Enzyme catalytic promiscuity: Lipase catalyzed synthesis of substituted 2H-chromenes by three-component reaction

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Supporting Information

1 Materials

Porcine pancreas lipase (PPL), *Candida antarctica* lipase B (CALB), *Pseudomonas sp.* lipase (PSL), *C. rugosa* lipase (CRL), Bovine serum albumin (BSA) and salicylaldehyde used in this study were purchased from Sigma (Beijing, China). These enzymes were used after lyophilization for enzymatic reaction without further purification. All the chemical reagents were purchased from Shanghai Chemical Reagent Company (Shanghai, China). Commercially available reagents and solvents were used without further purification. NMR spectra were recorded on an Inova 500 (1H, 500 MHz) spectrometer.

2 ^{1}H-NMR data of compounds 4a-4g

4a: ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.90 (s, 3H), 2.44 (s, 3H), 3.24 (s, 3H), 6.95 (m, 2H), 7.24 (d, *J* = 7.5Hz, 1H), 7.31 (t, *J* = 8.0Hz, 1H), 7.52 (s, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.5, 153.4, 136.9, 132.4, 132.2, 128.1, 121.7, 118.6, 116.3, 101.8, 50.0, 27.3, 24.9.

4b: ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.1 (t, J = 7.0 Hz, 3H), 1.89 (s, 3H), 2.45 (s, 3H), 3.48 (m, 2H), 6.94 (m, 2H), 7.23 (d, J = 7.5 Hz, 1H), 7.31 (t, J = 7.5 Hz, 1H), 7.51 (s, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.4,153.4,135.3, 132.5, 132.7, 129.2, 121.6, 119.0, 116.6, 101.2, 58.8, 27.5, 26.2, 15.1.

4c: ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.81 (t, J = 7.5 Hz, 3H), 1.20 (m, 2H), 1.47 (t, J = 7.5 Hz, 2H), 1.91 (s, 3H), 2.46 (s, 3H), 3.47 (m, 2H), 6.94 (m, 2H), 7.24 (d, J = 7.5 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.58 (s, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.7, 153.1, 135.5, 133.5, 132.1, 128.2, 121.6, 118.8, 116.4, 102.1, 63.2, 30.6, 27.4, 25.3, 18.9, 13.6.

4d: ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.81 (t, J = 7.0 Hz, 3H), 1.20 (m, 4H), 1.47 (t, J = 7.0 Hz, 2H), 1.91 (s, 3H), 2.46 (s, 3H), 3.40 (dd, J = 7.0 Hz, 15.5 Hz, 1H), 3.480 (dd, J = 6.5 Hz, 15.5 Hz, 1H), 6.95 (m, 2H), 7.24(d, J = 7.5 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.49 (s, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.9, 153.8, 135.9, 132.3, 131.5, 128.5, 120.2, 118.0, 115.3, 101.1, 64.1, 30.4, 28.1, 27.6, 23.6, 22.7, 14.1.

4e: ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.98 (d, J = 6.0 Hz, 3H), 1.13 (d, J = 6.0 Hz, 3H), 1.96 (s, 3H), 2.46 (s, 3H), 4.07 (t, J = 6.0 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.97 (t, J

= 7.5 Hz, 1H), 7.24 (d, J = 7.5 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.49 (s, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.5, 153.5, 136.9, 132.3, 131.5, 128.4, 121.2, 119.2, 116.3, 102.3, 63.8, 27.8, 24.6, 22.8, 22.8.

4f: ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.01 (s, 3H), 2.45 (s, 3H), 4.52 (d, J = 11.5Hz, 1H), 4.57 (d, J = 11.5 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.99 (t, J = 7.5 Hz, 1H), 7.21 (m, 5H), 7.33 (t, J = 7.5 Hz, 1H), 7.36 (d, J = 4.5 Hz, 1H), 7.53 (s, 1H) ; ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.5, 153.4, 141.8, 136.5, 132.9, 131.6, 129.1, 128.9, 128.6, 128.1, 127.8, 127.5, 120.2, 117.0, 116.3, 104.7, 62.6, 27.7, 24.4.

4g: ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.91 (s, 3H), 2.39 (s, 3H), 2.78 (m, 2H), 3.64 (dd, J = 8.5 Hz, J = 15.5 Hz, 1H), 3.70 (dd, J = 9.0 Hz, J = 15.5 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.95 (t, J = 7.5 Hz, 1H), 7.08 (d, J = 7.5 Hz, 2H), 7.13 (t, J = 7.5 Hz, 1H), 7.20 (m, 3H), 7.29 (t, J = 7.5 Hz, 1H), 7.47 (s, 1H); ^{13}C NMR (500 MHz, $CDCl_3$) δ 195.7, 153.8, 141.6, 136.2, 132.8, 131.5, 129.6, 128.4, 128.2, 127.9, 127.6, 127.1, 120.9, 117.3, 116.3, 105.1, 63.8, 35.7, 27.9, 24.8.