Generation of

6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxides
via a palladium-catalyzed reaction of
2-(2-alkynyl)benzenesulfonamide

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Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S2-S10).
3. 1H and 13C NMR spectra of compound 3 (S11-S40).
**General Materials and Methods:**

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63µm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. \(^1\)H and \(^{13}\)C NMR spectra were recorded in CDCl\(_3\) on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

**General procedure of the synthesis of 6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxides 3 via a palladium-catalyzed reaction of 2-(2-alkynyl)benzenesulfonamide 1 with 2-alkynylvinyl bromide 2**

\[
\begin{align*}
\text{O} & \text{S} \text{O} \text{NHR}^3 \text{R}^2 \text{R}^1 & + & \text{Br} \text{R}^4 \text{R}^3 & \xrightarrow{\text{Pd(OAc)}_2 (5 \text{ mol %}), \text{DPPP} (5 \text{ mol %}), \text{K}_2\text{CO}_3, 1,4\text{-dioxane}} & \text{O} & \text{S} \text{O} \text{N} \text{R}^3 \text{R}^5 \text{R}^4 \text{R}^1 \text{R}^2 \text{R}^4 \text{R}^3
\end{align*}
\]

2-(2-Alkynyl)benzenesulfonamide 1 (0.30 mmol) was added to a mixture of Pd(OAc)\(_2\) (5 mol%), DPPP (5 mol %), K\(_2\)CO\(_3\) (0.60 mmol), and 2-alkynylvinyl bromide 2 (0.36 mmol) in 1,4-dioxane (2.0 mL). The mixture was stirred under 100 °C. After completion of the reaction as indicated by TLC (~12 hours), the mixture was cooled and diluted by EtOAc (10 mL), washed with saturated brine (2 × 10 mL), and dried by anhydrous Na\(_2\)SO\(_4\). Evaporation of the solvent followed by purification on silica gel provided the product 3.
6-Methyl-7,10-diphenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3a): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.43 (t, $J = 7.3$ Hz, 3H), 0.73 (t, $J = 6.9$ Hz, 3H), 1.13-1.26 (m, 4H), 1.43-1.56 (m, 1H), 1.87-1.92 (m, 1H), 2.16-2.24 (m, 1H), 2.29-2.36 (m, 2H), 2.68 (s, 3H), 7.02 (d, $J = 6.4$ Hz, 1H), 7.90 (d, $J = 7.8$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.2, 14.5, 23.5, 25.5, 28.5, 29.0, 36.9, 125.3, 126.3, 127.0, 127.6, 128.3, 128.5, 128.8, 130.0, 130.6, 131.5, 133.2, 133.7, 134.0, 136.4, 136.0, 137.8, 142.6, 146.1, 146.5; HRMS (ESI) calcd for C$_{31}$H$_{31}$NO$_2$S: 504.1968 (M + Na$^+$), found: 504.1970.

2-Methoxy-6-methyl-7,10-diphenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3b): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.43 (t, $J = 6.9$ Hz, 3H), 0.73 (t, $J = 7.3$ Hz, 3H), 1.14-1.27 (m, 4H), 1.48-1.53 (m, 1H), 1.91-1.96 (m, 1H), 2.20-2.26 (m, 1H), 2.30-2.36 (m, 1H), 2.70 (s, 3H), 3.25 (s, 3H), 6.50 (s, 1H), 6.71 (d, $J = 8.2$ Hz, 2H), 7.26-7.54 (m, 9H), 7.80 (d, $J = 8.7$ Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.3, 14.5, 23.6, 25.6, 28.5, 29.0, 36.9, 55.1, 113.6, 116.7, 126.9, 127.6, 128.2, 128.3, 128.7, 128.8, 130.1, 130.6, 132.8, 133.7, 134.1, 135.8, 136.5, 138.4, 142.3, 146.0, 147.1, 161.6; HRMS (ESI) calcd for C$_{32}$H$_{33}$NO$_2$S: 534.2073 (M + Na$^+$), found: 534.2077.
2,6-Dimethyl-7,10-diphenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine
5,5-dioxide (3c): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.42 (t, $J$ = 7.3 Hz, 3H), 0.72 (t, $J$ = 7.3 Hz, 3H), 1.11-1.27 (m, 4H), 1.47-1.52 (m, 1H), 1.87-1.93 (m, 1H), 1.97 (s, 3H), 2.18-2.26 (m, 1H), 2.29-2.36 (m, 1H), 2.67 (s, 3H), 6.78 (s, 1H), 6.99 (d, $J$ = 7.8 Hz, 2H), 7.23-7.52 (m, 9H), 7.77 (d, $J$ = 7.8 Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.2, 14.5, 21.3, 23.6, 25.5, 28.5, 29.0, 36.8, 126.2, 126.4 126.9, 127.6, 128.2, 128.4, 128.8, 130.0, 130.5, 133.2, 133.6, 133.7, 133.9, 134.4, 136.5, 138.0, 142.0, 142.5, 145.9, 146.5; HRMS (ESI) calcd for C$_{32}$H$_{33}$NO$_2$S: 518.2124 (M + Na$^+$), found: 518.2142.

2-Chloro-6-methyl-7,10-diphenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3d): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.43 (t, $J$ = 7.3 Hz, 3H), 0.74 (t, $J$ = 7.3 Hz, 3H), 1.10-1.29 (m, 4H), 1.48-1.54 (m, 1H), 1.89-1.94 (m, 1H), 2.18-2.27 (m, 1H), 2.28-2.36 (m, 1H), 2.69 (s, 3H), 6.94 (s, 1H), 7.14 (d, $J$ = 8.2 Hz, 2H), 7.30 (d, $J$ = 6.4 Hz, 2H), 7.40-7.41 (m, 3H), 7.52-7.54 (m, 2H), 7.74-7.76 (m, 1H), 7.81 (d, $J$ = 8.7 Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.2, 14.5, 23.5, 25.5, 28.4, 29.0, 36.9, 125.6, 126.1 127.4, 127.7, 128.4, 128.7, 128.9, 129.9, 130.7, 133.1, 133.3, 133.7, 134.6, 134.8, 135.6, 136.1, 137.2, 137.8, 142.7, 146.7, 147.3; HRMS (ESI) calcd for C$_{31}$H$_{30}$ClNO$_2$S: 538.1578 (M + Na$^+$), found: 538.1569.
10-(4-Chlorophenyl)-2,6-dimethyl-7-phenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d] [1,2]thiazepine 5,5-dioxide (3e): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.42 (t, $J = 6.9$ Hz, 3H), 0.74 (t, $J = 7.3$ Hz, 3H), 1.09-1.25 (m, 4H), 1.42-1.53 (m, 1H), 1.85-1.92 (m, 1H), 2.03 (s, 3H), 2.17-2.24 (m, 1H), 2.26-2.34 (m, 1H), 2.67 (s, 3H), 6.78 (s, 1H), 7.02 (d, $J = 7.8$ Hz, 2H), 7.25-7.39 (m, 5H), 7.49-7.54 (m, 2H), 7.74-7.79 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.2, 14.5, 21.4, 23.6, 25.5, 28.5, 29.0, 36.9, 126.4, 126.5, 128.0, 128.3, 128.6, 128.9, 130.0, 130.6, 132.7, 133.4, 133.7, 133.9, 134.0, 134.3, 136.3, 136.6, 141.9, 142.2, 144.3, 147.1; HRMS (ESI) calcd for C$_{32}$H$_{32}$ClNO$_2$S: 552.1734 (M + Na$^+$), found: 552.1734.

10-(4-Methoxyphenyl)-2,6-dimethyl-7-phenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d] [1,2]thiazepine 5,5-dioxide (3f): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 0.42 (t, $J = 7.4$ Hz, 3H), 0.74 (t, $J = 7.3$ Hz, 3H), 1.10-1.25 (m, 4H), 1.47-1.54 (m, 1H), 1.86-1.92 (m, 1H), 2.01 (s, 3H), 2.18-2.25 (m, 1H), 2.29-2.38 (m, 1H), 2.66 (s, 3H), 6.83 (s, 1H), 6.99 (d, $J = 7.8$ Hz, 2H), 7.35-7.42 (m, 2H), 7.47-7.53 (m, 2H), 7.75-7.78 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.3, 14.6, 21.5, 23.6, 25.5, 28.6, 29.0, 36.8, 55.3, 113.9, 126.2, 126.4, 127.3, 128.2, 128.8, 130.0, 130.1, 130.5, 133.3, 133.6, 133.7, 133.8, 133.9, 134.3, 136.6, 140.0, 142.7, 145.6, 146.2, 158.7; HRMS (ESI) calcd for C$_{33}$H$_{35}$NO$_3$S: 548.2230 (M + Na$^+$), found: 548.2239.
10-Cyclopropyl-2,6-dimethyl-7-phenyl-8,9-dipropyl-6H-benzo[\(f\)]cyclopenta[\(d\)][1,2]thiazepine 5,5-dioxide (3g): Dark red solid; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) -1.20-0.15 (m, 1H), 0.37 (t, \(J = 7.3\) Hz, 3H), 0.40-0.45 (m, 1H), 0.60-0.66 (m, 1H), 0.92-1.77 (m, 6H), 1.47-1.54 (m, 2H), 1.66-1.80 (m, 3H), 2.32-2.40 (m, 1H), 2.45 (s, 3H), 2.50-2.58 (m, 1H), 2.60 (s, 3H), 7.16 (d, \(J = 7.8\) Hz, 2H), 7.33-7.36 (m, 2H), 7.47 (d, \(J = 6.9\) Hz, 2H), 7.65-7.69 (m, 2H), 7.8 (d, \(J = 7.8\) Hz, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 7.8, 10.1, 10.5, 14.1, 14.8, 21.7, 24.0, 25.3, 28.5, 28.8, 36.6, 126.1, 126.4, 127.3, 128.0, 128.8, 130.0, 130.1, 132.4, 133.0, 133.3, 133.4, 134.1, 136.8, 141.7, 144.5, 144.7, 146.0; HRMS (ESI) calcd for C\(_{29}\)H\(_{33}\)NO\(_2\): 482.2124 (M + Na\(^+\)), found: 482.2132.

10-Butyl-6-methyl-7-phenyl-8,9-dipropyl-6H-benzo[\(f\)]cyclopenta[\(d\)][1,2]thiazepine 5,5-dioxide (3h): Dark red oil; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 0.39 (t, \(J = 6.9\) Hz, 3H) 0.90 (t, \(J = 7.3\) Hz, 3H), 0.98 (t, \(J = 7.3\) Hz, 3H), 1.05-1.12 (m, 2H), 1.36-1.42 (m, 2H), 1.49-1.58 (m, 5H), 1.76-1.82 (m, 1H), 2.30 (t, \(J = 7.8\) Hz, 2H), 2.44-2.49 (m, 2H), 2.61 (s, 3H), 7.34-7.36 (m, 3H), 7.47-7.60 (m, 4H), 7.71 (d, \(J = 6.0\) Hz, 1H), 7.96 (d, \(J = 8.4\) Hz, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 13.7, 14.0, 14.7, 22.8, 24.2, 25.2, 26.9, 28.3, 28.7, 32.3, 36.4, 125.5, 126.6, 126.7, 127.9, 128.6, 129.8, 130.1, 131.2, 132.0, 133.3, 133.4, 133.7, 134.3, 136.3, 136.5, 142.8, 144.0, 146.1; HRMS (ESI) calcd for C\(_{29}\)H\(_{35}\)NO\(_2\): 500.2020 (M + K\(^+\)), found: 500.2001.
10-(4-Fluorophenyl)-6-methyl-7-phenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3i): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) δ 0.42 (t, $J$ = 6.9 Hz, 3H), 0.73 (t, $J$ = 6.8 Hz, 3H), 1.12-1.25 (m, 4H), 1.47-1.54 (m, 1H), 1.86-1.90 (m, 1H), 2.03 (s, 3H), 2.20-2.24 (m, 1H), 2.28-2.34 (m, 1H), 2.68 (s, 3H), 7.00 (d, $J$ = 7.8 Hz, 2H), 7.12 (t, $J$ = 7.8 Hz, 2H), 7.22 (t, $J$ = 7.3 Hz, 2H), 7.36-7.55 (m, 5H), 7.76 (d, $J$ = 5.5 Hz, 1H), 7.90 (d, $J$ = 7.8 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 14.2, 14.5, 23.5, 25.5, 28.6, 29.0, 36.9, 115.5 (d, $^2$JC = 21.0 Hz); 125.7, 126.4 127.8, 128.3, 128.9, 130.0, 130.7, 131.5, 131.7, 133.0, 133.5, 133.6, 133.8 (d, $^3$JC = 8.6 Hz), 136.3, 136.7, 142.2, 144.8, 146.8, 162.0 (d, $^1$JC = 245.0 Hz); HRMS (ESI) calcd for C$_{31}$H$_{30}$FNO$_2$S: 522.1873 (M + Na$^+$), found: 522.1874.

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6-Methyl-7-phenyl-8,9-dipropyl-10-(p-tolyl)-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3j): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) δ 0.43 (t, $J$ = 7.4 Hz, 3H), 0.74 (t, $J$ = 7.3 Hz, 3H), 1.12-1.27 (m, 4H), 1.49-1.56 (m, 1H), 1.87-1.95 (m, 1H), 2.18-2.24 (m, 1H), 2.30-2.35 (m, 4H), 2.67 (s, 3H), 7.05-7.12 (m, 5H), 7.20 (t, $J$ = 7.8 Hz, 2H), 7.37-7.44 (m, 2H), 7.76-7.54 (m, 2H), 7.77 (d, $J$ = 6.0 Hz, 1H), 7.90 (d, $J$ = 7.8 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 14.3, 14.6, 21.4, 23.6, 25.5, 28.5, 29.0, 36.9, 125.4, 126.3 127.4, 128.2, 128.8, 129.2, 130.0, 130.5, 131.6, 133.4, 133.7, 134.2, 134.7, 136.4, 136.5, 136.6, 142.8, 146.1, 146.2; HRMS (ESI) calcd for C$_{32}$H$_{33}$NO$_2$S: 518.2124 (M + Na$^+$), found: 518.2117.
8,9-Diethyl-6-methyl-7,10-diphenyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine
5,5-dioxide (3k): Dark red solid; \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 0.70 (t, \(J = 7.4\) Hz, 3H), 0.80 (t, \(J = 6.9\) Hz, 3H), 1.60-1.65 (m, 1H), 1.95-2.00 (m, 1H), 2.26-2.38 (m, 2H), 2.68 (s, 3H), 7.02 (d, \(J = 7.8\) Hz, 2H), 7.09 (t, \(J = 7.3\) Hz, 1H), 7.18-7.25 (m, 4H), 7.38-7.44 (m, 3H), 7.51 (d, \(J = 7.3\) Hz, 2H), 7.79 (d, \(J = 7.8\) Hz, 1H), 7.90 (d, \(J = 7.8\) Hz, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 14.8, 16.7, 19.3, 19.6, 36.9, 125.6, 126.3, 127.0, 127.6, 128.2, 128.5, 128.8, 129.9, 130.6, 131.6, 132.9, 133.6, 133.7, 134.0, 134.9, 136.5, 137.7, 143.8, 146.1, 146.4; HRMS (ESI) calcd for C\(_{29}\)H\(_{27}\)NO\(_2\)S: 476.1655 (M + Na\(^+\)), found: 476.1655.

6-Benzyl-7,10-diphenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine
5,5-dioxide (3l): Dark red solid; \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 0.43 (t, \(J = 7.3\) Hz, 3H), 0.73 (t, \(J = 6.8\) Hz, 3H), 1.13-1.28 (m, 4H), 1.42-1.49 (m, 1H), 1.84-1.91 (m, 1H), 2.18-2.24 (m, 1H), 2.29-2.38 (m, 1H), 4.31 (d, \(J = 16.0\) Hz, 2H), 4.82 (d, \(J = 16.0\) Hz, 2H), 6.45 (d, \(J = 7.8\), 2), 6.80 (t, \(J = 6.8\) Hz, 2H), 6.86-6.91 (m, 5H), 7.22-7.26 (m, 2H), 7.32-7.35 (m, 3H), 7.50-7.55 (m, 3H), 7.77 (d, \(J = 6.0\) Hz, 1H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 14.3, 14.6, 23.6, 25.6, 28.5, 29.1, 53.3, 125.5, 126.9, 127.2, 127.8, 127.9, 128.2, 128.3, 128.4, 128.6, 130.0, 130.4, 131.1, 133.2, 133.5, 133.7, 133.8, 133.9, 135.3, 136.0, 137.9, 139.2, 142.3, 145.7, 146.1; HRMS (ESI) calcd for C\(_{37}\)H\(_{35}\)NO\(_2\)S: 580.2281 (M + Na\(^+\)), found: 580.2281.
7-(4-Chlorophenyl)-6-methyl-10-phenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3m): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) δ 0.47 (t, $J = 6.9$ Hz, 3H), 0.72 (t, $J = 7.3$ Hz, 3H), 1.11-1.28 (m, 4H), 1.51-1.59 (m, 1H), 1.91-1.97 (m, 1H), 2.18-2.24 (m, 1H), 2.28-2.34 (m, 1H), 2.66 (s, 3H), 7.00 (d, $J = 7.8$ Hz, 1H), 7.09 (t, $J = 7.8$ Hz, 1H), 7.18-7.38 (m, 7H), 7.52 (d, $J = 8.2$ Hz, 1H), 7.71 (d, $J = 8.2$ Hz, 1H), 7.89 (d, $J = 7.8$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 14.2, 14.5, 23.5, 25.4, 28.5, 29.0, 36.9, 125.7, 126.4, 127.1, 127.6, 128.6, 129.2, 131.3, 131.6, 133.2, 133.6, 133.7, 133.8, 134.8, 134.9, 136.4, 136.9, 137.6, 143.2, 144.9, 146.4; HRMS (ESI) calcd for C$_{31}$H$_{30}$ClNO$_2$: 538.1578 (M + Na$^+$), found: 538.1572.

6-Methyl-10-phenyl-8,9-dipropyl-7-(p-tolyl)-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3n): Dark red solid; $^1$H NMR (400 MHz, CDCl$_3$) δ 0.45 (t, $J = 6.8$ Hz, 3H), 0.73 (t, $J = 7.3$ Hz, 3H), 1.13-1.27 (m, 4H), 1.55-1.61 (m, 1H), 1.90-1.98 (m, 1H), 2.19-2.26 (m, 1H), 2.30-2.38 (m, 1H), 2.45 (s, 3H), 2.69 (s, 3H), 7.01 (d, $J = 7.8$ Hz, 2H), 7.08 (t, $J = 7.4$ Hz, 1H), 7.14-7.26 (m, 4H), 7.31-7.36 (m, 3H), 7.65 (d, $J = 7.8$ Hz, 1H), 7.80 (d, $J = 7.8$ Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 14.2, 14.5, 21.6, 23.6, 25.5, 28.5, 29.0, 37.0, 125.4, 126.3, 126.9, 127.5, 128.5, 128.9, 129.6, 129.9, 131.5, 132.9, 133.5, 133.7, 133.8, 134.1, 136.6, 138.0, 141.0, 142.3, 145.8, 146.9; HRMS (ESI) calcd for C$_{32}$H$_{33}$NO$_2$: 518.2124 (M + Na$^+$), found: 518.2127.
7-(4-Methoxyphenyl)-2,6-dimethyl-10-phenyl-8,9-dipropyl-6H-benzo[f]cyclopenta[d][1,2]thiazepine 5,5-dioxide (3o): Dark red solid; \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 0.47 (t, \(J = 6.8\) Hz, 3H), 0.73 (t, \(J = 7.3\) Hz, 3H), 1.12-1.25 (m, 4H), 1.56-1.63 (m, 1H), 1.96-2.22 (m, 4H), 2.20-2.26 (m, 1H), 2.30-2.36 (m, 1H), 2.68 (s, 3H), 6.77 (s, 1H), 6.89 (d, \(J = 8.2\) Hz, 1H), 6.98 (d, \(J = 7.8\) Hz, 1H), 7.05 (d, \(J = 8.2\) Hz, 1H), 7.23-7.35 (m, 6H), 7.68 (d, \(J = 8.2\) Hz, 1H), 7.77 (d, \(J = 7.8\) Hz, 1H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 14.3, 14.6, 21.3, 23.7, 25.4, 28.5, 29.0, 37.0, 55.6, 113.4, 114.6, 126.1, 126.4, 126.8, 127.5, 128.3, 128.6, 130.2, 131.5, 132.5, 133.7, 133.8, 134.3, 135.6, 138.1, 141.9, 142.0, 145.4, 146.8; HRMS (ESI) calcd for C\(_{33}\)H\(_{38}\)NO\(_3\)S: 548.2230 (M + Na\(^+\)), found: 548.2230.
Electronic Supplementary Material (ESI) for Dalton Transactions
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