

Microwave-Assisted Synthesis of Benzofuran-3(2*H*)-ones

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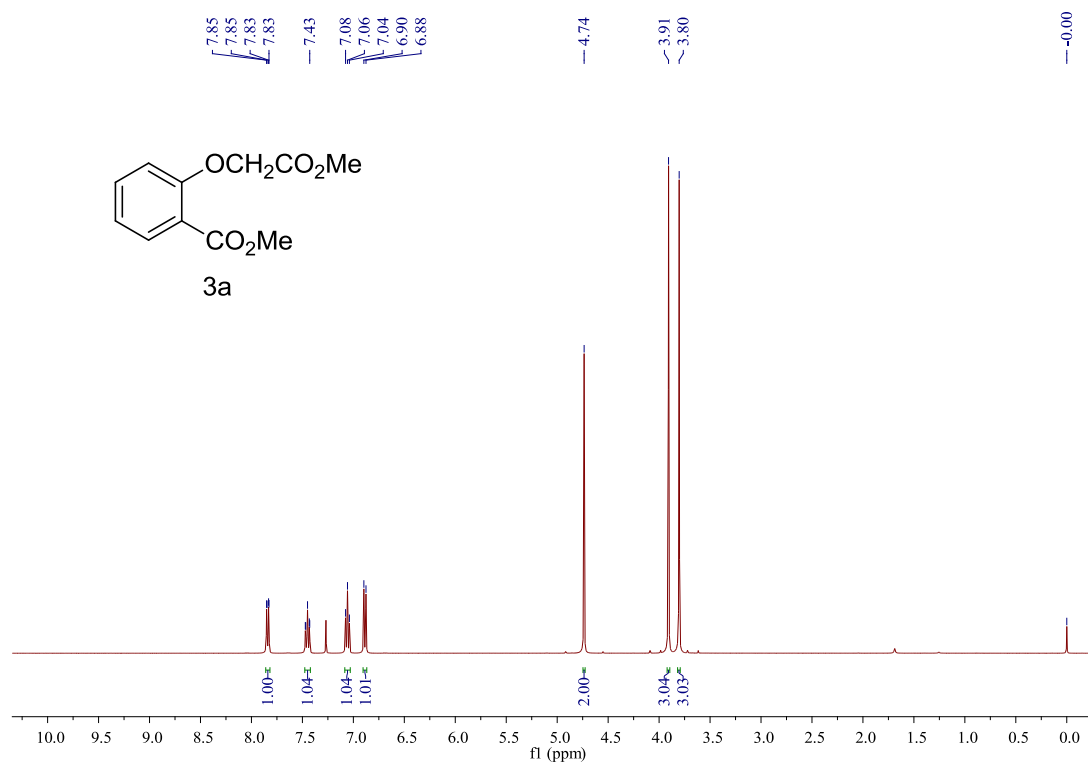
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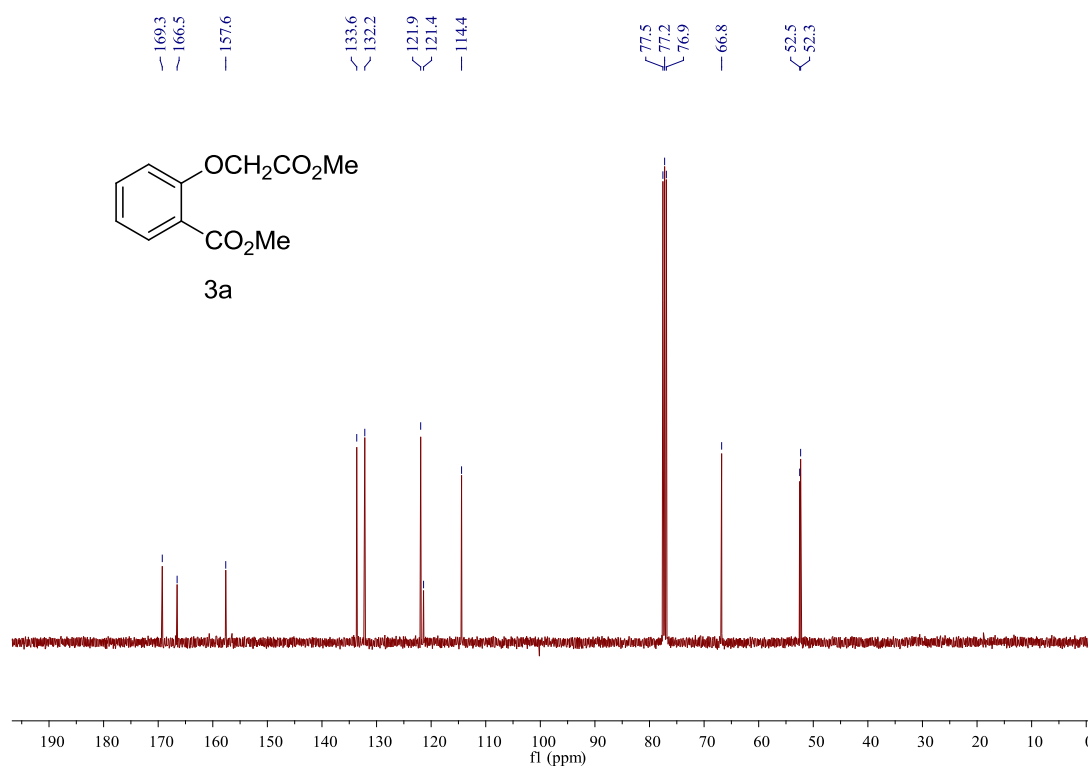
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NMR data for compounds **3a-3g**, and **4a-4g**.

^1H -NMR spectrum for 3a (in CDCl_3)



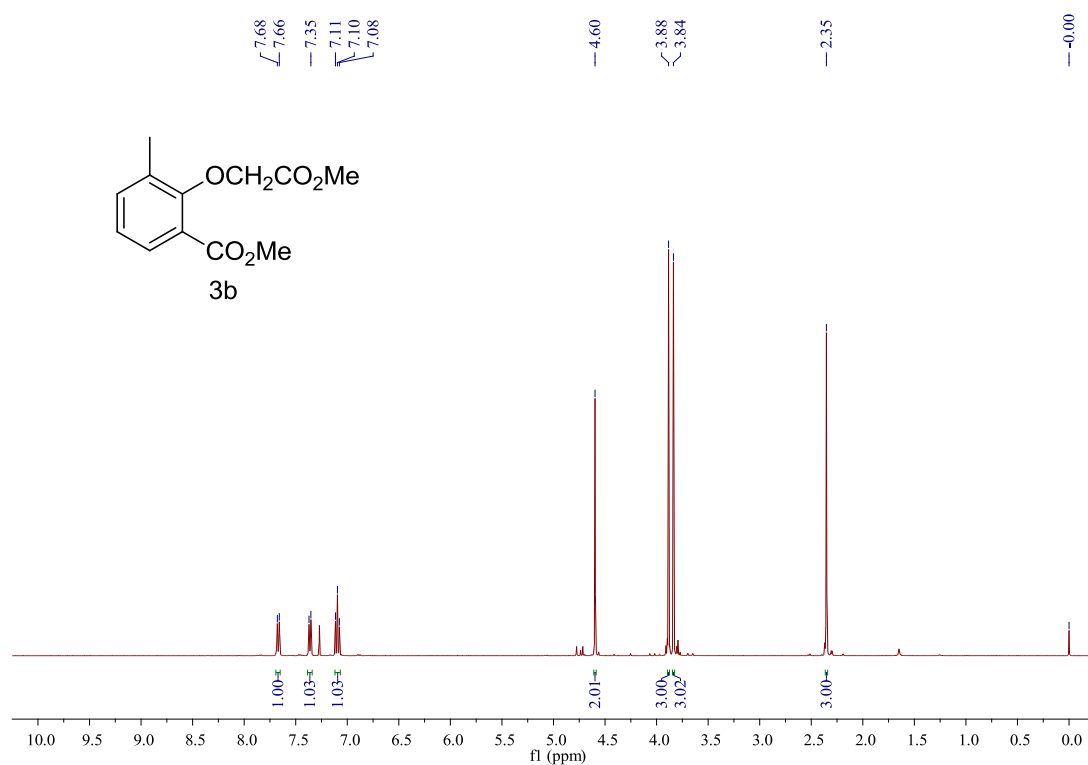
^{13}C -NMR spectrum for 3a (in CDCl_3)



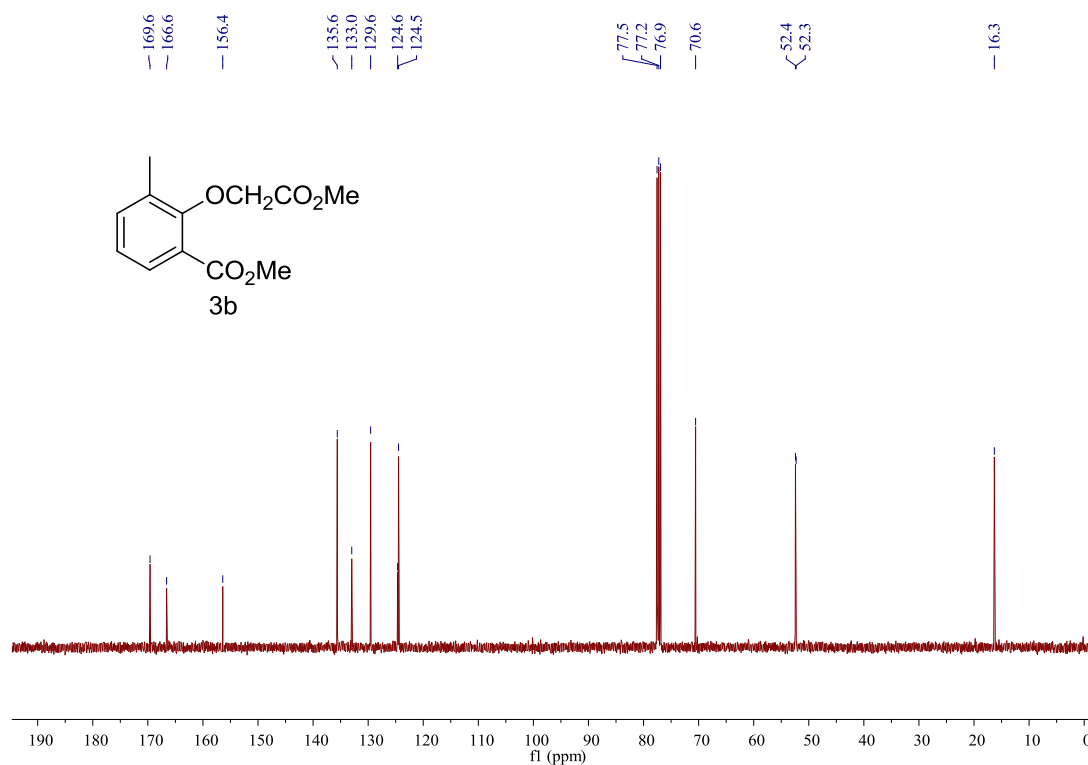
^1H NMR (400 MHz, CDCl_3): δ 7.84 (dd, $J_1 = 1.6$ Hz, $J_2 = 7.7$ Hz, 1H), 7.48-7.42 (m, 1H), 7.06 (t, $J = 7.6$ Hz, 1H), 6.89 (d, $J = 8.4$ Hz, 1H), 4.74 (s, 2H), 3.91 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 169.3, 166.5, 157.6, 133.6,

132.2, 121.9, 121.4, 114.4, 66.8, 52.5, 52.3; HRMS (ESI): calc. for $C_{11}H_{12}NaO_5$ $[M+Na]^+$: 247.0577; found: 247.0578.

1H -NMR spectrum for 3b (in $CDCl_3$)



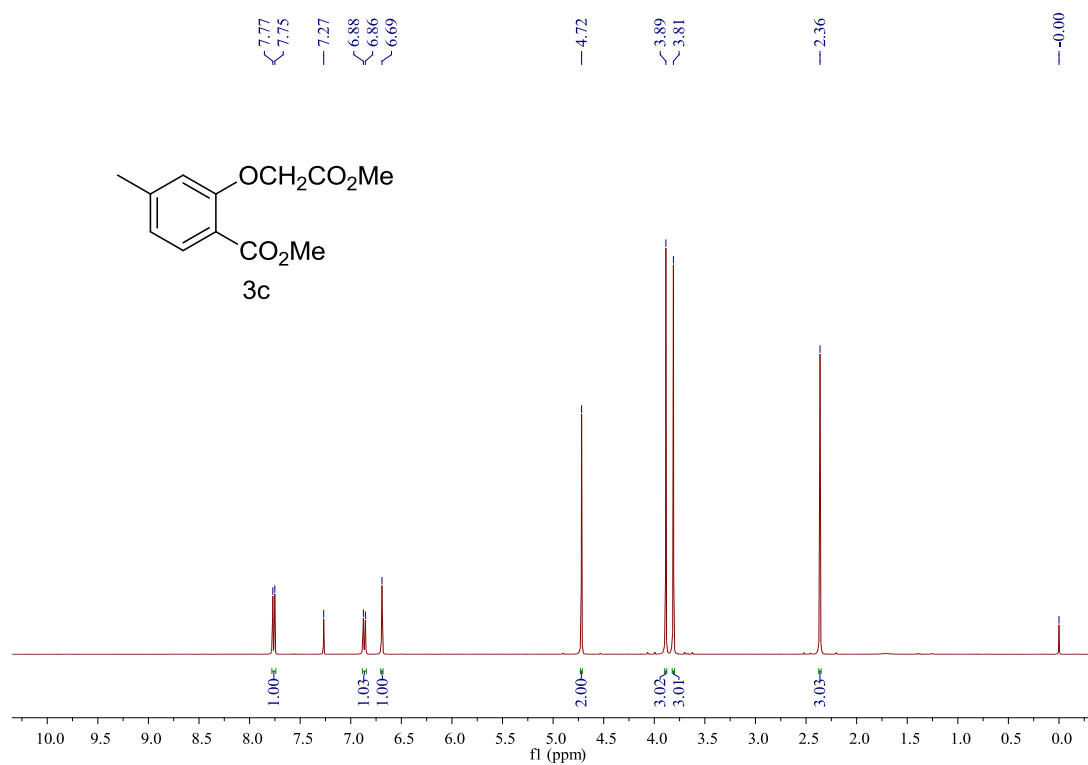
^{13}C -NMR spectrum for 3b (in $CDCl_3$)



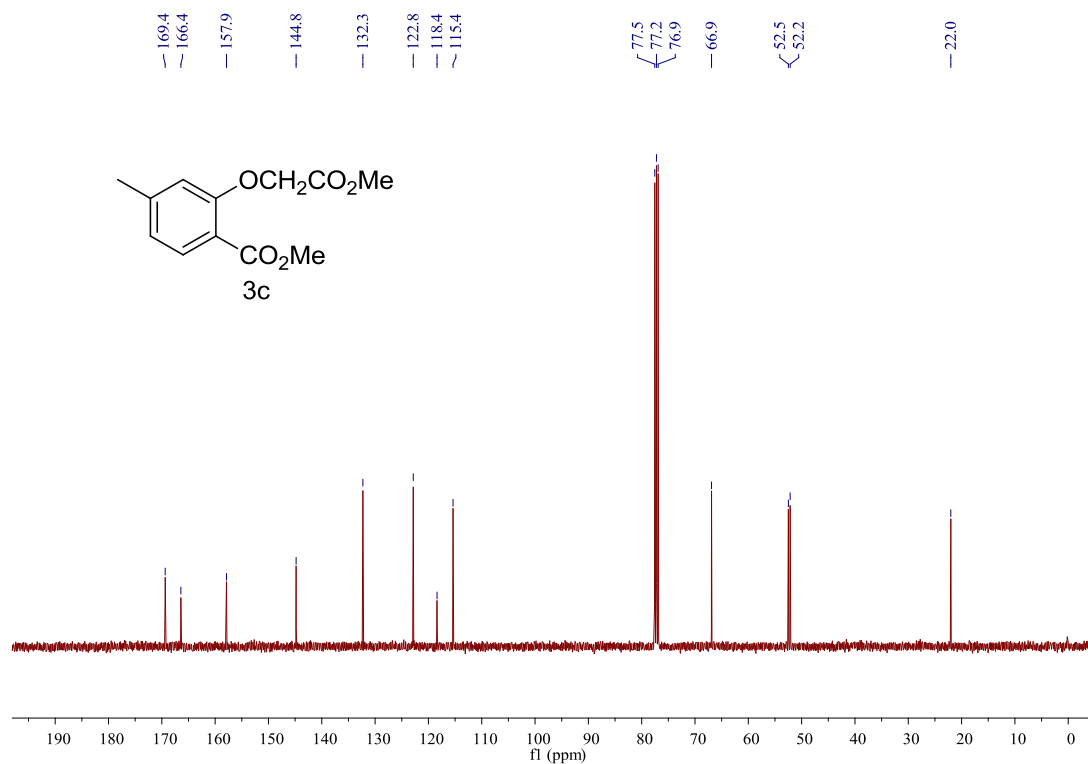
1H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, J = 7.5 Hz, 1H), 7.36 (d, J = 7.3 Hz, 1H), 7.10 (t, J = 7.6 Hz, 1H), 4.60 (s, 2H), 3.88 (s, 3H), 3.84 (s, 3H), 2.35 (s, 3H);

^{13}C NMR (100 MHz, CDCl_3): δ 169.6, 166.6, 156.4, 135.6, 133.0, 129.6, 124.6, 124.5, 70.6, 52.4, 52.3, 16.3; HRMS (ESI): calc. for $\text{C}_{12}\text{H}_{14}\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 261.0733; found: 261.0734.

^1H -NMR spectrum for 3c (in CDCl_3)

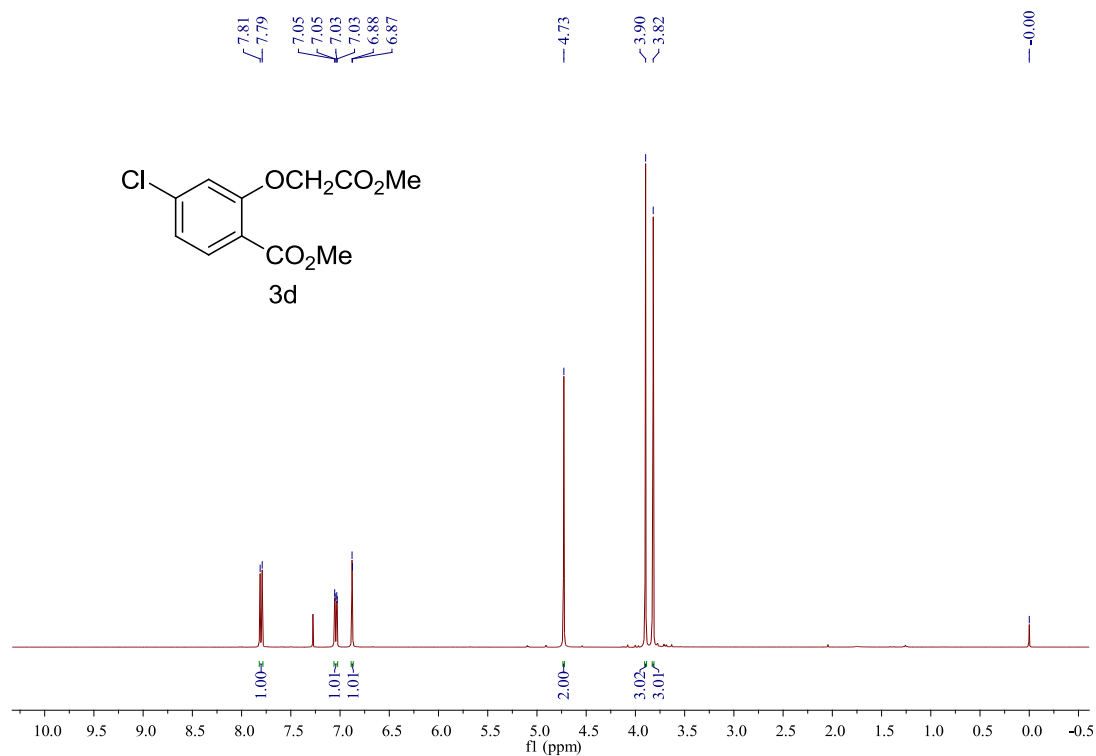


^{13}C -NMR spectrum for 3c (in CDCl_3)

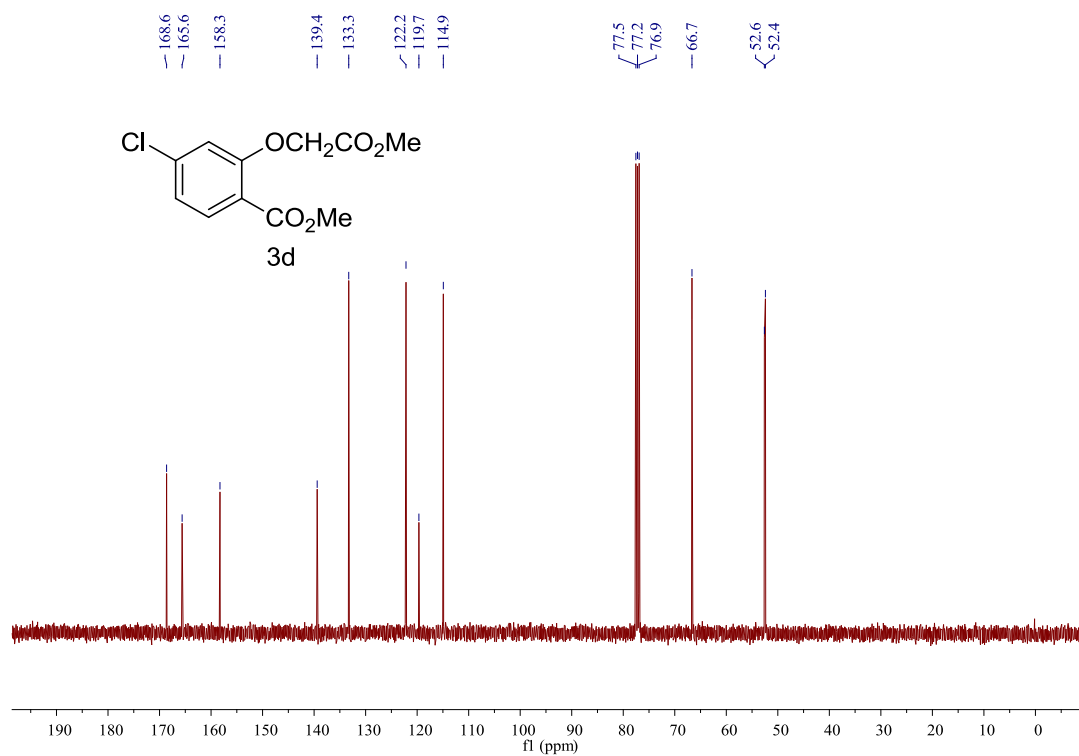


^1H NMR (400 MHz, CDCl_3): δ 7.76 (d, $J = 7.9$ Hz, 1H), 6.87 (d, $J = 7.9$ Hz, 1H), 6.69 (s, 1H), 4.72 (s, 2H), 3.89 (s, 3H), 3.81 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 169.4, 166.4, 157.9, 144.8, 132.3, 122.8, 122.8, 118.4, 115.4, 66.9, 52.5, 52.2, 22.0; HRMS (ESI): calc. for $\text{C}_{12}\text{H}_{14}\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 261.0733; found: 261.0737.

^1H -NMR spectrum for 3d (in CDCl_3)

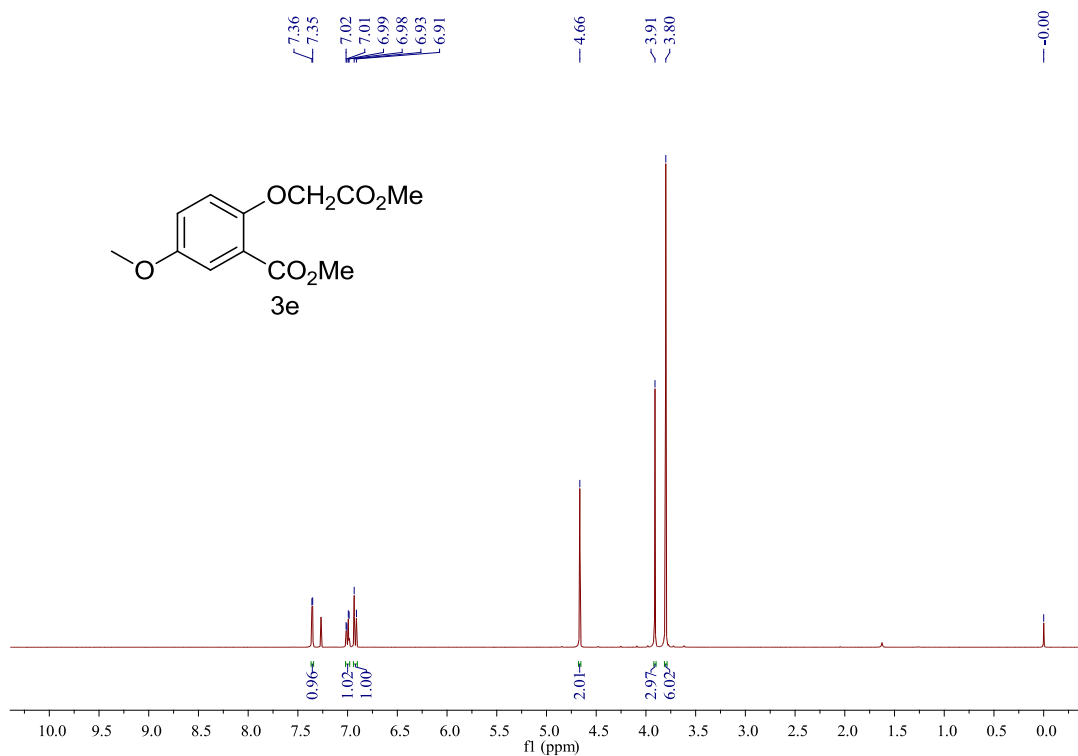


^{13}C -NMR spectrum for 3d (in CDCl_3)

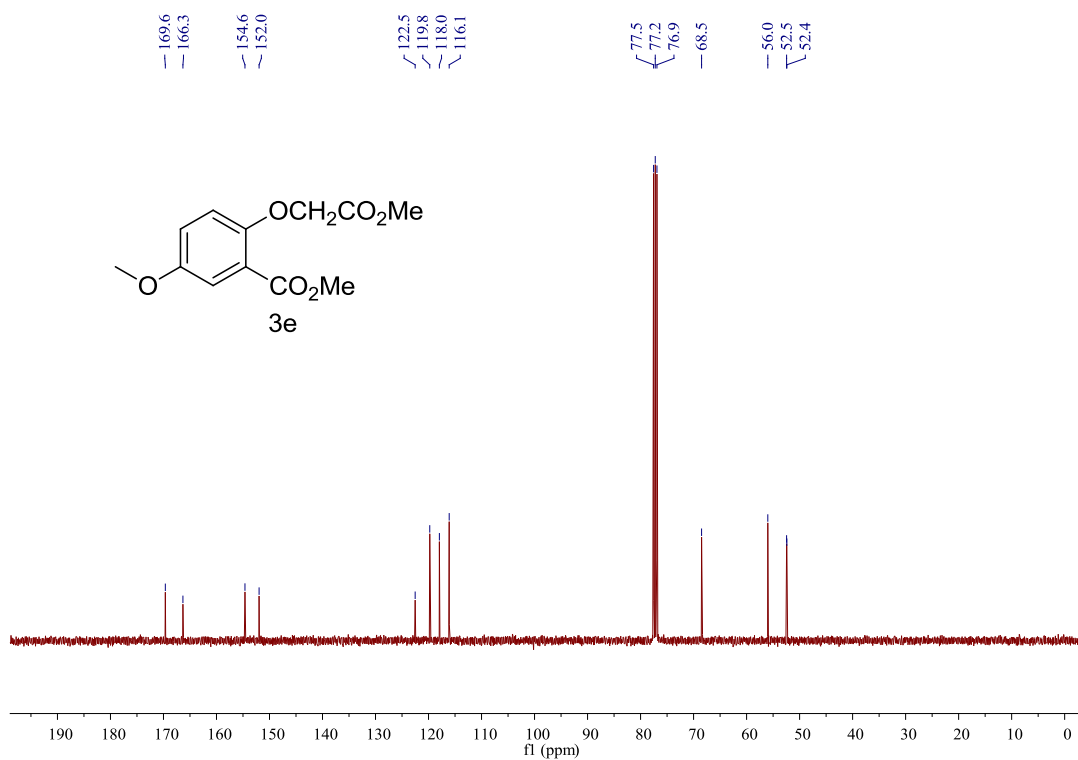


^1H NMR (400 MHz, CDCl_3): δ 7.80 (d, $J = 8.4$ Hz, 1H), 7.04 (dd, $J_1 = 8.4$, $J_2 = 1.8$, 1H), 6.88 (d, $J = 1.8$ Hz, 1H), 4.73 (s, 2H), 3.90 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 168.6, 165.6, 158.3, 139.4, 133.3, 122.2, 119.7, 114.9, 66.7, 52.6, 52.4; HRMS (ESI): calc. for $\text{C}_{11}\text{H}_{11}\text{ClNaO}_5$ $[\text{M}+\text{Na}]^+$: 281.0187; found: 281.0189.

^1H -NMR spectrum for **3e** (in CDCl_3)

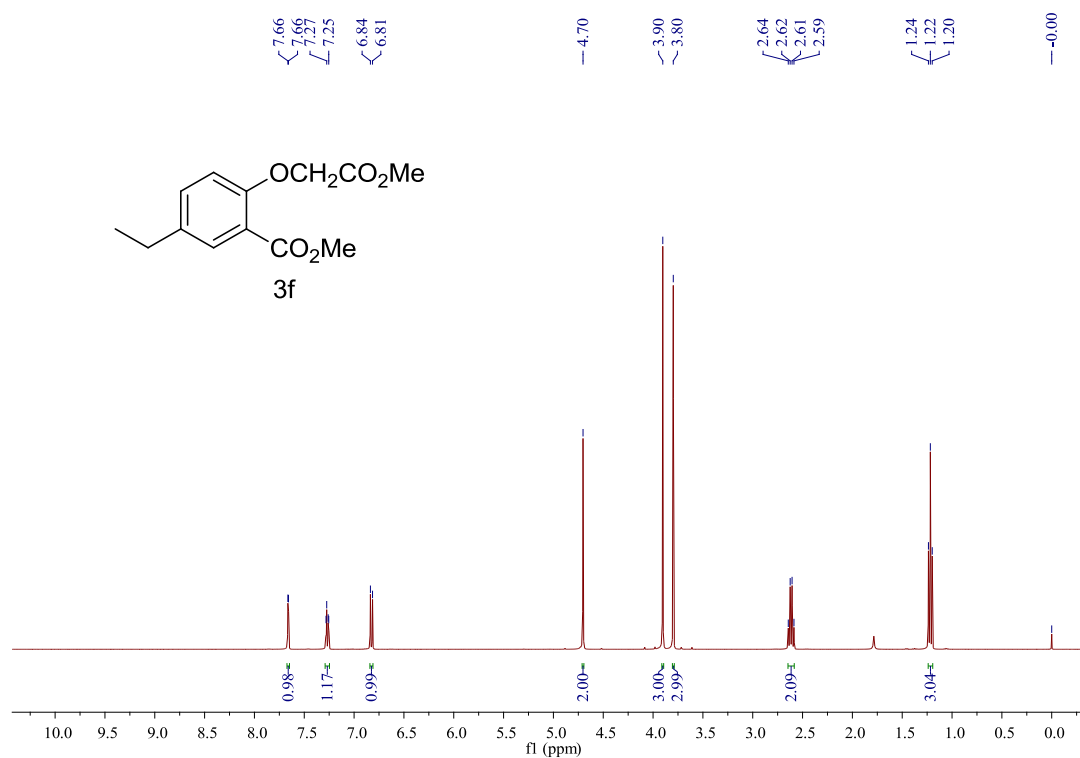


^{13}C -NMR spectrum for **3e** (in CDCl_3)

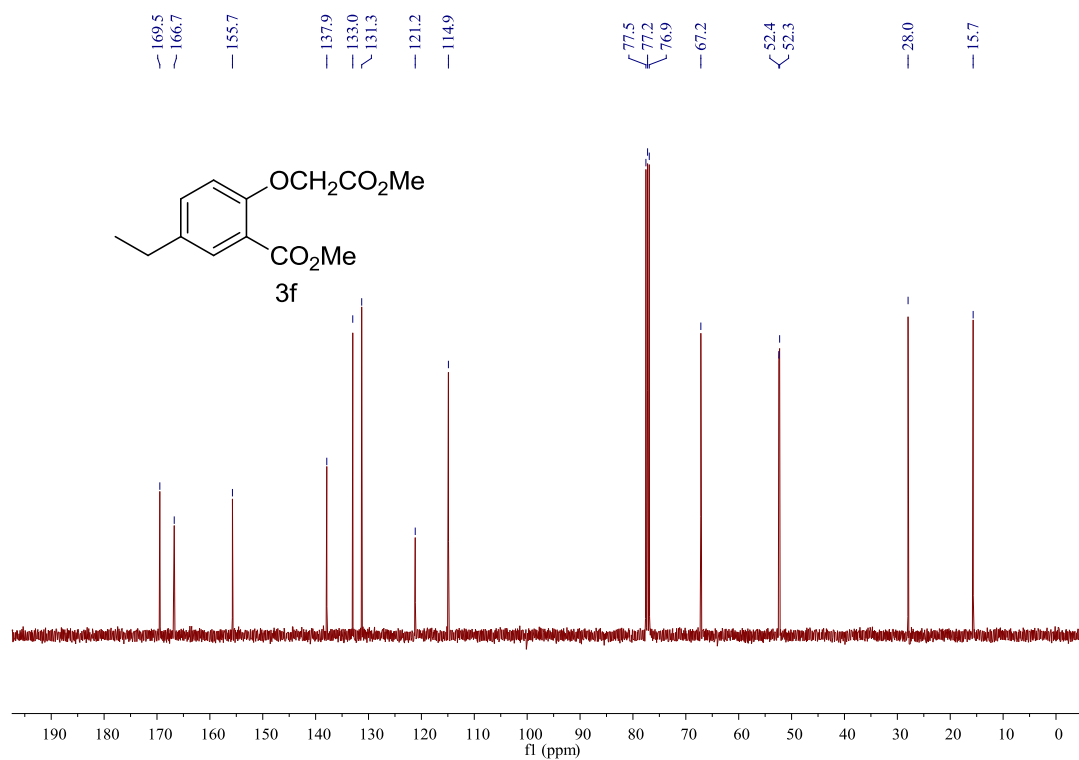


^1H NMR (400 MHz, CDCl_3): δ 7.35 (d, $J = 3.2$ Hz, 1H), 7.00 (dd, $J_1 = 3.2$ Hz, $J_2 = 9.0$ Hz, 1H), 6.92 (d, $J = 9.0$ Hz, 1H), 4.66 (s, 2H), 3.91 (s, 3H), 3.80 (s, 6H);
 ^{13}C NMR (100 MHz, CDCl_3): δ 169.6, 166.3, 154.6, 152.0, 122.5, 119.8, 118.0, 116.1, 68.5, 56.0, 52.5, 52.4; HRMS (ESI): calc. for $\text{C}_{12}\text{H}_{14}\text{NaO}_6$ $[\text{M}+\text{Na}]^+$: 277.0683; found: 277.0683.

^1H -NMR spectrum for 3f (in CDCl_3)

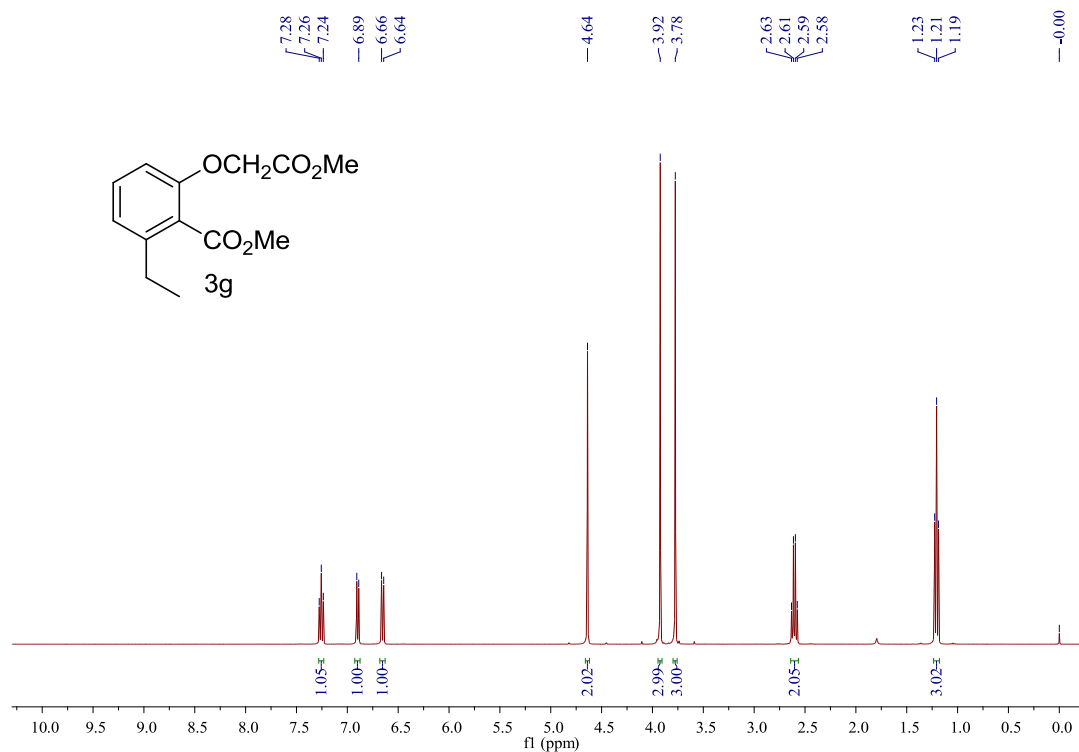


^{13}C -NMR spectrum for 3f (in CDCl_3)

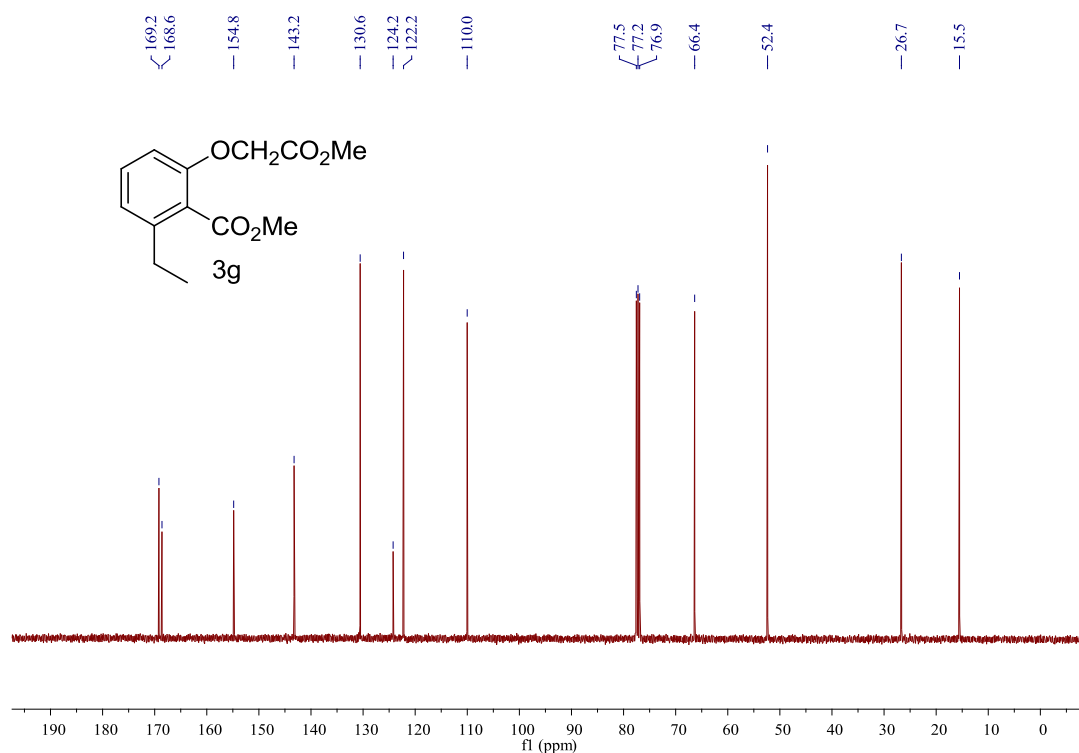


^1H NMR (400 MHz, CDCl_3): δ 7.66 (d, J = 2.3 Hz, 1H), 7.28-7.25 (m, 1H), 6.83 (d, J = 8.5 Hz, 1H), 4.70 (s, 2H), 3.90 (s, 3H), 3.80 (s, 3H), 2.61 (q, J = 7.6 Hz, 3H), 1.22 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 169.5, 166.7, 155.7, 137.9, 133.0, 131.3, 121.2, 114.9, 67.2, 52.4, 52.3, 28.0, 15.7; HRMS (ESI): calc. for $\text{C}_{13}\text{H}_{16}\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 275.0890; found: 275.0892.

^1H -NMR spectrum for 3g (in CDCl_3)

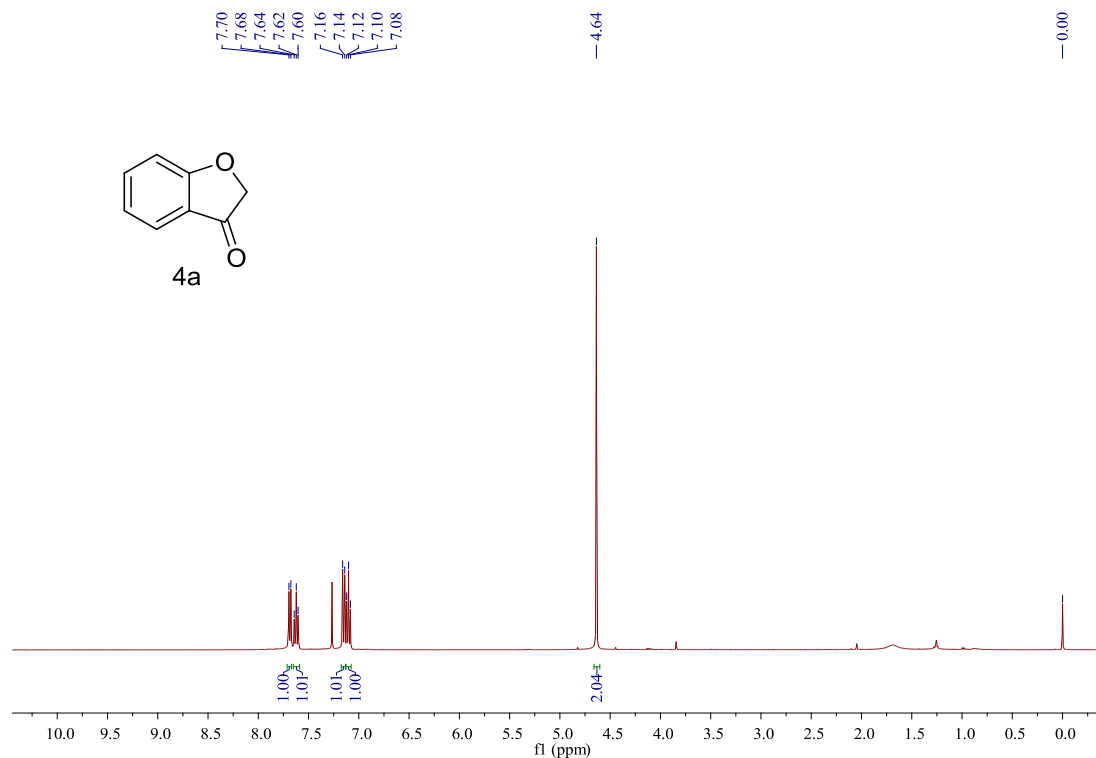


^{13}C -NMR spectrum for 3g (in CDCl_3)

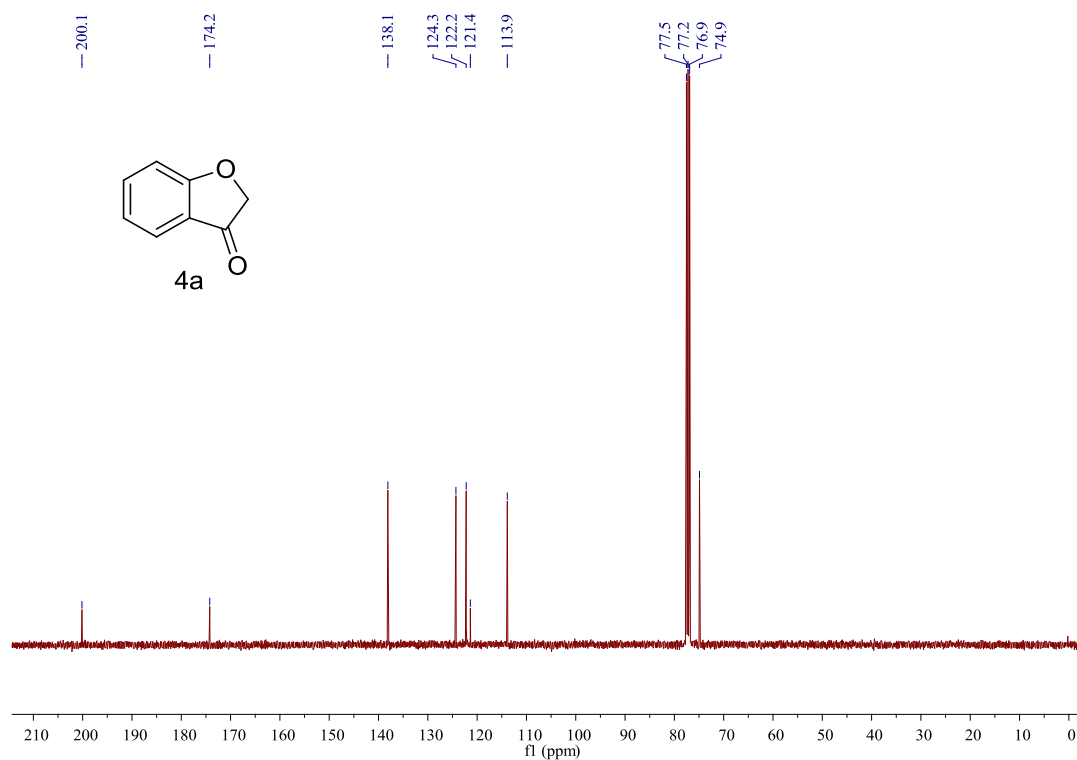


^1H NMR (400 MHz, CDCl_3): δ 7.26 (t, J = 8.0 Hz, 1H), 6.90 (d, J = 7.7 Hz, 1H), 6.65 (d, J = 8.3 Hz, 1H), 4.64 (s, 2H), 3.92 (s, 3H), 3.78 (s, 3H), 2.60 (q, J = 7.6 Hz, 3H), 1.21 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 169.2, 168.6, 154.8, 143.2, 130.6, 124.2, 122.2, 110.0, 66.4, 52.4, 52.4, 26.7, 15.5; HRMS (ESI): calc. for $\text{C}_{13}\text{H}_{16}\text{NaO}_5$ $[\text{M}+\text{Na}]^+$: 275.0890; found: 275.0887.

^1H -NMR spectrum for 4a (in CDCl_3)

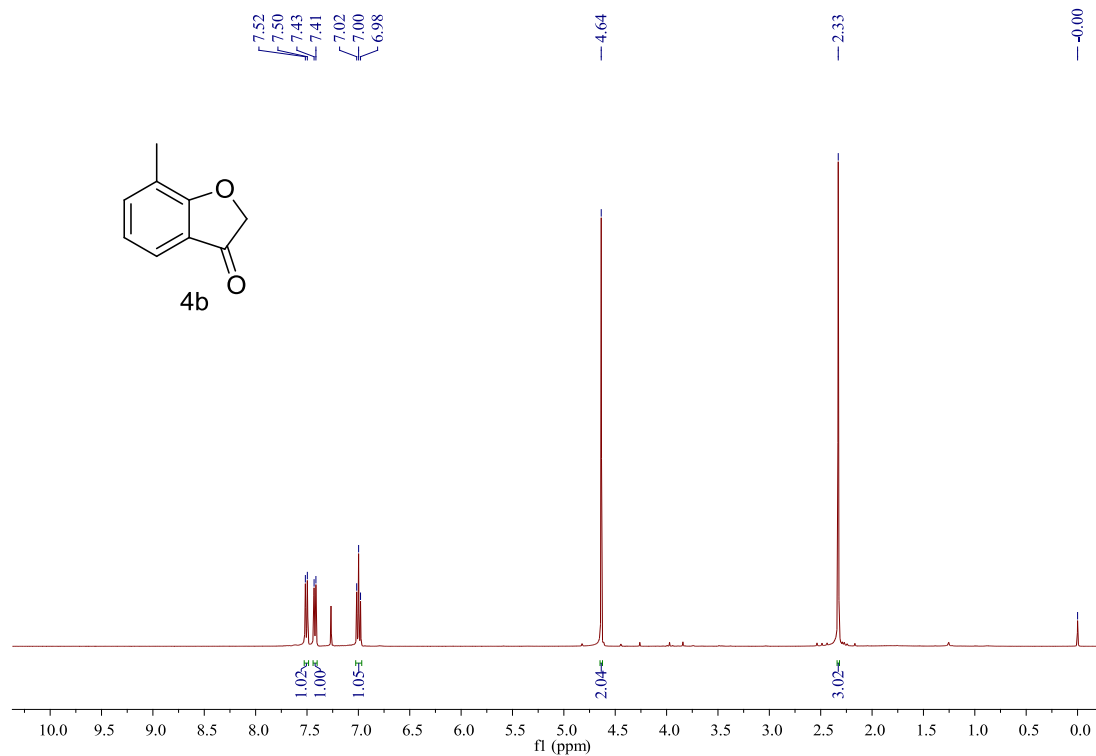


^{13}C -NMR spectrum for 10b (in CDCl_3)

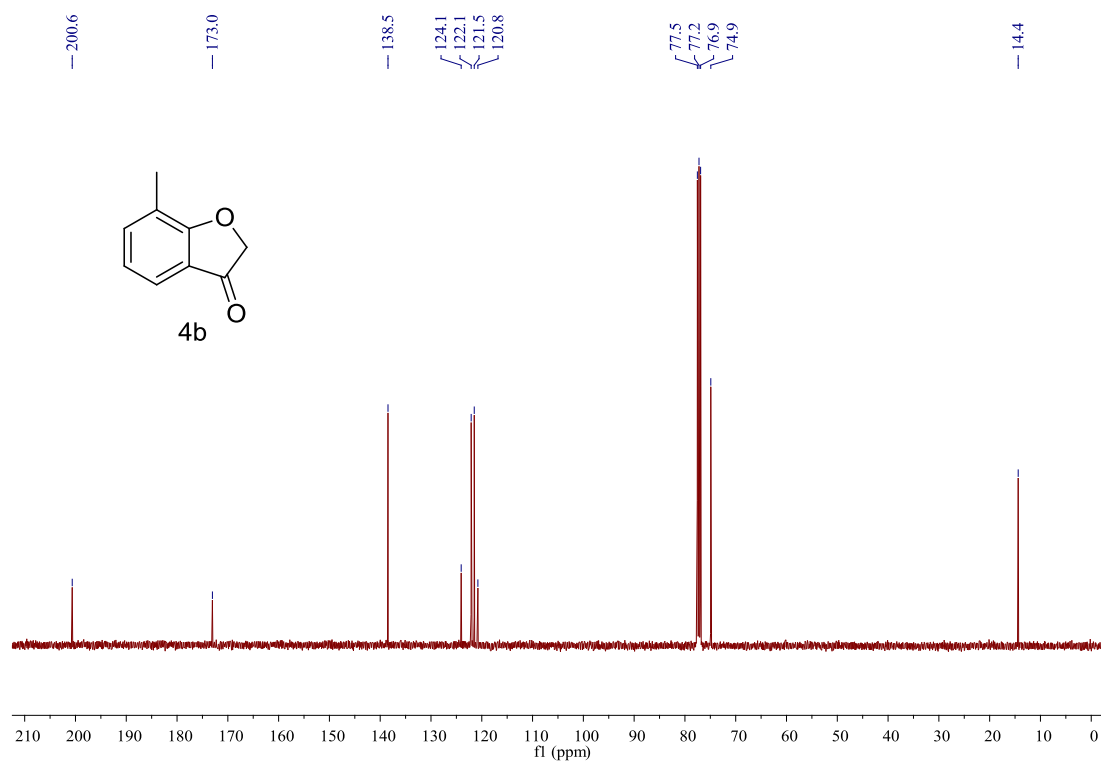


^1H NMR (400 MHz, CDCl_3): δ 7.69 (d, $J = 7.6$ Hz, 1H), 7.62 (t, $J = 8.4$ Hz, 1H), 7.15 (d, $J = 8.4$ Hz, 1H), 7.10 (t, $J = 7.6$ Hz, 1H), 4.64 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 200.1, 174.2, 138.1, 124.3, 122.2, 121.4, 113.9, 74.9; HRMS (ESI): calc. for $\text{C}_8\text{H}_7\text{O}_2$ $[\text{M}+\text{H}]^+$: 135.0441; found: 135.0444.

^1H -NMR spectrum for **4b** (in CDCl_3)

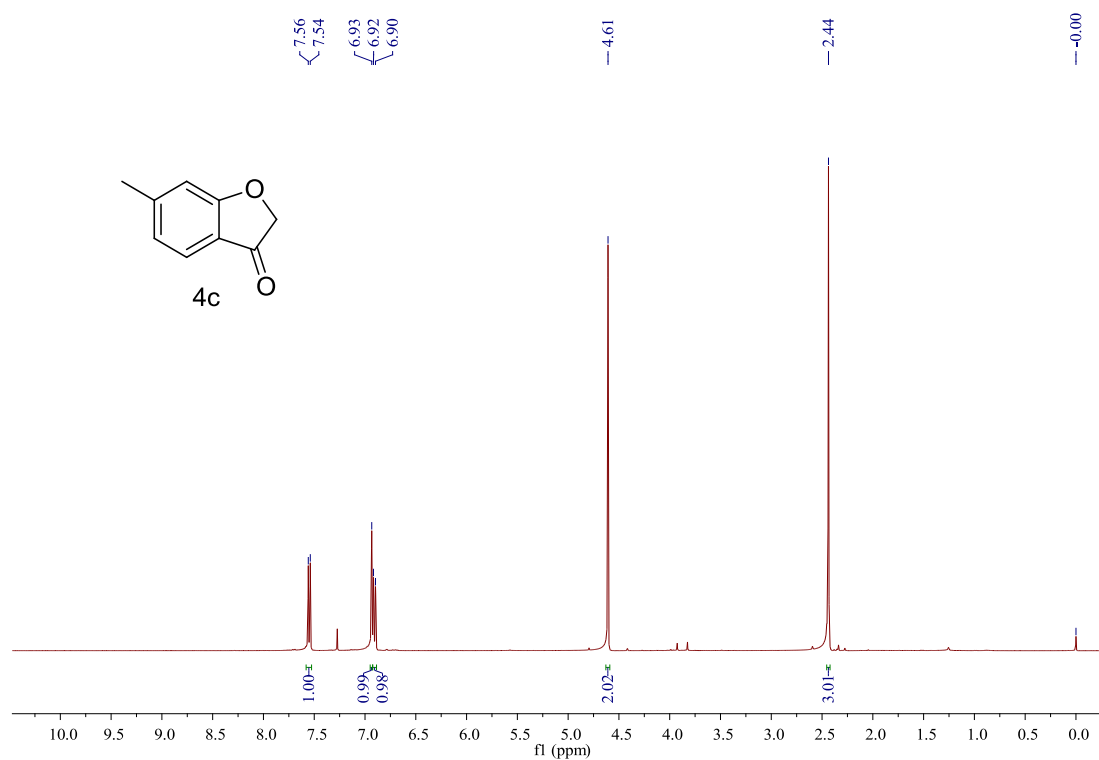


^{13}C -NMR spectrum for **4b** (in CDCl_3)

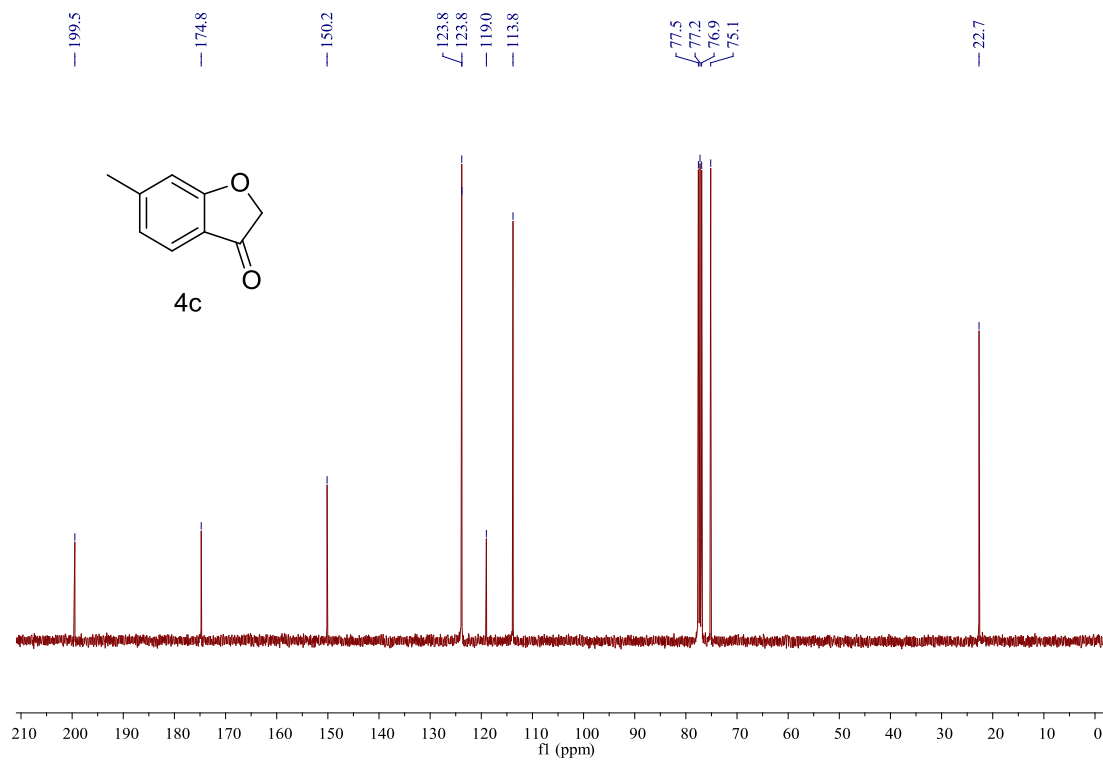


¹H NMR (400 MHz, CDCl₃): 7.51 (d, *J* = 7.7 Hz, 1H), 7.42 (d, *J* = 7.2 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 4.64 (s, 2H), 2.33 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 200.6, 173.0, 138.5, 124.1, 122.1, 121.5, 120.8, 74.9, 14.4; HRMS (ESI): calc. for C₉H₈NaO₂ [M+Na]⁺: 171.0417; found: 171.0414.

^1H -NMR spectrum for 4c (in CDCl_3)



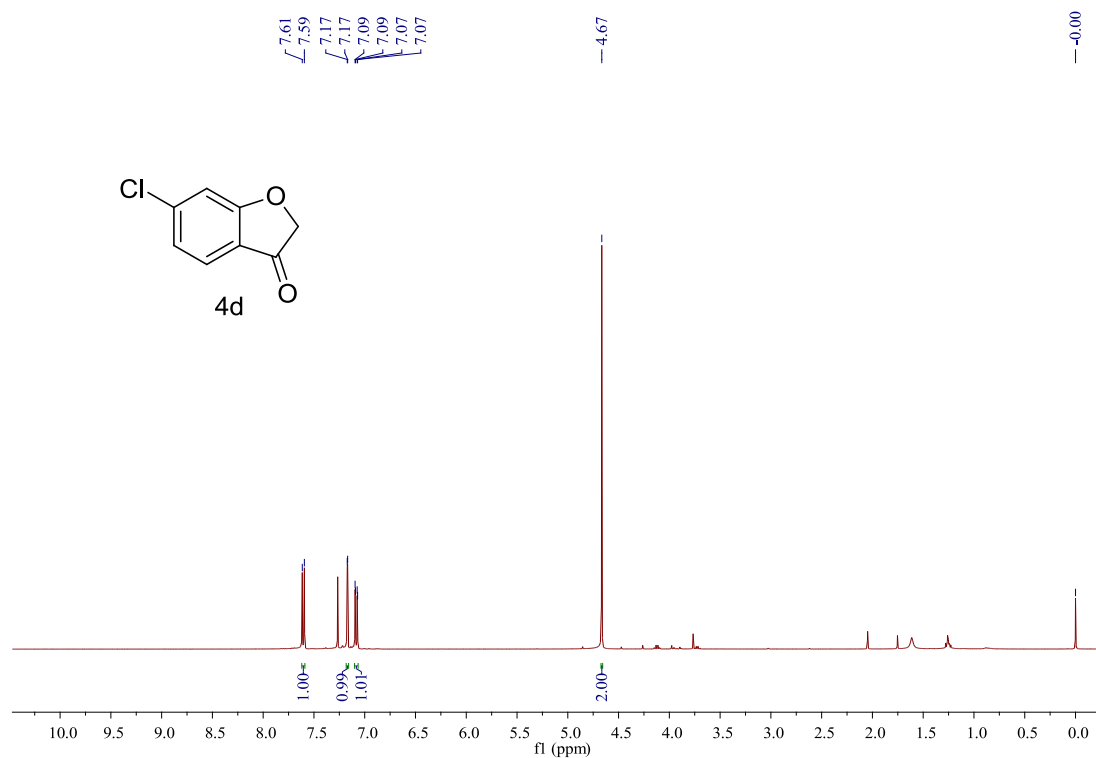
^{13}C -NMR spectrum for 4c (in CDCl_3)



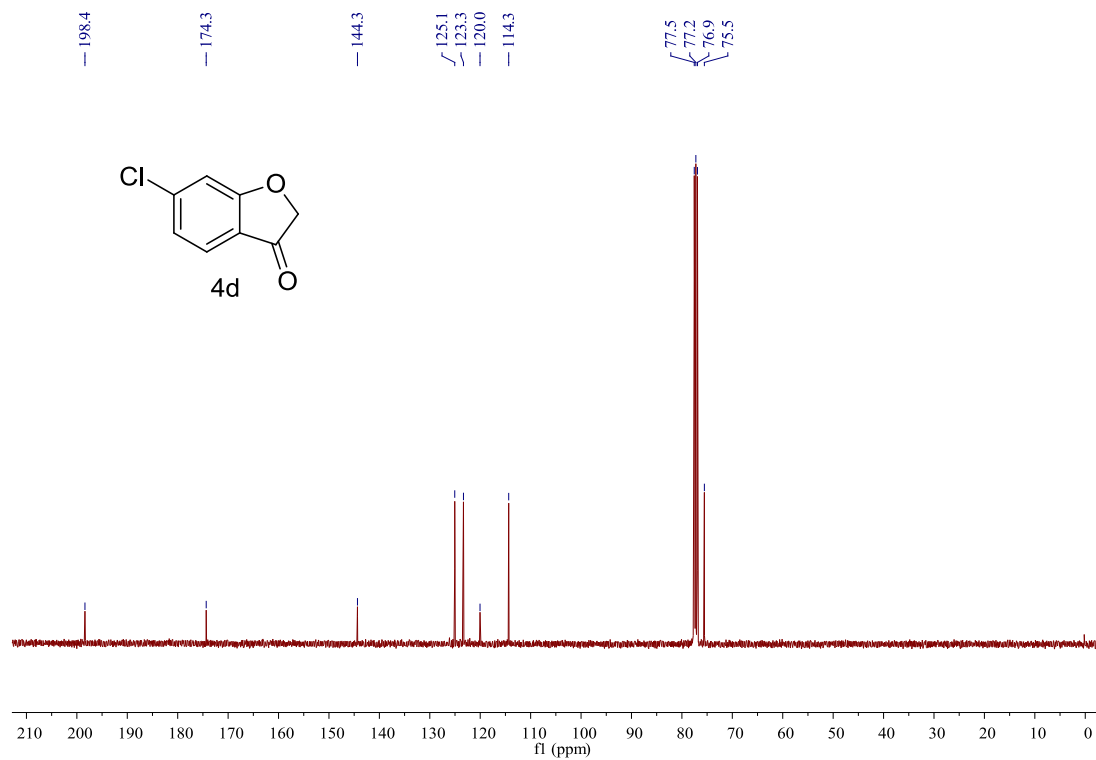
^1H NMR (400 MHz, CDCl_3): 7.55 (d, J = 7.9 Hz, 1H), 6.93 (s, 1H), 6.91 (d, J = 7.9 Hz, 1H), 4.61 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 199.5,

174.8, 150.2, 123.8, 123.8, 119.0, 113.8, 75.1, 22.7; HRMS (ESI): calc. for $C_9H_8NaO_2$ $[M+Na]^+$: 171.0417; found: 171.0422.

1H -NMR spectrum for 4d (in $CDCl_3$)

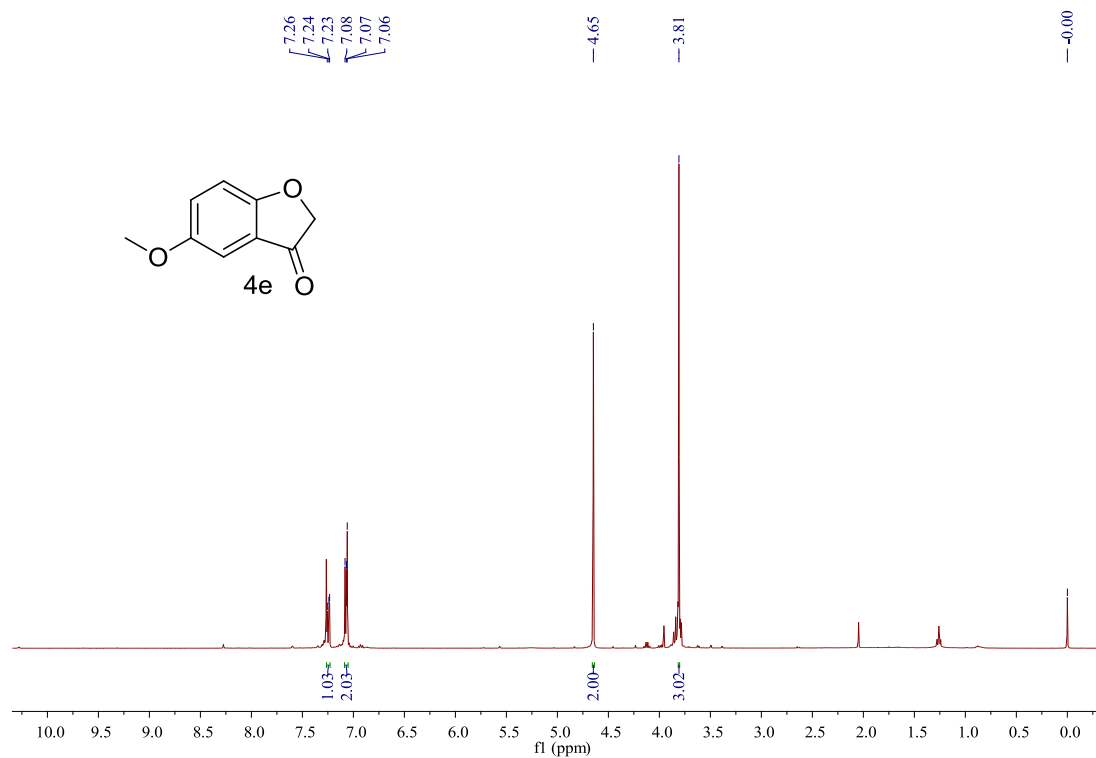


^{13}C -NMR spectrum for 4d (in $CDCl_3$)

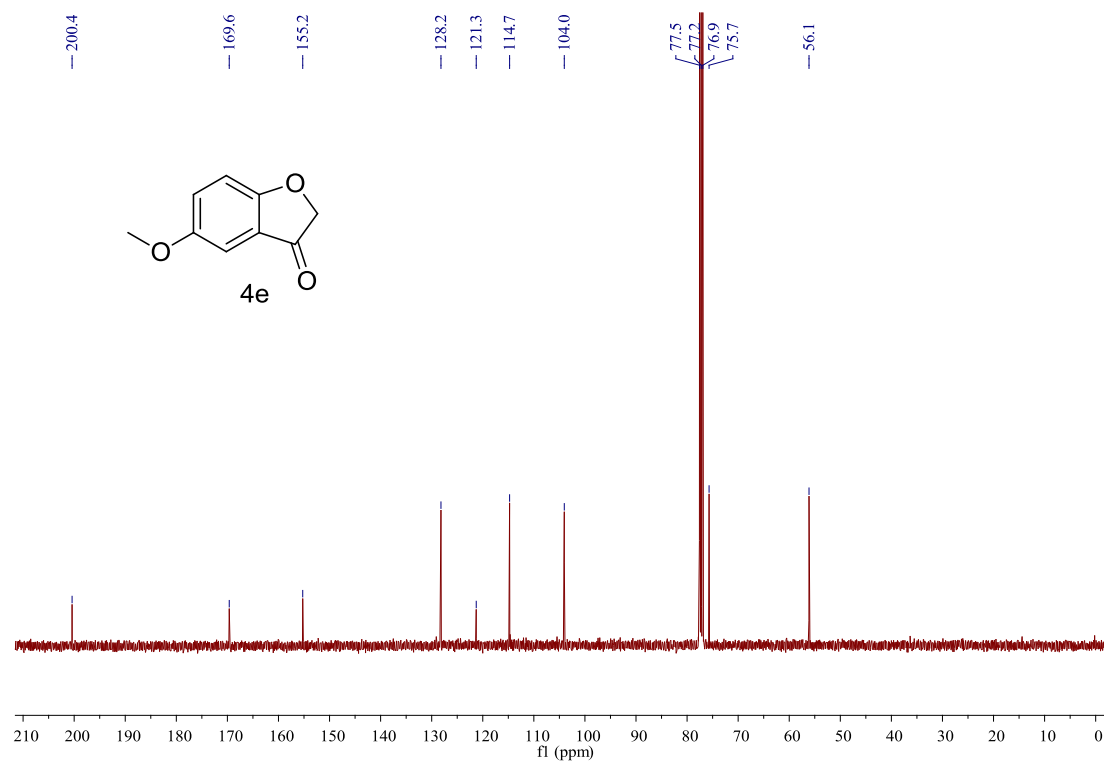


^1H NMR (400 MHz, CDCl_3): 7.60 (d, $J = 8.2$ Hz, 1H), 7.17 (d, $J = 1.6$ Hz, 1H), 7.08 (dd, $J_1 = 8.2$, $J_2 = 1.6$ Hz, 1H), 4.67 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 198.4, 174.3, 144.3, 125.1, 123.3, 120.0, 114.3, 75.5; HRMS (ESI): calc. for $\text{C}_{10}\text{H}_{11}\text{O}_2$ $[\text{M}+\text{H}]^+$: 163.0754; found: 163.0753.

^1H -NMR spectrum for 4e (in CDCl_3)

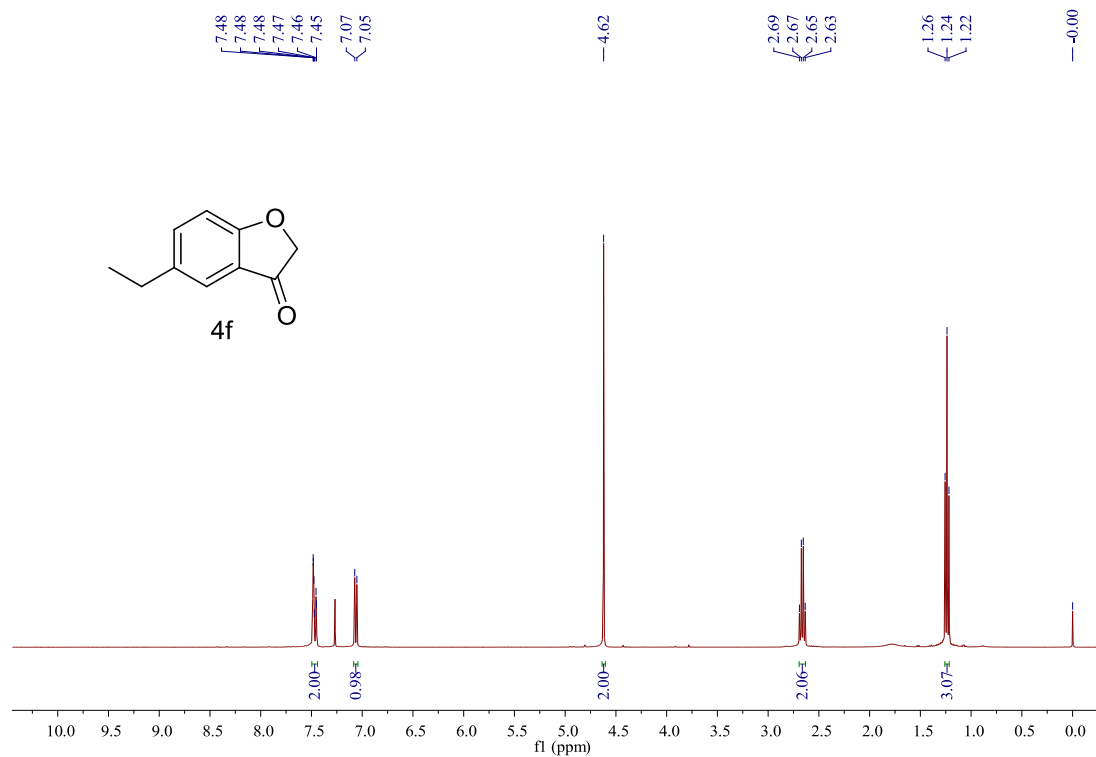


^{13}C -NMR spectrum for 4e (in CDCl_3)

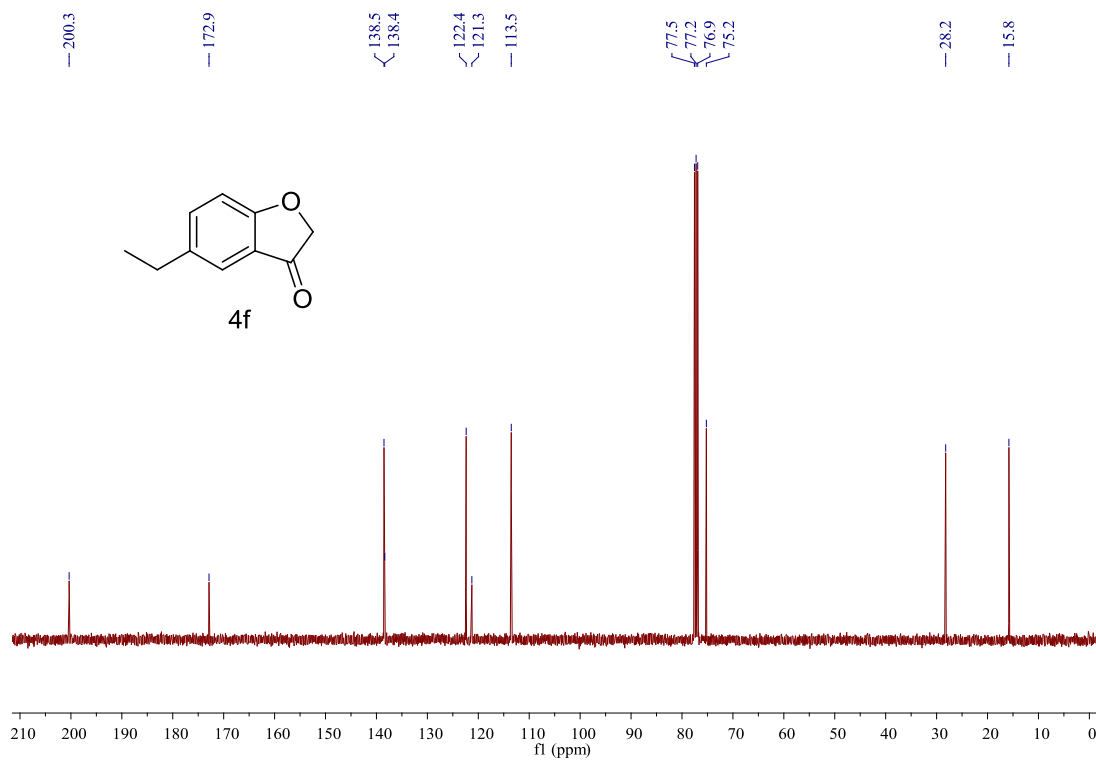


¹H NMR (400 MHz, CDCl₃): 7.26 – 7.23 (m, 1H), 7.09 – 7.05 (m, 2H), 4.65 (s, 2H), 3.81 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 200.4, 169.6, 155.2, 128.2, 121.3, 114.7, 104.0, 75.7, 56.1; HRMS (ESI): calc. for C₈H₇O₂ [M+H]⁺: 165.0546; found: 165.0549.

¹H-NMR spectrum for 4f (in CDCl₃)



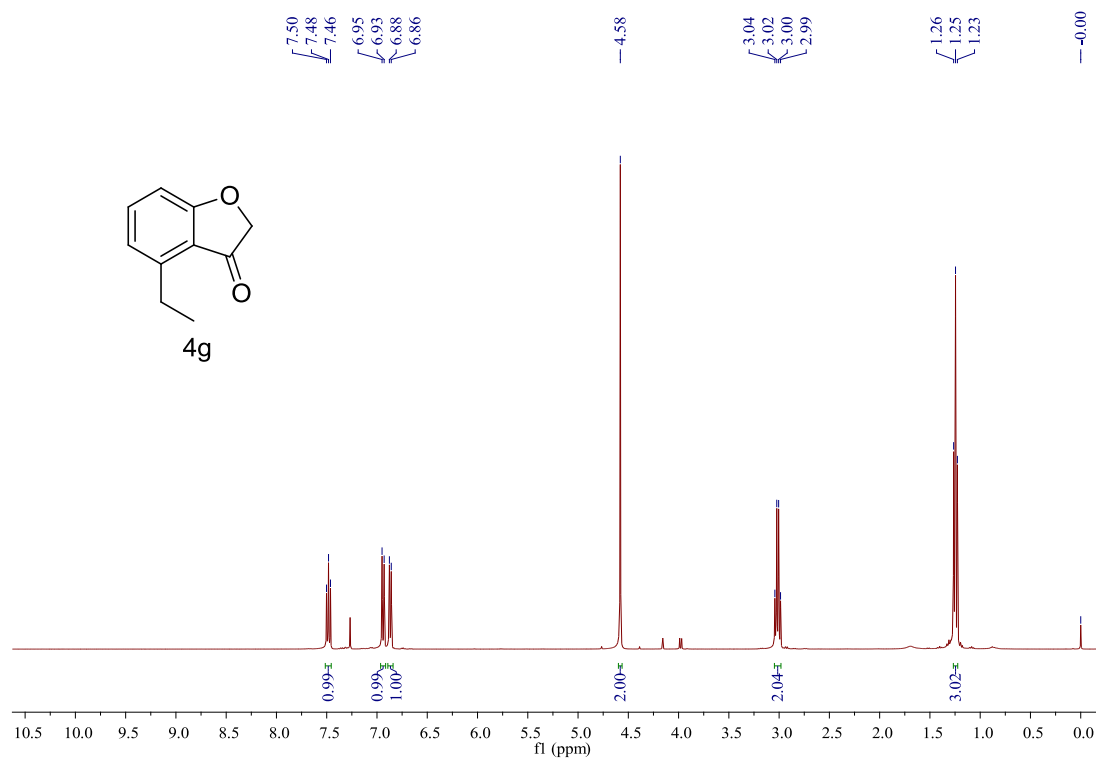
¹³C-NMR spectrum for 4f (in CDCl₃)



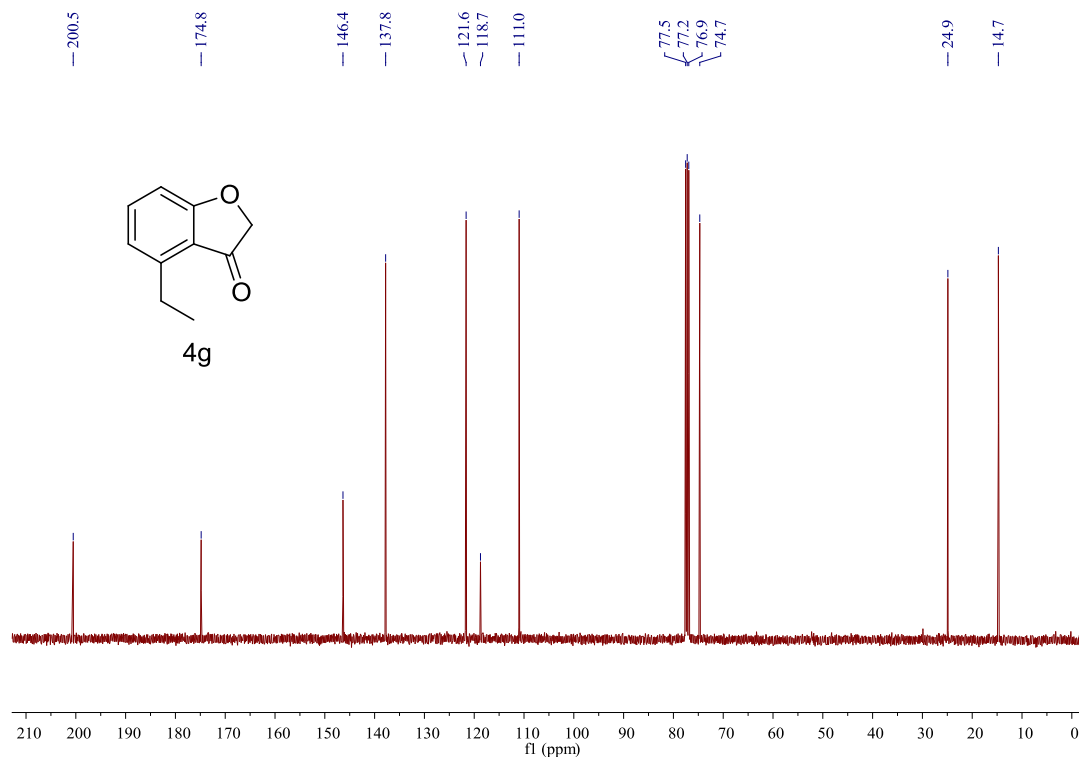
¹H NMR (400 MHz, CDCl₃): 7.50 – 7.44 (m, 2H), 7.06 (d, $J = 8.4$ Hz, 1H), 4.62 (s, 2H), 2.66 (q, $J = 7.6$ Hz, 2H), 1.24 (t, $J = 7.6$ Hz, 3H); ¹³C NMR (100 MHz,

CDCl₃): δ 200.3, 172.9, 138.5, 138.4, 122.4, 121.3, 113.5, 75.2, 28.2, 15.8; HRMS (ESI): calc. for C₁₀H₁₁O₂ [M+H]⁺: 163.0754; found: 163.0753.

¹H-NMR spectrum for 4g (in CDCl₃)



¹³C-NMR spectrum for 4g (in CDCl₃)



¹H NMR (400 MHz, CDCl₃): 7.51 – 7.46 (m, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 6.87 (d, *J* = 7.4 Hz, 1H), 4.58 (s, 2H), 3.01 (q, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.5 Hz,

3H); ^{13}C NMR (100 MHz, CDCl_3): δ 200.5, 174.8, 146.4, 137.8, 121.6, 118.7, 111.0, 74.7, 24.9, 14.7; HRMS (ESI): calc. for $\text{C}_{10}\text{H}_{11}\text{O}_2$ $[\text{M}+\text{H}]^+$: 163.0754; found: 163.0757.