Supplementary Information

Rare prenylated isoflavonoids from the young twigs of *Millettia extensa* and their cytotoxic activities

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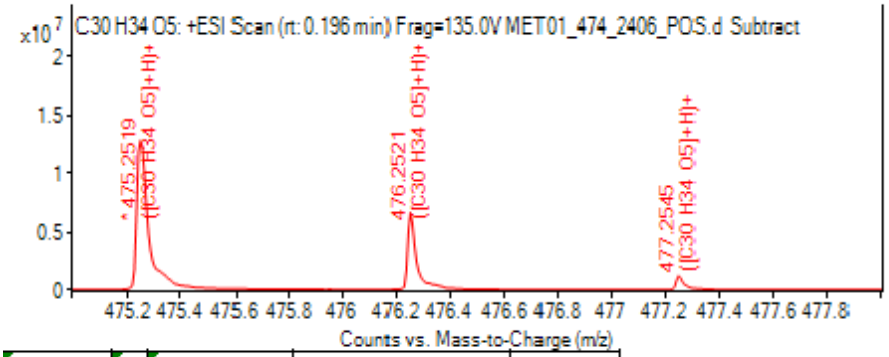
Data Filename	MET01_474_2406_POS.d	**Sample Name**	MET01_474_2406_POS
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	
Acq Method	POS_PURE_10012022_B_Tuning.m	**Acquired Tim**	17/1/2565 13:59:07 (UTC+07:00)
IRM Calibration Status	Success	**DA Method**	Default.m
Comment	C30H34O5		

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition Time (Local)**	17/1/2565 13:59:07 (UTC+07:00)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00	**QTOF Driver Version**	8.00.00
QTOF Firmware Version	25.712	**Tune Mass Range Max.**	3200

Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



407.1857	1	4689807.33	C26 H26 N O2	(M+Na)+
408.1887	1	1204718.42	C26 H26 N O2	(M+Na)+
475.2519	1	12830466.8	C30 H34 O5	(M+H)+
476.2521	1	6676667.11	C30 H34 O5	(M+H)+
477.2545	1	1209394.73	C30 H34 O5	(M+H)+
497.2299	1	2178385.48	C30 H34 O5	(M+Na)+
498.2334	1	651178.56	C30 H34 O5	(M+Na)+
971.4693	1	1785337.72	C52 H57 Cl N17 O	(M+H)+

Figure S1. HRESIMS ion peak of Compound **1**

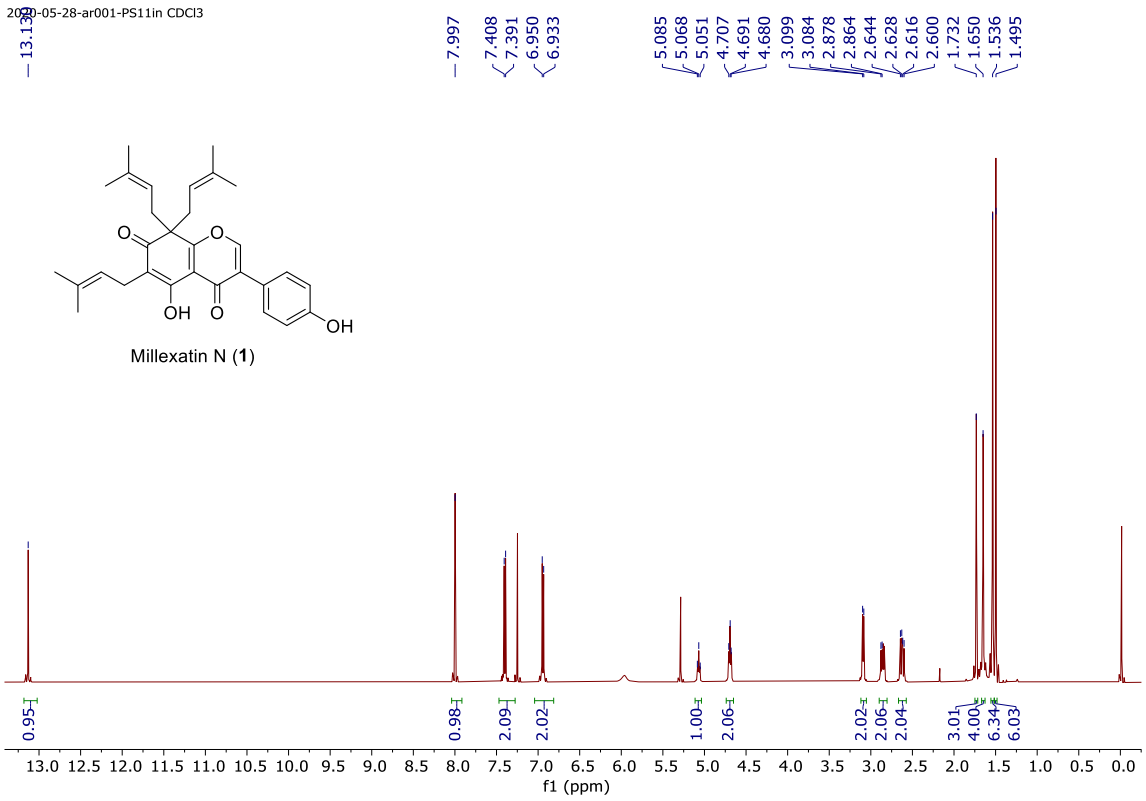


Figure S2. ^{1}H NMR (500 MHz) Spectrum of Millexatin N (**1**) in $CDCl_3$

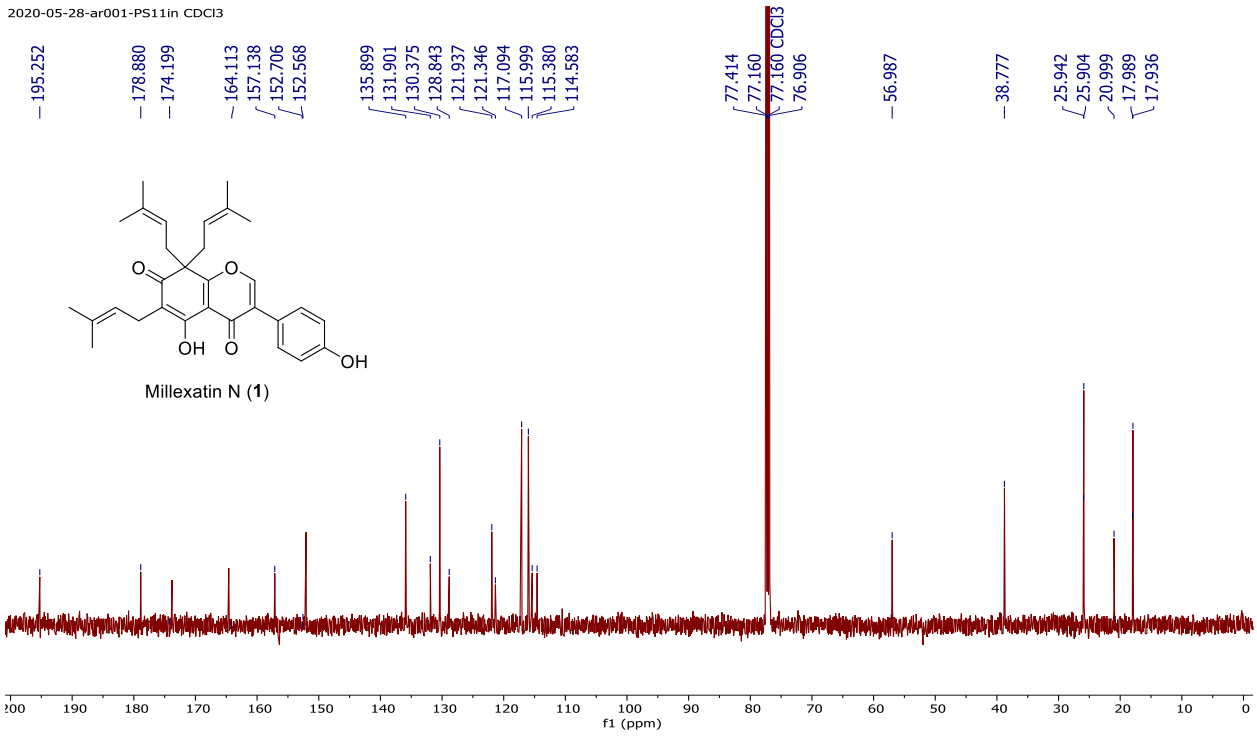


Figure S3. ^{13}C NMR (125 MHz) Spectrum of Millexatin N (**1**) in $CDCl_3$

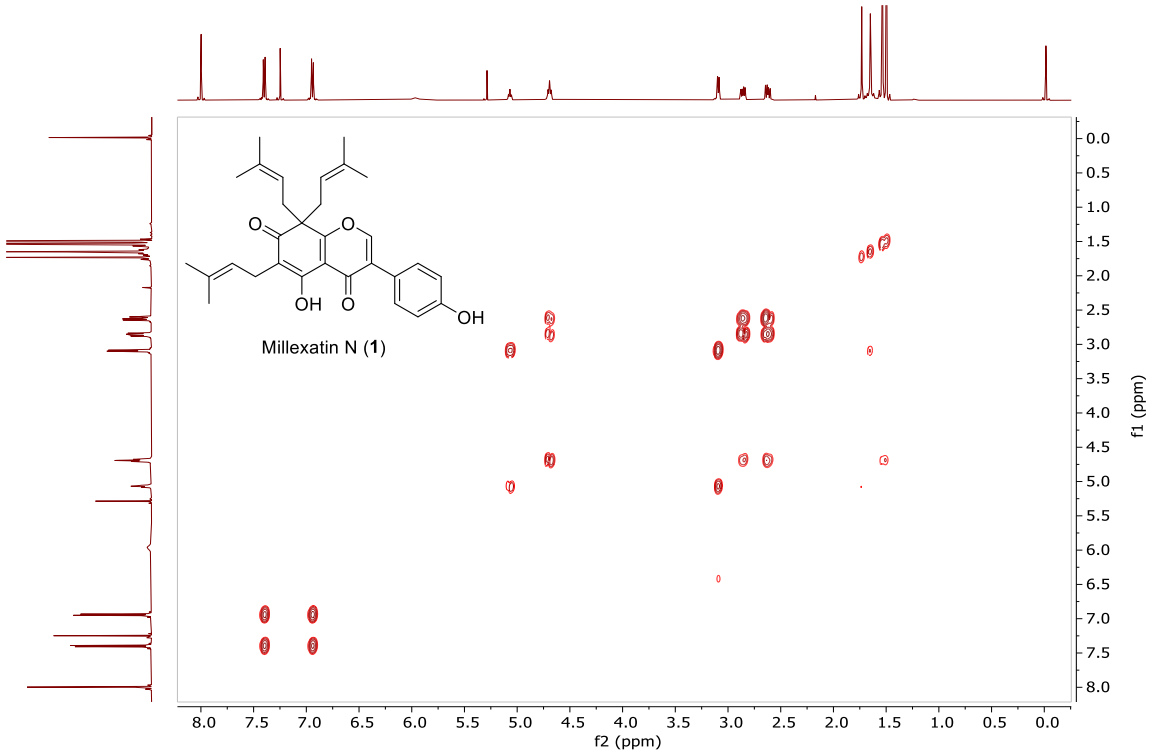


Figure S4. $^{1}H-^{1}H$ COSY Spectrum of Millexatin N (**1**)

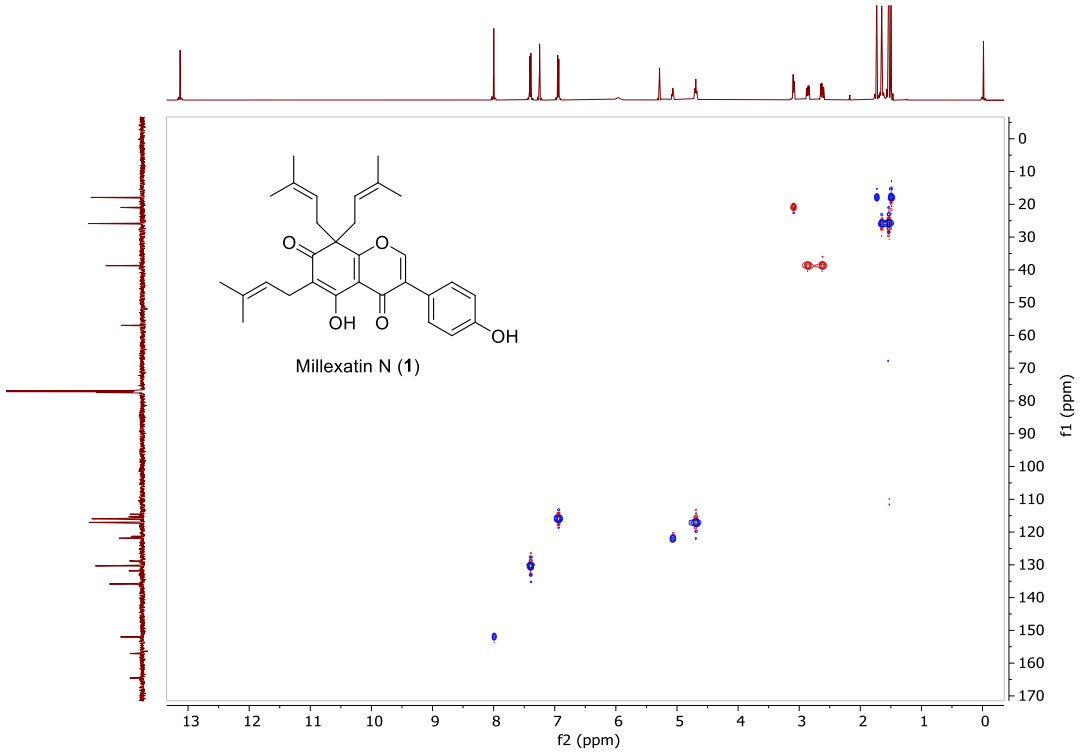


Figure S5. HSQC Spectrum of Millexatin N (**1**)

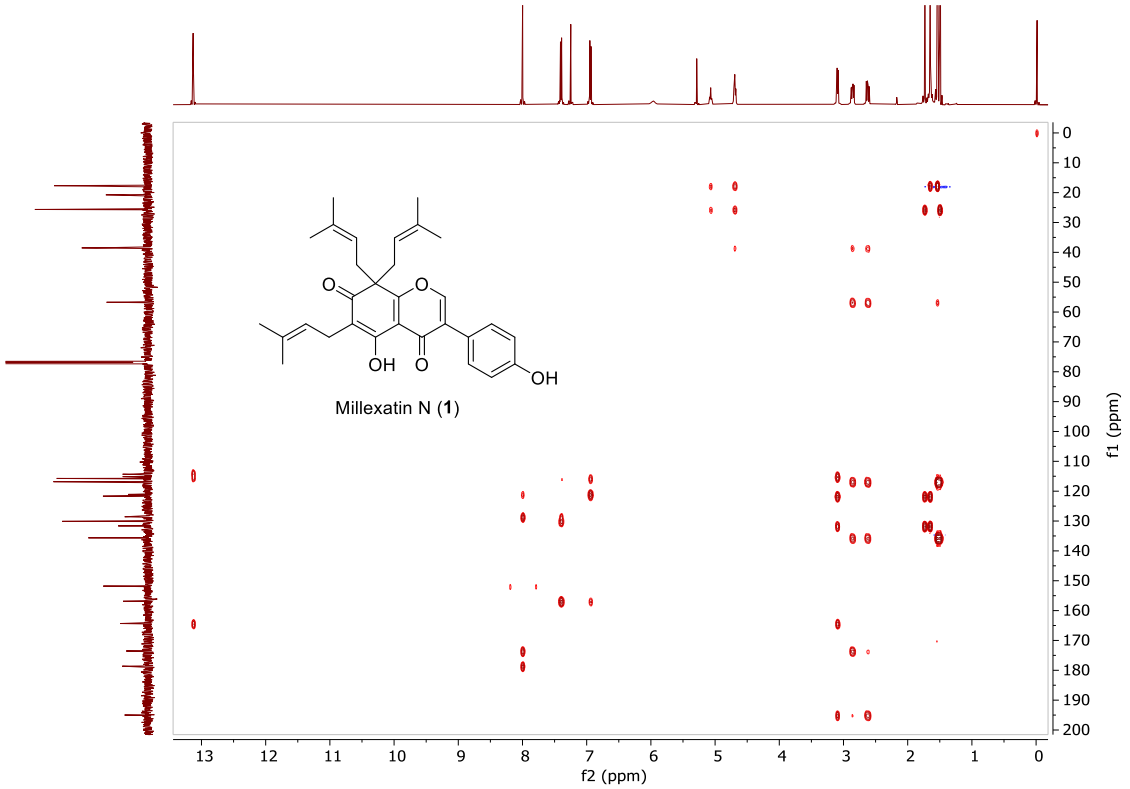


Figure S6. HMBC Spectrum of Millexatin N (**1**)

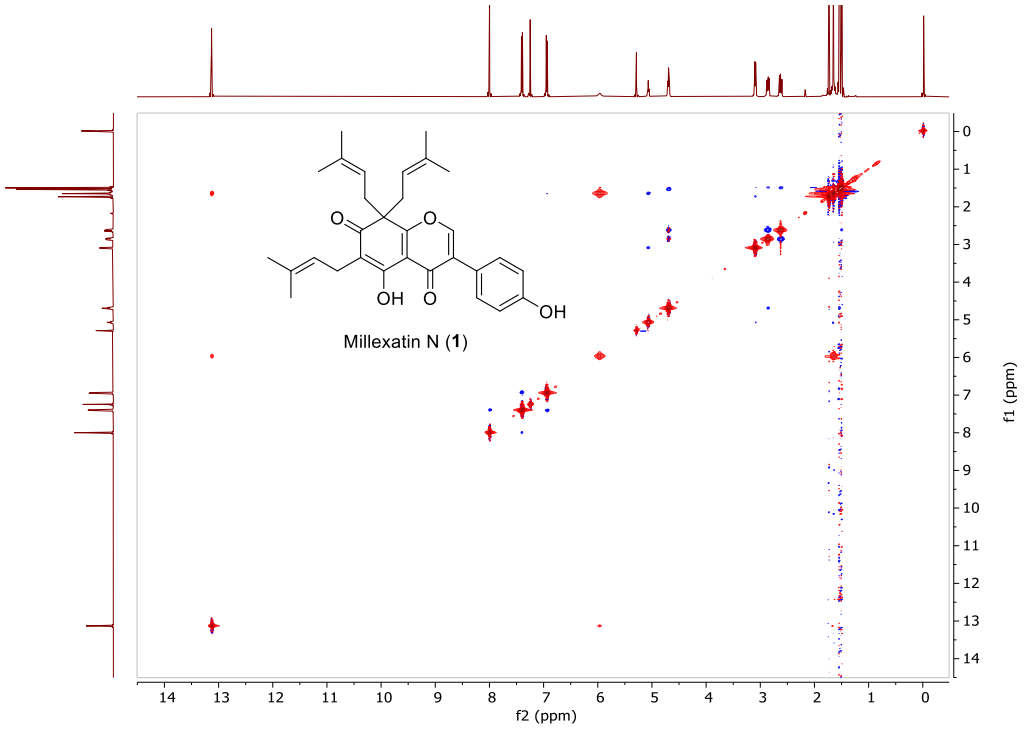
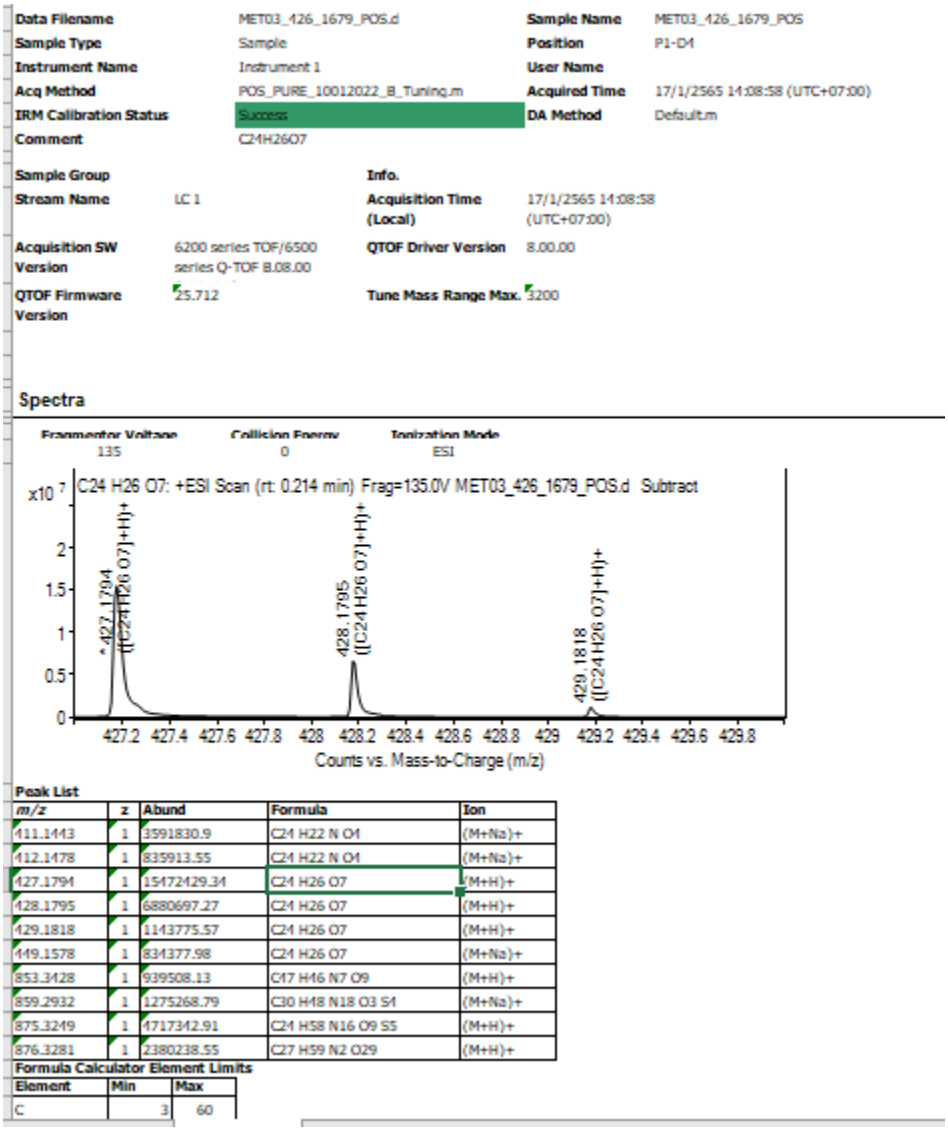


Figure S7. NOESY Spectrum of Millexatin N (**1**)



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Instrument Name	Instrument 1	**User Name**	
Acq Method	POS_PURE_10012022_B_Tuning.m	**Acquired Time**	17/1/2565 14:08:58 (UTC+07:00)
IRM Calibration Status	Success	**DA Method**	Default.m
Comment	C24H26O7		

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition Time (Local)**	17/1/2565 14:08:58 (UTC+07:00)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00	**QTOF Driver Version**	8.00.00
QTOF Firmware Version	25.712	**Tune Mass Range Max.**	3200

Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

Peak List

m/z	z	Abund	Formula	Ion
411.1443	1	3591830.9	C24 H22 N O4	(M+Na)+
412.1478	1	835913.55	C24 H22 N O4	(M+Na)+
427.1794	1	15472429.34	C24 H26 O7	(M+H)+
428.1795	1	6880697.27	C24 H26 O7	(M+H)+
429.1818	1	1143775.57	C24 H26 O7	(M+H)+
449.1578	1	834377.98	C24 H26 O7	(M+Na)+
853.3428	1	939508.13	C47 H46 N7 O9	(M+H)+
859.2932	1	1275268.79	C30 H48 N18 O3 S4	(M+Na)+
875.3249	1	1717342.91	C24 H58 N16 O9 S5	(M+H)+
876.3281	1	2380238.55	C27 H59 N2 O29	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	3	60

Figure S8. HRESIMS ion peak of Millexatin O (**2**)

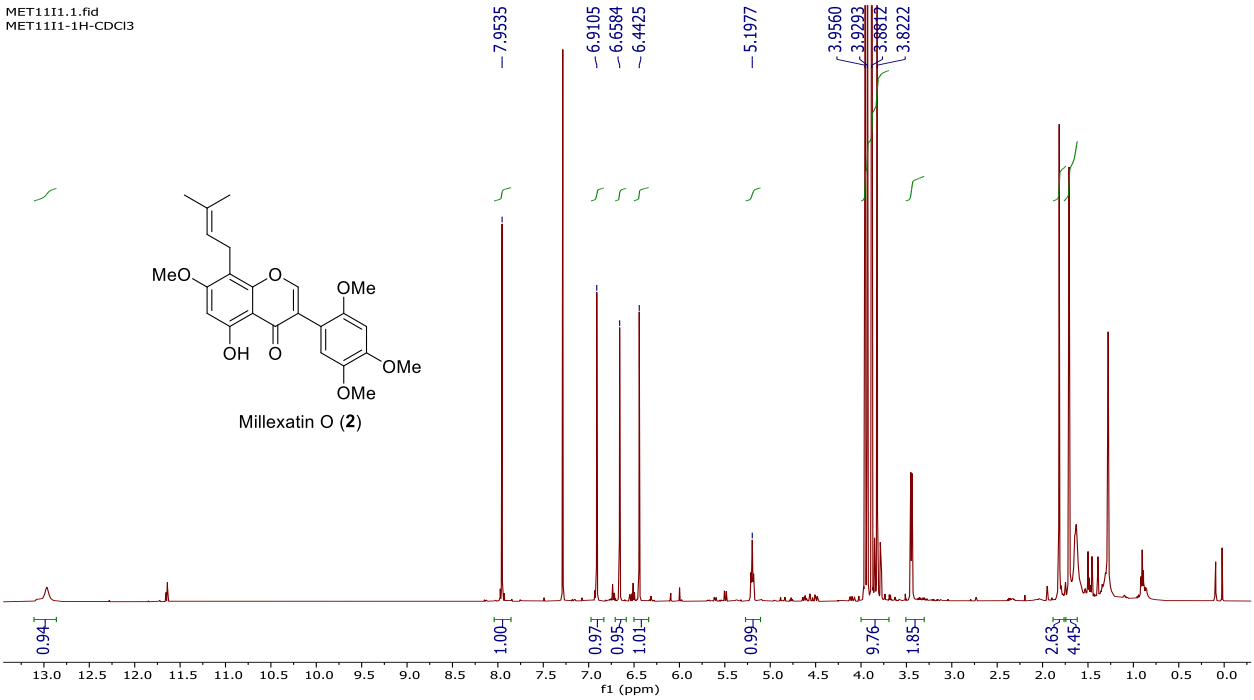

Figure S9. ^{1}H NMR (500 MHz) Spectrum of Millexatin O (**2**) in $CDCl_3$

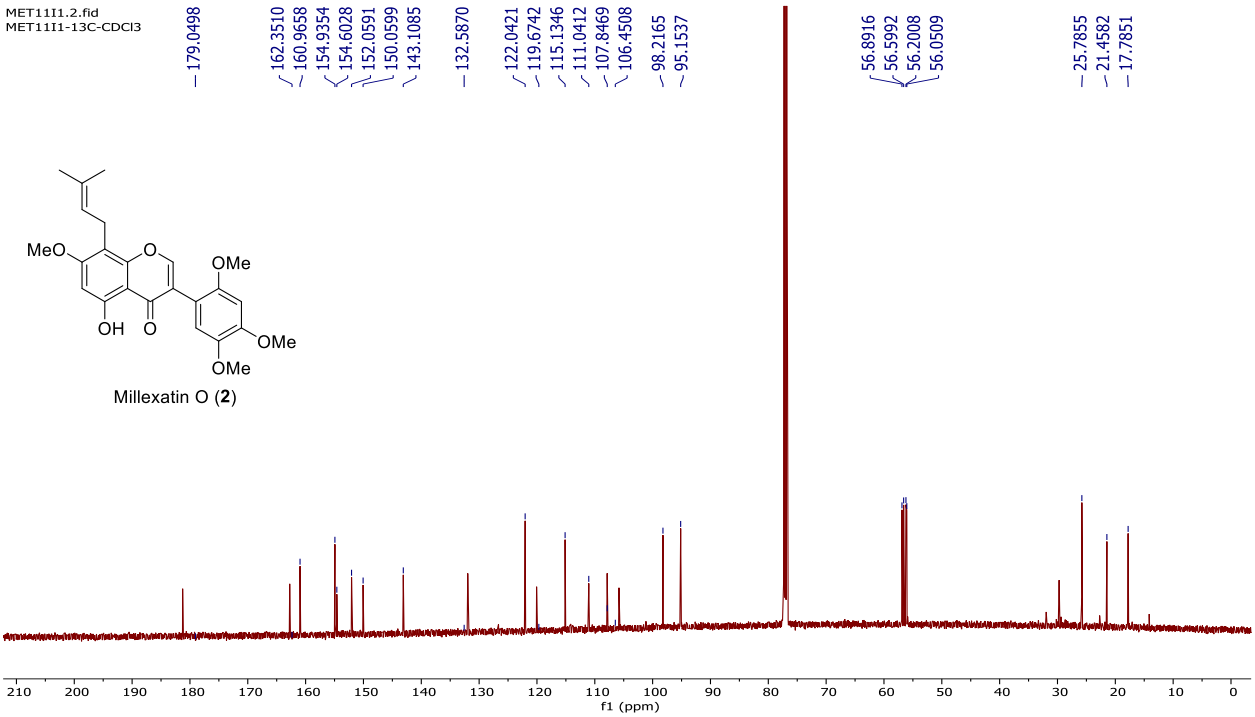

Figure S10. ^{13}C NMR (125 MHz) Spectrum of Millexatin O (**2**) in $CDCl_3$

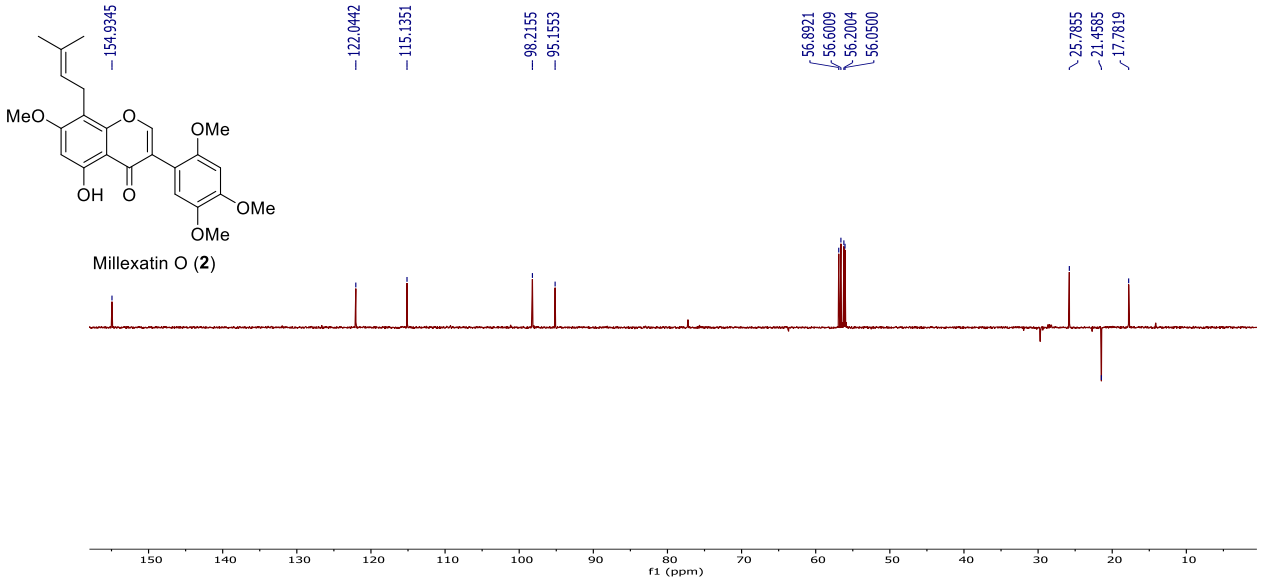

Figure S11. DEPT135 (125 MHz) Spectrum of Millexatin O (**2**)

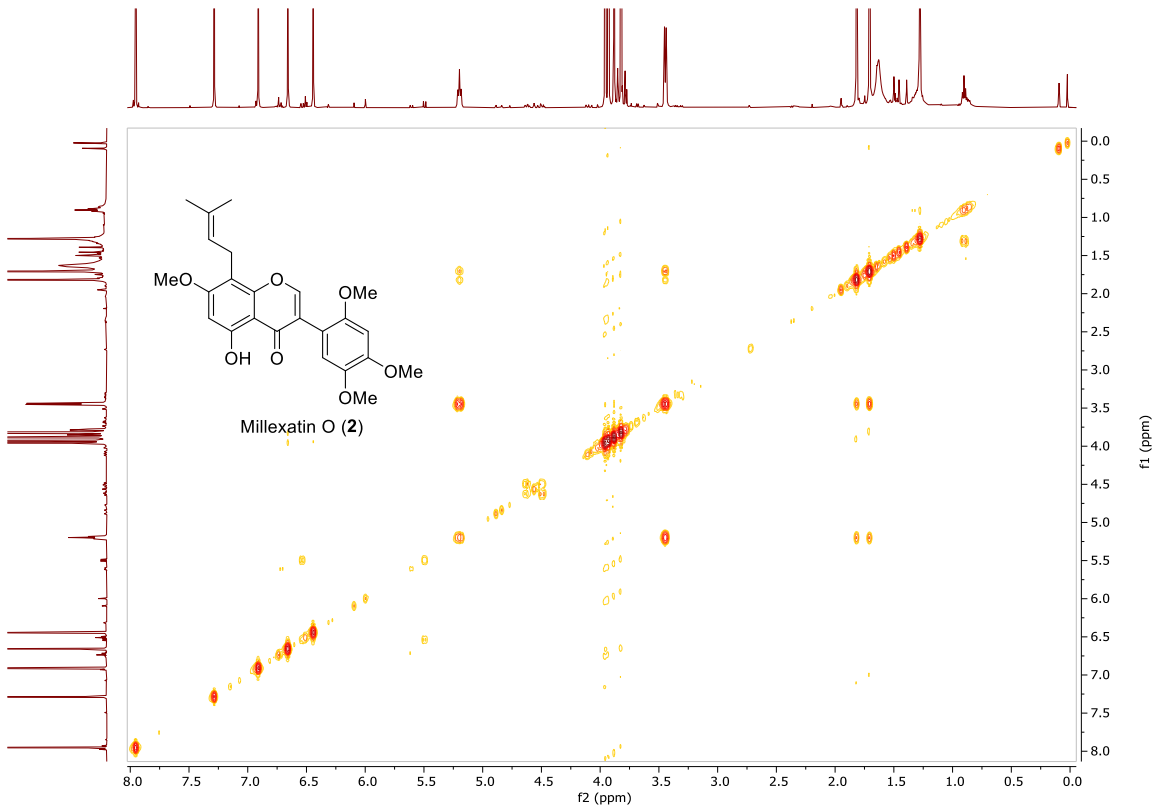

Figure S12. $^{1}H–^{1}H$ COSY Spectrum of Millexatin O (**2**)

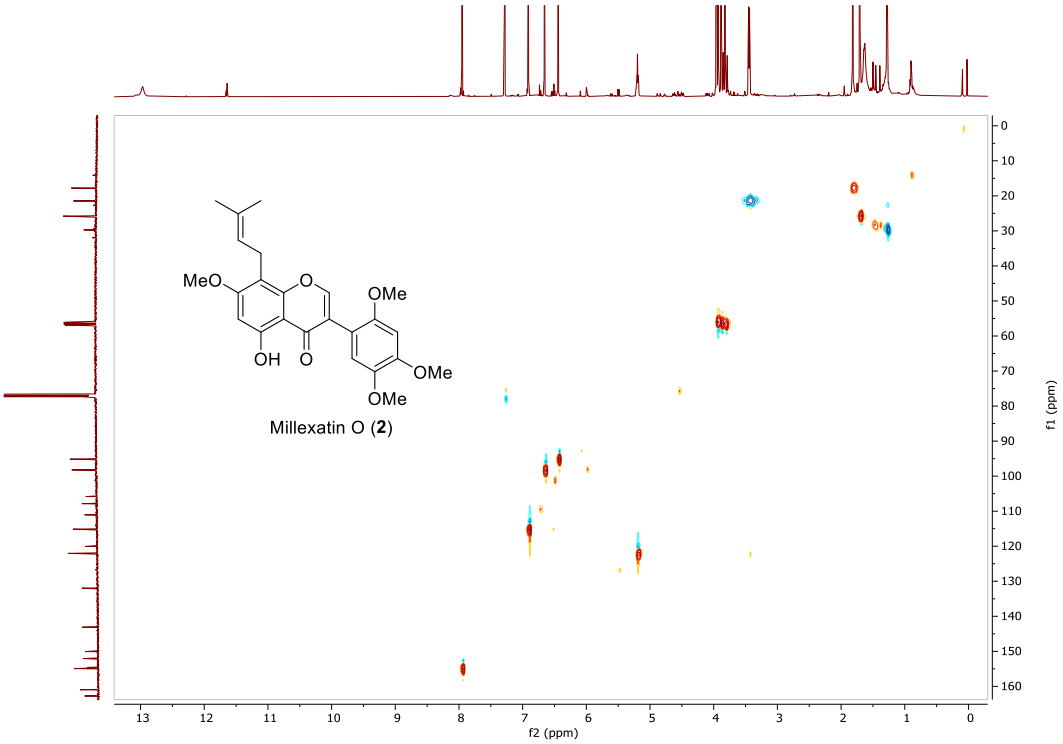

Figure S13. HSQC Spectrum of Millexatin O (**2**)

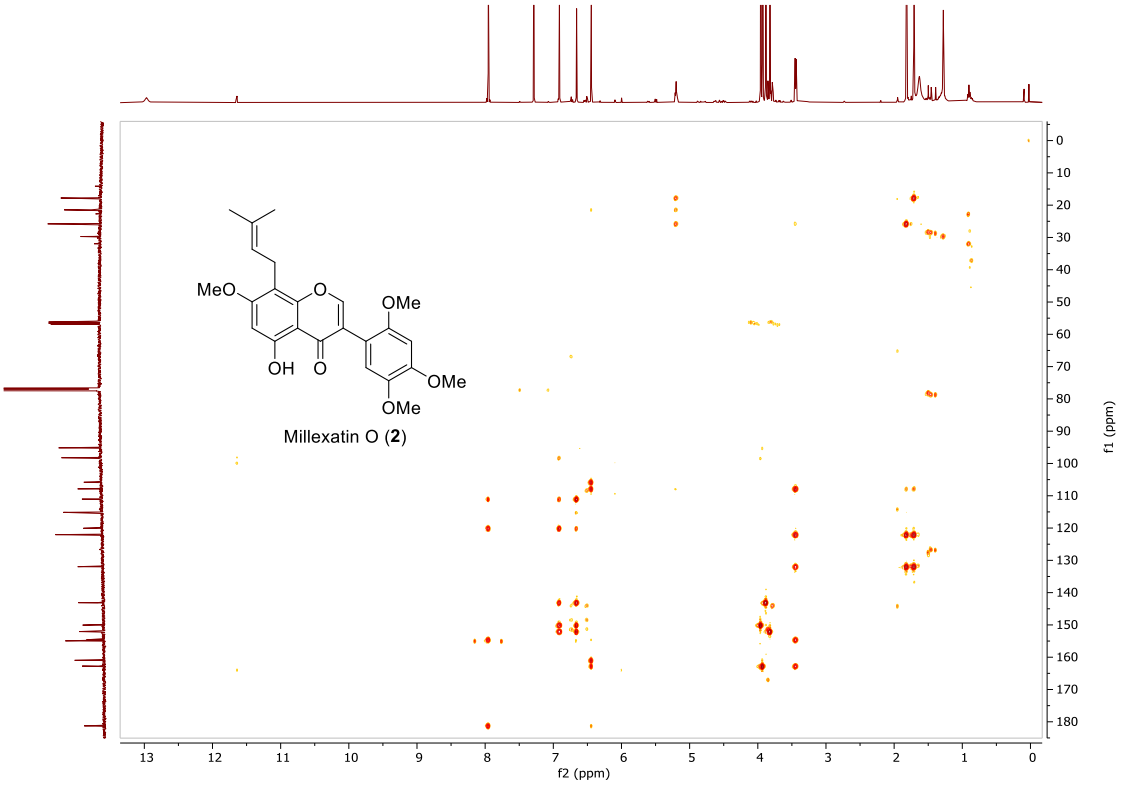

Figure S14. HMBC Spectrum of Millexatin O (**2**)

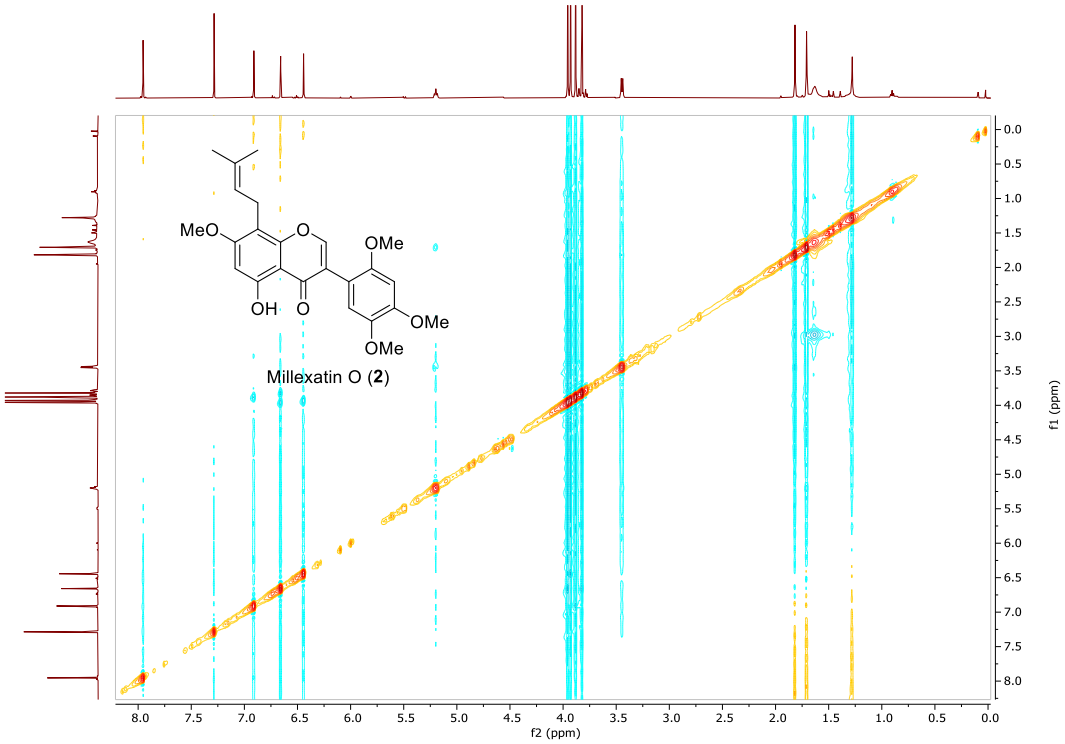

Figure S15. NOESY Spectrum of Millexatin O (**2**)

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Sample Type	Sample	**Position**	P1-D3
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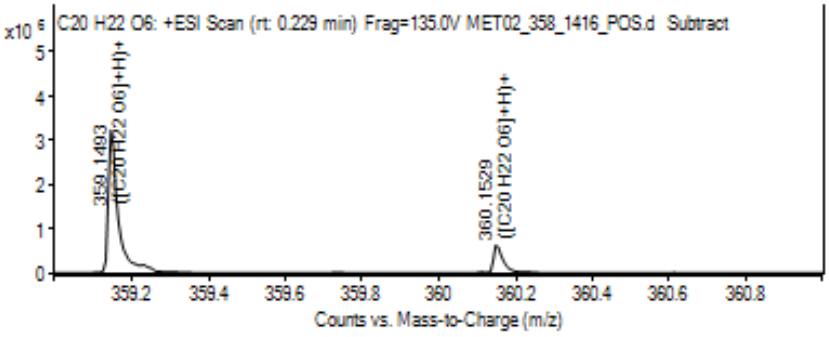
Acq Method	POS_PURE_10012022_B_Tuning.m	**Acquired Time**	17/1/2565 14:04:03 (UTC+07:00)
IRM Calibration Status	Success	**DA Method**	Default.m
Comment	C20H22O6		

Sample Group		**Info.**	
Stream Name	LC 1	**Acquisition Time (Local)**	17/1/2565 14:04:03 (UTC+07:00)
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00	**QTOF Driver Version**	8.00.00
QTOF Firmware Version	25.712	**Tune Mass Range Max.**	3200

Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
240.0788	2	268624.43	C19 H20 N11 O2	(M+2Na)+2
244.0971	1	344111.07	C15 H13 N2	(M+Na)+
341.139	1	5793674.39	C20 H20 O5	(M+H)+
342.142	1	1197013.04	C20 H20 O5	(M+H)+
359.1493	1	3310242.88	C20 H22 O6	(M+H)+
360.1529	1	657235.5	C20 H22 O6	(M+H)+
378.1234	2	375072.82	C17 H25 Cl2 N O4	(M+H)+
381.1321	1	788905.92	C20 H22 O6	(M+Na)+
557.1933	2	244332.46		
739.2722	1	308643.39	C19 H39 Cl N2 O3	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	3	60

Figure S16. HRESIMS ion peak of Millexatin P (**3**)

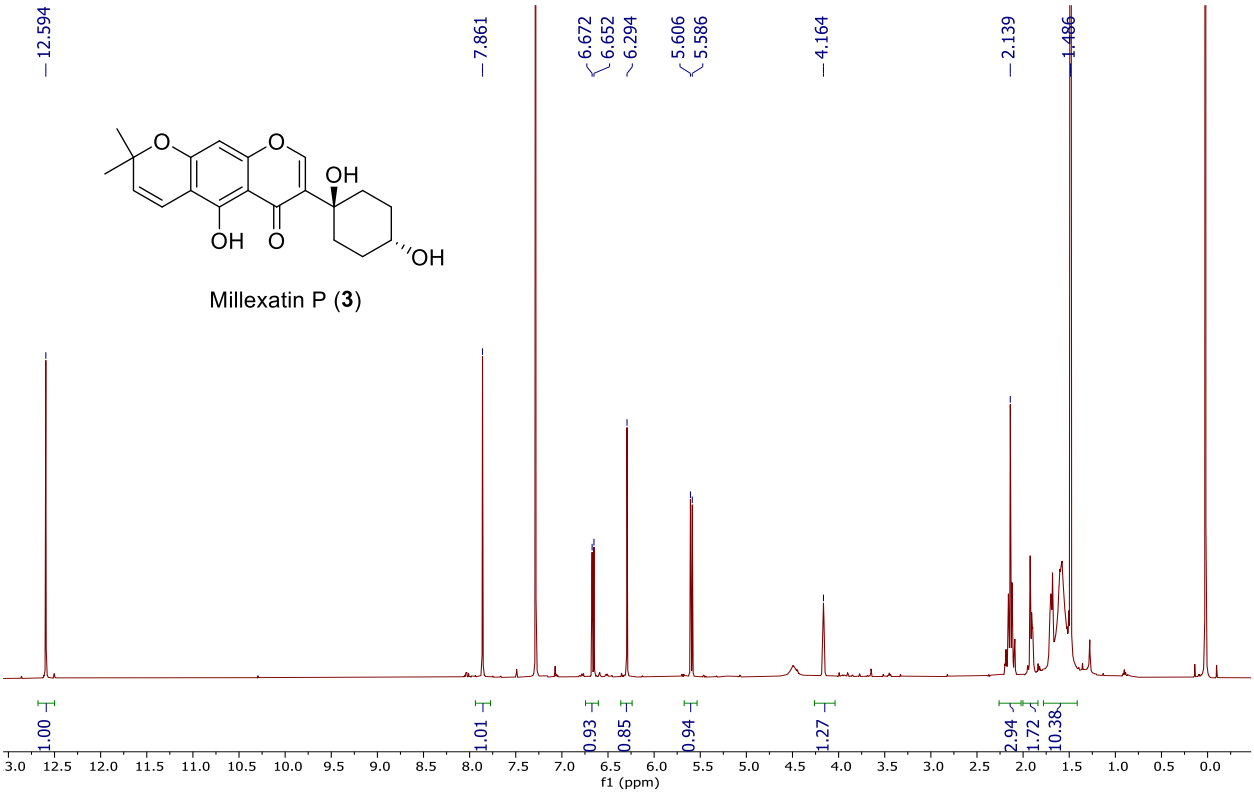


Figure S17. ^{1}H NMR (500 MHz) Spectrum of Millexatin P (**3**) in $CDCl_3$

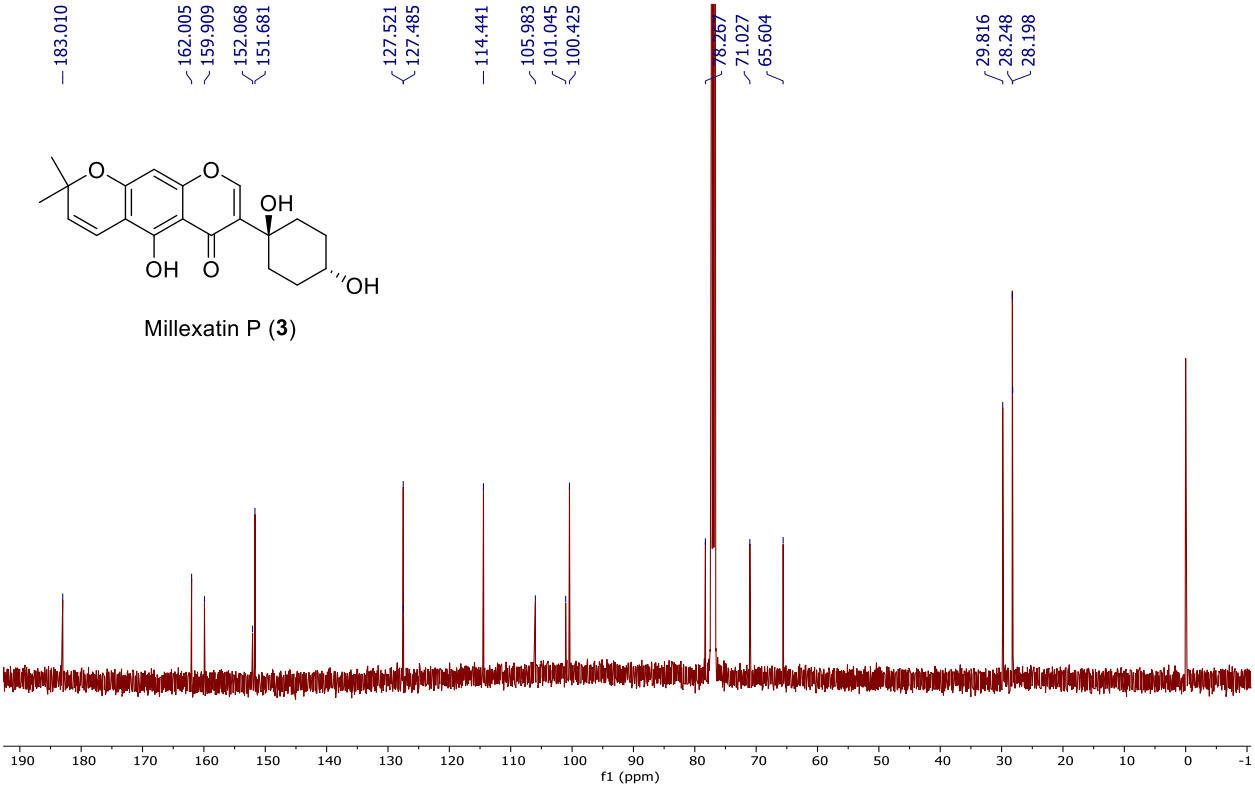


Figure S18. ^{13}C NMR (125 MHz) Spectrum of Millexatin P (**3**) in $CDCl_3$

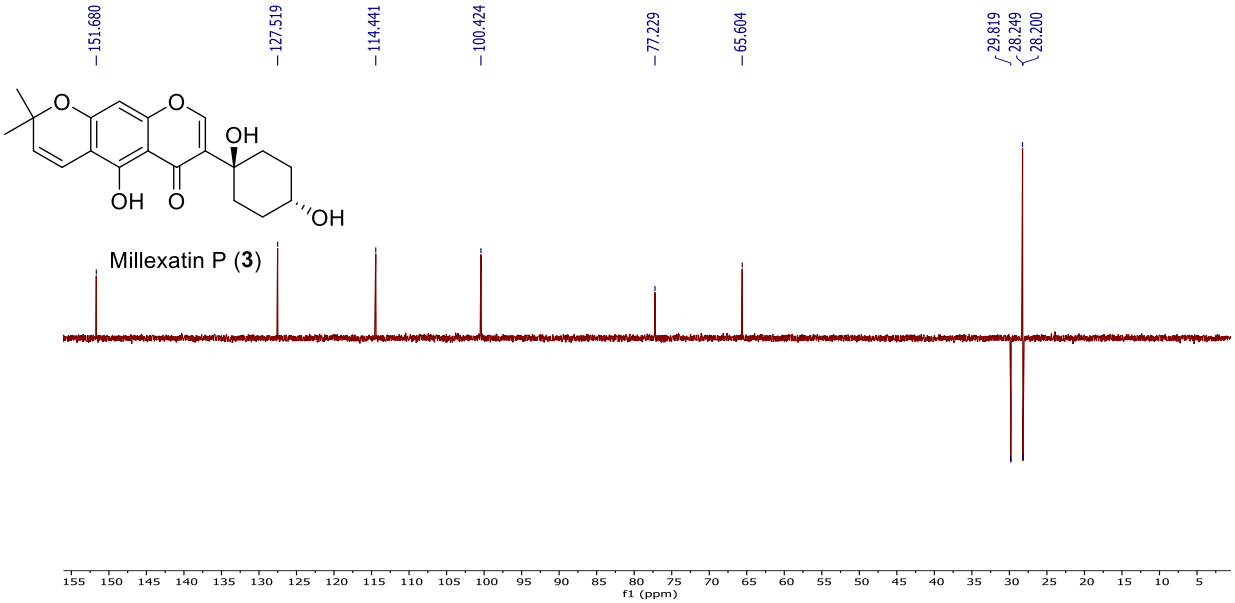


Figure S19. DEPT135 Spectrum of Millexatin P (**3**)

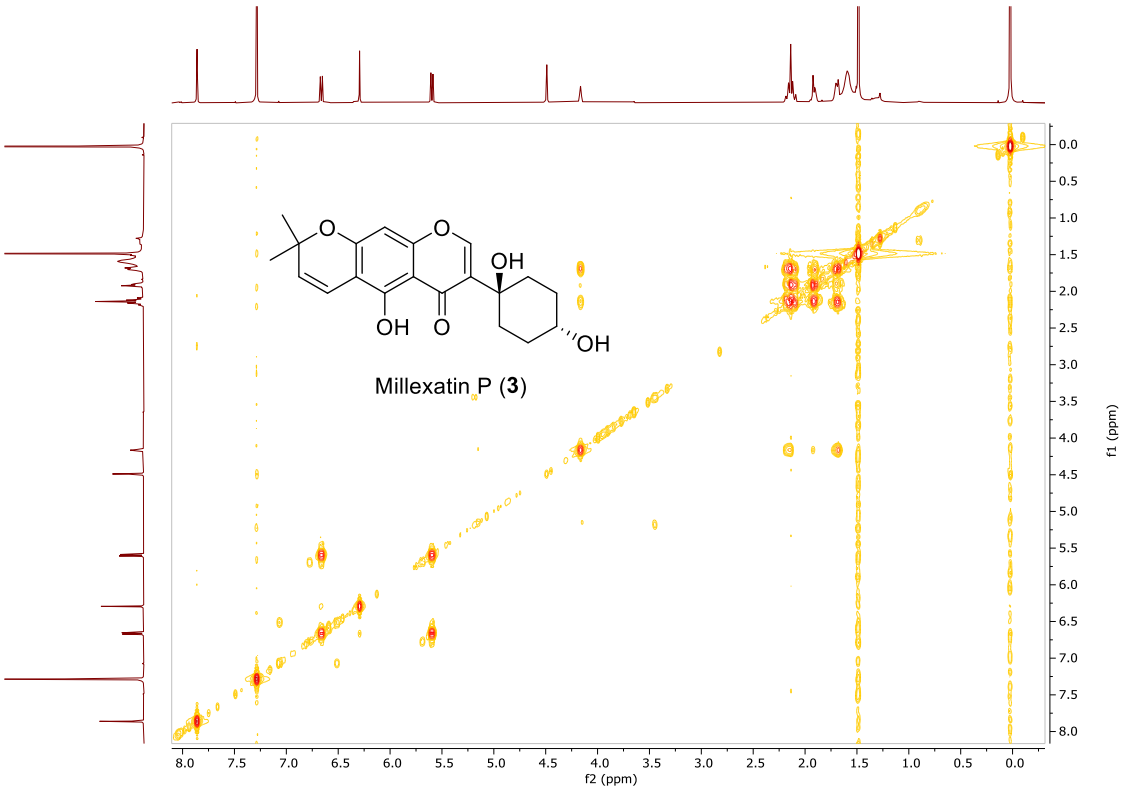


Figure S20. $^{1}H–^{1}H$ COSY Spectrum of Millexatin P (**3**)

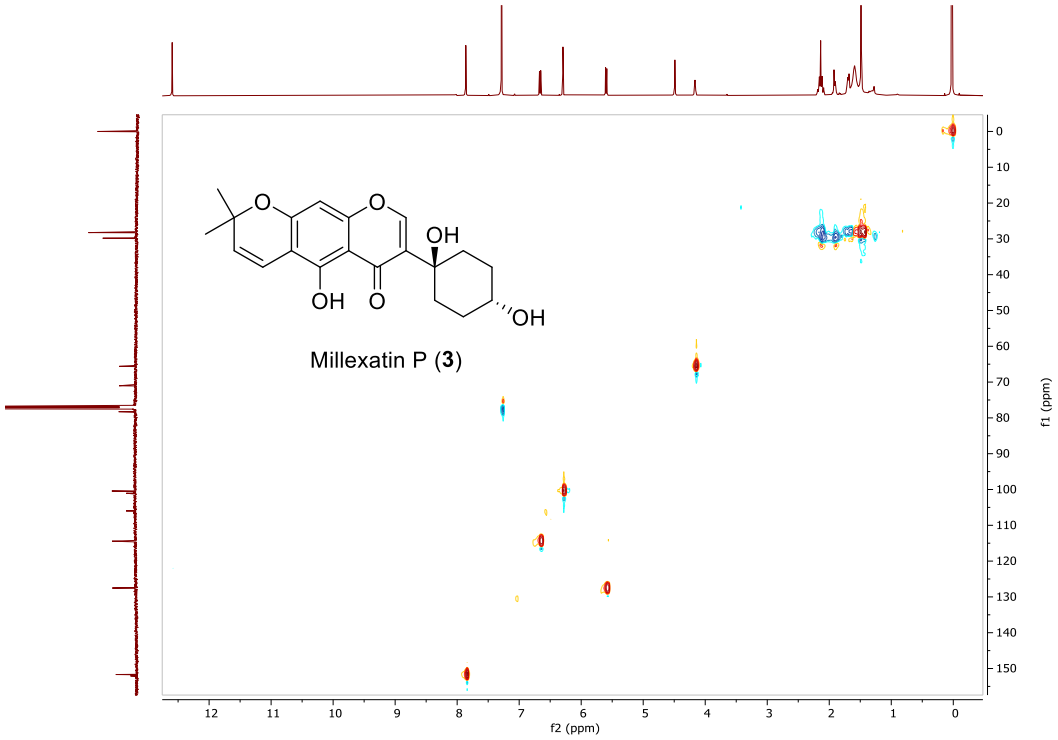


Figure S21. HSQC Spectrum of Millexatin P (**3**)

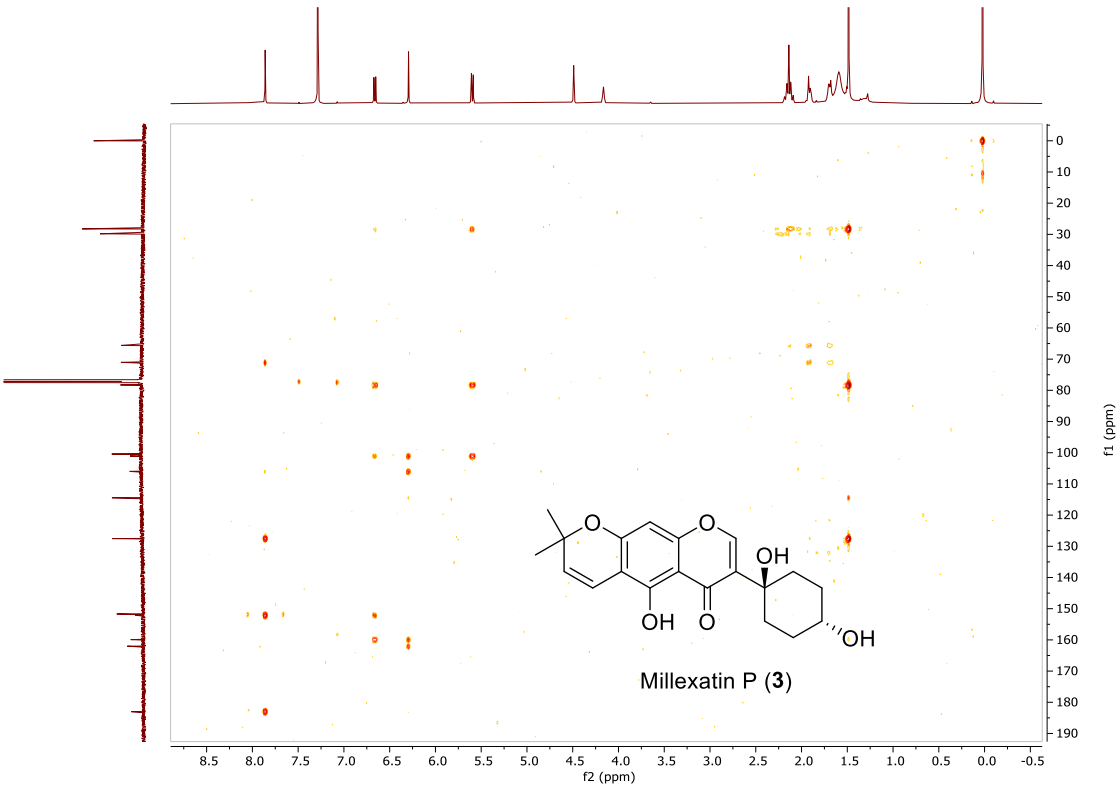


Figure S22. HMBC Spectrum of Millexatin P (**3**)

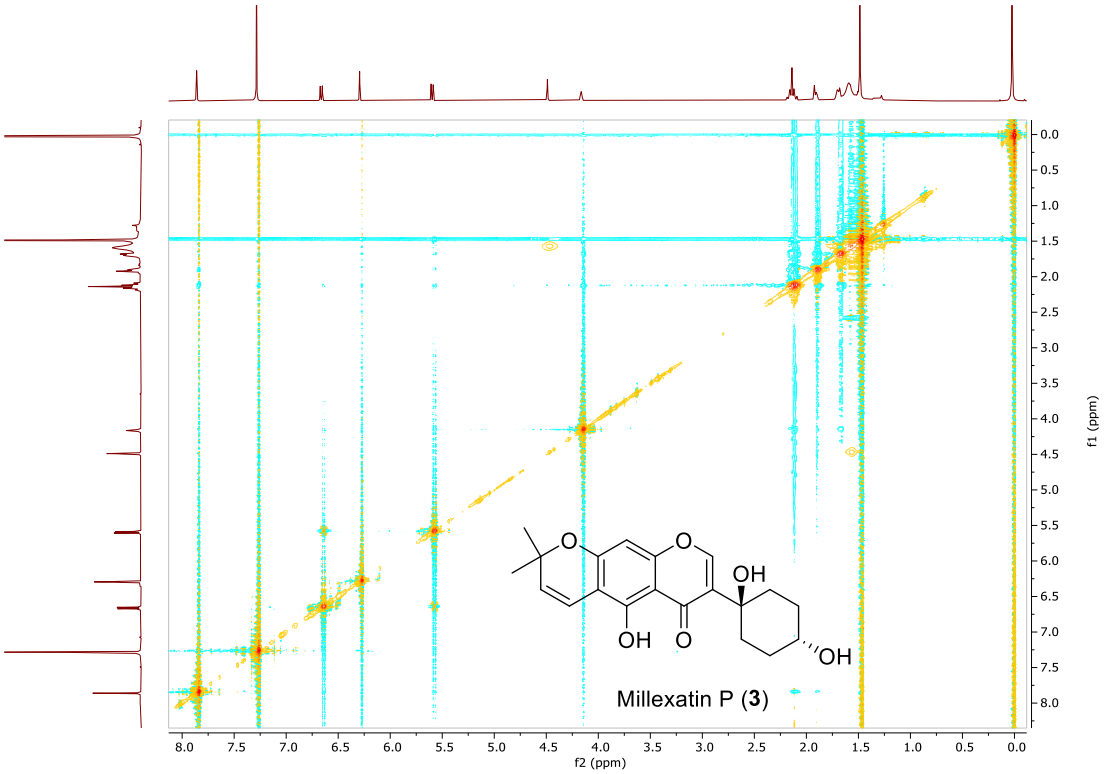


Figure S23. NOESY Spectrum of Millexatin P (**3**)

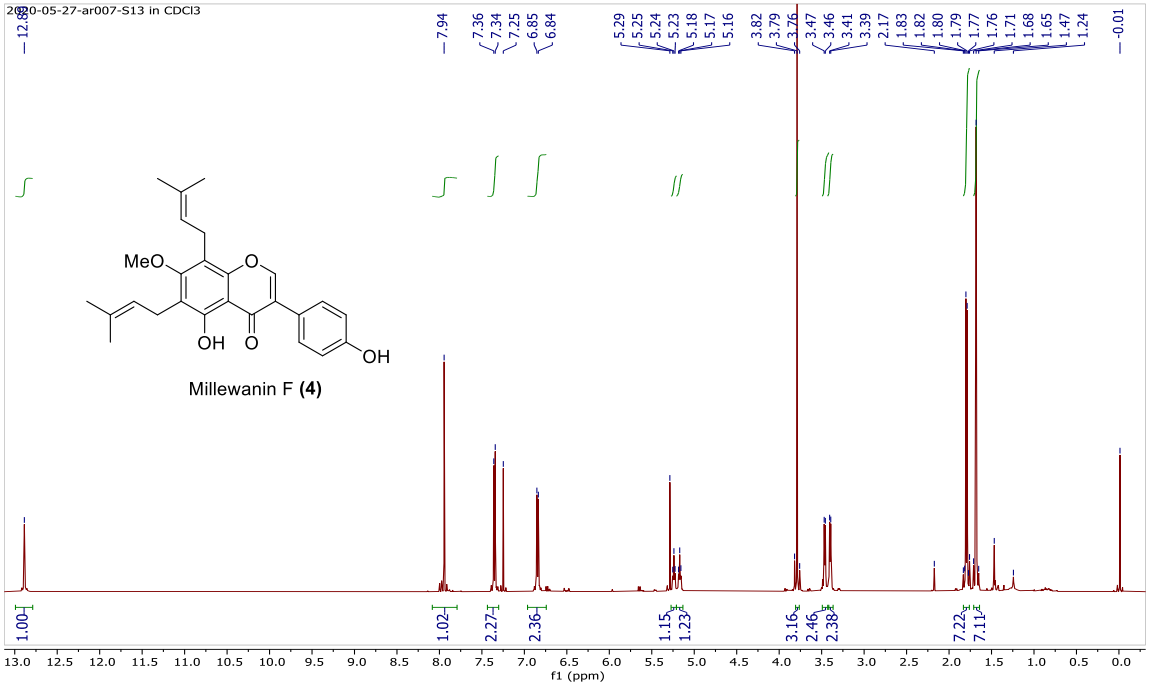


Figure S24. ^{1}H NMR (500 MHz) Spectrum of Millewanin F (**4**) in $CDCl_3$

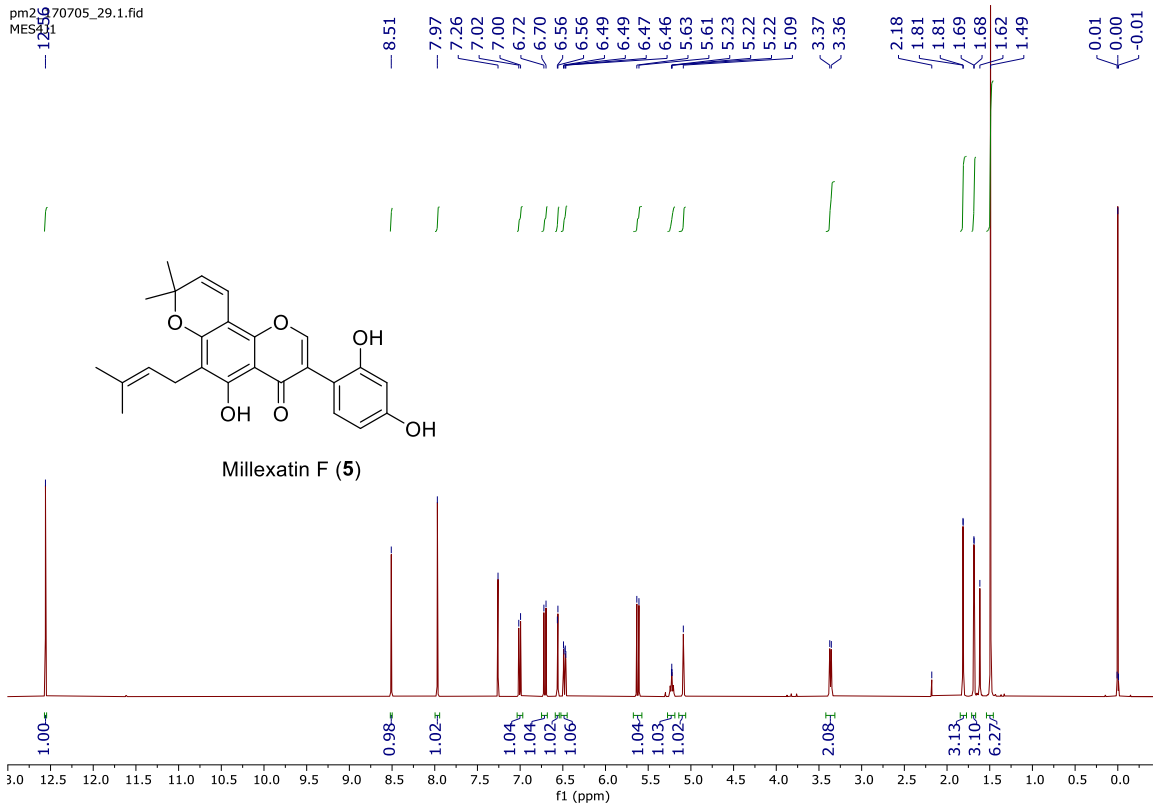


Figure S25. ^{1}H NMR (500 MHz) Spectrum of Millexatin F (**5**) in $CDCl_3$

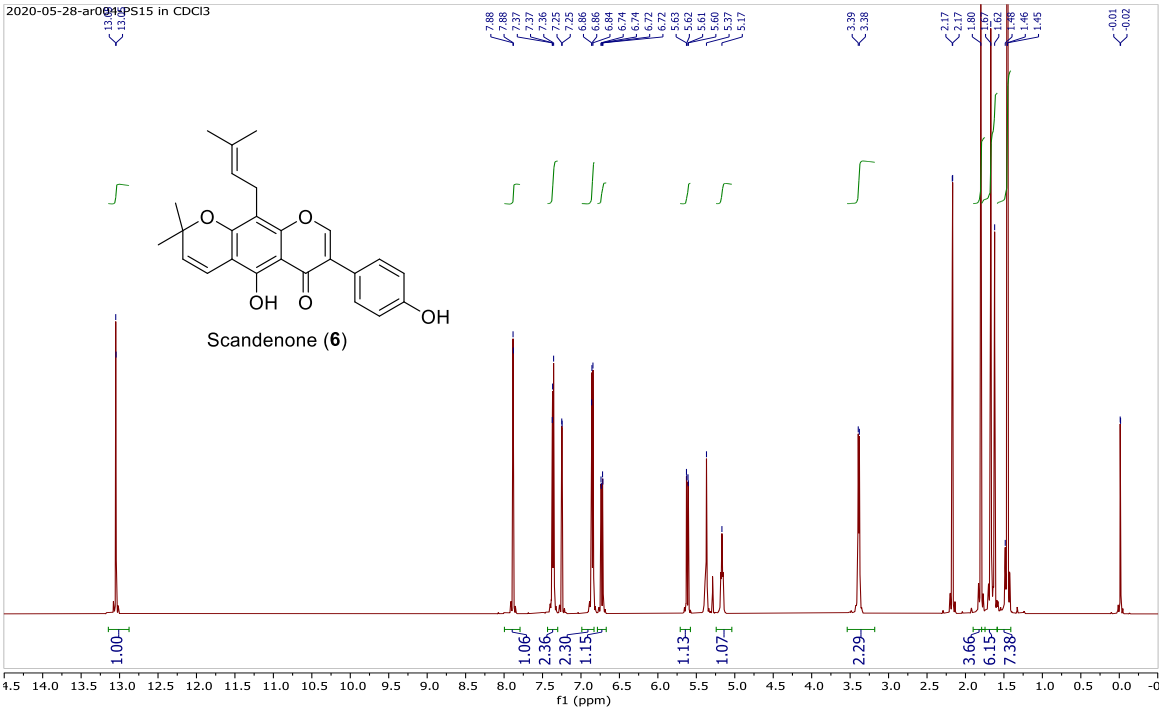


Figure S26. ^{1}H NMR (500 MHz) Spectrum of Scandenone (**6**) in $CDCl_3$

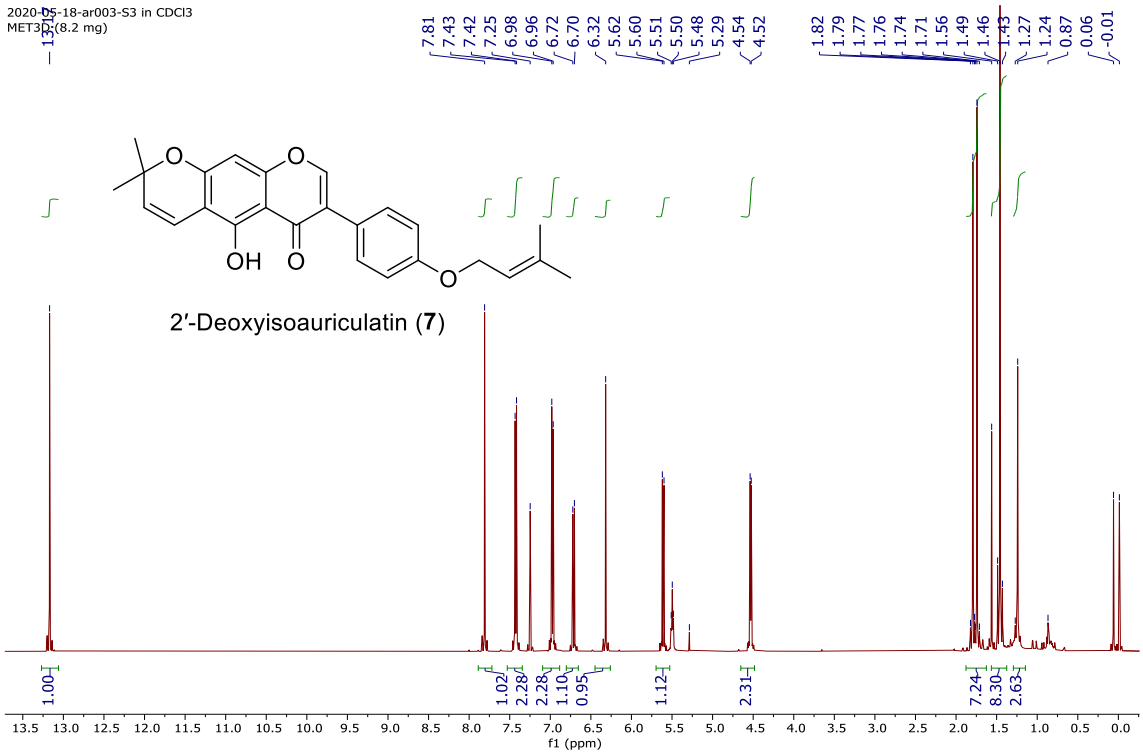


Figure S27. ^{1}H NMR (500 MHz) Spectrum of 2′-Deoxyisoauriculatin (**7**) in $CDCl_3$

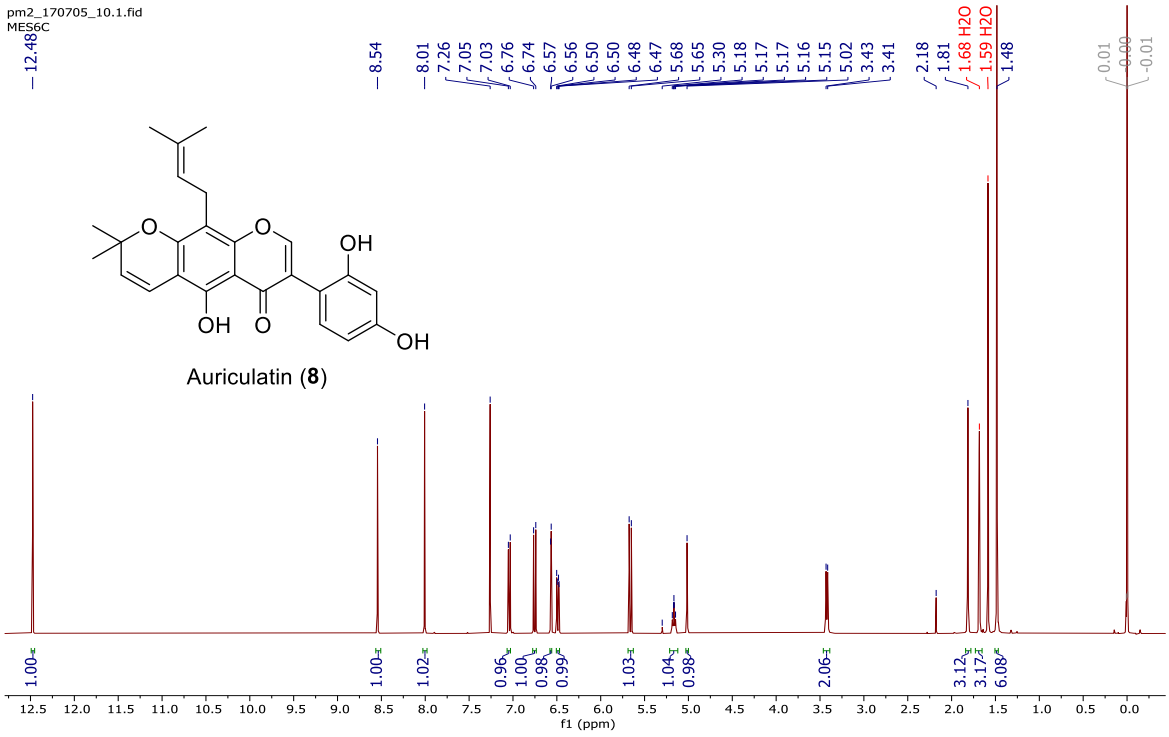


Figure S28. ^{1}H NMR (500 MHz) Spectrum of Auriculatin (**8**) in $CDCl_3$

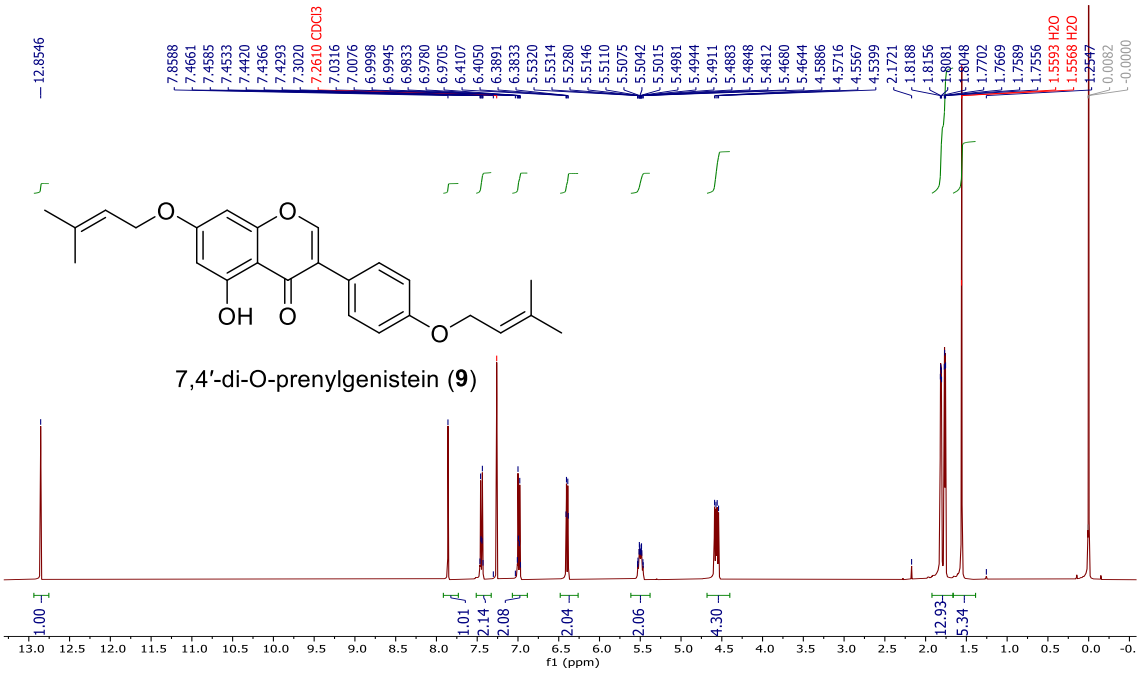


Figure S29. ^{1}H NMR (500 MHz) Spectrum of 7,4′-di-*O*-prenylgenistein (**9**) in $CDCl_3$

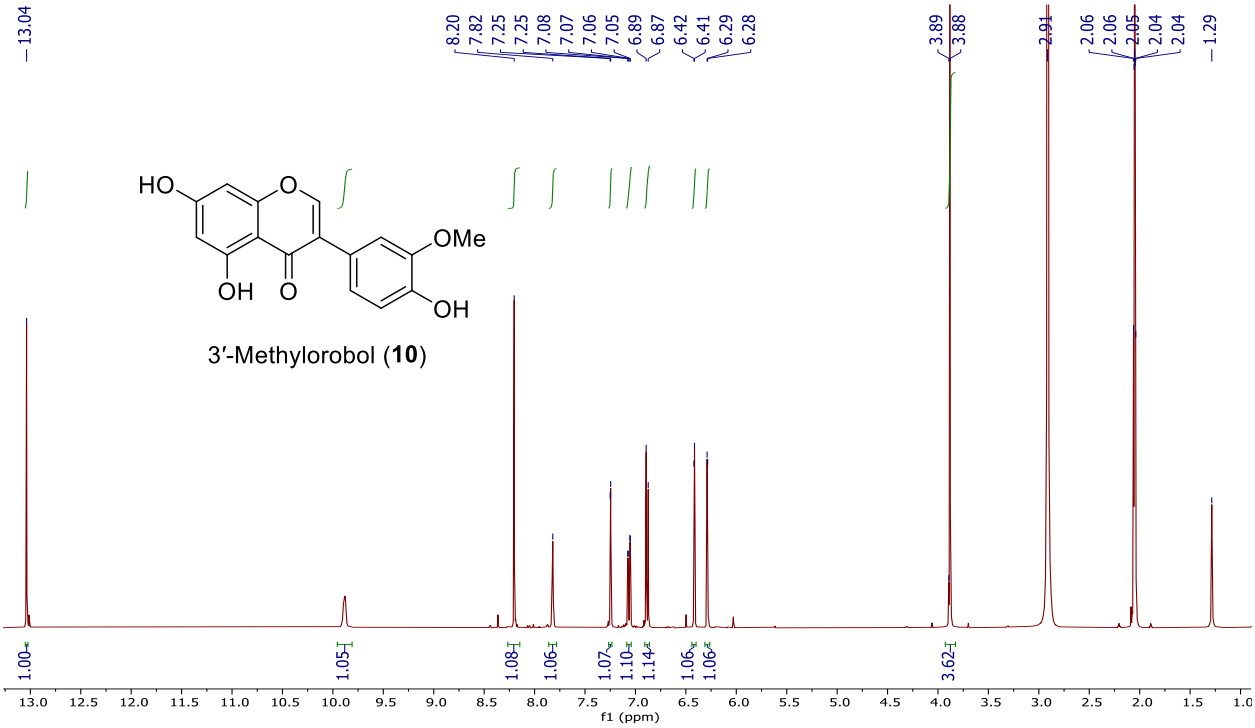


Figure S30. ^{1}H NMR (500 MHz) Spectrum of 3′-Methylorobol (**10**) in Acetone-d_6