

# New chromones from *Bouvardia ternifolia* (Cav.) Schltl with anti-inflammatory and immunomodulatory activity.

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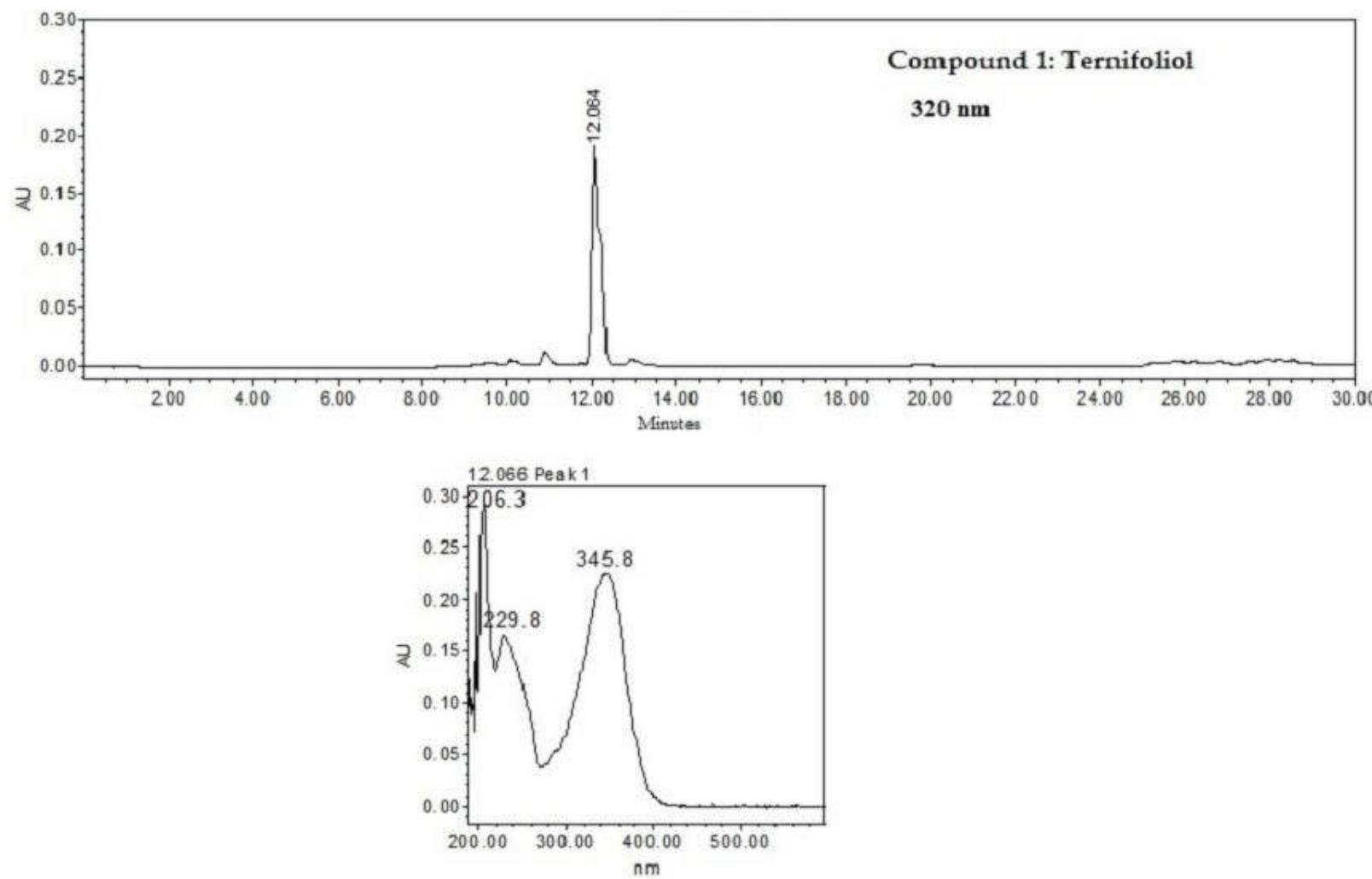


Figure S1. Spectrum UV of ternifoliol (**1**)

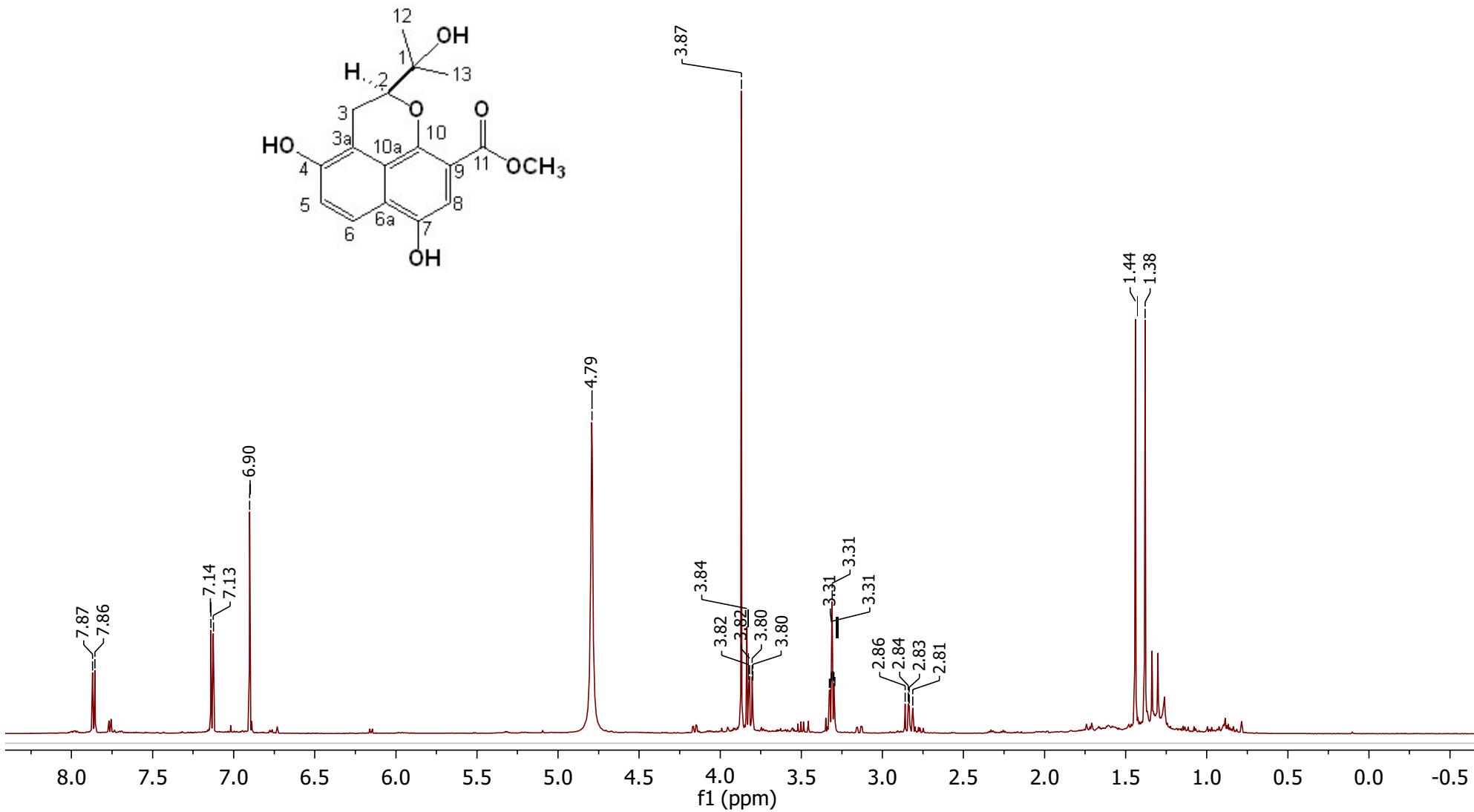
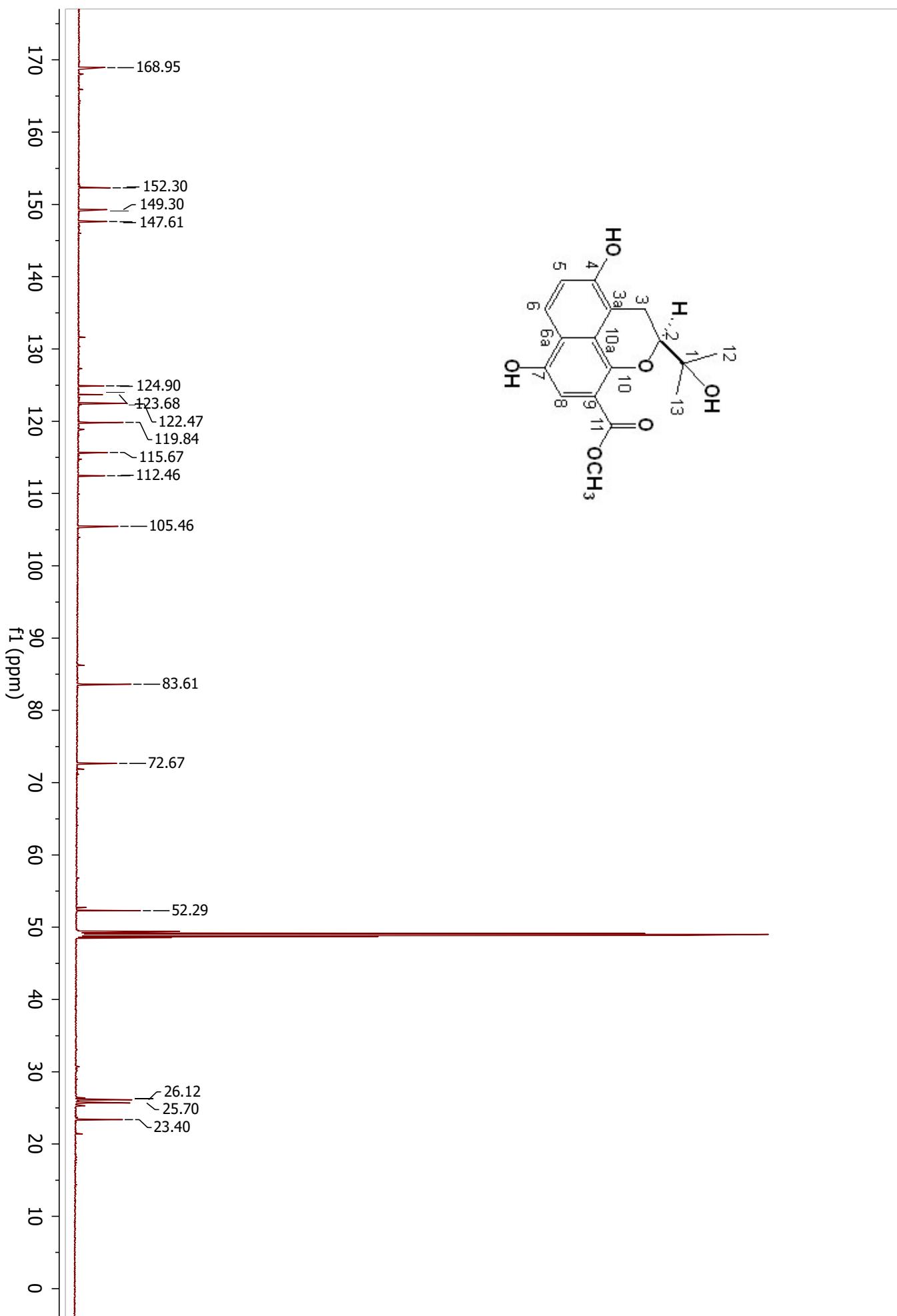


Figure S2.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz) of ternifoliol (**1**)

Figure S3.  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 125 MHz) of ternifoliol (**1**)



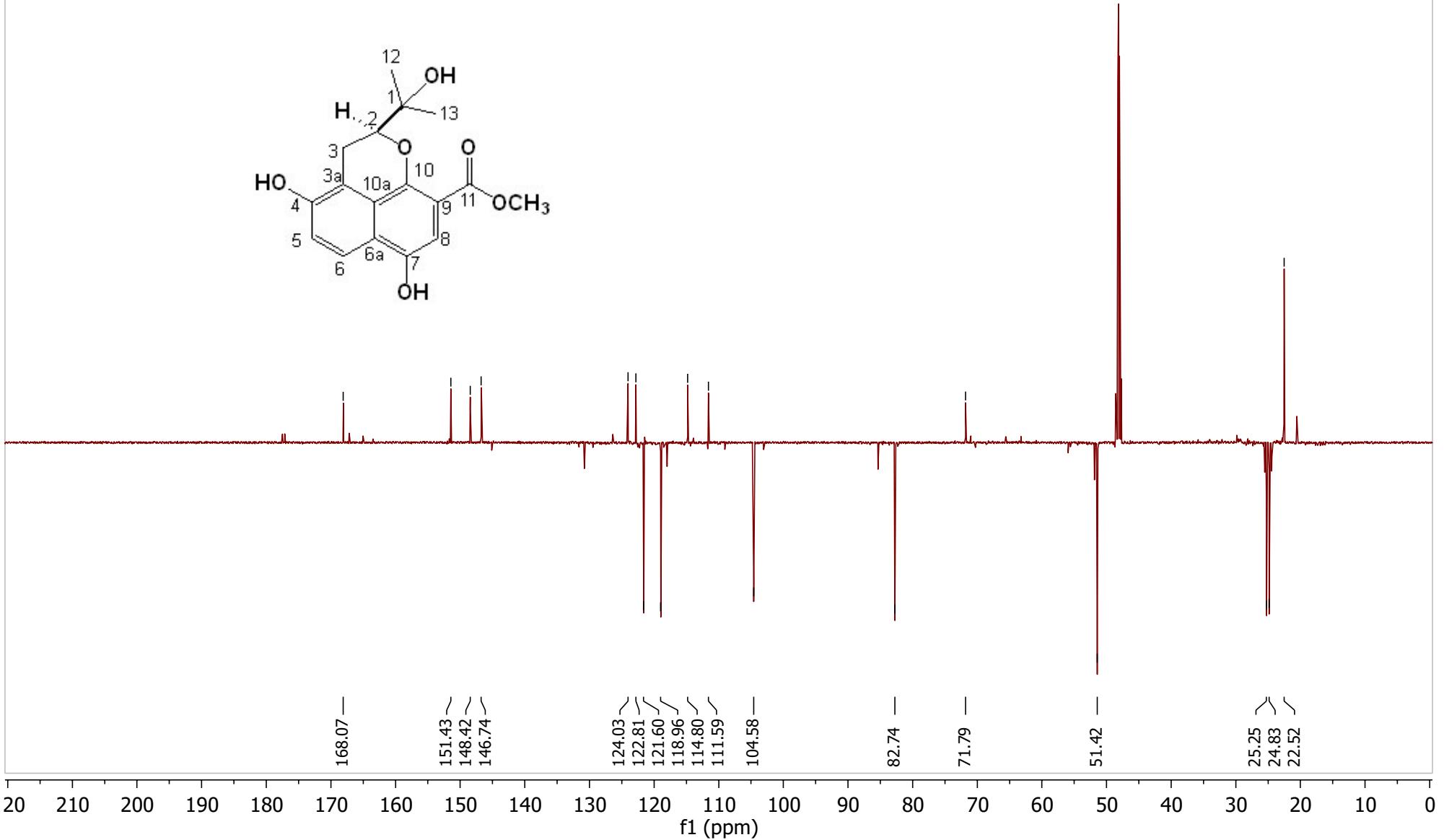


Figure S4.  $^{13}\text{C}$  DEPT ( $\text{CD}_3\text{OD}$ , 125 MHz) of ternifoliol (**1**)

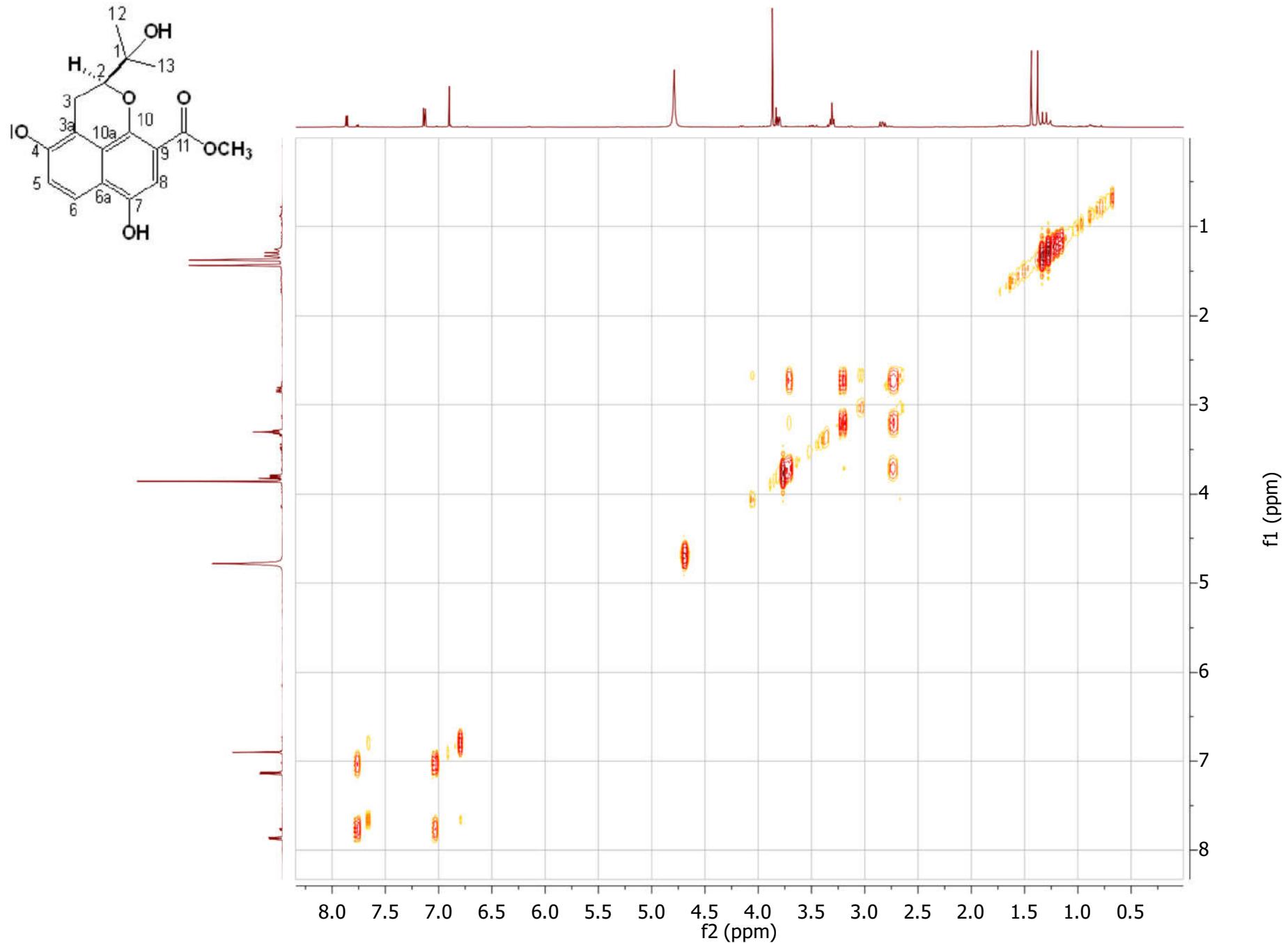


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of ternifoliol (**1**)

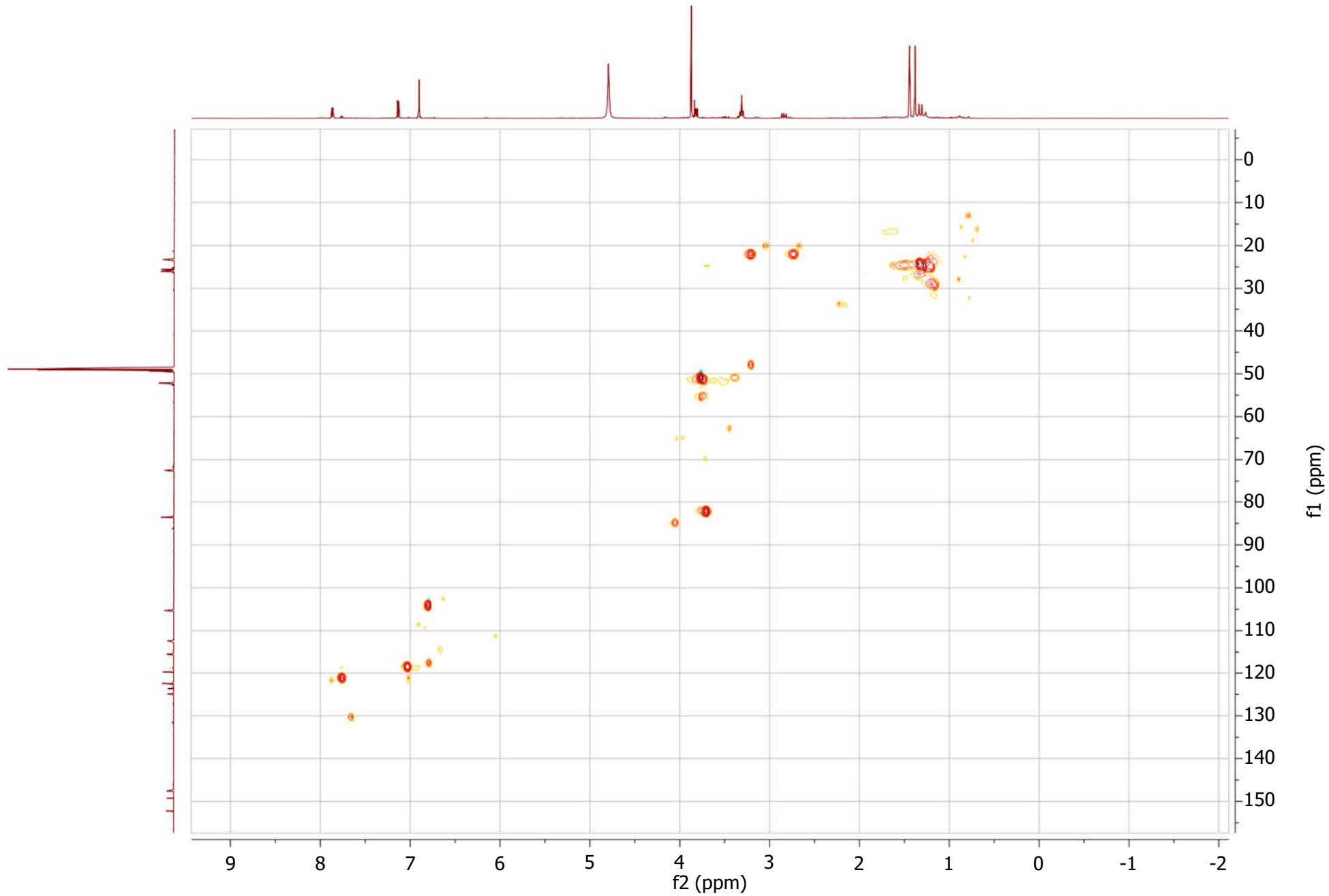


Figure S6.  $^1\text{H}$ - $^{13}\text{C}$  (HSQC) NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of ternifoliol (**1**)

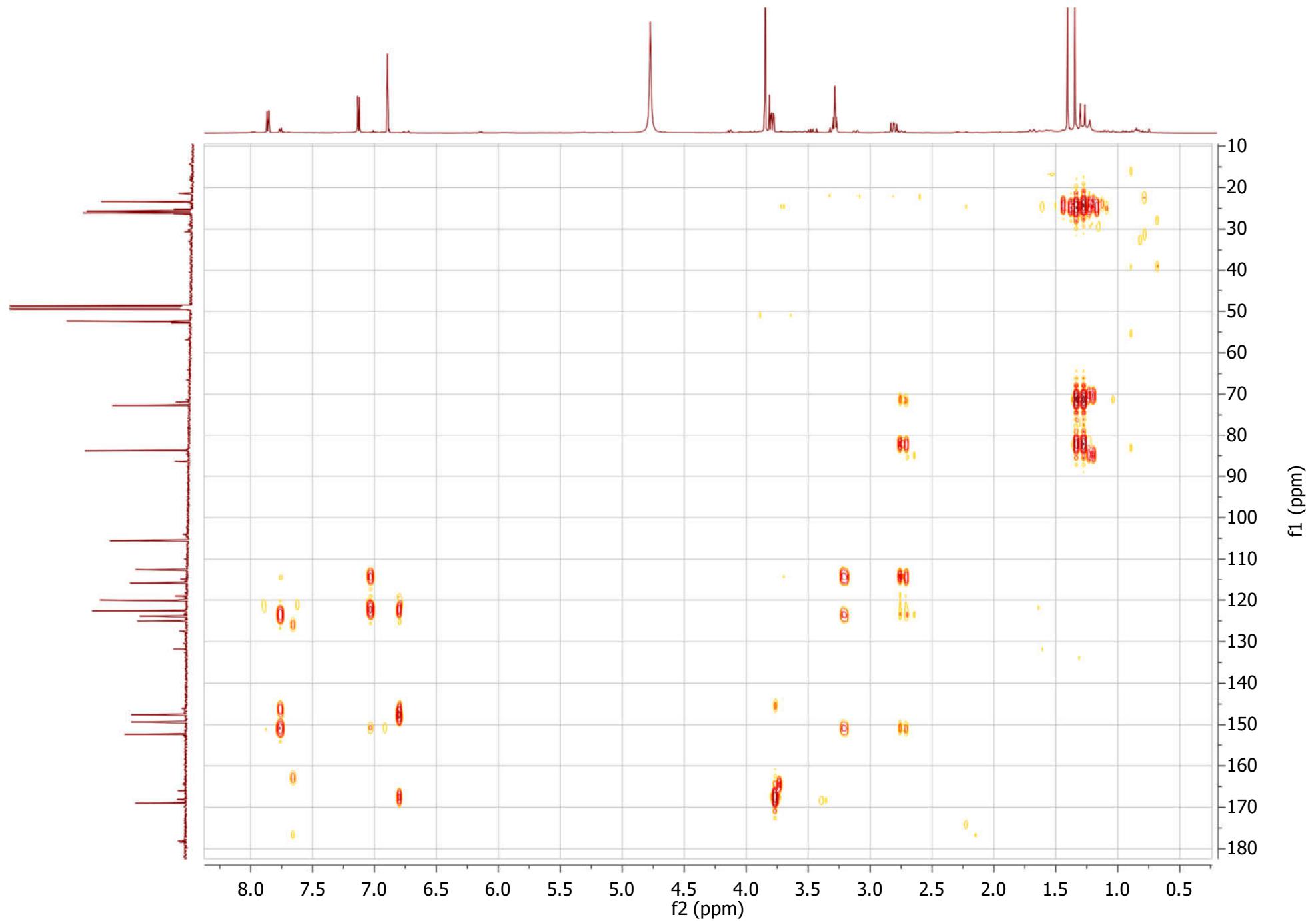


Figure S7.  $^1\text{H}$ - $^{13}\text{C}$  (HMBC) NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of ternifoliol (**1**)

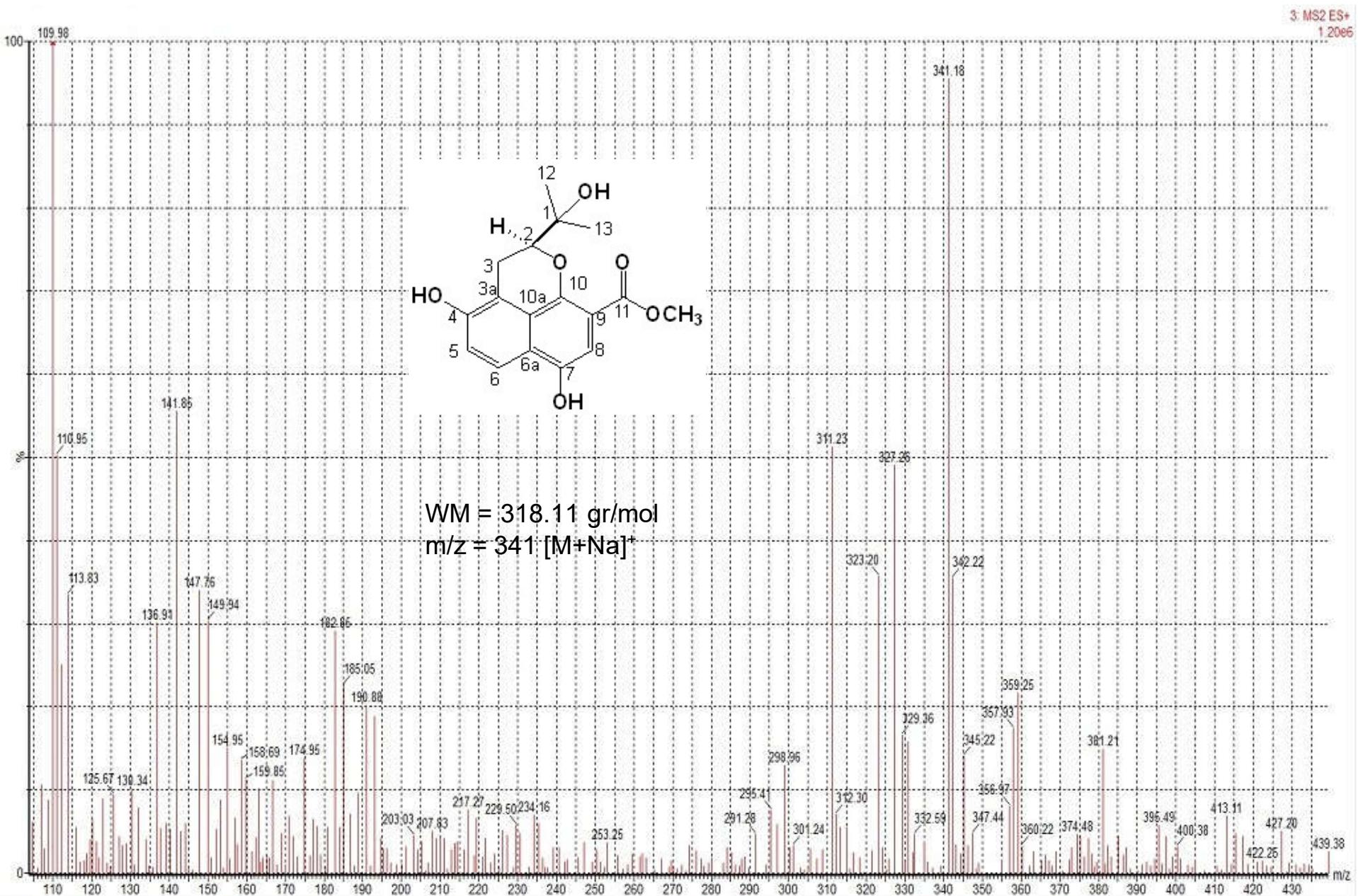


Figure S8. Mass spectrum (MS) of ternifoliol (1)

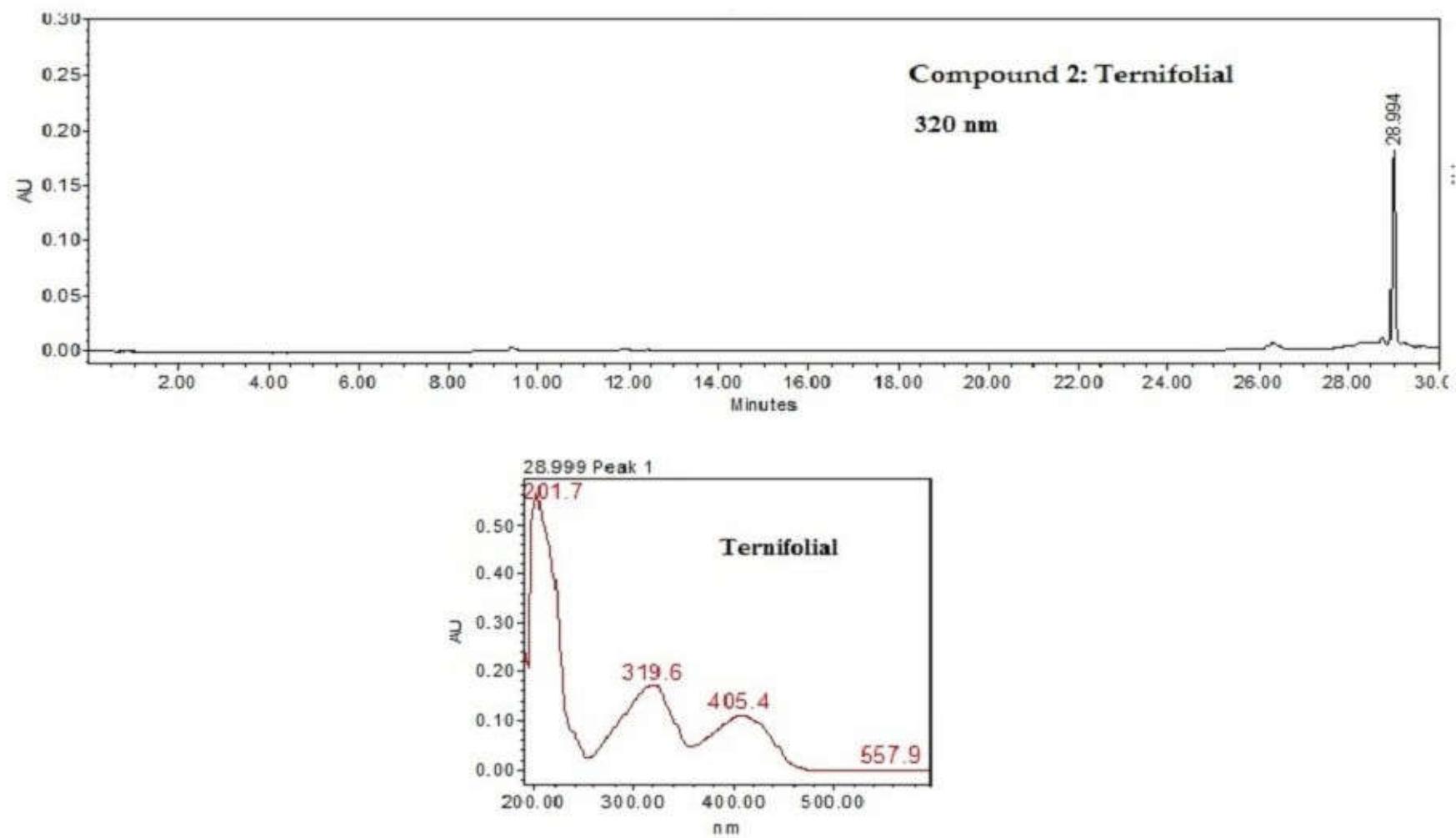


Figure S9. Spectrum UV of ternifolial (**2**)

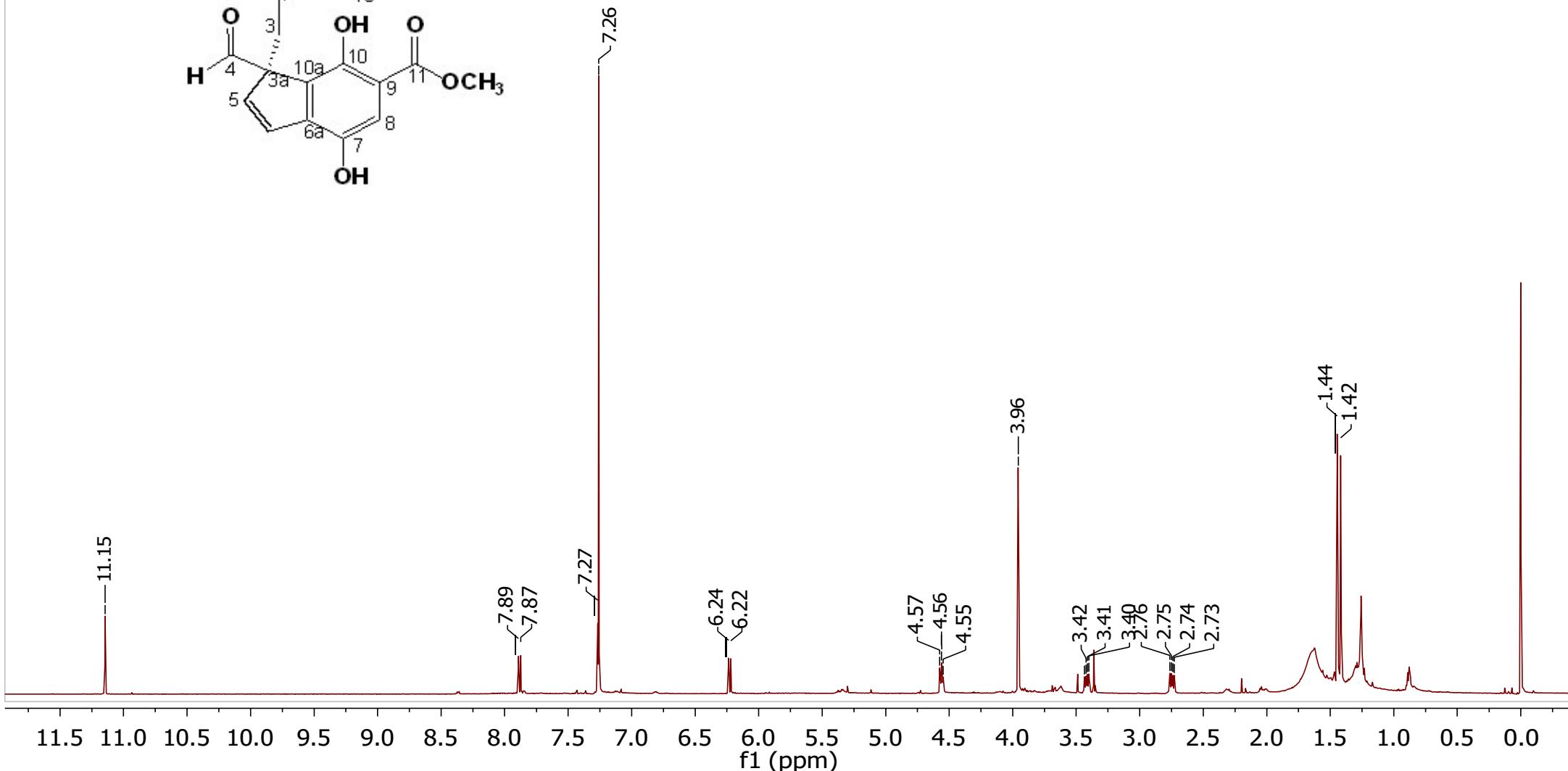
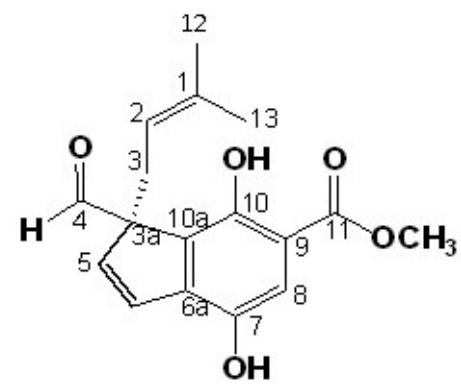


Figure S10.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz) of ternifolial (**2**)

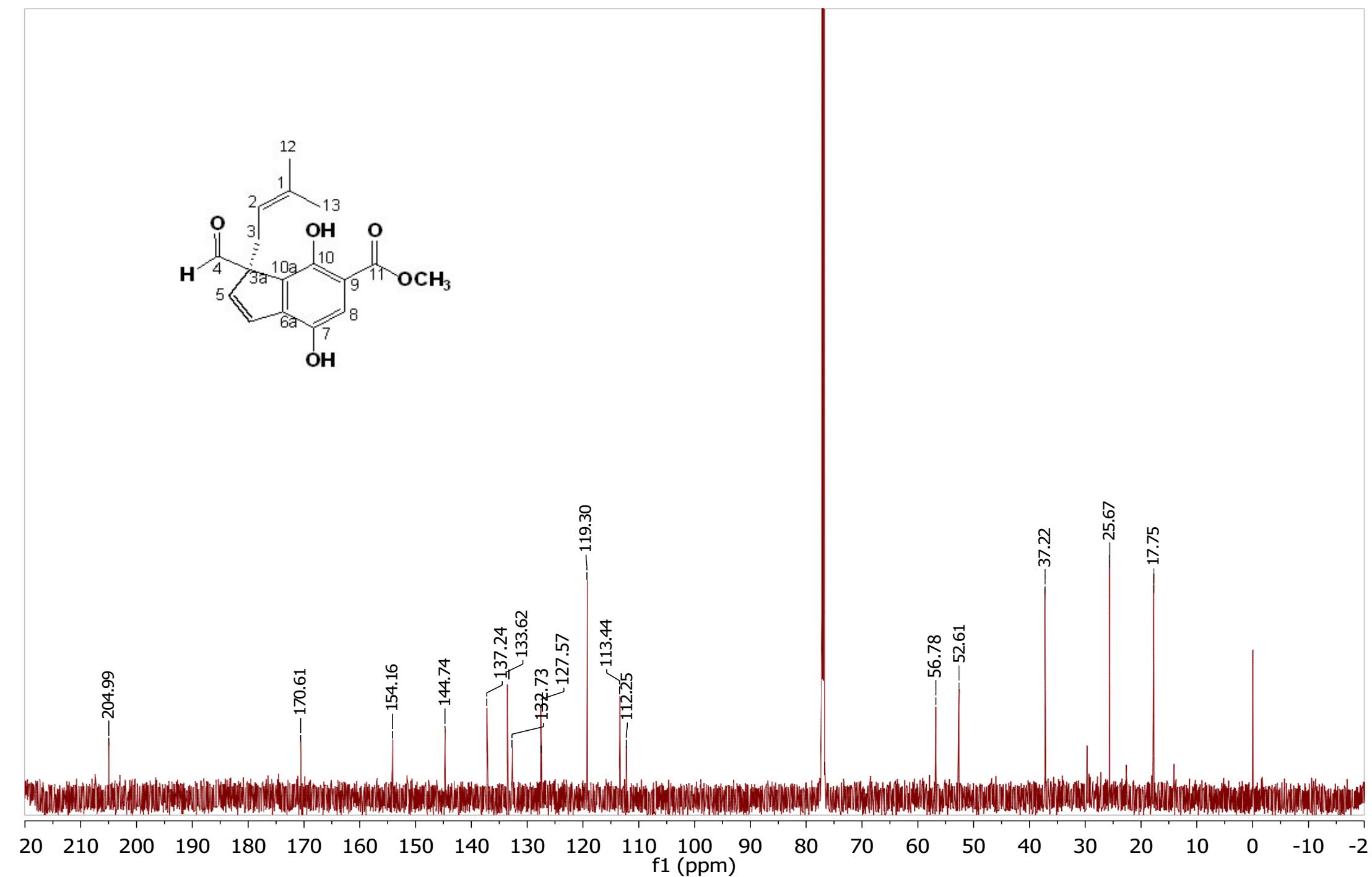
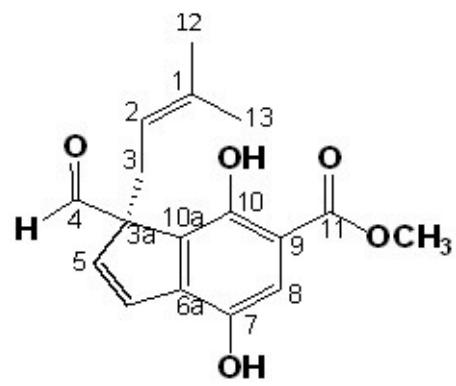


Figure S11. <sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz) of ternifolial (2)

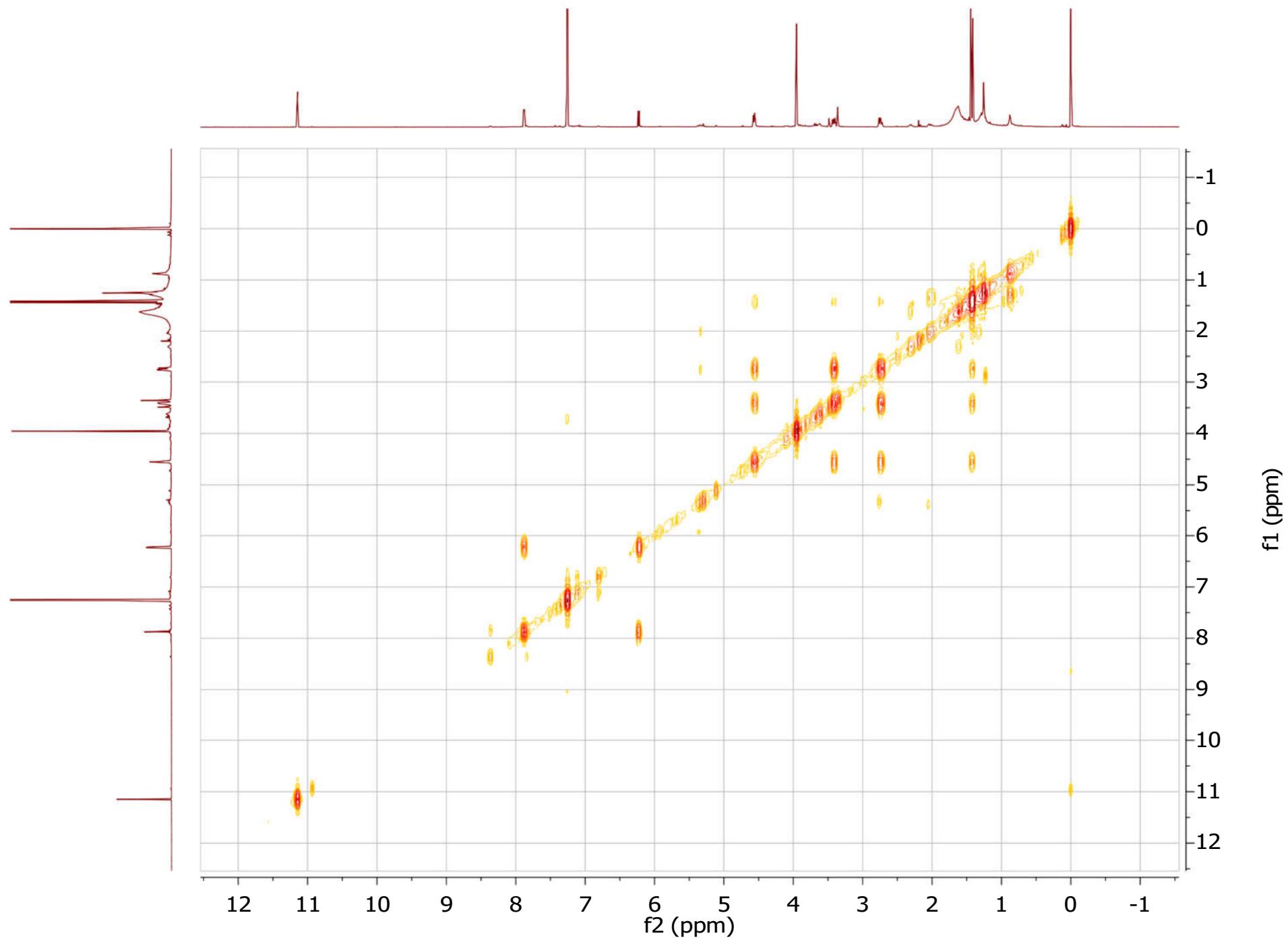


Figure S12.  $^1\text{H}$ - $^1\text{H}$  COSY NMR ( $\text{CDCl}_3$ , 600 MHz) of ternifolial (**2**)

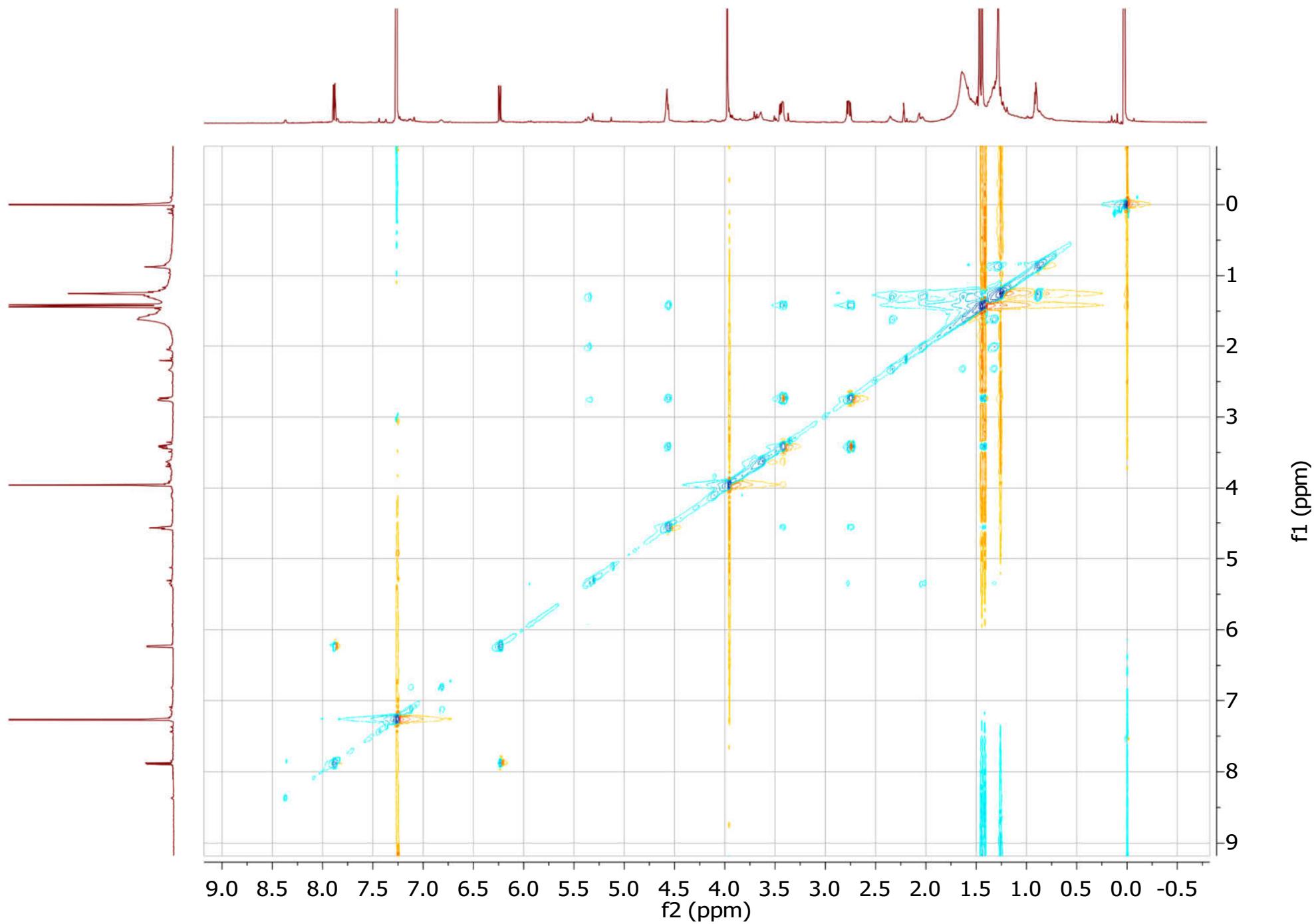


Figure S13.  $^1\text{H}$ - $^1\text{H}$  TOCSY NMR ( $\text{CDCl}_3$ , 600 MHz) of ternifolial (**2**)

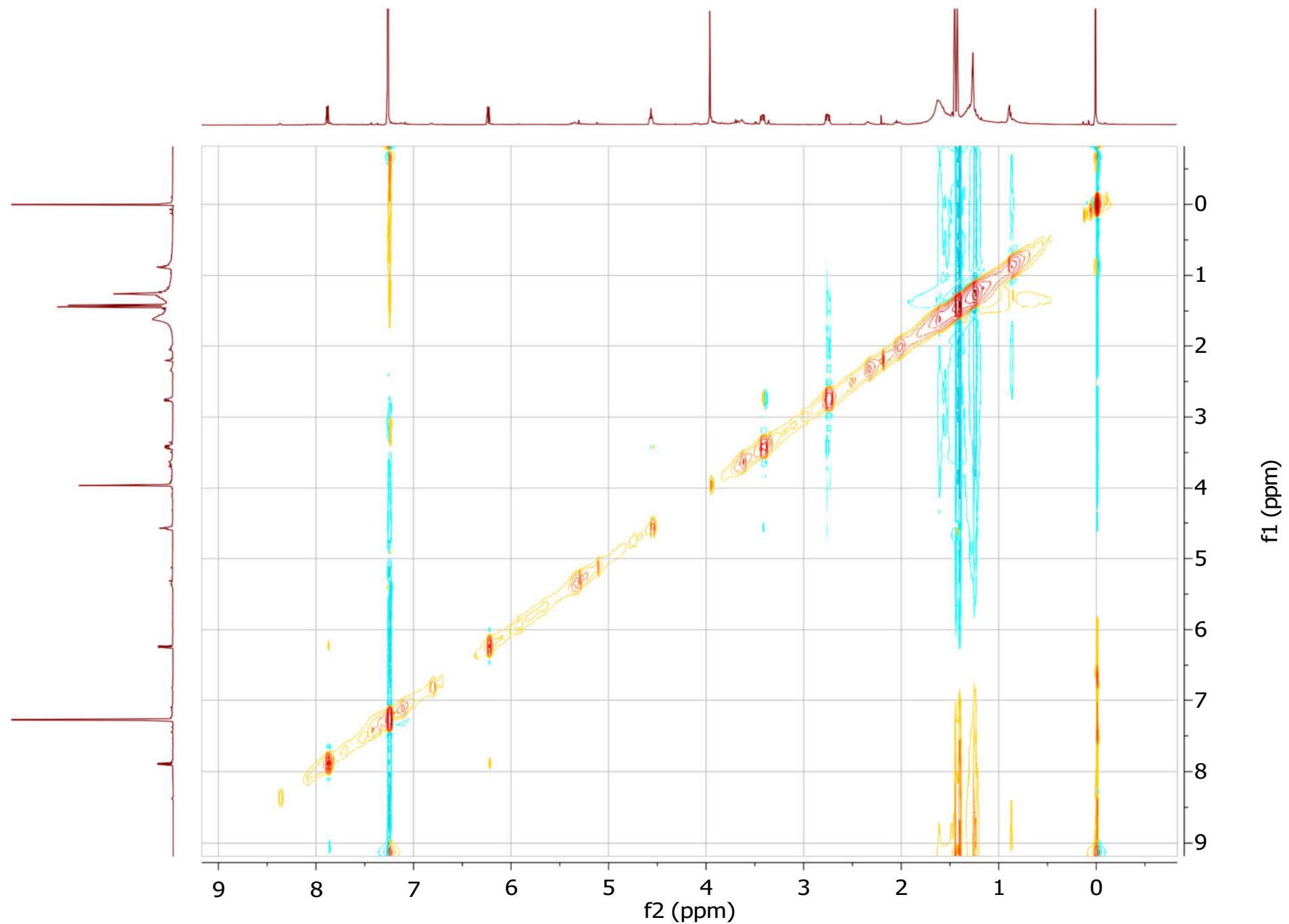


Figure S14.  $^1\text{H}$ - $^1\text{H}$  NOESY NMR ( $\text{CDCl}_3$ , 600 MHz) of ternifolial (**2**)

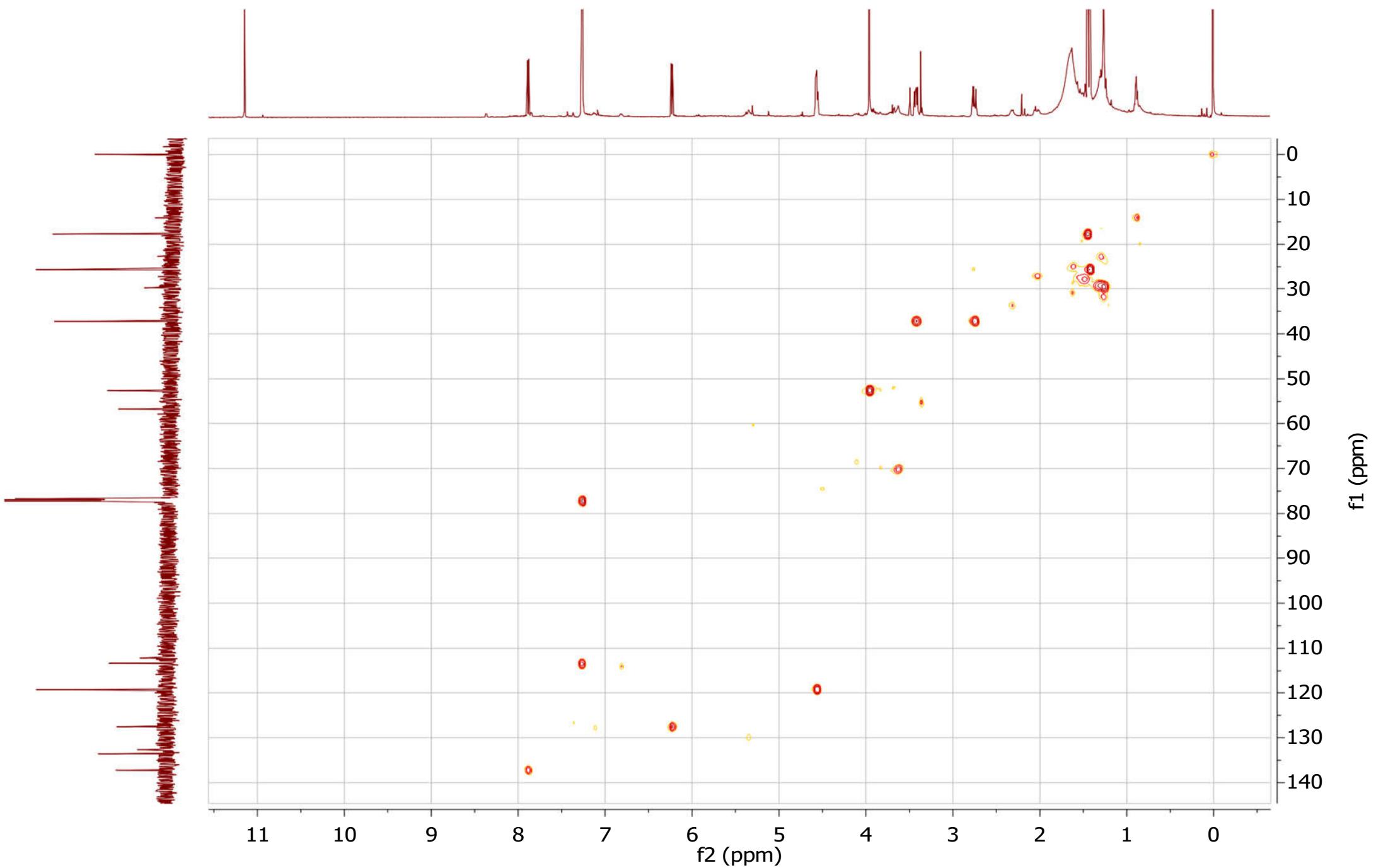


Figure S15.  $^1\text{H}$ - $^{13}\text{C}$  (HSQC) NMR ( $\text{CDCl}_3$ , 600 MHz) of ternifolial (**2**)

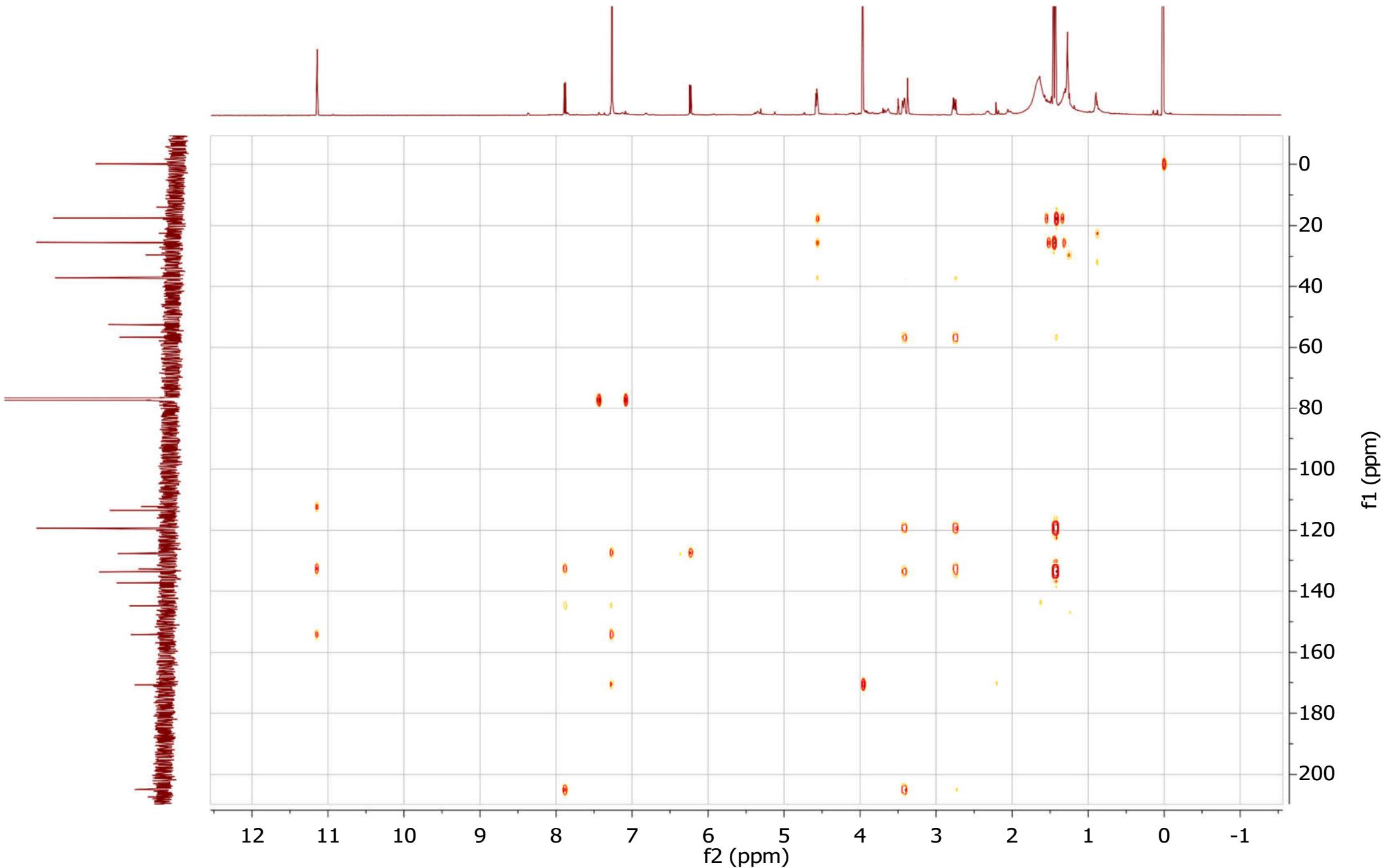


Figure S16.  $^1\text{H}$ - $^{13}\text{C}$  (HMBC) NMR ( $\text{CDCl}_3$ , 600 MHz) of ternifolial (**2**)

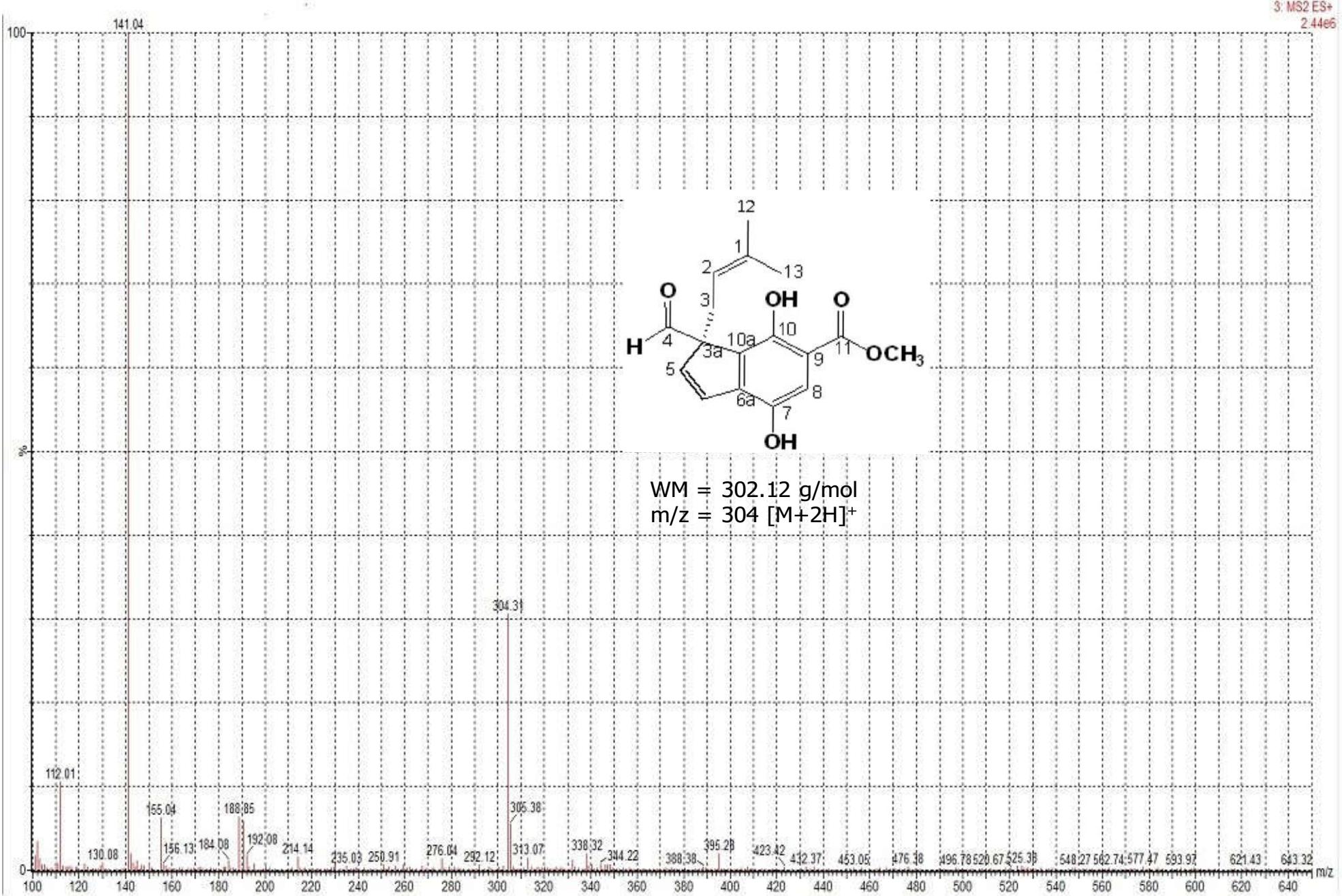


Figure S17. Mass spectrum (MS) of ternifolial (**2**)

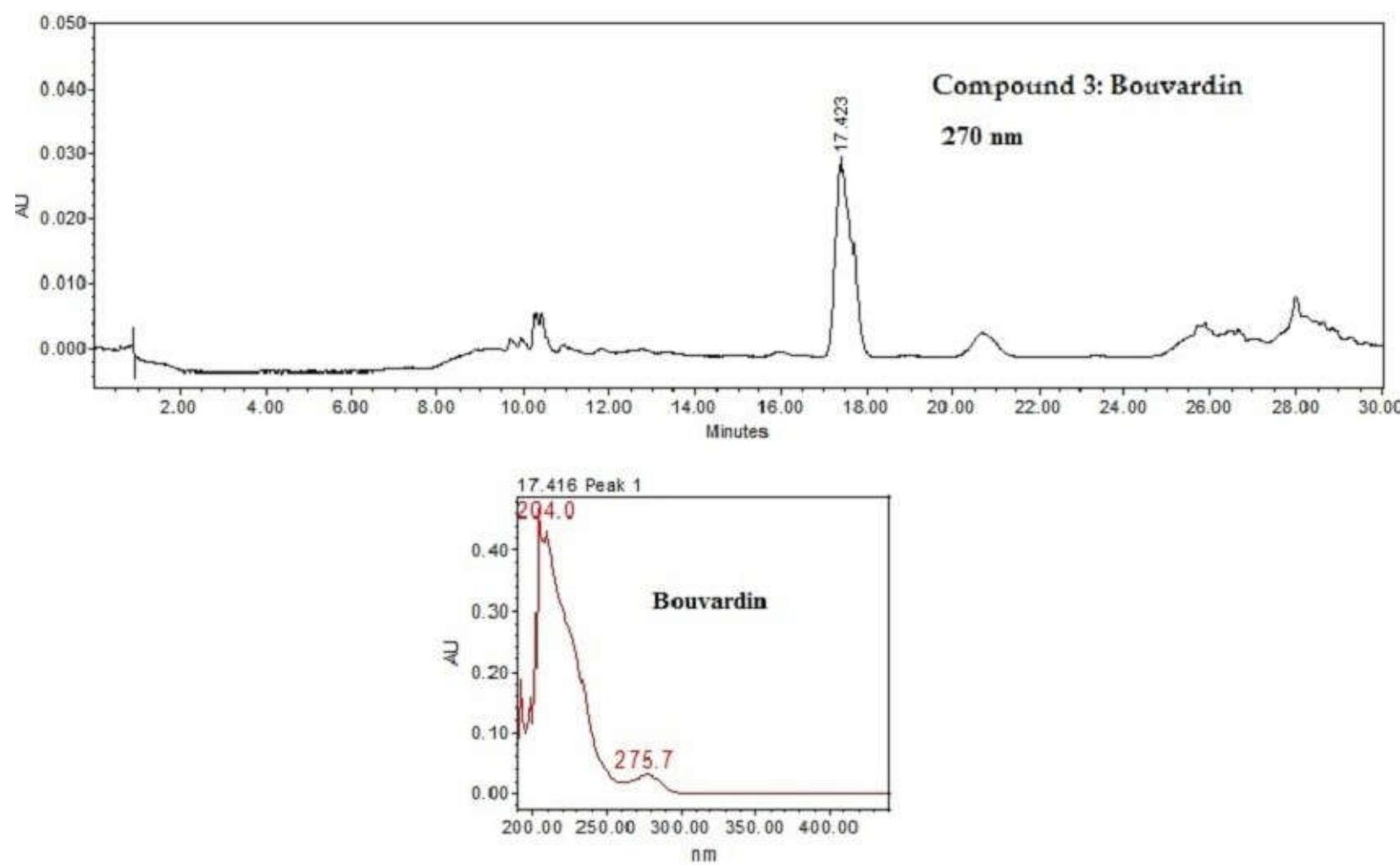


Figure S18. Spectrum UV of bouvardin (**3**)

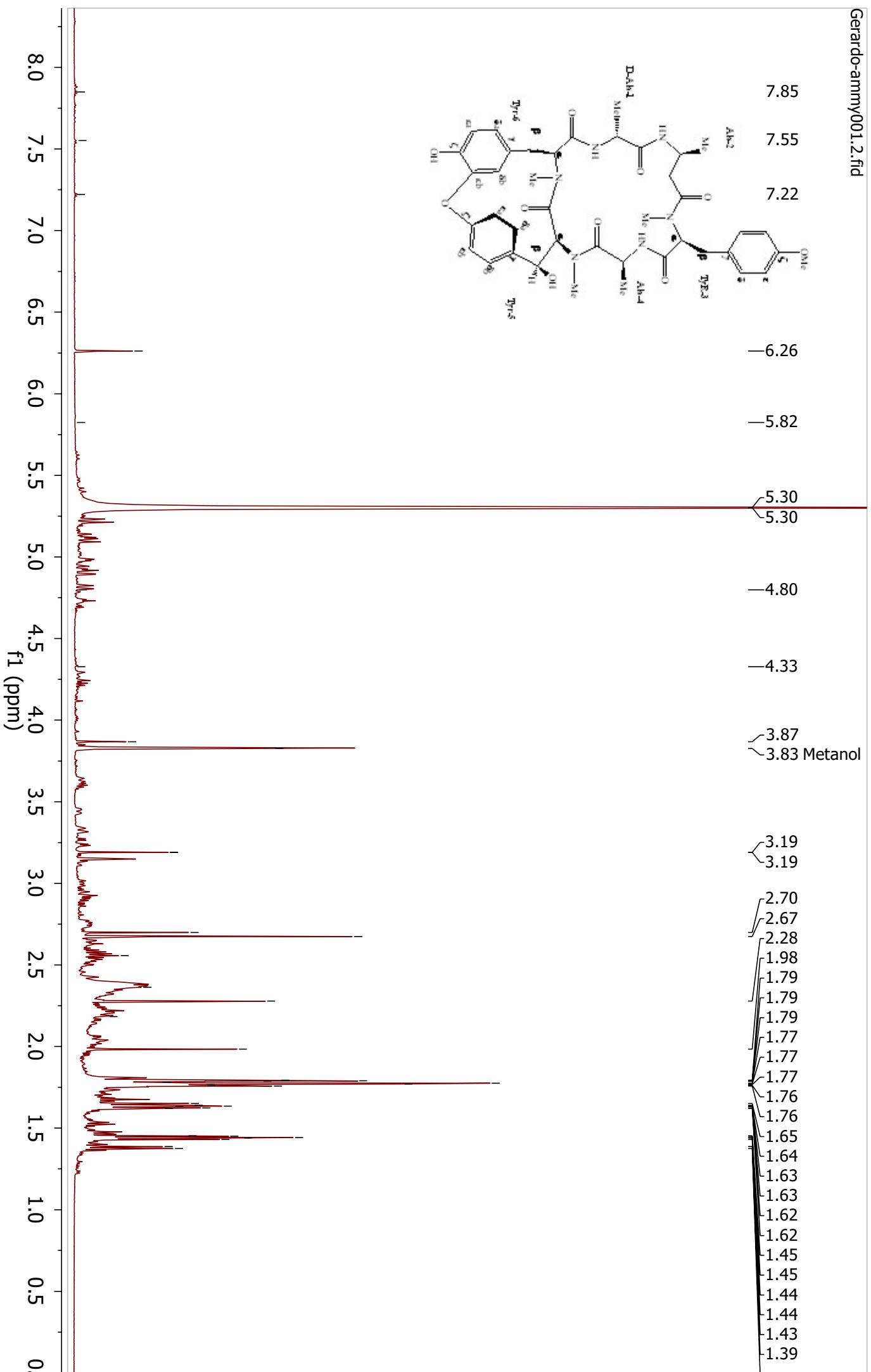


Figure S19.  $^1\text{H}$  NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of bouvardin (**3**)

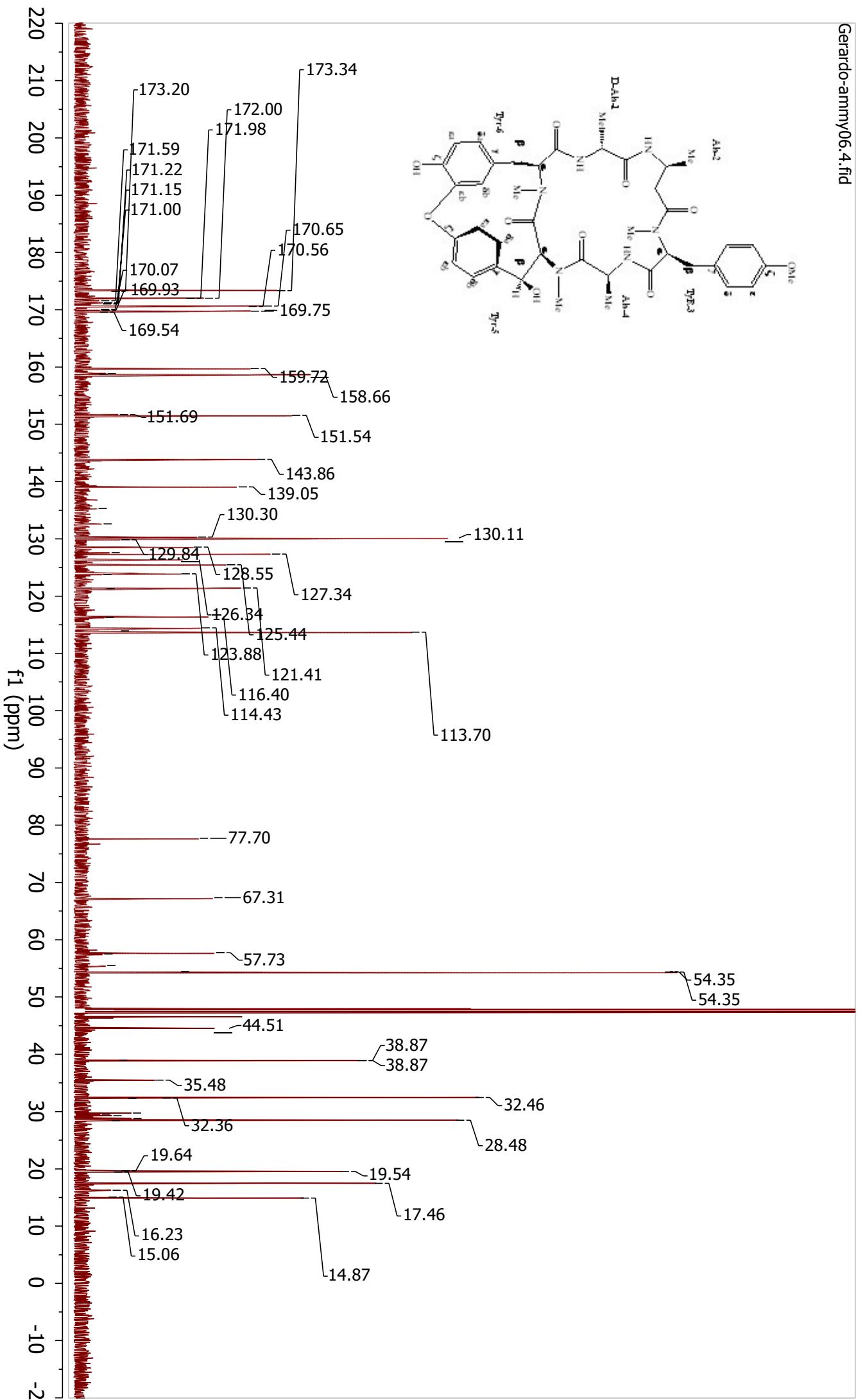
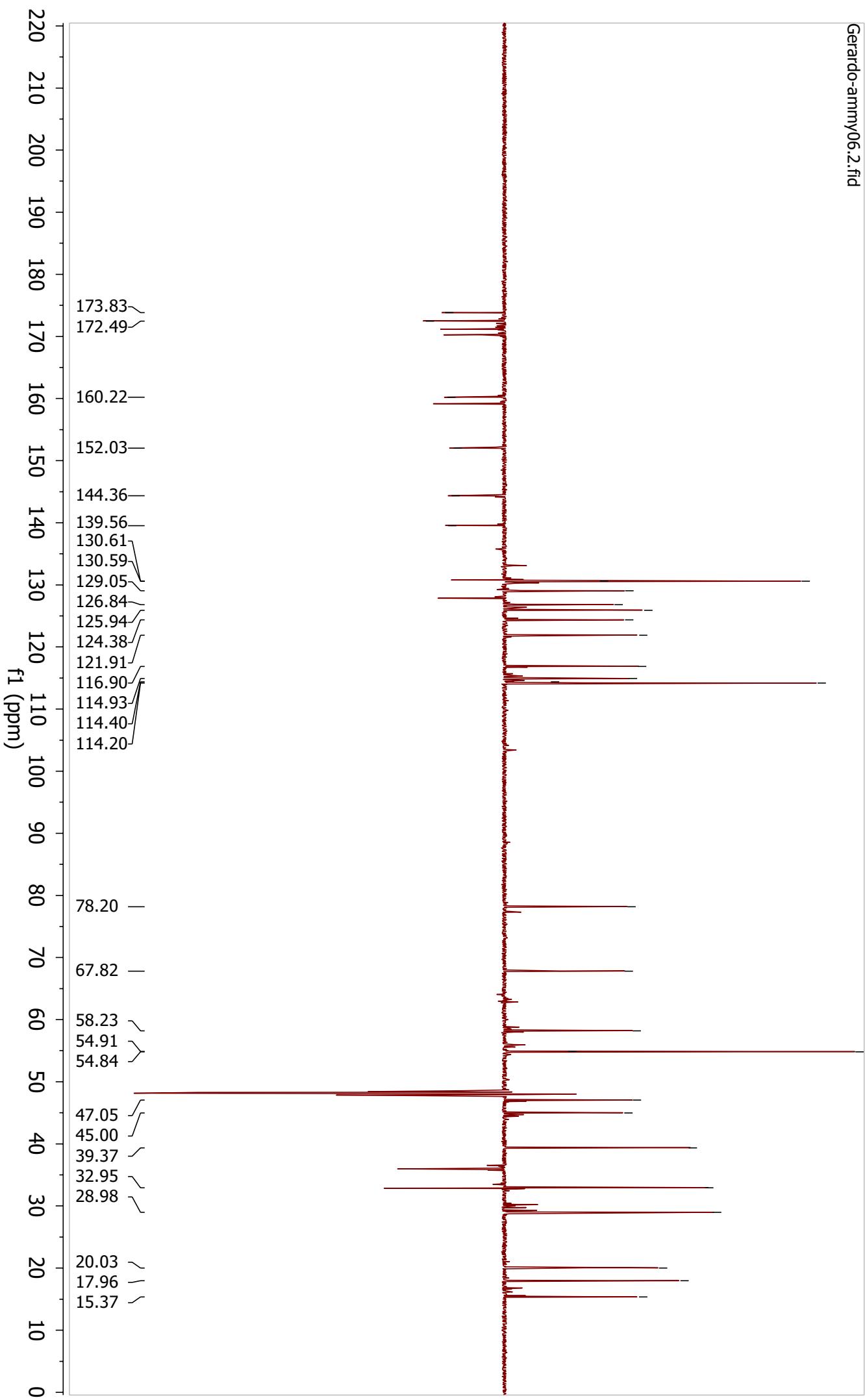
Figure S20.  $^{13}\text{C}$ NMR ( $\text{CD}_3\text{OD}$ , 100 MHz) of bouvardin (**3**)

Figure S21.  $^{13}\text{C}$  (DEPT) NMR ( $\text{CD}_3\text{OD}$ , 100 MHz) of bouvardin (**3**)



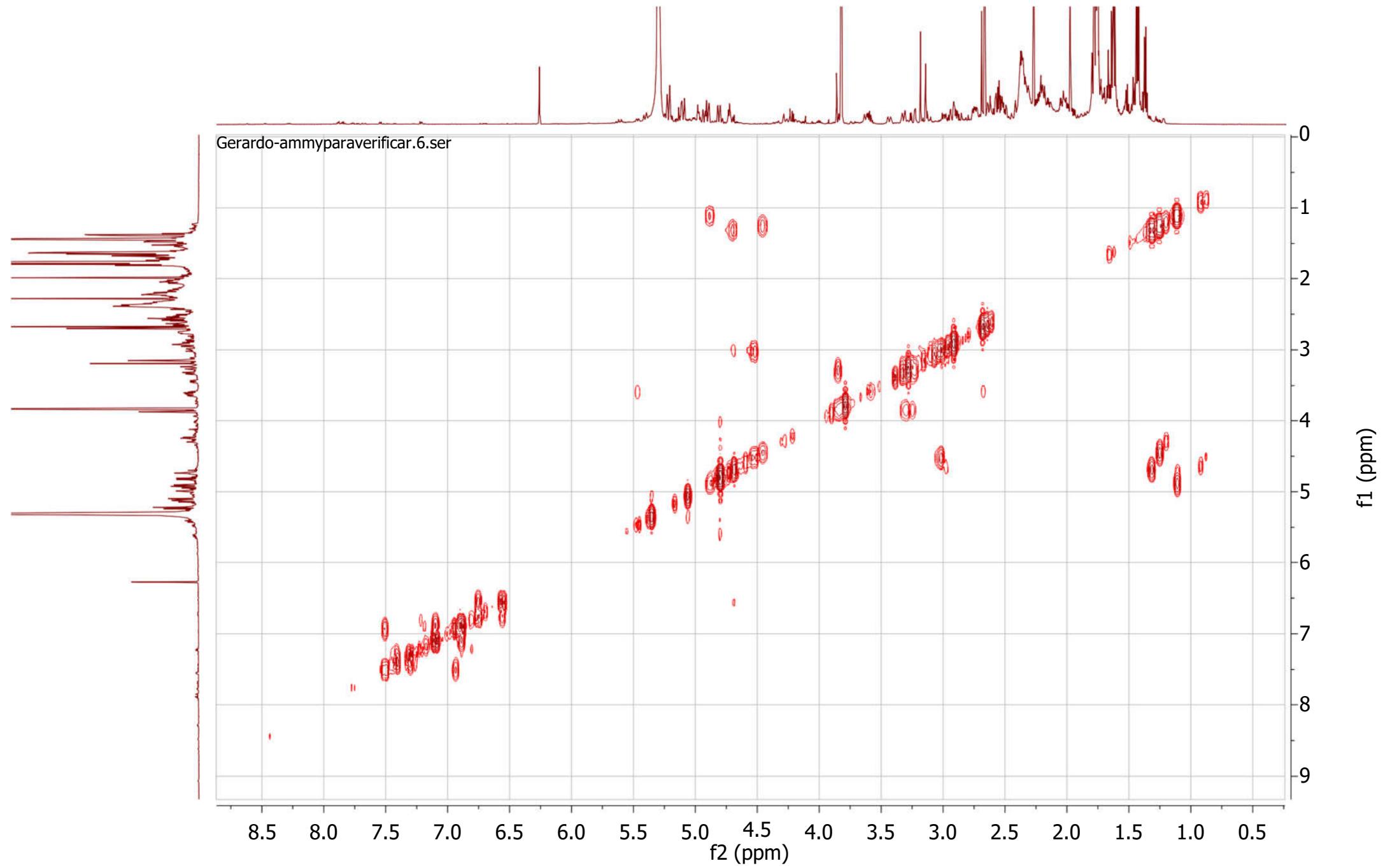


Figure S22.  $^1\text{H}$ - $^1\text{H}$  COSY NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of bouvardin (**3**)

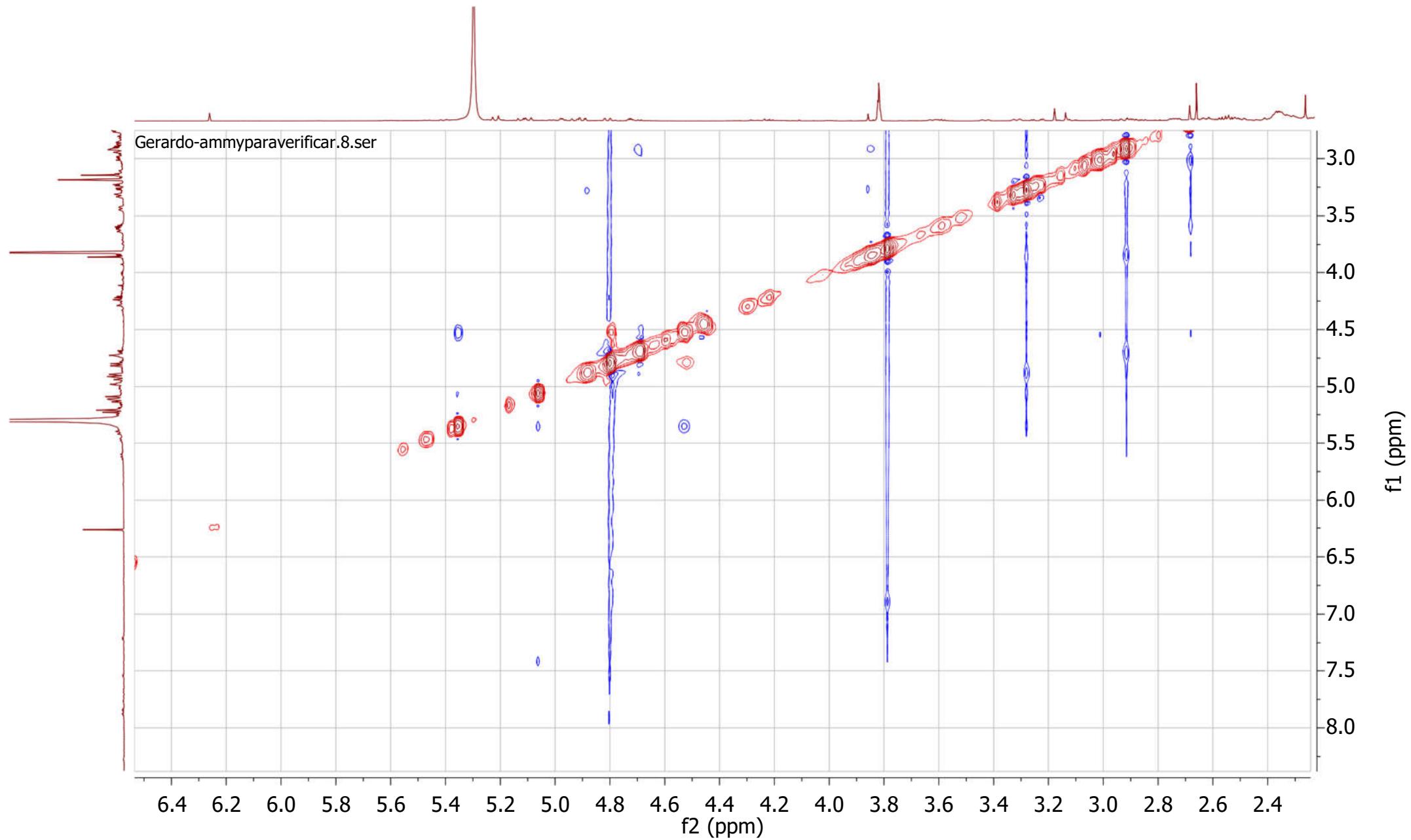


Figure S23.  $^1\text{H}$ - $^1\text{H}$  NOESY NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of bouvardin (**3**)

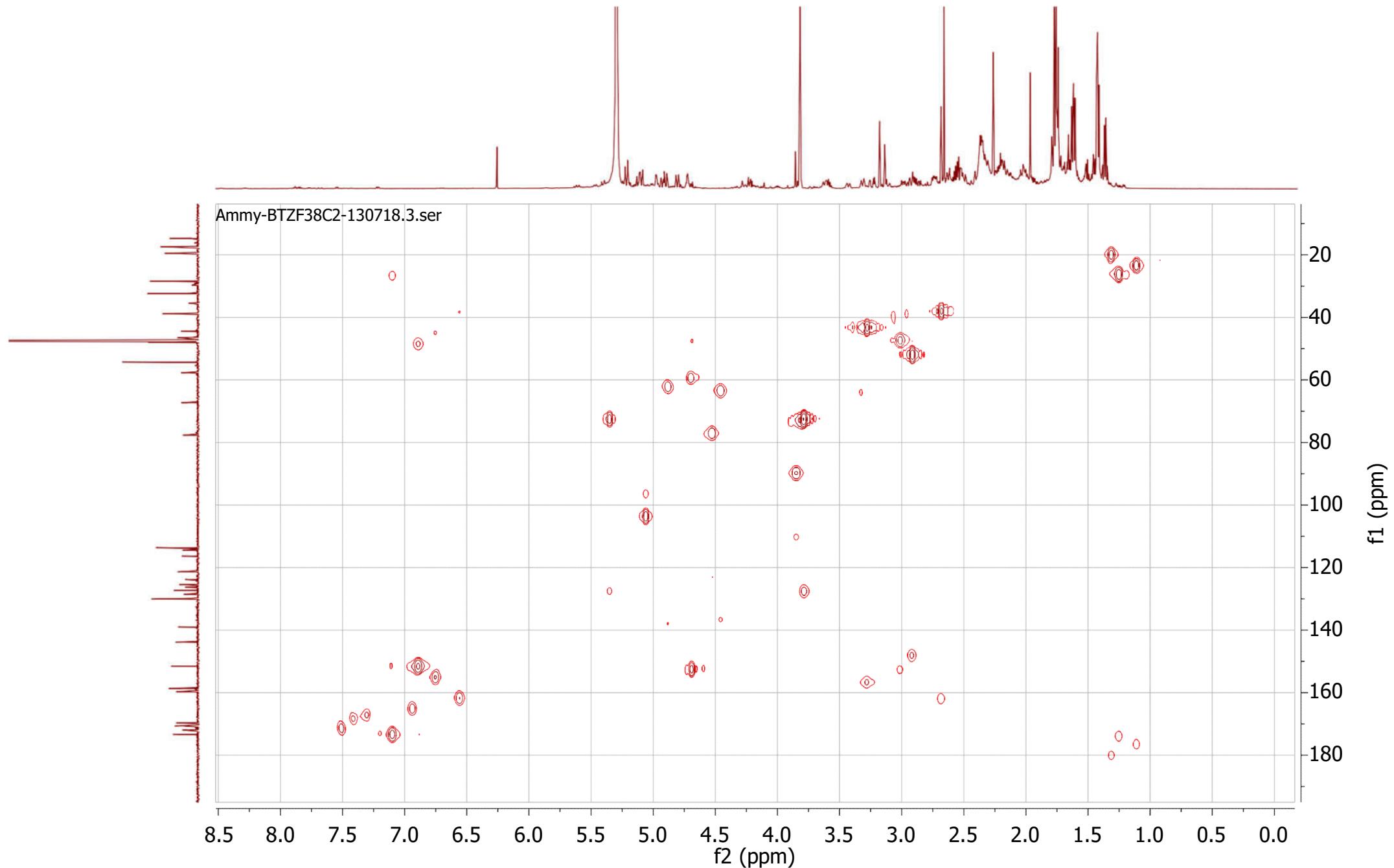


Figure S24.  $^1\text{H}$ - $^{13}\text{C}$  (HMBC) NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) of bouvardin (**3**)

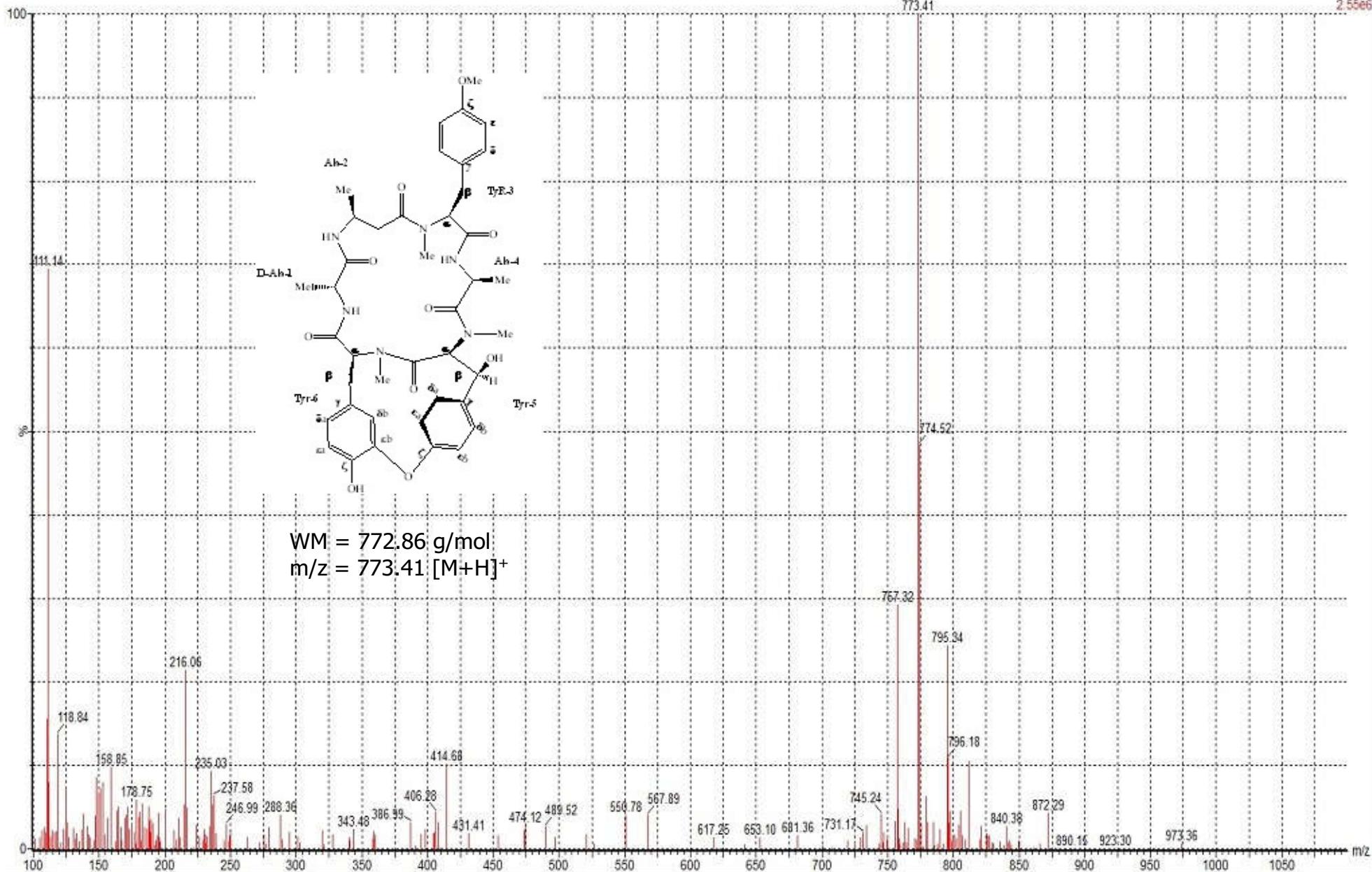


Figure S25. Mass spectrum (MS) of bouvardin (**3**)

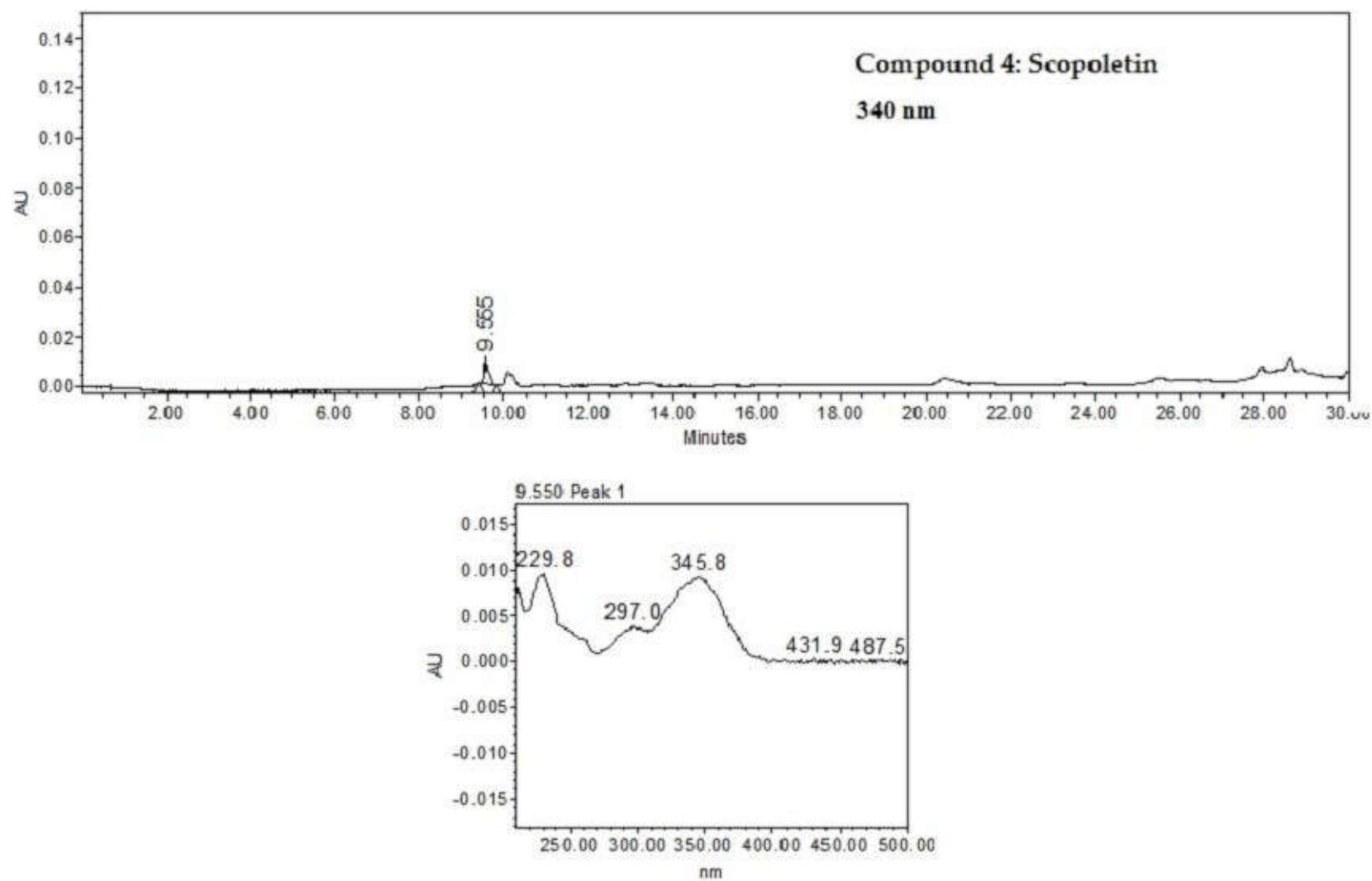


Fig S26. Spectrum UV of Scopoletin (**4**)

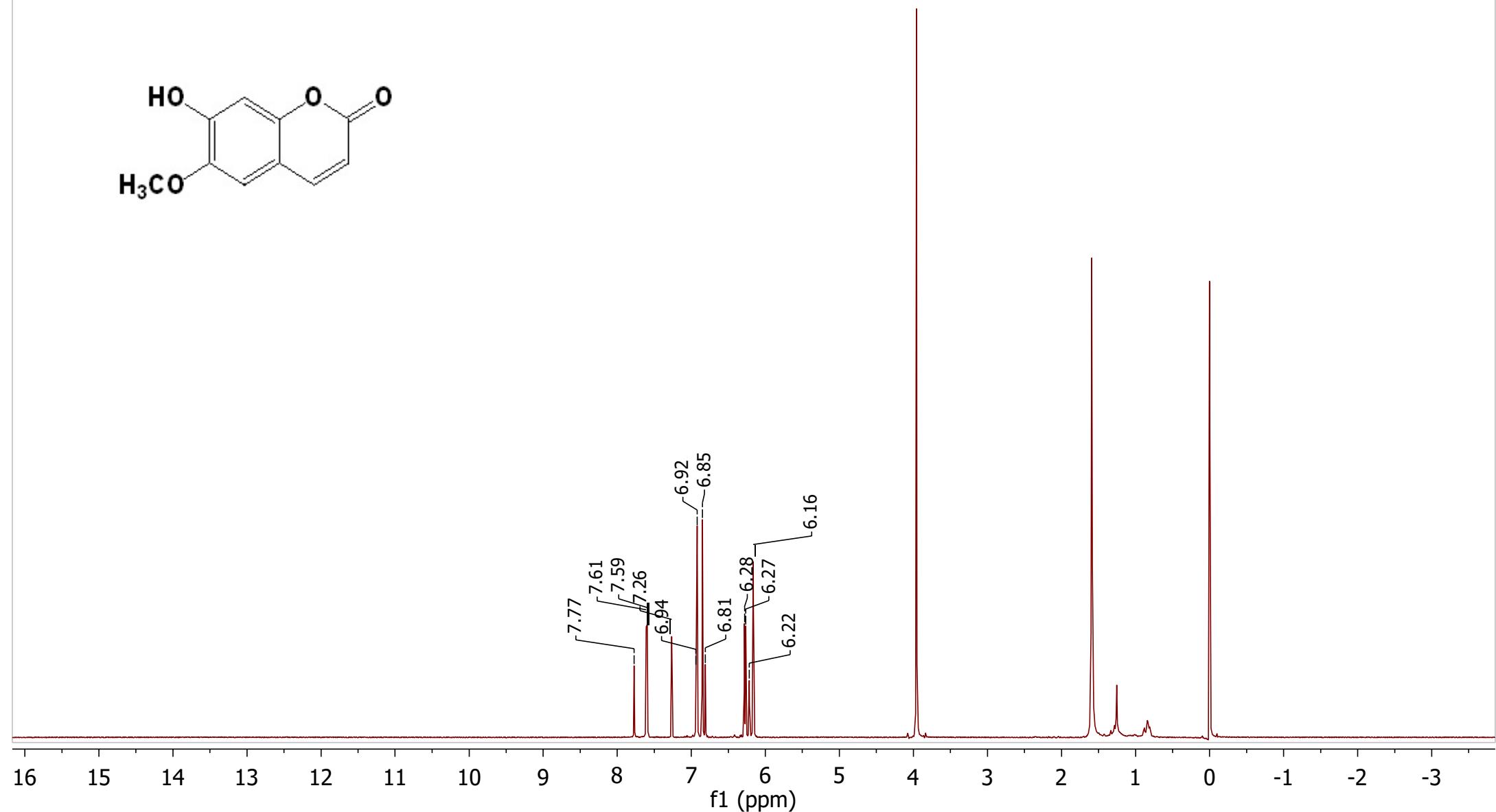
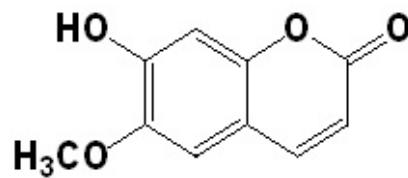


Figure S27.  $^1\text{H}$  NMR ( $\text{CD}_3\text{O}$ , 600 MHz) of scopoletin (**4**)

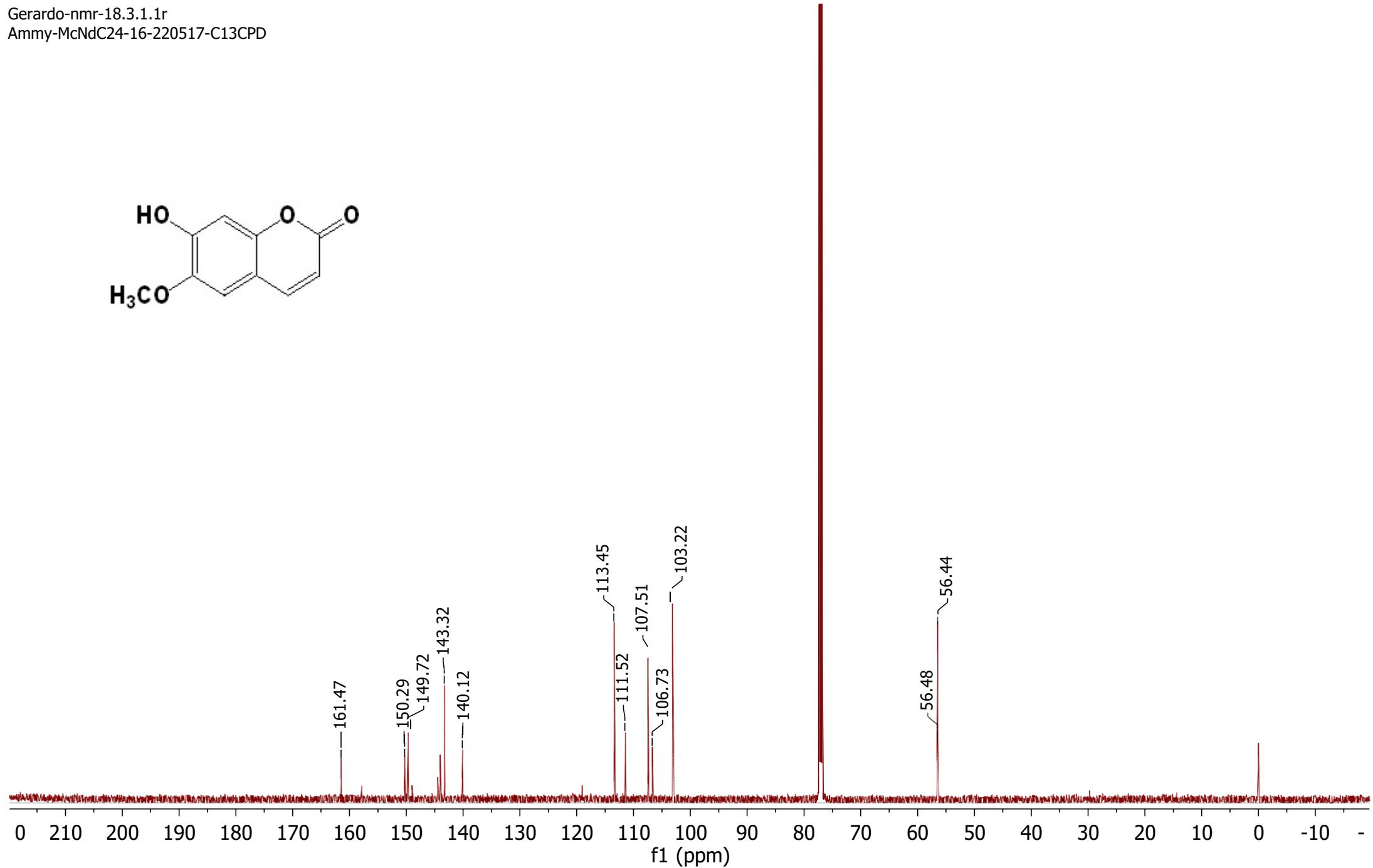
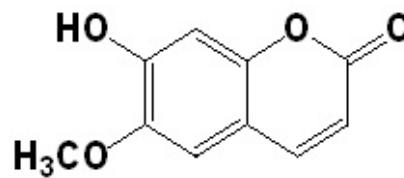


Figura S28.  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 150 MHz) of scopoletin (**4**)

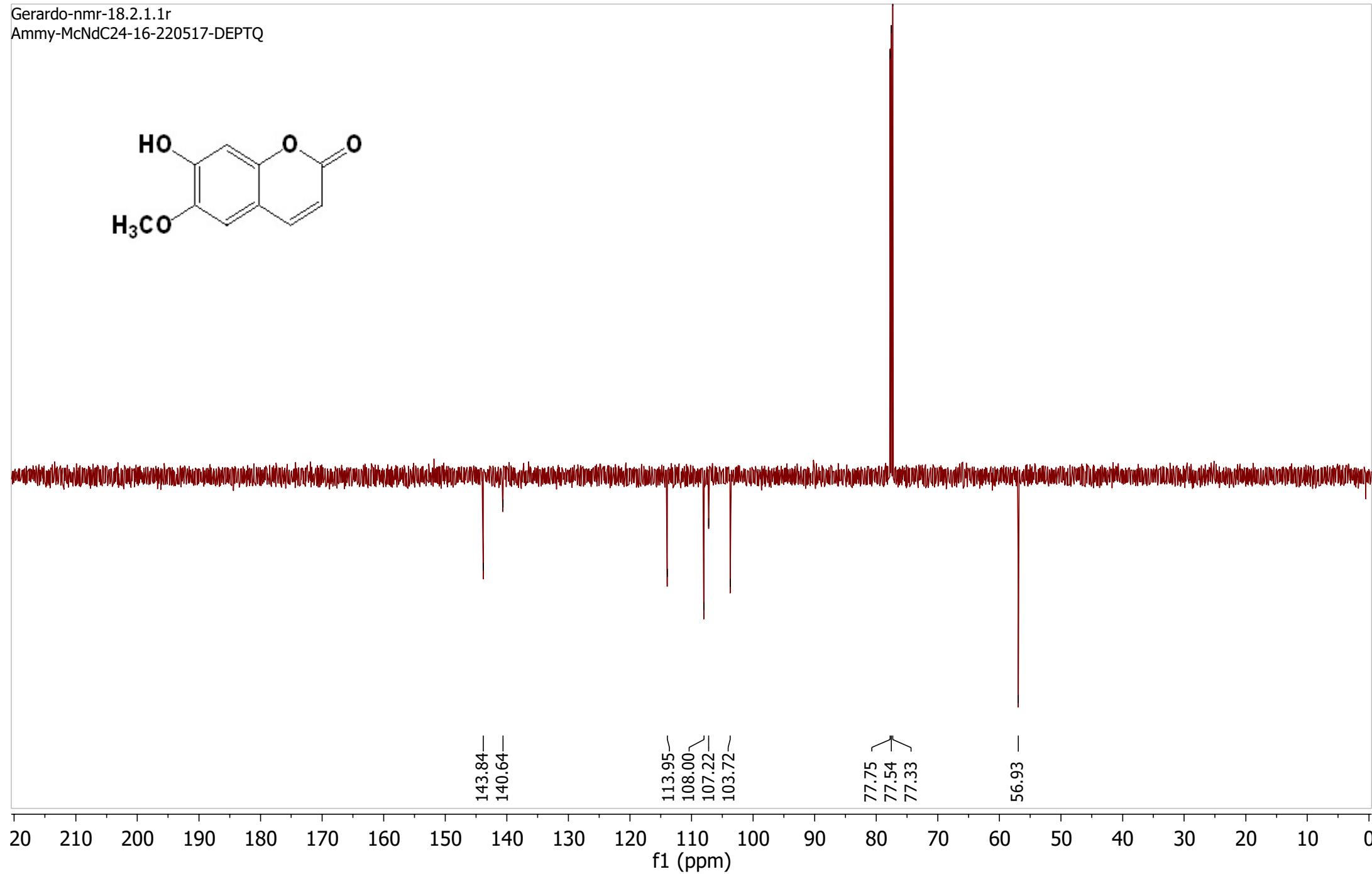
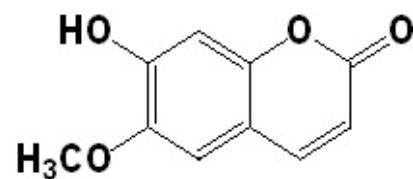


Figure S29.  $^{13}\text{C}$  (DEPT) NMR ( $\text{CD}_3\text{OD}$ , 150 MHz) of scopoletin (**4**)

**Table S1:**  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 100 MHz) of bouvardin (**3**),  $^1\text{H}$ - $^{13}\text{C}$  (HSQC) NMR ( $\text{CD}_3\text{OD}$ , 400 MHz) and  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , Bates *et al.*, 1983)

	Experimental	Referencia	
	$^{13}\text{C}$ NMR of Bouvardin ( <b>3</b> )	$^1\text{H}$ - $^{13}\text{C}$ (HSQC) NMR of Bouvardin ( <b>3</b> )	$^{13}\text{C}$ NMR Bouvardin (Bates <i>et al.</i> , 1983)
<b>Ala-2<math>\beta</math></b>	16.39	1.29 (d $J=7.03$ )	16.4q
<b>Ala-4<math>\beta</math></b>	18.93	1.08 (d $J=6.64$ )	18.5q
<b>Ala-1<math>\beta</math></b>	21.09	1.22 (d $J=6.64$ )	20.5q
<b>Tyr-6 N-Me</b>	30.01	2.67 (s)	29.2q
<b>Tyr-5 N-Me</b>	33.80	3.25 (s)	33.0q
<b>Tyr-3<math>\beta</math></b>	33.98		32.7t
<b>Tyr-6<math>\beta</math></b>	36.5	2.99 (s)	35.9t
<b>Tyr-5<math>\beta</math></b>	79.11	5.03 (s)	78.5 d
<b>Tyr-3 N-Me</b>	40.38	2.86 (s)	39.7q
<b>Ala- 1 <math>\alpha</math></b>	45.96	4.67 (s)	44.9d
<b>Ala-4<math>\alpha</math></b>	46.18		46.5d
<b>Ala-2<math>\alpha</math></b>	48.1	4.87 (s)	47.9d
<b>Tyr-5<math>\alpha</math></b>	55.74	5.32 (d $J=1.95$ )	53.9d
<b>Tyr-3 O-Me</b>	55.81	3.76 (s)	55.3d
<b>Tyr-6<math>\alpha</math></b>	59.11	4.45 (s)	57.8d
<b>Tyr-3<math>\alpha</math></b>	68.74	3.82 (s)	68.75d

<b>Tyr-6<math>\delta</math><sub>a</sub></b>	115.13	4.65 (s)	113.0d
<b>Tyr-3<math>\epsilon</math></b>	116.05	6.86 (d $J=8.60$ )	114.1d
<b>Tyr-6 <math>\epsilon</math><sub>a</sub></b>	117.87	6.73 (s)	116.1d
<b>Tyr-6<math>\delta</math><sub>b</sub></b>	122.89	6.53 (d $J=1.56$ )	124.2d
<b>Tyr-5<math>\epsilon</math><sub>a</sub></b>	125.37	6.90(dd $J=8.60; 10.55$ )	125.7d
<b>Tyr-6 <math>\gamma</math></b>	126.95	7.27(dd $J= 8.60; 10.55$ )	127.2s
<b>Tyr-3<math>\delta</math></b>	131.50	7.07(d $J= 8.60$ )	130.3d
<b>Tyr-3<math>\gamma</math></b>	131.71	7.48 (dd $J= 8.60; 10.55$ )	130.7s
<b>Tyr-5 <math>\delta</math><sub>a</sub></b>	127.17		126.9d
<b>Tyr-5 <math>\delta</math><sub>b</sub></b>	128.78		128.5d
<b>Tyr-5<math>\gamma</math></b>	140.54		139.8s
<b>Tyr-6<math>\zeta</math></b>	145.28		143.2s
<b>Tyr-6<math>\epsilon</math><sub>b</sub></b>	152.96		151.0s
<b>Tyr-5<math>\zeta</math></b>	160.06		158.9s
<b>Tyr-3<math>\zeta</math></b>	161.10		158.4s
<b>Tyr-6 CO</b>	167.81		168.3s
<b>Tyr-5 CO</b>	171.25		170.0s
<b>Tyr-3 CO</b>	171.98		170.8s
<b>Ala-4 CO</b>	172.10		172.2s
<b>Ala-1 CO</b>	173.39		172.2s
<b>Ala-2 CO</b>	174.78		172.5s

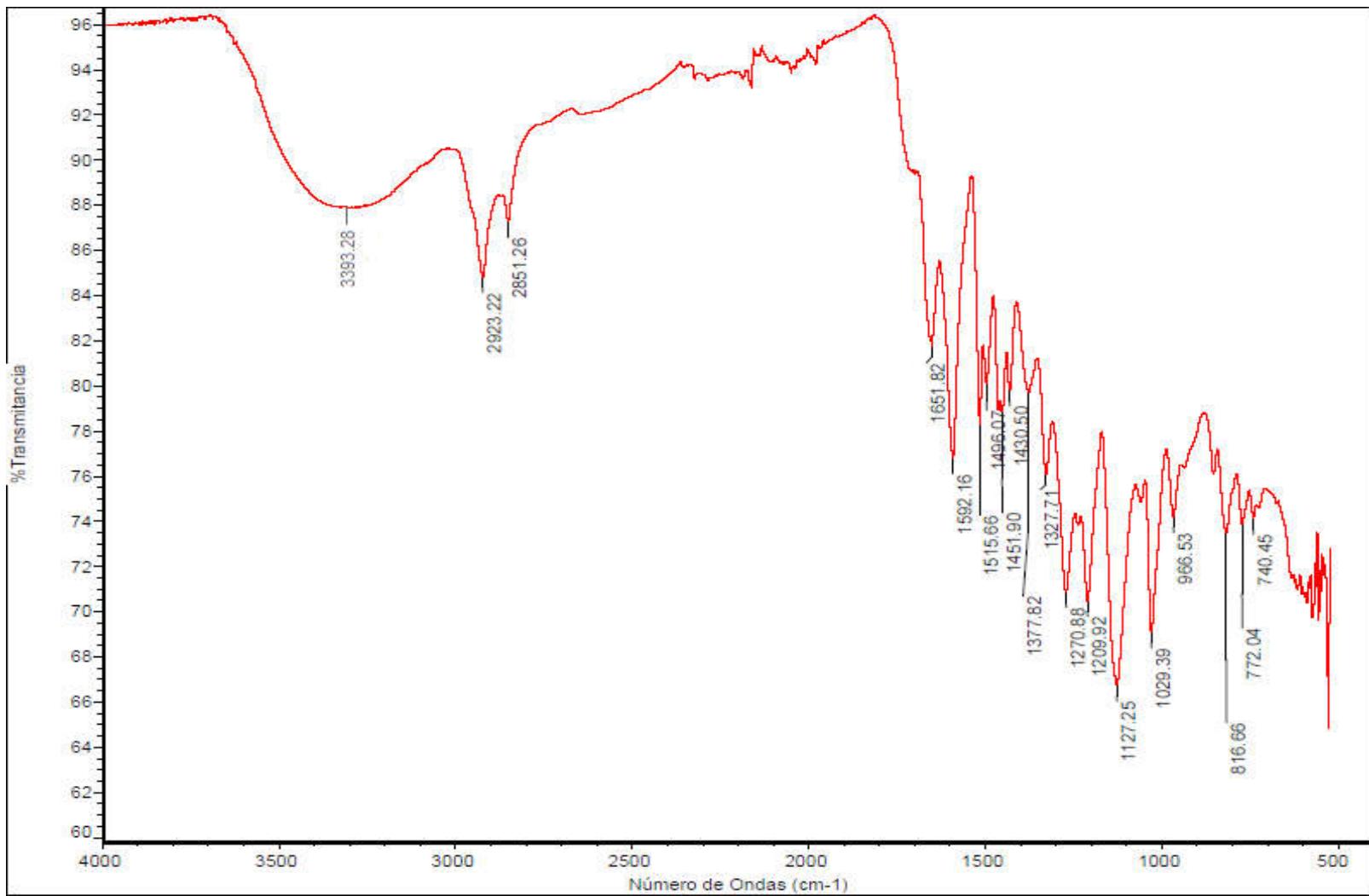


Figure S30. IF spectroscopy ternifoliol (**1**)

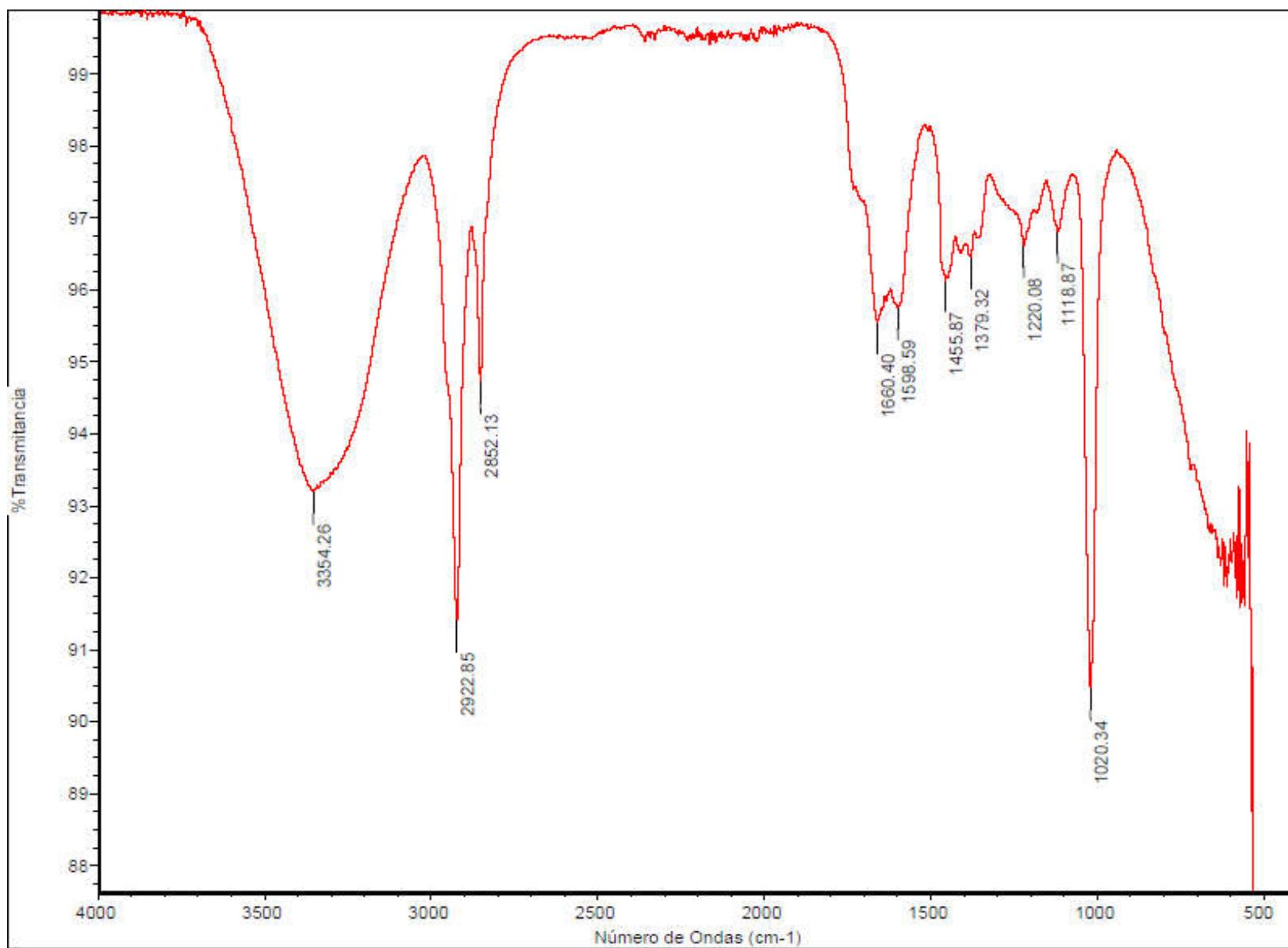


Figure S31. IF spectroscopy ternifolial (2)