Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Paired electrochemical C–H bromination of (hetero)arenes with 2-bromoethan-1-ol

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1. General Considerations

Unless otherwise noted, chemicals and materials were purchased from commercial suppliers and used without further purification. All ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker FT-NMR spectrometer. Data were reported as chemical shifts in ppm relative to TMS (0.00 ppm) or DMSO-d_6 (2.50 ppm) for ^{1}H NMR and $CDCl_3$ (77.2 ppm) or DMSO-d_6 (40.0 ppm) for ^{13}C NMR. The abbreviations used for explaining the multiplicities were as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. The coupling constants, *J*, are reported in Hertz (Hz). High resolution mass spectroscopy data of the product were collected on a Thermofisher Q Exactive Accurate-Mass Q-Orbitrap LC/MS (HESI). X-Ray data were collected on a Bruker SMART APEX Ⅱ instrument with an IμS Mo microsource (λ = 0.7107 A). Products were purified by flash chromatography on 200–300 mesh silica gels, SiO_2.

2. General Procedure for the Electrosynthesis

General procedure for the model reaction: A 20 mL three-necked beaker-type cell (Figure S1A) was charged with nBu$_4$NBF$_4$ (0.15 mmol). The cell was equipped with a reticulated vitreous carbon (RVC, 100 PPI, 1.2 cm x 0.8 cm x 0.8 cm) anode and a platinum plate (1.0 cm x 1.0 cm x 0.1 mm) cathode (Figure S1B). 1-Methoxy-4-propylbenzene (**1**, 0.30 mmol), 2-bromoethan-1-ol (**2**, 0.9 mmol), MeCN (7.0 mL) were added. The electrolysis was carried out at room temperature using a constant current of 10 mA for 3.0 h. The reaction mixture was concentrated under reduced pressure and the residue was chromatographed through silica gel eluting with ethyl acetate/petroleum ether to give the desired product.

General procedure for the gram-scale synthesis of 3: The gram-scale electrolysis was conducted in a 100 mL three-necked round-bottomed flask with a piece of RVC (1.2 cm x 2.0 cm x 2.0 cm) as the anode, a Pt plate as the cathode (1.5 cm x 1.5 cm x 0.3 mm), and a constant current of 62 mA for 10 h at room temperature (Figure S1C). The reaction mixture consisted 1-methoxy-4-propylbenzene (**1**, 0.90 g, 6.0 mmol), 2-

bromoethan-1-ol (**2**, 2.25 g, 9.0 mmol), nBu$_4$NBF$_4$ (0.99 g, 3.0 mmol), MeCN (90 mL). When the reaction was complete, the reaction mixture was concentrated under reduced pressure and the residue was chromatographed through silica gel eluting with ethyl acetate/petroleum ether to give the desired product **3** (0.67 g, 55% yield).

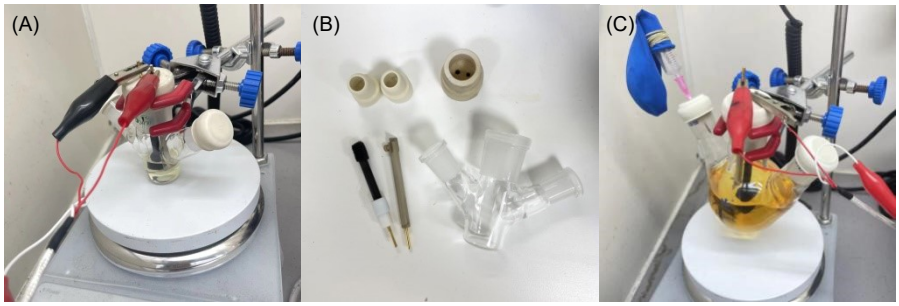


Figure S1. The electrolysis setup [The RVC is fixed on a sharpened graphite rod (∅ 6 mm)].

3. Mechanistic Studies

3.1 Cyclic voltammetry studies

The cyclic voltammograms were recorded in an electrolyte of nBu$_4$NBF$_4$ (0.1 M) in MeCN (5 mL) using a glassy carbon disk working electrode (diameter, 3 mm), a Pt wire auxiliary electrode and a Ag/AgCl reference electrode. The scan rate was 100 mV/s.

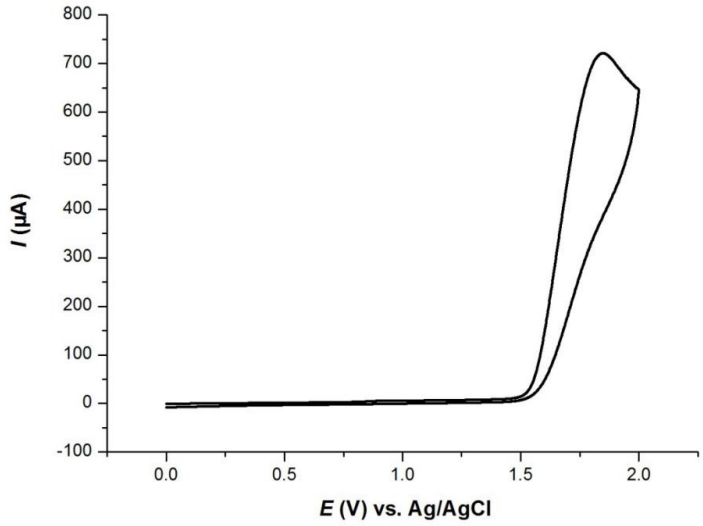


Figure S2. Cyclic voltammogram of 1-methoxy-4-propylbenzene in an electrolyte of nBu$_4$NBF$_4$ (0.1 M) in MeCN, $E_{p/2}$ = 1.66 V.

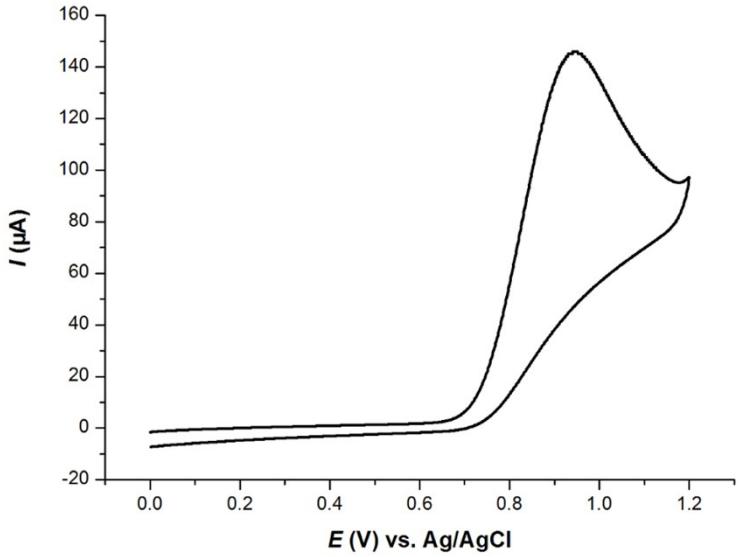


Figure S3. Cyclic voltammogram of nBu$_4$NBr in an electrolyte of nBu$_4$NBF$_4$ (0.1 M) in MeCN, $E_{p/2}$ = 0.82 V.

3.2 GC-MS analysis and detection of ethylene oxide

The reaction solution of **1** and **2** was detected by GC-MS analysis on a GCMS-QP2020 NX, and a peak of ethylene oxide was observed by comparison with standard diagram of spectral library. This proves that the bromide ion is formed by the reduction of 2-bromoethan-1-ol (**2**) at the cathode to release ethylene oxide.

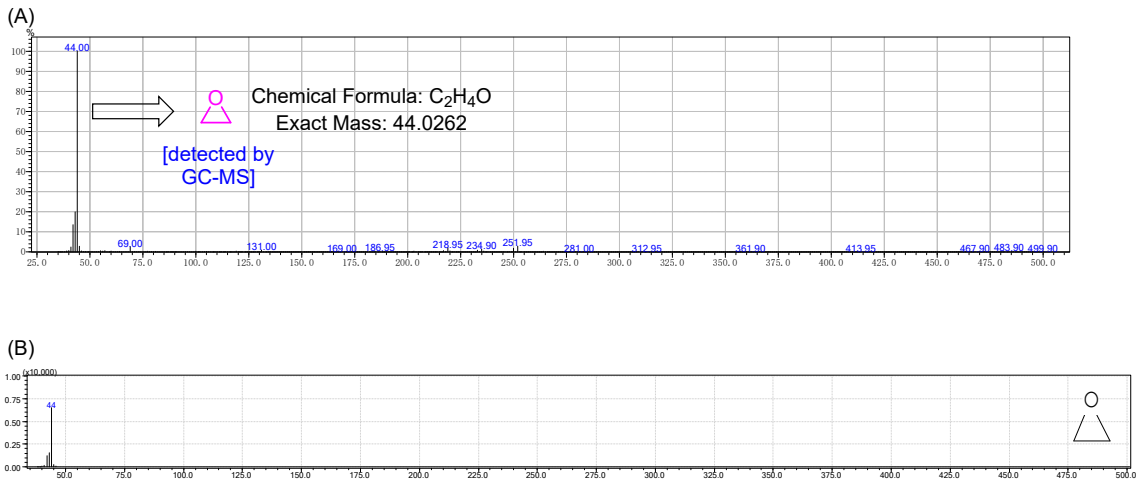


Figure S4. Test diagram (A) and standard diagram of spectral library (B)

4. Unsuccessful Substrates

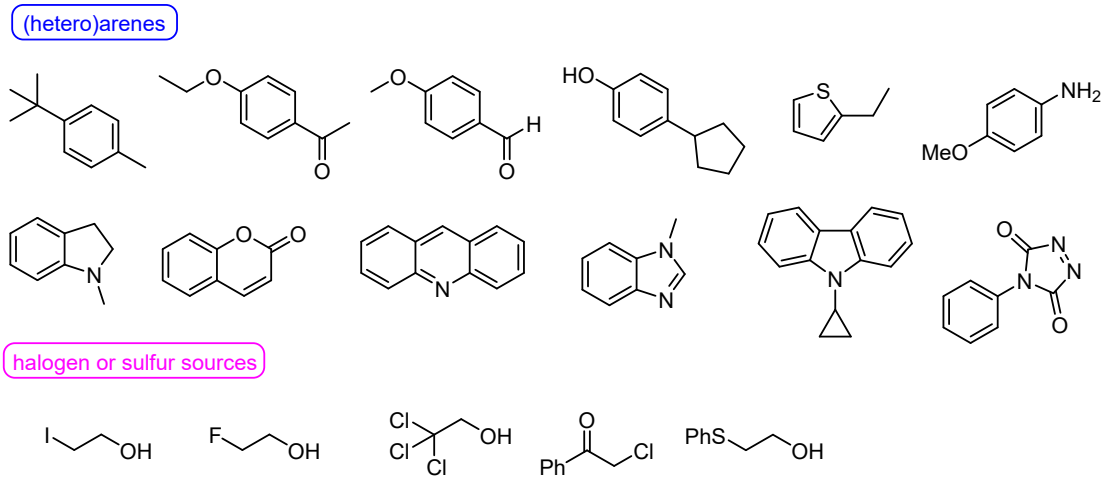
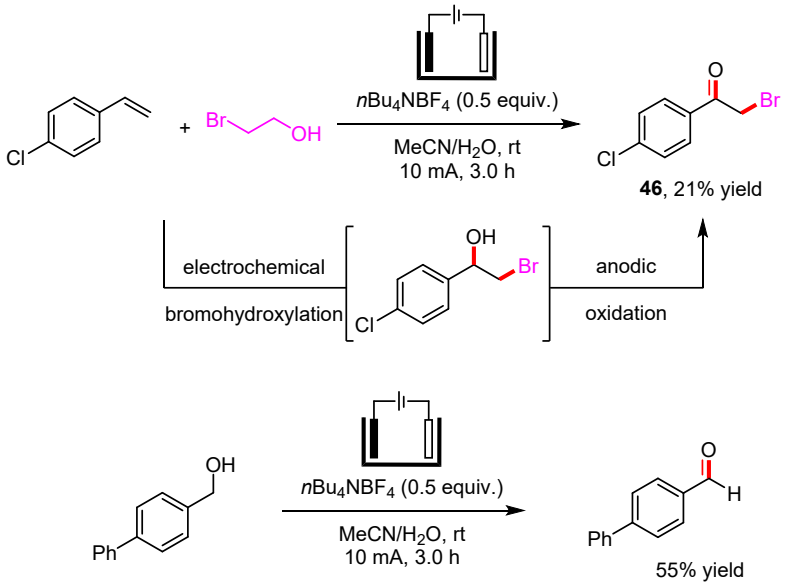


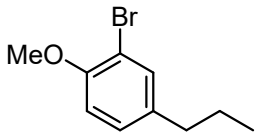
Figure S5. Unsuccessful substrates

5. Formation of Product 46

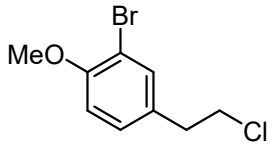


α-Bromoketone **46** may be formed by further oxidation of benzyl alcohol intermediate produced by the electrochemical bromohydroxylation of 4-chlorostyrene. [1,1'-biphenyl]-4-ylmethanol could be oxidized at the anode to form [1,1'-biphenyl]-4-carbaldehyde in 55% yield under electrochemical conditions. Benzyl alcohol moiety is more easily oxidized than alkyl alcohol, which allows the bromohydroxylation product **47** to be obtained.

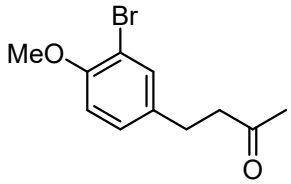
6. Characterization Data for the Electrolysis Products



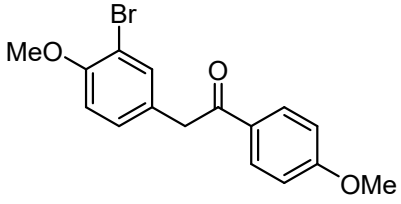
2-Bromo-1-methoxy-4-propylbenzene (3)[1]. Yellow oil (60.7 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 2.1 Hz, 1H), 7.05 (dd, J = 8.3, 2.1 Hz, 1H), 6.80 (d, J = 8.3 Hz, 1H), 3.85 (s, 3H), 2.49 (t, J = 7.6 Hz, 2H), 1.62–1.56 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 136.5, 133.3, 128.4, 111.9, 111.4, 56.4, 36.9, 24.7, 13.8.



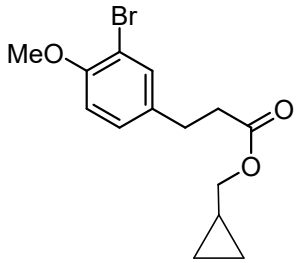
2-Bromo-4-(2-chloroethyl)-1-methoxybenzene (4)[2]. Colorless oil (64.0 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 2.1 Hz, 1H), 7.12 (dd, J = 8.4, 2.1 Hz, 1H), 6.84 (d, J = 8.4 Hz, 1H), 3.87 (s, 3H), 3.66 (t, J = 7.3 Hz, 2H), 2.98 (t, J = 7.3 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9, 133.7, 131.8, 129.0, 112.0, 111.7, 56.4, 45.1, 37.9.



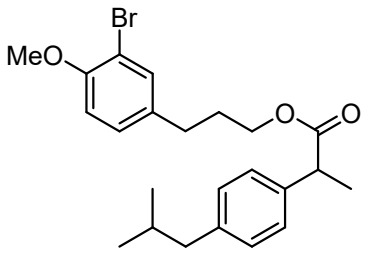
4-(3-Bromo-4-methoxyphenyl)butan-2-one (5)[3]. Yellow oil (66.0 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.09 (d, J = 8.4 Hz, 1H), 6.81 (d, J = 8.4 Hz, 1H), 3.86 (d, J = 1.2 Hz, 3H), 2.81 (t, J = 7.4 Hz, 2H), 2.72 (t, J = 7.4 Hz, 2H), 2.14 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.7, 154.2, 134.6, 133.0, 128.4, 111.9, 111.4, 56.2, 45.1, 30.2, 28.4.



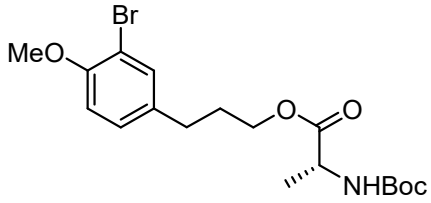
2-(3-Bromo-4-methoxyphenyl)-1-(4-methoxyphenyl)ethan-1-one (6). Yellow solid (58.0 mg, 58% yield); m.p. = 124.7−125.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 8.9 Hz, 2H), 7.44 (d, J = 2.1 Hz, 1H), 7.16 (dd, J = 8.4, 2.1 Hz, 1H), 6.93 (d, J = 8.9 Hz, 2H), 6.84 (d, J = 8.4 Hz, 1H), 4.14 (s, 2H), 3.88–3.86 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 163.8, 154.9, 134.3, 131.0, 129.6, 129.5, 128.5, 114.0, 112.1, 111.8, 56.4, 55.6, 43.9; HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{16}H_{16}BrO_3^+$: 335.0277, Found: 335.0271.



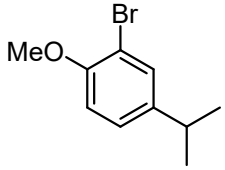
Cyclopropylmethyl 3-(3-bromo-4-methoxyphenyl)propanoate (7). Yellow oil (74.2 mg, 79% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 2.2 Hz, 1H), 7.11 (dd, J = 8.4, 2.2 Hz, 1H), 6.81 (d, J = 8.4 Hz, 1H), 3.89 (d, J = 7.3 Hz, 2H), 3.86 (s, 3H), 2.88 (t, J = 7.6 Hz, 2H), 2.61 (t, J = 7.6 Hz, 2H), 1.14–1.06 (m, 1H), 0.58–0.53 (m, 2H), 0.27–0.23 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 154.4, 134.3, 133.2, 128.4, 112.0, 111.5, 69.4, 56.3, 36.0, 29.8, 9.9, 3.4; HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{14}H_{18}BrO_3^+$: 313.0434, Found: 313.0430.



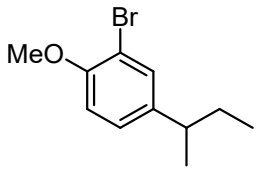
3-(3-Bromo-4-methoxyphenyl)propyl 3-(4-isobutylphenyl)-2-methylpropanoate (8). Yellow oil (87.2 mg, 67% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25–7.19 (m, 3H), 7.11 (d, J = 8.0 Hz, 2H), 6.91 (dd, J = 8.4, 2.1 Hz, 1H), 6.75 (d, J = 8.4 Hz, 1H), 4.09–3.97 (m, 2H), 3.84 (s, 3H), 3.70 (q, J = 7.2 Hz, 1H), 2.47–2.40 (m, 4H), 1.88–1.77 (m, 3H), 1.49 (d, J = 7.2 Hz, 3H), 0.88 (d, J = 6.6 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 154.2, 140.7, 137.9, 134.9, 133.2, 129.5, 128.4, 127.3, 111.9, 111.5, 63.6, 56.3, 45.3, 45.1, 30.7, 30.3, 22.5, 18.4; HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{23}H_{30}BrO_3^+$: 433.1373, Found: 433.1371.



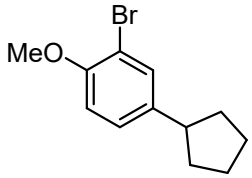
3-(3-Bromo-4-methoxyphenyl)propyl (*tert*-butoxycarbonyl)-*D*-alaninate (9). Yellow oil (86.3 mg, 69% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 2.1 Hz, 1H), 7.08 (dd, J = 8.4, 2.1 Hz, 1H), 6.83 (d, J = 8.4 Hz, 1H), 5.10 (s, 1H), 4.35–4.28 (m, 1H), 4.13 (t, J = 6.5 Hz, 2H), 3.87 (s, 3H), 2.62 (t, J = 7.4 Hz, 2H), 1.97–1.90 (m, 2H), 1.45 (s, 9H), 1.39 (d, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5, 155.3, 154.3, 134.7, 133.2, 128.5, 112.0, 111.6, 80.0, 64.4, 56.4, 49.4, 30.9, 30.3, 28.4, 18.8; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{18}H_{27}BrNO_5^+$: 416.1067, Found: 416.1063.



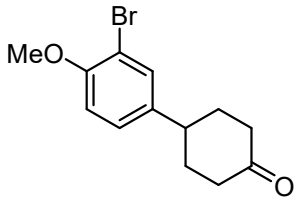
2-Bromo-4-(*iso*-propyl)-1-methoxybenzene (10)[4]. Yellow oil (68.9 mg, 69% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 2.2 Hz, 1H), 7.11 (dd, J = 8.4, 2.2 Hz, 1H), 6.82 (d, J = 8.4 Hz, 1H), 3.86 (s, 3H), 2.87–2.78 (m, 1H), 1.21 (d, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 142.8, 131.4, 126.4, 112.0, 111.5 , 56.4, 33.3, 24.2.



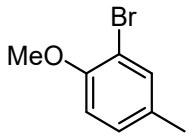
2-Bromo-4-(*sec*-butyl)-1-methoxybenzene (11). Yellow oil (50.0 mg 69% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 2.1 Hz, 1H), 7.07 (dd, J = 8.4, 2.1 Hz, 1H), 6.83 (d, J = 8.4 Hz, 1H), 3.87 (s, 3H), 2.56–2.48 (m, 1H), 1.59–1.51 (m, 2H), 1.20 (d, J = 7.0 Hz, 3H), 0.81 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 141.6, 131.9, 127.1, 111.9, 111.5, 56.4, 40.8, 31.4, 22.1, 12.3; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{11}H_{16}BrO^+$: 243.0379, Found: 243.0378.



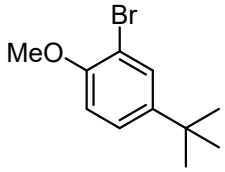
2-Bromo-4-cyclopentyl-1-methoxybenzene (12). Yellow oil (60.0 mg, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 2.1 Hz, 1H), 7.12 (dd, J = 8.4, 2.1 Hz, 1H), 6.81 (d, J = 8.4 Hz, 1H), 3.86 (s, 3H), 2.96–2.84 (m, 1H), 2.08–1.98 (m, 2H), 1.83–1.72 (m, 2H), 1.57–1.45 (m, 2H), 1.57–1.45 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9, 140.4, 132.0, 127.1, 111.9, 111.5, 56.4, 45.0, 34.8, 25.5; HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{12}H_{16}BrO^+$: 255.0379, Found: 253.0379.



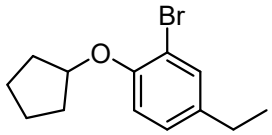
4-(3-Bromo-4-methoxyphenyl)cyclohexan-1-one (13). White solid (57.0 mg, 67% yield); m.p. = 81.5−82.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, J = 2.2 Hz, 1H), 7.15 (dd, J = 8.5, 2.2 Hz, 1H), 6.86 (d, J = 8.5 Hz, 1H), 3.88 (s, 3H), 3.01–2.93 (m, 1H), 2.53–2.45 (m, 4H), 2.24–2.14 (m, 2H), 1.96–1.81 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.0, 154.6, 138.6, 131.7, 126.7, 112.1, 111.7, 56.4, 41.7, 41.4, 34; HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{13}H_{16}BrO_2^+$: 283.0328 Found: 283.0323.



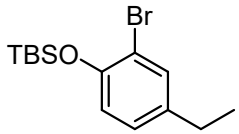
2-Bromo-1-methoxy-4-methylbenzene (14)[5]. Yellow oil (55.5 mg, 92% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 2.1 Hz, 1H), 7.05 (dd, J = 8.4, 2.1 Hz, 1H), 6.78 (d, J = 8.4 Hz, 1H), 3.85 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.8, 133.8, 131.5, 129.0, 111.9, 111.3, 56.4, 20.3.



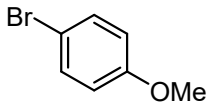
2-Bromo-1-(*tert*-butyl)-4-methylbenzene (15)[6]. Yellow oil (63.5 mg, 93% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 2.4 Hz, 1H), 7.27 (dd, J = 8.6, 2.4 Hz, 1H), 6.83 (d, J = 8.6 Hz, 1H), 3.87 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7, 145.2, 130.6, 125.4, 111.6, 111.4, 56.4, 34.3, 31.5.



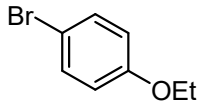
2-Bromo-1-(cyclopentyloxy)-4-ethylbenzene (16). Yellow oil (52.5 mg, 65% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 2.2 Hz, 1H), 7.03 (dd, J = 8.3, 2.2 Hz, 1H), 6.81 (d, J = 8.3 Hz, 1H), 4.80–4.74 (m, 1H), 2.55 (q, J = 7.6 Hz, 2H), 1.94–1.81 (m, 6H), 1.66–1.59 (m, 2H), 1.19 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.7, 137.7, 132.7, 127.6, 115.0, 113.1, 81.0, 32.9, 27.8, 24.1, 15.8; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{13}H_{18}BrO^+$: 269.0536, Found: 269.0534.



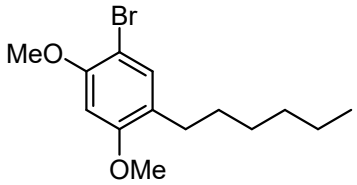
(2-Bromo-4-ethylphenoxy)(*tert*-butyl)dimethylsilane (17). Colorless oil (28.0 mg, 30% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (d, J = 2.2 Hz, 1H), 6.79 (dd, J = 8.2, 2.2 Hz, 1H), 6.60 (d, J = 8.2 Hz, 1H), 2.37 (q, J = 7.6 Hz, 2H), 1.01 (t, J = 7.6 Hz, 3H), 0.86 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.5, 138.6, 132.7, 127.7, 120.1, 115.1, 27.9, 25.9, 18.5, 15.8, –4.1; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{14}H_{24}BrOSi^+$: 315.0774, Found: 315.0774.



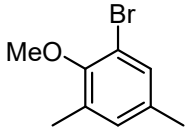
1-Bromo-4-methoxybenzene (18)[7]. Colorless oil (33.8 mg, 60% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.35 (m, 2H), 6.80–6.76 (m, 2H), 3.78 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8, 132.4, 115.9, 113.0, 55.6.



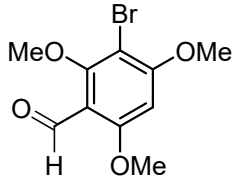
1-Bromo-4-ethoxybenzene (19)[8]. Yellow oil (32.0 mg, 53% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 6.4 Hz, 1H), 6.77 (d, J = 6.4 Hz, 1H), 3.99 (q, J = 7.0 Hz, 1H), 1.40 (t, J = 5.8 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 132.4, 116.4, 112.8, 63.9, 14.9.



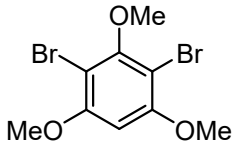
1-Bromo-5-hexyl-2,4-dimethoxybenzene (20). Yellow oil (64.0 mg, 71% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 1H), 6.45 (s, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 2.52–2.46 (m, 2H), 2.52–2.46 (m, 2H), 1.31–1.28 (m, 6H), 0.90–0.86 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 154.7, 133.4, 125.3, 101.4, 96.7, 56.5, 55.8, 31.9, 30.0, 29.3 (2C), 22.8, 14.3; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{14}H_{22}BrO_2^+$: 301.0798, Found: 301.0794.



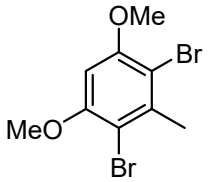
1-Bromo-2-methoxy-3,5-dimethylbenzene (21). Yellow oil (28.5 mg, 44% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (s, 1H), 6.96 (s, 1H), 3.79 (s, 3H), 2.29 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 132.6, 129.2, 125.9, 121.5, 114.2, 55.8, 21.9, 15.9; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_9H_{12}BrO^+$: 215.0066, Found: 215.0065.



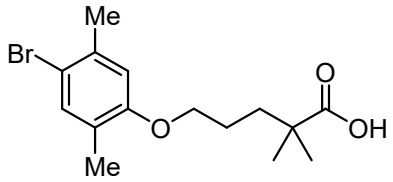
3-Bromo-2,4,6-trimethoxybenzaldehyde (22). Yellow solid (31.0 mg, 38% yield); m.p. = 115.1−116.0 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 6.32 (s, 1H), 3.99 (s, 3H), 3.95 (s, 3H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.4, 163.0, 162.1, 161.2, 113.8, 99.4, 92.1, 62.6, 56.7, 56.4; HRMS (ESI) ([M+H]$^{+}$) Calcd. for $C_{10}H_{12}BrO_4^{+}$: 274.9913, Found: 274.9912.



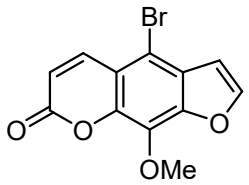
2,4-Dibromo-1,3,5-trimethoxybenzene (23)[9]. White solid (62.6 mg, 64% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.35 (s, 1H), 3.91 (s, 6H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 155.8, 99.0, 93.3, 60.6, 56.7.



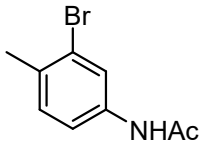
2,4-Dibromo-1,3-dimethoxy-5-methylbenzene (24)[10]. Yellow solid (64.0 mg, 69% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.41 (s, 1H), 3.90 (s, 6H), 2.61 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 139.3, 105.8, 94.8, 56.7, 24.3.



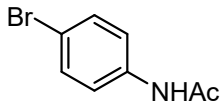
5-(4-Bromo-2,5-dimethylphenoxy)-2,2-dimethylpentanoic acid (25)[11]. Yellow solid (51.0 mg, 52% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 1H), 6.64 (s, 1H), 3.90 (t, J = 5.9 Hz, 2H), 2.33 (s, 3H), 2.14 (s, 3H), 1.83–1.70 (m, 4H), 1.25 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.9, 156.3, 135.7, 133.8, 126.4, 114.7, 113.5, 68.3, 42.1, 36.9, 25.2, 25.1, 23.1, 15.6.



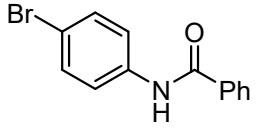
4-Bromo-9-methoxy-7*H*-furo[3,2-*g*]chromen-7-one (26)[9]. Yellow solid (37.0 mg, 42% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 9.8 Hz, 1H), 7.73 (d, J = 2.2 Hz, 1H), 6.88 (d, J = 2.2 Hz, 1H), 6.45 (d, J = 9.9 Hz, 1H), 4.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.0, 147.1, 146.8, 143.8, 142.8, 132.5, 128.1, 116.0, 115.8, 107.6, 105.7, 61.6.



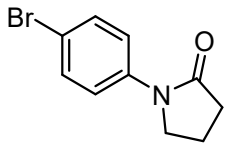
***N*-(2-Bromo-4-methylphenyl)acetamide (27)[8].** White solid (53.5 mg, 72% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 1H), 7.57 (s, 1H), 7.34 (s, 1H), 7.09 (dd, J = 8.4, 1.9 Hz, 1H), 2.29 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 135.4, 133.2, 132.5, 129.1, 122.2, 113.5, 24.9, 20.7.



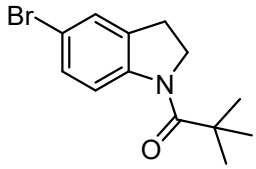
***N*-(4-Bromophenyl)acetamide (28)[5].** White solid (48.3 mg, 76% yield); ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.08 (s, 1H), 7.56 (d, J = 8.8 Hz, 2H), 7.47 (d, J = 8.8 Hz, 2H), 2.05 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.9, 139.1, 131.9, 121.3, 114.9, 24.5.



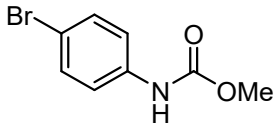
***N*-(4-Bromophenyl)benzamide (29)[12].** Yellow solid (39.2 mg, 48% yield); ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.40 (s, 1H), 7.97–7.92 (m, 2H), 7.80–7.75 (m, 2H), 7.64–7.52 (m, 5H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.2, 139.0, 135.2, 132.2, 131.9, 128.9, 128.2, 122.7, 115.8.



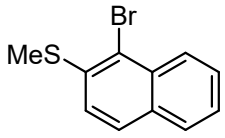
1-(4-Bromophenyl)pyrrolidin-2-one (30)[12]. Yellow solid (67.0 mg, 93% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.49 (m, 2H), 7.47–7.43 (m, 2H), 3.81 (t, J = 7.1 Hz, 2H), 2.59 (t, J = 8.1 Hz, 2H), 2.19–2.11 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4, 138.5, 131.8, 121.3, 117.2, 48.6, 32.7, 17.9.



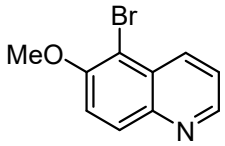
1-(5-Bromoindolin-1-yl)-2,2-dimethylpropan-1-one (31)[13]. Yellow solid (50.6 mg, 60% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 9.2 Hz, 1H), 7.32–7.25 (m, 2H), 4.23 (t, J = 8.2 Hz, 2H), 3.12 (t, J = 8.2 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.8, 144.1, 133.3, 130.3, 127.4, 119.8, 116.0, 49.6, 40.4, 29.2, 27.8.



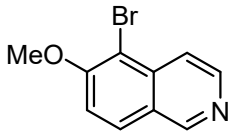
Methyl (4-bromophenyl)carbamate (32)[6]. Yellow solid (46.6 mg, 68% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.37 (m, 2H), 7.32–7.25 (m, 2H), 6.89 (s, 1H), 3.76 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.1, 137.1, 132.1, 120.4, 116.1, 52.6.



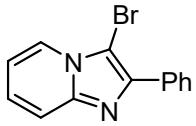
(1-Bromonaphthalen-2-yl)(methyl)sulfane (33)[5]. White solid (32 mg, 42% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.6 Hz, 1H), 7.76 (dd, J = 8.4, 3.3 Hz, 2H), 7.56 (ddd, J = 8.4, 6.9, 1.2 Hz, 1H), 7.43 (ddd, J = 8.4, 6.9, 1.2 Hz, 1H), 7.30 (d, J = 8.6 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.8, 132.7, 132.0, 128.3, 128.2, 128.1, 126.4, 125.8, 122.9, 120.4, 16.3.



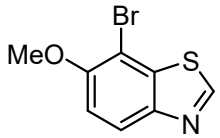
2-Bromo-6-methoxyquinoline (34)[14]. Yellow solid (55.3 mg, 77% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (dd, J = 4.2, 1.6 Hz, 1H), 8.50 (d, J = 8.6 Hz, 1H), 8.09 (d, J = 9.3 Hz, 1H), 7.53–7.41 (m, 2H), 4.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 148.8, 144.3, 134.6, 130.4, 128.7, 122.5, 116.5, 107.4, 57.1.



5-Bromo-6-methoxyisoquinoline (35)[15]. Yellow solid (23.8 mg, 33% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.54 (d, J = 6.1 Hz, 1H), 8.07 (d, J = 9.0 Hz, 1H), 8.03 (d, J = 9.0 Hz, 1H), 7.43 (d, J = 9.0 Hz, 1H), 4.11 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 151.1, 142.2, 137.0, 130.1, 124.8, 119.6, 115.1, 107.1, 57.2.

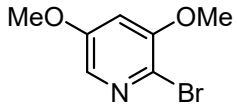


3-Bromo-2-phenyl-1,8*a*-dihydroimidazo[1,2-*a*]pyridine (36)[16]. Yellow oil (37.5 mg, 46% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19–8.11 (m, 3H), 7.64 (d, J = 9.1 Hz, 1H), 7.51–7.45 (m, 2H), 7.42–7.36 (m, 1H), 7.29–7.24 (m, 1H), 6.92 (t, J = 6.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 142.8, 133.0, 128.6, 128.5, 128.0, 125.3, 124.1, 117.8, 113.2, 91.9.



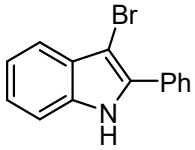
2-Bromo-6-methoxybenzo[*d*]thiazole (37). Yellow solid (45.7 mg, 62% yield); m.p. = 135.4–136.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.02 (d, J = 8.9 Hz, 1H), 7.15 (d, J = 8.9 Hz, 1H), 4.00 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.3, 152.4, 147.2, 138.9,

122.9, 111.7, 102.4, 57.3; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_8H_7BrNOS^+$: 243.9426, Found: 243.9421.

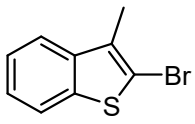


2-Bromo-3,5-dimethoxypyridine (38). Yellow solid (20.0 mg, 31% yield); m.p. = 78.2–79.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 2.5 Hz, 1H), 6.73 (d, J = 2.5 Hz, 1H), 3.90 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8, 153.3, 126.4, 123.2, 107.1, 56.4, 56.3; HRMS (ESI) ([M+H]$^+$) Calcd. for $C_7H_9BrNO_2^+$: 217.9811, Found: 217.9807.

3-Bromo-1*H*-indole (39)[17]. Yellow solid (38.6 mg, 66% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.34 (d, J = 7.6 Hz, 1H), 7.27–7.17 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.4, 127.0, 123.5, 123.3, 120.8, 119.3, 111.5, 91.8.

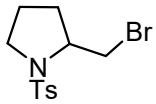


3-Bromo-2-phenyl-1*H*-indole (40)[9]. White solid (50.4 mg, 62% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.82–7.77 (m, 2H), 7.63–7.59 (m, 1H), 7.51–7.46 (m, 2H), 7.42–7.38 (m, 1H), 7.37–7.34 (m, 1H), 7.27–7.20 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.4, 134.4, 131.5, 129.0, 128.6, 127.9, 123.7, 121.1, 119.7, 111.3, 90.2.

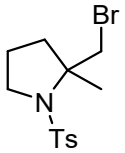


2-Bromo-3-methylbenzo[*b*]thiophene (41)[9]. Colorless oil (50.8 mg, 75% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 6.8 Hz, 1H), 7.59 (d, J = 6.8 Hz, 1H), 7.36–7.25 (m, 2H),

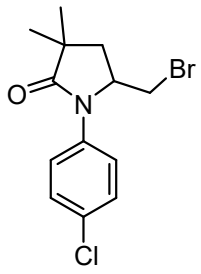
2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.7, 139.0, 131.9, 124.7, 124.6, 121.9, 121.8, 112.6, 13.3.



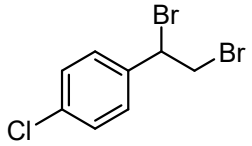
2-(Bromomethyl)-1-tosylpyrrolidine (42)[18]. Yellow oil (60.0 mg, 63% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 3.86–3.74 (m, 2H), 3.51–3.44 (m, 1H), 3.36 (t, J = 9.7 Hz, 1H), 3.18–3.13 (m, 1H), 2.44 (s, 3H), 1.98–1.80 (m, 2H), 1.76–1.71 (m, 1H), 1.60–1.51 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 134.1, 130.0, 127.7, 60.5, 50.0, 36.2, 30.4, 23.9, 21.7.



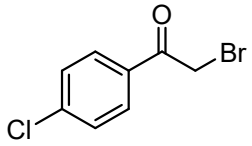
2-(Bromomethyl)-2-methyl-1-tosylpyrrolidine (43)[18]. Yellow oil (51.1 mg, 51% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.1 Hz, 2H), 7.29 (d, J = 8.1 Hz, 2H), 3.86 (d, J = 10.1 Hz, 1H), 3.76 (d, J = 10.1 Hz, 1H), 3.47–3.40 (m, 1H), 3.39–3.31 (m, 1H), 2.42 (s, 3H), 2.32–2.26 (m, 1H), 1.92–1.62 (m, 4H), 1.57 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 137.9, 129.6, 127.4, 67.5, 50.0, 41.2, 39.4, 24.2, 22.6, 21.6.



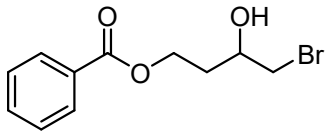
5-(Bromomethyl)-1-(4-chlorophenyl)-3,3-dimethylpyrrolidin-2-one (44). Yellow oil (52.9 mg, 56% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26–7.20 (m, 2H), 7.05–6.97 (m, 2H), 4.63–4.56 (m, 1H), 3.53–3.48 (m, 2H), 2.20 (dd, J = 12.7, 6.0 Hz, 1H), 1.94 (dd, J = 12.7, 9.7 Hz, 1H), 1.39 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 145.6, 128.8, 128.7, 124.3, 42.7, 41.7, 34.3, 27.0, 26.3; HRMS (ESI) ($[M+H]^+$) Calcd. For $C_{13}H_{16}BrNO^+$: 316.0098, Found: 316.0096.



1-Chloro-4-(1,2-dibromoethyl)benzene (45)[6]. Yellow oil (30.0 mg, 34% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.31 (m, 4H), 5.10 (dd, J = 10.7, 5.1 Hz, 1H), 4.06 (dd, J = 10.7, 5.1 Hz, 1H), 3.97 (t, J = 10.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.3, 135.1, 129.3, 129.2, 49.7, 34.8.



2-Bromo-1-(4-chlorophenyl)ethan-1-one (46)[6]. Yellow oil (14.6 mg, 21% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 8.6 Hz, 2H), 7.48 (d, J = 8.6 Hz, 2H), 4.42 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.4, 140.7, 132.4, 130.6, 129.4, 30.6.



4-Bromo-3-hydroxybutyl benzoate (47). Yellow oil (28.5 mg, 35% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11–8.07 (m, 2H), 7.65–7.56 (m, 1H), 7.50–7.45 (m, 2H), 5.50–5.44 (m, 1H), 3.80–3.62 (m, 4H), 2.11–1.97 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8, 133.7, 130.1, 129.6, 128.7, 70.7, 58.5, 36.1, 34.9; HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{11}H_{14}BrO_3^+$: 273.0121, Found: 273.0120.

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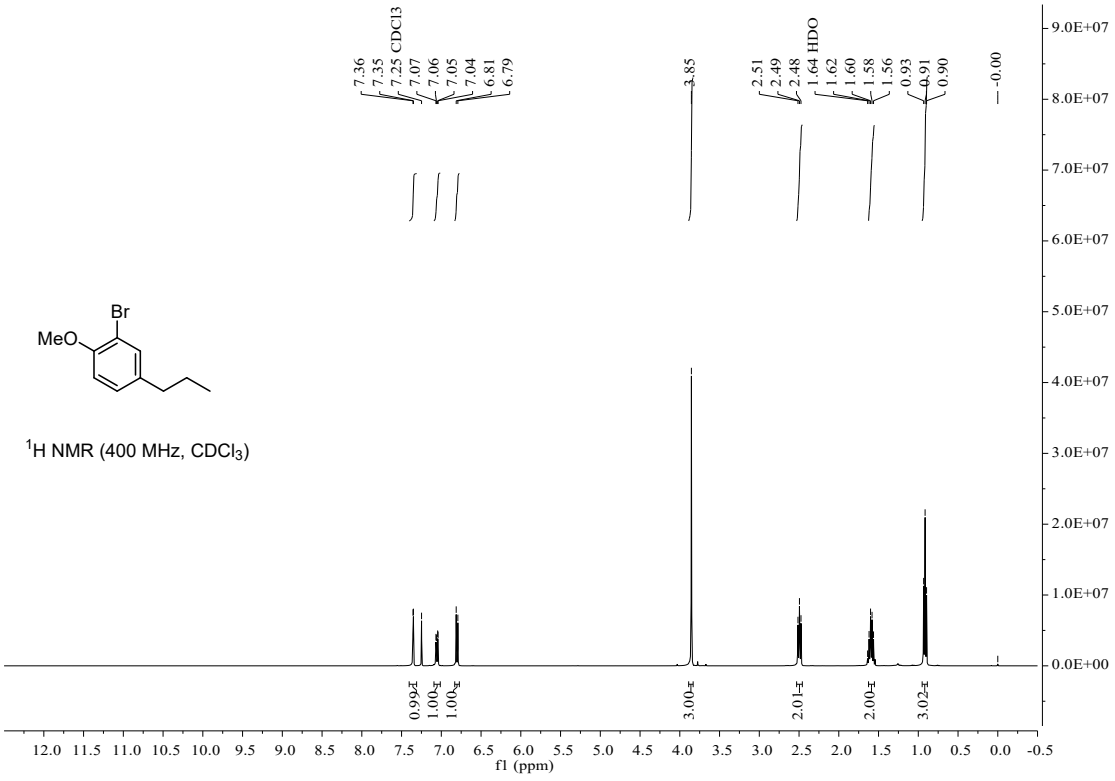
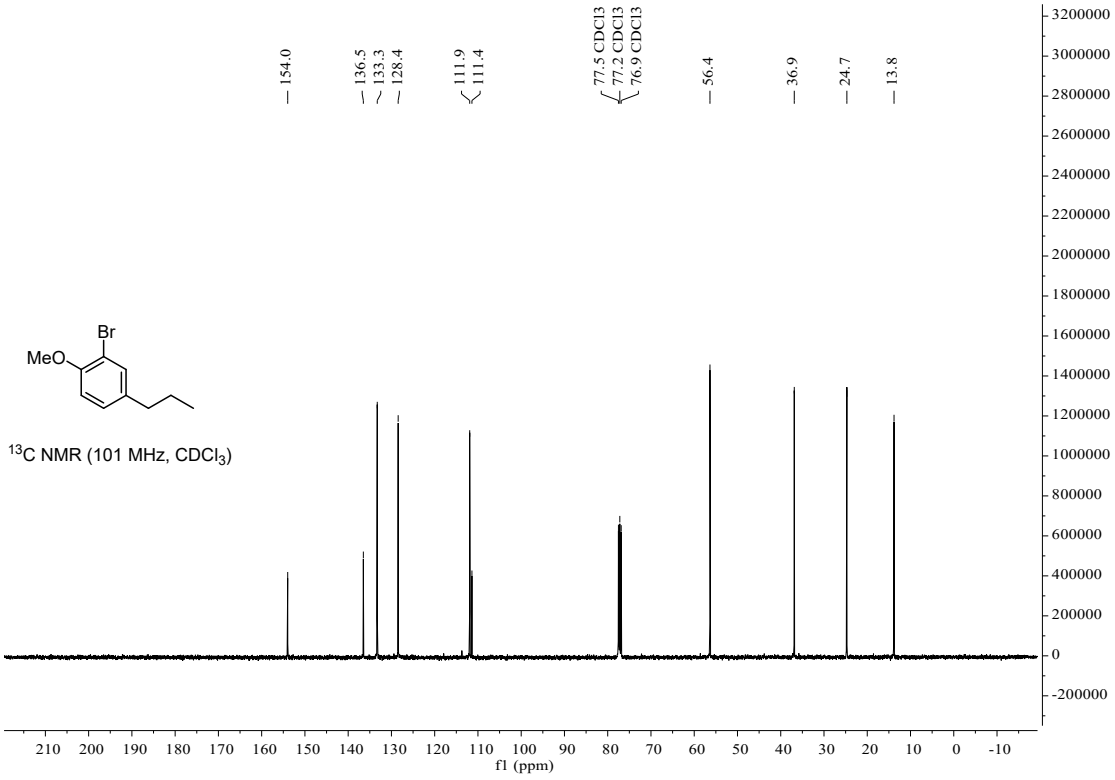
7. NMR Spectra for Products

Compound 3

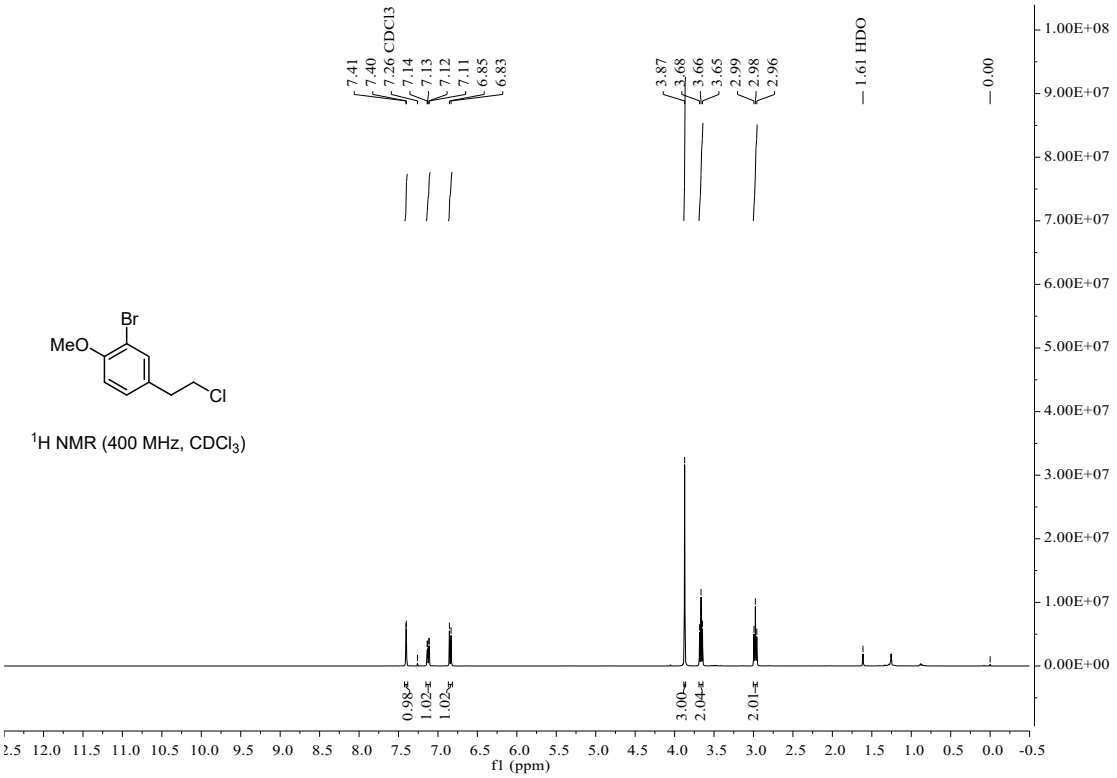


^{1}H NMR (400 MHz, $CDCl_3$)

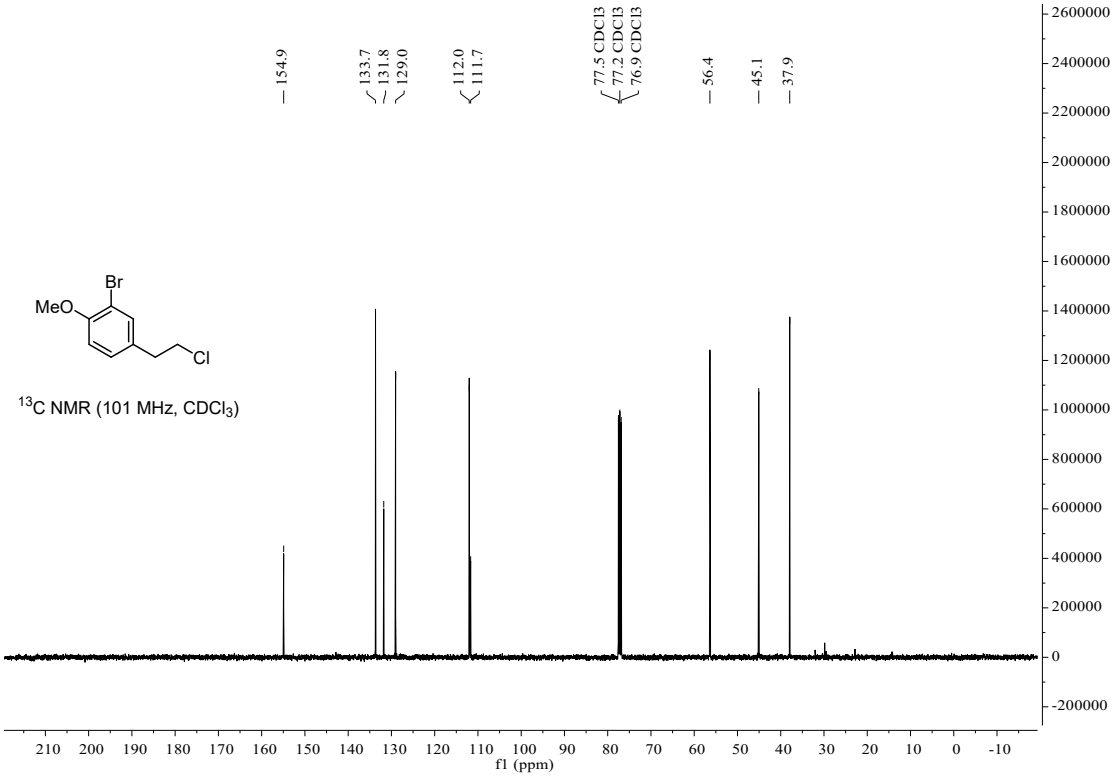


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 4

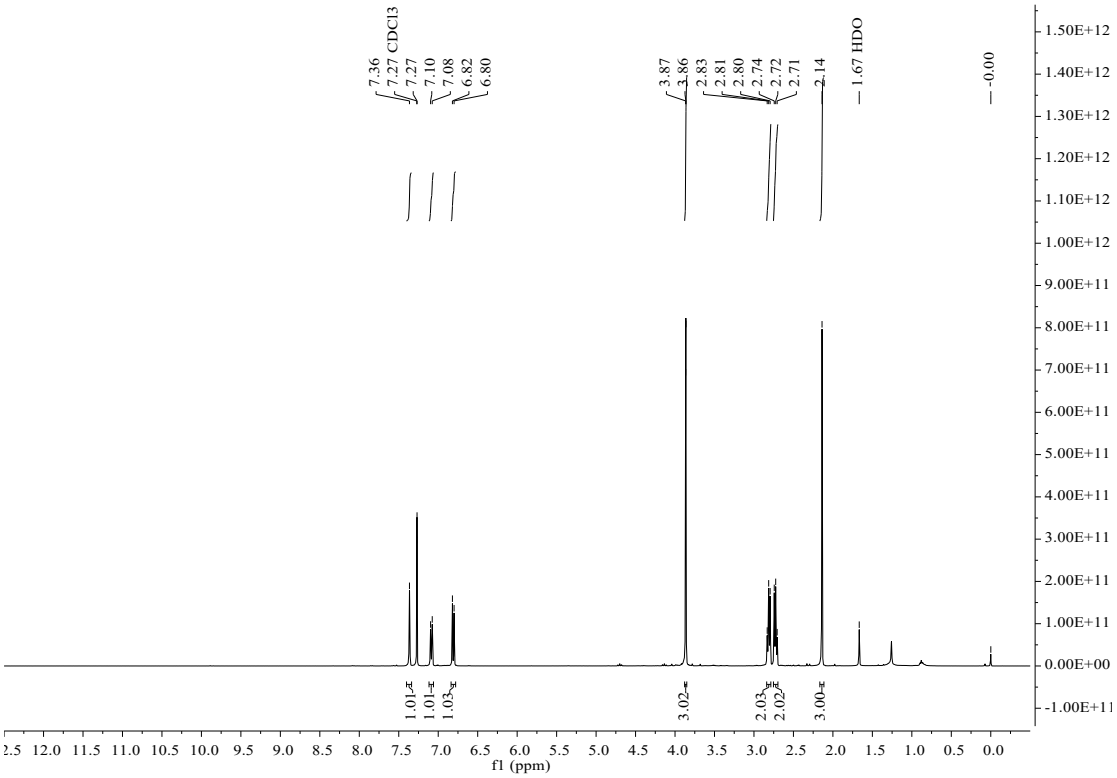


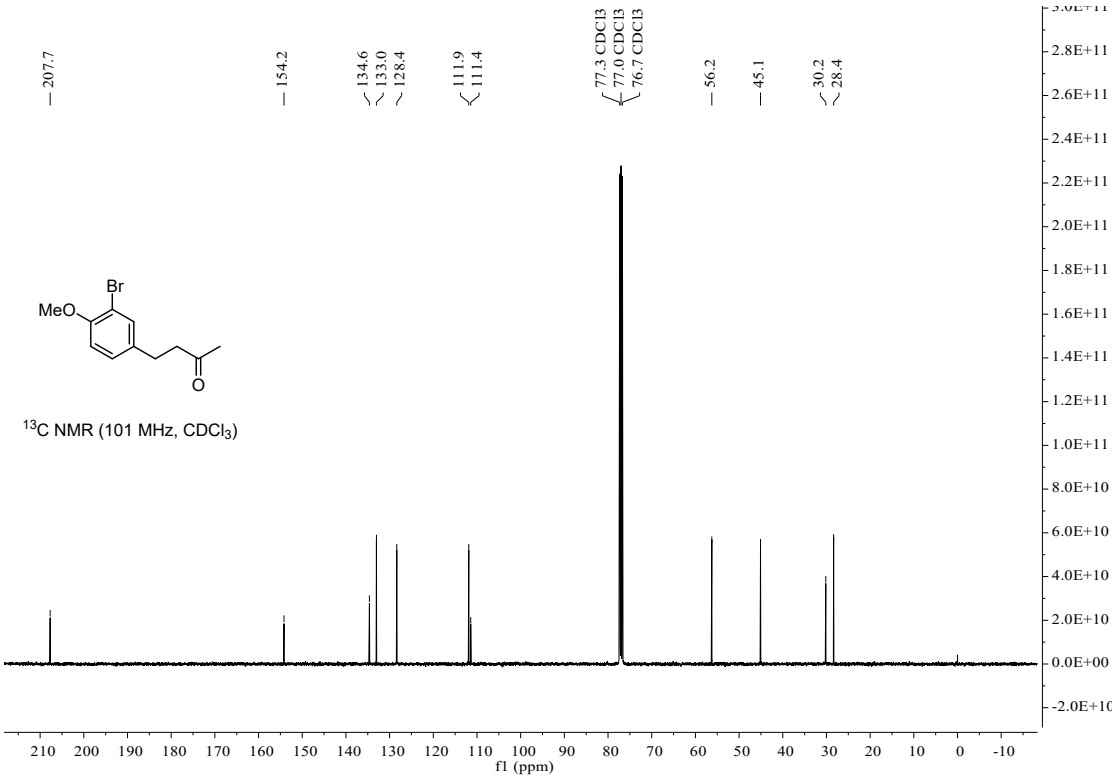
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

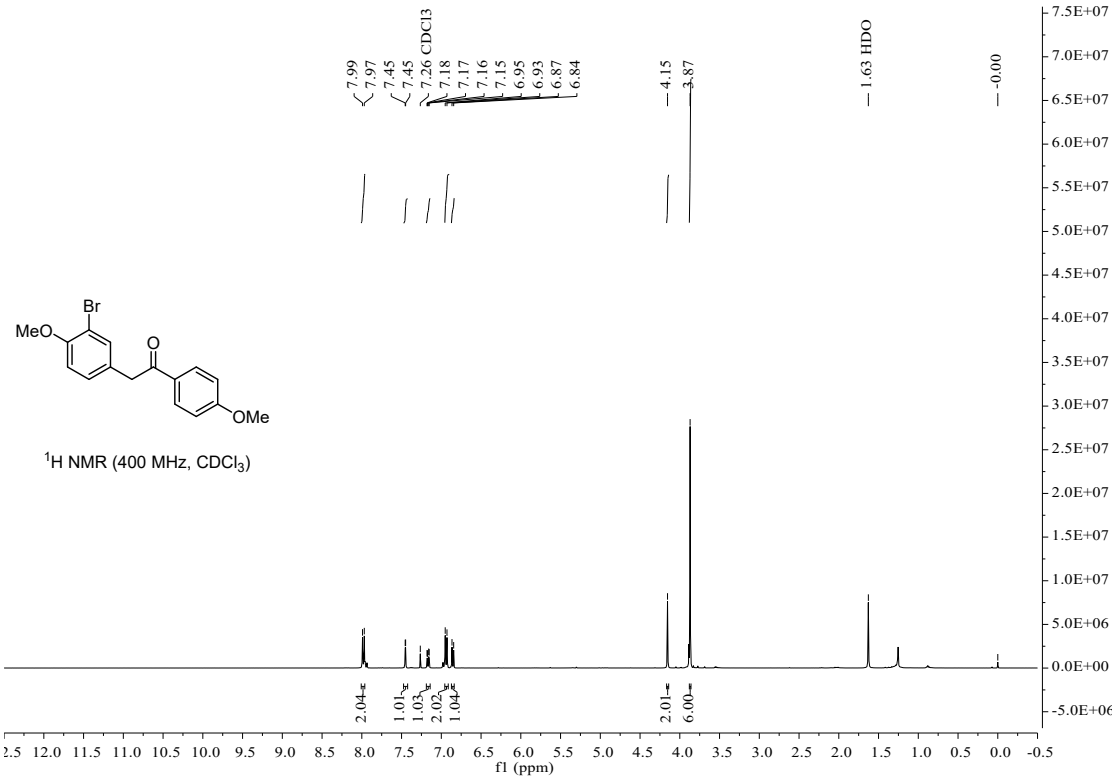
Compound 5

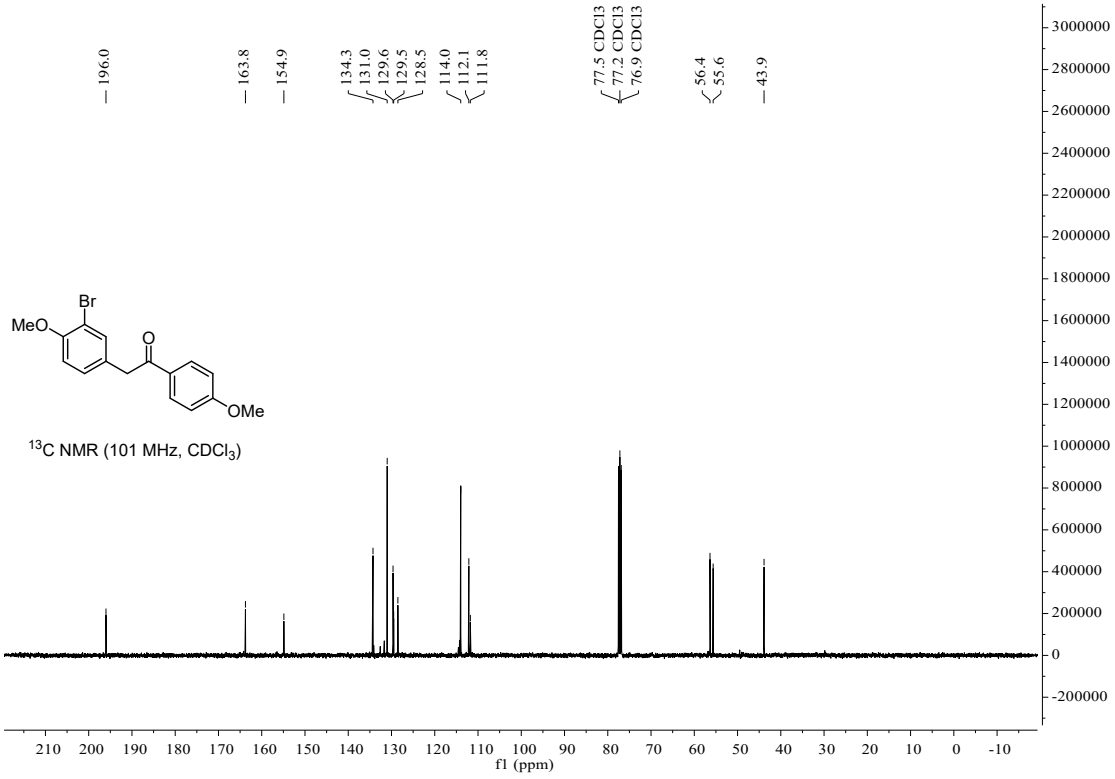




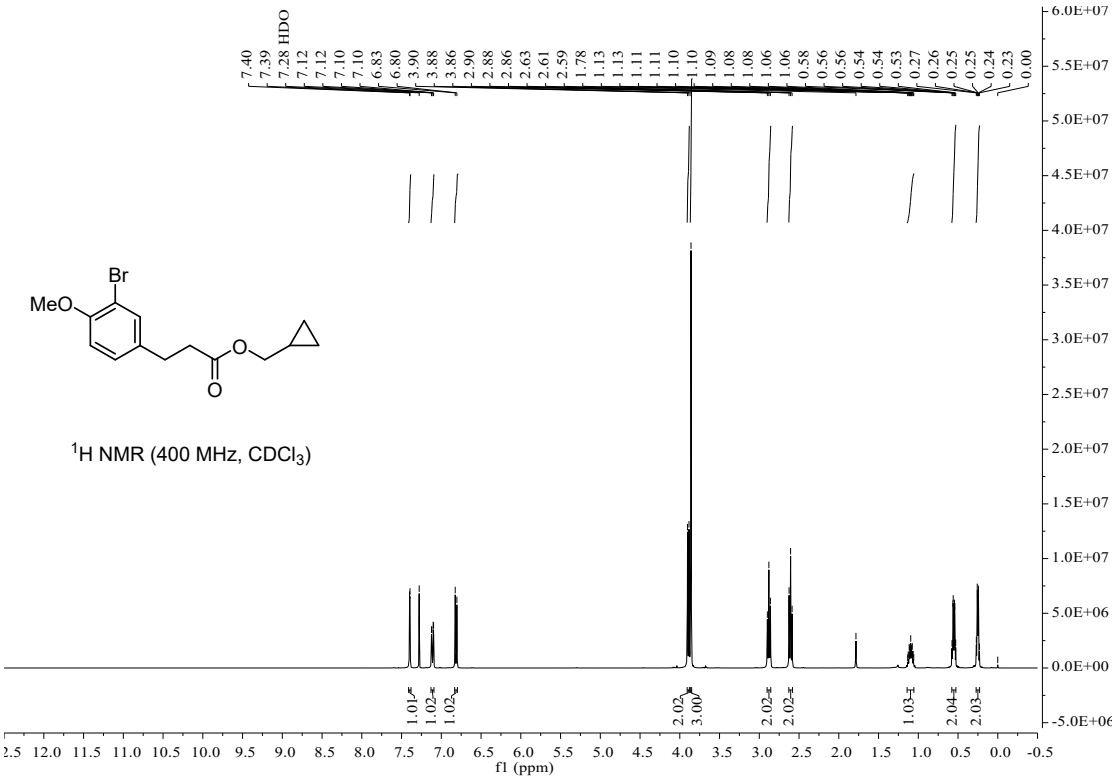
^{13}C NMR (101 MHz, $CDCl_3$)

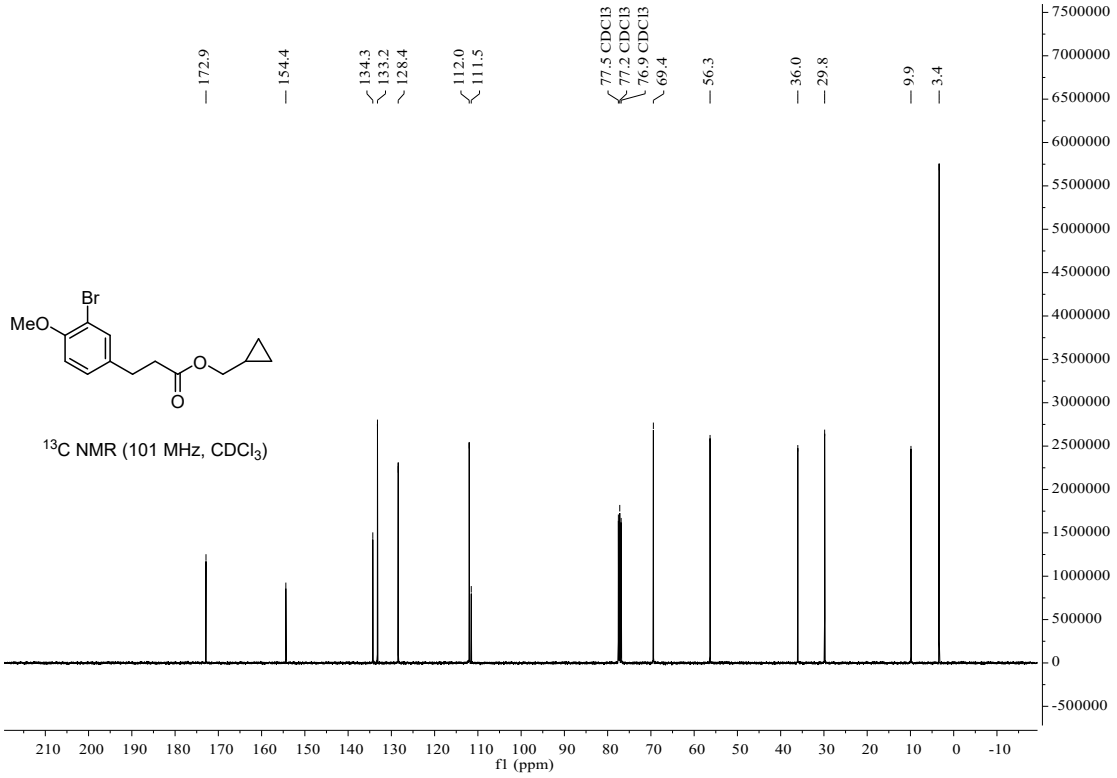
Compound 6


7.99
7.97
7.45
7.45
7.26 CDCl3
7.18
7.17
7.16
7.15
6.95
6.93
6.87
6.84
4.15
3.87
1.63 HDO
0.00
Br
MeO
O
OMe
1H NMR (400 MHz, CDCl3)
2.04
1.01
1.03
2.02
1.04
2.01
6.00
f1 (ppm)

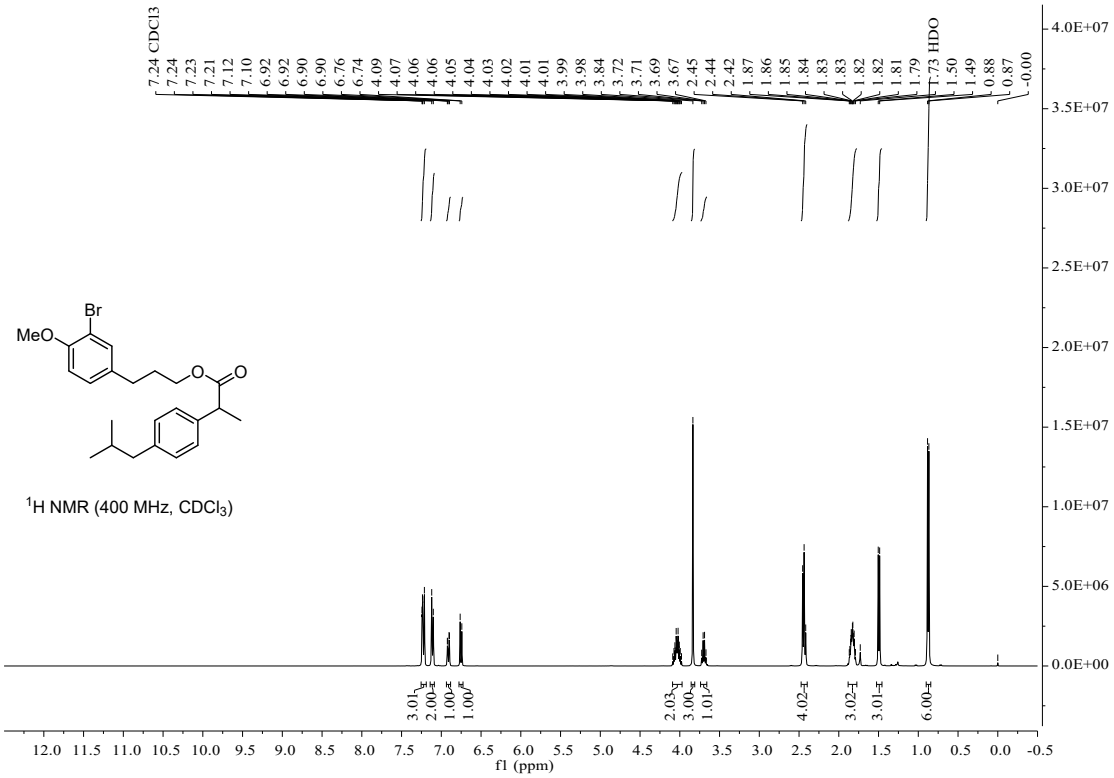

196.0
163.8
154.9
134.3
131.0
129.6
129.5
128.5
114.0
112.1
111.8
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
56.4
55.6
43.9
Br
MeO
O
OMe
13C NMR (101 MHz, CDCl3)
f1 (ppm)

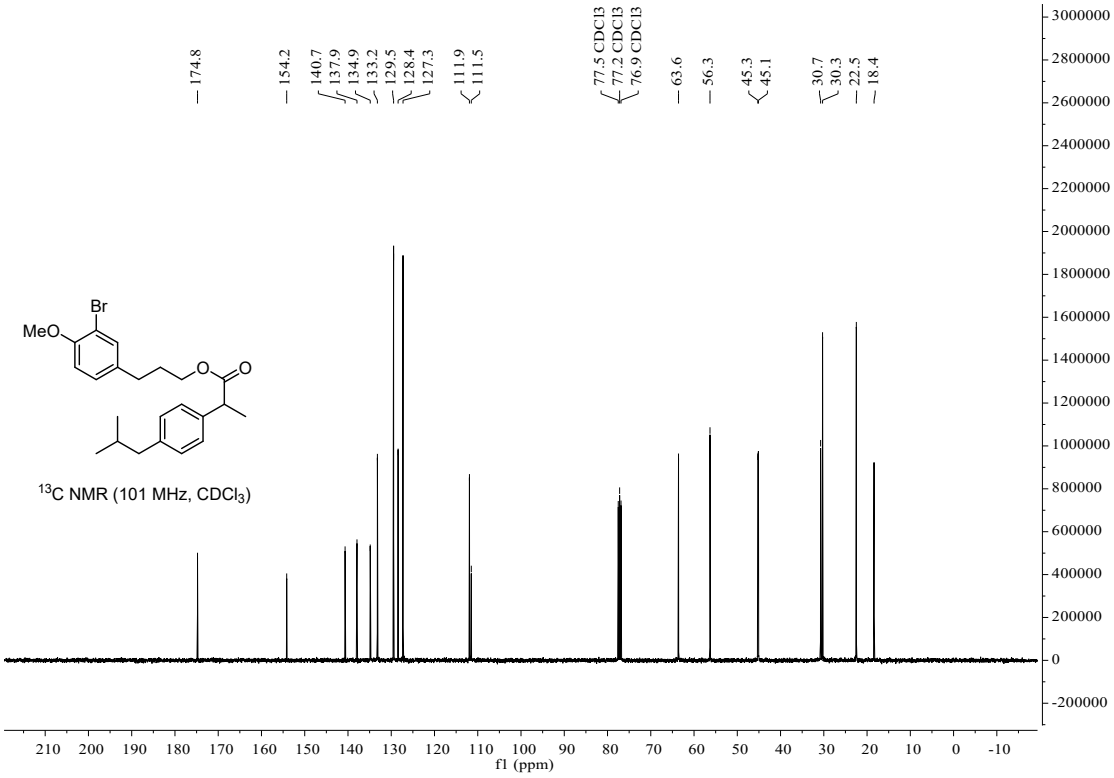
Compound 7


Br
MeO
O
O
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)

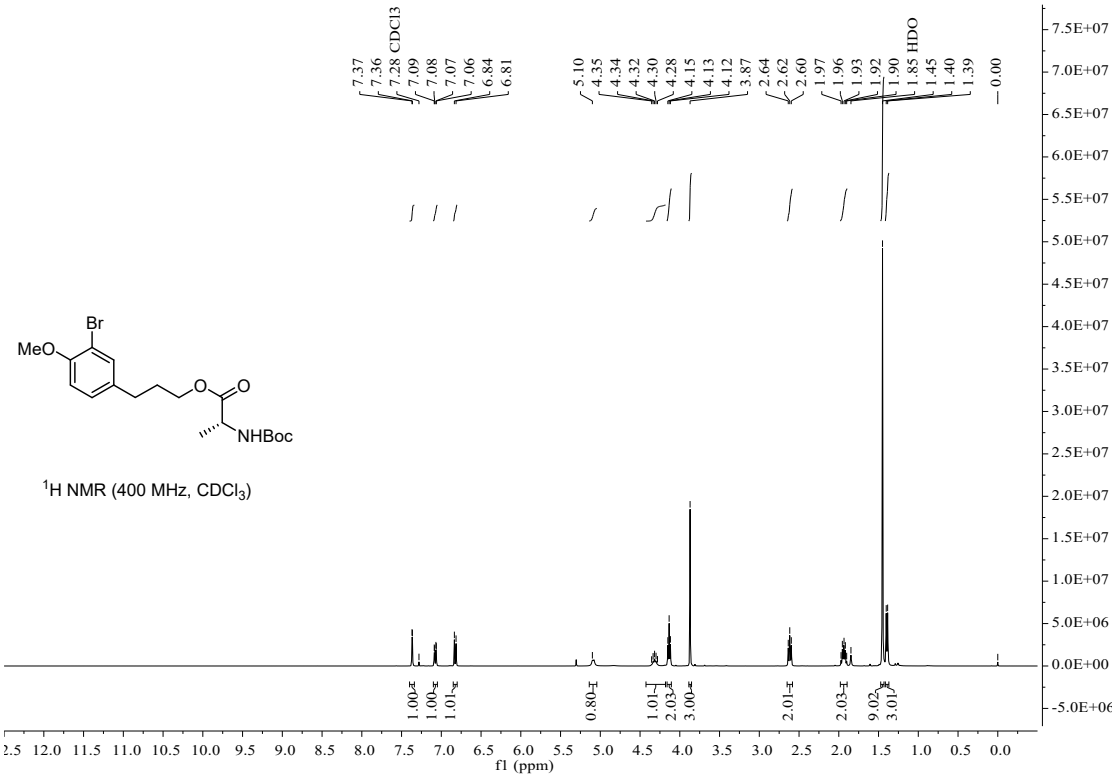

Br
MeO
O
O
^{13}C NMR (101 MHz, $CDCl_3$)
f1 (ppm)

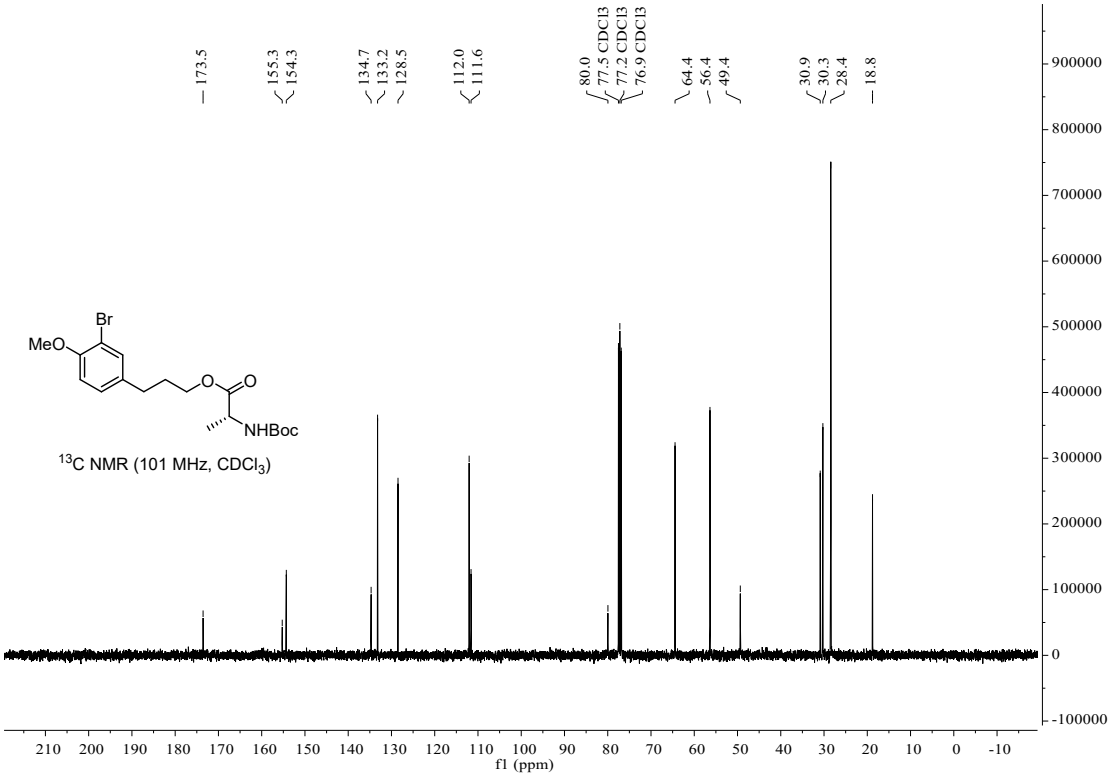
Compound 8


Br
MeO
O
O
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)

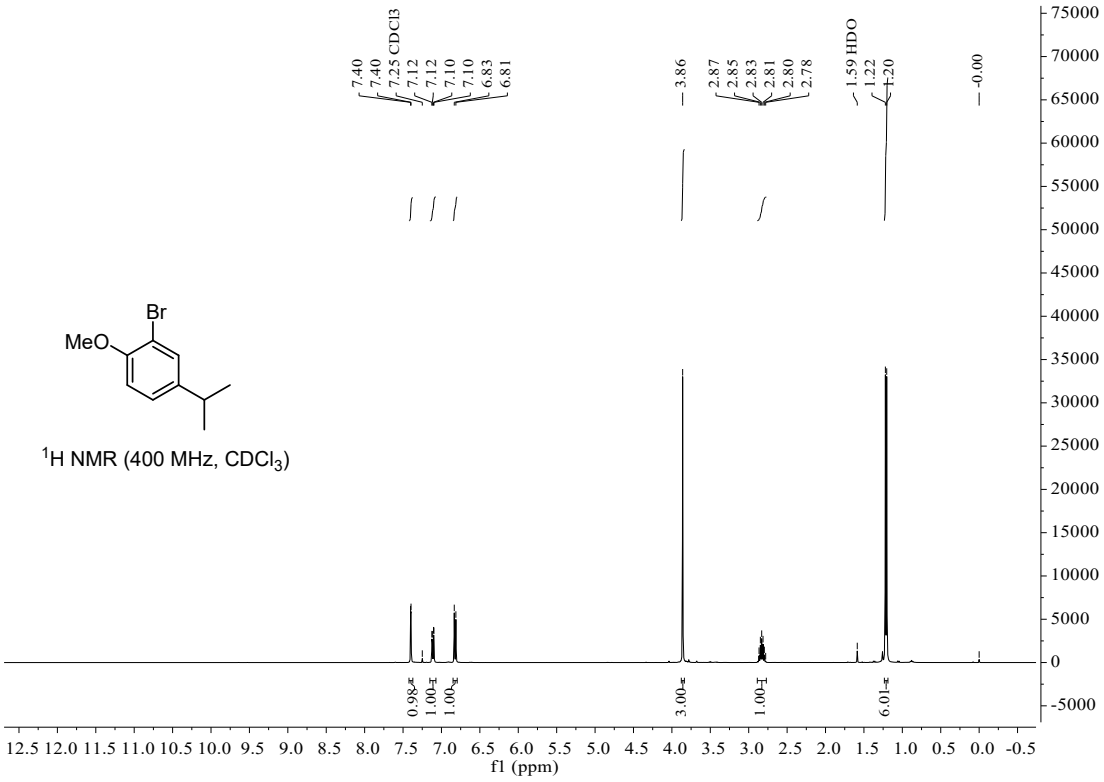

Br
MeO
O
O
^{13}C NMR (101 MHz, $CDCl_3$)
f1 (ppm)

Compound 9

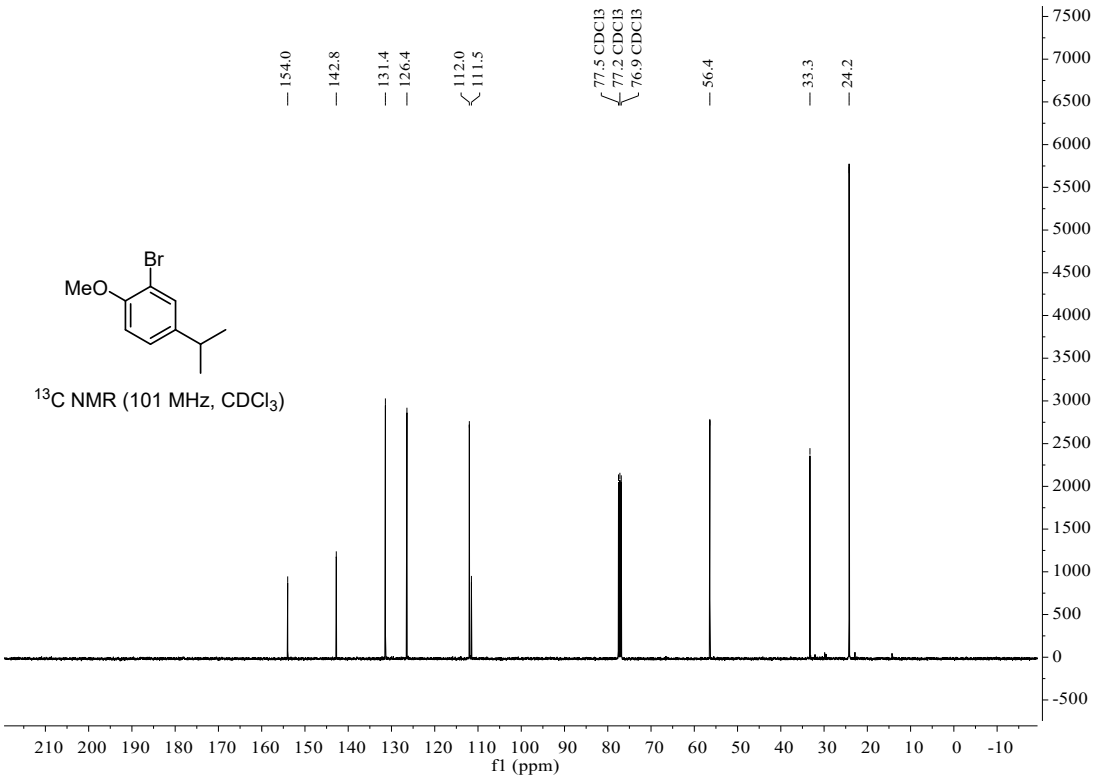

7.37
7.36
7.28 CDCl3
7.09
7.08
7.07
7.06
6.84
6.81
5.10
4.35
4.34
4.32
4.30
4.28
4.15
4.13
4.12
3.87
2.64
2.62
2.60
1.97
1.96
1.93
1.92
1.90
1.85 HDO
1.45
1.40
1.39
0.00
Br
MeO
O
O
NHBoc
1H NMR (400 MHz, CDCl3)
1.00
1.00
1.01
0.80
1.01
2.03
3.00
2.01
2.03
9.02
3.01
f1 (ppm)


173.5
155.3
154.3
134.7
133.2
128.5
112.0
111.6
80.0
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
64.4
56.4
49.4
30.9
30.3
28.4
18.8
Br
MeO
O
O
NHBoc
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 10

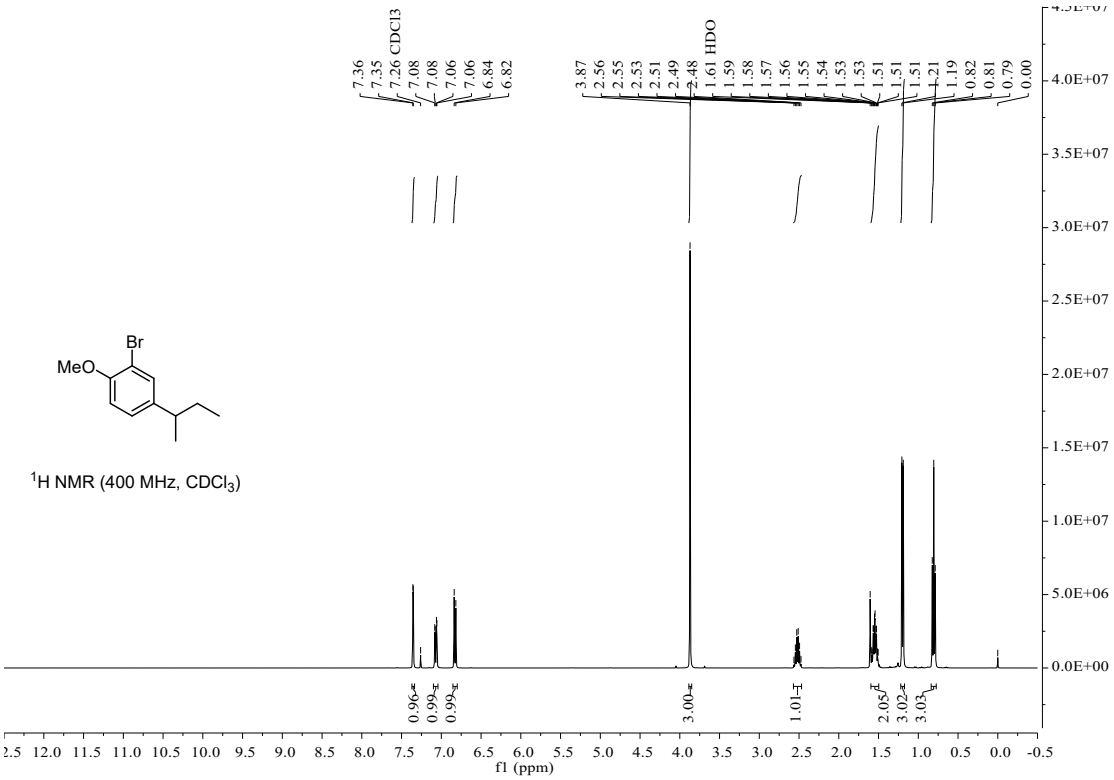


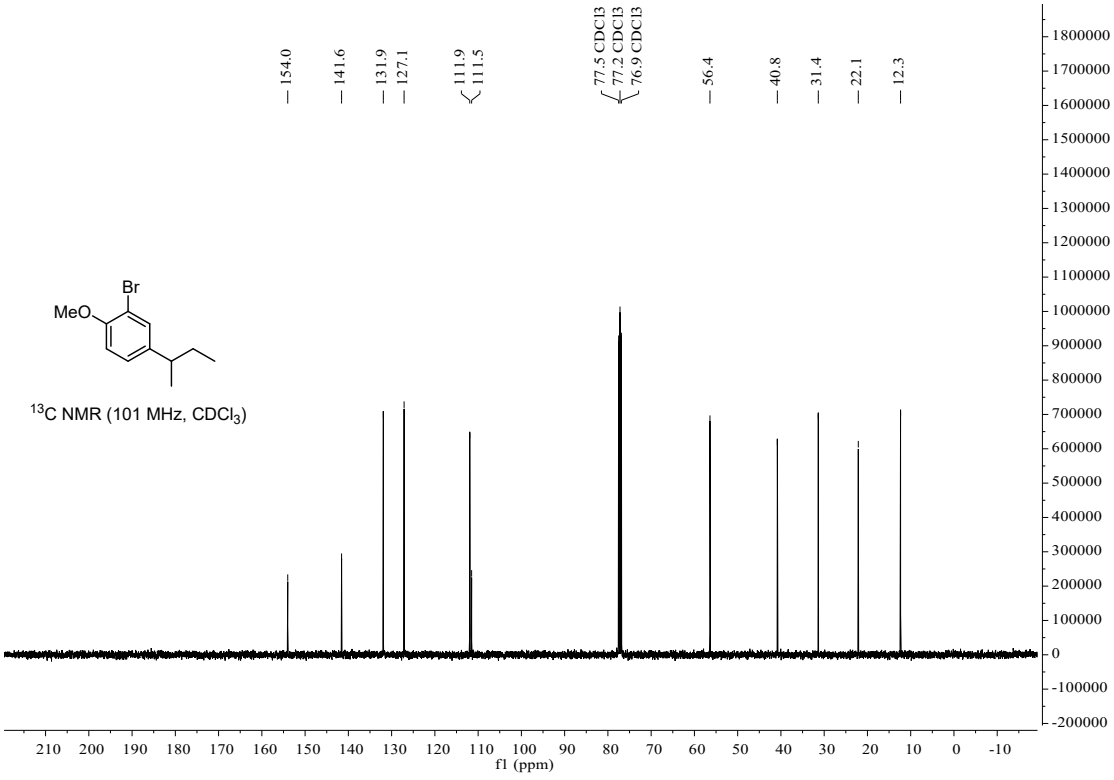
^{1}H NMR (400 MHz, $CDCl_3$)



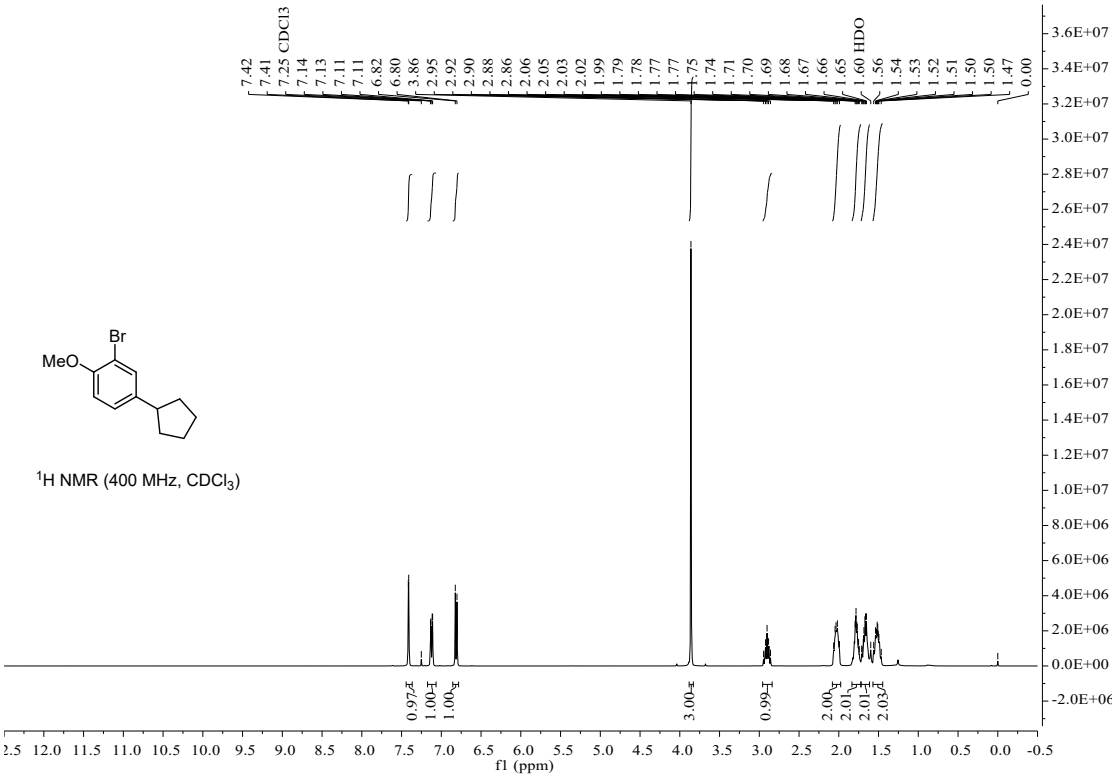
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 11

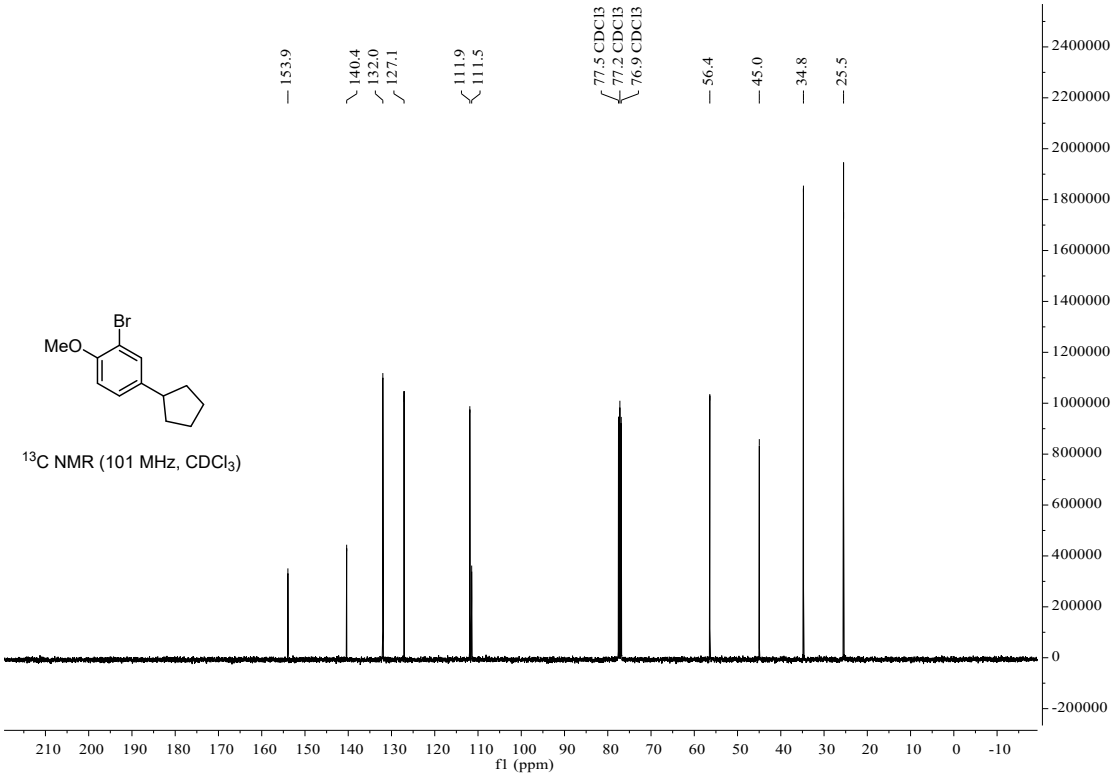

Br
MeO
1H NMR (400 MHz, CDCl3)
7.36
7.35
7.26 CDCl3
7.08
7.08
7.06
7.06
6.84
6.82
3.87
2.56
2.55
2.53
2.51
2.49
2.48
1.61 HDO
1.59
1.58
1.57
1.56
1.55
1.54
1.53
1.53
1.51
1.51
1.51
1.21
1.19
0.82
0.81
0.79
0.00
0.96
0.99
0.99
3.00
1.01
2.05
3.02
3.03
f1 (ppm)


Br
MeO
13C NMR (101 MHz, CDCl3)
154.0
141.6
131.9
127.1
111.9
111.5
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
56.4
40.8
31.4
22.1
12.3
f1 (ppm)

Compound 12

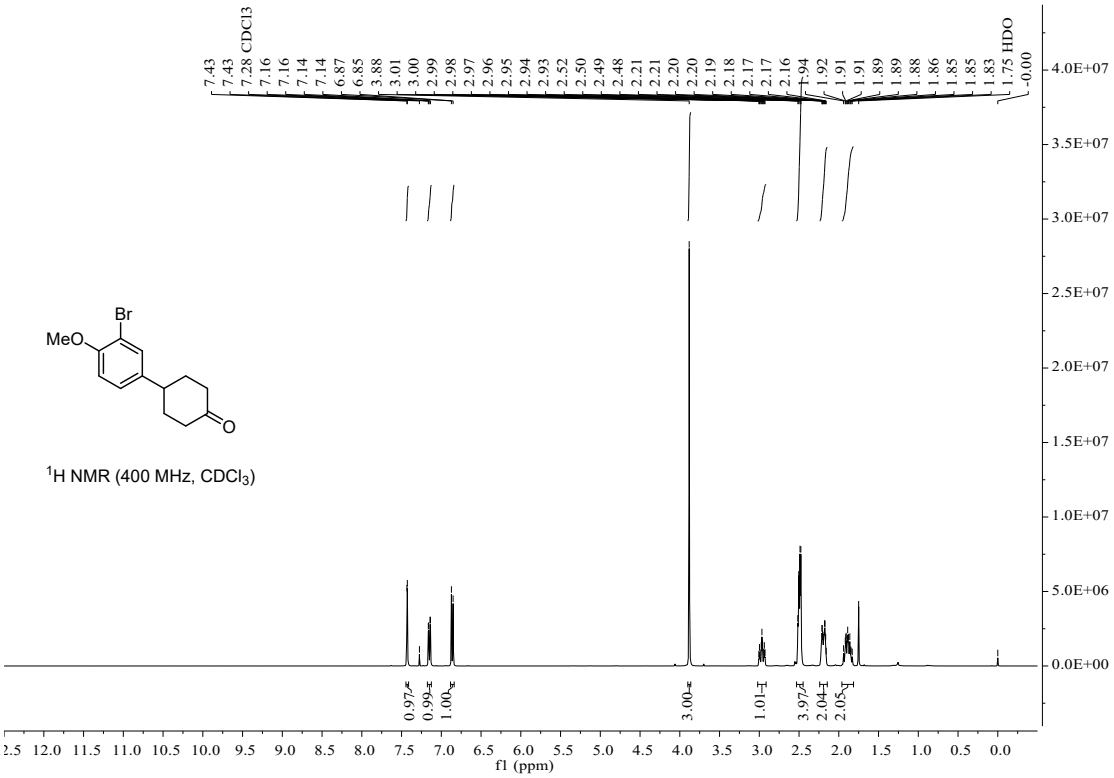


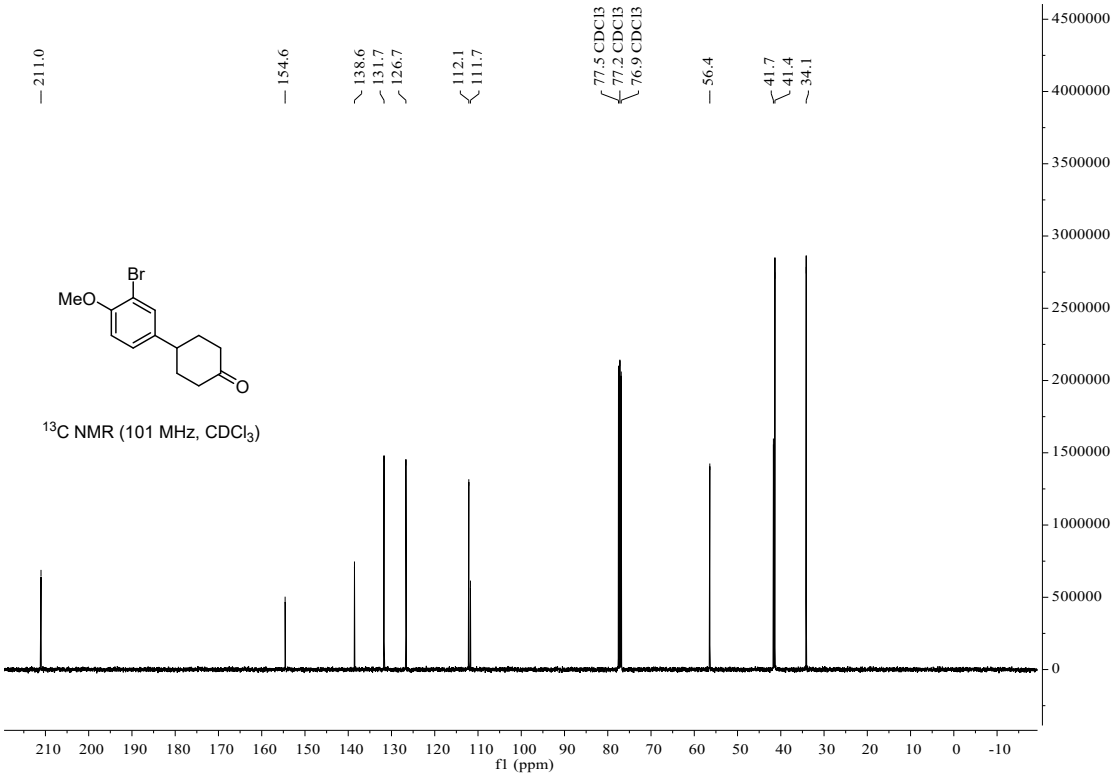
^{1}H NMR (400 MHz, $CDCl_3$)



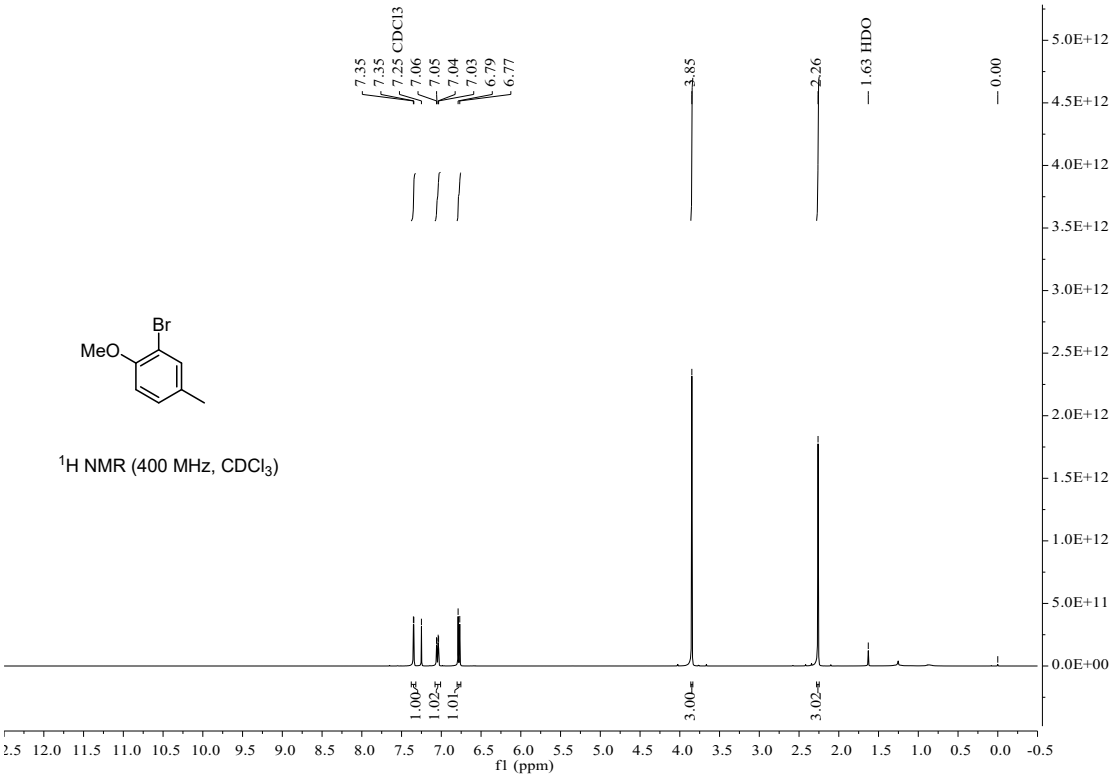
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 13

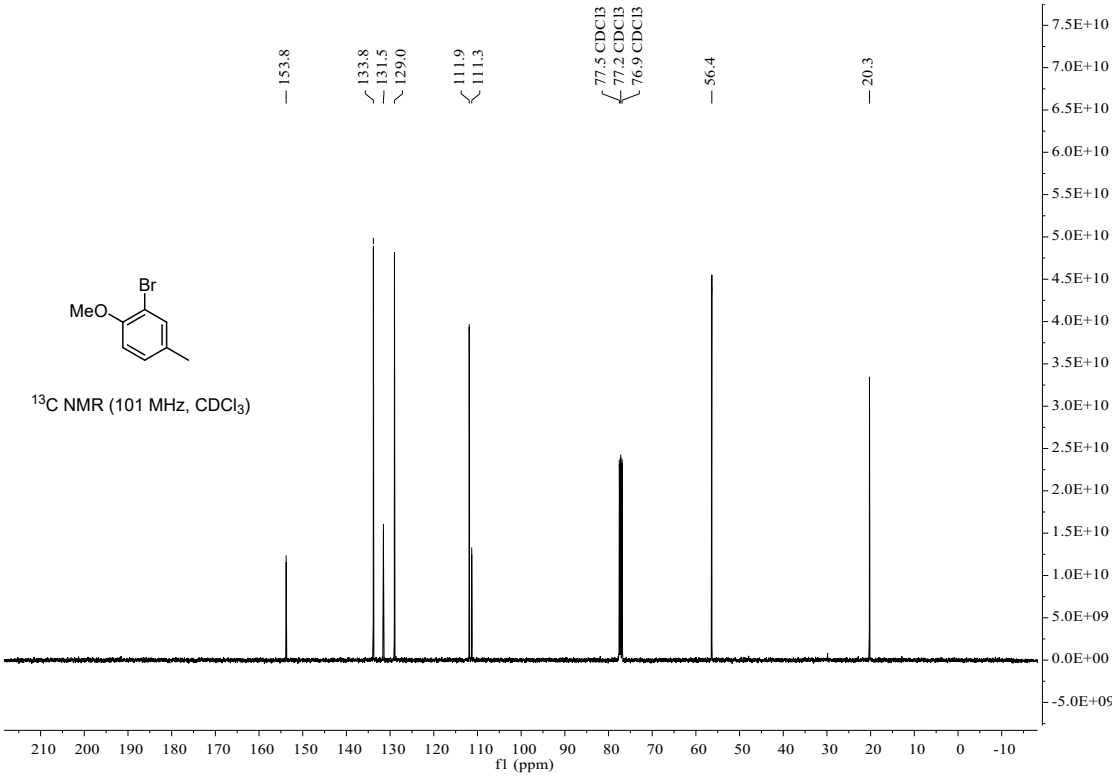

Br
MeO
O
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)


Br
MeO
O
^{13}C NMR (101 MHz, $CDCl_3$)
f1 (ppm)

Compound 14

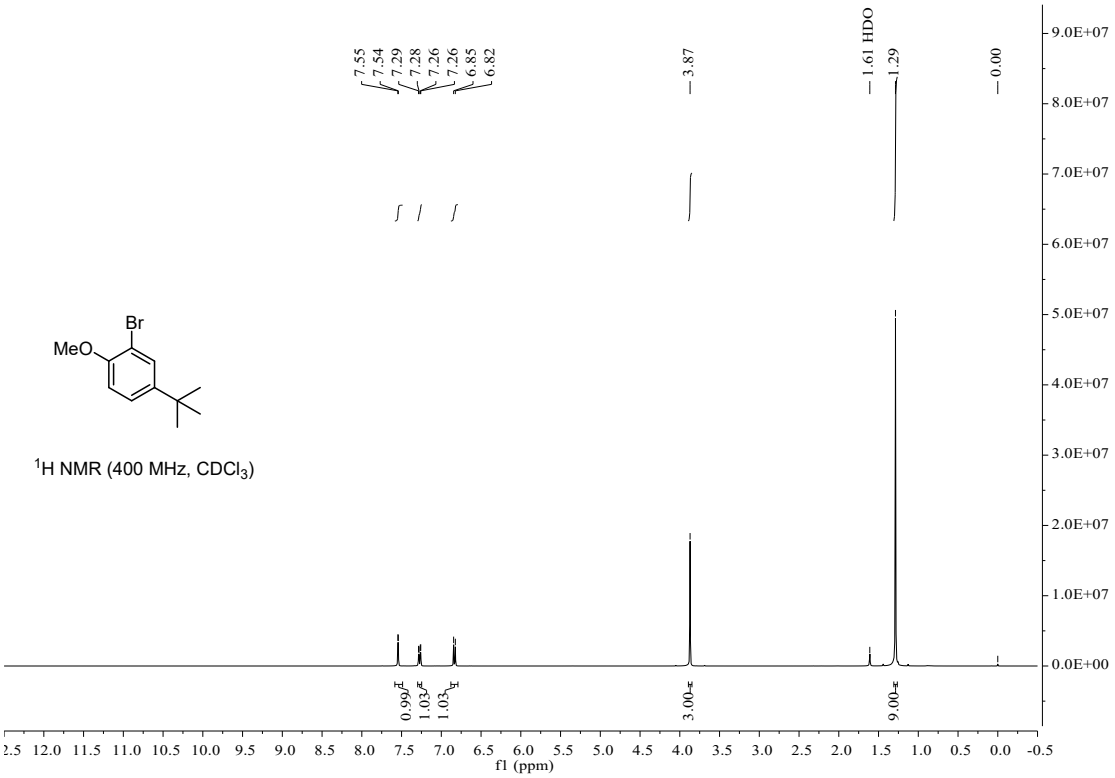


^{1}H NMR (400 MHz, $CDCl_3$)

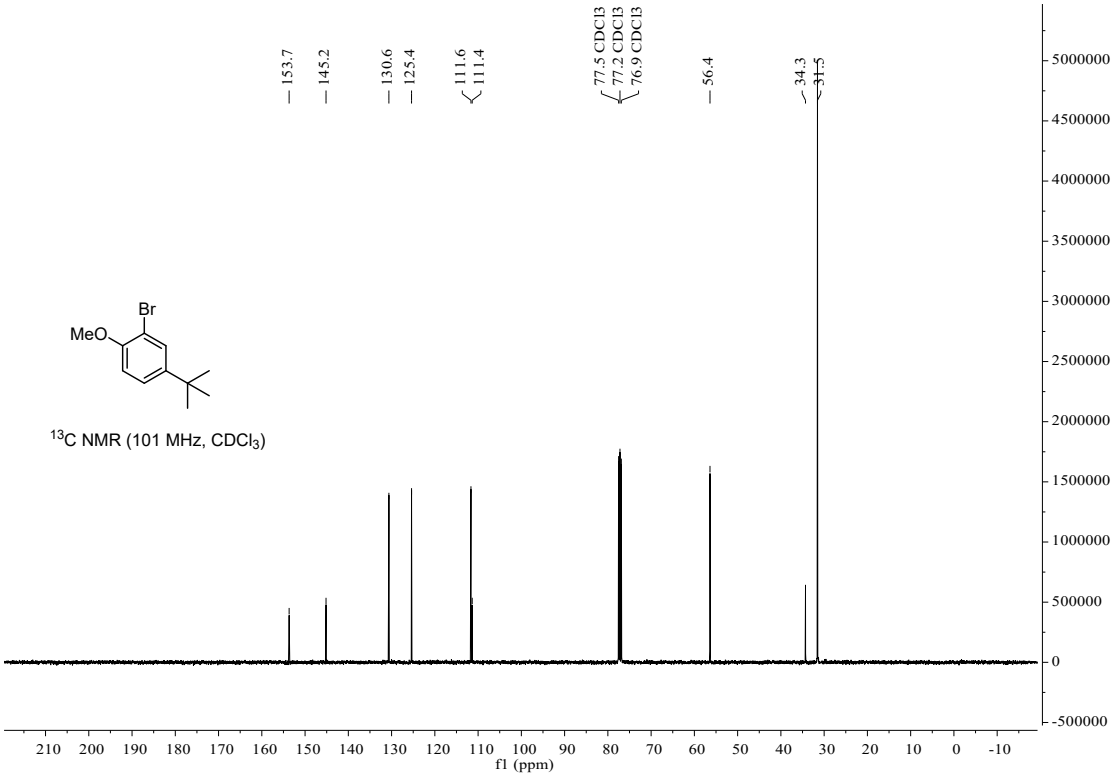


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 15

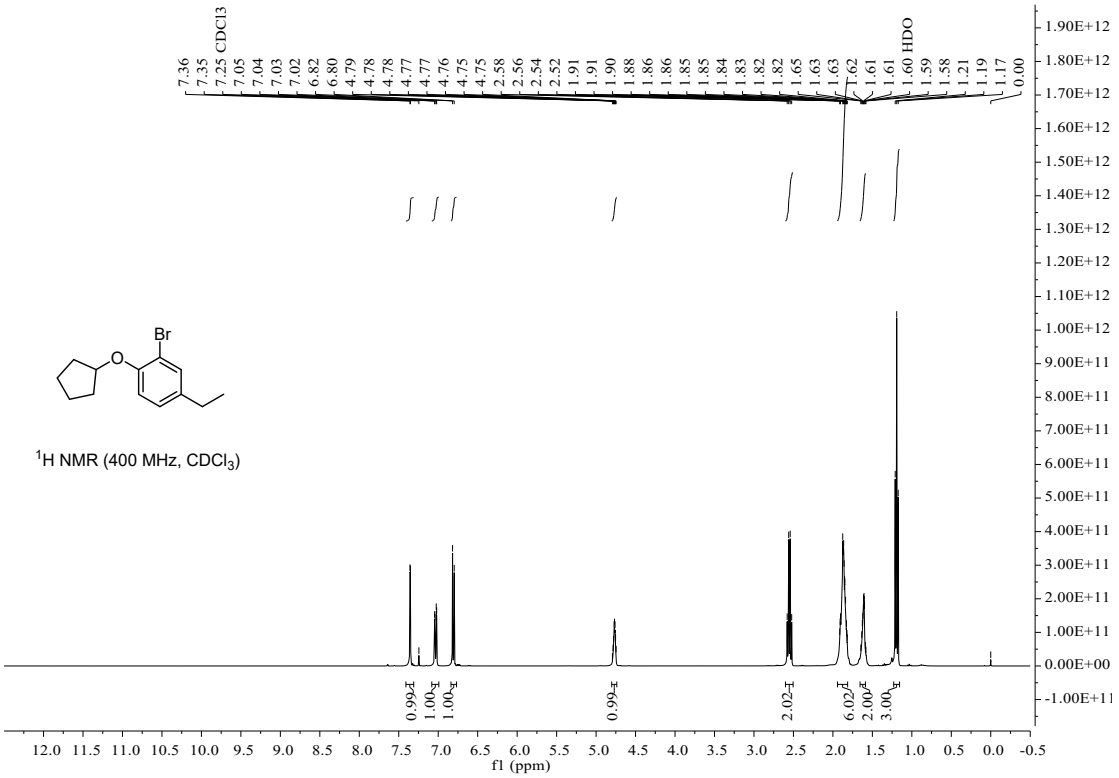


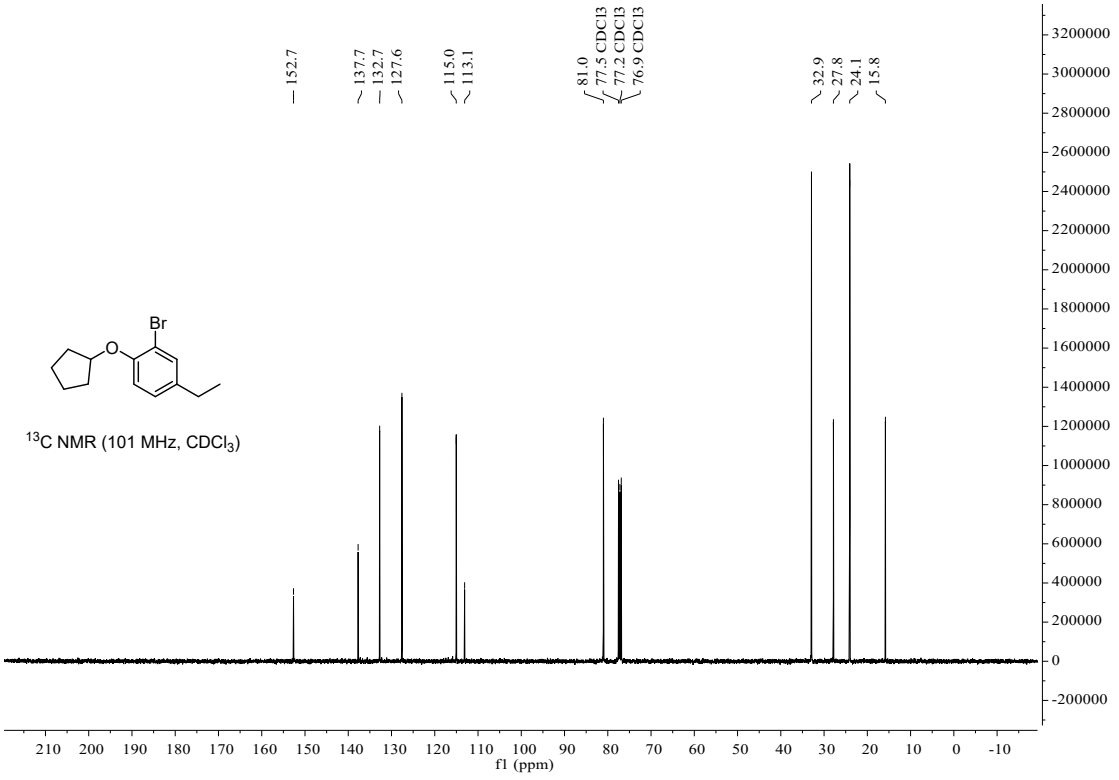
^{1}H NMR (400 MHz, $CDCl_3$)



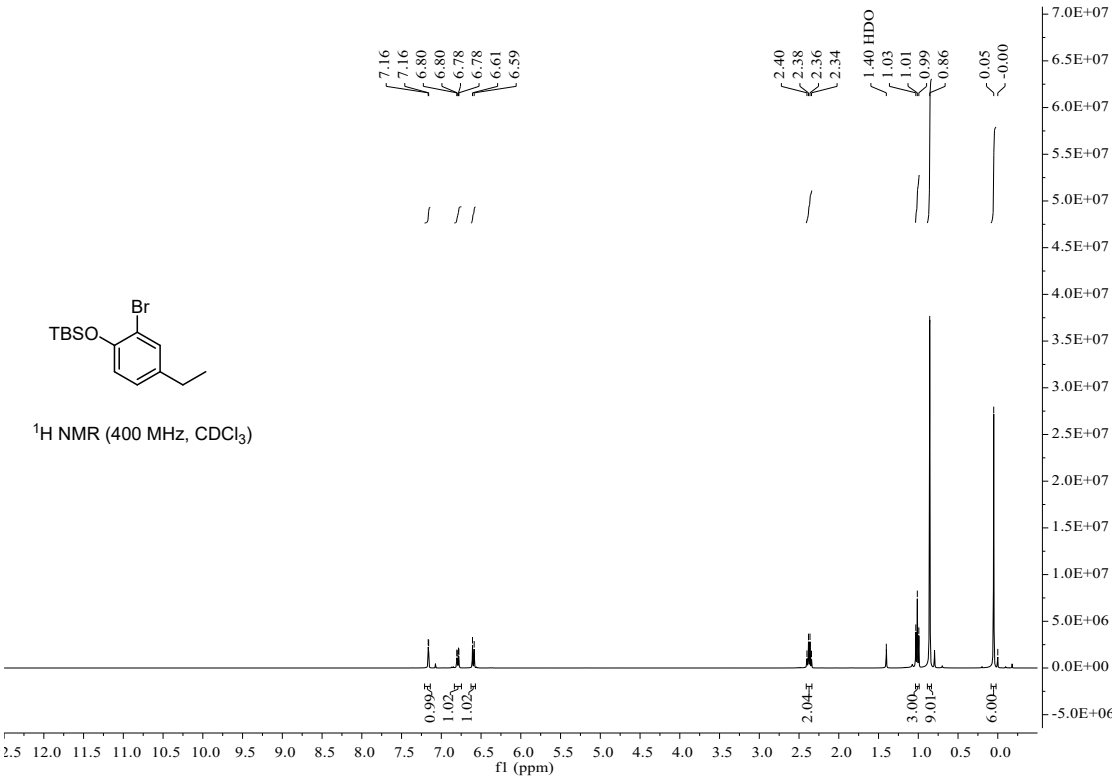
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 16

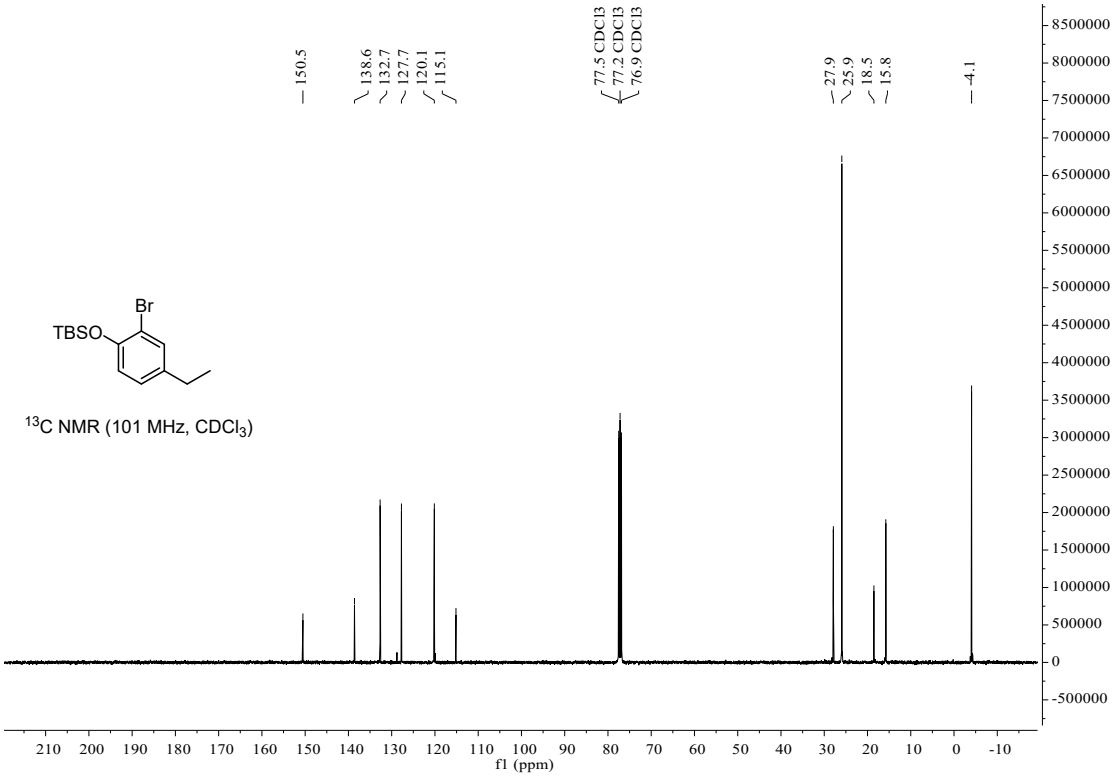

Br
O
^{1}H NMR (400 MHz, $CDCl_3$)
7.36
7.35
7.25 CDCl3
7.05
7.04
7.03
7.02
6.82
6.80
4.79
4.78
4.78
4.77
4.77
4.76
4.75
4.75
2.58
2.56
2.54
2.52
1.91
1.91
1.90
1.88
1.86
1.86
1.85
1.85
1.84
1.83
1.82
1.82
1.65
1.63
1.63
1.62
1.61
1.61
1.60 HDO
1.59
1.58
1.21
1.19
1.17
0.00
0.99
1.00
1.00
0.99
2.02
6.02
2.00
3.00
fl (ppm)


Br
O
^{13}C NMR (101 MHz, $CDCl_3$)
152.7
137.7
132.7
127.6
115.0
113.1
81.0
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
32.9
27.8
24.1
15.8
fl (ppm)

Compound 17

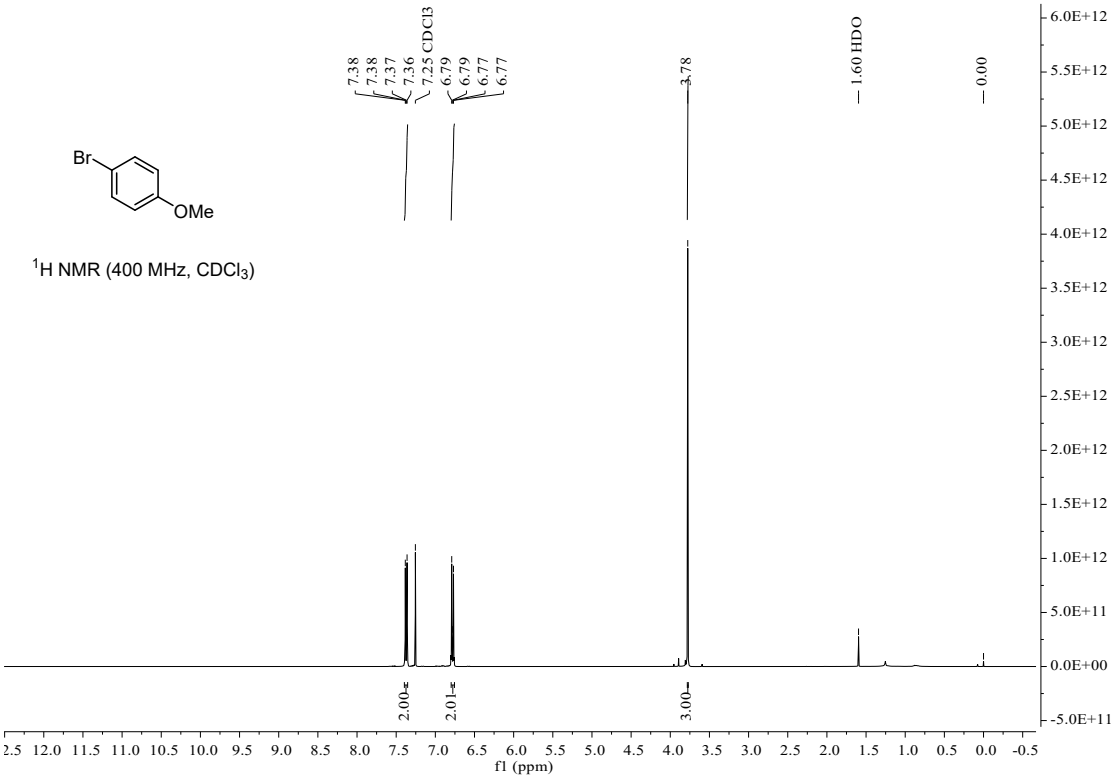


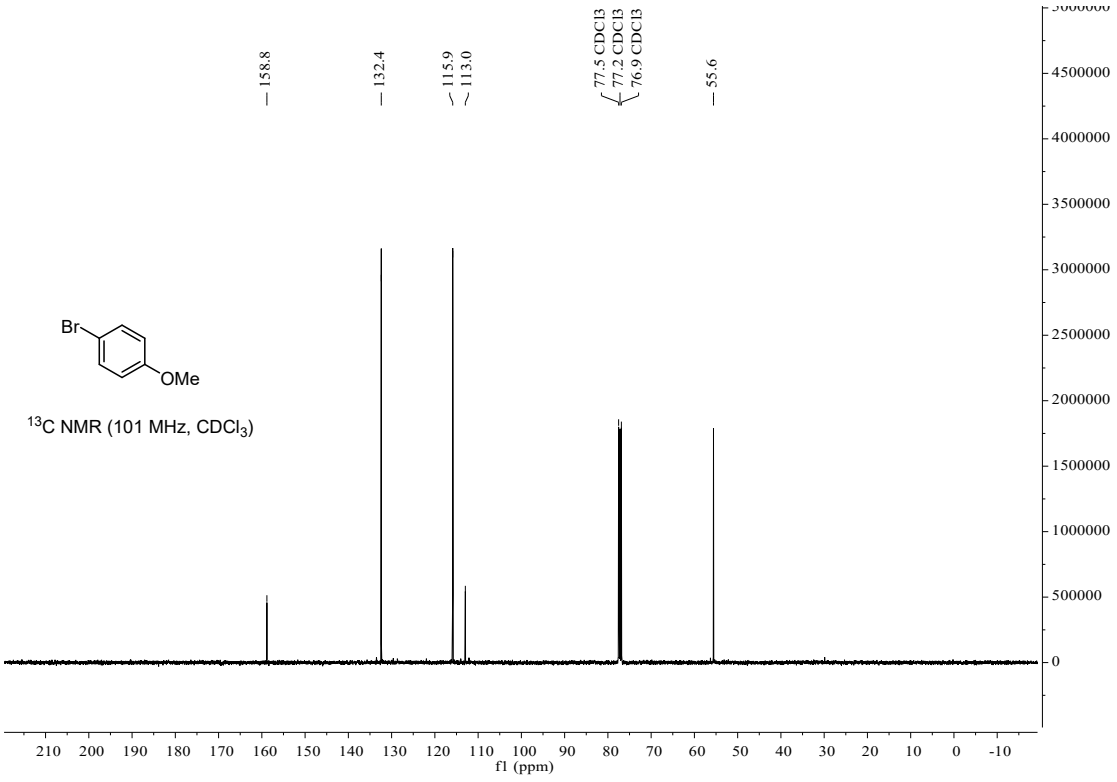
^{1}H NMR (400 MHz, $CDCl_3$)



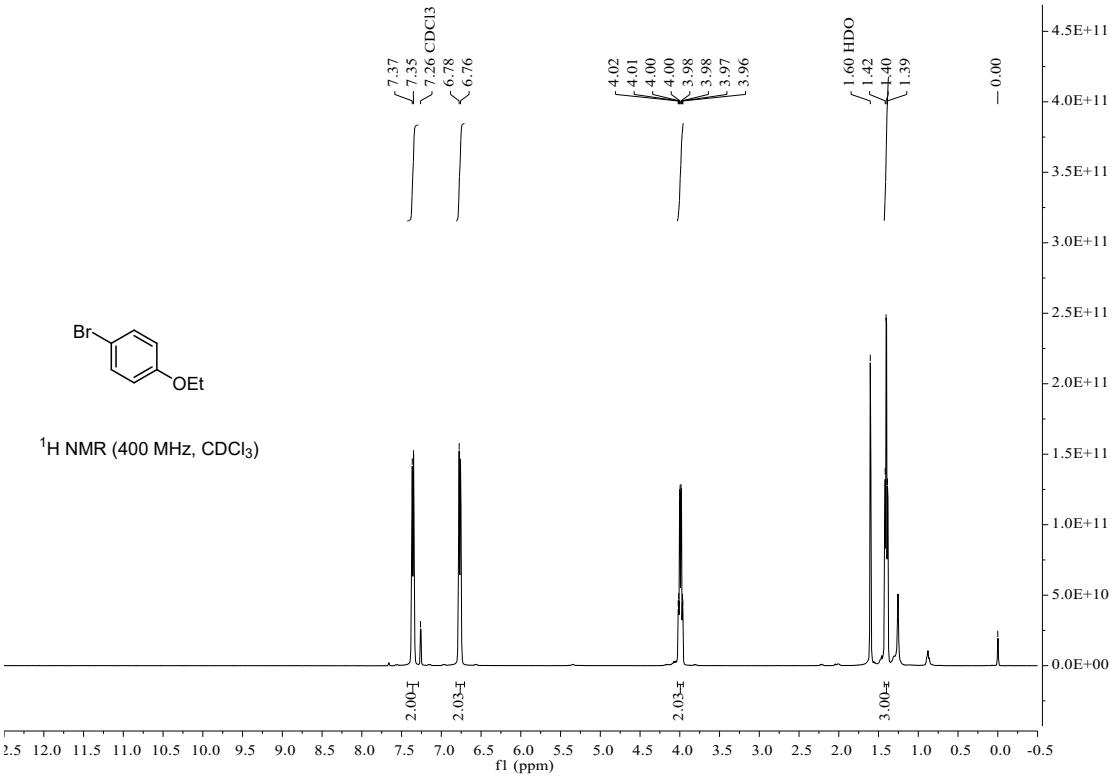
^{13}C NMR (101 MHz, $CDCl_3$)

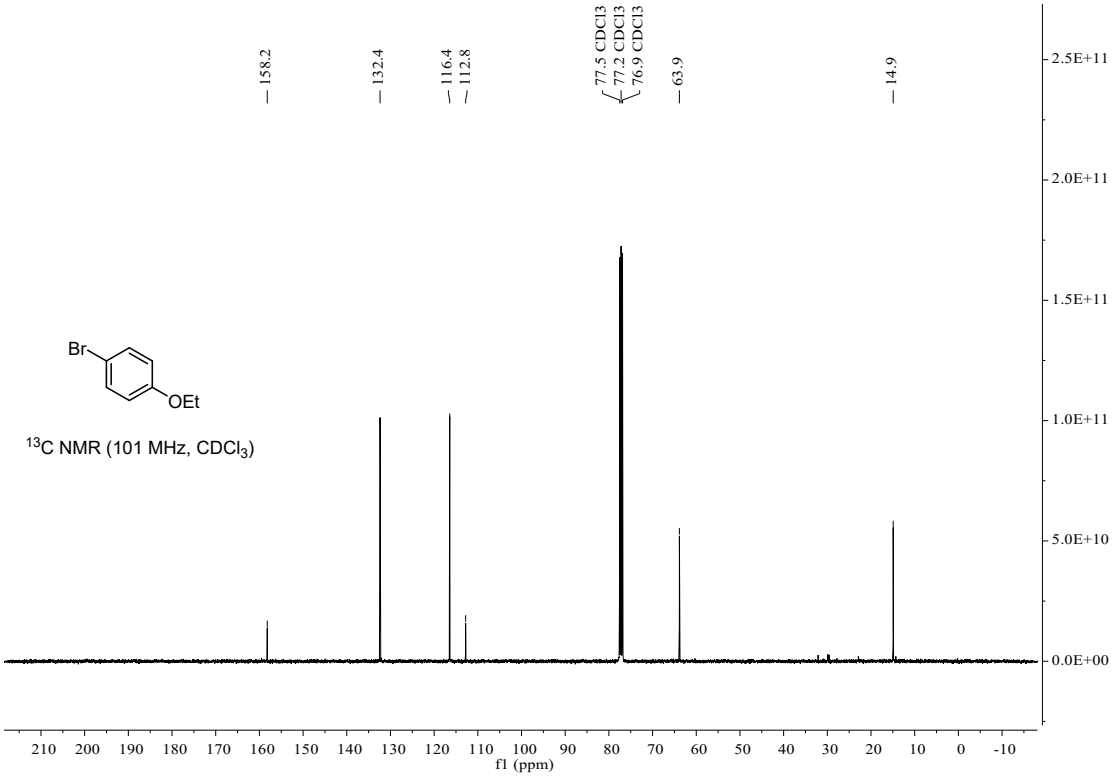
Compound 18


7.38
7.38
7.37
7.36
7.25 CDCl3
6.79
6.79
6.77
6.77
3.78
1.60 HDO
0.00
Br
OMe
1H NMR (400 MHz, CDCl3)
2.00
2.01
3.00
f1 (ppm)

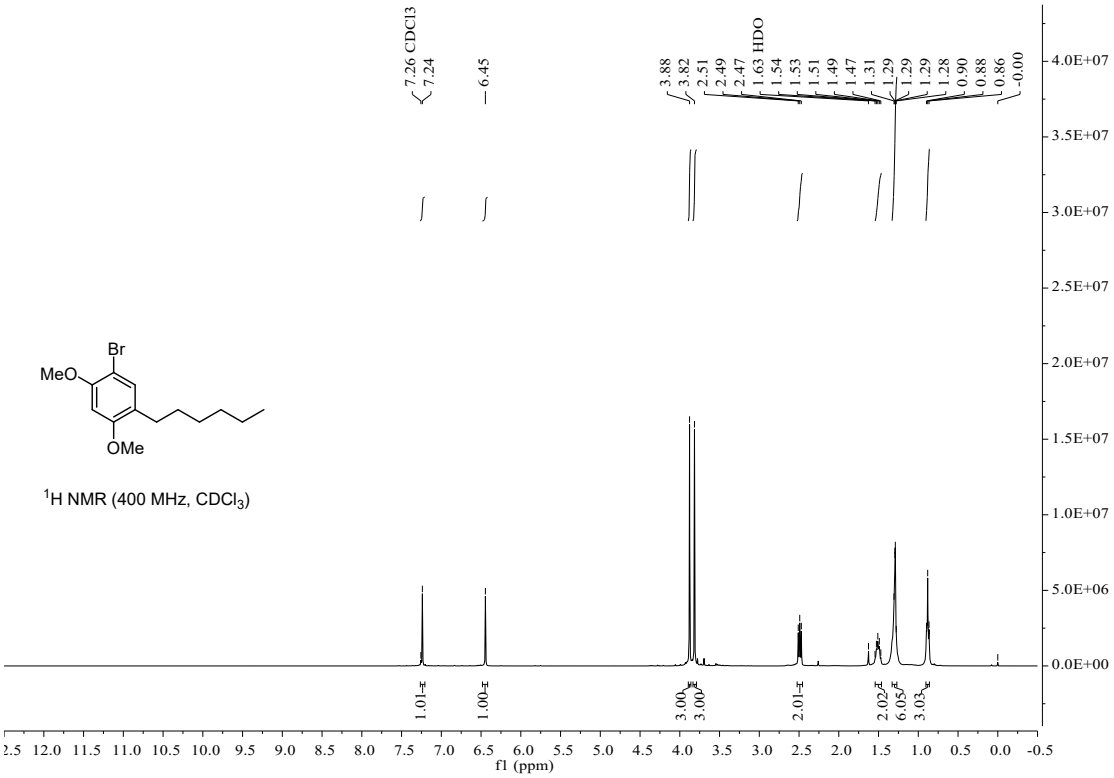

158.8
132.4
115.9
113.0
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
55.6
Br
OMe
13C NMR (101 MHz, CDCl3)
f1 (ppm)

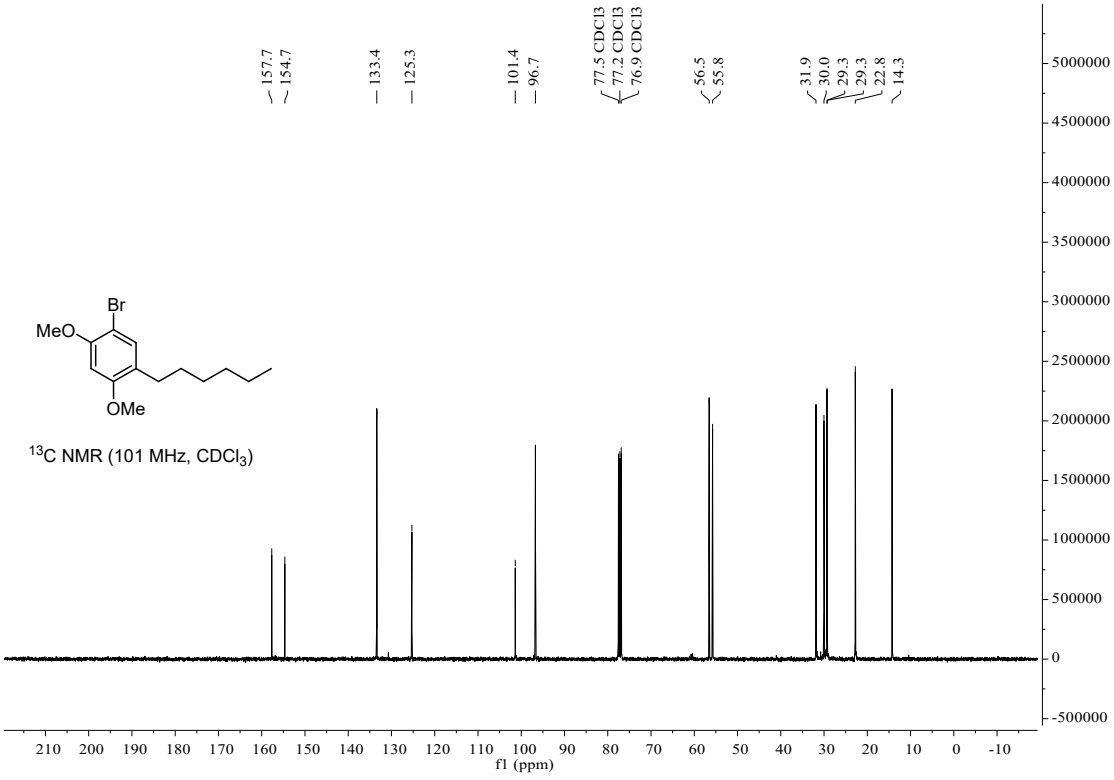
Compound 19


7.37
7.35
7.26 CDCl3
6.78
6.76
4.02
4.01
4.00
4.00
3.98
3.98
3.97
3.96
1.60 HDO
1.42
1.40
1.39
0.00
Br
OEt
1H NMR (400 MHz, CDCl3)
2.00
2.03
2.03
3.00
f1 (ppm)

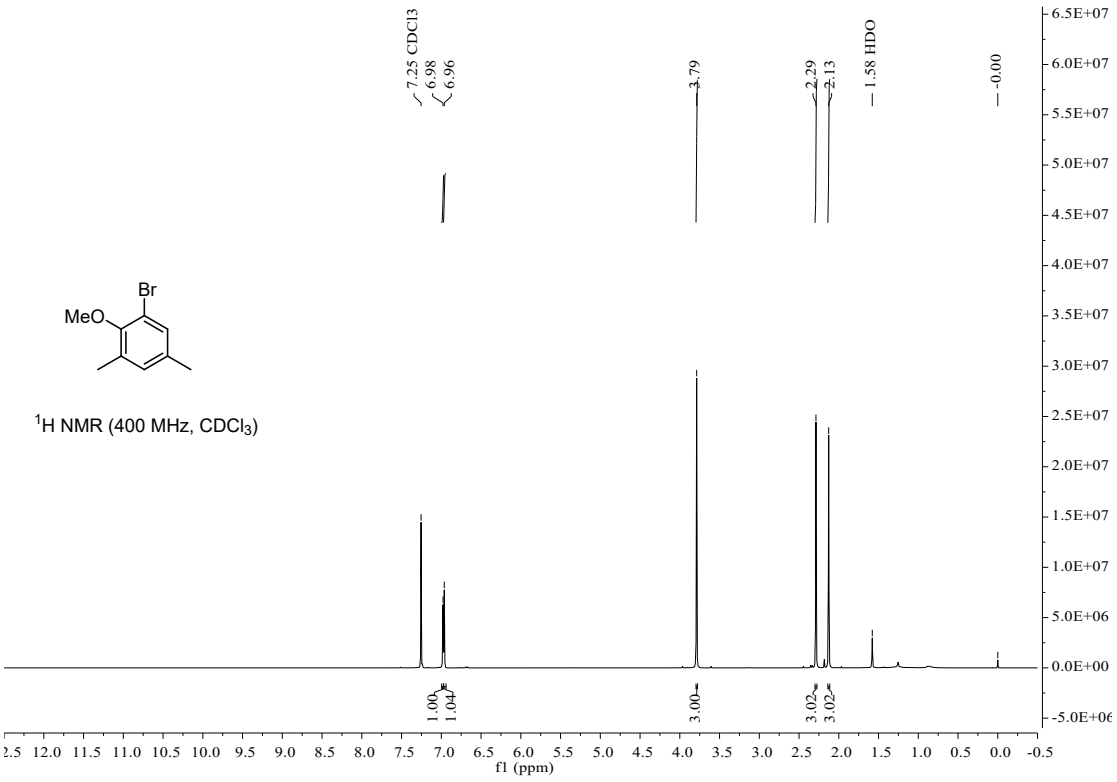

158.2
132.4
116.4
112.8
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
63.9
14.9
Br
OEt
13C NMR (101 MHz, CDCl3)
f1 (ppm)

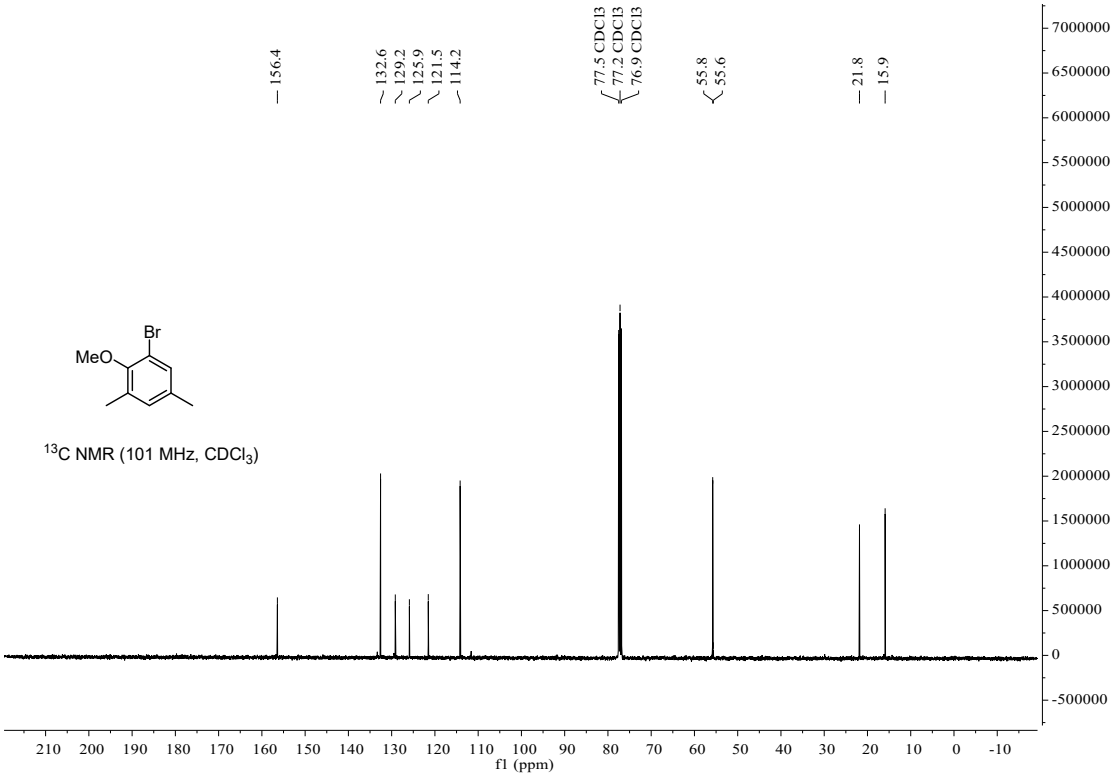
Compound 20


7.26 CDCl3
7.24
6.45
3.88
3.82
2.51
2.49
2.47
1.63 HDO
1.54
1.53
1.51
1.49
1.47
1.31
1.29
1.29
1.29
1.28
0.90
0.88
0.86
-0.00
Br
MeO
OMe
1H NMR (400 MHz, CDCl3)
1.01
1.00
3.00
3.00
2.01
2.02
6.05
3.03
f1 (ppm)

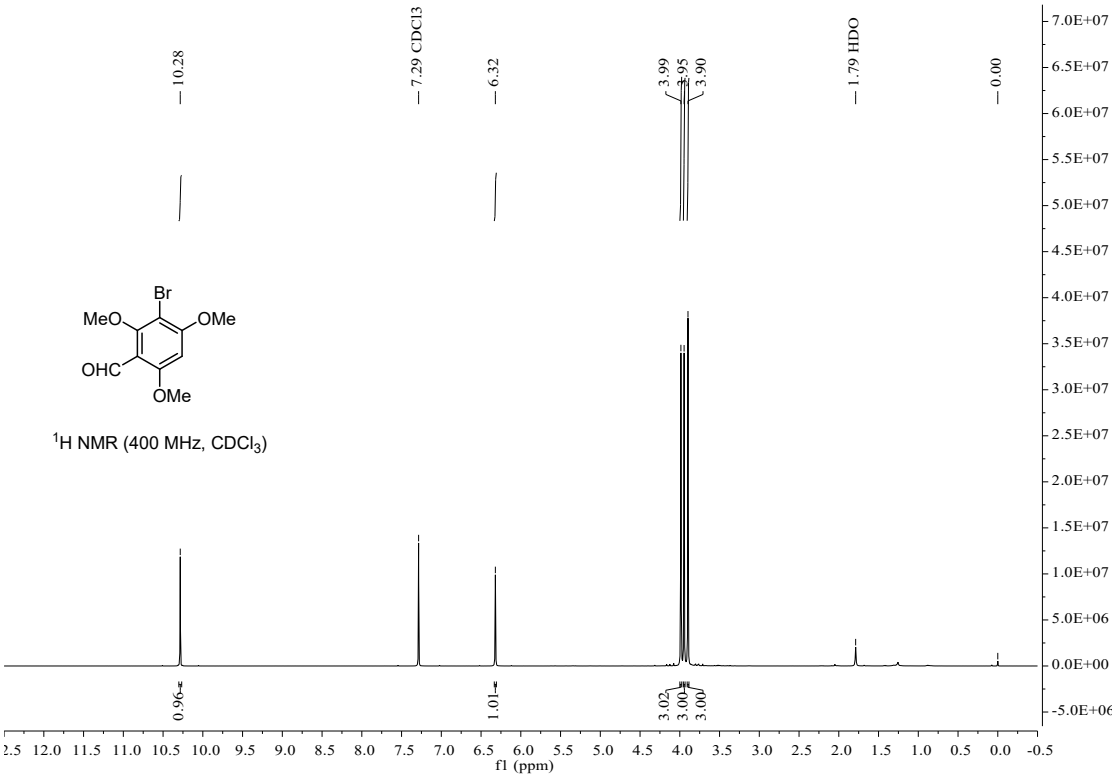

157.7
154.7
133.4
125.3
101.4
96.7
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
56.5
55.8
31.9
30.0
29.3
29.3
22.8
14.3
Br
MeO
OMe
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 21

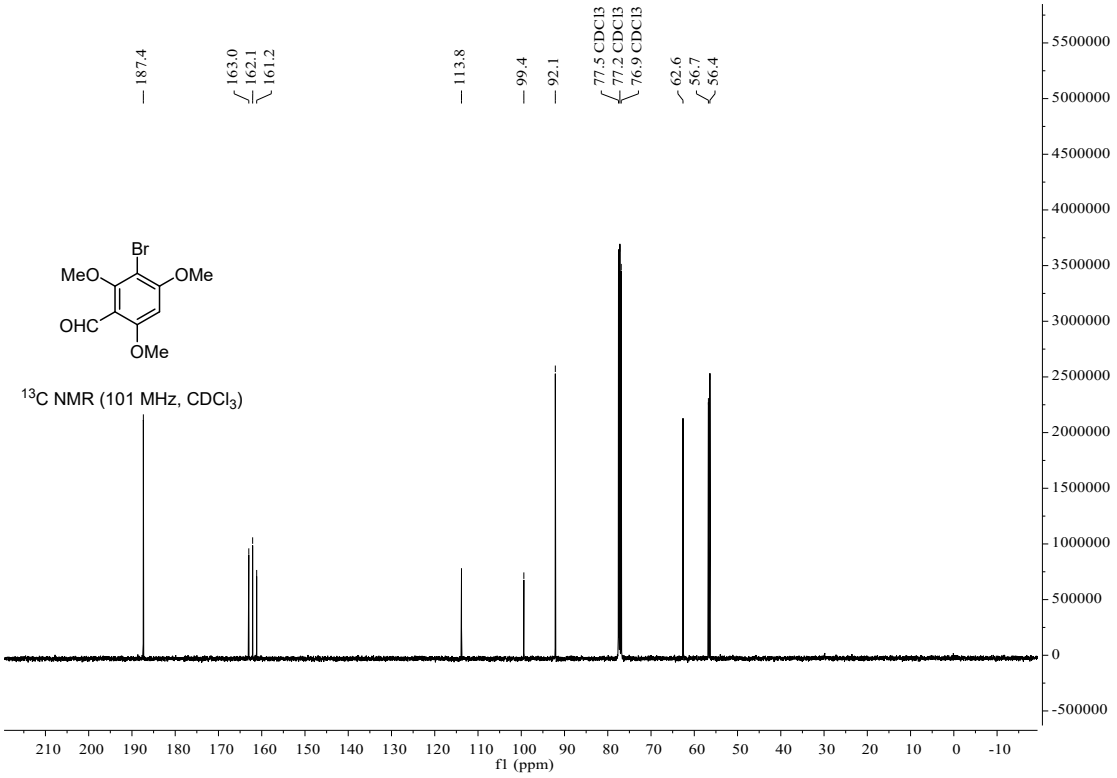

7.25 CDCl3
6.98
6.96
3.79
2.29
2.13
1.58 HDO
0.00
Br
MeO
1H NMR (400 MHz, CDCl3)
1.00
1.04
3.00
3.02
3.02
f1 (ppm)


156.4
132.6
129.2
125.9
121.5
114.2
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
55.8
55.6
21.8
15.9
Br
MeO
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 22

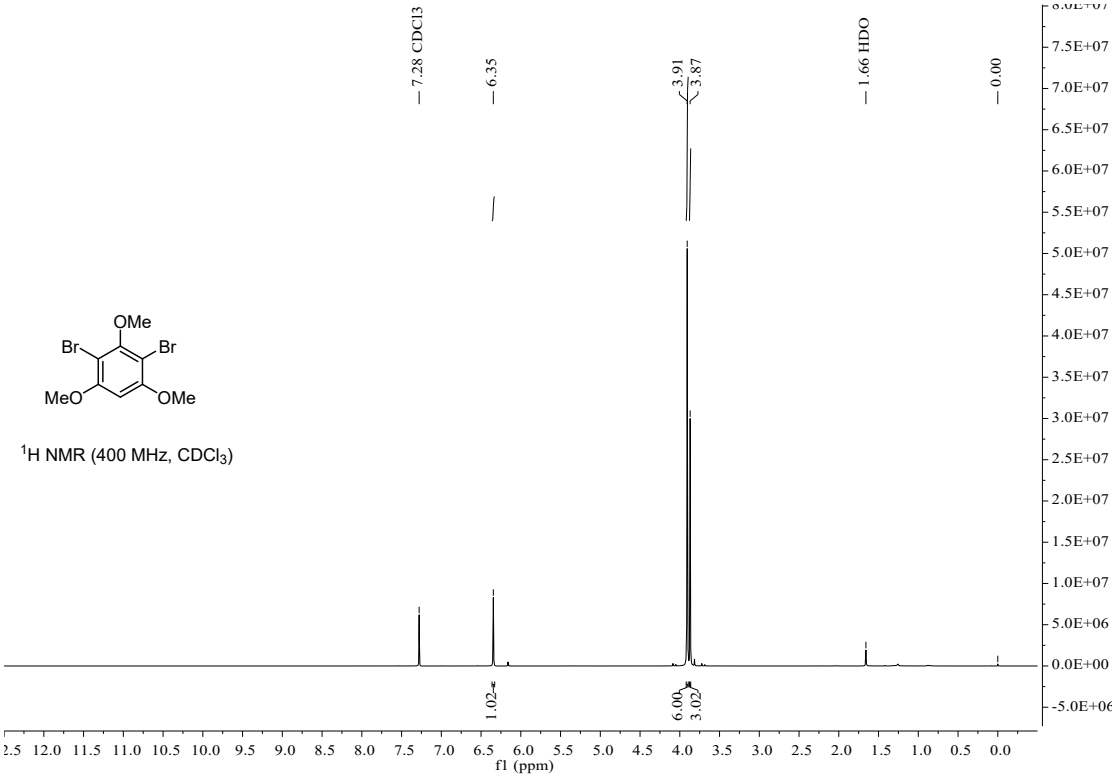


^{1}H NMR (400 MHz, $CDCl_3$)

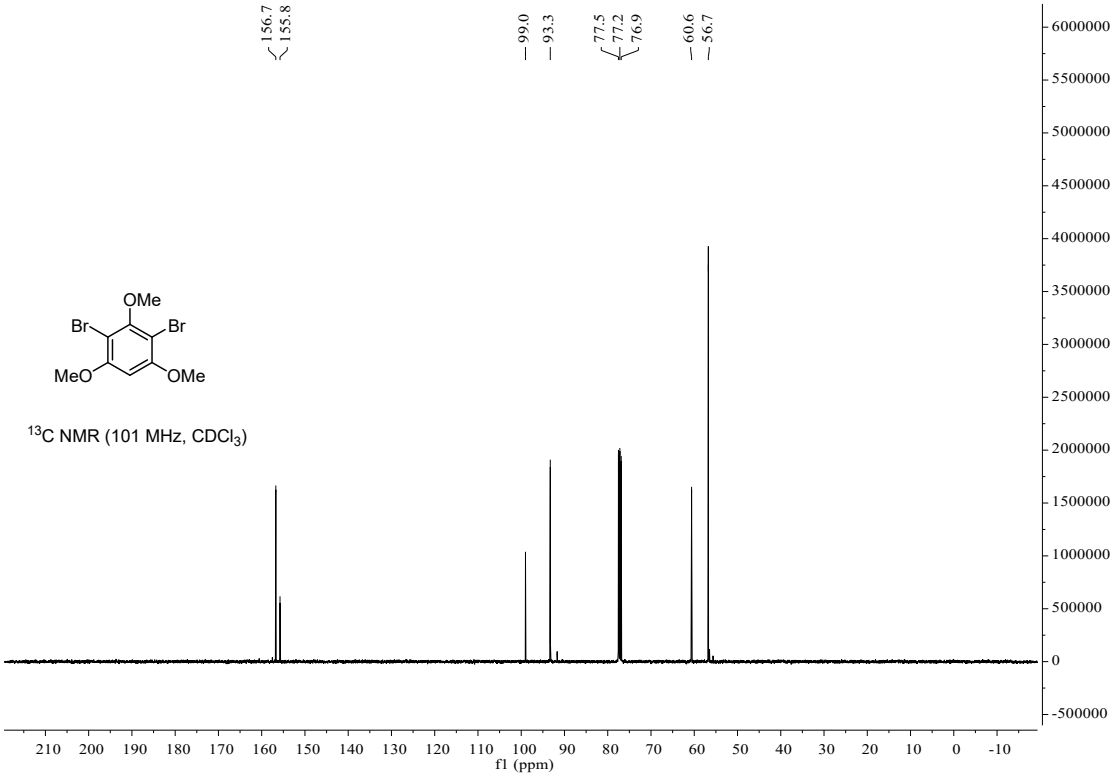


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 23

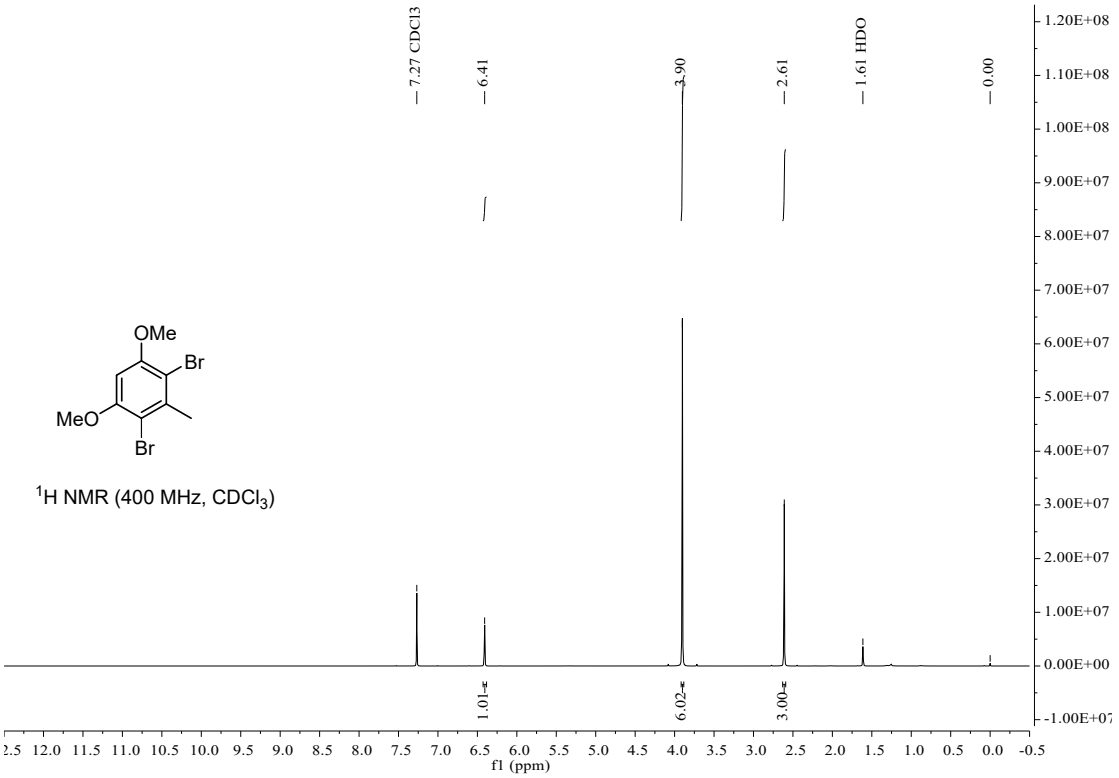


^{1}H NMR (400 MHz, $CDCl_3$)

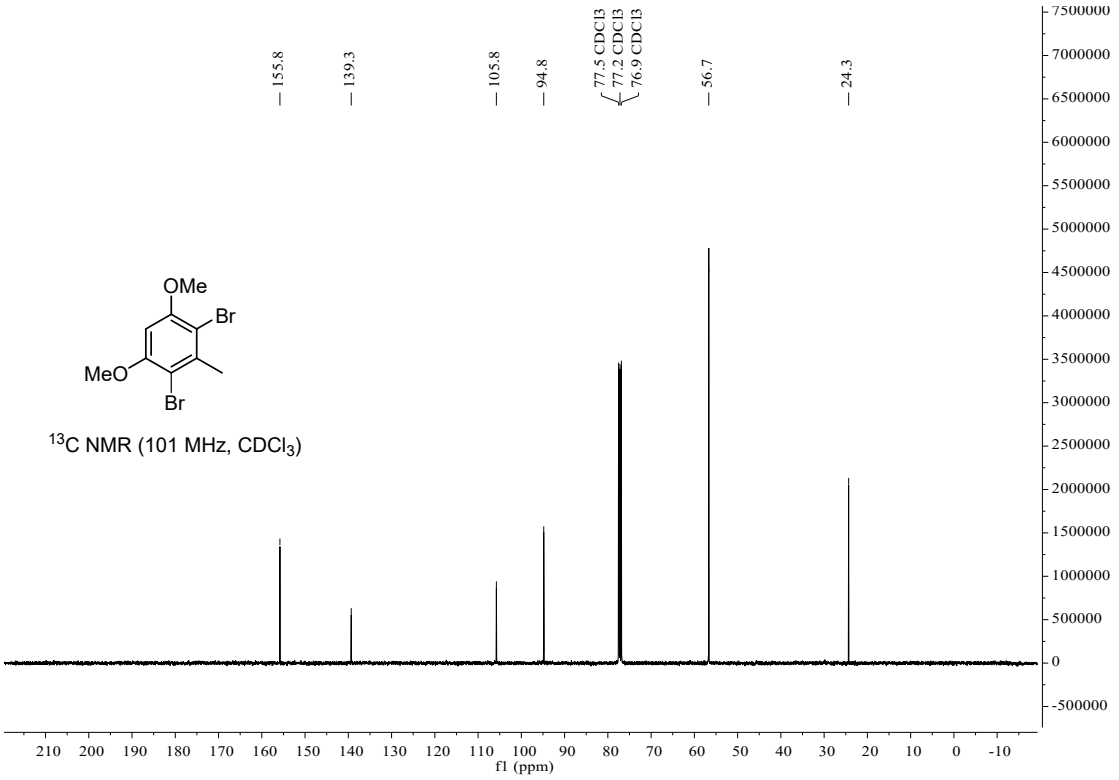


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 24

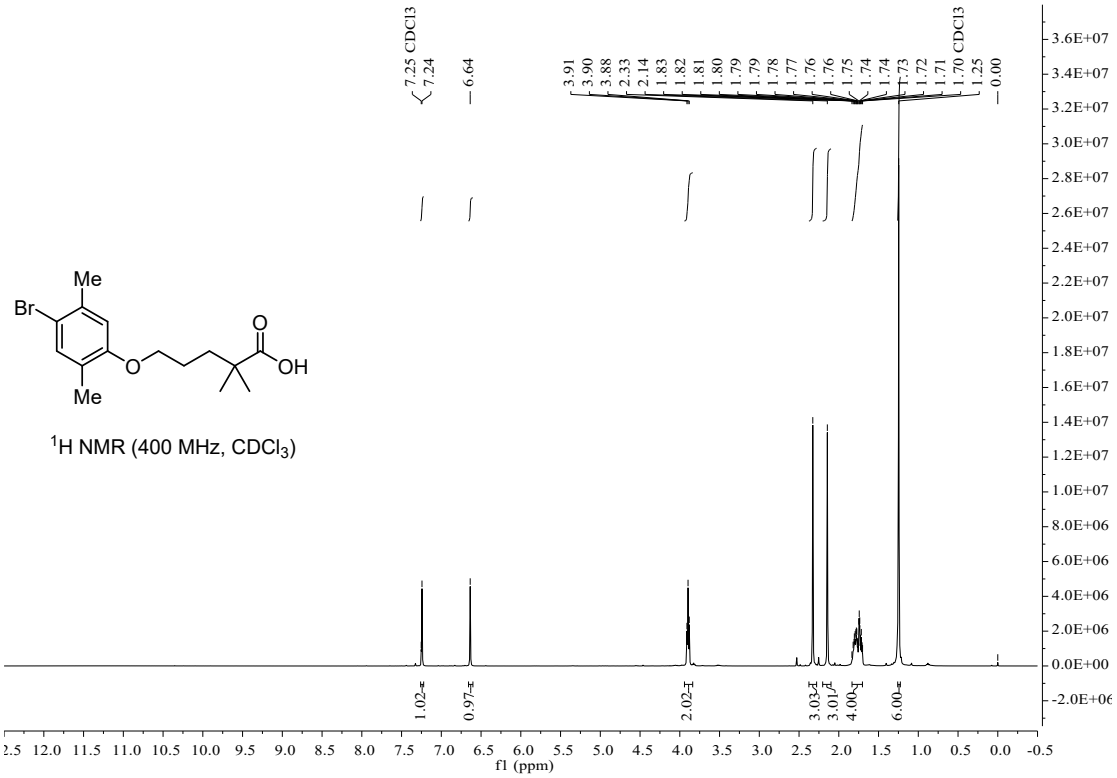


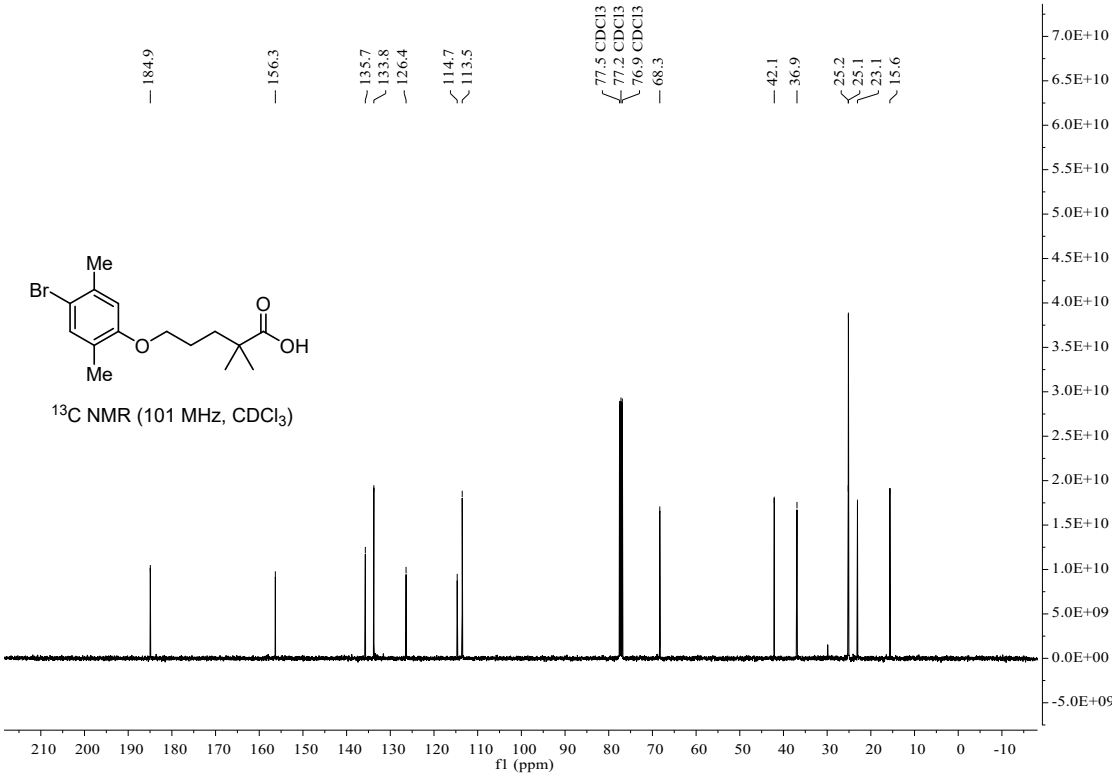
^{1}H NMR (400 MHz, $CDCl_3$)



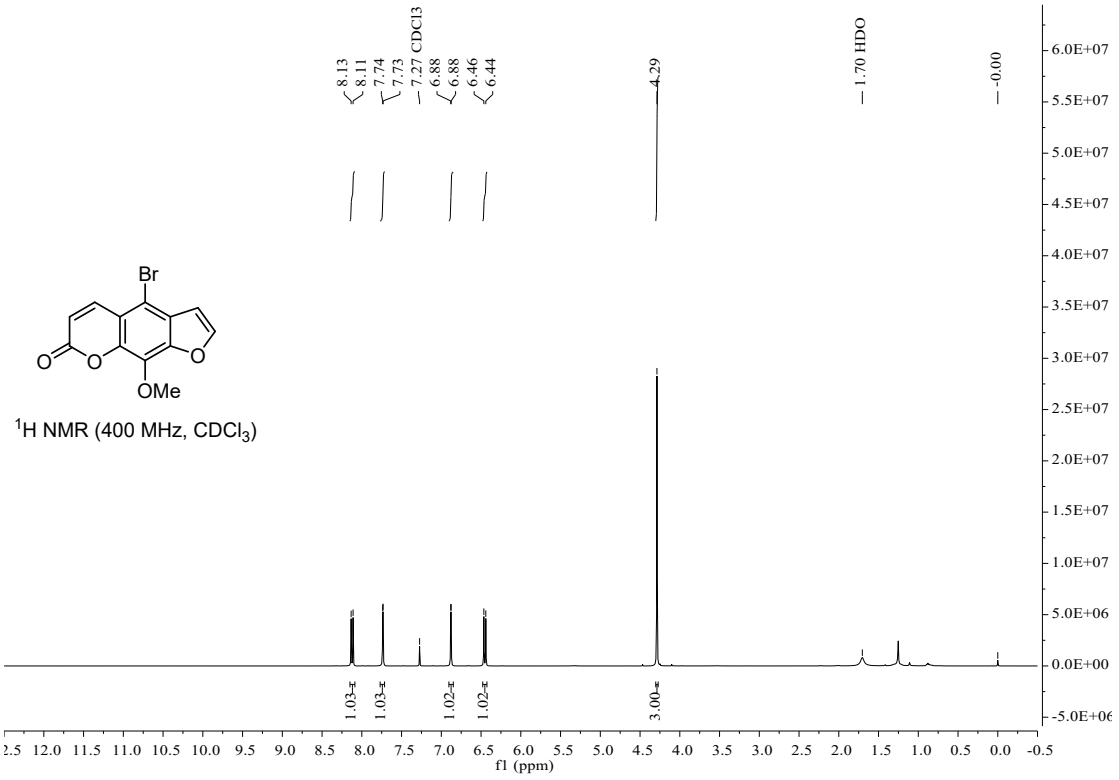
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 25

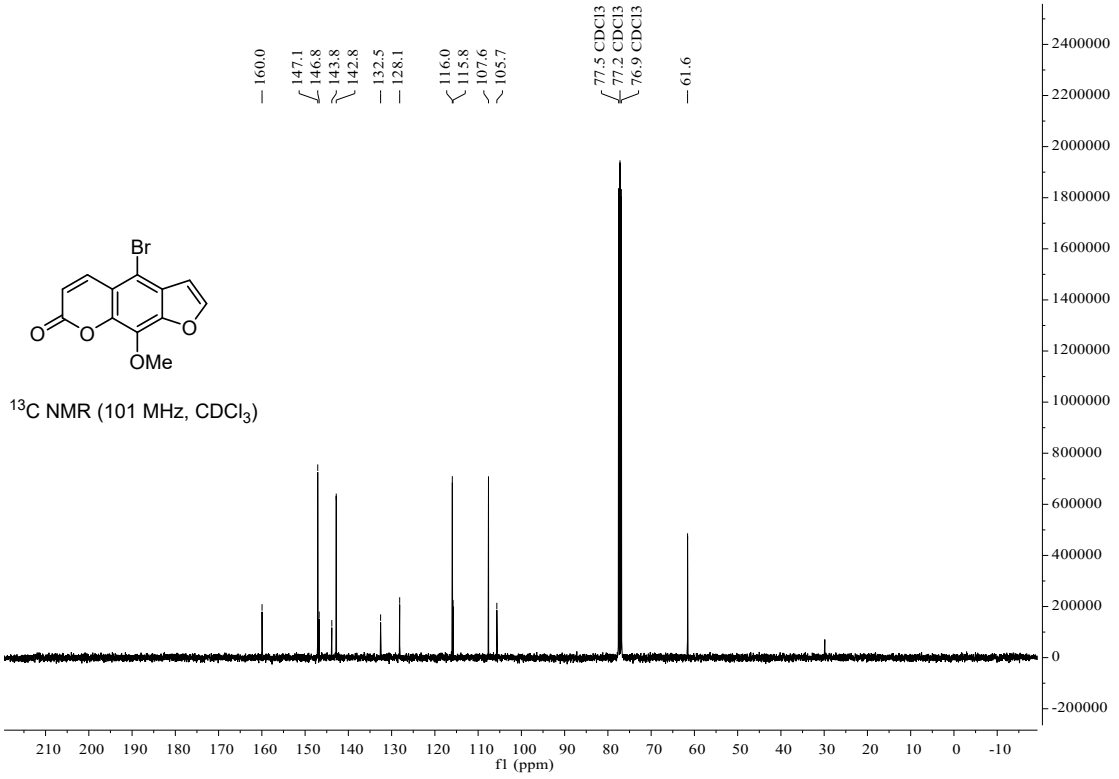

Me
Br
O
OH
Me
^{1}H NMR (400 MHz, $CDCl_3$)
7.25 CDCl3
7.24
6.64
3.91
3.90
3.88
2.33
2.14
1.83
1.82
1.81
1.80
1.79
1.79
1.78
1.77
1.76
1.76
1.75
1.74
1.74
1.73
1.72
1.71
1.70 CDCl3
1.25
0.00
1.02
0.97
2.02
3.03
3.01
4.00
6.00
f1 (ppm)


Me
Br
O
OH
Me
^{13}C NMR (101 MHz, $CDCl_3$)
184.9
156.3
135.7
133.8
126.4
114.7
113.5
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
68.3
42.1
36.9
25.2
25.1
23.1
15.6
f1 (ppm)

Compound 26

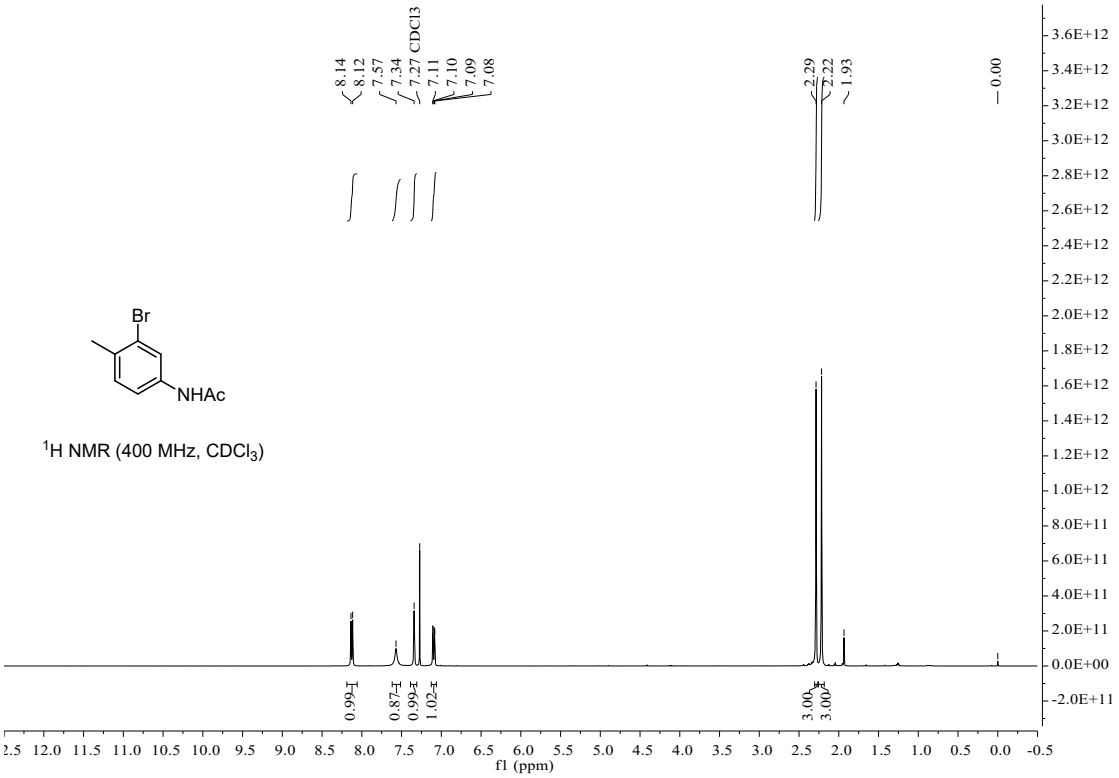


^{1}H NMR (400 MHz, $CDCl_3$)

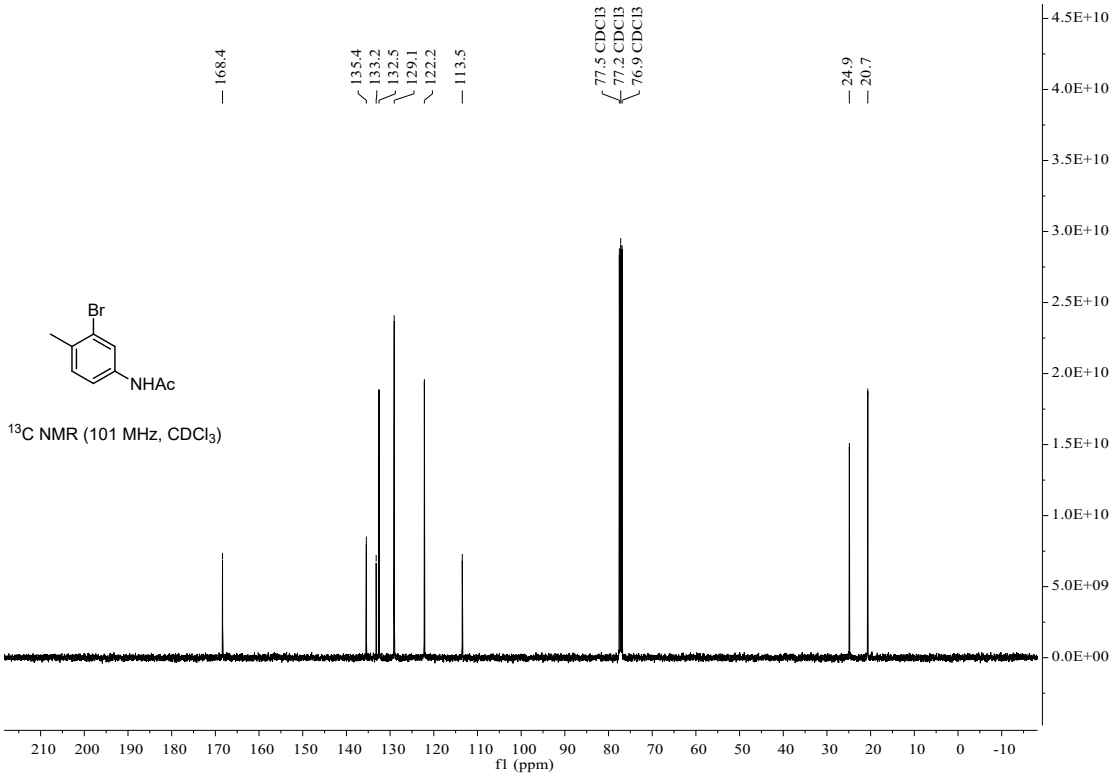


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 27

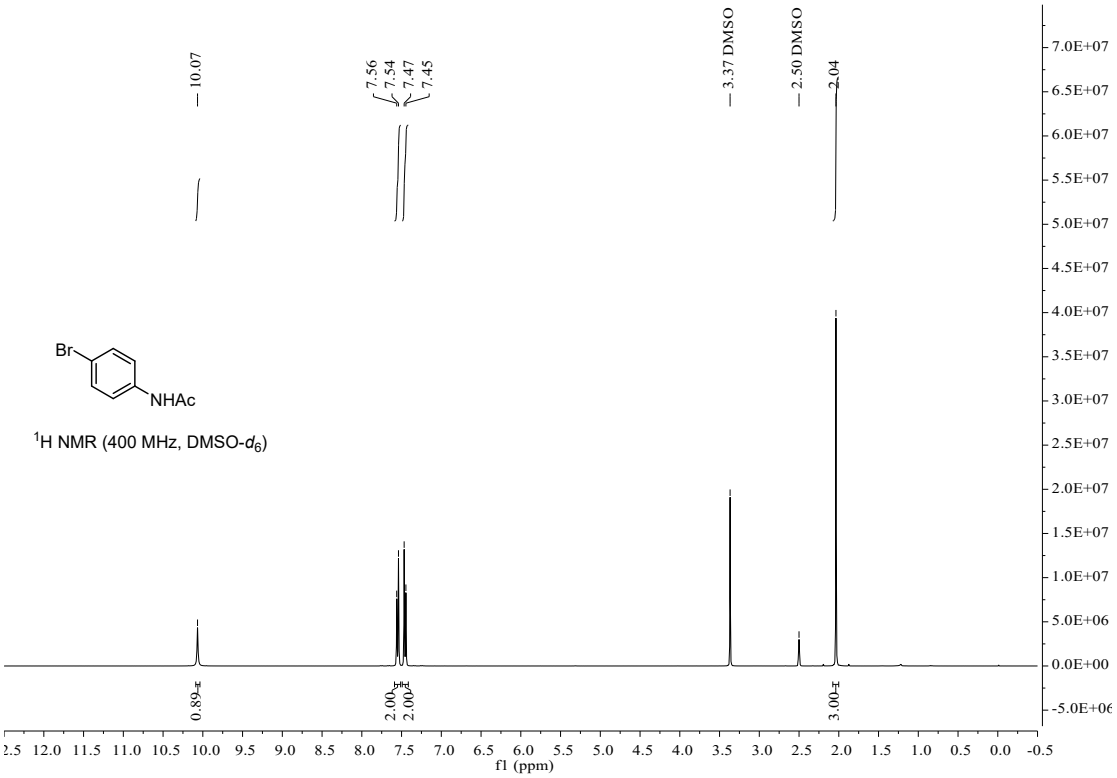


^{1}H NMR (400 MHz, $CDCl_3$)

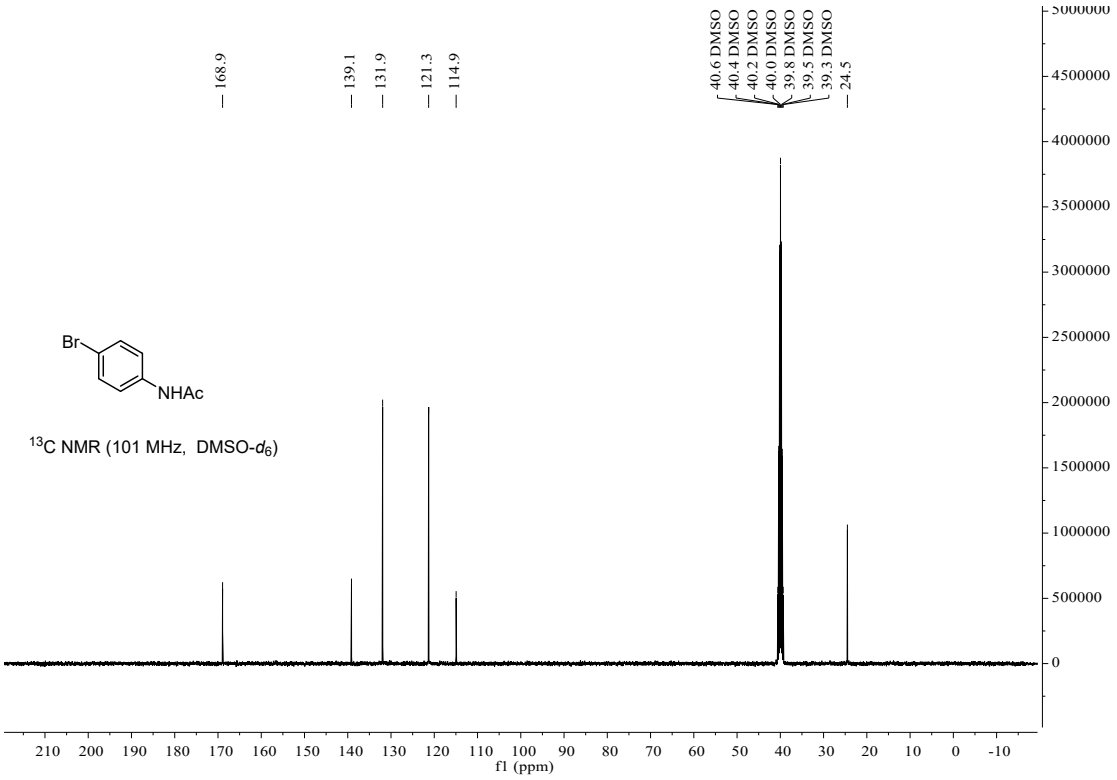


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 28

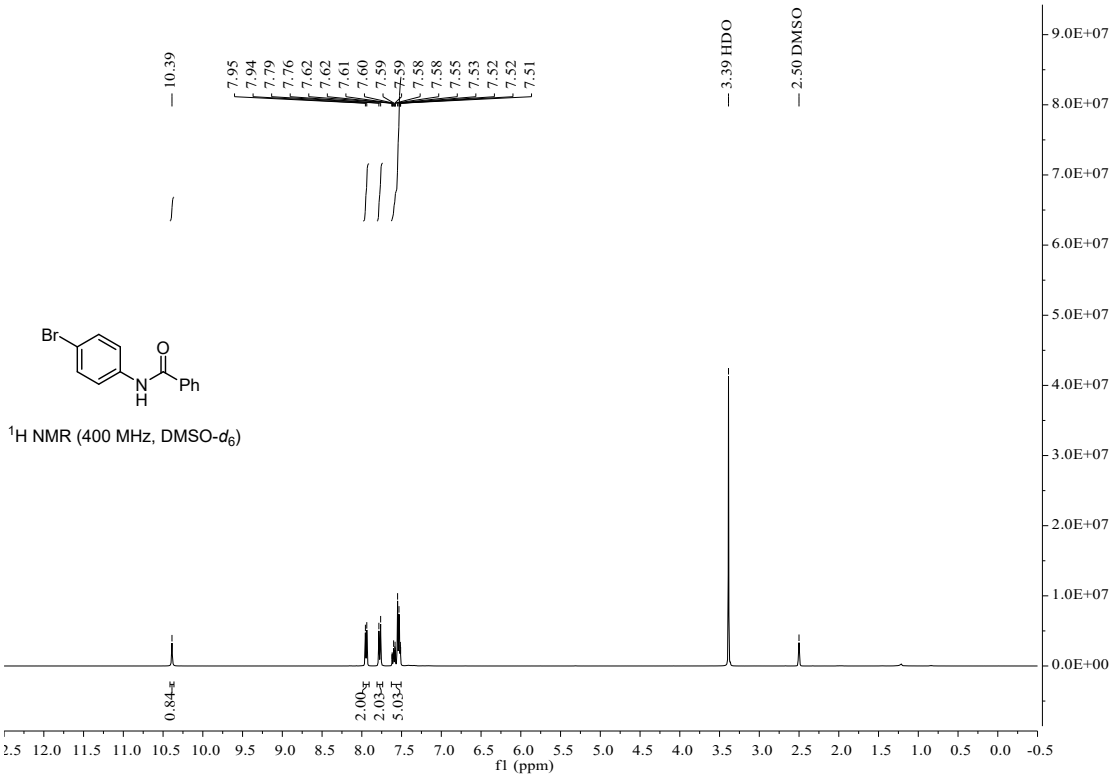


^{1}H NMR (400 MHz, DMSO-d_6)

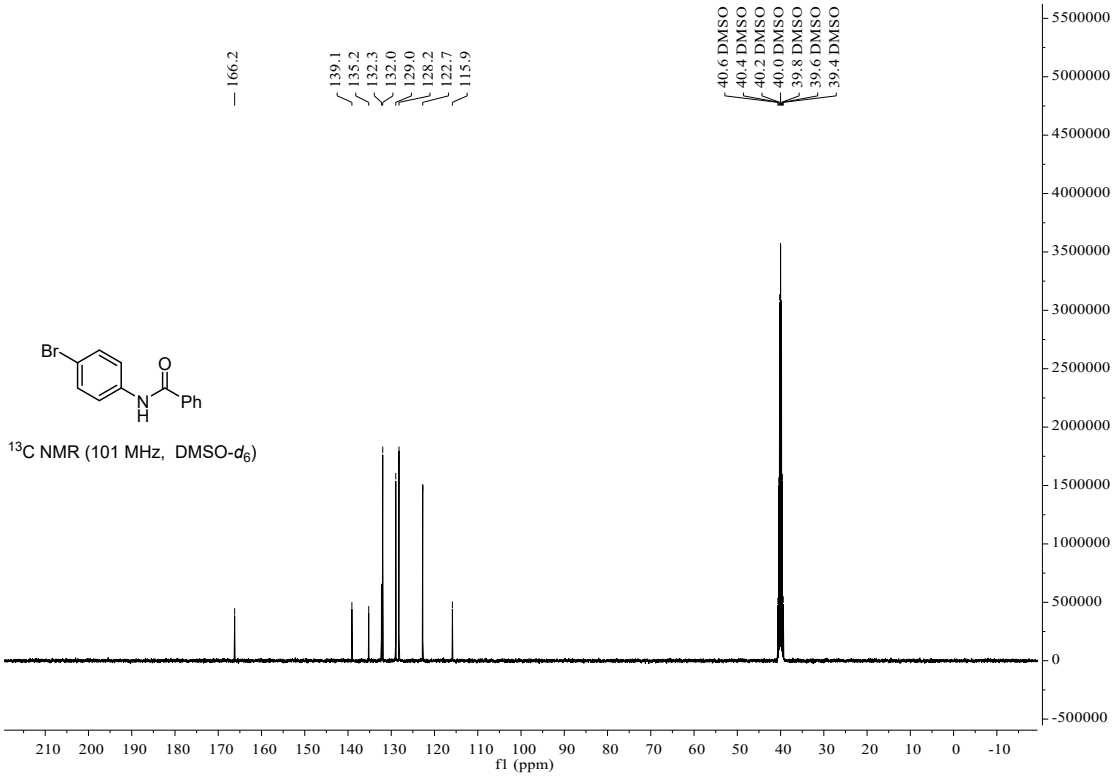


^{13}C NMR (101 MHz, DMSO-d_6)

Compound 29

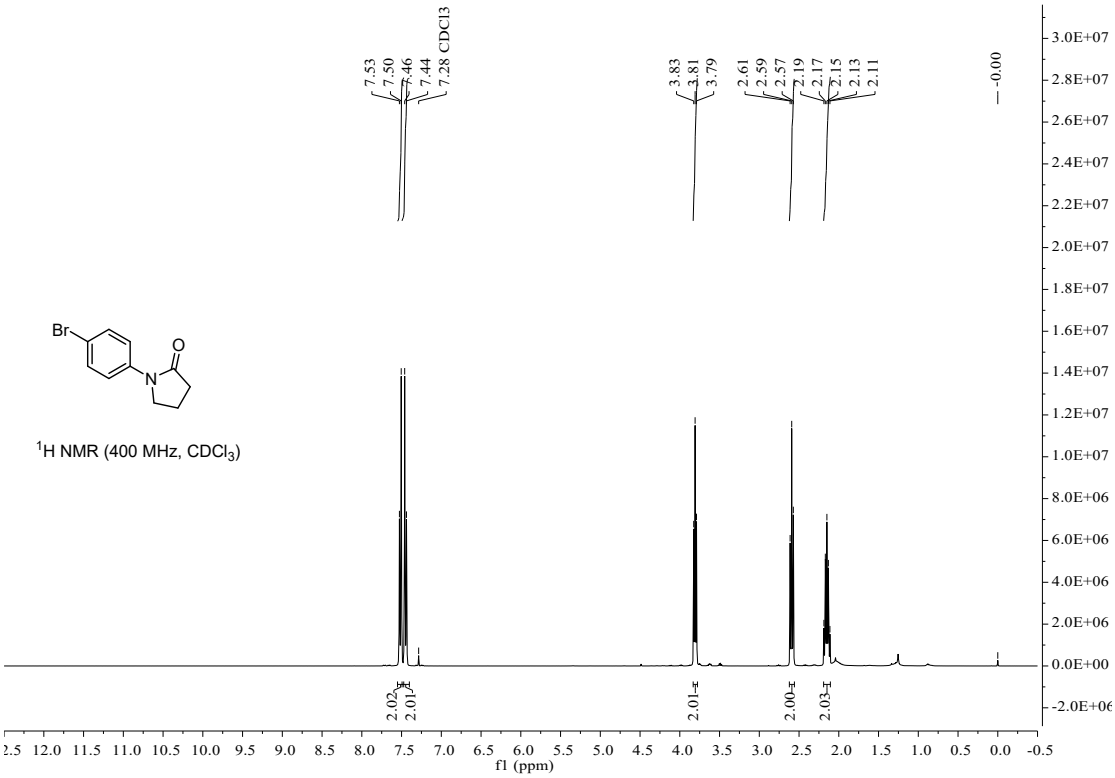


^{1}H NMR (400 MHz, DMSO-d_6)

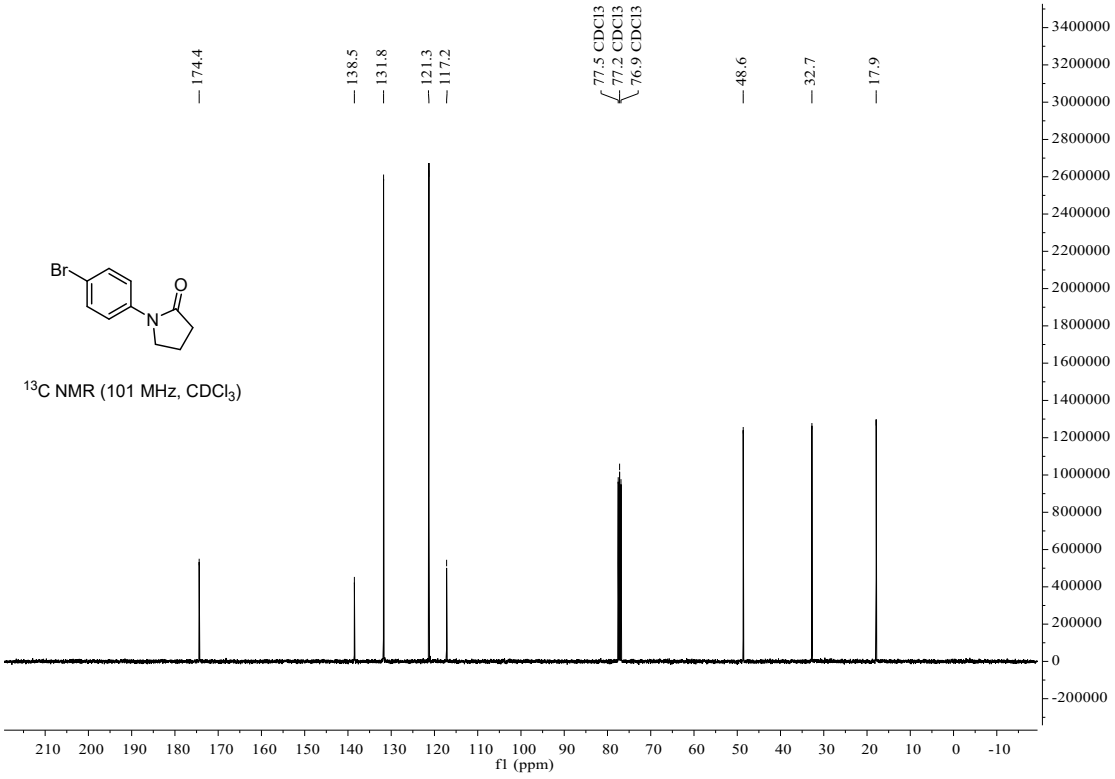


^{13}C NMR (101 MHz, DMSO-d_6)

Compound 30

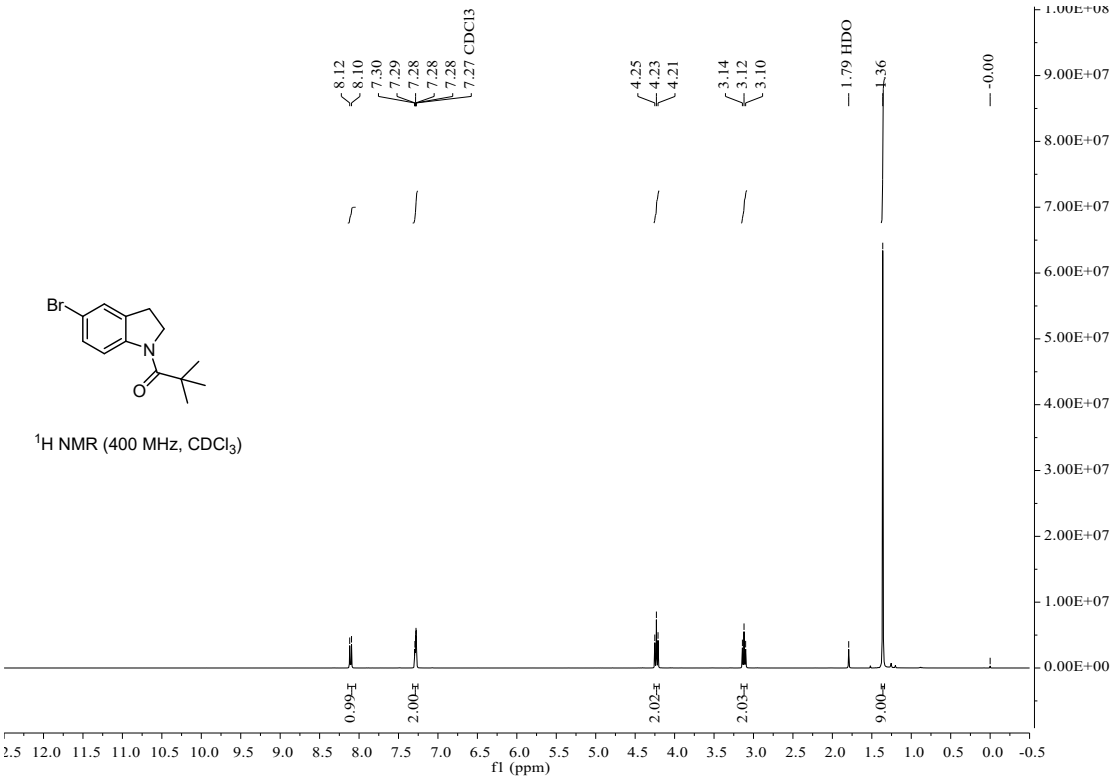


^{1}H NMR (400 MHz, $CDCl_3$)

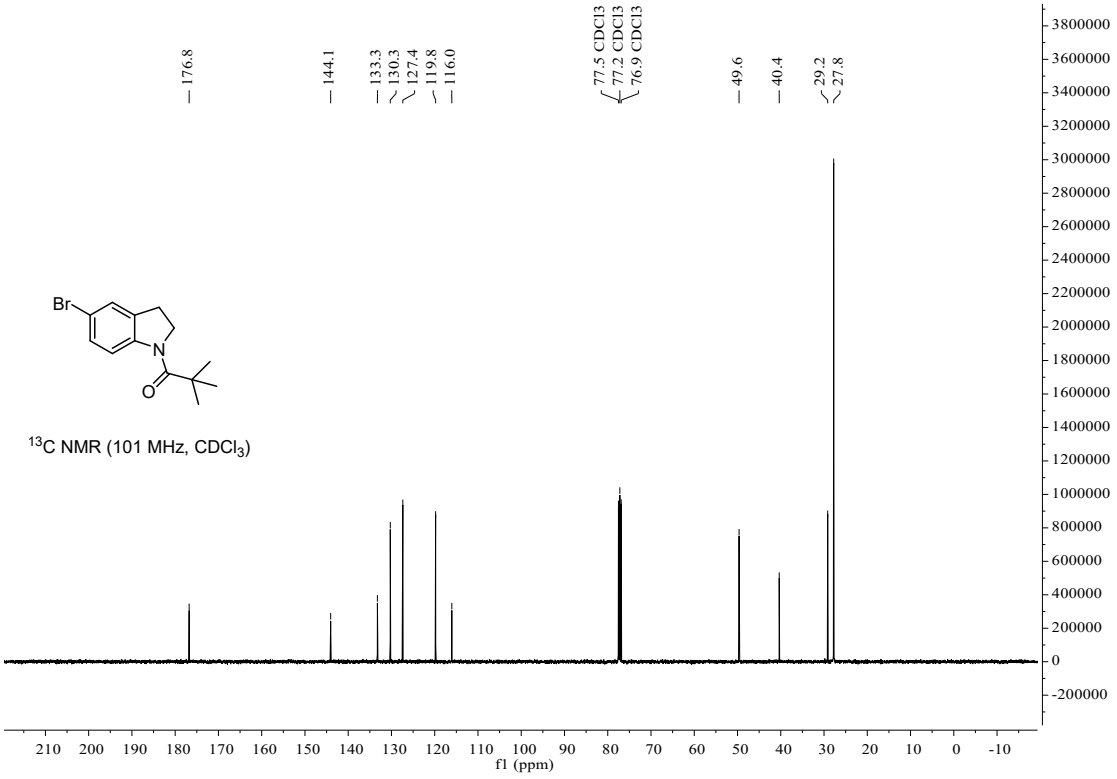


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 31

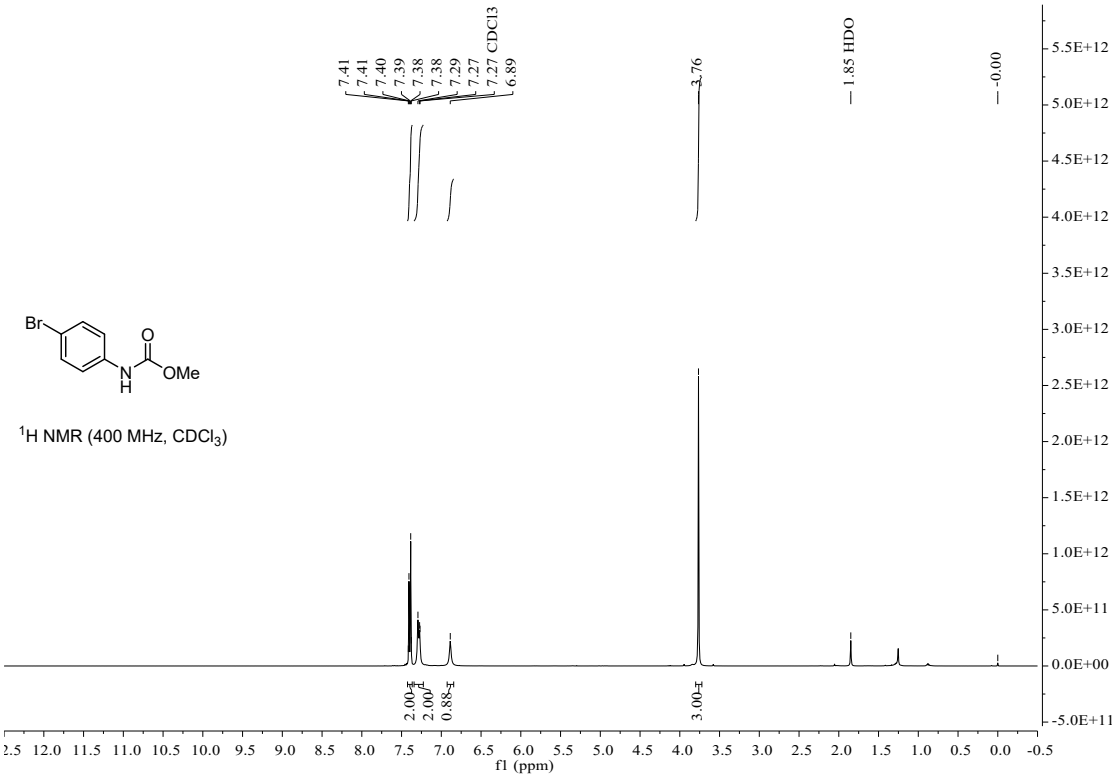


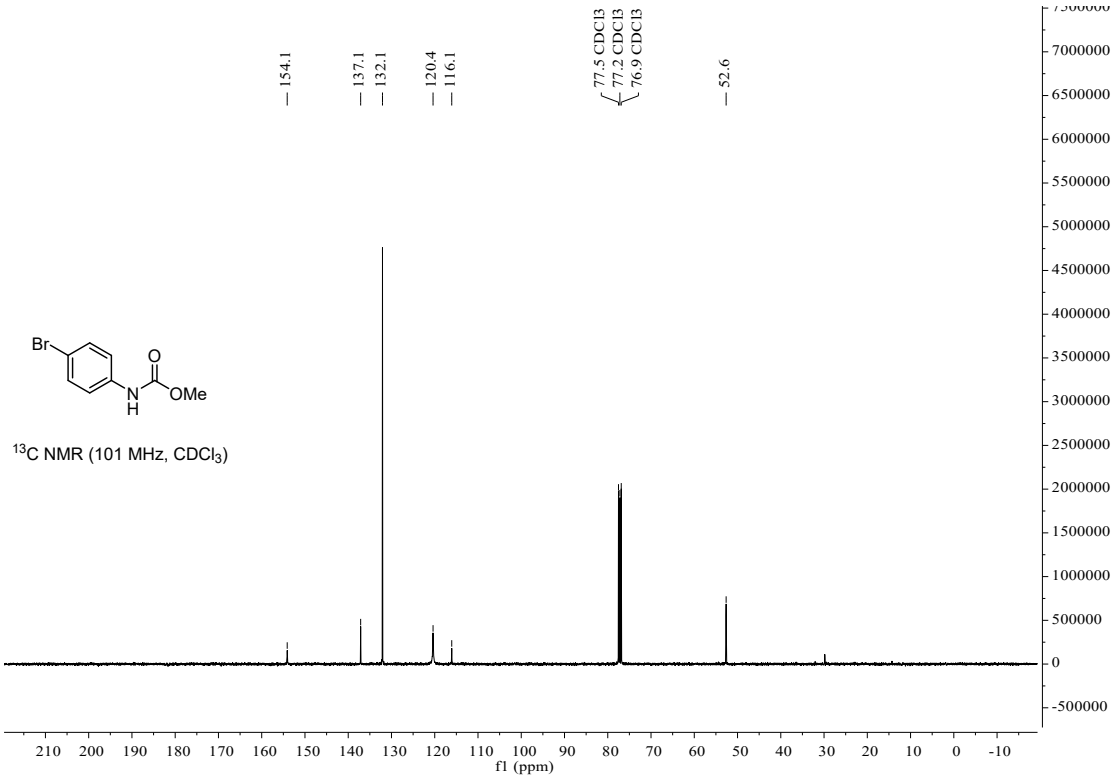
^{1}H NMR (400 MHz, $CDCl_3$)



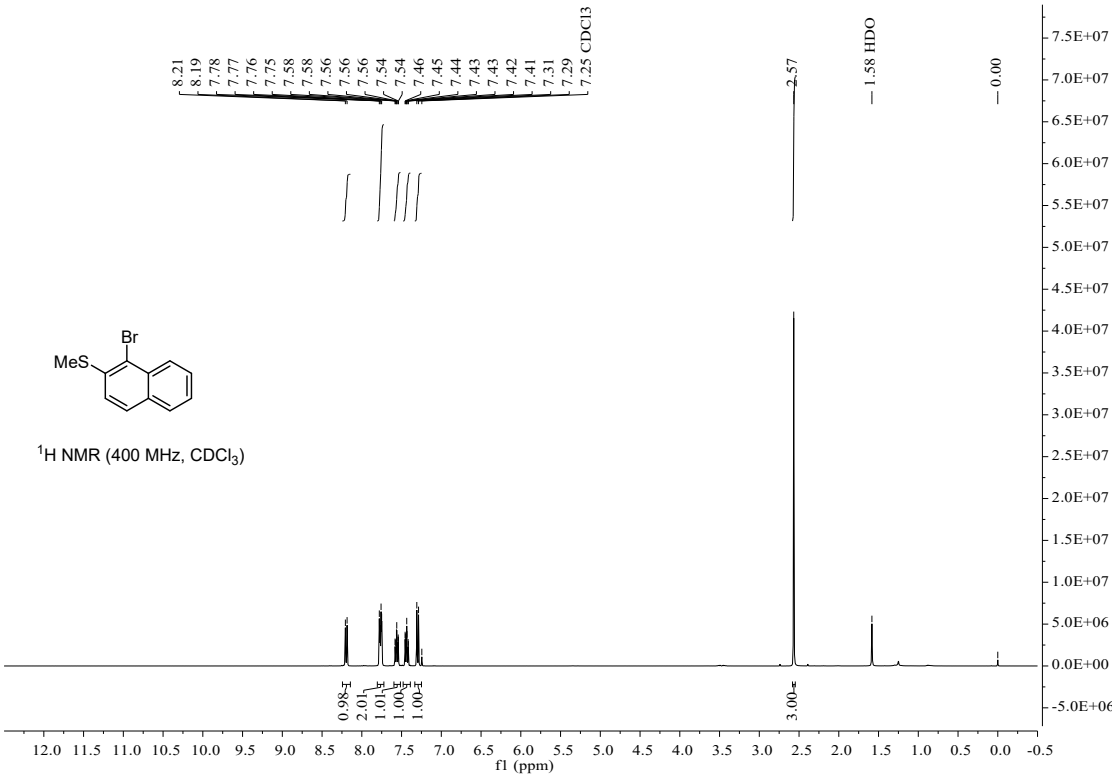
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 32

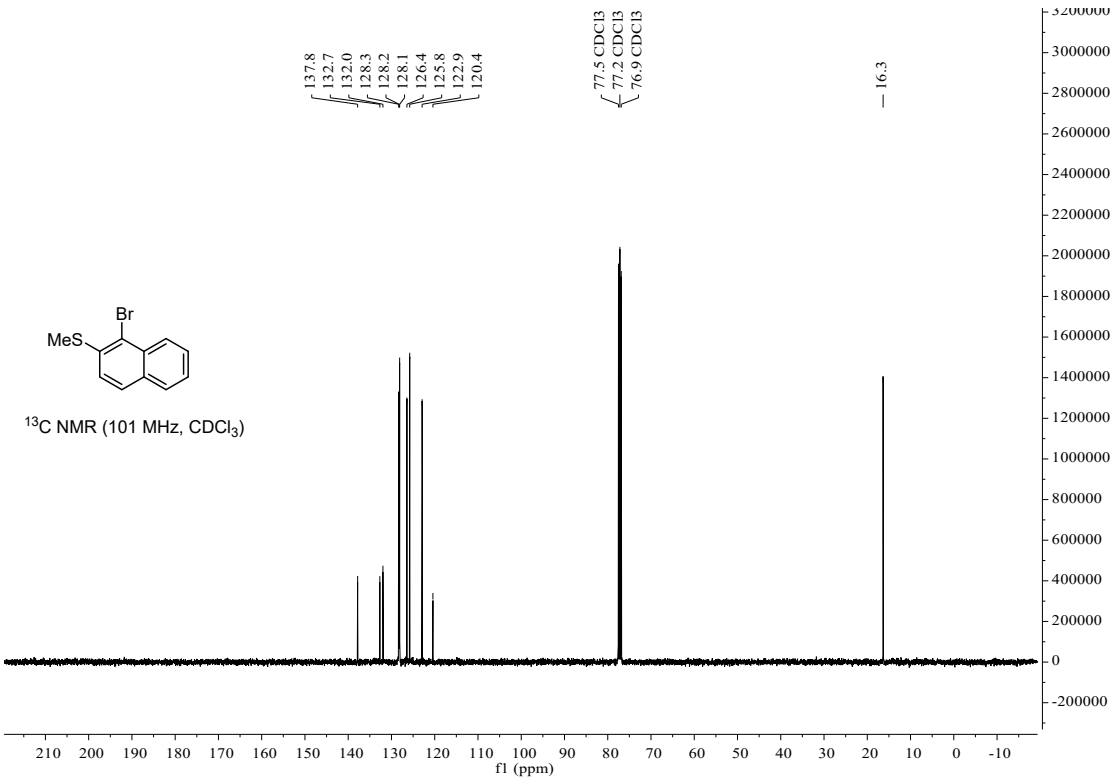

7.41
7.41
7.40
7.39
7.38
7.38
7.29
7.27
7.27 CDCl3
6.89
3.76
1.85 HDO
0.00
Br
O
N
H
OMe
1H NMR (400 MHz, CDCl3)
2.00
2.00
0.88
3.00
f1 (ppm)


154.1
137.1
132.1
120.4
116.1
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
52.6
Br
O
N
H
OMe
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 33

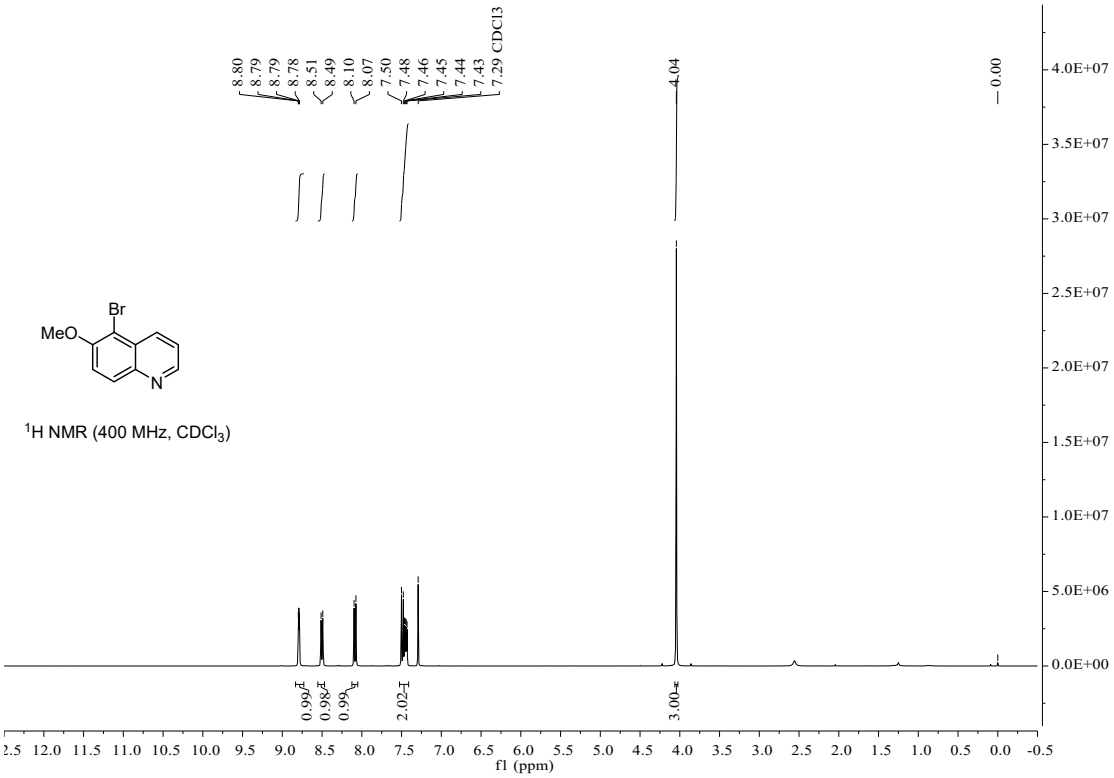


^{1}H NMR (400 MHz, $CDCl_3$)

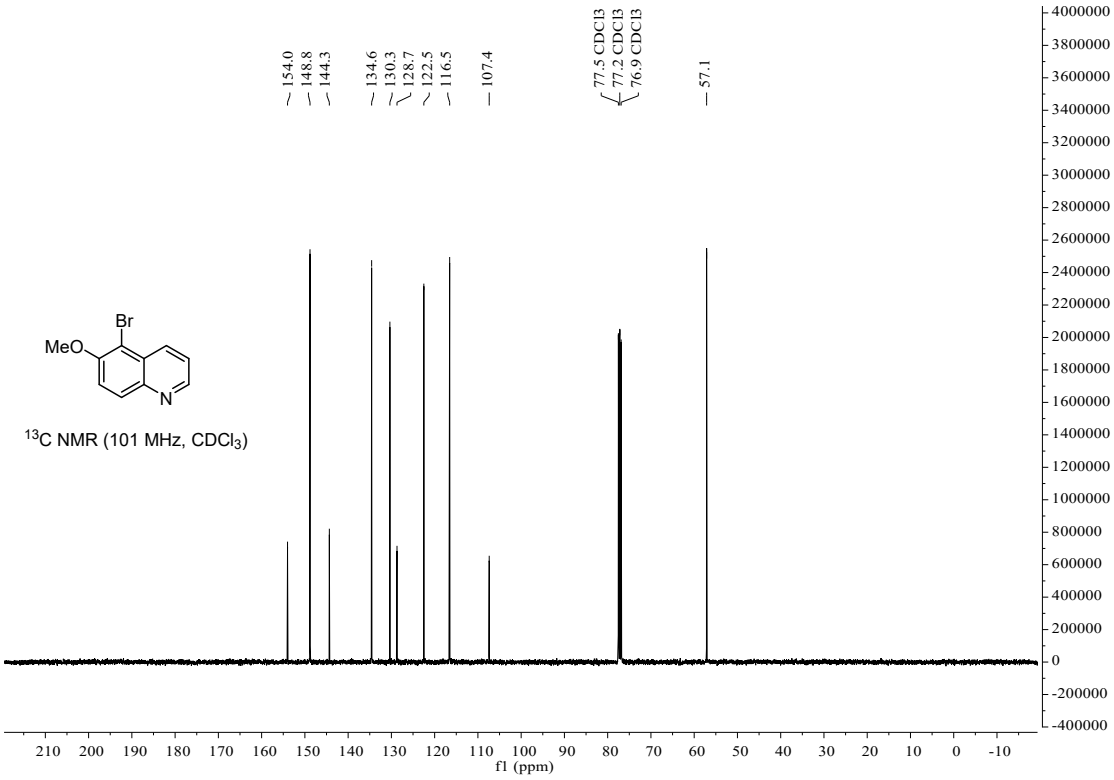


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 34

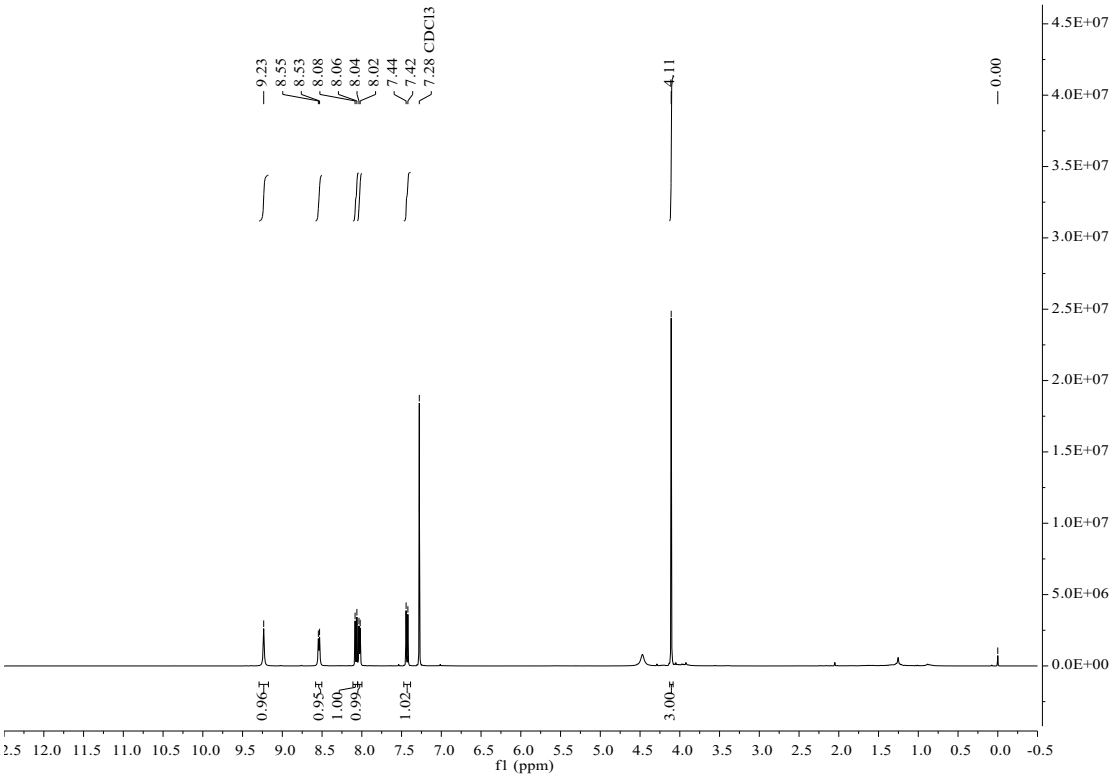


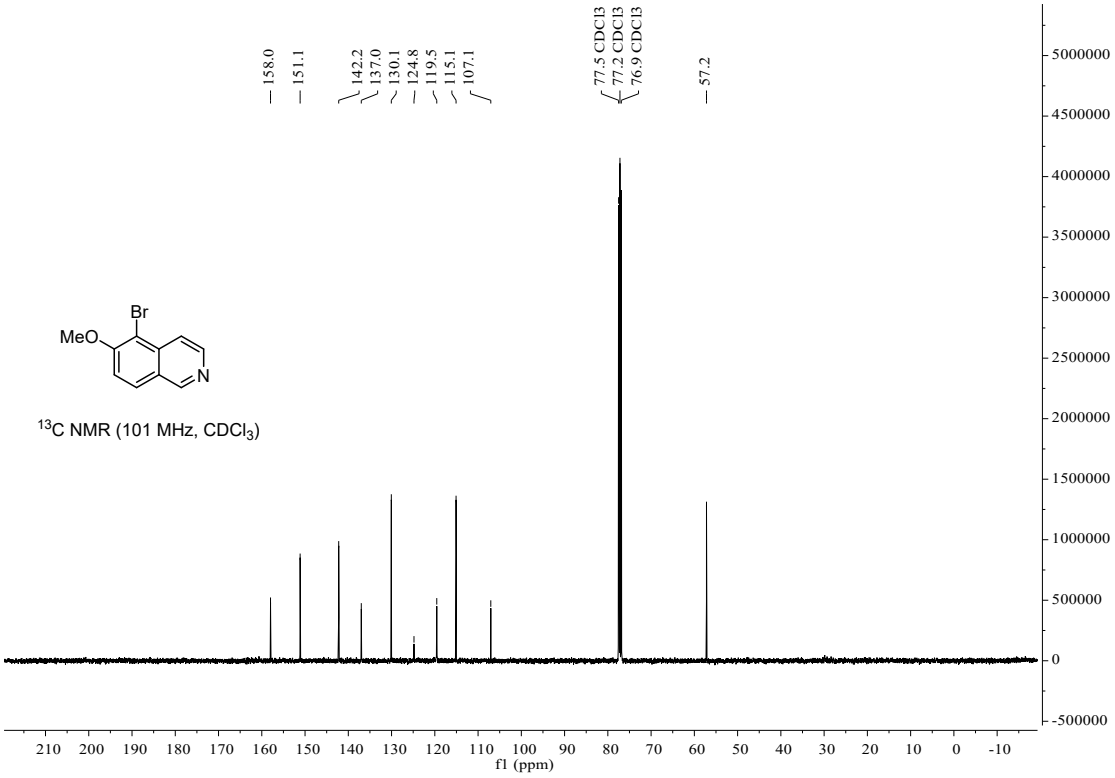
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

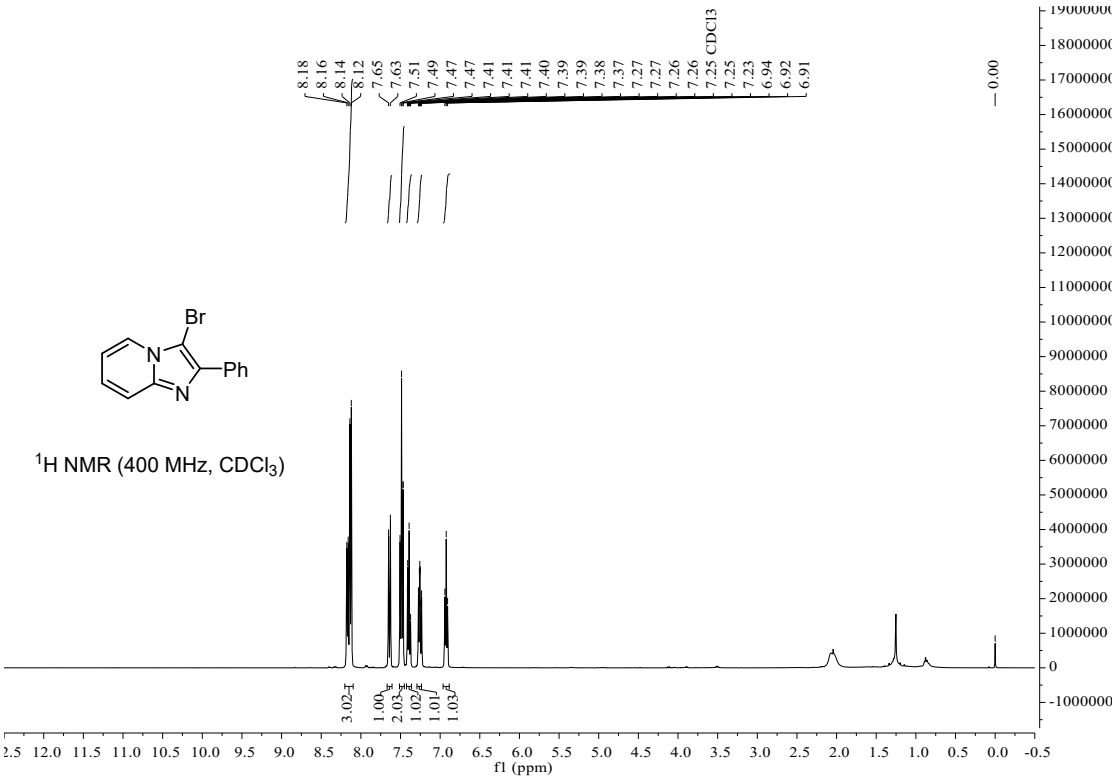
Compound 35

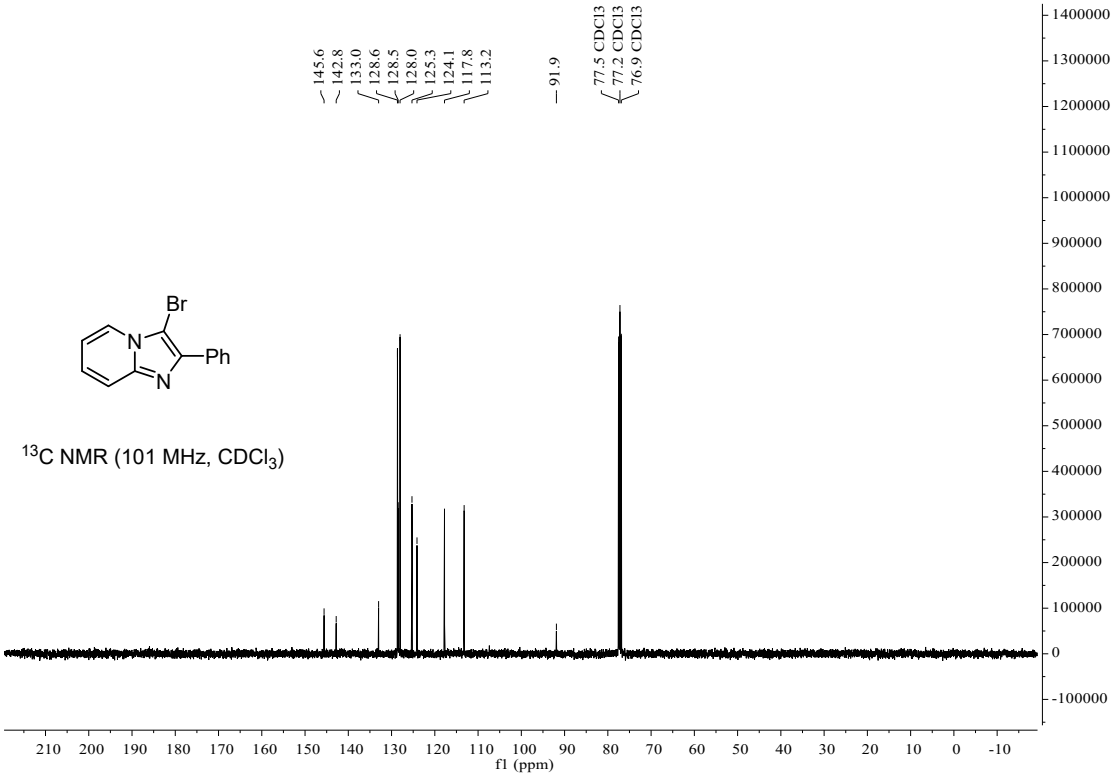




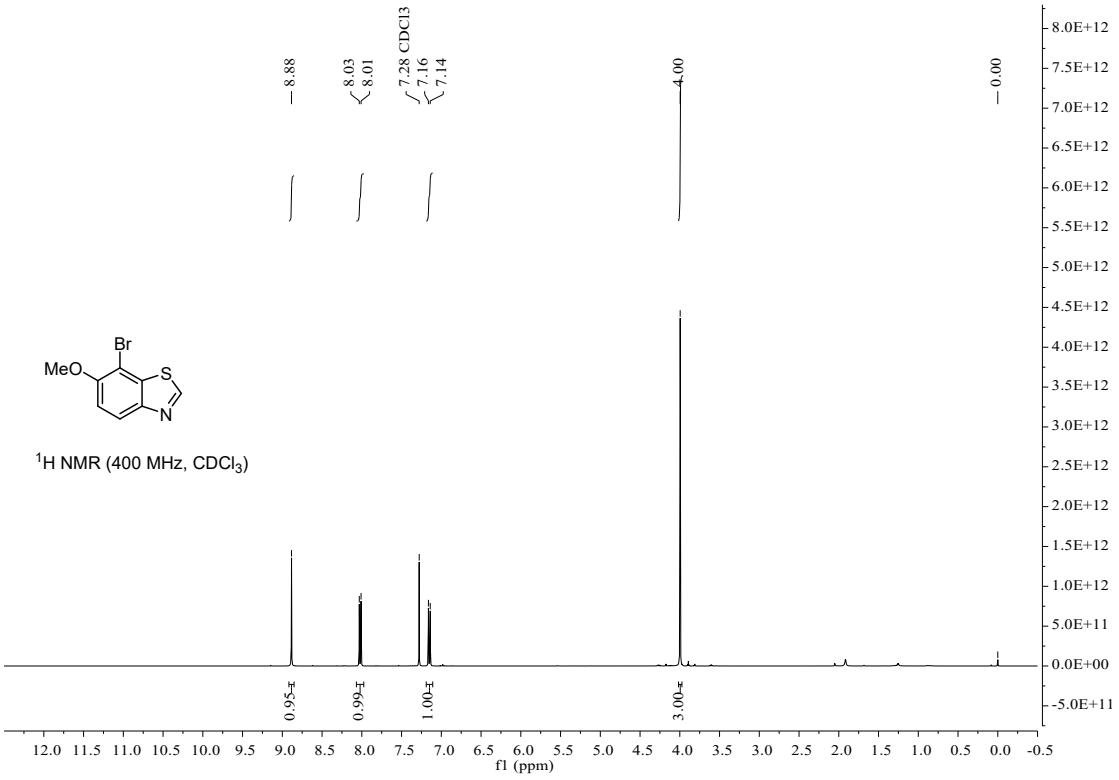
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 36

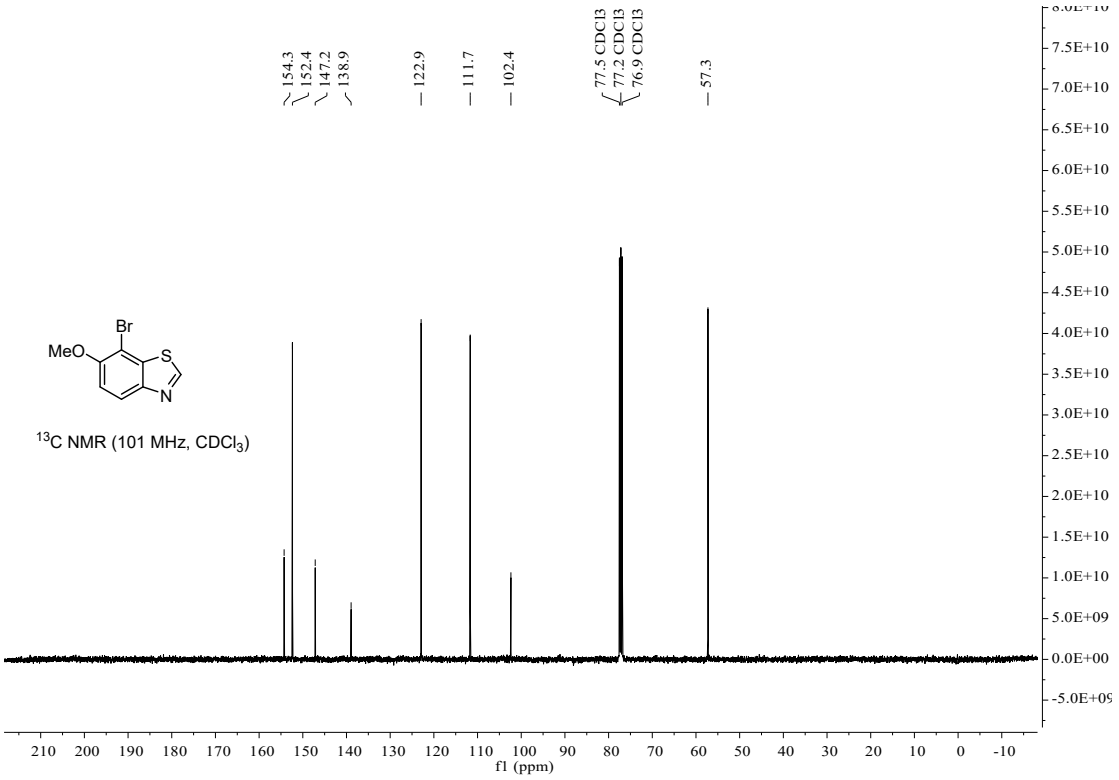

Br
N
Ph
N
^{1}H NMR (400 MHz, CDCl$_3$)
8.18
8.16
8.14
8.12
7.65
7.63
7.51
7.49
7.47
7.47
7.41
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.27
7.27
7.26
7.26
7.25 CDCl3
7.25
7.23
6.94
6.92
6.91
0.00
3.02
1.00
2.03
1.02
1.01
1.03
f1 (ppm)


Br
N
Ph
N
^{13}C NMR (101 MHz, CDCl$_3$)
145.6
142.8
133.0
128.6
128.5
128.0
125.3
124.1
117.8
113.2
91.9
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
f1 (ppm)

Compound 37

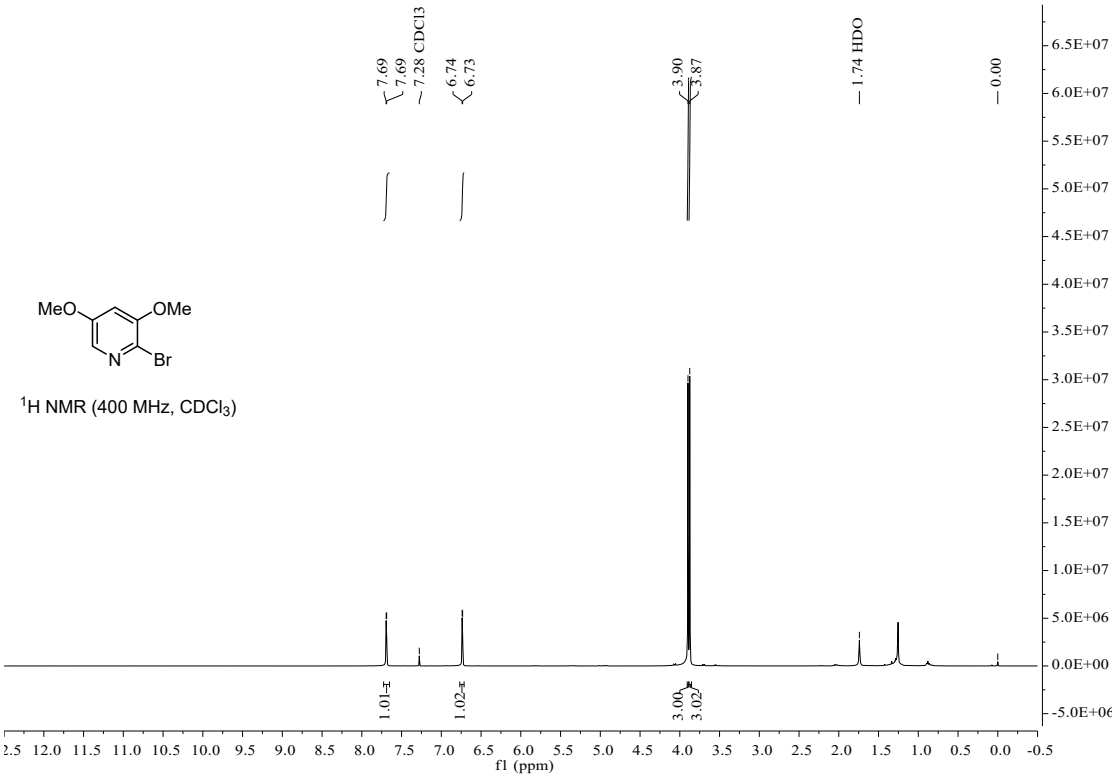


^{1}H NMR (400 MHz, $CDCl_3$)

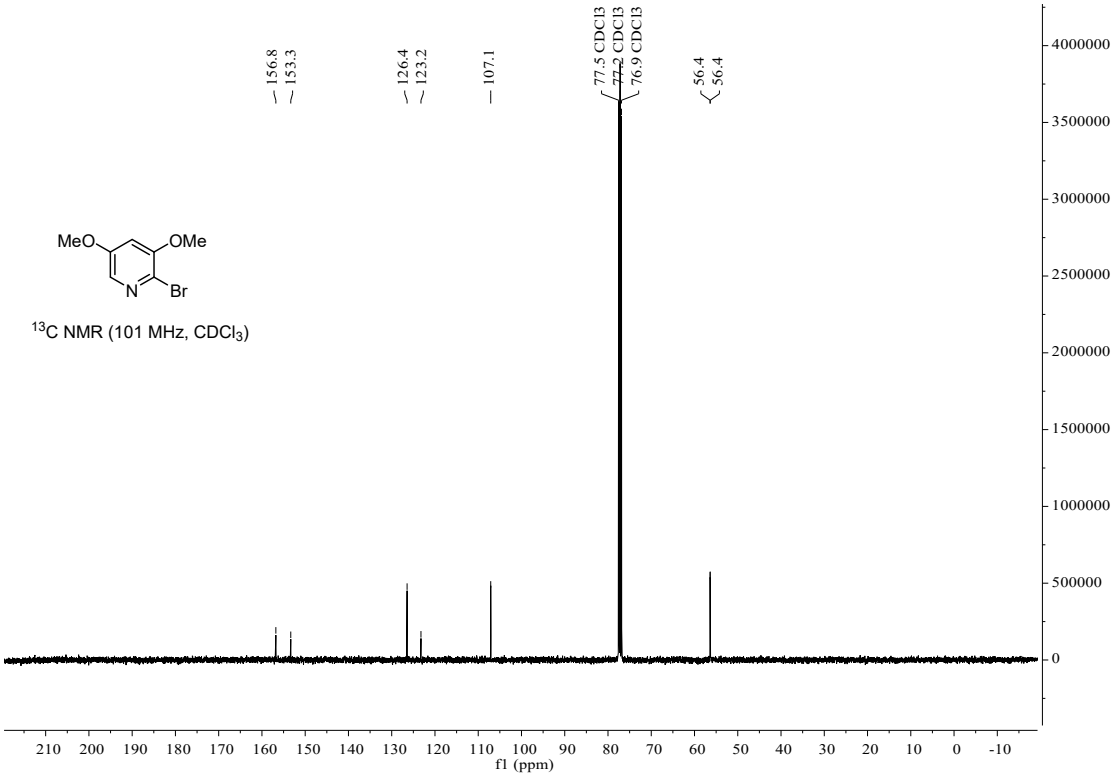


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 38

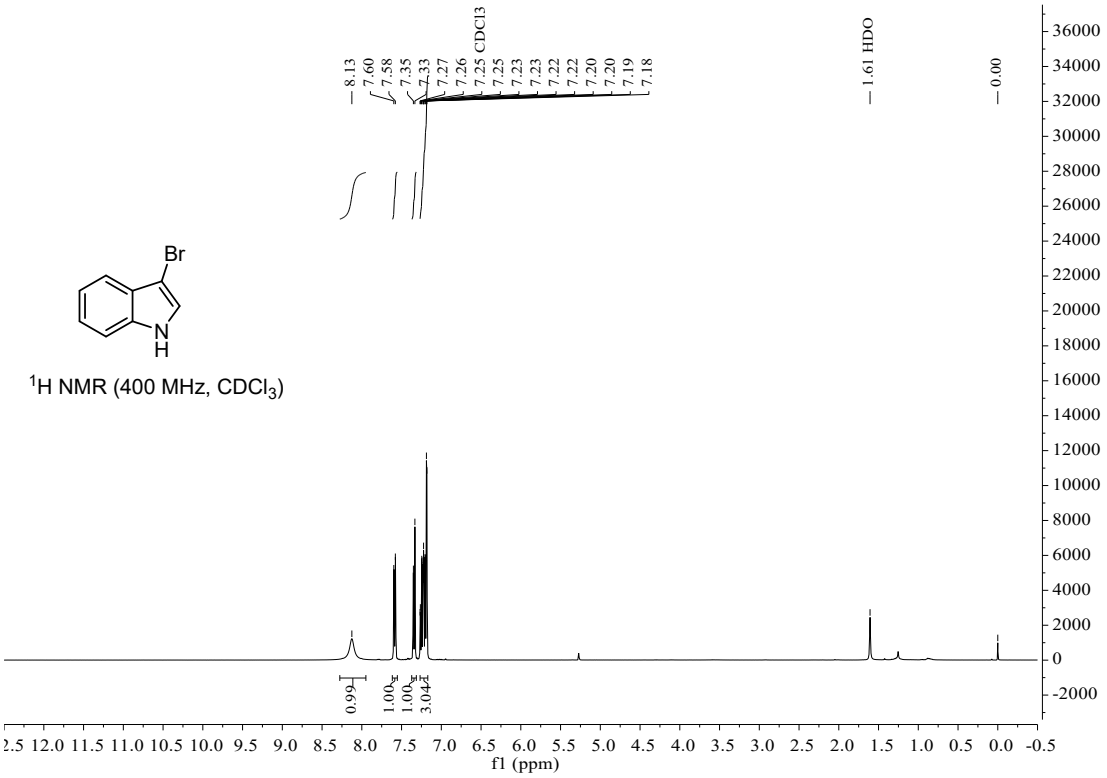


^{1}H NMR (400 MHz, $CDCl_3$)

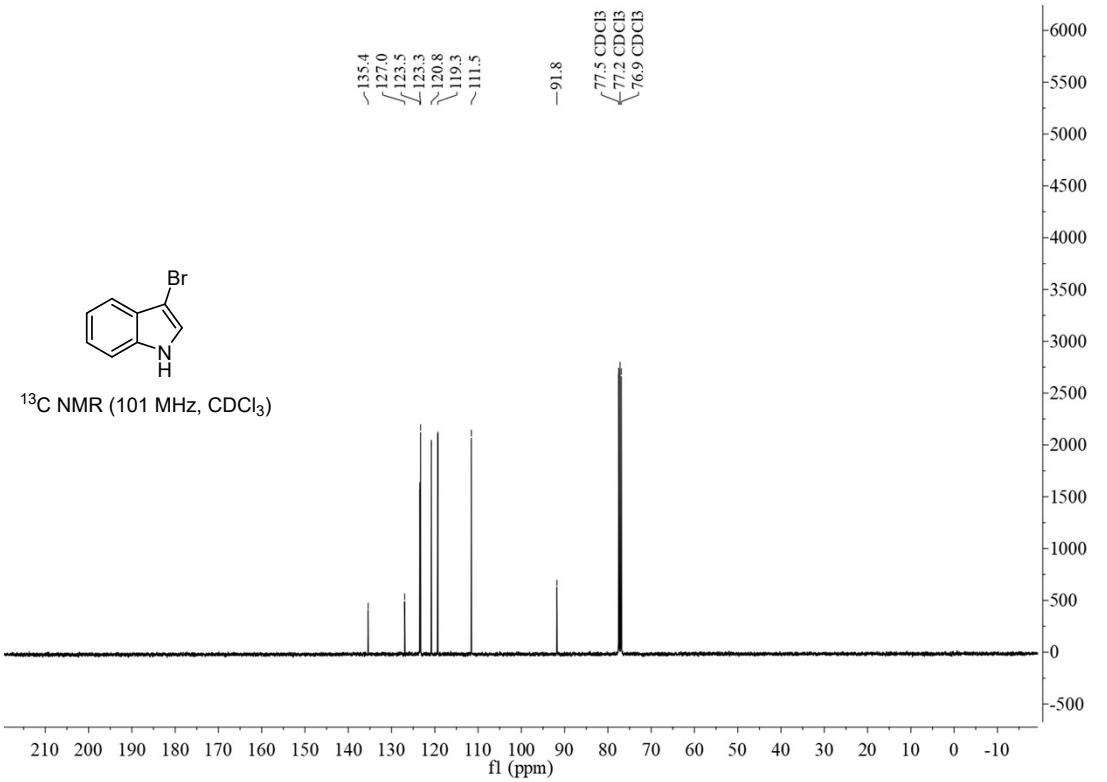


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 39

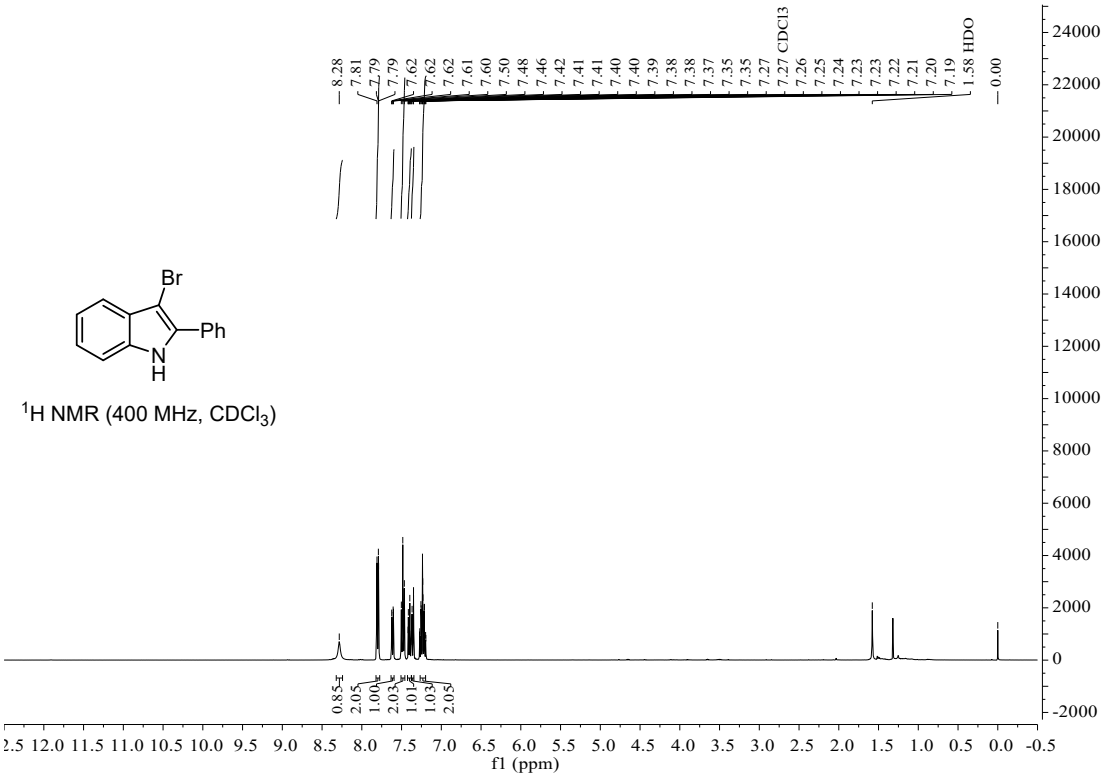


^{1}H NMR (400 MHz, $CDCl_3$)

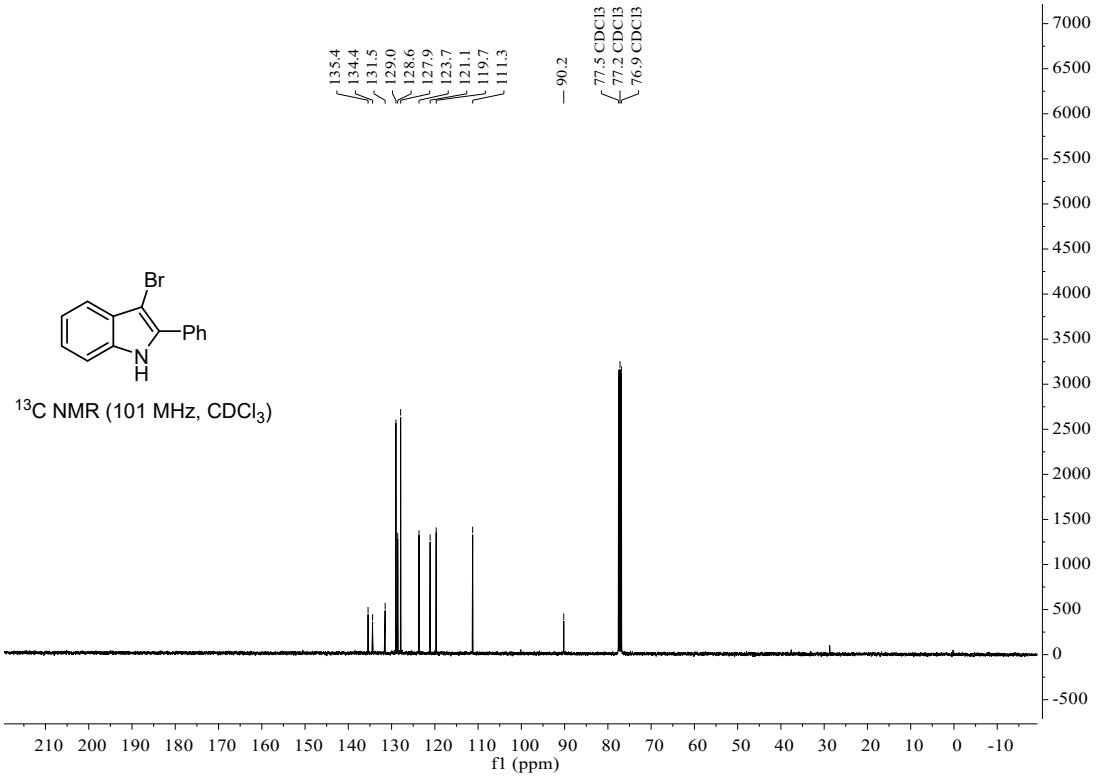


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 40

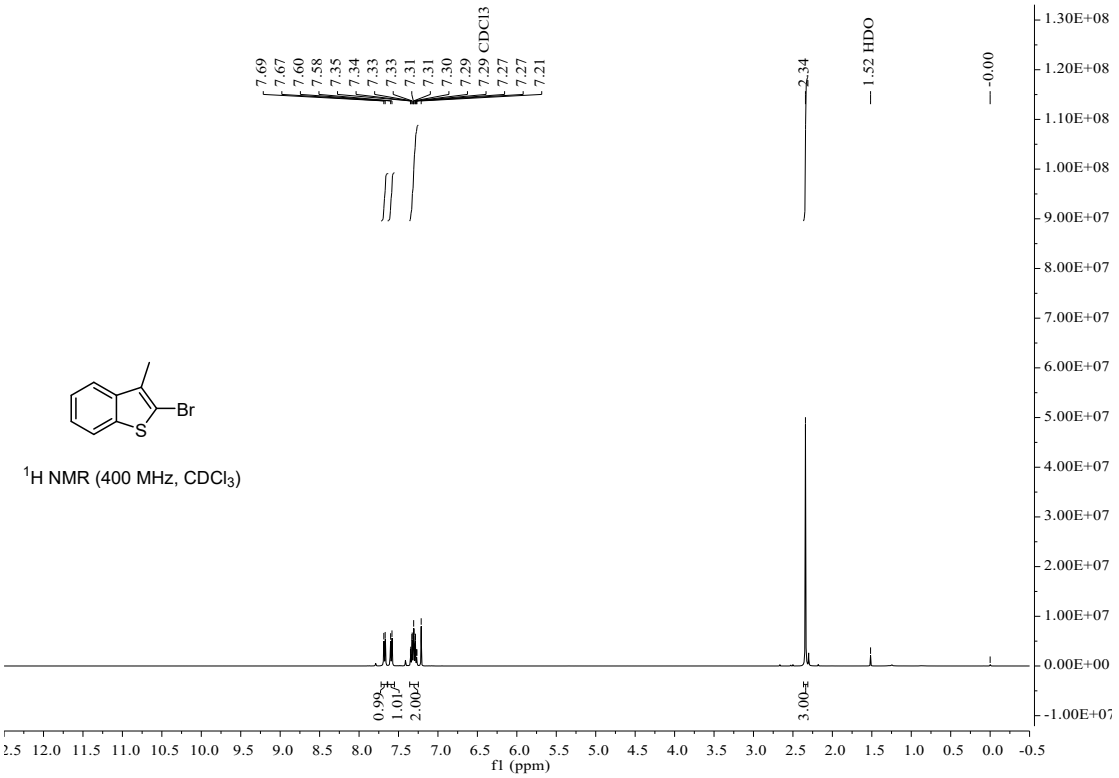


^{1}H NMR (400 MHz, $CDCl_3$)

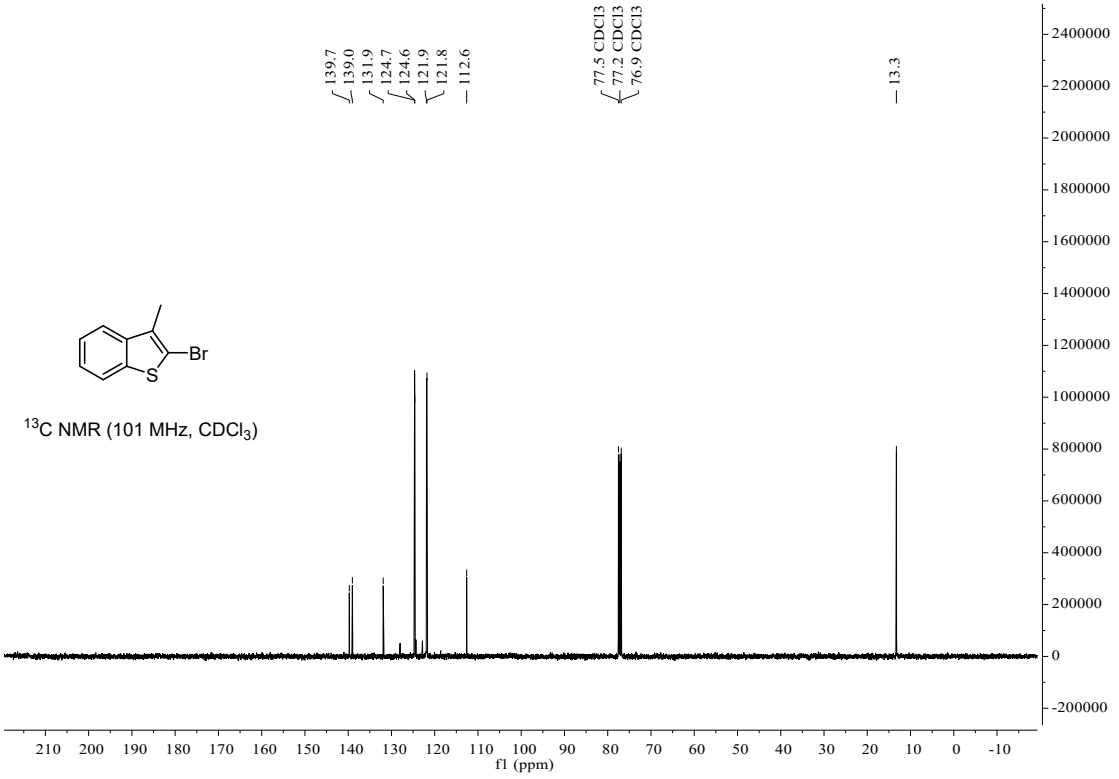


^{13}C NMR (101 MHz, $CDCl_3$)

Compound 41

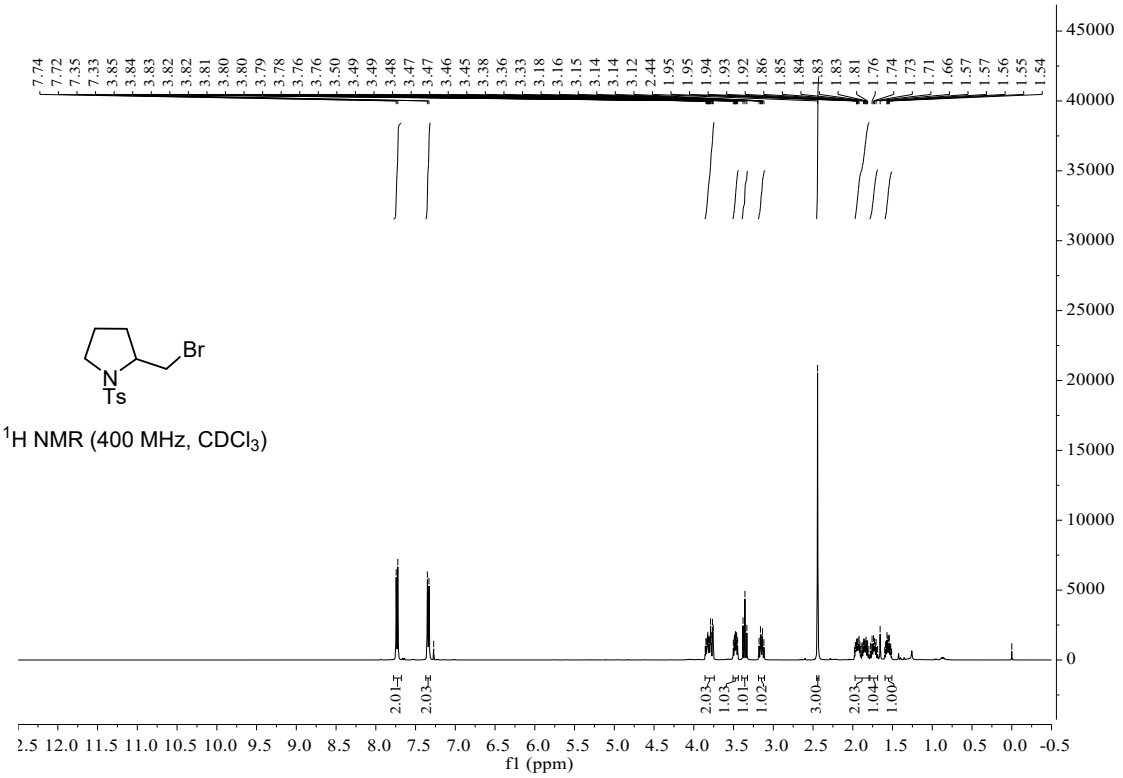


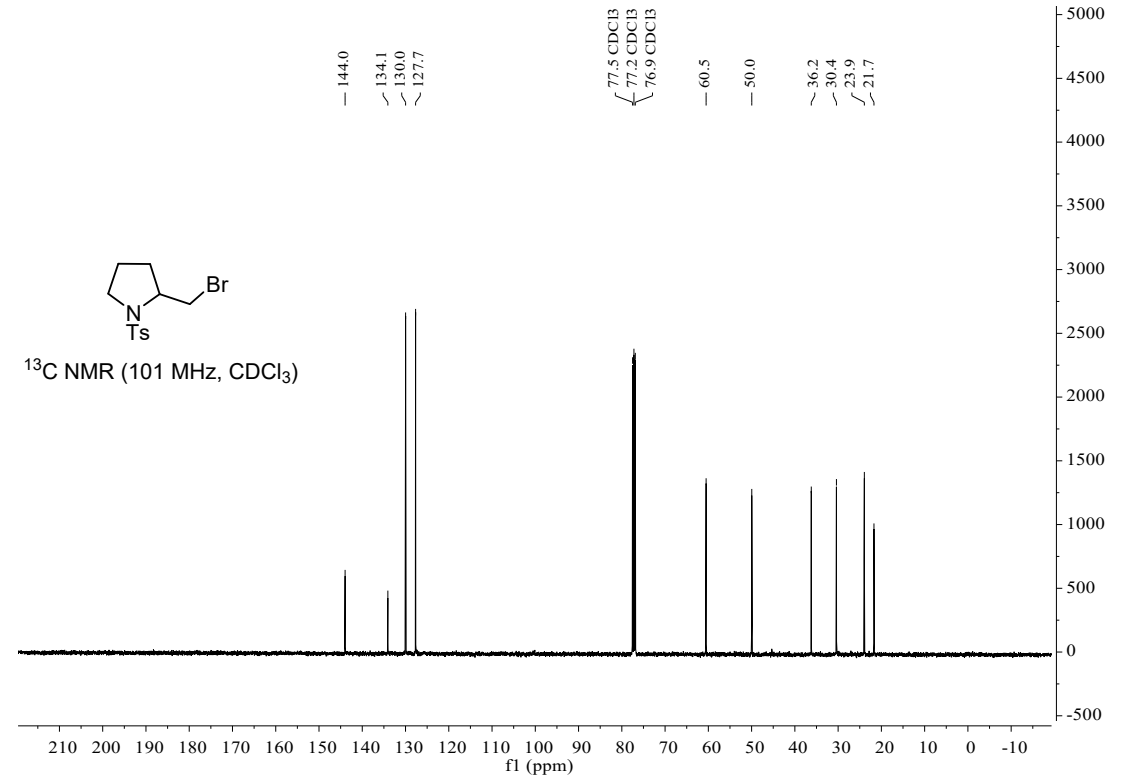
^{1}H NMR (400 MHz, $CDCl_3$)



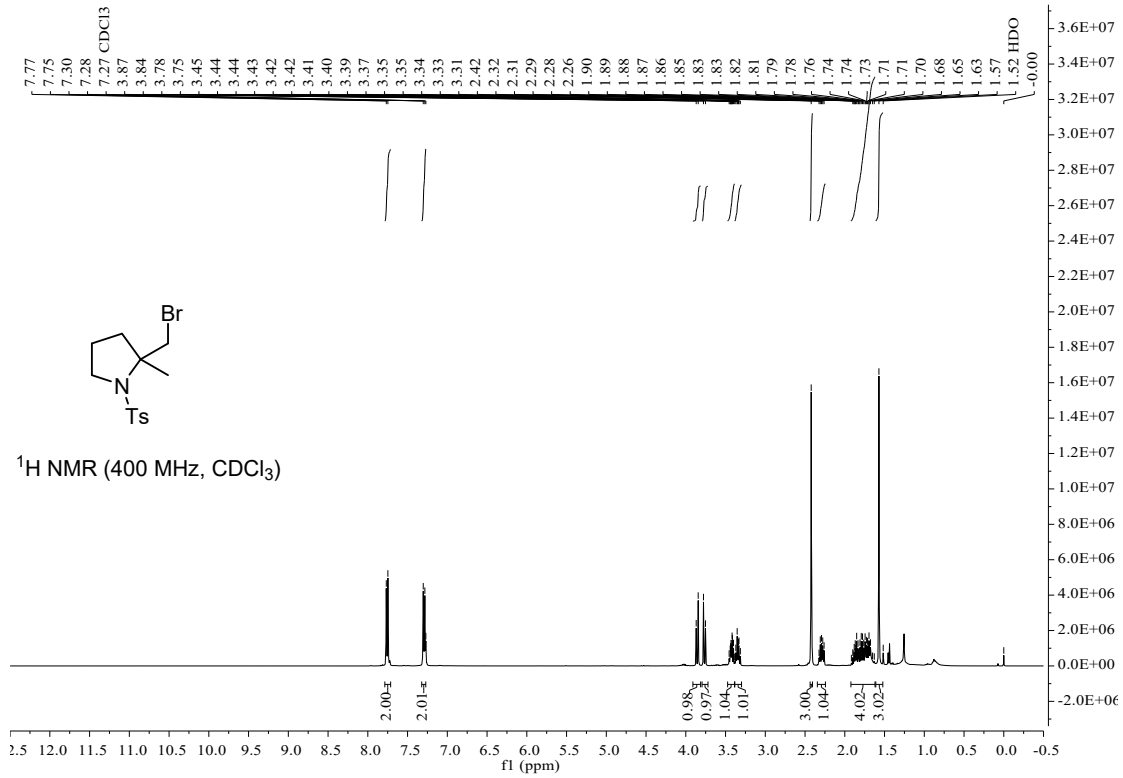
^{13}C NMR (101 MHz, $CDCl_3$)

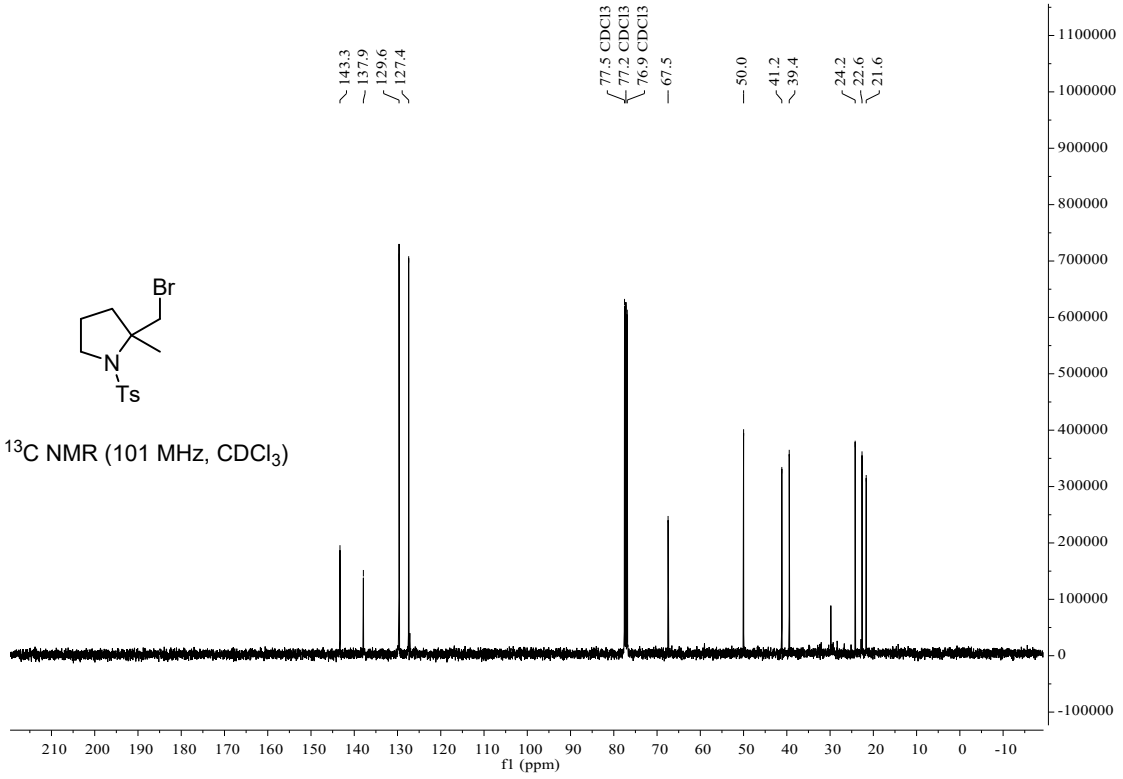
Compound 42


Br
N
Ts
1H NMR (400 MHz, CDCl3)
f1 (ppm)

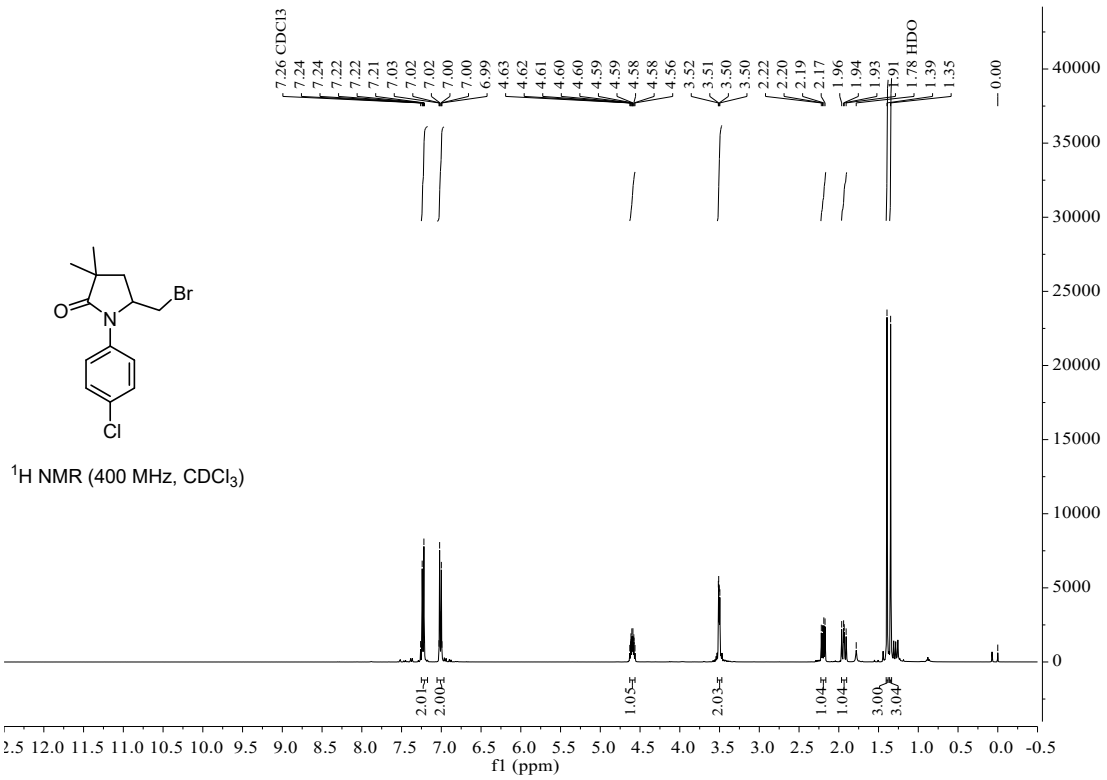

Br
N
Ts
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 43

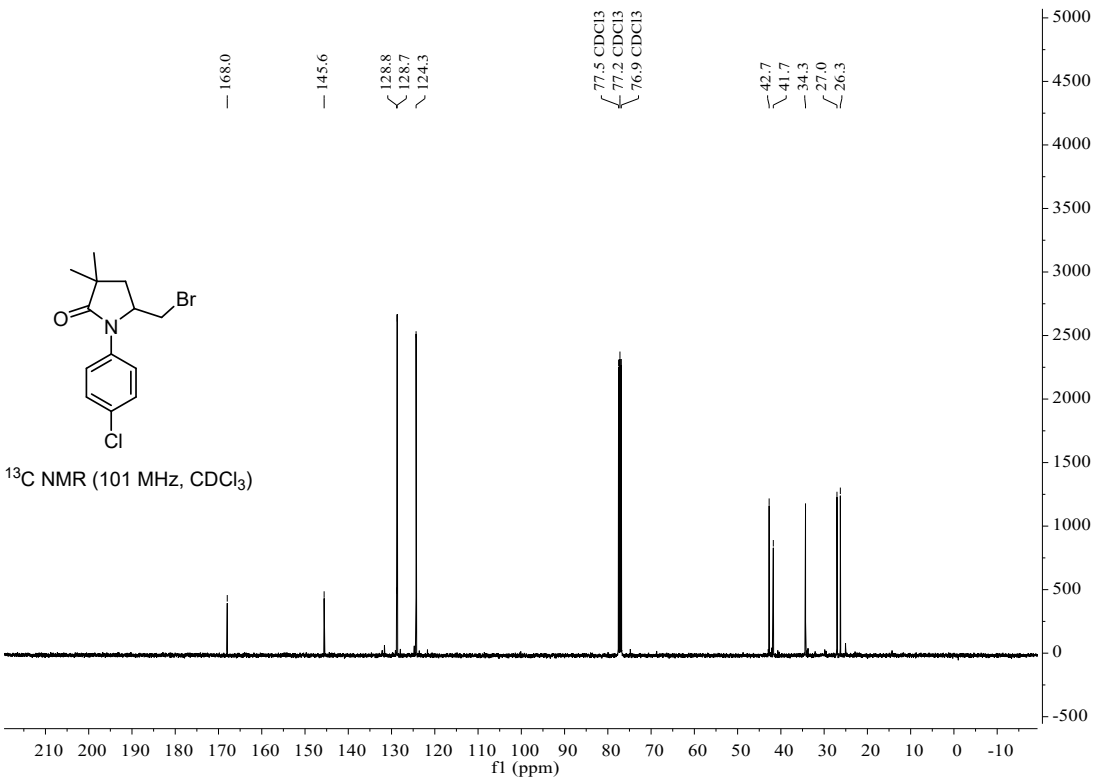

Br
N
Ts
1H NMR (400 MHz, CDCl3)
f1 (ppm)


Br
N
Ts
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 44

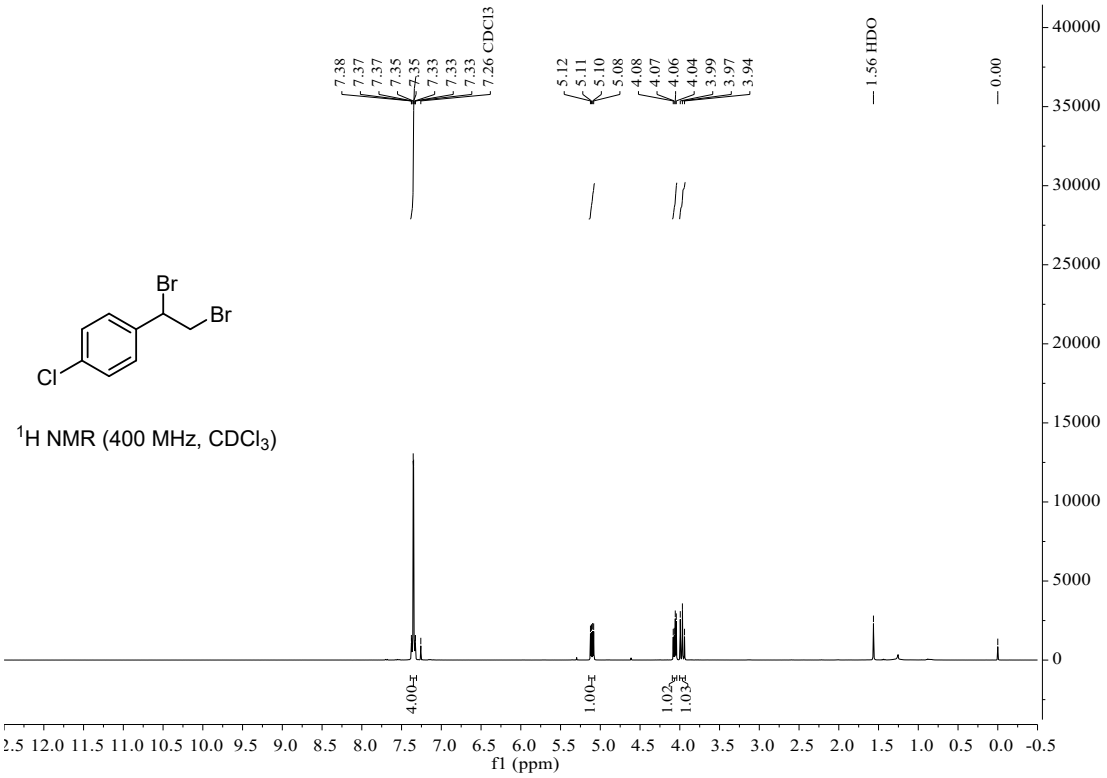


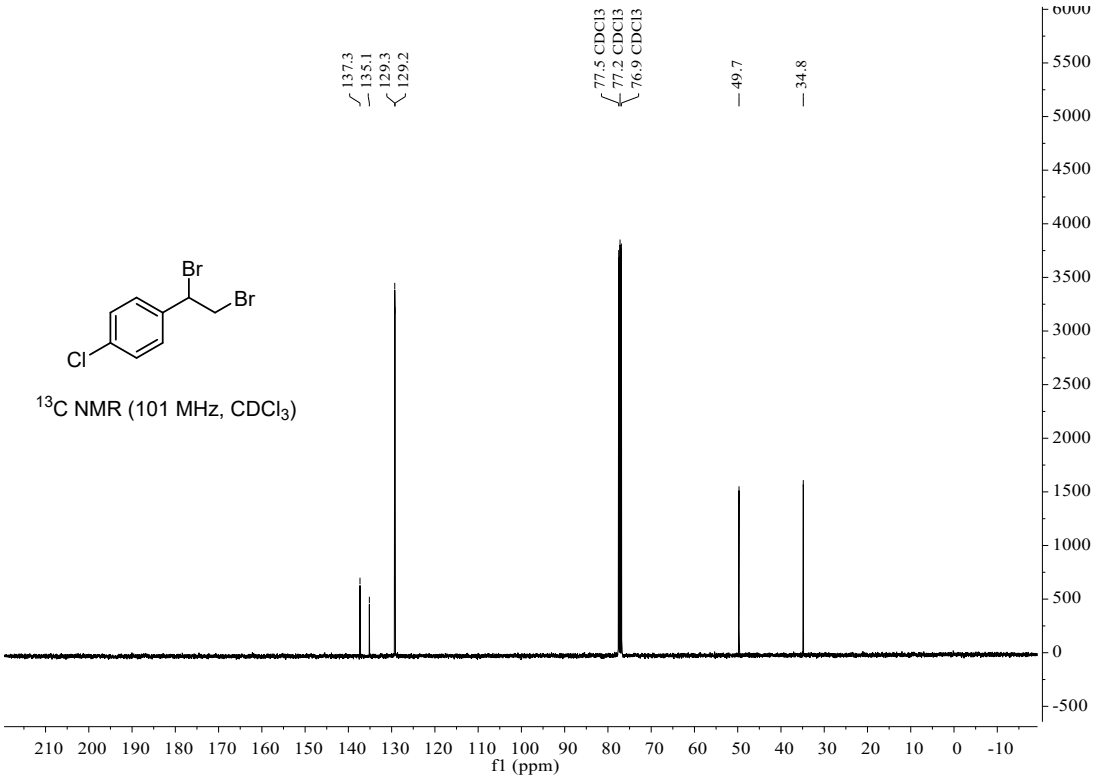
^{1}H NMR (400 MHz, $CDCl_3$)



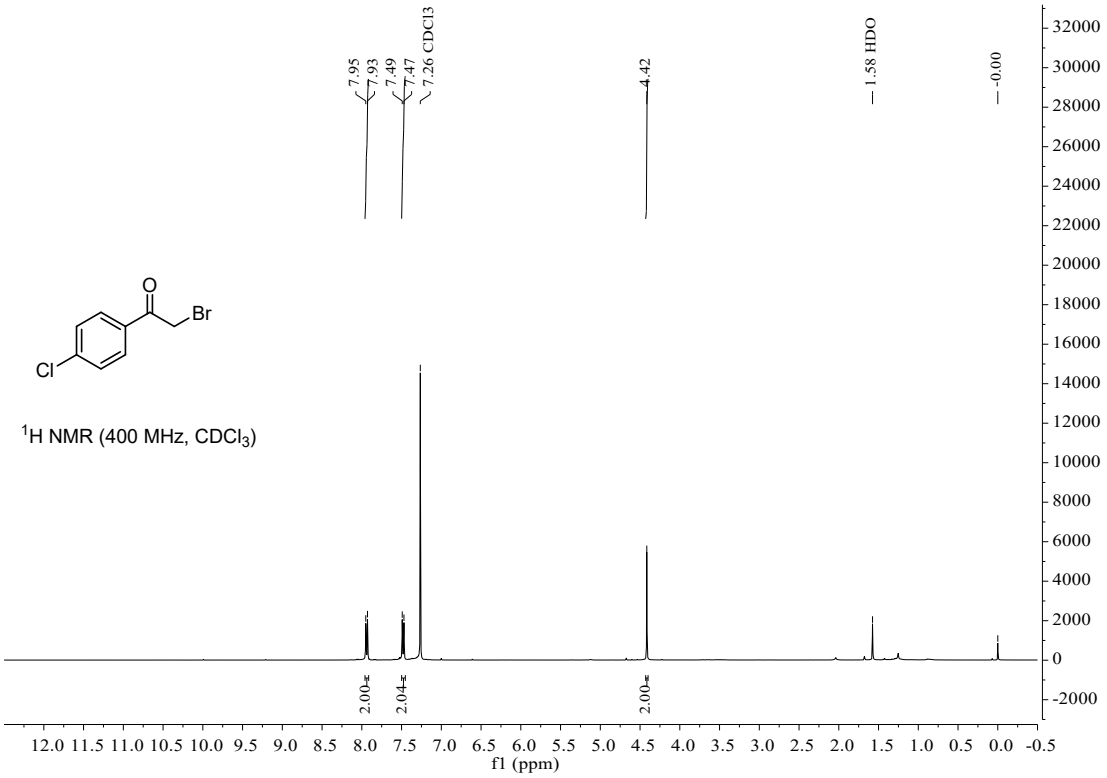
^{13}C NMR (101 MHz, $CDCl_3$)

Compound 45

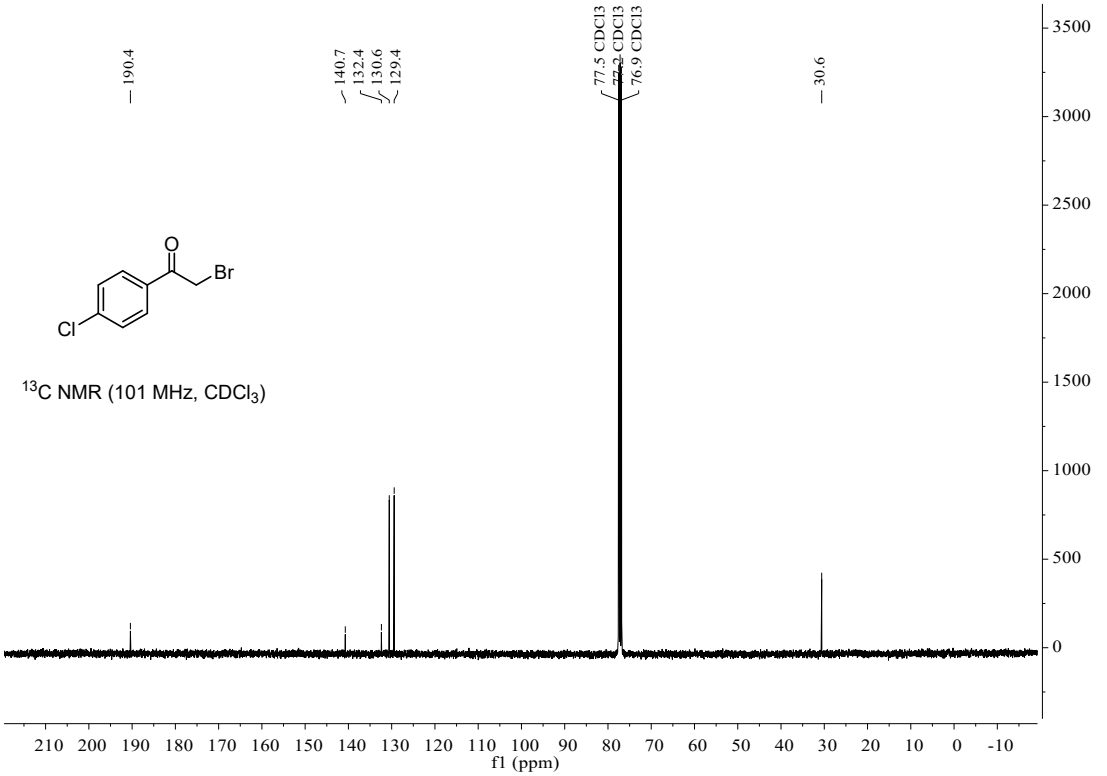

7.38
7.37
7.37
7.35
7.35
7.33
7.33
7.26 CDCl3
5.12
5.11
5.10
5.08
4.08
4.07
4.06
4.04
3.99
3.97
3.94
1.56 HDO
0.00
Br
Br
Cl
1H NMR (400 MHz, CDCl3)
4.00
1.00
1.02
1.03
f1 (ppm)


137.3
135.1
129.3
129.2
77.5 CDCl3
77.2 CDCl3
76.9 CDCl3
49.7
34.8
Br
Br
Cl
13C NMR (101 MHz, CDCl3)
f1 (ppm)

Compound 46

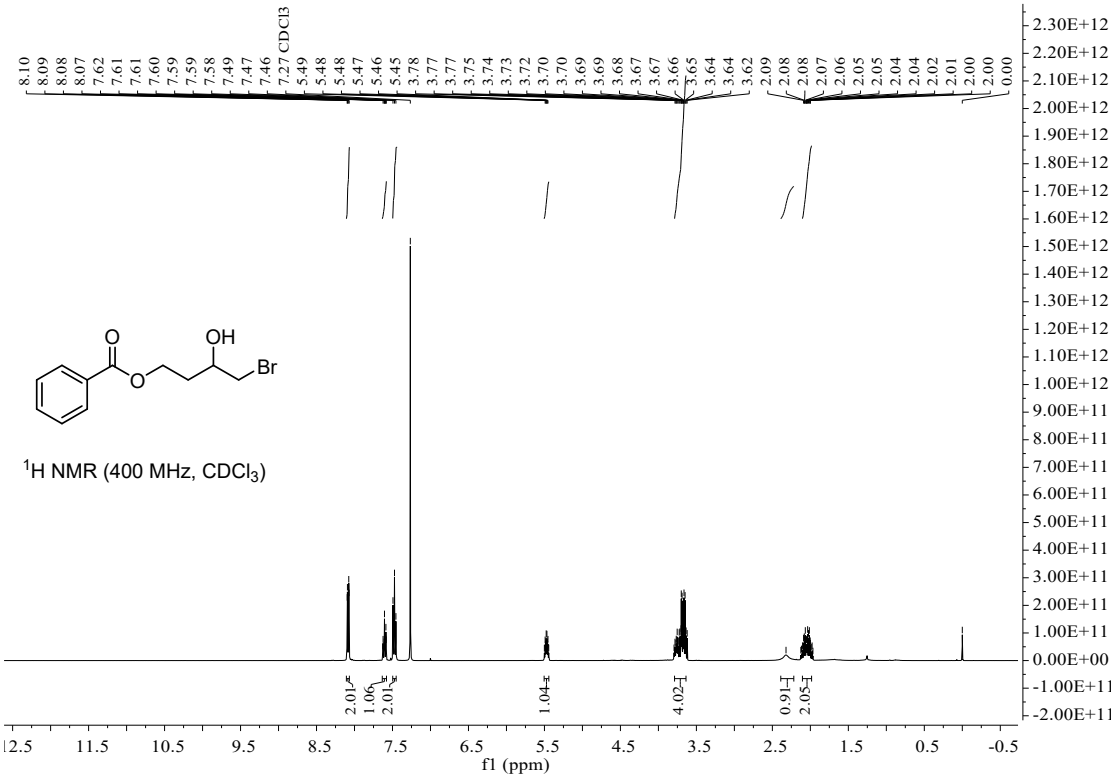


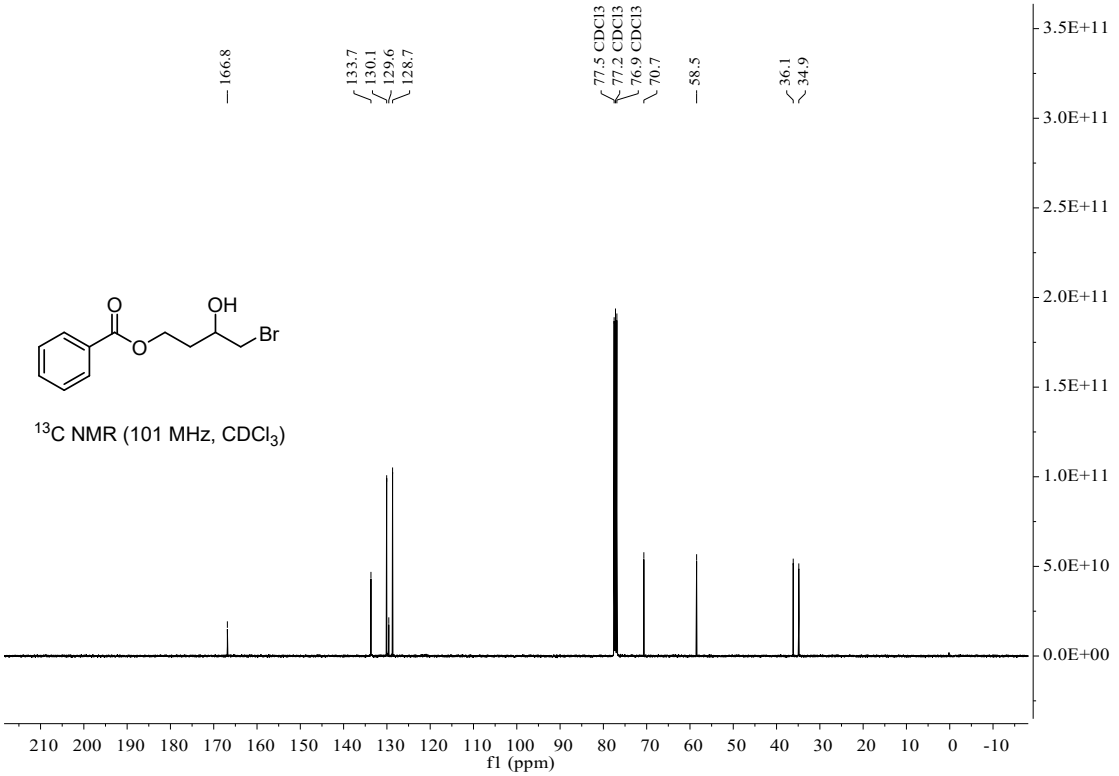
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

Compound 47


O
OH
O
Br
^{1}H NMR (400 MHz, $CDCl_3$)
f1 (ppm)


O
OH
O
Br
^{13}C NMR (101 MHz, $CDCl_3$)
f1 (ppm)