Supporting Information

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A New Ascochlorin Glycoside from Brittlestar-derived Fungus *Acremonium* sp. and Its Biological Activities

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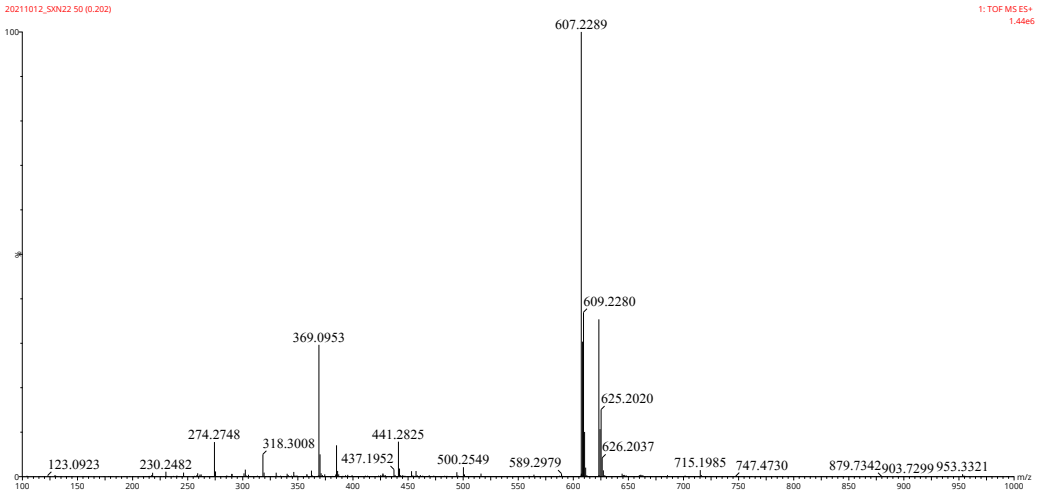

Figure S1: HR-ESI-MS spectrum of acremonoside (**1**)

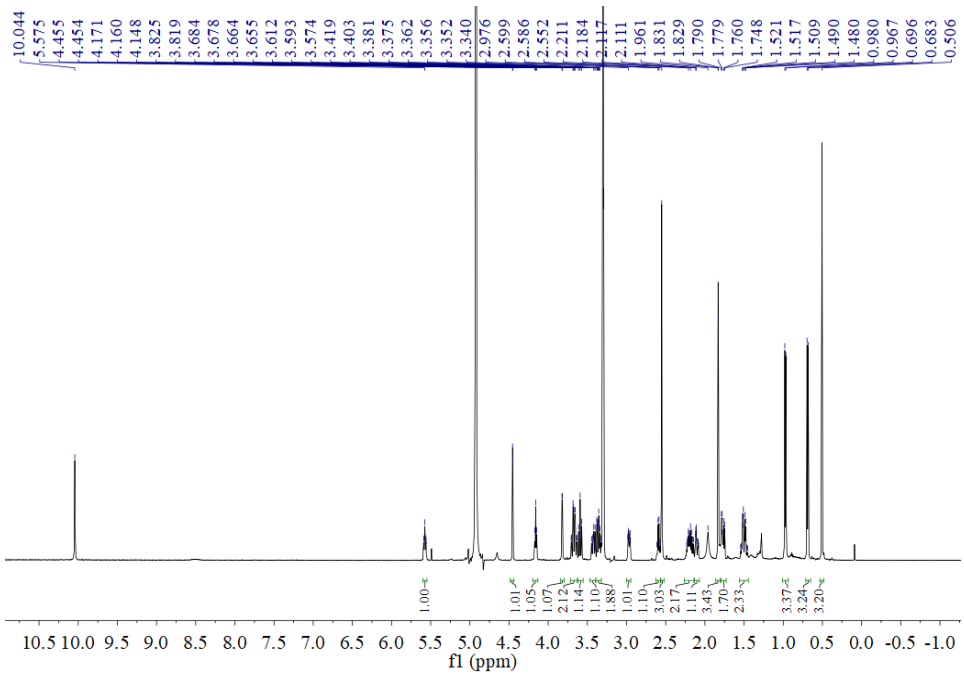

Figure S2: ^{1}H NMR (500 MHz, CD_3OD) spectrum of acremonoside (**1**)

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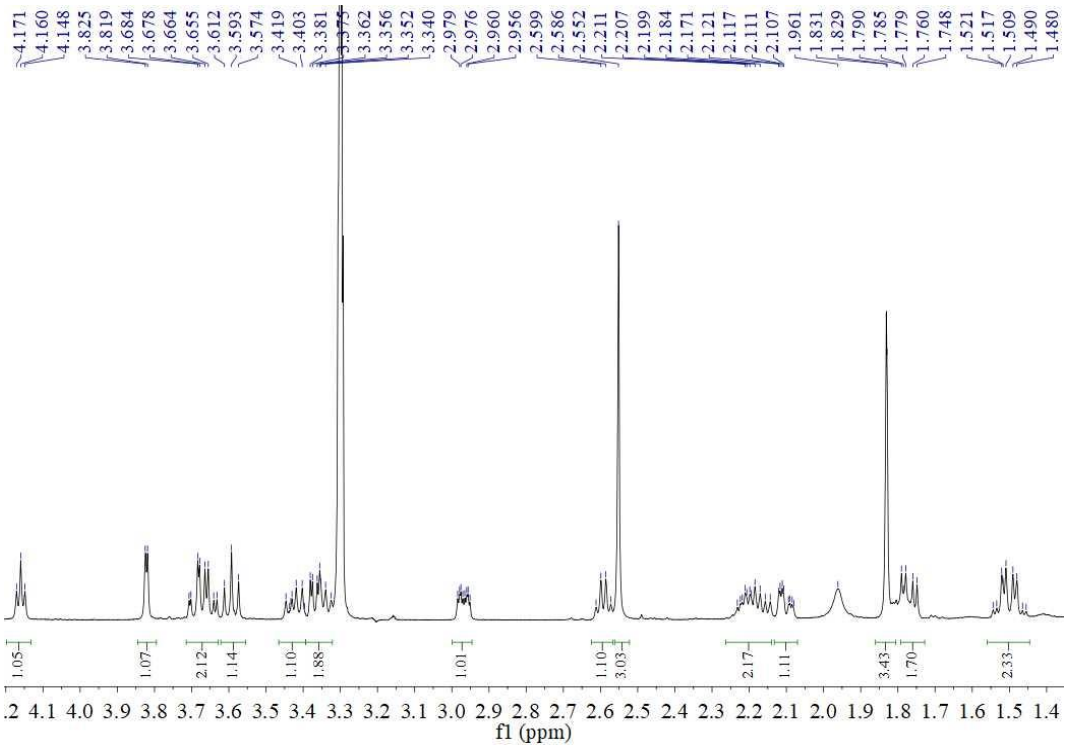

Figure S3: ^{1}H NMR (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (Enlarged)

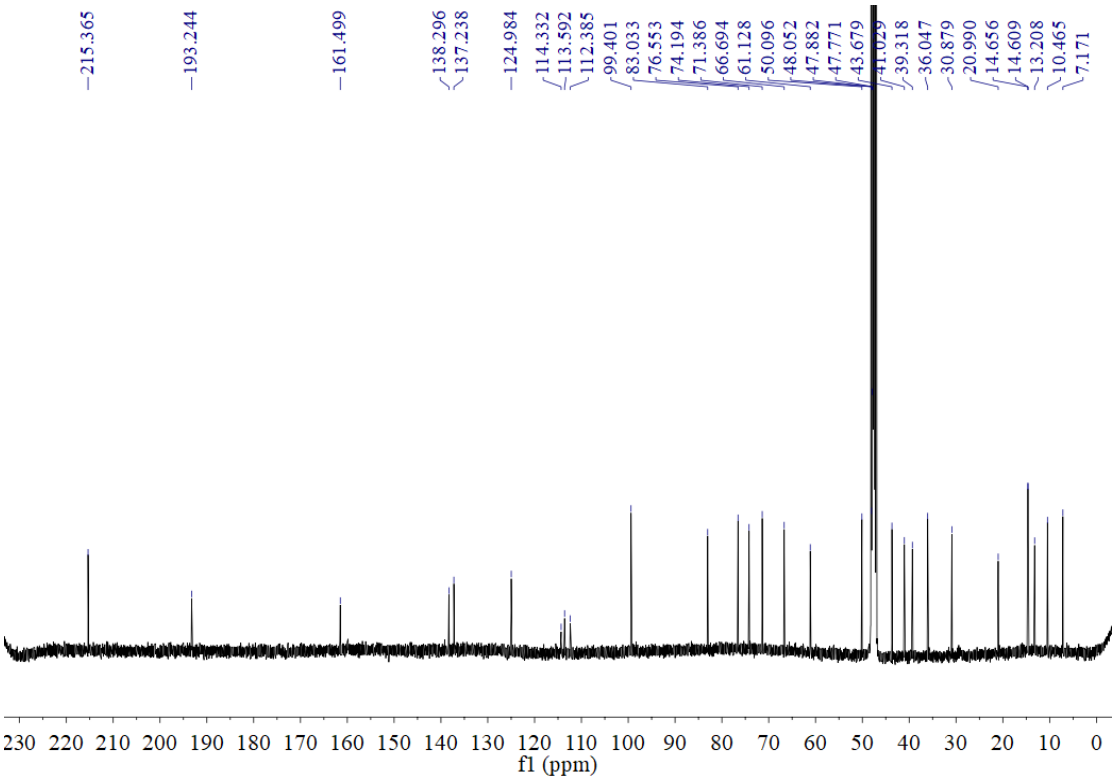

Figure S4: ^{13}C NMR (125 MHz, CD_3OD) spectrum of acremonoside (**1**)

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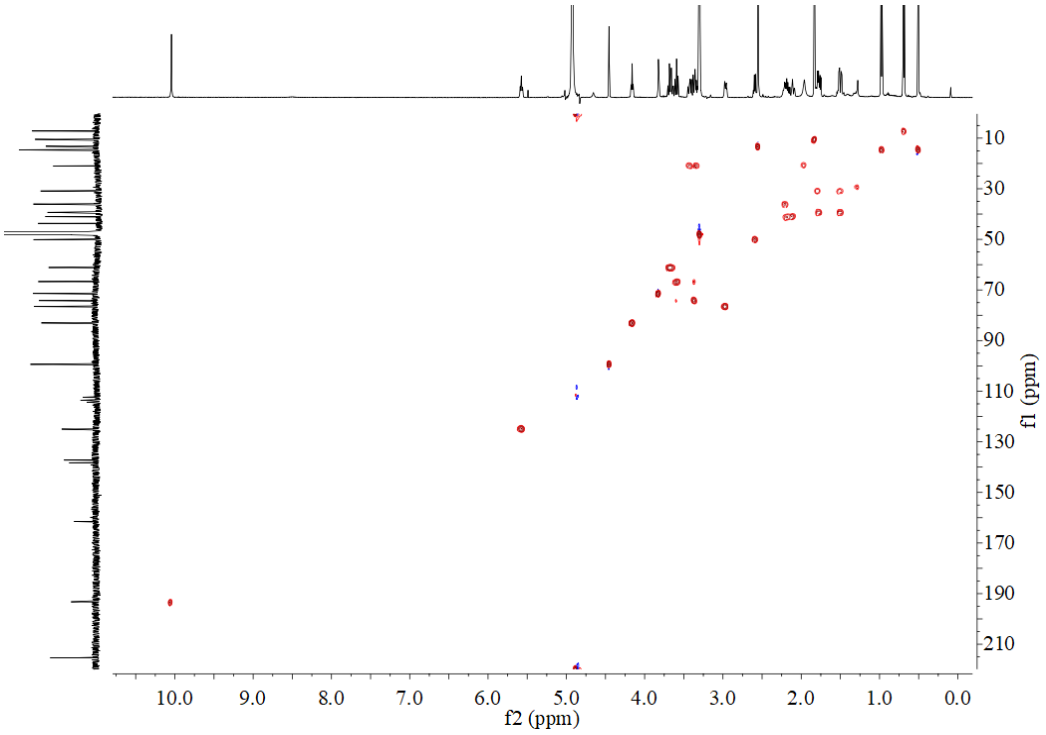

Figure S5: HSQC (500 MHz, CD_3OD) spectrum of acremonoside (**1**)

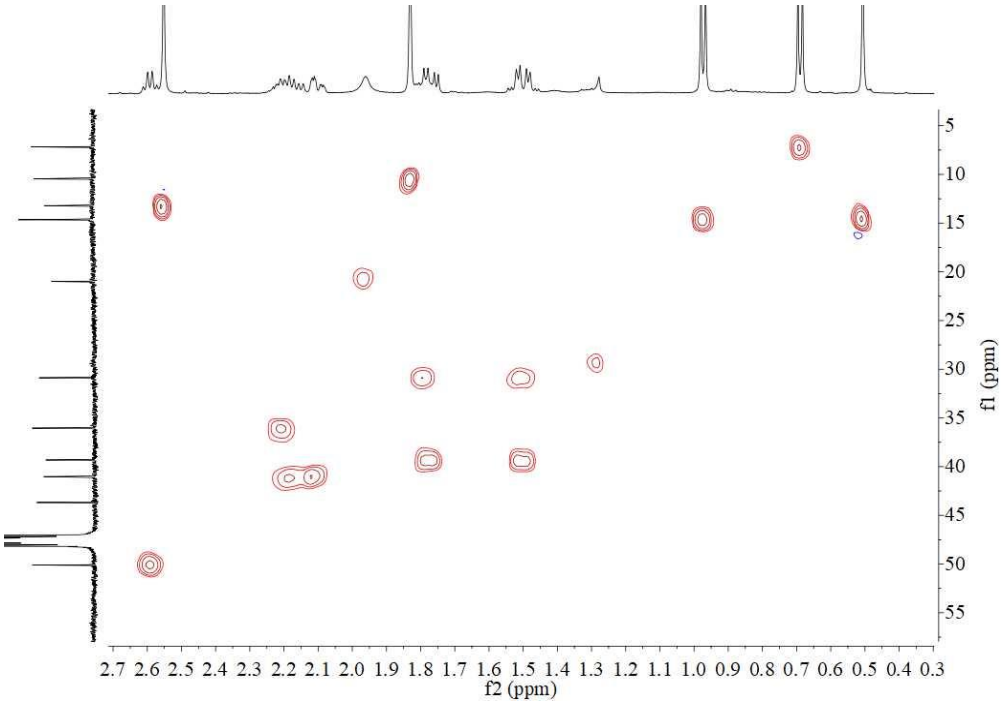

Figure S6: HSQC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.4-2.7, δ_C 5-55)

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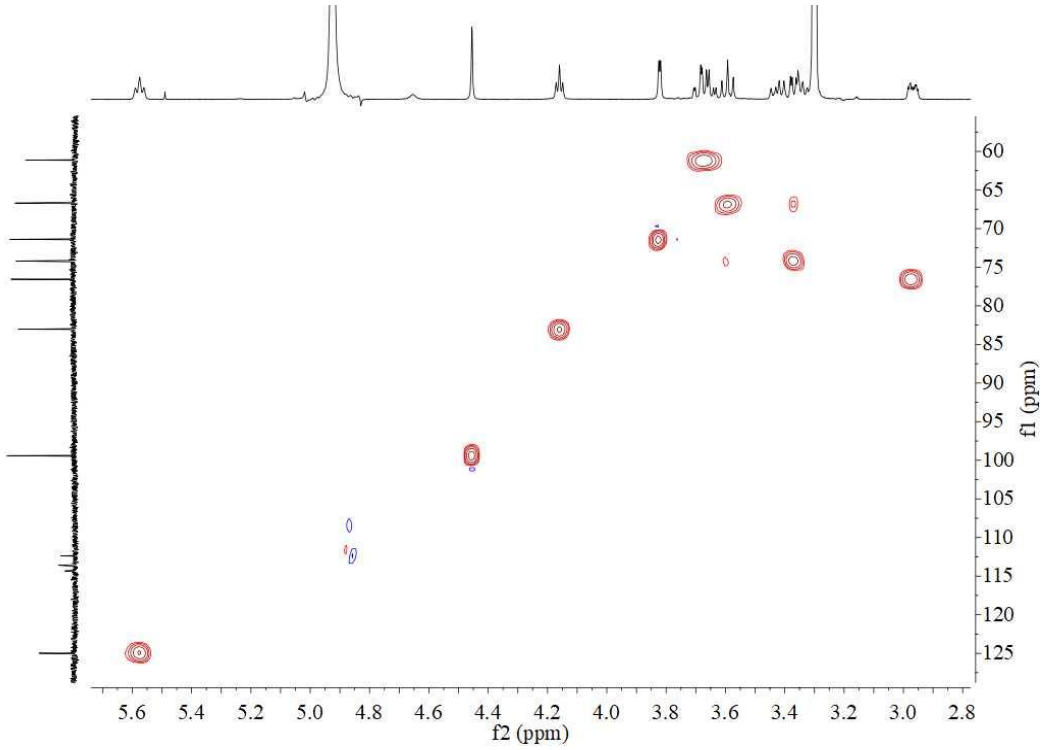

Figure S7: HSQC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 2.7-5.7, δ_C 55-126)

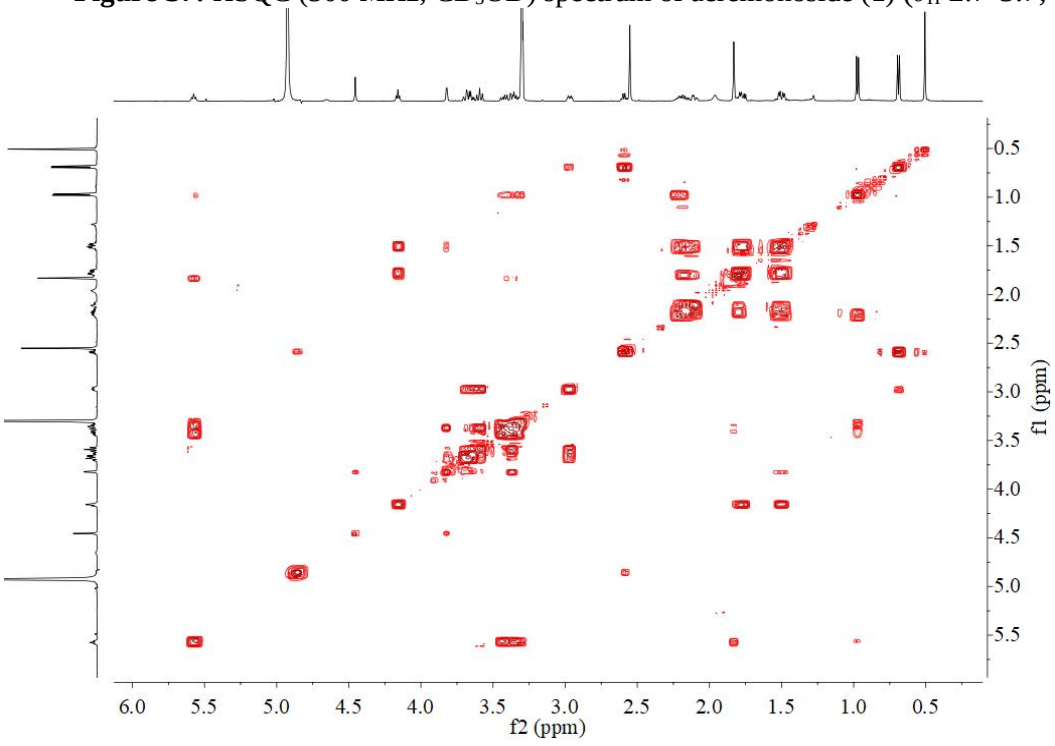

Figure S8: ^1H-^1H COSY (500 MHz, CD_3OD) spectrum of acremonoside (**1**)

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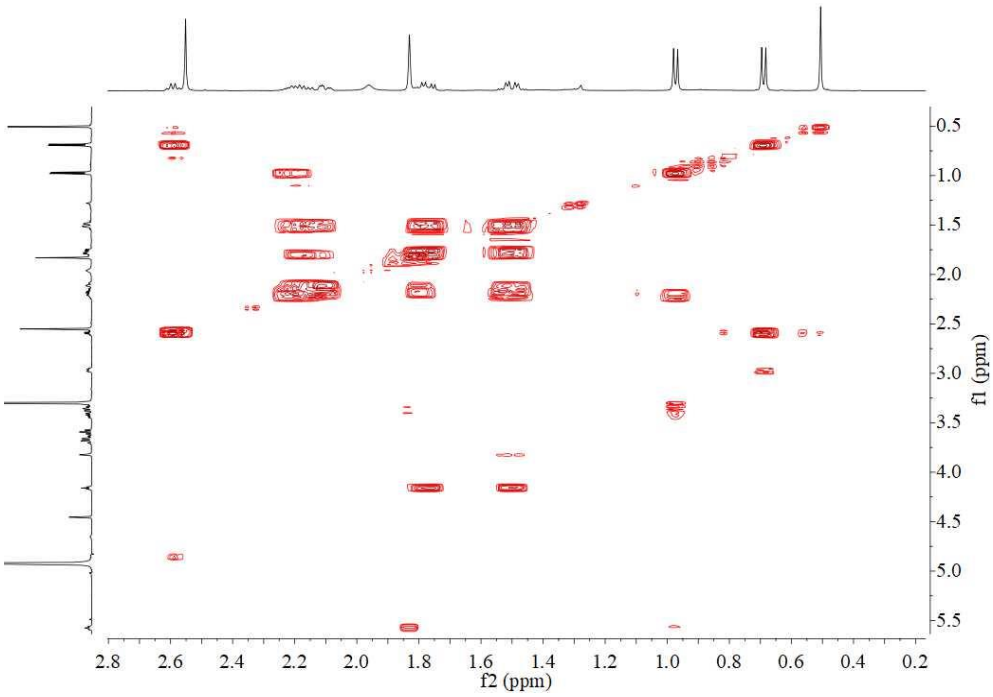

Figure S9: ^{1}H-^{1}H COSY (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.5-5.5, δ_H 0.2-2.8)

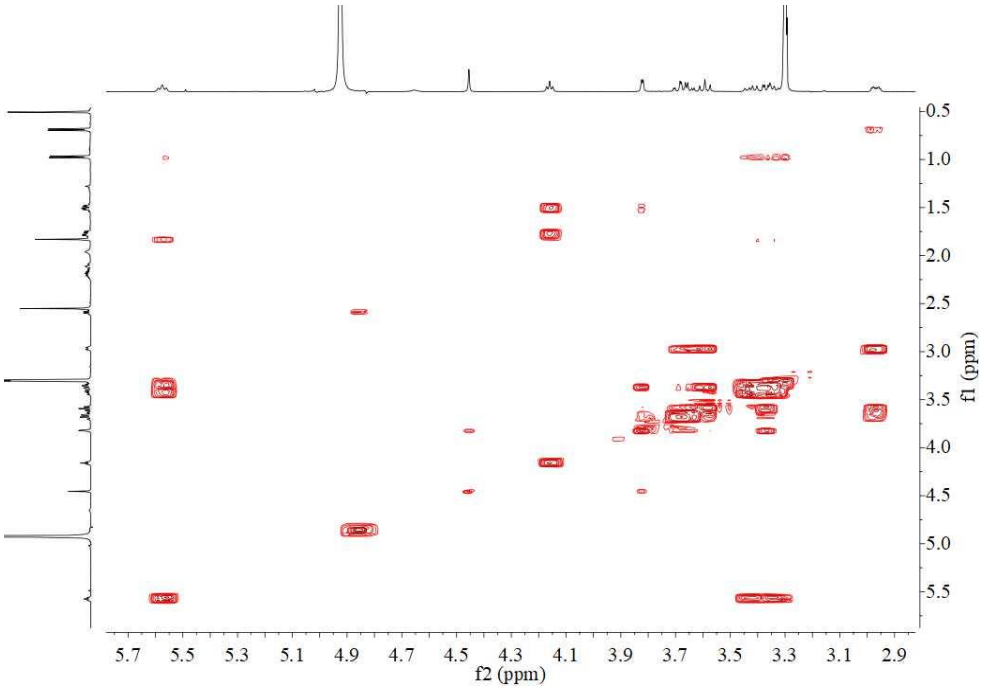

Figure S10: ^{1}H-^{1}H COSY (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.5-5.5, δ_H 2.8-5.8)

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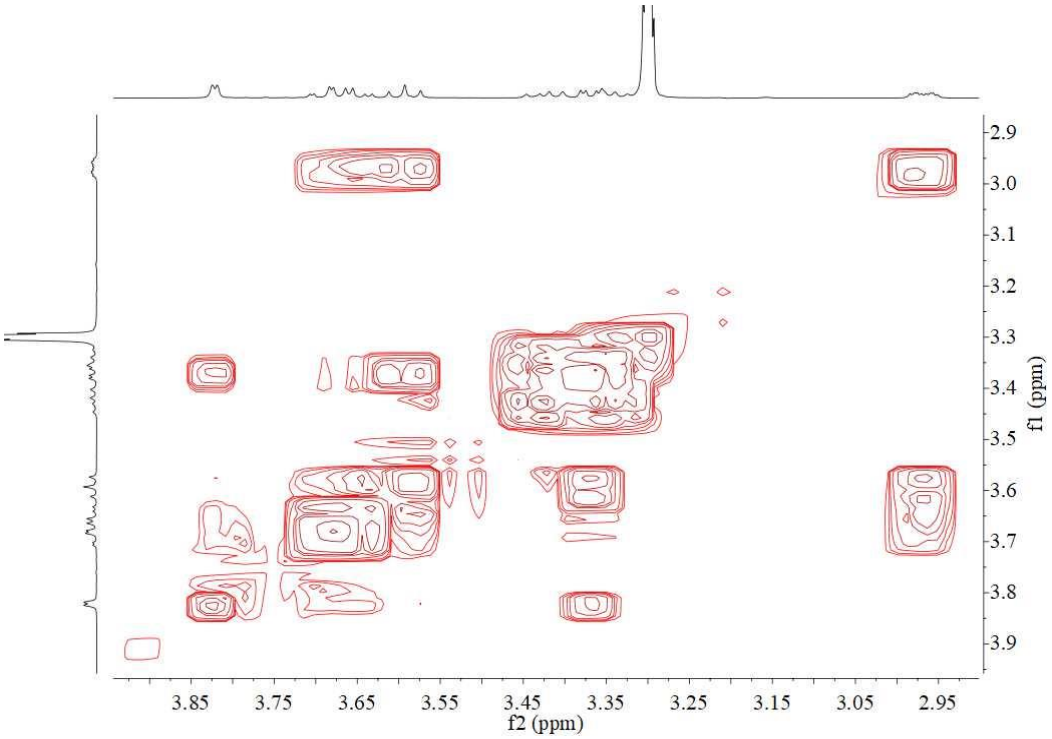

Figure S11: ^{1}H-^{1}H COSY (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 2.9-4.0, δ_H 2.9-3.9)

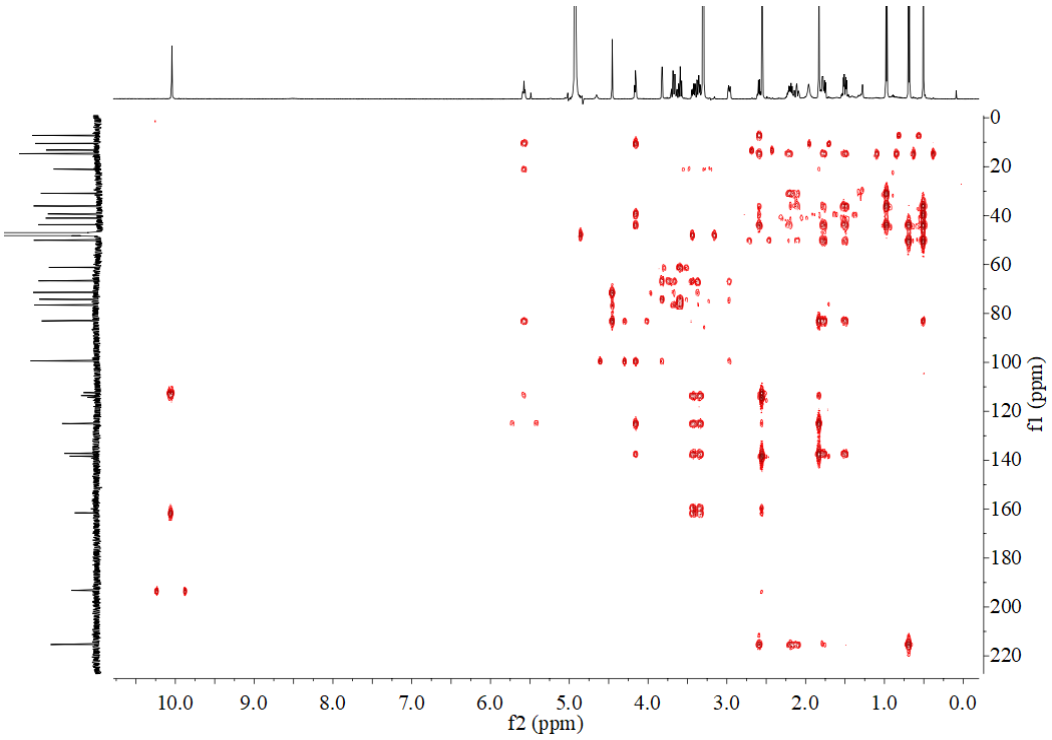

Figure S12: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**)

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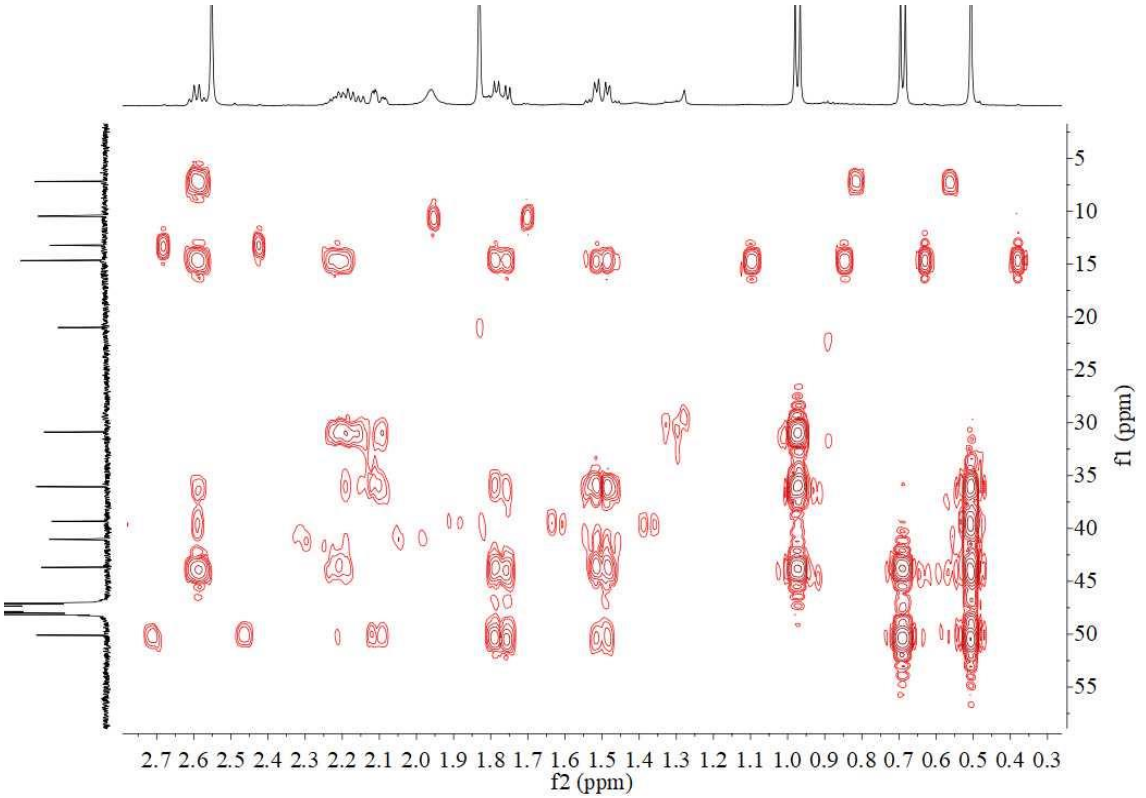

Figure S13: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.3-2.7, δ_C 5-58)

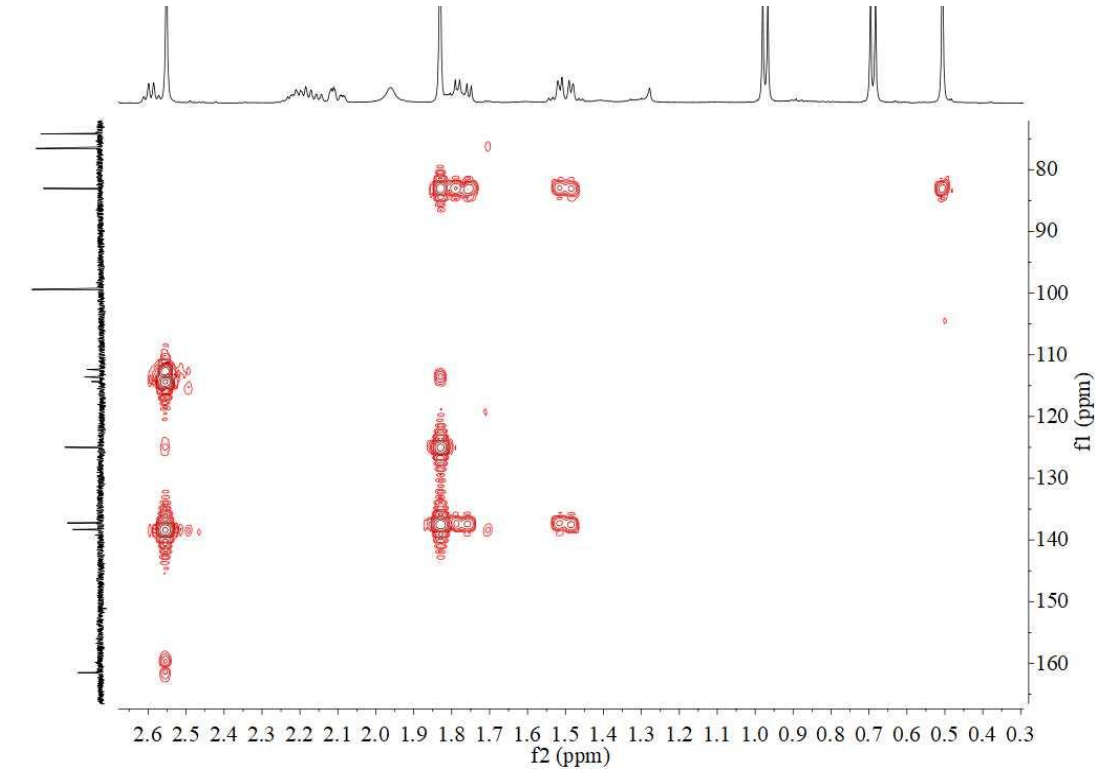

Figure S14:MBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.3-2.7, δ_C 70-166)

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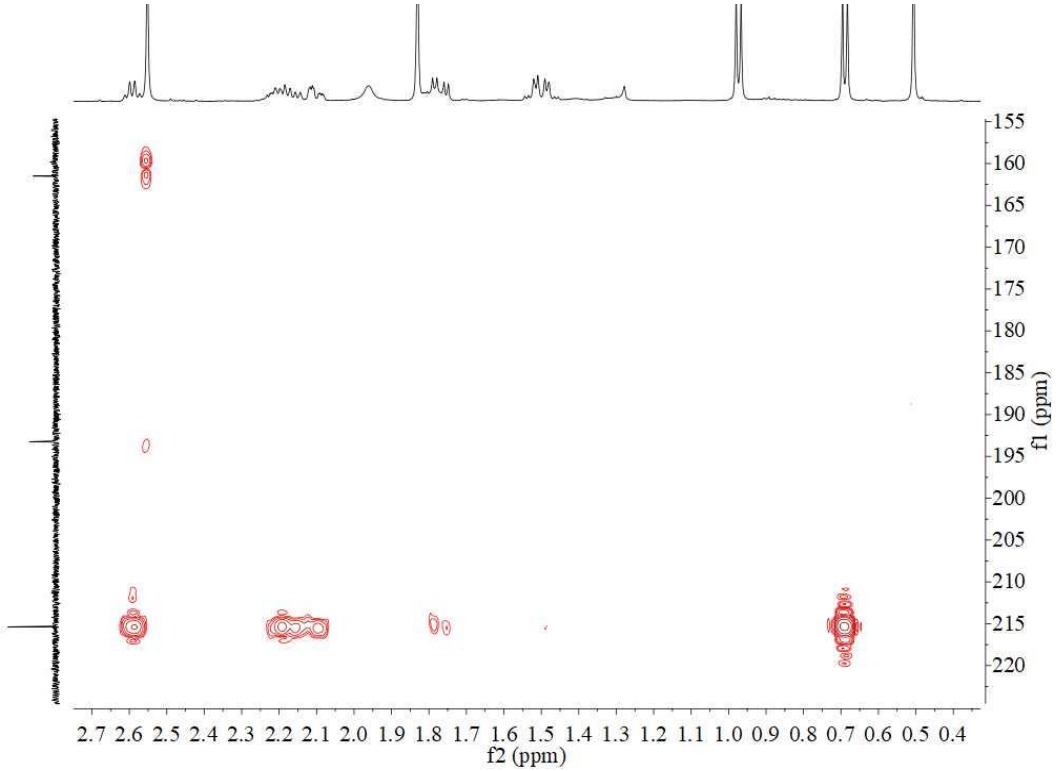

Figure S15: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.3-2.7, δ_C 155-220)

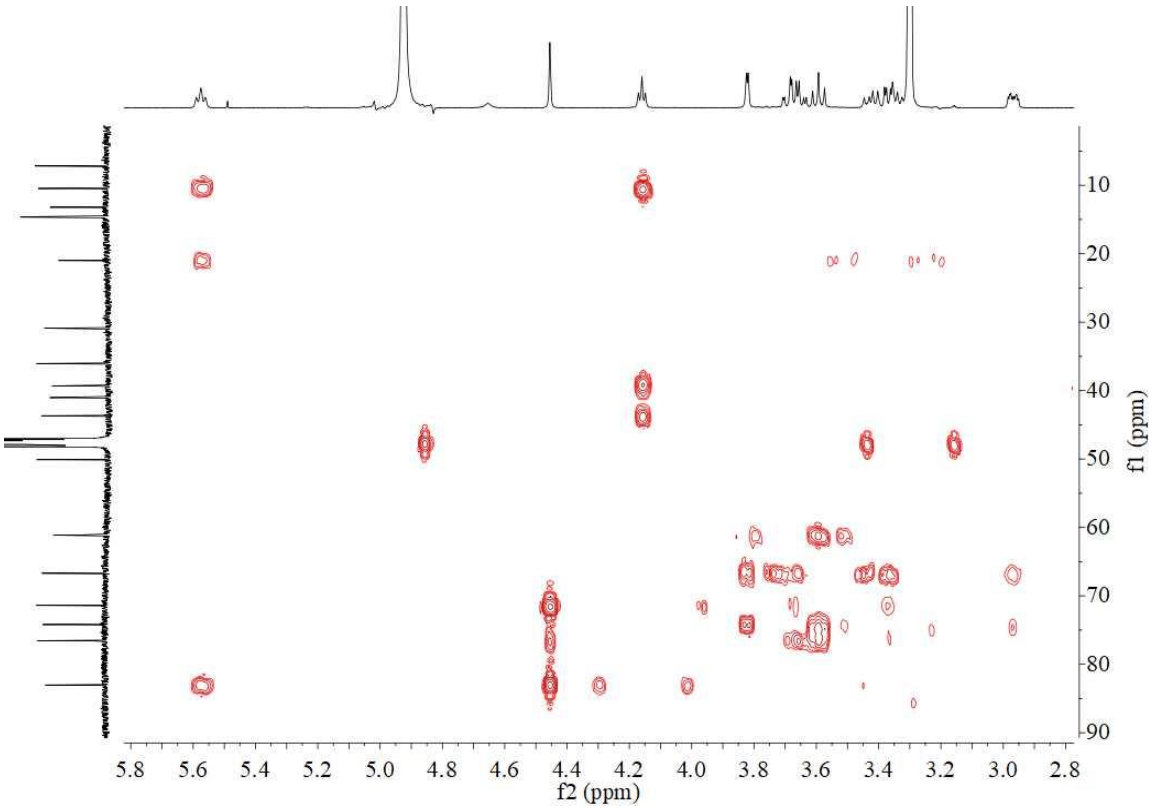

Figure S16: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 2.8-5.8, δ_C 5-90)

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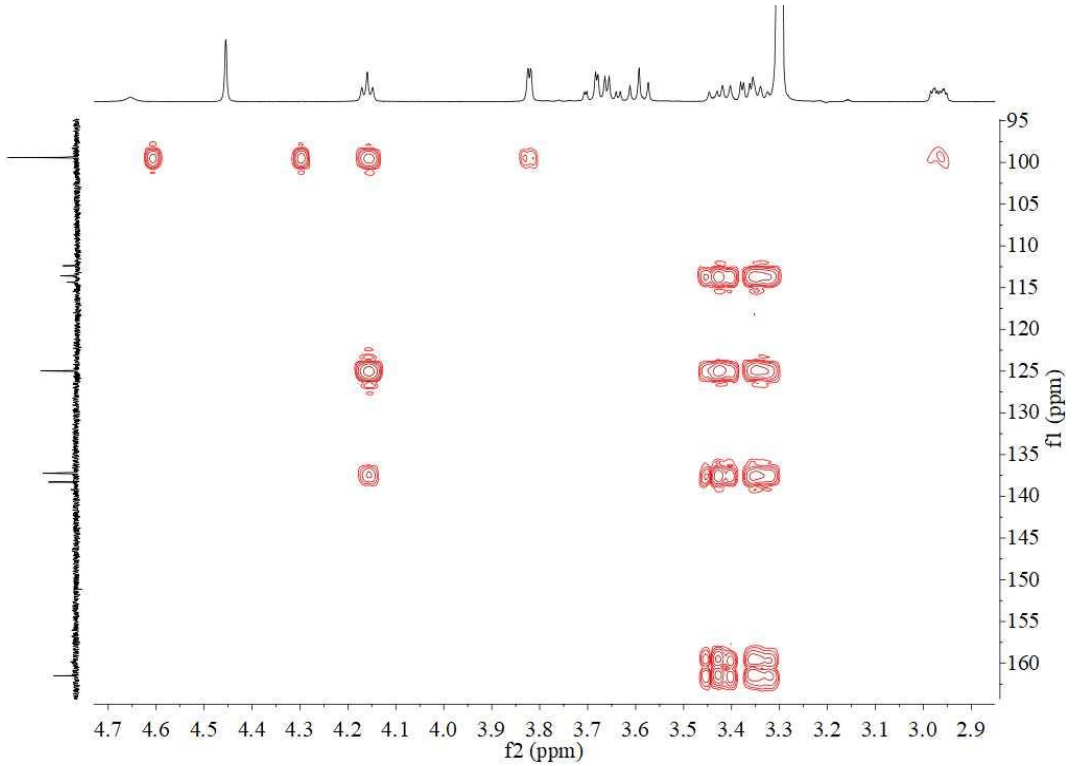

Figure S17: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 2.9-4.7, δ_C 95-167)

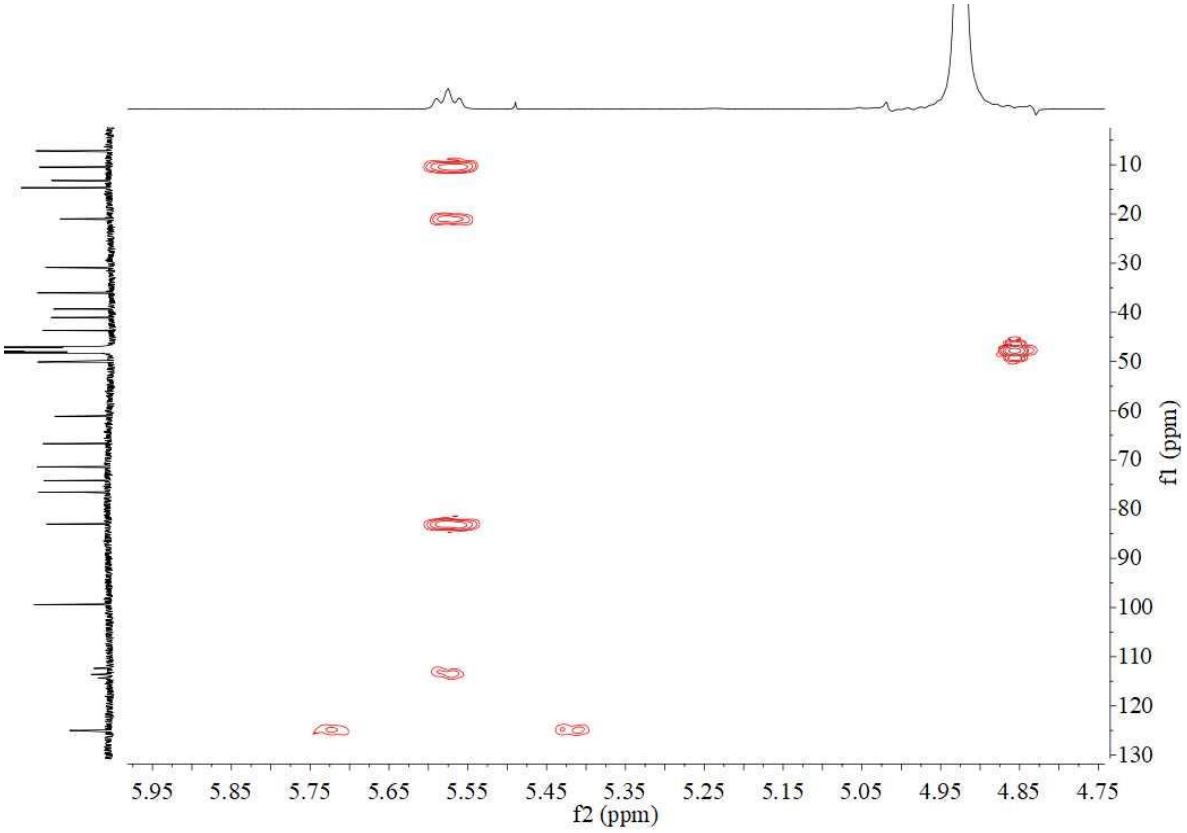

Figure S18: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 4.75-6.0, δ_C 5-130)

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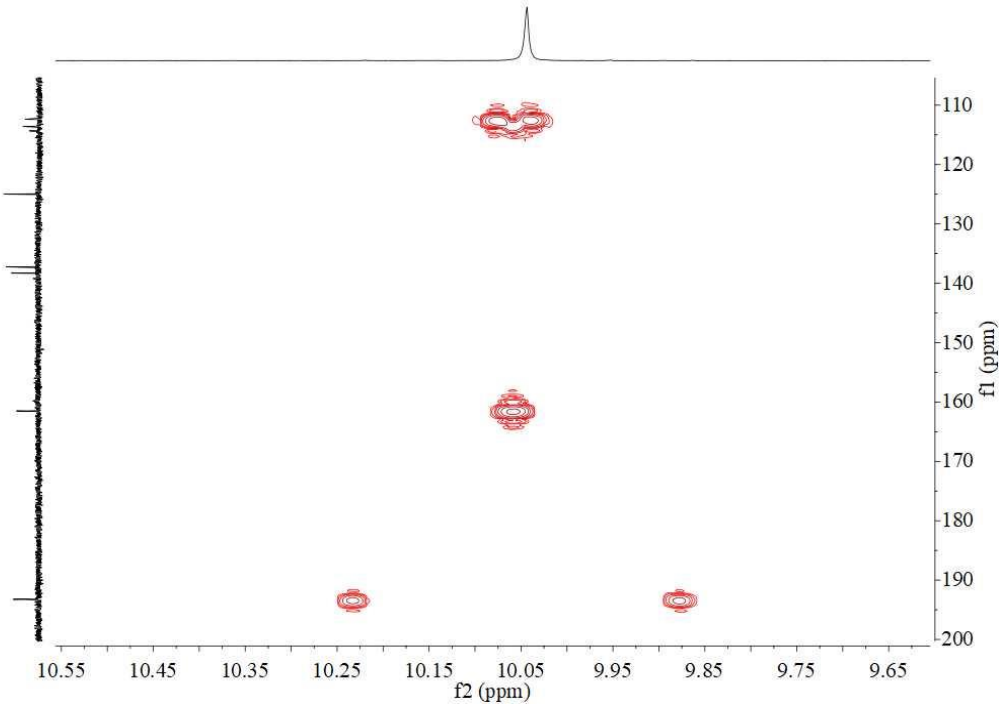

Figure S19: HMBC (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 9.6-10.6, δ_C 110-200)

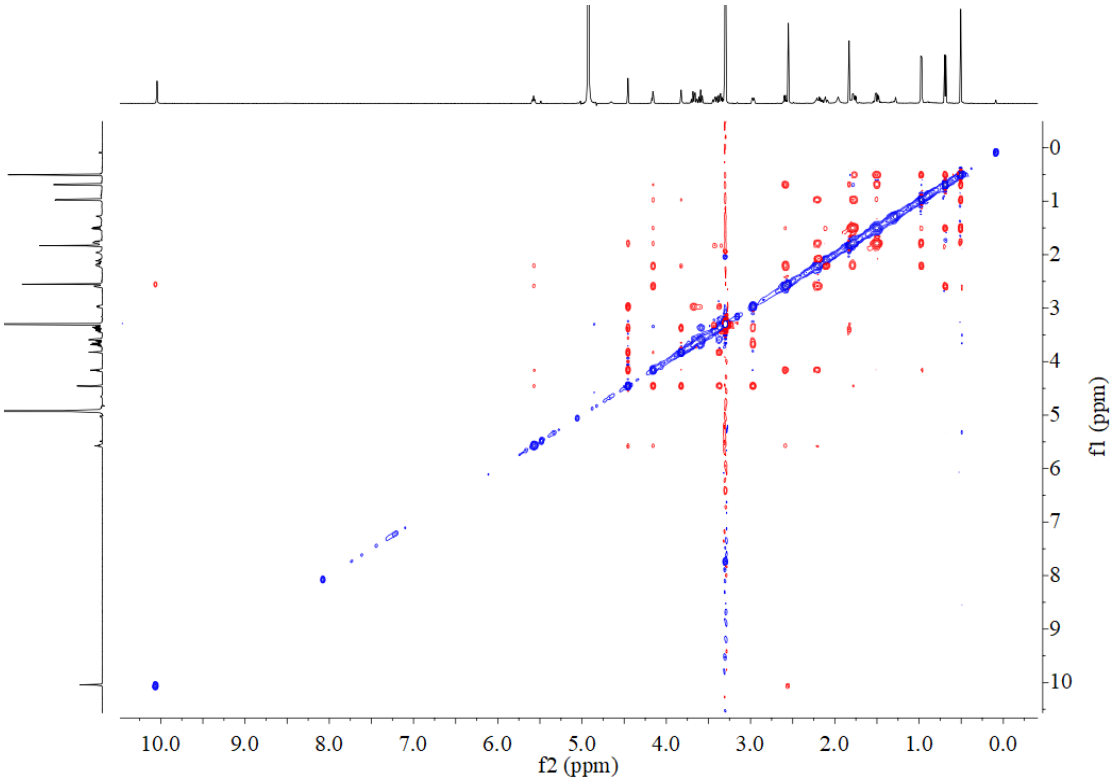

Figure S20: NOESY (500 MHz, CD_3OD) spectrum of acremonoside (**1**)

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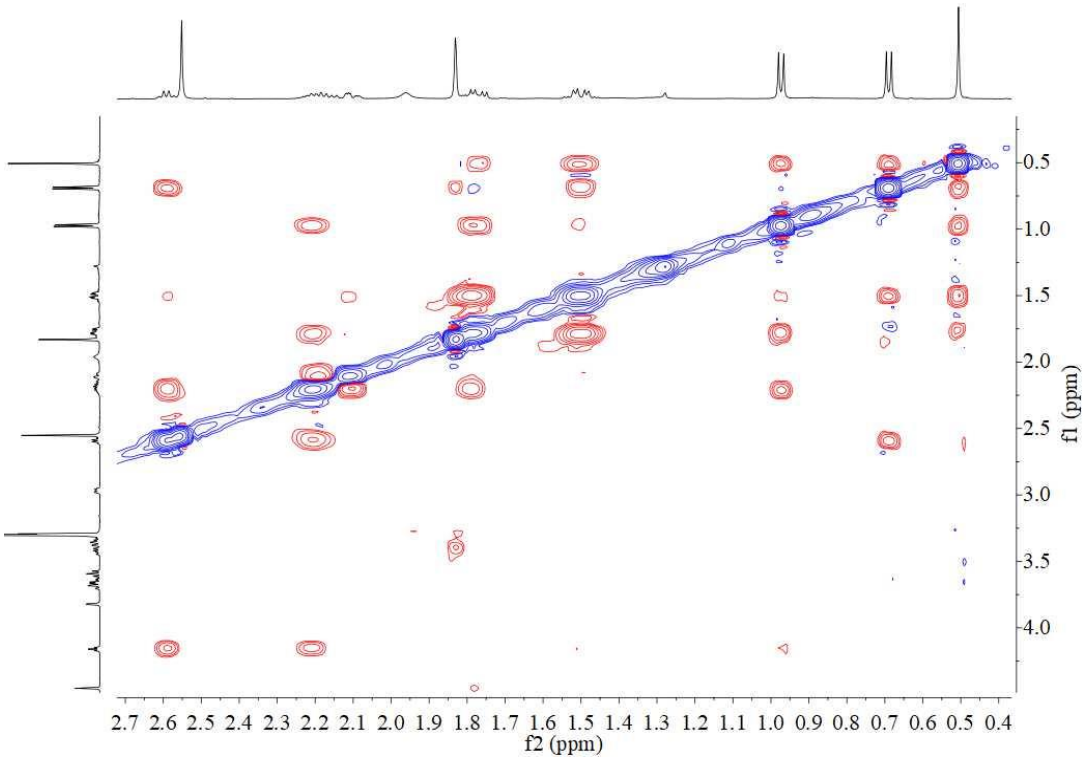

Figure S21: NOESY (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.5-5.0, δ_H 0.4-2.7)

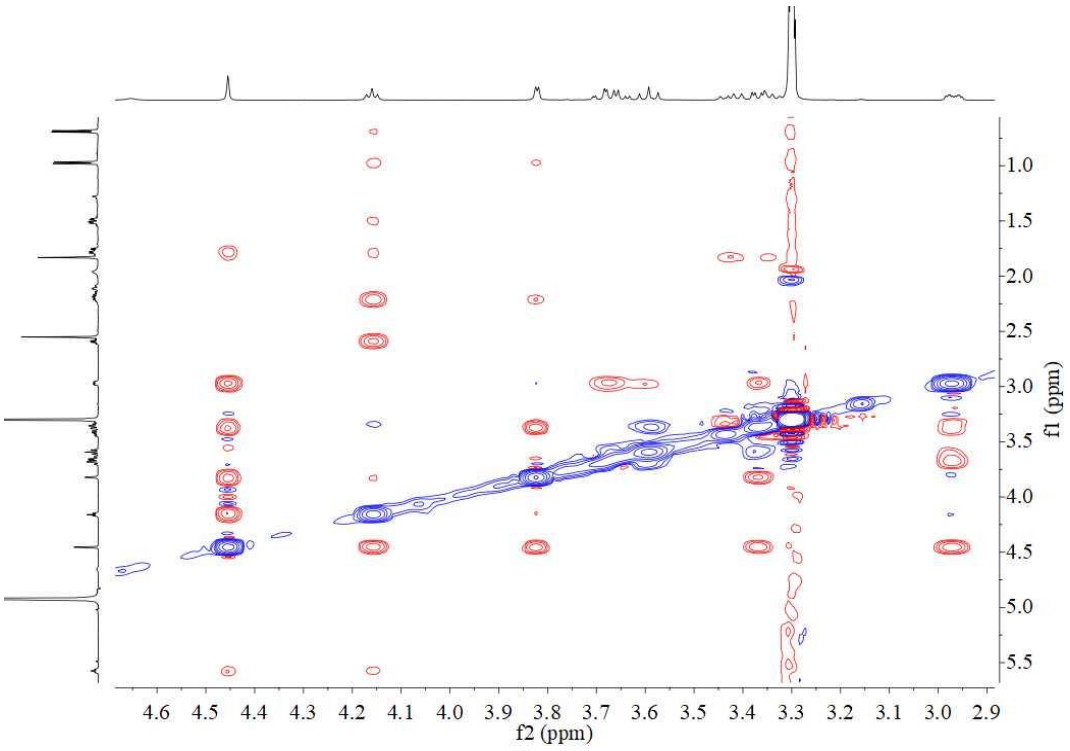

Figure S22: NOESY (500 MHz, CD_3OD) spectrum of acremonoside (**1**) (δ_H 0.5-5.5, δ_H 2.9-4.6)

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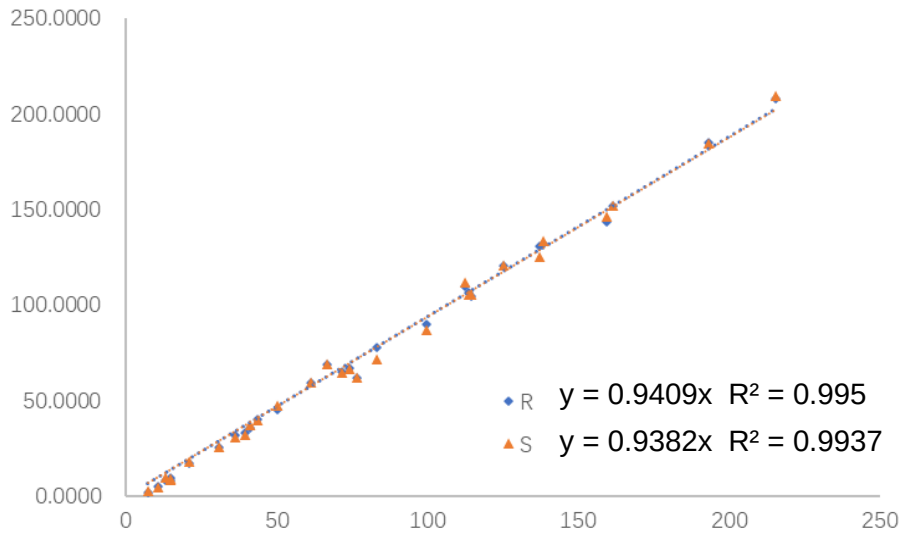

Figure S23: Linear correlation plots of experimental (**1**) versus calculated isomers (12*S*-**1** and 12*R*-**1**) ^{13}C NMR chemical shifts

Note : Density functional theory methods were employed to facilitate ^{13}C chemical shift assignments of **1**. Conformational analyses were carried out by random searching with an energy cutoff of 7 kcal/mol using the Schrödinger MacroModel software package. The MMFF94 force field was employed. The conformers were optimized in the gas phase at the PCM (solvent = methanol) B3LYP-GD3BJ/6-31G(d) level using the Gaussian 16 program. NMR chemical shifts of 12*R*-**1** and 12*S*-**1** were calculated by the GIAO method at the mpw1pw91/6-31+G(d, p) level of theory in the methanol. The computational ^{13}C-NMR data were obtained by linear regression.

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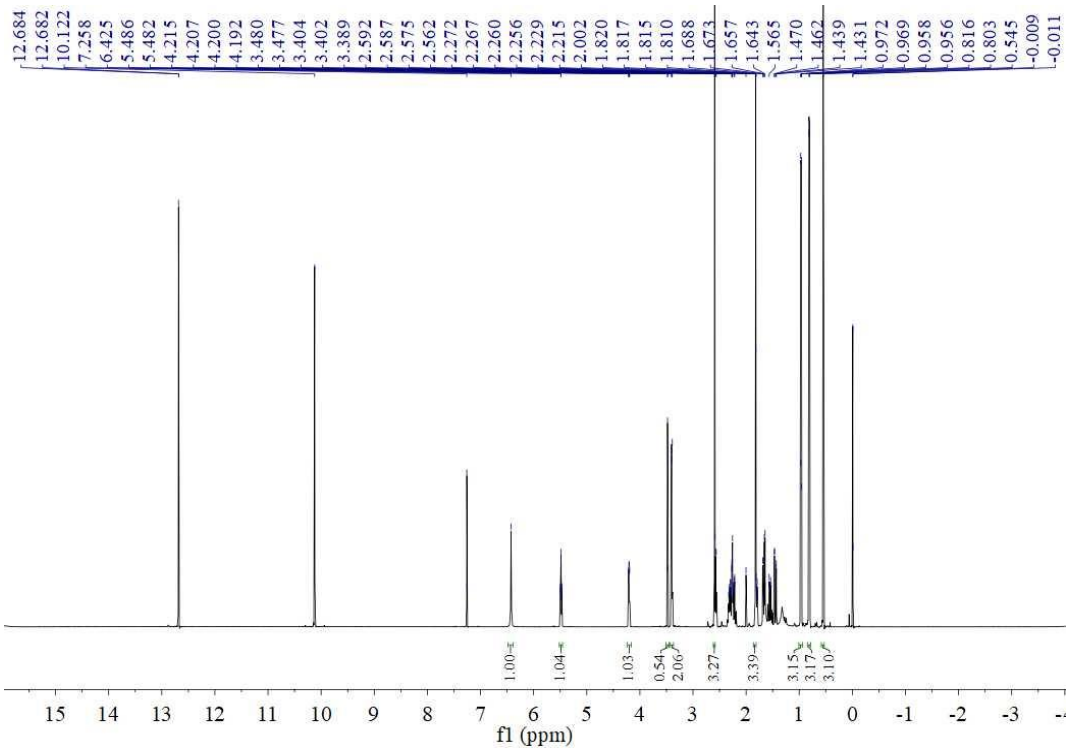

Figure S24: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **2**

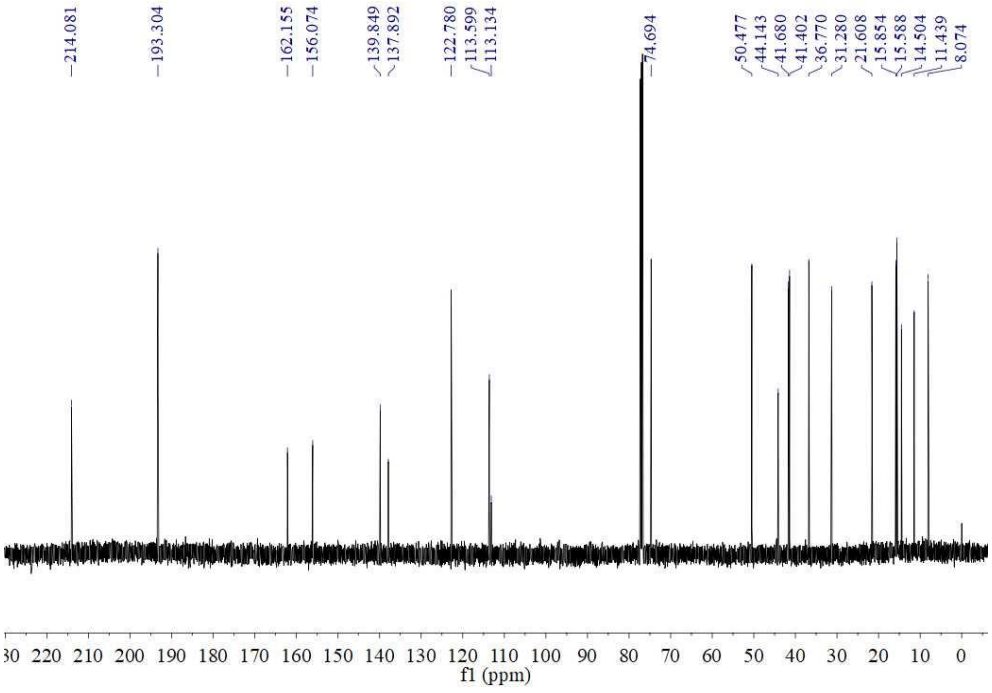

Figure S25: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **2**

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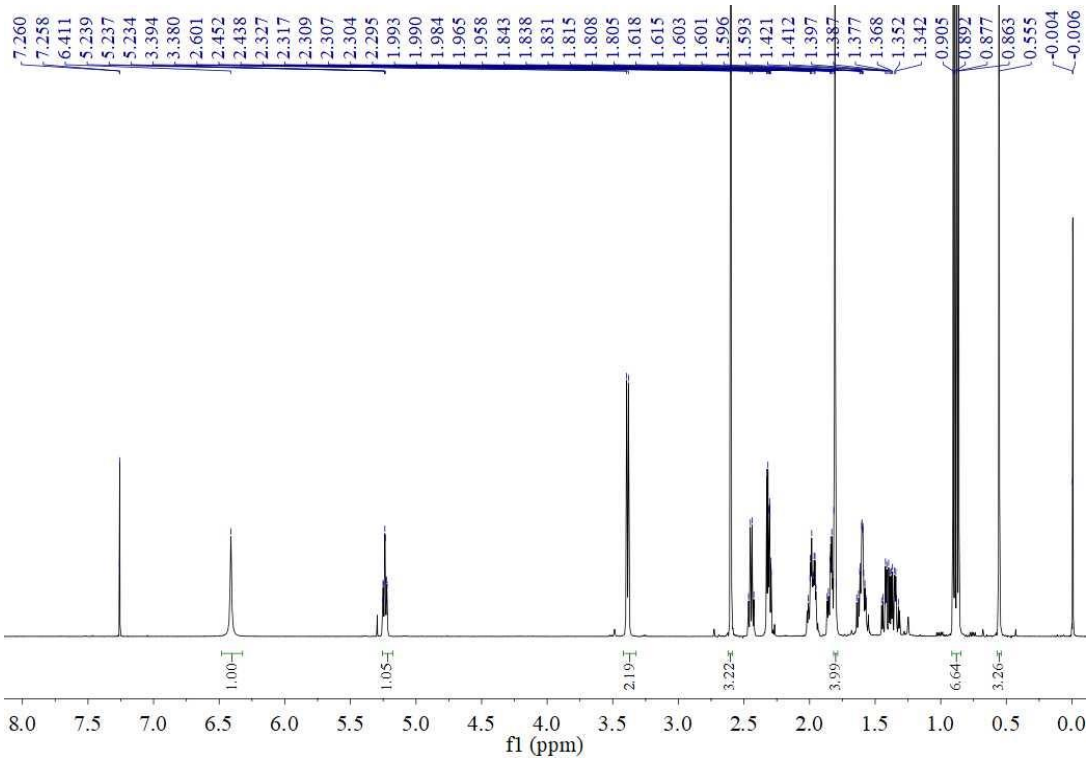

Figure S26: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **3**

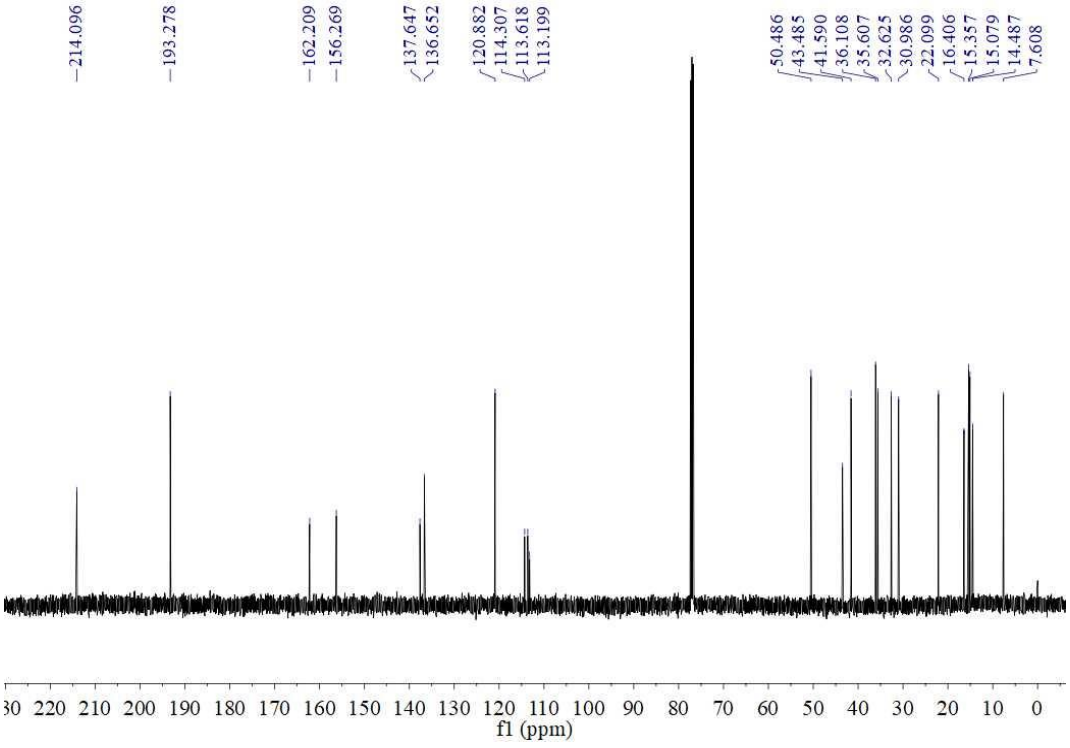

Figure S27: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **3**

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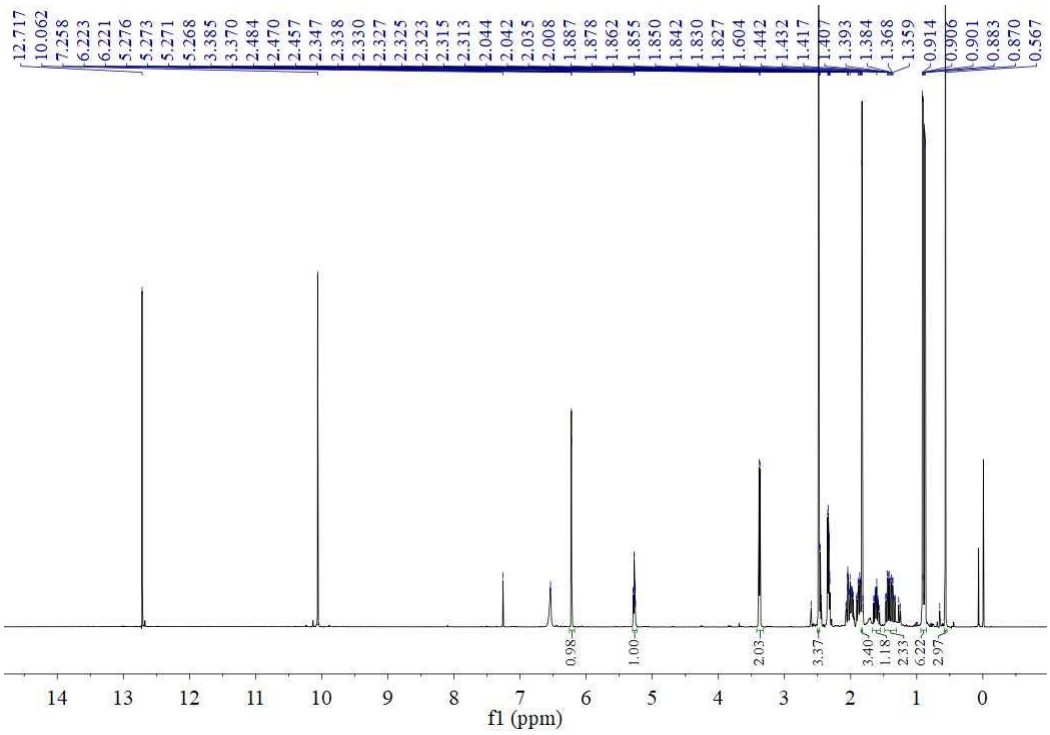

Figure S28: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **4**

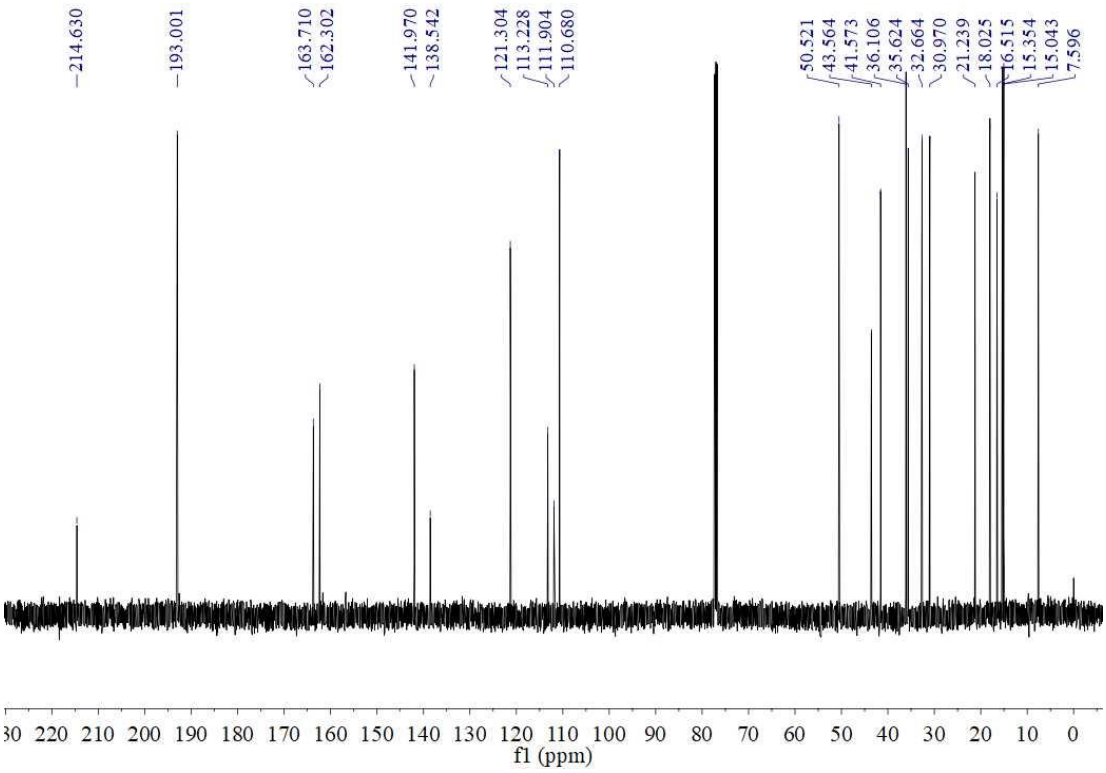

Figure S29: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **4**

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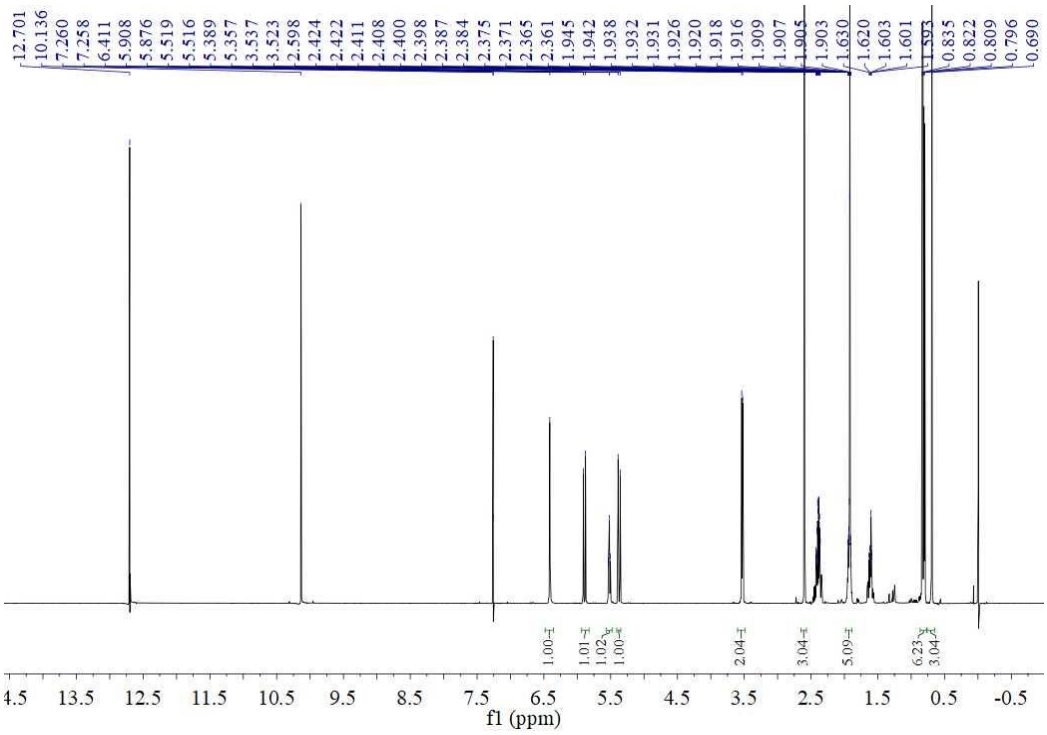

Figure S30: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **5**

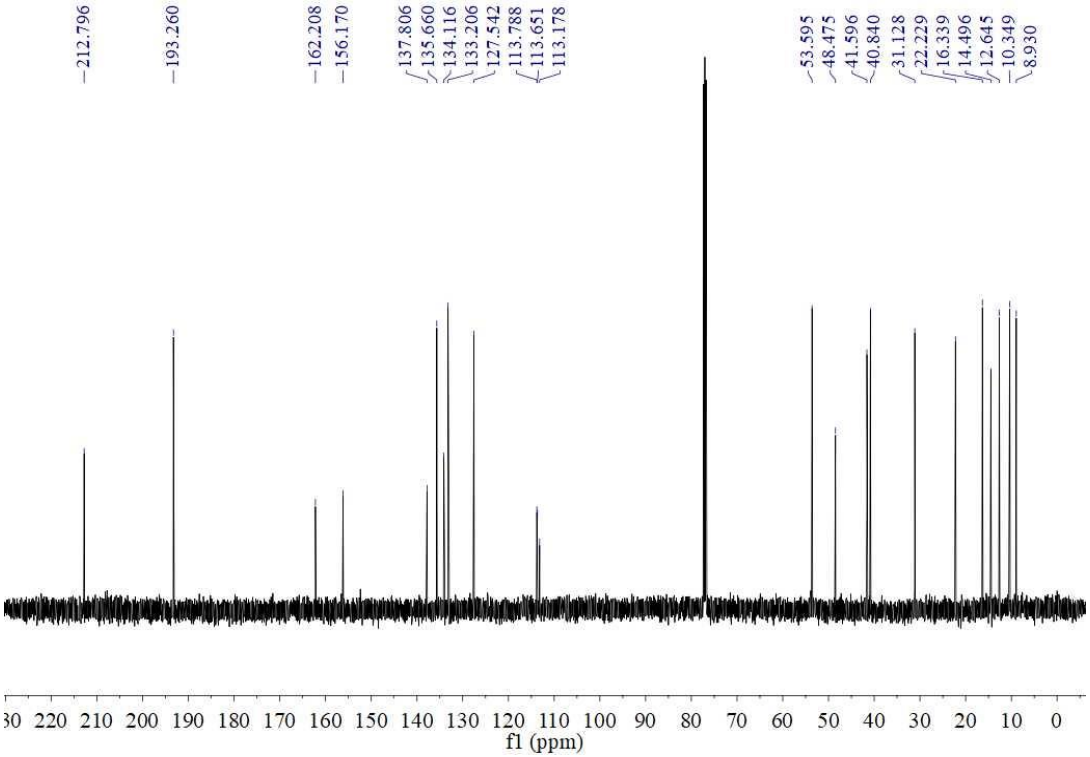

Figure S31: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **5**

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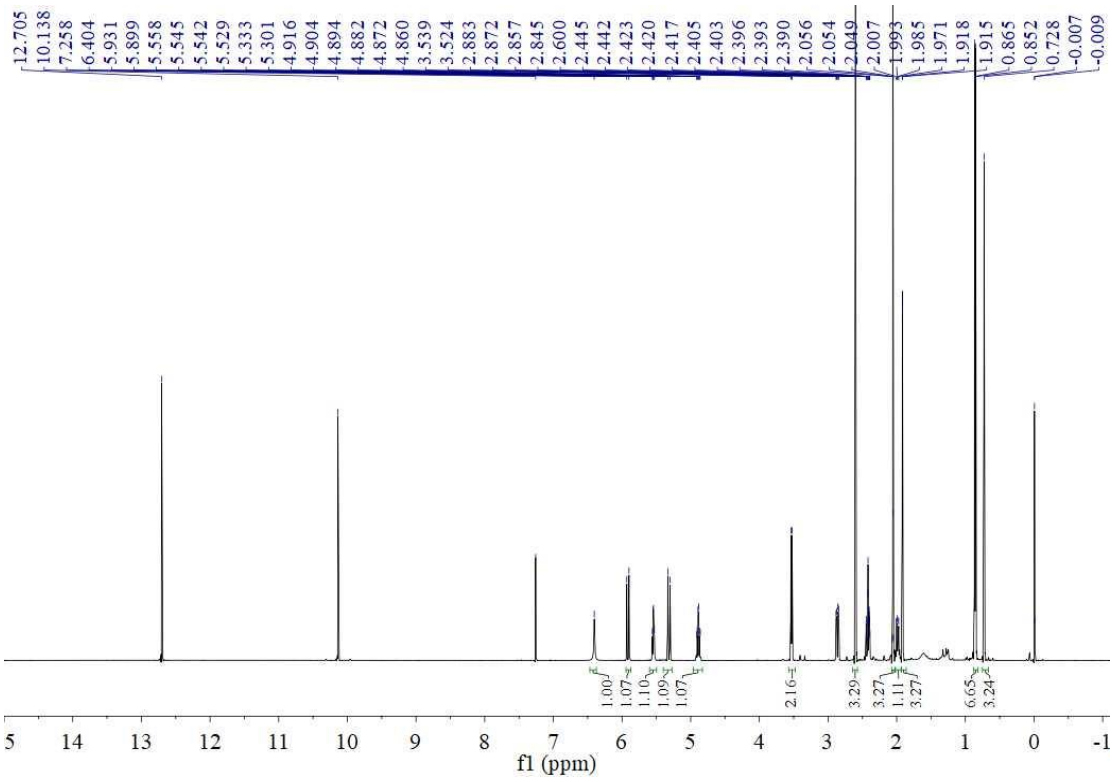

Figure S32: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **6**

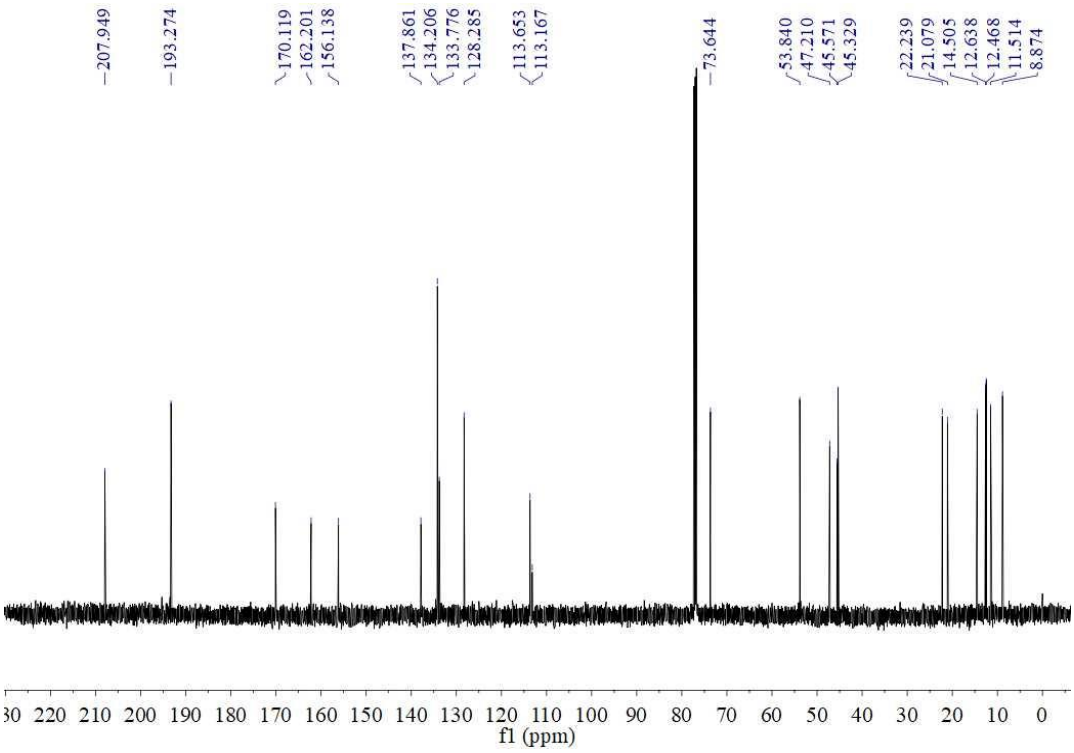

Figure S33: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **6**

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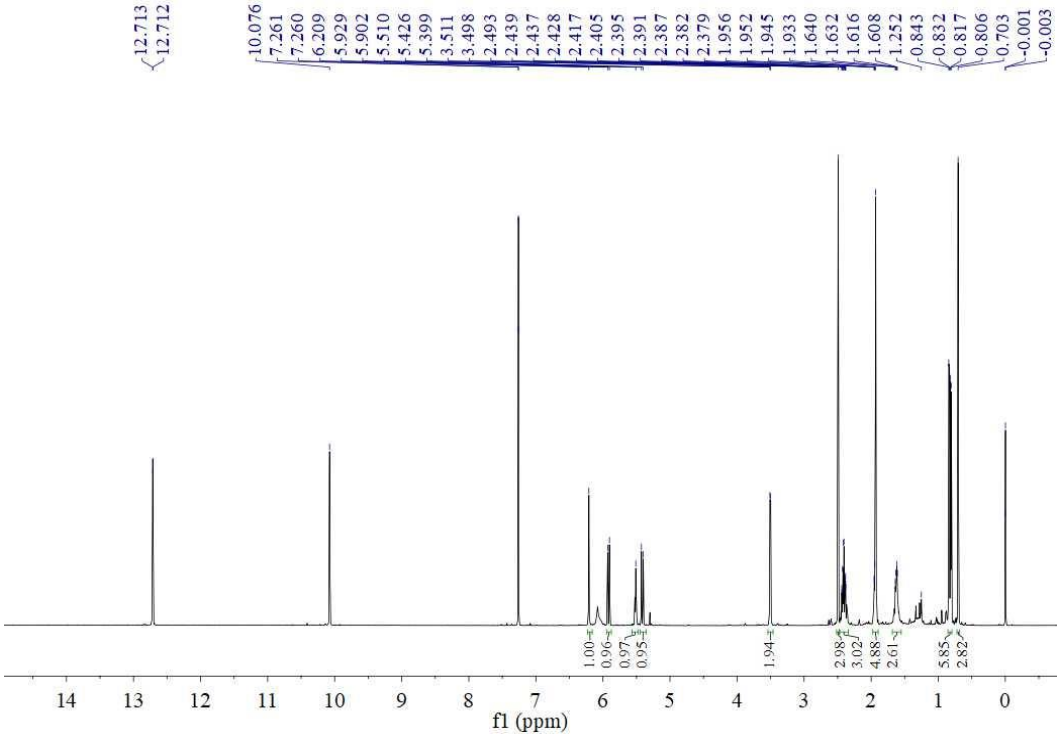

Figure S34: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **7**

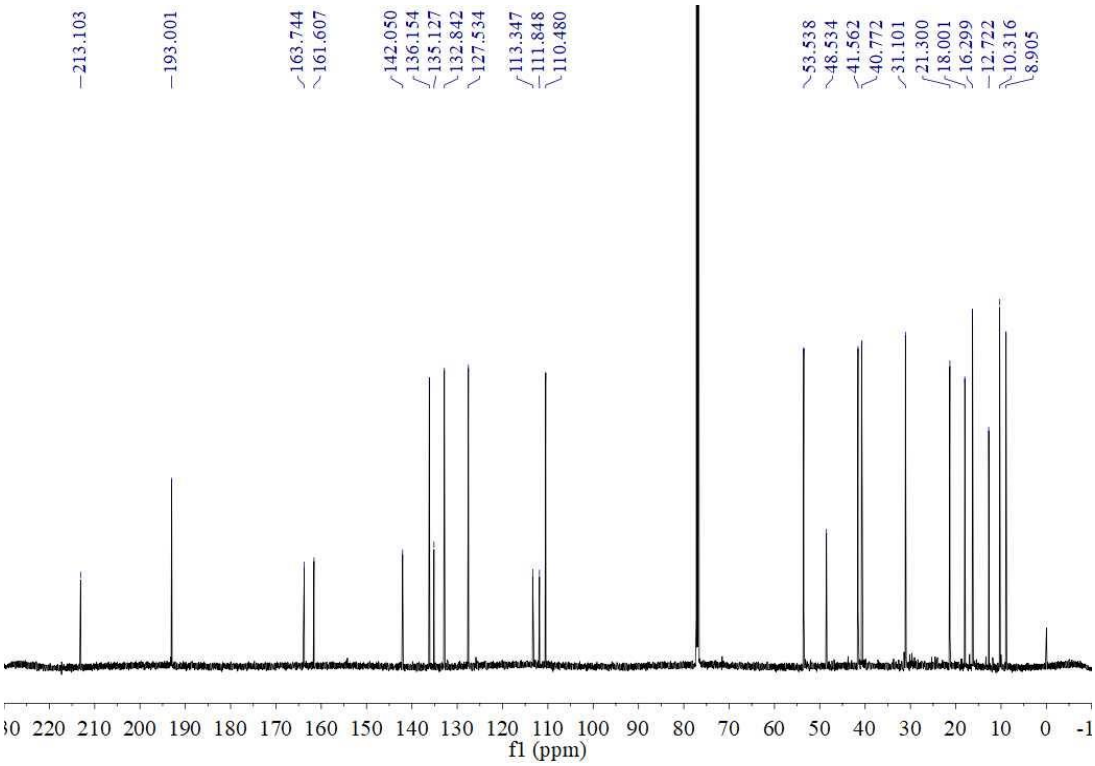

Figure S35: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **7**

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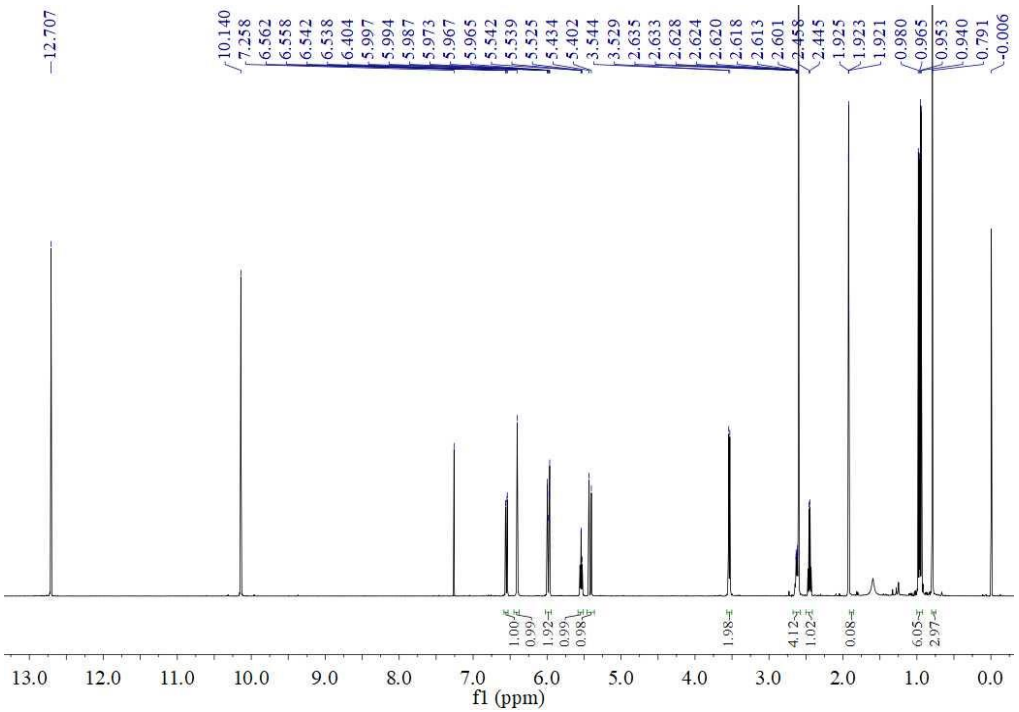

Figure S36: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **8**

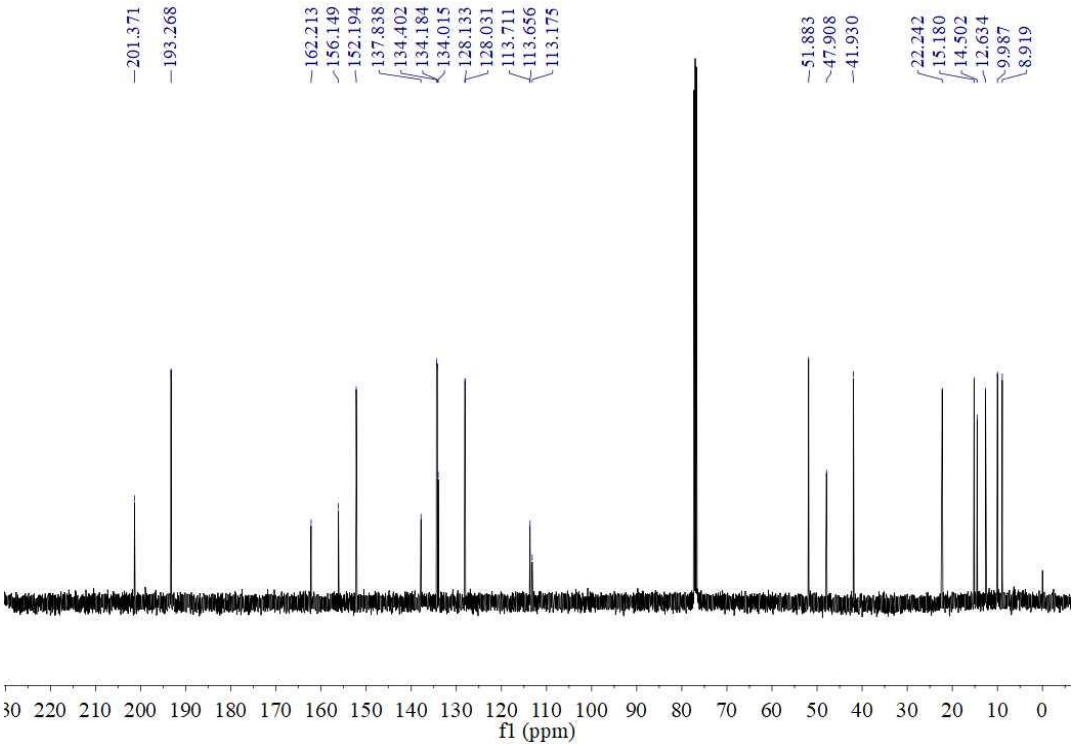

Figure S37: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **8**

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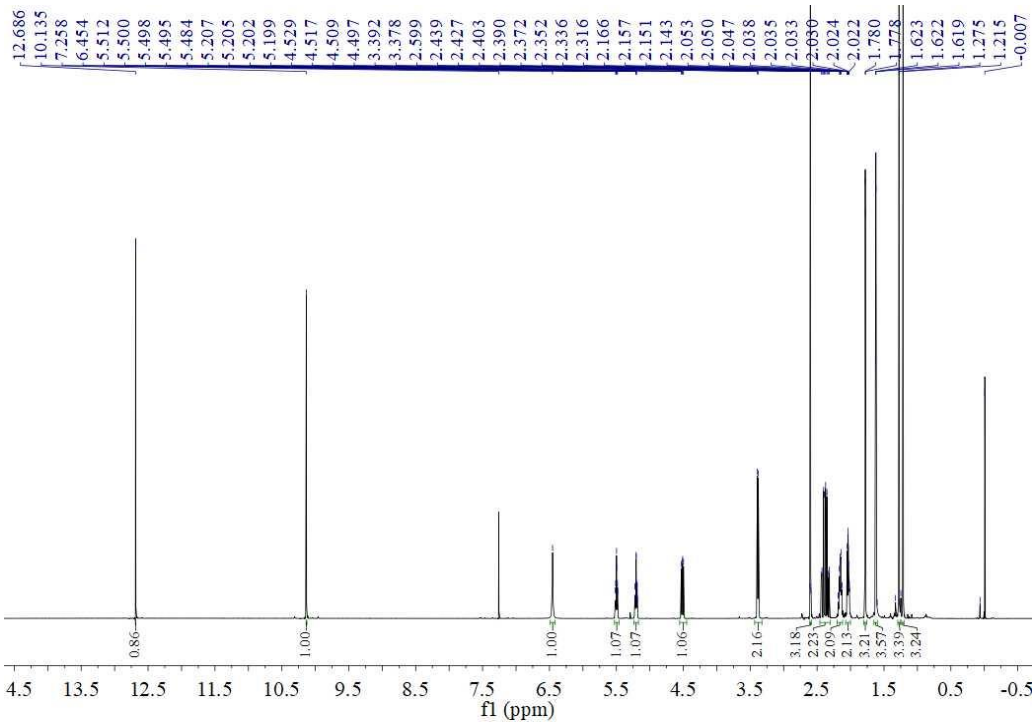

Figure S38: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **9**

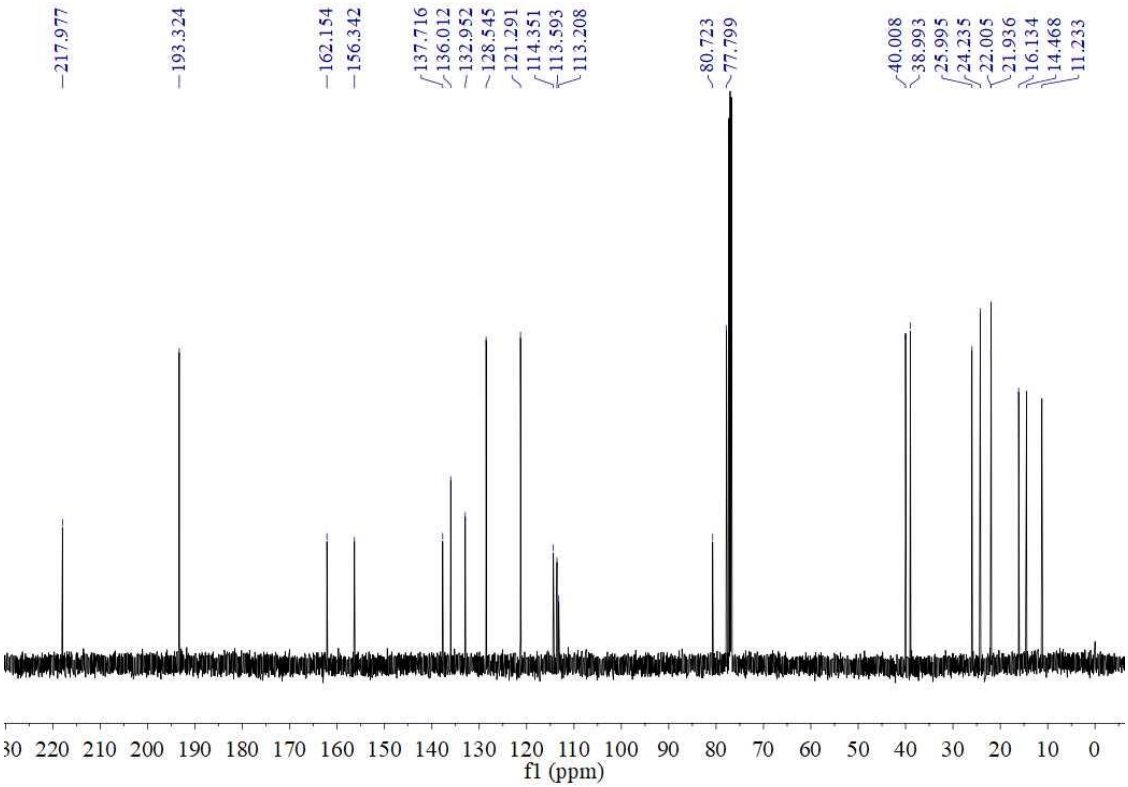

Figure S39: ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **9**

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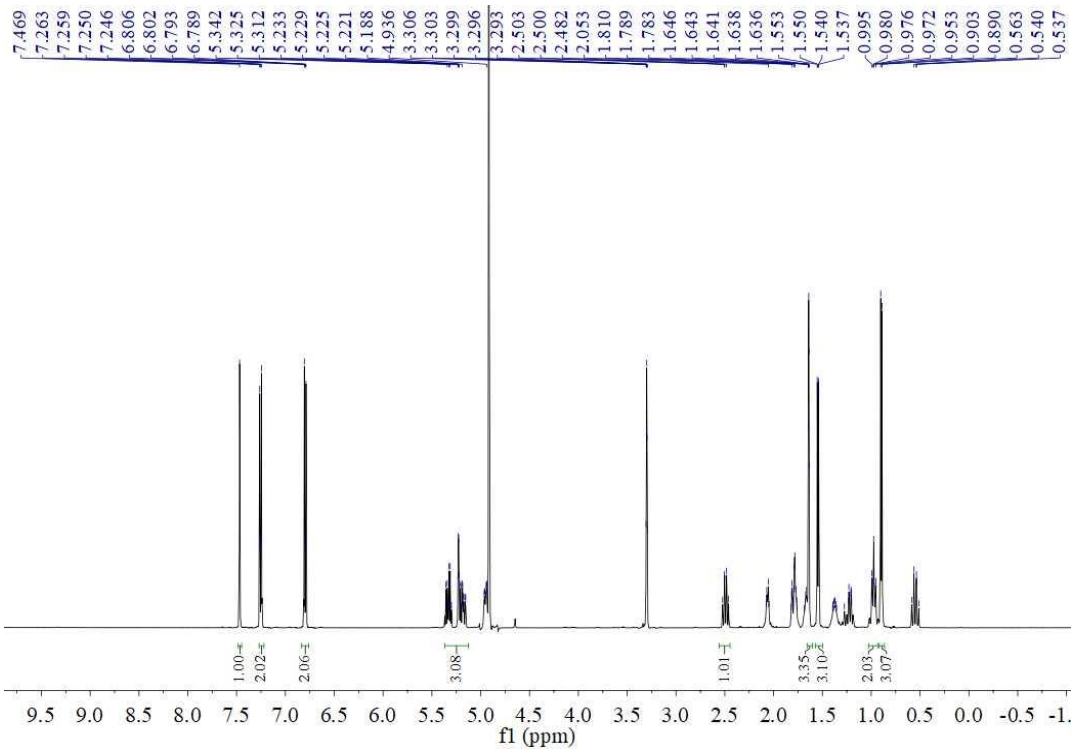

Figure S40: ^{1}H NMR (500 MHz, CD_3OD) spectrum of **10**

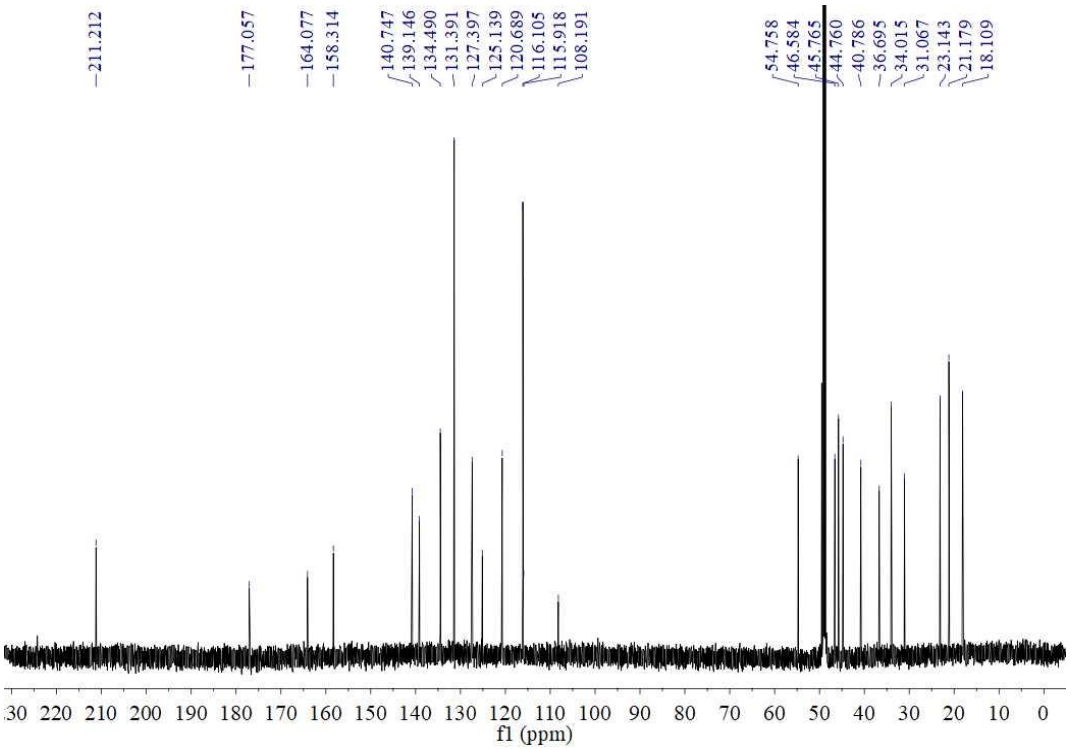

Figure S41: ^{13}C NMR (125 MHz, CD_3OD) spectrum of **10**

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Table S1 : Inhibitory effects of yeast α-glucosidase at the concentration of 10 mM

Compounds	Inhibitory rate (%)
1	62.7
2	6.1
3	26.6
7	59.9
8	54.6
10	56.1
Acarbose [a]	95.5

[a] positive control, the inhibitory rate was determined at the concentration of 4 μM.

Table S2 : Inhibitory activities of compounds **1**-**10** against tumor cells at the concentration of 40 μM

Compounds	Inhibitory rate (%)		
	DLD1	**SW1990**	**PANC1**
1	-	-	-
2	54.8	59.1	37.9
3	16.2	66.1	3.3
4	6.0	57.7	26.6
5	76.7	67.6	60.5
6	72.2	67.7	64.3
7	13.3	66.3	35.8
8	66.2	65.5	51.1
9	69.2	67.9	49.3
10	19.4	72.1	35.2

- inactive. DLD1 human colorectal carcinoma cells DLD1. SW1990 pancreatic cancer cell line SW1990. PANC1 pancreatic cancer cell line PANC1.

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Table S3 : Antibacterial activities of compounds **1-10**

compounds	MIC（μg/mL）					
	Actinomyces viscosus	***Staphylococcus epidermidis***	***Bacillus subtilis***	**MASR**	***Staphylococcus aureus***	***Micrococcus luteus***
1	-	-	-	-	-	-
2	31.25	15.625	62.500	-	125.000	-
3	7.81	3.90	3.90u0	62.500	7.810	3.90
4	7.81	7.81	7.810	7.810	15.6250	3.90
5	1.95	1.95	3.900	15.6250	7.810	7.81
6	1.95	3.90	7.810	-	15.6250	62.5
7	62.5	31.25	31.250	62.50	62.50	31.25
8	1.95	1.95	1.950	31.250	3.900	7.81
9	7.81	7.81	7.810	31.250	7.81	15.625
10	3.90	3.90	3.900	15.6250	-	1.95
Ciprofloxacin [a]	3.125	0.39	0.39	0.78	6.25	3.125

- no inhibitory activity at the concentration of 125 μg/mL. MRSA Methicillin-resistant *Staphylococcus aureus*. [a] positive control

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CAS SciFinder^{n}

Task History

Initiating Search

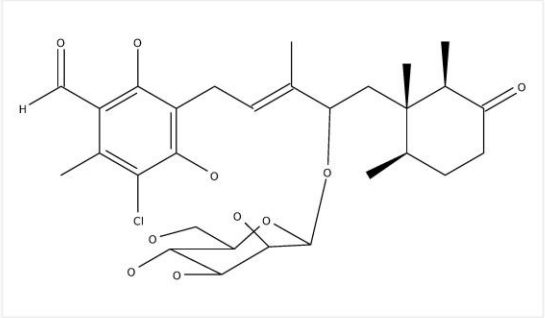
January 2, 2024, 4:09PM

Substances:

Filtered By:

Similarity: 95-98, 80-84

Number of Components: 1



Structure Match: **Similarity**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (16)	Substances	View Results

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Figure S43: Scifinder Search report for compound **1** (exact match)

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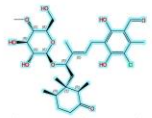
CAS SciFinder^{n}

Substances (4)

View in SciFinder^{n}

1 Similarity Score: 99

765956-86-3



Absolute stereochemistry shown
Double bond geometry shown

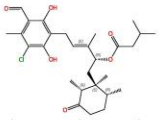
$C_{30}H_{43}ClO_{10}$

3-Chloro-4,6-dihydroxy-2-methyl-5-[(2*E*,4*R*)-3-methyl-4-[(4-*O*-methyl-β-D-glucopyranosyl)oxy]-5-[(1*S*,2*R*,6*R*)-1,2,6-trimethyl-3-oxocyclohexyl]-2-penten-1-yl]benzaldehyde

2 References | 0 Reactions | 0 Suppliers

2 Similarity Score: 83

165187-17-7



Absolute stereochemistry shown,
Rotation (+)
Double bond geometry shown

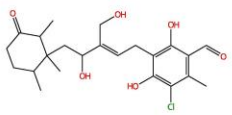
$C_{28}H_{39}ClO_{6}$

(1*R*,2*E*)-4-(3-Chloro-5-formyl-2,6-dihydroxy-4-methylphenyl)-2-methyl-1-[[(1*S*,2*R*,6*R*)-1,2,6-trimethyl-3-oxocyclohexyl]methyl]-2-buten-1-yl 3-methylbutanoate

4 References | 1 Reaction | 1 Supplier

3 Similarity Score: 83

2111912-99-1



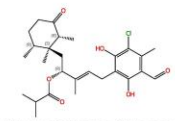
$C_{23}H_{31}ClO_{6}$

3-Chloro-4,6-dihydroxy-5-[4-hydroxy-3-(hydroxymethyl)-5-(1,2,6-trimethyl-3-oxocyclohexyl)-2-penten-1-yl]-2-methylbenzaldehyde

0 References | 0 Reactions | 1 Supplier

4 Similarity Score: 83

1214976-02-9



Relative stereochemistry shown
Double bond geometry unknown

$C_{27}H_{37}ClO_{6}$

rel-(1*S*)-4-(3-Chloro-5-formyl-2,6-dihydroxy-4-methylphenyl)-2-methyl-1-[[(1*R*,2*S*,6*S*)-1,2,6-trimethyl-3-oxocyclohexyl]methyl]-2-buten-1-yl 2-methylpropanoate

0 References | 0 Reactions | 0 Suppliers

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Figure S44: Scifinder Search report for compound **1** (>95 % match)

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Table S4: Comparison of NMR data between **1** and vertihemipterin A

Position	1 in CD_3OD		Vertihemipterin A in $CDCl_3$	
	δ_C (type)	δ_H (multiplicity, *J* in *Hz*)	δ_C (type)	δ_H (multiplicity, *J* in *Hz*)
1	114.3 (C)		113.5 (C)	
2	161.5 (C)		162.0 (C)	
3	113.6 (C)		113.3 (C)	
4	159.3 (C)		156.2 (C)	
5	112.4 (C)		113.3 (C)	
6	138.3 (C)		138.3 (C)	
7	13.2 (CH_3)	2.55 (s)	14.5 (CH_3)	2.60 (s)
8	193.2 (C)		193.3 (C)	
9	21.0 (CH_2)	3.40 (dd, 13.5, 8)	21.5 (CH_2)	3.40 (m) ; 3.37 (m)
10	125.0 (CH)	5.57 (t, 7.5)	124.4 (CH)	5.41 (t, 7.0)
11	137.2 (C)		138.3 (C)	
12	83.0 (CH)	4.16 (t, 6.0)	85.1 (CH)	6.42 (dd, 6.1, 4.2)
13	39.3 (CH_2)	1.77 (dd, 15.5, 6.0); 1.50 (dd, 15.5, 5.0)	40.6 (CH_2)	1.85 (dd, 15.6, 6.6) ; 1.4 (dd, 15.6, 3.9)
14	43.7 (C)		44.0 (C)	
15	36.0 (CH)	2.21 (m)	36.5 (CH)	2.22 (m)
16	30.9 (CH_2)	1.79 (m); 1.50 (dq, 12.5, 5.0)	31.1 (CH_2)	1.80 (m); 1.57 (dq, 13.0, 5.4)
17	41.0 (CH_2)	2.18 (m); 2.12 (m)	41.3 (CH_2)	2.28 (ddd, 13.5, 5.4, 2.4); 2.21 (m)
18	215.4 (C)		213.8 (C)	
19	50.1 (CH)	2.59 (q, 7.0)	50.4 (CH)	2.53 (q, 6.7)
20	14.6 (CH_3)	0.51 (s)	15.6 (CH_3)	0.57 (s)
21	14.7 (CH_3)	0.97 (d, 6.5)	15.8 (CH_3)	0.98 (d, 6.7)
22	7.2 (CH_3)	0.69 (d, 7.0)	8.1 (CH_3)	0.77 (d, 6.7)
23	10.5 (CH_3)	1.83 (s)	11.5 (CH_3)	1.82 (s)
1′	99.4 (CH)	4.45 (brs)	101.9 (CH)	4.22 (d, 7.9)
2′	71.4 (CH)	3.82 (d 3.0)	74.1 (CH)	3.38 (m)
3′	74.2 (CH)	3.37 (dd, 9.5, 3.0)	76.7 (CH)	3.56 (t, 8.8)
4′	66.7 (CH)	3.59 (t, 9.5)	79.9 (CH)	3.08 (dd, 9.5, 8.7)
5′	76.6 (CH)	2.97 (ddd, 9.5, 5.0, 3.0)	75.2 (CH)	3.14 (ddd, 9.5, 5.7, 2.8)
6′	61.1 (CH_2)	3.69 (dd, 11.5, 3.0); 3.65 (dd, 11.5, 5.0)	62.5 (CH_2)	3.79 (dd, 11.6, 2.7) 3.64 (dd, 11.6, 5.7)
4′-OCH_3			60.7 (CH_3)	3.55 (s)

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