

**Environmentally benign synthesis of 14-Phenyl-8H-Dibenzo[a,i]xanthene-8,13(14H)-Diones using CuI nanoparticles as an efficient catalyst**

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### Spectral Data:

**14-phenyl-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4a)** Orange powder; yield: 84 %, mp 294–296 °C, (lit.<sup>9</sup> 294–297 °C), IR (KBr):  $\nu_{\max}$  3052, 1702, 1657, 1475  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  5.95 (s, 1H); 7.10 (m, 1H), 7.18 (t, 2H,  $J = 14\text{Hz}$ ), 7.40–7.59 (m, 6H), 7.90 (m, 3H), 7.99 (d, 1H,  $J=8.4\text{Hz}$ ), 8.12 (d, 1H,  $J=7.5\text{ Hz}$ ), 8.15 (d, 1H,  $J=7.5\text{ Hz}$ ) ppm;  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  35.17, 116.56, 116.75, 116.88, 123.77, 124.53, 125.52, 126.84, 127.43, 128.55, 128.58, 129.38, 129.52, 130.01, 130.86, 131.01, 131.23, 131.89, 135.12, 143.13, 147.31, 157.19, 178.29, 178.34 ppm; Anal. Calcd. For  $\text{C}_{27}\text{H}_{16}\text{O}_3$ : C, 83.49; H, 4.15; Found C, 83.57, H 4.10; MS (EI) ( $m/z$ ): 388.

**14-(4-Chlorophenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4b)** Yellow powder; yield: 89 %, mp 281–283 °C, (lit.<sup>9</sup> 281–284 °C), IR (KBr):  $\nu_{\max}$  3039, 1699, 1665, 1461, 1366, 813  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  5.88 (s, 1H, CH), 7.15 (d, 2H,  $J=8\text{ Hz}$ ), 7.34–7.36 (d,  $J=8\text{ Hz}$ , 2H), 7.44–7.63 (m, 4H), 7.78 (t,  $J=8\text{ Hz}$ , 1H), 7.85–7.87 (d,  $J=8\text{Hz}$ , 1H), 7.90–7.93 (m, 2H), 8.13–8.18 (m, 2H) ppm;  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  34.62, 116.00, 116.26, 116.79, 123.57, 124.60, 125.67, 127.58, 128.65, 128.70, 129.47, 129.79, 129.96, 130.00, 130.68, 130.81, 131.39, 131.90, 132.65, 135.17, 141.59, 147.23, 157.30, 178.18, 178.24 ppm; Anal. Calcd. For  $\text{C}_{27}\text{H}_{15}\text{ClO}_3$ : C, 76.69; H, 3.58; Found C, 76.61; H, 3.61, MS (EI) ( $m/z$ ): 422.

**14-(4-fluorophenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4c)** Yellow powder; yield: 86 %, mp 299–301 °C, IR (KBr):  $\nu_{\max}$  3041, 1695, 1663, 1460, 1369, 811  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  5.91 (1H, s, CH), 7.25–7.35 (4H, m, H-Ar), 7.46 (2H, t,  $J= 6.7\text{ Hz}$ , H-Ar). 7.50–7.63 (2H, m, H-Ar), 7.81 (1H, t,  $J=7.6\text{ Hz}$ , H-Ar), 7.86–7.93 (3H, m, H-Ar), 8.11–8.21 (2H, m, H-Ar) ppm;  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  33.69, 115.63, 116.70, 116.84, 123.99, 124.68, 125.59, 127.12, 127.58, 128.26, 128.58, 129.42, 129.78, 130.14, 130.19, 130.84, 131.32, 131.37, 131.78, 133.35, 135.18, 147.14, 157.45, 178.15, 178.20 ppm; Anal. Calcd. For  $\text{C}_{27}\text{H}_{15}\text{FO}_3$ : C, 79.79; H, 3.72; Found C, 79.75; H, 3.65. MS (EI) ( $m/z$ ): 406.

**14-(4-nitrophenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4d)** Yellow powder; yield: 85 %, mp 325–327 °C, (lit.<sup>30</sup> >320 °C), IR (KBr):  $\nu_{\max}$  3045, 1695, 1632, 1460, 806, 550  $\text{cm}^{-1}$ ,  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  6.10 (1H, s, CH), 7.46–7.57 (m, 3H), 7.69–7.74 (m, 1H), 7.78–7.82 (m, 1H), 7.87–8.23 (m, 9H) ppm;  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  35.25, 115.03, 115.35, 116.83, 123.26, 123.88, 124.77, 125.91, 127.87, 128.83, 129.57, 129.63, 130.06, 130.32, 130.40, 130.65, 131.73, 131.99, 135.35, 146.68, 147.29, 150.06, 157.84,

177.98,178.15; Anal. Calcd. For C<sub>27</sub>H<sub>15</sub>NO<sub>5</sub>: C, 74.82; H, 3.49; N, 3.23; Found C, 74.75; H, 3.54,N, 3.15, MS (EI) (*m/z*): 433.

**14-(3-nitrophenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4e)** Yellow powder; yield: 82%, mp 300-302°C,(lit.<sup>8</sup> 304-305°C), IR (KBr):  $\nu_{\max}$ 3070, 1699, 1634, 1461, 1345, 813, 659, 555 cm<sup>-1</sup>, <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  6.04 (1H, s, CH), 7.44-7.52 (m, 3H), 7.67-7.71 (m, 1H), 7.78-7.80 (m, 1H), 7.85-8.25 (m, 9H) ppm; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  35.20, 115.19, 115.27, 116.97, 122.14, 123.26, 123.32, 124.88, 125.85, 127.82, 128.87, 129.38, 129.59, 130.09, 130.35, 130.42, 130.60, 131.68, 132.03, 135.08, 135.31, 145.09, 147.33, 148.56, 157.73, 178.02, 178.14; Anal. Calcd. ForC<sub>27</sub>H<sub>15</sub>NO<sub>5</sub>: C, 74.82; H, 3.49; N, 3.23; Found C,74.76; H, 3.56, N, 3.16, MS (EI) (*m/z*): 433.

**14-(4-methylphenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4f)** Yellow powder;yield: 79%, mp257-259°C,(lit.<sup>30</sup> 256-258°C), IR (KBr):  $\nu_{\max}$ 3055, 1692, 1631, 1455, 1340, 551 cm<sup>-1</sup>, <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  2.22 (s, 3H, CH<sub>3</sub>), 5.90 (s, 1H,CH), 7.35-7.65 (m, 5 H), 7.75-8.19 (m, 9 H) ppm, <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  20.96, 34.71, 116.70, 116.79, 117.03, 123.78, 124.49, 125.50, 127.44, 128.42, 128.53, 129.24, 129.34, 129.41, 129.99, 130.92, 131.02, 131.16, 131.87, 135.08, 136.48, 140.27, 147.24, 157.09, 178.21, 178.34 ppm; Anal. Calcd. For C<sub>28</sub>H<sub>18</sub>O<sub>3</sub>; C, 83.57; H, 4.51;Found C, 83.63; H, 4.49,MS (EI) (*m/z*): 402.

**14-(2,4-dichlorophenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4g)** Yellow powder; yield: 81 %, mp298–302 °C, (lit <sup>8</sup> 301-302°C); IR (KBr):  $\nu_{\max}$  3078, 1685, 1634, 1464, 1346, 810, 642, 550 cm<sup>-1</sup>, <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  6.12 (s, 1H, CH), 7.24 (m,1H), 7.28 (m, 2H), 7.48-8.16 (m, 9 H), 8.20 (m, 1H) ppm;<sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  33.24, 116.82, 123.71, 124.72, 125.69, 127.49, 127.69, 128.70, 129.47, 129.84, 130.01, 130.13, 130.60, 131.13, 131.52, 131.79, 132.61, 133.09, 134.02, 135.19, 139.20, 147.11, 157.55, 178.05, 178.10 ppm; Anal. Calcd. For C<sub>27</sub>H<sub>14</sub>Cl<sub>2</sub>O<sub>3</sub>: C, 70.91; H, 3.09, Found C, 70.87; H, 3.20, MS (EI) (*m/z*): 457.

**14-(4-Bromophenyl)-8H-dibenzo[a,i]xanthene-8,13(14H)-dione (4h)**Yellow powder; 84%, mp 292-294 °C, (lit.<sup>9</sup> 294-298 °C), IR (KBr):  $\nu_{\max}$ 3072, 1705, 1665, 1466, 1370cm<sup>-1</sup>, <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  5.90 (1H, s, CH), 7.26-7.30 (m, 4H), 7.46-7.63 (m, 4H), 7.80-7.92 (m, 4H), 8.13-8.18 (m, 2H) ppm; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  34.69, 116.05, 116.29, 116.79, 123.58, 124.62, 125.68, 127.58, 128.67, 128.72, 129.48, 129.79, 129.97, 130.06, 130.68, 130.84, 131.39, 131.92, 132.63, 135.18, 141.59, 147.25, 157.33,

178.18, 178.28 ppm; Anal. Calcd. For  $C_{27}H_{15}BrO_3$ : C, 69.39; H, 3.24; Found C, 69.45; H, 3.18, MS (EI) ( $m/z$ ): 468 ( $M^{+2}$ ), 466 ( $M^{+}$ ).

**14-(4-methoxyphenyl)-14H-dibenzo[a,i]xanthene-8,13-dione (4i)** Orange powder; 77%, mp 278-280 °C, (lit<sup>8</sup> 279-280 °C), IR (KBr):  $\nu_{max}$  2916, 1663, 1635, 1592, 1575, 1367  $cm^{-1}$ ;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  3.69 (s, 3H), 5.91 (s, 1H), 7.32 (d, 2H,  $J=8$ Hz), 7.62 (m, 5H), 7.80 (m, 4H), 7.98 (d, 1H,  $J=8$  Hz), 8.12 (d, 1H,  $J=7.5$  Hz), 8.17 (m, 1H) ppm;  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  34.28, 55.15, 113.91, 116.78, 117.07, 123.81, 124.51, 125.50, 127.42, 128.53, 129.39, 129.41, 129.58, 130.01, 130.96, 131.00, 131.16, 131.87, 135.11, 135.47, 147.23, 157.03, 158.26, 178.38, 178.42 ppm; Anal. Calcd. For  $C_{28}H_{18}O_4$ : C, 80.37; H, 4.34; Found C, 80.42; H, 4.39, MS (EI) ( $m/z$ ): 418.