

# Supplementary Materials: Six New Triterpene Derivatives from *Aralia chinensis* Var. *dasyphylloides*

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## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

75 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-10

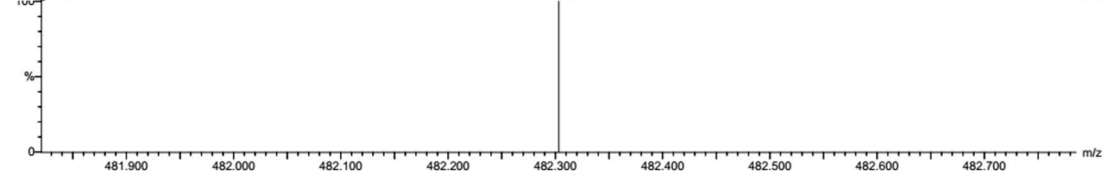
f44

10:24:36 26-Nov-2015

Voltage EI+

KIB  
M151126EA-01AFAMM 24 (2.203)  
482.3033

Autospec Premier  
P776  
362



Minimum:						
Maximum:	200.0	10.0	-10.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
482.3033	482.3032	0.1	0.2	10.0	5546199.0	C30 H42 O5

Figure S1. HR-EI-MS data of compound 1.

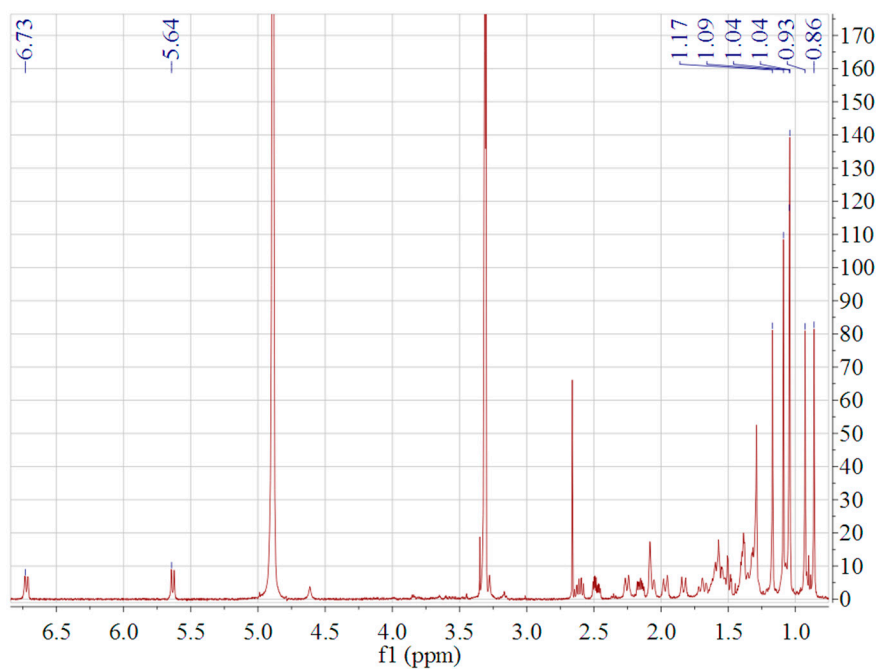


Figure S2. <sup>1</sup>H-NMR data of compound 1 (500 MHz, CD<sub>3</sub>OD).

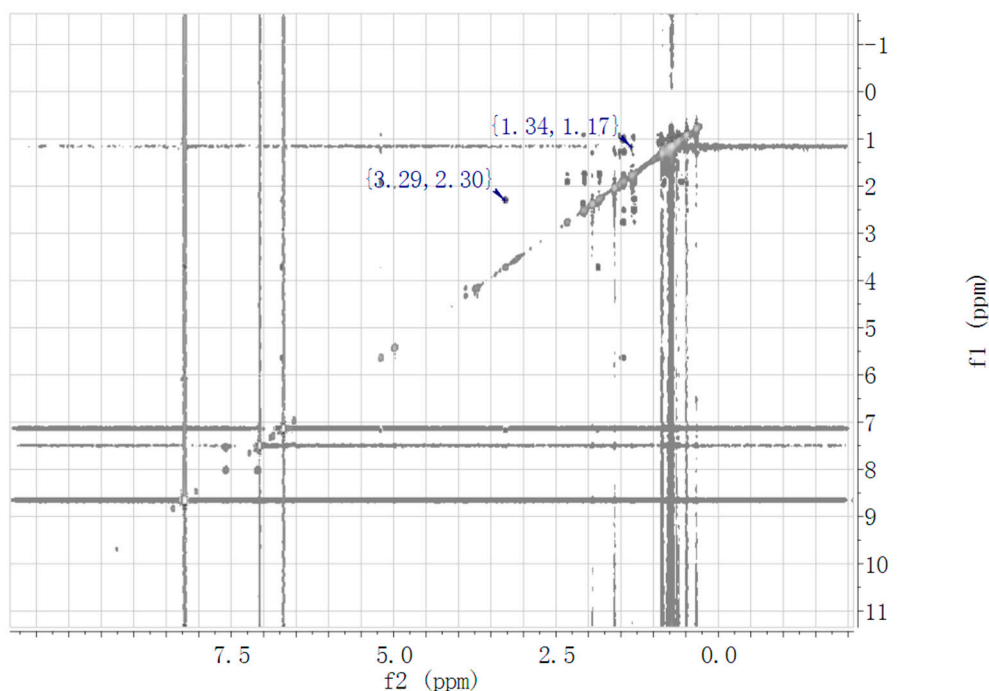


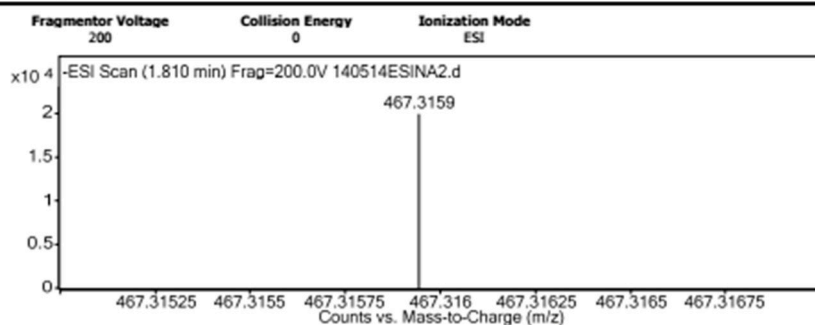
Figure S3. NOESY data of compound 1.

### Qualitative Analysis Report

<b>Data Filename</b>	140514ESINA2.d	<b>Sample Name</b>	f45
<b>Sample Type</b>	Sample	<b>Position</b>	
<b>Instrument Name</b>	Agilent G6230 TOF MS	<b>User Name</b>	KIB
<b>Acq Method</b>	ESIN.m	<b>Acquired Time</b>	5/14/2014 5:29:55 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	ESIN.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.1)	

#### User Spectra



#### Peak List

m/z	z	Abund
423.3268	1	141367.11

#### Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	2	20

#### Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff.(ppm)	DBE
C30 H43 O4	467.3161	467.3159	0.2	0.4	9.5

--- End Of Report ---

Figure S4. HR-ESI-MS data of compound 2.

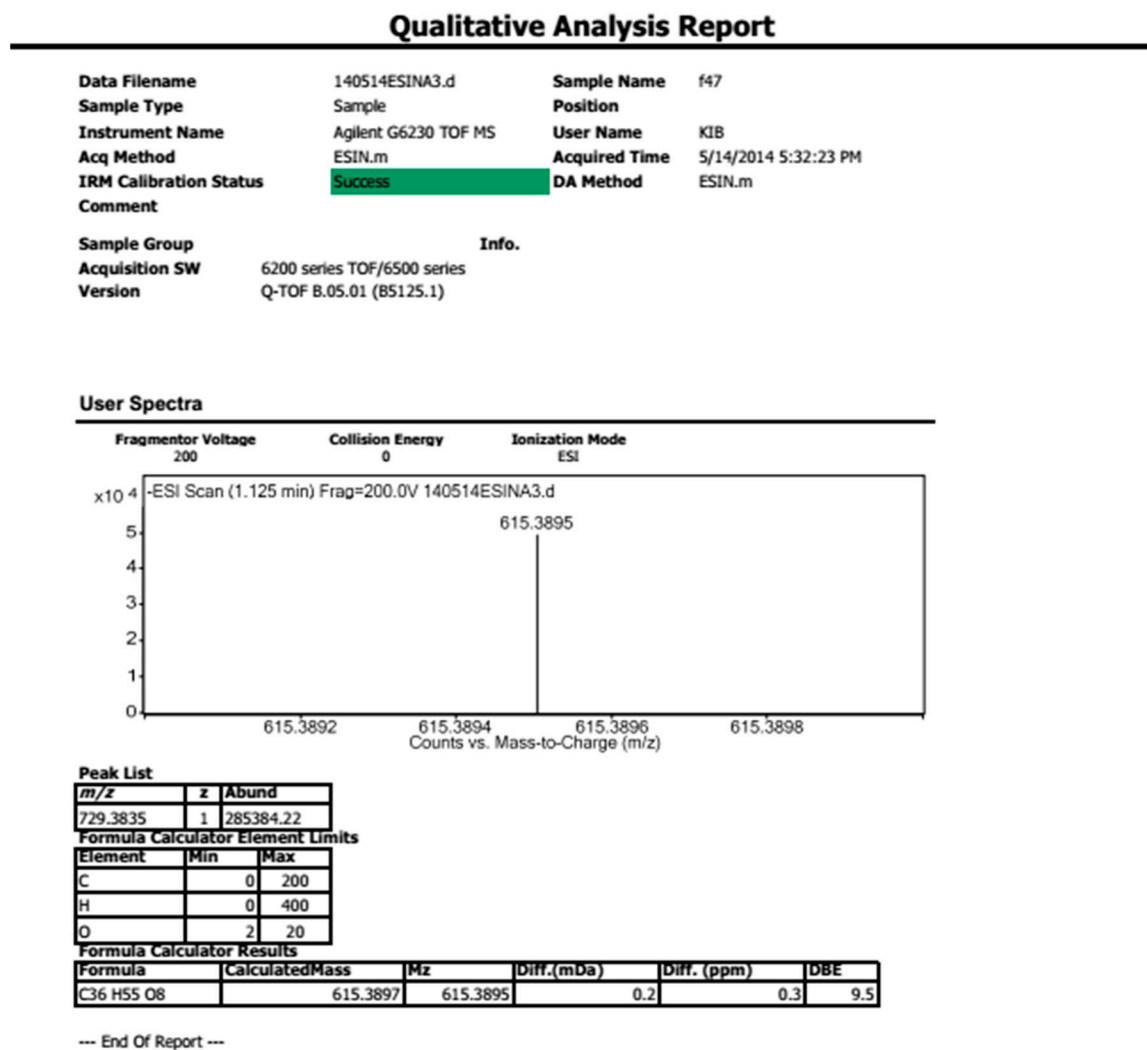


Figure S5. HR-ESI-MS data of compound 3.

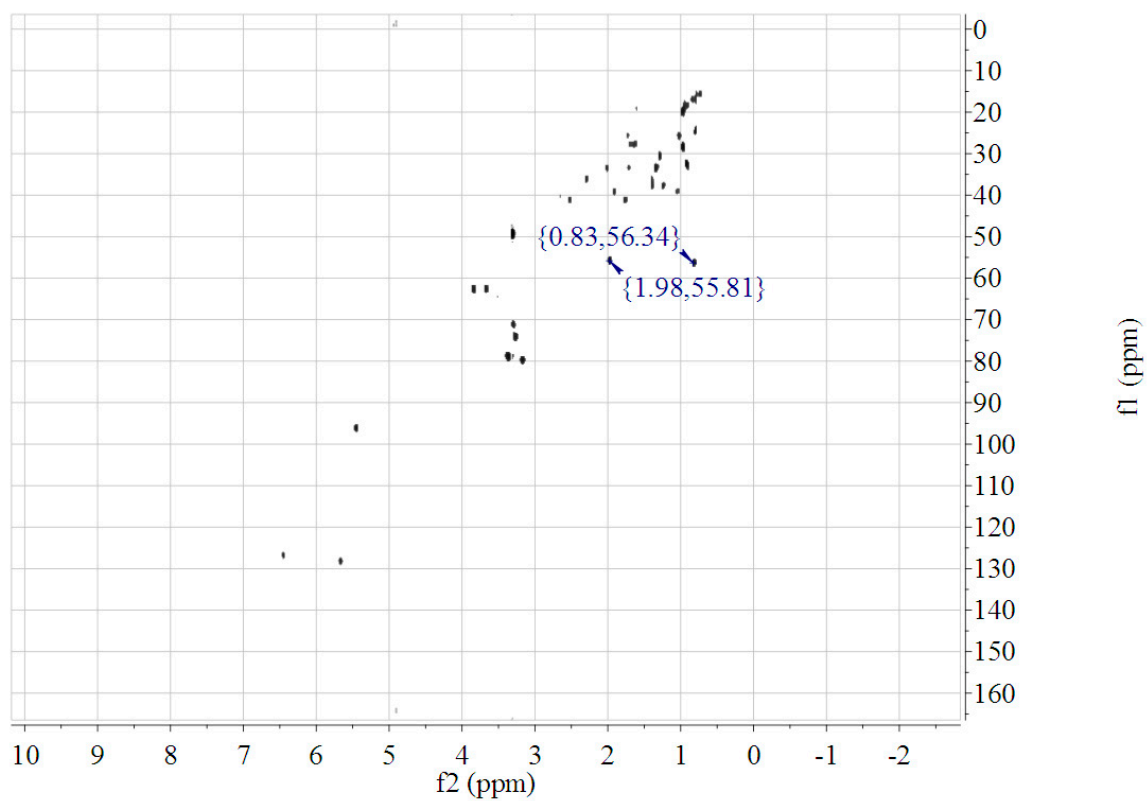


Figure S6. HSQC data of compound 3.

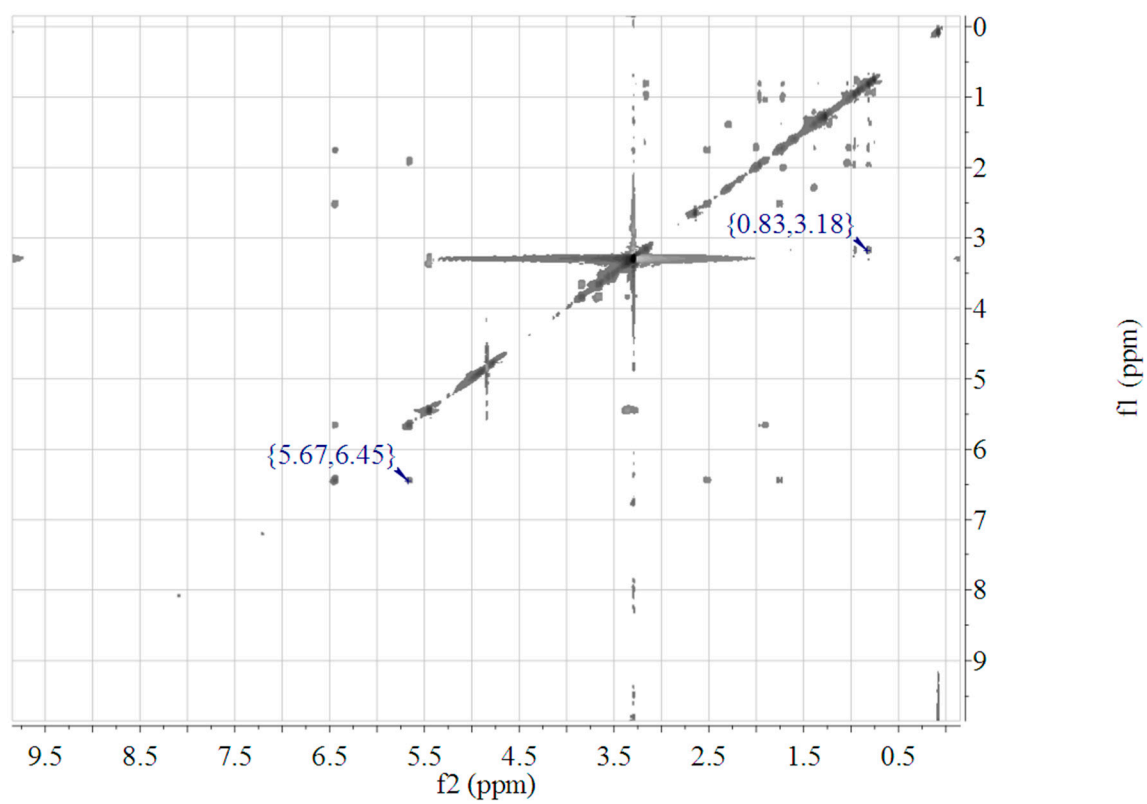
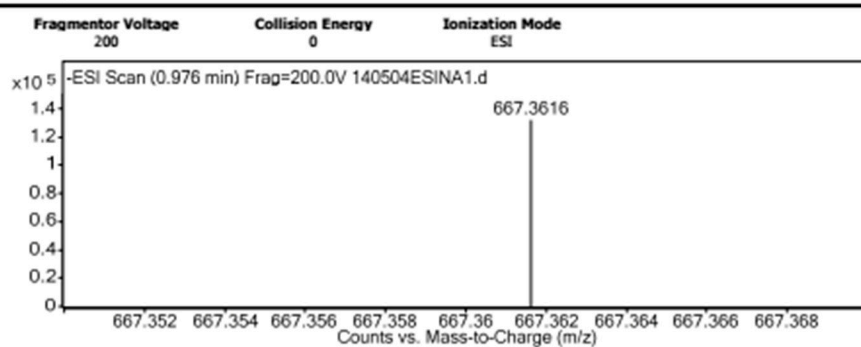


Figure S7. NOESY data of compound 3

## Qualitative Analysis Report

<b>Data Filename</b>	140504ESINA1.d	<b>Sample Name</b>	CP11
<b>Sample Type</b>	Sample	<b>Position</b>	
<b>Instrument Name</b>	Agilent G6230 TOF MS	<b>User Name</b>	KIB
<b>Acq Method</b>	ESIN.m	<b>Acquired Time</b>	5/4/2014 9:48:08 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	ESIN.m
<b>Comment</b>			
<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125.1)		

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
667.3616	1	131533.86	C36 H56 Cl O9	M-

### Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	2	20
Cl	0	1

### Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C36 H56 Cl O9	667.3613	667.3616	-0.3	0.4	8.5

--- End Of Report ---

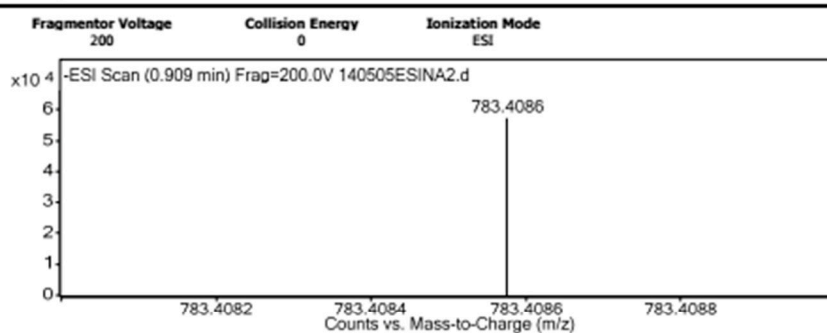
Figure S8. HR-ESI-MS data of compound 4.

## Qualitative Analysis Report

Data Filename	140505ESINA2.d	Sample Name	CP18
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESIN.m	Acquired Time	5/5/2014 9:44:20 AM
IRM Calibration Status	Success	DA Method	ESIN.m

Sample Group	Info.
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.1)

### User Spectra



#### Peak List

m/z	z	Abund
1033.9881	1	66713.21

#### Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	5	25
Cl	1	1

#### Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C41 H64 Cl O12	783.4086	783.4086	0.0	0.0	9.5

--- End Of Report ---

Figure S9. HR-ESI-MS data of compound 5.

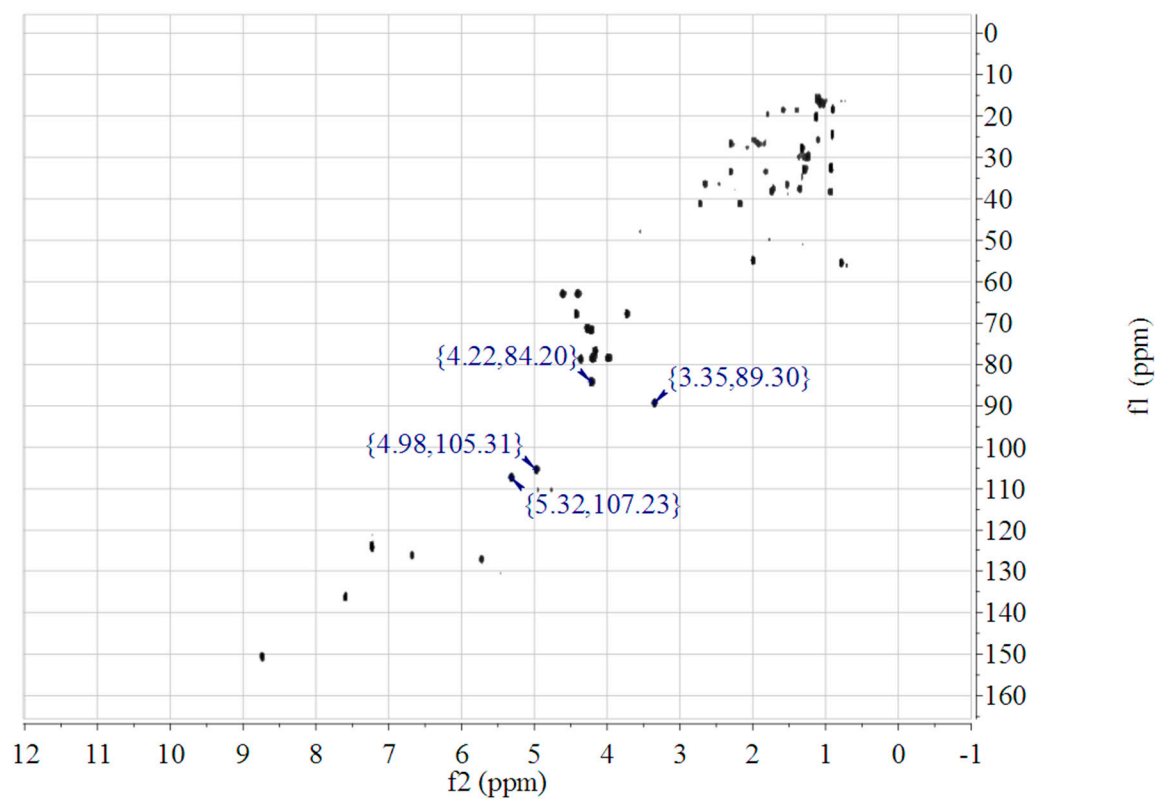


Figure S10. HSQC data of compound 5.

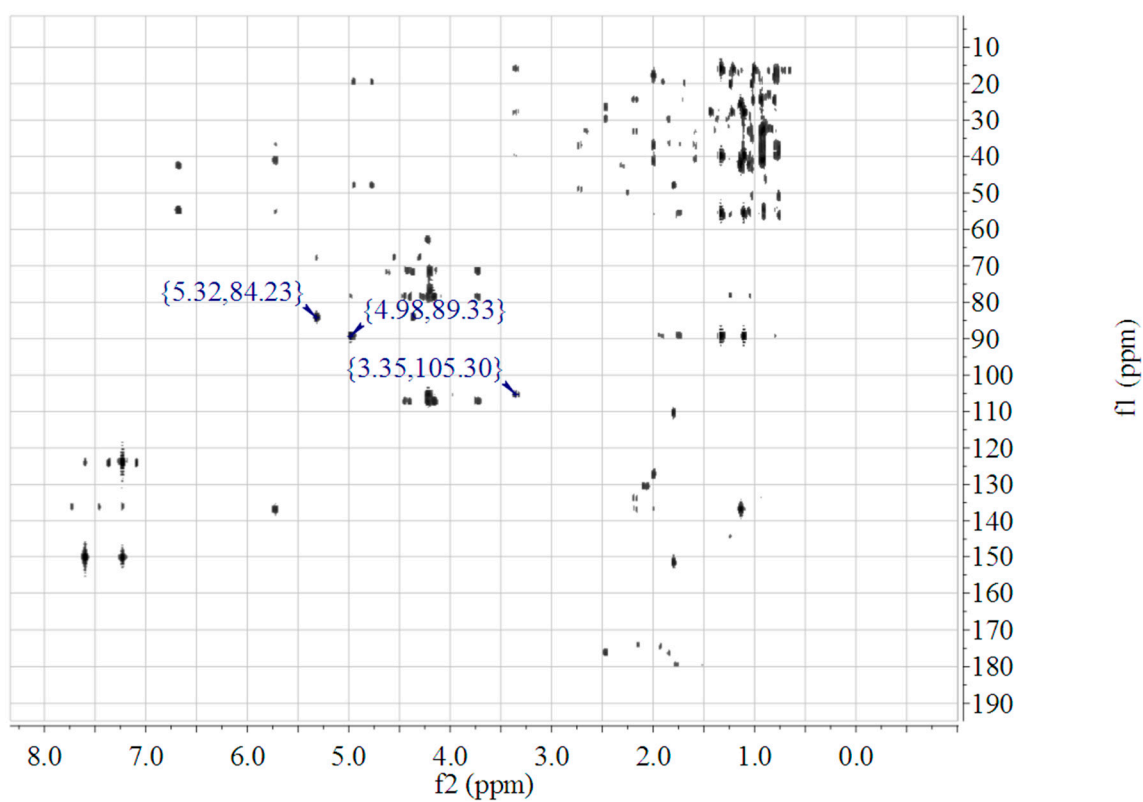


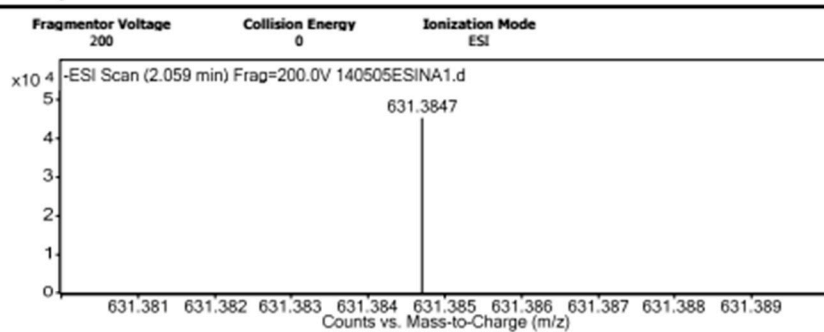
Figure S11. HMBC data of compound 5.

## Qualitative Analysis Report

<b>Data Filename</b>	140505ESINA1.d	<b>Sample Name</b>	CP10
<b>Sample Type</b>	Sample	<b>Position</b>	
<b>Instrument Name</b>	Agilent G6230 TOF MS	<b>User Name</b>	KIB
<b>Acq Method</b>	ESIN.m	<b>Acquired Time</b>	5/5/2014 9:37:19 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	ESIN.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.1)	

### User Spectra



#### Peak List

m/z	z	Abund
745.378	1	81054.69

#### Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	3	20

#### Formula Calculator Results

Formula	CalculatedMass	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C36 H55 O9	631.3846	631.3847	-0.1	0.2	9.5

--- End Of Report ---

Figure S12. HR-ESI-MS data of compound 6.



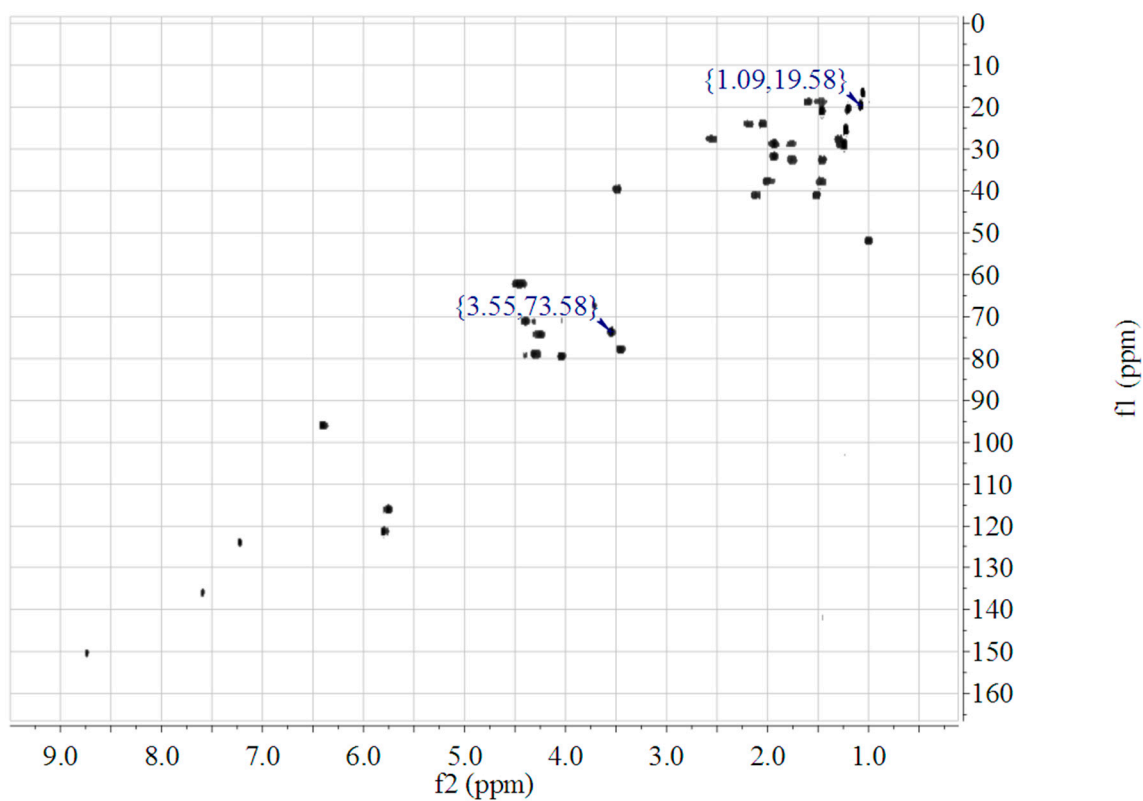


Figure S13. HSQC data of compound 6.

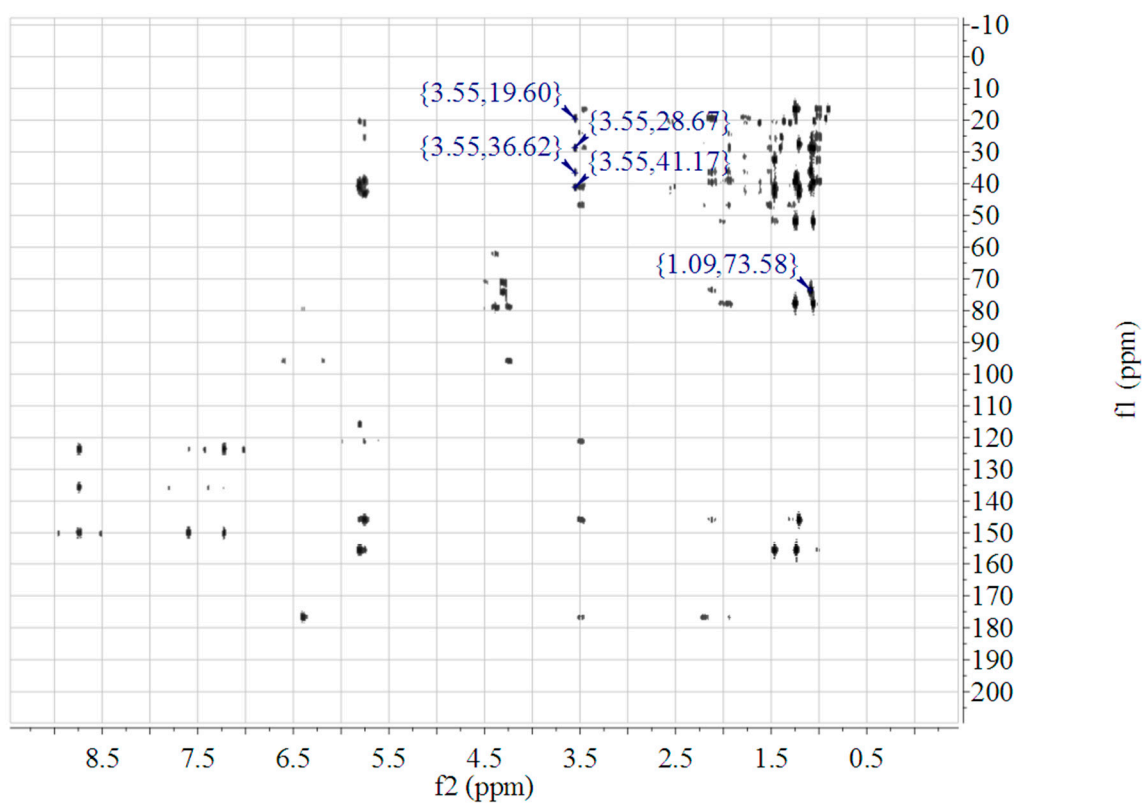


Figure S14. HMBC data of compound 6.

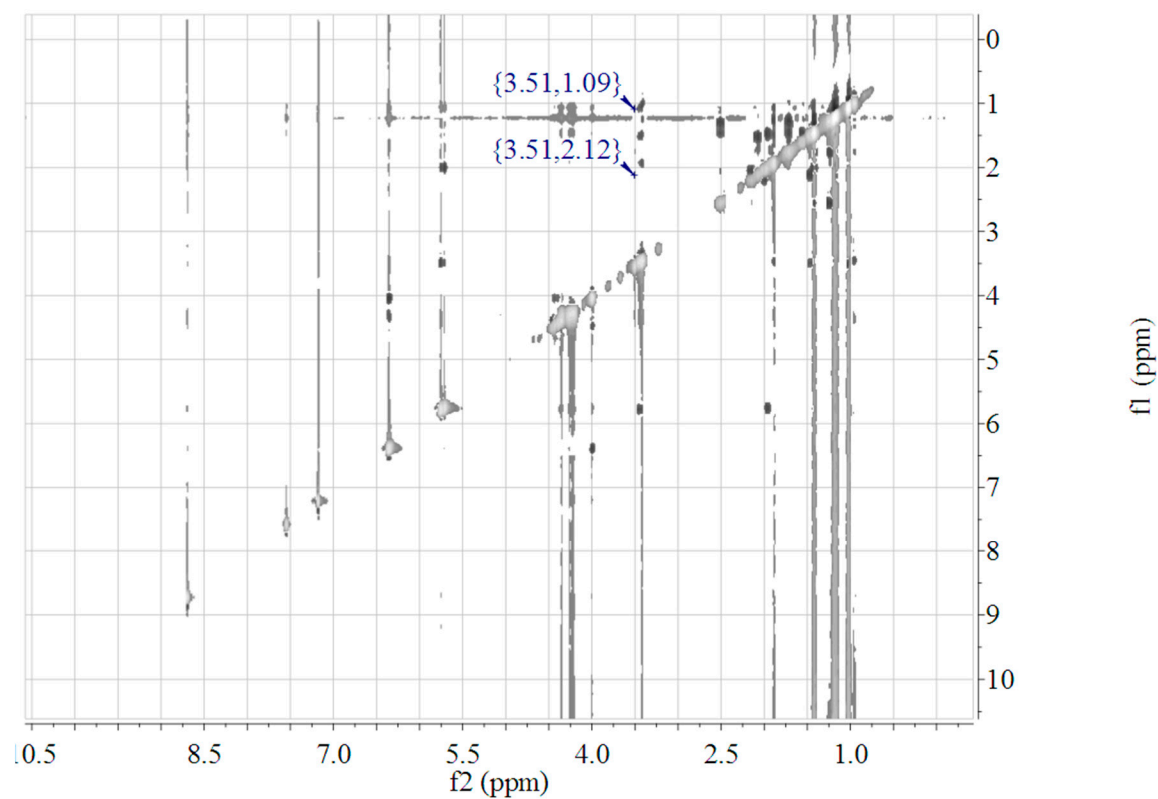


Figure S15. NOESY data of compound 6.

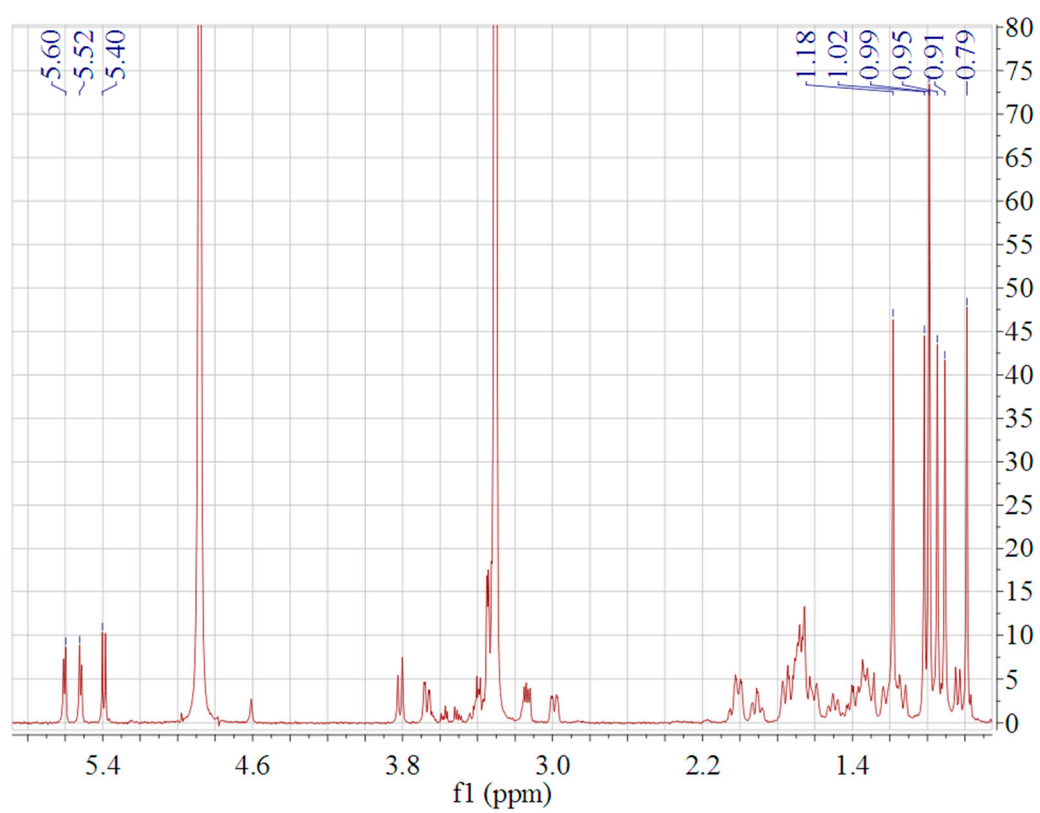


Figure S16. <sup>1</sup>H NMR data of compound 7 (500 MHz CD<sub>3</sub>OD).

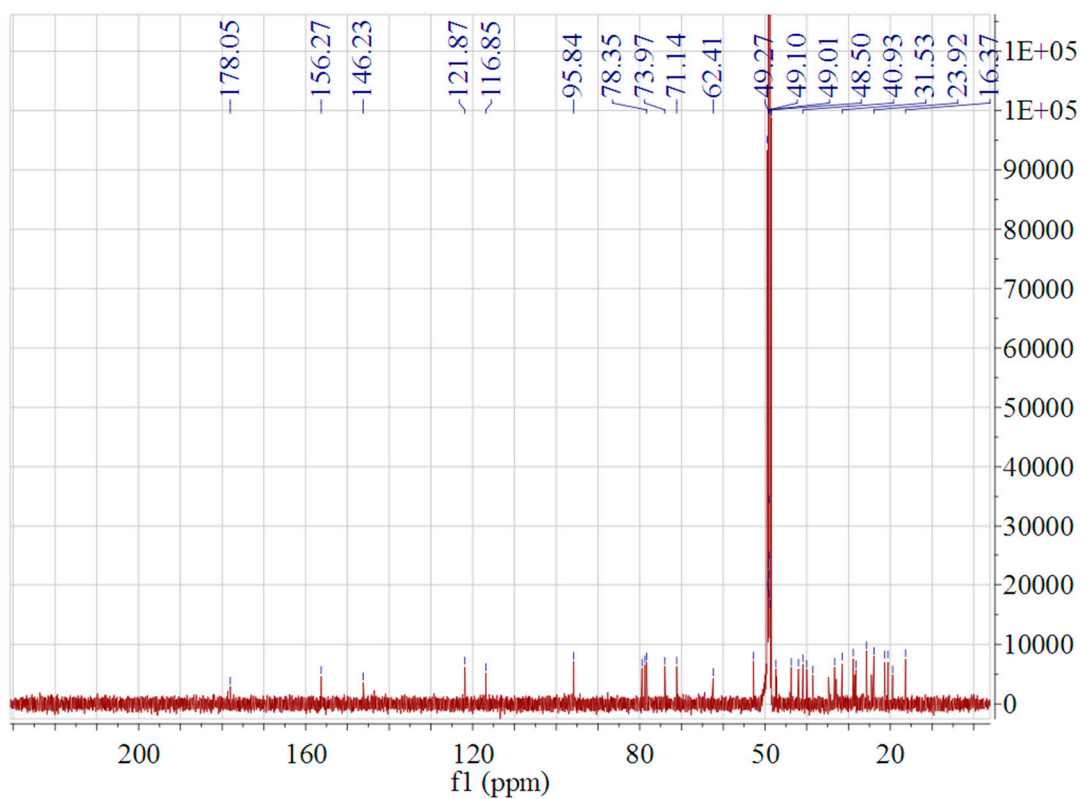


Figure S17.  $^{13}\text{C}$  NMR data of compound 7 (125 MHz  $\text{CD}_3\text{OD}$ ).

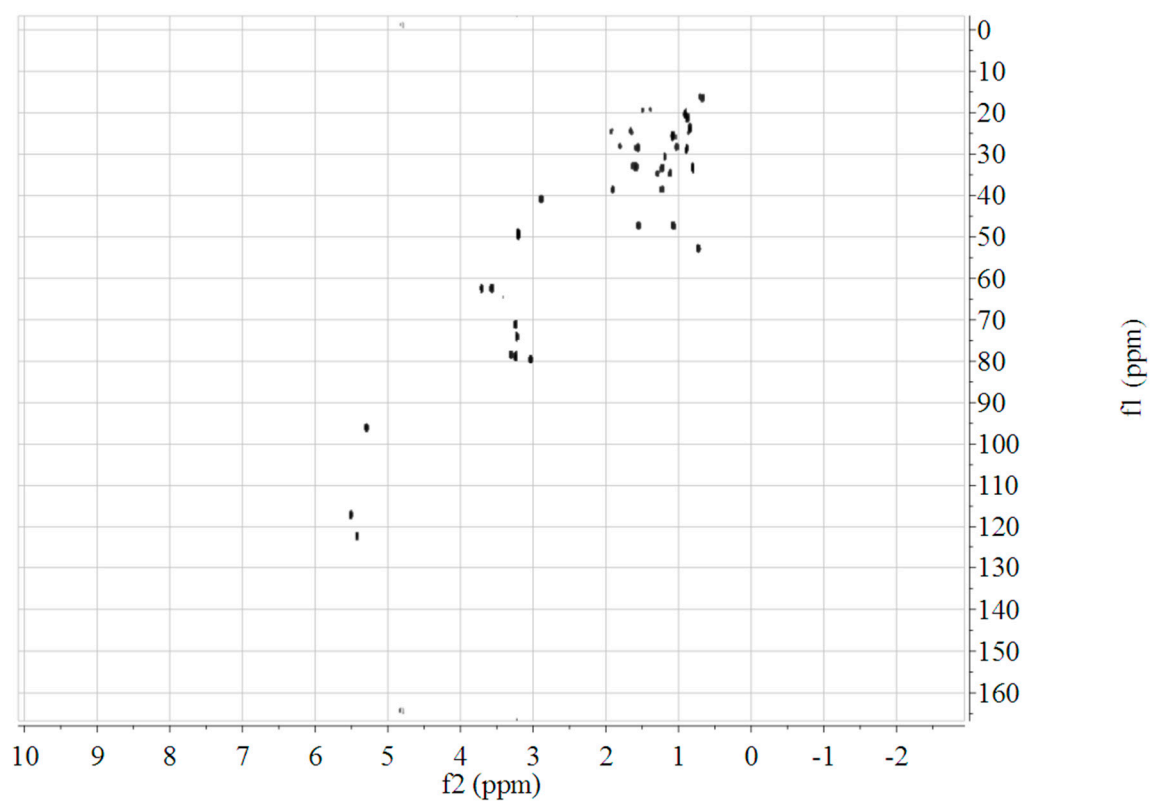


Figure S18. HSQC data of compound 7.

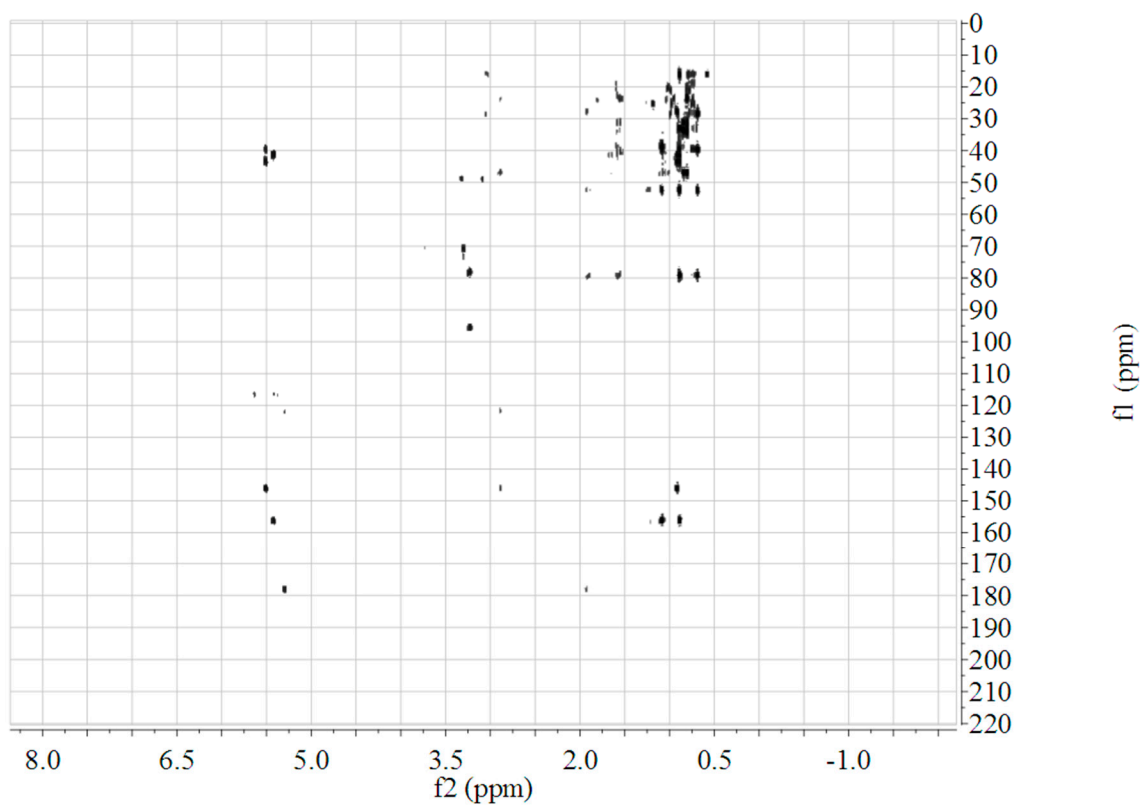


Figure S19. HMBC data of compound 7.

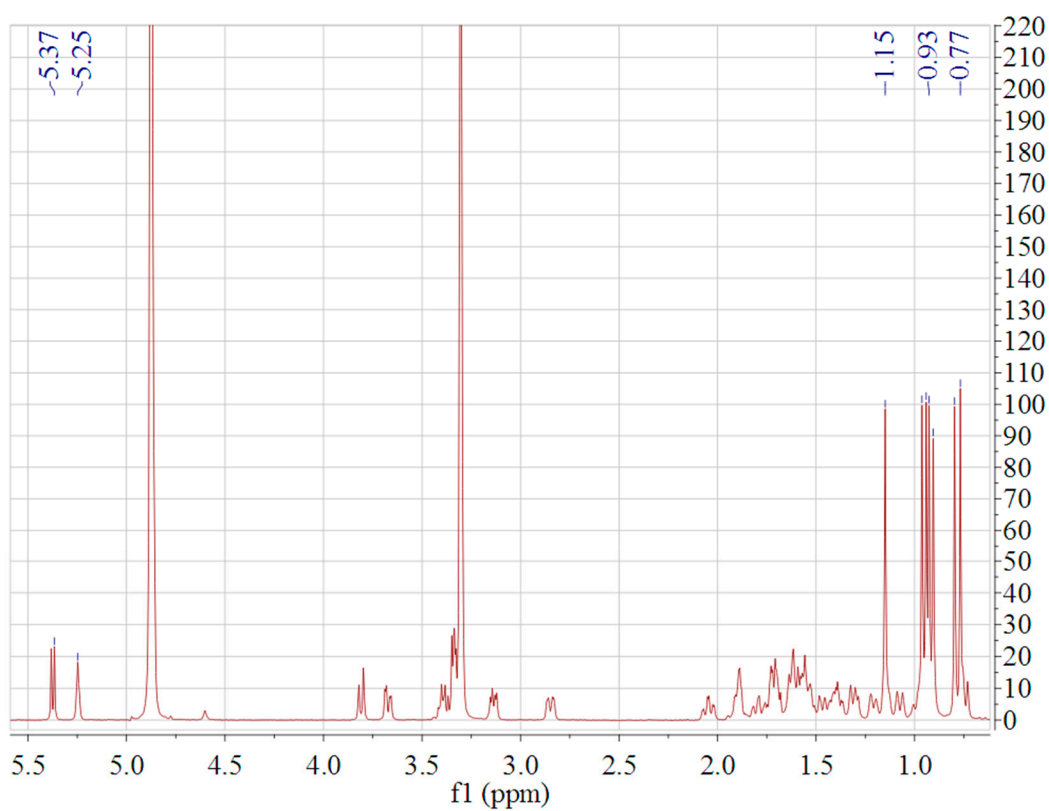


Figure S20. <sup>1</sup>H NMR data of compound 8 (500 MHz CD<sub>3</sub>OD).

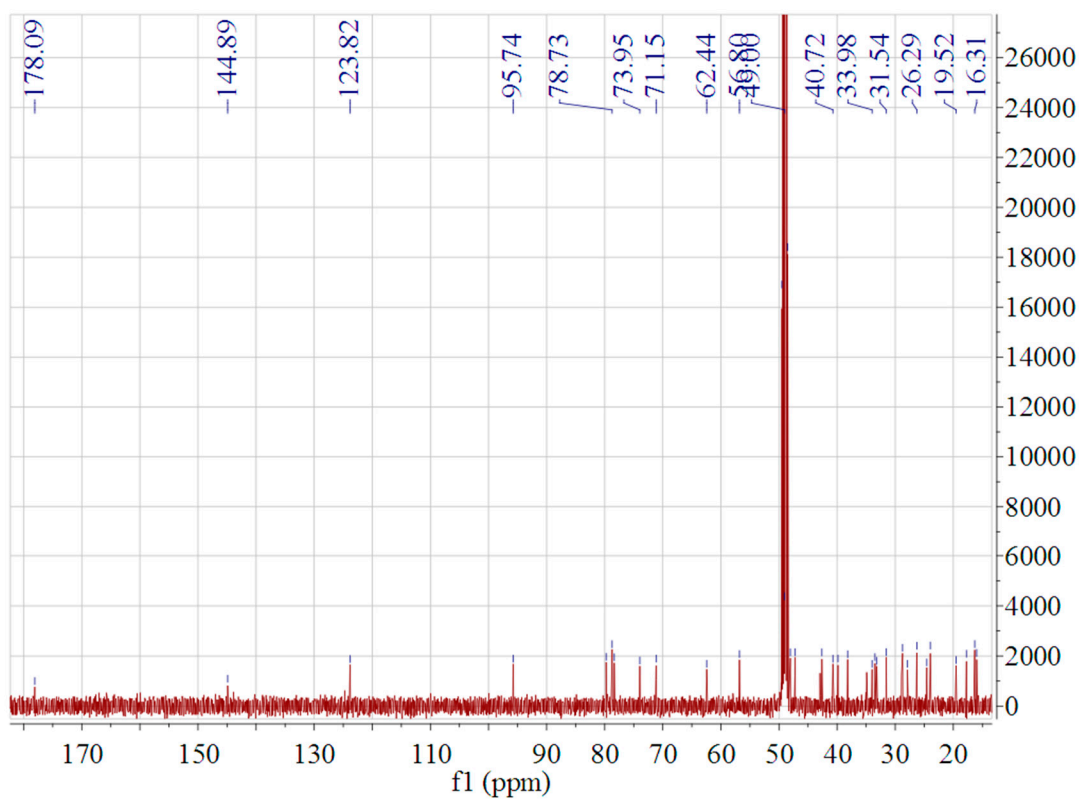


Figure S21.  $^{13}\text{C}$  NMR data of compound 8 (125 MHz  $\text{CD}_3\text{OD}$ ).

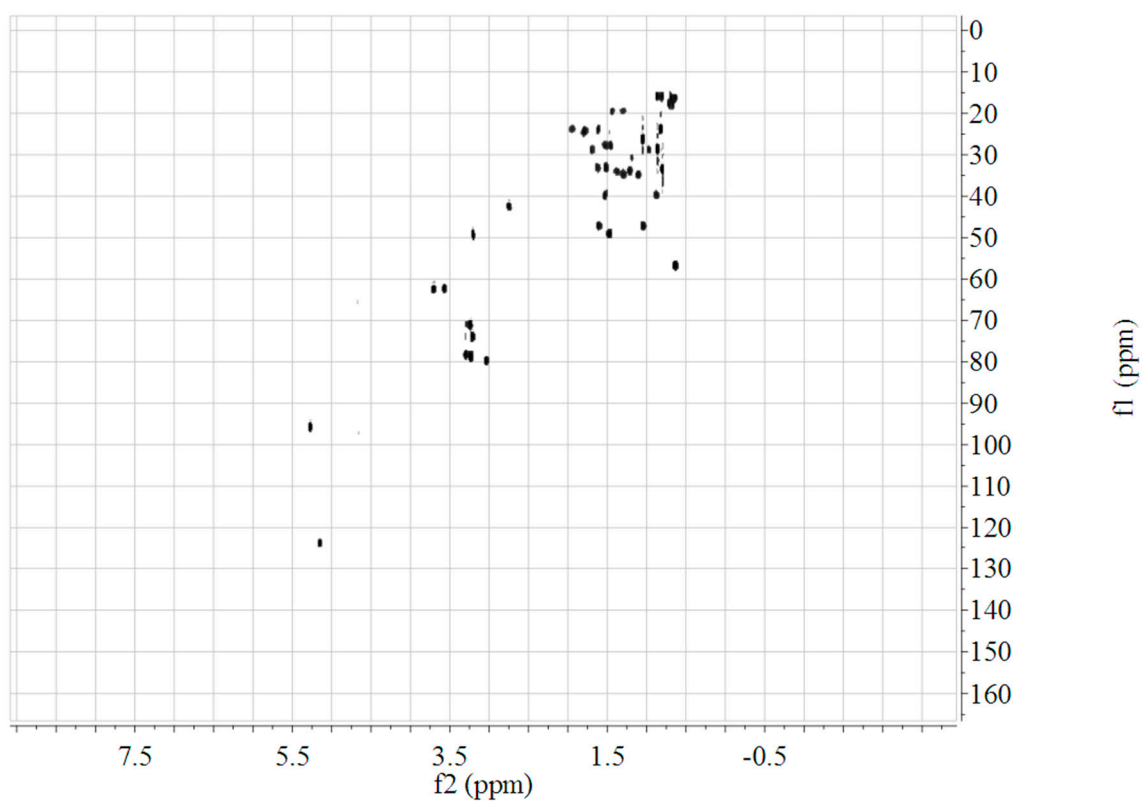


Figure S22. HSQC data of compound 7.

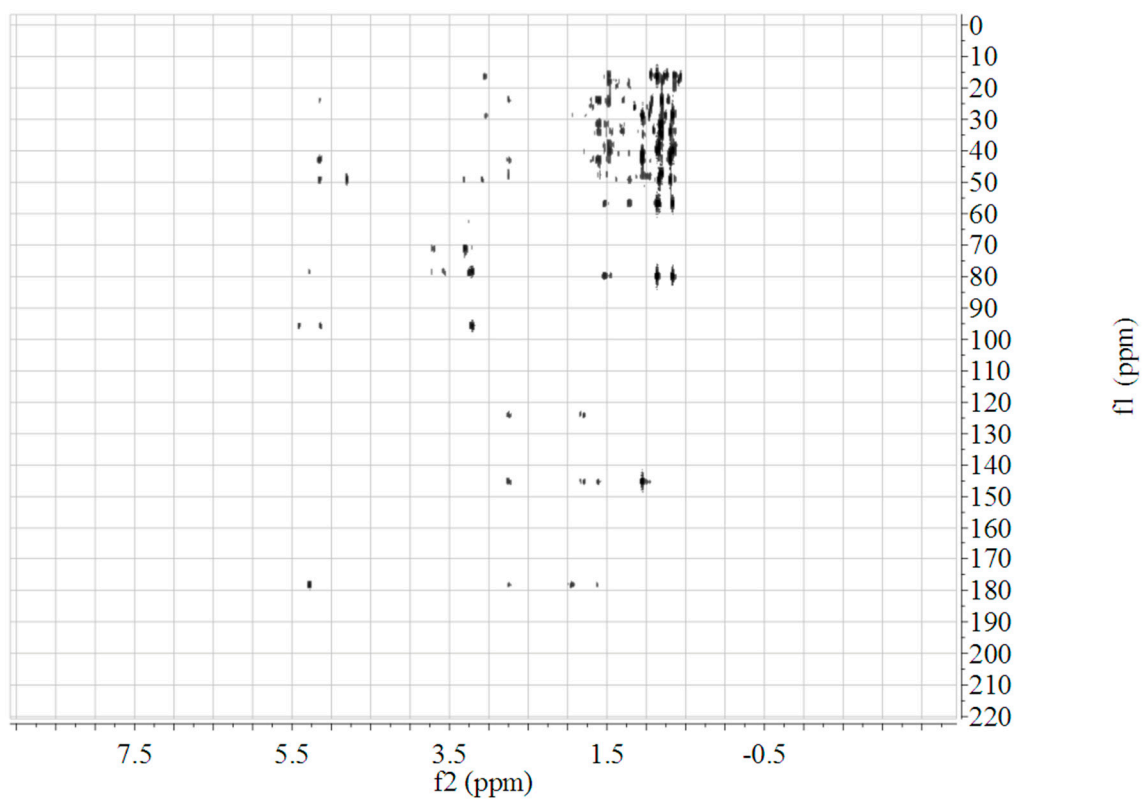


Figure S23. HMBC data of compound 8.