

Supporting Information

Characterization and bioactive potential of secondary metabolites isolated from *Piper sarmentosum* Roxb.

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4''-(3-Hydroxy-3-methylglutaroyl)-2''-β-D-glucopyranosyl vitexin

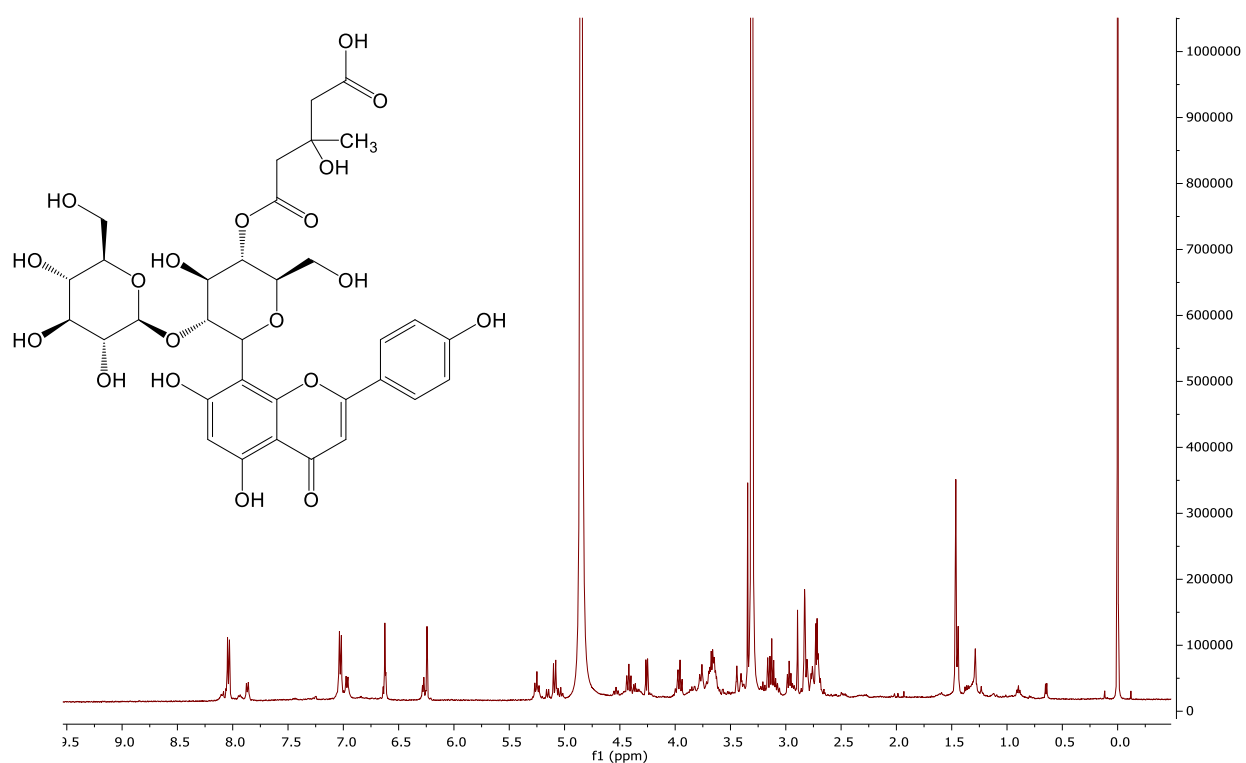


Figure S1: ¹H NMR spectrum of compound **1** (400 MHz, MeOH-*d*₄)

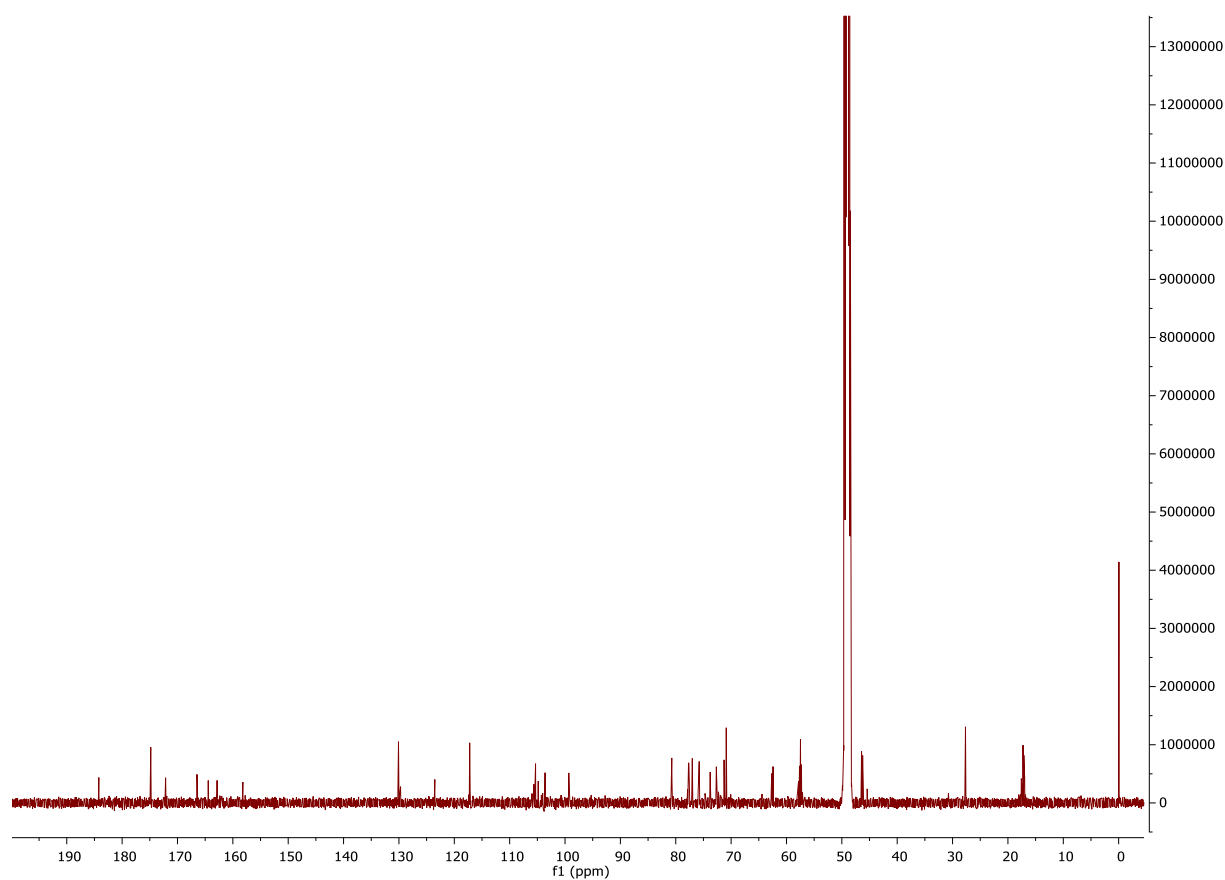


Figure S2: ¹³C NMR spectrum of compound **1** (100 MHz, MeOH-*d*₄)

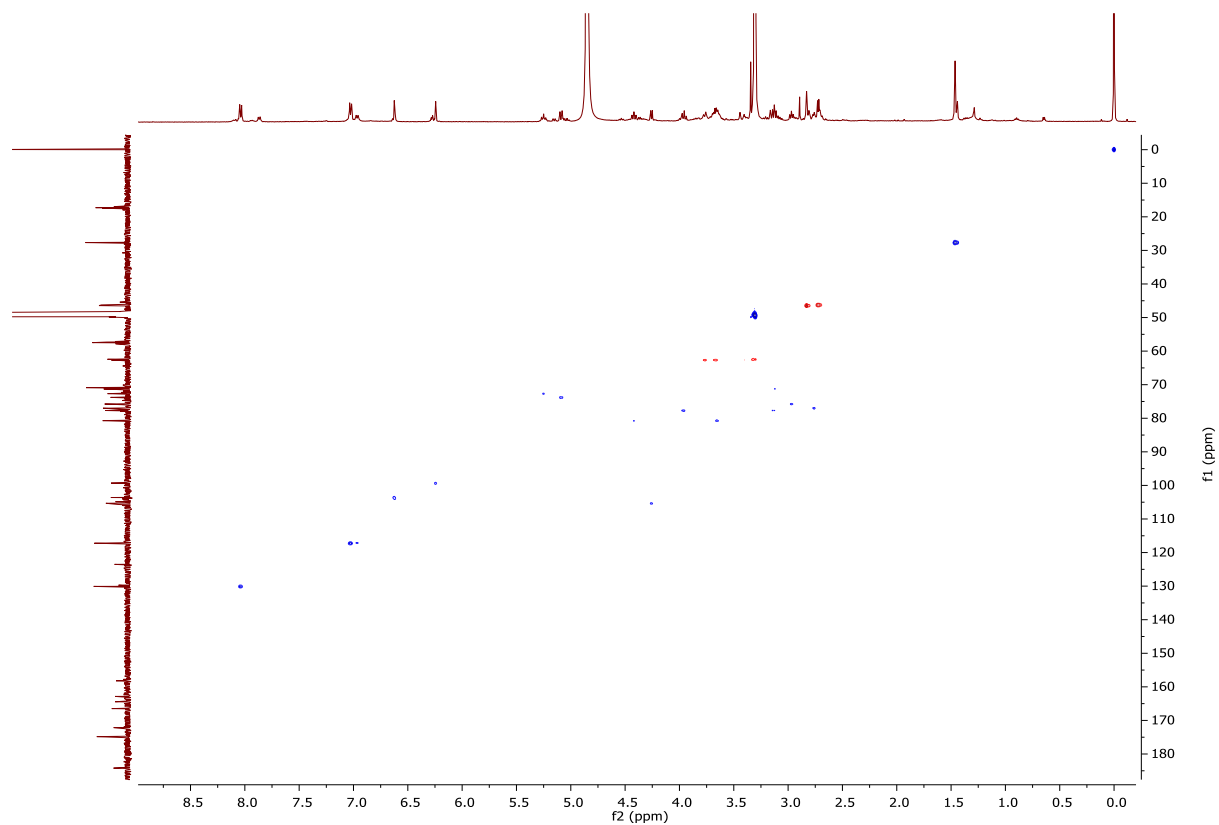


Figure S3: HSQC spectrum of compound **1** (400 MHz, MeOH-*d*₄)

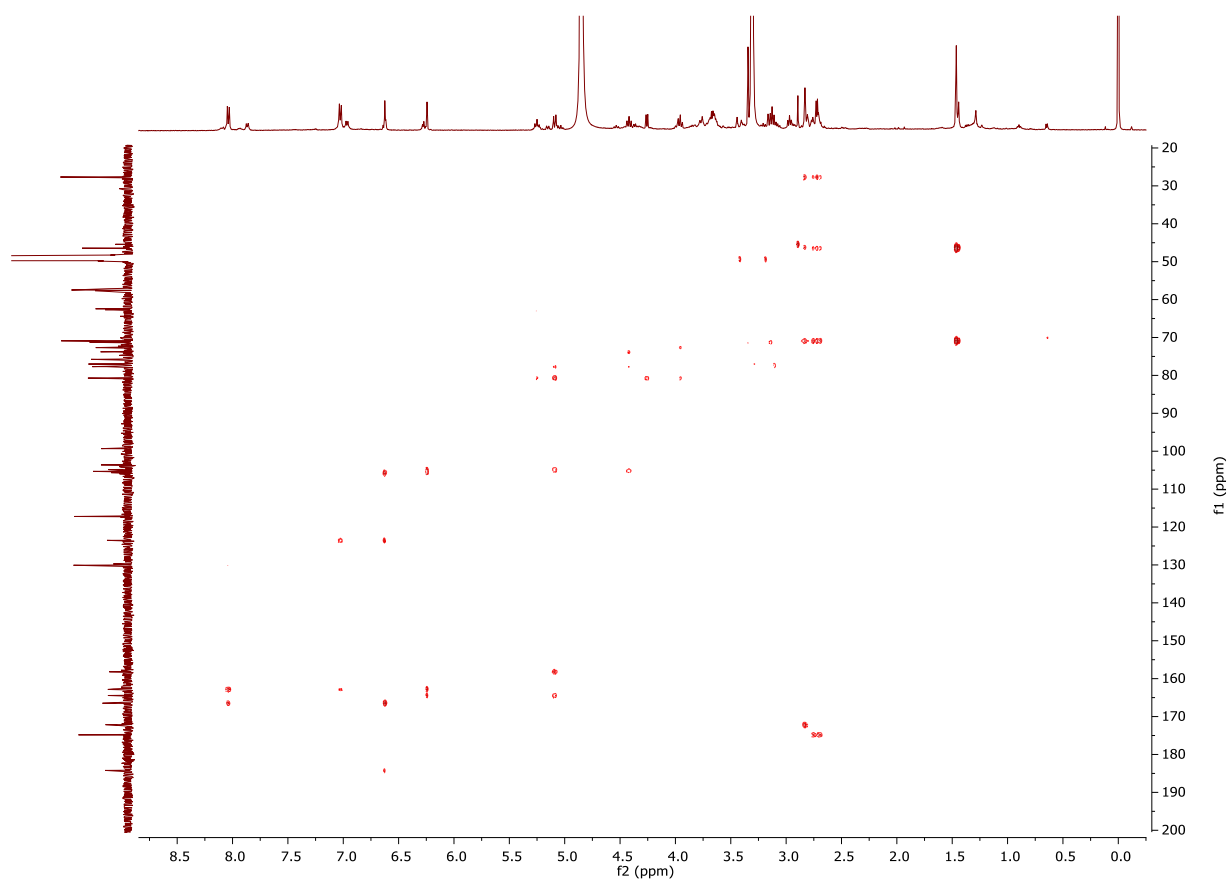


Figure S4: HMBC spectrum of compound **1** (400 MHz, MeOH-*d*₄)

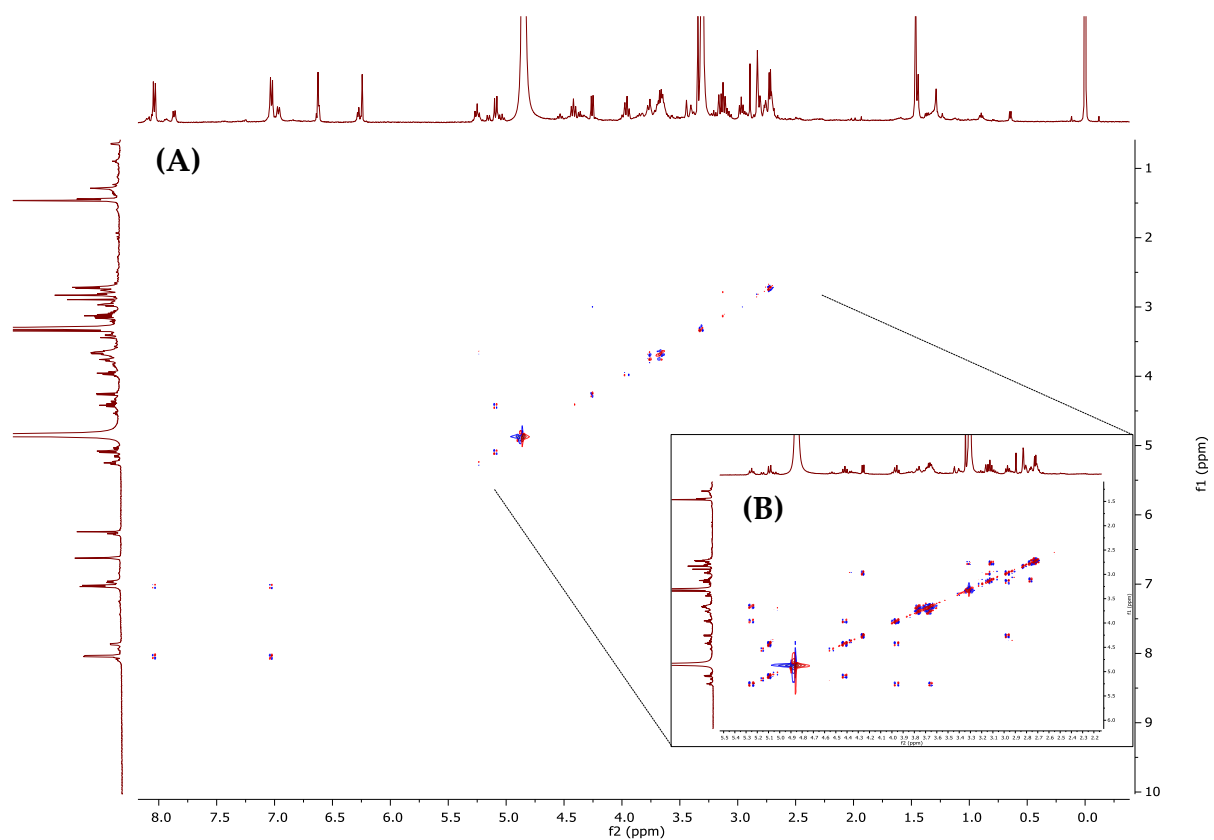


Figure S5: ^1H - ^1H COSY spectrum of compound **1**; A) full spectrum, B) glycoside region (400 MHz, $\text{MeOH-}d_4$)

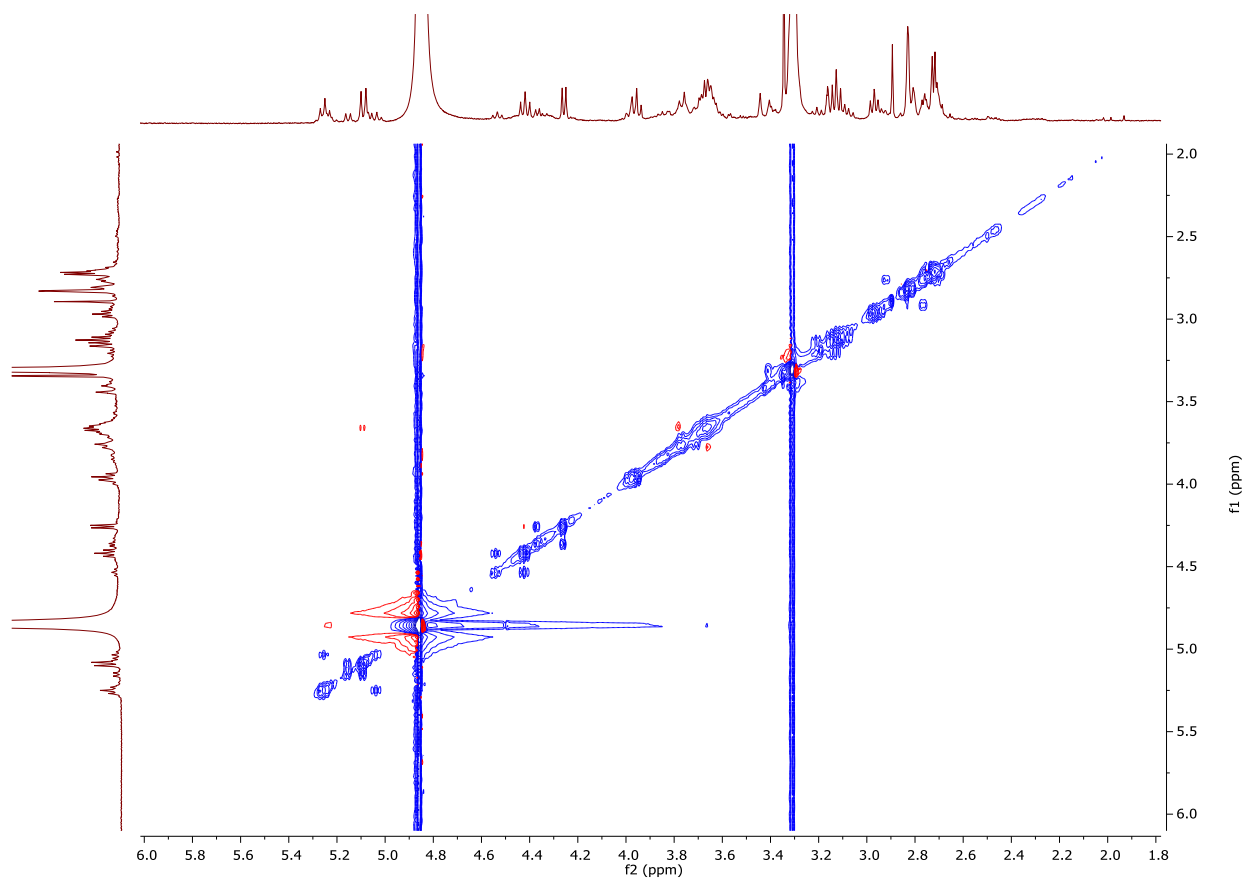


Figure S6: 2D-ROESY spectrum at glycoside region of compound **1** (400 MHz, $\text{MeOH-}d_4$)

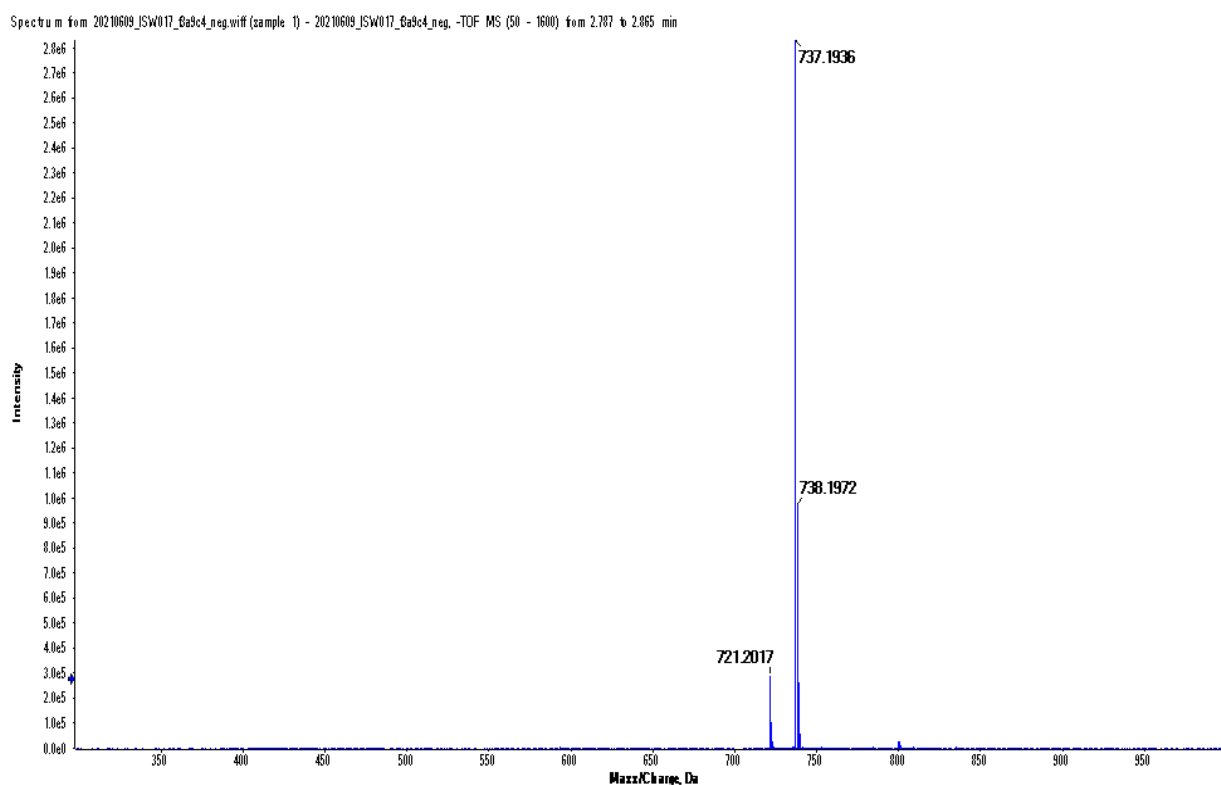


Figure S7: HR-ESI-MS spectrum of compound **1** in negative ion mode

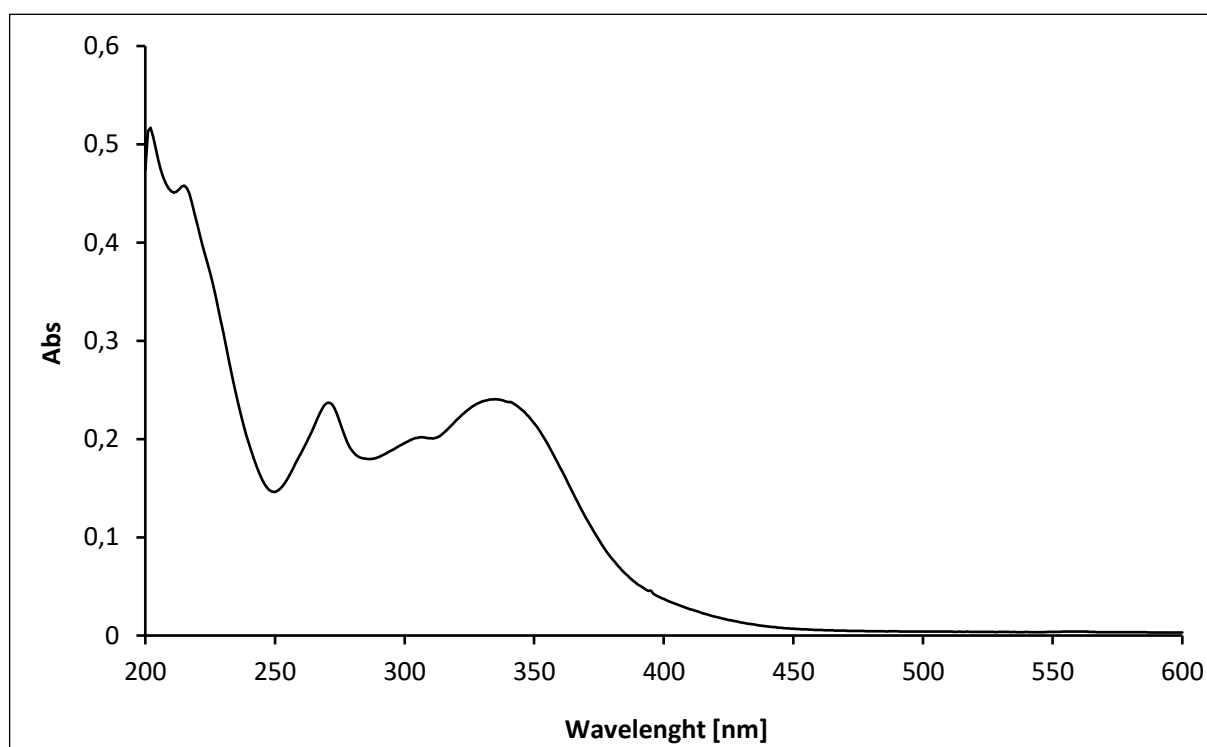


Figure S8: UV spectrum of compound **1** in MeOH

Table S1: Polarimeter data of compound 1.

Light Source	WI
Wavelength	589 nm
Sample Aperture	Ø 3.0
Light Aperture	Ø 1.0
D.I.T.	5 sec
Cycle Times	20
Cycle Interval	5 sec
Path Length	50 mm
Concentration	0.153 W/V%
Factor	1.0000
Temp. Correct	0
Sample	ISW017_f3a9c4
Comment	1.53 mg / 1 ml Methanol
Optical Rotation	
Average	-0.0084 deg
S.D.	0.0003 deg
R.S.D.	4.1097 %
Specific O.R.	
Average	-10.9346
S.D.	0.4494
Temperatur	23.5° C

4-Allyl-5-methoxy-2-(β -D-glucopyranosyloxy-3-(4-methoxyphenyl)propanoate
(Kadukoside)

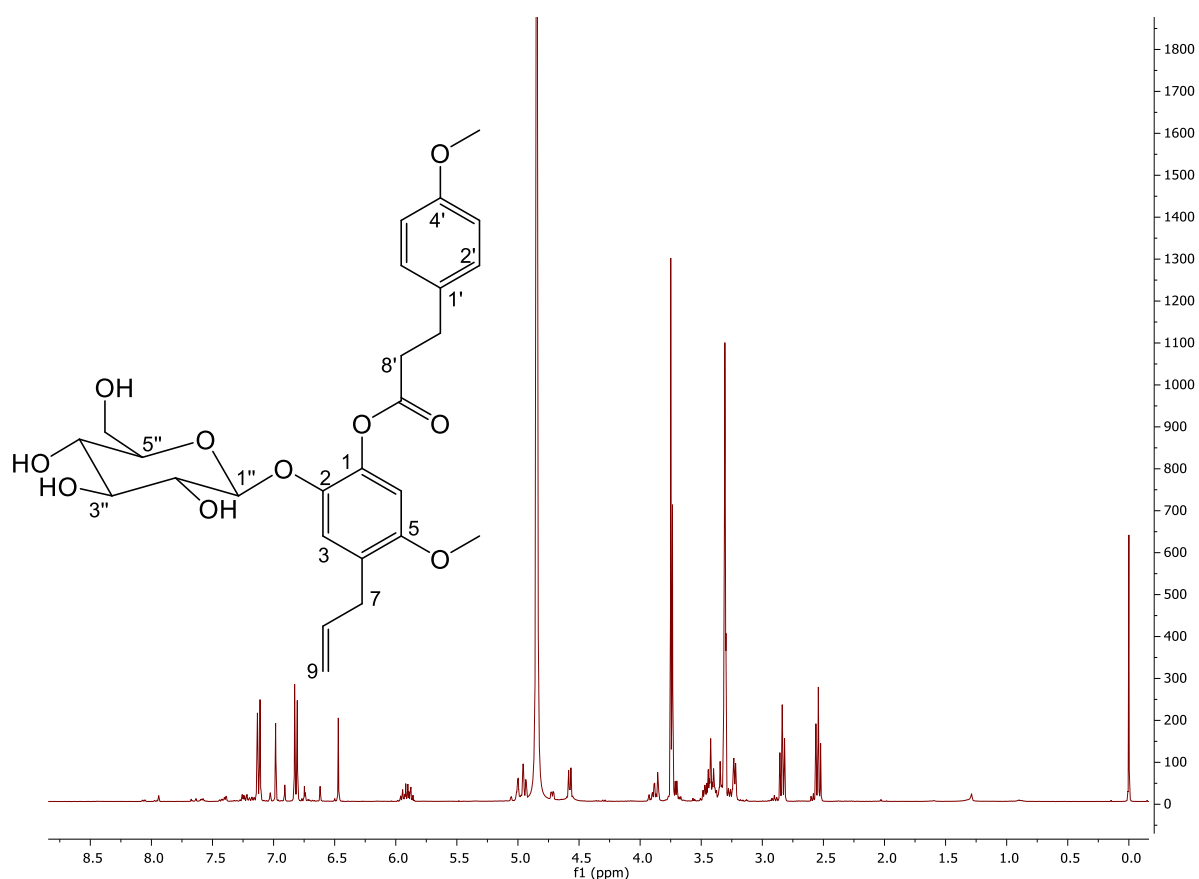


Figure S9: ^1H NMR spectrum of compound **2** (400 MHz, $\text{MeOH-}d_4$)

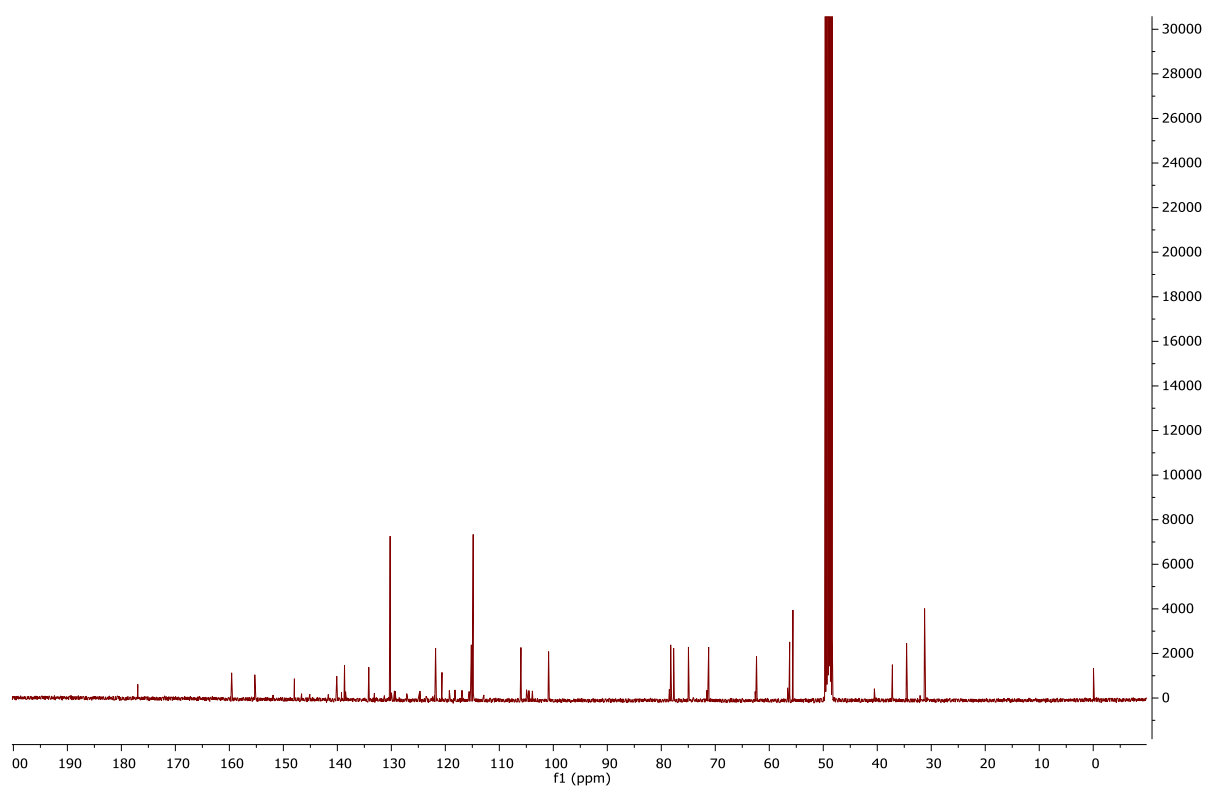


Figure S10 : ^{13}C NMR spectrum of compound **2** (400 MHz, $\text{MeOH-}d_4$)

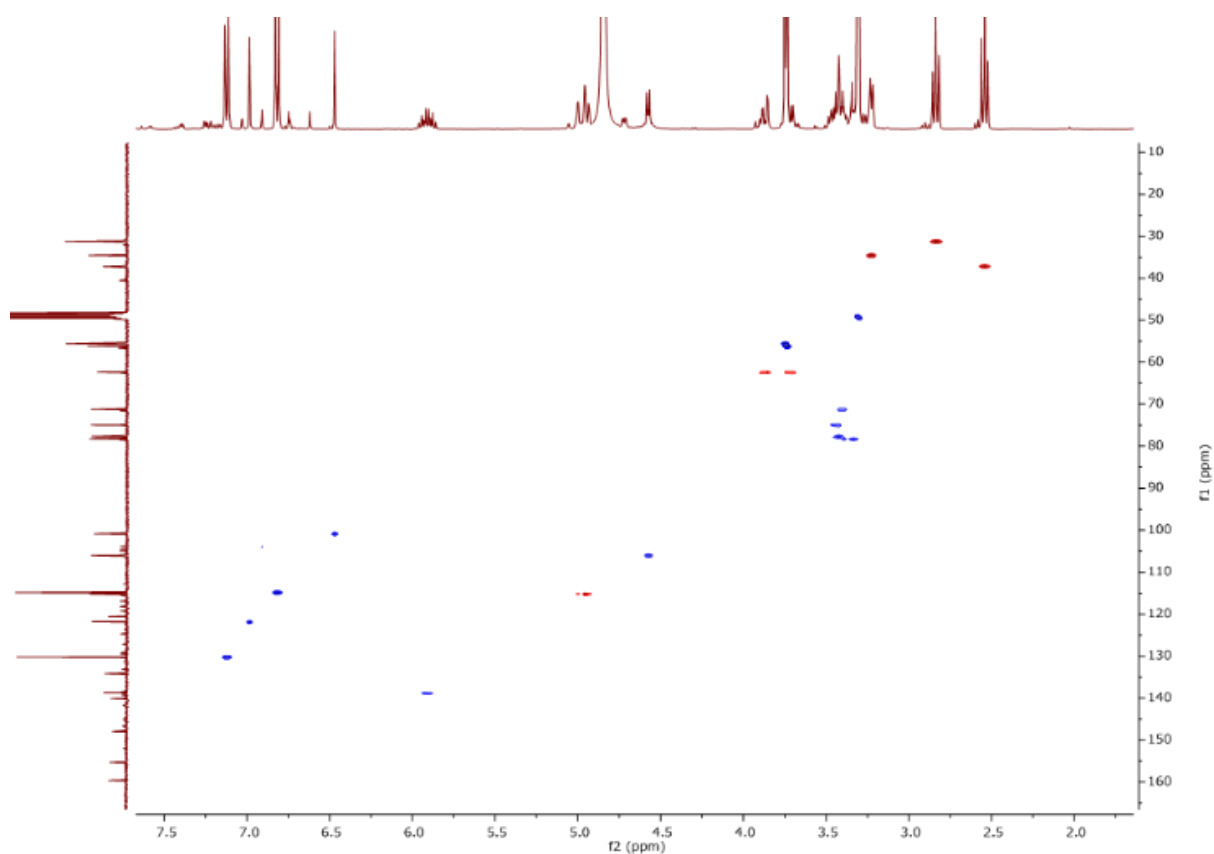


Figure S11: HSQC spectrum of compound **2** (400 MHz, MeOH-*d*₄)

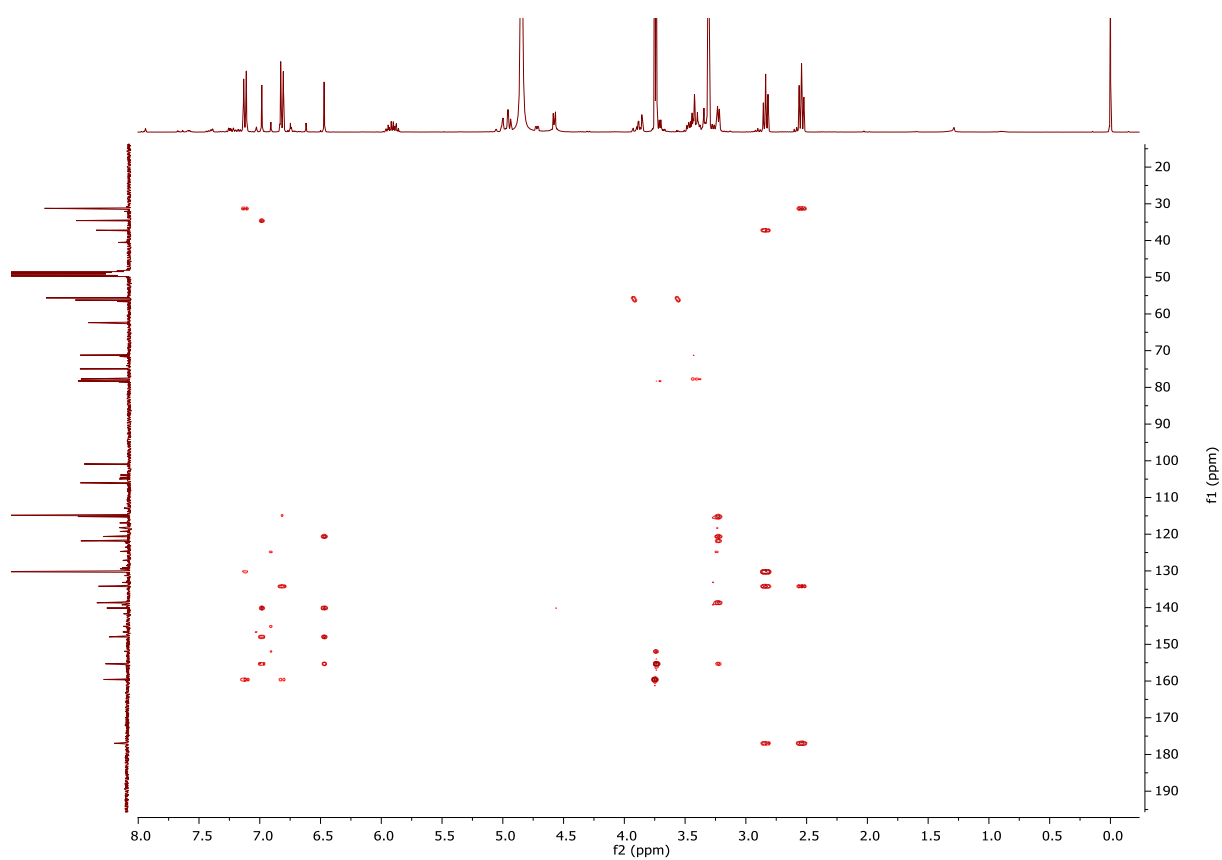


Figure S12: HMBC spectrum of compound **2** (400 MHz, MeOH-*d*₄)

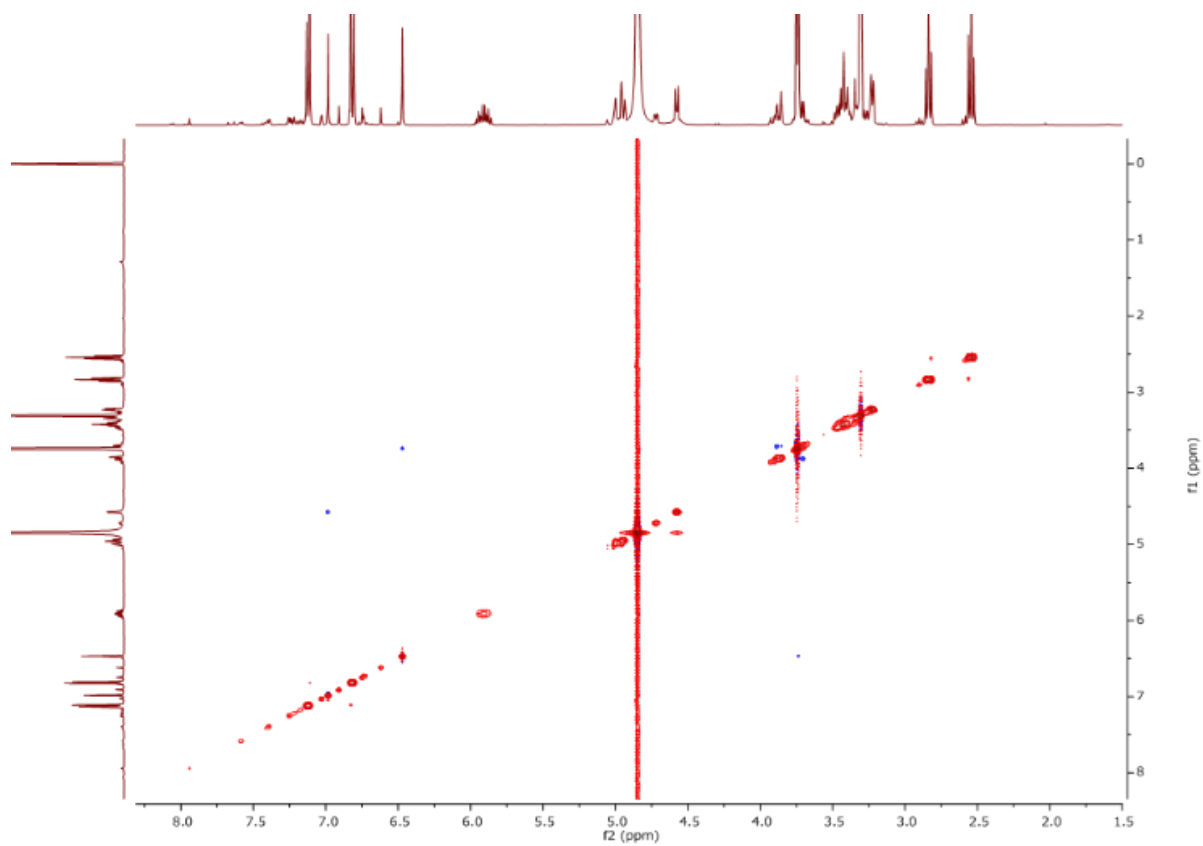


Figure S13: 2D-NOESY spectrum of compound **2** (400 MHz, MeOH-*d*₄)

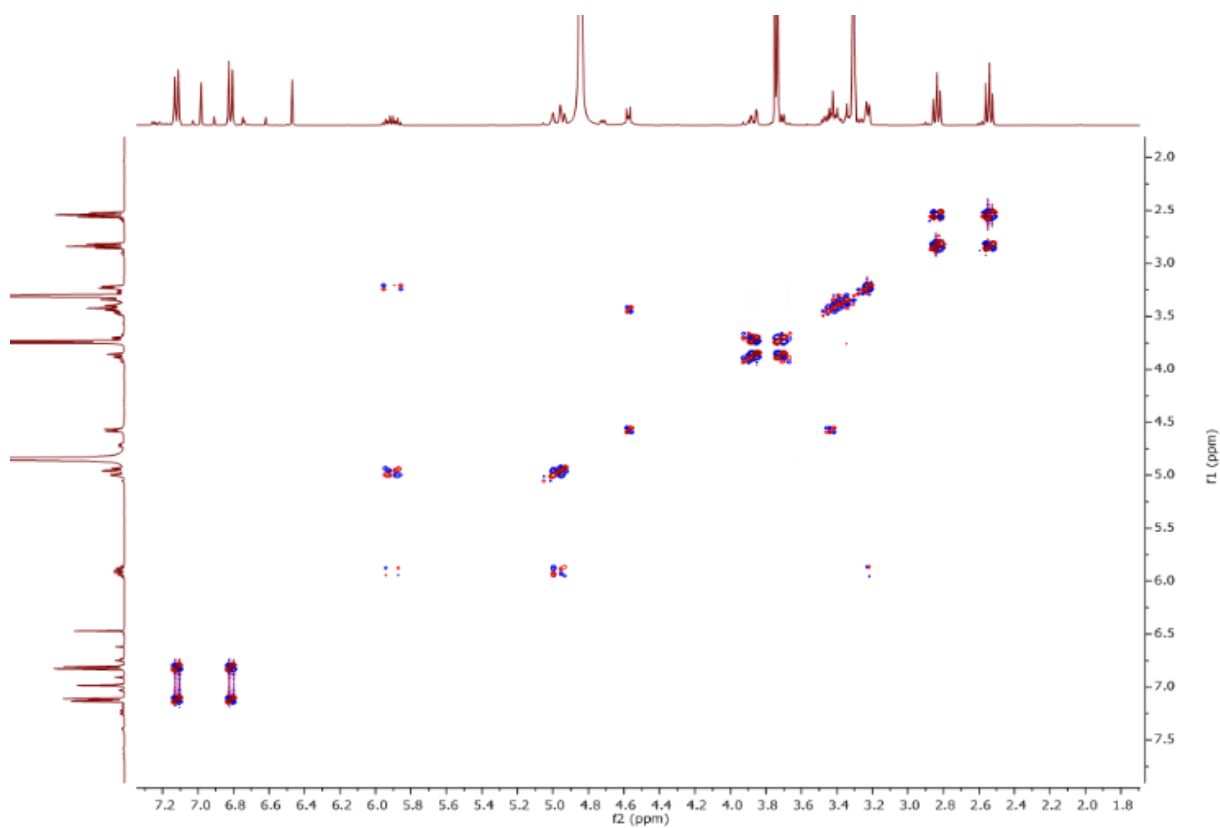


Figure S14: ^1H - ^1H COSY spectrum of compound **2** (400 MHz, MeOH-*d*₄)

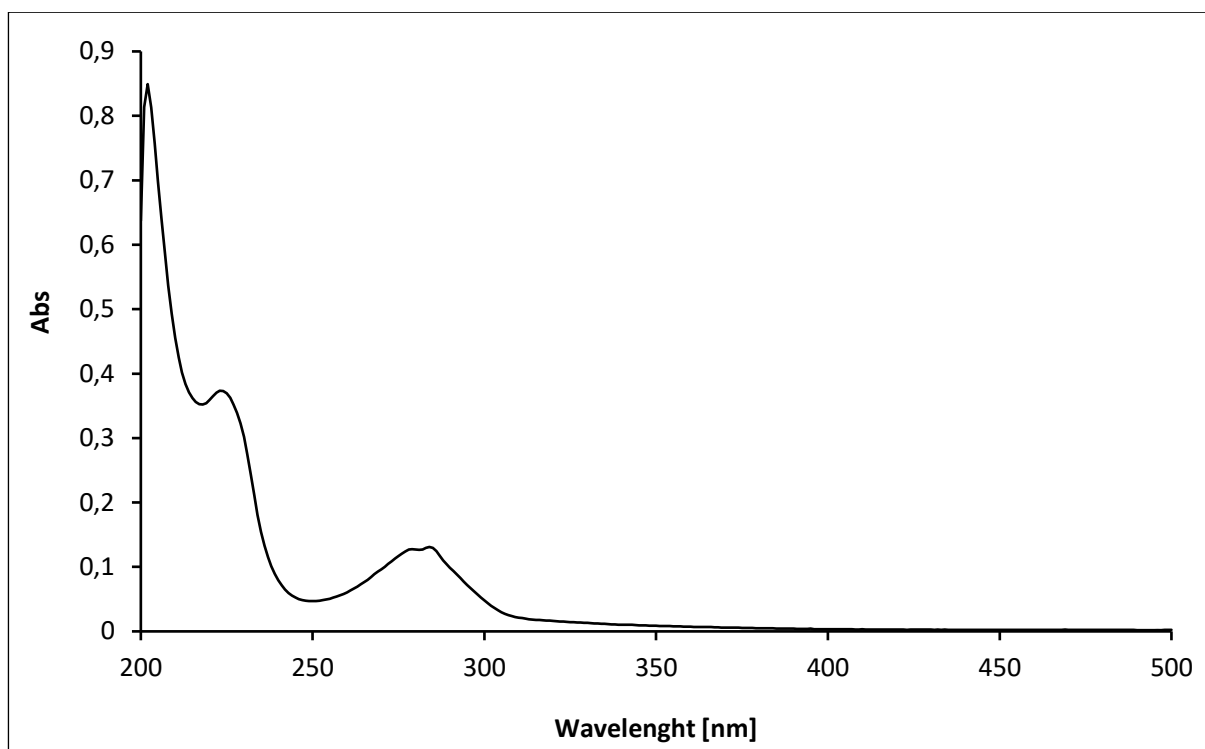


Figure S15: UV spectrum of compound 2 in MeOH

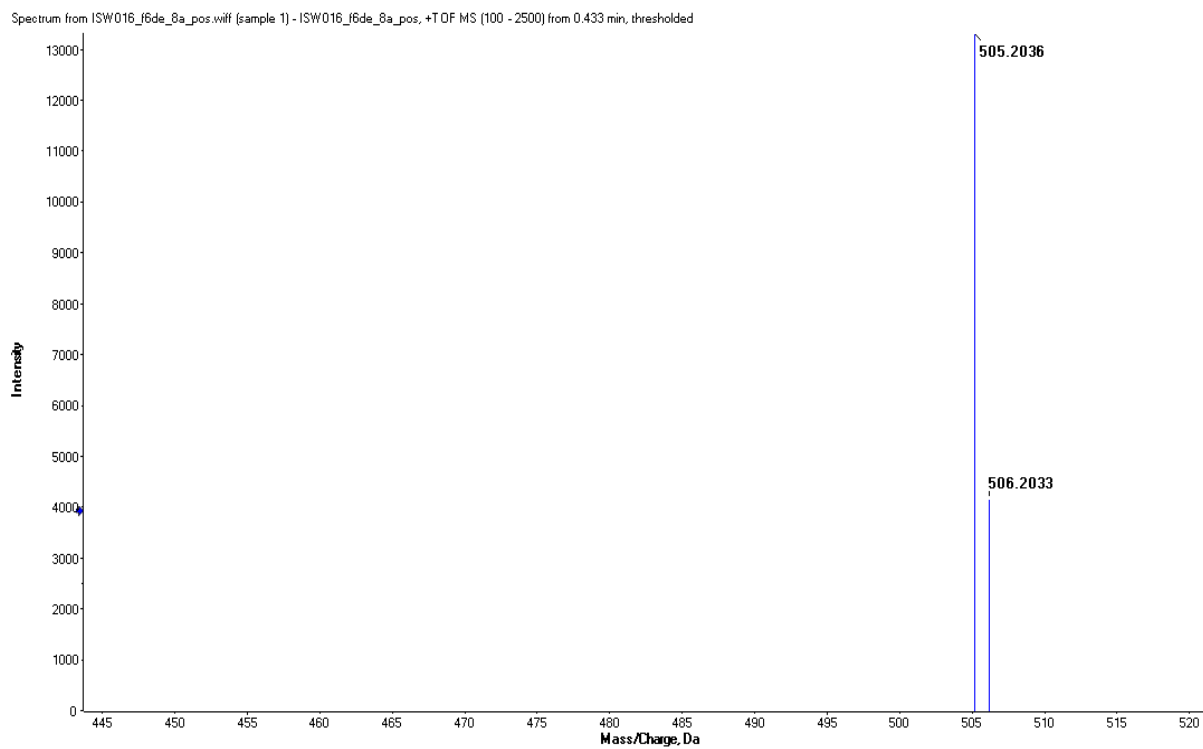


Figure S16: HR-ESI-MS spectrum of compound 2 in positive ion mode

6-*O-trans-p*-Coumaroyl-*D*-glucono-1,4-lactone

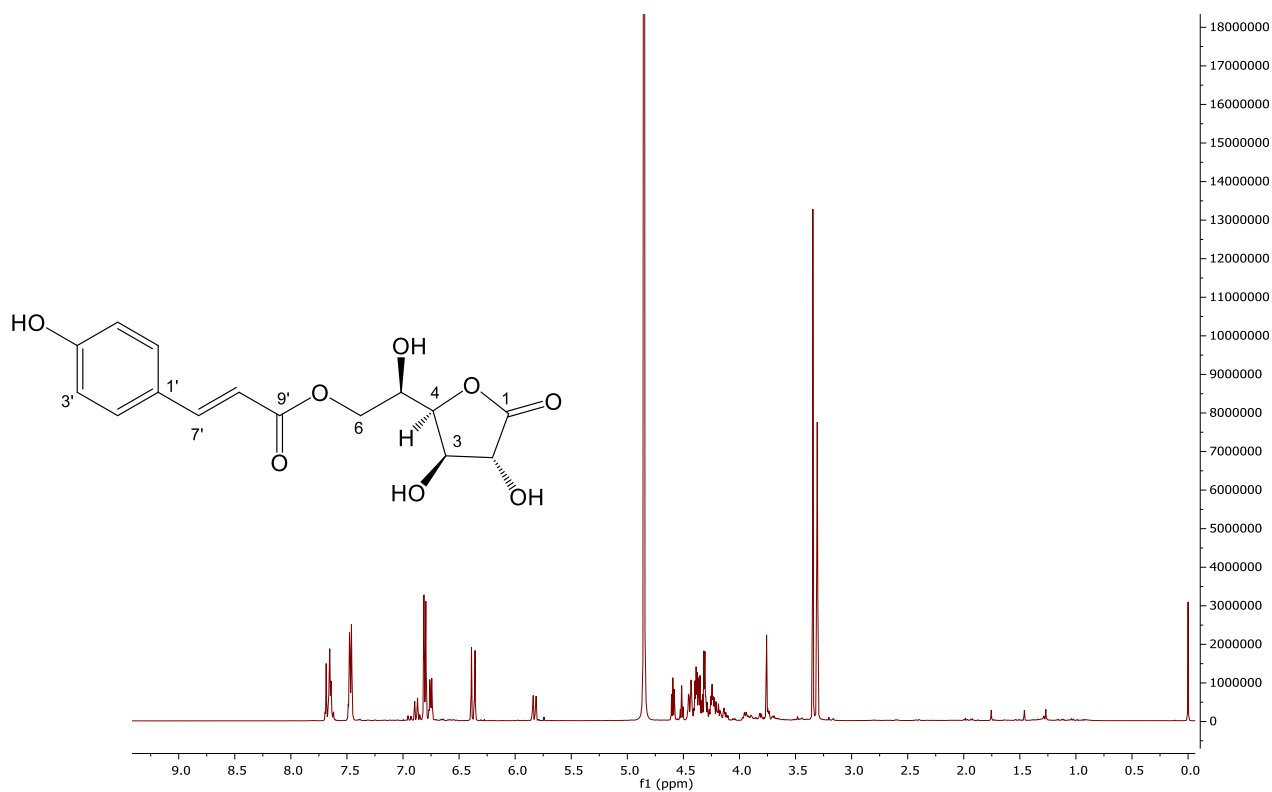


Figure S17: ¹H NMR spectrum of compound 3 (400 MHz, MeOH-*d*₄)

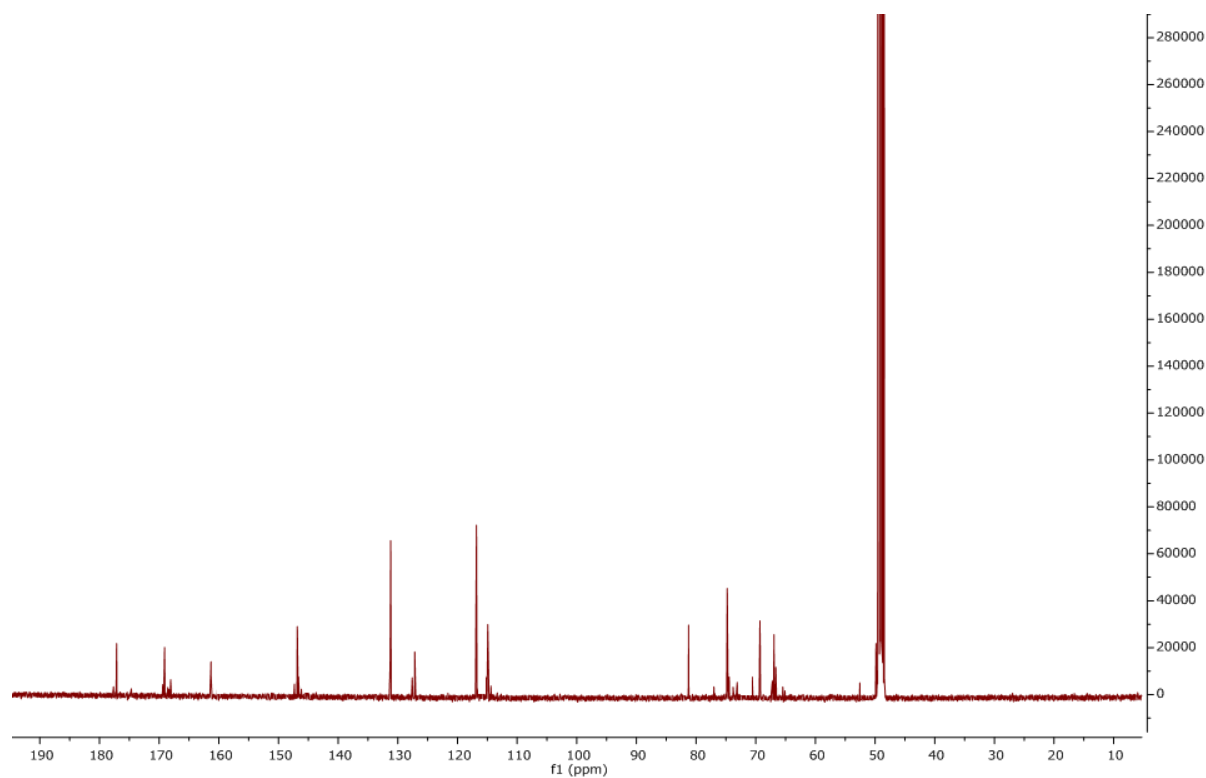


Figure S18: ¹³C NMR spectrum of compound 3 (100 MHz, MeOH-*d*₄)

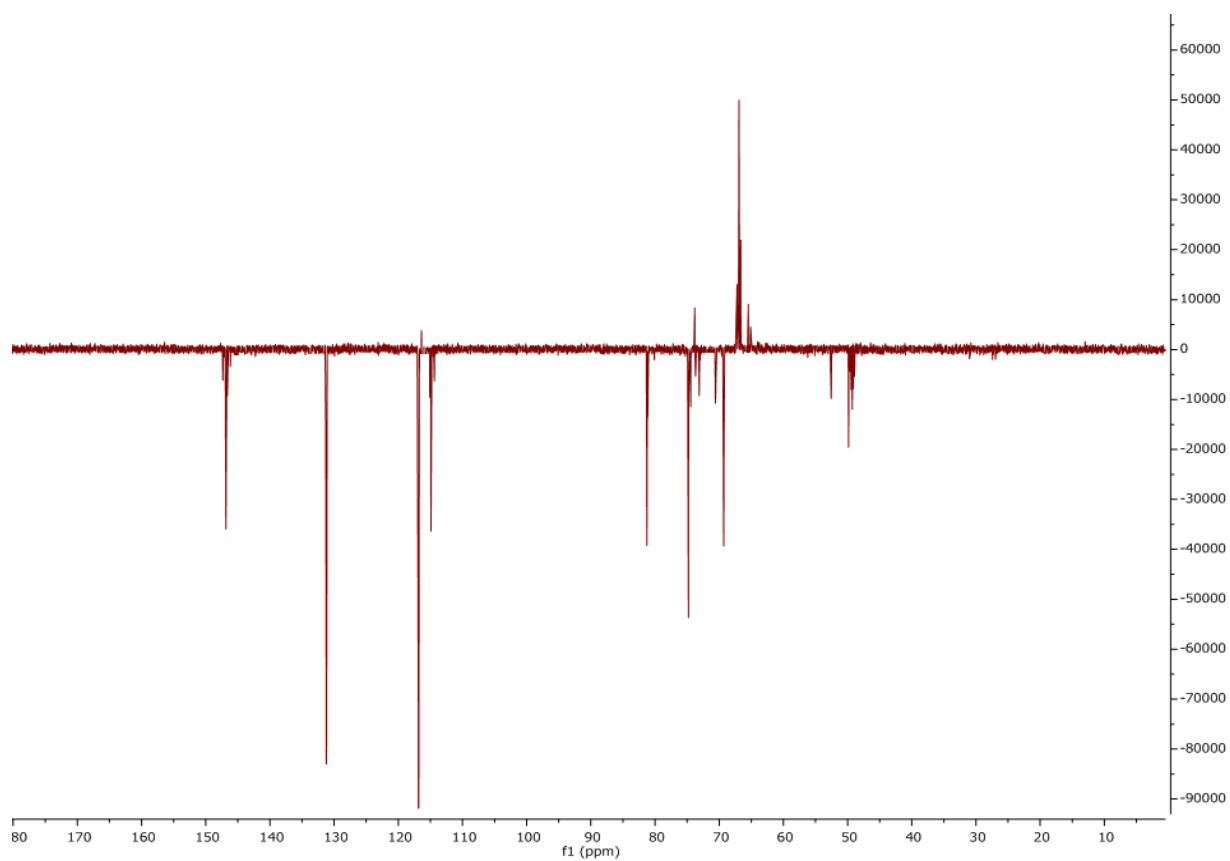


Figure S19: DEPT135 spectrum of compound **3** (100 MHz, MeOH-*d*₄)

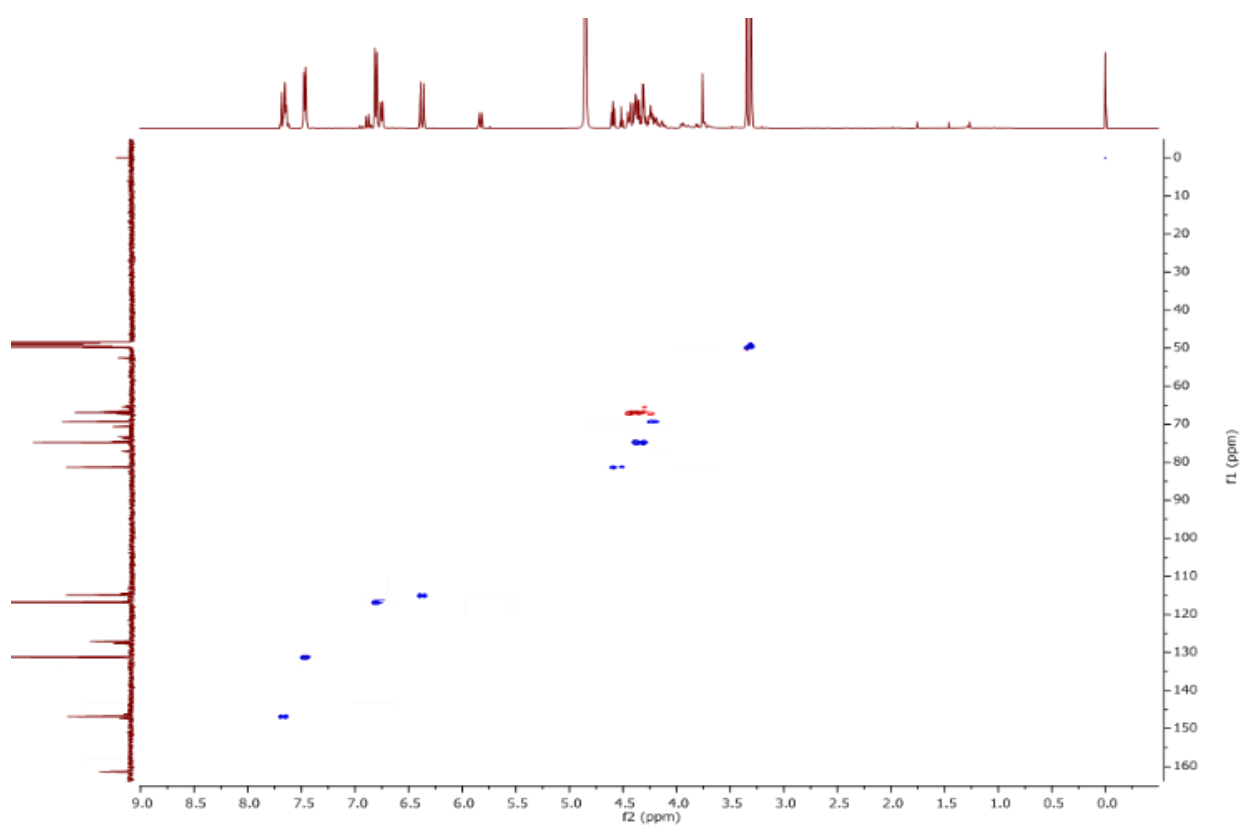


Figure S20: HSQC spectrum of compound **3** (400 MHz, MeOH-*d*₄)

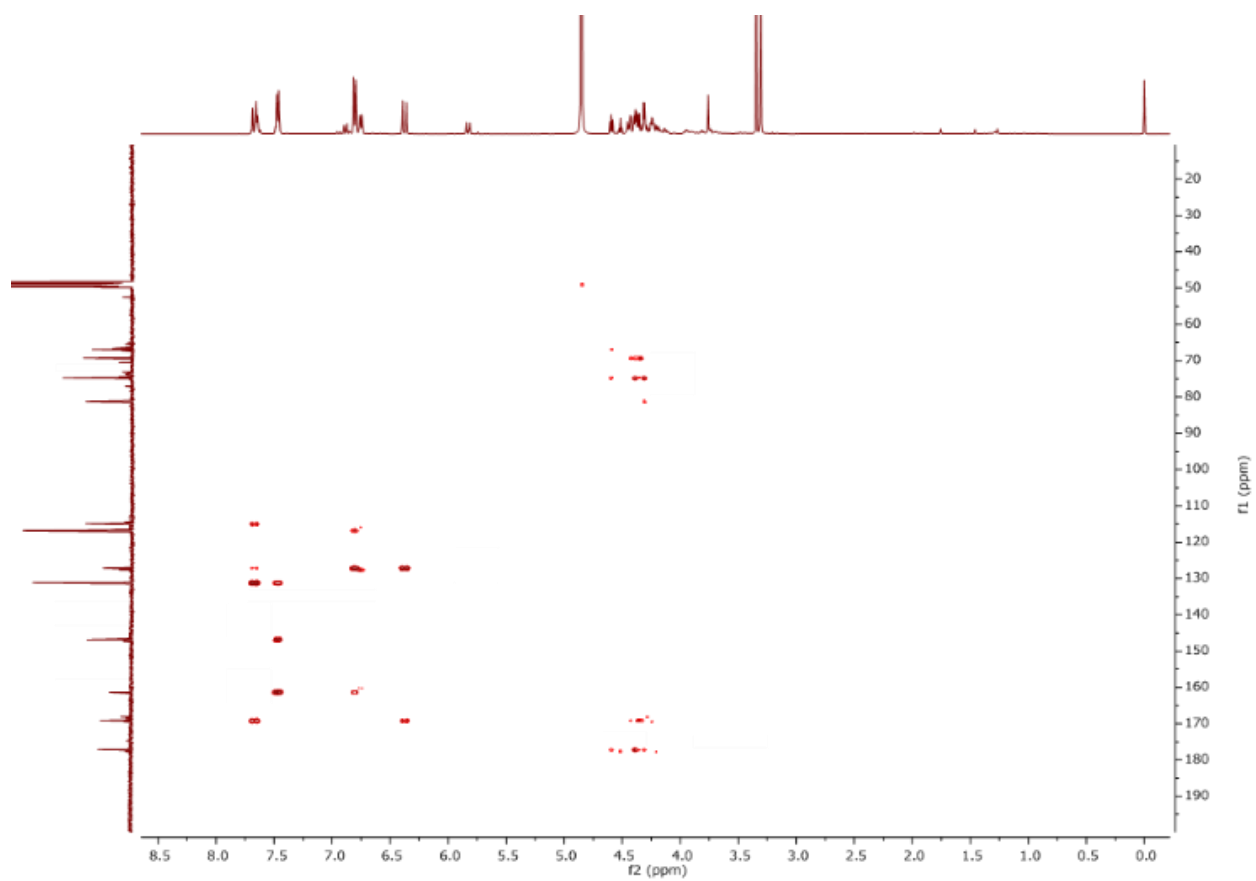


Figure S21: HMBC spectrum of compound **3** (400 MHz, MeOH-*d*₄)

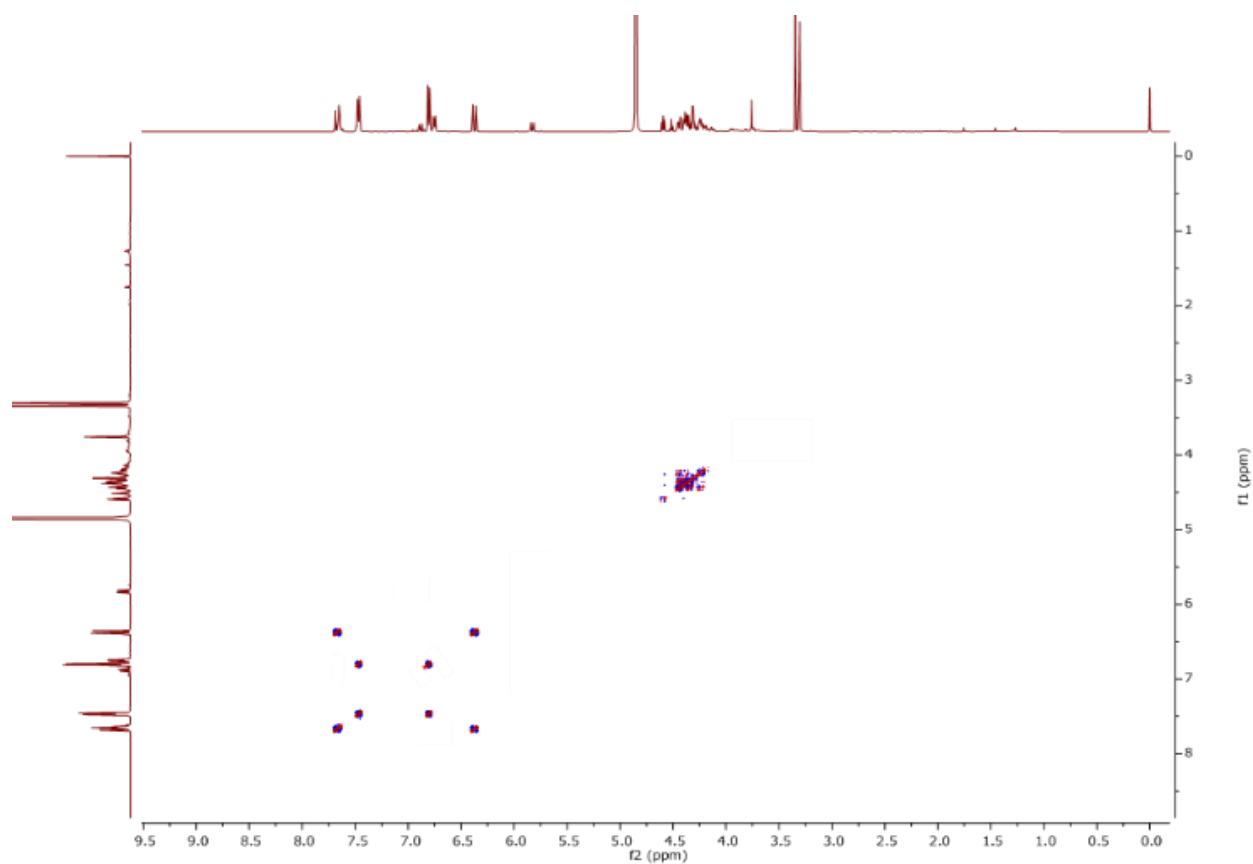


Figure S22: ^1H - ^1H COSY spectrum of compound **3** (400 MHz, MeOH-*d*₄)

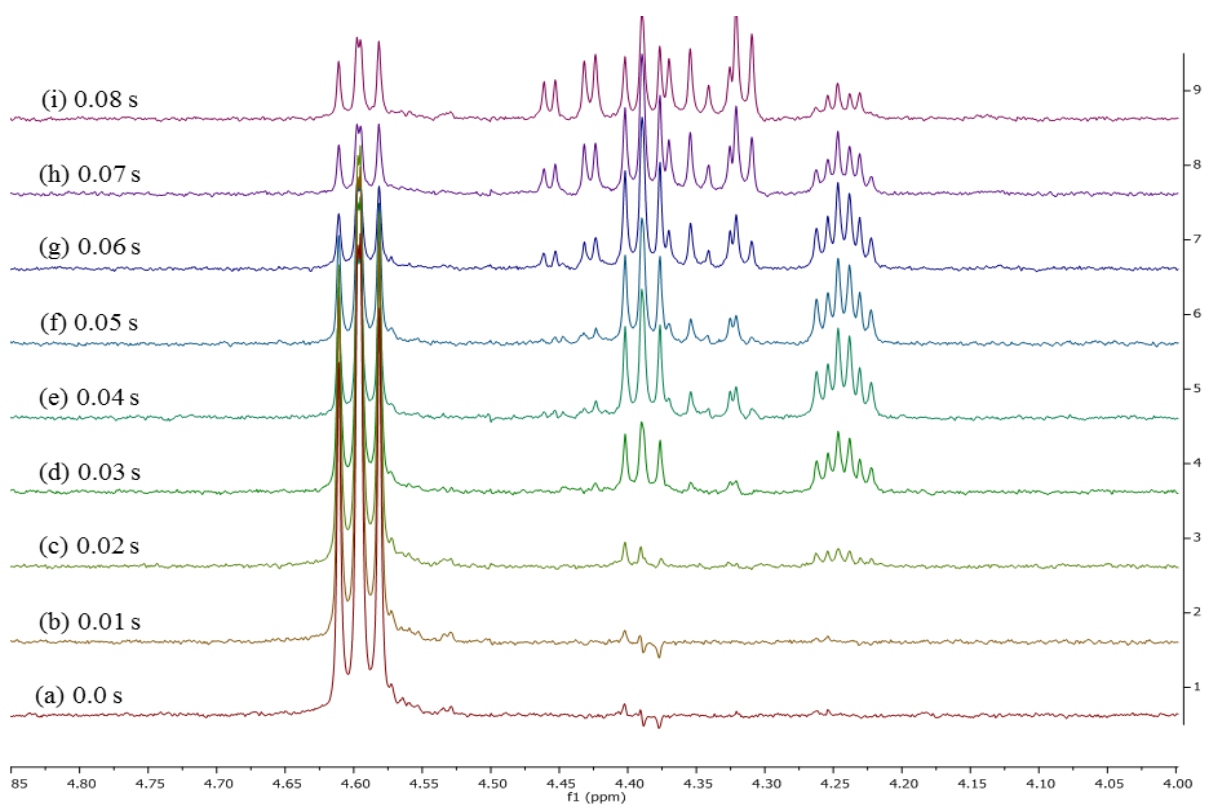


Figure S23: 1D-TOCSY spectrum of compound **3** with selective excitation of H-4 (δ_{H} 4.59) and mixing times (400 MHz, MeOH-*d*₄)

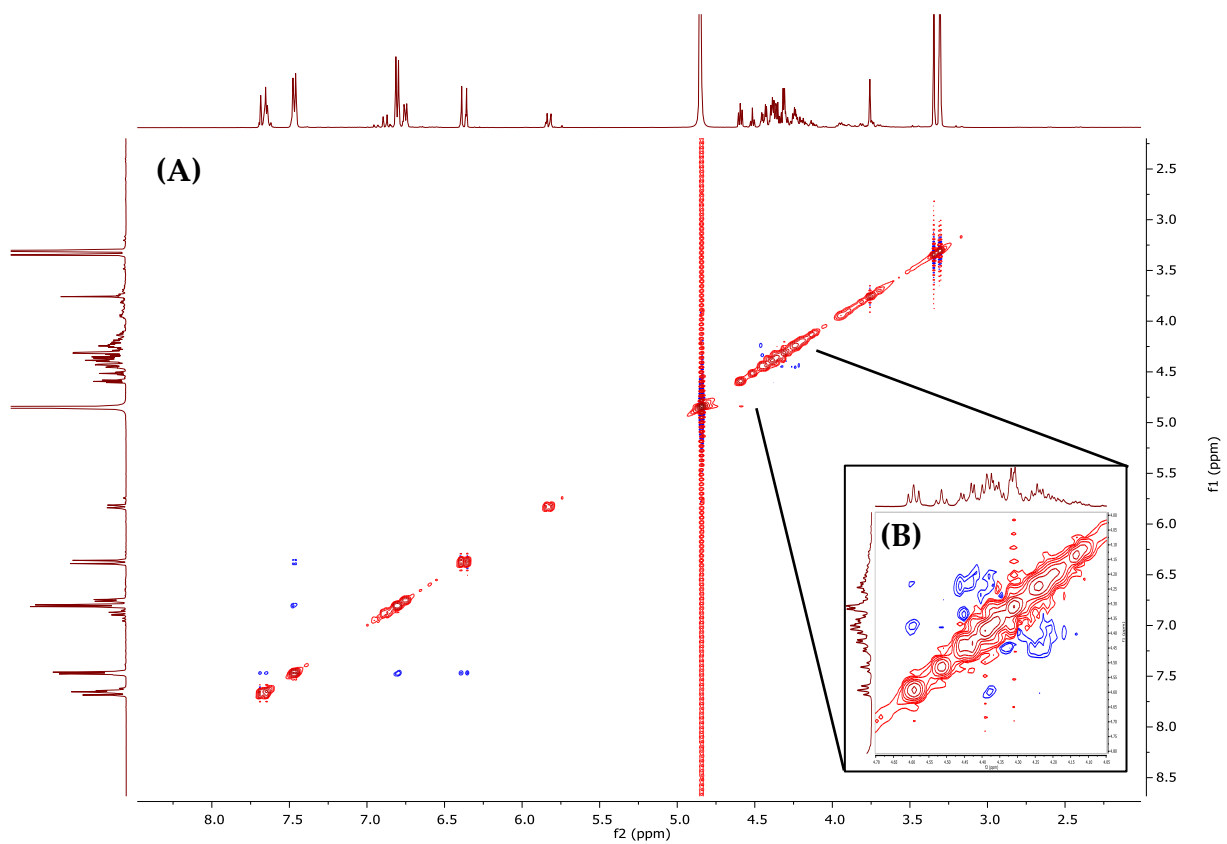
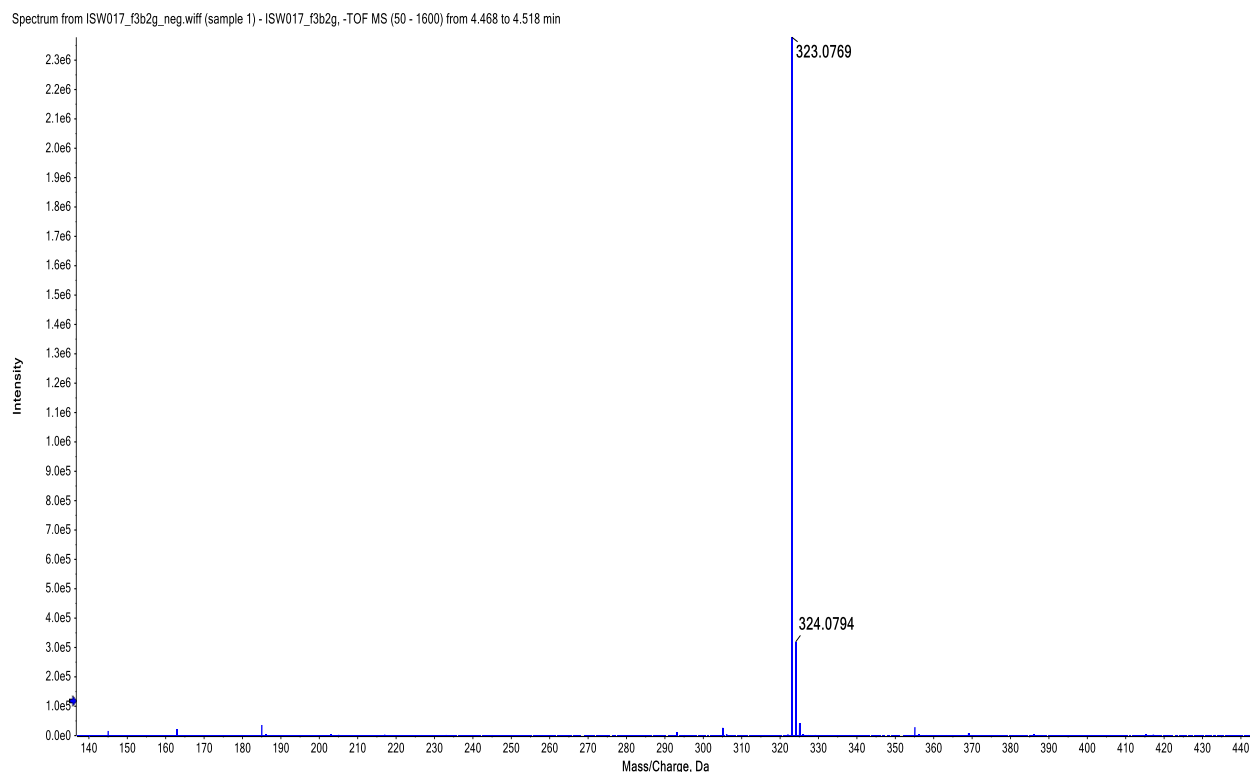


Figure S24: 2D-NOESY spectrum of compound **3**; A) full spectrum, B) glycoside region (400 MHz, MeOH-*d*₄)

Table S2. ^1H and ^{13}C NMR comparison data of compound **3** and similar structure (CD_3OD).

Pos.	Compound 3		Tanaka et al. [37]	
	δ_{H} Mult. J (Hz) (400 MHz)	δ_{C} (100 MHz)	δ_{H} Mult. J (Hz) (600 MHz)	δ_{C} (150 MHz)
1		177.1		176.0
2	4.32 d 4.7	74.8	4.38 d 8.7	75.6
3	4.39 dd 5.4, 4.7	74.9	4.33 t 8.7	74.4
4	4.59 dd 6.3, 5.4	81.3	4.19 dd 8.7, 2.4	81.4
5	4.24 ddd 6.3, 6.3, 3.3	69.3	4.07 m	67.8
6A	4.35 dd 11.7, 3.3	66.9	4.29 dd 11.1, 6.0	65.9
6B	4.44dd 11.7, 6.3	66.9	4.33 dd 11.1, 6.9	65.9
1'		127.2		127.1
2'	7.47 d 8.7	131.2	7.47 d 9.0	131.2
3'	6.81 d 8.7	116.8	6.81 d 9.0	116.8
4'		161.3		161.4
5'	6.81 d 8.7	116.8	6.81 d 9.0	116.8
6'	7.47 d 8.7	131.2	7.47 d 9.0	131.2
7'	7.67 d 16.0	146.9	7.67 d 15.9	147.0
8'	6.38 d 16.0	114.9	6.37 d 15.9	114.8
9'		169.1		168.9

[37] Tanaka, Y.; Yanagida, A.; Komeya, S.; Kawana, M.; Honma, D.; Tagashira, M.; Kanda, T.; Shibusawa, Y. Comprehensive separation and structural analyses of polyphenols and related compounds from bracts of hops (*Humulus lupulus* L.). *J Agric. Food Chem.* **2014**, 62, 2198-2206.

**Figure S25:** HR-ESI-MS spectrum of compound **3** in negative ion mode

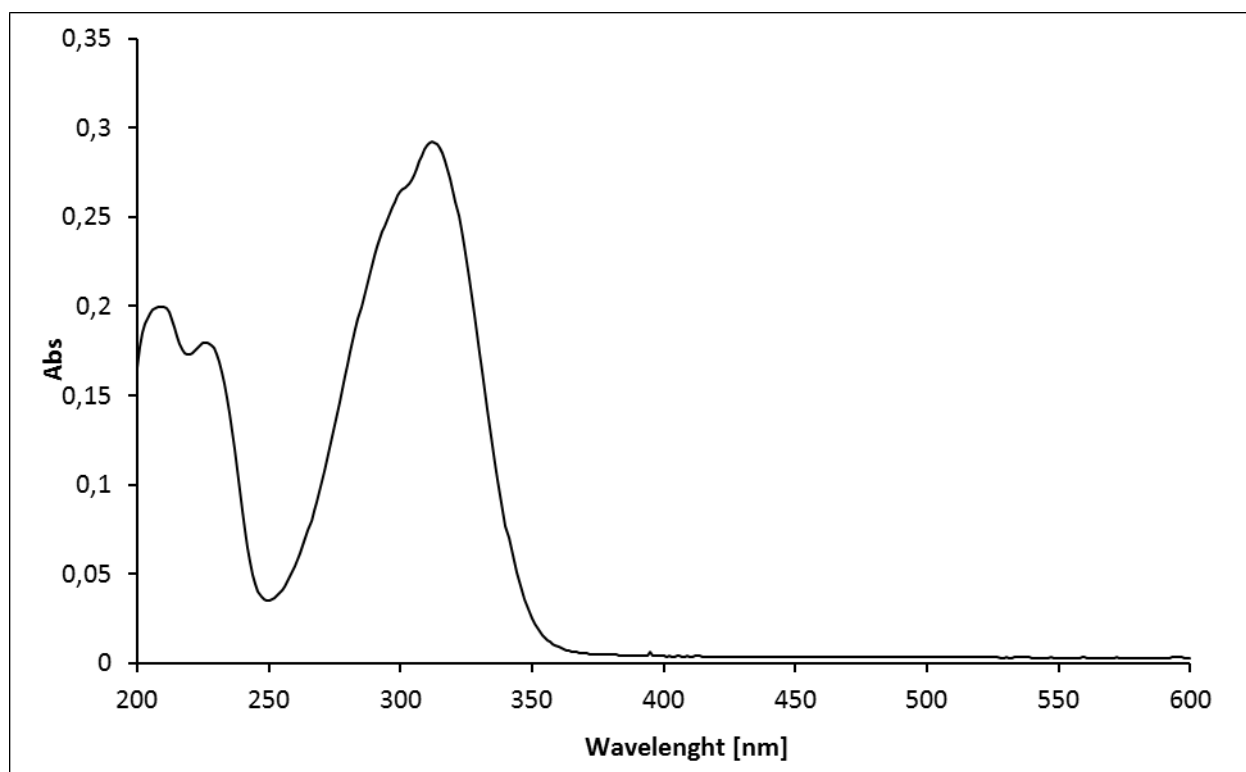


Figure S26: UV spectrum of compound **3** in MeOH

Table S3: Polarimeter data of compound **3**.

Light Source	WI
Wavelength	589 nm
Sample Aperture	Ø 3.0
Light Aperture	Ø 1.0
D.I.T.	5 sec
Cycle Times	20
Cycle Interval	5 sec
Path Length	50 mm
Concentration	0.247 W/V%
Factor	1.0000
Temp. Correct	0
Sample	ISW017_f3b2g
Comment	2.47 mg / 1 ml Methanol
Optical Rotation	
Average	0.0050 deg
S.D.	0.0002 deg
R.S.D.	4.2827 %
Specific O.R.	
Average	4.0445
S.D.	0.1732
Temperatur	23.2° C

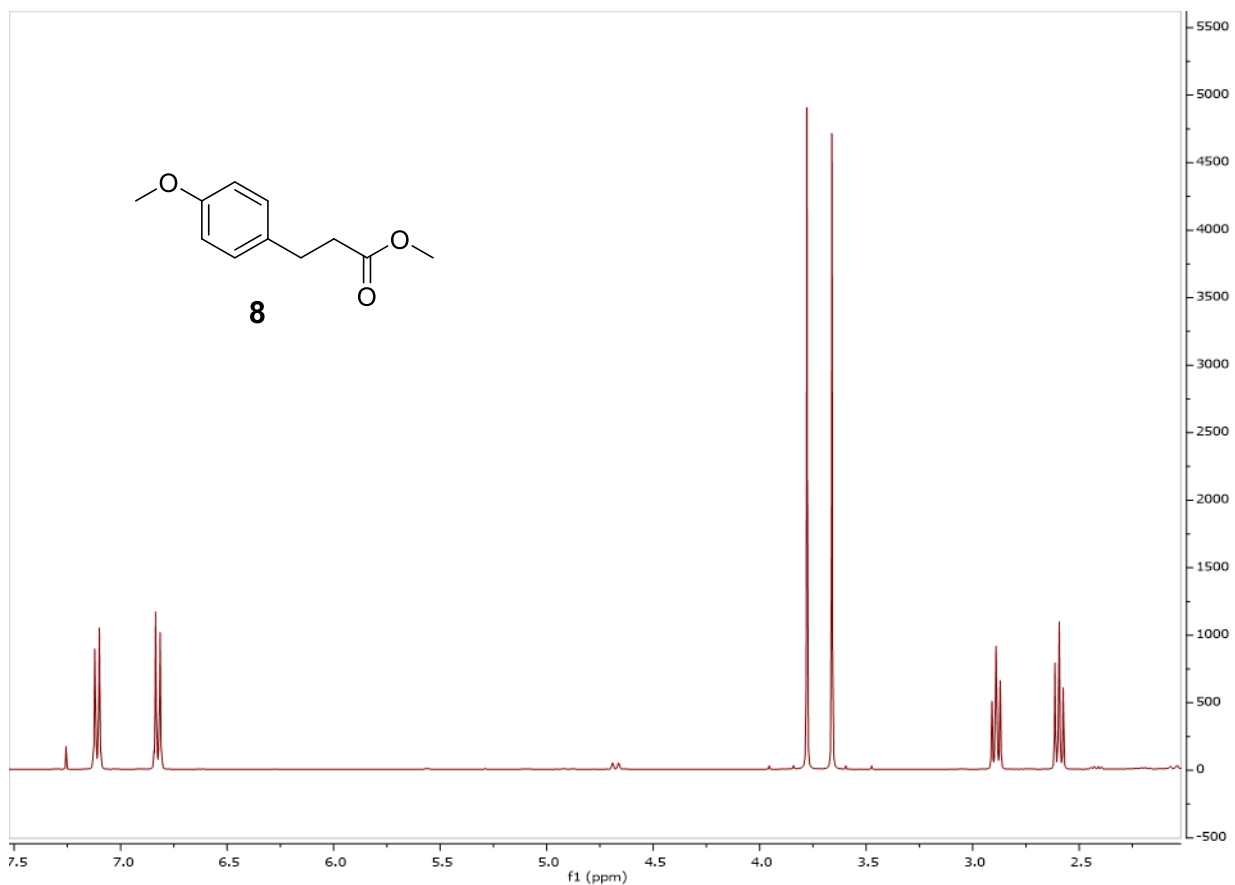


Figure S27: ¹H NMR spectrum of compound **8** (400 MHz, CDCl₃)

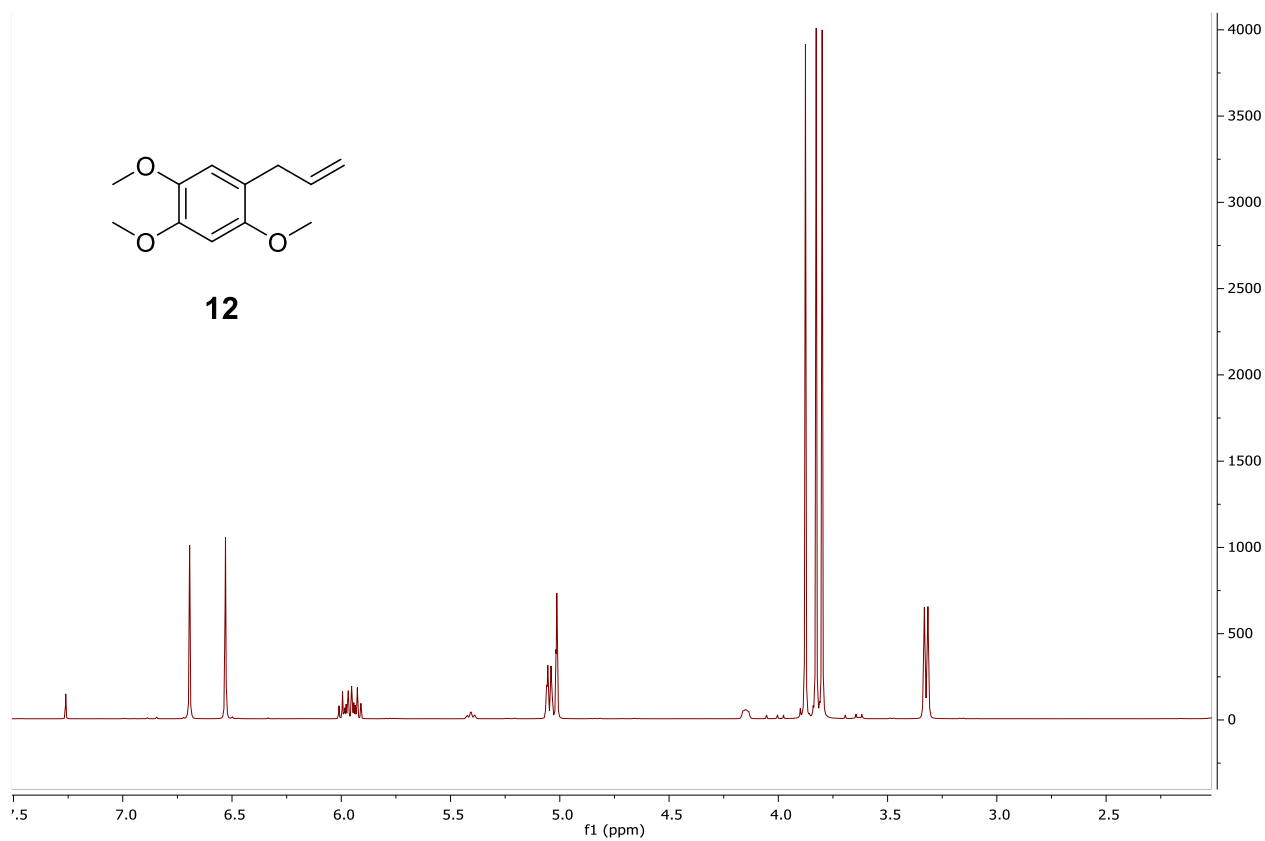


Figure S28: ¹H NMR spectrum of compound **12** (400 MHz, CDCl₃)

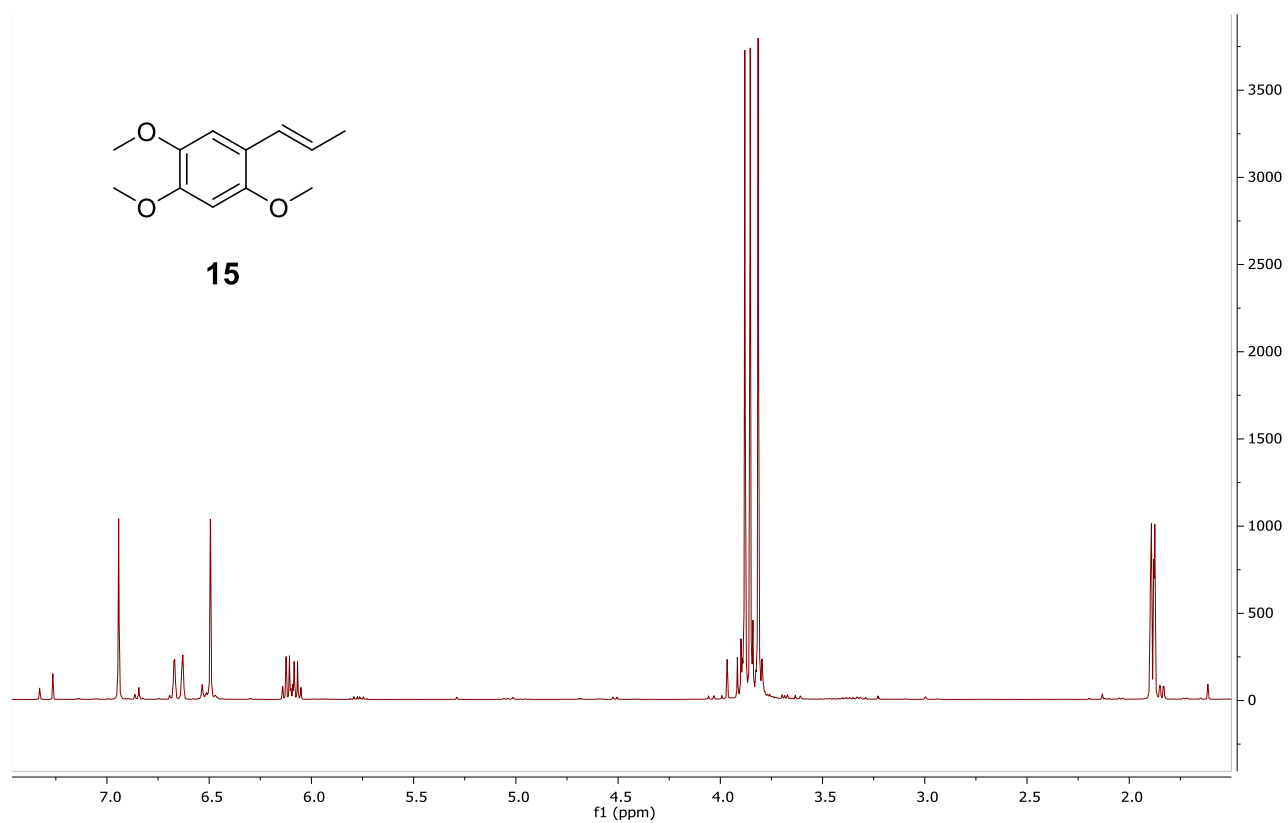


Figure S29: ¹H NMR spectrum of compound **15** (400 MHz, CDCl₃)

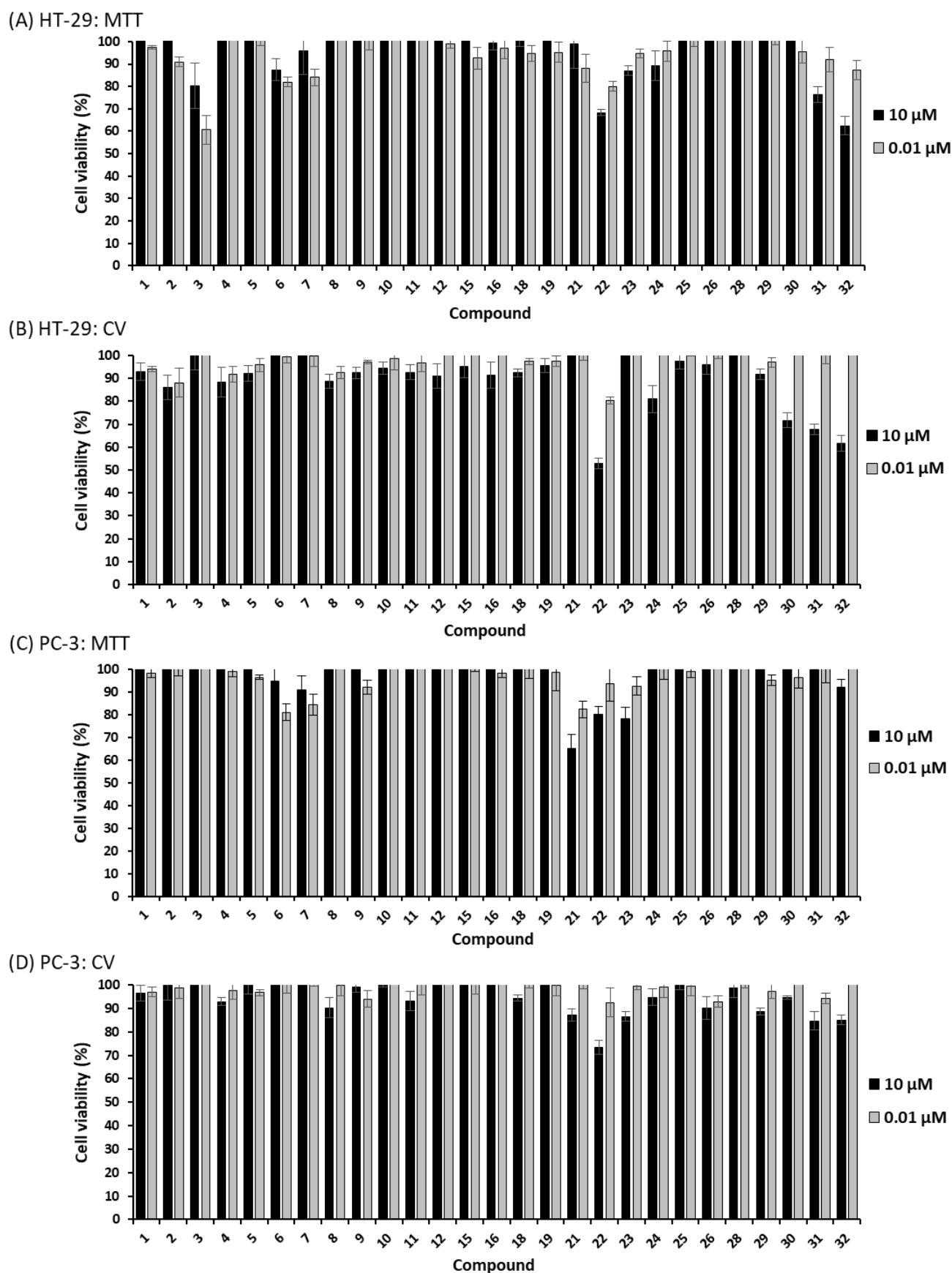


Figure S30: Antiproliferative and cytotoxic activities (MTT and CV) of compounds isolated from *P. sarmentosum* against human colorectal (HT-29) and prostate (PC-3) cancer cell lines. Digitonin (125 µM) was used as positive control compromising the cells to the point of 0% of cell viability after 48 h (data not shown).