

Supporting Information

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Two New Disaccharide Glycosides from the Root Cortex of *Paeonia ostii*

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Data File: E:\DATA\2021\0128\xff-11.lcd

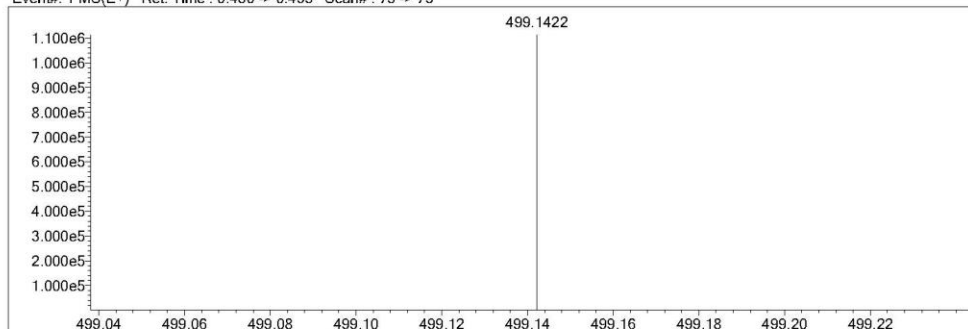
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	F	1	0	0	S	2	0	0	Br	1	0	2	H
2H	1	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	Na
C	4	5	50	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	0	Si	4	0	0	Cu	2	0	0	I	3	0	0	
O	2	0	30	P	3	0	0	Se	2	0	0					

Error Margin (ppm): 5
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

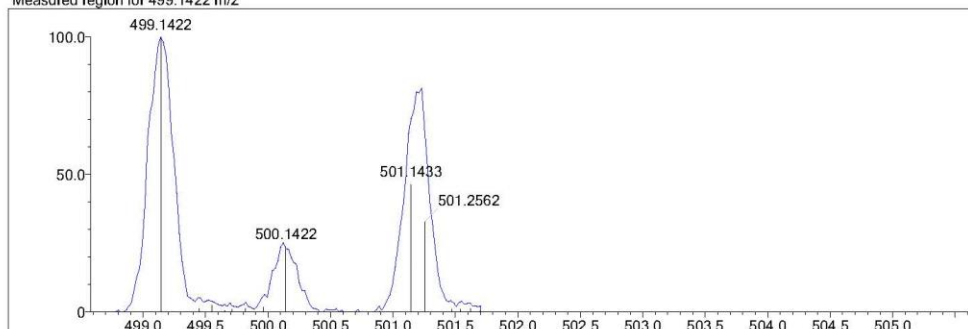
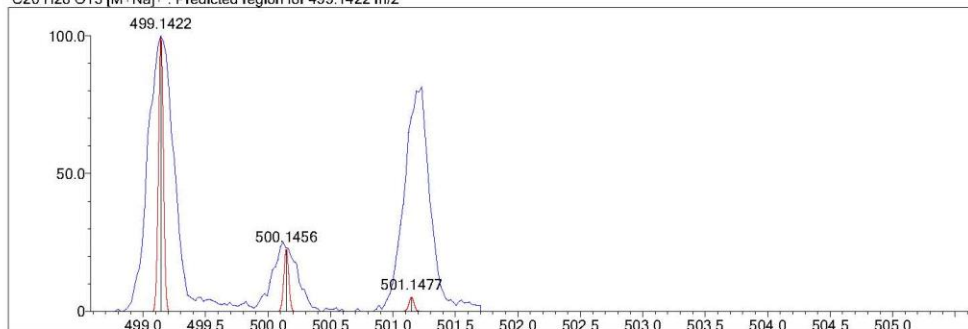
DBE Range: -2.0 - 100.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: OR

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 10000
 Max Results: 20

Event#: 1 MS(E+) Ret. Time : 0.480 -> 0.493 Scan#: 73 -> 75



Measured region for 499.1422 m/z

C20 H28 O13 [M+Na]⁺ : Predicted region for 499.1422 m/z

Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C20 H28 O13	[M+Na] ⁺	499.1422	499.1422	-0.0	0.00	7.0

Figure S1: HR-ESI-MS Spectrum of **1** (suffruticoside F)

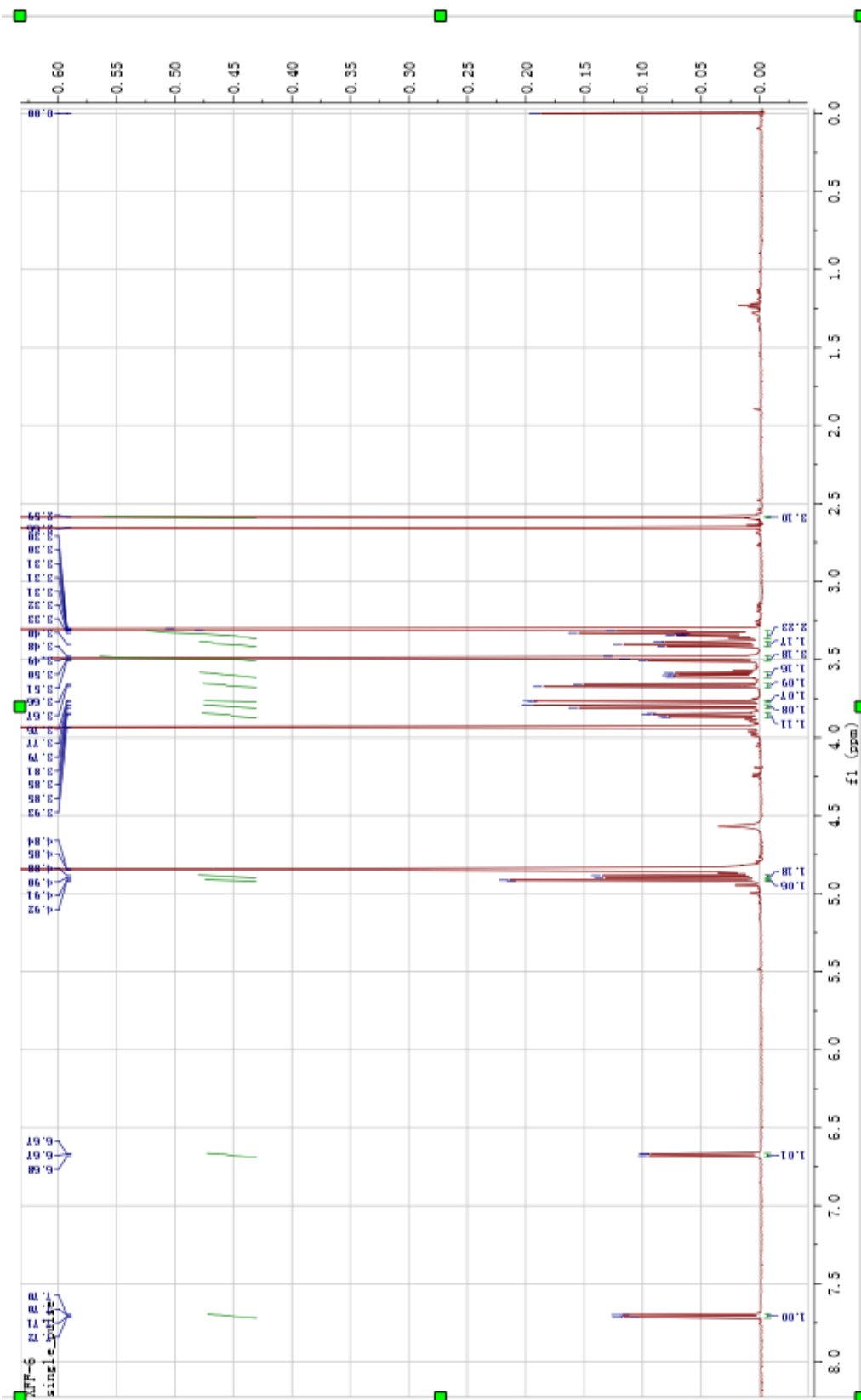


Figure S2: $^1\text{H-NMR}$ (500 MHz, MeOD) Spectrum of **1**(suffruticoside F)

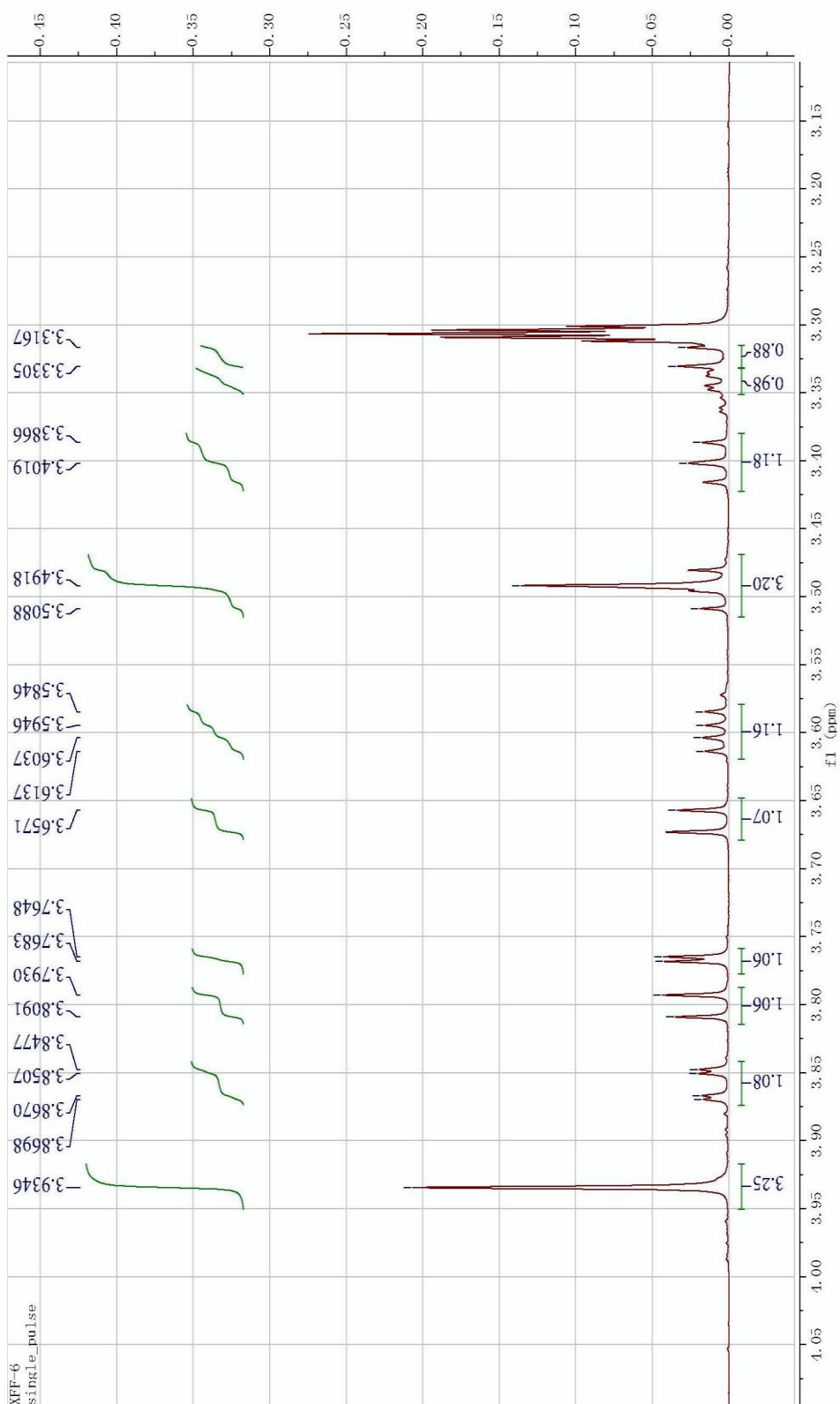


Figure S3: ¹H-NMR (500 MHz, MeOD) Spectrum of **1**(suffruticoside F) (δ 3.00-4.10 ppm)

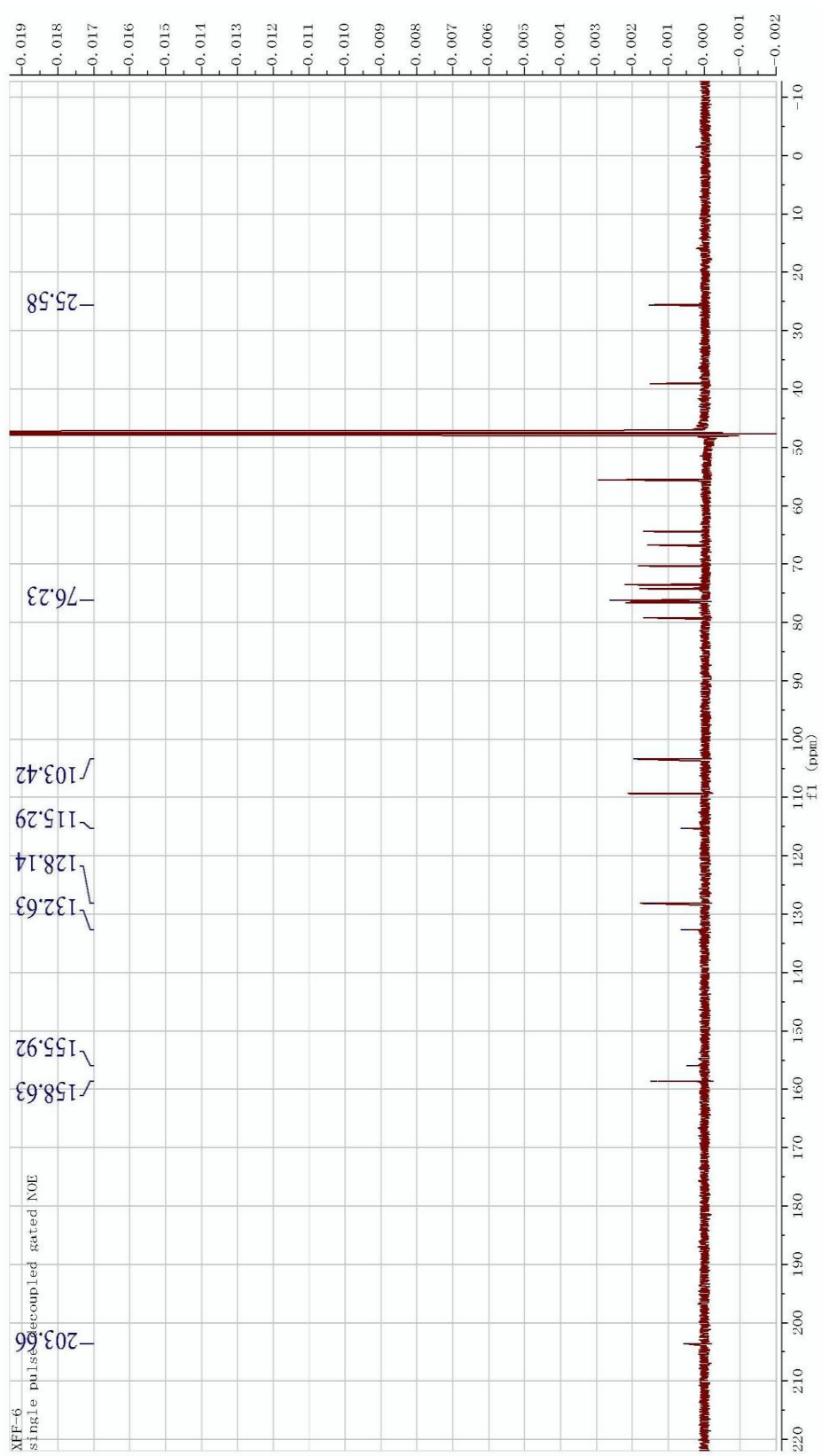


Figure S3: ^{13}C -NMR (150 MHz, MeOD) Spectrum of **1**(suffruticoside F)

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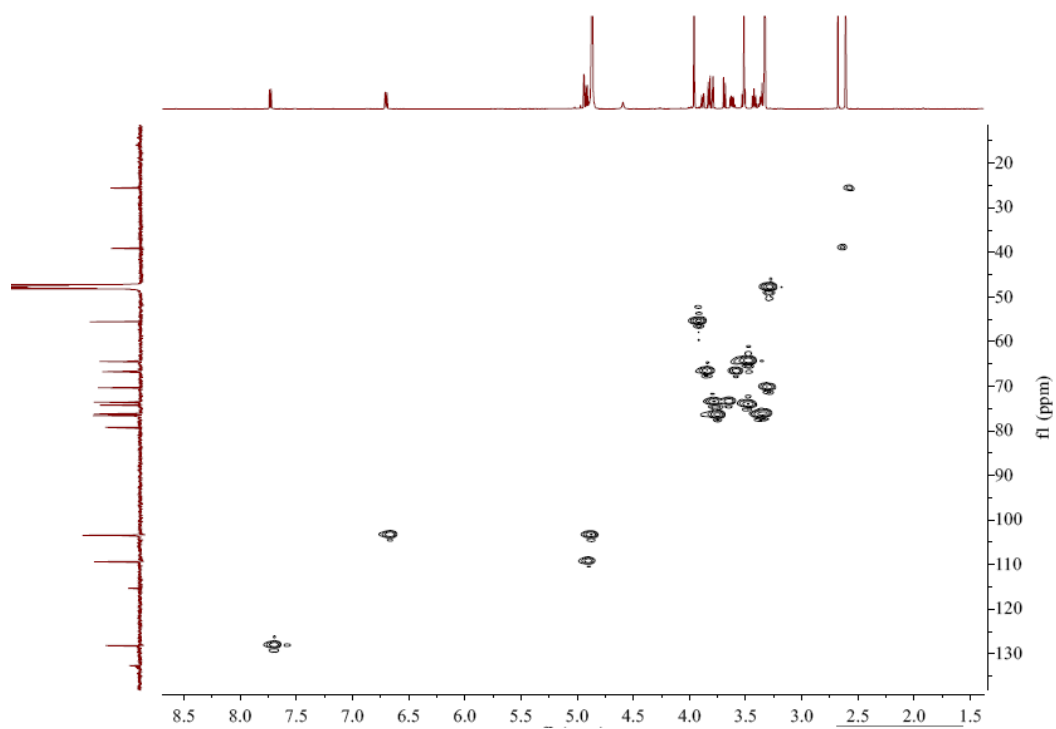


Figure S4: HSQC Spectrum of **1** (suffruticoside F)

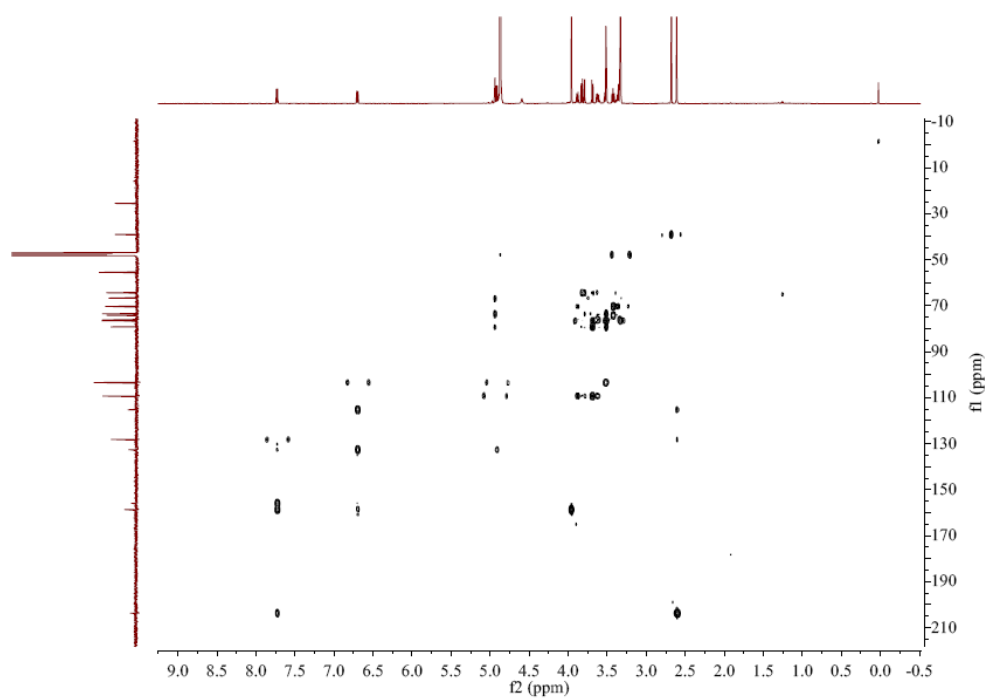


Figure S5: HMBC Spectrum of **1** (suffruticoside F)

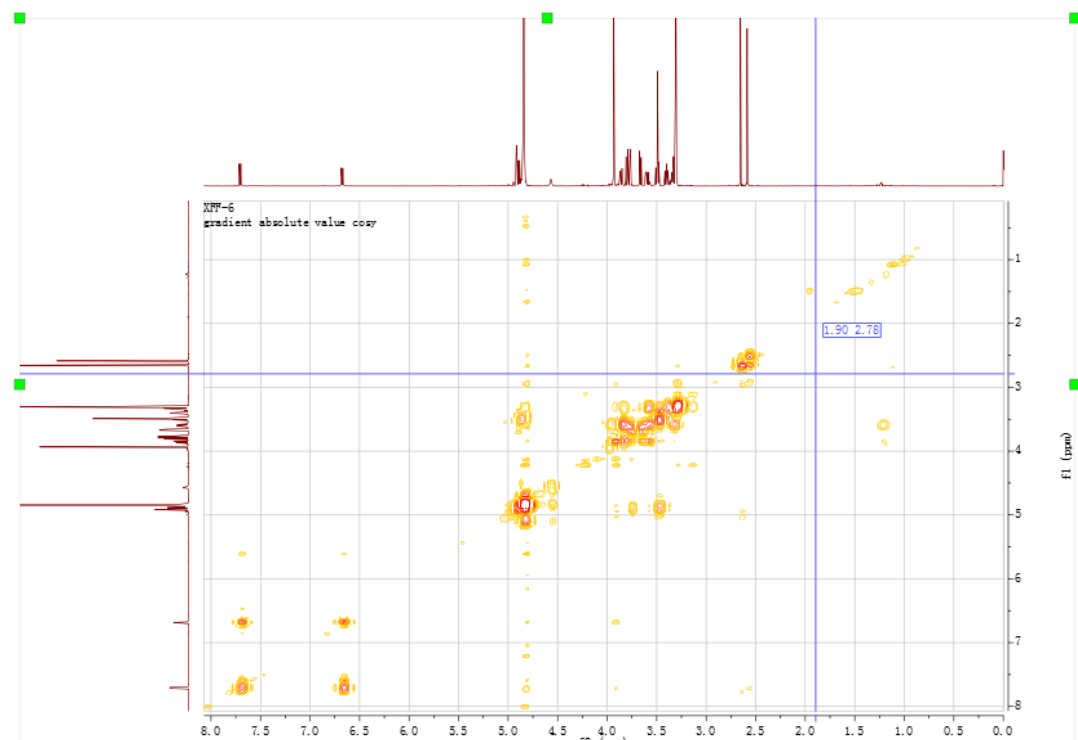
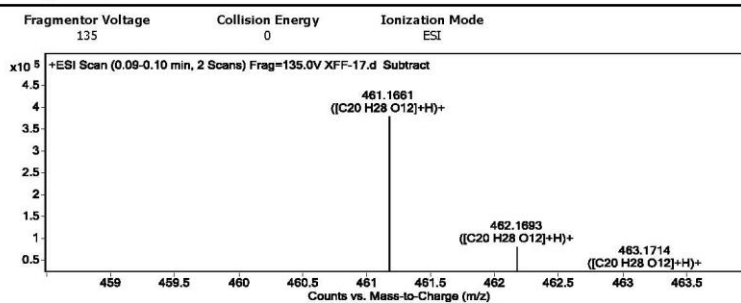


Figure S6: ^1H - ^1H COSY Spectrum of **1** (suffruticoside F)

Qualitative Analysis Report

Data Filename	XFF-17.d	Sample Name	XFF-17
Sample Type	Sample	Position	P1-D6
Instrument Name	Instrument 1	User Name	
Acq Method	s.m	Acquired Time	4/7/2021 1:58:23 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
153.0543	1	99436.89		
274.2741	1	49544.93		
315.1081	1	35117.43		
449.1636	1	49153.59		
461.1661	1	381992.34	C20 H28 O12	(M+H)+
462.1693	1	82304.79	C20 H28 O12	(M+H)+
483.1481	1	170172.06		
484.1514	1	35939.64		
943.3062	1	177757.41		
944.3091	1	78329.53		

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
C20 H28 O12	460.1581	461.1654	461.1661	-0.70	-1.52	7.0000

--- End Of Report ---

Figure S7: HR-ESI-MS Spectrum of 2 (suffruticoside G)

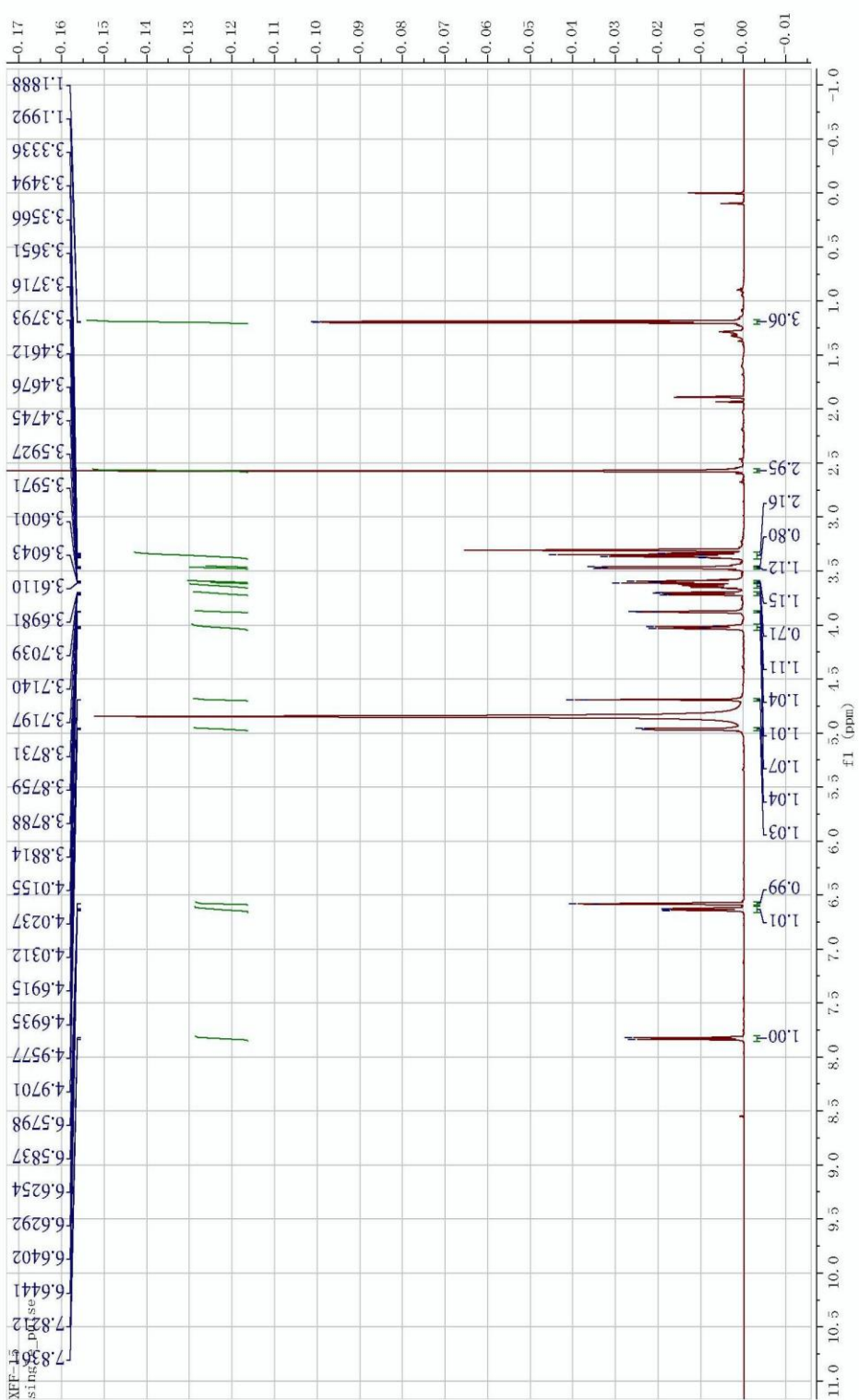


Figure S8: $^1\text{H-NMR}$ (500 MHz, MeOD) Spectrum of **2** (suffruticoside G)

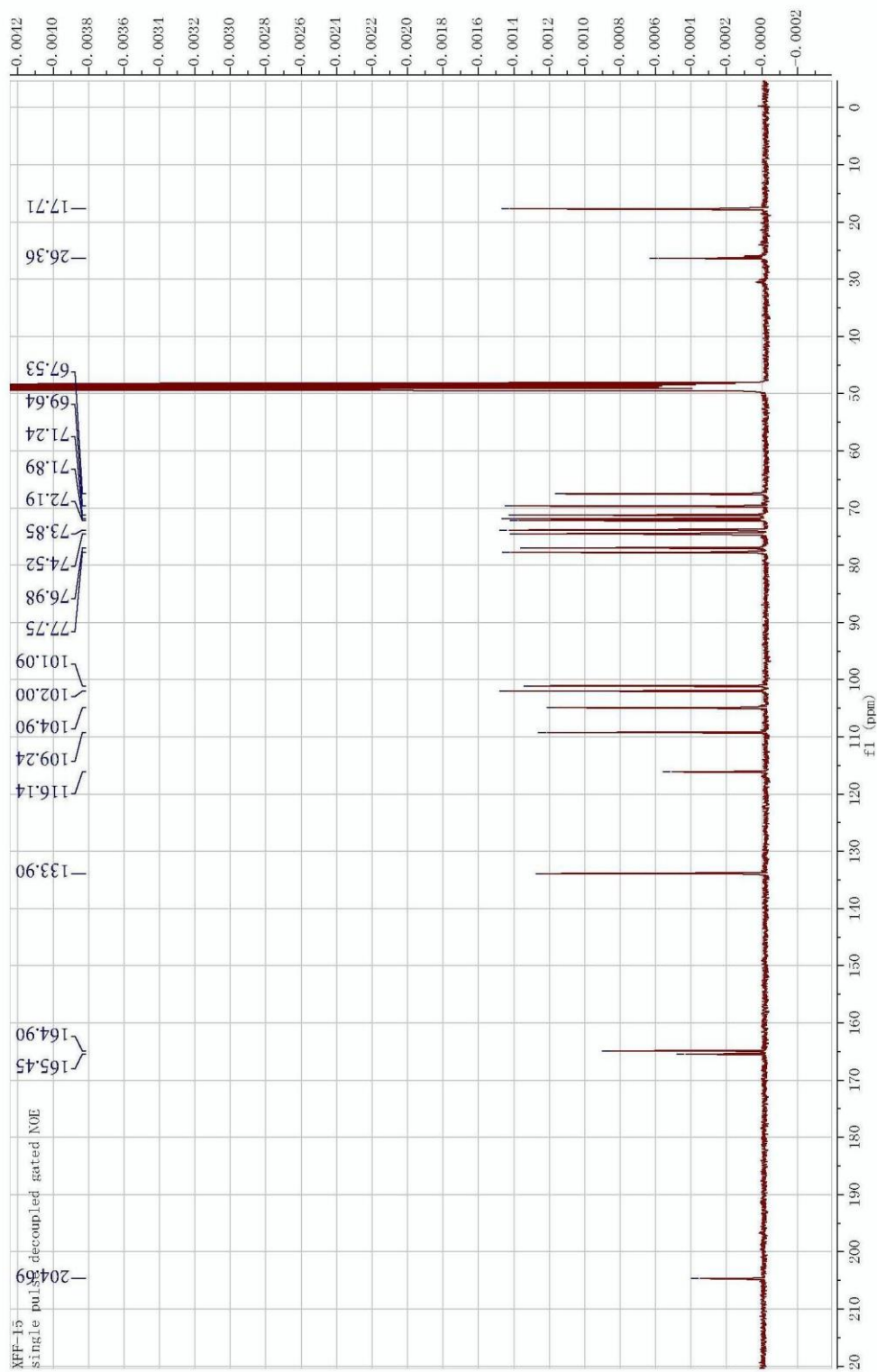


Figure S9: ^{13}C -NMR (125 MHz, MeOD) Spectrum of **2** (suffruticoside G)

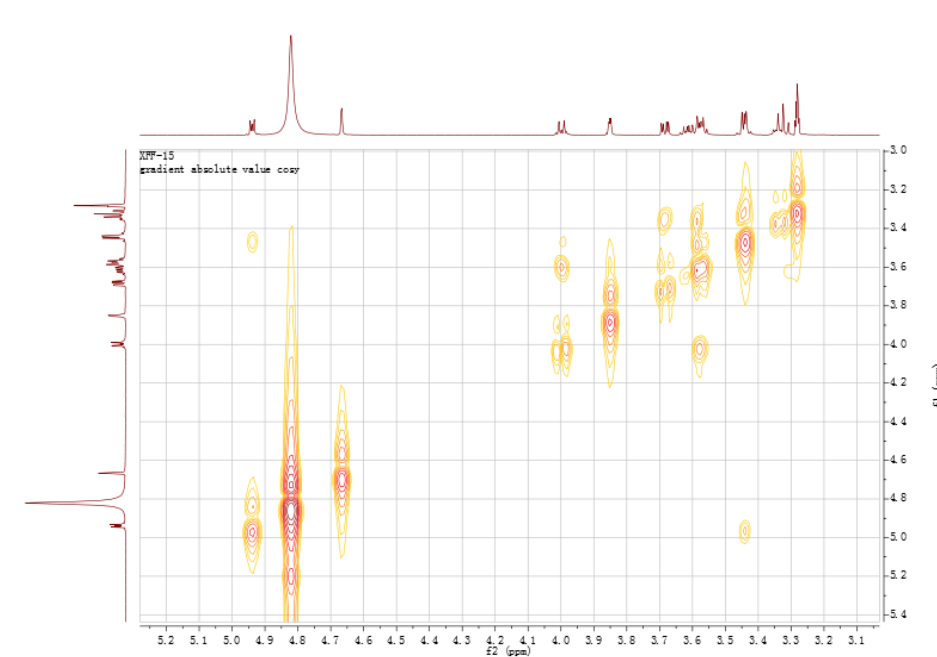


Figure S10: ^1H - ^1H COSY Spectrum of **2** (suffruticoside G)

Table S1 : The ¹H- and ¹³C-NMR data of compound **1** (CD₃OD, 600/150MHz)

Position	δ_C	δ_H	HMBC (H→C)
1	115.3	-	
2	155.9	-	
3	132.6	-	
4	158.6	-	
5	103.4	6.67 (1H, <i>d</i> , 9.0)	C-1, C-3, C-4
6	128.1	7.70 (1H, <i>d</i> , 9.0)	C-2, C-4, C-7
7	203.7	-	
8	25.6	2.59 (3H, <i>s</i>)	C-1, C-7
OCH ₃	55.6	3.93 (3H, <i>s</i>)	C-4
1'	103.4	4.89 (1H, <i>d</i> , 7.8)	C-3
2'	74.2	3.49 (1H, <i>dd</i> , 9.2, 7.8)	C-1'
3'	76.5	3.40 (1H, <i>t</i> , 9.2)	C-2', C-4'
4'	70.3	3.32 (1H, <i>t</i> , 8.0)	C-3'
5'	76.2	3.34 (1H, <i>ddd</i> , 9.6, 6.0, 1.8)	C-4'
6'	66.7	3.59 (1H, <i>dd</i> , 11.2, 6.0)	C-1'', C-5''
		3.86 (1H, <i>dd</i> , 11.2, 1.8)	C-1''
1''	109.3	4.92 (1H, <i>d</i> , 2.1)	C-6', C-3'', C-5''
2''	76.6	3.76 (1H, <i>d</i> , 2.1)	C-4''
3''	79.2	-	
4''	64.3	3.50 (2H, <i>s</i>)	C-2'', C-3'', C-5''
5''	73.6	3.79 (1H, <i>d</i> , 9.6)	C-4''
		3.66 (1H, <i>d</i> , 9.6)	C-2'', C-3'', C-1''