**Isolation and characterization of bis(2-ethylheptyl) phthalate from Cynodon dactylon (L.) and studies on catalytic activity of its Cu(II) complex in the green preparation of 1,8-dioxo-octahydroxanthenes**

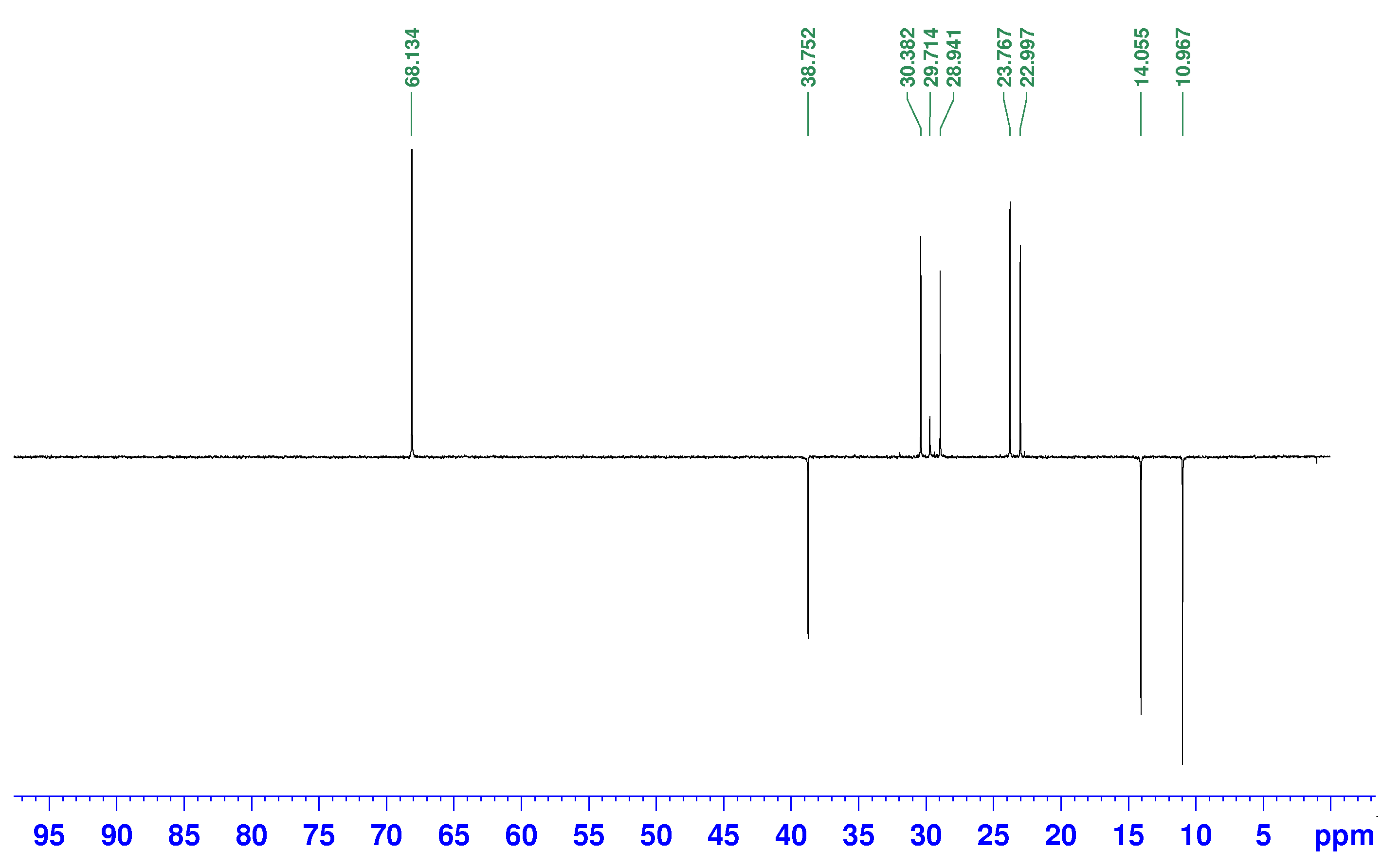
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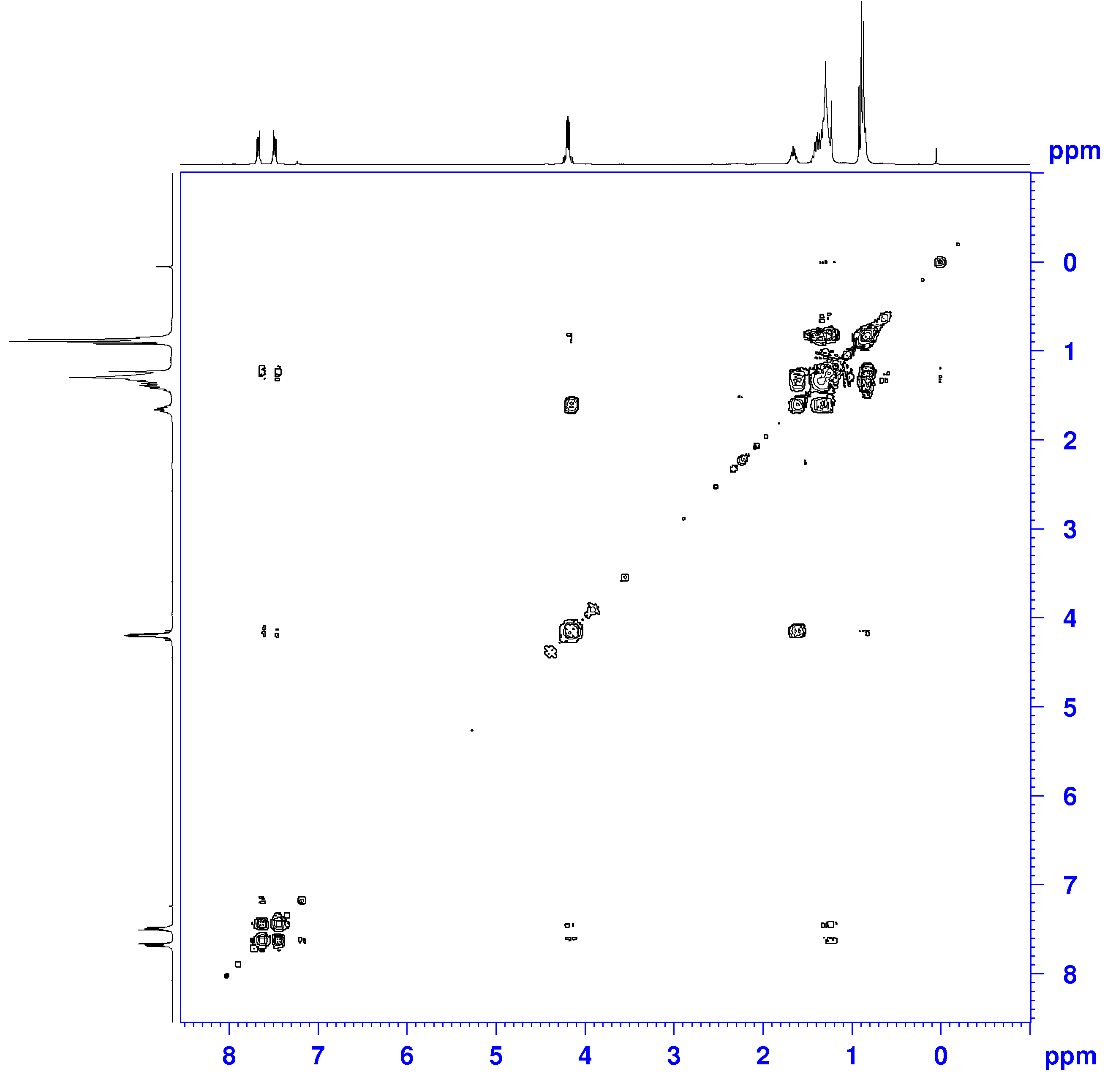
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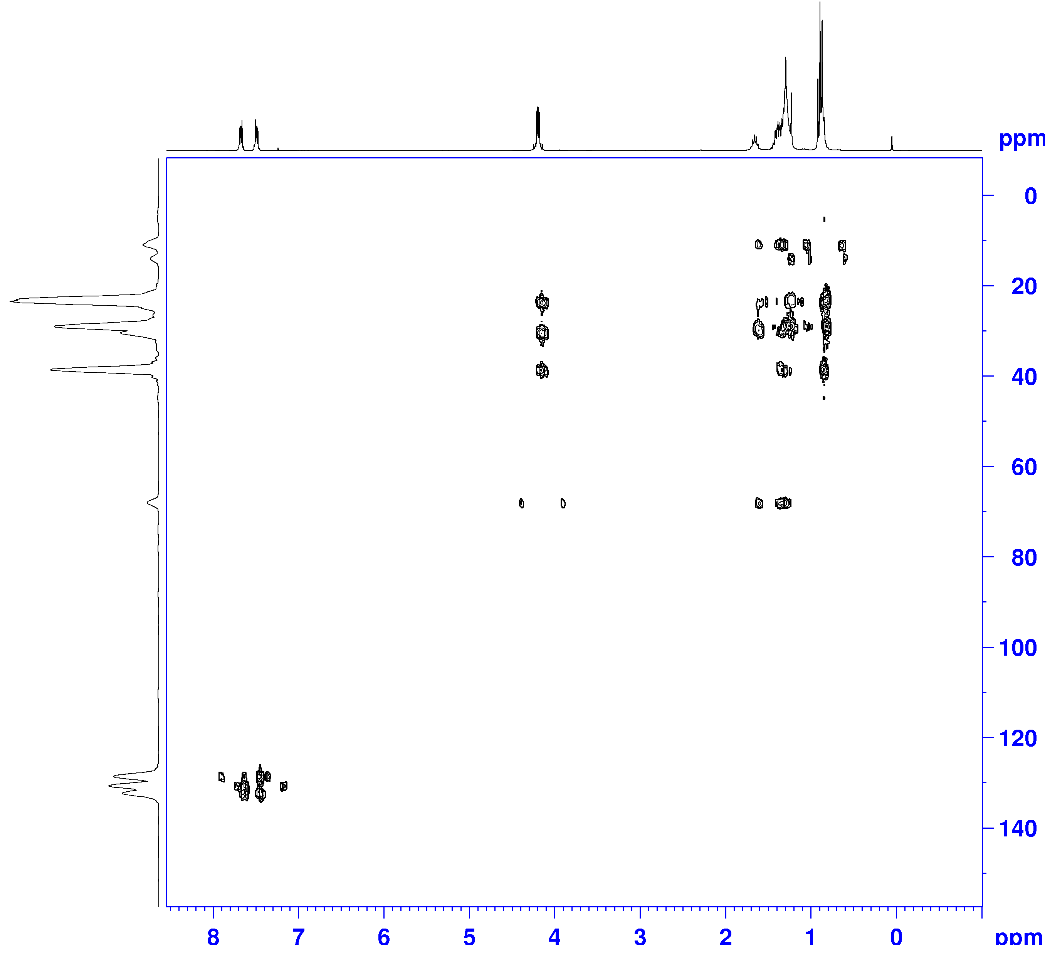
**Fig. S1** FTIR spectrum of bis(2-ethylheptyl) phthalate



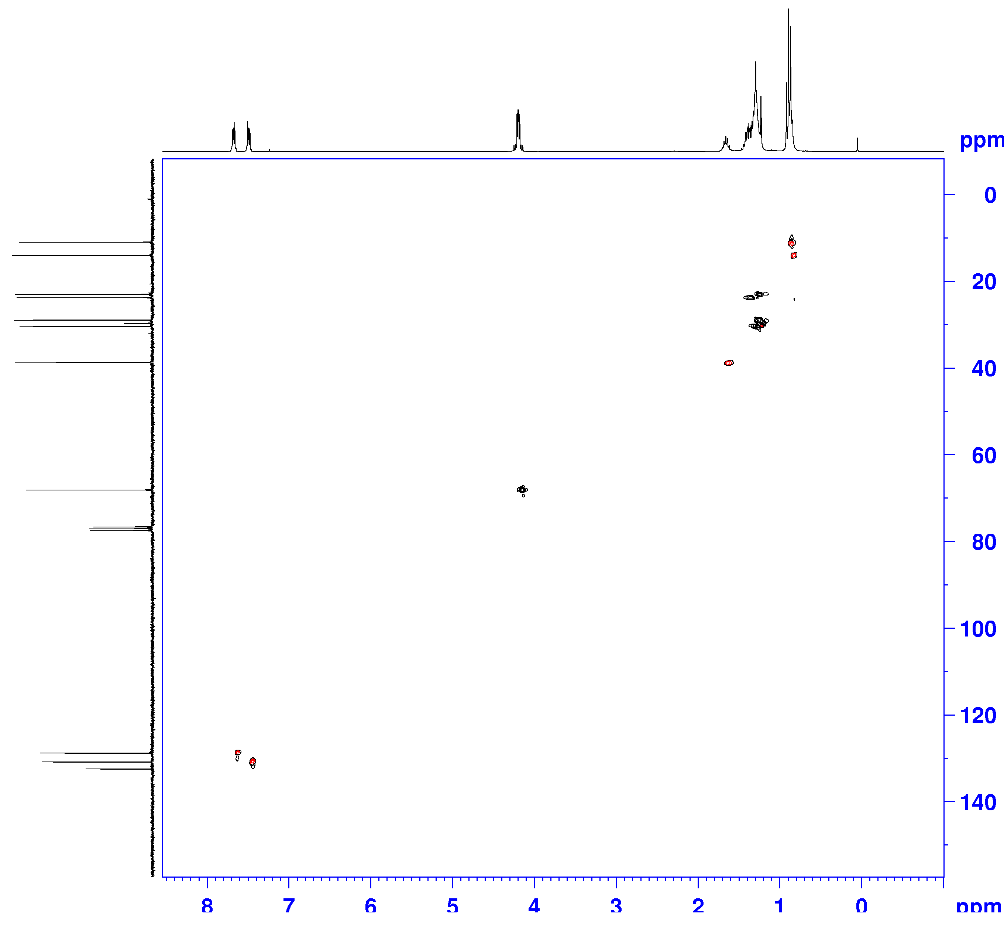
**Fig. S2** DEPT spectrum of bis(2-ethylheptyl) phthalate (75 MHz, CDCl3)



**Fig. S3** H-H COSY spectrum of bis(2-ethylheptyl) phthalate (300 MHz, CDCl3)



**Fig. S4** HMBC spectrum of bis(2-ethylheptyl) phthalate (CDCl3)



**Fig. S5** HSQC spectrum of bis(2-ethylheptyl) phthalate (CDCl3)

**Characterization data for xanthene derivatives**



9-(*p*-Tolyl)-3,4,5,6,7,9-hexahydro-1*H*-xanthene-1,8(2H)-dione (Table 3, **6a**)

M.P. 244-246 °C; IR (KBr, cm-1): 2977, 1662, 1533, 1364, 1329, 1220, 1158, 1132, 1081. 1H NMR (300 MHz, DMSO-*d6*, ppm): *δ* 1.95-2.08 (4H, m), 2.25 (3H, s), 2.30-2.44 (4H, m), 2.52-2.70 (4H, t, *J*= 6.2), 4.77 (1H, s), 7.03-7.08 (2H, d, *J*= 8 Hz), 7.12-7.25 (2H, d, *J*= 7.6 Hz) [1].



9-(4-chlorophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6b**)

IR (KBr, cm-1): 2951, 1660, 1512, 1373, 1333, 1218, 1191, 1135, 1008, 832, 733. 1H NMR (300 MHz, DMSO-*d6*, ppm): *δ* 1.56 (4H, m), 1.94 (4H, m), 2.96 (4H, t, *J*= 6.3), 3.98 (1H, s), 7.19 (4H, m) [2].



9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6c**)

IR (KBr, cm-1): 3143, 2954, 1720, 1587, 1375, 1199. 1H NMR (300 MHz, CDCl3, ppm): 2.20 (4H, m), 2.24 (3H, s), 2.45 (4H, m), 2.54 (4H, t, *J*= 6.1), 4.70 (1H, s), 7.00 (2H, s, *J*= 8.1 Hz), 7.15 (2H, d, *J*= 8.1 Hz) [3].



9-(4-hydroxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6d**)

M.P. 250 °C, IR (KBr, cm-1): 3498, 3078, 2933, 2929, 1719, 1645, 1577, 1384, 1166. 1H NMR (300 MHz, CDCl3, ppm): *δ* 2.12-2.24 (4H, m), 2.45 (4H, m), 3.15 (4H, t, *J*= 6.2), 4.61 (1H, s), 6.77 (2H, m) 6.93 (2H, m), 9.06 (1H, s) [4].



9-Phenyl-3,4,5,6,7,9-hexahydro-1*H*-xanthene-1,8(2H)-dione (Table 3, **6e**)

M. P. 214-216 °C; IR (KBr, cm-1): 3001, 1661, 1532, 1367, 1332, 1221, 1160, 1134, 1091, 841, 739. 1H NMR (300 MHz, DMSO-*d6*, ppm): *δ* 1.90-2.10 (4H, m), 2.27-2.28 (2H, t, *J*= 6.2), 2.31-2.40 (2H, t, *J*= 6.2 ), 2.52-2.65 (4H, m), 4.77 (1H, s), 7.05-7.09 (2H, t, *J*= 7.6 Hz), 7.12-7.13 (1H, d, *J*= 8.4 Hz), 7.23-7.31 (2H, dd, *J*= 8, 24.3) [1].



9-(2-hydroxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6f**)

Mp: 214°C; FT-IR (KBr, cm-1): 3030, 2965, 1677, 1669, 1643. 1H NMR (300 MHz, CDCl3, ppm): *δ* 2.21 (4H, m), 2.45 (4H, m), 2.55 (4H, t, *J*= 6.3), 4.67 (1H, s), 6.61 (2H, d, *J*= 8.0 Hz), 7.11 (2H, d, *J*= 8.0 Hz), 9.68 (1H, s) [4].



9-(4-nitrophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6g**)

M.P. 222 °C; FT-IR (KBr, cm-1): 3107, 3078, 2930, 2862, 1908, 1772, 1620, 1607, 1589, 1520, 1466, 1382, 1317, 1248. 1H NMR (300 MHz, CDCl3, ppm): *δ* 2.20 (2H, d, *J*= 16.3 Hz), 2.29 (2H, d, *J*= 16.3 Hz), 2.53 (4H, m), 2.57 (4H, t, *J*= 6.5 Hz), 4.86 (1H, s), 7.51 (2H, dd, *J1*= 7.0 Hz, *J2*= 1.7 Hz), 8.12 (2H, dd, *J1*= 7.0 Hz, *J2*= 1.7 Hz) [5].



9-(4-methoxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6h**)

M.P. >220 °C; FT-IR (KBr, cm-1): 3068, 2943, 2887, 1639, 1608, 1458, 1364, 1232, 1176. 1H NMR (300 MHz, CDCl3, ppm): *δ* 1.96-2.07 (4H, m), 2.29-2.42 (4H, m), 2.52-2.69 (4H, t, *J*= 6.2 Hz), 3.26 (1H, s), 3.56 (3H, s), 7.03-7.05 (2H, d, *J*= 8.0 Hz), 7.12-7.21 (2H, d, *J*= 7.6 Hz) [6].



4-(1,8-Dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)benzonitrile (Table 3, **6i**)

FT-IR (KBr, cm-1):3071, 3008, 2920, 2868, 1646, 1618, 1438, 1366, 1592, 1388, 1293, 1235, 1196, 1091. 1H NMR (300 MHz, CDCl3, ppm): δ 2.11 (4H, m), 2.49 (4H, m), 3.19 (4H, t, *J*= 6.4 Hz), 3.92 (1H, s), 7.71 (2H, d, *J*= 8.1 Hz), 7.50 (2H, d, *J*= 7.9 Hz).



9-(2-Furyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydro-2*H*-xanthene-1,8(5H,9H)-dione (Table 3, **6j**)

M.P. 180–181 °C; FT-IR (KBr, cm-1): 3092, 2962, 1660, 1621, 1470, 1199. 1H NMR (300 MHz, CDCl3, ppm): *δ* 1.01 (6H, s), 1.13 (6H, s), 2.18 (4H, s), 2.52 (4H, s), 4.85 (1H, s), 7.43 (1H, t, *J*= 6Hz), 7.84 (1H, d, *J*= 4Hz), 8.01 (1H, d, *J*= 6Hz) [1].



3,3,6,6-tetramethyl-9-(pyridin-2-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6k**)

M.P. 204-205 °C; IR (KBr, cm−1): 2958, 2930, 2874, 1681, 1657, 1623, 1199. 1H NMR (300 MHz, CDCl3): *δ* 0.99 (6H, s), 1.10 (6H, s), 2.15 (2H, d, *J=* 16.2), 2.23 (2H, d, *J=* 16.2), 2.44 (2H, d, *J=* 17.4), 2.52 (2H, d, *J=* 17.4), 4.85 (1H, s), 6.94–7.02 (1H, m), 7.55– 8.38 (3H, m) [7].



9-(1H-Indol-3-yl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6l**)

M.P. 204-205 °C; IR (KBr, cm−1): 3490, 3400, 3060, 2958, 2930, 2855, 2874, 1617, 1557, 1505, 1488, 1456, 1416, 1377, 1336, 1206, 1199, 1091, 1061. 1H NMR (300 MHz, CDCl3): *δ* 1.11 (6H, s), 1.19 (6H, s), 1.83 (4H, s), 2.01 (4H, s), 3.84 (1H, s), 6.94 (1H, t, *J*= 7.7 Hz), 7.06 (1H, t, *J*= 7.8 Hz), 7.17 (1H, s), 7.39 (1H, d, *J*= 8.0 Hz), 7.54 (1H, d, *J*= 8.2 Hz), 10.34 (1H, s).



3,3,6,6-tetramethyl-9-(thiophen-2-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione

(Table 3, **6m**)

M.P. 163-164 °C; IR (KBr, cm−1): 2957, 2895, 2872, 1659, 1622, 1371, 1360, 1200. 1H NMR (300 MHz, CDCl3): *δ* 1.06 (6H, s), 1.11 (6H, s), 2.26 (4H, s), 2.46 (4H, s), 5.15 (1H, s), 6.81–7.03 (3H, m) [8].



3,3,6,6-tetramethyl-9-(naphthalen-2-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6n**)

M.P. >300°C; IR (KBr, cm−1): 3059, 2954, 2922, 1649, 1608, 1491, 1364, 1221, 1171. 1H NMR (300 MHz, CDCl3): *δ* 0.99 (6H, s), 1.12 (6H, s), 2.13-2.18 (2H, d, *J*= 18 Hz), 2.21-2.23 (2H, d, *J*= 9.6 Hz), 2.52 (4H, s), 7.34- 7.38 (1H, d, *J*= 16), 7.46-7.47 (2H, d, *J*= 6.8 Hz), 7.73-7.79 (4H, m), 9.12 (1H, s) [9].



3,3,6,6-tetramethyl-9-(p-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6o**)

M.P. 215-217 °C; IR (KBr, cm−1): 3039, 2958, 1679, 1664, 1467, 1357, 1198, 1137. 1H NMR (300 MHz, CDCl3): *δ* 1.02 (6H, s), 1.12 (6H, s), 2.18 (2H, d, *J*= 16.2 Hz), 2.26 (2H, d, *J*= 16.2 Hz), 2.28 (3H, s), 2.48 (4H, s), 4.73 (1H, s), 7.04 (2H, d, *J*= 8.1 Hz), 7.20 (2H, d, *J*= 8.1 Hz) [10].



9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6p**)

M.P. 230–232 °C; FT-IR (KBr, cm-1): 3044, 2964, 1661, 1626, 1469, 1362, 1198. 1H NMR (300 MHz, CDCl3, ppm): *δ* 1.00 (6H, s), 1.11 (6H, s), 2.18 (2H, d, *J*= 16Hz), 2.25 (2H, d, *J*= 16Hz), 2.48 (4H, s), 4.72 (1H, s), 7.22 (2H, d, *J*= 4Hz), 7.27 (2H, d, *J*= 4Hz) [1].



9-(4-hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (Table 3, **6q**)

M.P. 250-251 °C;IR (KBr, cm−1): 3498, 3078, 2933,2929, 1719, 1645, 1577, 1384, 1166. 1H NMR (300 MHz, CDCl3): *δ* 1.00 (6H, s), 1.11 (6H, s), 2.12-2.24 (4H, s), 2.45 (4H, s), 4.61 (1H, s), 6.77 (2H, m), 6.93 (2H, m), 9.06 (1H, b) [11].



9-Phenyl-3,3,6,6-tetramethyl-3,4,6,7-tetrahydro-2H-xanthene-1,8(5H,9H)-dione (Table 3, **6r**)

M.P. 200–202 °C; FT-IR (KBr, cm-1): 3028, 2961, 1663, 1623,1454, 1359, 1197, 1000. 1H NMR (300 MHz, CDCl3, ppm): *δ* 1.00 (6H, s), 1.11 (6H, s), 2.17 (2H, d, *J*=16Hz), 2.25 (2H, d, *J=* 16Hz), 2.48 (4H, s), 4.76 (1H, s), 7.29 (5H, m) [1].



9-(2-Methoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydro-2*H*-xanthene-1,8(5H,9H)-dione (Table 3, **6s**)

M.P. 178–179 °C; FT-IR (KBr, cm-1): 3015, 2957, 1662, 1623, 1491, 1252, 1198; 1H NMR (300 MHz, CDCl3, ppm): *δ* 0.96 (6H, s), 1.01 (6H, s), 2.13 (2H, d, *J*= 18Hz), 2.21 (2H, d, *J*= 18Hz), 2.38 (2H, d, *J*=18Hz), 2.47 (2H, d, *J*= 18Hz), 3.78 (3H, s), 4.87 (1H, s), 6.76 (1H, d, *J*= 6Hz), 6.89 (1H, d, J= 4Hz), 7.42 (1H, d, *J*= 6Hz), 7.11 (1H, s) [1].



9-(4-Nitrophenyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydro-2*H*-xanthene-1,8(5H,9H)-dione (Table 3, **6t**)

M.P. 224–225 °C; FT-IR (KBr, cm-1): 3057, 2959, 1663, 1616, 1515, 1470, 1343, 1201. 1H NMR (300 MHz, CDCl3, ppm): *δ* 1.00 (6H, s), 1.12 (6H, s), 2.17 (2H, d, *J*= 16Hz), 2.27 (2H, d, *J*= 16Hz), 2.51 (4H, s), 4.83 (1H, s), 7.48 (2H, d, *J*= 9Hz), 8.09 (2H, d, *J*= 9Hz) [1].



9-(4-Methoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydro-2*H*-xanthene-1,8(5H,9H)-dione (Table 3, **6u**)

M.P. 240–242 °C; FT-IR (KBr, cm-1): 3050, 2959,1666, 1625, 1435, 1261, 1195. 1H NMR (300 MHz, CDCl3, ppm): *δ* 1.00 (6H, s), 1.11 (6H, s), 2.21 (4H, d, *J*= 4Hz), 2.47 (4H, s), 3.74 (3H, s), 4.71 (1H, s), 6.76 (2H, d, *J*= 9Hz), 7.22 (2H, d, *J*= 9Hz) [1].

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