

## Supporting Information

*Rec. Nat. Prod.* X:X (202X) XX-XX

### A New Sterol-Related Metabolite from the Soft Coral *Capnella imbricata*

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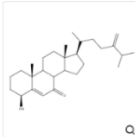
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February 19, 2024

Substances  
5:33 PM



As Drawn (0)  
Substructure (1)  
Similarity (416K)

Rerun Search

Edit Search

Search Within Results

Similarity

- >=99 (3)
- 95-98 (31)
- 90-94 (341)
- 85-89 (2,216)
- 80-84 (10K)

[View All](#)

Similarity >=99

1 100 \*\*\*

**851610-86-1**



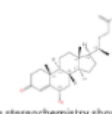
Absolute stereochemistry shown, Rotation (+)

$C_{28}H_{44}O_2$   
(6 $\beta$ )-6-Hydroxyergosta-4,24(28)-dien-3-one

2 References 0 Reactions 1 Supplier

2 100 \*\*\*

**851610-88-3**



Absolute stereochemistry shown, Rotation (+)

$C_{28}H_{44}O_2$   
Ergosta-4,24(28)-dien-3-one, 6-hydroxy-, (6 $\alpha$ -)

1 Reference 0 Reactions 1 Supplier

3 100 \*\*\*

**173681-52-2**



Absolute stereochemistry shown

$C_{29}H_{46}O_2$   
Stigmasta-4,25-dien-3-one, 6-hydroxy-, (6 $\beta$ ,24S)-

1 Reference 0 Reactions 1 Supplier

**Table 1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR data for the compounds showing high similarities.

position	1		851610-86-1	851610-88-3	173681-52-2
	$^1\text{H}$ (J in Hz) <sup>a</sup>	$^{13}\text{C}$ <sup>b</sup>	$^{13}\text{C}$ <sup>d</sup>	$^{13}\text{C}$ <sup>d</sup>	$^{13}\text{C}$ <sup>e</sup>
1a/b	1.73 m; 2.04 m	37.1	37.5	36.4	37.1
2	1.58 m	32.0	34.7	34.6	34.3
3a/b	1.26 m; 2.03 m	38.5	200.8	199.8	200.4
4	4.36 s	73.3	126.8	120.1	126.4
5		168.3	168.8	171.8	168.4
6	5.82 s	126.3	73.7	69.1	73.3
7		202.0	39.0	41.9	38.6
8	2.53 m	39.6	30.1	34.2	29.7
9	0.91 m	53.6	54.0	54.2	53.6
10		38.0	38.4	39.4	38.0
11	1.50 m	22.2	21.4	21.4	21.0
12a/b	1.17 m; 2.05m	39.6	40.0	39.9	39.6
13		42.6	43.0	42.9	42.5
14	1.35 m	50.8	56.3	56.0	55.9
15	1.65 m	24.1	28.6	28.5	24.1
16	1.89 m	28.1	24.5	24.6	28.1
17	1.16 m	55.9	56.4	56.3	56.1
18	0.75 s	12.0	12.4	12.3	12.5
19	1.38 s	19.5	19.9	18.7	19.5
20	1.43 m	35.8	36.1	36.1	35.5
21	0.96 d (6.6) <sup>c</sup>	18.7	19.1	19.0	18.6
22a/b	1.16 m; 1.53 m	31.0	35.1	35.0	33.6
23a/b	1.86 m; 2.18 m	34.6	31.4	31.3	29.4
24		156.8	157.2	157.2	49.5
25	2.21 m	33.8	34.2	34.2	147.5
26	1.02 d (3.0)	21.9	22.4	22.4	111.4
27	1.03 d (3.0)	22.0	22.3	22.3	17.8
28a/b	4.66 s; 4.72 s	106.0	106.4	106.4	26.5
29					12.1

<sup>a</sup>Spectroscopic data were recorded at 600 MHz in  $\text{CDCl}_3$  at 25 °C.

<sup>b</sup>Spectroscopic data was recorded at 150 MHz in  $\text{CDCl}_3$  at 25 °C.

<sup>c</sup>Attached protons were deduced by HSQC experiments.

<sup>d</sup>Data from the references (DOI: 10.1080/10286020310001617200).

<sup>e</sup>Data from the references (DOI: 10.1021/np50124a007).

Similarity <99

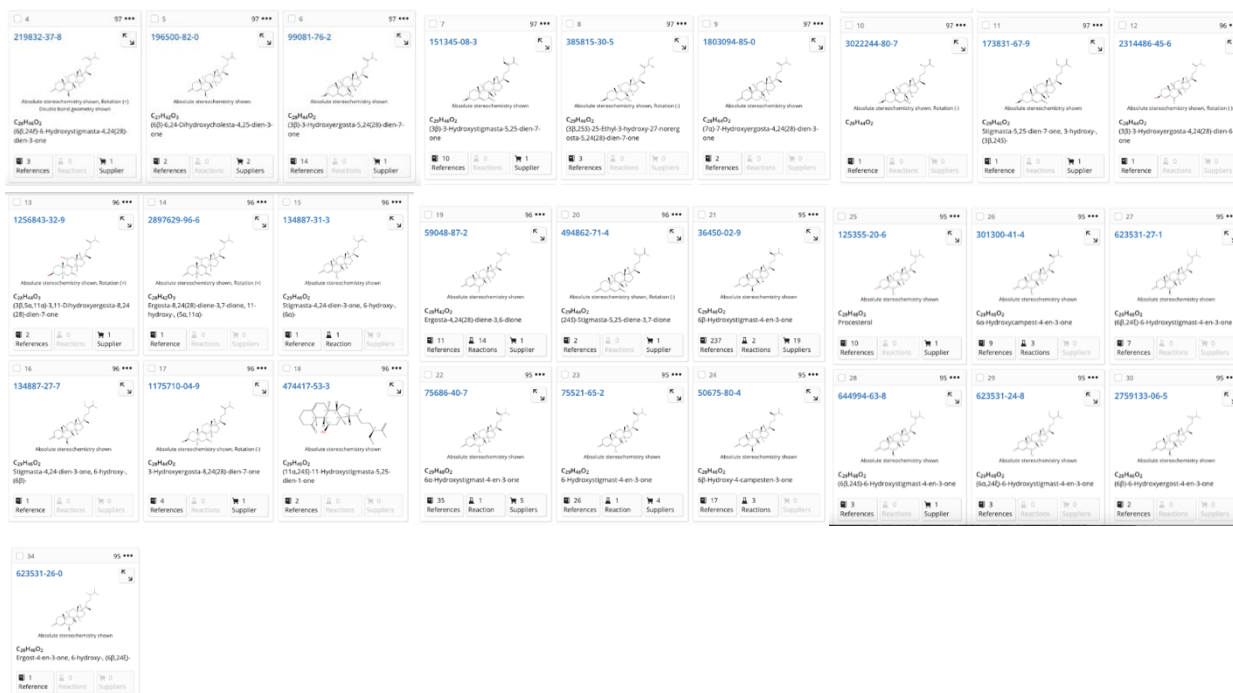
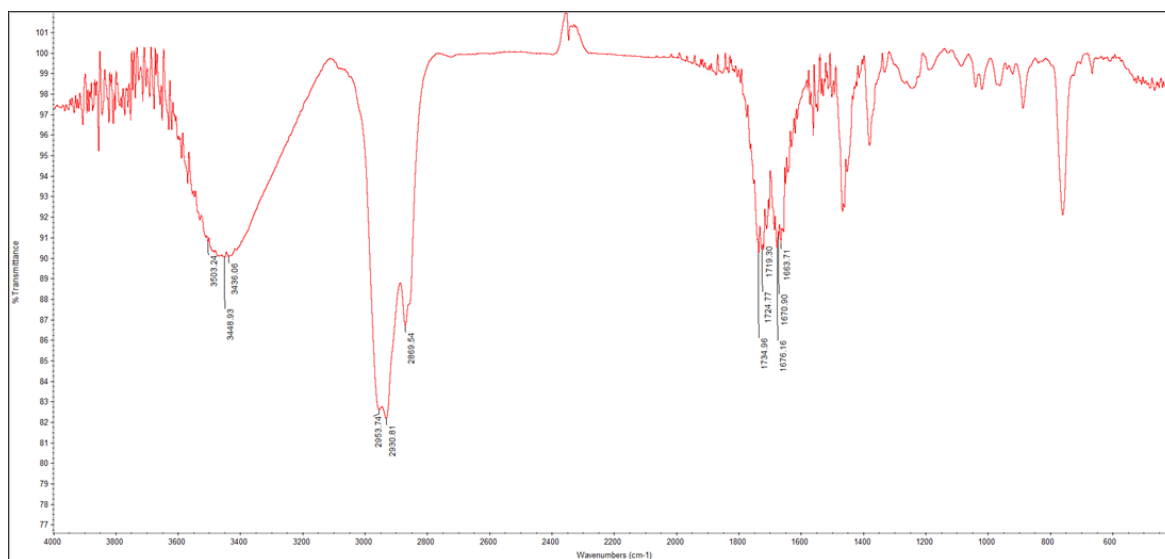
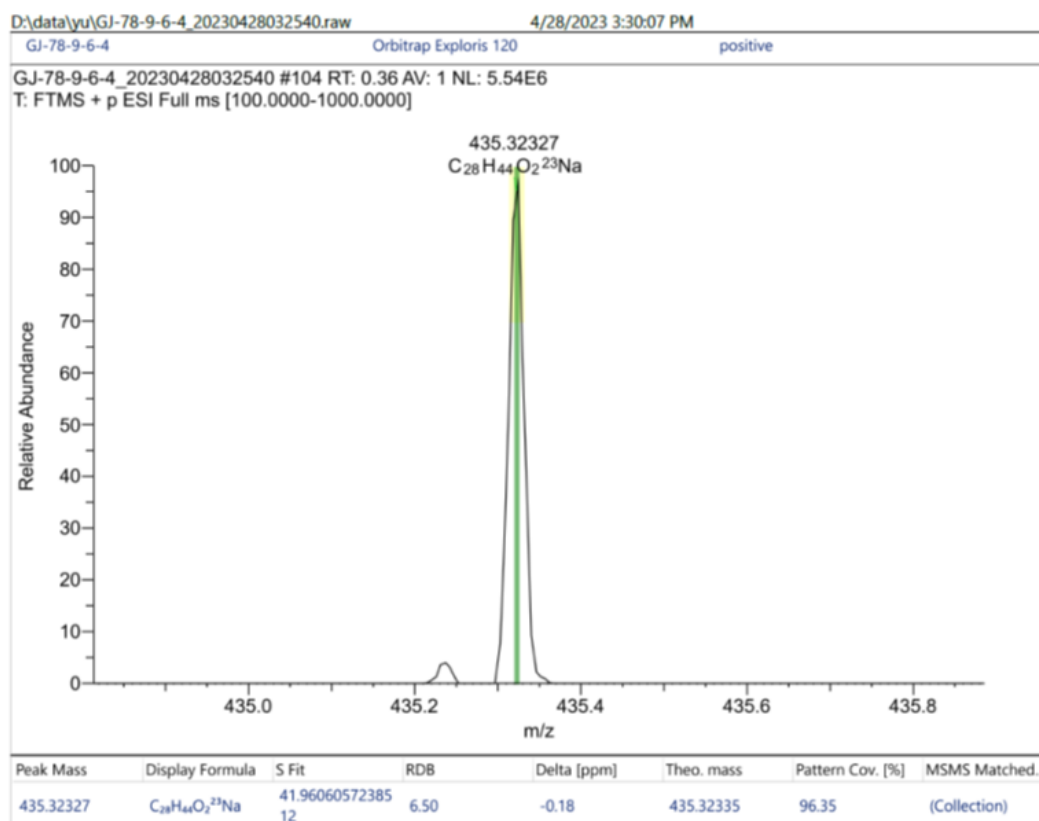


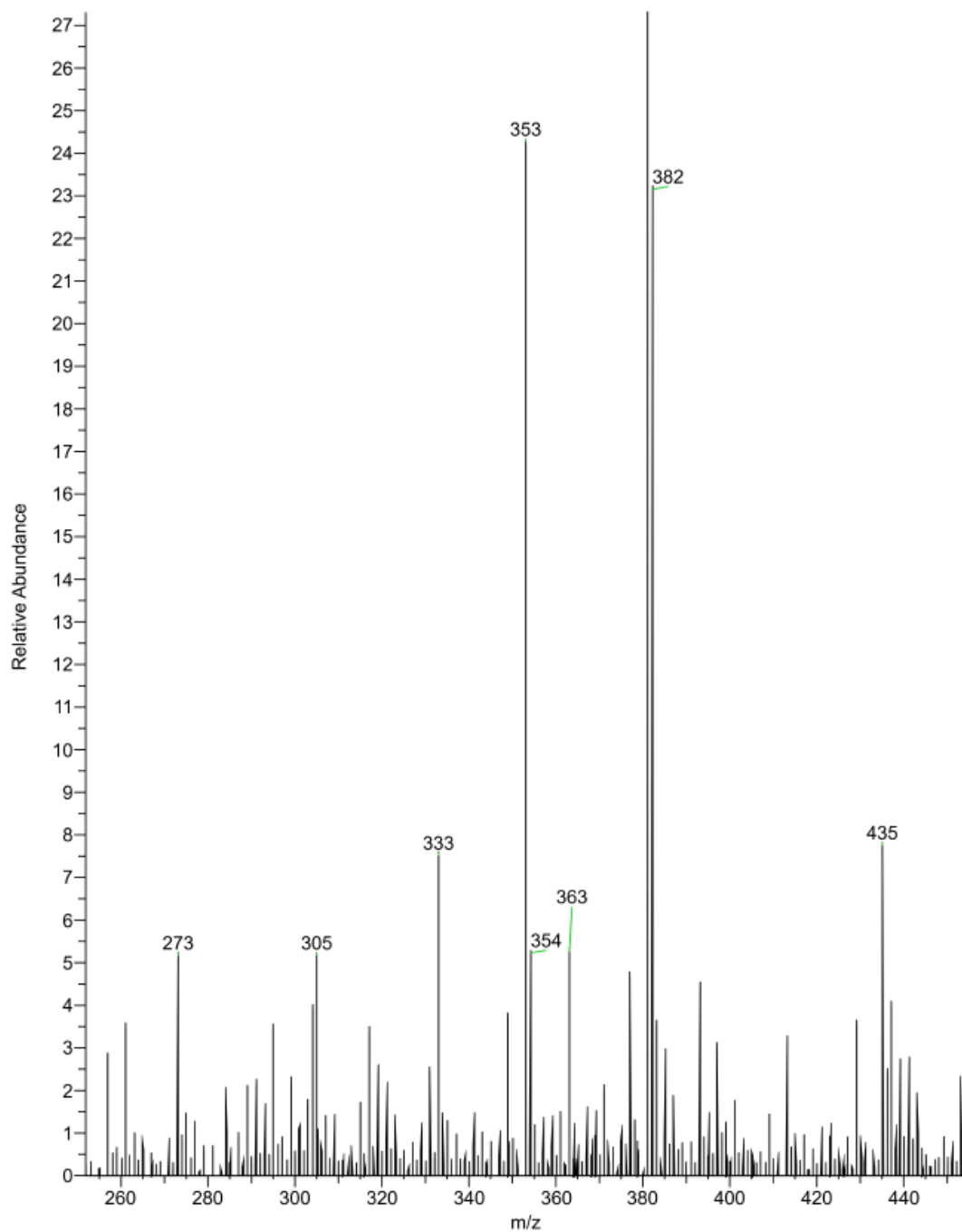
Figure S1: Scifinder Search Results of 1



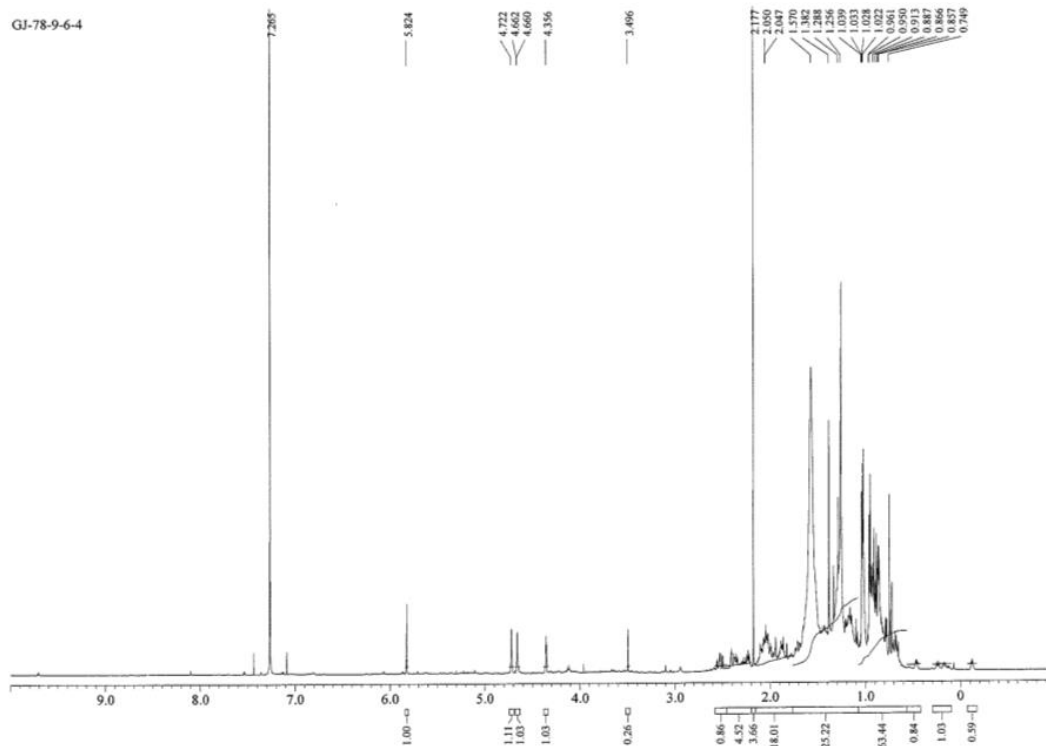
**Figure S2:** IR spectrum of **1**



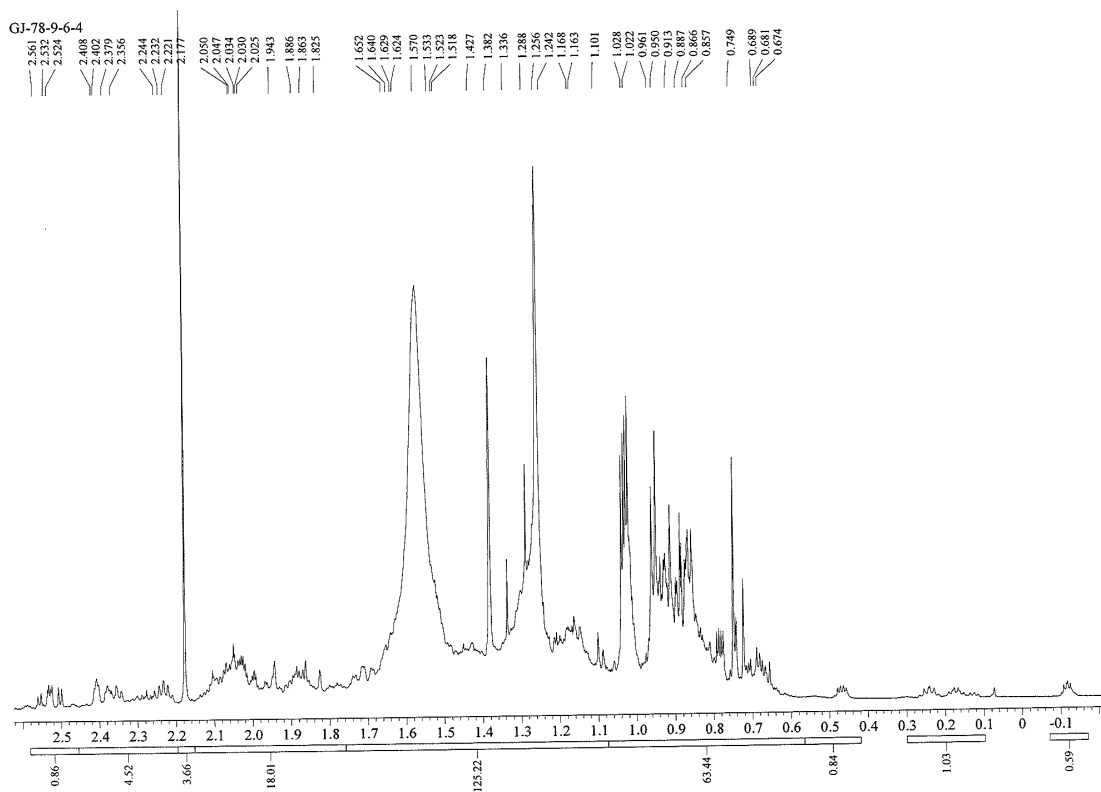
**Figure S3:** HRESIMS spectrum of **1**



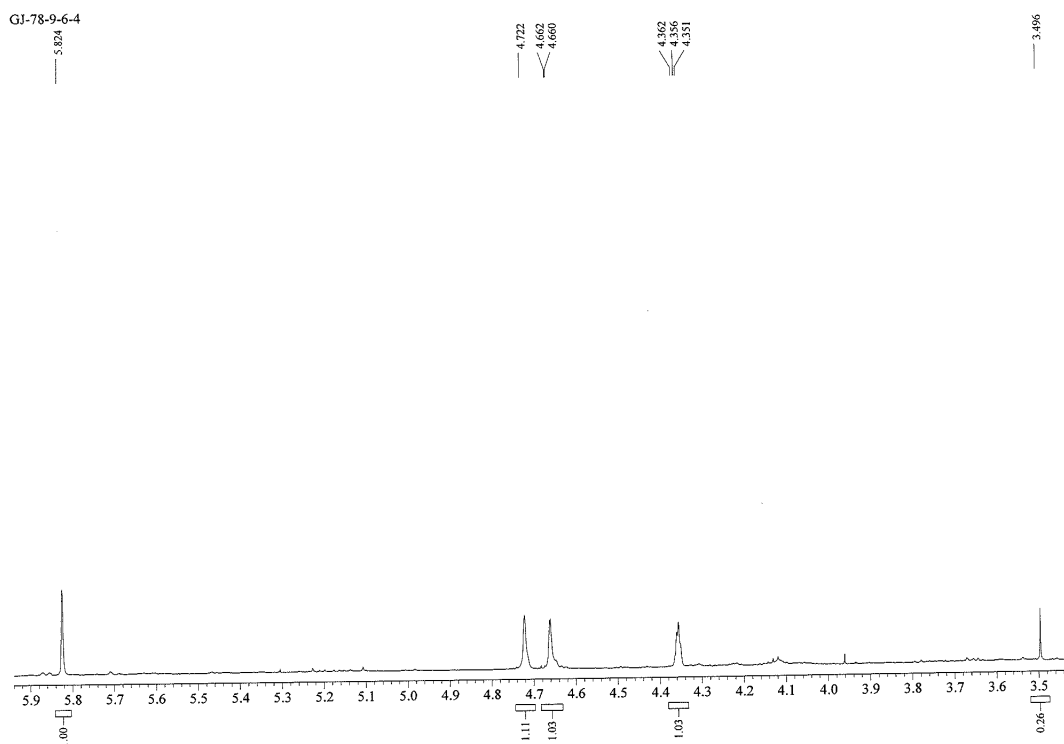
**Figure S4:**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 600 MHz



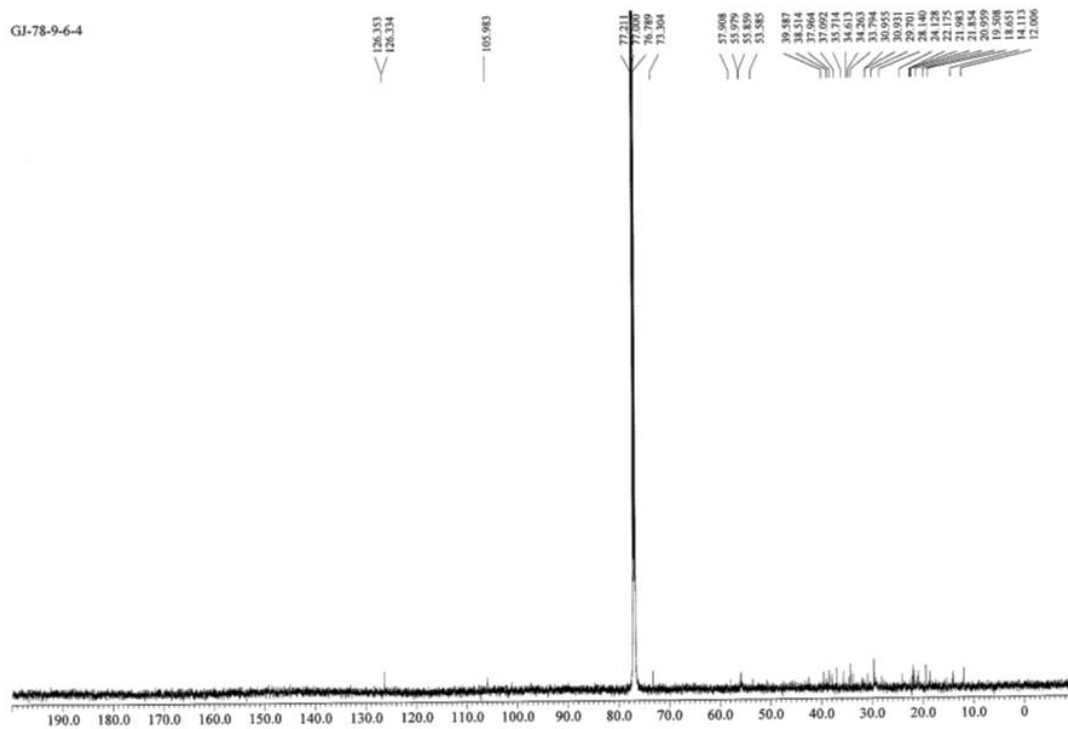
**Figure S5:**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 600 MHz



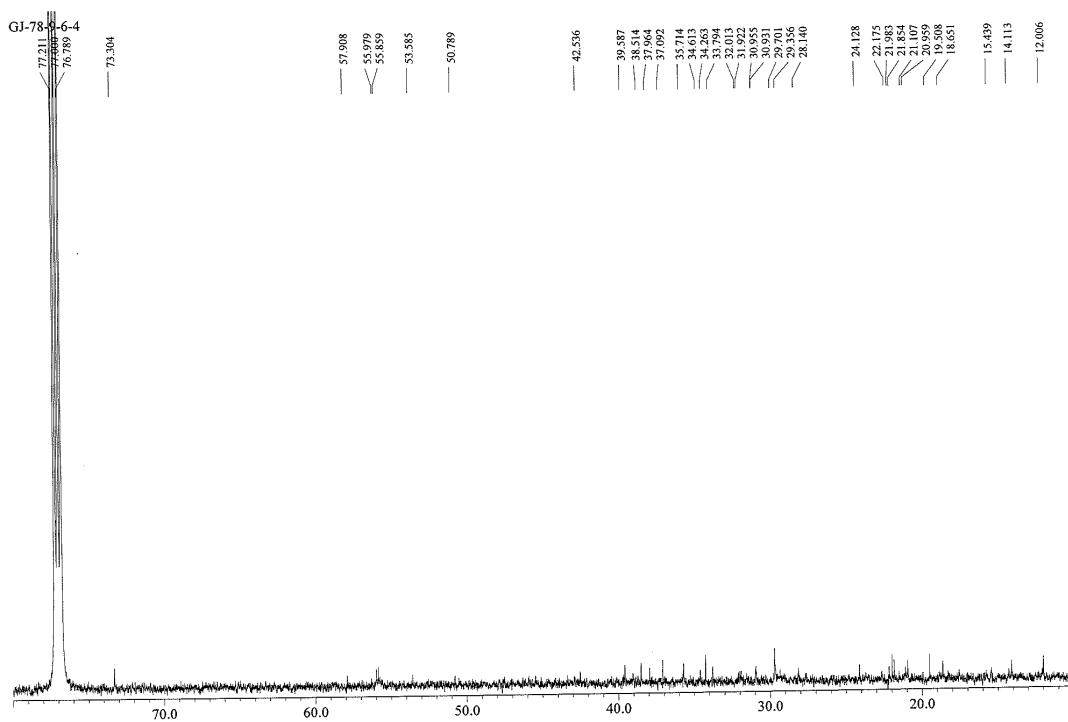
**Figure S6:**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 600 MHz (enlarged scale-1)



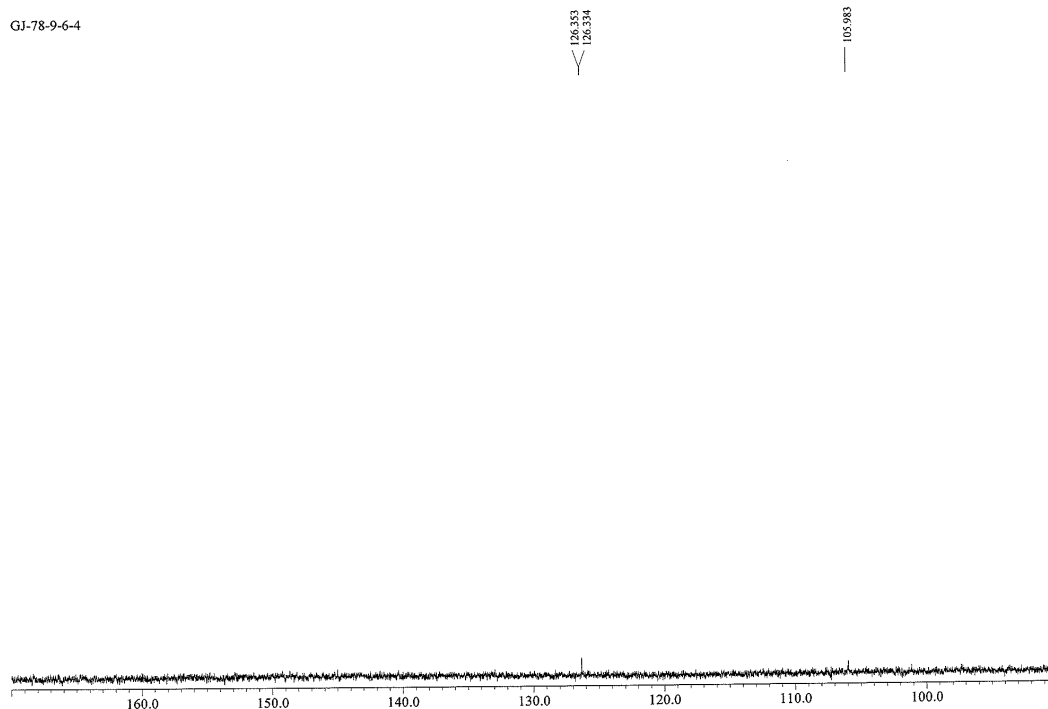
**Figure S7:**  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 600 MHz (enlarged scale-2)



**Figure S8:**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 150 MHz

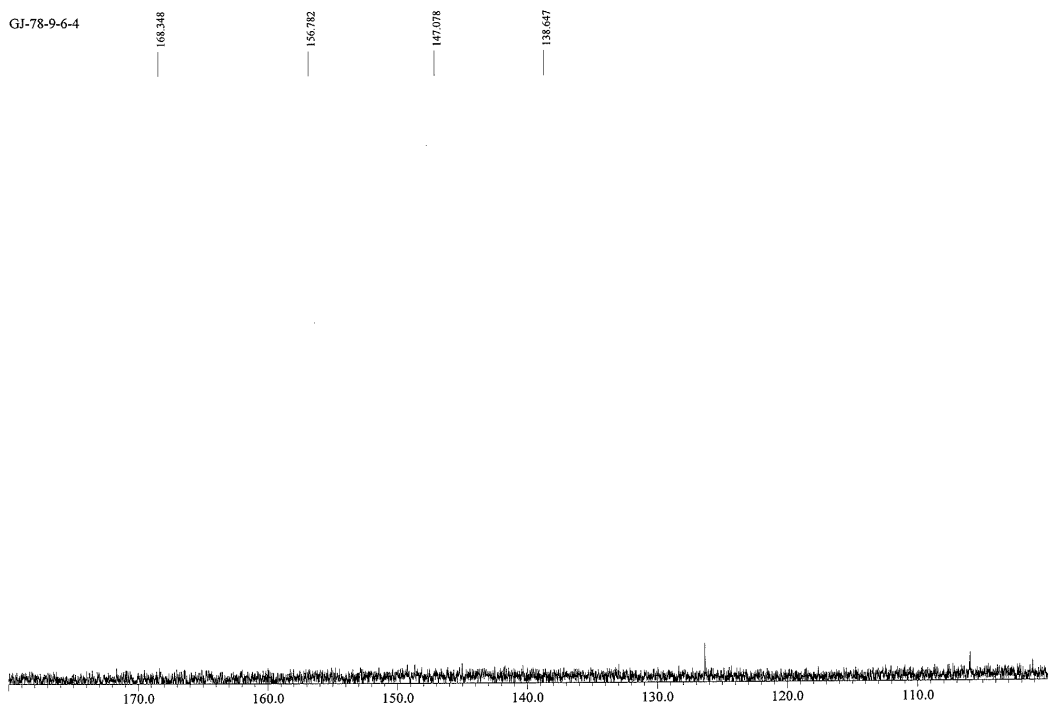


**Figure S9:**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 150 MHz (enlarged scale-1)

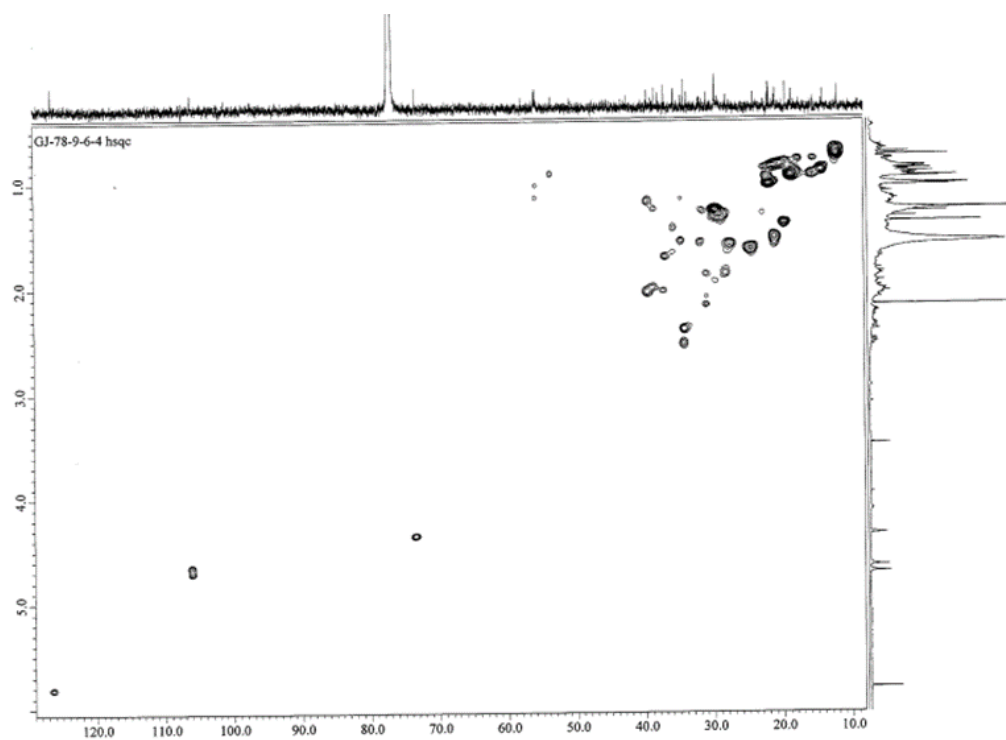


**Figure S10:**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 150 MHz (enlarged scale-2)

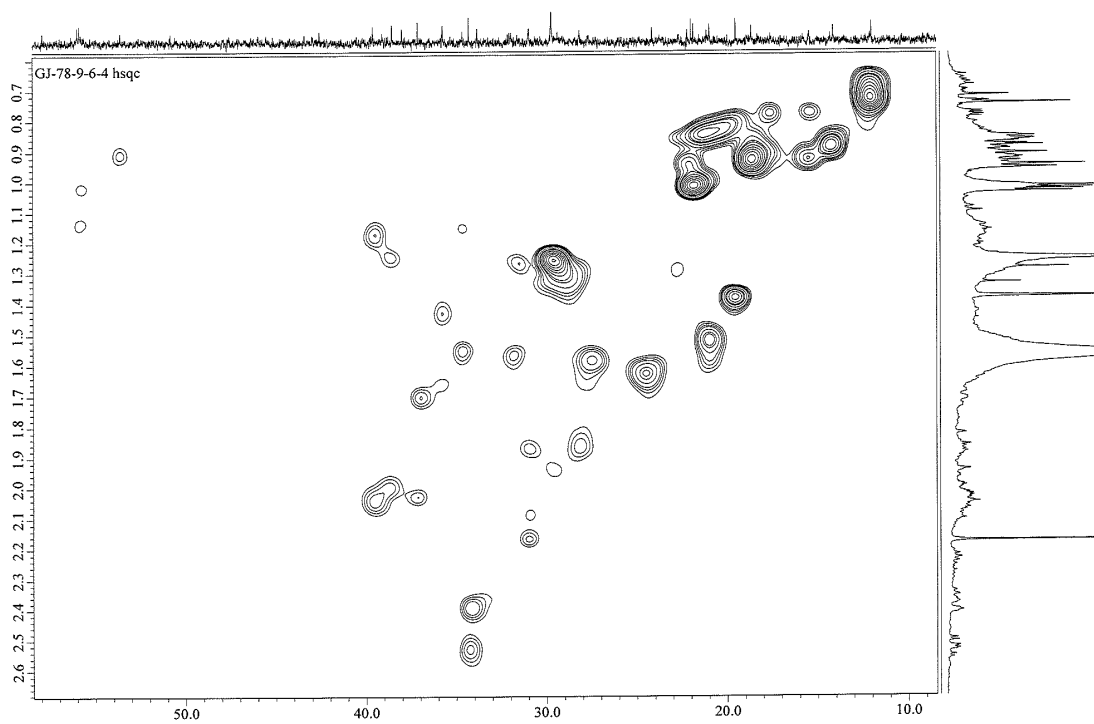




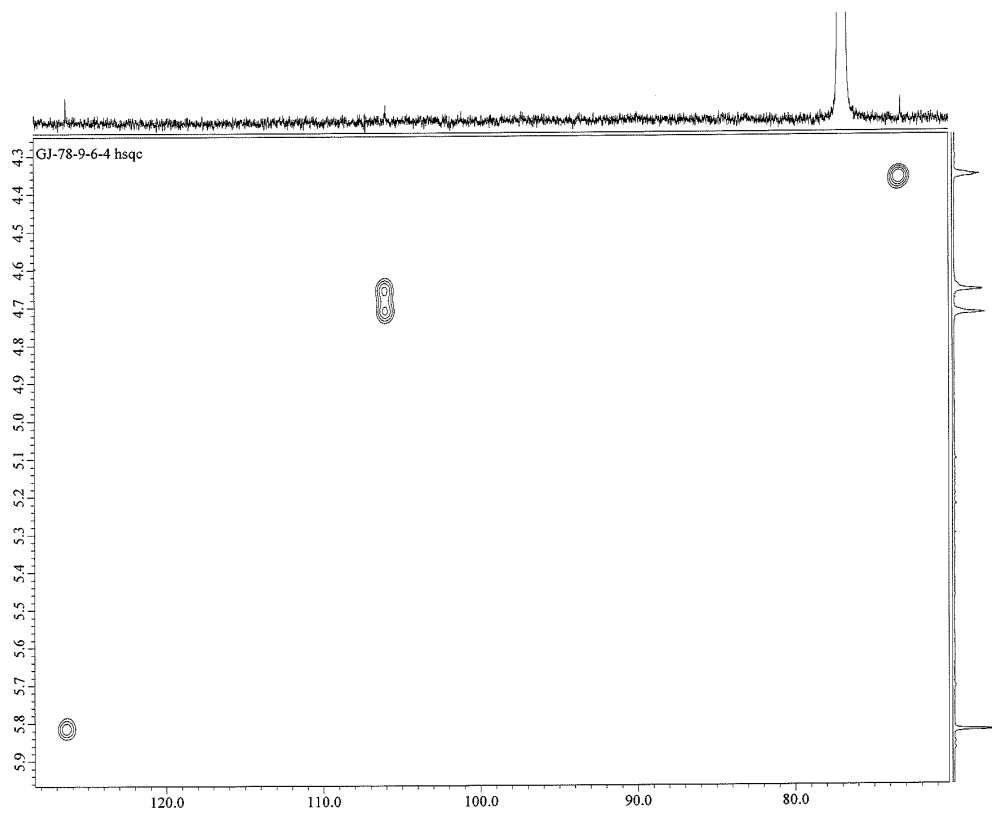
**Figure S11:**  $^{13}\text{C}$  NMR spectrum of **1** in  $\text{CDCl}_3$  at 150 MHz (enlarged scale-3)



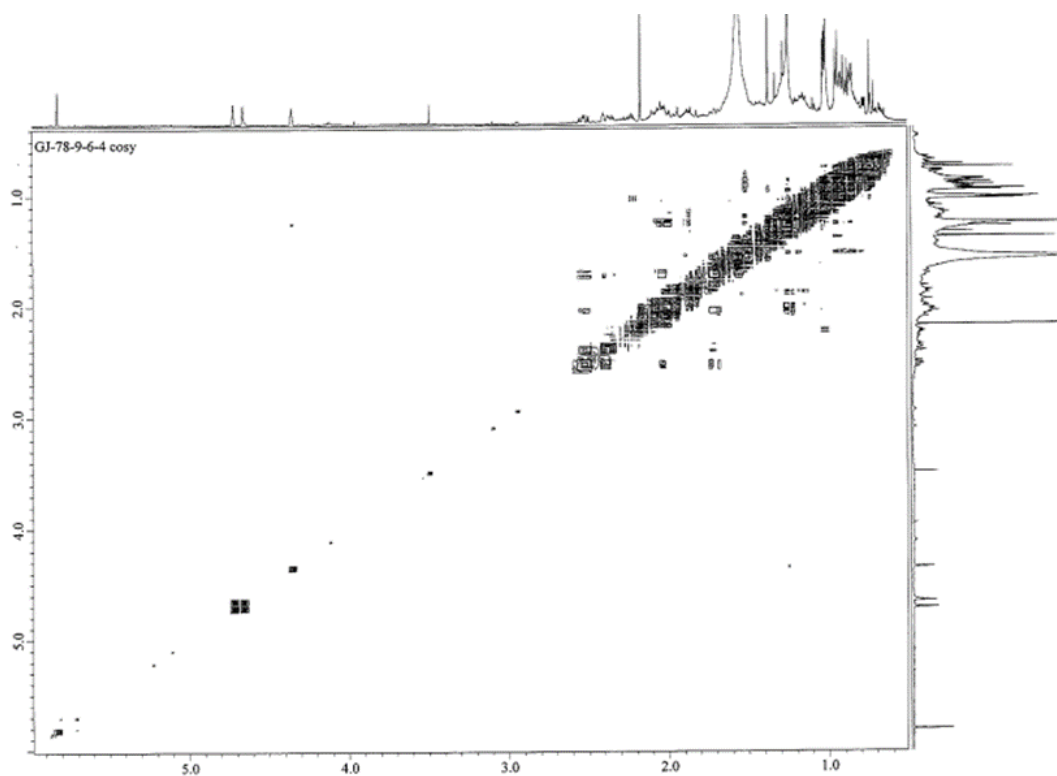
**Figure S12:** HSQC spectrum of **1**



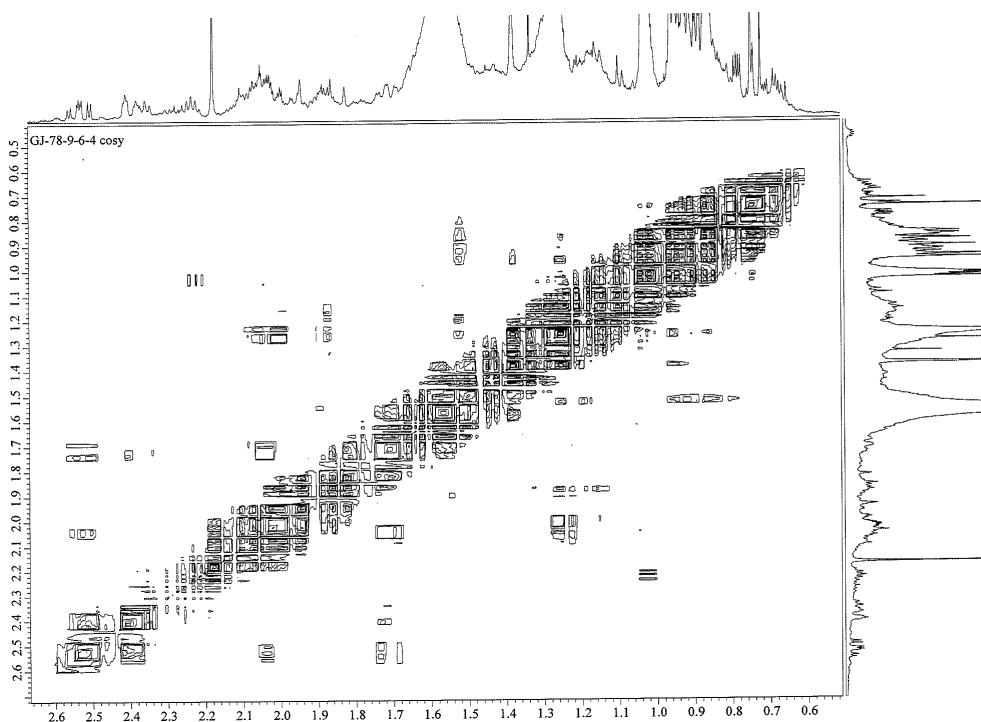
**Figure S13:** HSQC spectrum of **1** (enlarged scale-1)



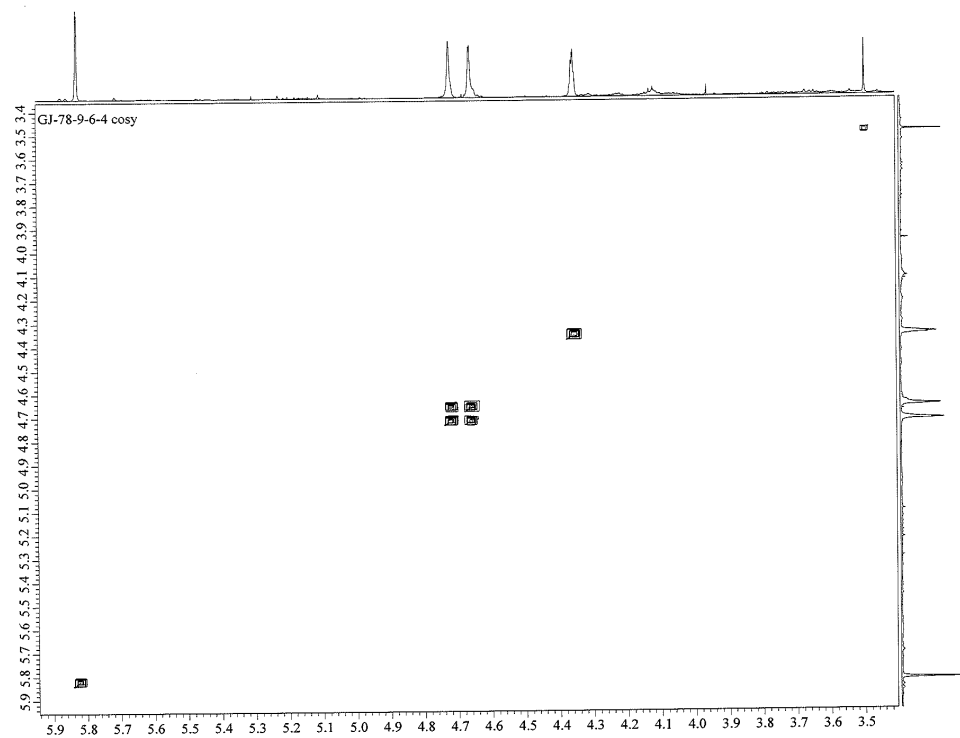
**Figure S14:** HSQC spectrum of **1** (enlarged scale-2)



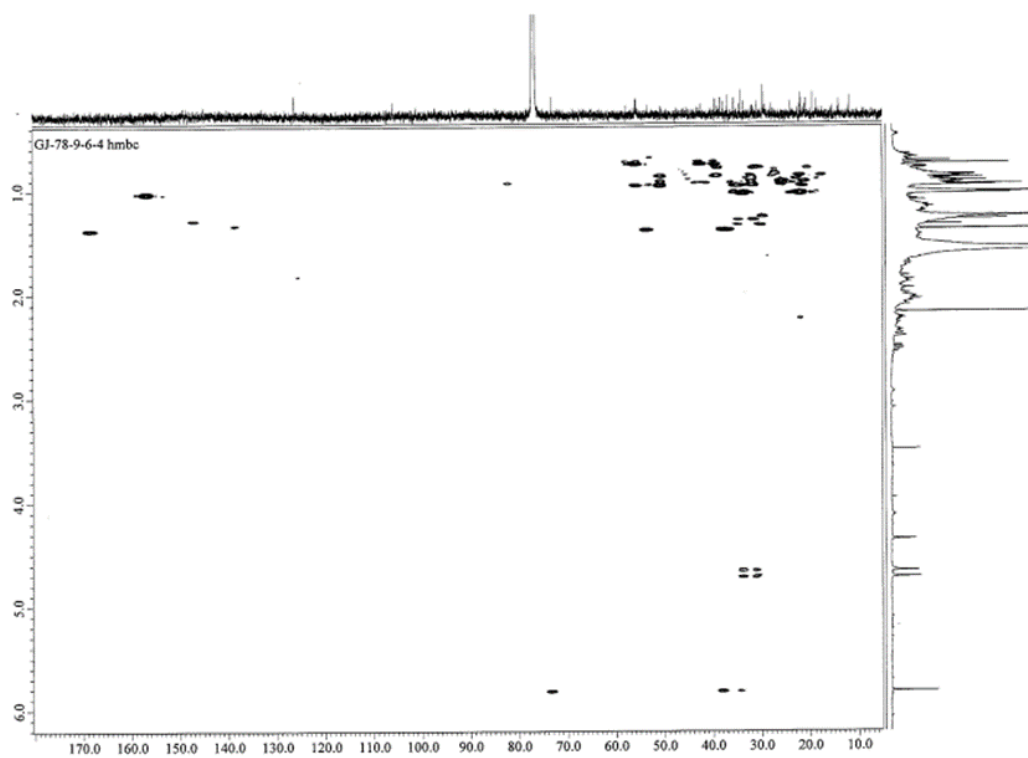
**Figure S15:** COSY spectrum of **1**



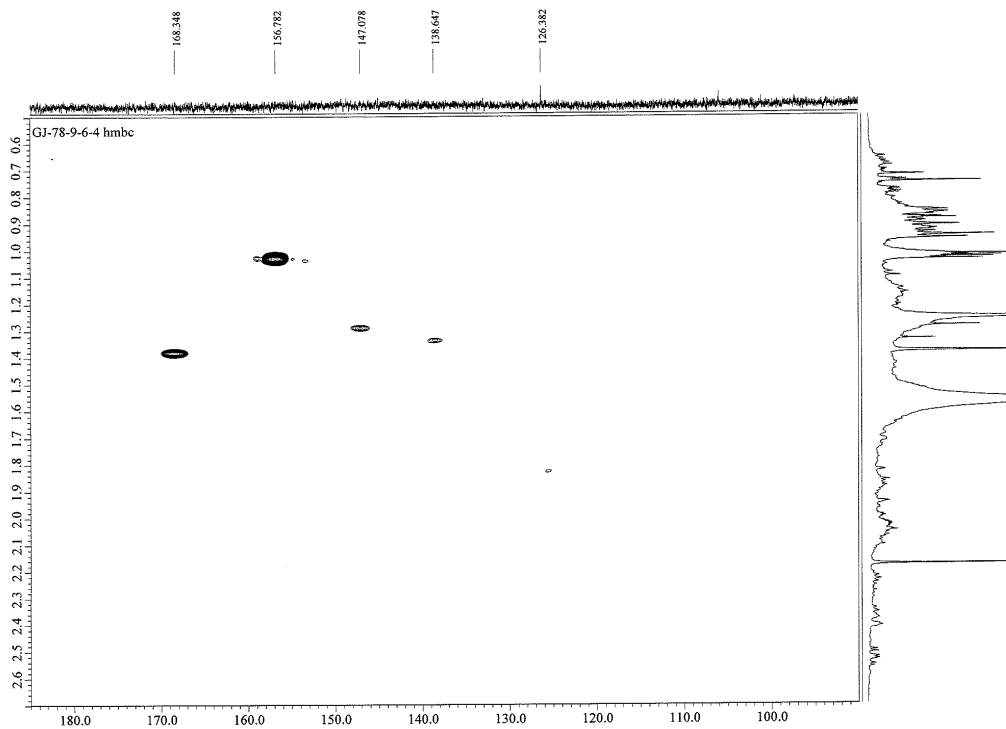
**Figure S16:** COSY spectrum of **1** (enlarged scale-1)



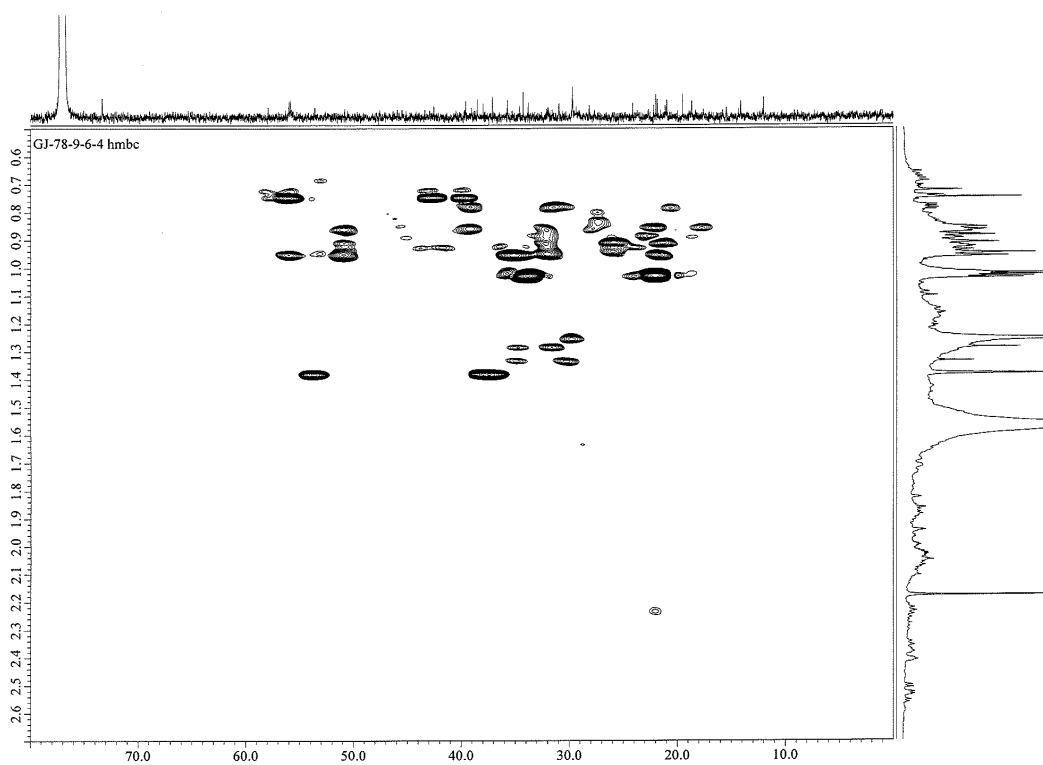
**Figure S17:** COSY spectrum of **1** (enlarged scale-2)



**Figure S18:** HMBC spectrum of **1**



**Figure S19:** HMBC spectrum of **1** (enlarged scale-1)



**Figure S20:** HMBC spectrum of **1** (enlarged scale-2)

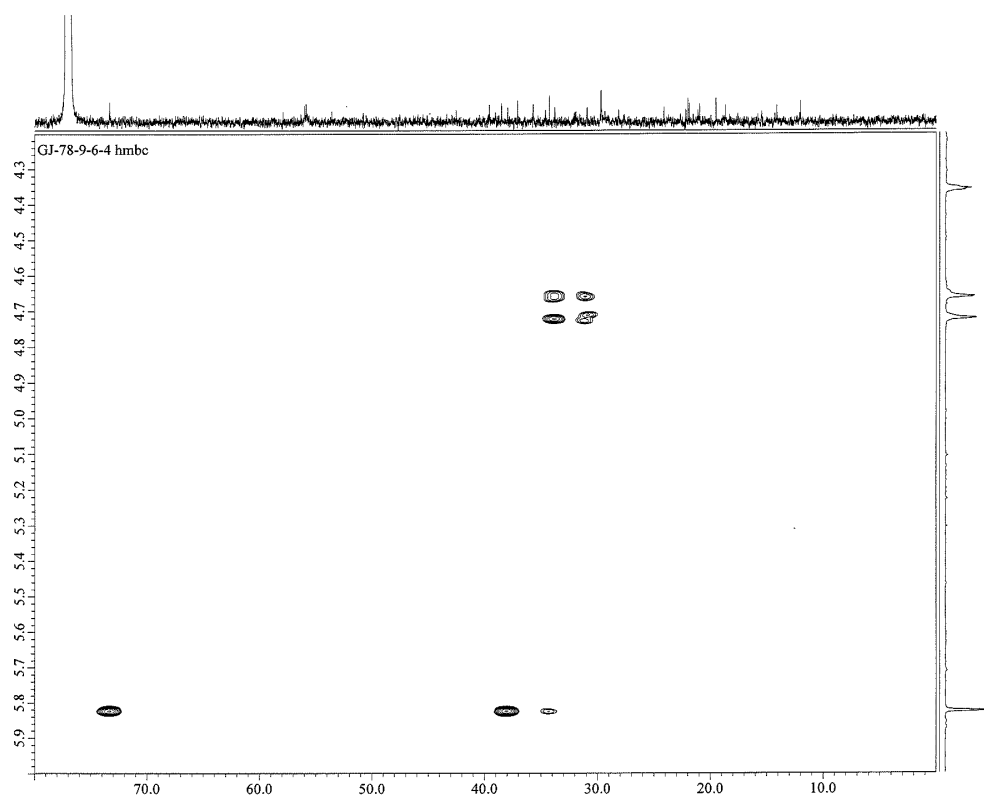


Figure S21: HMBC spectrum of **1** (enlarged scale-3)

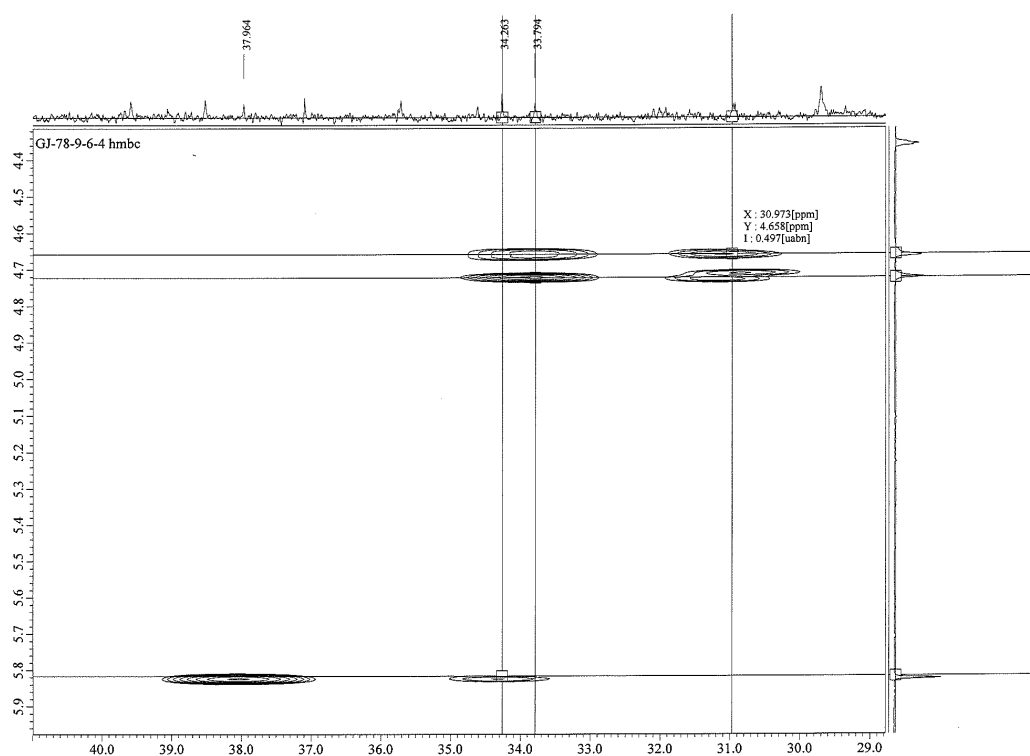
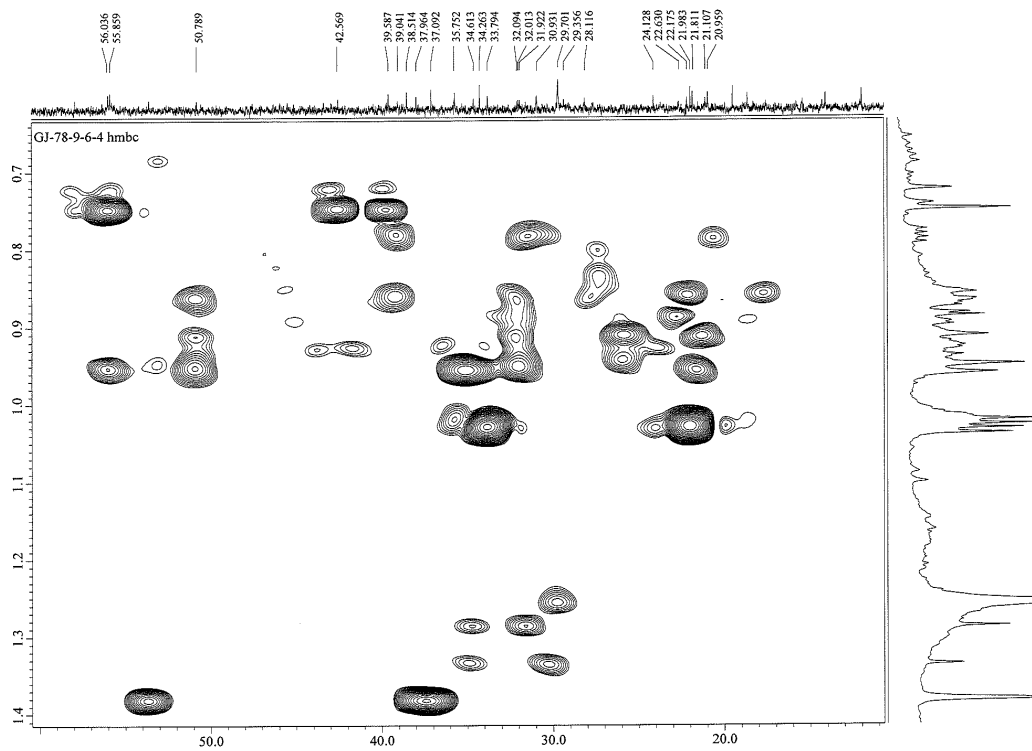
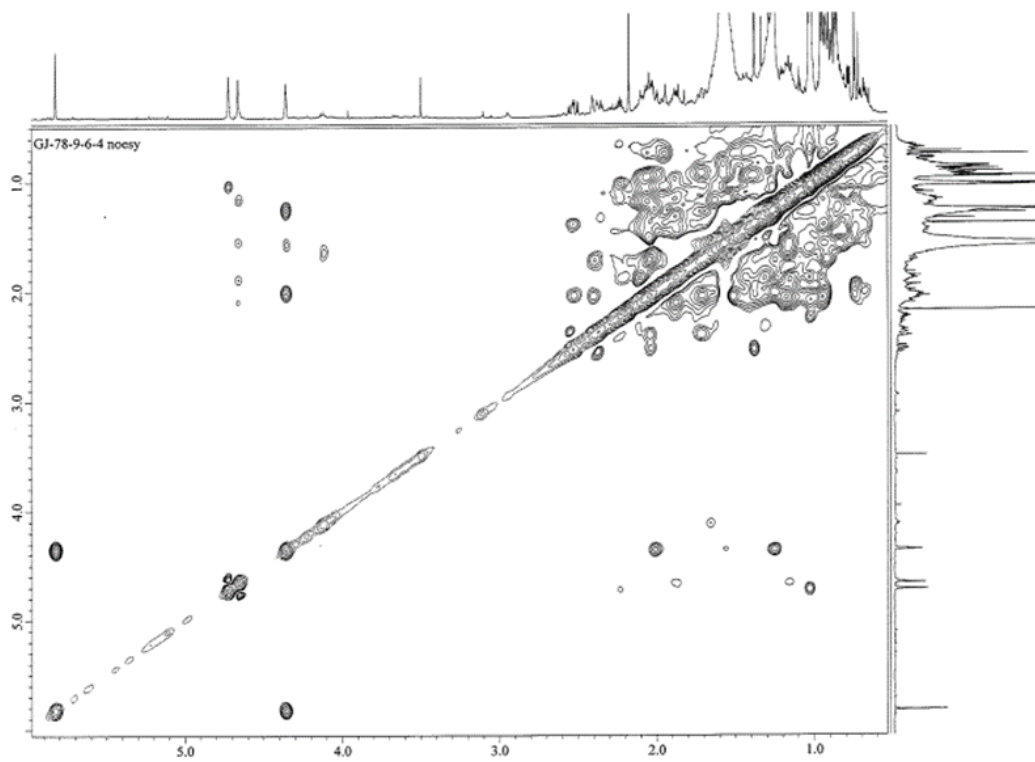


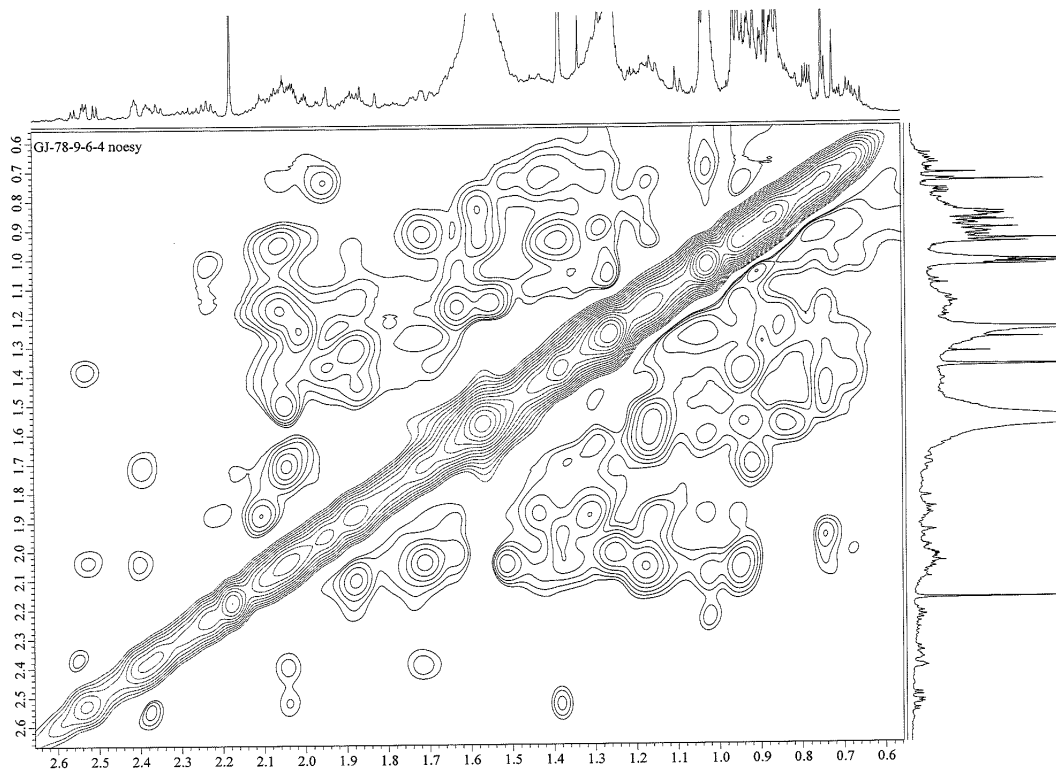
Figure S22: HMBC spectrum of **1** (enlarged scale-4)



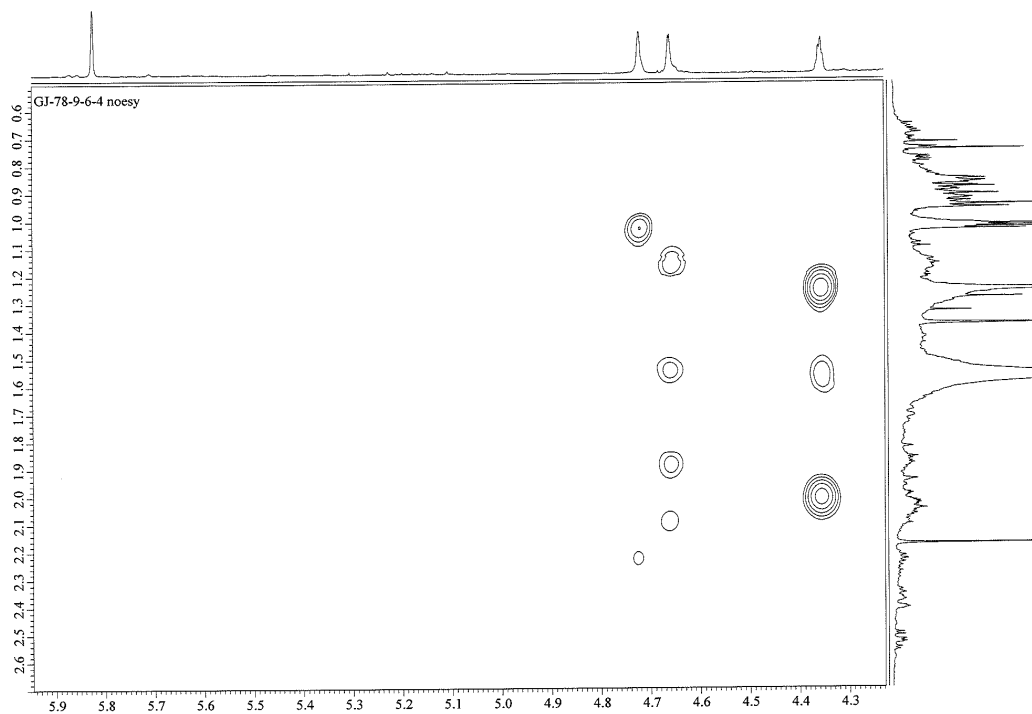
**Figure S23:** HMBC spectrum of **1** (enlarged scale-5)



**Figure S24:** NOESY spectrum of **1**

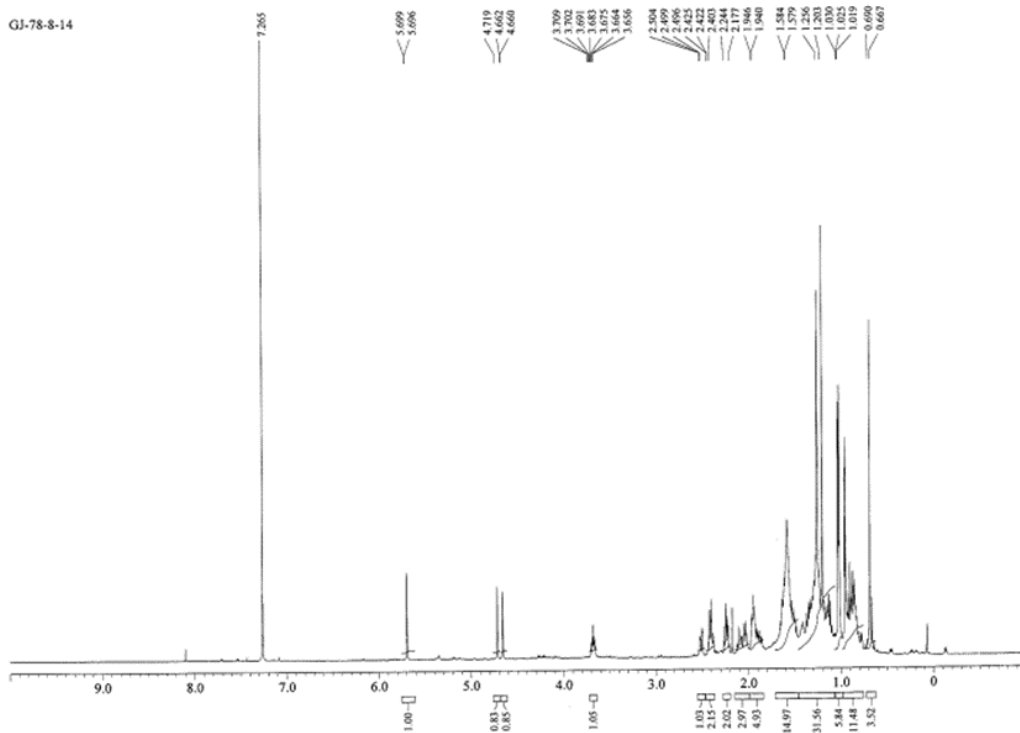


**Figure S25:** NOESY spectrum of **1** (enlarged scale-1)

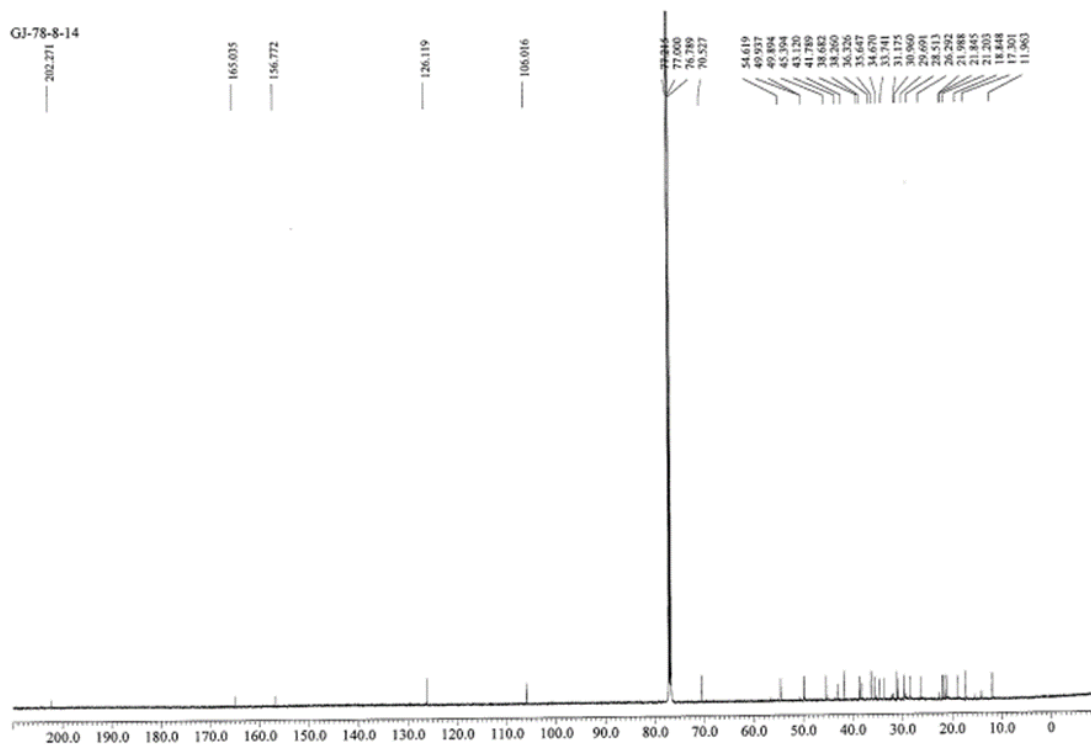


**Figure S26:** NOESY spectrum of **1** (enlarged scale-2)

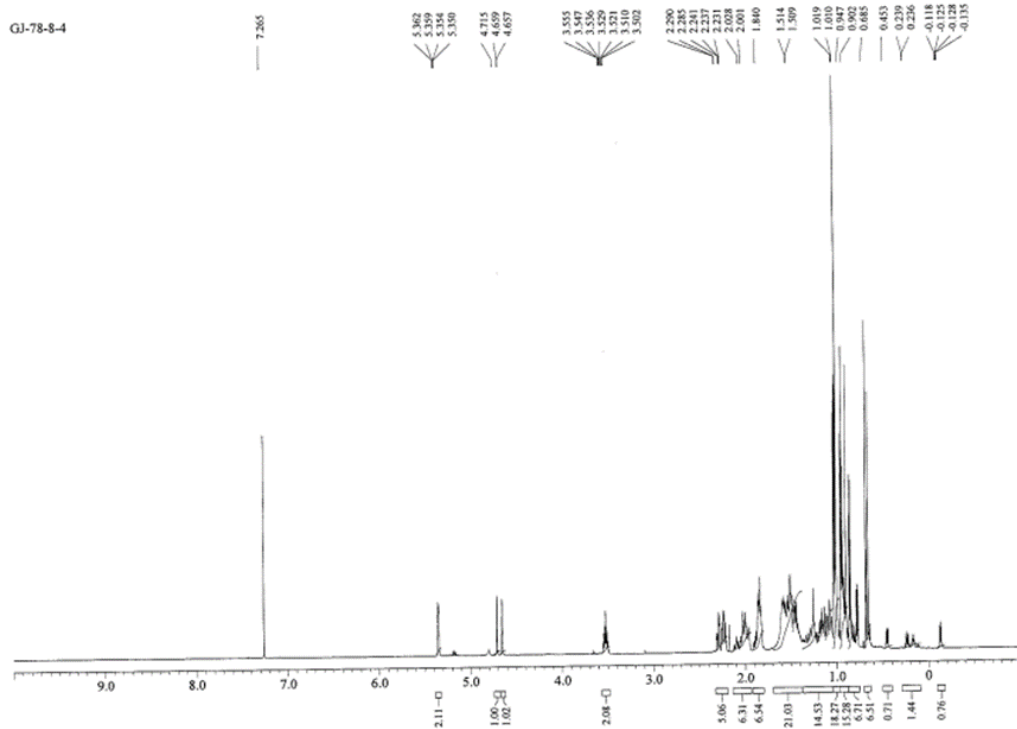




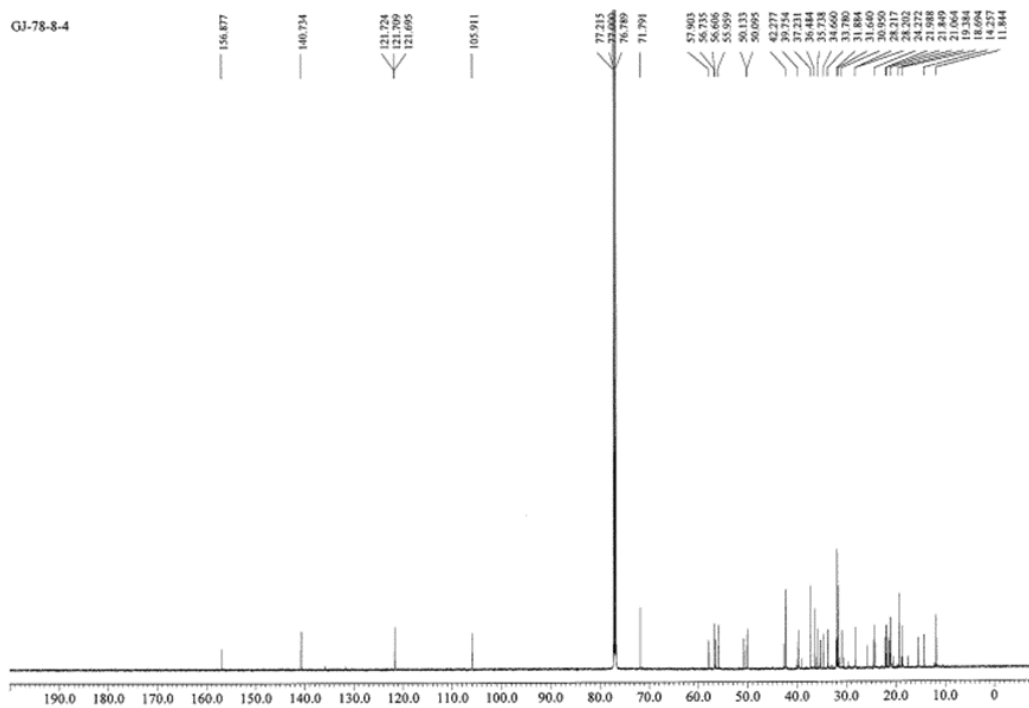
**Figure S27:**  $^1\text{H}$  NMR spectrum of **2** in  $\text{CDCl}_3$  at 600 MHz



**Figure S28:**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CDCl}_3$  at 150 MHz



**Figure S29:**  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at 600 MHz



**Figure S30:**  $^{13}\text{C}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at 125 MHz

**Datablock: ic21710**


---

Bond precision: C-C = 0.0138 Å Wavelength=0.71073  
 Cell: a=9.5322(4) b=7.4733(3) c=36.7188(15)  
 alpha=90 beta=90.4606(18) gamma=90  
 Temperature: 200 K

	Calculated	Reported
Volume	2615.65(19)	2615.65(19)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	2(C30 H48 O), H2 O	?
Sum formula	C60 H98 O3	C60 H98 O3
Mr	867.38	867.38
Dx, g cm <sup>-3</sup>	1.101	1.101
Z	2	2
Mu (mm <sup>-1</sup> )	0.065	0.065
F000	964.0	964.0
F000'	964.35	
h,k,lmax	11,9,45	11,9,45
Nref	10545[ 5696]	10421
Tmin,Tmax	0.986,0.996	0.696,0.959
Tmin'	0.967	

Correction method= # Reported T Limits: Tmin=0.696

Tmax=0.959 AbsCorr = MULTI-SCAN

Data completeness= 1.83/0.99 Theta(max)= 26.246

R(reflections)= 0.1095( 6802) wR2(reflections)=  
0.3425( 10421)

S = 1.056 Npar= 602

---

The following ALERTS were generated. Each ALERT has the format

[test-name\\_ALERT\\_alert-type\\_alert-level](#).

Click on the hyperlinks for more details of the test.

---

●Alert level B

[PLAT340 ALERT 3 B](#) Low Bond Precision on C-C Bonds .....  
0.01378 Ang.

---

● **Alert level C**

[STRVA01 ALERT 4 C](#) Flack test results are meaningless.  
From the CIF: `_refine_ls_abs_structure_Flack` -0.100  
From the CIF: `_refine_ls_abs_structure_Flack_su` 1.000

[PLAT082 ALERT 2 C](#) High R1 Value .....  
0.11 Report

[PLAT084 ALERT 3 C](#) High wR2 Value (i.e. > 0.25) .....  
0.34 Report

[PLAT220 ALERT 2 C](#) NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range  
5.5 Ratio

[PLAT220 ALERT 2 C](#) NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range  
4.4 Ratio

[PLAT222 ALERT 3 C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range  
6.9 Ratio

[PLAT222 ALERT 3 C](#) NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range  
5.3 Ratio

[PLAT234 ALERT 4 C](#) Large Hirshfeld Difference C53 --C60 .  
0.16 Ang.

And 3 other PLAT234 Alerts

More ...

[PLAT241 ALERT 2 C](#) High 'MainMol' Ueq as Compared to Neighbors of  
C30 Check

[PLAT242 ALERT 2 C](#) Low 'MainMol' Ueq as Compared to Neighbors of  
C52 Check

And 2 other PLAT242 Alerts

More ...

[PLAT415 ALERT 2 C](#) Short Inter D-H..H-X H3' ..H34B .  
2.10 Ang.

$-x, 1/2+y, 1-z =$

2\_556 Check

[PLAT790 ALERT 4 C](#) Centre of Gravity not Within Unit Cell: Resd. #  
1 Note

C30 H48 O

[PLAT911 ALERT 3 C](#) Missing FCF Refl Between Thmin & STh/L= 0.600  
12 Report

-3 0 2, -4 0 3, -5 0 4, -6 0 19, 5 0 20,  
-6 0 21,  
-1 0 25, -6 0 31, 2 1 31, 0 0 34, 1 0 34,  
-3 0 42,

[PLAT992 ALERT 5 C](#) Repd & Actual \_reflns\_number\_gt Values Differ by  
23 Check

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● Alert level G

[PLAT002 ALERT 2 G](#) Number of Distance or Angle Restraints on AtSite  
25 Note

[PLAT003 ALERT 2 G](#) Number of Uiso or Uij Restrained non-H Atoms ...  
17 Report

[PLAT007 ALERT 5 G](#) Number of Unrefined Donor-H Atoms .....  
4 Report

H2 H1 H3 H3'

[PLAT032 ALERT 4 G](#) Std. Uncertainty on Flack Parameter Value High .  
1.000 Report

[PLAT171 ALERT 4 G](#) The CIF-Embedded .res File Contains EADP Records  
8 Report

[PLAT172 ALERT 4 G](#) The CIF-Embedded .res File Contains DFIX Records  
7 Report

[PLAT175 ALERT 4 G](#) The CIF-Embedded .res File Contains SAME Records  
2 Report

[PLAT177 ALERT 4 G](#) The CIF-Embedded .res File Contains DELU Records  
13 Report

[PLAT186 ALERT 4 G](#) The CIF-Embedded .res File Contains ISOR Records  
1 Report

[PLAT192 ALERT 3 G](#) A Non-default DELU Restraint Value for First Par  
0.0010 Report

And 12 other PLAT192 Alerts

More ...

[PLAT301 ALERT 3 G](#) Main Residue Disorder .....(Resd 1)  
26% Note

[PLAT343 ALERT 2 G](#) Unusual sp? Angle Range in Main Residue for  
C25 Check

[PLAT367 ALERT 2 G](#) Long? C(sp?)-C(sp?) Bond C24 - C25 .  
1.51 Ang.

[PLAT367 ALERT 2 G](#) Long? C(sp?)-C(sp?) Bond C25 - C26 .  
 1.53 Ang.

[PLAT412 ALERT 2 G](#) Short Intra XH3 .. XHn H50 ..H59C .  
 1.92 Ang.  
 x,y,z =

1\_555 Check  
**And 2 other PLAT412 Alerts**  
 More ...

[PLAT413 ALERT 2 G](#) Short Inter XH3 .. XHn H26B ..H54B .  
 2.06 Ang.  
 x,y,z =

1\_555 Check

[PLAT413 ALERT 2 G](#) Short Inter XH3 .. XHn H28C ..H59F .  
 2.00 Ang.  
 -1+x,y,z =

1\_455 Check

[PLAT773 ALERT 2 G](#) Check long C-C Bond in CIF: C52 --C60'  
 1.83 Ang.

[PLAT790 ALERT 4 G](#) Centre of Gravity not Within Unit Cell: Resd. #  
 2 Note  
 C30 H48 O

[PLAT790 ALERT 4 G](#) Centre of Gravity not Within Unit Cell: Resd. #  
 3 Note  
 H2 O

[PLAT860 ALERT 3 G](#) Number of Least-Squares Restraints .....  
 133 Note

[PLAT883 ALERT 1 G](#) No Info/Value for \_atom\_sites\_solution\_primary .  
 Please Do !

[PLAT910 ALERT 3 G](#) Missing # of FCF Reflection(s) Below Theta(Min).  
 3 Note  
 0 0 1, 0 0 2, 0 0 3,

[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600  
 7 Note

[PLAT916 ALERT 2 G](#) Hooft y and Flack x Parameter Values Differ by .  
 1.00 Check

[PLAT941 ALERT 3 G](#) Average HKL Measurement Multiplicity .....  
 4.0 Low

[PLAT965\\_ALERT\\_2\\_G](#) The SHELXL WEIGHT Optimisation has not Converged  
Please Check

[PLAT967\\_ALERT\\_5\\_G](#) Note: Two-Theta Cutoff Value in Embedded .res ..  
52.5 Degree

[PLAT969\\_ALERT\\_5\\_G](#) The 'Henn et al.' R-Factor-gap value .....  
4.64 Note

Predicted wR2: Based on SigI\*\*2 7.39 or SHELX Weight  
33.43

[PLAT978\\_ALERT\\_2\\_G](#) Number C-C Bonds with Positive Residual Density.  
0 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

44 **ALERT level G** = General information/check it is not something unexpected

1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

22 **ALERT type 2** Indicator that the structure model may be wrong or deficient

22 **ALERT type 3** Indicator that the structure quality may be low

15 **ALERT type 4** Improvement, methodology, query or suggestion

4 **ALERT type 5** Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may



appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that [full publication checks](#) are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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PLATON version of 13/12/2023; check.def file version of 13/12/2023

### Datablock ic21710 - ellipsoid plot

