**Supporting Information**

# Selective oxidative intermolecular carbosulphenylation of aryl alkenes with thiols and nucleophiles via 1,2-dithioethane intermediate

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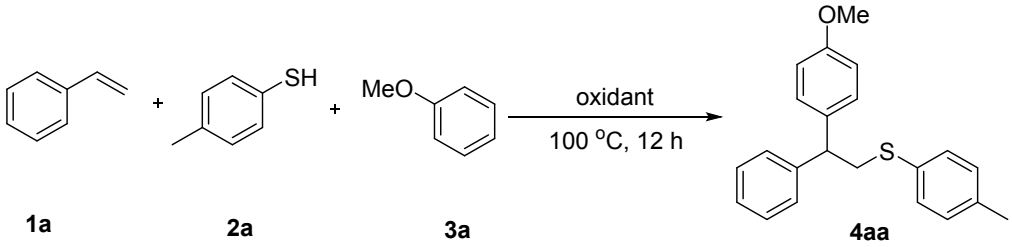
## Contents

## 1. General experiment details and materials

All non-aqueous reactions and manipulations were used by standard Schlenk techniques. All solvents before used were dried by standard methods and stored under nitrogen atmosphere. All reactions were monitored by TLC with silica gel-coated plates. NMR spectra were recorded on BRUKER AvanceIII (400 MHz) spectrometers. Chemical shifts were reported in parts per million (ppm) down field from tetramethylsilane (TMS) with the solvent resonance as the internal standard. Coupling constants (J) were reported in Hz and refered to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker Micro TOF-QII mass instrument (ESI). Gaschromatograph/massspectrometer (GC/MS) were recorded on Agilent 7890A/5975C system. Styrene derivates, thiophenol derivates and arene derivates used here were known compounds and commercially available.

## 2. Optimization of reaction conditions

**Table S1. Screening of oxidant**[a]

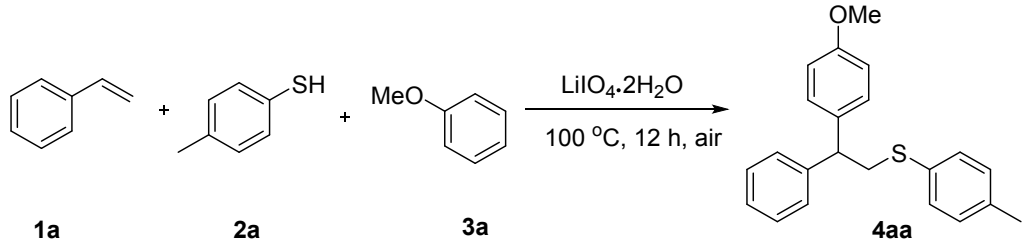



**1a** **2a** **3a** **4aa**

| Entry | Oxidant | Yield of **4aa** (%)[b] |
|---|---|---|
| 1 | air | trace |
| 2 | $O_2$ | trace |
| 3 | $PhI(OAc)_2$ | trace |
| 4 | TBHP | 0 |
| 5 | DDQ | trace |
| 6 | NFSI | trace |
| 7 | $NaIO_4$ | 0 |
| 8 | $NaCr_2O_7 \cdot 2H_2O$ | 0 |
| 9 | NaClO | 0 |
| 10 | $KIO_4$ | 0 |
| 11 | $LiClO_4$ | 6 |
| **12** | **$LiIO_4 \cdot 2H_2O$** | **67** |

[a]Reaction conditions: **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), oxidant (0.25 mmol, 50 mol %), anisole **3a** (2.0 mL), 100 °C, 12 h, air. [b]Yield was determined by GC using 1,3,5-trimethoxybenzene as the internal standard.

**Table S2. Screening of amount of oxidant**[a]

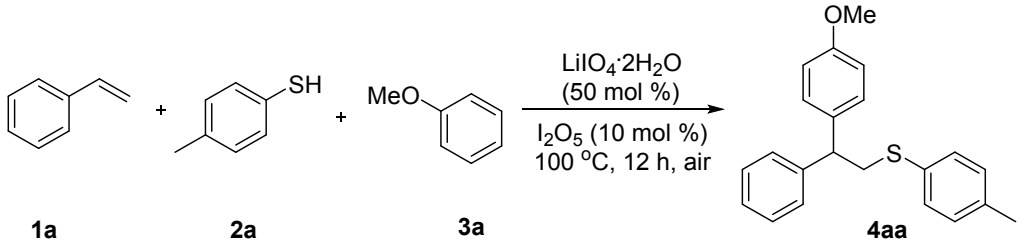



**1a** **2a** **3a** **4aa**

| Entry | $LiIO_4 \cdot 2H_2O$ (mmol) | Yield of **4aa** (%)[b] |
|---|---|---|
| 1 | 0.05 | trace |
| 2 | 0.1 | 20 |
| 3 | 0.15 | 37 |
| 4 | 0.2 | 54 |
| **5** | **0.25** | **67** |
| 6 | 0.3 | 61 |
| 7 | 0.5 | 54 |

[a]Reaction conditions: **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), anisole **3a** (2.0 mL), 100 °C, 12 h, air. [b]Yield was determined by GC using 1,3,5-trimethoxybenzene as the internal standard.

**Table S3. Controlled variable experiment**[a]

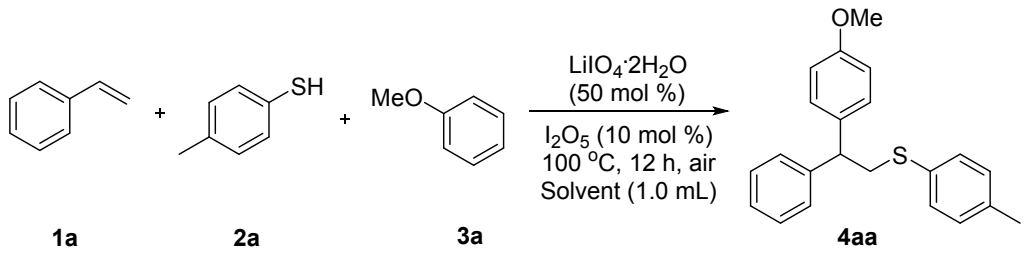



**1a** **2a** **3a** **4aa**

| Entry | $LiIO_4·2H_2O$ | $I_2O_5$ | Yield of **4aa** (%)[b] |
|---|---|---|---|
| 1 | / | / | trace |
| 2 | 0.5 equiv | / | 67 |
| 3 | 0.5 equiv | 10 mol % | 72 (75)[c] |

[a]Reaction conditions: **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), anisole **3a** (2.0 mL), $I_2O_5$ (0.05 mmol, 10 mol %), $LiIO_4·2H_2O$ (0.25 mmol, 50 mol %), 100 °C, 12 h, air. [b]Yield was determined by GC using 1,3,5-trimethoxybenzene as the internal standard. [c]Isolated yield.

**Table S4. Screening of solvent**[a]

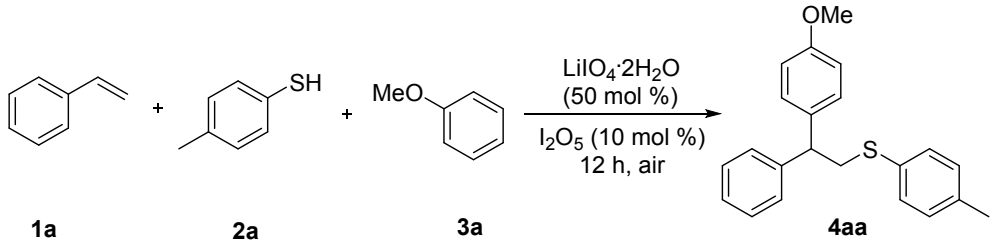



**1a** **2a** **3a** **4aa**

| Entry | Solvent (1.0 mL) | Yield of **4aa** (%)[b] |
|---|---|---|
| 1 | DMSO | 0 |
| 2 | DMF | 0 |
| 3 | DCE | 64 |
| 4 | benzotrifluoride | 63 |
| 5 | nitrobenzene | 62 |
| 6 | chlorobenzene | 55 |
| 7 | *m*-xylene | 28 |
| 8 | 1,2-dichlorobenzene | 65 |
| 9 | mesitylene | 23 |
| 10 | fluorobenzene | 70 |
| **11** | **anisole** | **72** |

[a]Reaction conditions: **1a** (0.75 mmol, 1 equiv), **2a** (0.5 mmol, 1 equiv), **3a** (7.5 mmol, 15 equiv), $I_2O_5$ (0.05 mmol, 10 mol %), $LiIO_4 \cdot 2H_2O$ (0.25 mmol, 50 mol %), slovent (1.0 mL), 100 °C, 12 h, air. [b]Yield was determined by GC using 1,3,5-trimethoxybenzene as the internal standard.

**Table S5. Screening of temperature**[a]

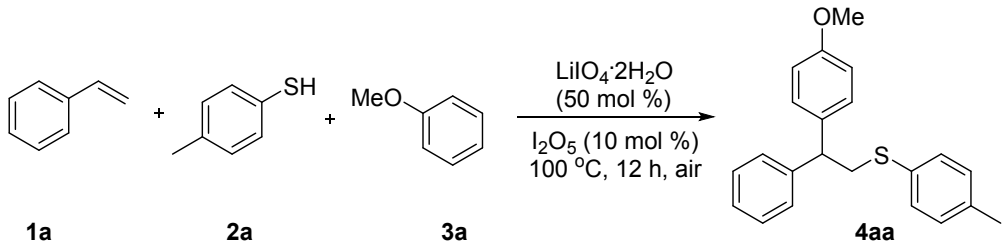



**1a** **2a** **3a** **4aa**

| Entry | Temp. (°C) | Yield of **4aa** (%)[b] |
|---|---|---|
| 1 | 60 | 29 |
| 2 | 80 | 67 |
| **3** | **100** | **72** |
| 4 | 120 | 70 |

[a]Reaction conditions: **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3a** (2.0 mL), $I_2O_5$ (0.05 mmol, 10 mol %), $LiIO_4 \cdot 2H_2O$ (0.25 mmol, 50 mol %), 12 h, air. [b]Yield was determined by GC using 1,3,5-trimethoxybenzene as the internal standard.

## 3. General procedure for the carbosulfuration of alkene

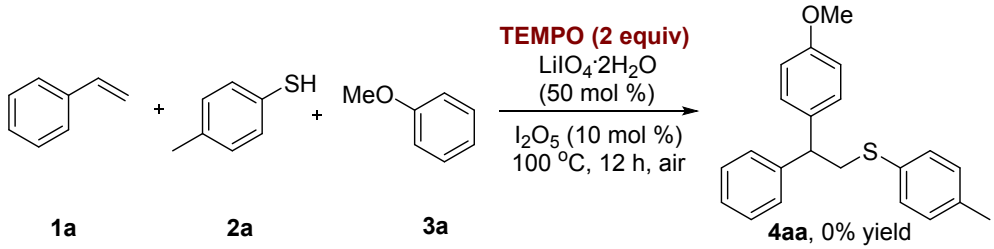



**1a** **2a** **3a** **4aa**

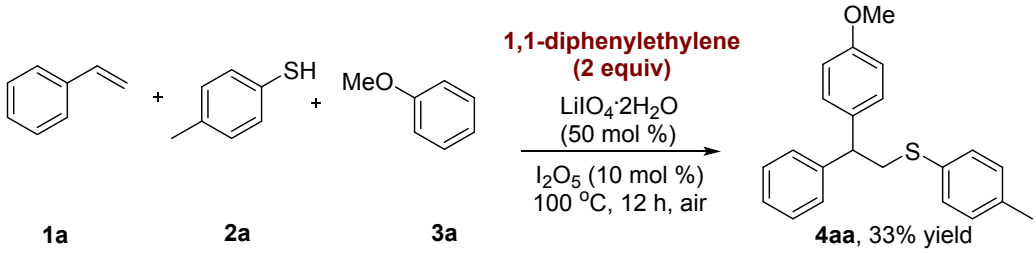
Under air atmosphere, styrene **1a** (86 μL, 0.75 mmol, 1.5 equiv), thiol **2a** (62.1 mg, 0.5 mmol, 1 equiv), $LiIO_4$ $2H_2O$ (58.5 mg, 0.25 mmol, 50 mol %), $I_2O_5$ (16.7 mg, 0.05 mmol, 10 mol %) and anisole **3a** (2.0 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the solvent was removed under reduced. Then the reaction mixture was purified by flash column chromatography on silica gel to give the desired product **4aa**.

## 4. Preliminary mechanistic studies

### (1) Radical trap experiments

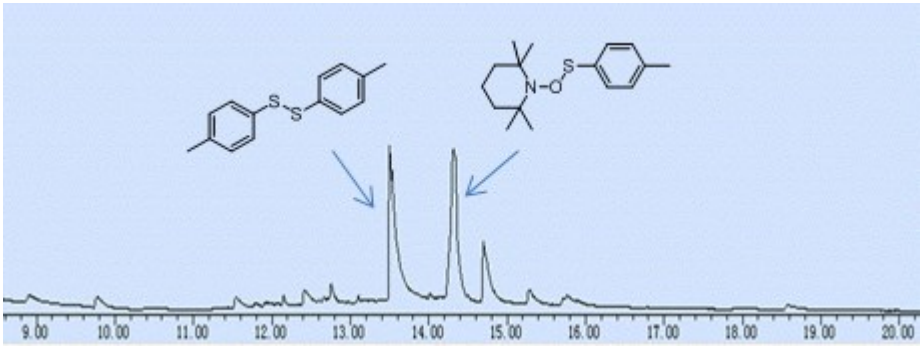


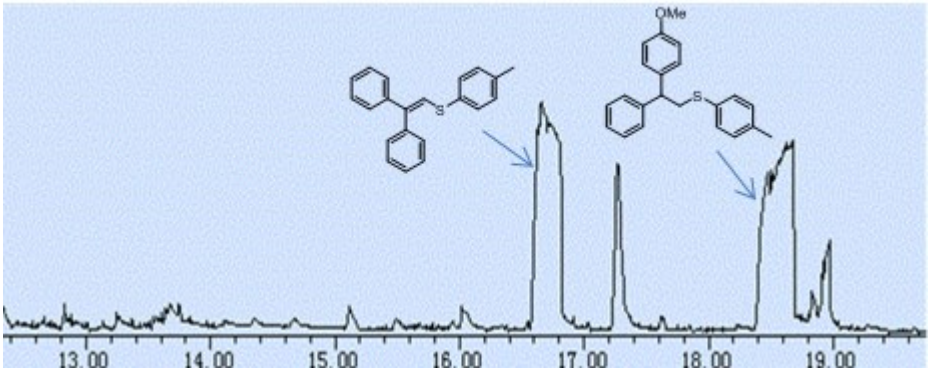

Under air atmosphere, **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), $LiIO_4$ $2H_2O$ (58.5 mg, 0.25 mmol, 50 mol %), $I_2O_5$ (16.7 mg, 0.05 mmol, 10 mol %), TEMPO (156 mg, 1.0 mmol, 2 equiv) and **3a** (2.0 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the solvent was detected by TLC and GC/MS. The product **4aa** could not be detected.



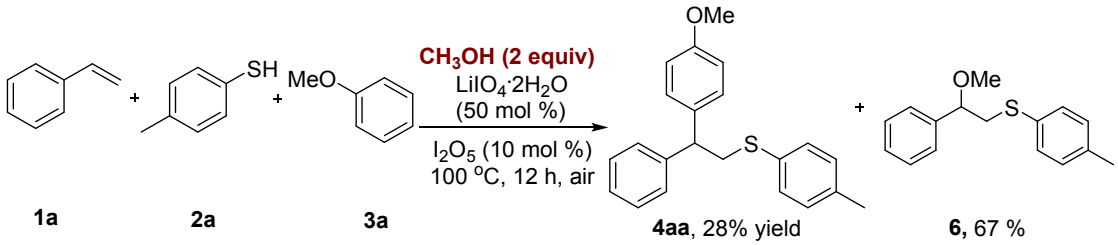

Under air atmosphere, **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), $LiIO_4$ $2H_2O$ (58.5 mg, 0.25 mmol, 50 mol %), $I_2O_5$ (16.7 mg, 0.05 mmol, 10 mol %), 1,1-diphenylethylene (180 mg, 1.0 mmol, 2 equiv) and anisole **3a** (2.0 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the reaction mixture was detected by GC using 1,3,5-trimethoxybenzene as the internal standard, giving 33% yield of product **4aa**.

Above results suggest that radical process might be involved into the reation.



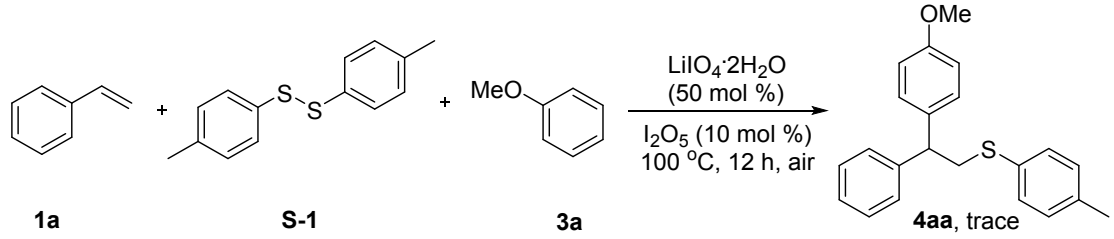




**(2) Cation trap experiment**

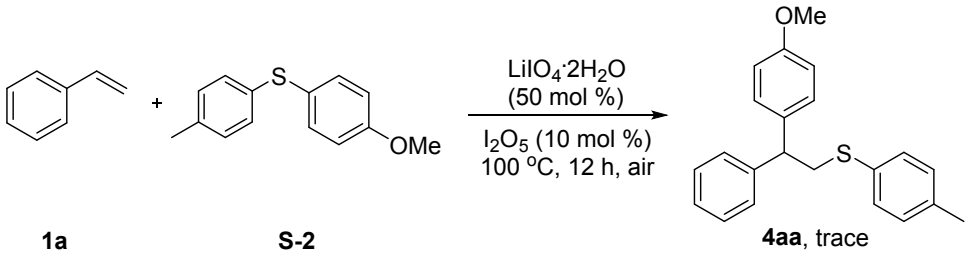



Under air atmosphere, **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), $LiIO_4$ $2H_2O$ (58.5 mg, 0.25 mmol, 50 mol %), $I_2O_5$ (16.7 mg, 0.05 mmol, 10 mol %), $CH_3OH$ (40.5 μL, 1.0 mmol, 2 equiv) and anisole **3a** (2.0 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the reaction mixture was detected by $^1H$ NMR using 1,3,5-trimethoxybenzene as the internal standard, giving 28% yield of product **4aa** and 67% yield of **6**, respectively. The result suggests that cation species might be involved into the reation.

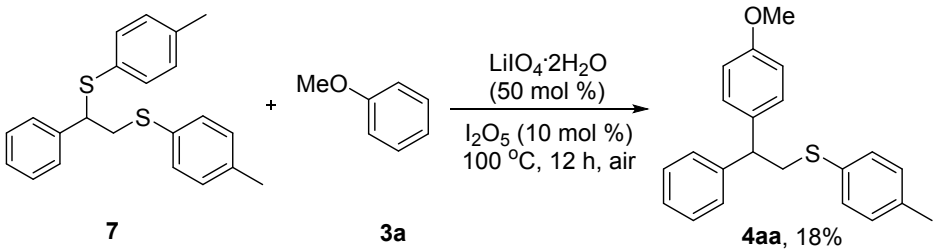
**(3) Possible intermediates:**



Under air atmosphere, **1a** (0.75 mmol, 1.5 equiv), **S-1** (0.25 mmol, 1 equiv), $LiIO_4$ $2H_2O$ (58.5 mg, 0.25 mmol, 50 mol %), $I_2O_5$ (16.7 mg, 0.05 mmol, 10 mol %) and anisole **3a** (2.0 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the reaction mixture was detected by GC using 1,3,5-trimethoxybenzene as the internal standard, giving trace amount of product **4aa**.

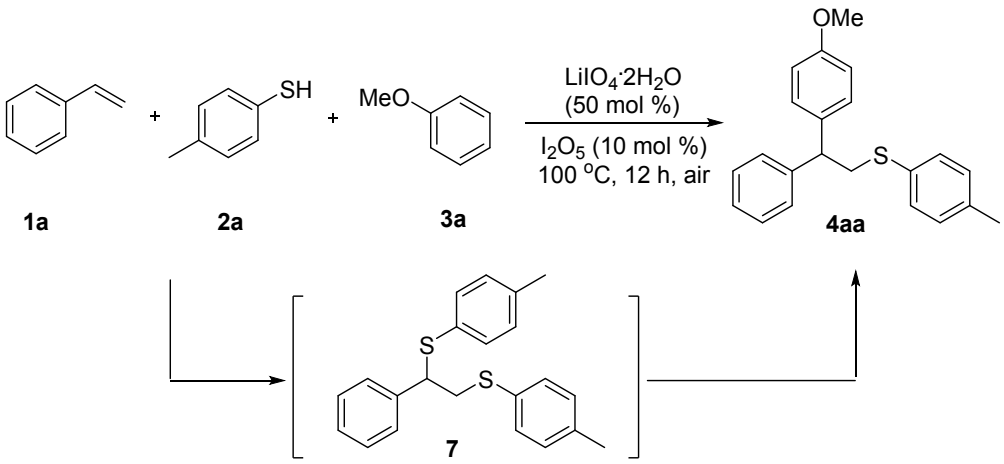



Under air atmosphere, **1a** (0.75 mmol, 1.5 equiv), **S-2** (0.5 mmol, 1 equiv), $LiIO_4$ $2H_2O$ (58.5 mg, 0.25 mmol, 50 mol %), $I_2O_5$ (16.7 mg, 0.05 mmol, 10 mol %) and **3a** (2.0 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the reaction mixture was detected by GC using 1,3,5-trimethoxybenzene as the internal standard, giving trace amount of product **4aa**.




Under air atmosphere, **7** (0.5 mmol, 1 equiv), **3a** (15 mmol, 30 equiv), $LiIO_4 \cdot 2H_2O$ (0.25 mmol, 50 mol %) and $I_2O_5$ (0.05 mmol, 10 mol %) were added into the reaction tube, and the mixture was stirred at 100 °C for 12 hours. After cooling to room temperature, the reaction mixture was detected by GC using 1,3,5-trimethoxybenzene as the internal standard, giving 18% yield of product **4aa**.

**(4) Reation profiles：**



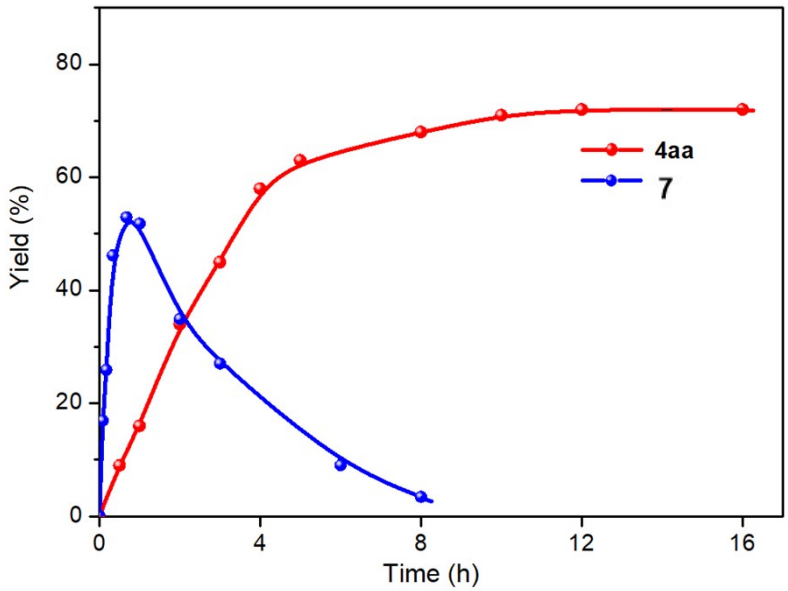




**Figure S1.** Reation profiles

Reaction profiles depicted in Figure S1 support the hypothesis of a consecutive reaction mechanism:

$$[R] \xrightarrow{k_1} [7] \xrightarrow{k_2} [4aa]$$

where R indicates the reactants (*i.e.* **1a**, **2a** and **3a**), and which can be solved analytically:

$$[7] = \frac{k_1}{k_2 - k_1}[R]_0(e^{-k_1 t} - e^{-k_2 t})$$

$$[4aa] = [R]_0\left[1 - \frac{1}{k_2 - k_1}\left(k_2 e^{-k_1 t} - k_1 e^{-k_2 t}\right)\right] \cong [R]_0\left[1 - e^{-k_2 t}\right]$$

The time where the intermediate's concentration is max is:

$$\tilde{t} = \frac{ln(\frac{k_1}{k_2})}{k_1 - k_2}$$

From the profile of concentration of the product **4aa**, the values of $[R]_0$ and of the kinetic constant $k_2$ (the rate determining step) can be readily determined upon non-linear least-square regression, *viz.* $[R]_0$ = (73.4 ± 1.4) % and $k_2$ = (19.8 ± 1.2) $min^{-1}$ (Adj-$R^2$ = 0.99108; Figure S2).

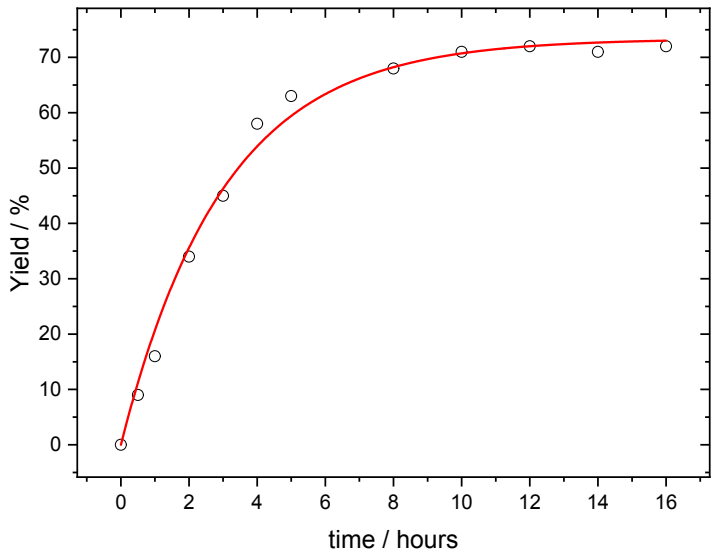



**Figure S2.** Product formation profile (circles) and fitting model (solid line).

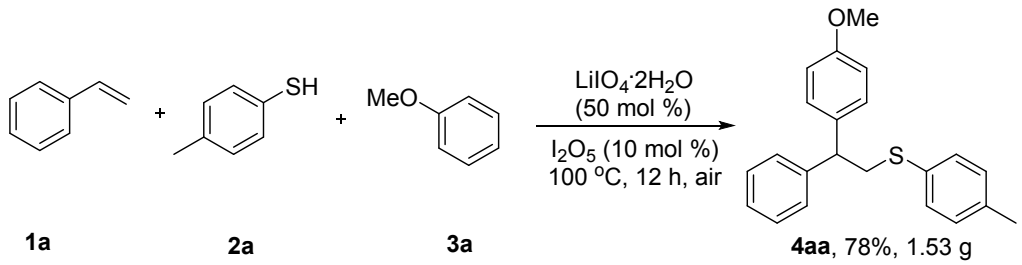
**Procedure for reaction profiles:**

Under air atmosphere, **1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), $LiIO_4 \cdot 2H_2O$ (0.25 mmol, 50 mol %), $I_2O_5$ (0.05 mmol, 10 mol %) and **3a** (2.0 mL)

were added into the reaction tube, and the mixture was stirred at 100 °C for 0~16 hours. After cooling to room temperature and then analyzed by GC (the yield of product **4aa** and intermediate **7** was determined by GC using 1,3,5-trimethoxybenzene as the internal standard).

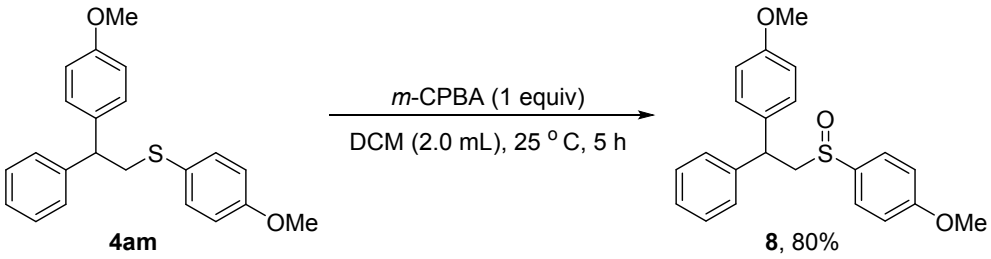
## 5. Synthetic applications

### (1) Gram scale experiment



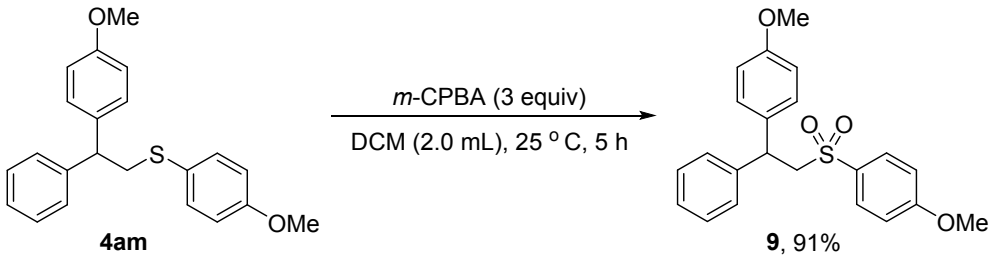

Under air atmosphere, **1a** (1.0 mL, 9 mmol, 1.5 equiv), **2a** (745 mg, 6 mmol, 1 equiv), $I_2O_5$ (200 mg, 0.6 mmol, 10 mol %), $LiIO_4 \cdot 2H_2O$ (702 mg, 3 mmol, 50 mol %) and **3a** (24 mL) were added into the reaction tube, and the mixture was stirred at 100 °C for 24 hours. After cooling to room temperature, the solvent was removed under reduced. Then the reaction mixture was purified by flash column chromatography on silica gel to give the desired product **4aa** in 78% yield (1.53 g).

### (2) Synthesis of sulfoxide



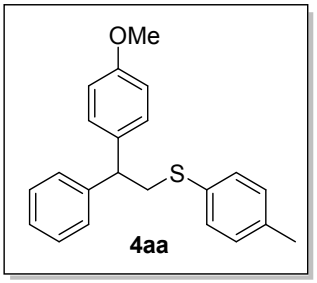

Under air atmosphere, **4am** (175 mg, 0.5 mmol, 1 equiv) and DCM (2.0 mL) were added into the reaction tube, *m*-CPBA (86.0 mg, 0.5 mmol, 1 equiv) was added under stirring at -15 °C. The mixture was stirred at 25 °C for 5 hours, then the reaction was quenched by 10 mL of NaOH saturated solution. The aqueous phase extracted with NaOH saturated solution (2×10 mL) and combined organic phases dried with $Na_2SO_4$. The solvent was removed under reduced pressure, then the reaction mixture was purified by flash column chromatography on silica gel and eluted with ethyl acetate/ petroleum ether (1/5~1/1) to give sulfoxide **8** (146 mg, 80% yield, a white solid).

### (3) Synthesis of sulfone

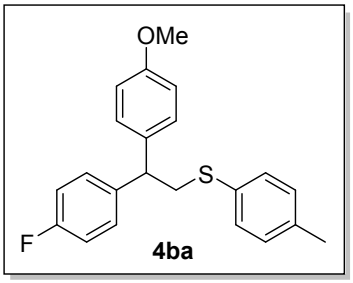



Under air atmosphere, **4am** (175.0 mg, 0.5 mmol, 1 equiv) and DCM (2.0 mL) were added into the reaction tube, *m*-CPBA (258 mg, 1.5 mmol, 3 equiv) was added under stirring at -4 °C. The mixture was stirred at 25 °C for 5 hours, then the reaction was quenched by 10 mL of NaOH saturated solution. The aqueous phase extracted with NaOH saturated solution (2×10 mL) and combined organic phases dried with $Na_2SO_4$. The solvent was removed under reduced pressure, then the reaction mixture was purified by flash column chromatography on silica gel and eluted with ethyl acetate/ petroleum ether (1/10~2/1) to give sulfone **9** (174 mg, 91% yield, a white solid).

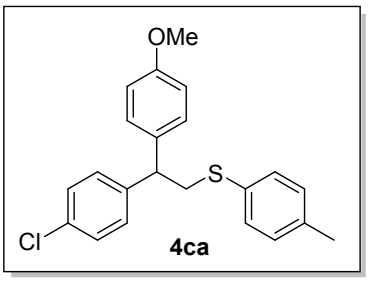
## 6. Experimental characterization data for products



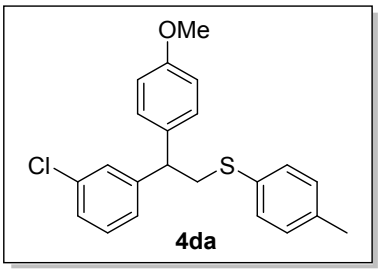

**(2-(4-Methoxyphenyl)-2-phenylethyl)(*p*-tolyl)sulfane (4aa):** A yellow oil, 125 mg, 75% yield. $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.20 (t, $J$ = 7.6 Hz, 2H), 7.15-7.11 (m, 5H), 7.06 (d, $J$ = 8.5 Hz, 2H), 7.00 (d, $J$ = 7.9 Hz, 2H), 6.75 (d, $J$ = 8.6 Hz, 2H), 4.05 (t, $J$ = 7.9 Hz, 1H), 3.68 (s, 3H), 3.44 (d, $J$ = 7.9 Hz, 2H), 2.23 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 143.6, 136.3, 135.3, 132.8, 130.3, 129.8, 129.0, 128.6, 127.9, 126.6, 113.9, 55.3, 49.8, 40.6, 21.1; HRMS (ESI) calcd for $C_{22}H_{23}OS$ [M+H]: 335.1464, found: 335.1455.



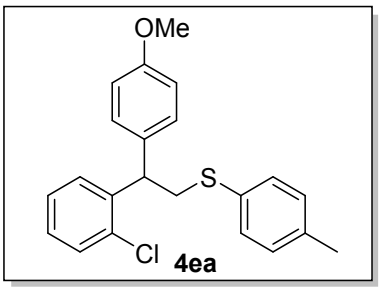

**(2-(4-Fluorophenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4ba):** A yellow oil, 146 mg, 83% yield. $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.23-7.20 (m, 2H), 7.17-7.13 (m, 2H), 7.12-7.08 (m, 4H), 6.98-6.94 (m, 2H), 6.85-6.81 (m, 2H), 4.10 (t, $J$ = 7.9 Hz, 1H), 3.76 (s, 3H), 3.53-3.43 (m, 2H), 2.32 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.6 (d, $J$ = 243.3 Hz), 158.4, 139.2 (d, $J$ = 3.3 Hz), 136.4, 135.2, 132.5, 130.4, 129.8, 129.4 (d, $J$ = 7.8 Hz), 128.8, 115.4 (d, $J$ = 21.1 Hz), 114.0, 55.3, 49.0, 40.8, 21.1, $^{19}$F NMR (376 MHz, $CDCl_3$) $\delta$ -116.4; HRMS (ESI) calcd for $C_{22}H_{22}FOS$ [M+H]: 353.1370, found: 353.1363.




**(2-(4-Chlorophenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4ca):** A yellow oil, 138 mg, 75% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.13-7.09 (m, 4H), 7.02-6.96 (m, 6H), 6.71 (d, $J$ = 8.5 Hz, 2H), 3.98 (t, $J$ = 7.9 Hz, 1H), 3.62 (s, 3H), 3.41-3.31 (m, 2H), 2.19 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 142.0, 136.5, 134.9, 132.5, 132.4, 130.5, 129.9, 129.4, 128.9, 128.7, 114.1, 55.3, 49.2, 40.5, 21.2; HRMS (ESI) calcd for $C_{22}H_{21}ClNaOS$ [M+Na]: 391.0894, found: 391.0887.

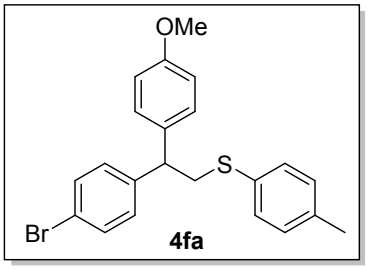



**(2-(3-Chlorophenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4da):** A yellow oil, 65.5 mg, 36% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.20-7.17 (m, 3H), 7.12 (d, $J$ = 5.3 Hz, 2H), 7.08-7.03 (m, 5H), 6.79 (d, $J$ = 8.3 Hz, 2H), 4.06 (t, $J$ = 7.9 Hz, 1H), 3.68 (s, 3H), 3.44 (d, $J$ = 8.0 Hz, 2H), 2.26 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.6, 145.8, 136.6, 134.6, 134.4, 132.6, 130.6, 130.0, 129.9, 129.0, 128.2, 126.9, 126.3, 114.2, 55.3, 49.7, 40.5, 21.2; HRMS (ESI) calcd for $C_{22}H_{21}ClNaOS$ [M+Na]: 391.0894, found: 391.0897.

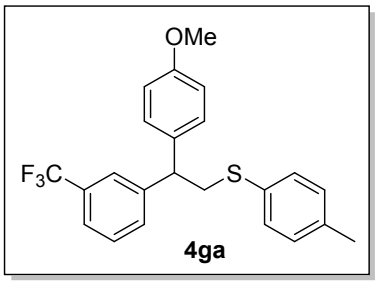



**(2-(2-Chlorophenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4ea):** A yellow oil, 117 mg, 62% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.29-7.20 (m, 4H), 7.16-7.11 (m,

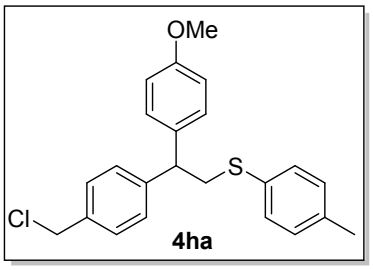
3H), 7.07-7.02 (m, 3H), 6.78 (d, $J$ = 8.0 Hz, 2H), 4.68 (t, $J$ = 6.2 Hz, 1H), 3.66 (s, 3H), 3.52-3.39 (m, 2H), 2.25 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 140.9, 136.6, 134.4, 133.9, 132.7, 130.9, 130.0, 129.9, 129.5, 128.8, 128.0, 127.1, 114.1, 55.3, 46.0, 40.1, 21.3; HRMS (ESI) calcd for $C_{22}H_{21}ClNaOS$ [M+Na]: 391.0894, found: 391.0894.



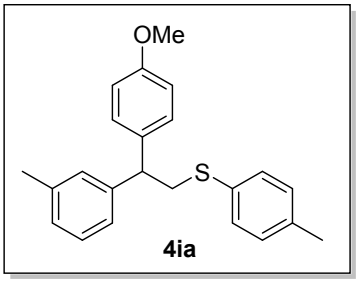

**(2-(4-Bromophenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4fa):** A yellow oil, 143 mg, 69% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34 (d, $J$ = 8.0 Hz, 2H), 7.18 (d, $J$ = 7.8 Hz, 2H), 7.04 (q, $J$ = 7.6 Hz, 2H), 6.79 (d, $J$ = 8.3 Hz, 2H), 4.05 (t, $J$ = 7.8 Hz, 1H), 3.69 (s, 3H), 3.48-3.39 (m, 2H), 2.27 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 142.7, 136.5, 134.9, 132.6, 131.7, 130.5, 130.0, 129.9, 129.0, 120.6, 114.2, 55.3, 49.4, 40.5, 21.2; HRMS (ESI) calcd for $C_{22}H_{21}BrNaOS$ [M+Na]: 435.0389, found: 435.0391.



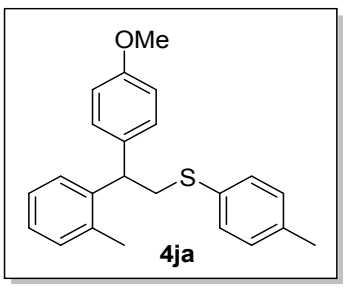

**(2-(4-Methoxyphenyl)-2-(3-(trifluoromethyl)phenyl)ethyl)(*p*-tolyl)sulfane (4ga):** A yellow oil, 48.1 mg, 24% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.46-7.38 (m, 4H), 7.21 (d, $J$ = 8.0 Hz, 2H), 7.04 (dd, $J_1$ = 8.6 Hz, $J_2$ = 12.3 Hz, 4H), 6.84 (d, $J$ = 8.7 Hz, 2H), 4.16 (t, $J$ = 7.8 Hz, 1H), 3.77 (s, 3H), 3.56-3.46 (m, 2H), 2.32 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 144.4, 136.7, 134.4, 132.1, 131.3, 130.9, 130.7, 130.6, 129.8, 129.7, 129.0, 128.9, 124.1 (dd, $J_1$ = 75.9 Hz, $J_2$ = 197.9 Hz), 55.3, 49.7, 40.5, 21.1. $^{19}$F NMR (376 MHz, $CDCl_3$) $\delta$ -62.3; HRMS (ESI) calcd for $C_{23}H_{22}F_3OS$ [M+H]: 403.1338, found: 403.1330.




**(2-(4-(Chloromethyl)phenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4ha):** A yellow oil, 39.1 mg, 20% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30-7.07 (m, 10H), 6.82 (d, $J$ = 8.2 Hz, 2H), 4.53 (s, 2H), 4.12 (t, $J$ = 7.9 Hz, 1H), 3.75 (s, 3H), 3.49 (d, $J$ = 7.8 Hz, 2H), 2.31 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.4, 143.9, 136.4, 135.7, 135.0, 132.6, 130.4, 129.8, 128.9, 128.9, 128.3, 114.0, 55.3, 49.5, 46.1, 40.5, 21.1; HRMS (ESI) calcd for $C_{23}H_{23}ClNaOS$ [M+Na]: 405.1050, found: 405.1038.

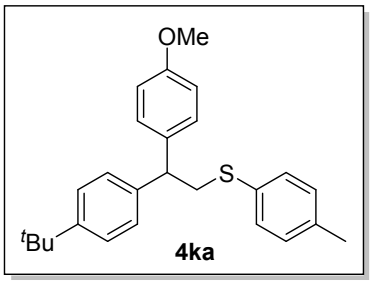



**(2-(4-Methoxyphenyl)-2-(*m*-tolyl)ethyl)(*p*-tolyl)sulfane (4ia):** A yellow oil, 128 mg, 74% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.22 (d, $J$ = 8.2 Hz, 2H), 7.17-7.13 (m, 3H), 7.07 (d, $J$ = 7.9 Hz, 2H), 7.03-6.99 (m, 3H), 6.82 (d, $J$ = 8.7 Hz, 2H), 4.09 (t, $J$ = 7.9 Hz, 1H), 3.75 (s, 3H), 3.54-3.48 (m, 2H), 2.30 (d, $J$ = 5.5 Hz, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 143.5, 138.1, 136.2, 135.4, 132.9, 130.2, 129.7, 129.0, 128.7, 128.5, 127.4, 124.8, 113.9, 55.3, 49.8, 40.6, 21.6, 21.1; HRMS (ESI) calcd for $C_{23}H_{25}OS$ [M+H]: 349.1621, found: 349.1621.

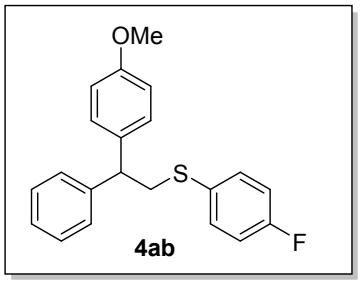



**(2-(4-Methoxyphenyl)-2-(*o*-tolyl)ethyl)(*p*-tolyl)sulfane (4ja):** A yellow oil, 147 mg, 84% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30 (d, $J$ = 7.6 Hz, 1H), 7.20 (t, $J$ = 8.0 Hz,

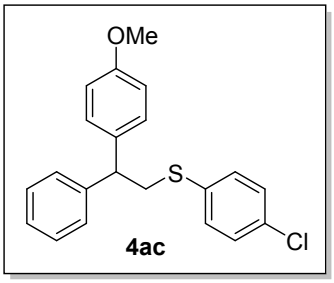
3H), 7.14-7.06 (m, 6H), 6.79 (d, $J$ = 8.6 Hz, 2H), 4.30 (t, $J$ = 7.8 Hz, 1H), 3.73 (s, 3H), 3.53-3.42 (m, 2H), 2.30 (s, 3H), 2.14 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.2, 141.2, 136.4, 136.3, 134.9, 132.9, 130.7, 130.4, 129.8, 129.3, 126.6, 126.6, 126.1, 113.9, 55.3, 45.5, 40.8, 21.1, 19.8; HRMS (ESI) calcd for $C_{23}H_{25}OS$ [M+H]: 349.1621, found: 349.1618.



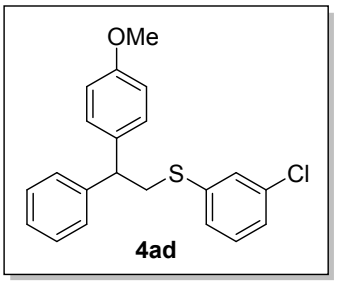

**(2-(4-(*tert*-Butyl)phenyl)-2-(4-methoxyphenyl)ethyl)(*p*-tolyl)sulfane (4ka):** A yellow oil, 147 mg, 75% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.28 (d, $J$ = 8.4 Hz, 2H), 7.21 (d, $J$ = 7.8 Hz, 2H), 7.16-7.12 (m, 4H), 7.06 (d, $J$ = 7.8 Hz, 2H), 6.82 (d, $J$ = 8.7 Hz, 2H), 4.11 (t, $J$ = 7.8 Hz, 1H), 3.74 (s, 3H), 3.56-3.46 (m, 2H), 2.29 (s, 3H),1.27 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 149.3, 140.6, 136.1, 135.4, 133.0, 130.2, 129.7, 129.0, 127.4, 125.5, 113.9, 55.3, 49.5, 40.7, 34.5, 31.5, 21.1; HRMS (ESI) calcd for $C_{26}H_{31}OS$ [M+H]: 391.2090, found: 391.2081.



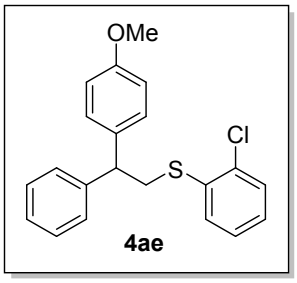

**(4-Fluorophenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ab):** A yellow oil, 109 mg, 64% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30-7.26 (m, 4H), 7.19 (d, $J$ = 6.8 Hz, 3H), 7.13 (d, $J$ = 8.7 Hz, 2H), 6.95 (t, $J$ = 8.6 Hz, 2H), 6.82 (d, $J$ = 8.7 Hz, 2H), 4.10 (t, $J$ = 7.9 Hz, 1H), 3.75 (s, 3H), 3.50 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.8 (d, $J$ = 244.9 Hz), 158.4, 143.4, 135.0, 132.6 (d, $J$ = 7.8 Hz), 131.4 (d, $J$ = 3.3 Hz), 128.9, 128.6, 127.9, 126.7, 116.1 (d, $J$ = 21.9 Hz), 114.0, 55.3, 49.9, 41.3, $^{19}$F NMR (376 MHz, $CDCl_3$) $\delta$ -115.4; HRMS (ESI) calcd for $C_{21}H_{19}FNaOS$ [M+Na]: 361.1033, found: 361.1021.




**(4-Chlorophenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ac):** A yellow oil, 108 mg, 61% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30-7.26 (m, 2H), 7.21-7.17 (m, 7H), 7.13 (d, $J$ = 8.2 Hz, 2H), 6.82 (d, $J$ = 8.6 Hz, 2H), 4.12 (t, $J$ = 7.9 Hz, 1H), 3.75 (s, 3H), 3.52 (d, $J$ = 8.0 Hz, 2H), $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.4, 143.3, 135.2, 134.9, 132.0, 130.8, 129.1, 128.9, 128.7, 127.8, 126.8, 114.0, 55.3, 49.8, 40.2; HRMS (ESI) calcd for $C_{21}H_{19}ClNaOS$ [M+Na]: 377.0737, found: 377.0732.

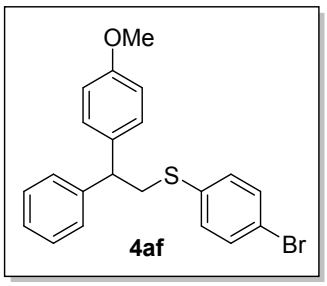



**(3-Chlorophenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ad):** A yellow oil, 98.3 mg, 56% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.26-7.15 (m, 6H), 7.14-7.05 (m, 5H), 6.81-6.77 (m, 2H), 4.13 (t, $J$ = 7.9 Hz, 1H), 3.67 (s, 3H), 3.50 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.6, 143.4, 139.3, 135.0, 134.8, 130.1, 129.1, 128.8, 128.5, 128.0, 127.0, 127.0, 126.1, 114.2, 53.3, 49.9, 39.6; HRMS (ESI) calcd for $C_{21}H_{19}ClNaOS$ [M+Na]: 377.0737, found: 377.0739.

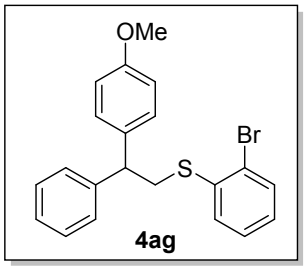



**(2-Chlorophenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ae):** A yellow oil, 57.3 mg, 32% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.32-7.21 (m, 6H), 7.19-7.11 (m, 4H), 7.06-7.02 (m, 1H), 6.83-6.79 (m, 2H), 4.20 (t, $J$ = 7.9 Hz, 1H), 3.71 (s, 3H), 3.53

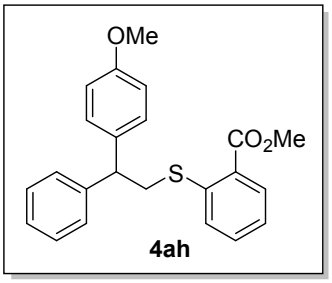
(d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 143.4, 136.1, 135.0, 134.0, 129.8, 129.2, 129.0, 128.7, 127.9, 127.2, 126.8, 126.8, 114.1, 55.3, 49.7, 38.9; HRMS (ESI) calcd for $C_{21}H_{19}ClNaOS$ [M+Na]: 377.0737, found: 377.0737.



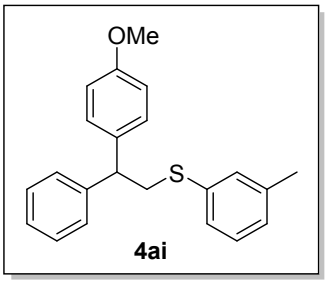

**(4-Bromophenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4af):** A yellow oil, 122 mg, 61% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.31 (d, $J$ = 8.4 Hz, 2H), 7.26-7.22 (m, 2H), 7.19-7.14 (m, 3H), 7.09 (t, $J$ = 8.8 Hz, 4H), 6.79 (d, $J$ = 8.5 Hz, 2H), 4.11 (t, $J$ = 7.8 Hz, 1H), 3.69 (s, 3H), 3.49 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 143.2, 135.9, 134.8, 131.9, 130.7, 128.9, 128.6, 127.8, 126.7, 119.7, 114.0, 55.2, 49.7, 39.8; HRMS (ESI) calcd for $C_{21}H_{19}BrNaOS$ [M+Na]: 421.0232, found: 421.0223.



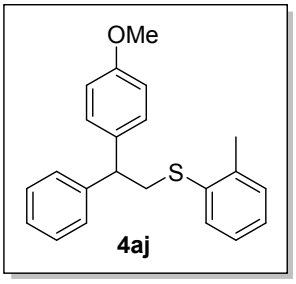

**(2-Bromophenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ag):** A yellow oil, 39.4 mg, 29% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.49 (dd, $J_1$ = 1.3 Hz, $J_2$ = 8.0 Hz, 1H), 7.30-7.14 (m, 9H), 6.99-6.95 (m, 1H), 6.82 (d, $J$= 8.7 Hz, 2H), 4.22 (t, $J$ = 7.8 Hz, 1H), 3.73 (s, 3H), 3.54 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 143.4, 138.2, 135.0, 133.1, 129.0, 128.9, 128.7, 127.9, 127.8, 126.9, 126.8, 124.2, 114.1, 55.3, 49.6, 39.3; HRMS (ESI) calcd for $C_{21}H_{19}BrNaOS$ [M+Na]: 421.0232, found: 421.0226.




**Methyl 2-((2-(4-methoxyphenyl)-2-phenylethyl)thio)benzoate (4ah):** A yellow solid, 113 mg, 60% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.92 (d, $J$ = 7.7 Hz, 1H), 7.42-7.34 (m, 2H), 7.31-7.25 (m, 4H), 7.22-7.18 (m, 3H), 7.13 (t, $J$ = 7.6 Hz, 1H), 6.83 (d, $J$ = 8.6 Hz, 2H), 4.27 (t, $J$ = 7.7 Hz, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 3.55 (d, $J$ = 7.7 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 166.9, 158.4, 143.6, 141.7, 135.2, 132.3, 131.2, 128.9, 128.7, 128.2, 127.8, 126.7, 126.2, 124.1, 114.0, 55.3, 52.1, 49.2, 38.6; HRMS (ESI) calcd for $C_{23}H_{23}O_3S$ [M+H]: 379.1362, found: 379.1361.

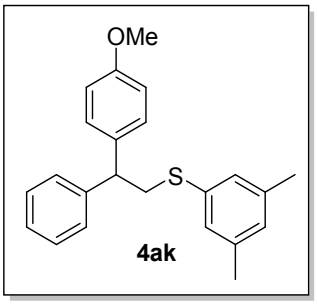



**(2-(4-Methoxyphenyl)-2-phenylethyl)(*m*-tolyl)sulfane (4ai):** A yellow oil, 131 mg, 78% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.29-7.24 (m, 2H), 7.22-7.17 (m, 3H), 7.16-7.08 (m, 5H), 6.97-6.94 (m, 1H), 6.83-6.79 (m, 2H), 4.15 (t, $J$ = 7.9 Hz, 1H), 3.72 (s, 3H), 3.54 (d, $J$ = 8.0 Hz, 2H), 2.29 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.4, 143.6, 138.8, 136.6, 135.3, 130.1, 129.0, 128.9, 128.7, 128.0, 127.0, 126.7, 126.4, 114.0, 55.3, 49.9, 39.9, 21.5; HRMS (ESI) calcd for $C_{22}H_{23}OS$ [M+H]: 335.1464, found: 335.1463.

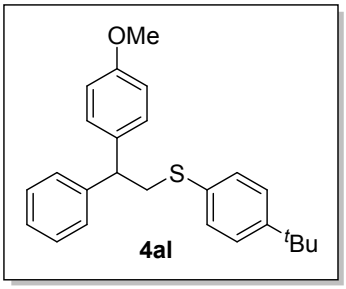



**(2-(4-Methoxyphenyl)-2-phenylethyl)(*o*-tolyl)sulfane (4aj):** A yellow oil, 117 mg,

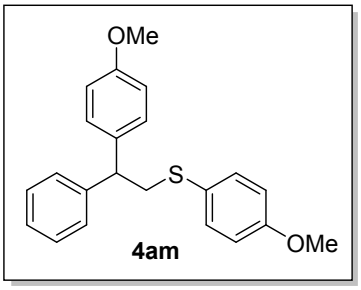
70% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.26-7.16 (m, 5H), 7.15-7.06 (m, 5H), 7.04-6.99 (m, 1H), 6.77 (d, $J$ = 8.6 Hz, 2H), 4.14 (t, $J$ = 7.8 Hz, 1H), 3.63 (s, 3H), 3.47 (d, $J$ = 8.0 Hz, 2H), 2.23 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.6, 143.9, 138.1, 136.3, 135.5, 130.4, 129.2, 128.8, 128.6, 128.1, 126.7, 126.7, 126.1, 114.2, 55.4, 50.0, 39.4, 20.7; HRMS (ESI) calcd for $C_{22}H_{22}NaOS$ [M+Na]: 357.1284, found: 357.1280.



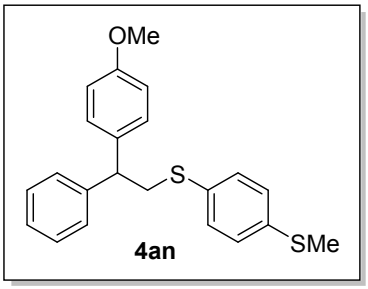

**(3,5-Dimethylphenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ak):** A yellow solid, 108 mg, 62% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.24-7.17 (m, 4H), 7.15-7.09 (m, 3H), 6.90 (s, 2H), 6.76 (t, $J$ = 8.6 Hz, 3H), 4.15 (t, $J$ = 7.8 Hz, 1H), 3.64 (s, 3H), 3.51 (d, $J$ = 7.8 Hz, 2H), 2.20 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 143.9, 143.9, 138.7, 136.6, 136.6, 135.5, 129.2, 128.8, 128.1, 127.2, 126.8, 114.2, 55.3, 50.2, 50.2, 40.0, 21.5; HRMS (ESI) calcd for $C_{23}H_{25}OS$ [M+H]: 349.1621, found: 349.1623.



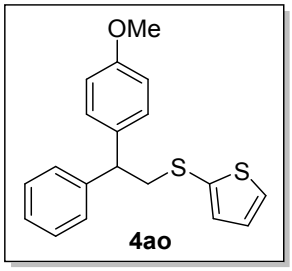

**(4-(*tert*-Butyl)phenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4al):** A yellow oil, 115 mg, 61% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.28-7.11 (m, 10H), 6.79 (d, $J$ = 8.6 Hz, 2H), 4.15 (t, $J$ = 7.8 Hz, 1H), 3.68 (s, 3H), 3.51 (d, $J$ = 7.7 Hz, 2H), 1.27 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.5, 149.4, 143.8, 135.4, 133.3, 129.8, 129.1, 128.7, 128.1, 126.8, 126.2, 114.1, 55.3, 50.1, 40.5, 34.6, 31.5; HRMS (ESI) calcd for $C_{25}H_{29}OS$ [M+H]: 377.1934, found: 377.1931.




**(4-Methoxyphenyl)(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4am):** A yellow oil, 131 mg, 75% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.27 (dd, $J_1$ = 8.5 Hz, $J_2$ = 15.1 Hz, 4H), 7.18 (d, $J$ = 7.6 Hz, 3H), 7.12 (d, $J$ = 8.5 Hz, 2H), 6.81 (d, $J$ = 8.6 Hz, 4H), 4.08 (t, $J$ = 7.9 Hz, 1H), 3.74 (d, $J$ = 9.0 Hz, 6H), 3.45 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 159.0, 158.3, 143.6, 135.3, 133.4, 129.0, 128.6, 127.9, 126.6, 126.6, 114.7, 114.0, 55.4, 55.3, 49.9, 42.0; HRMS (ESI) calcd for $C_{22}H_{23}O_2S$ [M+H]: 351.1413, found: 351.1410.

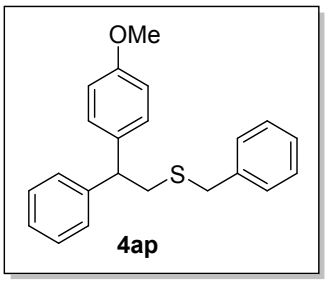



**(2-(4-Methoxyphenyl)-2-phenylethyl)(4-(methylthio)phenyl)sulfane (4an):** A yellow solid, 135 mg, 74% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.29-7.12 (m, 11H), 6.82 (d, $J$ = 8.2 Hz, 2H), 4.12 (t, $J$ = 7.9 Hz, 1H), 3.74 (s, 3H), 3.51 (d, $J$ = 7.9 Hz, 2H), 2.43 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 143.4, 136.7, 135.1, 132.9, 130.6, 128.9, 128.6, 127.9, 127.2, 126.7, 114.0, 55.3, 49.8, 40.5, 16.0; HRMS (ESI) calcd for $C_{22}H_{22}NaOS_2$ [M+Na]: 389.1004, found: 389.1006.

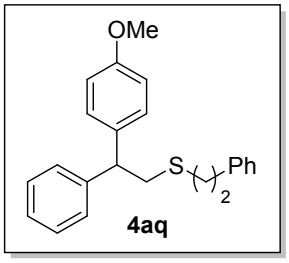



**2-((2-(4-Methoxyphenyl)-2-phenylethyl)thio)thiophene (4ao):** A yellow oil, 50.6 mg,

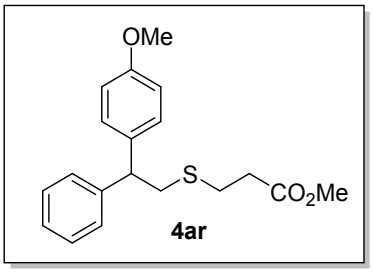
31% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.34-7.26 (m, 3H), 7.23-7.19 (m, 3H), 7.13 (d, $J$ = 8.5 Hz, 2H), 7.05-7.03 (m, 1H), 6.96-6.94 (m, 1H), 6.83 (d, $J$ = 8.6 Hz, 2H), 4.15 (t, $J$ = 7.9 Hz, 1H), 3.76 (s, 3H), 3.44 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 143.2, 134.9, 134.6, 133.6, 129.3, 129.0, 128.6, 127.9, 127.6, 126.7, 114.0, 55.3, 49.8, 44.8; HRMS (ESI) calcd for $C_{19}H_{19}OS_2$ [M+H]: 327.0872, found: 327.0868.



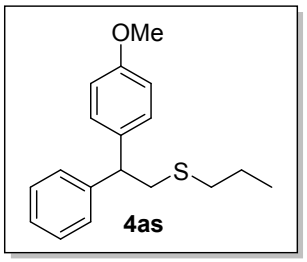

**Benzyl(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4ap):** A yellow oil, 65.4 mg, 39% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.27-7.21 (m, 7H), 7.16-7.11 (m, 3H), 7.05 (d, $J$ = 8.6 Hz, 2H), 6.77 (d, $J$ = 8.6 Hz, 2H), 4.00 (t, $J$ = 7.8 Hz, 1H), 3.66 (s, 3H), 3.57 (s, 2H), 3.02 (d, $J$ = 7.9 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.4, 144.0, 138.6, 135.6, 129.1, 129.1, 128.6, 128.6, 128.0, 127.2, 126.7, 114.0, 53.3, 50.6, 37.5, 37.2; HRMS (ESI) calcd for $C_{22}H_{23}OS$ [M+H]: 335.1464, found: 335.1460.



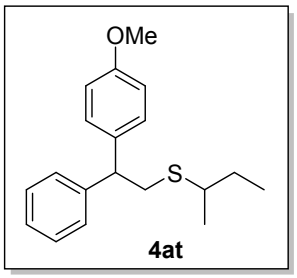

**(2-(4-Methoxyphenyl)-2-phenylethyl)(phenethyl)sulfane (4aq):** A yellow oil, 104 mg, 60% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.28-7.15 (m, 7H), 7.14-7.10 (m, 4H), 6.81 (d, $J$ = 8.6 Hz, 2H), 4.10 (t, $J$ = 7.8 Hz, 1H), 3.70 (s, 3H), 3.15 (d, $J$ = 7.8 Hz, 2H), 2.83-2.79 (m, 2H), 2.69-2.65 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.4, 144.0, 140.7, 135.7, 129.0, 128.7, 128.6, 128.6, 128.0, 126.7, 126.5, 114.1, 53.3, 50.9, 38.6, 36.5, 34.6; HRMS (ESI) calcd for $C_{23}H_{25}OS$ [M+H]: 349.1621, found: 349.1622.




**Methyl3-((2-(4-methoxyphenyl)-2-phenylethyl)thio)propanoate (4ar):** A yellow oil, 115 mg, 70% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30-7.26 (m, 2H), 7.23-7.14 (m, 5H), 6.82 (d, $J$ = 8.8 Hz, 2H), 4.12 (t, $J$ = 7.9 Hz, 1H), 3.73 (s, 3H), 3.65 (s, 2H), 3.18 (d, $J$ = 7.9 Hz, 2H), 2.72 (t, $J$ = 7.2 Hz, 2H), 2.55 (t, $J$ = 7.3 Hz, 2H);$^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 172.4, 158.3, 143.7, 135.4, 128.9, 128.6, 127.8, 126.6, 114.0, 55.2, 51.8, 50.6, 38.4, 34.7, 27.8; HRMS (ESI) calcd for $C_{19}H_{23}O_3S$ [M+H]: 331.1362, found: 331.1357.

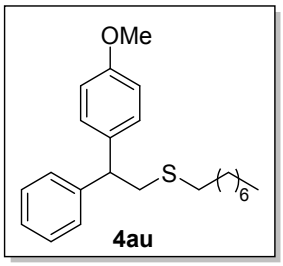



**(2-(4-Methoxyphenyl)-2-phenylethyl)(propyl)sulfane (4as):** A yellow oil, 76.4 mg, 53% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.29-7.22 (m, 4H), 7.19-7.15 (m, 3H), 6.82 (d, $J$ = 8.5Hz, 2H), 4.12 (t, $J$ = 7.9 Hz, 1H), 3.73 (s, 3H), 3.15 (d, $J$ = 7.9 Hz, 2H), 2.43 (t, $J$ = 7.2 Hz, 2H), 1.61-1.52 (m, 2H), 0.93 (t, $J$ = 7.3 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.3, 144.0, 135.7, 128.9, 128.6, 127.9, 126.6, 113.9, 55.3, 50.8, 38.3, 35.1, 23.0, 12.6; HRMS (ESI) calcd for $C_{18}H_{23}OS$ [M+H]: 287.1464, found: 287.1464.



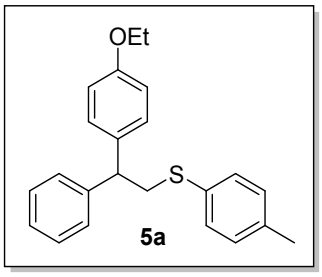

**Sec-butyl(2-(4-methoxyphenyl)-2-phenylethyl)sulfane (4at):** A yellow oil, 98.6 mg, 66% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30-7.22 (m, 4H), 7.20-7.16 (m, 3H), 6.83

(d, $J$ = 8.6 Hz, 2H), 4.12 (t, $J$ = 7.9 Hz, 1H), 3.75 (s, 3H), 3.16 (d, $J$ = 7.9 Hz, 2H), 2.62 (q, $J$ = 6.6 Hz, 1H), 1.62-1.41 (m, 2H), 1.23 (d, $J$ = 6.7 Hz, 3H), 0.92 (t, $J$ = 7.4 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.2, 144.1, 144.0, 135.8, 135.7, 128.9, 128.9, 128.5, 127.8, 127.8, 126.5, 113.9, 55.2, 51.1, 42.7, 36.4, 29.8, 20.9, 20.9, 11.5, 11.5; HRMS (ESI) calcd for $C_{19}H_{25}OS$ [M+H]: 301.1621, found: 301.1619.



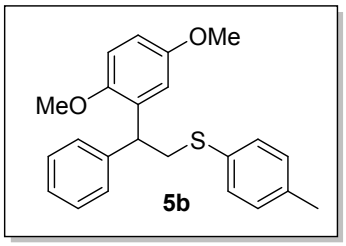
**4au**

**(2-(4-Methoxyphenyl)-2-phenylethyl)(octyl)sulfane (4au):** A yellow oil, 107 mg, 60% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.30-7.22 (m, 4H), 7.21-7.15 (m, 3H), 6.83 (d, $J$ = 8.7Hz, 2H), 4.12 (t, $J$ = 7.8 Hz, 1H), 3.75 (s, 3H), 3.16 (d, $J$ = 7.8 Hz, 2H), 2.44 (t, $J$ = 7.4 Hz, 2H), 1.58-1.50 (m, 2H), 1.34-1.25 (m, 10H), 0.88 (t, $J$ = 6.4 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 158.2, 144.0, 135.7, 128.9, 128.5, 127.8, 126.5, 113.9, 55.2, 50.8, 38.3, 33.0, 31.9, 29.7, 29.2, 29.0, 22.7, 14.2; HRMS (ESI) calcd for $C_{23}H_{33}OS$ [M+H]: 357.2247, found: 357.2240.

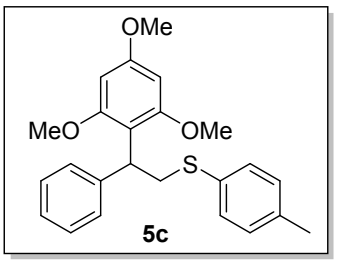


**5a**

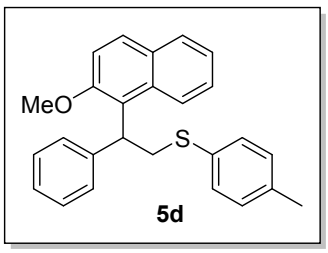
**(2-(4-Ethoxyphenyl)-2-phenylethyl)(*p*-tolyl)sulfane (5a):** A yellow oil, 146 mg, 84% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3b** (7.5 mmol, 15 equiv), fluorobenzene (1.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.27 (t, $J$ =7.5 Hz, 2H), 7.22-7.18 (m, 5H), 7.11 (d, $J$ = 8.7Hz, 2H), 7.06 (d, $J$ = 7.9 Hz, 2H), 6.80 (d, $J$ = 8.6 Hz, 2H), 4.16 (t, $J$ = 7.9 Hz, 1H), 3.96 (q, $J$ = 7.0 Hz, 2H), 3.51 (d, $J$ = 7.9 Hz, 2H), 2.30 (s, 3H), 1.36 (t, $J$ = 7.0 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.7, 143.6, 136.2, 135.1, 132.9, 130.3, 129.8, 129.0, 128.6, 128.0, 126.6, 114.5, 63.4, 49.8, 40.6, 21.1, 15.0; HRMS (ESI) calcd for $C_{23}H_{25}OS$ [M+H]: 349.1621, found: 349.1619.



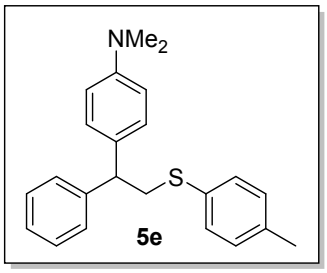

**(2-(2,5-Dimethoxyphenyl)-2-phenylethyl)(*p*-tolyl)sulfane (5b):** A yellow oil, 106 mg, 58% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3c** (7.5 mmol, 15 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$, 7.27-7.22 (m, 6H), 7.20-7.17 (m, 1H), 7.07 (d, $J$ = 7.5 Hz, 2H), 6.77-6.67 (m, 3H), 4.62 (t, $J$ = 8.1 Hz, 1H), 3.70 (d, $J$ = 4.8 Hz, 6H), 3.57 (dd, $J_1$ = 7.3 Hz, $J_2$ = 12.8 Hz, 1H), 3.44 (dd, $J_1$ = 8.6 Hz, $J_2$ = 12.8 Hz, 1H), 2.30 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 153.5, 151.4, 142.5, 136.0, 133.2, 133.0, 130.1, 129.6, 128.4, 128.4, 126.5, 115.3, 111.8, 111.2, 56.1, 55.6, 43.9, 39.1, 21.1; HRMS (ESI) calcd for $C_{23}H_{25}O_2S$ [M+H]: 365.1570, found: 365.1566.



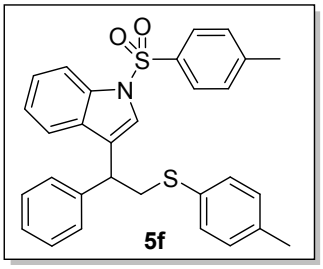

**(2-Phenyl-2-(2,4,6-trimethoxyphenyl)ethyl)(*p*-tolyl)sulfane (5c):** A yellow oil, 105 mg, 53% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3d** (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.31 (d, $J$ =7.6 Hz, 2H), 7.22-7.19 (m, 4H), 7.10 (t, $J$ = 7.3 Hz, 1H), 7.03 (d, $J$ = 7.8 Hz, 2H), 6.09 (s, 2H), 4.85 (t, $J$ = 7.8 Hz, 1H), 3.83 (dd, $J_1$ = 9.1 Hz, $J_2$ = 12.6 Hz, 1H), 3.74 (s, 3H), 3.69 (d, $J$ = 7.1 Hz, 1H), 3.67 (s, 6H), 2.27(s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.0, 159.3, 143.9, 135.6, 133.7, 130.1, 129.4, 128.0, 127.8, 125.7, 112.0, 91.2, 55.7, 55.3, 39.5, 37.7, 21.1; HRMS (ESI) calcd for $C_{24}H_{27}O_3S$ [M+H]: 395.1675, found: 395.1675.



**(2-(2-Methoxynaphthalen-1-yl)-2-phenylethyl)(*p*-tolyl)sulfane (5d):** A yellow solid, 119 mg, 62% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3e** (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.84-7.68 (m, 3H), 7.32-7.09 (m, 10H), 6.97 (d, $J$ = 7.8 Hz, 2H), 5.25 (s, 1H), 3.98-3.88 (m, 2H), 3.65 (s, 3H), 2.24 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 155.7, 143.4, 136.1, 133.3, 130.4, 129.8, 129.8, 129.4, 129.0, 128.2, 128.0, 126.6, 126.1, 124.6, 123.7, 123.4, 114.5, 56.5, 41.9, 38.1, 21.2; HRMS (ESI) calcd for $C_{26}H_{24}NaOS$ [M+Na]: 407.1440, found: 407.1433.

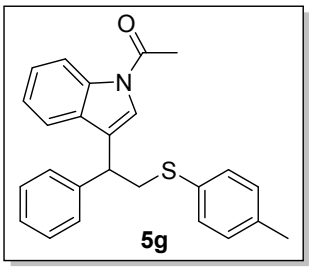



***N,N*-Dimethyl-4-(1-phenyl-2-(*p*-tolylthio)ethyl)aniline (5e):** A yellow solid, 13.8 mg, 8% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3f** (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.27-7.25 (m, 2H), 7.23-7.21 (m, 4H), 7.19-7.16 (m, 1H), 7.11-7.06 (m, 4H), 4.09 (t, $J$ = 7.9 Hz, 1H), 3.52 (d, $J$ = 7.6 Hz, 2H), 2.90 (s, 6H), 2.31 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 149.4, 143.9, 136.0, 133.1, 131.2, 130.1, 129.7, 128.6, 128.5, 127.9, 126.4, 112.7, 49.7, 10.7, 40.6, 21.1; HRMS (ESI) calcd for $C_{23}H_{26}NS$ [M+H]: 348.1780, found: 348.1775.

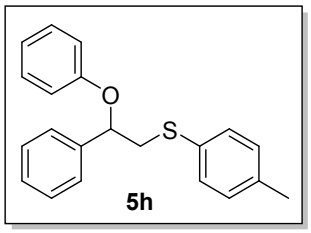



**1-(3-(1-Phenyl-2-(p-tolylthio)ethyl)-1*H*-indol-1-yl)ethan-1-one (5f):** A white solid, 19.9 mg, 8% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3e** (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL), $LiIO_4$ $2H_2O$ (50 mol %), $I_2O_5$ (10 mol %)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.85 (d, $J$ = 8.3 Hz, 1H), 7.66 (d, $J$ = 8.1 Hz, 2H), 7.45 (s, 1H), 7.18-7.09 (m, 10H), 7.05-6.94 (m, 4H), 4.09 (t, $J$ = 7.9 Hz, 1H), 3.55-3.50 (m,

1H), 3.37-3.32 (m, 1H), 2.22 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.9, 141.7, 136.8, 135.6, 135.1, 132.5, 130.7, 130.4, 129.9, 129.8, 128.7, 127.9, 127.1, 126.9, 124.8, 124.6, 123.6, 123.2, 120.0, 113.8, 42.5, 40.6, 21.6, 21.1; HRMS (ESI) calcd for $C_{30}H_{27}NNaO_2S_2$ [M+Na]: 520.1375, found: 520.1372.

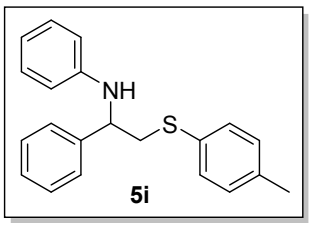



**3-(1-Phenyl-2-(p-tolylthio)ethyl)-1-tosyl-1*H*-indole (5g):** A white solid, 25.0 mg, 13% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3e** (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL), $LiIO_4$ $2H_2O$ (50 mol %), $I_2O_5$ (10 mol %)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.30 (s, 1H), 7.22-7.11 (m, 10H), 7.05-6.97 (m, 3H), 4.28 (t, $J$ = 7.5 Hz, 1H), 3.56 (dd, $J_1$ = 7.5 Hz, $J_2$ = 13.0 Hz, 1H), 3.38 (dd, $J_1$ = 7.4 Hz, $J_2$ = 13.0 Hz, 1H), 2.48 (s, 3H), 2.21 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 168.5, 141.9, 136.7, 136.1, 132.6, 130.7, 130.0, 129.9, 128.8, 128.0, 127.1, 125.4, 124.3, 123.5, 122.4, 119.5, 116.6, 42.7, 40.6, 24.1, 21.1; HRMS (ESI) calcd for $C_{25}H_{24}NOS$ [M+H]: 386.1573, found: 386.1574.

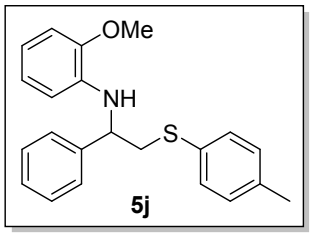



**(2-Phenoxy-2-phenylethyl)(p-tolyl)sulfane (5h):** A yellow oil, 84.8 mg, 53% yield. (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3i** (7.5 mmol, 15 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.29-7.19 (m, 7H), 7.08 (t, $J$ = 7.7 Hz, 2H), 7.01 (d, $J$ = 7.9 Hz, 2H), 6.79 (t, $J$ = 7.3 Hz, 1H), 6.71 (d, $J$ = 8.1 Hz, 2H), 5.12 (dd, $J_1$ = 4.9 Hz, $J_2$ = 8.0 Hz, 1H), 3.39 (dd, $J_1$ = 8.1 Hz, $J_2$ = 13.7 Hz, 1H), 3.16 (dd, $J_1$ = 4.9 Hz, $J_2$ = 13.7 Hz, 1H), 2.25 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.89, 140.32, 136.60, 132.37, 130.74, 129.78, 129.32, 128.70, 128.11, 126.27,

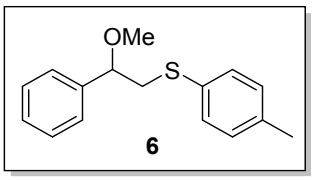
121.06, 116.09, 79.23, 42.80, 21.09; HRMS (ESI) calcd for $C_{21}H_{20}NaOS$ [M+Na]: 343.1127, found: 343.1112.



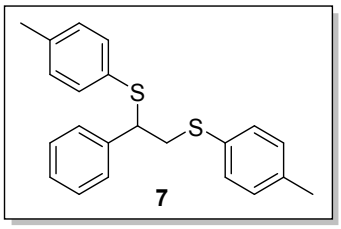

**(2-Phenoxy-2-phenylethyl)(p-tolyl)sulfane (5i):** A yellow oil, 65.3 mg, 41% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3j** (7.5 mmol, 15 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.35-7.21 (m, 7H), 7.06 (dd, $J_1$ = 7.4 Hz, $J_2$ = 14.6 Hz, 4H), 6.65 (t, $J$ = 7.3 Hz, 1H), 6.45 (d, $J$ = 8.0 Hz, 2H), 4.54 (br, 1H), 4.32 (dd, $J_1$ = 4.3 Hz, $J_2$ = 9.4 Hz, 1H), 3.32 (dd, $J_1$ = 4.4 Hz, $J_2$ = 13.6 Hz, 1H), 3.07 (dd, $J_1$ = 9.4 Hz, $J_2$ = 13.6 Hz, 1H), 2.31 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 147.35, 142.61, 137.27, 131.52, 131.14, 130.01, 129.10, 128.89, 127.58, 126.43, 117.87, 113.89, 57.31, 43.47, 21.18; HRMS (ESI) calcd for $C_{21}H_{22}NS$ [M+H]: 320.1467, found: 320.1458.



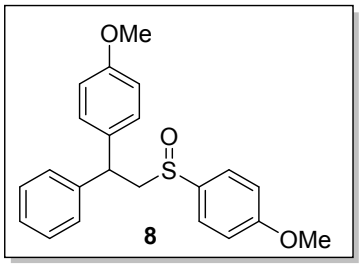

**(2-Phenoxy-2-phenylethyl)(p-tolyl)sulfane (5j):** A yellow oil, 34.9 mg, 20% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), **3k** (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.29-7.15 (m, 7H), 7.00 (d, $J$ = 7.8 Hz, 2H), 6.70-6.67 (m, 1H), 6.54 (t, $J$ = 3.9 Hz, 2H), 6.13-6.11 (m, 1H), 5.11 (br, 1H), 4.28 (dd, $J_1$ = 4.6 Hz, $J_2$ = 9.0 Hz, 1H), 3.80 (s, 3H), 3.26 (dd, $J_1$ = 4.6 Hz, $J_2$ = 13.4 Hz, 1H), 3.16 (dd, $J_1$ = 9.0 Hz, $J_2$ = 13.5 Hz, 1H), 2.24 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 147.13, 142.67, 137.12, 136.94, 131.57, 131.26, 129.86, 128.78, 127.48, 126.46, 121.01, 116.90, 111.36, 109.39, 57.27, 55.57, 43.34, 21.12; HRMS (ESI) calcd for $C_{22}H_{24}NOS$ [M+H]: 350.1573, found: 350.1567.




**2-Methoxy-2-phenylethyl-(*p*-tolyl)sulfane (6)[1]:** A yellow oil, 106 mg, 82% yield (**1a** (0.75 mmol, 1.5 equiv), **2a** (0.5 mmol, 1 equiv), methanol (0.75 mmol, 1.5 equiv), fluorobenzene (2.0 mL)). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.37-7.27 (m, 7H), 7.08 (d, $J$ = 7.9 Hz, 2H), 4.26 (dd, $J_1$ = 4.9 Hz, $J_2$ = 8.2 Hz, 1H), 3.27 (dd, $J_1$ = 8.2 Hz, $J_2$ = 13.3 Hz, 1H), 3.23 (s, 3H), 3.08 (dd, $J_1$ = 5.0 Hz, $J_2$ = 13.3 Hz, 1H), 2.31 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 140.6, 136.2, 132.7, 130.2, 129.7, 128.6, 128.1, 126.8. 82.5, 57.1, 42.3, 21.1.

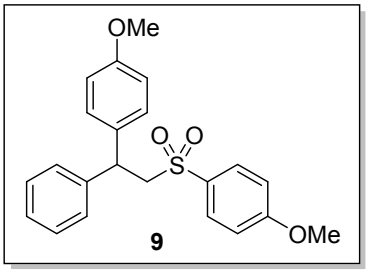



**1-Phenylethane-1,2-diyl-bis(*p*-tolylsulfane) (7)[3]:** A yellow solid, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.31-7.21 (m, 5H), 7.16 (d, $J$ = 8.0 HZ, 2H), 7.08-7.01 (m, 6H), 4.17 (dd, $J_1$ = 4.9 Hz, $J_2$ = 10.2 Hz, 1H), 4.17 (dd, $J_1$ = 4.9 Hz, $J_2$ = 10.2 Hz, 1H), 3.44 (dd, $J_1$ = 4.9 Hz, $J_2$ = 13.5 Hz, 1H), 3.29 (dd, $J_1$ = 10.2 Hz, $J_2$ = 13.6 Hz, 1H), 2.31 (d, $J$ = 2.2 HZ, 6H), $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 139.8, 137.8, 136.5, 133.4, 131.8, 130.6, 130.4, 129.7, 129.6, 128.5, 128.1, 127.7, 52.6, 40.0, 21.2, 21.1.



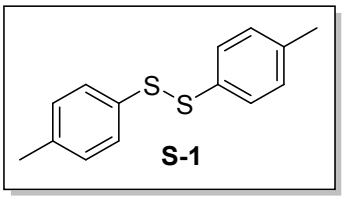

**1-Methoxy-4-((2-(4-methoxyphenyl)-2-phenylethyl)sulfinyl)benzene (8):** A white solid, 146 mg, 80% yield (dr = 50:50, which was determined by $^1$H NMR according to the crude reaction). $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.55 (d, $J$ = 8.3 Hz, 2H), 7.35-7.18 (m, 6H), 7.14 (d, $J$ = 8.3 Hz, 1H), 7.00 (d, $J$ = 8.4 Hz, 2H), 6.87 (d, $J$ = 8.2 Hz, 1H),

6.81 (d, $J$ = 8.2 Hz, 1H), 4.49-4.40 (m, 1H), 3.84 (s, 3H), 3.77 (d, $J$ = 11.6 Hz, 3H), 3.52-3.46 (m, 1H), 3.36-3.29 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 162.1, 162.1, 158.6, 158.4, 142.8, 141.9, 135.2, 135.1, 134.4, 133.5, 129.2, 128.9, 128.7, 128.7, 128.0, 127.6, 127.1, 126.8, 126.1, 126.1, 114.8, 114.1, 114.1, 64.9, 64.8, 55.6, 55.3, 44.8, 44.7; HRMS (ESI) calcd for $C_{22}H_{23}O_3S$ [M+H]: 367.1362, found: 367.1361.



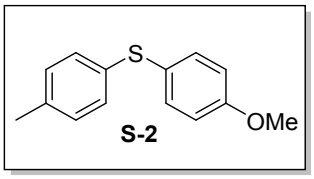
**9**

**1-Methoxy-4-((2-(4-methoxyphenyl)-2-phenylethyl)sulfonyl)benzene (9):** A white solid, 174 mg, 91% yield. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.54 (d, $J$ = 8.9 Hz, 2H), 7.21-7.17 (m, 2H), 7.14-7.10 (m, 3H), 7.02 (d, $J$ = 8.7 Hz, 2H), 6.77 (d, $J$ = 8.9 Hz, 2H), 6.71 (d, $J$ = 8.7 Hz, 2H), 4.55 (t, $J$ = 7.2 Hz, 1H), 3.85 (d, $J$ = 7.2 Hz, 2H), 3.81 (s, 3H), 3.73 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 163.3, 158.4, 141.9, 133.46, 131.2, 130.1, 128.7, 128.7. 127.5, 126.8, 114.1, 61.9, 55.6, 55.2, 45.6; HRMS (ESI) calcd for $C_{22}H_{23}O_4S$ [M+H]: 383.1312, found: 383.1305.



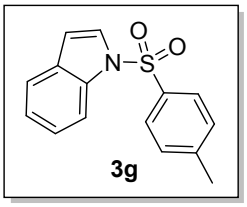
**S-1**

**1,2-di-*p*-Tolyldisulfane (S-1)[2]:** A white solid. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.37 (d, $J$ = 8.2 HZ, 4H), 7.09 (d, $J$ = 8.0 HZ, 4H), 2.30 (s, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 137.5, 133.9, 129.8, 128.6, 21.1.

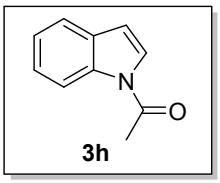


**S-2**

**4-Methoxyphenyl-(*p*-tolyl)sulfane (S-2)[2]:** A yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.38-7.34 (m, 2H), 7.13 (d, $J$ = 8.2 HZ, 2H), 7.06 (d, $J$ = 8.0 HZ, 2H), 6.88-6.84 (m, 2H), 3.80 (s, 3H), 2.29 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 159.5, 136.1, 134.4, 129.8, 129.4, 125.6, 114.9, 55.4. 21.0.

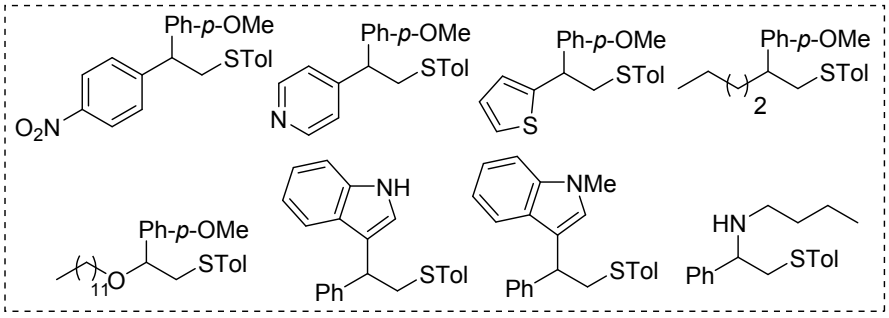



**1-Tosyl-1*H*-indole (S-2)[4]:** A colorless solid. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.05 (d, $J$ = 8.2 Hz, 1H), 7.80 (d, $J$ = 8.5 Hz, 2H), 7.61 (d, $J$ = 3.7 Hz, 1H), 7.59 (d, $J$ = 7.8 Hz, 1H), 7.35 (t, $J$ = 7.6 Hz, 1H), 7.28 (t, $J$ = 7.4 Hz, 1H), 7.23 (d, $J$ = 8.1 Hz, 2H), 6.69 (d, $J$ = 3.1 Hz, 1H), 2.33 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 145.0, 135.3, 134.9, 130.8, 129.9, 126.8, 126.4, 124.6, 123.3, 121.4, 113.6, 109.1, 21.5.




**1-(1*H*-indol-1-yl)ethan-1-one (3h)[5]:** A pale yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.51 (d, $J$ = 8.4 Hz, 1H), 7.61 (d, $J$ = 7.5 Hz, 1H), 7.41-7.30 (m, 3H), 6.63 (d, $J$ = 3.3 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 168.8, 135.6, 130.5, 125.4, 125.1, 123.7, 120. 9, 116.6, 109.1, 23.9.

The compouds were not attained under the optimal reaction conditions:



**X-ray crystal structure determination of 5d:**

Diffraction data for the complexes were collected with a Bruker SMART APEX II area detector at low temperature (100 K) with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). An empirical absorption correction using SADABS[6] was applied for all data. The structure was solved by direct methods using the SHELXS program. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on $F^2$ by the use of the program SHELXL[7]. Crystallographic data for the complexes are summarized in Table S6. CCDC 2076131 contain the supplementary crystallographic data for the structures reported in this paper. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

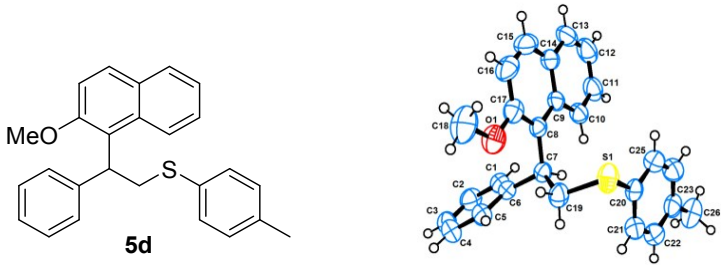



**Figure S3.** The X-ray Diffraction Configuration of **5d**. Thermal ellipsoids are set at 50% probability. Crystal of compound **5d** was grown by slow evaporation of its solution with petroleum ether/ethyl acetate under -20 °C.

**Table S6. Crystallographic data for compound 5d**.

| | |
|---|---|
| compound | **5d** |
| formula | $C_{26}H_{24}OS$ |
| *F*w | 384.51 |
| crystal system | orthorhombic |
| space group | *P*2(1)/*c* |
| *a* /Å | 7.6661(19) |
| *b* /Å | 13.863(3) |
| *c* /Å | 19.578(5) |
| *α* /° | 90 |

| | |
|---|---|
| $\beta$ /° | 90 |
| $\gamma$ /° | 90 |
| $V$ /Å$^3$ | 2080.7(9) |
| $Z$ | 4 |
| $D_{calc}$ /g cm$^{-3}$ | 1.227 |
| $F$(000) | 816 |
| $\mu$ /mm$^{-1}$ | 0.169 |
| $\theta$ range /° | 1.800~28.965 |
| reflns collected ($R_{int}$) | 17187 (17187) |
| independent reflns | 5153 |
| observed reflns [$I > 2\sigma(I)$] | 3389 |
| $R_1$; $wR_2$ [$I > 2\sigma(I)$] | 0.0442, 0.0998 |
| $R_1$; w$R_2$ (all data) | 0.0802, 0.1155 |
| GOF ($F^2$) | 1.000 |

## 7. Computational details and results

The molecular geometry of each system in solution was fully optimised and harmonic frequencies were subsequently computed along with the thermochemical quantities at $T$ = 298.15 K and $p$ = 1.00 atm. No imaginary frequencies were found for minima and one negative frequency was found for transition states. The calculations were performed at the Density Functional Theory (DFT) level, by using M06-2X[8] hybrid functional coupled with the triple-ζ 6-311++G** basis set for all the elements, except for Iodine, for which the DGDZVP basis set was adopted. The differences in thermochemicals describing the possible reactions were calculated (Table S7).

Solvent effects were taken into account via the implicit polarizable continuum model in its integral equation formalism (IEF−PCM)[9]. Truhlar and coworkers' SMD solvation model[10] was used to build up the cavity and compute the non-electrostatic terms. The solvent used was anisole, and its standard values for dielectric constant and refractive index were always assumed.

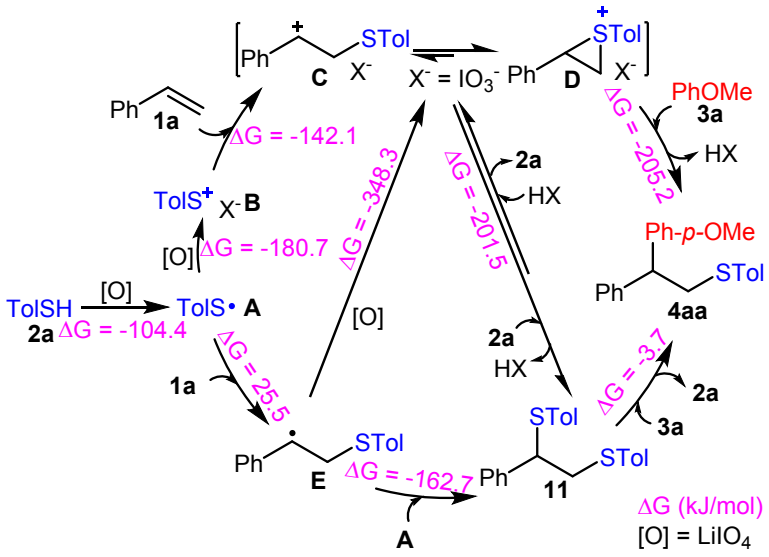
The full Natural Bond Orbital (NBO) analysis[11] of the total density was systematically performed at the same level of theory. Natural Atomic Charges were also computed.

For all calculations integration grid for the electronic density was set to 250 radial shells and 974 angular points all the atomic species. Accuracy for the two-electron integrals and their derivatives was set to $10^{-14}$ a.u. The Self-Consistent Field (SCF) algorithm used was the quadratically convergent procedure designed by Bacskay[12], a method which is acknowledged to be slower but more reliable than regular SCF with DIIS extrapolation. The convergence criteria for SCF were set to $10^{-12}$ for root mean square (RMS) change in density matrix and $10^{-10}$ for maximum change in density matrix. Convergence criteria for geometry optimizations were set to $2 \times 10^{-6}$ a.u. for maximum force, $1 \times 10^{-6}$ a.u. for RMS force, $6 \times 10^{-6}$ a.u. for maximum displacement and $4 \times 10^{-6}$ a.u. for RMS displacement.

All calculations were performed using GAUSSIAN G16.A03 package[13].

**Table S7. Differences in thermochemicals computed at $T$ = 298.15 K and $p$ = 1.00 atm, for plausible pathways.**

| Plausible pathways | Δ$H$ / (kJ/mol) | Δ$G$ / (kJ/mol) |
|---|---|---|
| $2TolSH + IO_4^- = 2TolS^\bullet + IO_3^- + H_2O$ | -168.2 | -208.8 |
| $2TolS^\bullet + IO_4^- + 2H_3O^+ = 2TolS^+ + IO_3^- + 3H_2O$ | −321.3 | −361.3 |
| $Ph\text{-}CH{=}CH_2 + TolS^\bullet = [Ph\text{-}CH\text{-}CH_2\text{-}STol]^\bullet_{(linear)}$ | -25.4 | 25.5 |
| $Ph\text{-}CH{=}CH_2 + TolS^+ = [Ph\text{-}CH\text{-}CH_2\text{-}STol]^+_{(cycl)}$ | -203.5 | -142.1 |
| $[Ph\text{-}CH\text{-}CH_2\text{-}STol]^+_{(cycl)} + IO_3^- + TolSH = Tol_2S_2CHCH_2Ph + HIO_3$ | -244.4 | -201.5 |
| $2[Ph\text{-}CH\text{-}CH_2\text{-}STol]^\bullet_{(linear)} + 2H^+ + IO_4^- = 2[Ph\text{-}CH\text{-}CH_2\text{-}STol]^+_{(cycl)} + IO_3^- + H_2O$ | -677.6 | -696.6 |
| $TolS^\bullet + [Ph\text{-}CH\text{-}CH_2\text{-}STol]^\bullet_{(linear)} = Tol_2S_2CHCH_2Ph$ | -220.1 | -162.7 |
| $[Ph\text{-}CH\text{-}CH_2\text{-}STol]^+_{(cycl)} + IO_3^- + AniH = TolSAniCHCH_2Ph + HIO_3$ | -248.7 | -205.2 |
| $AniH + Tol_2S_2CHCH_2Ph = TolSAniCHCH_2Ph + TolSH$ | -4.3 | -3.7 |



## Cartesian Coordinates of the Optimised Geometries

$[Ani]^-$

| | | | |
|---|---|---|---|
| 6 | -1.221616 | -0.216035 | -0.006976 |
| 6 | -2.460754 | -0.855752 | -0.027298 |
| 6 | -3.633257 | -0.098268 | 0.013813 |
| 6 | -3.689945 | 1.317421 | 0.076860 |
| 6 | -2.401158 | 1.886238 | 0.093722 |
| 6 | -1.188209 | 1.173351 | 0.054324 |
| 1 | -2.482181 | -1.941582 | -0.075236 |
| 1 | -4.564202 | -0.668267 | -0.005412 |
| 1 | -2.298397 | 2.972475 | 0.141152 |
| 1 | -0.245656 | 1.709953 | 0.071996 |
| 6 | 1.147833 | -0.389529 | -0.029957 |
| 1 | 1.292274 | 0.190256 | 0.888385 |
| 1 | 1.893682 | -1.183040 | -0.069906 |
| 1 | 1.280760 | 0.269229 | -0.895251 |
| 8 | -0.110123 | -1.024789 | -0.049963 |

AniH

| | | | |
|---|---|---|---|
| 6 | -1.223045 | -0.205879 | -0.017042 |
| 6 | -2.460675 | -0.857686 | -0.046363 |
| 6 | -3.633041 | -0.119975 | -0.026706 |
| 6 | -3.593150 | 1.274691 | 0.022317 |
| 6 | -2.362409 | 1.915366 | 0.051211 |
| 6 | -1.171614 | 1.187317 | 0.031990 |
| 1 | -2.475588 | -1.940701 | -0.084347 |
| 1 | -4.586541 | -0.635557 | -0.049765 |
| 1 | -4.511451 | 1.849026 | 0.037591 |
| 1 | -2.314438 | 2.997879 | 0.089351 |
| 1 | -0.225323 | 1.711383 | 0.055307 |
| 6 | 1.144578 | -0.389479 | -0.011018 |
| 1 | 1.281592 | 0.192029 | 0.905530 |
| 1 | 1.872694 | -1.197835 | -0.035479 |
| 1 | 1.291000 | 0.254630 | -0.883182 |
| 8 | -0.129970 | -1.008789 | -0.039397 |

$[Ani]^+$

| | | | |
|---|---|---|---|
| 6 | -1.229646 | -0.207047 | -0.006526 |
| 6 | -2.467913 | -0.873678 | -0.028045 |
| 6 | -3.691190 | -0.174780 | 0.010799 |
| 6 | -3.338328 | 1.101633 | 0.065034 |

| | | | |
|---|---|---|---|
| 6 | -2.357663 | 1.980231 | 0.097602 |
| 6 | -1.174399 | 1.191303 | 0.055031 |
| 1 | -2.512515 | -1.956423 | -0.075697 |
| 1 | -4.668801 | -0.639359 | -0.003458 |
| 1 | -2.371987 | 3.060701 | 0.145534 |
| 1 | -0.241963 | 1.742327 | 0.073407 |
| 6 | 1.134910 | -0.372774 | -0.029132 |
| 1 | 1.273926 | 0.194579 | 0.894715 |
| 1 | 1.854056 | -1.186404 | -0.069800 |
| 1 | 1.262331 | 0.274083 | -0.900939 |
| 8 | -0.151764 | -0.992731 | -0.048273 |

[Ani]•

| | | | |
|---|---|---|---|
| 6 | -1.232188 | -0.203567 | -0.007075 |
| 6 | -2.465785 | -0.866757 | -0.030041 |
| 6 | -3.651712 | -0.141247 | 0.010623 |
| 6 | -3.551278 | 1.231421 | 0.073194 |
| 6 | -2.371434 | 1.926050 | 0.097940 |
| 6 | -1.178624 | 1.189984 | 0.056745 |
| 1 | -2.473599 | -1.949651 | -0.079840 |
| 1 | -4.608667 | -0.650670 | -0.006961 |
| 1 | -2.338890 | 3.008696 | 0.147576 |
| 1 | -0.232309 | 1.714721 | 0.075101 |
| 6 | 1.137172 | -0.382838 | -0.029854 |
| 1 | 1.284092 | 0.188572 | 0.891652 |
| 1 | 1.865793 | -1.190103 | -0.071484 |
| 1 | 1.273127 | 0.270897 | -0.896696 |
| 8 | -0.136645 | -1.003850 | -0.050630 |

$HIO_3$

| | | | |
|---|---|---|---|
| 53 | -0.034625 | -0.059213 | 0.283115 |
| 8 | 1.517541 | -0.387266 | 1.177762 |
| 8 | 0.582858 | 1.328993 | -0.982219 |
| 8 | -0.288711 | -1.452176 | -0.861842 |
| 1 | 1.360490 | 0.992172 | -1.459939 |

$LiIO_3$

| | | | |
|---|---|---|---|
| 53 | -0.216686 | -0.068577 | 0.125224 |
| 8 | 1.572436 | -0.133367 | 0.688393 |
| 8 | 0.225355 | 1.175513 | -1.208626 |
| 8 | -0.521655 | -1.646202 | -0.746726 |

| | | | |
|---|---|---|---|
| 3 | 2.078103 | 1.095144 | -0.701389 |

$[IO_3]^-$

| | | | |
|---|---|---|---|
| 53 | 0.000462 | -0.000681 | -0.231558 |
| 8 | -1.624894 | 0.487764 | 0.511985 |
| 8 | 1.234737 | 1.164938 | 0.511371 |
| 8 | 0.390616 | -1.653215 | 0.511178 |

$HIO_4$

| | | | |
|---|---|---|---|
| 53 | 0.071839 | -0.023406 | -0.137014 |
| 8 | 0.263164 | -0.200843 | 1.785994 |
| 8 | -0.050392 | -1.768194 | -0.558504 |
| 8 | -1.432579 | 0.951561 | -0.339559 |
| 8 | 1.583872 | 0.818367 | -0.647627 |
| 1 | 0.347932 | 0.675061 | 2.206710 |

$LiIO_4$

| | | | |
|---|---|---|---|
| 53 | 0.043666 | -0.069716 | 0.000046 |
| 8 | -0.651666 | 1.632546 | -0.102457 |
| 8 | -1.375195 | -1.194199 | 0.074409 |
| 8 | 1.049097 | -0.310124 | -1.492194 |
| 8 | 1.051947 | -0.120218 | 1.508523 |
| 3 | -0.146129 | 3.328557 | -0.181273 |

$[IO_4]^-$

| | | | |
|---|---|---|---|
| 53 | 0.000000 | 0.000000 | 0.000000 |
| 8 | 0.000000 | 0.000000 | 1.825018 |
| 8 | 0.000000 | -1.720643 | -0.608339 |
| 8 | -1.490121 | 0.860322 | -0.608339 |
| 8 | 1.490121 | 0.860322 | -0.608339 |

MeOH

| | | | |
|---|---|---|---|
| 6 | 0.000145 | 0.016899 | 0.014459 |
| 1 | -0.000210 | -1.017271 | -0.329120 |
| 1 | -0.891247 | 0.514537 | -0.380880 |
| 1 | 0.891493 | 0.514128 | -0.381494 |
| 8 | 0.000626 | -0.014479 | 1.433121 |
| 1 | 0.000948 | 0.891120 | 1.754369 |

[MeOPhCHPhCH$_2$STol]$^+$

| | | | |
|---|---|---|---|
| 6 | 1.365291 | 0.370118 | -0.234969 |
| 6 | 0.390101 | 1.379324 | 0.049425 |
| 6 | -0.891952 | 1.048617 | 0.579271 |
| 6 | -1.186978 | -0.242549 | 0.833866 |
| 6 | -0.277911 | -1.353361 | 0.477431 |
| 6 | 1.043040 | -0.923894 | -0.018275 |
| 1 | 2.337726 | 0.643693 | -0.620836 |
| 1 | -1.576839 | 1.857499 | 0.799068 |
| 1 | -2.151851 | -0.504958 | 1.257825 |
| 1 | 1.766325 | -1.702245 | -0.244829 |
| 8 | 0.599935 | 2.641187 | -0.145580 |
| 6 | 1.858519 | 3.119400 | -0.669784 |
| 1 | 2.036528 | 2.689370 | -1.655147 |
| 1 | 1.740739 | 4.195975 | -0.744357 |
| 1 | 2.663991 | 2.875213 | 0.022499 |
| 1 | -0.769284 | -1.803229 | -0.411475 |
| 6 | -0.212079 | -2.531158 | 1.508782 |
| 1 | -1.237907 | -2.676612 | 1.862736 |
| 6 | 0.676288 | -2.211992 | 2.710250 |
| 1 | 0.715554 | -3.081722 | 3.368045 |
| 1 | 1.693425 | -1.961951 | 2.403285 |
| 6 | 0.208058 | -3.814290 | 0.808126 |
| 6 | 1.521091 | -4.285849 | 0.817250 |
| 6 | -0.760551 | -4.538388 | 0.107521 |
| 6 | 1.857400 | -5.454290 | 0.135514 |
| 1 | 2.294021 | -3.756418 | 1.363294 |
| 6 | -0.427557 | -5.703268 | -0.572503 |
| 1 | -1.789049 | -4.189208 | 0.105042 |
| 6 | 0.886901 | -6.164109 | -0.561388 |
| 1 | 2.880693 | -5.810763 | 0.156725 |
| 1 | -1.194582 | -6.255577 | -1.102890 |
| 1 | 1.148993 | -7.075129 | -1.086330 |
| 16 | 0.017285 | -0.797808 | 3.667429 |
| 6 | 1.298920 | -0.680069 | 4.907586 |
| 6 | 2.494192 | -0.016377 | 4.627402 |
| 6 | 1.104119 | -1.244404 | 6.166366 |
| 6 | 3.485770 | 0.067664 | 5.596944 |
| 1 | 2.644122 | 0.434483 | 3.652102 |
| 6 | 2.101058 | -1.147731 | 7.132256 |
| 1 | 0.176880 | -1.759590 | 6.389276 |
| 6 | 3.303993 | -0.493004 | 6.864755 |
| 1 | 4.413443 | 0.583333 | 5.370296 |

| | | | |
|---|---|---|---|
| 1 | 1.940118 | -1.590958 | 8.109372 |
| 6 | 4.367827 | -0.366181 | 7.921116 |
| 1 | 5.366451 | -0.436229 | 7.486002 |
| 1 | 4.294535 | 0.602696 | 8.423713 |
| 1 | 4.264477 | -1.142990 | 8.680150 |

$[MeOPhCHPhCH_2STol]^+$ - TS

| | | | |
|---|---|---|---|
| 6 | 1.324881 | 0.766712 | 1.289079 |
| 6 | 0.275728 | 1.406594 | 0.574926 |
| 6 | -0.737476 | 0.650939 | -0.098788 |
| 6 | -0.685771 | -0.693884 | -0.075450 |
| 6 | 0.393604 | -1.445086 | 0.602457 |
| 6 | 1.329831 | -0.588185 | 1.360336 |
| 1 | 2.079808 | 1.344551 | 1.804251 |
| 1 | -1.523216 | 1.195574 | -0.607319 |
| 1 | -1.442487 | -1.276282 | -0.592643 |
| 1 | 2.122270 | -1.073577 | 1.922625 |
| 8 | 0.149826 | 2.693886 | 0.487375 |
| 6 | 1.095959 | 3.573403 | 1.130660 |
| 1 | 2.091102 | 3.415219 | 0.714340 |
| 1 | 0.749144 | 4.577237 | 0.904957 |
| 1 | 1.086549 | 3.403690 | 2.207545 |
| 1 | 1.033771 | -1.802976 | -0.231723 |
| 6 | -0.139772 | -2.743294 | 1.314512 |
| 1 | -1.229437 | -2.662771 | 1.329251 |
| 6 | 0.320781 | -2.873181 | 2.772165 |
| 1 | -0.087985 | -3.796515 | 3.183090 |
| 1 | 1.407352 | -2.922398 | 2.850301 |
| 6 | 0.218014 | -4.006828 | 0.554613 |
| 6 | 1.555177 | -4.323550 | 0.296736 |
| 6 | -0.778342 | -4.887023 | 0.137536 |
| 6 | 1.887382 | -5.495707 | -0.371046 |
| 1 | 2.342910 | -3.646937 | 0.619746 |
| 6 | -0.447302 | -6.062904 | -0.533161 |
| 1 | -1.819262 | -4.654612 | 0.339174 |
| 6 | 0.884279 | -6.368677 | -0.788645 |
| 1 | 2.927363 | -5.730690 | -0.565607 |
| 1 | -1.231933 | -6.737507 | -0.855592 |
| 1 | 1.142775 | -7.282570 | -1.310388 |
| 16 | -0.276288 | -1.457287 | 3.765584 |
| 6 | 1.182344 | -0.975319 | 4.669718 |
| 6 | 2.051745 | -1.908247 | 5.231123 |
| 6 | 1.423994 | 0.387709 | 4.853974 |

| | | | |
|---|---|---|---|
| 6 | 3.170237 | -1.475763 | 5.938028 |
| 1 | 1.854108 | -2.969897 | 5.132939 |
| 6 | 2.531876 | 0.804441 | 5.581527 |
| 1 | 0.741310 | 1.117852 | 4.431938 |
| 6 | 3.431184 | -0.117929 | 6.124507 |
| 1 | 3.841997 | -2.211876 | 6.367005 |
| 1 | 2.706178 | 1.866283 | 5.726137 |
| 6 | 4.644904 | 0.350269 | 6.881168 |
| 1 | 5.155835 | -0.484776 | 7.361966 |
| 1 | 5.355719 | 0.839963 | 6.209690 |
| 1 | 4.370602 | 1.074200 | 7.651739 |

PhTolSCHCH$_2$Ani

| | | | |
|---|---|---|---|
| 6 | -1.848432 | 2.594913 | 0.105006 |
| 1 | -2.300479 | 2.193942 | -0.807796 |
| 1 | -2.204220 | 1.981486 | 0.936753 |
| 6 | -2.332480 | 4.048823 | 0.261886 |
| 1 | -1.815120 | 4.666760 | -0.473749 |
| 6 | -3.819272 | 4.233750 | 0.090623 |
| 6 | -4.737923 | 3.326492 | 0.624769 |
| 6 | -4.299223 | 5.351863 | -0.594613 |
| 6 | -6.105284 | 3.533803 | 0.475289 |
| 1 | -4.387070 | 2.455593 | 1.168313 |
| 6 | -5.666626 | 5.560109 | -0.745839 |
| 1 | -3.592793 | 6.063212 | -1.011967 |
| 6 | -6.574570 | 4.651100 | -0.210760 |
| 1 | -6.806281 | 2.821396 | 0.895592 |
| 1 | -6.022129 | 6.431673 | -1.283985 |
| 1 | -7.640282 | 4.811258 | -0.327466 |
| 16 | -1.794852 | 4.734329 | 1.906691 |
| 6 | -0.772312 | 6.105507 | 1.393732 |
| 6 | 0.527188 | 5.886423 | 0.927617 |
| 6 | -1.260012 | 7.408888 | 1.471457 |
| 6 | 1.315119 | 6.960739 | 0.534155 |
| 1 | 0.917454 | 4.874354 | 0.876010 |
| 6 | -0.457534 | 8.478524 | 1.082704 |
| 1 | -2.269953 | 7.584107 | 1.824474 |
| 6 | 0.837945 | 8.273339 | 0.607777 |
| 1 | 2.320650 | 6.777693 | 0.168012 |
| 1 | -0.849423 | 9.488896 | 1.144751 |
| 6 | 1.710764 | 9.433776 | 0.211653 |
| 1 | 1.111609 | 10.282749 | -0.121749 |
| 1 | 2.315670 | 9.768202 | 1.059757 |

| | | | |
|---|---|---|---|
| 1 | 2.394928 | 9.156556 | -0.592165 |
| 6 | -0.346511 | 2.519025 | 0.006131 |
| 6 | 0.443011 | 2.117848 | 1.077570 |
| 6 | 0.300036 | 2.932504 | -1.165260 |
| 6 | 1.837647 | 2.129061 | 1.005870 |
| 1 | -0.031396 | 1.796051 | 1.998620 |
| 6 | 1.680967 | 2.955935 | -1.256303 |
| 1 | -0.292822 | 3.248477 | -2.018969 |
| 6 | 2.461455 | 2.558457 | -0.164779 |
| 1 | 2.414712 | 1.808273 | 1.862952 |
| 1 | 2.179757 | 3.276009 | -2.163903 |
| 8 | 3.806428 | 2.615384 | -0.342519 |
| 6 | 4.632125 | 2.234237 | 0.744158 |
| 1 | 5.657132 | 2.355700 | 0.399701 |
| 1 | 4.464750 | 2.876768 | 1.613785 |
| 1 | 4.465824 | 1.189225 | 1.022030 |

Sty

| | | | |
|---|---|---|---|
| 6 | -1.001482 | -0.422552 | 0.000000 |
| 6 | 0.000274 | 0.557327 | 0.000000 |
| 6 | 1.336002 | 0.141908 | 0.000000 |
| 6 | 1.667441 | -1.209678 | 0.000000 |
| 6 | 0.663326 | -2.171387 | 0.000000 |
| 6 | -0.672556 | -1.770974 | 0.000000 |
| 1 | -2.045776 | -0.131870 | 0.000000 |
| 1 | 2.122093 | 0.890338 | 0.000000 |
| 1 | 2.709242 | -1.509267 | 0.000000 |
| 1 | 0.915766 | -3.225441 | 0.000000 |
| 1 | -1.460495 | -2.515717 | 0.000000 |
| 6 | -0.294059 | 2.003341 | 0.000000 |
| 1 | 0.583593 | 2.645567 | 0.000000 |
| 6 | -1.499412 | 2.571608 | 0.000000 |
| 1 | -2.419597 | 1.997145 | 0.000000 |
| 1 | -1.599073 | 3.650796 | 0.000000 |

TEMPOH

| | | | |
|---|---|---|---|
| 6 | -1.276553 | 0.080036 | -0.058156 |
| 6 | 1.287476 | 0.079812 | -0.057810 |
| 6 | 1.250589 | -1.380636 | -0.530970 |
| 6 | 0.005269 | -2.126730 | -0.062673 |
| 6 | -1.239794 | -1.380419 | -0.531305 |
| 1 | 1.277246 | -1.387872 | -1.626730 |

| | | | |
|---|---|---|---|
| 1 | 2.161308 | -1.874619 | -0.178923 |
| 1 | 0.005235 | -3.141464 | -0.469573 |
| 1 | 0.005114 | -2.229218 | 1.026812 |
| 1 | -1.266156 | -1.387650 | -1.627072 |
| 1 | -2.150694 | -1.874243 | -0.179504 |
| 6 | 2.398250 | 0.812711 | -0.816505 |
| 1 | 2.531809 | 1.827455 | -0.436050 |
| 1 | 3.344527 | 0.278702 | -0.696075 |
| 1 | 2.161162 | 0.863874 | -1.882266 |
| 6 | 1.592795 | 0.169171 | 1.446407 |
| 1 | 2.653420 | -0.040996 | 1.609960 |
| 1 | 1.387250 | 1.175248 | 1.816961 |
| 1 | 1.022698 | -0.543937 | 2.040477 |
| 6 | -1.582261 | 0.169448 | 1.445980 |
| 1 | -1.376639 | 1.175490 | 1.816590 |
| 1 | -2.642967 | -0.040533 | 1.609247 |
| 1 | -1.012450 | -0.543760 | 2.040203 |
| 6 | -2.386994 | 0.813130 | -0.817149 |
| 1 | -3.333397 | 0.279286 | -0.696974 |
| 1 | -2.520479 | 1.827896 | -0.436730 |
| 1 | -2.149610 | 0.864251 | -1.882847 |
| 7 | 0.005572 | 0.706089 | -0.470047 |
| 8 | 0.005627 | 2.053755 | -0.001401 |
| 1 | 0.005781 | 2.577959 | -0.808625 |

TEMPO

| | | | |
|---|---|---|---|
| 6 | 1.315309 | 0.674382 | -0.265589 |
| 6 | -1.320936 | 0.641166 | -0.269231 |
| 6 | -1.225523 | -0.822116 | 0.177686 |
| 6 | 0.022306 | -1.526882 | -0.340831 |
| 6 | 1.254373 | -0.793271 | 0.174271 |
| 1 | -1.218393 | -0.853955 | 1.273359 |
| 1 | -2.135155 | -1.330749 | -0.154749 |
| 1 | 0.034966 | -2.562206 | 0.008430 |
| 1 | 0.022244 | -1.564962 | -1.434776 |
| 1 | 1.251283 | -0.828848 | 1.269821 |
| 1 | 2.174634 | -1.279550 | -0.162003 |
| 6 | -2.364312 | 1.367906 | 0.578289 |
| 1 | -2.536002 | 2.379521 | 0.211169 |
| 1 | -3.304854 | 0.812963 | 0.536702 |
| 1 | -2.039198 | 1.426219 | 1.619662 |
| 6 | -1.707027 | 0.747405 | -1.750737 |
| 1 | -2.756390 | 0.465904 | -1.871331 |

| | | | |
|---|---|---|---|
| 1 | -1.585057 | 1.776809 | -2.094720 |
| 1 | -1.109656 | 0.091093 | -2.384931 |
| 6 | 1.702856 | 0.806070 | -1.744218 |
| 1 | 1.610225 | 1.847644 | -2.059353 |
| 1 | 2.742992 | 0.496275 | -1.875144 |
| 1 | 1.082778 | 0.189682 | -2.396102 |
| 6 | 2.338397 | 1.418029 | 0.592055 |
| 1 | 3.293748 | 0.889437 | 0.543336 |
| 1 | 2.482547 | 2.438977 | 0.239524 |
| 1 | 2.011910 | 1.452165 | 1.634102 |
| 7 | -0.011282 | 1.325761 | -0.046657 |
| 8 | -0.026784 | 2.595577 | -0.115115 |

$Tol_2S_2CHCH_2Ph$

| | | | |
|---|---|---|---|
| 6 | 0.040519 | -0.042788 | 0.202989 |
| 6 | 1.141647 | -0.818186 | -0.178867 |
| 6 | 0.991595 | -2.174680 | -0.422137 |
| 6 | -0.253839 | -2.801588 | -0.306041 |
| 6 | -1.340775 | -2.018684 | 0.073540 |
| 6 | -1.203753 | -0.655511 | 0.334059 |
| 1 | 2.115908 | -0.354082 | -0.290784 |
| 1 | 1.857528 | -2.758818 | -0.718658 |
| 1 | -2.319251 | -2.477024 | 0.176440 |
| 1 | -2.073636 | -0.089777 | 0.643513 |
| 16 | 0.345357 | 1.677168 | 0.537340 |
| 6 | -0.399339 | -4.273614 | -0.586096 |
| 1 | -0.125105 | -4.505239 | -1.618730 |
| 1 | 0.252089 | -4.862269 | 0.065048 |
| 1 | -1.426479 | -4.604961 | -0.426721 |
| 6 | -1.333059 | 2.385236 | 0.425749 |
| 1 | -1.820064 | 1.973460 | -0.460858 |
| 1 | -1.910657 | 2.111348 | 1.310362 |
| 6 | -1.263068 | 3.903369 | 0.272622 |
| 1 | -0.631161 | 4.145795 | -0.584212 |
| 6 | -2.628014 | 4.510996 | 0.062209 |
| 6 | -3.664302 | 4.310079 | 0.978277 |
| 6 | -2.854699 | 5.324637 | -1.047138 |
| 6 | -4.905337 | 4.902230 | 0.778538 |
| 1 | -3.493424 | 3.706539 | 1.863672 |
| 6 | -4.097155 | 5.922479 | -1.246599 |
| 1 | -2.049606 | 5.498928 | -1.753994 |
| 6 | -5.125320 | 5.711578 | -0.335072 |
| 1 | -5.701706 | 4.738158 | 1.495715 |

| | | | |
|---|---|---|---|
| 1 | -4.257369 | 6.555656 | -2.111761 |
| 1 | -6.092791 | 6.176278 | -0.486746 |
| 16 | -0.429997 | 4.624782 | 1.764096 |
| 6 | -0.529845 | 6.348667 | 1.310452 |
| 6 | 0.401601 | 6.898142 | 0.429306 |
| 6 | -1.557162 | 7.148475 | 1.809446 |
| 6 | 0.296466 | 8.230762 | 0.047179 |
| 1 | 1.204866 | 6.280511 | 0.042480 |
| 6 | -1.649714 | 8.482356 | 1.425986 |
| 1 | -2.289234 | 6.722285 | 2.485928 |
| 6 | -0.727261 | 9.043606 | 0.540842 |
| 1 | 1.023565 | 8.647920 | -0.642370 |
| 1 | -2.456201 | 9.094909 | 1.815955 |
| 6 | -0.811562 | 10.495420 | 0.152689 |
| 1 | -1.835099 | 10.865967 | 0.229772 |
| 1 | -0.186174 | 11.105287 | 0.811529 |
| 1 | -0.462511 | 10.650797 | -0.869776 |

TolSAniCHCH$_2$Ph

| | | | |
|---|---|---|---|
| 6 | -0.038655 | 0.302315 | 0.125176 |
| 6 | 1.156026 | -0.252483 | -0.345194 |
| 6 | 1.280248 | -1.626579 | -0.493652 |
| 6 | 0.222077 | -2.489073 | -0.192688 |
| 6 | -0.962968 | -1.923609 | 0.273983 |
| 6 | -1.099018 | -0.546961 | 0.439040 |
| 1 | 1.988738 | 0.395491 | -0.597664 |
| 1 | 2.216445 | -2.037727 | -0.858348 |
| 1 | -1.799505 | -2.568737 | 0.523599 |
| 1 | -2.031487 | -0.150875 | 0.821372 |
| 16 | -0.087040 | 2.066122 | 0.339864 |
| 6 | 0.355181 | -3.975257 | -0.394163 |
| 1 | 0.176848 | -4.243252 | -1.439855 |
| 1 | 1.357937 | -4.320123 | -0.133729 |
| 1 | -0.365764 | -4.521849 | 0.216093 |
| 6 | -1.879240 | 2.399692 | 0.358152 |
| 1 | -2.335747 | 1.865331 | -0.477904 |
| 1 | -2.302509 | 2.034658 | 1.296036 |
| 6 | -2.108027 | 3.908349 | 0.215390 |
| 1 | -1.594026 | 4.234808 | -0.694608 |
| 6 | -3.580395 | 4.261520 | 0.043522 |
| 6 | -4.621389 | 3.381488 | 0.335832 |
| 6 | -3.899594 | 5.546528 | -0.408069 |
| 6 | -5.950770 | 3.777295 | 0.182276 |

| | | | |
|---|---|---|---|
| 1 | -4.411769 | 2.376366 | 0.684081 |
| 6 | -5.220842 | 5.942029 | -0.565265 |
| 1 | -3.096136 | 6.241916 | -0.632284 |
| 6 | -6.255133 | 5.055447 | -0.267928 |
| 1 | -6.747199 | 3.079425 | 0.415030 |
| 1 | -5.445761 | 6.941578 | -0.919769 |
| 1 | -7.287842 | 5.361724 | -0.388360 |
| 6 | -1.501532 | 4.675478 | 1.380319 |
| 6 | -2.021078 | 4.534796 | 2.673672 |
| 6 | -0.412959 | 5.517073 | 1.198835 |
| 6 | -1.464157 | 5.208248 | 3.744990 |
| 1 | -2.881447 | 3.892994 | 2.839817 |
| 6 | 0.164518 | 6.210167 | 2.267084 |
| 1 | 0.008506 | 5.639816 | 0.205825 |
| 6 | -0.362892 | 6.054117 | 3.550531 |
| 1 | -1.866553 | 5.101519 | 4.745602 |
| 1 | 1.011728 | 6.855661 | 2.082405 |
| 8 | 0.111247 | 6.676232 | 4.667886 |
| 6 | 1.217091 | 7.553119 | 4.530680 |
| 1 | 1.422520 | 7.938935 | 5.527407 |
| 1 | 2.099619 | 7.023610 | 4.159851 |
| 1 | 0.980513 | 8.387007 | 3.863166 |

TolSAniCHCH$_2$Ph

| | | | |
|---|---|---|---|
| 6 | -3.042355 | -0.527293 | -0.347303 |
| 6 | -3.948804 | -1.451903 | -0.882107 |
| 6 | -5.292463 | -1.389299 | -0.549955 |
| 6 | -5.783586 | -0.406345 | 0.317081 |
| 6 | -4.873314 | 0.506349 | 0.841215 |
| 6 | -3.516020 | 0.452648 | 0.522062 |
| 1 | -3.596778 | -2.220703 | -1.562165 |
| 1 | -5.978124 | -2.115576 | -0.975882 |
| 1 | -5.222578 | 1.279137 | 1.518572 |
| 1 | -2.845084 | 1.178532 | 0.962968 |
| 16 | -1.339795 | -0.719290 | -0.816041 |
| 6 | -7.248224 | -0.350936 | 0.661461 |
| 1 | -7.855740 | -0.197559 | -0.234388 |
| 1 | -7.577735 | -1.285193 | 1.123447 |
| 1 | -7.458899 | 0.463467 | 1.356206 |
| 6 | -0.576910 | 0.803279 | -0.172515 |
| 1 | -1.170797 | 1.657749 | -0.503949 |
| 1 | -0.573475 | 0.765113 | 0.919112 |
| 6 | 0.851360 | 0.914022 | -0.718070 |

| | | | |
|---|---|---|---|
| 1 | 0.789070 | 0.878445 | -1.810748 |
| 6 | 1.512751 | 2.238185 | -0.354642 |
| 6 | 1.024462 | 3.097673 | 0.628357 |
| 6 | 2.686654 | 2.592765 | -1.028043 |
| 6 | 1.694979 | 4.283198 | 0.932712 |
| 1 | 0.115742 | 2.857475 | 1.168726 |
| 6 | 3.353709 | 3.773022 | -0.730337 |
| 1 | 3.079438 | 1.926711 | -1.790573 |
| 6 | 2.858877 | 4.624894 | 0.256461 |
| 1 | 1.300785 | 4.938680 | 1.701111 |
| 1 | 4.260098 | 4.029962 | -1.266835 |
| 1 | 3.378396 | 5.546402 | 0.492536 |
| 6 | 1.712260 | -0.258320 | -0.274389 |
| 6 | 2.055700 | -0.420692 | 1.073606 |
| 6 | 2.163992 | -1.204219 | -1.184522 |
| 6 | 2.816956 | -1.496058 | 1.491330 |
| 1 | 1.728018 | 0.313362 | 1.804034 |
| 6 | 2.937221 | -2.296668 | -0.782916 |
| 1 | 1.908906 | -1.100914 | -2.234753 |
| 6 | 3.263210 | -2.444344 | 0.562531 |
| 1 | 3.085602 | -1.623145 | 2.533531 |
| 1 | 3.270044 | -3.011984 | -1.523329 |
| 8 | 4.006212 | -3.462715 | 1.064718 |
| 6 | 4.488892 | -4.434401 | 0.153754 |
| 1 | 5.057666 | -5.148334 | 0.746301 |
| 1 | 3.665367 | -4.954846 | -0.344456 |
| 1 | 5.146050 | -3.982723 | -0.595567 |

TolSAni

| | | | |
|---|---|---|---|
| 6 | -0.028490 | 0.339061 | 0.087387 |
| 6 | 1.217494 | -0.259651 | -0.114905 |
| 6 | 1.323770 | -1.642063 | -0.187043 |
| 6 | 0.199773 | -2.463951 | -0.068315 |
| 6 | -1.035321 | -1.849835 | 0.134752 |
| 6 | -1.158632 | -0.464827 | 0.215542 |
| 1 | 2.105565 | 0.355656 | -0.216496 |
| 1 | 2.299929 | -2.090844 | -0.342178 |
| 1 | -1.925361 | -2.463030 | 0.236334 |
| 1 | -2.133946 | -0.021957 | 0.379077 |
| 16 | -0.054270 | 2.122758 | 0.203313 |
| 6 | 0.318244 | -3.960061 | -0.188945 |
| 1 | 0.283887 | -4.268158 | -1.238299 |
| 1 | 1.262209 | -4.315961 | 0.228371 |

| | | | |
|---|---|---|---|
| 1 | -0.498712 | -4.463464 | 0.330989 |
| 6 | -1.796349 | 2.488742 | 0.166118 |
| 6 | -2.481189 | 2.752537 | 1.346311 |
| 6 | -2.486733 | 2.532503 | -1.050815 |
| 6 | -3.841536 | 3.058232 | 1.331029 |
| 1 | -1.953651 | 2.717703 | 2.292575 |
| 6 | -3.837020 | 2.827331 | -1.077646 |
| 1 | -1.958948 | 2.330441 | -1.975966 |
| 6 | -4.523509 | 3.092465 | 0.114476 |
| 1 | -4.347705 | 3.260295 | 2.265312 |
| 1 | -4.383718 | 2.863256 | -2.012536 |
| 8 | -5.839450 | 3.374209 | -0.012325 |
| 6 | -6.577049 | 3.645834 | 1.169200 |
| 1 | -6.180732 | 4.523118 | 1.688408 |
| 1 | -7.596558 | 3.847959 | 0.847563 |
| 1 | -6.573269 | 2.784316 | 1.843032 |

TolSCH$_2$CH$_2$Ph

| | | | |
|---|---|---|---|
| 6 | -0.094539 | 0.320425 | -0.021106 |
| 6 | 1.194891 | -0.227071 | -0.037086 |
| 6 | 1.372763 | -1.601005 | -0.027394 |
| 6 | 0.281130 | -2.476755 | -0.001594 |
| 6 | -0.993864 | -1.919965 | 0.014066 |
| 6 | -1.190508 | -0.538486 | 0.004610 |
| 1 | 2.059645 | 0.428357 | -0.057173 |
| 1 | 2.380513 | -2.004986 | -0.040102 |
| 1 | -1.860901 | -2.572677 | 0.034164 |
| 1 | -2.201729 | -0.153145 | 0.017545 |
| 16 | -0.208669 | 2.092173 | -0.035482 |
| 6 | 0.493731 | -3.967345 | 0.008601 |
| 1 | 1.044524 | -4.291184 | -0.878541 |
| 1 | 1.073211 | -4.275043 | 0.883124 |
| 1 | -0.458324 | -4.499853 | 0.028984 |
| 6 | -2.002048 | 2.392210 | -0.009027 |
| 1 | -2.451512 | 1.926932 | -0.888671 |
| 1 | -2.422496 | 1.943259 | 0.893158 |
| 6 | -2.225909 | 3.899593 | -0.019194 |
| 1 | -1.751861 | 4.329017 | -0.907652 |
| 1 | -1.723316 | 4.345079 | 0.845345 |
| 6 | -3.680650 | 4.323641 | 0.000610 |
| 6 | -4.742321 | 3.420043 | 0.026179 |
| 6 | -3.973499 | 5.692193 | -0.007163 |
| 6 | -6.062411 | 3.871491 | 0.043539 |

| | | | |
|---|---|---|---|
| 1 | -4.554443 | 2.352316 | 0.032905 |
| 6 | -5.285901 | 6.145063 | 0.010058 |
| 1 | -3.156436 | 6.407243 | -0.027022 |
| 6 | -6.339553 | 5.232452 | 0.035580 |
| 1 | -6.873297 | 3.152025 | 0.063337 |
| 1 | -5.488857 | 7.210078 | 0.003603 |
| 1 | -7.365235 | 5.582471 | 0.049075 |

$TolSCH_2CHOMePh$

| | | | |
|---|---|---|---|
| 6 | -0.035035 | 0.289727 | 0.292696 |
| 6 | 1.094297 | -0.393805 | -0.172551 |
| 6 | 1.122303 | -1.780304 | -0.177228 |
| 6 | 0.029238 | -2.532012 | 0.266697 |
| 6 | -1.089633 | -1.840425 | 0.724337 |
| 6 | -1.127123 | -0.446924 | 0.748123 |
| 1 | 1.950142 | 0.164600 | -0.536893 |
| 1 | 2.008082 | -2.291145 | -0.542478 |
| 1 | -1.952000 | -2.395368 | 1.079960 |
| 1 | -2.009861 | 0.049584 | 1.132145 |
| 16 | 0.042797 | 2.066146 | 0.322463 |
| 6 | 0.076650 | -4.036897 | 0.250583 |
| 1 | 0.245476 | -4.413973 | -0.761502 |
| 1 | 0.891468 | -4.409136 | 0.877233 |
| 1 | -0.856633 | -4.464524 | 0.619984 |
| 6 | -1.723553 | 2.520943 | 0.337486 |
| 1 | -2.265134 | 1.843307 | -0.324631 |
| 1 | -2.127849 | 2.441929 | 1.348889 |
| 6 | -1.885438 | 3.949437 | -0.166366 |
| 1 | -1.494347 | 4.013722 | -1.191704 |
| 6 | -3.356995 | 4.325629 | -0.178310 |
| 6 | -4.105913 | 4.202704 | -1.346983 |
| 6 | -3.980887 | 4.759027 | 0.992188 |
| 6 | -5.466226 | 4.500760 | -1.347143 |
| 1 | -3.621237 | 3.874362 | -2.261656 |
| 6 | -5.338430 | 5.062166 | 0.992237 |
| 1 | -3.393192 | 4.867895 | 1.897828 |
| 6 | -6.084365 | 4.931930 | -0.177334 |
| 1 | -6.040369 | 4.403894 | -2.261595 |
| 1 | -5.815144 | 5.403151 | 1.904300 |
| 1 | -7.141852 | 5.170037 | -0.176987 |
| 8 | -1.122677 | 4.779629 | 0.682597 |
| 6 | -0.958574 | 6.089773 | 0.176468 |
| 1 | -0.440527 | 6.070874 | -0.789784 |

| | | | |
|---|---|---|---|
| 1 | -1.920790 | 6.599880 | 0.055691 |
| 1 | -0.352304 | 6.639086 | 0.895927 |

[TolSCHCH$_2$Ph]$_{(cyc)}^+$

| | | | |
|---|---|---|---|
| 6 | -0.820958 | 0.601370 | -0.949644 |
| 6 | 0.061246 | 0.791899 | 0.109880 |
| 6 | 0.853539 | -0.273578 | 0.516930 |
| 6 | 0.783955 | -1.512958 | -0.124632 |
| 6 | -0.106620 | -1.667816 | -1.192064 |
| 6 | -0.907559 | -0.617796 | -1.617270 |
| 1 | 0.128961 | 1.749913 | 0.613474 |
| 1 | 1.537966 | -0.138225 | 1.346919 |
| 1 | -0.171641 | -2.623609 | -1.700365 |
| 1 | -1.588267 | -0.750222 | -2.451075 |
| 16 | -1.771906 | 1.998028 | -1.522047 |
| 6 | 1.667677 | -2.649988 | 0.302914 |
| 1 | 2.569257 | -2.677448 | -0.316066 |
| 1 | 1.978844 | -2.538348 | 1.342183 |
| 1 | 1.159650 | -3.608641 | 0.188486 |
| 6 | -3.513338 | 1.393484 | -1.387350 |
| 1 | -4.143236 | 1.837964 | -2.149070 |
| 1 | -3.555484 | 0.313890 | -1.310150 |
| 6 | -3.177672 | 2.162514 | -0.194686 |
| 6 | -3.643039 | 3.536331 | 0.068548 |
| 6 | -4.244787 | 4.324286 | -0.917748 |
| 6 | -3.465411 | 4.048424 | 1.356699 |
| 6 | -4.663106 | 5.611792 | -0.611420 |
| 1 | -4.390713 | 3.944975 | -1.923059 |
| 6 | -3.894626 | 5.333844 | 1.660390 |
| 1 | -3.000225 | 3.431798 | 2.118622 |
| 6 | -4.490436 | 6.116429 | 0.675892 |
| 1 | -5.128011 | 6.222106 | -1.376100 |
| 1 | -3.763086 | 5.723931 | 2.662395 |
| 1 | -4.823386 | 7.120620 | 0.910392 |
| 1 | -2.854101 | 1.590423 | 0.670036 |

[TolSCHCH$_2$Ph]$_{(cyc)}^{\bullet}$

| | | | |
|---|---|---|---|
| 6 | -0.140551 | 1.243559 | -1.413974 |
| 6 | -0.010049 | 1.249715 | -0.023332 |
| 6 | -0.619391 | 0.262008 | 0.738888 |
| 6 | -1.363216 | -0.756813 | 0.136210 |
| 6 | -1.460589 | -0.771616 | -1.255726 |

| | | | |
|---|---|---|---|
| 6 | -0.855460 | 0.216521 | -2.027705 |
| 1 | 0.547890 | 2.045097 | 0.457739 |
| 1 | -0.529109 | 0.287994 | 1.820556 |
| 1 | -2.021883 | -1.561732 | -1.744145 |
| 1 | -0.950399 | 0.198289 | -3.108084 |
| 16 | 0.543649 | 2.574040 | -2.386522 |
| 6 | -2.055054 | -1.792053 | 0.981094 |
| 1 | -1.361502 | -2.246090 | 1.692729 |
| 1 | -2.863356 | -1.333926 | 1.558697 |
| 1 | -2.484064 | -2.584582 | 0.366470 |
| 6 | -0.938769 | 3.715991 | -2.416423 |
| 1 | -0.598385 | 4.542479 | -3.042368 |
| 1 | -1.740445 | 3.194276 | -2.936952 |
| 6 | -1.300174 | 4.174249 | -1.061948 |
| 6 | -2.264886 | 3.562191 | -0.218313 |
| 6 | -3.100137 | 2.496796 | -0.638958 |
| 6 | -2.383075 | 3.991629 | 1.128508 |
| 6 | -3.971721 | 1.885723 | 0.245277 |
| 1 | -3.045977 | 2.136559 | -1.658722 |
| 6 | -3.257339 | 3.373927 | 2.004444 |
| 1 | -1.756543 | 4.808680 | 1.471615 |
| 6 | -4.055438 | 2.311083 | 1.573267 |
| 1 | -4.589202 | 1.062824 | -0.098300 |
| 1 | -3.319296 | 3.715287 | 3.031750 |
| 1 | -4.735700 | 1.823814 | 2.261832 |
| 1 | -0.696345 | 4.969474 | -0.636589 |

$[TolSCHCH_2Ph]_{(lin)}^{+}$

| | | | |
|---|---|---|---|
| 6 | -1.484467 | 0.003731 | -0.619282 |
| 6 | -0.222882 | 0.557300 | -0.411973 |
| 6 | 0.813890 | -0.277561 | -0.020945 |
| 6 | 0.610615 | -1.650185 | 0.155768 |
| 6 | -0.663326 | -2.175305 | -0.075020 |
| 6 | -1.716629 | -1.359704 | -0.467474 |
| 1 | -0.050508 | 1.618664 | -0.552443 |
| 1 | 1.799508 | 0.143027 | 0.146124 |
| 1 | -0.834004 | -3.238992 | 0.047258 |
| 1 | -2.697924 | -1.783005 | -0.652065 |
| 16 | -2.789492 | 1.066211 | -1.211868 |
| 6 | 1.740471 | -2.533369 | 0.602369 |
| 1 | 2.665493 | -2.275590 | 0.083696 |
| 1 | 1.917884 | -2.407448 | 1.674301 |
| 1 | 1.517328 | -3.584632 | 0.418739 |

| | | | |
|---|---|---|---|
| 6 | -4.107372 | 0.848269 | 0.065484 |
| 1 | -5.095510 | 0.949592 | -0.367922 |
| 1 | -3.941582 | -0.041174 | 0.660991 |
| 6 | -3.332049 | 2.044505 | 0.373077 |
| 6 | -3.799721 | 3.422574 | 0.137152 |
| 6 | -4.929760 | 3.706824 | -0.636136 |
| 6 | -3.071658 | 4.465645 | 0.715964 |
| 6 | -5.322800 | 5.024632 | -0.824239 |
| 1 | -5.507144 | 2.911436 | -1.094168 |
| 6 | -3.474783 | 5.781909 | 0.532300 |
| 1 | -2.197203 | 4.239193 | 1.316965 |
| 6 | -4.598168 | 6.061549 | -0.240037 |
| 1 | -6.197586 | 5.244156 | -1.424171 |
| 1 | -2.912691 | 6.587138 | 0.989612 |
| 1 | -4.912515 | 7.088169 | -0.386602 |
| 1 | -2.532730 | 1.925280 | 1.098733 |

$[TolSCHCH_2Ph]_{(lin)}^{\bullet}$

| | | | |
|---|---|---|---|
| 6 | -0.133533 | 0.296672 | -0.103169 |
| 6 | 1.173513 | -0.206267 | -0.135366 |
| 6 | 1.399385 | -1.572127 | -0.080614 |
| 6 | 0.340320 | -2.482702 | 0.011414 |
| 6 | -0.952574 | -1.969608 | 0.044372 |
| 6 | -1.197868 | -0.597333 | -0.013771 |
| 1 | 2.014184 | 0.476952 | -0.199777 |
| 1 | 2.419959 | -1.941867 | -0.105382 |
| 1 | -1.795415 | -2.649768 | 0.116149 |
| 1 | -2.221810 | -0.248004 | 0.011193 |
| 16 | -0.310184 | 2.061011 | -0.193083 |
| 6 | 0.603985 | -3.964139 | 0.060370 |
| 1 | 1.016624 | -4.319022 | -0.888249 |
| 1 | 1.326074 | -4.209422 | 0.843046 |
| 1 | -0.313419 | -4.520795 | 0.257688 |
| 6 | -2.099672 | 2.298083 | 0.032469 |
| 1 | -2.634705 | 1.813632 | -0.790201 |
| 1 | -2.405062 | 1.811614 | 0.967327 |
| 6 | -2.394587 | 3.760809 | 0.068537 |
| 6 | -3.714545 | 4.277355 | 0.034895 |
| 6 | -4.857551 | 3.441719 | -0.023613 |
| 6 | -3.925059 | 5.679451 | 0.061806 |
| 6 | -6.131624 | 3.985018 | -0.056026 |
| 1 | -4.737639 | 2.364286 | -0.038015 |
| 6 | -5.201154 | 6.210110 | 0.027974 |

| | | | |
|---|---|---|---|
| 1 | -3.062395 | 6.335987 | 0.107973 |
| 6 | -6.315318 | 5.368175 | -0.032517 |
| 1 | -6.992500 | 3.327323 | -0.099849 |
| 1 | -5.336711 | 7.285552 | 0.047810 |
| 1 | -7.314471 | 5.786362 | -0.059524 |
| 1 | -1.573562 | 4.463783 | 0.160318 |

TolSH

| | | | |
|---|---|---|---|
| 6 | -0.002981 | 0.511963 | -0.010081 |
| 6 | 1.204139 | -0.188921 | -0.050642 |
| 6 | 1.201922 | -1.577111 | -0.040107 |
| 6 | 0.008762 | -2.303332 | 0.009769 |
| 6 | -1.186910 | -1.587710 | 0.051335 |
| 6 | -1.201520 | -0.195736 | 0.041557 |
| 1 | 2.145403 | 0.348821 | -0.088706 |
| 1 | 2.148761 | -2.107348 | -0.071033 |
| 1 | -2.129495 | -2.123905 | 0.093071 |
| 1 | -2.148821 | 0.331060 | 0.076141 |
| 16 | 0.062366 | 2.290545 | -0.023407 |
| 1 | -1.264240 | 2.491798 | 0.025114 |
| 6 | 0.024007 | -3.808771 | 0.001296 |
| 1 | 0.326526 | -4.189117 | -0.978558 |
| 1 | 0.730744 | -4.200081 | 0.736699 |
| 1 | -0.963547 | -4.213454 | 0.227553 |

TolSLi

| | | | |
|---|---|---|---|
| 6 | -0.019713 | 0.520569 | -0.014754 |
| 6 | 1.185258 | -0.199861 | -0.050718 |
| 6 | 1.198126 | -1.588198 | -0.038428 |
| 6 | 0.014333 | -2.330445 | 0.009619 |
| 6 | -1.184454 | -1.620373 | 0.047855 |
| 6 | -1.202968 | -0.227593 | 0.035334 |
| 1 | 2.121326 | 0.346197 | -0.087094 |
| 1 | 2.151037 | -2.109403 | -0.066678 |
| 1 | -2.124884 | -2.162013 | 0.089011 |
| 1 | -2.163958 | 0.278032 | 0.067286 |
| 16 | 0.018207 | 2.294893 | -0.031547 |
| 6 | 0.043255 | -3.836516 | 0.002341 |
| 1 | 0.351924 | -4.219302 | -0.974936 |
| 1 | 0.750055 | -4.222463 | 0.741039 |
| 1 | -0.941370 | -4.250552 | 0.226771 |
| 3 | -2.127144 | 2.937566 | 0.044899 |

[TolS]$^-$

| | | | |
|---|---|---|---|
| 6 | 0.013165 | 0.559493 | -0.001603 |
| 6 | 1.205888 | -0.186568 | 0.063605 |
| 6 | 1.207193 | -1.579028 | 0.065947 |
| 6 | 0.022108 | -2.313010 | 0.003388 |
| 6 | -1.170700 | -1.584903 | -0.060992 |
| 6 | -1.177771 | -0.196122 | -0.063673 |
| 1 | 2.149083 | 0.347248 | 0.113944 |
| 1 | 2.156622 | -2.105961 | 0.118201 |
| 1 | -2.117020 | -2.118763 | -0.110113 |
| 1 | -2.123616 | 0.333010 | -0.114218 |
| 16 | 0.003482 | 2.317615 | -0.004917 |
| 6 | 0.016018 | -3.820667 | -0.001099 |
| 1 | -0.398588 | -4.216293 | -0.933461 |
| 1 | 1.027953 | -4.216895 | 0.106981 |
| 1 | -0.588885 | -4.220741 | 0.818011 |

[TolS]$^+$

| | | | |
|---|---|---|---|
| 6 | 0.009275 | 0.522513 | -0.009965 |
| 6 | 1.266942 | -0.217574 | 0.020810 |
| 6 | 1.260963 | -1.572983 | 0.039696 |
| 6 | 0.025391 | -2.285228 | 0.030584 |
| 6 | -1.218986 | -1.585677 | 0.000606 |
| 6 | -1.240380 | -0.231402 | -0.019706 |
| 1 | 2.191187 | 0.348670 | 0.029229 |
| 1 | 2.186300 | -2.135292 | 0.064520 |
| 1 | -2.138227 | -2.158946 | -0.004592 |
| 1 | -2.170696 | 0.324292 | -0.041980 |
| 16 | 0.002287 | 2.152200 | -0.038638 |
| 6 | 0.024750 | -3.756874 | 0.018357 |
| 1 | -0.118810 | -4.068473 | -1.029271 |
| 1 | 0.967593 | -4.176829 | 0.364469 |
| 1 | -0.822655 | -4.159984 | 0.575883 |

[TolS]$^\bullet$

| | | | |
|---|---|---|---|
| 6 | 0.012067 | 0.527010 | -0.005783 |
| 6 | 1.227201 | -0.194525 | 0.039496 |
| 6 | 1.225661 | -1.576980 | 0.048595 |
| 6 | 0.024053 | -2.296714 | 0.012222 |
| 6 | -1.186055 | -1.585343 | -0.031287 |

| | | | |
|---|---|---|---|
| 6 | -1.199246 | -0.205823 | -0.041127 |
| 1 | 2.161462 | 0.353907 | 0.068725 |
| 1 | 2.166348 | -2.115689 | 0.085089 |
| 1 | -2.122291 | -2.133365 | -0.057445 |
| 1 | -2.137547 | 0.335422 | -0.074313 |
| 16 | 0.005263 | 2.243683 | -0.016371 |
| 6 | 0.019097 | -3.796691 | 0.001401 |
| 1 | -0.268042 | -4.166580 | -0.987818 |
| 1 | 1.003176 | -4.199918 | 0.241339 |
| 1 | -0.706213 | -4.189980 | 0.717277 |

TolSSTol

| | | | |
|---|---|---|---|
| 6 | -1.901760 | -0.360839 | 0.173431 |
| 6 | -3.176643 | -0.424453 | 0.740598 |
| 6 | -4.125879 | 0.533881 | 0.414928 |
| 6 | -3.837288 | 1.564726 | -0.484424 |
| 6 | -2.562284 | 1.604470 | -1.045394 |
| 6 | -1.593513 | 0.657175 | -0.720937 |
| 1 | -3.429031 | -1.222848 | 1.430779 |
| 1 | -5.113620 | 0.474832 | 0.861276 |
| 1 | -2.311415 | 2.392646 | -1.747765 |
| 1 | -0.610692 | 0.716770 | -1.173740 |
| 16 | -0.741274 | -1.611839 | 0.718987 |
| 16 | 0.740587 | -1.615141 | -0.707462 |
| 6 | 1.901398 | -0.362075 | -0.167365 |
| 6 | 3.176264 | -0.428493 | -0.734249 |
| 6 | 1.593416 | 0.659908 | 0.722555 |
| 6 | 4.125749 | 0.531006 | -0.412760 |
| 6 | 2.562433 | 1.608357 | 1.042879 |
| 6 | 3.837426 | 1.565838 | 0.482088 |
| 1 | 3.428444 | -1.229955 | -1.420942 |
| 1 | 0.610610 | 0.721732 | 1.175093 |
| 1 | 5.113474 | 0.469755 | -0.858846 |
| 1 | 2.311769 | 2.399654 | 1.741807 |
| 6 | -4.885991 | 2.584533 | -0.839837 |
| 1 | -5.709264 | 2.120147 | -1.389453 |
| 1 | -5.308234 | 3.041260 | 0.058498 |
| 1 | -4.469783 | 3.377744 | -1.462275 |
| 6 | 4.886394 | 2.586912 | 0.833053 |
| 1 | 5.709546 | 2.124713 | 1.384689 |
| 1 | 5.308754 | 3.039608 | -0.067266 |
| 1 | 4.470392 | 3.382938 | 1.452025 |

```
TolSSTol•Sty - TS
      6       -0.450154   1.320606  -0.937962
      6       -1.505664   1.410060  -0.031461
      6       -1.293456   1.997459   1.211924
      6       -0.042461   2.504718   1.560804
      6        1.007491   2.402452   0.636302
      6        0.818069   1.803698  -0.596523
      1       -2.482499   1.020228  -0.294079
      1       -2.113954   2.062436   1.918129
      1        1.989565   2.779775   0.902588
      1        1.650218   1.685103  -1.282981
     16       -0.709512   0.423398  -2.436202
     16        0.784735  -1.401591  -2.424923
      6        0.115787  -1.869821  -0.826874
      6       -1.051395  -2.628298  -0.714159
      6        0.799106  -1.501412   0.336601
      6       -1.530107  -2.996596   0.538479
      6        0.315422  -1.877253   1.583787
      6       -0.857973  -2.626241   1.705867
      1       -1.586665  -2.924555  -1.609926
      1        1.709134  -0.917162   0.256833
      1       -2.440316  -3.583254   0.611036
      1        0.855193  -1.581514   2.478377
      6        0.193498   3.146724   2.899051
      1       -0.699117   3.101457   3.523576
      1        1.010756   2.649131   3.426979
      1        0.475332   4.196041   2.778043
      6       -1.367493  -3.031708   3.062743
      1       -0.702819  -3.768498   3.522482
      1       -1.415874  -2.171852   3.735146
      1       -2.363468  -3.471725   2.996056
      6        0.286255   1.240736  -3.875222
      6        1.105836   0.212505  -4.495131
      1        0.815704   2.067566  -3.405476
      1       -0.526970   1.621560  -4.495161
      1        0.620380  -0.433487  -5.217747
      6        2.527627   0.139668  -4.401501
      6        3.196830  -0.973130  -4.972311
      6        3.334554   1.068350  -3.697149
      6        4.568098  -1.140365  -4.849718
      1        2.611453  -1.706194  -5.518769
      6        4.705458   0.892863  -3.584173
      1        2.886185   1.950834  -3.254148
```

| | | | |
|---|---|---|---|
| 6 | 5.341979 | -0.210616 | -4.155388 |
| 1 | 5.039506 | -2.006721 | -5.302091 |
| 1 | 5.290676 | 1.631895 | -3.046438 |
| 1 | 6.413537 | -0.339863 | -4.062938 |

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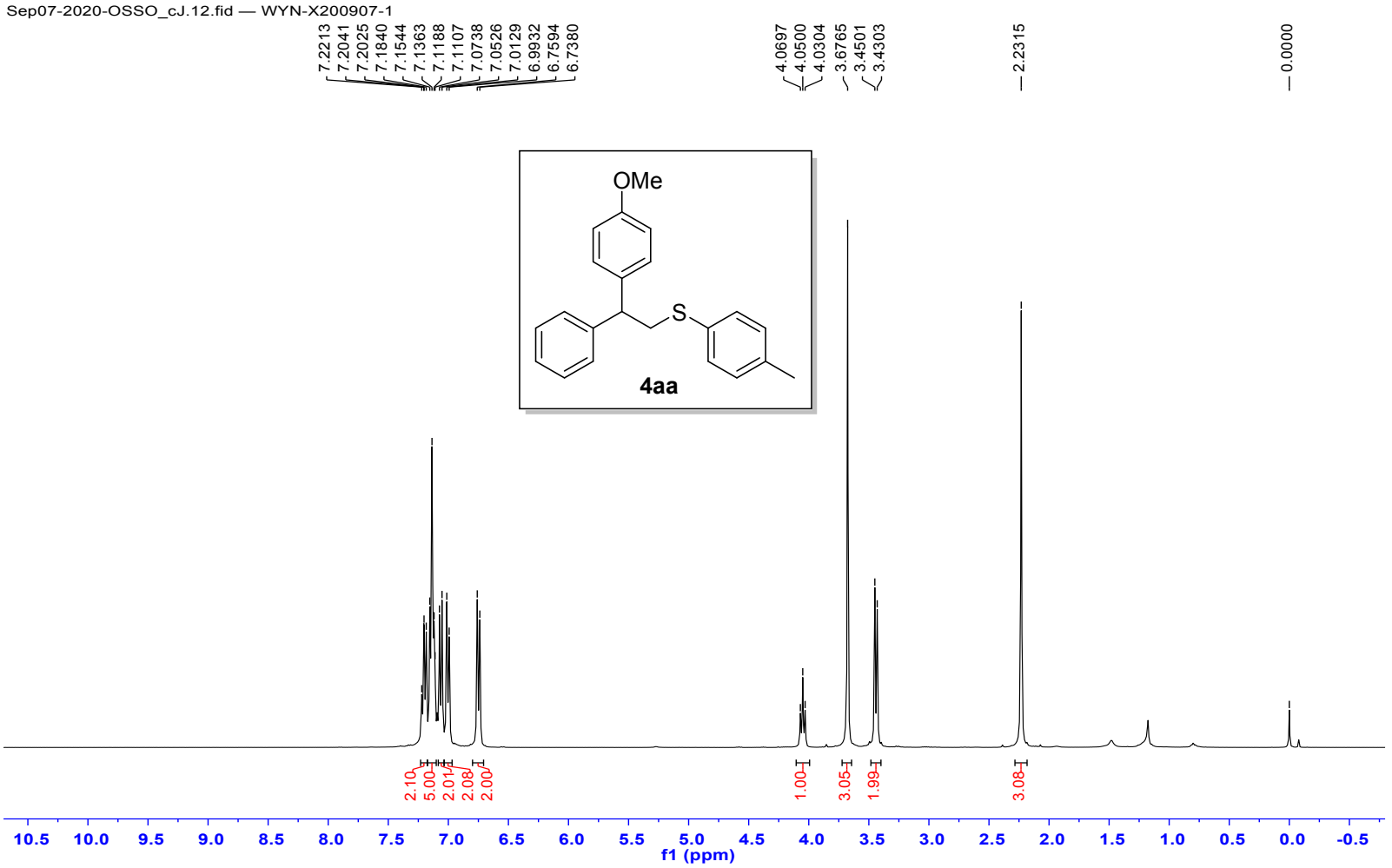
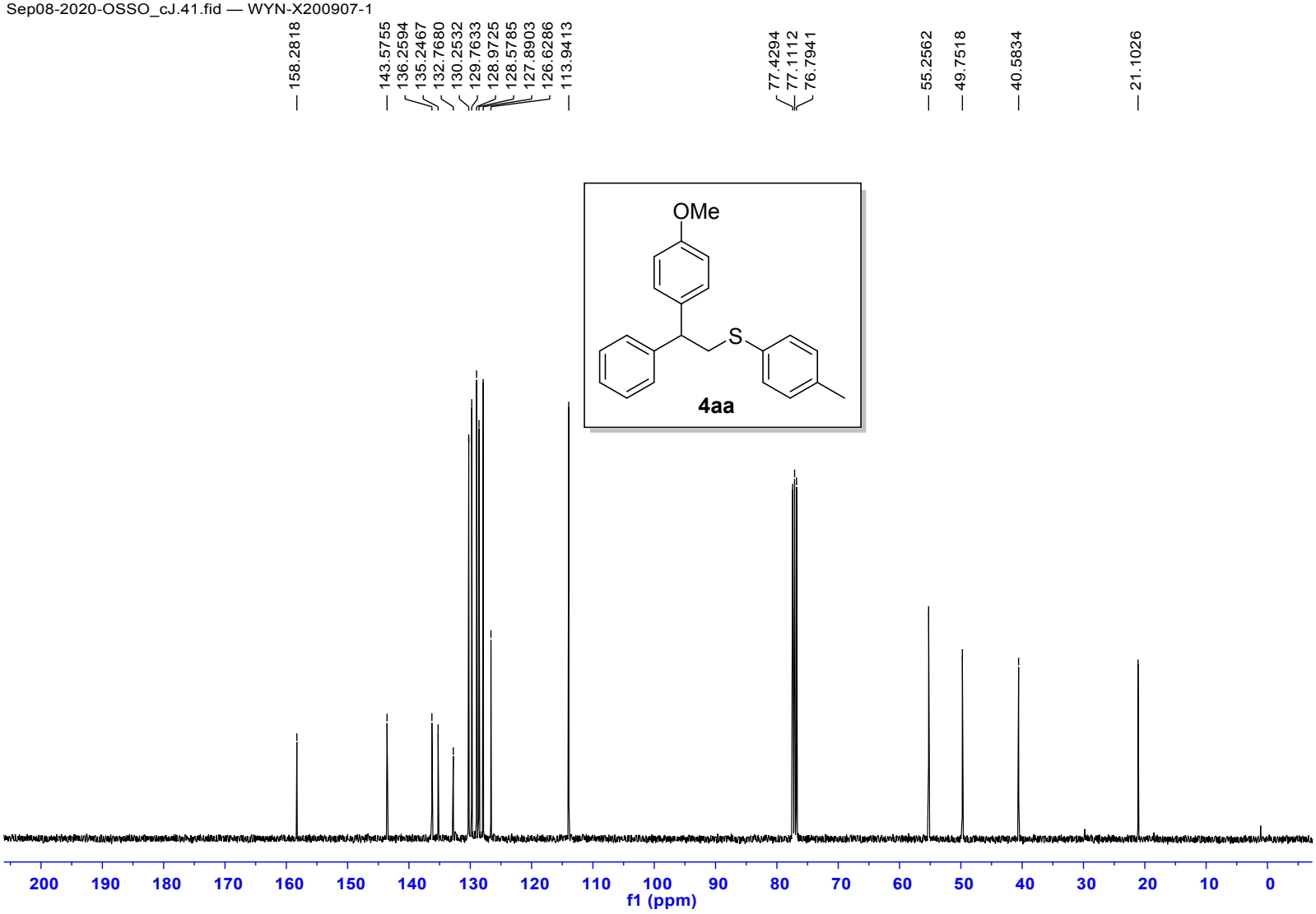
# 9. Copies of NMR spectra of the products

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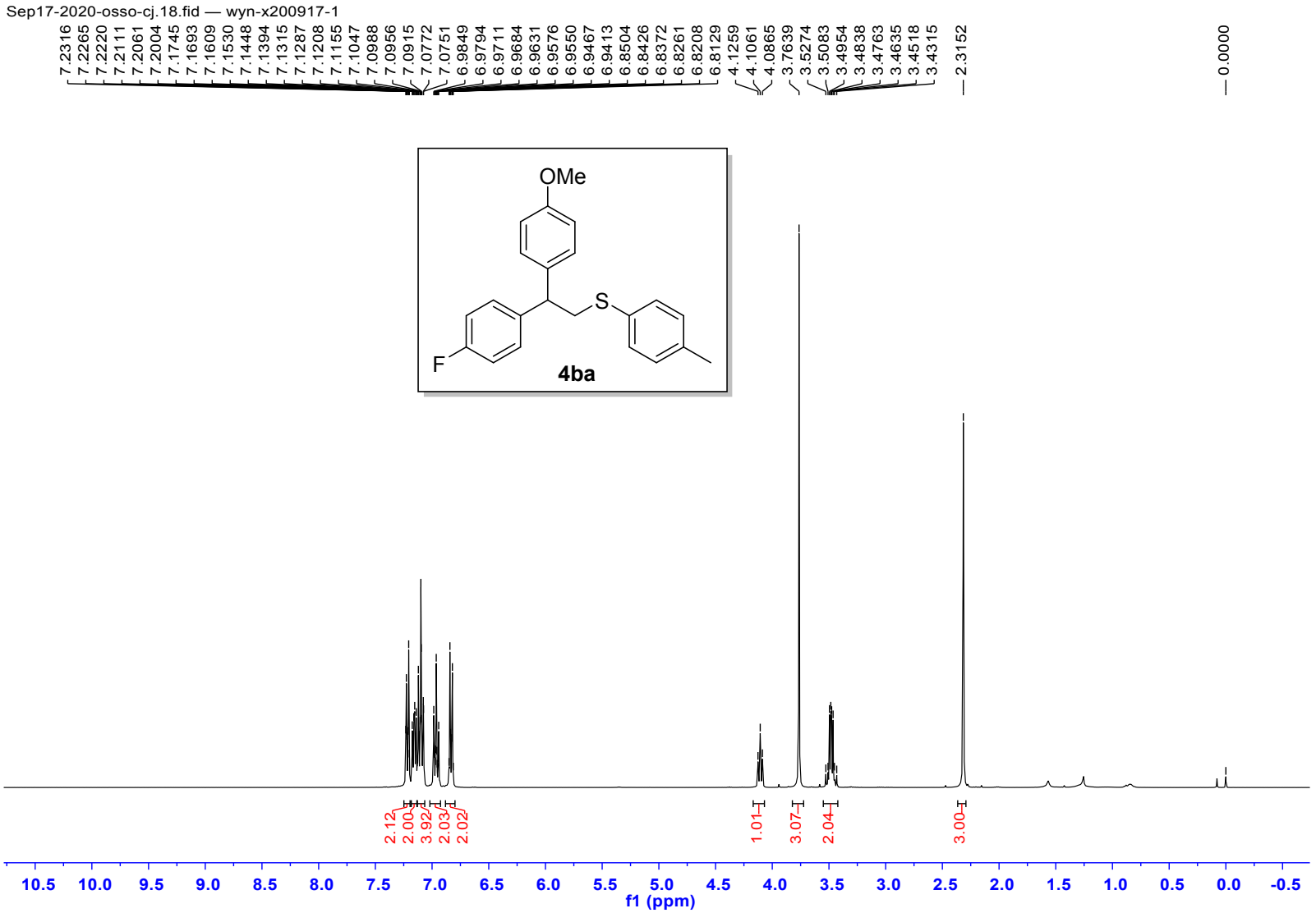
128.5785
127.8903
126.6286
113.9413
77.4294
77.1112
76.7941
55.2562
49.7518
40.5834
21.1026
OMe
S
4aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.1609
7.1530
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7.1394
7.1315
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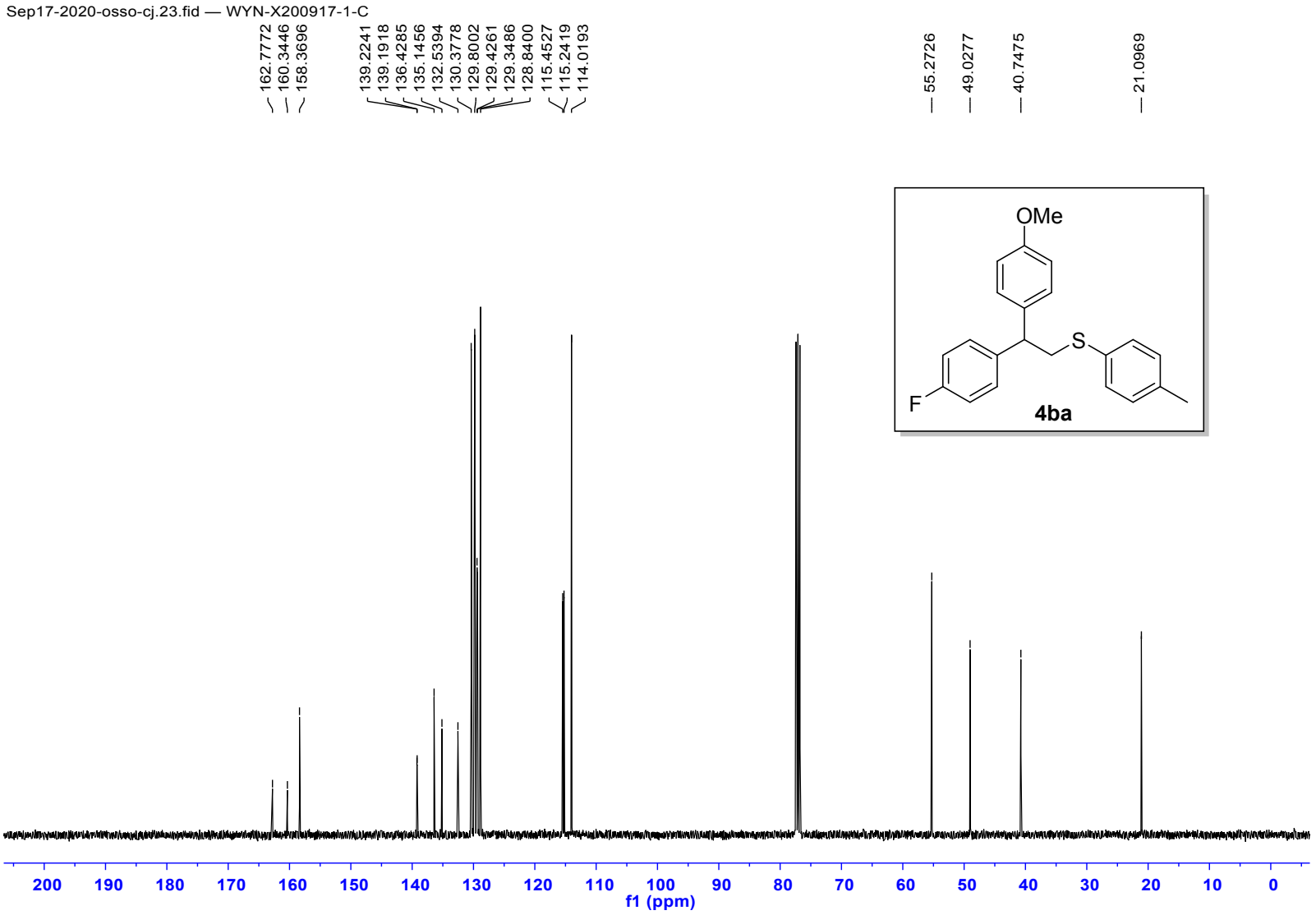
7.1208
7.1155
7.1047
7.0988
7.0956
7.0915
7.0772
7.0751
6.9849
6.9794
6.9711
6.9684
6.9631
6.9576
6.9550
6.9467
6.9413
6.8504
6.8426
6.8372
6.8261
6.8208
6.8129
4.1259
4.1061
4.0865
3.7639
3.5274
3.5083
3.4954
3.4838
3.4763
3.4635
3.4518
3.4315
2.3152
0.0000
OMe
S
F
4ba
2.12
2.00
3.92
2.03
2.02
1.01
3.07
2.04
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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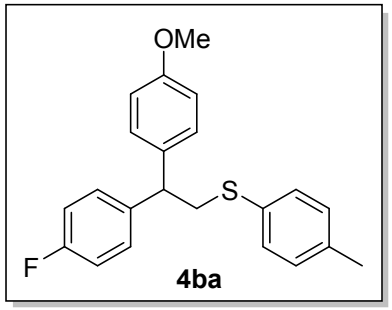
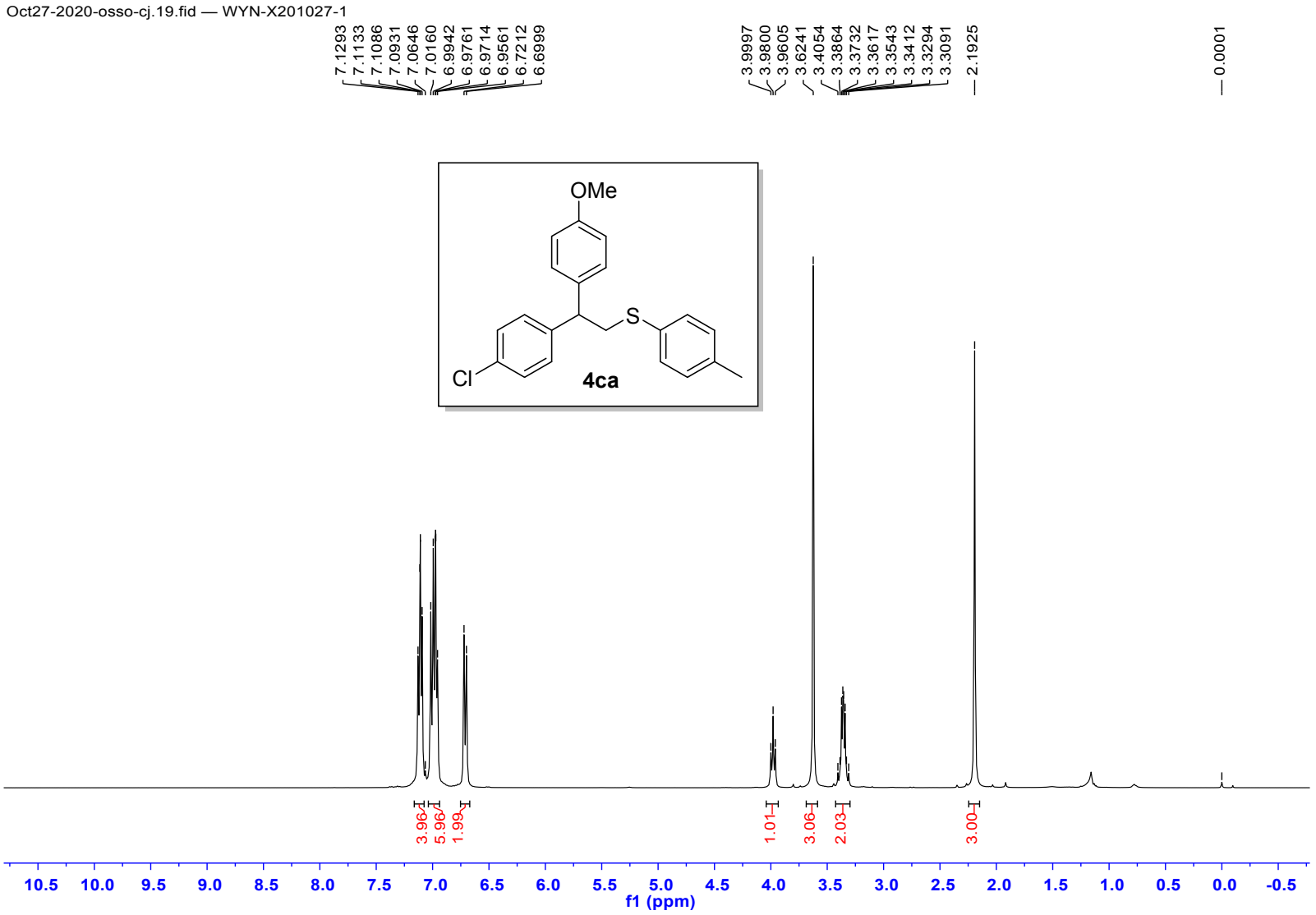
135.1456
132.5394
130.3778
129.8002
129.4261
129.3486
128.8400
115.4527
115.2419
114.0193
55.2726
49.0277
40.7475
21.0969
OMe
S
F
4ba
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Sep17-2020-OSSO_cJ.24.fid — WYN-X200917-1-F




**4ba**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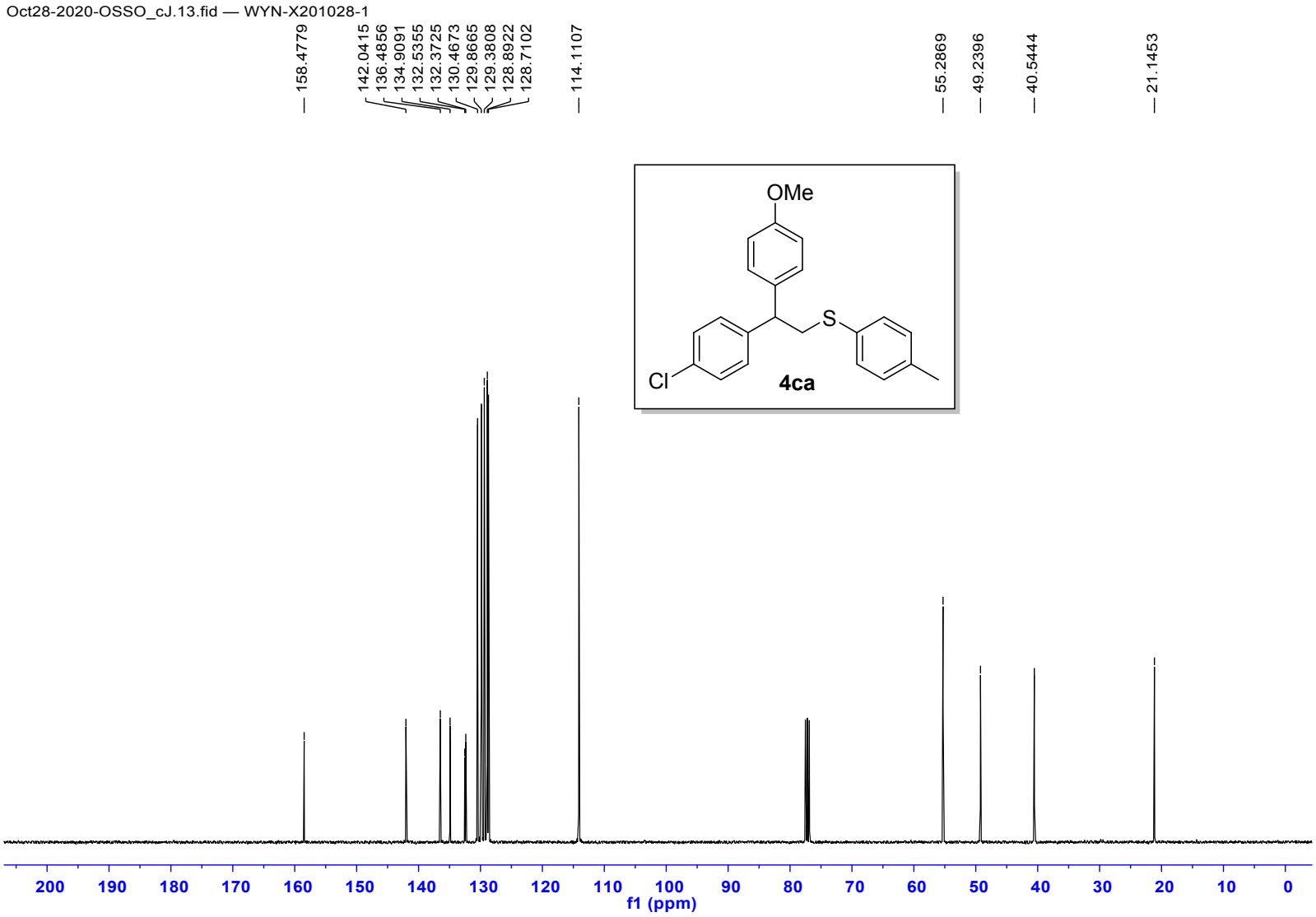
6.9714
6.9561
6.7212
6.6999
3.9997
3.9800
3.9605
3.6241
3.4054
3.3864
3.3732
3.3617
3.3543
3.3412
3.3294
3.3091
2.1925
0.0001
OMe
S
Cl
4ca
3.96
5.96
1.99
1.01
3.06
2.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.9091
132.5355
132.3725
130.4673
129.8665
129.3808
128.8922
128.7102
114.1107
55.2869
49.2396
40.5444
21.1453
OMe
S
Cl
4ca
200
190
180
170
160
150
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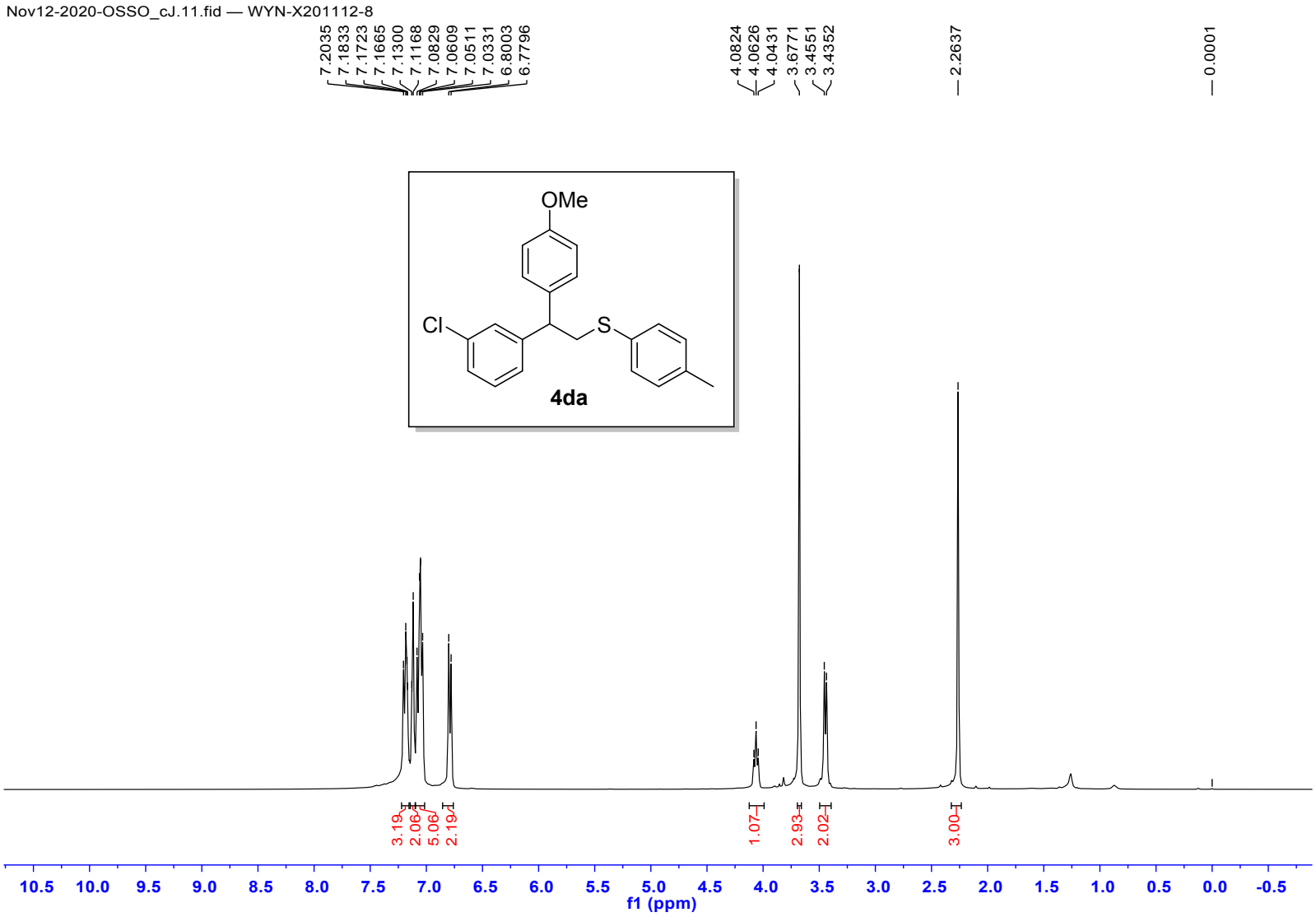
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.0331
6.8003
6.7796
4.0824
4.0626
4.0431
3.6771
3.4551
3.4352
2.2637
0.0001
OMe
Cl
S
4da
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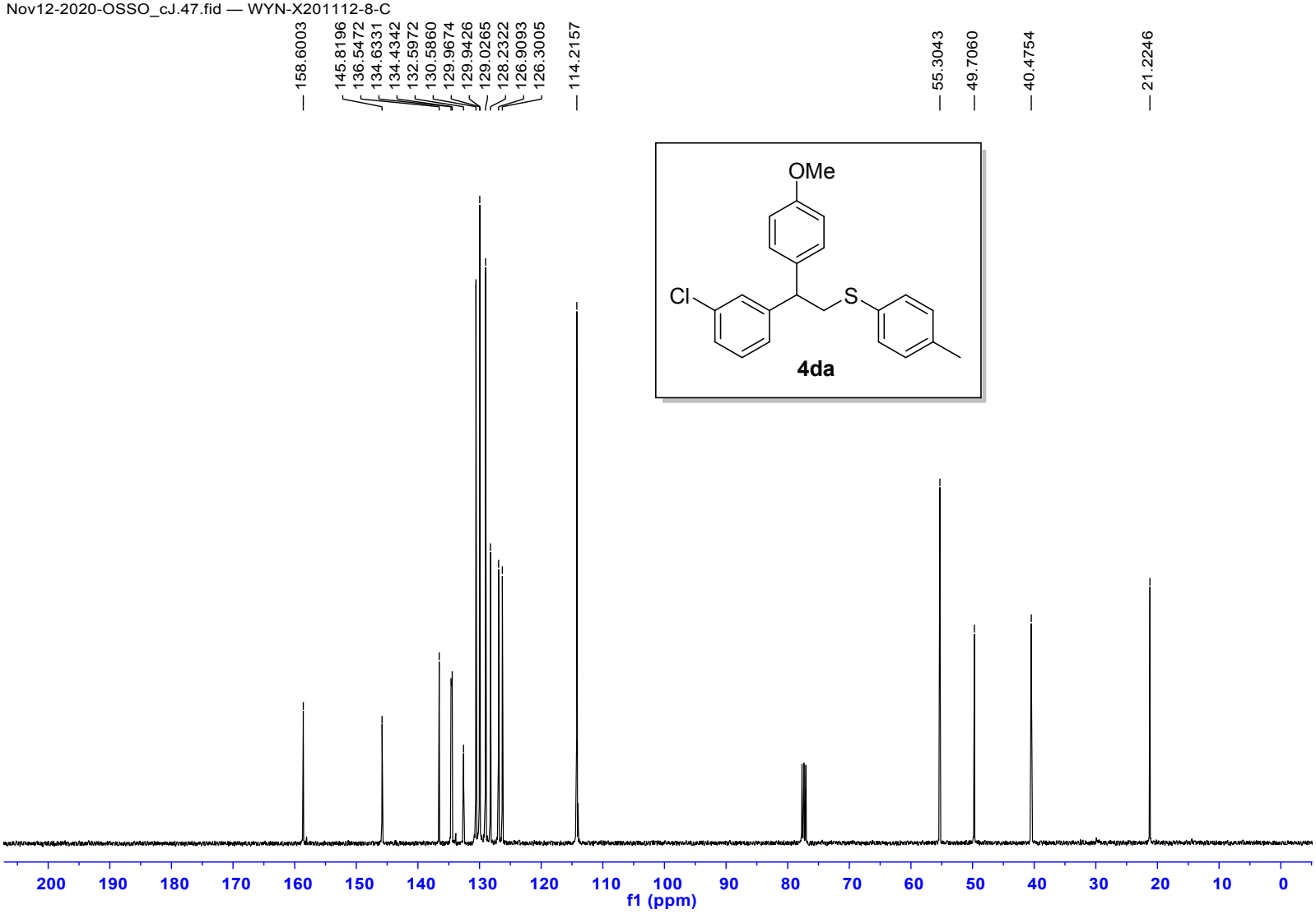
2.06
5.06
2.19
1.07
2.93
2.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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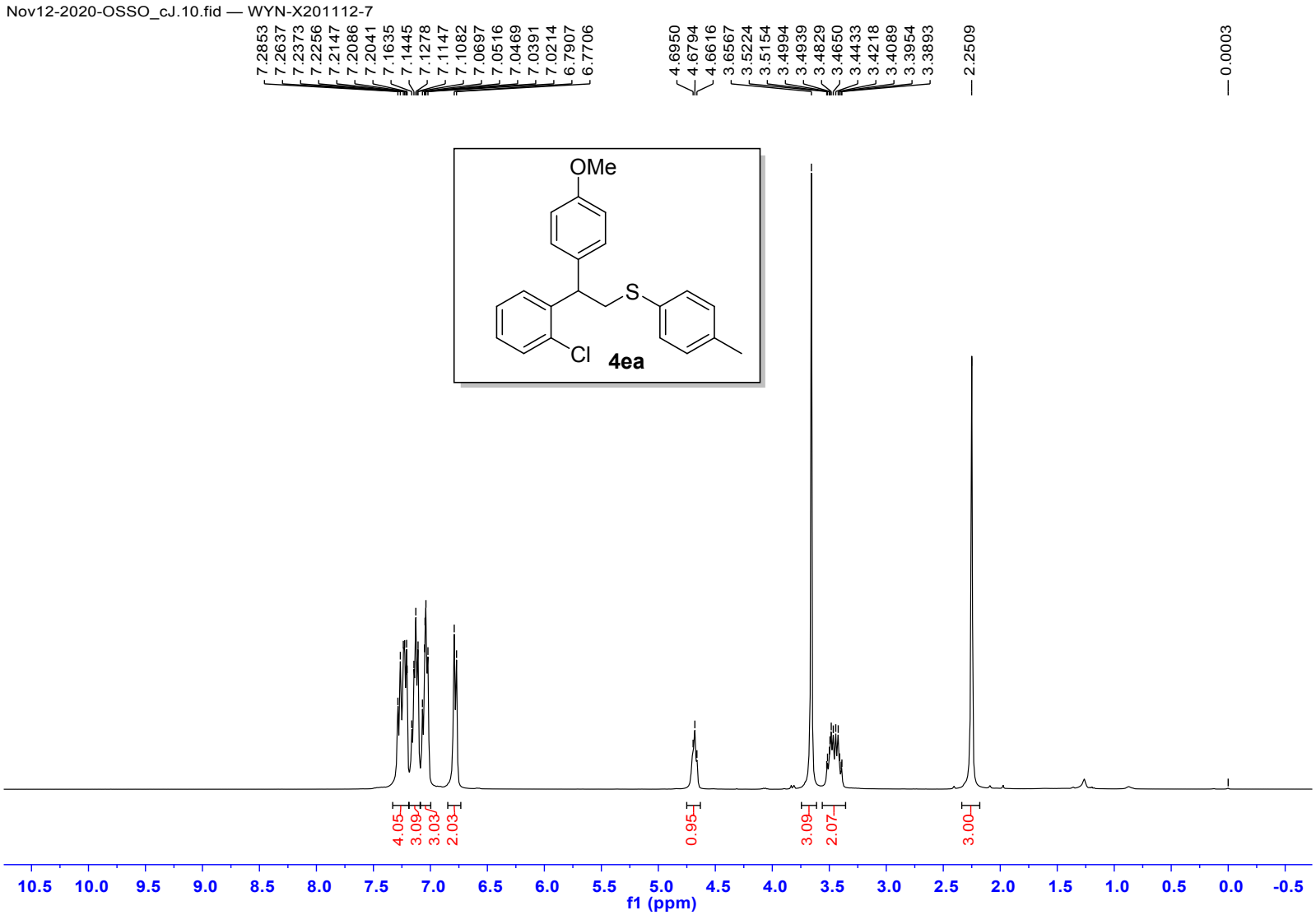
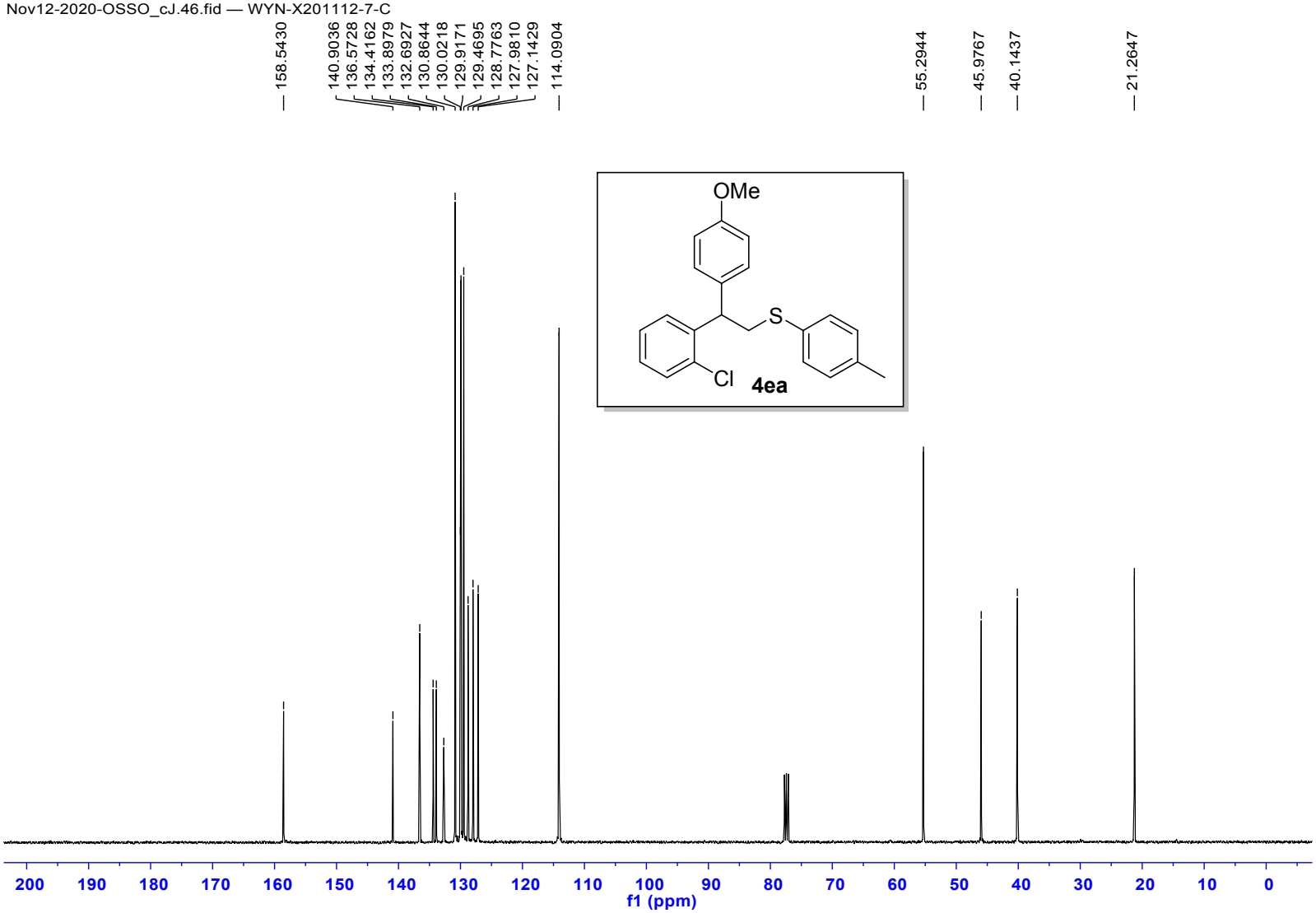
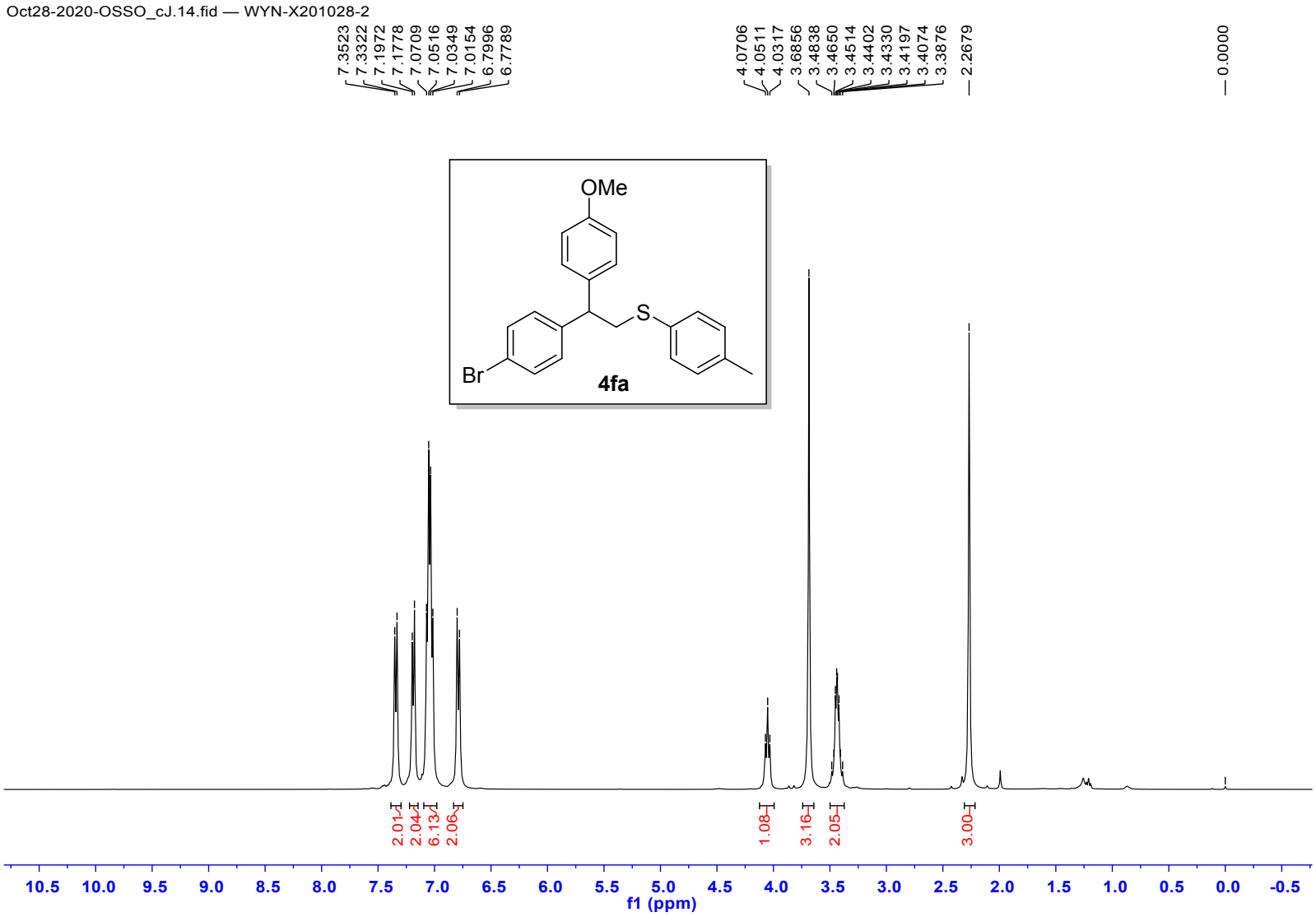
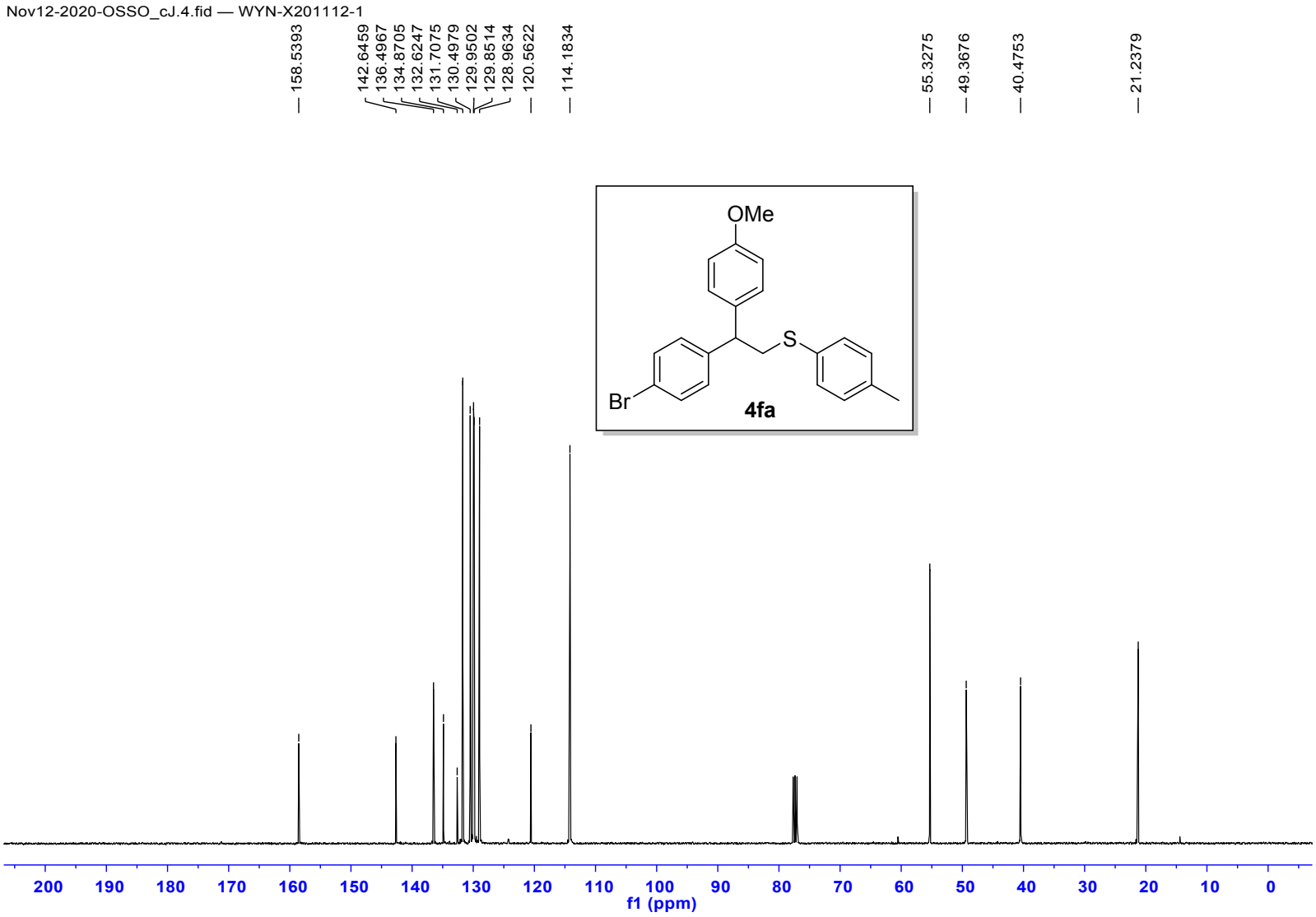
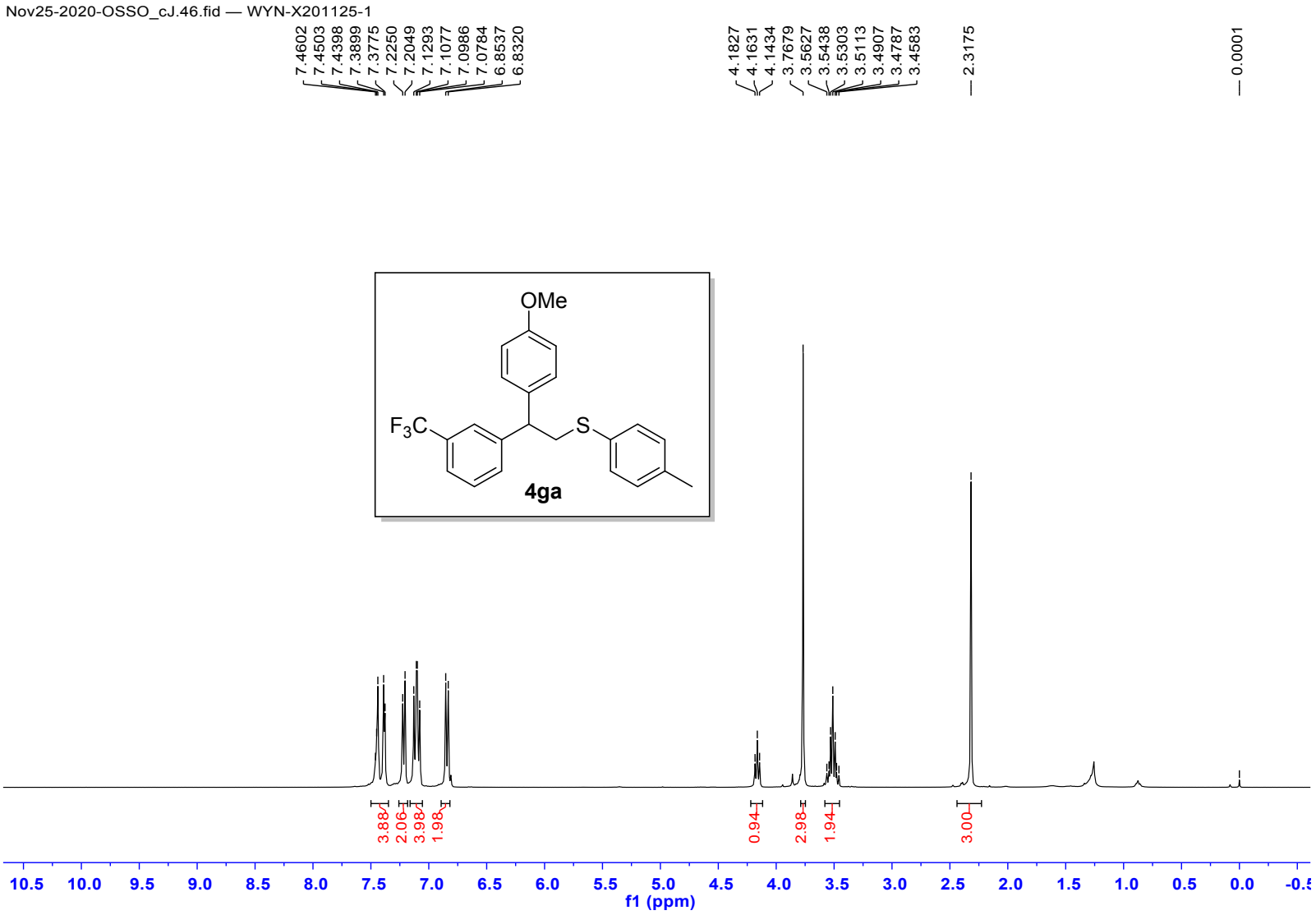
129.0265
128.2322
126.9093
126.3005
114.2157
55.3043
49.7060
40.4754
21.2246
OMe
Cl
S
4da
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

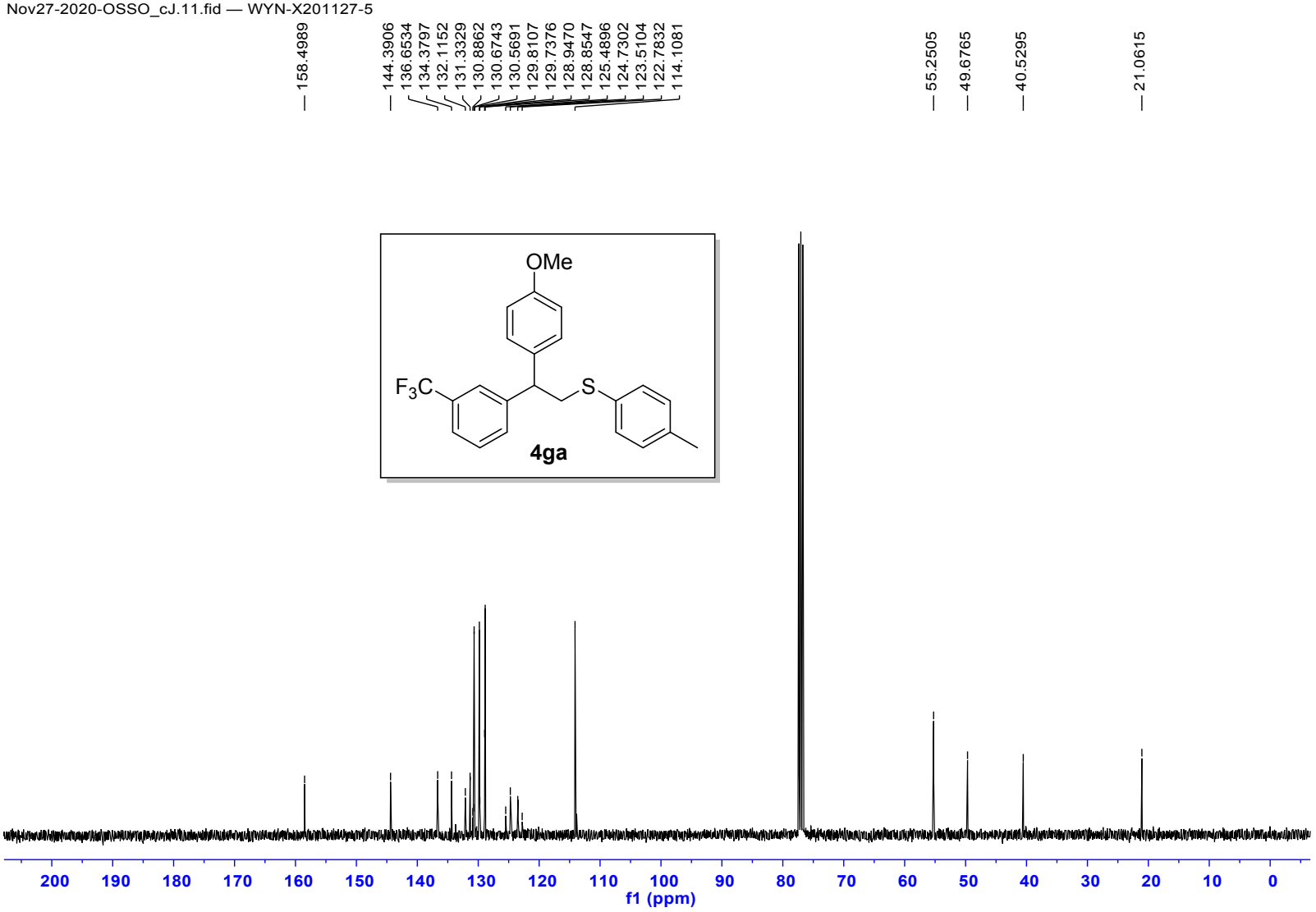

Nov12-2020-OSSO_cJ.10.fid — WYN-X201112-7
7.2853
7.2637
7.2373
7.2256
7.2147
7.2086
7.2041
7.1635
7.1445
7.1278
7.1147
7.1082
7.0697
7.0516
7.0469
7.0391
7.0214
6.7907
6.7706
4.6950
4.6794
4.6616
3.6567
3.5224
3.5154
3.4994
3.4939
3.4829
3.4650
3.4433
3.4218
3.4089
3.3954
3.3893
2.2509
0.0003
OMe
S
Cl
4ea
4.05
3.09
3.03
2.03
0.95
3.09
2.07
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Nov12-2020-OSSO_cJ.46.fid — WYN-X201112-7-C
158.5430
140.9036
136.5728
134.4162
133.8979
132.6927
130.8644
130.0218
129.9171
129.4695
128.7763
127.9810
127.1429
114.0904
55.2944
45.9767
40.1437
21.2647
OMe
S
Cl
4ea
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

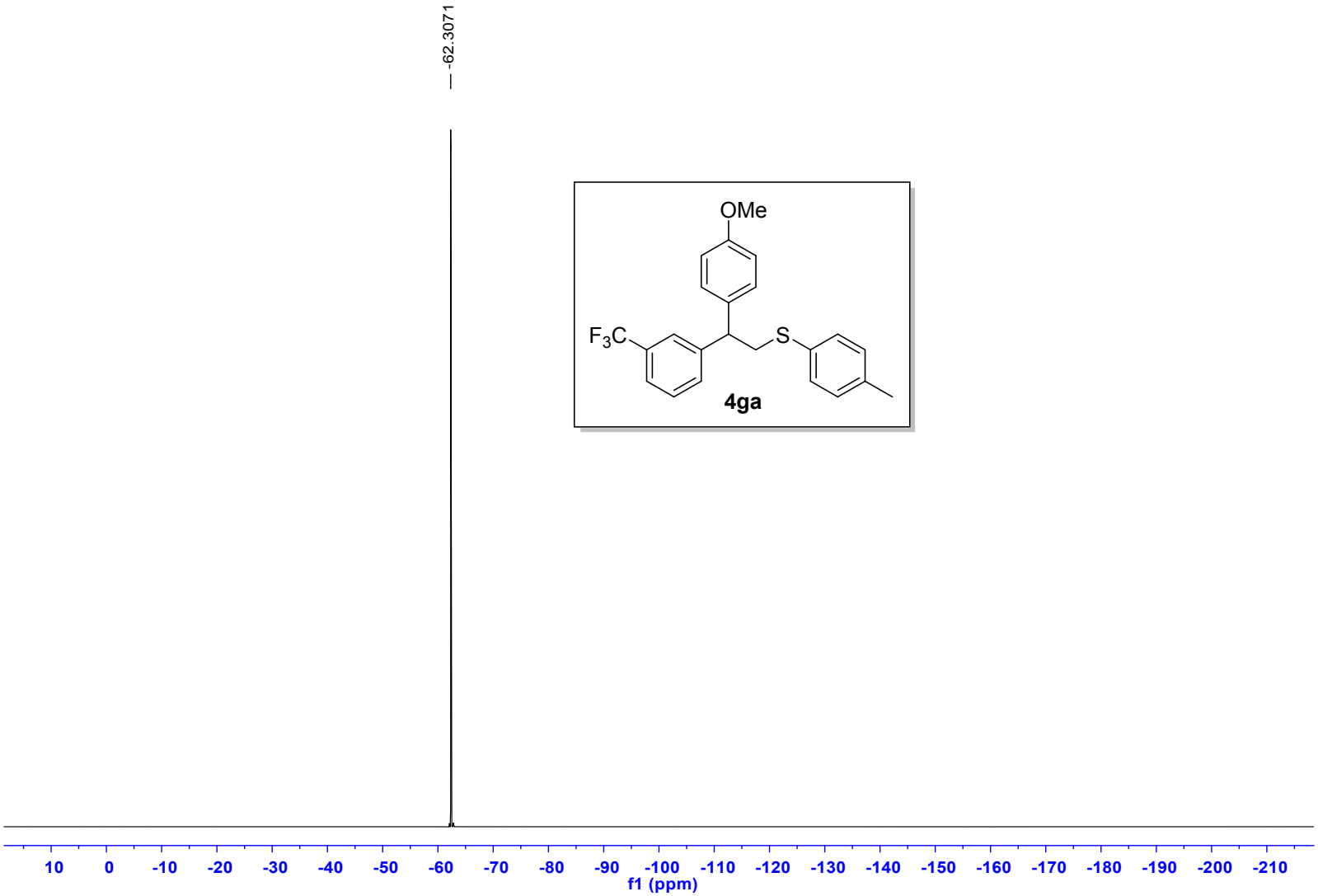

Oct28-2020-OSSO_cJ.14.fid — WYN-X201028-2
7.3523
7.3322
7.1972
7.1778
7.0709
7.0516
7.0349
7.0154
6.7996
6.7789
4.0706
4.0511
4.0317
3.6856
3.4838
3.4650
3.4514
3.4402
3.4330
3.4197
3.4074
3.3876
2.2679
0.0000
OMe
S
Br
4fa
2.01
2.04
6.13
2.06
1.08
3.16
2.05
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

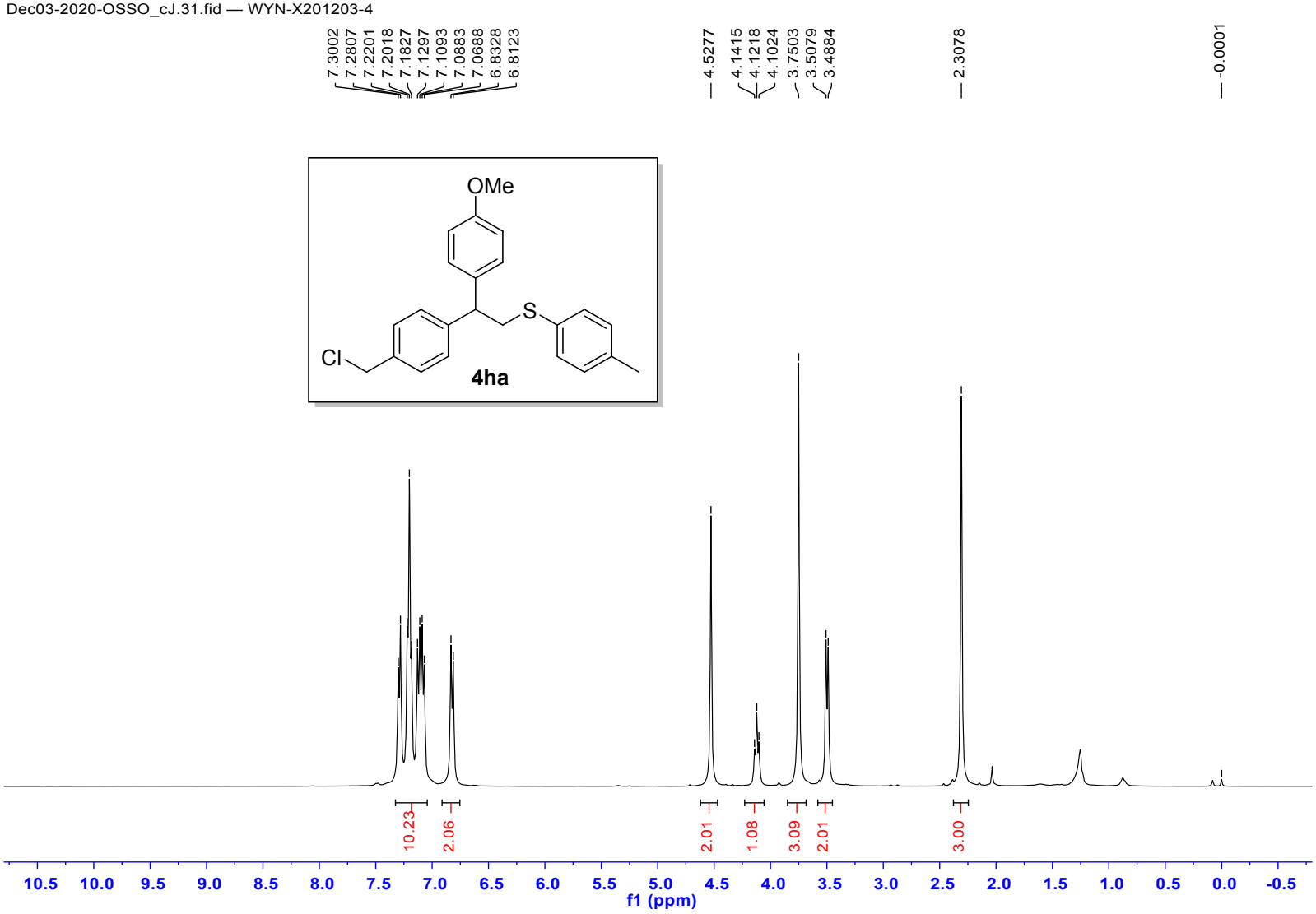

Nov12-2020-OSSO_cJ.4.fid — WYN-X201112-1
158.5393
142.6459
136.4967
134.8705
132.6247
131.7075
130.4979
129.9502
129.8514
128.9634
120.5622
114.1834
55.3275
49.3676
40.4753
21.2379
OMe
S
Br
4fa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov25-2020-OSSO_cJ.46.fid — WYN-X201125-1
7.4602
7.4503
7.4398
7.3899
7.3775
7.2250
7.2049
7.1293
7.1077
7.0986
7.0784
6.8537
6.8320
4.1827
4.1631
4.1434
3.7679
3.5627
3.5438
3.5303
3.5113
3.4907
3.4787
3.4583
2.3175
0.0001
OMe
F3C
S
4ga
3.88
2.06
3.98
1.98
0.94
2.98
1.94
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Nov27-2020-OSSO_cJ.11.fid — WYN-X201127-5
158.4989
144.3906
136.6534
134.3797
132.1152
131.3329
130.8862
130.6743
130.5691
129.8107
129.7376
128.9470
128.8547
125.4896
124.7302
123.5104
122.7832
114.1081
55.2505
49.6765
40.5295
21.0615
OMe
F3C
S
4ga
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

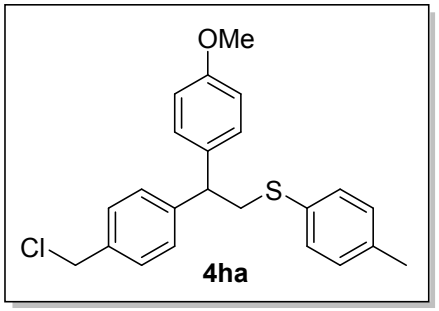
Nov12-2020-OSSO_cJ.49.fid — WYN-X201112-9-F



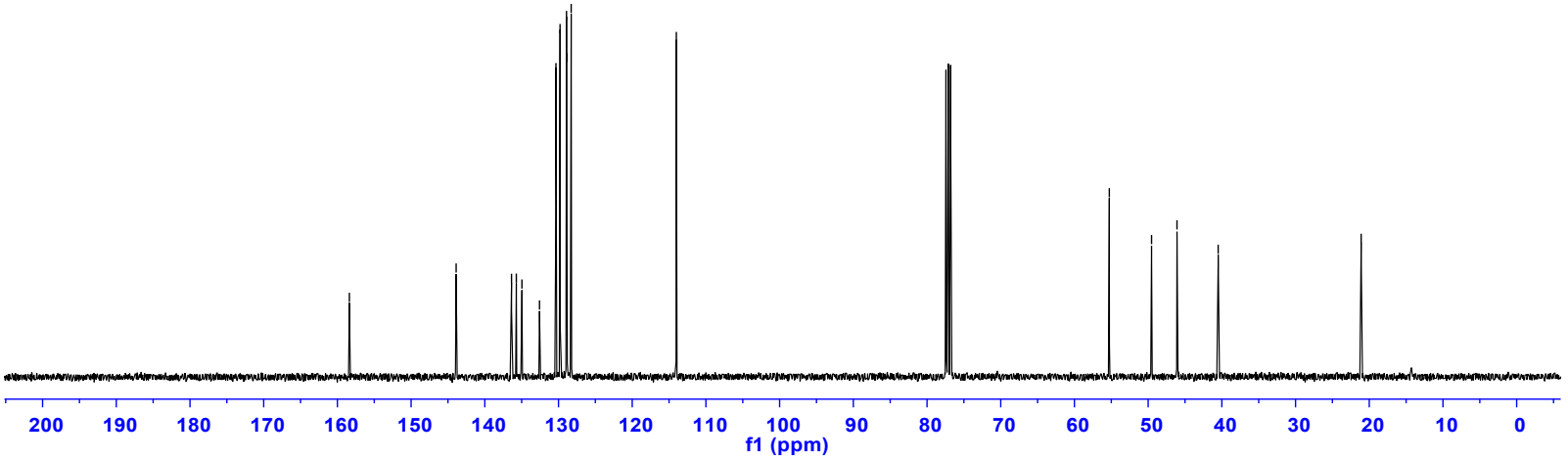

Dec03-2020-OSSO_cJ.31.fid — WYN-X201203-4
7.3002
7.2807
7.2201
7.2018
7.1827
7.1297
7.1093
7.0883
7.0688
6.8328
6.8123
4.5277
4.1415
4.1218
4.1024
3.7503
3.5079
3.4884
2.3078
-0.0001
OMe
S
Cl
4ha
10.23
2.06
2.01
1.08
3.09
2.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

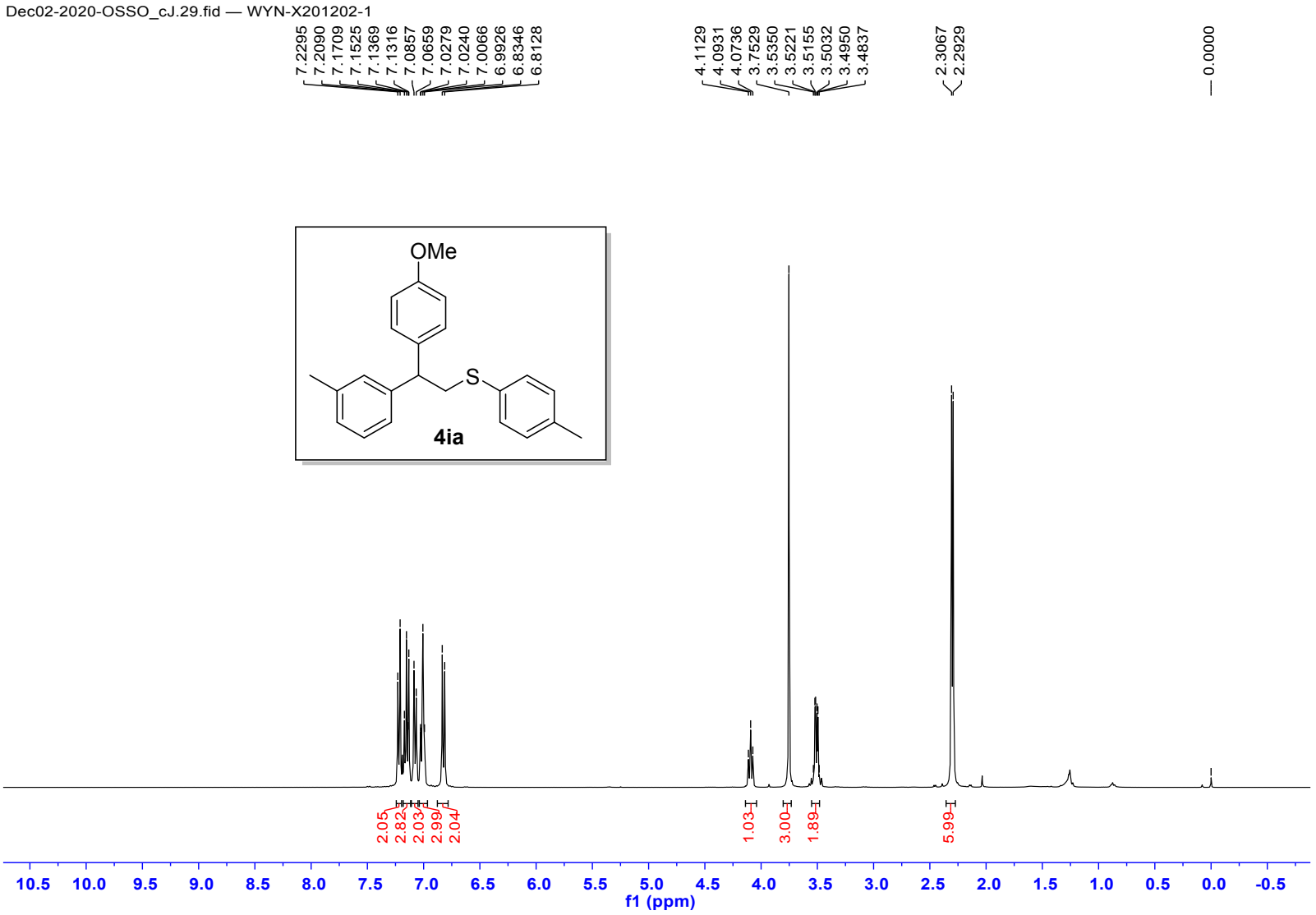
Dec04-2020-OSSO_cJ.10.fid — WYN-X201204-4

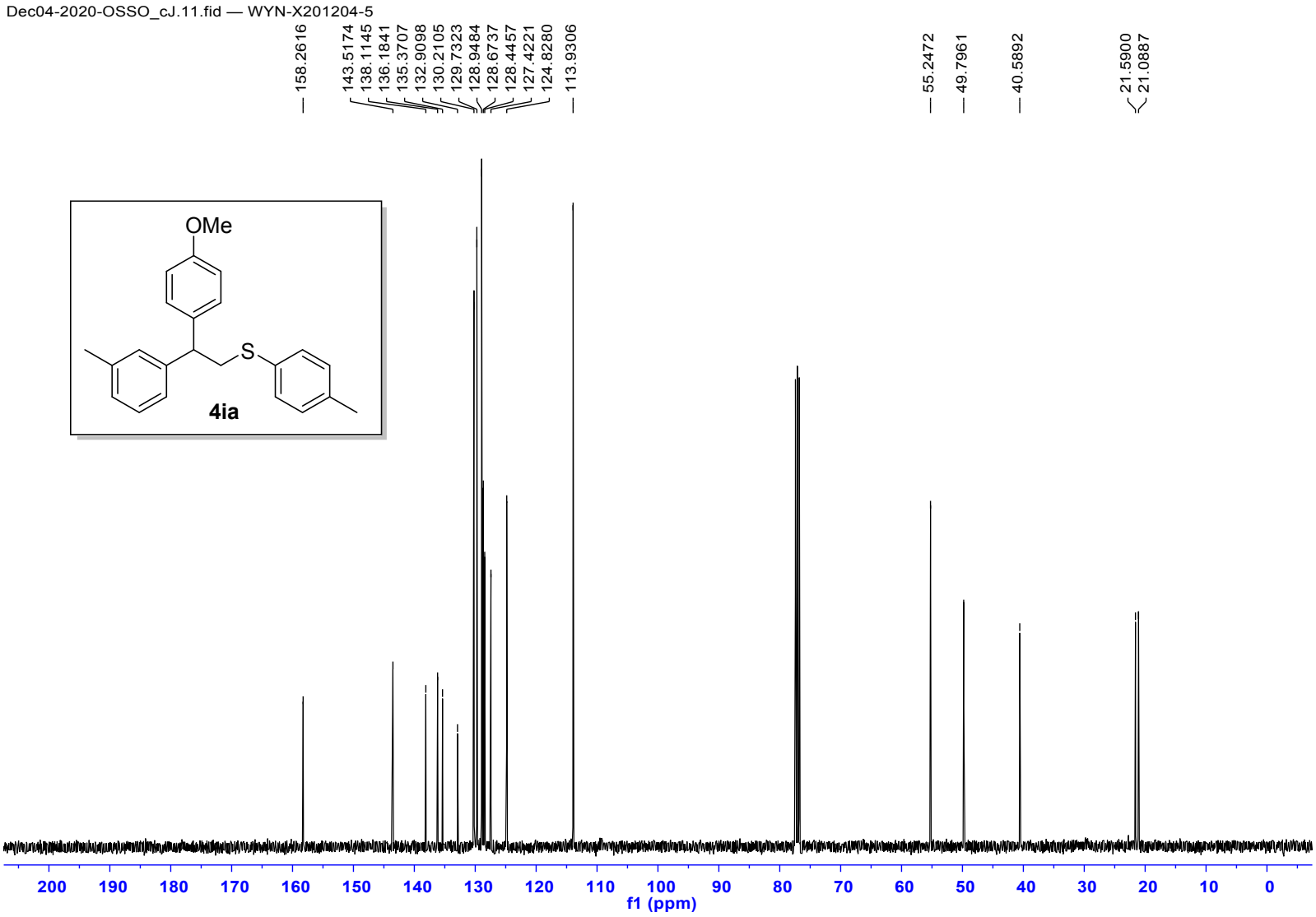
158.3776
143.8888
136.3735
135.7228
134.9622
132.5770
130.3491
129.7895
128.9155
128.8522
128.2800
114.0133
55.2682
49.5361
46.0863
40.4974
21.0983

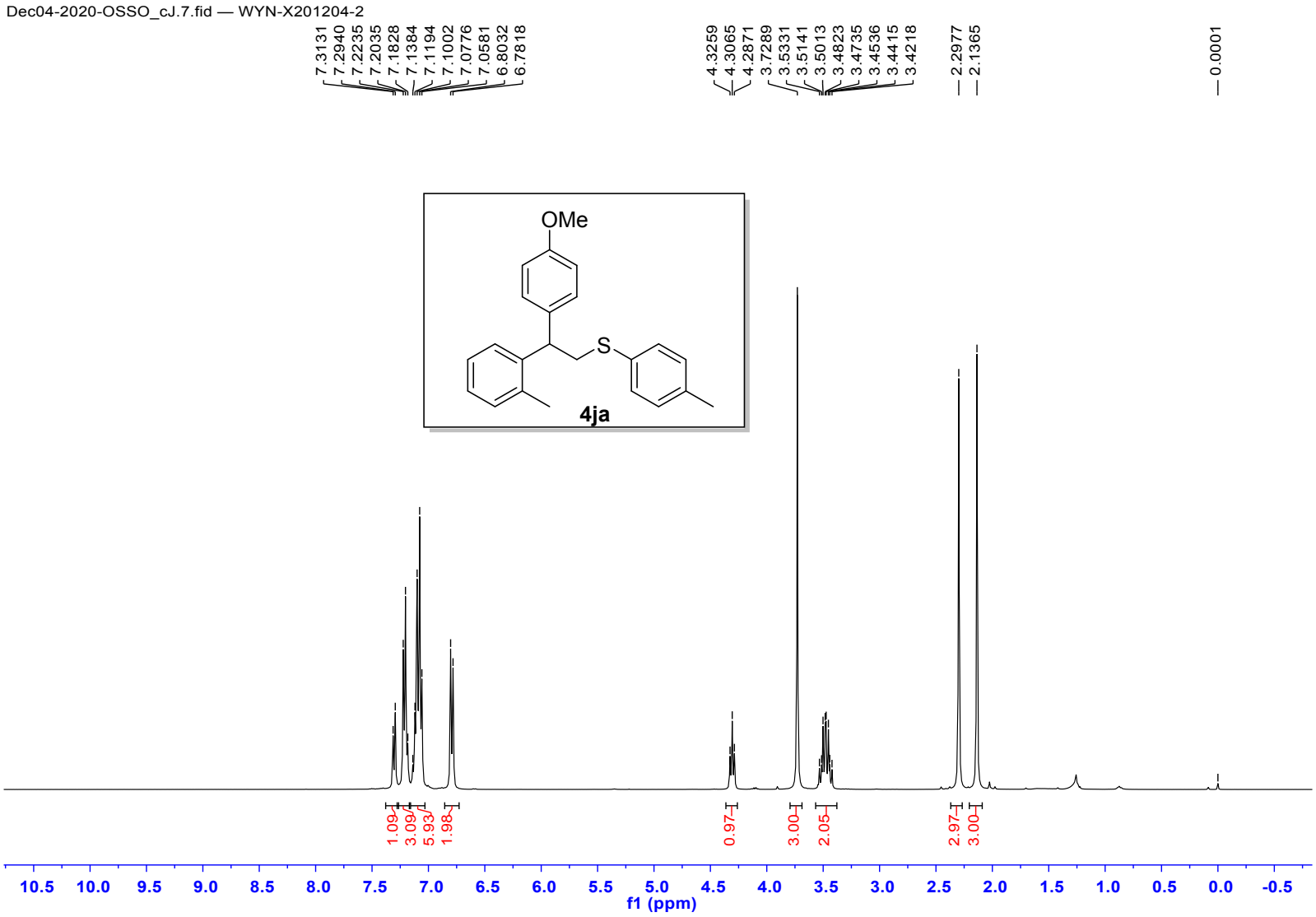


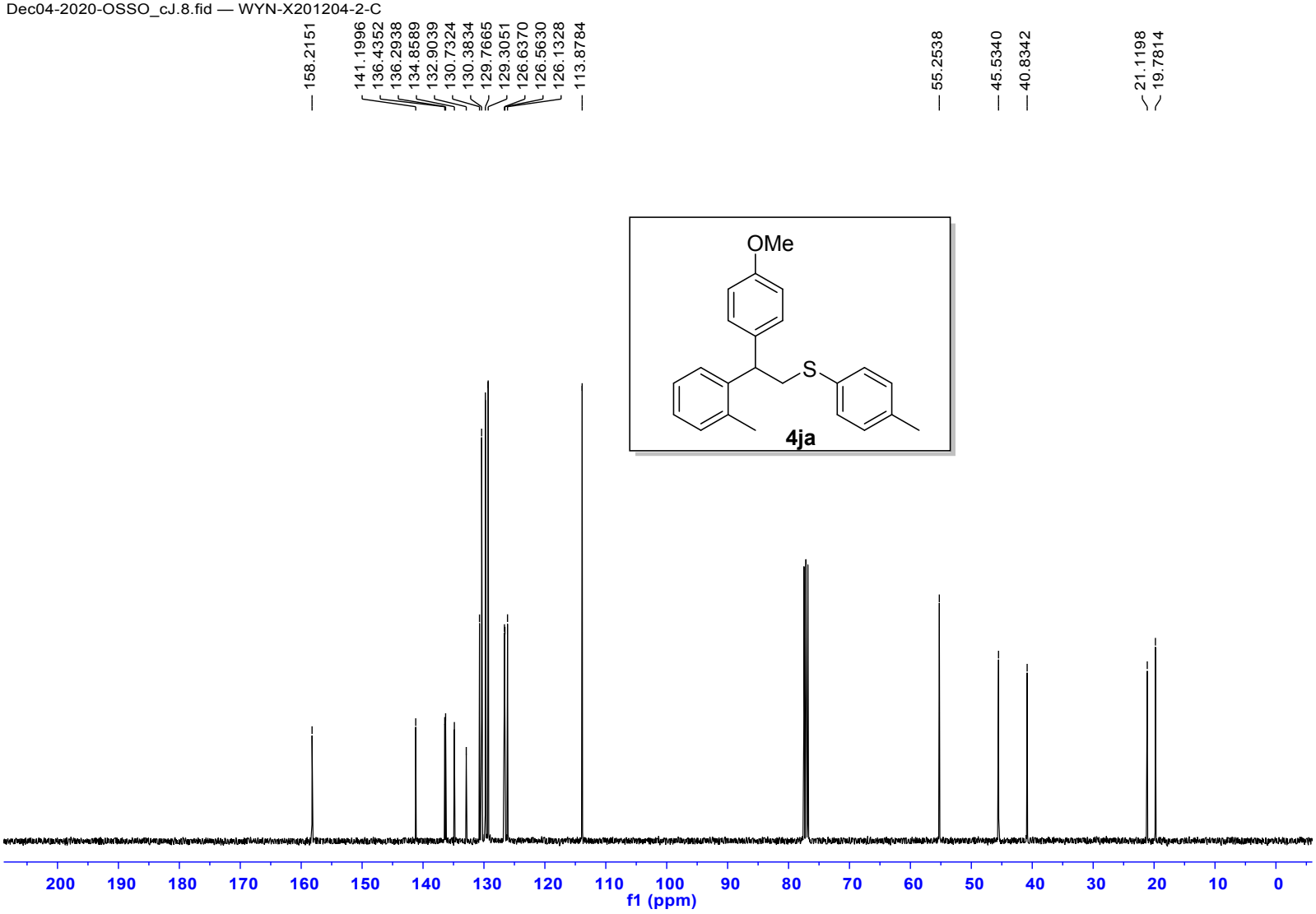

**4ha**

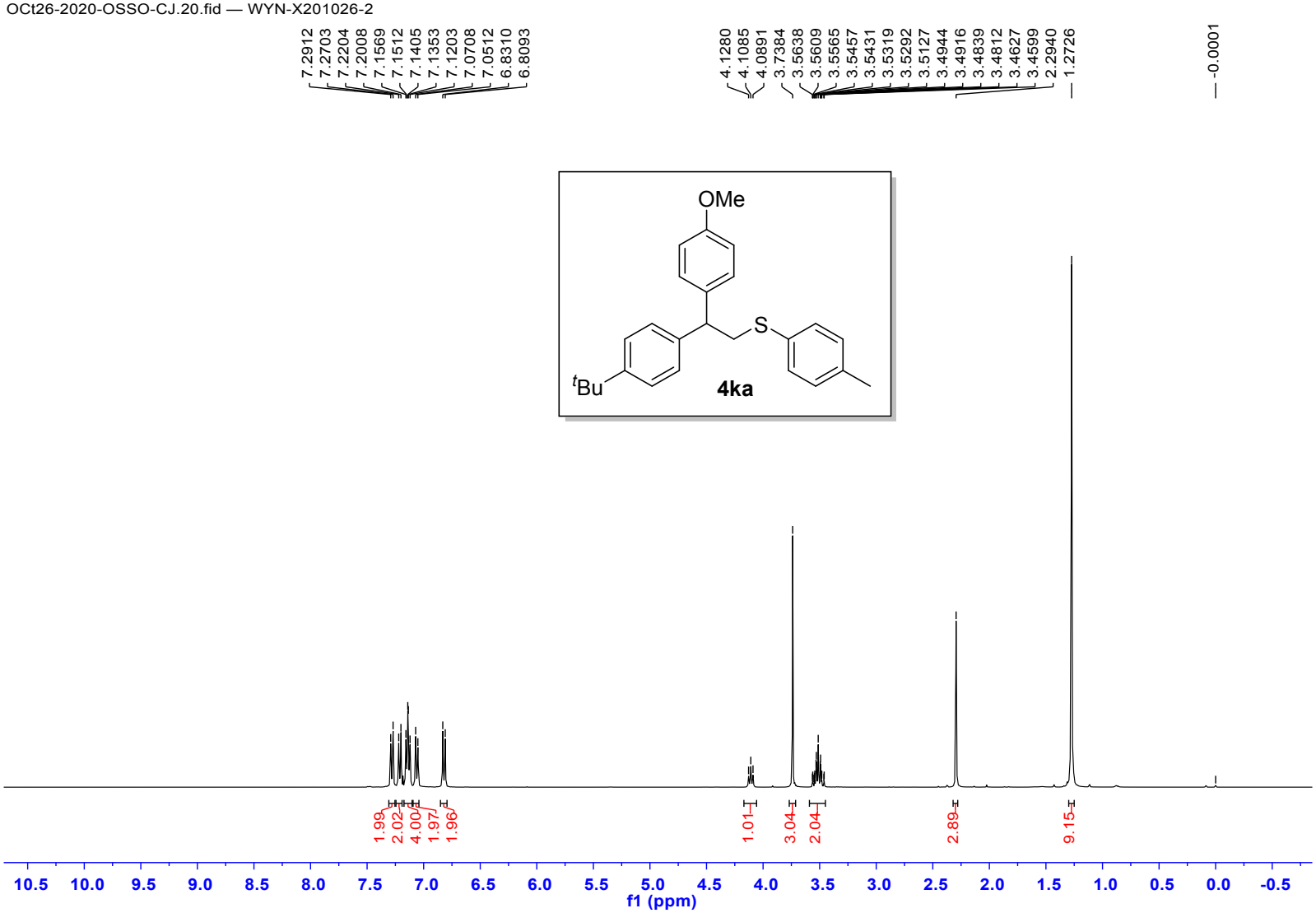


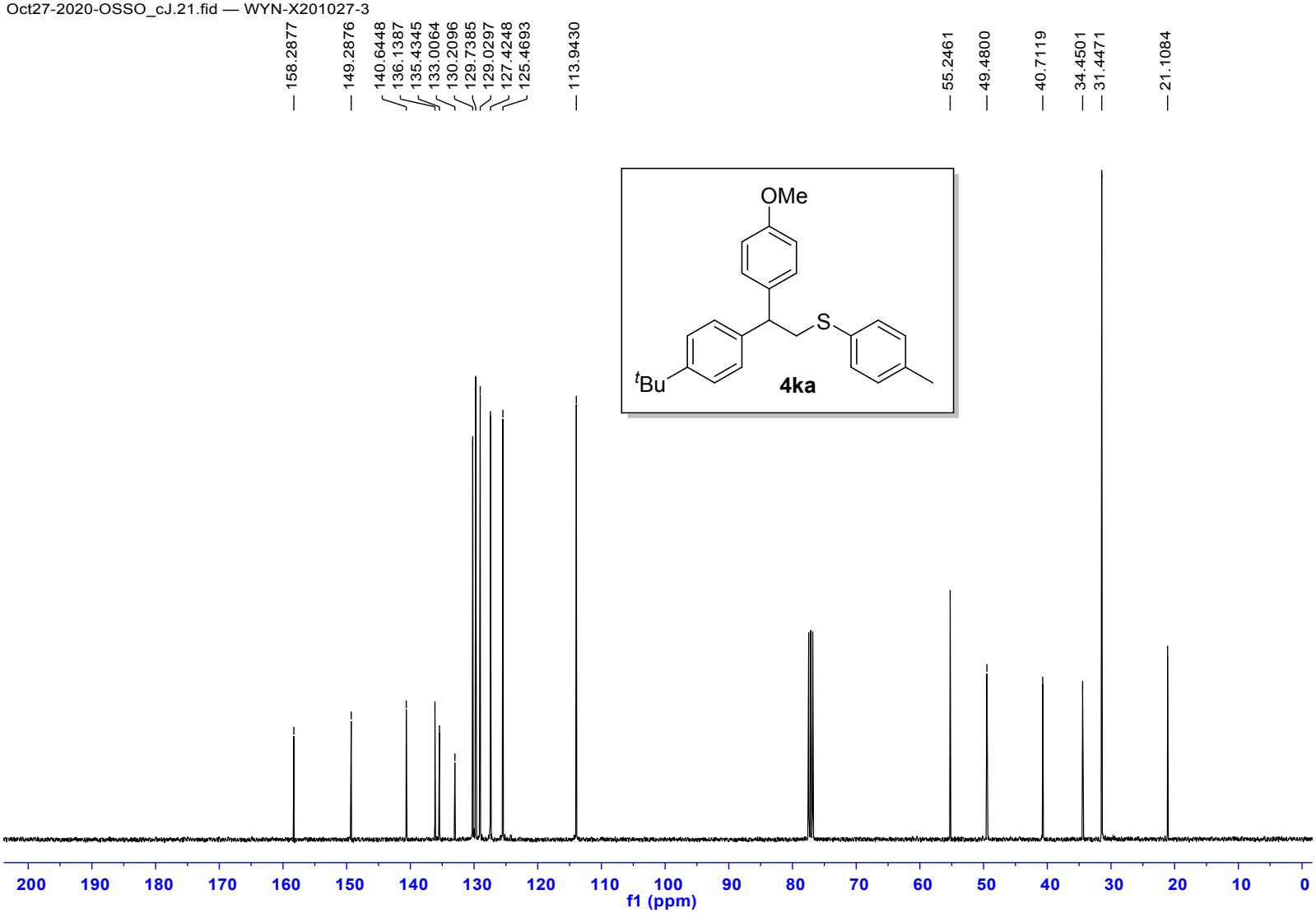

Dec02-2020-OSSO_cJ.29.fid — WYN-X201202-1
7.2295
7.2090
7.1709
7.1525
7.1369
7.1316
7.0857
7.0659
7.0279
7.0240
7.0066
6.9926
6.8346
6.8128
4.1129
4.0931
4.0736
3.7529
3.5350
3.5221
3.5155
3.5032
3.4950
3.4837
2.3067
2.2929
0.0000
OMe
S
4ia
2.05
2.82
2.03
2.99
2.04
1.03
3.00
1.89
5.99
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

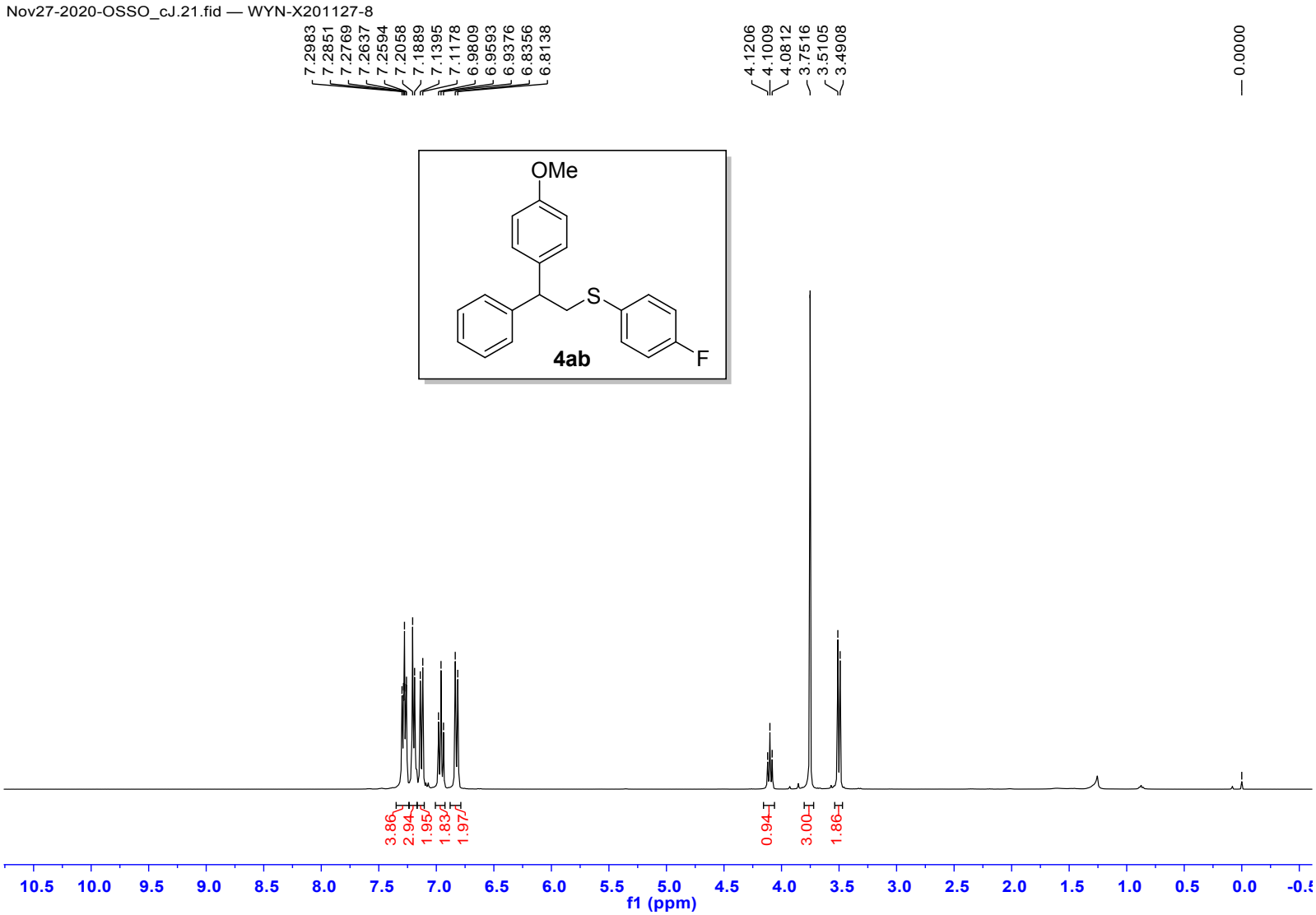

Dec04-2020-OSSO_cJ.11.fid — WYN-X201204-5
158.2616
143.5174
138.1145
136.1841
135.3707
132.9098
130.2105
129.7323
128.9484
128.6737
128.4457
127.4221
124.8280
113.9306
55.2472
49.7961
40.5892
21.5900
21.0887
OMe
S
4ia
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Dec04-2020-OSSO_cJ.7.fid — WYN-X201204-2
7.3131
7.2940
7.2235
7.2035
7.1828
7.1384
7.1194
7.1002
7.0776
7.0581
6.8032
6.7818
4.3259
4.3065
4.2871
3.7289
3.5331
3.5141
3.5013
3.4823
3.4735
3.4536
3.4415
3.4218
2.2977
2.1365
0.0001
OMe
S
4ja
1.09
3.09
5.93
1.98
0.97
3.00
2.05
2.97
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

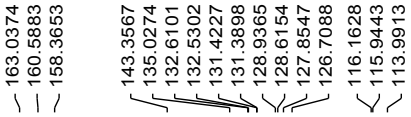

Dec04-2020-OSSO_cJ.8.fid — WYN-X201204-2-C
158.2151
141.1996
136.4352
136.2938
134.8589
132.9039
130.7324
130.3834
129.7665
129.3051
126.6370
126.5630
126.1328
113.8784
55.2538
45.5340
40.8342
21.1198
19.7814
OMe
S
4ja
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

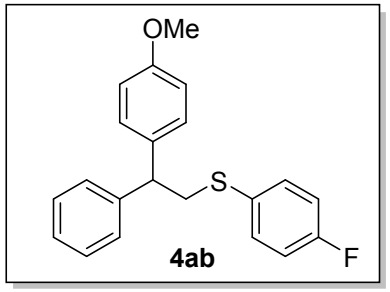

OCt26-2020-OSSO-CJ.20.fid — WYN-X201026-2
7.2912
7.2703
7.2204
7.2008
7.1569
7.1512
7.1405
7.1353
7.1203
7.0708
7.0512
6.8310
6.8093
4.1280
4.1085
4.0891
3.7384
3.5638
3.5609
3.5565
3.5457
3.5431
3.5319
3.5292
3.5127
3.4944
3.4916
3.4839
3.4812
3.4627
3.4599
2.2940
1.2726
-0.0001
OMe
S
tBu
4ka
1.99
2.02
4.00
1.97
1.96
1.01
3.04
2.04
2.89
9.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

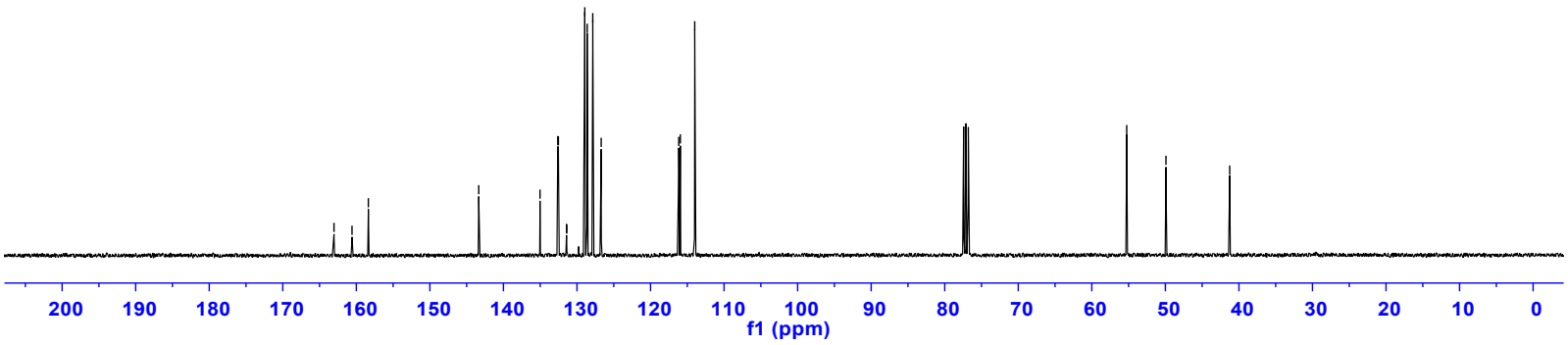

Oct27-2020-OSSO_cJ.21.fid — WYN-X201027-3
158.2877
149.2876
140.6448
136.1387
135.4345
133.0064
130.2096
129.7385
129.0297
127.4248
125.4693
113.9430
55.2461
49.4800
40.7119
34.4501
31.4471
21.1084
OMe
S
tBu
4ka
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov27-2020-OSSO_cJ.21.fid — WYN-X201127-8
7.2983
7.2851
7.2769
7.2637
7.2594
7.2058
7.1889
7.1395
7.1178
6.9809
6.9593
6.9376
6.8356
6.8138
4.1206
4.1009
4.0812
3.7516
3.5105
3.4908
0.0000
OMe
S
F
4ab
3.86
2.94
1.95
1.83
1.97
0.94
3.00
1.86
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

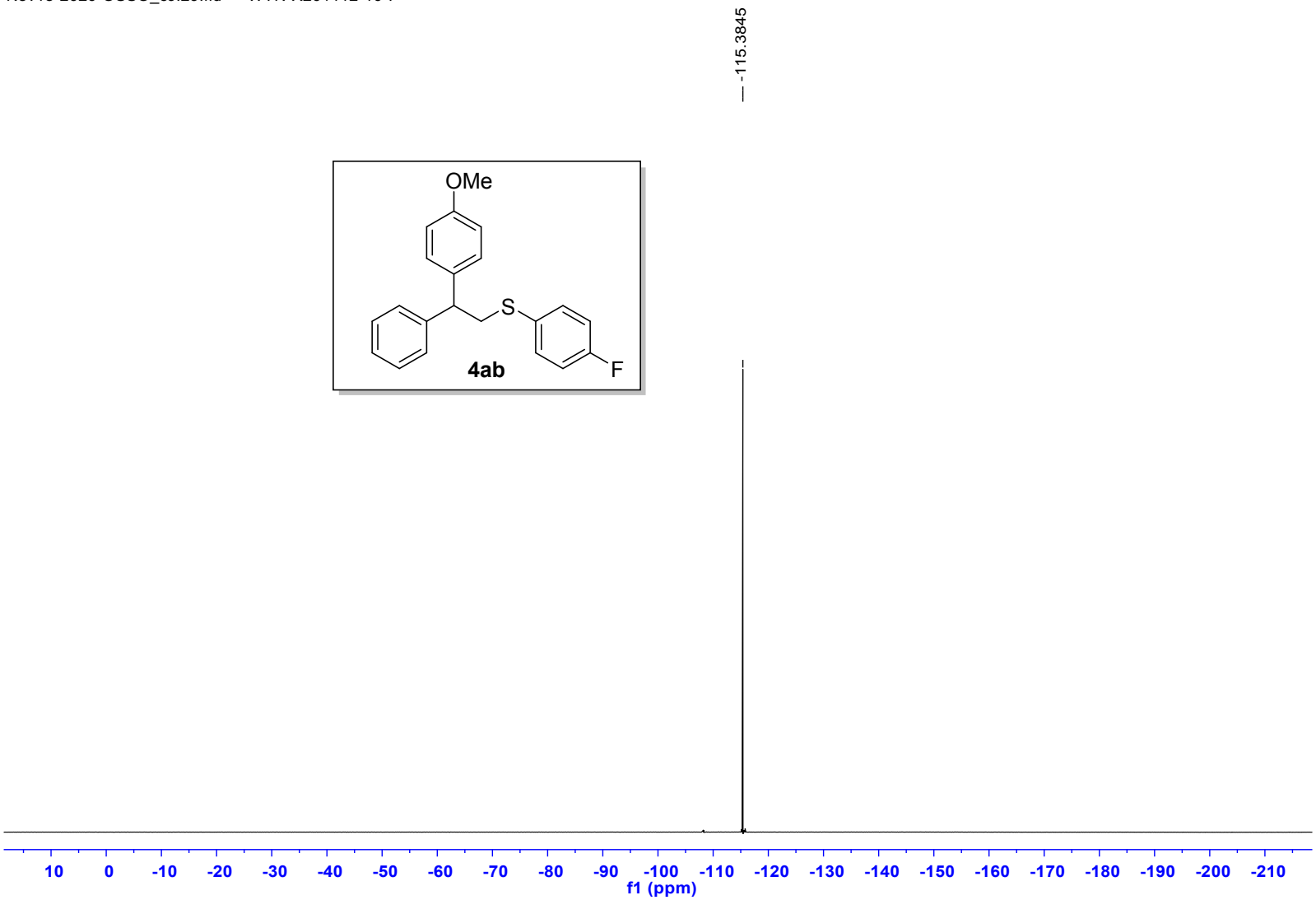
Nov30-2020-OSSO_cJ.14.fid — WYN-X201130-6

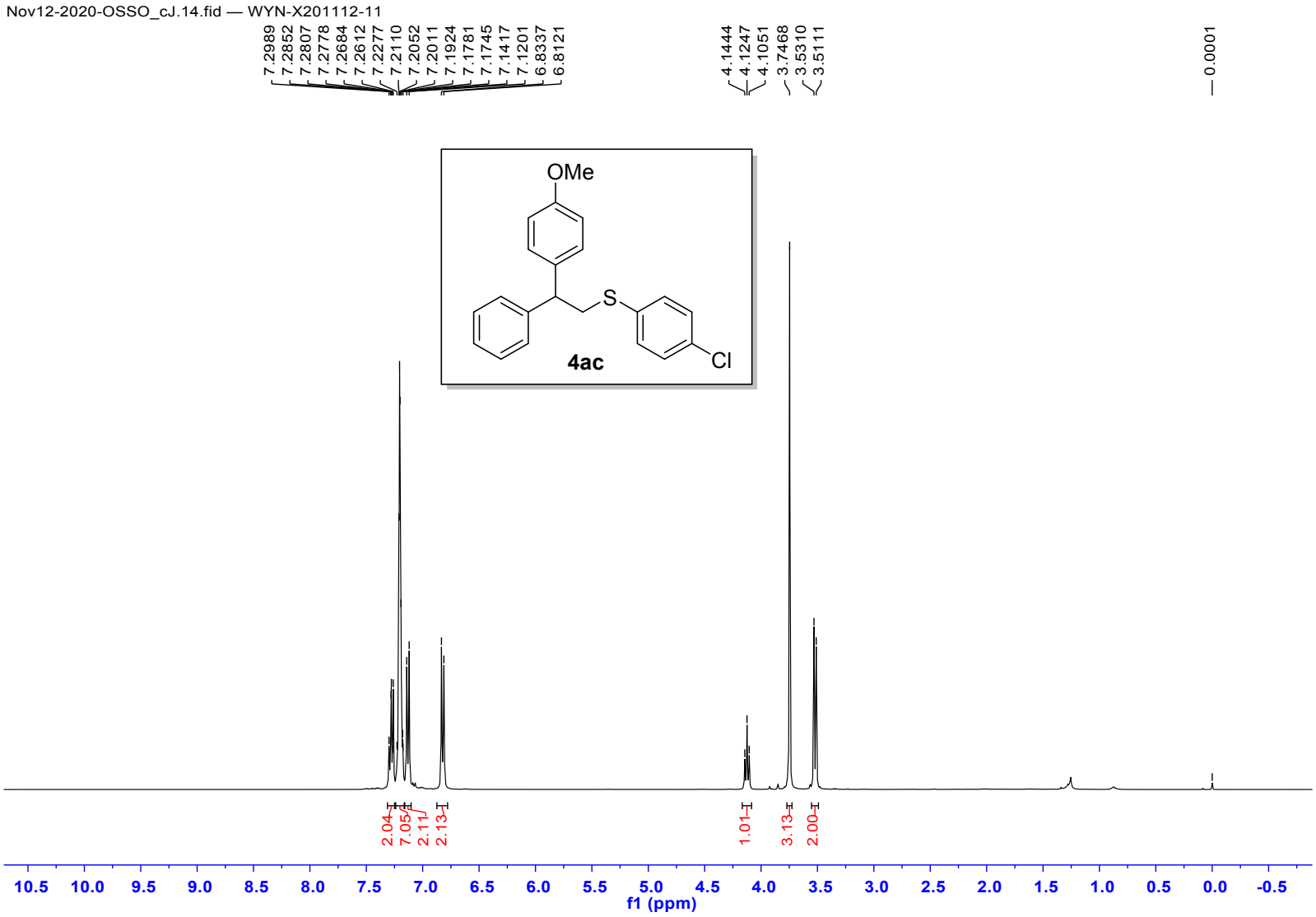


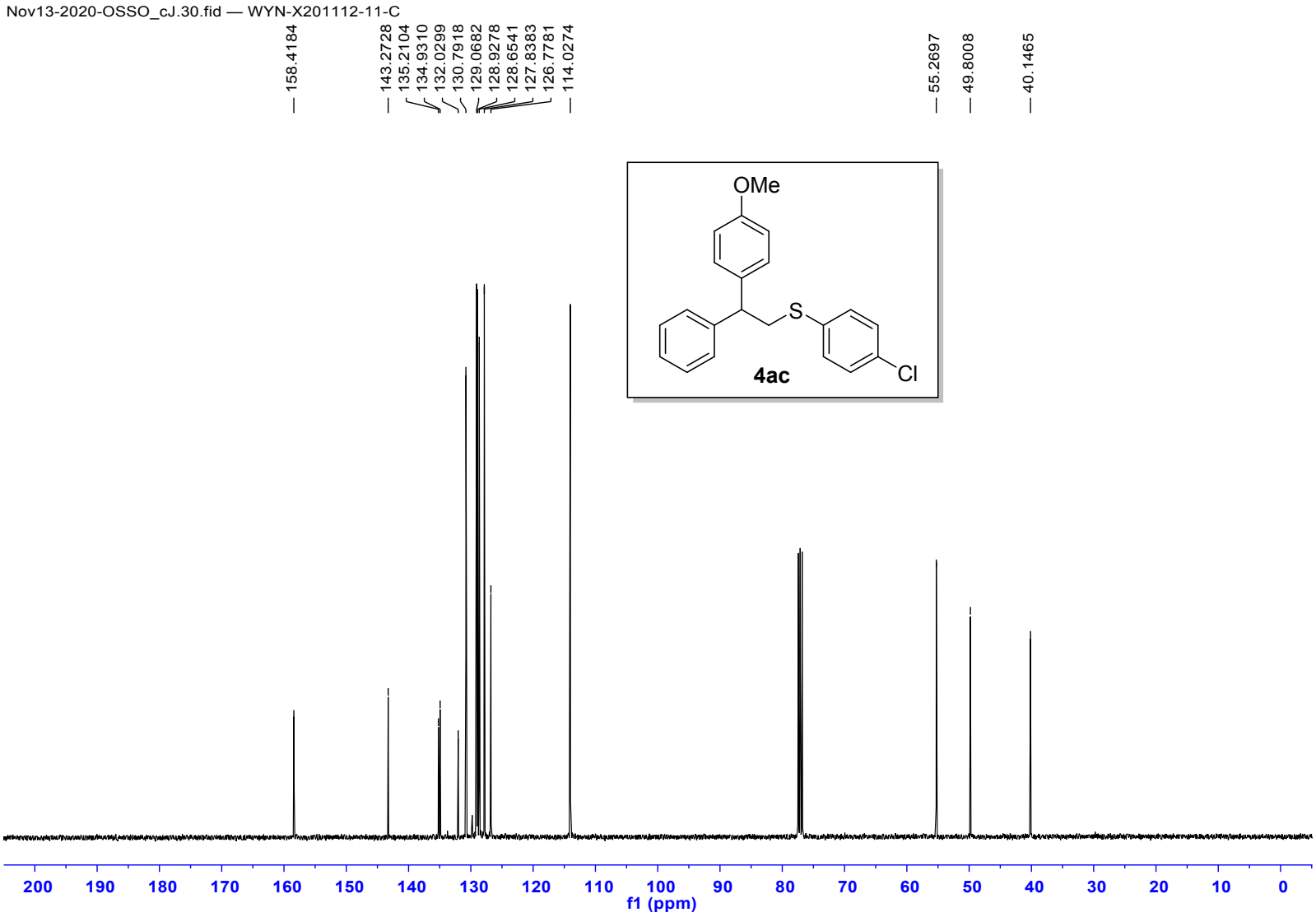



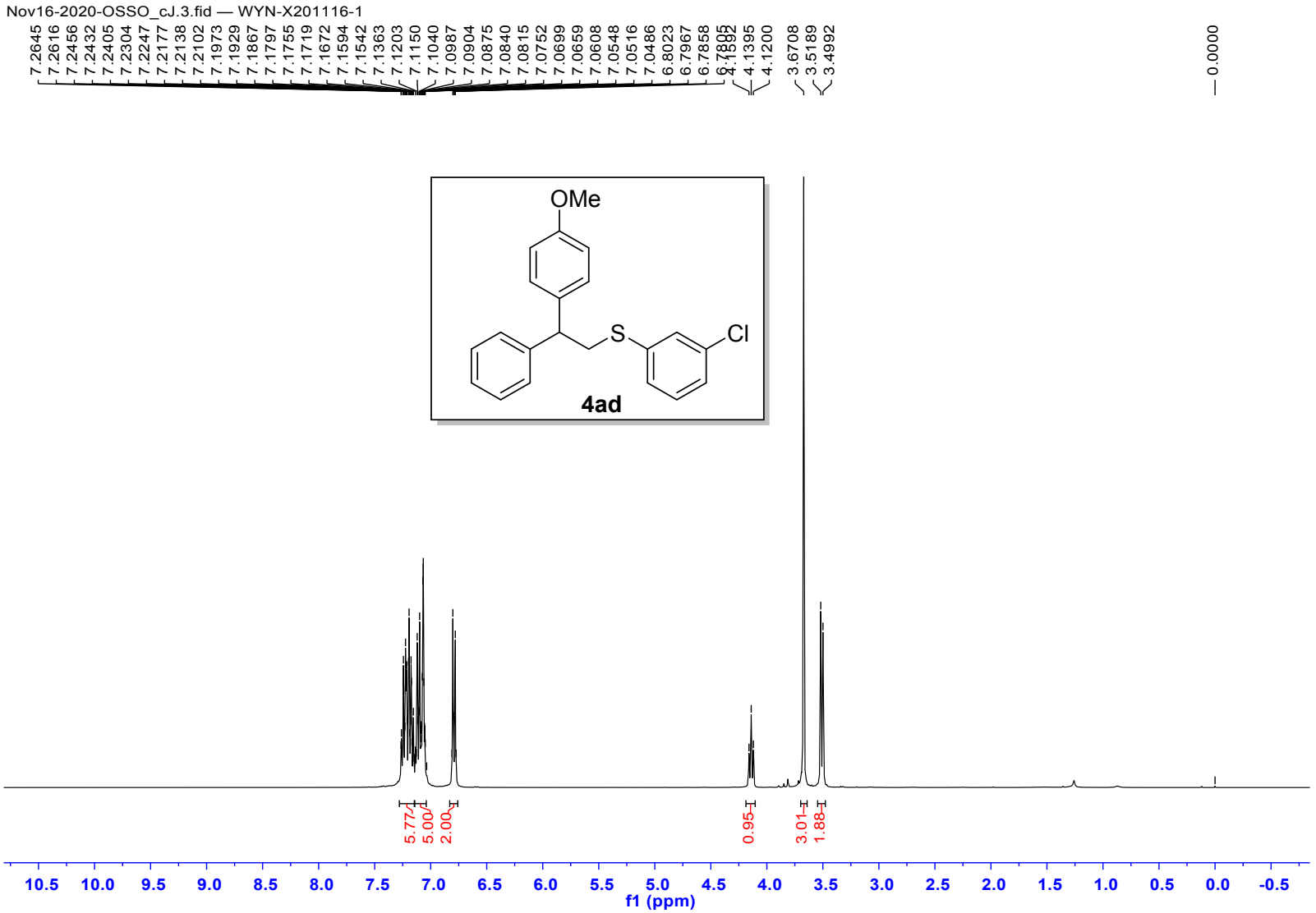



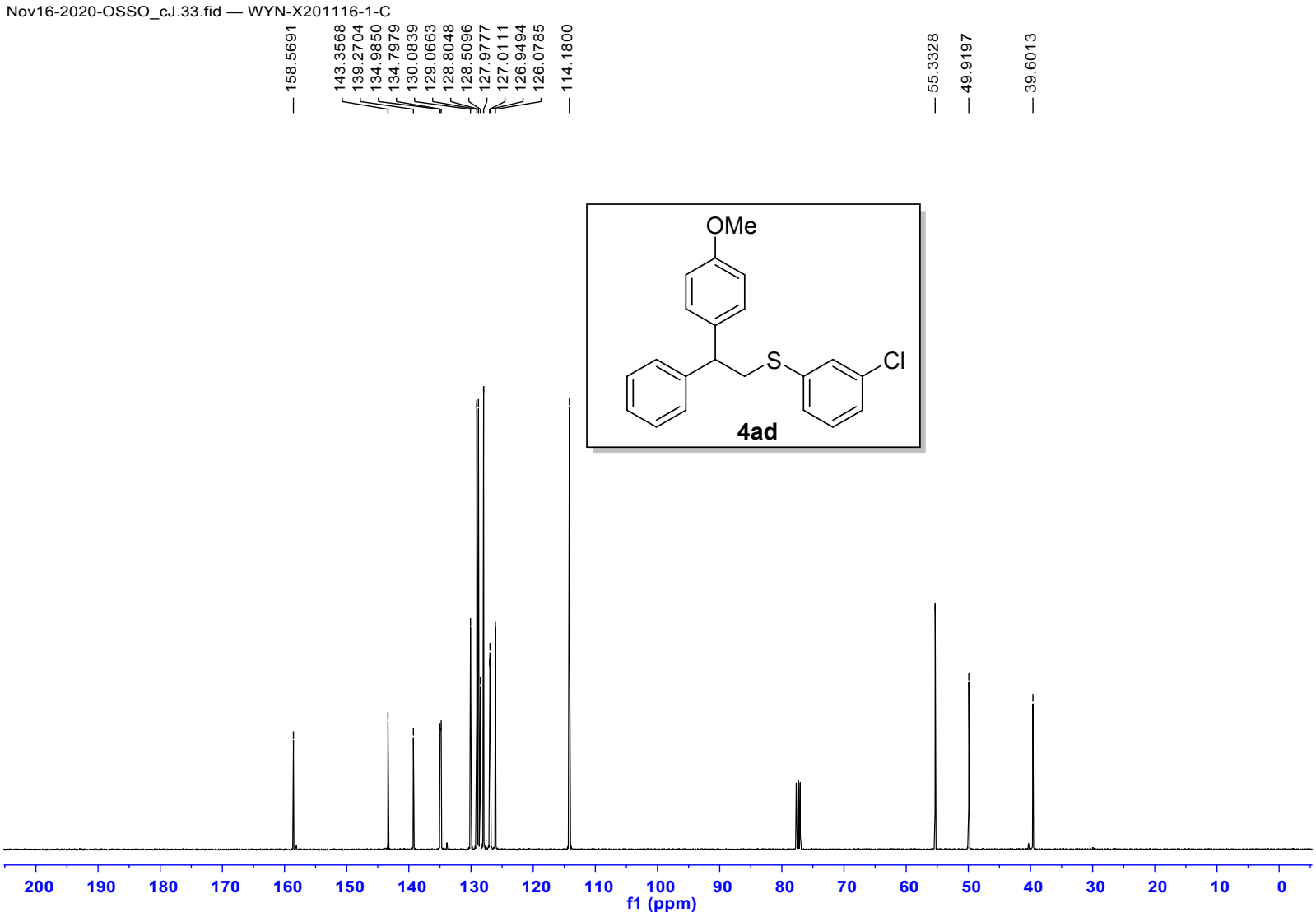
Nov13-2020-OSSO_cJ.29.fid — WYN-X201112-10-F

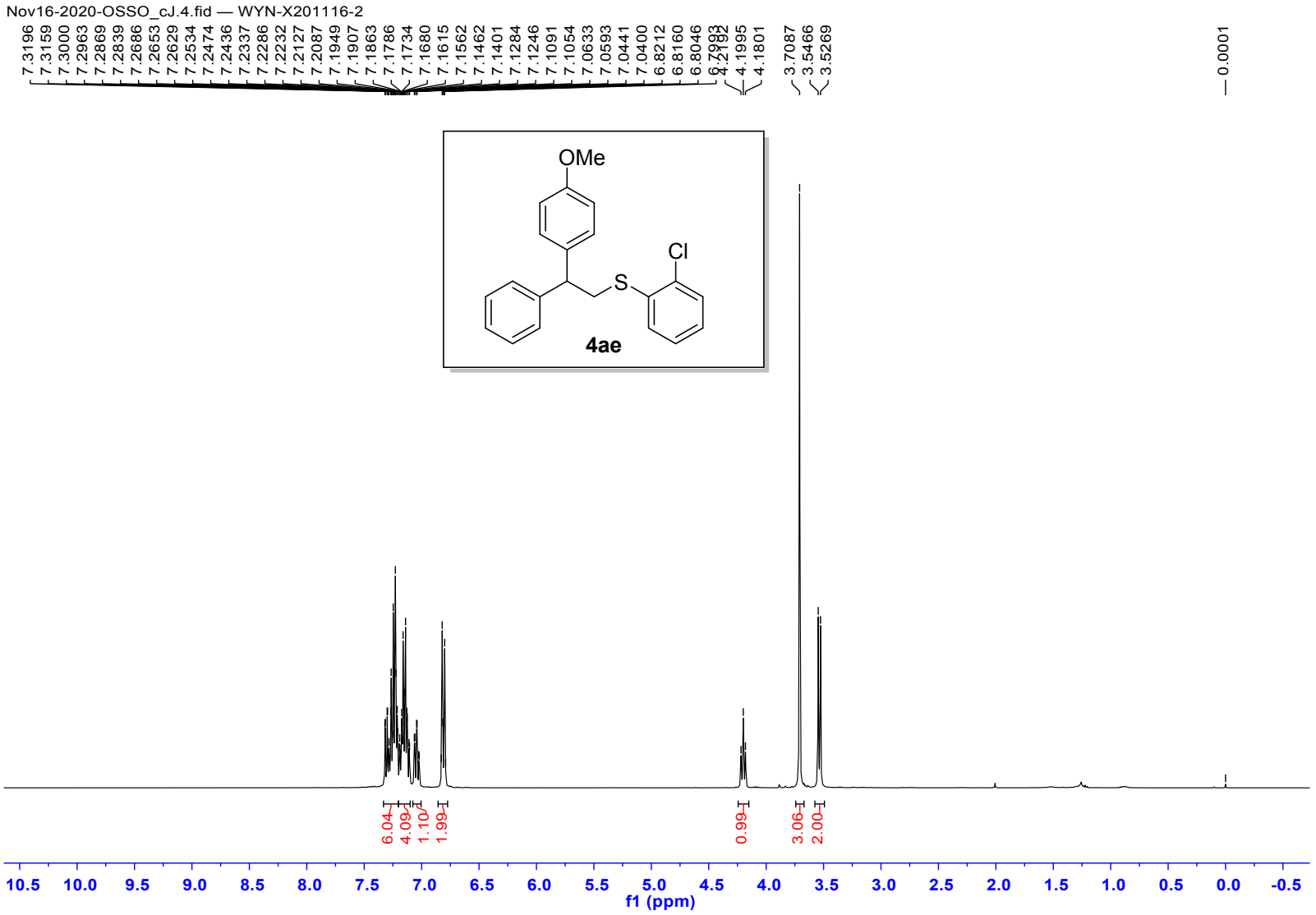


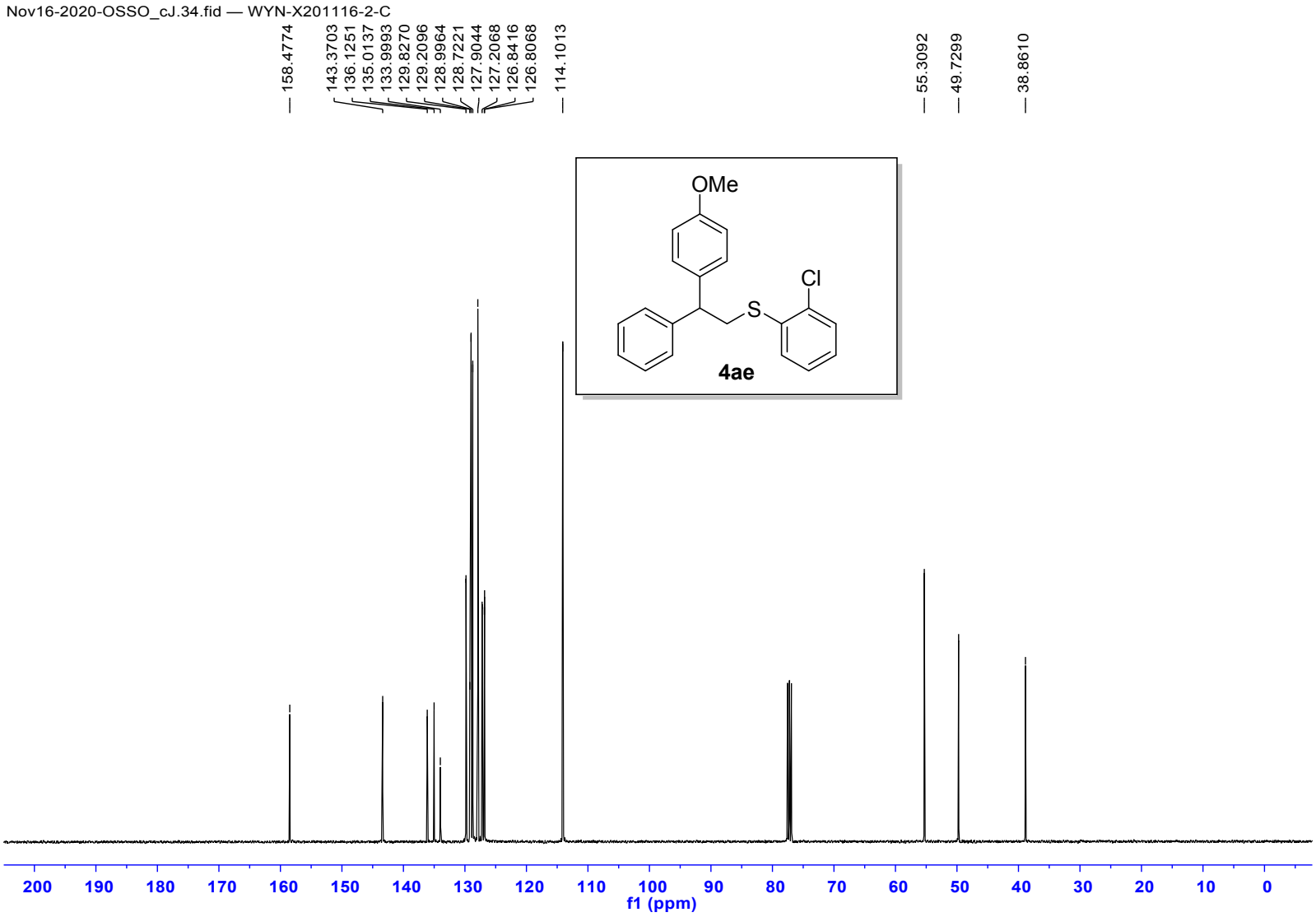

Nov12-2020-OSSO_cJ.14.fid — WYN-X201112-11
7.2989
7.2852
7.2807
7.2778
7.2684
7.2612
7.2277
7.2110
7.2052
7.2011
7.1924
7.1781
7.1745
7.1417
7.1201
6.8337
6.8121
4.1444
4.1247
4.1051
3.7468
3.5310
3.5111
0.0001
OMe
S
Cl
4ac
2.04
7.05
2.11
2.13
1.01
3.13
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

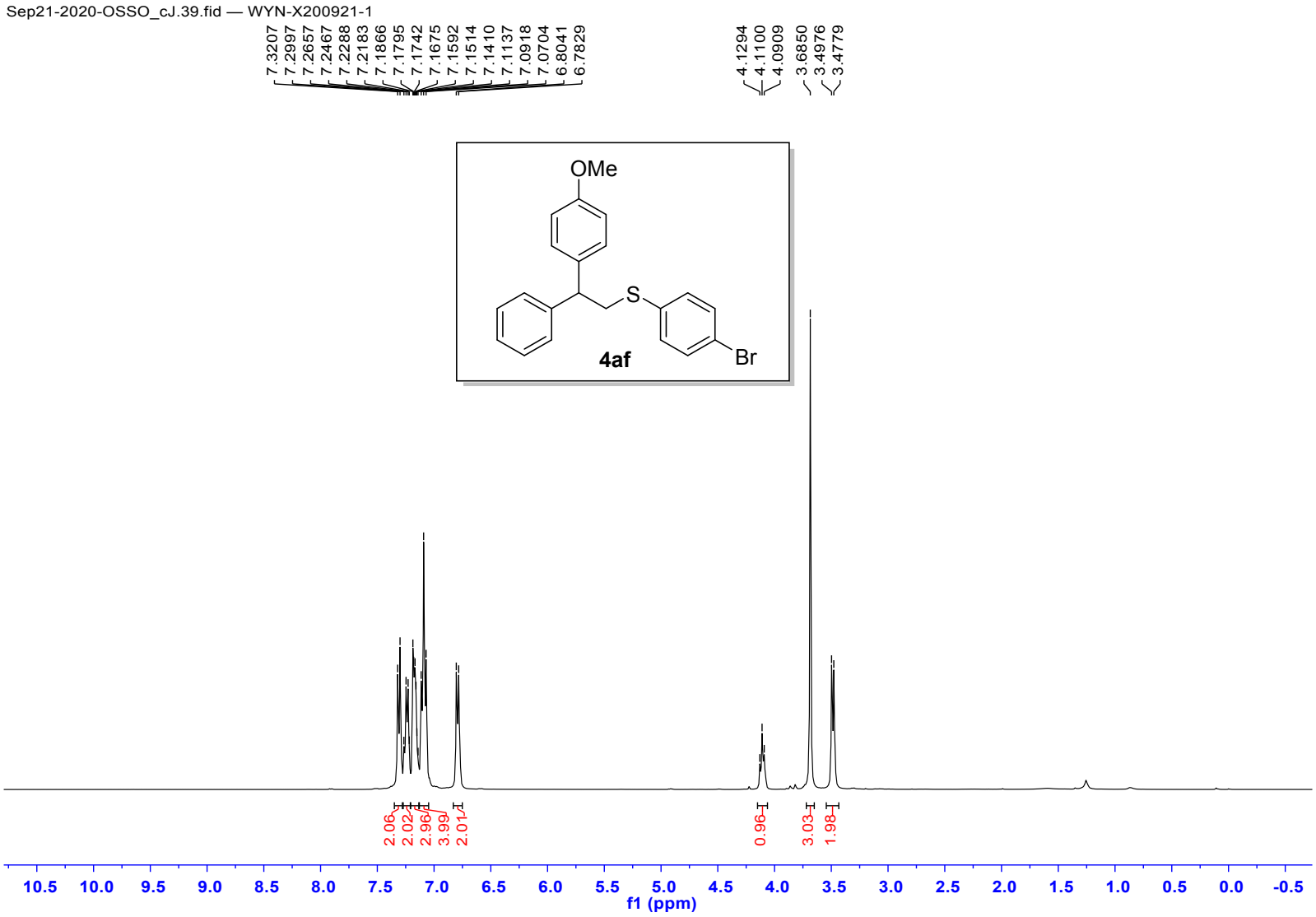

Nov13-2020-OSSO_cJ.30.fid — WYN-X201112-11-C
158.4184
143.2728
135.2104
134.9310
132.0299
130.7918
129.0682
128.9278
128.6541
127.8383
126.7781
114.0274
55.2697
49.8008
40.1465
OMe
S
Cl
4ac
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

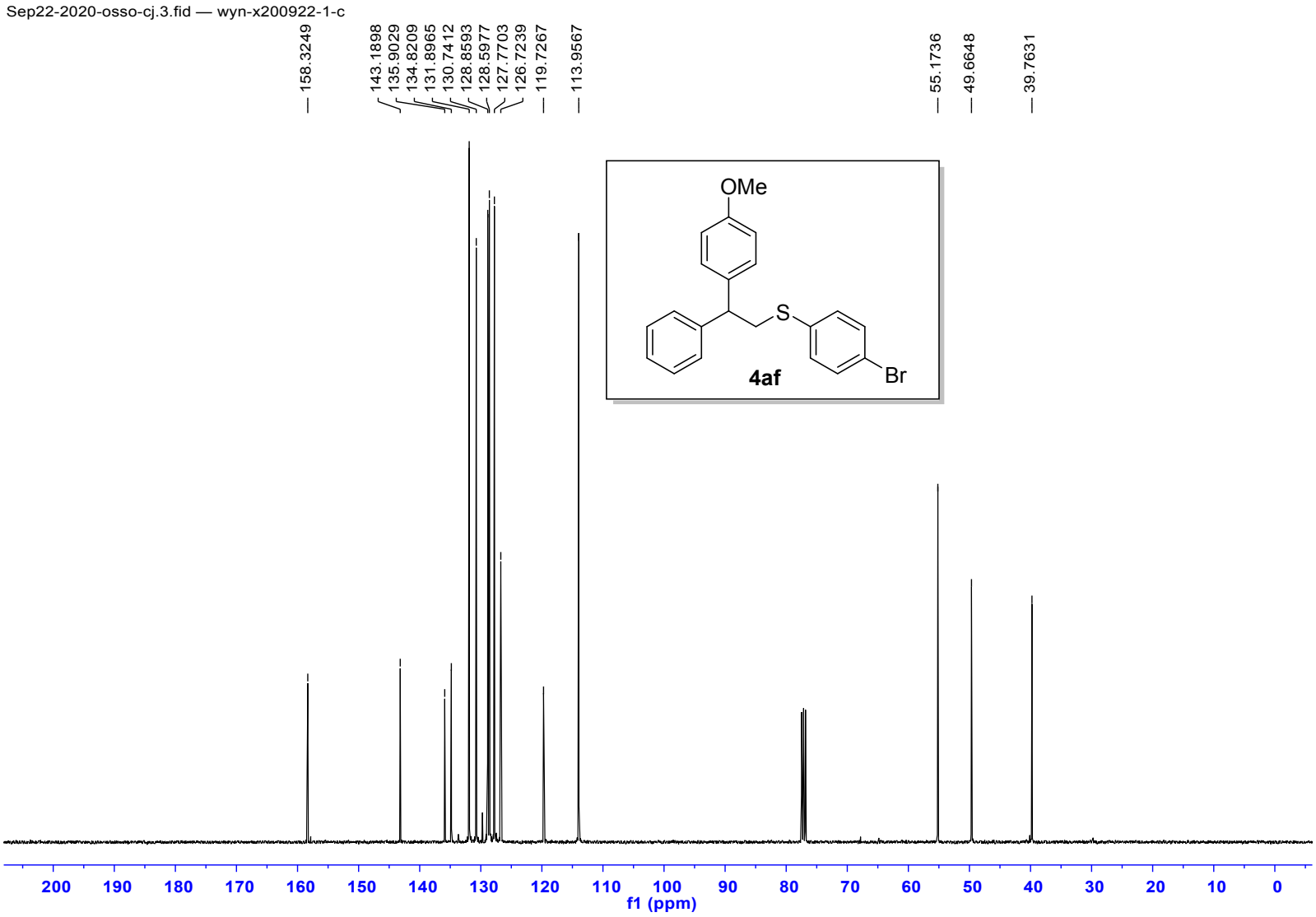

Nov16-2020-OSSO_cJ.3.fid — WYN-X201116-1
7.2645
7.2616
7.2456
7.2432
7.2405
7.2304
7.2247
7.2177
7.2138
7.2102
7.1973
7.1929
7.1867
7.1797
7.1755
7.1719
7.1672
7.1594
7.1542
7.1363
7.1203
7.1150
7.1040
7.0987
7.0904
7.0875
7.0840
7.0815
7.0752
7.0699
7.0659
7.0608
7.0548
7.0516
7.0486
6.8023
6.7967
6.7858
4.1395
4.1200
3.6708
3.5189
3.4992
0.0000
OMe
S
Cl
4ad
5.77
5.00
2.00
0.95
3.01
1.88
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

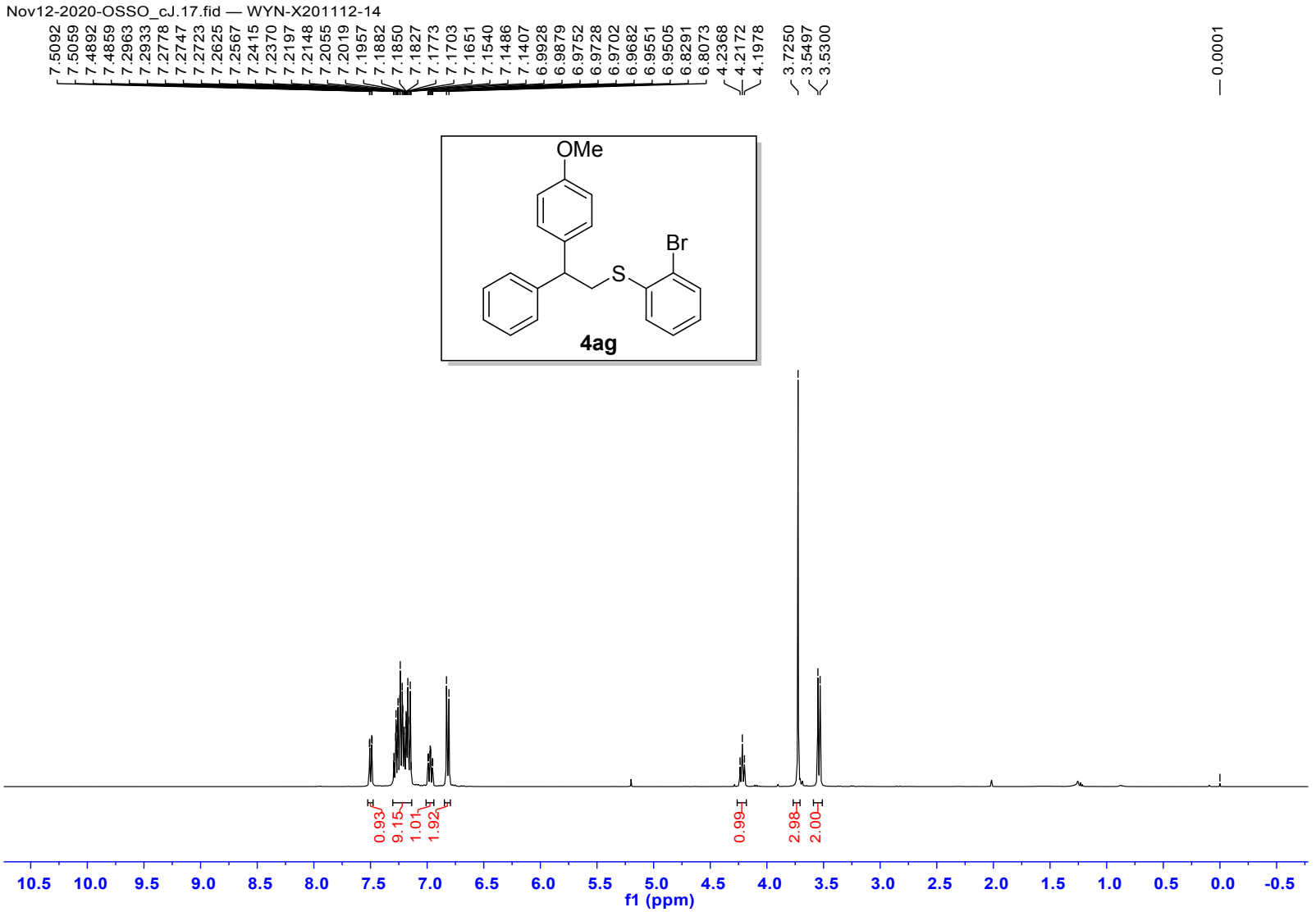

Nov16-2020-OSSO_cJ.33.fid — WYN-X201116-1-C
158.5691
143.3568
139.2704
134.9850
134.7979
130.0839
129.0663
128.8048
128.5096
127.9777
127.0111
126.9494
126.0785
114.1800
55.3328
49.9197
39.6013
OMe
S
Cl
4ad
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

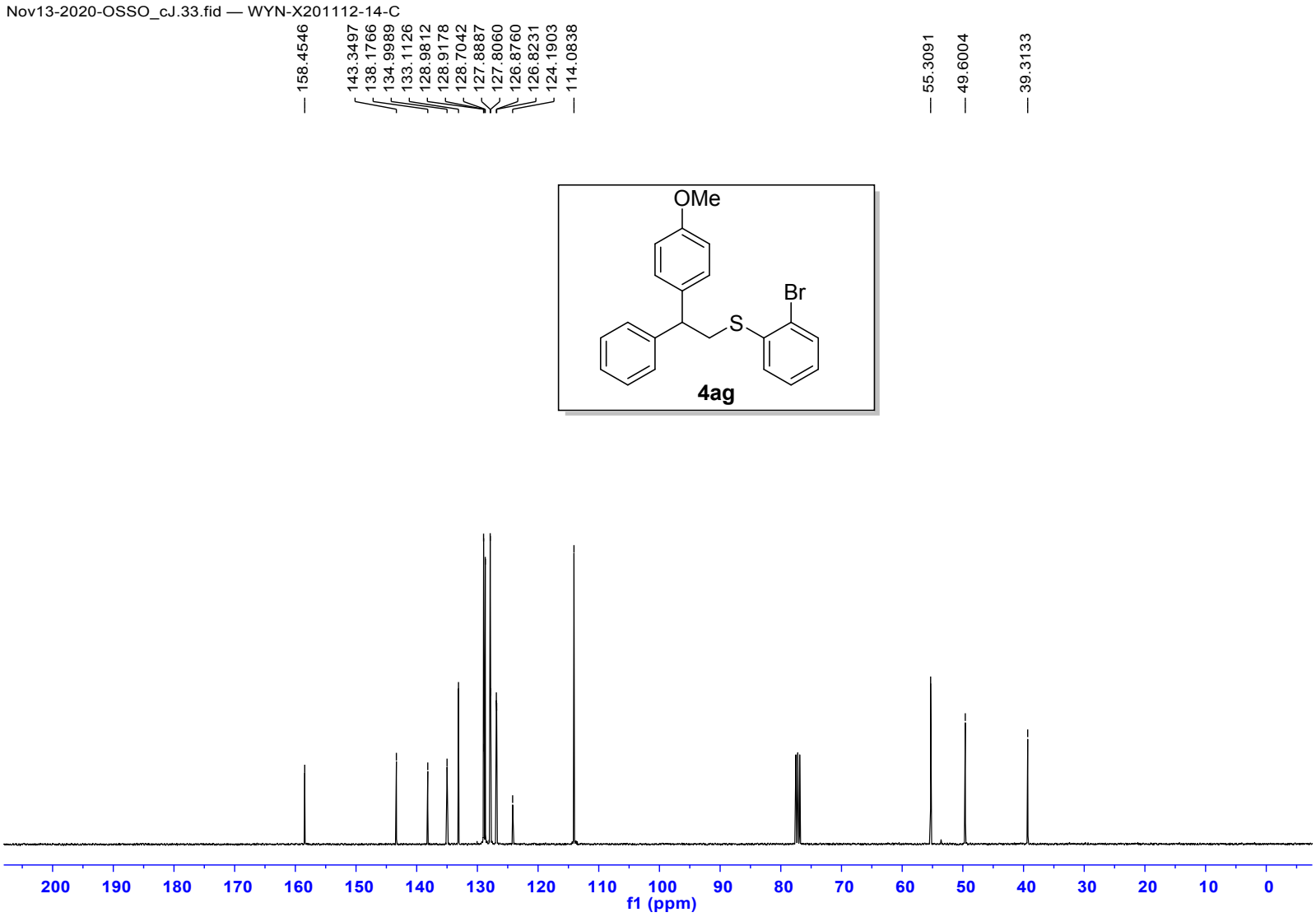

Nov16-2020-OSSO_cJ.4.fid — WYN-X201116-2
7.3196
7.3159
7.3000
7.2963
7.2869
7.2839
7.2686
7.2653
7.2629
7.2534
7.2474
7.2436
7.2337
7.2286
7.2232
7.2127
7.2087
7.1949
7.1907
7.1863
7.1786
7.1734
7.1680
7.1615
7.1562
7.1462
7.1401
7.1284
7.1246
7.1091
7.1054
7.0633
7.0593
7.0441
7.0400
6.8212
6.8160
6.8046
4.1995
4.1801
3.7087
3.5466
3.5269
0.0001
OMe
Cl
S
4ae
6.04
4.09
1.10
1.99
0.99
3.06
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

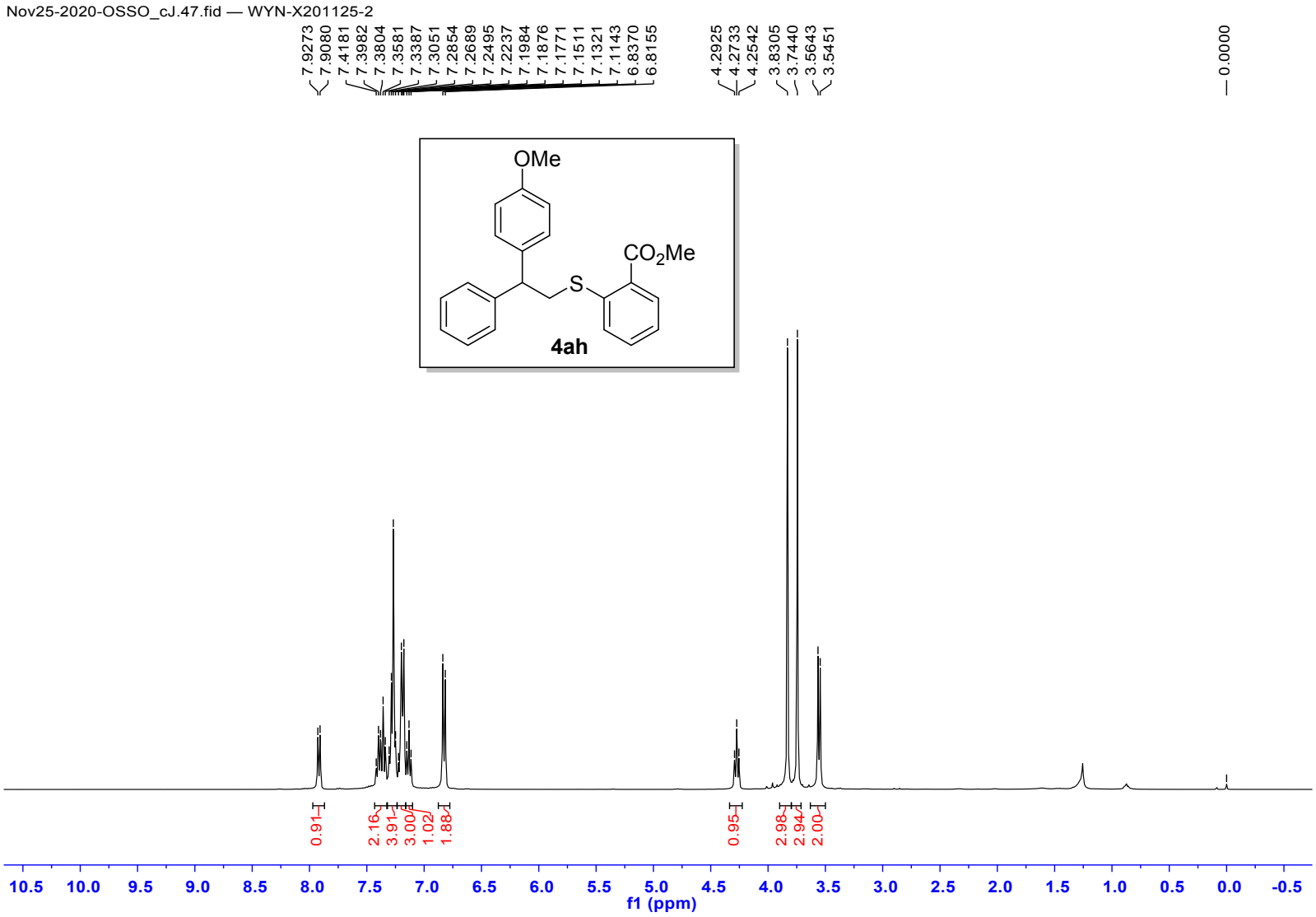

Nov16-2020-OSSO_cJ.34.fid — WYN-X201116-2-C
158.4774
143.3703
136.1251
135.0137
133.9993
129.8270
129.2096
128.9964
128.7221
127.9044
127.2068
126.8416
126.8068
114.1013
55.3092
49.7299
38.8610
OMe
Cl
S
4ae
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

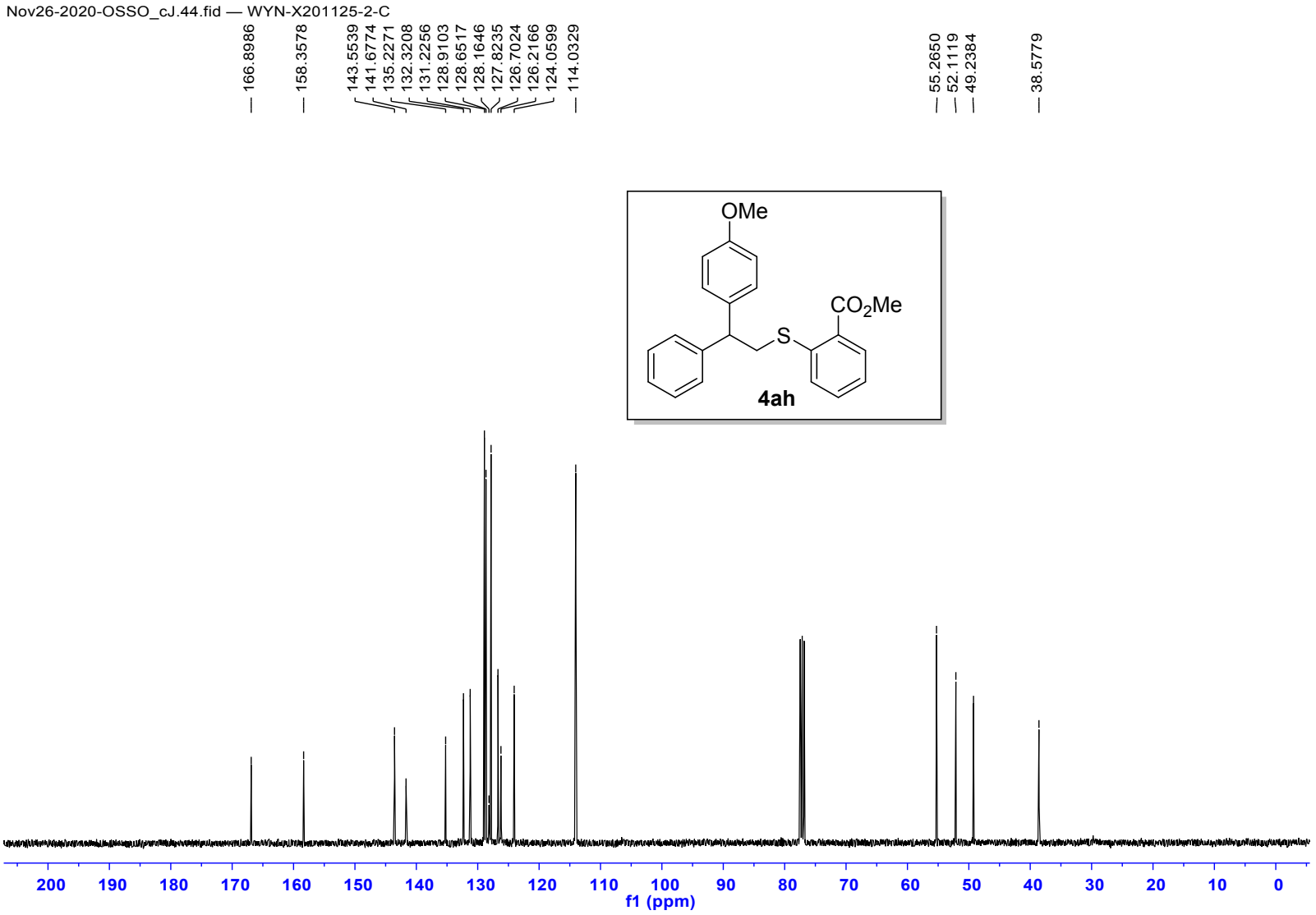

Sep21-2020-OSSO_cJ.39.fid — WYN-X200921-1
7.3207
7.2997
7.2657
7.2467
7.2288
7.2183
7.1866
7.1795
7.1742
7.1675
7.1592
7.1514
7.1410
7.1137
7.0918
7.0704
6.8041
6.7829
4.1294
4.1100
4.0909
3.6850
3.4976
3.4779
OMe
S
Br
4af
2.06
2.02
2.96
3.99
2.01
0.96
3.03
1.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

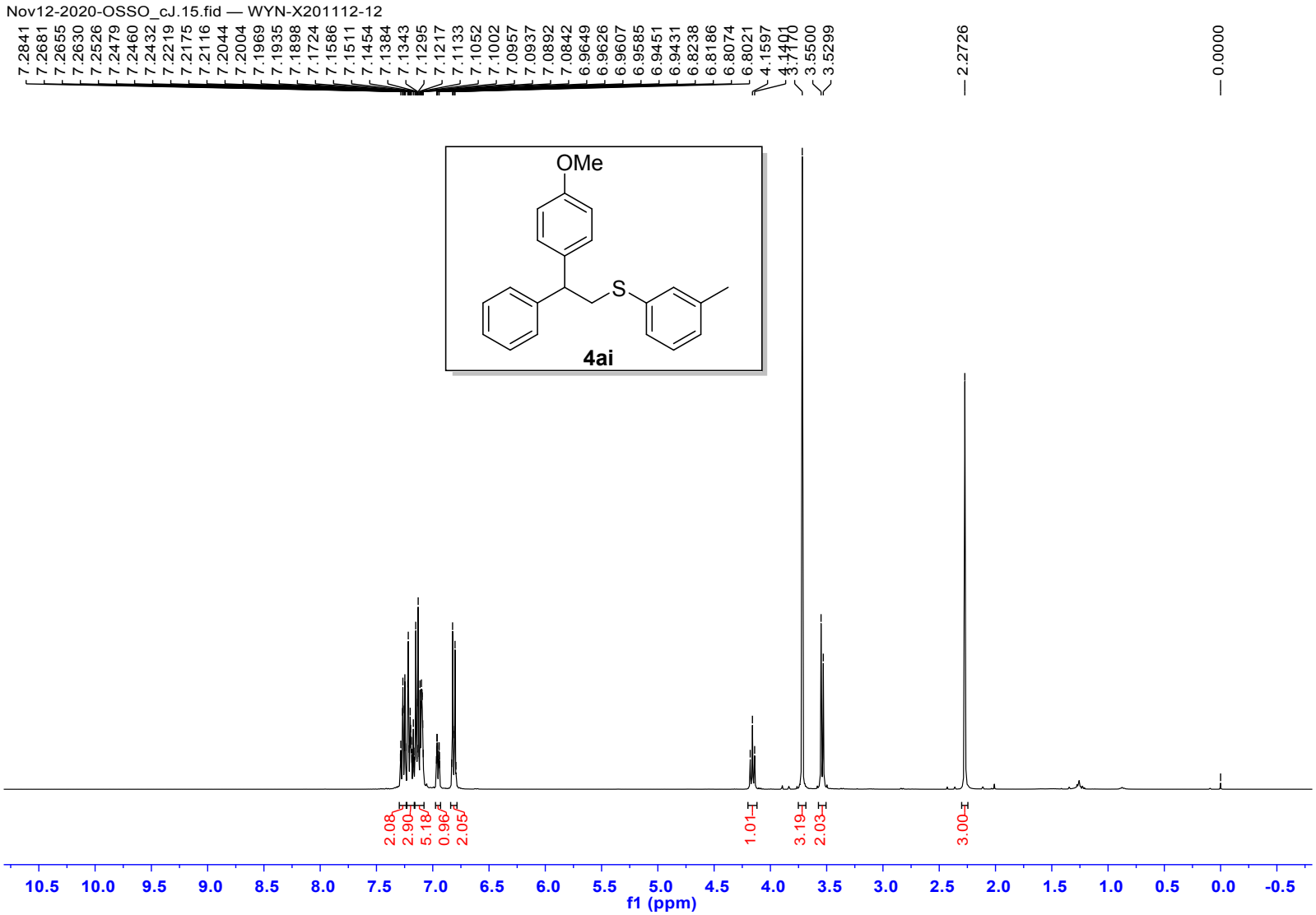

Sep22-2020-osso-cj.3.fid — wyn-x200922-1-c
158.3249
143.1898
135.9029
134.8209
131.8965
130.7412
128.8593
128.5977
127.7703
126.7239
119.7267
113.9567
55.1736
49.6648
39.7631
OMe
S
Br
4af
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

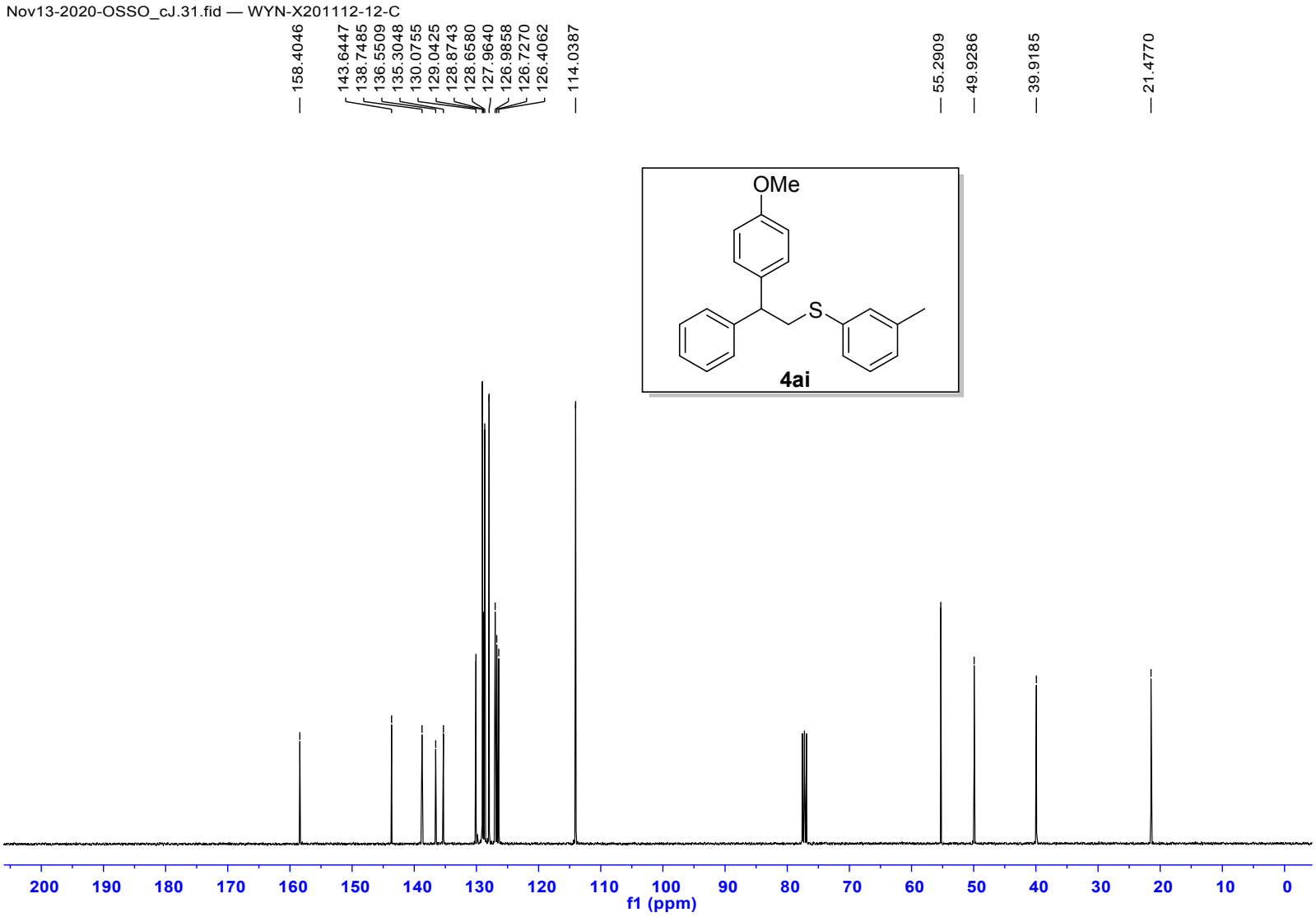

Nov12-2020-OSSO_cJ.17.fid — WYN-X201112-14
7.5092
7.5059
7.4892
7.4859
7.2963
7.2933
7.2778
7.2747
7.2723
7.2625
7.2567
7.2415
7.2370
7.2197
7.2148
7.2055
7.2019
7.1957
7.1882
7.1850
7.1827
7.1773
7.1703
7.1651
7.1540
7.1486
7.1407
6.9928
6.9879
6.9752
6.9728
6.9702
6.9682
6.9551
6.9505
6.8291
6.8073
4.2368
4.2172
4.1978
3.7250
3.5497
3.5300
0.0001
OMe
Br
S
4ag
0.93
9.15
1.01
1.92
0.99
2.98
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

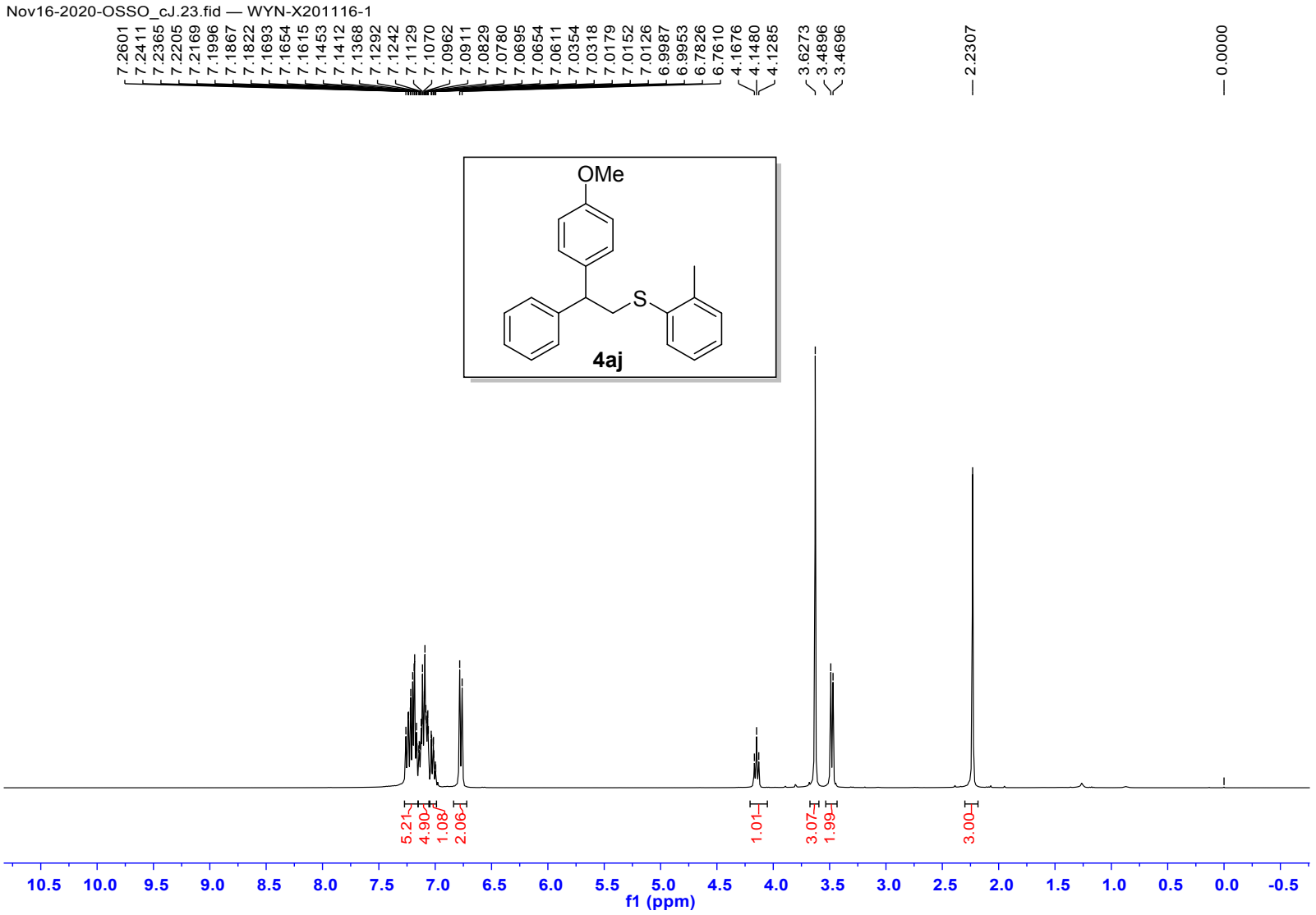

Nov13-2020-OSSO_cJ.33.fid — WYN-X201112-14-C
158.4546
143.3497
138.1766
134.9989
133.1126
128.9812
128.9178
128.7042
127.8887
127.8060
126.8760
126.8231
124.1903
114.0838
55.3091
49.6004
39.3133
OMe
Br
S
4ag
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

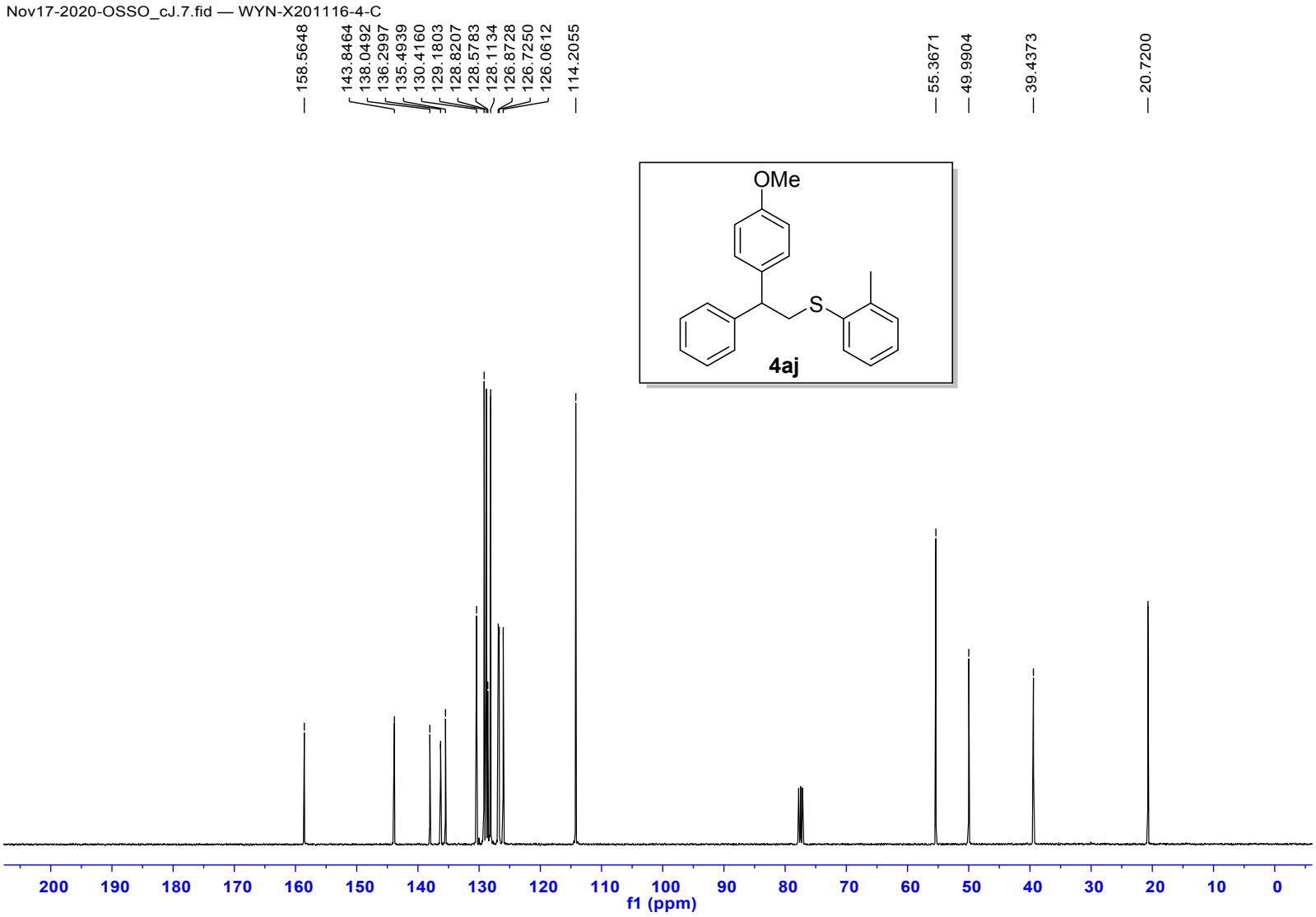

Nov25-2020-OSSO_cJ.47.fid — WYN-X201125-2
7.9273
7.9080
7.4181
7.3982
7.3804
7.3581
7.3387
7.3051
7.2854
7.2689
7.2495
7.2237
7.1984
7.1876
7.1771
7.1511
7.1321
7.1143
6.8370
6.8155
4.2925
4.2733
4.2542
3.8305
3.7440
3.5643
3.5451
0.0000
OMe
CO2Me
S
4ah
0.91
2.16
3.91
3.00
1.02
1.88
0.95
2.98
2.94
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

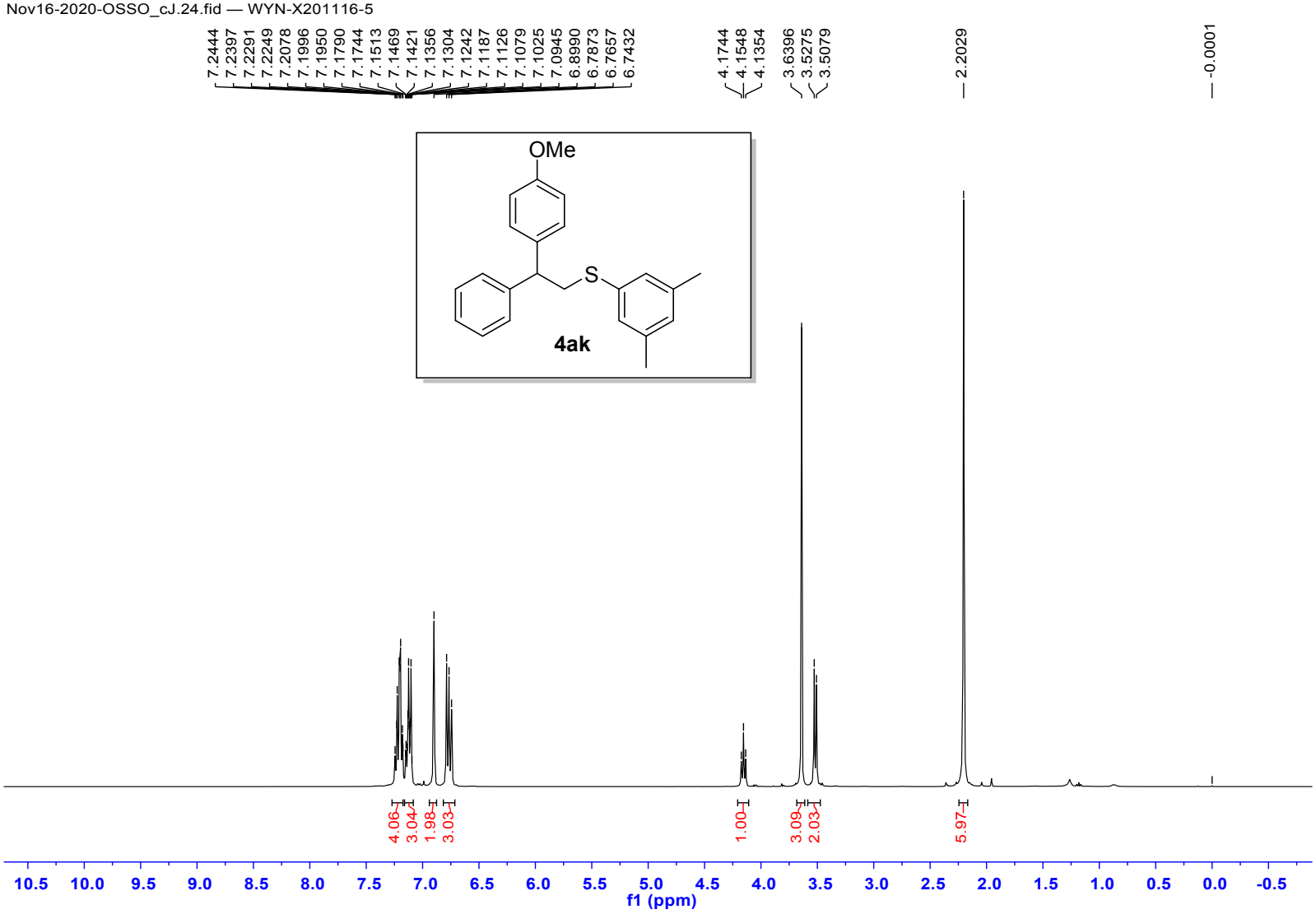

Nov26-2020-OSSO_cJ.44.fid — WYN-X201125-2-C
166.8986
158.3578
143.5539
141.6774
135.2271
132.3208
131.2256
128.9103
128.6517
128.1646
127.8235
126.7024
126.2166
124.0599
114.0329
55.2650
52.1119
49.2384
38.5779
OMe
CO2Me
S
4ah
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

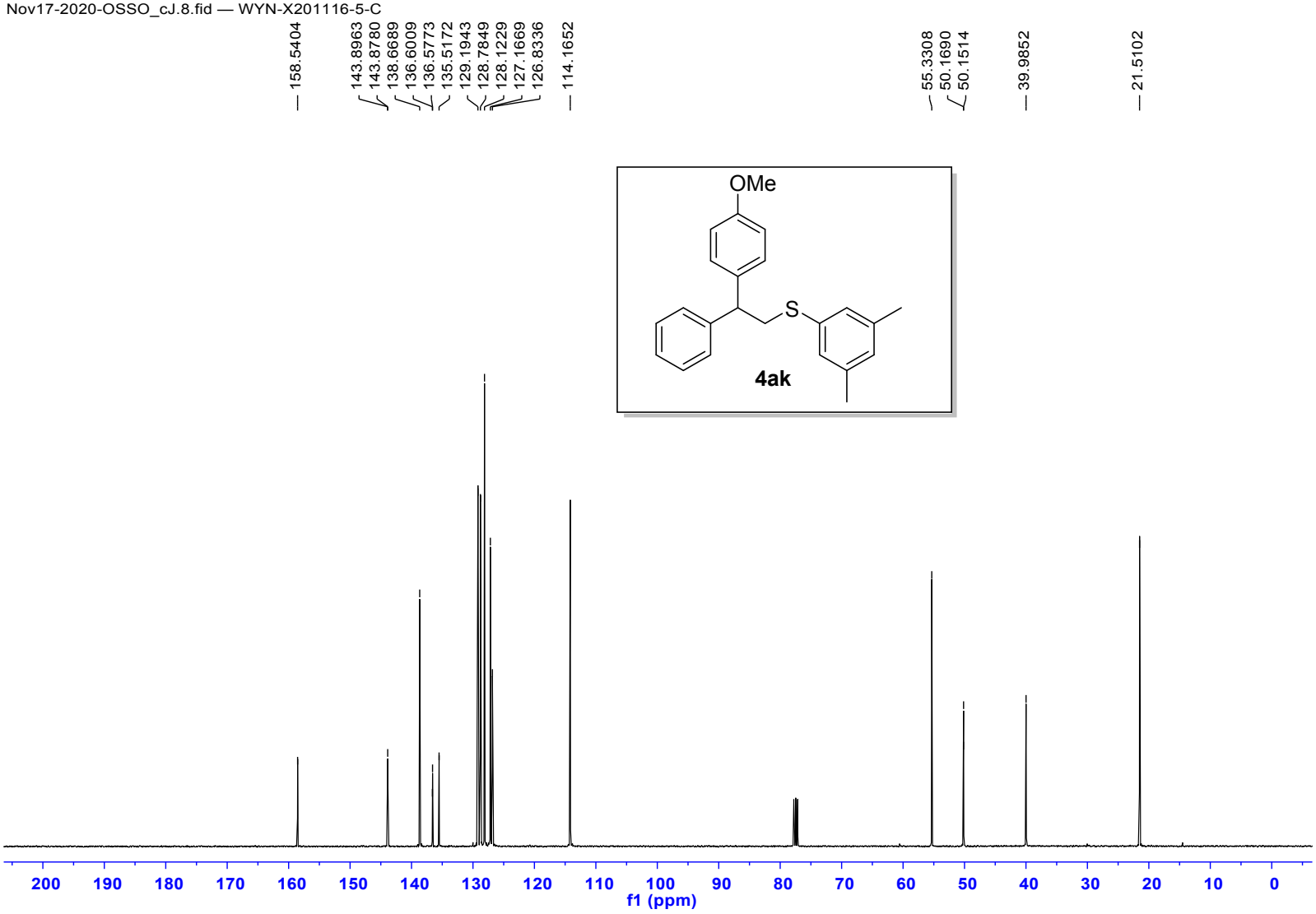

Nov12-2020-OSSO_cJ.15.fid — WYN-X201112-12
7.2841
7.2681
7.2655
7.2630
7.2526
7.2479
7.2460
7.2432
7.2219
7.2175
7.2116
7.2044
7.2004
7.1969
7.1935
7.1898
7.1724
7.1586
7.1511
7.1454
7.1384
7.1343
7.1295
7.1217
7.1133
7.1052
7.1002
7.0957
7.0937
7.0892
7.0842
6.9649
6.9626
6.9607
6.9585
6.9451
6.9431
6.8238
6.8186
6.8074
6.8021
4.1597
4.1401
4.1170
3.5500
3.5299
2.2726
0.0000
OMe
S
4ai
2.08
2.90
5.18
0.96
2.05
1.01
3.19
2.03
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

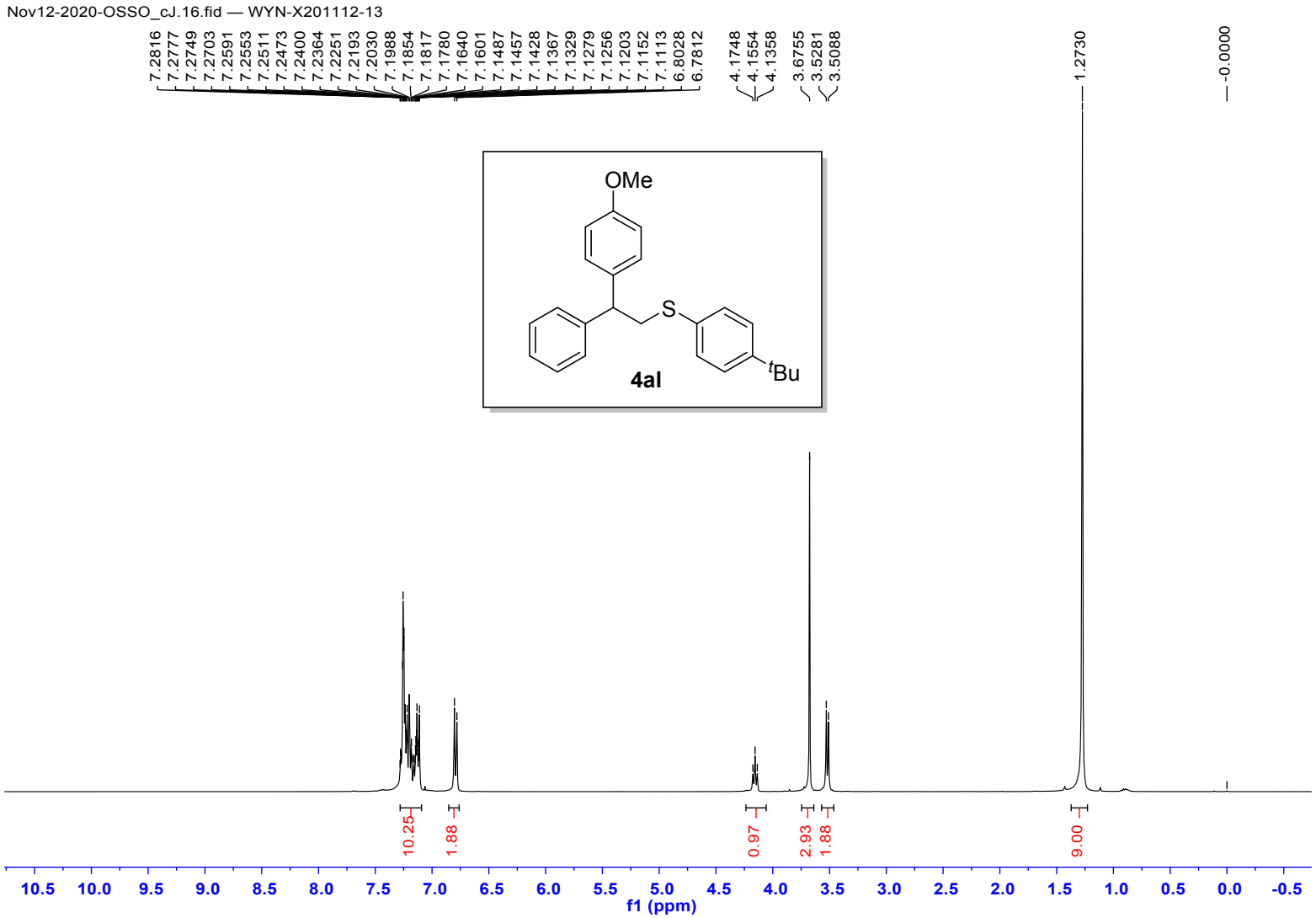

Nov13-2020-OSSO_cJ.31.fid — WYN-X201112-12-C
158.4046
143.6447
138.7485
136.5509
135.3048
130.0755
129.0425
128.8743
128.6580
127.9640
126.9858
126.7270
126.4062
114.0387
55.2909
49.9286
39.9185
21.4770
OMe
S
4ai
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

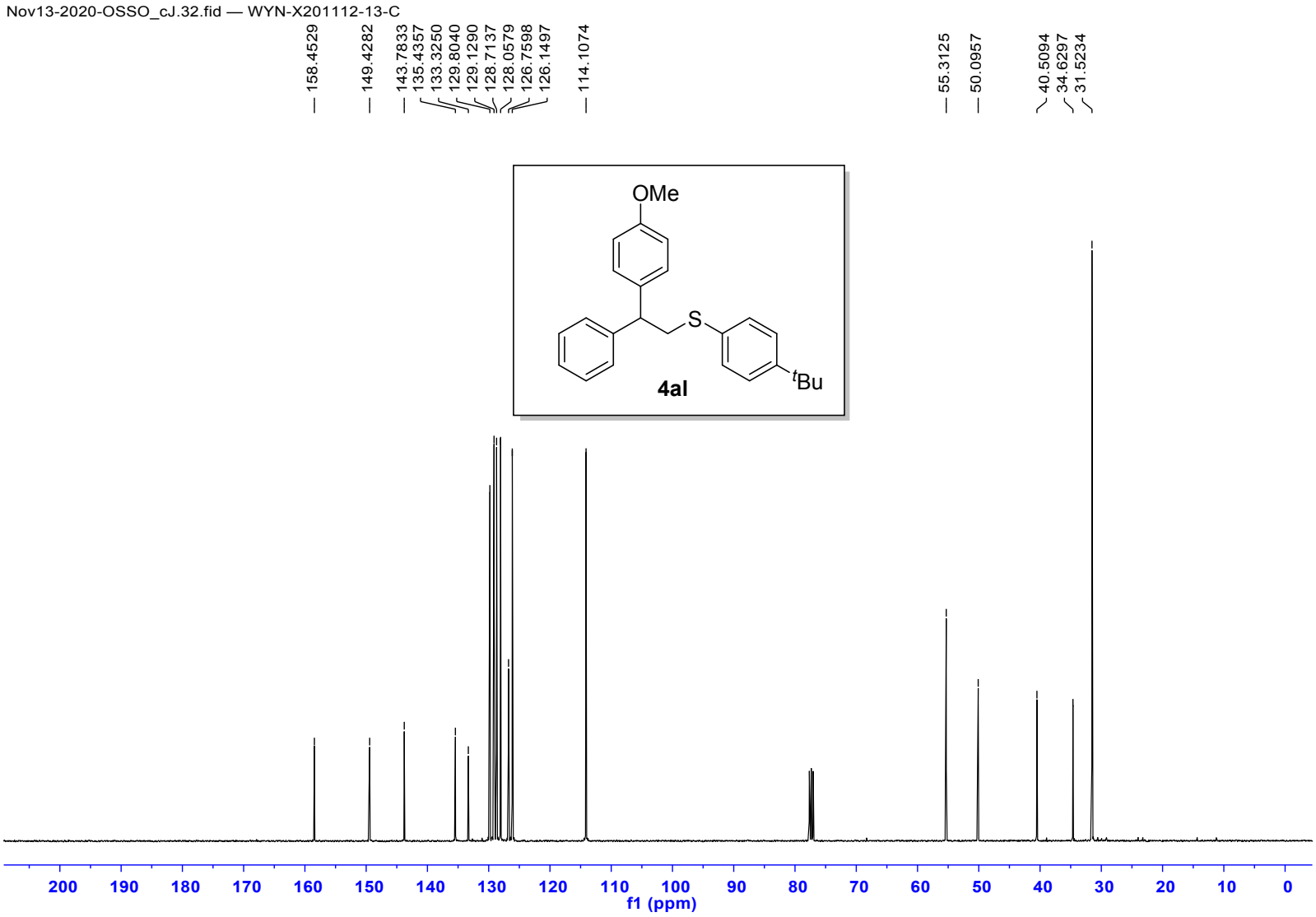

Nov16-2020-OSSO_cJ.23.fid — WYN-X201116-1
7.2601
7.2411
7.2365
7.2205
7.2169
7.1996
7.1867
7.1822
7.1693
7.1654
7.1615
7.1453
7.1412
7.1368
7.1292
7.1242
7.1129
7.1070
7.0962
7.0911
7.0829
7.0780
7.0695
7.0654
7.0611
7.0354
7.0318
7.0179
7.0152
7.0126
6.9987
6.9953
6.7826
6.7610
4.1676
4.1480
4.1285
3.6273
3.4896
3.4696
2.2307
0.0000
OMe
S
4aj
5.21
4.90
1.08
2.06
1.01
3.07
1.99
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Nov17-2020-OSSO_cJ.7.fid — WYN-X201116-4-C
158.5648
143.8464
138.0492
136.2997
135.4939
130.4160
129.1803
128.8207
128.5783
128.1134
126.8728
126.7250
126.0612
114.2055
55.3671
49.9904
39.4373
20.7200
OMe
S
4aj
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov16-2020-OSSO_cJ.24.fid — WYN-X201116-5
7.2444
7.2397
7.2291
7.2249
7.2078
7.1996
7.1950
7.1790
7.1744
7.1513
7.1469
7.1421
7.1356
7.1304
7.1242
7.1187
7.1126
7.1079
7.1025
7.0945
6.8990
6.7873
6.7657
6.7432
4.1744
4.1548
4.1354
3.6396
3.5275
3.5079
2.2029
-0.0001
OMe
S
4ak
4.06
3.04
1.98
3.03
1.00
3.09
2.03
5.97
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Nov17-2020-OSSO_cJ.8.fid — WYN-X201116-5-C
158.5404
143.8963
143.8780
138.6689
136.6009
136.5773
135.5172
129.1943
128.7849
128.1229
127.1669
126.8336
114.1652
55.3308
50.1690
50.1514
39.9852
21.5102
OMe
S
4ak
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov12-2020-OSSO_cJ.16.fid — WYN-X201112-13
7.2816
7.2777
7.2749
7.2703
7.2591
7.2553
7.2511
7.2473
7.2400
7.2364
7.2251
7.2193
7.2030
7.1988
7.1854
7.1817
7.1780
7.1640
7.1601
7.1487
7.1457
7.1428
7.1367
7.1329
7.1279
7.1256
7.1203
7.1152
7.1113
6.8028
6.7812
4.1748
4.1554
4.1358
3.6755
3.5281
3.5088
1.2730
-0.0000
OMe
S
tBu
4al
10.25
1.88
0.97
2.93
1.88
9.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Nov13-2020-OSSO_cJ.32.fid — WYN-X201112-13-C
158.4529
149.4282
143.7833
135.4357
133.3250
129.8040
129.1290
128.7137
128.0579
126.7598
126.1497
114.1074
55.3125
50.0957
40.5094
34.6297
31.5234
OMe
S
tBu
4al
200
190
180
170
160
150
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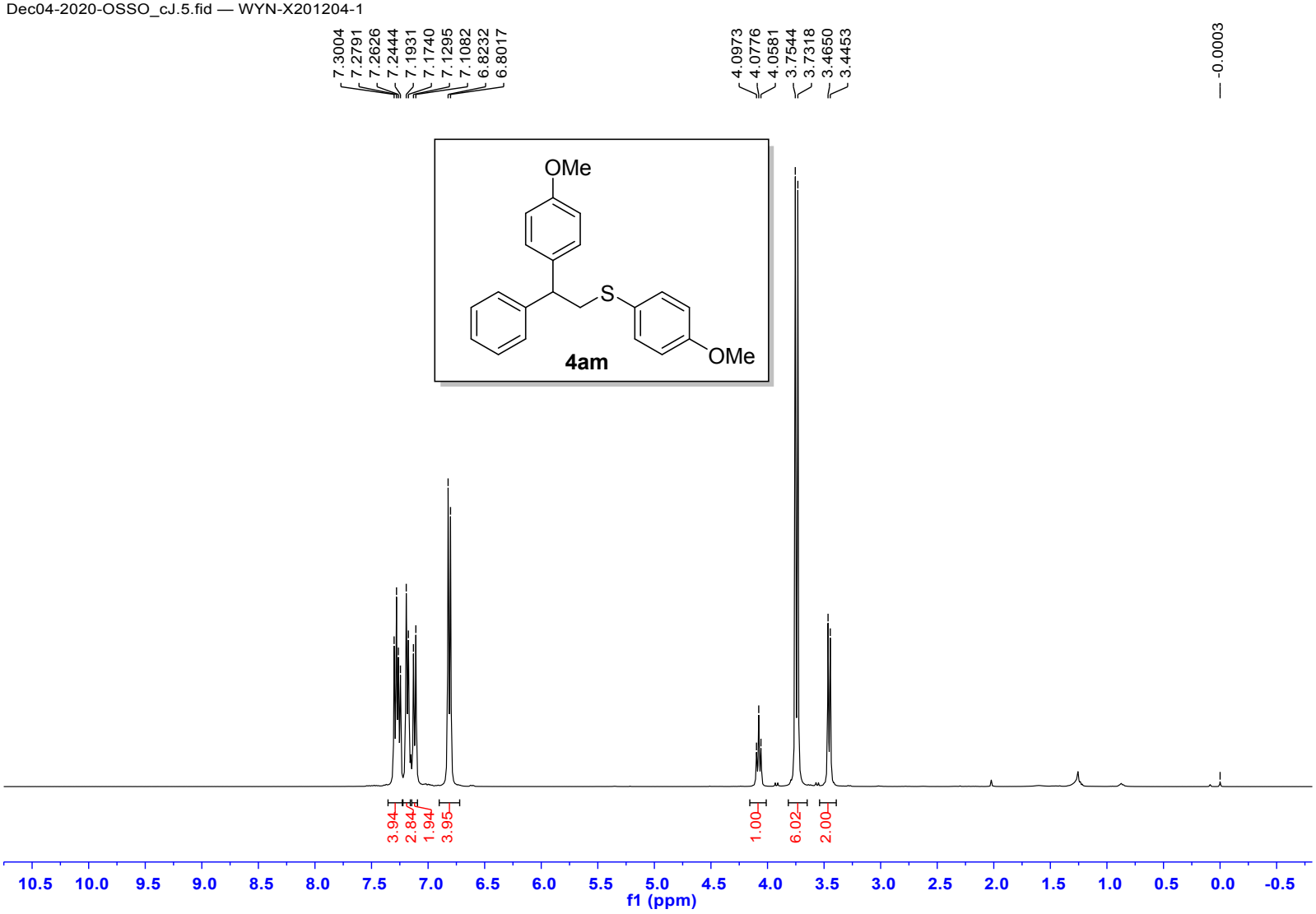
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Dec04-2020-OSSO_cJ.5.fid — WYN-X201204-1
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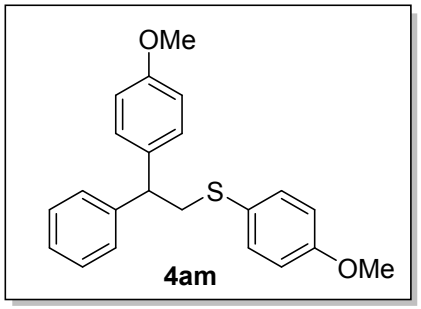
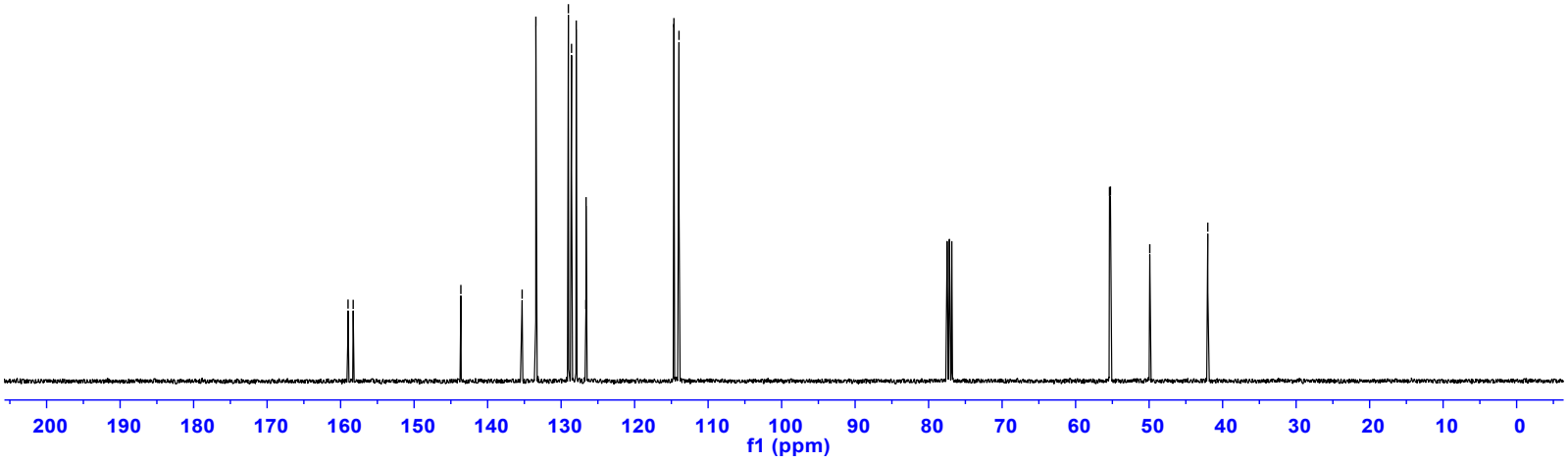
7.2791
7.2626
7.2444
7.1931
7.1740
7.1295
7.1082
6.8232
6.8017
4.0973
4.0776
4.0581
3.7544
3.7318
3.4650
3.4453
-0.0003
OMe
S
OMe
4am
3.94
2.84
1.94
3.95
1.00
6.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

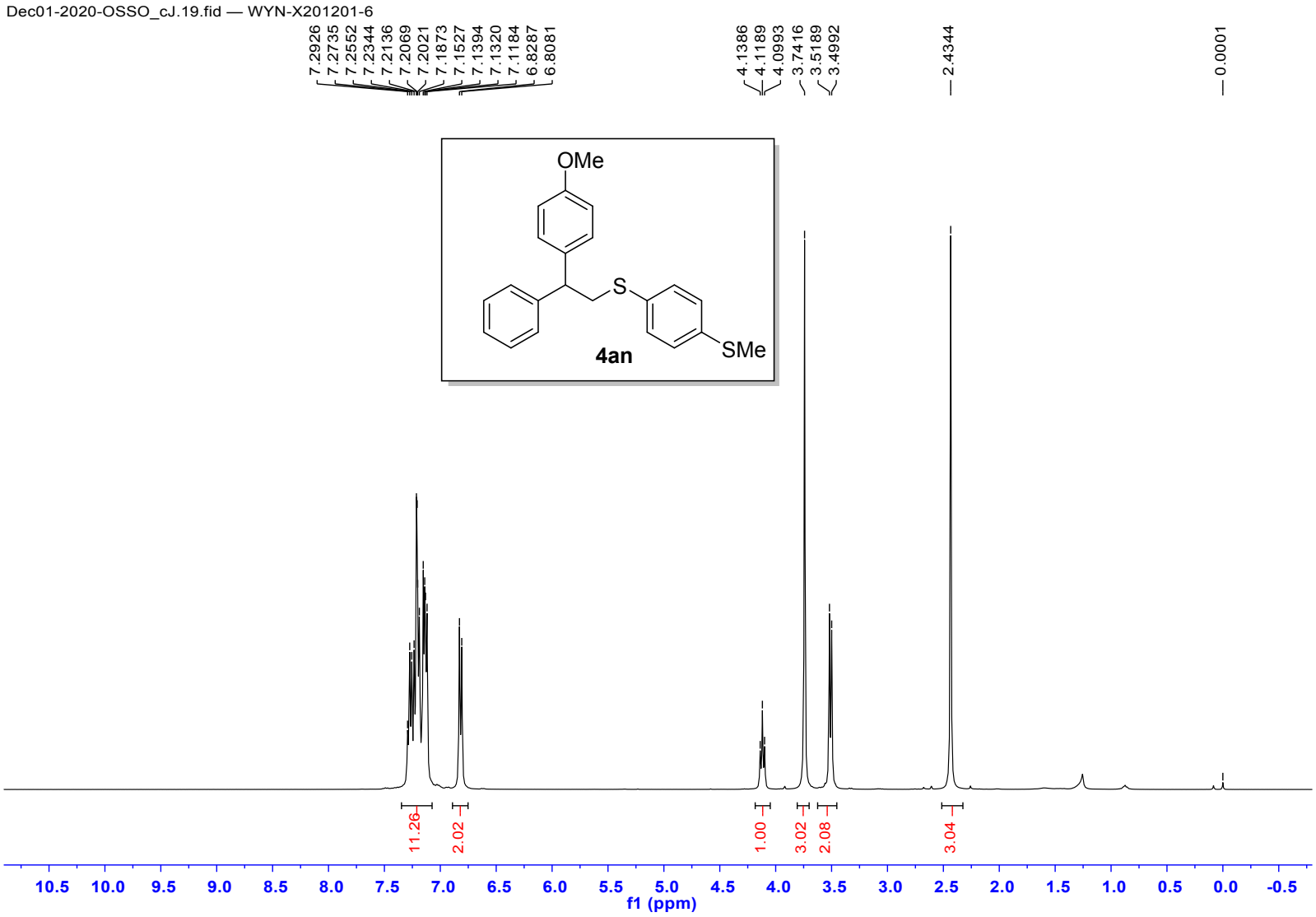
Dec04-2020-OSSO_cJ.6.fid — WYN-X201204-1-C

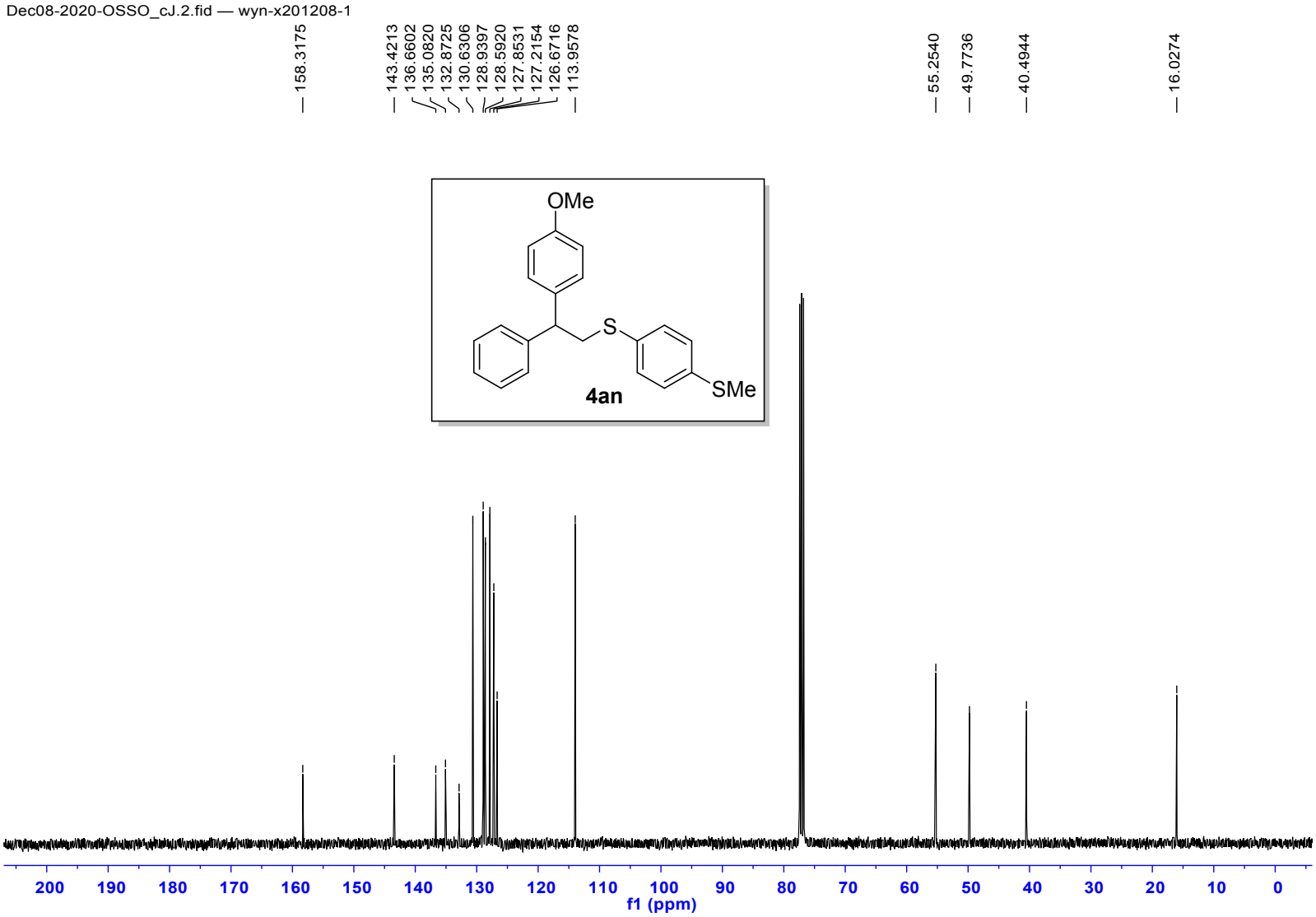
158.9888
158.2876
143.6383
135.3040
133.4338
129.0127
128.5825
127.9395
126.6286
126.6045
114.6530
113.9613
55.3884
55.2637
49.9096
42.0180

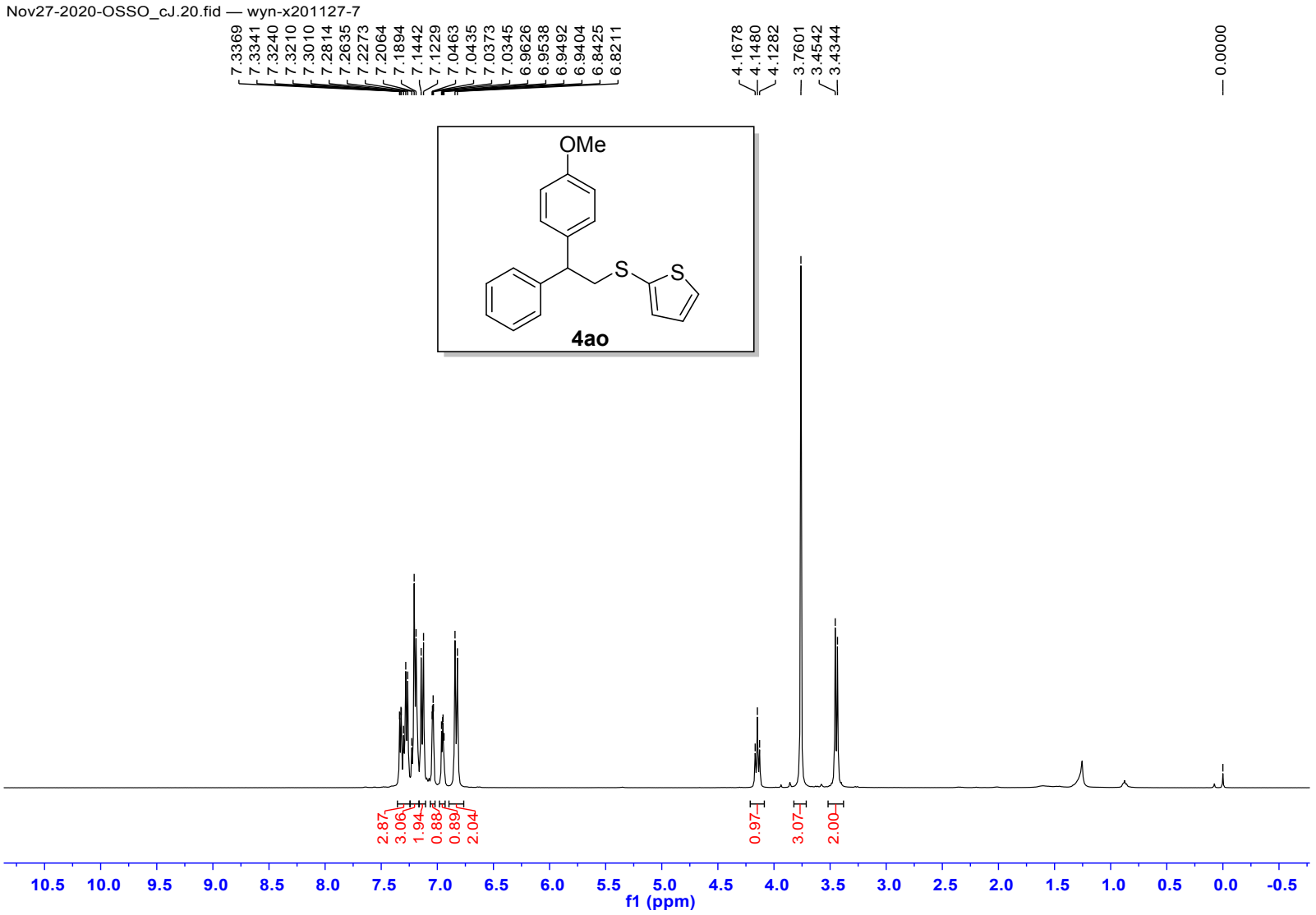


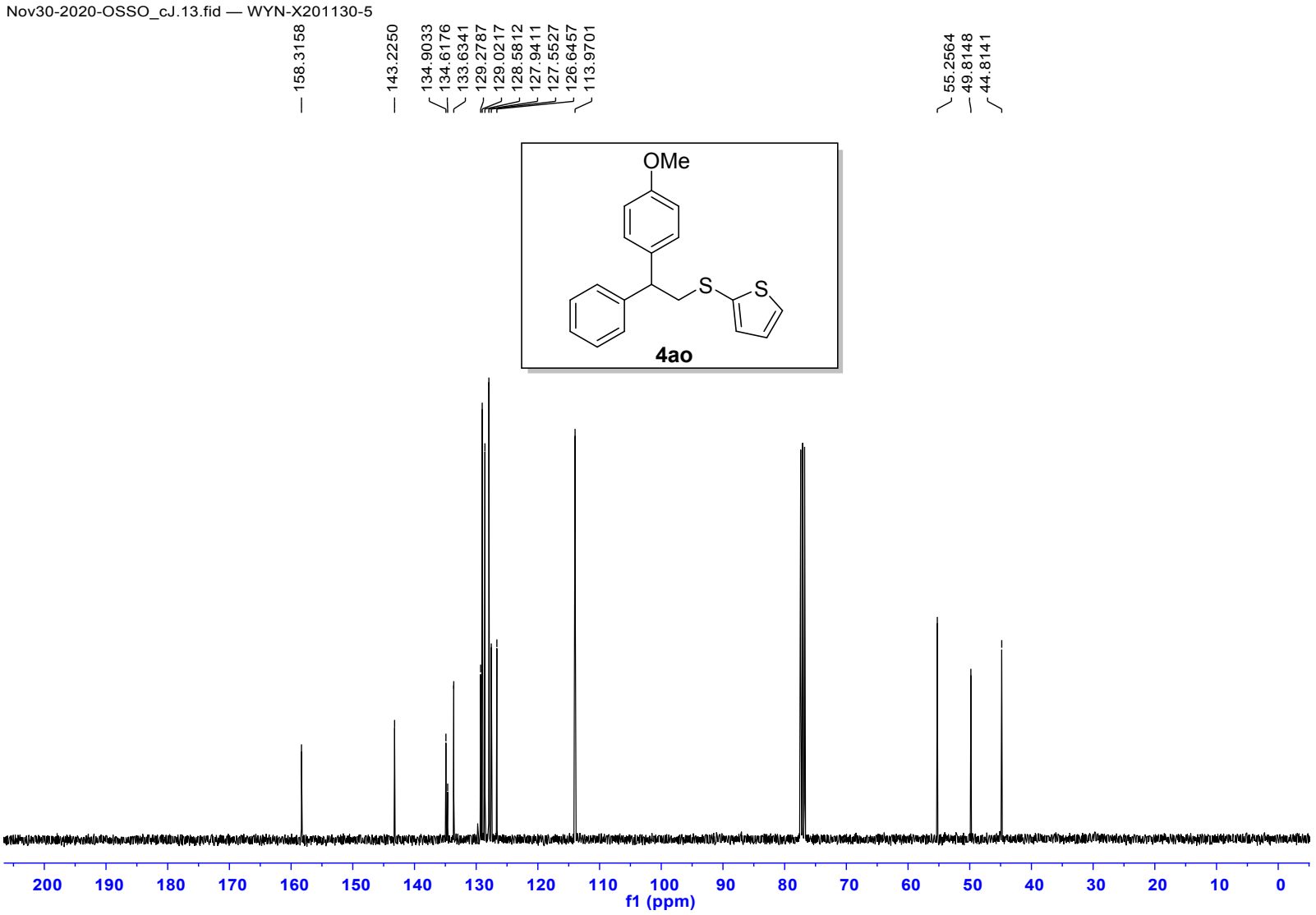

**4am**

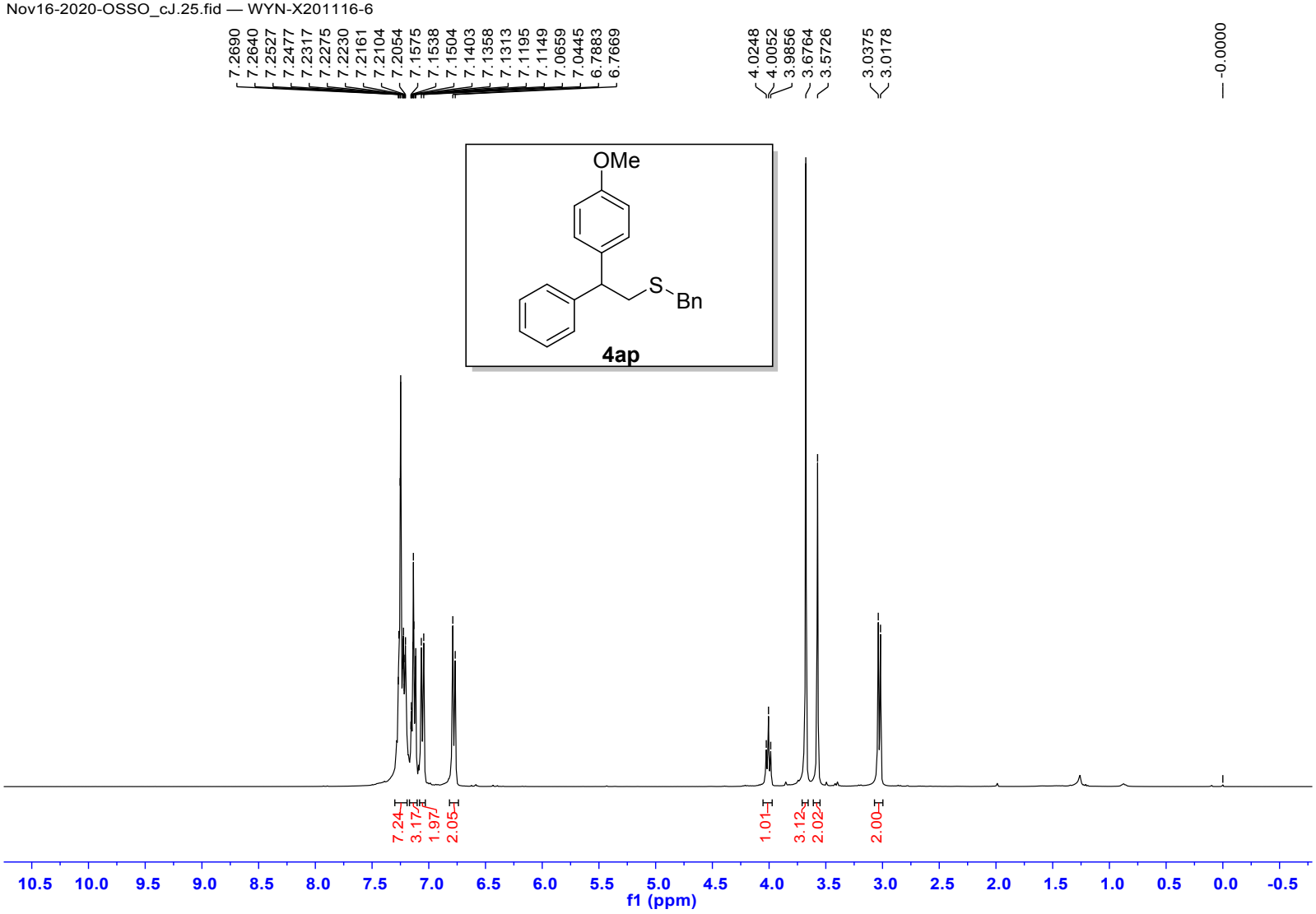


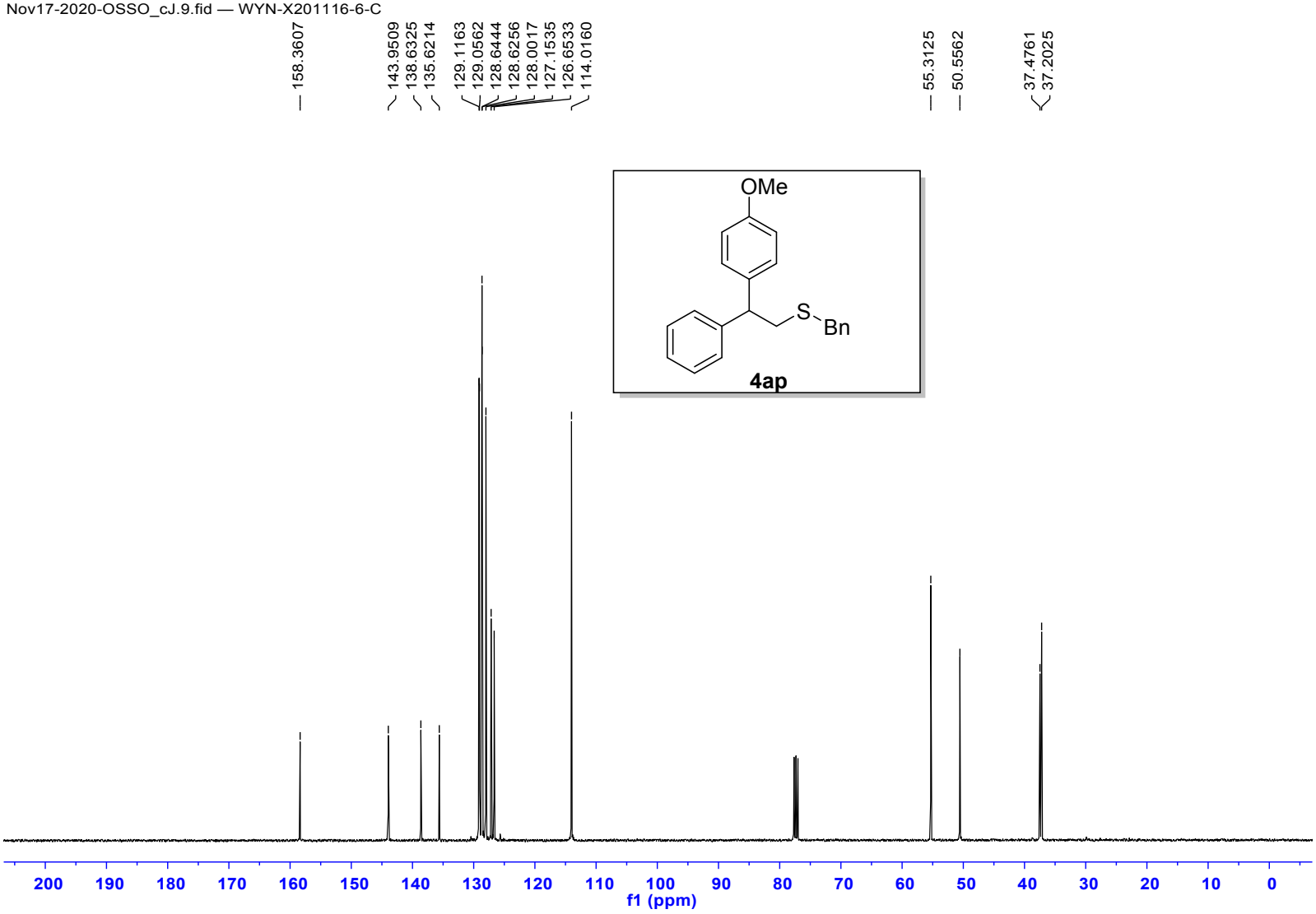

Dec01-2020-OSSO_cJ.19.fid — WYN-X201201-6
7.2926
7.2735
7.2552
7.2344
7.2136
7.2069
7.2021
7.1873
7.1527
7.1394
7.1320
7.1184
6.8287
6.8081
4.1386
4.1189
4.0993
3.7416
3.5189
3.4992
2.4344
0.0001
OMe
S
SMe
4an
11.26
2.02
1.00
3.02
2.08
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

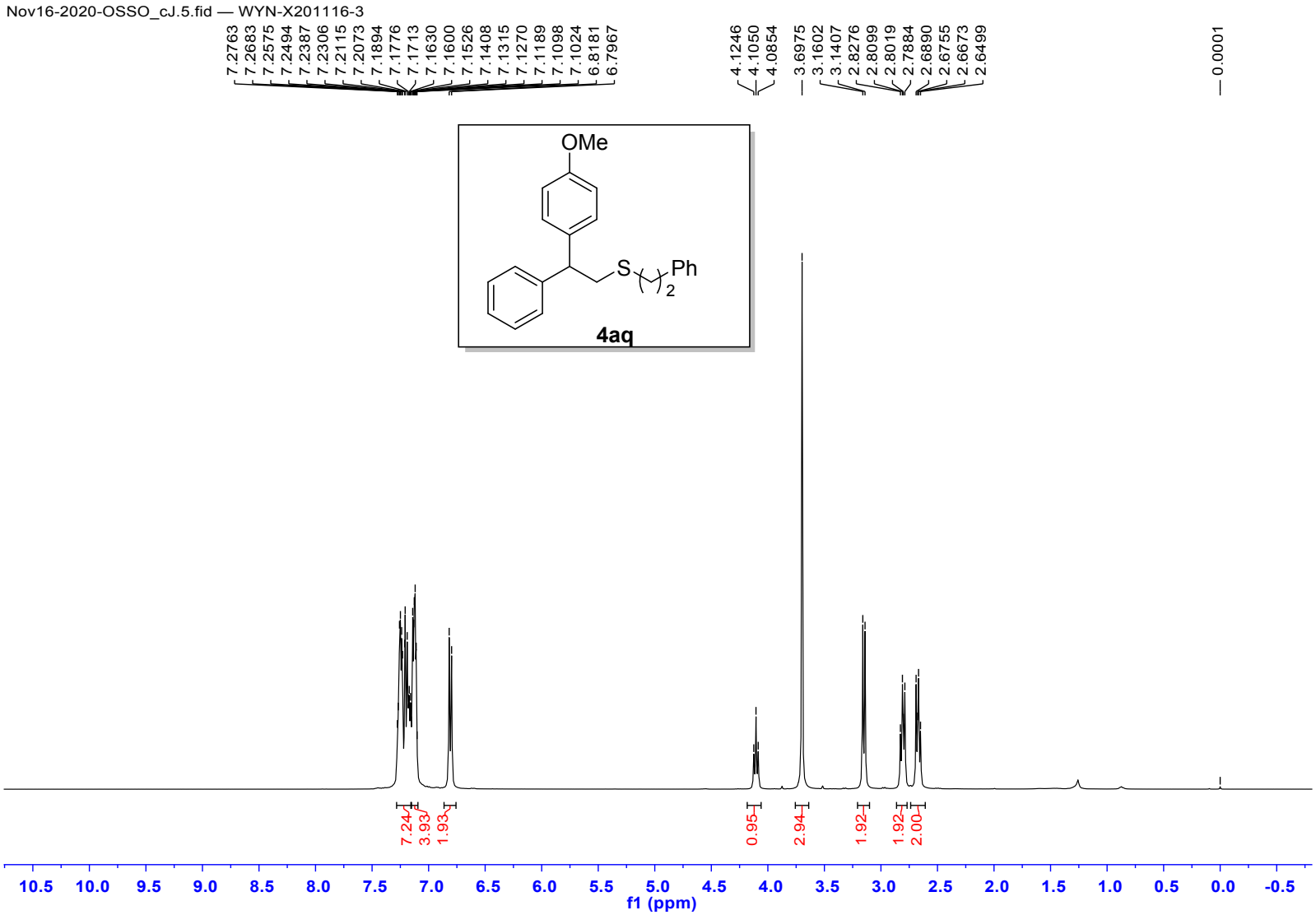

Dec08-2020-OSSO_cJ.2.fid — wyn-x201208-1
158.3175
143.4213
136.6602
135.0820
132.8725
130.6306
128.9397
128.5920
127.8531
127.2154
126.6716
113.9578
55.2540
49.7736
40.4944
16.0274
OMe
S
SMe
4an
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

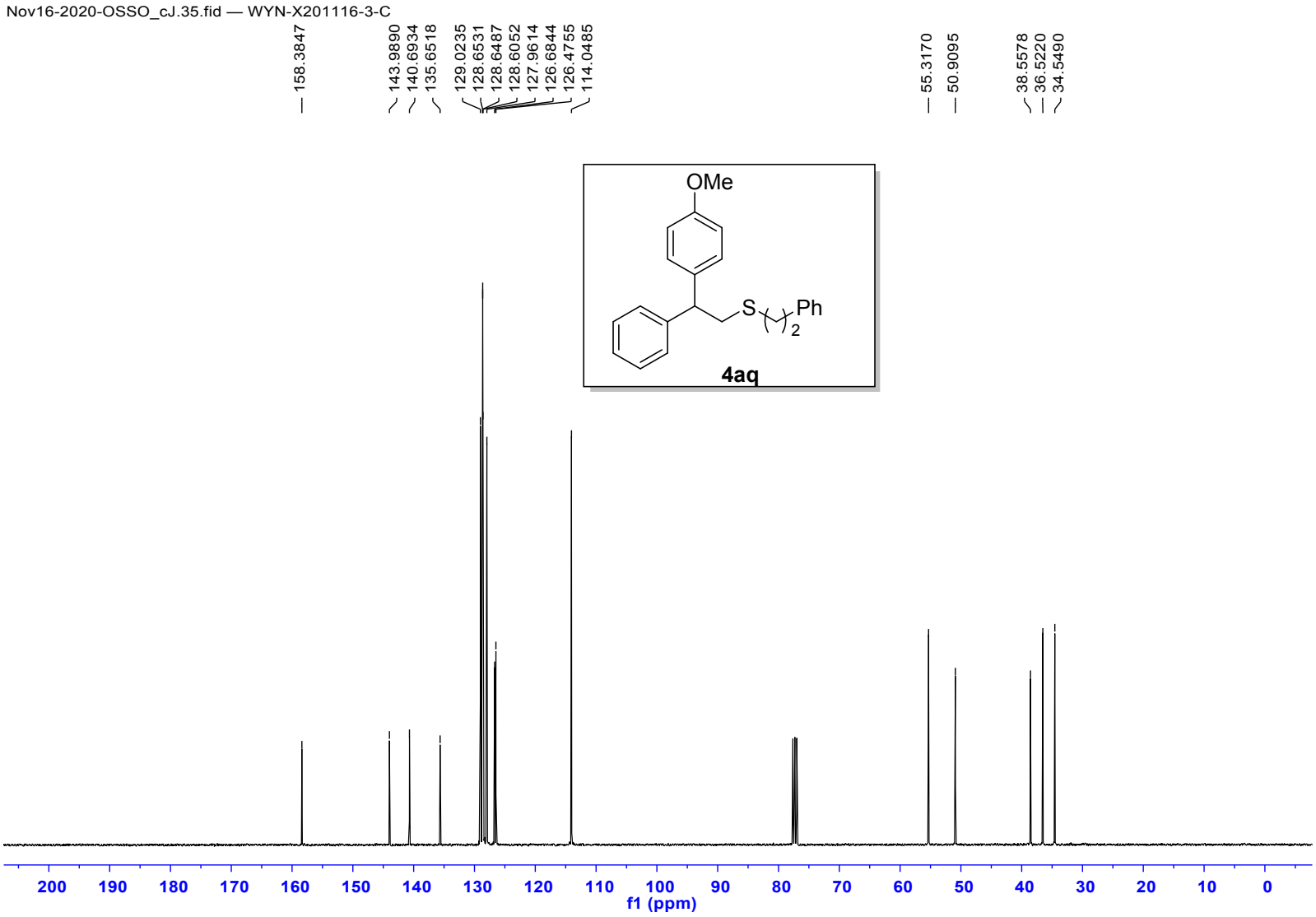

Nov27-2020-OSSO_cJ.20.fid — wyn-x201127-7
7.3369
7.3341
7.3240
7.3210
7.3010
7.2814
7.2635
7.2273
7.2064
7.1894
7.1442
7.1229
7.0463
7.0435
7.0373
7.0345
6.9626
6.9538
6.9492
6.9404
6.8425
6.8211
4.1678
4.1480
4.1282
3.7601
3.4542
3.4344
0.0000
OMe
S
S
4ao
2.87
3.06
1.94
0.88
0.89
2.04
0.97
3.07
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

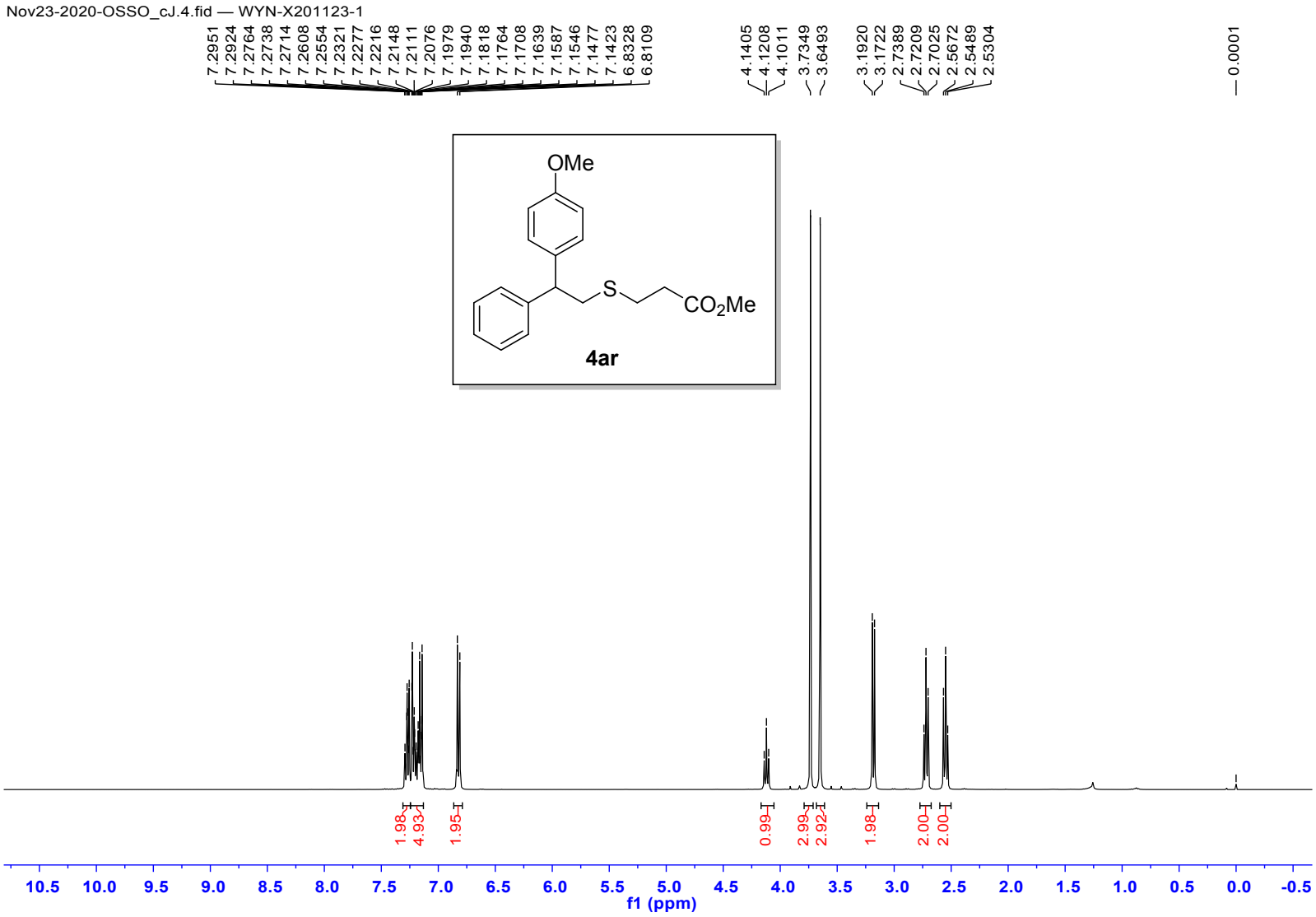

Nov30-2020-OSSO_cJ.13.fid — WYN-X201130-5
158.3158
143.2250
134.9033
134.6176
133.6341
129.2787
129.0217
128.5812
127.9411
127.5527
126.6457
113.9701
55.2564
49.8148
44.8141
OMe
S
S
4ao
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

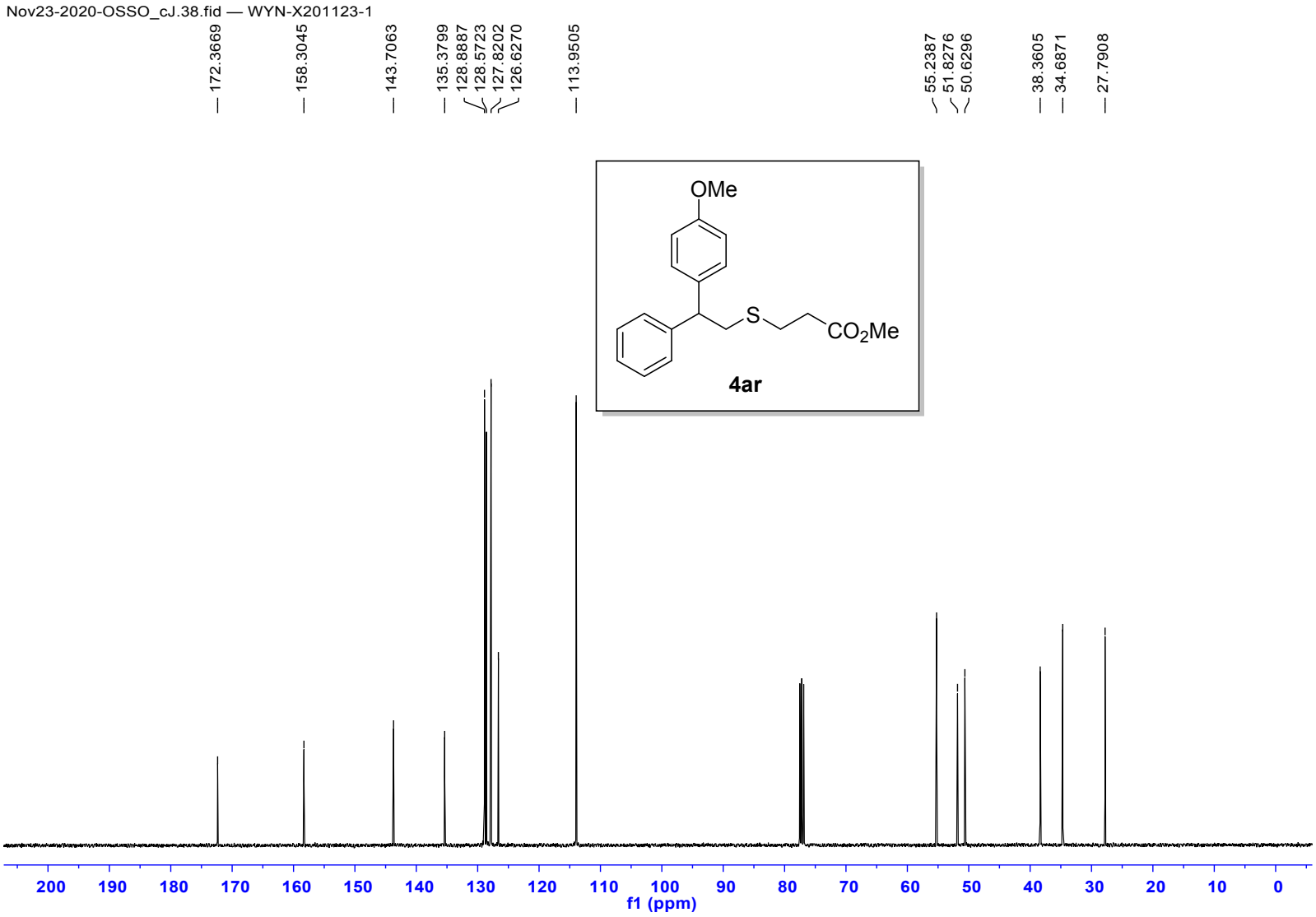

Nov16-2020-OSSO_cJ.25.fid — WYN-X201116-6
7.2690
7.2640
7.2527
7.2477
7.2317
7.2275
7.2230
7.2161
7.2104
7.2054
7.1575
7.1538
7.1504
7.1403
7.1358
7.1313
7.1195
7.1149
7.0659
7.0445
6.7883
6.7669
4.0248
4.0052
3.9856
3.6764
3.5726
3.0375
3.0178
-0.0000
OMe
S
Bn
4ap
7.24
3.17
1.97
2.05
1.01
3.12
2.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

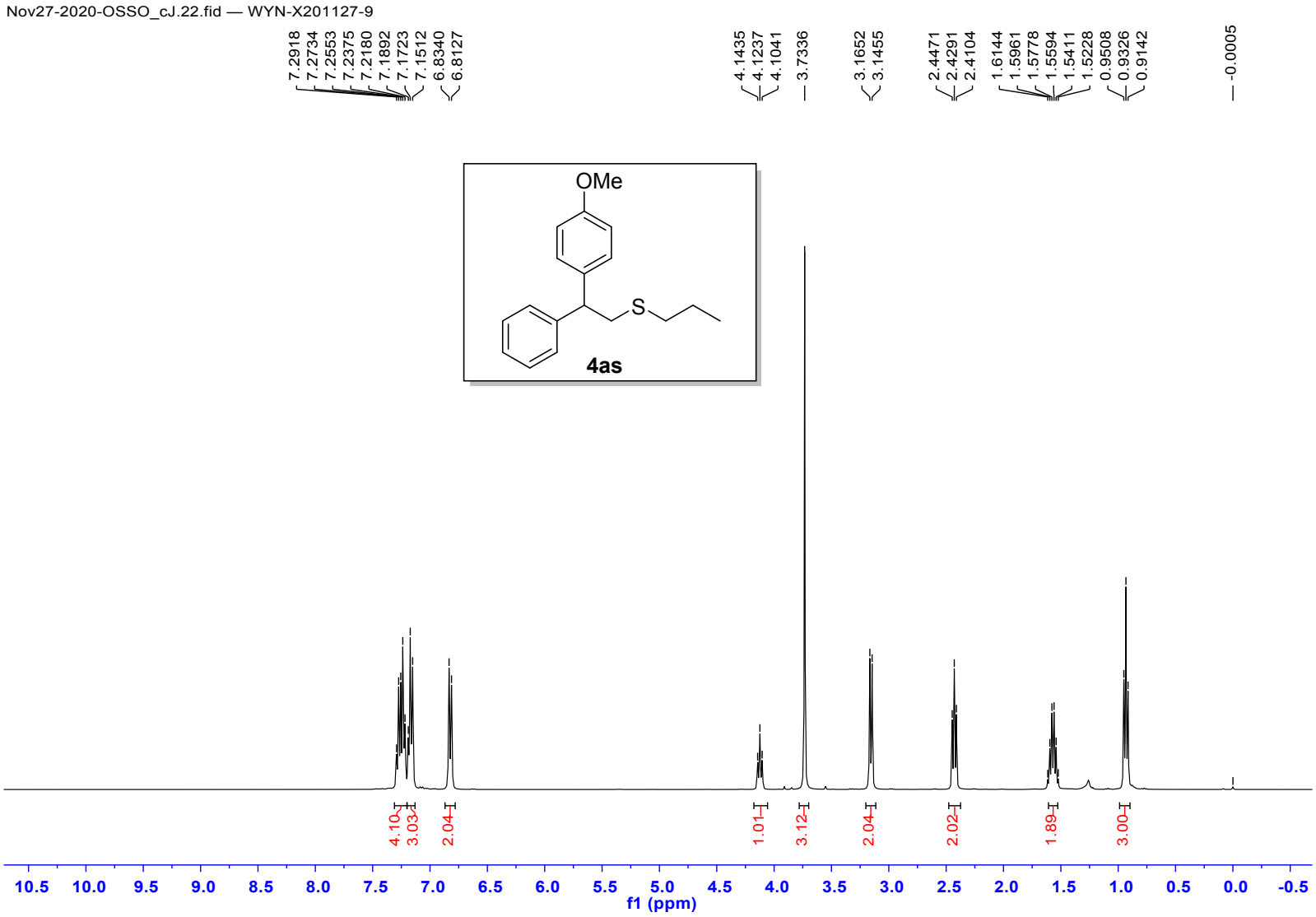

Nov17-2020-OSSO_cJ.9.fid — WYN-X201116-6-C
158.3607
143.9509
138.6325
135.6214
129.1163
129.0562
128.6444
128.6256
128.0017
127.1535
126.6533
114.0160
55.3125
50.5562
37.4761
37.2025
OMe
S
Bn
4ap
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

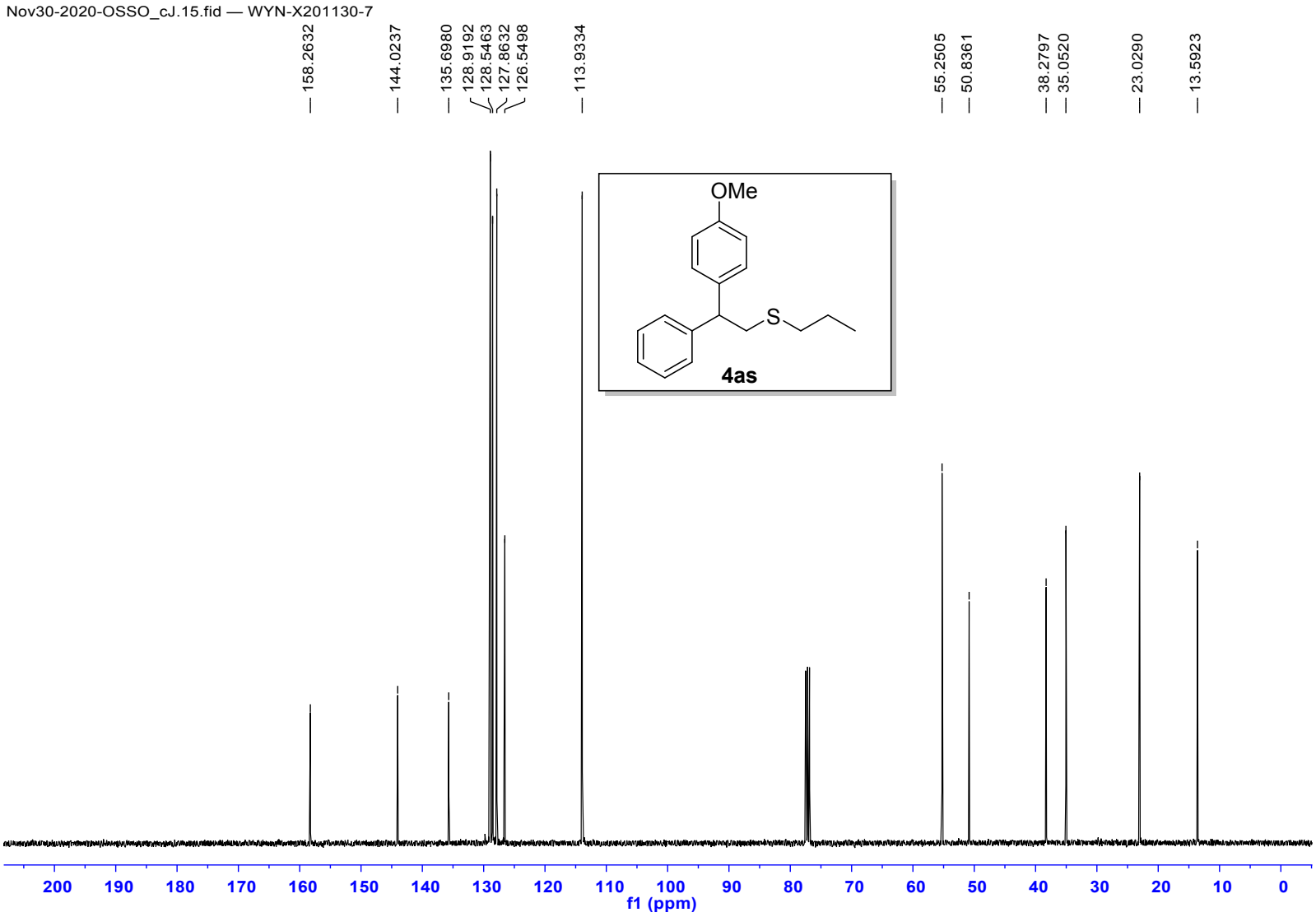

Nov16-2020-OSSO_cJ.5.fid — WYN-X201116-3
7.2763
7.2683
7.2575
7.2494
7.2387
7.2306
7.2115
7.2073
7.1894
7.1776
7.1713
7.1630
7.1600
7.1526
7.1408
7.1315
7.1270
7.1189
7.1098
7.1024
6.8181
6.7967
4.1246
4.1050
4.0854
3.6975
3.1602
3.1407
2.8276
2.8099
2.8019
2.7884
2.6890
2.6755
2.6673
2.6499
0.0001
OMe
S
Ph
2
4aq
7.24
3.93
1.93
0.95
2.94
1.92
1.92
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

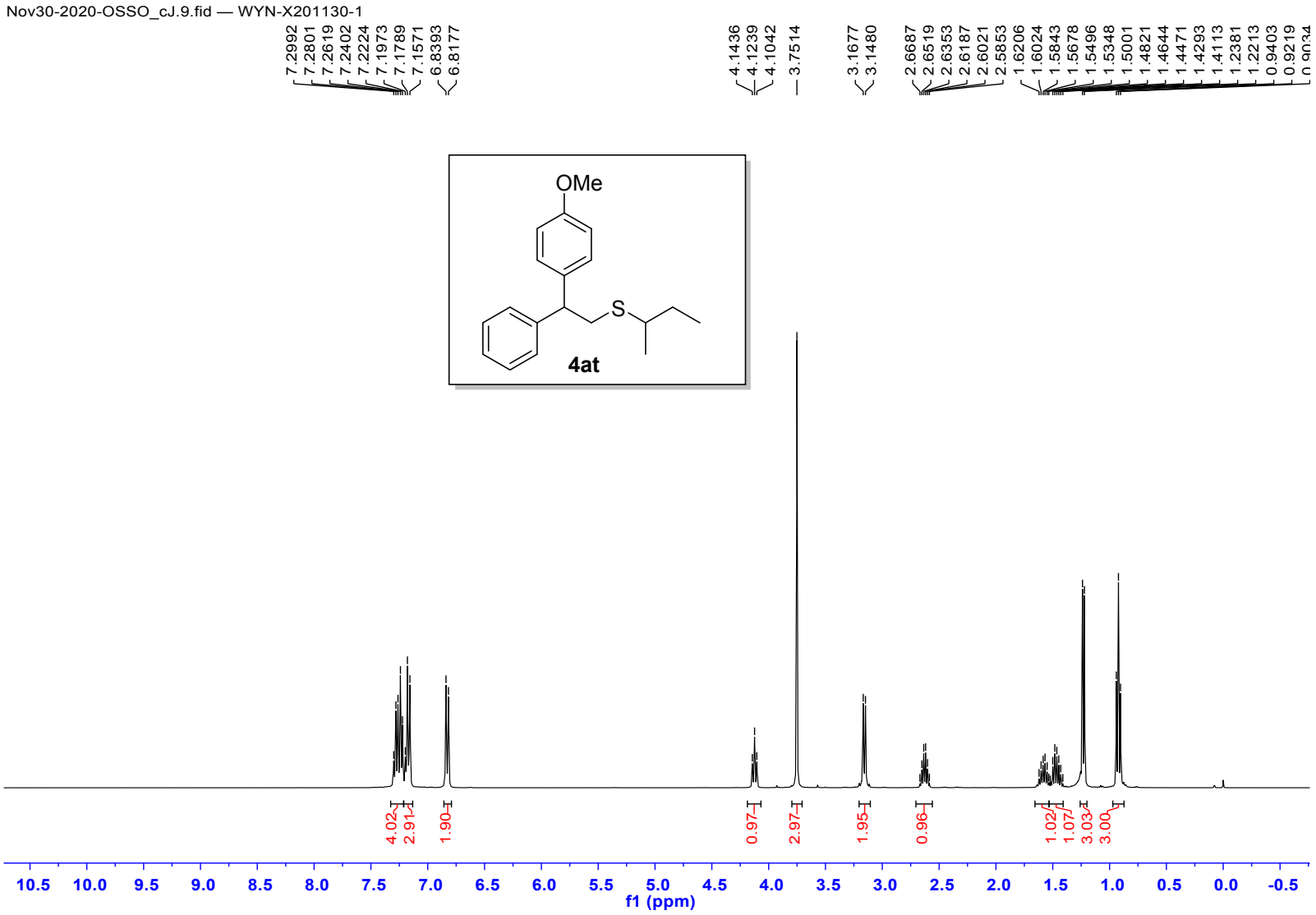

Nov16-2020-OSSO_cJ.35.fid — WYN-X201116-3-C
158.3847
143.9890
140.6934
135.6518
129.0235
128.6531
128.6487
128.6052
127.9614
126.6844
126.4755
114.0485
55.3170
50.9095
38.5578
36.5220
34.5490
OMe
S
Ph
2
4aq
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov23-2020-OSSO_cJ.4.fid — WYN-X201123-1
7.2951
7.2924
7.2764
7.2738
7.2714
7.2608
7.2554
7.2321
7.2277
7.2216
7.2148
7.2111
7.2076
7.1979
7.1940
7.1818
7.1764
7.1708
7.1639
7.1587
7.1546
7.1477
7.1423
6.8328
6.8109
4.1405
4.1208
4.1011
3.7349
3.6493
3.1920
3.1722
2.7389
2.7209
2.7025
2.5672
2.5489
2.5304
0.0001
OMe
S
CO2Me
4ar
1.98
4.93
1.95
0.99
2.99
2.92
1.98
2.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Nov23-2020-OSSO_cJ.38.fid — WYN-X201123-1
172.3669
158.3045
143.7063
135.3799
128.8887
128.5723
127.8202
126.6270
113.9505
55.2387
51.8276
50.6296
38.3605
34.6871
27.7908
OMe
S
CO2Me
4ar
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov27-2020-OSSO_cJ.22.fid — WYN-X201127-9
7.2918
7.2734
7.2553
7.2375
7.2180
7.1892
7.1723
7.1512
6.8340
6.8127
4.1435
4.1237
4.1041
3.7336
3.1652
3.1455
2.4471
2.4291
2.4104
1.6144
1.5961
1.5778
1.5594
1.5411
1.5228
0.9508
0.9326
0.9142
-0.0005
OMe
S
4as
4.10
3.03
2.04
1.01
3.12
2.04
2.02
1.89
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Nov30-2020-OSSO_cJ.15.fid — WYN-X201130-7
158.2632
144.0237
135.6980
128.9192
128.5463
127.8632
126.5498
113.9334
55.2505
50.8361
38.2797
35.0520
23.0290
13.5923
OMe
S
4as
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov30-2020-OSSO_cJ.9.fid — WYN-X201130-1
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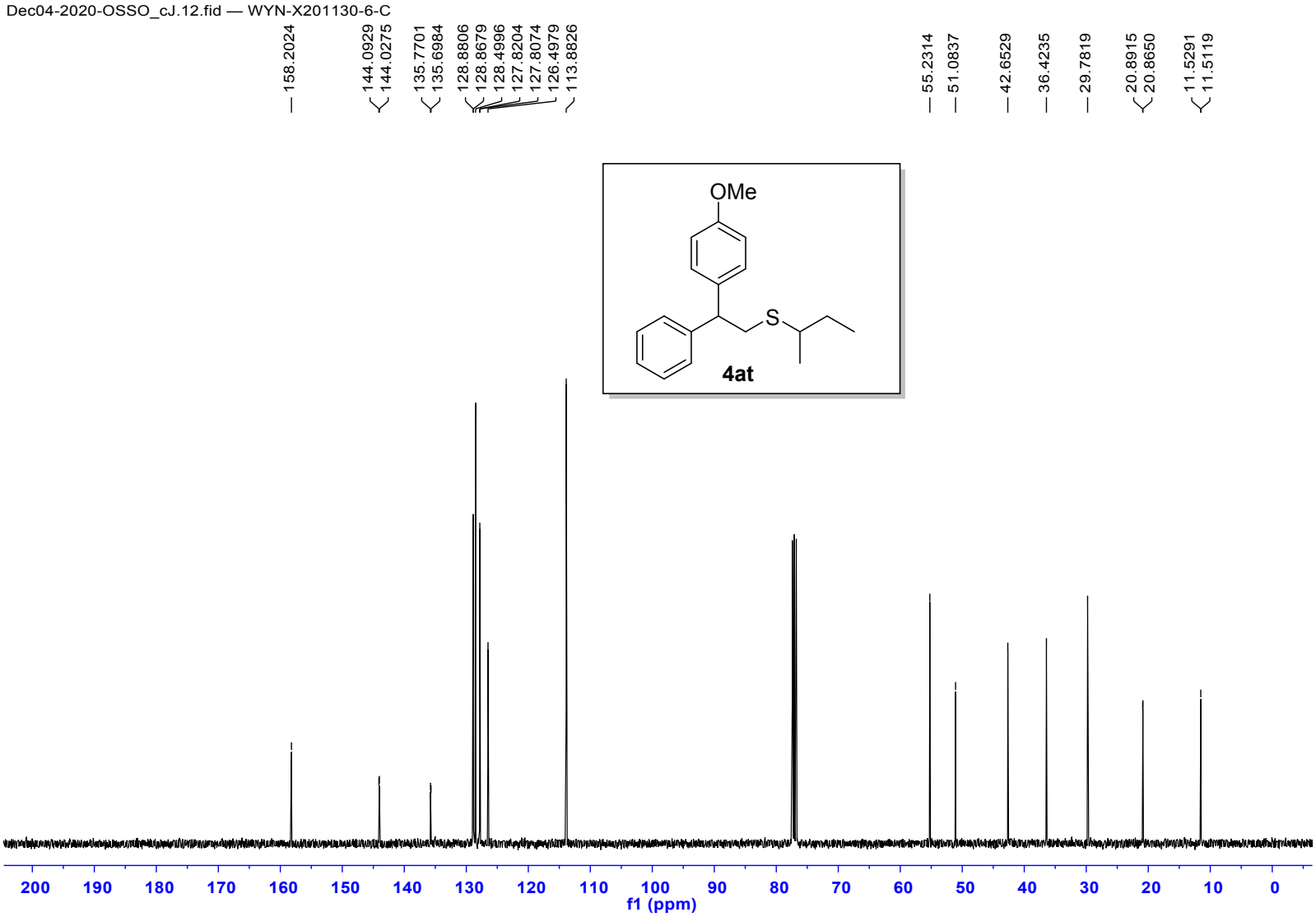
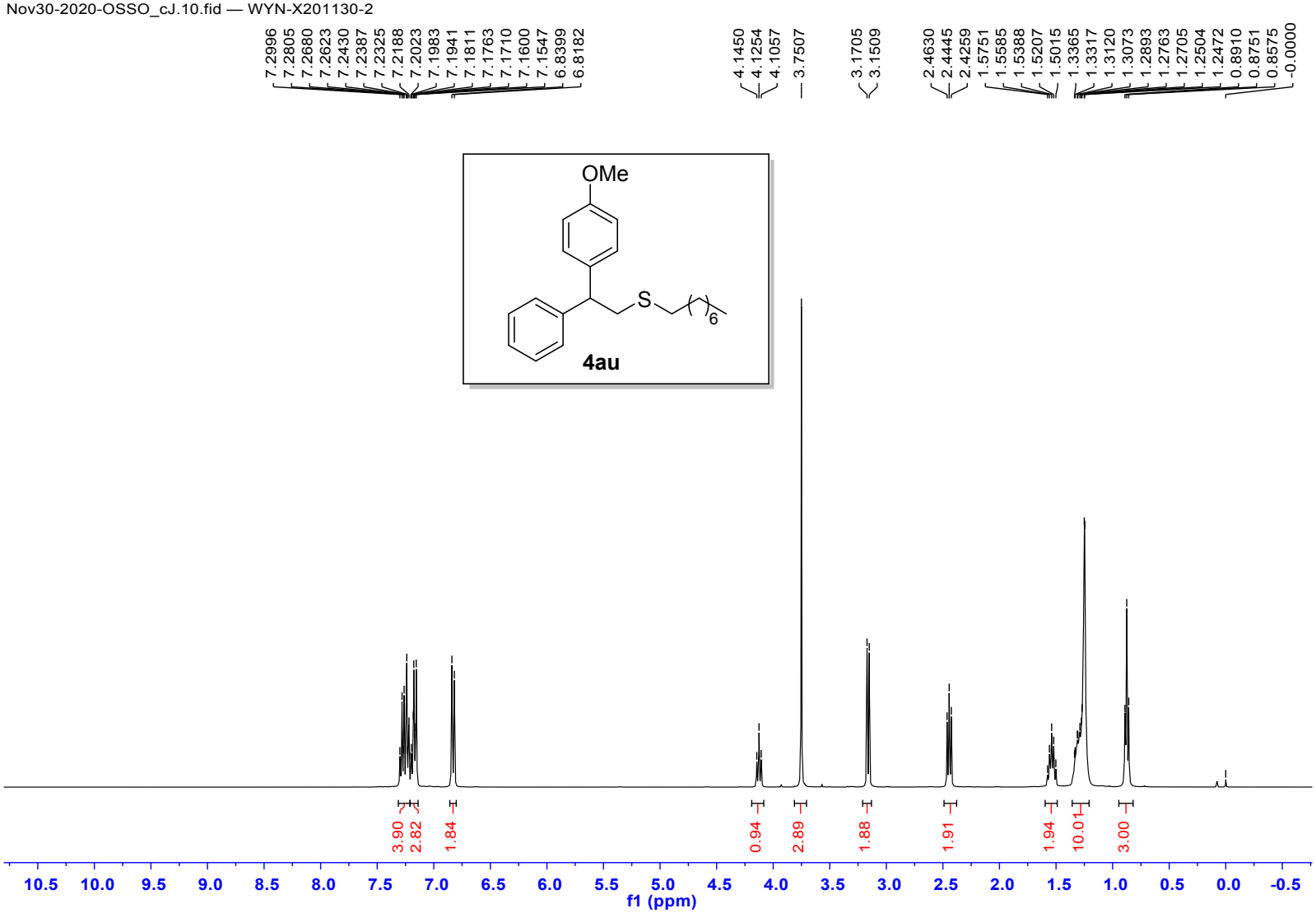
7.2801
7.2619
7.2402
7.2224
7.1973
7.1789
7.1571
6.8393
6.8177
4.1436
4.1239
4.1042
3.7514
3.1677
3.1480
2.6687
2.6519
2.6353
2.6187
2.6021
2.5853
1.6206
1.6024
1.5843
1.5678
1.5496
1.5348
1.5001
1.4821
1.4644
1.4471
1.4293
1.4113
1.2381
1.2213
0.9403
0.9219
OMe
S
4at
4.02
2.91
1.90
0.97
2.97
1.95
0.96
1.02
1.07
3.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Dec04-2020-OSSO_cJ.12.fid — WYN-X201130-6-C
158.2024
144.0929
144.0275
135.7701
135.6984
128.8806
128.8679
128.4996
127.8204
127.8074
126.4979
113.8826
55.2314
51.0837
42.6529
36.4235
29.7819
20.8915
20.8650
11.5291
11.5119
OMe
S
4at
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov30-2020-OSSO_cJ.10.fid — WYN-X201130-2
7.2996
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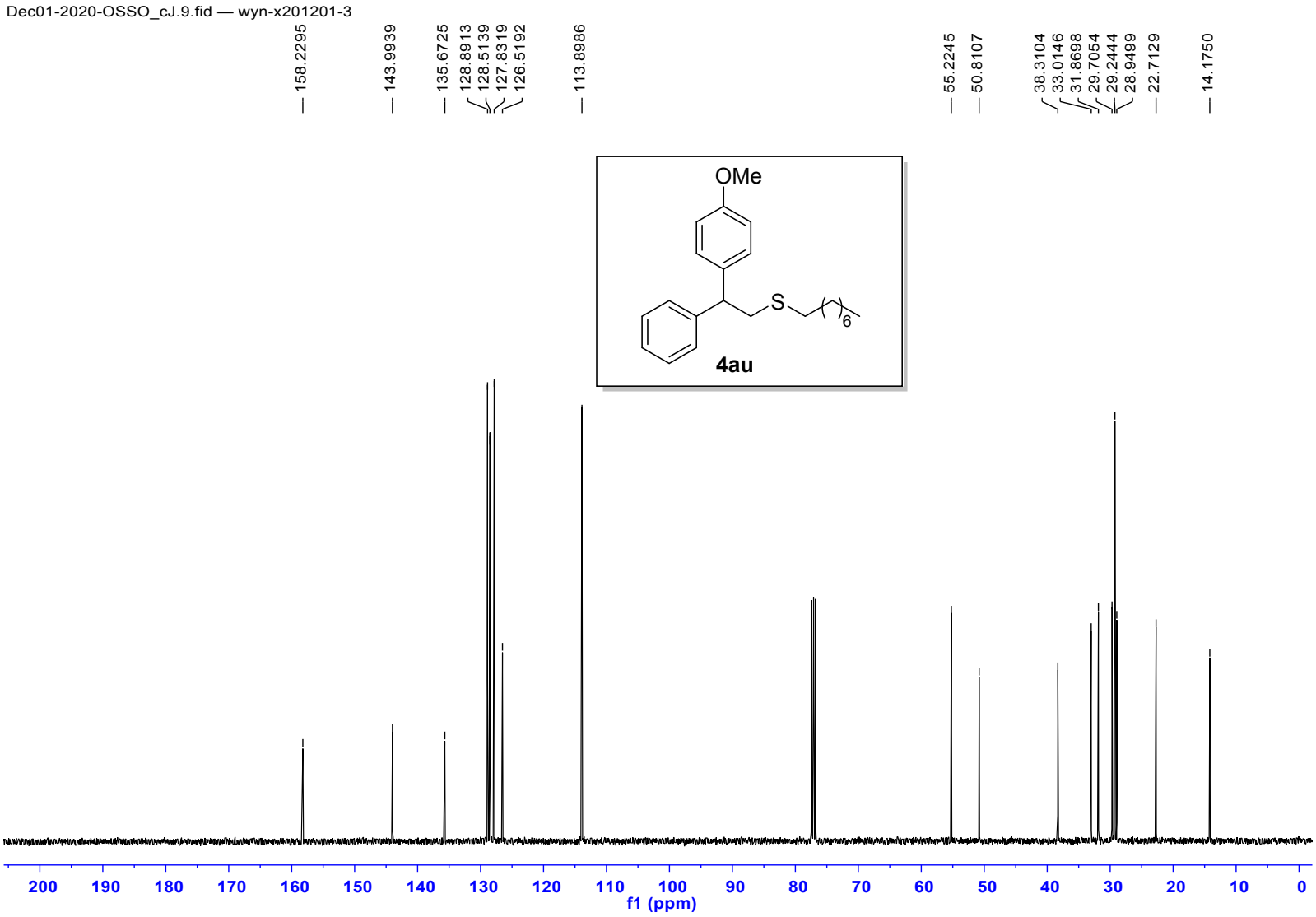
7.2680
7.2623
7.2430
7.2387
7.2325
7.2188
7.2023
7.1983
7.1941
7.1811
7.1763
7.1710
7.1600
7.1547
6.8399
6.8182
4.1450
4.1254
4.1057
3.7507
3.1705
3.1509
2.4630
2.4445
2.4259
1.5751
1.5585
1.5388
1.5207
1.5015
1.3365
1.3317
1.3120
1.3073
1.2893
1.2763
1.2705
1.2504
1.2472
0.8910
0.8751
0.8575
-0.0000
OMe
S
6
4au
3.90
2.82
1.84
0.94
2.89
1.88
1.91
1.94
10.01
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Dec01-2020-OSSO_cJ.9.fid — wyn-x201201-3
158.2295
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135.6725
128.8913
128.5139
127.8319
126.5192
113.8986
55.2245
50.8107
38.3104
33.0146
31.8698
29.7054
29.2444
28.9499
22.7129
14.1750
OMe
S
6
4au
200
190
180
170
160
150
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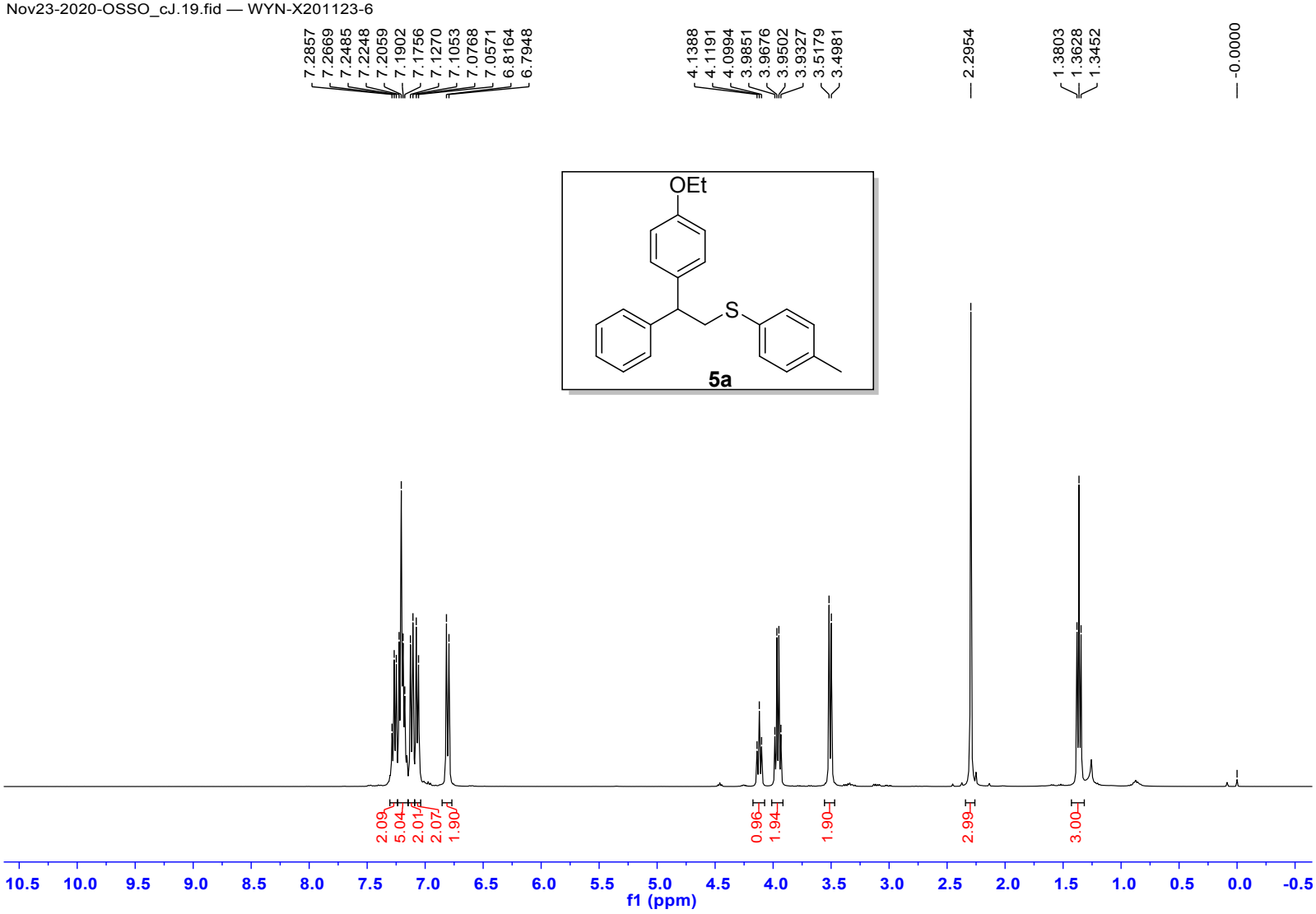
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov23-2020-OSSO_cJ.19.fid — WYN-X201123-6
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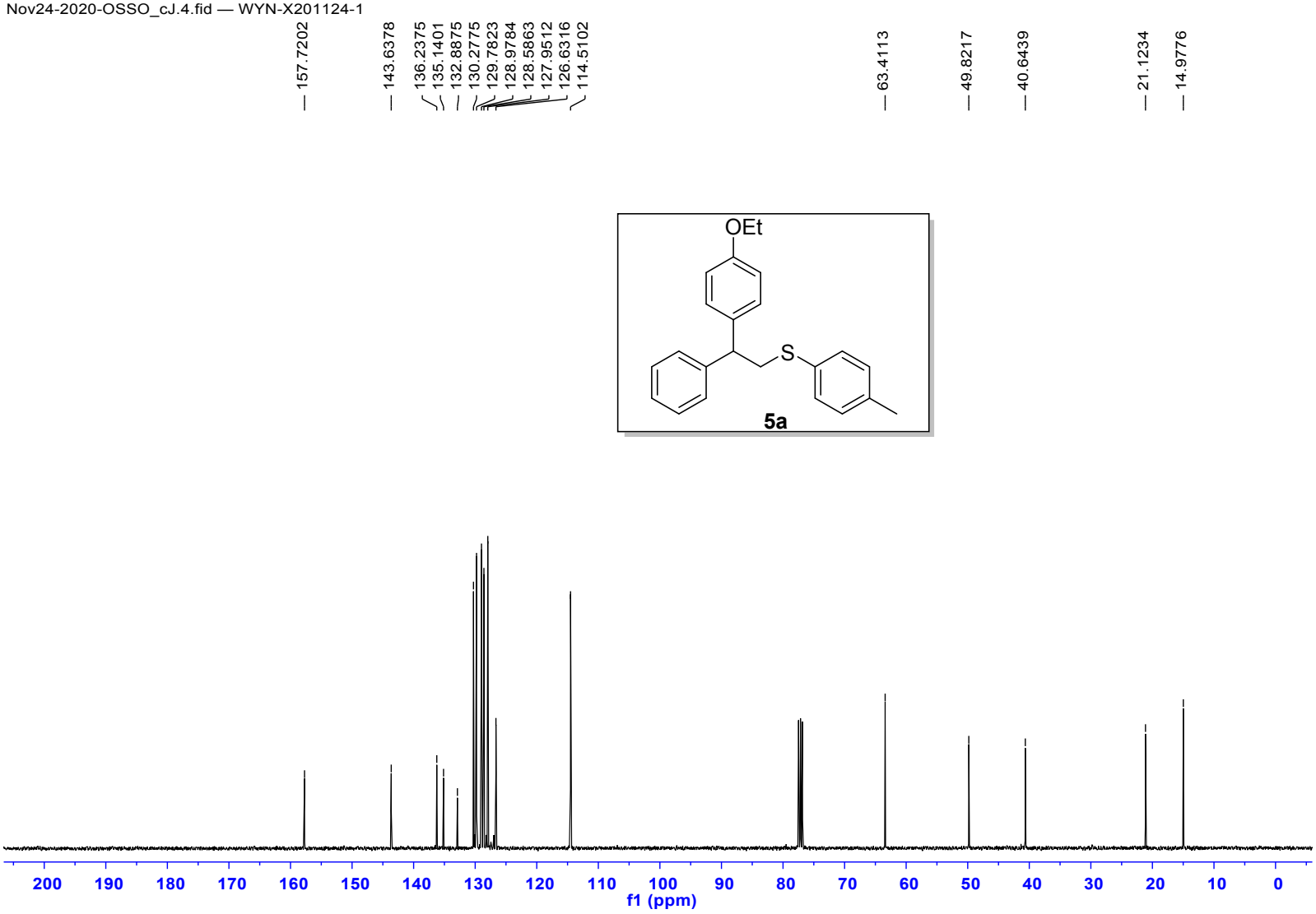
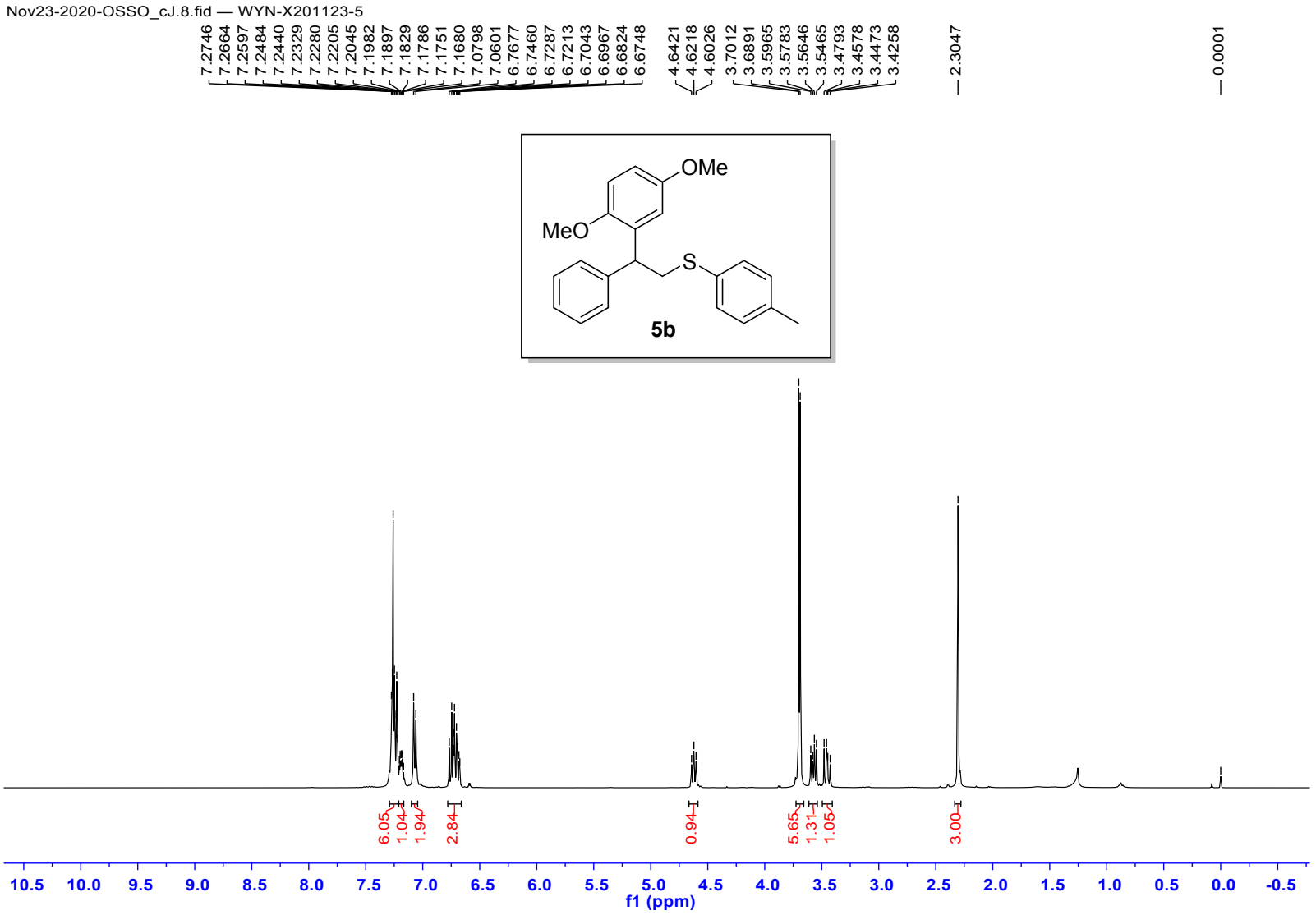
7.2485
7.2248
7.2059
7.1902
7.1756
7.1270
7.1053
7.0768
7.0571
6.8164
6.7948
4.1388
4.1191
4.0994
3.9851
3.9676
3.9502
3.9327
3.5179
3.4981
2.2954
1.3803
1.3628
1.3452
-0.0000
OEt
S
5a
2.09
5.04
2.01
2.07
1.90
0.96
1.94
1.90
2.99
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Nov24-2020-OSSO_cJ.4.fid — WYN-X201124-1
157.7202
143.6378
136.2375
135.1401
132.8875
130.2775
129.7823
128.9784
128.5863
127.9512
126.6316
114.5102
63.4113
49.8217
40.6439
21.1234
14.9776
OEt
S
5a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov23-2020-OSSO_cJ.8.fid — WYN-X201123-5
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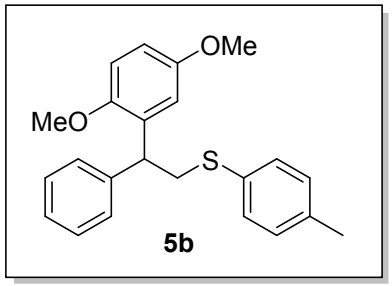
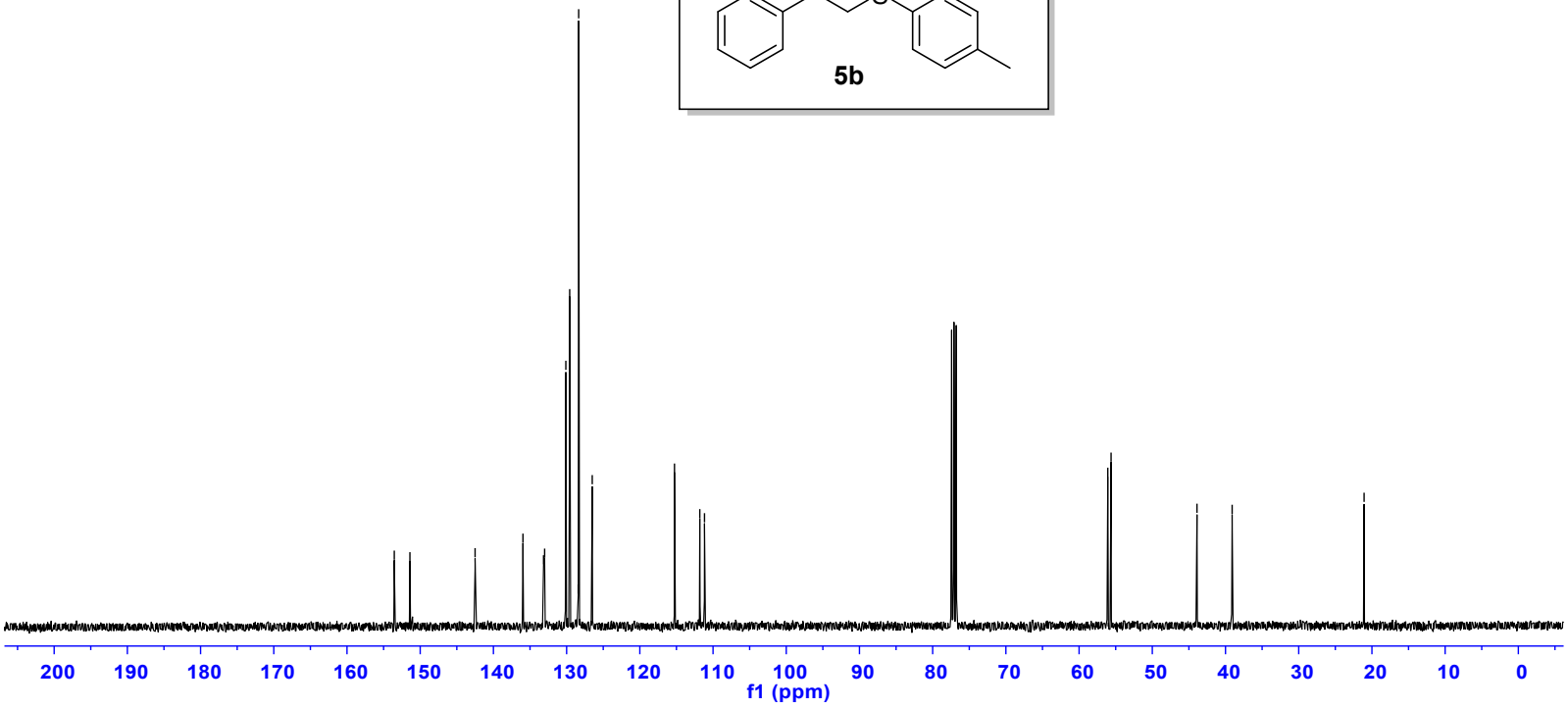
7.2484
7.2440
7.2329
7.2280
7.2205
7.2045
7.1982
7.1897
7.1829
7.1786
7.1751
7.1680
7.0798
7.0601
6.7677
6.7460
6.7287
6.7213
6.7043
6.6967
6.6824
6.6748
4.6421
4.6218
4.6026
3.7012
3.6891
3.5965
3.5783
3.5646
3.5465
3.4793
3.4578
3.4473
3.4258
2.3047
0.0001
OMe
MeO
S
5b
6.05
1.04
1.94
2.84
0.94
5.65
1.31
1.05
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

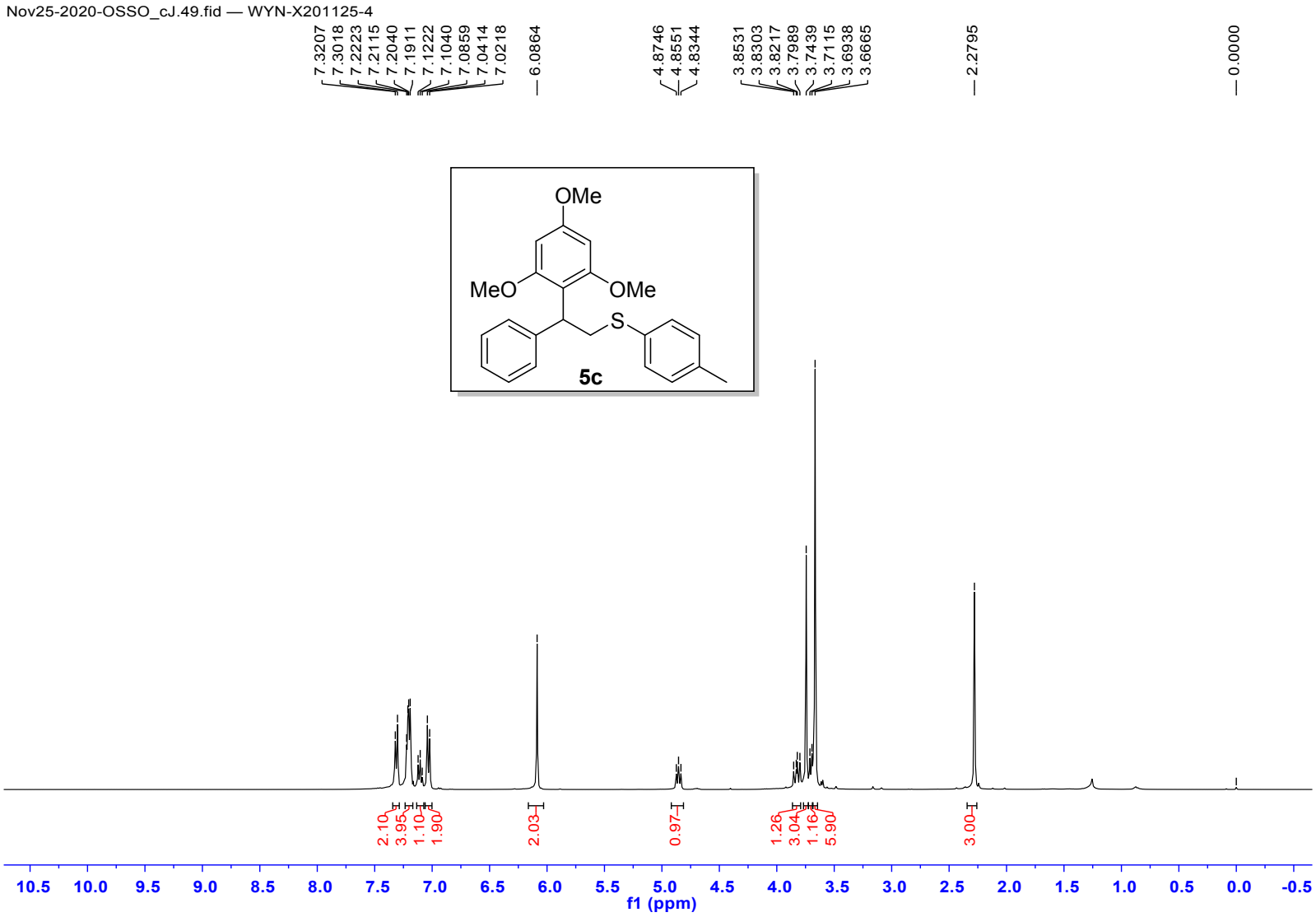
Nov23-2020-OSSO_cJ.40.fid — WYN-X201123-5

153.5409
151.4044
142.5032
135.9648
133.1529
133.0034
130.1062
129.5818
128.4148
128.3528
126.5010
115.2655
111.8092
111.1675
56.0809
55.6300
43.8966
39.0933
21.0687



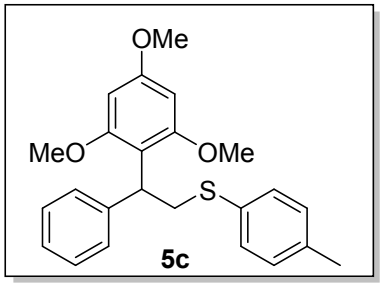

**5b**



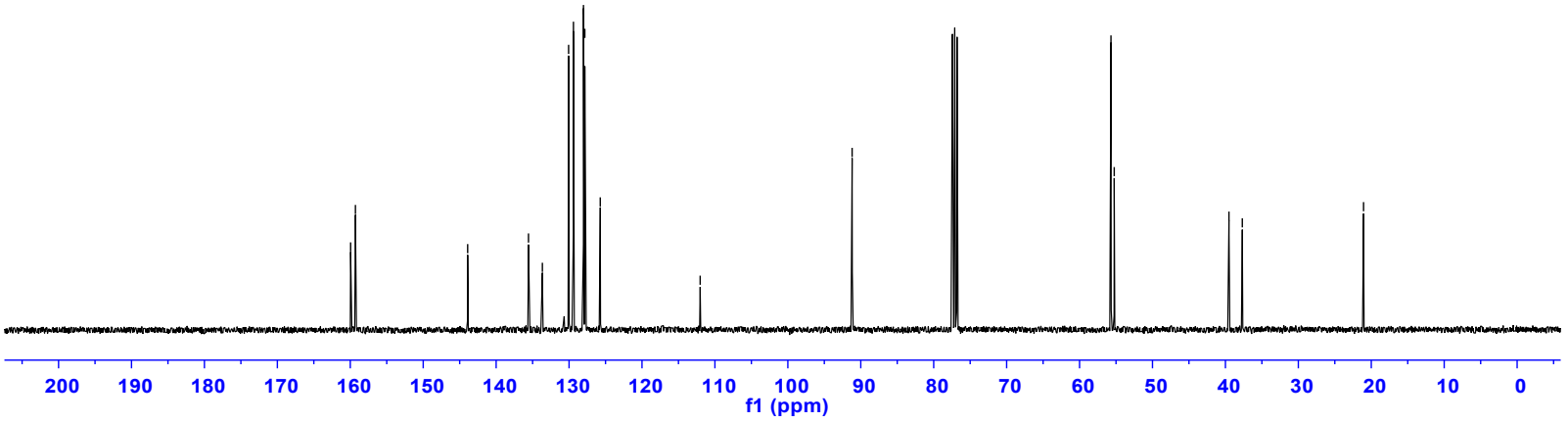

Nov25-2020-OSSO_cJ.49.fid — WYN-X201125-4
7.3207
7.3018
7.2223
7.2115
7.2040
7.1911
7.1222
7.1040
7.0859
7.0414
7.0218
6.0864
4.8746
4.8551
4.8344
3.8531
3.8303
3.8217
3.7989
3.7439
3.7115
3.6938
3.6665
2.2795
0.0000
OMe
MeO
OMe
S
5c
2.10
3.95
1.10
1.90
2.03
0.97
1.26
3.04
1.16
5.90
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

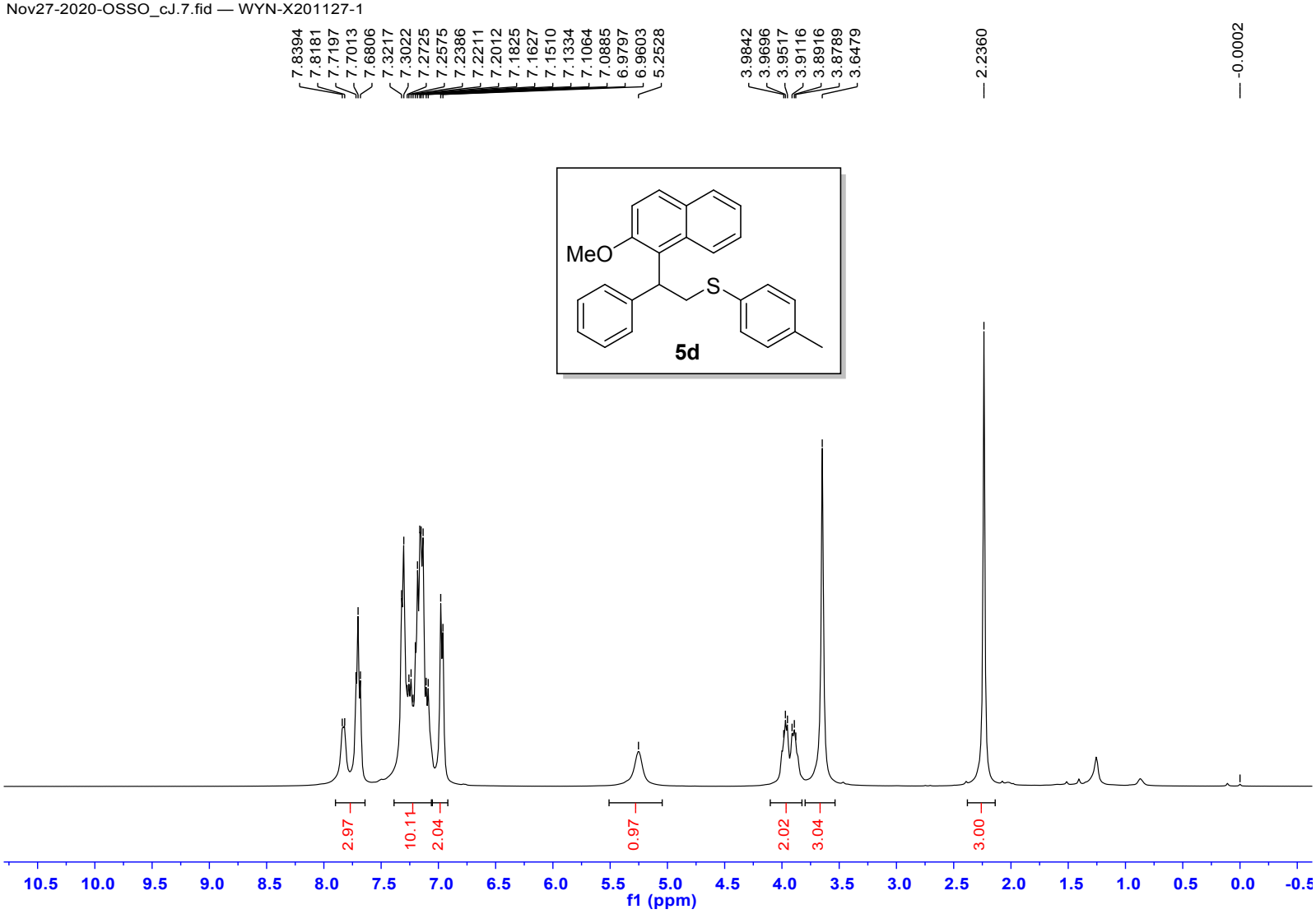
Nov27-2020-OSSO_cJ.12.fid — WYN-X201127-6

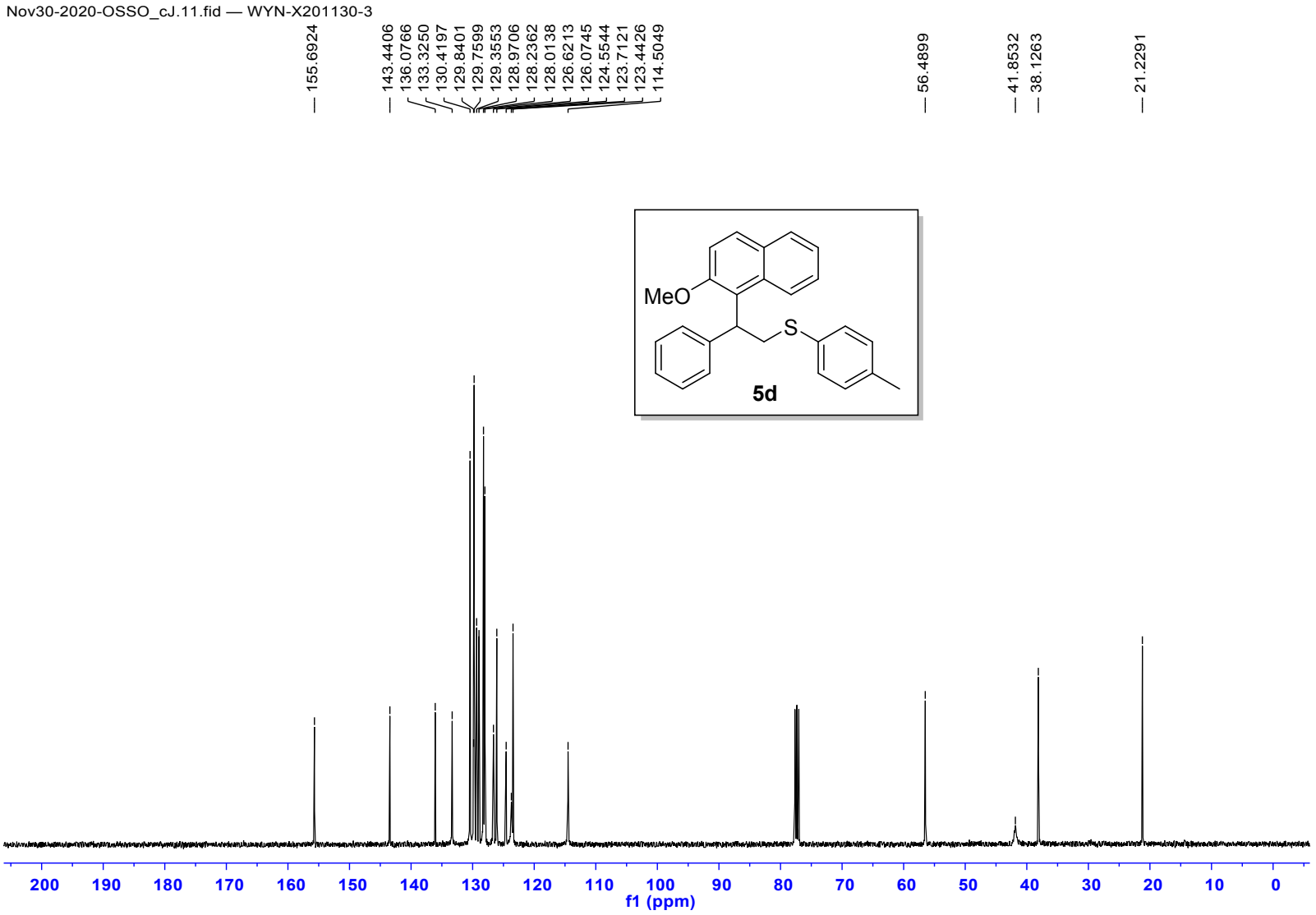
159.9521
159.2946
143.9040
135.5631
133.6588
130.0626
129.3983
128.0240
127.8387
125.7235
112.0222
91.1864
55.6922
55.2456
39.5156
37.6840
21.0578

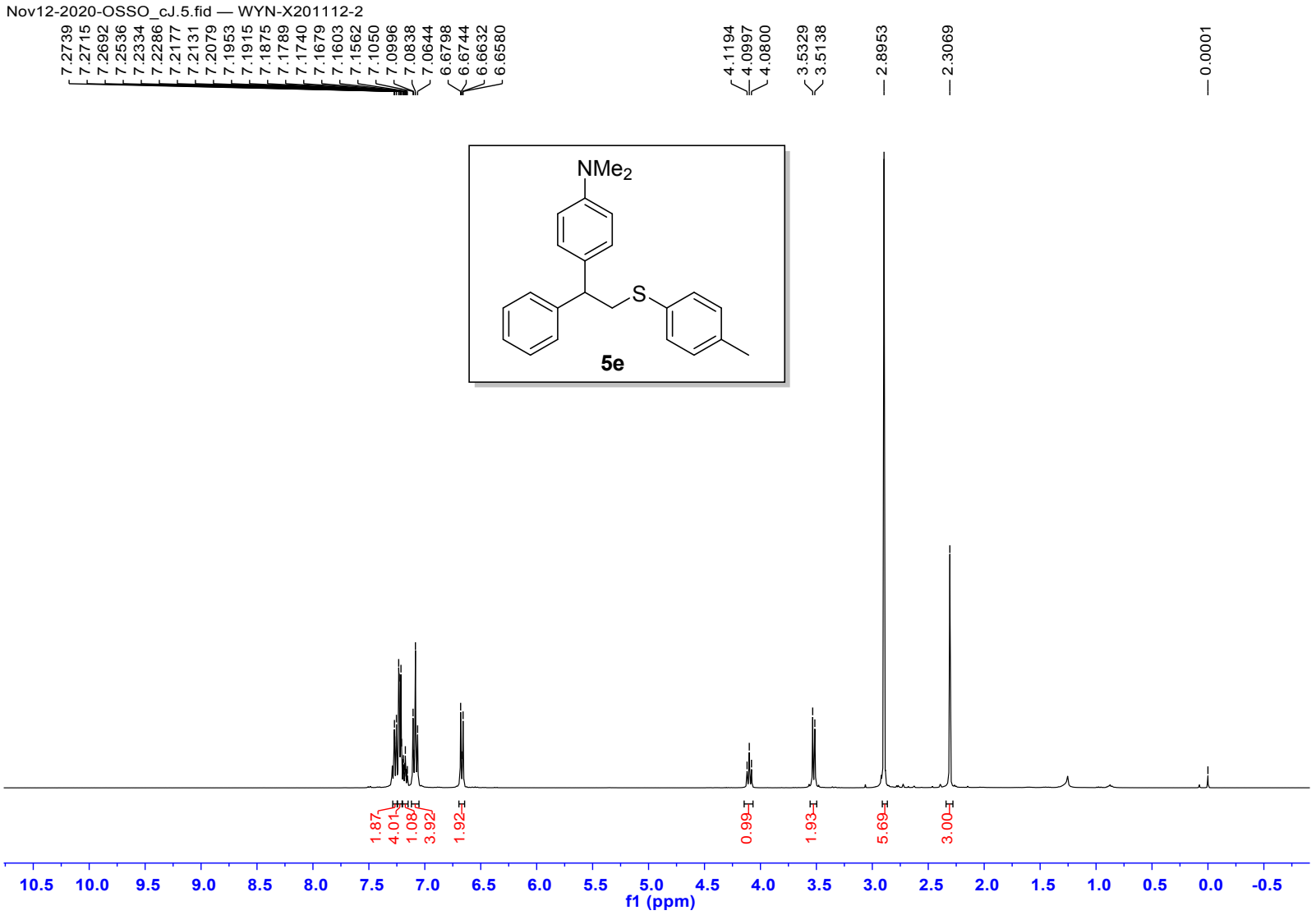


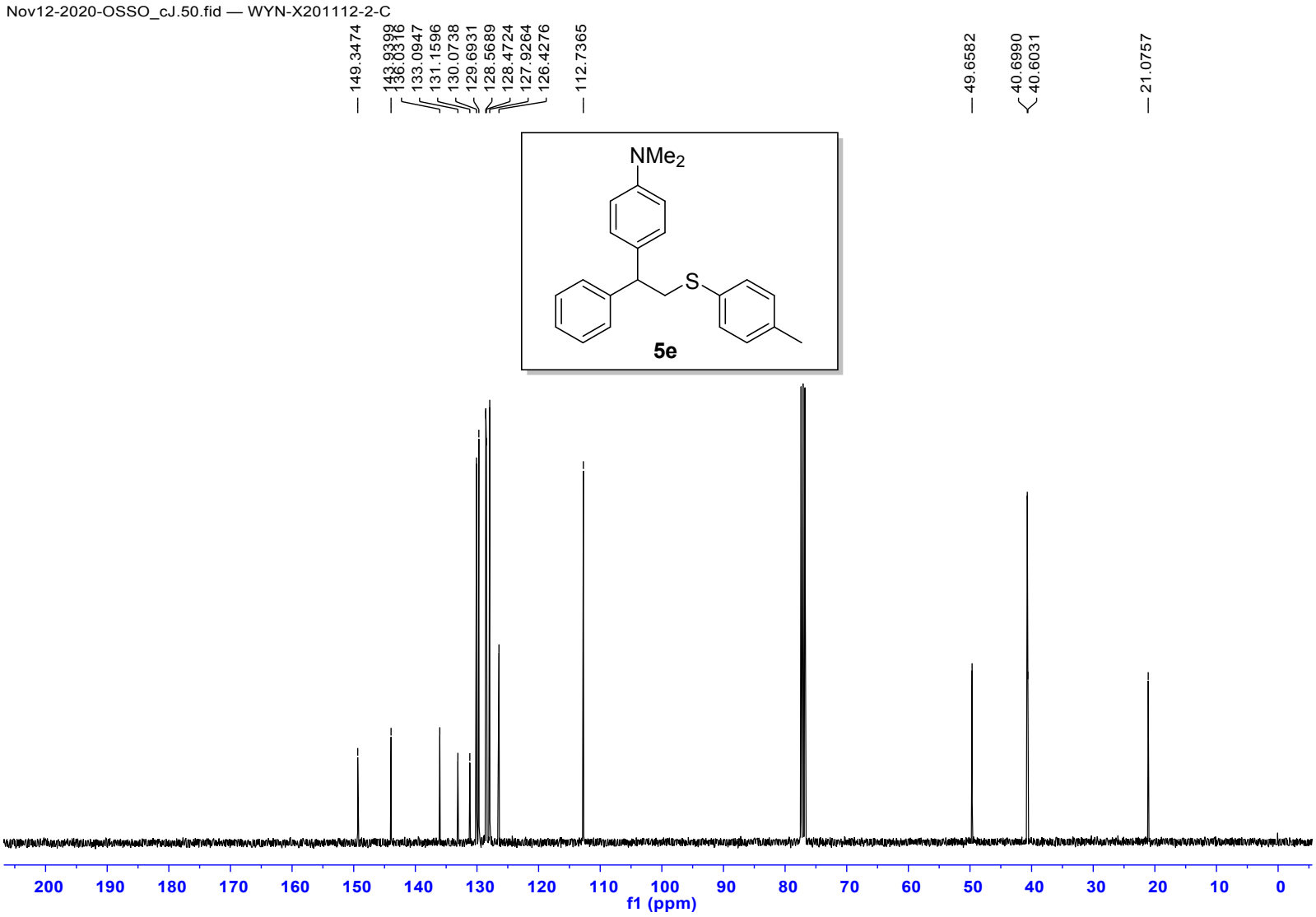

**5c**

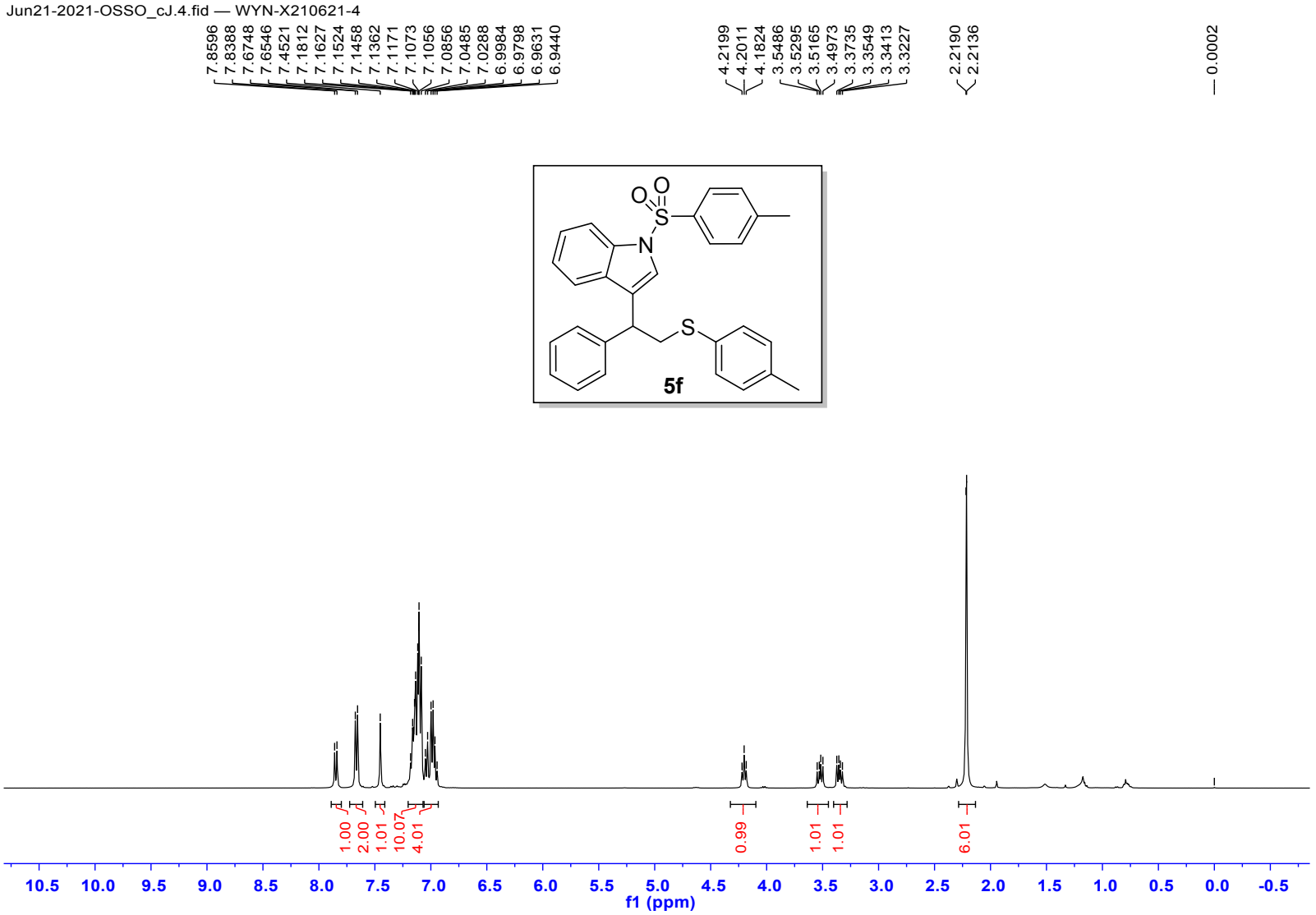


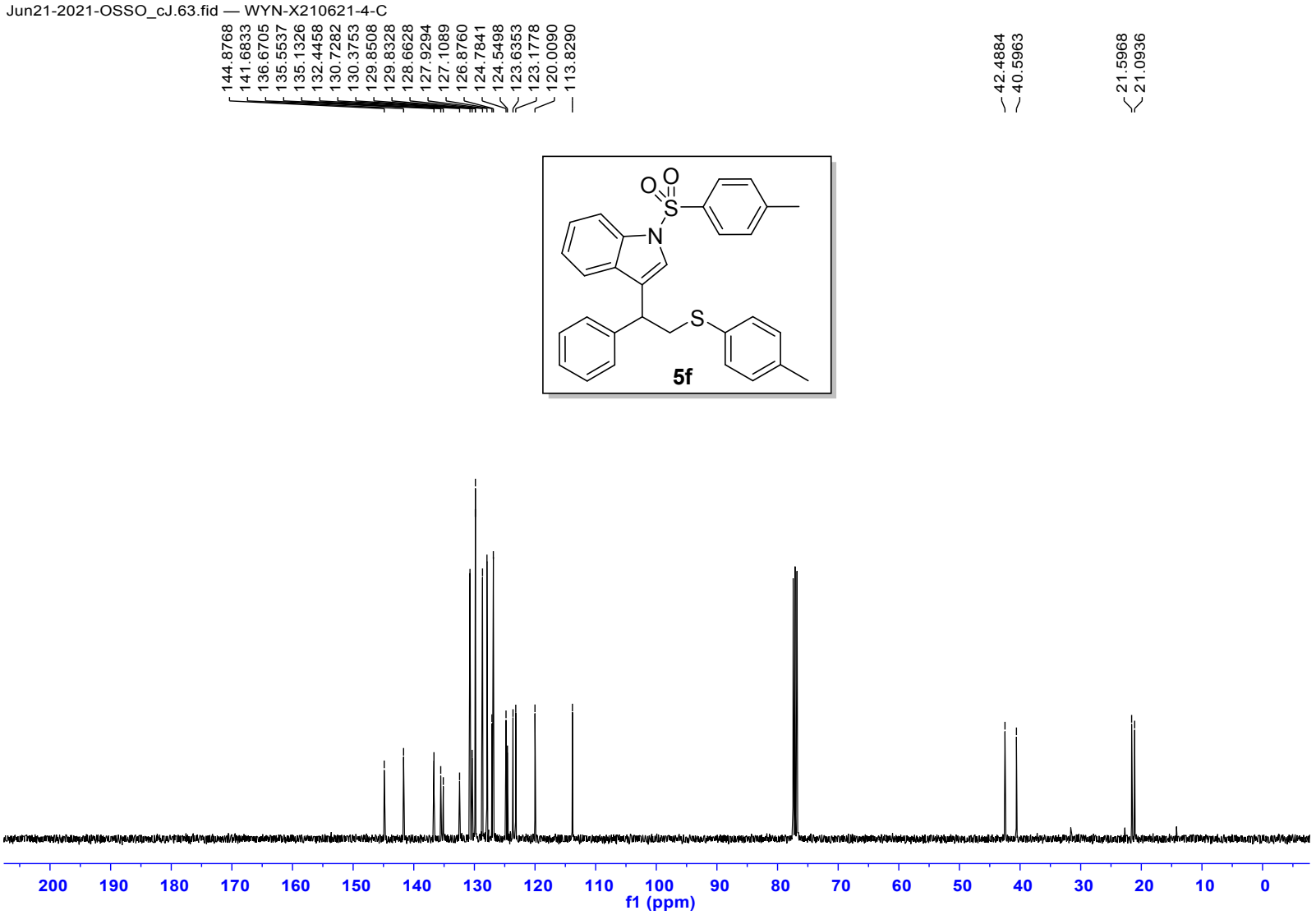

Nov27-2020-OSSO_cJ.7.fid — WYN-X201127-1
7.8394
7.8181
7.7197
7.7013
7.6806
7.3217
7.3022
7.2725
7.2575
7.2386
7.2211
7.2012
7.1825
7.1627
7.1510
7.1334
7.1064
7.0885
6.9797
6.9603
5.2528
3.9842
3.9696
3.9517
3.9116
3.8916
3.8789
3.6479
2.2360
-0.0002
MeO
S
5d
2.97
10.11
2.04
0.97
2.02
3.04
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

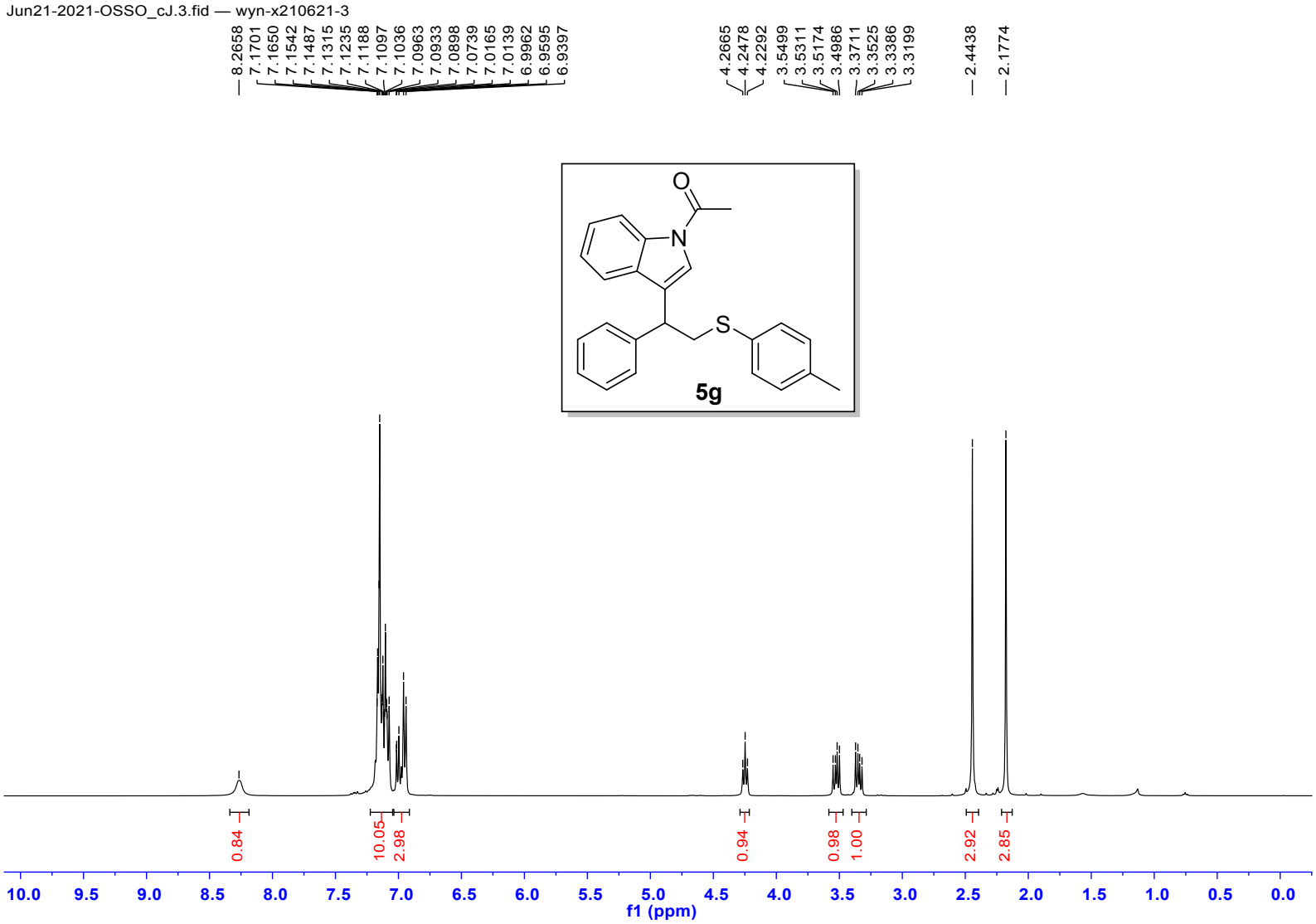

Nov30-2020-OSSO_cJ.11.fid — WYN-X201130-3
155.6924
143.4406
136.0766
133.3250
130.4197
129.8401
129.7599
129.3553
128.9706
128.2362
128.0138
126.6213
126.0745
124.5544
123.7121
123.4426
114.5049
56.4899
41.8532
38.1263
21.2291
MeO
S
5d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

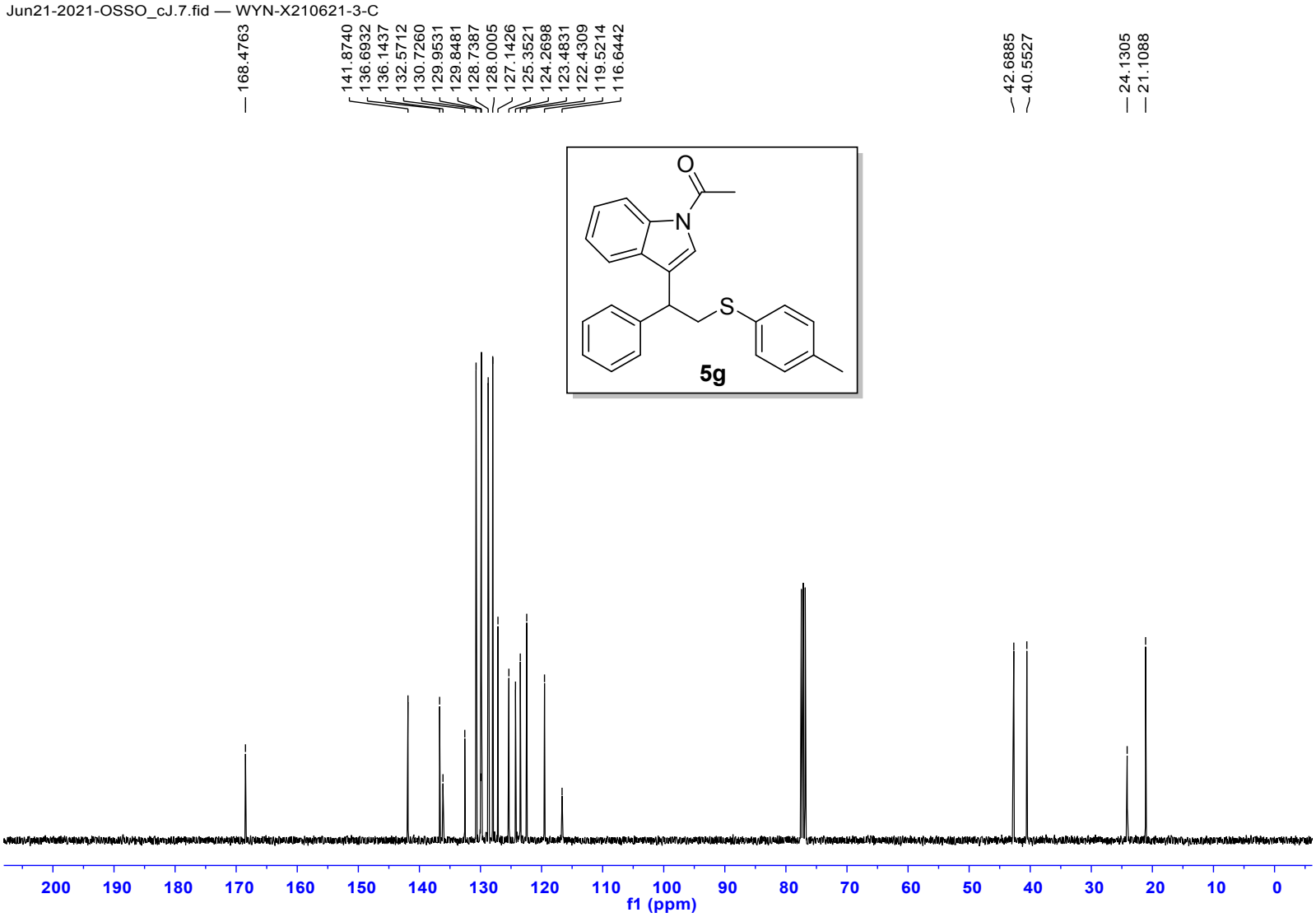

Nov12-2020-OSSO_cJ.5.fid — WYN-X201112-2
7.2739
7.2715
7.2692
7.2536
7.2334
7.2286
7.2177
7.2131
7.2079
7.1953
7.1915
7.1875
7.1789
7.1740
7.1679
7.1603
7.1562
7.1050
7.0996
7.0838
7.0644
6.6798
6.6744
6.6632
6.6580
4.1194
4.0997
4.0800
3.5329
3.5138
2.8953
2.3069
0.0001
NMe2
S
5e
1.87
4.01
1.08
3.92
1.92
0.99
1.93
5.69
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

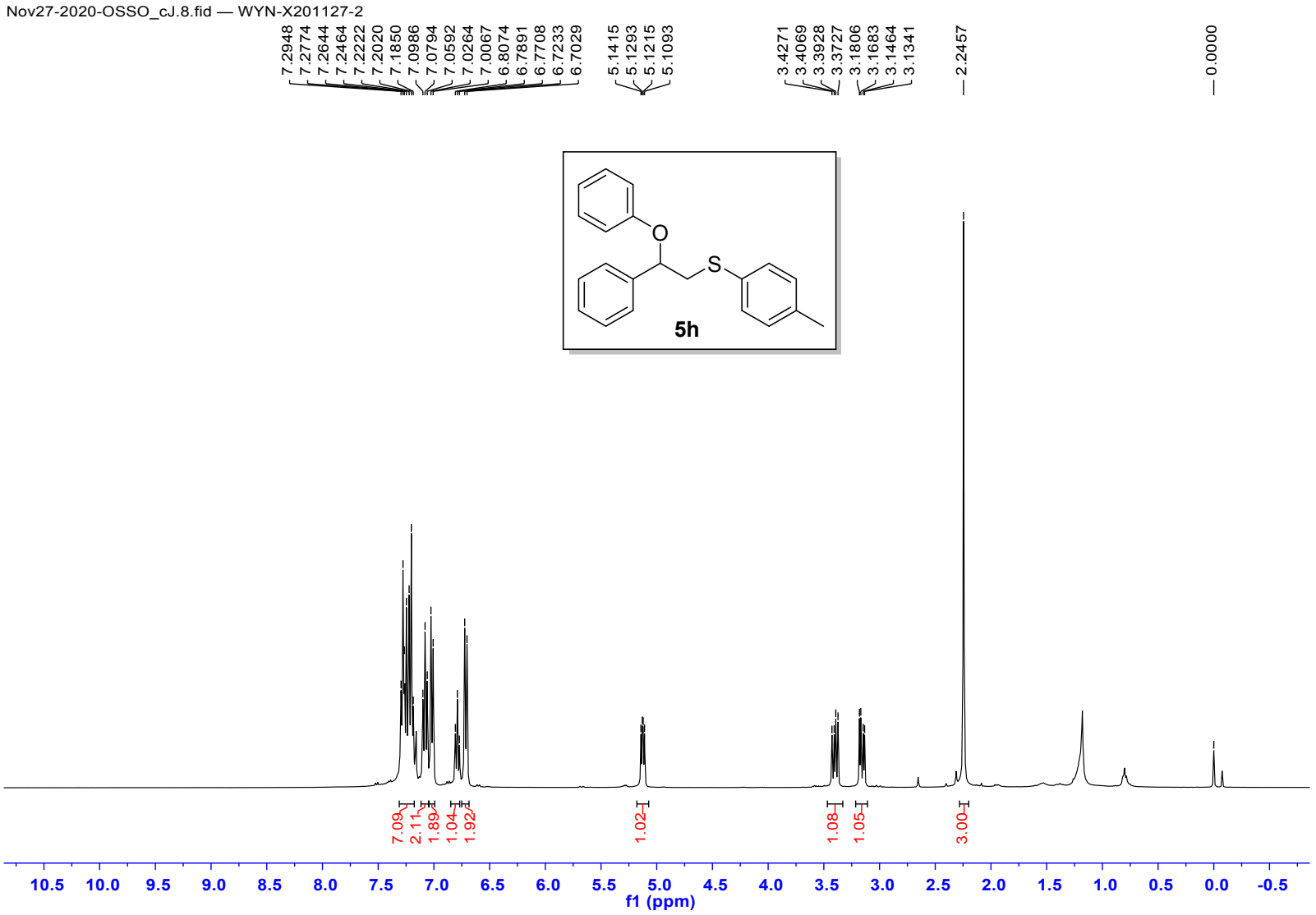

Nov12-2020-OSSO_cJ.50.fid — WYN-X201112-2-C
149.3474
143.9399
136.0316
133.0947
131.1596
130.0738
129.6931
128.5689
128.4724
127.9264
126.4276
112.7365
49.6582
40.6990
40.6031
21.0757
NMe2
S
5e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

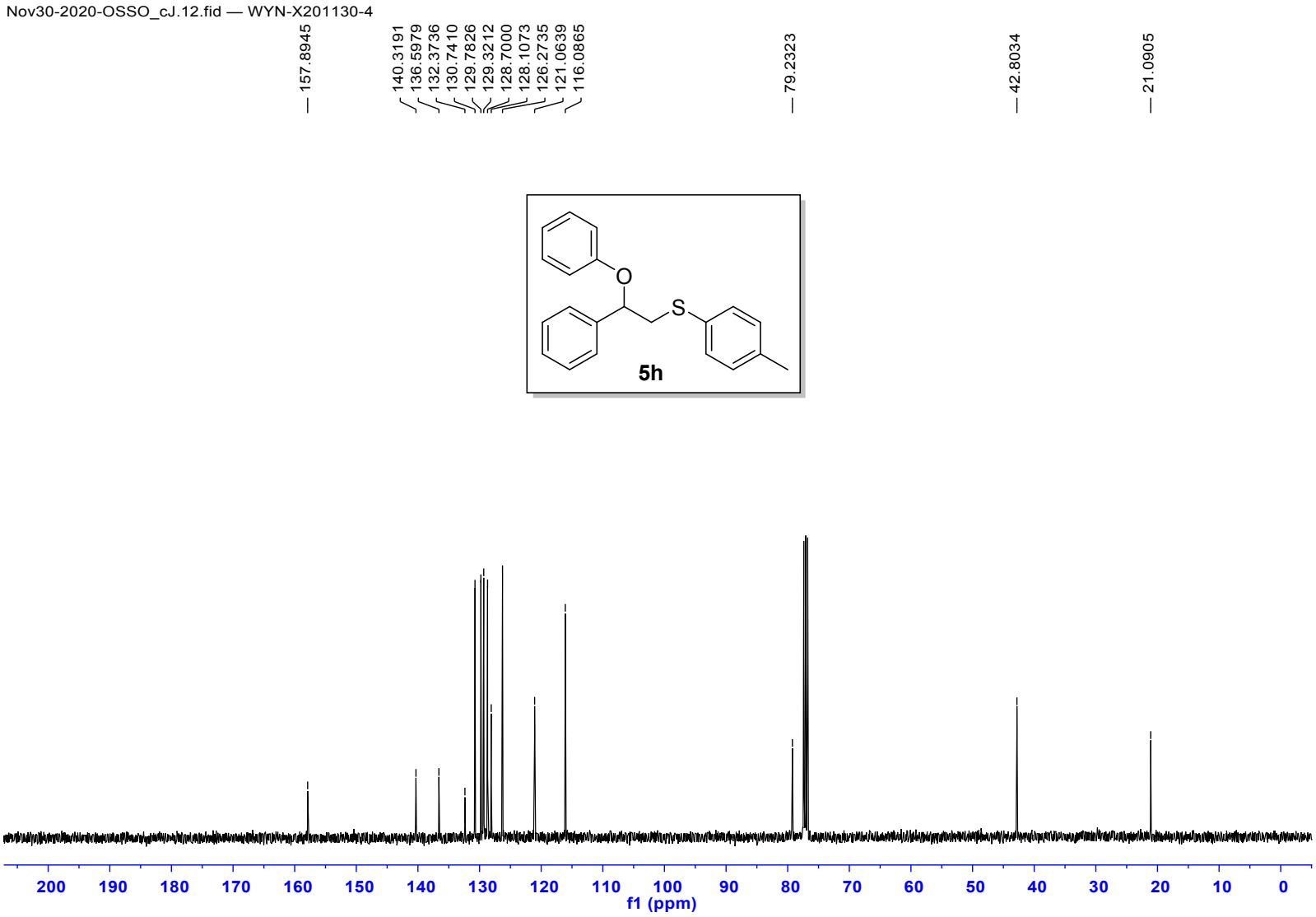

Jun21-2021-OSSO_cJ.4.fid — WYN-X210621-4
7.8596
7.8388
7.6748
7.6546
7.4521
7.1812
7.1627
7.1524
7.1458
7.1362
7.1171
7.1073
7.1056
7.0856
7.0485
7.0288
6.9984
6.9798
6.9631
6.9440
4.2199
4.2011
4.1824
3.5486
3.5295
3.5165
3.4973
3.3735
3.3549
3.3413
3.3227
2.2190
2.2136
0.0002
O
O
S
N
S
5f
1.00
2.00
1.01
10.07
4.01
0.99
1.01
1.01
6.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

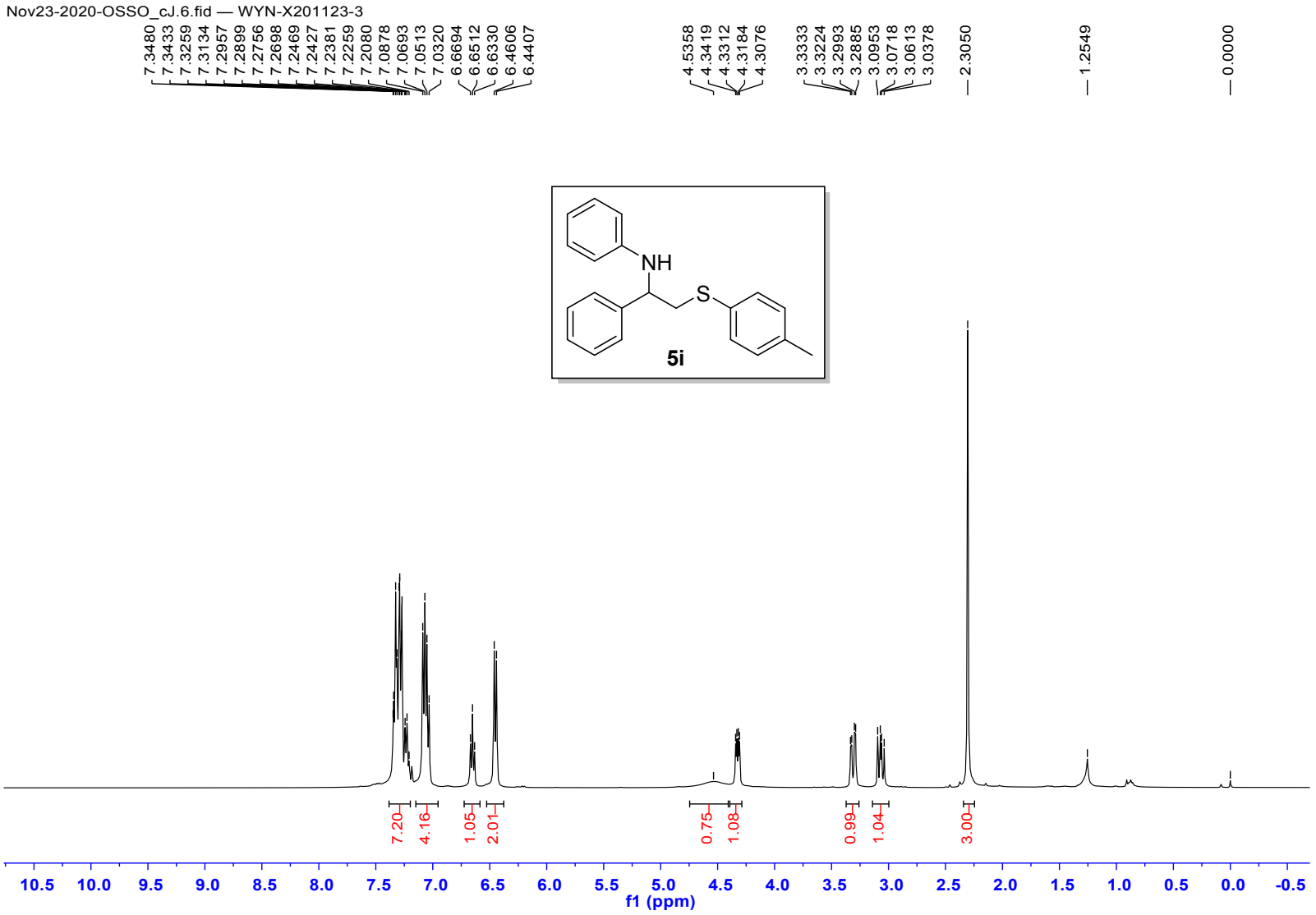

Jun21-2021-OSSO_cJ.63.fid — WYN-X210621-4-C
144.8768
141.6833
136.6705
135.5537
135.1326
132.4458
130.7282
130.3753
129.8508
129.8328
128.6628
127.9294
127.1089
126.8760
124.7841
124.5498
123.6353
123.1778
120.0090
113.8290
42.4884
40.5963
21.5968
21.0936
O
O
S
N
S
5f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

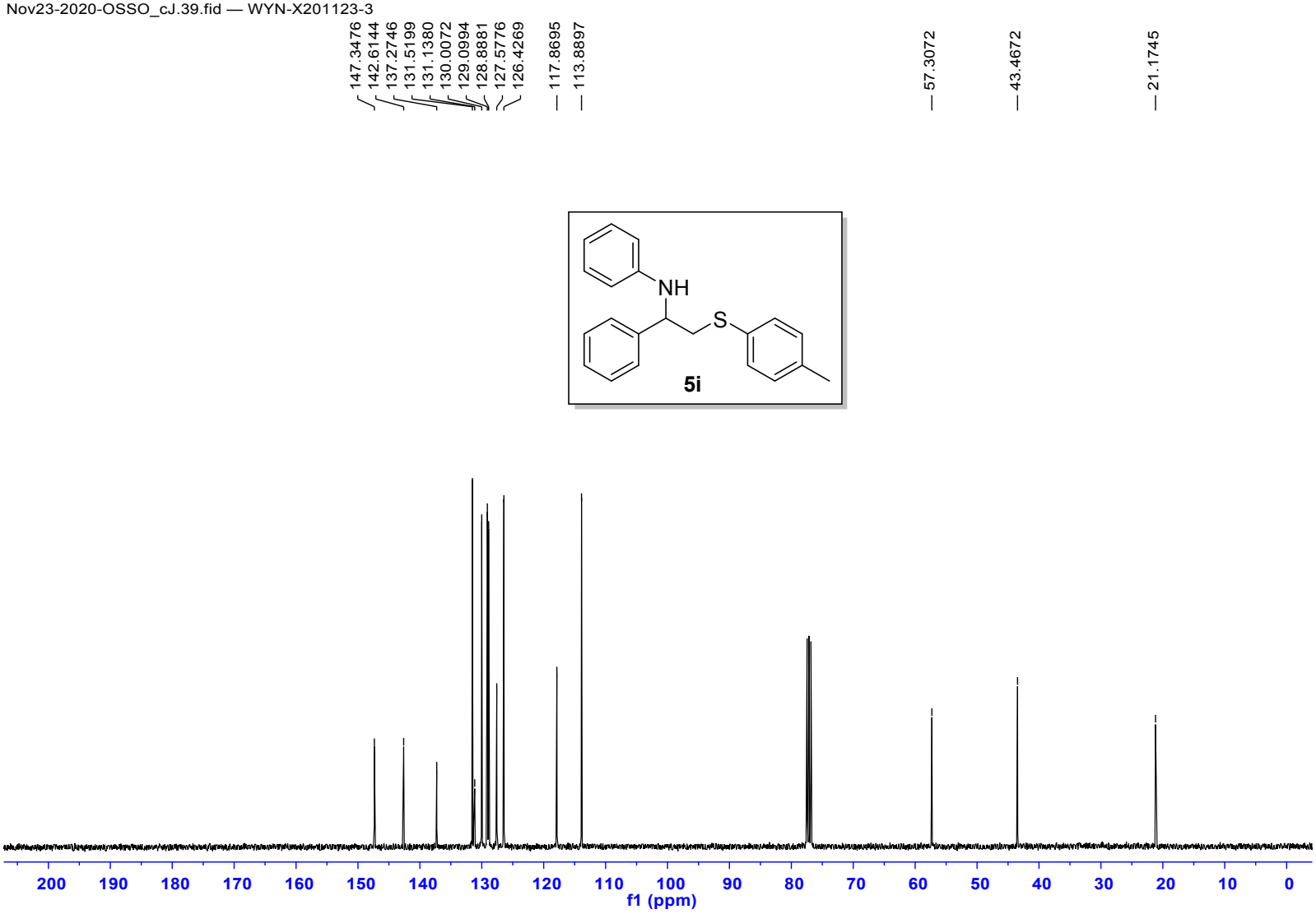

Jun21-2021-OSSO_cJ.3.fid — wyn-x210621-3
8.2658
7.1701
7.1650
7.1542
7.1487
7.1315
7.1235
7.1188
7.1097
7.1036
7.0963
7.0933
7.0898
7.0739
7.0165
7.0139
6.9962
6.9595
6.9397
4.2665
4.2478
4.2292
3.5499
3.5311
3.5174
3.4986
3.3711
3.3525
3.3386
3.3199
2.4438
2.1774
O
N
S
5g
0.84
10.05
2.98
0.94
0.98
1.00
2.92
2.85
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

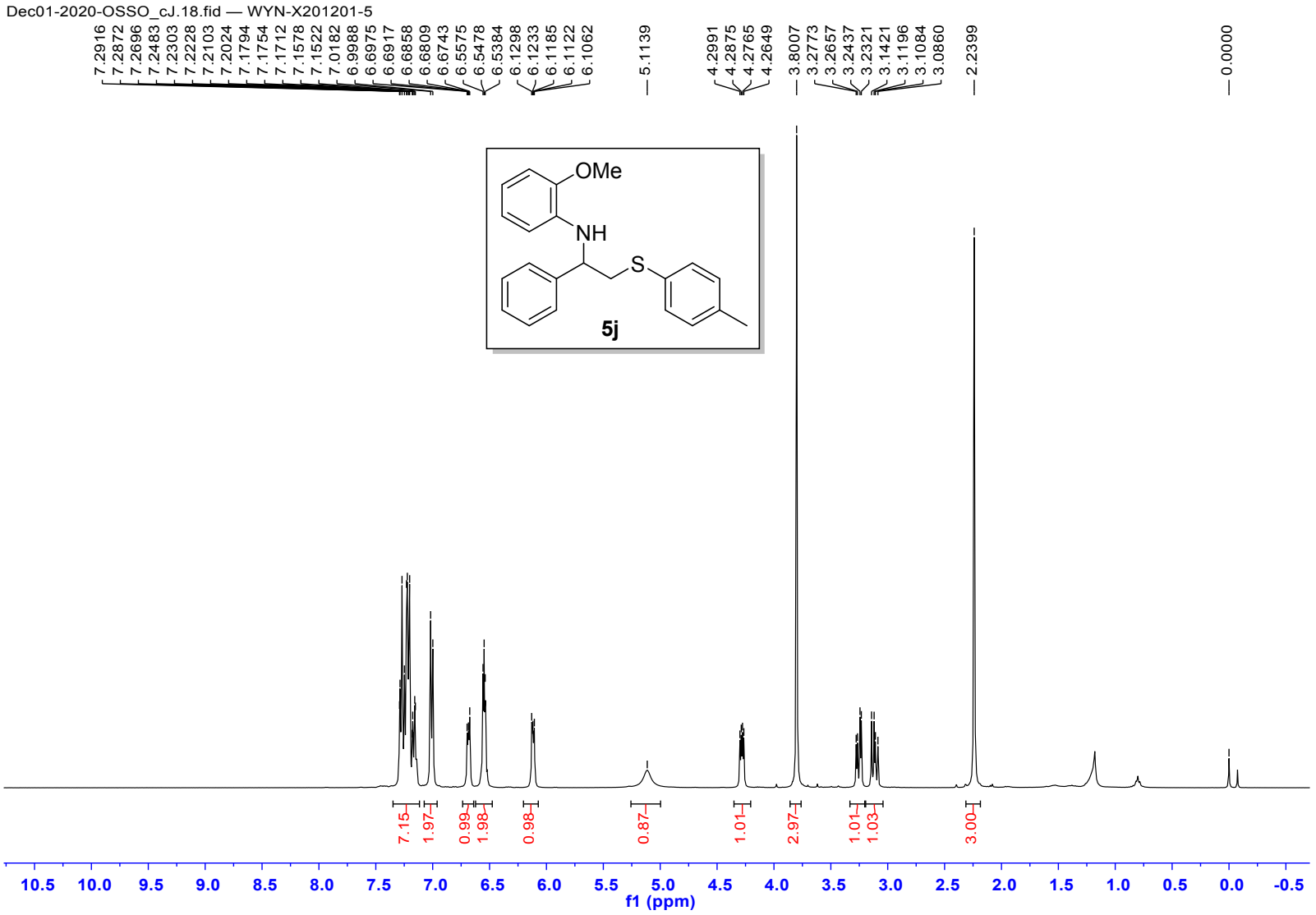

Jun21-2021-OSSO_cJ.7.fid — WYN-X210621-3-C
168.4763
141.8740
136.6932
136.1437
132.5712
130.7260
129.9531
129.8481
128.7387
128.0005
127.1426
125.3521
124.2698
123.4831
122.4309
119.5214
116.6442
42.6885
40.5527
24.1305
21.1088
O
N
S
5g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov27-2020-OSSO_cJ.8.fid — WYN-X201127-2
7.2948
7.2774
7.2644
7.2464
7.2222
7.2020
7.1850
7.0986
7.0794
7.0592
7.0264
7.0067
6.8074
6.7891
6.7708
6.7233
6.7029
5.1415
5.1293
5.1215
5.1093
3.4271
3.4069
3.3928
3.3727
3.1806
3.1683
3.1464
3.1341
2.2457
0.0000
O
S
5h
7.09
2.11
1.89
1.04
1.92
1.02
1.08
1.05
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Nov30-2020-OSSO_cJ.12.fid — WYN-X201130-4
157.8945
140.3191
136.5979
132.3736
130.7410
129.7826
129.3212
128.7000
128.1073
126.2735
121.0639
116.0865
79.2323
42.8034
21.0905
O
S
5h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

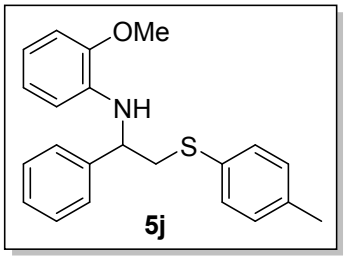

Nov23-2020-OSSO_cJ.6.fid — WYN-X201123-3
7.3480
7.3433
7.3259
7.3134
7.2957
7.2899
7.2756
7.2698
7.2469
7.2427
7.2381
7.2259
7.2080
7.0878
7.0693
7.0513
7.0320
6.6694
6.6512
6.6330
6.4606
6.4407
4.5358
4.3419
4.3312
4.3184
4.3076
3.3333
3.3224
3.2993
3.2885
3.0953
3.0718
3.0613
3.0378
2.3050
1.2549
0.0000
NH
S
5i
7.20
4.16
1.05
2.01
0.75
1.08
0.99
1.04
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Nov23-2020-OSSO_cJ.39.fid — WYN-X201123-3
147.3476
142.6144
137.2746
131.5199
131.1380
130.0072
129.0994
128.8881
127.5776
126.4269
117.8695
113.8897
57.3072
43.4672
21.1745
NH
S
5i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

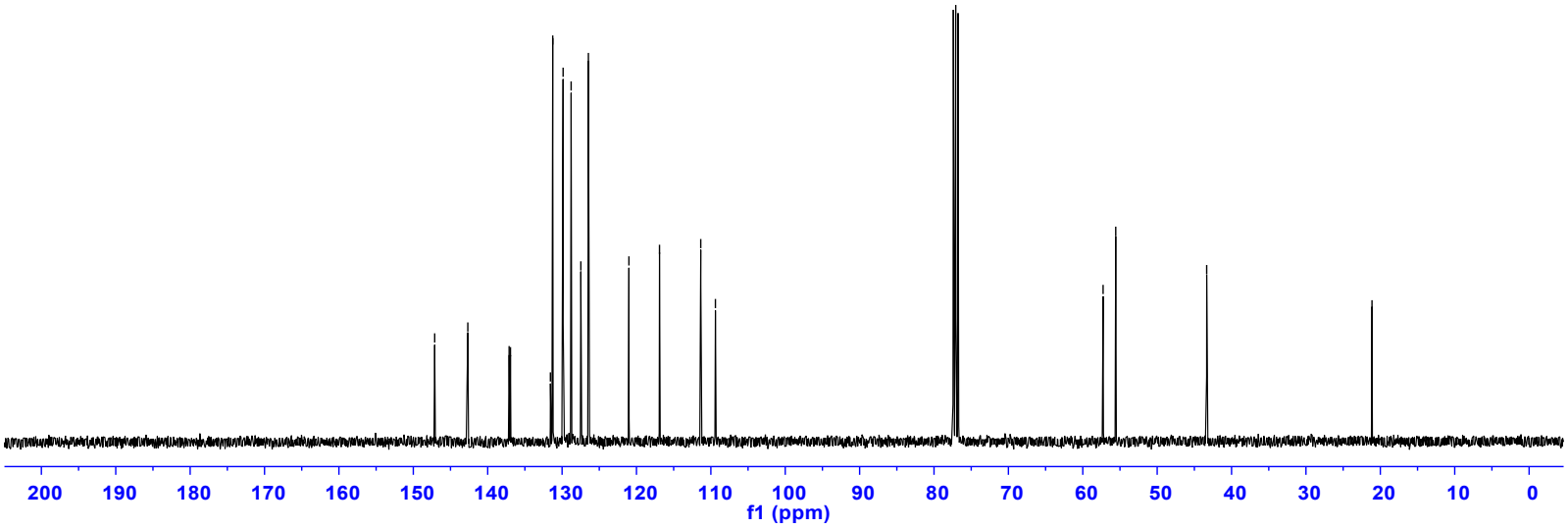

Dec01-2020-OSSO_cJ.18.fid — WYN-X201201-5
7.2916
7.2872
7.2696
7.2483
7.2303
7.2228
7.2103
7.2024
7.1794
7.1754
7.1712
7.1578
7.1522
7.0182
6.9988
6.6975
6.6917
6.6858
6.6809
6.6743
6.5575
6.5478
6.5384
6.1298
6.1233
6.1185
6.1122
6.1062
5.1139
4.2991
4.2875
4.2765
4.2649
3.8007
3.2773
3.2657
3.2437
3.2321
3.1421
3.1196
3.1084
3.0860
2.2399
0.0000
OMe
NH
S
5j
7.15
1.97
0.99
1.98
0.98
0.87
1.01
2.97
1.01
1.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

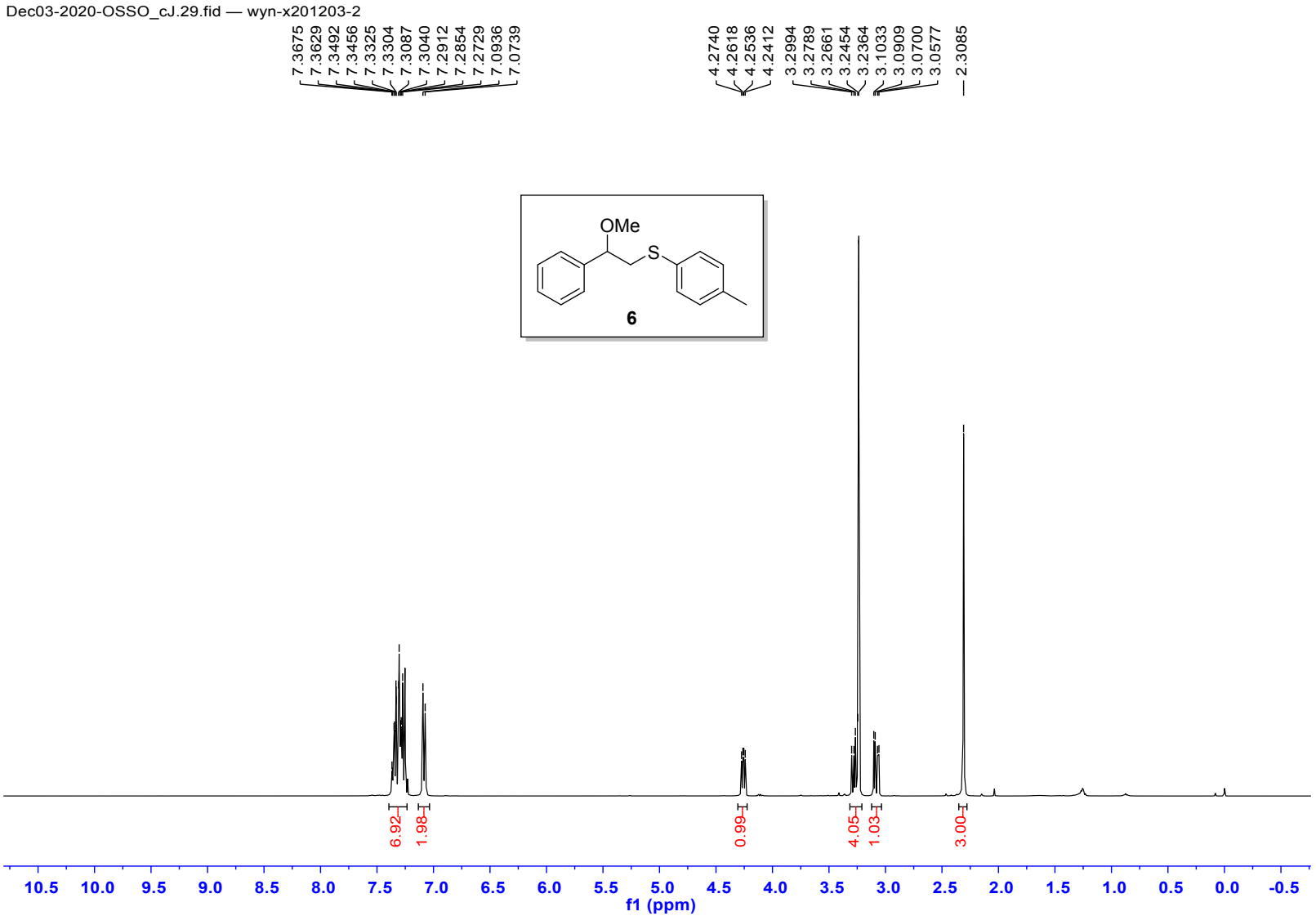
Dec04-2020-OSSO_cJ.14.fid — WYN-X201201-5-C

147.1260
142.6709
137.1183
136.9390
131.5689
131.2574
129.8620
128.7830
127.4774
126.4633
121.0149
116.9020
111.3584
109.3865
57.2700
55.5710
43.3442
21.1209



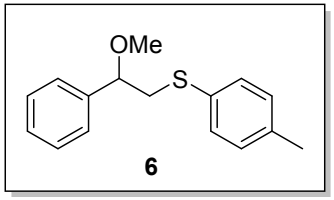

**5j**



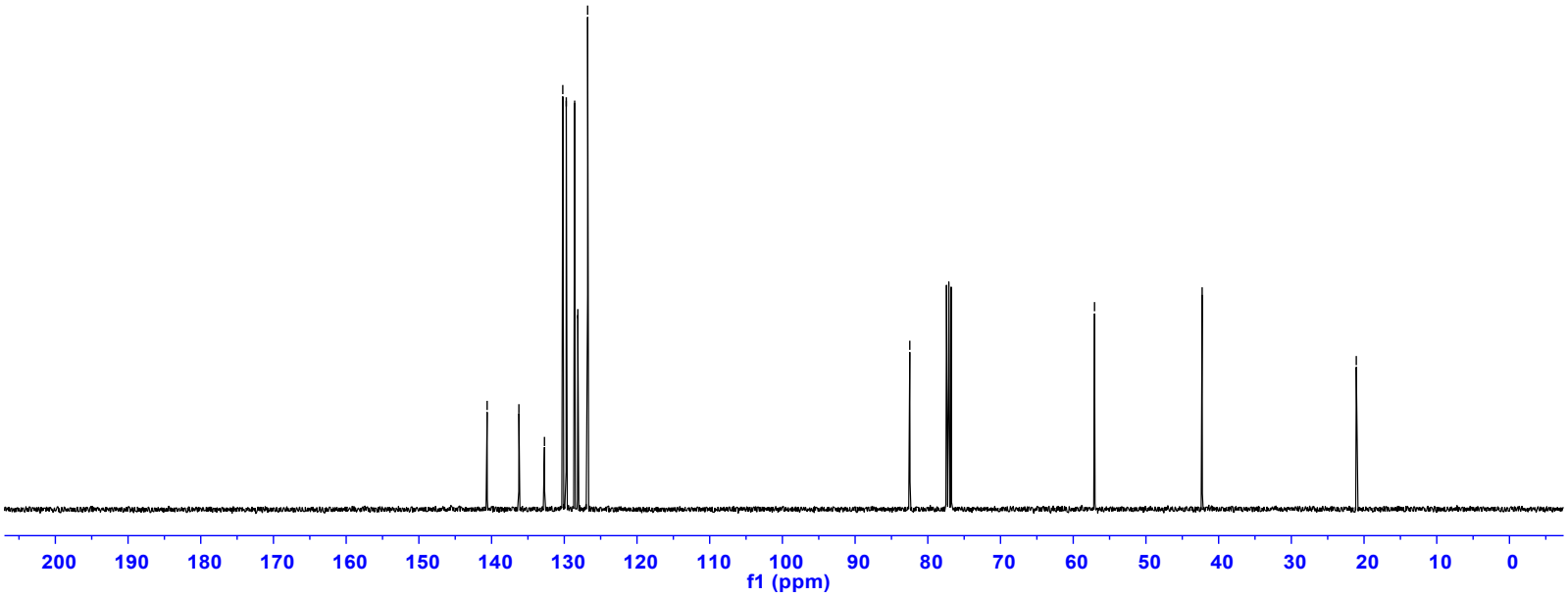

Dec03-2020-OSSO_cJ.29.fid — wyn-x201203-2
7.3675
7.3629
7.3492
7.3456
7.3325
7.3304
7.3087
7.3040
7.2912
7.2854
7.2729
7.0936
7.0739
4.2740
4.2618
4.2536
4.2412
3.2994
3.2789
3.2661
3.2454
3.2364
3.1033
3.0909
3.0700
3.0577
2.3085
OMe
S
6
6.92
1.98
0.99
4.05
1.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

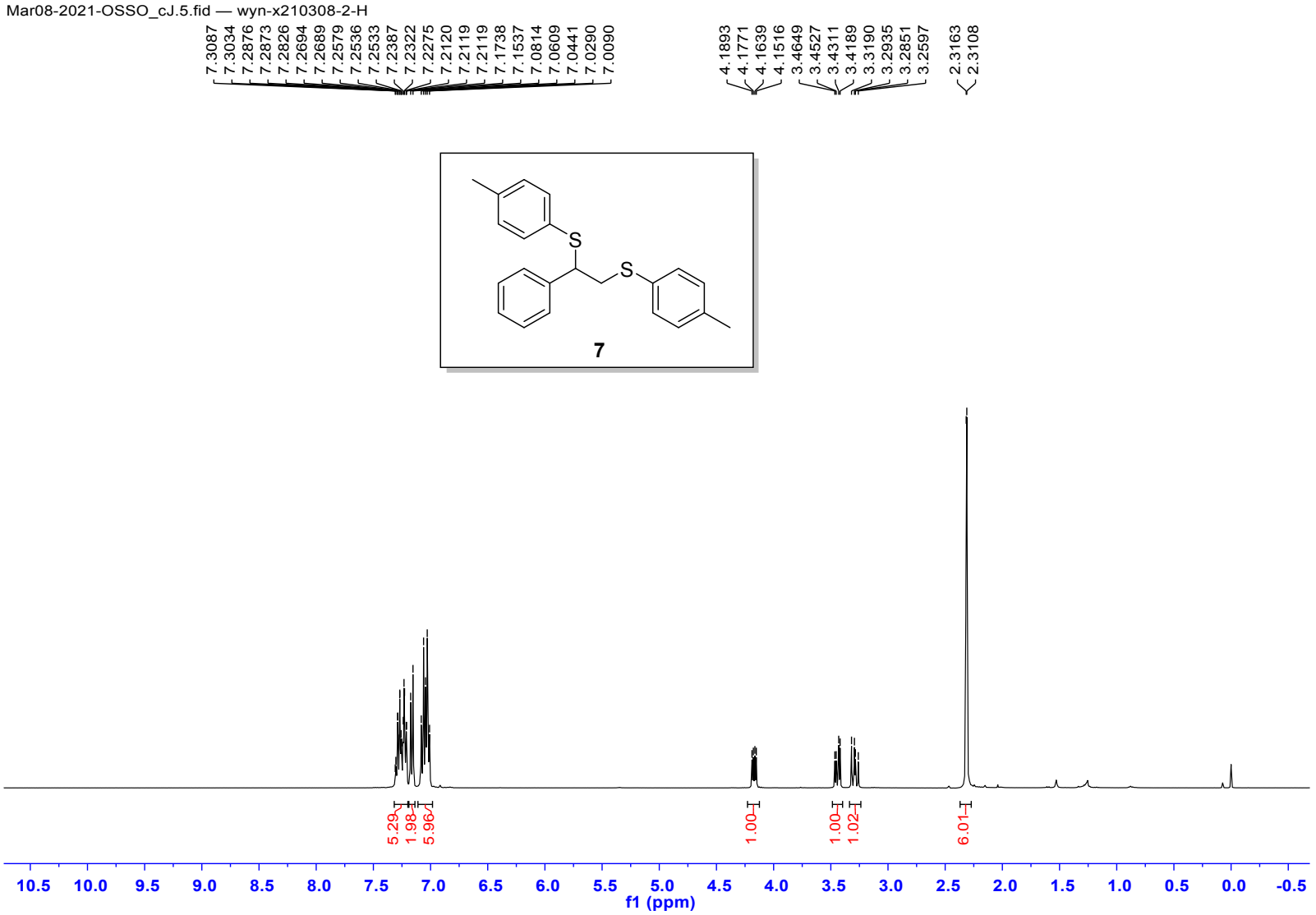
Dec04-2020-OSSO_cJ.72.fid — wyn-x201204-6

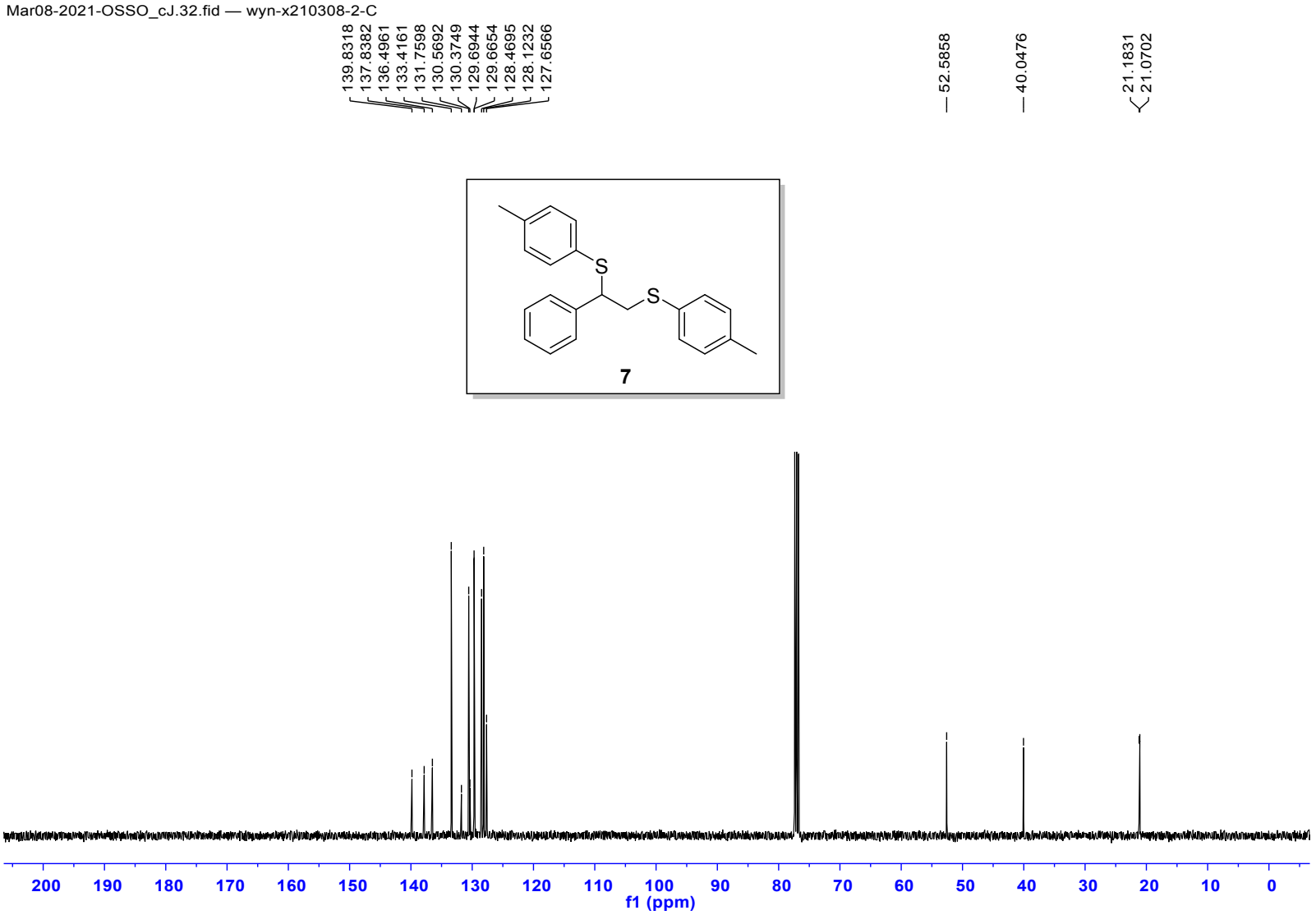
140.6119
136.2434
132.7262
130.2083
129.7274
128.5719
128.1389
126.7890
82.4807
57.0695
42.2683
21.0681

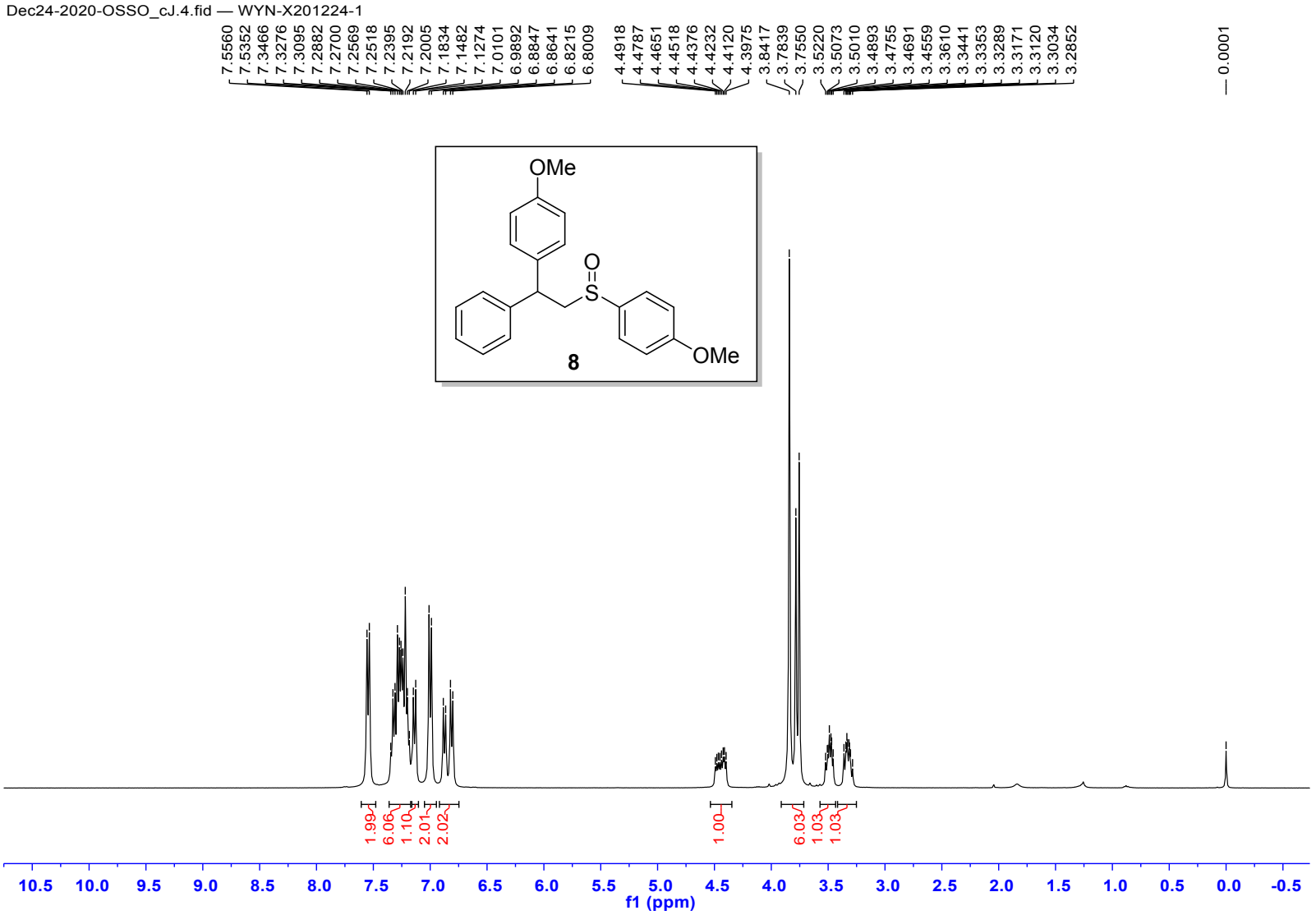


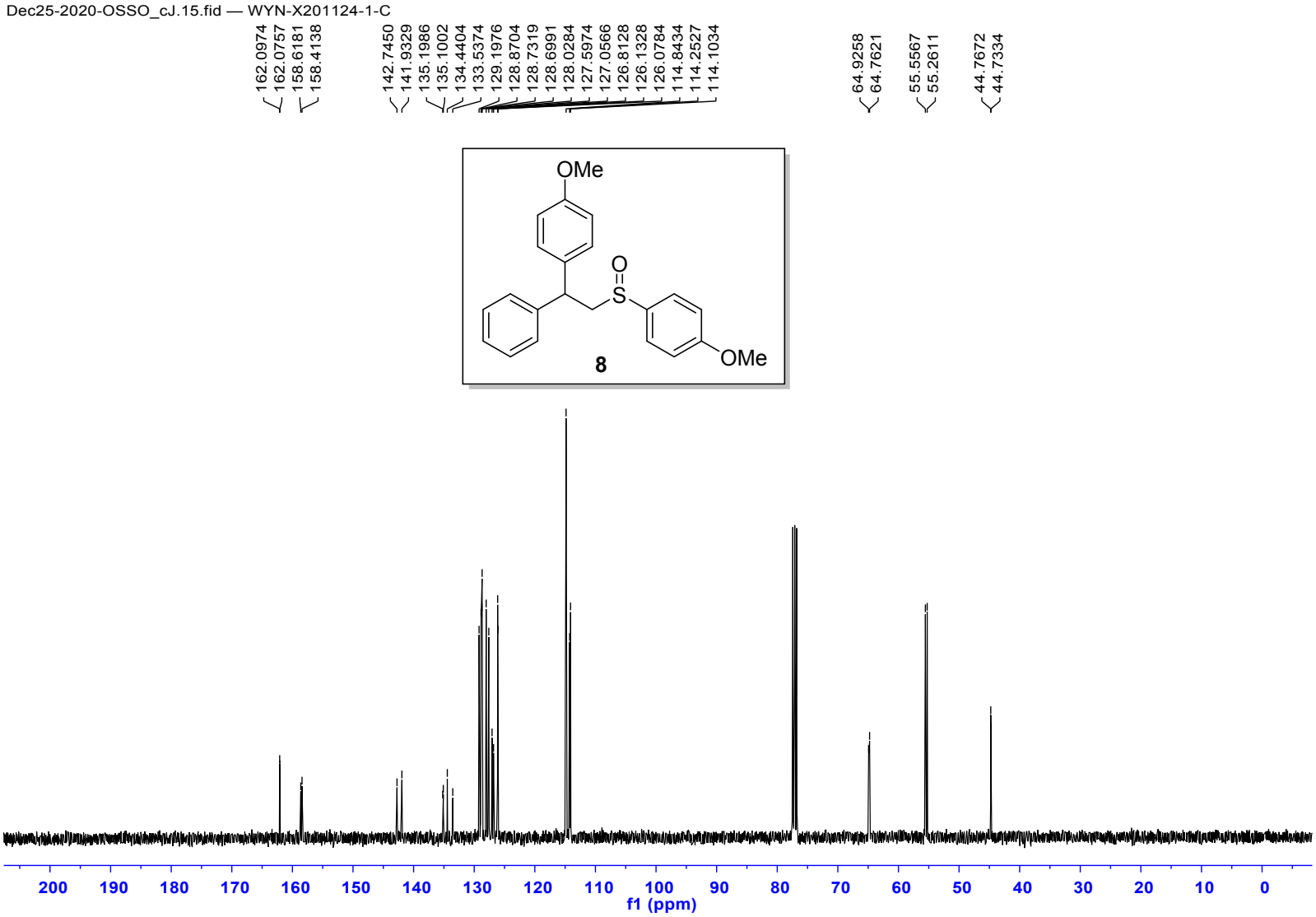

**6**

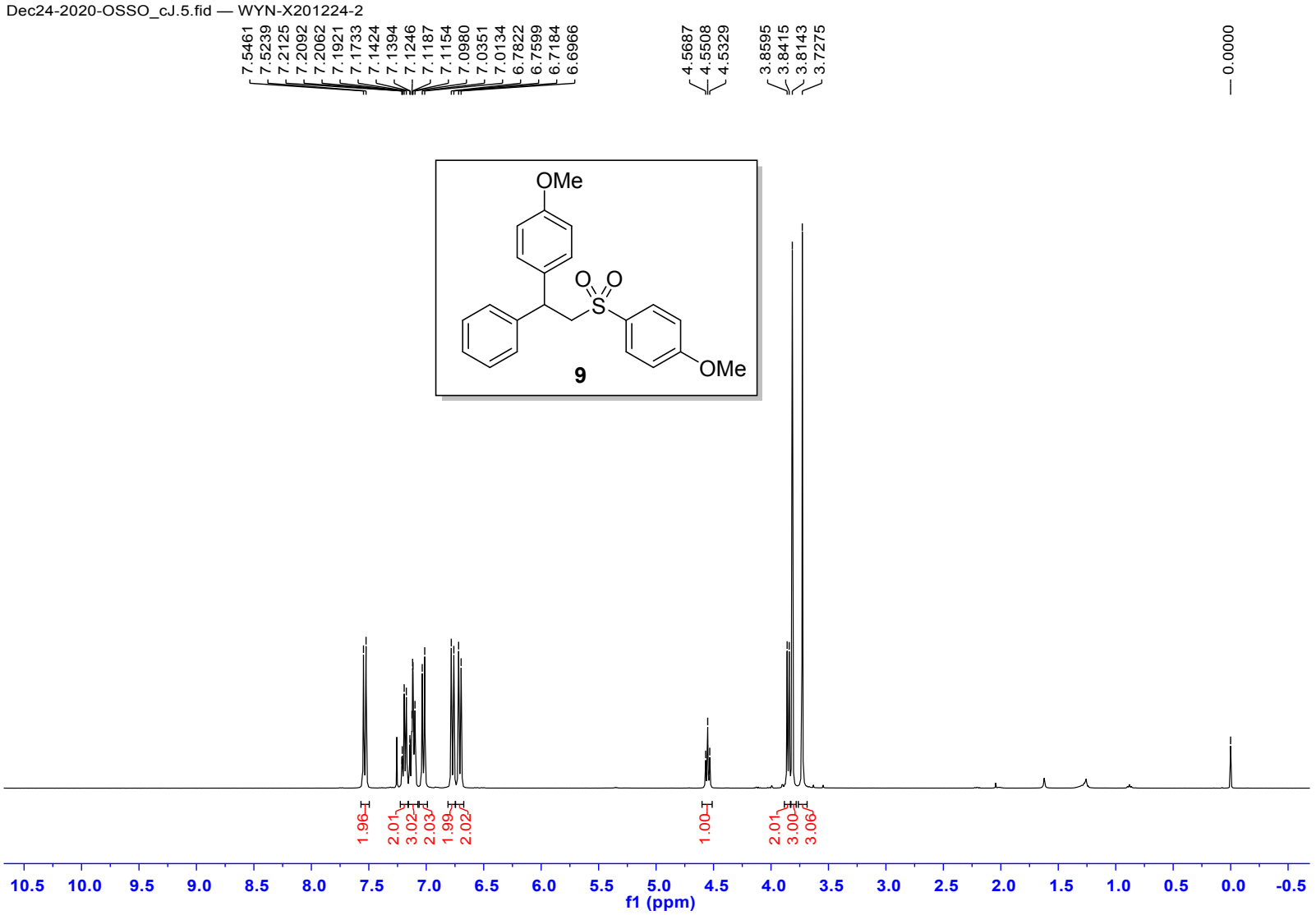


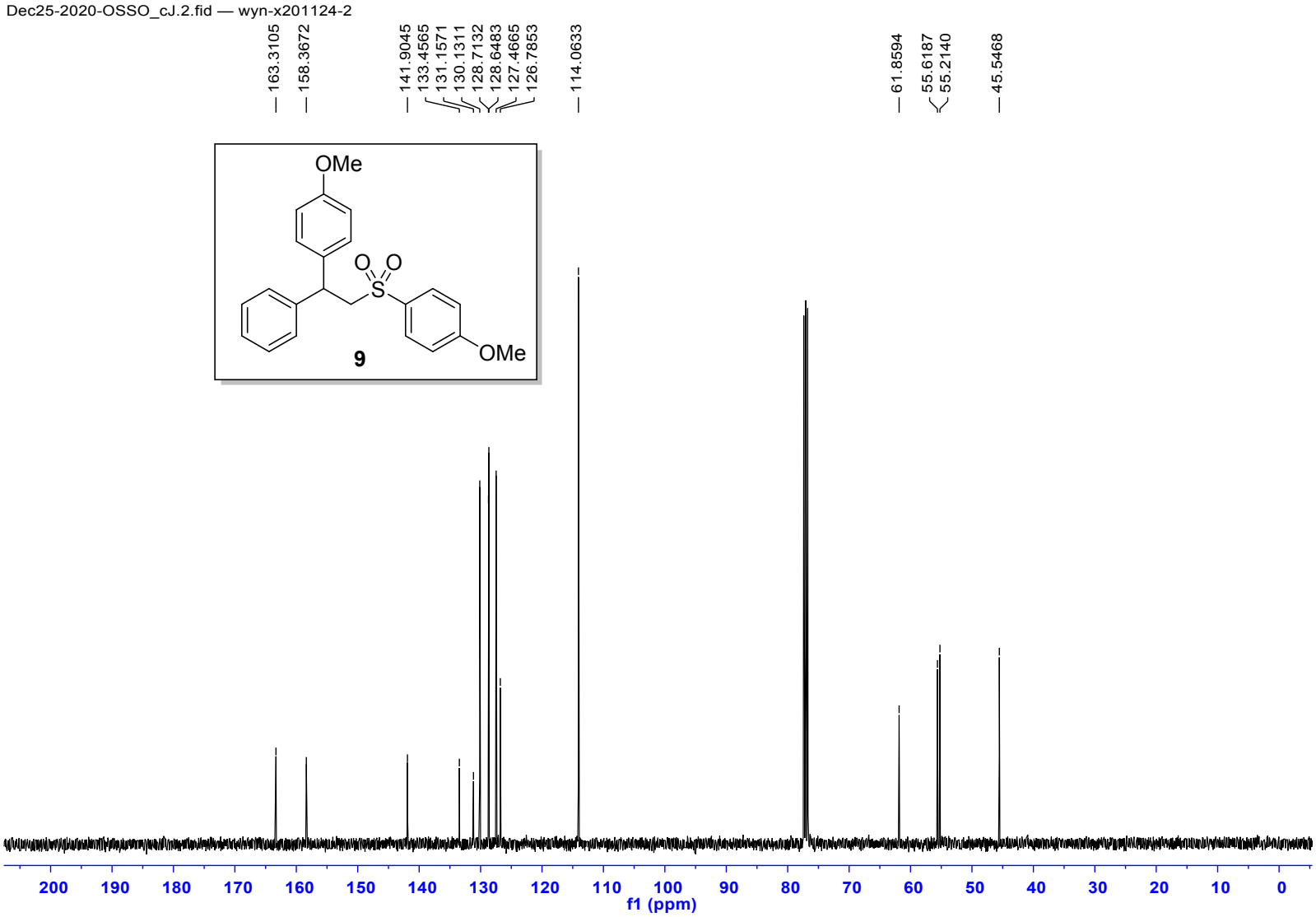

Mar08-2021-OSSO_cJ.5.fid — wyn-x210308-2-H
7.3087
7.3034
7.2876
7.2873
7.2826
7.2694
7.2689
7.2579
7.2536
7.2533
7.2387
7.2322
7.2275
7.2120
7.2119
7.2119
7.1738
7.1537
7.0814
7.0609
7.0441
7.0290
7.0090
4.1893
4.1771
4.1639
4.1516
3.4649
3.4527
3.4311
3.4189
3.3190
3.2935
3.2851
3.2597
2.3163
2.3108
S
S
7
5.29
1.98
5.96
1.00
1.00
1.02
6.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

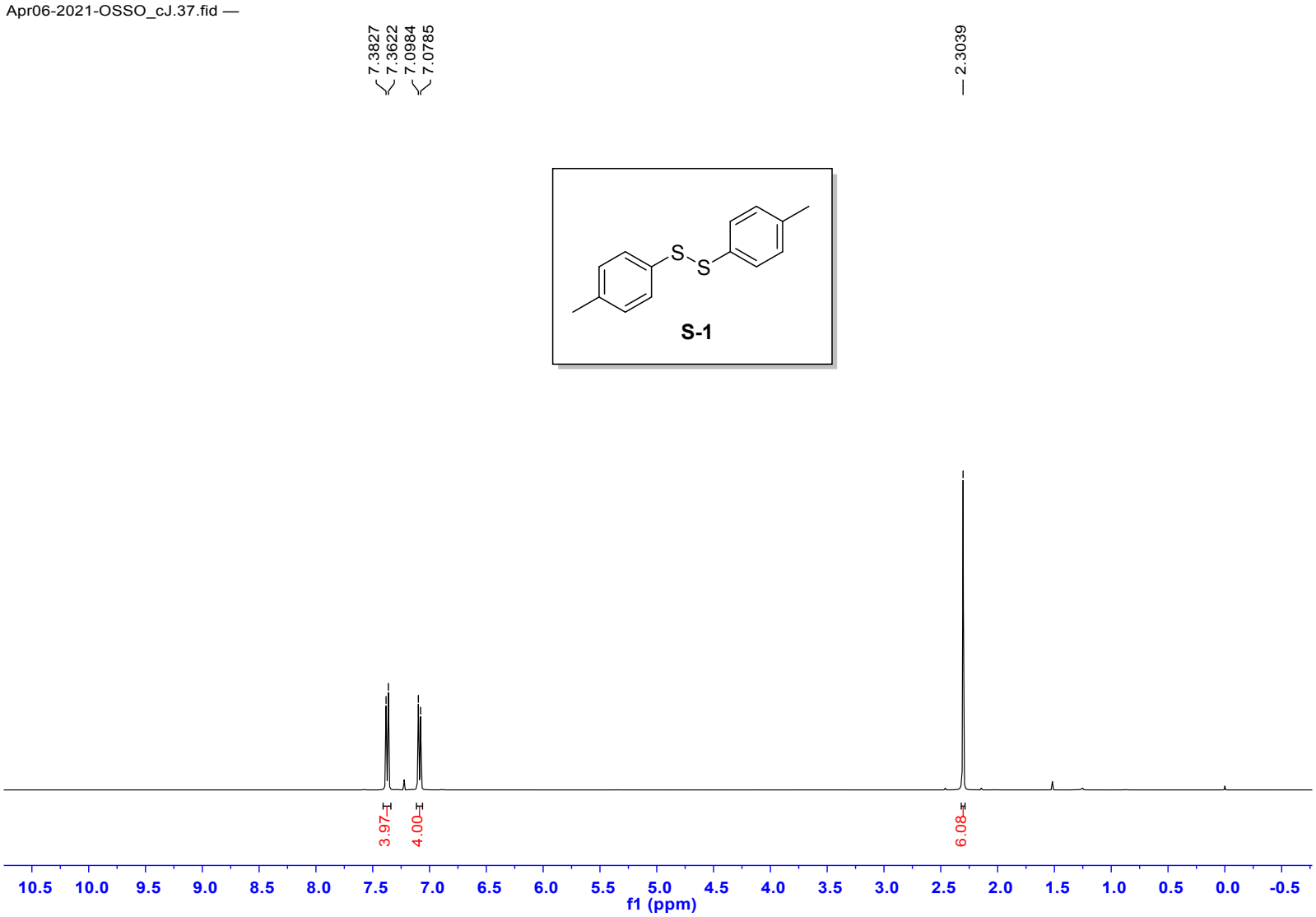

Mar08-2021-OSSO_cJ.32.fid — wyn-x210308-2-C
139.8318
137.8382
136.4961
133.4161
131.7598
130.5692
130.3749
129.6944
129.6654
128.4695
128.1232
127.6566
52.5858
40.0476
21.1831
21.0702
S
S
7
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

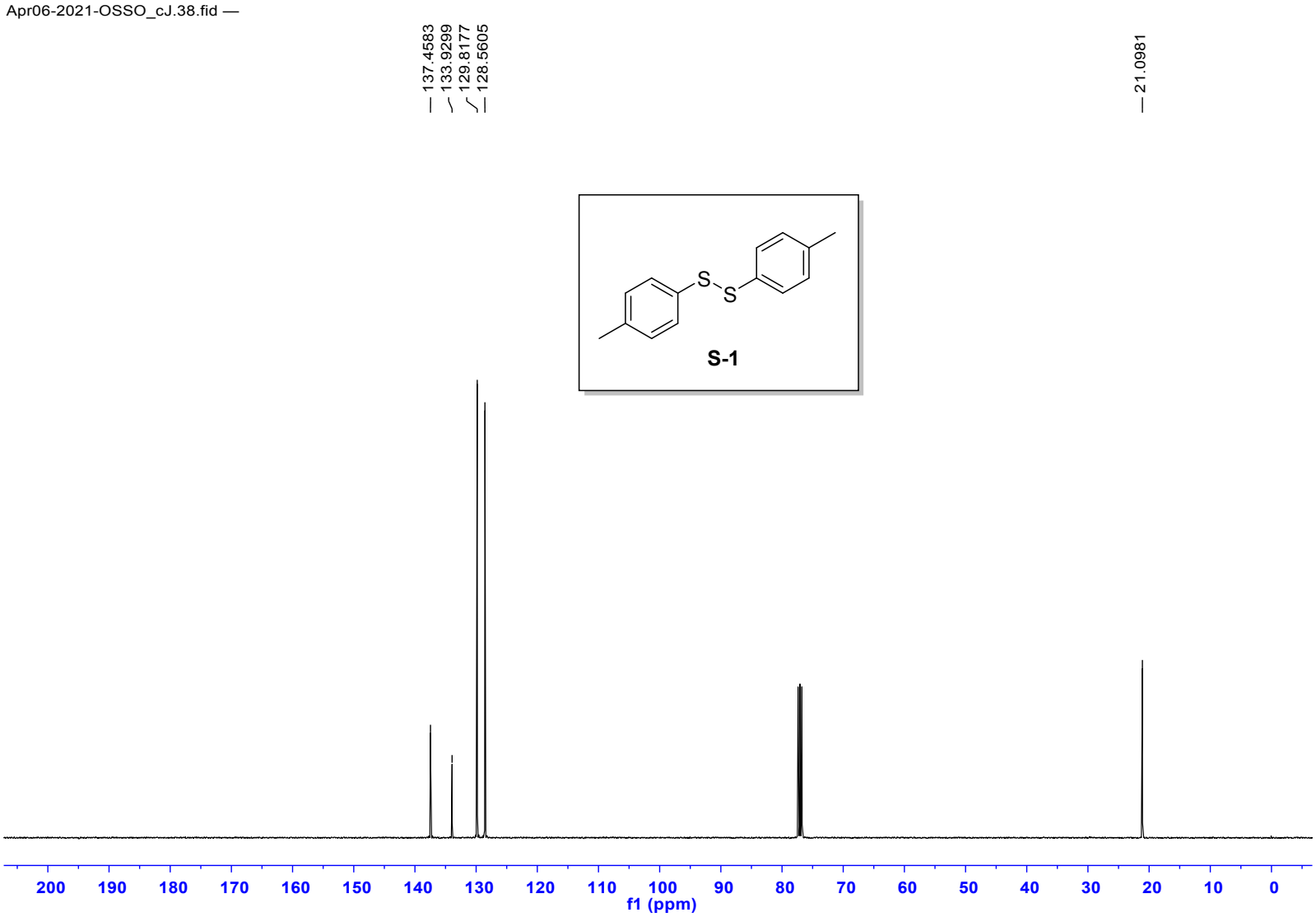

Dec24-2020-OSSO_cJ.4.fid — WYN-X201224-1
7.5560
7.5352
7.3466
7.3276
7.3095
7.2882
7.2700
7.2569
7.2518
7.2395
7.2192
7.2005
7.1834
7.1482
7.1274
7.0101
6.9892
6.8847
6.8641
6.8215
6.8009
4.4918
4.4787
4.4651
4.4518
4.4376
4.4232
4.4120
4.3975
3.8417
3.7839
3.7550
3.5220
3.5073
3.5010
3.4893
3.4755
3.4691
3.4559
3.3610
3.3441
3.3353
3.3289
3.3171
3.3120
3.3034
3.2852
0.0001
OMe
O
S
OMe
8
1.99
6.06
1.10
2.01
2.02
1.00
6.03
1.03
1.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

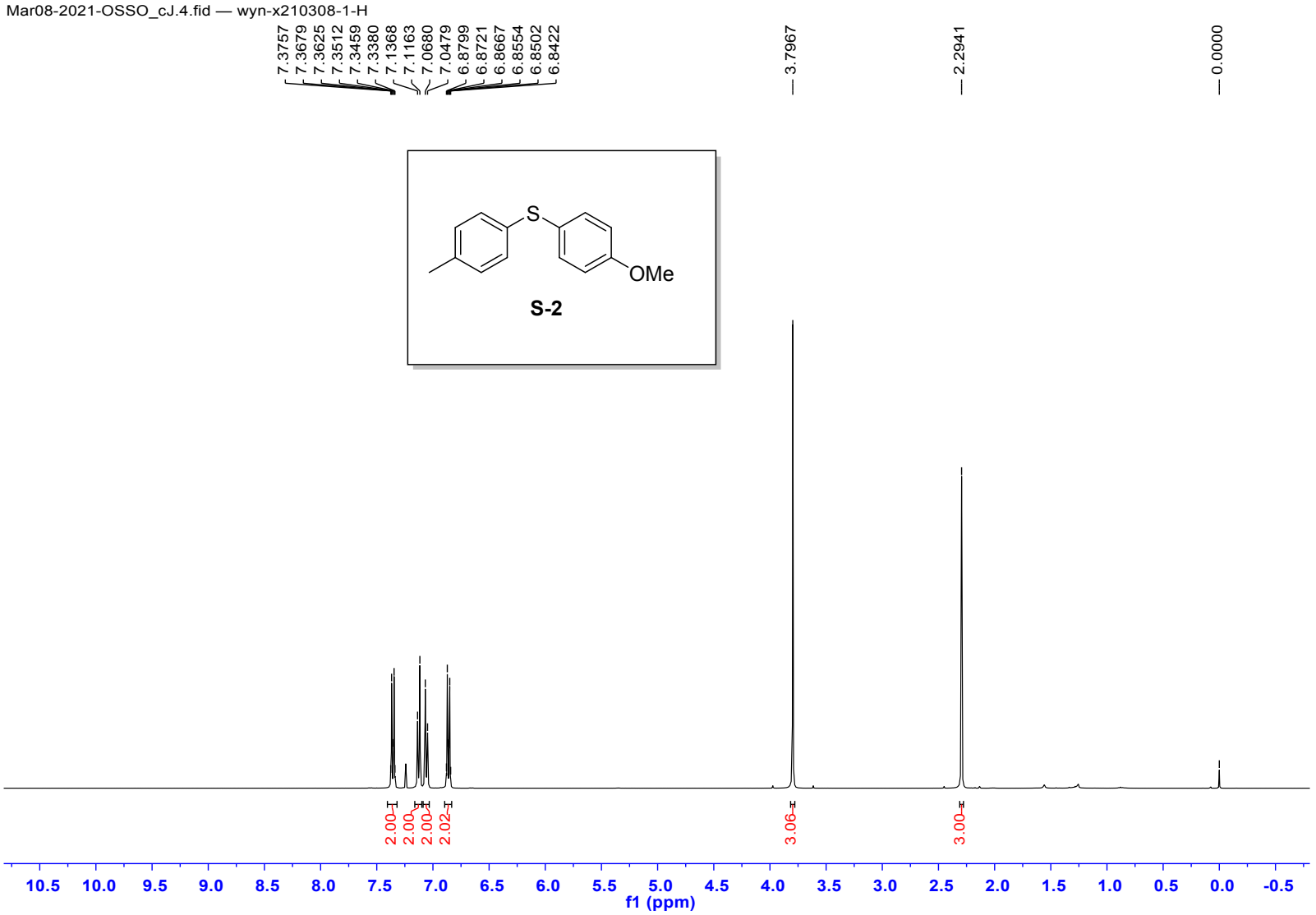

Dec25-2020-OSSO_cJ.15.fid — WYN-X201124-1-C
162.0974
162.0757
158.6181
158.4138
142.7450
141.9329
135.1986
135.1002
134.4404
133.5374
129.1976
128.8704
128.7319
128.6991
128.0284
127.5974
127.0566
126.8128
126.1328
126.0784
114.8434
114.2527
114.1034
64.9258
64.7621
55.5567
55.2611
44.7672
44.7334
OMe
O
S
OMe
8
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Dec24-2020-OSSO_cJ.5.fid — WYN-X201224-2
7.5461
7.5239
7.2125
7.2092
7.2062
7.1921
7.1733
7.1424
7.1394
7.1246
7.1187
7.1154
7.0980
7.0351
7.0134
6.7822
6.7599
6.7184
6.6966
4.5687
4.5508
4.5329
3.8595
3.8415
3.8143
3.7275
0.0000
OMe
O
O
S
OMe
9
1.96
2.01
3.02
2.03
1.99
2.02
1.00
2.01
3.00
3.06
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


Dec25-2020-OSSO_cJ.2.fid — wyn-x201124-2
163.3105
158.3672
141.9045
133.4565
131.1571
130.1311
128.7132
128.6483
127.4665
126.7853
114.0633
61.8594
55.6187
55.2140
45.5468
OMe
O
O
S
OMe
9
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

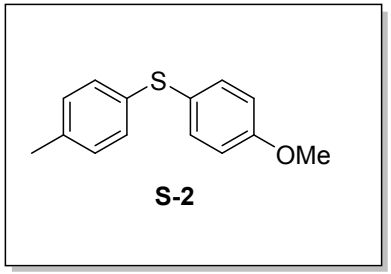

Apr06-2021-OSSO_cJ.37.fid
7.3827
7.3622
7.0984
7.0785
2.3039
S
S
S-1
3.97
4.00
6.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Apr06-2021-OSSO_cJ.38.fid
137.4583
133.9299
129.8177
128.5605
21.0981
S
S
S-1
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

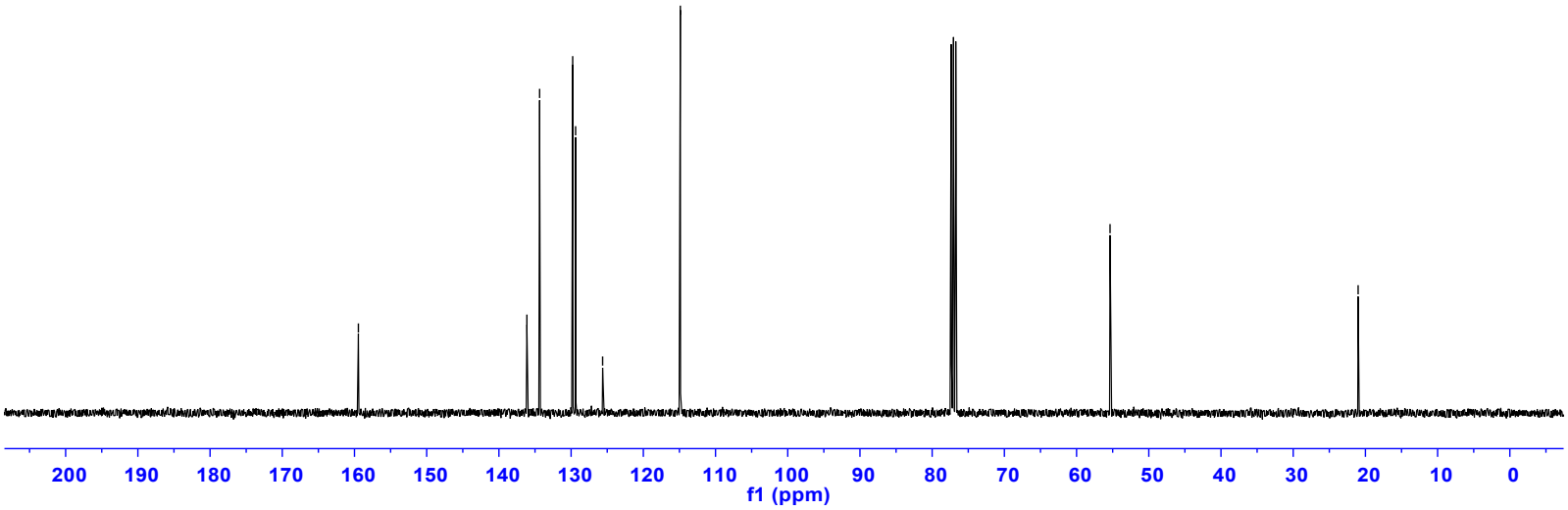

Mar08-2021-OSSO_cJ.4.fid — wyn-x210308-1-H
7.3757
7.3679
7.3625
7.3512
7.3459
7.3380
7.1368
7.1163
7.0680
7.0479
6.8799
6.8721
6.8667
6.8554
6.8502
6.8422
3.7967
2.2941
0.0000
S
OMe
S-2
2.00
2.00
2.00
2.02
3.06
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

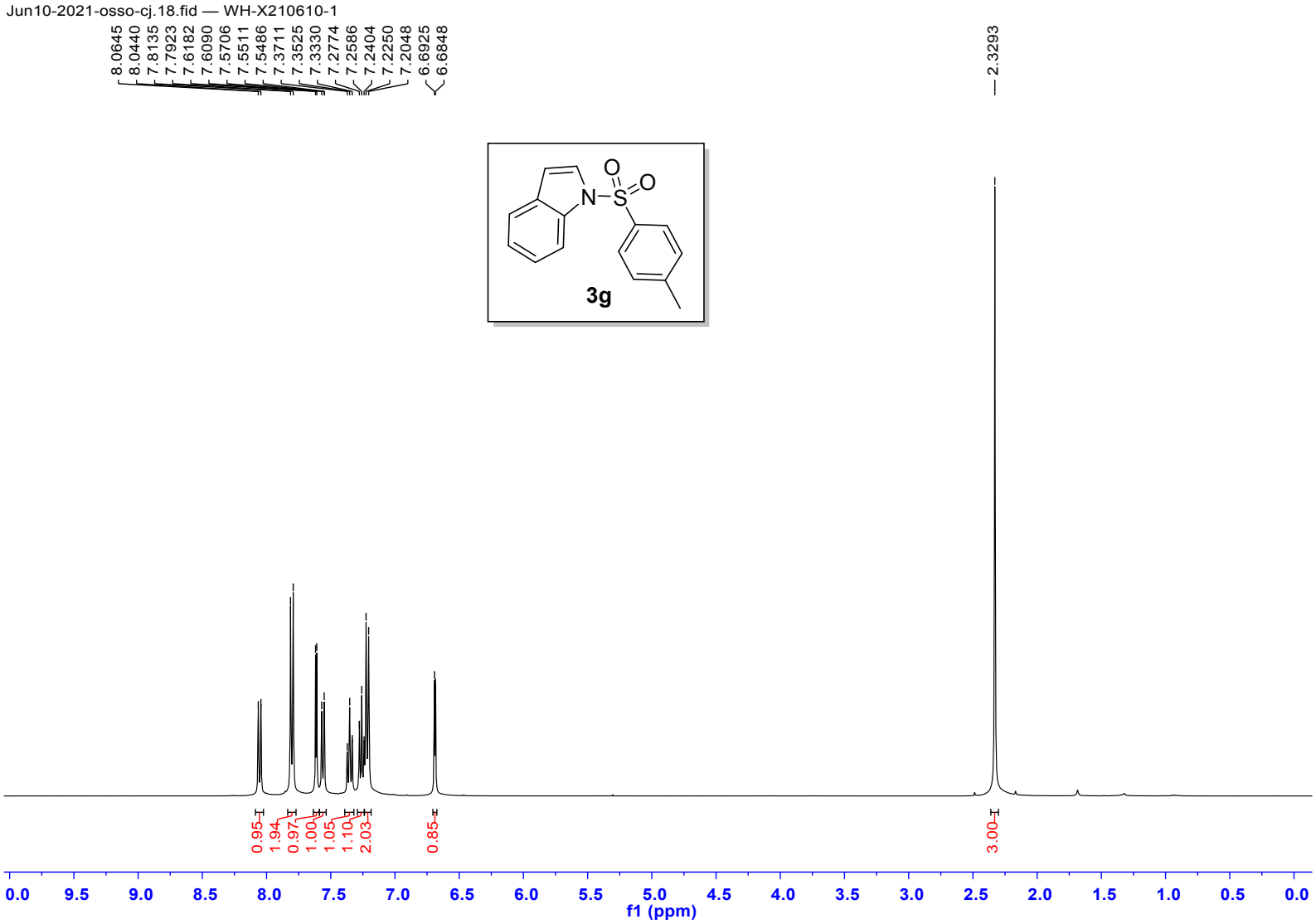
Mar08-2021-OSSO_cJ.31.fid — wyn-x210308-1-C

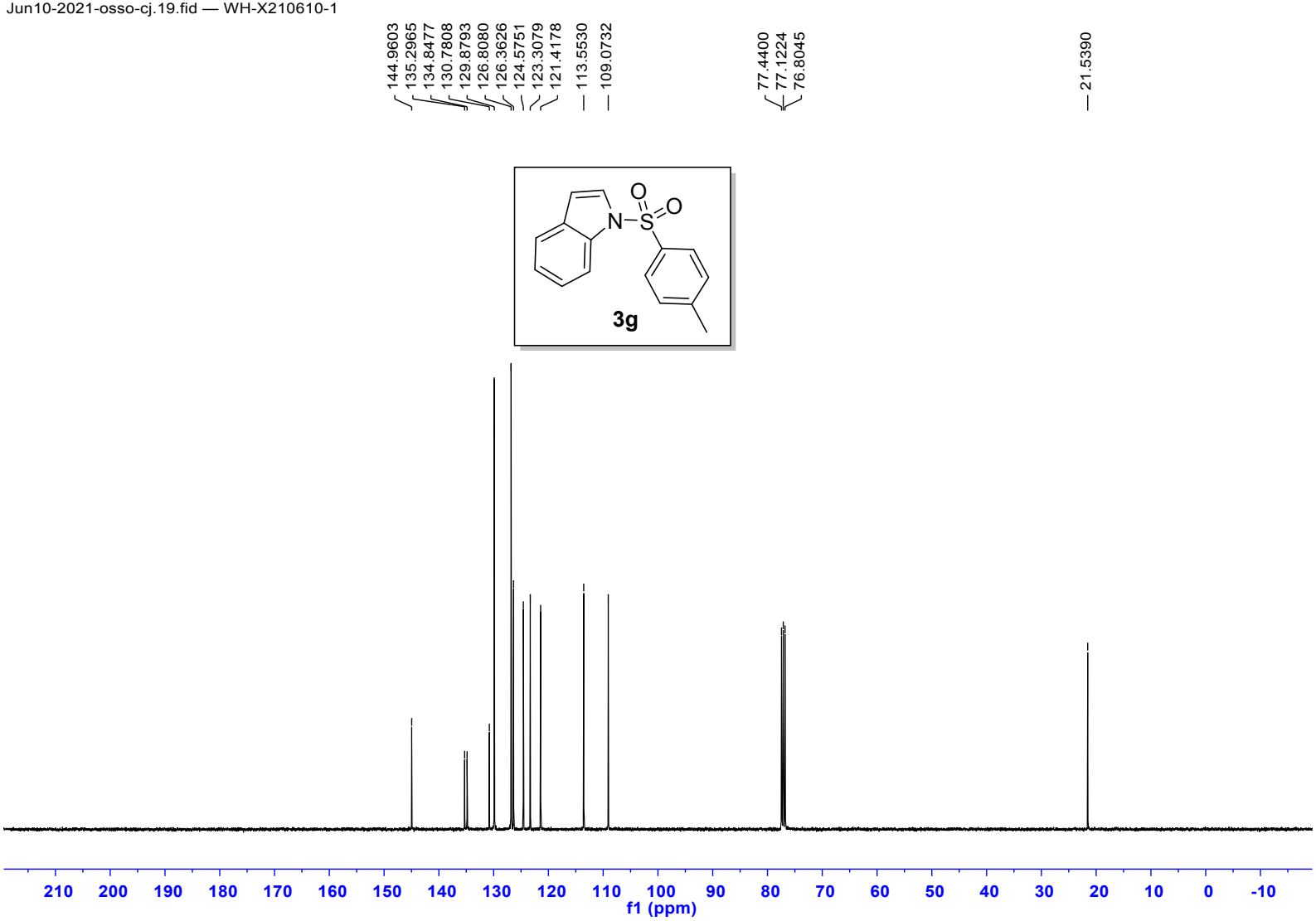
159.4575
136.1234
134.3639
129.7810
129.3773
125.6380
114.8720
55.3664
21.0104

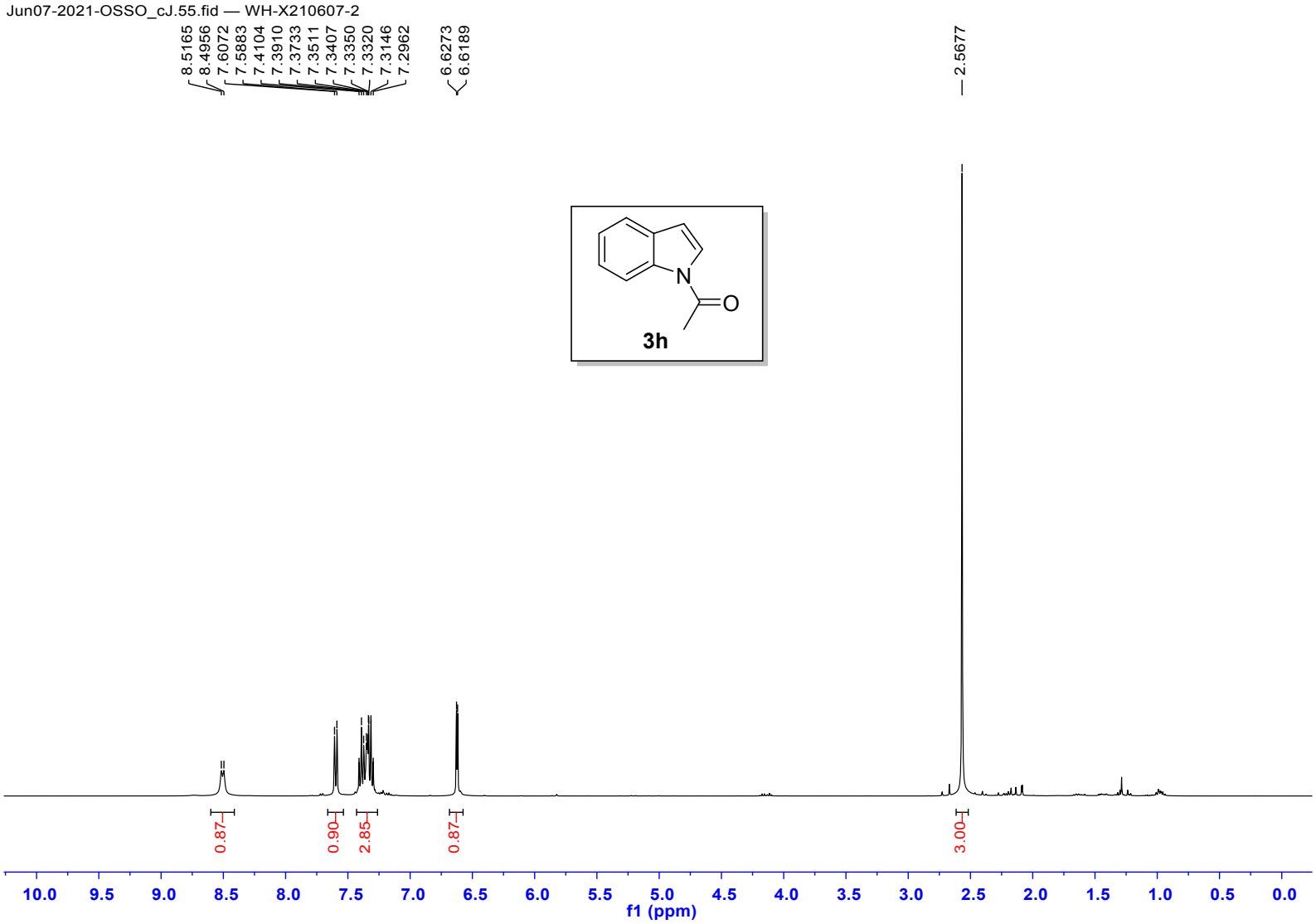


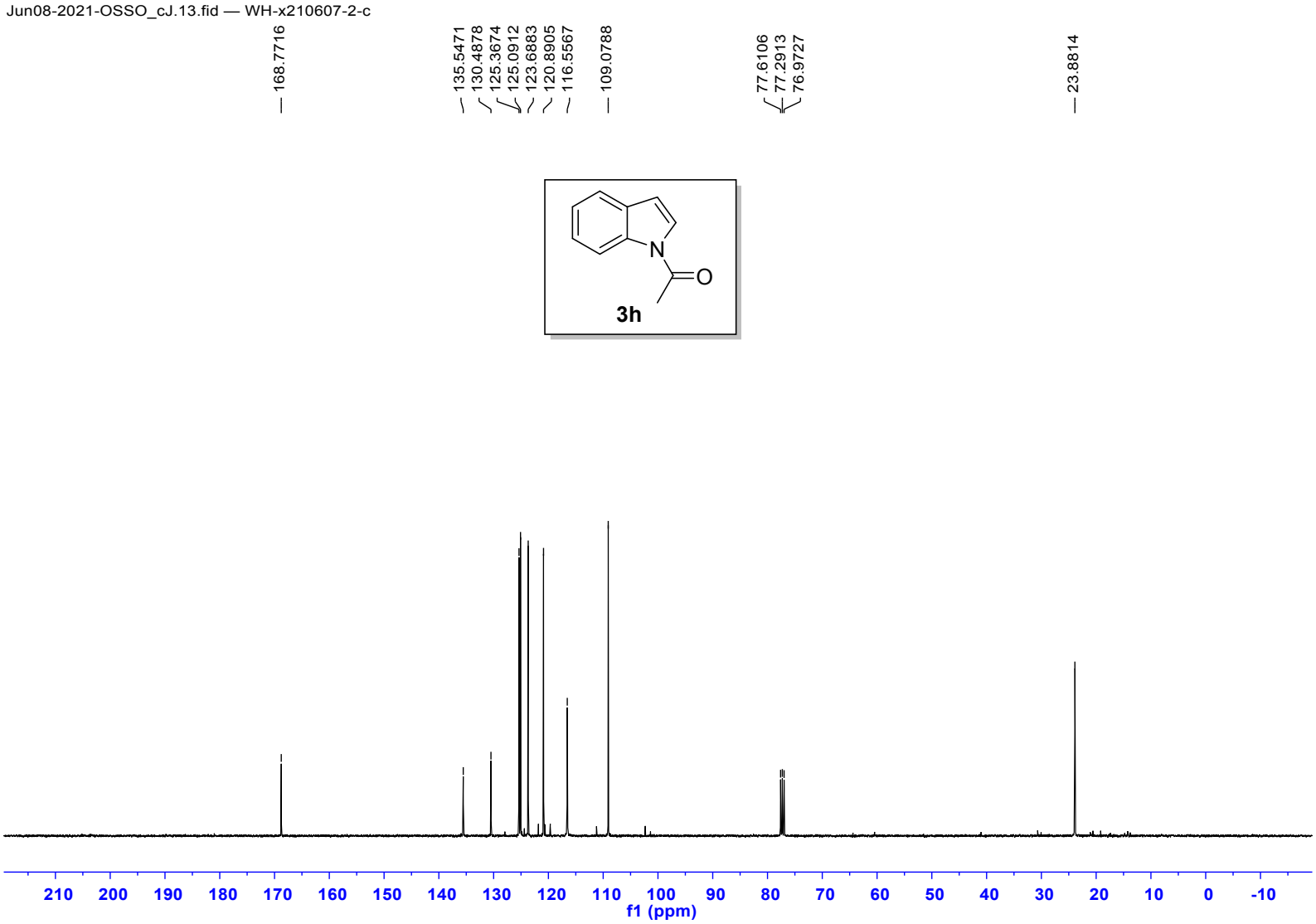

**S-2**




Jun10-2021-osso-cj.18.fid — WH-X210610-1
8.0645
8.0440
7.8135
7.7923
7.6182
7.6090
7.5706
7.5511
7.5486
7.3711
7.3525
7.3330
7.2774
7.2586
7.2404
7.2250
7.2048
6.6925
6.6848
2.3293
3g
0.95
1.94
0.97
1.00
1.05
1.10
2.03
0.85
3.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Jun10-2021-osso-cj.19.fid — WH-X210610-1
144.9603
135.2965
134.8477
130.7808
129.8793
126.8080
126.3626
124.5751
123.3079
121.4178
113.5530
109.0732
77.4400
77.1224
76.8045
21.5390
O
N
S
O
3g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Jun07-2021-OSSO_cJ.55.fid — WH-X210607-2
8.5165
8.4956
7.6072
7.5883
7.4104
7.3910
7.3733
7.3511
7.3407
7.3350
7.3320
7.3146
7.2962
6.6273
6.6189
2.5677
N
O
3h
0.87
0.90
2.85
0.87
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Jun08-2021-OSSO_cJ.13.fid — WH-x210607-2-c
168.7716
135.5471
130.4878
125.3674
125.0912
123.6883
120.8905
116.5567
109.0788
77.6106
77.2913
76.9727
23.8814
N
O
3h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)