SUPPLEMENTARY MATERIAL

Title: New Iridoid Glycosides from *Anarrhinum pubescens*

Authors:

Ehab Mahran[a,b], Mohammed Hosny[b], Atef El-Hela[b] and Arezue Boroujerdi[a]

Affiliations:

[a]*Chemistry Department, Claflin University, Orangeburg, SC 29115, USA*

[b]*Department of Pharmacognosy, Faculty of Pharmacy, Al-Azhar University, Cairo 11371, Egypt*

Corresponding author:

Arezue Boroujerdi

Address: 898 Goff Ave, Orangeburg, SC 29115, USA

Phone: +1 (803) 5355536 Fax: +1 (803) 535 5776

e-mail: aboroujerdi@claflin.edu

Abstract:

Six metabolites (**1**-**6**) were isolated from the aerial parts of *Anarrhinum pubescens* Fresen. (Plantaginaceae) growing in Saint Catherine region in Egypt; two of them (**1** and **4**) are here reported to be newly identified naturally occurring iridoids. The isolated metabolites were identified as 6-*O*-foliamenthoyl-(6'-*O*-cinnamoyl)-antirrhinoside (**1**), 6'-*O*-cinnamoyl-antirrhinoside (**2**), the iridoid dimer, pubescensoside (**4**), antirrhinoside (**5**), 10-hydroxy-antirrhinoside (**6**), and the flavonoid, diosmin (**3**). Identification of the new metabolites was based on analysis of their collected spectroscopic data (NMR and HR-ESI-MS). Furthermore, compounds (**1, 4,** and **5**) were subjected to cytotoxic testing against the human lung carcinoma cell line (A-549); compound **4** showed better cytotoxic activity as indicated by the obtained (IC_{50}).

Keywords:

Iridoids, *Anarrhinum pubescens*, Plantaginaceae, and Secondary Metabolites.

Table S1. ^{1}H and ^{13}C NMR data of compound 1 and 4 in (CD_3OD, δ in ppm).

Compound (1)						Compound (4)					
Position	δ_H multi(*J* in Hz)	δ_C	Position	δ_H multi(*J* in Hz)	^{13}C	Position	δ_H multi(*J* in Hz)	δ_C	Position	δ_H multi(*J* in Hz)	^{13}C
1	5.24 d (7.75)	94.0	**Cinnamoyl**			**Part (a)**			**part (b)**		
3	6.35 d (6.25)	141.47	**1"**	-	166.9	**1a**	5.27 d (3.5)	94.1	**1b**	5.25 d (5.6)	94.1
4	4.86 d (6.25)	106.0	**2"**	6.57 d (16.01)	117.0	**3a**	6.1 dd (6.29, 1.91)	139.54	**3b**	7.4 d (0.9)	150.9
5	-	73.0	**3"**	7.72 d (16.01)	145.0	**4a**	4.7 *	106.0	**4b**	-	111.8
6	4.94 d (1.64)	78.6	**4"**	-	134.0	**5a**	2.84 m	29.08	**5b**	3.17 m	31.0
7	3.48 br.s	62.63	**5" & 9"**	7.39 m	128.66	**$6a_1$**	1.72 m	39.0	**$6b_1$**	2.27 m	29.61
8	-	62.61	**6" & 8"**	7.61 m	127.96	**$6a_2$**	1.82 m	39.0	**$6b_2$**	1.36 m	
9	2.42 d (7.75)	52.27	**7"**	7.74 m	130.0	**7a**	4.48 br.t (4.5)	72.7	**7b**	1.66 t (7.8)	38.0
10	1.45 s	16.24	**Foliamenthoyl**			**8a**	-	152.0	**8b**	-	79.5
Glucose			**1'"**	-	167.4	**9a**	2.93 br.m	43.8	**9b**	2.1 dd (8.5, 5.6)	51.0
1'	4.7 d (7.9)	98.0	**2'"**	-	127.24	**$10a_1$**	5.31 t (2.23)	110.23	**10b**	1.29 s	23.0
2'	3.25 m	73.0	**3'"**	6.86 td (7.4, 1.3)	142.6	**$10a_2$**	5.18 t (2.23)		**11b**	-	167.3
3'	3.40 m	76.0	**4'"**	2.33 q (15.29, 7.65)	27.1	**1'a**	4.65 d (8.0)	98.2	**1'b**	4.74 d (7.9)	98.4
4'	3.38 m	70.0	**5'"**	2.23 t (7.65)	30.1	**2'a**	3.22 m	73.39	**2'b**	3.24 m	73.40
5'	3.59 m	74.0	**6'"**	-	137.2	**3'a**	3.38 m	76.44	**3'b**	3.39 m	76.44
6'a	4.53 dd (12.01, 2.5)	63.07	**7'"**	5.4 br.t (6.9)	125.12	**4'a**	3.33 m	70.39	**4'b**	3.38 m	70.21
6'b	4.41 dd (12.01, 6.1)		**8'"**	4.05 d (6.9)	57.75	**5'a**	3.48 m	74.23	**5'b**	3.57 m	74.27
			9'"	1.84 s	11.1	**$6'a_1$**	4.16 dd (11.9, 6.0)	62.93	**$6'b_1$**	4.14 dd (11.9, 5.9)	62.76
			10'"	1.76 s	22.08	**$6'a_2$**	4.52 dd (11.9, 2.2)		**$6'b_2$**	4.55 dd (11.9, 2.3)	
									1"b	-	166.9
									2"b	6.52 d (16.1)	117.3
									3"b	7.70 d (16.1)	145.2
									4"b	-	134.0
									5"b,9"b	7.60 m	127.9
									6"b,8"b	7.41 m	128.7
									7"b	7.44 m	130.2

* Overlapped

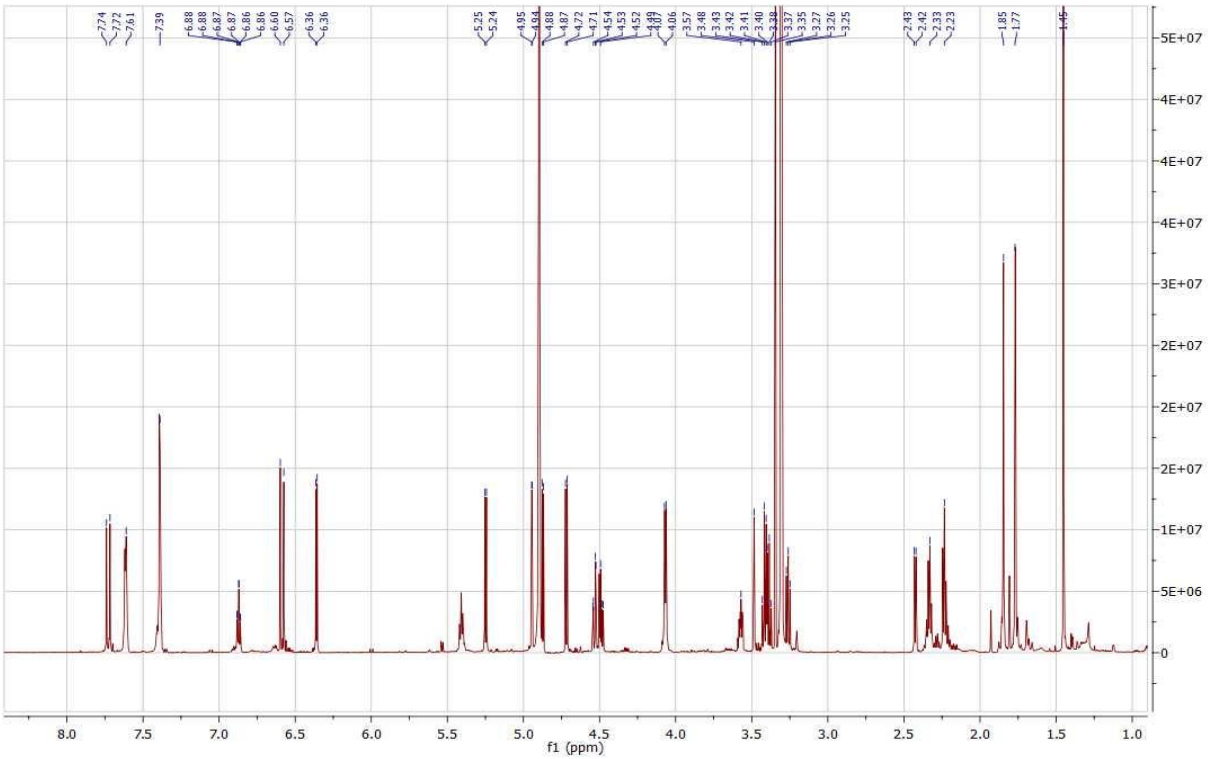

Figure S2: ^{1}H NMR spectrum (700 MHz) of compound 1 (in CD3OD)

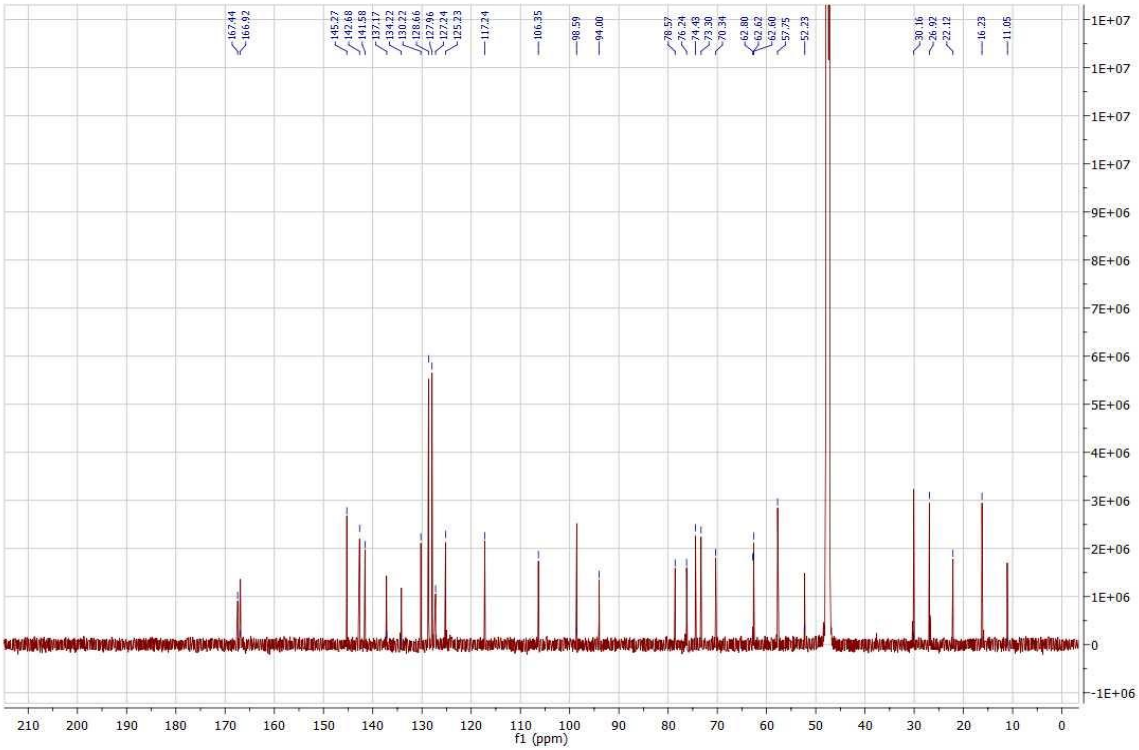

Figure S3: ^{13}C NMR (175 MHz) spectrum of compound 1 (in CD3OD)

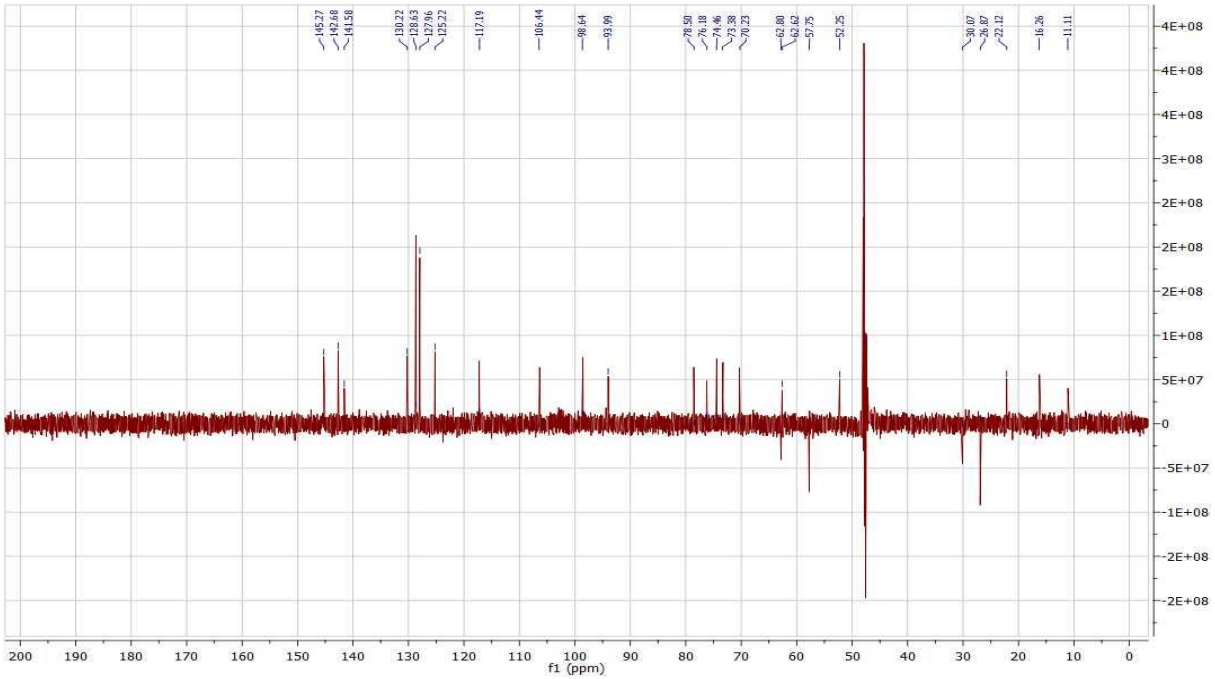

Figure S4: DEPT spectrum of compound 1

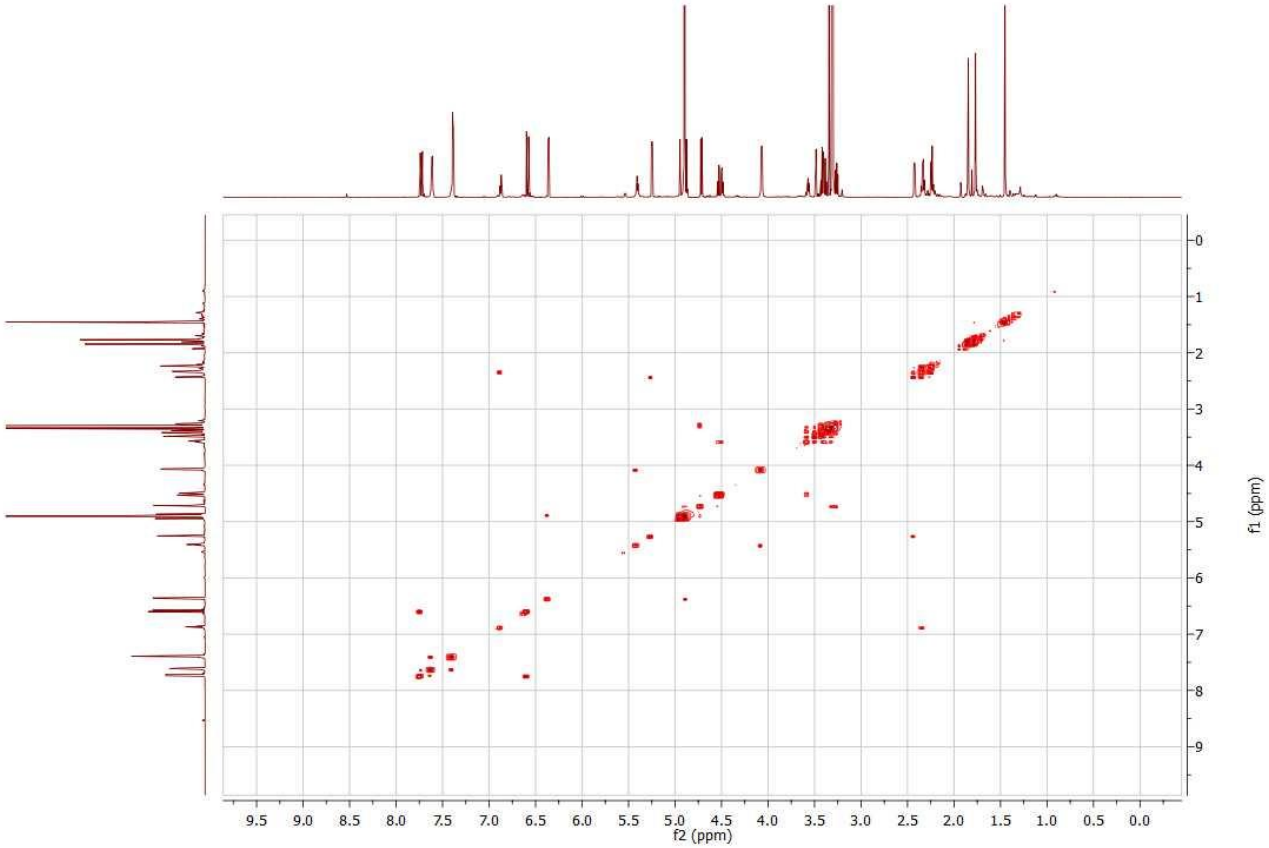

Figure S5: ^{1}H-^{1}H COSY spectrum of compound 1

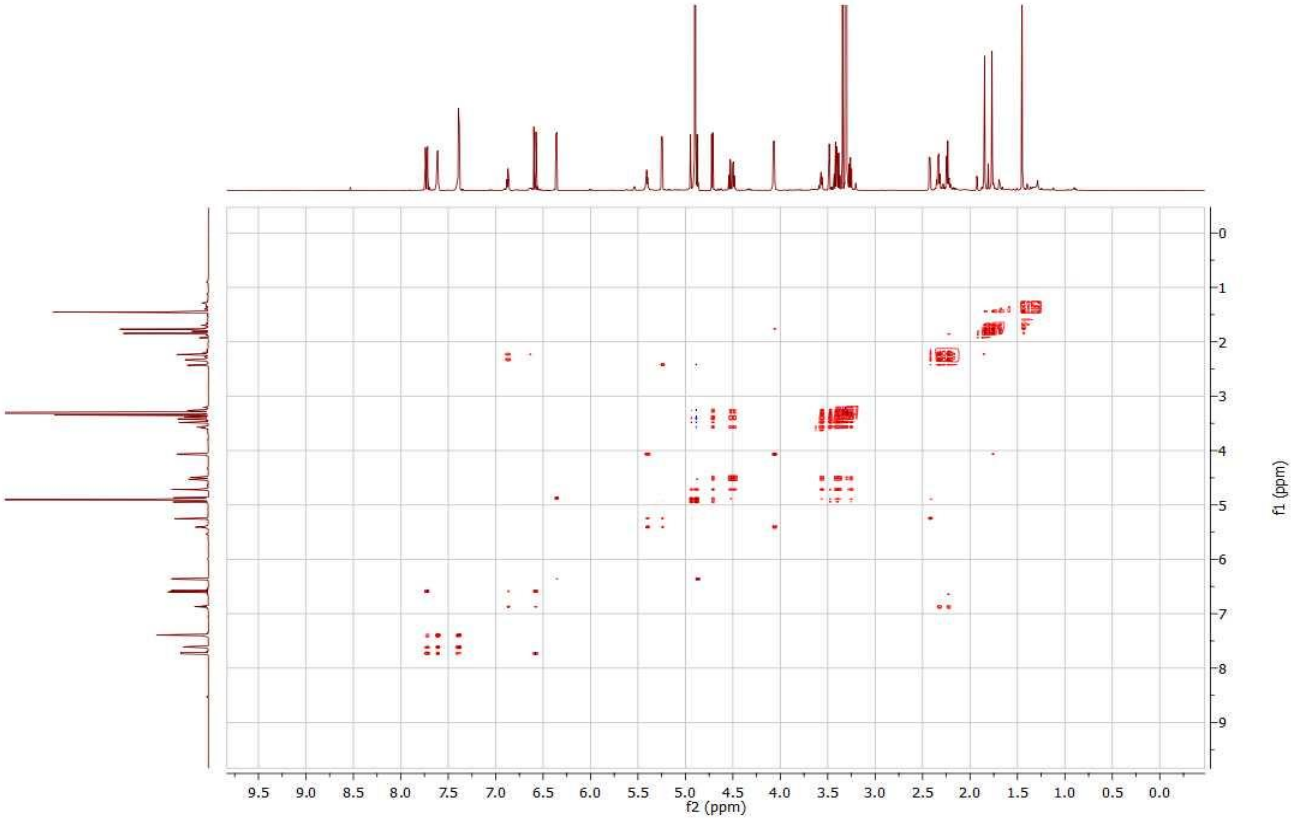

Figure S6: TOCSY spectrum of compound 1

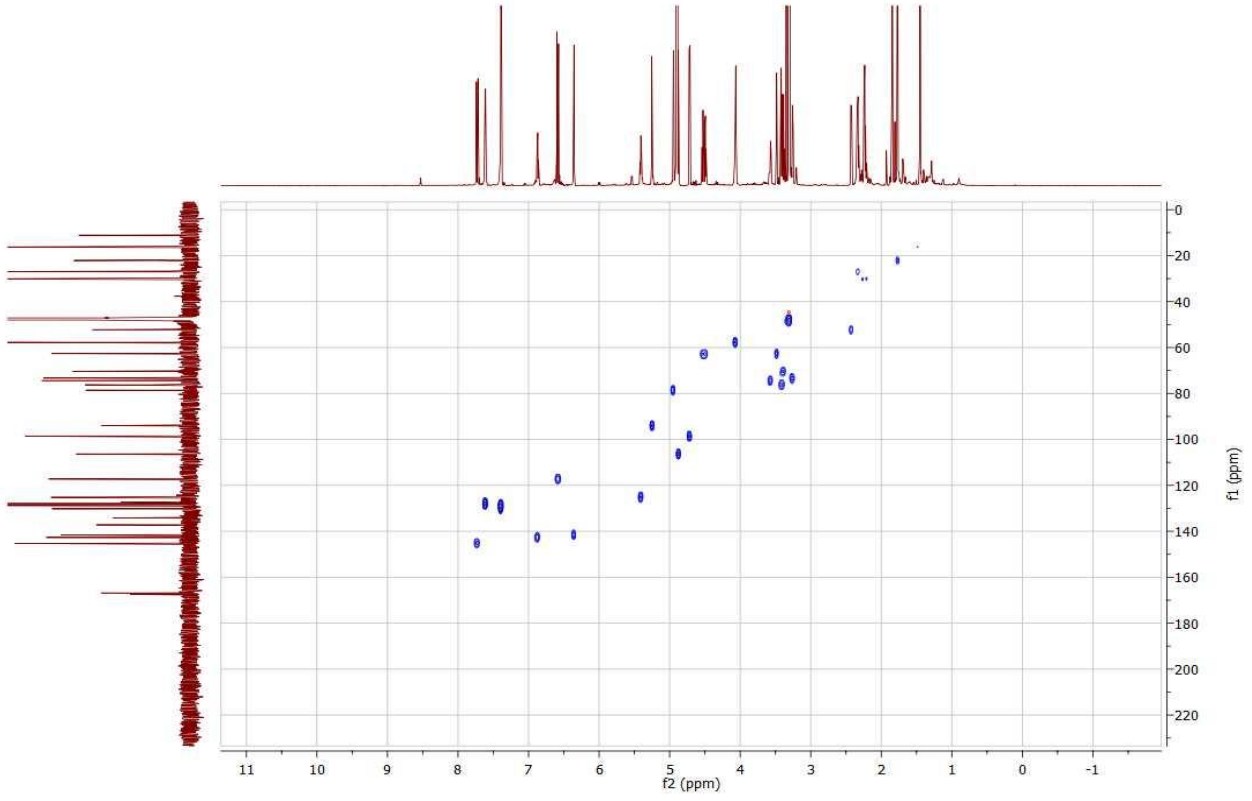

Figure S7: HSQC spectrum of compound 1

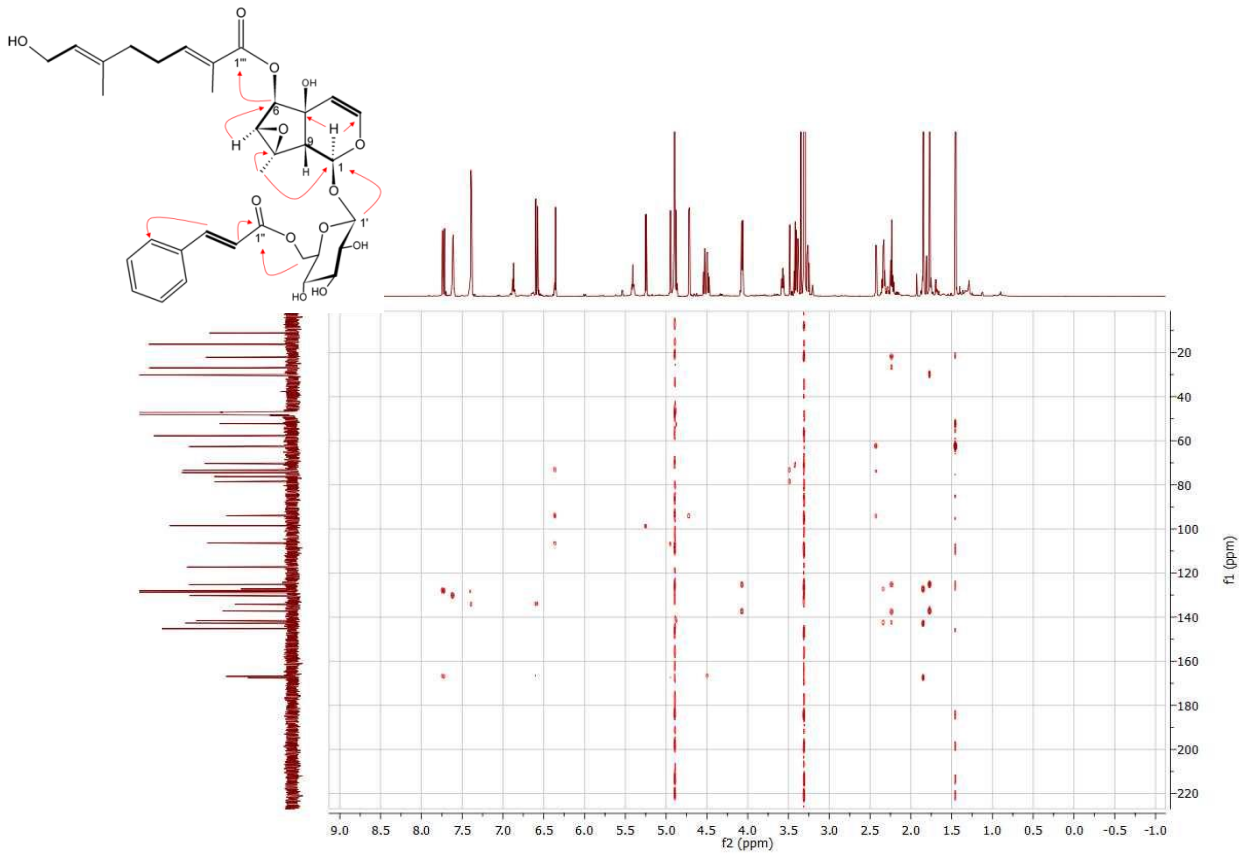

Figure S8: HMBC spectrum of compound 1

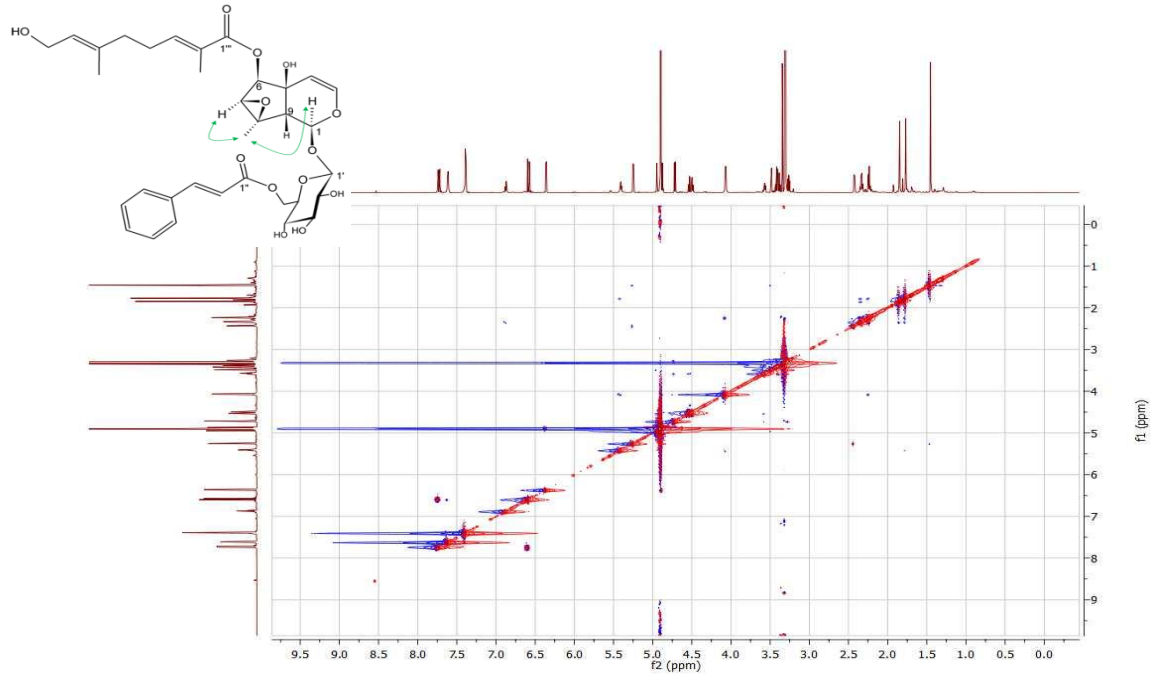

Figure S9: 2D-NOESY spectrum of compound 1

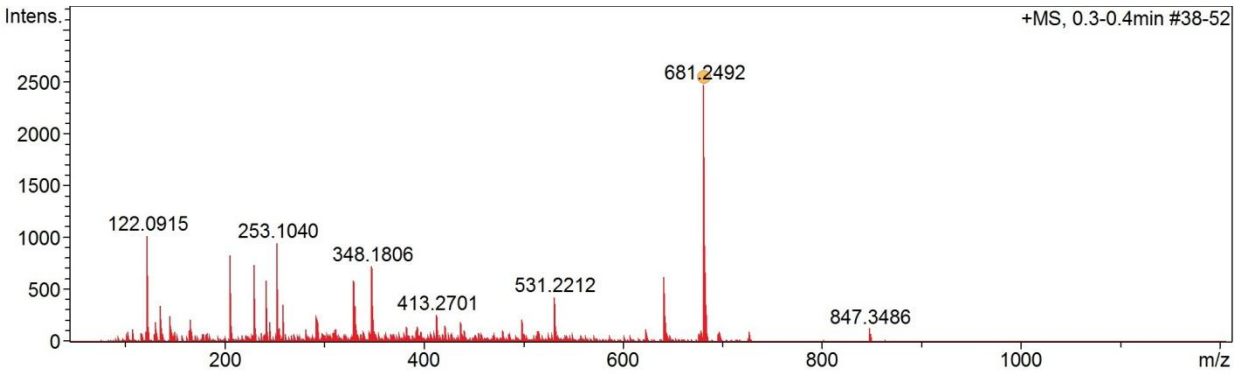

Figure S10: HR-MS of compound 1

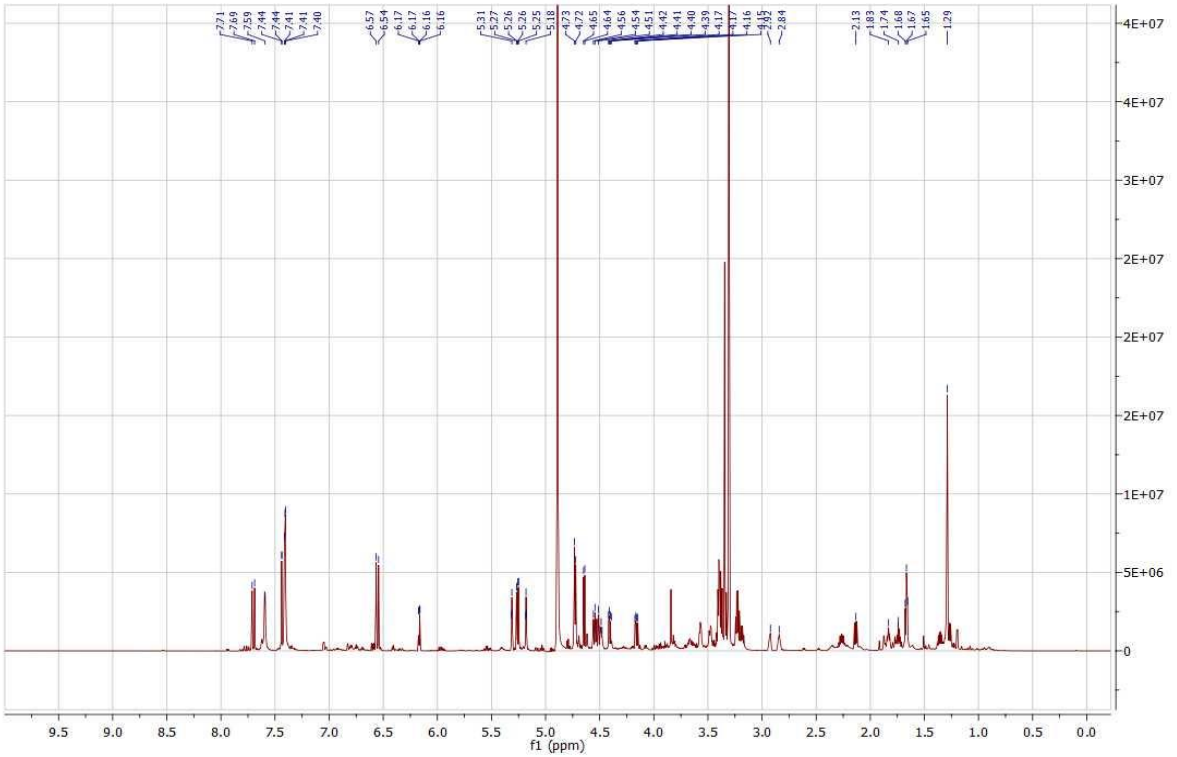

Figure S11: ^{1}NMR (700 MHz) spectrum of compound 4 in CD_3OD

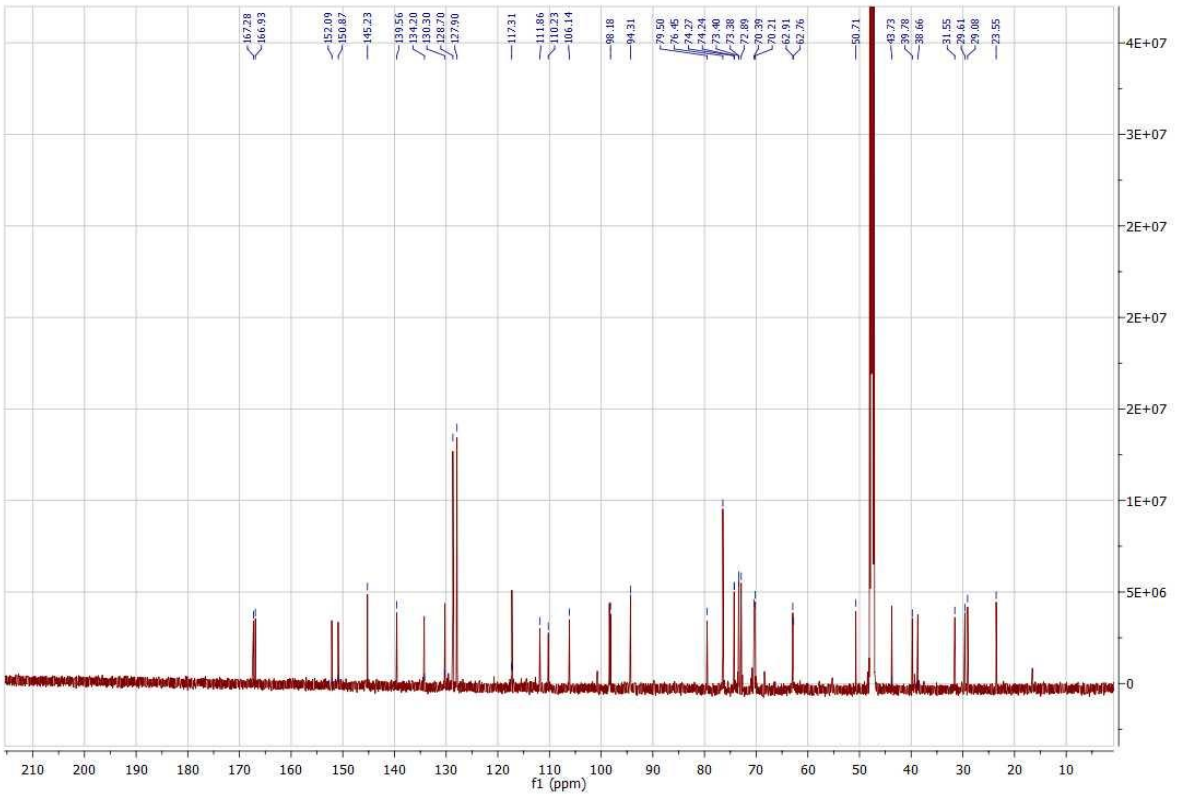

Figure S12: ^{13}C NMR (175 MHz) spectrum of compound 4 in CD_3OD

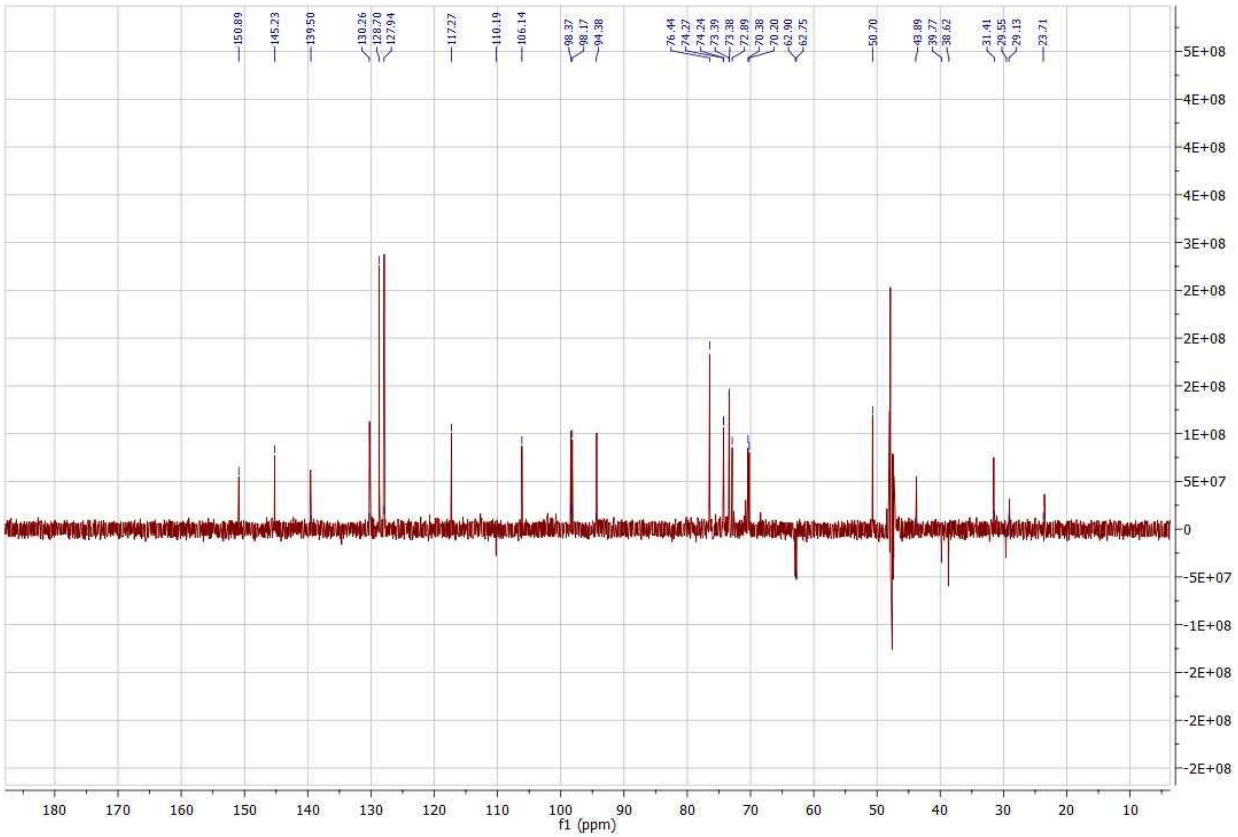

Figure S13: DEPT spectrum of compound 4

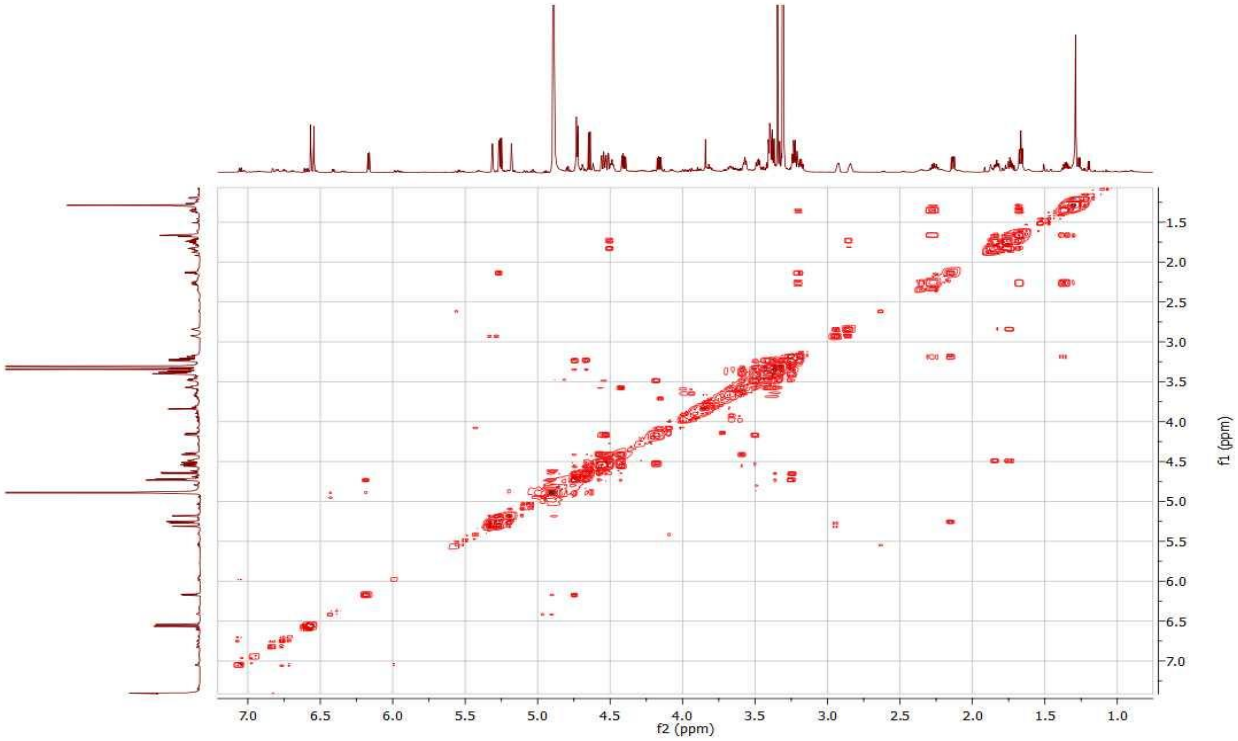

Figure S14: ^{1}H-^{1}H COSY spectrum of compound 4

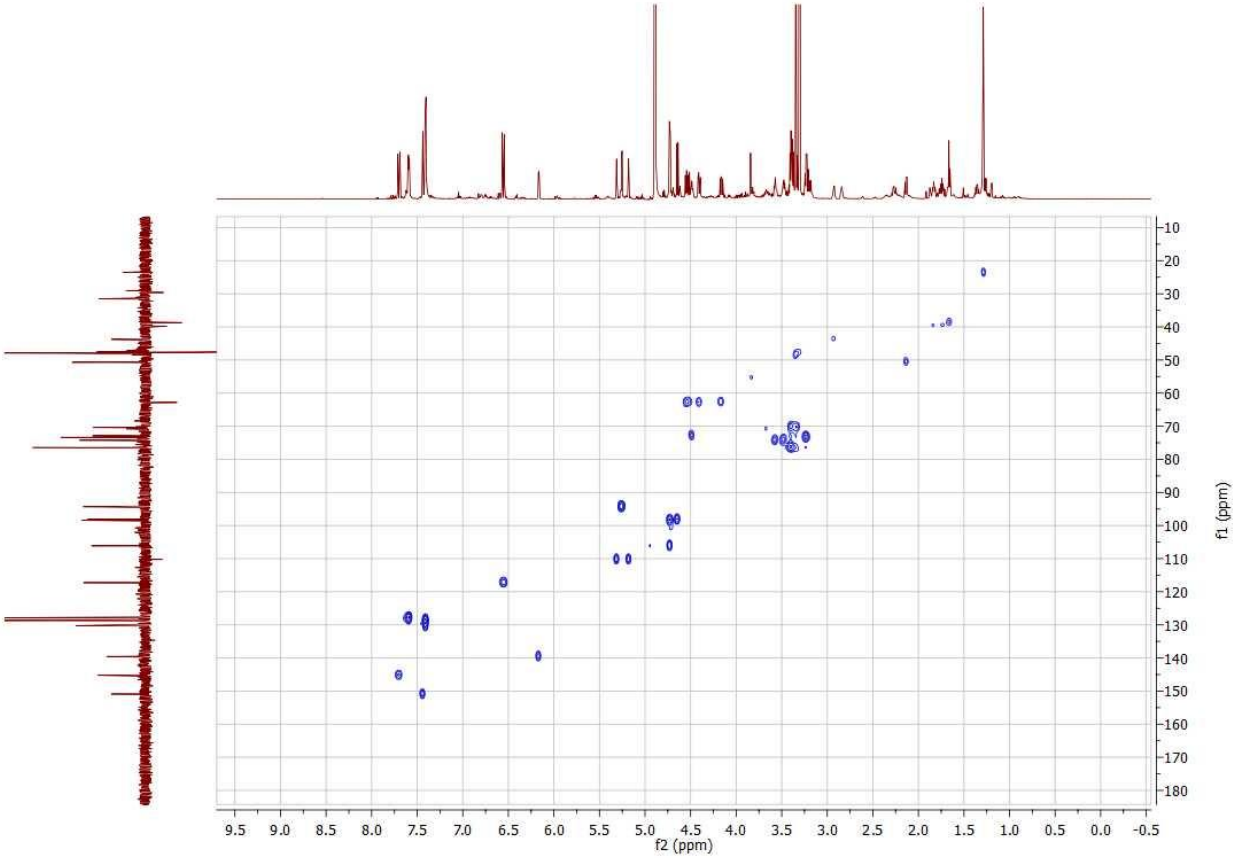

Figure S15: HSQC spectrum of compound 4

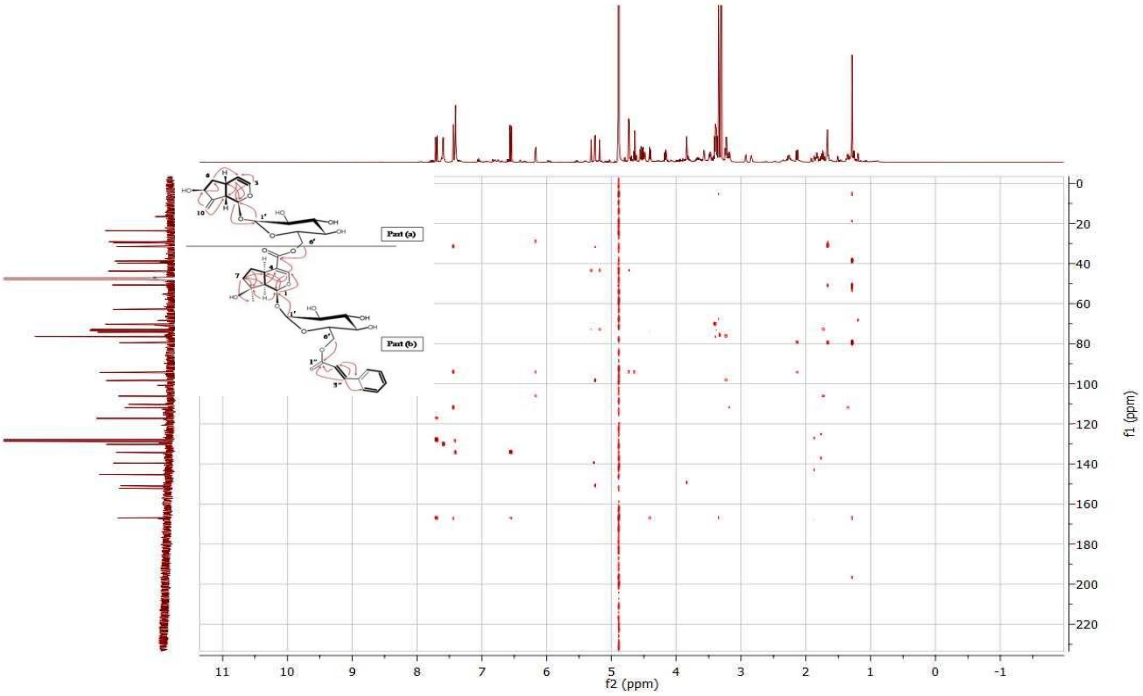

Figure S16: HMBC spectrum of compound 4

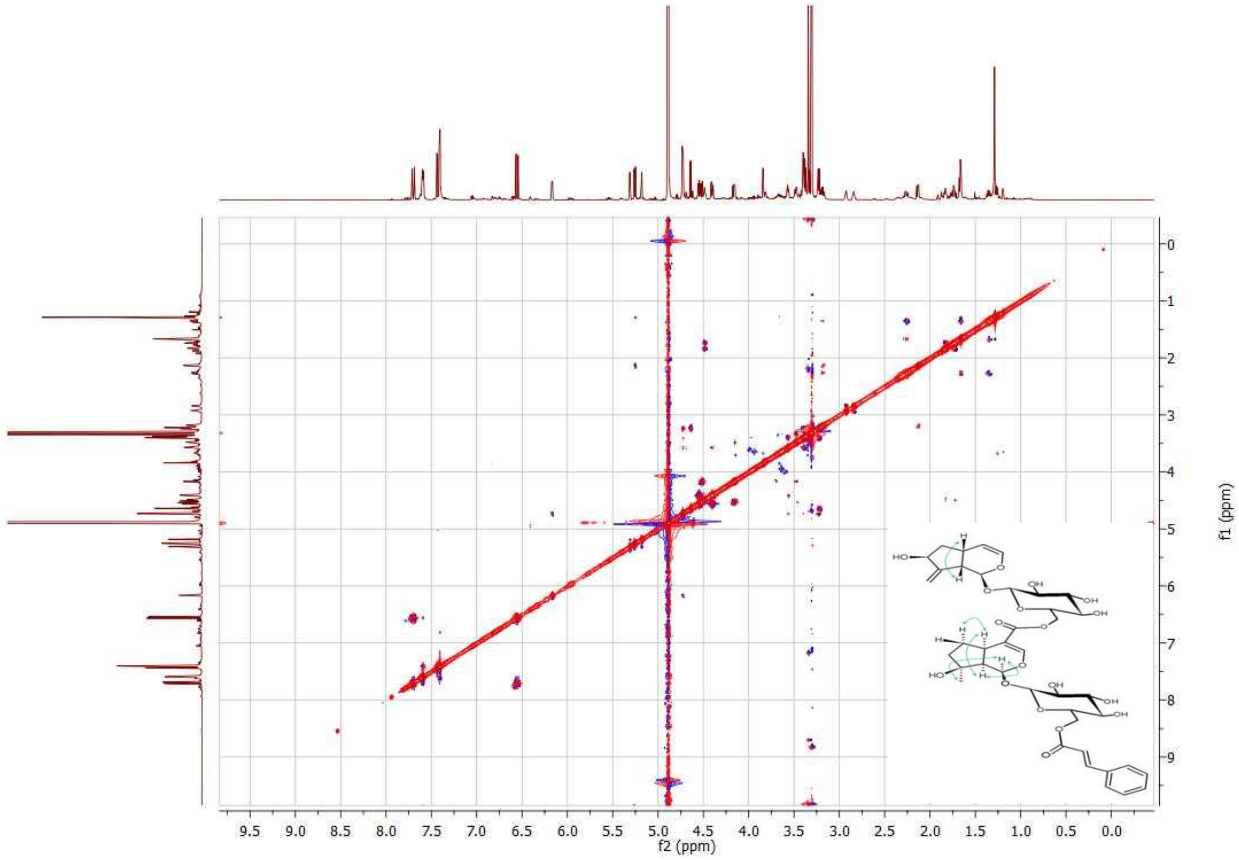

Figure S17: 2D-NOESY spectrum of compound 4

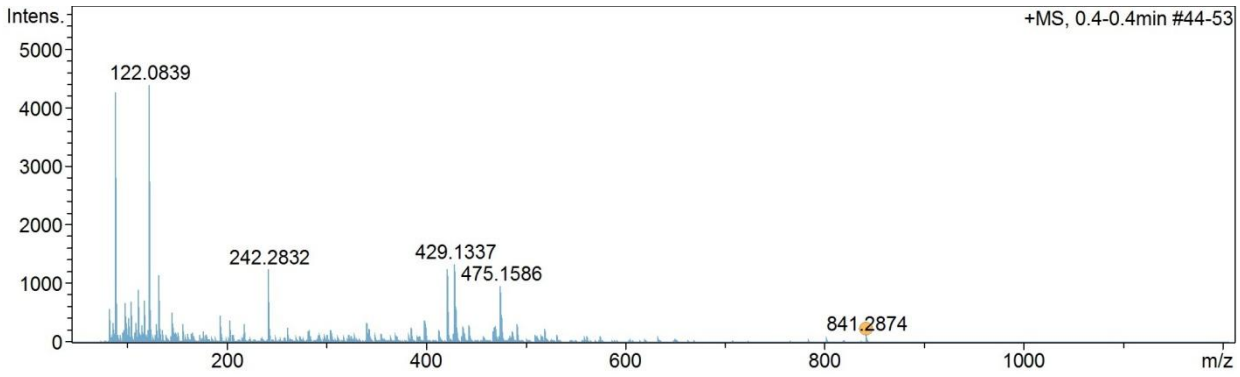

Figure S18: HR-ESI-MS of compound 4