Supporting Information

***Rec. Nat. Prod*. 20:4 (2026):e25113727**

Bioactive compounds from the cultured lichen mycobiont of *Nigrovothelium inspersotropicum*

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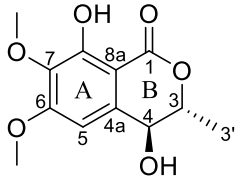
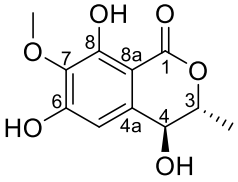
Table S1. ^{1}H-NMR and ^{13}C-NMR data of **1** in Acetone-d_6, **Lignicol** in CD_3OD, and **(3*R*, 4*R*)-6,7-dimethoxy-4-hydroxymellein** in $CDCl_3$.

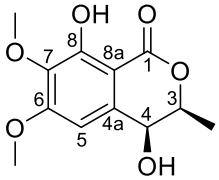
No.	**1**		**Lignicol (3)**		**(3*R*, 4*R*)-6,7-dimethoxy-4-hydroxymellein**	
	δ_H (ppm, *J* in Hz) (Acetone-d_6, 500 MHz)	δ_C (ppm) (Acetone-d_6, 125 MHz)	δ_H (ppm, *J* in Hz) (CD_3OD, 500 MHz)	δ_C (ppm) (CD_3OD, 125 MHz)	δ_H (ppm, *J* in Hz) ($CDCl_3$, 500 MHz)	δ_C (ppm) ($CDCl_3$, 125 MHz)
1		-		170.5		170.9
3	4.53 (*m*)	80.7	4.50 (*m*)	81.4	4.65 (*dd*, 2.1, 6.7)	79.8
4	4.63 (*t*, 7.5)	69.1	4.50 (*m*)	65.9	4.50 (*d*, 1.9)	67.7
4a		136.7*		140.2		139.3
5	6.84 (*s*)	103.8	6.67 (*s*)	106.9	6.70 (*s*)	104.3
6		160.5*		158.8		160.2
7		136.5*		135.7		134.2
8		156.4*		157.4		156.7
8a		117.4*		100.9		102.9
3′	1.47 (*d*, 6.5)	18.1	1.50 (*d*, 6.0)	18.1	1.49 (*d*, 6.6)	16.3
4-OH	5.23 (*d*, 7.0)		2.06 (*d*, 6.0)			
6-OMe	3.94 (*s*)	56.5			3.94 (*s*)	56.8
7-OMe	3.77 (*s*)	60.3	4.03 (*s*)	60.9	3.80 (*s*)	60.9
8-OH	11.16 (*s*)		11.36 (*s*)			



2



Lignicol (3)

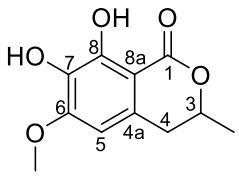


(3*R*,4*R*)-6,7-dimethoxy-4-hydroxymellein

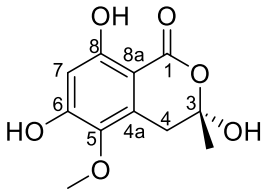
*determined by HMBC correlations

Table S2. ^{1}H-NMR and ^{13}C-NMR data of **2**, **Embeurekol A** in in DMSO-d_6, and **(3*R*)-methyl-8-hydroxy-6-(hydroxymethyl)-7-methoxydihydro isocoumarin** in $CDCl_3$.

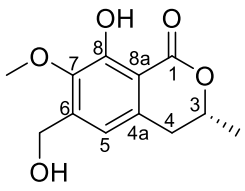
No.	**2**		**Embeurekol A**		**(3*R*)-methyl-8-hydroxy-6-(hydroxymethyl)-7-methoxydihydro isocoumarin**	
	δ_H (ppm, *J* in Hz) (DMSO-d_6, 500 MHz)	δ_C (ppm) (DMSO-d_6, 125 MHz)	δ_H (ppm, *J* in Hz) (DMSO-d_6, 600 MHz)	δ_C (ppm) (DMSO-d_6, 150 MHz)	δ_H (ppm, *J* in Hz) ($CDCl_3$, 400 MHz)	δ_C (ppm) ($CDCl_3$, 100 MHz)
1		171.7		168.2		169.3
3	4.39 (*m*)	73.7		105.1	4.67 (*m*)	75.8
4*α*	2.71 (*d*, 2.0)	33.2	3.10 (*d*, 16.9)	32.2	2.87 (*m*)	34.7
4*β*	2.56 (*m*)		3.18 (*d*, 16.9)		2.87 (*m*)	
4a		133.9		130.9		134.0
5	6.46 (*s*)	126.0		137.8	6.68 (*s*)	122.3
6		157.3		158.3		133.2
7		127.8	6.29 (*s*)	101.6		146.2
8		156.8		159.1		152.4
8a		111.2		98.5		114.1
3′	1.34 (*d*, 6.5)	20.5	1.62 (*s*)	22.3	1.51 (*d*, 6.3)	20.7
5-OMe			3.63 (*s*)	60.2		
6-OMe	3.83 (*s*)	56.0				
6-OH			10.70 (*s*)			
7-OMe					3.86 (*s*)	60.9
8-OH	15.30 (*s*)		10.90 (*s*)		11.14 (*s*)	



3



Embeurekol A



(3*R*)-methyl-8-hydroxy-6-(hydroxymethyl)-7-methoxydihydroisocoumarin

Table S3. ^{1}H-NMR and ^{13}C-NMR data of **5** in Acetone-d_6 and **Aspermytin A** in Pyridine-d_5.

No.	5		Aspermytin A	
	$\delta_{H,}$ (ppm, *J* in Hz) (Acetone-d_6, 500 MHz)	δ_C (ppm) (Acetone-d_6, 125 MHz)	$\delta_{H,}$ (ppm, *J* in Hz) (Pyridine-d_5, 500 MHz)	δ_C (ppm) (Pyridine-d_5, 125 MHz)
1	3.76 (2H, *m*)	58.4	4.30 (2H, *m*)	57.6
2	2.65 (1H, *dt*, 18.0, 6.0) 3.08 (1H, *dt*, 18.0, 6.0)	45.1	3.05 (1H, *dt*, 18.1, 6.4) 3.65 (1H, *dt*, 18.1, 6.4)	45.6
3		214.6		214.1
4		57.6		57.7
5	1.79 (1H, *m*)	44.3	2.07 (1H, *dt*, 2.1, 10.9)	43.7
6	1.18 (1H, *m*) 1.70 (1H, *m*)	28.2	1.00 (1H, *dq*, 2.0, 10.9) 1.82 (1H. *m*)	27.8
7	0.99 (2H, *t*, 10.0)	36.5	1.02 (1H, *dq*, 2.0, 10.9) 1.63 (1H, *m*)	35.7
8	1.47 (1H, *m*)	34.2	1.35 (1H, *m*)	33.4
9	0.77 (1H, *q*, 12.0) 1.56 (1H, *d*, 7.5)	42.6	0.78 (1H, *q*, 12.2) 1.66 (1H, *m*)	41.9
10	1.78 (1H, *m*)	39.4	1.77 (1H, *ddd*, 12.2, 10.9, 2.1)	38.7
11	5.30 (1H, *dd*, 10.0, 2.0)	130.2	5.37 (1H, *dd*, 9.8, 1.0)	129.5
12	5.36 (1H, *dd*, 9.5, 2.5)	135.4	5.71 (1H, *dd*, 9.8, 2.9)	135.5
13		73.7		73.2
14	1.05 (3H, *s*)	28.4	1.49 (3H, *s*)	28.5
15	1.31 (3H, *s*)	12.5	1.54 (3H, *s*)	12.6
16	0.89 (3H, *d*, 6.5)	22.8	0.84 (3H, *d*, 6.8)	22.5
1-OH	3.45 (1H, *q*, 5.0)		5.94 (1H, *t*, 5.4)	
13-OH	3.93 (1H, *d*, 2.5)		6.46 (1H, *s*)	

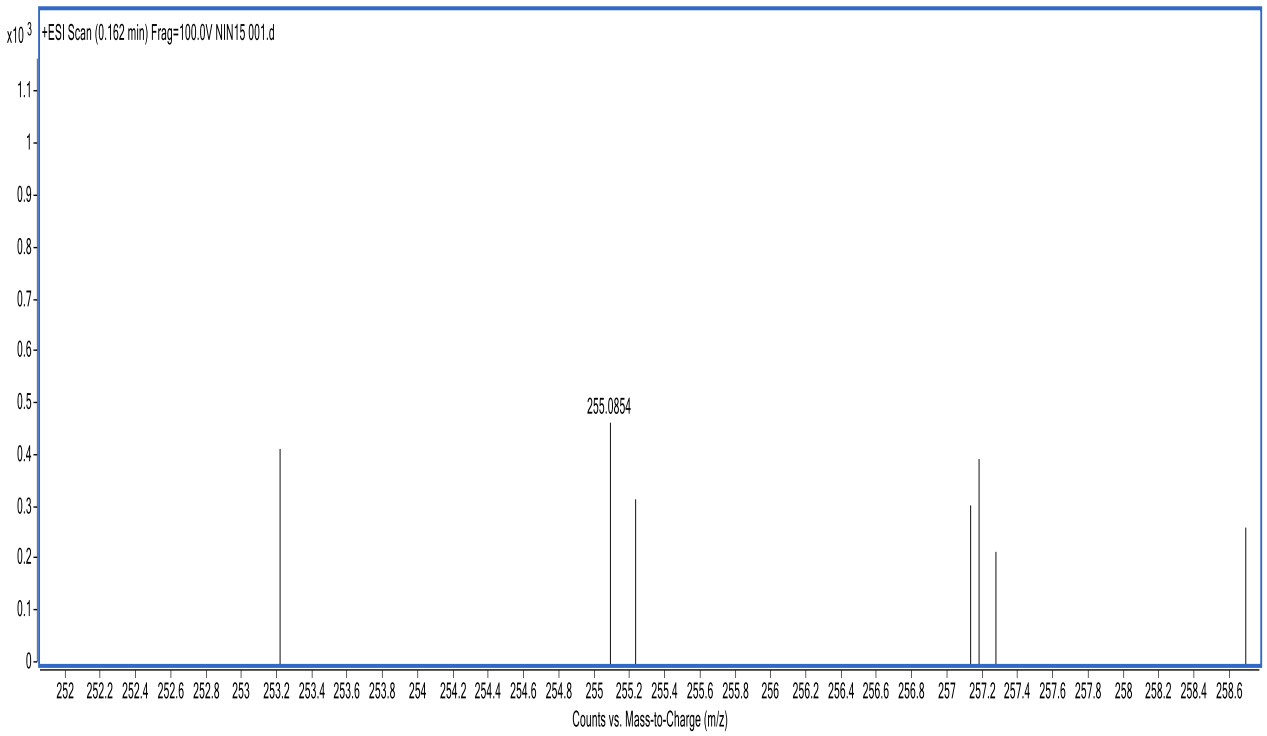


Figure S1.1. HRESIMS spectrum of **1.**

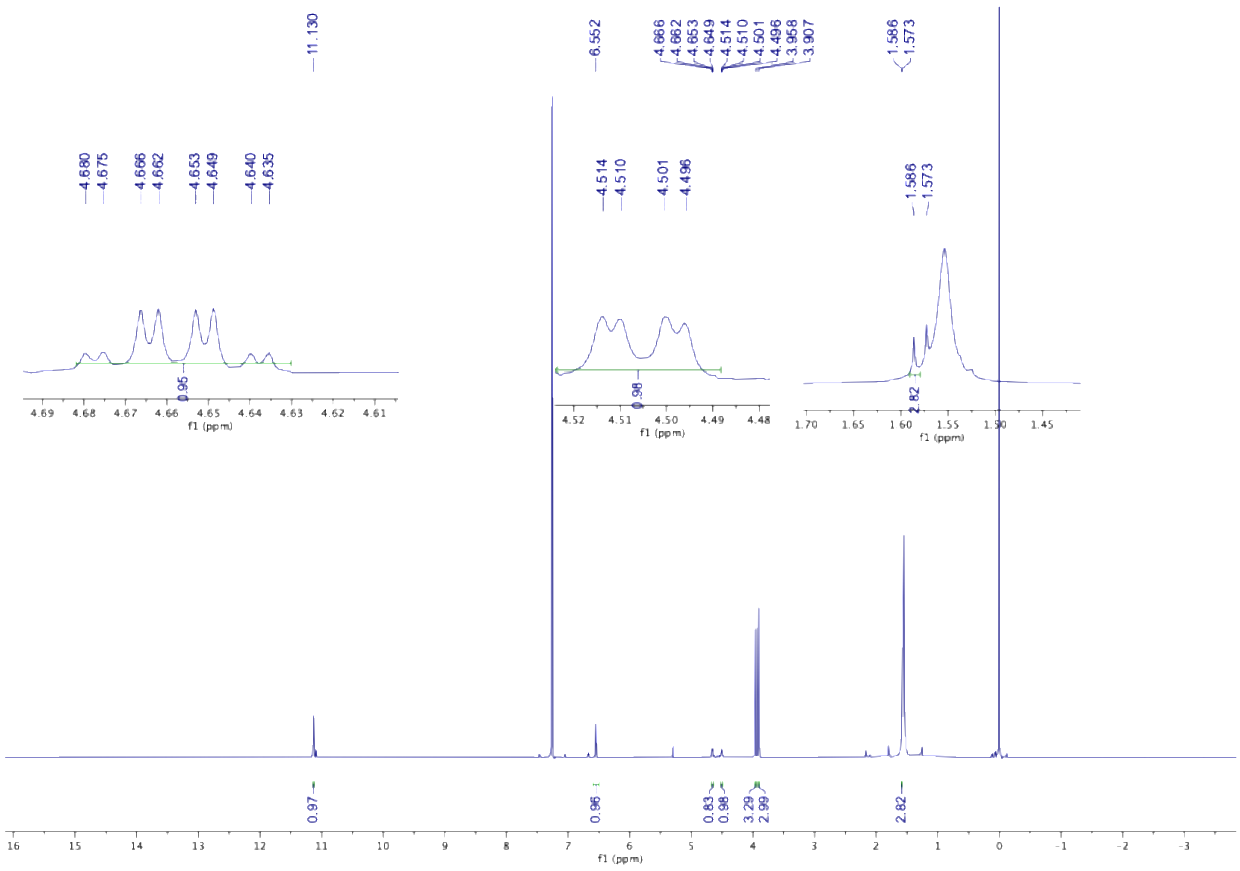


Figure S1.2. ^{1}H-NMR (chloroform-*d*$_1$, 500 MHz) spectrum of **1.**

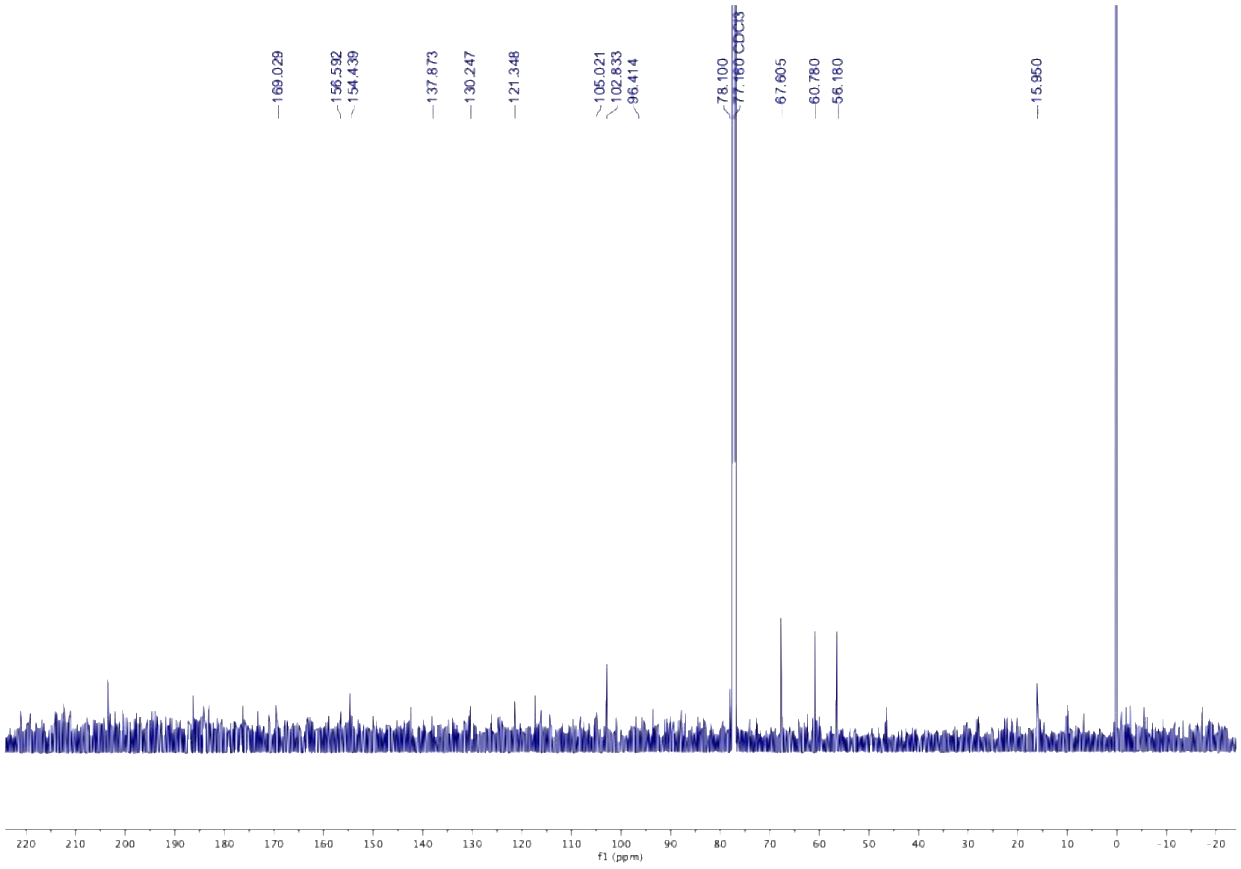


Figure S1.3. ^{13}C-NMR (chloroform-*d*$_1$, 125 MHz) spectrum of **1.**

Figure S1.4. The HSQC (chloroform-d_1) spectrum of **1.**

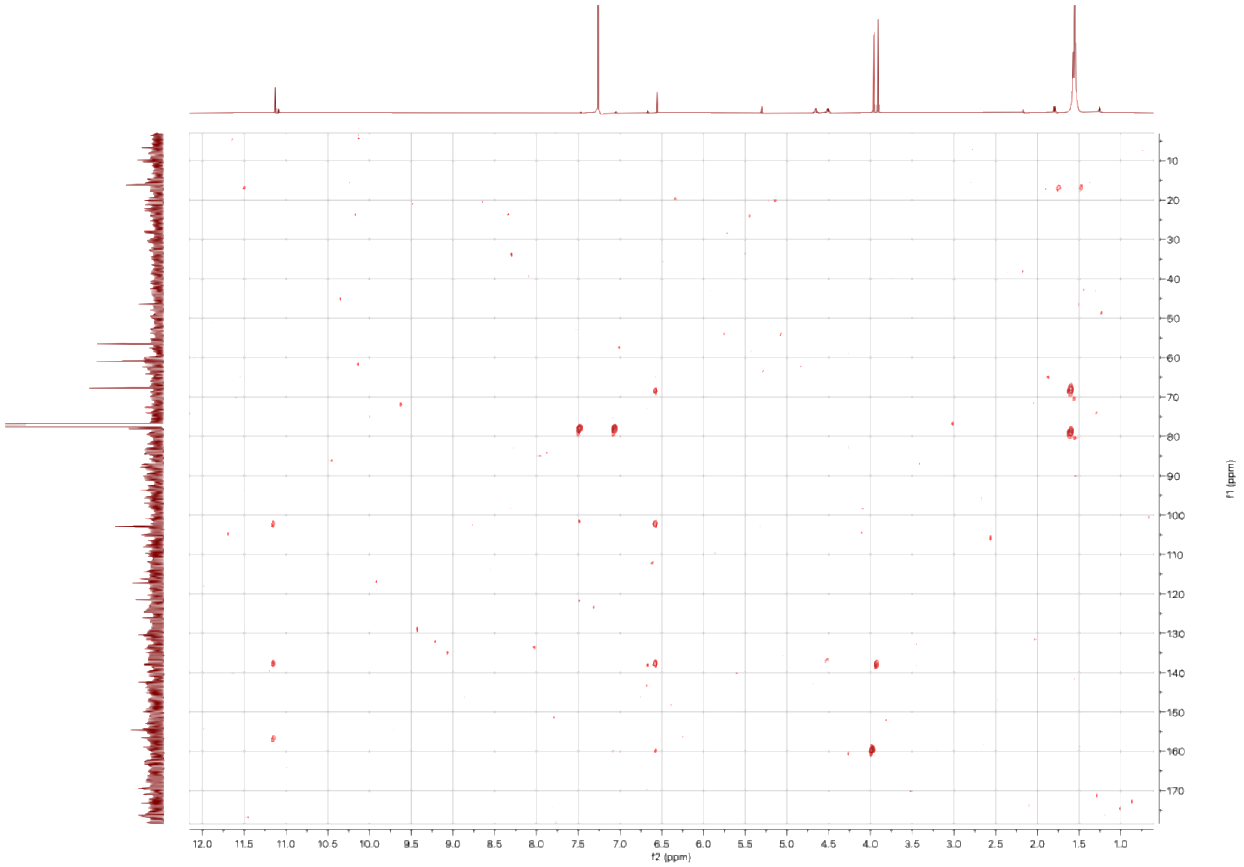


Figure S1.5. The HMBC (chloroform-d_1) spectrum of **1.**

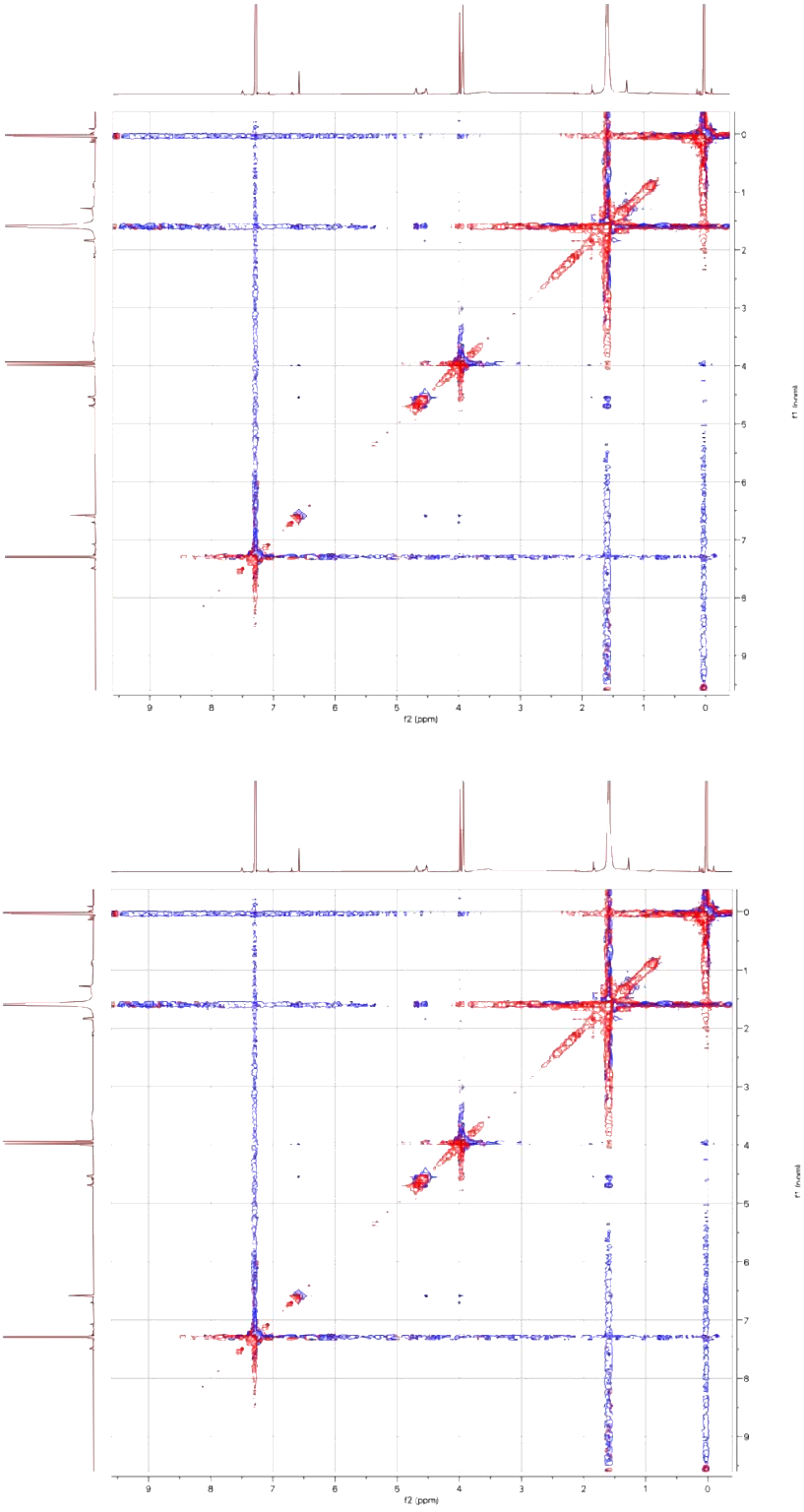


Figure S1.6. The NOESY (chloroform-d_1) spectrum of **1.**

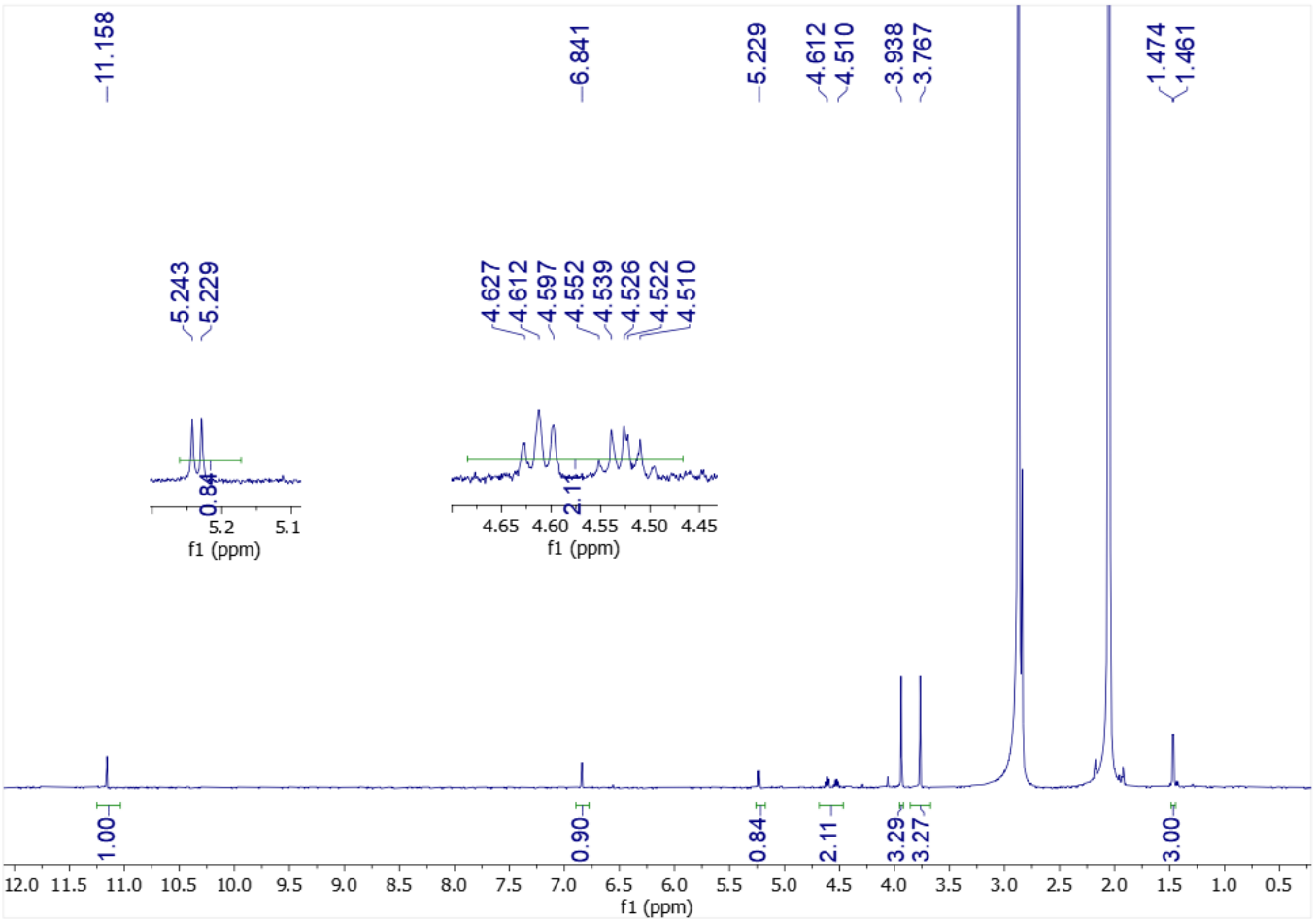


Figure S1.7. ^{1}H-NMR (acetone-d_6, 500 MHz) spectrum of **1.**

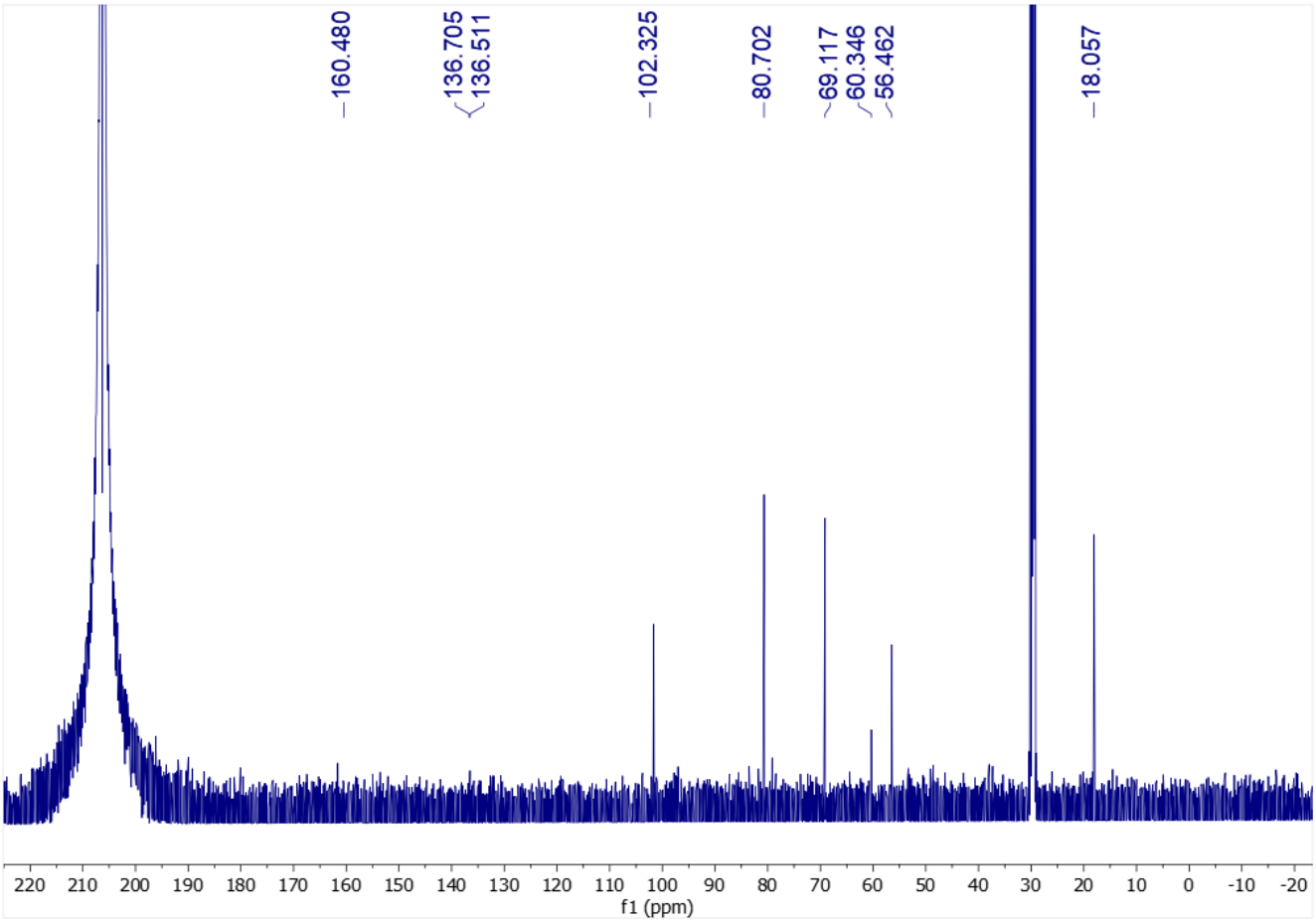


Figure S1.8. ^{13}C-NMR (acetone-d_6, 125 MHz) spectrum of **1.**

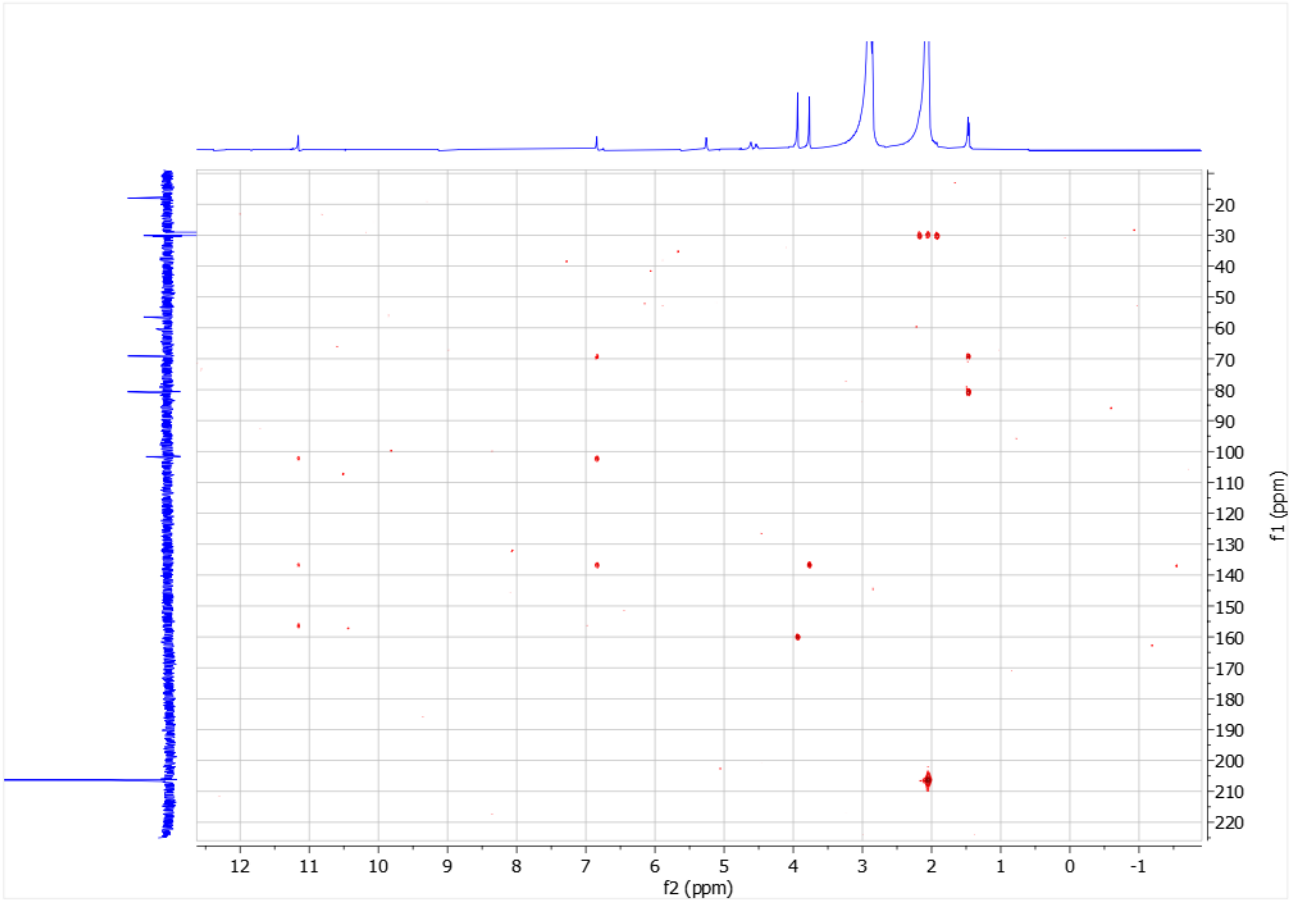


Figure S1.9. The HMBC (acetone-d_6) spectrum of **1.**

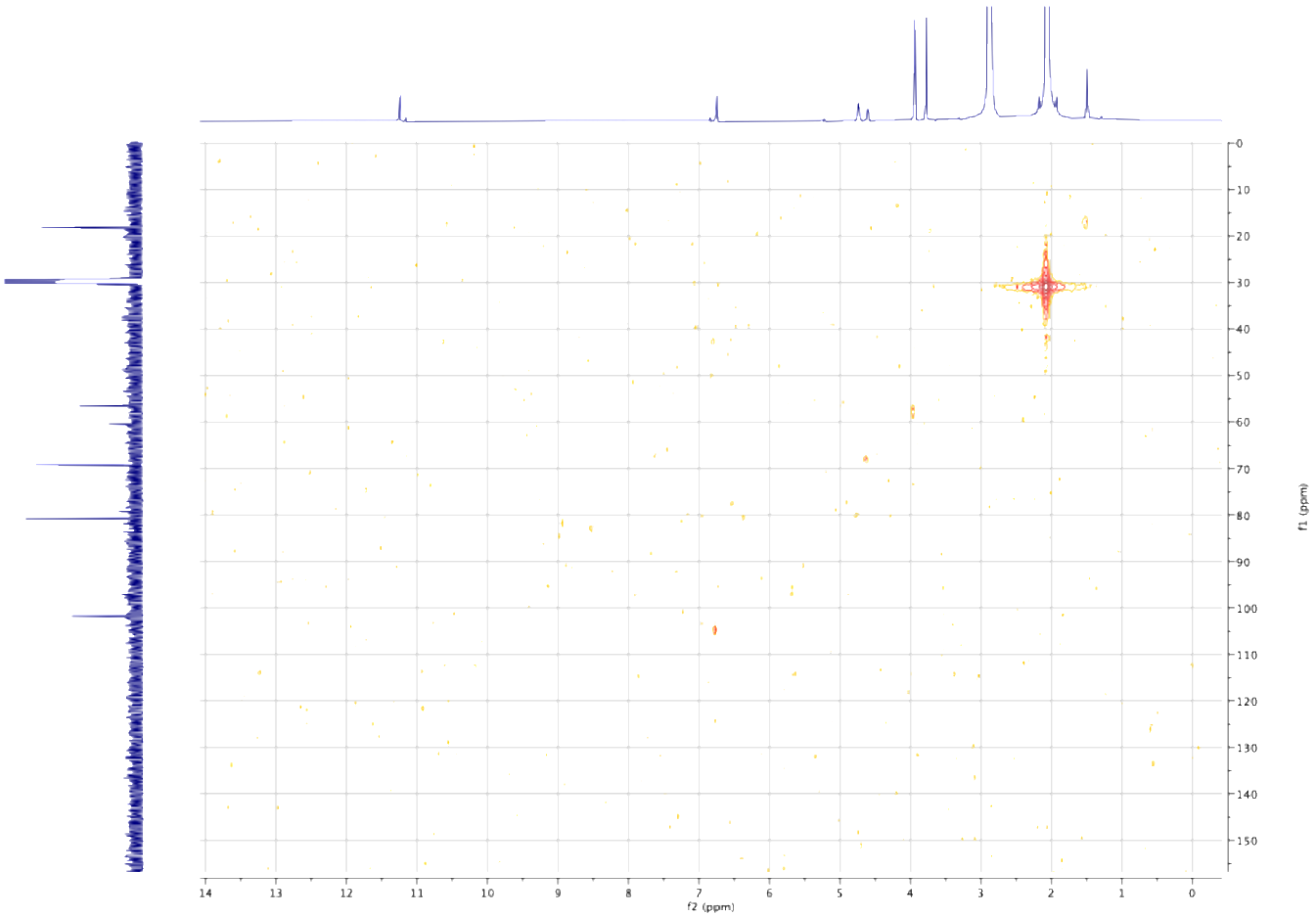


Figure S1.10. The HSQC (acetone-d_6) spectrum of **1.**

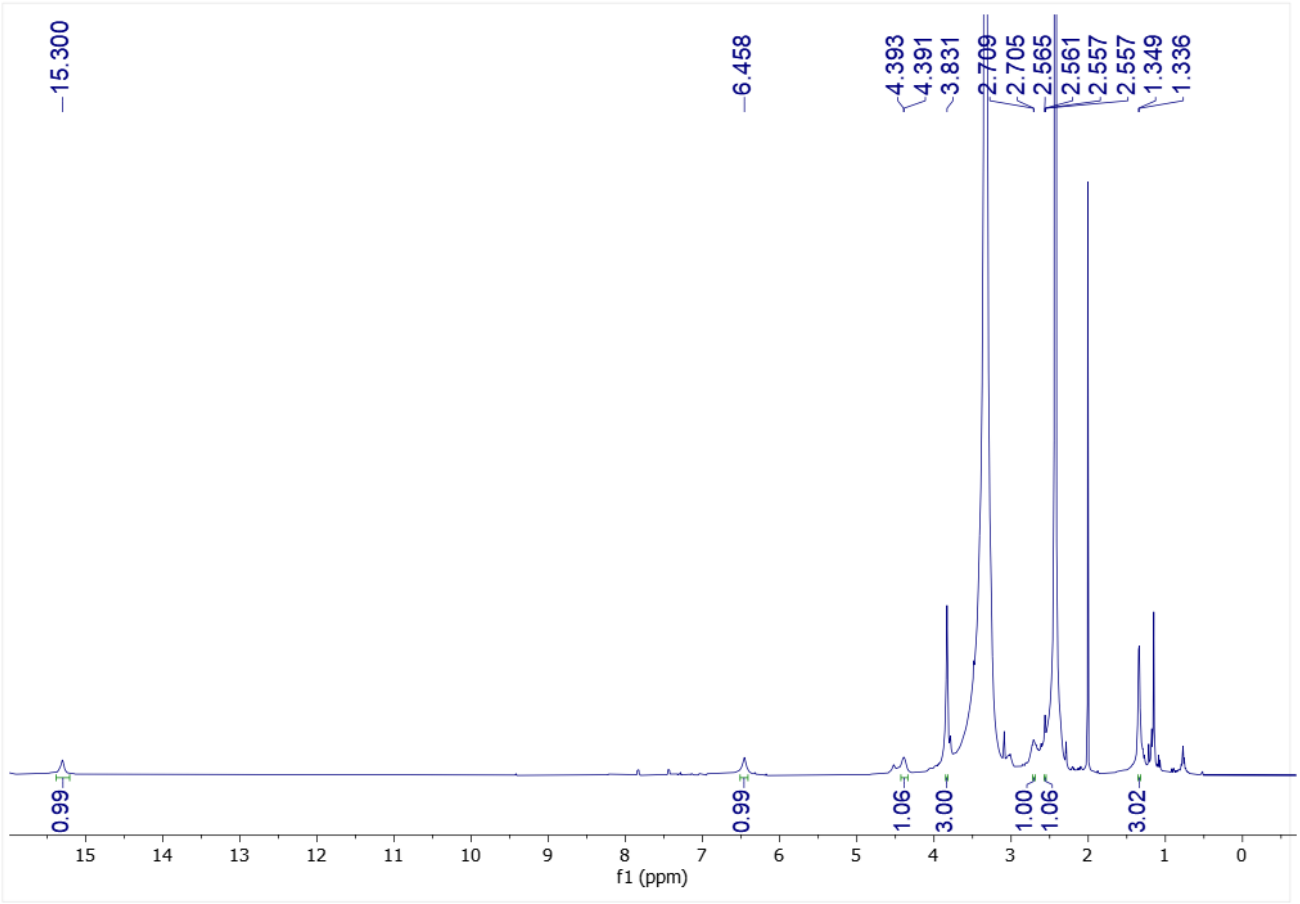


Figure S2.1. ^{1}H-NMR (DMSO-d_6, 500MHz) spectrum of **2.**

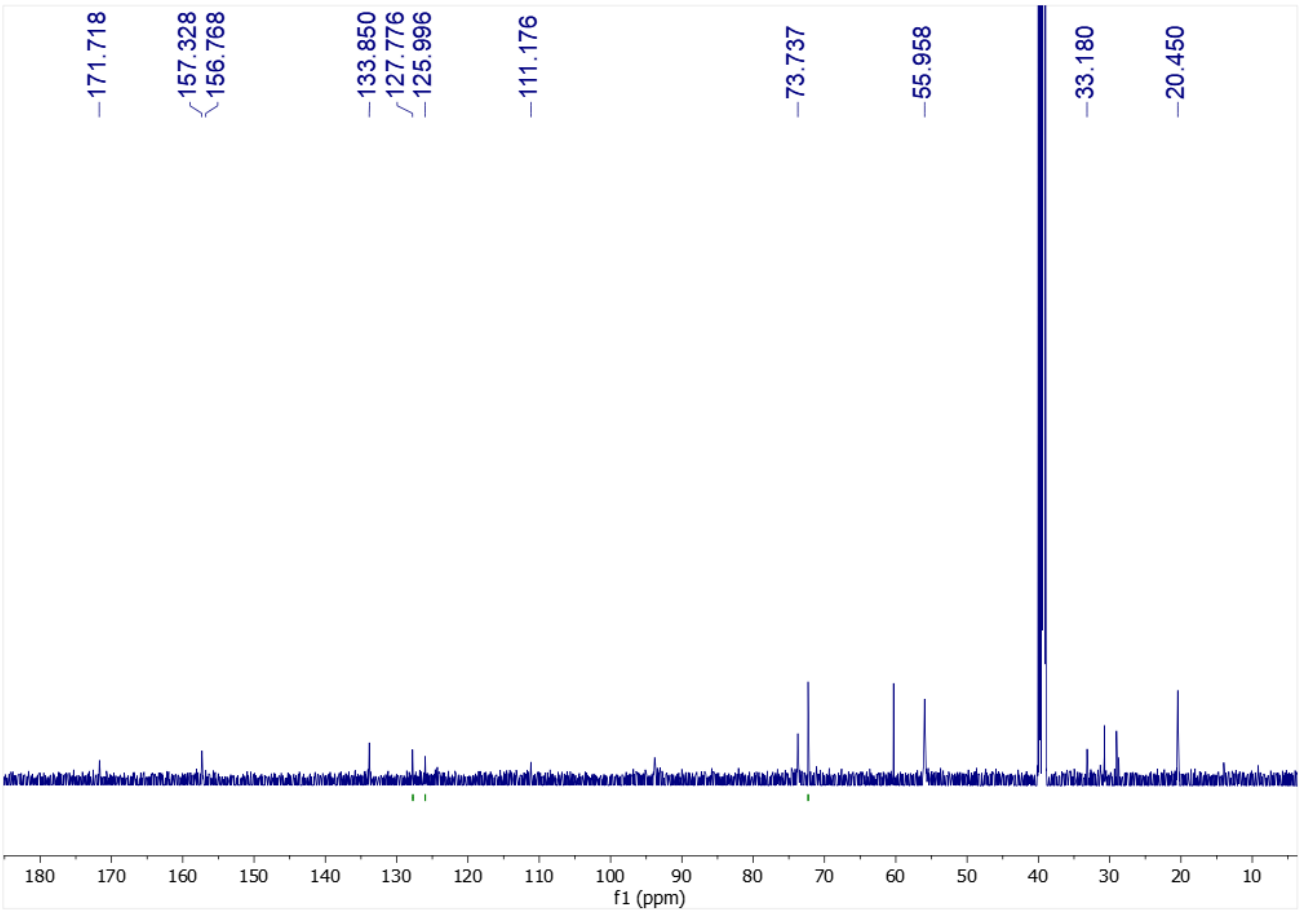


Figure S2.2. ^{13}C-NMR (DMSO-d_6, 125 MHz) spectrum of **2.**

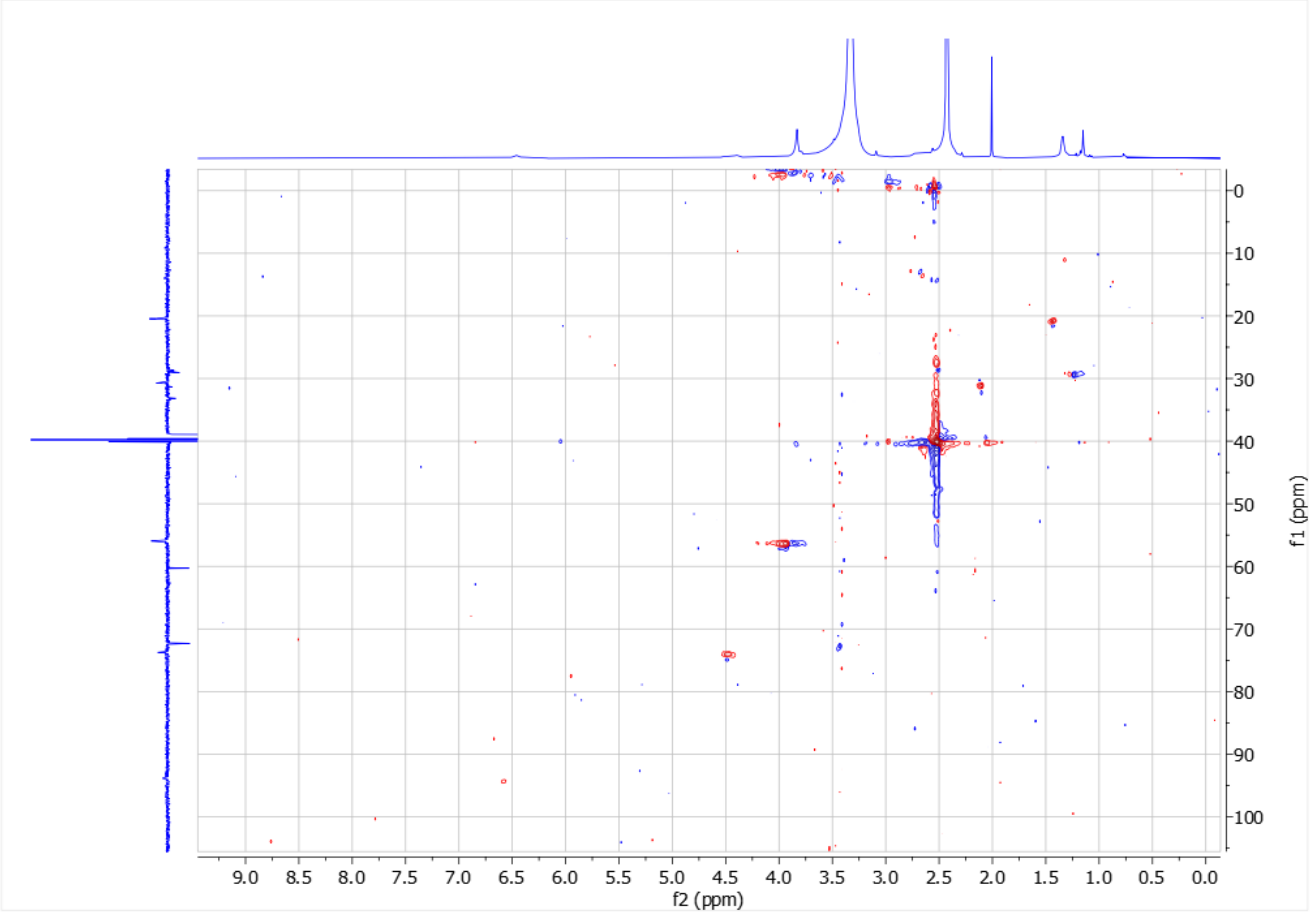


Figure S2.3. The HSQC (DMSO-d_6) spectrum of **2.**

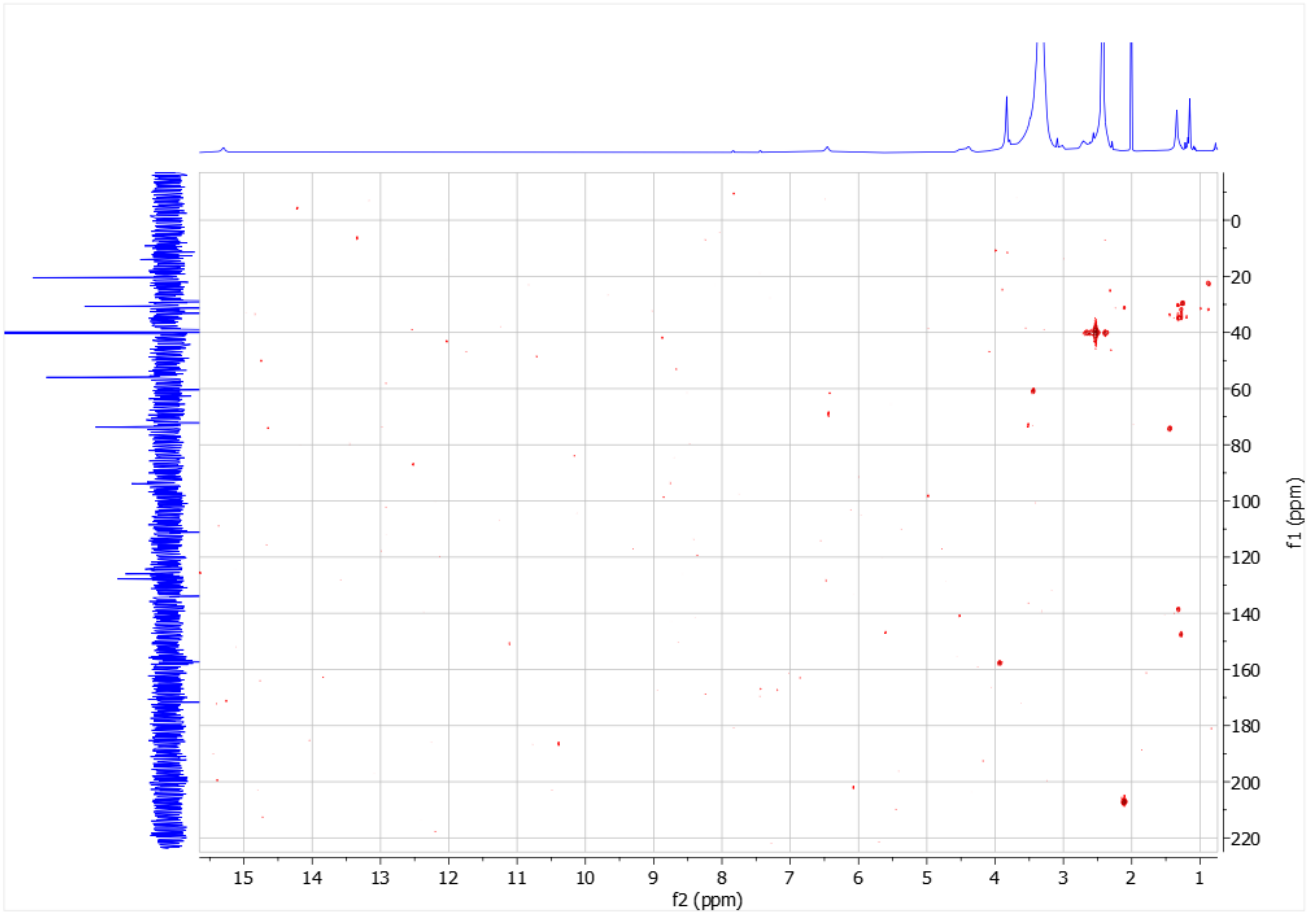


Figure S2.4. The HMBC (DMSO-d_6) spectrum of **2.**

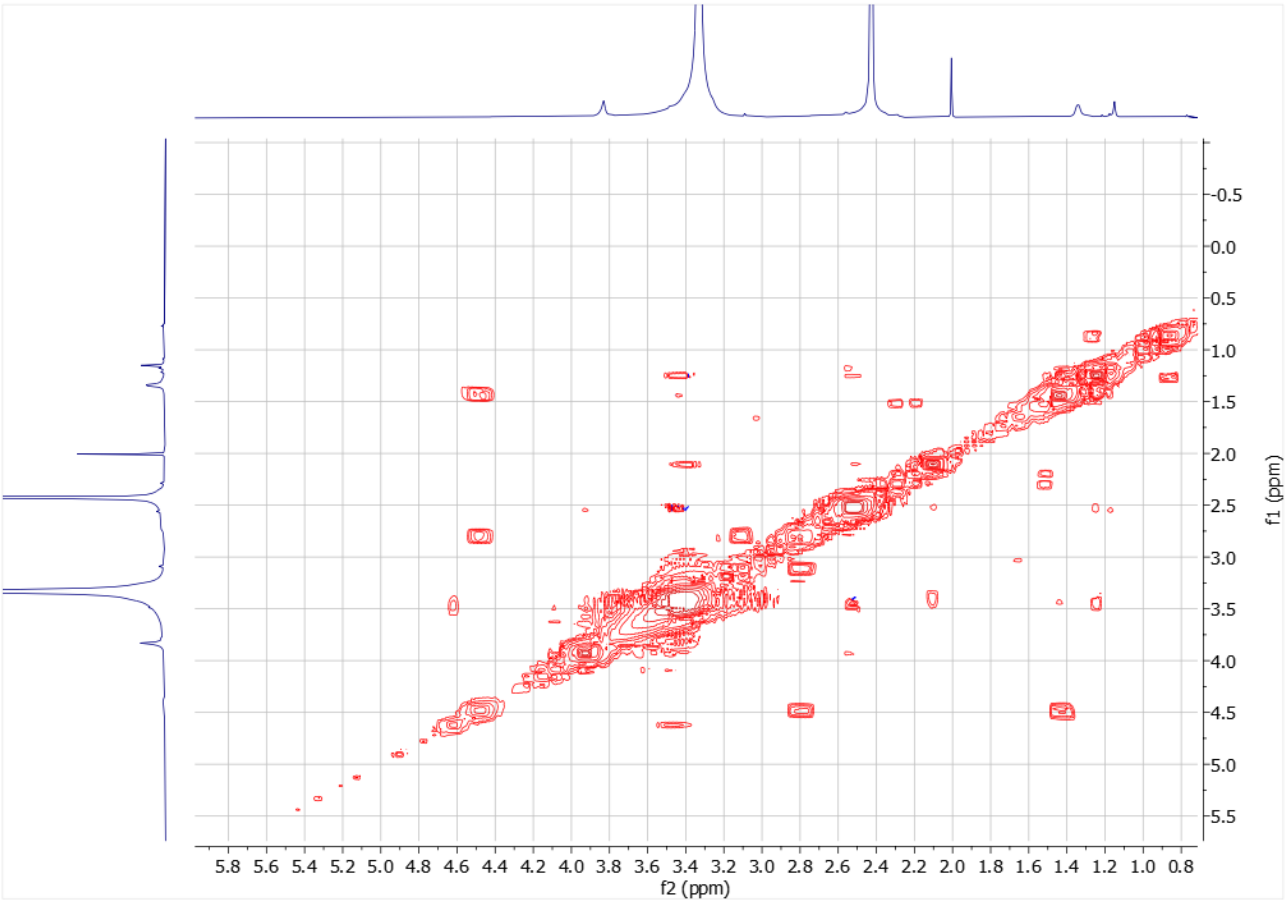


Figure S2.5. The COSY (DMSO-d_6) spectrum of **2.**

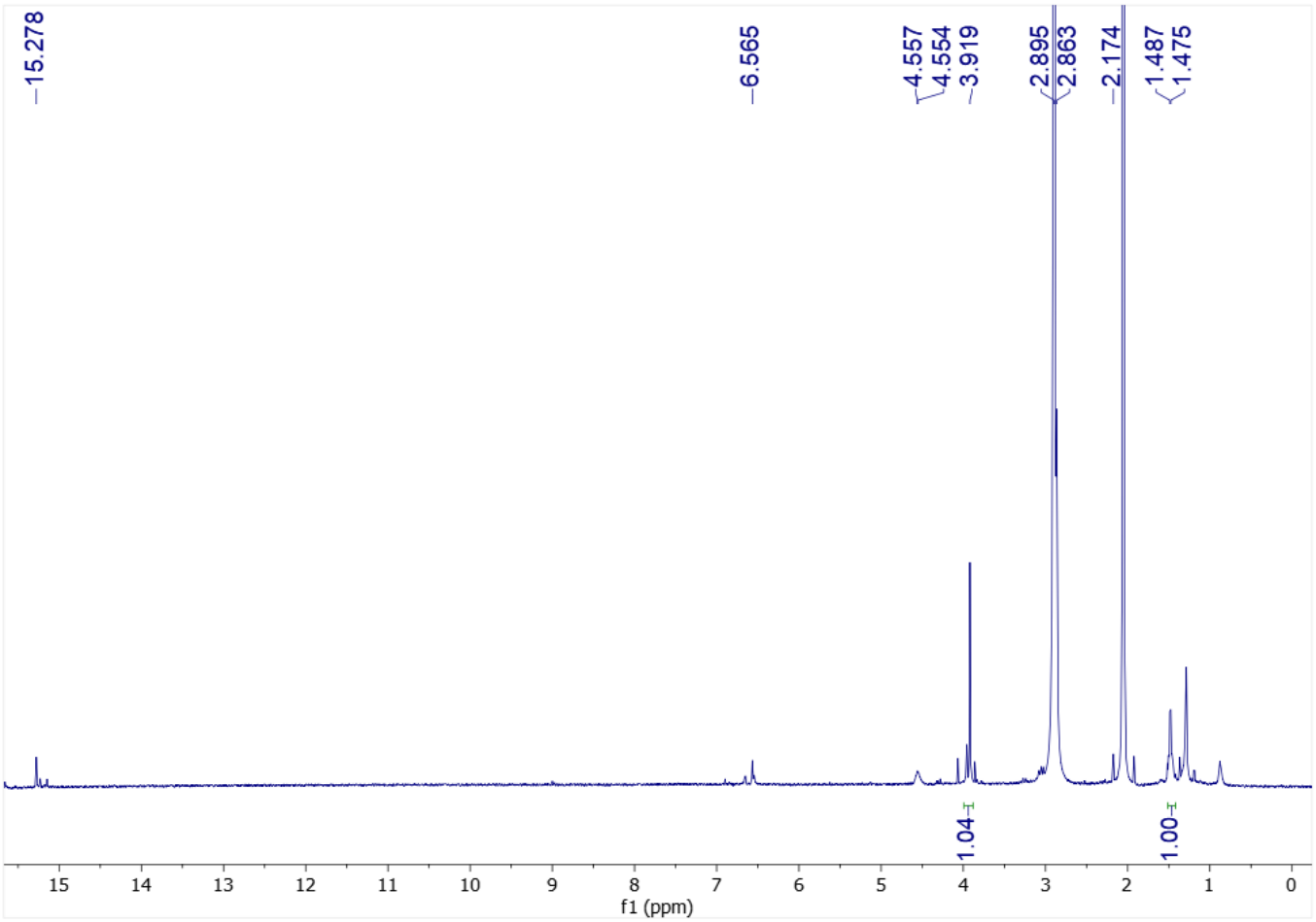


Figure S2.6. ^{1}H-NMR (Acetone-d_6, 500MHz) spectrum of **2.**

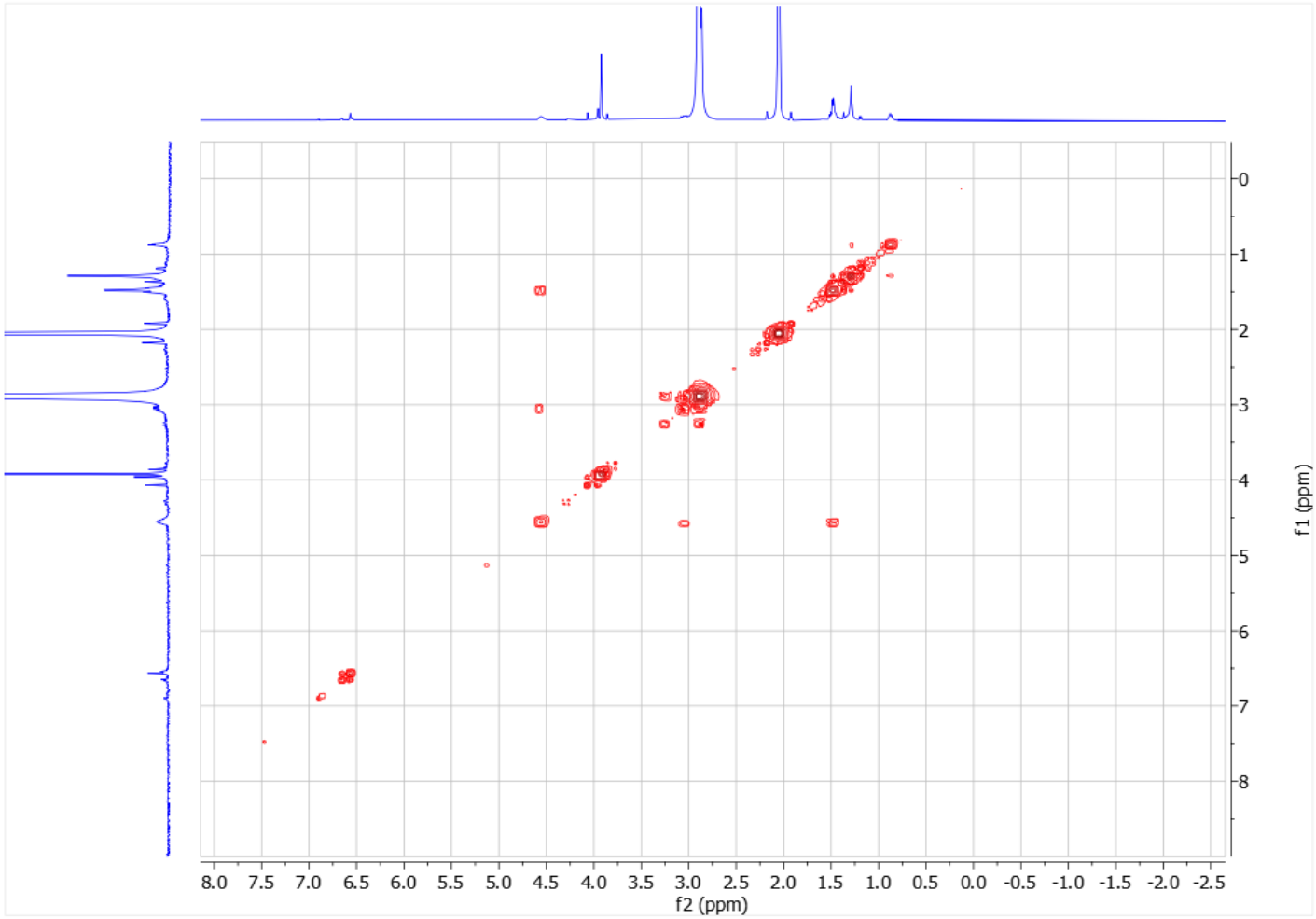


Figure S2.7. The COSY (Acetone-d_6) spectrum of **2.**

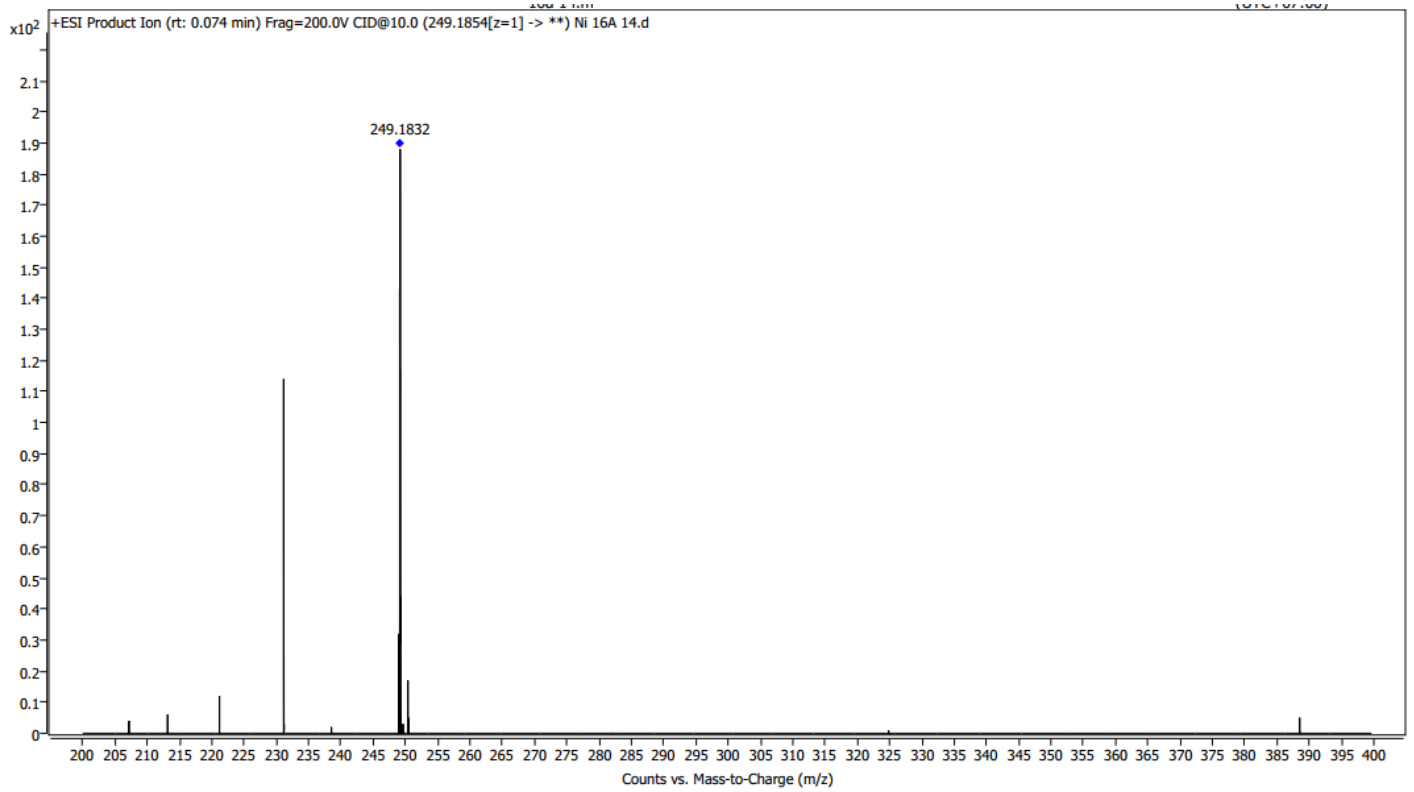


Figure S3.1. HRESIMS spectrum of **5.**

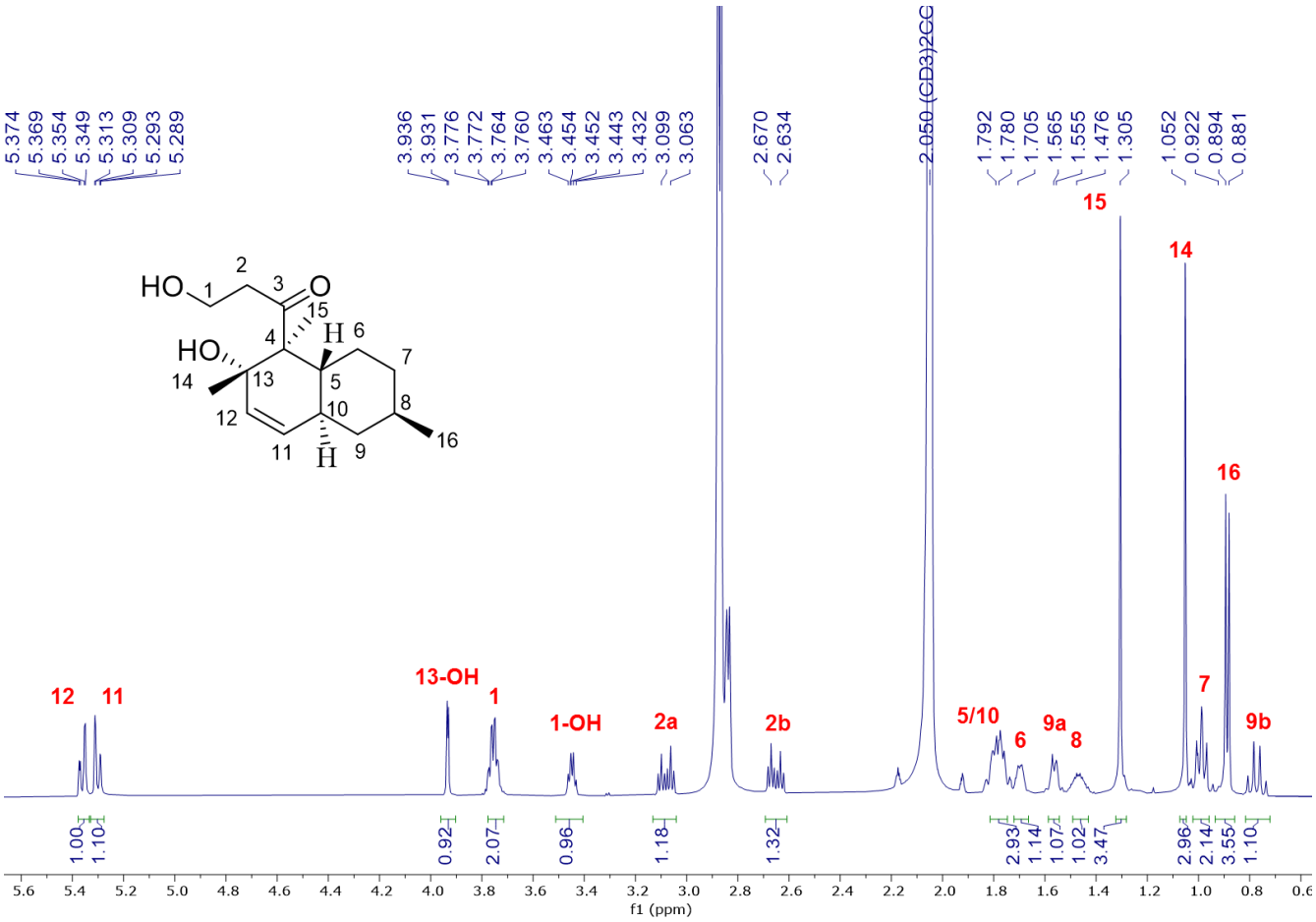


Figure S3.2. ^{1}H-NMR (Acetone-d_6, 500MHz) spectrum of **5**.

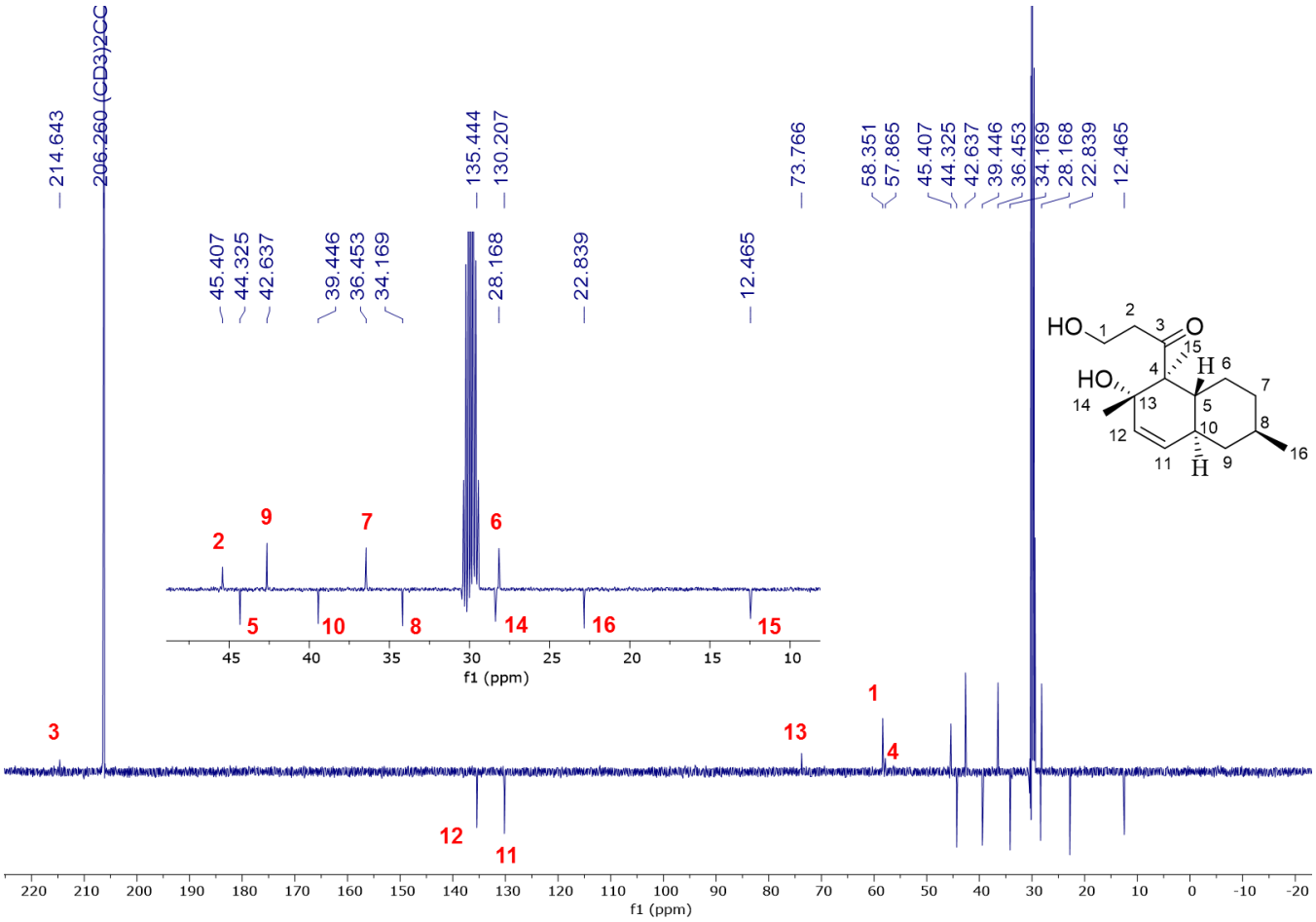


Figure S3.3. JMOD (acetone-d_6, 125 MHz) spectrum of **5**.

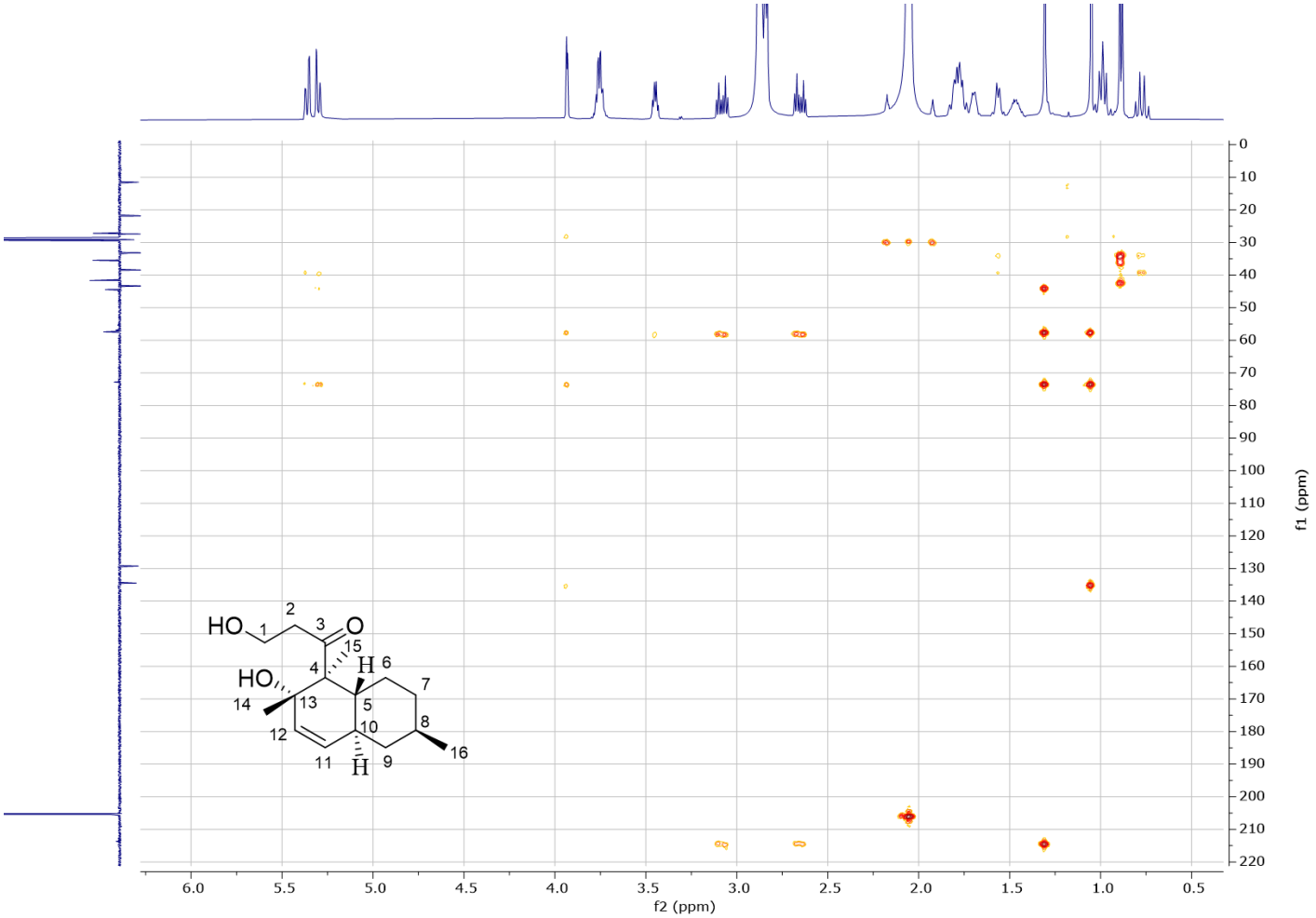


Figure S3.4. The HMBC (acetone-d_6) spectrum of **5**.

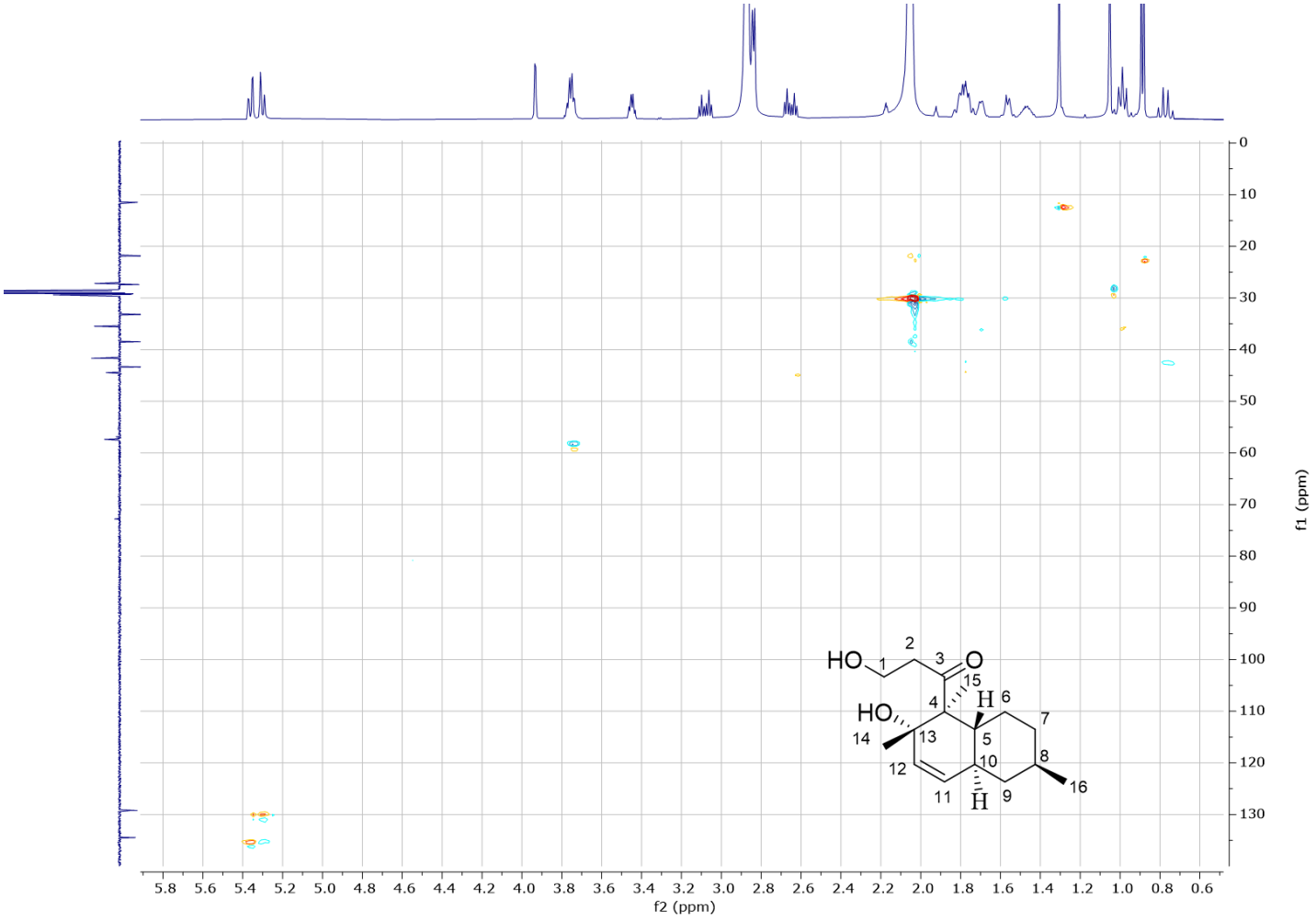


Figure S3.5. The HSQC (acetone-d_6) spectrum of **5**.

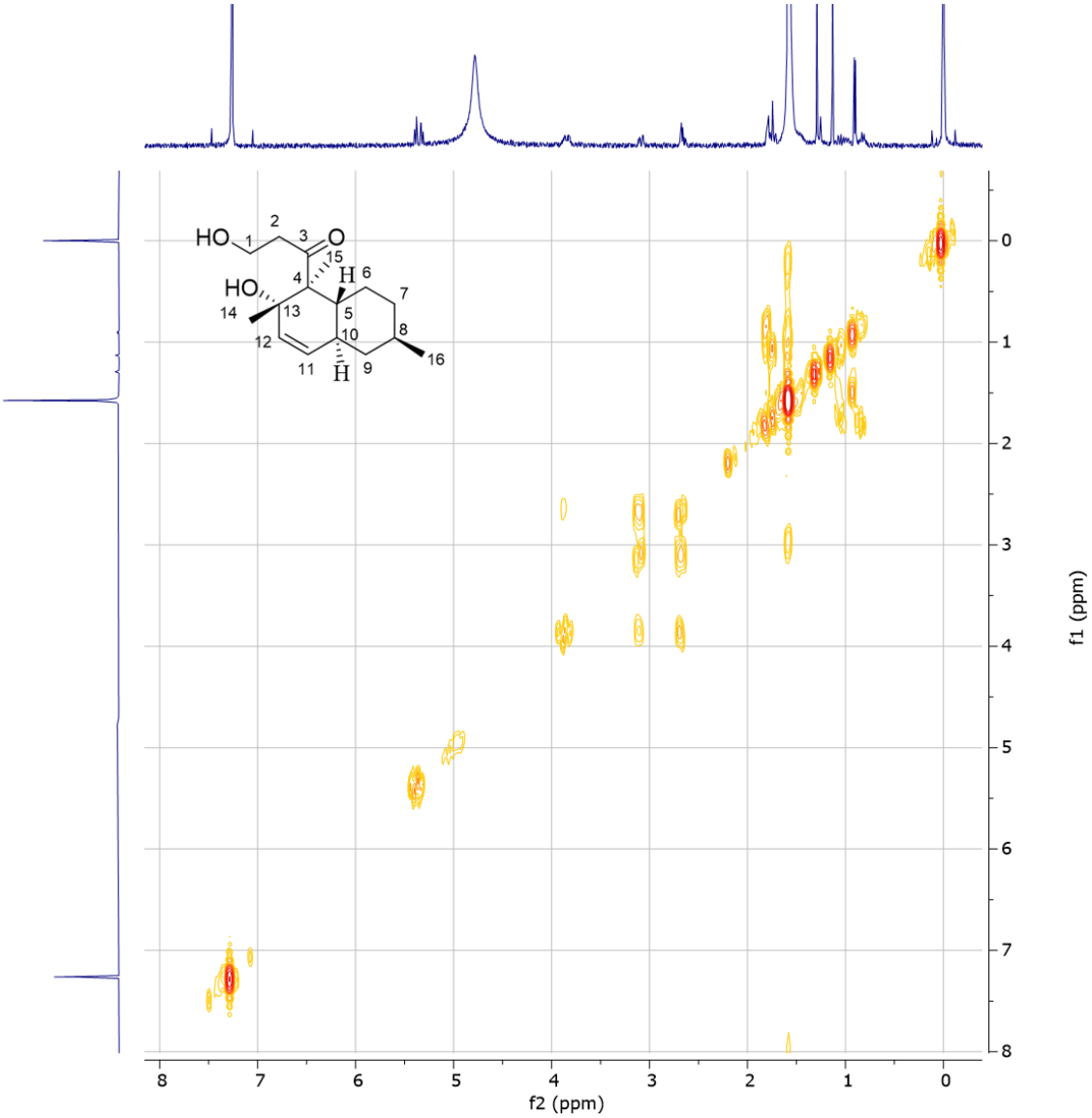


Figure S3.6. The COSY (Chloroform-*d*) spectrum of **5**.

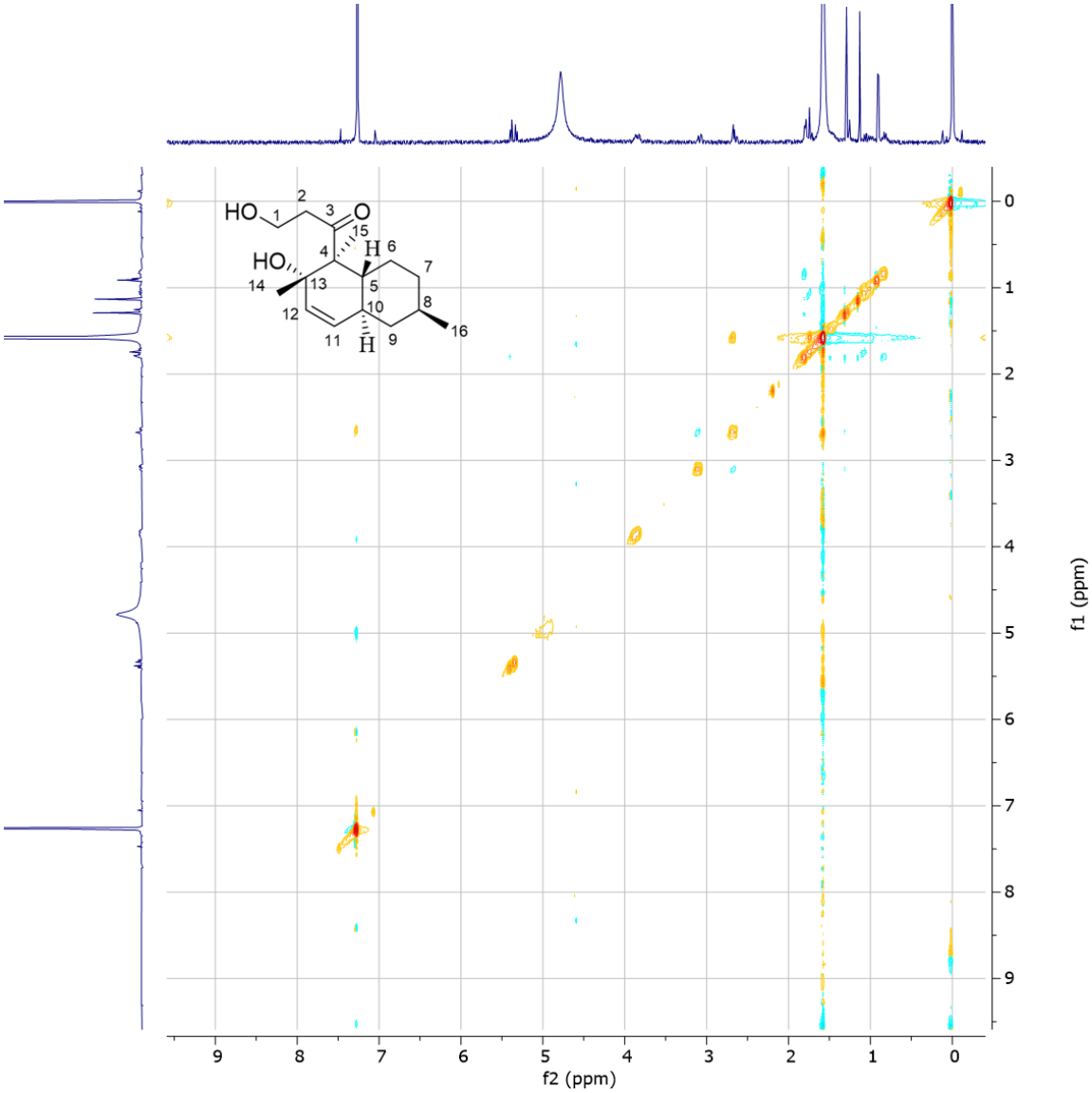


Figure S3.7. The NOESY (Chloroform-*d*) spectrum of **5**.

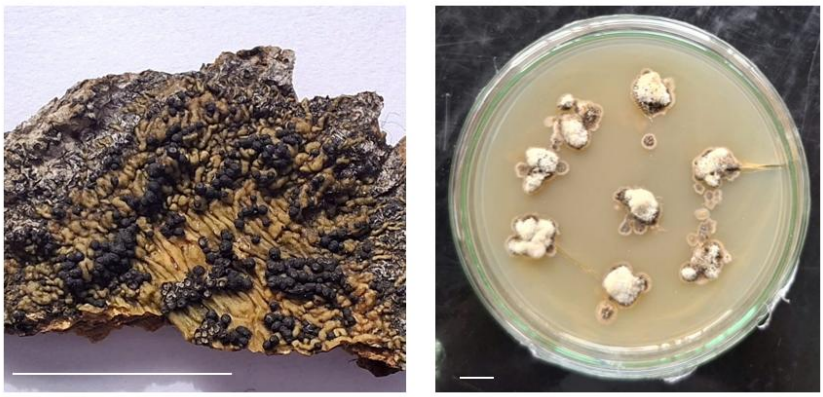


Figure S4. *Nigrovothelium inspersotropicum* thallus (A) and its mycobiont (B)