Electronic Supplementary Material (ESI) for ChemComm.


# Pyridine-borane complex catalysed thioesterification: the direct conversion of carboxylic acids into thioesters

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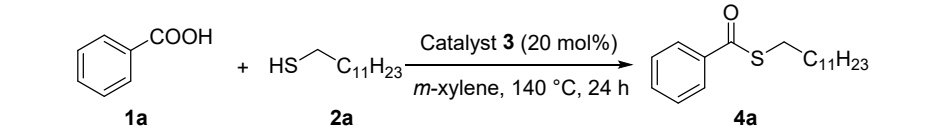
# Contents

# 1. General Information

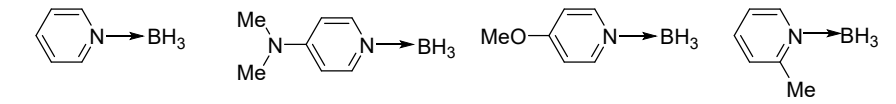
Unless otherwise noted, all manipulations were carried out under argon atmosphere. $^{11}B$, $^{13}C$ $^{19}F$ and $^{1}H$ NMR spectra were recorded at ambient temperature, on a Bruker Avance III 400 MHz NMR with Autosampler. Spectral data is reported in ppm using solvents as the reference ($CDCl_3$ at 7.26 ppm and DMSO at 2.50 ppm for $^{1}H$ NMR/$CDCl_3$ at 77.16 ppm, and DMSO at 39.52 ppm for $^{13}C$ NMR). Spectral data is reported as: δ value, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant(s) in Hz and integration. The $^{11}B$ NMR spectrum measured for the compound **3i** was hydrogen decoupled. All solvents for routine isolation of products were reagent-grade and were purchased from Sinopharm. The high-resolution mass spectra (HRMS) were measured on Bruker micrOTOF-II mass spectrometer by ESI using a positive electrospray ionization (ESI+). Measured values are reported to 4 decimal places of the calculated value. The calculated values are based on the most abundant isotope. Sodium borohydride was purchased from Sinopharm and used without further purification. All pyridines, thiols, thiophenols, carboxylic acids, benzylamine and ammonia-borane complex were purchased from Energy Chemical, Bidepharm and Aladdin and used without further purification. All reactions requiring heating were using an aluminum heating block except that the gram-scale reactions were heated in an oil bath.

# 2. Optimization Tables

**Table S1.** Survey of the catalysts for the synthesis of *S*-dodecyl benzothioate (**4a**).




**1a** **2a** **4a**



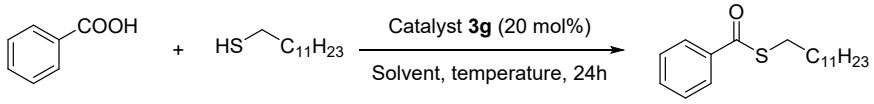

**3a**, 20% **3b**, 9% **3c**, 5% **3d**, 11%

**3e**, 7% **3f**, 15% **3g**, 31% **3h**, 25%

**3i**, 26% **3j**, 23% No Cat. N. R.

Reaction conditions: **1a** (2.0 mmol, 2.0 equiv), **2a** (1.0 mmol, 1.0 equiv), catalyst **3** (0.2 mmol, 20 mol%), *m*-xylene (2.0 mL), at 140 ℃ under argon, and yields reported are $^1$H NMR yields and determined by using 1,3,5-trimethoxybenzene as an internal standard. N.R. = No reaction.

**Table S2.** Optimization of solvents and the effect of temperature.

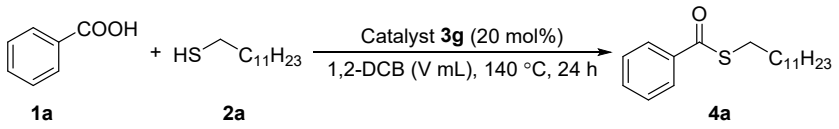



**1a** **2a** **4a**

| Entry | Solvent | Temperature (℃) | Yield (%) |
|---|---|---|---|
| 1 | *M*-xylene | 140 | 31 |
| 2 | Mesitylene | 140 | 24 |
| 3 | DMSO | 140 | 0 |
| 4 | DMF | 140 | Trace |
| **5** | **Dodecane** | **140** | **35** |
| 6 | Nitrobenzene | 140 | 31 |
| **7** | **1,2-DCB** | **140** | **35** |
| 8 | *M*-xylene | 120 | 11 |
| 9 | 1,2-DCB | 150 | 41 |

Reaction conditions: **1a** (2.0 mmol, 2.0 equiv), **2a** (1.0 mmol, 1.0 equiv), catalyst **3g** (0.2 mmol, 20 mol%), solvent (2.0 mL), under argon, and yields reported are $^1$H NMR yields and determined by using 1,3,5-trimethoxybenzene as an internal standard. 1,2-DCB = 1,2-dichlorobenzene, DMF = *N*,*N*-dimethylformamide, DMSO = dimethyl sulfoxide.

**Table S3.** Dosage proportional and concentration optimization table for the synthesis of **4a.**

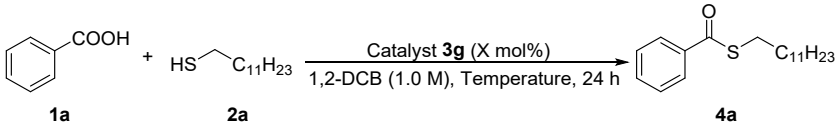



**1a** **2a** **4a**

| Entry | **1a** (equiv) | **2a** (equiv) | V (mL) | Concentration (M) | Yield (%) |
|---|---|---|---|---|---|
| 1 | 1.0 | 1.0 | 2.0 | 0.5 | 17 |
| 2 | 1.0 | 2.0 | 2.0 | 0.5 | 20 |
| 3 | 2.0 | 1.0 | 2.0 | 0.5 | 35 |
| 4 | 3.0 | 1.0 | 2.0 | 0.5 | 22 |
| 5 | 4.0 | 1.0 | 2.0 | 0.5 | 30 |
| 6 | 2.0 | 1.0 | 4.0 | 0.25 | 18 |
| **7** | **2.0** | **1.0** | **1.0** | **1.0** | **40** |
| 8 | 2.0 | 1.0 | 2.0 | 2.0 | 24 |

Reaction conditions: **1a**, **2a**, catalyst **3g** (0.2 mmol, 20 mol%), 1,2-DCB, at 140 °C, under argon, and yields reported are $^1$H NMR yields and determined by using 1,3,5-trimethoxybenzene as an internal standard.

**Table S4.** Survey of the catalyst's loading amount for the synthesis of **4a** and effects of temperature.



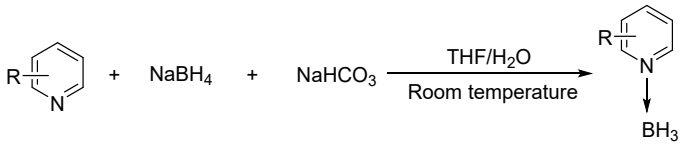

**1a** **2a** **4a**

| Entry | Temperature (°C) | X | Yield (%) |
|---|---|---|---|
| 1 | 140 | 20 | 40 |
| **2** | **140** | **50** | **74 (60)**[a] |
| 3 | 140 | 40 | 46 |
| 4 | 140 | 60 | 73 |
| 5 | 140 | 80 | 77 |
| 6 | 150 | 50 | 48 |
| 7 | 140 | 100 | 74 |

Reaction conditions: **1a** (2.0 mmol, 2.0 equiv), **2a** (1.0 mmol, 1.0 equiv), catalyst **3g** (0.2 mmol, 20 mol%), 1,2-DCB (1.0 mL), at 140 °C under argon, and yields reported are $^1$H NMR yields and determined by using 1,3,5-trimethoxybenzene as an internal standard. [a]Isolated yield.

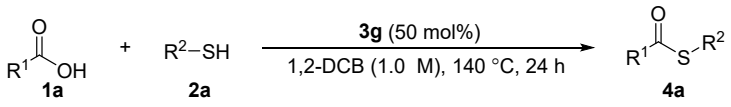
# 3. Experimental Procedures

## 3.1 Experimental procedures for the synthesis of pyridine-borane complexes.




The pyridine-borane complexes were synthesized according to the reported procedure. [1a] Sodium borohydride (0.28 g, 7.5 mmol) and powdered sodium bicarbonate (1.26 g, 15 mmol) were added to a 50 mL dry round bottom flask. The corresponding pyridine was charged into the reaction flask followed by the addition of reagent-grade THF (1.9 mL for liquid pyridines) at ambient temperature. Under vigorous stirring, 1.9 mL of 14.4% v/v solution water in THF was added dropwise. The reaction was monitored by TLC. Upon completion (4 - 12 h), the reaction was filtered through sodium sulfate and celite and the solid residue was washed with 50 mL THF. Remove the solvent *in vacuo* and the residue was purified with flash chromatography with 200-300 mesh silica gel, eluting with petroleum, ether and ethyl acetate.

## 3.2 Experimental procedures of thioesters.

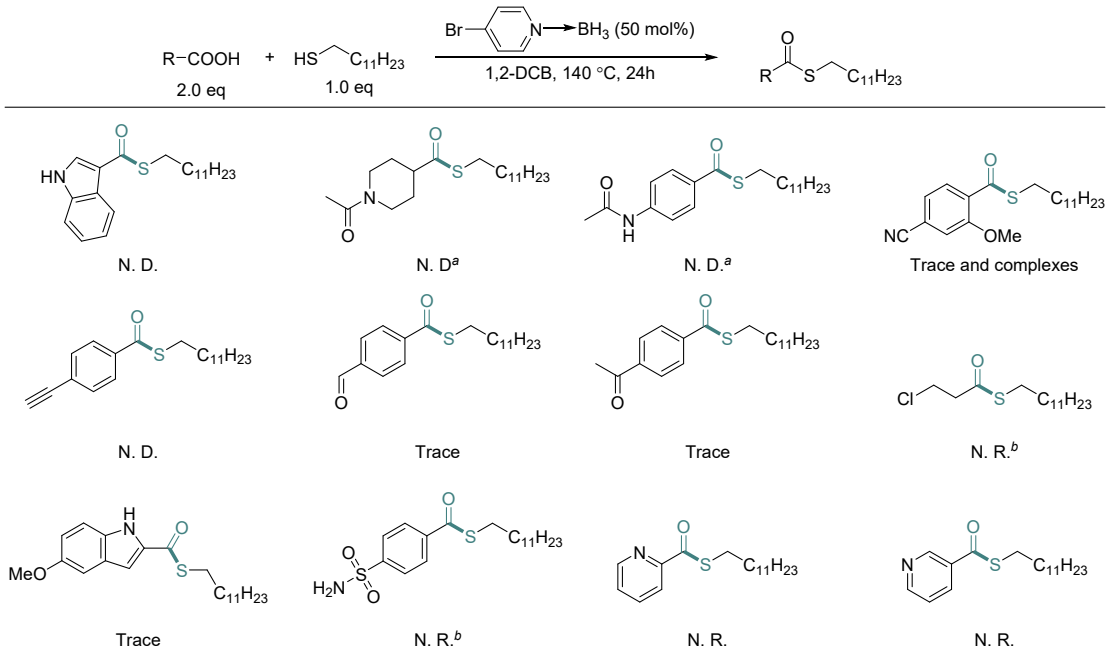



To a 25 mL Schlenk tube was added carboxylic acids (2.0 mmol), thiols or thiophenols (1.0 mmol), and pyridine-borane complex **3g** (0.5 mmol, 50 mol%) under argon atmosphere. Then 1,2-DCB was added into the tube (1.0 mL, 1.0 M with respect to thiols or thiophenols), and the reaction was then heated to 140 ℃ for 24 hours. When completed, the mixture was cooled to room temperature and extracted with ethyl acetate (10 mL × 3), then the combined organic layer was washed with brine and then dried over $Na_2SO_4$. Filtered and concentrated *in vacuo.* The residue was purified with flash chromatography with 200-300 mesh silica gel, eluting with petroleum ether and dichloromethane, to afford desired thioesters.

### 3.3 Experimental procedures of gram-scale reactions

To a 50 mL round-bottom flask, carboxylic acids (20.0 mmol), thiols (10.0 mmol), and pyridine-borane complex **3g** (5.0 mmol, 50 mol%) were added under argon atmosphere. Then 1,2-DCB was added into the flask (10.0 mL, 1.0 M with respect to thiols). The reaction was heated to 140 ℃ for 24 hours. When the reaction was completed, the reaction mixture was cooled to room temperature, then washed with water and extracted with ethyl acetate (20 mL × 3). The combined organic layer was washed with brine, and then dried over $Na_2SO_4$. Filtered and concentrated *in vacuo* and purified with 200-300 mesh silica gel, eluting with petroleum ether and dichloromethane, to afford desired thioesters.

### 3.4 Unsuccessful examples.

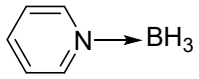



N. D. = Not detected. N. R. = No reaction. [a]*S*-dodecyl ethanethioate as the product was obtained, and yields < 10%. [b]Carboxylic acid could not dissolve in the solvent.

# 4. Characterization data of catalysts, thioesters and amide products

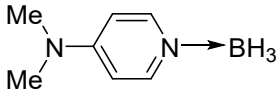
## 4.1 Characterization data of pyridine-borane complexes.

**3a** Pyridine-Borane complex



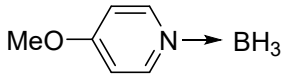
The title compound was isolated as a colorless oil. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 9.03 – 8.28 (m, 2H), 7.93 (t, *J* = 7.7 Hz, 1H), 7.58 – 7.37 (m, 2H), 2.59 (br, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 147.5, 139.2, 125.4. Characterization is in agreement with previous reports for this compound. [1a]

**3b** 4-Dimethlaminopyridine-Borane complex



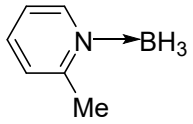
The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.05 (d, *J* = 7.3 Hz, 2H), 6.48 (d, *J* = 7.5 Hz, 2H), 3.09 (s, 6H), 2.86 – 1.97 (br, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.7, 146.8, 106.5, 39.6. Characterization is in agreement with previous reports for this compound. [1a]

**3c** 4-Methoxypyridine-Borane complex



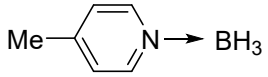
The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.39 (d, *J* = 7.0 Hz, 2H), 6.92 (d, *J* = 7.2 Hz, 2H), 3.94 (s, 3H), 2.95 – 2.10 (br, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 167.4, 149.0, 111.0, 56.4. Characterization is in agreement with previous reports for this compound. [1c]

**3d** 2-Methylpyridine-Borane complex



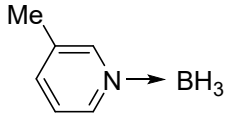
The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.74 (d, *J* = 5.7 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 6.7 Hz, 1H), 2.76 (s, 3H), 2.83 – 2.12 (br, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 157.9, 148.8, 139.6, 126.9, 122.5, 22.6. Characterization is in agreement with previous reports for this compound. [1a]

**3e** 4-Methylpyridine-Borane complex



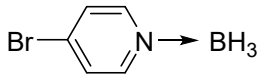
The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.43 (d, *J* = 6.3 Hz, 2H), 7.29 (d, *J* = 6.1 Hz, 2H), 2.48 (s, 3H), 3.03 – 2.09 (br, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 151.6, 147.0, 126.1, 21.4. Characterization is in agreement with previous reports for this compound. [1c]

**3f** 3-Methylpyridine-Borane complex



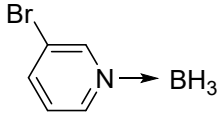

The title compound was isolated as a colorless oil. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.44 – 8.25 (m, 2H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.37 (dd, *J* = 7.8, 5.7 Hz, 1H), 3.05 – 2.04 (br, 3H), 2.36 (s, 3H). **$^{13}$C NMR** (101 MHz, $CDCl_3$) δ 147.4, 144.5, 139.7, 135.8, 124.9, 18.4. Characterization is in agreement with previous reports for this compound. [1c]

**3g** 4-Bromopyridine-Borane complex



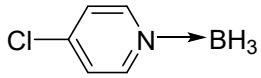

The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.43 (d, *J* = 6.4 Hz, 2H), 7.67 (d, *J* = 6.8Hz, 2H), 3.02–1.94 (br, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 148.3, 136.6, 129.1. Characterization is in agreement with previous reports for this compound. [1c]

**3h** 3-Bromopyridine-Borane complex




The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.76 (s, 1H), 8.57 (d, *J* = 5.6 Hz, 1H), 8.07 (d, *J* = 8.2 Hz, 1H), 7.42 (dd, *J* = 8.2, 5.7 Hz, 1H), 3.09 – 2.09 (3H, br). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 149.2, 146.1, 142.0, 126.2, 121.2. Characterization is in agreement with previous reports for this compound. [1c]

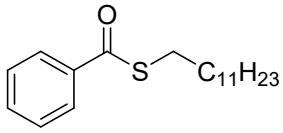
**3i** 4-Chloropyridine-Borane complex




The title compound was isolated as a white solid. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.53 (d, *J* = 6.4 Hz, 2H), 7.50 (d, *J* = 6.9 Hz, 2H), 2.99 – 2.14 (m, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 148.5, 147.8, 126.0. **$^{11}$B NMR (128 MHz, $CDCl_3$)** δ -12.03. **HRMS (ESI)** *m/z*: calculated for $C_5H_7BBrN[Na]^+$: 149.0253; found: 149.0255.

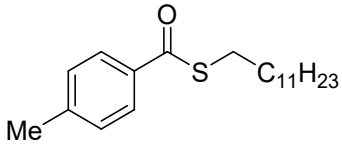
# 4.2 Characterization data of thioesters.

**4a** *S*-dodecyl benzothioate



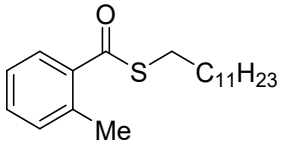

The title compound was isolated as a colorless oil (184 mg, 60% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.97 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 3.07 (t, *J* = 7.4 Hz, 2H), 1.67 (m, 2H), 1.46 – 1.38 (m, 2H), 1.33 – 1.22 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 192.3, 137.4, 133.3, 128.7, 127.3, 32.1, 29.8, 29.8, 29.7, 29.7, 29.6, 29.5, 29.3, 29.2, 29.1, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2a]

**4b** *S*-dodecyl 4-methylbenzothioate



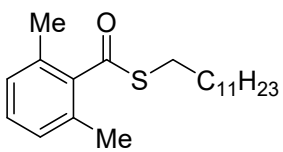

The title compound was isolated as a colorless oil (199 mg, 62% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.87 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 3.05 (t, *J* = 7.4 Hz, 2H), 2.40 (s, 3H), 1.66 (p, *J* = 7.4 Hz, 2H), 1.42 (p, *J* = 6.8 Hz, 2H), 1.32 – 1.22 (m, 16H), 0.88 (t, *J* = 6.9 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.9, 144.1, 134.9, 129.3, 127.4, 32.1, 29.8, 29.8, 29.8, 29.7, 29.6, 29.5, 29.3, 29.1, 22.8, 21.8, 14.3. Characterization is in agreement with previous reports for this compound. [2b]

**4c** *S*-dodecyl 2-methylbenzothioate




The title compound was isolated as a colorless oil (237 mg, 74% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.80 – 7.72 (m, 1H), 7.40 – 7.31 (m, 1H), 7.22 (t, *J* = 7.1 Hz, 2H), 3.02 (t, *J* = 7.4 Hz, 2H), 2.47 (s, 3H), 1.66 (p, *J* = 7.4 Hz, 2H), 1.42 (p, *J* = 6.7 Hz, 2H), 1.32 – 1.22 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 194.7, 138.0, 136.7, 131.6, 131.5, 128.5, 125.8, 32.1, 29.8, 29.8, 29.7, 29.7, 29.5, 29.3, 29.1, 22.8, 20.7, 14.3. Characterization is in agreement with previous reports for this compound. [2b]

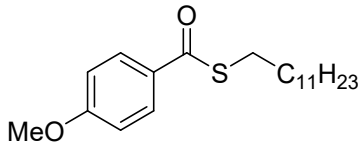
**4d** *S*-dodecyl 2,6-dimethylbenzothioate




The title compound was isolated as a colorless oil (261 mg, 78% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.18 (t, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 7.6 Hz, 2H), 3.07 (t, *J* = 7.3 Hz, 2H), 2.33 (s, 6H), 1.70 (p, *J* = 7.4 Hz, 2H), 1.44 (p, *J* = 6.7 Hz, 2H), 1.35 – 1.25 (m, 16H), 0.90 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz,**

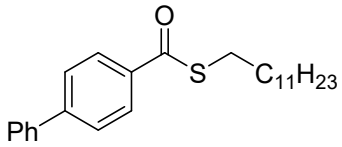
**$CDCl_3$)** δ 198.0, 140.6, 133.7, 129.3, 127.7, 32.1, 29.8, 29.7, 29.6, 29.6, 29.5, 29.3, 29.0, 22.8, 19.1, 14.2. **HRMS (ESI)** *m/z:* calculated for $C_{21}H_{34}OS[H]^+$: 335.2404; found: 335.2409.

**4e** *S*-dodecyl 4-methoxybenzothioate



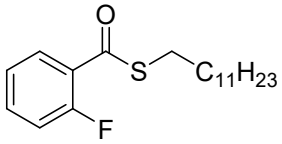

The title compound was isolated as a colorless oil (281 mg, 83% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.95 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 3.85 (s, 3H), 3.04 (t, *J* = 7.4 Hz, 2H), 1.65 (p, *J* = 7.5 Hz, 2H), 1.40 (q, *J* = 7.3, 6.3 Hz, 2H), 1.32 – 1.22 (m, 16H), 0.88 (t, *J* = 6.7 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 190.8, 163.7, 130.3, 129.4, 113.8, 55.6, 32.1, 29.8, 29.8, 29.7, 29.7, 29.7, 29.5, 29.3, 29.1, 29.1, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2c]

**4f** *S*-dodecyl [1,1'-biphenyl]-4-carbothioate



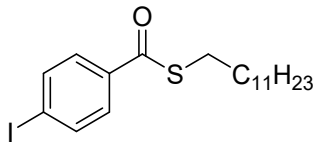

The title compound was isolated as a white solid (233 mg, 61% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.04 (d, *J* = 8.5 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 7.1 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 3.09 (t, *J* = 7.4 Hz, 2H), 1.69 (p, *J* = 7.4 Hz, 2H), 1.44 (p, *J* = 6.7 Hz, 2H), 1.32 – 1.22 (s, 16H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.8, 146.1, 134.0, 136.1, 129.1, 128.3, 127.9, 127.4, 127.3, 32.1, 29.8, 29.8, 29.7, 29.7, 29.5, 29.3, 29.2, 29.1, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2d]

**4g** *S*-dodecyl 2-fluorobenzothioate



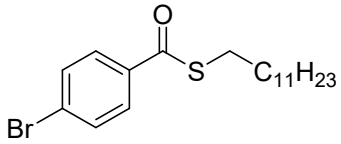

The title compound was isolated as a yellow oil (193 mg, 59% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.85 (td, *J* = 7.6, 1.8 Hz, 1H), 7.49 (dddd, *J* = 8.3, 7.2, 5.0, 1.8 Hz, 1H), 7.20 (td, *J* = 7.7, 1.0 Hz, 1H), 7.13 (ddd, *J* = 10.7, 8.3, 0.9 Hz, 1H), 3.06 (t, *J* = 7.4 Hz, 2H), 1.77 – 1.59 (m, 2H), 1.42 (p, *J* = 6.8 Hz, 2H), 1.33 – 1.22 (m, 16H), 0.87 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 189.1 (d, *J* = 4.6 Hz), 160.4 (d, *J* = 257.7 Hz), 134.2 (d, *J* = 8.8 Hz), 129.8 (d, *J* = 1.4 Hz), 126.0 (d, *J* = 11.3 Hz), 124.2 (d, *J* = 3.5 Hz), 117.0 (d, *J* = 22.4 Hz), 32.0, 29.8, 29.7, 29.6, 29.5, 29.5, 29.4, 29.3, 29.1, 22.8, 14.2. **$^{19}$F NMR (377 MHz, $CDCl_3$)** δ -111.00 (ddd, *J* = 11.1, 6.9, 4.3 Hz). **HRMS (ESI)** *m/z*: calculated for $C_{19}H_{29}FOS[H]^+$: 325.1996; found: 325.1990.

**4h** *S*-dodecyl 4-iodobenzothioate



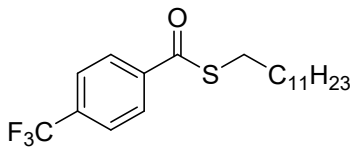

The title compound was isolated as a white solid (208 mg, 48% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.5 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 3.05 (t, *J* = 7.4 Hz, 2H), 1.65 (p, *J* = 7.4 Hz, 2H), 1.46 – 1.34 (m, 2H), 1.32 – 1.22 (s, 16H), 0.87 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.5, 137.9, 136.7, 128.6, 101.0, 32.0, 29.8, 29.7, 29.6, 29.6, 29.5, 29.3, 29.0, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2e]

**4i** *S*-dodecyl 4-bromobenzothioate



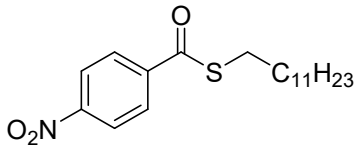

The title compound was isolated as a yellow oil (160 mg, 42% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.83 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 3.06 (t, *J* = 7.4 Hz, 2H), 1.66 (p, *J* = 7.4 Hz, 2H), 1.40 (q, *J* = 7.2 Hz, 2H), 1.33-1.22 (m, 16H), 0.88 (t, *J* = 6.7 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.3, 136.2, 132.0, 128.8, 128.3, 32.1, 29.8, 29.7, 29.6, 29.6, 29.5, 29.3, 29.3, 29.1, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2e]

**4j** *S*-dodecyl 4-(trifluoromethyl)benzothioate



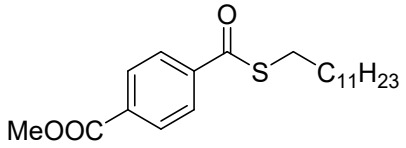

The title compound was isolated as a yellow oil (153 mg, 41% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 3.10 (t, *J* = 7.3 Hz, 2H), 1.69 (p, *J* = 7.4 Hz, 2H), 1.49 – 1.38 (m, 2H), 1.31 – 1.22 (m, 16H), 0.88 (t, *J* = 6.7 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.3, 140.1, 134.7 (q, *J* = 32.7 Hz), 127.6, 125.8 (q, *J* = 3.7 Hz), 123.7 (d, *J* = 272.6 Hz), 32.1, 29.9, 29.8, 29.7, 29.7, 29.6, 29.5, 29.5, 29.3, 29.1, 22.8, 14.2. Characterization is in agreement with previous reports for this compound. [2e]

**4k** *S*-dodecyl 4-nitrobenzothioate



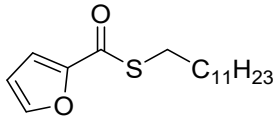

The title compound was isolated as a awhite solid (107 mg, 30% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.29 (d, *J* = 8.8 Hz, 2H), 8.11 (d, *J* = 8.9 Hz, 2H), 3.11 (t, *J* = 7.3 Hz, 2H), 1.69 (p, *J* = 7.4 Hz, 2H), 1.42 (dt, *J* = 14.6, 6.7 Hz, 2H), 1.31– 1.25 (br, 16H), 0.87 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 190.8, 150.6, 142.0, 128.3, 124.0, 32.0, 29.8, 29.7, 29.6, 29.5, 29.4, 29.2, 29.0, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2p]

**4l** methyl 4-((dodecylthio)carbonyl)benzoate



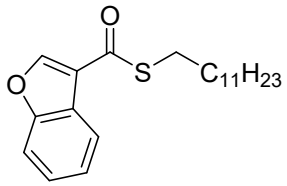

The title compound was isolated as a white solid (179 mg, 49% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.10 (d, *J* = 8.4 Hz, 2H), 8.01 (d, *J* = 8.5 Hz, 2H), 3.95 (s, 3H), 3.09 (t, *J* = 7.3 Hz, 2H), 1.68 (p, *J* = 7.3 Hz, 2H), 1.42 (p, *J* = 6.9 Hz, 2H), 1.36 – 1.25 (m, 16H), 0.87 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.8, 166.3, 140.7, 134.1, 130.0, 127.2, 52.6, 32.1, 29.8, 29.8, 29.7, 29.6, 29.6, 29.5, 29.5, 29.3, 29.1, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2q]

**4o** *S*-dodecyl furan-2-carbothioate



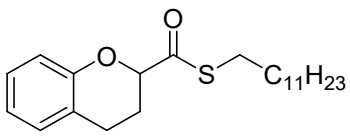

The title compound was isolated as a yellow oil (160 mg, 54% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.60 – 7.46 (m, 1H), 7.15 (d, *J* = 3.4 Hz, 1H), 6.50 (dd, *J* = 3.6, 1.7 Hz, 1H), 3.03 (t, *J* = 7.3 Hz, 2H), 1.64 (p, *J* = 7.4 Hz, 2H), 1.39 (p, *J* = 6.7 Hz, 2H), 1.32 – 1.22 (m, 16H) 0.86 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 180.8, 151.2, 146.0, 115.3, 112.2, 32.0, 29.7, 29.7, 29.6, 29.4, 29.2, 29.0, 28.2, 22.8, 14.2. Characterization is in agreement with previous reports for this compound. [2e]

**4p** *S*-dodecyl benzofuran-3-carbothioate




The title compound was isolated as a white solid (216 mg, 62% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.69 (d, *J* = 7.8 Hz, 1H), 7.58 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.51 (d, *J* = 1.0 Hz, 1H), 7.46 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 1H), 7.33 – 7.27 (m, 1H), 3.11 (t, *J* = 7.3 Hz, 2H), 1.69 (p, *J* = 7.4 Hz, 2H), 1.43 (p, *J* = 6.8 Hz, 2H), 1.38 – 1.26 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 182.6, 155.5, 151.5, 128.1, 127.1, 124.1, 123.2, 112.5, 111.0, 32.0, 29.8, 29.8, 29.7, 29.6, 29.6, 29.5, 29.3, 29.0, 28.6, 22.8, 14.3. **HRMS (ESI)** *m/z*: calculated for $C_{21}H_{30}O_2S[H]^+$: 347.2040; found: 347.2039.

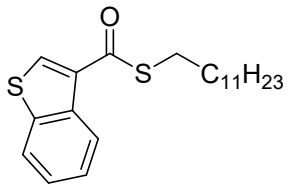
**4q** *S*-dodecyl chromane-2-carbothioate




The title compound was isolated as a white solid (219 mg, 60% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.15 (t, *J* = 7.7 Hz, 1H), 7.04 (d, *J* = 6.0 Hz, 1H), 6.96 (d, *J* = 7.1 Hz, 1H), 6.89 (t, *J* = 7.4 Hz, 1H), 4.72 (dd, *J* = 6.8, 4.3 Hz, 1H), 2.96 – 2.81 (m, 2H), 2.80 – 2.74 (m, 2H), 2.30 – 2.15 (m, 2H), 1.64 – 1.51 (m, 2H),1.38 – 1.26 (m, 18H), 0.89 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 201.9, 153.2, 129.6, 127.8, 121.8, 121.1, 117.0, 80.3, 32.0, 29.8, 29.8, 29.7, 29.6, 29.5, 29.4, 29.2, 29.0, 28.4, 25.0, 23.0, 22.8,

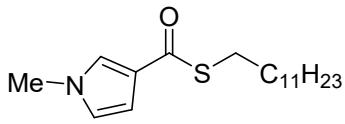
14.3. **HRMS (ESI)** *m/z*: calculated for $C_{22}H_{34}O_2S[K]^+$: 385.2172; found: 385.2161.

**4r** *S*-dodecyl benzo[*b*]thiophene-3-carbothioate



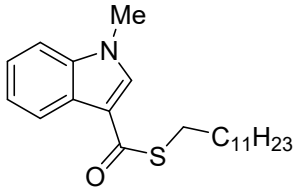
The title compound was isolated as a yellow oil (298 mg, 55% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.58 (d, *J* = 8.1 Hz, 1H), 8.39 (s, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.52 – 7.45 (m, 1H), 7.45 – 7.37 (m, 1H), 3.10 (t, *J* = 7.4, 2H), 1.71 (p, *J* = 7.4 Hz, 2H), 1.45 (p, *J* = 6.7 Hz, 2H), 1.35 – 1.25 (m, 16H), 0.90 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 186.4, 140.0, 135.9, 135.1, 135.0, 125.9, 125.6, 125.0, 122.5, 32.1, 29.9, 29.8, 29.8, 29.7, 29.7, 29.5, 29.3, 29.1, 29.1, 22.8, 14.3. **HRMS (ESI)** *m/z*: calculated for $C_{21}H_{30}OS_2[Na]^+$: 385.1631; found: 385.1631.

**4s** *S*-dodecyl 1-methyl-1H-pyrrole-3-carbothioate



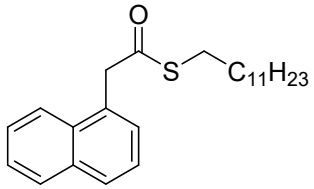
The title compound was isolated as a white solid (107 mg, 35% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.07 (dd, *J* = 4.1, 1.7 Hz, 1H), 6.78 (t, *J* = 2.1 Hz, 1H), 6.10 (dd, *J* = 4.1, 2.5 Hz, 1H), 3.90 (s, 3H), 2.96 (t, *J* = 7.3 Hz, 2H), 1.63 (p, *J* = 6.8 Hz, 2H), 1.39 (q, *J* = 6.5, 5.7 Hz, 2H), 1.38 – 1.26 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 182.3, 130.2, 129.7, 118.1, 108.4, 37.2, 32.0, 30.1, 29.8, 29.8, 29.7, 29.7, 29.5, 29.3, 29.1, 28.4, 22.8, 14.3. **HRMS (ESI)** *m/z*: calculated for $C_{18}H_{31}NOS[H]^+$: 310.2200; found: 310.2199.

**4t** *S*-dodecyl 1-methyl-1H-indole-3-carbothioate



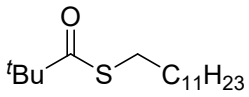
The title compound was isolated as a yellow solid (204 mg, 57% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.32 – 8.21 (m, 1H), 7.85 (s, 1H), 7.39 – 7.26 (m, 3H), 3.83 (s, 3H), 3.08 (t, *J* = 7.4 Hz, 2H), 1.79 – 1.60 (m, 2H), 1.44 (p, *J* = 6.6 Hz, 2H), 1.34 – 1.26 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 185.0, 137.4, 134.3, 125.6, 123.4, 122.6, 122.2, 116.0, 109.9, 33.7, 32.1, 30.3, 29.8, 29.8, 29.7, 29.7, 29.5, 29.4, 29.1, 28.3, 22.8, 14.3. **HRMS (ESI)** *m/z*: calculated for $C_{22}H_{33}NOS[H]^+$: 360.2356; found: 360.2338.

**4u** *S*-dodecyl 2-(naphthalen-1-yl)ethanethioate



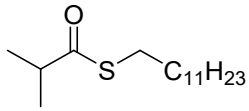
The title compound was isolated as a colorless oil (266 mg, 71% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.98 (d, *J* = 8.3 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.82 (dd, *J* = 6.4, 3.1 Hz, 1H), 7.57 – 7.47 (m, 2H), 7.44 (q, *J* = 3.5 Hz, 2H), 4.28 (s, 2H), 2.94 – 2.65 (m, 2H), 1.51 (p, *J* = 7.3 Hz, 2H), 1.32 – 1.22 (d, *J* = 8.51 Hz, 18H), 0.88 (t, *J* = 6.9 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 198.0, 134.0, 132.3, 130.4, 128.9, 128.9, 128.5, 126.6, 126.0, 125.6, 124.1, 48.5, 32.1, 29.8, 29.68, 29.6, 29.5, 29.4, 29.2, 28.9, 22.8, 14.3. Characterization is in agreement with previous reports for this compound. [2o]

**4v** *S*-dodecyl 2,2-dimethylpropanethioate



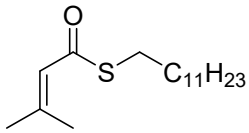
The title compound was isolated as a colorless oil (171 mg, 60% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 2.84 – 2.76 (m, 2H), 1.53 (dt, *J* = 15.0, 7.4 Hz, 2H), 1.36 – 1.18 (m, 27H), 0.86 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 207.1, 46.5, 32.1, 29.8, 29.7, 29.7, 29.6, 29.5, 29.3, 29.1, 28.7, 27.5, 22.8, 14.2. Characterization is in agreement with previous reports for this compound. [2f]

**4w** *S*-dodecyl 2-methylpropanethioate



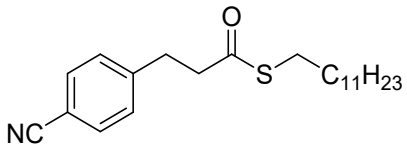
The title compound was isolated as a colorless oil (169 mg, 62% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 2.83 (t, *J* = 7.4 Hz, 2H), 2.76 – 2.66 (m, 1H), 1.58 – 1.50 (m, 2H), 1.36 – 1.21 (m, 18H), 1.17 (d, *J* = 6.9 Hz, 6H), 0.86 (t, *J* = 6.7 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 204.5, 43.2, 32.0, 29.8, 29.7, 29.7, 29.6, 29.5, 29.3, 29.0, 28.7, 22.8, 19.5, 14.2. Characterization is in agreement with previous reports for this compound. [2r]

**4x** *S*-dodecyl 3-methylbut-2-enethioate



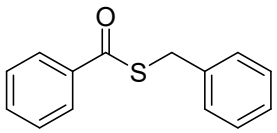
The title compound was isolated as a colorless oil (200 mg, 70% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 5.97 (t, *J* = 1.4 Hz, 1H), 2.87 (t, *J* = 7.4 Hz, 2H), 2.15 (d, *J* = 1.2 Hz, 3H), 1.86 (d, *J* = 1.3 Hz, 3H), 16.0 – 1.53 (m, 2H), 1.40 – 1.16 (m, 18H), 0.87 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 189.6, 153.3, 123.5, 32.0, 29.9, 29.8, 29.8, 29.7, 29.6, 29.5, 29.3, 29.1, 28.9, 27.3, 22.8, 21.2, 14.2. **HRMS (ESI)** *m/z*: calculated for $C_{17}H_{32}OS[H]^+$: 285.2247; found: 285.2247.

**4y** *S*-dodecyl 3-(4-cyanophenyl)propanethioate



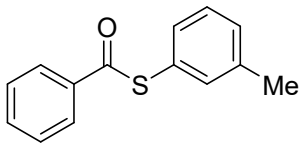

The title compound was isolated as a white solid (231 mg, 64% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.57 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 3.03 (t, *J* = 7.5 Hz, 2H), 2.89 – 2.77 (m, 4H), 1.53 (p, *J* = 7.8, 7.2 Hz, 2H), 1.33 – 1.25 (m, 18H), 0.87 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 198.2, 145.9, 132.5, 129.4, 119.0, 110.5, 44.6, 32.0, 31.5, 29.8, 29.7, 29.6, 29.6, 29.5, 29.2, 29.1, 28.9, 22.8, 14.3. **HRMS (ESI)** *m/z*: calculated for $C_{22}H_{33}NOS[H]^+$: 360.2356; found: 360.2356.

**4z** *S*-benzyl benzothioate



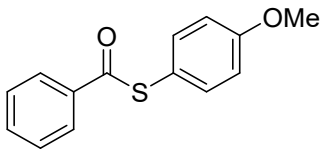

The title compound was isolated as a colorless oil (132 mg, 58% yield; gram-scale reaction: 1.152g, 50% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.96 (dt, *J* = 8.5, 1.6 Hz, 2H), 7.53 (tt, *J* = 6.9, 1.2 Hz, 1H),) 7.39 – 7.32 (m, 3H), 7.30 – 7.25 (m, 1H), 7.32 – 7.27 (m, 2H), 7.26 – 7.19 (m, 1H), 4.30 (s, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.3, 137.6, 136.8, 133.5, 129.1, 128.7, 128.7, 127.4, 127.4, 33.4. Characterization is in agreement with previous reports for this compound. [2g]

**4aa** *S*-(*m*-tolyl) benzothioate



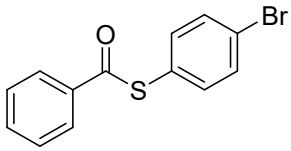

The title compound was isolated as a colorless oil (113 mg, 49% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.05 (dt, *J* = 8.5, 1.7 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.38 – 7.26 (m, 4H), 2.41 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 190.5, 139.2, 136.8, 135.8, 133.7, 132.2, 130.5, 129.2, 128.9, 127.6, 127.1, 21.4. Characterization is in agreement with previous reports for this compound. [2h]

**4ab** *S*-(4-methoxyphenyl) benzothioate



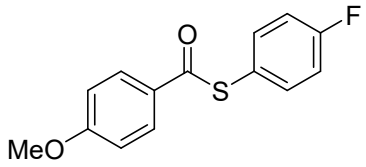

The title compound was isolated as a colorless oil (89 mg, 36% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.42 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 191.2, 160.9, 136.8, 133.7, 128.9, 127.6, 118.0, 115.1, 55.5. Characterization is in agreement with previous reports for this compound. [2i]

**4ac** *S*-(4-bromophenyl) benzothioate



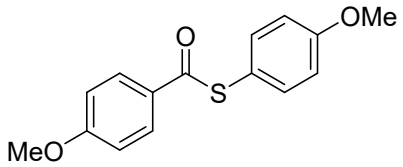

The title compound was isolated as a white solid (86 mg, 30% yield), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 7.3 Hz, 2H), 7.65 – 7.57 (m, 3H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 189.5, 136.6, 136.4, 133.9, 132.5, 128.9, 127.6, 126.6, 124.3, Characterization is in agreement with previous reports for this compound. [2j]

**4ad** *S*-(4-fluorophenyl) 4-methoxybenzothioate



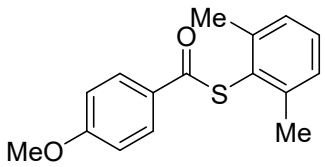

The title compound was isolated as a white solid (79 mg, 30% yield), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.00 (d, *J* = 8.9 Hz, 2H), 7.57 – 7.41 (m, 2H), 7.14 (t, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 188.6, 164.2, 163.6 (d, *J* = 249.8 Hz), 137.3 (d, *J* = 8.6 Hz), 129.8, 129.2, 123.0 (d, *J* = 3.8 Hz), 116.5 (d, *J* = 22.1 Hz), 114.0, 55.6. Characterization is in agreement with previous reports for this compound. [2k]

**4ae** *S*-(4-methoxyphenyl) 4-methoxybenzothioate



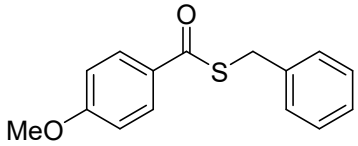

The title compound was isolated as a white solid (89 mg, 32% yield), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.34 – 7.75 (m, 2H), 7.42 (d, *J* = 8.8 Hz, 2H), 7.11 – 6.85 (m, 4H), 3.86 (s, 3H), 3.84 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 189.5, 164.0, 160.7, 136.8, 129.7, 129.5, 118.2, 114.9, 113.9, 55.6, 55.4. Characterization is in agreement with previous reports for this compound. [2l]

**4af** *S*-(2,6-dimethylphenyl) 4-methoxybenzothioate



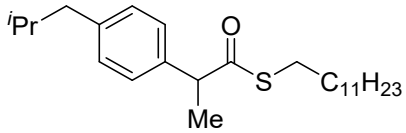

The title compound was isolated as a colorless oil (76 mg, 28% yield), **$^{1}$H NMR (400 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 8.9 Hz, 2H), 7.29 – 7.24 (m, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 2.40 (s, 6H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 187.7, 164.0, 143.4, 129.9, 129.9, 128.4, 128.3, 127.0, 113.9, 55.6, 21.9. Characterization is in agreement with previous reports for this compound. [2m]

**4ag** *S*-benzyl 4-methoxybenzothioate



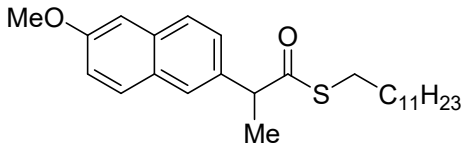

The title compound was isolated as a colorless oil (Gram-scale reaction: 1.453 g, 56% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.95 (d, *J* = 9.0 Hz, 2H), 7.38 (d, *J* = 6.9 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.28 – 7.23 (m, 1H), 6.91 (d, *J* = 8.9 Hz, 2H), 4.30 (s, 2H), 3.85 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 189.9, 163.9, 137.9, 129.8, 129.6, 129.1, 128.7, 127.4, 113.9, 55.6, 33.3. Characterization is in agreement with previous reports for this compound. [2g]

**4ah** *S*-dodecyl 2-(4-isobutylphenyl)propanethioate



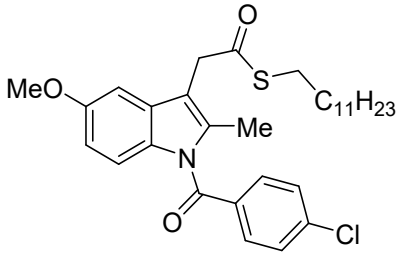

The title compound was isolated as a colorless oil (229 mg, 59% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.22 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H), 3.86 (q, *J* = 7.1 Hz, 1H), 2.93 – 2.70 (m, 2H), 2.46 (d, *J* = 7.2 Hz, 2H), 1.86 (dp, *J* = 13.6, 6.7 Hz, 1H), 1.53 (d, *J* = 7.1 Hz, 5H), 1.35 – 1.19 (m, 18H), 0.87 – 0.92 (m, 9H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 201.7, 140.9, 137.4, 129.5, 127.7, 54.0, 45.2, 32.1, 30.3, 29.8, 29.7, 29.6, 29.6, 29.5, 29.2, 29.2, 29.0, 22.8, 22.5, 18.6, 14.3. **HRMS (ESI)** *m/z:* calculated for $C_{25}H_{42}OS[H]^+$: 391.3030; found: 391.3014.

**4ai** *S*-dodecyl 2-(6-methoxynaphthalen-2-yl)propanethioate




The title compound was isolated as a colorless oil (208 mg, 50% yield), **$^1$H NMR (400 MHz, $CDCl_3$)** δ 7.78 – 7.64 (m, 3H), 7.41 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.19 – 7.07 (m, 2H), 4.02 (q, *J* = 7.1 Hz, 1H), 3.92 (s, 3H), 2.83 (tt, *J* = 13.3, 6.6 Hz, 2H), 1.62 (d, *J* = 7.1 Hz, 3H), 1.52 (p, *J* = 7.5, 7.0 Hz, 2H), 1.30 – 1.24 (m, 18H), 0.89 (t, *J* = 6.9 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 201.6, 157.8, 135.3, 134.0, 129.5, 129.1, 127.3, 126.7, 126.5, 119.1, 105.7, 55.4, 54.3, 32.0, 29.8, 29.7, 29.6, 29.5, 29.5, 29.3, 29.2, 29.0, 22.8, 18.6, 14.3. **HRMS (ESI)** *m/z:* calculated for $C_{26}H_{38}O_2S[H]^+$: 415.2666; found: 415.2657.

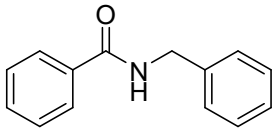
**4aj** *S*-dodecyl 3-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)propanethioate



The title compound was isolated as a yellow oil (225 mg, 40% yield), **$^{1}$H NMR (101 MHz, $CDCl_3$)** δ 7.66 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 6.95 (d, *J* = 2.5 Hz, 1H), 6.89 (d, *J* = 9.0 Hz, 1H), 6.68 (dd, *J* = 9.0, 2.5 Hz, 1H), 3.85 (s, 2H), 3.84 (s, 3H), 2.85 (t, *J* = 7.4 Hz, 2H), 2.39 (s, 3H), 1.54 (p, *J* = 7.5, 7.0 Hz, 2H), 1.32 – 1.22 (s, 18H), 0.88 (t, *J* = 6.8 Hz, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 197.4, 168.4, 156.2, 139.4, 136.6, 133.9, 131.3, 130.9, 130.7, 129.2, 115.1, 112.5, 111.9, 101.3, 55.8, 39.5, 32.0, 29.7, 29.7, 29.7, 29.6, 29.5, 29.5, 29.4, 29.2, 29.0, 22.8, 14.2, 13.6. **HRMS (ESI)** *m/z:* calculated for $C_{31}H_4OClNO_3S[Na]^+$: 654.2310; found: 654.2304.

# 4.3 Characterization data of amide.

**5** *N*-benzylbenzamide



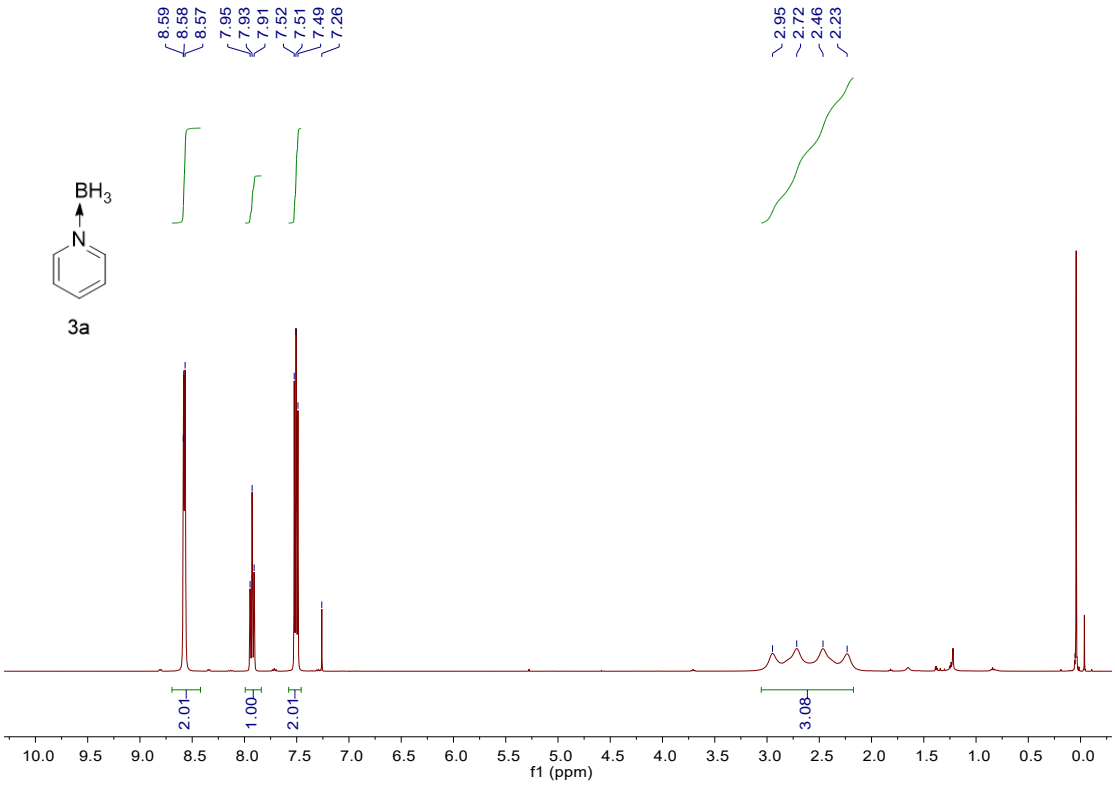

The title compound was isolated as a white solid (49 mg, 77% yield), **$^{1}$H NMR (101 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 7.2 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.22 (m, 5H), 6.79 (s, 1H), 4.58 (d, *J* = 5.7 Hz, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 167.6, 138.3, 134.4, 131.6, 128.8, 128.6, 127.9, 127.6, 127.1, 44.1. Characterization is in agreement with previous reports for this compound. [2n]

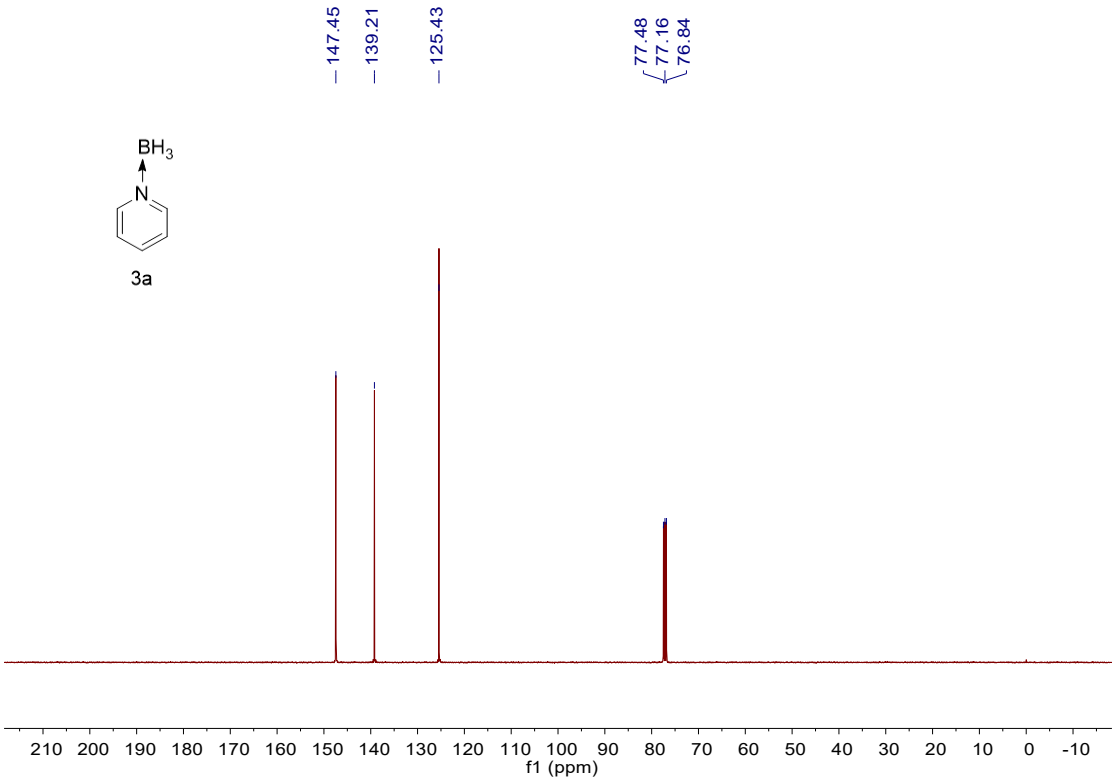
# 5. References

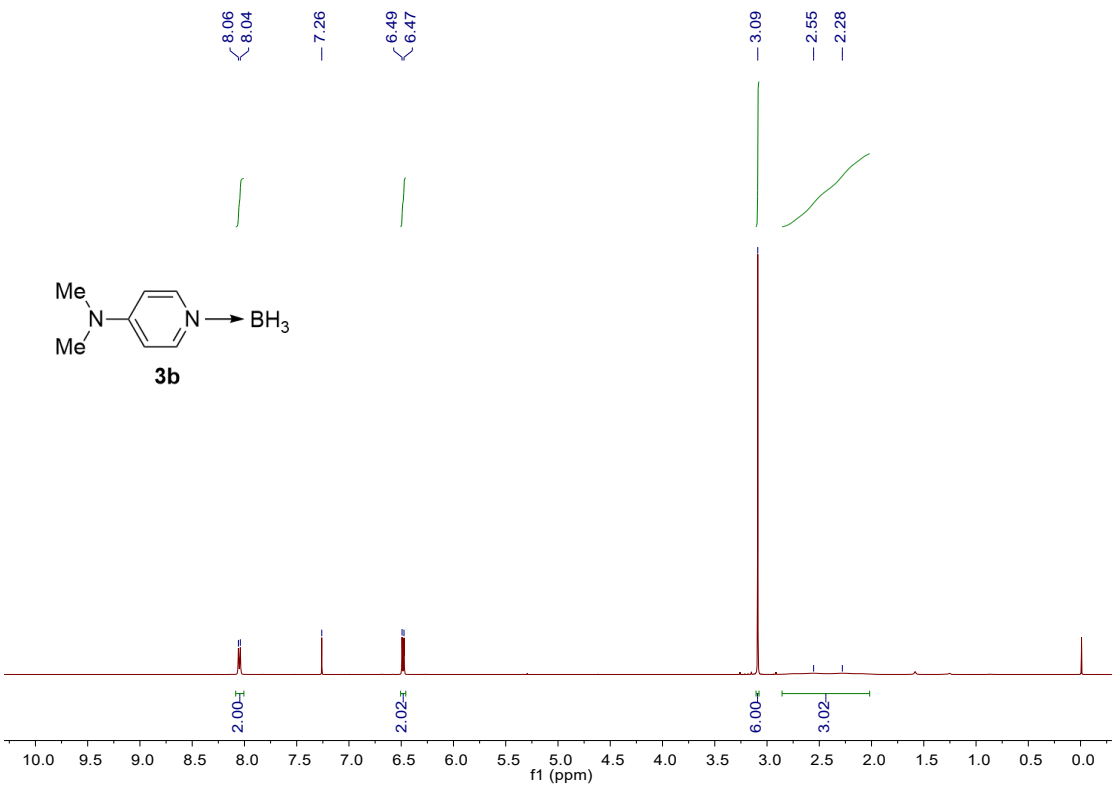

[1] a): P. V. Ramachandran, A. S. Kulkarni, Y. Zhao and J. G. Mei, *Chem. Commun.,* **2016**, *52*, 11885. b): E. Jeong, J. Heo, S. Park, and S. Chang, *Chem.- Eur. J.*, **2019**, *25*, 6320. c): M.-C. Wang, J.-Y. F, J.-F. Zhou, W.-X. Zhang, and B.-J. Li. *Chemistryselect*, **2024**, *9*, e202400325.

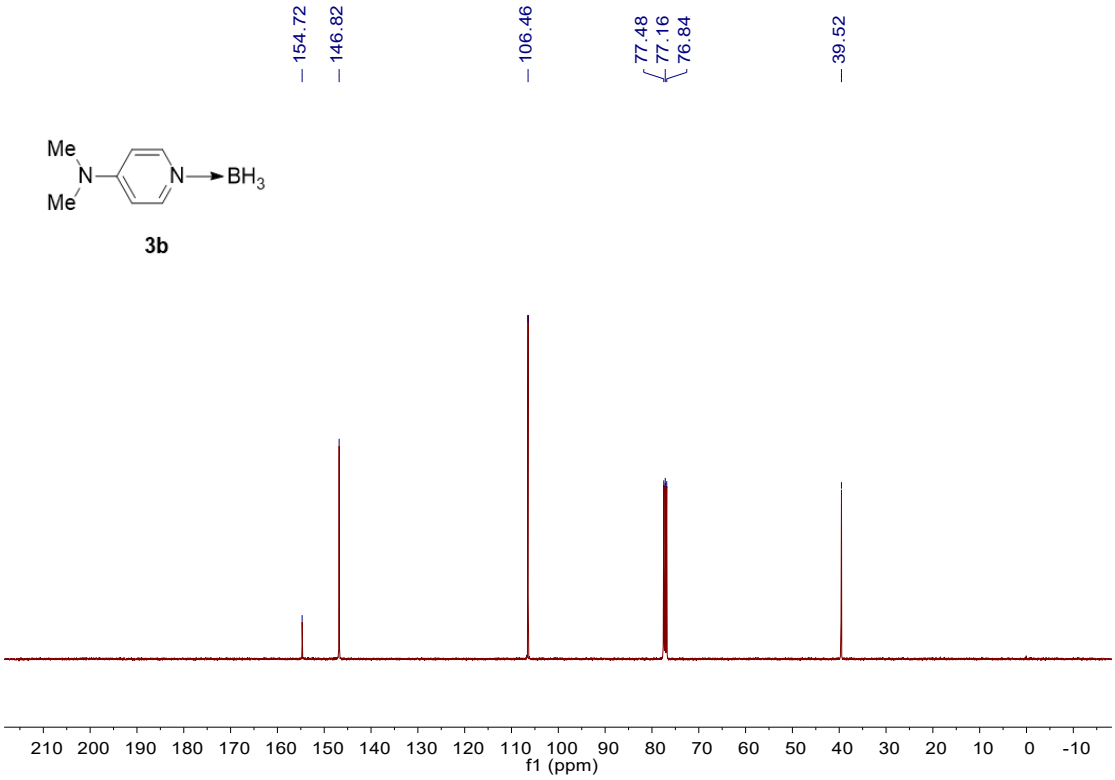
[2] a): M. Xuan, C. Lu, M. Liu, and B.-L. Lin, *J. Org. Chem.*, **2019**, *84*, 7694. b): Y.-T. Huang, S.-Y. Lu, C.-L. Yi, and C.-F. Lee, *J. Org. Chem*., **2014**, *79*, 4561. c): Y.-J. Lin, Y.-P. Wu, M. Thul, M.-W. Hung, S.-H. Chou, W.-T. Chen, W. Lin, M. Lin, D. M. Reddy, H.-R. Wu, W.-Y. Ho, and S.-Y. Luo, *Molecules,* **2020**, *25*, 352. d): Y. Hu, J. Liu, Z. Lü, X. Luo, H. Zhang, Y. Lan, A. Lei, *J. Am. Chem. Soc.,* **2010**, *132*, 3153. e): D. Kato, T. Murase, J. Talode, H. Nagae, H. Tsurugi, M. Seki, K. Mashima, *Chem.- Eur. J.*, **2022**, *28*, e202200474. f): A. Temperini, D. Annesi, L. Testaferri, M. Tiecco, *Tetrahedron Lett*., **2010**, *51*, 5368. g): P. Singh, and R. K. Peddinti, *Tetrahedron lett*., **2017**, *58*, 1875. h): X. Qi, Z.-P. Bao, X.-T. Yao, and X.-F. Wu, *Org. Lett.*, **2020**, *22*, 6671. i): Y. Shi, X. Liu, H. Cao, F. Bie, Y. Han, P. Yan, R. Szostak, M. Szostak, and C. Liu, *Org. Biomol. Chem*., **2021**, *19*, 2991. j): M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, M. Babaghanbari, M. Zarea, L. Shariati, and S. A. Taghavi, *J. Iran. Chem. Soc.*, **2009**, *6*, 523. k): X. Qi, Z.-P. Bao, and X.-F. Wu, *Org. Chem. Front*., **2020**, *7*, 885. l): S. Xie, L. Su, M. Mo, W. Zhou, Y. Zhou, and J. Dong, *J. Org. Chem*., **2021**, *86*, 739. m): M. N. Burhardt, R. H. Taaning, and T. Skrydstrup, *Org. Lett.*, **2013**, 15, 948. n): P. V. Ramachandran, and H. J. Hamann, *Org. Lett.*, **2021**, *23*, 2938. o): M. Asadi, S. Bonke, A. Polyzos, and D. W. Lupton, *ACS Catal*., **2014**, *4*, 2070. p): T.-J. Chai, X.-S. Chiou, N.-X. Lin, Y.-T. Kuo, and C.-K. Lin, *Org. Biomol. Chem.*, **2023**, *21*, 7541. q): Z. Zhu, Y. Gong, W. Tong, W. Xue, and H. Gong, *Org. Lett*., **2021**, *23*, 2158. r): S. Naik, V. Kavala, R. Gopinath, and B. K. Patel, *ARKIVOC*, **2006**, *2006*, 21.

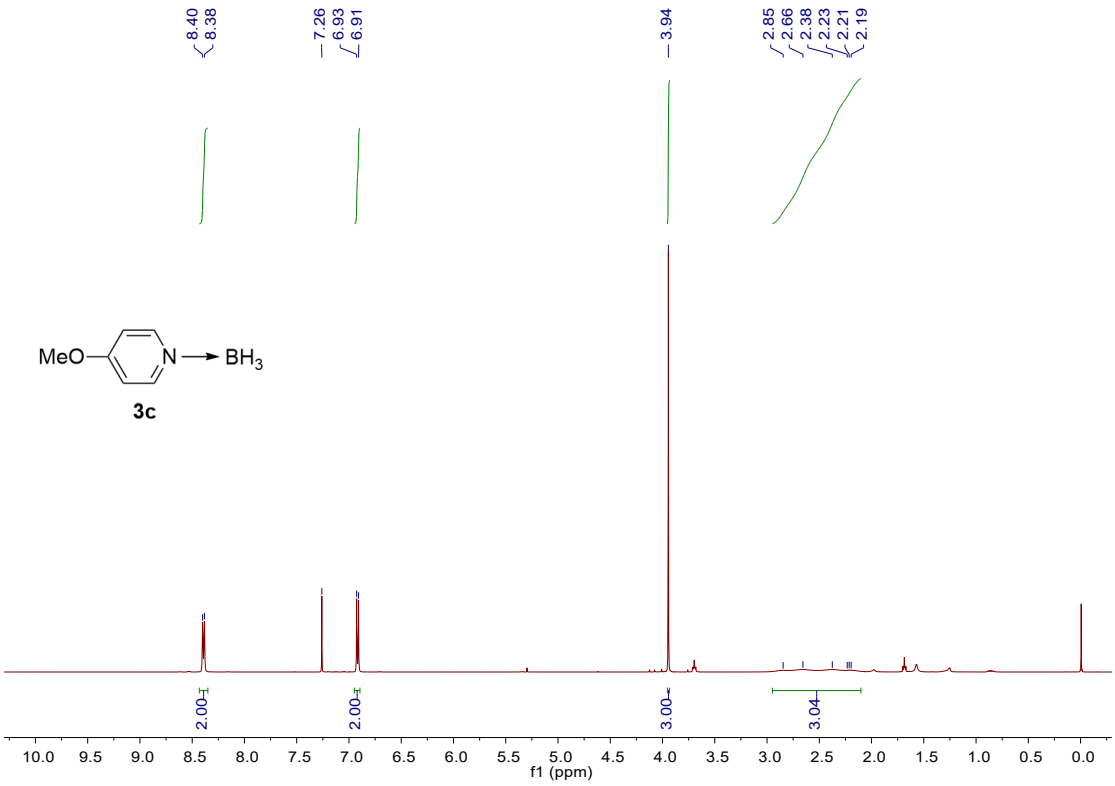
# 6. NMR spectra




8.06
8.04
7.26
6.49
6.47
3.09
2.55
2.28
Me
N
Me
N
BH3
3b
2.00
2.02
6.00
3.02
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)


154.72
146.82
106.46
77.48
77.16
76.84
39.52
Me
N
Me
N
BH3
3b
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)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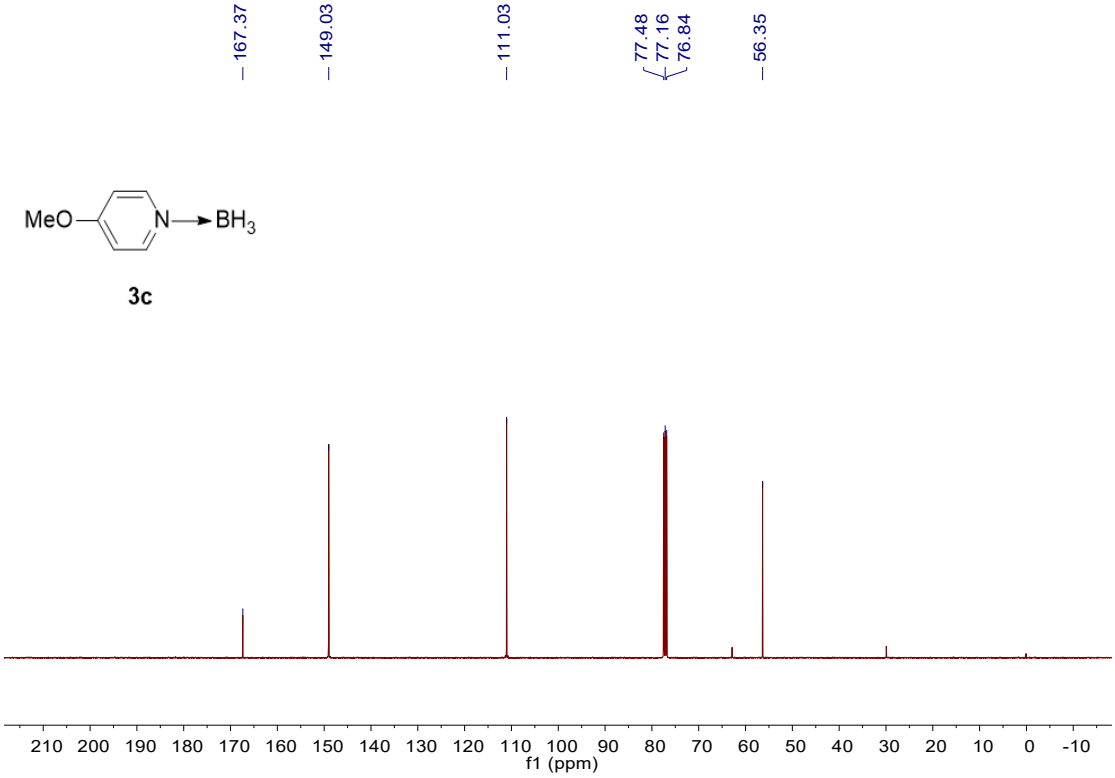
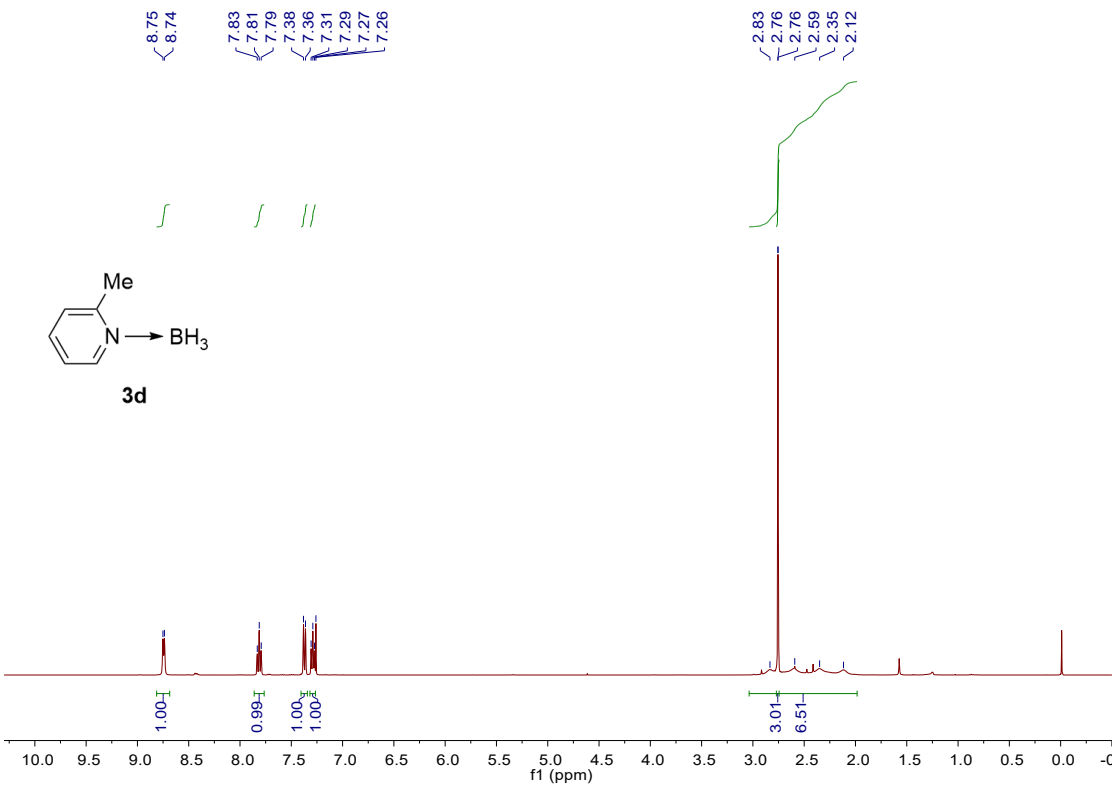
8.38
7.26
6.93
6.91
3.94
2.85
2.66
2.38
2.23
2.21
2.19
MeO
N
BH3
2.00
2.00
3.00
3.04
f1 (ppm)

**3c**


167.37
149.03
111.03
77.48
77.16
76.84
56.35
MeO
N
BH3
f1 (ppm)

**3c**


8.75
8.74
7.83
7.81
7.79
7.38
7.36
7.31
7.29
7.27
7.26
2.83
2.76
2.76
2.59
2.35
2.12
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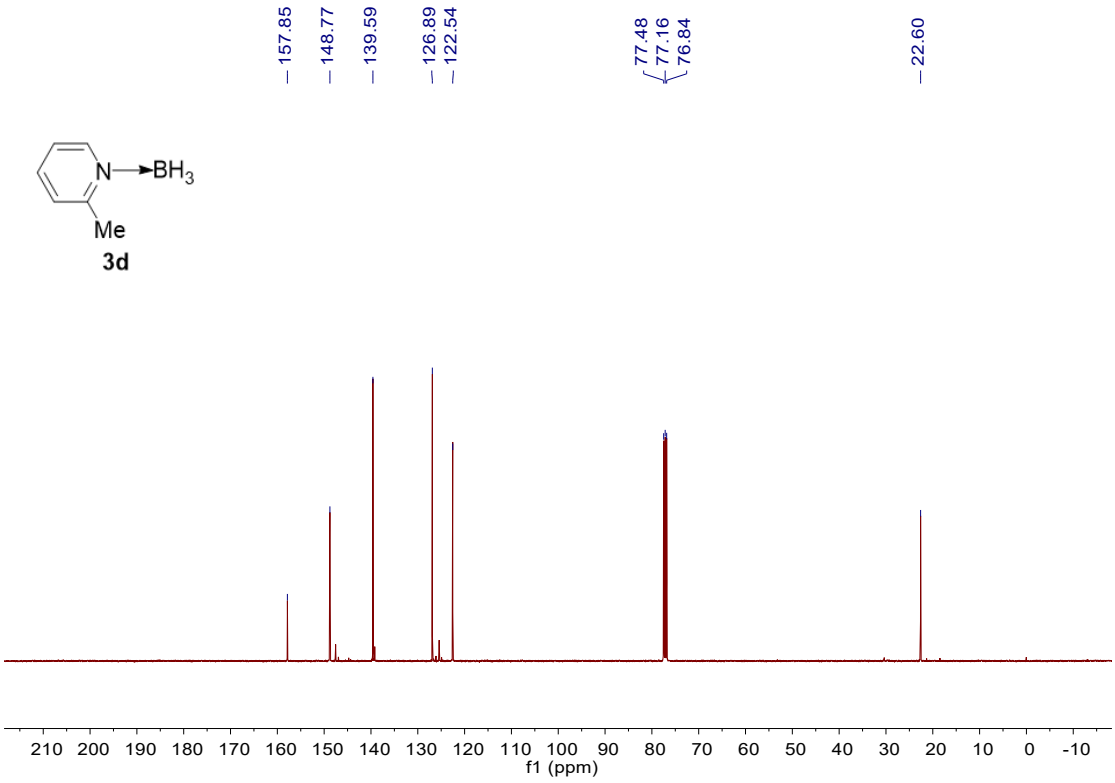
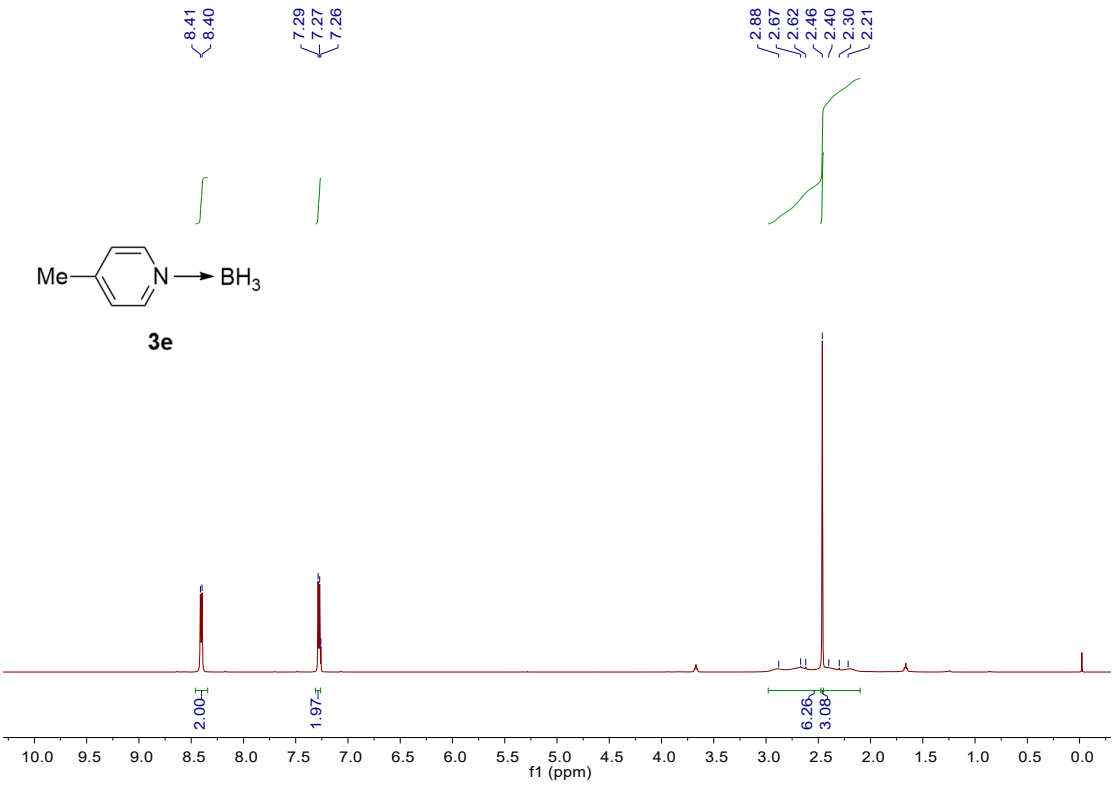
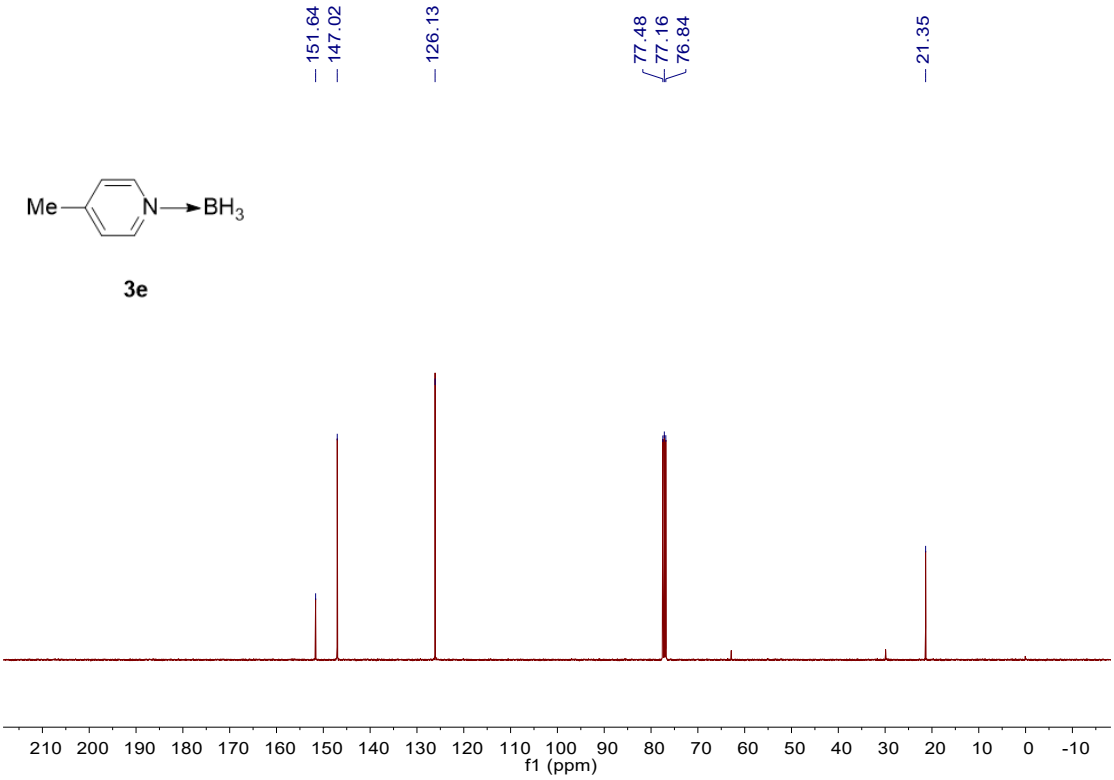
N
BH3
3d
1.00
0.99
1.00
1.00
3.01
6.51
f1 (ppm)

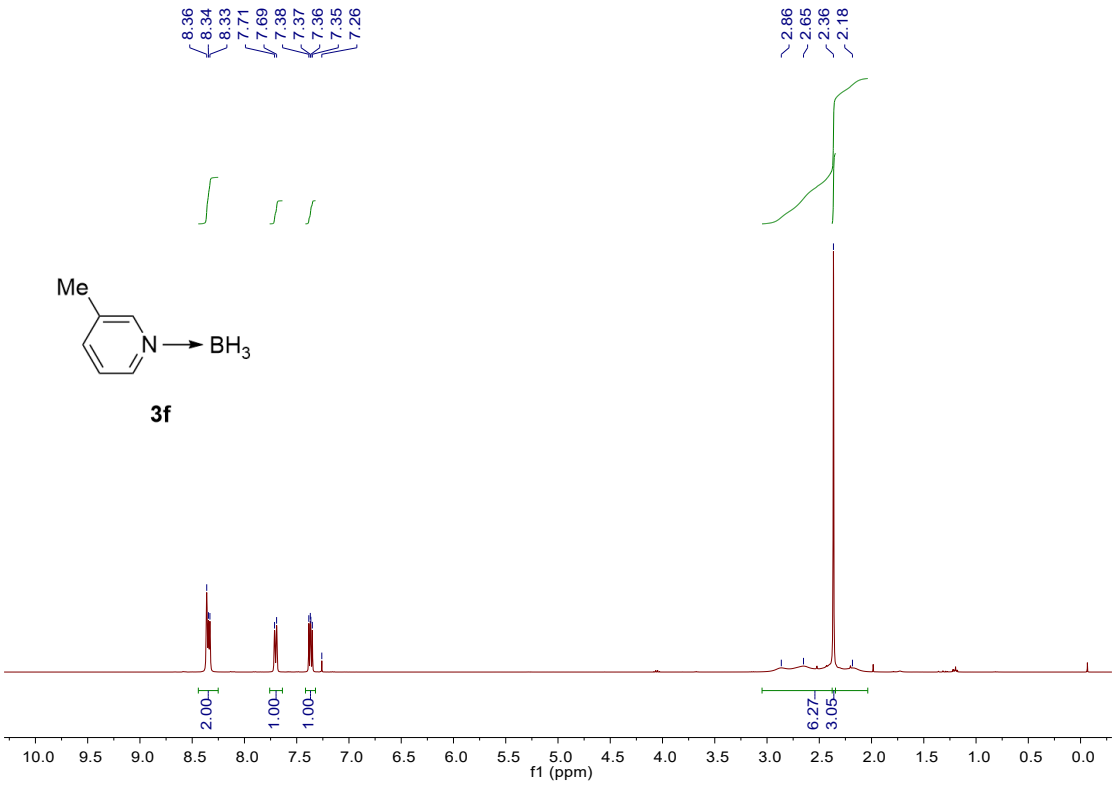

157.85
148.77
139.59
126.89
122.54
77.48
77.16
76.84
22.60
N
BH3
Me
3d
f1 (ppm)

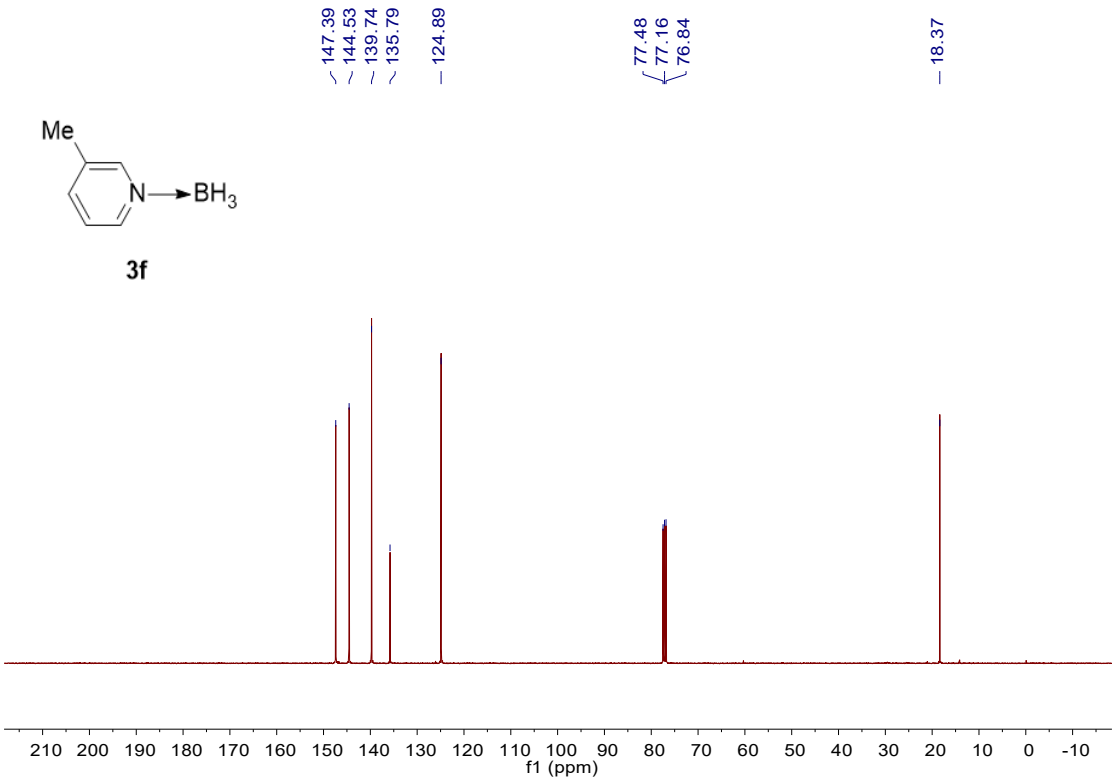

8.41
8.40
7.29
7.27
7.26
2.88
2.67
2.62
2.46
2.40
2.30
2.21
Me
N
BH3
2.00
1.97
6.26
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

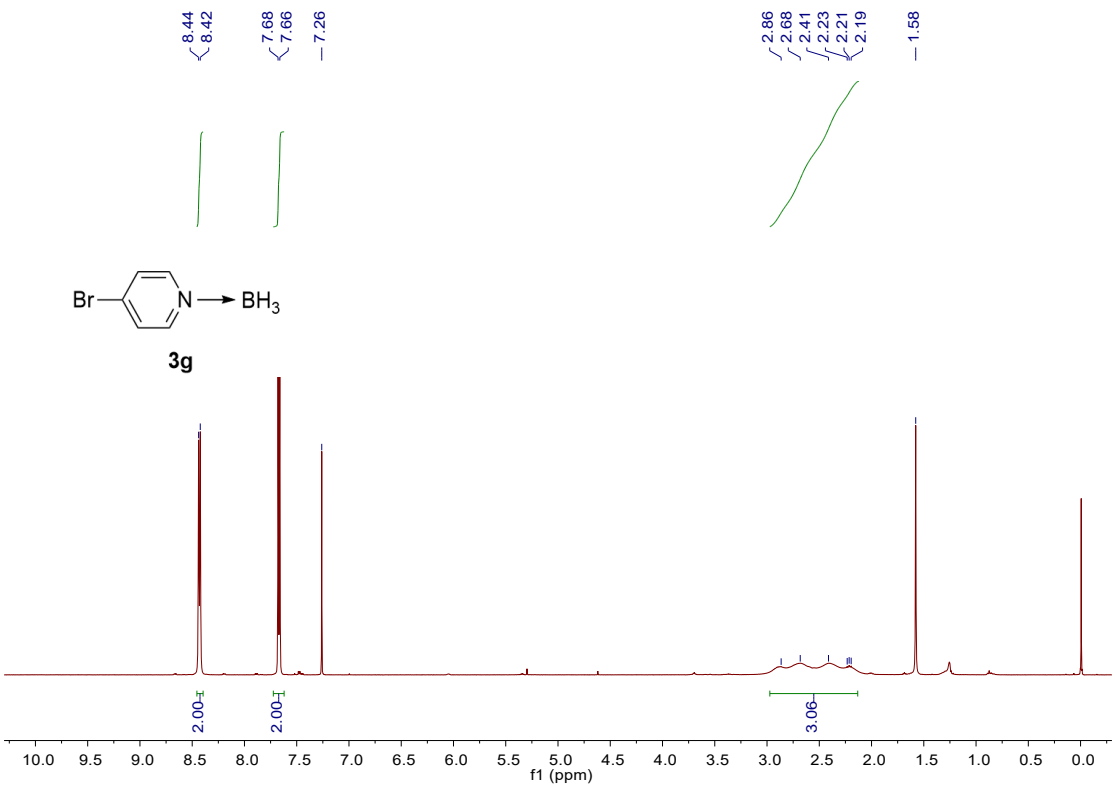
**3e**

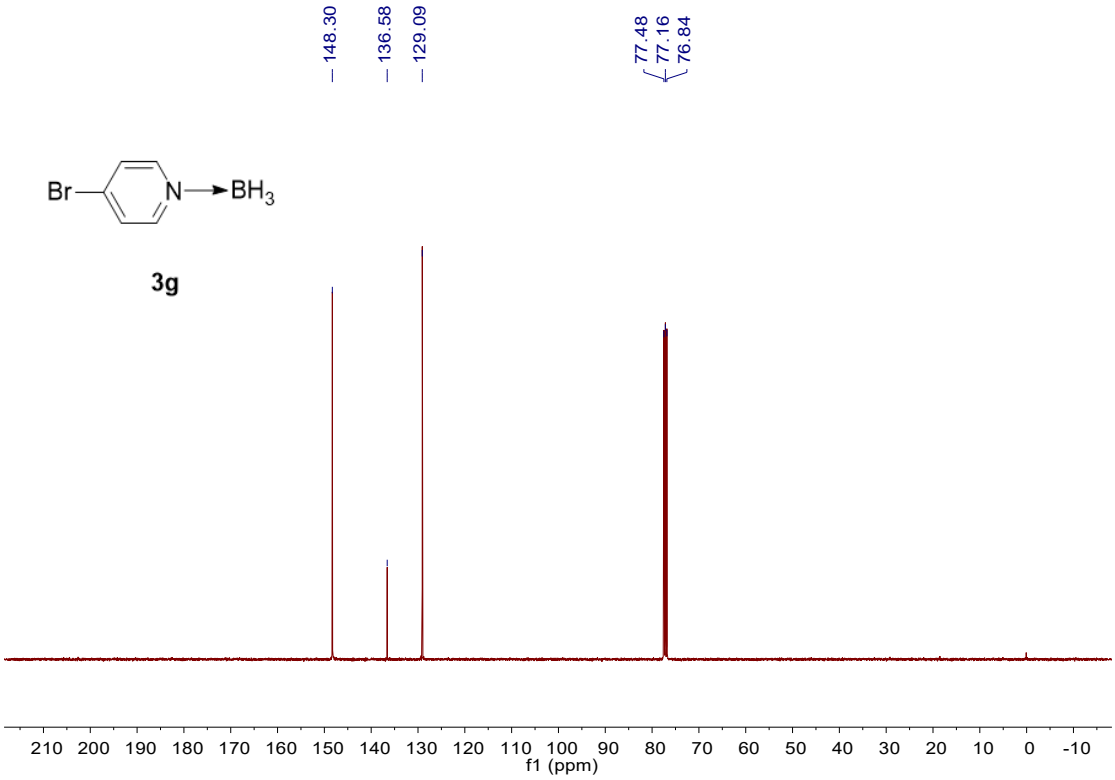

151.64
147.02
126.13
77.48
77.16
76.84
21.35
Me
N
BH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

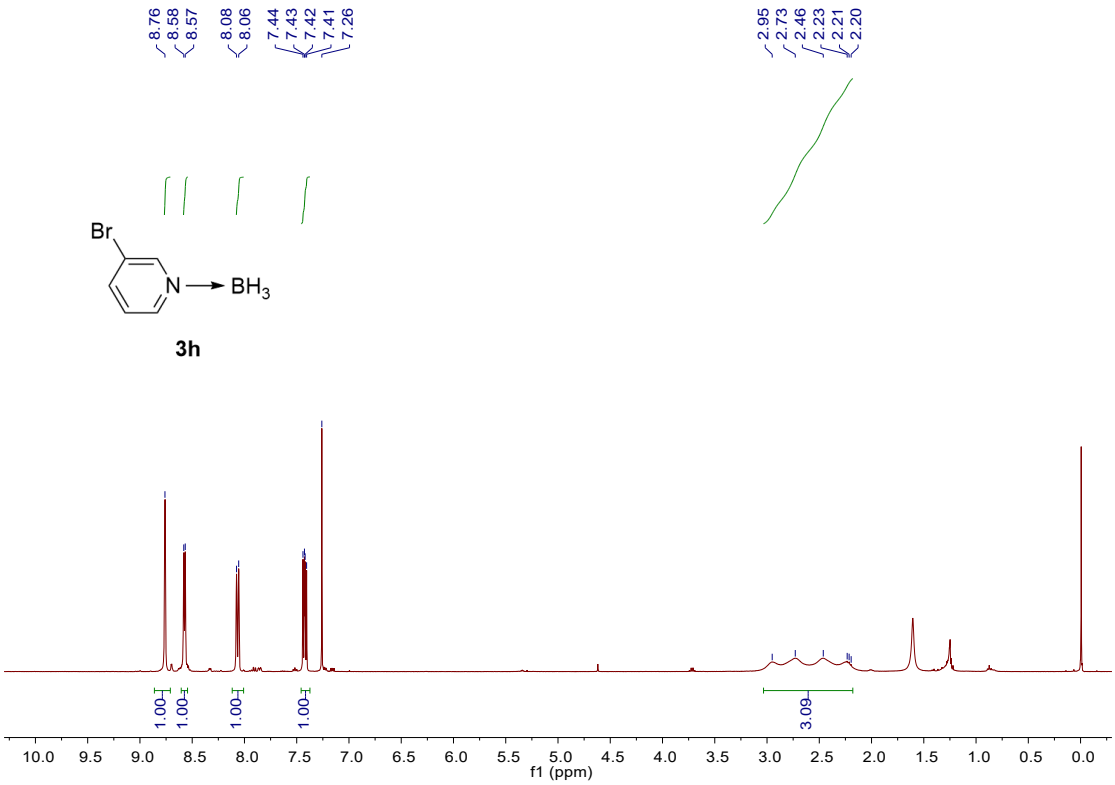
**3e**

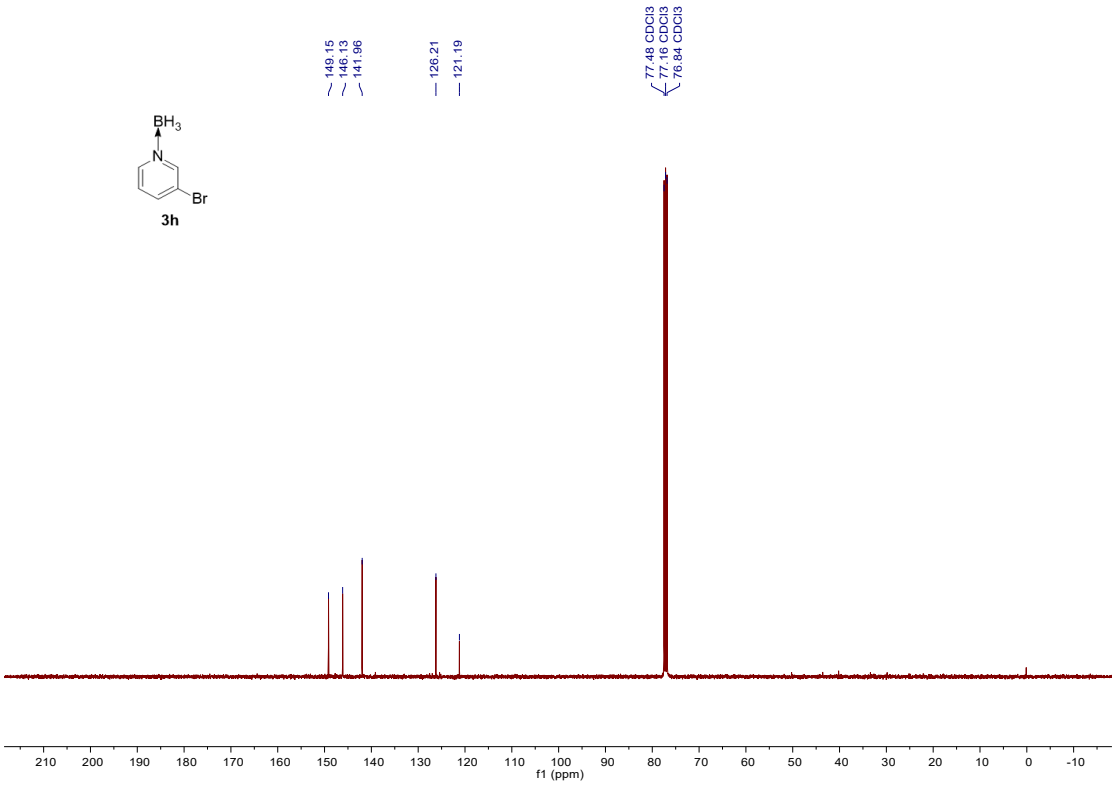

8.36
8.34
8.33
7.71
7.69
7.38
7.37
7.36
7.35
7.26
2.86
2.65
2.36
2.18
Me
N
BH3
3f
2.00
1.00
1.00
6.27
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

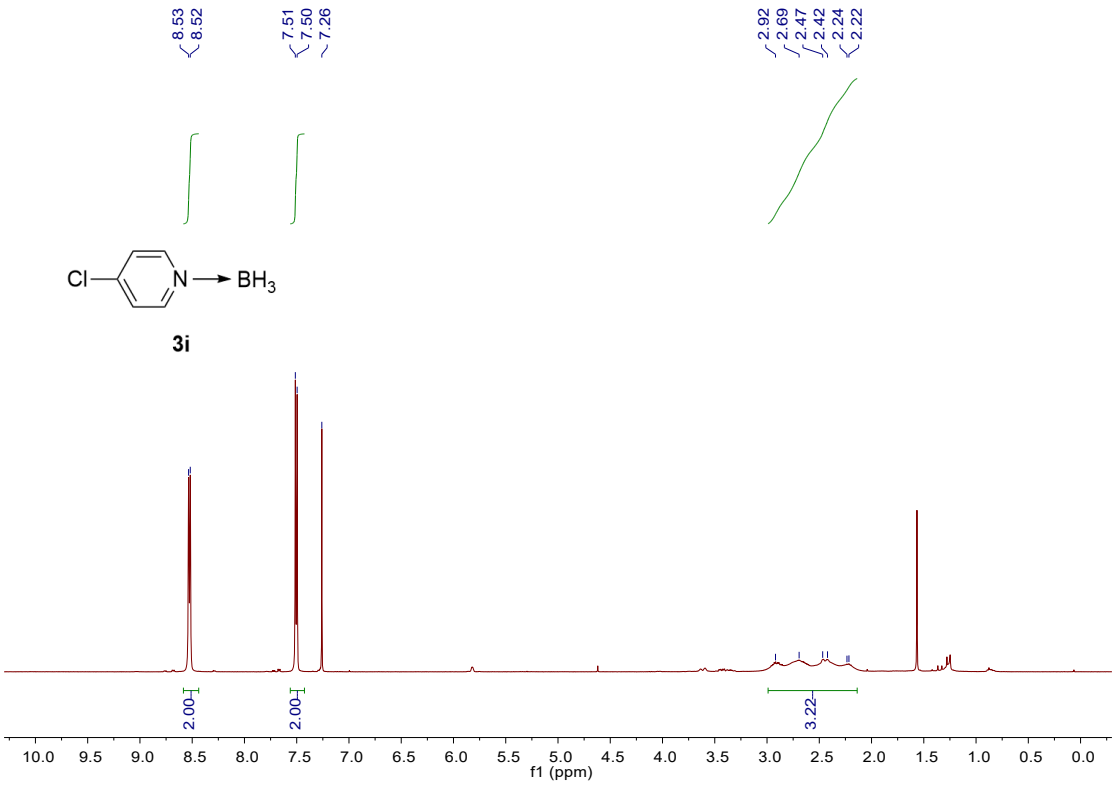

147.39
144.53
139.74
135.79
124.89
77.48
77.16
76.84
18.37
Me
N
BH3
3f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.44
8.42
7.68
7.66
7.26
2.86
2.68
2.41
2.23
2.21
2.19
1.58
Br
N
BH3
3g
2.00
2.00
3.06
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)

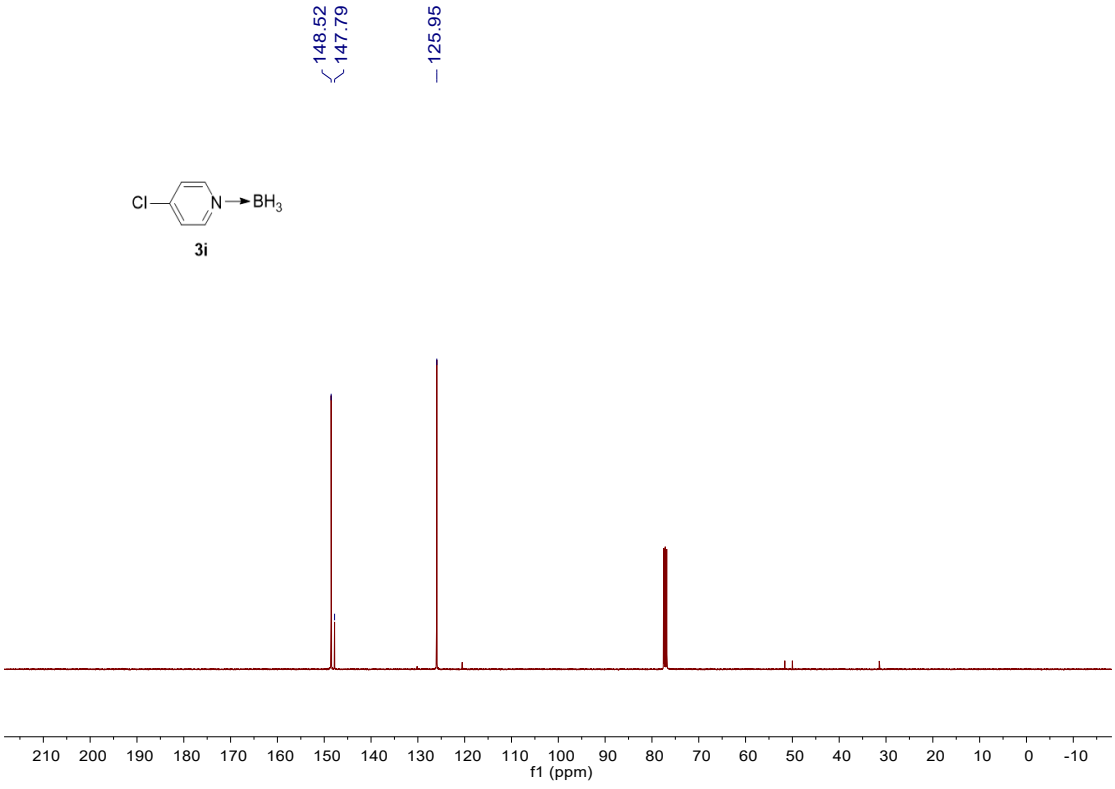

148.30
136.58
129.09
77.48
77.16
76.84
Br
N
BH3
3g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.76
8.58
8.57
8.08
8.06
7.44
7.43
7.42
7.41
7.26
2.95
2.73
2.46
2.23
2.21
2.20
Br
N
BH3
3h
1.00
1.00
1.00
1.00
3.09
f1 (ppm)

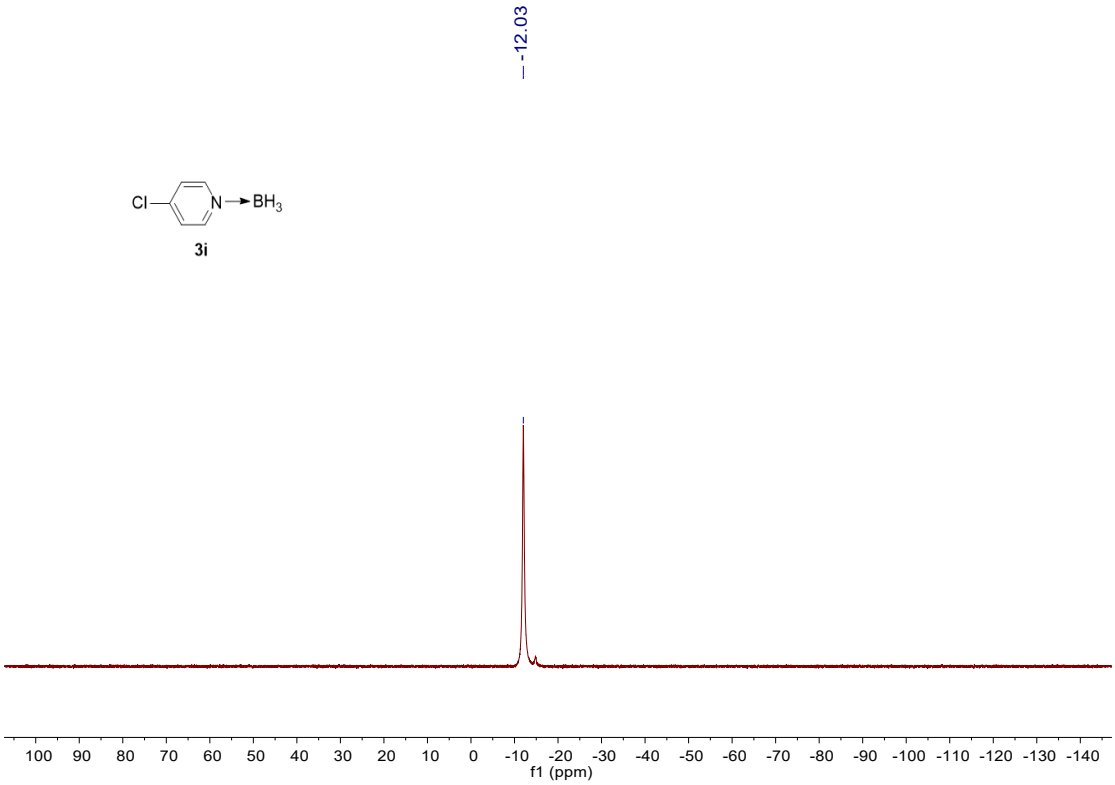

149.15
146.13
141.96
126.21
121.19
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
BH3
N
Br
3h
f1 (ppm)

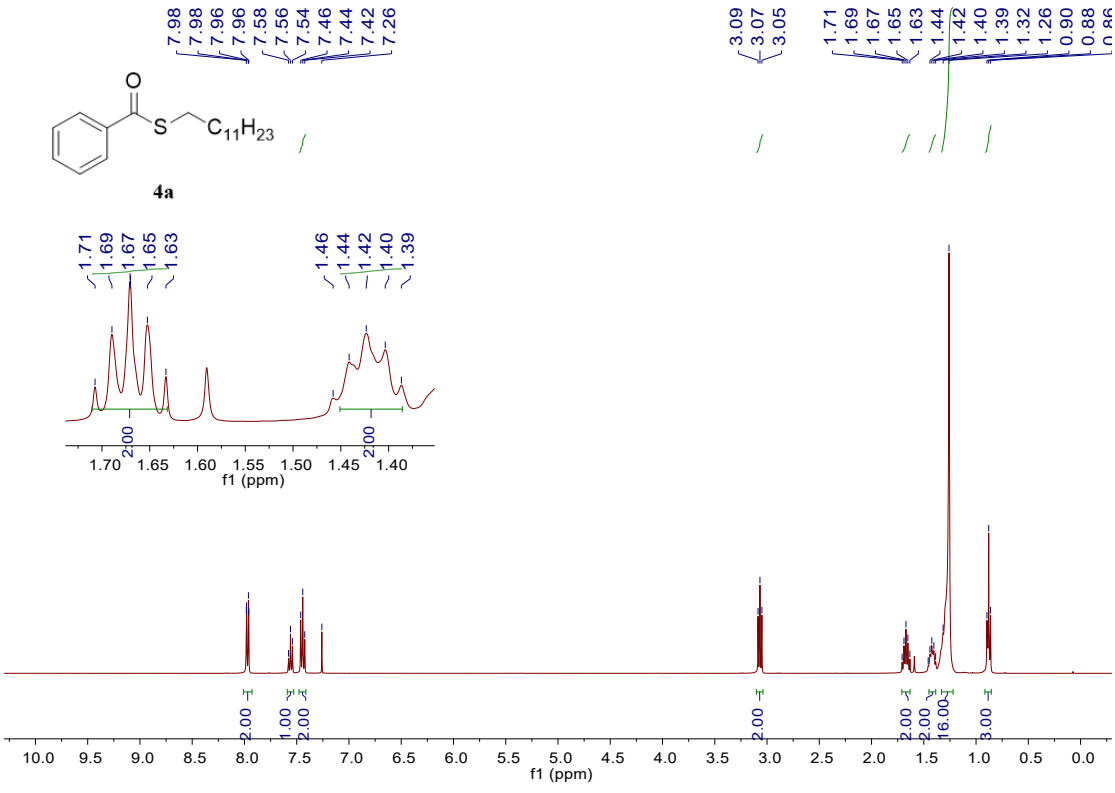

8.53
8.52
7.51
7.50
7.26
2.92
2.69
2.47
2.42
2.24
2.22
Cl
N
BH3
2.00
2.00
3.22
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

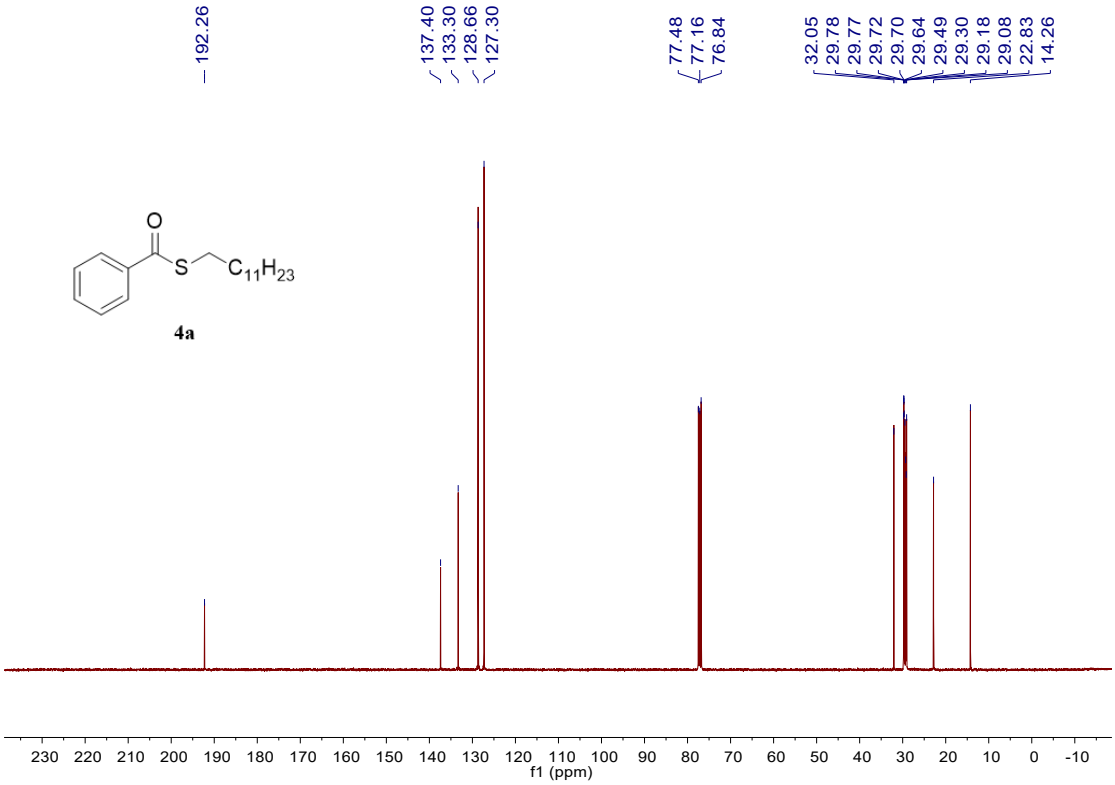
**3i**

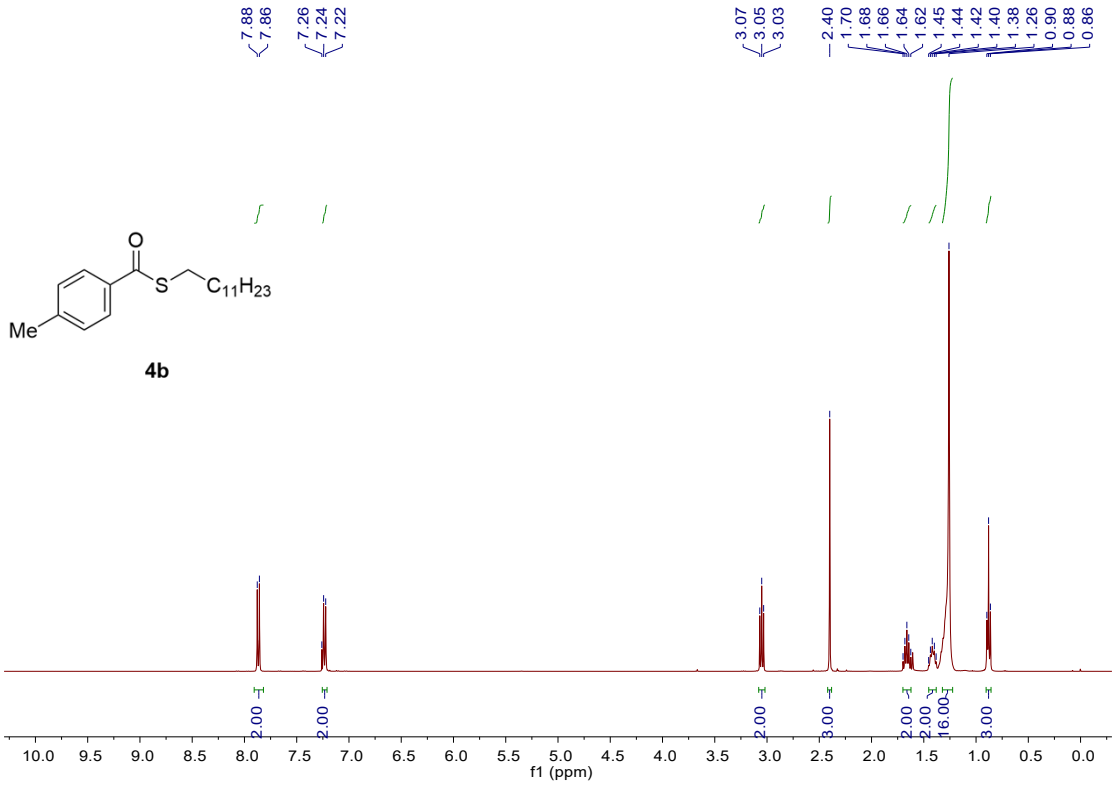

148.52
147.79
125.95
Cl
N
BH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

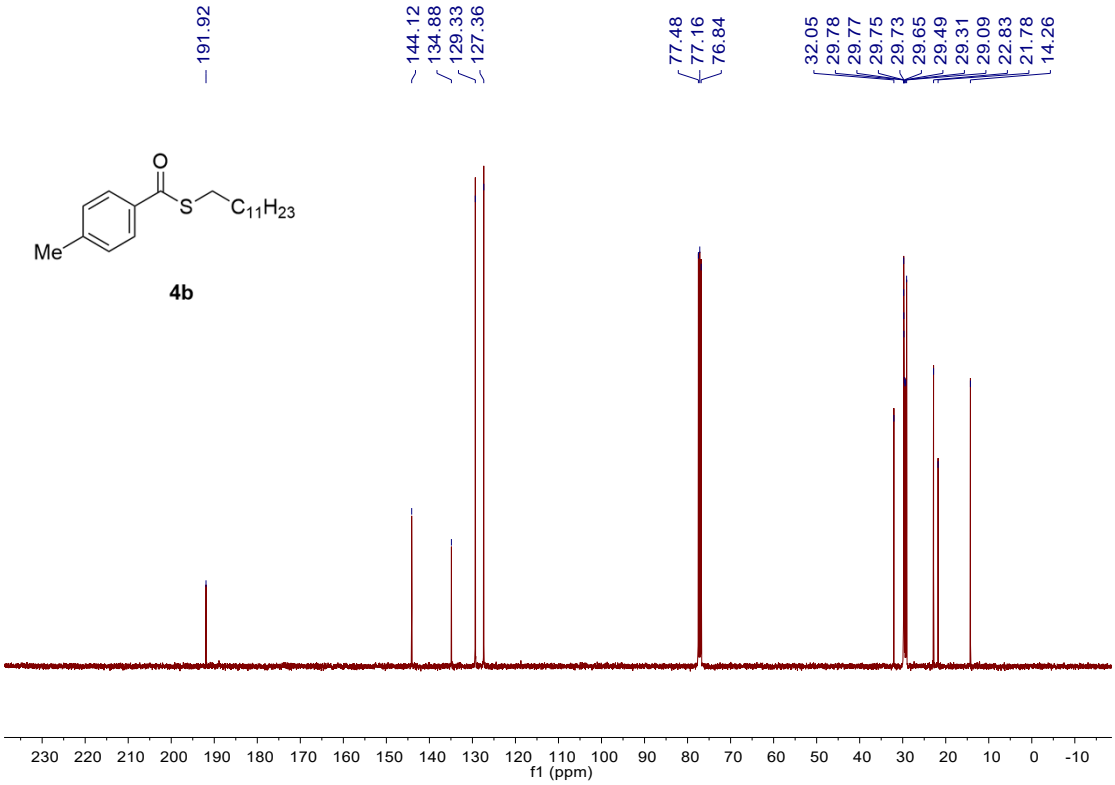
**3i**

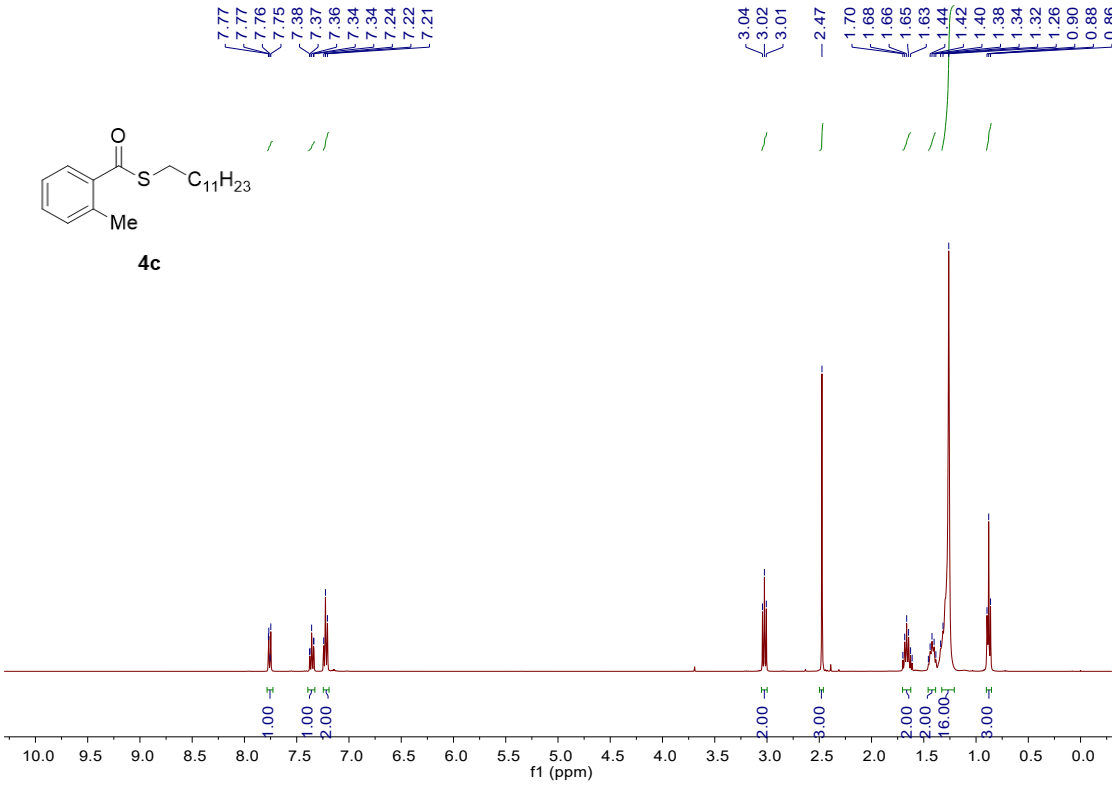

-12.03
Cl
N
BH3
3i
100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140
f1 (ppm)

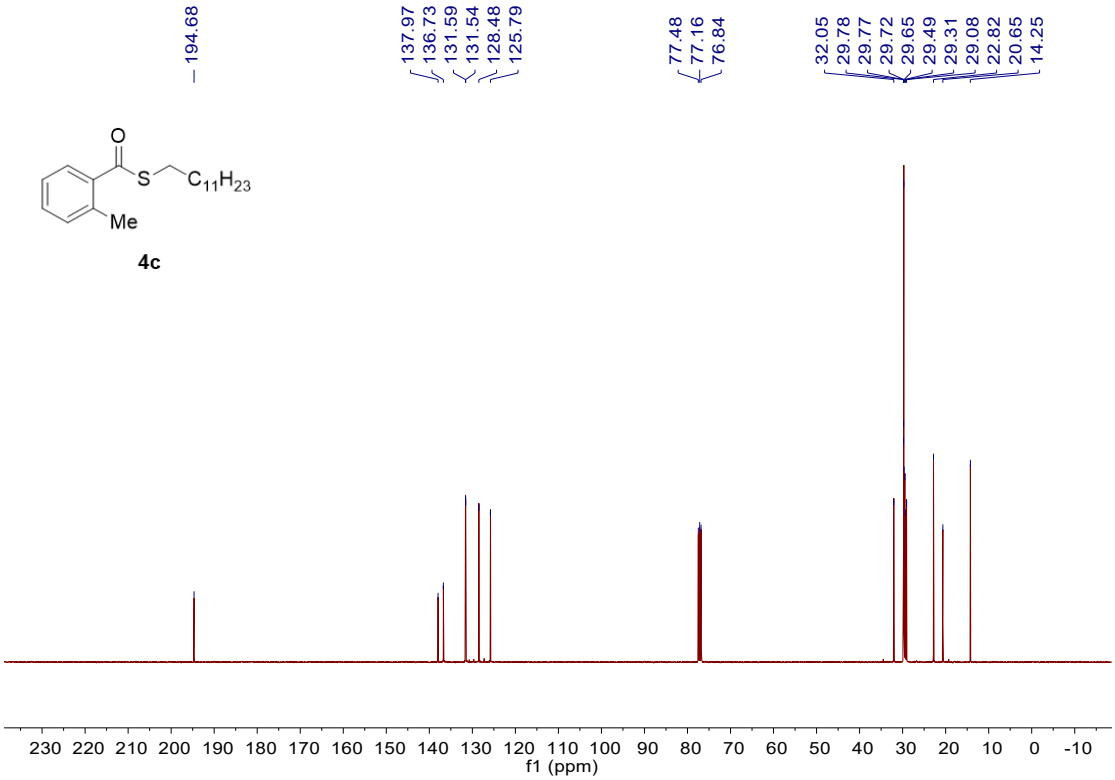

7.98 7.98 7.96 7.96 7.58 7.56 7.54 7.46 7.44 7.42 7.26
3.09 3.07 3.05
1.71 1.69 1.67 1.65 1.63 1.44 1.42 1.40 1.39 1.32 1.26 0.90 0.88
O
S
C11H23
4a
1.71 1.69 1.67 1.65 1.63
1.46 1.44 1.42 1.40 1.39
2.00 2.00
1.70 1.65 1.60 1.55 1.50 1.45 1.40
f1 (ppm)
2.00 1.00 2.00 2.00 2.00 2.00 16.00 3.00
10.0 9.5 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)


192.26
137.40
133.30
128.66
127.30
77.48
77.16
76.84
32.05
29.78
29.77
29.72
29.70
29.64
29.49
29.30
29.18
29.08
22.83
14.26
O
S
C11H23
4a
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

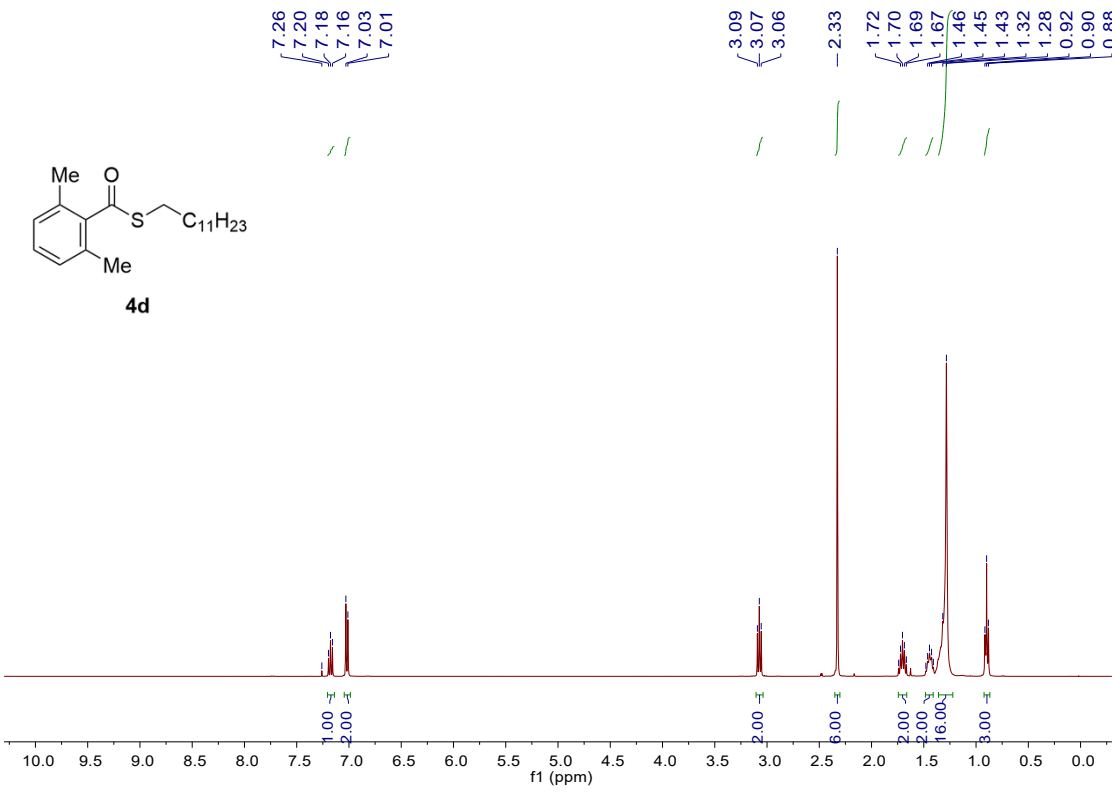

7.88
7.86
7.26
7.24
7.22
3.07
3.05
3.03
2.40
1.70
1.68
1.66
1.64
1.62
1.45
1.44
1.42
1.40
1.38
1.26
0.90
0.88
0.86
O
S
C11H23
Me
4b
2.00
2.00
2.00
3.00
2.00
2.00
16.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


191.92
144.12
134.88
129.33
127.36
77.48
77.16
76.84
32.05
29.78
29.77
29.75
29.73
29.65
29.49
29.31
29.09
22.83
21.78
14.26
O
S
C11H23
Me
4b
f1 (ppm)

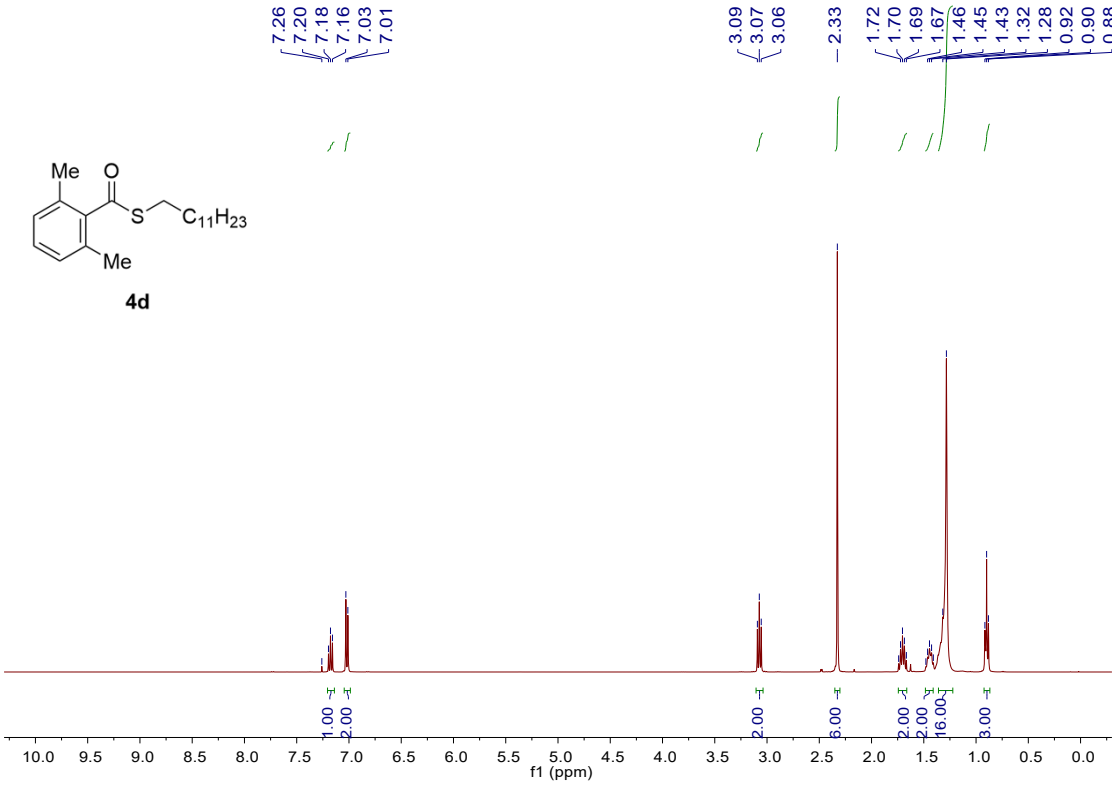

7.77
7.77
7.76
7.75
7.38
7.37
7.36
7.34
7.34
7.24
7.22
7.21
3.04
3.02
3.01
2.47
1.70
1.68
1.66
1.65
1.63
1.44
1.42
1.40
1.38
1.34
1.32
1.26
0.90
0.88
O
S
C11H23
Me
4c
1.00
1.00
2.00
2.00
3.00
2.00
2.00
16.00
3.00
f1 (ppm)


194.68
137.97
136.73
131.59
131.54
128.48
125.79
77.48
77.16
76.84
32.05
29.78
29.77
29.72
29.65
29.49
29.31
29.08
22.82
20.65
14.25
O
S
C11H23
Me
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

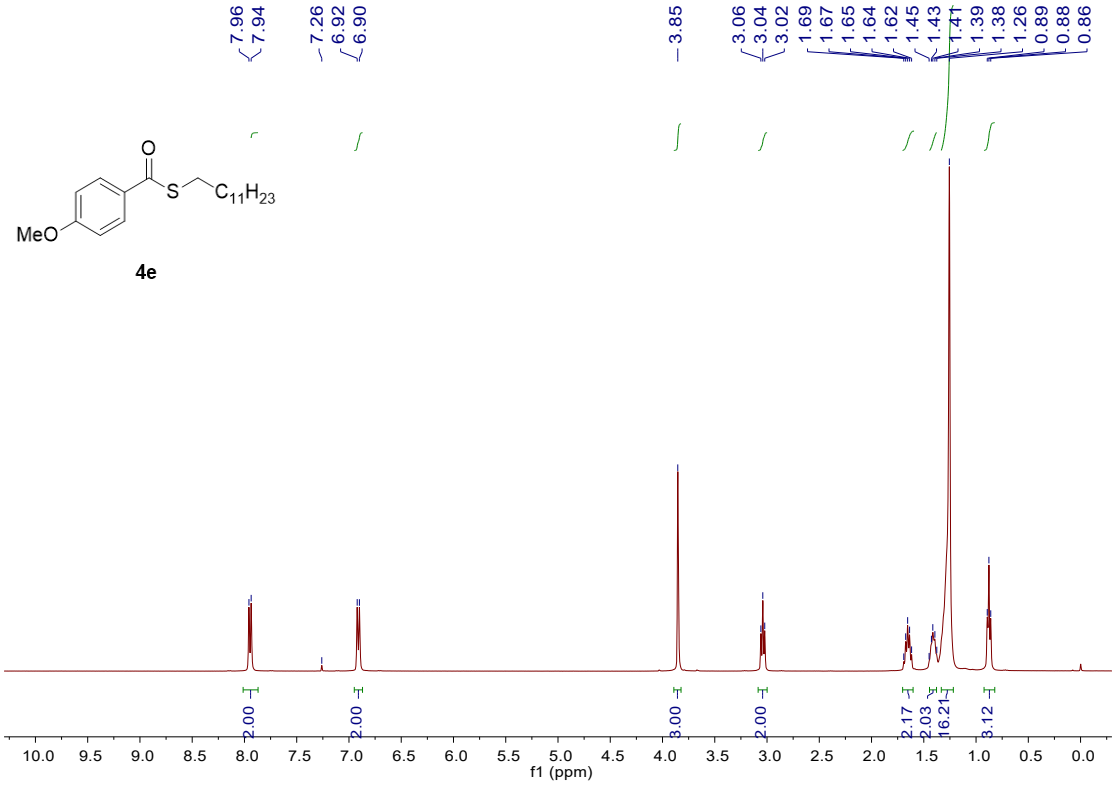
**4c**


7.26
7.20
7.18
7.16
7.03
7.01
3.09
3.07
3.06
2.33
1.72
1.70
1.69
1.67
1.46
1.45
1.43
1.32
1.28
0.92
0.90
Me
O
S
C11H23
Me
1.00
2.00
2.00
6.00
2.00
2.00
16.00
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)

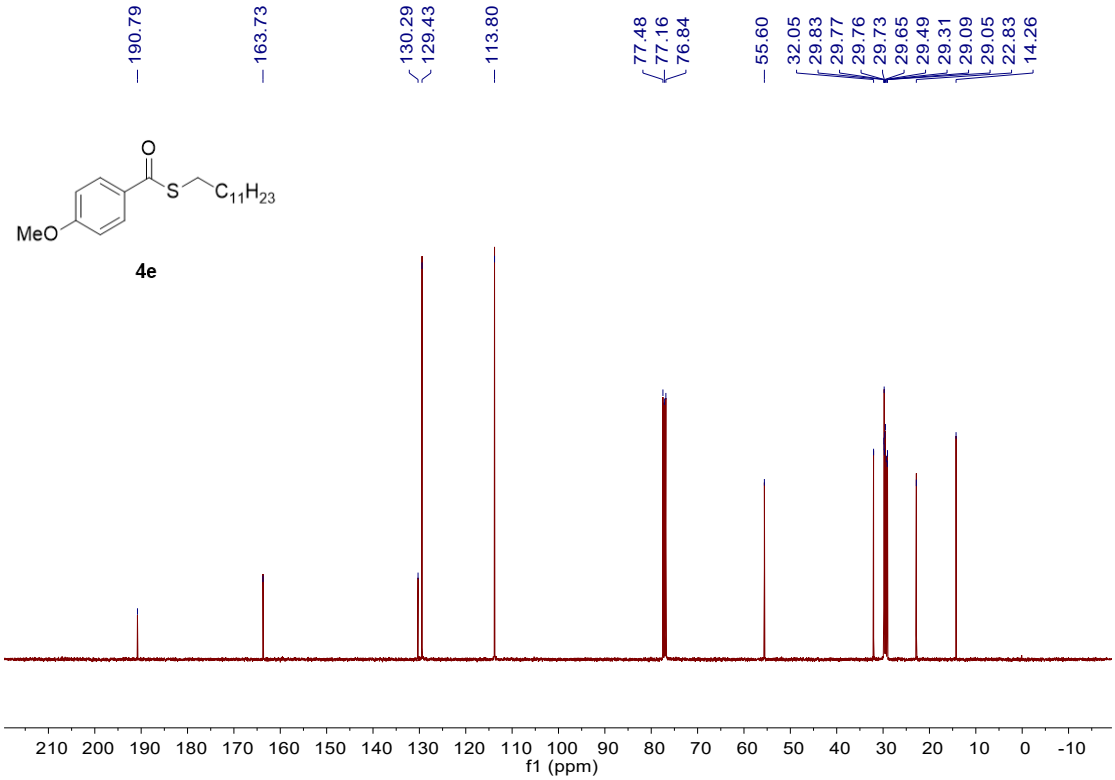
**4d**

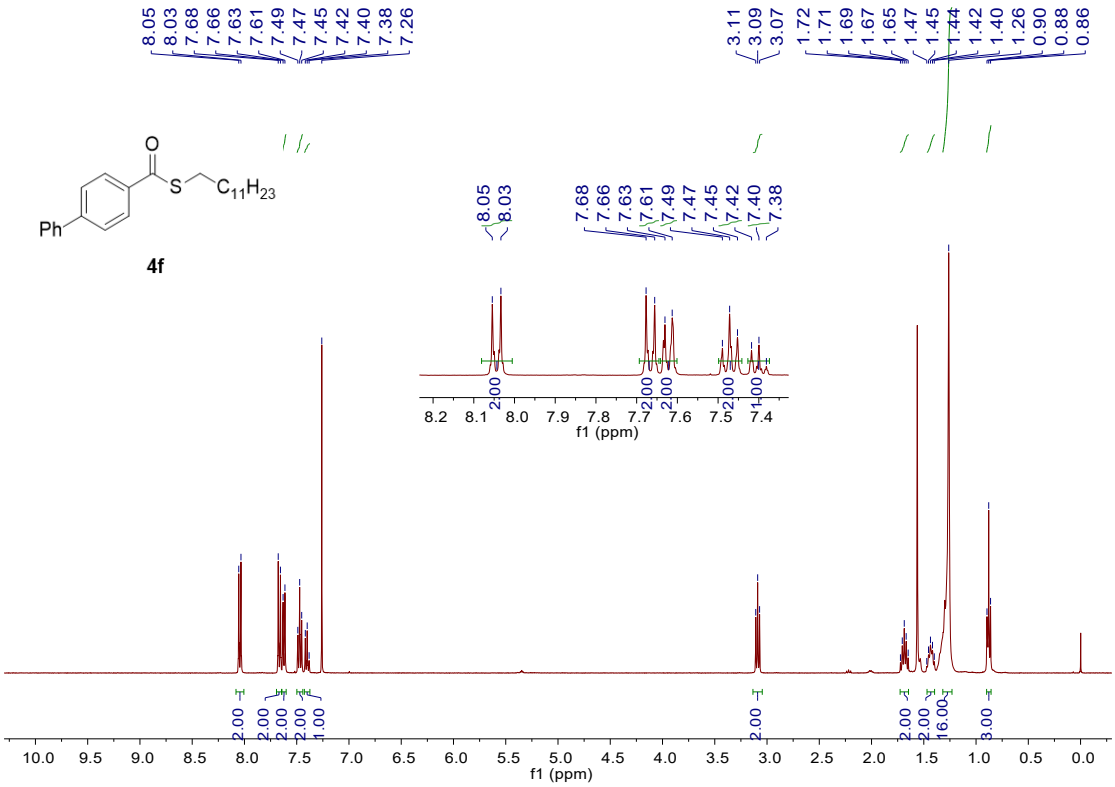

7.26
7.20
7.18
7.16
7.03
7.01
3.09
3.07
3.06
2.33
1.72
1.70
1.69
1.67
1.46
1.45
1.43
1.32
1.28
0.92
0.90
Me
O
S
C11H23
Me
1.00
2.00
2.00
6.00
2.00
2.00
16.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

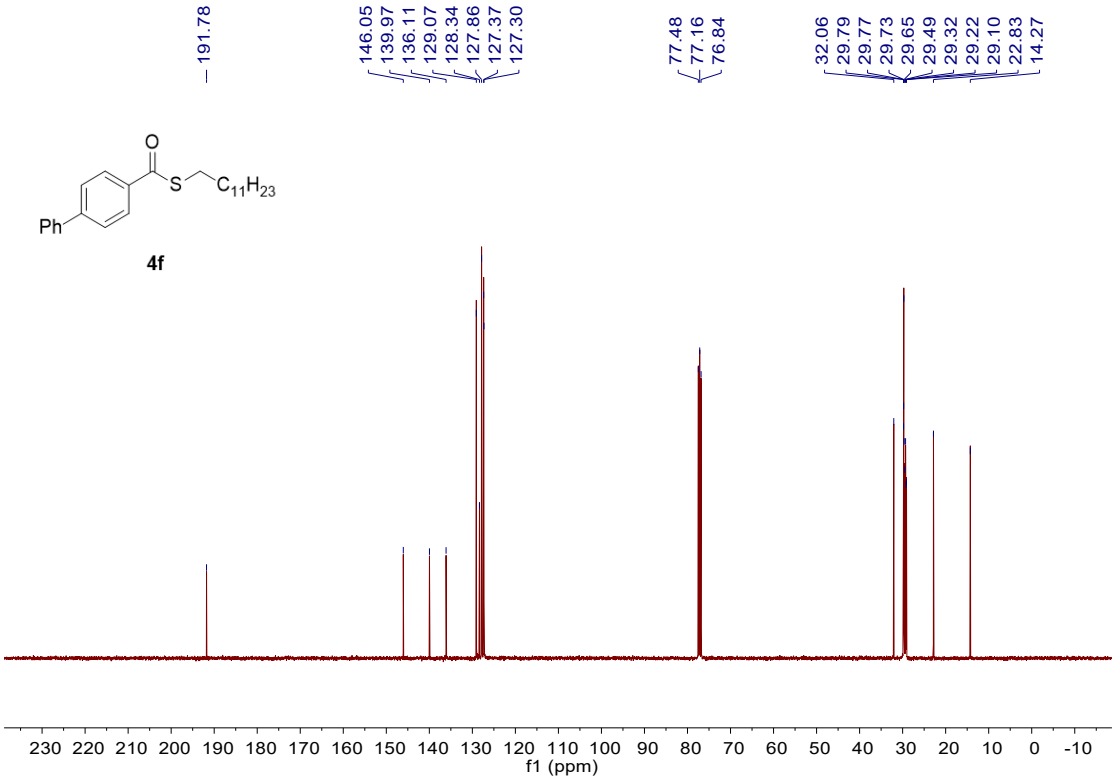
**4d**

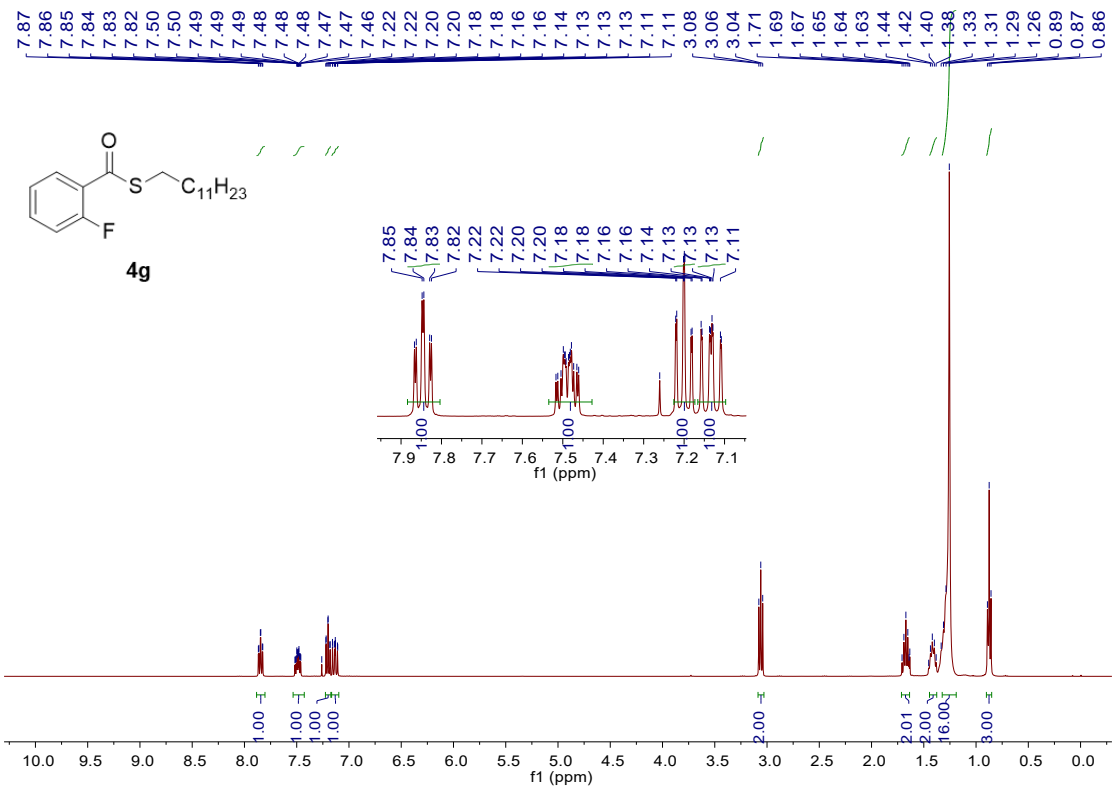

7.96
7.94
7.26
6.92
6.90
3.85
3.06
3.04
3.02
1.69
1.67
1.65
1.64
1.62
1.45
1.43
1.41
1.39
1.38
1.26
0.89
0.88
0.86
O
S
C11H23
MeO
2.00
2.00
3.00
2.00
2.17
2.03
16.21
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

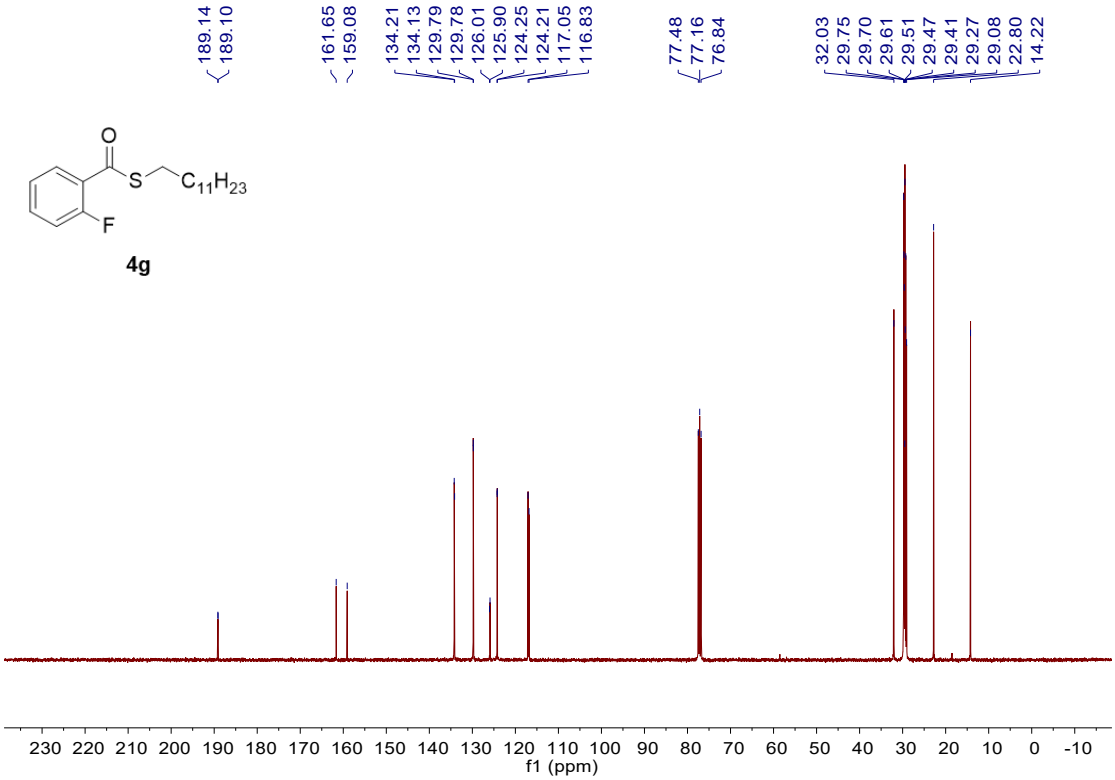
**4e**

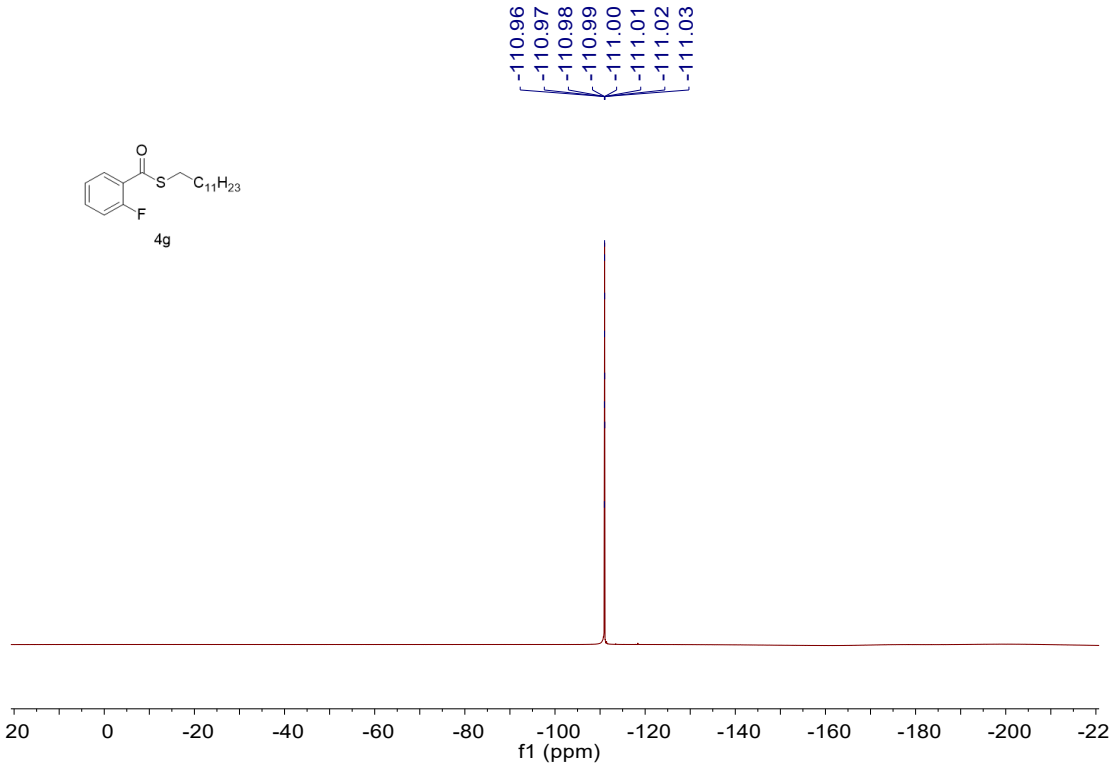

190.79
163.73
130.29
129.43
113.80
77.48
77.16
76.84
55.60
32.05
29.83
29.77
29.76
29.73
29.65
29.49
29.31
29.09
29.05
22.83
14.26
O
S
C11H23
MeO
4e
f1 (ppm)

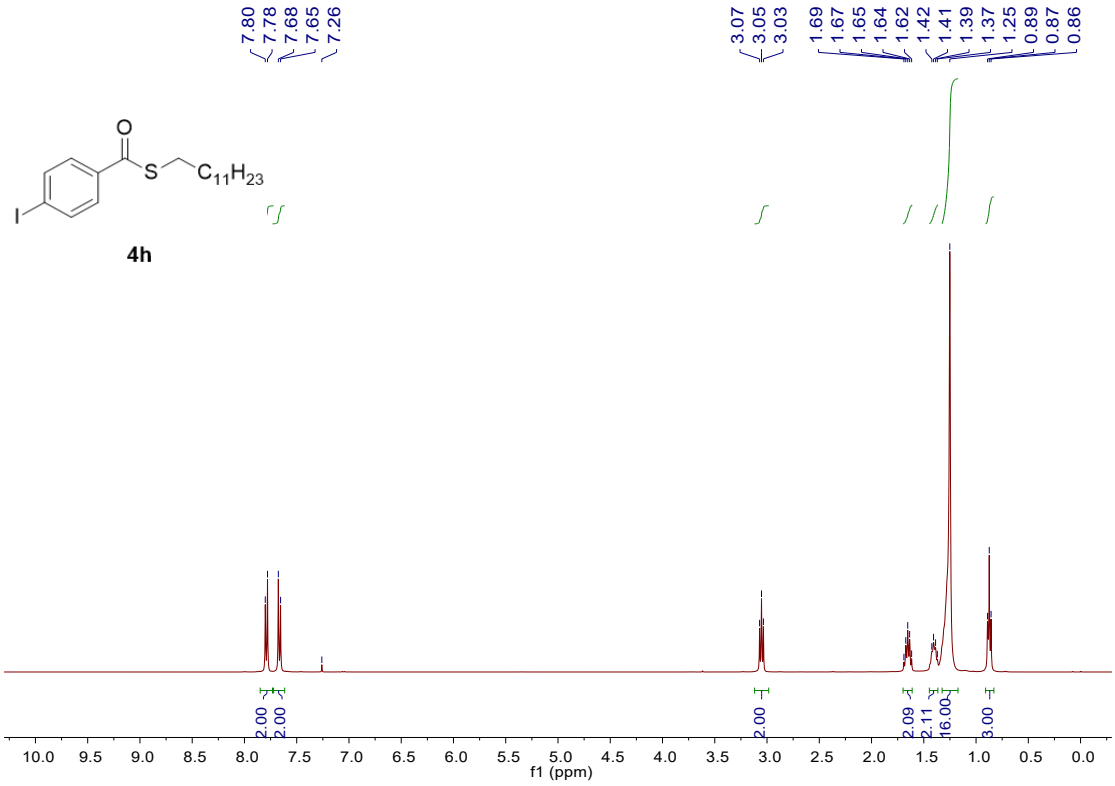

8.05
8.03
7.68
7.66
7.63
7.61
7.49
7.47
7.45
7.42
7.40
7.38
7.26
3.11
3.09
3.07
1.72
1.71
1.69
1.67
1.65
1.47
1.45
1.44
1.42
1.40
1.26
0.90
0.88
0.86
O
S
C11H23
Ph
4f
f1 (ppm)

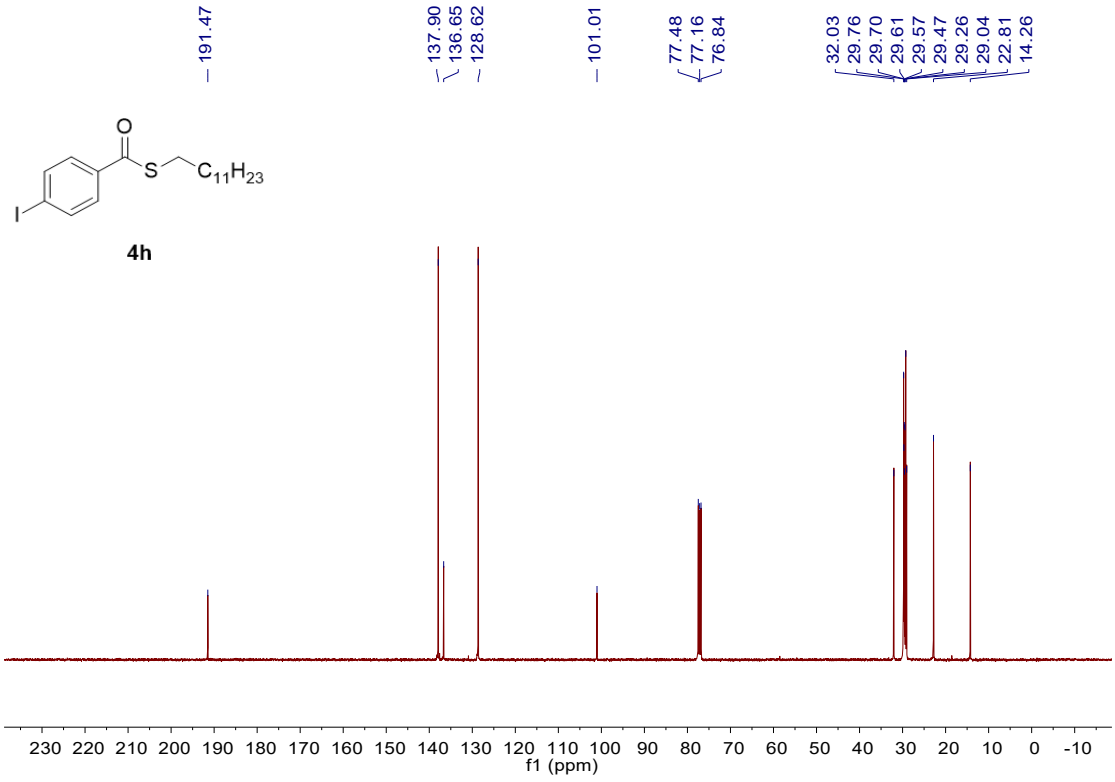

191.78
146.05
139.97
136.11
129.07
128.34
127.86
127.37
127.30
77.48
77.16
76.84
32.06
29.79
29.77
29.73
29.65
29.49
29.32
29.22
29.10
22.83
14.27
O
S
C11H23
Ph
4f
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.87
7.86
7.85
7.84
7.83
7.82
7.50
7.50
7.49
7.49
7.49
7.48
7.48
7.48
7.47
7.47
7.46
7.22
7.20
7.20
7.18
7.18
7.16
7.16
7.14
7.13
7.13
7.11
7.11
3.08
3.06
3.04
1.71
1.69
1.67
1.65
1.64
1.63
1.44
1.42
1.40
1.38
1.33
1.31
1.29
1.26
0.89
0.87
0.86
O
S
C11H23
F
4g
7.85
7.84
7.83
7.82
7.22
7.22
7.20
7.20
7.18
7.18
7.16
7.16
7.14
7.13
7.13
7.13
7.11
1.00
1.00
1.00
1.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
1.00
1.00
1.00
1.00
2.00
2.01
2.00
16.00
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)


189.14
189.10
161.65
159.08
134.21
134.13
129.79
129.78
126.01
125.90
124.25
124.21
117.05
116.83
77.48
77.16
76.84
32.03
29.75
29.70
29.61
29.51
29.47
29.41
29.27
29.08
22.80
14.22
O
S
C11H23
F
4g
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-110.96
-110.97
-110.98
-110.99
-111.00
-111.01
-111.02
-111.03
O
S
C11H23
F
4g
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -22
f1 (ppm)


7.80
7.78
7.68
7.65
7.26
3.07
3.05
3.03
1.69
1.67
1.65
1.64
1.62
1.42
1.41
1.39
1.37
1.25
0.89
0.87
0.86
O
S
C11H23
I
4h
2.00
2.00
2.00
2.09
2.11
16.00
3.00
f1 (ppm)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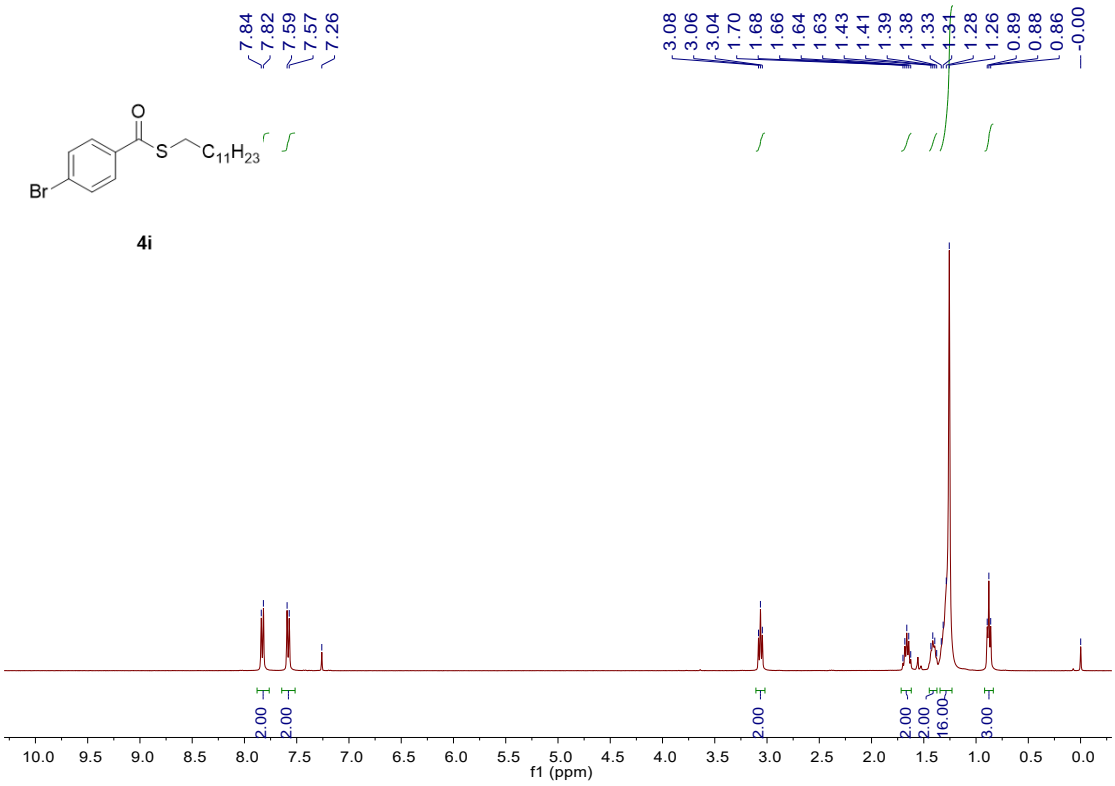
137.90
136.65
128.62
101.01
77.48
77.16
76.84
32.03
29.76
29.70
29.61
29.57
29.47
29.26
29.04
22.81
14.26
O
S
C11H23
I
4h
f1 (ppm)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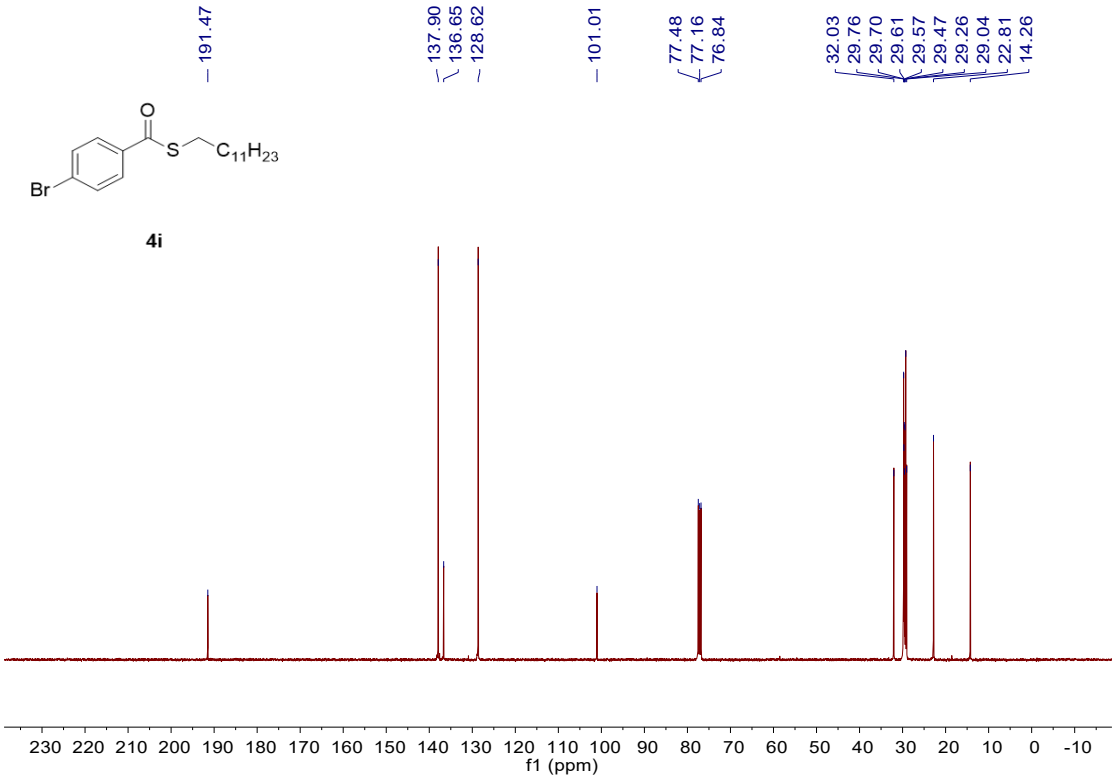
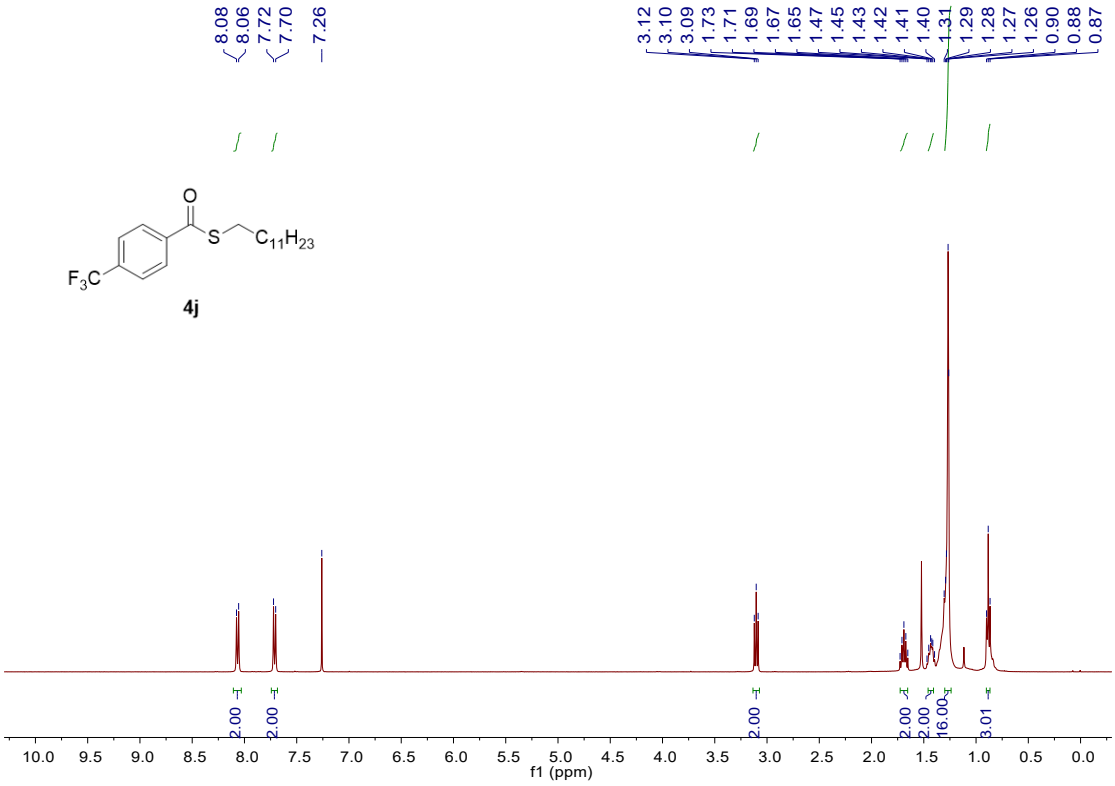
7.82
7.59
7.57
7.26
3.08
3.06
3.04
1.70
1.68
1.66
1.64
1.63
1.43
1.41
1.39
1.38
1.33
1.31
1.28
1.26
0.89
0.88
0.86
-0.00
O
S
C11H23
Br
4i
2.00
2.00
2.00
2.00
2.00
16.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


191.47
137.90
136.65
128.62
101.01
77.48
77.16
76.84
32.03
29.76
29.70
29.61
29.57
29.47
29.26
29.04
22.81
14.26
O
S
C11H23
Br
4i
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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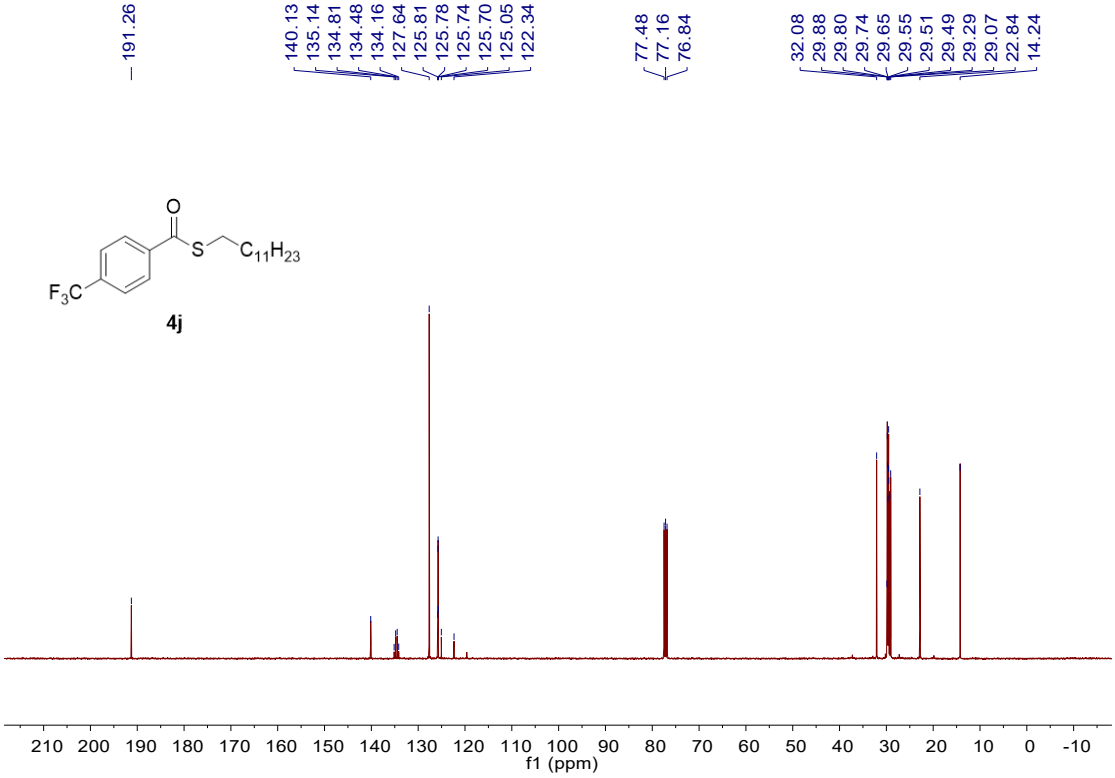
8.06
7.72
7.70
7.26
3.12
3.10
3.09
1.73
1.71
1.69
1.67
1.65
1.47
1.45
1.43
1.42
1.41
1.40
1.31
1.29
1.28
1.27
1.26
0.90
0.88
0.87
O
S
C11H23
F3C
4j
2.00
2.00
2.00
2.00
2.00
16.00
3.01
f1 (ppm)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140.13
135.14
134.81
134.48
134.16
127.64
125.81
125.78
125.74
125.70
125.05
122.34
77.48
77.16
76.84
32.08
29.88
29.80
29.74
29.65
29.55
29.51
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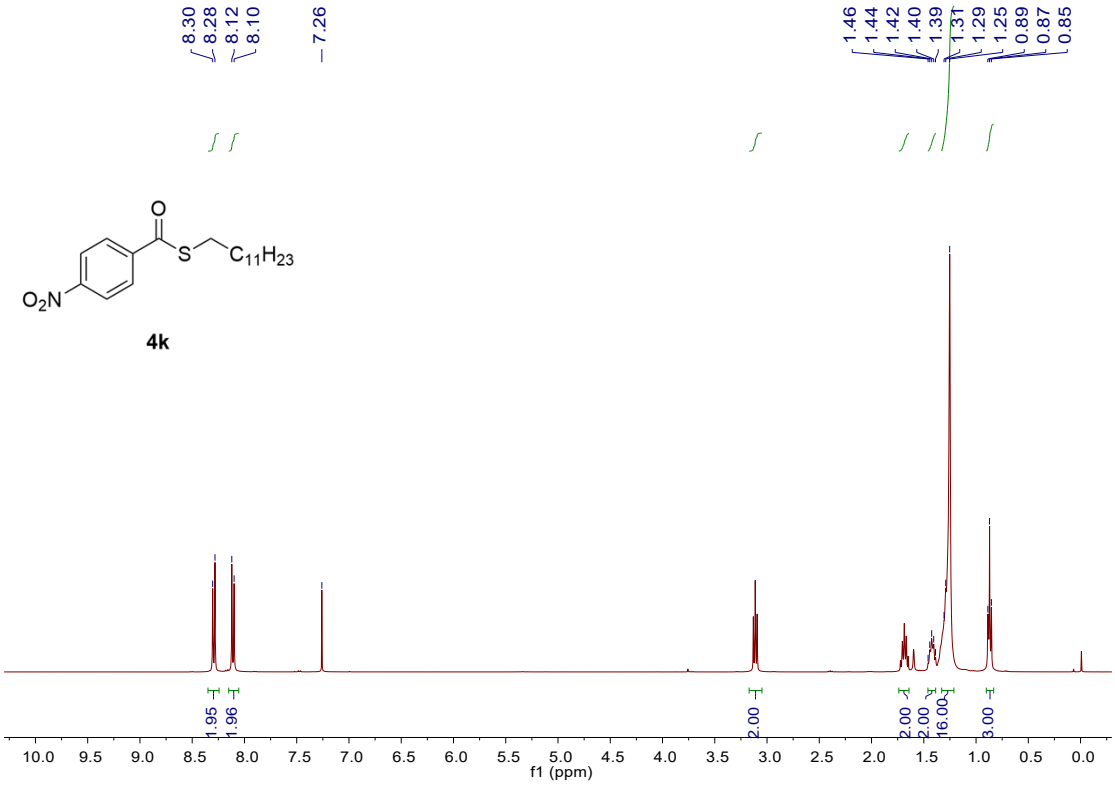
29.29
29.07
22.84
14.24
O
S
C11H23
F3C
4j
f1 (ppm)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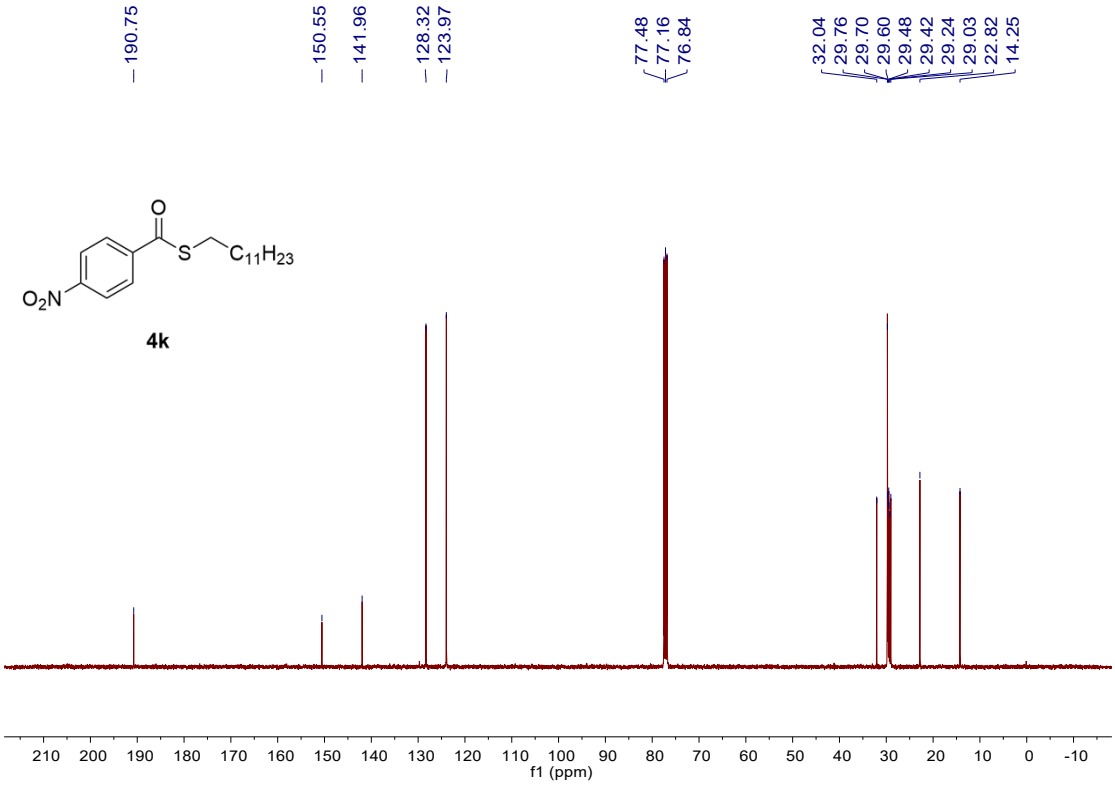
8.28
8.12
8.10
7.26
1.46
1.44
1.42
1.40
1.39
1.31
1.29
1.25
0.89
0.87
0.85
O
S
C11H23
O2N
4k
1.95
1.96
2.00
2.00
2.00
16.00
3.00
f1 (ppm)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150.55
141.96
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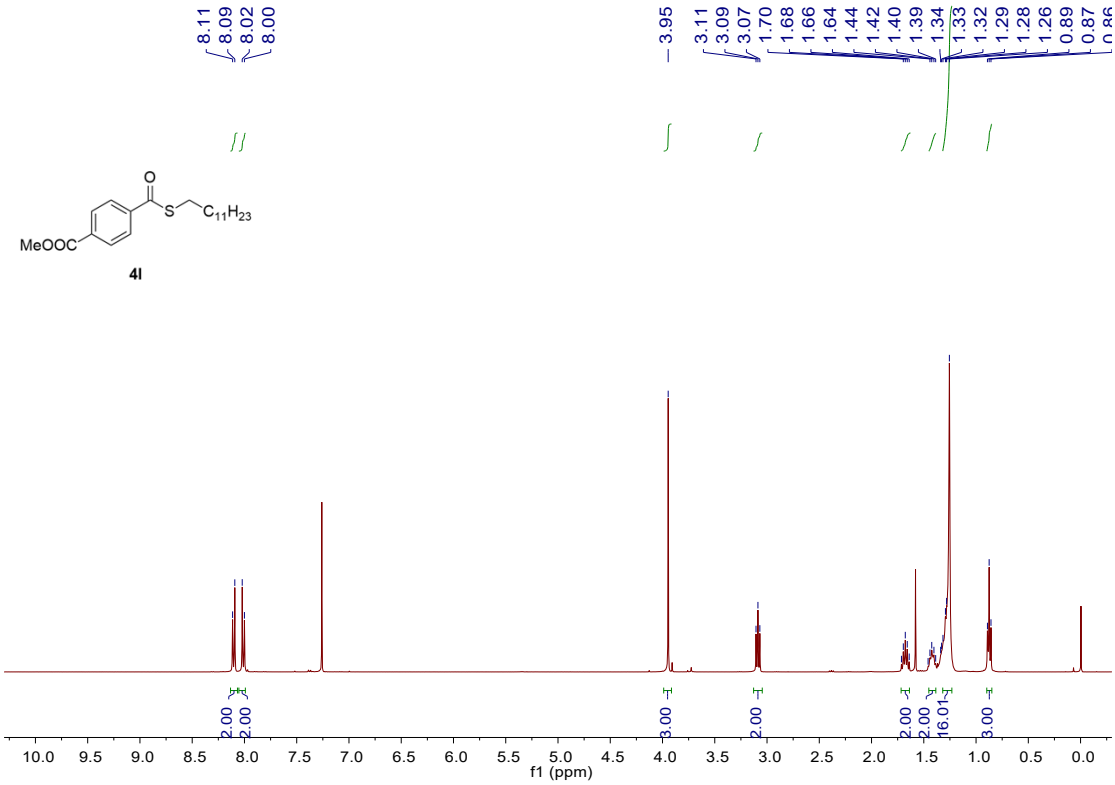
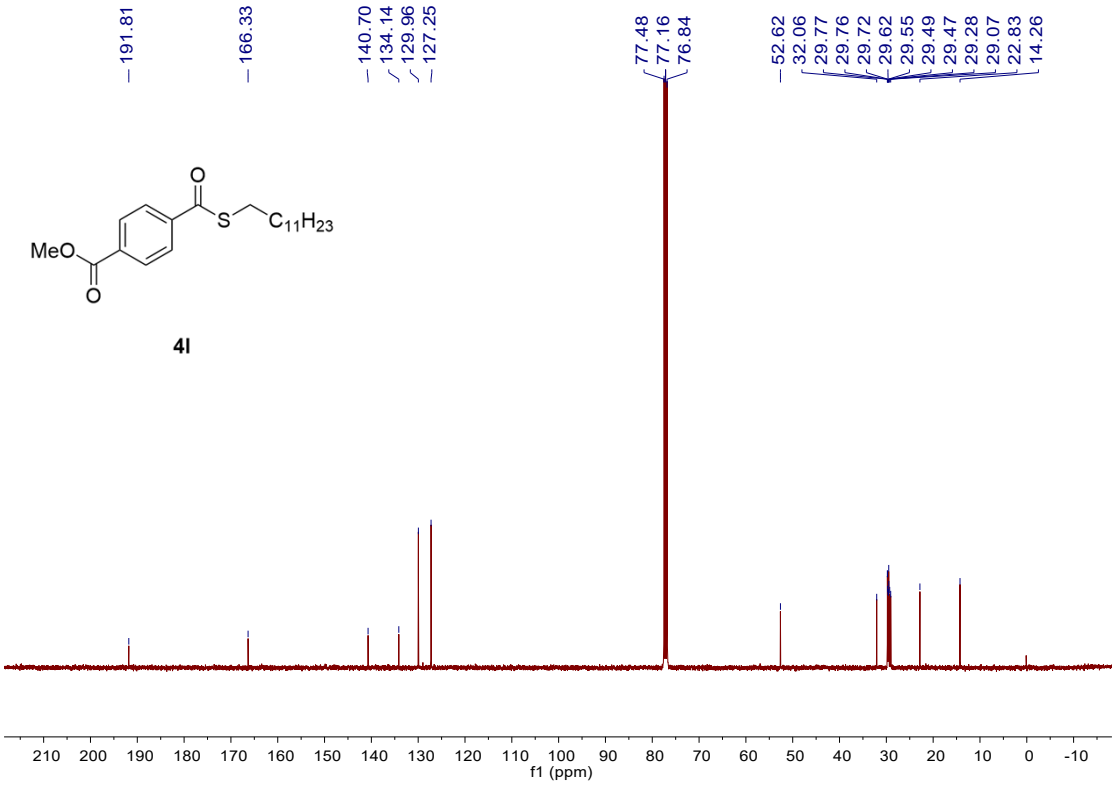
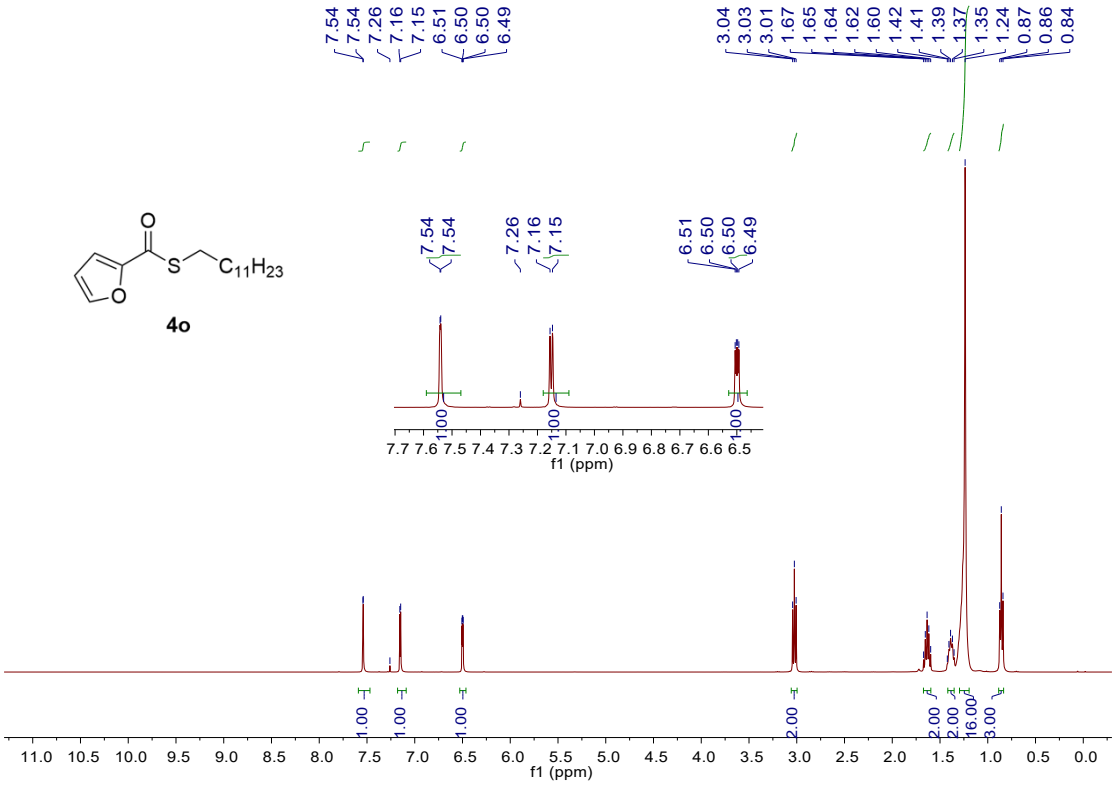
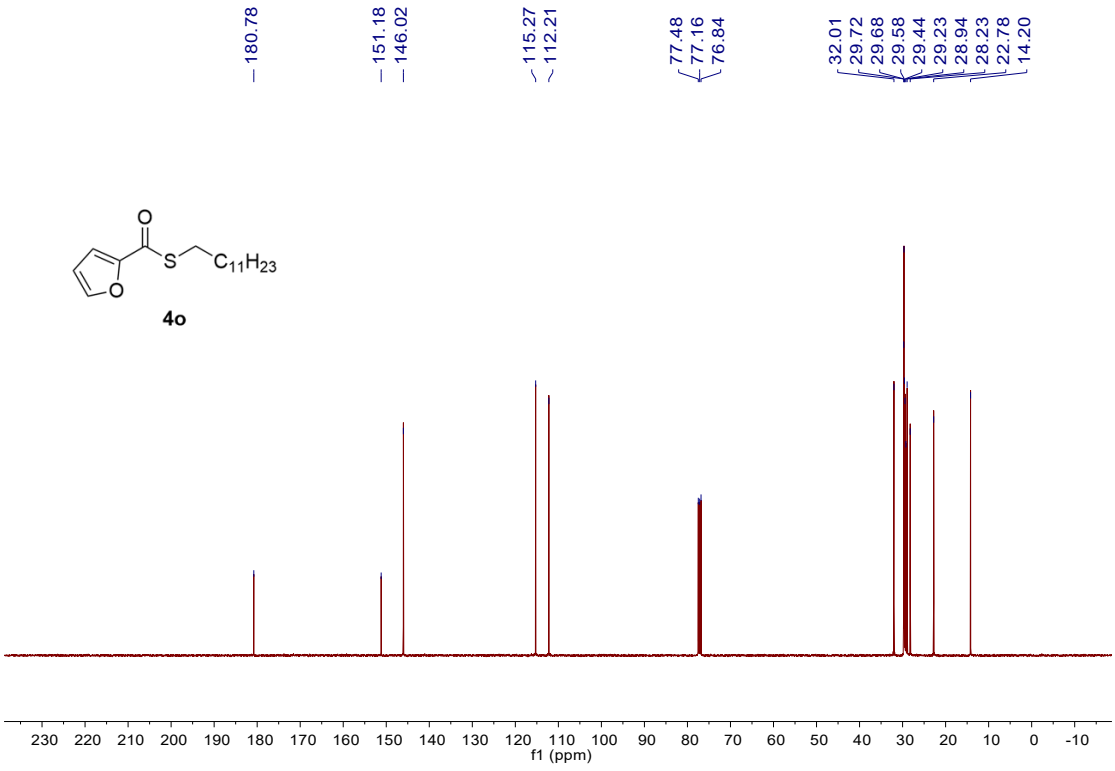
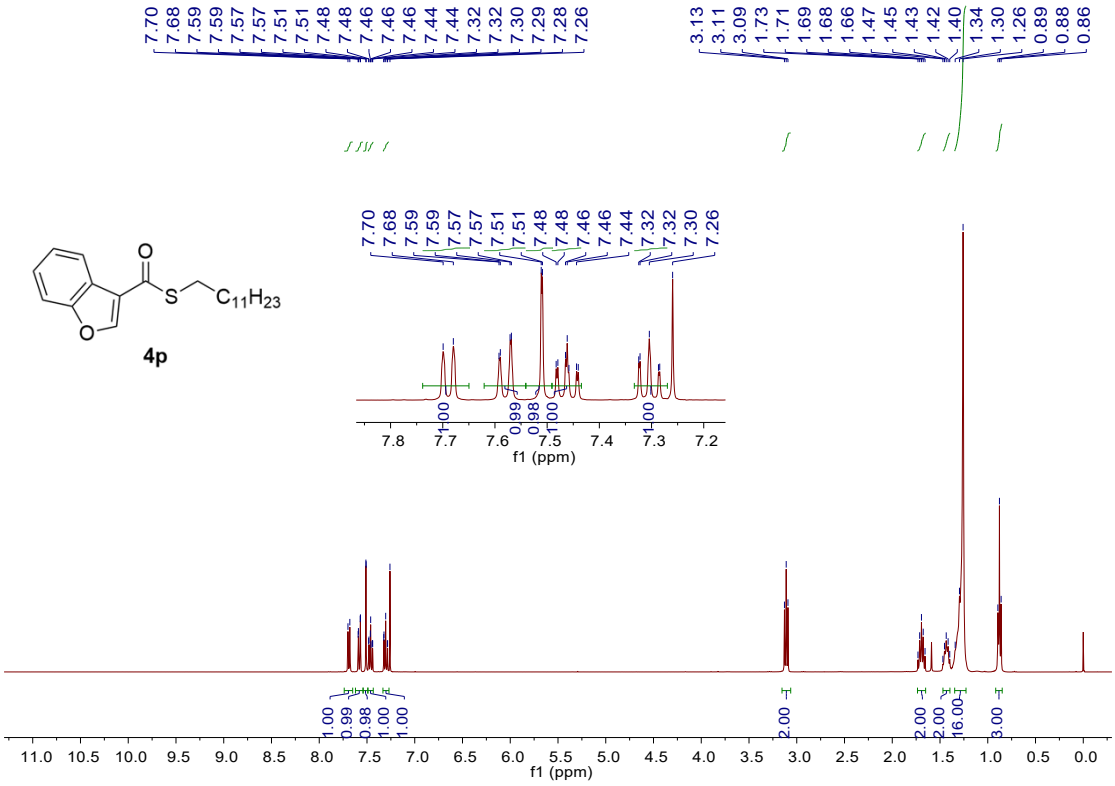
123.97
77.48
77.16
76.84
32.04
29.76
29.70
29.60
29.48
29.42
29.24
29.03
22.82
14.25
O
S
C11H23
O2N
4k
f1 (ppm)


8.11
8.09
8.02
8.00
3.95
3.11
3.09
3.07
1.70
1.68
1.66
1.64
1.44
1.42
1.40
1.39
1.34
1.33
1.32
1.29
1.28
1.26
0.89
0.87
MeOOC
O
S
C11H23
4l
2.00
2.00
3.00
2.00
2.00
2.00
16.01
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)


191.81
166.33
140.70
134.14
129.96
127.25
77.48
77.16
76.84
52.62
32.06
29.77
29.76
29.72
29.62
29.55
29.49
29.47
29.28
29.07
22.83
14.26
MeO
O
S
C11H23
O
4l
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)


7.54
7.54
7.26
7.16
7.15
6.51
6.50
6.50
6.49
3.04
3.03
3.01
1.67
1.65
1.64
1.62
1.60
1.42
1.41
1.39
1.37
1.35
1.24
0.87
0.86
0.84
O
S
C11H23
O
4o
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
f1 (ppm)
1.00
1.00
1.00
2.00
2.00
2.00
16.00
3.00
11.0 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)


180.78
151.18
146.02
115.27
112.21
77.48
77.16
76.84
32.01
29.72
29.68
29.58
29.44
29.23
28.94
28.23
22.78
14.20
O
S
C11H23
O
4o
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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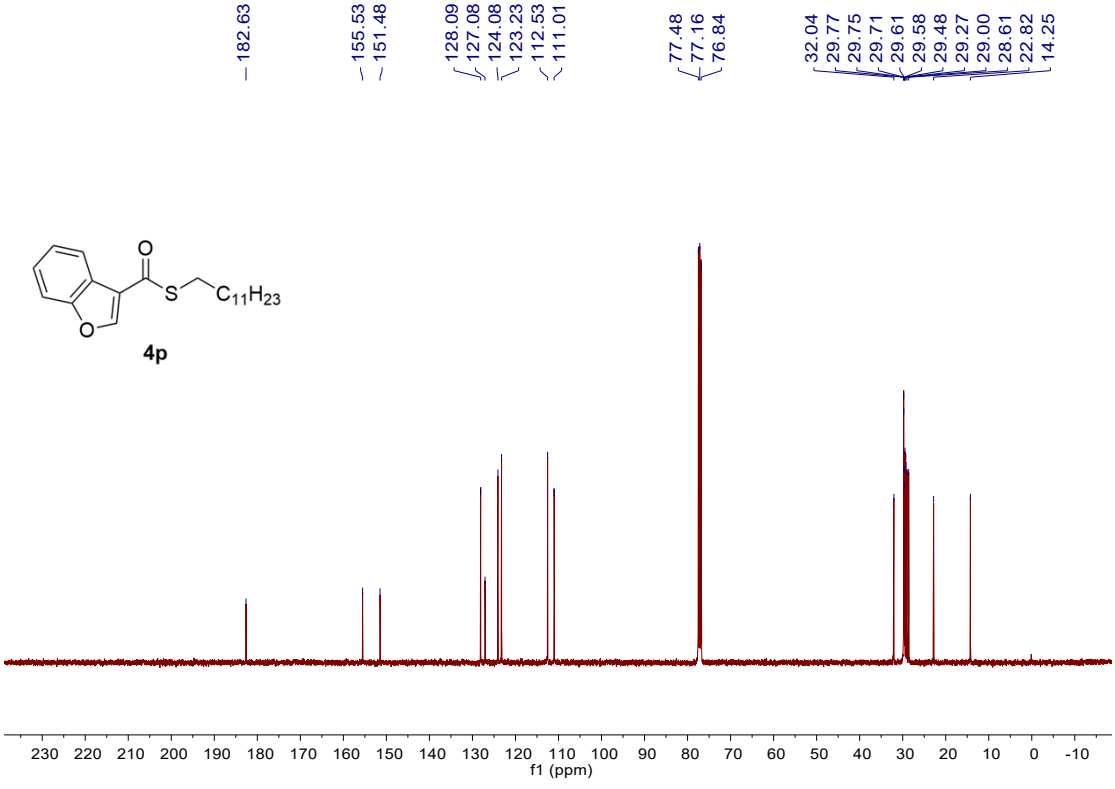
7.68
7.59
7.59
7.57
7.57
7.51
7.51
7.48
7.48
7.46
7.46
7.46
7.44
7.44
7.32
7.32
7.30
7.29
7.28
7.26
3.13
3.11
3.09
1.73
1.71
1.69
1.68
1.66
1.47
1.45
1.43
1.42
1.40
1.34
1.30
1.26
0.89
0.88
0.86
O
S
C11H23
O
4p
1.00
0.99
0.98
1.00
1.00
2.00
2.00
2.00
16.00
3.00
f1 (ppm)


182.63
155.53
151.48
128.09
127.08
124.08
123.23
112.53
111.01
77.48
77.16
76.84
32.04
29.77
29.75
29.71
29.61
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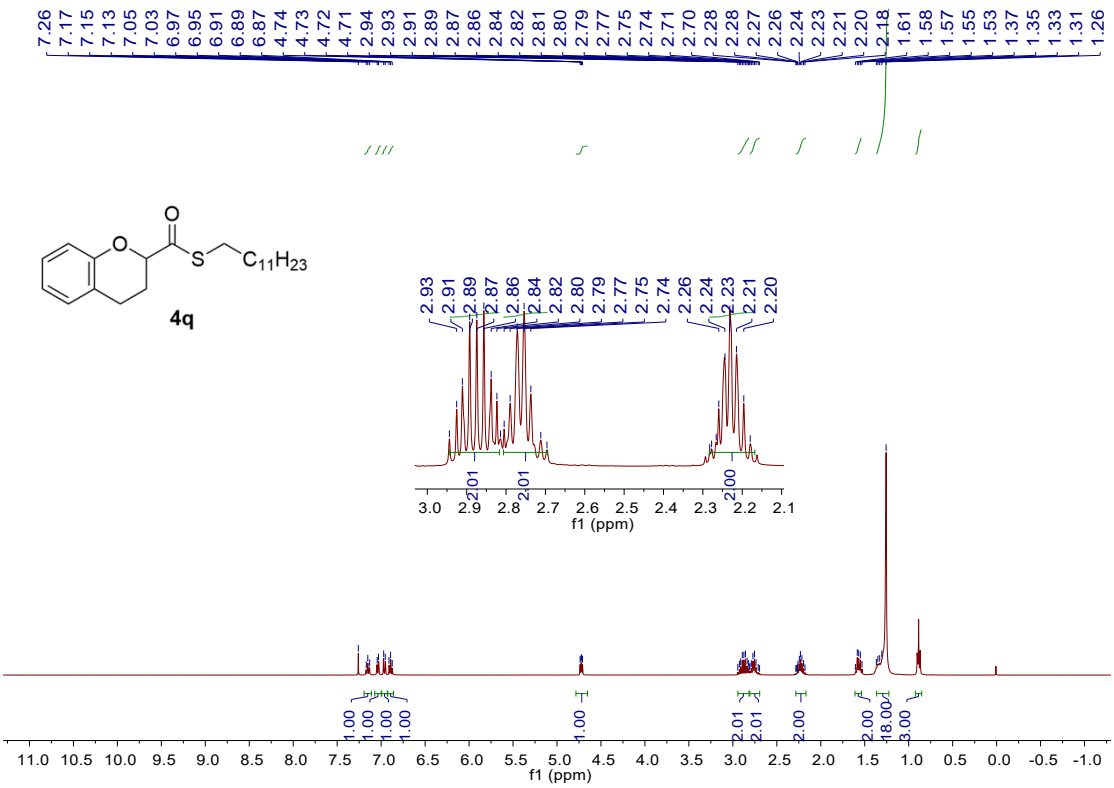
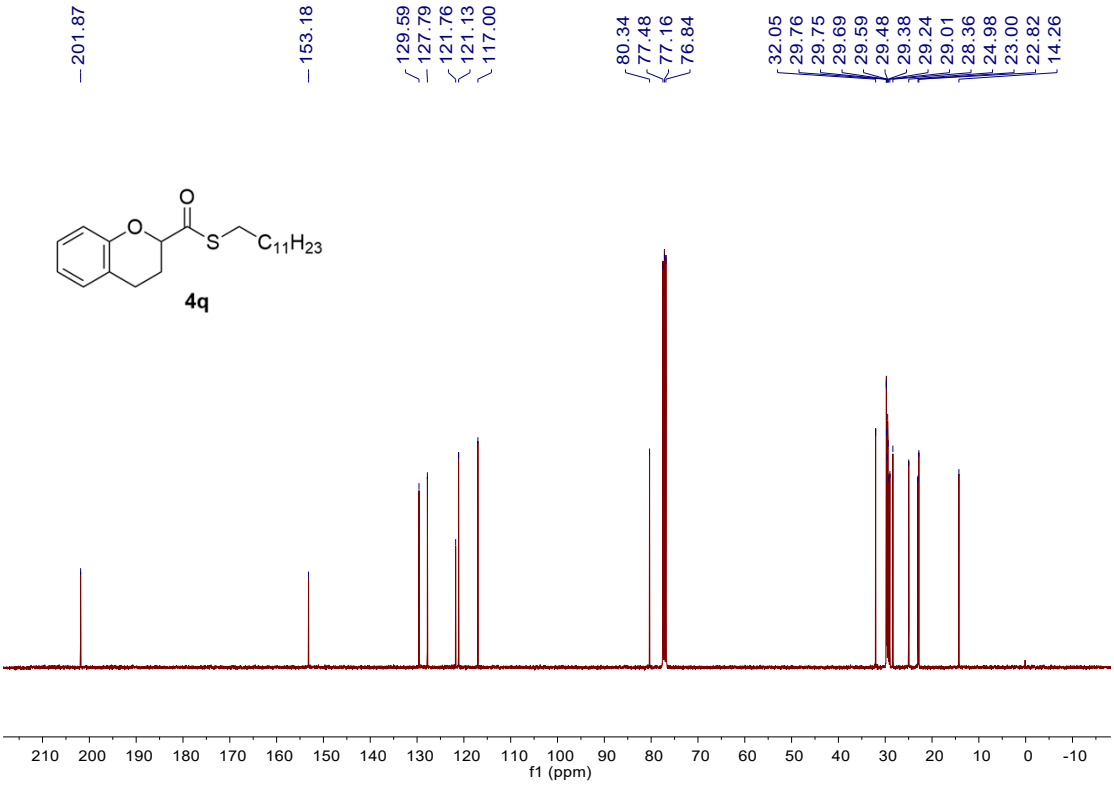
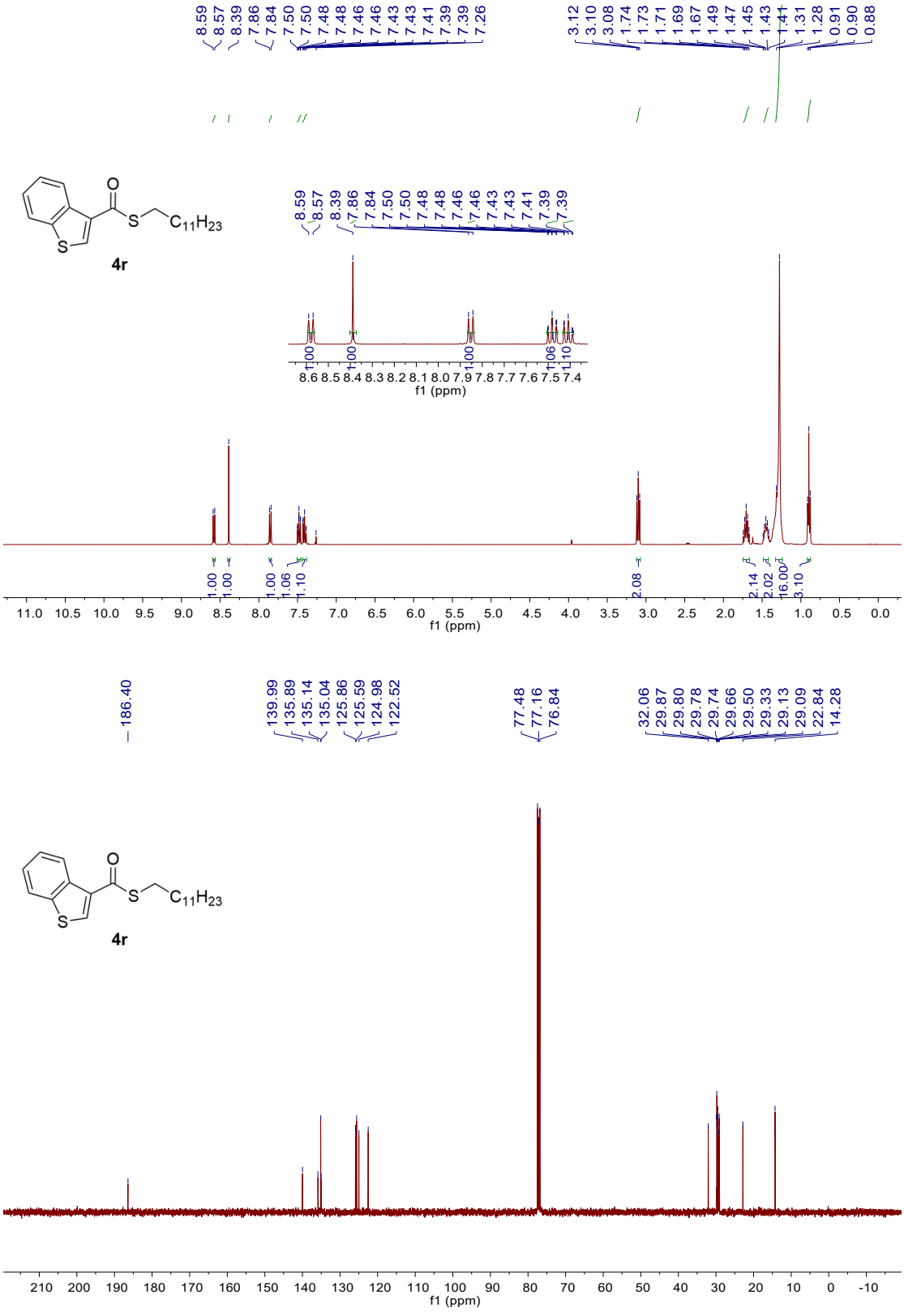
O
S
C11H23
O
4p
f1 (ppm)


7.26 7.17 7.15 7.13 7.05 7.03 6.97 6.95 6.91 6.89 6.87 4.74 4.73 4.72 4.71 2.94 2.93 2.91 2.89 2.87 2.86 2.84 2.82 2.81 2.80 2.79 2.77 2.75 2.74 2.71 2.70 2.28 2.28 2.27 2.26 2.24 2.23 2.21 2.20 2.18 1.61 1.58 1.57 1.55 1.53 1.37 1.35 1.33 1.31 1.26
O
O
S
C11H23
4q
2.93 2.91 2.89 2.87 2.86 2.84 2.82 2.80 2.79 2.77 2.75 2.74 2.26 2.24 2.23 2.21 2.20
2.01 2.01 2.00
3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1
f1 (ppm)
1.00 1.00 1.00 1.00 1.00 2.01 2.01 2.00 2.00 18.00 3.00
11.0 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 -1.0
f1 (ppm)


201.87
153.18
129.59 127.79 121.76 121.13 117.00
80.34 77.48 77.16 76.84
32.05 29.76 29.75 29.69 29.59 29.48 29.38 29.24 29.01 28.36 24.98 23.00 22.82 14.26
O
O
S
C11H23
4q
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)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8.57
8.39
7.86
7.84
7.50
7.48
7.48
7.46
7.46
7.43
7.43
7.41
7.39
7.39
7.26
3.12
3.10
3.08
1.74
1.73
1.71
1.69
1.67
1.49
1.47
1.45
1.43
1.41
1.31
1.28
0.91
0.90
0.88
O
S
C11H23
S
4r
f1 (ppm)
f1 (ppm)


186.40
139.99
135.89
135.14
135.04
125.86
125.59
124.98
122.52
77.48
77.16
76.84
32.06
29.87
29.80
29.78
29.74
29.66
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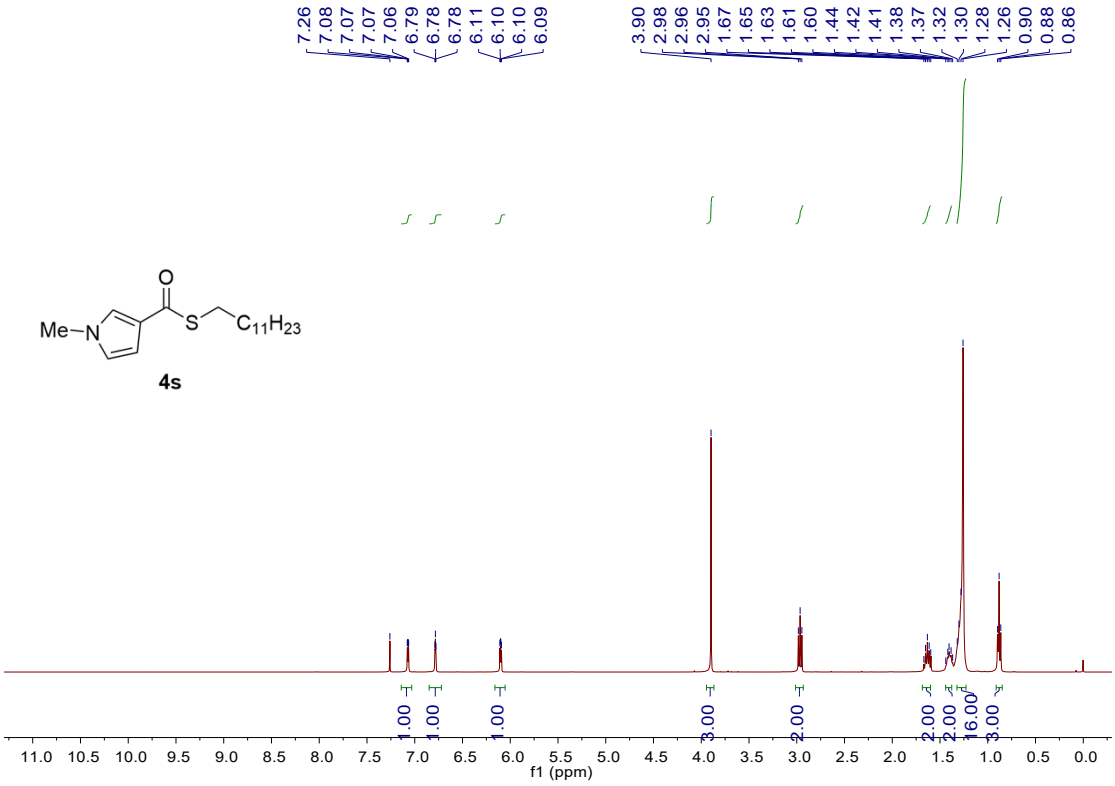
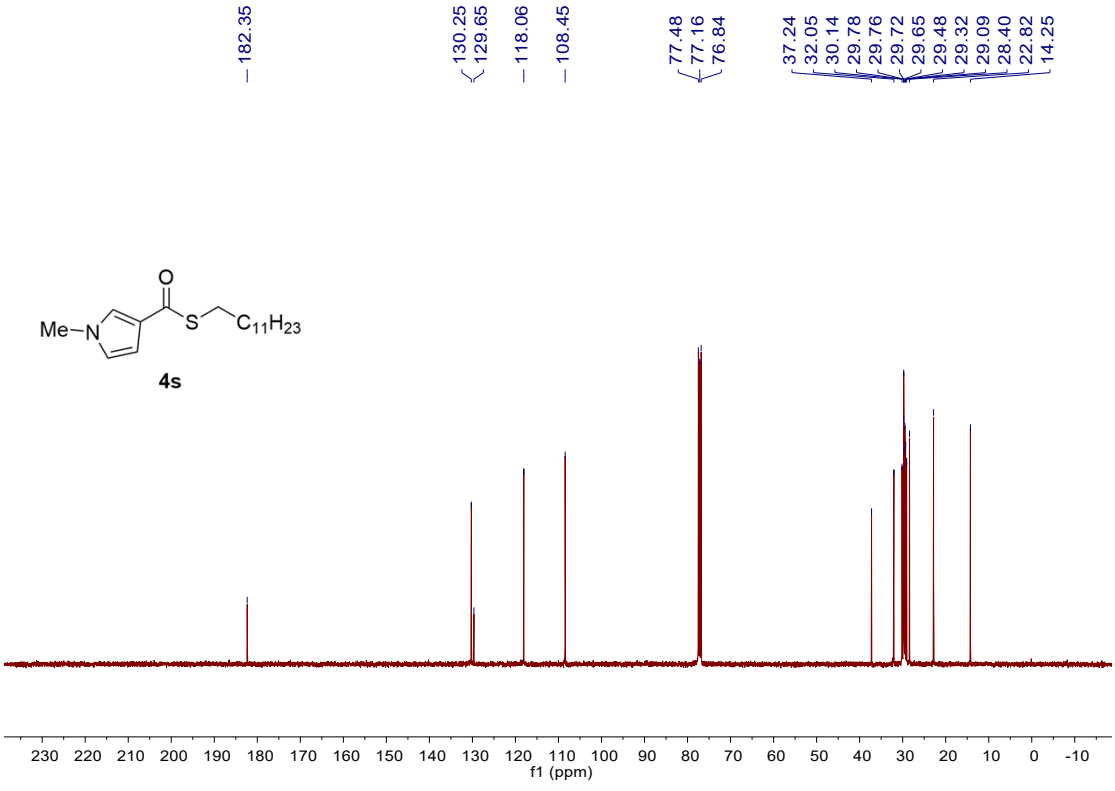
29.33
29.13
29.09
22.84
14.28
O
S
C11H23
S
4r
f1 (ppm)


7.26
7.08
7.07
7.07
7.06
6.79
6.78
6.78
6.11
6.10
6.10
6.09
3.90
2.98
2.96
2.95
1.67
1.65
1.63
1.61
1.60
1.44
1.42
1.41
1.38
1.37
1.32
1.30
1.28
1.26
0.90
0.88
0.86
Me
N
O
S
C11H23
4s
1.00
1.00
1.00
3.00
2.00
2.00
2.00
16.00
3.00
11.0 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)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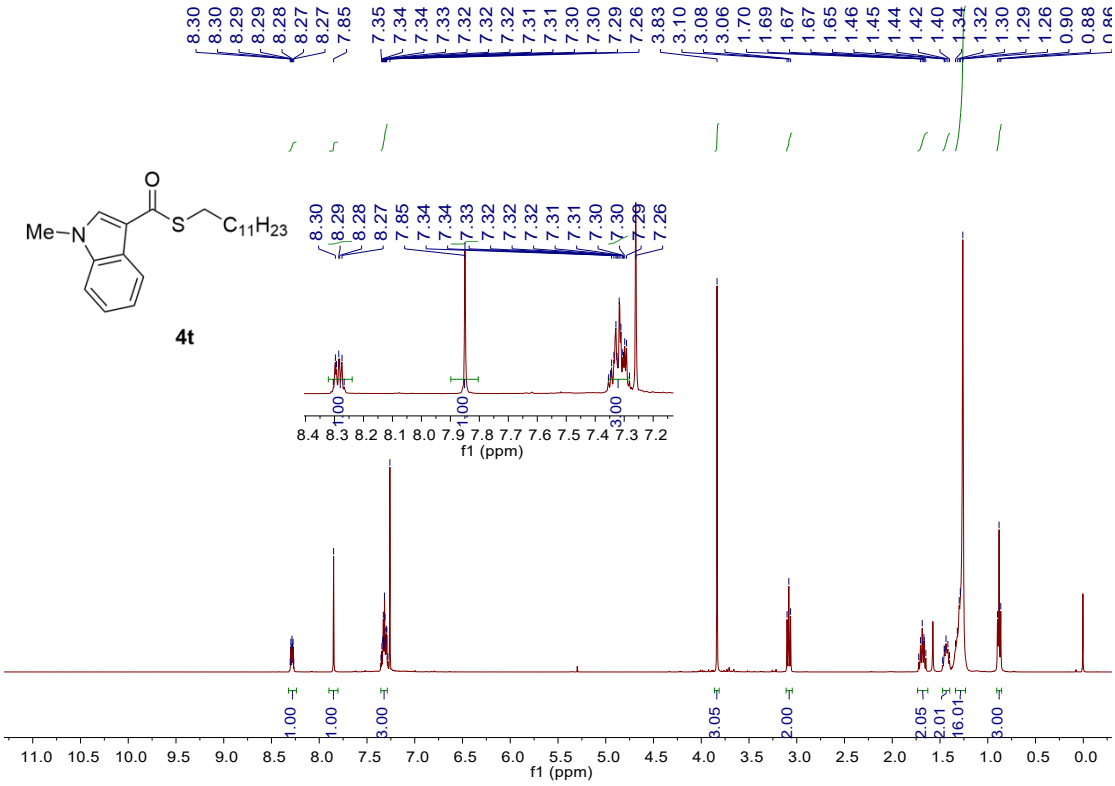
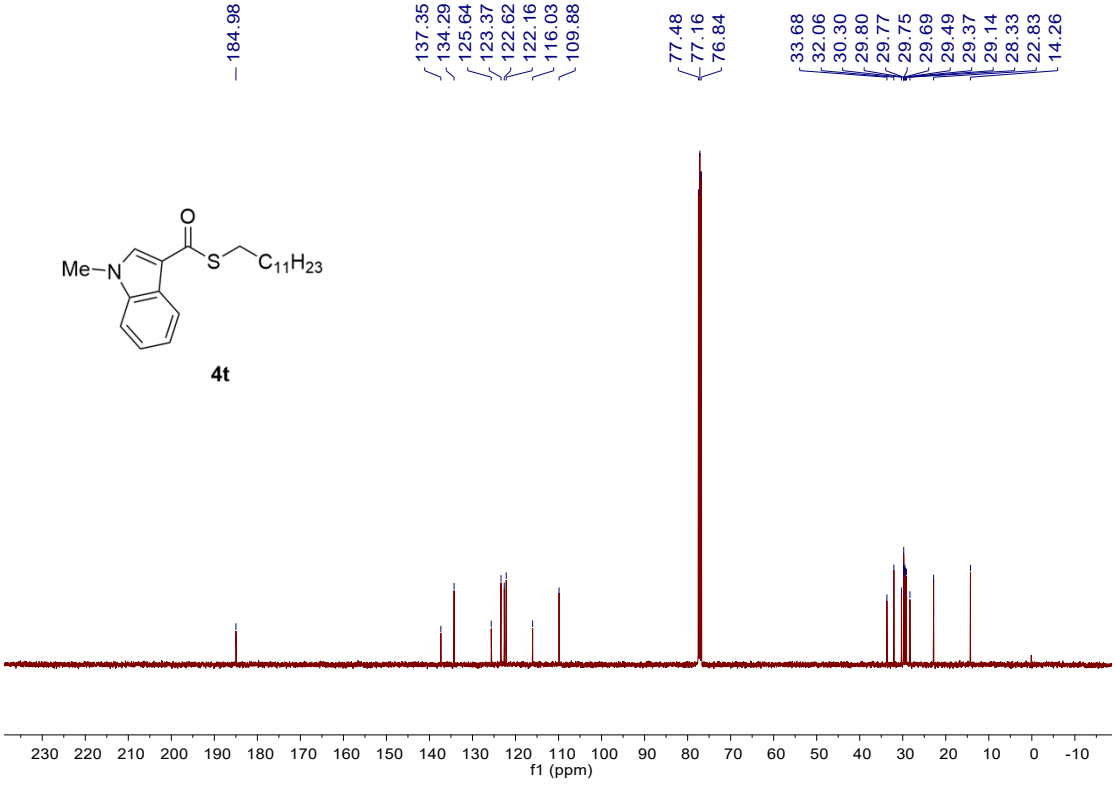
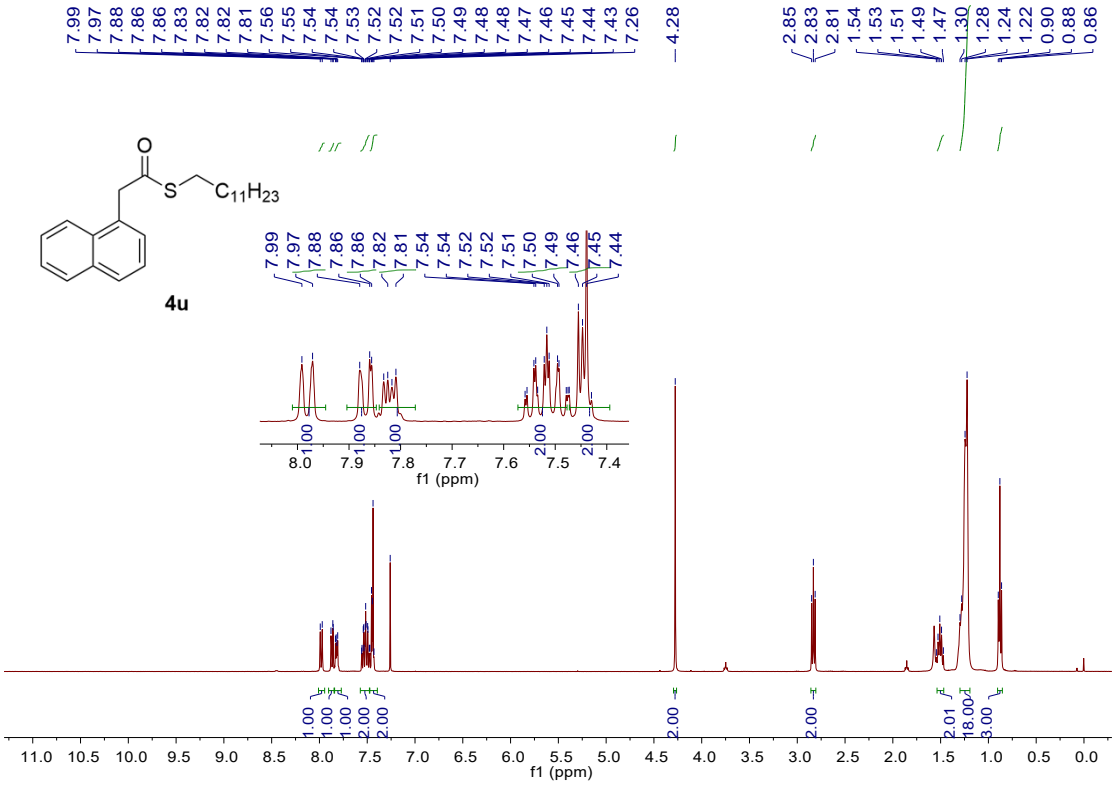
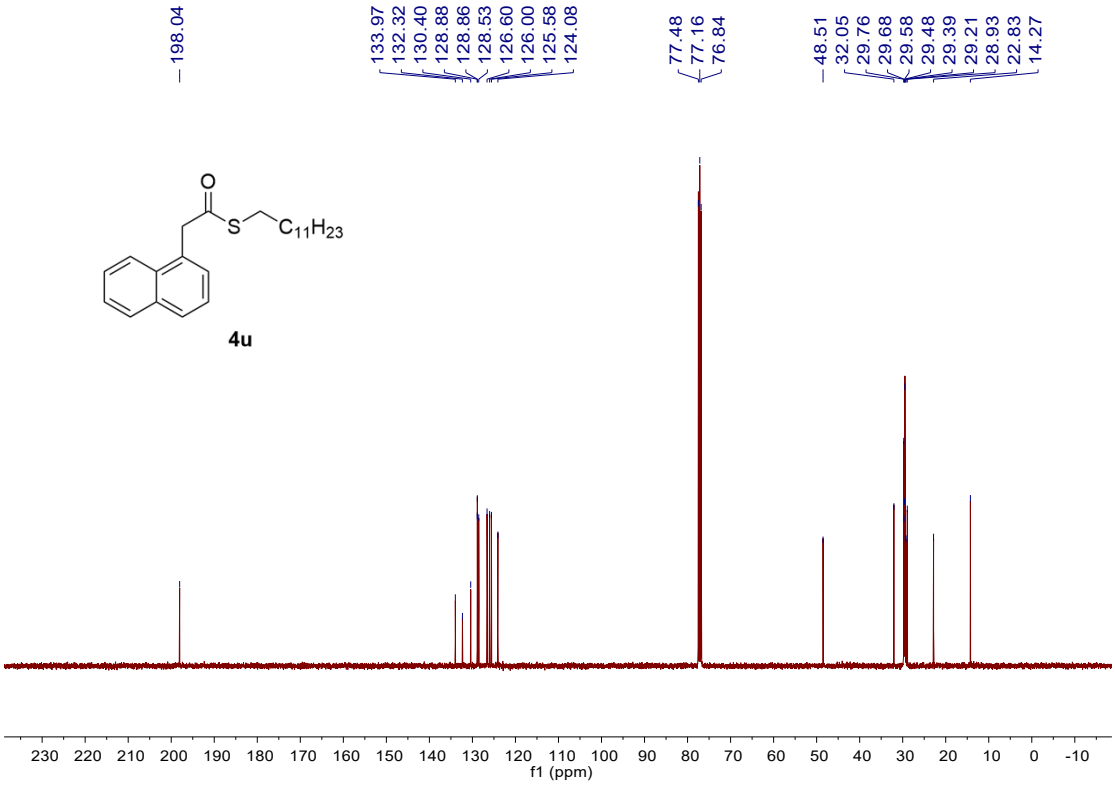
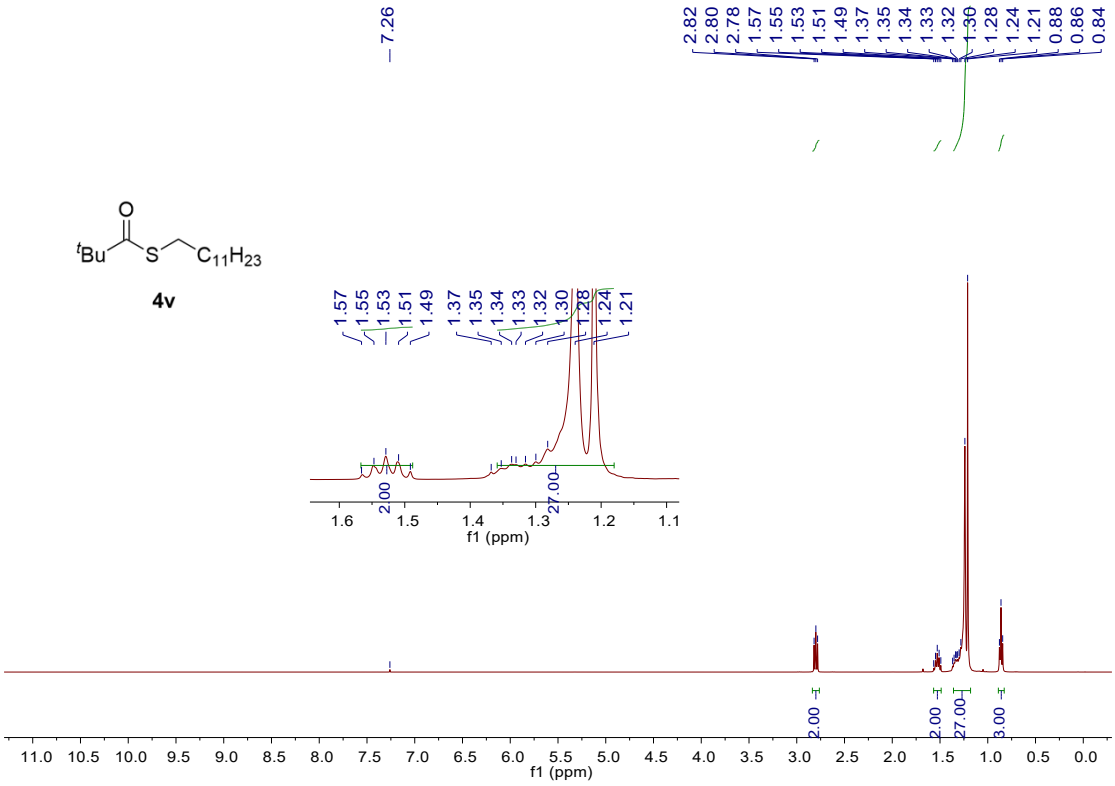
129.65
118.06
108.45
77.48
77.16
76.84
37.24
32.05
30.14
29.78
29.76
29.72
29.65
29.48
29.32
29.09
28.40
22.82
14.25
Me
N
O
S
C11H23
4s
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Me–N
O
S
C11H23
4t
f1 (ppm)


Me–N
O
S
C11H23
4t
f1 (ppm)


7.99 7.97 7.88 7.86 7.86 7.83 7.82 7.82 7.81 7.56 7.55 7.54 7.54 7.53 7.52 7.52 7.51 7.50 7.49 7.48 7.48 7.47 7.46 7.45 7.44 7.43 7.26
4.28
2.85 2.83 2.81 1.54 1.53 1.51 1.49 1.47 1.30 1.28 1.24 1.22 0.90 0.88 0.86
O
S
C11H23
4u
f1 (ppm)
f1 (ppm)


198.04
133.97 132.32 130.40 128.88 128.86 128.53 126.60 126.00 125.58 124.08
77.48 77.16 76.84
48.51 32.05 29.76 29.68 29.58 29.48 29.39 29.21 28.93 22.83 14.27
O
S
C11H23
4u
f1 (ppm)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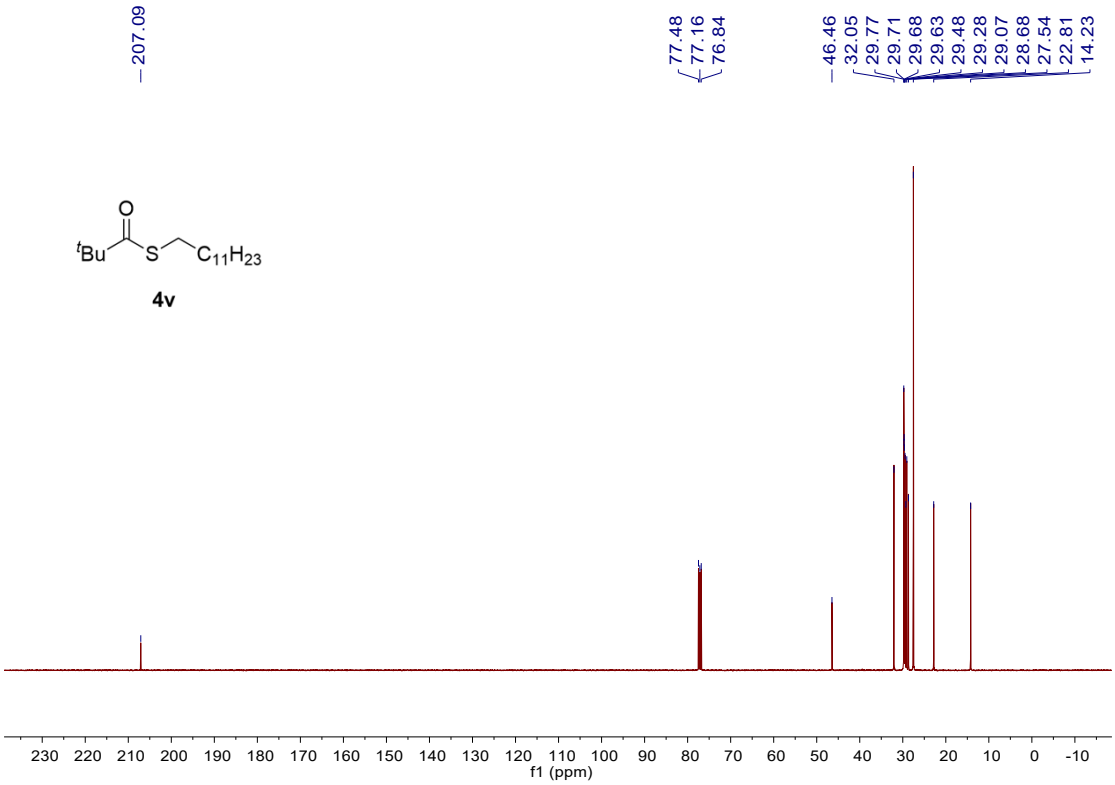
2.80
2.78
1.57
1.55
1.53
1.51
1.49
1.37
1.35
1.34
1.33
1.32
1.30
1.28
1.24
1.21
0.88
0.86
0.84
O
tBu
S
C11H23
4v
2.00
27.00
3.00
f1 (ppm)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76.84
46.46
32.05
29.77
29.71
29.68
29.63
29.48
29.28
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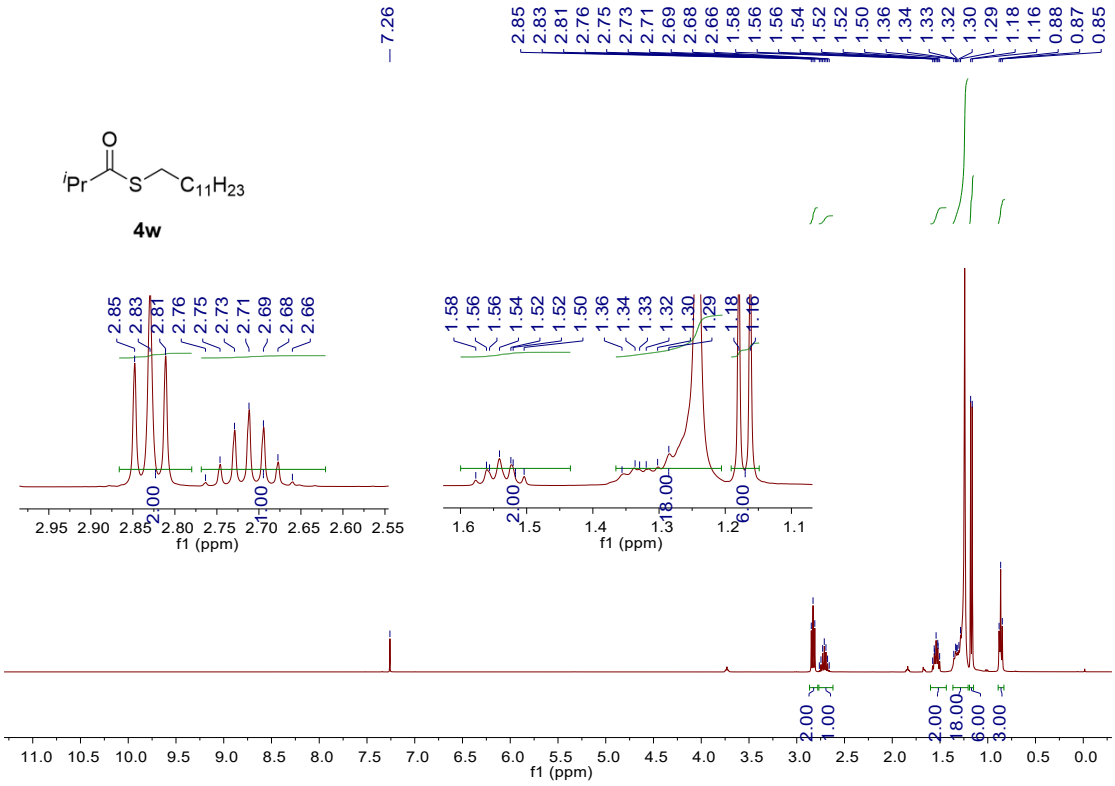
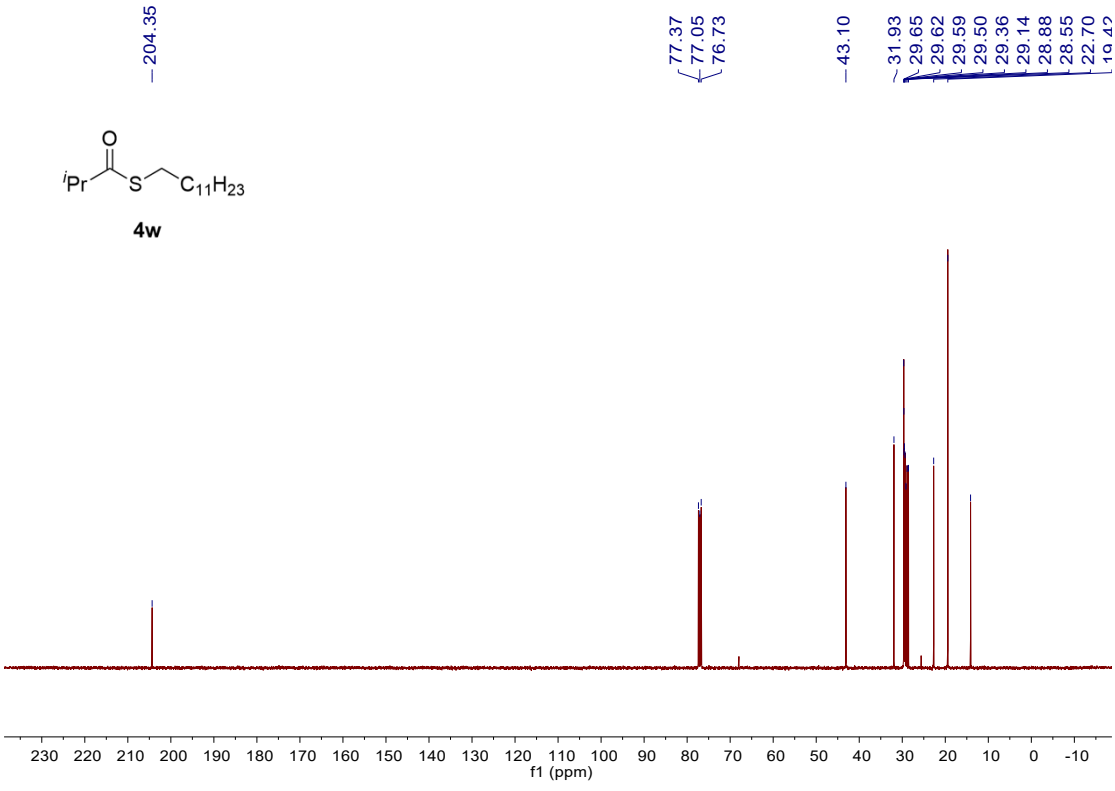
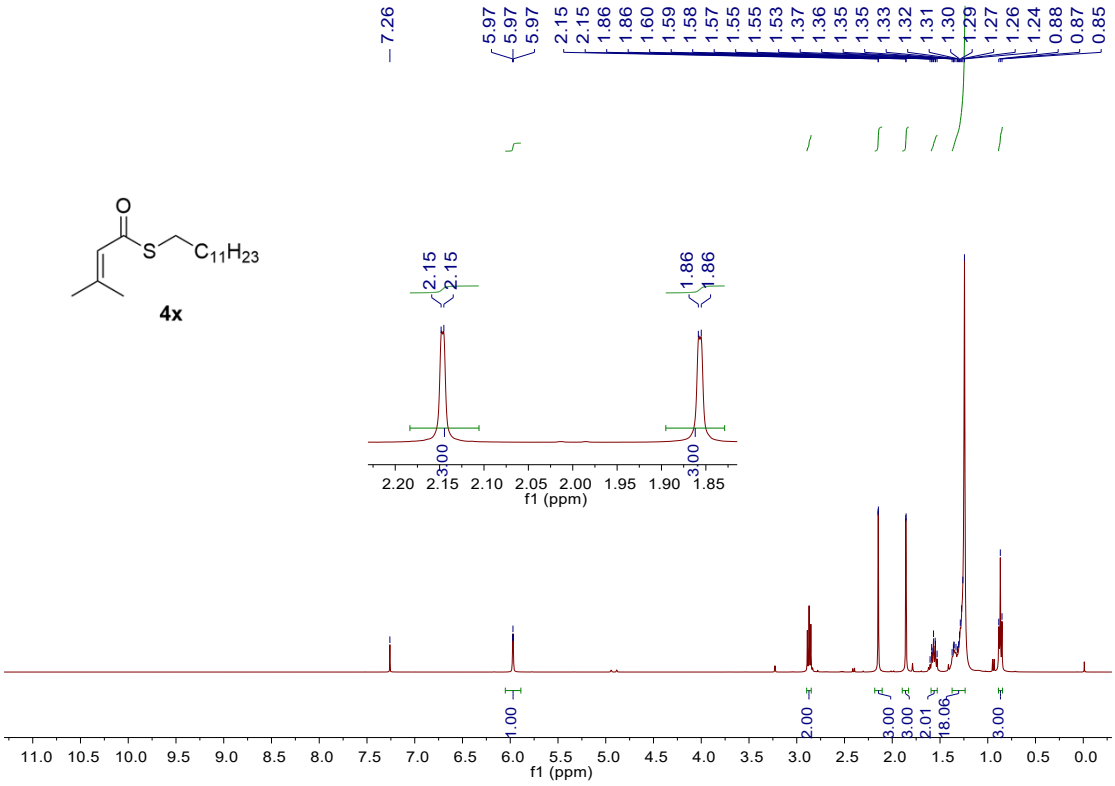
O
tBu
S
C11H23
4v
f1 (ppm)


7.26
2.85 2.83 2.81 2.76 2.75 2.73 2.71 2.69 2.68 2.66 1.58 1.56 1.56 1.54 1.52 1.52 1.50 1.36 1.34 1.33 1.32 1.30 1.29 1.18 1.16 0.88 0.87 0.85
O
iPr S C11H23
4w
2.00 1.00 2.00 18.00 6.00 3.00
f1 (ppm)


204.35
77.37 77.05 76.73
43.10
31.93 29.65 29.62 29.59 29.50 29.36 29.14 28.88 28.55 22.70
O
iPr S C11H23
4w
f1 (ppm)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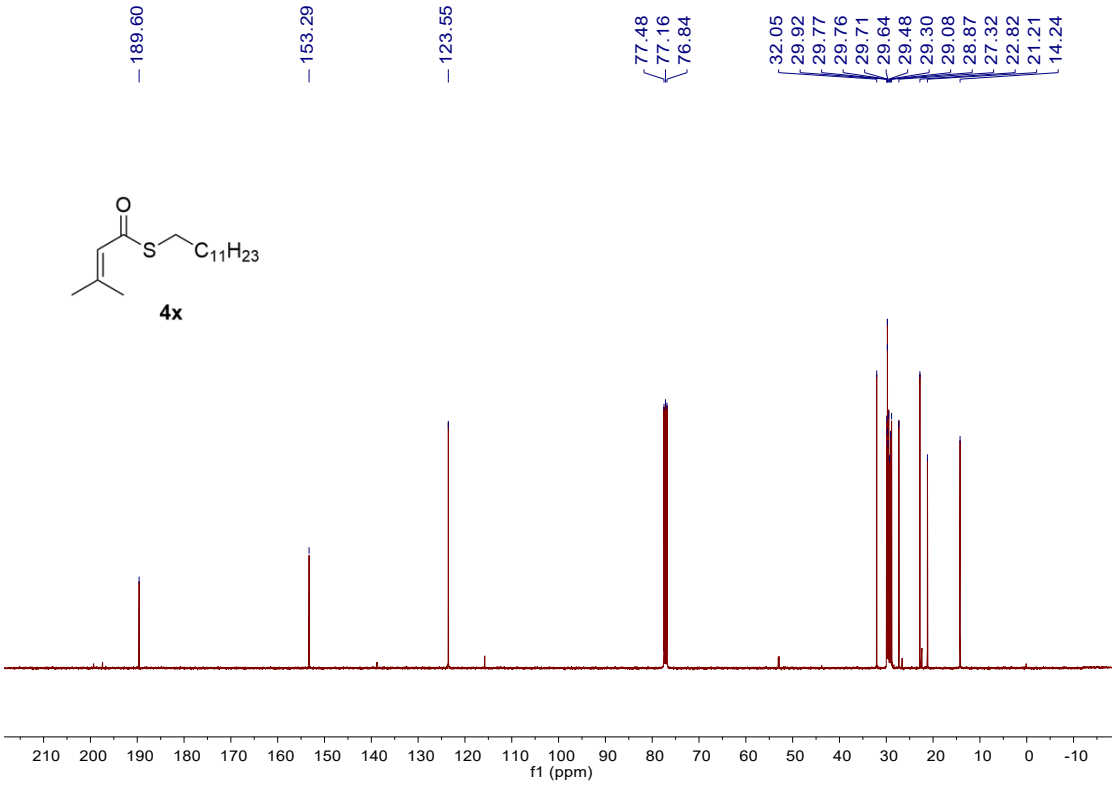
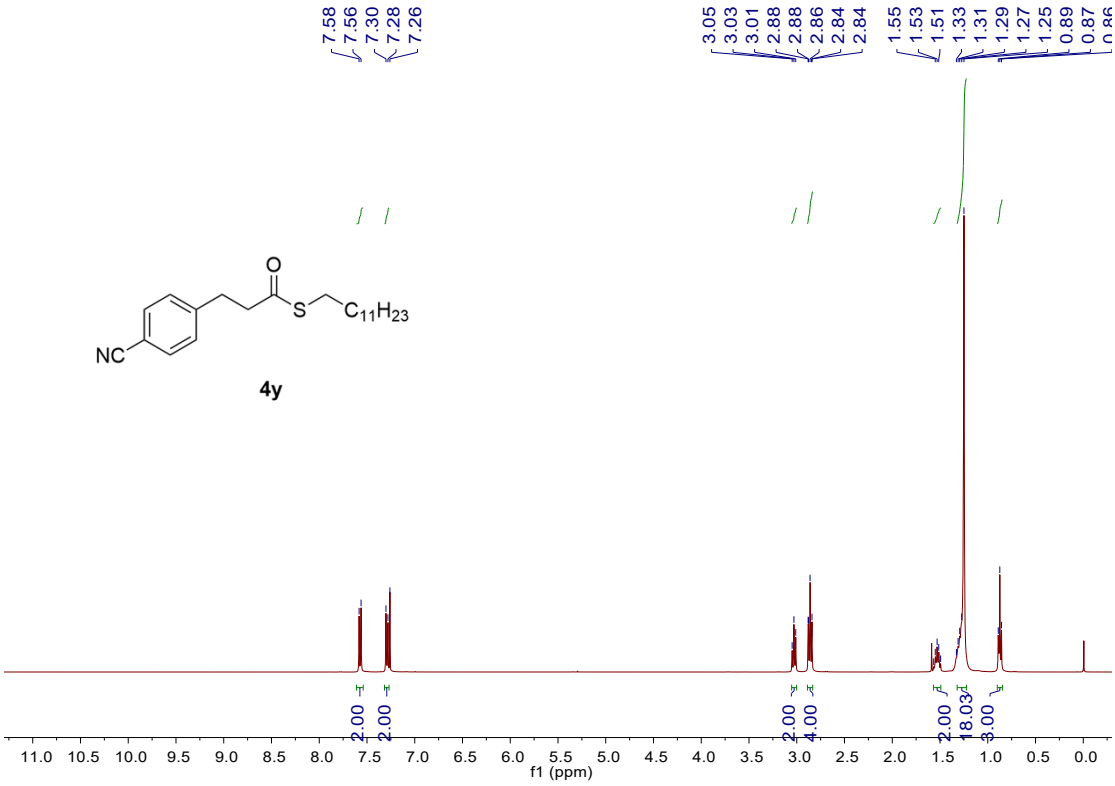
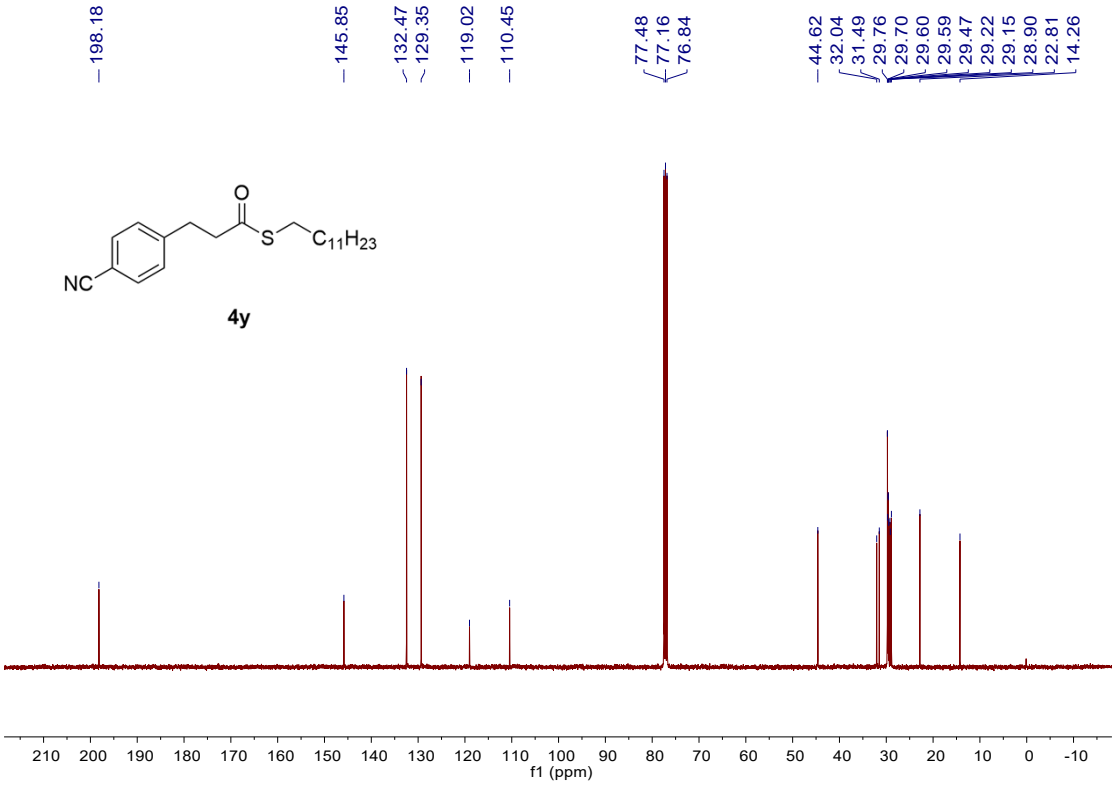
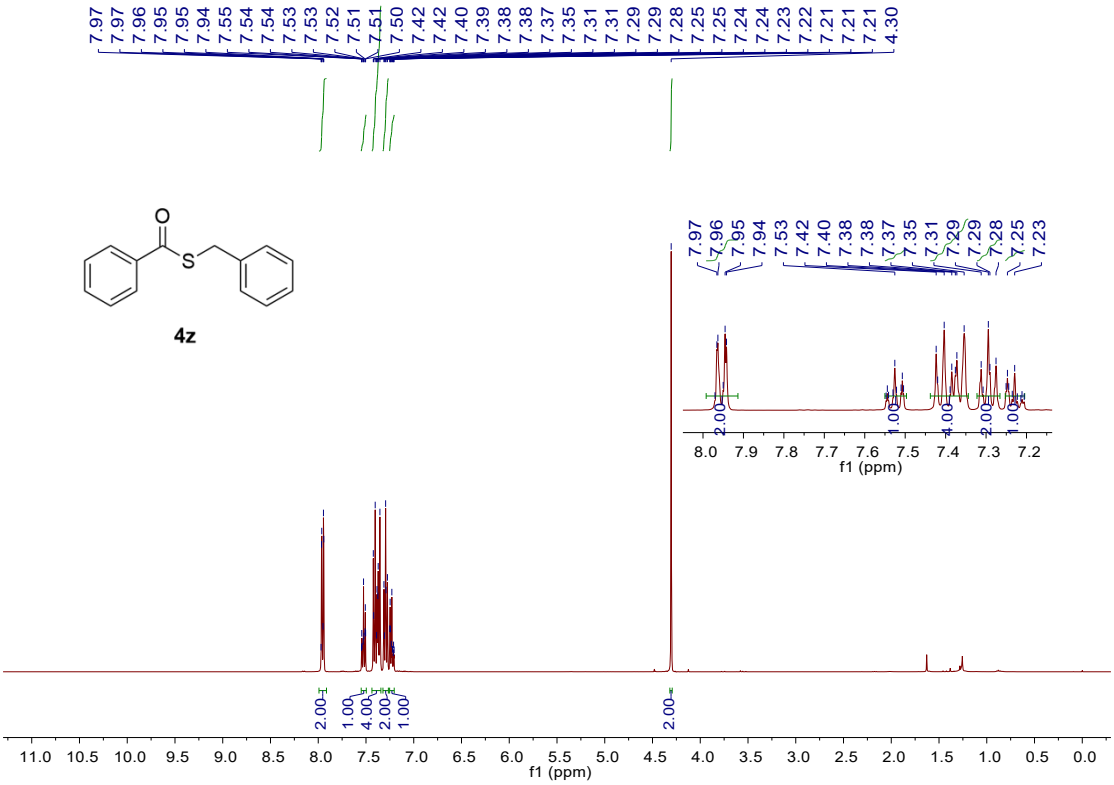
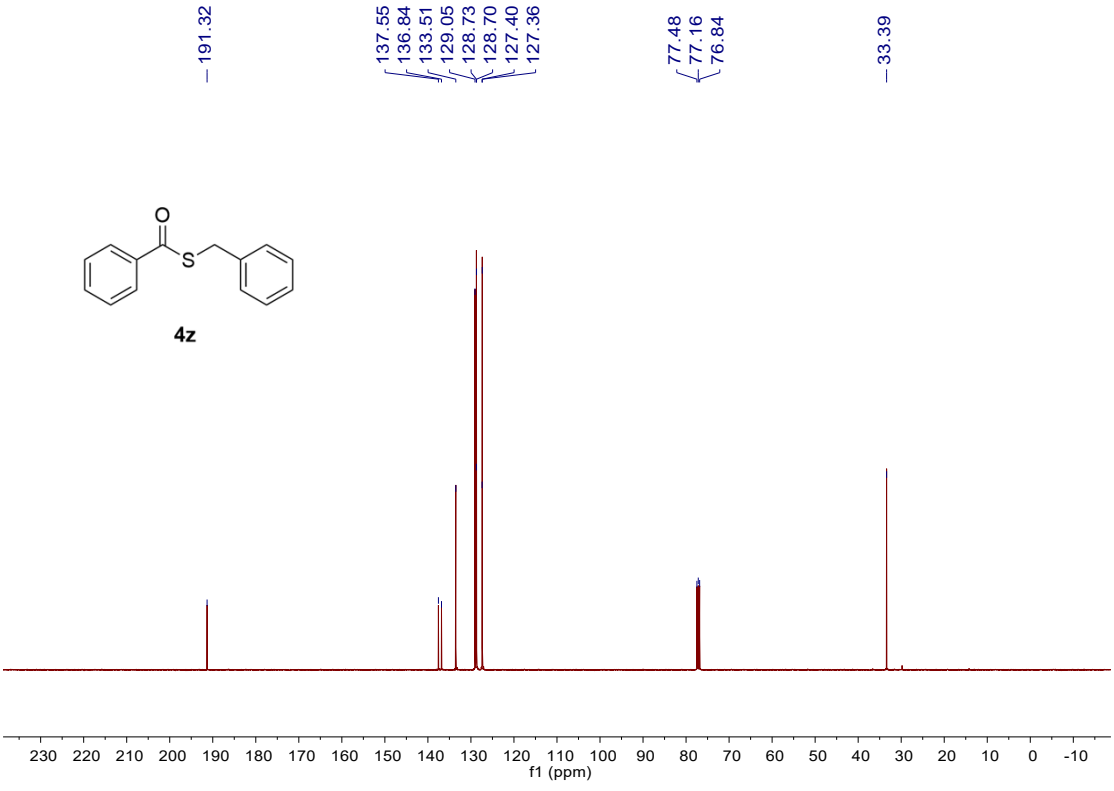
5.97
5.97
5.97
2.15
2.15
1.86
1.86
1.60
1.59
1.58
1.57
1.55
1.55
1.53
1.37
1.36
1.35
1.35
1.33
1.32
1.31
1.30
1.29
1.27
1.26
1.24
0.88
0.87
0.85
O
S
C11H23
4x
2.15
2.15
1.86
1.86
3.00
3.00
2.20 2.15 2.10 2.05 2.00 1.95 1.90 1.85
f1 (ppm)
1.00
2.00
3.00
3.00
2.01
18.06
3.00
11.0 10.5 10.0 9.5 9.0 8.5 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)

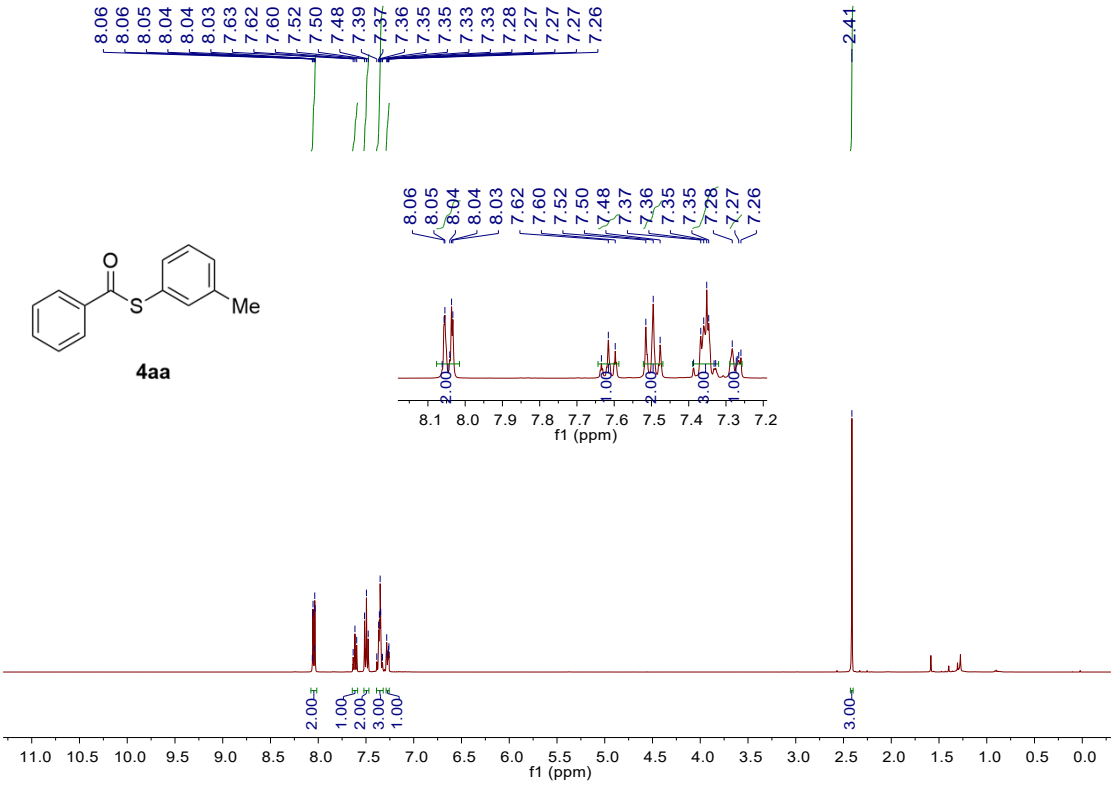

189.60
153.29
123.55
77.48
77.16
76.84
32.05
29.92
29.77
29.76
29.71
29.64
29.48
29.30
29.08
28.87
27.32
22.82
21.21
14.24
O
S
C11H23
4x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

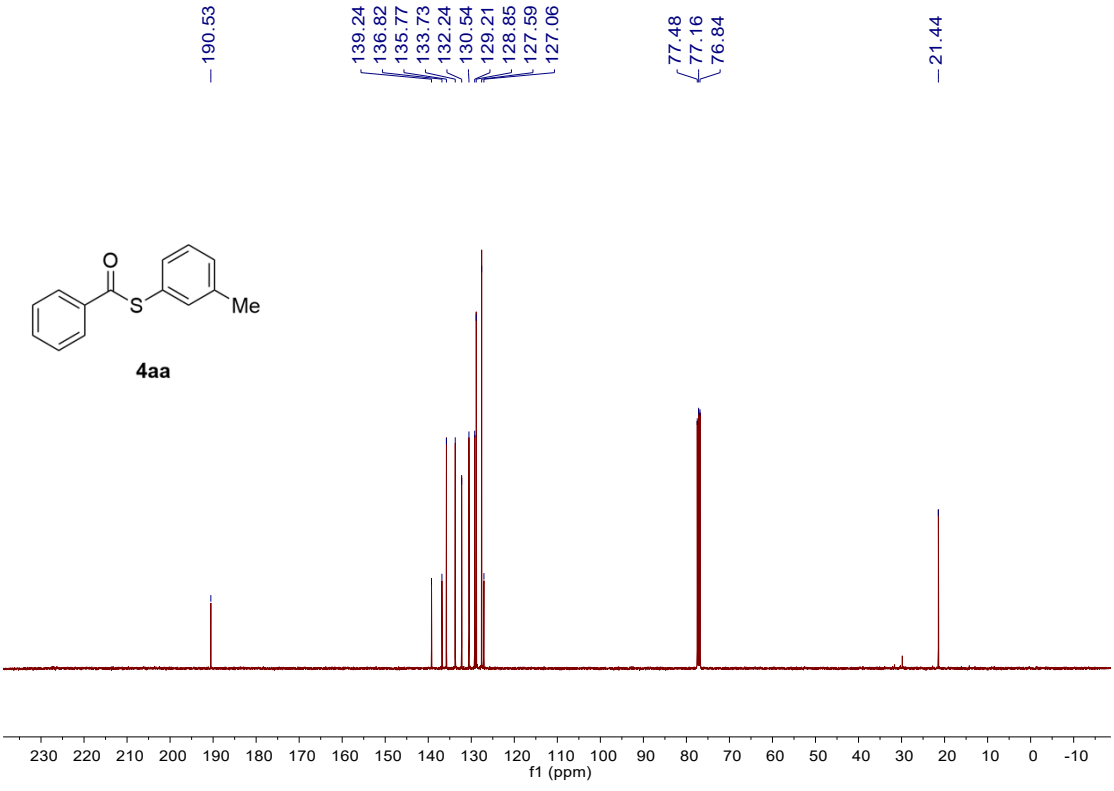

7.58
7.56
7.30
7.28
7.26
3.05
3.03
3.01
2.88
2.88
2.86
2.84
2.84
1.55
1.53
1.51
1.33
1.31
1.29
1.27
1.25
0.89
0.87
O
S
C11H23
NC
4y
2.00
2.00
2.00
4.00
2.00
18.03
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

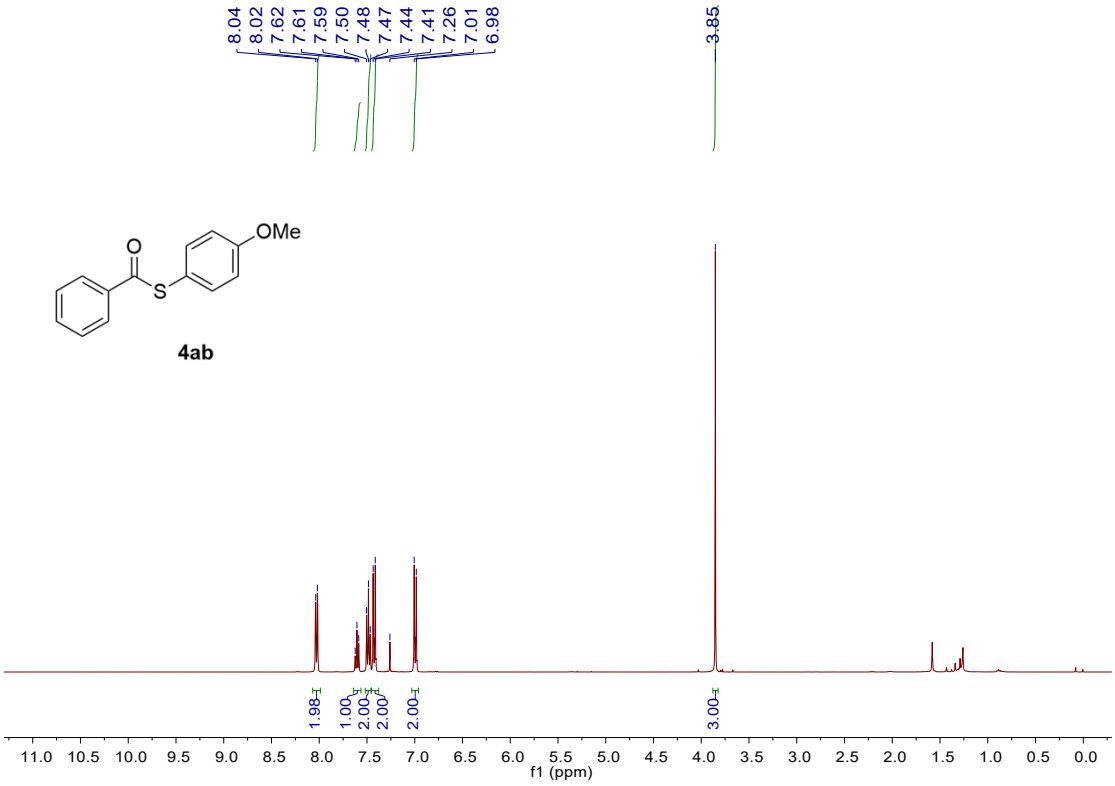

198.18
145.85
132.47
129.35
119.02
110.45
77.48
77.16
76.84
44.62
32.04
31.49
29.76
29.70
29.60
29.59
29.47
29.22
29.15
28.90
22.81
14.26
O
S
C11H23
NC
4y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

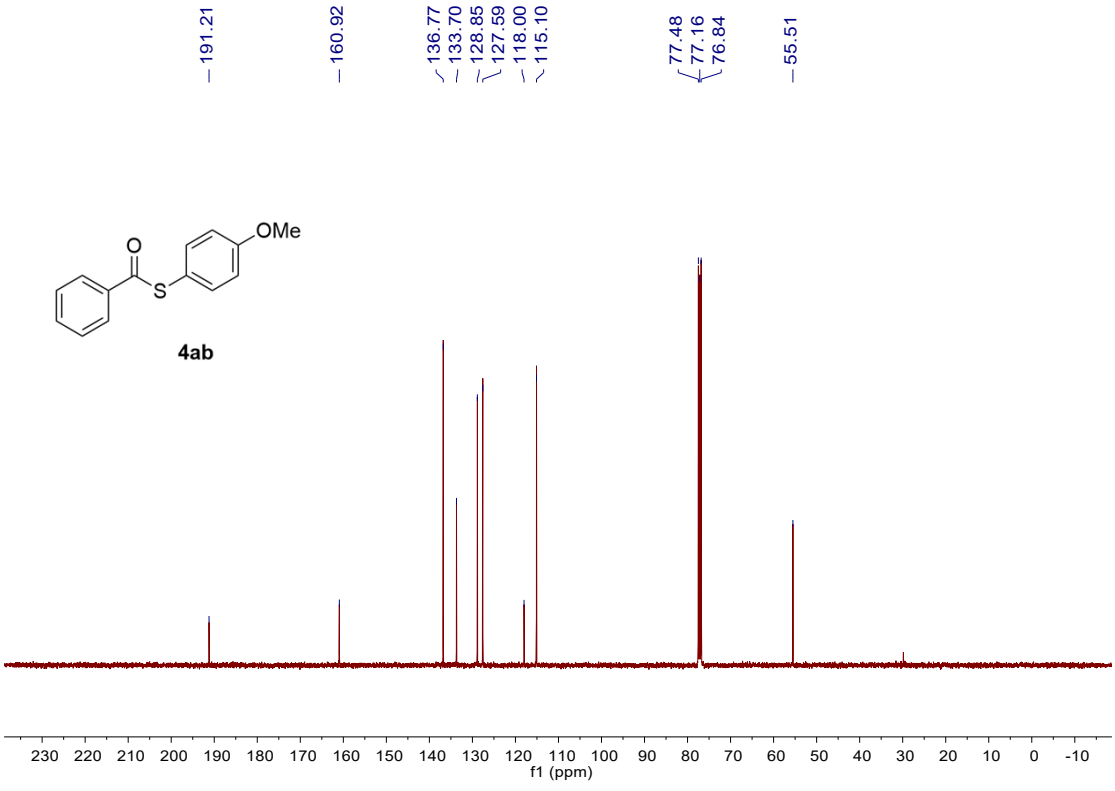

7.97 7.97 7.96 7.95 7.95 7.94 7.55 7.54 7.54 7.53 7.53 7.52 7.51 7.51 7.50 7.42 7.42 7.40 7.39 7.38 7.38 7.37 7.35 7.31 7.31 7.29 7.29 7.28 7.25 7.25 7.24 7.24 7.23 7.22 7.21 7.21 7.21 4.30
O
S
4z
7.97 7.96 7.95 7.94 7.53 7.42 7.40 7.38 7.38 7.37 7.35 7.31 7.29 7.29 7.28 7.25 7.23
2.00 1.00 4.00 2.00 1.00
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
2.00 1.00 4.00 2.00 1.00 2.00
11.0 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)

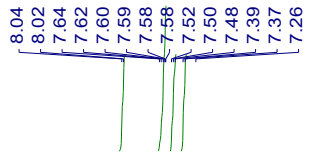

191.32
137.55 136.84 133.51 129.05 128.73 128.70 127.40 127.36
77.48 77.16 76.84
33.39
O
S
4z
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

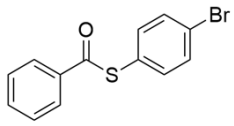

8.06
8.06
8.05
8.04
8.04
8.03
7.63
7.62
7.60
7.52
7.50
7.48
7.39
7.37
7.36
7.35
7.35
7.33
7.33
7.28
7.27
7.27
7.26
2.41
O
S
Me
4aa
2.00
1.00
2.00
3.00
1.00
3.00
f1 (ppm)


190.53
139.24
136.82
135.77
133.73
132.24
130.54
129.21
128.85
127.59
127.06
77.48
77.16
76.84
21.44
O
S
Me
4aa
f1 (ppm)

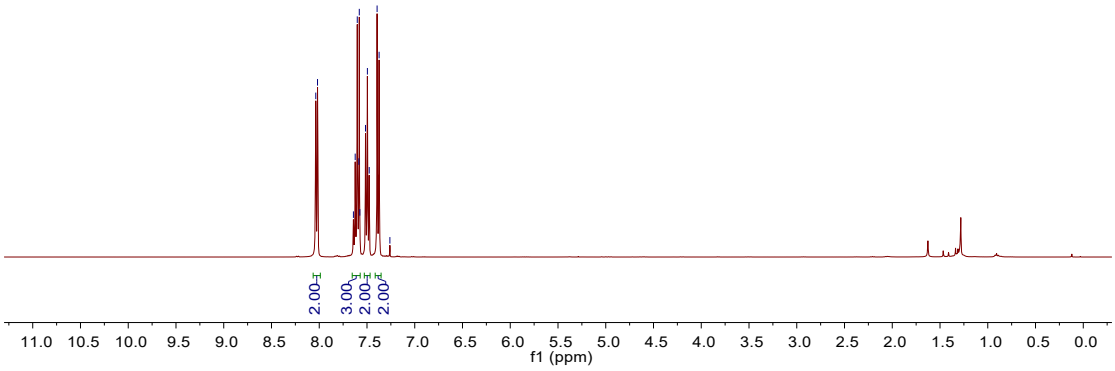

8.04
8.02
7.62
7.61
7.59
7.50
7.48
7.47
7.44
7.41
7.26
7.01
6.98
3.85
OMe
O
S
4ab
1.98
1.00
2.00
2.00
2.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

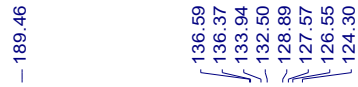

191.21
160.92
136.77
133.70
128.85
127.59
118.00
115.10
77.48
77.16
76.84
55.51
OMe
O
S
4ab
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

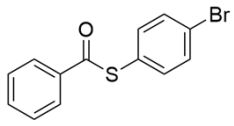

8.04
8.02
7.64
7.62
7.60
7.59
7.58
7.58
7.52
7.50
7.48
7.39
7.37
7.26


O
S
Br

**4ac**

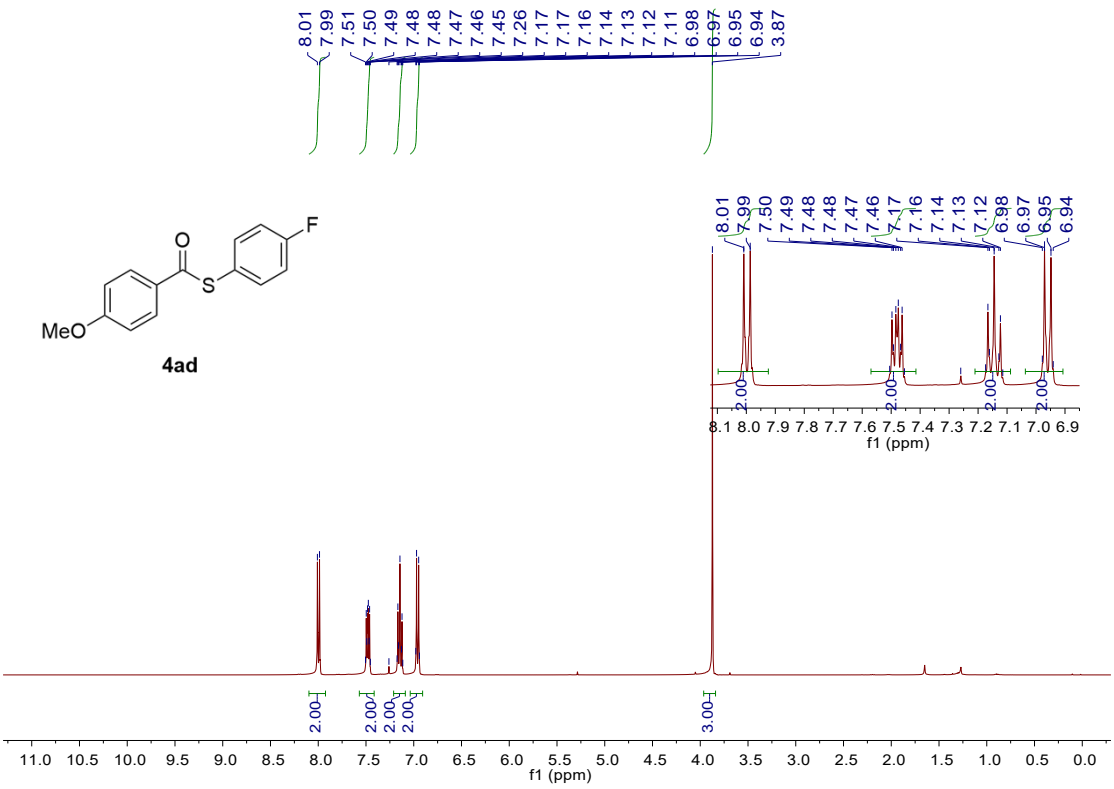

2.00
3.00
2.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

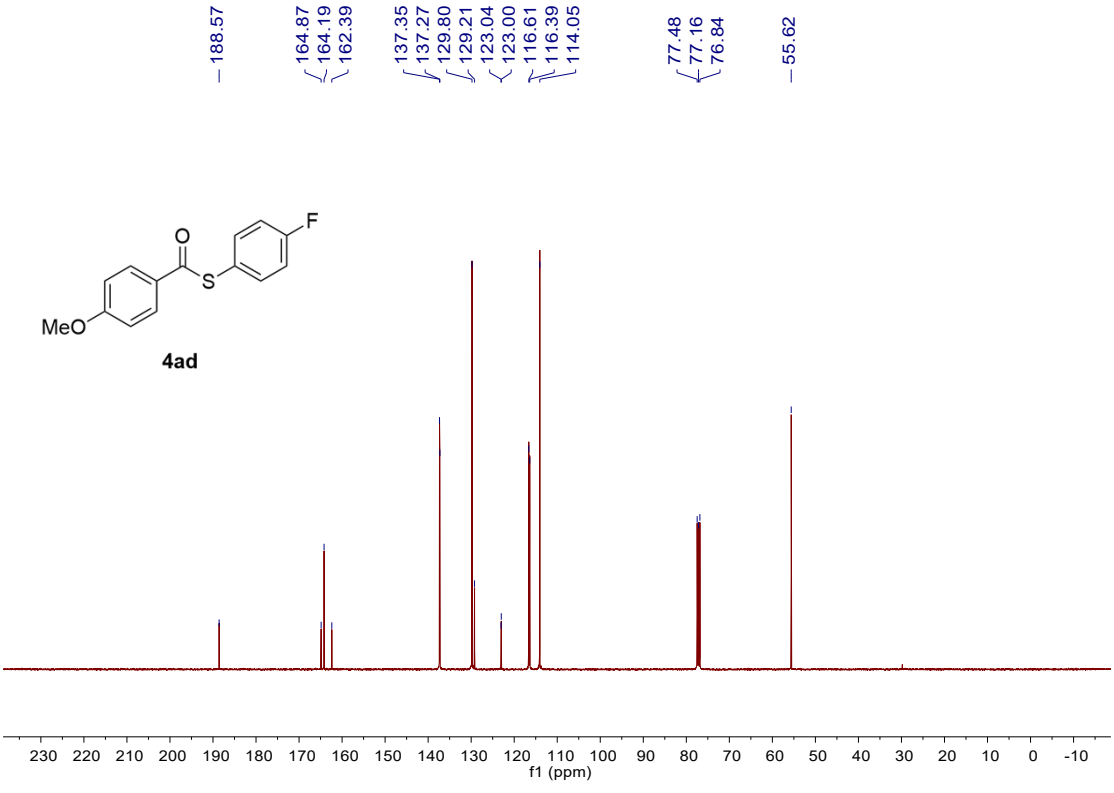

189.46
136.59
136.37
133.94
132.50
128.89
127.57
126.55
124.30
77.48
77.16
76.84

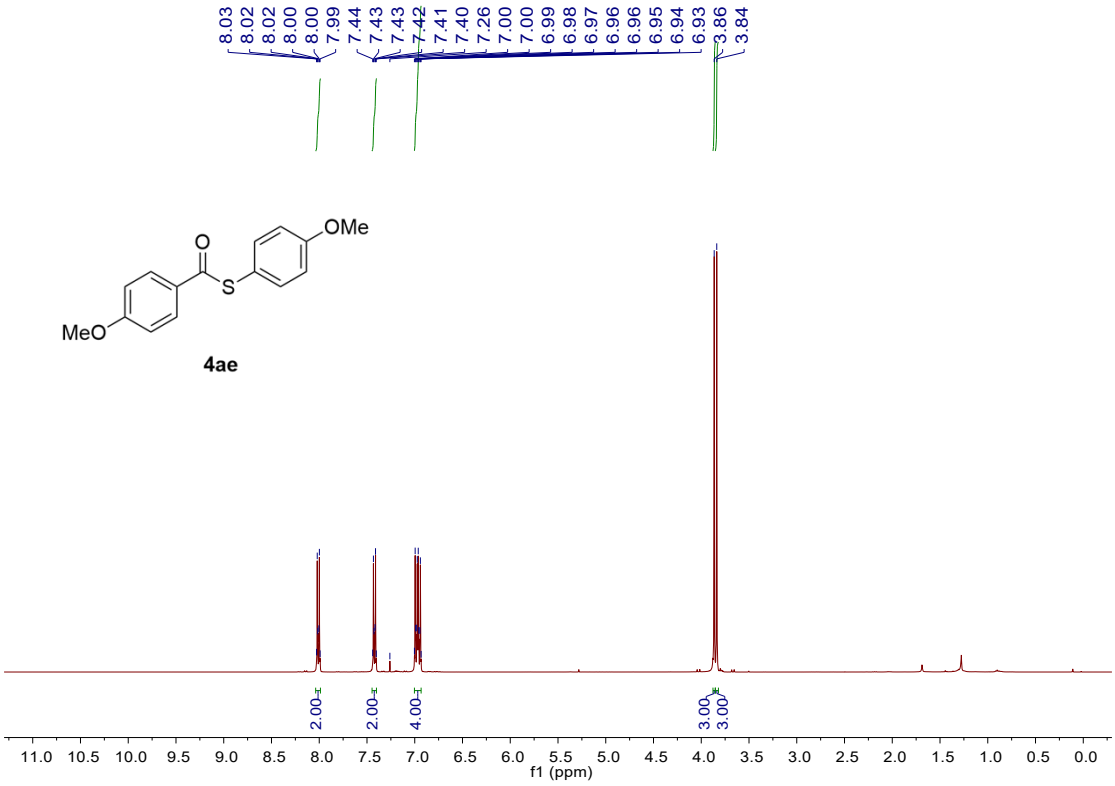

O
S
Br

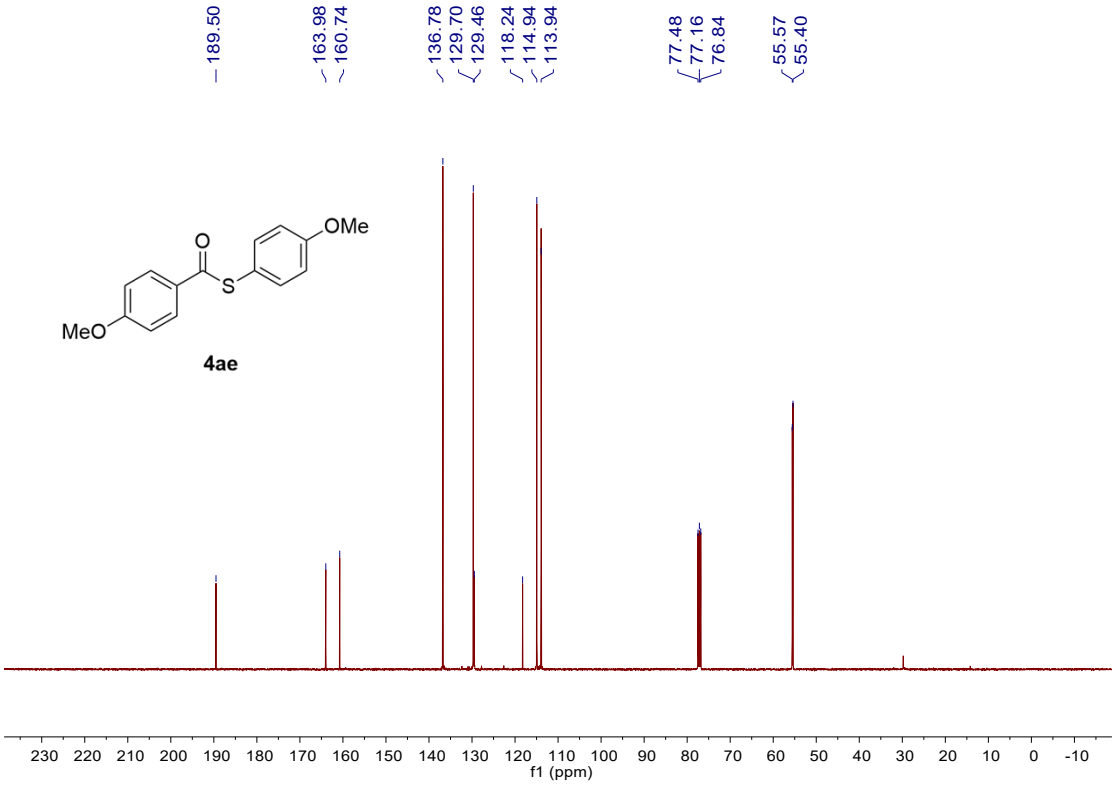
**4ac**

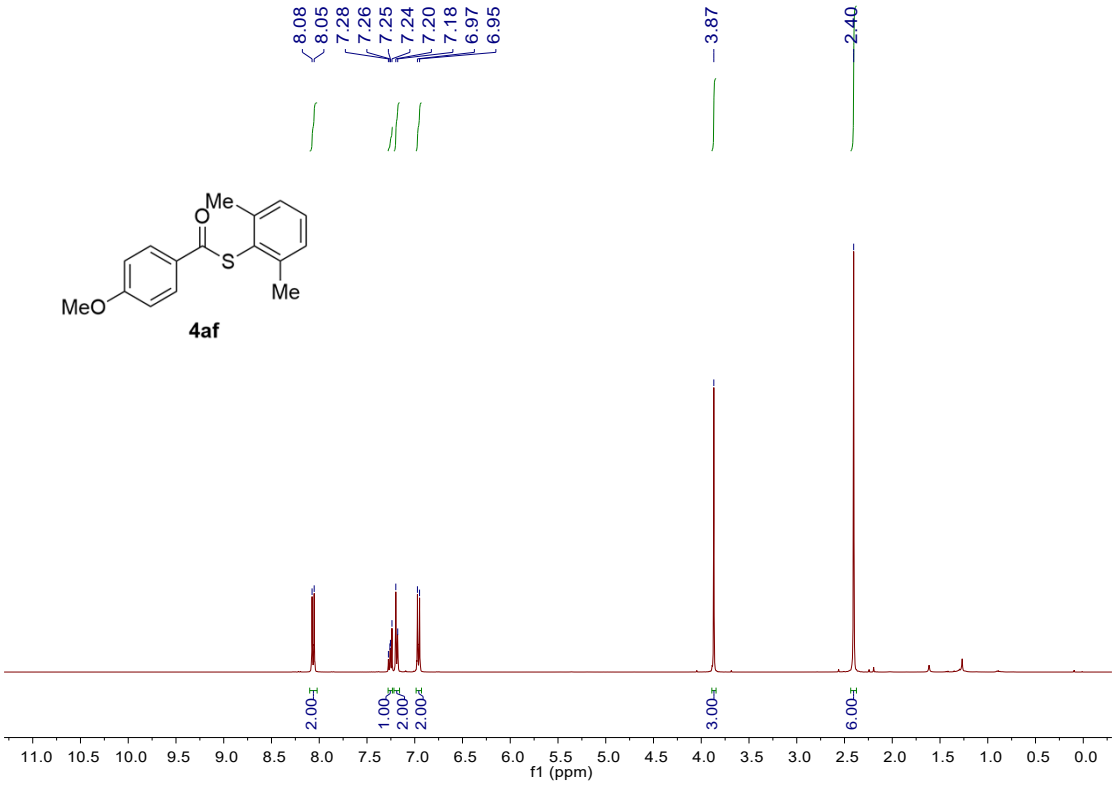

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

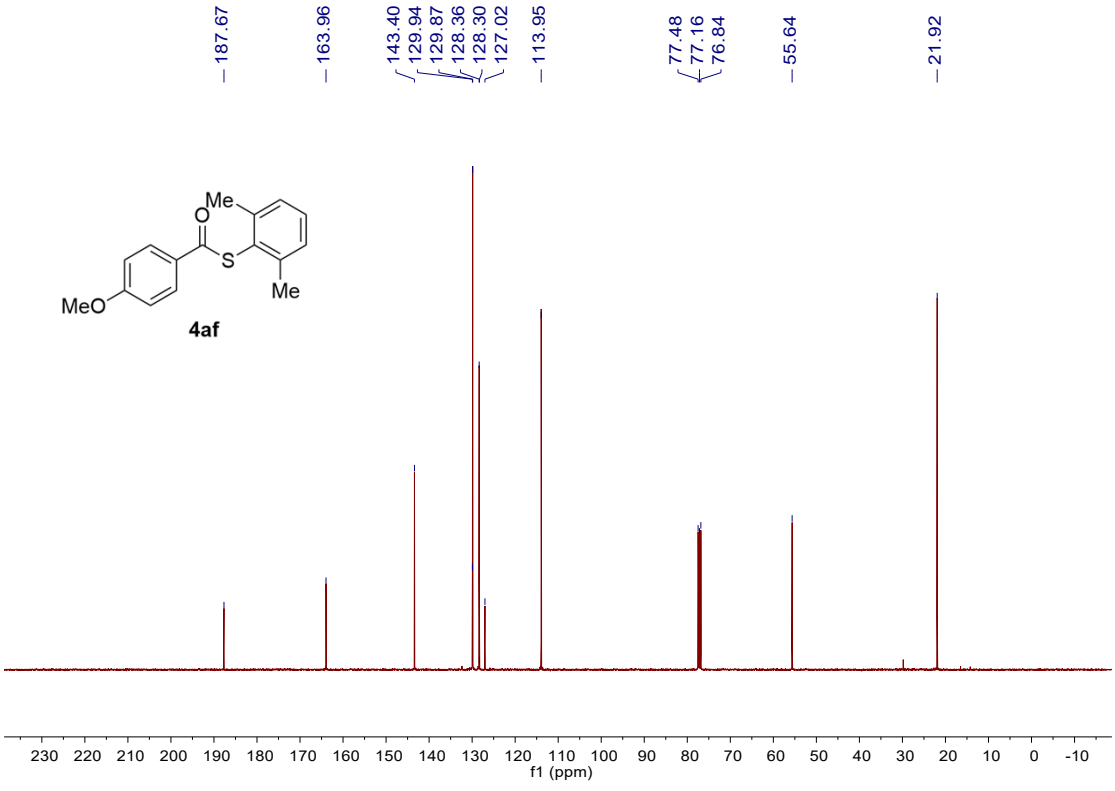

8.01
7.99
7.51
7.50
7.49
7.48
7.48
7.47
7.46
7.45
7.26
7.17
7.17
7.16
7.14
7.13
7.12
7.11
6.98
6.97
6.95
6.94
3.87
F
O
S
MeO
4ad
2.00
2.00
2.00
2.00
3.00
f1 (ppm)

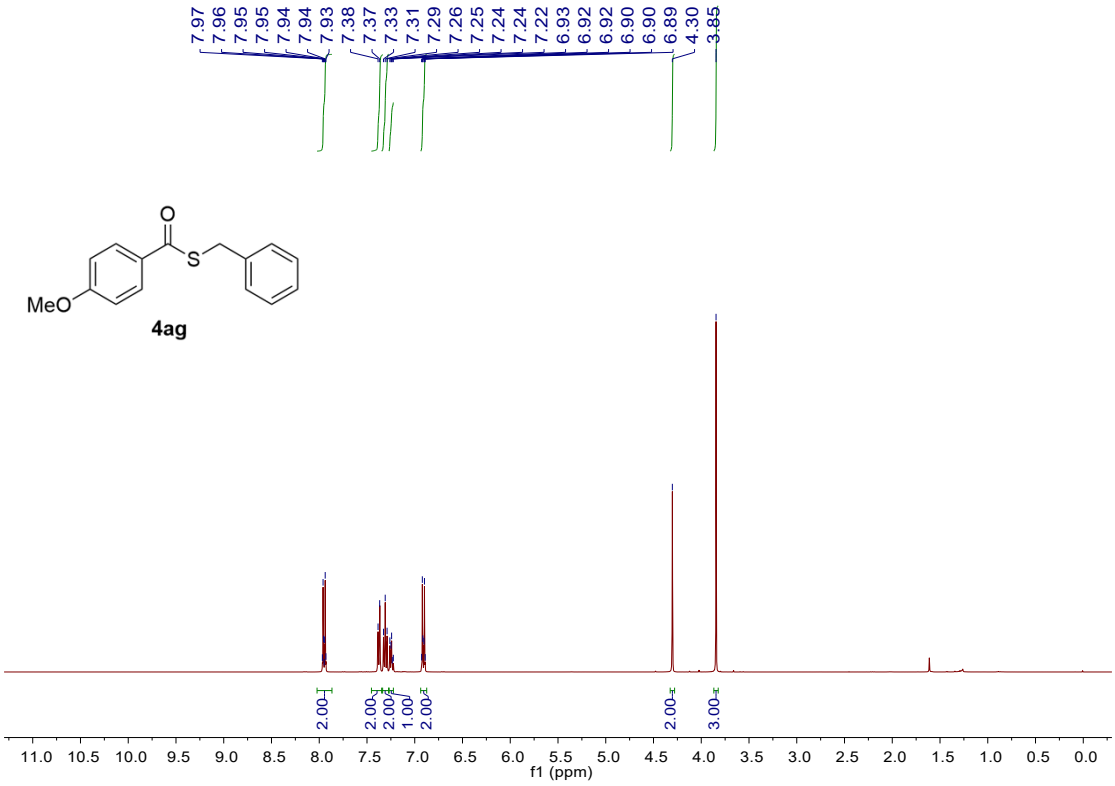

188.57
164.87
164.19
162.39
137.35
137.27
129.80
129.21
123.04
123.00
116.61
116.39
114.05
77.48
77.16
76.84
55.62
F
O
S
MeO
4ad
f1 (ppm)

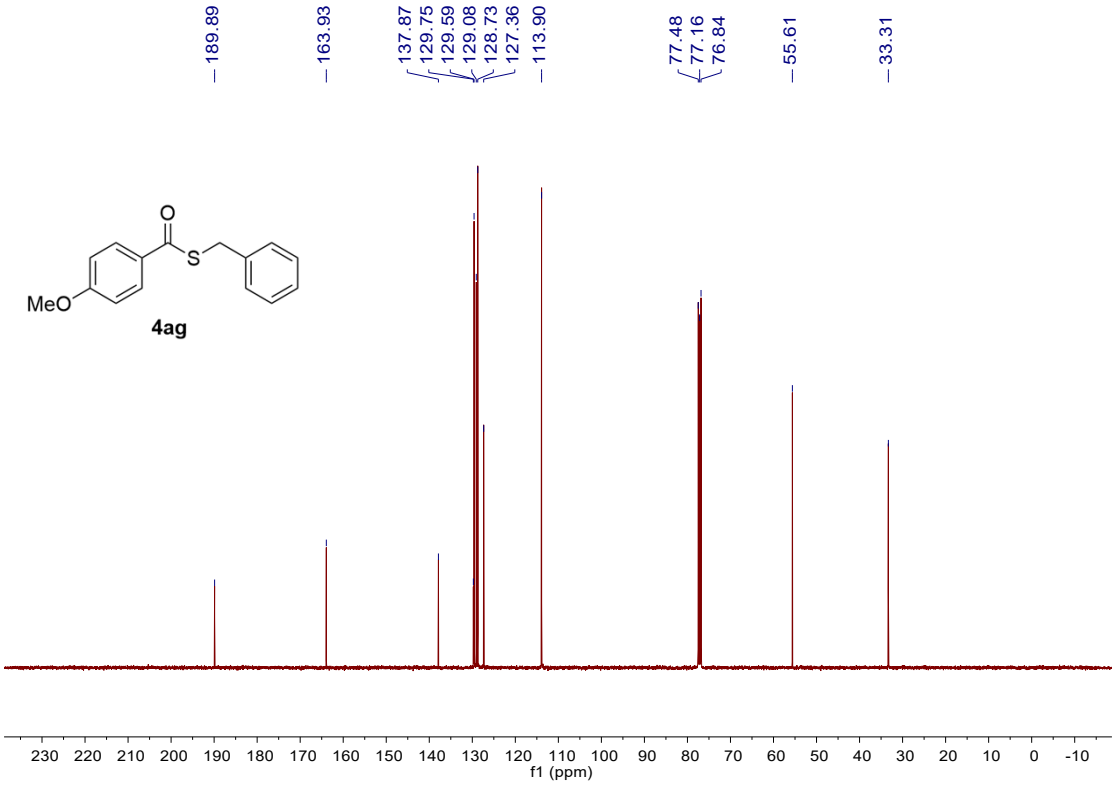

8.03
8.02
8.02
8.00
8.00
7.99
7.44
7.43
7.43
7.42
7.41
7.40
7.26
7.00
7.00
6.99
6.98
6.97
6.96
6.96
6.95
6.94
6.93
3.86
3.84
OMe
O
S
MeO
4ae
2.00
2.00
4.00
3.00
3.00
f1 (ppm)

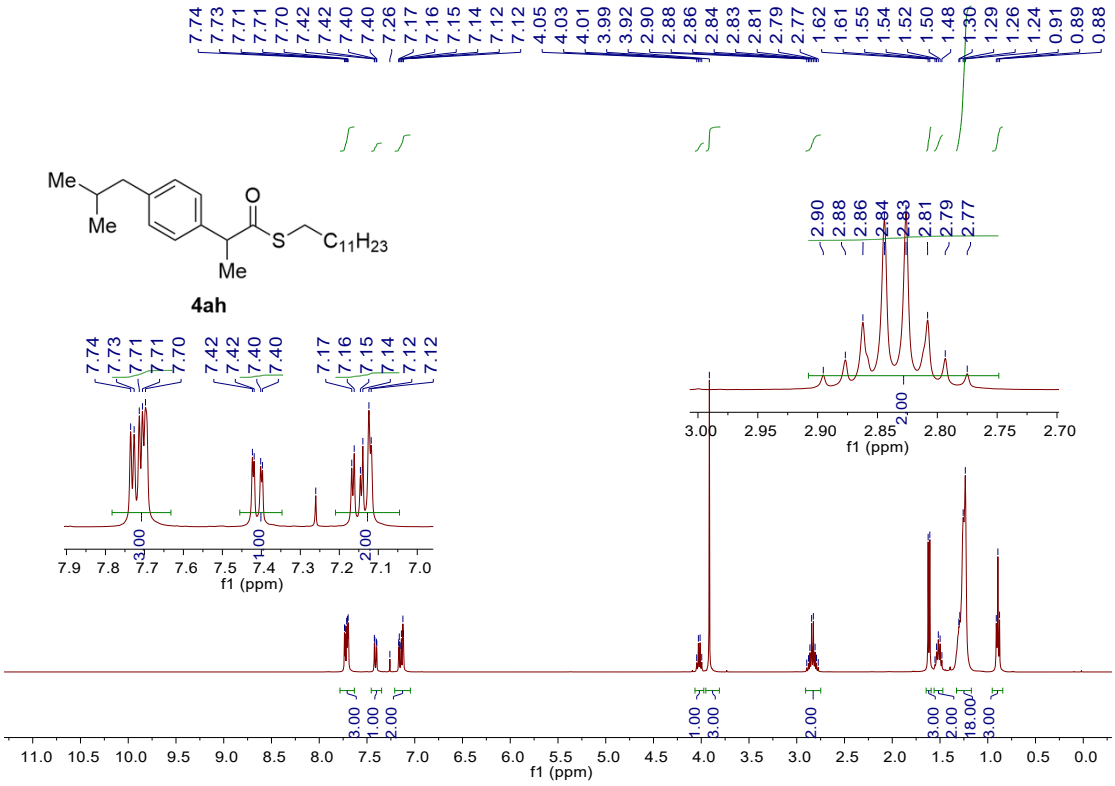

189.50
163.98
160.74
136.78
129.70
129.46
118.24
114.94
113.94
77.48
77.16
76.84
55.57
55.40
OMe
O
S
MeO
4ae
f1 (ppm)

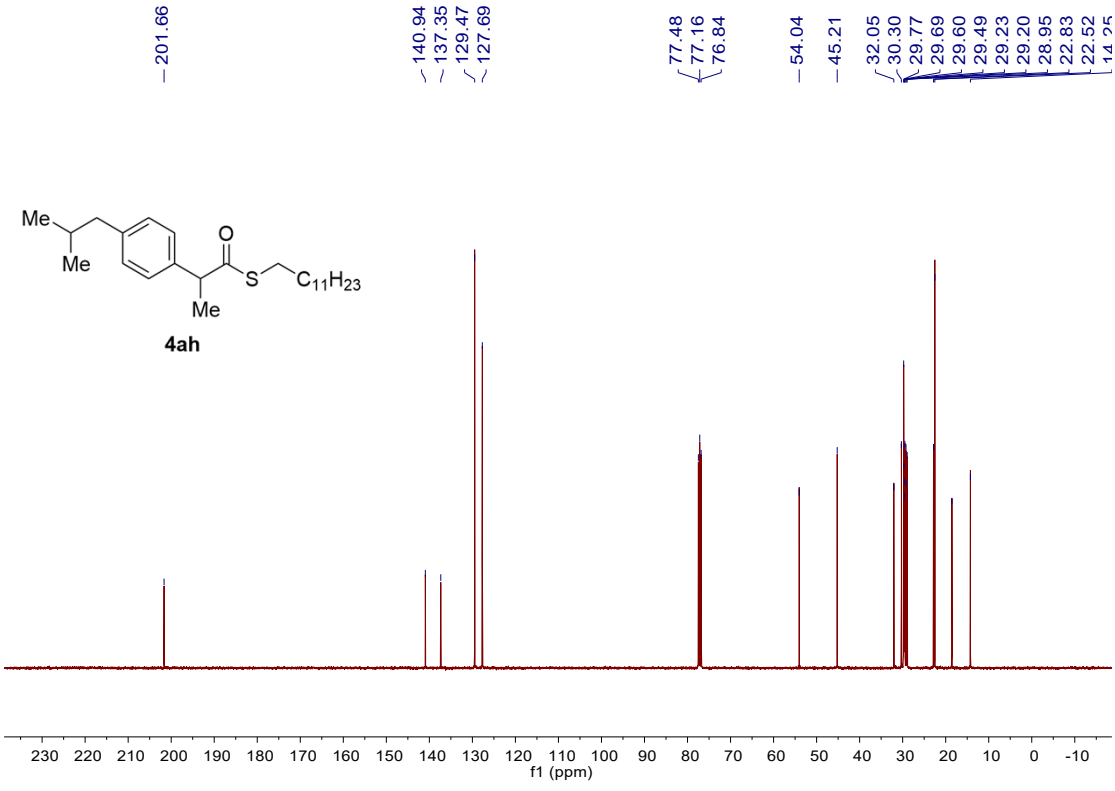

8.08
8.05
7.28
7.26
7.25
7.24
7.20
7.18
6.97
6.95
3.87
2.40
Me
O
S
Me
MeO
4af
2.00
1.00
2.00
2.00
3.00
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

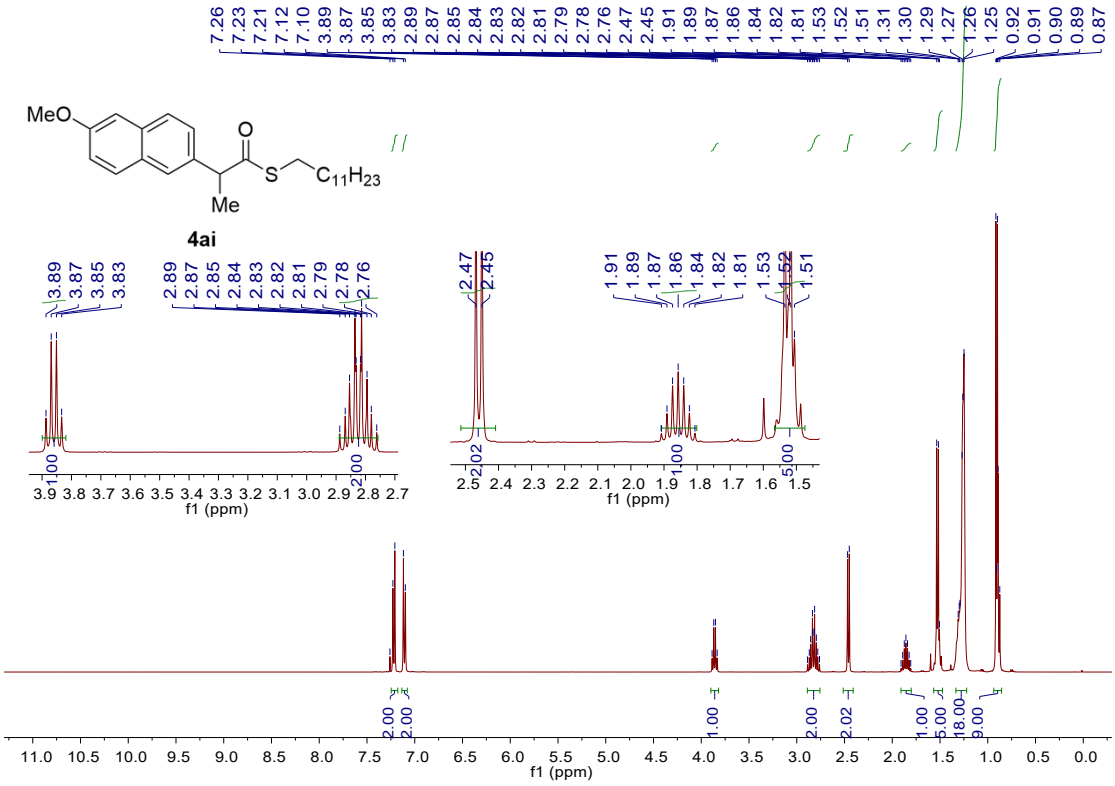

187.67
163.96
143.40
129.94
129.87
128.36
128.30
127.02
113.95
77.48
77.16
76.84
55.64
21.92
Me
O
S
Me
MeO
4af
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

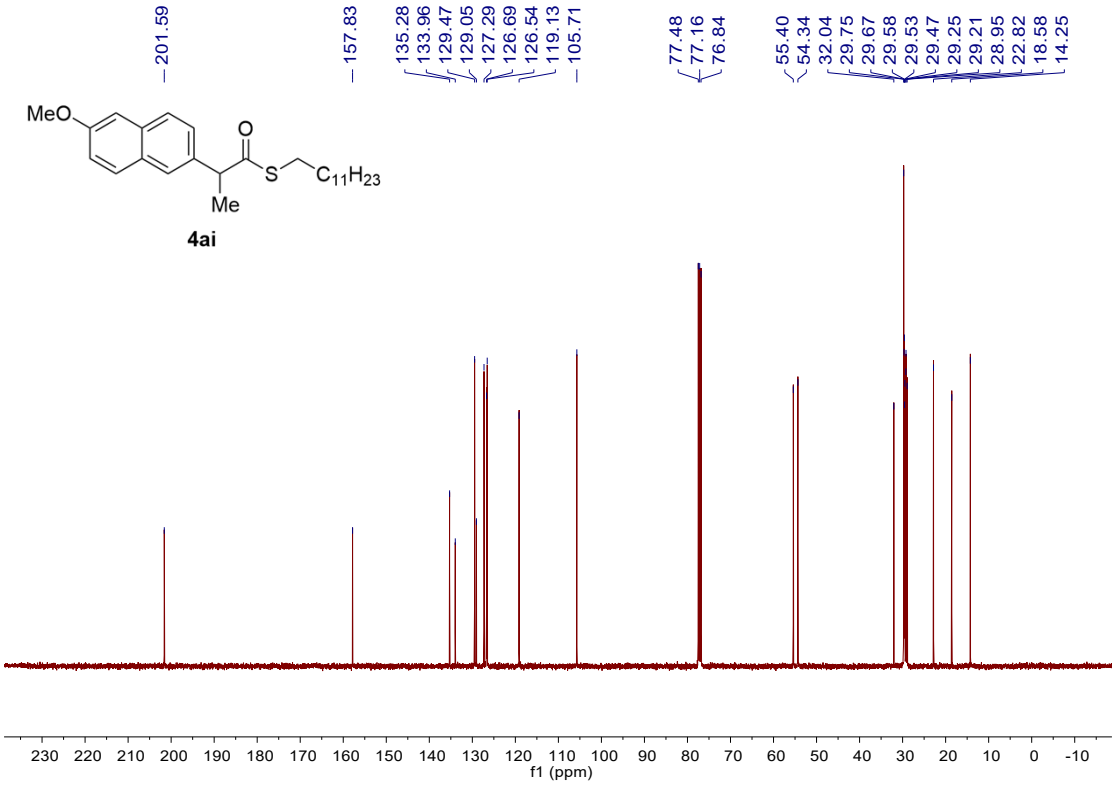

7.97
7.96
7.95
7.95
7.94
7.94
7.93
7.38
7.37
7.33
7.31
7.29
7.26
7.25
7.24
7.24
7.22
6.93
6.92
6.92
6.90
6.90
6.89
4.30
3.85
O
S
MeO
4ag
2.00
2.00
2.00
1.00
2.00
2.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

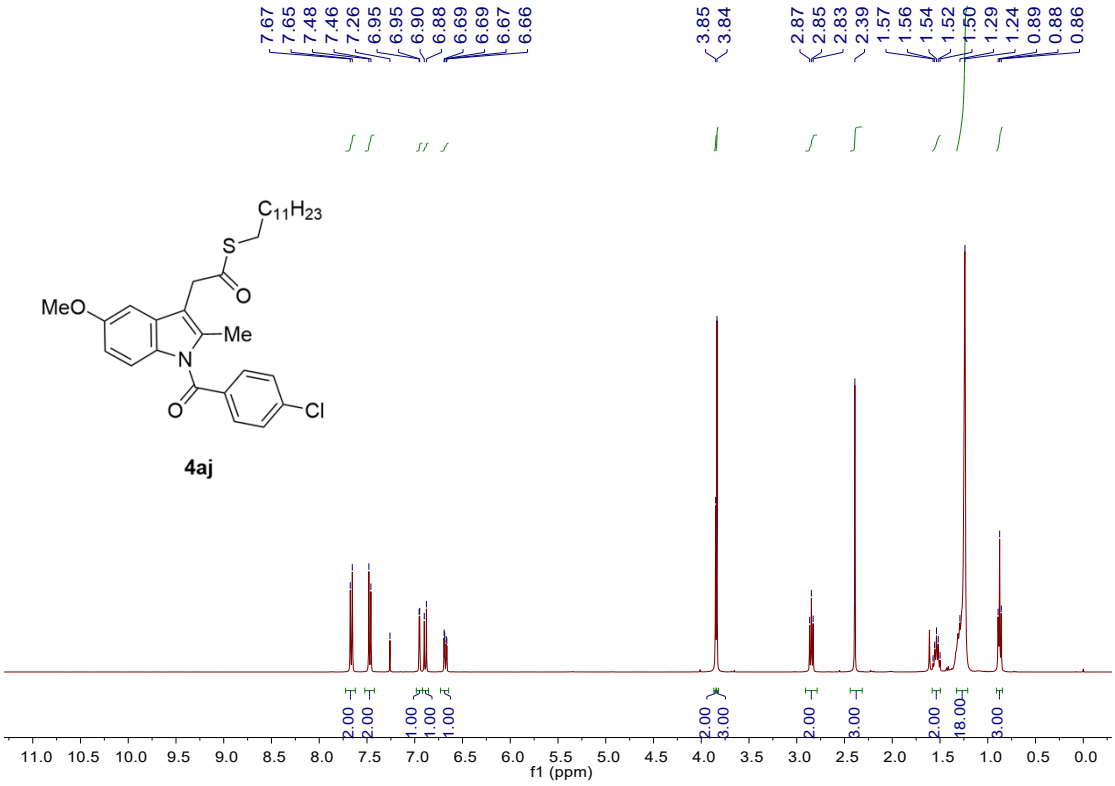

189.89
163.93
137.87
129.75
129.59
129.08
128.73
127.36
113.90
77.48
77.16
76.84
55.61
33.31
O
S
MeO
4ag
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

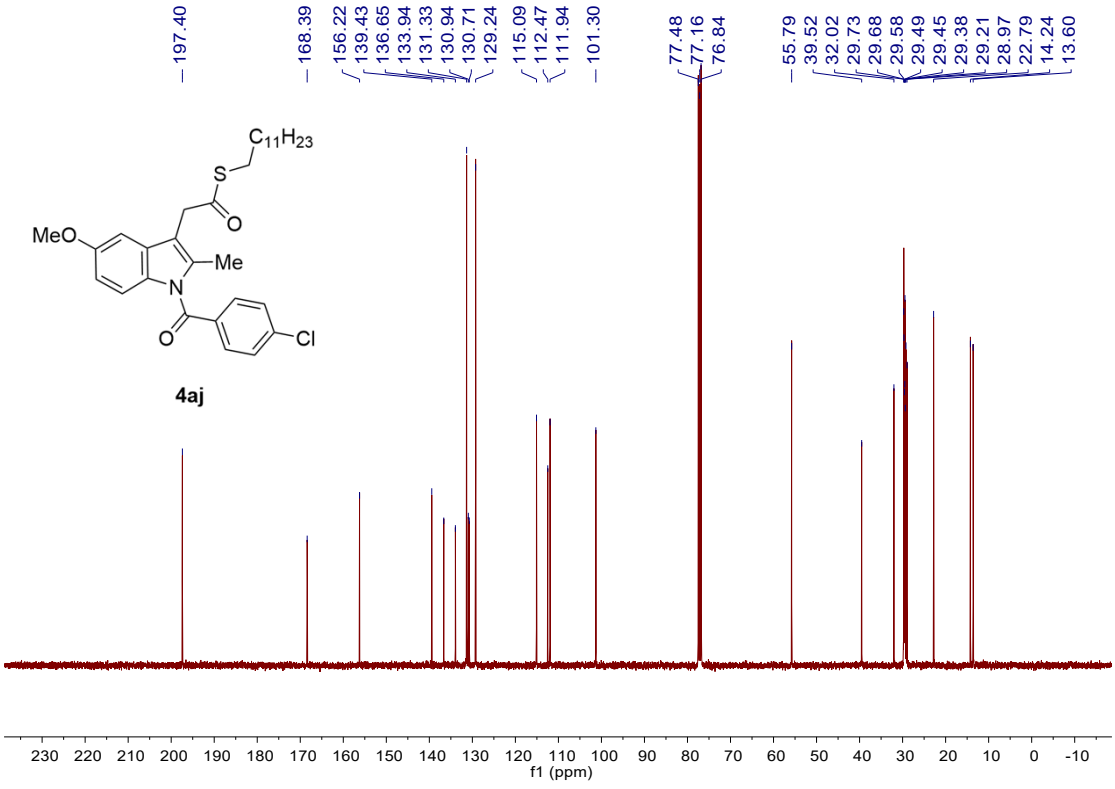

7.74 7.73 7.71 7.71 7.70 7.42 7.42 7.40 7.40 7.26 7.17 7.16 7.15 7.14 7.12 7.12
4.05 4.03 4.01 3.99 3.92 2.90 2.88 2.86 2.84 2.83 2.81 2.79 2.77 1.62 1.61 1.55 1.54 1.52 1.50 1.48 1.30 1.29 1.26 1.24 0.91 0.89 0.88
Me
Me
O
S
C11H23
Me
4ah
f1 (ppm)

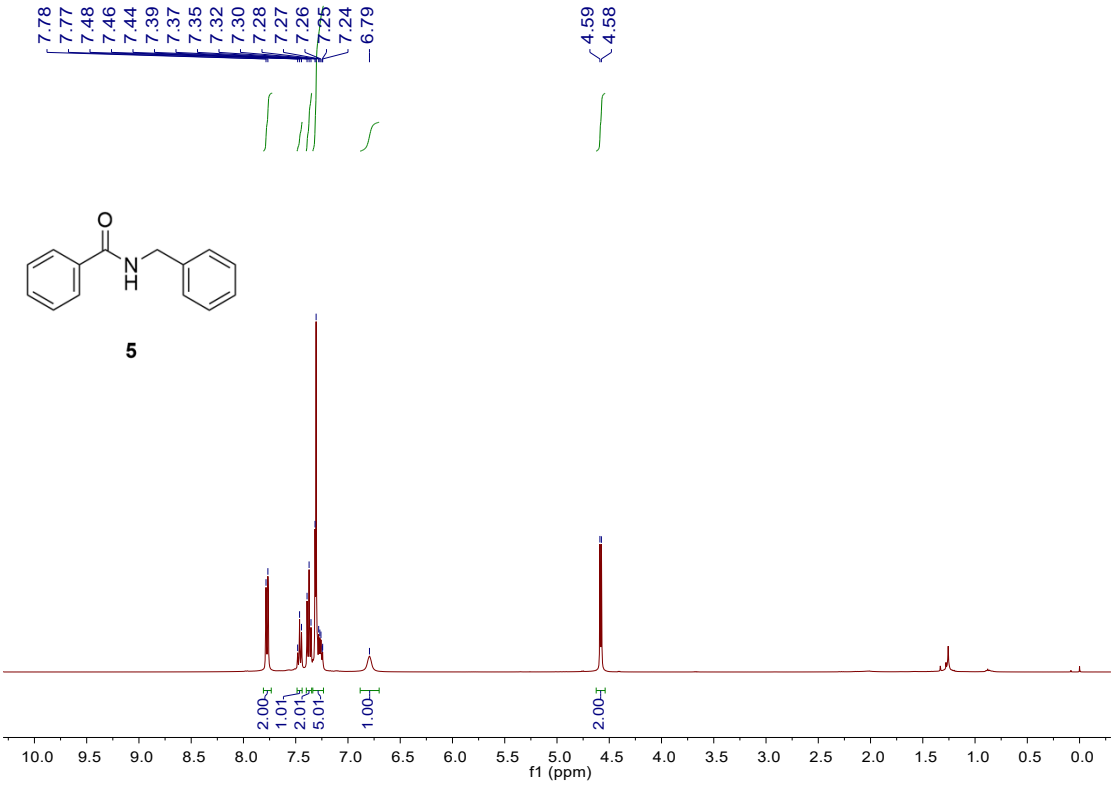

201.66
140.94 137.35 129.47 127.69
77.48 77.16 76.84
54.04 45.21
32.05 30.30 29.77 29.69 29.60 29.49 29.23 29.20 28.95 22.83 22.52
Me
Me
O
S
C11H23
Me
4ah
f1 (ppm)

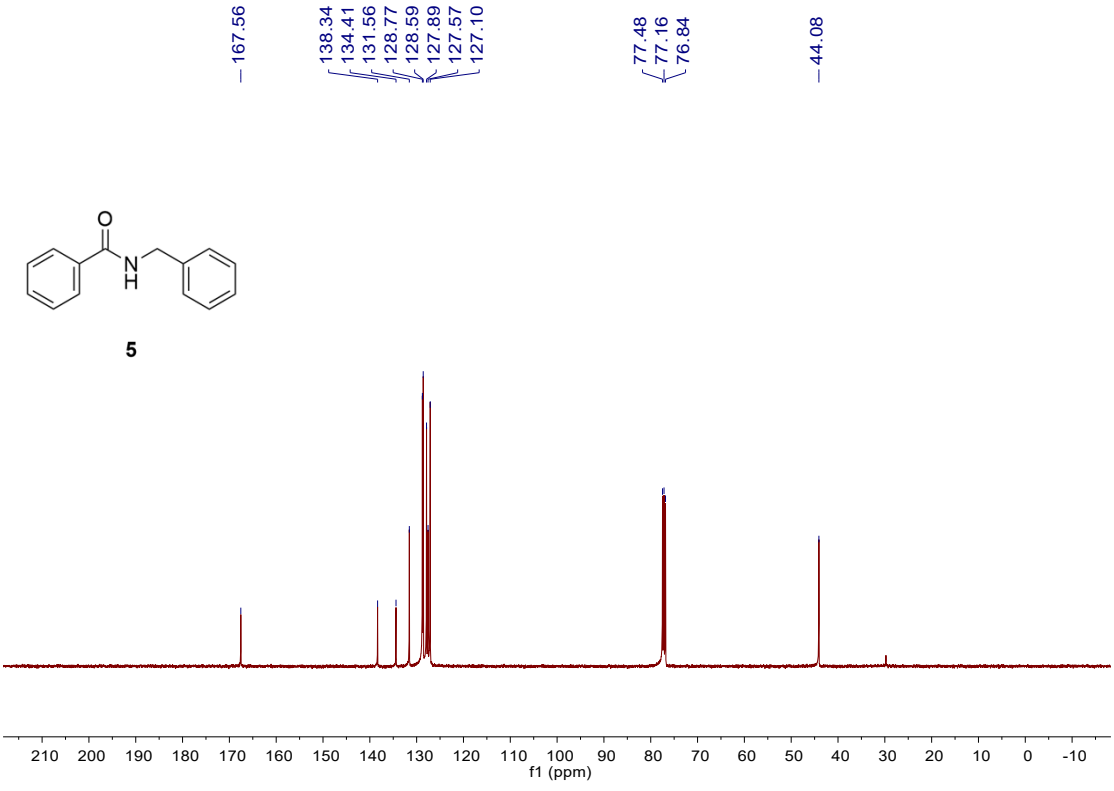

MeO
O
S
$C_{11}H_{23}$
Me
4ai
f1 (ppm)


MeO
O
S
$C_{11}H_{23}$
Me
4ai
f1 (ppm)


7.67
7.65
7.48
7.46
7.26
6.95
6.95
6.90
6.88
6.69
6.69
6.67
6.66
3.85
3.84
2.87
2.85
2.83
2.39
1.57
1.56
1.54
1.52
1.50
1.29
1.24
0.89
0.88
0.86
C11H23
S
O
MeO
Me
N
O
Cl
4aj
2.00
2.00
1.00
1.00
1.00
2.00
3.00
2.00
3.00
2.00
18.00
3.00
11.0 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)


197.40
168.39
156.22
139.43
136.65
133.94
131.33
130.94
130.71
129.24
115.09
112.47
111.94
101.30
77.48
77.16
76.84
55.79
39.52
32.02
29.73
29.68
29.58
29.49
29.45
29.38
29.21
28.97
22.79
14.24
13.60
C11H23
S
O
MeO
Me
N
O
Cl
4aj
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.78
7.77
7.48
7.46
7.44
7.39
7.37
7.35
7.32
7.30
7.28
7.27
7.26
7.25
7.24
6.79
4.59
4.58
O
N
H
5
2.00
1.01
2.01
5.01
1.00
2.00
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)


167.56
138.34
134.41
131.56
128.77
128.59
127.89
127.57
127.10
77.48
77.16
76.84
44.08
O
N
H
5
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)