

S1 HRTOFMS of brachyantheraoside A₇ (**4**)

S2 ¹H NMR spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (**4**)

S3 ¹³C NMR spectrum (150 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (**4**)

S4 HSQC (600 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (**4**)

S5 HMBC spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (**4**)

S6 HRTOFMS of brachyantheraoside A₈ (**5**)

S7 ¹H NMR spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)

S8 ¹³C NMR spectrum (150 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)

S9 HSQC spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)

S10 HMBC spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)

S11 TOCOSY spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\20131218-CEYANG\PPL-1_1-a,6_01_2470.d

Acquisition Date 12/18/2013 1:49:23 PM

Method 20131026_ceyang.m

Operator Bruker Customer

Sample Name PPL-1

Instrument / Ser# micrOTOF-Q 125

Comment

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.

Tolerance

Charge

Formula, max.

Minimum

Maximum

Measured m/z

Electron Configuration

Check Valence

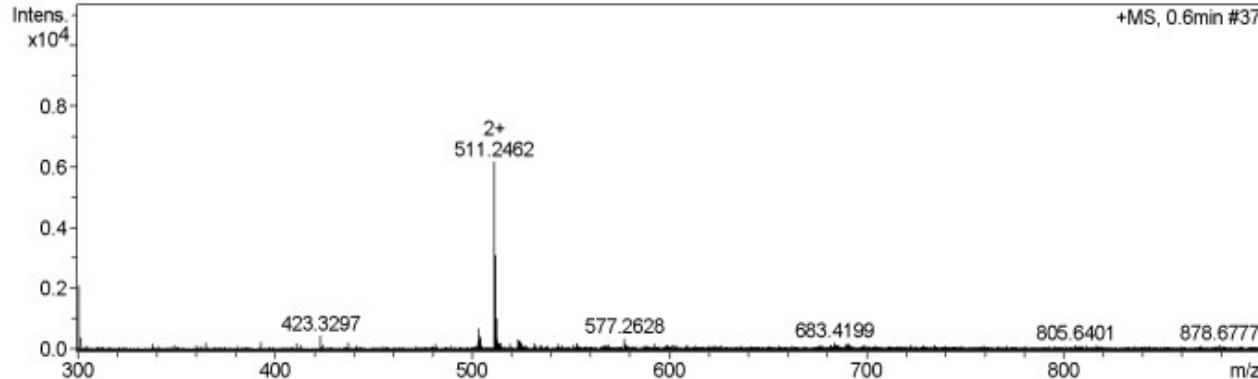
Minimum

Maximum

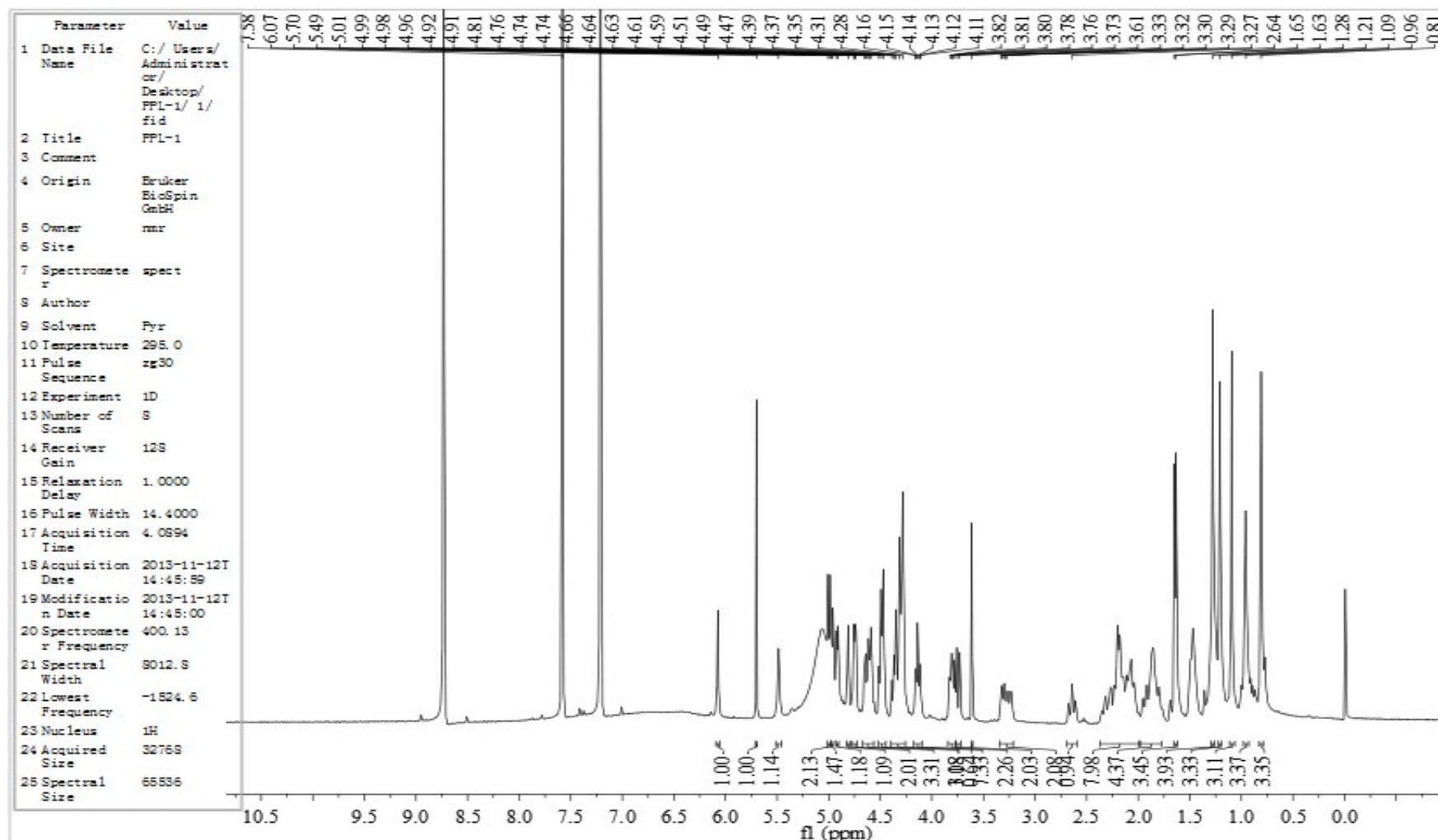
Nitrogen Rule

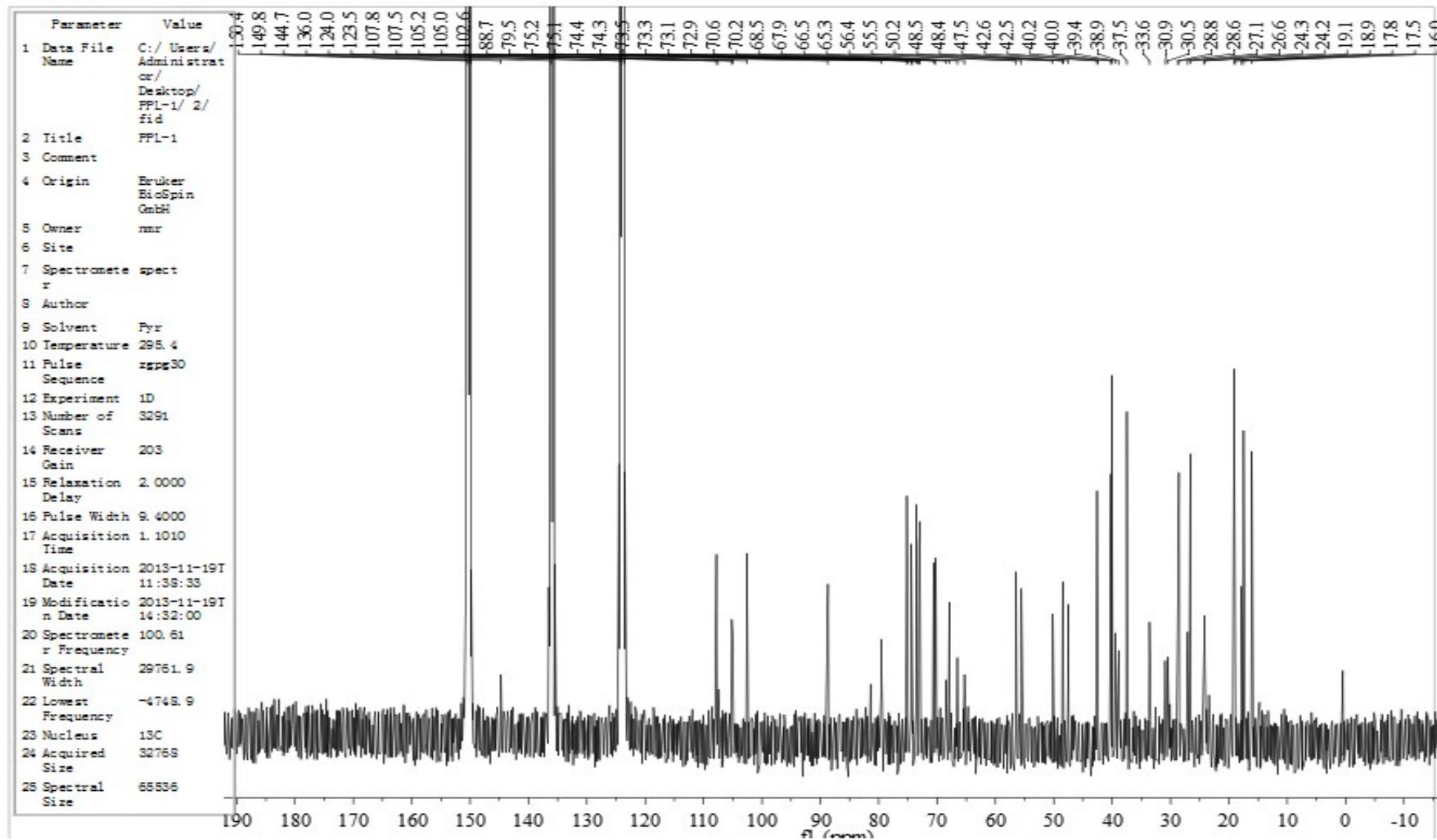
Filter H/C Ratio

Estimate Carbon

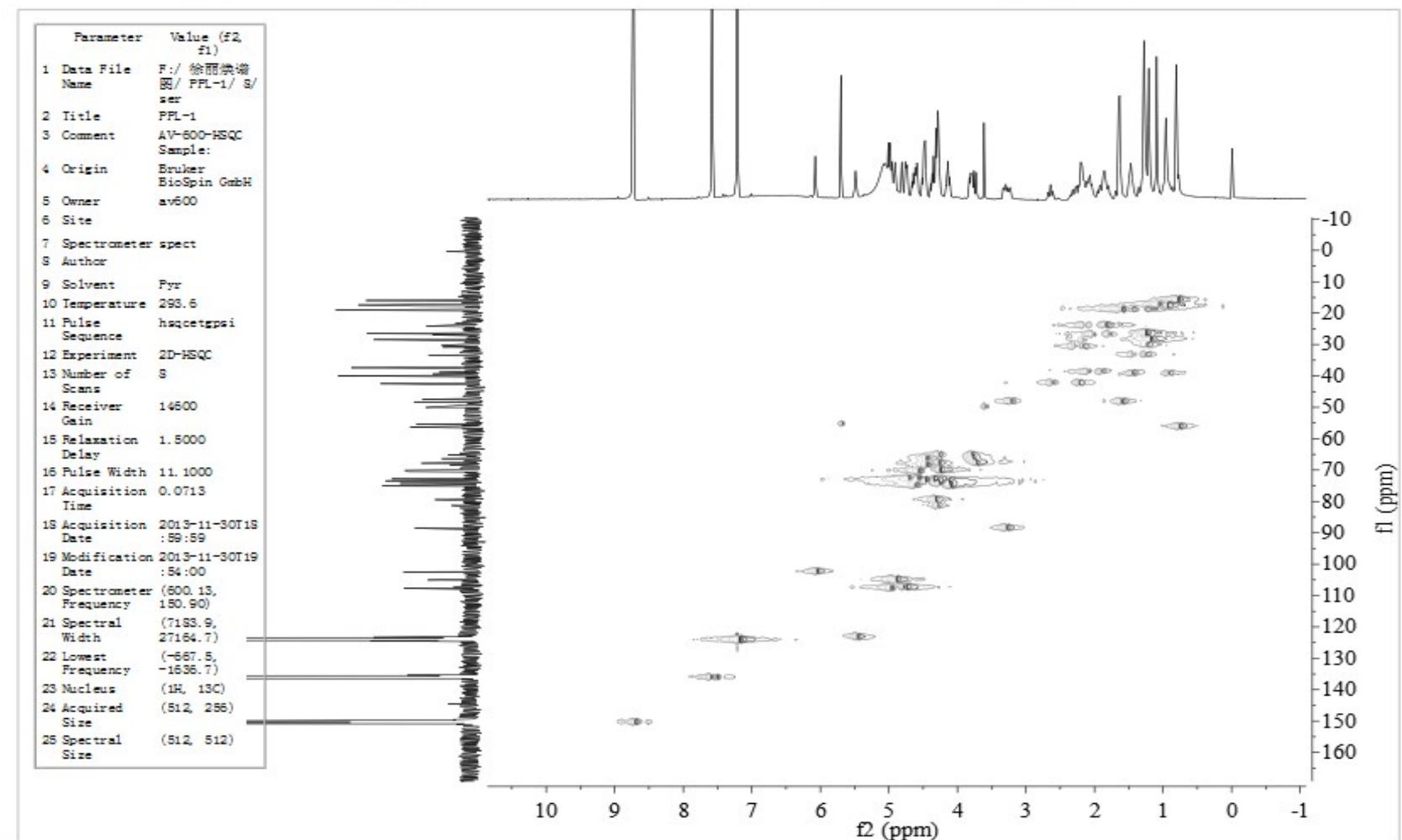


S1 HRTOFMS of brachyantheraoside A₇ (4)

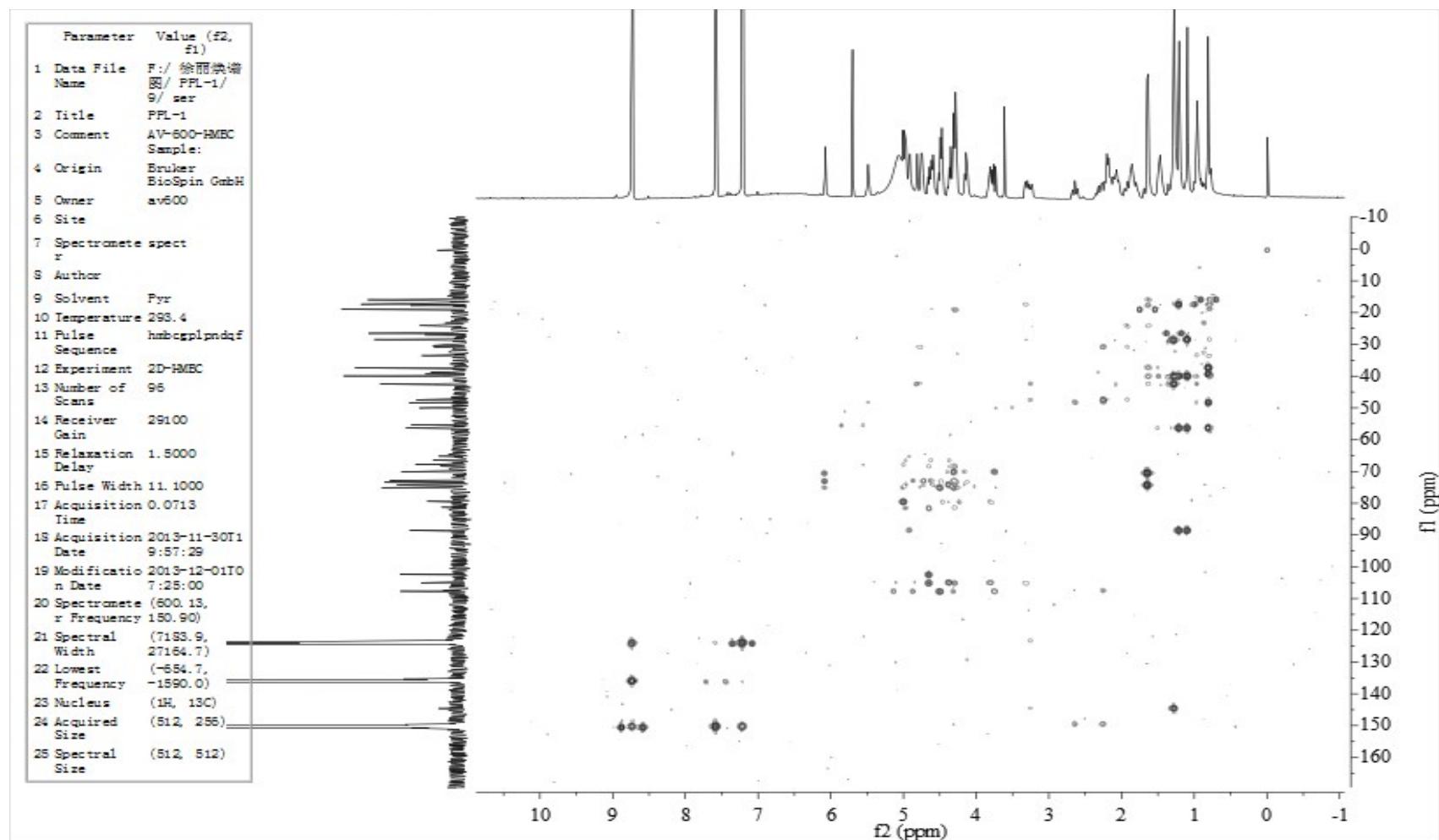




S3 ¹³C NMR spectrum (150 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (4)



S4 HSQC (600 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (**4**)



S5 HMBC spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₇ (**4**)

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\20131218-CEYANG\HA18C-5.d
Method tune_high_pos.m
Sample Name HA18C-5
Comment

Acquisition Date 12/18/2013 5:25:08 PM
Operator Bruker Customer
Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

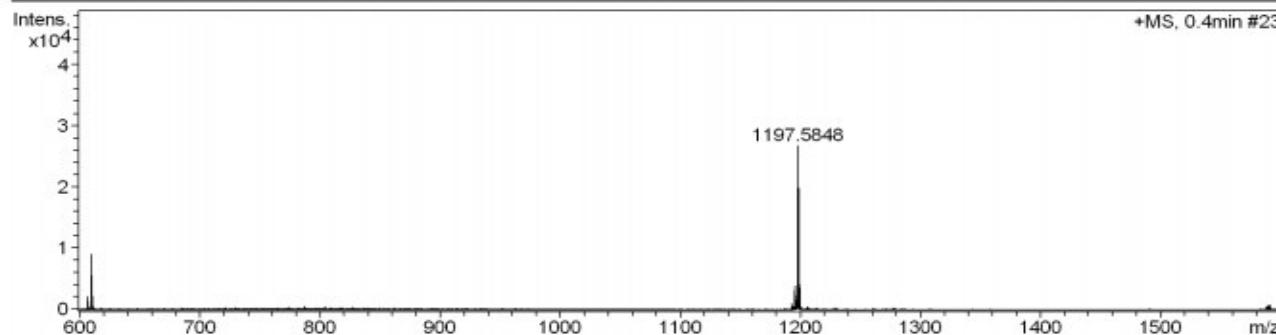
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min. C 57 H 90 O25

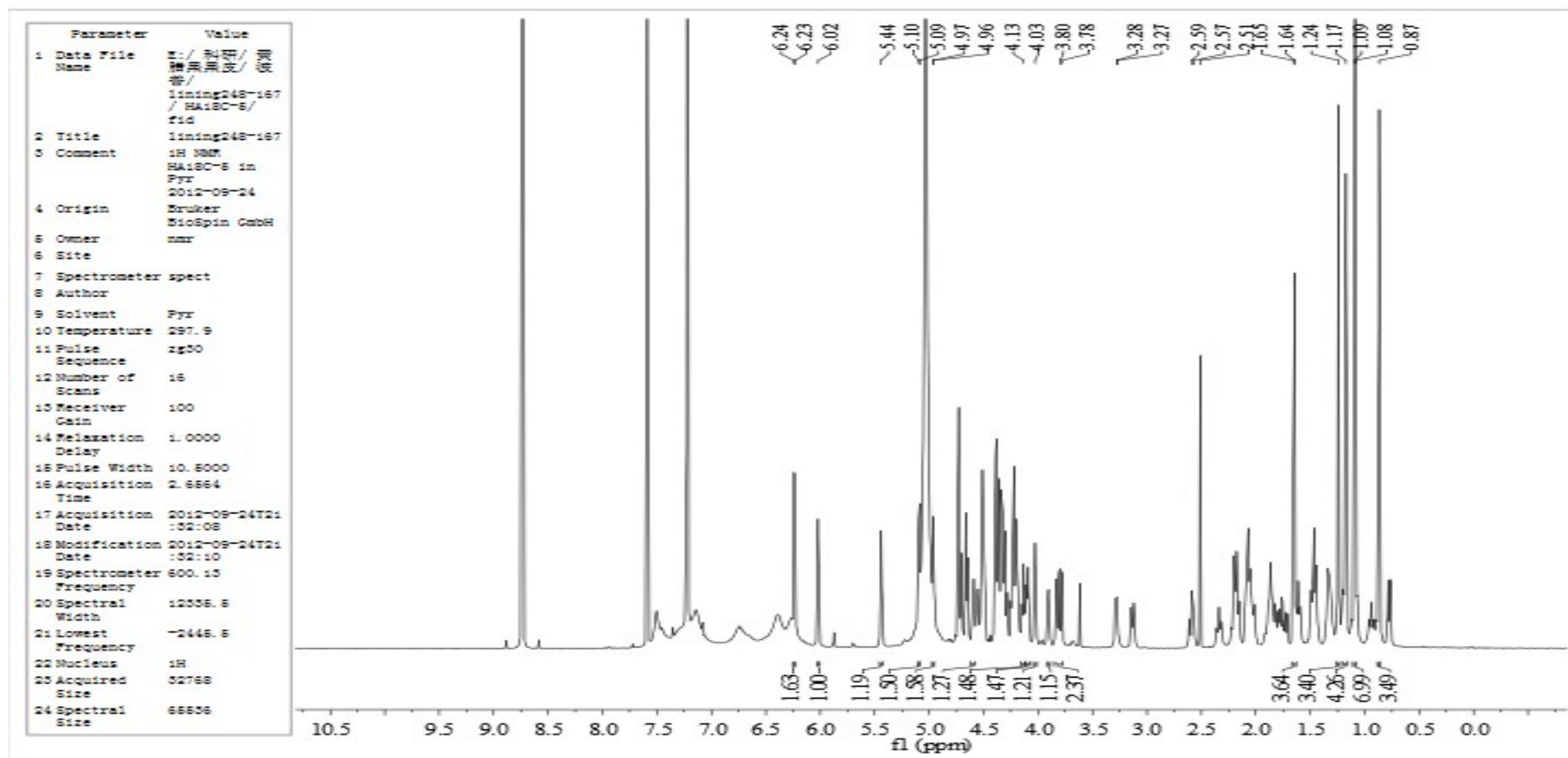
Formula, max.

Measured m/z	1197.578	Tolerance	5	ppm	Charge	1
Check Valence	no	Minimum	0		Maximum	0
Nirogen Rule	no	Electron Configuration				
Filter H/C Ratio	no	Minimum	0		Maximum	3
Estimate Carbon	yes					

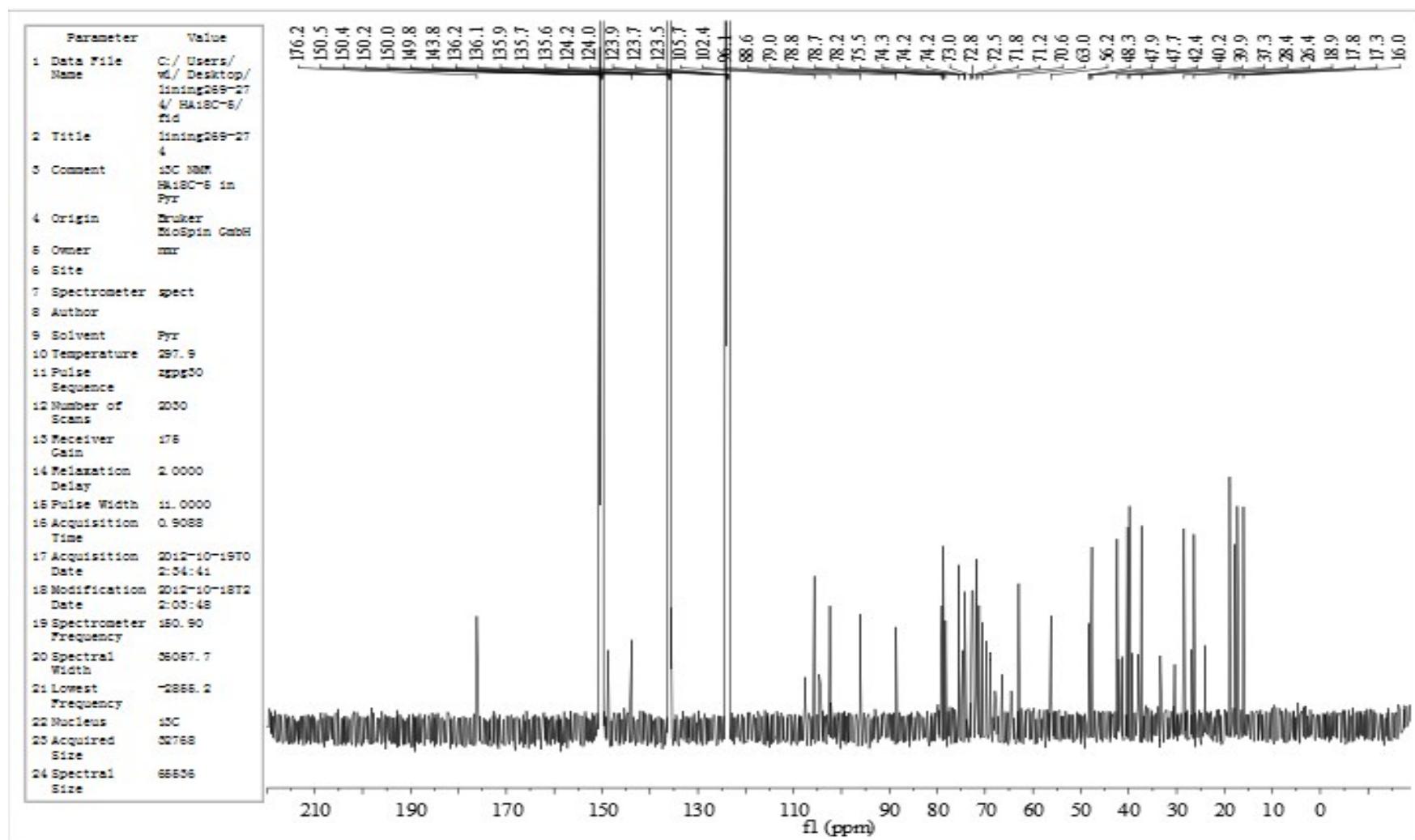


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 57 H 90 O25 Na1	0.021	1197.5771	-0.008	0.425	-0.007	14.50	ok	even

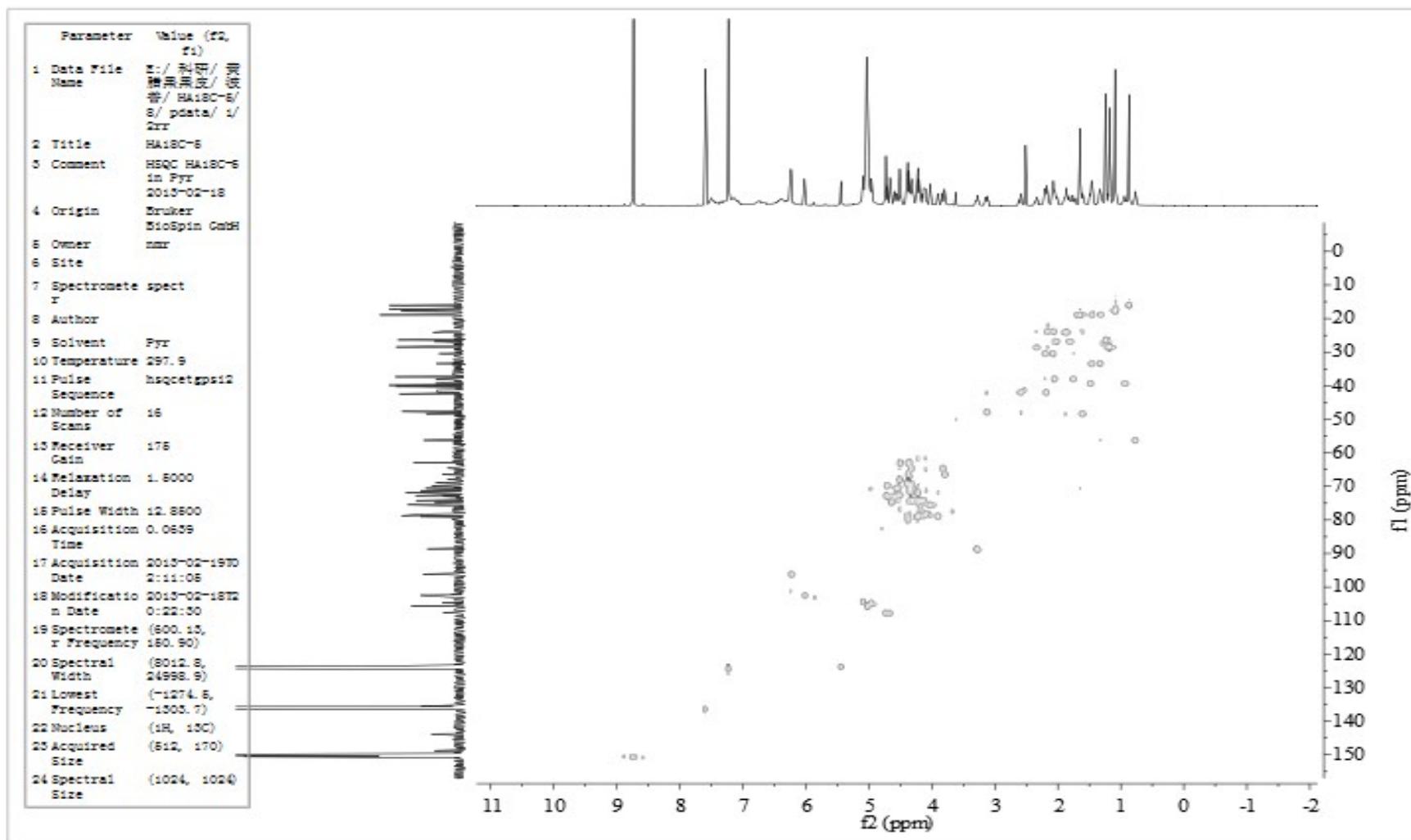
S6 HRTOFMS of brachyantheraoside A₈ (**5**)



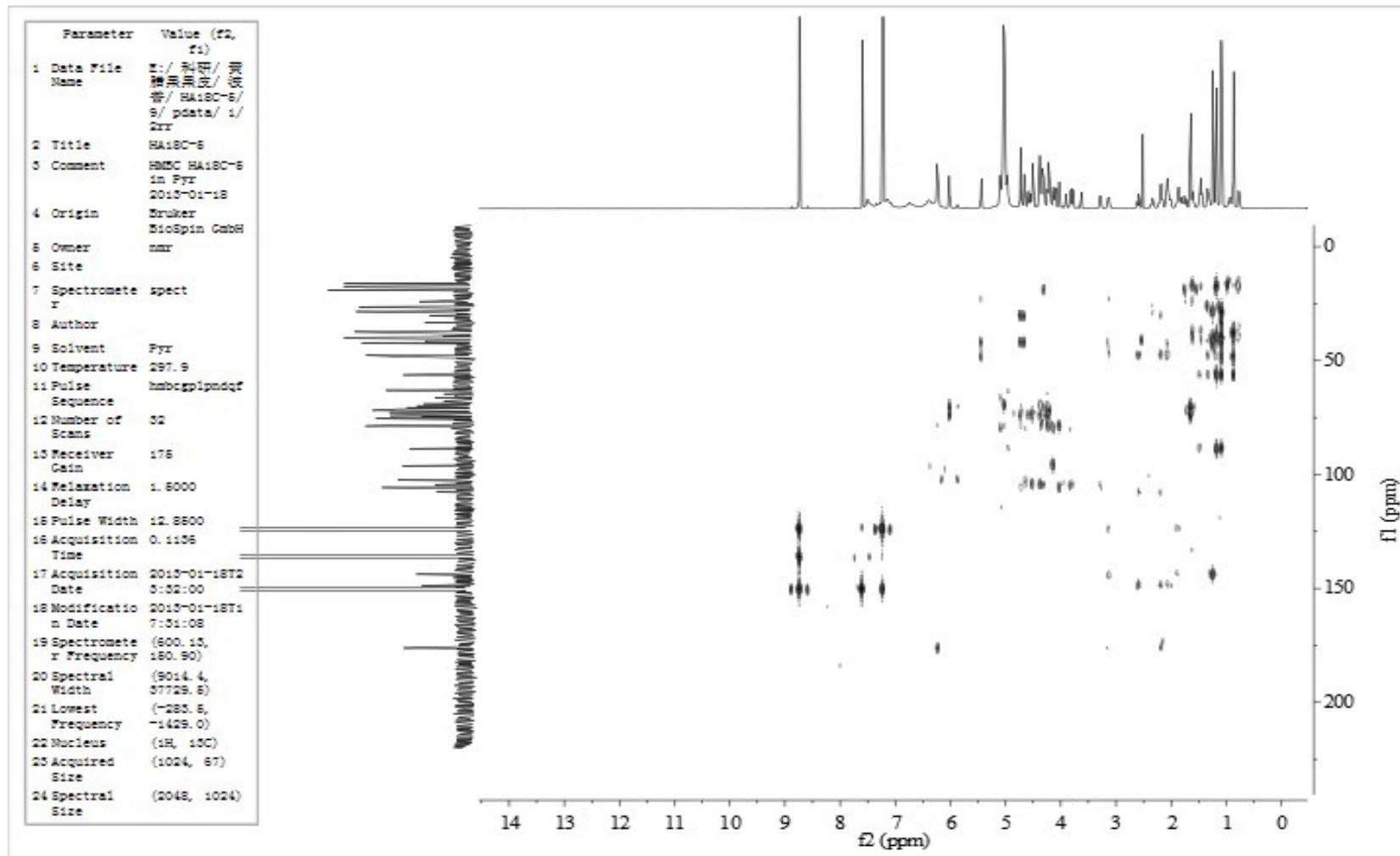
S7 ^1H NMR spectrum (600 MHz, pyridine- d_5) of brachyantheraoside A₈ (**5**)



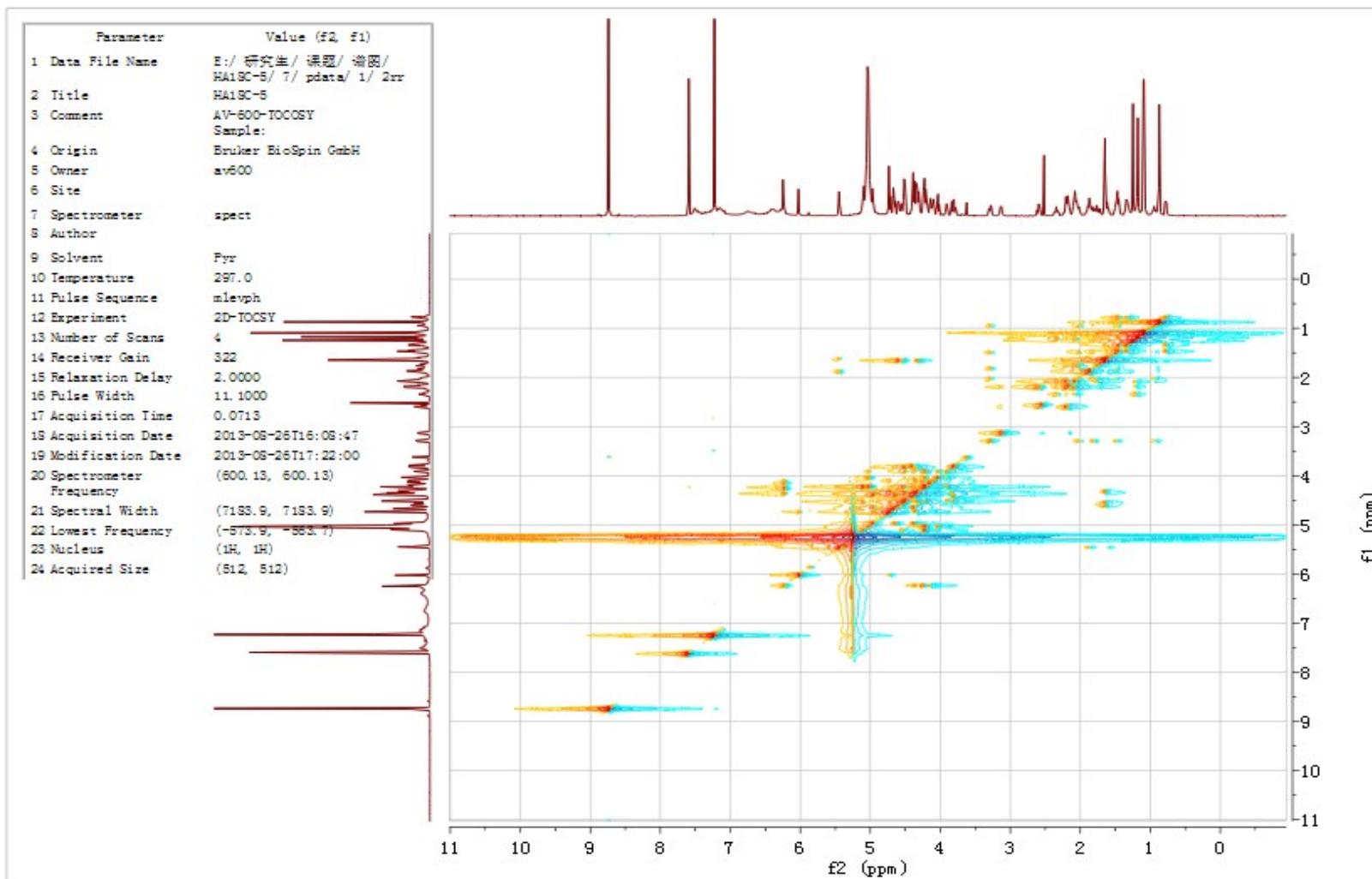
S8 ¹³C NMR spectrum (150 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)



S9 HSQC spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)



S10 HMBC spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)



S₁₁ TOCOSY spectrum (600 MHz, pyridine-*d*₅) of brachyantheraoside A₈ (**5**)