

SUPPLEMENTARY MATERIAL

Bodinosides S – Y, Seven New Triterpenoid Saponins from *Elsholtzia bodinieri* and Their Anti-Influenza Activities

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Abstract

Investigation of the n-BuOH extract of the aerial parts of *Elsholtzia bodinieri* led to the isolation of seven new triterpenoid saponins, Bodinosides S - Y (**1** – **7**, resp.). Their structures were elucidated on the basis of spectroscopic techniques, including HSQC, HSBC, and HSQC-TOCSY experiments, together with acid hydrolysis and GC analysis. Anti-influenza activities of compounds **1** - **7** were evaluated against A/WSN/33/2009 (H1N1) virus in MDCK cells. As the results, compounds **2** and **5** exhibited potent anti-influenza activities against A/WSN/33/2009 (H1N1), with inhibition rate of 35.33% and 24.08%, respectively.

Keywords: *Elsholtzia bodinieri*; triterpenoid saponins; anti-influenza virus activities; Bodinosides S – Y;

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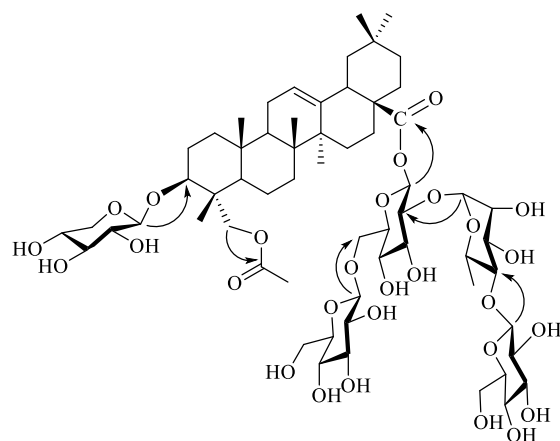


Figure S1 Key HMBC correlation of compound **1**

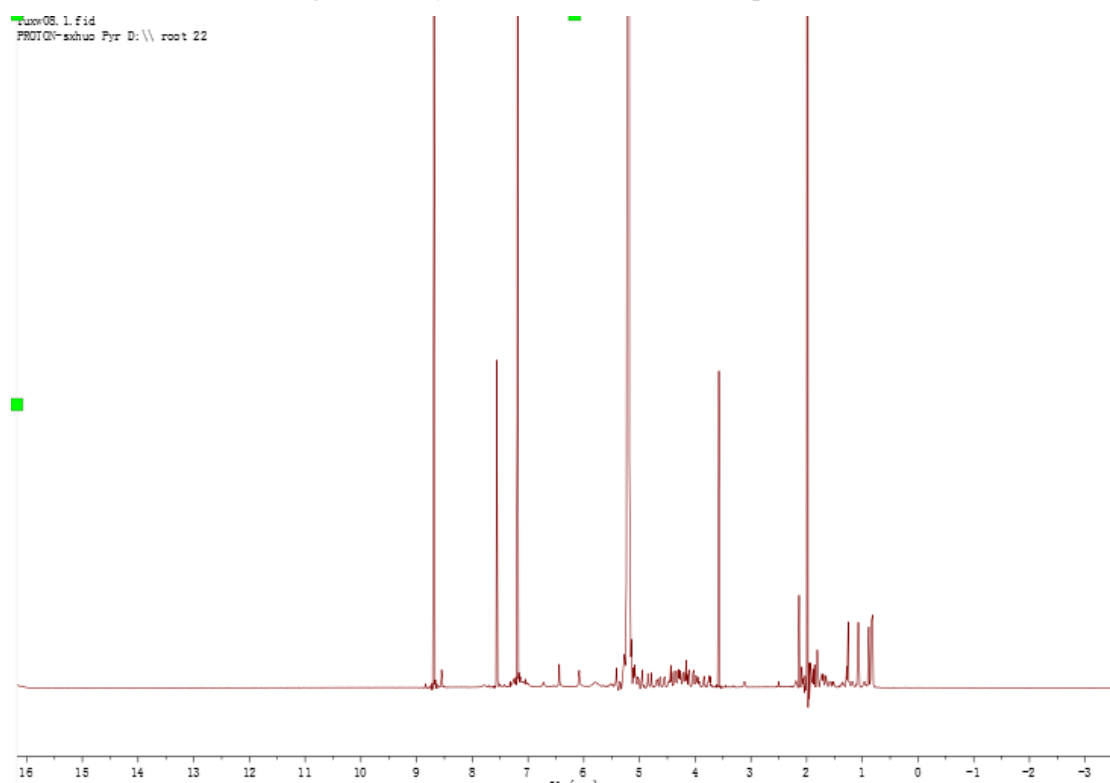


Figure S2 ¹H NMR spectrum of compound **1** (600 MHz, pyridine-*d*₅)

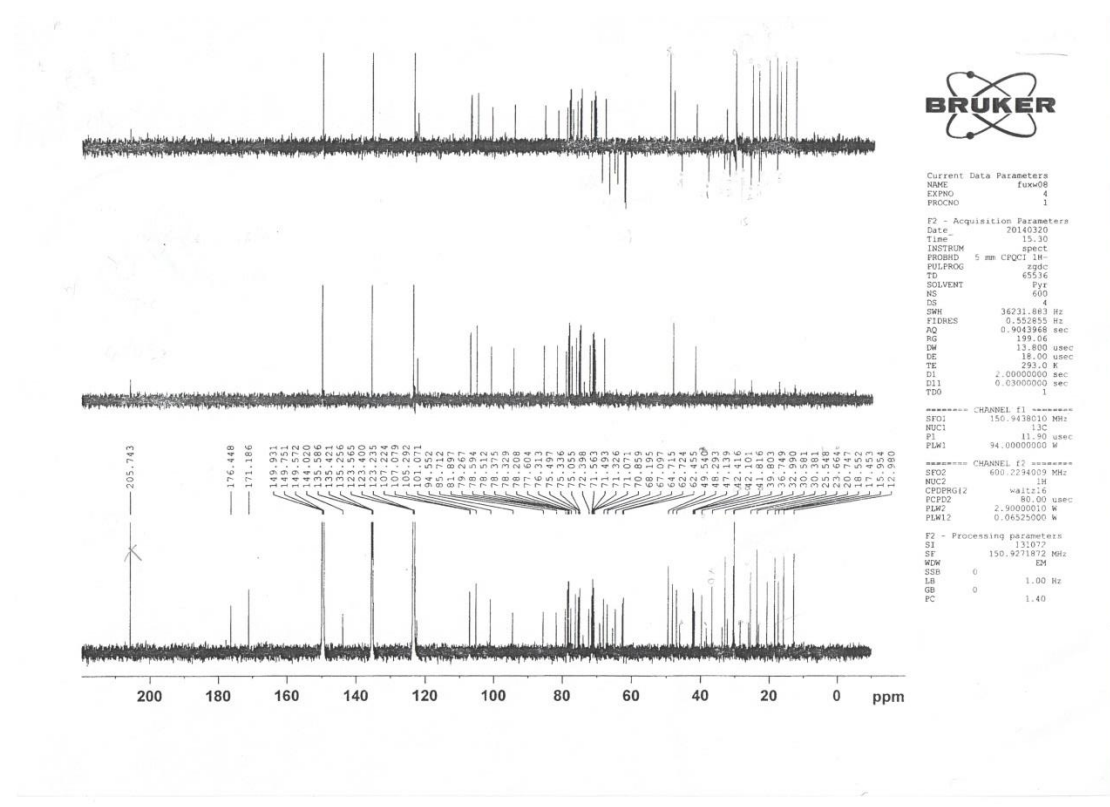


Figure S3 ^{13}C NMR spectrum of compound **1** (150 MHz, pyridine- d_5)

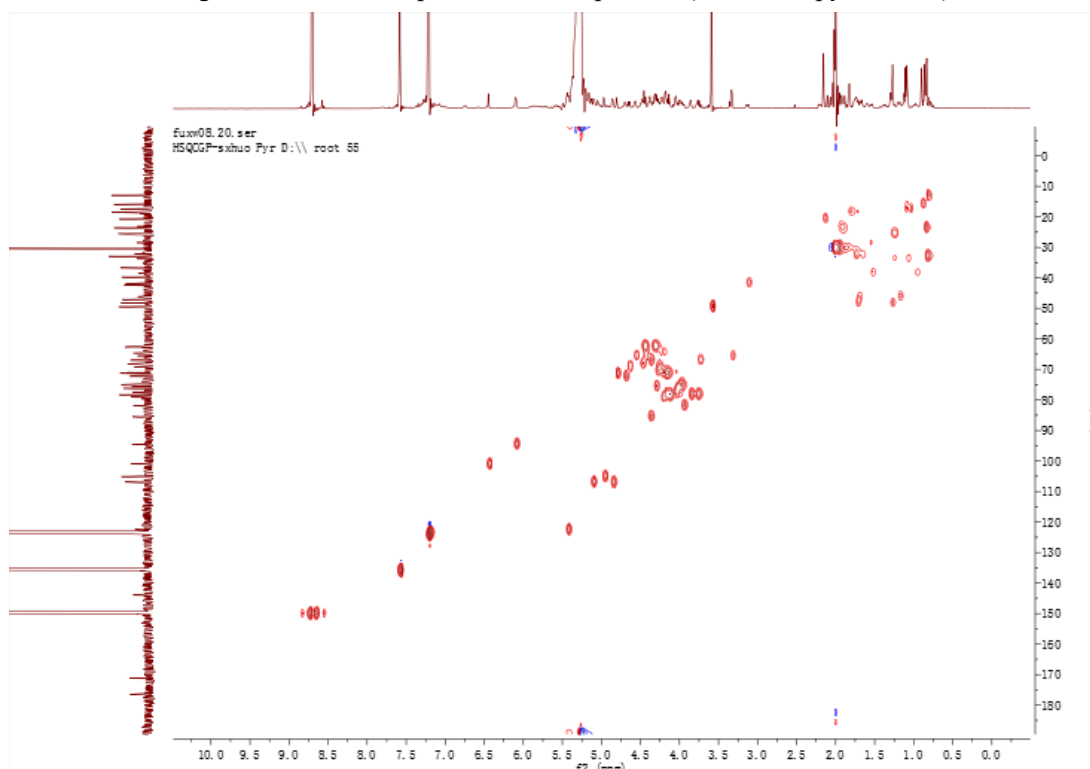


Figure S4 HSQC spectrum of compound **1**

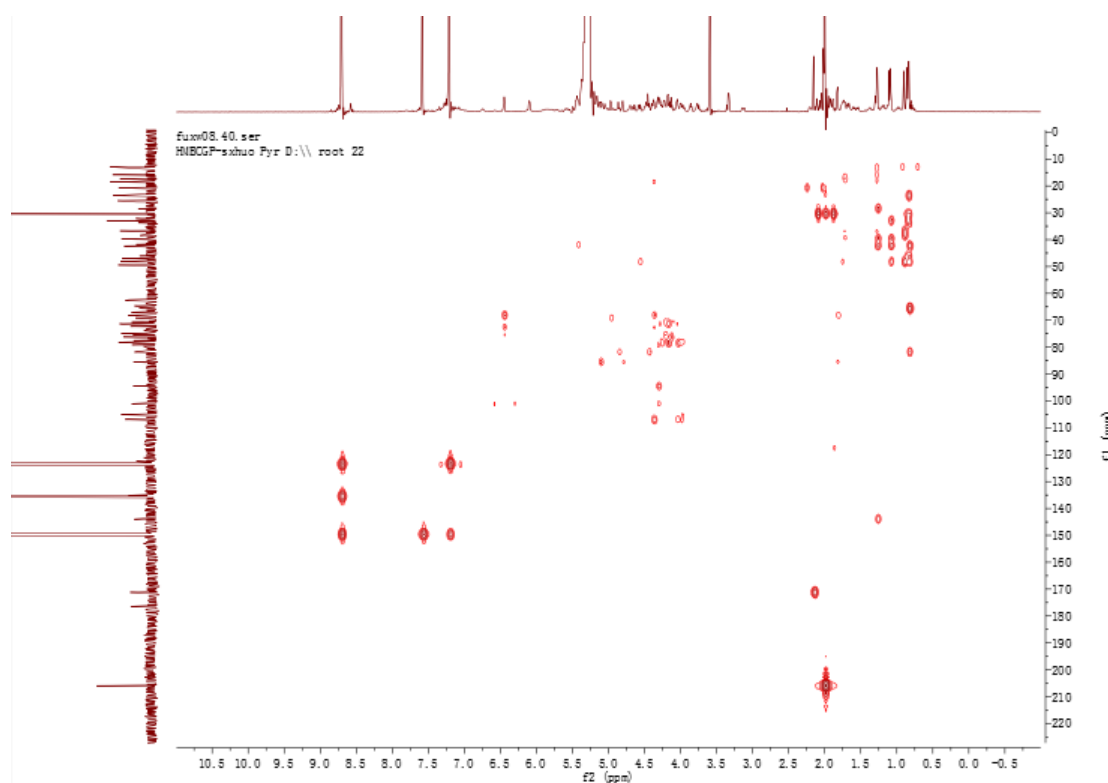


Figure S5 HMBC spectrum of compound **1**

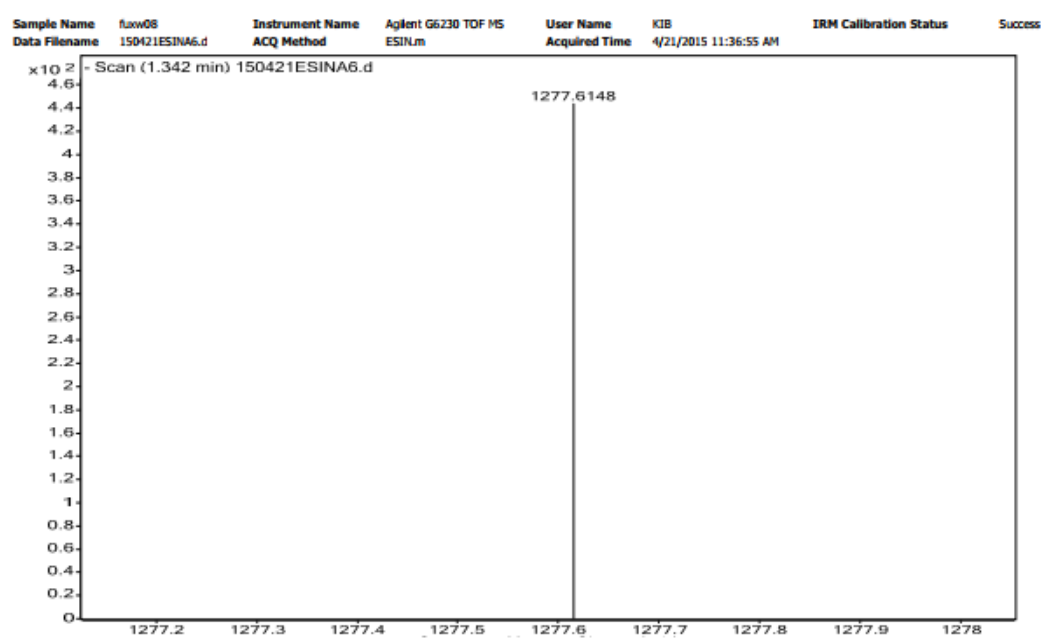


Figure S6 HRESIMS spectrum of compound **1**

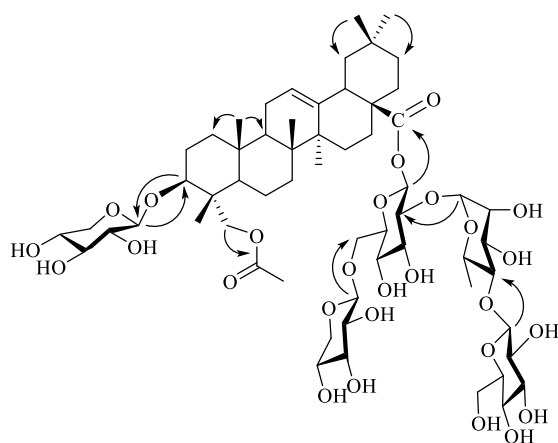


Figure S7 Key HMBC correlation of compound **2**

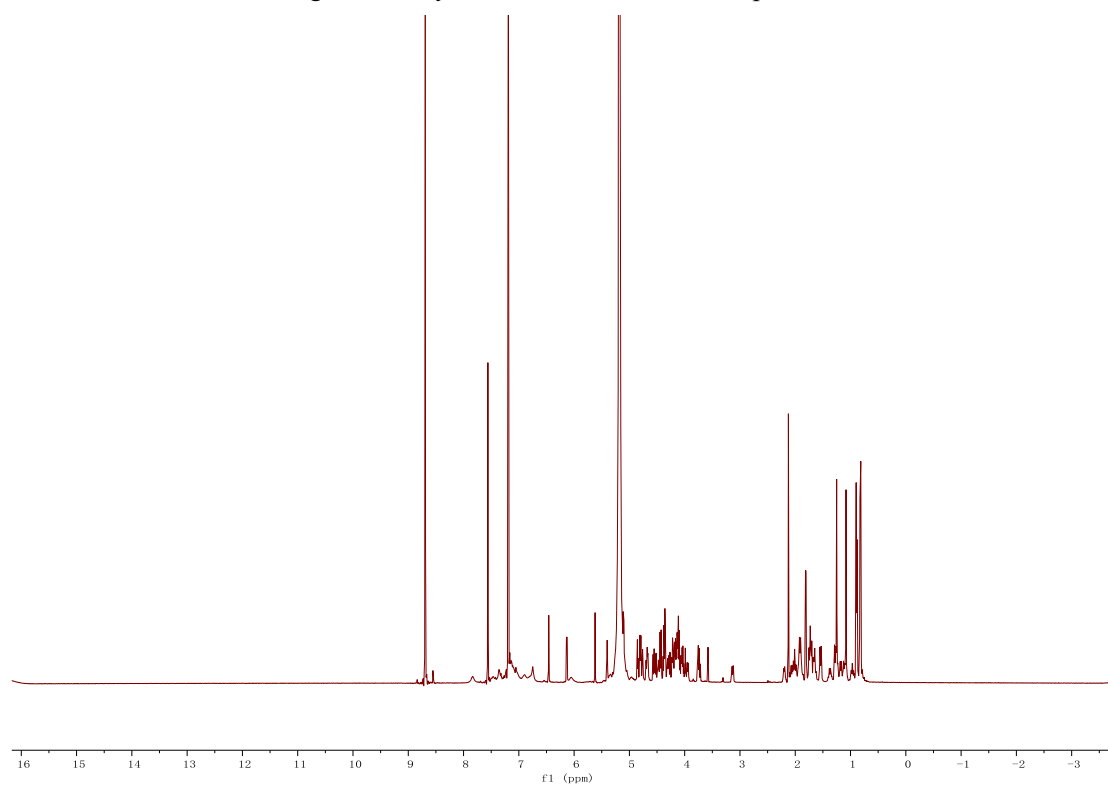


Figure S8 ^1H NMR spectrum of compound **2** (600 MHz, $\text{pyridine-}d_5$)

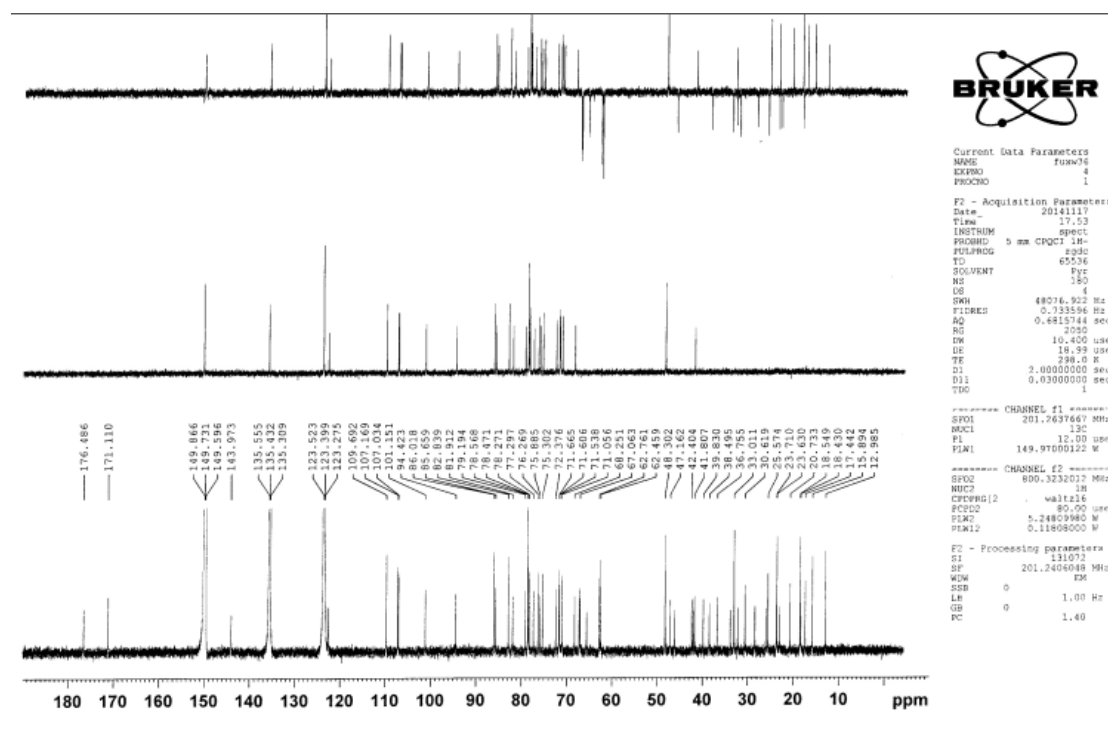


Figure S9 ^{13}C NMR spectrum of compound **2** (150 MHz, pyridine- d_5)

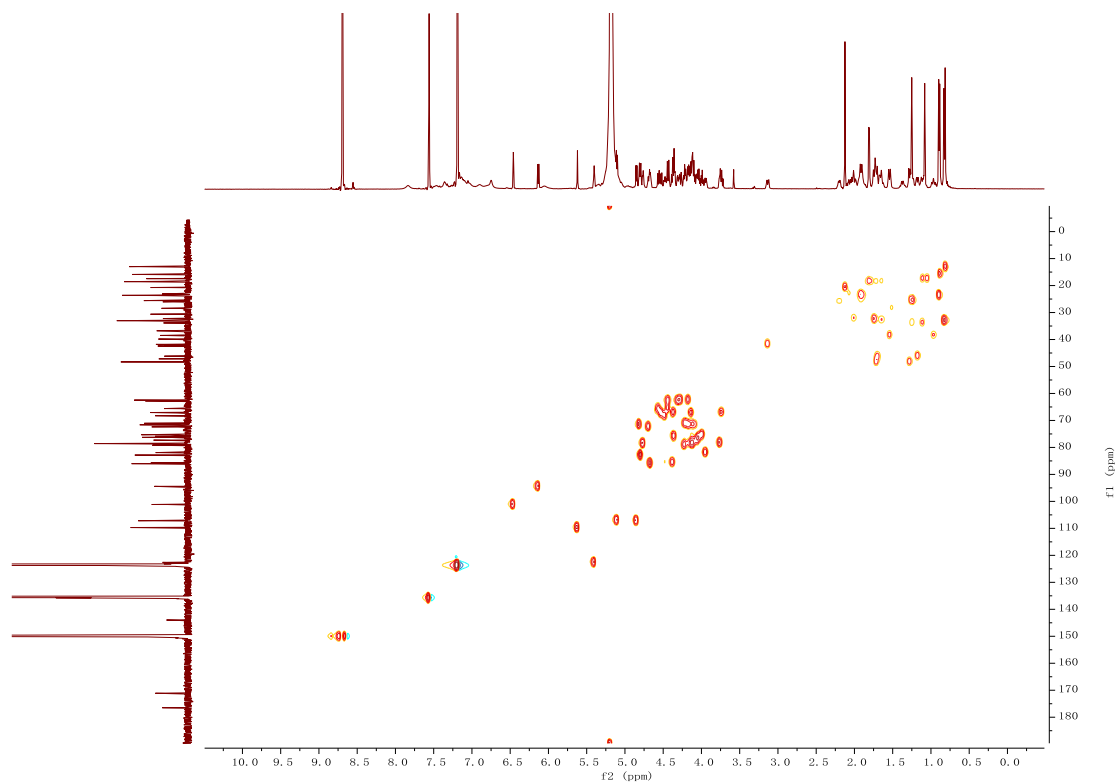


Figure S10 HSQC spectrum of compound **2**

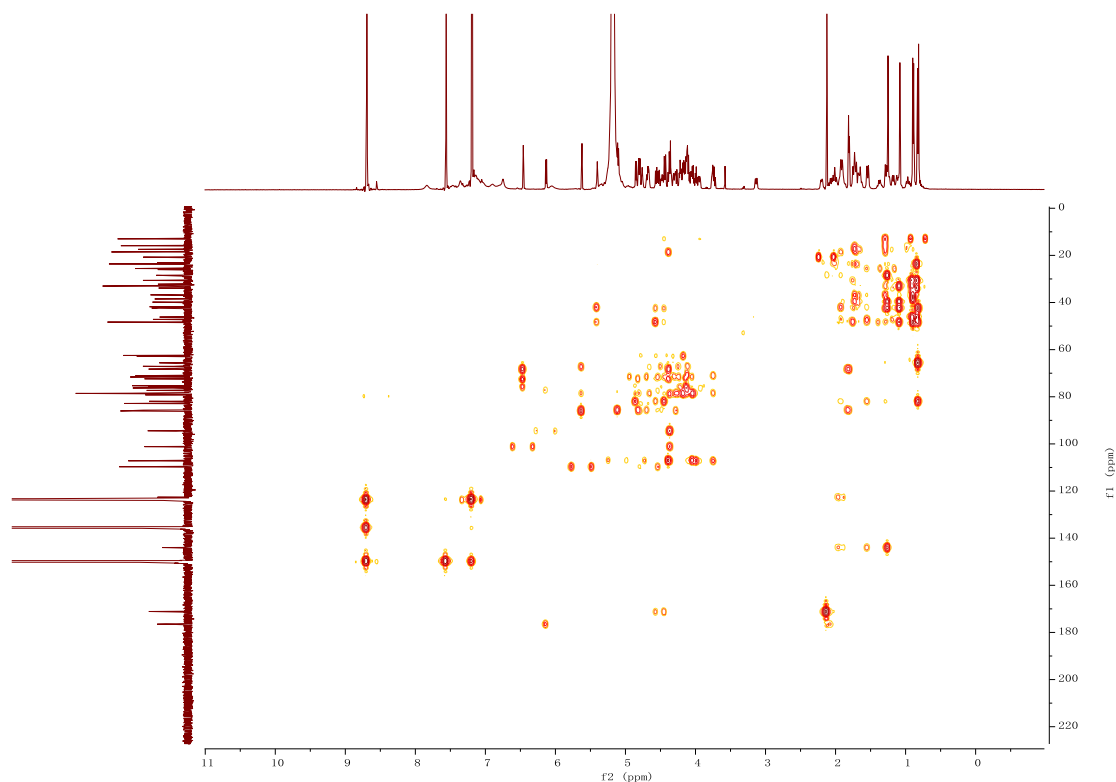
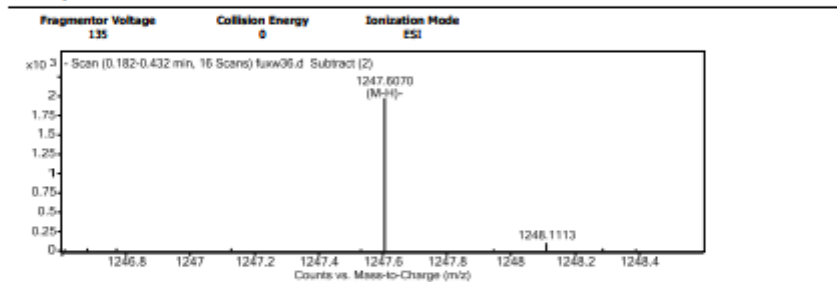


Figure S11 HMBC spectrum of compound **2**

Qualitative Analysis Report

Data Filename	fluxw36.d	Sample Name	fluxw36
Sample Type	Sample	Position	P1-A7
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU-ESI-Lm	Acquired Time	9/22/2015 3:56:44 PM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
623.2991	2	1121.34		
646.3021	2	1139.5		
646.805	2	870.68		
1247.607	1	1958.22	C60 H96 O27	[M-H]-
1248.608	1	1383.56	C60 H96 O27	[M-H]-
1293.6099	1	913.5		
1361.5953	1	1281.46		
1362.5957	1	773.62		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	Calculated Mass	Calculated Mz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C60 H96 O27	1248.6139	1247.6066	1247.6070	0.8	0.6	13.0000

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Figure S12 HRESIMS spectrum of compound **2**

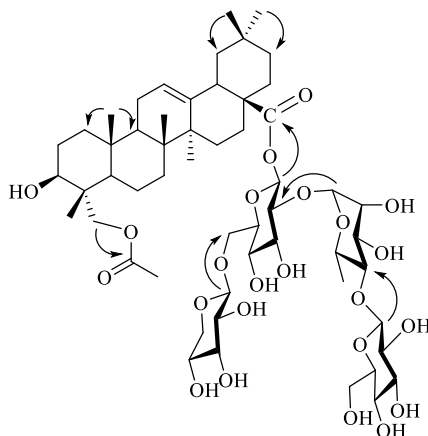


Figure S13 Key HMBC correlation of compound **3**

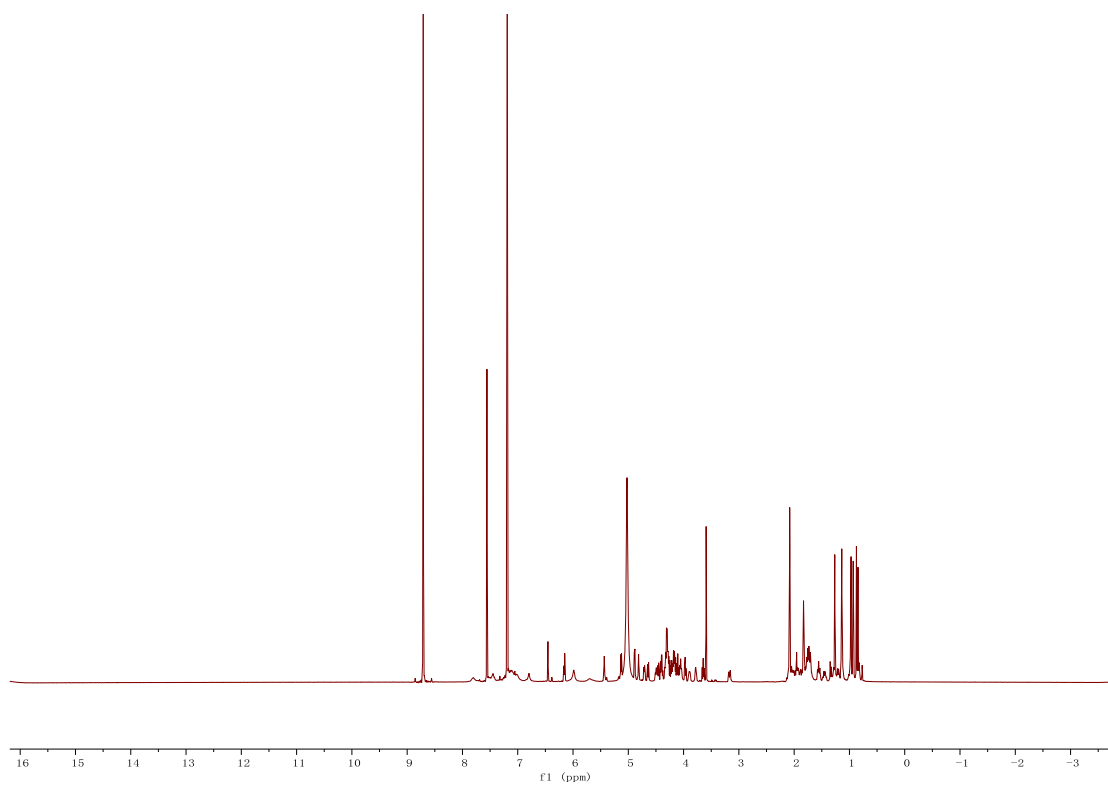


Figure S14 ¹H NMR spectrum of compound **3** (600 MHz, pyridine-*d*₅)

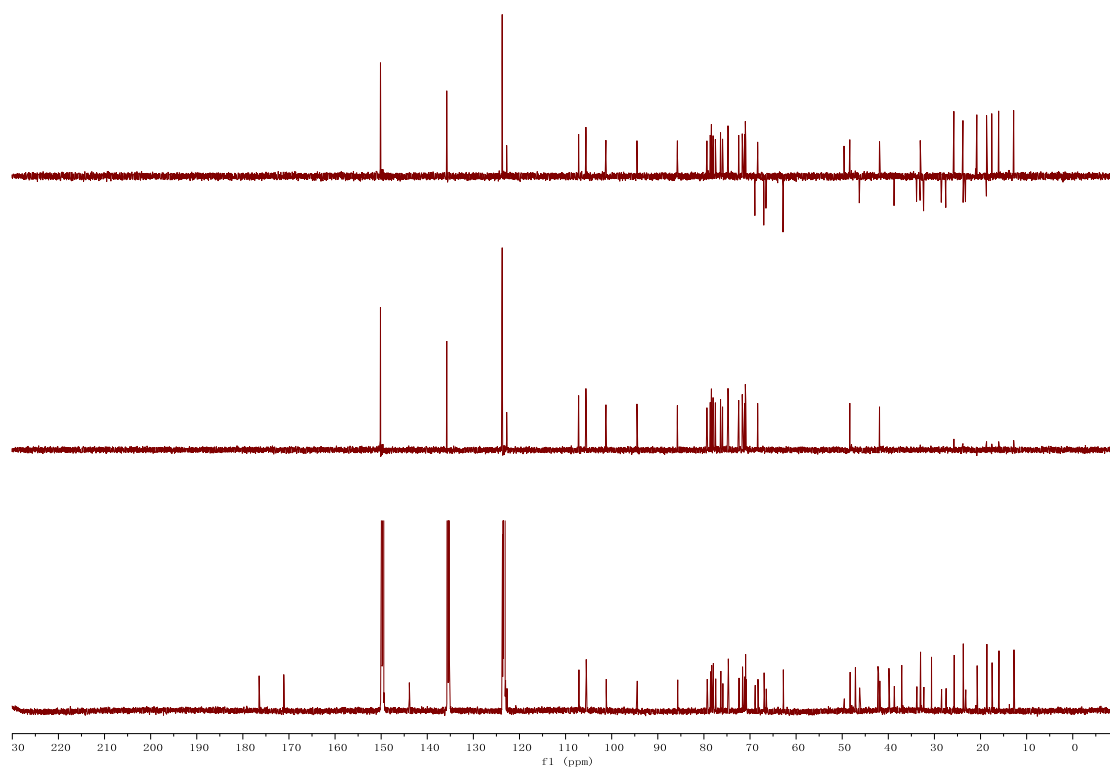


Figure S15 ^{13}C NMR spectrum of compound **3** (150 MHz, pyridine- d_5)

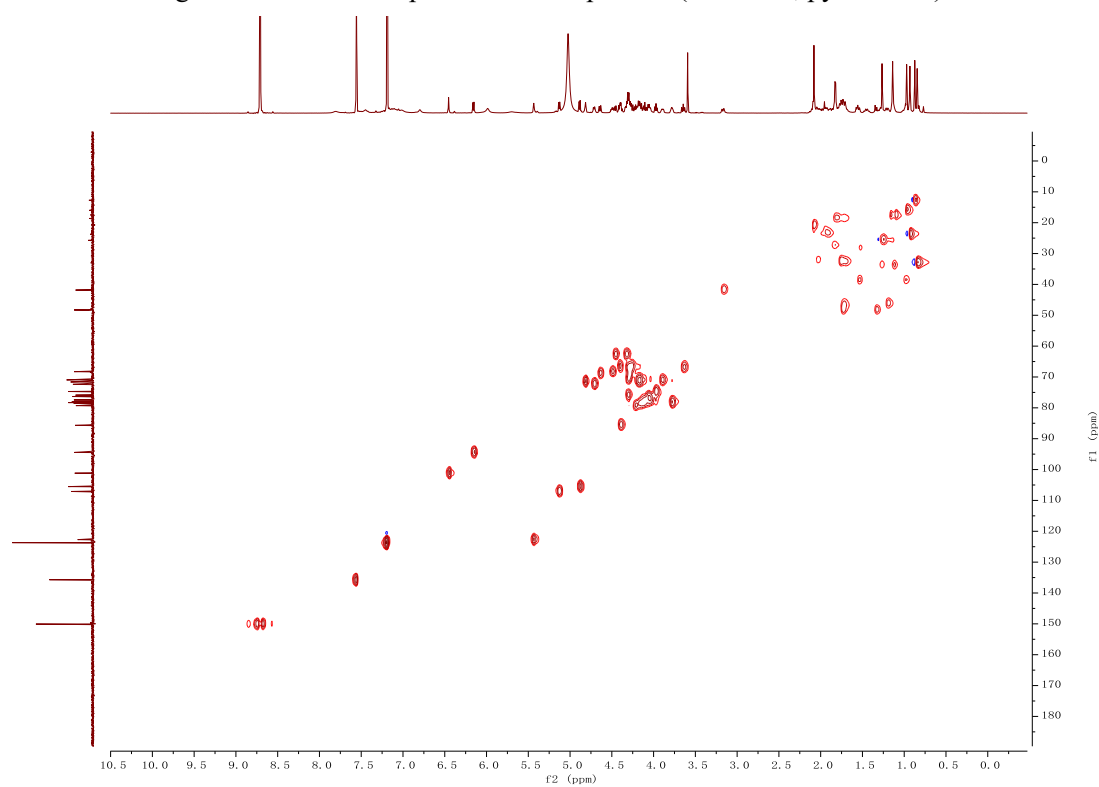


Figure S16 HSQC spectrum of compound **3**

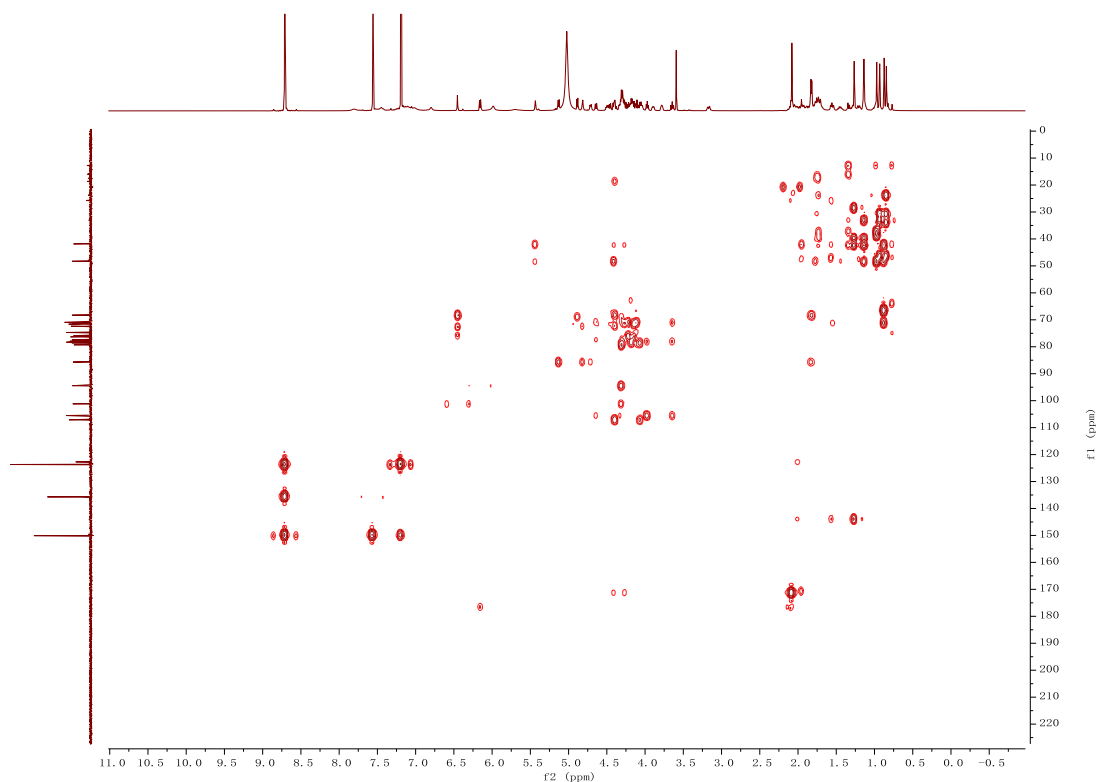
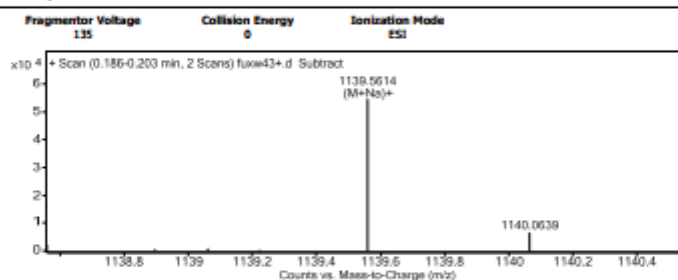


Figure S17 HMBC spectrum of compound **3**

Qualitative Analysis Report

Data Filename	fluxw43+.d	Sample Name	fluxw43
Sample Type	Sample	Position	P1-D6
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	11/5/2015 10:23:27 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			
Sample Group	Info.		
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
570.2806	2	11468.18		
578.2691	2	33672.49		
578.7708	2	21226.05		
1139.5614	1	54369.45	CS5 H88 O23	(M+Na)+
1140.565	1	32070.97	CS5 H88 O23	(M+Na)+
1141.5679	1	11161.86	CS5 H88 O23	(M+Na)+
1155.5347	1	15864.92		
1156.5377	1	9860.31		

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
CS5 H88 O23	1116.5716	1139.5609	1139.5614	-0.5	-0.4	12.0000

Figure S18 HRESIMS spectrum of compound **3**

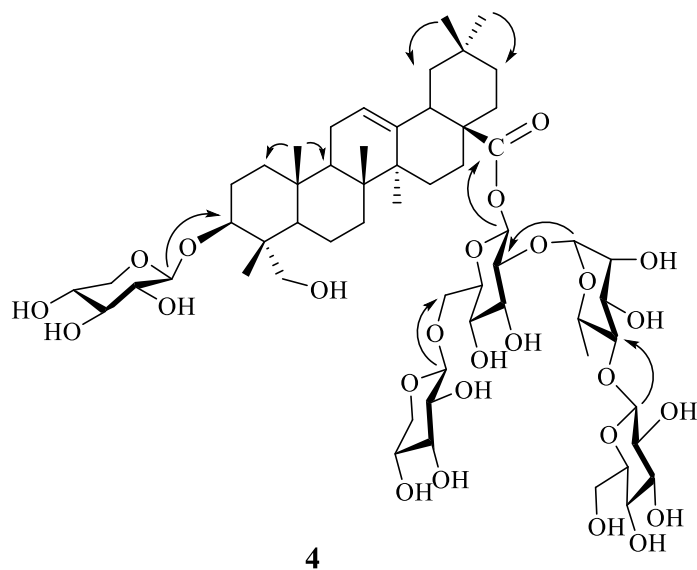


Figure S19 Key HMBC correlation of compound **4**

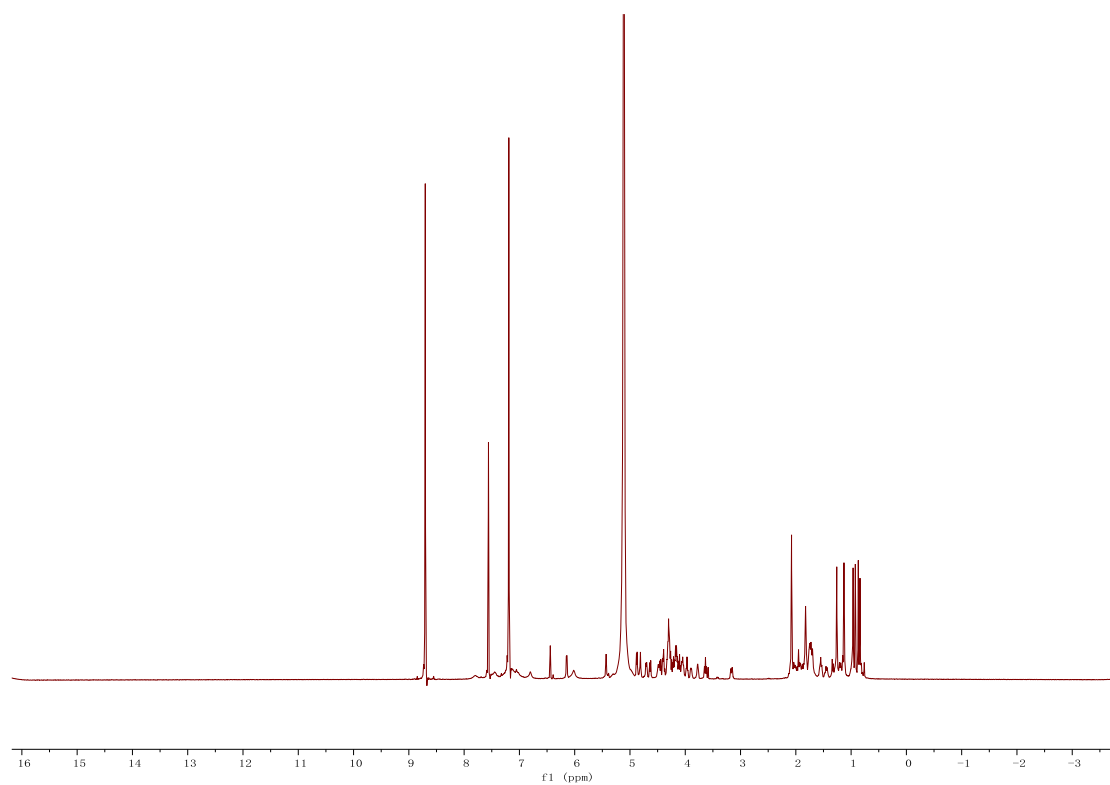


Figure S20 ¹H NMR spectrum of compound **4** (600 MHz, pyridine-*d*₅)

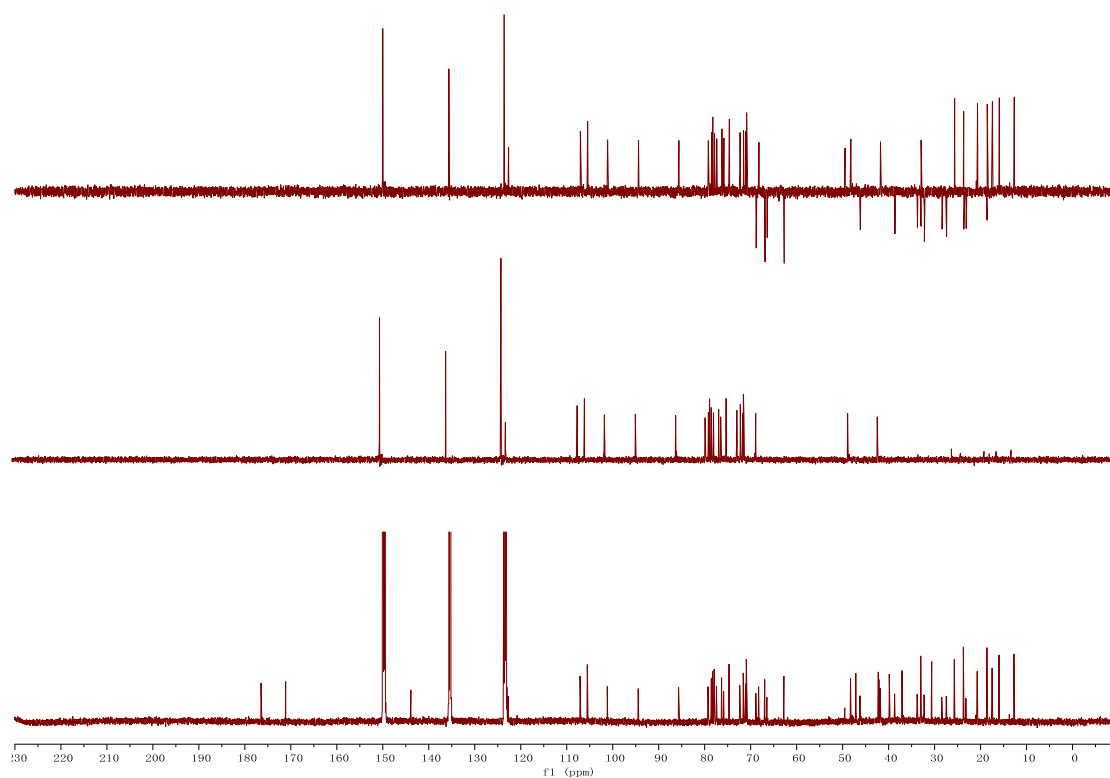


Figure S21 ^{13}C NMR spectrum of compound **4**(150 MHz, pyridine- d_5)

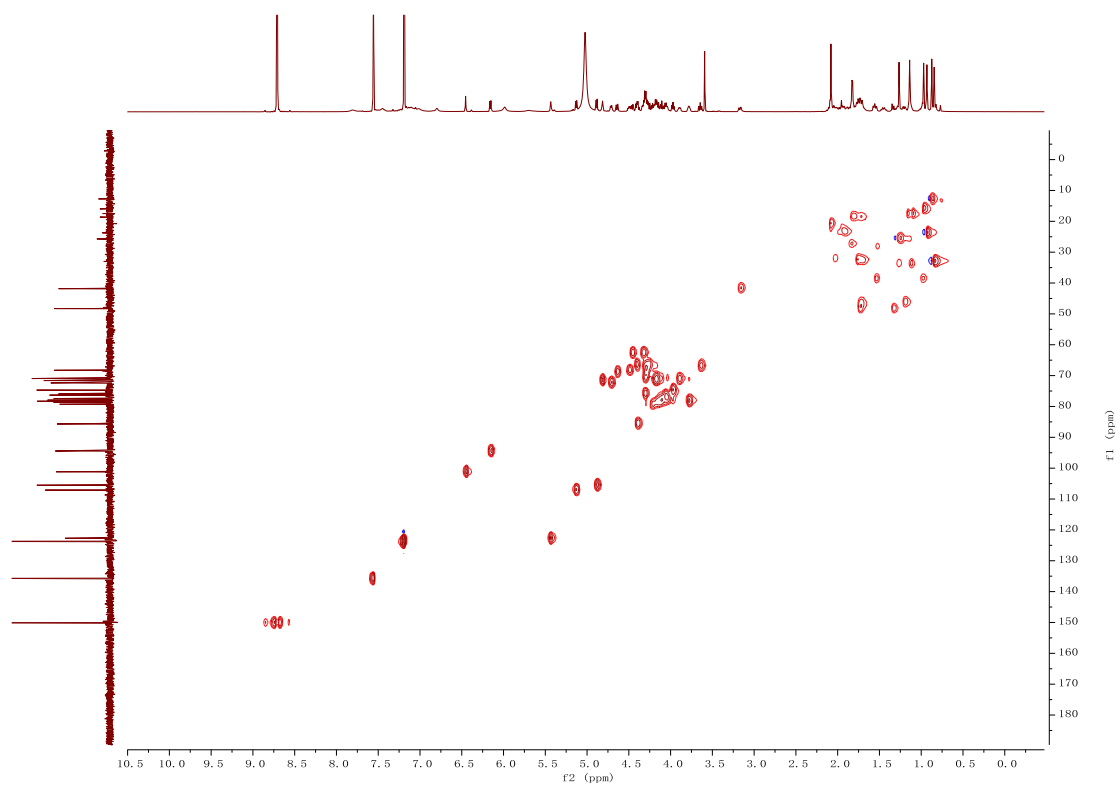


Figure S22 HSQC spectrum of compound **4**

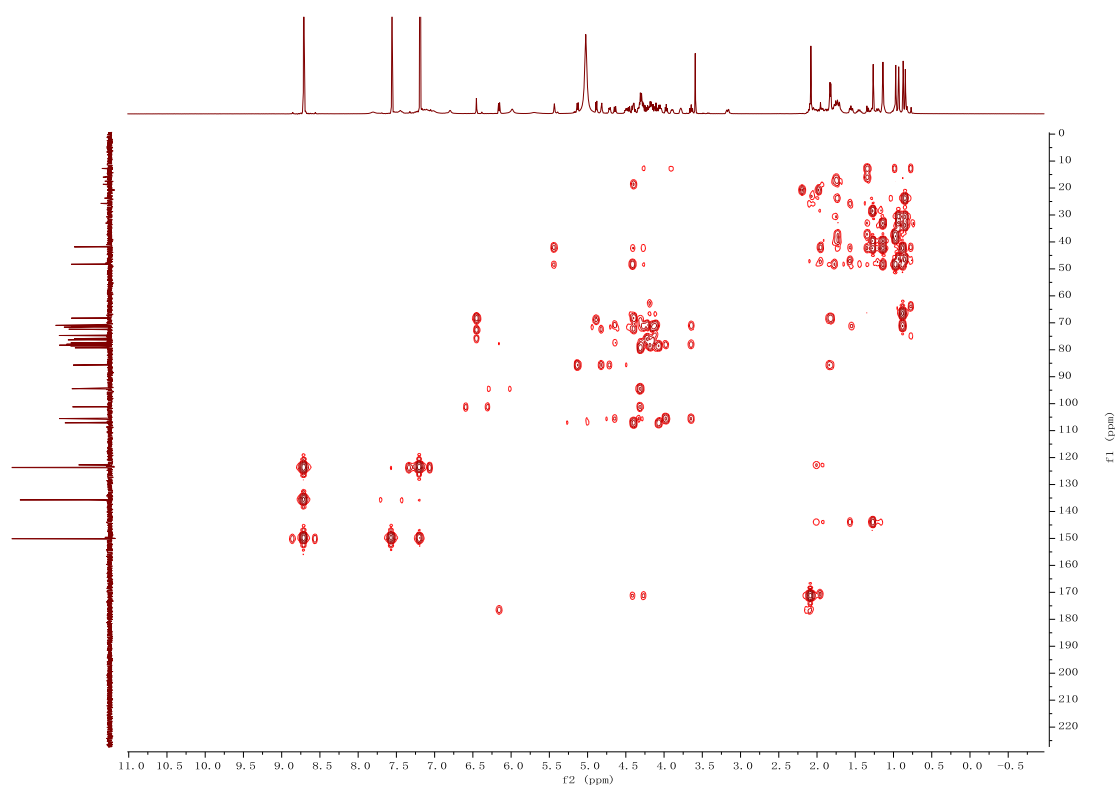


Figure S23 HMBC spectrum of compound **4**

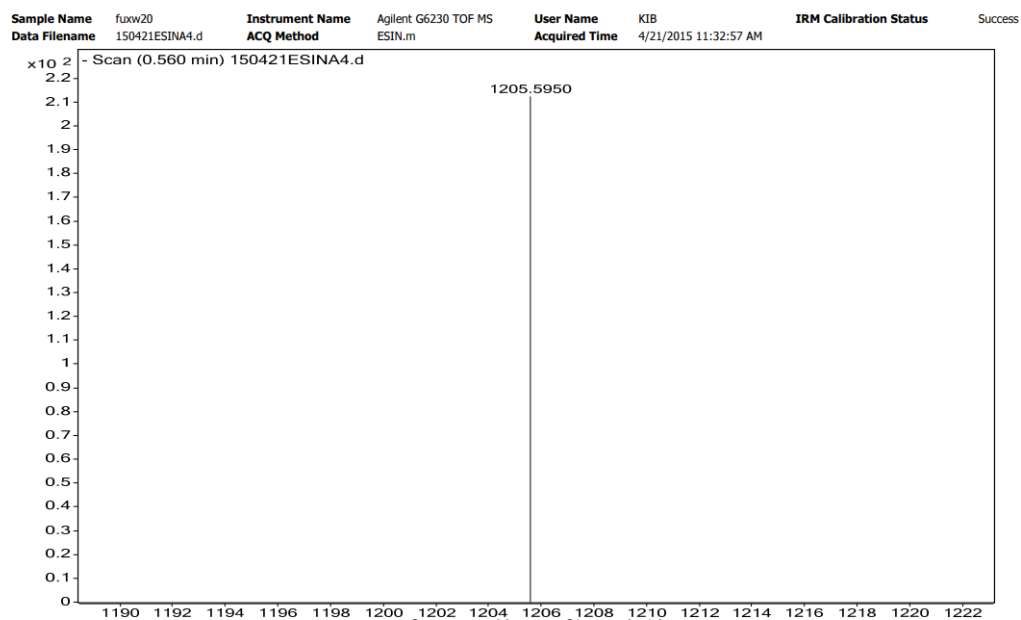


Figure S24 HRESIMS spectrum of compound **4**

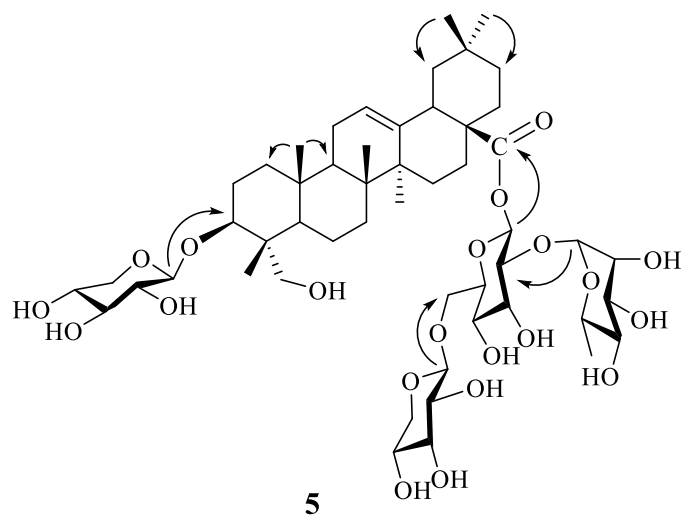


Figure S25 Key HMBC correlation of compound **5**

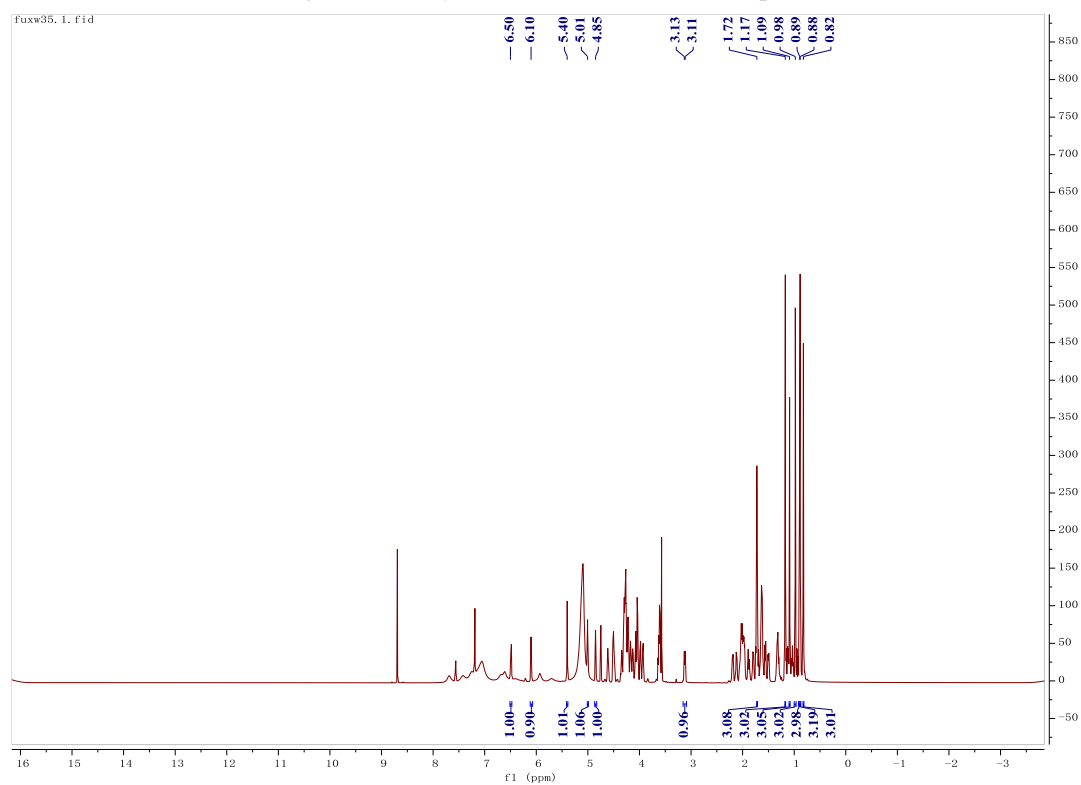


Figure S26 ^1H NMR spectrum of compound **5** (600 MHz, pyridine- d_5)

fuxw35. 6. fid

fuxw35. 8. fid

fuxw35. 4. fid

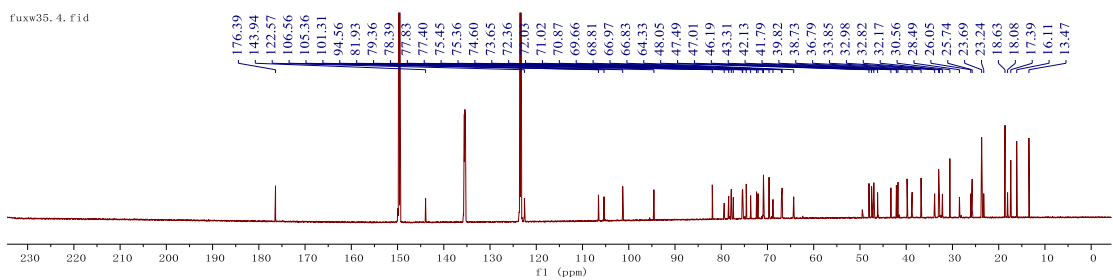


Figure S27 ^{13}C NMR spectrum of compound **5** (150 MHz, pyridine- d_5)

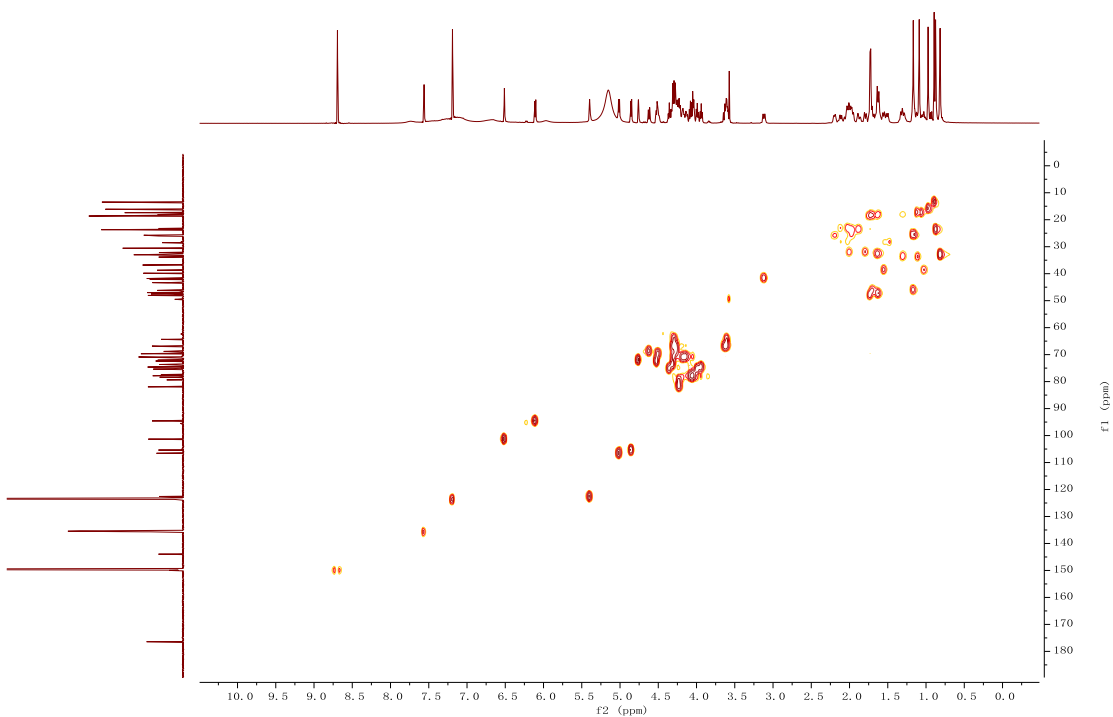


Figure S28 HSQC spectrum of compound **5**

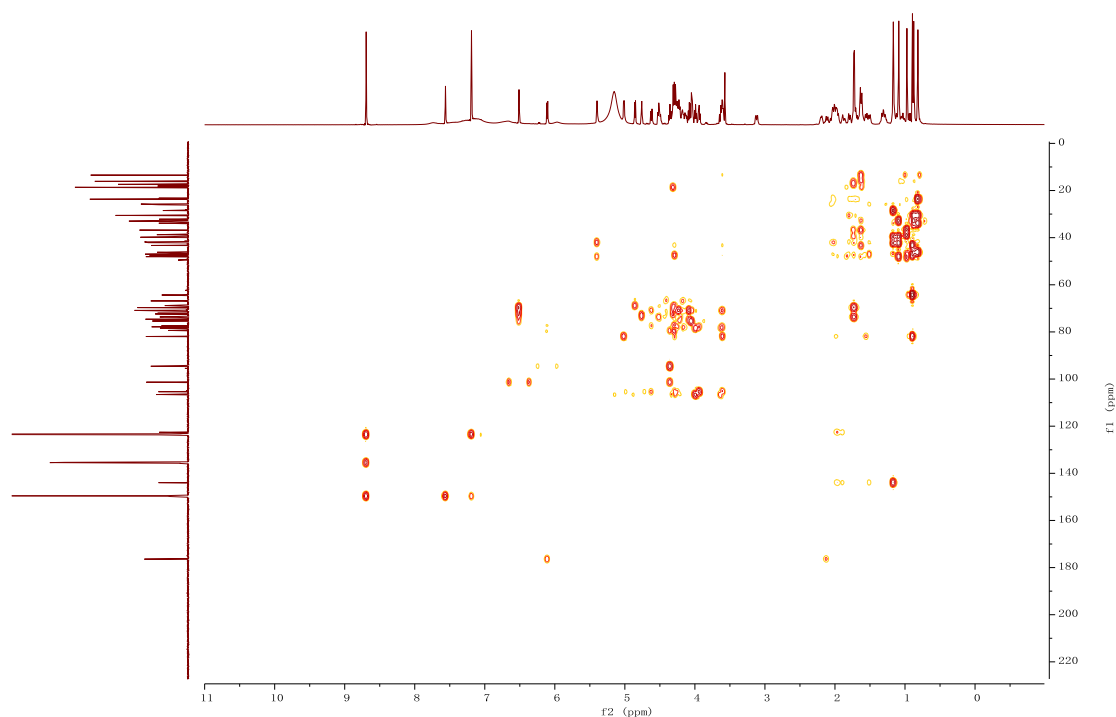
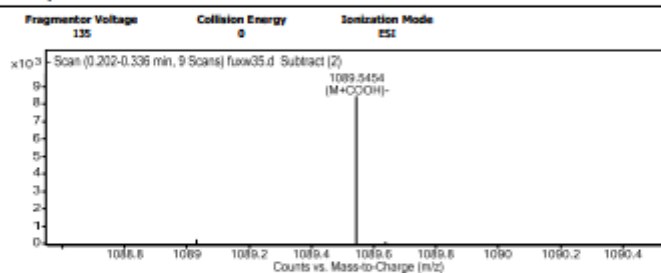


Figure S29 HMBC spectrum of compound **5**

Qualitative Analysis Report

Data Filename	fuwx35.d	Sample Name	fuwx35
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU-ESI-Lm	Acquired Time	9/22/2015 3:55:13 PM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF 8.05.01 (BS125.2)		

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
362.9406	1	5479.9		
1043.5417	2	15203.24		
1044.546	2	8454.5		
1089.5454	1	8421.02	C52 H84 O21	(M+COOH)-
1090.5505	1	5362.31	C52 H84 O21	(M+COOH)-
1106.5393	1	6732.35		
1157.5343	1	13300.13		
1158.5396	1	7422.3		

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C52 H84 O21	1044.5505	1089.5487	1089.5454	2.1	2.0	11.0000

Figure S30 HRESIMS spectrum of compound **5**

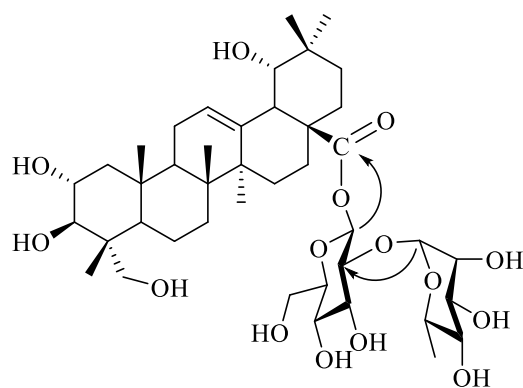


Figure S31 Key HMBC correlation of compound **6**

fuya19_1.fid

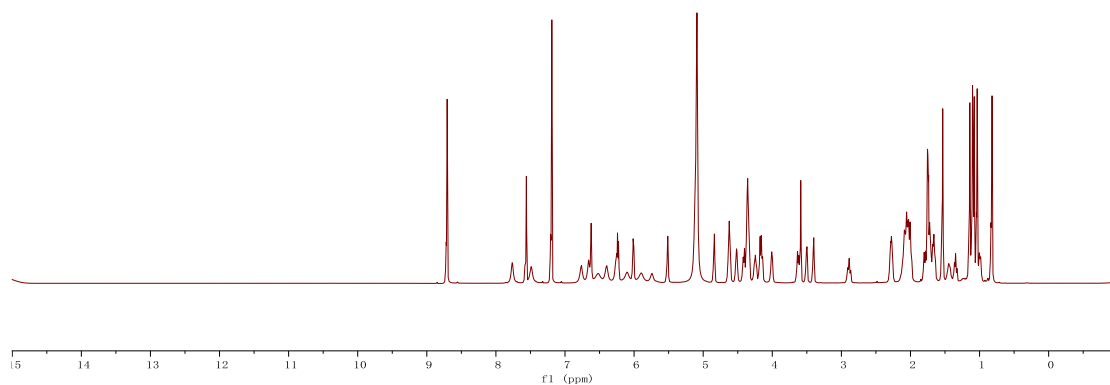


Figure S32 ¹H NMR spectrum of compound **6** (600 MHz, pyridine-*d*₅)

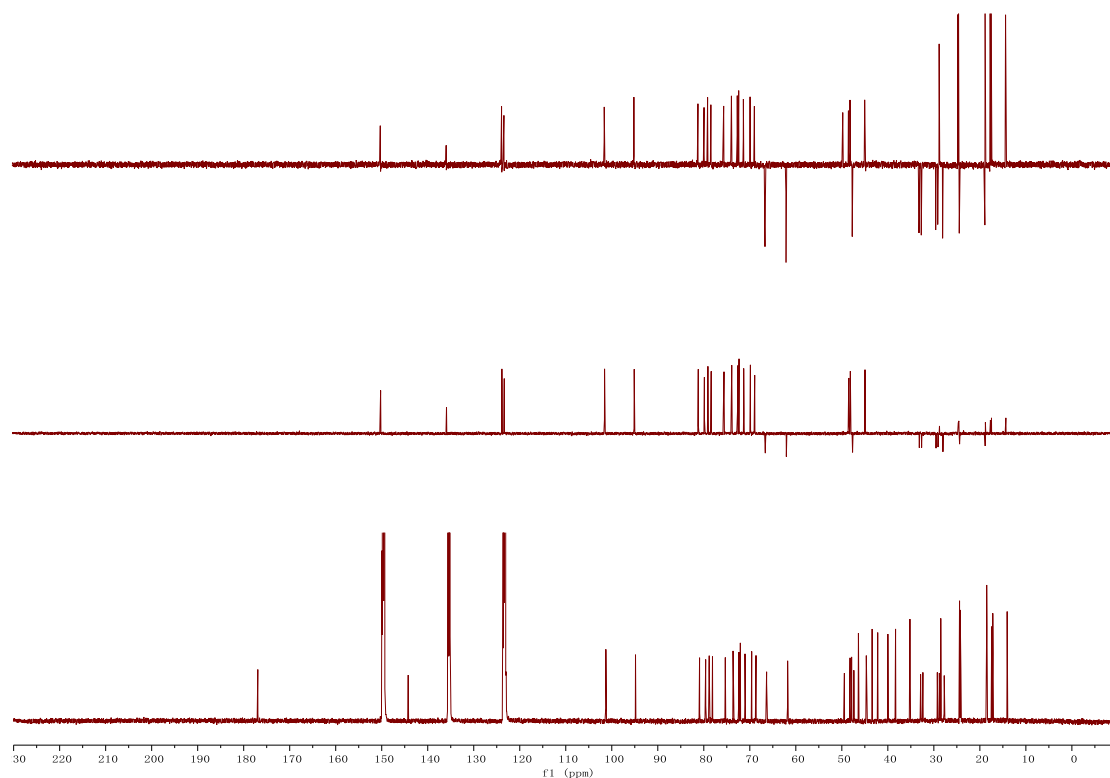


Figure S33 ^{13}C NMR spectrum of compound **6** (150 MHz, $\text{pyridine-}d_5$)

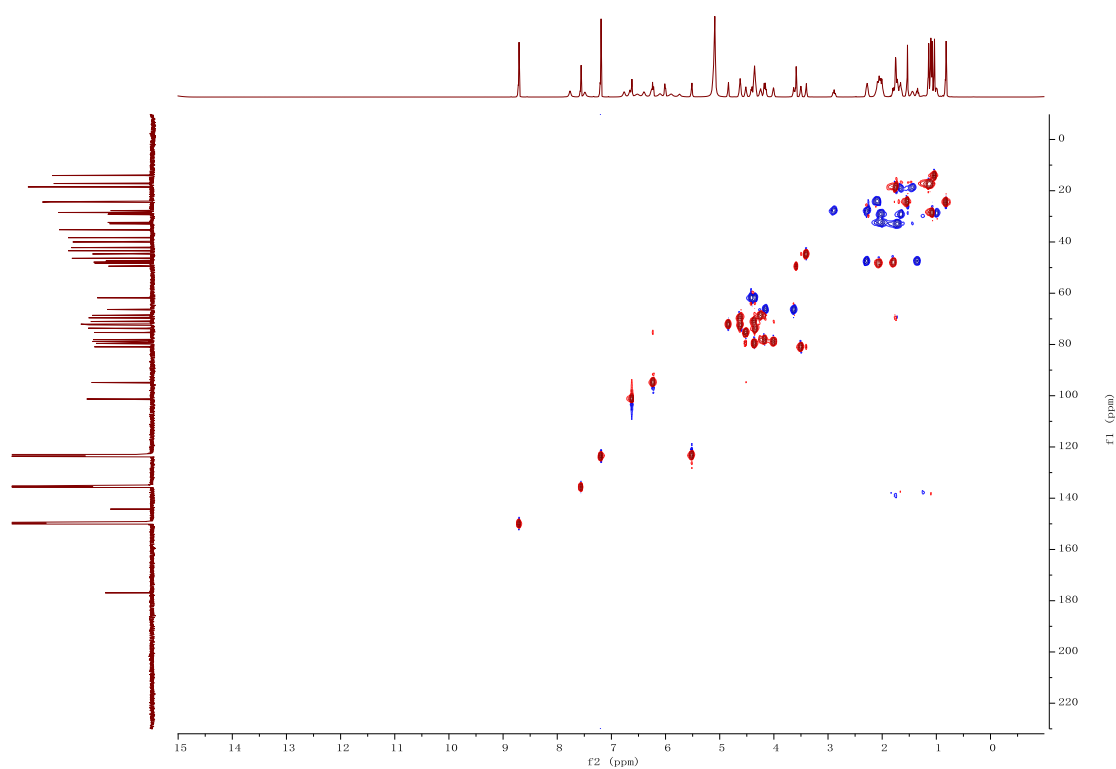


Figure S34 HSQC spectrum of compound **6**

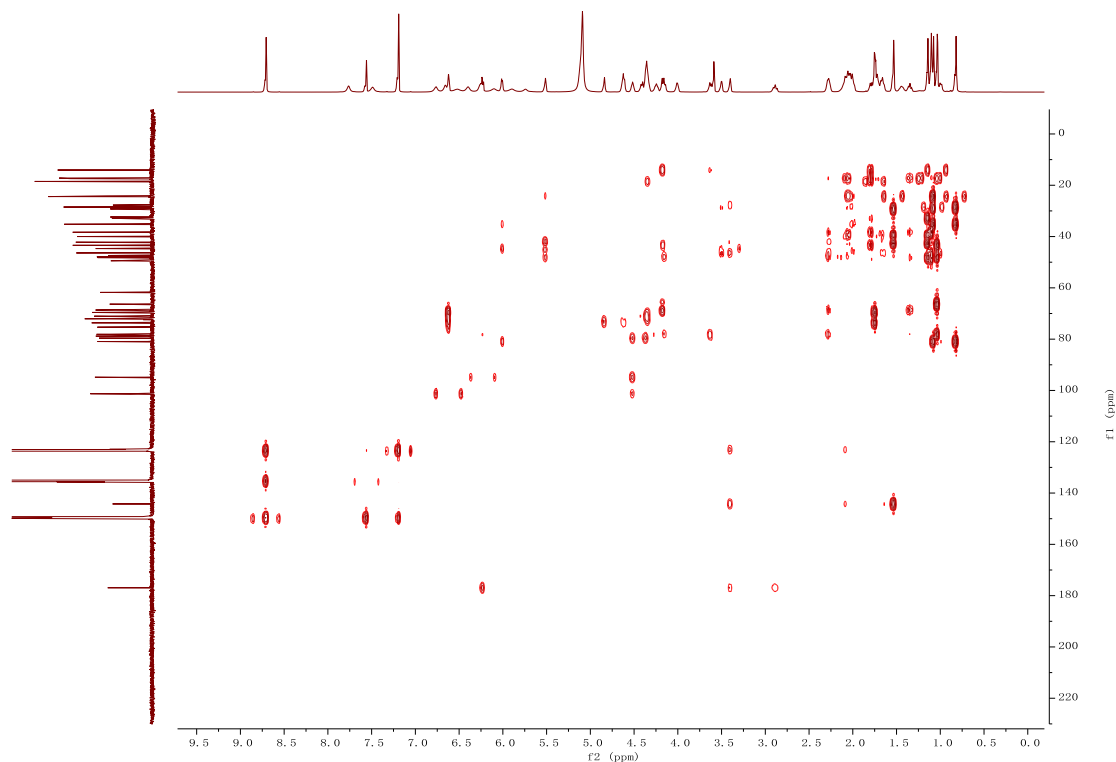
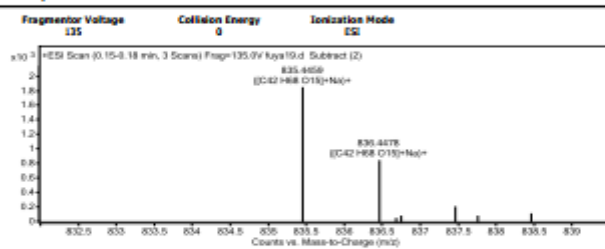


Figure S35 HMBC spectrum of compound **6**

Qualitative Analysis Report

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Sample Type	Sample	Position	P1-C1
Instrument Name	Instrument 1	User Name	
Acq Method	s.m	Acquired Time	7/30/2019 11:49:39 AM
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW	6300 series TOF/6500 series		
Version	Q-TOF 8.05.01 (85125.2)		

User Spectra



Peak List	m/z	z	Abund	Formula	Ion
	100.1277	1	4945.02		
	104.107		1894.2		
	353.2642	1	1477.43		
	369.2396		2653.37		
	381.2961	1	1377.17		
	397.2715	1	2374.74		
	453.1668	1	1293.8		
	575.3535	1	1042.65		
	835.4459	1	1856.69	C42 H68 O15	(H+Na)+
	836.4478	1	858.99	C42 H68 O15	(H+Na)+

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedHz	H/z	Diff. (mDa)	Diff. (ppm)	DBE
C42 H68 O15	812.4558	835.4450	835.4459	-0.90	-1.08	9.0000

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Figure S36 HRESIMS spectrum of compound **6**

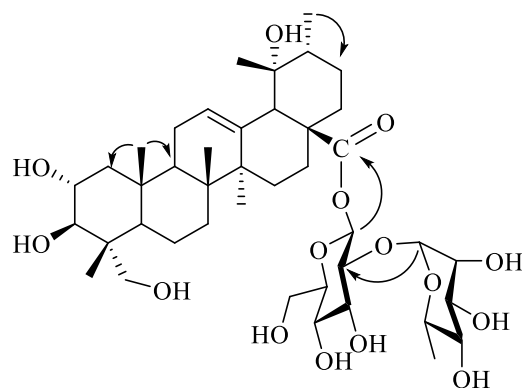


Figure S37 Key HMBC correlation of compound **7**

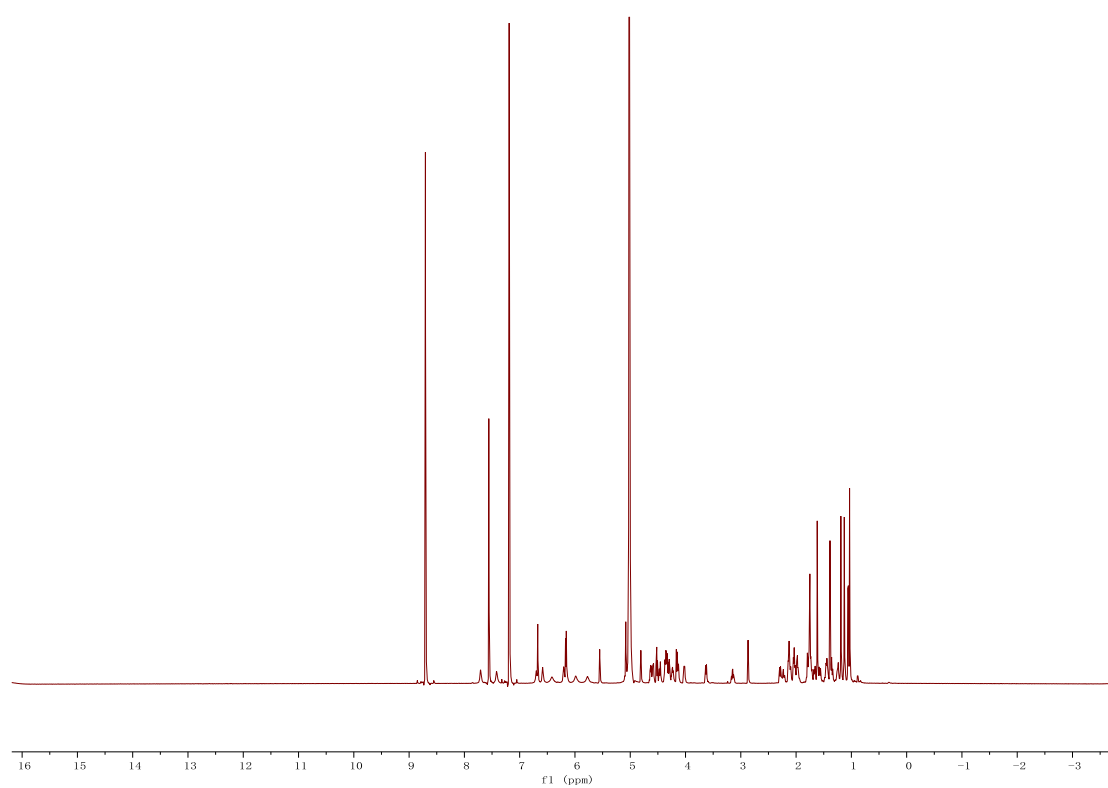


Figure S38 ^1H NMR spectrum of compound **7** (600 MHz, pyridine- d_5)

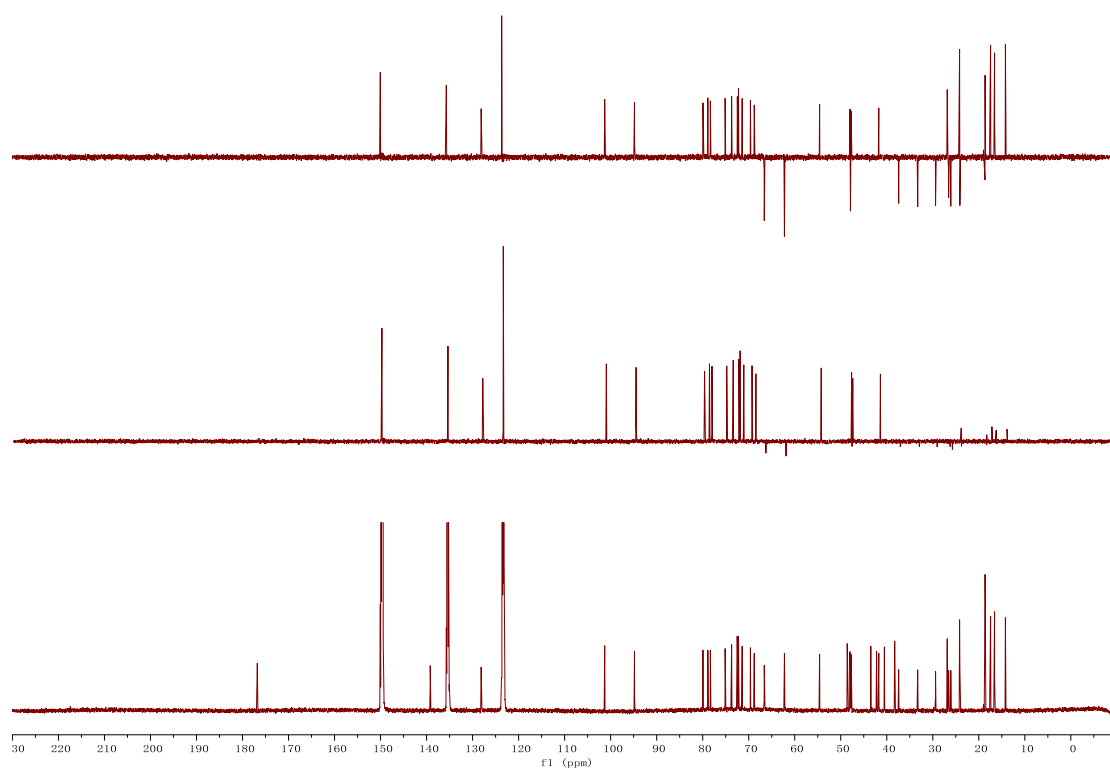


Figure S39 ^{13}C NMR spectrum of compound **7**(150 MHz, $\text{pyridine-}d_5$)

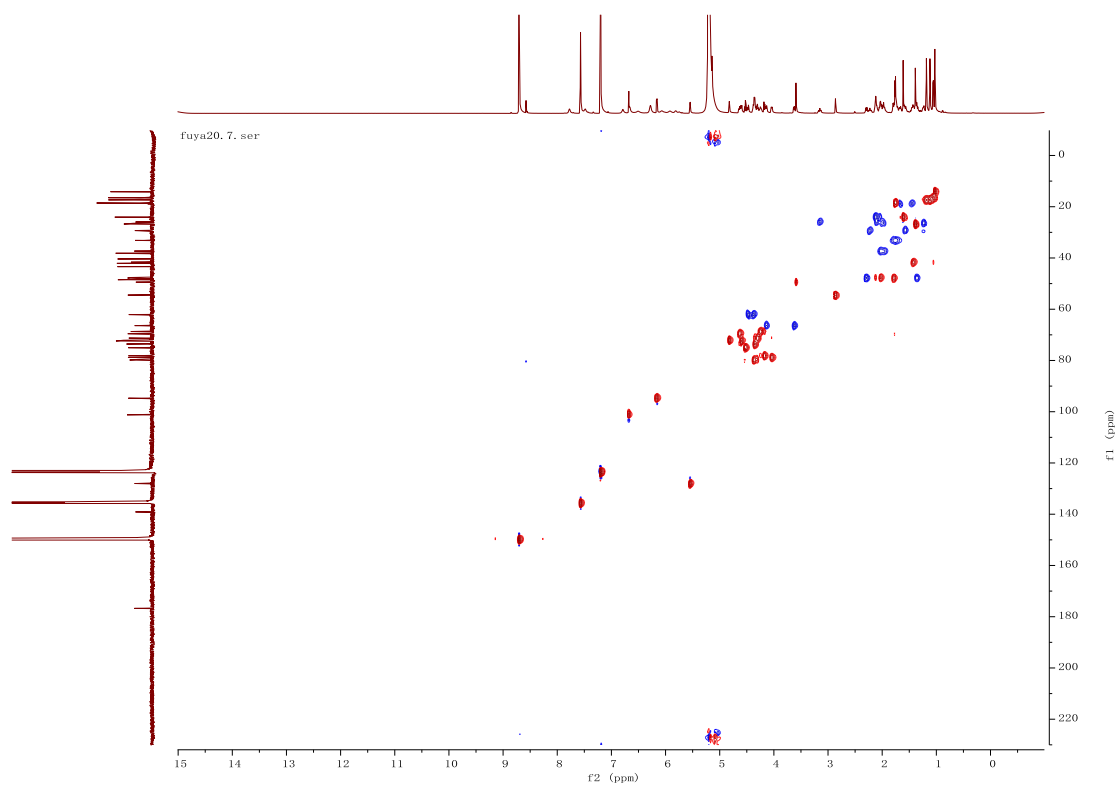


Figure S40 HSQC spectrum of compound **7**

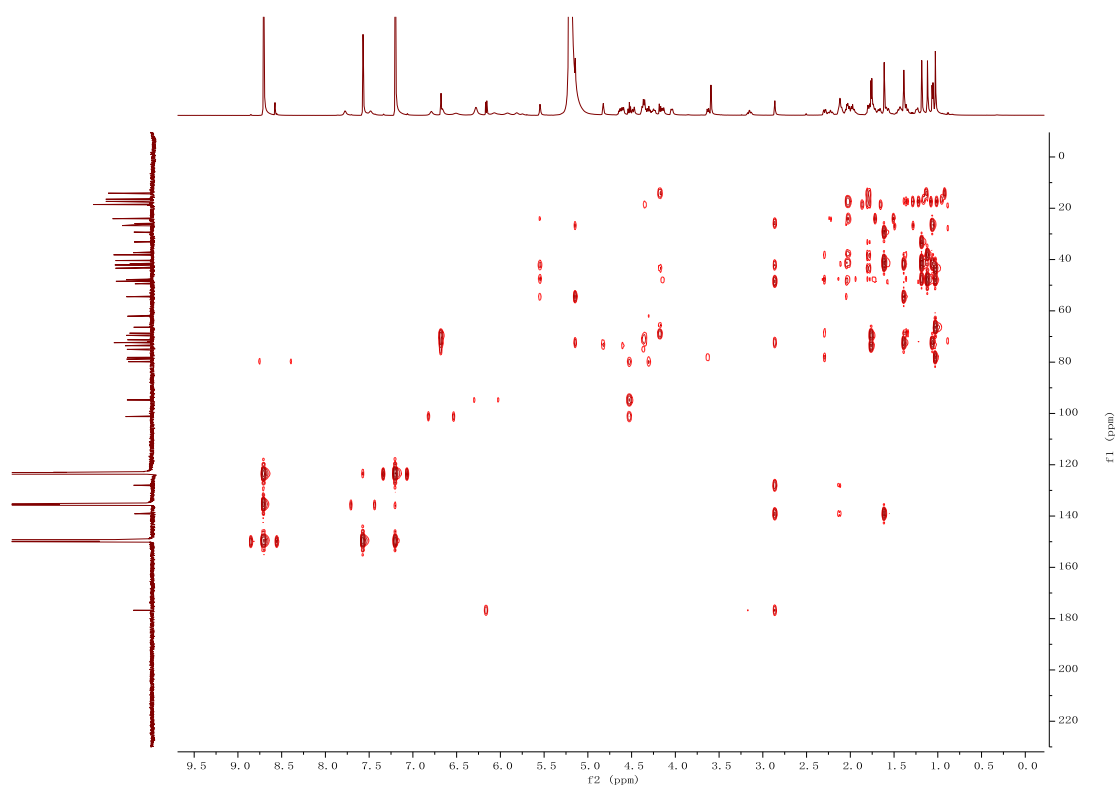


Figure S41 HMBC spectrum of compound **7**

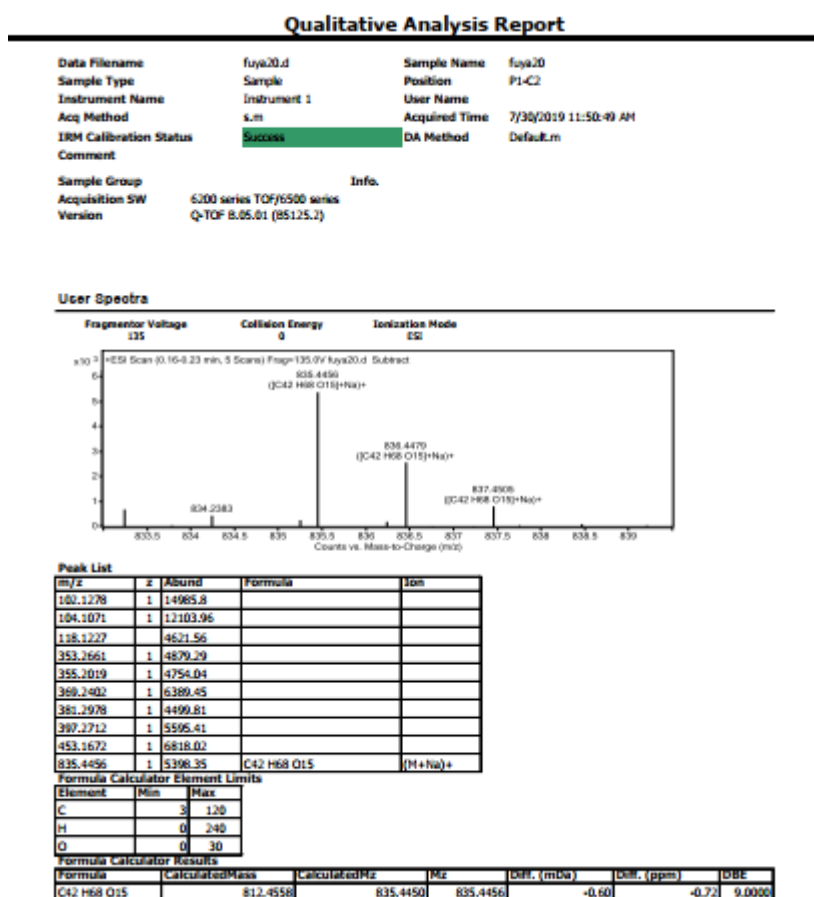


Figure S42 HRESIMS spectrum of compound **7**