; column, Supelco, Ascentis-C18, 250 × 21.2 mm, 5 µm particle size; flow, 12 mL/min; eluent, aqueous: 0.1 vol% TFA in water; organic: acetonitrile; gradient 1: 0–5 min, 10% organic; 5–7 min, linear increase of organic to 15%; 5–7 min, linear increase of organic to 25% organic; 7–12 min, 25% organic; 12–20 min, linear increase of organic to 90% organic; 20–28 min, 90% organic; 28–32 min, linear decrease of organic to 10% organic; 32–37 min, 10% organic; gradient 2: 0–5 min, 10% organic; 5–22 min, linear increase of organic to 50%; 22–27 min, 50% organic; 27–29 min, linear decrease of organic to 10% organic; 29–32 min, 10% organic.

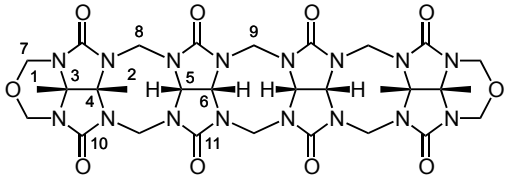
The following abbreviations are used: TBTA, tris[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]amin; NaAsc, sodiumascorbate; PyCloP, chlorotripyrrolidinophosphonium hexafluorophosphate; DIPEA, diisopropylethylamine.

Preparation of Eaton's Reagent. Eaton's reagent was prepared by following the literature procedure.[3] Specifically, 10 wt.% phosphorus pentoxide (dried under high vacuum) was added to freshly distilled $MeSO_3H$ under rapid stirring. The mixture was stirred overnight under N_2 until the solid was dissolved completely. If not completely dissolved, the mixture was filtrated to obtain a colorless solution.

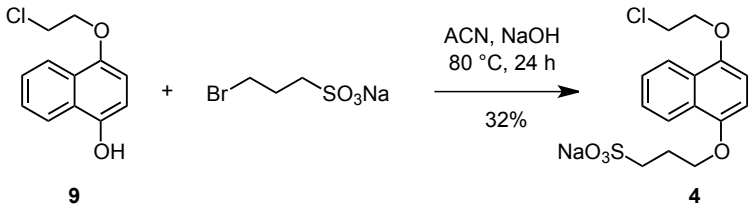
Tetramer 3



Dimer **8** (11.0 g, 27.9 mmol) was dissolved in Eaton's Reagent[3] (80 mL) and the solution was heated to 50 °C. Diether **6** (40.0 g, 157 mmol) was added and the reaction mixture was stirred for 3 h at 50 °C. Afterwards, the dark red solution was poured into H_2O (800 mL). The precipitate was collected by centrifugation (4400 rpm, 15 min). The solid was suspended with small volumes of water and centrifugated until the supernatant solution was almost colorless. After drying *in vacuo*, the light red solid was dissolved in TFA (32 mL) and precipitated by the addition of H_2O (180 mL). This procedure was repeated once more, the resulting solid was washed with H_2O (120 mL) and acetone (2 × 120 mL), and dried *in vacuo*. Yield: 15.5 g (19.9 mmol, 56%), colorless solid; m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 5.68 (d, 2H, ^2J = 14.4 Hz, H9^{exo}), 5.48–5.61 (m, 8H, H5/H6/H8^{exo}), 5.16 (d, 4H, ^2J = 10.7 Hz, H7^{exo}), 4.83 (d, 4H, ^2J = 11.0 Hz, H7^{endo}), 4.27 (m, 6H, 8H^{endo}/H9^{endo}), 1.81 (s, 6H, H1), 1.63 (s, 6H, H2) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 155.35 (C10), 154.81 (C11), 77.18 (C7), 72.44 (C3), 70.79 + 70.55 + 70.14 (C4/C5/C6), 52.94 (C9), 48.46 (C8), 17.77 (C1), 15.73 (C2) ppm; MS (MALDI/TOF pos. mode): *m/z* (%) = 803.5 $[M+Na]^+$ (100).

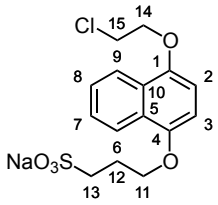


Naphthalene Derivative 4

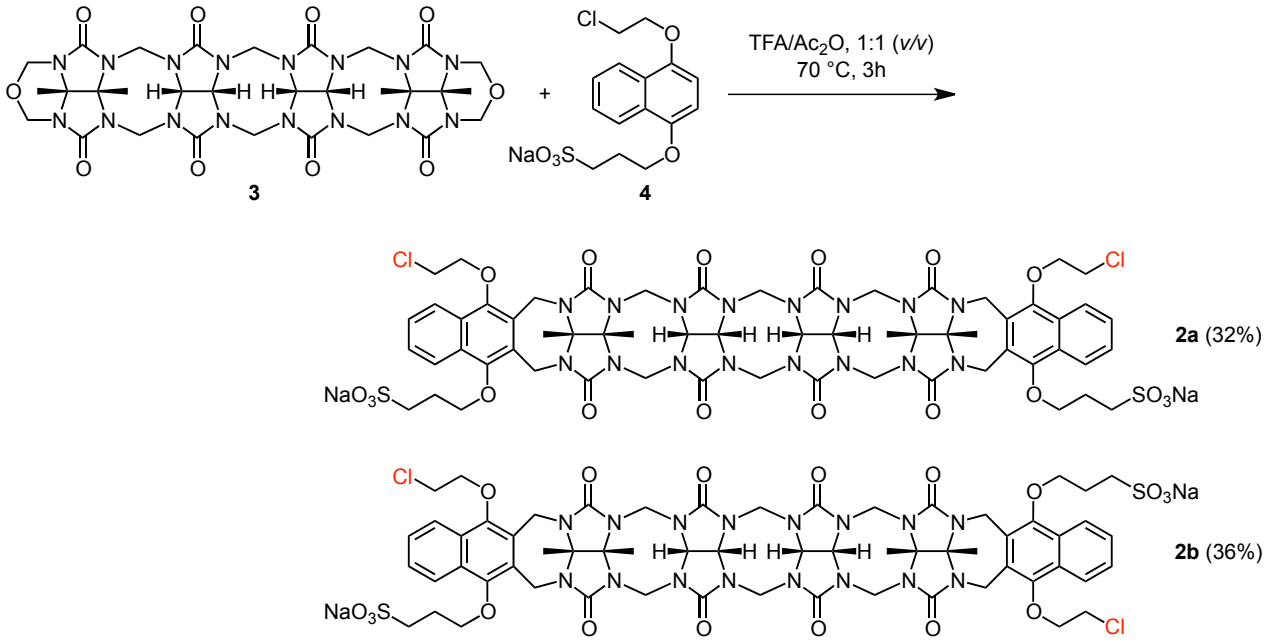


9 **4**

The monosubstituted naphthohydroquinone **9**[4] (4.30 g, 19.3 mmol) and NaOH (928 mg, 23.2 mmol) were dissolved in acetonitrile (230 mL). Sodium 3-bromopropane-1-sulfonate (4.34 g, 19.3 mmol) was added and the reaction mixture was stirred at 80 °C for 24 h. The precipitate was filtered off, washed with acetonitrile (4 × 30 mL) and dissolved in a small amount of hot water. The precipitate formed after the solution reached room temperature was collected by centrifugation and recrystallized from water. Yield: 2.26 g (6.16 mmol, 32%), off-white solid; m.p. >250 °C, ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.11–8.17 (m, 2H, H6/H9), 7.53–7.56 (m, 2H, H7/H8), 6.89 (d, ^{3}J = 8.4 Hz, 1H, H2), 6.83 (d, ^{3}J = 8.4 Hz, 1H, H3), 4.36 (t, ^{3}J = 5.1 Hz, 2H, H14), 4.18 (t, ^{3}J = 6.4 Hz, 2H, H11), 4.06 (t, ^{3}J = 5.0 Hz, 2H, H15), 2.68 (t, ^{3}J = 8.0 Hz, 2H, H13), 2.08–2.18 (m, 2H, H12) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 148.37 (C1), 147.19 (C4), 126.00 + 125.77 (C9/C6), 121.53 + 121 48 (C5/C10), 105.91 (C2), 104.80 (C3), 68.71 (C14), 67.22 (C11), 48.22 (C13), 43.46 (C15), 25.46 (C12) ppm; MS (MALDI/TOF pos. mode): *m/z* (%) = 389.0 $[M+Na]^+$ (100), 755.2 $[2M+Na]^+$ (28); CHN calcd (%) for $C_{15}H_{16}ClNaO_5S \cdot H_2O$ (M.W. 384.81): C 46.82, H 4.71, S 8.33, found C 47.28, H 4.66, S 8.41.



Dichlorides 2a and 2b

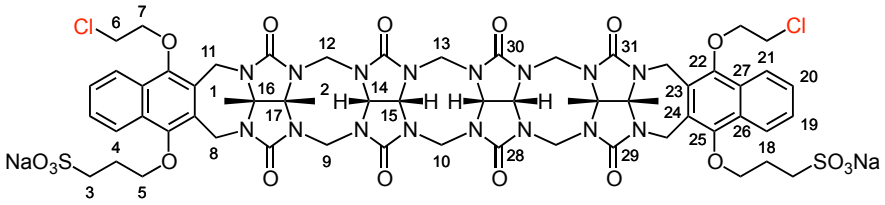


Compound **3** (1.86 g, 2.38 mmol) was dissolved in TFA/Ac_2O, 1:1 (*v/v*) (19 mL) and the mixture was heated to 70 °C. Sulfonate **4** (2.10 g, 5.73 mmol) was added and the solution was stirred for 3 h at 70 °C. Afterwards, the still warm reaction mixture was poured slowly into MeOH (75 mL). The precipitate was centrifuged (4400 rpm, 15 min). It was suspended in small volumes of MeOH and centrifuged until the supernatant became almost colorless. The crude was refluxed in EtOH overnight, centrifuged and dried *in vacuo* to yield 3.12 g (80%) of the mixture of regioisomers **2a** and **2b**.

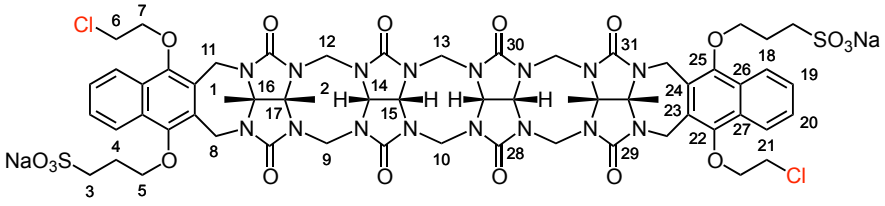
Both isomers were separated by dissolving the obtained product mixture in hot water (5 mL). The pH of the solution was adjusted to 10–11 with 0.5 M aqueous NaOH, the precipitated solid separated by centrifugation, washed with MeOH (3 × 15 mL), and dried *in vacuo* to afford **2a**. The aqueous layer was treated with EtOH (15 mL), thus precipitated **2b** was separated by centrifugation, washed with MeOH (3 × 15 mL), and dried. This way, both isomers were obtained in >85% purity. For further purification, they were repeatedly dissolved in H_2O and precipitated by the addition of EtOH or, if pure enough, recrystallized from EtOH/H_2O, 2:1 (*v/v*).

Achiral Isomer **2a**: Yield: 1.13 g (0.76 mmol, 32%), colorless solid; m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.10 (d, 2H, ^2J = 8.3 Hz, H21), 7.94 (d, 2H, ^2J = 8.3 Hz, H18), 7.68–7.74 (m, 4H, H19/H20), 5.46–5.59 (m, 8H, $H9^{exo}$/$H12^{exo}$/$H10^{exo}$/$H13^{exo}$/H14), 5.30–5.38 (m, 6H, $H8^{exo}$/$H11^{exo}$/H15), 4.54–4.58 (m, 2H, H7), 4.35–4.41 (m, 4H, $H8^{endo}$/$H11^{endo}$), 4.10–4.18 (m, 8H, H5/H6/$H9^{endo}$/$H10^{endo}$/$H12^{endo}$/$H13^{endo}$), 3.95–4.05 (m, 6H, H6/H7), 3.85–3.87 (m, 2H, H5), 2.76–

2.80 (m, 4H, H3), 2.05–2.12 (m, 4H, H4), 1.73–1.75 (m, 12H, H1/H2) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 155.77 + 155.20 + 154.45 + 154.12 (C28/C29/C30/C31), 148.73 + 147.16 (C22/C25), 127.83 + 127.71 + 127.50 + 127.31 (C23/C24/C26/C27), 126.83 + 126.78 (C19/C20), 122.74 + 122.57 (C18/C21), 77.57 (C16), 76.23 (C17), 74.11 (C5/C7), 70.84 + 70.49 (C14/C15), 48.51 + 48.31 (C3/C9/C10/C12/C13), 44.73 (C6), 35.95 + 35.80 (C8/C11), 26.33 (C4), 16.05 + 15.66 (C1/C2) ppm; MS (ESI/TOF neg. mode): *m/z* (%) = 715.2 $[M–2Na]^{2–}$ (100), 962.3 $[M_2–3Na]^{3–}$ (72), 1085.2 $[M_3–4Na]^{4–}$ (29), 1453.3 $[M–Na]^{–}$ (20); CHN calcd (%) for $C_{60}H_{64}Cl_2N_{16}Na_2O_{18}S_2·9H_2O$ (M.W. 1640.42): C 43.93, H 5.04, N 13.66, S 3.91, found C 43.72, H 4.88, N 13.60, S 3.83.



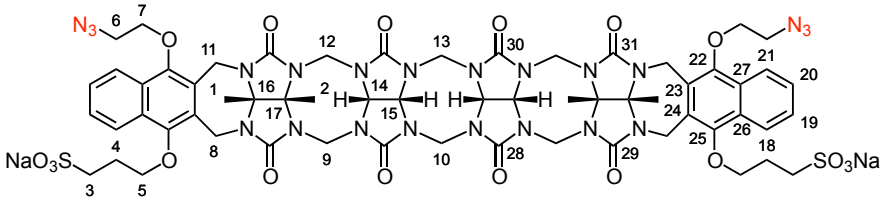
Chiral Isomer **2b**: Yield: 1.26 g (0.85 mmol, 36%), colorless solid; m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.12 (d, 2H, ^{2}J = 8.3 Hz, H21), 7.98 (d, 2H, ^{2}J = 8.3 Hz, H18), 7.70 (t, 2H, ^{3}J = 8.1 Hz, H20) 7.63 (t, 2H, ^{3}J = 8.1 Hz, H19), 5.55 (d, 4H, ^{2}J = 14.8 Hz, $H9^{exo}$/$H12^{exo}$), 5.40–5.44 (m, 4H, $H10^{exo}$/$H13^{exo}$/H14), 5.27–5.37 (m, 6H, $H8^{exo}$/$H11^{exo}$/H15), 4.30–4.40 (m, 8H, H5/H7/$H8^{endo}$/$H11^{endo}$), 4.06–4.12 (m, 6H, $H9^{endo}$/$H10^{endo}$/$H12^{endo}$/$H13^{endo}$), 3.87–3.98 (m, 6H, H5/H6/H7), 3.76–3.80 (m, 2H, H6), 2.78–2.82 (m, 4H, H3), 2.08–2.22 (m, 4H, H4), 1.72–1.74 (m, 12H, H1/H2) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 155.67 + 155.27 + 154.85 + 153.63 (C28/C29/C30/C31), 148.95 + 147.03 (C22/C25), 127.85 + 127.82 + 127.45 + 127.24 (C23/C24/C26/C27), 126.67 + 126.66 (C19/C20), 122.73 + 122.69 (C18/C21), 77.59 (C16), 76.23 (C17), 74.17 + 74.04 (C5/C7), 70.91 + 70.53 (C14/C15), 48.67 + 48.58 + 48.30 (C3/C9/C10/C12/C13), 44.84 (C6), 36.25 + 35.54 (C8/C11), 26.52 (C4), 16.00 + 15.57 (C1/C2) ppm; MS (ESI/TOF neg. mode): *m/z* (%) = 715.0 $[M–2Na]^{2–}$ (100); CHN calcd (%) for $C_{60}H_{64}Cl_2N_{16}Na_2O_{18}S_2·9H_2O$ (M.W. 1640.42): C 43.93, H 5.04, N 13.66, S 3.91, found C 43.78, H 4.87, N 13.77, S 3.93.



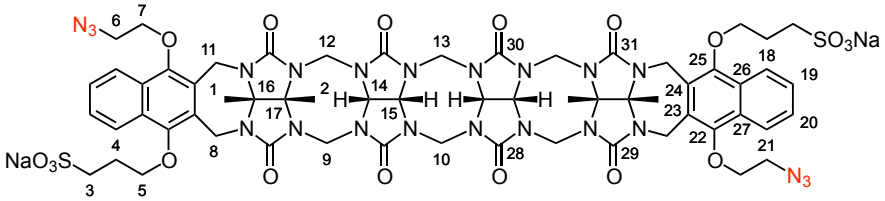
Diazides 10a and 10b

General Procedure. The dichloride **2a** or **2b** was dissolved in DMSO (6 mL/mmol) and the solution was heated to 80 °C. NaN_3 (10 eq) was added and the resulting mixture was stirred for 20 h at 80 °C. Afterwards, the still hot mixture was added dropwise to MeCN (40 mL/mmol). The precipitate was collected by centrifugation and washed with MeOH (3 × 30 mL/mmol). For further purification, the solids where either repeatedly dissolved in H_2O and precipitated by the addition of EtOH or, if already pure enough, recrystallized from EtOH/H_2O, 2:1 (*v/v*).

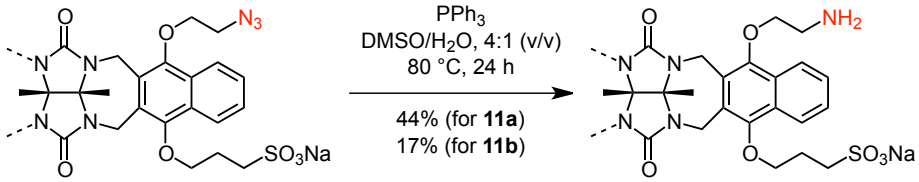
Achiral Isomer **10a**: Compound **10a** was prepared from **2a** (0.72 g, 0.49 mmol) according to the general procedure. Yield: 0.66 g (0.44 mmol, 90%), colorless solid; m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.05 (d, ^3J = 8.3 Hz, 2H, H21), 7.94 (d, 2H, ^3J = 8.3 Hz, H18), 7.70–7.76 (m, 4H, H19/H20), 5.46–5.58 (m, 8H, H9^{exo}/H10^{exo}/H12^{exo}/H13^{exo}/H14), 5.30–5.36 (m, 6H, H8^{exo}/H11^{exo}/H14 or H15), 4.45–4.47 (m, 2H, H7), 4.35–4.40 (m, 4H, H8^{endo}/H11^{endo}), 4.11–4.16 (m, 8H, H5/H9^{endo}/H10^{endo}/H12^{endo}/H13^{endo}), 3.88–3.90 (m, 2H, H7), 3.83–3.84 (m, 2H, H5), 3.71–3.74 (m, 2H, H6), 3.58–3.63 (m, 2H, H6), 2.76–2.78 (m, 4H, H3), 2.01–2.11 (m, 4H, H4), 1.73–1.75 (m, 12H, H1/H2) ppm; ^{13}C NMR (151 MHz, DMSO-d_6): δ = 155.92 + 155.27 + 154.48 + 154.28 (C28/C29/C30/C31), 148.68 + 147.40 (C22/C25), 127.87 + 127.61 + 127.46 + 127.40 (C23/C24/C26/C27), 126.85 (C19/C20), 122.80 + 122.48 (C18/C21), 77.65 (C16), 76.31 (C17), 74.14 (C5), 73.48 (C7), 70.84 + 70.51 (C14/C15), 50.95 (C6), 48.51 + 48.45 + 48.30 (C3/C9/C10/C12/C13), 35.93 + 35.87 (C8/C11), 26.28 (C4), 16.06 + 15.70 (C1/C2) ppm; IR (ATR): $\tilde{\upsilon}$ = 2107 [m, ν(azide)] cm^{-1}; MS (ESI/TOF neg. mode): *m/z* (%) = 722.1 [M–2Na]$^{2-}$ (100); CHN calcd (%) for $C_{60}H_{64}N_{22}Na_2O_{18}S_2 \cdot 6H_2O$ (M.W. 1599.51): C 45.06, H 4.79, N 19.27, S 4.01, found C 44.92, H 4.82, N 19.43, S 4.00.



Chiral Isomer **10b**: Compound **10b** was prepared from **2b** (0.44 g, 0.29 mmol) according to the general procedure. Yield: 0.38 g (0.25 mmol, 86%), colorless solid; m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.06 (d, 2H, ^{3}J = 8.3 Hz, H21), 7.99 (d, 2H, ^{3}J = 8.3 Hz, H18), 7.73 (t, 2H, ^{3}J = 7.8 Hz, H20), 7.64 (t, 2H, ^{3}J = 7.4 Hz, H19), 5.55 (d, 4H, ^{2}J = 14.8 Hz, H9^{exo}/H12^{exo}), 5.39–5.45 (m, 4H, H10^{exo}/H13^{exo}/H14), 5.27–5.37 (m, 6H, H8^{exo}/H11^{exo}/ H14 or H15), 4.26–4.40 (m, 8H, H5/H7/H8^{endo}/H11^{endo}), 4.05–4.12 (m, 6H, H9^{endo}/H10^{endo}/H12^{endo}/H13^{endo}), 3.94–3.99 (m, 2H, H7), 3.80–3.85 (m, 2H, H5), 3.56–3.61 (m, 2H, H6), 3.42–3.44 (m, 2H, H6), 2.79–2.83 (m, 4H, H3), 2.14–2.17 (m, 4H, H4), 1.73–1.75 (m, 12H, H1/H2) ppm; ^{13}C NMR (151 MHz, DMSO-d_6): δ = 155.68 + 155.25 + 154.87 + 153.59 (C28/C29/C30/C31), 148.94 + 147.21 (C22/C25), 127.89 + 127.75 + 127.36 + 127.28 (C23/C24/C26/C27), 126.87 (C19/C20), 122.81 + 122.59 (C18/C21), 77.58 (C16), 76.22 (C17), 74.05 (C5), 73.68 (C7), 70.92 + 70.52 (C14/C15), 50.90 (C6), 48.70 + 48.59 + 48.29 (C3/C9/C10/C12/C13), 36.28 + 35.50 (C8/C11), 26.52 (C4), 16.04 + 15.60 (C1/C2) ppm; IR (ATR): ῡ = 2106 [m, ν(azide)] cm^{-1}; MS (ESI/TOF neg. mode): *m/z* (%) = 722.1 [M–2Na]$^{2-}$ (100); CHN calcd (%) for $C_{60}H_{64}N_{22}Na_2O_{18}S_2 \cdot 8H_2O$ (M.W. 1635.54): C 44.06, H 4.93, N 18.84, S 3.92, found C 44.23, H 4.82, N 19.08, S 3.99.



Diamines 11a and 11b



10a or **10b**

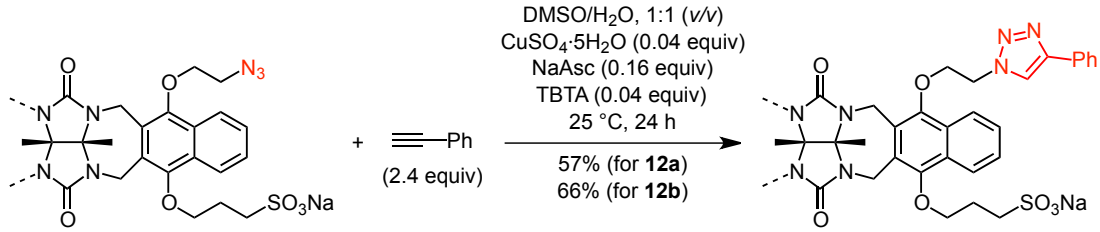
General Procedure. The diazide **10a** or **10b** (800 mg, 0.54 mmol) and triphenylphosphine (1.12 g, 4.29 mmol) were dissolved in DMSO/H_2O, 4:1 (*v/v*) (18 mL) and the mixture was heated to 80 °C for 24 h. Afterwards, the still hot mixture was added slowly into acetone (100 mL). The precipitate was collected by centrifugation and washed with acetone (3 × 30 mL). The solid was dissolved twice

in hot water (ca. 2 mL), the precipitate was collected by centrifugation and dried.

Achiral Isomer **11a**: Yield: 337 mg (0.24 mmol, 44%), colorless solid; m.p. >250 °C; MS (ESI/TOF neg. mode): *m/z* (%) = 696.1 $[M–2Na]^{2–}$ (100).

Chiral Isomer **11b**: The product was dissolved in a small amount of water and the solution was subjected to preparative HPLC (gradient 2). Pure fractions were collected and the solvent was evaporated to a volume of ca. 2 mL. The pH of the resulting solution was adjusted to 14 by adding aqueous NaOH (1 M), the precipitate was collected by centrifugation, washed with ethanol (2 × 10 mL) and dried in vacuo. Yield: 65 mg (0.05 mmol, 17%), colorless solid; m.p. >250 °C; MS (ESI/TOF neg. mode): *m/z* (%) = 696.1 $[M–2Na]^{2–}$ (100).

Triazoles 12 and 12b



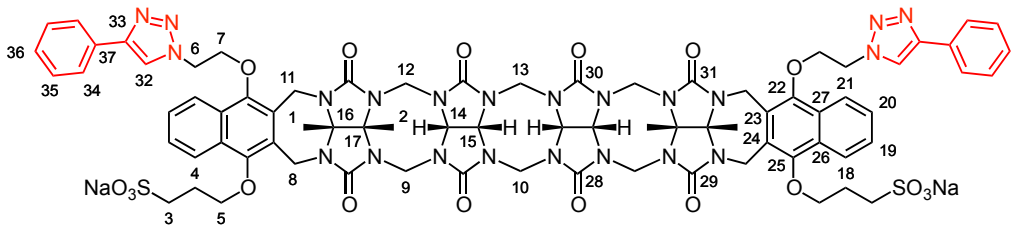
10a or **10b**

General Procedure. The diazide **10a** or **10b** (100 mg, 0.7 mmol) was dissolved in DMSO/H_2O, 1:1 (*v/v*) (2 mL) under a N_2 atmosphere and the solution was heated to 70 °C. Stock solutions of $CuSO_4·5H_2O$ (17.2 mM in H_2O), sodium ascorbate (62.5 mM in H_2O), TBTA (40.5 mM in DMSO) and phenylacetylene (1.33 M in DMSO) were prepared. The necessary quantities of these solutions were added [$CuSO_4·5H_2O$ (81 µl), sodium ascorbate (81 µl), TBTA (33 µl) and phenylacetylene (120 µl)] and the resulting mixture was stirred for 20 h at 70 °C. The progress of the reaction was followed by HPLC. The reaction mixture was cooled to room temperature. The precipitate was collected by centrifugation and washed with DMSO/H_2O, 1:1 (*v/v*) (1 mL). If no precipitate was formed, the mixture was added dropwise to MeCN (20 mL) and collected by centrifugation. The crude product was washed with MeOH (3 × 15 mL) and Et_2O (3 × 10 mL) and then dried *in vacuo*. For further purification, the solid was either repeatedly dissolved in H_2O and precipitated by the addition of EtOH or, if pure enough, recrystallized from EtOH/H_2O, 2:1 (*v/v*).

If the free acid of diazides **10a** or **10b** is used for the reaction instead of the sodium salt, the amount

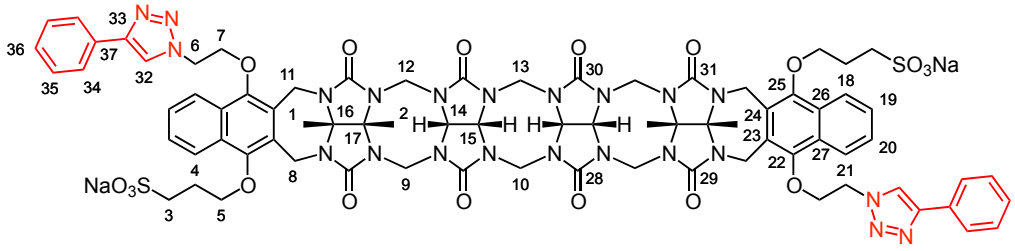
of solvent can be decreased and the product precipitates from the hot reaction mixture. To then convert the product to the sodium salt, the reaction mixture should be centrifuged and the crude product dissolved in H_2O (40 mL). After adjusting the pH to 9–10 by the addition of 0.5 M aqueous NaOH, the solvent should be evaporated ca. 5 mL and the solution treated with EtOH (15 mL). The product can then be collected by centrifugation and is obtained in pure form by washing with MeOH (3 × 15 mL) and Et_2O (3 × 15 mL) and drying *in vacuo*.

Achiral Isomer **12a**: Compound **12a** was prepared from **10a** (100 mg, 0.7 mmol) according to the general procedure. Yield: 64 mg (38 µmol, 57%), colorless solid; m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.78 (s, 2H, H32), 7.90–7.94 (m, 6H, H21/H34), 7.70 (d, 2H, ^3J = 8.3 Hz, H18), 7.60 (t, 2H, ^3J = 7.2 Hz, H20), 7.51 (t, 2H, ^3J = 7.7 Hz, H19), 7.46 (t, 4H, ^3J = 7.8 Hz, H35), 7.35 (t, 2H, ^3J = 7.4 Hz, H36), 5.45–5.63 (m, 8H, H9^{exo}/H10^{exo}/H12^{exo}/H13^{exo}/H14 or H15), 5.28–5.35 (m, 4H, H8^{exo}/H11^{exo}/H14 or H15), 5.10 (d, 2H, ^2J = 16.0 Hz, H8^{exo}/H11^{exo}), 4.87–4.90 (m, 2H, H6), 4.77–4.81 (m, 2H, H6), 4.65–4.68 (m, 2H, H7), 4.07–4.36 (m, 14H, H5/H7/H8^{endo}/H9^{endo}/H10^{endo}/H11^{endo}/H12^{endo}/H13^{endo}), 3.89–3.91 (m, 2H, H5), 2.77–2.81 (m, 4H, H3), 2.06–2.14 (m, 4H, H4), 1.68–1.73 (m, 12H, H1/H2) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 155.79 + 155.31 + 154.45 + 154.23 (C28/C29/C30/C31), 148.77 (C22), 147.23 (C25), 146.50 (C33), 131.06 (C37), 128.94 (C35), 127.86 + 127.76 + 127.55 + 127.28 +127.26 (C23/C24/C26/C27/C36), 126.76 + 126.66 (C19/C20), 125.32 (C34), 122.78 + 122.44 (C18/C21), 122.03 (C32), 77.57 (C16), 76.31 (C17), 74.12 (C5), 72.65 (C7), 71.00 + 70.59 (C14/C15), 50.43 (C6), 48.60 + 48.55 + 48.35 (C3/C9/C10/C12/C13), 36.00 + 35.72 (C8/C11), 26.37 (C4), 16.07 + 15.61 (C1/C2) ppm; MS (ESI/TOF neg. mode): *m/z* (%) = 824.1 [M–2Na]$^{2-}$ (100), 994.1 [M_3–5Na]$^{5-}$ (12%), 1107.1 [M_2–3Na]$^{3-}$ (19%); CHN calcd (%) for $C_{76}H_{76}N_{22}Na_2O_{18}S_2$·13$H_2O$ (M.W. 1929.89): C 47.30, H 5.33, N 15.97, S 3.32, found C 47.03, H 5.37, N 15.97, S 3.20.

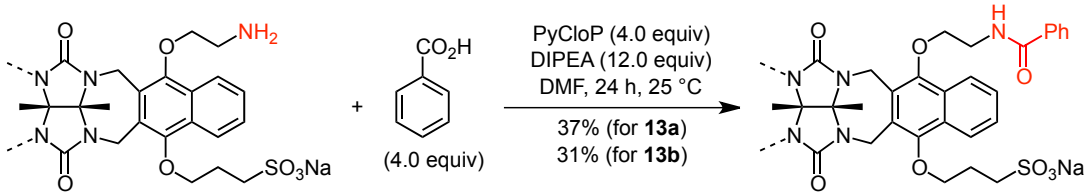


Chiral Isomer **12b**: Compound **12b** was prepared from **10b** (100 mg, 0.7 mmol) according to the general procedure. The ^{1}H NMR spectrum indicated that the product contained ca. 15% of isomer

12a, reflecting the composition of the starting material used for the reaction. The product was not obtained in analytically pure form. Yield: 74 mg (44 µmol, 66%), colorless solid. m.p. >250 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.87 (s, 2H, H32), 7.87–7.97 (m, 6H, H21/H34), 7.79 (d, 2H, ^{3}J = 8.4 Hz, H18), 7.43 –7.50 (m, 6H, H20/H35), 7.29–7.37 (m, 4H, H19/H36), 5.42–5.60 (m, 8H, H9^{exo}/H10^{exo}/H12^{exo}/ H13^{exo}/H14 or H15), 5.24–5.32 (m, 4H, H8^{exo}/H11^{exo}/H14 or H15), 5.13 (d, 2H, ^{2}J = 15.8 Hz, H8^{exo}/H11^{exo}), 4.93–4.99 (m, 2H, H6), 4.71–4.78 (m, 2H, H6), 4.55–4.60 (m, 2H, H7), 4.40–4.45 (m, 2H, H7), 4.21–4.36 (m, 6H, H5/H8^{endo}/H11^{endo}), 4.09–4.15 (m, 6H, H9^{endo}/H10^{endo}/H12^{endo}/H13^{endo}), 3.84–3.90 (m, 2H, H5), 2.77 (t, 4H, ^{3}J = 8.2 Hz, H3), 2.08–2.13 (m, 4H, H4), 1.68–1.73 (m, 12H, H1/H2) ppm; ^{13}C NMR (151 MHz, DMSO-d_6): δ = 155.75 + 155.35 + 154.79 + 153.92 (C28/C29/C30/C31), 148.94 (C22), 147.07 (C25), 146.43 (C33), 131.18 (C37), 128.98 (C35), 127.80 + 127.67 + 127.29 + 127.18 (C23/C24/C26/C27/C36), 126.59 + 126.33 (C19/C20), 125.33 (C34), 122.78 + 122.76 (C18/C21), 122.10 (C32), 77.65 (C16), 76.33 (C17), 74.06 (C5), 72.49 (C7), 71.04 + 70.62 (C14/C15), 50.51 (C6), 48.66 + 48.58 + 48.46 (C3/C9/C10/C12/C13), 36.21 + 35.50 (C8/C11), 26.49 (C4), 15.91 + 15.49 (C1/C2) ppm; MS (ESI/TOF neg. mode): *m/z* (%) = 824.1 $[M–2Na]^{2–}$ (100).



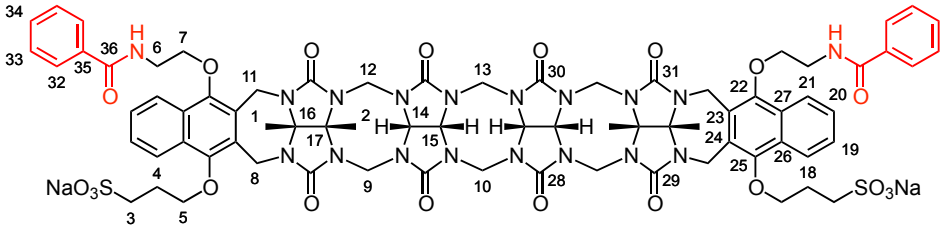
Diamides 13a and 13b



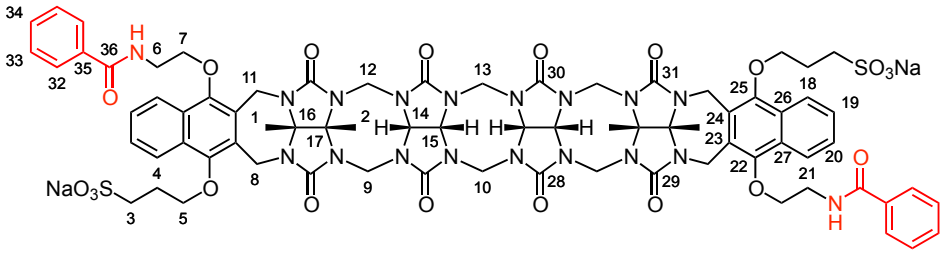
General Procedure. The diamine **11a** or **11b** (200 mg, 0.14 mmol), benzoic acid (68 mg, 0.56 mmol) and PyCloP (246 mg, 0.56 mmol) were dissolved in DMF (9 mL). DIPEA (217 mg, 292 µl, 1.68 mmol) was added dropwise and the resulting mixture was stirred for 24 h at room temperature. Afterwards, the reaction mixture was added dropwise to Et_2O (200 mL), the precipitate was filtered off, and washed with ethyl acetate (3 × 20 mL) and Et_2O (2 × 20 mL). The residue was dissolved in hot water (ca. 3 mL) and the pH of the resulting solution was adjusted to 14 with aqueous NaOH (1 M). The precipitate was collected by centrifugation and dried *in vacuo*.

Achiral Isomer **13a**: Compound **13a** was prepared from **11a** (200 mg, 0.14 mmol) according to the general procedure. The product was dissolved in a small amount of water and the solution was subjected to preparative HPLC (gradient 1). Pure fractions were collected and the solvent was evaporated to a volume of ca. 2 mL. The pH of the solution was adjusted to 14 by adding aqueous NaOH (1 M), the precipitate was collected by centrifugation, washed with ethanol (2 × 10 mL), and dried *in vacuo*. Yield: 84 mg (0.5 mmol, 37%), colorless solid; m.p. >250 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ = 8.79–8.80 (m, 2H, NH), 8.01–8.02 (m, 2H, H21), 7.94–7.95 (m, 6H, H18/H32), 7.63 (t, ^3J = 9.0 Hz, 2H, H20), 7.54–7.57 (m, 2H, H19), 7.52–7.53 (m, 2H, H34), 7.47–7.49 (m, 4H, H33), 5.45–5.58 (m, 8H, H9/H10/H12/H13/H14/H15), 5.29–5.36 (m, 6H, H8/H11/H14/H15), 4.30–4.38 (m, 4H, H8/H11), 4.08–4.18 (m, 10H, H9/H10/H12/H13/H5/H7), 3.98–3.99 (m, 2H, H5), 3.88–3.90 (m, 2H, H7), 3.80–3.81 (m, 2H, H6), 3.54–3.55 (m, 2H, H6), 2.77–2.78 (m, 4H, H3), 2.05–2.12 (m, 4H, H4), 1.69–1.74 (m, 12H, H1/H2) ppm; ^{13}C NMR (151 MHz, DMSO-d_6): δ = 166.56 (C36), 155.74 + 155.31 + 154.47 + 154.25 (C28/ C29/C30/C31), 148.50 + 147.81 (C22/C25), 134.49 (C35), 131.09 (C34), 128.31 (C33), 127.88 + 127.70 + 127.09 (C23/C24/C26/C27), 127.37 (C32), 126.64 + 126.54 (C19/C20), 122.77 + 122.64 (C18/C21), 77.61 + 76.39 (C16/C17), 74.08 + 73.61 (C5/C7), 70.97 + 70.54 (C14/C15), 48.54 + 48.33 (C3/C6/C9/C10/C12/C13), 36.04 + 35.66 (C8/C11), 26.37 (C4), 16.06 + 15.61 (C1/C2) ppm; MS (ESI/TOF neg. mode): *m/z* (%) = 800.6 $[M–2Na]^{2–}$ (100);

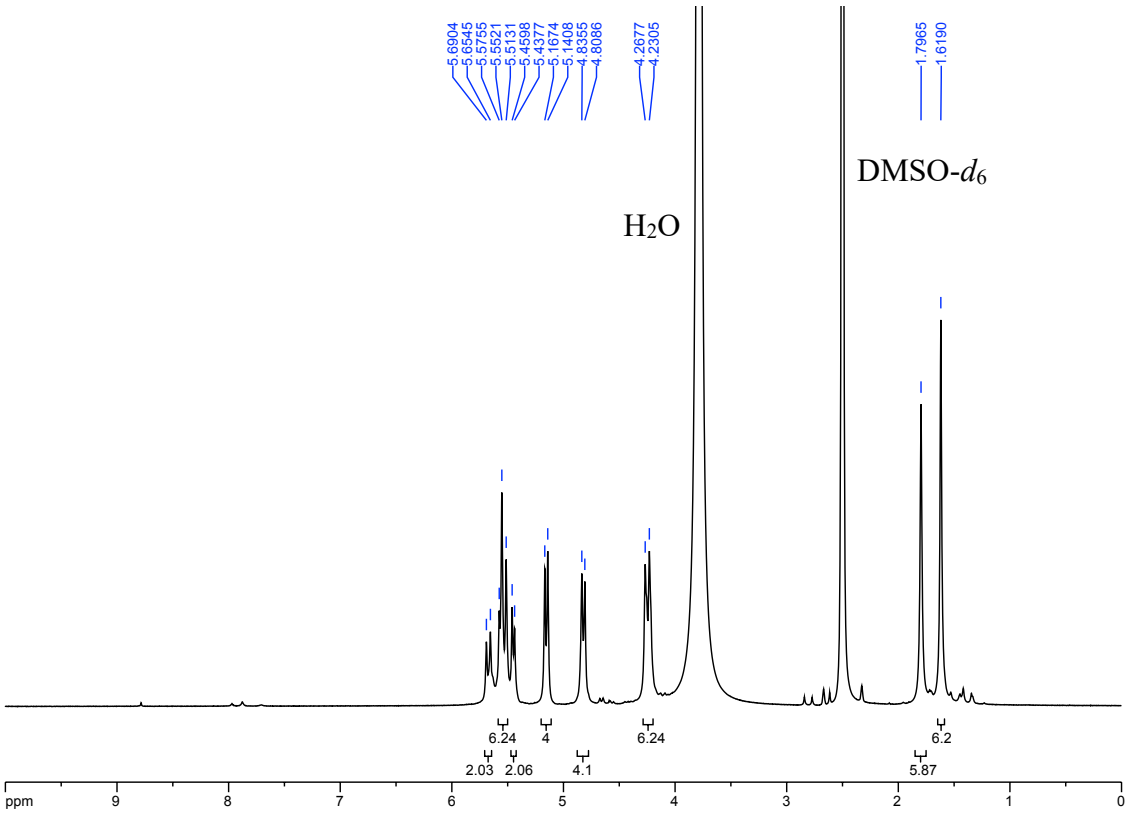
CHN calcd for $C_{74}H_{76}N_{18}Na_2O_{20}S_2 \cdot 11H_2O$ (M.W. 1845.78) C 48.15, H 5.35, N 13.66, S 3.47, found C 48.07, H 4.99, N 14.00, S 3.47.



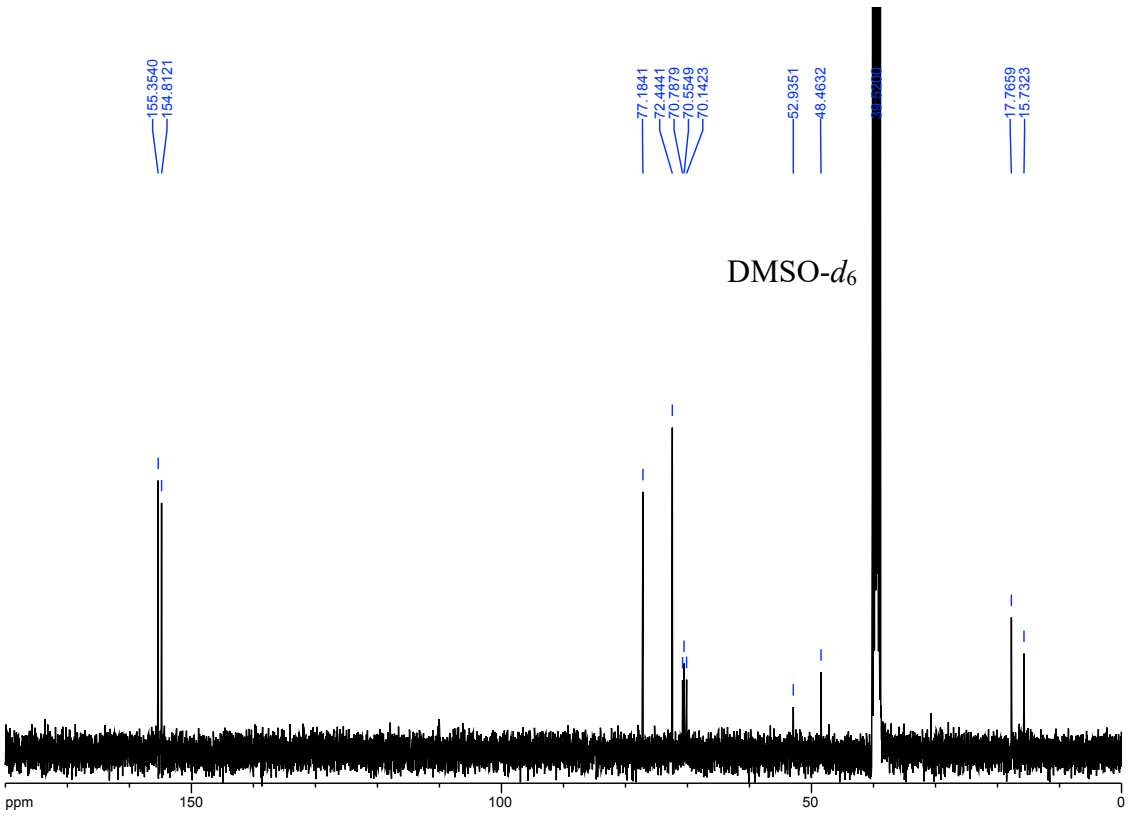
Chiral Isomer **13b**: Compound **13b** was prepared from **11b** (200 mg, 0.14 mmol) according to the general procedure. The crude product was recrystallized from water but could not be obtained in analytically pure form. Yield: 23 mg (0.014 mmol, 31%), colorless solid; m.p. >250 °C; ^{1}H NMR (600 MHz, DMSO-d_6): δ = 8.88–8.90 (m, 2H, NH), 8.09–8.10 (m, 2H, H21), 7.94–8.01 (m, 4H, H18/H32), 7.86–7.88 (m, 2H, H18/H32), 7.60–7.62 (m, 2H, H20), 7.47–7.57 (m, 8H, H19/H33/H34), 5.42–5.58 (m, 8H, H9/H10/H12/H13/H14/H15), 5.29–5.36 (m, 6H, H8/H11/H14/H15), 4.32–4.35 (m, 4H, H8/H11), 4.25–4.27 (m, 2H, H7), 4.08–4.13 (m, 10H, H9/H10/H12/H13/H5/H7), 3.72–3.82 (m, 6H, H5/H6), 2.77–2.79 (m, 4H, H3), 2.10–2.17 (m, 4H, H4), 1.70–1.74 (m, 12H, H1/H2) ppm; ^{13}C NMR (151 MHz, DMSO-d_6): δ = 166.48 (C36), 155.56 + 155.53 + 154.37 + 154.29 (C28/C29/C30/C31), 148.38 + 147.86 (C22/C25), 134.49 (C35), 131.08 (C34), 128.30 (C33), 127.84 + 127.72 + 127.29 + 127.22 (C23/C24/C26/C27), 127.44 (C32), 126.56 (C19/C20), 122.87 + 122.63 (C18/C21), 77.60 + 76.33 (C16/C17), 74.15 + 73.56 (C5/C7), 70.84 + 70.45 (C14/C15), 48.60 + 48.43 + 48.38 + 48.36 (C3/C6/C9/C10/C12/C13), 35.90 + 35.85 (C8/C11), 26.44 (C4), 16.11 + 15.67 (C1/C2) ppm; MS (ESI/TOF neg. mode): *m/z* (%) = 800.1 $[M–2Na]^{2–}$ (100).



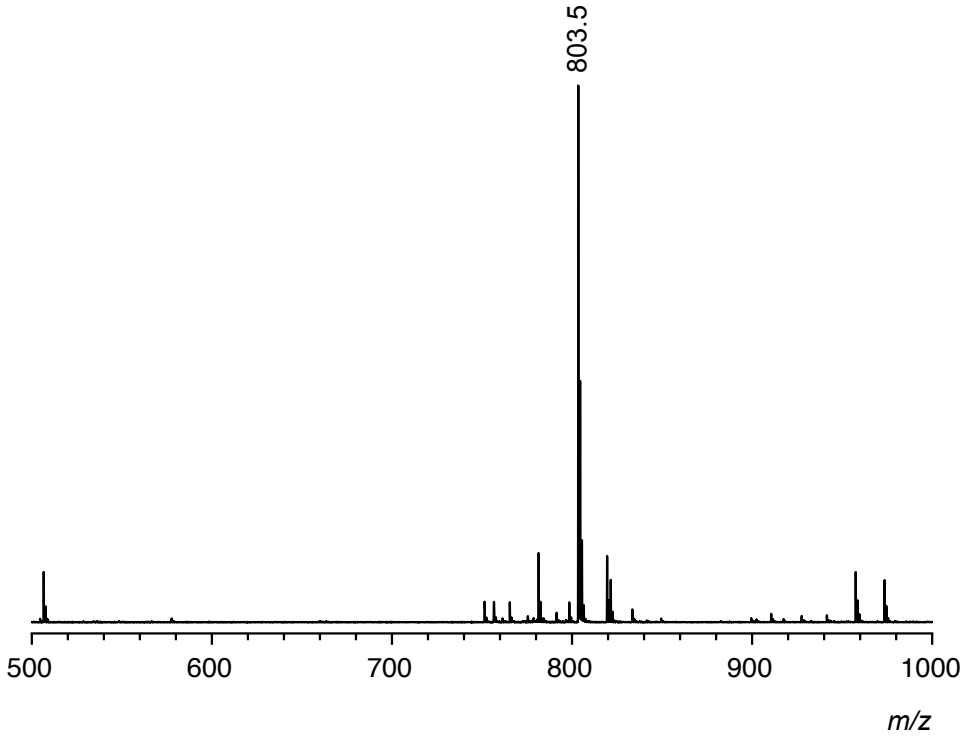
^{1}H NMR: **3** (400 MHz, DMSO-d_6).



^{13}C NMR: **3** (101 MHz, DMSO-d_6).

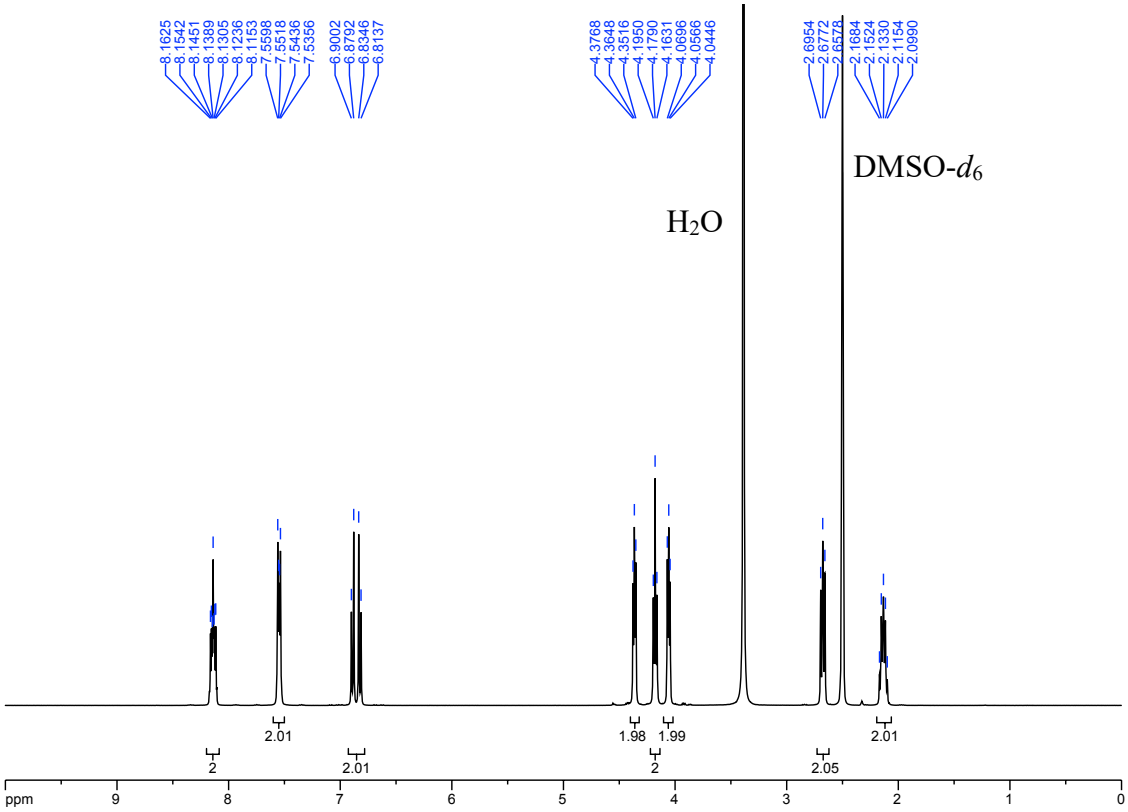


ESI-TOF MS: **3** (MALDI/TOF pos. mode).

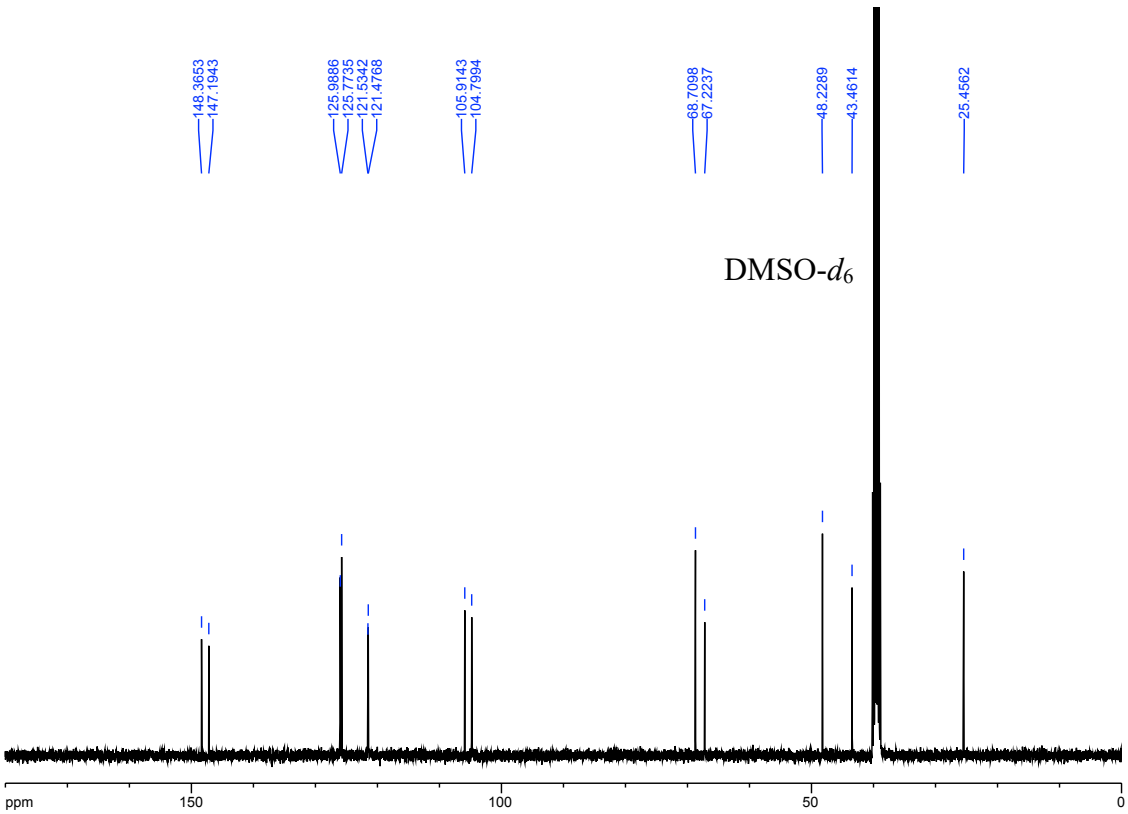


		m/z calcd.	*m/z exp.*
$[M+Na]^+$	$C_{30}H_{36}N_{16}O_{10} + H^+$	803.3	803.5

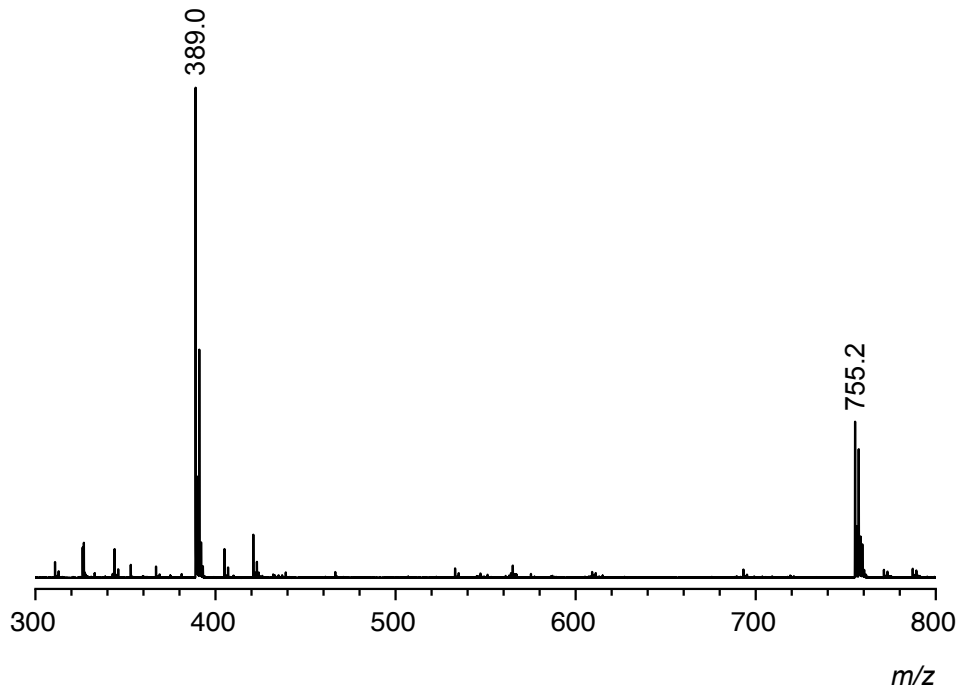
^{1}H NMR: **4** (400 MHz, DMSO-d_6).



^{13}C NMR: **4** (101 MHz, DMSO-d_6).

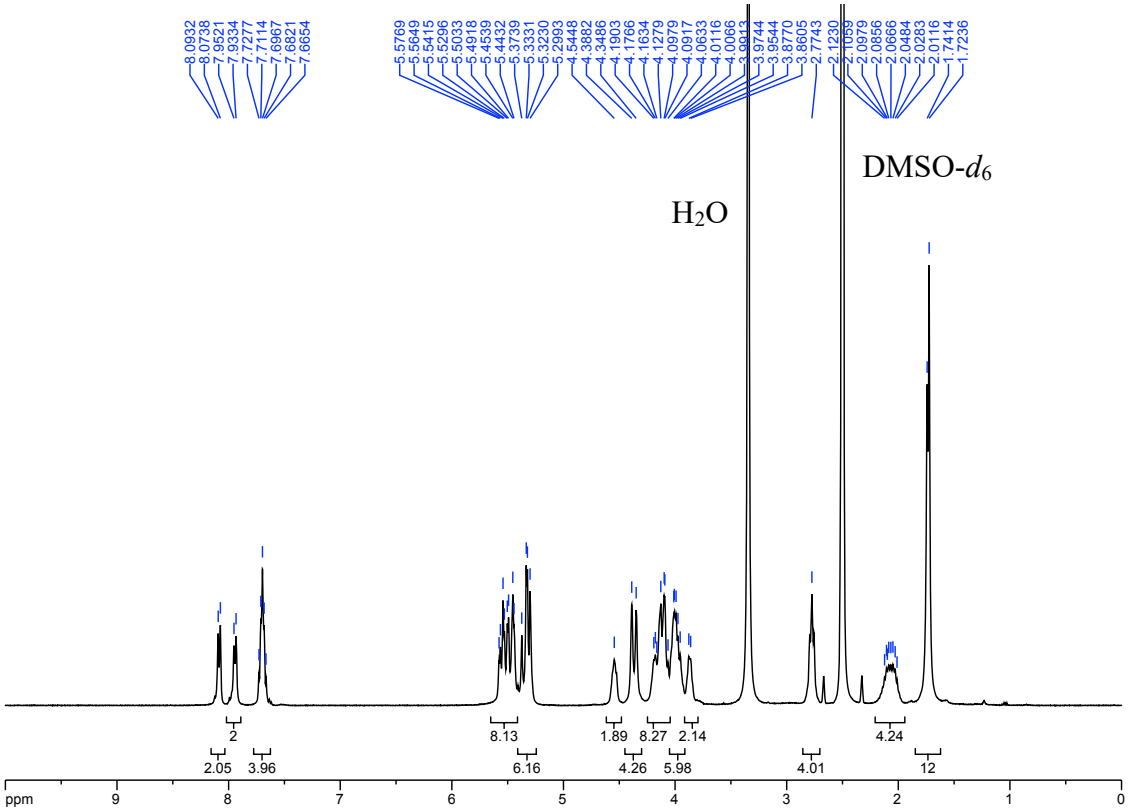


ESI-TOF MS: **4** (MALDI/TOF pos. mode).

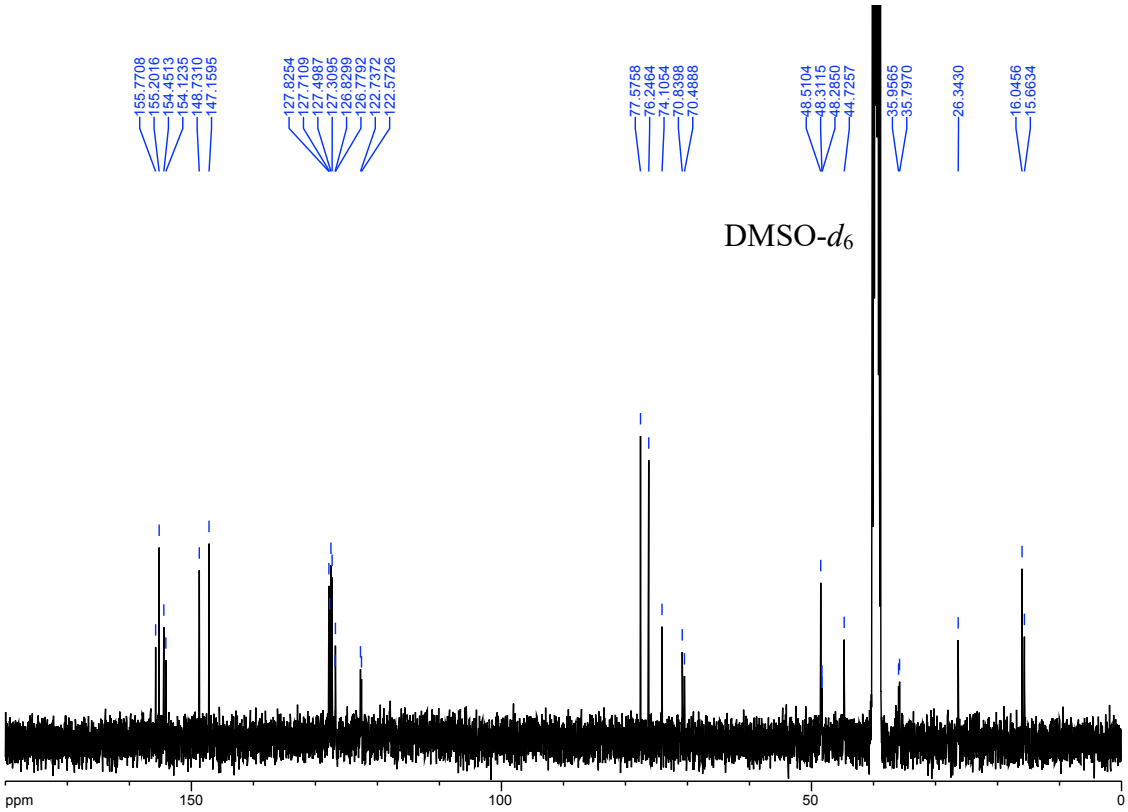


		m/z calcd.	*m/z exp.*
$[M+Na]^+$	$C_{15}H_{16}ClNaO_5S + Na^+$	389.0	389.0
$[2M+Na]^+$	$(C_{15}H_{16}ClNaO_5S)_2 + Na^+$	755.1	755.2

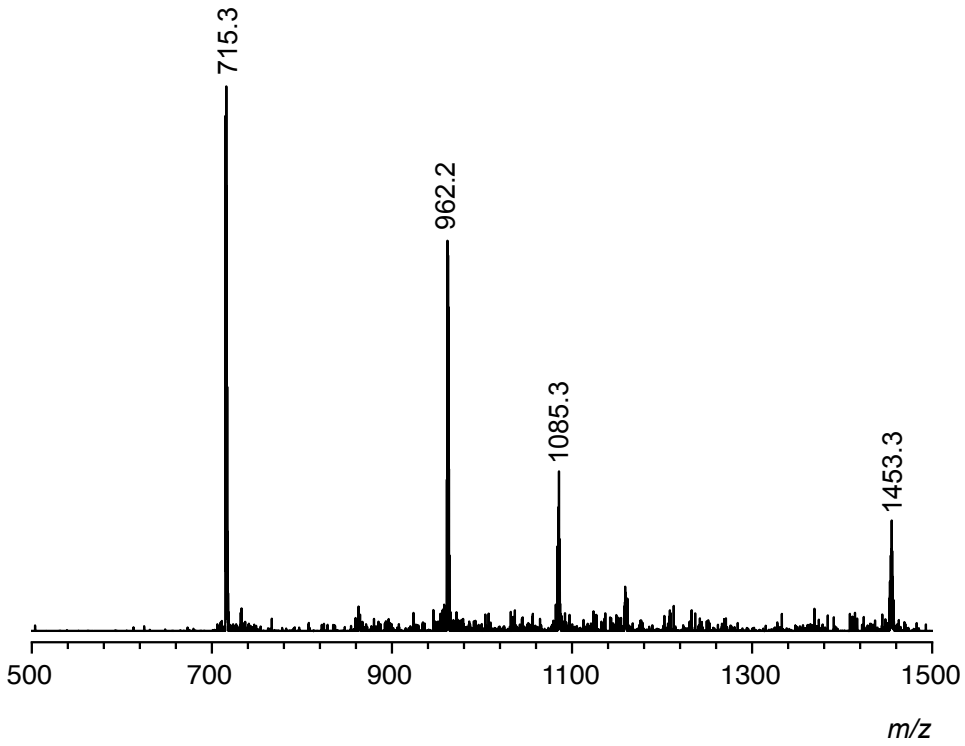
^{1}H NMR: **2a** (400 MHz, DMSO-d_6).



^{13}C NMR: **2a** (101 MHz, DMSO-d_6).

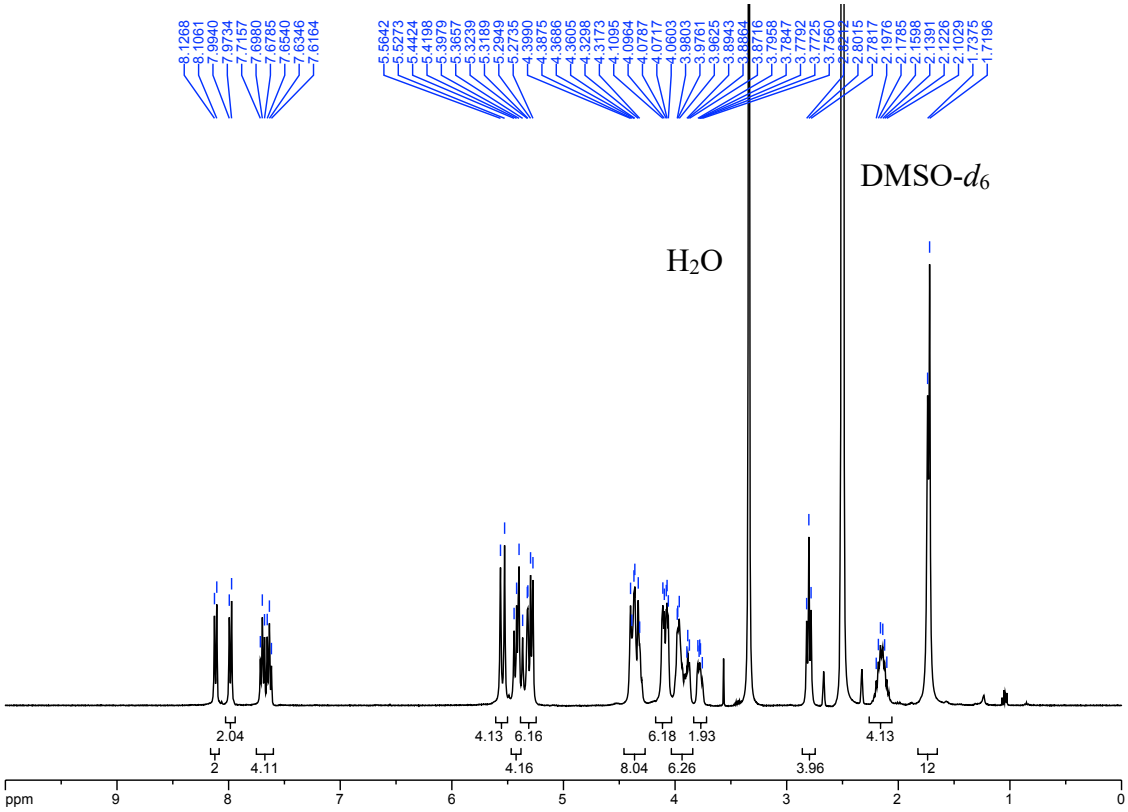


ESI-TOF MS: **2a** (ESI/TOF neg. mode).

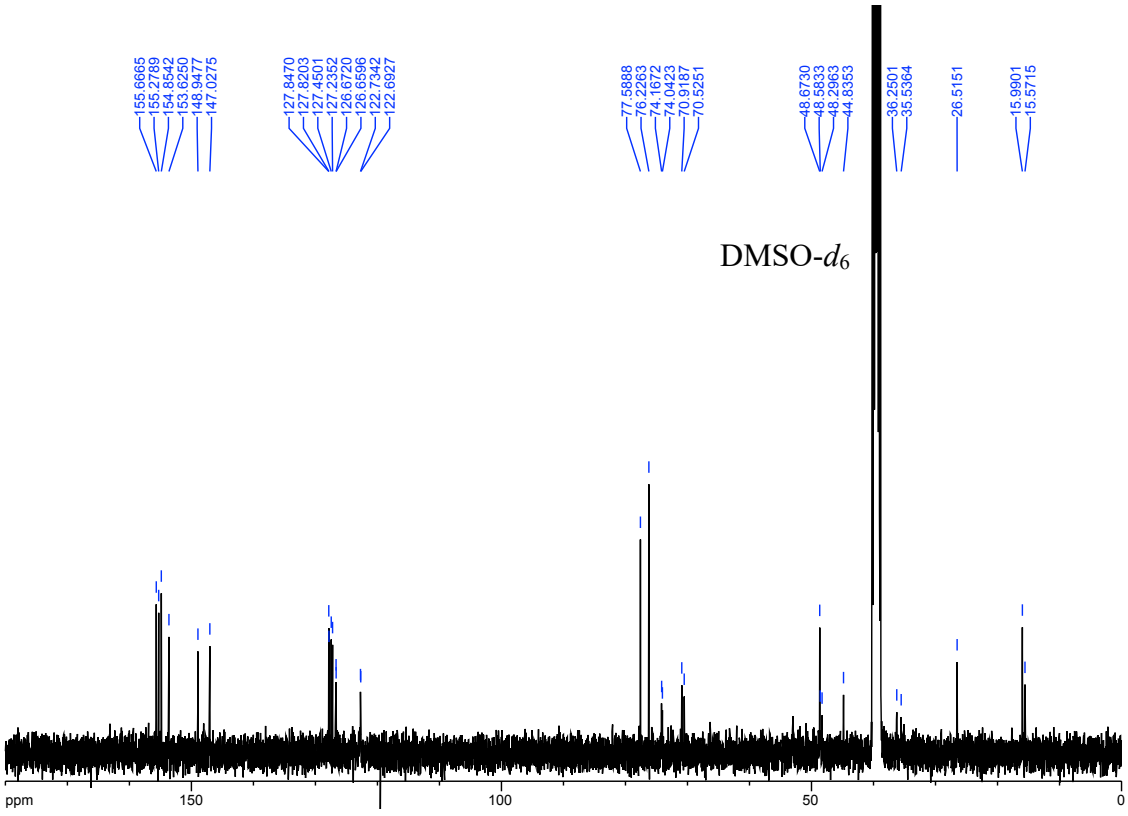


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{60}H_{64}Cl_2N_{16}O_{18}S_2^{2–}$	715.2	715.2
$[M_2–3Na]^{3–}$	$(C_{60}H_{64}Cl_2N_{16}O_{18}S_2^{2–})_2Na$	962.2	962.3
$[M_3–4Na]^{4–}$	$(C_{60}H_{64}Cl_2N_{16}O_{18}S_2^{2–})_3(Na)_2$	1085.3	1085.2
$[M–Na]^{–}$	$C_{60}H_{64}Cl_2N_{16}NaO_{18}S_2^{–}$	1453.3	1453.3

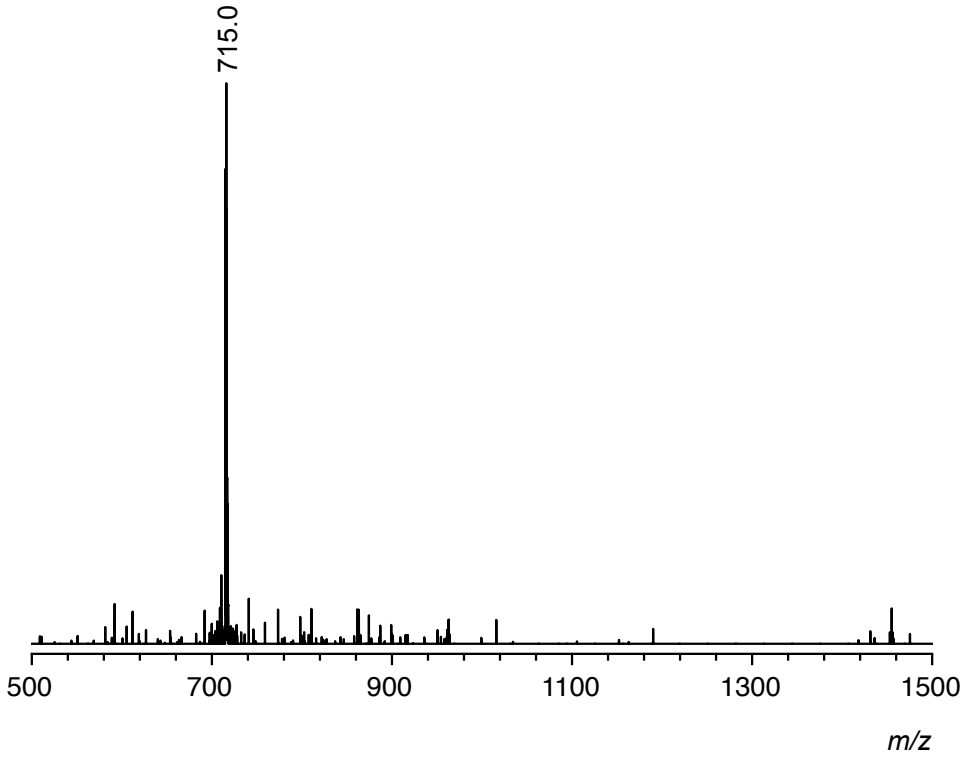
^{1}H NMR: **2b** (400 MHz, DMSO-d_6).



^{13}C NMR: **2b** (101 MHz, DMSO-d_6).

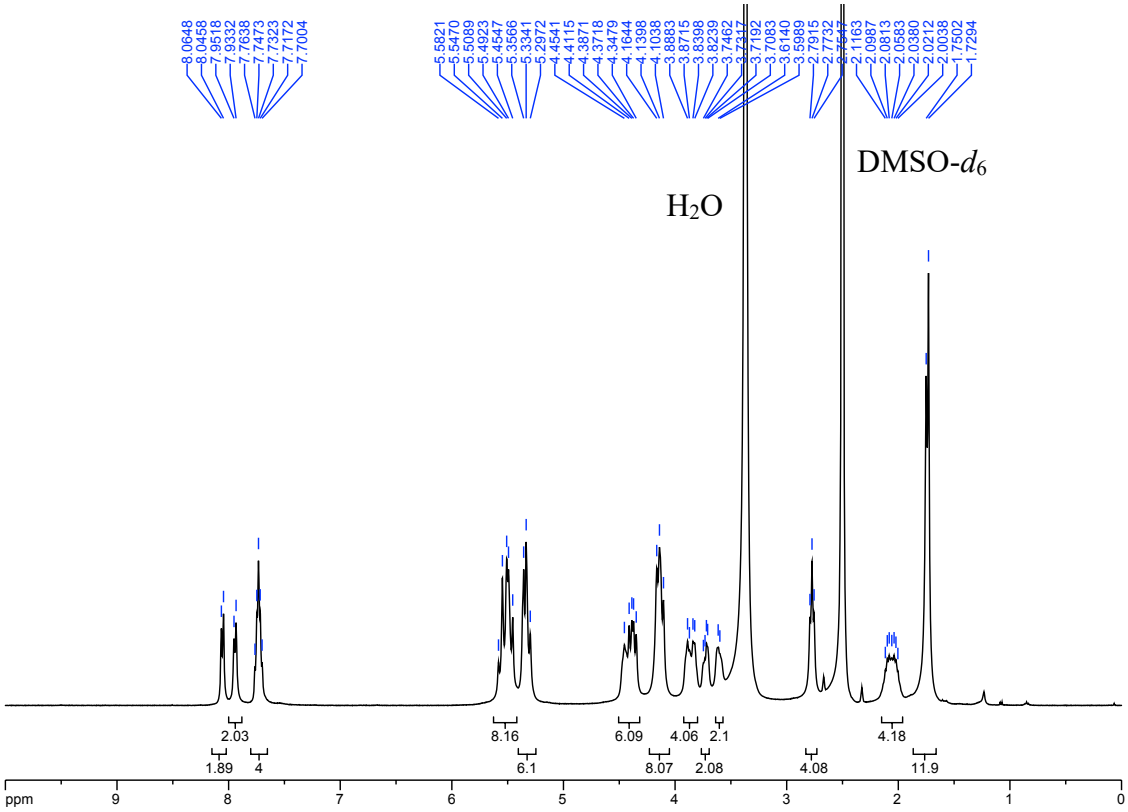


ESI-TOF MS: **2b** (ESI/TOF neg. mode).

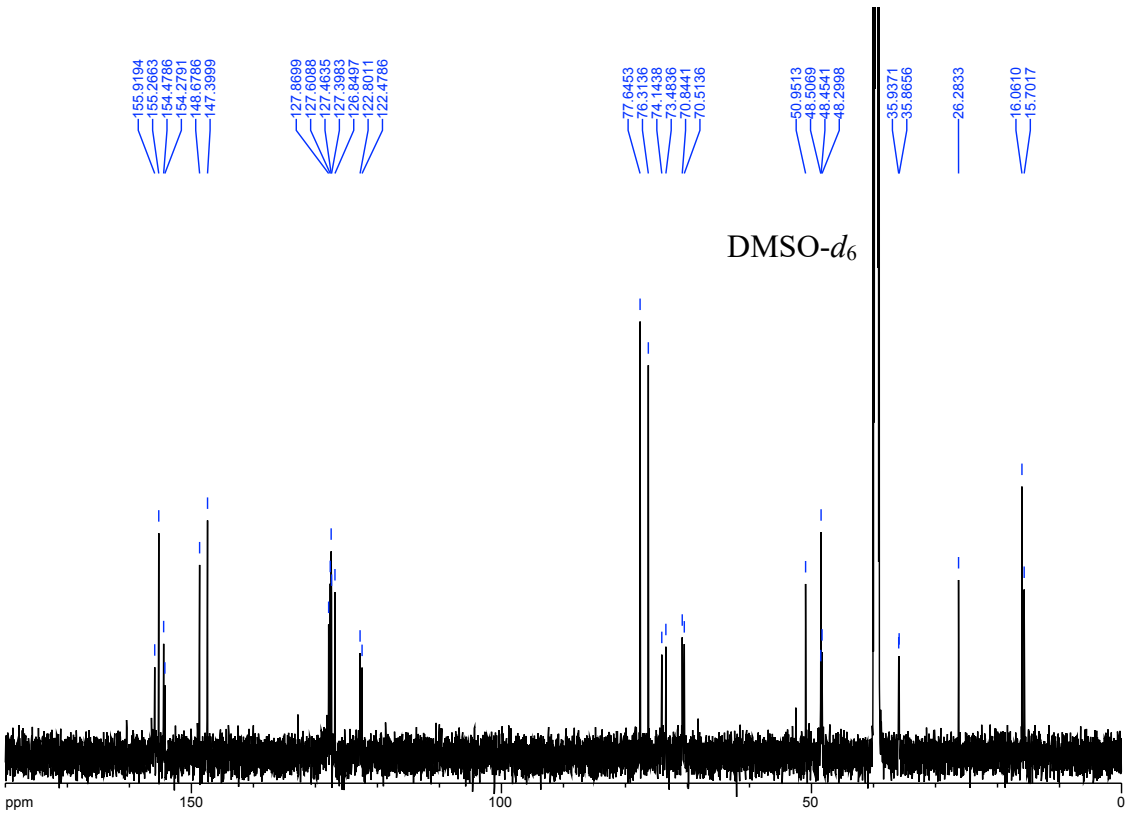


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{60}H_{64}Cl_2N_{16}O_{18}S_2^{2–}$	715.2	715.0

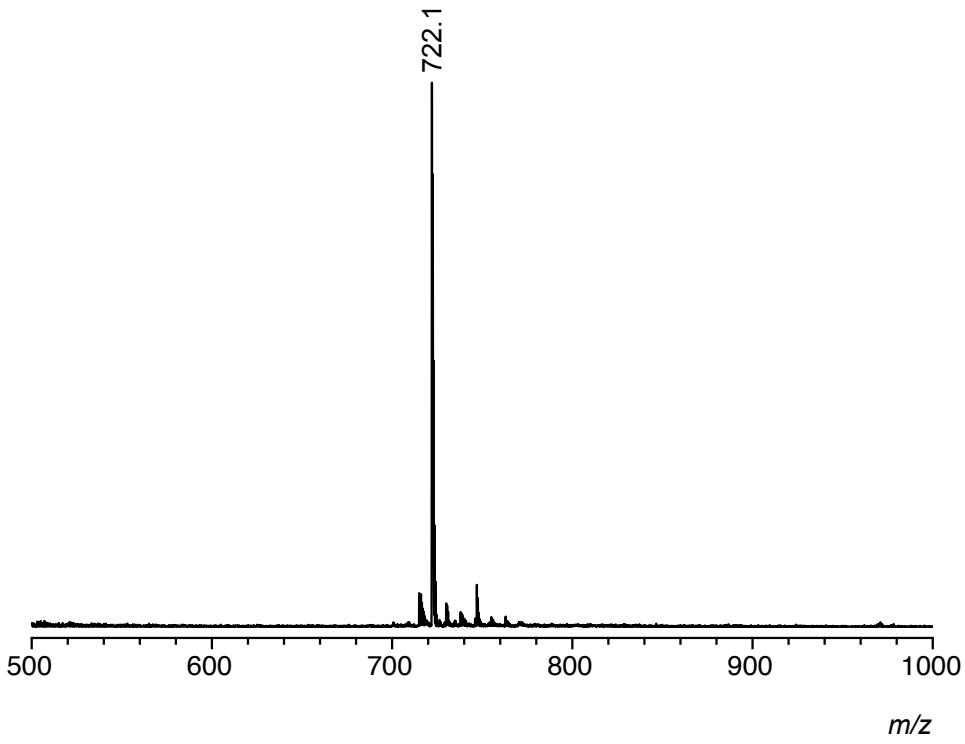
^{1}H NMR: **10a** (400 MHz, DMSO-d_6).



^{13}C NMR: **10a** (151 MHz, DMSO-d_6).

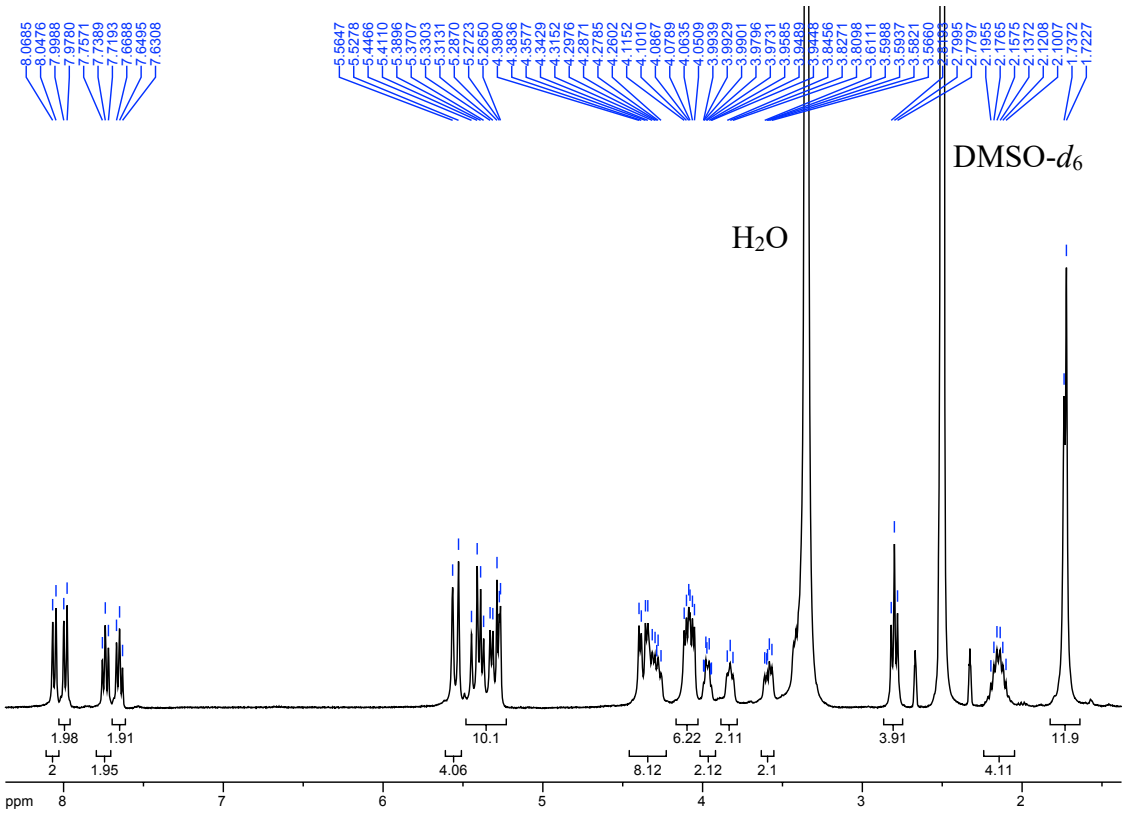


ESI-TOF MS: **10a** (ESI/TOF neg. mode).

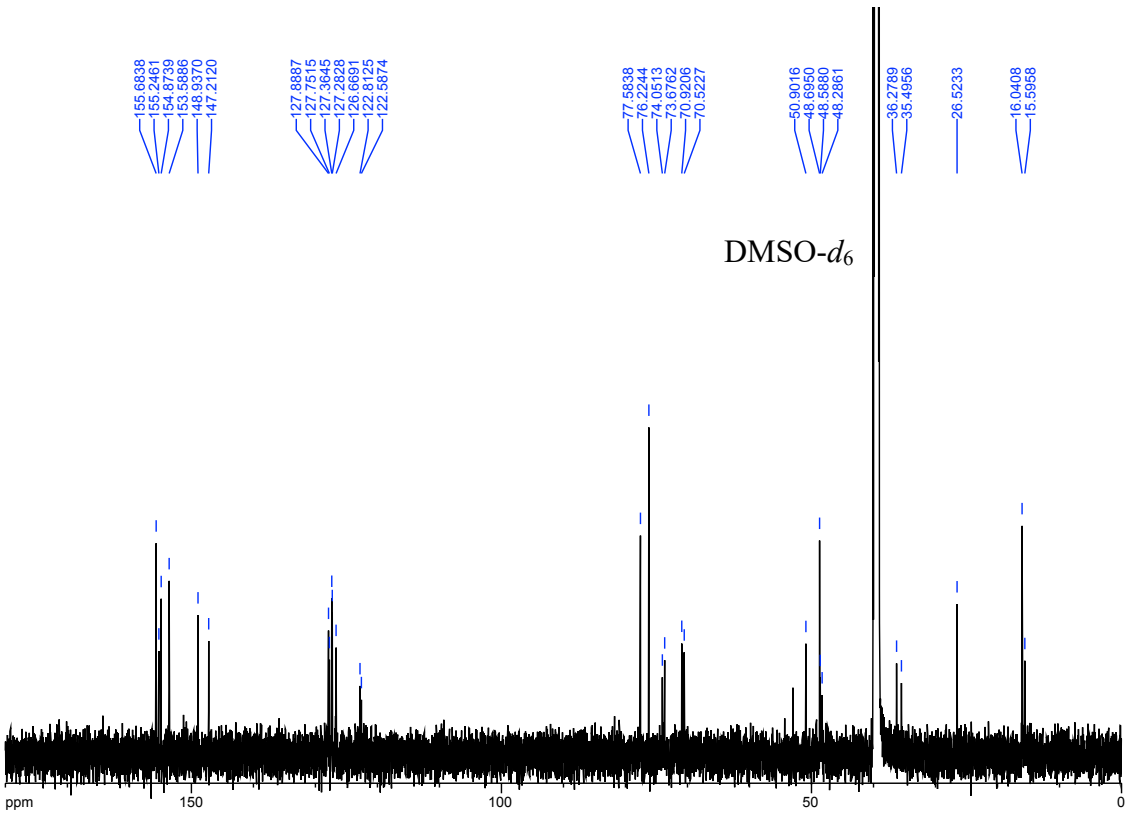


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{60}H_{64}N_{22}O_{18}S_2^{2–}$	722.2	722.1

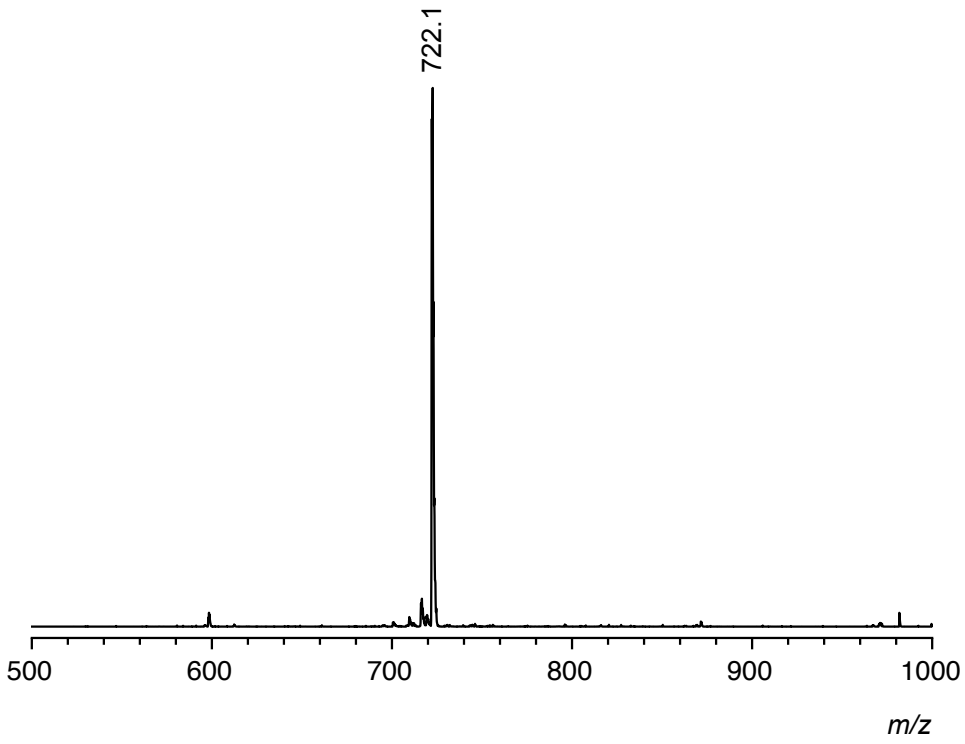
^{1}H NMR: **10b** (400 MHz, DMSO-d_6).



^{13}C NMR: **10b** (151 MHz, DMSO-d_6).

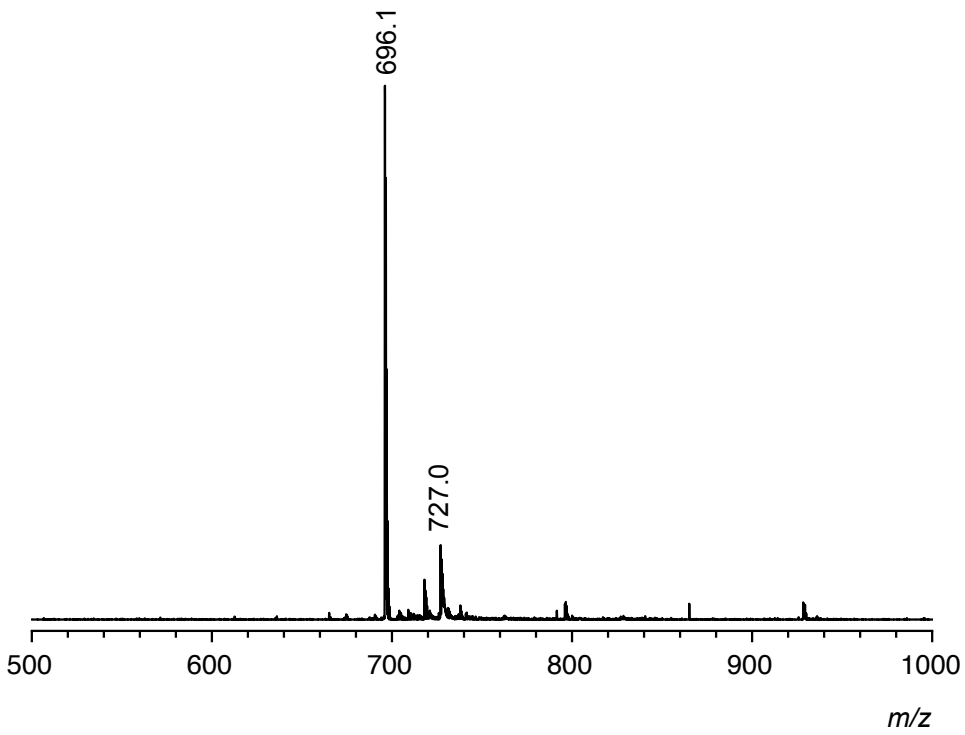


ESI-TOF MS: **10b** (ESI/TOF neg. mode).



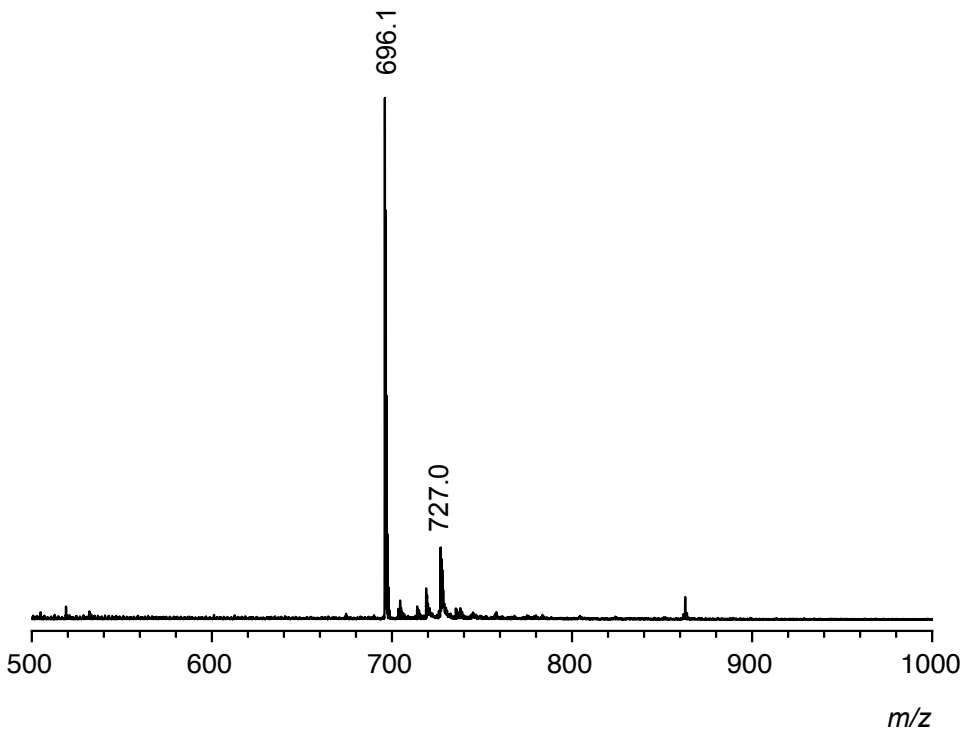
		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{60}H_{64}N_{22}O_{18}S_2^{2–}$	722.2	722.1

ESI-TOF MS: **11a** (ESI/TOF neg. mode).



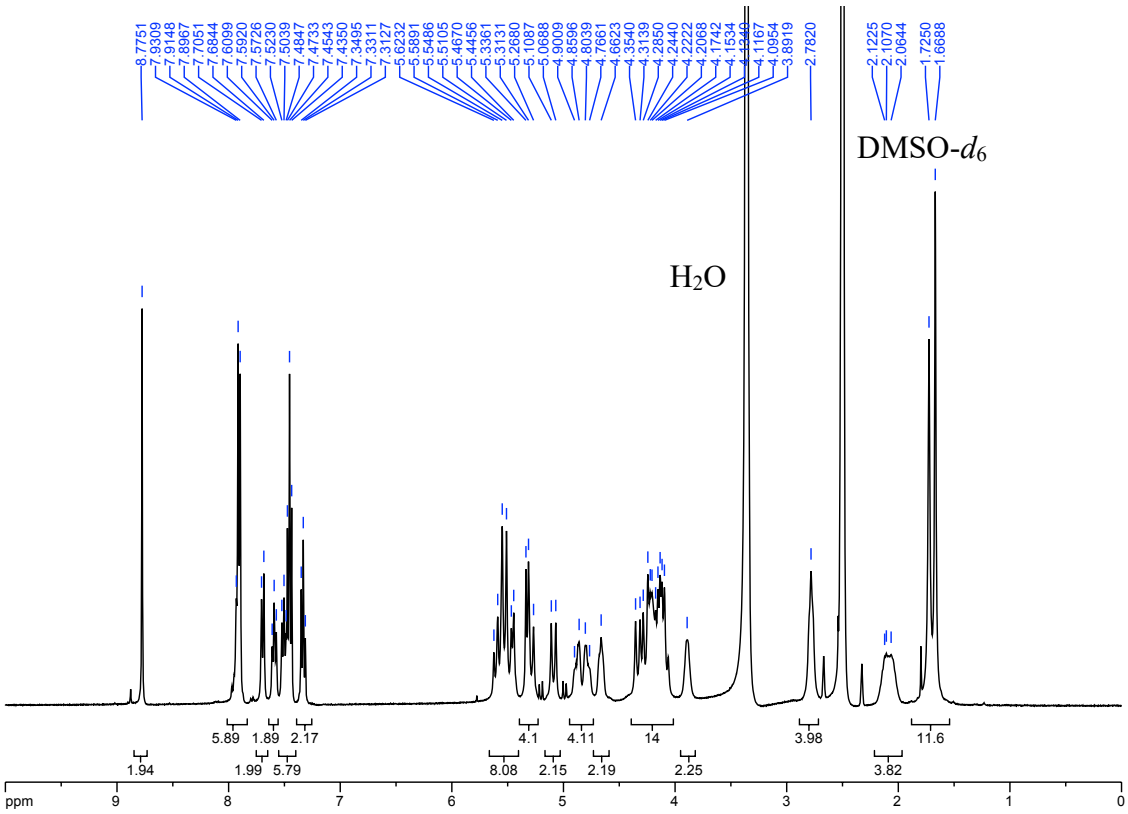
		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{60}H_{68}N_{18}O_{18}S_2^{2–}$	696.2	696.1
	peak could not be assigned		727.0

ESI-TOF MS: **11b** (ESI/TOF neg. mode).

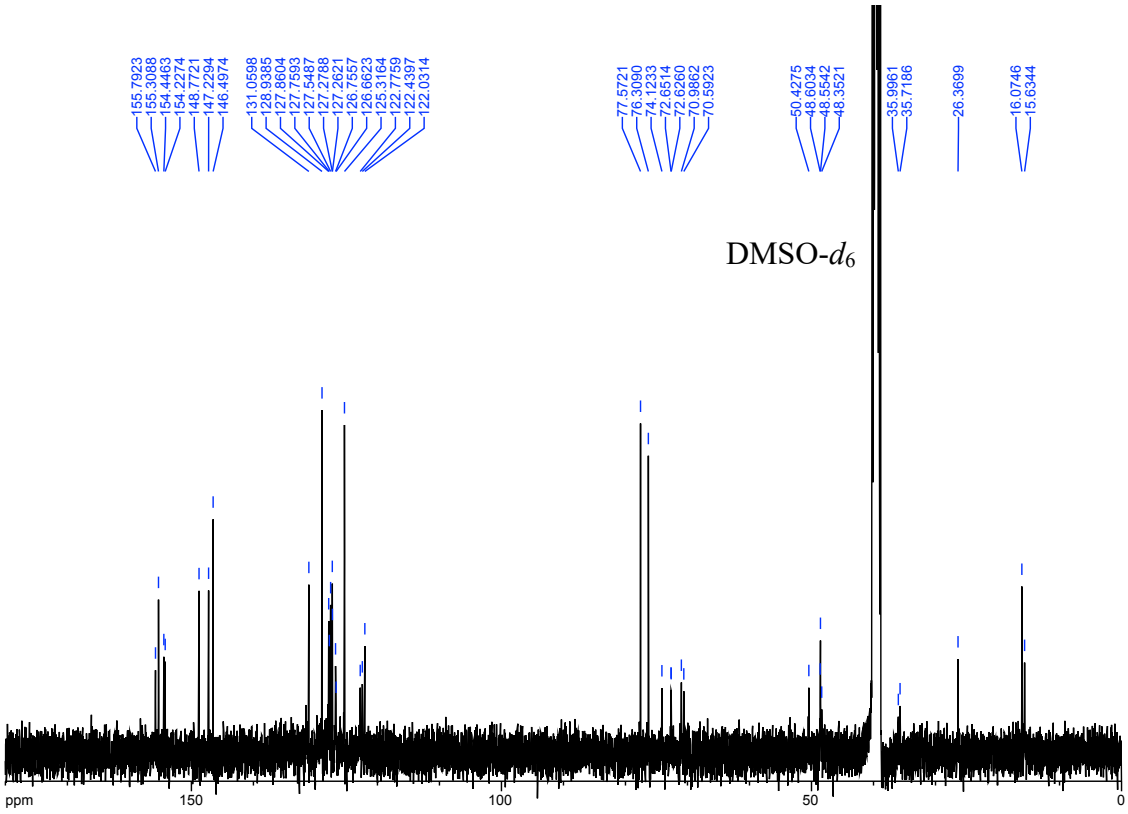


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{60}H_{68}N_{18}O_{18}S_2^{2–}$	696.2	696.1
	peak could not be assigned		727.0

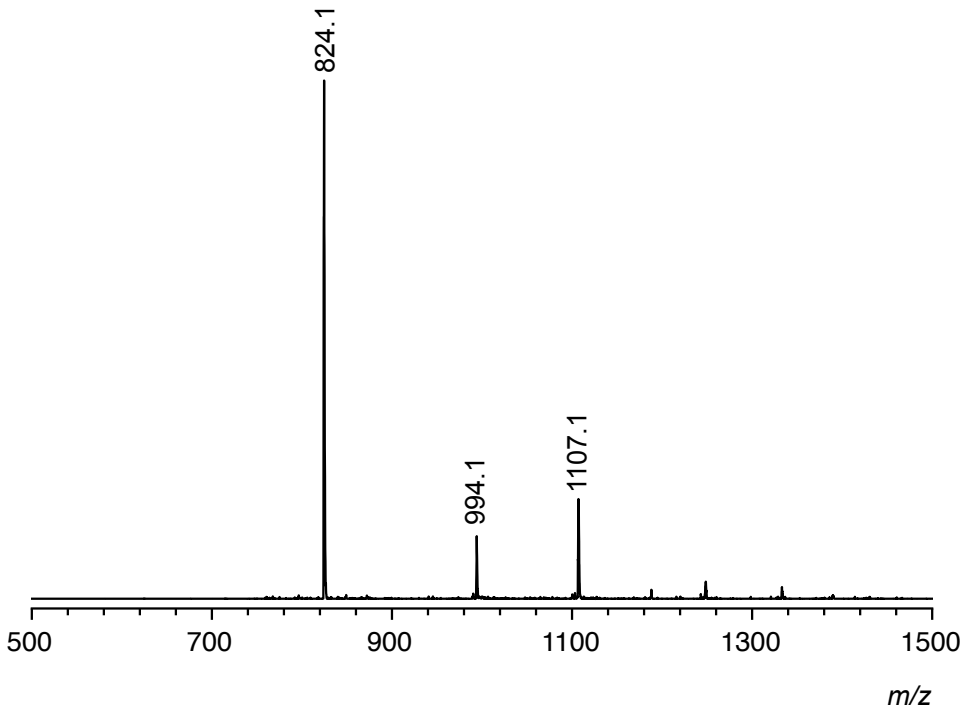
^{1}H NMR: **12a** (400 MHz, DMSO-d_6).



^{13}C NMR: **12a** (101 MHz, DMSO-d_6).

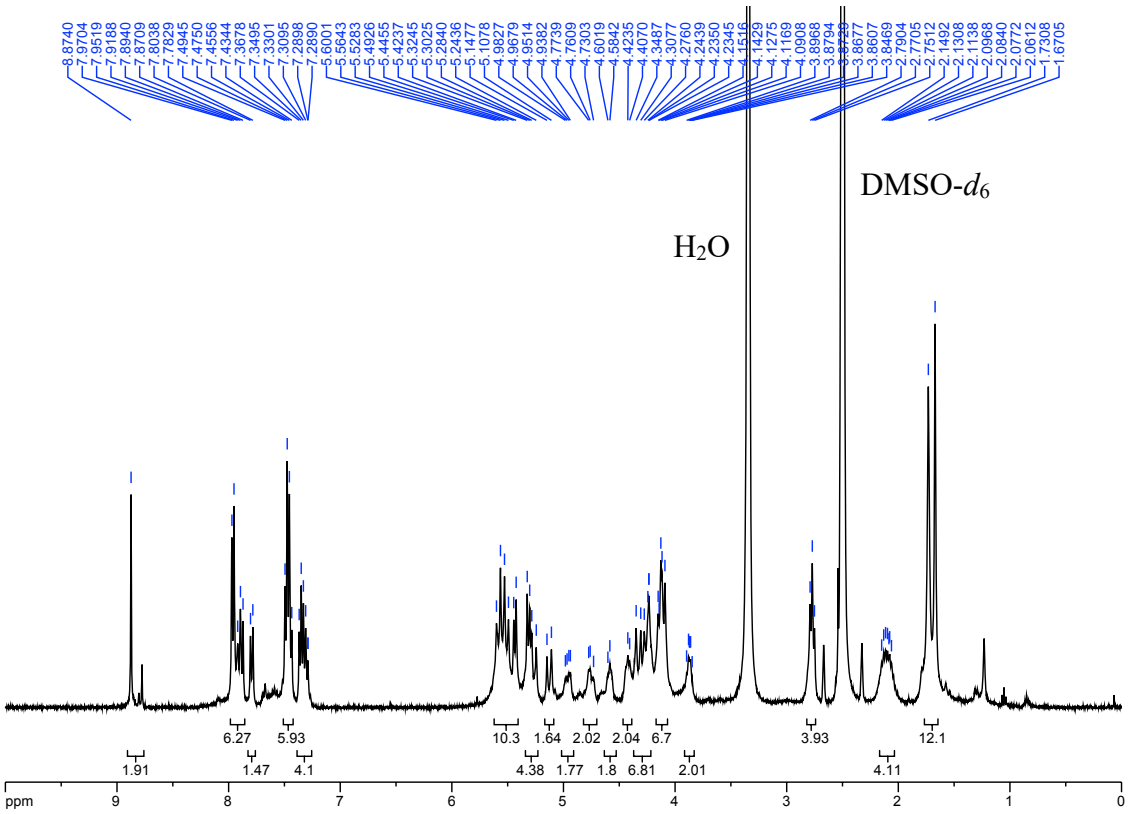


ESI-TOF MS: **12a** (ESI/TOF neg. mode).

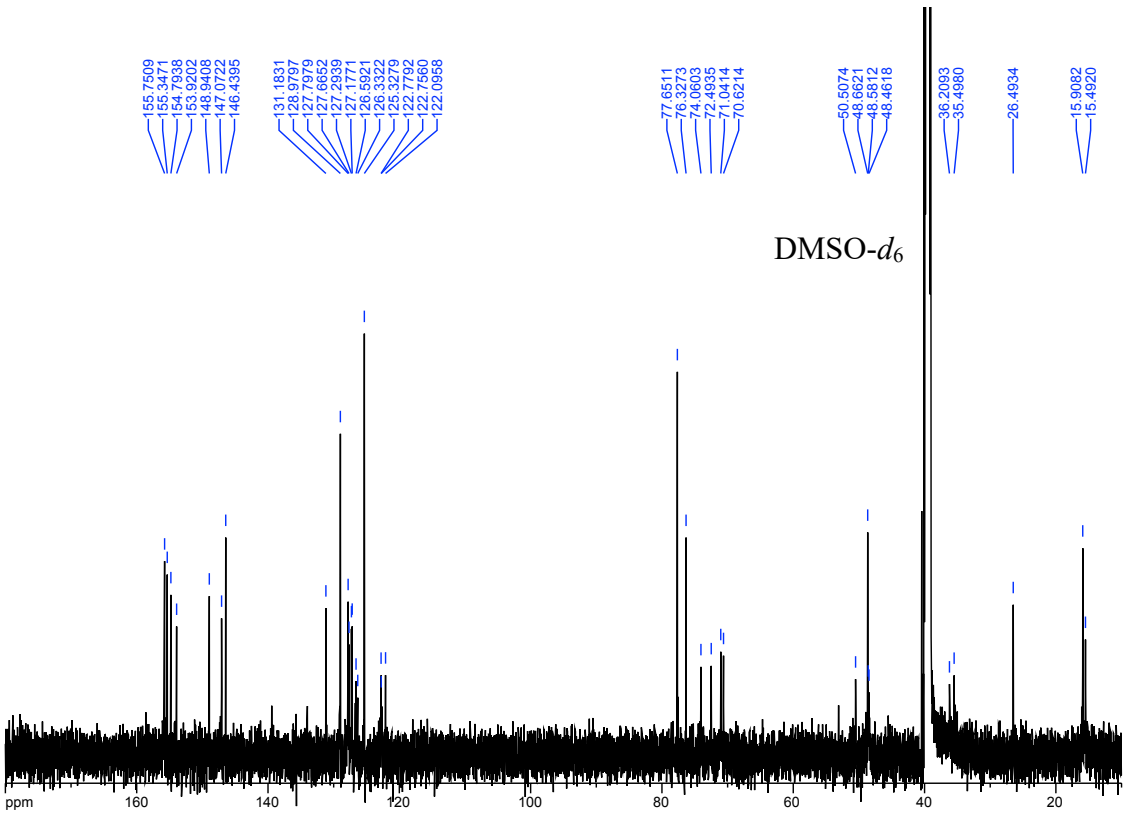


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{76}H_{76}N_{22}Na_2O_{18}S_2^{2–}$	824.3	824.1
$[M_3–5Na]^{5–}$	$[(C_{76}H_{76}N_{22}Na_2O_{18}S_2^{2–})_3Na]^{5–}$	994.3	994.1
$[M_2–3Na]^{3–}$	$[(C_{76}H_{76}N_{22}Na_2O_{18}S_2^{2–})_2Na]^{3–}$	1107.0	1107.1

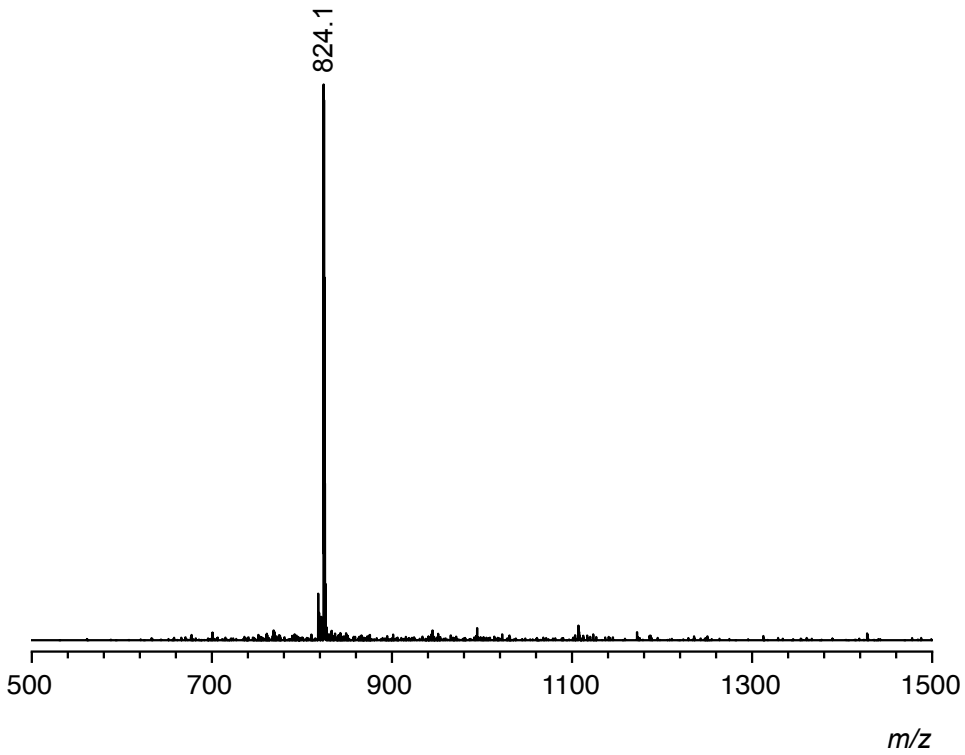
^{1}H NMR: **12b** (400 MHz, DMSO-d_6).



^{13}C NMR: **12b** (101 MHz, DMSO-d_6).

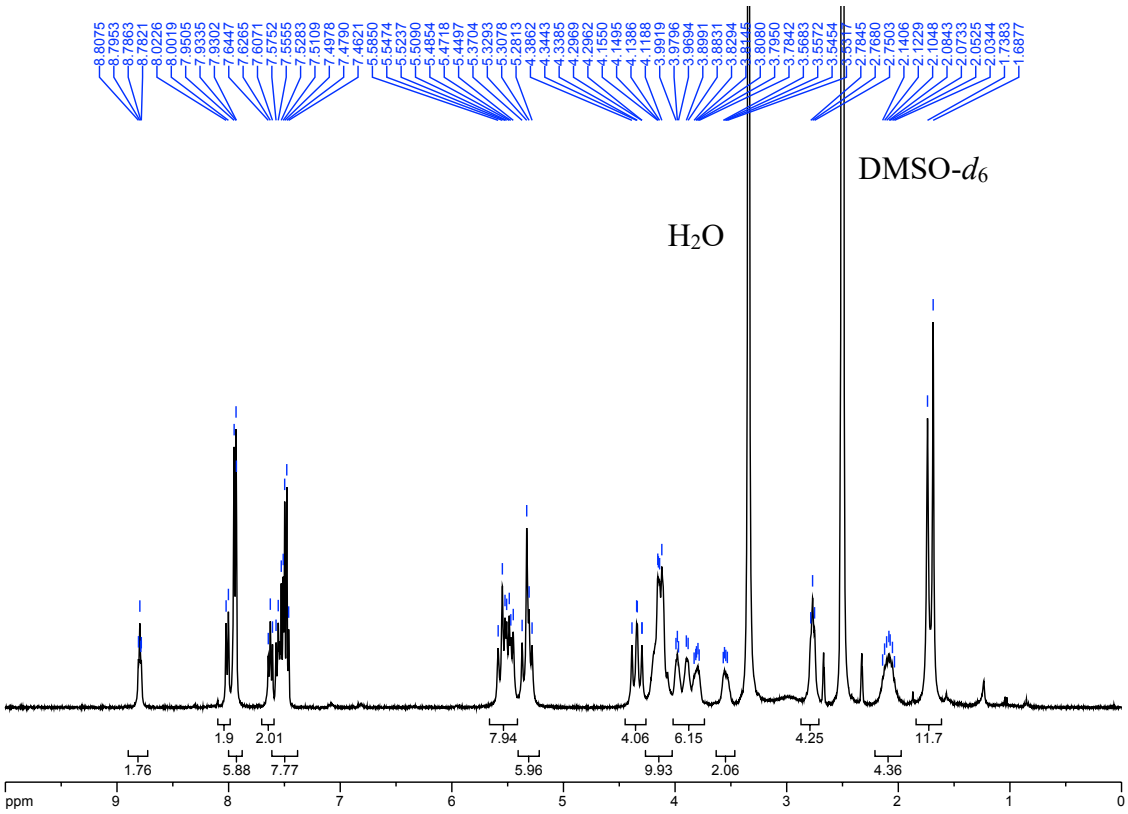


ESI-TOF MS: **12b** (ESI/TOF neg. mode).

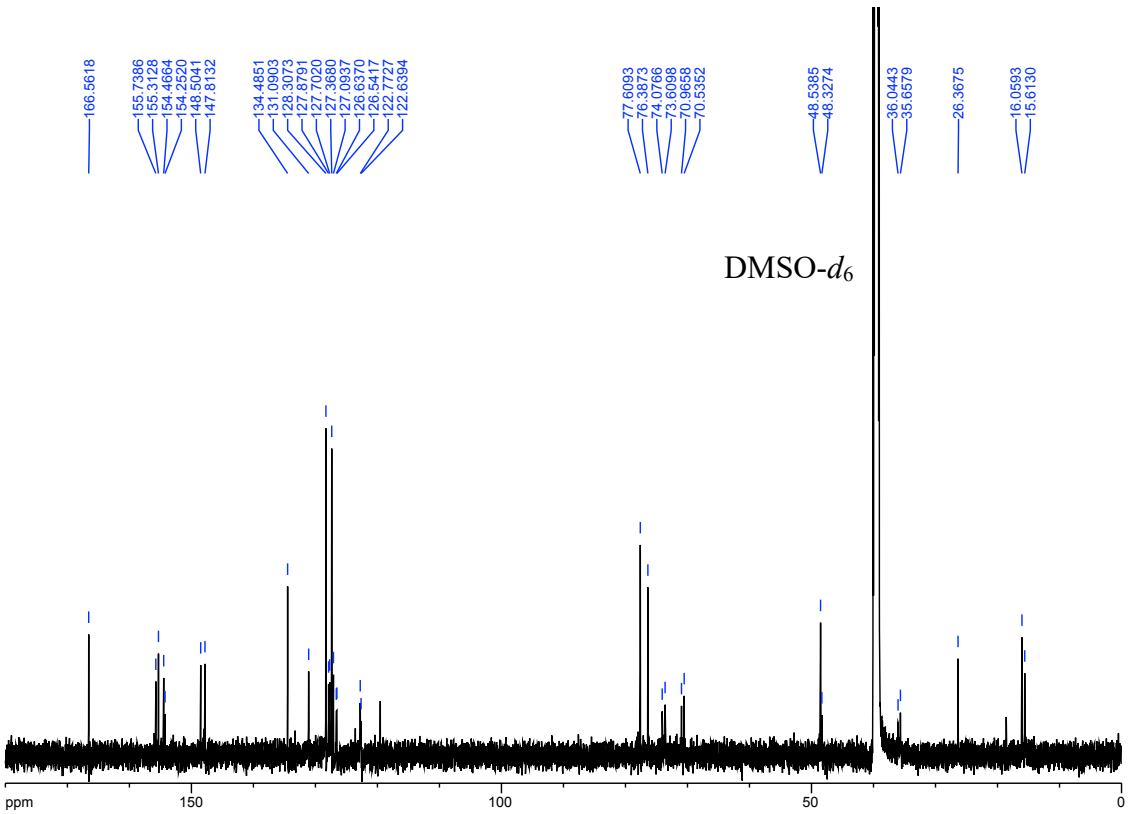


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{76}H_{76}N_{22}Na_2O_{18}S_2^{2–}$	824.3	824.1

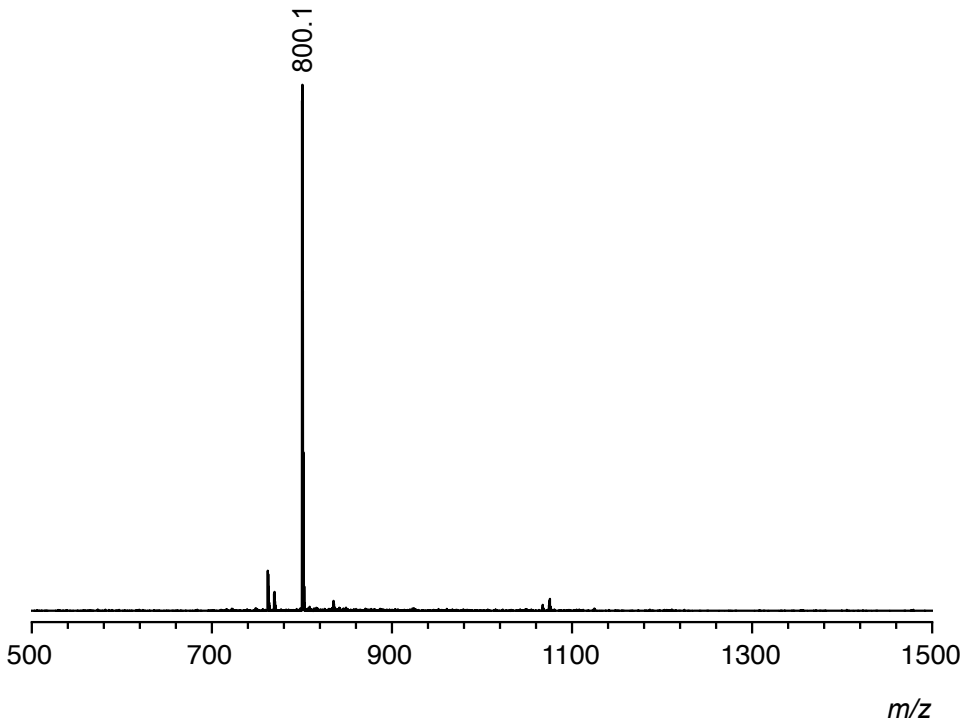
^{1}H NMR: **13a** (600 MHz, DMSO-d_6).



^{13}C NMR: **13a** (151 MHz, DMSO-d_6).

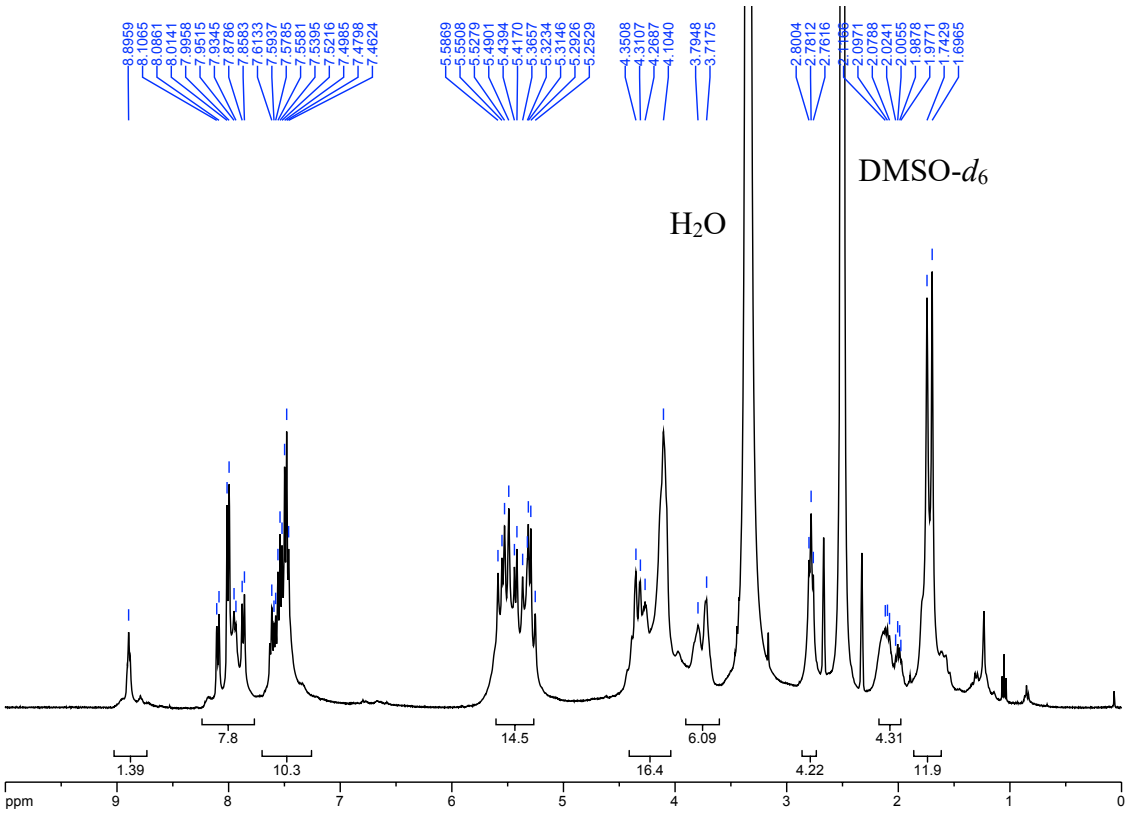


ESI-TOF MS: **13a** (ESI/TOF neg. mode).

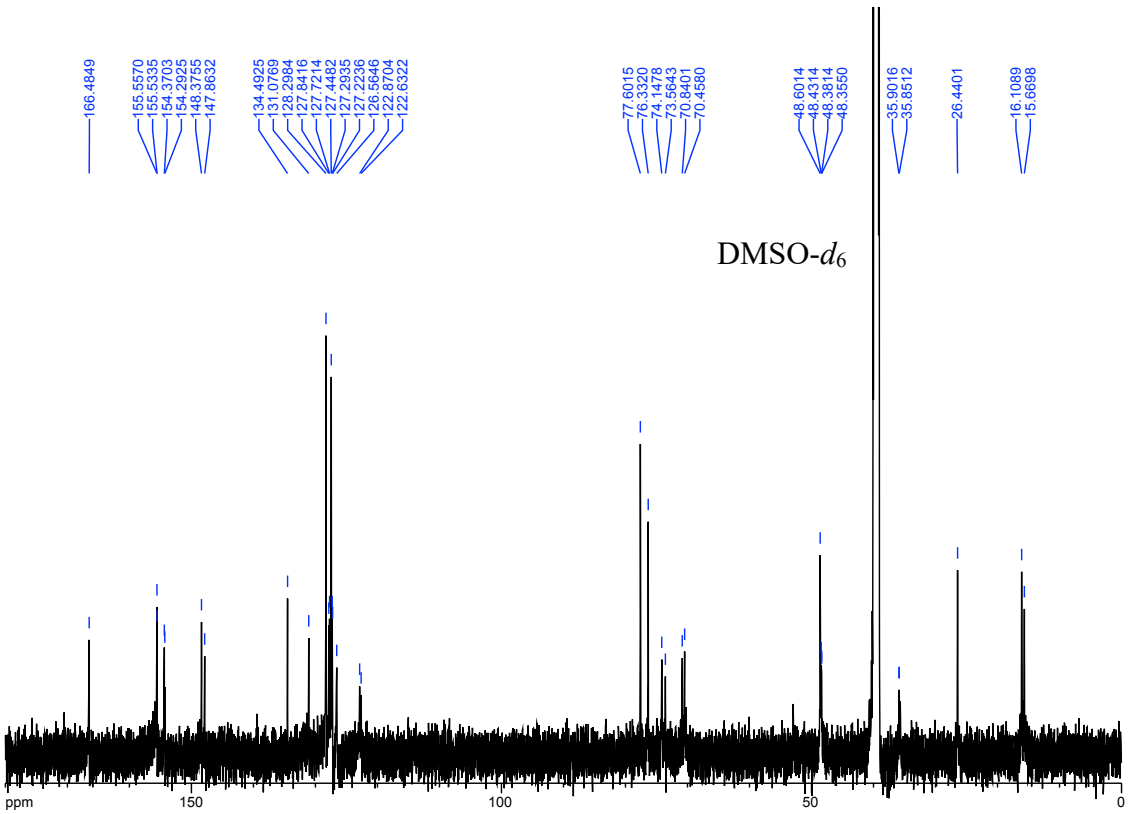


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{74}H_{76}N_{18}Na_2O_{20}S_2^{2–}$	800.3	800.1

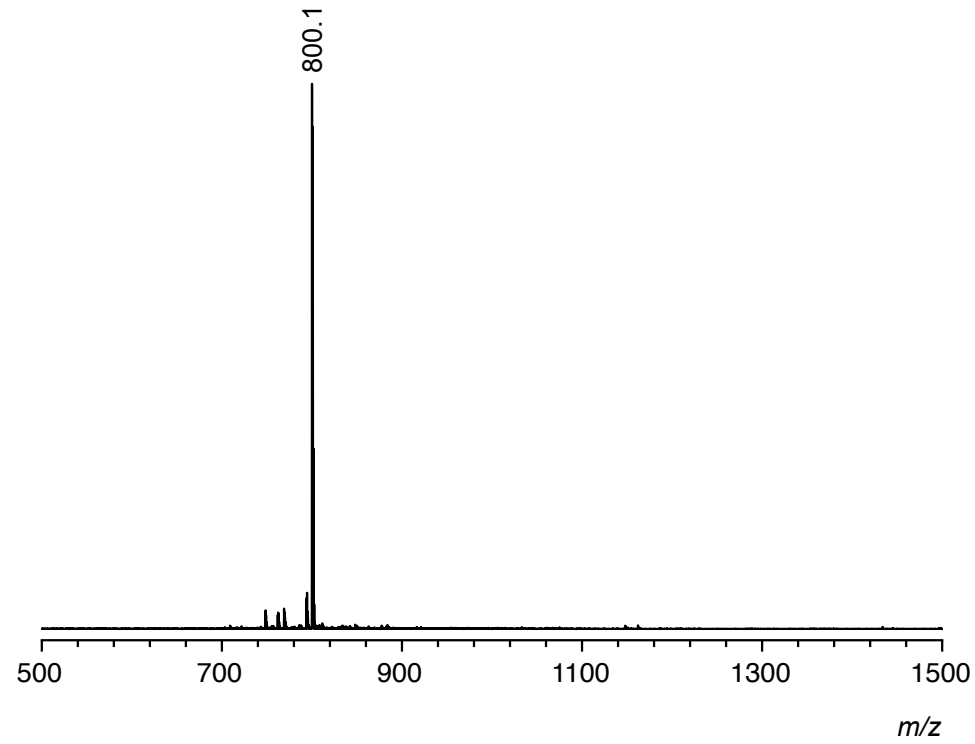
^{1}H NMR: **13b** (600 MHz, DMSO-d_6).



^{13}C NMR: **13b** (151 MHz, DMSO-d_6).

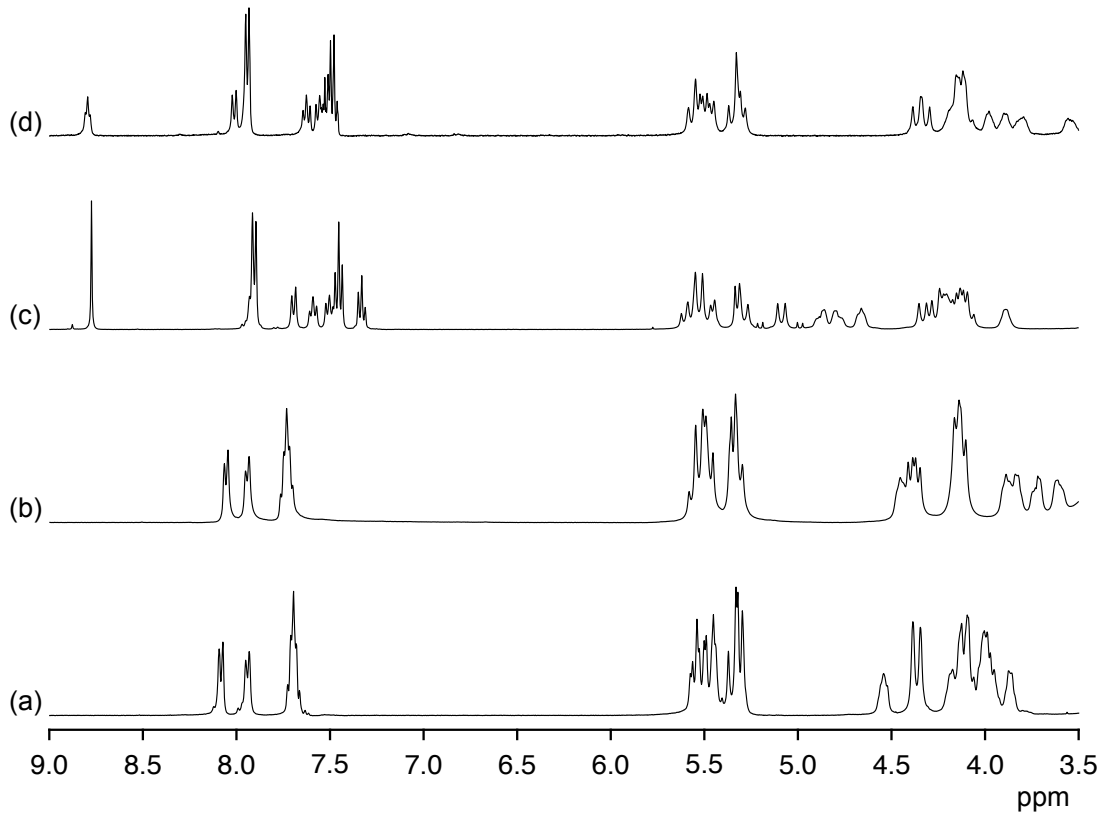


ESI-TOF MS: **13b** (ESI/TOF neg. mode).

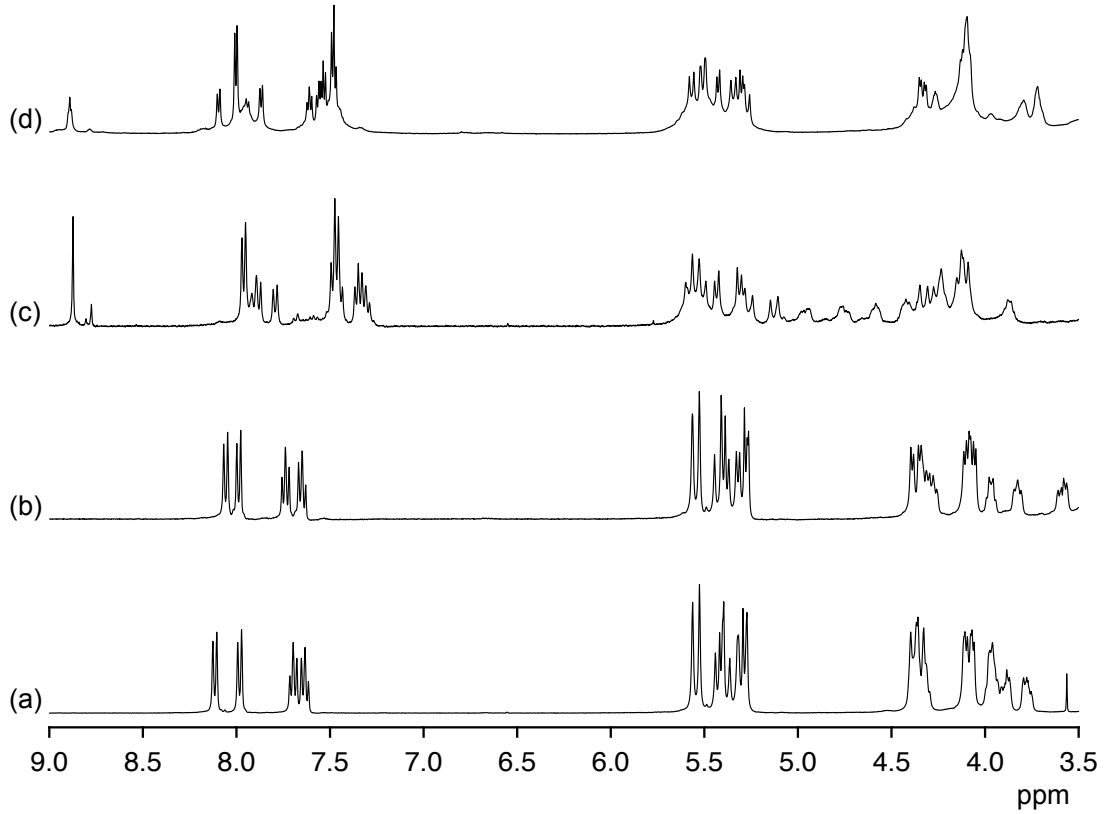


		m/z calcd.	*m/z exp.*
$[M–2Na]^{2–}$	$C_{74}H_{76}N_{18}Na_2O_{20}S_2^{2–}$	800.3	800.1

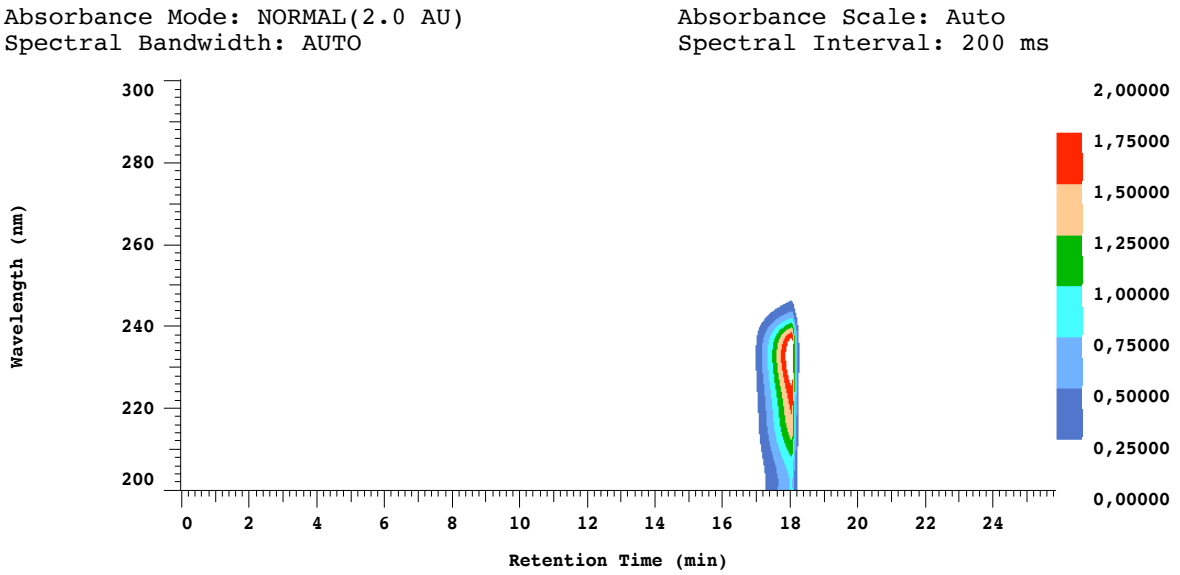
Comparison of the ^{1}H NMR spectra of **2a** (a), **10a** (b), **12a** (c), and **13a** (d) (400 MHz, DMSO-d_6).

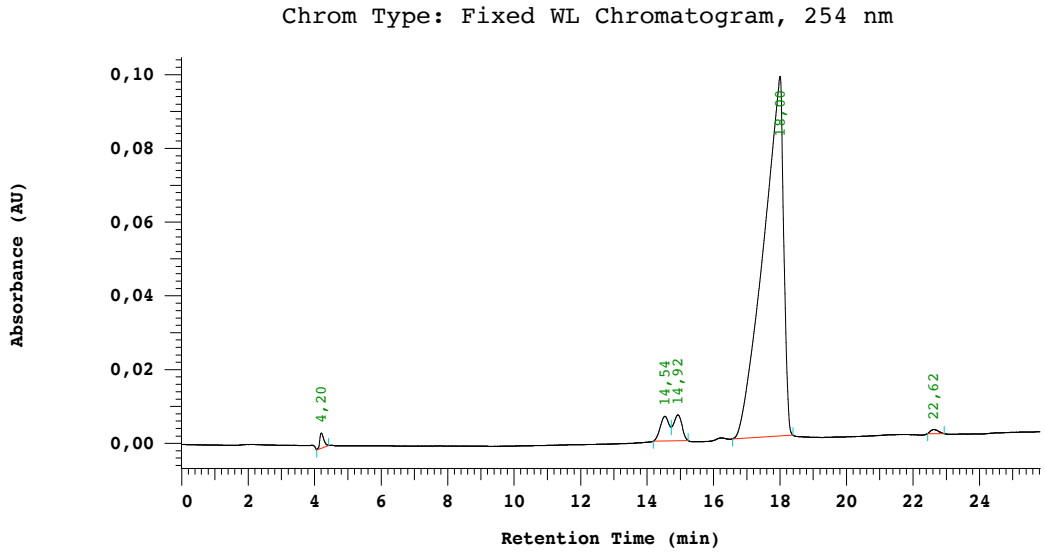


Comparison of the ^{1}H NMR spectra of **2b** (a), **10b** (b), **12b** (c), and **13b** (d) (400 MHz, DMSO-d_6).



Chiral HPLC Chromatogram of **2a**.



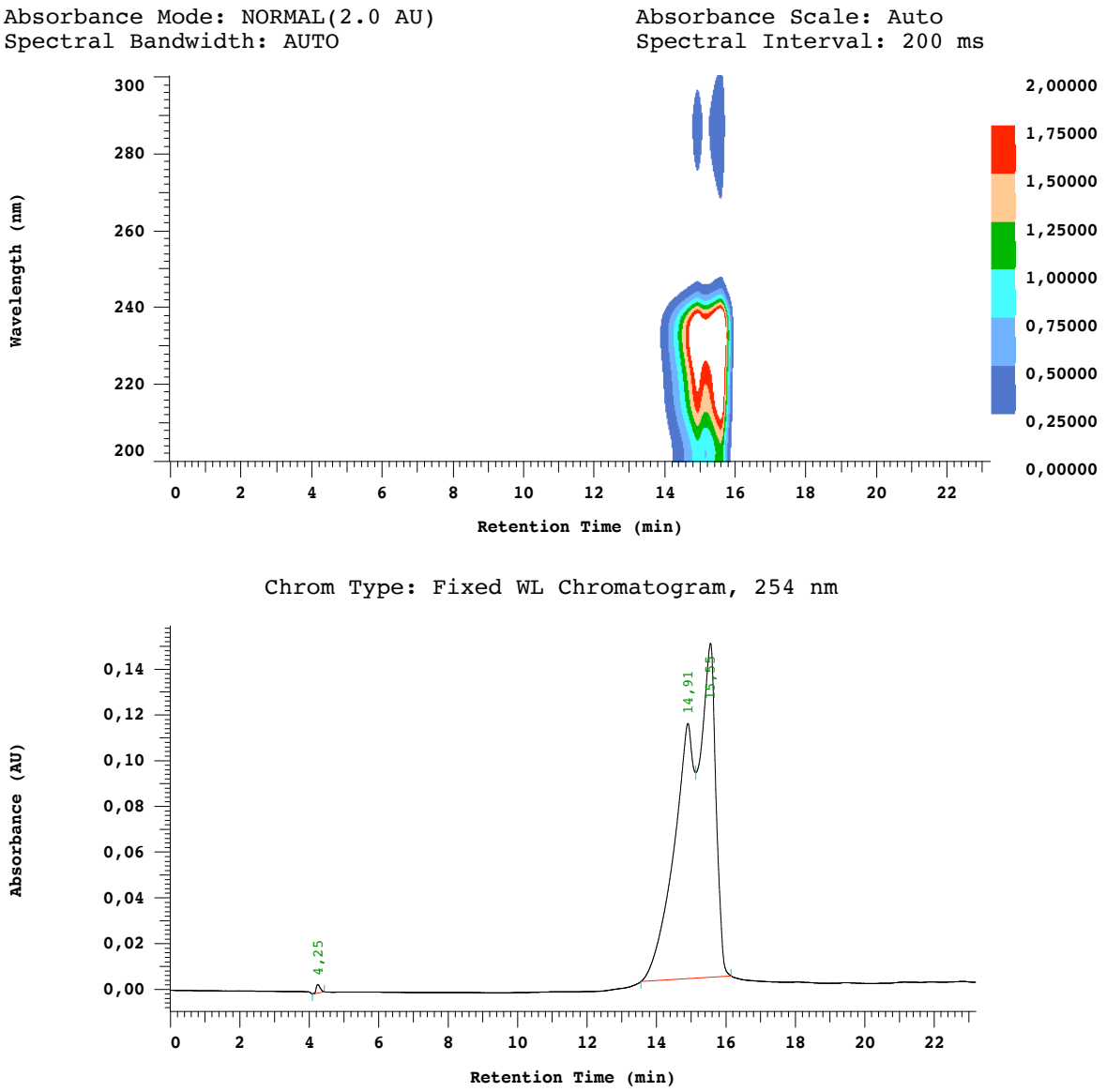


D-7000 HSM: Samples | Series: 0313 | Report: original | System: Sys 1

No.	RT	Area	Conc 1	BC
1	4,20	16650	0,758	BB
2	14,54	60783	2,765	BV
3	14,92	62349	2,837	VB
4	18,00	2049693	93,252	BB
5	22,62	8540	0,389	BB
		2198015	100,000	

Peak rejection level: 0

Chiral HPLC Chromatogram of **2b**.



D-7000 HSM: Samples Series: 0310 Report: original System: Sys 1

No.	RT	Area	Conc 1	BC
1	4,25	14911	0,329	BB
2	14,91	2262387	49,976	BV
3	15,55	2249685	49,695	VB
		4526983	100,000	

Peak rejection level: 0

ITC Titrations:

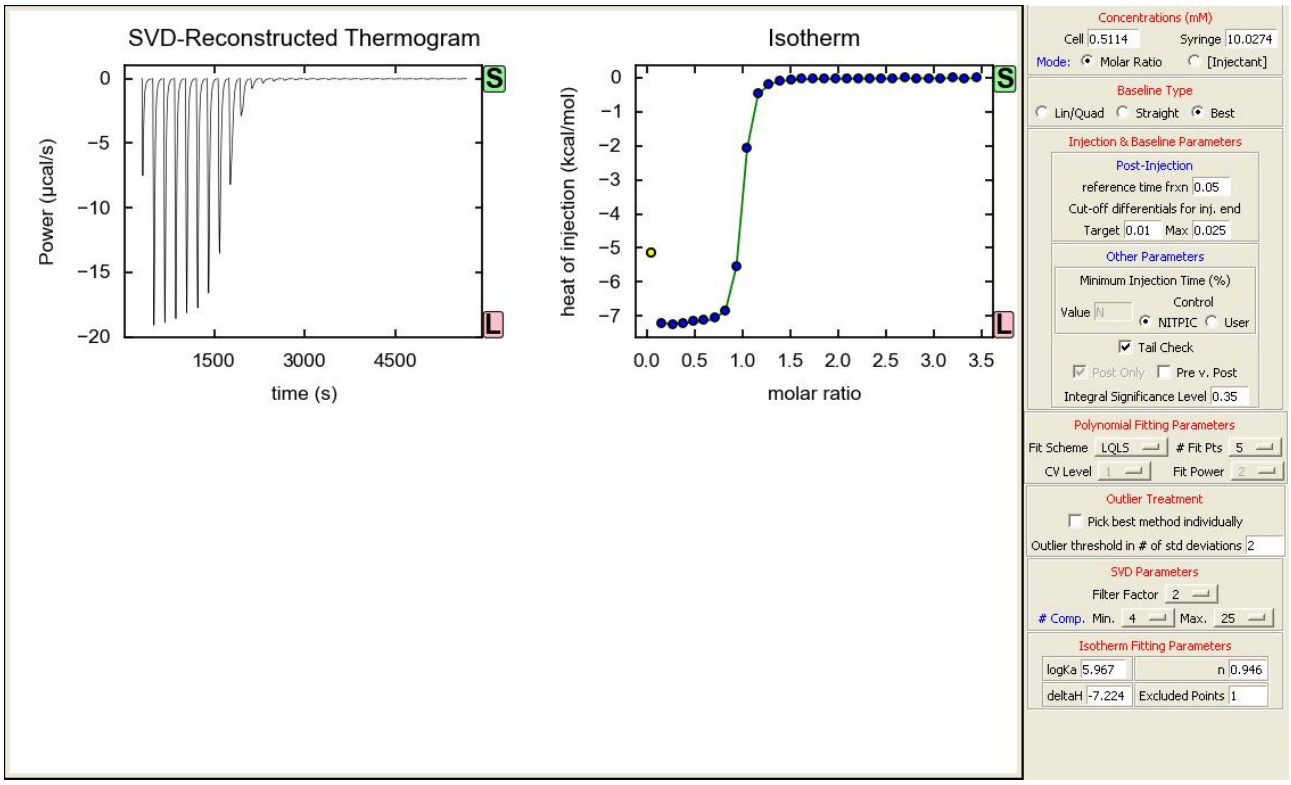
The ITC experiments were carried out in water. Acetylcholine was used as its chloride salt. The salt and receptors **10a**, **10b** and **14** were weighed using an analytical precision balance, dissolved in known volumes of water, and loaded into the system for immediate analysis. The concentrations of the binding partners used in the individual measurements are summarized in Table S1. The measurements were carried out at 25 °C using a reference power of 30.0–34.8 µCal/s, a stirring speed of 307 rpm, a filter period of 2 s, an injection delay of 8 s, and a spacing time of 180 s. For the first 15 injections, an injection volume of 4 µL was used and for injections 16 to 30 an injection volume of 6 µL. Automated baseline assignment and peak integration of raw thermograms were accomplished by singular value decomposition and peak-shape analysis using NITPIC.[5]

Table S1. Concentrations and experimental parameters of the individual titrations.

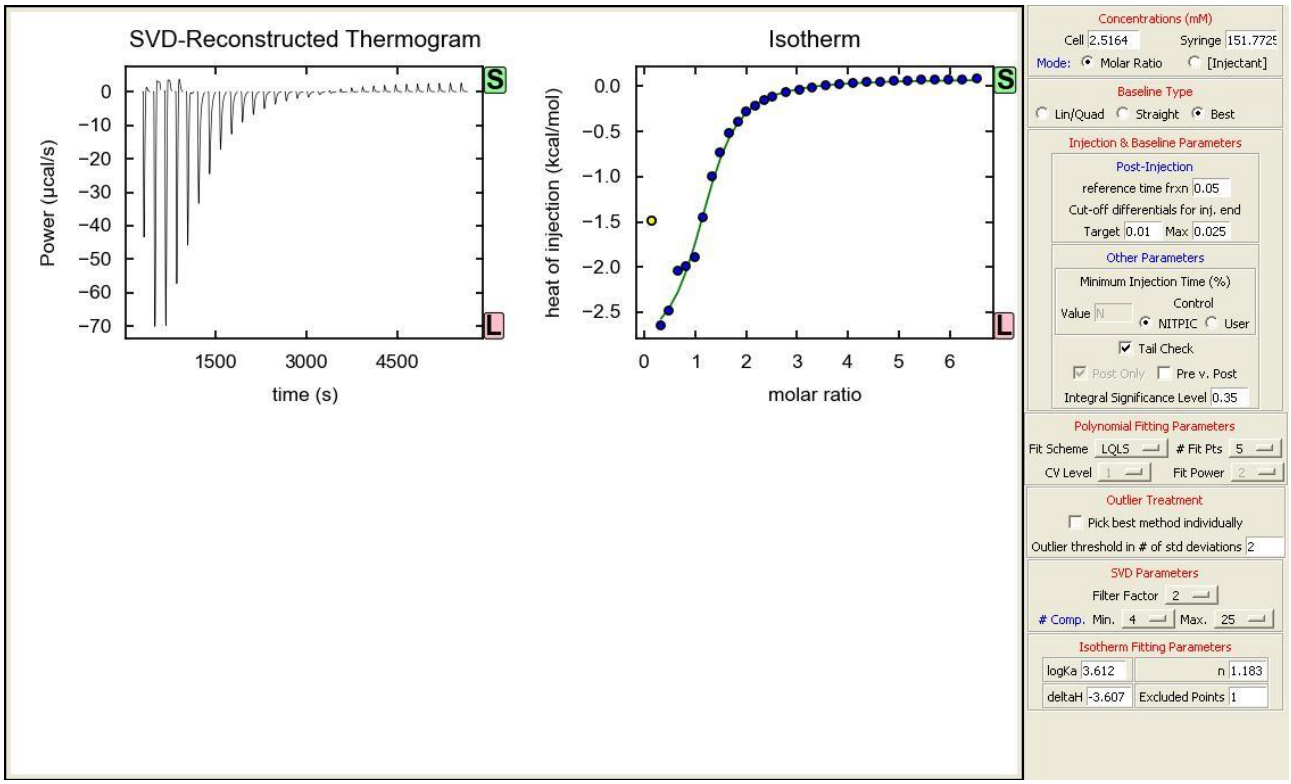
receptor	c(receptor) / mM	c(ACh·Cl) / mM
14	0.5	10
10a	2.5	150
10b	2.5	150

Obtained thermograms and binding isotherms are shown in the following figures.

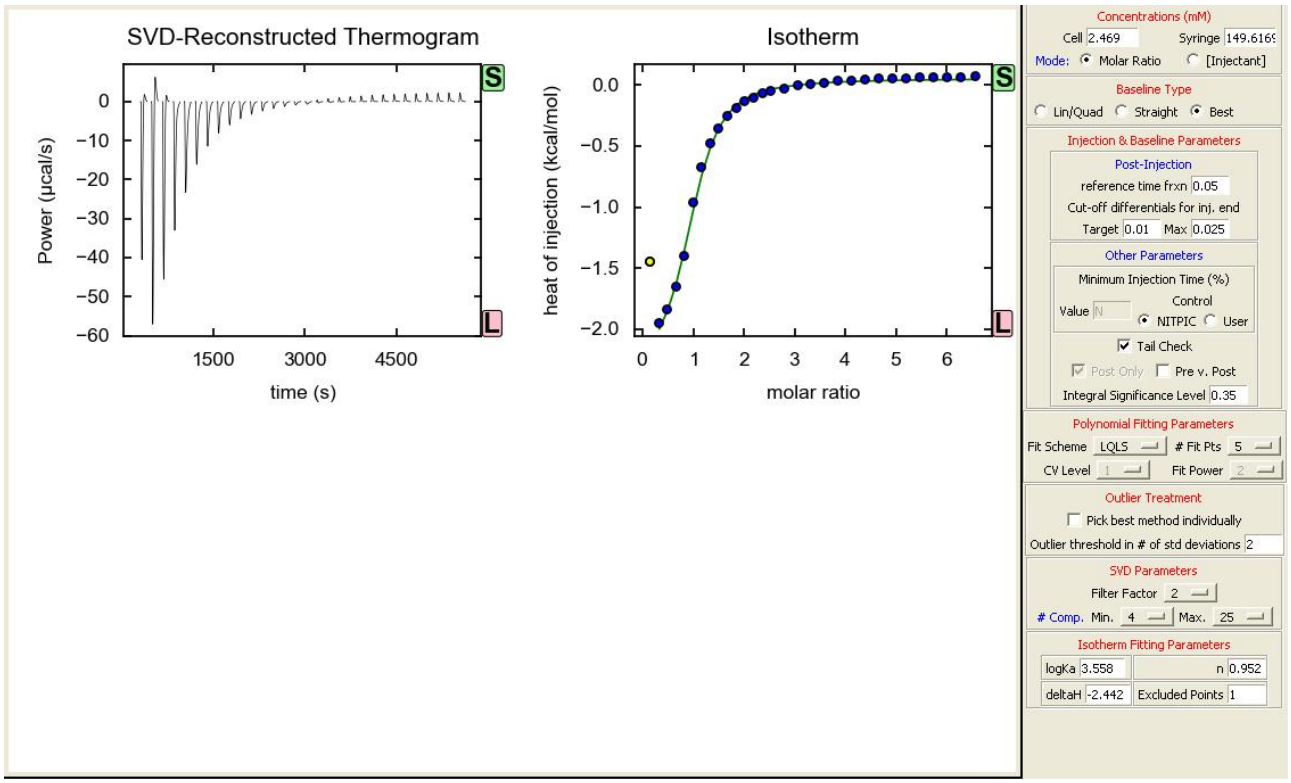
Thermogram and Binding Isotherm: Titration of **14** with acetylcholine chloride in H_2O.



Thermogram and Binding Isotherm: Titration of **10a** with acetylcholine chloride in H_2O.



Thermogram and Binding Isotherm: Titration of **10b** with acetylcholine chloride in H_2O.



X-Ray Data Collection and Refinement

Single crystal X-ray diffraction studies were performed using suitable crystals of **2b** and **10a**. The single crystal was mounted on a MiTeGen Dual Thickness MicroMount™ with Fomblin Y oil and transferred to a N_2 cold stream (100 K) by an OXFORD CRYOSYSTEMS 700 low temperature system. Data were collected at low temperatures (100 K) using φ- and ω-scans on a BRUKER D8 Venture system equipped with dual IμS microfocus sources and a PHOTON100 detector. Cu-K_α radiation with wavelength 1.54178 Å and a collimating Quazar multilayer mirror were used. Semi-empirical absorption corrections from equivalents were calculated with SADABS-2016/2.[6] The space groups were determined using *XPREP*[7] through analysis of the Laue symmetry and systematic absences. The structures were solved with *SHELXT*.[8] The structures were refined by full-matrix least-squares based on F^2 using *SHELXL* (Re. 859)[9] and *SHELXle*[10] as a graphical interface. Both structures were checked for a higher symmetry using *PLATON*.[11] All non-hydrogen atoms were located and refined anisotropically. Hydrogen atoms were assigned to idealized positions and given thermal parameters equal to either 1.5 (methyl hydrogen atoms and water hydrogen atoms) or 1.2 (non-methyl hydrogen atoms) times the thermal displacement parameters of the atoms to which they were attached. Advanced rigid-bond restraints were applied to all atoms in the structures. Similarity restraints on 1,2 distances were used to model disorder components. U_{ij} components of disordered atoms were restrained with similar ADP restraints. The behavior of the U_{ij} components of disordered atoms in **10a** was additionally approximated to isotropic behavior.

Crystal Structure of 2b. **2b** crystallized as colorless needles while slowly diffusing acetonitrile into a solution in EtOH/H_2O, 2:1 (*v/v*) containing a few drops of TFA. The compound crystallized as a polymer in the orthorhombic space group *Pbcn*. The asymmetric unit contains two half molecules of the organic ligand bridged *via* two sodium ions that are coordinated by two additional acetonitrile molecules and one water molecule (Figure S1). Na2 is coordinated in a distorted trigonal bipyramidal mode by five atoms. One organic ligand binds as a tridentate ligand *via* one sulfonate oxygen donor and two carbonyl oxygen donors, one of which (O38) bridges both sodium ions. The coordination sphere is completed by another carbonyl oxygen donor (O8) from the second organic ligand and one acetonitrile solvent molecule. Na1 is coordinated by six atoms in an octahedral fashion. Similar to Na2, three oxygen donors derive from the same ligand and a forth oxygen donor (O38) derives from the opposite ligand. The coordination sphere is saturated by one acetonitrile (N61) and one water molecule (O81). The positions of the H-atoms of H2O81 were taken from the Fourier synthesis and assigned to idealized positions. Their U_{ij} components were set to 1.5 times the thermal displacement parameters of the oxygen atoms they are attached to.

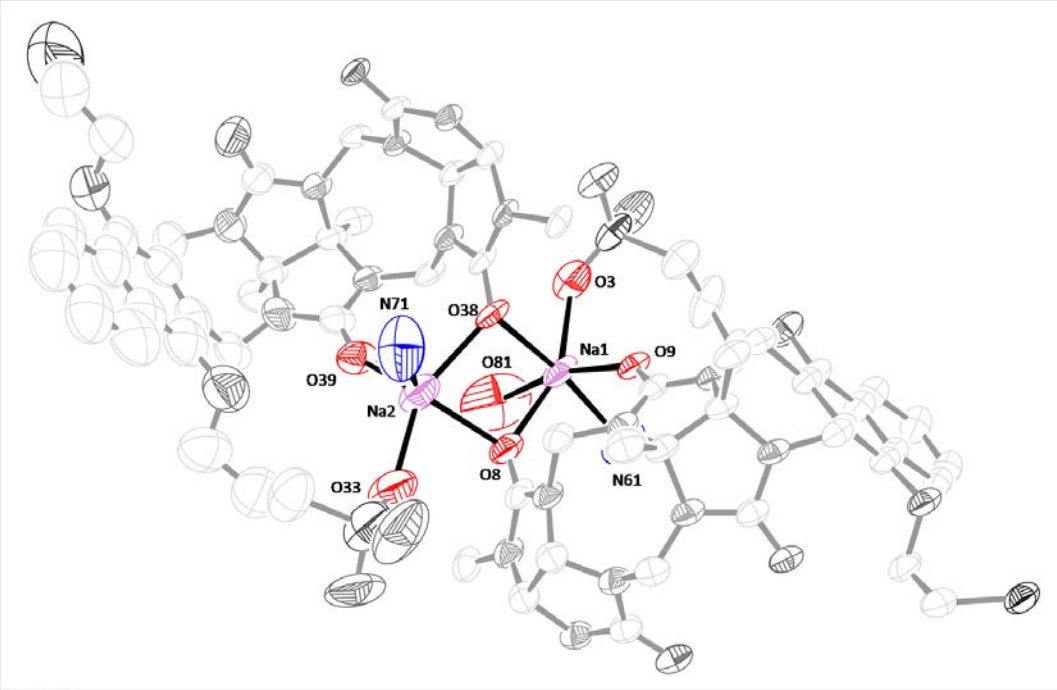


Figure S1: ORTEP-plot of the asymmetric unit of **2b** with the bridging sodium water motif highlighted. Thermal ellipsoids set at 50% probability. Hydrogen atoms and acetonitrile carbon atoms are omitted for clarity.

The positions of the sodium ions, the coordinated water molecule, and one acetonitrile molecule are rather well defined. The organic ligands, however, display a whole molecule disorder. Each half ligand was treated independently and modeled across two positions. The main occupied species refined to 82.2% (esd 0.3%) and 68.1% (esd 0.5%), respectively (Figure S2). The disorder, however, is not resolved well. Even though similar ADP restraints have been applied, the thermal ellipsoids of one half ligand are not well behaved. A stronger set of restraints was applied during the refinement, however, it did not lead to any improvement and accordingly was not included in the final refinement model. One of the coordinated acetonitrile molecules shows an additional, independent disorder. It was modeled across two positions. The main occupied species refined to 87.5% (esd 0.7%).

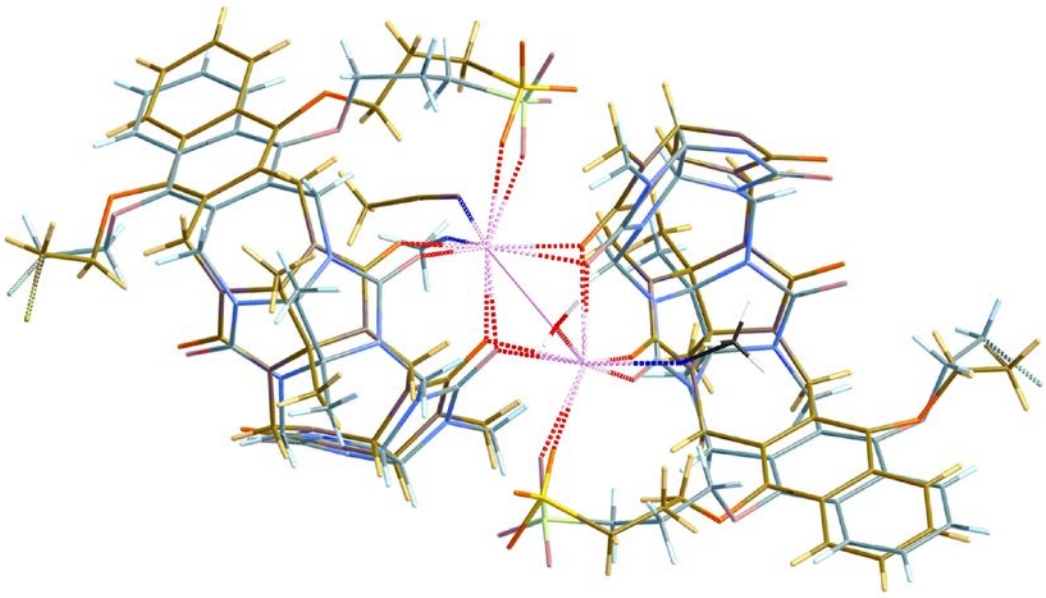


Figure S2: Stick model of all disorder components in the asymmetric unit. Main occupied components are highlighted in blue, minor occupied components in yellow.

Several free solvent molecules were found in the lattice. Their positions were rather poorly defined, thus, SQUEEZE as implemented in PLATON[11] was used to handle this solvent disorder. SQUEEZE found two solvent accessible voids that are located at -0.099 0.000 0.224 and -0.003 0.500 0.731 (Figure S3). Both voids have a volume of 2993 $Å^3$ and contain 328 electrons. It is impossible to determine the exact solvent composition based on the crystal structure alone because a solvent mixture has been used to crystallize **2b**. One possible combination comprises 9 acetonitrile and 13 water molecules (a total of 328 electrons) per unit cell.

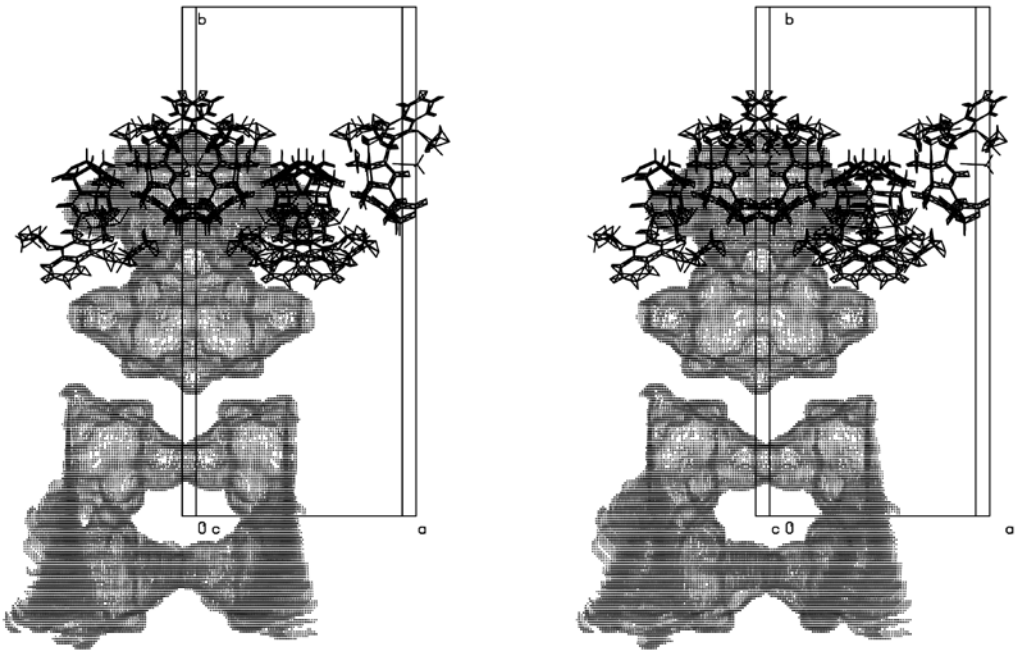


Figure S3: Stereo view of the solvent accessible voids in the unit cell. All disorder components of **2b** are shown.

In general, the dataset is of a rather mediocre quality, as demonstrated by a low mean I and mean I/s at high resolutions so that it had to be truncated at 0.82 Å. Intensity statistic, crystal data, and refinement parameters are listed below.

Table S2: Crystal data and structure refinement for **2b**.

CCDC number	1890949	
Empirical formula	$C_{64}H_{72}Cl_2N_{18}Na_2O_{19}S_2$	
Formula weight	1578.39	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	*Pbcn*	
Unit cell dimensions	a = 19.1042(9) Å	α = 90°
	b = 43.808(2) Å	β = 90°
	c = 23.0275(11) Å	γ = 90°
Volume	19272.3(16) $Å^3$	

Z	8
Density (calculated)	1.088 Mg/m^3
Absorption coefficient	1.635 mm^{-1}
F(000)	6576
Crystal size	0.121 x 0.083 x 0.055 mm^3
Theta range for data collection	2.523 to 70.067°
Index ranges	–22<=h<=23, –53<=k<=53, –28<=l<=28
Reflections collected	389997
Independent reflections	18294 [R(int) = 0.0971]
Completeness to theta = 67.679°	99.9%
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18294 / 6516 / 1871
Goodness-of-fit on F^2	2.172
Final R indices [I>2sigma(I)]	R1 = 0.1112, wR2 = 0.3068
R indices (all data)	R1 = 0.1383, wR2 = 0.3181
Extinction coefficient	0.00029(4)
Largest diff. peak and hole	0.714 and -0.911 $e.Å^{-3}$

Table S3: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2b**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	*U*(eq)
Na(1)	2110(1)	6773(1)	7955(1)	65(1)
Na(2)	2873(1)	6044(1)	8032(1)	85(1)
Cl(1)	–1089(1)	7570(1)	3883(1)	64(1)
S(1)	2975(1)	7480(1)	8377(1)	65(1)
O(1)	1495(2)	7776(2)	6857(2)	56(1)
O(2)	–74(4)	7564(2)	4877(3)	48(1)
O(3)	2707(3)	7173(2)	8488(3)	102(2)
O(4)	2823(3)	7717(2)	8789(2)	101(2)
O(5)	3713(2)	7492(1)	8242(2)	76(1)
O(6)	357(3)	6769(2)	4950(5)	46(2)
O(7)	–515(3)	6230(2)	5941(4)	51(2)

O(8)	1810(4)	6280(1)	7756(3)	58(1)
O(9)	2220(3)	6927(1)	6928(2)	42(1)
N(1)	2105(3)	7058(1)	5957(2)	38(1)
N(2)	1456(3)	6975(1)	5076(3)	38(1)
N(3)	1246(3)	6513(1)	5428(3)	45(1)
N(4)	674(3)	6148(1)	6061(3)	47(1)
N(5)	–55(3)	5976(1)	6734(3)	47(2)
N(6)	873(3)	5986(1)	7458(2)	50(2)
N(7)	1588(3)	6179(1)	6796(2)	46(1)
N(8)	2111(3)	6569(1)	6200(2)	41(1)
C(1)	2093(3)	7388(1)	6009(3)	42(1)
C(2)	1365(4)	7524(2)	5948(3)	40(2)
C(3)	1096(4)	7704(2)	6371(3)	43(1)
C(4)	429(3)	7845(2)	6330(3)	48(1)
C(5)	178(3)	8060(2)	6747(3)	52(2)
C(6)	–460(3)	8199(2)	6662(3)	60(2)
C(7)	–868(3)	8133(2)	6186(3)	56(2)
C(8)	–643(3)	7930(2)	5778(3)	50(1)
C(9)	14(3)	7782(2)	5829(3)	44(1)
C(10)	299(3)	7596(2)	5392(2)	42(2)
C(11)	961(3)	7468(1)	5436(2)	36(2)
C(12)	1269(4)	7289(1)	4930(3)	41(1)
C(13)	961(3)	6754(2)	5134(4)	41(1)
C(14)	884(4)	6224(2)	5477(3)	49(2)
C(15)	–19(3)	6126(2)	6221(3)	46(2)
C(16)	620(3)	5851(1)	6924(3)	50(1)
C(17)	1129(3)	5986(1)	6458(3)	48(1)
C(18)	704(5)	5862(2)	8032(3)	57(2)
C(19)	1458(3)	6159(1)	7373(3)	49(2)
C(20)	2231(3)	6312(1)	6565(3)	46(2)
C(21)	2151(4)	6859(1)	6415(2)	39(1)
C(22)	1989(3)	6564(1)	5573(2)	42(1)
C(23)	2089(3)	6901(1)	5397(2)	40(1)
C(24)	2460(5)	6330(2)	5270(4)	53(2)
C(25)	2745(4)	6975(2)	5045(3)	46(2)
C(26)	1339(4)	7581(2)	7356(2)	66(2)
C(27)	1824(4)	7671(3)	7822(3)	94(3)
C(28)	2531(3)	7606(2)	7725(3)	75(2)
C(29)	–614(4)	7329(2)	4898(3)	53(2)
C(30)	–783(3)	7253(1)	4281(3)	55(1)
Cl(1A)	–454(8)	7296(3)	3750(6)	130(4)
S(1A)	2792(6)	7373(3)	8570(4)	69(2)
O(1A)	1715(12)	7758(7)	6826(9)	56(4)
O(2A)	–62(19)	7562(11)	4970(13)	49(4)

O(3A)	2778(8)	7155(4)	8093(7)	57(3)
O(4A)	2740(11)	7310(5)	9144(6)	76(5)
O(5A)	3463(9)	7566(5)	8511(10)	76(1)
O(6A)	293(15)	6671(7)	4980(20)	41(6)
O(7A)	–561(16)	6130(9)	6000(20)	51(7)
O(8A)	1820(20)	6186(6)	7736(13)	66(4)
O(9A)	2168(17)	6810(5)	6896(8)	45(4)
N(1A)	2049(17)	6962(4)	5946(9)	42(3)
N(2A)	1380(13)	6890(5)	5084(13)	39(3)
N(3A)	1185(12)	6424(5)	5449(14)	40(3)
N(4A)	633(13)	6051(7)	6076(12)	46(4)
N(5A)	–53(13)	5879(8)	6776(14)	48(4)
N(6A)	895(15)	5887(7)	7450(11)	53(4)
N(7A)	1588(13)	6072(6)	6774(10)	49(4)
N(8A)	2108(16)	6465(4)	6168(9)	39(3)
C(1A)	2110(13)	7287(5)	6006(14)	37(4)
C(2A)	1411(17)	7452(9)	5977(14)	40(4)
C(3A)	1225(15)	7653(10)	6412(13)	45(4)
C(4A)	582(12)	7811(8)	6382(11)	47(4)
C(5A)	427(11)	8037(7)	6785(10)	51(4)
C(6A)	–202(12)	8196(6)	6748(11)	51(4)
C(7A)	–675(11)	8128(7)	6309(13)	54(4)
C(8A)	–520(12)	7902(8)	5906(11)	49(4)
C(9A)	109(14)	7743(8)	5943(11)	45(4)
C(10A)	297(15)	7541(9)	5483(13)	43(4)
C(11A)	953(15)	7388(7)	5506(12)	39(4)
C(12A)	1209(17)	7209(5)	4978(11)	36(4)
C(13A)	894(14)	6668(6)	5170(20)	39(4)
C(14A)	830(18)	6134(6)	5498(12)	48(4)
C(15A)	–47(13)	6036(10)	6271(16)	46(4)
C(16A)	626(13)	5743(6)	6926(11)	57(4)
C(17A)	1107(12)	5884(6)	6450(10)	51(4)
C(18A)	730(20)	5760(10)	8022(13)	53(6)
C(19A)	1487(18)	6053(9)	7353(10)	62(4)
C(20A)	2213(13)	6206(6)	6513(12)	41(4)
C(21A)	2140(20)	6753(5)	6382(8)	37(3)
C(22A)	1945(12)	6467(5)	5546(9)	39(3)
C(23A)	2029(12)	6807(5)	5387(9)	41(3)
C(24A)	2378(19)	6234(8)	5216(17)	49(7)
C(25A)	2650(18)	6887(9)	4998(17)	48(8)
C(26A)	1795(16)	7588(8)	7342(8)	66(4)
C(27A)	1668(14)	7608(12)	7934(9)	69(4)
C(28A)	2162(12)	7661(6)	8380(9)	70(4)
C(29A)	–700(20)	7376(13)	4865(11)	62(5)

C(30A)	–987(12)	7443(9)	4269(10)	77(5)
Cl(3)	7717(6)	5543(2)	10453(6)	294(5)
S(31)	2197(3)	5379(1)	7446(3)	127(2)
O(31)	4006(5)	5235(2)	8561(4)	118(2)
O(32)	6339(5)	5314(2)	9994(5)	128(3)
O(33)	2186(5)	5643(2)	7805(5)	117(3)
O(34)	2252(7)	5415(3)	6847(4)	174(4)
O(35)	1543(5)	5193(3)	7597(7)	169(4)
O(36)	5937(6)	6118(4)	9973(8)	104(5)
O(37)	6289(7)	6632(5)	8726(8)	50(4)
O(38)	3213(6)	6570(2)	7954(6)	51(2)
O(39)	3239(5)	5989(2)	8904(4)	72(2)
N(31)	3856(5)	5860(2)	9720(4)	68(2)
N(32)	4884(4)	5942(2)	10308(5)	72(2)
N(33)	4915(5)	6381(2)	9818(5)	51(2)
N(34)	5155(6)	6728(3)	9021(5)	40(2)
N(35)	5459(6)	6853(4)	8123(5)	39(2)
N(36)	4231(6)	6846(3)	7830(4)	38(2)
N(37)	3948(5)	6698(3)	8714(4)	40(2)
N(38)	3691(5)	6355(2)	9517(4)	49(2)
C(31)	3827(6)	5533(2)	9662(4)	79(2)
C(32)	4523(6)	5400(3)	9481(5)	89(3)
C(33)	4561(6)	5227(3)	8970(5)	105(3)
C(34)	5194(6)	5088(3)	8816(5)	108(3)
C(35)	5257(8)	4904(3)	8290(5)	129(3)
C(36)	5828(8)	4744(3)	8152(7)	131(4)
C(37)	6416(8)	4762(4)	8500(7)	136(4)
C(38)	6393(7)	4937(4)	9014(6)	123(4)
C(39)	5792(6)	5107(4)	9161(6)	109(3)
C(40)	5748(6)	5283(3)	9670(5)	101(3)
C(41)	5113(5)	5439(3)	9834(5)	89(2)
C(42)	5099(6)	5624(2)	10389(5)	86(3)
C(43)	5303(6)	6146(3)	10022(10)	69(3)
C(44)	5252(7)	6660(3)	9623(5)	48(2)
C(45)	5692(6)	6724(5)	8627(6)	40(2)
C(46)	4767(6)	6983(3)	8186(5)	40(2)
C(47)	4550(5)	6890(3)	8810(4)	38(2)
C(48)	4061(9)	6961(4)	7253(5)	42(2)
C(49)	3746(6)	6692(3)	8148(4)	40(2)
C(50)	3473(5)	6612(2)	9190(4)	45(2)
C(51)	3570(7)	6061(2)	9331(4)	60(2)
C(52)	4179(5)	6362(2)	10007(4)	50(2)
C(53)	4146(5)	6021(2)	10215(4)	62(2)
C(54)	3992(9)	6602(3)	10451(5)	61(3)

C(55)	3719(6)	5974(3)	10769(5)	77(3)
C(56)	3477(7)	5006(3)	8660(6)	126(3)
C(57)	2821(7)	5099(4)	8375(6)	135(4)
C(58)	2895(7)	5153(3)	7750(6)	125(3)
C(59)	6865(7)	5466(4)	9565(8)	155(4)
C(60)	7564(8)	5408(4)	9791(8)	197(5)
Cl(3A)	7236(10)	5700(4)	10995(8)	243(7)
S(31A)	2040(8)	5308(4)	7638(8)	156(4)
O(31A)	3883(10)	5036(5)	8779(7)	123(4)
O(32A)	6459(11)	5222(5)	9761(11)	136(4)
O(33A)	2273(13)	5550(4)	8008(11)	129(5)
O(34A)	1692(16)	5399(7)	7128(12)	198(8)
O(35A)	1622(15)	5090(7)	8008(15)	212(10)
O(36A)	6029(9)	6068(6)	9944(13)	64(5)
O(37A)	6296(15)	6569(11)	8789(15)	43(5)
O(38A)	3247(13)	6507(5)	8049(11)	48(3)
O(39A)	3397(13)	5894(4)	8972(9)	75(4)
N(31A)	3974(12)	5774(4)	9790(9)	72(3)
N(32A)	5021(9)	5861(4)	10307(11)	74(3)
N(33A)	4978(10)	6322(5)	9892(12)	51(3)
N(34A)	5177(11)	6677(7)	9114(10)	37(3)
N(35A)	5461(13)	6809(9)	8223(11)	35(3)
N(36A)	4243(13)	6795(7)	7927(9)	38(3)
N(37A)	3971(11)	6633(6)	8812(8)	39(3)
N(38A)	3767(11)	6269(4)	9592(8)	51(3)
C(31A)	3938(12)	5444(4)	9775(10)	85(4)
C(32A)	4584(10)	5310(6)	9490(11)	91(4)
C(33A)	4526(10)	5136(6)	8990(10)	105(4)
C(34A)	5114(10)	4982(6)	8771(10)	116(4)
C(35A)	5035(13)	4762(5)	8309(10)	129(5)
C(36A)	5590(15)	4609(6)	8086(12)	134(5)
C(37A)	6244(15)	4676(8)	8293(15)	137(5)
C(38A)	6344(13)	4879(8)	8759(14)	128(5)
C(39A)	5775(11)	5040(7)	8998(12)	113(4)
C(40A)	5844(10)	5243(7)	9475(12)	109(4)
C(41A)	5239(11)	5371(8)	9745(12)	96(4)
C(42A)	5293(13)	5549(5)	10309(10)	86(4)
C(43A)	5401(10)	6085(6)	10040(20)	62(4)
C(44A)	5282(15)	6610(6)	9713(11)	43(3)
C(45A)	5714(14)	6685(11)	8721(12)	36(4)
C(46A)	4765(12)	6942(6)	8291(10)	33(3)
C(47A)	4557(11)	6834(6)	8912(9)	37(3)
C(48A)	4060(20)	6914(10)	7355(11)	42(2)
C(49A)	3763(13)	6638(7)	8256(9)	42(3)

C(50A)	3518(11)	6518(5)	9283(9)	49(3)
C(51A)	3660(15)	5974(4)	9416(10)	61(3)
C(52A)	4250(10)	6277(4)	10084(8)	54(3)
C(53A)	4276(9)	5938(4)	10272(8)	64(3)
C(54A)	4030(20)	6511(6)	10532(11)	62(6)
C(55A)	3886(15)	5865(7)	10831(10)	82(7)
C(56A)	3640(16)	5180(6)	8244(11)	129(4)
C(57A)	3158(15)	4969(6)	7950(12)	139(5)
C(58A)	2807(12)	5090(7)	7449(11)	146(5)
C(59A)	6821(19)	5508(6)	9964(13)	153(5)
C(60A)	7060(20)	5398(6)	10552(13)	182(6)
N(61)	870(2)	6920(2)	7928(2)	92(2)
C(61)	358(2)	6909(1)	8174(2)	61(1)
C(62)	–276(3)	6898(1)	8496(2)	68(1)
N(71)	3809(5)	5936(2)	7360(4)	132(3)
C(71)	4225(6)	5938(2)	6994(4)	120(3)
C(72)	4706(6)	5943(2)	6561(4)	141(5)
N(71A)	3300(20)	5749(7)	7650(20)	117(5)
C(71A)	3880(20)	5695(13)	7530(30)	127(6)
C(72A)	4600(20)	5657(17)	7550(30)	128(7)
O(81)	1797(5)	6549(3)	8785(2)	190(4)

Table S4: Bond lengths [Å] and angles [°] for **2b**.

Na(1)-O(3A)	2.129(16)
Na(1)-O(81)	2.230(7)
Na(1)-O(8)	2.281(6)
Na(1)-O(38)	2.289(13)
Na(1)-O(3)	2.425(8)
Na(1)-O(9A)	2.449(19)
Na(1)-N(61)	2.454(5)
Na(1)-O(9)	2.470(4)
Na(1)-O(38A)	2.48(3)
Na(1)-O(8A)	2.68(2)
Na(1)-S(1A)	3.255(12)
Na(1)-Na(2)	3.519(3)
Na(2)-N(71A)	1.76(3)
Na(2)-O(39)	2.140(7)
Na(2)-O(38A)	2.15(2)
Na(2)-O(8A)	2.21(4)
Na(2)-O(33)	2.254(9)
Na(2)-O(8)	2.367(7)
Na(2)-O(38)	2.405(9)

Na(2)-N(71)	2.412(8)
Na(2)-O(33A)	2.45(2)
Na(2)-O(39A)	2.474(16)
Na(2)-C(71A)	2.72(3)
Na(2)-C(19A)	3.08(3)
Cl(1)-C(30)	1.762(6)
S(1)-O(4)	1.436(5)
S(1)-O(5)	1.444(5)
S(1)-O(3)	1.461(6)
S(1)-C(28)	1.810(6)
O(1)-C(3)	1.390(6)
O(1)-C(26)	1.462(7)
O(2)-C(10)	1.391(6)
O(2)-C(29)	1.459(7)
O(6)-C(13)	1.231(6)
O(7)-C(15)	1.233(6)
O(8)-C(19)	1.231(7)
O(9)-C(21)	1.225(6)
N(1)-C(21)	1.370(6)
N(1)-C(1)	1.454(7)
N(1)-C(23)	1.461(6)
N(2)-C(13)	1.361(6)
N(2)-C(23)	1.454(6)
N(2)-C(12)	1.460(7)
N(3)-C(13)	1.365(7)
N(3)-C(14)	1.447(7)
N(3)-C(22)	1.476(6)
N(4)-C(15)	1.377(6)
N(4)-C(14)	1.443(7)
N(4)-C(17)	1.448(7)
N(5)-C(15)	1.353(7)
N(5)-C(18)#1	1.441(11)
N(5)-C(16)	1.467(6)
N(6)-C(19)	1.364(7)
N(6)-C(16)	1.448(7)
N(6)-C(18)	1.465(7)
N(7)-C(19)	1.354(6)
N(7)-C(17)	1.446(7)
N(7)-C(20)	1.460(6)
N(8)-C(21)	1.365(7)
N(8)-C(20)	1.421(7)
N(8)-C(22)	1.462(6)
C(1)-C(2)	1.518(7)
C(1)-H(1A)	0.9900

C(1)-H(1AB)	0.9900
C(2)-C(3)	1.356(7)
C(2)-C(11)	1.430(6)
C(3)-C(4)	1.419(7)
C(4)-C(9)	1.426(7)
C(4)-C(5)	1.428(7)
C(5)-C(6)	1.377(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.376(8)
C(6)-H(6)	0.9500
C(7)-C(8)	1.362(8)
C(7)-H(7)	0.9500
C(8)-C(9)	1.419(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.406(7)
C(10)-C(11)	1.387(6)
C(11)-C(12)	1.521(6)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(16)-C(17)	1.565(7)
C(16)-H(16)	1.0000
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(22)-C(24)	1.534(7)
C(22)-C(23)	1.542(7)
C(23)-C(25)	1.527(6)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-C(27)	1.470(10)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.398(10)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9900

C(28)-H(28B)	0.9900
C(29)-C(30)	1.497(8)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
Cl(1A)-C(30A)	1.698(18)
S(1A)-O(4A)	1.356(14)
S(1A)-O(3A)	1.454(12)
S(1A)-O(5A)	1.542(15)
S(1A)-C(28A)	1.796(15)
O(1A)-C(26A)	1.411(16)
O(1A)-C(3A)	1.413(16)
O(2A)-C(10A)	1.370(16)
O(2A)-C(29A)	1.480(17)
O(6A)-C(13A)	1.227(15)
O(7A)-C(15A)	1.234(15)
O(8A)-C(19A)	1.238(15)
O(9A)-C(21A)	1.211(14)
N(1A)-C(21A)	1.371(15)
N(1A)-C(1A)	1.438(15)
N(1A)-C(23A)	1.455(15)
N(2A)-C(13A)	1.360(15)
N(2A)-C(12A)	1.455(15)
N(2A)-C(23A)	1.469(14)
N(3A)-C(13A)	1.367(15)
N(3A)-C(14A)	1.446(15)
N(3A)-C(22A)	1.480(14)
N(4A)-C(15A)	1.376(14)
N(4A)-C(14A)	1.429(15)
N(4A)-C(17A)	1.449(15)
N(5A)-C(15A)	1.350(15)
N(5A)-C(16A)	1.469(16)
N(5A)-C(18A)#1	1.48(5)
N(6A)-C(19A)	1.365(15)
N(6A)-C(16A)	1.454(15)
N(6A)-C(18A)	1.465(15)
N(7A)-C(19A)	1.348(14)
N(7A)-C(17A)	1.444(15)
N(7A)-C(20A)	1.460(15)
N(8A)-C(21A)	1.356(15)
N(8A)-C(20A)	1.401(15)
N(8A)-C(22A)	1.464(14)
C(1A)-C(2A)	1.519(15)

C(1A)-H(1AA)	0.9900
C(1A)-H(1AC)	0.9900
C(2A)-C(3A)	1.379(15)
C(2A)-C(11A)	1.422(15)
C(3A)-C(4A)	1.412(14)
C(4A)-C(5A)	1.3900
C(4A)-C(9A)	1.3900
C(5A)-C(6A)	1.3900
C(5A)-H(5A)	0.9500
C(6A)-C(7A)	1.3900
C(6A)-H(6A)	0.9500
C(7A)-C(8A)	1.3900
C(7A)-H(7A)	0.9500
C(8A)-C(9A)	1.3900
C(8A)-H(8A)	0.9500
C(9A)-C(10A)	1.427(14)
C(10A)-C(11A)	1.421(15)
C(11A)-C(12A)	1.526(15)
C(12A)-H(12C)	0.9900
C(12A)-H(12D)	0.9900
C(14A)-H(14C)	0.9900
C(14A)-H(14D)	0.9900
C(16A)-C(17A)	1.557(15)
C(16A)-H(16A)	1.0000
C(17A)-H(17A)	1.0000
C(18A)-H(18C)	0.9900
C(18A)-H(18D)	0.9900
C(20A)-H(20C)	0.9900
C(20A)-H(20D)	0.9900
C(22A)-C(24A)	1.518(15)
C(22A)-C(23A)	1.542(15)
C(23A)-C(25A)	1.525(15)
C(24A)-H(24D)	0.9800
C(24A)-H(24E)	0.9800
C(24A)-H(24F)	0.9800
C(25A)-H(25D)	0.9800
C(25A)-H(25E)	0.9800
C(25A)-H(25F)	0.9800
C(26A)-C(27A)	1.387(17)
C(26A)-H(26C)	0.9900
C(26A)-H(26D)	0.9900
C(27A)-C(28A)	1.413(18)
C(27A)-H(27C)	0.9900
C(27A)-H(27D)	0.9900

C(28A)-H(28C)	0.9900
C(28A)-H(28D)	0.9900
C(29A)-C(30A)	1.509(19)
C(29A)-H(29C)	0.9900
C(29A)-H(29D)	0.9900
C(30A)-H(30C)	0.9900
C(30A)-H(30D)	0.9900
Cl(3)-C(60)	1.660(16)
S(31)-O(34)	1.391(11)
S(31)-O(33)	1.420(8)
S(31)-O(35)	1.532(11)
S(31)-C(58)	1.805(10)
O(31)-C(33)	1.420(11)
O(31)-C(56)	1.443(12)
O(32)-C(40)	1.361(11)
O(32)-C(59)	1.560(13)
O(36)-C(43)	1.222(9)
O(37)-C(45)	1.231(8)
O(38)-C(49)	1.232(8)
O(39)-C(51)	1.212(8)
N(31)-C(51)	1.370(9)
N(31)-C(31)	1.442(10)
N(31)-C(53)	1.449(9)
N(32)-C(43)	1.370(9)
N(32)-C(42)	1.465(10)
N(32)-C(53)	1.468(9)
N(33)-C(43)	1.352(9)
N(33)-C(44)	1.455(8)
N(33)-C(52)	1.475(8)
N(34)-C(45)	1.369(8)
N(34)-C(44)	1.429(8)
N(34)-C(47)	1.441(8)
N(35)-C(48)#2	1.35(2)
N(35)-C(45)	1.365(8)
N(35)-C(46)	1.446(8)
N(36)-C(49)	1.362(8)
N(36)-C(46)	1.443(8)
N(36)-C(48)	1.456(7)
N(37)-C(49)	1.359(7)
N(37)-C(47)	1.442(8)
N(37)-C(50)	1.473(8)
N(38)-C(51)	1.375(9)
N(38)-C(50)	1.417(8)
N(38)-C(52)	1.463(8)

C(31)-C(32)	1.512(11)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(41)	1.399(11)
C(32)-C(33)	1.402(12)
C(33)-C(34)	1.399(12)
C(34)-C(39)	1.395(12)
C(34)-C(35)	1.458(12)
C(35)-C(36)	1.337(13)
C(35)-H(35)	0.9500
C(36)-C(37)	1.382(14)
C(36)-H(36)	0.9500
C(37)-C(38)	1.412(13)
C(37)-H(37)	0.9500
C(38)-C(39)	1.410(12)
C(38)-H(38)	0.9500
C(39)-C(40)	1.406(12)
C(40)-C(41)	1.442(11)
C(41)-C(42)	1.513(11)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(46)-C(47)	1.551(8)
C(46)-H(46)	1.0000
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(52)-C(54)	1.510(10)
C(52)-C(53)	1.569(9)
C(53)-C(55)	1.529(9)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-C(57)	1.471(14)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.465(14)
C(57)-H(57A)	0.9900

C(57)-H(57B)	0.9900
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(60)	1.456(15)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
Cl(3A)-C(60A)	1.704(18)
S(31A)-O(34A)	1.408(15)
S(31A)-O(33A)	1.430(14)
S(31A)-O(35A)	1.507(16)
S(31A)-C(58A)	1.802(15)
O(31A)-C(33A)	1.391(15)
O(31A)-C(56A)	1.458(16)
O(32A)-C(40A)	1.349(15)
O(32A)-C(59A)	1.506(16)
O(36A)-C(43A)	1.224(14)
O(37A)-C(45A)	1.230(13)
O(38A)-C(49A)	1.237(13)
O(39A)-C(51A)	1.193(13)
N(31A)-C(51A)	1.365(14)
N(31A)-C(53A)	1.445(13)
N(31A)-C(31A)	1.447(14)
N(32A)-C(43A)	1.365(13)
N(32A)-C(42A)	1.463(14)
N(32A)-C(53A)	1.465(13)
N(33A)-C(43A)	1.363(13)
N(33A)-C(44A)	1.445(14)
N(33A)-C(52A)	1.473(13)
N(34A)-C(45A)	1.368(13)
N(34A)-C(44A)	1.427(13)
N(34A)-C(47A)	1.445(13)
N(35A)-C(45A)	1.358(13)
N(35A)-C(46A)	1.460(13)
N(35A)-C(48A)#2	1.68(5)
N(36A)-C(49A)	1.374(13)
N(36A)-C(46A)	1.454(13)
N(36A)-C(48A)	1.459(13)
N(37A)-C(49A)	1.339(13)
N(37A)-C(47A)	1.443(13)
N(37A)-C(50A)	1.477(13)
N(38A)-C(51A)	1.370(14)
N(38A)-C(50A)	1.385(14)

N(38A)-C(52A)	1.462(13)
C(31A)-C(32A)	1.515(15)
C(31A)-H(31C)	0.9900
C(31A)-H(31D)	0.9900
C(32A)-C(33A)	1.388(14)
C(32A)-C(41A)	1.408(14)
C(33A)-C(34A)	1.402(15)
C(34A)-C(39A)	1.391(14)
C(34A)-C(35A)	1.445(15)
C(35A)-C(36A)	1.355(15)
C(35A)-H(35A)	0.9500
C(36A)-C(37A)	1.370(16)
C(36A)-H(36A)	0.9500
C(37A)-C(38A)	1.406(16)
C(37A)-H(37A)	0.9500
C(38A)-C(39A)	1.408(15)
C(38A)-H(38A)	0.9500
C(39A)-C(40A)	1.420(15)
C(40A)-C(41A)	1.428(15)
C(41A)-C(42A)	1.515(15)
C(42A)-H(42C)	0.9900
C(42A)-H(42D)	0.9900
C(44A)-H(44C)	0.9900
C(44A)-H(44D)	0.9900
C(46A)-C(47A)	1.557(13)
C(46A)-H(46A)	1.0000
C(47A)-H(47A)	1.0000
C(48A)-H(48C)	0.9900
C(48A)-H(48D)	0.9900
C(50A)-H(50C)	0.9900
C(50A)-H(50D)	0.9900
C(52A)-C(54A)	1.515(14)
C(52A)-C(53A)	1.548(14)
C(53A)-C(55A)	1.522(14)
C(54A)-H(54D)	0.9800
C(54A)-H(54E)	0.9800
C(54A)-H(54F)	0.9800
C(55A)-H(55D)	0.9800
C(55A)-H(55E)	0.9800
C(55A)-H(55F)	0.9800
C(56A)-C(57A)	1.469(17)
C(56A)-H(56C)	0.9900
C(56A)-H(56D)	0.9900
C(57A)-C(58A)	1.435(18)

C(57A)-H(57C)	0.9900
C(57A)-H(57D)	0.9900
C(58A)-H(58C)	0.9900
C(58A)-H(58D)	0.9900
C(59A)-C(60A)	1.509(18)
C(59A)-H(59C)	0.9900
C(59A)-H(59D)	0.9900
C(60A)-H(60C)	0.9900
C(60A)-H(60D)	0.9900
N(61)-C(61)	1.133(6)
C(61)-C(62)	1.420(6)
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
N(71)-C(71)	1.157(8)
C(71)-C(72)	1.357(9)
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
N(71A)-C(71A)	1.161(13)
C(71A)-C(72A)	1.390(13)
C(72A)-C(72A)#2	1.54(8)
C(72A)-H(72D)	0.9800
C(72A)-H(72E)	0.9800
C(72A)-H(72F)	0.9800
O(81)-H(81A)	0.89(2)
O(81)-H(81B)	0.89(2)

O(3A)-Na(1)-O(81)	112.3(5)
O(81)-Na(1)-O(8)	71.8(3)
O(81)-Na(1)-O(38)	94.4(4)
O(8)-Na(1)-O(38)	82.1(3)
O(81)-Na(1)-O(3)	90.6(3)
O(8)-Na(1)-O(3)	154.7(2)
O(38)-Na(1)-O(3)	81.2(3)
O(3A)-Na(1)-O(9A)	94.0(7)
O(81)-Na(1)-O(9A)	153.5(6)
O(3A)-Na(1)-N(61)	112.2(4)
O(81)-Na(1)-N(61)	83.1(3)
O(8)-Na(1)-N(61)	90.0(3)
O(38)-Na(1)-N(61)	172.1(3)
O(3)-Na(1)-N(61)	106.2(2)
O(9A)-Na(1)-N(61)	90.0(8)
O(81)-Na(1)-O(9)	164.6(3)

O(8)-Na(1)-O(9)	94.9(2)
O(38)-Na(1)-O(9)	91.4(3)
O(3)-Na(1)-O(9)	104.4(2)
N(61)-Na(1)-O(9)	89.22(19)
O(3A)-Na(1)-O(38A)	80.3(6)
O(81)-Na(1)-O(38A)	87.3(6)
O(9A)-Na(1)-O(38A)	94.5(10)
N(61)-Na(1)-O(38A)	166.5(5)
O(3A)-Na(1)-O(8A)	154.8(10)
O(81)-Na(1)-O(8A)	71.5(7)
O(9A)-Na(1)-O(8A)	83.4(7)
N(61)-Na(1)-O(8A)	92.9(9)
O(38A)-Na(1)-O(8A)	75.0(10)
O(3A)-Na(1)-S(1A)	20.1(5)
O(81)-Na(1)-S(1A)	95.2(3)
O(9A)-Na(1)-S(1A)	111.2(5)
N(61)-Na(1)-S(1A)	100.8(3)
O(38A)-Na(1)-S(1A)	89.5(5)
O(8A)-Na(1)-S(1A)	159.8(7)
O(3A)-Na(1)-Na(2)	117.2(4)
O(81)-Na(1)-Na(2)	70.6(3)
O(8)-Na(1)-Na(2)	41.72(18)
O(38)-Na(1)-Na(2)	42.7(2)
O(3)-Na(1)-Na(2)	115.86(16)
O(9A)-Na(1)-Na(2)	95.2(7)
N(61)-Na(1)-Na(2)	129.72(18)
O(9)-Na(1)-Na(2)	105.03(15)
O(38A)-Na(1)-Na(2)	37.2(4)
O(8A)-Na(1)-Na(2)	38.8(8)
S(1A)-Na(1)-Na(2)	123.0(2)
N(71A)-Na(2)-O(38A)	122.9(19)
N(71A)-Na(2)-O(8A)	118.5(18)
O(38A)-Na(2)-O(8A)	92.3(8)
O(39)-Na(2)-O(33)	108.7(4)
O(39)-Na(2)-O(8)	125.5(4)
O(33)-Na(2)-O(8)	77.2(3)
O(39)-Na(2)-O(38)	95.1(3)
O(33)-Na(2)-O(38)	152.6(3)
O(8)-Na(2)-O(38)	77.9(3)
O(39)-Na(2)-N(71)	109.8(4)
O(33)-Na(2)-N(71)	97.5(4)
O(8)-Na(2)-N(71)	123.3(3)
O(38)-Na(2)-N(71)	86.5(5)
N(71A)-Na(2)-O(33A)	64.0(18)

O(38A)-Na(2)-O(33A)	171.5(9)
O(8A)-Na(2)-O(33A)	79.5(7)
N(71A)-Na(2)-O(39A)	93.0(17)
O(38A)-Na(2)-O(39A)	95.8(7)
O(8A)-Na(2)-O(39A)	135.4(11)
O(33A)-Na(2)-O(39A)	88.5(7)
N(71A)-Na(2)-C(71A)	17.5(13)
O(38A)-Na(2)-C(71A)	107.6(16)
O(8A)-Na(2)-C(71A)	132.2(15)
O(33A)-Na(2)-C(71A)	80.0(15)
O(39A)-Na(2)-C(71A)	86.4(14)
N(71A)-Na(2)-C(19A)	99.1(18)
O(38A)-Na(2)-C(19A)	106.4(9)
O(8A)-Na(2)-C(19A)	19.5(9)
O(33A)-Na(2)-C(19A)	66.3(8)
O(39A)-Na(2)-C(19A)	142.8(8)
C(71A)-Na(2)-C(19A)	113.7(14)
O(4)-S(1)-O(5)	108.3(3)
O(4)-S(1)-O(3)	118.6(5)
O(5)-S(1)-O(3)	114.3(4)
O(4)-S(1)-C(28)	103.4(3)
O(5)-S(1)-C(28)	105.6(3)
O(3)-S(1)-C(28)	105.2(4)
C(3)-O(1)-C(26)	112.9(6)
C(10)-O(2)-C(29)	113.8(6)
S(1)-O(3)-Na(1)	137.8(4)
C(19)-O(8)-Na(1)	133.7(5)
C(19)-O(8)-Na(2)	118.1(5)
Na(1)-O(8)-Na(2)	98.4(2)
C(21)-O(9)-Na(1)	148.1(4)
C(21)-N(1)-C(1)	124.9(4)
C(21)-N(1)-C(23)	112.4(4)
C(1)-N(1)-C(23)	122.7(4)
C(13)-N(2)-C(23)	111.6(4)
C(13)-N(2)-C(12)	121.6(4)
C(23)-N(2)-C(12)	122.1(4)
C(13)-N(3)-C(14)	121.5(5)
C(13)-N(3)-C(22)	112.3(4)
C(14)-N(3)-C(22)	125.1(5)
C(15)-N(4)-C(14)	122.2(5)
C(15)-N(4)-C(17)	112.0(4)
C(14)-N(4)-C(17)	122.3(5)
C(15)-N(5)-C(18)#1	122.6(6)
C(15)-N(5)-C(16)	113.4(4)

C(18)#1-N(5)-C(16)	121.0(6)
C(19)-N(6)-C(16)	112.2(4)
C(19)-N(6)-C(18)	121.2(5)
C(16)-N(6)-C(18)	122.7(5)
C(19)-N(7)-C(17)	112.2(4)
C(19)-N(7)-C(20)	122.5(5)
C(17)-N(7)-C(20)	123.2(5)
C(21)-N(8)-C(20)	120.8(4)
C(21)-N(8)-C(22)	112.2(4)
C(20)-N(8)-C(22)	126.8(5)
N(1)-C(1)-C(2)	113.3(5)
N(1)-C(1)-H(1A)	108.9
C(2)-C(1)-H(1A)	108.9
N(1)-C(1)-H(1AB)	108.9
C(2)-C(1)-H(1AB)	108.9
H(1A)-C(1)-H(1AB)	107.7
C(3)-C(2)-C(11)	119.3(5)
C(3)-C(2)-C(1)	120.5(5)
C(11)-C(2)-C(1)	120.2(5)
C(2)-C(3)-O(1)	120.2(5)
C(2)-C(3)-C(4)	123.0(5)
O(1)-C(3)-C(4)	116.6(5)
C(3)-C(4)-C(9)	118.1(5)
C(3)-C(4)-C(5)	122.8(5)
C(9)-C(4)-C(5)	119.0(5)
C(6)-C(5)-C(4)	119.6(5)
C(6)-C(5)-H(5)	120.2
C(4)-C(5)-H(5)	120.2
C(7)-C(6)-C(5)	121.4(6)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	120.6(6)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	121.3(5)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
C(10)-C(9)-C(8)	123.3(5)
C(10)-C(9)-C(4)	118.4(5)
C(8)-C(9)-C(4)	118.1(5)
C(11)-C(10)-O(2)	119.3(5)
C(11)-C(10)-C(9)	122.4(5)
O(2)-C(10)-C(9)	118.0(5)
C(10)-C(11)-C(2)	118.8(5)

C(10)-C(11)-C(12)	120.3(5)
C(2)-C(11)-C(12)	120.8(5)
N(2)-C(12)-C(11)	113.7(5)
N(2)-C(12)-H(12A)	108.8
C(11)-C(12)-H(12A)	108.8
N(2)-C(12)-H(12B)	108.8
C(11)-C(12)-H(12B)	108.8
H(12A)-C(12)-H(12B)	107.7
O(6)-C(13)-N(2)	125.3(5)
O(6)-C(13)-N(3)	125.9(6)
N(2)-C(13)-N(3)	108.8(4)
N(4)-C(14)-N(3)	114.2(5)
N(4)-C(14)-H(14A)	108.7
N(3)-C(14)-H(14A)	108.7
N(4)-C(14)-H(14B)	108.7
N(3)-C(14)-H(14B)	108.7
H(14A)-C(14)-H(14B)	107.6
O(7)-C(15)-N(5)	126.6(6)
O(7)-C(15)-N(4)	125.0(6)
N(5)-C(15)-N(4)	108.4(5)
N(6)-C(16)-N(5)	113.3(5)
N(6)-C(16)-C(17)	102.8(4)
N(5)-C(16)-C(17)	101.6(4)
N(6)-C(16)-H(16)	112.7
N(5)-C(16)-H(16)	112.7
C(17)-C(16)-H(16)	112.7
N(7)-C(17)-N(4)	114.5(5)
N(7)-C(17)-C(16)	103.2(4)
N(4)-C(17)-C(16)	104.1(4)
N(7)-C(17)-H(17)	111.5
N(4)-C(17)-H(17)	111.5
C(16)-C(17)-H(17)	111.5
N(5)#1-C(18)-N(6)	113.5(6)
N(5)#1-C(18)-H(18A)	108.9
N(6)-C(18)-H(18A)	108.9
N(5)#1-C(18)-H(18B)	108.9
N(6)-C(18)-H(18B)	108.9
H(18A)-C(18)-H(18B)	107.7
O(8)-C(19)-N(7)	125.1(6)
O(8)-C(19)-N(6)	125.7(5)
N(7)-C(19)-N(6)	109.2(5)
N(8)-C(20)-N(7)	113.3(5)
N(8)-C(20)-H(20A)	108.9
N(7)-C(20)-H(20A)	108.9

N(8)-C(20)-H(20B)	108.9
N(7)-C(20)-H(20B)	108.9
H(20A)-C(20)-H(20B)	107.7
O(9)-C(21)-N(8)	125.5(5)
O(9)-C(21)-N(1)	126.4(5)
N(8)-C(21)-N(1)	108.1(4)
N(8)-C(22)-N(3)	112.3(5)
N(8)-C(22)-C(24)	111.4(5)
N(3)-C(22)-C(24)	111.0(5)
N(8)-C(22)-C(23)	103.2(4)
N(3)-C(22)-C(23)	101.8(4)
C(24)-C(22)-C(23)	116.7(5)
N(2)-C(23)-N(1)	111.2(4)
N(2)-C(23)-C(25)	111.4(4)
N(1)-C(23)-C(25)	110.7(5)
N(2)-C(23)-C(22)	104.2(4)
N(1)-C(23)-C(22)	102.6(4)
C(25)-C(23)-C(22)	116.3(5)
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(1)-C(26)-C(27)	106.8(7)
O(1)-C(26)-H(26A)	110.4
C(27)-C(26)-H(26A)	110.4
O(1)-C(26)-H(26B)	110.4
C(27)-C(26)-H(26B)	110.4
H(26A)-C(26)-H(26B)	108.6
C(28)-C(27)-C(26)	116.1(7)
C(28)-C(27)-H(27A)	108.3
C(26)-C(27)-H(27A)	108.3
C(28)-C(27)-H(27B)	108.3
C(26)-C(27)-H(27B)	108.3
H(27A)-C(27)-H(27B)	107.4
C(27)-C(28)-S(1)	112.5(5)
C(27)-C(28)-H(28A)	109.1

S(1)-C(28)-H(28A)	109.1
C(27)-C(28)-H(28B)	109.1
S(1)-C(28)-H(28B)	109.1
H(28A)-C(28)-H(28B)	107.8
O(2)-C(29)-C(30)	106.2(5)
O(2)-C(29)-H(29A)	110.5
C(30)-C(29)-H(29A)	110.5
O(2)-C(29)-H(29B)	110.5
C(30)-C(29)-H(29B)	110.5
H(29A)-C(29)-H(29B)	108.7
C(29)-C(30)-Cl(1)	112.8(6)
C(29)-C(30)-H(30A)	109.0
Cl(1)-C(30)-H(30A)	109.0
C(29)-C(30)-H(30B)	109.0
Cl(1)-C(30)-H(30B)	109.0
H(30A)-C(30)-H(30B)	107.8
O(4A)-S(1A)-O(3A)	126.9(14)
O(4A)-S(1A)-O(5A)	105.0(12)
O(3A)-S(1A)-O(5A)	108.0(12)
O(4A)-S(1A)-C(28A)	109.4(13)
O(3A)-S(1A)-C(28A)	105.4(10)
O(5A)-S(1A)-C(28A)	98.6(13)
O(4A)-S(1A)-Na(1)	103.3(10)
O(3A)-S(1A)-Na(1)	30.2(8)
O(5A)-S(1A)-Na(1)	137.6(10)
C(28A)-S(1A)-Na(1)	101.1(9)
C(26A)-O(1A)-C(3A)	118(2)
C(10A)-O(2A)-C(29A)	121(3)
S(1A)-O(3A)-Na(1)	129.7(12)
C(19A)-O(8A)-Na(2)	124(3)
C(19A)-O(8A)-Na(1)	134(3)
Na(2)-O(8A)-Na(1)	91.6(8)
C(21A)-O(9A)-Na(1)	163.4(17)
C(21A)-N(1A)-C(1A)	125.6(17)
C(21A)-N(1A)-C(23A)	109.9(13)
C(1A)-N(1A)-C(23A)	123.2(17)
C(13A)-N(2A)-C(12A)	123.9(19)
C(13A)-N(2A)-C(23A)	109.4(14)
C(12A)-N(2A)-C(23A)	120.5(17)
C(13A)-N(3A)-C(14A)	122.1(17)
C(13A)-N(3A)-C(22A)	111.8(13)
C(14A)-N(3A)-C(22A)	124.1(18)
C(15A)-N(4A)-C(14A)	124.4(18)
C(15A)-N(4A)-C(17A)	111.8(13)

C(14A)-N(4A)-C(17A)	121.1(18)
C(15A)-N(5A)-C(16A)	113.7(15)
C(19A)-N(6A)-C(16A)	112.8(14)
C(19A)-N(6A)-C(18A)	122(2)
C(16A)-N(6A)-C(18A)	121(2)
C(19A)-N(7A)-C(17A)	112.8(13)
C(19A)-N(7A)-C(20A)	123.2(17)
C(17A)-N(7A)-C(20A)	122.4(17)
C(21A)-N(8A)-C(20A)	122.7(16)
C(21A)-N(8A)-C(22A)	111.0(13)
C(20A)-N(8A)-C(22A)	126.3(16)
N(1A)-C(1A)-C(2A)	113(2)
N(1A)-C(1A)-H(1AA)	108.9
C(2A)-C(1A)-H(1AA)	108.9
N(1A)-C(1A)-H(1AC)	108.9
C(2A)-C(1A)-H(1AC)	108.9
H(1AA)-C(1A)-H(1AC)	107.7
C(3A)-C(2A)-C(11A)	121.5(15)
C(3A)-C(2A)-C(1A)	119.8(16)
C(11A)-C(2A)-C(1A)	118.7(15)
C(2A)-C(3A)-C(4A)	120.1(14)
C(2A)-C(3A)-O(1A)	121.8(18)
C(4A)-C(3A)-O(1A)	116.7(16)
C(5A)-C(4A)-C(9A)	120.0
C(5A)-C(4A)-C(3A)	120.2(12)
C(9A)-C(4A)-C(3A)	119.8(12)
C(6A)-C(5A)-C(4A)	120.0
C(6A)-C(5A)-H(5A)	120.0
C(4A)-C(5A)-H(5A)	120.0
C(5A)-C(6A)-C(7A)	120.0
C(5A)-C(6A)-H(6A)	120.0
C(7A)-C(6A)-H(6A)	120.0
C(6A)-C(7A)-C(8A)	120.0
C(6A)-C(7A)-H(7A)	120.0
C(8A)-C(7A)-H(7A)	120.0
C(9A)-C(8A)-C(7A)	120.0
C(9A)-C(8A)-H(8A)	120.0
C(7A)-C(8A)-H(8A)	120.0
C(8A)-C(9A)-C(4A)	120.0
C(8A)-C(9A)-C(10A)	118.9(12)
C(4A)-C(9A)-C(10A)	120.6(12)
O(2A)-C(10A)-C(11A)	120(2)
O(2A)-C(10A)-C(9A)	118(2)
C(11A)-C(10A)-C(9A)	119.2(14)

C(10A)-C(11A)-C(2A)	118.5(15)
C(10A)-C(11A)-C(12A)	119.6(16)
C(2A)-C(11A)-C(12A)	120.8(17)
N(2A)-C(12A)-C(11A)	115.6(19)
N(2A)-C(12A)-H(12C)	108.4
C(11A)-C(12A)-H(12C)	108.4
N(2A)-C(12A)-H(12D)	108.4
C(11A)-C(12A)-H(12D)	108.4
H(12C)-C(12A)-H(12D)	107.5
O(6A)-C(13A)-N(2A)	125.6(19)
O(6A)-C(13A)-N(3A)	123.8(18)
N(2A)-C(13A)-N(3A)	110.4(13)
N(4A)-C(14A)-N(3A)	115(2)
N(4A)-C(14A)-H(14C)	108.6
N(3A)-C(14A)-H(14C)	108.6
N(4A)-C(14A)-H(14D)	108.6
N(3A)-C(14A)-H(14D)	108.6
H(14C)-C(14A)-H(14D)	107.5
O(7A)-C(15A)-N(5A)	127(2)
O(7A)-C(15A)-N(4A)	125(2)
N(5A)-C(15A)-N(4A)	108.3(14)
N(6A)-C(16A)-N(5A)	109(2)
N(6A)-C(16A)-C(17A)	101.9(13)
N(5A)-C(16A)-C(17A)	101.2(13)
N(6A)-C(16A)-H(16A)	114.3
N(5A)-C(16A)-H(16A)	114.3
C(17A)-C(16A)-H(16A)	114.3
N(7A)-C(17A)-N(4A)	115(2)
N(7A)-C(17A)-C(16A)	103.6(13)
N(4A)-C(17A)-C(16A)	104.5(13)
N(7A)-C(17A)-H(17A)	111.2
N(4A)-C(17A)-H(17A)	111.2
C(16A)-C(17A)-H(17A)	111.2
N(6A)-C(18A)-H(18C)	109.8
N(5A)#1-C(18A)-H(18C)	109.8
N(6A)-C(18A)-H(18D)	109.8
N(5A)#1-C(18A)-H(18D)	109.8
H(18C)-C(18A)-H(18D)	108.2
O(8A)-C(19A)-N(7A)	127(2)
O(8A)-C(19A)-N(6A)	124.4(19)
N(7A)-C(19A)-N(6A)	108.2(14)
O(8A)-C(19A)-Na(2)	36(2)
N(7A)-C(19A)-Na(2)	112.3(18)
N(6A)-C(19A)-Na(2)	128(2)

N(8A)-C(20A)-N(7A)	116(2)
N(8A)-C(20A)-H(20C)	108.2
N(7A)-C(20A)-H(20C)	108.2
N(8A)-C(20A)-H(20D)	108.2
N(7A)-C(20A)-H(20D)	108.2
H(20C)-C(20A)-H(20D)	107.4
O(9A)-C(21A)-N(8A)	123.5(18)
O(9A)-C(21A)-N(1A)	125.5(19)
N(8A)-C(21A)-N(1A)	110.4(13)
N(8A)-C(22A)-N(3A)	110.8(17)
N(8A)-C(22A)-C(24A)	111.6(18)
N(3A)-C(22A)-C(24A)	111.9(17)
N(8A)-C(22A)-C(23A)	102.6(12)
N(3A)-C(22A)-C(23A)	100.9(12)
C(24A)-C(22A)-C(23A)	118.3(18)
N(1A)-C(23A)-N(2A)	109.0(17)
N(1A)-C(23A)-C(25A)	113.2(18)
N(2A)-C(23A)-C(25A)	108.7(18)
N(1A)-C(23A)-C(22A)	103.9(12)
N(2A)-C(23A)-C(22A)	105.3(12)
C(25A)-C(23A)-C(22A)	116.2(18)
C(22A)-C(24A)-H(24D)	109.5
C(22A)-C(24A)-H(24E)	109.5
H(24D)-C(24A)-H(24E)	109.5
C(22A)-C(24A)-H(24F)	109.5
H(24D)-C(24A)-H(24F)	109.5
H(24E)-C(24A)-H(24F)	109.5
C(23A)-C(25A)-H(25D)	109.5
C(23A)-C(25A)-H(25E)	109.5
H(25D)-C(25A)-H(25E)	109.5
C(23A)-C(25A)-H(25F)	109.5
H(25D)-C(25A)-H(25F)	109.5
H(25E)-C(25A)-H(25F)	109.5
C(27A)-C(26A)-O(1A)	141(3)
C(27A)-C(26A)-H(26C)	101.8
O(1A)-C(26A)-H(26C)	101.8
C(27A)-C(26A)-H(26D)	101.8
O(1A)-C(26A)-H(26D)	101.8
H(26C)-C(26A)-H(26D)	104.7
C(26A)-C(27A)-C(28A)	127(2)
C(26A)-C(27A)-H(27C)	105.4
C(28A)-C(27A)-H(27C)	105.4
C(26A)-C(27A)-H(27D)	105.4
C(28A)-C(27A)-H(27D)	105.4

H(27C)-C(27A)-H(27D)	106.0
C(27A)-C(28A)-S(1A)	121(2)
C(27A)-C(28A)-H(28C)	107.2
S(1A)-C(28A)-H(28C)	107.2
C(27A)-C(28A)-H(28D)	107.2
S(1A)-C(28A)-H(28D)	107.2
H(28C)-C(28A)-H(28D)	106.8
O(2A)-C(29A)-C(30A)	110(2)
O(2A)-C(29A)-H(29C)	109.7
C(30A)-C(29A)-H(29C)	109.7
O(2A)-C(29A)-H(29D)	109.7
C(30A)-C(29A)-H(29D)	109.7
H(29C)-C(29A)-H(29D)	108.2
C(29A)-C(30A)-Cl(1A)	110(2)
C(29A)-C(30A)-H(30C)	109.6
Cl(1A)-C(30A)-H(30C)	109.6
C(29A)-C(30A)-H(30D)	109.6
Cl(1A)-C(30A)-H(30D)	109.6
H(30C)-C(30A)-H(30D)	108.1
O(34)-S(31)-O(33)	119.2(8)
O(34)-S(31)-O(35)	110.3(8)
O(33)-S(31)-O(35)	106.8(7)
O(34)-S(31)-C(58)	113.0(7)
O(33)-S(31)-C(58)	103.4(6)
O(35)-S(31)-C(58)	102.7(8)
C(33)-O(31)-C(56)	113.6(10)
C(40)-O(32)-C(59)	103.2(10)
S(31)-O(33)-Na(2)	139.4(7)
C(49)-O(38)-Na(1)	126.3(10)
C(49)-O(38)-Na(2)	127.6(7)
Na(1)-O(38)-Na(2)	97.1(4)
C(51)-O(39)-Na(2)	154.6(8)
C(51)-N(31)-C(31)	124.3(7)
C(51)-N(31)-C(53)	110.7(6)
C(31)-N(31)-C(53)	124.8(7)
C(43)-N(32)-C(42)	121.1(8)
C(43)-N(32)-C(53)	109.7(7)
C(42)-N(32)-C(53)	120.9(7)
C(43)-N(33)-C(44)	120.4(7)
C(43)-N(33)-C(52)	112.2(6)
C(44)-N(33)-C(52)	124.1(8)
C(45)-N(34)-C(44)	122.9(7)
C(45)-N(34)-C(47)	112.6(6)
C(44)-N(34)-C(47)	122.2(8)

C(48)#2-N(35)-C(45)	118.0(12)
C(48)#2-N(35)-C(46)	123.3(12)
C(45)-N(35)-C(46)	112.1(6)
C(49)-N(36)-C(46)	112.5(6)
C(49)-N(36)-C(48)	120.7(7)
C(46)-N(36)-C(48)	122.2(8)
C(49)-N(37)-C(47)	112.7(6)
C(49)-N(37)-C(50)	122.3(7)
C(47)-N(37)-C(50)	121.7(7)
C(51)-N(38)-C(50)	122.0(7)
C(51)-N(38)-C(52)	111.5(6)
C(50)-N(38)-C(52)	125.4(6)
N(31)-C(31)-C(32)	112.0(8)
N(31)-C(31)-H(31A)	109.2
C(32)-C(31)-H(31A)	109.2
N(31)-C(31)-H(31B)	109.2
C(32)-C(31)-H(31B)	109.2
H(31A)-C(31)-H(31B)	107.9
C(41)-C(32)-C(33)	120.8(9)
C(41)-C(32)-C(31)	120.1(9)
C(33)-C(32)-C(31)	119.0(9)
C(34)-C(33)-C(32)	119.6(10)
C(34)-C(33)-O(31)	119.2(10)
C(32)-C(33)-O(31)	120.4(10)
C(39)-C(34)-C(33)	122.5(10)
C(39)-C(34)-C(35)	116.0(10)
C(33)-C(34)-C(35)	121.5(11)
C(36)-C(35)-C(34)	123.7(13)
C(36)-C(35)-H(35)	118.1
C(34)-C(35)-H(35)	118.1
C(35)-C(36)-C(37)	119.7(14)
C(35)-C(36)-H(36)	120.1
C(37)-C(36)-H(36)	120.1
C(36)-C(37)-C(38)	119.4(13)
C(36)-C(37)-H(37)	120.3
C(38)-C(37)-H(37)	120.3
C(39)-C(38)-C(37)	121.0(12)
C(39)-C(38)-H(38)	119.5
C(37)-C(38)-H(38)	119.5
C(34)-C(39)-C(40)	117.3(10)
C(34)-C(39)-C(38)	119.9(11)
C(40)-C(39)-C(38)	122.6(11)
O(32)-C(40)-C(39)	117.4(10)
O(32)-C(40)-C(41)	120.6(10)

C(39)-C(40)-C(41)	121.9(9)
C(32)-C(41)-C(40)	117.8(9)
C(32)-C(41)-C(42)	122.8(9)
C(40)-C(41)-C(42)	119.3(9)
N(32)-C(42)-C(41)	114.1(9)
N(32)-C(42)-H(42A)	108.7
C(41)-C(42)-H(42A)	108.7
N(32)-C(42)-H(42B)	108.7
C(41)-C(42)-H(42B)	108.7
H(42A)-C(42)-H(42B)	107.6
O(36)-C(43)-N(33)	126.0(9)
O(36)-C(43)-N(32)	123.9(10)
N(33)-C(43)-N(32)	110.1(7)
N(34)-C(44)-N(33)	114.6(8)
N(34)-C(44)-H(44A)	108.6
N(33)-C(44)-H(44A)	108.6
N(34)-C(44)-H(44B)	108.6
N(33)-C(44)-H(44B)	108.6
H(44A)-C(44)-H(44B)	107.6
O(37)-C(45)-N(35)	126.5(9)
O(37)-C(45)-N(34)	125.1(9)
N(35)-C(45)-N(34)	108.3(6)
N(36)-C(46)-N(35)	115.4(9)
N(36)-C(46)-C(47)	103.1(6)
N(35)-C(46)-C(47)	103.5(6)
N(36)-C(46)-H(46)	111.4
N(35)-C(46)-H(46)	111.4
C(47)-C(46)-H(46)	111.4
N(34)-C(47)-N(37)	113.9(8)
N(34)-C(47)-C(46)	103.2(6)
N(37)-C(47)-C(46)	103.0(6)
N(34)-C(47)-H(47)	112.0
N(37)-C(47)-H(47)	112.0
C(46)-C(47)-H(47)	112.0
N(35)#2-C(48)-N(36)	108.4(13)
N(35)#2-C(48)-H(48A)	110.0
N(36)-C(48)-H(48A)	110.0
N(35)#2-C(48)-H(48B)	110.0
N(36)-C(48)-H(48B)	110.0
H(48A)-C(48)-H(48B)	108.4
O(38)-C(49)-N(37)	126.2(8)
O(38)-C(49)-N(36)	125.5(8)
N(37)-C(49)-N(36)	108.3(6)
N(38)-C(50)-N(37)	114.7(7)

N(38)-C(50)-H(50A)	108.6
N(37)-C(50)-H(50A)	108.6
N(38)-C(50)-H(50B)	108.6
N(37)-C(50)-H(50B)	108.6
H(50A)-C(50)-H(50B)	107.6
O(39)-C(51)-N(31)	124.8(8)
O(39)-C(51)-N(38)	125.8(8)
N(31)-C(51)-N(38)	109.3(6)
N(38)-C(52)-N(33)	112.5(7)
N(38)-C(52)-C(54)	112.7(8)
N(33)-C(52)-C(54)	112.6(8)
N(38)-C(52)-C(53)	101.0(5)
N(33)-C(52)-C(53)	100.5(6)
C(54)-C(52)-C(53)	116.5(7)
N(31)-C(53)-N(32)	111.6(8)
N(31)-C(53)-C(55)	112.8(7)
N(32)-C(53)-C(55)	111.0(7)
N(31)-C(53)-C(52)	103.7(6)
N(32)-C(53)-C(52)	103.4(5)
C(55)-C(53)-C(52)	113.8(7)
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
O(31)-C(56)-C(57)	109.6(11)
O(31)-C(56)-H(56A)	109.8
C(57)-C(56)-H(56A)	109.8
O(31)-C(56)-H(56B)	109.8
C(57)-C(56)-H(56B)	109.8
H(56A)-C(56)-H(56B)	108.2
C(58)-C(57)-C(56)	113.6(12)
C(58)-C(57)-H(57A)	108.8
C(56)-C(57)-H(57A)	108.8
C(58)-C(57)-H(57B)	108.8
C(56)-C(57)-H(57B)	108.8
H(57A)-C(57)-H(57B)	107.7

C(57)-C(58)-S(31)	113.5(10)
C(57)-C(58)-H(58A)	108.9
S(31)-C(58)-H(58A)	108.9
C(57)-C(58)-H(58B)	108.9
S(31)-C(58)-H(58B)	108.9
H(58A)-C(58)-H(58B)	107.7
C(60)-C(59)-O(32)	106.8(12)
C(60)-C(59)-H(59A)	110.4
O(32)-C(59)-H(59A)	110.4
C(60)-C(59)-H(59B)	110.4
O(32)-C(59)-H(59B)	110.4
H(59A)-C(59)-H(59B)	108.6
C(59)-C(60)-Cl(3)	115.3(14)
C(59)-C(60)-H(60A)	108.4
Cl(3)-C(60)-H(60A)	108.4
C(59)-C(60)-H(60B)	108.4
Cl(3)-C(60)-H(60B)	108.4
H(60A)-C(60)-H(60B)	107.5
O(34A)-S(31A)-O(33A)	115.7(17)
O(34A)-S(31A)-O(35A)	113.6(18)
O(33A)-S(31A)-O(35A)	107.4(16)
O(34A)-S(31A)-C(58A)	109.3(16)
O(33A)-S(31A)-C(58A)	106.4(14)
O(35A)-S(31A)-C(58A)	103.4(15)
C(33A)-O(31A)-C(56A)	116.2(19)
C(40A)-O(32A)-C(59A)	120(2)
S(31A)-O(33A)-Na(2)	144.5(17)
C(49A)-O(38A)-Na(2)	135.2(18)
C(49A)-O(38A)-Na(1)	121(2)
Na(2)-O(38A)-Na(1)	98.7(8)
C(51A)-O(39A)-Na(2)	147.5(15)
C(51A)-N(31A)-C(53A)	109.9(12)
C(51A)-N(31A)-C(31A)	127.2(14)
C(53A)-N(31A)-C(31A)	122.3(14)
C(43A)-N(32A)-C(42A)	119.1(16)
C(43A)-N(32A)-C(53A)	109.0(12)
C(42A)-N(32A)-C(53A)	124.2(14)
C(43A)-N(33A)-C(44A)	119.9(14)
C(43A)-N(33A)-C(52A)	112.4(11)
C(44A)-N(33A)-C(52A)	125.6(16)
C(45A)-N(34A)-C(44A)	122.6(15)
C(45A)-N(34A)-C(47A)	113.0(11)
C(44A)-N(34A)-C(47A)	121.7(15)
C(45A)-N(35A)-C(46A)	113.3(12)

C(49A)-N(36A)-C(46A)	111.2(12)
C(49A)-N(36A)-C(48A)	121.6(16)
C(46A)-N(36A)-C(48A)	121.5(17)
C(49A)-N(37A)-C(47A)	111.9(11)
C(49A)-N(37A)-C(50A)	122.3(13)
C(47A)-N(37A)-C(50A)	123.1(14)
C(51A)-N(38A)-C(50A)	122.8(14)
C(51A)-N(38A)-C(52A)	110.2(11)
C(50A)-N(38A)-C(52A)	126.4(14)
N(31A)-C(31A)-C(32A)	111.0(16)
N(31A)-C(31A)-H(31C)	109.4
C(32A)-C(31A)-H(31C)	109.4
N(31A)-C(31A)-H(31D)	109.4
C(32A)-C(31A)-H(31D)	109.4
H(31C)-C(31A)-H(31D)	108.0
C(33A)-C(32A)-C(41A)	121.5(14)
C(33A)-C(32A)-C(31A)	120.5(15)
C(41A)-C(32A)-C(31A)	118.0(14)
C(32A)-C(33A)-O(31A)	122.2(16)
C(32A)-C(33A)-C(34A)	119.9(14)
O(31A)-C(33A)-C(34A)	115.6(16)
C(39A)-C(34A)-C(33A)	120.4(15)
C(39A)-C(34A)-C(35A)	119.6(14)
C(33A)-C(34A)-C(35A)	120.1(15)
C(36A)-C(35A)-C(34A)	121.8(18)
C(36A)-C(35A)-H(35A)	119.1
C(34A)-C(35A)-H(35A)	119.1
C(35A)-C(36A)-C(37A)	118.5(19)
C(35A)-C(36A)-H(36A)	120.8
C(37A)-C(36A)-H(36A)	120.8
C(36A)-C(37A)-C(38A)	121.7(19)
C(36A)-C(37A)-H(37A)	119.2
C(38A)-C(37A)-H(37A)	119.2
C(37A)-C(38A)-C(39A)	120.7(18)
C(37A)-C(38A)-H(38A)	119.7
C(39A)-C(38A)-H(38A)	119.7
C(34A)-C(39A)-C(38A)	117.6(15)
C(34A)-C(39A)-C(40A)	119.3(15)
C(38A)-C(39A)-C(40A)	123.0(16)
O(32A)-C(40A)-C(39A)	114.4(16)
O(32A)-C(40A)-C(41A)	121.3(18)
C(39A)-C(40A)-C(41A)	120.6(15)
C(32A)-C(41A)-C(40A)	117.5(14)
C(32A)-C(41A)-C(42A)	121.0(15)

C(40A)-C(41A)-C(42A)	121.3(15)
N(32A)-C(42A)-C(41A)	116.9(17)
N(32A)-C(42A)-H(42C)	108.1
C(41A)-C(42A)-H(42C)	108.1
N(32A)-C(42A)-H(42D)	108.1
C(41A)-C(42A)-H(42D)	108.1
H(42C)-C(42A)-H(42D)	107.3
O(36A)-C(43A)-N(33A)	125.5(17)
O(36A)-C(43A)-N(32A)	124.1(17)
N(33A)-C(43A)-N(32A)	110.3(12)
N(34A)-C(44A)-N(33A)	113.6(17)
N(34A)-C(44A)-H(44C)	108.8
N(33A)-C(44A)-H(44C)	108.8
N(34A)-C(44A)-H(44D)	108.8
N(33A)-C(44A)-H(44D)	108.8
H(44C)-C(44A)-H(44D)	107.7
O(37A)-C(45A)-N(35A)	126.5(17)
O(37A)-C(45A)-N(34A)	125.7(18)
N(35A)-C(45A)-N(34A)	107.4(12)
N(36A)-C(46A)-N(35A)	112.7(18)
N(36A)-C(46A)-C(47A)	102.7(11)
N(35A)-C(46A)-C(47A)	102.1(11)
N(36A)-C(46A)-H(46A)	112.8
N(35A)-C(46A)-H(46A)	112.8
C(47A)-C(46A)-H(46A)	112.8
N(37A)-C(47A)-N(34A)	113.4(17)
N(37A)-C(47A)-C(46A)	103.6(11)
N(34A)-C(47A)-C(46A)	103.3(10)
N(37A)-C(47A)-H(47A)	111.9
N(34A)-C(47A)-H(47A)	111.9
C(46A)-C(47A)-H(47A)	111.9
N(36A)-C(48A)-H(48C)	107.4
N(35A)#2-C(48A)-H(48C)	107.4
N(36A)-C(48A)-H(48D)	107.4
N(35A)#2-C(48A)-H(48D)	107.4
H(48C)-C(48A)-H(48D)	107.0
O(38A)-C(49A)-N(37A)	126.8(15)
O(38A)-C(49A)-N(36A)	123.4(15)
N(37A)-C(49A)-N(36A)	109.7(11)
N(38A)-C(50A)-N(37A)	116.5(16)
N(38A)-C(50A)-H(50C)	108.2
N(37A)-C(50A)-H(50C)	108.2
N(38A)-C(50A)-H(50D)	108.2
N(37A)-C(50A)-H(50D)	108.2

H(50C)-C(50A)-H(50D)	107.3
O(39A)-C(51A)-N(31A)	122.5(15)
O(39A)-C(51A)-N(38A)	126.3(16)
N(31A)-C(51A)-N(38A)	110.8(12)
N(38A)-C(52A)-N(33A)	111.5(14)
N(38A)-C(52A)-C(54A)	111.6(15)
N(33A)-C(52A)-C(54A)	112.1(16)
N(38A)-C(52A)-C(53A)	102.4(10)
N(33A)-C(52A)-C(53A)	100.5(10)
C(54A)-C(52A)-C(53A)	117.8(14)
N(31A)-C(53A)-N(32A)	108.3(14)
N(31A)-C(53A)-C(55A)	110.5(15)
N(32A)-C(53A)-C(55A)	112.3(14)
N(31A)-C(53A)-C(52A)	104.4(10)
N(32A)-C(53A)-C(52A)	105.6(10)
C(55A)-C(53A)-C(52A)	115.1(14)
C(52A)-C(54A)-H(54D)	109.5
C(52A)-C(54A)-H(54E)	109.5
H(54D)-C(54A)-H(54E)	109.5
C(52A)-C(54A)-H(54F)	109.5
H(54D)-C(54A)-H(54F)	109.5
H(54E)-C(54A)-H(54F)	109.5
C(53A)-C(55A)-H(55D)	109.5
C(53A)-C(55A)-H(55E)	109.5
H(55D)-C(55A)-H(55E)	109.5
C(53A)-C(55A)-H(55F)	109.5
H(55D)-C(55A)-H(55F)	109.5
H(55E)-C(55A)-H(55F)	109.5
O(31A)-C(56A)-C(57A)	108.6(17)
O(31A)-C(56A)-H(56C)	110.0
C(57A)-C(56A)-H(56C)	110.0
O(31A)-C(56A)-H(56D)	110.0
C(57A)-C(56A)-H(56D)	110.0
H(56C)-C(56A)-H(56D)	108.3
C(58A)-C(57A)-C(56A)	116(2)
C(58A)-C(57A)-H(57C)	108.4
C(56A)-C(57A)-H(57C)	108.4
C(58A)-C(57A)-H(57D)	108.4
C(56A)-C(57A)-H(57D)	108.4
H(57C)-C(57A)-H(57D)	107.4
C(57A)-C(58A)-S(31A)	112.4(18)
C(57A)-C(58A)-H(58C)	109.1
S(31A)-C(58A)-H(58C)	109.1
C(57A)-C(58A)-H(58D)	109.1

S(31A)-C(58A)-H(58D)	109.1
H(58C)-C(58A)-H(58D)	107.9
O(32A)-C(59A)-C(60A)	98.9(17)
O(32A)-C(59A)-H(59C)	112.0
C(60A)-C(59A)-H(59C)	112.0
O(32A)-C(59A)-H(59D)	112.0
C(60A)-C(59A)-H(59D)	112.0
H(59C)-C(59A)-H(59D)	109.7
C(59A)-C(60A)-Cl(3A)	110.5(18)
C(59A)-C(60A)-H(60C)	109.5
Cl(3A)-C(60A)-H(60C)	109.5
C(59A)-C(60A)-H(60D)	109.5
Cl(3A)-C(60A)-H(60D)	109.5
H(60C)-C(60A)-H(60D)	108.1
C(61)-N(61)-Na(1)	144.0(4)
N(61)-C(61)-C(62)	178.6(7)
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(71)-N(71)-Na(2)	167.0(8)
N(71)-C(71)-C(72)	179.2(13)
C(71)-C(72)-H(72A)	109.5
C(71)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(71A)-N(71A)-Na(2)	135(4)
N(71A)-C(71A)-C(72A)	163(6)
N(71A)-C(71A)-Na(2)	27(2)
C(72A)-C(71A)-Na(2)	139(4)
C(71A)-C(72A)-C(72A)#2	166(7)
C(71A)-C(72A)-H(72D)	109.5
C(72A)#2-C(72A)-H(72D)	57.9
C(71A)-C(72A)-H(72E)	109.5
C(72A)#2-C(72A)-H(72E)	81.6
H(72D)-C(72A)-H(72E)	109.5
C(71A)-C(72A)-H(72F)	109.5
C(72A)#2-C(72A)-H(72F)	73.0
H(72D)-C(72A)-H(72F)	109.5
H(72E)-C(72A)-H(72F)	109.5

Na(1)-O(81)-H(81A)	118(6)
Na(1)-O(81)-H(81B)	131(7)
H(81A)-O(81)-H(81B)	95(3)

Symmetry transformations used to generate equivalent atoms: #1 –x,y,-z+3/2 #2 –x+1,y,–z+3/2.

Table S5: Anisotropic displacement parameters (Å^2 x 10^3) for **2b**. The anisotropic displacement factor exponent takes the form: –2p^2[h^2 a*^{2} U^{11} + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Na(1)	25(1)	107(2)	62(1)	19(1)	–4(1)	1(1)
Na(2)	69(1)	98(2)	88(2)	–16(1)	–33(1)	10(1)
Cl(1)	38(1)	97(1)	57(1)	24(1)	–12(1)	–15(1)
S(1)	51(1)	97(2)	47(1)	–17(1)	–17(1)	20(1)
O(1)	48(3)	88(3)	33(2)	–5(2)	–7(2)	9(3)
O(2)	28(2)	78(3)	37(2)	6(2)	–4(2)	–7(2)
O(3)	82(4)	118(4)	105(5)	24(4)	–34(3)	–3(3)
O(4)	89(4)	155(5)	58(3)	–35(3)	–24(2)	33(3)
O(5)	48(2)	104(4)	78(3)	–16(3)	–20(2)	8(2)
O(6)	31(2)	63(5)	43(3)	–2(4)	–8(2)	–6(2)
O(7)	31(2)	70(6)	51(3)	–11(3)	–3(2)	1(2)
O(8)	33(2)	86(3)	55(2)	15(2)	–6(2)	–4(3)
O(9)	24(2)	72(3)	30(2)	1(2)	–2(1)	–2(3)
N(1)	25(2)	59(3)	29(2)	0(2)	–1(2)	–4(2)
N(2)	23(2)	60(3)	32(2)	–1(2)	1(2)	–5(2)
N(3)	26(2)	60(3)	49(2)	–1(3)	–2(2)	–2(2)
N(4)	31(2)	54(4)	54(2)	2(2)	–1(2)	–3(2)
N(5)	27(2)	57(4)	57(3)	–3(3)	2(2)	0(2)
N(6)	31(2)	68(4)	52(2)	15(2)	2(2)	3(2)
N(7)	24(2)	61(4)	52(2)	8(2)	0(2)	1(2)
N(8)	26(2)	58(3)	41(2)	0(2)	–1(2)	3(3)
C(1)	31(2)	63(3)	33(2)	0(3)	–1(2)	–4(3)
C(2)	29(2)	62(4)	30(2)	6(3)	1(2)	–4(2)
C(3)	34(3)	66(4)	29(2)	3(2)	0(2)	2(2)
C(4)	32(3)	74(4)	37(3)	9(2)	9(2)	3(2)
C(5)	43(4)	78(4)	35(2)	2(2)	8(3)	10(3)
C(6)	49(4)	86(4)	45(3)	11(3)	12(3)	16(3)
C(7)	42(3)	77(4)	49(3)	14(3)	9(2)	14(3)
C(8)	33(3)	74(4)	45(3)	16(3)	4(2)	3(2)
C(9)	30(3)	66(3)	36(3)	11(3)	6(2)	–3(2)
C(10)	26(2)	67(4)	33(3)	11(3)	4(2)	–7(2)
C(11)	24(2)	57(4)	28(2)	9(2)	2(2)	–5(2)
C(12)	29(3)	67(3)	26(2)	4(2)	2(2)	–4(3)

C(13)	33(3)	59(4)	31(3)	–4(3)	0(2)	–3(3)
C(14)	37(3)	57(4)	53(3)	–5(3)	–1(2)	–3(3)
C(15)	34(2)	52(5)	51(3)	–8(3)	2(2)	2(2)
C(16)	35(2)	52(4)	62(3)	4(3)	9(2)	6(2)
C(17)	34(2)	53(4)	58(3)	1(3)	8(2)	5(2)
C(18)	39(3)	69(6)	62(3)	18(3)	6(2)	11(4)
C(19)	24(2)	68(4)	55(3)	15(3)	2(2)	8(2)
C(20)	27(2)	62(4)	51(3)	5(3)	5(2)	4(3)
C(21)	20(2)	59(3)	38(2)	0(2)	0(2)	3(3)
C(22)	25(2)	64(3)	39(2)	–3(2)	1(2)	0(2)
C(23)	24(2)	62(3)	34(2)	–2(2)	1(2)	–3(2)
C(24)	41(4)	65(5)	55(4)	–8(3)	7(3)	3(3)
C(25)	22(3)	74(6)	42(3)	–3(3)	6(2)	0(3)
C(26)	73(4)	97(4)	29(2)	6(2)	8(2)	34(3)
C(27)	102(5)	134(6)	45(4)	–2(4)	–11(3)	57(5)
C(28)	68(3)	106(5)	52(3)	–8(3)	–13(3)	11(3)
C(29)	27(3)	70(4)	62(3)	8(3)	–9(2)	1(3)
C(30)	38(3)	65(4)	63(3)	–2(3)	–6(2)	–6(3)
Cl(1A)	134(9)	145(10)	110(8)	–1(7)	–6(7)	0(8)
S(1A)	57(4)	98(6)	53(4)	1(5)	–16(4)	2(4)
O(1A)	52(8)	81(8)	37(6)	–2(6)	–8(6)	13(8)
O(2A)	29(7)	70(8)	48(7)	12(7)	–5(6)	–1(7)
O(3A)	35(6)	101(7)	34(6)	–20(6)	–18(6)	17(5)
O(4A)	85(11)	88(11)	53(6)	–17(7)	–35(7)	–20(9)
O(5A)	48(2)	104(4)	78(3)	–16(3)	–20(2)	8(2)
O(6A)	33(7)	48(15)	40(10)	6(12)	–16(7)	–22(8)
O(7A)	37(8)	59(19)	58(12)	–9(11)	–4(8)	1(10)
O(8A)	35(7)	105(8)	59(7)	24(7)	–3(7)	–15(7)
O(9A)	24(7)	70(9)	40(5)	–9(6)	–5(5)	–11(9)
N(1A)	28(6)	58(6)	40(5)	–3(5)	–5(5)	–1(6)
N(2A)	24(5)	59(6)	35(6)	5(6)	0(5)	–12(5)
N(3A)	23(5)	57(7)	41(7)	–1(6)	–2(5)	–6(5)
N(4A)	33(5)	50(8)	54(6)	2(6)	3(5)	–1(6)
N(5A)	38(6)	52(10)	54(7)	–3(7)	6(5)	–4(7)
N(6A)	36(6)	65(8)	58(6)	18(6)	3(5)	7(6)
N(7A)	26(6)	63(8)	59(5)	5(6)	5(5)	1(6)
N(8A)	22(6)	57(6)	38(5)	–6(5)	–1(5)	0(6)
C(1A)	23(6)	61(7)	28(7)	1(7)	–2(6)	–4(6)
C(2A)	30(6)	62(7)	28(6)	7(6)	3(5)	1(6)
C(3A)	32(7)	72(7)	30(6)	5(6)	1(5)	12(6)
C(4A)	34(7)	75(7)	33(6)	7(6)	6(5)	8(6)
C(5A)	34(8)	81(8)	39(7)	6(6)	13(7)	14(7)
C(6A)	34(9)	81(8)	37(7)	8(7)	13(7)	12(7)
C(7A)	37(8)	80(8)	45(8)	13(7)	6(7)	8(7)

C(8A)	30(7)	75(8)	43(8)	16(7)	3(6)	1(7)
C(9A)	28(6)	70(7)	38(7)	15(6)	7(5)	1(6)
C(10A)	28(6)	63(7)	37(6)	15(6)	0(5)	–3(6)
C(11A)	25(6)	63(8)	30(6)	11(6)	5(5)	–5(6)
C(12A)	21(7)	61(7)	25(7)	9(6)	7(6)	–17(6)
C(13A)	28(6)	55(7)	33(7)	1(7)	–1(6)	–12(6)
C(14A)	34(7)	56(8)	55(7)	–2(7)	–1(6)	–10(7)
C(15A)	32(6)	53(10)	53(7)	–7(7)	2(5)	0(7)
C(16A)	40(6)	64(8)	65(6)	8(6)	6(5)	0(6)
C(17A)	33(6)	58(8)	62(6)	5(6)	0(5)	1(6)
C(18A)	29(9)	69(13)	60(8)	15(9)	14(7)	15(11)
C(19A)	44(6)	82(8)	60(5)	12(6)	3(5)	–7(6)
C(20A)	20(6)	57(8)	46(7)	0(7)	–4(6)	6(7)
C(21A)	15(6)	58(6)	38(5)	–3(5)	–2(5)	–1(7)
C(22A)	24(5)	59(6)	36(5)	–5(5)	1(5)	–6(5)
C(23A)	24(5)	60(6)	37(5)	–4(5)	–1(5)	–6(5)
C(24A)	30(11)	68(13)	49(12)	–19(12)	1(10)	0(12)
C(25A)	29(10)	58(17)	59(13)	–6(12)	6(10)	–14(11)
C(26A)	57(8)	105(8)	37(6)	2(6)	–8(6)	21(8)
C(27A)	56(8)	117(10)	35(6)	–5(8)	–8(6)	25(8)
C(28A)	59(7)	108(8)	45(7)	–14(7)	–13(6)	24(7)
C(29A)	35(8)	75(9)	75(8)	8(8)	–12(7)	–3(8)
C(30A)	50(9)	92(11)	89(8)	10(9)	–26(7)	–8(9)
Cl(3)	313(11)	207(7)	362(11)	88(8)	–139(9)	–16(7)
S(31)	117(3)	103(3)	161(4)	–59(3)	–48(3)	38(2)
O(31)	139(5)	105(5)	110(5)	13(4)	–17(4)	–18(4)
O(32)	103(5)	93(6)	187(8)	41(5)	–12(5)	–1(4)
O(33)	83(4)	104(5)	166(8)	–55(5)	–45(5)	20(4)
O(34)	177(9)	207(10)	137(6)	–49(7)	–88(6)	58(8)
O(35)	115(6)	142(9)	251(12)	–57(8)	–87(7)	–32(6)
O(36)	56(4)	132(10)	126(8)	73(7)	6(5)	2(5)
O(37)	27(3)	79(10)	45(4)	29(4)	–11(2)	–5(3)
O(38)	24(3)	91(5)	37(4)	9(3)	–10(2)	–2(3)
O(39)	75(5)	96(6)	47(3)	4(3)	–12(3)	–24(4)
N(31)	76(4)	70(4)	57(4)	21(3)	1(3)	–17(3)
N(32)	59(4)	82(5)	75(4)	37(4)	–1(3)	–10(3)
N(33)	37(3)	76(5)	39(4)	24(3)	–3(3)	–12(3)
N(34)	28(3)	66(5)	27(4)	16(3)	–6(2)	–5(3)
N(35)	32(3)	60(6)	24(4)	13(3)	–9(3)	–5(3)
N(36)	27(2)	60(5)	26(4)	8(3)	–8(2)	5(3)
N(37)	26(3)	70(5)	26(4)	10(3)	–3(2)	–2(3)
N(38)	40(3)	71(4)	36(3)	16(3)	–4(2)	–17(3)
C(31)	101(5)	76(5)	62(5)	29(4)	3(4)	–25(4)
C(32)	109(5)	75(6)	83(4)	35(4)	8(4)	–14(4)

C(33)	122(5)	106(7)	88(5)	28(5)	14(4)	–9(5)
C(34)	123(5)	95(7)	105(5)	48(5)	35(4)	–6(5)
C(35)	146(7)	123(8)	119(6)	35(6)	51(6)	–4(6)
C(36)	140(8)	131(9)	123(7)	39(7)	29(6)	16(7)
C(37)	143(8)	137(9)	128(8)	38(7)	40(6)	21(7)
C(38)	133(7)	118(8)	118(8)	51(6)	34(6)	17(6)
C(39)	117(5)	96(7)	114(6)	52(5)	31(5)	9(5)
C(40)	101(5)	85(6)	117(6)	53(5)	14(5)	0(4)
C(41)	96(5)	84(6)	87(5)	40(4)	14(4)	–16(4)
C(42)	82(6)	83(6)	93(5)	36(4)	–1(5)	–7(4)
C(43)	49(4)	88(6)	70(5)	33(5)	0(5)	–9(4)
C(44)	33(3)	77(5)	33(5)	19(3)	–10(3)	–16(4)
C(45)	26(3)	64(6)	31(5)	14(4)	–7(3)	–10(3)
C(46)	35(3)	60(5)	26(4)	6(3)	–6(3)	2(3)
C(47)	31(3)	56(5)	28(4)	8(3)	–7(3)	–1(3)
C(48)	36(2)	67(6)	24(4)	8(3)	–7(3)	12(3)
C(49)	26(3)	69(5)	27(4)	7(3)	–8(3)	8(3)
C(50)	23(3)	81(5)	32(4)	11(3)	2(2)	–2(3)
C(51)	60(4)	79(5)	41(4)	14(3)	1(3)	–26(4)
C(52)	38(3)	76(4)	36(3)	19(3)	–4(2)	–16(3)
C(53)	55(4)	78(5)	54(3)	31(3)	–7(3)	–17(3)
C(54)	52(5)	93(7)	36(4)	11(5)	2(4)	–21(5)
C(55)	77(7)	97(9)	56(5)	28(5)	4(5)	–31(6)
C(56)	134(7)	136(7)	109(7)	–8(6)	–14(6)	–28(6)
C(57)	142(8)	126(8)	137(7)	–17(7)	–14(7)	3(7)
C(58)	128(6)	119(7)	129(6)	–32(6)	–33(6)	37(6)
C(59)	113(7)	116(8)	235(10)	65(8)	3(8)	–9(6)
C(60)	145(8)	157(10)	289(12)	80(10)	–20(10)	1(9)
Cl(3A)	252(15)	226(13)	252(14)	46(10)	–91(12)	–99(11)
S(31A)	134(7)	145(7)	188(8)	–38(6)	–35(6)	10(5)
O(31A)	143(8)	125(9)	102(7)	2(7)	4(7)	–9(8)
O(32A)	119(7)	107(8)	183(9)	49(7)	–5(7)	–3(7)
O(33A)	104(9)	103(7)	180(11)	–32(8)	–39(8)	23(7)
O(34A)	170(16)	202(17)	222(15)	–28(13)	–88(13)	16(14)
O(35A)	174(18)	161(17)	300(20)	–16(16)	11(17)	–19(14)
O(36A)	45(6)	67(9)	81(10)	12(8)	–16(6)	–16(6)
O(37A)	28(5)	60(13)	39(10)	11(9)	–1(5)	2(6)
O(38A)	20(5)	96(6)	29(7)	10(6)	–8(4)	1(5)
O(39A)	76(8)	98(9)	53(6)	7(6)	–4(5)	–11(7)
N(31A)	77(7)	84(6)	56(6)	22(5)	–1(5)	–19(6)
N(32A)	60(6)	83(7)	79(6)	36(6)	–8(5)	–14(5)
N(33A)	37(5)	77(7)	40(6)	25(5)	–7(5)	–12(5)
N(34A)	25(4)	65(8)	22(6)	13(5)	–4(4)	–6(5)
N(35A)	24(4)	58(8)	24(7)	12(6)	0(5)	–4(5)

N(36A)	28(5)	69(7)	18(5)	8(5)	–7(4)	–1(5)
N(37A)	24(5)	73(7)	21(5)	13(5)	–3(4)	–4(5)
N(38A)	42(5)	79(6)	33(5)	19(5)	–5(4)	–16(5)
C(31A)	100(7)	82(7)	74(8)	30(7)	9(7)	–13(7)
C(32A)	103(6)	88(8)	82(6)	38(6)	9(5)	–13(6)
C(33A)	126(6)	96(8)	92(7)	32(6)	16(6)	–4(6)
C(34A)	133(6)	108(9)	106(7)	38(7)	32(6)	–3(7)
C(35A)	146(9)	119(10)	122(8)	25(8)	38(8)	1(8)
C(36A)	144(10)	129(11)	127(9)	30(9)	36(8)	9(9)
C(37A)	150(10)	131(11)	129(11)	32(9)	31(9)	8(10)
C(38A)	140(8)	120(9)	125(10)	39(8)	32(8)	9(7)
C(39A)	123(6)	98(8)	117(7)	57(6)	26(6)	7(6)
C(40A)	107(6)	91(8)	130(8)	51(6)	17(6)	2(6)
C(41A)	100(6)	85(8)	102(7)	42(6)	8(6)	–11(6)
C(42A)	79(8)	85(7)	95(7)	41(6)	–7(7)	–9(6)
C(43A)	45(6)	81(7)	60(7)	28(7)	–12(6)	–10(5)
C(44A)	37(6)	72(7)	21(6)	15(6)	–7(5)	–8(6)
C(45A)	29(5)	58(9)	23(7)	11(6)	–7(5)	–7(5)
C(46A)	28(5)	52(7)	19(6)	7(5)	–4(4)	0(4)
C(47A)	32(5)	62(7)	17(5)	8(5)	–1(4)	0(5)
C(48A)	36(2)	67(6)	24(4)	8(3)	–7(3)	12(3)
C(49A)	20(5)	79(7)	28(6)	7(5)	–2(4)	2(5)
C(50A)	31(6)	83(8)	34(6)	14(6)	2(5)	–11(6)
C(51A)	60(7)	80(7)	43(6)	16(5)	1(5)	–18(6)
C(52A)	40(5)	83(6)	38(5)	18(5)	–6(4)	–15(5)
C(53A)	56(6)	84(6)	52(5)	29(5)	–9(5)	–18(5)
C(54A)	62(11)	94(12)	31(8)	12(9)	8(7)	–22(11)
C(55A)	84(13)	113(17)	49(8)	37(10)	1(8)	–8(12)
C(56A)	142(9)	125(9)	120(8)	–1(8)	–14(7)	0(8)
C(57A)	143(9)	137(10)	138(9)	–18(9)	–15(8)	12(8)
C(58A)	151(9)	128(10)	159(10)	–34(9)	–32(8)	24(8)
C(59A)	118(9)	114(9)	227(11)	59(9)	–22(9)	–15(8)
C(60A)	150(11)	150(11)	246(12)	55(10)	–45(10)	–23(10)
N(61)	41(2)	160(5)	76(3)	17(3)	12(2)	15(3)
C(61)	39(2)	91(4)	53(3)	17(2)	4(2)	10(2)
C(62)	55(3)	87(4)	63(3)	7(3)	24(2)	8(3)
N(71)	153(6)	137(6)	105(5)	12(5)	37(4)	56(5)
C(71)	163(7)	111(6)	85(5)	1(5)	40(5)	49(6)
C(72)	224(12)	90(6)	110(7)	4(5)	81(7)	34(7)
N(71A)	131(9)	126(10)	93(11)	–10(10)	3(10)	44(9)
C(71A)	145(9)	132(11)	103(11)	–1(11)	22(9)	53(9)
C(72A)	147(10)	134(13)	105(13)	3(12)	30(12)	56(11)
O(81)	191(7)	339(11)	41(2)	8(4)	15(3)	–62(7)

Table S6: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **2b**.

	x	y	z	*U*(eq)
H(1A)	2400	7477	5707	51
H(1AB)	2286	7447	6392	51
H(5)	450	8107	7081	63
H(6)	–622	8344	6938	72
H(7)	–1310	8230	6142	67
H(8)	–933	7887	5452	61
H(12A)	925	7286	4609	49
H(12B)	1692	7396	4789	49
H(14A)	463	6230	5228	59
H(14B)	1194	6061	5328	59
H(16)	624	5623	6934	59
H(17)	1396	5821	6255	58
H(18A)	676	5637	8004	68
H(18B)	1088	5913	8304	68
H(20A)	2533	6375	6893	56
H(20B)	2486	6154	6342	56
H(24A)	2389	6342	4849	80
H(24B)	2340	6124	5406	80
H(24C)	2951	6373	5361	80
H(25A)	2727	6866	4673	69
H(25B)	3160	6910	5262	69
H(25C)	2767	7195	4973	69
H(26A)	1407	7364	7254	80
H(26B)	848	7611	7483	80
H(27A)	1776	7893	7887	112
H(27B)	1678	7567	8184	112
H(28A)	2766	7792	7575	91
H(28B)	2570	7445	7425	91
H(29A)	–1035	7406	5102	64
H(29B)	–440	7147	5106	64
H(30A)	–1145	7091	4274	66
H(30B)	–359	7171	4090	66
H(1AA)	2417	7366	5694	44
H(1AC)	2336	7334	6382	44
H(5A)	750	8083	7086	62
H(6A)	–308	8350	7024	61
H(7A)	–1105	8236	6283	64
H(8A)	–844	7855	5605	59
H(12C)	842	7218	4674	43
H(12D)	1630	7312	4822	43
H(14C)	403	6141	5255	58

H(14D)	1139	5973	5340	58
H(16A)	627	5515	6937	68
H(17A)	1360	5721	6229	61
H(18C)	1104	5816	8302	63
H(18D)	713	5534	7999	63
H(20C)	2542	6260	6829	49
H(20D)	2443	6047	6272	49
H(24D)	2277	6251	4800	74
H(24E)	2260	6029	5352	74
H(24F)	2876	6273	5284	74
H(25D)	2663	6746	4667	73
H(25E)	3085	6868	5221	73
H(25F)	2600	7097	4857	73
H(26C)	1556	7394	7242	80
H(26D)	2300	7537	7334	80
H(27C)	1429	7416	8040	83
H(27D)	1314	7772	7978	83
H(28C)	1896	7710	8737	85
H(28D)	2427	7847	8274	85
H(29C)	–1054	7423	5163	74
H(29D)	–579	7156	4895	74
H(30C)	–1028	7667	4216	92
H(30D)	–1460	7353	4232	92
H(31A)	3468	5479	9369	95
H(31B)	3684	5442	10038	95
H(35)	4870	4898	8031	155
H(36)	5830	4618	7816	157
H(37)	6833	4657	8394	163
H(38)	6789	4941	9264	148
H(42A)	4774	5525	10666	103
H(42B)	5572	5621	10564	103
H(44A)	5068	6833	9855	57
H(44B)	5760	6645	9702	57
H(46)	4776	7210	8139	48
H(47)	4435	7071	9056	46
H(48A)	3588	6891	7138	51
H(48B)	4066	7187	7253	51
H(50A)	3425	6788	9456	55
H(50B)	3005	6569	9025	55
H(54A)	4072	6805	10285	91
H(54B)	4286	6576	10796	91
H(54C)	3499	6581	10559	91
H(55A)	3232	6034	10699	115
H(55B)	3915	6100	11082	115

H(55C)	3735	5759	10882	115
H(56A)	3398	4982	9082	152
H(56B)	3635	4808	8501	152
H(57A)	2466	4938	8437	162
H(57B)	2647	5288	8561	162
H(58A)	2910	4953	7548	150
H(58B)	3346	5257	7678	150
H(59A)	6815	5377	9172	186
H(59B)	6777	5689	9541	186
H(60A)	7910	5499	9522	236
H(60B)	7644	5185	9795	236
H(31C)	3517	5380	9556	102
H(31D)	3897	5365	10176	102
H(35A)	4581	4723	8158	155
H(36A)	5527	4459	7792	160
H(37A)	6640	4583	8118	164
H(38A)	6800	4908	8914	154
H(42C)	5042	5432	10613	104
H(42D)	5792	5556	10423	104
H(44C)	5076	6776	9950	52
H(44D)	5791	6605	9793	52
H(46A)	4765	7169	8251	40
H(47A)	4430	7010	9169	44
H(48C)	4083	7140	7378	51
H(48D)	3572	6858	7275	51
H(50C)	3436	6687	9561	59
H(50D)	3060	6462	9113	59
H(54D)	4007	6713	10351	94
H(54E)	4369	6514	10850	94
H(54F)	3566	6457	10685	94
H(55D)	3392	5827	10744	123
H(55E)	3924	6038	11100	123
H(55F)	4091	5683	11011	123
H(56C)	4043	5226	7989	155
H(56D)	3396	5373	8335	155
H(57C)	3425	4786	7829	167
H(57D)	2799	4902	8233	167
H(58C)	2669	4920	7191	175
H(58D)	3135	5223	7231	175
H(59C)	6494	5682	9994	184
H(59D)	7219	5563	9710	184
H(60C)	7490	5273	10507	219
H(60D)	6695	5269	10729	219
H(62A)	–563	6727	8357	103

H(62B)	–532	7090	8445	103
H(62C)	–169	6868	8909	103
H(72A)	4847	6154	6484	212
H(72B)	4502	5854	6208	212
H(72C)	5116	5823	6676	212
H(72D)	4801	5676	7164	193
H(72E)	4710	5454	7711	193
H(72F)	4805	5814	7808	193
H(81A)	1380(40)	6460(40)	8800(40)	286
H(81B)	1780(70)	6620(30)	9140(20)	286

Table S7: Intensity statistics for **2b**.

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	Rmerge	R(sigma)
Inf - 3.60	295	296	99.7	25.30	45.07	64.59	0.0373	0.0113
3.60 - 2.31	692	693	99.9	26.09	21.56	60.42	0.0393	0.0120
2.31 - 1.81	1007	1007	100.0	23.33	8.10	38.17	0.0625	0.0172
1.81 - 1.57	988	988	100.0	31.40	5.02	36.61	0.0863	0.0188
1.57 - 1.42	1003	1003	100.0	32.92	2.74	28.38	0.1255	0.0261
1.42 - 1.32	942	942	100.0	28.08	1.87	20.21	0.1593	0.0378
1.32 - 1.23	1109	1109	100.0	25.90	1.53	17.39	0.1659	0.0449
1.23 - 1.17	939	939	100.0	25.12	1.49	17.01	0.1751	0.0469
1.17 - 1.12	937	937	100.0	23.70	1.38	15.60	0.1815	0.0511
1.12 - 1.07	1125	1125	100.0	22.46	1.21	13.68	0.1975	0.0579
1.07 - 1.03	1070	1070	100.0	21.45	1.00	11.88	0.2377	0.0693
1.03 - 1.00	887	887	100.0	18.88	0.75	9.36	0.2557	0.0904
1.00 - 0.97	1039	1039	100.0	16.51	0.59	7.41	0.2948	0.1199
0.97 - 0.95	747	747	100.0	17.08	0.42	6.06	0.3706	0.1499
0.95 - 0.92	1253	1253	100.0	16.62	0.34	5.37	0.4004	0.1709
0.92 - 0.90	941	941	100.0	15.66	0.26	4.31	0.4824	0.2218
0.90 - 0.88	1003	1003	100.0	15.00	0.22	3.89	0.4958	0.2508
0.88 - 0.86	1125	1125	100.0	14.06	0.18	3.24	0.5545	0.2984
0.86 - 0.85	596	596	100.0	13.30	0.18	3.20	0.5729	0.2980
0.85 - 0.83	1269	1269	100.0	12.34	0.16	2.80	0.5851	0.3442
0.83 - 0.82	699	699	100.0	10.86	0.17	2.67	0.5997	0.3509
0.92 - 0.82	5633	5633	100.0	13.63	0.20	3.36	0.5358	0.2859
Inf - 0.82	19666	19668	100.0	20.67	2.84	15.62	0.0894	0.0292

Merged [A], lowest resolution = 23.03 Angstroms.

Crystal Structure of 10a. **10a** crystallized as colorless needles from ethanol/water, 2:1 (*v/v*) containing a few drops of TFA *via* ethanol diffusion. The compound crystallized in the triclinic space group $P\bar{1}$ with one molecule of **10a**, two free water solvent molecules, one free ethanol solvent molecule, and one sodium ion in the asymmetric unit. One of the azide residues of **10a** displays disorder that was modeled across three positions. The main occupied species refined to an occupancy of 59.0% (esd 0.3%). The minor occupied species refined to occupancies of 22.8% (esd 0.3%) and 18.2% (esd 0.3%), respectively. The occupancies were restrained to unity using the SUMP command in *SHELXL*.[9]

Application of the crystallographic symmetry operator generates a dimer of **10a** that is bridged *via* two sodium ions (Figure S4). Each sodium ion is coordinated by six oxygen atoms that form a distorted octahedron. Three of these oxygen donors are carbonyl groups of **10a**, the other three oxygen atoms derive from solvent water molecules: the sodium ions are bridged *via* two μ_2-OH_2 molecules (H_2O20). In addition, one water molecule (H_2O21) is coordinated in an end-on fashion to each sodium ion.

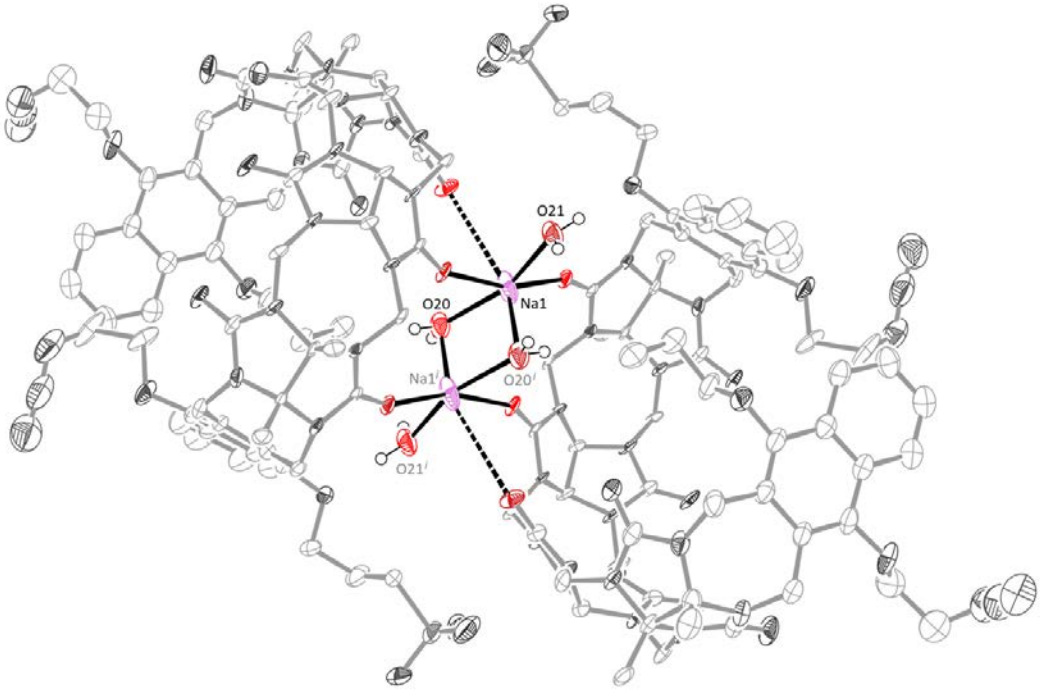


Figure S4: ORTEP-plot of the dimer of **10a** with the bridging sodium water motif highlighted. Thermal ellipsoids set at 50% probability. Hydrogen atoms, the $S1O_3$ residue, and the ethanol molecule are omitted for clarity.

The positions of the H-atoms of H_2O21 and H_2O20 were taken from the Fourier synthesis and assigned to idealized positions. Their U_{ij} components were set to 1.5 times the thermal displacement parameters of the oxygen atoms they are attached to. Additional support for the assignment of hydrogen atoms to H_2O20 (and thus generating a bridging H_2O species) comes from a comparison of the Na-O bond distance with known values from the CSD.[12] Examples of bridging μ_2-OH species are very rare and display Na–O bond distances of 2.25–2.29 Å. Bridging μ_2-OH_2 species are much more common. Their Na–O bond distances are found to be 2.30–3.0 Å with an average distance of 2.42 Å. The bond distance observed for the bridging oxygen species in **10a** refines to 2.358 Å (esd 0.002 Å), thus falling into the typically observed range of bridging μ_2-OH_2 species. Both water molecules are a part of an extensive hydrogen bond network with proximal ether and sulfonate groups.

Several other free solvent water and ethanol molecules were found in the lattice; however all but one ethanol molecule located in the cavity of the bonded **10a** were defined poorly because of extensive disorder and movement of these solvent molecules in the crystal. Thus, *SQUEEZE* as implemented in *PLATON*[11] was applied. *SQUEEZE* found one solvent accessible void at the origin of the unit cell. The volume is 1486 $Å^3$ and comprises 453 electrons (Figure S5). It is impossible to determine the exact number of solvent molecules based on the electron count alone because there are multiple possible combinations of solvent molecules that match the number of electrons determined. For example, a possible combination comprises 14 ethanol and 11 water molecules (a total of 452 electrons) per unit cell.

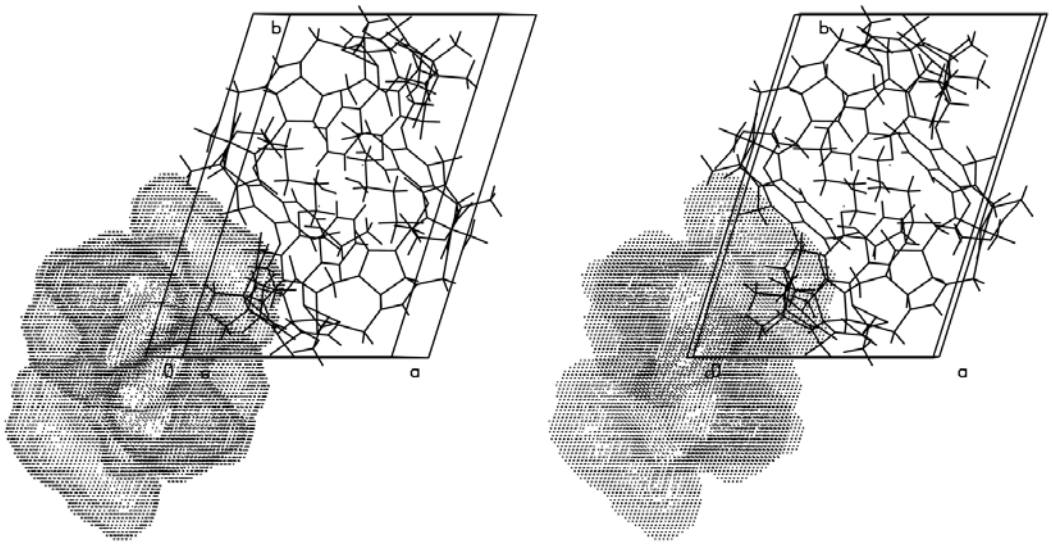


Figure S5: Stereo view of the solvent accessible void located at the origin of the unit cell.

Application of SQUEEZE, however, led to a non-charge balanced structure. **10a** has a negative charge of –2 and crystallized with one positively charged sodium ion per molecule. In total, this leads to a missing positive charge. **10a** has been crystallized from an ethanol water mixture with the addition of a few drops of TFA (trifluoroacetic acid). Thus, it seems to be reasonable that the missing positive charge refers to a proton that participates in the water ethanol hydrogen bond network in the void found by *SQUEEZE*.

In general, the quality of the data set is rather mediocre (Rint = 0.1574, R1 = 0.1246, wR2 = 0.2820) as usually observed for large macrocyclic compounds. That is because of a high number of free electron pairs, weak scatterers, and a high solvent content (usually highly disordered and of poor definition). Detection of a proton in a hydrogen bonding network, however, requires a very good dataset. Intensity statistic, crystal data, and refinement parameters are listed below.

Table S8: Crystal data and structure refinement for **10a**.

CCDC number	1890948	
Empirical formula	$C_{62}H_{74}N_{22}NaO_{21}S_2$	
Formula weight	1550.54	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.4931(5) Å	α = 89.537(2)°
	b = 18.1989(7) Å	β = 87.890(3)°
	c = 20.9673(8) Å	γ = 72.498(2)°
Volume	4543.3(3) Å^3	
Z	2	
Density (calculated)	1.133 Mg/m^3	
Absorption coefficient	1.184 mm^{-1}	
F(000)	1622	
Crystal size	0.242 x 0.045 x 0.023 mm^3	
Theta range for data collection	2.546 to 66.596°	
Index ranges	–12<=h<=14, –21<=k<=21, –24<=l<=24	
Reflections collected	54274	

Independent reflections	15565 [R(int) = 0.1574]
Completeness to theta = 66.596°	97.0%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7536 and 0.4028
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15565 / 1464 / 1077
Goodness-of-fit on F^2	1.037
Final R indices [I > 2sigma(I)]	R1 = 0.1246, wR2 = 0.2820
R indices (all data)	R1 = 0.1890, wR2 = 0.3217
Largest diff. peak and hole	0.822 and –0.889 e.Å^{-3}

Table S9: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **10a**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	*U*(eq)
S(1)	7396(2)	3949(1)	7255(1)	45(1)
S(2)	3316(2)	1184(1)	5523(1)	54(1)
Na(1)	5665(3)	5598(2)	4711(2)	56(1)
O(1)	5806(5)	5775(3)	8804(3)	50(2)
O(2)	7366(6)	3353(4)	7722(3)	64(2)
O(3)	8505(5)	3925(3)	7084(3)	55(2)
O(4)	6763(6)	3919(4)	6701(3)	63(2)
O(5)	4192(6)	8502(4)	10178(3)	64(2)
C(14)	3070(30)	8850(30)	9920(30)	76(5)
C(15)	2420(40)	9660(30)	10260(30)	75(5)
N(1)	3270(40)	10060(30)	10330(20)	79(5)
N(2)	3910(40)	9780(30)	10750(20)	81(5)
N(3)	4300(50)	9620(40)	11270(20)	87(8)
C(14A)	3250(20)	9138(12)	9994(10)	70(4)
C(15A)	3214(19)	9767(12)	10521(10)	74(4)
N(1A)	2986(14)	9526(11)	11155(8)	82(4)
N(2A)	3791(15)	9233(12)	11478(9)	81(4)
N(3A)	4495(15)	8903(12)	11844(8)	94(5)
C(14B)	3220(50)	9040(30)	9880(30)	75(5)
C(15B)	2780(50)	9890(30)	10200(20)	77(5)
N(1B)	2680(30)	9800(30)	10882(17)	80(5)
N(2B)	3560(30)	9630(30)	11170(20)	78(5)
N(3B)	4240(40)	9300(30)	11560(30)	85(9)
O(6)	6859(4)	6710(3)	7242(2)	34(1)
O(7)	4368(4)	9483(3)	8574(3)	45(1)

O(8)	6087(4)	7048(3)	5619(2)	33(1)
O(9)	2640(4)	9644(3)	7158(2)	37(1)
O(10)	3836(3)	6301(3)	5071(2)	22(1)
O(11)	354(4)	8773(3)	6624(2)	32(1)
O(12)	2419(4)	4773(3)	5594(2)	23(1)
O(13)	–343(4)	7125(3)	7243(2)	29(1)
O(14)	3002(4)	3314(3)	6847(2)	25(1)
O(15)	2747(7)	723(3)	5883(3)	61(2)
O(16)	2911(8)	1368(4)	4885(3)	80(2)
O(17)	4523(7)	834(4)	5517(4)	84(2)
O(18)	674(5)	5533(3)	8596(2)	41(1)
N(4)	6909(5)	7450(4)	8116(3)	33(1)
N(5)	6898(4)	7967(3)	7165(2)	23(1)
N(6)	6150(5)	8661(4)	8663(3)	35(1)
N(7)	5597(5)	9095(3)	7705(3)	29(1)
N(8)	5757(4)	8173(3)	6233(3)	21(1)
N(9)	4551(4)	8122(3)	5490(3)	23(1)
N(10)	4474(4)	9276(3)	6764(3)	26(1)
N(11)	3168(4)	9053(3)	6177(3)	24(1)
N(12)	3085(4)	7625(3)	5178(3)	21(1)
N(13)	1930(4)	6894(3)	5196(2)	18(1)
N(14)	1679(4)	8607(3)	5797(3)	26(1)
N(15)	543(4)	7879(3)	5813(3)	26(1)
N(16)	1011(4)	5933(3)	5517(2)	16(1)
N(17)	638(4)	4980(3)	6049(2)	16(1)
N(18)	–362(4)	6923(3)	6153(2)	20(1)
N(19)	–314(4)	5962(3)	6810(2)	22(1)
N(20)	–605(8)	6596(5)	9510(4)	70(2)
N(21)	–864(9)	5995(6)	9616(4)	75(3)
N(22)	–1260(10)	5514(6)	9725(5)	92(3)
C(1)	4057(6)	7257(5)	9926(3)	35(2)
C(2)	3233(8)	7314(6)	10396(4)	48(2)
C(3)	2833(8)	6692(6)	10532(4)	52(2)
C(4)	3241(8)	6010(6)	10185(4)	49(2)
C(5)	4039(7)	5935(5)	9713(4)	40(2)
C(6)	4495(6)	6550(4)	9575(3)	34(2)
C(7)	5406(7)	6477(5)	9122(3)	37(2)
C(8)	5914(7)	7045(4)	9036(3)	34(2)
C(9)	5476(7)	7768(4)	9381(3)	34(2)
C(10)	4577(7)	7853(5)	9800(3)	40(2)
C(11)	5189(10)	5745(5)	8237(4)	58(3)
C(12)	5636(8)	4968(5)	7918(5)	56(2)
C(13)	6809(8)	4851(5)	7671(5)	58(2)
C(16)	6959(7)	6893(5)	8616(4)	43(2)

C(17)	6014(8)	8396(5)	9322(3)	41(2)
C(18)	7064(6)	8215(5)	8246(3)	32(2)
C(19)	6775(6)	8630(4)	7580(3)	25(1)
C(20)	8220(7)	8146(5)	8482(4)	44(2)
C(21)	7506(6)	9119(4)	7373(3)	30(2)
C(22)	5266(6)	9120(5)	8335(3)	34(2)
C(23)	6903(6)	7317(4)	7486(3)	32(2)
C(24)	6886(5)	7986(4)	6473(3)	24(1)
C(25)	4923(6)	9638(4)	7249(3)	30(2)
C(26)	5070(5)	8962(4)	6182(3)	22(1)
C(27)	4143(5)	8901(4)	5733(3)	22(1)
C(28)	5527(5)	7712(4)	5767(3)	23(1)
C(29)	3348(5)	9356(4)	6748(3)	25(1)
C(30)	4053(5)	7841(4)	4981(3)	24(1)
C(31)	2041(5)	9267(4)	5926(4)	30(2)
C(32)	1956(5)	8184(4)	5205(3)	23(1)
C(33)	1172(5)	7675(3)	5217(3)	18(1)
C(34)	3025(5)	6884(4)	5137(3)	16(1)
C(35)	815(5)	8460(4)	6131(3)	25(1)
C(36)	1581(5)	6240(4)	5004(3)	16(1)
C(37)	–491(5)	7717(4)	5973(3)	20(1)
C(38)	–163(5)	6272(4)	5717(3)	18(1)
C(39)	–353(5)	5630(4)	6181(3)	18(1)
C(40)	–934(6)	6463(4)	5157(3)	25(1)
C(41)	–1430(5)	5424(4)	6104(3)	24(1)
C(42)	1465(5)	5198(4)	5722(3)	16(1)
C(43)	–330(5)	6708(4)	6785(3)	22(1)
C(44)	923(5)	4307(4)	6478(3)	20(1)
C(45)	–314(6)	5543(4)	7399(3)	26(2)
C(46)	1294(7)	5042(4)	8123(3)	32(2)
C(47)	841(6)	5009(4)	7549(3)	22(1)
C(48)	1426(6)	4419(4)	7095(3)	22(1)
C(49)	2451(6)	3926(4)	7258(3)	22(1)
C(50)	2962(6)	3971(4)	7838(3)	29(2)
C(51)	4016(7)	3472(5)	7992(4)	46(2)
C(52)	4476(9)	3504(6)	8581(5)	65(3)
C(53)	3834(9)	4039(6)	9033(5)	64(3)
C(54)	2820(9)	4550(6)	8899(4)	56(2)
C(55)	2351(7)	4532(4)	8290(3)	37(2)
C(56)	2775(7)	2601(4)	7055(3)	34(2)
C(57)	3465(8)	1967(5)	6618(4)	43(2)
C(58)	3009(7)	2080(4)	5927(3)	32(2)
C(59)	952(8)	6254(5)	8668(4)	49(2)
C(60)	587(9)	6516(6)	9352(4)	69(3)

O(19)	5011(5)	6226(3)	6679(3)	45(1)
C(61)	3933(7)	6769(6)	6771(4)	50(2)
C(62)	3055(9)	6339(7)	6804(5)	69(3)
O(20)	5606(5)	5093(3)	5746(3)	49(2)
O(21)	5186(5)	6436(4)	3855(3)	46(2)

Table S10: Bond lengths [Å] and angles [°] for **10a**.

S(1)-O(3)	1.407(6)
S(1)-O(4)	1.440(8)
S(1)-O(2)	1.463(6)
S(1)-C(13)	1.800(9)
S(2)-O(15)	1.445(6)
S(2)-O(16)	1.449(7)
S(2)-O(17)	1.449(9)
S(2)-C(58)	1.774(7)
Na(1)-O(21)	2.321(6)
Na(1)-O(12)#1	2.349(5)
Na(1)-O(10)	2.357(5)
Na(1)-O(20)	2.358(6)
Na(1)-O(20)#1	2.520(8)
Na(1)-Na(1)#1	3.309(7)
O(1)-C(7)	1.389(9)
O(1)-C(11)	1.451(11)
O(5)-C(10)	1.379(10)
O(5)-C(14A)	1.446(16)
O(5)-C(14B)	1.47(2)
O(5)-C(14)	1.48(2)
C(14)-C(15)	1.61(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-N(1)	1.46(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
N(1)-N(2)	1.222(12)
N(2)-N(3)	1.208(12)
C(14A)-C(15A)	1.59(2)
C(14A)-H(14C)	0.9900
C(14A)-H(14D)	0.9900
C(15A)-N(1A)	1.44(2)
C(15A)-H(15C)	0.9900
C(15A)-H(15D)	0.9900
N(1A)-N(2A)	1.215(10)

N(2A)-N(3A)	1.203(10)
C(14B)-C(15B)	1.60(3)
C(14B)-H(14E)	0.9900
C(14B)-H(14F)	0.9900
C(15B)-N(1B)	1.45(3)
C(15B)-H(15E)	0.9900
C(15B)-H(15F)	0.9900
N(1B)-N(2B)	1.224(12)
N(2B)-N(3B)	1.216(12)
O(6)-C(23)	1.236(9)
O(7)-C(22)	1.210(9)
O(8)-C(28)	1.235(8)
O(9)-C(29)	1.212(8)
O(10)-C(34)	1.232(7)
O(11)-C(35)	1.222(8)
O(12)-C(42)	1.231(7)
O(13)-C(43)	1.226(7)
O(14)-C(49)	1.403(8)
O(14)-C(56)	1.468(8)
O(18)-C(46)	1.387(8)
O(18)-C(59)	1.465(10)
N(4)-C(23)	1.347(9)
N(4)-C(16)	1.442(10)
N(4)-C(18)	1.491(10)
N(5)-C(23)	1.355(9)
N(5)-C(24)	1.453(8)
N(5)-C(19)	1.460(8)
N(6)-C(22)	1.372(10)
N(6)-C(18)	1.452(9)
N(6)-C(17)	1.480(9)
N(7)-C(22)	1.367(9)
N(7)-C(25)	1.464(9)
N(7)-C(19)	1.475(8)
N(8)-C(28)	1.386(9)
N(8)-C(26)	1.440(8)
N(8)-C(24)	1.456(8)
N(9)-C(28)	1.371(9)
N(9)-C(30)	1.427(8)
N(9)-C(27)	1.445(8)
N(10)-C(29)	1.372(9)
N(10)-C(25)	1.435(9)
N(10)-C(26)	1.436(8)
N(11)-C(29)	1.374(9)
N(11)-C(31)	1.461(8)

N(11)-C(27)	1.464(8)
N(12)-C(34)	1.376(8)
N(12)-C(30)	1.426(8)
N(12)-C(32)	1.469(8)
N(13)-C(34)	1.363(8)
N(13)-C(36)	1.450(8)
N(13)-C(33)	1.451(8)
N(14)-C(35)	1.356(8)
N(14)-C(31)	1.436(8)
N(14)-C(32)	1.441(8)
N(15)-C(35)	1.386(8)
N(15)-C(37)	1.438(8)
N(15)-C(33)	1.440(8)
N(16)-C(42)	1.360(8)
N(16)-C(38)	1.457(8)
N(16)-C(36)	1.466(8)
N(17)-C(42)	1.373(8)
N(17)-C(39)	1.452(8)
N(17)-C(44)	1.476(8)
N(18)-C(43)	1.377(8)
N(18)-C(37)	1.453(8)
N(18)-C(38)	1.458(8)
N(19)-C(43)	1.352(9)
N(19)-C(45)	1.445(8)
N(19)-C(39)	1.465(8)
N(20)-N(21)	1.246(11)
N(20)-C(60)	1.478(14)
N(21)-N(22)	1.146(11)
C(1)-C(2)	1.379(11)
C(1)-C(6)	1.434(11)
C(1)-C(10)	1.440(12)
C(2)-C(3)	1.391(13)
C(2)-H(2)	0.9500
C(3)-C(4)	1.392(13)
C(3)-H(3)	0.9500
C(4)-C(5)	1.357(11)
C(4)-H(4)	0.9500
C(5)-C(6)	1.424(12)
C(5)-H(5)	0.9500
C(6)-C(7)	1.431(11)
C(7)-C(8)	1.373(11)
C(8)-C(9)	1.451(10)
C(8)-C(16)	1.503(11)
C(9)-C(10)	1.372(11)

C(9)-C(17)	1.493(11)
C(11)-C(12)	1.507(12)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.490(13)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(20)	1.513(11)
C(18)-C(19)	1.584(10)
C(19)-C(21)	1.506(10)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.548(9)
C(26)-H(26)	1.0000
C(27)-H(27)	1.0000
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.536(9)
C(32)-H(32)	1.0000
C(33)-H(33)	1.0000
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-C(40)	1.518(9)
C(38)-C(39)	1.579(9)
C(39)-C(41)	1.516(9)
C(40)-H(40A)	0.9800

C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(44)-C(48)	1.500(9)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(47)	1.520(10)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.359(10)
C(46)-C(55)	1.421(11)
C(47)-C(48)	1.444(9)
C(48)-C(49)	1.377(9)
C(49)-C(50)	1.409(10)
C(50)-C(51)	1.404(11)
C(50)-C(55)	1.419(10)
C(51)-C(52)	1.390(12)
C(51)-H(51)	0.9500
C(52)-C(53)	1.406(14)
C(52)-H(52)	0.9500
C(53)-C(54)	1.364(14)
C(53)-H(53)	0.9500
C(54)-C(55)	1.427(11)
C(54)-H(54)	0.9500
C(56)-C(57)	1.509(10)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.565(11)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(60)	1.526(12)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
O(19)-C(61)	1.418(10)
O(19)-HO19	0.89(2)
C(61)-C(62)	1.526(14)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900

C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
O(20)-HO1A	0.841(10)
O(20)-HO1B	0.841(10)
O(21)-HO2A	0.839(10)
O(21)-HO2B	0.839(10)

O(3)-S(1)-O(4)	111.3(4)
O(3)-S(1)-O(2)	111.6(4)
O(4)-S(1)-O(2)	112.5(4)
O(3)-S(1)-C(13)	105.1(4)
O(4)-S(1)-C(13)	110.5(5)
O(2)-S(1)-C(13)	105.5(4)
O(15)-S(2)-O(16)	113.8(5)
O(15)-S(2)-O(17)	111.1(4)
O(16)-S(2)-O(17)	111.7(5)
O(15)-S(2)-C(58)	106.7(3)
O(16)-S(2)-C(58)	105.6(4)
O(17)-S(2)-C(58)	107.5(5)
O(21)-Na(1)-O(12)#1	92.5(2)
O(21)-Na(1)-O(10)	81.5(2)
O(12)#1-Na(1)-O(10)	163.9(3)
O(21)-Na(1)-O(20)	159.4(2)
O(12)#1-Na(1)-O(20)	104.7(2)
O(10)-Na(1)-O(20)	78.9(2)
O(21)-Na(1)-O(20)#1	86.3(2)
O(12)#1-Na(1)-O(20)#1	120.0(2)
O(10)-Na(1)-O(20)#1	74.7(2)
O(20)-Na(1)-O(20)#1	94.6(2)
O(21)-Na(1)-Na(1)#1	128.1(3)
O(12)#1-Na(1)-Na(1)#1	124.1(2)
O(10)-Na(1)-Na(1)#1	70.30(15)
O(20)-Na(1)-Na(1)#1	49.4(2)
O(20)#1-Na(1)-Na(1)#1	45.24(16)
C(7)-O(1)-C(11)	112.5(6)
C(10)-O(5)-C(14A)	120.7(10)
C(10)-O(5)-C(14B)	108.9(18)
C(10)-O(5)-C(14)	101(2)
O(5)-C(14)-C(15)	112(3)
O(5)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14A)	109.2
O(5)-C(14)-H(14B)	109.2
C(15)-C(14)-H(14B)	109.2

H(14A)-C(14)-H(14B)	107.9
N(1)-C(15)-C(14)	105(3)
N(1)-C(15)-H(15A)	110.6
C(14)-C(15)-H(15A)	110.6
N(1)-C(15)-H(15B)	110.6
C(14)-C(15)-H(15B)	110.6
H(15A)-C(15)-H(15B)	108.8
N(2)-N(1)-C(15)	111(3)
N(3)-N(2)-N(1)	162(5)
O(5)-C(14A)-C(15A)	102.1(14)
O(5)-C(14A)-H(14C)	111.3
C(15A)-C(14A)-H(14C)	111.3
O(5)-C(14A)-H(14D)	111.3
C(15A)-C(14A)-H(14D)	111.3
H(14C)-C(14A)-H(14D)	109.2
N(1A)-C(15A)-C(14A)	112.6(16)
N(1A)-C(15A)-H(15C)	109.1
C(14A)-C(15A)-H(15C)	109.1
N(1A)-C(15A)-H(15D)	109.1
C(14A)-C(15A)-H(15D)	109.1
H(15C)-C(15A)-H(15D)	107.8
N(2A)-N(1A)-C(15A)	117.0(18)
N(3A)-N(2A)-N(1A)	171(2)
O(5)-C(14B)-C(15B)	116(3)
O(5)-C(14B)-H(14E)	108.4
C(15B)-C(14B)-H(14E)	108.4
O(5)-C(14B)-H(14F)	108.4
C(15B)-C(14B)-H(14F)	108.4
H(14E)-C(14B)-H(14F)	107.4
N(1B)-C(15B)-C(14B)	108(3)
N(1B)-C(15B)-H(15E)	110.0
C(14B)-C(15B)-H(15E)	110.0
N(1B)-C(15B)-H(15F)	110.0
C(14B)-C(15B)-H(15F)	110.0
H(15E)-C(15B)-H(15F)	108.4
N(2B)-N(1B)-C(15B)	117(3)
N(3B)-N(2B)-N(1B)	158(4)
C(34)-O(10)-Na(1)	154.8(4)
C(42)-O(12)-Na(1)#1	159.2(4)
C(49)-O(14)-C(56)	110.7(5)
C(46)-O(18)-C(59)	115.1(6)
C(23)-N(4)-C(16)	125.8(7)
C(23)-N(4)-C(18)	111.7(6)
C(16)-N(4)-C(18)	121.7(6)

C(23)-N(5)-C(24)	120.5(6)
C(23)-N(5)-C(19)	113.6(5)
C(24)-N(5)-C(19)	125.5(6)
C(22)-N(6)-C(18)	113.0(6)
C(22)-N(6)-C(17)	122.4(6)
C(18)-N(6)-C(17)	120.1(6)
C(22)-N(7)-C(25)	120.6(6)
C(22)-N(7)-C(19)	113.4(6)
C(25)-N(7)-C(19)	124.2(5)
C(28)-N(8)-C(26)	111.8(5)
C(28)-N(8)-C(24)	119.5(5)
C(26)-N(8)-C(24)	120.8(5)
C(28)-N(9)-C(30)	124.2(6)
C(28)-N(9)-C(27)	111.8(5)
C(30)-N(9)-C(27)	123.7(5)
C(29)-N(10)-C(25)	121.7(5)
C(29)-N(10)-C(26)	112.5(5)
C(25)-N(10)-C(26)	124.2(6)
C(29)-N(11)-C(31)	120.0(5)
C(29)-N(11)-C(27)	112.5(5)
C(31)-N(11)-C(27)	119.4(6)
C(34)-N(12)-C(30)	123.5(5)
C(34)-N(12)-C(32)	110.8(5)
C(30)-N(12)-C(32)	121.9(5)
C(34)-N(13)-C(36)	121.3(5)
C(34)-N(13)-C(33)	111.7(5)
C(36)-N(13)-C(33)	122.7(5)
C(35)-N(14)-C(31)	122.2(5)
C(35)-N(14)-C(32)	112.8(5)
C(31)-N(14)-C(32)	122.6(6)
C(35)-N(15)-C(37)	119.9(5)
C(35)-N(15)-C(33)	112.2(5)
C(37)-N(15)-C(33)	124.7(5)
C(42)-N(16)-C(38)	113.7(5)
C(42)-N(16)-C(36)	120.0(5)
C(38)-N(16)-C(36)	124.2(5)
C(42)-N(17)-C(39)	111.8(5)
C(42)-N(17)-C(44)	120.8(5)
C(39)-N(17)-C(44)	120.6(5)
C(43)-N(18)-C(37)	120.9(5)
C(43)-N(18)-C(38)	112.9(5)
C(37)-N(18)-C(38)	126.0(5)
C(43)-N(19)-C(45)	123.7(5)
C(43)-N(19)-C(39)	113.1(5)

C(45)-N(19)-C(39)	123.1(5)
N(21)-N(20)-C(60)	117.6(9)
N(22)-N(21)-N(20)	169.9(12)
C(2)-C(1)-C(6)	119.3(8)
C(2)-C(1)-C(10)	123.3(8)
C(6)-C(1)-C(10)	117.2(7)
C(1)-C(2)-C(3)	120.6(9)
C(1)-C(2)-H(2)	119.7
C(3)-C(2)-H(2)	119.7
C(2)-C(3)-C(4)	120.3(8)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	120.9(9)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	120.2(8)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	122.4(7)
C(5)-C(6)-C(1)	118.5(7)
C(7)-C(6)-C(1)	118.9(7)
C(8)-C(7)-O(1)	121.5(7)
C(8)-C(7)-C(6)	122.1(7)
O(1)-C(7)-C(6)	116.2(7)
C(7)-C(8)-C(9)	119.8(7)
C(7)-C(8)-C(16)	119.5(7)
C(9)-C(8)-C(16)	120.6(7)
C(10)-C(9)-C(8)	118.4(7)
C(10)-C(9)-C(17)	119.4(7)
C(8)-C(9)-C(17)	122.1(7)
C(9)-C(10)-O(5)	120.5(8)
C(9)-C(10)-C(1)	123.5(7)
O(5)-C(10)-C(1)	115.7(7)
O(1)-C(11)-C(12)	110.5(8)
O(1)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11A)	109.5
O(1)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
C(13)-C(12)-C(11)	110.1(9)
C(13)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12B)	109.6

H(12A)-C(12)-H(12B)	108.2
C(12)-C(13)-S(1)	113.2(7)
C(12)-C(13)-H(13A)	108.9
S(1)-C(13)-H(13A)	108.9
C(12)-C(13)-H(13B)	108.9
S(1)-C(13)-H(13B)	108.9
H(13A)-C(13)-H(13B)	107.8
N(4)-C(16)-C(8)	114.8(6)
N(4)-C(16)-H(16A)	108.6
C(8)-C(16)-H(16A)	108.6
N(4)-C(16)-H(16B)	108.6
C(8)-C(16)-H(16B)	108.6
H(16A)-C(16)-H(16B)	107.5
N(6)-C(17)-C(9)	115.2(6)
N(6)-C(17)-H(17A)	108.5
C(9)-C(17)-H(17A)	108.5
N(6)-C(17)-H(17B)	108.5
C(9)-C(17)-H(17B)	108.5
H(17A)-C(17)-H(17B)	107.5
N(6)-C(18)-N(4)	109.5(6)
N(6)-C(18)-C(20)	114.1(6)
N(4)-C(18)-C(20)	112.4(6)
N(6)-C(18)-C(19)	102.6(6)
N(4)-C(18)-C(19)	101.4(5)
C(20)-C(18)-C(19)	115.8(6)
N(5)-C(19)-N(7)	113.6(5)
N(5)-C(19)-C(21)	113.6(5)
N(7)-C(19)-C(21)	112.1(6)
N(5)-C(19)-C(18)	100.6(5)
N(7)-C(19)-C(18)	100.9(5)
C(21)-C(19)-C(18)	114.9(6)
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(7)-C(22)-N(7)	127.4(7)

O(7)-C(22)-N(6)	125.0(7)
N(7)-C(22)-N(6)	107.6(6)
O(6)-C(23)-N(4)	125.5(7)
O(6)-C(23)-N(5)	125.7(7)
N(4)-C(23)-N(5)	108.8(6)
N(5)-C(24)-N(8)	112.8(5)
N(5)-C(24)-H(24A)	109.0
N(8)-C(24)-H(24A)	109.0
N(5)-C(24)-H(24B)	109.0
N(8)-C(24)-H(24B)	109.0
H(24A)-C(24)-H(24B)	107.8
N(10)-C(25)-N(7)	113.6(6)
N(10)-C(25)-H(25A)	108.8
N(7)-C(25)-H(25A)	108.8
N(10)-C(25)-H(25B)	108.8
N(7)-C(25)-H(25B)	108.8
H(25A)-C(25)-H(25B)	107.7
N(10)-C(26)-N(8)	113.9(5)
N(10)-C(26)-C(27)	104.5(5)
N(8)-C(26)-C(27)	102.7(5)
N(10)-C(26)-H(26)	111.7
N(8)-C(26)-H(26)	111.7
C(27)-C(26)-H(26)	111.7
N(9)-C(27)-N(11)	115.2(5)
N(9)-C(27)-C(26)	103.9(5)
N(11)-C(27)-C(26)	101.4(5)
N(9)-C(27)-H(27)	111.9
N(11)-C(27)-H(27)	111.9
C(26)-C(27)-H(27)	111.9
O(8)-C(28)-N(9)	125.0(6)
O(8)-C(28)-N(8)	127.1(6)
N(9)-C(28)-N(8)	107.8(5)
O(9)-C(29)-N(10)	126.4(7)
O(9)-C(29)-N(11)	126.3(6)
N(10)-C(29)-N(11)	107.3(5)
N(12)-C(30)-N(9)	113.5(5)
N(12)-C(30)-H(30A)	108.9
N(9)-C(30)-H(30A)	108.9
N(12)-C(30)-H(30B)	108.9
N(9)-C(30)-H(30B)	108.9
H(30A)-C(30)-H(30B)	107.7
N(14)-C(31)-N(11)	112.3(6)
N(14)-C(31)-H(31A)	109.1
N(11)-C(31)-H(31A)	109.1

N(14)-C(31)-H(31B)	109.1
N(11)-C(31)-H(31B)	109.1
H(31A)-C(31)-H(31B)	107.9
N(14)-C(32)-N(12)	113.8(6)
N(14)-C(32)-C(33)	103.8(5)
N(12)-C(32)-C(33)	103.6(5)
N(14)-C(32)-H(32)	111.7
N(12)-C(32)-H(32)	111.7
C(33)-C(32)-H(32)	111.7
N(15)-C(33)-N(13)	114.1(5)
N(15)-C(33)-C(32)	103.4(5)
N(13)-C(33)-C(32)	104.2(5)
N(15)-C(33)-H(33)	111.5
N(13)-C(33)-H(33)	111.5
C(32)-C(33)-H(33)	111.5
O(10)-C(34)-N(13)	125.3(6)
O(10)-C(34)-N(12)	125.2(5)
N(13)-C(34)-N(12)	109.4(5)
O(11)-C(35)-N(14)	127.1(6)
O(11)-C(35)-N(15)	125.4(6)
N(14)-C(35)-N(15)	107.5(5)
N(13)-C(36)-N(16)	113.7(5)
N(13)-C(36)-H(36A)	108.8
N(16)-C(36)-H(36A)	108.8
N(13)-C(36)-H(36B)	108.8
N(16)-C(36)-H(36B)	108.8
H(36A)-C(36)-H(36B)	107.7
N(15)-C(37)-N(18)	114.6(5)
N(15)-C(37)-H(37A)	108.6
N(18)-C(37)-H(37A)	108.6
N(15)-C(37)-H(37B)	108.6
N(18)-C(37)-H(37B)	108.6
H(37A)-C(37)-H(37B)	107.6
N(16)-C(38)-N(18)	114.0(5)
N(16)-C(38)-C(40)	112.5(5)
N(18)-C(38)-C(40)	111.8(5)
N(16)-C(38)-C(39)	101.3(5)
N(18)-C(38)-C(39)	101.2(4)
C(40)-C(38)-C(39)	115.1(5)
N(17)-C(39)-N(19)	111.1(5)
N(17)-C(39)-C(41)	112.1(5)
N(19)-C(39)-C(41)	111.9(5)
N(17)-C(39)-C(38)	102.9(5)
N(19)-C(39)-C(38)	102.2(5)

C(41)-C(39)-C(38)	116.1(5)
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-H(41A)	109.5
C(39)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(39)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
O(12)-C(42)-N(16)	126.5(6)
O(12)-C(42)-N(17)	125.2(6)
N(16)-C(42)-N(17)	108.0(5)
O(13)-C(43)-N(19)	126.2(6)
O(13)-C(43)-N(18)	126.0(6)
N(19)-C(43)-N(18)	107.8(5)
N(17)-C(44)-C(48)	115.5(5)
N(17)-C(44)-H(44A)	108.4
C(48)-C(44)-H(44A)	108.4
N(17)-C(44)-H(44B)	108.4
C(48)-C(44)-H(44B)	108.4
H(44A)-C(44)-H(44B)	107.5
N(19)-C(45)-C(47)	112.8(5)
N(19)-C(45)-H(45A)	109.0
C(47)-C(45)-H(45A)	109.0
N(19)-C(45)-H(45B)	109.0
C(47)-C(45)-H(45B)	109.0
H(45A)-C(45)-H(45B)	107.8
C(47)-C(46)-O(18)	120.0(7)
C(47)-C(46)-C(55)	122.5(7)
O(18)-C(46)-C(55)	117.2(6)
C(46)-C(47)-C(48)	119.4(6)
C(46)-C(47)-C(45)	120.9(6)
C(48)-C(47)-C(45)	119.5(6)
C(49)-C(48)-C(47)	118.0(6)
C(49)-C(48)-C(44)	119.9(6)
C(47)-C(48)-C(44)	122.0(6)
C(48)-C(49)-O(14)	119.3(6)
C(48)-C(49)-C(50)	123.6(6)
O(14)-C(49)-C(50)	117.0(6)
C(51)-C(50)-C(49)	122.9(7)

C(51)-C(50)-C(55)	119.4(7)
C(49)-C(50)-C(55)	117.6(6)
C(52)-C(51)-C(50)	121.8(9)
C(52)-C(51)-H(51)	119.1
C(50)-C(51)-H(51)	119.1
C(51)-C(52)-C(53)	117.9(9)
C(51)-C(52)-H(52)	121.1
C(53)-C(52)-H(52)	121.1
C(54)-C(53)-C(52)	122.4(8)
C(54)-C(53)-H(53)	118.8
C(52)-C(53)-H(53)	118.8
C(53)-C(54)-C(55)	120.1(9)
C(53)-C(54)-H(54)	120.0
C(55)-C(54)-H(54)	120.0
C(50)-C(55)-C(46)	118.8(6)
C(50)-C(55)-C(54)	118.4(8)
C(46)-C(55)-C(54)	122.8(7)
O(14)-C(56)-C(57)	106.9(6)
O(14)-C(56)-H(56A)	110.3
C(57)-C(56)-H(56A)	110.3
O(14)-C(56)-H(56B)	110.3
C(57)-C(56)-H(56B)	110.3
H(56A)-C(56)-H(56B)	108.6
C(56)-C(57)-C(58)	110.7(6)
C(56)-C(57)-H(57A)	109.5
C(58)-C(57)-H(57A)	109.5
C(56)-C(57)-H(57B)	109.5
C(58)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	108.1
C(57)-C(58)-S(2)	110.9(5)
C(57)-C(58)-H(58A)	109.5
S(2)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
S(2)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	108.0
O(18)-C(59)-C(60)	105.2(8)
O(18)-C(59)-H(59A)	110.7
C(60)-C(59)-H(59A)	110.7
O(18)-C(59)-H(59B)	110.7
C(60)-C(59)-H(59B)	110.7
H(59A)-C(59)-H(59B)	108.8
N(20)-C(60)-C(59)	113.8(8)
N(20)-C(60)-H(60A)	108.8
C(59)-C(60)-H(60A)	108.8

N(20)-C(60)-H(60B)	108.8
C(59)-C(60)-H(60B)	108.8
H(60A)-C(60)-H(60B)	107.7
C(61)-O(19)-HO19	142(6)
O(19)-C(61)-C(62)	108.8(8)
O(19)-C(61)-H(61A)	109.9
C(62)-C(61)-H(61A)	109.9
O(19)-C(61)-H(61B)	109.9
C(62)-C(61)-H(61B)	109.9
H(61A)-C(61)-H(61B)	108.3
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
Na(1)-O(20)-Na(1)#1	85.4(2)
Na(1)-O(20)-HO1A	142(6)
Na(1)#1-O(20)-HO1A	109(7)
Na(1)-O(20)-HO1B	115(6)
Na(1)#1-O(20)-HO1B	68(8)
HO1A-O(20)-HO1B	103(4)
Na(1)-O(21)-HO2A	110(7)
Na(1)-O(21)-HO2B	127(6)
HO2A-O(21)-HO2B	107(4)

Symmetry transformations used to generate equivalent atoms: #1 –x+1,–y+1,–z+1.

Table S11: Anisotropic displacement parameters (Å^2 x 10^3) for **10a**. The anisotropic displacement factor exponent takes the form: –2p^2[h^2 a*^{2} U^{11} + ... + 2 h k a* b* U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	39(1)	34(1)	51(1)	6(1)	19(1)	4(1)
S(2)	93(2)	22(1)	40(1)	–9(1)	28(1)	–10(1)
Na(1)	31(2)	66(2)	53(2)	20(2)	22(2)	13(2)
O(1)	71(4)	26(3)	42(3)	–4(2)	16(3)	–2(3)
O(2)	78(5)	44(4)	60(4)	8(3)	26(3)	–6(3)
O(3)	47(3)	31(3)	78(4)	–7(3)	27(3)	1(3)
O(4)	57(4)	54(4)	72(4)	–5(3)	13(3)	–10(3)
O(5)	81(4)	60(4)	45(3)	–31(3)	27(3)	–15(3)
C(14)	78(7)	68(7)	77(8)	–6(7)	14(7)	–17(6)
C(15)	76(7)	70(7)	76(7)	–5(6)	8(6)	–18(5)
N(1)	81(7)	74(7)	80(7)	–7(6)	3(6)	–21(5)

N(2)	84(7)	77(7)	81(7)	–5(6)	2(5)	–22(6)
N(3)	94(13)	85(14)	83(9)	–4(11)	–1(9)	–26(12)
C(14A)	76(6)	60(6)	73(6)	–7(5)	21(5)	–21(5)
C(15A)	83(6)	65(5)	72(5)	–8(5)	7(5)	–20(5)
N(1A)	90(6)	76(7)	73(5)	–11(5)	14(5)	–16(5)
N(2A)	86(7)	79(7)	75(6)	–12(6)	13(5)	–22(6)
N(3A)	99(10)	101(11)	79(9)	–17(8)	0(7)	–24(9)
C(14B)	78(7)	65(7)	78(7)	–4(6)	16(6)	–19(6)
C(15B)	79(7)	69(6)	80(6)	–7(6)	2(6)	–19(6)
N(1B)	82(6)	75(7)	80(6)	–7(6)	3(5)	–19(6)
N(2B)	81(7)	74(7)	77(7)	–11(6)	3(6)	–21(6)
N(3B)	88(12)	83(14)	81(12)	–14(11)	–4(10)	–22(11)
O(6)	38(3)	27(3)	35(3)	–8(2)	10(2)	–4(2)
O(7)	29(3)	57(4)	44(3)	–21(3)	16(2)	–6(3)
O(8)	21(2)	18(2)	57(3)	–10(2)	2(2)	1(2)
O(9)	23(3)	31(3)	51(3)	–4(2)	15(2)	1(2)
O(10)	13(2)	25(2)	27(2)	–16(2)	4(2)	–2(2)
O(11)	21(2)	32(3)	45(3)	–30(2)	6(2)	–11(2)
O(12)	18(2)	23(2)	25(2)	–9(2)	7(2)	–3(2)
O(13)	26(2)	32(3)	27(2)	–20(2)	0(2)	–7(2)
O(14)	24(2)	21(2)	29(2)	–4(2)	6(2)	–4(2)
O(15)	115(6)	28(3)	48(3)	–7(3)	18(4)	–35(4)
O(16)	168(8)	35(4)	32(3)	–8(3)	8(4)	–24(4)
O(17)	101(5)	44(4)	86(5)	–5(4)	56(4)	2(4)
O(18)	56(4)	39(3)	25(3)	–17(2)	–2(2)	–11(3)
N(4)	33(3)	33(3)	27(3)	–3(2)	5(2)	–2(3)
N(5)	20(3)	25(3)	23(2)	–13(2)	–1(2)	–5(2)
N(6)	38(3)	41(4)	24(3)	–10(2)	6(2)	–7(3)
N(7)	28(3)	29(3)	22(3)	–14(2)	4(2)	4(2)
N(8)	10(2)	18(3)	32(3)	–11(2)	1(2)	–2(2)
N(9)	16(3)	21(3)	33(3)	–15(2)	2(2)	–7(2)
N(10)	17(2)	29(3)	27(3)	–19(2)	6(2)	3(2)
N(11)	9(2)	15(3)	49(3)	–9(2)	5(2)	–3(2)
N(12)	9(2)	18(3)	35(3)	–21(2)	6(2)	–4(2)
N(13)	17(2)	11(2)	27(3)	–11(2)	2(2)	–4(2)
N(14)	15(2)	20(2)	43(2)	–24(2)	9(2)	–7(2)
N(15)	15(2)	20(2)	43(2)	–24(2)	9(2)	–7(2)
N(16)	16(2)	18(2)	17(2)	–11(2)	4(2)	–10(2)
N(17)	14(2)	19(3)	16(2)	–11(2)	–1(2)	–5(2)
N(18)	20(3)	14(2)	26(2)	–12(2)	2(2)	–4(2)
N(19)	17(3)	28(3)	20(2)	–9(2)	7(2)	–5(2)
N(20)	82(5)	49(5)	56(5)	–14(4)	–8(4)	14(4)
N(21)	94(7)	60(6)	49(5)	–10(5)	5(5)	12(5)
N(22)	109(9)	78(7)	71(6)	13(6)	11(6)	0(6)

C(1)	30(4)	42(4)	29(4)	–9(3)	–2(3)	–5(3)
C(2)	46(5)	57(5)	37(4)	–4(4)	3(3)	–9(4)
C(3)	45(5)	71(5)	39(5)	–3(4)	5(4)	–16(4)
C(4)	46(5)	65(5)	36(4)	4(4)	–5(3)	–16(4)
C(5)	41(4)	50(5)	30(4)	–7(3)	–7(3)	–15(4)
C(6)	35(4)	37(4)	26(3)	–1(3)	–8(3)	–5(3)
C(7)	47(4)	33(4)	26(4)	–8(3)	0(3)	–4(3)
C(8)	40(4)	26(3)	28(4)	–4(3)	1(3)	0(3)
C(9)	41(4)	33(4)	24(3)	–6(3)	2(3)	–4(3)
C(10)	46(4)	50(4)	23(4)	–13(3)	2(3)	–14(3)
C(11)	103(8)	33(5)	28(4)	–11(3)	11(4)	–7(5)
C(12)	63(5)	37(5)	61(6)	–13(4)	17(5)	–7(4)
C(13)	61(5)	29(4)	71(6)	–5(4)	16(5)	3(4)
C(16)	50(5)	33(4)	36(4)	–2(3)	10(3)	2(4)
C(17)	57(5)	38(4)	29(4)	–11(3)	6(3)	–15(4)
C(18)	24(3)	42(4)	28(3)	–5(3)	1(3)	–7(3)
C(19)	23(3)	26(3)	25(3)	–13(3)	–1(2)	–5(3)
C(20)	35(4)	56(5)	35(4)	–8(4)	–10(3)	–7(4)
C(21)	35(4)	27(4)	30(4)	–15(3)	1(3)	–14(3)
C(22)	30(3)	39(4)	30(3)	–12(3)	6(3)	–8(3)
C(23)	23(4)	30(3)	35(3)	–10(3)	5(3)	3(3)
C(24)	10(3)	33(4)	27(3)	–11(3)	5(2)	–4(3)
C(25)	26(4)	24(4)	33(3)	–18(3)	1(3)	4(3)
C(26)	13(3)	18(3)	32(3)	–4(3)	2(2)	0(2)
C(27)	17(3)	15(3)	32(3)	–14(3)	–1(2)	–4(2)
C(28)	12(3)	20(3)	36(4)	–6(3)	3(2)	–3(2)
C(29)	14(3)	17(3)	43(3)	–6(3)	5(2)	–3(2)
C(30)	17(3)	24(4)	35(4)	–21(3)	6(3)	–12(3)
C(31)	9(3)	22(3)	58(5)	–24(3)	–1(3)	–4(3)
C(32)	17(3)	14(3)	40(4)	–15(3)	5(3)	–6(2)
C(33)	18(3)	14(3)	24(3)	–6(2)	–4(2)	–6(2)
C(34)	15(2)	20(2)	16(2)	–14(2)	2(2)	–9(2)
C(35)	8(3)	23(3)	43(4)	–18(3)	3(2)	–5(2)
C(36)	15(2)	20(2)	16(2)	–14(2)	2(2)	–9(2)
C(37)	9(3)	15(3)	36(4)	–13(3)	0(2)	–5(2)
C(38)	21(3)	20(3)	16(3)	–14(2)	6(2)	–10(2)
C(39)	17(3)	20(3)	16(3)	–12(2)	4(2)	–6(2)
C(40)	25(3)	22(4)	30(3)	–2(3)	–5(3)	–12(3)
C(41)	19(3)	22(4)	33(4)	–6(3)	1(3)	–11(3)
C(42)	16(3)	19(3)	18(3)	–13(2)	4(2)	–11(2)
C(43)	18(3)	22(3)	25(3)	–14(2)	1(3)	–4(3)
C(44)	21(3)	19(3)	20(3)	–7(2)	–1(2)	–7(3)
C(45)	30(3)	24(4)	21(3)	–9(3)	7(3)	–4(3)
C(46)	50(4)	26(4)	19(3)	–7(3)	0(3)	–13(3)

C(47)	29(3)	17(3)	20(3)	–6(2)	4(2)	–8(3)
C(48)	24(3)	21(3)	23(3)	–3(2)	3(2)	–8(2)
C(49)	25(3)	19(3)	23(3)	–6(2)	8(2)	–7(2)
C(50)	33(4)	23(4)	32(3)	–3(3)	0(3)	–11(3)
C(51)	46(4)	42(5)	50(4)	1(4)	–17(4)	–11(4)
C(52)	66(6)	58(6)	65(5)	–12(5)	–33(5)	–7(5)
C(53)	70(6)	68(7)	50(5)	–2(4)	–36(4)	–9(5)
C(54)	70(6)	59(6)	36(4)	–8(4)	–18(4)	–10(4)
C(55)	53(4)	31(4)	27(3)	–5(3)	–9(3)	–14(3)
C(56)	50(5)	17(3)	35(4)	–2(3)	3(3)	–11(3)
C(57)	52(5)	24(4)	46(4)	–8(3)	0(4)	–3(4)
C(58)	43(4)	21(3)	32(3)	–8(3)	15(3)	–11(3)
C(59)	68(6)	33(4)	46(4)	–20(4)	–27(4)	–9(4)
C(60)	75(6)	62(6)	55(5)	–46(5)	–22(4)	5(5)
O(19)	43(3)	42(3)	49(3)	–11(3)	9(3)	–13(3)
C(61)	37(4)	60(6)	47(5)	–2(4)	4(4)	–8(4)
C(62)	52(6)	101(9)	63(6)	13(6)	–1(5)	–35(6)
O(20)	50(4)	38(3)	42(3)	6(3)	16(3)	7(3)
O(21)	35(3)	54(4)	46(3)	4(3)	17(3)	–11(3)

Table S12: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 × 10^3) for **10a**.

	x	y	z	*U*(eq)
H(14A)	2614	8494	9988	91
H(14B)	3143	8935	9459	91
H(15A)	1802	9968	9999	90
H(15B)	2104	9579	10688	90
H(14C)	2543	8992	10007	84
H(14D)	3371	9323	9560	84
H(15C)	3945	9875	10511	89
H(15D)	2628	10251	10419	89
H(14E)	2592	8814	9901	90
H(14F)	3414	9098	9427	90
H(15E)	3319	10176	10092	92
H(15F)	2043	10172	10030	92
H(2)	2936	7782	10628	58
H(3)	2279	6734	10864	62
H(4)	2957	5591	10281	59
H(5)	4294	5470	9473	48
H(11A)	5258	6152	7936	70
H(11B)	4383	5845	8355	70
H(12A)	5620	4559	8229	67
H(12B)	5154	4936	7561	67

H(13A)	7286	4871	8033	70
H(13B)	6820	5278	7378	70
H(16A)	7598	6879	8887	52
H(16B)	7114	6377	8419	52
H(17A)	5558	8843	9578	50
H(17B)	6764	8214	9509	50
H(20A)	8791	7876	8162	65
H(20B)	8333	7855	8883	65
H(20C)	8286	8662	8555	65
H(21A)	8281	8789	7300	45
H(21B)	7484	9497	7707	45
H(21C)	7230	9388	6977	45
H(24A)	7337	7476	6302	29
H(24B)	7243	8372	6314	29
H(25A)	4294	10013	7485	36
H(25B)	5394	9929	7042	36
H(26)	5506	9298	5998	26
H(27)	4022	9290	5383	26
H(30A)	3840	8245	4650	28
H(30B)	4618	7388	4785	28
H(31A)	1506	9604	6239	36
H(31B)	2031	9564	5528	36
H(32)	1829	8536	4828	28
H(33)	669	7783	4846	22
H(36A)	2251	5826	4848	20
H(36B)	1070	6396	4645	20
H(37A)	–980	7846	5602	23
H(37B)	–879	8057	6330	23
H(40A)	–738	6849	4887	37
H(40B)	–1715	6668	5315	37
H(40C)	–847	5995	4906	37
H(41A)	–1451	5241	5667	36
H(41B)	–2076	5880	6187	36
H(41C)	–1459	5017	6407	36
H(44A)	1458	3869	6247	24
H(44B)	232	4163	6578	24
H(45A)	–843	5235	7369	31
H(45B)	–587	5915	7754	31
H(51)	4426	3103	7686	55
H(52)	5200	3175	8676	78
H(53)	4117	4046	9446	77
H(54)	2425	4917	9210	68
H(56A)	1966	2654	7025	41
H(56B)	2990	2484	7503	41

H(57A)	3439	1462	6785	51
H(57B)	4258	1968	6605	51
H(58A)	3355	2425	5685	39
H(58B)	2186	2327	5950	39
H(59A)	543	6644	8360	59
H(59B)	1769	6167	8596	59
H(60A)	1061	6140	9648	82
H(60B)	720	7019	9422	82
HO19	5710(30)	6190(50)	6540(40)	54
H(61A)	3782	7140	6413	59
H(61B)	3901	7060	7172	59
H(62A)	2312	6705	6896	104
H(62B)	3236	5952	7142	104
H(62C)	3054	6085	6394	104
HO1A	6020(60)	4810(50)	6010(30)	73
HO1B	4970(30)	5220(60)	5930(40)	73
HO2A	4670(60)	6350(60)	3650(30)	70
HO2B	5620(60)	6550(60)	3590(30)	70

Table S13: Intensity statistics for **10a**.

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R(int)	R(sigma)
Inf–2.25	802	841	95.4	4.04	58.1	16.86	0.0536	0.0456
2.25–1.75	866	922	93.9	3.80	24.5	11.64	0.0867	0.0718
1.75–1.55	781	785	99.5	5.07	14.1	10.62	0.1180	0.0731
1.55–1.40	891	901	98.9	5.00	10.3	8.58	0.1567	0.0886
1.40–1.30	867	878	98.7	4.62	8.1	7.06	0.2066	0.1210
1.30–1.20	1179	1187	99.3	4.41	7.7	6.49	0.2496	0.1299
1.20–1.10	1631	1636	99.7	4.03	7.5	5.78	0.2612	0.1460
1.10–1.05	1055	1065	99.1	3.49	6.5	4.94	0.2493	0.1729
1.05–1.00	1284	1305	98.4	3.22	5.5	4.11	0.3298	0.2116
1.00–0.95	1518	1576	96.3	2.79	3.6	2.80	0.5049	0.3471
0.95–0.90	1867	1949	95.8	2.49	2.6	2.23	0.6284	0.4275
0.90–0.85	2310	2451	94.2	2.01	2.3	1.79	0.7021	0.4990
0.85–0.84	516	551	93.6	1.65	1.9	1.44	0.7851	0.5919
0.95–0.84	4693	4951	94.8	2.16	2.3	1.93	0.6647	0.4761
Inf–0.84	15567	16047	97.0	3.38	9.4	5.56	0.1574	0.1287

Merged [A], lowest resolution = 20.95 Å, 1064 outliers down-weighted.

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