Electronic Supplementary Material (ESI) for RSC Advances.

Barrigenol triterpenes from the husks of *Xanthoceras sorbifolia* Bunge and their antitumor activities

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Figure S1. ^{1}H-NMR Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1) in C_5D_5N.

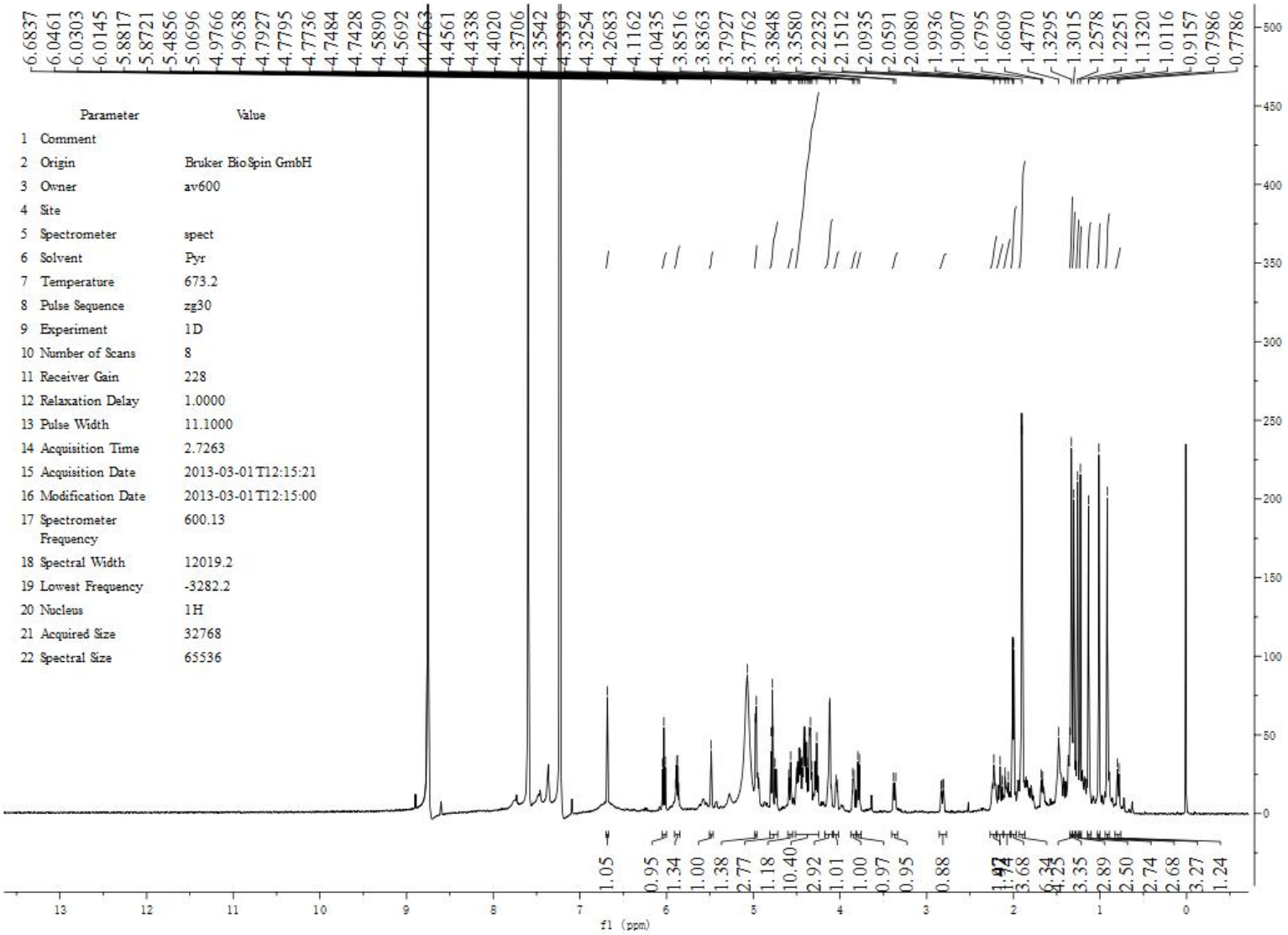


Figure S2. ^{13}C-NMR Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1) in C_5D_5N.

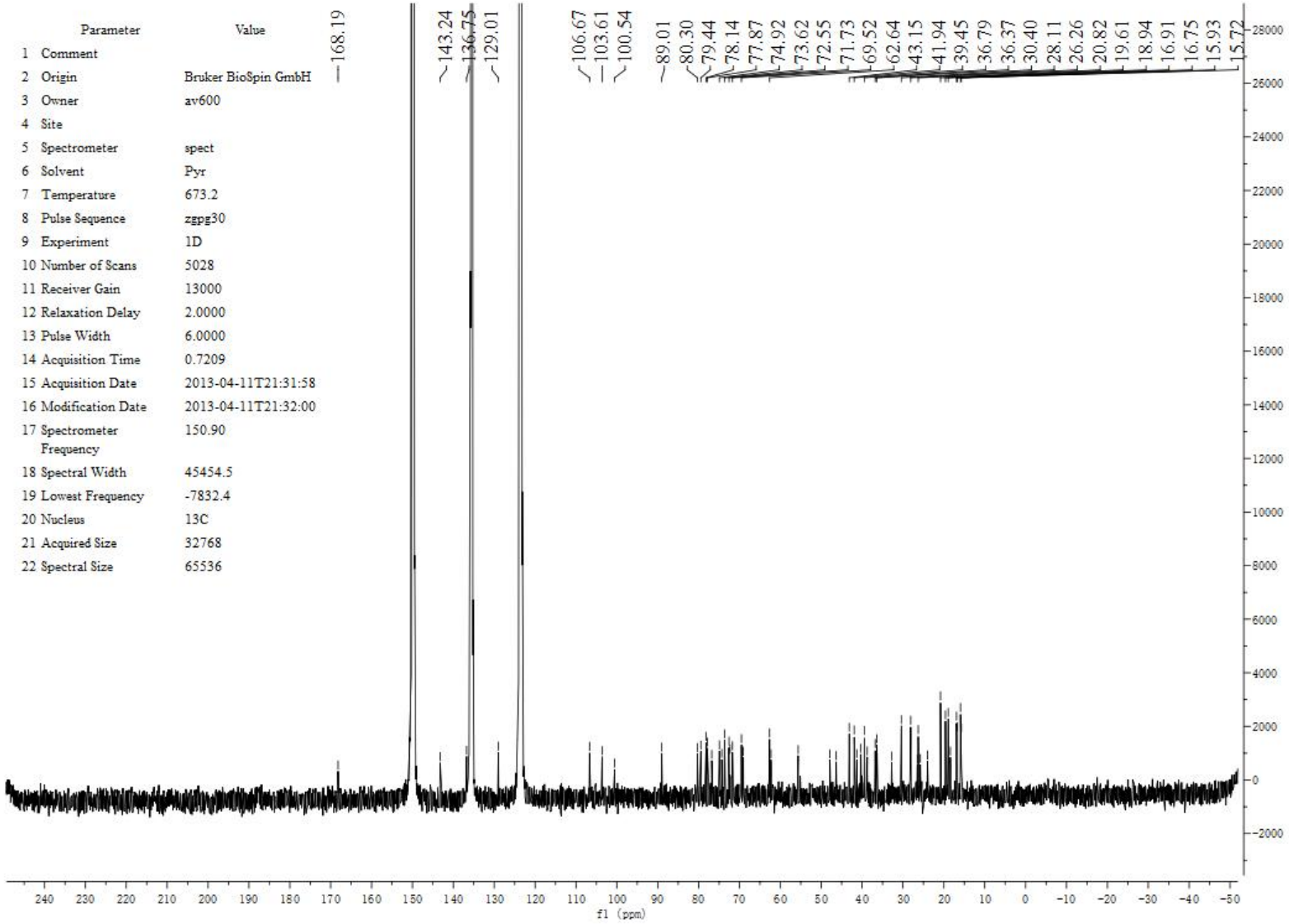


Figure S3. HR-ESI-MS Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1).

Mass Spectrum Molecular Formula Report

Analysis Info

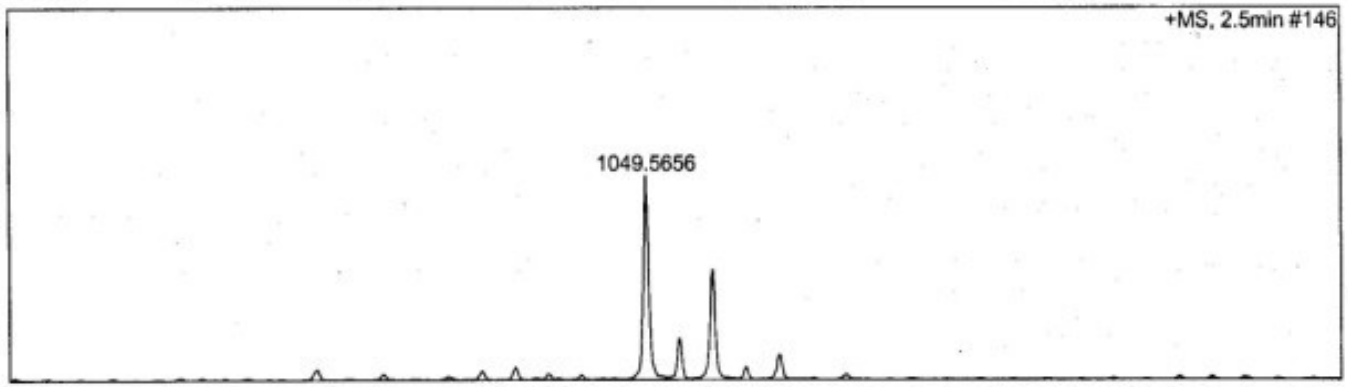
Analysis Name	D:\Data\20130428\3.1.d	Acquisition Date	4/28/2013 9:22:54 AM
Method	MA250-550POS.m	Operator	Bruker Customer
Sample Name	3.1	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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	600.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C53H86O19Na						
Formula, max.							
Measured m/z	1049.57	Tolerance	4	mDa	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
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 53 H 86 Na 1 O 19	0.281	1049.5656	-0.06	-0.06	-0.07	10.50	ok	even

Figure S4. HMBC Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1) in C_5D_5N.

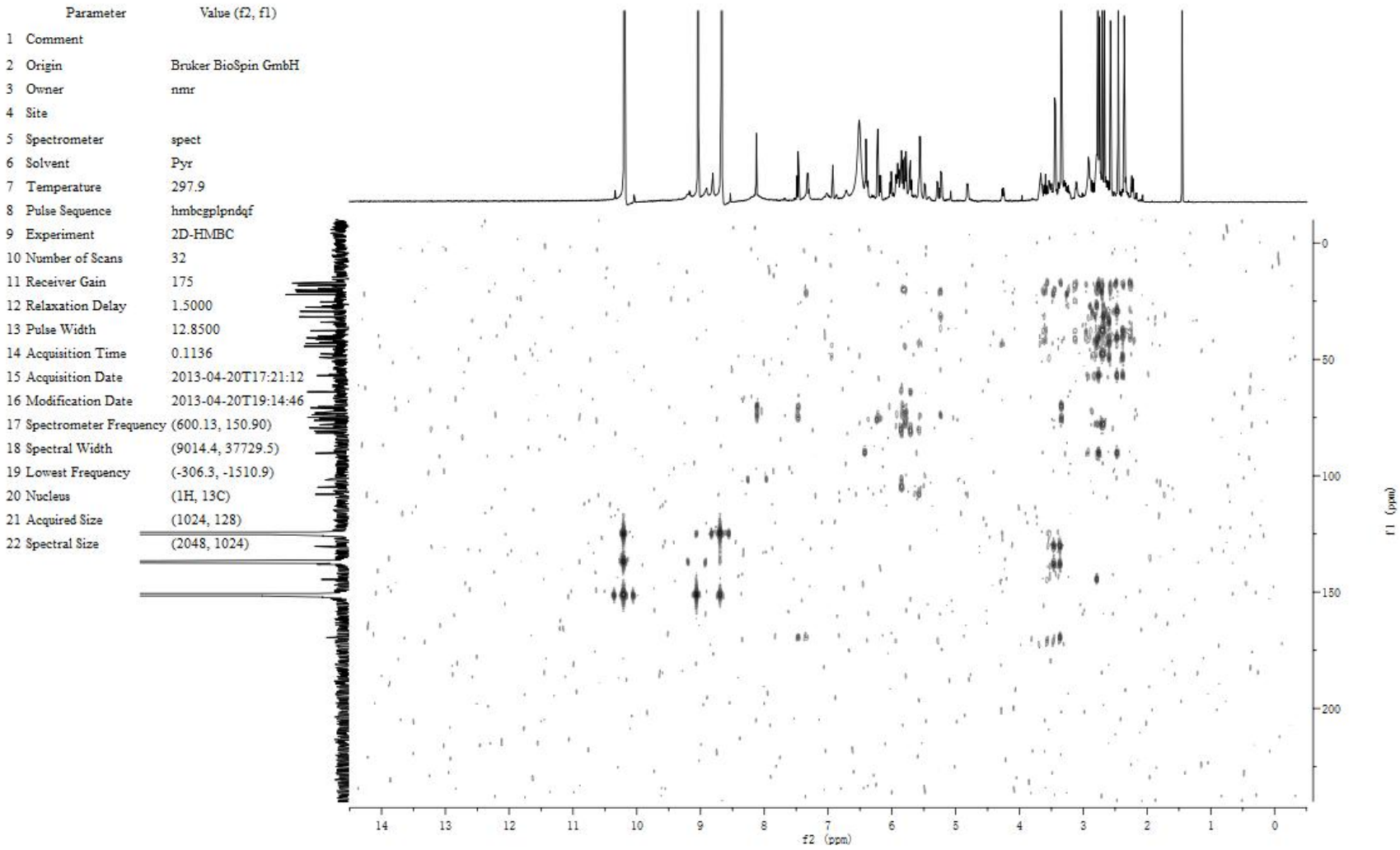


Figure S5. HSQC Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1) in C_5D_5N.

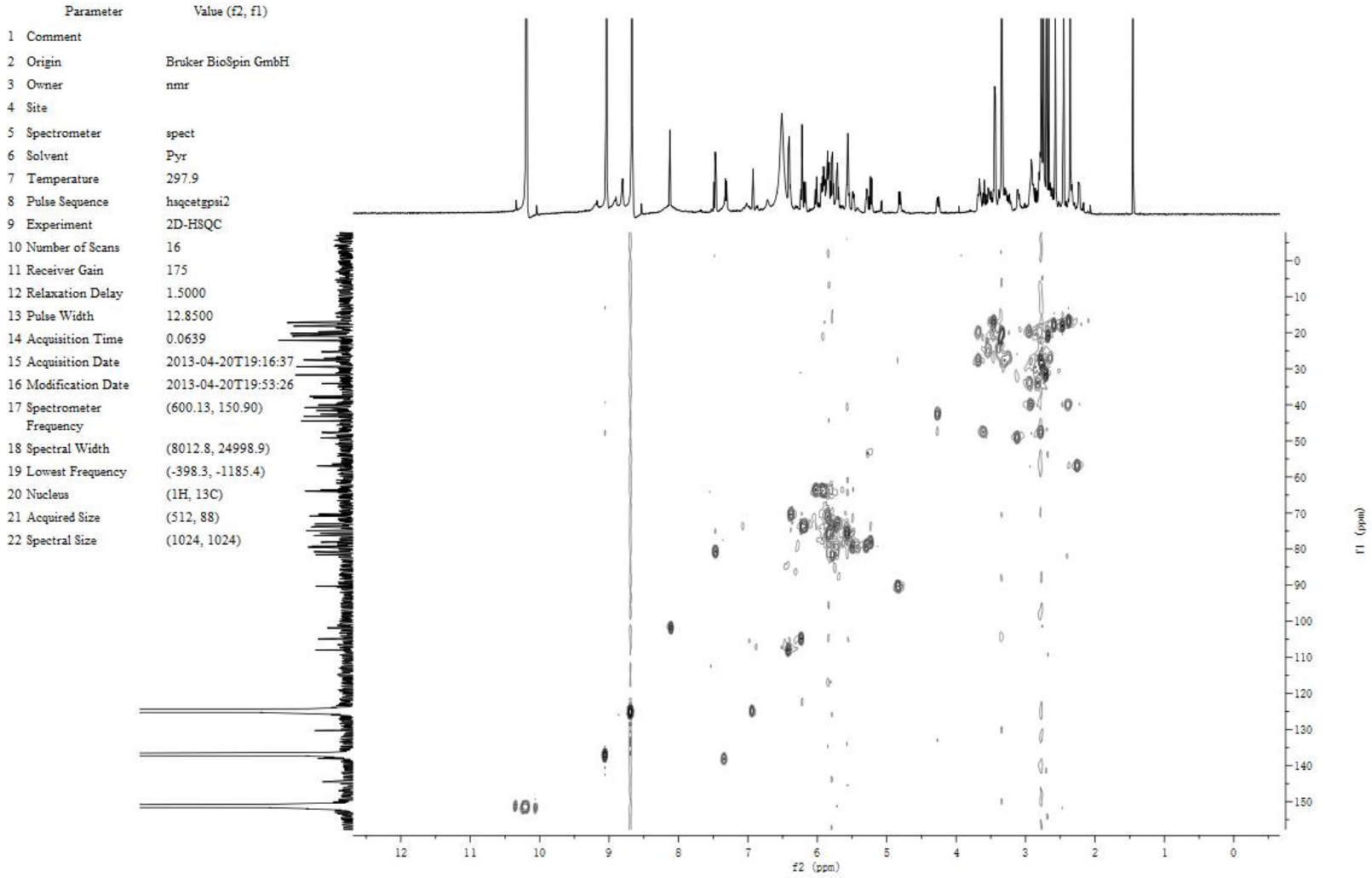


Figure S6. NOESY Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1) in C_5D_5N.

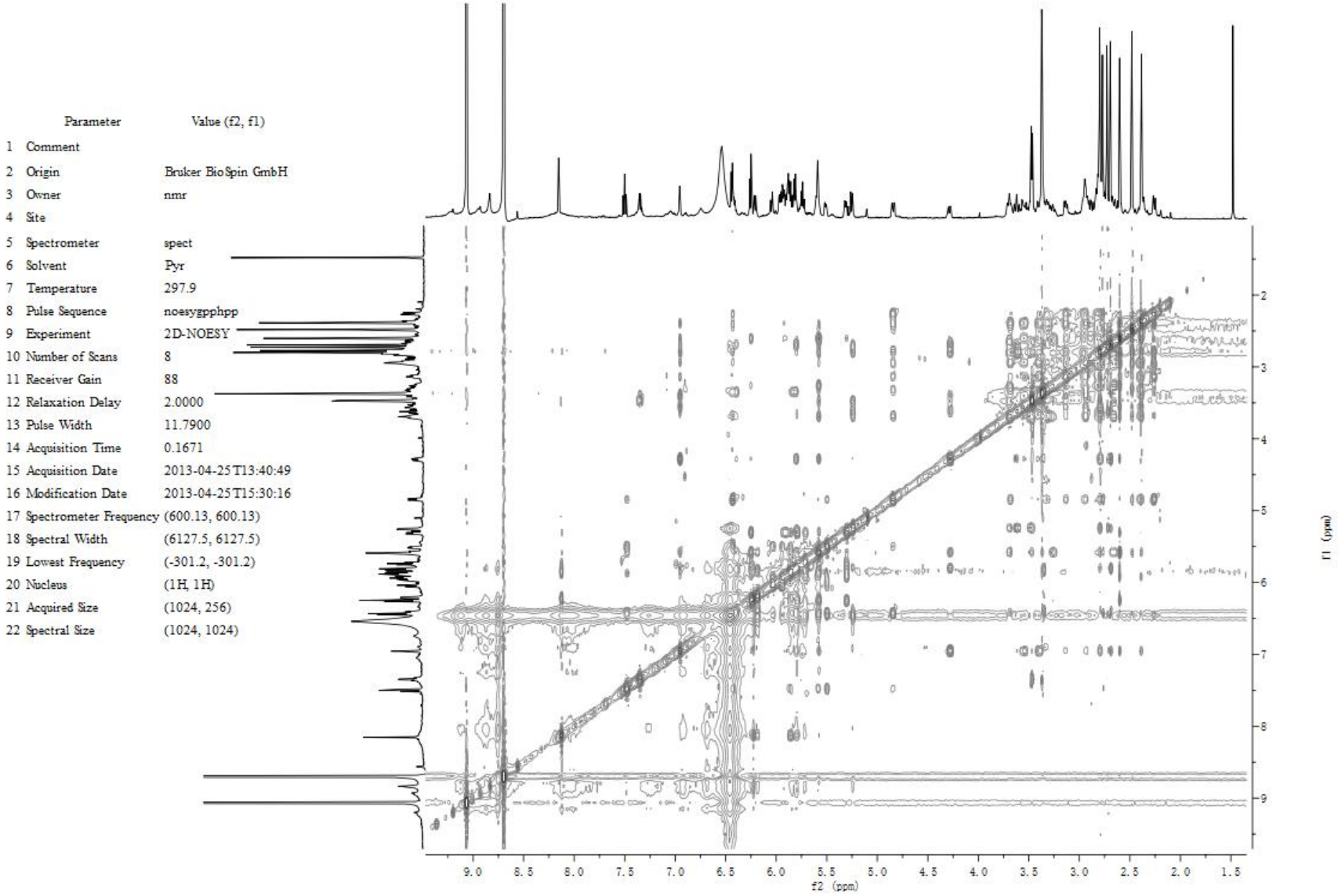
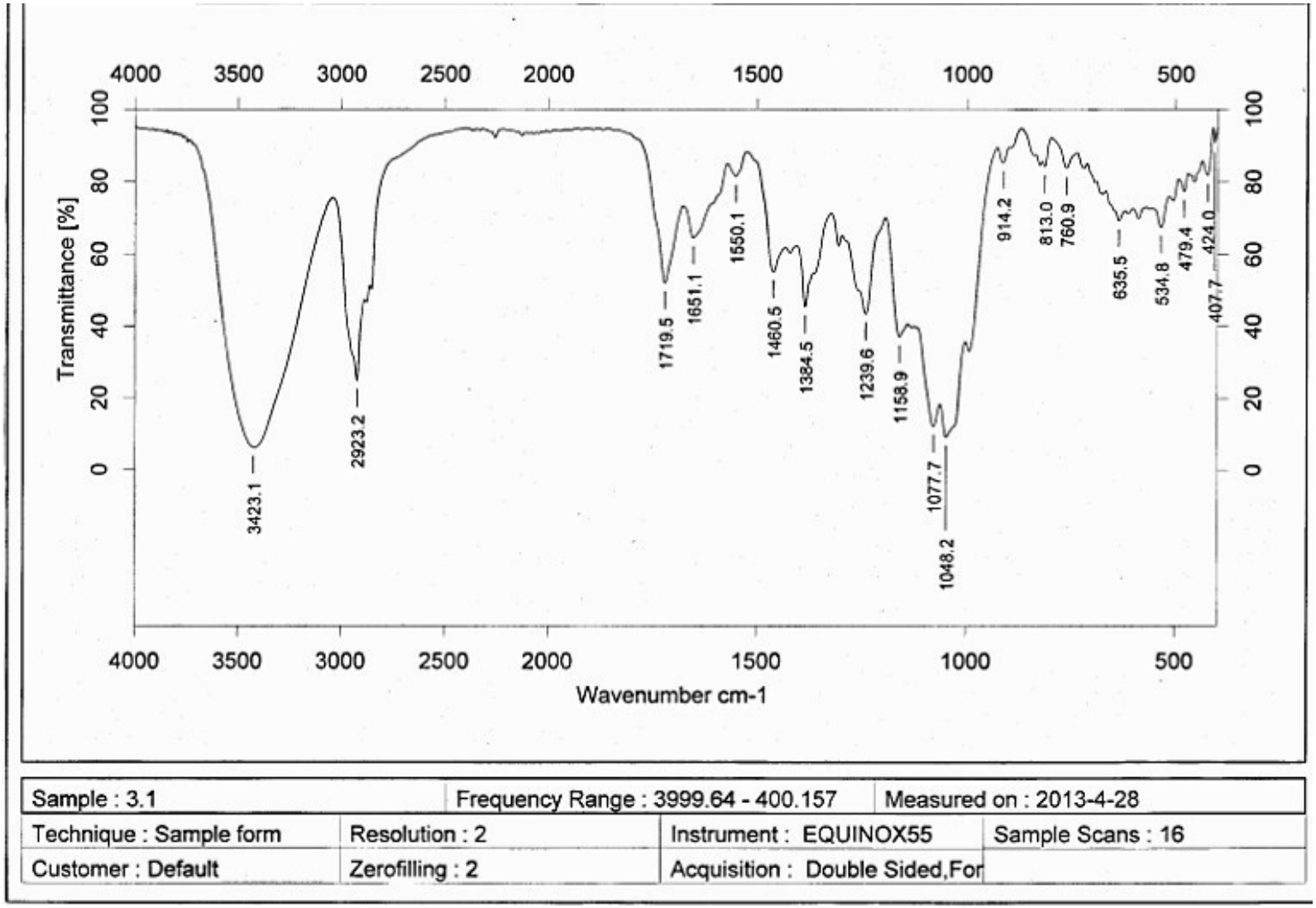


Figure S7. IR Spectrum of 3-*O*-(3′-*O*-angeloyl)-*β*-*D*-glucopyranosyl-28-*O*- [*α*-*L*-rhamnopyranosyl(1→2)]-*β*-*D*-glucopyranosyl-3*β*, 21*β*, 22*α*, 28-tetrahydroxy-olean-12-ene (1).



Sample : 3.1	Frequency Range : 3999.64 - 400.157	Measured on : 2013-4-28	
Technique : Sample form	Resolution : 2	Instrument : EQUINOX55	Sample Scans : 16
Customer : Default	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S8. ^{1}H-NMR Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2) in C_5D_5N.

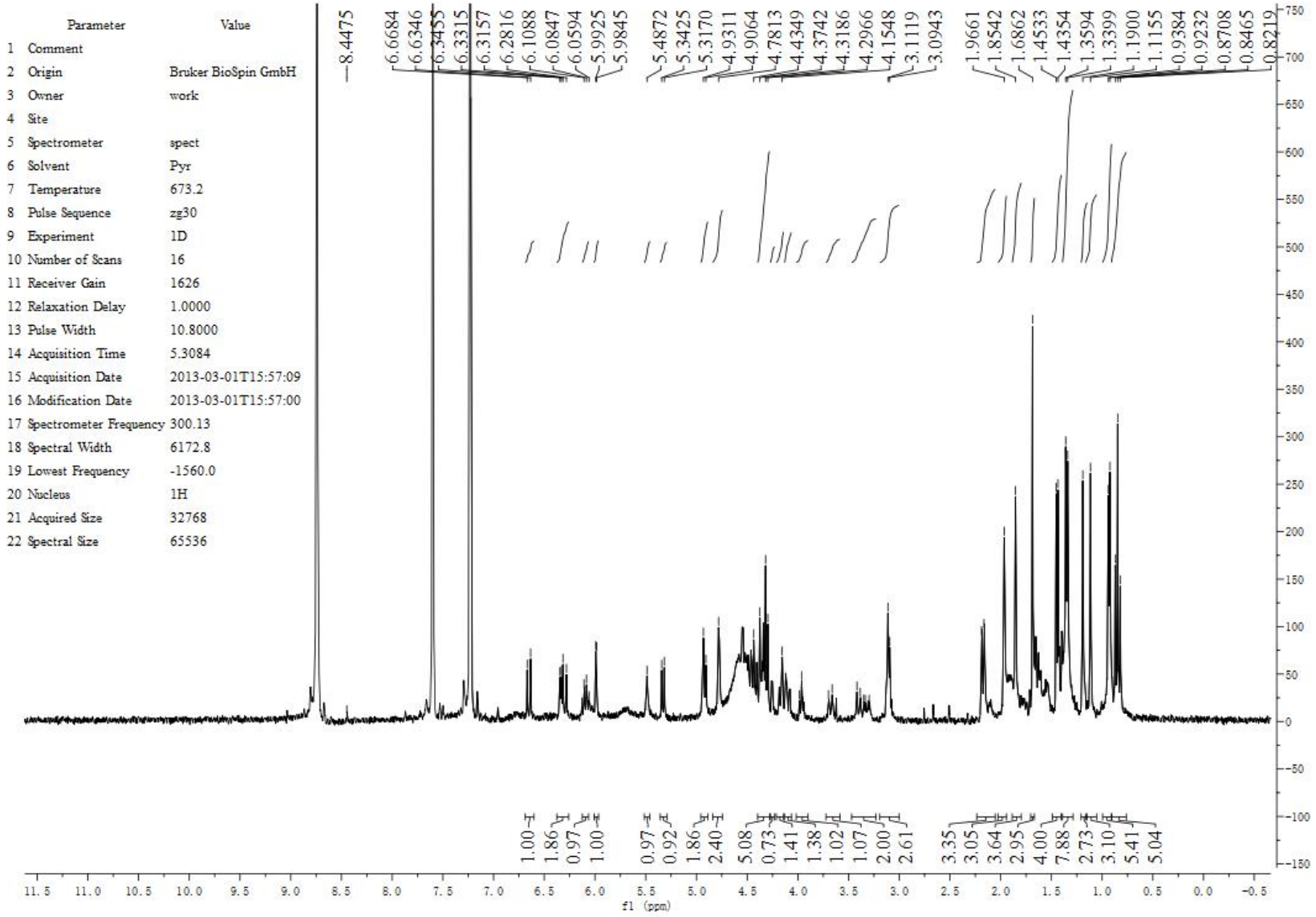


Figure S9. ^{13}C-NMR Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2)in C_5D_5N.

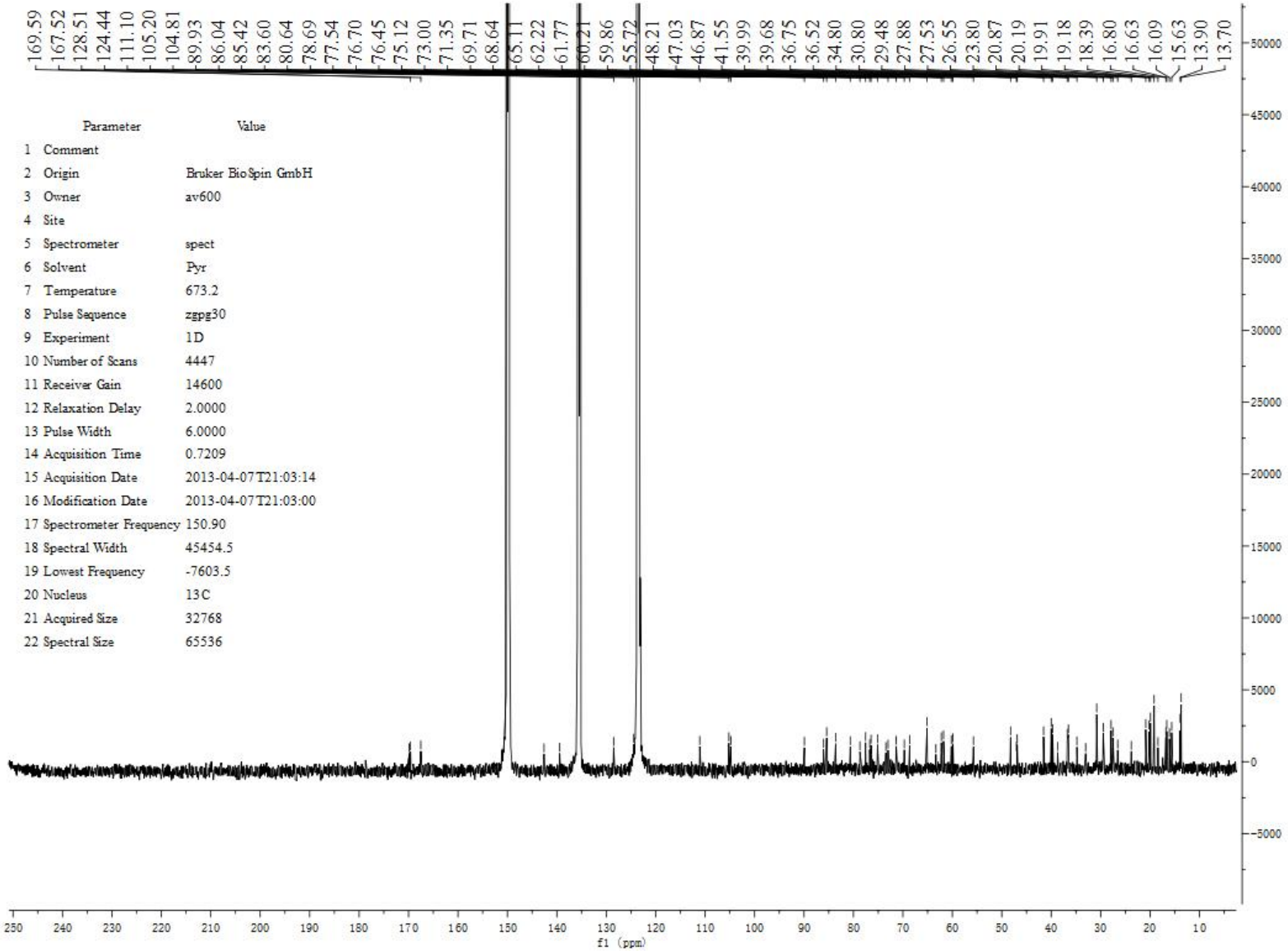


Figure S10. HR-ESI-MS Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2).

Mass Spectrum Molecular Formula Report

Analysis Info

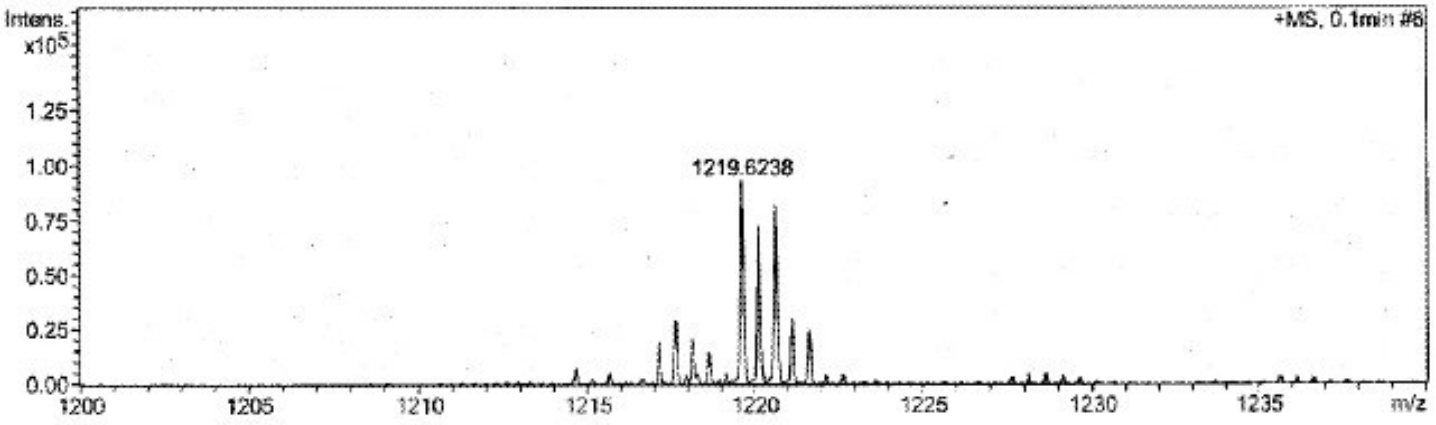
Analysis Name	D:\Data\20130428\16.5--.d	Acquisition Date	4/28/2013 9:16:41 AM
Method	MA250-550POS.m	Operator	Bruker Customer
Sample Name	16.5--	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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.	C61H96O23Na						
Formula, max.							
Measured m/z	1219.62	Tolerance	4	mDa	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nitrogen Rule	no	Electron Configuration	both				
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 61 H 96 Na 1 O 23	0.330	1219.6235	-0.27	-0.27	-0.33	13.50	ok	even

Figure S11. HMBC Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2) in C_5D_5N.

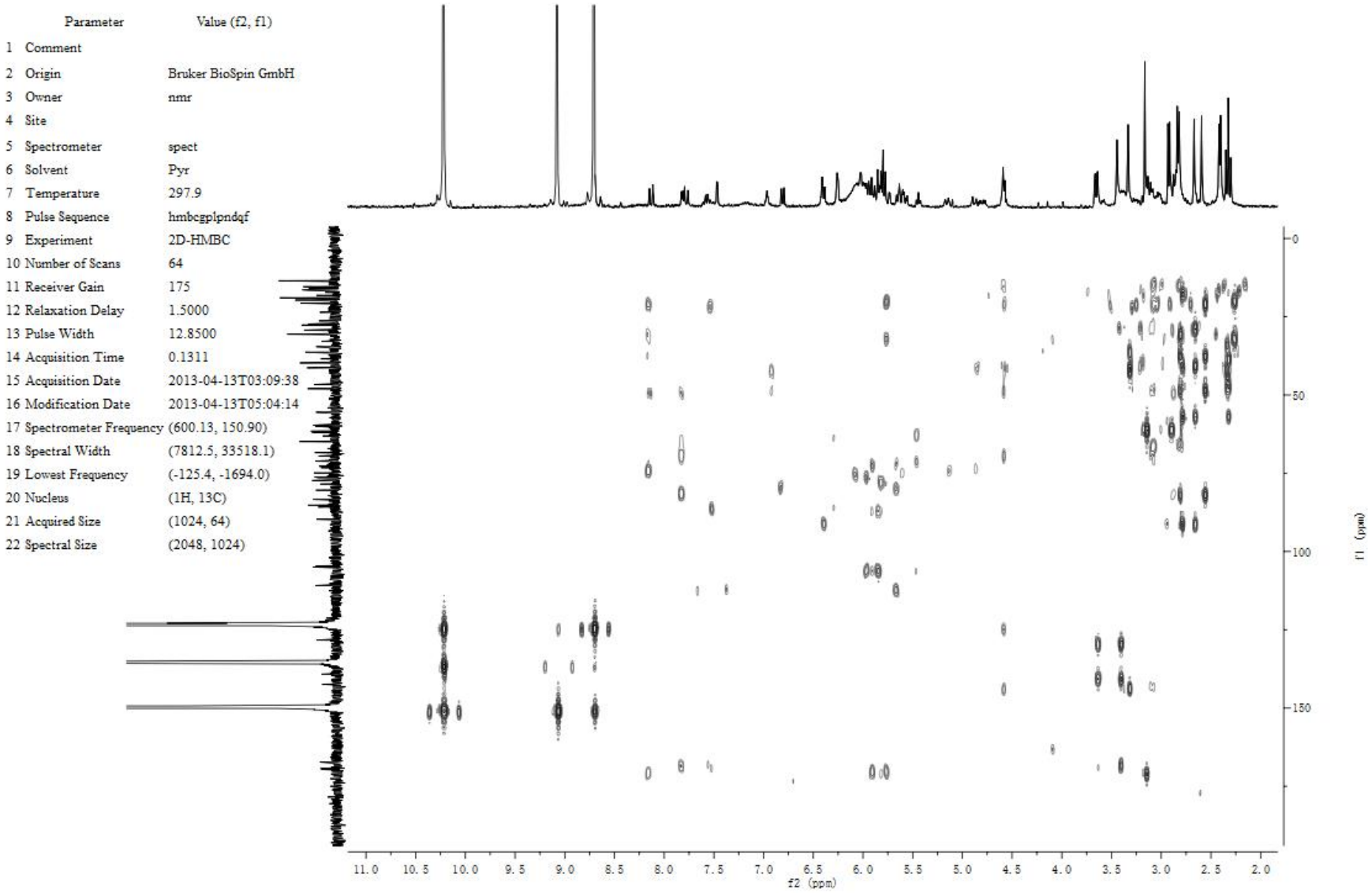


Figure S12. HSQC Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2) in C_5D_5N.

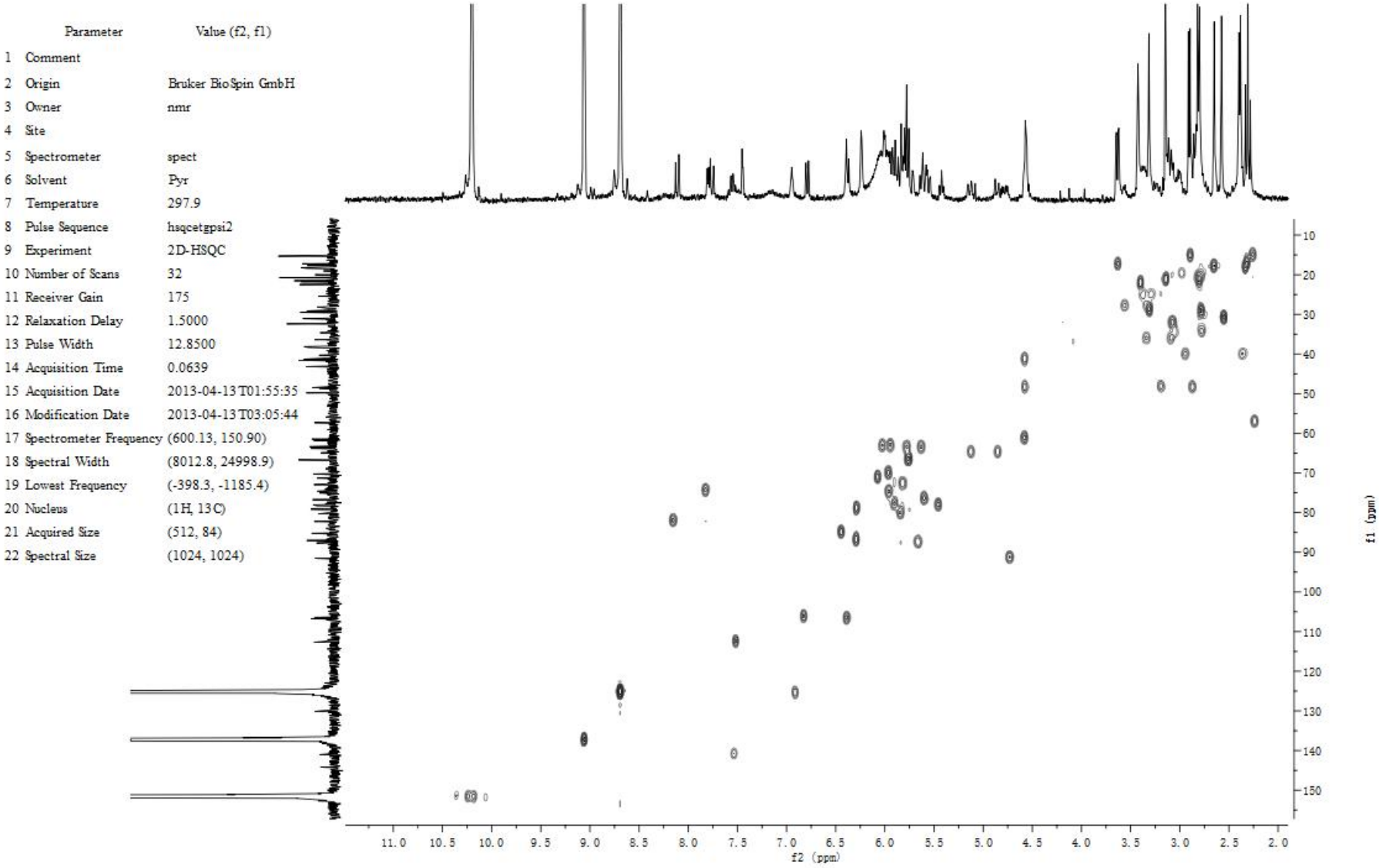


Figure S13. NOESY Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2) in C_5D_5N.

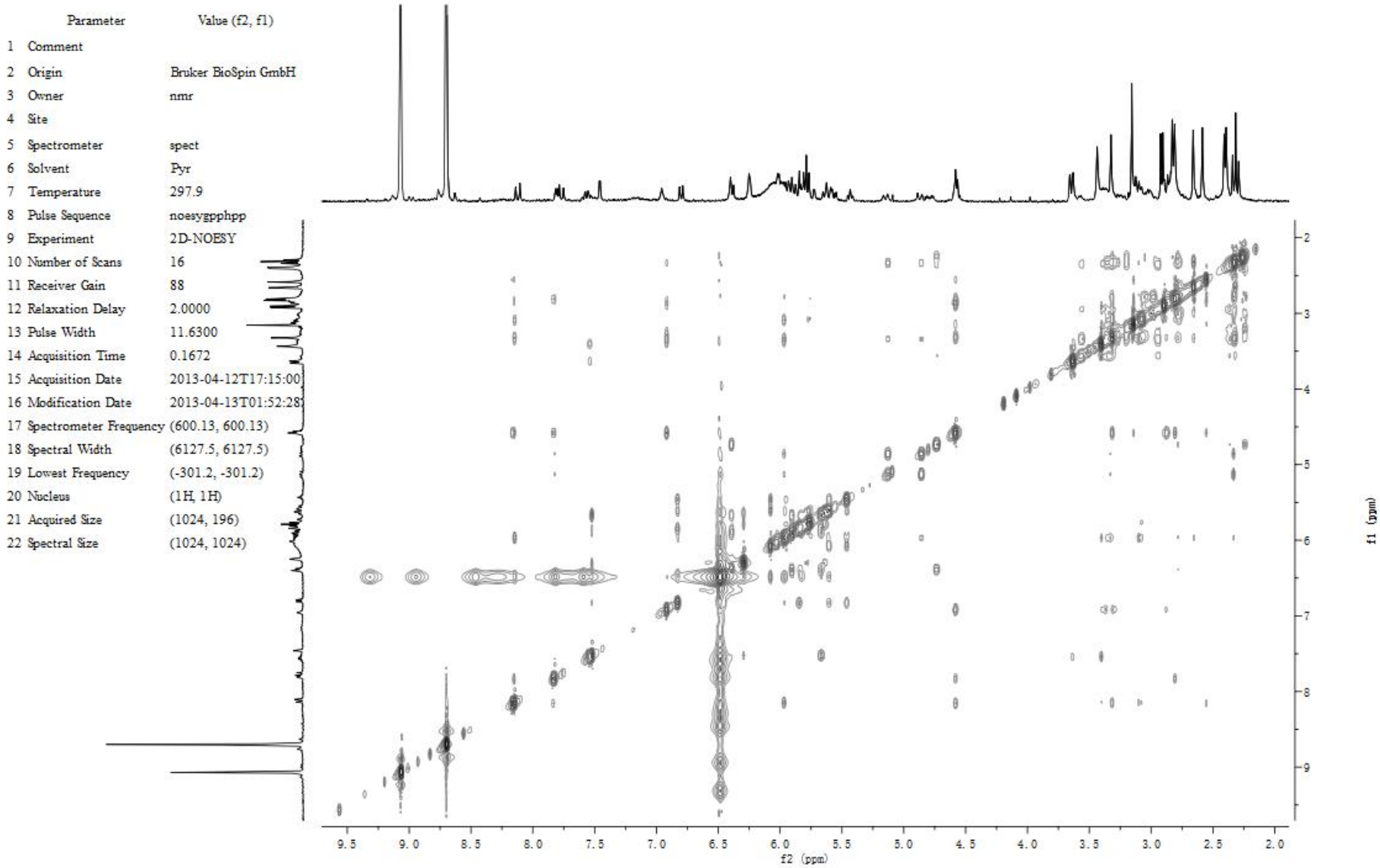


Figure S14. IR Spectrum of 3-*O*-[*α*-*L*-arabinofuranosyl(1→3)]-*β*-*D*-galactopyranosyl(1→2)-*β*-*D*-6′- *n*-butyl-glucuronic acid-21-*O*-epoxyangeloyl-22-*O*-angeloyl-3*β*, 16*α*, 21*β*, 22*α*, 28-pentahydroxy-olean-12-ene (2).

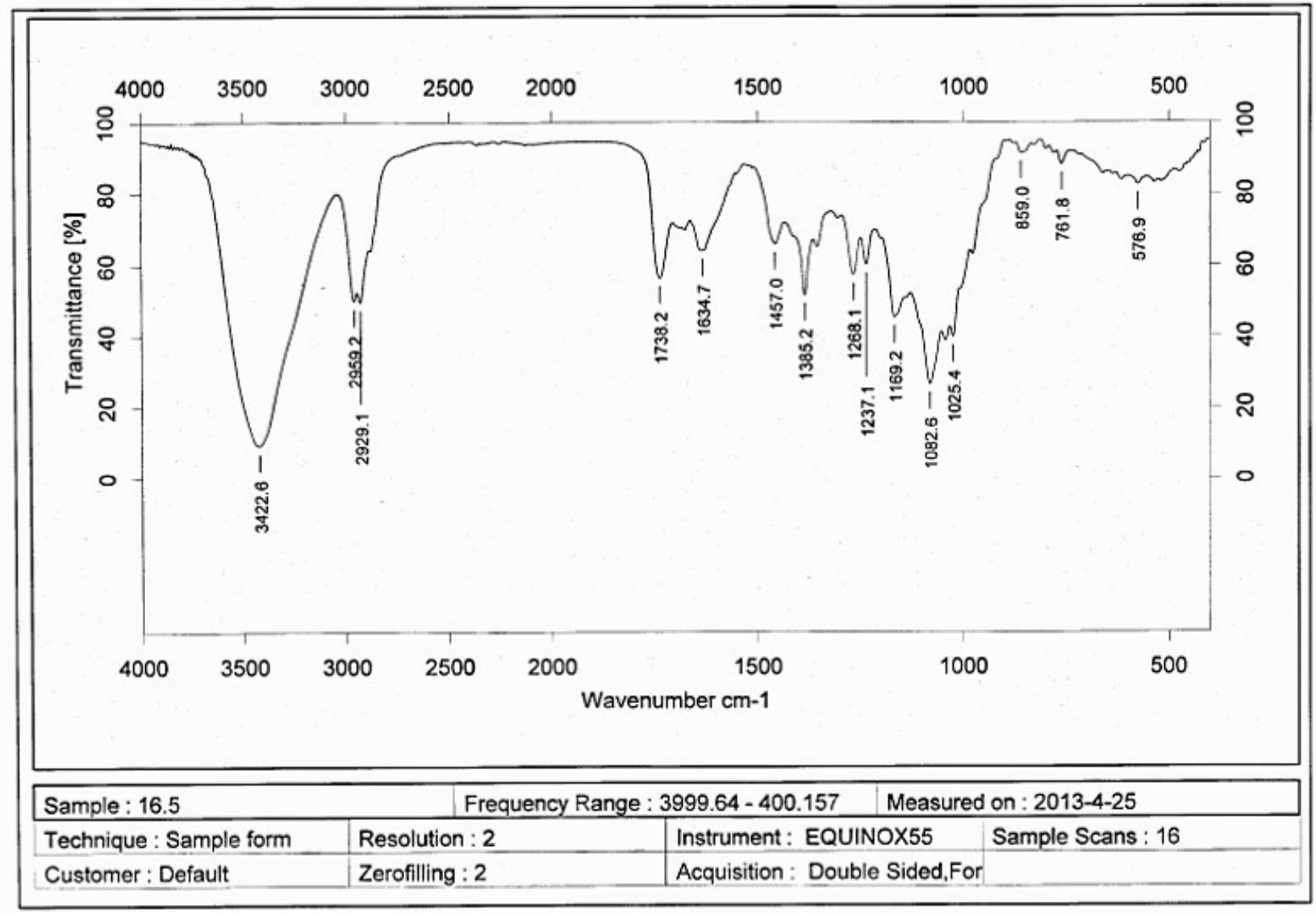


Figure S15. ^{1}H-NMR Spectrum of 6′-methylester-O-Xanifolia-Y5 (3) in C_5D_5N.

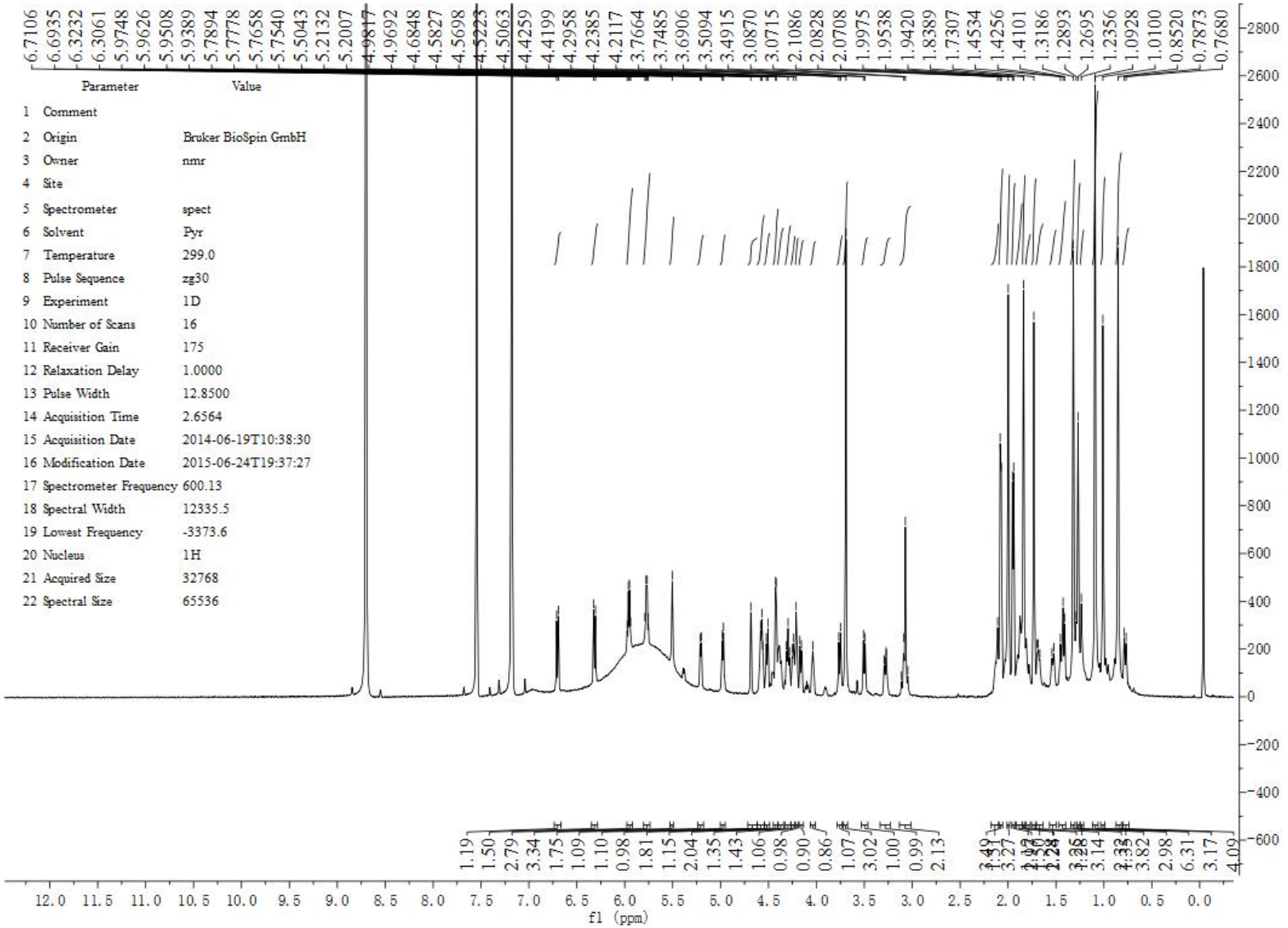


Figure S16. ^{13}C-NMR Spectrum of 6′-methylester-O-Xanifolia-Y5 (3) in C_5D_5N.

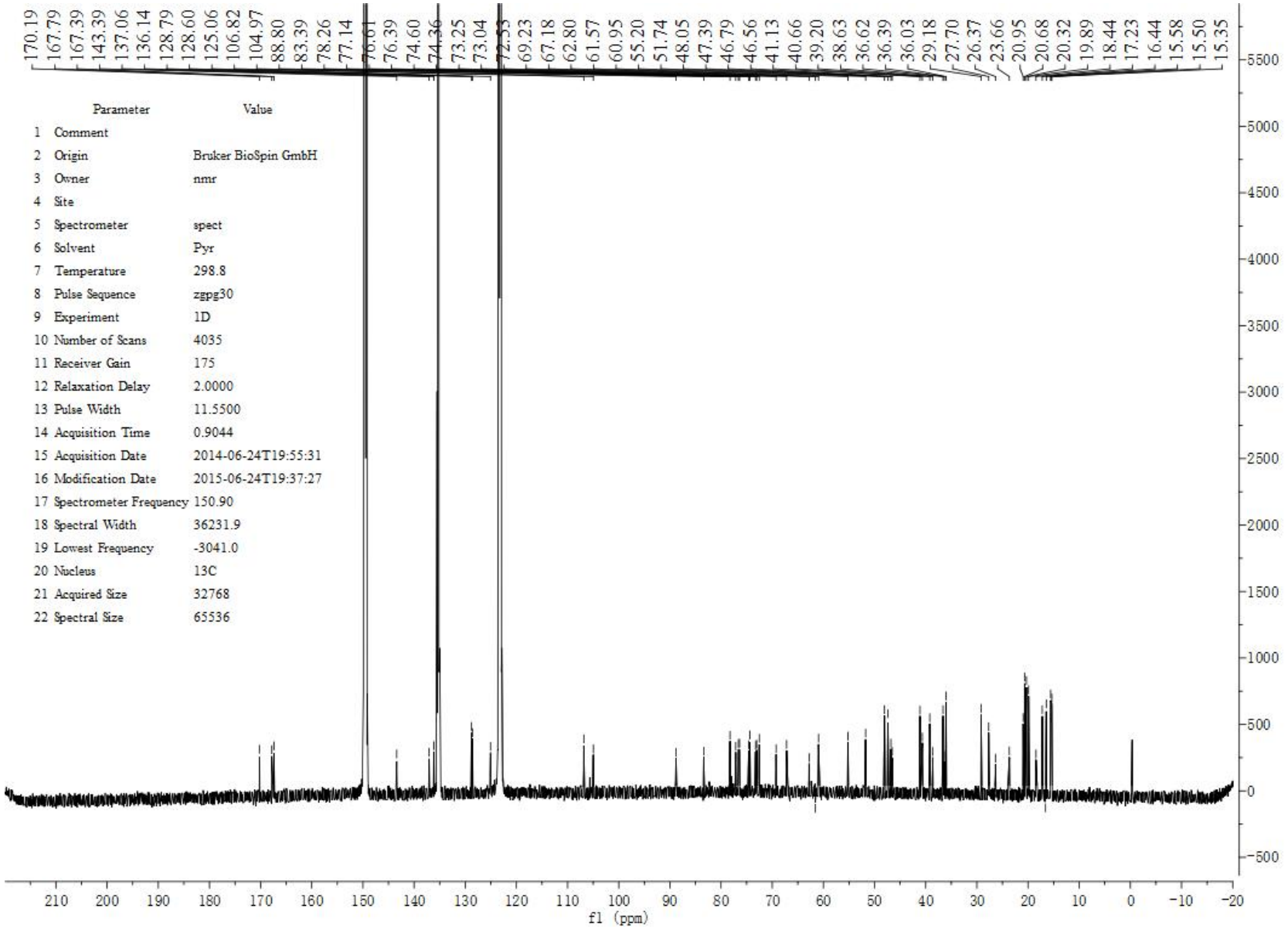


Figure S17. HR-ESI-MS Spectrum of 6′-methylester-O-Xanifolia-Y5 (3).

Mass Spectrum Molecular Formula Report

Analysis Info

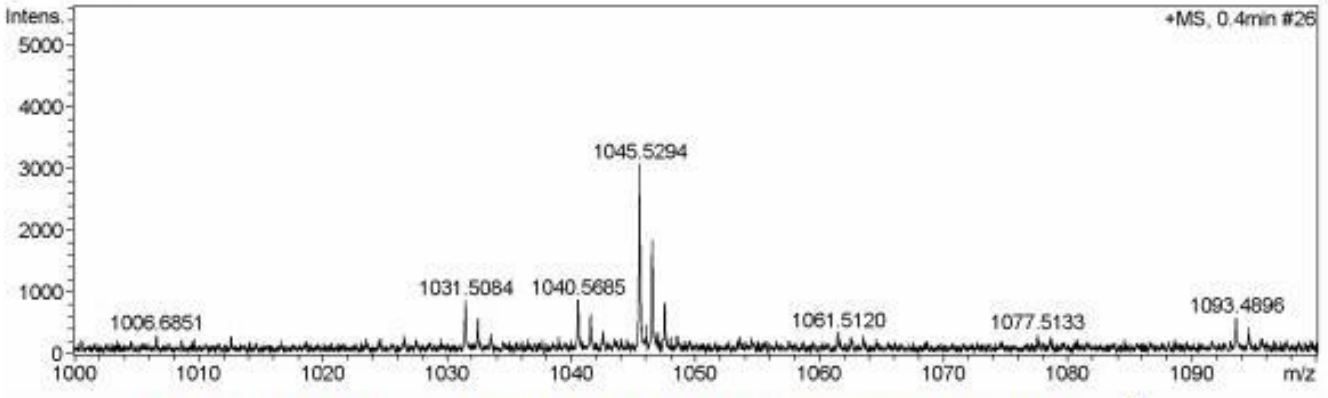
Analysis Name	D:\Data\20151118CEYANG\WD-12_1-a,5_01_5982.d	Acquisition Date	11/18/2015 12:21:31 PM
Method	20131026_ceyang.m	Operator	micrOTOF-Q
Sample Name	WD-12	Instrument / Ser#	Bruker Customer 125
Comment			

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	3000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C53H82O19Na				
Formula, max.					
Measured m/z	1045.53	Tolerance	5 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
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 53 H 82 Na 1 O 19	0.039	1045.5343	4.66	7.66	4.87	12.50	ok	even

Figure S18. HMBC Spectrum of 6′-methylester-O-Xanifolia-Y5 (3) in C_5D_5N.

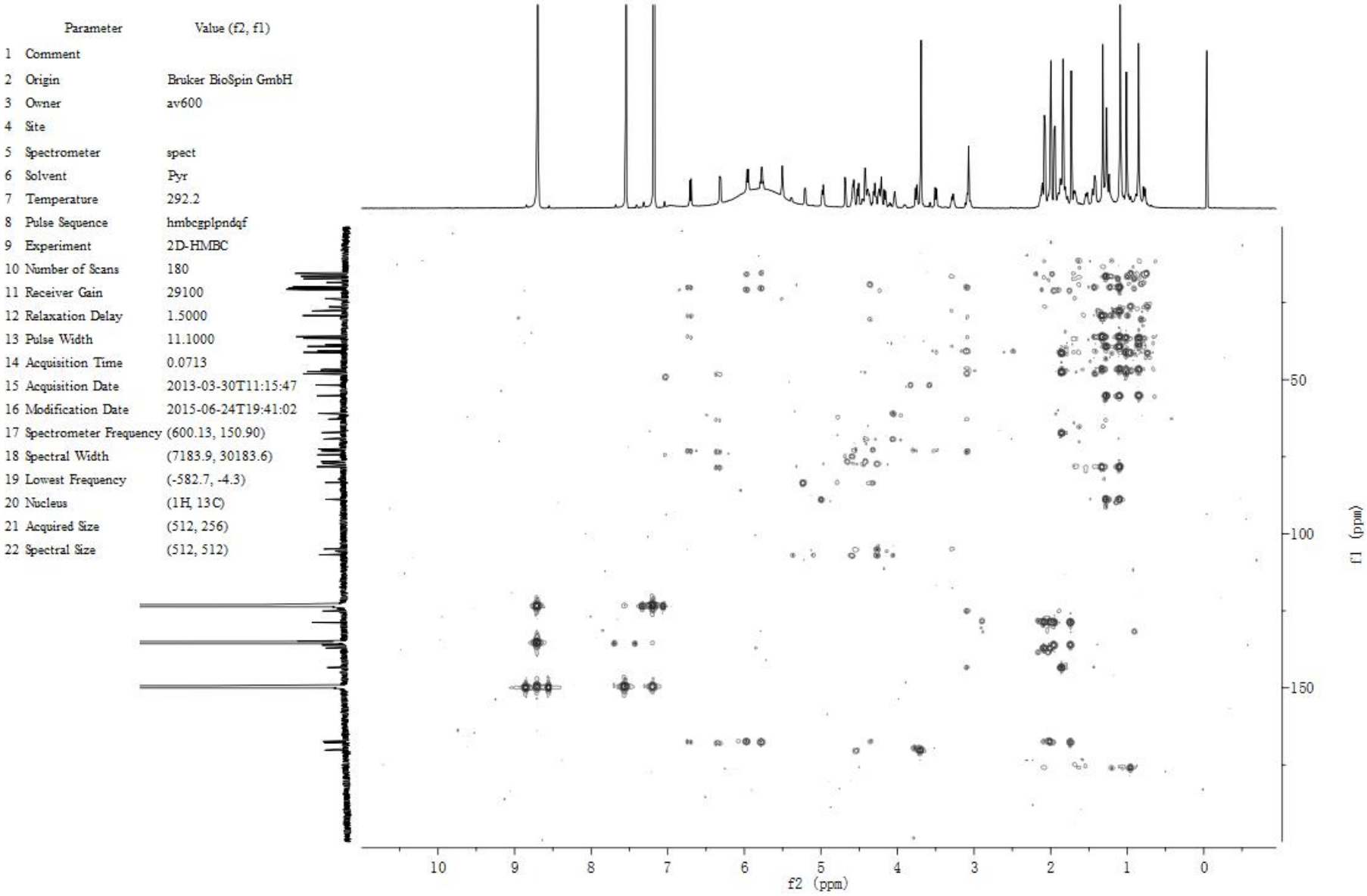


Figure S19. HSQC Spectrum of 6′-methylester-O-Xanifolia-Y5 (3) in C_5D_5N.

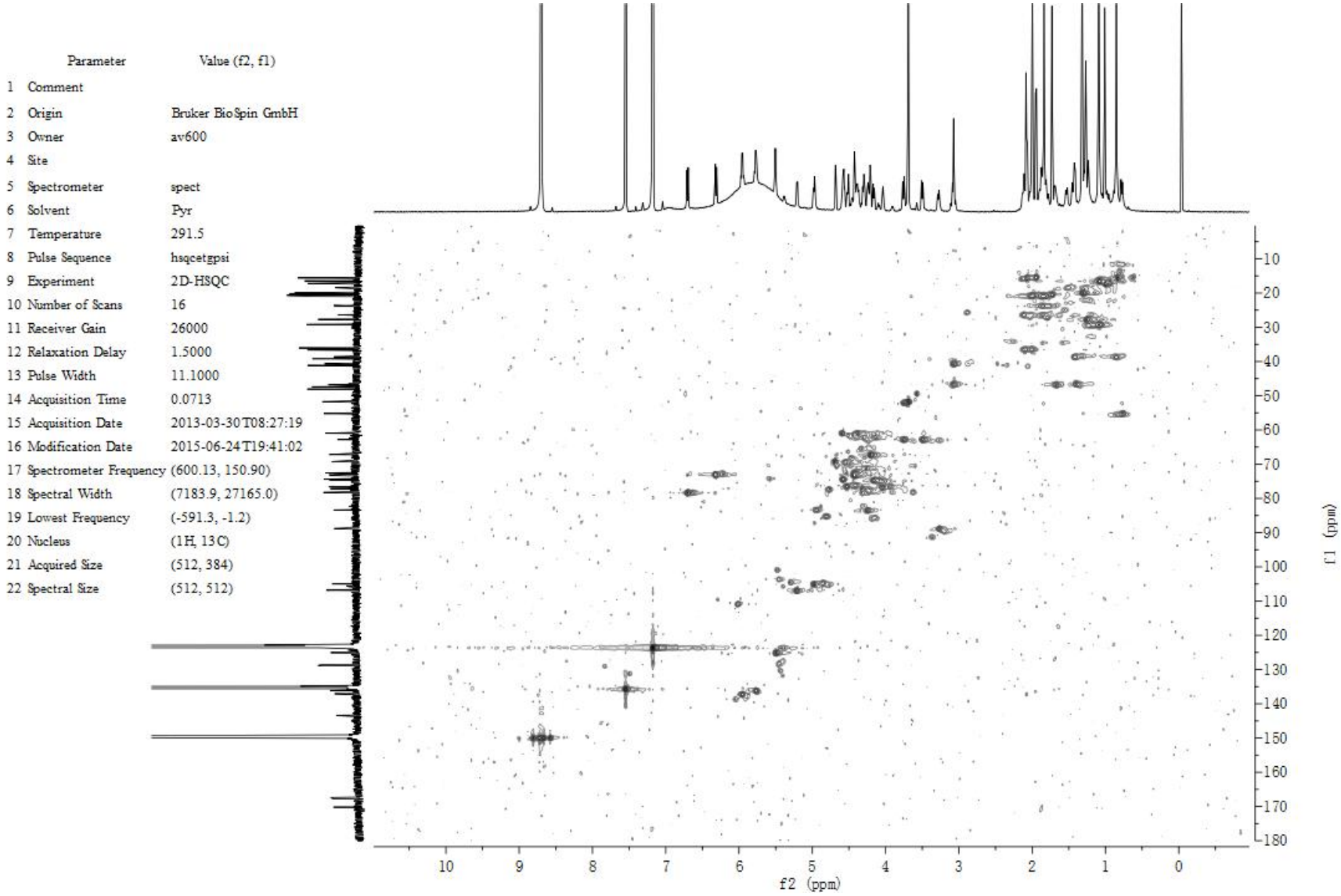


Figure S20. IR Spectrum of 6′-methylester-O-Xanifolia-Y5 (3).

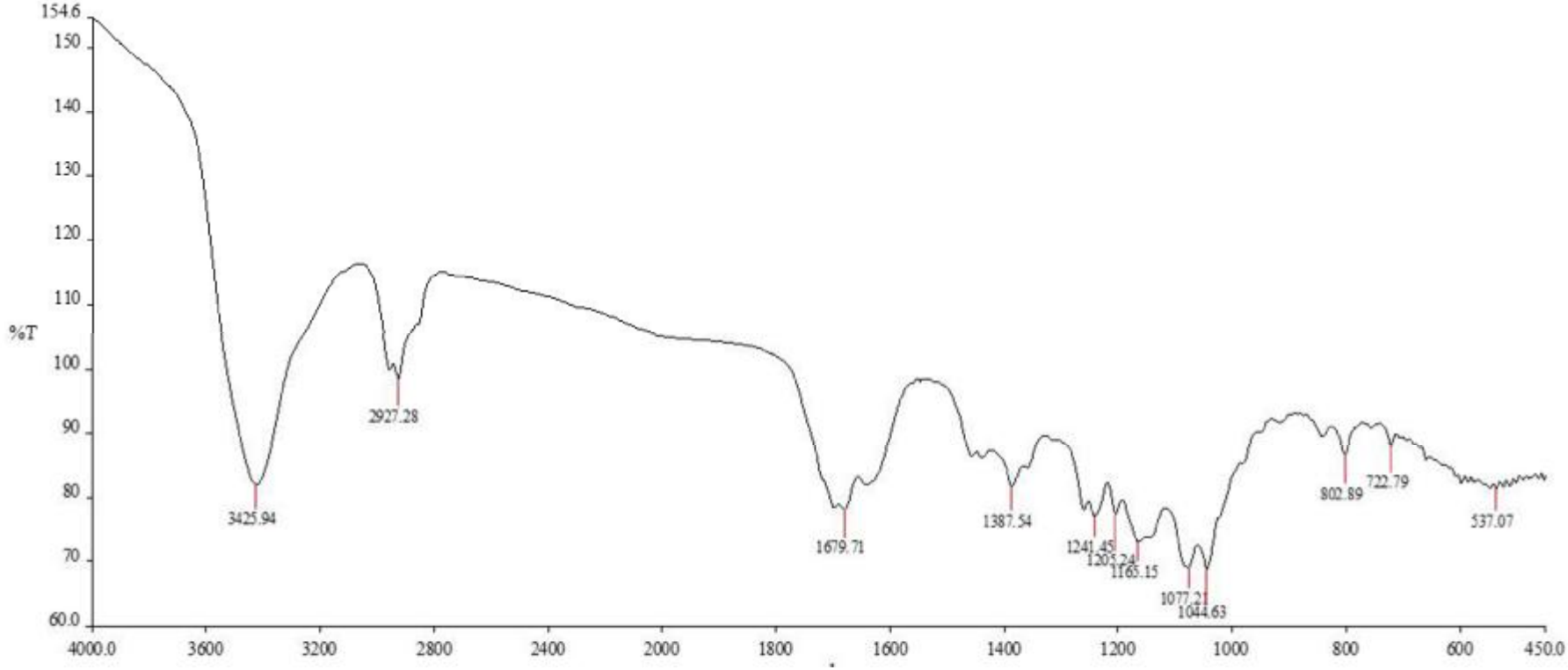


Figure S21. ^{1}H-NMR Spectrum of 16-*O*-acetyl-aesculioside G12 (4) in C_5D_5N.

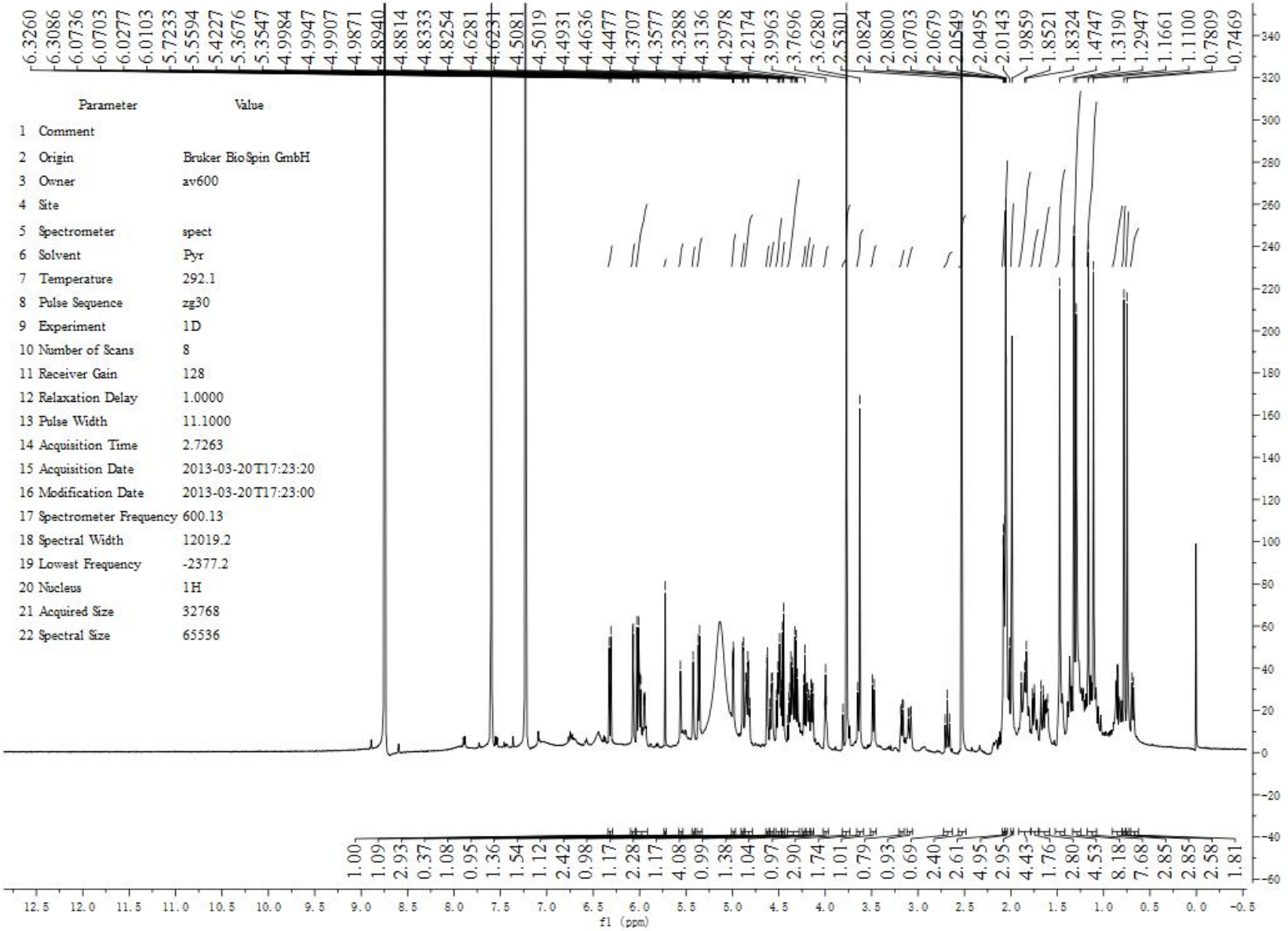


Figure S22. ^{13}C-NMR Spectrum of 16-*O*-acetyl-aesculioside G12 (4) in C_5D_5N.

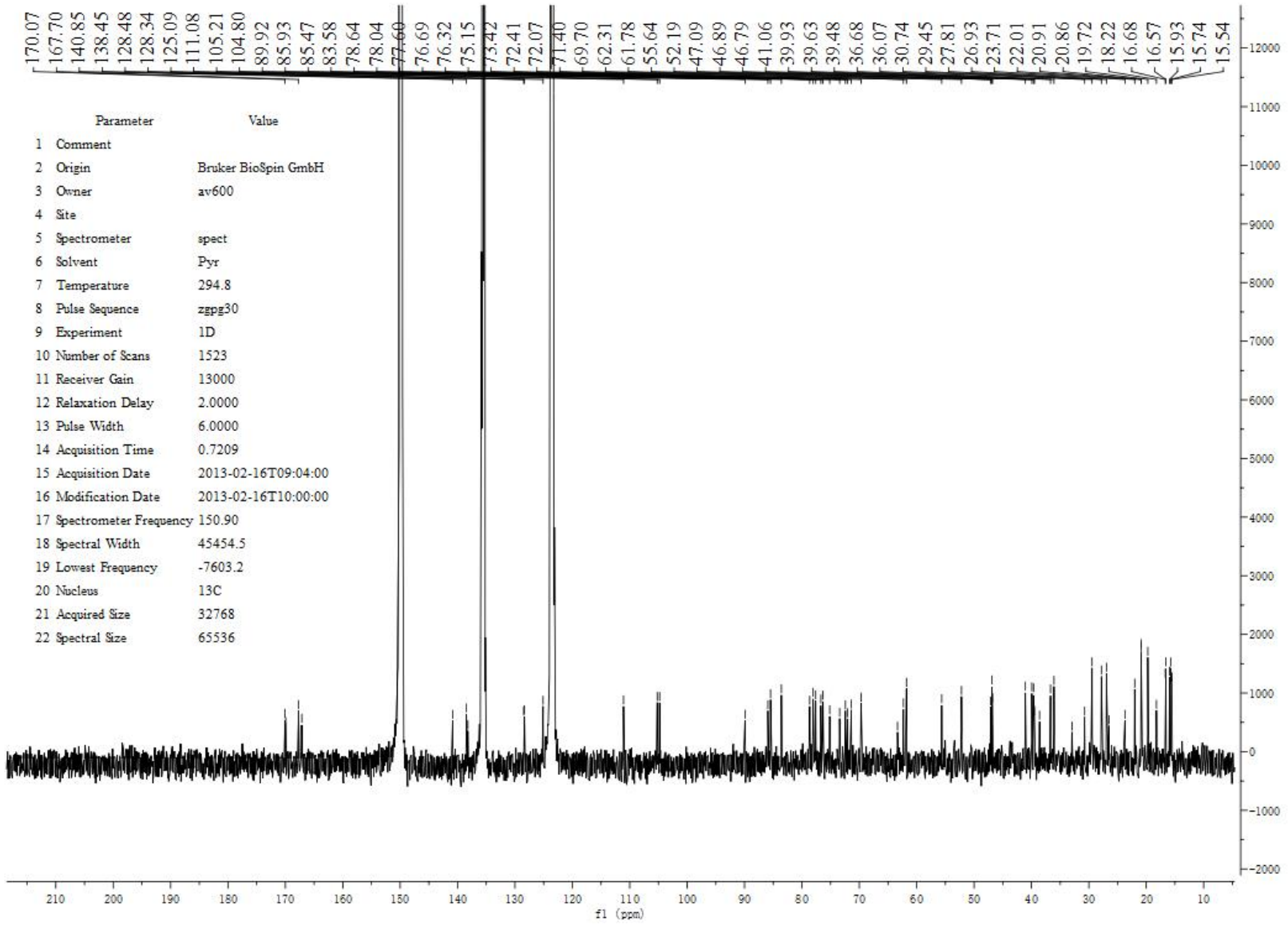


Figure S23. HR-ESI-MS Spectrum of 16-*O*-acetyl-aesculioside G12 (4).

Mass Spectrum Molecular Formula Report

Analysis Info

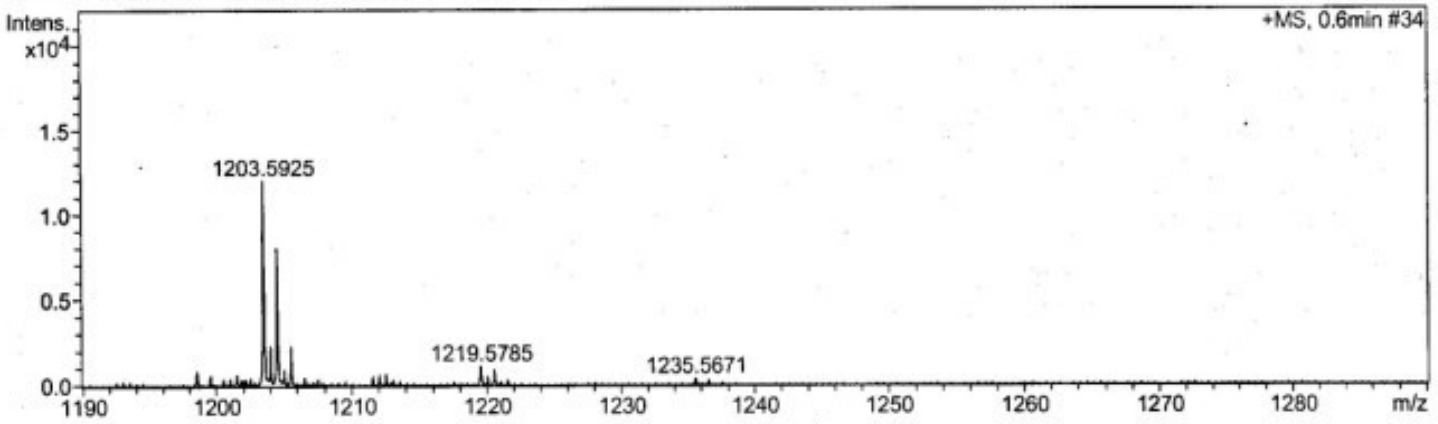
Analysis Name	D:\Data\ZL-M.d	Acquisition Date	4/10/2013 3:09:35 PM
Method	LIU 250-550POS.m	Operator	Bruker Customer
Sample Name	ZL-M	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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	500.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C60H92O23Na				
Formula, max.					
Measured m/z	1203.59	Tolerance	5 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
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 60 H 92 Na 1 O 23	0.036	1203.5922	-0.29	0.59	-0.35	14.50	ok	even

Figure S24. HMBC Spectrum of 16-*O*-acetyl-aesculioside G12 (4) in C_5D_5N.

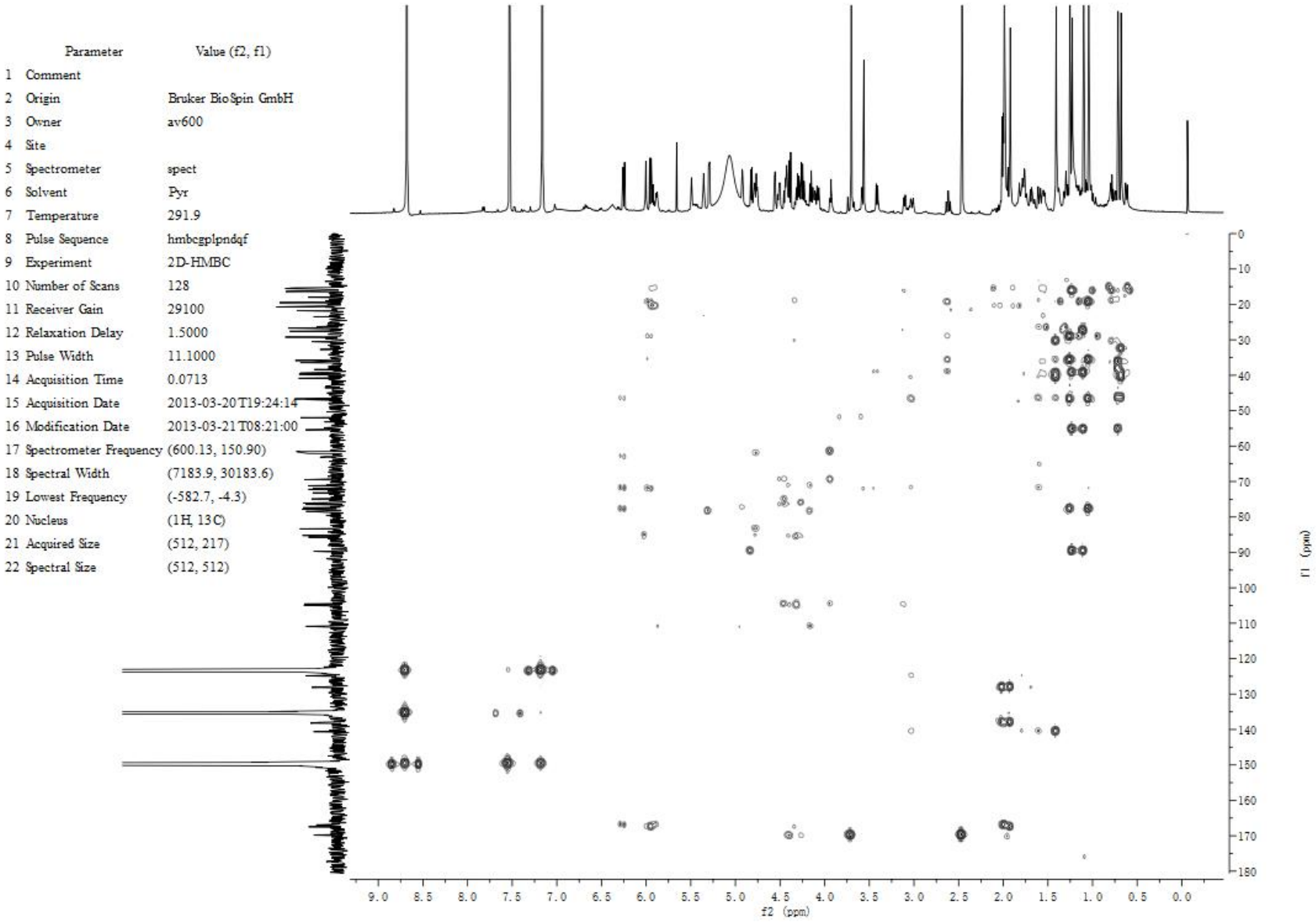


Figure S25. HSQC Spectrum of 16-*O*-acetyl-aesculioside G12 (4) in C_5D_5N.

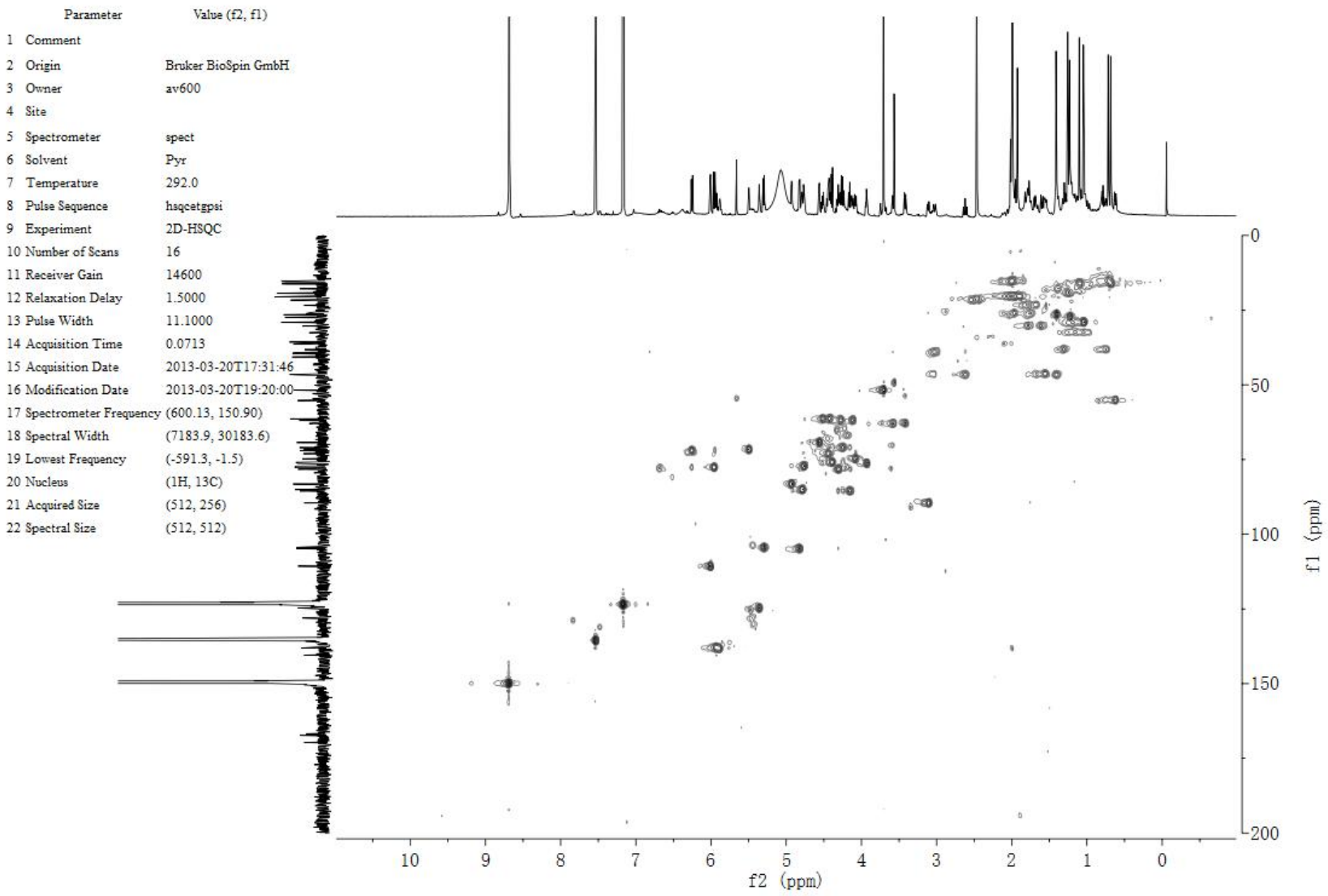


Figure S26. NOESYS pectrum of 16-*O*-acetyl-aesculioside G12 (4) in C_5D_5N.

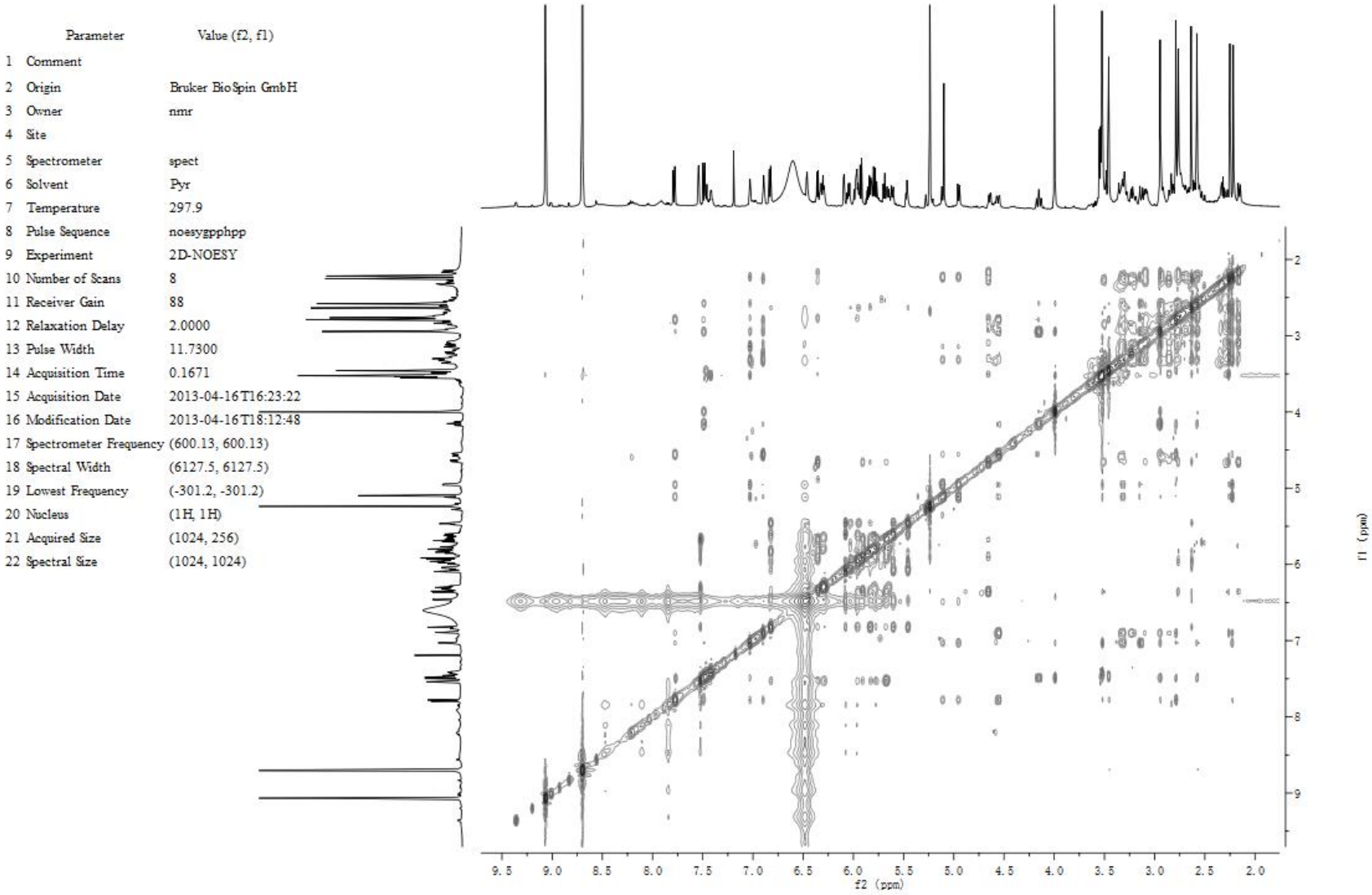
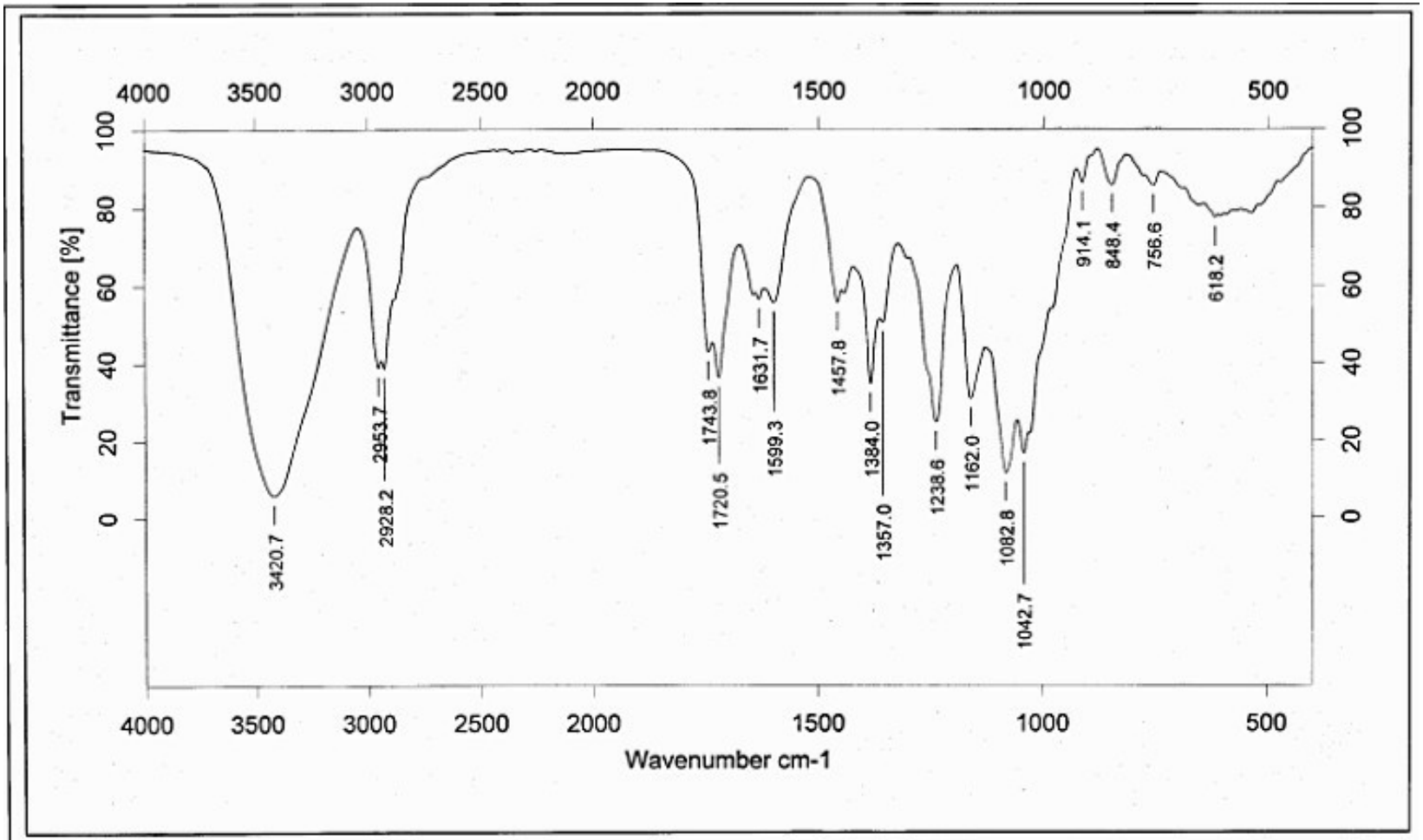


Figure S27. IR Spectrum of 16-*O*-acetyl-aesculioside G12 (4).



Sample : M	Frequency Range : 3999.64 - 400.157	Measured on : 2013-4-25	
Technique : Sample form	Resolution : 2	Instrument : EQUINOX55	Sample Scans : 16
Customer : Default	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S28. ^{1}H-NMR Spectrum of 3-O-[α-L-arabinofuranosyl(1→3)]-β-D-galactopyranosyl(1→2)-β-D-6′-methyl-glucuronic acid-21-O-(3′′′′,4′′′′-O-diangeloyl)-β-D-fucopyranosyl-28-O-acetyl-3β, 16α, 21β, 22α, 28-pentahydroxy-olean-12-ene (5) in C_5D_5N.

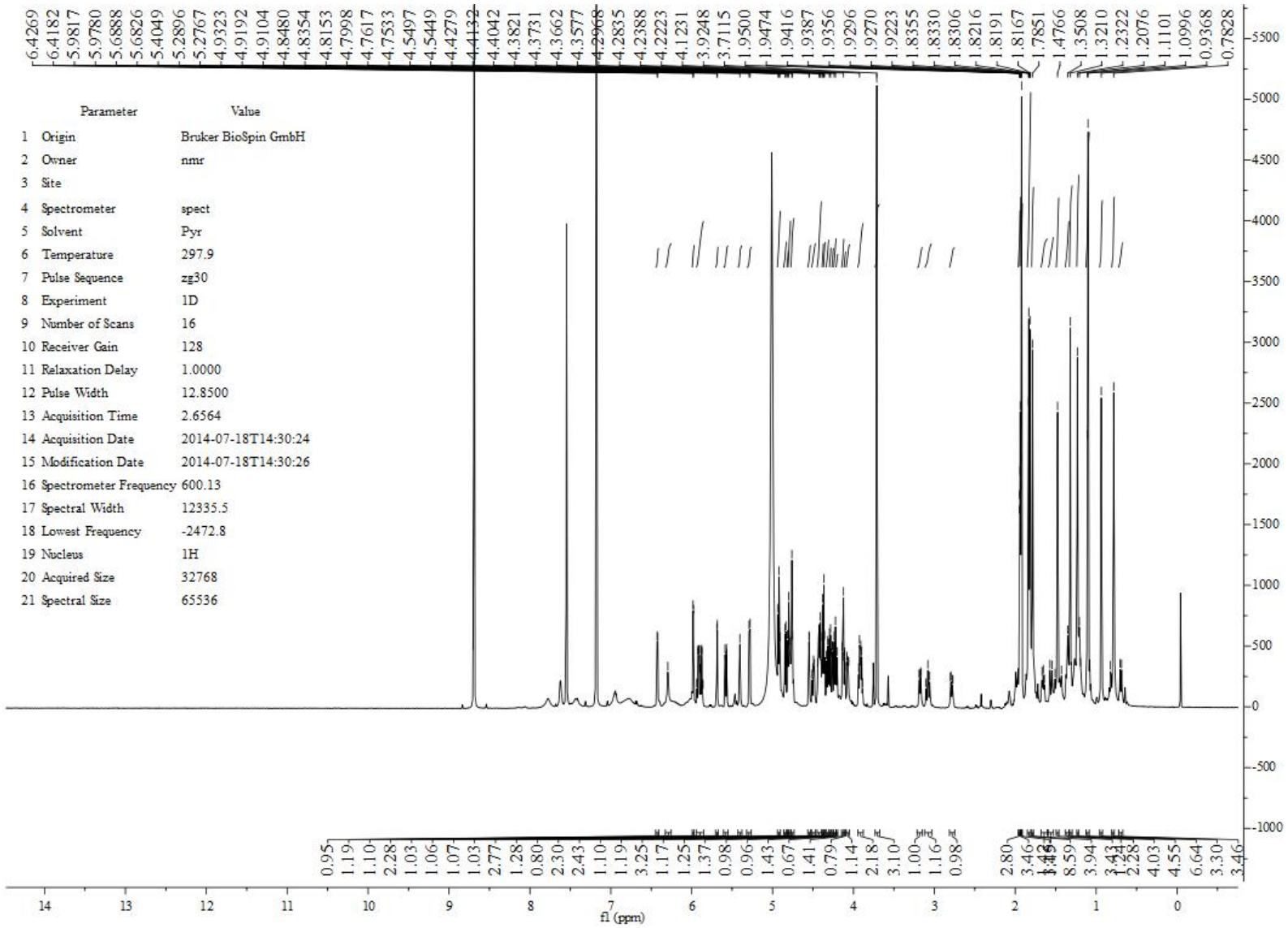


Figure S29. ^{13}C-NMR Spectrum of 3-O-[α-L-arabinofuranosyl(1→3)]-β-D-galactopyranosyl(1→2)-β-D-6′-methyl-glucuronic acid-21-O-(3′′′′,4′′′′-O-diangeloyl)-β-D-fucopyranosyl-28-O-acetyl-3β, 16α, 21β, 22α, 28-pentahydroxy-olean-12-ene (5) in C_5D_5N.

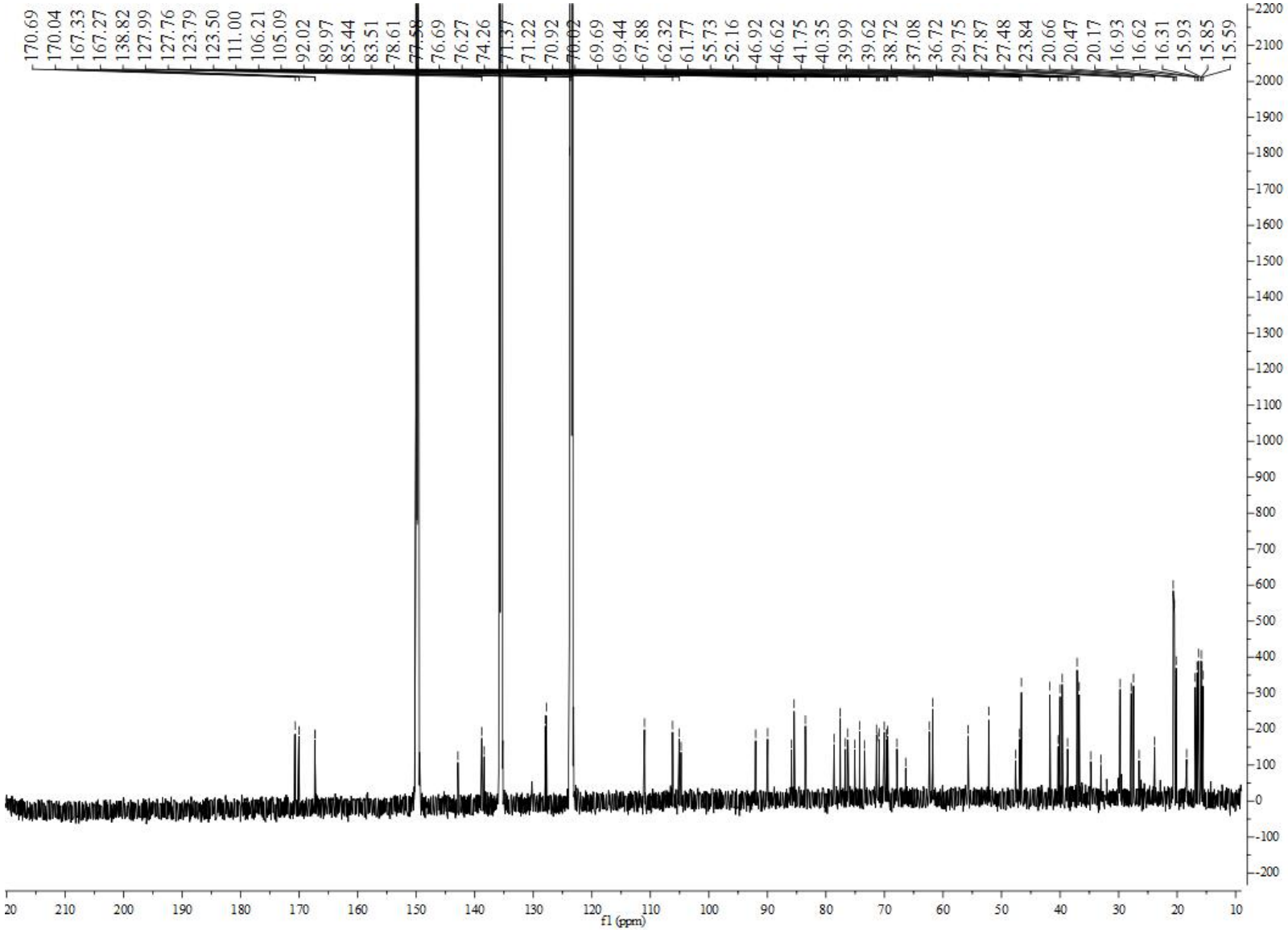


Figure S30. HR-ESI-MS Spectrum of 3-O-[α-L-arabinofuranosyl(1→3)]-β-D-galactopyranosyl(1→2)-β-D-6′-methyl-glucuronic acid-21-O-(3‴′,4‴′-O-diangeloyl)-β-D-fucopyranosyl-28-O-acetyl-3β, 16α, 21β, 22α, 28-pentahydroxy-olean-12-ene (5).

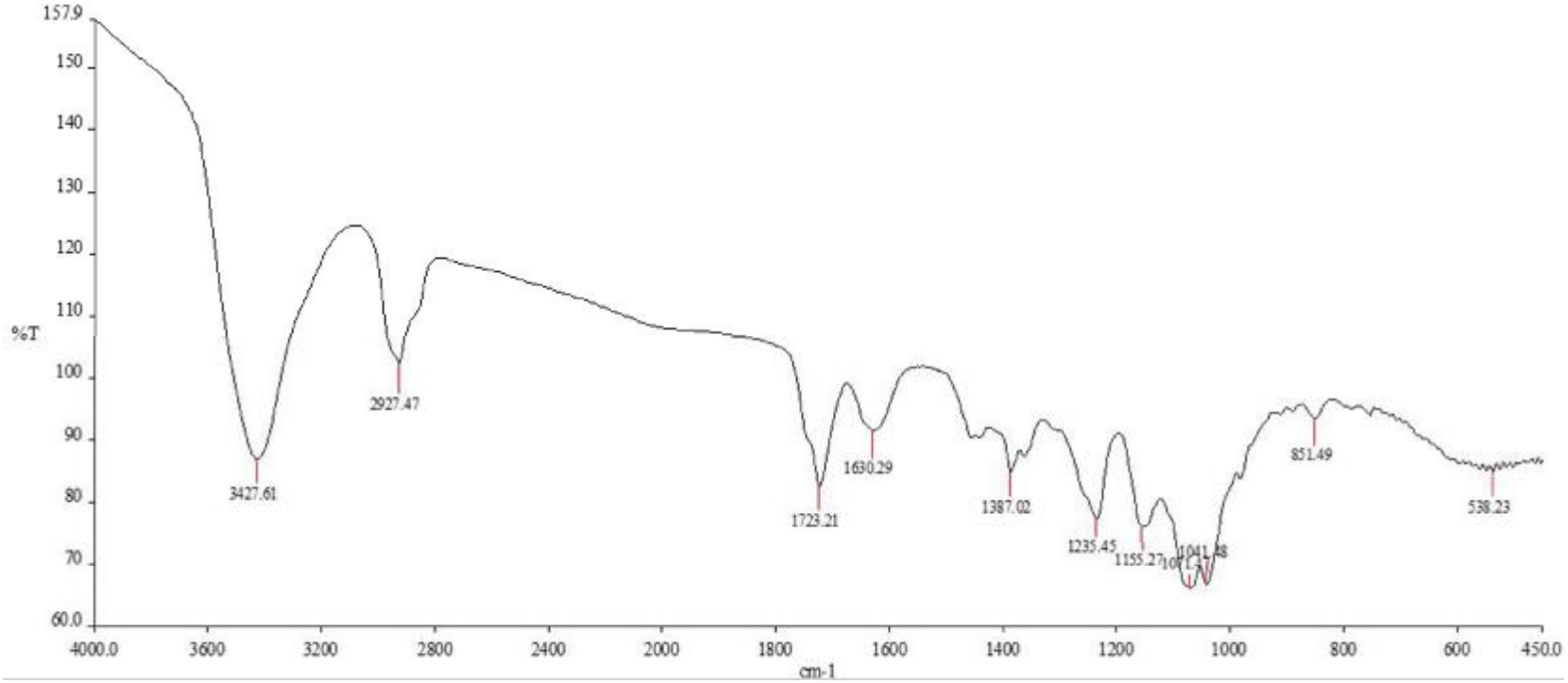


Figure S31. HMBC Spectrum of 3-O-[α-L-arabinofuranosyl(1→3)]-β-D-galactopyranosyl(1→2)-β-D-6′-methyl-glucuronic acid-21-O-(3′′′′,4′′′′-O-diangeloyl)-β-D-fucopyranosyl-28-O-acetyl-3β, 16α, 21β, 22α, 28-pentahydroxy-olean-12-ene (5) in C_5D_5N.

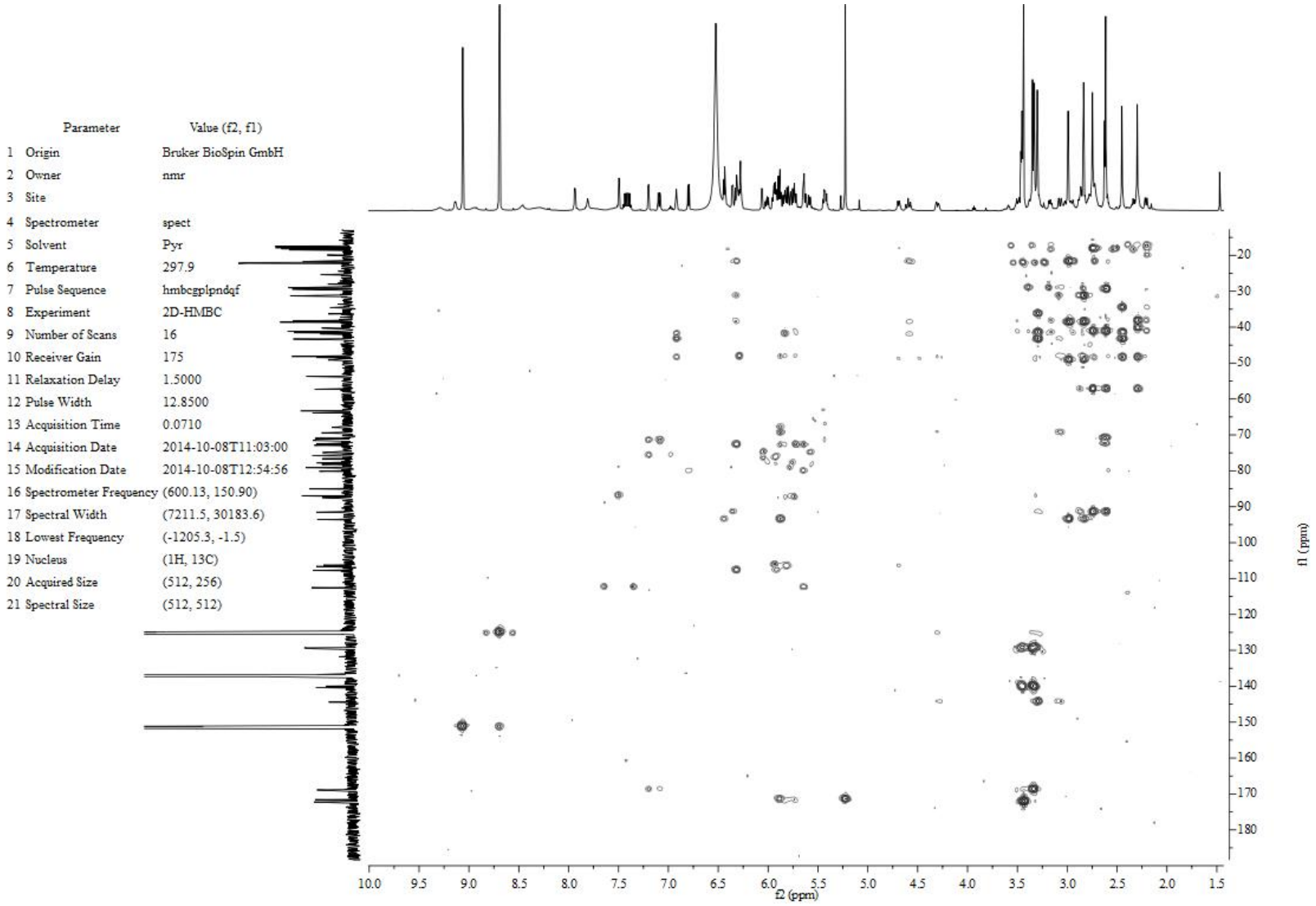


Figure S32. HSQC Spectrum of 3-O-[α-L-arabinofuranosyl(1→3)]-β-D-galactopyranosyl(1→2)-β-D-6′-methyl-glucuronic acid-21-O-(3′′′′,4′′′′-O-diangeloyl)-β-D-fucopyranosyl-28-O-acetyl-3β, 16α, 21β, 22α, 28-pentahydroxy-olean-12-ene (5) in C_5D_5N.

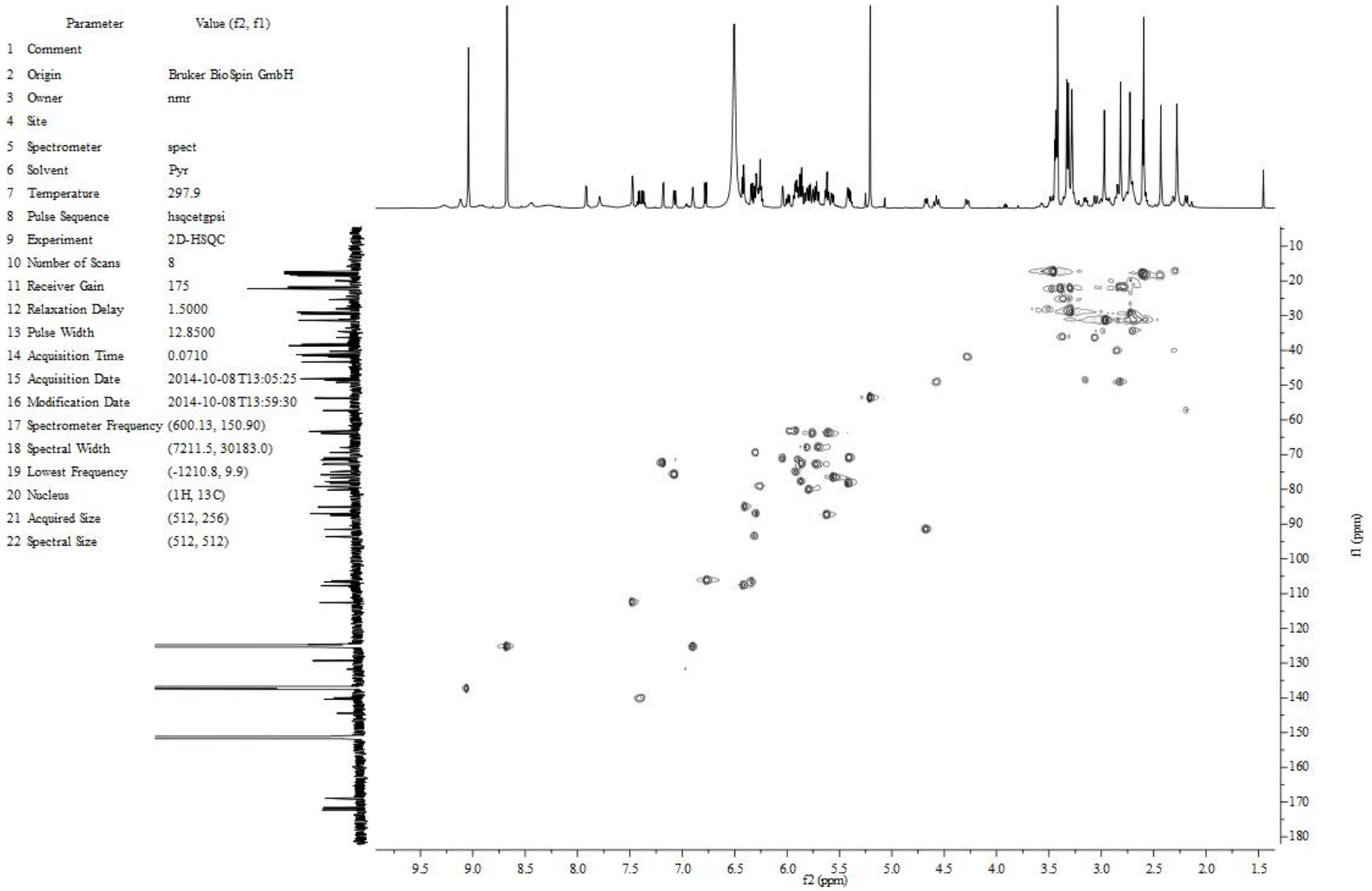


Figure S33. IR Spectrum of 3-O-[α-L-arabinofuranosyl(1→3)]-β-D-galactopyranosyl(1→2)-β-D-6′-methyl-glucuronic acid-21-O-(3′′′′,4′′′′-O-diangeloyl)-β-D-fucopyranosyl-28-O-acetyl-3β, 16α, 21β, 22α, 28-pentahydroxy-olean-12-ene (5) in C_5D_5N.

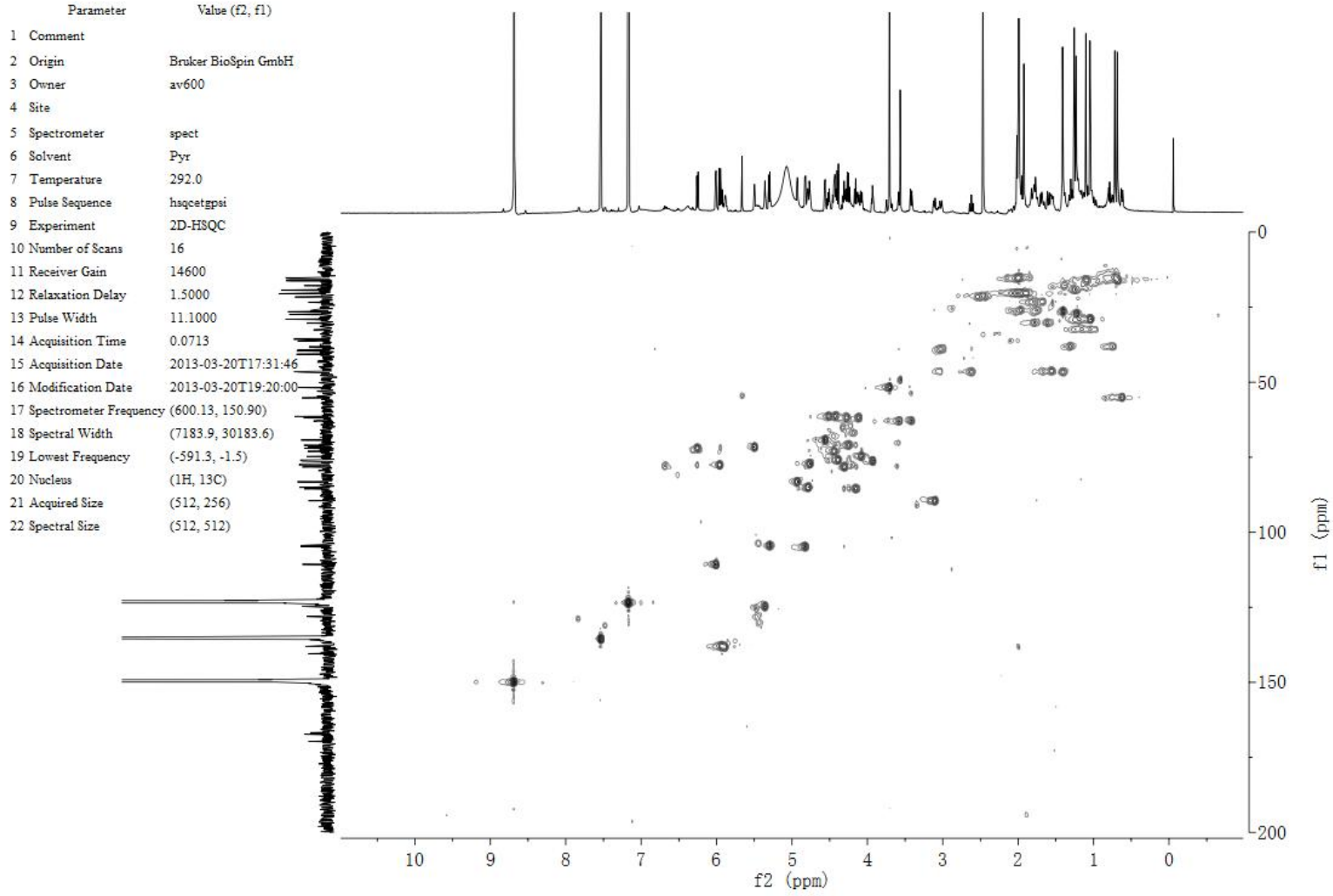


Figure S34. ^{1}H-NMR Spectrum of 6′-methylester-O-Xanifolia-Y2 (6) in C_5D_5N.

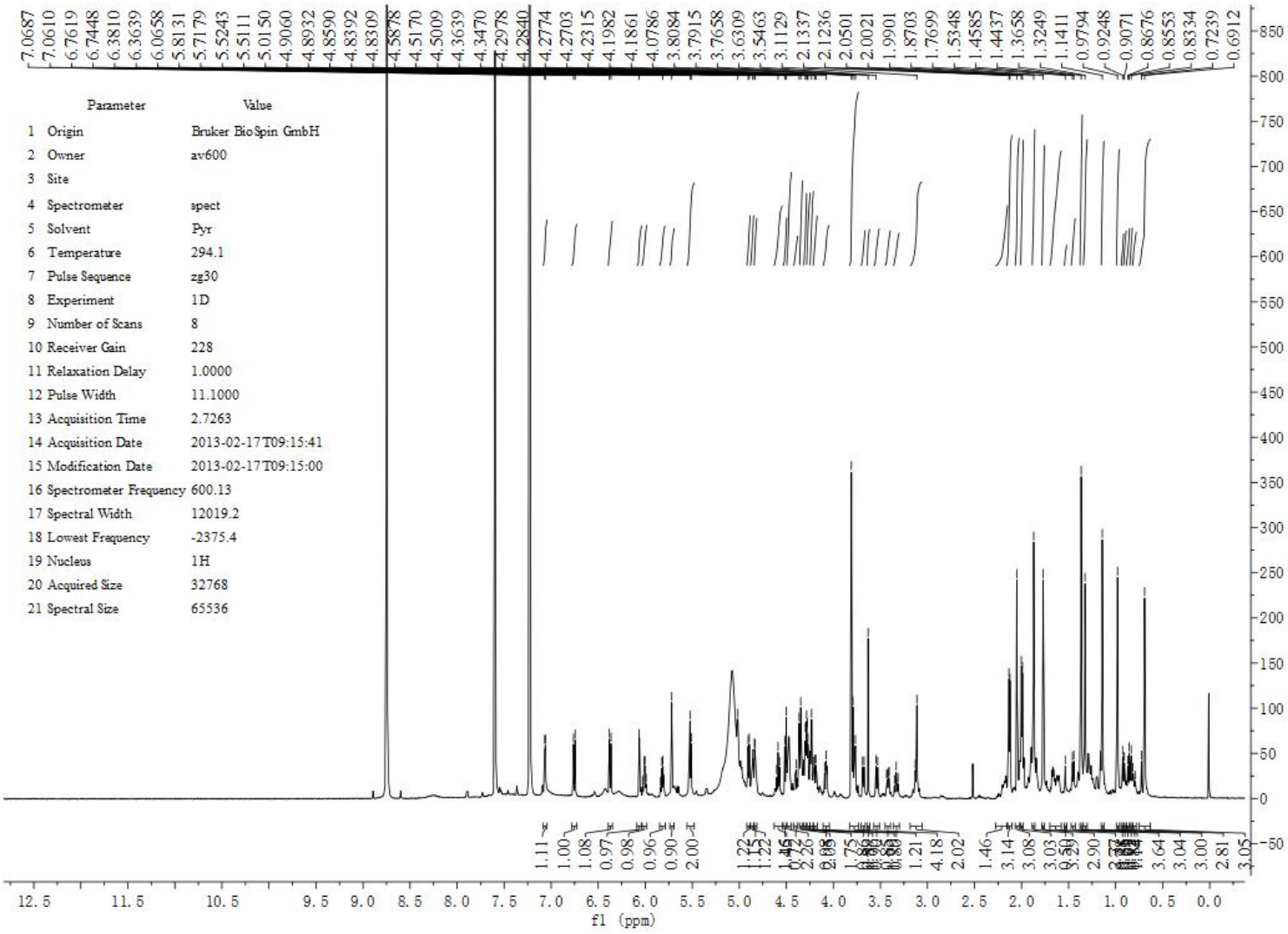


Figure S35. ^{13}C-NMR Spectrum of 6′-methylester-O-Xanifolia-Y2 (6) in C_5D_5N.

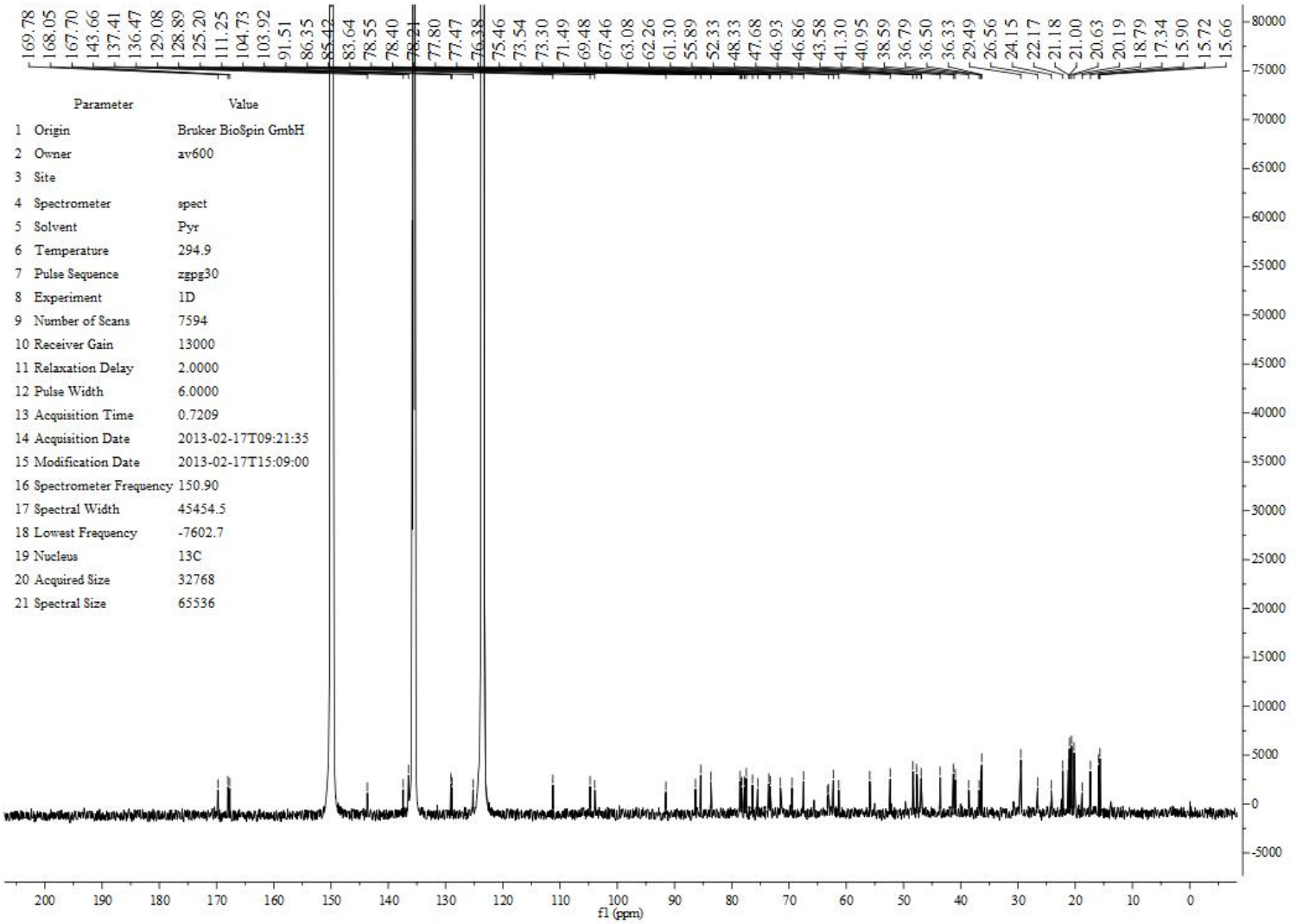


Figure S36. HR-ESI-MS Spectrum of 6′-methylester-O-Xanifolia-Y2 (6).

Mass Spectrum Molecular Formula Report

Analysis Info

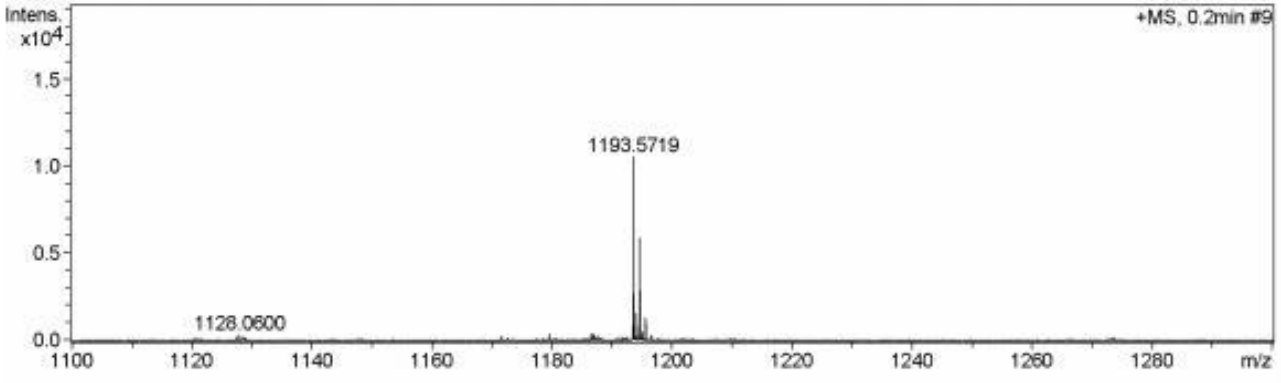
Analysis Name	D:\Data\20140312ceyang\ZL-9.d	Acquisition Date	3/12/2014 7:32:01 PM
Method	tune_high_pos.m	Operator	Bruker Customer
Sample Name	ZL-9	Instrument / Ser#	micrOTOF-Q 125
Comment			

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

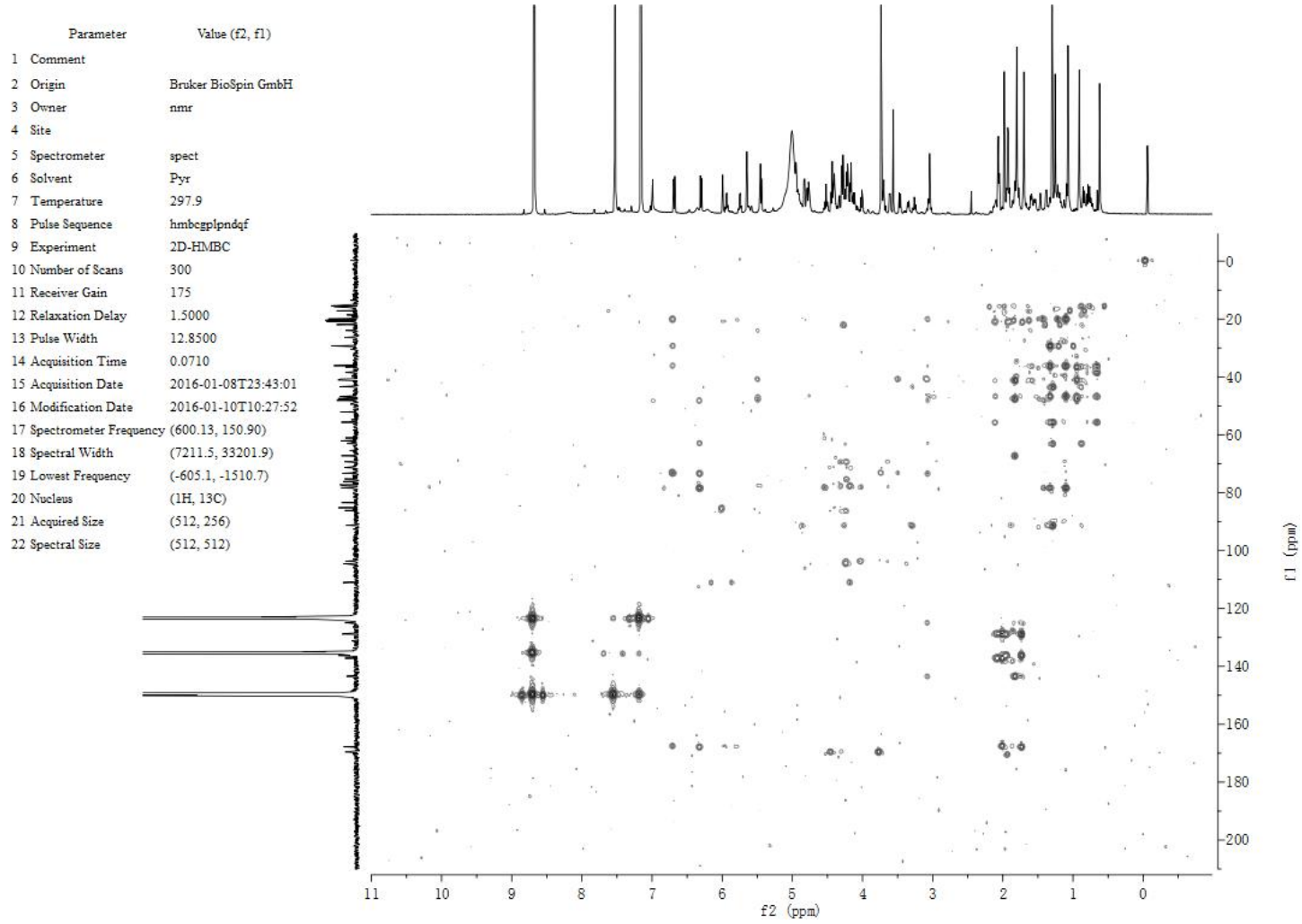
Generate Molecular Formula Parameter

Formula, min.	C58H90O24Na				
Formula, max.					
Measured m/z	1193.57	Tolerance	5 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
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 58 H 90 Na 1 O 24	0.073	1193.5714	-0.42	-0.30	-0.50	13.50	ok	even

Figure S37. HMBC Spectrum of 6′-methylester-O-Xanifolia-Y2 (6) in C_5D_5N.



Parameter	Value (f2, f1)
1 Comment	
2 Origin	Bruker BioSpin GmbH
3 Owner	nmr
4 Site	
5 Spectrometer	spect
6 Solvent	Pyr
7 Temperature	297.9
8 Pulse Sequence	hmbcgplpndqf
9 Experiment	2D-HMBC
10 Number of Scans	300
11 Receiver Gain	175
12 Relaxation Delay	1.5000
13 Pulse Width	12.8500
14 Acquisition Time	0.0710
15 Acquisition Date	2016-01-08T23:43:01
16 Modification Date	2016-01-10T10:27:52
17 Spectrometer Frequency	(600.13, 150.90)
18 Spectral Width	(7211.5, 33201.9)
19 Lowest Frequency	(-605.1, -1510.7)
20 Nucleus	(1H, 13C)
21 Acquired Size	(512, 256)
22 Spectral Size	(512, 512)

Figure S38. HSQC Spectrum of 6′-methylester-O-Xanifolia-Y2 (6) in C_5D_5N.

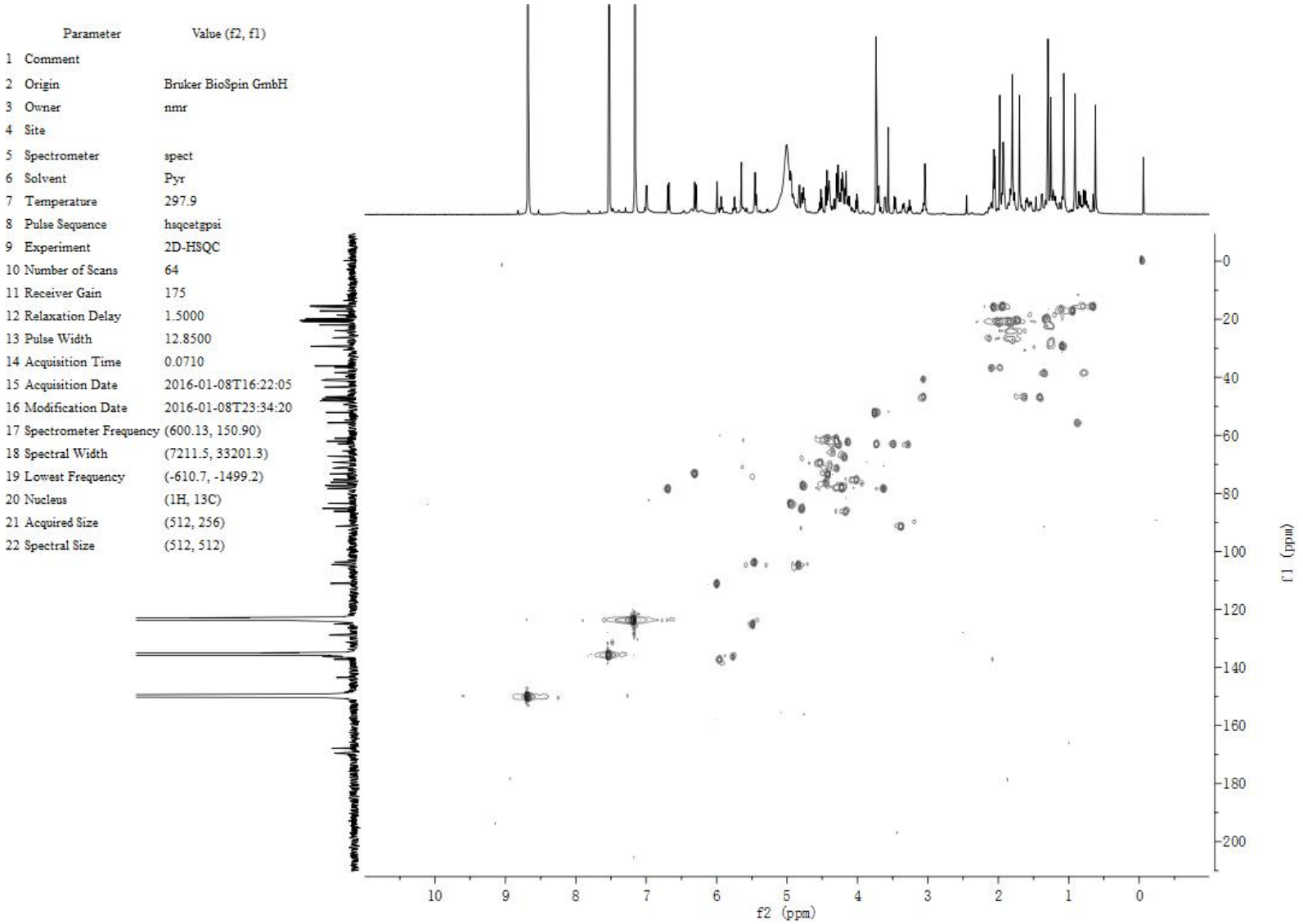


Figure S39. IR Spectrum of 6′-methylester-O-Xanifolia-Y2 (6).

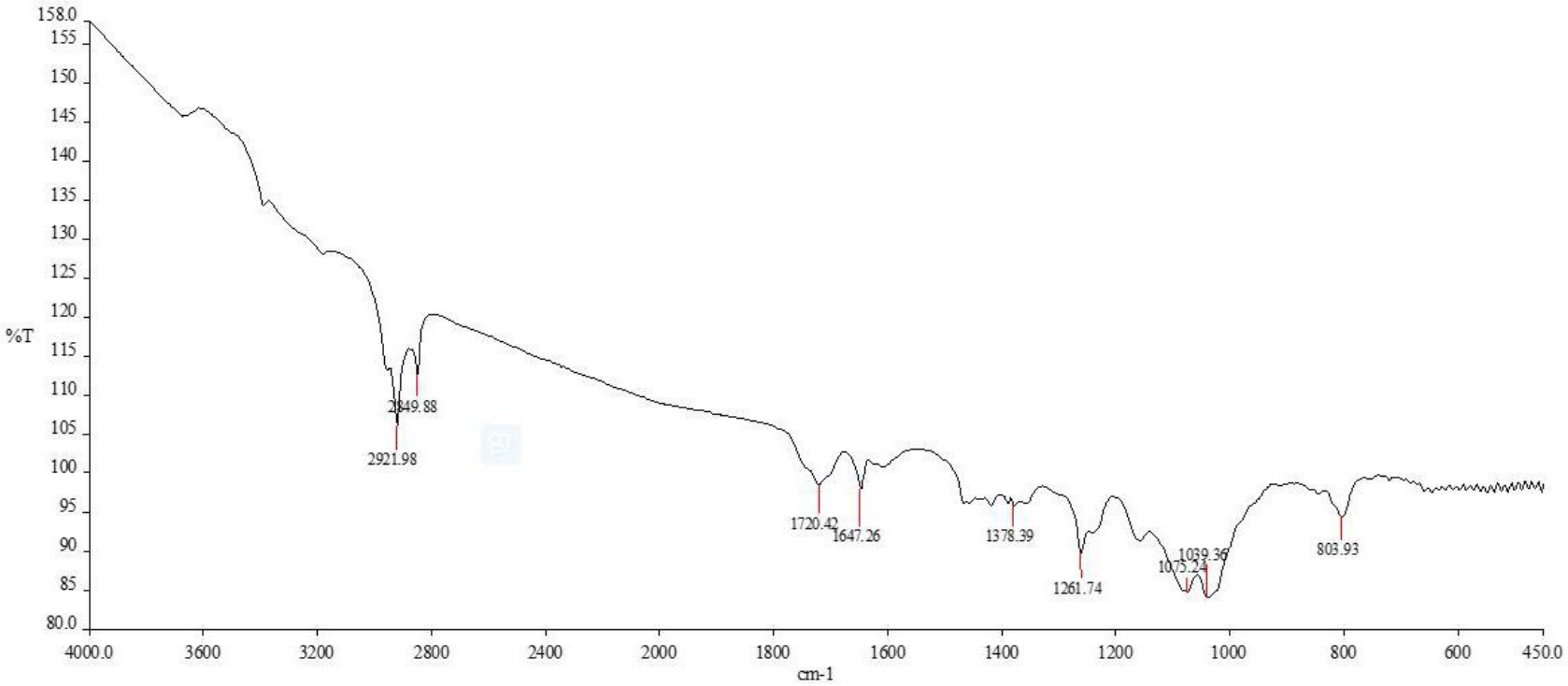


Figure S40. ^{1}H-NMR Spectrum of 6′-methylester-O-Xanifolia-Y8 (7) in C_5D_5N.

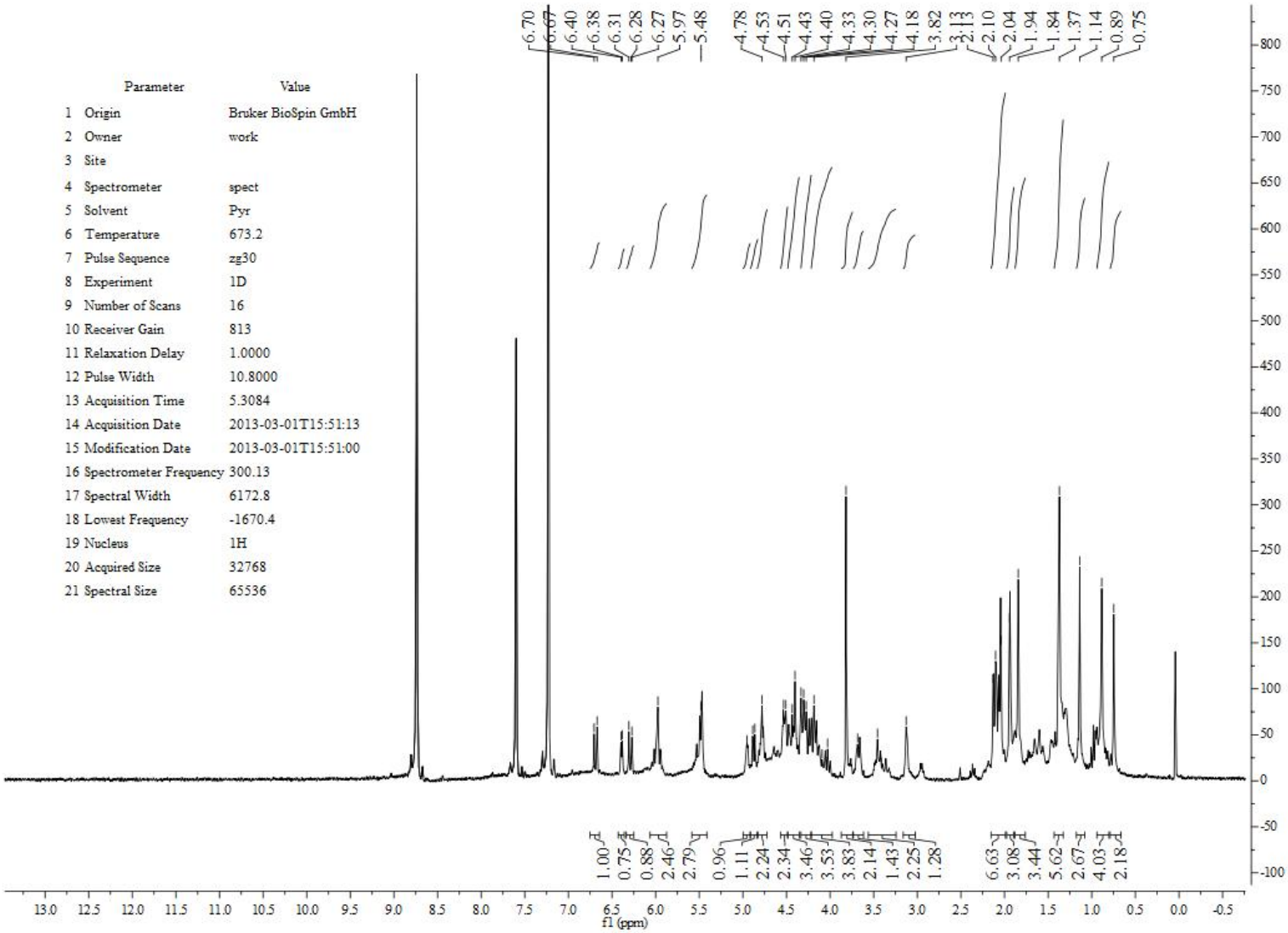


Figure S41. ^{13}C-NMR Spectrum of 6′-methylester-O-Xanifolia-Y8 (7) in C_5D_5N.

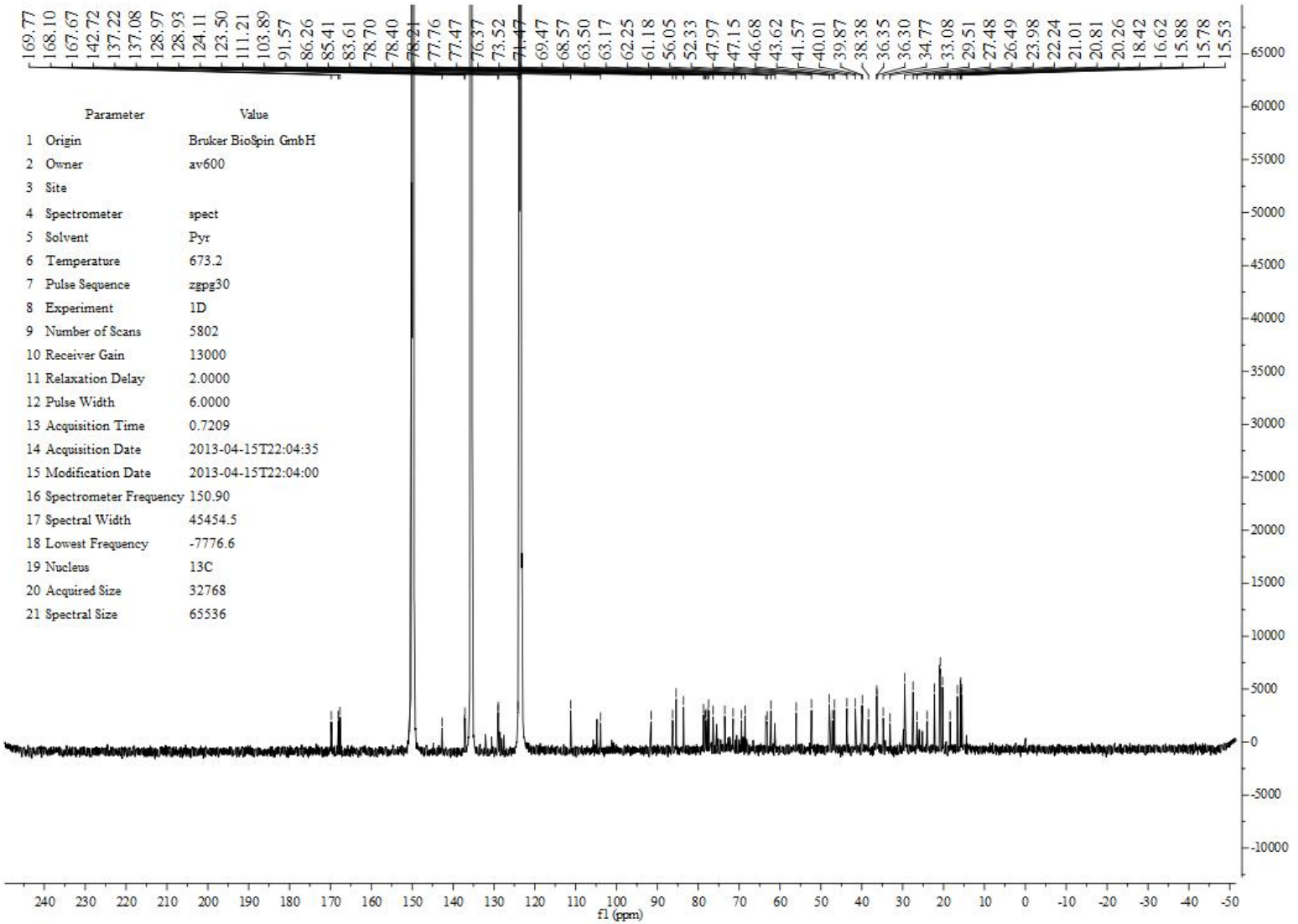


Figure S42. HR-ESI-MS Spectrum of 6′-methylester-O-Xanifolia-Y8 (7).

Mass Spectrum Molecular Formula Report

Analysis Info

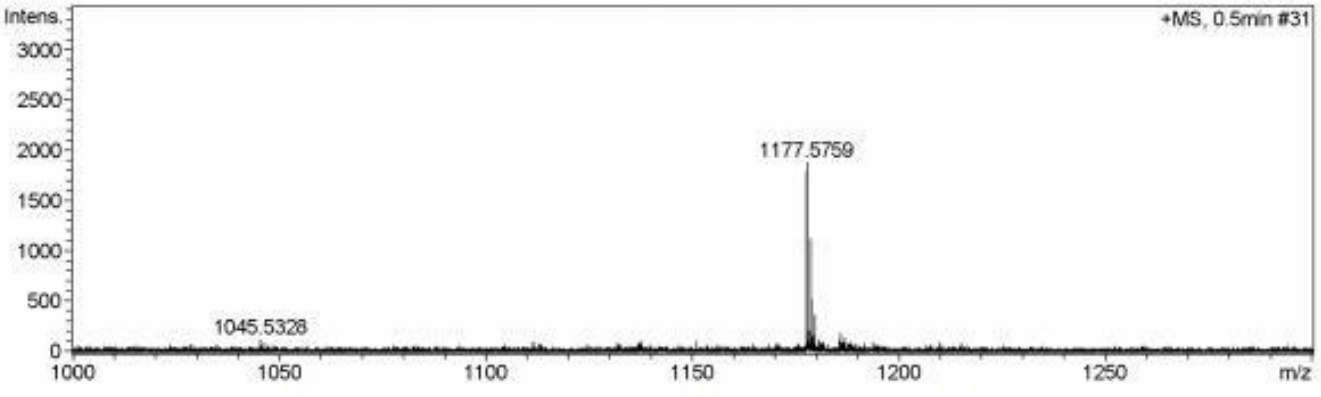
Analysis Name	D:\Data\20140312ceyang\ZL-10.d	Acquisition Date	3/12/2014 7:28:36 PM
Method	tune_high_pos.m	Operator	Bruker Customer
Sample Name	ZL-10	Instrument / Ser#	micrOTOF-Q 125
Comment			

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.	C58H90O23Na						
Formula, max.							
Measured m/z	1177.58	Tolerance	5	ppm	Charge	1	
Check Valence	no	Minimum	0		Maximum	0	
Nirogen Rule	no	Electron Configuration	both				
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 58 H 90 Na 1 O 23	0.047	1177.5765	0.51	-0.26	0.60	13.50	ok	even

Figure S43. HMBC Spectrum of 6′-methylester-O-Xanifolia-Y8 (7) in C_5D_5N.

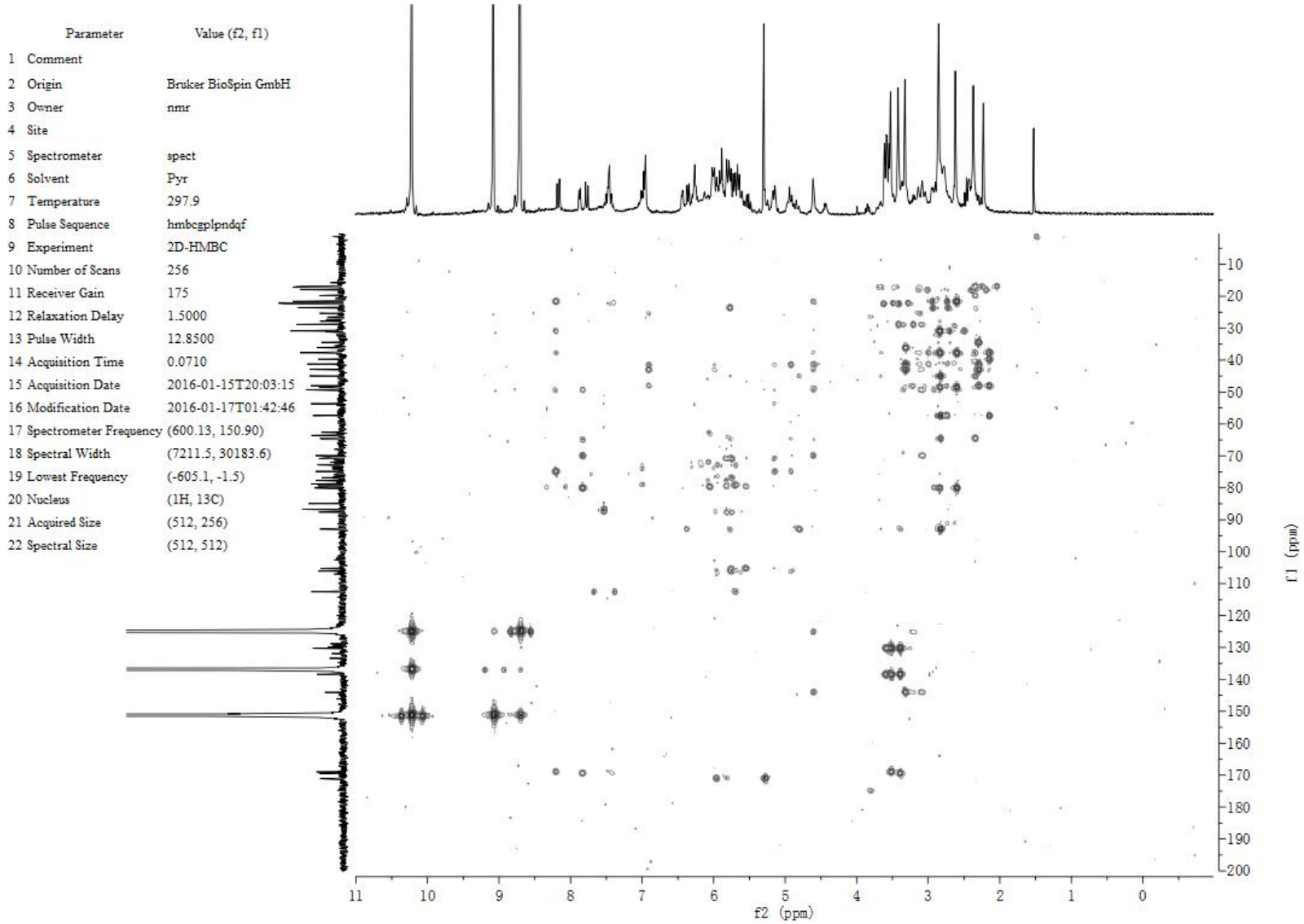


Figure S44. HSQC Spectrum of 6′-methylester-O-Xanifolia-Y8 (7) in C_5D_5N.

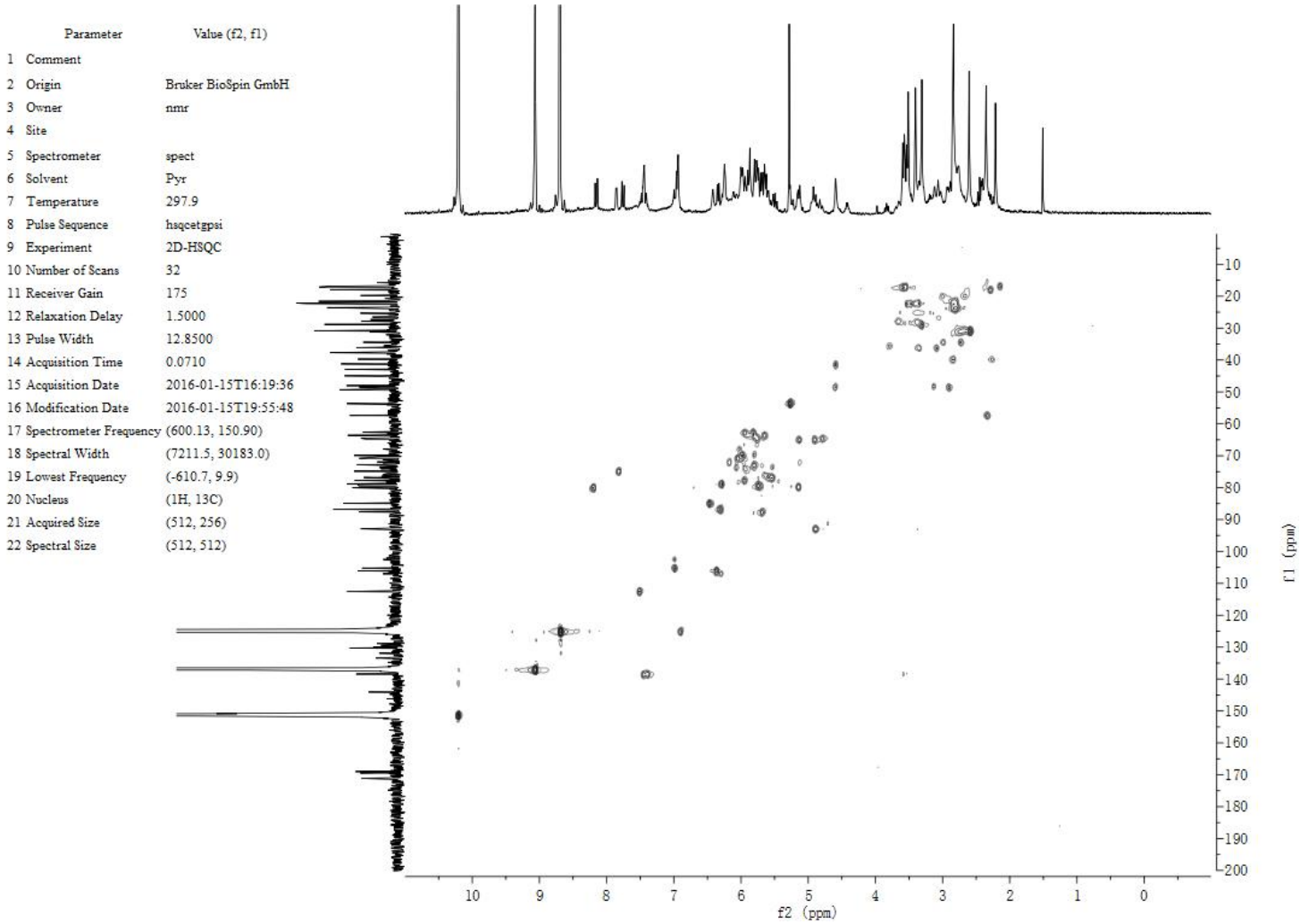


Figure S45. IR Spectrum of 6′-methylester-O-Xanifolia-Y8 (7).

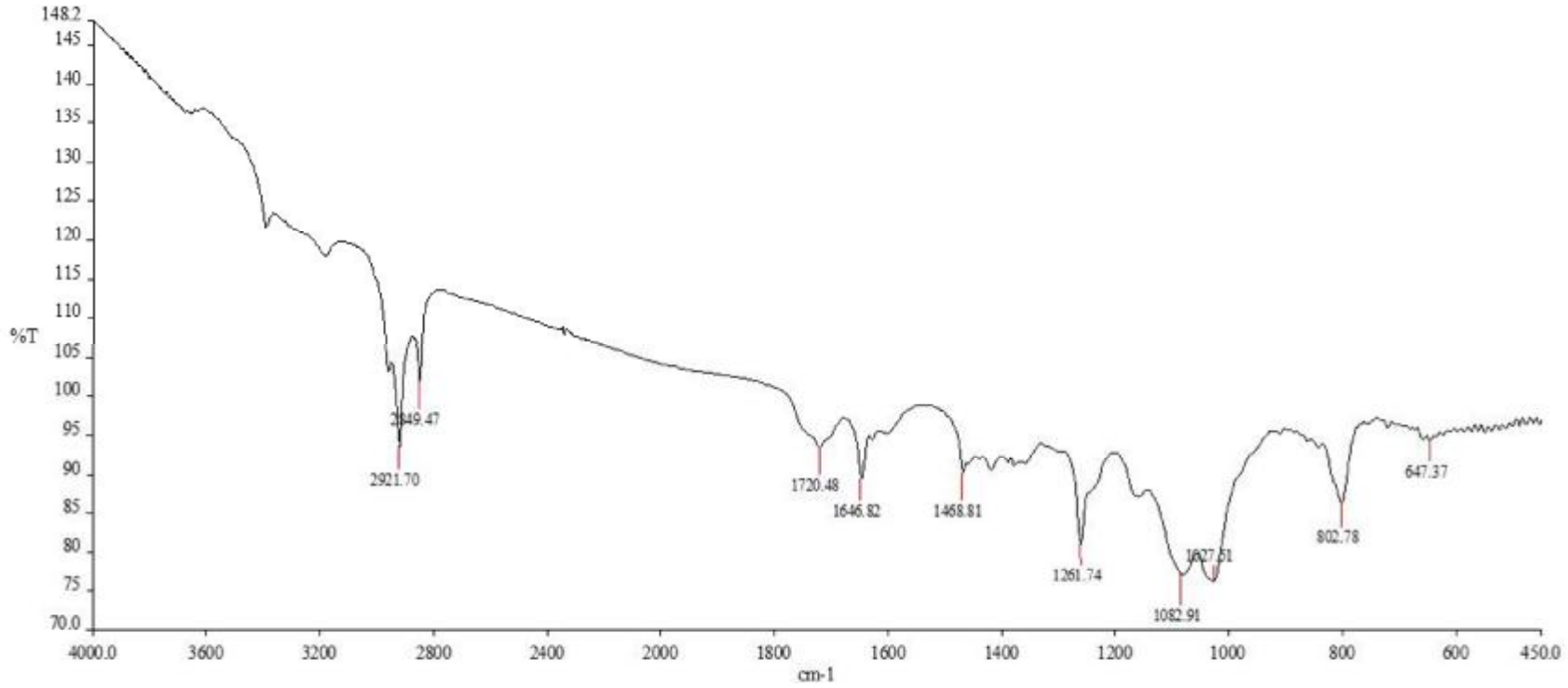


Figure S46. ^{1}H-NMR Spectrum of Xanifolia Y (8) in C_5D_5N.

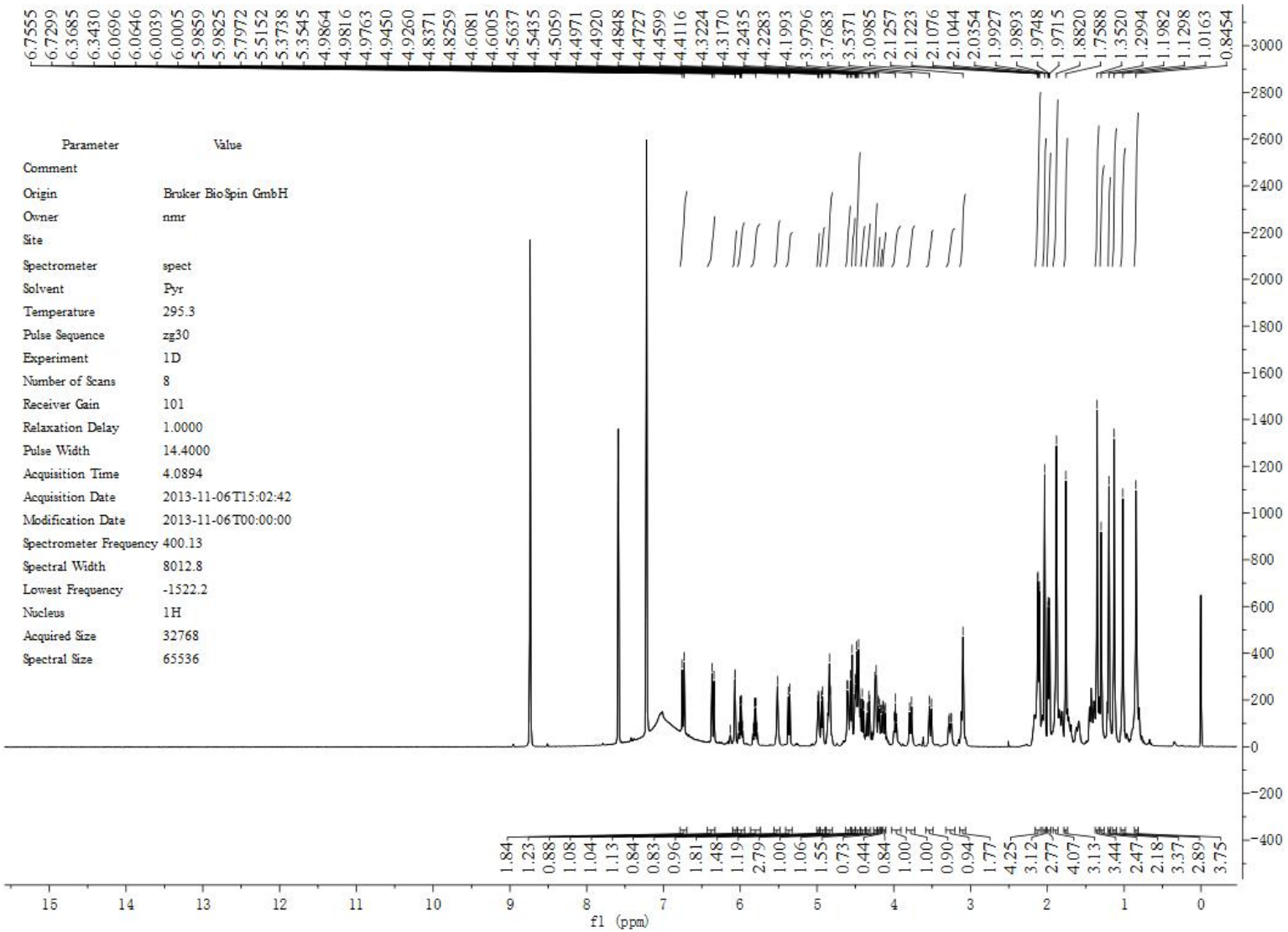


Figure S47. ^{13}C-NMR Spectrum of Xanifolia Y (8) in C_5D_5N.

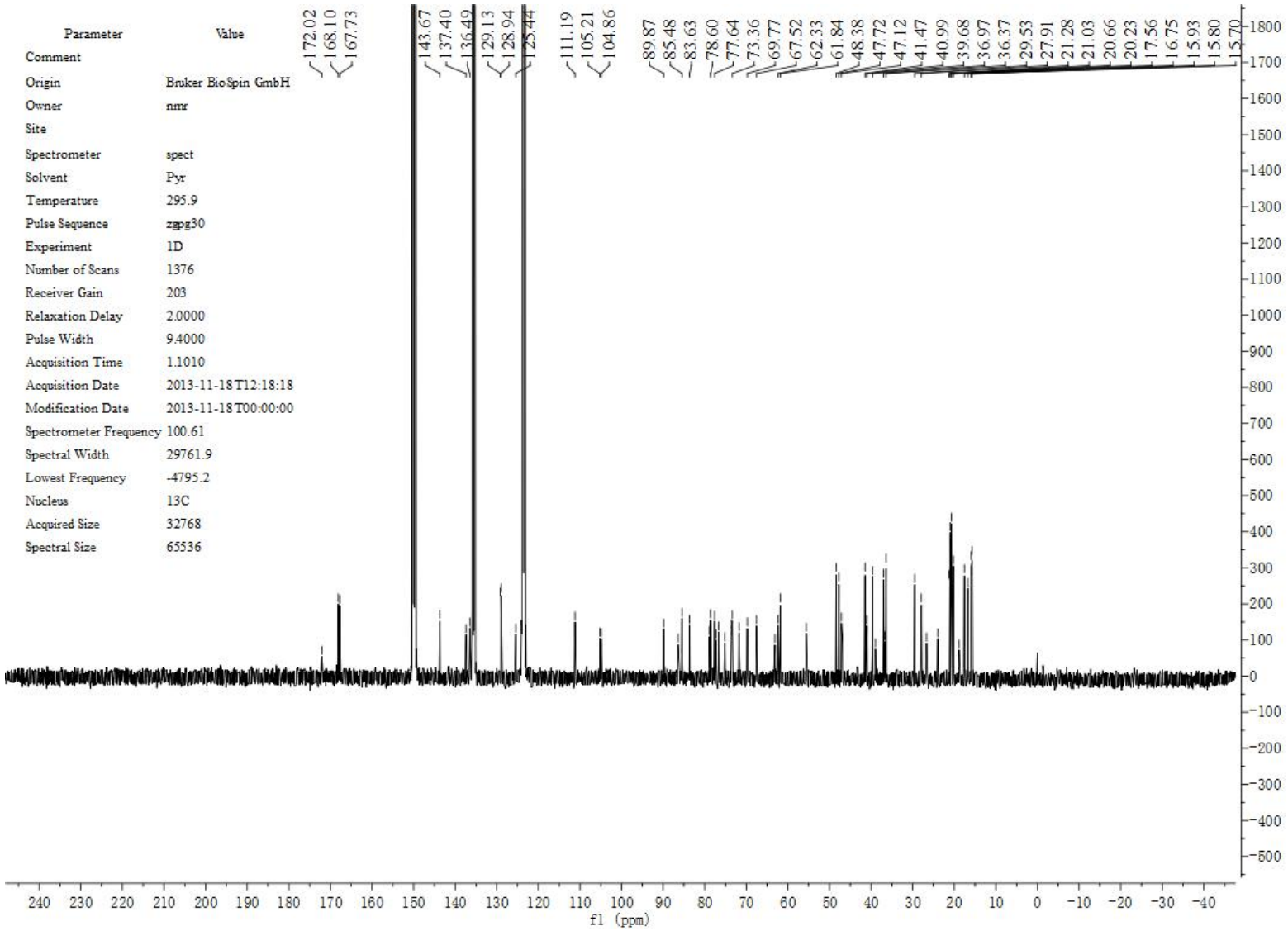


Figure S48. ^{1}H-NMR Spectrum of Xanifolia ACH-Y (9) in C_5D_5N.

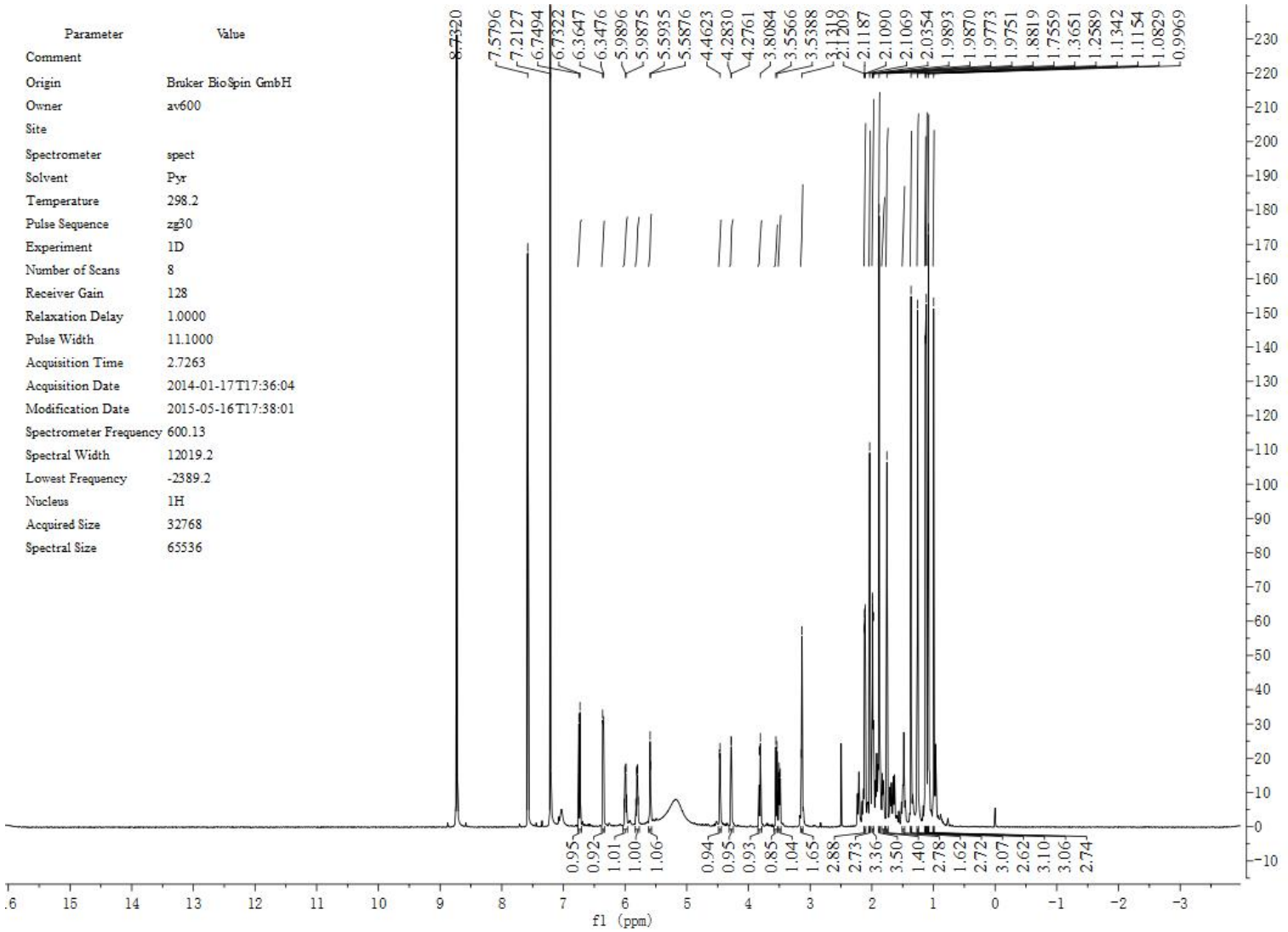


Figure S49. ^{13}C-NMR Spectrum of Xanifolia ACH-Y (9) in C_5D_5N.

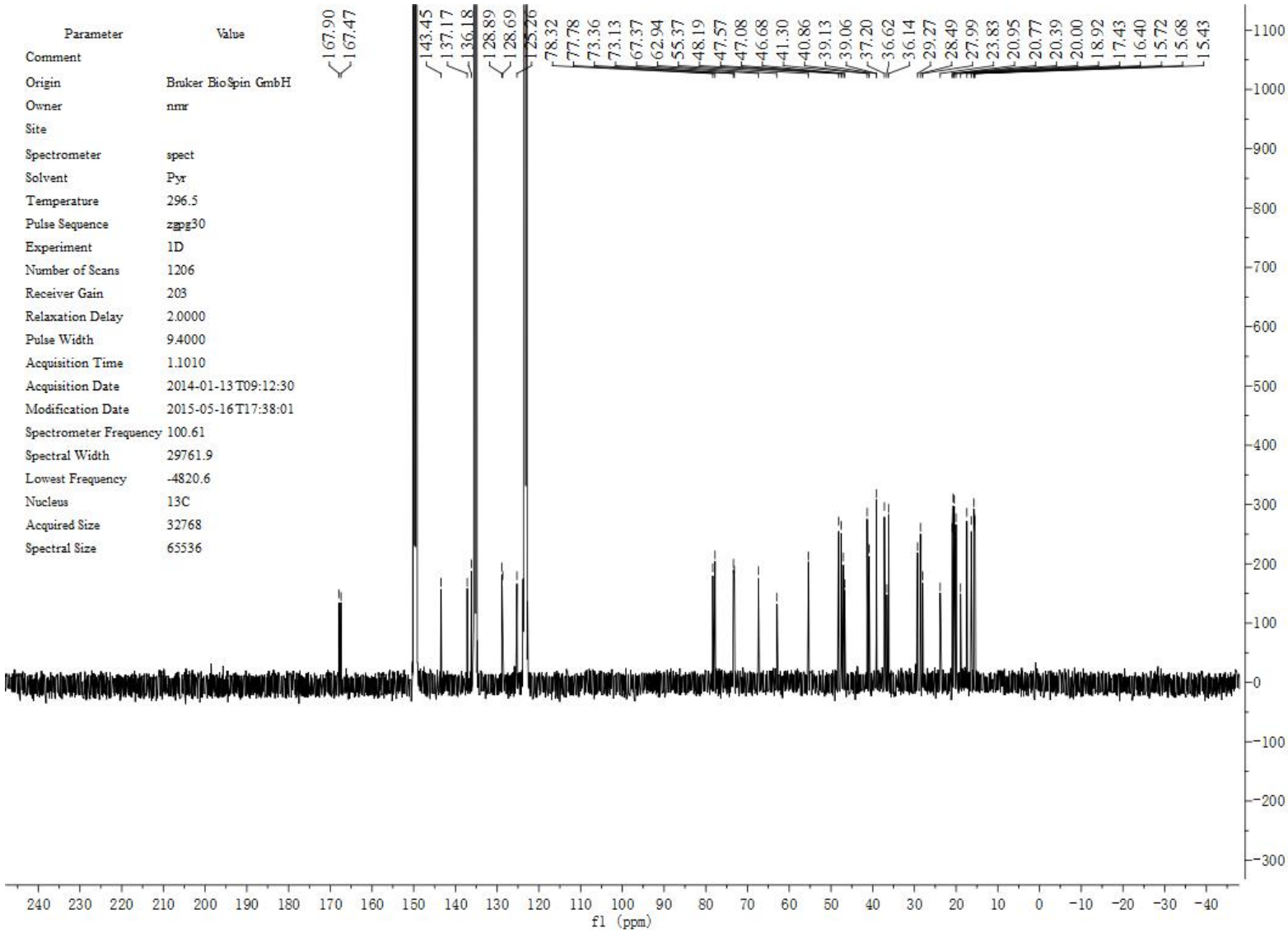


Figure S50. ^{1}H-NMR Spectrum of Xanifolia Y2 (10) in C_5D_5N.

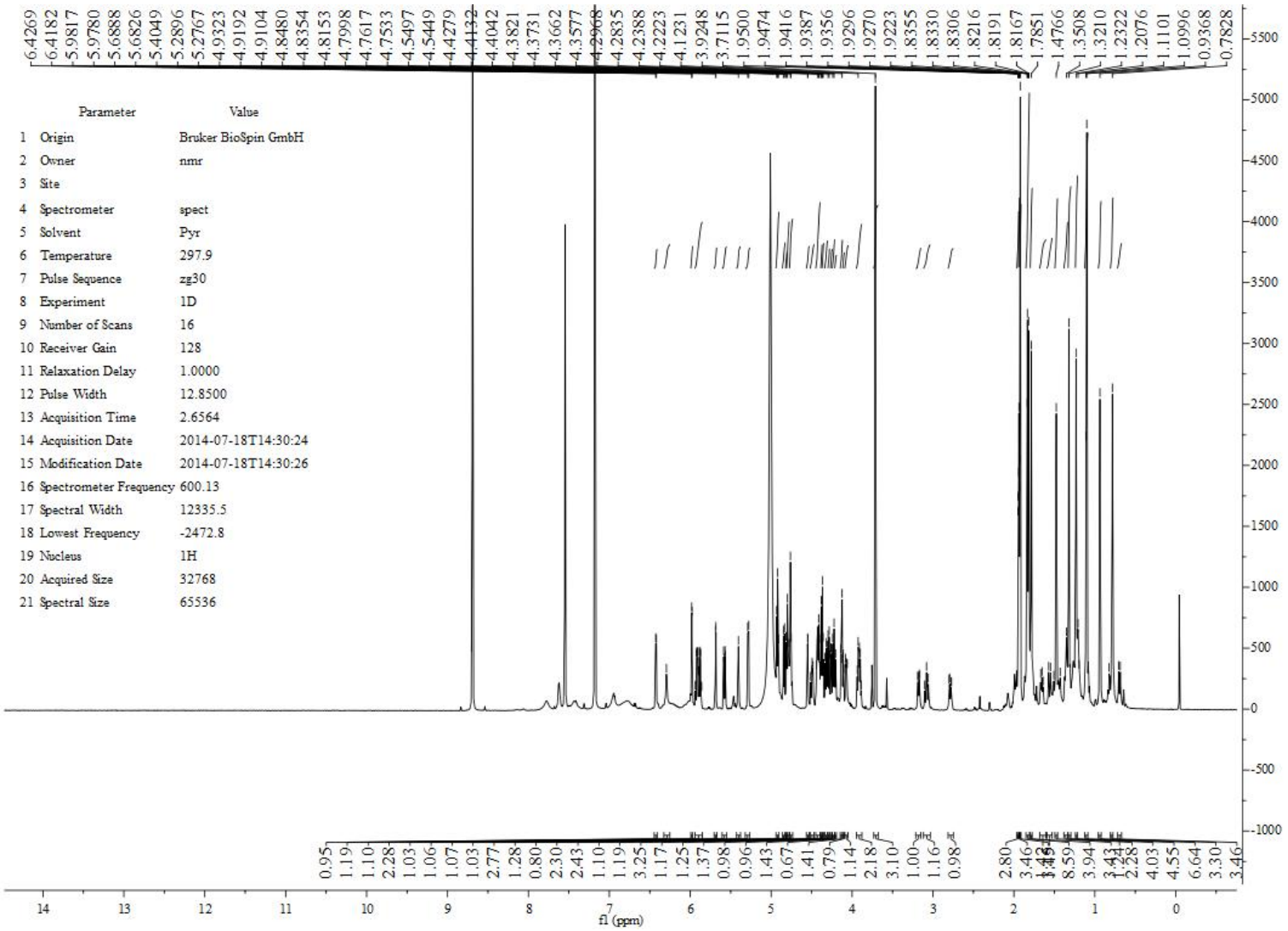


Figure S51. ^{13}C-NMR Spectrum of Xanifolia Y2 (10) in C_5D_5N.

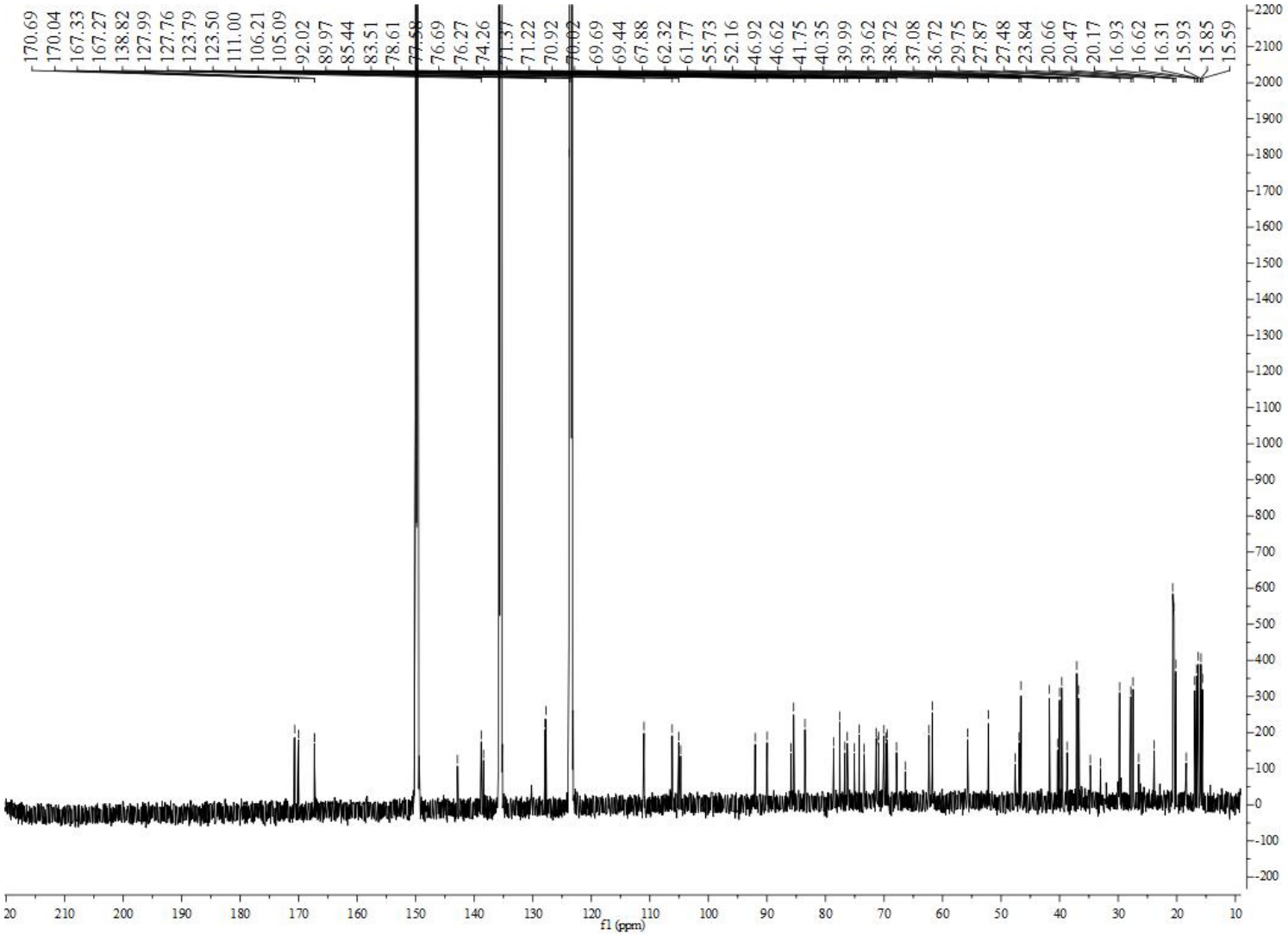


Figure S52. HR-ESI-MSSpectrum of Xanifolia Y2 (10) in C_5D_5N.

Mass Spectrum Molecular Formula Report

Analysis Info

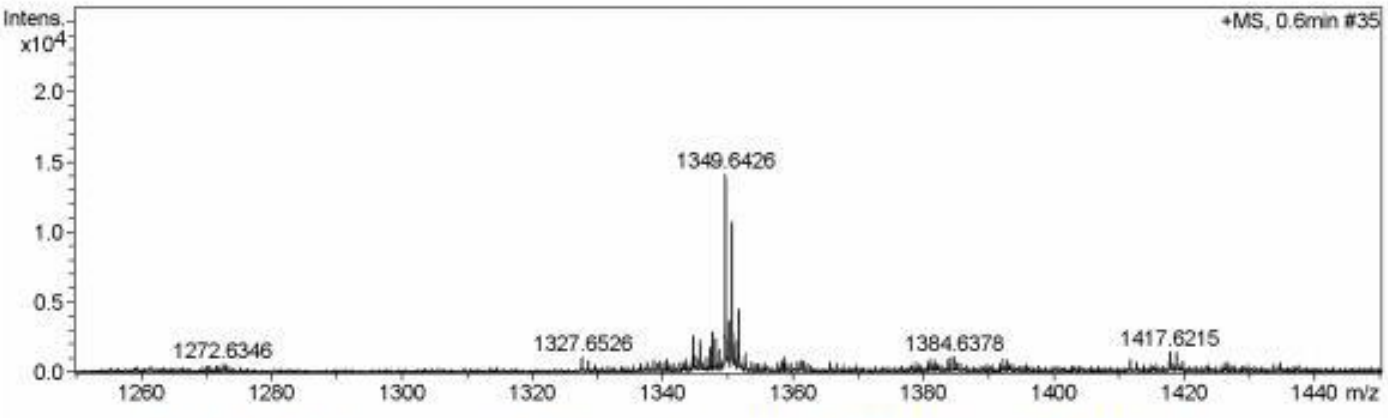
Analysis Name	D:\Data\20150605CEYANG\wd-15_1-a,7_01_5269.d	Acquisition Date	5/6/2015 12:37:12 PM
Method	20131026_ceyang.m	Operator	micrOTOF-Q
Sample Name	wd-15	Instrument / Ser#	Bruker Customer 125
Comment			

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	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

Formula, min.	C66H102O27Na				
Formula, max.					
Measured m/z	1349.64	Tolerance	6 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
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 66 H 102 Na 1 O 27	0.018	1349.6501	5.54	7.44	7.47	15.50	ok	even