Supplementary material

Xylaropyrones B and C, new γ-pyrones from the endophytic fungus *Xylaria* sp. SC1440

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ABSTRACT

Two new γ-pyrones, xylaropyrones B (**1**) and C (**2**), together with three known compounds, xylaropyrone (**3**), annularin A (**4**), and annularin C (**5**), were isolated from solid cultures of the endophytic fungus *Xylaria* sp. SC1440. The structures of these compounds were determined mainly by analysis of their NMR spectroscopic data. The relative configurations of **1** and **2** were assigned on the basis of *J*-based configurational analysis, and the absolute configurations were established by experimental and TDDFT calculated ECD spectra. The isolated compounds were evaluated for cytotoxic and tyrosinase inhibitory activity.

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Table S1. The ^{1}H and ^{13}C NMR data of **1** and **2** (δ in ppm, J in Hz, $CDCl_3$)

	xylaropyrone B (**1**)		xylaropyrone C (**2**)	
No.	δ_C, type	δ_H, mult. (J in Hz)	δ_C, type	δ_H, mult. (J in Hz)
2	172.4, C		172.1, C	
3	111.7, CH	6.41, s	112.0, CH	6.41, s
4	180.3, C		180.3, C	
5	127.6, C		127.6, C	
6	152.5, CH	7.81, s	152.7, CH	7.83, s
7	58.0, CH_2	4.44, s	57.8, CH_2	4.43, s
8	68.9, CH	4.51, dd (9.7, 3.7)	69.3, CH	4.50, dd (8.3, 5.3)
9	42.3, CH_2	1.73, ddd (13.8, 9.7, 4.1)	42.3, CH_2	1.71, ddd (13.4, 8.3, 4.9)
		1.48, ddd (13.8, 9.4, 3.7)		1.58, dd (13.4, 5.3)
10	30.7, CH	1.64, m	30.9, CH	1.54, m
11	30.2, CH_2	1.35, m	28.8, CH_2	1.44, m
		1.24, m		1.16, m
12	11.4, CH_3	0.89, t (7.4)	11.1, CH_3	0.87, t (7.4)
13	18.6, CH_3	0.94, d (6.6)	19.7, CH_3	0.92, d (6.4)

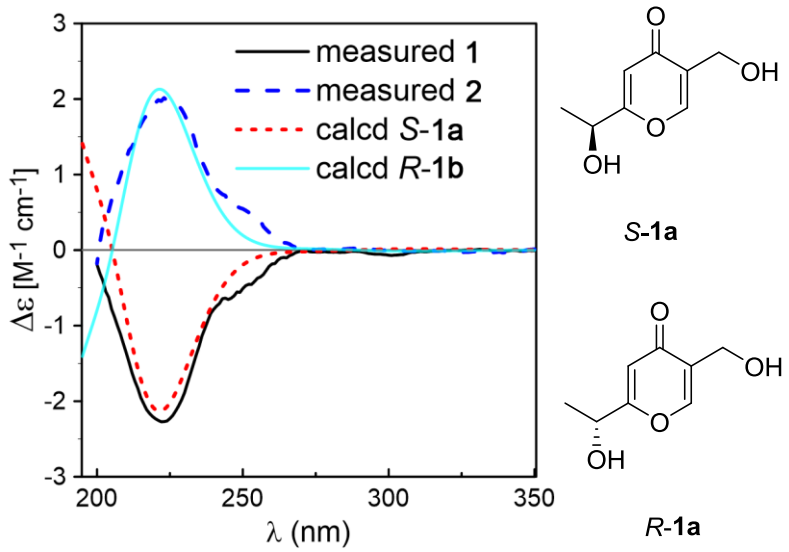


Figure S1. Comparison of the measured ECD spectra of **1** and **2** with PBE0/TZVP calculated spectra of *S*-**1a** and *R*-**1a** in MeOH (σ = 0.38 eV, shift = -3 nm for both isomers).

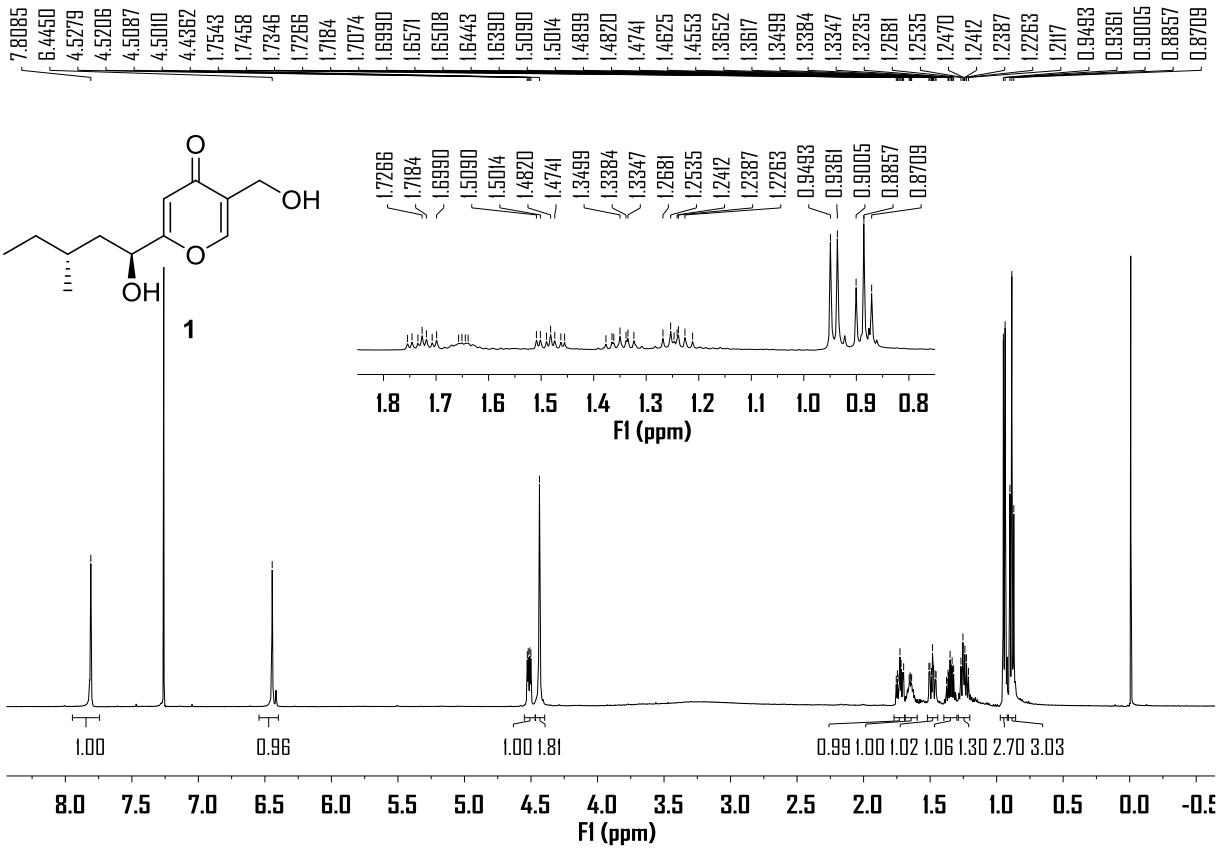


Figure S2. ^{1}H NMR spectrum of xylaropyrone B (**1**) in $CDCl_3$.

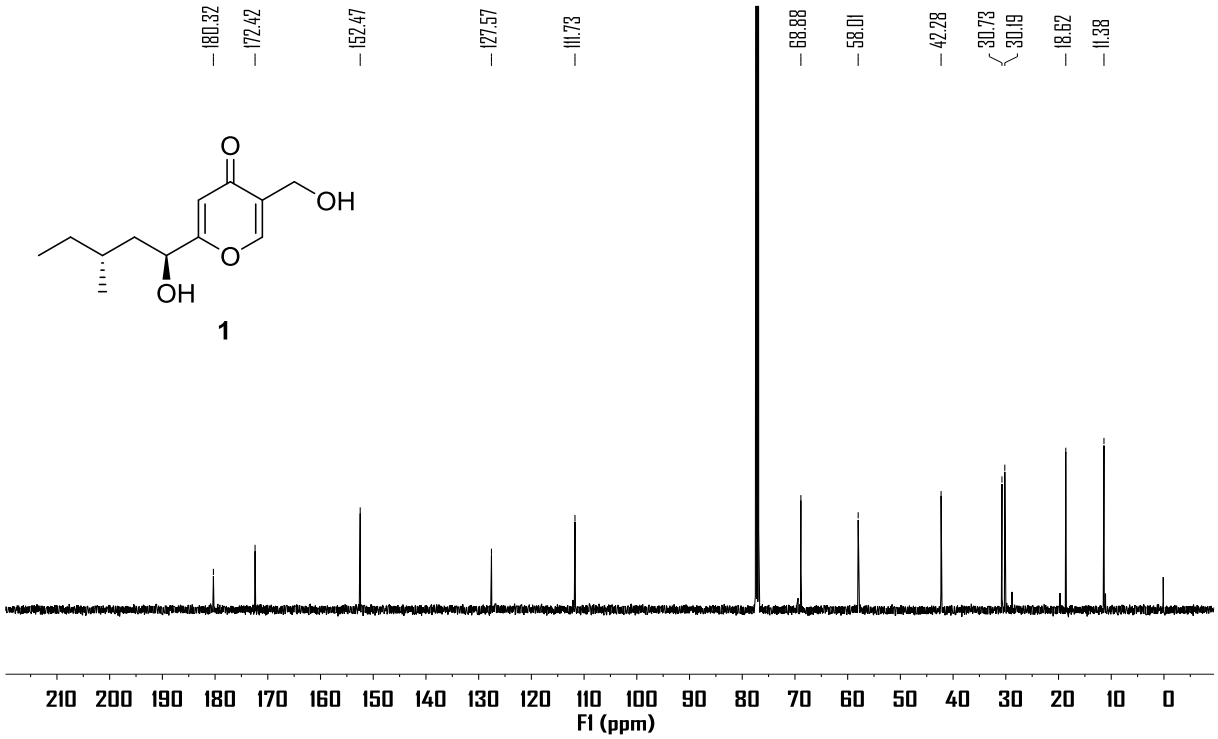


Figure S3. ^{13}C NMR spectrum of xylaropyrone B (**1**) in $CDCl_3$.

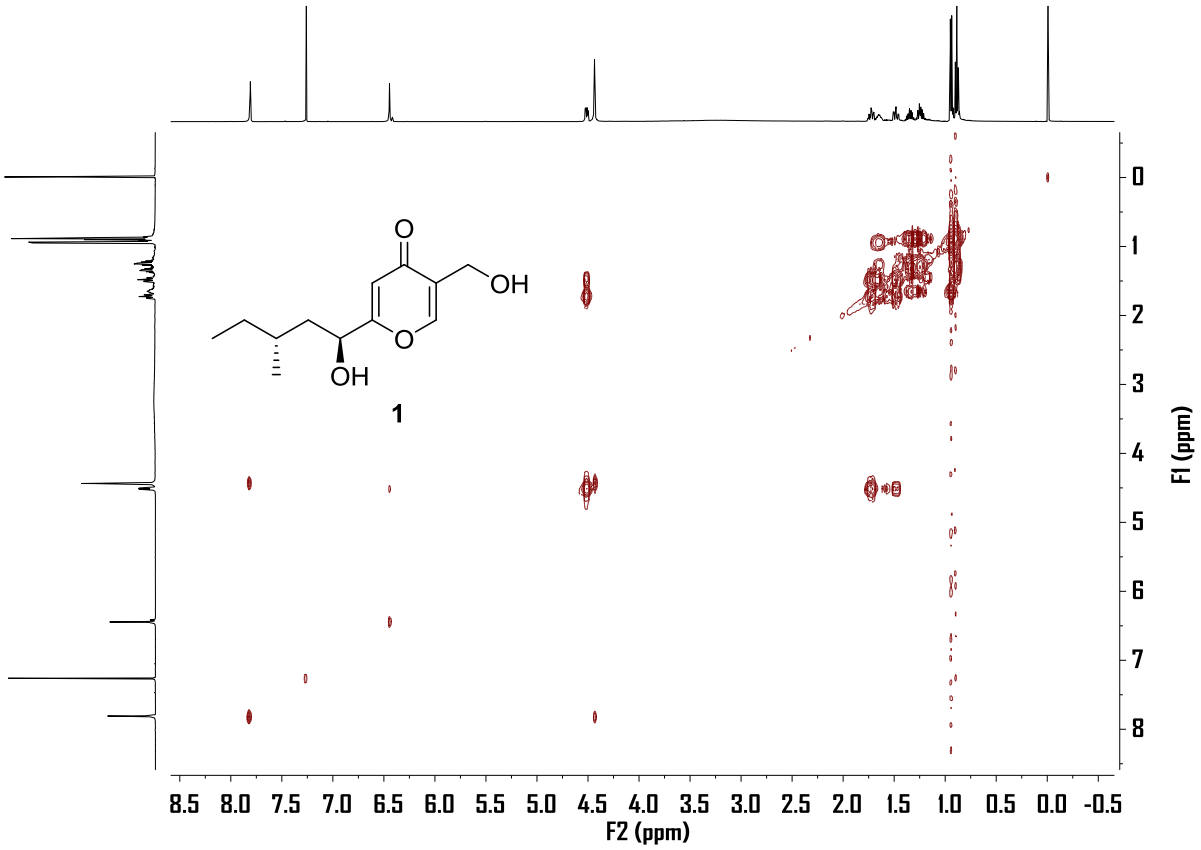


Figure S4. ^{1}H–^{1}H COSY NMR spectrum of xylaropyrone B (**1**) in $CDCl_3$.

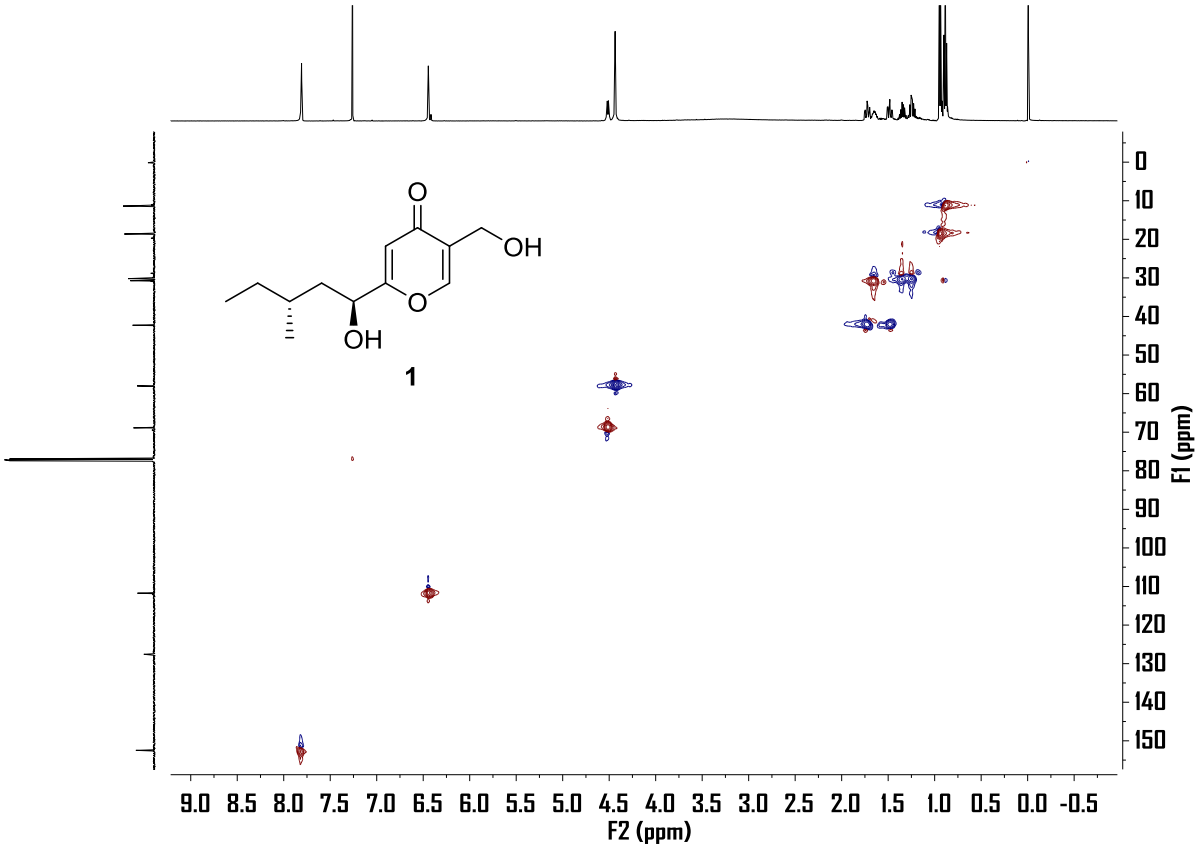


Figure S5. HSQC NMR spectrum of xylaropyrone B (**1**) in $CDCl_3$.

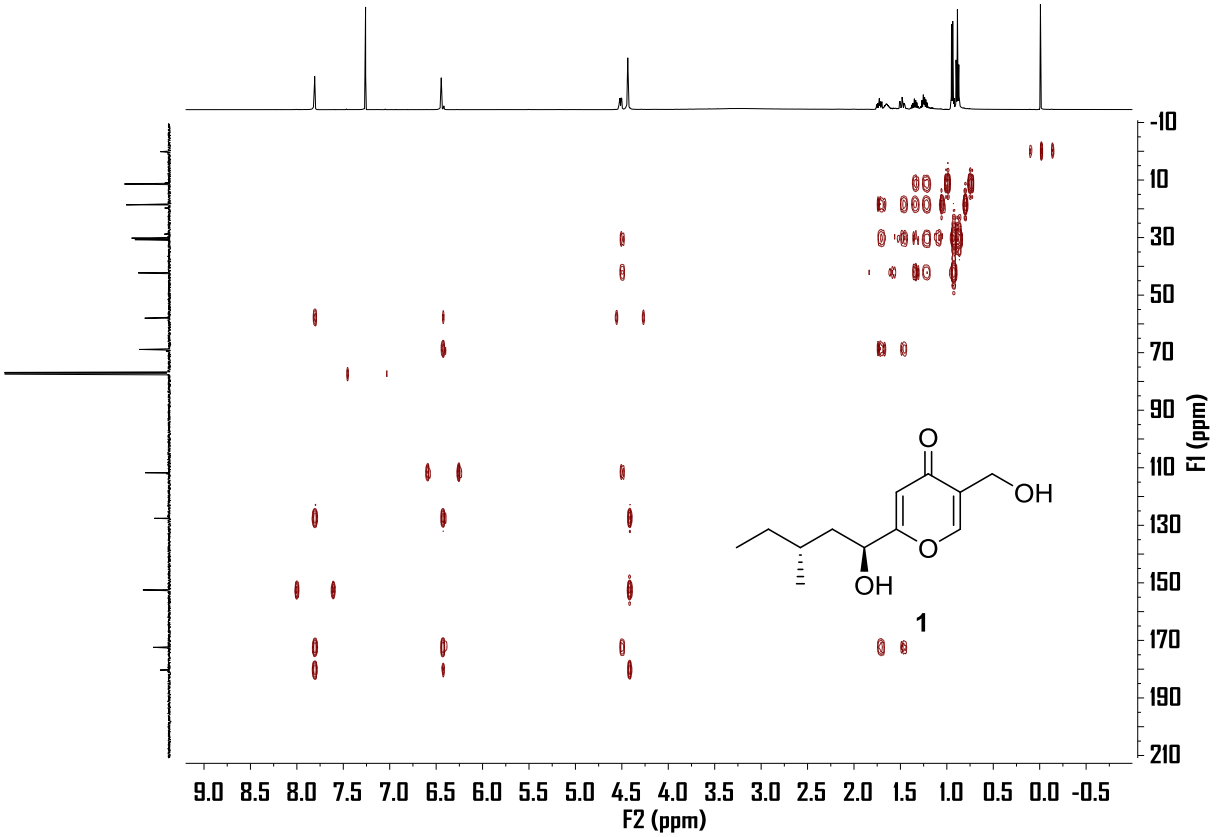


Figure S6. HMBC NMR spectrum of xylaropyrone B (**1**) in $CDCl_3$.

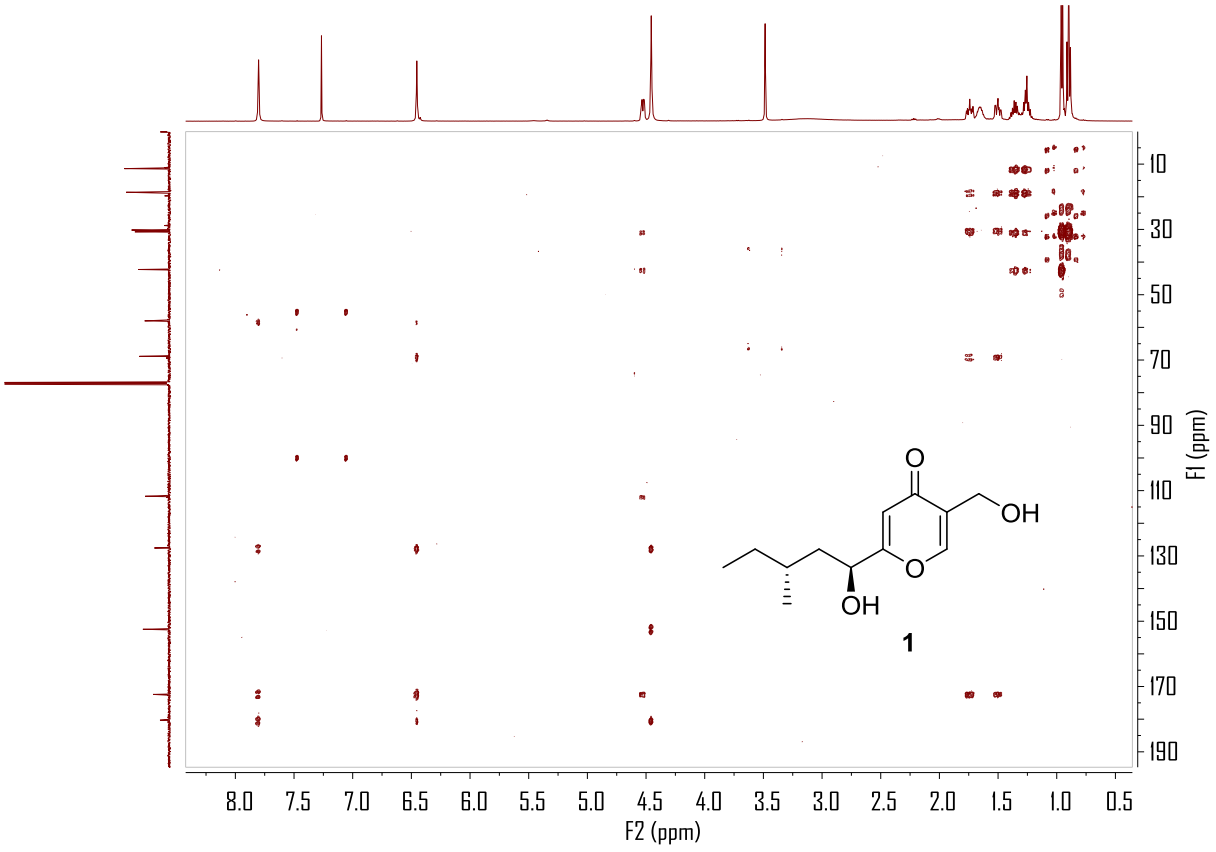


Figure S7. *J*-resolved HMBC-2 spectrum of xylaropyrone B (**1**) in $CDCl_3$.

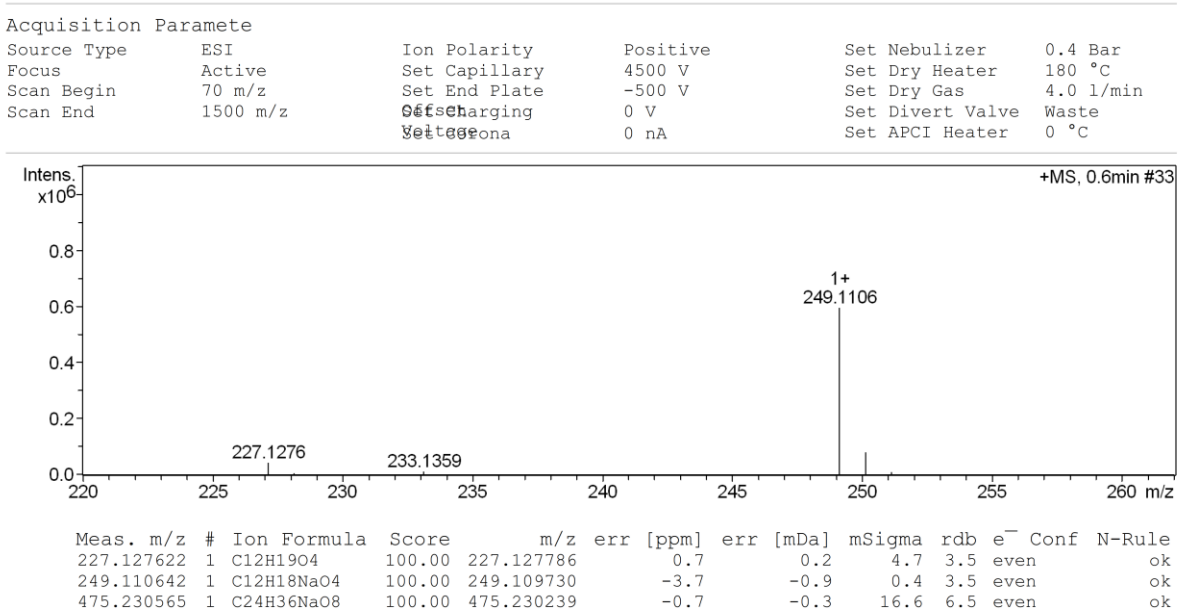


Figure S8. HRESIMS of xylaropyrone B (**1**).

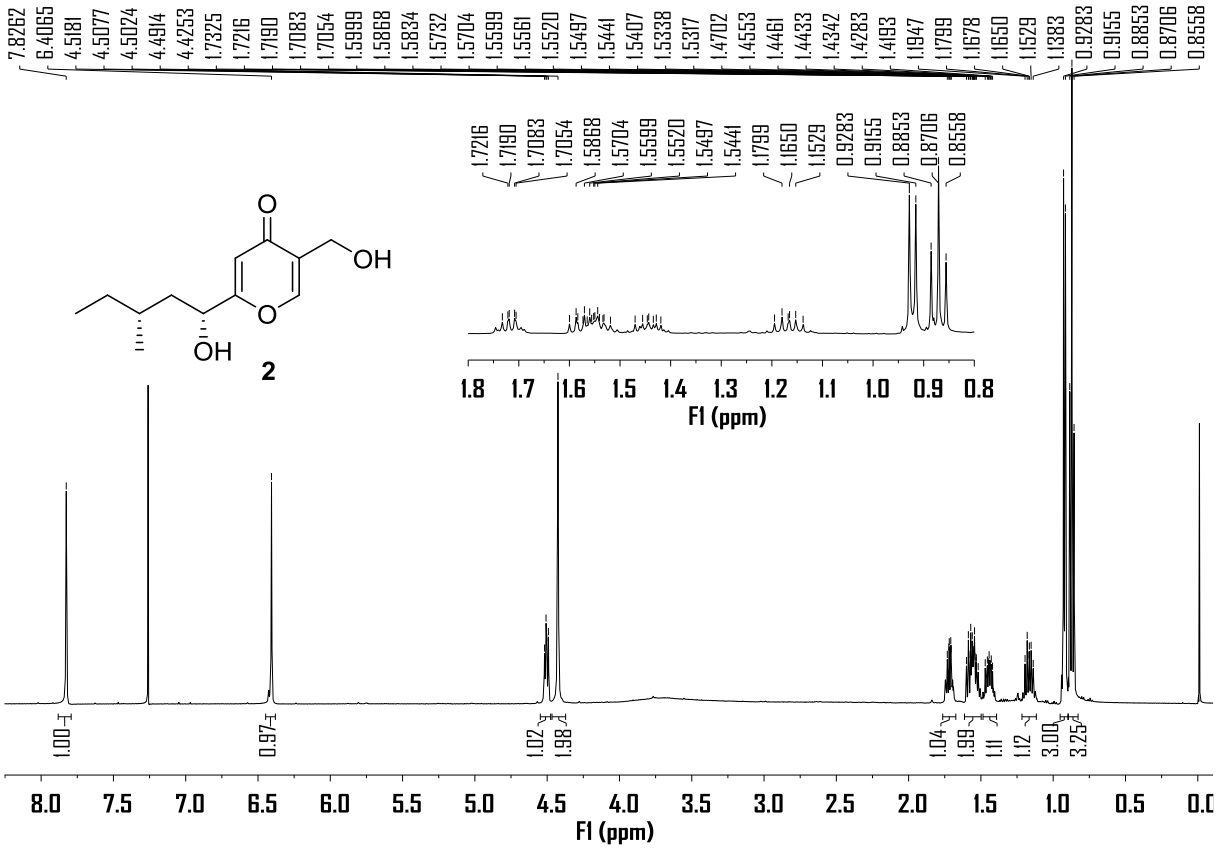


Figure S9. ^{1}H NMR spectrum of xylaropyrone C (**2**) in $CDCl_3$.

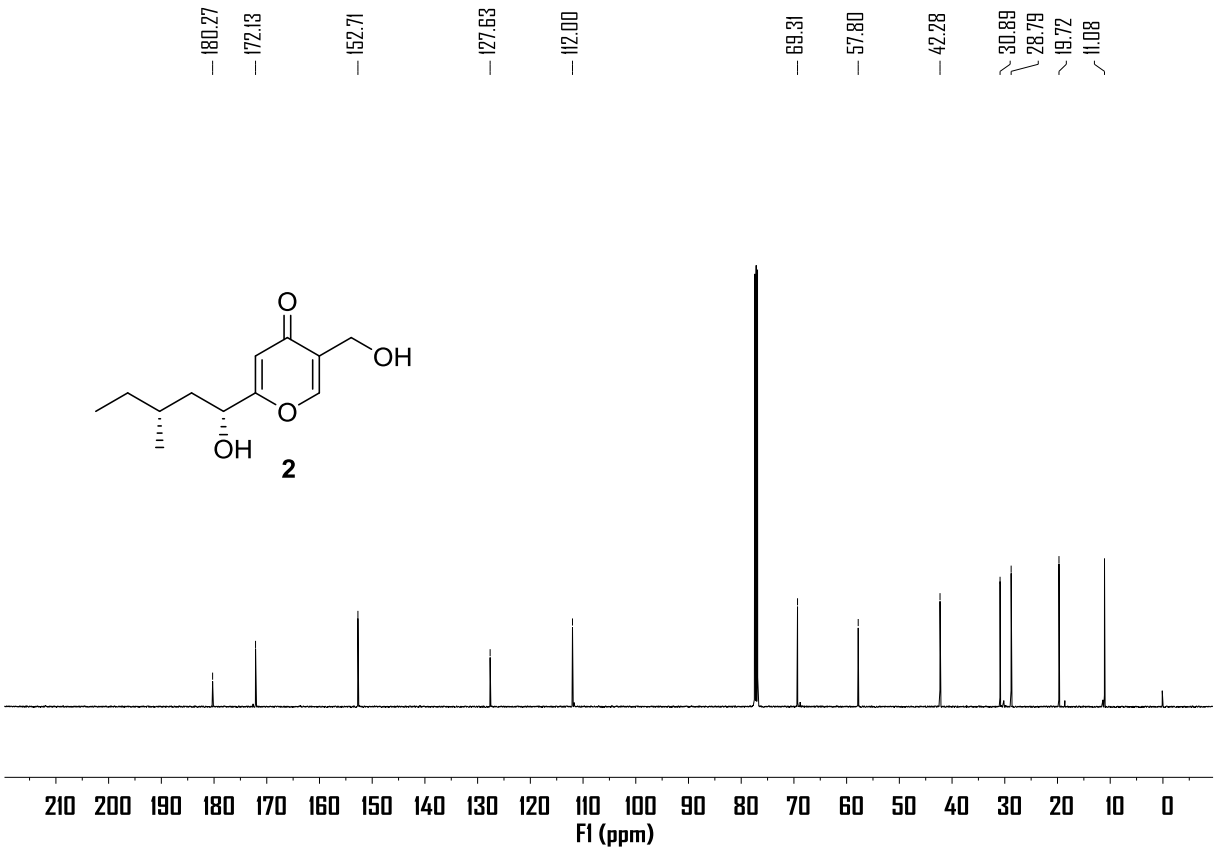


Figure S10. ^{13}C NMR spectrum of xylaropyrone C (**2**) in $CDCl_3$.

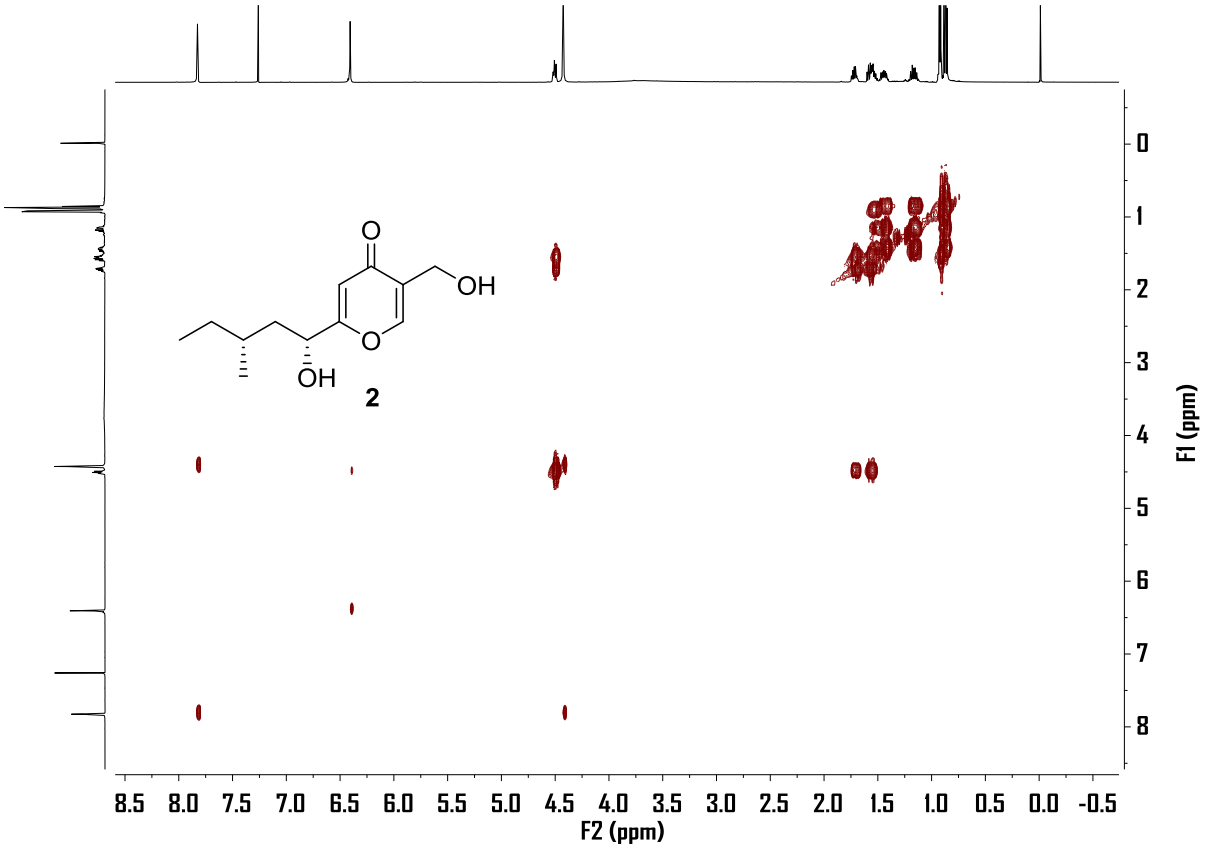


Figure S11. $^{1}H–^{1}H$ COSY NMR spectrum of xylaropyrone C (**2**) in $CDCl_3$.

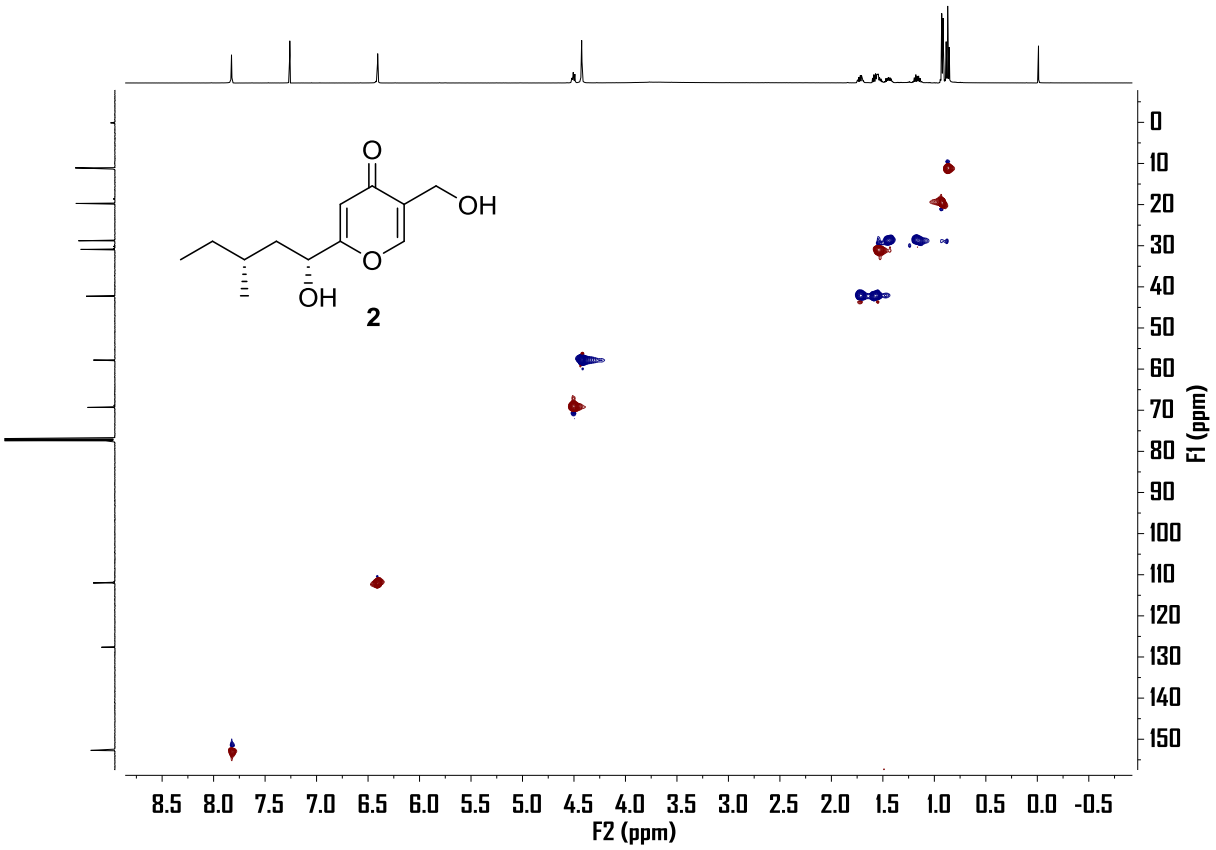


Figure S12. HSQC NMR spectrum of xylaropyrone C (**2**) in $CDCl_3$.

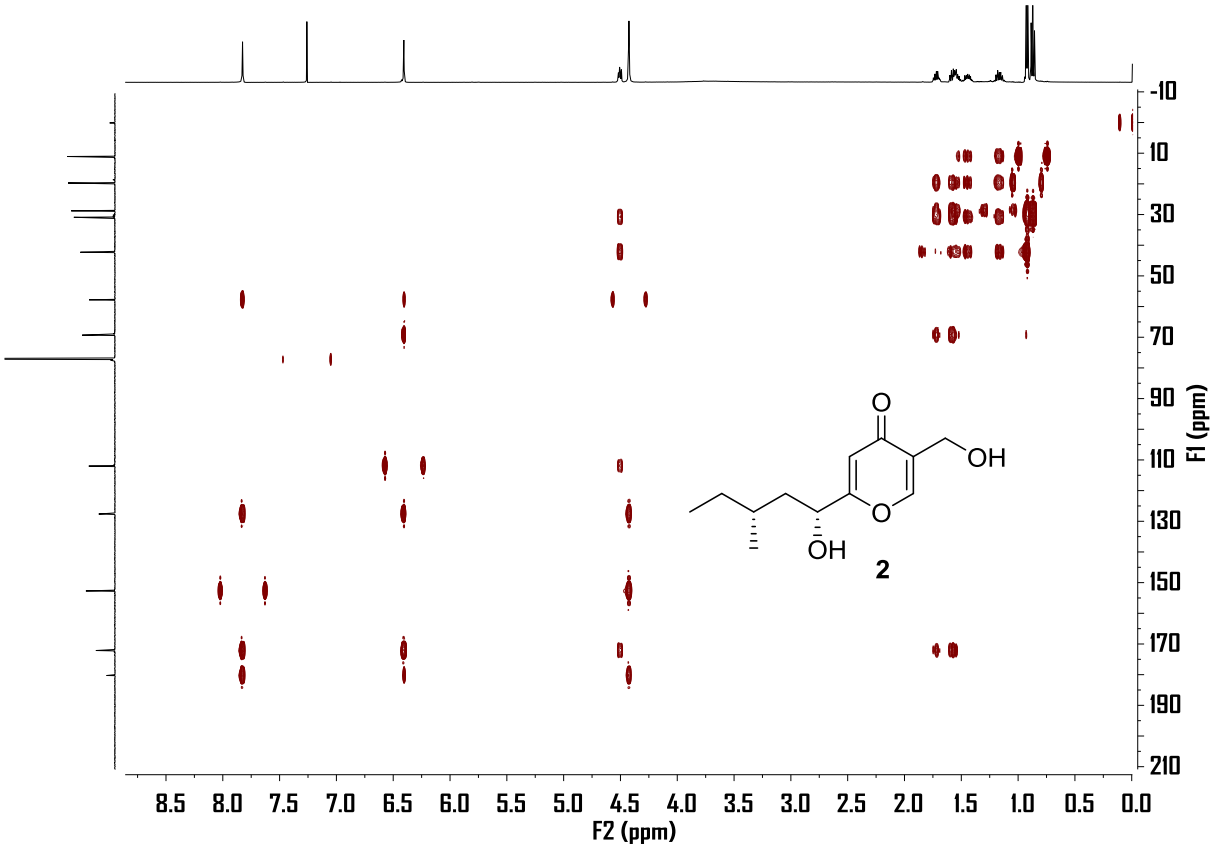
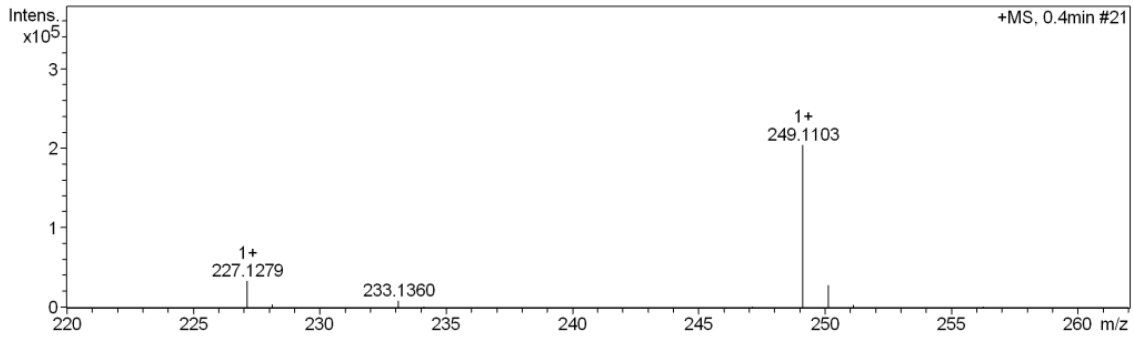


Figure S13. HMBC NMR spectrum of xylaropyrone C (**2**) in $CDCl_3$.

Acquisition Paramete

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e¯ Conf	N-Rule
227.127910	1	C12H19O4	100.00	227.127786	-0.5	-0.1	3.6	3.5	even	ok
249.110305	1	C12H18NaO4	100.00	249.109730	-2.3	-0.6	1.9	3.5	even	ok
475.230348	1	C24H36NaO8	100.00	475.230239	0.2	0.1	17.1	6.5	even	ok

Figure S14. HRESIMS of xylaropyrone C (**2**).