Supporting Information

General Remarks

Most of chemicals were purchased from Sigma-Aldrich, Strem, Acros, TCI or Alfa Aesar and used as such unless stated otherwise. Solvents (Anhydrous and under inert atmosphere) were collected from The Solventpurification system by M BRAUN and used under standard schlenk technique. NMR spectra were recorded on Bruker Avance 600 and Bruker ARX 400 spectrometers. Chemical shifts (ppm) are given relative to solvent: references for CDCl₃ were 7.26 ppm (¹H NMR) and 77.00 ppm (¹³C NMR). Multiplets were assigned as s (singlet), d (doublet), t (triplet), q (quartet), p (pentet) dd (doublet of doublet), m (multiplet) and br. s (broad singlet). GC-yields were calculated using isooctane as internal standard. All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (m/z). Gas chromatography analysis was performed on an Agilent HP-7890A instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d., 0.25 μm film thickness) using argon as carrier gas. The products were isolated from the reaction mixture by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck).

A. General Procedure of Thiomethylation and Carbonylative Thiomethylation

Under an N₂ atmosphere, a 25 mL pressure tube was charged with ArX (0.2 mmol), PdCl₂ (1.8 mg, 5 mol%), Xantphos (5.8 mg, 5 mol%), KO'Bu (44.8mg, 2 equiv) and an oven-dried stirring bar. Then 2 (0.6 mmol) and xylene (2 mL) were injected by syringe. The pressure tube was sealed and the reaction was allowed to be heated under 120 °C for 12 hours. Afterwards, the reaction was cooled to room temperature. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).

Under an N₂ atmosphere, a 4 mL screwcap vial was charged with ArX (0.2 mmol), PdCl₂ (1.8 mg, 5 mol%), Xantphos (5.8 mg, 5 mol%), KO'Bu (67.2 mg, 3 equiv) and an oven-dried stirring bar. Then 4-(methylthio)butan-2-one (70.8 mg, 0.6 mmol) and xylene (2 mL) were injected by syringe. The vial was closed by a Teflon septum and a phenolic cap and connected to the atmosphere through a needle. Then the vial was fixed in an alloy plate and put into Parr 4560 series autoclave (300 mL). At room temperature, the autoclave was flushed with carbon monoxide for three times and 20 bar of carbon monoxide was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction was heated at 130 °C for 16 hours. Afterwards, the autoclave was cooled to room temperature and the pressure was carefully released. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: eluent: pentane/ethyl acetate = 100:1).
General Procedure of Thiomethylation and Carbonylative Thiomethylation

A 25 mL pressure tube was charged with ArX (0.2 mmol), PdCl₂ (1.8 mg, 5 mol%), Xantphos (5.8 mg, 5 mol%), KOtBu (67.2 mg, 3 equiv) and an oven-dried stirring bar. After exchange N₂, 2 (0.6 mmol) and xylene (2 mL) were injected by syringe. The reaction was allowed to be heated under 140 °C for 12 hours. Afterwards, the reaction was cooled to room temperature. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).

A 25 mL tube was charged with ArX (0.2 mmol), PdCl₂ (1.8 mg, 5 mol%), Xantphos (5.8 mg, 5 mol%), NaOMe (32.4 mg, 3 equiv) and an oven-dried stirring bar. After exchange N₂, S-methyl butanethioate (70.8 mg, 0.6 mmol) and xylene (2 mL) were injected by syringe. The reaction was allowed to be heated under 140 °C for 12 hours. Afterwards, the reaction was cooled to room temperature. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).

Under an N₂ atmosphere, a 4 mL screwcap vial was charged with ArX (0.2 mmol), PdCl₂ (1.8 mg, 5 mol%), Xantphos (5.8 mg, 5 mol%), KO'Bu (67.2 mg, 3 equiv) and an oven-dried stirring bar. Then S-methyl butanethioate (70.8 mg, 0.6 mmol) and xylene (1 mL) were injected by syringe. The vial was closed by a Teflon septum and a phenolic cap and connected to the atmosphere through a needle. Then the vial was fixed in an alloy plate and put into Parr 4560 series autoclave (300 mL). At room temperature, the autoclave was flushed with carbon monoxide for three times and 20 bar of carbon monoxide was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction was heated at 130 °C for 16 hours. Afterwards, the autoclave was cooled to room temperature and the pressure was carefully released. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: eluent: pentane/ethyl acetate = 100:1).

Pd-Catalyzed Thiomethylation of Aryl Iodide with different Alkyl sulfides

A 25 mL pressure tube was charged with ArI (0.2 mmol), PdCl₂ (5 mol%), Xantphos (5 mol%), KO'Bu (2 equiv) and an oven-dried stirring bar. Then, 2 (0.6 mmol) and xylene (2 mL) were injected by syringe. The reaction was
allowed to be heated under 120 °C for 12 hours. Afterwards, the reaction was cooled to room temperature. Yields were determined by GC using n-dodecane as internal standard. Or after removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).

Pd-Catalyzed Thiomethylation of Aryl halide with Methionine and Selenomethionine

\[
\begin{align*}
\text{Methionine:} & \quad \text{A 25 mL pressure tube was charged with PdCl}_2 (1.8 \text{ mg, 5 mol\%), Xantphos (5.8mg, 5 mol\%), KO'Bu (67 mg, 3 equiv) and an oven-dried stirring bar. After exchange N}_2 \text{ ArX (0.2 mmol), Methionine (0.6 mmol) and xylene (2 mL) were injected by syringe. The reaction was allowed to be heated under 130 °C for 24 hours. Afterwards, the reaction was cooled to room temperature. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).} \\
\text{Selenomethionine:} & \quad \text{A 25 mL pressure tube was charged with PdCl}_2 (1.8 \text{ mg, 5 mol\%), Xantphos (5.8mg, 5 mol\%), KO'Bu (67 mg, 3 equiv) and an oven-dried stirring bar. After exchange N}_2 \text{ ArX (0.2 mmol), Selenomethionine (0.6 mmol) and xylene (2 mL) were injected by syringe. The reaction was allowed to be heated under 140 °C for 24 hours. Afterwards, the reaction was cooled to room temperature. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).} \\
\end{align*}
\]

Control experiment

\[
\begin{align*}
\text{A 25 mL pressure tube was charged with PdCl}_2 (1.8 \text{ mg, 5 mol\%), Xantphos (5.8mg, 5 mol\%), KO'Bu (45 mg, 2 equiv) and an oven-dried stirring bar. After exchange N}_2 \text{ dodecyl methyl sulfide (43.2 mg, 0.2 mmol) and xylene (2 mL) were injected by syringe. The reaction was allowed to be heated under 120 °C for 12 hours. Afterwards, the reaction was cooled to room temperature. Yield was determined by GC using n-dodecane as internal standard.}
\end{align*}
\]
Gram-scale experiment

A 25 mL pressure tube was charged with ArI (0.2 mmol), PdCl₂ (1.8 mg, 5 mol%), Xantphos (5.8 mg, 5 mol%), KO'Bu (44.8mg, 2 equiv) and an oven-dried stirring bar. After exchange N₂, 2-mercaptoethanol (55.2 mg, 0.6 mmol) and xylene (2 mL) were injected by syringe. The reaction was allowed to be heated under 120 °C for 12 hours. Afterwards, the reaction was cooled to room temperature. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 100:1).
Analytic Data of Products

(3,5-Dimethylphenyl)(methyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 6.89 (s, 3H), 6.78 (s, 1H), 2.47 (s, 3H), 2.29 (s, 6H).
\]

\[
\text{\textsuperscript{13}C NMR (151 MHz, CDCl}_3) \delta 138.40, 137.90, 126.97, 124.37, 21.23, 21.21, 15.86, 15.84.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 152(M+, 100), 119(60), 105(30), 91(45), 77(20).}
\]

Methyl(naphthalen-1-yl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 8.33 – 8.28 (m, 1H), 7.85 (dd, J = 8.0, 1.5 Hz, 1H), 7.69 – 7.54 (dddd, J = 8.0, 1.1 Hz, 1H). 7.54 (dddd, J = 20.5, 8.1, 6.8, 1.4 Hz, 2H), 7.47 – 7.38 (m, 2H), 2.59 (s, 3H).
\]

\[
\text{\textsuperscript{13}C NMR (151 MHz, CDCl}_3) \delta 135.81, 133.65, 131.74, 128.50, 126.19, 126.10, 125.88, 125.64, 124.32, 123.86, 16.29.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 174(M+, 100), 159(50), 141(18), 128(10), 115(80), 87(10), 77(7).}
\]

(3,5-Dimethoxyphenyl)(methyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 6.41 (d, J = 2.2 Hz, 2H), 6.24 (t, J = 2.2 Hz, 2H), 3.78 (s, 6H), 2.47 (s, 3H).
\]

\[
\text{\textsuperscript{13}C NMR (151 MHz, CDCl}_3) \delta 160.95, 140.59, 104.46, 97.42, 55.33, 55.31, 15.60.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 184(M+, 100), 151(78), 141(10), 121(15), 108(20), 91(10).}
\]

(4-Ethoxyphenyl)(methyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 7.29 – 7.24 (m, 2H), 6.87 – 6.81 (m, 2H), 4.01 (qd, J = 6.9, 1.5 Hz, 2H), 2.44 (d, J = 1.6 Hz, 3H), 1.40 (td, J = 7.0, 1.6 Hz, 3H).
\]

\[
\text{\textsuperscript{13}C NMR (151 MHz, CDCl}_3) \delta 157.56, 130.23, 128.57, 115.20, 115.18, 63.57, 18.09, 14.78.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 168(M+, 100), 140(78), 139(30), 125(95), 111(12), 97(10), 81(8), 77(10), 65(10).}
\]

1,4-Bis(methylthio)benzene

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 7.20 (s, 3H), 2.46 (s, 3H).
\]

\[
\text{\textsuperscript{13}C NMR (151 MHz, CDCl}_3) \delta 135.20, 127.68, 127.66, 16.40.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 170(M+, 100), 155(82), 108(10).}
\]
5-(Methylthio)benzo[d][1,3]dioxole

\[
\text{H NMR (600 MHz, Chloroform-}d\text{)} \delta 7.18 (d, J = 1.9 \text{ Hz}, 1H), 7.14 (dd, J = 8.1, 1.9 \text{ Hz}, 1H), 7.08 (d, J = 8.1 \text{ Hz}, 1H), 6.28 (s, 2H), 2.78 (s, 3H).
\]

\[
\text{13C NMR (151 MHz, CDCl}_3\text{)} \delta 148.04, 146.22, 130.50, 121.92, 121.89, 109.41, 109.39, 108.70, 101.13, 18.01.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 168(M+, 100), 153(72), 123(18), 95(30).}
\]

Methyl(4-phenoxyphenyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-}d\text{)} \delta 7.35 – 7.31 (m, 2H), 7.29 – 7.26 (m, 2H), 7.10 (tt, J = 7.5, 1.1 \text{ Hz}, 1H), 7.01 – 6.98 (m, 2H), 6.97 – 6.93 (m, 2H), 2.48 (s, 3H).
\]

\[
\text{13C NMR (151 MHz, CDCl}_3\text{)} \delta 157.25, 155.33, 132.27, 129.71, 129.28, 123.22, 119.57, 118.66, 17.19.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 216(M+, 100), 201(42), 129(23), 77(25), 51(15).}
\]

(4-(Benzyloxy)phenyl)(methyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-}d\text{)} \delta 7.42 (d, J = 7.4 \text{ Hz}, 2H), 7.40 – 7.36 (m, 2H), 7.33 (t, J = 7.2 \text{ Hz}, 1H), 7.27 (d, J = 8.5 \text{ Hz}, 2H), 6.95 – 6.90 (m, 2H), 5.05 (s, 2H), 2.45 (d, J = 1.0 \text{ Hz}, 3H).
\]

\[
\text{13C NMR (151 MHz, CDCl}_3\text{)} \delta 157.15, 136.86, 133.15, 130.05, 128.57, 127.97, 127.41, 115.59, 70.16, 17.93.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 230(M+, 35), 139(17), 91(100), 65(12).}
\]

(4-Chloro-3-(4-ethoxybenzyl)phenyl)(methyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-}d\text{)} \delta 7.27 (t, J = 6.5 \text{ Hz}, 1H), 7.09 (d, J = 8.5 \text{ Hz}, 2H), 7.06 – 7.01 (m, 2H), 6.83 (d, J = 8.6 \text{ Hz}, 2H), 4.01 (dd, J = 12.6, 5.6 \text{ Hz}, 5H), 2.41 (s, 3H), 1.41 (t, J = 7.0 \text{ Hz}, 3H).
\]

\[
\text{13C NMR (151 MHz, CDCl}_3\text{)} \delta 157.49, 139.54, 137.12, 130.97, 129.86, 129.73, 129.01, 125.66, 114.52, 63.40, 38.32, 16.03, 14.86.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 292(M+, 100), 264(18), 257(20), 229(33), 217(17), 182(28), 165(10), 152(20), 115(12), 107(28), 77(10).}
\]

\[
\text{HRMS(EI): calcd. for [C}_{16}\text{H}_{17}\text{ClOS}: 262.0662 found: 262.0658.}
\]

(4-((tert-Butyl)phenyl)(methyl)sulfane

\[
\text{H NMR (600 MHz, Chloroform-}d\text{)} \delta 7.34 – 7.30 (m, 2H), 7.23 (d, J = 8.5 \text{ Hz}, 2H), 2.48 (s, 3H), 1.31 (s, 9H).
\]

\[
\text{13C NMR (151 MHz, CDCl}_3\text{)} \delta 148.35, 134.78, 126.88, 125.84, 34.35, 31.29, 16.30, 16.26.
\]

\[
\text{GC-MS (EI, 70ev): m/z(%) = 180(M+, 50), 165(100), 150(10), 137(20), 117(30), 115(13), 91(10), 77(5).}
\]
[1,1'-Biphenyl]-4-yl(methyl)sulfane¹

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 7.59 - 7.56 \text{ (m, 2H), 7.53 (d, } J = 8.4 \text{ Hz, 2H), 7.44 (t, } J = 7.7 \text{ Hz, 2H), 7.37 - 7.31 \text{ (m, 3H), 2.53 (s, 3H).}
\]

¹C NMR (151 MHz, CDCl₃) δ 140.53, 138.06, 137.57, 128.78, 127.46, 127.18, 127.00, 126.82, 15.93.

GC-MS (EI, 70ev): m/z(%) = 200(M⁺, 100), 185(50), 152(25), 115(12), 100(10).

(3-Chlorophenyl)(methyl)sulfane⁶

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 7.20 \text{ (dd, } J = 13.8, 4.9 \text{ Hz, 2H), 7.11 (dd, } J = 10.5, 8.5 \text{ Hz, 2H), 2.48 (s, 3H).}
\]

¹H NMR (600 MHz, Chloroform-d) δ 7.20 (dd, J = 13.8, 4.9 Hz, 2H), 7.11 (dd, J = 10.5, 8.5 Hz, 2H), 2.48 (s, 3H).

¹C NMR (151 MHz, CDCl₃) δ 140.68, 134.74, 129.73, 125.92, 125.01, 124.51, 15.58.

GC-MS (EI, 70ev): m/z(%) = 158(M⁺, 100), 143(18), 125(73), 112(27), 108(42), 75(13).

N,N-Dimethyl-4-(methylthio)aniline⁴

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 7.31 - 7.26 \text{ (m, 2H), 6.68 (dd, } J = 9.4, 2.5 \text{ Hz, 2H), 2.94 (s, 6H), 2.42 (d, } J = 4.1 \text{ Hz, 3H).}
\]

¹H NMR (600 MHz, Chloroform-d) δ 7.31 - 7.26 (m, 2H), 6.68 (dd, J = 9.4, 2.5 Hz, 2H), 2.94 (s, 6H), 2.42 (d, J = 4.1 Hz, 3H).

¹C NMR (151 MHz, CDCl₃) δ 149.47, 131.35, 123.45, 113.18, 40.56, 19.16.

GC-MS (EI, 70ev): m/z(%) = 167(M⁺, 75), 152(100), 136(5), 108(12), 83(11), 77(10).

(4-Methoxyphenyl)(methyl)sulfane¹

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 7.28 \text{ (d, } J = 8.6 \text{ Hz, 2H), 6.84 (t, } J = 9.0 \text{ Hz, 2H), 3.81 (d, } J = 17.6 \text{ Hz, 3H), 2.44 (s, 3H).}
\]

¹H NMR (600 MHz, Chloroform-d) δ 7.28 (d, J = 8.6 Hz, 2H), 6.84 (t, J = 9.0 Hz, 2H), 3.81 (d, J = 17.6 Hz, 3H), 2.44 (s, 3H).

¹C NMR (151 MHz, CDCl₃) δ 158.19, 130.20, 128.76, 114.59, 55.37, 55.32, 18.09, 18.07.

GC-MS (EI, 70ev): m/z(%) = 154(M⁺, 90), 139(100), 124(12), 111(15), 95(10), 77(10).

6-(Methylthio)quinoline⁴

\[
\text{H NMR (600 MHz, Chloroform-d)} \delta 8.80 \text{ (dd, } J = 4.0, 1.3 \text{ Hz, 1H), 8.01 (d, } J = 8.2 \text{ Hz, 1H), 7.97 (d, } J = 8.9 \text{ Hz, 1H), 7.57 \text{ (dd, } J = 8.8, 2.0 \text{ Hz, 1H), 7.50 \text{ (d, } J = 1.8 \text{ Hz, 1H), 7.35 \text{ (dd, } J = 8.3, 4.2 \text{ Hz, 1H), 2.57 (s, 3H).}
\]

¹H NMR (600 MHz, Chloroform-d) δ 8.80 (dd, J = 4.0, 1.3 Hz, 1H), 8.01 (d, J = 8.2 Hz, 1H), 7.97 (d, J = 8.9 Hz, 1H), 7.57 (dd, J = 8.8, 2.0 Hz, 1H), 7.50 (d, J = 1.8 Hz, 1H), 7.35 (dd, J = 8.3, 4.2 Hz, 1H), 2.57 (s, 3H).

¹C NMR (151 MHz, CDCl₃) δ 149.45, 146.48, 137.48, 134.69, 129.58, 128.99, 128.75, 122.51, 121.60, 15.64.

GC-MS (EI, 70ev): m/z(%) = 175(M⁺, 100), 165(50), 142(22), 129(25), 116(30), 102(10), 89(17), 77(11).
**Naphthalen-1-yl(phenyl)sulfane**<sup>7</sup>

![Naphthalen-1-yl(phenyl)sulfane structure]

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 8.40 (dt, $J = 6.3, 3.5$ Hz, 1H), 7.92 – 7.84 (m, 2H), 7.68 (d, $J = 7.2$ Hz, 1H), 7.53 (dd, $J = 6.4, 3.3$ Hz, 2H), 7.44 (t, $J = 7.7$ Hz, 1H), 7.28 – 7.13 (m, 5H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 136.91, 134.24, 133.60, 132.51, 131.28, 129.16, 129.04, 129.01, 128.53, 127.90, 126.59, 126.12, 126.06.

GC-MS (EI, 70ev): m/z(%): 236 (M$^+$, 100), 221 (10), 202 (15), 127 (15), 115 (30), 77 (20), 51 (18).

**N-Methyl-4-(methylthio)benzamide**<sup>8</sup>

![N-Methyl-4-(methylthio)benzamide structure]

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.70 – 7.62 (m, 2H), 7.23 (d, $J = 8.4$ Hz, 2H), 6.29 (s, 1H), 2.98 (d, $J = 4.8$ Hz, 3H), 2.49 (s, 3H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 167.65, 143.15, 130.83, 127.21, 125.51, 26.74, 15.08, 15.06.

GC-MS (EI, 70ev): m/z(%): 181 (M$^+$, 80), 151 (100), 123 (15), 77 (20).

**7-(Methylthio)-1H-indole**

![7-(Methylthio)-1H-indole structure]

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 8.50 (s, 1H), 7.58 (d, $J = 7.9$ Hz, 1H), 7.32 – 7.21 (m, 2H), 7.13 (t, $J = 7.7$ Hz, 1H), 6.61 (s, 1H), 2.52 (s, 3H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 136.16, 127.70, 124.21, 120.47, 119.89, 118.82, 103.37, 103.35, 18.05.

HR-MS (ESI-TOF) calcd. for C$_9$H$_9$NS [M+H$^+$]: 164.0456; found: 164.0466.

**1-(4-(Methylthio)phenyl)ethan-1-one**<sup>9</sup>

![1-(4-(Methylthio)phenyl)ethan-1-one structure]

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.91 – 7.80 (m, 2H), 7.31 – 7.18 (m, 2H), 2.56 (s, 3H), 2.51 (s, 3H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 197.01, 145.82, 133.57, 128.68, 125.02, 26.33, 26.31, 14.78, 14.76.

GC-MS (EI, 70ev): m/z(%): 166 (M$^+$, .70), 151 (100), 123 (27), 108 (18), 79 (15).

**2-(Methylthio)benzo[d]thiazole**<sup>10</sup>

![2-(Methylthio)benzo[d]thiazole structure]

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.87 (d, $J = 8.2$ Hz, 1H), 7.75 (dd, $J = 8.1, 1.3$ Hz, 1H), 7.41 (ddd, $J = 8.4, 7.2, 1.3$ Hz, 1H), 7.28 (td, $J = 7.6, 7.2, 1.2$ Hz, 1H), 2.79 (s, 4H).
$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 167.97, 153.38, 135.17, 126.01, 124.06, 121.39, 120.91, 15.91.

GC-MS (EI, 70ev): m/z(%) = 181(M+,100), 148(75), 122(18), 108(35), 69(18).

(1,2,3,6,7,8-Hexahydropyren-4-yl)(methyl)sulfane

![Hexahydropyren-4-yl](image)

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.19 (s, 1H), 7.13 (d, $J = 7.1$ Hz, 1H), 7.09 (d, $J = 7.1$ Hz, 1H), 3.08 (ddt, $J = 28.2, 15.9, 6.2$ Hz, 8H), 2.55 (s, 2H), 2.07 (td, $J = 6.3, 2.2$ Hz, 4H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 134.57, 134.12, 133.50, 131.73, 131.32, 130.32, 128.22, 124.13, 123.00, 122.39, 31.51, 31.31, 31.22, 28.44, 23.23, 22.84, 16.33.

GC-MS (EI, 70ev): m/z(%) = 254(M+,100), 239(40), 206(22), 178(25), 89(15).

HRMS(EI): calcd. for [C$_{17}$H$_{18}$S]$: 254.1123$, found: 254.1119.

4-(Methylthio)benzonitrile

![Methylthiobenzonitrile](image)

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.57 – 7.47 (m, 2H), 7.25 (d, $J = 8.4$ Hz, 2H), 2.50 (s, 3H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 146.09, 132.12, 125.54, 125.52, 118.88, 107.72, 14.69.

GC-MS (EI, 70ev): m/z(%) = 149(M+,100), 134(28), 116(53), 104(22), 90(13), 75(12).

4,4,5,5-Tetramethyl-2-(4-(methylthio)phenyl)-1,3,2-dioxaborolane

![Tetramethyl-2-(4-(methylthio)phenyl)-1,3,2-dioxaborolane](image)

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.77 – 7.63 (m, 2H), 7.23 (d, $J = 8.2$ Hz, 2H), 2.48 (s, 3H), 1.34 (s, 12H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 142.52, 135.05, 125.12, 83.69, 24.82, 15.11.

GC-MS (EI, 70ev): m/z(%) = 250(M+,100), 235(28), 164(42), 150(80), 117(18), 85(12).

Cyclohexyl(4-methoxyphenyl)sulfane

![Cyclohexyl(4-methoxyphenyl)sulfane](image)

$^1$H NMR (600 MHz, Chloroform-$d$) $\delta$ 7.64 – 7.21 (m, 2H), 6.97 – 6.62 (m, 2H), 3.79 (s, 3H), 2.90 (ddd, $J = 10.7, 6.9, 3.7$ Hz, 1H), 1.92 (dd, $J = 10.2, 5.2$ Hz, 2H), 1.75 (dt, $J = 12.5, 3.6$ Hz, 2H), 1.60 (q, $J = 7.1, 5.4$ Hz, 1H), 1.42 – 1.12 (m, 5H).

$^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 159.29, 135.55, 135.50, 125.04, 114.26, 55.30, 55.23, 47.89, 33.37, 26.09, 25.76.

GC-MS (EI, 70ev): m/z(%) = 222(M+,38), 140(100), 125(25), 55(20).
Decyl(4-methoxyphenyl)sulfane

\[
\begin{align*}
\text{O} & \quad \text{S} \\
\end{align*}
\]

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 7.48 – 7.17 (m, 2H), 6.84 (d, \(J = 8.3\) Hz, 2H), 3.79 (s, 3H), 2.81 (t, \(J = 7.4\) Hz, 2H), 1.62 – 1.53 (m, 2H), 1.38 (t, \(J = 7.5\) Hz, 2H), 1.26 (s, 11H), 0.88 (t, \(J = 7.0\) Hz, 3H).

\(^1^3\)C NMR (151 MHz, cdcl\(_3\)) \(\delta\) 158.70, 132.88, 132.85, 132.83, 127.04, 114.47, 55.31, 55.25, 35.82, 31.87, 29.52, 29.49, 29.36, 29.28, 29.16, 28.69, 22.65, 14.07.

GC-MS (EI, 70ev): m/z(%) = 280 (M+, 100), 153(10), 140(78), 125(15), 55(10).

S-(\(p\)-Tolyl) quinoline-6-carbothioate\(^{14}\)

\[
\begin{align*}
\text{O} & \quad \text{S} \\
\end{align*}
\]

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 8.83 (dd, \(J = 4.2, 1.8\) Hz, 1H), 8.03 – 7.91 (m, 2H), 7.59 (d, \(J = 2.1\) Hz, 1H), 7.53 (dd, \(J = 8.9, 2.1\) Hz, 1H), 7.38 (d, \(J = 7.8\) Hz, 2H), 7.33 (dd, \(J = 8.3, 4.2\) Hz, 1H), 7.18 (d, \(J = 7.8\) Hz, 2H), 2.36 (s, 3H).

\(^1^3\)C NMR (151 MHz, cdcl\(_3\)) \(\delta\) 150.00, 146.96, 138.36, 136.45, 135.10, 133.10, 130.61, 130.33, 130.05, 128.63, 126.51, 121.54, 21.20.

S-Methyl benzothioate\(^{15}\)

\[
\begin{align*}
\text{O} & \quad \text{S} \\
\end{align*}
\]

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 8.00 – 7.92 (m, 2H), 7.60 – 7.53 (m, 1H), 7.47 – 7.40 (m, 2H), 2.48 (s, 3H).

\(^1^3\)C NMR (151 MHz, cdcl\(_3\)) \(\delta\) 192.42, 137.06, 133.22, 128.57, 127.10, 11.68.

S-Methyl naphthalene-2-carbothioate

\[
\begin{align*}
\text{O} & \quad \text{S} \\
\end{align*}
\]

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 8.53 (d, \(J = 1.7\) Hz, 1H), 8.00 (dd, \(J = 8.6, 1.8\) Hz, 1H), 7.97 (d, \(J = 8.1\) Hz, 1H), 7.88 (t, \(J = 8.8\) Hz, 2H), 7.59 (dd, \(J = 8.2, 6.8, 1.4\) Hz, 1H), 7.55 (dd, \(J = 8.1, 6.8, 1.3\) Hz, 1H), 2.53 (s, 3H).

\(^1^3\)C NMR (151 MHz, cdcl\(_3\)) \(\delta\) 192.29, 135.71, 134.38, 132.46, 129.52, 128.43, 128.41, 128.36, 127.77, 126.86, 123.11, 11.81.

GC-MS (EI, 70ev): m/z(%) = 202(M+, 18), 155(100), 127(90), 101(10), 77(12).

S-Methyl 3,5-dimethoxybenzothioate

\[
\begin{align*}
\text{O} & \quad \text{S} \\
\end{align*}
\]

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 7.10 (d, \(J = 2.4\) Hz, 2H), 6.65 (t, \(J = 2.3\) Hz, 1H), 3.83 (s, 6H), 2.46 (s, 3H).

\(^1^3\)C NMR (151 MHz, cdcl\(_3\)) \(\delta\) 192.26, 160.81, 139.02, 105.65, 104.88, 55.57, 55.56, 11.81.

GC-MS (EI, 70ev): m/z(%) = 212(M+, 17), 137(28), 122(27), 107(18), 77(15).
S-Methyl 4-methyl-3-(trifluoromethyl)benzothioate

\[
\text{CF}_3 \\
\text{O} \\
\text{S} 
\]

\(^1^H\) NMR (600 MHz, Chloroform-\text{d}) \(\delta\) 8.20 (d, \textit{J} = 1.9 Hz, 1H), 8.01 (dd, \textit{J} = 8.0, 1.8 Hz, 1H), 7.38 (d, \textit{J} = 7.9 Hz, 1H), 7.26 (s, 1H), 2.54 (d, \textit{J} = 1.9 Hz, 3H), 2.49 (s, 3H).

\(^1^3^C\) NMR (151 MHz, Chloroform-\text{d}) \(\delta\) 191.01, 142.37, 134.93, 132.28, 130.04, 129.41 (d, \textit{J} = 30.3 Hz), 124.82, 124.64 (q, \textit{J} = 5.6 Hz), 123.00, 19.54, 11.72.

S-Methyl 4-chloro-3-(4-ethoxybenzyl)benzothioate

\[
\text{Cl} \\
\text{O} \\
\text{S} 
\]

\(^1^H\) NMR (600 MHz, Chloroform-\text{d}) \(\delta\) 7.84 – 7.67 (m, 2H), 7.44 (d, \textit{J} = 8.2 Hz, 1H), 7.10 (d, \textit{J} = 8.4 Hz, 2H), 6.92 – 6.74 (m, 2H), 4.08 (s, 2H), 4.01 (qd, \textit{J} = 6.9, 0.9 Hz, 2H), 2.45 (d, \textit{J} = 1.1 Hz, 3H), 1.40 (td, \textit{J} = 6.9, 0.9 Hz, 3H).

\(^1^3^C\) NMR (151 MHz, cdcl\text{3}) \(\delta\) 191.32, 157.65, 139.83, 139.47, 135.72, 130.45, 129.82, 129.80, 129.38, 126.14, 114.68, 63.41, 38.35, 38.33, 38.31, 14.82, 11.69, 11.67.

GC-MS (EI, 70ev): m/z(%) = 320 (M\text{+}, 32), 273(100), 107(18), 135(14), 123(12), 152(10), 181(10).

S-Methyl 4-cyanobenzothioate

\[
\text{NC} \\
\text{O} \\
\text{S} 
\]

\(^1^H\) NMR (600 MHz, Chloroform-\text{d}) \(\delta\) 8.16 – 7.94 (m, 2H), 7.83 – 7.68 (m, 2H), 2.52 (d, \textit{J} = 1.3 Hz, 3H).

\(^1^3^C\) NMR (151 MHz, cdcl\text{3}) \(\delta\) 191.04, 140.09, 132.47, 127.55, 117.78, 116.56, 11.94.

GC-MS (EI, 70ev): m/z(%) =177(M\text{+}, 10), 130(100), 102(40), 75(10).

S-Methyl 2-chloro-4-fluorobenzothioate

\[
\text{Cl} \\
\text{F} \\
\text{O} \\
\text{S} 
\]

\(^1^H\) NMR (600 MHz, Chloroform-\text{d}) \(\delta\) 7.70 (dd, \textit{J} = 8.7, 5.9 Hz, 1H), 7.19 (dd, \textit{J} = 8.4, 2.5 Hz, 1H), 7.03 (ddd, \textit{J} = 8.7, 7.7, 2.5 Hz, 1H), 2.49 (s, 3H).

\(^1^3^C\) NMR (151 MHz, cdcl\text{3}) \(\delta\) 191.16, 164.62, 162.92, 133.78, 133.76, 132.68, 132.61, 131.08, 131.02, 118.51, 118.35, 114.10, 113.96, 12.64.

GC-MS (EI, 70ev): m/z(%) = 204 (M\text{+}, 10), 157(100), 129(34), 159(32).

S-Methyl 4-methylbenzothioate
\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 7.91 – 7.82 (m, 2H), 7.24 (d, \(J = 8.0\) Hz, 2H), 2.46 (s, 3H), 2.40 (s, 3H).
\(^{13}\)C NMR (151 MHz, \(\text{cdcl}_3\)) \(\delta\) 192.02, 144.05, 134.55, 129.22, 127.16, 21.62, 11.60, 11.58.
GC-MS (EI, 70ev): m/z(%) = 166(M+, 10), 119(100), 91(50), 65(16).

S-Methyl 4-(dimethylamino)benzothioate\(^{17}\)

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 8.04 – 7.71 (m, 2H), 6.78 – 6.49 (m, 2H), 3.04 (s, 6H), 2.43 (s, 3H).
\(^{13}\)C NMR (151 MHz, \(\text{cdcl}_3\)) \(\delta\) 190.17, 153.63, 129.15, 124.80, 110.60, 40.01, 39.99, 11.33.
GC-MS (EI, 70ev): m/z(%) = 195(M+, 22), 148(100), 120(12), 105(10), 77(12), 91(10).

S-Methyl 4-(methylcarbamoyl)benzothioate

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 8.02 – 7.97 (m, 2H), 7.82 (d, \(J = 8.5\) Hz, 2H), 3.02 (d, \(J = 4.7\) Hz, 3H), 2.49 (s, 3H).
\(^{13}\)C NMR (151 MHz, \(\text{cdcl}_3\)) \(\delta\) 191.76, 167.11, 139.11, 138.69, 127.32, 127.15, 26.93, 11.82.
GC-MS (EI, 70ev): m/z(%) = 209(M+, 10), 162(100), 134(18), 103(25), 76(20).

S-Methyl 3-fluoro-4-methoxybenzothioate

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 7.77 (d, \(J = 8.5\) Hz, 1H), 7.69 (d, \(J = 11.7\) Hz, 1H), 7.02 – 6.94 (m, 1H), 3.94 (s, 3H), 2.45 (s, 3H).
\(^{13}\)C NMR (151 MHz, \(\text{cdcl}_3\)) \(\delta\) 190.16, 152.68, 152.00, 151.92, 151.04, 124.23, 124.20, 114.95, 114.82, 112.42, 56.29, 11.67.
GC-MS (EI, 70ev): m/z(%) = 200(M+, 18), 153(100), 125(22), 110(10), 95(18), 82(12).

S-Methyl 4-(benzyloxy)benzothioate

\(^1\)H NMR (600 MHz, Chloroform-\(d\)) \(\delta\) 8.04 – 7.81 (m, 2H), 7.49 – 7.34 (m, 2H), 7.23 – 7.13 (m, 1H), 7.12 – 7.02 (m, 2H), 6.99 (d, \(J = 8.9\) Hz, 2H), 2.46 (s, 3H).
\(^{13}\)C NMR (151 MHz, \(\text{cdcl}_3\)) \(\delta\) 190.97, 162.13, 155.47, 131.63, 130.02, 129.26, 124.59, 120.12, 117.33, 11.64.
GC-MS (EI, 70ev): m/z(%) = 244(M+, 10), 197(100), 141(18), 115(18), 77(10).
S-Methyl [1,1’-biphenyl]-4-carbothioate

\[
\begin{align*}
\text{H NMR} & (600 \text{ MHz, Chloroform-}d) \quad \delta 8.05 (d, J = 8.5 \text{ Hz, 2H}, 7.70 – 7.65 \text{ (m, 2H)}, 7.64 – 7.60 \text{ (m, 2H)}, 7.50 – 7.44 \text{ (m, 2H)}, 7.43 – 7.38 \text{ (m, 1H)}, 2.50 \text{ (s, 3H)}. \\
\text{C NMR} & (151 \text{ MHz, cdcl}_{3}) \quad \delta 191.91, 146.01, 139.80, 135.78, 128.94, 128.22, 127.66, 127.23, 127.22, 11.71. \\
\text{GC-MS} (\text{EI, 70ev}): m/z(\%) = 228(\text{M}^{+}, 15), 182(12), 181(100), 153(25), 152(46), 76(10).
\end{align*}
\]

S-Methyl 4-(pyrrolidin-1-yl)benzothioate

\[
\begin{align*}
\text{H NMR} & (600 \text{ MHz, Chloroform-}d) \quad \delta 7.86 (d, J = 8.9 \text{ Hz, 2H}), 6.48 (d, J = 8.9 \text{ Hz, 2H}), 3.50 – 3.18 \text{ (m, 4H)}, 2.42 \text{ (s, 4H)}, 2.12 – 1.87 \text{ (m, 3H)}. \\
\text{C NMR} & (151 \text{ MHz, cdcl}_{3}) \quad \delta 190.03, 151.22, 129.31, 124.26, 110.63, 47.54, 25.41, 11.32. \\
\text{GC-MS} (\text{EI, 70ev}): m/z(\%) = 221(\text{M}^{+}, 23), 174(100), 146(18), 117(10), 104(12), 77(10).
\end{align*}
\]

S-Methyl 4-hexylbenzothioate

\[
\begin{align*}
\text{H NMR} & (600 \text{ MHz, Chloroform-}d) \quad \delta 7.98 – 7.75 \text{ (m, 2H)}, 7.33 – 7.11 \text{ (m, 2H)}, 2.64 (t, J = 7.8 \text{ Hz, 2H}), 2.46 \text{ (s, 3H)}, 1.70 – 1.49 \text{ (m, 2H)}, 1.43 – 1.15 \text{ (m, 6H)}, 1.02 – 0.79 \text{ (m, 3H)}. \\
\text{C NMR} & (151 \text{ MHz, cdcl}_{3}) \quad \delta 192.04, 149.02, 134.72, 128.58, 127.18, 35.99, 31.63, 31.04, 31.02, 28.88, 22.54, 14.04, 14.03, 11.59.
\end{align*}
\]

S-Methyl 4-methoxybenzothioate

\[
\begin{align*}
\text{H NMR} & (600 \text{ MHz, Chloroform-}d) \quad \delta 8.00 – 7.87 \text{ (m, 2H)}, 6.92 (d, J = 8.9 \text{ Hz, 2H}), 3.86 \text{ (s, 3H)}, 2.45 \text{ (s, 3H)}. \\
\text{C NMR} & (151 \text{ MHz, cdcl}_{3}) \quad \delta 190.93, 163.65, 129.98, 129.24, 113.72, 55.47, 55.45, 11.56. \\
\text{GC-MS} (\text{EI, 70ev}): m/z(\%) = 182(\text{M}^{+}, 10), 135(100), 107(18), 92(17), 77(30).
\end{align*}
\]

S-Methyl 4-morpholinobenzothioate

\[
\begin{align*}
\text{H NMR} & (600 \text{ MHz, Chloroform-}d) \quad \delta 7.89 (d, J = 9.0 \text{ Hz, 2H}), 6.84 (d, J = 9.1 \text{ Hz, 2H}), 3.84 \text{ (dd, } J = 5.8, 4.1 \text{ Hz, 4H}), 3.29 \text{ (dd, } J = 5.8, 4.0 \text{ Hz, 4H}), 2.44 \text{ (s, 3H)}.
\end{align*}
\]
$^{13}$C NMR (151 MHz, cdcl$_3$) δ 190.48, 154.45, 129.00, 127.70, 113.31, 66.53, 47.54, 11.44. 
GC-MS (EI, 70ev): m/z(%) = 237(M+, .12), 190(100), 132(10), 91(12), 77(11).

**S-Methyl 4-(tert-butyl)benzothioate**

![Structure](image)

$^1$H NMR (600 MHz, Chloroform-d) δ 8.04 – 7.76 (m, 2H), 7.55 – 7.33 (m, 2H), 2.46 (s, 3H), 1.34 (s, 9H).

$^{13}$C NMR (151 MHz, cdcl$_3$) δ 192.01, 157.01, 134.47, 127.00, 125.50, 35.11, 31.06, 11.58. 
GC-MS (EI, 70ev): m/z(%) = 208(M+, .10), 161(100), 146(18), 118(17), 91(12).

**S-Methyl benzofuran-5-carbothioate**

![Structure](image)

$^1$H NMR (600 MHz, Chloroform-d) δ 8.28 (t, J = 2.0 Hz, 1H), 7.96 (dt, J = 8.7, 2.0 Hz, 1H), 7.69 (s, 1H), 7.59 – 7.50 (m, 1H), 6.86 (td, J = 2.5, 1.1 Hz, 1H), 2.67 – 2.41 (m, 3H).

$^{13}$C NMR (151 MHz, cdcl$_3$) δ 191.95, 157.60, 146.43, 132.57, 127.52, 123.79, 121.19, 111.46, 107.23, 11.83. 
GC-MS (EI, 70ev): m/z(%) = 192(M+, .14), 145(100), 117(48), 89(25), 63(14).

**S-Methyl quinoline-6-carbothioate**

![Structure](image)

$^1$H NMR (600 MHz, Chloroform-d) δ 9.00 (dd, J = 4.2, 1.7 Hz, 1H), 8.49 (d, J = 2.0 Hz, 1H), 8.32 – 8.26 (m, 1H), 8.23 (dd, J = 8.8, 2.0 Hz, 1H), 8.15 (d, J = 8.8 Hz, 1H), 7.48 (dd, J = 8.3, 4.2 Hz, 1H), 2.54 (s, 3H).

$^{13}$C NMR (151 MHz, cdcl$_3$) δ 191.74, 152.54, 150.20, 137.46, 134.83, 130.13, 128.14, 126.83, 122.01, 11.93. 
GC-MS (EI, 70ev): m/z(%) = 203(M+, .15), 156(100), 128(70), 101(25), 75(18).

**S-Methyl 1H-indole-7-carbothioate**

![Structure](image)

$^1$H NMR (600 MHz, Chloroform-d) δ 10.08 (s, 0H), 8.01 – 7.92 (m, 1H), 7.90 – 7.86 (m, 1H), 7.36 – 7.28 (m, 1H), 7.16 (t, J = 7.7 Hz, 1H), 6.59 (dd, J = 3.2, 2.2 Hz, 1H), 2.52 (s, 3H).

$^{13}$C NMR (151 MHz, cdcl$_3$) δ 193.07, 133.46, 129.40, 126.88, 125.70, 122.91, 119.85, 119.04, 102.39, 11.28. 
GC-MS (EI, 70ev): m/z(%) = 191(M+, .44), 144(100), 116(76), 89(28).
S-Methyl 4-(benzyloxy)benzothioate

\[
\text{CH}_3\text{S-} \quad \text{O} \quad \text{S-} \quad \text{O}
\]

\[
^1H \text{ NMR (600 MHz, Chloroform-}d) \delta 7.99 – 7.89 (m, 2H), 7.46 – 7.37 (m, 4H), 7.37 – 7.32 (m, 1H), 7.03 – 6.94 (m, 2H), 5.12 (s, 2H), 2.45 (s, 3H).
\]

\[
^{13}C \text{ NMR (151 MHz, CDCl}_3) \delta 190.88, 162.81, 136.14, 130.21, 129.26, 128.67, 128.22, 127.43, 114.61, 70.18, 11.57.
\]

GC-MS (EI, 70ev): m/z(%) = 158(M+, 10), 211(52), 91(100), 65(15).

S-Methyl benzo[d][1,3]dioxole-5-carbothioate\(^{19}\)

\[
\text{CH}_3\text{S-} \quad \text{O} \quad \text{S-} \quad \text{O}
\]

\[
^1H \text{ NMR (600 MHz, Chloroform-}d) \delta 7.60 (dt, J = 8.2, 1.4 Hz, 1H), 7.48 – 7.30 (m, 1H), 6.93 – 6.78 (m, 1H), 6.04 (d, J = 1.1 Hz, 2H), 2.44 (d, J = 1.2 Hz, 3H).
\]

\[
^{13}C \text{ NMR (151 MHz, CDCl}_3) \delta 190.65, 151.88, 148.00, 131.65, 123.12, 107.98, 107.14, 101.88, 11.75.
\]

GC-MS (EI, 70ev): m/z(%) = 196(M+, 18), 149(100), 121(28), 91(10), 65(22).

(4-Methoxyphenyl)(methyl)selane\(^{20}\)

\[
\text{O} \quad \text{Se} \quad \text{O}
\]

\[
^1H \text{ NMR (600 MHz, Chloroform-}d) \delta 7.49 – 7.36 (m, 2H), 6.91 – 6.72 (m, 2H), 3.79 (s, 3H), 2.30 (s, 3H).
\]

\[
^{13}C \text{ NMR (151 MHz, CDCl}_3) \delta 158.83, 133.45, 121.53, 114.80, 55.30, 55.25, 8.67, 8.65.
\]

GC-MS (EI, 70ev): m/z(%) = 202(M+, 100), 200(50), 189(22), 187(96), 185(46), 183(22), 172(18), 144(18), 121(15), 78(28), 69(19).

S-Methyl 4-(methylthio)benzothioate

\[
\text{S-} \quad \text{O} \quad \text{S-} \quad \text{O}
\]

\[
^1H \text{ NMR (600 MHz, Chloroform-}d) \delta 7.94 – 7.81 (m, 2H), 7.29 – 7.12 (m, 2H), 2.51 (s, 3H), 2.46 (s, 3H).
\]

\[
^{13}C \text{ NMR (151 MHz, CDCl}_3) \delta 191.33, 146.05, 133.34, 127.46, 127.44, 125.05, 125.00, 14.84, 14.79, 11.61, 11.56.
\]

GC-MS (EI, 70ev): m/z(%) = 198(M+, 18), 151(100), 123(20), 108(16), 79(10).
Reference
