Supporting Information

***Rec. Nat. Prod*. 16:4 (2022) 316-323**

Two New Seco-abietanoids with Xanthine Oxidase Inhibitory Activity from *Cryptomeria japonica*

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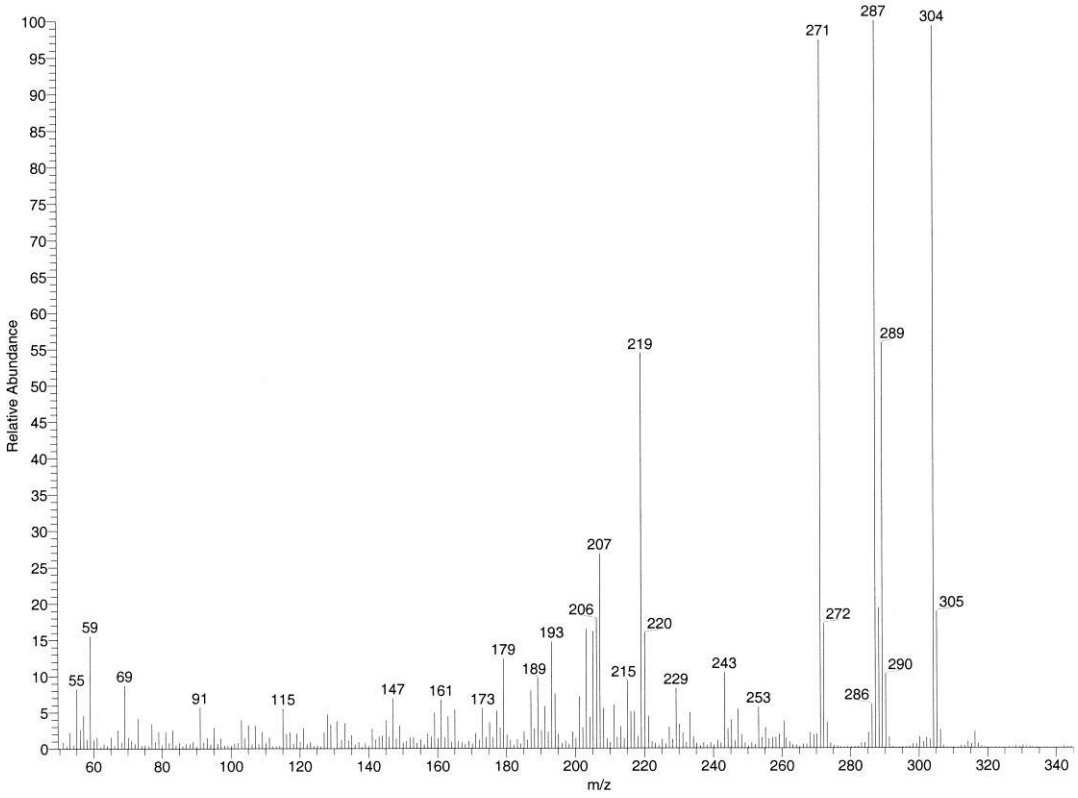

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Instrument : MStation
Sample : CJD63
Note :
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.00 min Scan# : 1 Temp : 3276.7 deg.C
BP : m/z 287.2006 Int. : 20.73 (217402)
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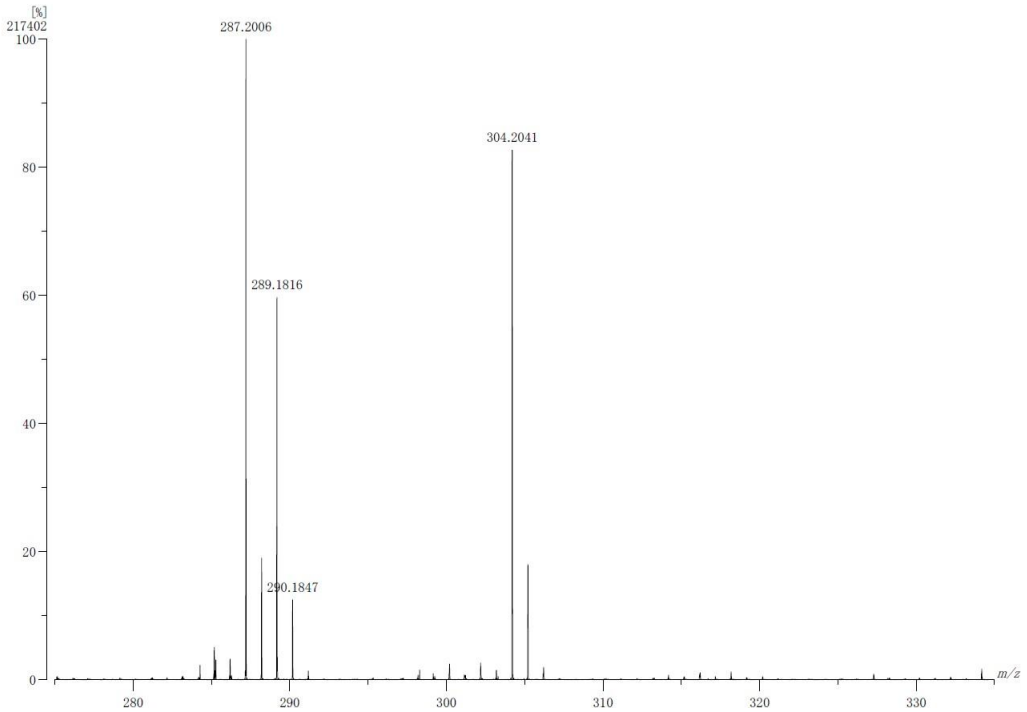

Figure S1: Mass Spectrum of compound **1** (EI-MS Spectrum and HR-EI-MS data)

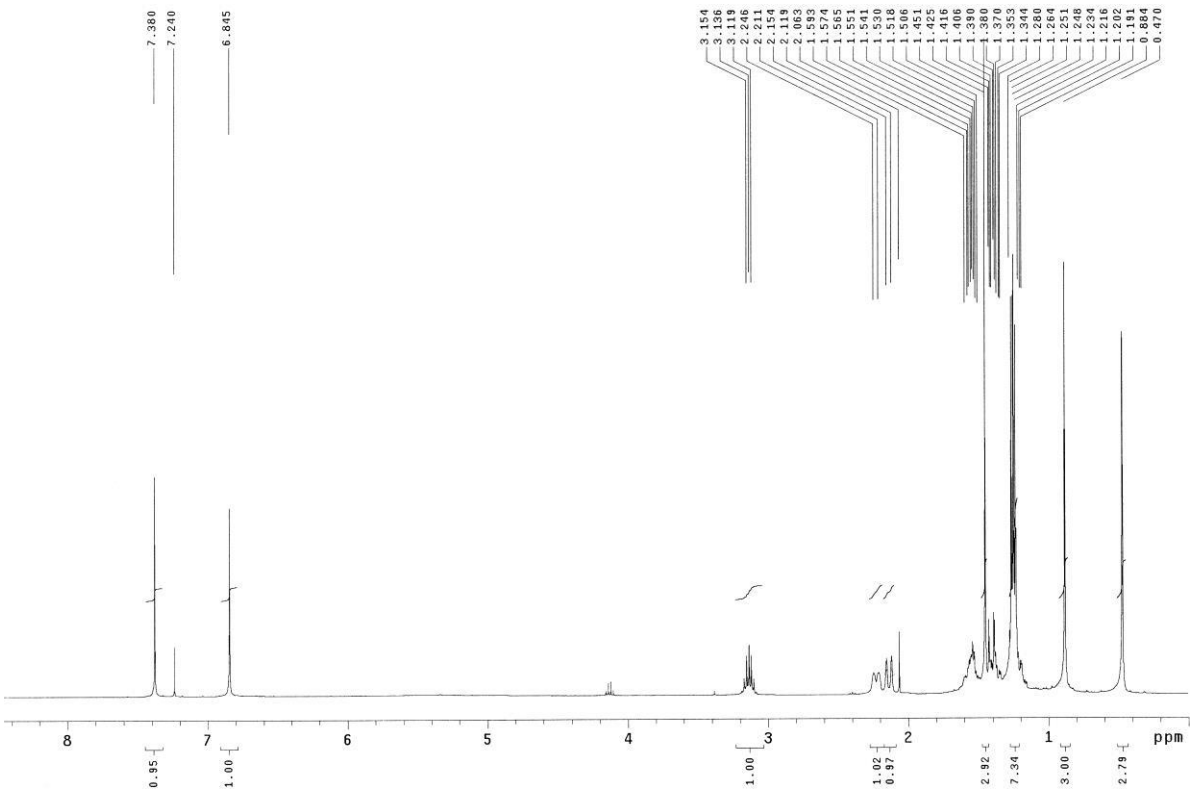

Figure S2: ^{1}H-NMR spectrum of compound **1** in $CDCl_3$

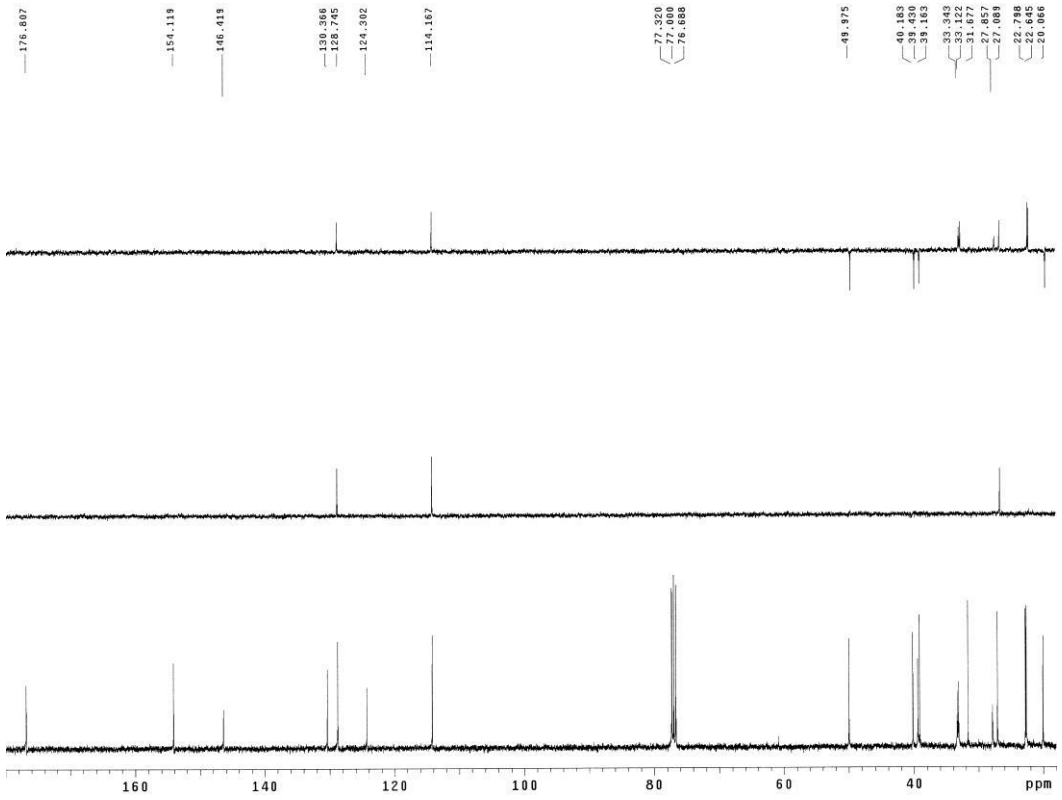

Figure S3: ^{13}C-NMR spectrum and DEPT of compound **1** in $CDCl_3$

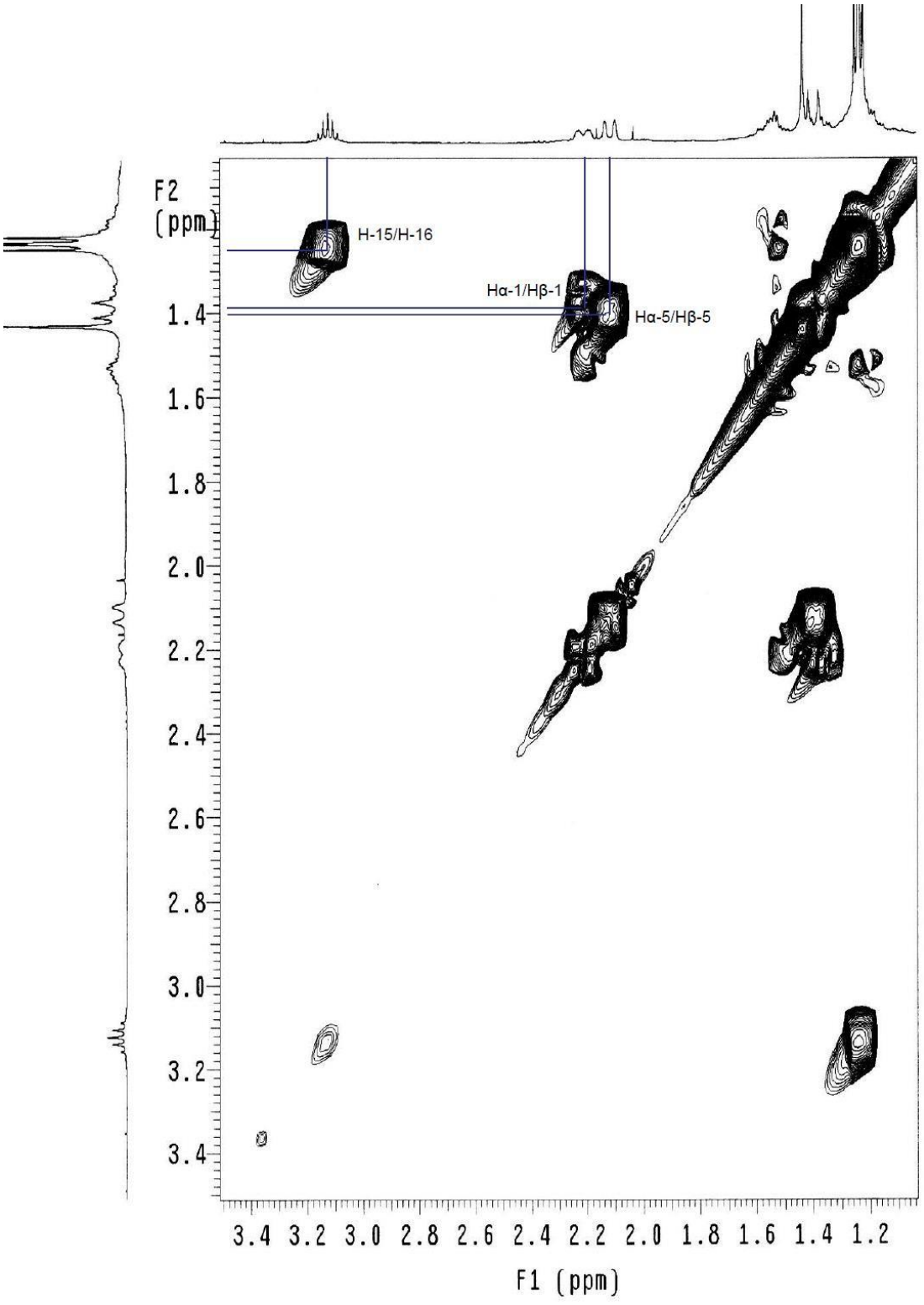

Figure S4: ^{1}H-^{1}H COSY spectrum of compound **1** in $CDCl_3$

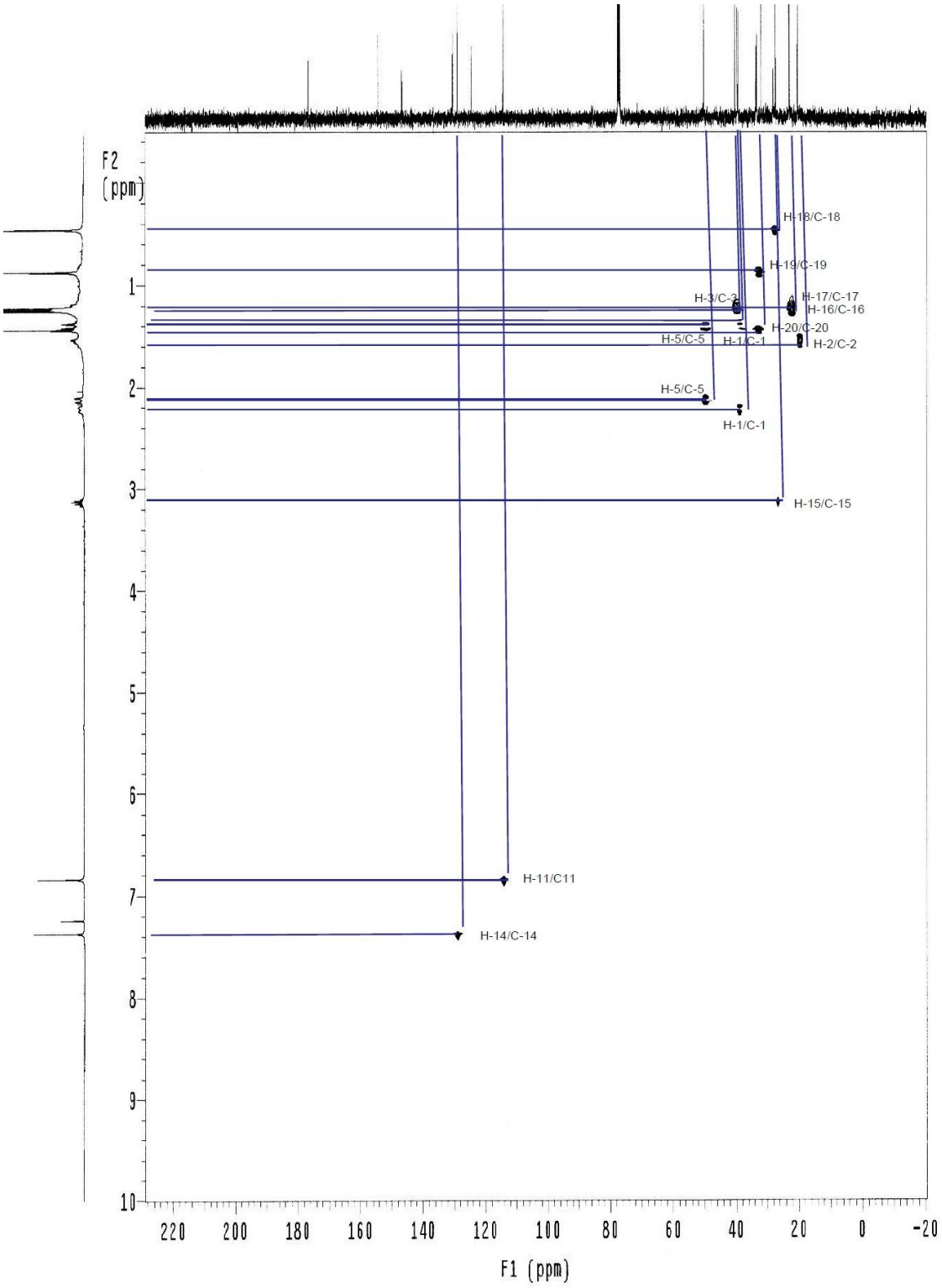

Figure S5: HMQC spectrum of compound **1** in $CDCl_3$

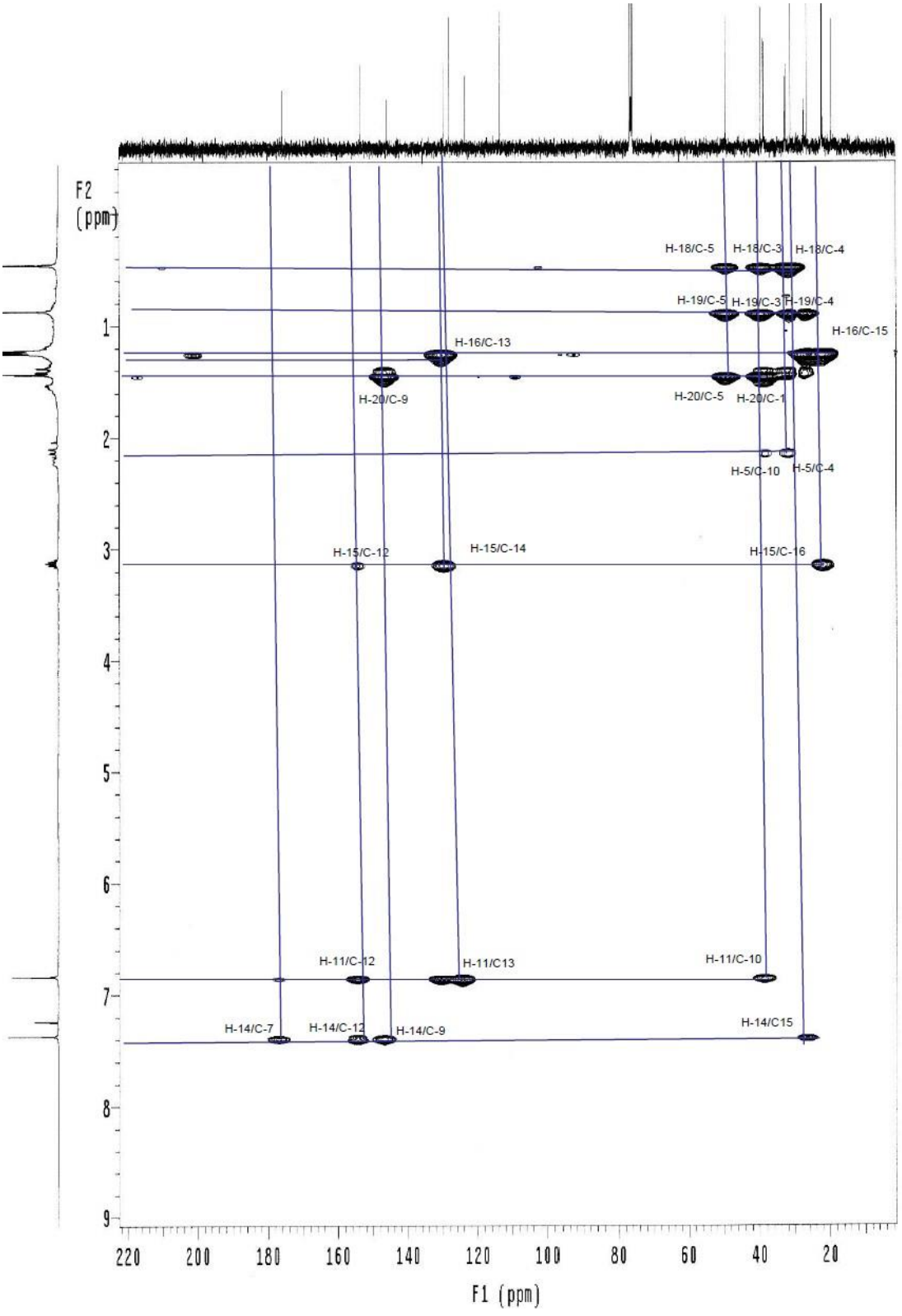

Figure S6: HMBC spectrum of compound **1**in $CDCl_3$

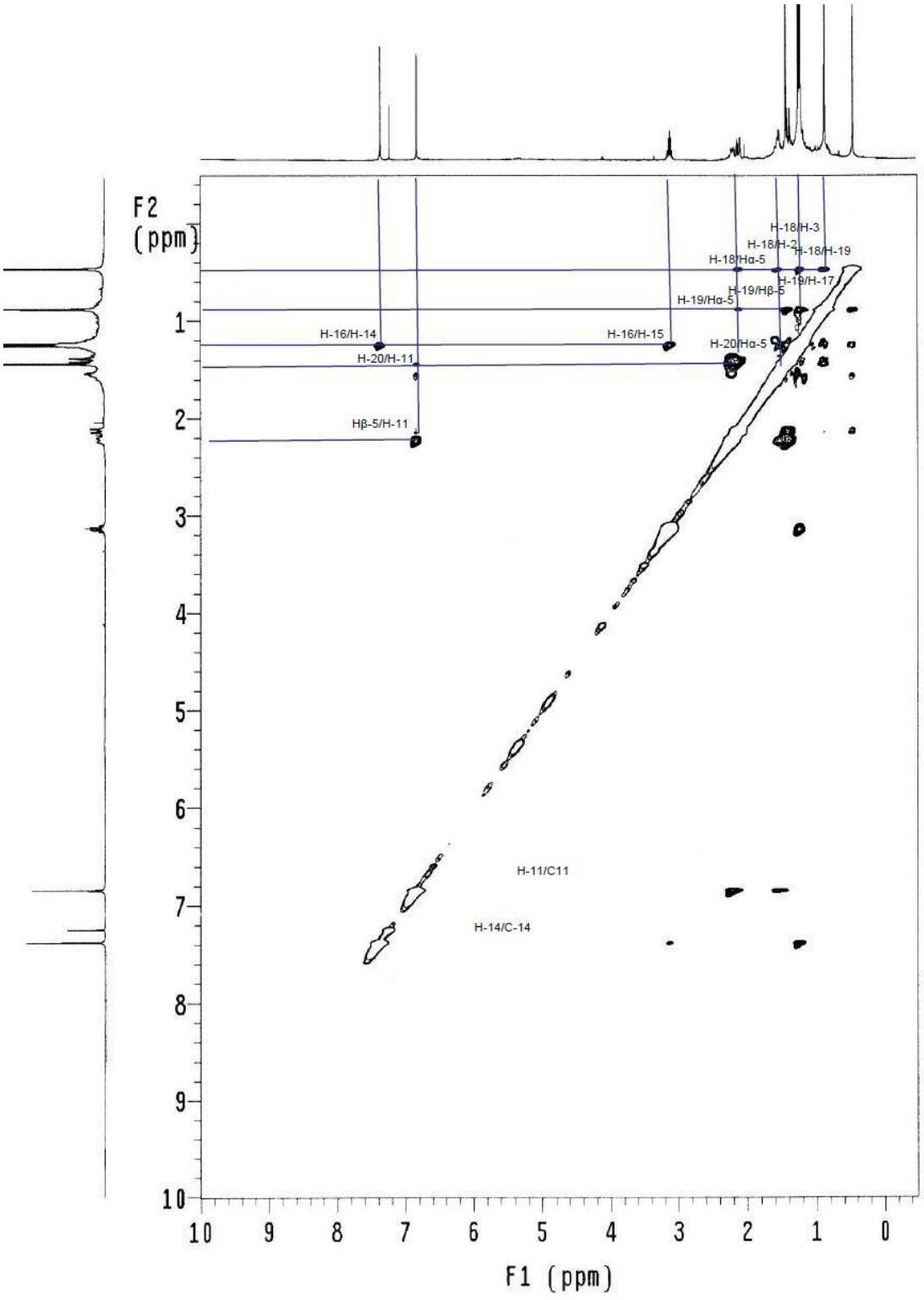

Figure S7: NOSEY spectrum of compound **1** in $CDCl_3$

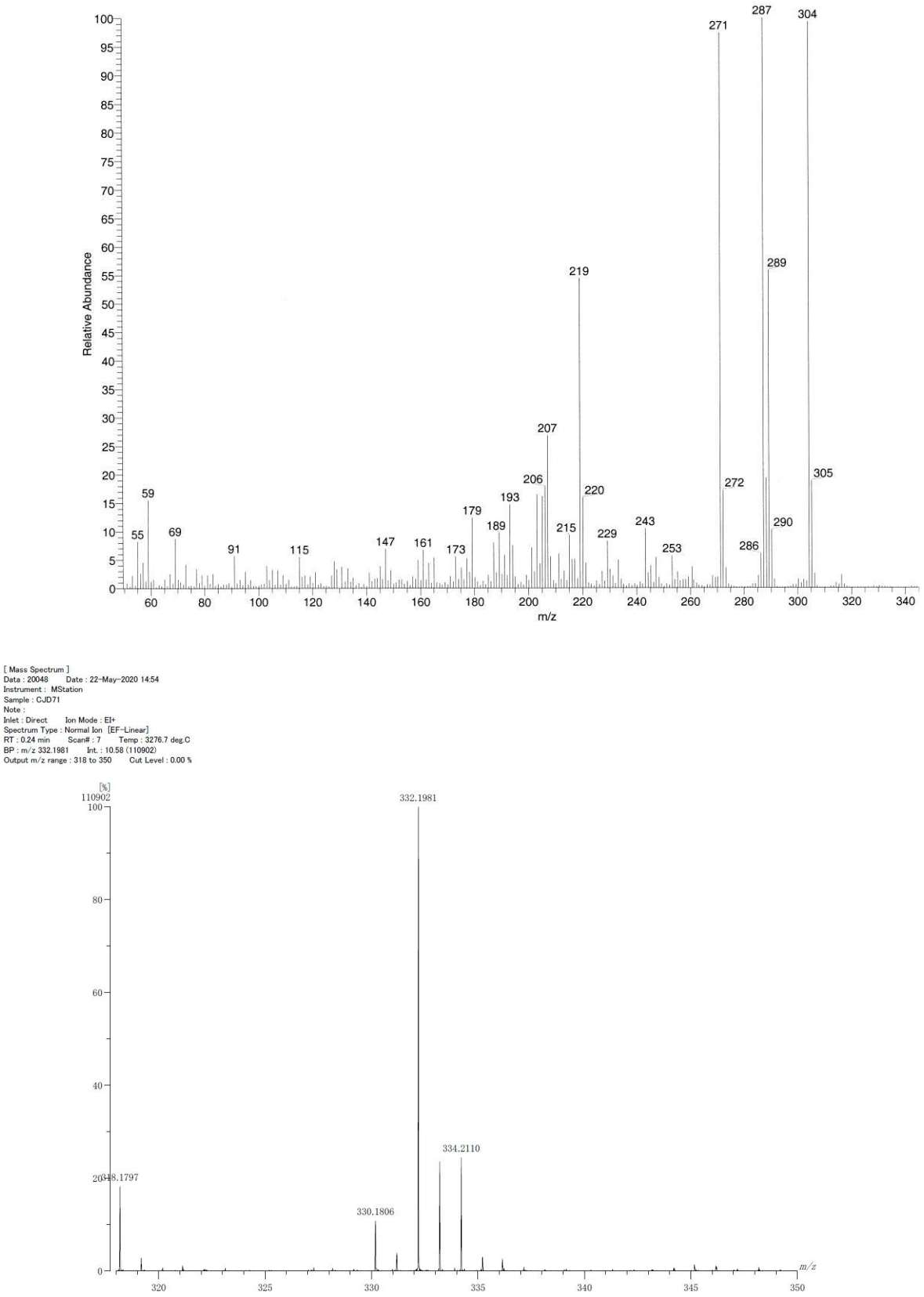

Figure S8: Mass Spectrum of compound **3** (EI-MS Spectrum and HR-EI-MS data)

CAS SciFinder

Task History

Initiating Search

September 29, 2021, 9:22AM

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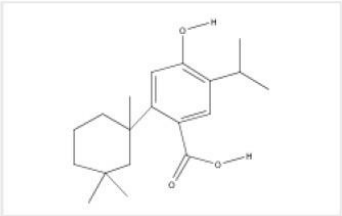
Filtered By:

Structure Match:	**Similarity**
Similarity:	**85-89, >=99**
Number of Components:	**1**



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

CAS SciFinder

Substances (16)

View in SciFinder

1 Similarity Score: **100**

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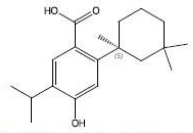

Absolute stereochemistry shown

$C_{19}H_{28}O_3$

4-Hydroxy-5-(1-methylethyl)-2-[(1*S*)-1,3,3-trimethylcyclohexyl]benzoic acid

2 References | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	304.42	-
Boiling Point (Predicted)	439.8±45.0 °C	Press: 760 Torr
Density (Predicted)	1.055±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	4.55±0.36	Most Acidic Temp: 25 °C

Figure S9: Scifinder report for compound **1**

		1		reference compound
Position	δ_C	δ_H	δ_C*	δ_H
1	39.1	2.23 br d (14.0), 1.38 m		2.14 m, 1.40 m
2	20.0	1.56 m, 1.58 m		1.56 m
3	40.1	1.20 m, 1.24 m		1.60 m
4	31.6			
5	49.9	1.41 d (14.0), 2.13 d (14.0)		
6				
7	176.8			
8	124.3			
9	146.4			
10	39.4			
11	114.1	6.84 s		6.84 s
12	154.1			
13	130.3			
14	128.7	7.38 s		7.36 s
15	27.0	3.13 sept (7.0)		
16	22.7	1.24 d (7.0)	1.25 d (6.8)	
17	22.6	1.26 d (7.0)	1.26 d (6.8)	
18	27.8	0.47 s		0.47 s
19	33.1	0.88 s		0.88 s
20	33.3	1.45 s		1.45 s
7-OH				

Table S1: ^{1}H and ^{13}C NMR data for compounds **1** and reference compound.
* ^{13}C NMR data are unavailable.

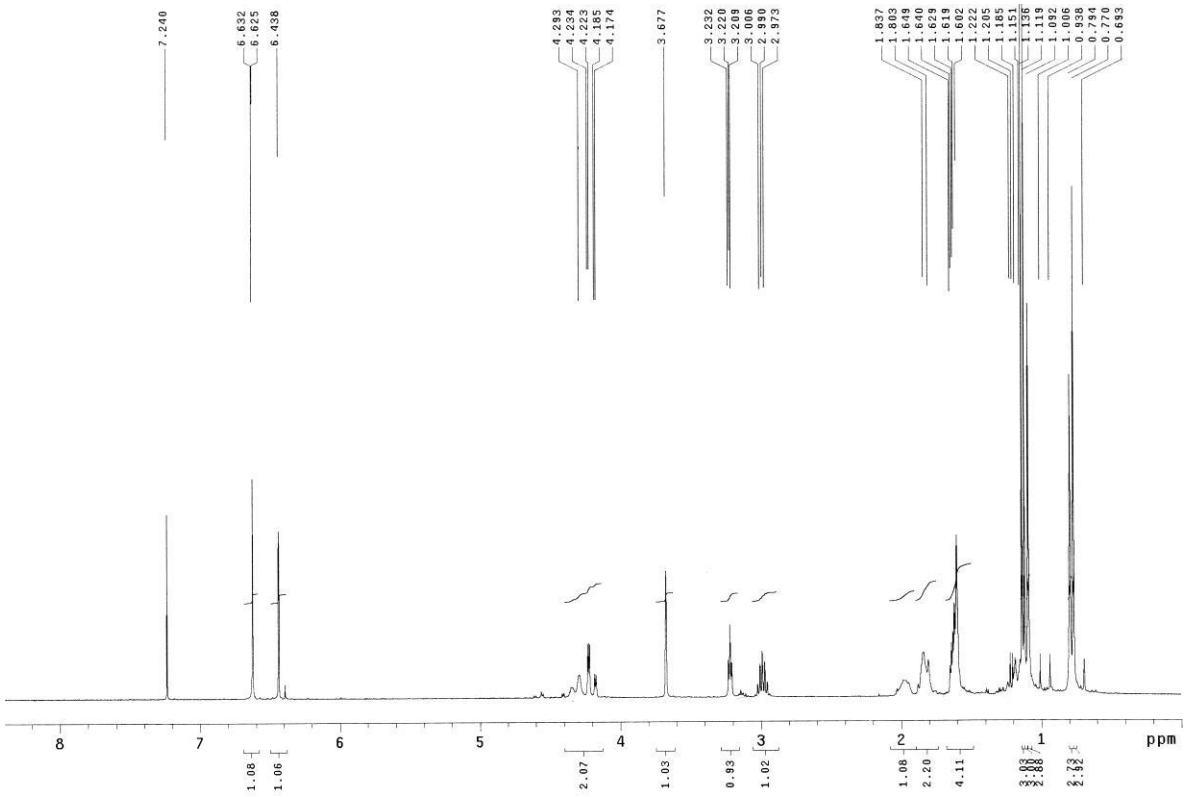

Figure S10: ^{1}H-NMR spectrum of compound **3** in $CDCl_3$

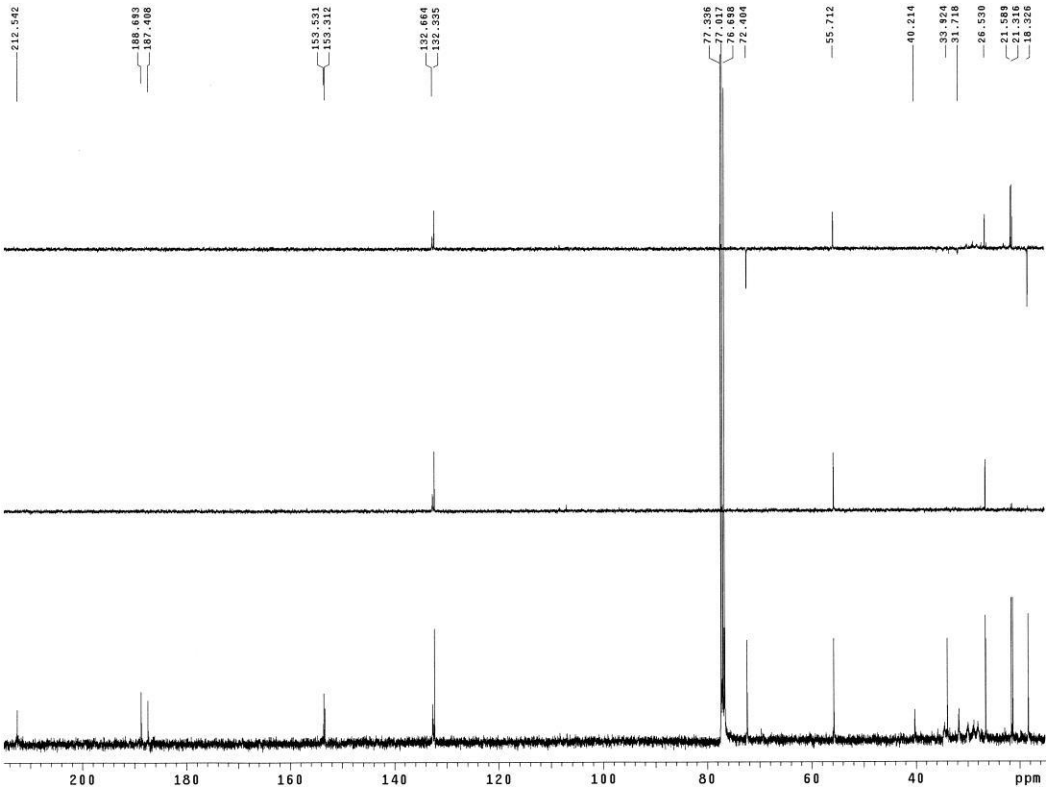

Figure S11: ^{13}C-NMR spectrum and DEPT of compound **3** in $CDCl_3$

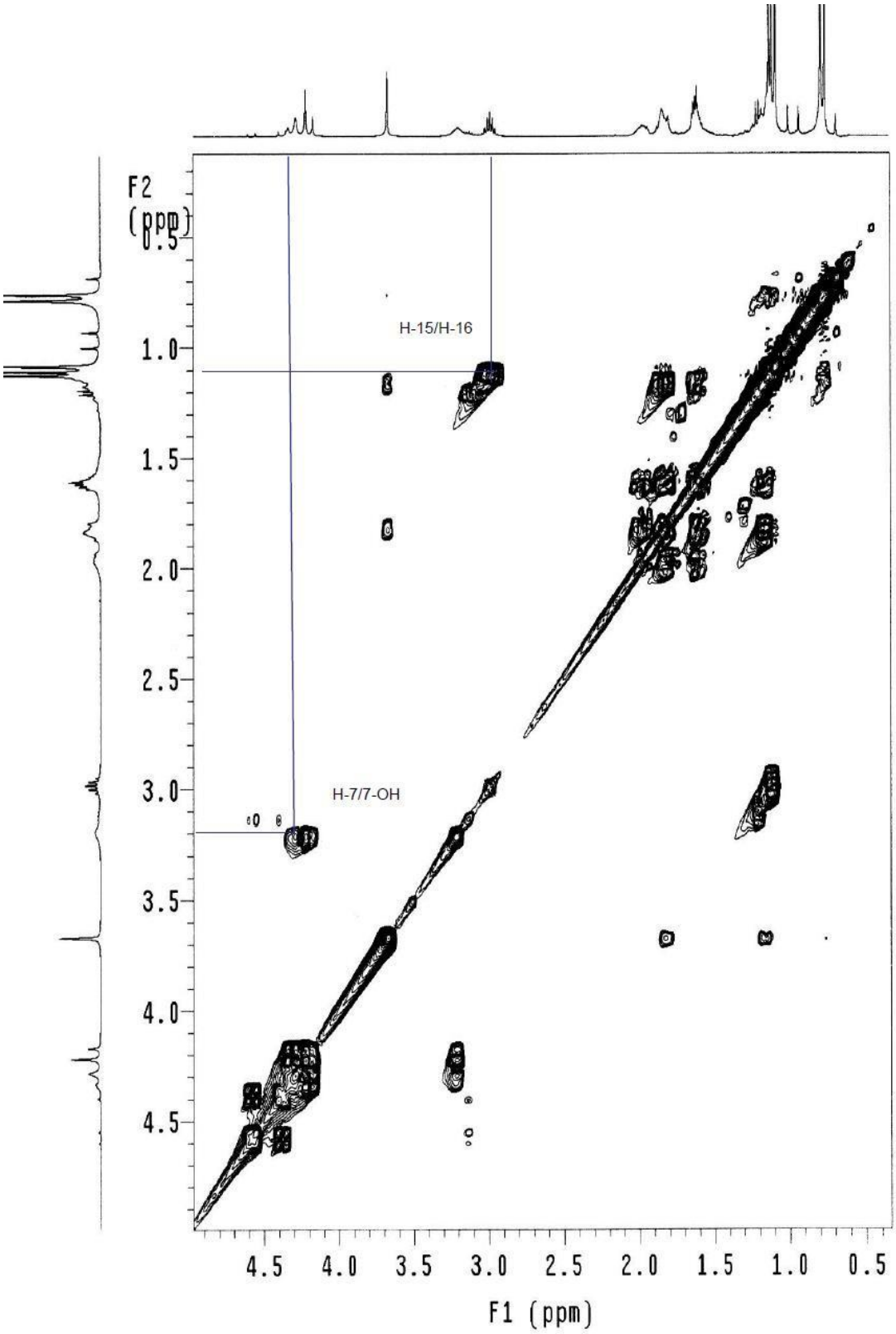

Figure S12: ^{1}H-^{1}H COSY spectrum of compound **3** in $CDCl_3$

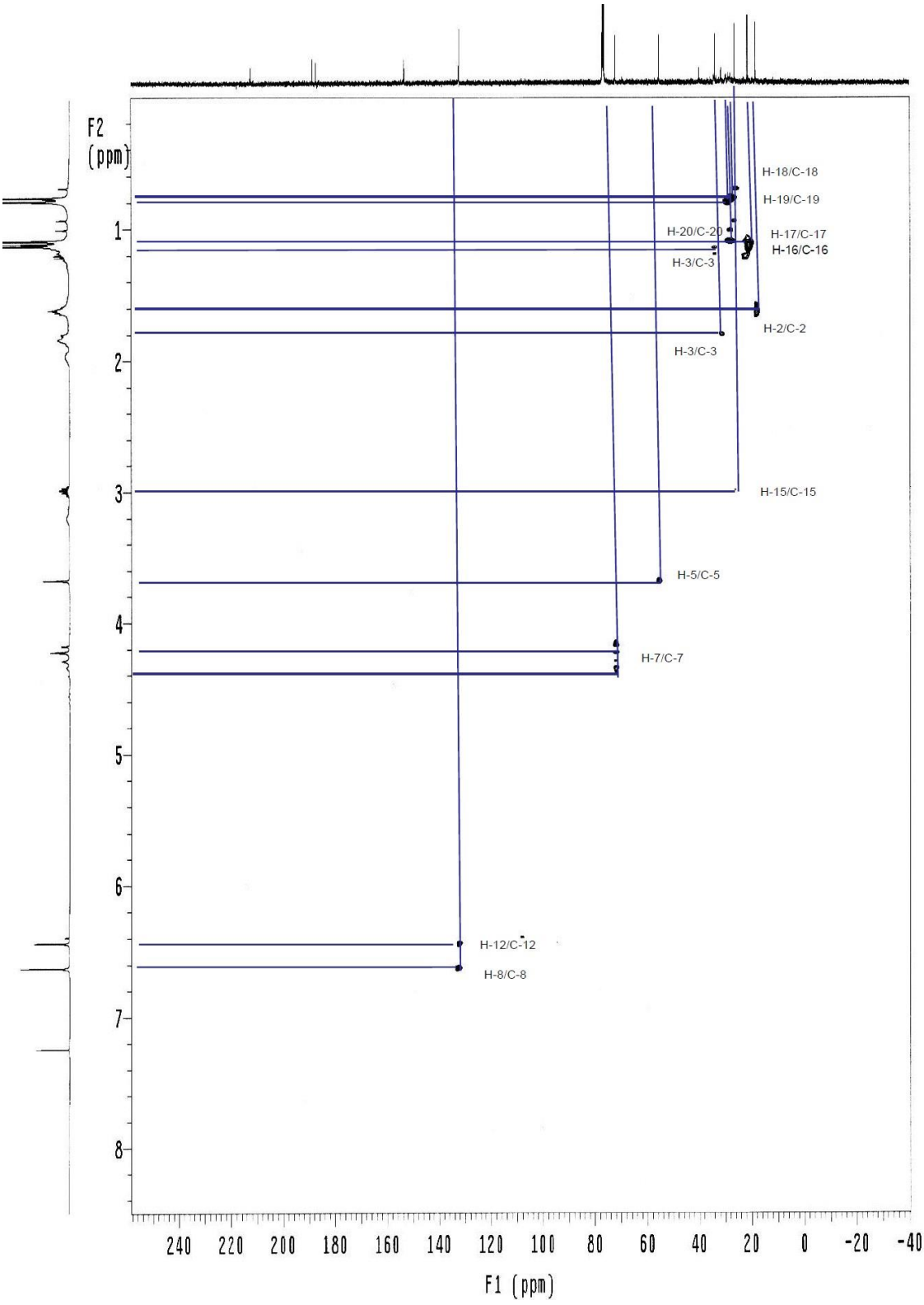

Figure S13: HMQC spectrum of compound **3** in $CDCl_3$

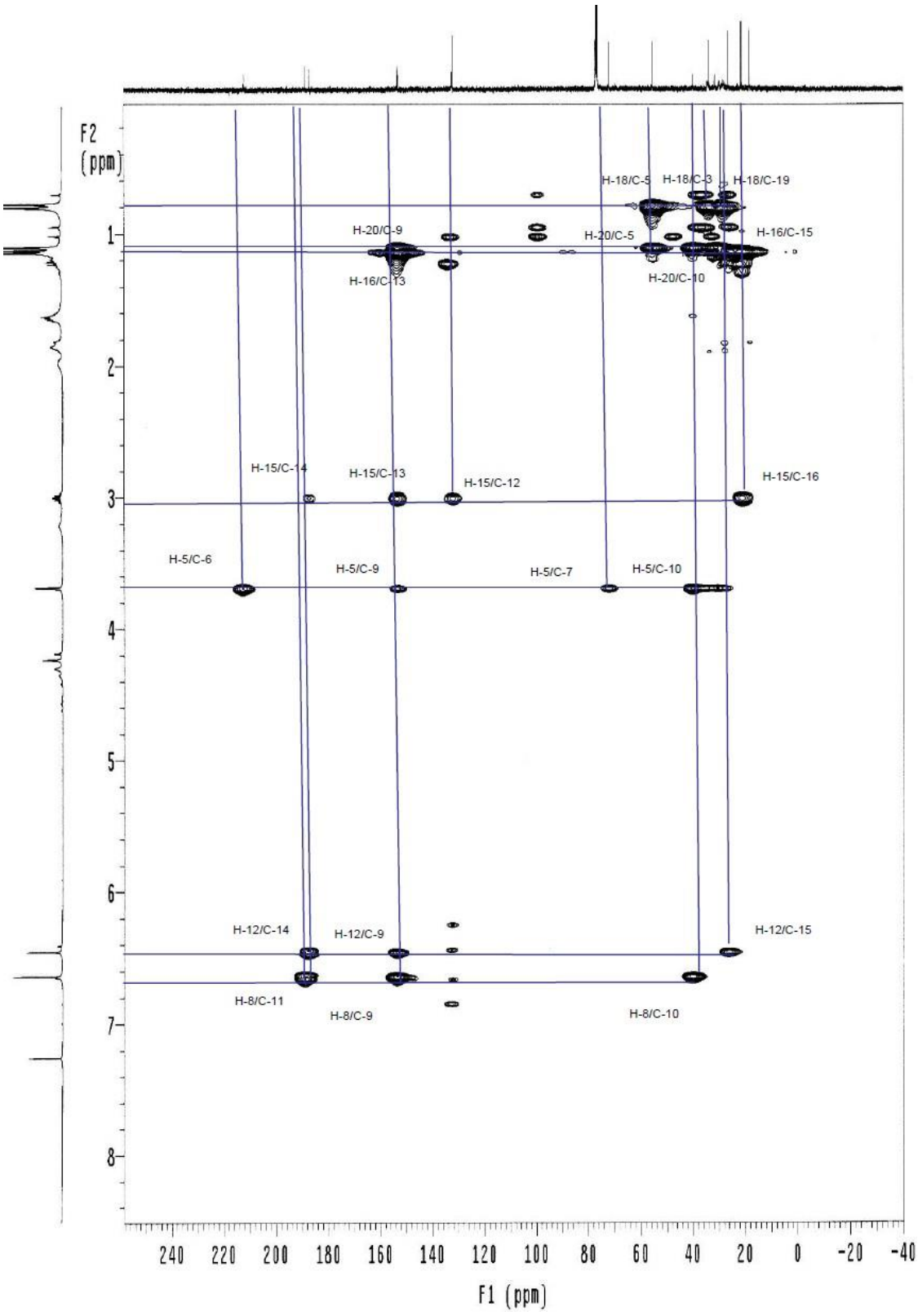

Figure S14: HMBC spectrum of compound **3** in $CDCl_3$

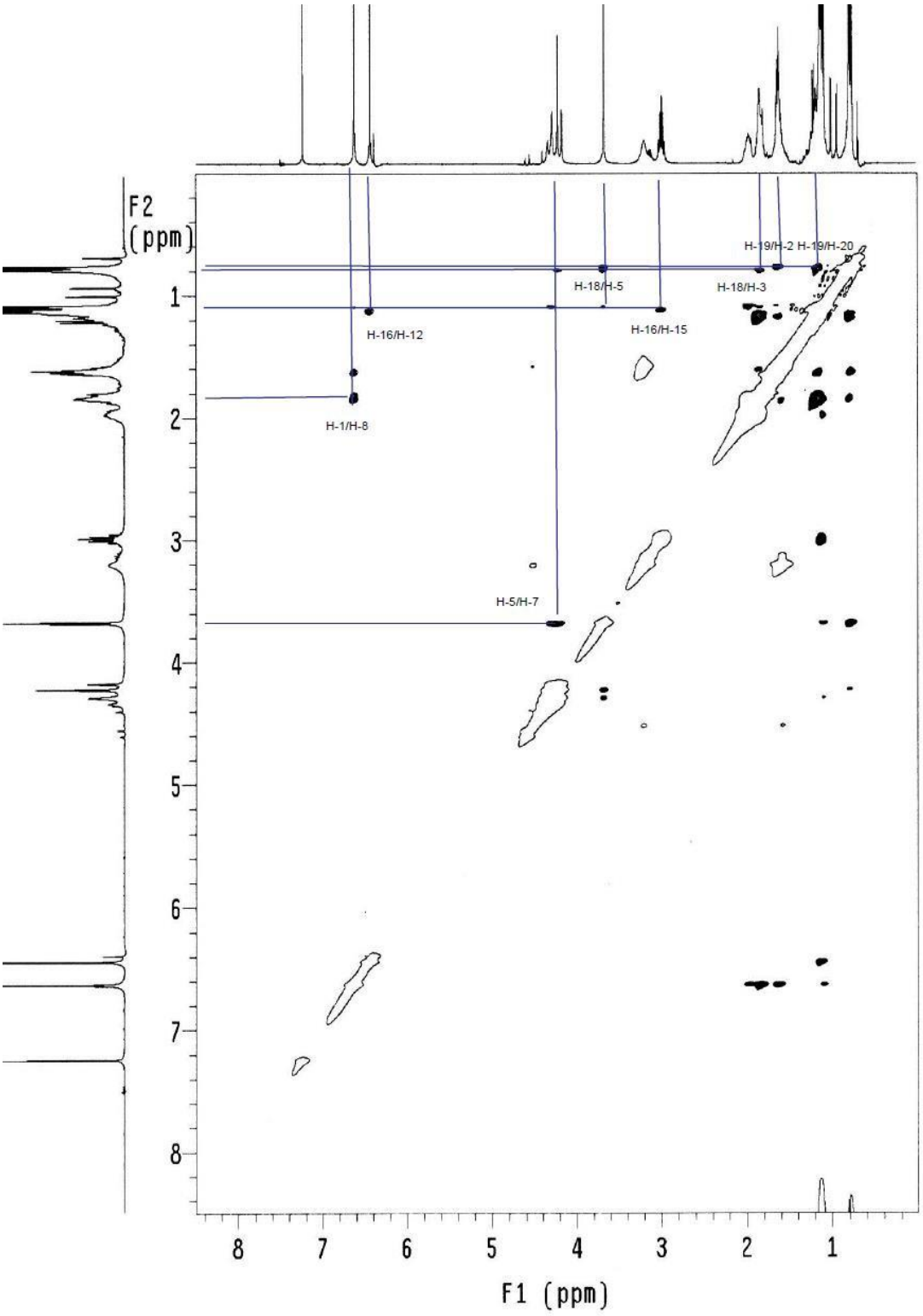

Figure S15: NOSEY spectrum of compound **3** in $CDCl_3$

CAS SciFinder^{n}

Task History

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September 29, 2021, 9:27AM

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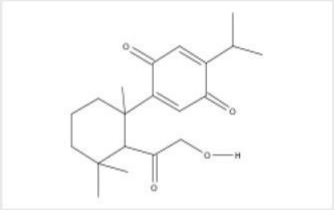

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters	**Substances**	View Results

CAS SciFinder^n

Substances (6)

View in SciFinder^n

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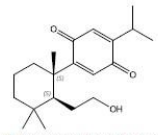
2697170-39-9



Absolute stereochemistry shown

$C_{20}H_{30}O_3$

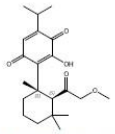
2,5-Cyclohexadiene-1,4-dione, 2-[(1*S*,2*S*)-2-(2-hydroxyethyl)-1,3,3-trimethylcyclohexyl]-5-(1-methylethyl)-

1 Reference | 1 Reaction | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	318.45	-
Boiling Point (Predicted)	418.4±14.0 °C	Press: 760 Torr
Density (Predicted)	1.040±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	15.14±0.10	Most Acidic Temp: 25 °C

2 Similarity Score: **91**

1879065-67-4



Absolute stereochemistry shown, Rotation (+)

$C_{21}H_{30}O_5$

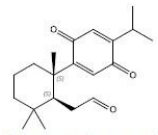
3-Hydroxy-2-[(1*S*,2*S*)-2-(2-methoxyacetyl)-1,3,3-trimethylcyclohexyl]-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione

3 References | 0 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	362.46	-
Boiling Point (Predicted)	483.7±45.0 °C	Press: 760 Torr
Density (Predicted)	1.132±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	3.19±0.50	Most Acidic Temp: 25 °C

3 Similarity Score: **91**

453510-93-5



Absolute stereochemistry shown

$C_{20}H_{28}O_3$

(1*S*,6*S*)-2,2,6-Trimethyl-6-[4-(1-methylethyl)-3,6-dioxo-1,4-cyclohexadien-1-yl]cyclohexaneacetaldehyde

4 References | 2 Reactions | 1 Supplier

Key Physical Properties	Value	Condition
Molecular Weight	316.43	-
Boiling Point (Predicted)	413.3±14.0 °C	Press: 760 Torr
Density (Predicted)	1.034±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
Spectra		

Figure S16: Scifinder report for compound **3**