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## Supporting Information

### Efficient synthesis of esters through oxone-catalyzed dehydrogenation of carboxylic acids and alcohols

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## General Experimental Details.

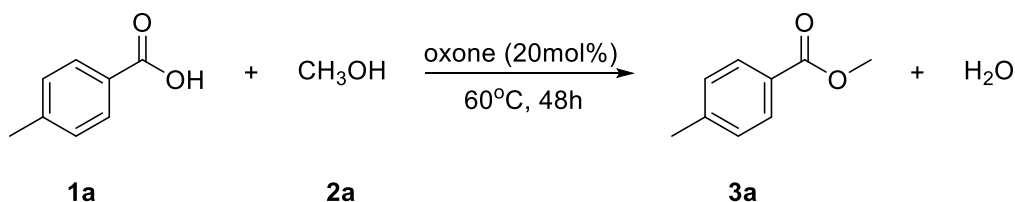
### 1. General

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR data analyses were performed with a Varian Mercury plus-400 instrument and plus-600 instrument unless otherwise specified. Dual-beam infrared spectrophotometer  $\text{CDCl}_3$  as solvent and tetramethylsilane (TMS) as the internal standard were employed. Chemical shifts were reported in units (ppm) by assigning TMS resonance in the  $^1\text{H}$  NMR spectrum as 0.00 ppm. The data of  $^1\text{H}$  NMR was reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant (J values) in Hz and integration. Chemical shift for  $^{13}\text{C}$  NMR spectra were recorded in ppm from TMS using the central peak of  $\text{CDCl}_3$  (77.0 ppm) as the internal standard. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Melting points were measured with an XT-4 apparatus. High-resolution mass spectra (HRMS) (ESI) were obtained with a Bruker Daltonics APEX II 47e and Orbitrap Elite mass spectrometer. Column chromatography was generally performed on silica gel (200–300 mesh) and TLC analyses were conducted on silica gel GF254 plates.

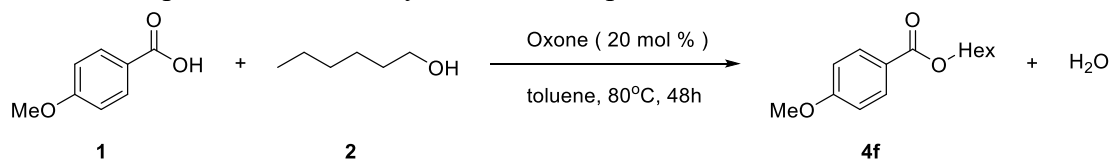
### 2. Experimental details.

The mixture of **1a** (0.50 mmol, 68 mg), Methanol (3mL), Oxone (20 mol %, 60 mg) and was stirred at 60 °C for 48 h under air atmosphere. After the reaction completing monitored by TLC analysis, 3.0 mL  $\text{NaHCO}_3$  solution were added to the mixture to quench the reaction and extracted with ethyl acetate ( $3 \times 10$  mL). The combined organic layers were dried by  $\text{MgSO}_4$ . The residue was purified by column chromatography on silica gel (ethyl acetate: petroleum ether = 1:6) to give the corresponding product **3a** as white solid, (66 mg, 88% yield). All of the products were synthesized according to above described procedure; when isopropyl alcohol and tert-butyl alcohol are used as a solvent, the reaction needs to be performed under a condition of 80 °C. Use high-boiling alcohol as a substrate, toluene is used as a solvent, the target product was obtained under the condition of 80 °C.

#### 2.1 General procedure for the synthesis of compound **3a**.



The mixture of **1a** (0.50 mmol, 68 mg), methanol (3mL), oxone (20 mol %, 60 mg) and was stirred at 60 °C for 48 h under air atmosphere. After the reaction completing monitored by TLC analysis, 3.0 mL  $\text{NaHCO}_3$  solution were added to the mixture to quench the reaction and extracted with ethyl acetate ( $3 \times 10$  mL). The combined organic layers were dried by  $\text{MgSO}_4$ . The residue was purified by column chromatography on silica gel (ethyl acetate: petroleum ether = 1:6) to give the corresponding product **3a** as white solid (66 mg, 88% yield).

2.2 General procedure for the synthesis of compound **4f**.

The mixture of **1c** (0.50 mmol, 76 mg), toluene (3mL), oxone (20 mol %, 60 mg) and was stirred at 80 °C for 48 h under air atmosphere. After the reaction completing monitored by TLC analysis, 3.0 mL NaHCO<sub>3</sub> solution were added to the mixture to quench the reaction and extracted with ethyl acetate (3×10 mL). The combined organic layers were dried by MgSO<sub>4</sub>. The residue was purified by column chromatography on silica gel (ethyl acetate: petroleum ether = 1:6) to give the corresponding product **4f** as colorless liquid (71 mg, 60% yield).

**Methyl 4-methylbenzoate (3a):**<sup>5b</sup> Colorless oil (66 mg, 88% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 7.92 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H), 2.39 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 167.12, 143.49, 129.56, 129.03, 127.41, 51.88, 21.59. HRMS (ESI) *m/z*: ([M+H]<sup>+</sup>) Calcd for C<sub>9</sub>H<sub>10</sub>O<sub>2</sub> 151.0754; Found 151.0752.

**Methyl benzoate (3b):**<sup>3</sup> Colorless liquid (61 mg, 89% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 8.02–8.04(m, 2H), 7.56–7.52 (m, 1H), 7.40–7.43 (m, 2H), 3.90 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 167.03, 132.85, 130.14, 129.52, 128.30, 52.02. HRMS (ESI) *m/z*: ([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>8</sub>O<sub>2</sub> 137.0597; Found 137.0595.

**Methyl 4-methoxybenzoate (3c):**<sup>5b</sup> White solid (72 mg, 87% yield), mp: 47–48 °C (lit 47–49 °C).<sup>5b</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 7.97 (d, *J* = 9.0Hz, 2H), 6.89 (d, *J* = 8.4Hz, 2H), 3.86 (s, 3H), 3.83 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 166.80, 163.29, 131.54, 122.58, 113.56, 55.36, 51.80. HRMS (ESI) *m/z*: ([M+H]<sup>+</sup>) Calcd for C<sub>9</sub>H<sub>10</sub>O<sub>3</sub> 167.0703; Found 167.0701.

**Methyl 4-nitrobenzoate (3d):**<sup>5b</sup> White solid (75 mg, 82% yield), mp: 95–96 °C (lit 93–95 °C).<sup>5b</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ ppm; 8.29–8.21 (m, 2H), 8.21–8.15 (m, 2H), 3.95 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ ppm; 165.06, 150.41, 135.38, 130.61, 123.44, 52.76. HRMS (ESI) *m/z*: ([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>7</sub>NO<sub>4</sub> 182.0448; Found 182.0445.

**Methyl 4-chlorobenzoate (3e):**<sup>5c</sup> White solid (73 mg, 86% yield), mp: 37–39 °C (lit 36–38 °C).<sup>5c</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 7.96 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 9.0 Hz, 2H), 3.90 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 166.17, 139.33, 130.93, 128.67, 128.57, 52.23. HRMS (ESI) *m/z*: ([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>7</sub>ClO<sub>2</sub> 171.0207; Found 171.0205.

**Methyl 4-bromobenzoate (3f):**<sup>7n</sup> White solid (91 mg, 85% yield), mp: 77–80 °C (lit 76–78 °C).<sup>7n</sup> <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ ppm; 7.90 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 3.91 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ ppm; 166.31, 131.67, 131.07, 129.01, 128.00, 52.26. HRMS (ESI) *m/z*: ([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>7</sub>BrO<sub>2</sub> 214.9702; Found 214.9704.

**4-Iodobenzoic acid methyl ester (3g):**<sup>4, 7n</sup> White solid (118 mg, 90% yield), mp: 113–115 °C (lit 113.8–114.7 °C).<sup>7n</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 7.77 (d, *J* =

8.4 Hz, 2H), 7.72 (d,  $J = 8.4$  Hz, 2H), 3.89 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.51, 137.68, 130.99, 129.58, 100.70, 52.26. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_8\text{H}_7\text{IO}_2$  262.9563; Found 262.9565.

**Methyl 3-methylbenzoate (3h):**<sup>6</sup> Colorless liquid (65 mg, 87% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.83 (t,  $J = 7.8$  Hz, 2H), 7.34 (d,  $J = 7.2$  Hz, 1H), 7.30 (t,  $J = 7.2$  Hz, 1H), 3.89 (s, 3H), 2.38 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 167.48, 138.33, 133.88, 130.32, 130.28, 128.46, 126.91, 52.24, 21.47. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_9\text{H}_{10}\text{O}_2$  151.0754; Found 151.0756.

**Methyl 3-methoxybenzoate (3i):**<sup>5c</sup> Colorless liquid (73 mg, 88% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.61 (d,  $J = 7.2$  Hz, 1H), 7.54 (d,  $J = 1.8$  Hz, 1H), 7.32 (t,  $J = 7.2$  Hz, 1H), 7.08 (dd,  $J = 8.4, 2.4$  Hz, 1H), 3.89 (s, 3H), 3.82 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.90, 159.52, 131.41, 129.33, 121.92, 119.42, 113.93, 55.36, 52.10. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_9\text{H}_{10}\text{O}_3$  167.0703; Found 167.0700.

**Methyl 3-nitrobenzoate (3j):**<sup>1, 7p</sup> White solid (74 mg, 82% yield), mp: 76–78 °C (lit 77–79 °C).<sup>7p</sup>  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 8.83 (t,  $J = 2.4$  Hz, 1H), 8.39 – 8.37 (m, 1H), 8.34 (dt,  $J = 7.2, 1.2$  Hz, 1H), 7.64 (t,  $J = 7.8$  Hz, 1H), 3.96 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 164.89, 148.23, 135.21, 131.83, 129.61, 127.33, 124.53, 52.75. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_8\text{H}_7\text{NO}_4$  182.0448; Found 182.0450.

**Methyl 3-iodobenzoate (3k):**<sup>4, 7o</sup> White solid (114 mg, 81% yield), mp: 55–57 °C (lit 50–52 °C).<sup>7o</sup>  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 8.36 (t,  $J = 1.2$  Hz, 1H), 7.99–7.97 (m, 1H), 7.87–7.85 (m, 1H), 7.17 (t,  $J = 7.6$  Hz, 1H), 3.91 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 165.75, 141.94, 138.67, 132.19, 130.27, 128.95, 94.05, 52.64. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_8\text{H}_7\text{IO}_2$  262.9563; Found 262.9561.

**Methyl 3-hydroxybenzoate (3l):**<sup>1, 7q</sup> White solid (66 mg, 87% yield), mp: 72–73 °C (lit 67 °C).<sup>7q</sup>  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.61 (t,  $J = 1.8$  Hz, 1H), 7.57 (dt,  $J = 7.8, 1.2$  Hz, 1H), 7.28 (t,  $J = 7.8$  Hz, 1H), 7.10 (dd,  $J = 2.4, 0.6$  Hz, 1H), 7.08 (s, 1H), 3.90 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 168.17, 156.38, 131.24, 130.00, 121.97, 120.85, 116.67, 52.77. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_8\text{H}_8\text{O}_3$  153.0546; Found 153.0543.

**Methyl 2-methoxybenzoate (3m):**<sup>6</sup> Colorless liquid (74 mg, 97% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 8.62 (t,  $J = 1.8$  Hz, 1H), 8.16 (dd,  $J = 7.8, 1.8$  Hz, 2H), 7.47 (t,  $J = 1.8$  Hz, 1H), 3.89 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.66, 133.46, 131.59, 120.08, 120.01, 111.98, 55.93, 51.94. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_9\text{H}_{10}\text{O}_3$  167.0703; Found 167.0705.

**Methyl 2-chlorobenzoate (3n):**<sup>1</sup> Colorless liquid (63 mg, 74% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.80 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.43 (dd,  $J = 7.8, 1.2$  Hz, 1H), 7.40–7.37 (m, 1H), 7.29–7.27 (m, 1H), 3.91 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.08, 133.62, 132.48, 131.32, 131.00, 130.03, 126.50, 52.35. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_8\text{H}_7\text{ClO}_2$  171.0207; Found 171.0205.

**Methyl 2-bromobenzoate (3o):**<sup>6</sup> Colorless liquid (86 mg, 81% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.76 (dd,  $J = 7.8, 2.4$  Hz, 1H), 7.63 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.34–7.31 (m, 1H), 7.30–7.27 (m, 1H), 3.90 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.55, 134.29, 132.51, 131.25, 127.11, 121.60, 52.41. HRMS (ESI)  $m/z$ :

([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>7</sub>BrO<sub>2</sub> 214.9702; Found 214.9700.

**Methyl 2-iodobenzoate (3p):**<sup>1</sup> Colorless liquid (94 mg, 72% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ ppm; 7.99 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 3.93 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ ppm; 166.91, 141.28, 135.08, 132.61, 130.90, 127.86, 94.04, 52.46. HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>7</sub>IO<sub>2</sub> 262.9563; Found 262.9561.

**Methyl [1,1'-biphenyl]-2-carboxylate (3q):**<sup>7m</sup> Colorless liquid (82 mg, 77% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ ppm; 7.82 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.51 (td, *J* = 1.6, 1.2, 1.2 Hz, 1H), 7.42–7.34 (m, 5H), 7.31–7.29 (m, 2H), 3.62 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ ppm; 169.39, 142.71, 141.55, 131.51, 131.10, 130.95, 130.02, 128.55, 128.29, 127.48, 127.41, 52.19. HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>14</sub>H<sub>12</sub>O<sub>2</sub> 213.0910; Found 213.0913.

**Methyl 3,5-dinitrobenzoate (3r):**<sup>1, 7r</sup> White solid (110 mg, 98% yield), mp: 107–109 °C (lit 104–106 °C).<sup>7r</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 9.19 (t, *J* = 2.4 Hz, 1H), 9.14 (d, *J* = 1.8 Hz, 2H), 4.05 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 162.94 (d, *J* = 6.0 Hz), 148.62, 133.68 (d, *J* = 5.3 Hz), 129.38 (d, *J* = 5.6 Hz), 122.32 (d, *J* = 5.7 Hz), 53.51 (d, *J* = 6.1 Hz). HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>6</sub> 227.0299; Found 227.0296.

**Methyl 3-chloro-4-methoxybenzoate (3s):**<sup>8</sup> White solid (75 mg, 75% yield), mp: 92–94 °C (lit 93–97 °C).<sup>22g</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 8.05 (d, *J* = 2.4 Hz, 1H), 7.93 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 3.95 (s, 3H), 3.89 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 165.81, 158.60, 131.63, 129.83, 123.32, 122.47, 111.16, 56.30, 52.10. HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>9</sub>H<sub>9</sub>ClO<sub>3</sub> 201.0313; Found 201.0315.

**Methyl cinnamate (3t):**<sup>2, 3</sup> White solid (70 mg, 86% yield), mp: 31–34 °C (lit 34–38 °C).<sup>3</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 7.69 (d, *J* = 15.6 Hz, 1H), 7.51 (dd, *J* = 7.2, 3.6 Hz, 2H), 7.39–7.35 (m, 3H), 6.44 (d, *J* = 15.6 Hz, 1H), 3.80 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 167.37, 144.83, 134.37, 130.26, 128.86, 128.04, 117.79, 51.65. HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>10</sub>H<sub>10</sub>O<sub>2</sub> 163.0754; Found 163.0751.

**Methyl 1-naphthoate (3u):**<sup>5c</sup> Colorless liquid (83 mg, 89% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 8.96 (d, *J* = 9.0 Hz, 1H), 8.20 (dd, *J* = 7.2, 1.2 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.64–7.61 (m, 1H), 7.55–7.52 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 4.01 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm; 167.99, 133.84, 133.36, 131.35, 130.23, 128.54, 127.75, 127.07, 126.20, 125.83, 124.47, 52.12. HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>12</sub>H<sub>10</sub>O<sub>2</sub> 187.0754; Found 187.0751.

**Methyl thiophene-2-carboxylate (3v):**<sup>5a</sup> Colorless liquid (19 mg, 27% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ ppm; 7.80 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.55 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.11–7.08 (m, 1H), 3.89 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ ppm; 162.93, 133.69, 133.77, 132.58, 127.97, 52.38. HRMS (ESI) m/z: ([M+H]<sup>+</sup>) Calcd for C<sub>6</sub>H<sub>6</sub>O<sub>2</sub>S 143.0161; Found 143.0163.

**Methyl furan-2-carboxylate (3w):**<sup>5c</sup> Colorless liquid (18 mg, 28% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ ppm; 7.57 (dd, *J* = 1.8, 0.6 Hz, 1H), 7.17 (dd, *J* = 3.6, 1.2 Hz, 1H), 6.50 (q, *J* = 1.8 Hz, 1H), 3.89 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ ppm;

159.09, 146.23, 144.58, 117.88, 111.80, 51.88. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_6H_6O_3$  127.0390; Found 127.0392.

**Methyl adamantane-1-carboxylate (3x):**<sup>7f</sup> White solid (80 mg, 82% yield), mp: 34–36 °C (lit 38–39 °C).<sup>7f</sup>  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 3.63 (s, 3H), 1.99 (s, 3H), 1.87 (d,  $J = 3.0$  Hz, 6H), 1.65–1.72 (m, 7H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 178.15, 51.48, 40.67, 38.82, 36.47, 27.91. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_{12}H_{18}O_2$  195.1380; Found 195.1383.

**Dimethyl isophthalate (3y):**<sup>4</sup> Colorless liquid (76 mg, 78% yield).  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 7.76 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.45–7.41 (m, 1H), 6.96–6.92 (m, 2H), 3.86 (d,  $J = 4.8$  Hz, 6H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 166.64, 159.05, 133.45, 131.57, 120.06, 111.97, 55.91, 51.92. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_{10}H_{10}O_4$  195.0652; Found 195.0650.

**Dimethyl malonate (3z):**<sup>7b</sup> Colorless liquid (53 mg, 81% yield).  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 3.74 (s, 6H), 3.38 (s, 2H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 166.88, 52.51, 41.09. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_5H_8O_4$  133.0495; Found 133.0493.

**Dimethyl cyclopropane-1,1-dicarboxylate (3aa):**<sup>7c</sup> Colorless liquid (67 mg, 85% yield).  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 3.65 (t,  $J = 4.2$  Hz, 6H), 1.37 (t,  $J = 4.8$  Hz, 4H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 169.99, 52.41, 27.75, 16.49. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_7H_{10}O_4$  159.0652; Found 159.0654.

**Methyl stearate (3ab):**<sup>2,9</sup> White solid (143 mg, 96% yield), mp: 39–41 °C (lit 38–40 °C).<sup>9</sup>  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  ppm; 3.66 (s, 3H), 2.30 (t,  $J = 7.6$  Hz, 2H), 1.65–1.58 (m, 2H), 1.26 (s, 28H), 0.88 (t,  $J = 6.8$  Hz, 3H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  ppm; 51.29, 34.03, 31.89, 29.66, 29.64, 29.62, 29.61, 29.56, 29.42, 29.33, 29.22, 29.12, 24.91, 22.64, 14.03. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_{19}H_{38}O_2$  299.2945; Found 299.2948.

**Ethyl 4-hydroxybenzoate (4a):**<sup>1, 7s</sup> White solid (60 mg, 72% yield), mp: 113–115 °C (lit 117–117 °C).<sup>7s</sup>  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 7.95 (d,  $J = 9.0$  Hz, 2H), 6.87 (d,  $J = 9.0$  Hz, 2H), 6.16 (s, 1H), 4.35 (q,  $J = 7.2$  Hz, 2H), 1.38 (t,  $J = 7.2$  Hz, 3H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 166.93, 160.17, 131.87, 122.60, 115.20, 60.92, 14.30. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_9H_{10}O_3$  167.0703; Found 167.0705.

**Ethyl 4-methoxybenzoate (4b):**<sup>7d</sup> Colorless liquid (66 mg, 72% yield),  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 7.98 (d,  $J = 9.0$  Hz, 2H), 6.89 (d,  $J = 9.0$  Hz, 2H), 6.15 (s, 1H), 4.33 (q,  $J = 8.4$  Hz, 2H), 3.83 (s, 3H), 1.36 (t,  $J = 7.2$  Hz, 3H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 166.33, 163.21, 131.48, 122.93, 113.50, 60.57, 55.35, 14.34. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_{10}H_{12}O_3$  181.0859; Found 181.0857.

**Propyl 4-methoxybenzoate (4c):**<sup>7e</sup> Colorless liquid (73 mg, 76% yield).  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 7.99 (d,  $J = 8.4$  Hz, 2H), 6.91 (d,  $J = 9.0$  Hz, 2H), 4.24 (t,  $J = 6.6$  Hz, 2H), 3.85 (s, 3H), 1.79–1.74 (m, 2H), 1.01 (t,  $J = 7.2$  Hz, 3H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  ppm; 166.41, 163.21, 131.49, 122.96, 113.52, 66.20, 55.38, 22.14, 10.50. HRMS (ESI)  $m/z$ : ( $[M+H]^+$ ) Calcd for  $C_{11}H_{14}O_3$  195.1016; Found 195.1018.

**Butyl 4-methoxybenzoate (4d):**<sup>7f</sup> Colorless liquid (68 mg, 66% yield).  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  ppm; 7.99 (d,  $J = 9.0$  Hz, 2H), 6.91 (d,  $J = 9.0$  Hz, 2H), 4.28 (t,  $J = 6.6$  Hz, 2H), 3.85 (s, 3H), 1.75–1.70 (m, 2H), 1.49–1.43 (m, 2H), 0.97 (t,  $J = 7.2$  Hz,

3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 163.45, 131.75, 123.20, 113.76, 64.75, 55.63, 31.06, 19.52, 14.01. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{12}\text{H}_{16}\text{O}_3$  209.1172; Found 209.1170.

**Isopentyl 4-methoxybenzoate (4e):**<sup>7g</sup> Colorless liquid (38 mg, 34% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.98 (d,  $J = 9.0$  Hz, 2H), 6.91 (d,  $J = 8.8$  Hz, 2H), 4.31 (t,  $J = 6.6$  Hz, 2H), 3.85 (s, 3H), 1.81–1.75 (m, 1H), 1.64 (q,  $J = 6.6$  Hz, 2H), 0.96 (d,  $J = 7.8$  Hz, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 163.21, 131.49, 122.97, 113.52, 63.30, 55.38, 37.47, 25.22, 22.51. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{13}\text{H}_{18}\text{O}_3$  223.1329; Found 223.1327.

**Hexyl 4-methoxybenzoate (4f):**<sup>7g</sup> Colorless liquid (71 mg, 60% yield).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.97 (d,  $J = 6.0$  Hz, 2H), 6.88 (d,  $J = 6.0$  Hz, 2H), 4.25 (t,  $J = 4.4$  Hz, 2H), 3.81 (s, 3H), 1.74–1.69 (m, 2H), 1.43–1.38 (m, 2H), 1.32–1.29 (m, 4H), 0.89 (t,  $J = 4.8$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.41, 163.20, 131.49, 122.98, 113.52, 64.81, 55.37, 31.46, 28.72, 25.70, 22.53, 13.98. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{14}\text{H}_{20}\text{O}_3$  237.1485; Found 237.1487.

**Isopropyl benzoate (4g):**<sup>10</sup> Colorless liquid (52 mg, 63% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 8.02–8.04 (m, 2H), 7.54–7.51 (m, 1H), 7.42 (t,  $J = 7.8$  Hz, 2H), 5.28–5.22 (m, 1H), 1.36 (d,  $J = 6.0$  Hz, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 166.06, 132.63, 130.90, 129.46, 128.21, 68.28, 21.92. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{10}\text{H}_{12}\text{O}_2$  165.0910; Found 165.0912.

**Isopropyl 4-methoxybenzoate (4h):**<sup>5b</sup> Colorless liquid (66 mg, 68% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.98 (d,  $J = 9.0$  Hz, 2H), 6.89 (d,  $J = 9.0$  Hz, 2H), 5.24–5.17 (m, 1H), 3.84 (s, 3H), 1.34 (d,  $J = 6.0$  Hz, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 165.82, 163.13, 131.44, 123.35, 113.44, 67.88, 55.35, 21.96. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{11}\text{H}_{14}\text{O}_3$  195.1016; Found 195.1018.

**Isopropyl 3-nitrobenzoate (4i):**<sup>5c</sup> Colorless liquid (83 mg, 80% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 8.78 (t,  $J = 1.8$  Hz, 1H), 8.36–8.34 (m, 1H), 8.32 (dt,  $J = 7.2, 1.2$  Hz, 1H), 7.61 (t,  $J = 7.8$  Hz, 1H), 5.28–5.22 (m, 1H), 1.37 (d,  $J = 6.6$  Hz, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 163.84, 148.18, 135.18, 132.59, 129.47, 127.09, 124.37, 76.95 (d,  $J = 31.9$  Hz), 21.79. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{10}\text{H}_{11}\text{NO}_4$  210.0761; Found 210.0763.

**Isopropyl 2-methoxybenzoate (4j):**<sup>7t</sup> Colorless liquid (65 mg, 67% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.72 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.42–7.38 (m, 1H), 6.94–6.91 (m, 2H), 5.24–5.18 (m, 1H), 3.85 (s, 3H), 1.32 (d,  $J = 6.6$  Hz, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 165.63, 159.01, 133.07, 131.20, 120.95, 120.00, 112.03, 67.99, 55.91, 21.87. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{11}\text{H}_{14}\text{O}_3$  195.1016; Found 195.1014.

**Isopropyl 2-nitrobenzoate (4k):**<sup>7u</sup> Colorless liquid (52 mg, 45% yield).  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 7.89 (dd,  $J = 7.8, 1.2$  Hz, 1H), 7.73 (dd,  $J = 7.2, 1.2$  Hz, 1H), 7.67–7.64 (m, 1H), 7.61–7.58 (m, 1H), 5.28–5.22 (m, 1H), 1.34 (d,  $J = 6.3$  Hz, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 1645.11, 148.42, 133.04, 131.72, 130.03, 128.43, 124.00, 70.65, 21.59. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{10}\text{H}_{11}\text{NO}_4$  210.0761; Found 210.0764.

**Isopropyl 2-bromobenzoate (4l):**<sup>7h</sup> Colorless liquid (62 mg, 51% yield).  $^1\text{H}$  NMR

(600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 7.72 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.63 (dd,  $J = 7.8, 1.2$  Hz, 1H), 7.35–7.32 (m, 1H), 7.30–7.27 (m, 1H), 5.29–5.23 (m, 1H), 1.38 (d,  $J = 6.3$  Hz, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 129.64, 128.56, 127.69, 126.46, 122.59, 116.81, 64.94, 17.32. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>10</sub>H<sub>11</sub>BrO<sub>2</sub> 243.0015; Found 243.0012.

**Isopropyl 3-methoxybenzoate (4m):**<sup>7v</sup> Colorless liquid (62 mg, 65% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  = 7.62 (dt,  $J = 7.8, 1.2$  Hz, 1H), 7.55 (dd,  $J = 3.0, 1.8$  Hz, 1H), 7.32 (t,  $J = 7.8$  Hz, 1H), 7.08–7.06 (m, 1H), 5.26–5.20 (m, 1H), 3.84 (s, 3H), 1.36 (d,  $J = 6.6$  Hz, 6H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  = 165.92, 159.48, 132.22, 129.23, 121.85, 119.05, 114.04, 68.41, 55.37, 21.89. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>11</sub>H<sub>14</sub>O<sub>3</sub> 195.1016; Found 195.1013.

**Tert-butyl 4-methoxybenzoate (4n):**<sup>5d</sup> Colorless liquid (26 mg, 25% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 7.93 (d,  $J = 9.0$  Hz, 2H), 6.89 (d,  $J = 9.0$  Hz, 2H), 3.84 (s, 3H), 1.57 (s, 9H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 165.57, 162.91, 131.33, 124.49, 113.34, 80.47, 55.36, 28.23. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>12</sub>H<sub>16</sub>O<sub>3</sub> 209.1172; Found 209.1170.

**Tert-butyl 2-bromobenzoate(4o):**<sup>7i</sup> Colorless liquid (31 mg, 24% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 7.67 (dd,  $J = 7.8, 1.8$  Hz, 1H), 7.61 (dd,  $J = 7.8, 1.2$  Hz, 1H), 7.34–7.31 (m, 1H), 7.27 (dd,  $J = 7.2, 1.8$  Hz, 1H), 1.60 (s, 9H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 165.68, 134.32, 133.99, 131.79, 130.76, 127.04, 120.95, 82.55, 28.13. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>11</sub>H<sub>13</sub>BrO<sub>2</sub> 257.0172; Found 257.0174.

**Tert-butyl 3-nitrobenzoate (4p):**<sup>7j</sup> Colorless liquid (23 mg, 21% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 8.78 (t,  $J = 2.4$  Hz, 1H), 8.38–8.36 (m, 1H), 8.31 (dt,  $J = 7.2, 1.2$  Hz, 1H), 7.61 (t,  $J = 8.4$  Hz, 1H), 1.62 (s, 9H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 163.48, 135.11, 133.75, 129.33, 126.87, 124.39, 82.60, 28.09. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>11</sub>H<sub>13</sub>NO<sub>4</sub> 224.0917; Found 224.0914.

**Diisopropyl isophthalate (4q):**<sup>4</sup> Colorless liquid (64 mg, 51% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 8.64 (t,  $J = 1.8$  Hz, 1H), 8.18 (dd,  $J = 7.8, 1.8$  Hz, 2H), 7.48 (t,  $J = 7.8$  Hz, 1H), 5.28–5.21 (m, 2H), 1.36 (d,  $J = 6.6$  Hz, 12H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 165.29, 133.47, 131.22, 130.49, 128.32, 68.78, 21.86. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>14</sub>H<sub>18</sub>O<sub>4</sub> 251.1278; Found 251.1275.

**Diisopropyl malonate (4r):**<sup>7k</sup> Colorless liquid (81 mg, 86% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 5.03–4.97 (m, 2H), 3.24 (s, 2H), 1.20 (d,  $J = 6.6$  Hz, 12H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 166.12, 68.88, 42.23, 21.55. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>9</sub>H<sub>16</sub>O<sub>4</sub> 189.1121; Found 189.1123.

**Ethyl 4-phenylbutanoate (4s):**<sup>7l</sup> Colorless liquid (83 mg, 86% yield). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 7.29 (t,  $J = 7.2$  Hz, 2H), 7.20 (t,  $J = 7.8$  Hz, 3H), 4.13 (q,  $J = 7.2$  Hz, 2H), 2.66 (t,  $J = 7.8$  Hz, 2H), 2.33 (t,  $J = 7.8$  Hz, 2H), 1.97 (p,  $J = 7.8$  Hz, 2H), 1.26 (t,  $J = 7.2$  Hz, 4H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 173.46, 141.42, 128.47, 128.35, 125.94, 60.23, 35.14, 33.67, 26.54, 14.24. HRMS (ESI)  $m/z$ : ([M+H]<sup>+</sup>) Calcd for C<sub>12</sub>H<sub>16</sub>O<sub>2</sub> 193.1223; Found 193.1226.

**Isopropyl 2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoate (4t):**<sup>11</sup> White solid (144 mg, 80% yield), mp: 78–80 °C (lit 80–81 °C).<sup>1d</sup> <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  ppm; 7.71 (d,  $J = 8.4$  Hz, 2H), 7.68 (d,  $J = 8.4$  Hz, 2H), 7.43 (d,  $J = 8.4$  Hz, 2H), 6.85



(d,  $J = 9.0$  Hz, 2H), 5.10–5.03 (m, 1H), 1.64 (s, 6H), 1.19 (d,  $J = 6.6$  Hz, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  ppm; 194.16, 173.03, 159.70, 138.29, 136.40, 131.89, 131.11, 130.19, 128.49, 117.23, 79.39, 69.29, 25.34, 21.49. HRMS (ESI)  $m/z$ : ( $[\text{M}+\text{H}]^+$ ) Calcd for  $\text{C}_{20}\text{H}_{21}\text{ClO}_4$  361.1201; Found 361.1200.

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