

# Supplementary Materials

## *Anti-Mycobacterium tuberculosis* Terpenoids from *Resina Commiphora*

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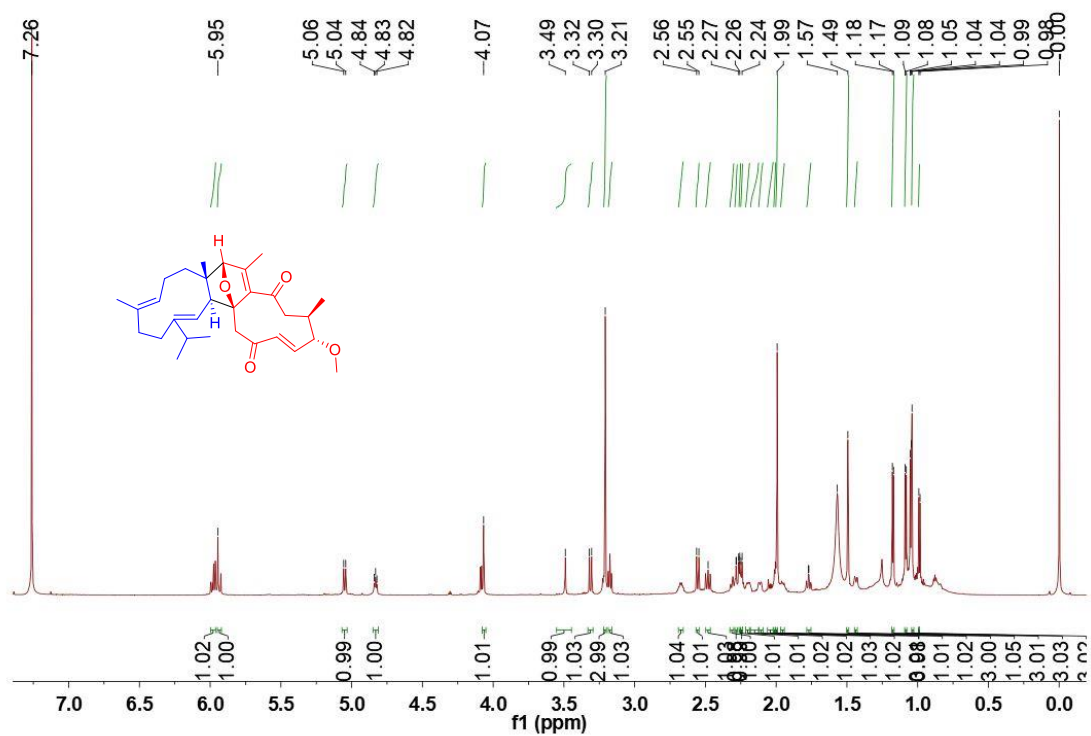


Figure S1.  $^1\text{H}$  NMR spectrum of **1** in  $\text{CDCl}_3$ .

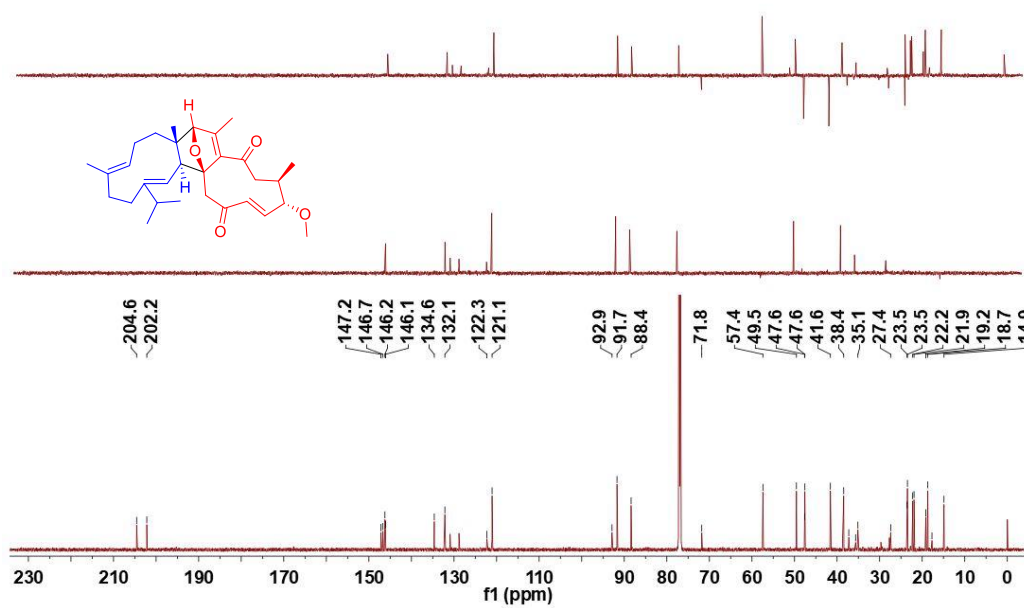
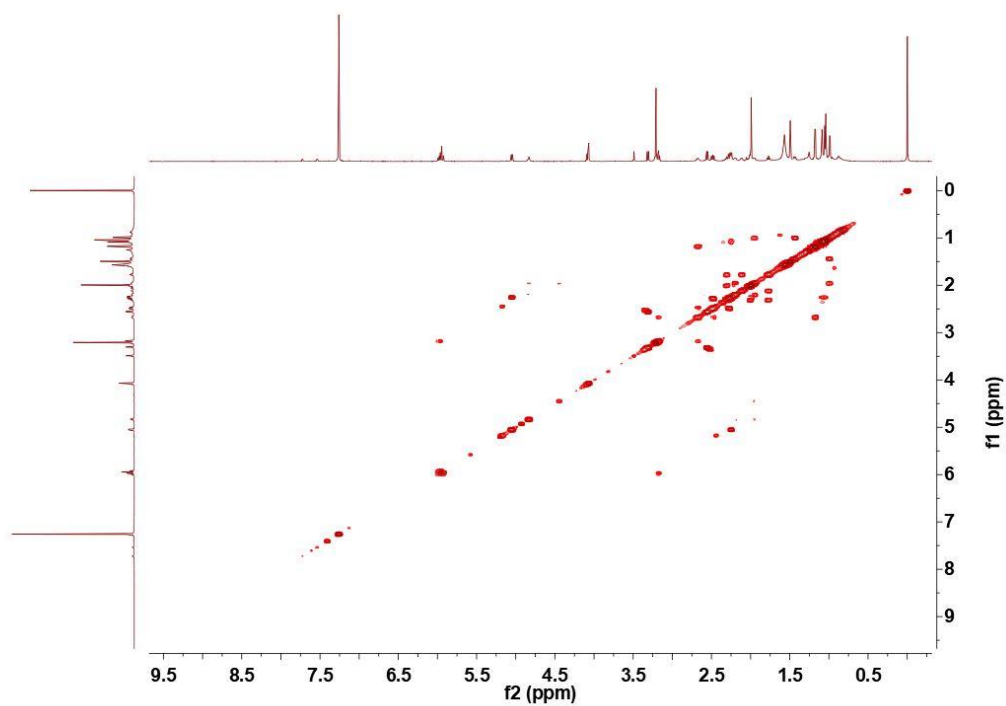
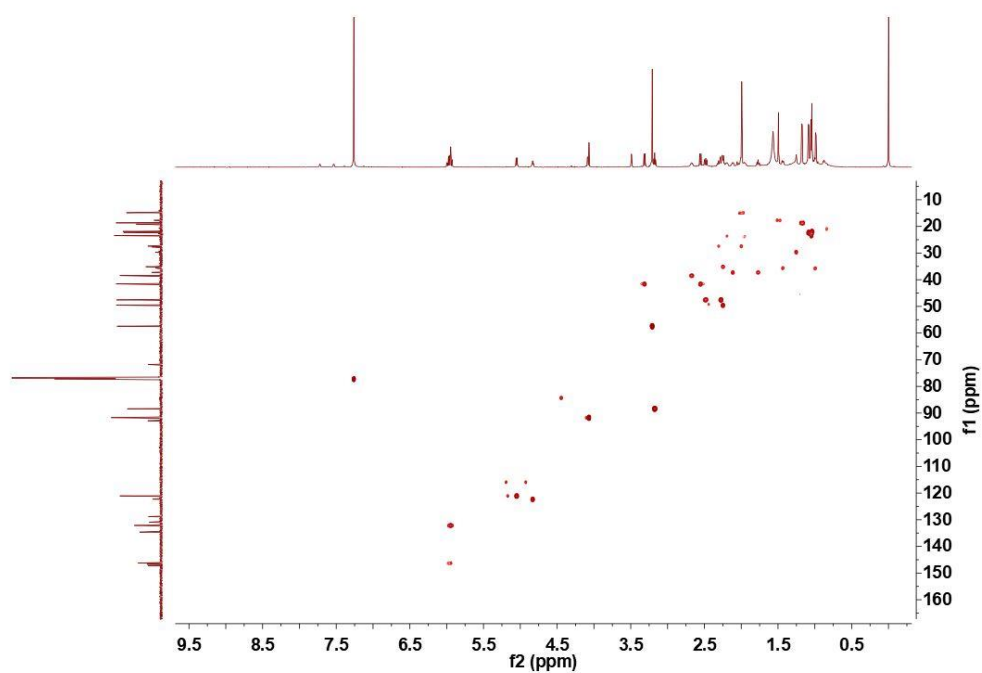


Figure S2.  $^{13}\text{C}$  NMR and DEPT spectra of **1** in  $\text{CDCl}_3$ .



**Figure S3.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{CDCl}_3$ .



**Figure S4.** HSQC Spectrum of **1** in  $\text{CDCl}_3$ .

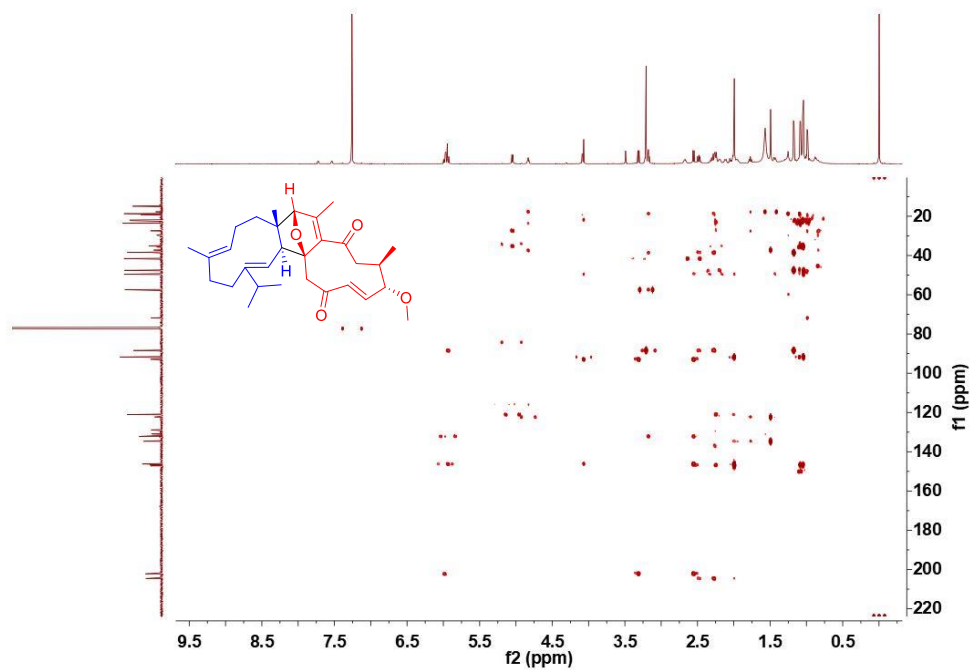


Figure S5. HMBC spectrum of **1** in CDCl<sub>3</sub>.

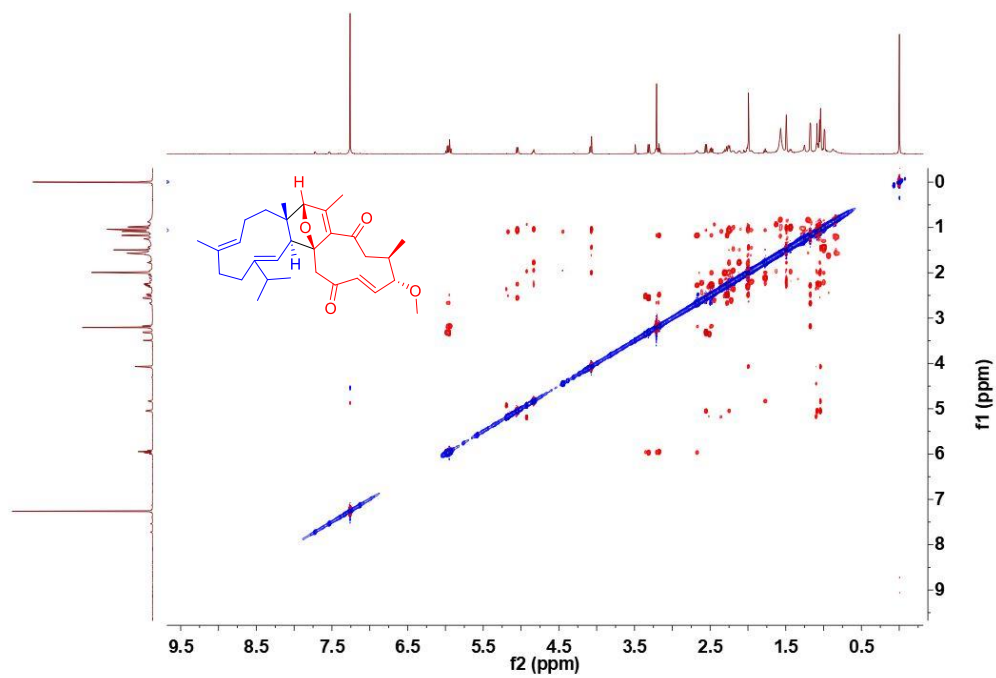
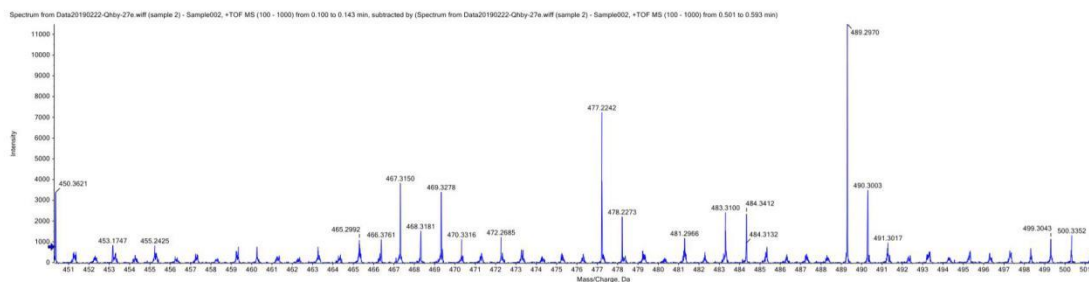


Figure S6. ROESY spectrum of **1** in CDCl<sub>3</sub>.



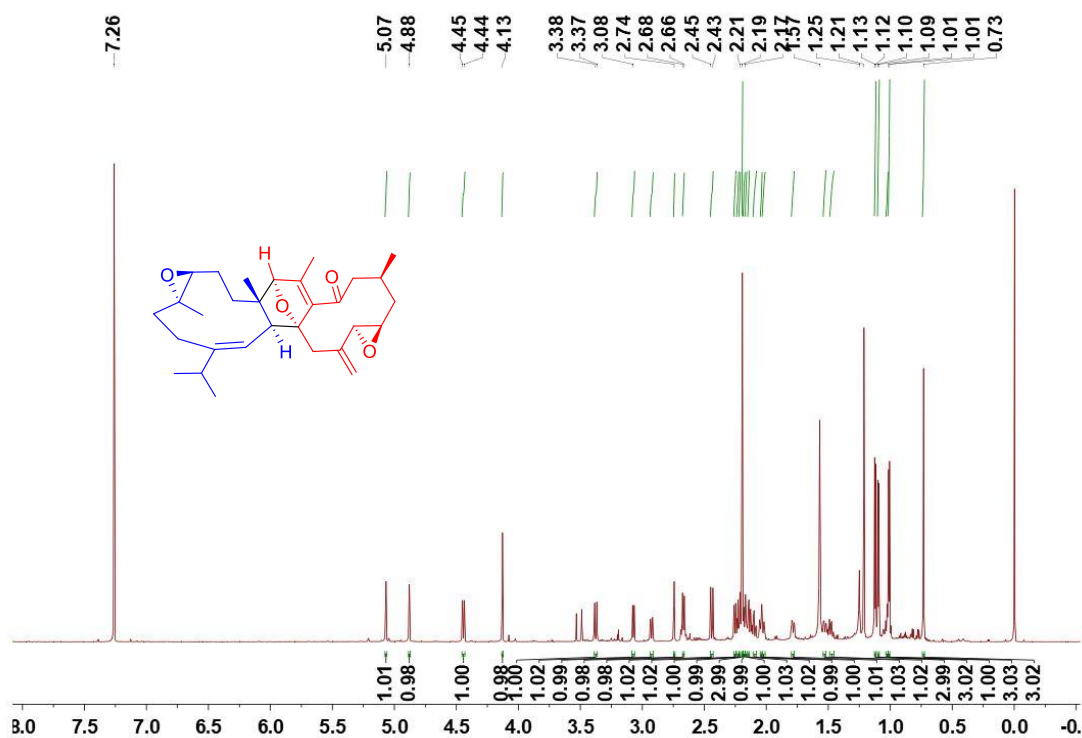
[M+H]<sup>+</sup> m/z 467.3150

Hit	Formula	m/z	RDB	ppm
1	C <sub>30</sub> H <sub>43</sub> O <sub>4</sub>	467.3156	10.0	-1.3

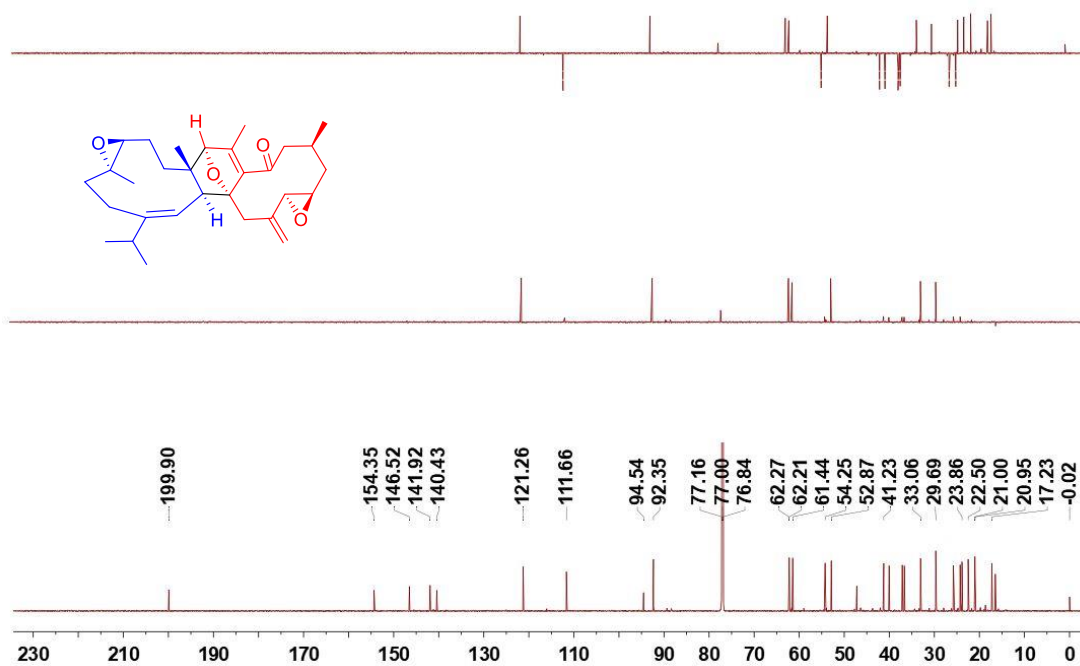
Elements from ~ to C<sub>60</sub>H<sub>120</sub>O<sub>6</sub>

Mass tolerance 5 ppm

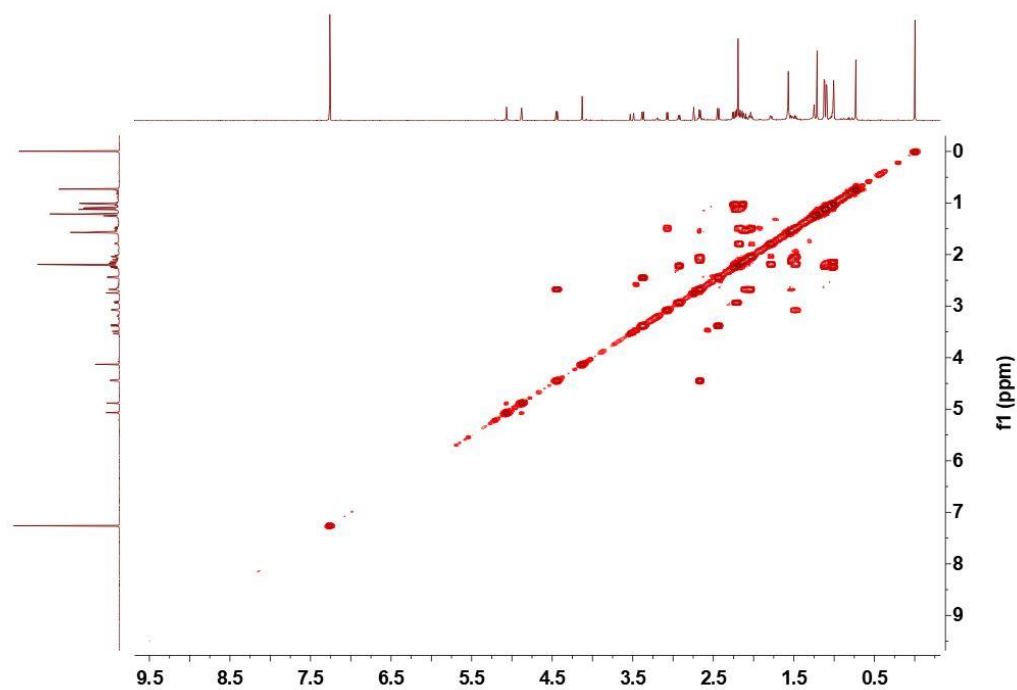
**Figure S7.** HRESIMS of **1**.



**Figure S8.** <sup>1</sup>H NMR spectrum of **2** in CDCl<sub>3</sub>.



**Figure S9.**  $^{13}\text{C}$  NMR and DEPT spectra of **2** in  $\text{CDCl}_3$ .



**Figure S10.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{CDCl}_3$ .

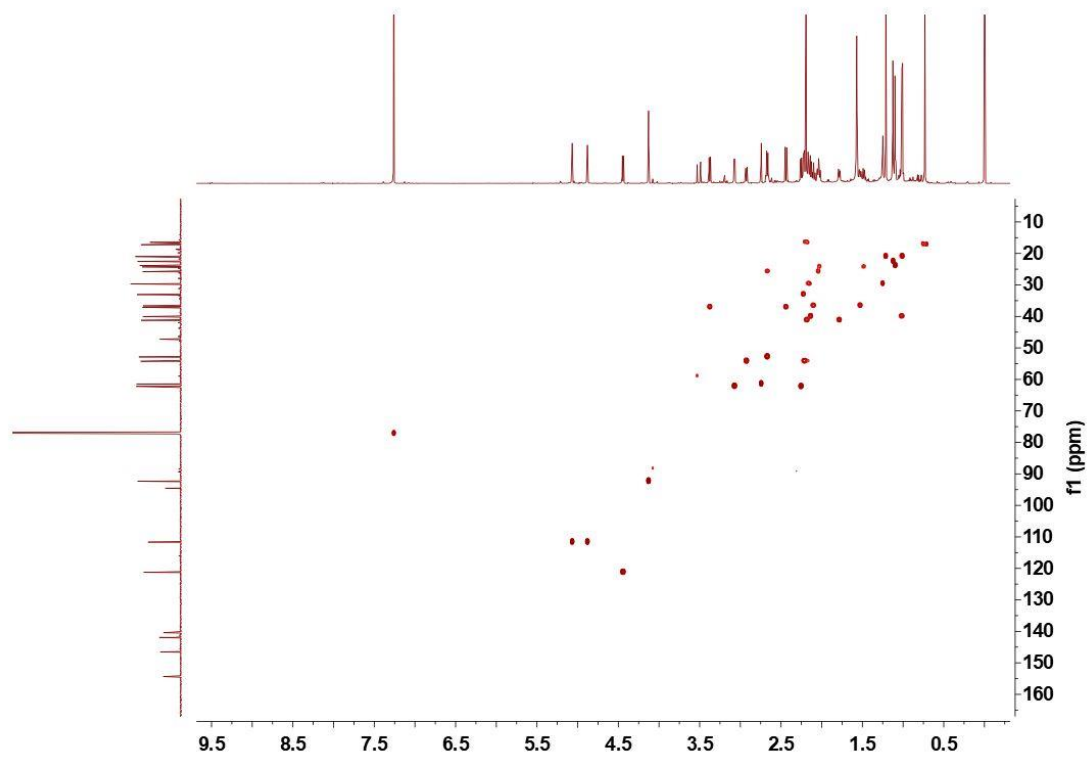


Figure S11. HSQC Spectrum of **2** in  $\text{CDCl}_3$ .

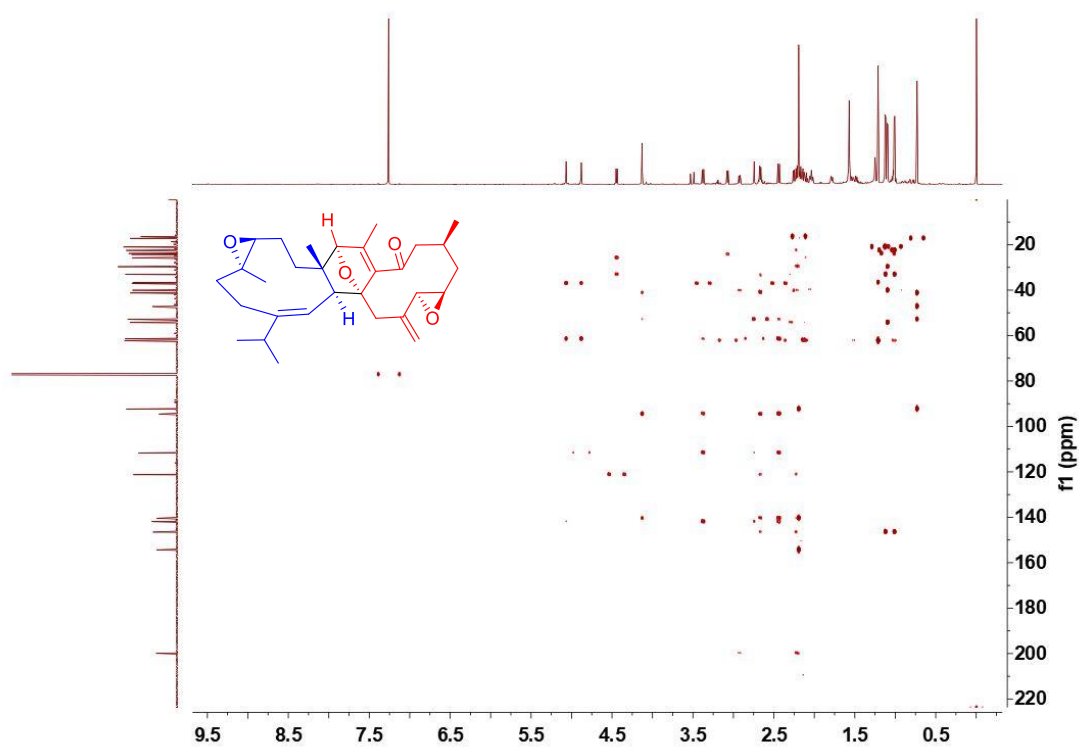


Figure S12. HMBC spectrum of **2** in  $\text{CDCl}_3$ .



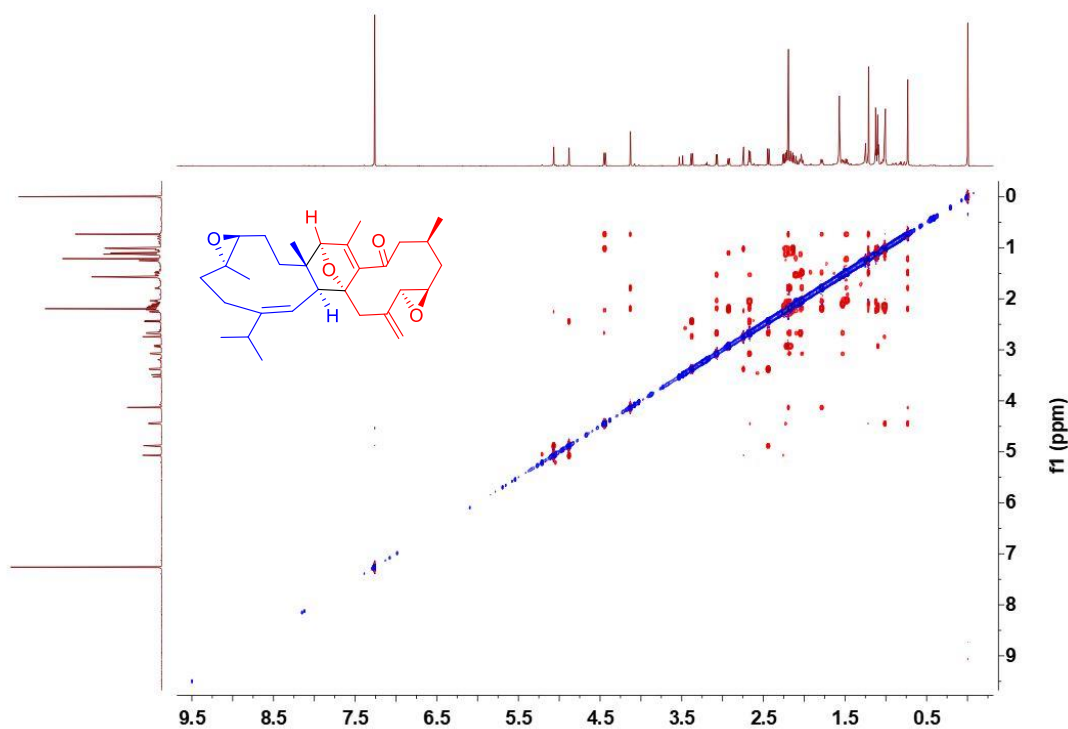
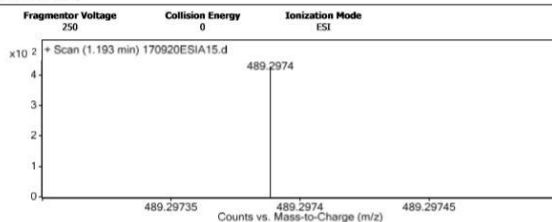


Figure S13. ROESY spectrum of 2 in CDCl<sub>3</sub>.

#### Qualitative Analysis Report

Data Filename	170920ESIA15.d	Sample Name	qjw-58d
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESL.m	Acquired Time	9/19/2017 6:28:58 PM
IRM Calibration Status	Success	DA Method	ESL.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

#### User Spectra



m/z	z	Abund
121.0509	1	9492.1
256.2626	1	8474.39
274.2738	1	15405.78
318.2998	1	14130.2
362.3261	1	4403.11
384.3077	1	3165.42
437.1929	1	4847.29
521.3206	1	2700.71
922.0098	1	44952.27
923.01	1	5919.36

Element	Min	Max
C	0	200
H	0	400
O	4	10
Na	1	1

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff.(ppm)	DBE
C30 H42 Na O4	489.2981	489.2974	0.7	1.4	9.5

— End Of Report —

Figure S14. HRESIMS of 2.

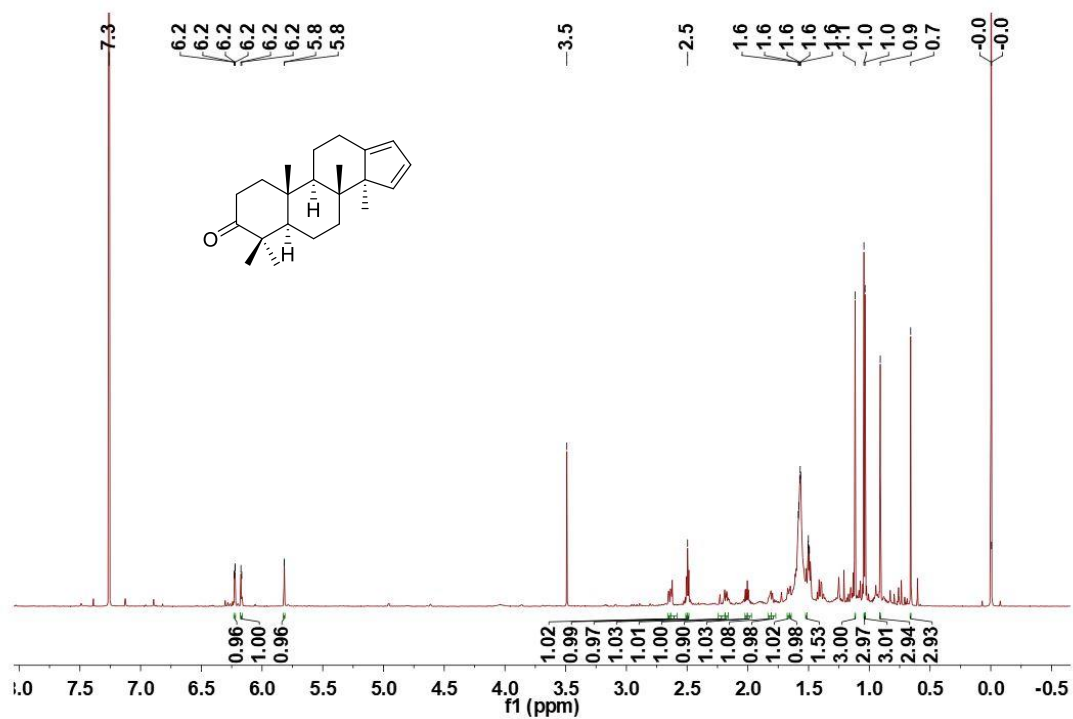


Figure Figure S15.  $^1\text{H}$  NMR spectrum of 3 in  $\text{CDCl}_3$ .

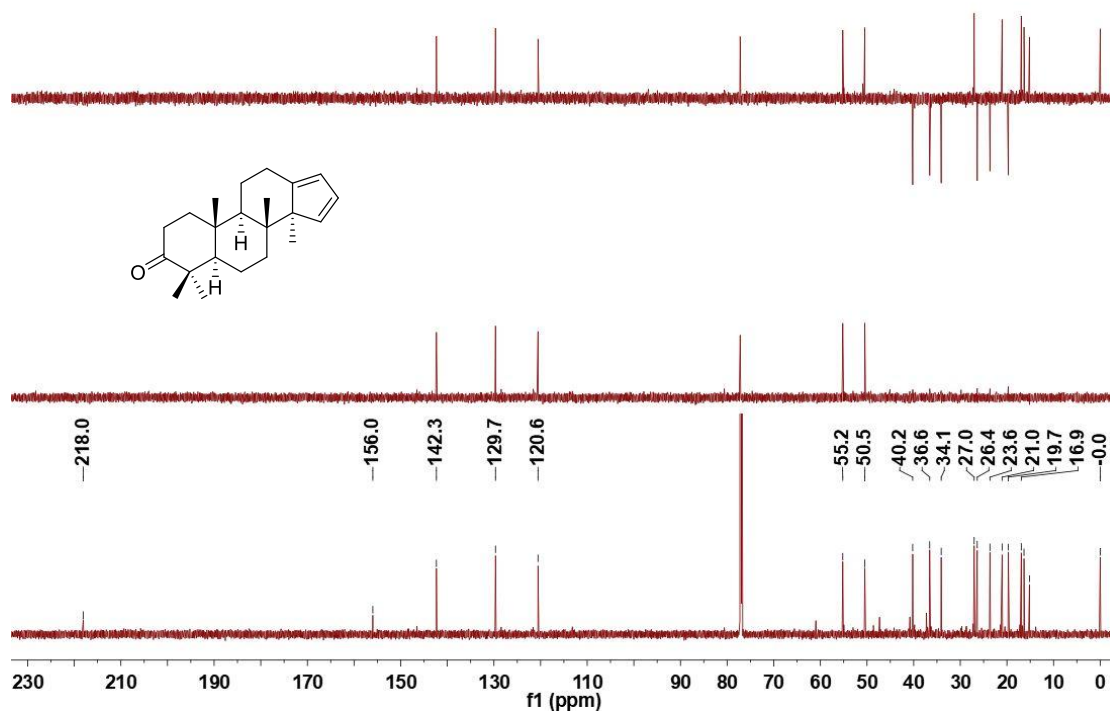


Figure S16.  $^{13}\text{C}$  NMR and DEPT spectra of 3 in  $\text{CDCl}_3$ .

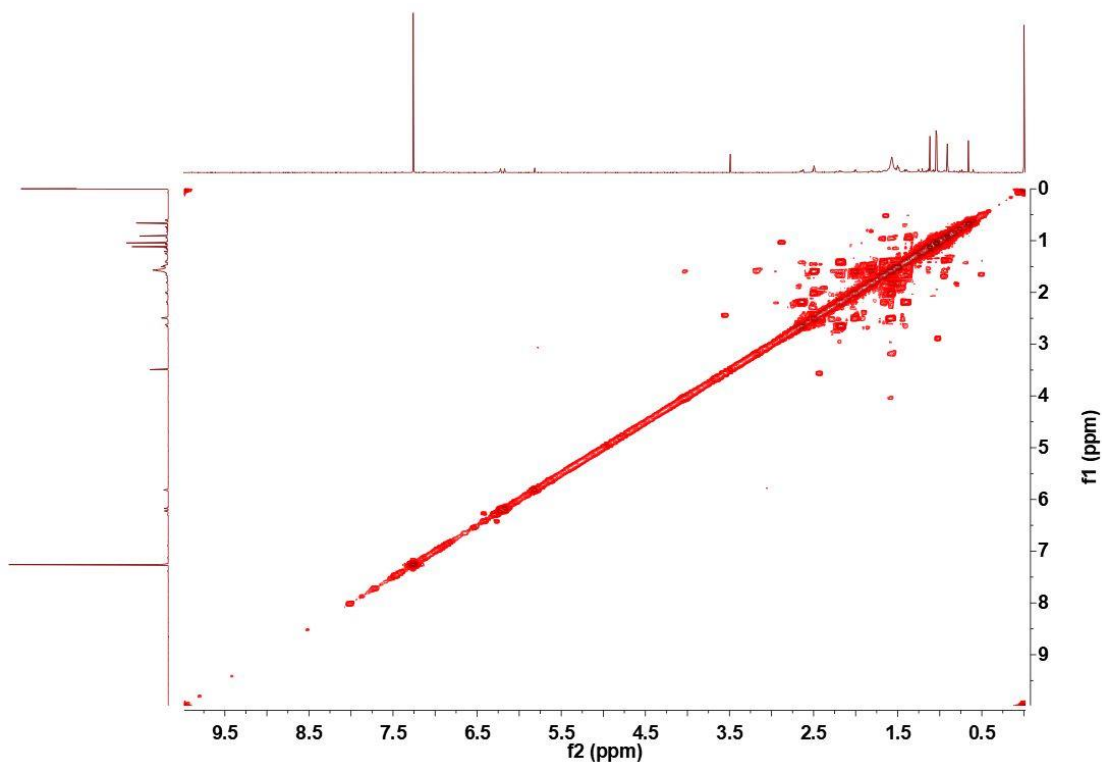


Figure S17.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{CDCl}_3$ .

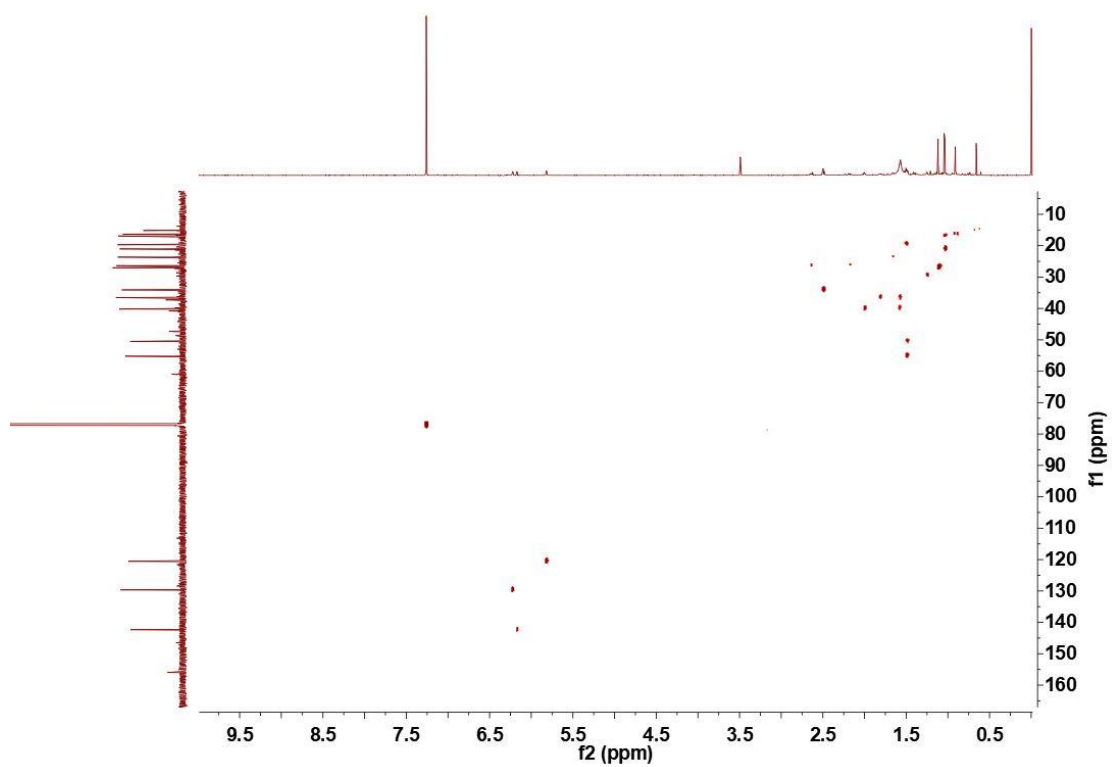
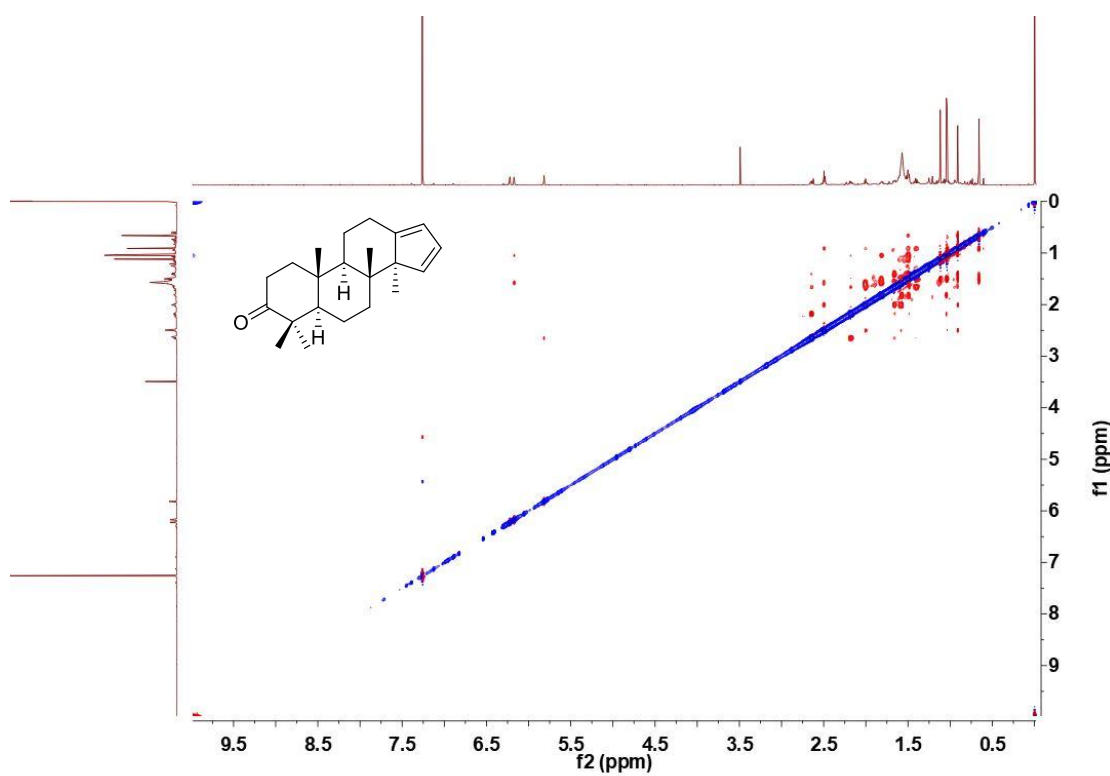
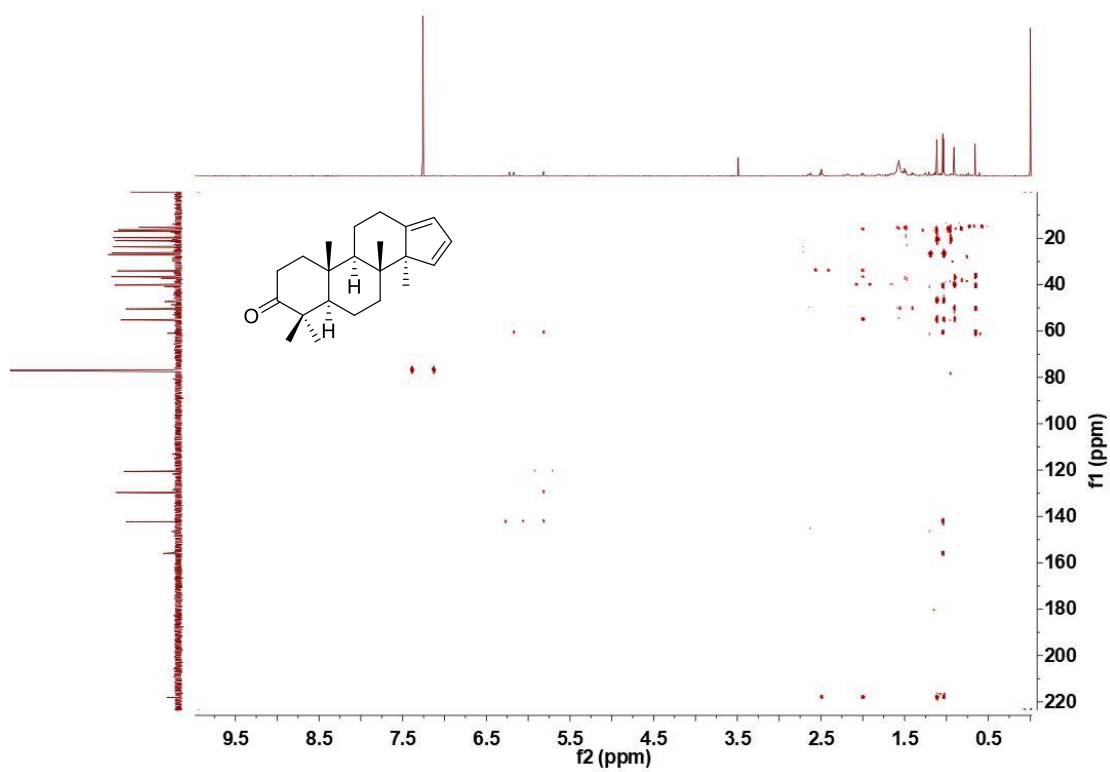


Figure S18. HSQC Spectrum of **3** in  $\text{CDCl}_3$ .



## Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

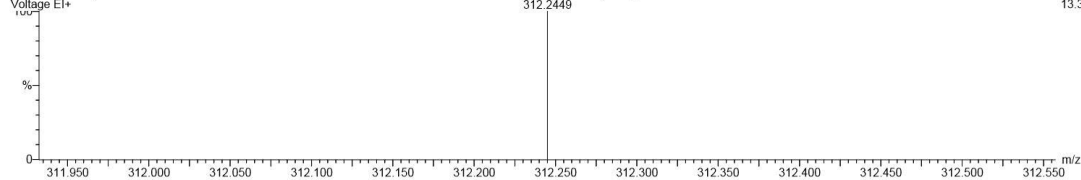
17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-2

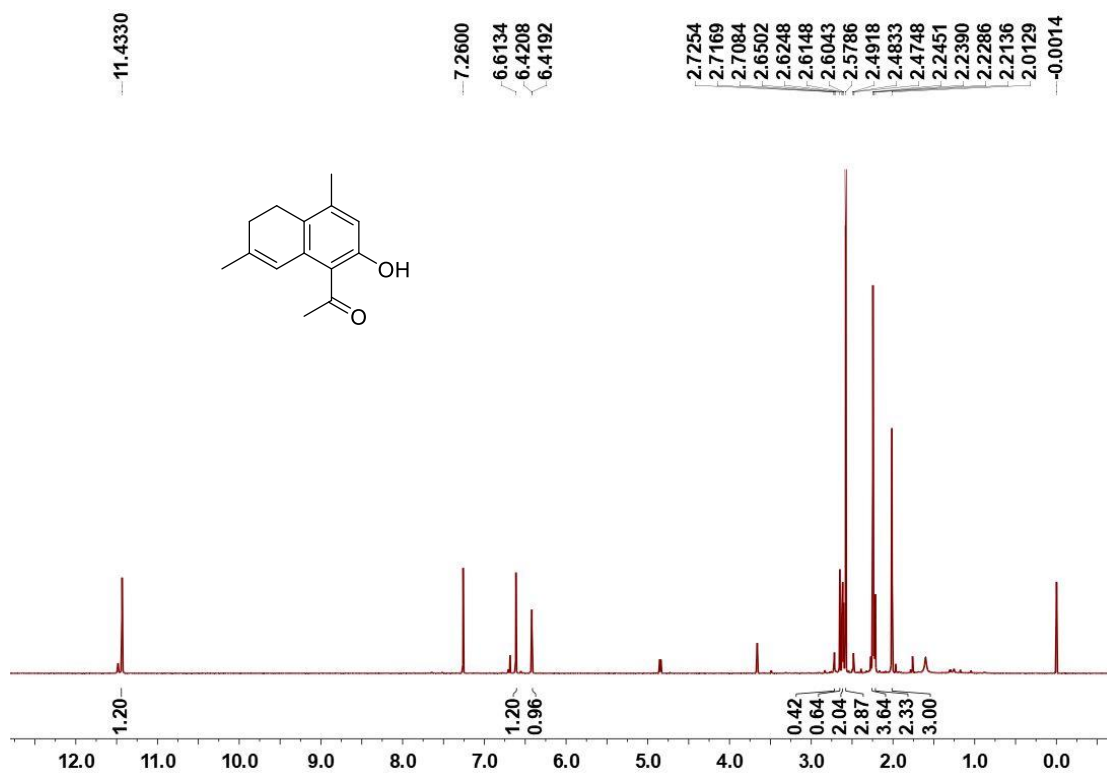
09/08/23 20-Sep-2017

Voltage EI+



Minimum:	200.0	10.0	-10.0			
Maximum:			120.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
312.2449	312.2453	-0.4	-1.3	7.0	5546026.5	C22 H32 O

Figure S21. HRESIMS of 3

Figure Figure S22. <sup>1</sup>H NMR spectrum of 4 in CDCl<sub>3</sub>.

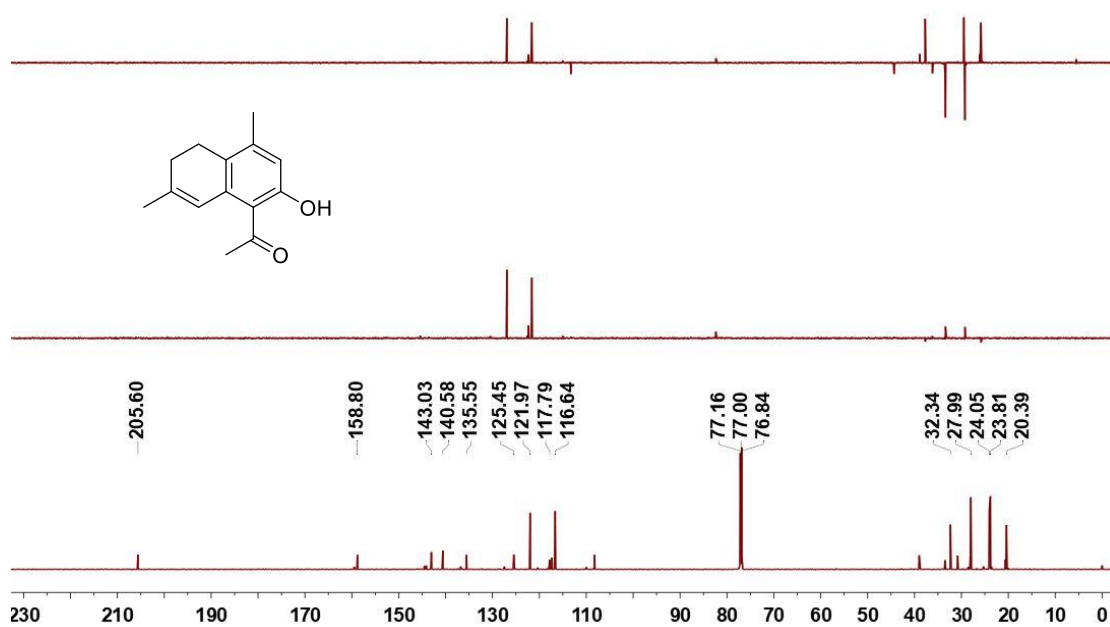


Figure S23.  $^{13}\text{C}$  NMR and DEPT spectra of 4 in  $\text{CDCl}_3$ .

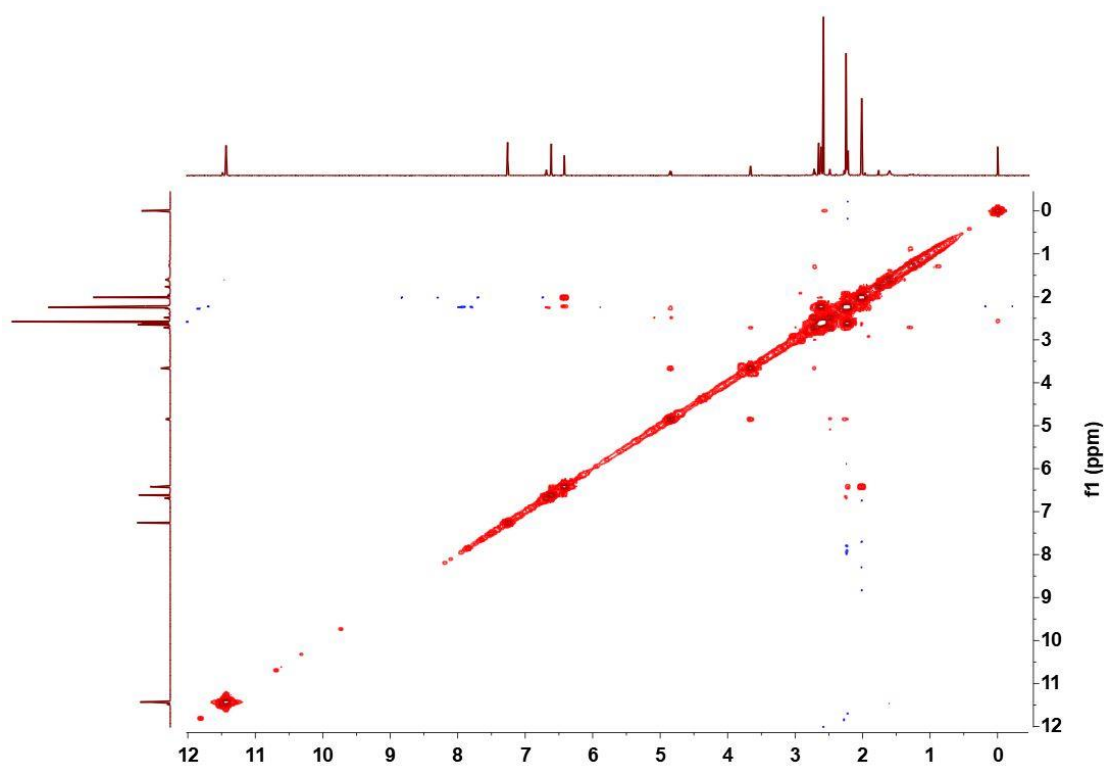
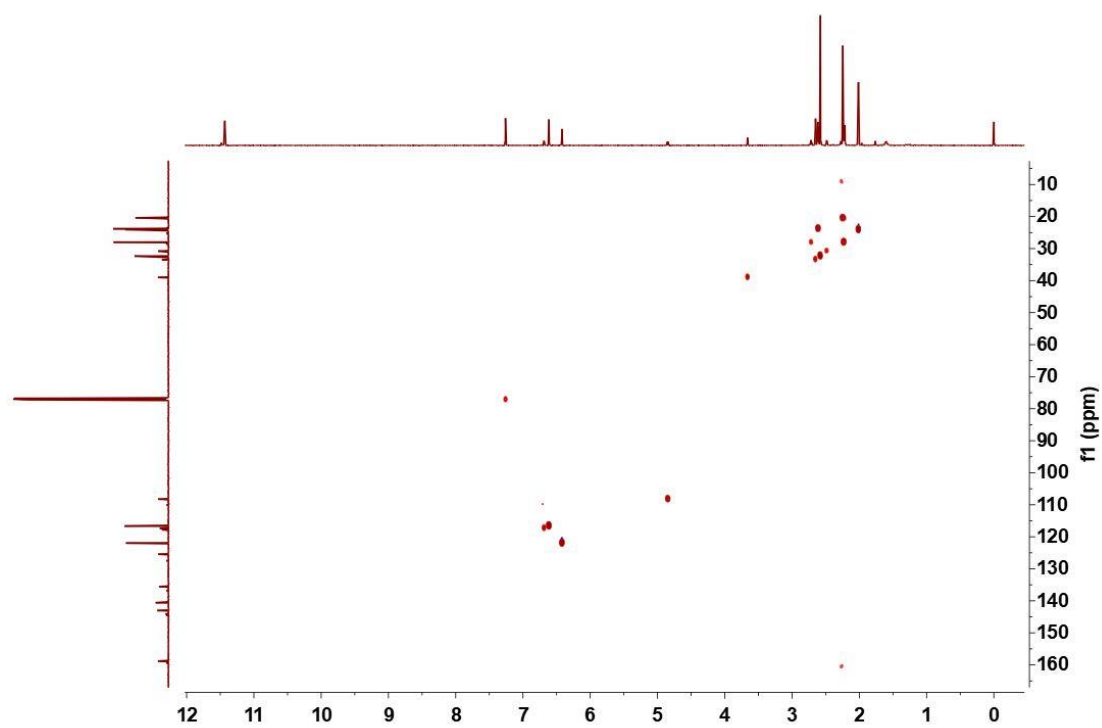
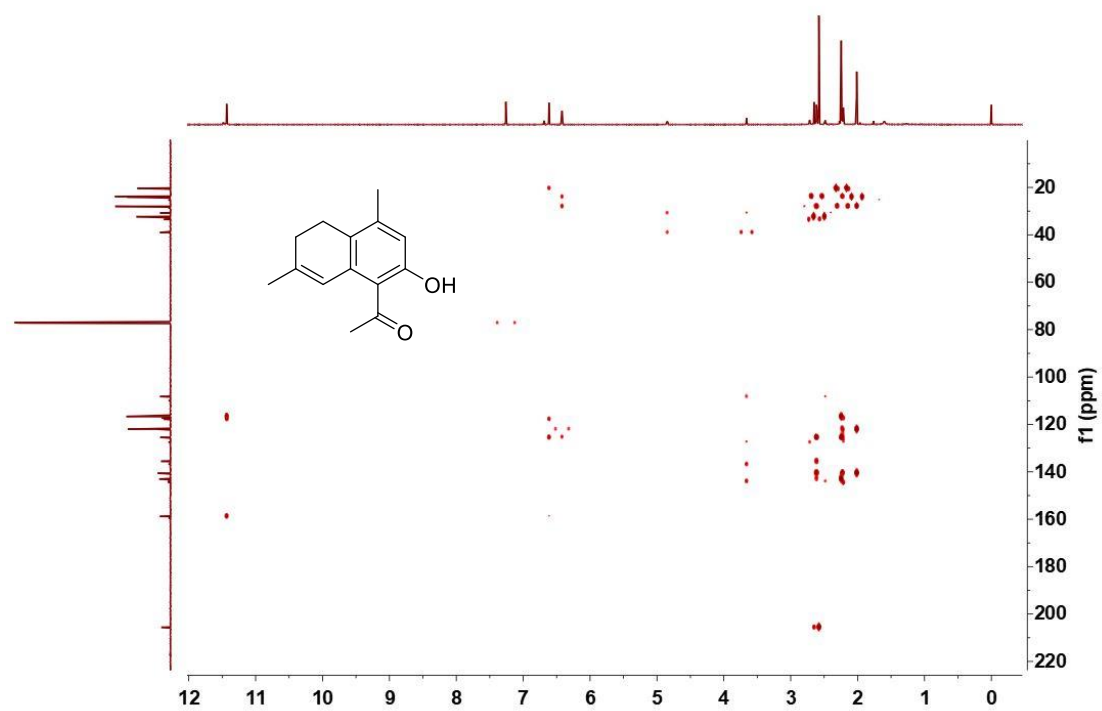


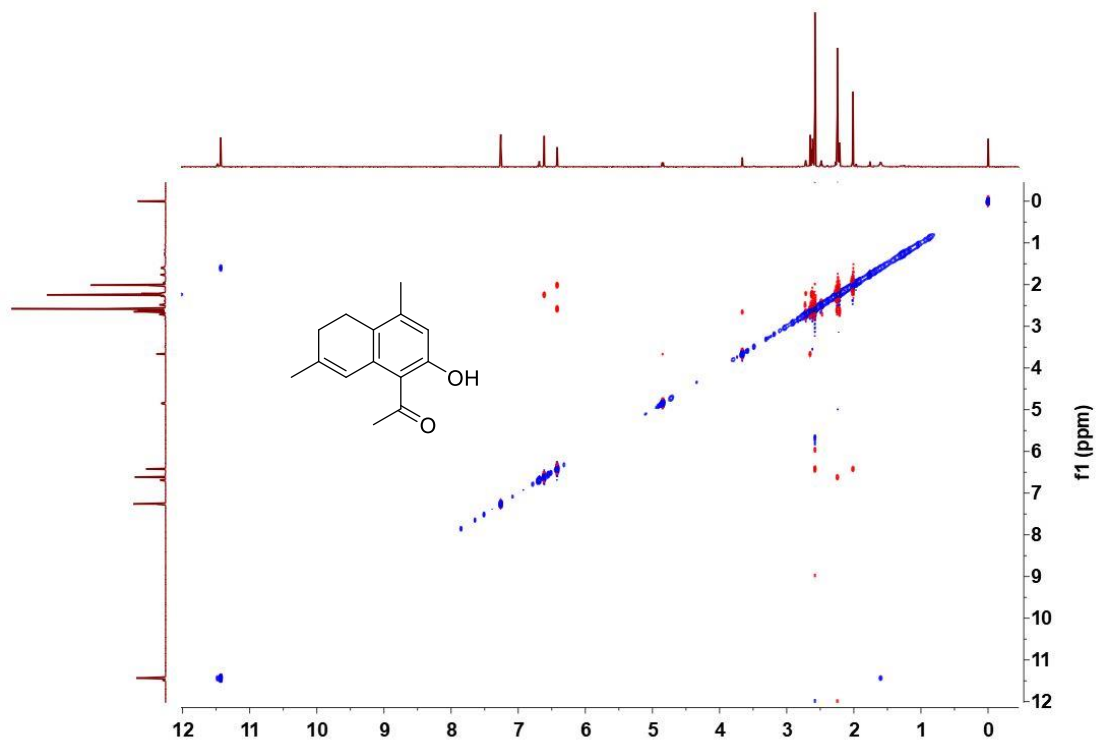
Figure S24.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 4 in  $\text{CDCl}_3$ .



**Figure S25.** HSQC Spectrum of **4** in  $\text{CDCl}_3$ .



**Figure S26.** HMBC spectrum of **4** in  $\text{CDCl}_3$ .



**Figure S27.** ROESY spectrum of **4** in CDCl<sub>3</sub>.

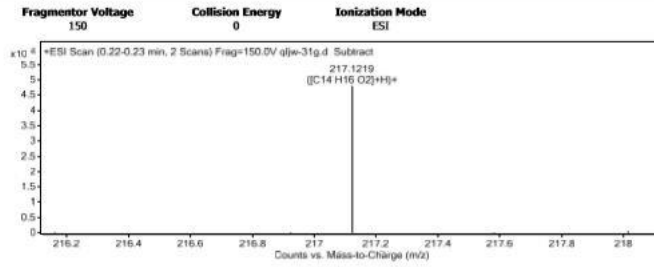


## Qualitative Analysis Report

Data Filename	qjw-31g.d	Sample Name	qjw-31g
Sample Type	Sample	Position	P1-A5
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Acq Method	SIBU.m	Acquired Time	5/15/2017 4:37:48 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (85125.2)	

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
128.0384	2	21256.65		
148.5519	2	7633.8		
217.1219	1	47814.5	C14 H16 O2	(M+H)+
227.1063		7368.16		
239.1041	1	40431.36		
255.0699	1	7581.44		
255.0965		7992.23		
267.0987	1	10794.19		

### Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

### Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C14 H16 O2	216.1150	217.1223	217.1219	0.3	1.4	7.0000

-- End Of Report --

**Figure S28.** HRESIMS of 4.