

# Supplementary Information

## Solvent-Dependent Regioselective Oxidation of *trans*-Chalcones using Aqueous Hydrogen Peroxide

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Table S1. The NMR data of compounds 2a-2l

	( <i>E</i> )-Cinnamic acid ( <b>2a</b> ): mp 132-133 °C (132-134 °C); <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.58 (d, 1H, <i>J</i> 16 Hz), 7.42-7.69 (m, 5H), 6.53 (d, 1H, <i>J</i> 16 Hz); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 167.7, 144.0, 134.3, 130.3, 128.9, 128.2, 119.3.
	( <i>E</i> )-3-(2,4-Dichlorophenyl)acrylic acid ( <b>2b</b> ): mp 232-233 °C; <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.95 (d, 1H, <i>J</i> 8.5 Hz), 7.81 (d, 1H, <i>J</i> 16 Hz), 7.70 (d, 1H, <i>J</i> 5.8 Hz), 7.47 (dd, 1H, <i>J</i> 8.5 Hz), 6.64 (d, 1H, <i>J</i> 16 Hz); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ): δ 166.9, 137.4, 135.2, 134.3, 130.9, 129.4, 129.3, 127.9, 122.9; HRMS (ESI) calcd for C <sub>9</sub> H <sub>7</sub> Cl <sub>2</sub> O <sub>2</sub> ([M + H] <sup>+</sup> ) 218.0561, found 218.0558.
	( <i>E</i> )-3-(4-Fluorophenyl)acrylic acid ( <b>2c</b> ): mp 208-209 °C (209 °C); <sup>2</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.71 (m, 2H), 7.48 (d, 1H, <i>J</i> 16 Hz), 7.21 (m, 2H), 6.45 (d, 1H, <i>J</i> 16 Hz); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 171.6, 164.2, 145.8, 130.3, 130.2, 117.1, 116.2.
	( <i>E</i> )-3-(2-Nitrophenyl)acrylic acid ( <b>2d</b> ): mp 244-245 °C (243-245 °C); <sup>3</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 8.04 (dd, 1H, <i>J</i> 8.1 Hz, 1.2 Hz), 7.91 (dd, 1H, <i>J</i> 7.6 Hz, 1.1 Hz), 7.84 (d, 1H, <i>J</i> 15.8 Hz), 7.75 (t, 1H, <i>J</i> 7.4 Hz), 7.65 (t, 1H, <i>J</i> 8.1 Hz), 6.54 (d, 1H, <i>J</i> 15.8 Hz); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 157.7, 140.6, 131.9, 127.4, 124.5, 123.1, 123.0, 118.9, 118.2.
	( <i>E</i> )-3-(3-nitrophenyl)acrylic acid ( <b>2e</b> ): mp 204-205 °C (202-204 °C); <sup>4</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 8.50 (s, 1H), 8.20 (dd, 1H, <i>J</i> 8.2, 1.7 Hz), 8.16 (d, 1H, <i>J</i> 8.0 Hz), 7.67 (m, 2H), 6.74 (d, 1H, <i>J</i> 15.8 Hz); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 158.0, 140.5, 134.3, 129.4, 127.6, 124.0, 118.6, 117.1, 116.7.
	( <i>E</i> )-3-( <i>p</i> -tolyl)acrylic acid ( <b>2f</b> ): mp 198-199 °C (196-198 °C); <sup>4</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.56 (m, 3H), 7.23 (d, 2H, <i>J</i> 7.9 Hz), 6.48 (d, 1H, <i>J</i> 16 Hz), 2.33 (s, 3H); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 167.5, 143.7, 140.0, 131.5, 129.4, 128.1, 118.1, 21.0.
	( <i>E</i> )-3-( <i>m</i> -tolyl)acrylic acid ( <b>2g</b> ): mp 117-118 °C (116-118 °C); <sup>3</sup> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) δ 7.75 (d, 1H, <i>J</i> 16 Hz), 7.29 (m, 4H), 6.43 (d, 1H, <i>J</i> 16 Hz), 2.35 (s, 3H); <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) δ 173.1, 147.6, 138.7, 134.3, 132.0, 129.1, 129.0, 125.8, 117.5, 21.6.

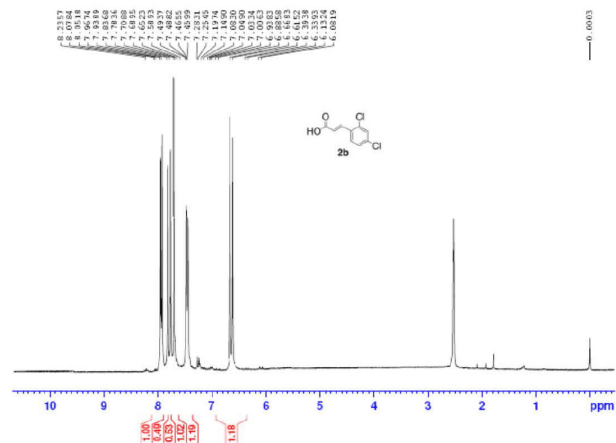
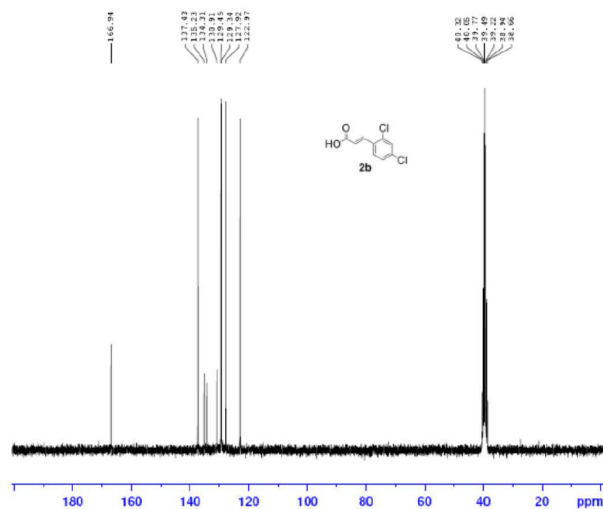
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Table S1. continuation

	( <i>E</i> )-3-(4-methoxyphenyl)acrylic acid ( <b>2h</b> ): mp 173-174 °C (173-175 °C); <sup>4</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.61 (d, 2H, <i>J</i> 8.7 Hz), 7.56 (d, 1H, <i>J</i> 16 Hz), 6.97 (d, 2H, <i>J</i> 8.7 Hz), 6.38 (d, 2H, <i>J</i> 16 Hz), 3.76 (s, 3H); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 167.9, 161.0, 143.6, 130.1, 126.9, 116.5, 114.5, 55.2.
	( <i>E</i> )-3-(2-methoxyphenyl)acrylic acid ( <b>2i</b> ): mp 184-185 °C (182-184 °C); <sup>3</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 12.27 (s, 1H), 7.81 (d, 1H, <i>J</i> 16 Hz), 7.64 (dd, 1H, <i>J</i> 7.8, 7.6 Hz), 7.38-7.42 (m, 1H), 7.08 (d, 1H, <i>J</i> 8.1 Hz), 6.94 (t, 1H, <i>J</i> 7.4 Hz), 6.49 (d, 1H, <i>J</i> 16 Hz), 3.85 (s, 3H); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 167.9, 157.8, 138.7, 132.0, 128.6, 122.5, 120.7, 119.3, 111.7, 55.6.
	( <i>E</i> )-3-(3,4-dimethoxyphenyl)acrylic acid ( <b>2j</b> ): mp 180-181 °C (179-181 °C); <sup>5</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.50 (d, 1H, <i>J</i> 16 Hz), 7.29 (s, 1H), 7.19 (d, 1H, <i>J</i> 8.0 Hz), 6.95 (d, 1H, <i>J</i> 8.0 Hz), 6.41 (d, 1H, <i>J</i> 16 Hz), 3.78 (s, 3H), 3.77 (s, 3H); <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) δ 172.3, 151.9, 149.6, 147.0, 127.4, 123.1, 115.1, 111.4, 110.6, 56.1.
	( <i>E</i> )-3-(4-(dimethylamino)phenyl)acrylic acid ( <b>2k</b> ): mp 225-226 °C (227-230 °C); <sup>6</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.47 (d, 2H, <i>J</i> 9.1 Hz), 7.43 (d, 1H, <i>J</i> 16 Hz), 6.64 (d, 2H, <i>J</i> 9.1 Hz), 6.15 (d, 1H, <i>J</i> 15.9 Hz), 2.97 (s, 6H); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 168.0, 151.5, 144.3, 129.4, 121.6, 112.9, 111.7, 39.6.
	( <i>E</i> )-3-(benzo[d][1,3]dioxol-5-yl)acrylic acid ( <b>2l</b> ): mp 242-243 °C (243-244 °C); <sup>7</sup> <sup>1</sup> H NMR (300 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 7.47 (d, 1H, <i>J</i> 16 Hz), 7.34 (d, 1H, <i>J</i> 1.7 Hz), 7.13 (d, 1H, <i>J</i> 8.2, 1.7 Hz), 6.92 (d, 1H, <i>J</i> 8.2 Hz), 6.38 (d, 1H, <i>J</i> 16 Hz), 6.07 (s, 2H); <sup>13</sup> C NMR (75 MHz, DMSO- <i>d</i> <sub>6</sub> ) δ 167.8, 149.1, 148.0, 143.7, 128.9, 124.6, 117.0, 108.3, 106.7, 101.5.

## References

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Figure S1. <sup>1</sup>H NMR spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of compound **2b**.Figure S2. <sup>13</sup>C NMR spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of compound **2b**.