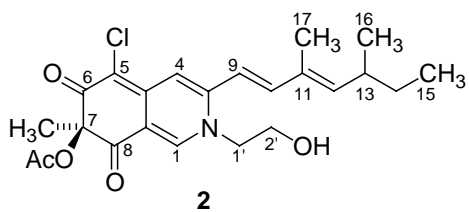


5 **Experimental Data** (to be included as supplementary information)

**(+)-Isochromophilone VI (2):** [Acetic acid 5-chloro-3-(3,5-dimethyl-hepta-1,3-dienyl)-2-(2-hydroxy-ethyl)-7-methyl-6,8-dioxo-2,6,7,8-tetrahydro-isoquinolin-7-yl ester]



10 TLC:  $R_f$  0.24 [Si, MeOH/DCM 5:95 (v/v)].

U.V. (MeOH)  $\lambda_{\max}$  ( $\epsilon$ ): 231 (6,100); 372 (7,361); 475 (866).

$[\alpha]_D^{20} +128$  (c. 0.10, MeOH).

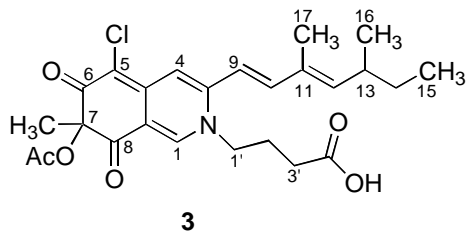
IR:  $\nu$  ( $\text{cm}^{-1}$ ) 3373 (br), 3084 (br), 2908 (m), 1681 (s), 1643 (m), 1203 (s), 1136 (m).

ESI-MS (+ve ion, cv 70V)  $m/z$  (%): 436 [M+H ( $^{37}\text{Cl}$ )] (20); 434 [M+H ( $^{35}\text{Cl}$ )] (58); 394 [M-  
15  $\text{C}_2\text{H}_2\text{O}+\text{H}$  ( $^{37}\text{Cl}$ )] (3); 392 [M- $\text{C}_2\text{H}_2\text{O}+\text{H}$  ( $^{35}\text{Cl}$ )] (8); 348 [M-  $\text{C}_4\text{H}_7\text{O}_2+\text{H}$  ( $^{37}\text{Cl}$ )] (35); 346 [M- $\text{C}_4\text{H}_7\text{O}_2+\text{H}$  ( $^{35}\text{Cl}$ )] (100). HRFAB-MS: found 434.1733;  $\text{C}_{23}\text{H}_{29}\text{NO}_5^{35}\text{Cl}$  calcd 434.1734.

$^1\text{H}$  NMR (500MHz,  $\text{CDCl}_3$ ):  $\delta$ (ppm), mult,  $J$ , Assignment: 7.91, s, 1-H; 7.05, s, 4-H; 6.94, d, 15.3 Hz, 10-H; 6.27, d, 15.3 Hz, 9-H; 5.71, br d, 9.6 Hz, 12-H; 4.05, ddd, 14.4, 4.8, 4.8 Hz, 1'-Ha; 4.02, ddd, 14.4, 4.8, 4.8 Hz, 1'Hb; 3.92, ddd, 12.9, 4.8, 4.8 Hz, 2'-Ha; 3.91, ddd, 12.9, 4.8, 4.8 Hz, 2'Hb; 2.47, m, 13-H; 2.15, s, 7-Ac Me; 1.84, s, 17- $\text{H}_3$ ; 1.54, s, 18- $\text{H}_3$ ; 1.44, ddq, 13.5, 7.5, 7.2 Hz, 14-Ha; 1.34, ddq, 13.5, 7.5, 5.4 Hz, 14-Hb; 1.02, d, 6.0 Hz, 16- $\text{H}_3$ ; 0.88, dd, 7.5, 7.5 Hz, 15- $\text{H}_3$ .

$^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) mult, Assignment: 193.9, s, C-8; 184.2, s, C-6; 170.4, s, 7-Ac C=O; 149.0, s, C-4a; 148.3, d, C-12; 145.5, s, C-3; 145.5, d, C-10; 142.3, d, C-1; 131.7, s, C-11; 114.9, d, C-9; 114.7, s, C-8a; 111.9, d, C-4; 101.6, s, C-5; 84.8, s, C-7; 60.7, t, C-2'; 55.7, t, C-1'; 35.0, d, C-13; 30.0, t, C-14; 23.3, q, C-18; 20.3, q, C-7 Ac Me; 20.2, q, C-16; 12.6, q, C-17; 12.0, q, C-15.

(+)-**Isochromophilone IX (3)** [4-[7-Acetoxy-5-chloro-3-(3,5-dimethyl-hepta-1,3-dienyl)-7-methyl-6,8-dioxo-7,8-dihydro-6H-isoquinolin-2-yl]-butyric acid]



TLC:  $R_f$  0.47 [Si, MeOH/DCM 10:90 (v/v)].

U.V. (EtOH)  $\lambda_{max}$  ( $\epsilon$ ): 233 (17,100); 376 (17,100); 481 (1880).

$[\alpha]_D^{20}$  +430 (c. 0.10, MeOH).

IR:  $\nu$  ( $\text{cm}^{-1}$ ) 2935 (m), 2927 (m), 1737 (s), 1706 (s), 1576 (s), 1491 (s), 1235 (m), 1149 (m).

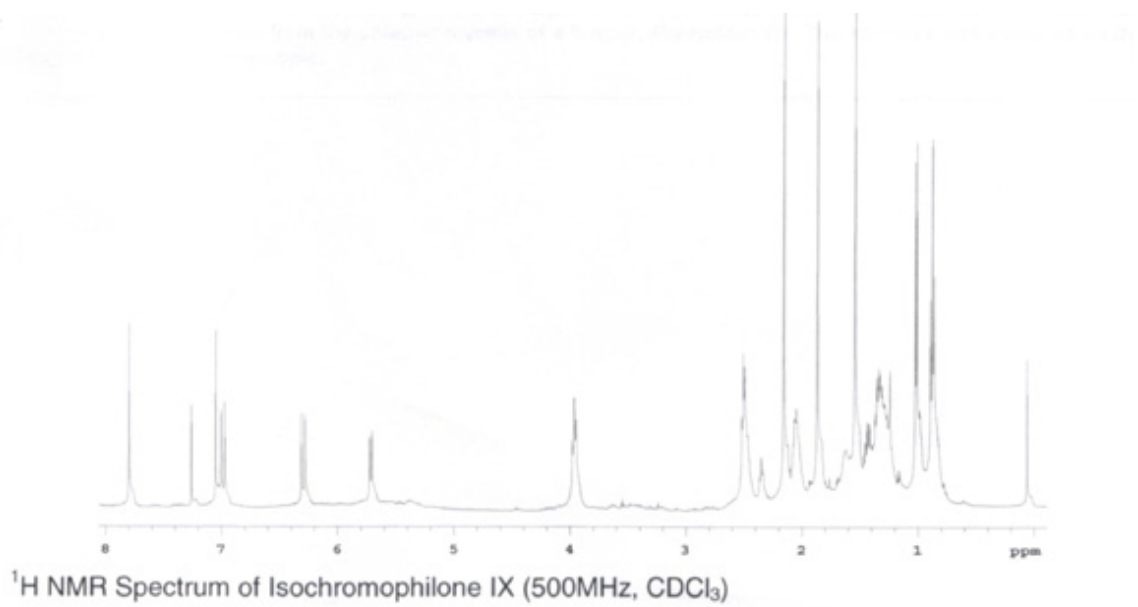
ESI-MS (+ve ion, cv 60V)  $m/z$  (%): 478 [M+H ( $^{37}\text{Cl}$ )] (18); 476 [M+H ( $^{35}\text{Cl}$ )] (45); 390 [M-C<sub>4</sub>H<sub>7</sub>O<sub>2</sub>+H ( $^{37}\text{Cl}$ )] (33); 388 [M-C<sub>4</sub>H<sub>7</sub>O<sub>2</sub>+H ( $^{35}\text{Cl}$ )] (100). HREI-MS: found 475.1761; C<sub>25</sub>H<sub>30</sub>NO<sub>6</sub><sup>35</sup>Cl calcd 475.1763. found 477.1732; C<sub>25</sub>H<sub>30</sub>NO<sub>6</sub><sup>37</sup>Cl calcd 477.1717.

<sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>):  $\delta$ (ppm), mult,  $J$ , Assignment: 7.80, s, 1-H; 7.05, s, 4-H; 6.99, d, 15.0 Hz, 10-H; 6.28, d, 15.0 Hz, 9-H; 5.71, br d, 9.5 Hz, 12-H; 3.96, t, 7.5 Hz, 1'-H<sub>2</sub>; 2.51, t, 6.5 Hz, 3'-H<sub>2</sub>; 2.47, m, 13-H; 2.16, s, 7-Ac Me; 2.05, m, 2'-H<sub>2</sub>; 1.87, s, 17-H<sub>3</sub>; 1.55, s, 18-H<sub>3</sub>; 1.44, ddq, 13.0, 8.0, 6.0 Hz, 14-Ha; 1.34, ddq, 13.0, 8.0, 6.0 Hz, 14-Hb; 1.02, d, 6.5 Hz, 16-H<sub>3</sub>; 0.88, dd, 8.0, 8.0 Hz, 15-H<sub>3</sub>.

<sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>)  $\delta$  (ppm) mult, Assignment: 193.8, s, C-8; 184.4, s, C-6; 175.2, s, C-4'; 170.2, s, 7-Ac C=O; 148.4, d, C-12; 148.1, s, C-3; 145.5, d, C-10; 144.7, s, C-4a; 141.2, d, C-1; 132.0, s, C-11; 114.9, s, C-8a; 114.3, d, C-9; 111.5, d, C-4; 102.1, s, C-5; 84.7, s, C-7; 53.4, t, C-1'; 35.0, d, C-13; 30.0, t, C-14; 30.0, t, C-3'; 25.0, t, C-2'; 23.2, q, C-18; 20.3, q, 7-Ac Me; 20.2, q, C-16; 12.5, q, C-17; 12.0, q, C-15.

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## Spectra



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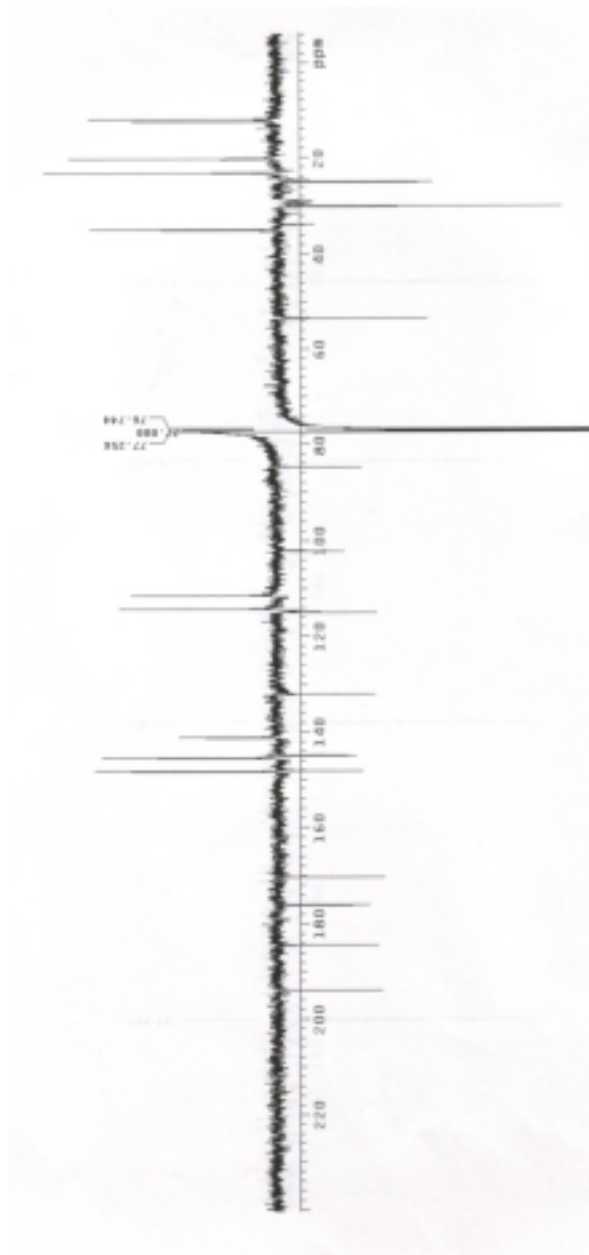
90

95

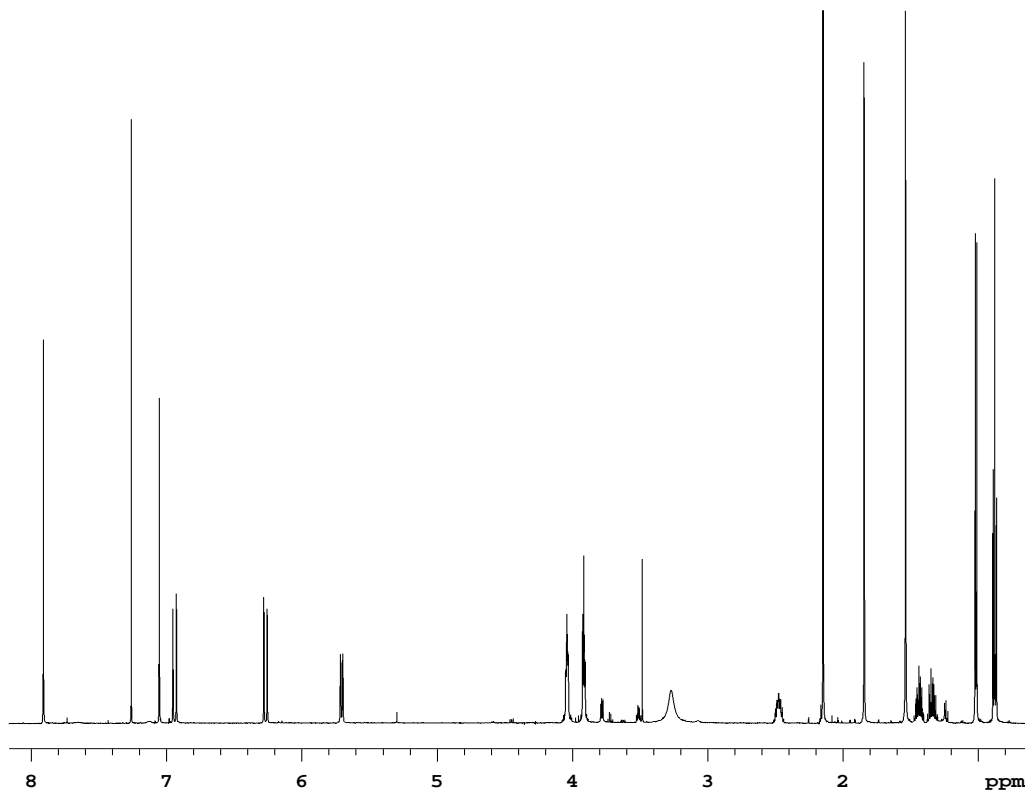
100

105

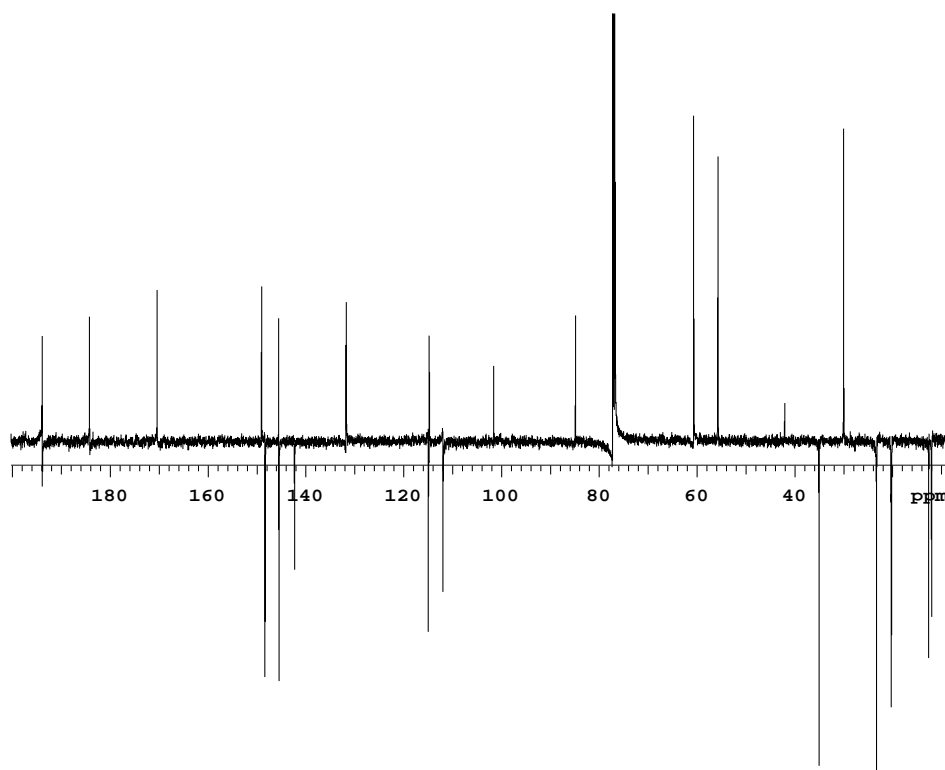
110



$^{13}\text{C}$  (APT) NMR Spectrum of (+)-isochromophilone IX (**3**) (125 MHz,  $\text{CDCl}_3$ )



<sup>1</sup>H NMR spectrum of (+)-isochromophilone VI (**2**) (500MHz, CDCl<sub>3</sub>)



115 <sup>13</sup>C NMR (APT) spectrum of (+)-isochromophilone VI (**2**) (125MHz, CDCl<sub>3</sub>)