



SUPPLEMENTARY MATERIAL TO

Synthesis of 2-azetidinones substituted coumarin derivatives

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PHYSICAL, ANALYTIC AND SPECTRAL DATA FOR THE SYNTHESIZED
COMPOUNDS

Compound 1. White crystals; yield: 92 %; m.p. 170–172 °C; Anal. Calcd. for $C_{14}H_{10}O_2$; C, 79.98; H, 4.79 %. Found: C, 79.96; H, 4.83 %; IR (KBr, cm^{-1}): 3065 (arom-CH), 1711 (C=O); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.5 (1H, *d*, $J = 1.2$ Hz, CH_3), 6.4 (1H, *q*, $J = 1.2$ Hz, C_3 -H), 7.6–8.6 (6H, *m*, Ar-H); ^{13}C -NMR (100.622 MHz, $CDCl_3$, δ / ppm): 22.1, 112.6, 120.9, 121.5, 123.0, 124.8, 126.2, 126.9, 127.1, 128.6, 133.8, 153.1, 153.6, 161.3; mass (m/z): 210 [M^+].

Compound 2. White crystals; yield: 78 %; m.p. 198–200 °C; Anal. Calcd. for $C_{14}H_8O_3$; C, 75.00; H, 3.60 %; Found: C, 75.05; H, 3.61 %; IR (KBr, cm^{-1}): 3057 (arom-CH), 1727 (C=O), 1706 (C=O); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 7.0 (1H, *s*, C_3 -H), 7.6–8.6 (6H, *m*, Ar-H), 10.23 (1H, *s*, CHO); ^{13}C -NMR (100.622 MHz, $CDCl_3$, δ / ppm): 121.7, 122.3, 123.1, 124.4, 125.9, 126.2, 126.9, 127.1, 128.6, 133.8, 153.6, 161.3, 162.3, 185.8; mass (m/z): 224 [M^+].

4-[(3-Nitrophenyl)imino]methyl}-2H-benzo[h]chromen-2-one (3a). Yellow crystals; yield 84 %; m.p. 265 °C; Anal. Calcd. for $C_{20}H_{12}N_2O_4$; C, 69.76; H, 3.51; N, 8.14 %. Found: C, 69.80; H, 3.56; N, 8.19 %; IR (KBr, cm^{-1}): 3078 (arom-CH), 1708 (C=O), 1634 (C=N); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 7.0 (1H, *s*, C_3 -H), 7.6–8.6 (10H, *m*, Ar-H), 8.8 (1H, *s*, CH=N); ^{13}C -NMR (100.622 MHz, $CDCl_3$, δ / ppm): 112.2, 117.8, 118.3, 120.9, 121.5, 123.0, 124.3, 126.2, 126.9, 127.1, 128.8, 129.3, 131.5, 133.6, 146.5, 149.1, 149.3, 153.6, 161.3, 163.3; mass (m/z): 344 [M^+].

4-[(4-Methoxyphenyl)imino]methyl}-2H-benzo[h]chromen-2-one (3b). Yellow crystals; yield: 80 %; m.p. 182 °C; Anal. Calcd. for $C_{21}H_{15}NO_3$; C, 76.58; H, 4.59; N, 4.25 %. Found: C, 76.62; H, 4.62; N, 4.29 %; IR (KBr, cm^{-1}): 3080 (arom-CH), 1706 (C=O), 1628 (C=N); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 3.9 (3H, *s*, OCH_3), 6.9 (1H, *s*, C_3 -H), 7.0–8.7 (10H, *m*, Ar-H), 8.79 (1H, *s*, CH=N);

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^{13}C -NMR (100.622 MHz, CDCl_3 , δ / ppm): 54.9, 112.2, 115.9, 120.9, 121.5, 123.0, 123.3, 124.3, 126.2, 126.9, 127.7, 128.8, 133.6, 140.6, 146.5, 153.6, 160.0, 161.3, 163.3; mass (m/z): 329 [M^+].

4-[(4-Chlorophenyl)imino]methyl-2H-benzo[h]chromen-2-one (**3c**). Brown crystals; yield: 82 %; m.p. 243 °C; Anal. Calcd. for $\text{C}_{20}\text{H}_{12}\text{ClNO}_2$: C, 71.97; H, 3.62; N, 4.20 %. Found: C, 71.96; H, 3.64; N, 4.25 %; IR (KBr, cm^{-1}): 3079 (arom-CH), 1707 (C=O) 1633 (C=N); ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 6.9 (1H, s, $\text{C}_3\text{-H}$), 7.25–8.60 (10H, m, Ar-H), 8.75 (1H, s, CH=N); ^{13}C -NMR (100.622 MHz, CDCl_3 , δ / ppm): 112.2, 120.9, 121.5, 123.0, 124.1, 124.3, 126.2, 126.9, 127.7, 128.8, 129.6, 133.6, 145.2, 146.5, 147.8, 153.6, 161.3, 163.3; mass (m/z): 333 [M^+].

4-[(4-Fluorophenyl)imino]methyl-2H-benzo[h]chromen-2-one (**3d**). Yellow crystals; yield: 81 %; m.p. 230 °C; Anal. Calcd. for $\text{C}_{20}\text{H}_{12}\text{FNO}_2$: C, 75.70; H, 3.81; N, 4.41 %. Found: C, 75.73; H, 3.86; N, 4.43 %; IR (KBr, cm^{-1}): 3082 (arom-CH), 1704 (C=O), 1622 (C=N); ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 6.70 (1H, s, $\text{C}_3\text{-H}$), 6.90–8.76 (10H, m, Ar-H), 8.92 (1H, s, CH=N); ^{13}C -NMR (100.622 MHz, CDCl_3 , δ / ppm): 112.2, 115.2, 120.9, 121.5, 123.0, 124.1, 124.3, 126.2, 126.9, 127.7, 128.8, 133.6, 145.1, 146.5, 153.6, 160.9, 162.0, 163.3; mass (m/z): 317 [M^+].

1-(4-Fluorophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)-3-phenylazetid-2-one (**4a**). White crystals; yield: 58 %; m.p. 241–243 °C; Anal. Calcd. for $\text{C}_{28}\text{H}_{18}\text{FNO}_3$: C, 77.23; H, 4.17; N, 3.22 %. Found: C, 77.26; H, 4.15; N, 3.14 %; IR (KBr, cm^{-1}): 3055, 1758, 1726, 1606, 1559, 1509; ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 4.3 (1H, d, $J = 2.8$ Hz, $\text{C}_3\text{-H}$), 5.3 (1H, d, $J = 2.8$ Hz, $\text{C}_4\text{-H}$), 6.4 (1H, s, CH=C), 7.1–7.7 (15H, m, Ar-H); ^{13}C -NMR (100.622 MHz, CDCl_3 , δ / ppm): 59.9, 64.4, 110.9, 112.0, 116.3, 116.5, 118.5, 118.6, 119.1, 122.6, 123.1, 124.7, 127.7, 127.9, 129.3, 129.5, 132.8, 133.3, 134.8, 151.3, 151.5, 158.3, 160.8, 163.9; mass (m/z): 435 [M^+].

1-(4-Chlorophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)-3-phenylazetid-2-one (**4b**). White crystals; yield: 52 %; m.p. 236–238 °C; Anal. Calcd. for $\text{C}_{28}\text{H}_{18}\text{ClNO}_3$: C, 74.42; H, 4.01; N, 3.10 %. Found: C, 74.3; H, 4.11; N, 3.19 %; IR (KBr, cm^{-1}): 3066, 1760, 1722, 1594, 1561, 1494; ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 4.3 (1H, d, $J = 2.8$ Hz, $\text{C}_3\text{-H}$), 5.8 (1H, d, $J = 2.8$ Hz, $\text{C}_4\text{-H}$), 6.3 (1H, s, CH=C), 7.1–8.6 (15H, m, Ar-H); ^{13}C -NMR (100.622 MHz, CDCl_3 , δ / ppm): 59.9, 64.4, 112.5, 122.1, 122.7, 123.6, 124.0, 125.8, 127.0, 127.6, 127.8, 128.5, 128.7, 130.1, 130.3, 130.7, 130.9, 135.1, 137.3, 140.6, 155.3, 158.3, 160.8, 163.9; mass (m/z): 451 [M^+].

1-(4-Methoxyphenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)-3-phenylazetid-2-one (**4c**). White crystals; yield: 49 %; m.p. 247–249 °C; Anal. Calcd. for $\text{C}_{29}\text{H}_{21}\text{NO}_4$: C, 77.84; H, 4.73; N, 3.13 %. Found: C, 77.70; H, 4.58; N, 3.04 %; IR (KBr, cm^{-1}): 3066, 1749, 1720, 1607, 1560, 1512; ^1H -NMR (400 MHz,

CDCl₃, δ / ppm): 3.7 (3H, s, OCH₃), 5.2 (1H, d, J = 6.0 Hz, C₃-H), 5.8 (1H, d, J = 6.0 Hz, C₄-H), 6.3 (1H, s, CH=C), 6.9–7.7 (15H, m, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 43.3, 59.9, 64.4, 112.5, 115.8, 122.2, 122.7, 123.0, 123.6, 125.9, 127.1, 127.6, 127.8, 128.6, 128.7, 130.3, 130.7, 135.0, 135.1, 137.4, 153.4, 154.8, 157.0, 160.8, 163.9; mass (m/z): 447 [M⁺].

1-(3-Nitrophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)-3-phenylazetidin-2-one (4d). White crystals; yield: 51 %; m.p. 201–203 °C; Anal. Calcd. for C₂₈H₁₈N₂O₅: C, 72.72; H, 3.92; N, 6.06 %. Found: C, 72.56; H, 3.79; N, 5.89 %; IR (KBr, cm⁻¹): 3050, 1773, 1726, 1612, 1560, 1452; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 4.4 (1H, d, J = 2.8 Hz, C₃-H), 5.4 (1H, d, J = 2.8 Hz, C₄-H), 6.4 (1H, s, CH=C), 7.0–8.6 (15H, m, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 59.9, 64.5, 116.5, 112.5, 117.8, 122.1, 122.7, 123.8, 124.0, 125.9, 127.1, 127.7, 127.9, 128.5, 128.8, 130.5, 130.7, 130.9, 135.2, 137.4, 149.6, 150.6, 152.3, 154.8, 160.8, 163.9; mass (m/z): 462 [M⁺].

3-(4-Chlorophenyl)-1-(4-fluorophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)-azetidin-2-one (4e). White crystals; yield: 44 %; m.p. 212–214 °C; Anal. Calcd. for C₂₈H₁₇ClFNO₃: C, 71.57; H, 3.65; N, 2.98 %. Found: C, 71.35; H, 3.72; N, 2.85 %; IR (KBr, cm⁻¹): 3071, 1768, 1730, 1607, 1559, 1514; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 4.3 (1H, d, J = 2.8 Hz, C₃-H), 5.3 (1H, d, J = 2.8 Hz, C₄-H), 6.4 (1H, s, CH=C), 7.1–8.6 (14H, m, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 59.9, 64.4, 112.6, 116.9, 122.1, 122.7, 123.6, 124.2, 125.9, 127.0, 127.7, 127.9, 128.5, 130.6, 132.3, 134.2, 135.1, 135.5, 138.3, 151.3, 154.3, 158.3, 160.8, 163.9; mass (m/z): 469 [M⁺].

1,3-Bis(4-chlorophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetidin-2-one (4f). White crystals; yield: 48 %; m.p. 293–295 °C; Anal. Calcd. for C₂₈H₁₇Cl₂NO₃: C, 69.15; H, 3.52; N, 2.88 %. Found: C, 69.26; H, 3.61; N, 2.95 %; IR (KBr, cm⁻¹): 3085, 1754, 1719, 1598, 1559, 1492; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 4.3 (1H, d, J = 2.8 Hz, C₃-H), 5.3 (1H, d, J = 2.8 Hz, C₄-H), 6.4 (1H, s, CH=C), 7.1–7.8 (14H, m, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 59.9, 64.4, 112.5, 122.2, 122.7, 123.6, 124.0, 125.9, 127.0, 127.7, 127.9, 128.7, 130.2, 130.4, 130.9, 132.2, 134.2, 135.2, 135.5, 140.8, 154.3, 158.4, 160.8, 163.9; mass (m/z): 486 [M⁺].

3-(4-Chlorophenyl)-1-(4-methoxyphenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetidin-2-one (4g). White crystals; yield: 53 %; m.p. 248–250 °C; Anal. Calcd. for C₂₉H₂₀ClNO₄: C, 72.27; H, 4.18; N, 2.91 %. Found: C, 72.39; H, 4.25; N, 3.04 %; IR (KBr, cm⁻¹): 3075, 1759, 1713, 1611, 1561, 1498; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.8 (3H, s, OCH₃), 5.1 (1H, d, J = 6.0 Hz, C₃-H), 5.8 (1H, d, J = 6.0 Hz, C₄-H), 6.3 (1H, s, CH=C), 6.9–8.4 (14H, m, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 43.3, 59.9, 64.4, 112.5, 115.5, 122.3, 122.9, 123.8, 125.9, 127.0, 127.8, 127.9, 128.5, 130.6, 134.2, 134.3, 135.0, 135.1, 135.5, 141.0, 154.3, 155.8, 157.3, 160.8, 163.9; mass (m/z): 481 [M⁺].

3-(4-Chlorophenyl)-1-(3-nitrophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetid-2-one (4h). White crystals; yield: 42 %; m.p. 205–207 °C; Anal. Calcd. for C₂₈H₁₇ClN₂O₅: C, 67.68; H, 3.45; N, 5.64 %. Found: C, 67.72; H, 3.34; N, 5.74 %; IR (KBr, cm⁻¹): 3072, 1770, 1732, 1608, 1535, 1505; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 4.4 (1H, *d*, *J* = 2.8 Hz, C₃-H), 5.4 (1H, *d*, *J* = 2.8 Hz, C₄-H), 6.4 (1H, *s*, CH=C), 7.1–8.1 (14H, *m*, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 59.9, 64.4, 112.5, 116.5, 116.8, 121.3, 122.7, 123.7, 125.8, 127.2, 127.7, 127.9, 128.6, 128.8, 130.6, 131.0, 132.5, 133.3, 135.1, 135.7, 143.6, 149.6, 154.4, 154.9, 160.8, 163.9; mass (*m/z*): 496 [M⁺].

1-(4-Fluorophenyl)-3-(4-methoxyphenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetid-2-one (4i). White crystals; yield: 56 %; m.p. 249–250 °C; Anal. Calcd. for C₂₉H₂₀FNO₄: C, 74.83; H, 4.33; N, 3.01 %. Found: C, 74.72; H, 4.25; N, 2.88 %; IR (KBr, cm⁻¹): 3073, 1762, 1730, 1610, 1560, 1506; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.6 (3H, *s*, OCH₃), 5.2 (1H, *d*, *J* = 6.0 Hz, C₃-H), 5.8 (1H, *d*, *J* = 6.0 Hz, C₄-H), 6.3 (1H, *s*, CH=C), 6.5–8.4 (14H, *m*, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 55.2, 57.4, 60.0, 112.8, 113.1, 113.7, 116.4, 116.8, 119.5, 121.4, 122.0, 122.4, 123.5, 124.3, 127.9, 129.4, 131.1, 134.0, 134.7, 150.2, 151.1, 157.9, 159.0, 159.4, 165.7; mass (*m/z*): 465 [M⁺].

1-(4-Chlorophenyl)-3-(4-methoxyphenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetid-2-one (4j). White crystals; yield: 53 %; m.p. 208–210 °C; Anal. Calcd. for C₂₉H₂₀ClNO₄: C, 72.27; H, 4.18; N, 2.91 %. Found: C, 72.32; H, 4.30; N, 2.82 %; IR (KBr, cm⁻¹): 3075, 1745, 1711, 1612, 1560, 1508; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.6 (3H, *s*, OCH₃), 5.2 (1H, *d*, *J* = 6.0 Hz, C₃-H), 5.8 (1H, *d*, *J* = 6.0 Hz, C₄-H), 6.3 (1H, *s*, CH=C), 6.5–7.8 (14H, *m*, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 55.2, 57.4, 60.0, 110.5, 113.8, 122.2, 122.7, 123.6, 124.0, 126.0, 127.0, 127.6, 127.8, 128.5, 129.8, 130.1, 131.0, 131.7, 135.2, 141.0, 154.4, 155.9, 160.7, 161.8, 165.7; mass (*m/z*): 481 [M⁺].

1,3-Bis(4-methoxyphenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetid-2-one (4k). White crystals; yield: 57 %; m.p. 254–256 °C; Anal. Calcd. for C₃₀H₂₃NO₅: C, 75.46; H, 4.85; N, 2.93 %. Found: C, 75.32; H, 4.92; N, 2.84 %; IR (KBr, cm⁻¹): 3050, 1746, 1714, 1611, 1560, 1508; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.6 (3H, *s*, OCH₃), 3.8 (3H, *s*, OCH₃), 5.1 (1H, *d*, *J* = 6.0 Hz, C₃-H), 5.8 (1H, *d*, *J* = 6.0 Hz, C₄-H), 6.3 (1H, *s*, CH=C), 6.5–8.4 (14H, *m*, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 55.1, 55.2, 57.4, 60.0, 112.5, 113.5, 115.8, 122.3, 122.7, 123.5, 123.6, 125.8, 127.0, 127.6, 128.0, 128.6, 130.0, 131.7, 133.2, 135.0, 135.2, 154.4, 155.8, 160.6, 161.8, 165.7; mass (*m/z*): 477 [M⁺].

3-(4-Methoxyphenyl)-1-(3-nitrophenyl)-4-(2-oxo-2H-benzo[h]chromen-4-yl)azetid-2-one (4l). White crystals; yield: 42 %; m.p. 257–258 °C; Anal. Calcd. for C₂₉H₂₀N₂O₆: C, 70.73; H, 4.09; N, 5.69 %. Found: C, 70.79; H, 4.18; N, 5.54 %; IR (KBr, cm⁻¹): 3053, 1763, 1723, 1612, 1561, 1515; ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.8 (3H, *s*, OCH₃), 4.3 (1H, *d*, *J* = 2.8 Hz, C₃-H), 5.4

(1H, *d*, *J* = 2.8 Hz, C₄-H), 6.3 (1H, *s*, CH=C), 6.9–8.1 (14H, *m*, Ar-H); ¹³C-NMR (100.622 MHz, CDCl₃, δ / ppm): 55.2, 57.4, 60.0, 110.6, 113.6, 114.3, 115.6, 122.2, 122.8, 123.7, 126.0, 127.0, 127.8, 128.0, 128.6, 128.8, 130.0, 131.0, 131.8, 135.2, 143.8, 149.8, 154.4, 155.9, 160.6, 161.8, 165.7; mass (*m/z*): 492 [M⁺].