

A Complete and Unambiguous ^1H and ^{13}C NMR Signals Assignment of *para*-Naphthoquinones, *ortho*- and *para*-Furanonaphthoquinones

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Signals assignments were based on chemical shifts (δ , ppm) of ^1H and ^{13}C , and the multiplicity patterns of proton resonances depicted by the J couplings (Hz).

(*E*)-2-Hydroxy-3-(prop-1-en-1-yl)naphthalene-1,4-dione (**4a**)

Mp 85-87 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.09 (d, 1H, J 7.6, CH), 8.03 (d, 1H, J 7.52, CH), 7.78 (s, 1H, OH), 7.72 (t, 1H, J 7.52, CH), 7.65 (t, 1H, J 7.52, CH), 7.10-7.00 (m, 1H, CH), 6.60 (d, 1H, J 16.12, CH), 1.97 (3H, d, J 6.84, CH_3); ^{13}C NMR (400 MHz, CDCl_3) δ 181.58, 151.40, 118.87, 184.40, 127.20, 135.01, 133.17, 126.04, 129.64, 132.89, 120.18, 138.97, 20.70.

(*E*)-2-Hydroxy-3-(but-1-en-1-yl)naphthalene-1,4-dione (**4b**)

Mp 88-91 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.11 (dd, 1H, J 7.02 and 1.07, CH), 8.05 (dd, 1H, J 7.34 and J 1.36, CH), 7.82 (s, 1H, OH), 7.77-7.62 (m, 2H, 2xCH), 7.18-6.98 (m, 1H, CH), 6.60 (d, 1H, J 16.22, CH), 2.32 (2H, quint, J 7.40, CH_2), 1.12 (3H, m, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 181.57, 151.47, 118.91, 184.51, 126.11, 135.06, 133.21, 127.20, 129.61, 132.87, 117.98, 145.61, 28.19, 13.49.

(*E*)-2-Hydroxy-3-(pent-1-en-1-yl)naphthalene-1,4-dione (**4c**)

Mp 78-80 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.11 (dd, 1H, J 7.02 and 1.07, CH), 8.05 (dd, 1H, J 7.34 and 1.36, CH), 7.81 (s, 1H, OH), 7.78-7.62 (m, 2H, 2xCH), 7.14-6.98 (m, 1H, CH), 6.61 (d, 1H, J 16.20, CH), 2.27 (2H, q, J 6.80, CH_2), 1.53 (2H, st, J 7.3, CH_2), 0.97 (3H, t, J 7.30, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 181.61, 151.47, 119.00, 184.53, 126.12, 135.06, 133.21, 127.22, 129.64, 132.90, 118.88, 144.20, 37.30, 22.52, 13.99.

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(E)-2-Hydroxy-3-(hex-1-en-1-yl)naphthalene-1,4-dione (4d)

Mp 78-80 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.10 (dd, 1H, *J* 7.39 and 1.18, CH), 8.04 (dd, 1H, *J* 7.14 and *J* 1.42, CH), 7.80 (s, 1H, OH), 7.77-7.61 (m, 2H, 2xCH), 7.10-7.03 (m, 1H, CH), 6.60 (d, 1H, *J* 16.40, CH), 2.27 (2H, q, *J* 6.90, CH₂), 1.56-1.32 (m, 4H, 2xCH₂), 0.93 (3H, t, *J* 6.94, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ 181.56, 151.44, 118.88, 184.48, 126.10, 135.02, 133.19, 127.19, 129.62, 132.87, 118.84, 144.40, 34.95, 31.45, 22.53, 14.14.

(E)-2-Hydroxy-3-(3-methylbut-1-en-1-yl)naphthalene-1,4-dione (4e)

Mp 118-119 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, 1H, *J* 7.60, CH), 8.06 (d, 1H, *J* 7.40, CH), 7.80 (s, 1H, OH), 7.71-7.64 (m, 2H, 2xCH), 7.04 (dd, 1H, *J* 16.34 and 7.20, CH), 6.60 (d, 1H, *J* 16.34, CH), 2.53 (m, 1H, CH), 1.12 (d, 6H, *J* 6.72, 2xCH₃); ¹³C NMR (100 MHz, CDCl₃) δ 181.55, 151.50, 118.98, 184.54, 126.11, 135.06, 133.20, 127.20, 129.60, 132.92, 116.15, 150.66, 33.64, 22.38.

(E)-2-Hydroxy-3-(3-phenylprop-1-en-1-yl)naphthalene-1,4-dione (4f)

Mp 140-141 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.12 (d, 1H, *J* 7.40, CH), 8.05 (d, 1H, *J* 7.20, CH), 7.82 (s, 1H, OH), 7.73-7.65 (m, 2H, 2xCH), 7.35-7.12 (m, 6H), 6.71 (d, 1H, *J* 16.10, CH); ¹³C NMR (100 MHz, CDCl₃) δ 181.17, 151.50, 118.92, 184.31, 127.37, 135.14, 133.37, 126.23, 129.76, 132.90, 117.57, 139.46, 39.70, 128.89, 127.36, 126.80, 127.23.

(E)-2-Hydroxy-3-styrylnaphthalene-1,4-dione (4g)

Mp 162-163 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.14 (d, 1H, *J* 7.30, CH), 8.06 (d, 1H, *J* 7.60, CH), 7.90 (s, 1H, OH), 7.78-7.56 (m, 4H), 7.94 (s, 1H, CH), 7.41-7.1 (m, 4H, 2xCH₂), 6.71 (d, 1H, *J* 16.10, CH); ¹³C NMR (100 MHz, CDCl₃) δ 181.50, 151.76, 119.98, 184.33, 126.45, 135.14, 133.27, 126.17, 129.56, 132.89, 118.50, 141.76, 41.48, 139.80, 128.88, 128.74.

(E)-2-(4-Chlorostyryl)-3-hydroxynaphthalene-1,4-dione (4h)

¹H NMR (400 MHz, CDCl₃) δ 8.16 (dd, 1H, *J* 7.66 and 0.70, CH), 8.11 (dd, 1H, *J* 8.11 and 0.84, CH), 7.78 (t, 1H, *J* 7.58, CH), 7.71 (t, 1H, *J* 7.58, CH), 7.99 (s, 1H, OH), 7.38-7.34 (m, 3H), 7.94 (d, 1H, *J* 16.68, CH), 7.53 (d, 2H, *J* 8.44, CH); ¹³C NMR (100 MHz, CDCl₃) δ 181.36, 152.26, 118.65, 184.31, 127.45, 135.34, 133.50, 126.39, 129.81, 132.99, 118.24, 138.04, 136.59, 128.54, 129.15, 134.59.

2-Methylnaphtho[1,2-*b*]furan-4,5-dione (5a)

¹H NMR (400 MHz, CDCl₃) δ: 7.62-7.57 (m, 2H, 2xCH), 7.78 (t, 1H, *J* 7.20, CH), 8.00 (d, 1H, *J* 7.72, CH), 6.40 (s, 1H, CH), 2.40 (s, 3H, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ 180.76, 174.44, 122.70, 156.08, 122.07, 135.49, 129.91, 130.51, 128.75, 128.64, 104.60, 159.70, 13.70.

2-Ethyl-naphtho[1,2-*b*]furan-4,5-dione (5b)

¹H NMR (400 MHz, CDCl₃) δ 7.64-7.58 (m, 2H, 2xCH), 7.40 (t, 1H, *J* 7.20, CH), 8.01 (d, 1H, *J* 7.60, CH), 6.43 (s, 1H, CH), 2.75 (q, 2H, *J* 7.47, CH₂), 1.32 (t, 3H, *J* 7.60, CH₃); ¹³C NMR (100 MHz, CDCl₃) δ 180.94, 174.61, 122.60, 159.64, 122.10, 135.46, 129.92, 130.54, 128.90, 128.79, 103.10,

161.60, 21.45, 11.80.

2-Propylnaphtho[1,2-*b*]furan-4,5-dione (5c)

^1H NMR (400 MHz, CDCl_3) δ 7.66-7.57 (m, 2H, 2xCH), 7.45-7.37 (m, 1H, CH), 8.03 (d, 1H, J 7.60, CH), 6.44 (s, 1H, CH), 2.70 (t, 2H, J 7.65, CH), 1.74 (st, 2H, J 7.40, CH_2), 1.03 (t, 3H, J 7.28 Hz, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 180.94, 174.66, 122.66, 159.76, 122.19, 135.53, 129.95, 130.61, 128.94, 128.76, 104.00, 160.30, 29.98, 21.06, 13.77.

2-Butylnaphtho[1,2-*b*]furan-4,5-dione (5d)

^1H NMR (400 MHz, CDCl_3) δ 7.65-7.56 (m, 2H, 2xCH), 7.40 (t, 1H, J 7.40, CH), 8.02 (d, 1H, J 7.60, CH), 6.43 (s, 1H, CH), 2.71 (t, 2H, J 7.60, CH), 1.70 (quint, 2H, J 7.40 Hz, CH_2), 1.43 (s, 2H, J 7.40, CH_2), 0.97 (t, 3H, J 7.40, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 180.89, 174.60, 122.68, 159.65, 122.15, 135.46, 129.90, 130.55, 128.92, 128.78, 103.84, 160.49 (C-2'), 27.70, 29.71, 22.28, 13.85.

2-Isopropylnaphtho[1,2-*b*]furan-4,5-dione (5e)

^1H NMR (400 MHz, CDCl_3) δ 7.66-7.56 (m, 2H, 2xCH), 7.44-7.36 (m, 1H, CH), 8.01 (d, 1H, J 7.54, CH), 6.42 (s, 1H, CH), 3.01 (ht, 1H, J 6.83 Hz, CH), 1.32 (d, 6H, J 6.83 Hz, 2x CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 183.90, 180.90, 122.40, 159.69, 122.18, 135.47, 129.95, 130.57, 128.92, 128.77, 102.01, 165.55, 28.30, 20.60.

2-Benzyl naphtho[1,2-*b*]furan-4,5-dione (5f)

^1H NMR (400 MHz, CDCl_3) δ 7.51 (s, 2H, 2xCH), 7.30-7.21 (m, 6H), 7.91 (d, 1H, J 7.50, CH), 6.33 (s, 1H, CH), 3.95 (s, 2H, CH_2); ^{13}C NMR (100 MHz, CDCl_3) δ 180.69, 174.50, 122.58, 158.59, 122.30, 135.49, 130.09, 130.58, 128.77, 128.68, 105.34, 160.20, 34.52, 136.17, 128.98, 128.93, 127.33.

2-Phenylnaphtho[1,2-*b*]furan-4,5-dione (5g)

^1H NMR (400 MHz, CDCl_3) δ 7.73-7.41 (m, 2H, 2xCH), 7.67 (t, 1H, J 7.50, CH), 8.06 (d, 1H, J 7.68, CH), 7.01 (s, 1H, CH), 7.48-7.36 (m, 4H, 4xCH), 7.78-7.77 (m, 1H, CH); ^{13}C NMR (100 MHz, CDCl_3) δ 180.69, 174.50, 122.58, 158.59, 122.30, 135.49, 130.09, 130.58, 128.77, 128.68, 105.34, 160.20, 34.52, 136.17, 128.98, 128.93, 127.33.

2-(4-Chlorophenyl)naphtho[1,2-*b*]furan-4,5-dione (5h)

^1H NMR (400 MHz, CDCl_3) δ 8.11 (d, 1H, J 7.68, CH), 7.81 (d, 1H, J 7.60, CH), 7.71 (s, 1H, CH), 7.49 (t, 1H, J 7.72, CH), 7.05 (s, 1H, CH), 7.69-7.67 (m, 2H, 2xCH), 7.48-7.44 (m, 2H, 2xCH).

2-Methylnaphtho[2,3-*b*]furan-4,9-dione (6a)

^1H NMR (400 MHz, CDCl_3) δ 8.15-8.13 (m, 1H, CH), 7.75-7.70 (m, 1H, CH), 7.40 (t, 1H, J 7.20, CH), 8.00 (d, 1H, J 7.72, CH), 6.40 (s, 1H, CH), 2.40 (s, 3H, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 173.27, 151.84, 132.10, 181.02, 126.96, 133.99, 133.74, 127.05, 132.68, 133.20, 105.17, 160.66, 14.30.

2-Ethyl naphtho[2,3-*b*]furan-4,9-dione (**6b**)

^1H NMR (400 MHz, CDCl_3) δ 8.18-8.09 (m, 2H, 2xCH), 7.73-7.68 (m, 2H, 2xCH), 6.59 (s, 1H, CH), 2.83 (q, 2H, J 7.53, CH_2); 1.34 (t, 3H, J 7.53, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 173.30, 151.68, 131.91, 181.04, 126.92, 133.95, 133.70, 126.98, 132.69, 133.21, 103.66, 166.05, 21.95, 11.76.

2-Propyl naphtho[2,3-*b*]furan-4,9-dione (**6c**)

^1H NMR (400 MHz, CDCl_3) δ 8.20-8.11 (m, 2H, 2xCH), 7.77-7.70 (m, 2H, 2xCH), 6.61 (s, 1H, CH), 2.79 (t, 2H, J 7.48, CH_2); 1.80 (st, 2H, J 7.39, CH_2); 1.02 (t, 3H, J 7.39, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 173.25, 151.71, 131.90, 181.07, 126.92, 133.95, 133.68, 126.97, 132.71, 133.23, 104.30, 164.78, 21.04, 30.40, 13.78.

2-Butyl naphtho[2,3-*b*]furan-4,9-dione (**6d**)

^1H NMR (400 MHz, CDCl_3) δ 8.15-8.13 (m, 2H, 2xCH), 7.73-7.68 (m, 2H, 2xCH), 6.60 (s, 1H, CH), 2.81 (t, 2H, J 7.60, CH_2), 1.75 (quint, 2H, J 7.57 CH_2), 1.43 (t, 2H, 7.41, CH_2), 0.96 (t, 3H, J 7.40, CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 173.23, 151.72, 131.95, 181.06, 126.90, 133.93, 133.66, 126.93, 132.78, 133.28, 104.30, 164.99, 28.20, 29.68, 22.74, 13.83.

2-Isopropyl naphtho[2,3-*b*]furan-4,9-dione (**6e**)

^1H NMR (400 MHz, CDCl_3) δ 8.19-8.09 (m, 2H, 2xCH), 7.72-7.68 (m, 2H, 2xCH), 6.58 (s, 1H, CH), 3.11 (ht, 1H, J 6.90, CH); 1.35 (d, 6H, J 6.90, 2x CH_3); ^{13}C NMR (100 MHz, CDCl_3) δ 173.31, 151.61, 131.79, 181.10, 126.91, 133.94, 133.66, 126.95, 133.19, 132.73, 102.46, 169.87, 28.52, 20.87.

2-Benzyl naphtho[2,3-*b*]furan-4,9-dione (**6f**)

^1H NMR (400 MHz, CDCl_3) δ 7.51 (s, 2H, 2xCH), 7.30-7.21 (m, 6H), 7.91 (d, 1H, J 7.50, CH), 6.33 (s, 1H, CH), 3.95 (s, 2H, J 6.90, CH_2); ^{13}C NMR (100 MHz, CDCl_3) δ 173.35, 152.07, 131.81, 180.88, 126.96, 134.00, 133.78, 127.02, 133.17, 132.6, 105.55, 163.14, 34.99, 135.64, 129.11.

2-Phenyl naphtho[2,3-*b*]furan-4,9-dione (**6g**)

^1H NMR (400 MHz, CDCl_3) δ 8.24 (dd, 1H, J 6.72 and 1.62, CH), 7.79-7.73 (m, 2H, 2xCH), 8.19 (dd, 1H, J 6.78 and J 1.66, CH), 7.19 (s, 1H, CH), 7.90 (d, 2H, J 7.60, 2xCH), 7.54-7.43 (m, 3H, 2xCH); ^{13}C NMR (100 MHz, CDCl_3) δ 173.26, 151.78, 130.49, 181.04, 127.17, 134.20, 133.83, 127.12, 133.09, 132.64, 103.14, 160.56, 133.31, 129.31, 125.77, 128.53.

2-(4-Chlorophenyl) naphtho[2,3-*b*]furan-4,9-dione (**6h**)

^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, 1H, J 7.62, CH), 7.91 (d, 1H, J 7.64, CH), 7.72 (s, 1H, CH), 7.60 (t, 1H, J 7.72, CH), 7.06 (s, 1H, CH), 7.70-7.68 (m, 2H, 2xCH), 7.49-7.44 (m, 2H, 2xCH); ^{13}C NMR (100 MHz, CDCl_3) δ 71.64, 151.84, 130.89, 181.57, 126.71, 135.45, 132.61, 128.97, 133.10, 132.58, 103.66, 160.17, 135.69, 125.71, 129.34, 135.69.

Table S1. ¹H NMR chemical shifts (δ), multiplicities and coupling constants (J) for compounds **4a-h** and lapachol (**1**)

δ / ppm (multiplicity, J / Hz)									
	Lapachol	4a	4b	4c	4d	4e	4f	4g	4h
H-5	8.11(d, 7.50)	8.09 (d,7.60)	8.11 (dd, 7.30; 1.40)	8.11(dd, 7.30; 1.30)	8.11 (d, 7.60)	8.12 (d, 7.60)	8.12 (d, 7.40)	8.14 (d, 7.30)	8.16(dd, 7.70; 0.70)
H-6	7.74 (dt, 0.88; 7.50)	7.72 (t,7.50)	7.77-7.61 (m)	7.78- 7.62 (m)	7.73 (t, 7.40)	7.71- 7.64 (m)	7.73- 7.65 (m)	7.78- 7.56 (m)	7.71 (dt, 7.60; 1.30)
H-7	7.66 (dt, 0.84; 7.50)	7.65 (t,7.50)	7.77-7.61 (m)	7.78- 7.62 (m)	7.64 (t, 7.40)	7.71- 7.64 (m)	7.73- 7.65 (m)	7.78- 7.56 (m)	7.71 (dt, 7.60; 1.30)
H-8	8.05 (d, 7.50)	8.03 (d, 7.50)	8.05 (dd, 7.00; 1.00)	8.04 (dd, 7.30; 1.40)	8.04 (d, 7.60)	8.06 (d, 7.40)	8.05 (d, 7.20)	8.06 (d, 7.60)	8.11 (dd, 8.10; 0.80)
H-1'	3.30 (d, 7.40)	6.60 (d, 16.10)	6.60 (d, 16.20)	6.61 (d, 16.20)	6.60 (d, 16.00)	6.60 (d, 16.30)	6.71 (d, 16.10)	7.78- 7.56 (m)	7.38- 7.34 (m)
H-2'	5.21 (t, 7.40)	7.10- 7.00 (m)	7.17- 6.98 (m)	7.17- 6.98 (m)	7.10- 7.03 (m)	7.04 (dd, 7.20; 16.30)	7.35- 7.12 (m)	7.94 (br)	7.94 (d, 16.70)
H-3'	—	1.97 (d, 6.80)	2.32 (quint,7.40)	2.27 (q, 7.30)	2.30 (q, 7.00)	2.53 (m)	3.63 (d, 7.00)	—	—
H-4'	1.49 (s)	—	1.12 (t)	1.53 (st, 6.80)	1.49 (quint, 7.20)	1.12 (d, 7.00)	—	7.41- 7.8 (m)	7.38- 7.34 (m)
H-5'	1.68 (s)	—	—	0.97 (t, 7.30)	1.38 (st, 7.20)	—	7.35- 7.12 (m)	—	7.78- 7.56 (m)
H-6'	—	—	—	—	0.93 (t, 7.20)	—	—	—	—
H-7'	—	—	—	—	—	—	—	—	—

s: singlet; d: doublet; t: triplet; q: quartet; quint: quintet; s: sextet; m: multiplet; dd: doublet of doublets; dt: doublet of triplets; br: broad singlet.

Table S2. ^{13}C NMR chemical shifts (δ) for compounds **4a-h**

		δ / ppm							
	Lapachol	4a	4b	4c	4d	4e	4f	4g	4h
C1	181.88	181.58	181.57	181.61	181.56	181.55	181.17	181.50	181.36
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)
C2	152.90	151.40	151.47	151.46	151.47	151.50	151.50	151.76	152.26
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)
C3	123.68	120.18	118.91	119.00	120.18	118.98	118.92	119.98	118.65
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)
C4	184.75	184.40	184.51	184.53	184.50	184.54	184.31	184.33	184.31
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)
C5	126.95	127.21	127.20	127.22	127.19	127.20	127.37	126.45	127.45
	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)
C6	135.00	135.01	135.06	135.06	135.02	135.06	135.14	135.14	135.34
	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)
C7	133.10	133.17	133.21	133.22	133.16	133.20	133.37	133.27	133.50
	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)
C8	126.22	126.04	126.11	126.12	126.08	126.11	126.23	126.17	126.39
	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)
C9	129.64	129.64	129.61	129.63	129.62	129.60	129.76	129.56	129.81
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)
C10	133.02	132.89	132.87	132.90	132.87	132.92	132.90	132.89	132.99
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)
C1'	25.92	118.87	117.98	118.88	118.80	116.15	117.57	118.50	118.24
	(CH ₂)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)
C2'	119.86	138.97	145.61	144.20	144.40	150.66	139.46	141.76	138.07
	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)	(CH)
C3'	134.00	20.70	28.19	37.30	34.95	33.64	39.70	141.49	136.59
	(C)	(CH ₃)	(CH ₂)	(CH ₂)	(CH ₂)	(CH)	(CH ₂)	(C)	(C)
C4'	18.06	–	13.49	22.52	31.45	22.38	128.89	139.80	124.54
	(CH ₃)	–	(CH ₃)	(CH ₂)	(CH ₂)	(CH ₃)	(C)	(CH)	(CH)
C5'	22.80	–	–	13.99	22.55	–	127.36	128.88	129.15
	(CH ₃)	–	–	(CH ₃)	(CH ₂)	–	(CH)	(CH)	(CH)
C6'	–	–	–	–	14.14	–	126.80	128.74	134.50
	–	–	–	–	(CH ₃)	–	(CH)	(CH)	(C)
C7'	–	–	–	–	–	–	127.23 (CH)	–	–

Table S3. ¹H NMR chemical shifts (δ), multiplicities and coupling constants (J) for compounds **5a-h**

δ / ppm (multiplicity, J / Hz)								
	5a	5b	5c	5d	5e	5f	5g	5h
H-5	7.59 (d, 7.70)	8.18-8.09 (m)	7.66-7.57 (m)	7.64- 7.58 (m)	7.66- 7.56 (m)	7.52 (br)	7.78 (d, 7.60)	7.81 (d, 7.60)
H-6	7.59 (d, 7.70)	7.73-7.68 (m)	7.66-7.57 (m)	7.64- 7.58 (m)	7.66- 7.56 (m)	7.52 (br)	7.72 (br)	7.50 (t, 7.70)
H-7	7.43- 7.37 (m)	7.73-7.68 (m)	7.45-7.37 (m)	7.40 (t, 7.80)	7.44- 7.36 (m)	7.30-7.21 (m)	7.72 (br)	7.71 (br)
H-8	7.99 (d, 7.70)	8.18-8.09 (m)	8.03 (d, 7.70)	8.00 (d, 7.80)	8.01 (d, 7.50)	7.92 (d, 7.50)	8.06 (d, 7.70)	8.11 (d, 7.70)
H-1'	6.40 (s)	6.59 (s)	6.44 (s)	6.42 (s)	6.42 (s)	6.33 (s)	7.01 (s)	—
H-3'	2.40 (s)	2.83 (q, 7.50)	2.69 (t, 7.60)	2.71 (t, 7.60)	3.01 (h, 6.80)	3.95 (s)	—	—
H-4'	—	1.34 (t, 7.6)	1.75 (s, 7.40)	1.70 (qt, 7.60)	1.32 (d, 6.90)	—	7.47- 7.58 (m)	7.69-7.68 (m)
H-5'	—	—	1.03 (t, 7.50)	1.44 (st, 7.60)	—	7.30-7.21 (m)	—	7.48-7.44 (m)
H-6'	—	—	—	0.97 (t, 7.60)	—	—	7.66 (t, 7.60)	—
H-7'	—	—	—	—	—	7.30-7.20 (m)	—	—

s: singlet; d: doublet; t: triplet; q: quartet; quint: quintet; s: sextet; m: multiplet; dd: doublet of doublets; dt: doublet of triplets; br: broad singlet.

Table S4. ¹³C NMR chemical shifts (δ) for compounds **5a-h**

	δ / ppm							
	5a	5b	5c	5d	5e	5f	5g	5h
C1	180.76 (C)	180.94 (C)	180.94 (C)	180.89 (C)	183.91 (C)	180.69 (C)	180.55 (C)	180.57 (C)
C2	174.44 (C)	174.61 (C)	174.66 (C)	174.60 (C)	180.92 (C)	174.50 (C)	174.63 (C)	174.64 (C)
C3	122.77 (C)	122.67 (C)	122.66 (C)	122.68 (C)	122.49 (C)	122.58 (C)	123.51 (C)	123.56 (C)
C4	156.08 (C)	159.76 (C)	159.65 (C)	159.65 (C)	158.09 (C)	159.59 (C)	156.94 (C)	155.91 (C)
C5	122.07 (CH)	122.14 (CH)	122.19 (CH)	122.15 (CH)	122.18 (CH)	122.30 (CH)	122.41 (CH)	122.51 (CH)
C6	135.49 (CH)	135.46 (CH)	135.53 (CH)	135.46 (CH)	135.47 (CH)	135.49 (CH)	135.63 (CH)	135.45 (CH)
C7	129.91 (CH)	129.92 (CH)	129.95 (CH)	130.55 (CH)	129.95 (CH)	130.09 (CH)	129.42 (CH)	130.61 (CH)
C8	126.04 (CH)	126.11 (CH)	126.12 (CH)	129.90 (CH)	126.11 (CH)	126.23 (CH)	126.17 (CH)	126.39 (CH)
C9	128.75 (C)	128.90 (C)	128.94 (C)	128.92 (C)	128.92 (C)	128.77 (C)	129.08 (C)	129.57 (C)
C10	128.64 (C)	128.79 (C)	128.76 (C)	128.78 (C)	128.77 (C)	128.68 (C)	128.85 (C)	128.55 (C)
C1'	104.69 (CH)	103.17 (CH)	104.00 (CH)	103.84 (CH)	102.01 (CH)	105.34 (CH)	103.02 (CH)	103.65 (CH)
C2'	159.70 (C)	161.64 (C)	160.30 (C)	160.49 (C)	165.55 (C)	160.20 (C)	159.91 (C)	160.16 (C)
C3'	13.70 (CH ₃)	21.45 (CH ₂)	29.98 (CH ₂)	27.70 (CH ₂)	28.03 (CH)	34.52 (CH ₂)	128.63 (C)	125.93 (C)
C4'	—	11.81 (CH ₃)	21.06 (CH ₂)	29.71 (CH ₂)	20.86 (CH ₃)	136.17 (C)	129.21 (CH)	125.70 (CH)
C5'	—	—	13.77 (CH ₃)	22.28 (CH ₂)	—	128.98 (CH)	124.61 (CH)	129.35 (CH)
C6'	—	—	—	13.85 (CH ₃)	—	128.93 (CH)	130.80 (CH)	135.70 (C)
C7'	—	—	—	—	—	127.33 (CH)	—	—

Table S5. ¹H NMR chemical shifts (δ), multiplicities and coupling constants (J) for compounds **6a-h**

δ / ppm (multiplicity, J / Hz)								
	6a	6b	6c	6d	6e	6f	6g	6h
H-5	8.20- 8.18 (m)	8.19 (d, 7.64)	8.21-8.11 (m)	8.19 (dd, 3.00; 6.00)	8.19-8.09 (m)	8.11-8.01 (m)	8.21 (br)	8.12 (d, 7.6)
H-6	8.16- 8.14 (m)	7.75- 7.69 (m)	7.77-7.70 (m)	7.75-7.69 (m)	7.72-7.68 (m)	7.64-7.60 (m)	7.91-7.88 (m)	7.60 (t, 7.7)
H-7	8.16- 8.14 (m)	7.75- 7.69 (m)	7.77-7.70 (m)	7.75-7.69 (m)	7.72-7.68 (m)	7.64-7.60 (m)	7.91-7.88 (m)	7.72 (br)
H-8	8.20- 8.18 (m)	8.14 (d, 6.32)	8.21-8.11 (m)	8.14 (dd, 3.00; 6.00)	8.19-8.09 (m)	8.11-8.01 (m)	8.21 (br)	7.91 (d, 7.60)
H-1'	6.60 (s)	6.61 (s)	6.61 (s)	6.60 (s)	6.58 (s)	6.45 (s)	7.26-7.19 (m)	7.06 (s)
H-3'	2.52 (s)	2.85 (q, 7.50)	2.79 (t, 7.48)	2.81 (t, 7.60)	3.11 (h, 6.90)	4.04 (s)	—	—
H-4'	—	1.36 (t, 7.50)	1.80 (st, 7.40)	1.75 (qt, 7.60)	1.35 (d, 6.90)	—	7.77-7.75 (m)	7.70-7.68 (m)
H-5	—	—	1.02 (t, 7.36)	1.43 (st, 7.50)	—	7.26-7.22 (m)	7.49-7.46 (m)	7.49-7.44 (m)
H-6'	—	—	—	0.96 (t, 7.50)	—	—	—	—
H-7'	—	—	—	—	—	—	—	—

s: singlet; d: doublet; t: triplet; q: quartet; quint: quintet; s: sextet; m: multiplet; dd: doublet of doublets; dt: doublet of triplets; br: broad singlet.

Table S6. ^{13}C NMR chemical shifts (δ) for compounds **6a-h**

[illegible]

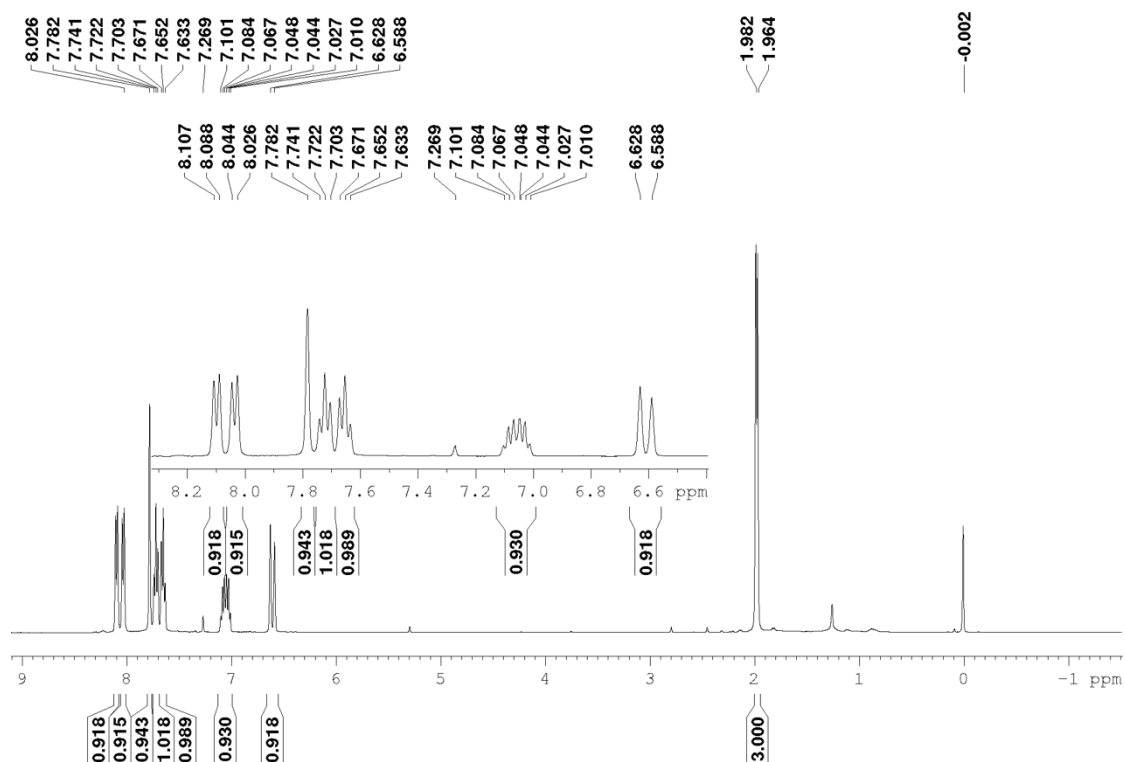


Figure S1. ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-2-hydroxy-3-(prop-1-en-1-yl)naphthalene-1,4-dione (**4a**).

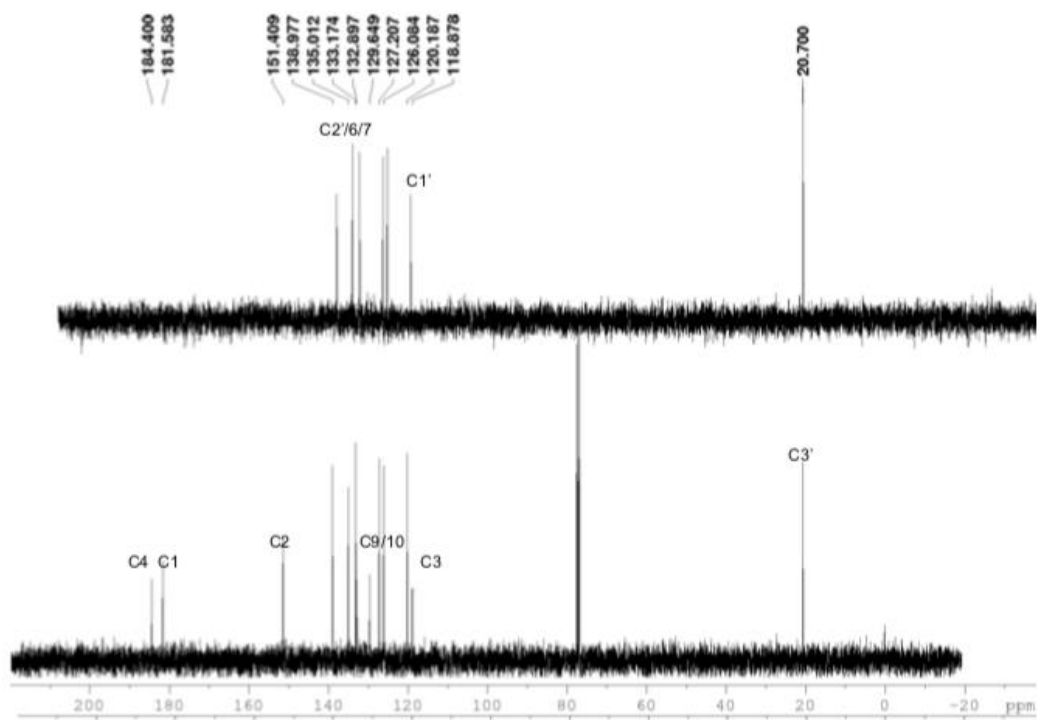


Figure S2. ¹³C NMR spectrum (100 MHz, CDCl₃) and distortionless enhancement by polarization transfer (DEPT) 135 of (*E*)-2-hydroxy-3-(prop-1-en-1-yl)naphthalene-1,4-dione (**4a**).

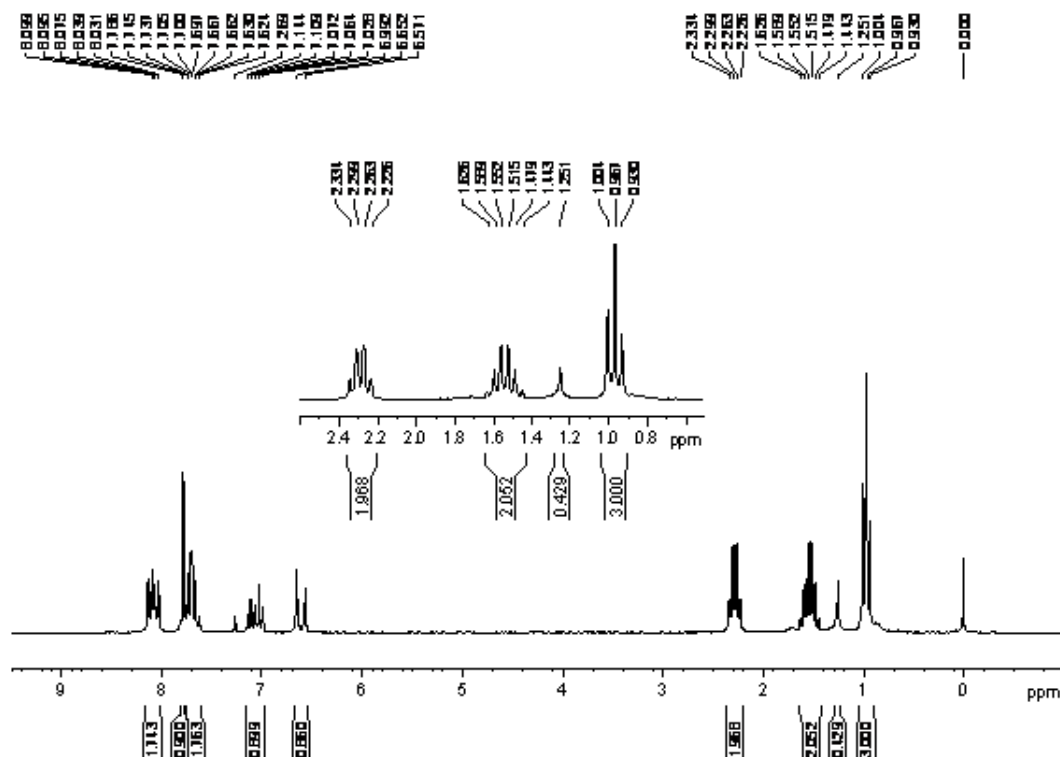


Figure S5. ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-2-hydroxy-3-(pent-1-en-1-yl)naphthalene-1,4-dione (**4c**).

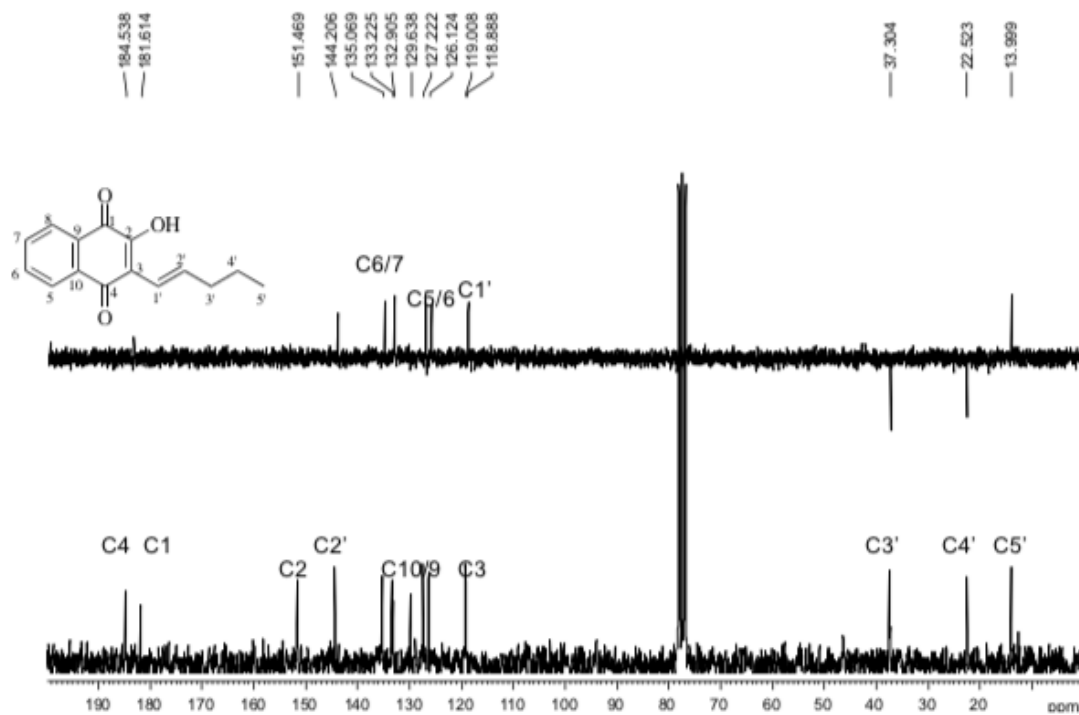


Figure S6. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of (*E*)-2-hydroxy-3-(pent-1-en-1-yl)naphthalene-1,4-dione (**4c**).

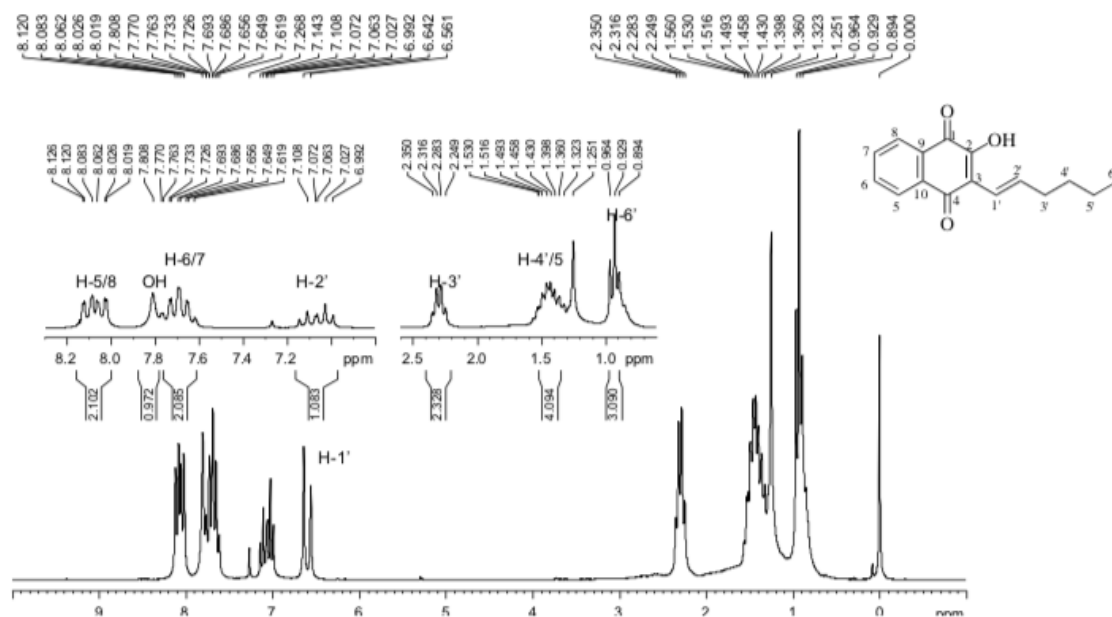


Figure S7. ¹H NMR spectrum (400 MHz, CDCl₃) of (E)-2-hydroxy-3-(hex-1-en-1-yl)naphthalene-1,4-dione (**4d**).

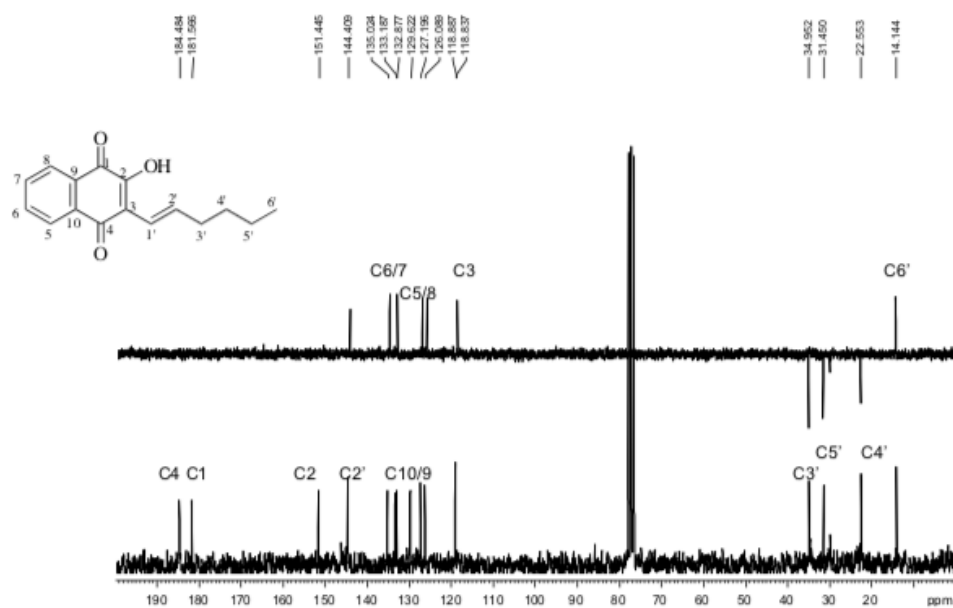


Figure S8. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of (E)-2-hydroxy-3-(hex-1-en-1-yl)naphthalene-1,4-dione (**4c**).

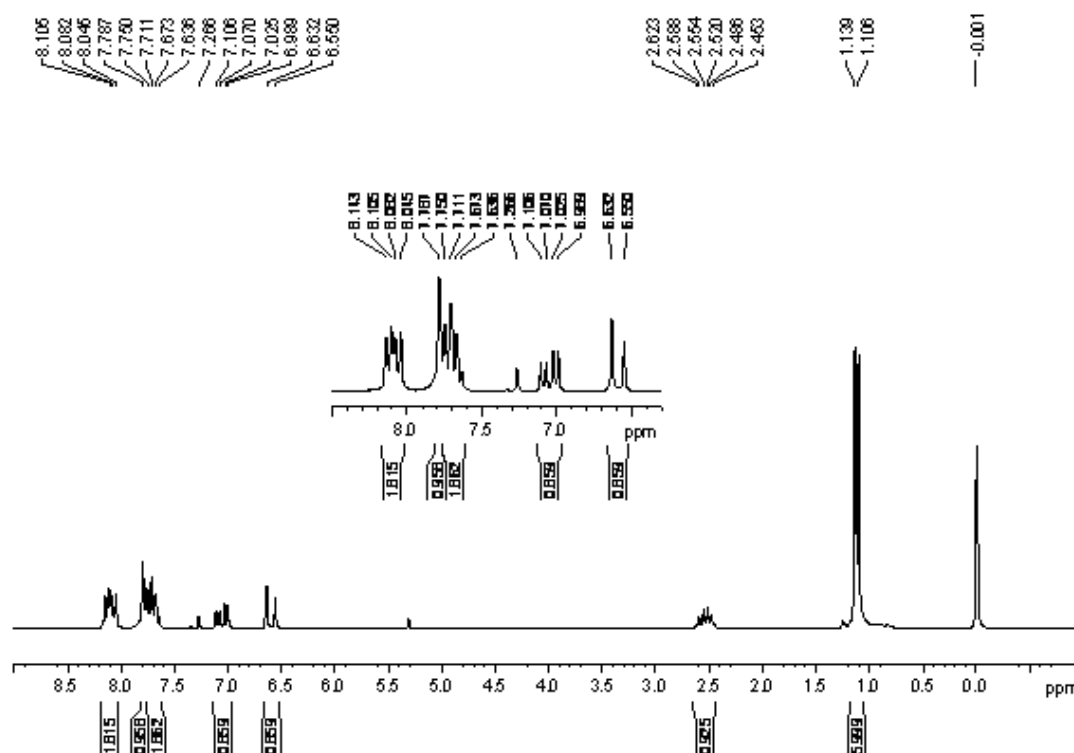


Figure S9. ¹H NMR spectrum (400 MHz, CDCl₃) of (*E*)-2-hydroxy-3-(3-methylbut-1-en-1-yl)naphthalene-1,4-dione (**4e**).

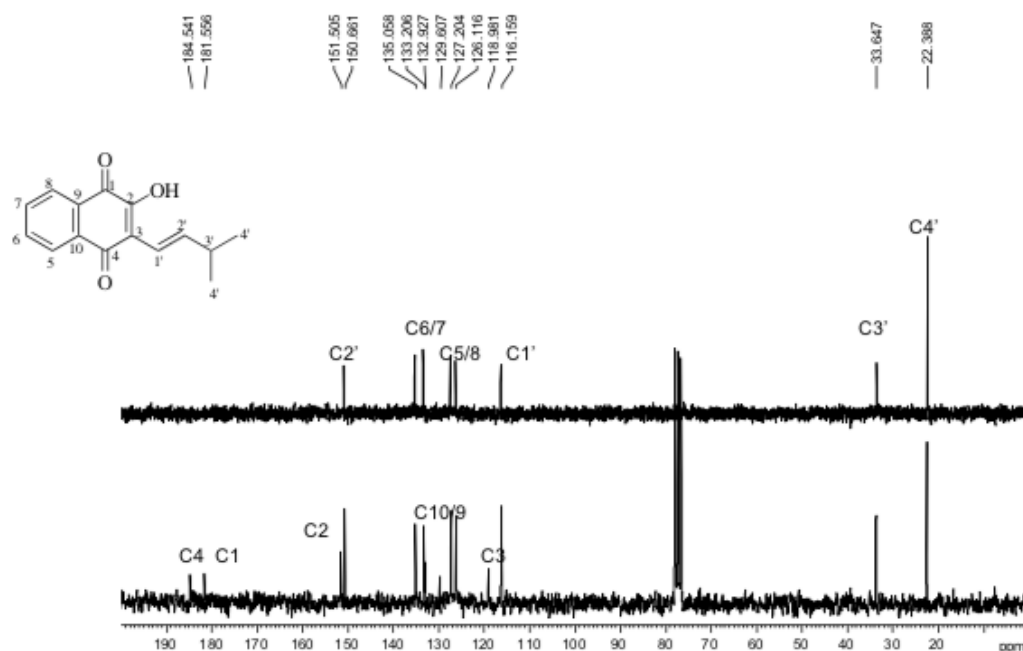


Figure S10. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of (*E*)-2-hydroxy-3-(3-methylbut-1-en-1-yl)naphthalene-1,4-dione (**4e**).

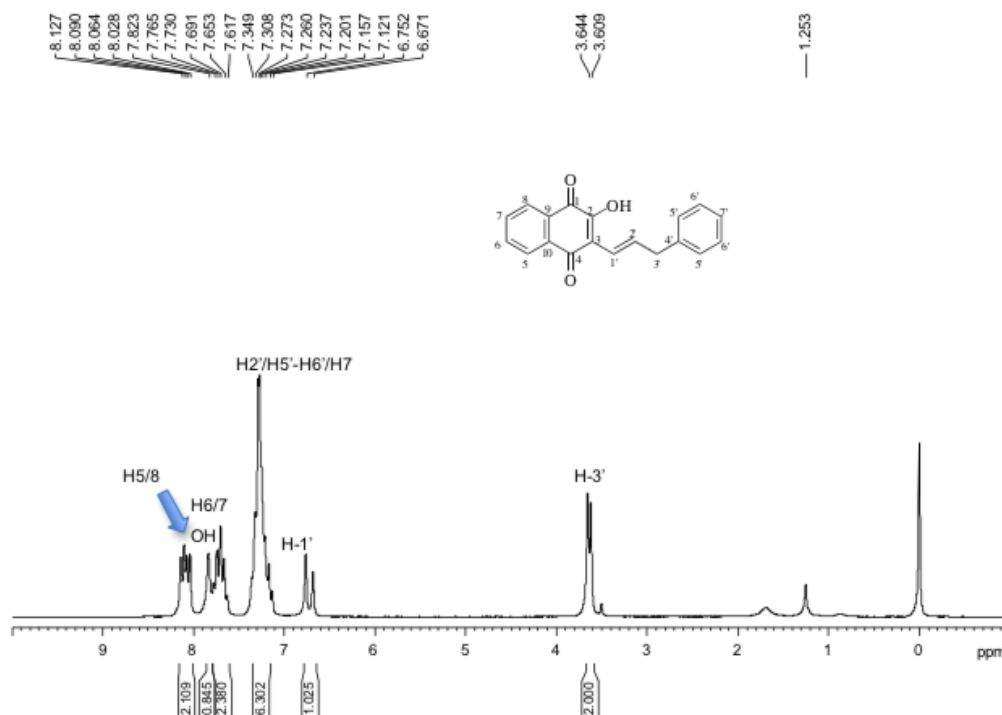


Figure S11. ^1H NMR spectrum (400 MHz, CDCl_3) of (*E*)-2-hydroxy-3-(3-phenylprop-1-en-1-yl)naphthalene-1,4-dione (**4f**).

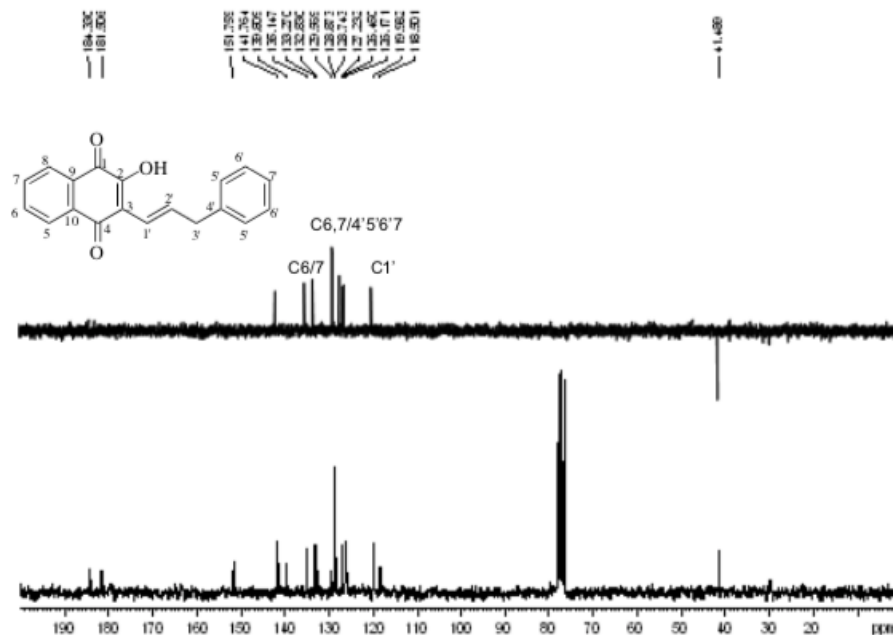


Figure S12. ^{13}C NMR spectrum (100 MHz, CDCl_3) and DEPT 135 of (*E*)-2-hydroxy-3-(3-phenylprop-1-en-1-yl)naphthalene-1,4-dione (**4f**).

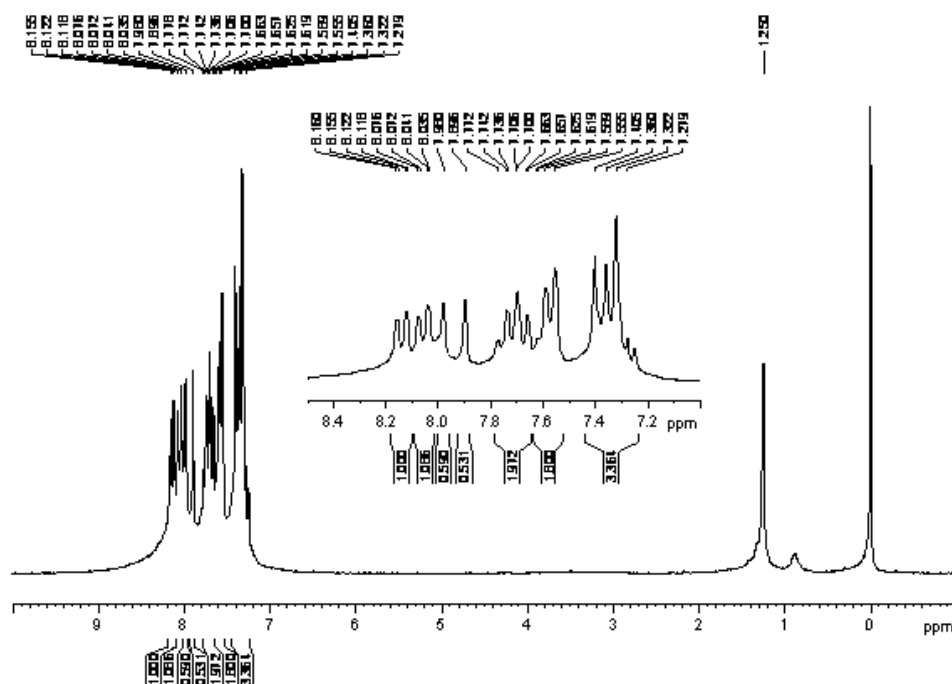


Figure S13. ¹H NMR spectrum (400 MHz, CDCl₃) of (E)-2-hydroxy-3-styrylnaphthalene-1,4-dione (**4g**).

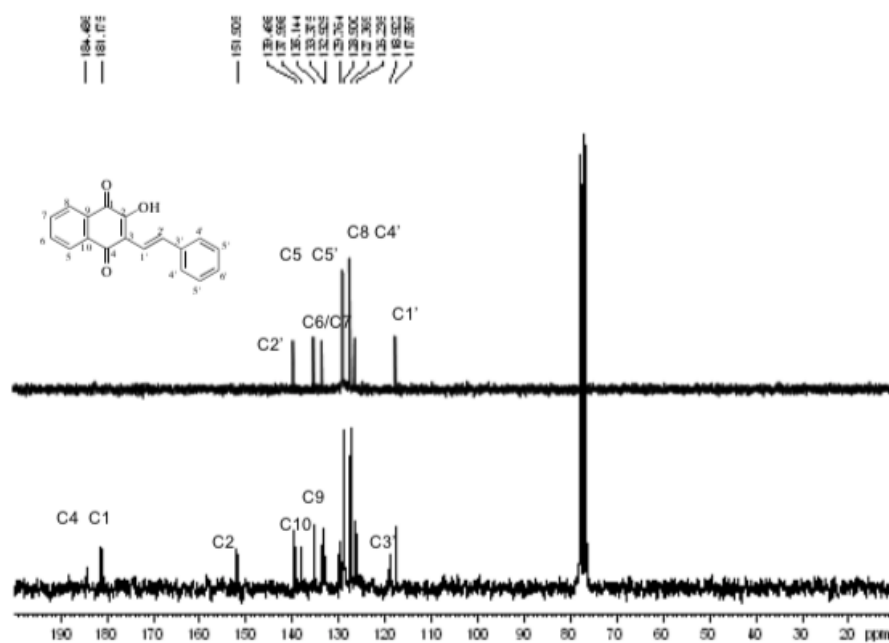


Figure S14. ¹³C NMR spectrum (100 MHz, CDCl₃) and of DEPT 135 of (E)-2-hydroxy-3-styrylnaphthalene-1,4-dione (**4g**).

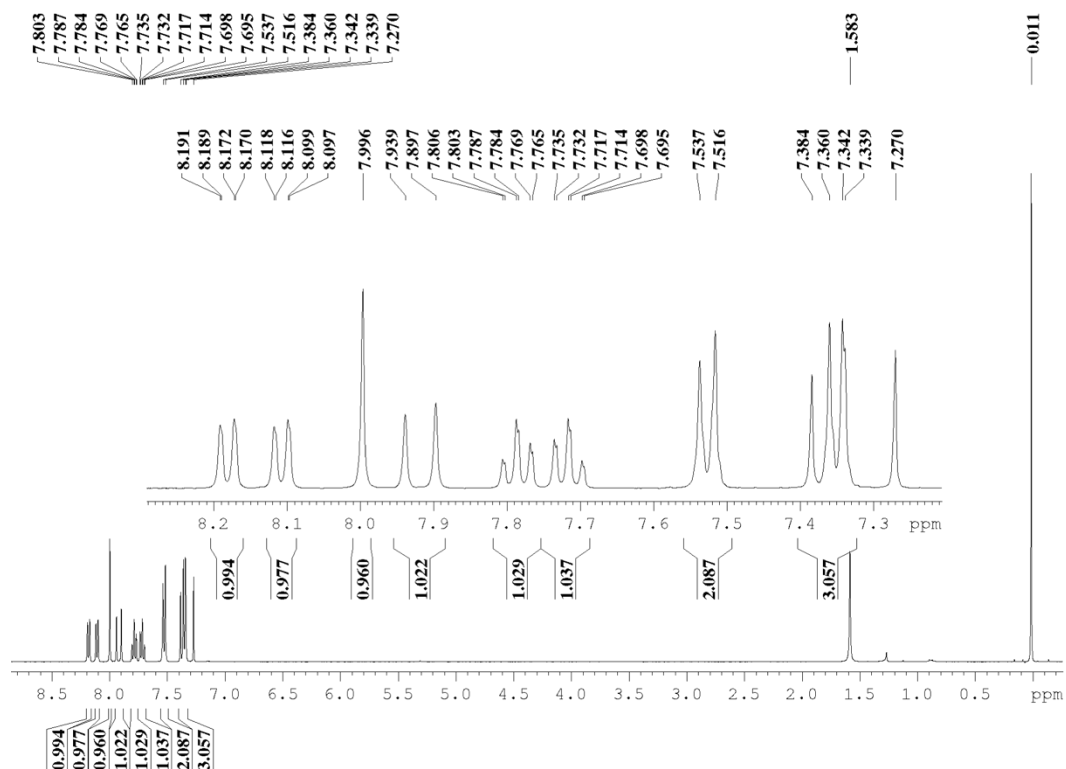


Figure S15. ¹H NMR spectrum (400 MHz, CDCl₃) of (E)-2-(4-chlorostyryl)-3-hydroxynaphthalene-1,4-dione (4h).

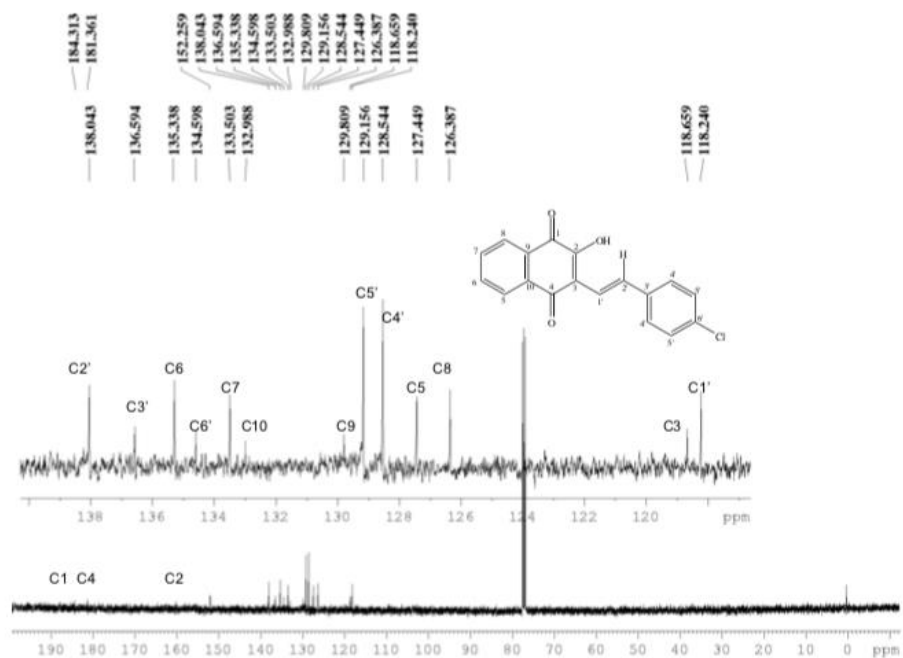


Figure S16. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT of 135 (E)-2-(4-chlorostyryl)-3-hydroxynaphthalene-1,4-dione (4h).

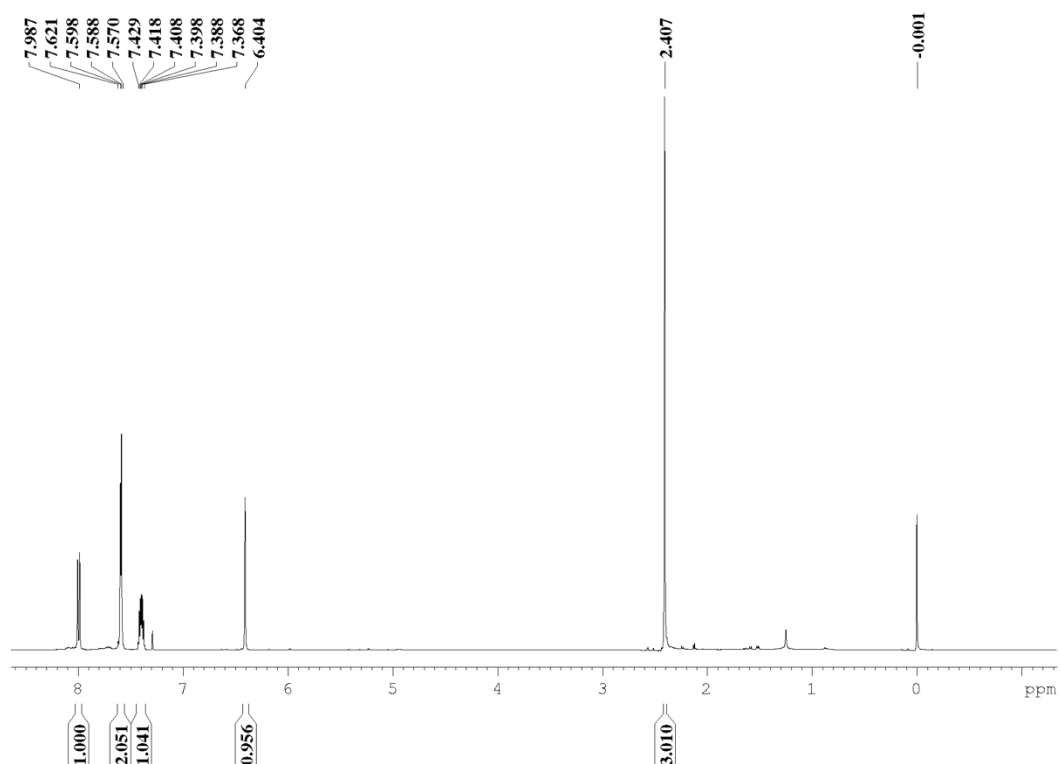


Figure S17. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-methylnaphtho[1,2-*b*]furan-4,5-dione (5a).

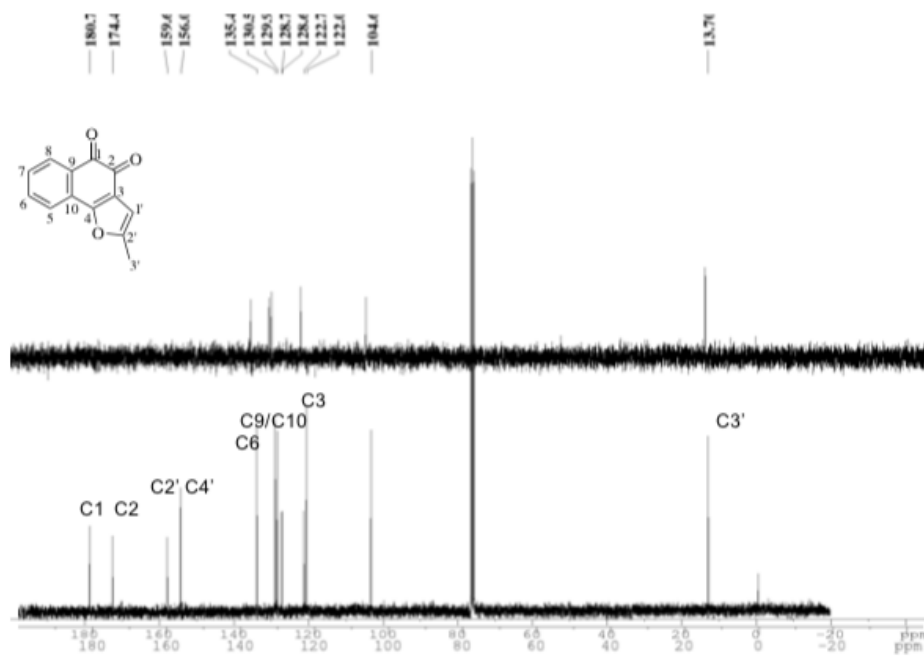


Figure S18. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-methylnaphtho[1,2-*b*]furan-4,5-dione (5a).

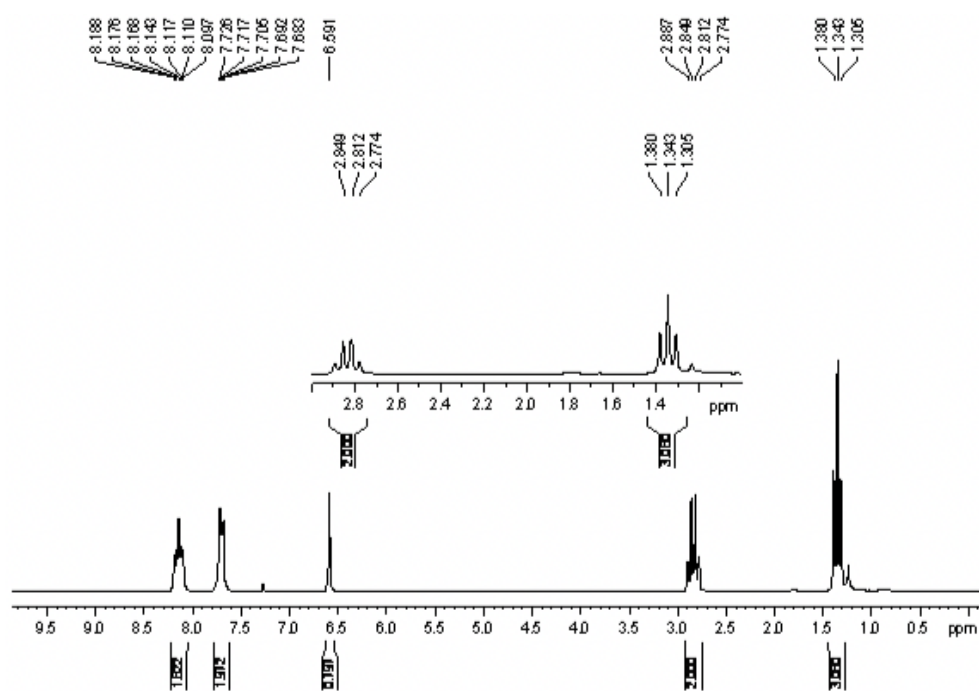


Figure S19. ^1H NMR spectrum (400 MHz, CDCl_3) of 2-ethylnaphtho[1,2-*b*]furan-4,5-dione (**5b**).

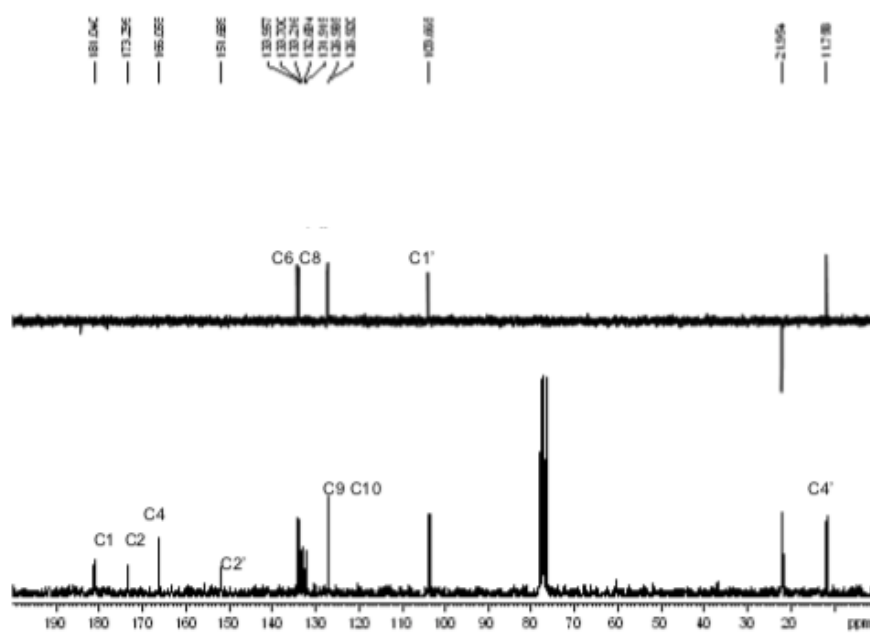


Figure S20. ^{13}C NMR spectrum (100 MHz, CDCl_3) and DEPT 135 of 2-ethylnaphtho[1,2-*b*]furan-4,5-dione (**5b**).

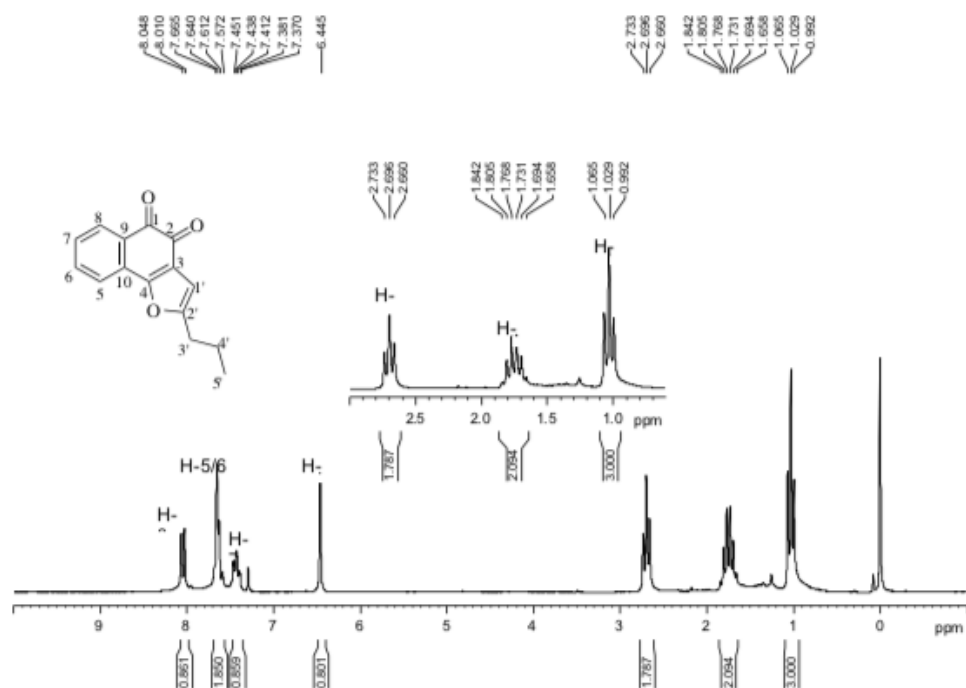


Figure S21. ^1H NMR spectrum (400 MHz, CDCl_3) of 2-propylnaphtho[1,2-*b*]furan-4,5-dione (5c).

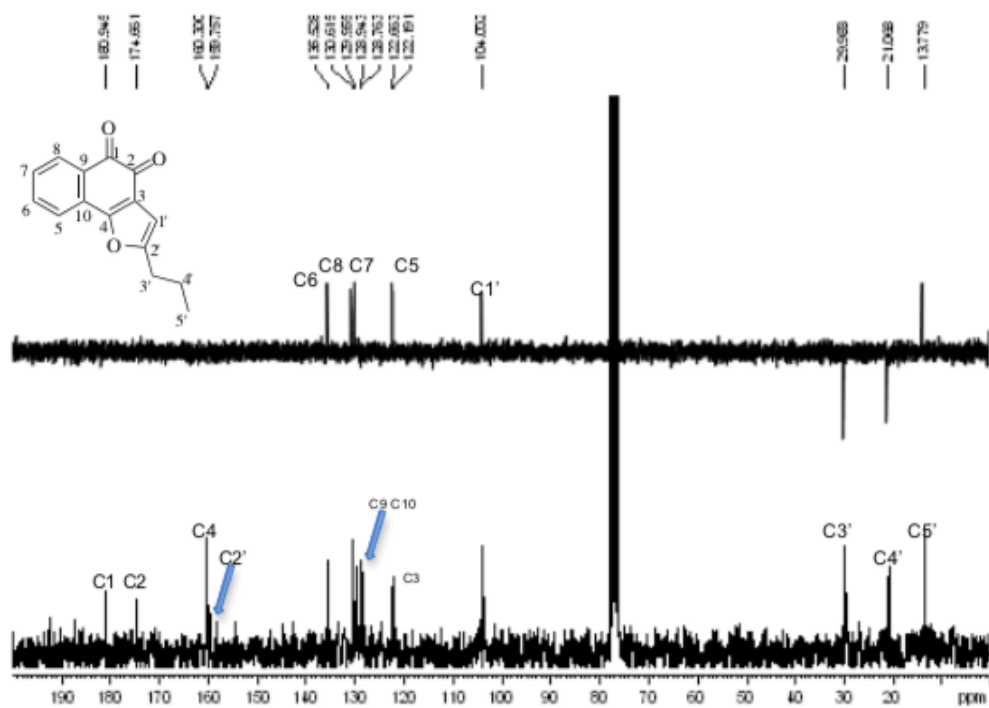


Figure S22. ^{13}C NMR spectrum (100 MHz, CDCl_3) and DEPT 135 of 2-propylnaphtho[1,2-*b*]furan-4,5-dione (5c).

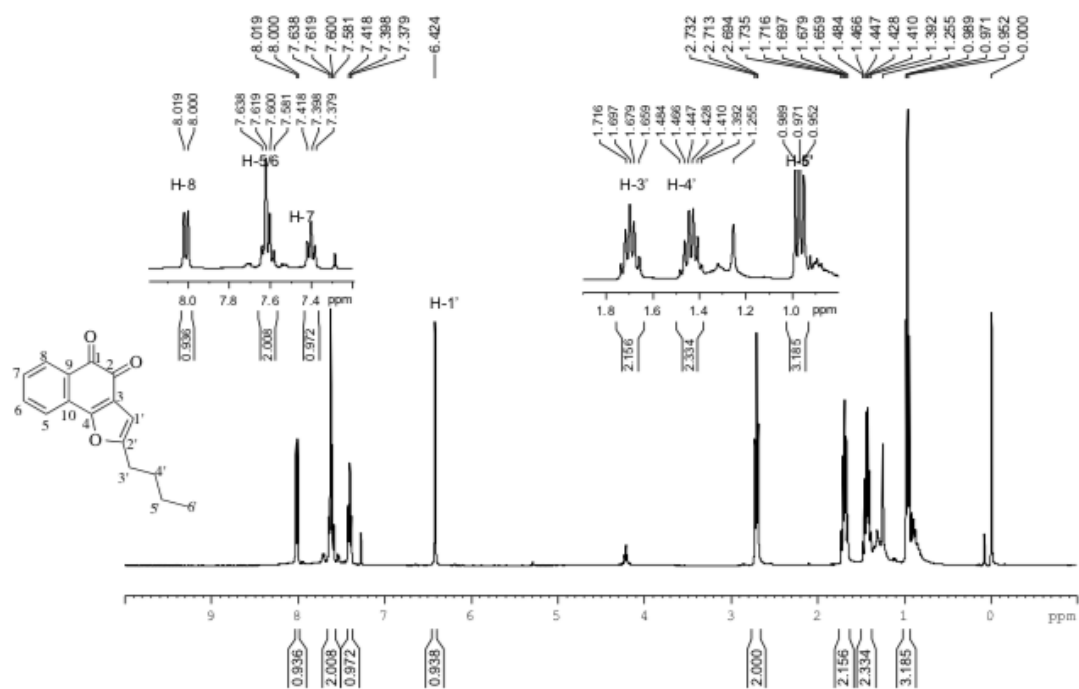


Figure S23. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-butyl-naphtho[1,2-*b*]furan-4,5-dione (5d).

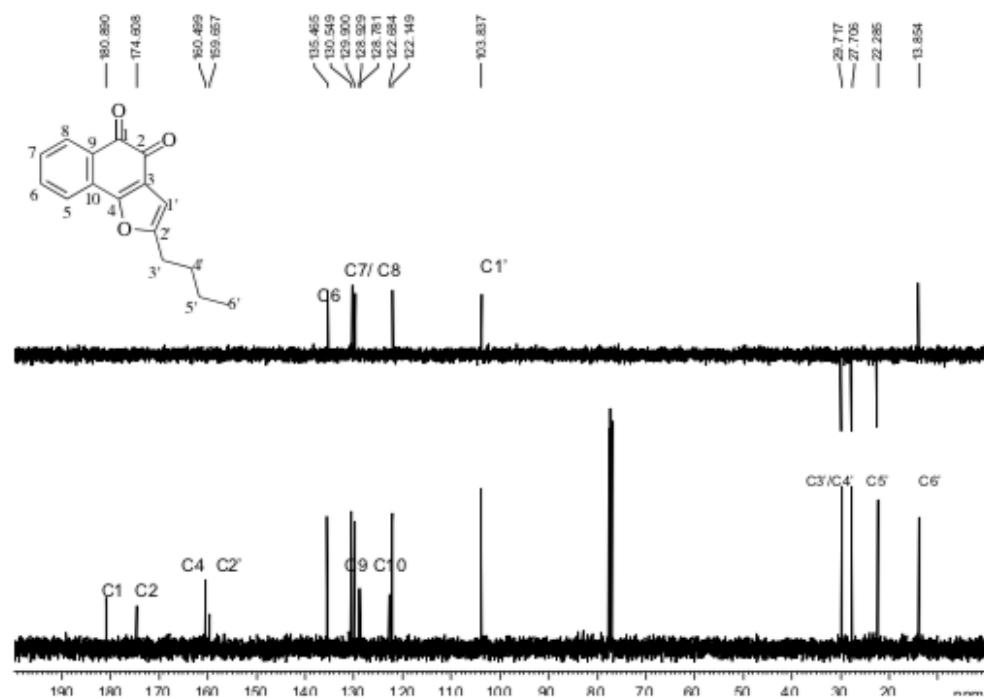


Figure S24. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-butyl-naphtho[1,2-*b*]furan-4,5-dione (5d).

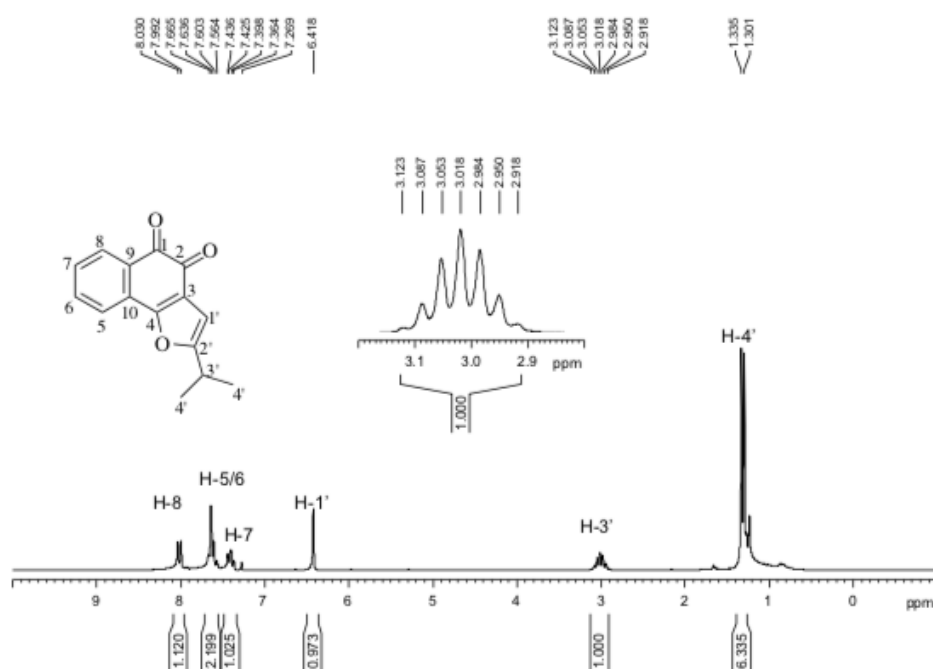


Figure S25. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-isopropyl-naphtho[1,2-*b*]furan-4,5-dione (5e).

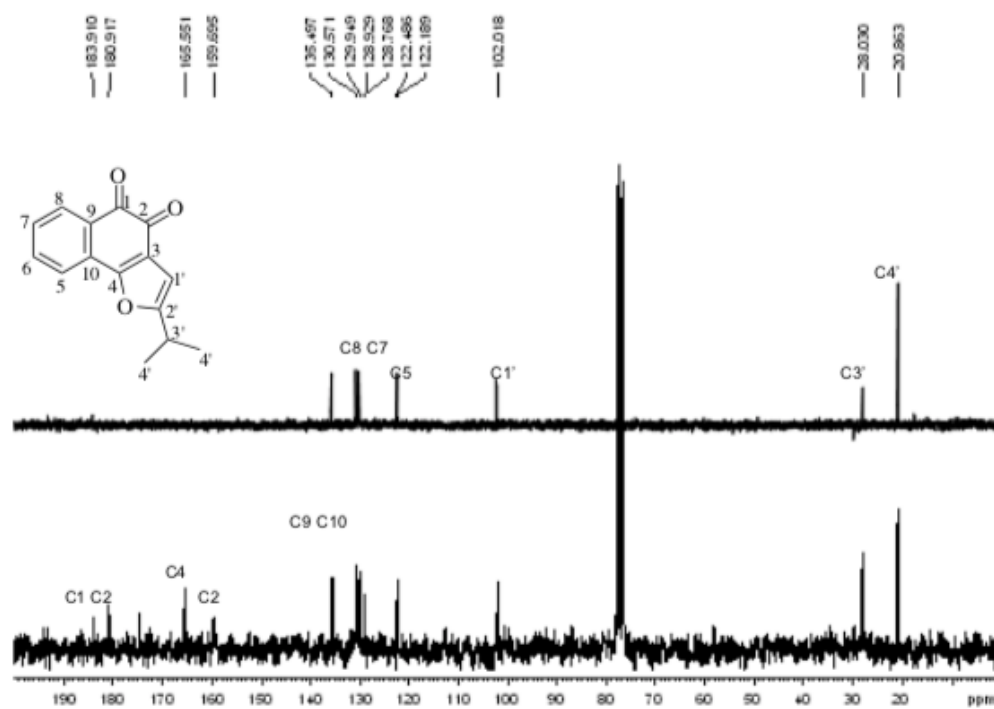


Figure S26. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-isopropyl-naphtho[1,2-*b*]furan-4,5-dione (5e).

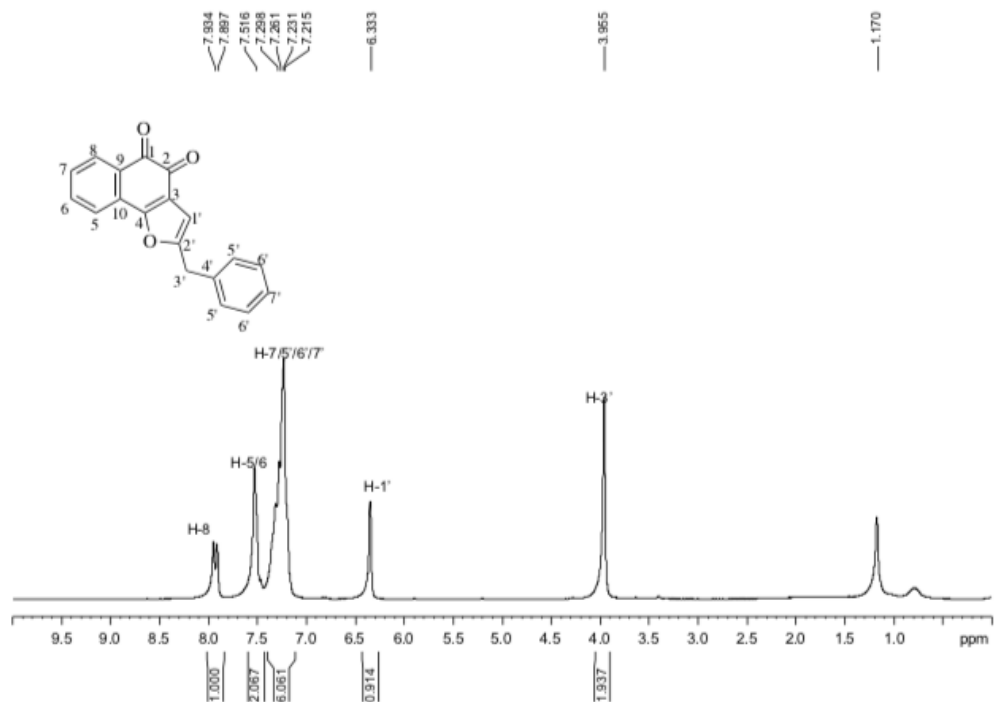


Figure S27. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-benzylphthalophthalide (5f).

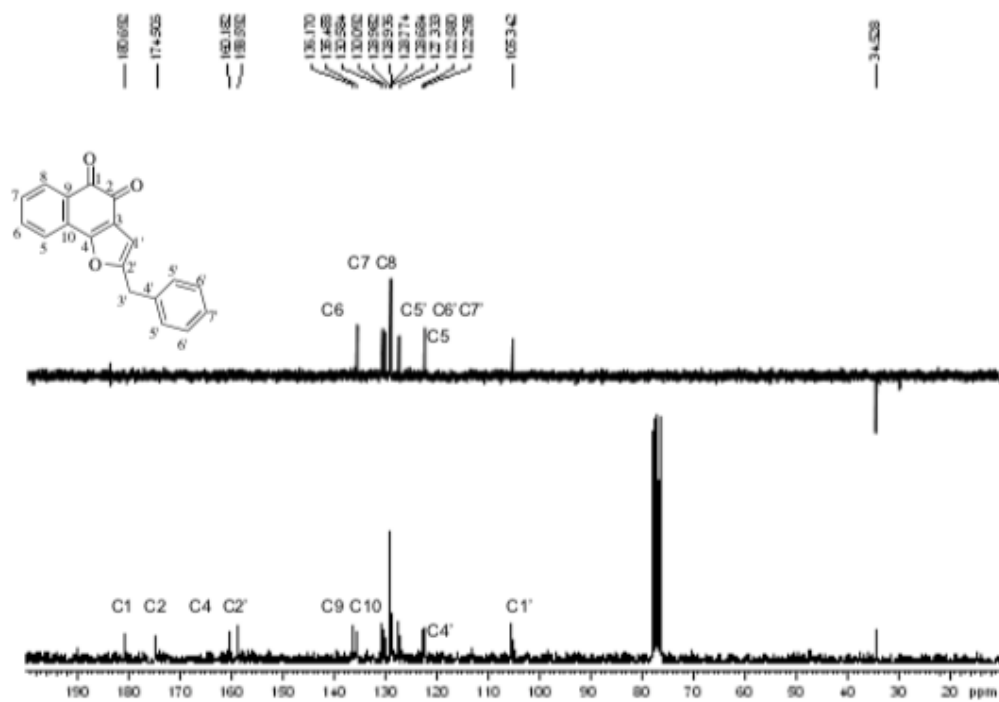


Figure S28. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-benzylphthalophthalide (5f).

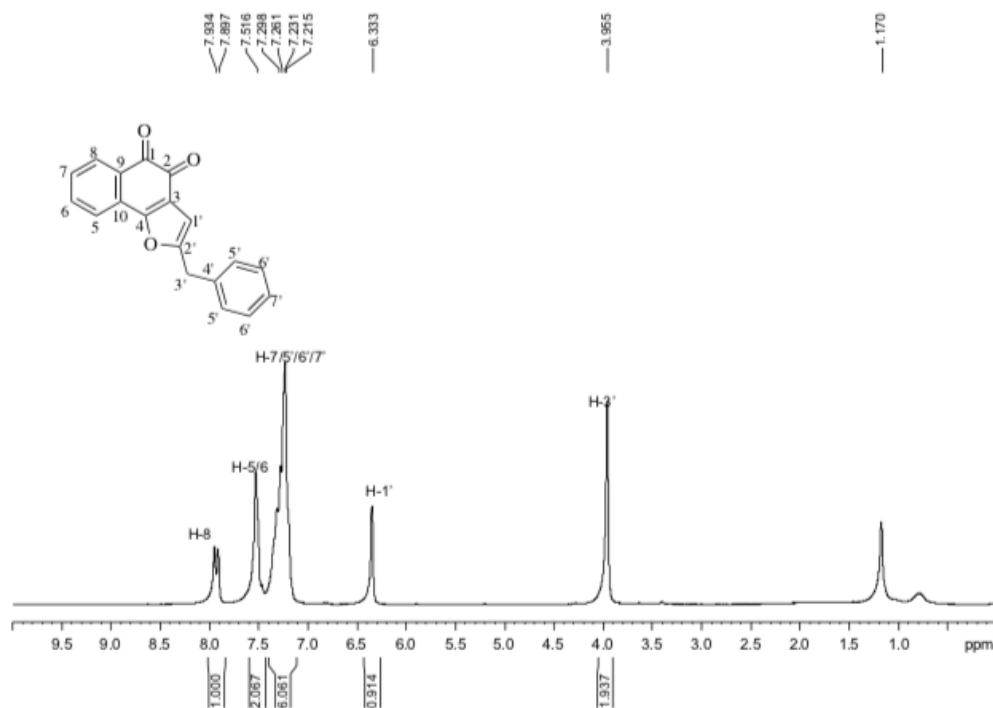


Figure S29. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-phenylnaphtho[1,2-*b*]furan-4,5-dione (5f).

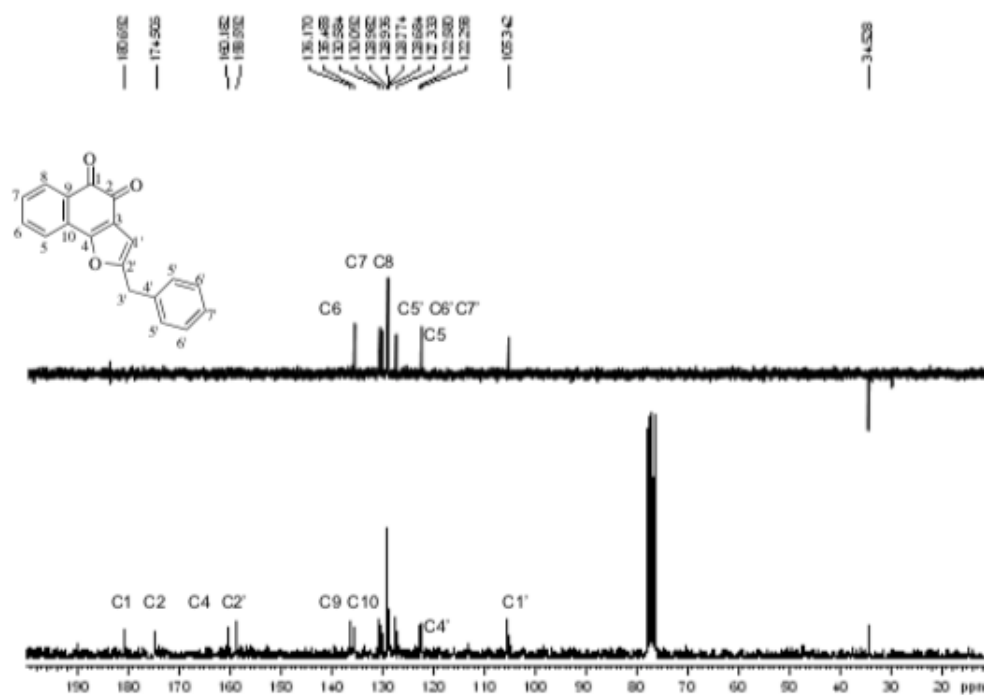


Figure S30. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-phenylnaphtho[1,2-*b*]furan-4,5-dione (5f).

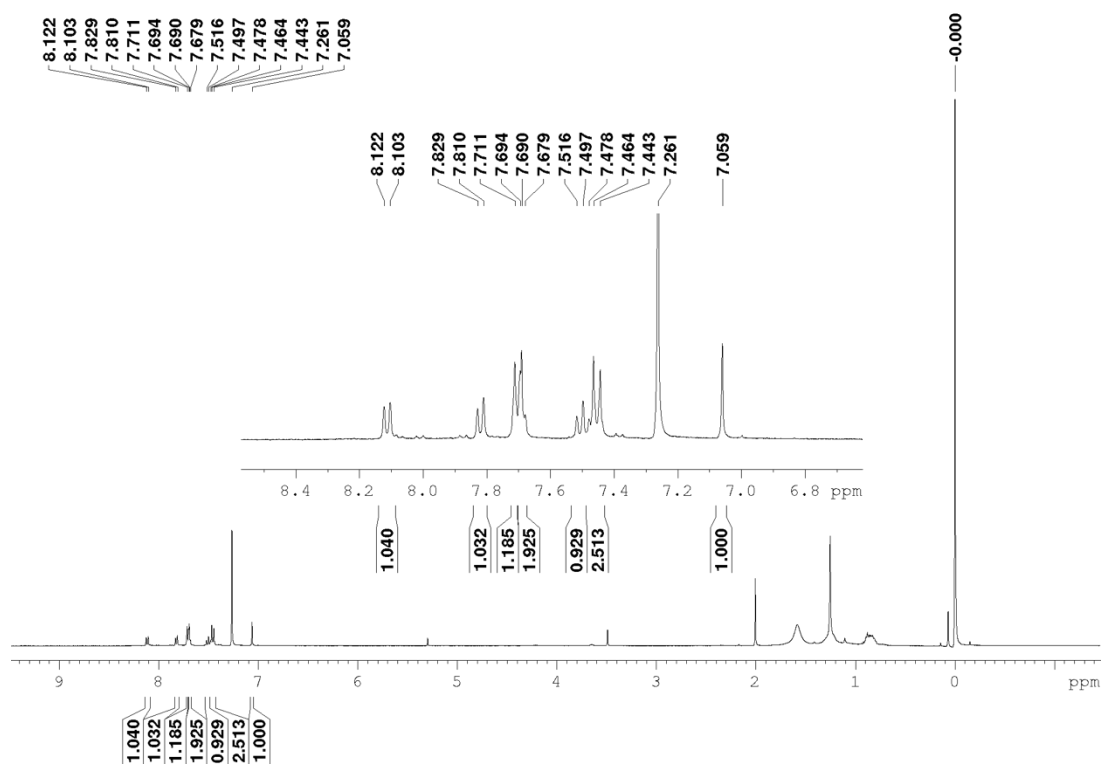


Figure S31. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-(4-chlorophenyl)naphtho[1,2-*b*]furan-4,5-dione (5h).

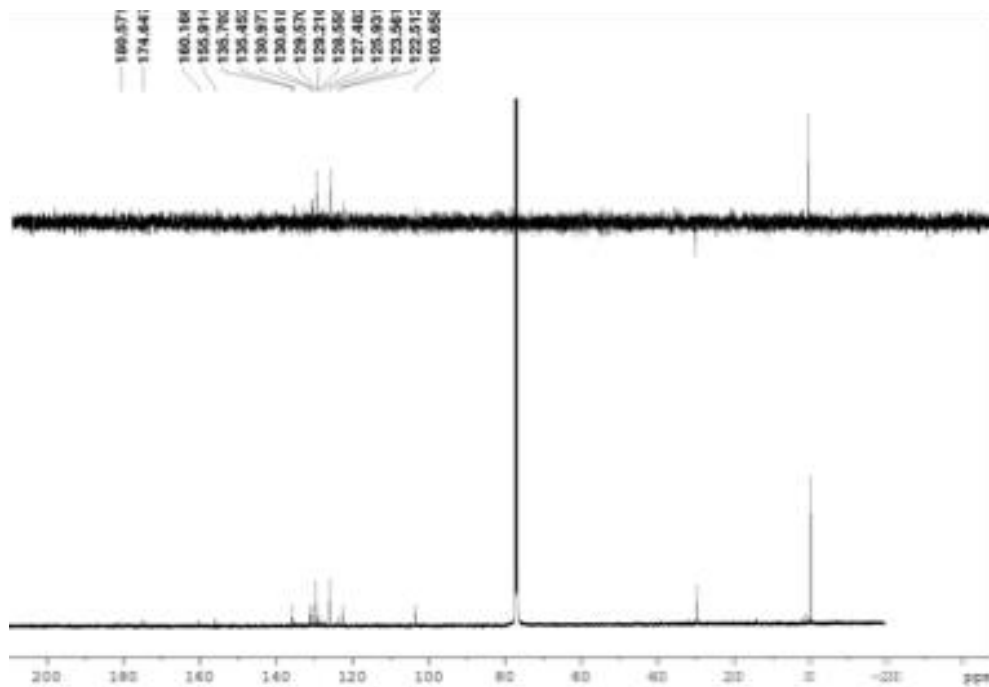


Figure S32. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-(4-chlorophenyl)naphtho[1,2-*b*]furan-4,5-dione (5h).

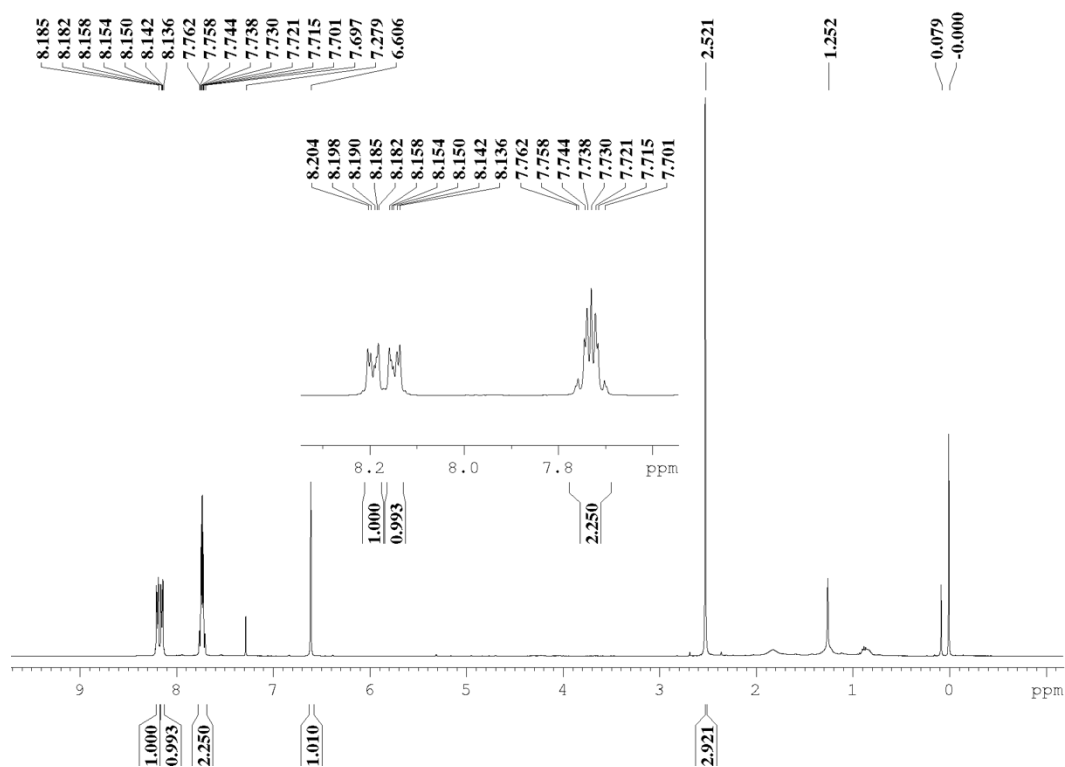


Figure S33. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-methylnaphtho[2,3-*b*]furan-4,9-dione (**6a**).

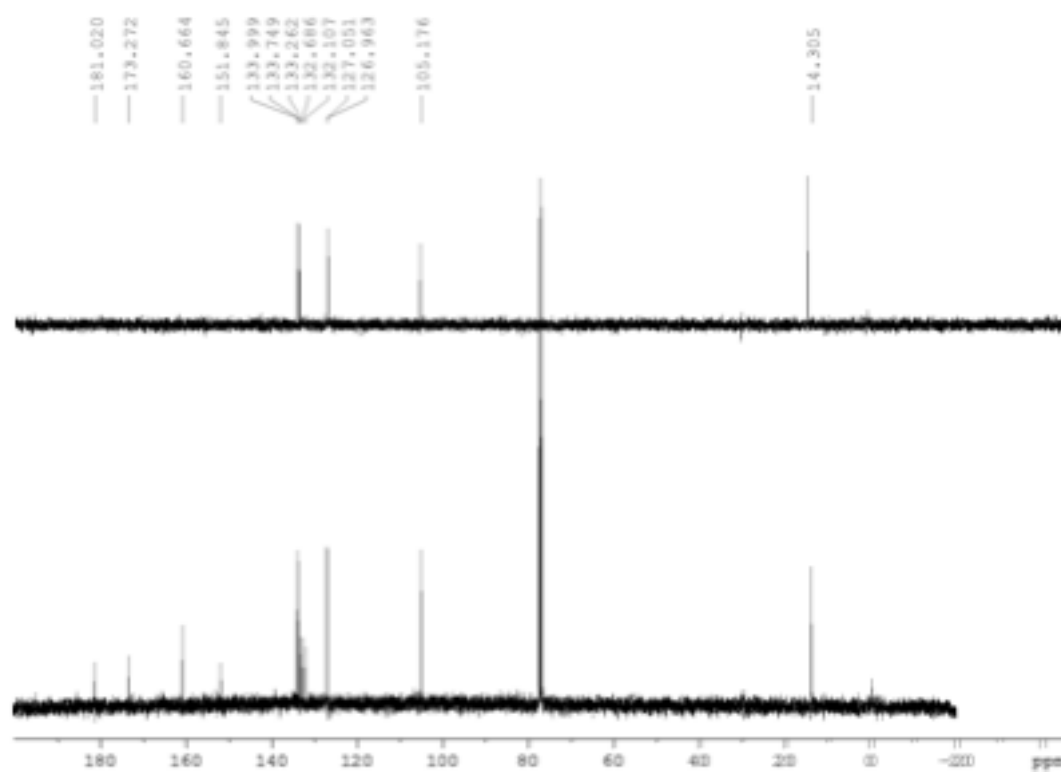


Figure S34. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-methylnaphtho[2,3-*b*]furan-4,9-dione (**6a**).

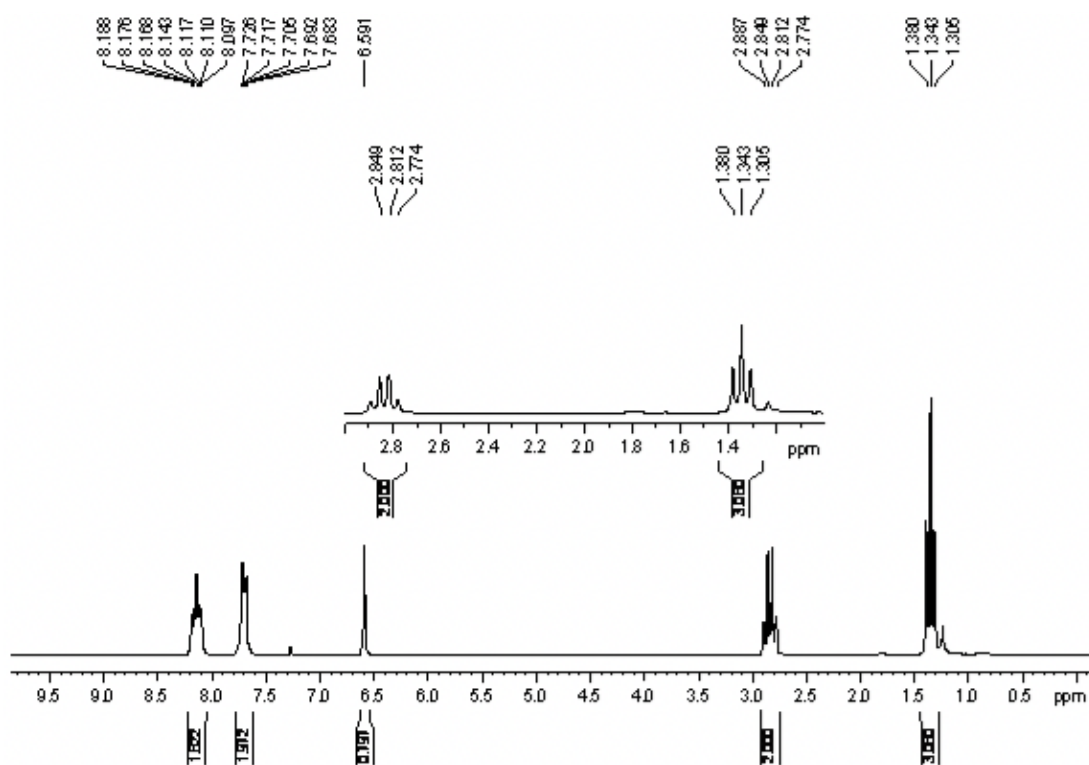


Figure S35. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-ethylnaphtho[2,3-*b*]furan-4,9-dione (**6b**).

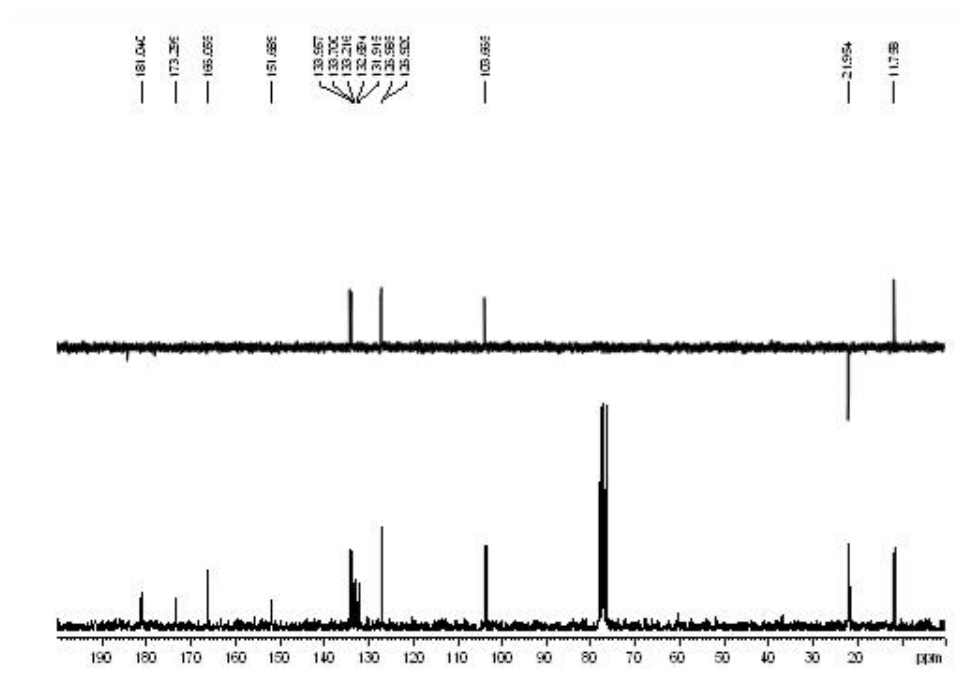


Figure S36. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-ethylnaphtho[2,3-*b*]furan-4,9-dione (**6b**).

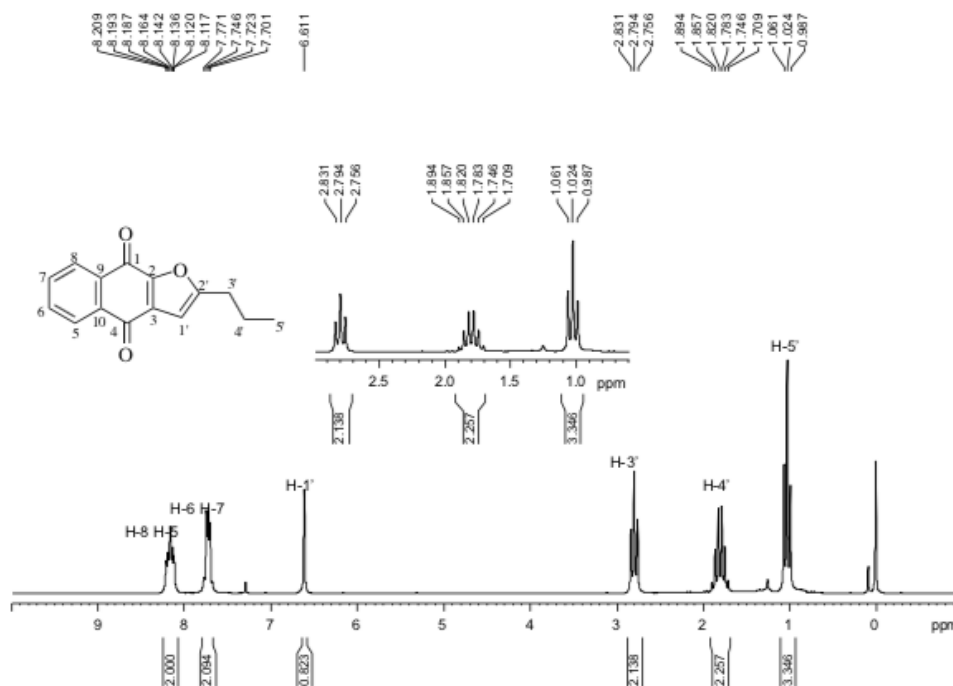


Figure S37. ^1H NMR spectrum (400 MHz, CDCl_3) of 2-propylnaphtho[2,3-*b*]furan-4,9-dione (6c).

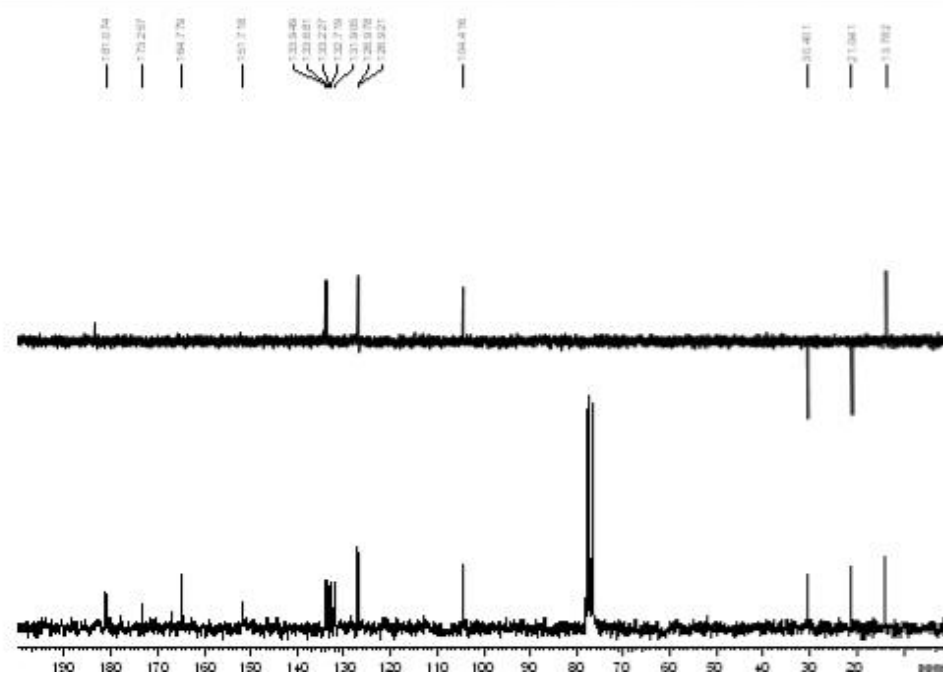


Figure S38. ^{13}C NMR spectrum (100 MHz, CDCl_3) and DEPT 135 of 2-propylnaphtho[2,3-*b*]furan-4,9-dione (6c).

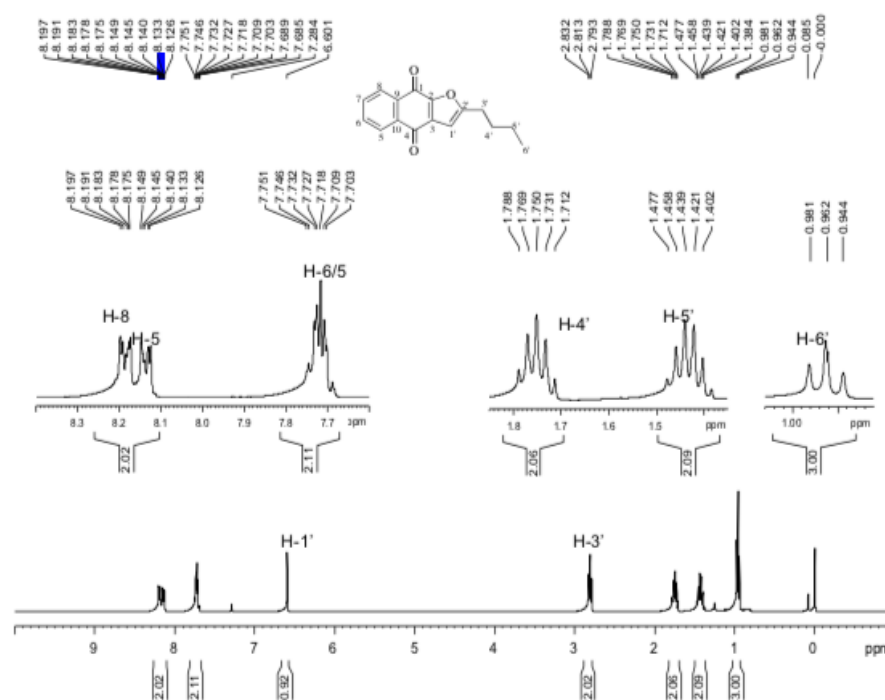


Figure S39. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-butyl-naphtho[2,3-*b*]furan-4,9-dione (6d).

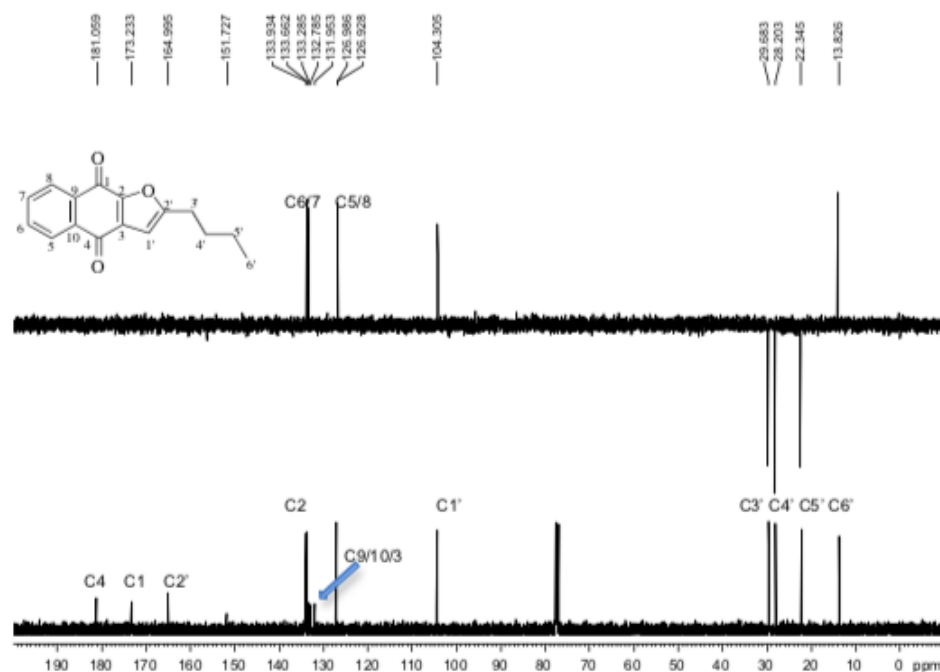


Figure S40. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-butyl-naphtho[2,3-*b*]furan-4,9-dione (6d).

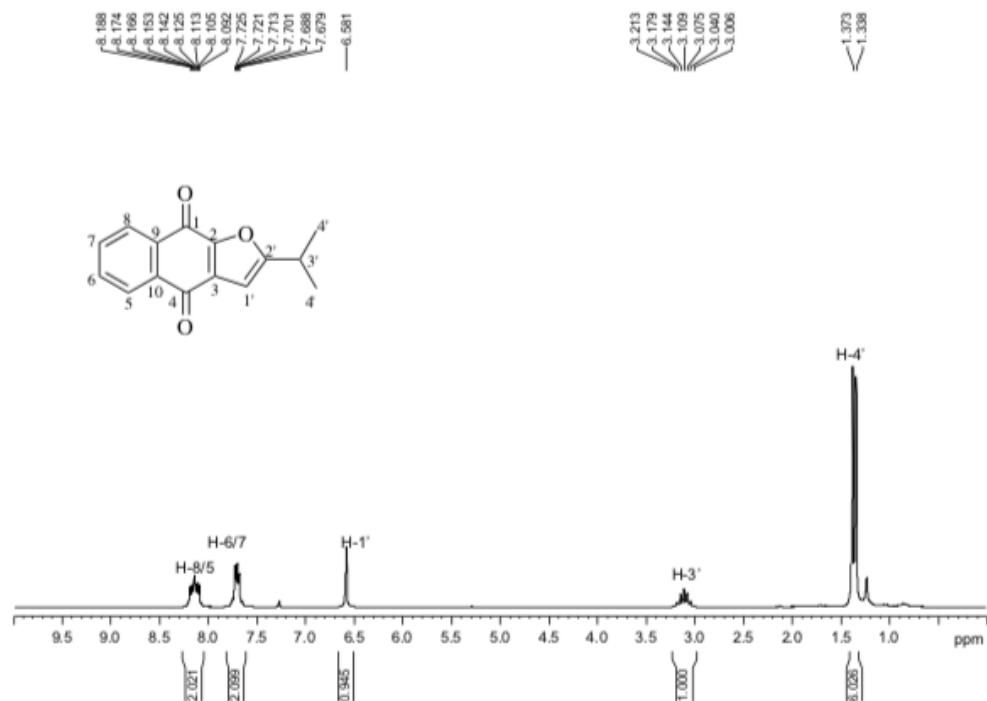


Figure S41. ^1H NMR spectrum (400 MHz, CDCl_3) of 2-isopropynaphtho[2,3-*b*]furan-4,9-dione (**6e**).

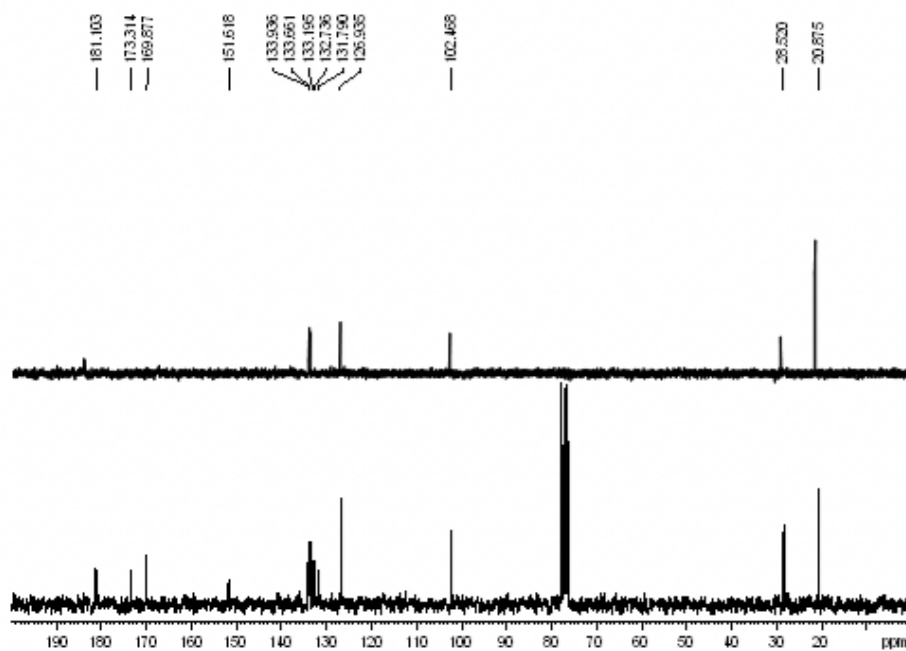


Figure S42. ^{13}C NMR spectrum (100 MHz, CDCl_3) and DEPT 135 of 2-isopropynaphtho[2,3-*b*]furan-4,9-dione (**6e**).

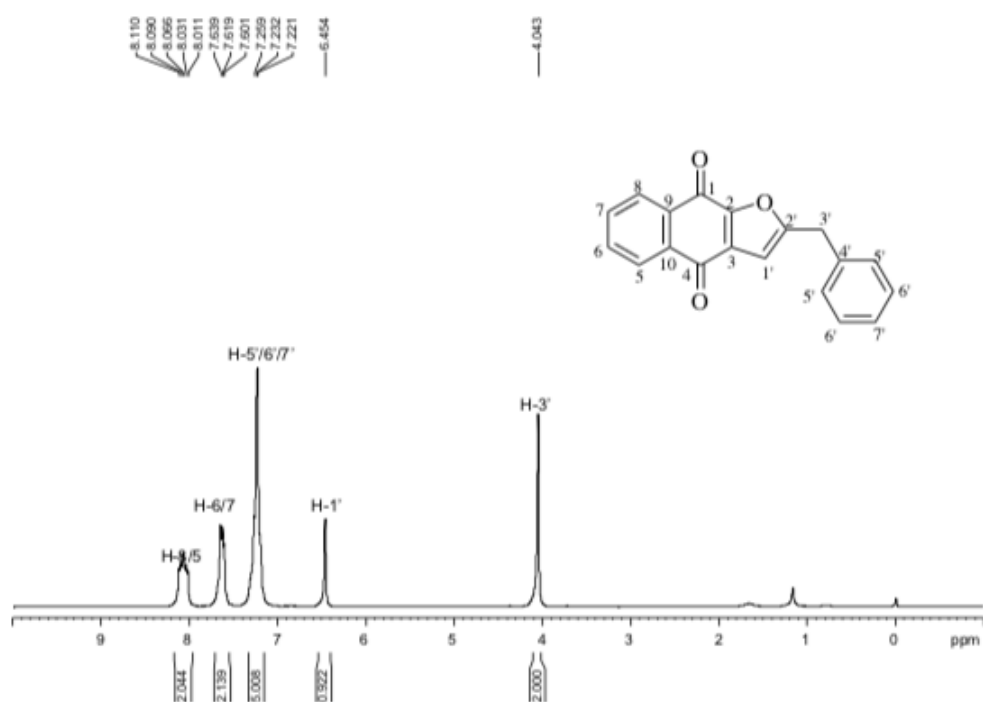


Figure S43. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-benzyl-naphtho[2,3-*b*]furan-4,9-dione (**6f**).

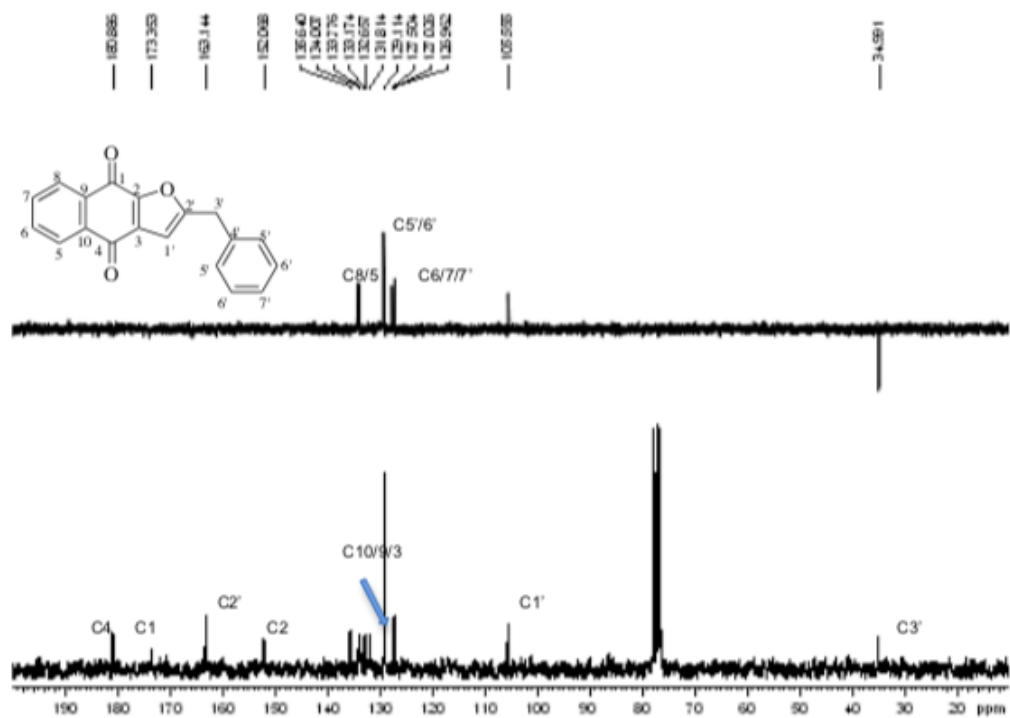


Figure S44. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-benzyl-naphtho[2,3-*b*]furan-4,9-dione (**6f**).

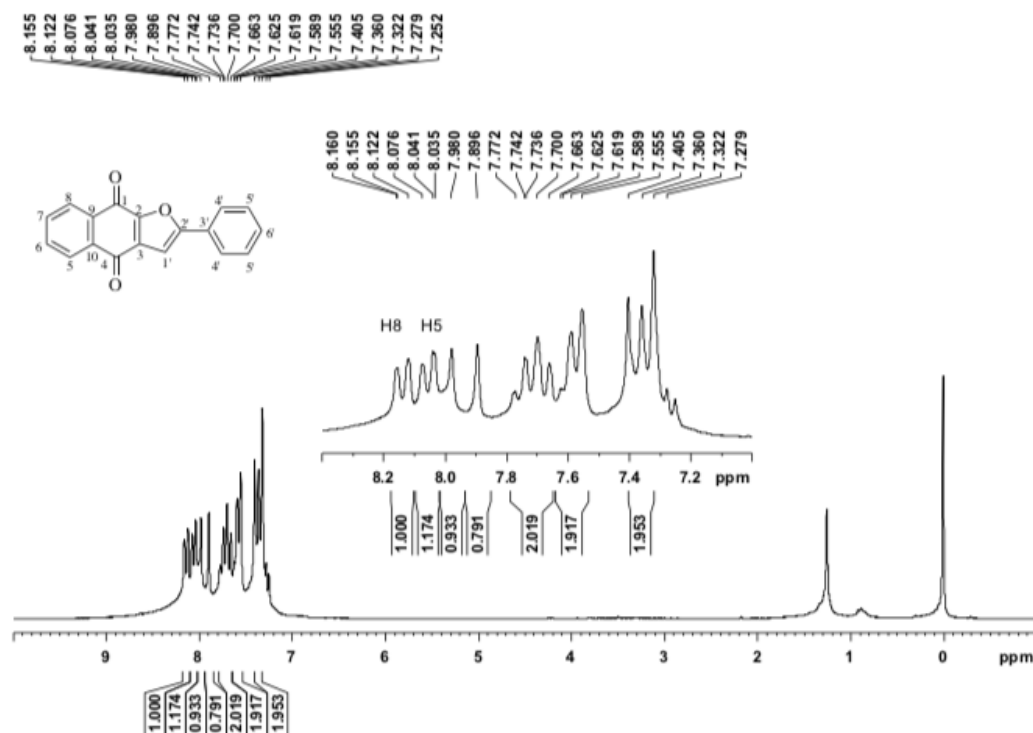


Figure S45. ¹H NMR spectrum (400 MHz, CDCl₃) of 2-phenylnaphtho[2,3-*b*]furan-4,9-dione (**6g**).

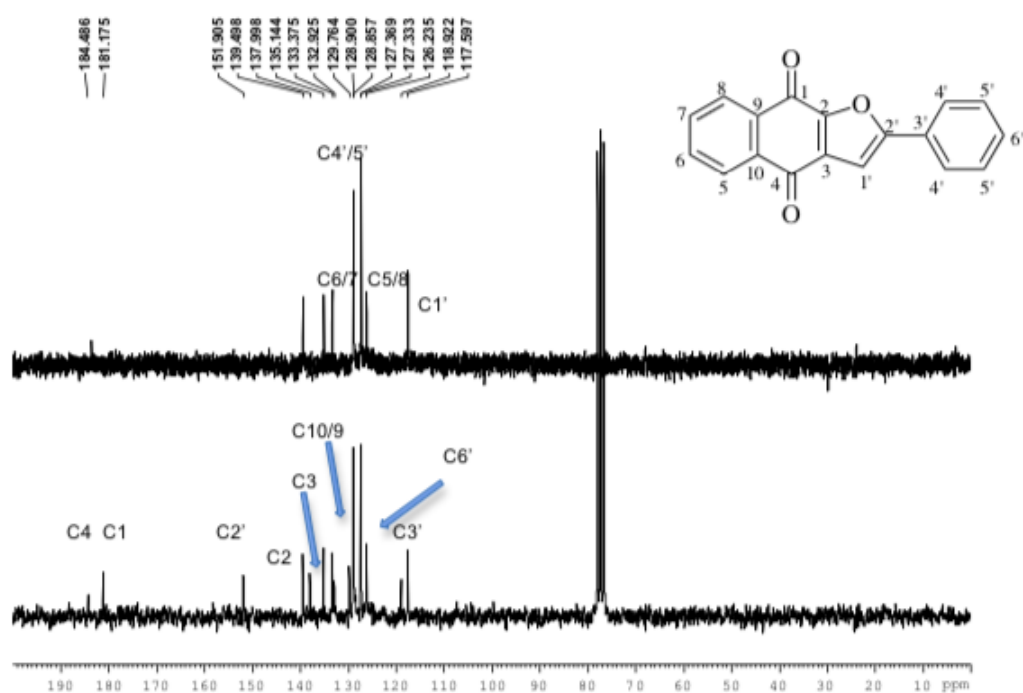


Figure S46. ¹³C NMR spectrum (100 MHz, CDCl₃) and DEPT 135 of 2-phenylnaphtho[2,3-*b*]furan-4,9-dione (**6g**).

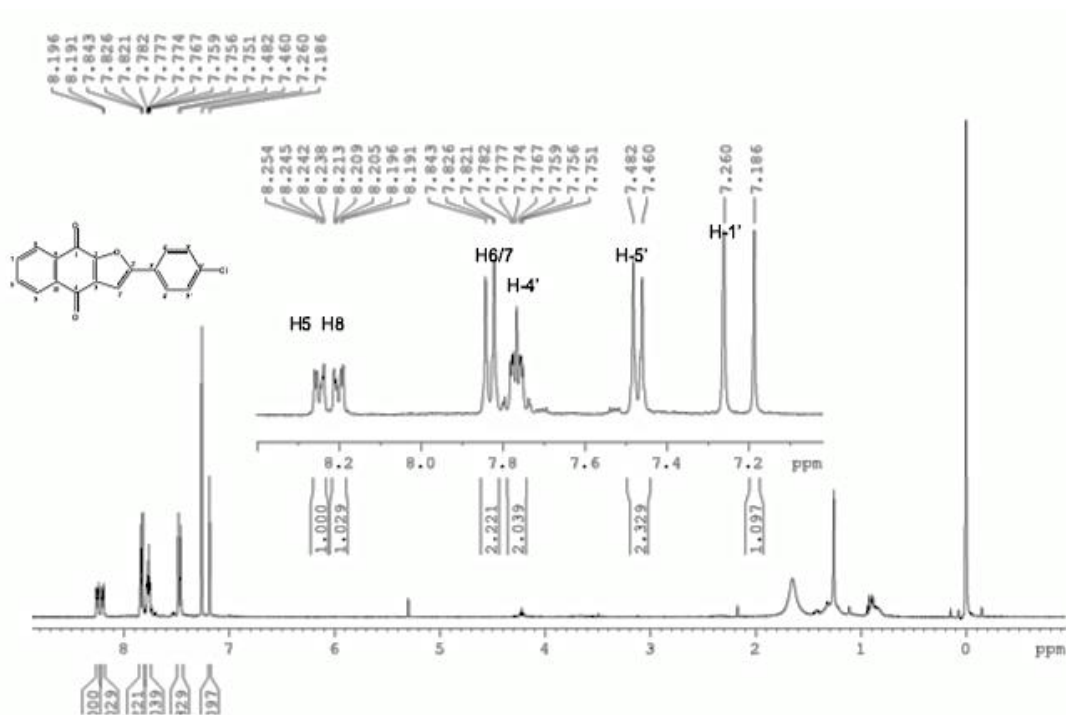


Figure S47. ^1H NMR spectrum (400 MHz, CDCl_3) of 2-(4-chlorophenyl)naphtho[2,3-*b*]furan-4,9-dione (6h).

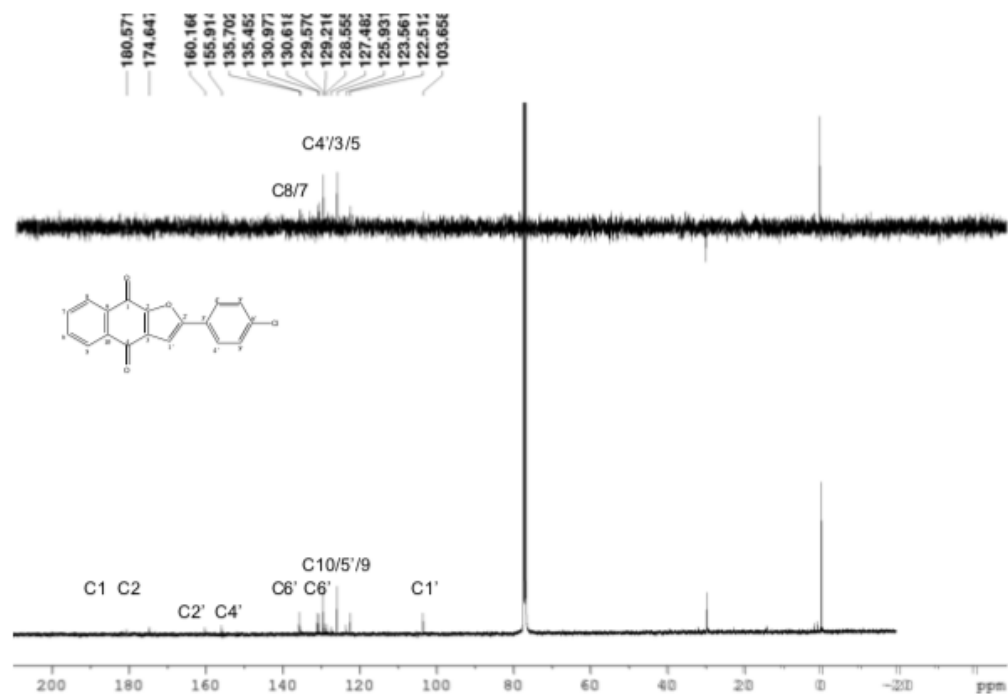


Figure S48. ^{13}C NMR spectrum (100 MHz, CDCl_3) and DEPT 135 of 2-(4-chlorophenyl)naphtho[2,3-*b*]furan-4,9-dione (6h).