

Supplementary Information

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Table S1.1. HPLC method- salicinoids from *Populus trichocarpa* × *deltoides* Beaupré.

HPLC Method for Isolation of Salicinoids (1–3) (Sample Concentration 3 mg/mL)			
Column Temp.	35 °C	Injection Volume	40 µL
Flow Rate	0.8 mL/min	<i>Isis Nucleodur 250 mm × 4.6 mm; 5 µm; MN</i>	
Time	Solvent A	Solvent B	
t [min]	H₂O (0.1% FA) in %	MeOH (0.1% FA) in %	
0	100	0	
5	100	0	
10	85	15	
35	70	30	
85	50	50	
90	0	100	
100	0	100	
110	100	0	
115	100	0	

Retention times: salicortin (1): 42.6 min; HCH-salicortin (2): 63.6 min; tremulacin (3): 87.8 min.

Table S1.2. HPLC method- salicinoids from *Idesia polycarpa*.

HPLC Method for Isolation of Idescarpin (4) (Sample Concentration 115 mg/mL)			
Column Temp.	40 °C	Injection Volume	5 µL
Flow Rate	0.8 mL/min	<i>Isis Nucleodur 250 mm × 4.6 mm; 5 µm; MN</i>	
Time	Solvent A	Solvent B	
t [min]	H₂O (0.1% FA) in %	MeOH (0.1% FA) in %	
0	67.5	32.5	
1	67.5	32.5	
21	32	68	
25	0	100	
30	0	100	
35	67.5	32.5	
40	67.5	32.5	

Retention times: idescarpin (4): 21.7 min.

Table S1.3. Specific optical rotation of salicortin (**1**) and idescarpin (**4**).

Measurement	Salicortin (1)		Idescarpin (4)
	$[\alpha]_{\text{D}}^{22}$ (c 0.72; MeOH)	$[\alpha]_{\text{D}}^{22}$ (c 0.65; H ₂ O)	$[\alpha]_{\text{D}}^{22}$ (c 0.73; MeOH)
1	−123.91°	−119.06°	−57.12°
2	−123.67°	−118.84°	−56.97°
3	−124.06°	−118.55°	−57.59°
4	−124.06°	−118.83°	−57.44°
5	−124.10°	−118.87°	−57.66°
6	−123.53°	−118.22°	−56.90°
7	−124.18°	−118.43°	−57.48°
8	−123.95°	−118.98°	−57.40°
9	−123.87°	−118.42°	−57.60°
10	−123.62°	−118.06°	−57.27°
mean $[\alpha]_{\text{D}}$	−123.89°	−118.63°	−57.34°
stdev.	±0.22°	±0.34°	±0.27°

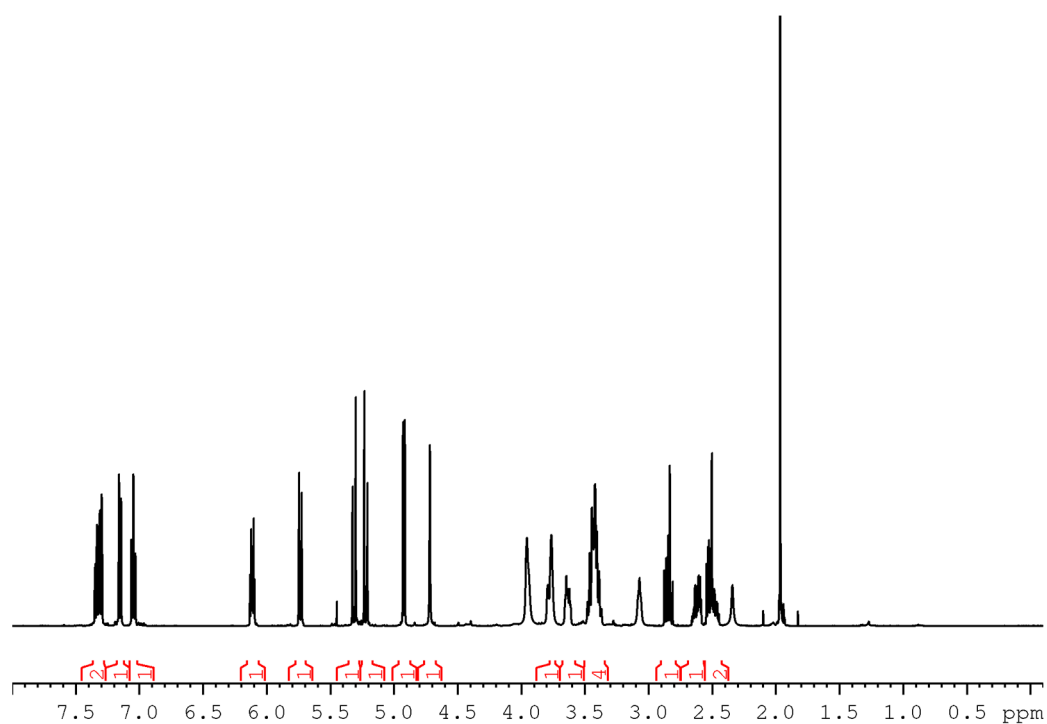


Figure S2.1. Salicortin (**1**), ¹H-NMR spectrum (500 MHz, MeCN-*d*₃).

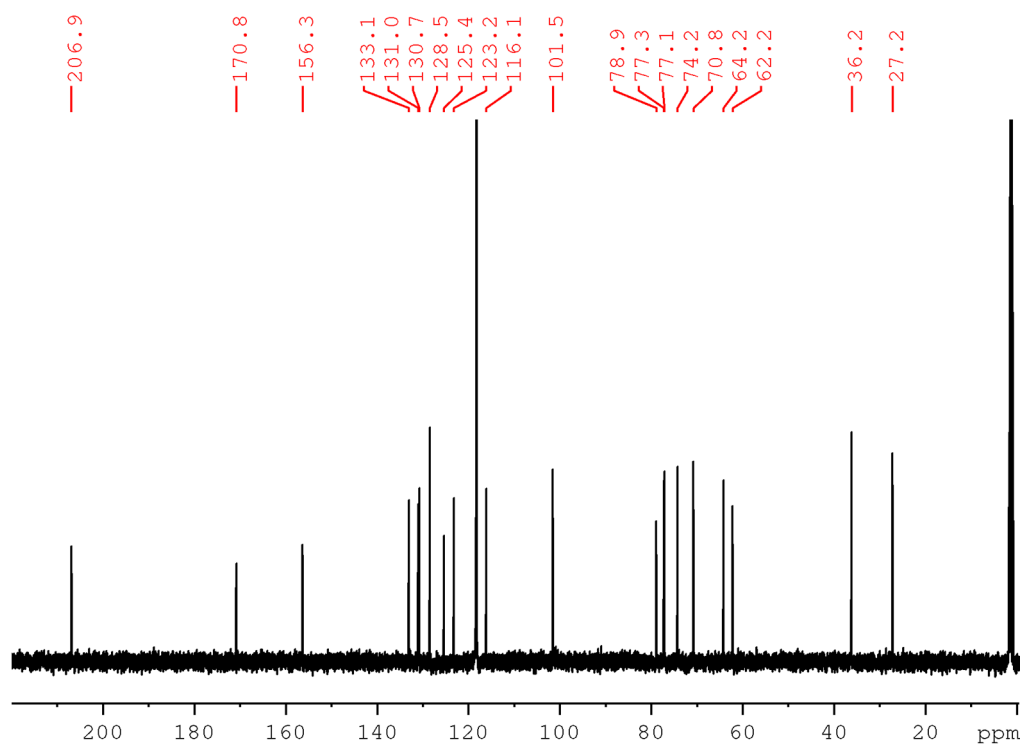


Figure S2.2. Salicortin (1), ¹³C-NMR spectrum (125 MHz, MeCN-*d*₃).

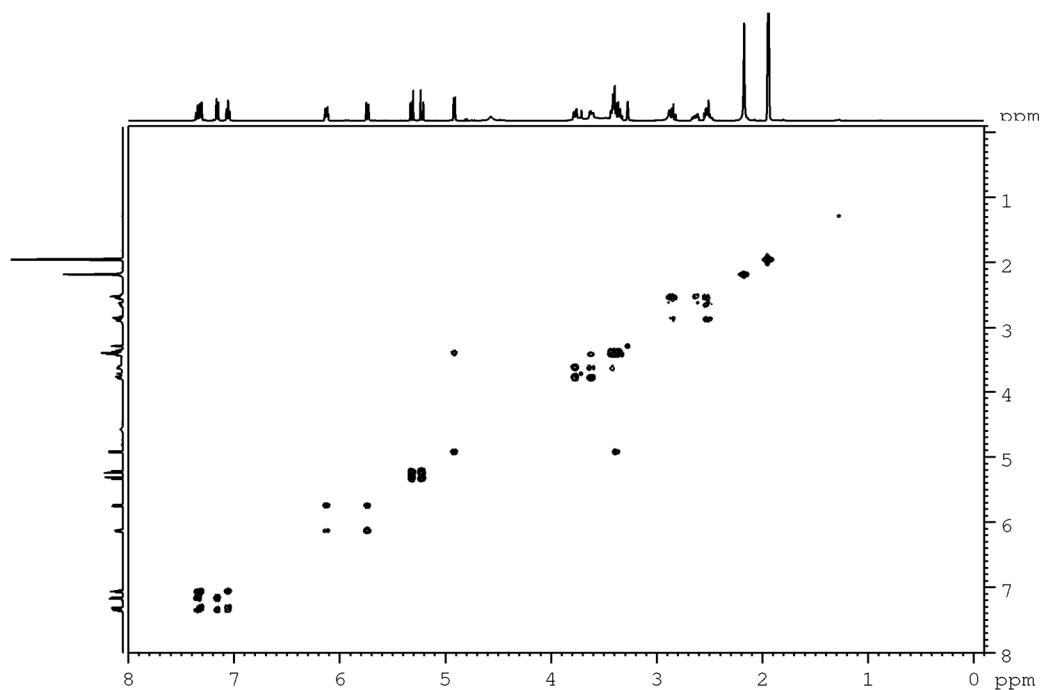


Figure S2.3. Salicortin (1), ¹H-¹H COSY spectrum (500 MHz, MeCN-*d*₃).

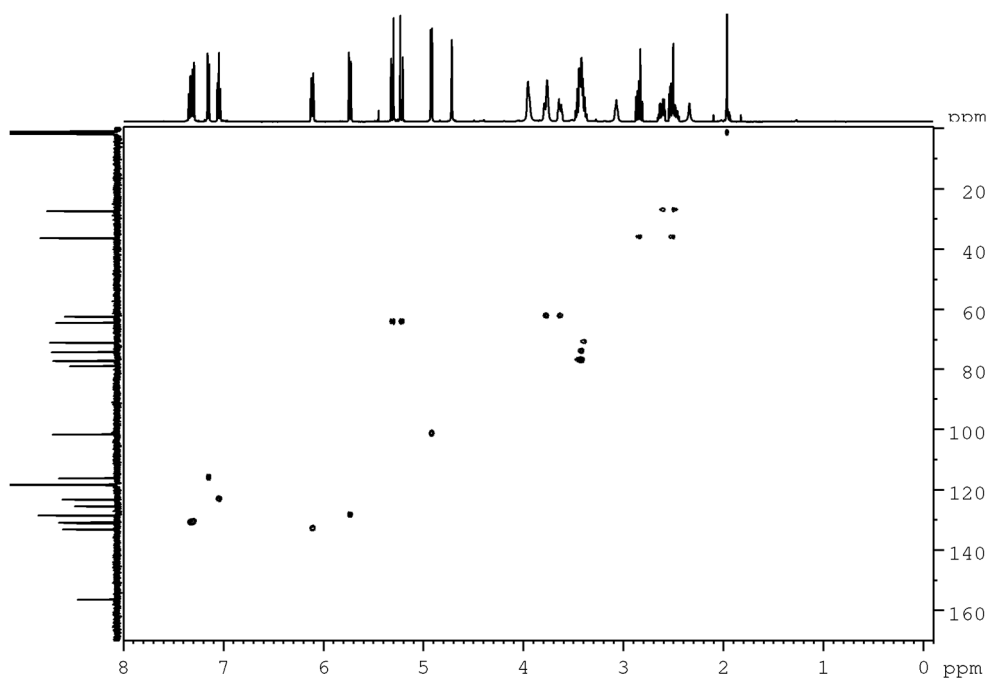


Figure S2.4. Salicortin (1), ^1H - ^{13}C HSQC spectrum (500 MHz, $\text{MeCN-}d_3$).

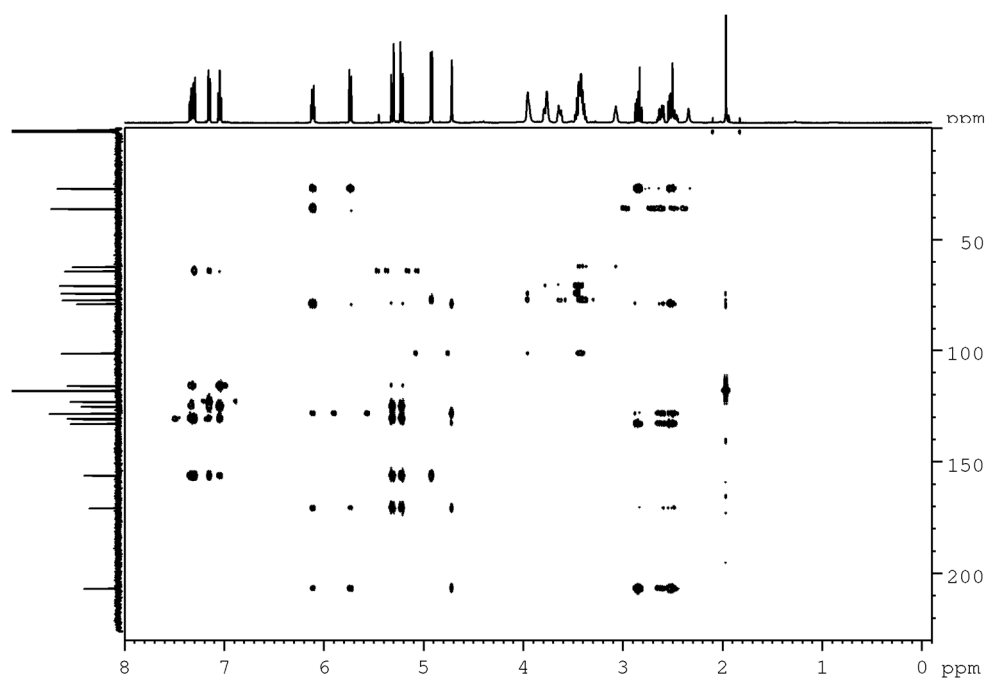


Figure S2.5. Salicortin (1), ^1H - ^{13}C HMBC spectrum (500 MHz, $\text{MeCN-}d_3$).

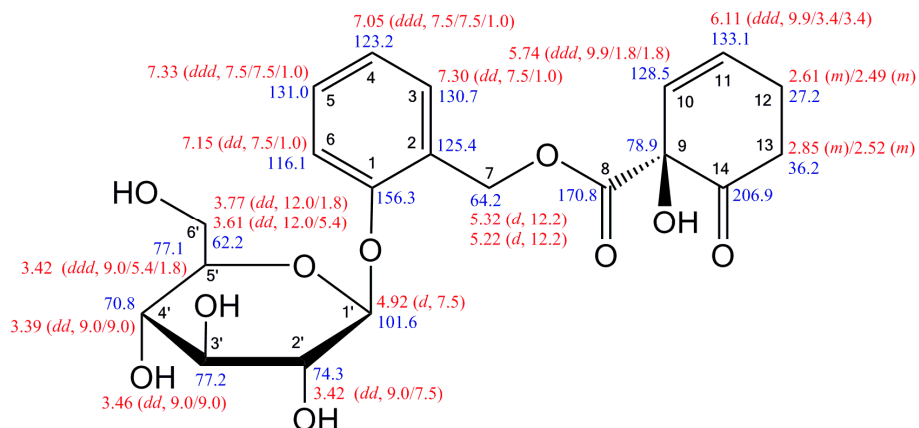


Figure S2.6. Salicortin (1), structure with chemical shifts (MeCN- d_3), multiplicities and coupling constants (J in Hz). Red: ^1H -NMR (500 MHz); blue: ^{13}C -NMR (125 MHz).

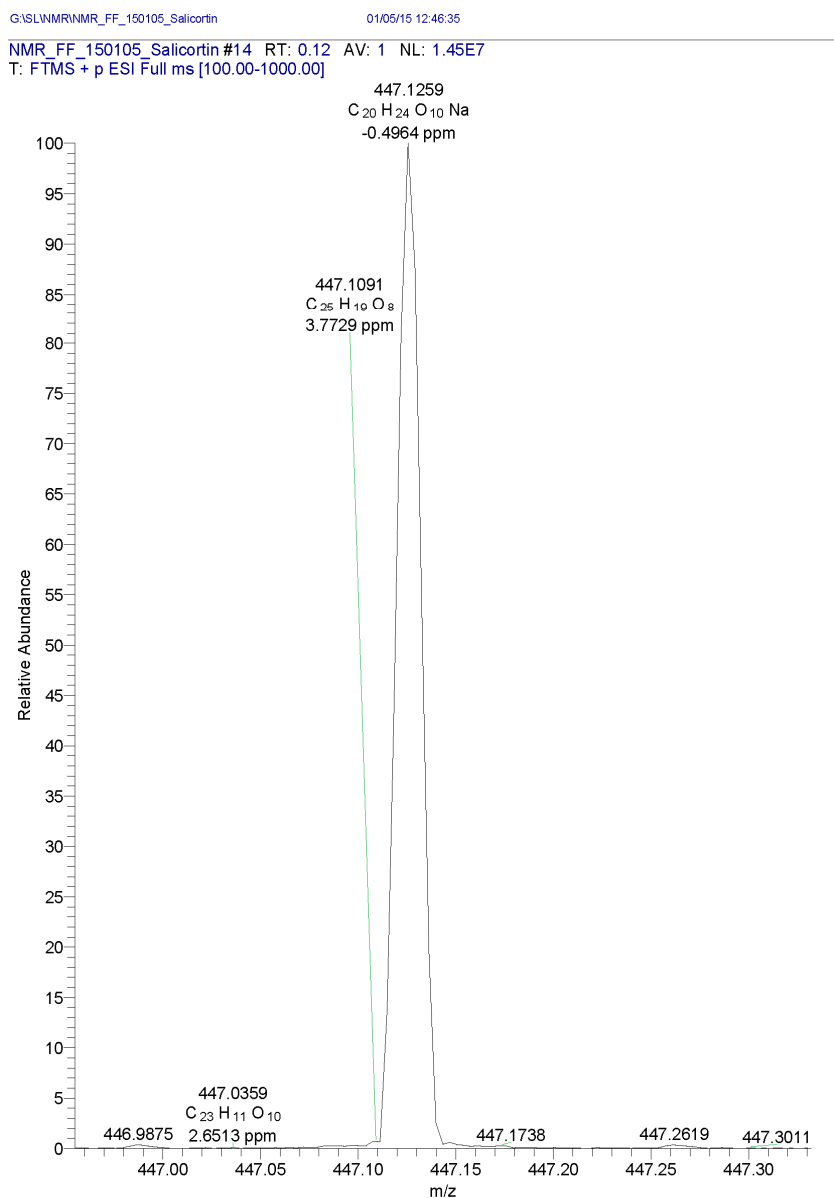


Figure S2.7. Salicortin (1), result of the HRMS measurement.

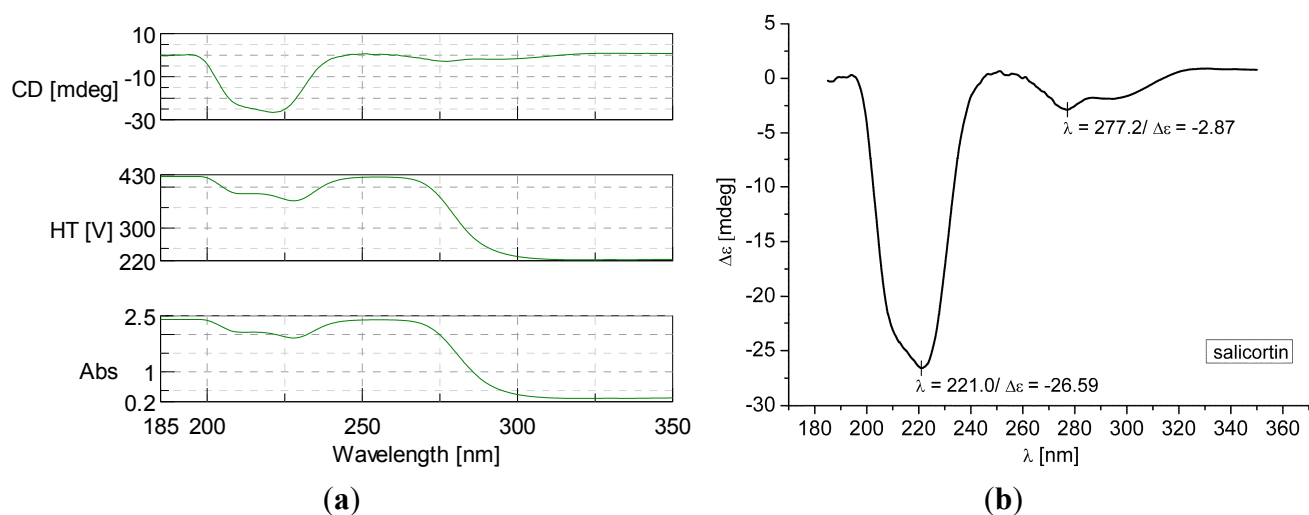


Figure S2.8. Salicortin (1), (a) results of the CD measurement (concentration 0.70 mg/mL (1.66 mM in MeOH), cuvette width 1 mm). (b) Molar circular dichroism $\Delta\epsilon$ at maximum wavelengths.

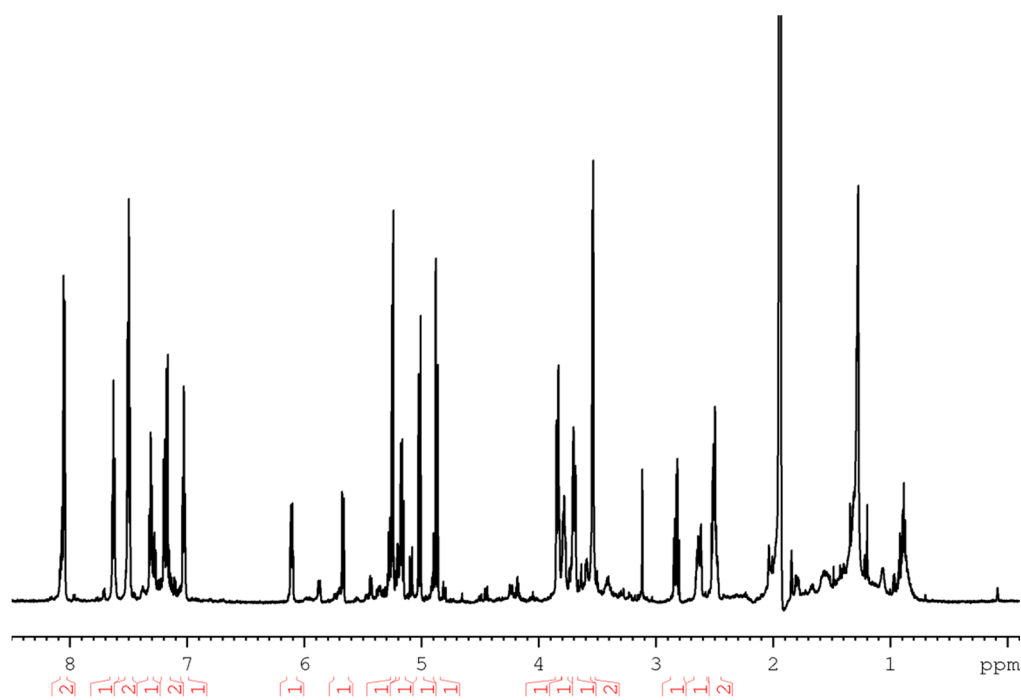


Figure S3.1. Tremulacin (2), ^1H -NMR spectrum (700 MHz, $\text{MeCN-}d_3$).

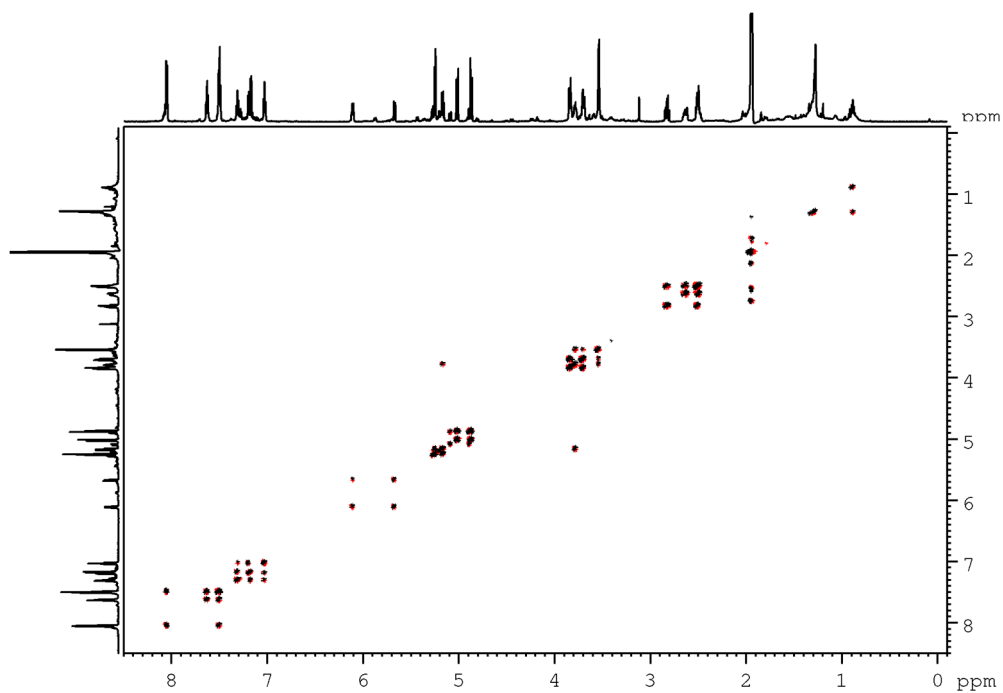


Figure S3.2. Tremulacin (2), ^1H - ^1H COSY spectrum (700 MHz, $\text{MeCN-}d_3$).

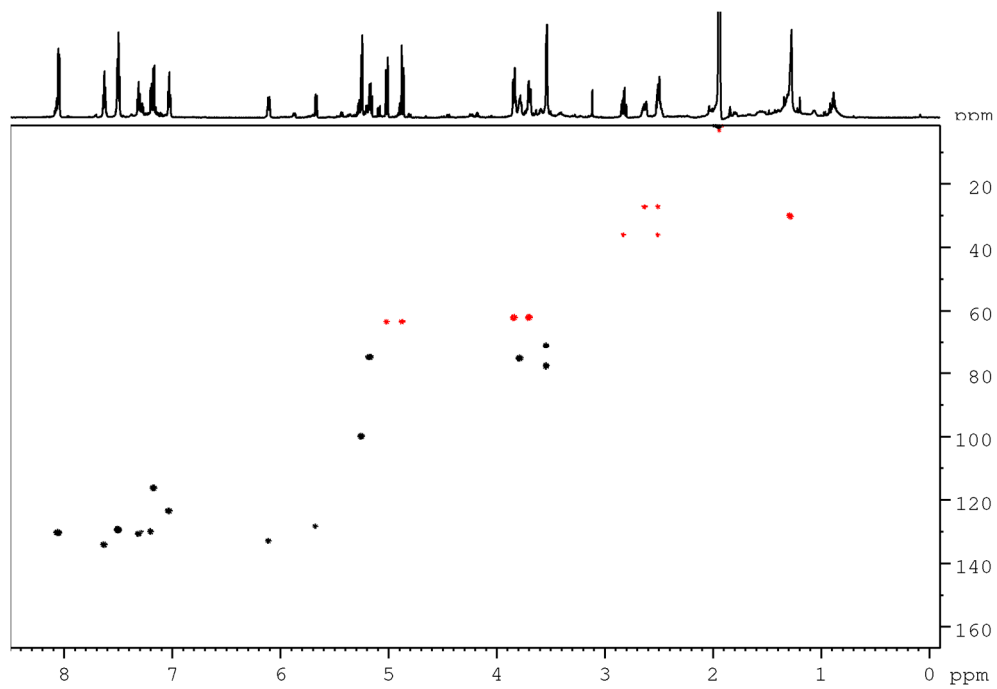


Figure S3.3. Tremulacin (2), ^1H - ^{13}C HSQC spectrum (700 MHz, $\text{MeCN-}d_3$).

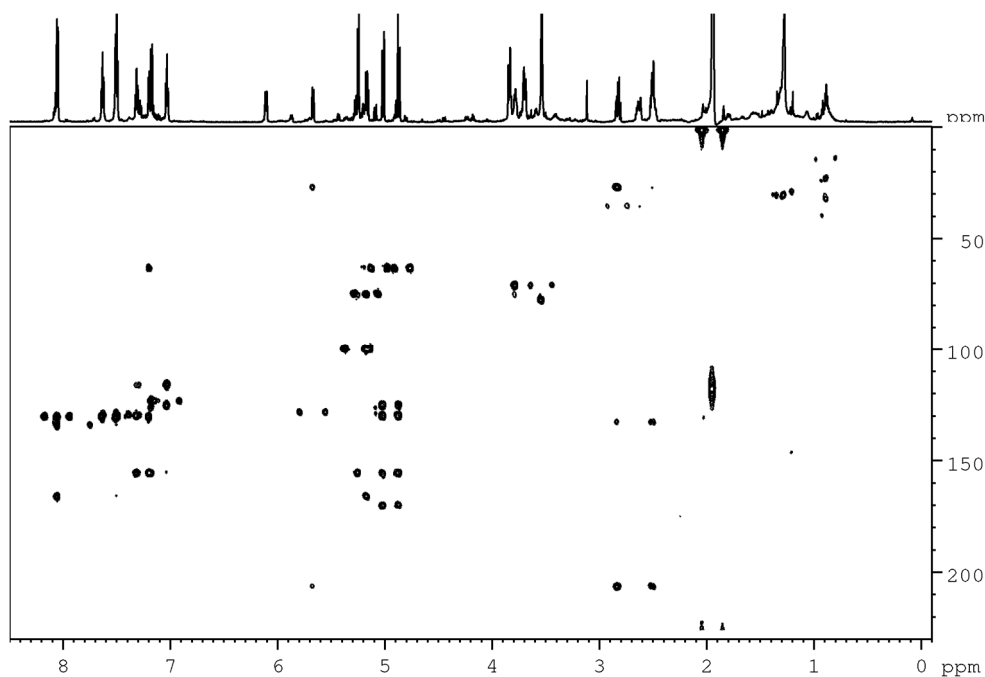


Figure S3.4. Tremulacin (**2**), ^1H - ^{13}C HMBC spectrum (700 MHz, $\text{MeCN-}d_3$).

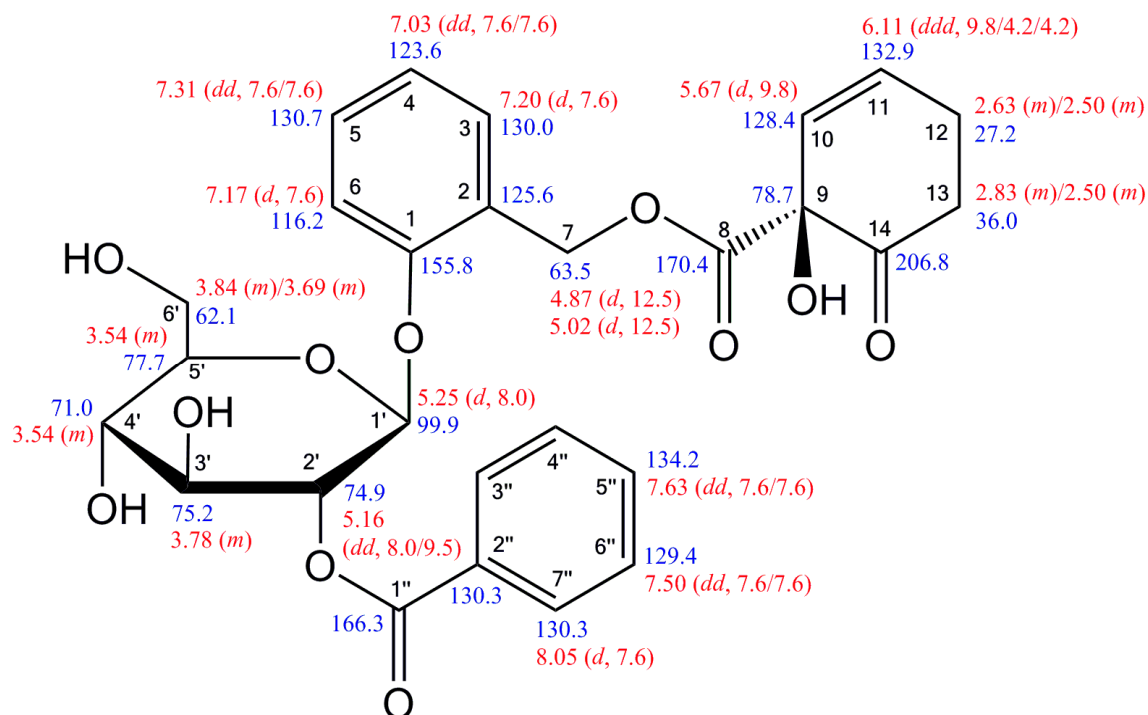


Figure S3.5. Tremulacin (**2**), structure with chemical shifts (MeCN- d_3), multiplicities and coupling constants (J in Hz). Red: ^1H -NMR (700 MHz); blue: ^{13}C -NMR (175 MHz).

G:\SL\NMR\NMR_FF_150107_Tremulacin

01/08/15 12:07:33

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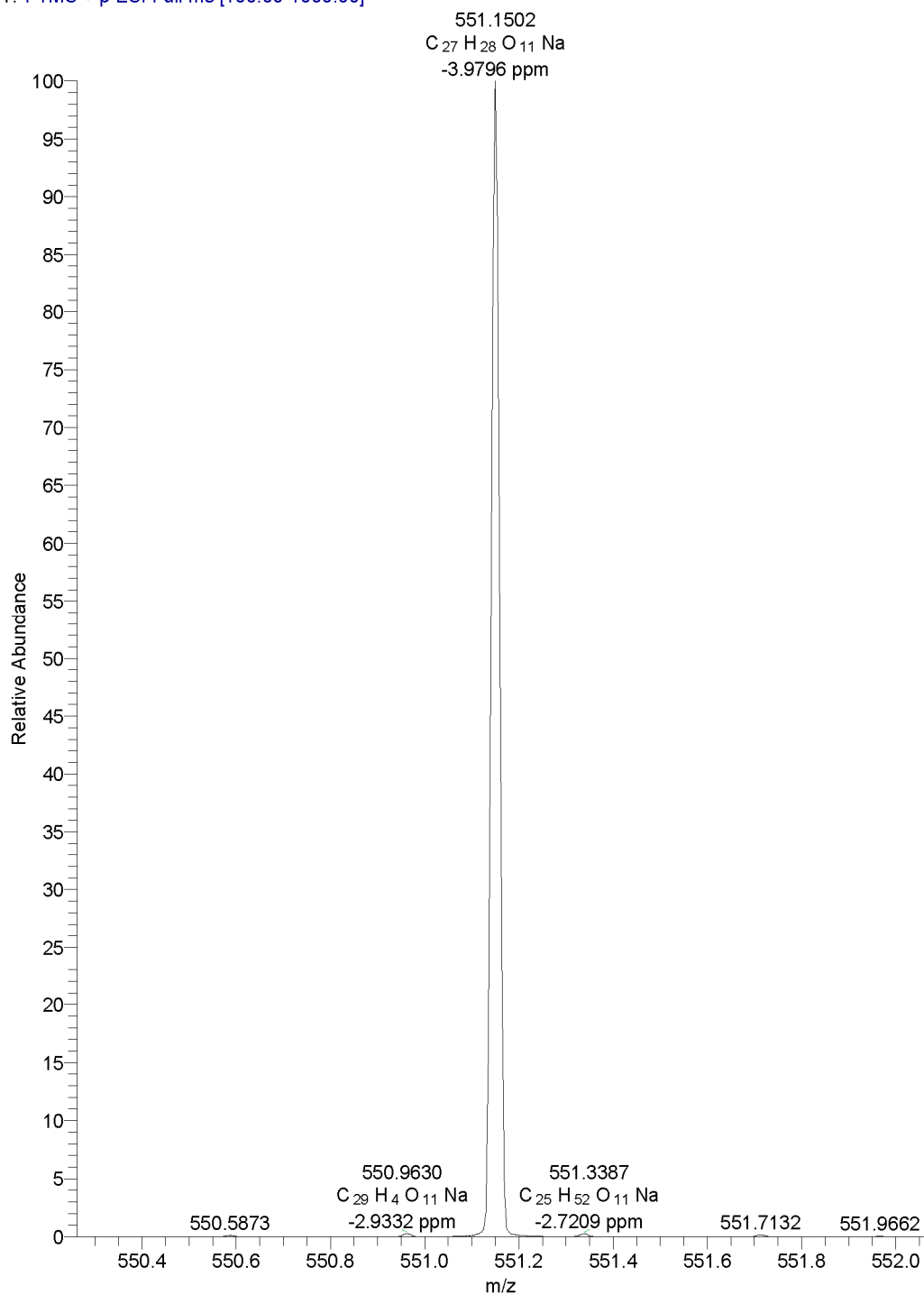


Figure S3.6. Tremulacin (2), result of the HRMS measurement.



Figure S3.7. Tremulacin (**2**), **(a)** results of the CD measurement (concentration 0.76 mg/mL (1.44 mM in MeOH), cuvette width 1 mm). **(b)** Molar circular dichroism $\Delta\epsilon$ at maximum wavelengths.

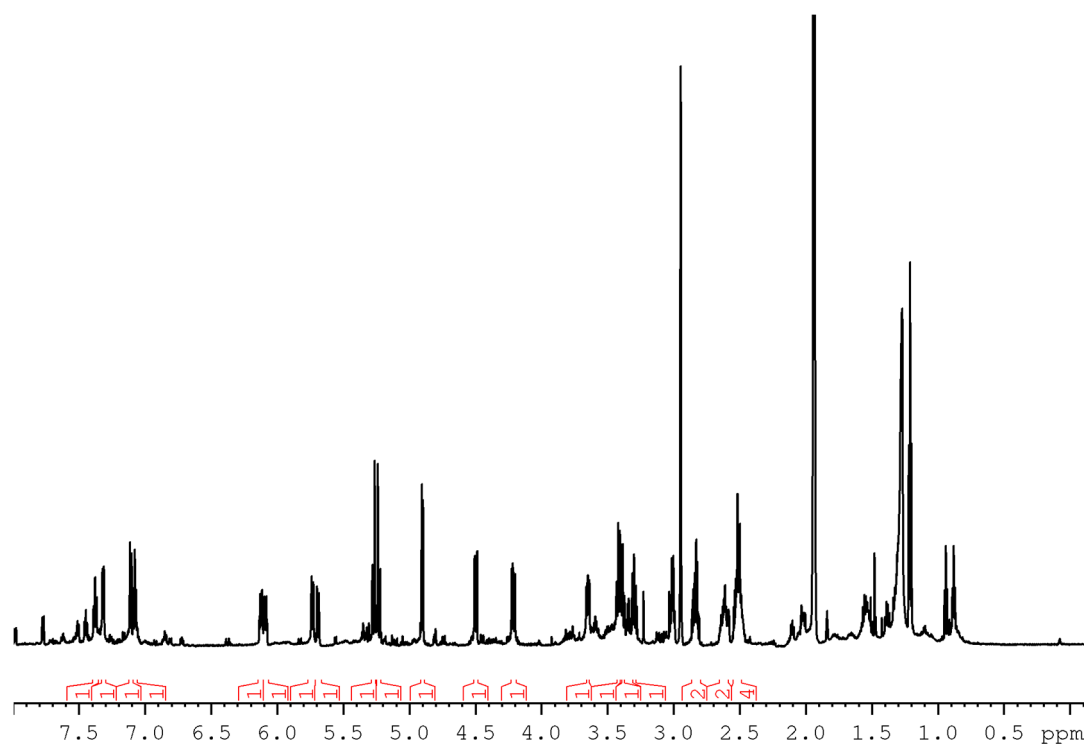


Figure S4.1. HCH-Salicortin (**3**), ¹H-NMR spectrum (700 MHz, MeCN-*d*₃).

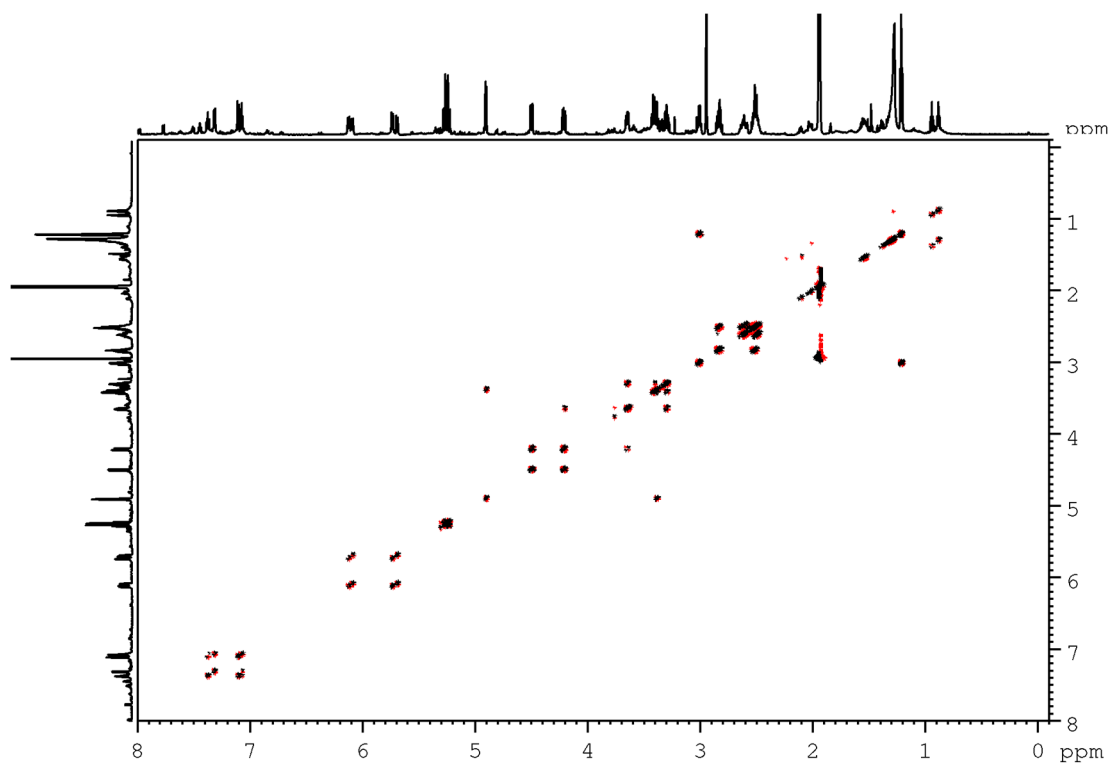


Figure S4.2. HCH-Salicortin (**3**), ^1H - ^1H COSY spectrum (700 MHz, $\text{MeCN-}d_3$).

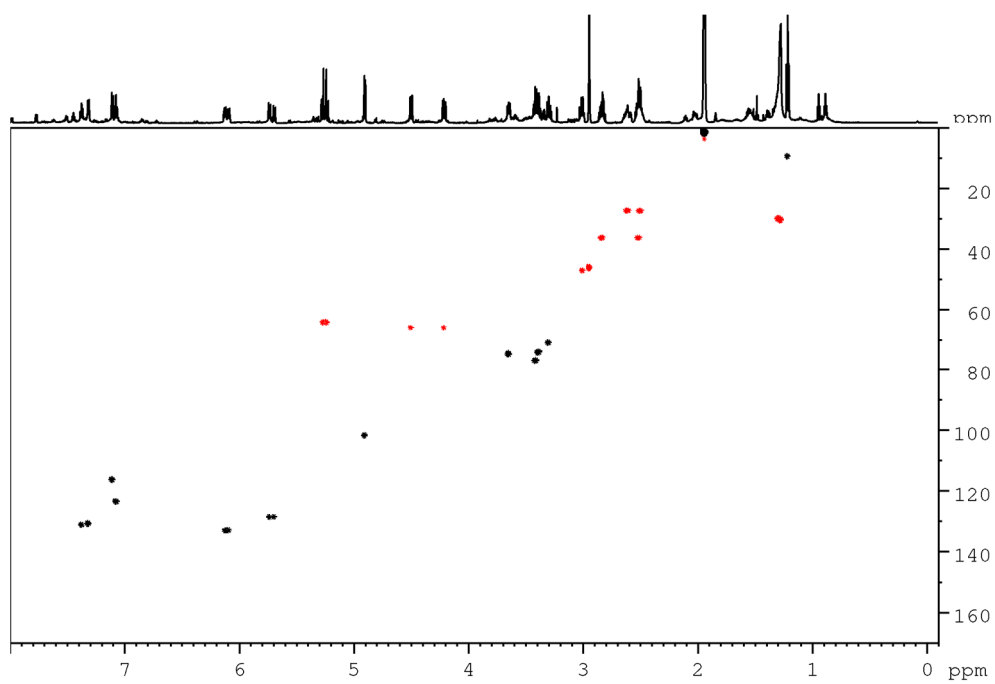


Figure S4.3. HCH-Salicortin (**3**), ^1H - ^{13}C HSQC spectrum (700 MHz, $\text{MeCN-}d_3$).

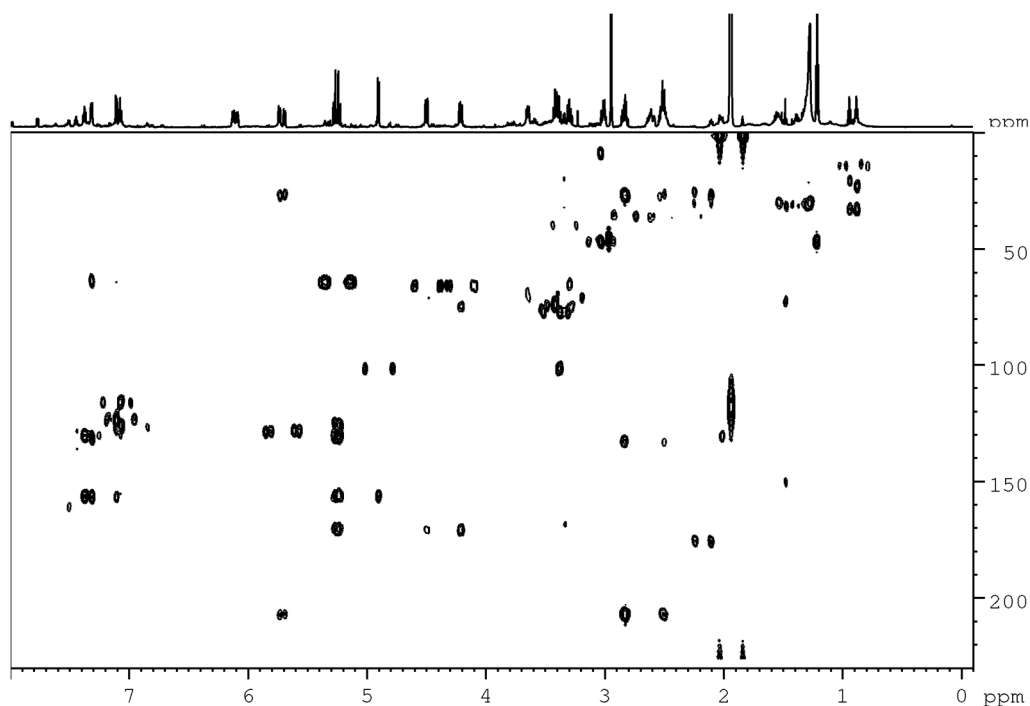


Figure S4.4. HCH-Salicortin (**3**), ^1H - ^{13}C HMBC spectrum (700 MHz, $\text{MeCN-}d_3$).

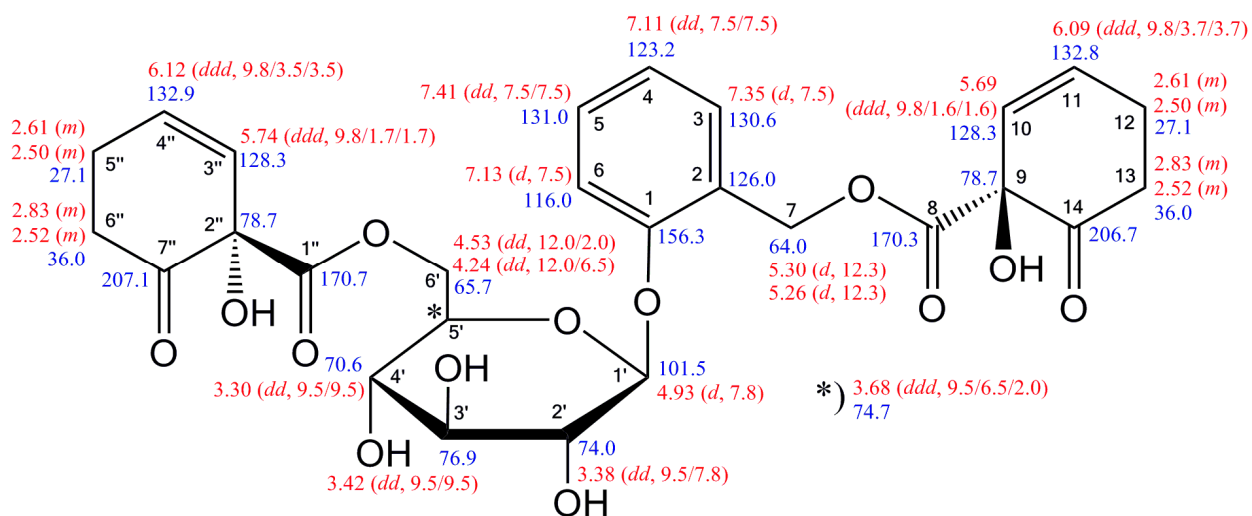


Figure S4.5. HCH-Salicortin (**3**), structure with chemical shifts ($\text{MeCN-}d_3$) multiplicities and coupling constants (J in Hz). Red: ^1H -NMR (700 MHz); blue: ^{13}C -NMR (175 MHz).

G:\SL\NMR\NMR_FF_150107_HCH-Salicortin

01/08/15 11:32:09

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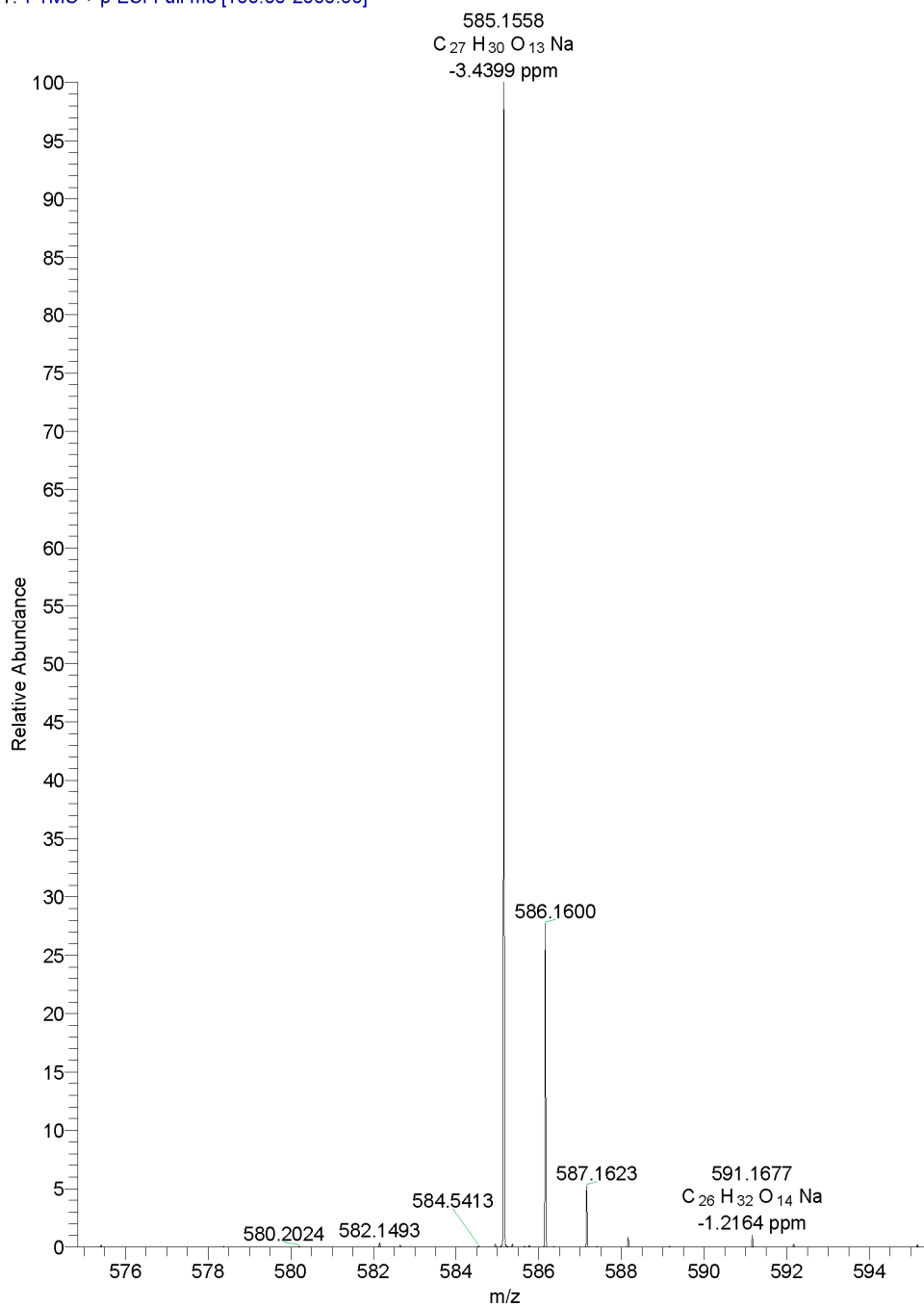


Figure S4.6. HCH-Salicortin (**3**), result of the HRMS measurement.

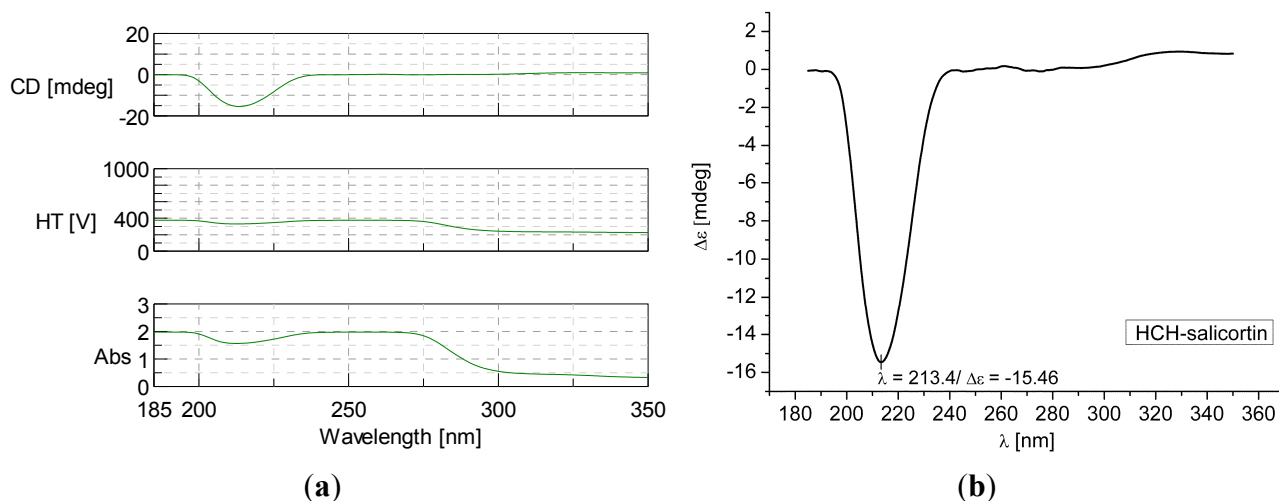


Figure S4.7. HCH-Salicortin (**3**), (a) results of the CD measurement (concentration 0.67 mg/mL (1.19 mM in MeOH), cuvette width 1 mm). (b) Molar circular dichroism $\Delta\epsilon$ at maximum wavelength.

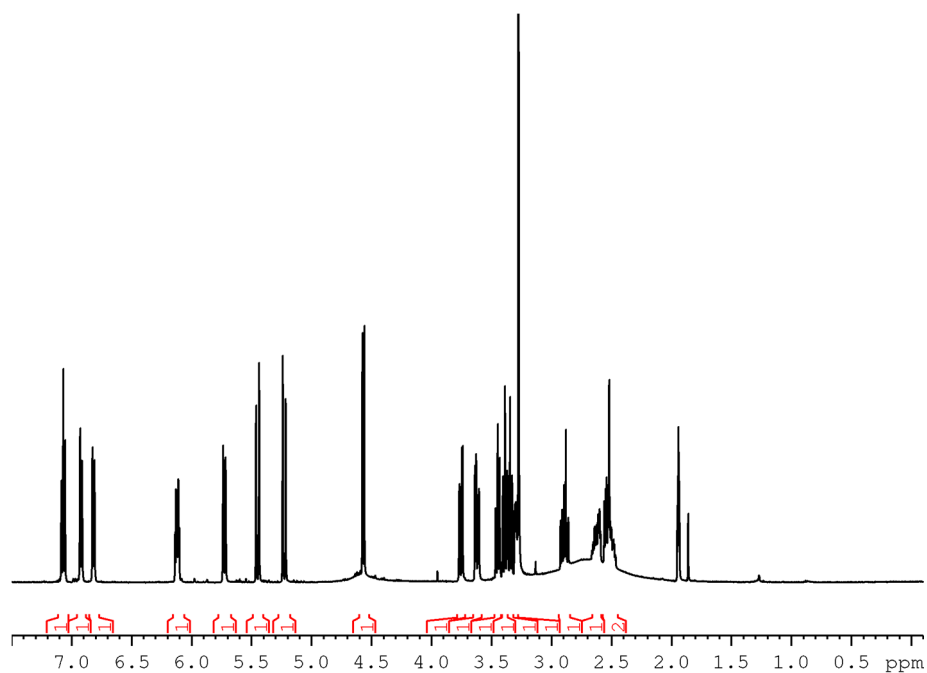


Figure S5.1. Idescarpin (**4**), ^1H -NMR spectrum (500 MHz, $\text{MeCN-}d_3$).

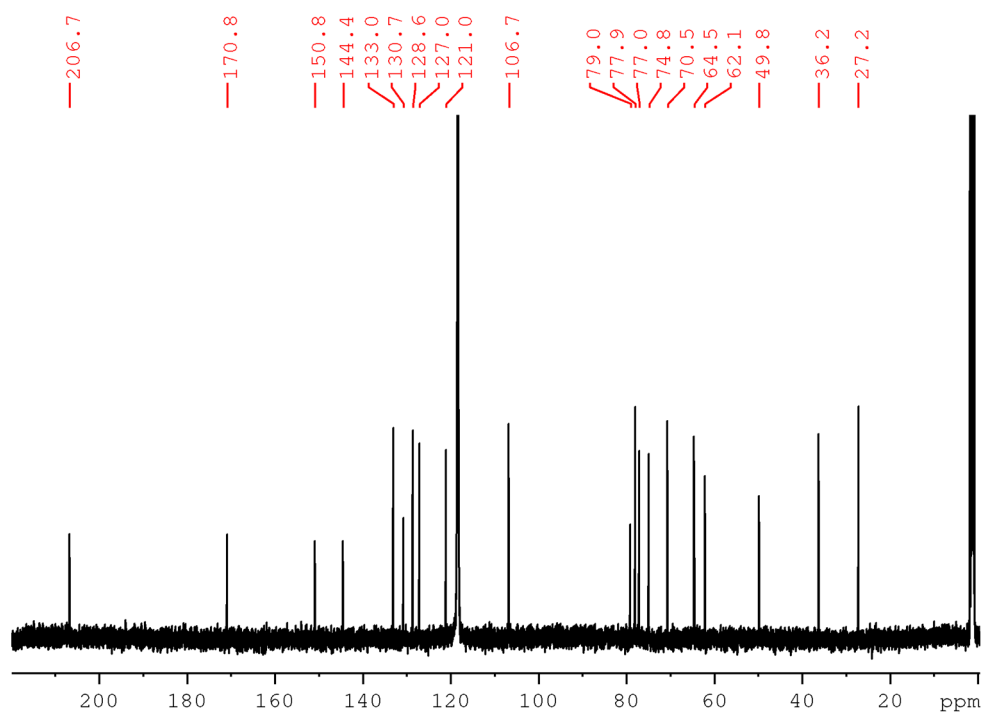


Figure S5.2. Idescarpin (**4**), ^{13}C -NMR spectrum (125 MHz, $\text{MeCN-}d_3$).

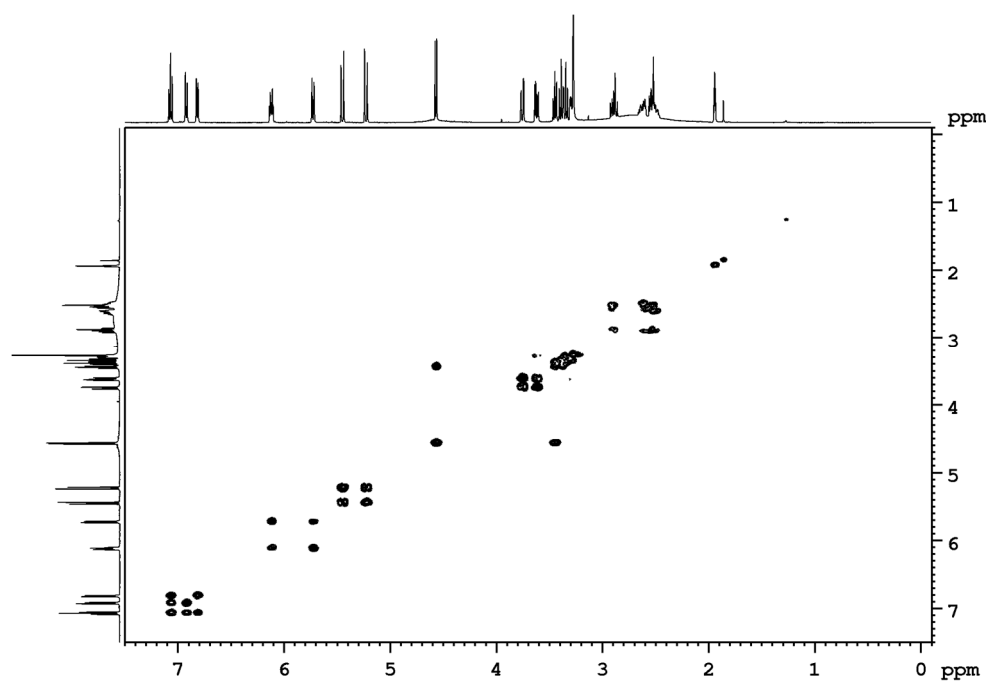


Figure S5.3. Idescarpin (**4**), ^1H - ^1H COSY spectrum (500 MHz, $\text{MeCN-}d_3$).

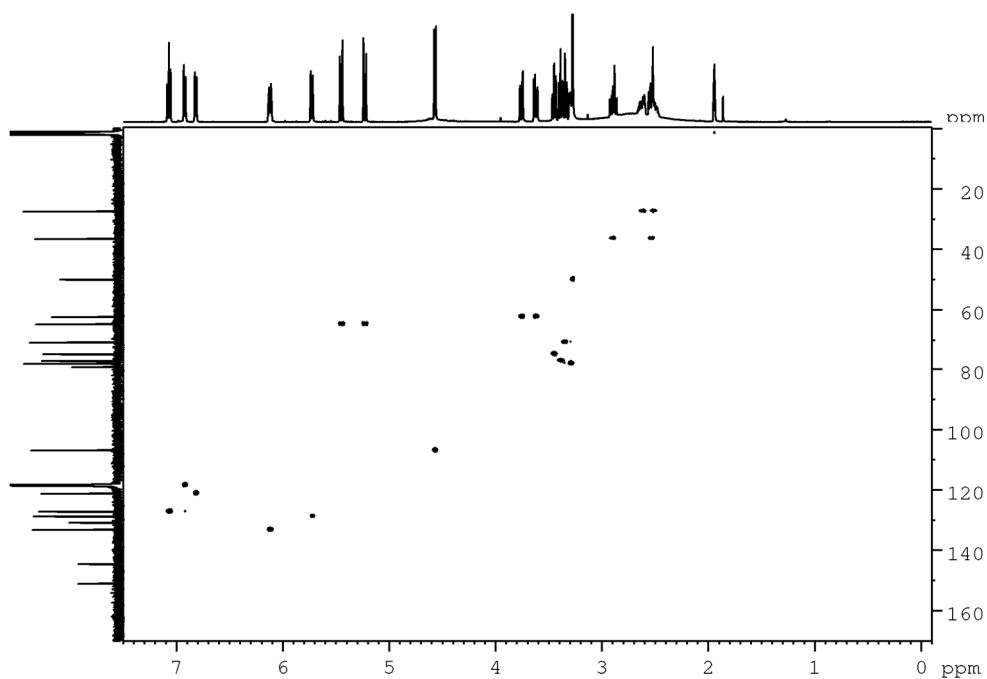


Figure S5.4. Idescarpin (4), ^1H - ^{13}C HSQC spectrum (500 MHz, $\text{MeCN-}d_3$).

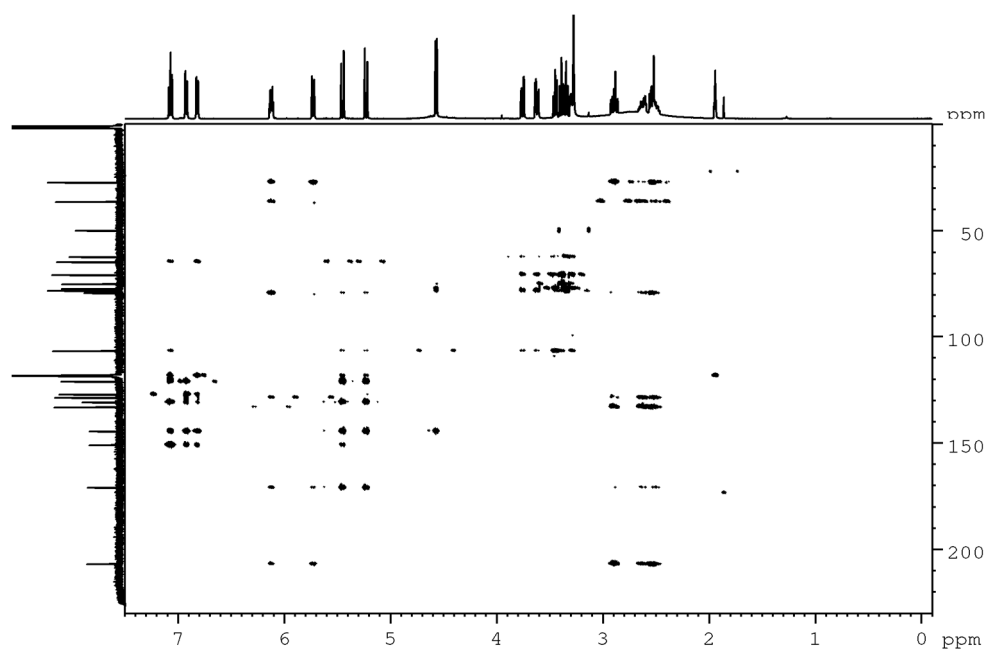


Figure S5.5. Idescarpin (4), ^1H - ^{13}C HMBC spectrum (500 MHz, $\text{MeCN-}d_3$).

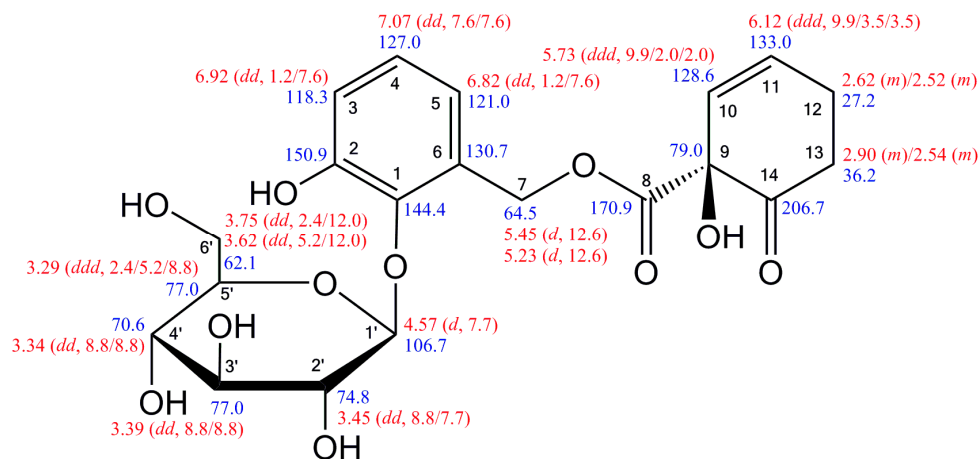


Figure S5.6. Idescarpin (4), structure with chemical shifts (MeCN- d_3), multiplicities and coupling constants (J in Hz). Red: ^1H -NMR (500 MHz); blue: ^{13}C -NMR (125 MHz).

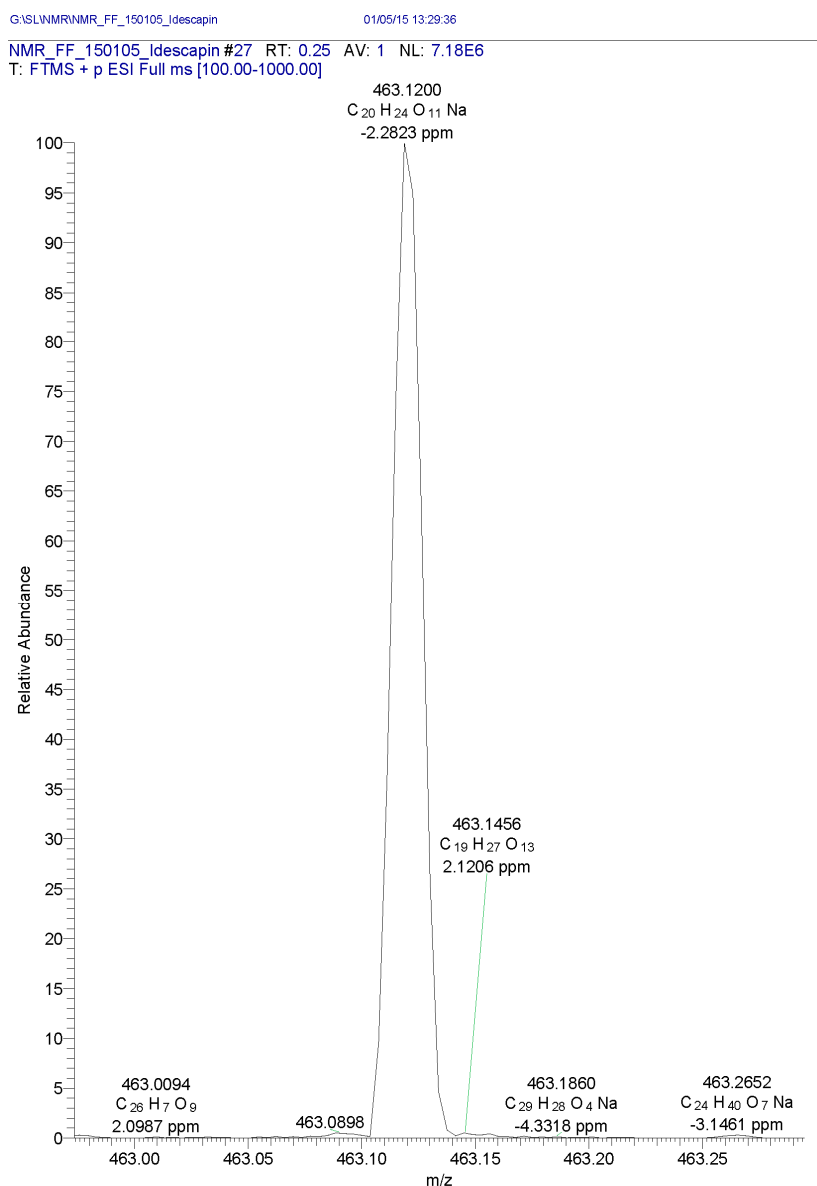


Figure S5.7. Idescarpin (4), result of the HRMS measurement.

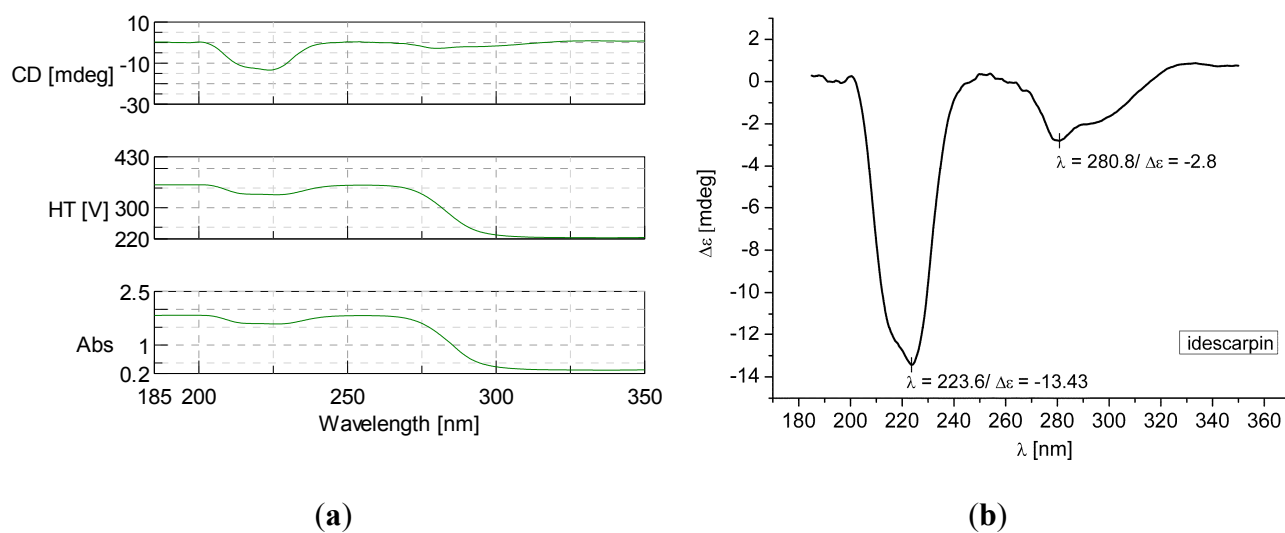


Figure S5.8. Idescarpin (**4**), (a) results of the CD measurement (concentration 0.71 mg/mL (1.61 mM in MeOH), cuvette width 1 mm). (b) Molar circular dichroism $\Delta\epsilon$ at maximum wavelengths.