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SUPPLEMENTARY MATERIAL TO

One-pot synthesis of carbazole based 3-hydroxy-4*H*-chromen-4--ones by a modified Algar–Flynn–Oyamada reaction and their antimicrobial activity

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PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR COMPOUNDS **3a**–**i**

*2-(9-Ethyl-9*H*-carbazol-3-yl)-3-hydroxy-4*H*-chromen-4-one* ***(3a)***. Anal. Calcd. for $C_{23}H_{17}NO_3$: C, 77.73; H, 4.82; N, 3.94 %. Found: C, 77.78; H, 4.86; N, 3.97 %; IR (KBr, cm^{-1}): 3446 (–OH), 1632 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.48 (3H, *t*, *J* = 7.27 Hz, CH_3), 4.42 (2H, *q*, *J* = 7.27 Hz, N–CH_2), 7.08 (1H, *brs*, OH), 7.29–7.33 (1H, *m*, Ar-H), 7.41–7.54 (4H, *m*, Ar-H), 7.66–7.74 (2H, *m*, Ar-H), 8.24–8.29 (2H, *m*, Ar-H), 8.42 (1H, *dd*, *J* = 1.7, 8.7 Hz, Ar-H), 9.03 (1H, *d*, *J* = 1.5 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 37.7, 108.4, 108.8, 114.6, 118.2, 119.6, 120.7, 120.8, 121.7, 123.1, 124.3, 125.3, 125.5, 126.2, 133.1, 137.6, 140.5, 140.8, 146.7, 155.3, 173.0; ESI-MS (*m*/*z*): 356 ($[M+H]^+$, 100 %).

*2-(9-Ethyl-9*H*-carbazol-3-yl)-6-fluoro-3-hydroxy-4*H*-chromen-4-one* ***(3b)***. Anal. Calcd. for $C_{23}H_{16}FNO_3$: C, 73.99; H, 4.32; N, 3.75 %. Found: C, 74.05; H, 4.36; N, 3.79 %; IR (KBr, cm^{-1}): 3441 (–OH), 1631 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.49 (3H, *t*, *J* = 7.25 Hz, CH_3), 4.43 (2H, *q*, *J* = 7.20 Hz, N–CH_2), 7.00 (1H, *brs*, OH), 7.30–7.33 (1H, *m*, Ar-H), 7.42–7.45 (2H, *m*, Ar-H), 7.52–7.55 (2H, *m*, Ar-H), 7.90 (1H, *dd*, *J* = 4.0, 9.2 Hz, Ar-H), 8.22 (2H, *d*, *J* = 7.7 Hz, Ar-H), 8.41 (1H, *dd*, *J* = 1.7, 8.7 Hz, Ar-H), 9.02 (1H, *d*, *J* = 1.5 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 37.8, 108.5, 108.9, 109.7, 119.7, 120.2, 120.4, 120.8, 121.7, 121.8, 123.1, 123.2, 125.5, 126.3, 137.3, 140.5, 147.2, 151.6, 157.8, 160.2, 172.3; ESI-MS (*m*/*z*): 374 ($[M+H]^+$, 100 %).

*6-Chloro-2-(9-ethyl-9*H*-carbazol-3-yl)-3-hydroxy-4*H*-chromen-4-one* ***(3c)***. Anal. Calcd. for $C_{23}H_{16}ClNO_3$: C, 70.86; H, 4.14; N, 3.59 %. Found: C, 70.91; H, 4.19; N, 3.63 %; IR (KBr, cm^{-1}): 3442 (–OH), 1630 (C=O); ^{1}H-NMR (400

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MHz, $CDCl_3$, δ / ppm): 1.48 (3H, *t*, *J* = 7.20 Hz, CH_3), 4.42 (2H, *q*, *J* = 7.02 Hz, N–CH_2), 7.02 (1H, *brs*, OH), 7.29–7.33 (1H, *m*, Ar-H), 7.45–7.62 (5H, *m*, Ar-H), 8.21 (2H, *d*, *J* = 7.5 Hz, Ar-H), 8.39 (1H, *d*, *J* = 8.5 Hz, Ar-H), 9.00 (1H, *d*, *J* = 1.2 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 37.8, 108.5, 108.9, 119.7, 119.9, 120.7, 120.8, 121.2, 121.7, 123.0, 123.2, 124.6, 125.5, 126.4, 130.4, 133.4, 137.7, 140.5, 140.9, 147.2, 153.6, 171.8; ESI-MS (*m*/*z*): 390 ($[M+H]^+$, 100 %).

*6-Bromo-2-(9-ethyl-9*H*-carbazol-3-yl)-3-hydroxy-4*H*-chromen-4-one* ***(3d)***. Anal. Calcd. for $C_{23}H_{16}BrNO_3$: C, 63.61; H, 3.71; N, 3.23 %. Found: C, 63.65; H, 3.75; N, 3.27 %; IR (KBr, cm^{-1}): 3440 (–OH), 1632 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.48 (3H, *t*, *J* = 7.20 Hz, CH_3), 4.42 (2H, *q*, *J* = 7.20 Hz, N–CH_2), 6.99 (1H, *brs*, OH), 7.30–7.34 (1H, *m*, Ar-H), 7.50–7.56 (4H, *m*, Ar-H), 7.64 (1H, *s*, Ar-H), 8.22 (2H, *d*, *J* = 7.5 Hz, Ar-H), 8.40 (1H, *d*, *J* = 8.5 Hz, Ar-H), 9.01 (1H, *s*, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 37.8, 108.5, 108.9, 109.1, 119.7, 119.9, 120.3, 120.7, 120.8, 121.2, 123.0, 123.1, 124.6, 125.6, 126.4, 126.7, 130.2, 133.4, 137.7, 140.5, 140.9, 147.4, 151.0, 153.6, 171.9; ESI-MS (*m*/*z*): 434 ($[M+H]^+$, 100 %).

*2-(9-Ethyl-9*H*-carbazol-3-yl)-3-hydroxy-6-methyl-4H-chromen-4-one* ***(3e)***. Anal. Calcd. for $C_{24}H_{19}NO_3$: C, 78.03; H, 5.18; N, 3.79 %. Found: C, 71.41; H, 4.51; N, 3.51 %; IR (KBr, cm^{-1}): 3444 (–OH), 1628 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.47 (3H, *t*, *J* = 7.02 Hz, CH_3), 2.48 (3H, *s*, Ar-CH_3), 4.40 (2H, *q*, *J* = 7.02 Hz, N–CH_2), 7.09 (1H, *brs*, OH), 7.28–7. 32 (1H, *m*, Ar-H), 7.43––7.56 (5H, *m*, Ar-H), 8.04 (1H, *s*, Ar-H), 8.21 (1H, *d*, *J* = 7.7 Hz, Ar-H), 8.40 (1H, *dd*, *J* = 1.7, 8.7 Hz, Ar-H), 9.01 (1H, *d*, *J* = 1.5 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 29.6, 37.9, 108.4, 108.6, 108.8, 109.1, 117.9, 119.6, 120.3, 120.7, 120.8, 123.0, 123.1, 123.2, 124.0, 124.5, 125.6, 126.2, 126.7, 127.2, 128.5, 134.6, 140.5, 140.7, 143.6, 160.4, 172.7. ESI-MS (*m*/*z*): 370 ($[M+H]^+$, 100 %).

*6-Chloro-2-(9-ethyl-9*H*-carbazol-3-yl)-3-hydroxy-7-methyl-4*H*-chromen-4-one* ***(3f)***. Anal. Calcd. for $C_{24}H_{18}ClNO_3$: C, 71.38; H, 4.49; N, 3.47 %. Found: C, 71.41; H, 4.51; N, 3.51 %; IR (KBr, cm^{-1}): 3445 (–OH), 1632 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.48 (3H, *t*, *J* = 7.02 Hz, CH_3), 2.55 (3H, *s*, Ar-CH_3), 4.43 (2H, *q*, *J* = 7.02 Hz, N–CH_2), 7.21 (1H, *s*, OH), 7.29–7.33 (1H, *m*, Ar-H), 7.45–7.57 (4H, *m*, *J* = 4.0, 9.2 Hz, Ar-H), 8.15–8.23 (2H, *m*, Ar-H), 8.40 (1H, *d*, *J* = 8.7 Hz, Ar-H), 8.99 (1H, *d*, *J* = 1.5 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 29.7, 37.9, 108.7, 109.0, 109.1, 116.1, 119.9, 120.3, 120.5, 120.7, 120.8, 122.1, 123.1, 123.2, 124.0, 125.5, 126.5, 126.7, 126.8, 127.2, 128.5, 129.1, 140.7, 141.8, 143.6, 145.0, 147.7, 162.0, 172.3; ESI-MS (*m*/*z*): 404 ($[M+H]^+$, 100 %).

*6,8-Dichloro-2-(9-ethyl-9*H*-carbazol-3-yl)-3-hydroxy-4*H*-chromen-4-one* ***(3g)***. Anal. Calcd. for $C_{23}H_{15}Cl_2NO_3$: C, 65.11; H, 3.56; N, 3.30 %. Found: C,

65.15; H, 3.61; N, 3.35 %; IR (KBr, cm^{-1}): 3445 (–OH), 1629 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.50 (3H, *t*, *J* = 7.02 Hz, CH_3), 4.43 (2H, *q*, *J* = 7.02 Hz, N–CH_2), 6.31 (1H, *brs*, OH), 7.33–7.66 (6H, *m*, Ar-H), 8.03 (1H, *d*, *J* = 7.8 Hz, Ar-H), 8.18 (1H, *d*, *J* = 7.8 Hz, Ar-H), 8.63 (1H, *s*, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 37.9, 108.4, 108.6, 109.1, 119.1, 119.8, 120.3, 120.6, 120.8, 120.9, 123.0, 123.2, 123.3, 124.2, 125.6, 126.2, 126.5, 126.7, 127.2, 128.3, 128.8, 135.9, 140.7, 143.7, 155.4, 155.7, 171.9; ESI-MS (*m*/*z*): 424 ($[M+H]^+$, 100 %).

*2-(9-Ethyl-9*H*-carbazol-3-yl)-3-hydroxy-7-methoxy-4*H*-chromen-4-one* ***(3h)***. Anal. Calcd. for $C_{24}H_{19}NO_4$: C, 74.79; H, 4.97; N, 3.63 %. Found: C, 74.85; H, 5.01; N, 3.67 %; IR (KBr, cm^{-1}): 3440 (–OH), 1625 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.48 (3H, *t*, *J* = 7.27 Hz, CH_3), 3.97 (3H, *s*, O–CH_3), 4.42 (2H, *q*, *J* = 7.27 Hz, N–CH_2), 6.99–7.07 (3H, *m*, OH & Ar-H), 7.29–7.32 (1H, *m*, Ar-H), 7.45–7.54 (3H, *m*, Ar-H), 8.16 (1H, *d*, Ar-H), 8.23 (1H, *d*, *J* = 7.7 Hz, Ar-H), 8.40 (1H, *dd*, *J* = 1.5, 8.7 Hz, Ar-H), 8.98 (1H, *d*, *J* = 1.25 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 37.7, 55.8, 99.8, 108.4, 108.8, 114.6, 114.7, 119.5, 120.3, 120.7, 121.8, 123.0, 123.1, 125.4, 126.2, 126.6, 137.2, 140.4, 140.6, 146.1, 157.2, 163.9, 172.5. ESI-MS (*m*/*z*): 386 ($[M+H]^+$, 100 %).

*7-Ethoxy-2-(9-ethyl-9*H*-carbazol-3-yl)-3-hydroxy-4*H*-chromen-4-one* ***(3i)***. Anal. Calcd. for $C_{25}H_{21}NO_4$: C, 75.17; H, 5.30; N, 3.51 %. Found: C, 75.21; H, 5.35; N, 3.54 %; IR (KBr, cm^{-1}): 3442 (–OH), 1628 (C=O); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 1.45–1.48 (6H, *m*, 2×CH_3), 4.12 (2H, *q*, *J* = 7.02 Hz, O–CH_2), 4.42 (2H, *q*, *J* = 7.02 Hz, N–CH_2), 6.98–7.06 (3H, *m*, OH & Ar-H), 7.28–7.31 (1H, *m*, Ar-H), 7.42–7.52 (3H, *m*, Ar-H), 8.13 (1H, *d*, Ar-H), 8.21 (1H, *d*, *J* = 7.4 Hz, Ar-H), 8.38 (1H, *dd*, *J* = 1.6, 8.6 Hz, Ar-H), 8.96 (1H, *d*, *J* = 1.4 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 13.8, 14.5, 37.8, 62.8, 99.9, 108.2, 109.4, 114.6, 114.7, 119.5, 120.2, 120.7, 121.9, 122.6, 123.0, 125.4, 126.2, 126.6, 137.6, 140.1, 140.3, 144.7, 157.0, 162.7, 172.3; ESI-MS (*m*/*z*): 400 ($[M+H]^+$, 100 %).