

**Anti-Adipogenic Lanostane-Type Triterpenoids from the Edible and Medicinal Mushroom *Ganoderma applanatum***

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## Section S1: 1D and 2D NMR spectra of compound 1

Figure S1.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 1.

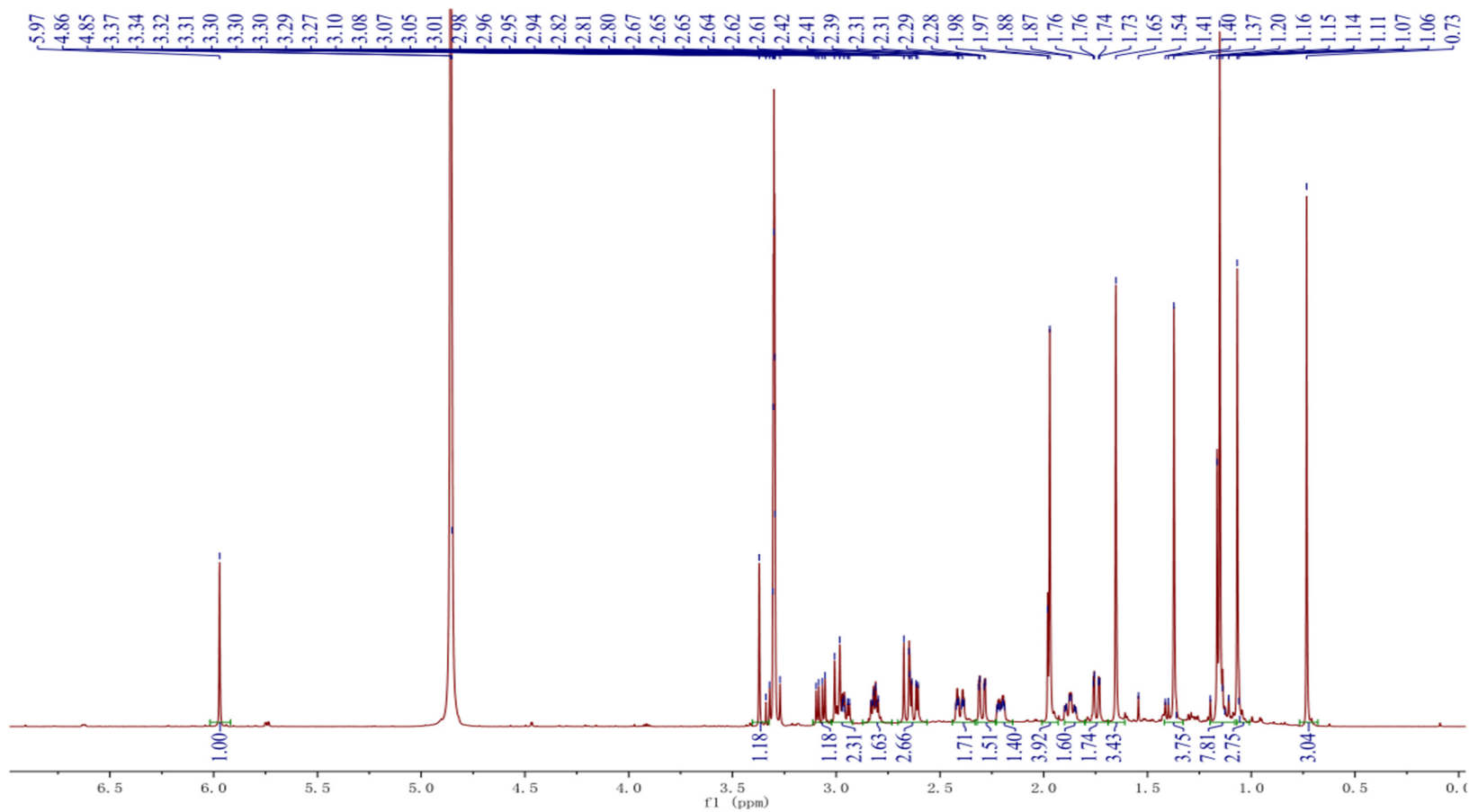


Figure S2.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 1.

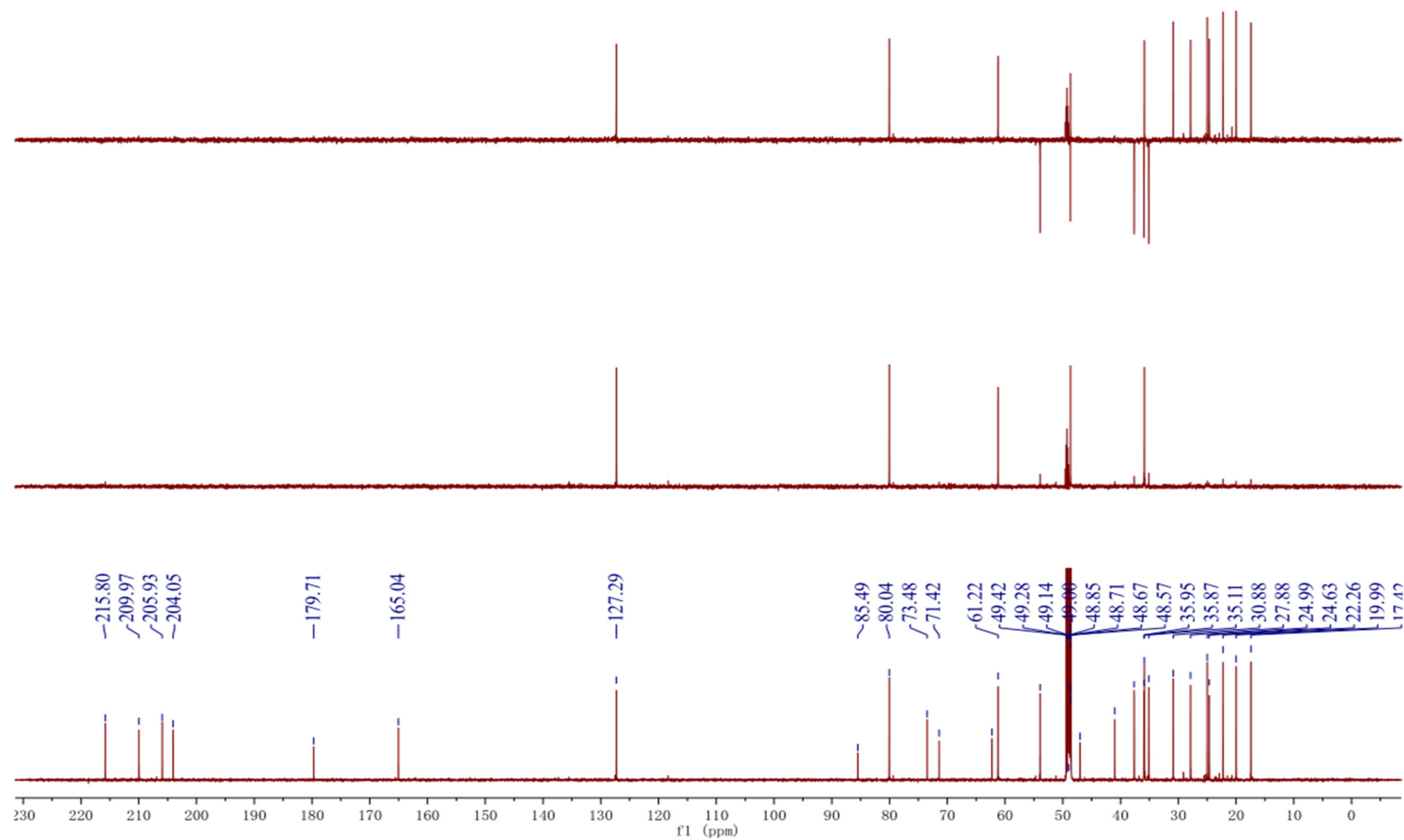


Figure S3.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 1.

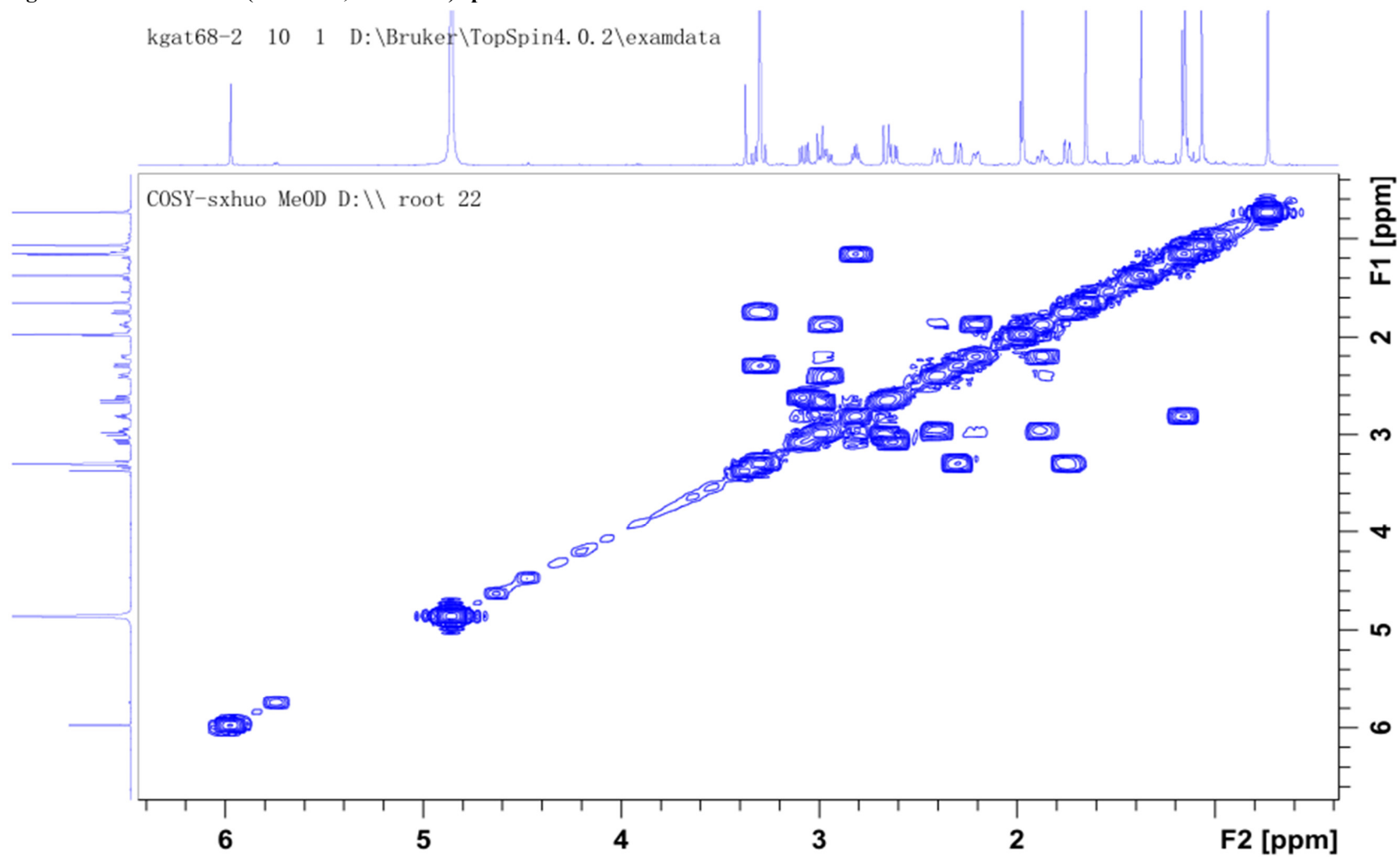


Figure S4. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 1.

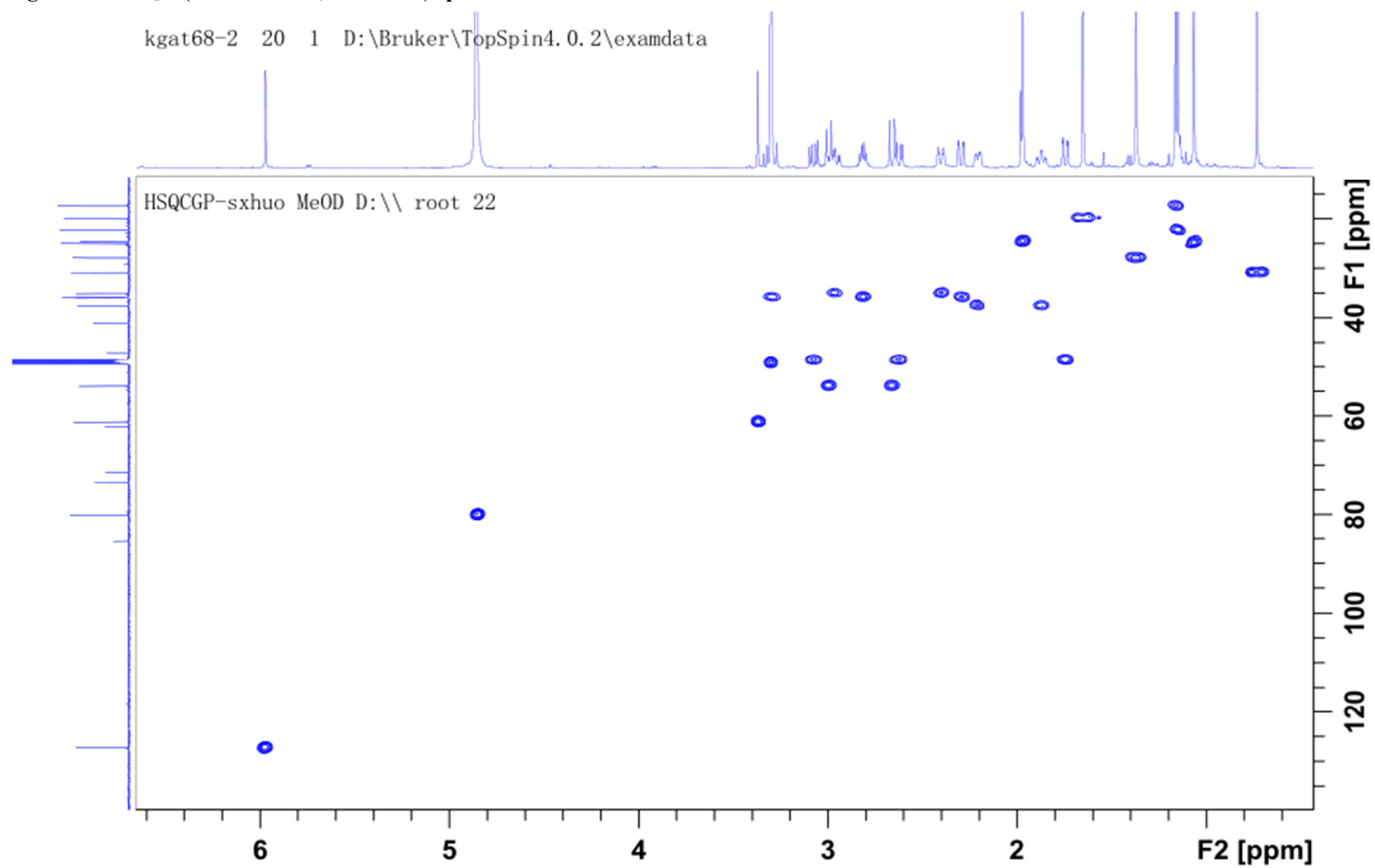


Figure S5. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 1.

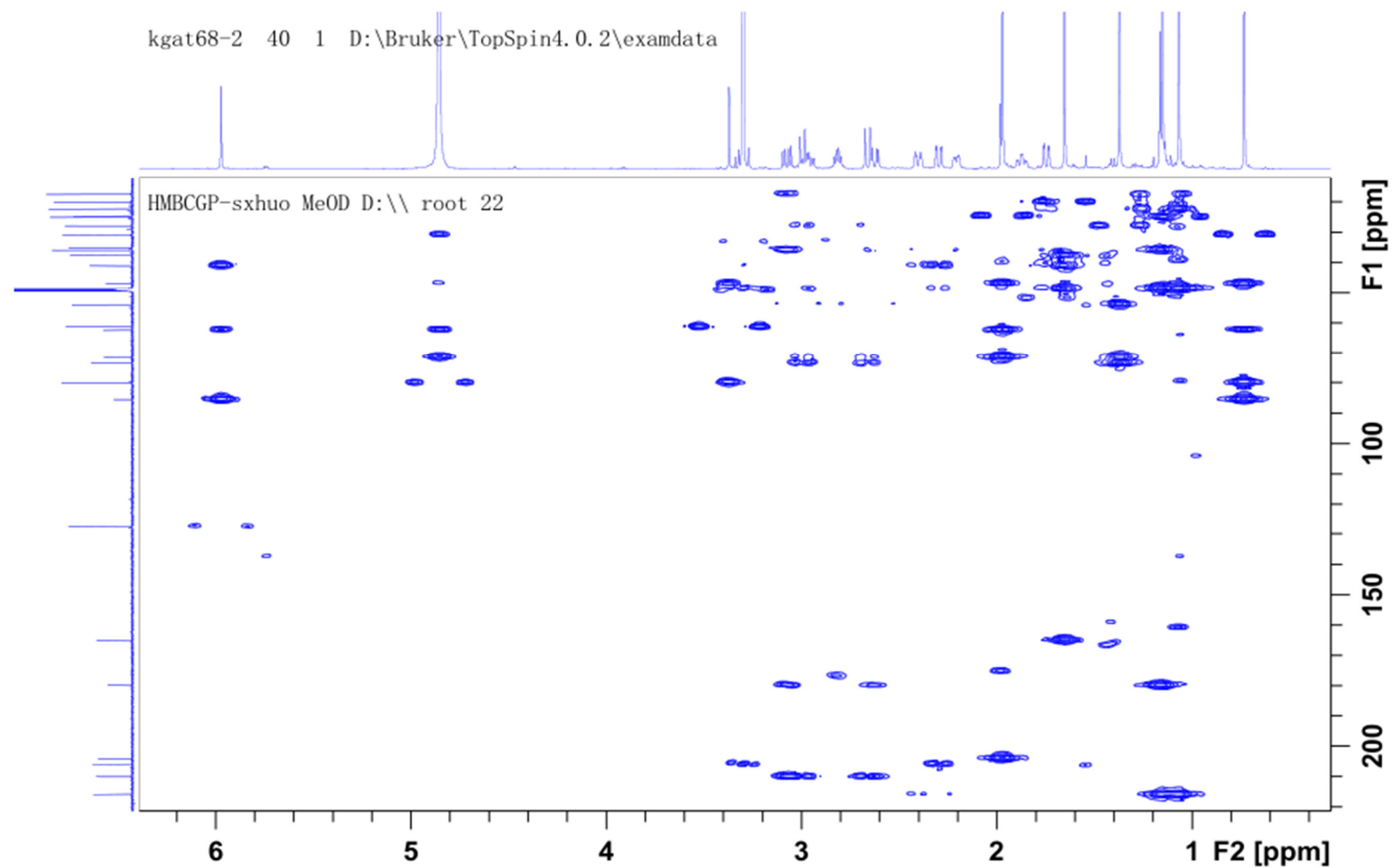
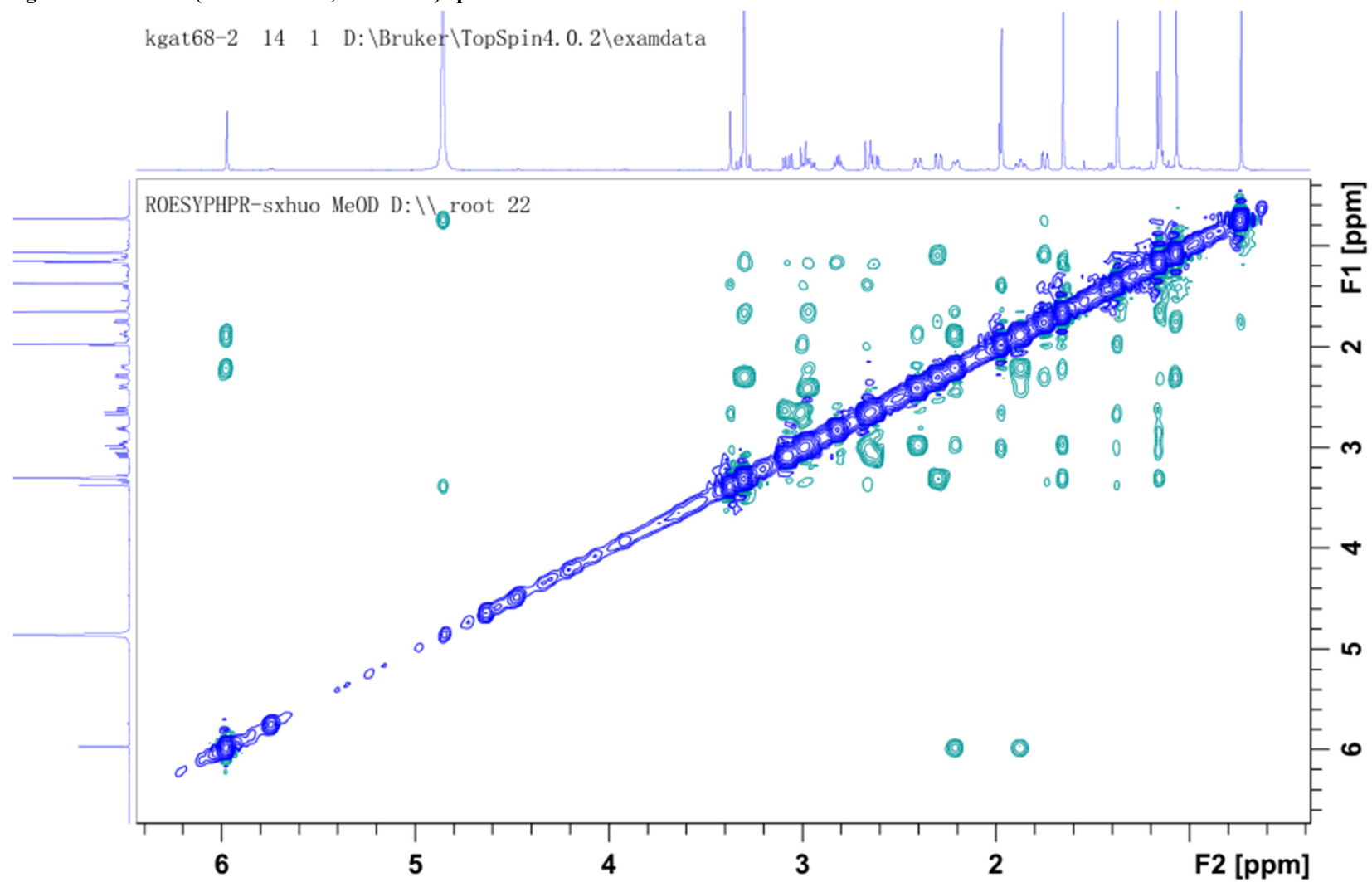


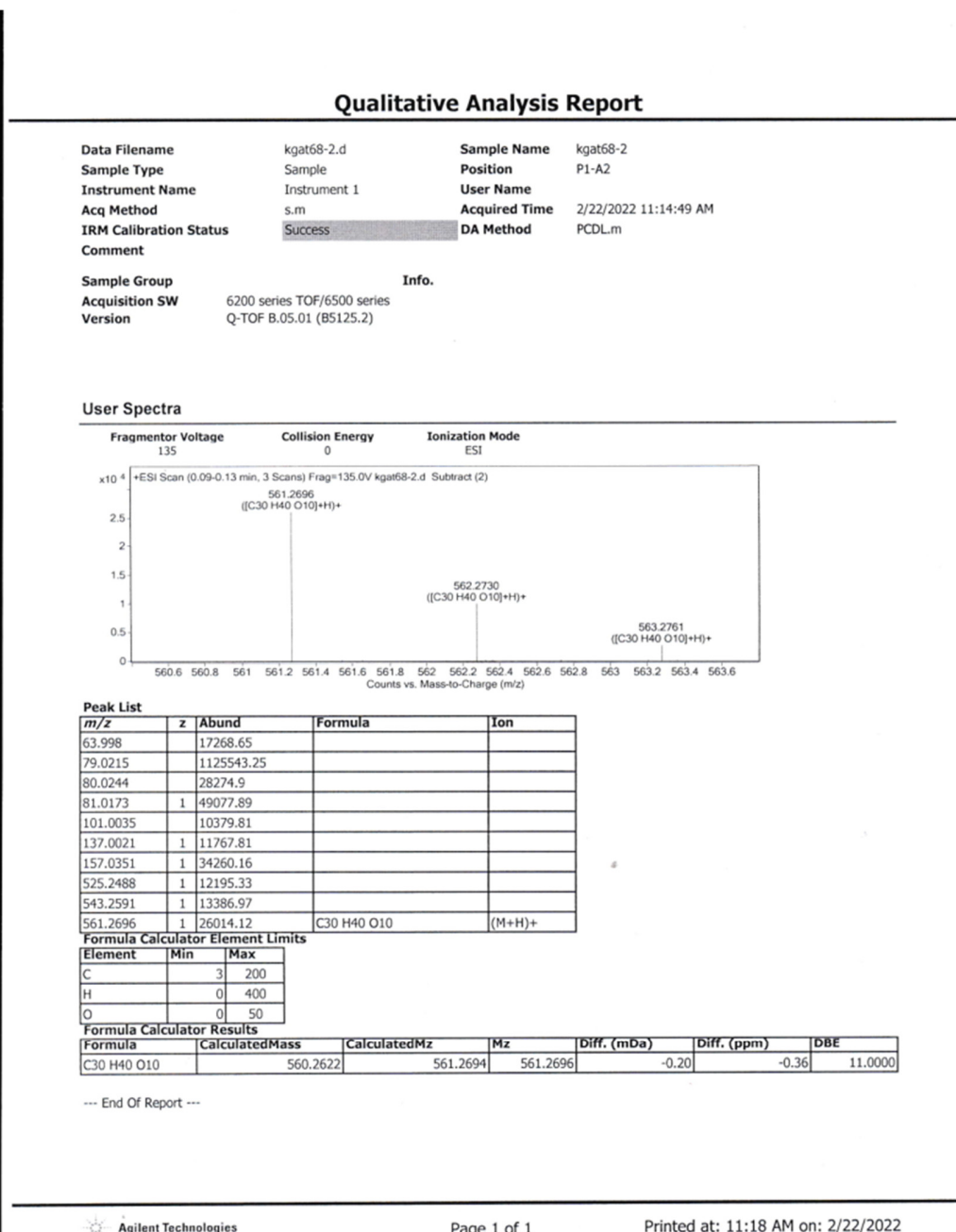


Figure S6. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 1.

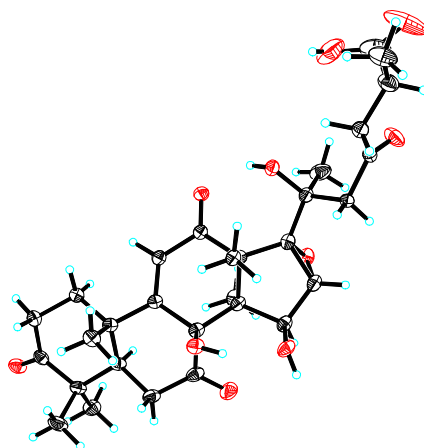


## Section S2: HRESIMS spectrum of 1

Figure S7. HRESIMS spectrum of 1.



### Section S3: X-ray crystallographic data of 1



View of a molecule of 1 with the atom-labelling scheme.  
Displacement ellipsoids are drawn at the 30% probability level.

**Table S1. Crystal data and structure refinement for 1.**

Identification code	global
Empirical formula	C <sub>31</sub> H <sub>46</sub> O <sub>12</sub>
Formula weight	610.68
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 13.9761(7) Å, $\alpha$ = 90°; b = 6.9089(3) Å, $\beta$ = 90.948(2)°; c = 15.8732(7) Å, $\gamma$ = 90°
Volume	1532.50(12) Å <sup>3</sup>
Z	2
Density (calculated)	1.323 Mg/m <sup>3</sup>
Absorption coefficient	0.844 mm <sup>-1</sup>
F(000)	656
Crystal size	1.050 x 0.140 x 0.120 mm <sup>3</sup>
Theta range for data collection	2.78 to 72.57°
Index ranges	-17 ≤ h ≤ 17, -8 ≤ k ≤ 8, -19 ≤ l ≤ 19
Reflections collected	26208
Independent reflections	5973 [R(int) = 0.0593]
Completeness to theta = 72.57°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.91 and 0.62
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5973 / 352 / 506
Goodness-of-fit on F <sup>2</sup>	1.042
Final R indices [I > 2σ(I)]	R1 = 0.0504, wR2 = 0.1381
R indices (all data)	R1 = 0.0543, wR2 = 0.1436
Absolute structure parameter	0.07(9)
Largest diff. peak and hole	0.372 and -0.254 e.Å <sup>-3</sup>

## Section S4: 1D and 2D NMR spectra of compound 2

Figure S8.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 2.

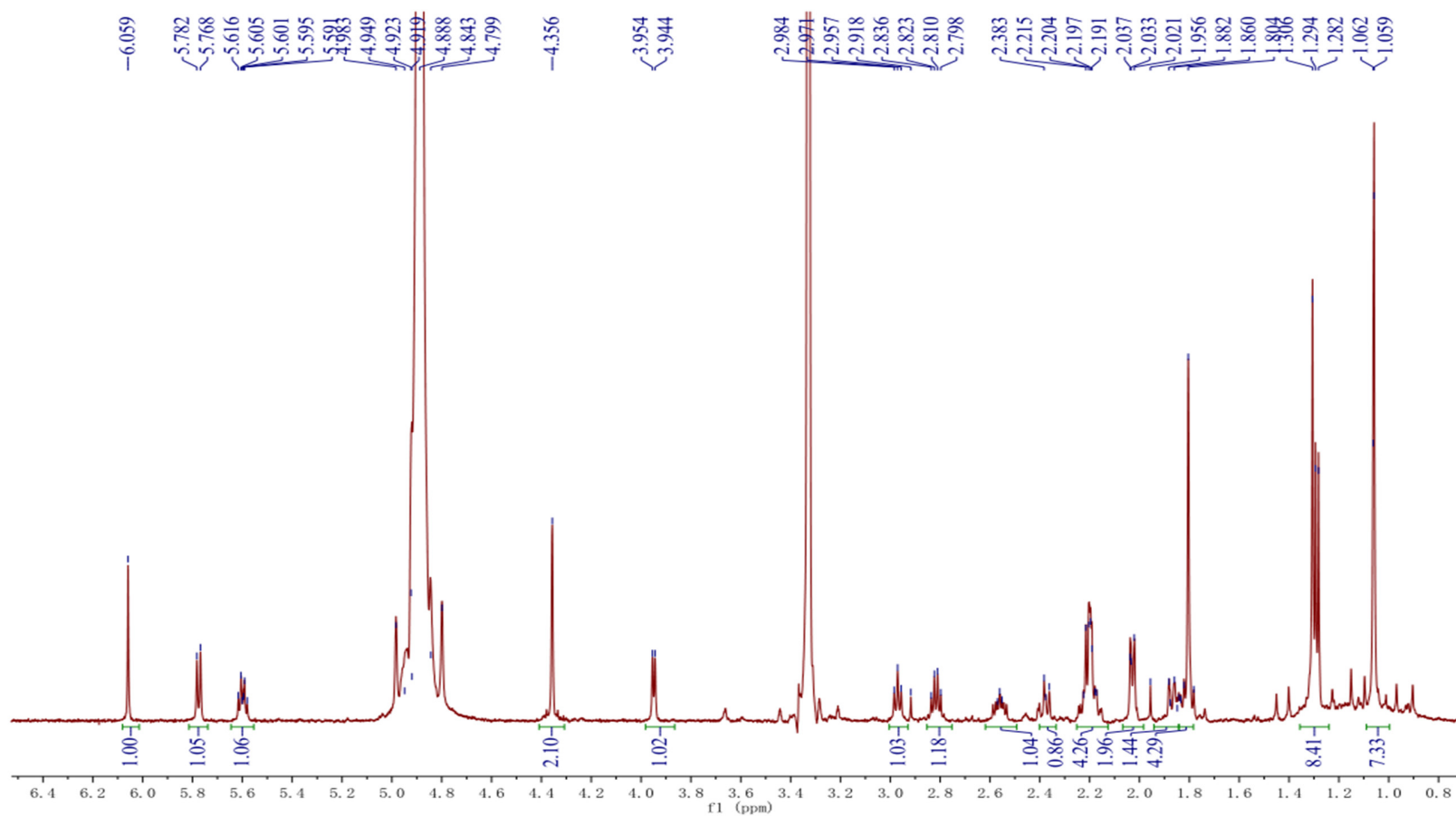


Figure S9.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 2.

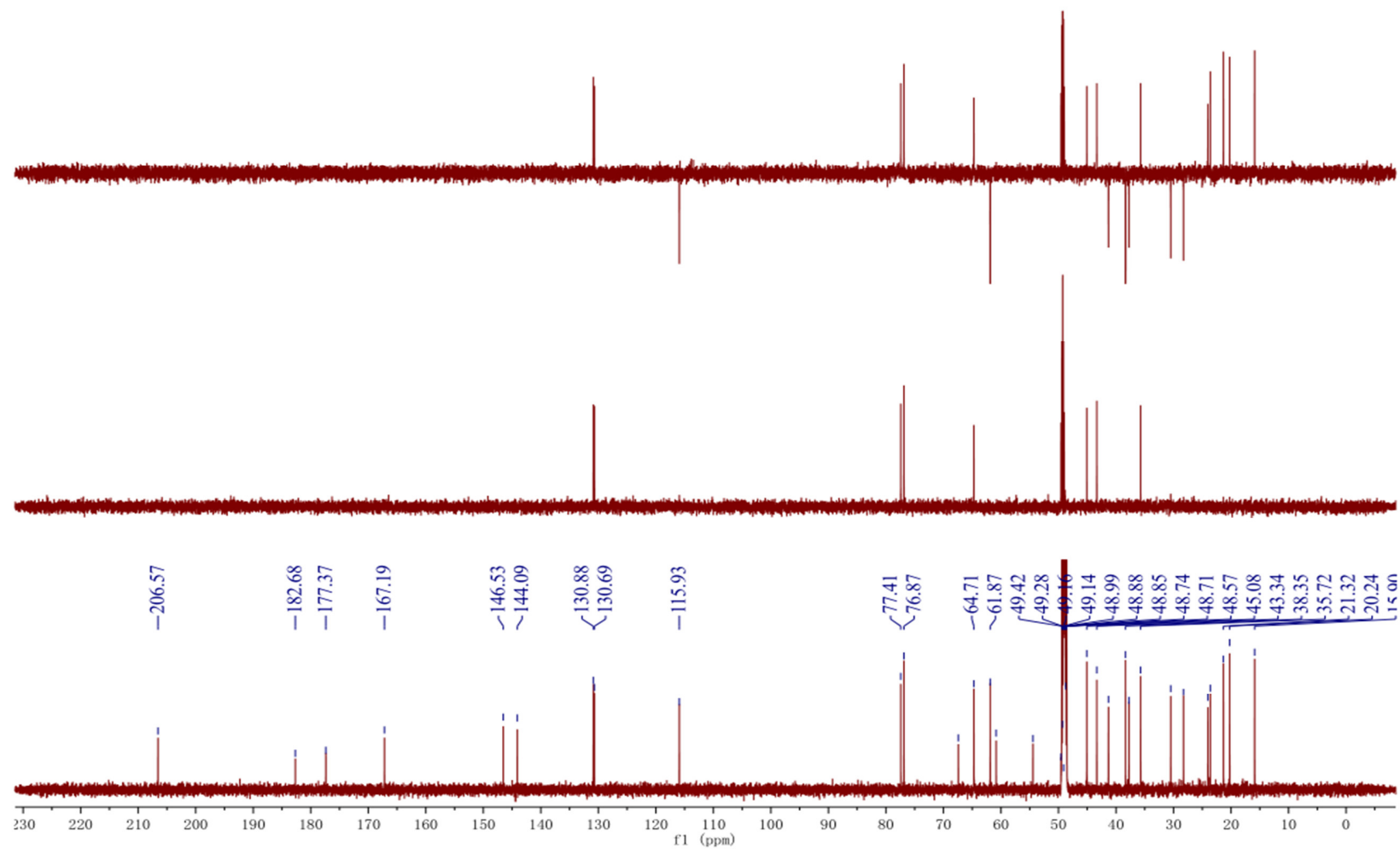


Figure S10.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 2.

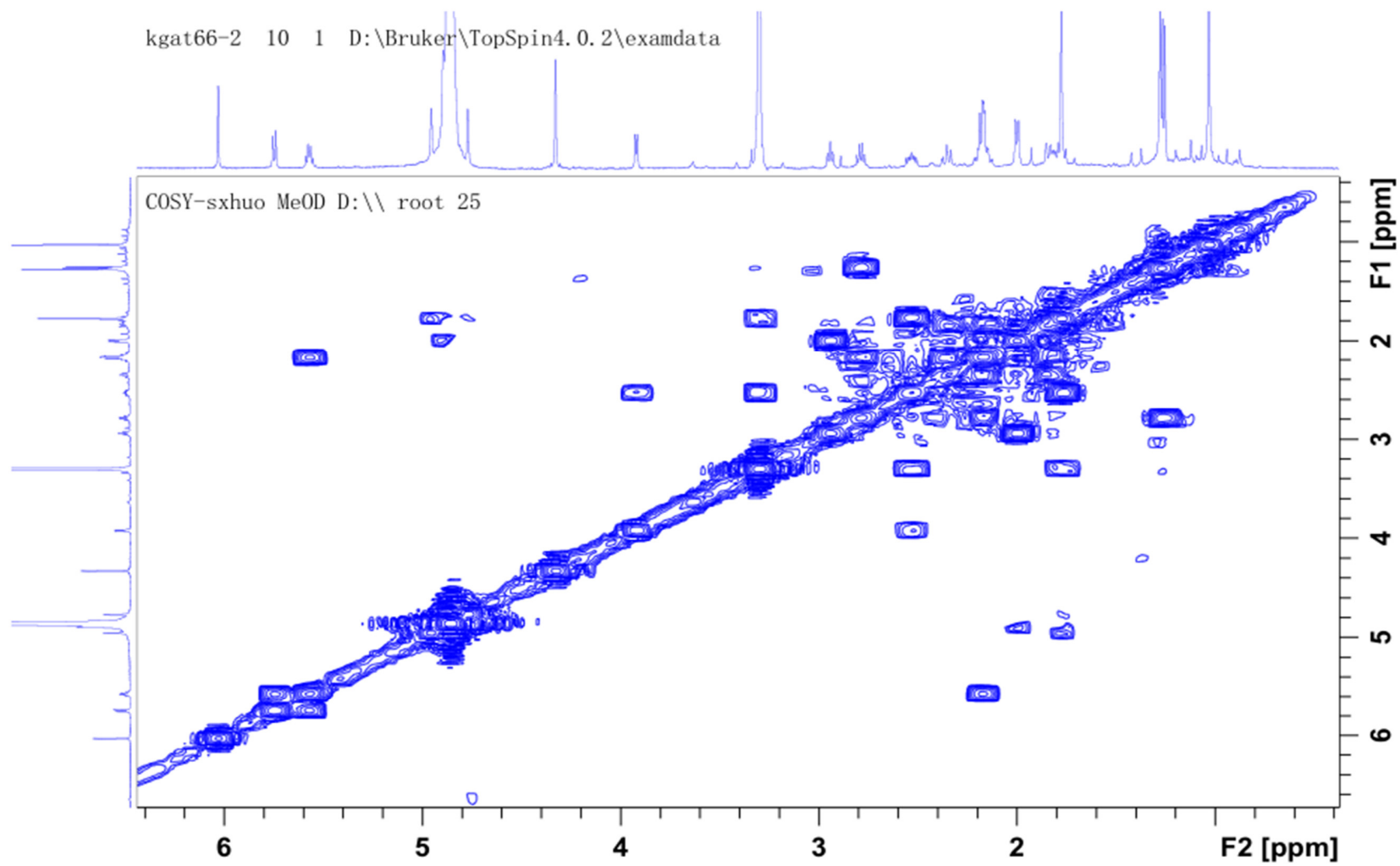


Figure S11. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 2.

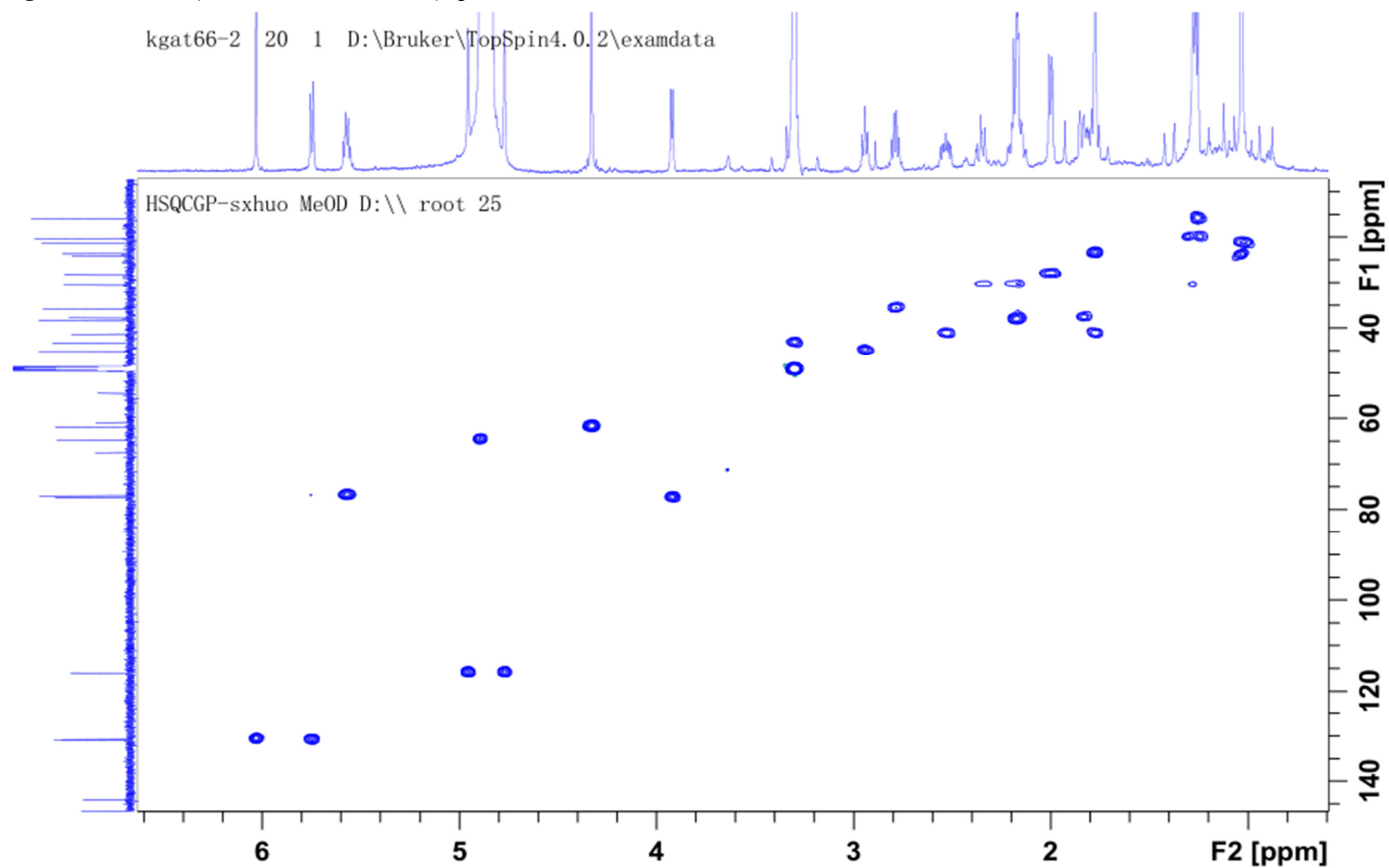
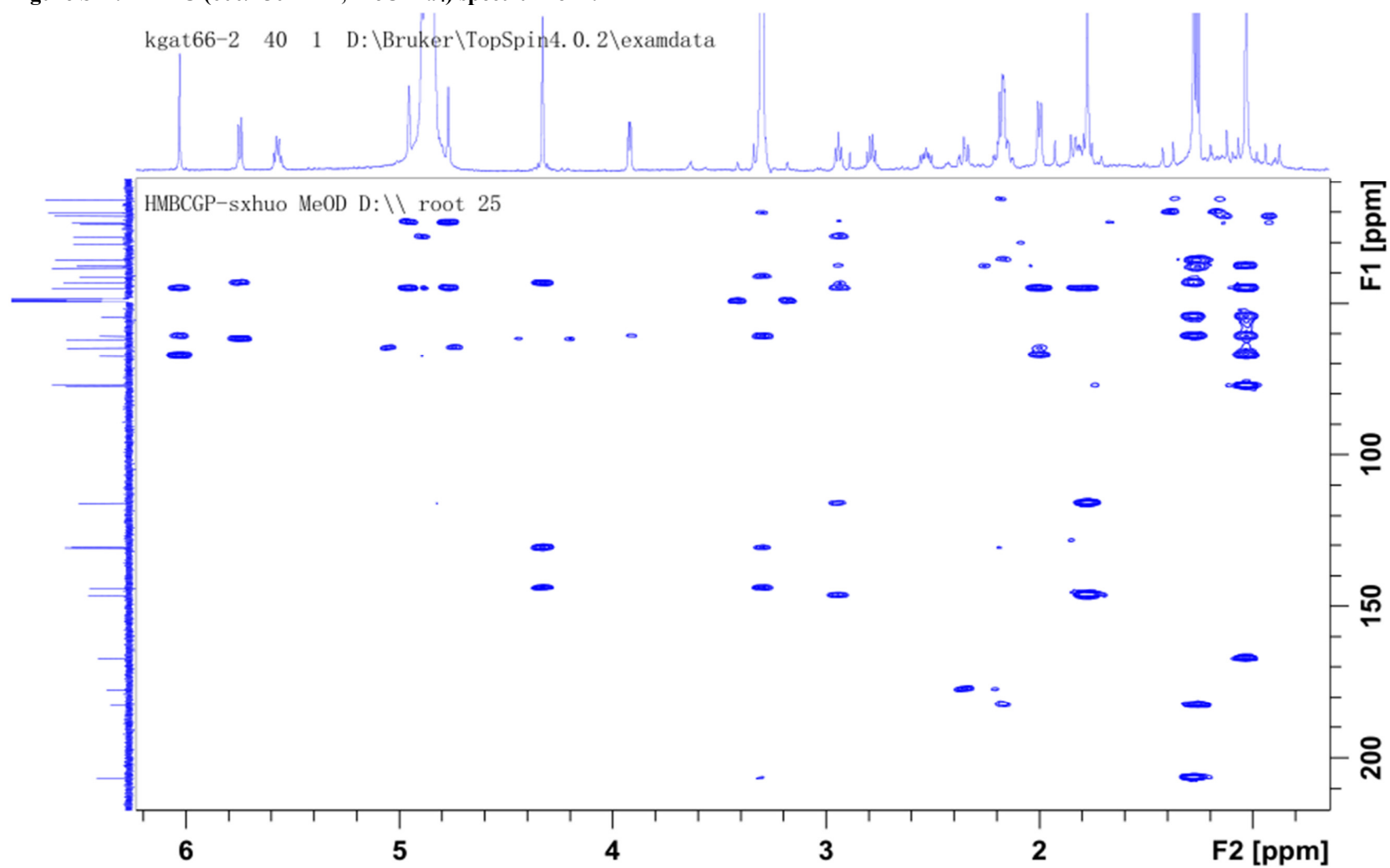




Figure S12. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 2.





**Section S5: HRESIMS spectrum of 2**

**Figure S14. HRESIMS spectrum of 2.**

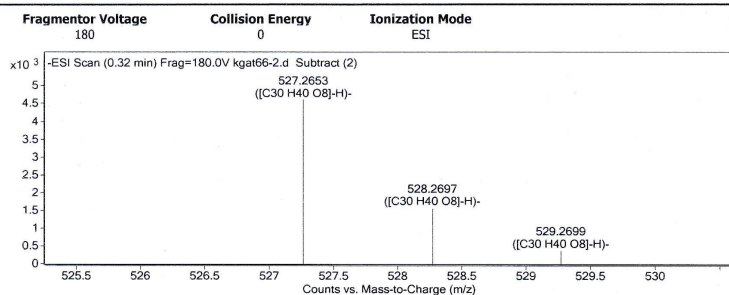
### Qualitative Analysis Report

<b>Data Filename</b>	kgat66-2.d	<b>Sample Name</b>	kgat66-2
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s-.m	<b>Acquired Time</b>	7/9/2021 2:54:52 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

#### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
324.9885		348.81		
447.5934		347.95		
448.9755		365.66		
500.3118		352.77		
527.2653	1	4608.72	C30 H40 O8	(M-H)-
528.2697	1	1573.13	C30 H40 O8	(M-H)-
529.2699	1	360.96	C30 H40 O8	(M-H)-
573.2709		593.19		
595.2445		440.07		
948.0079		444.48		
1071.9621		314.56		
1306.9568		366.34		

#### 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
C30 H40 O8	528.2723	527.2650	527.2653	-0.30	-0.57	11.0000

--- End Of Report ---

## Section S6: 1D and 2D NMR spectra of compound 3

Figure S15.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 3.

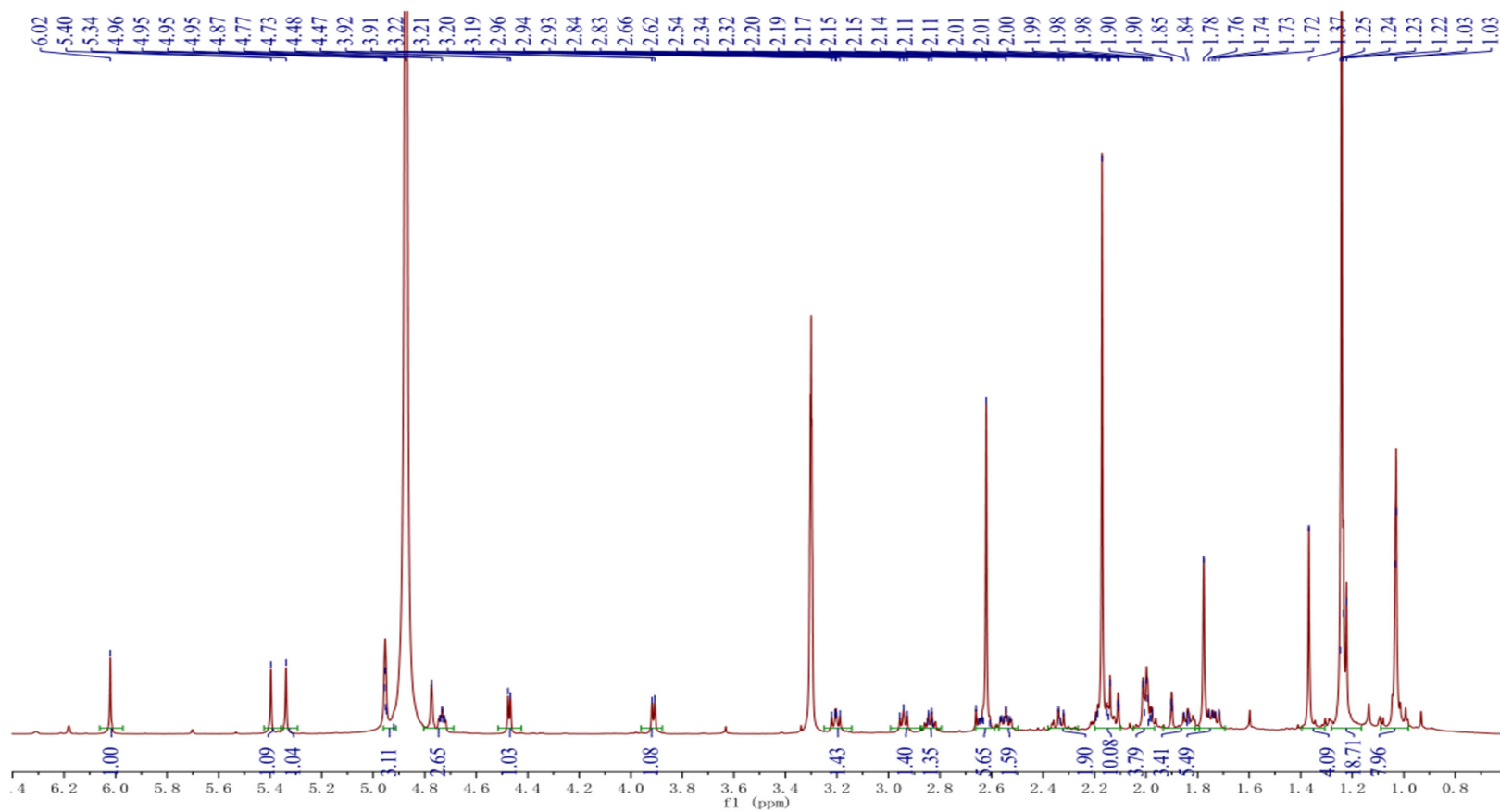


Figure S16.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 3.

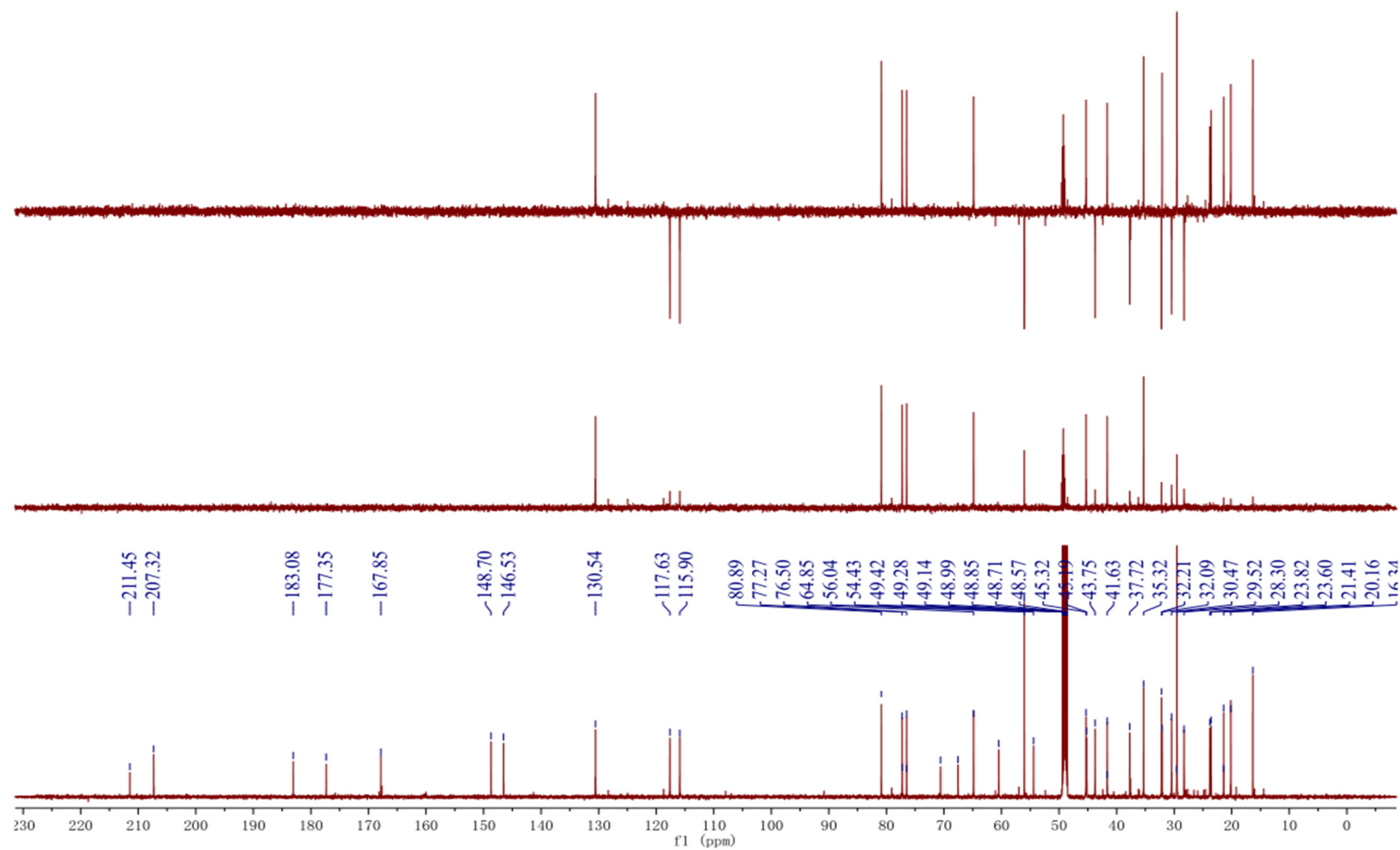


Figure S17.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 3.

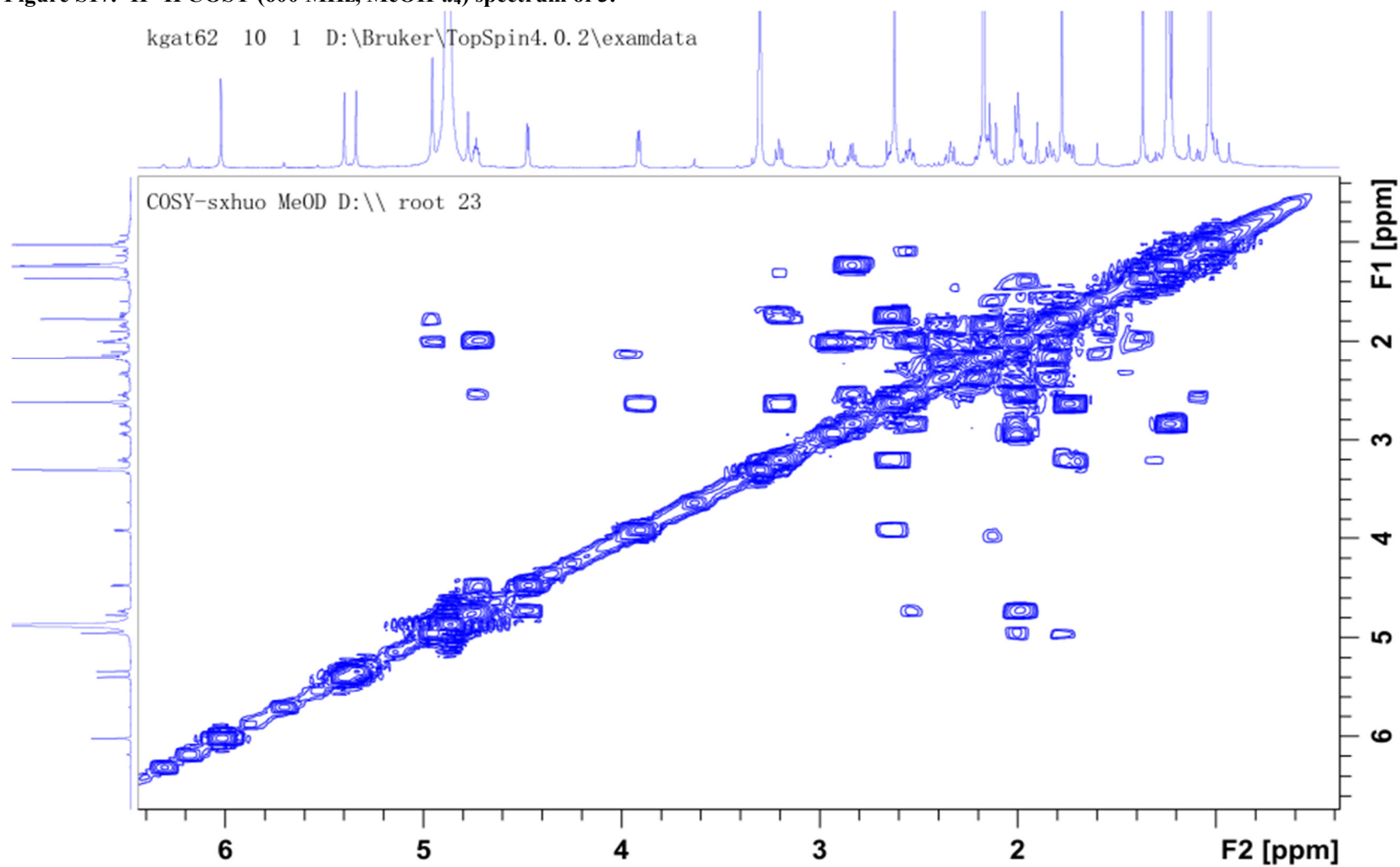


Figure S18. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 3.

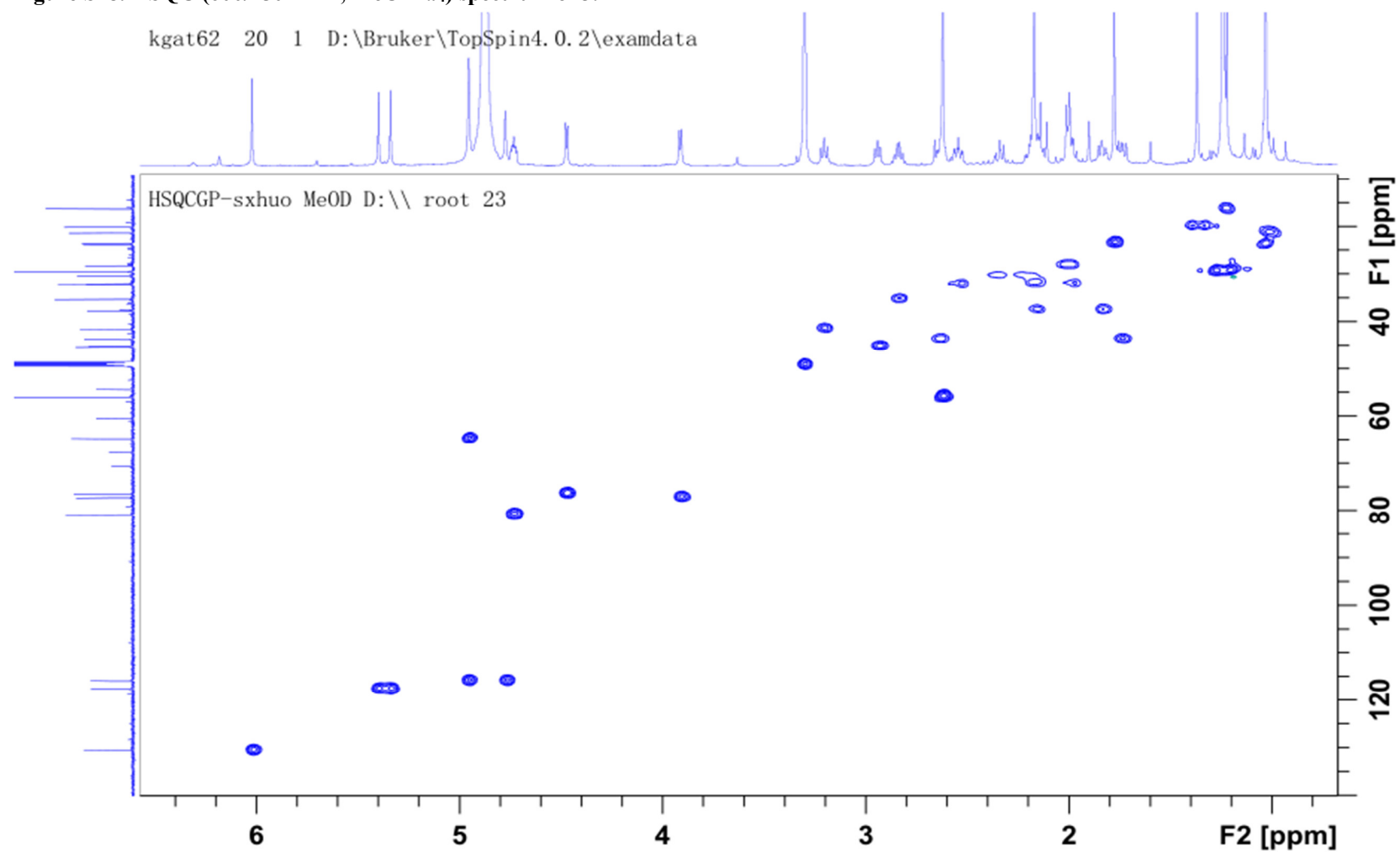


Figure S19. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 3.

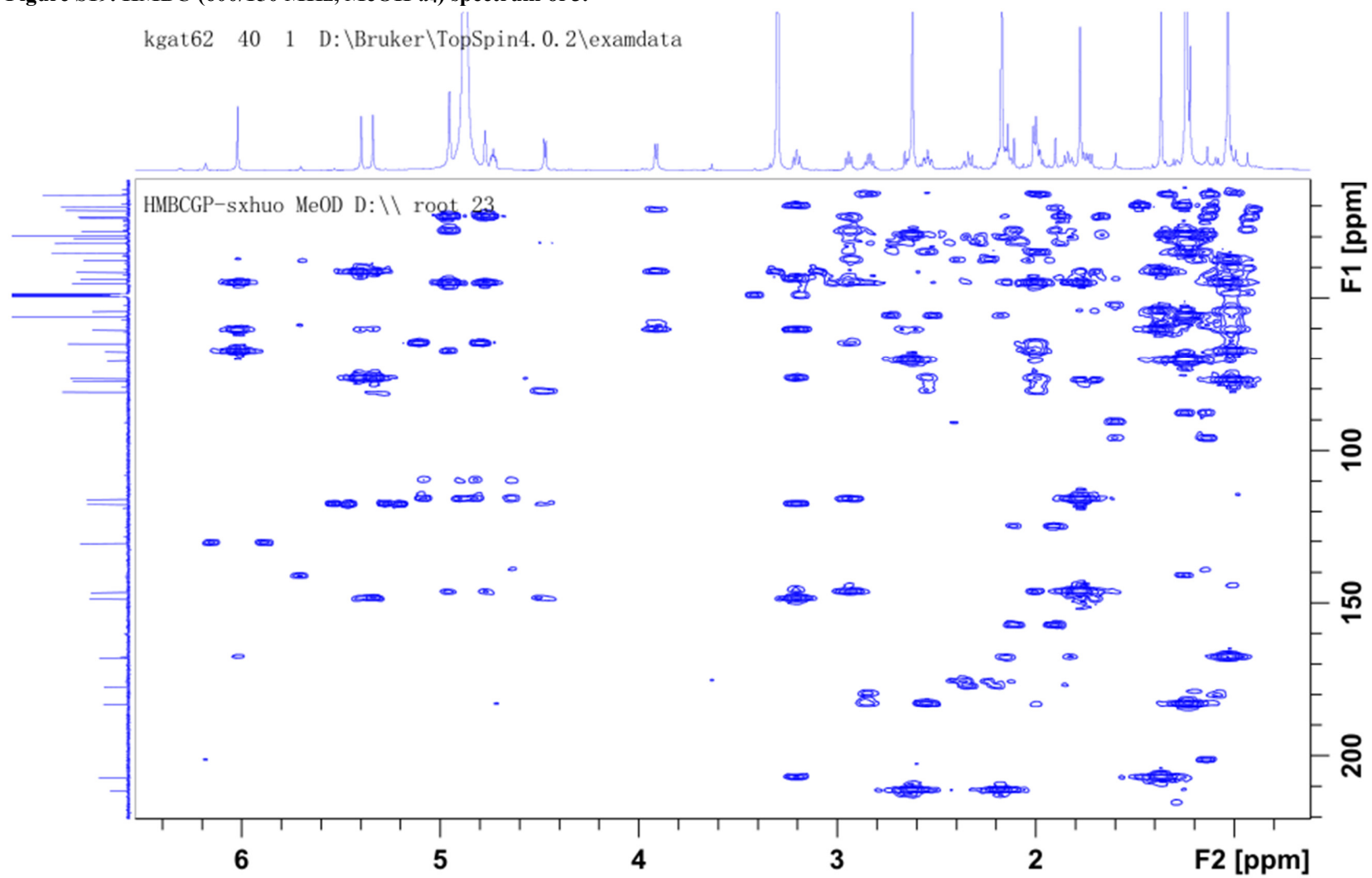
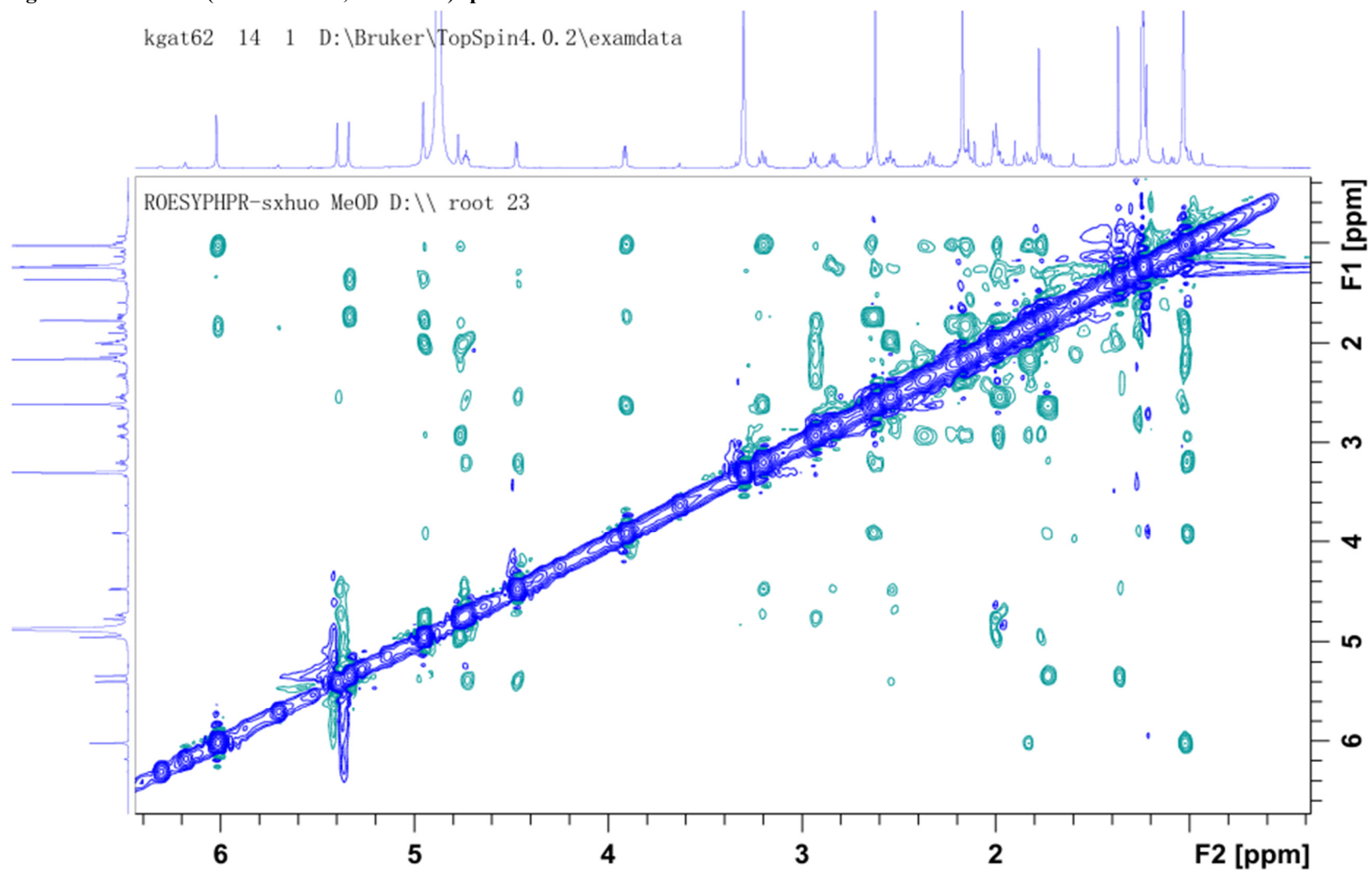




Figure S20. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 3.



## Section S7: HRESIMS spectrum of 3

Figure S21. HRESIMS spectrum of 3.

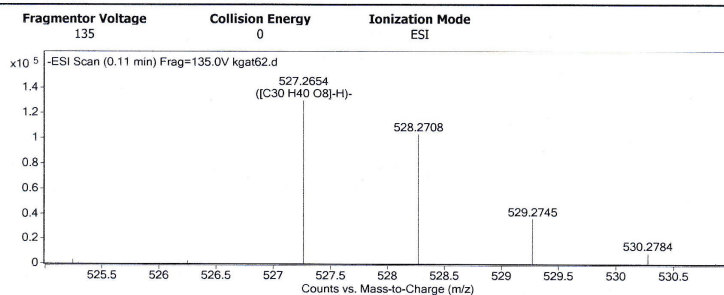
### Qualitative Analysis Report

<b>Data Filename</b>	kgat62.d	<b>Sample Name</b>	kgat62
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s-.m	<b>Acquired Time</b>	5/19/2021 10:40:04 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
112.9856		326571.84		
527.2654		129859.75	C30 H40 O8	(M-H)-
528.2708	1	102946.99		
544.2997		99789.67		
545.306	1	271520.28		
573.2709	1	99540.22		
590.3058	1	644088.69		
591.309	1	201983.73		
1033.9885	1	247649.55		
1055.5377	1	109539.64		
1072.572	1	365939.16		
1073.5753	1	247403.97		

### 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
C30 H40 O8	528.2723	527.2650	527.2654	-0.40	-0.76	11.0000

--- End Of Report ---

## Section S8: 1D and 2D NMR spectra of compound 4

Figure S22.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 4.

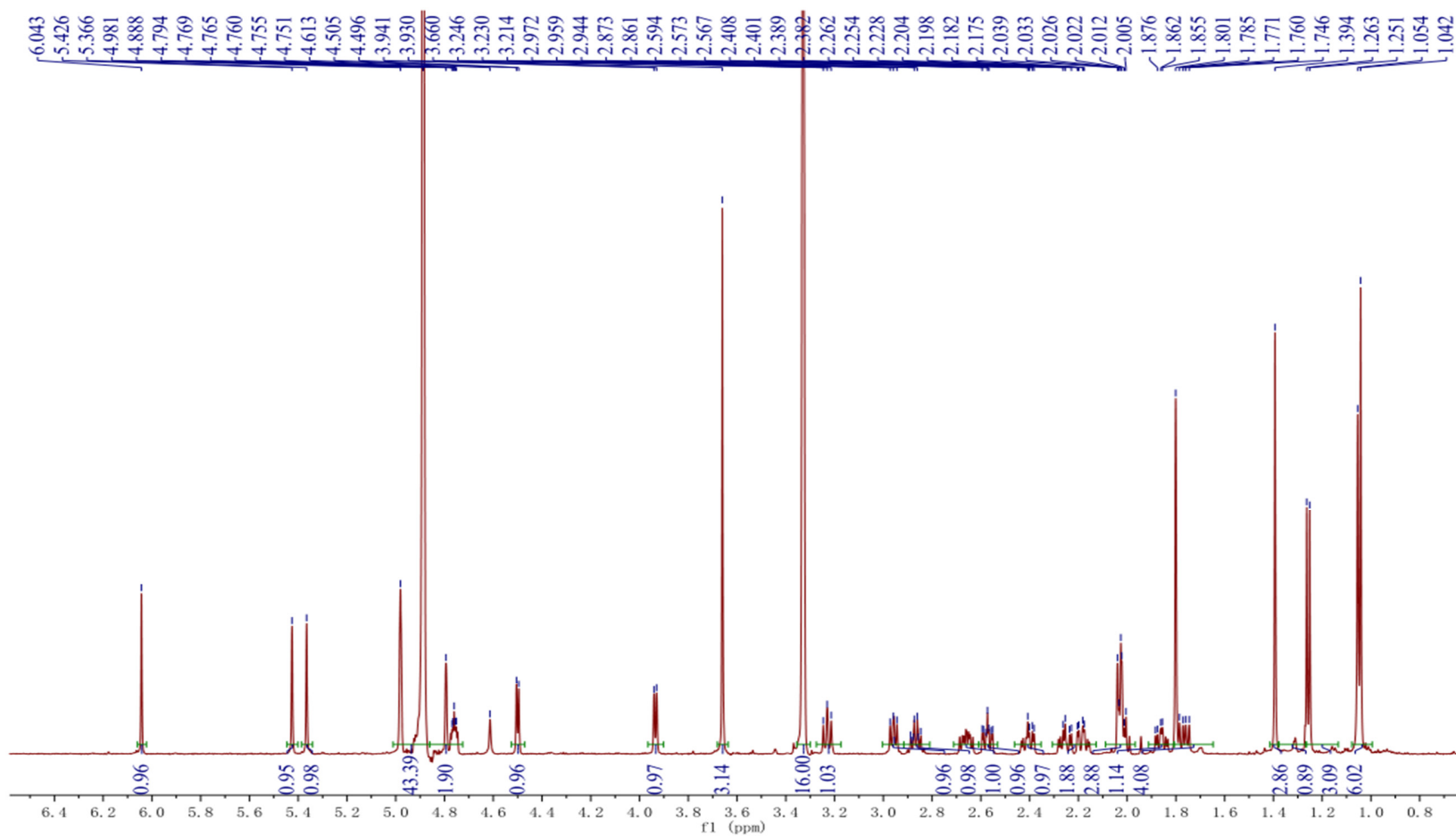


Figure S23.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 4.

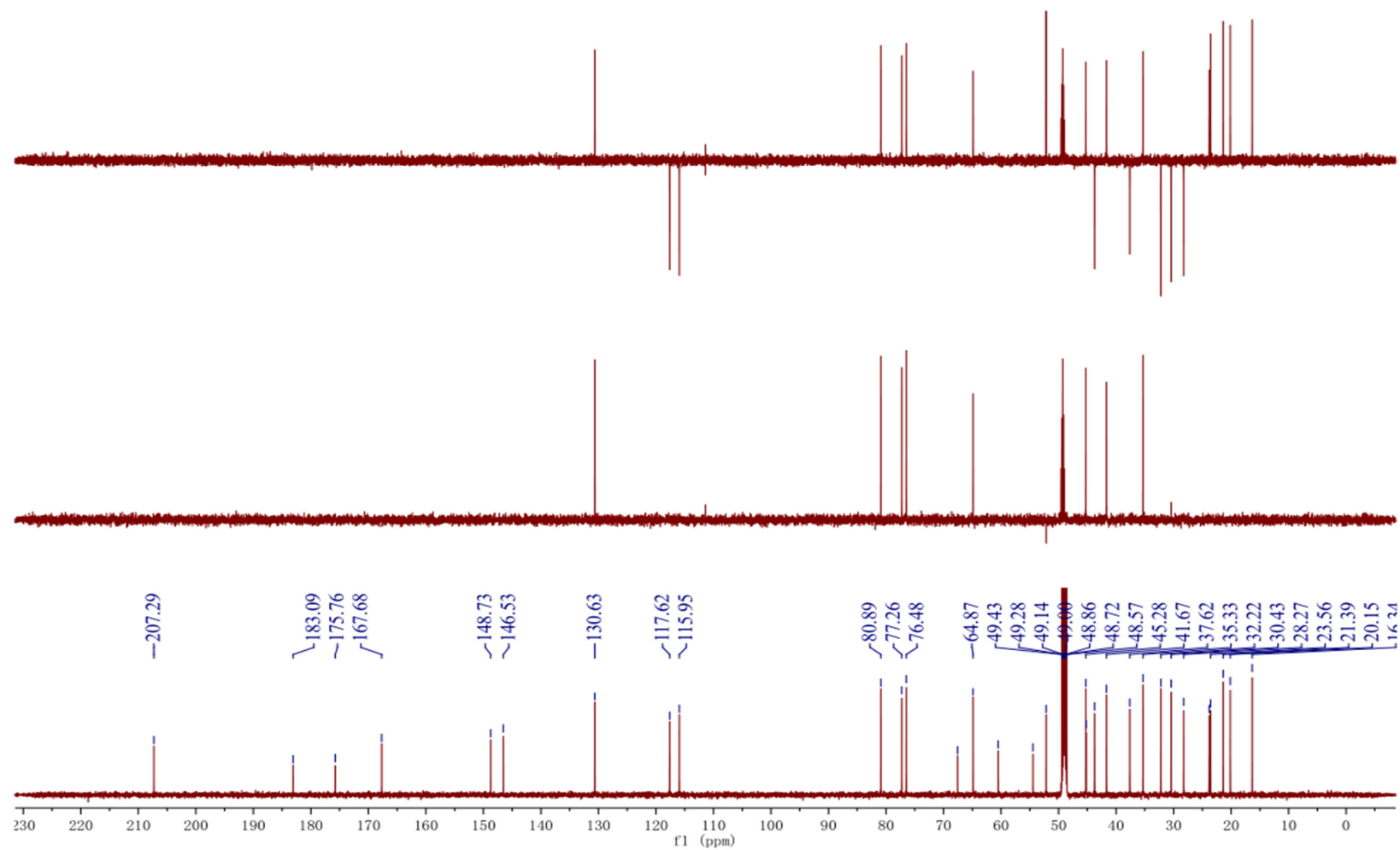


Figure S24.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 4.

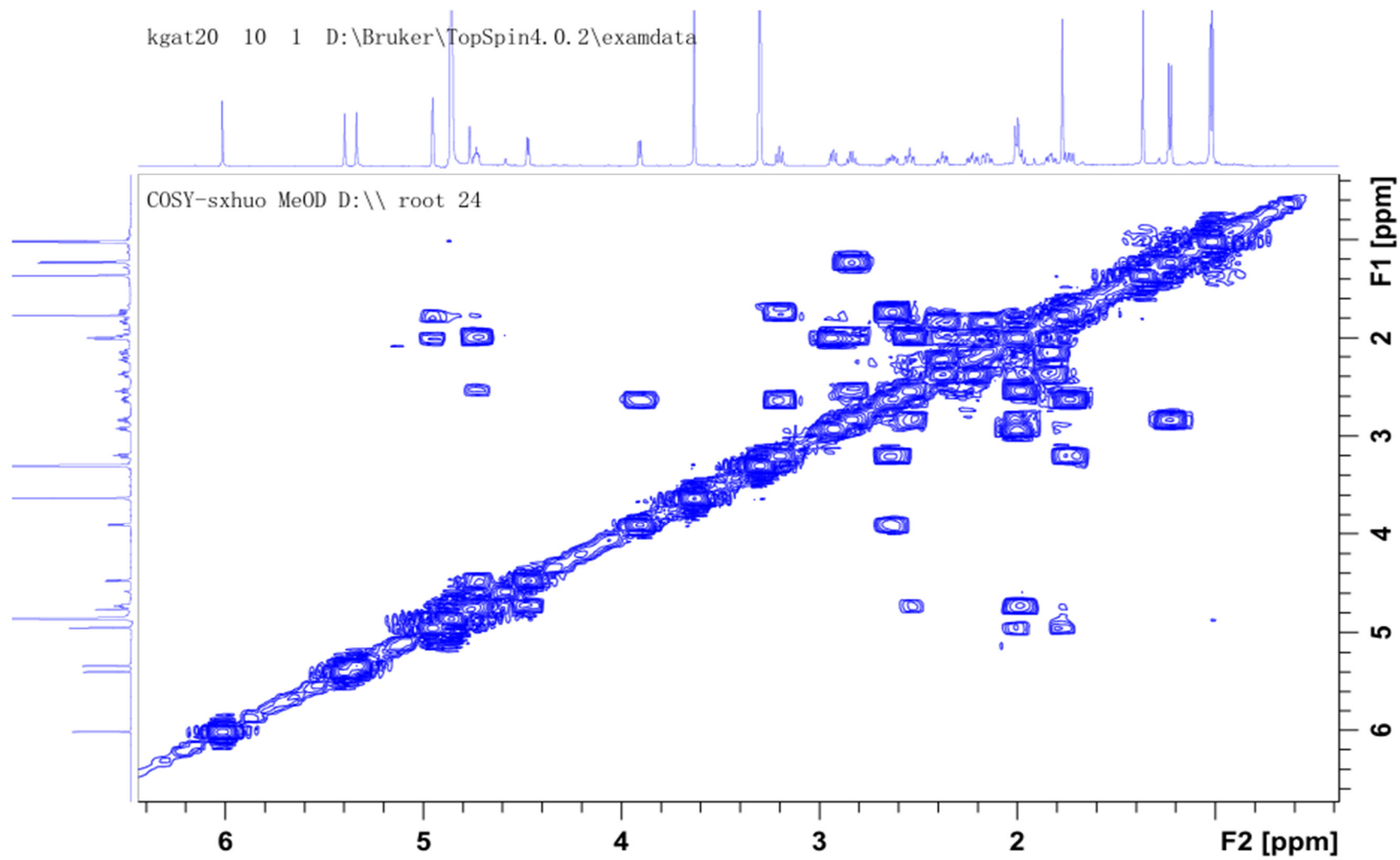


Figure S25. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 4.

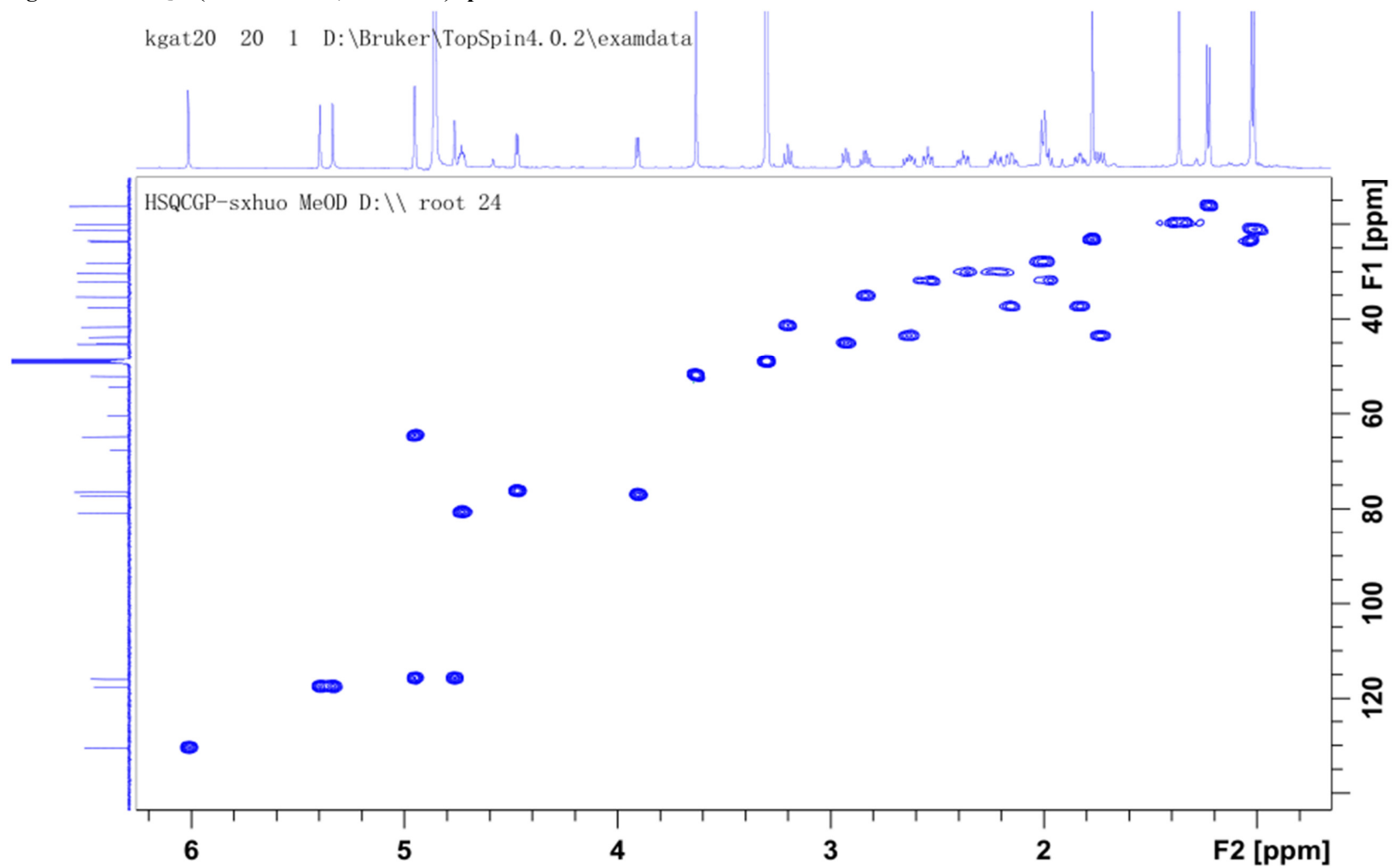


Figure S26. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 4.

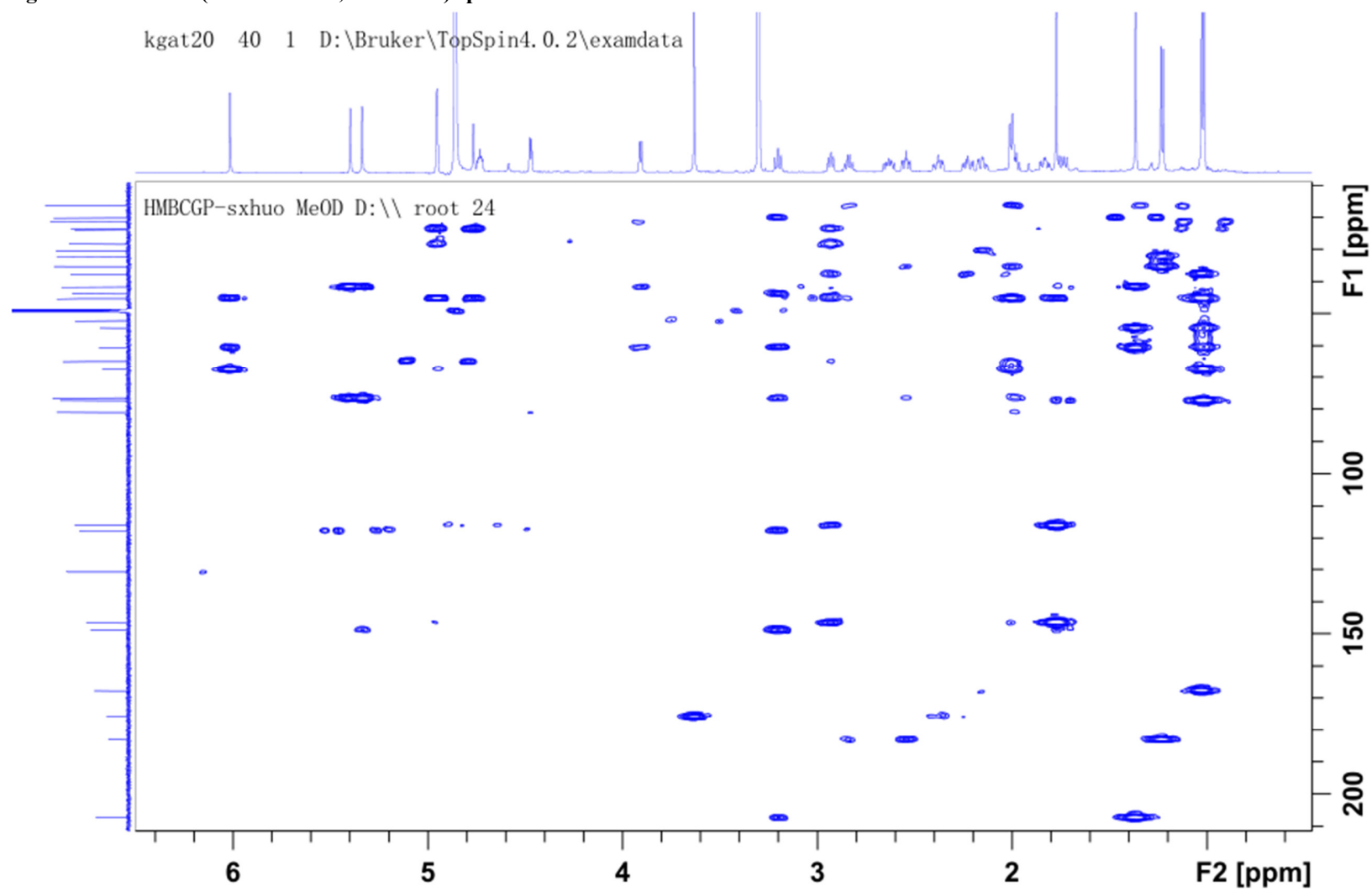
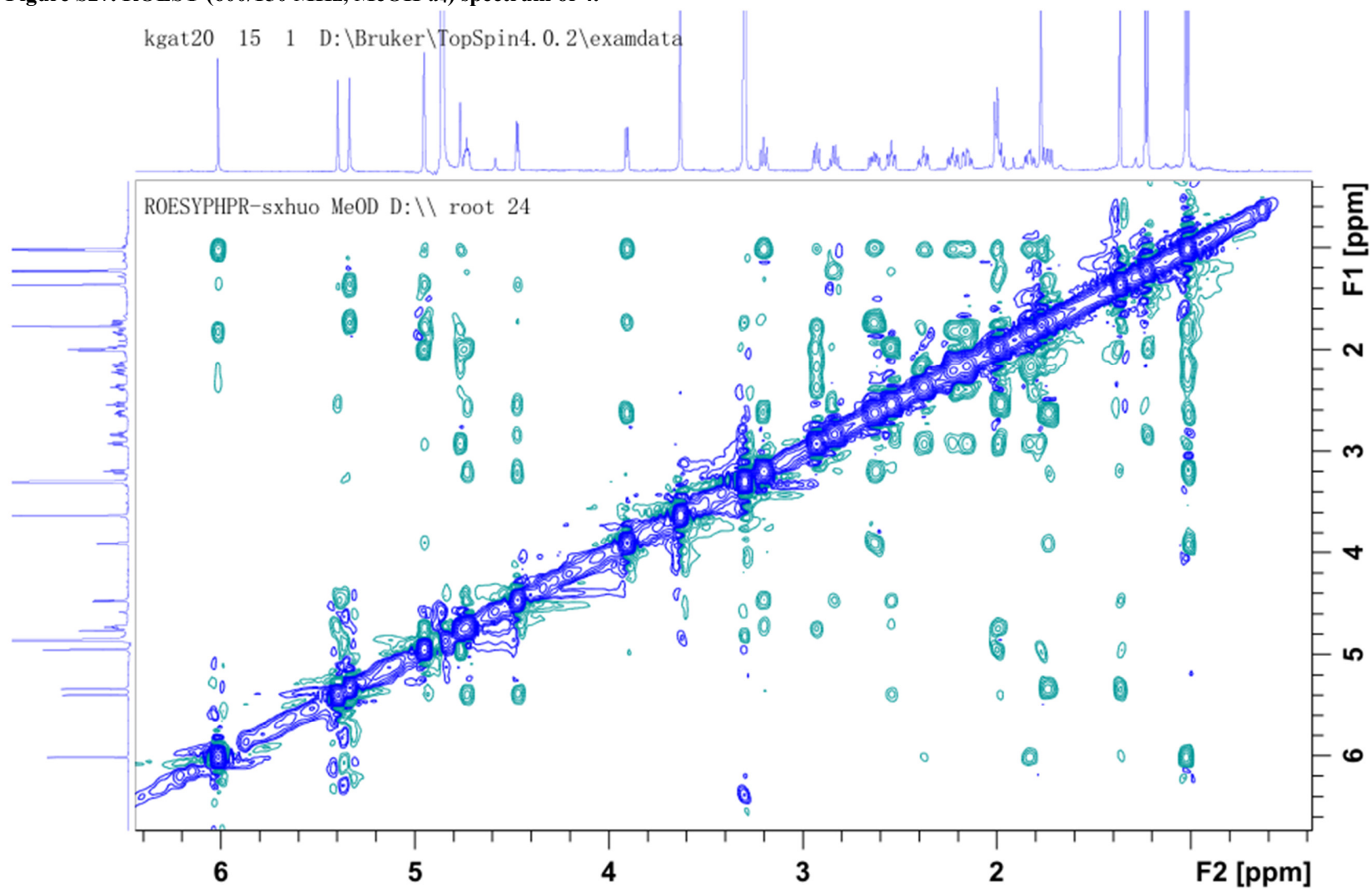


Figure S27. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 4.





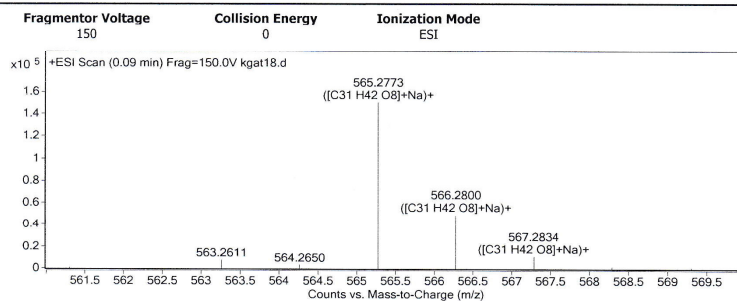
**Section S9: HRESIMS spectrum of 4**

**Figure S28. HRESIMS spectrum of 4.**

### Qualitative Analysis Report

<b>Data Filename</b>	kgat18.d	<b>Sample Name</b>	kgat18
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A7
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:44:06 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			
<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125.2)		

#### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
102.1273	1	57547.51		
146.0803	1	27420.7		
172.0935	1	43954.79		
535.3023	1	28773.45		
543.2954	1	32063.38		
565.2773	1	150467.63	C31 H42 O8	(M+Na)+
566.28	1	49360.54	C31 H42 O8	(M+Na)+
714.3826	1	25285.37		
1107.565	1	43101.66		
1108.5688	1	28253.28		

#### Formula Calculator Element Limits

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

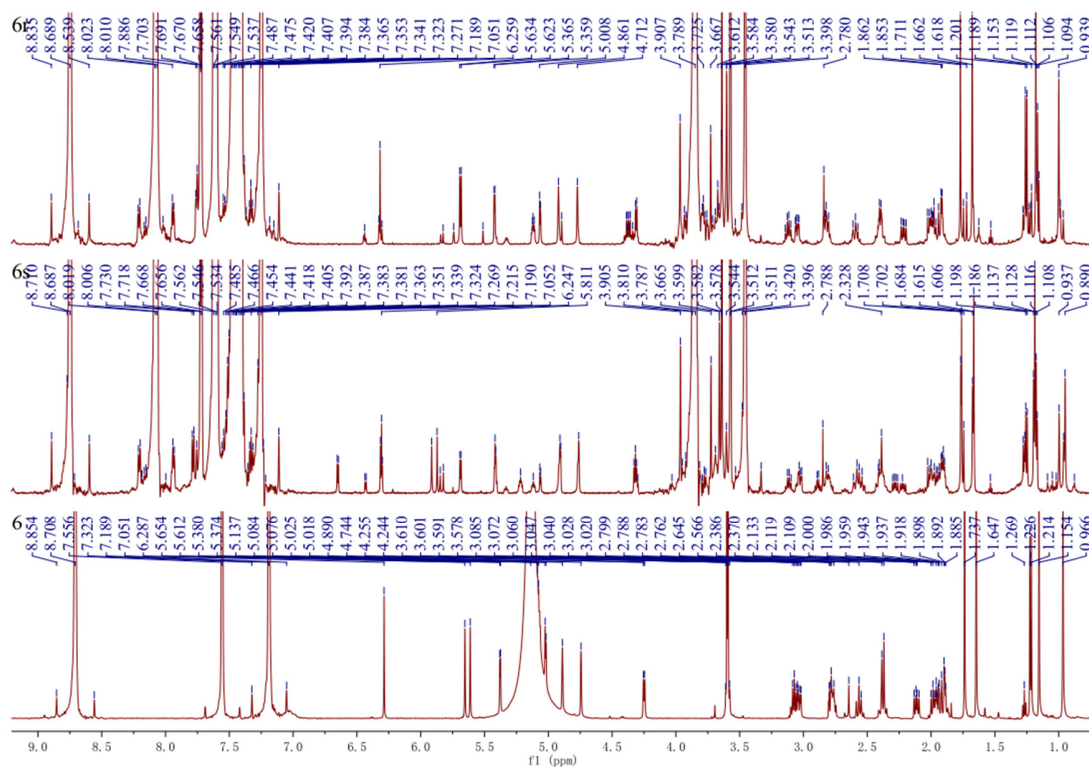
#### Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C31 H42 O8	542.2880	565.2772	565.2773	-0.10	-0.18	11.0000

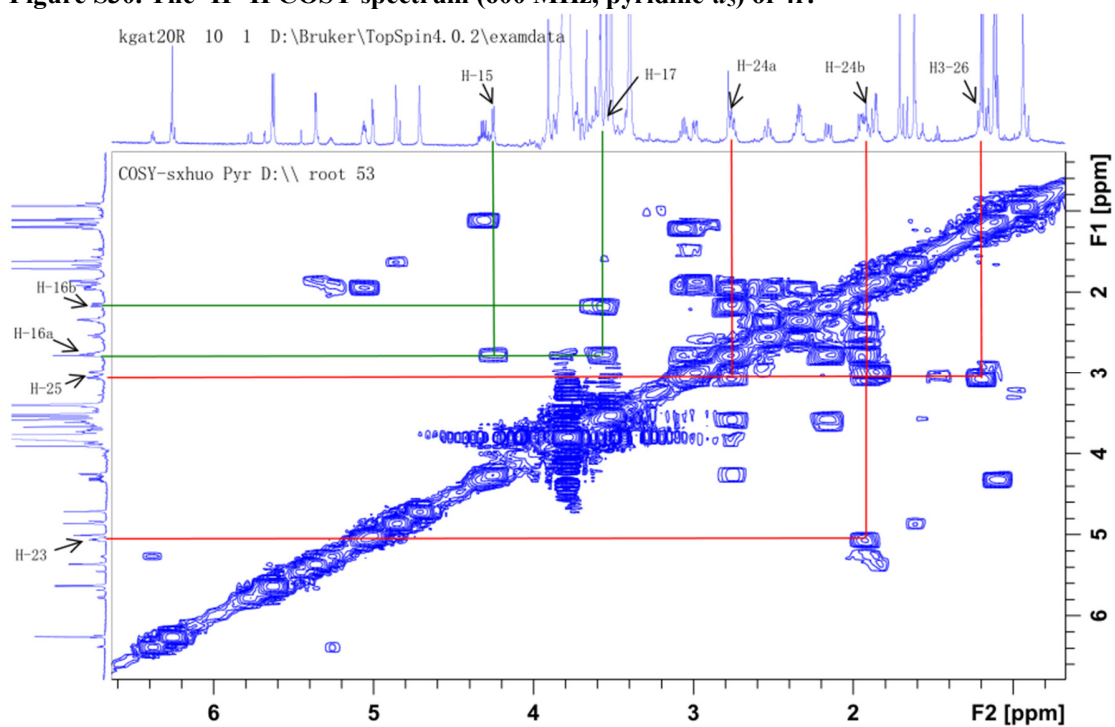
--- End Of Report ---

**Section S10: Comparison of  $^1\text{H}$  NMR and  $^1\text{H}$ - $^1\text{H}$  COSY spectra between 4r and 4s**

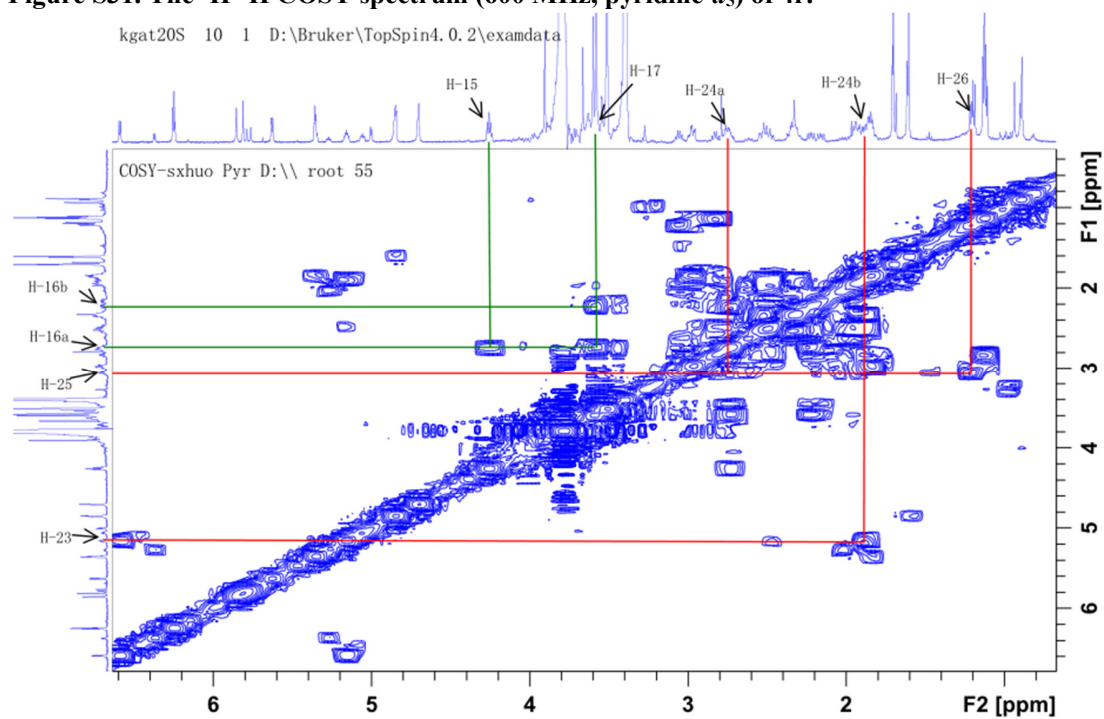
**Figure S29. Comparison of  $^1\text{H}$  NMR spectra (600 MHz, pyridine- $d_5$ ) between 4r and 4s.**



**Figure S30.** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz, pyridine- $d_5$ ) of 4r.



**Figure S31.** The  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (600 MHz, pyridine- $d_5$ ) of 4r.



# Section S11: 1D and 2D NMR spectra of compound 5

Figure S32.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 5.

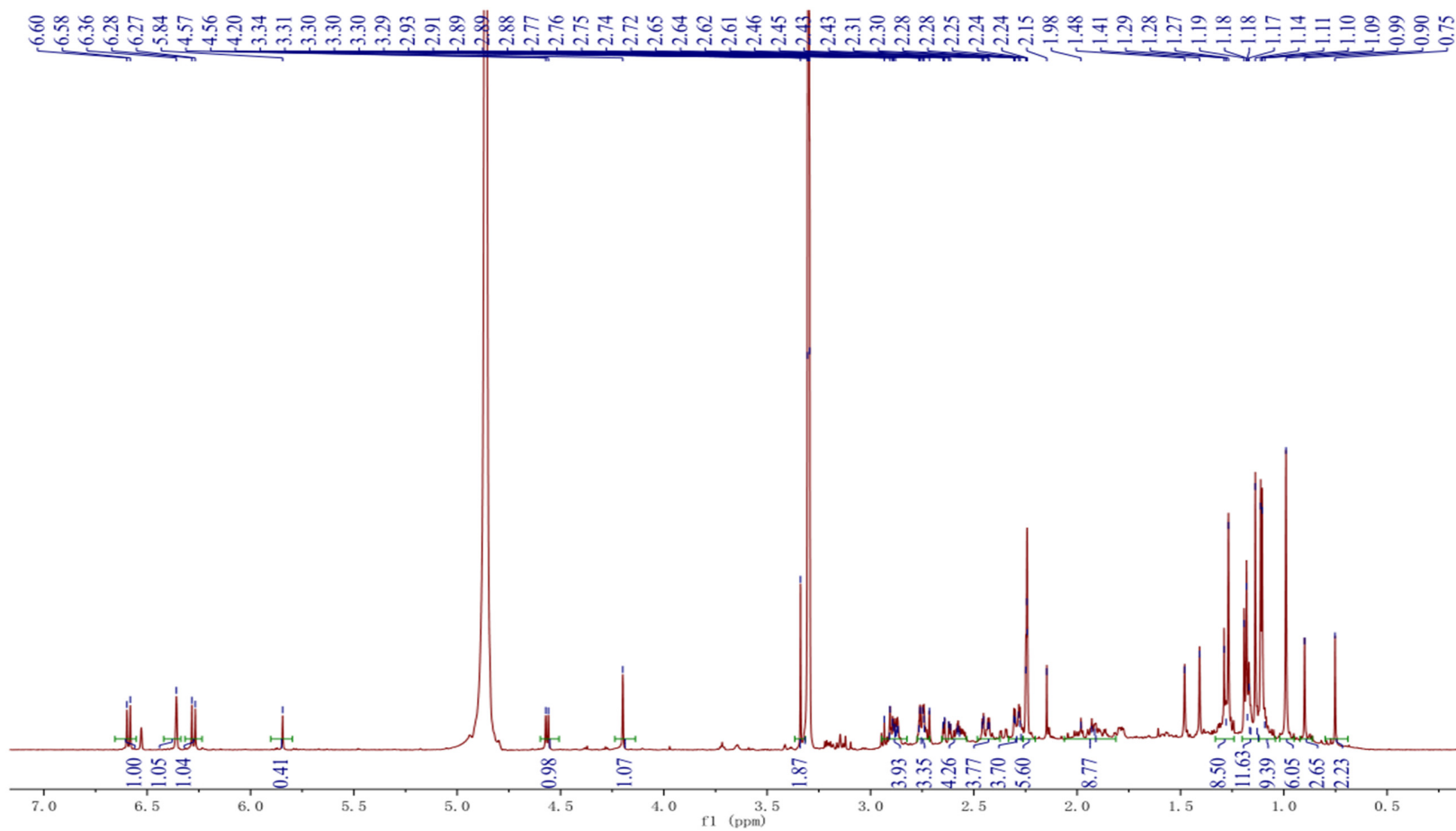


Figure S33.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 5.

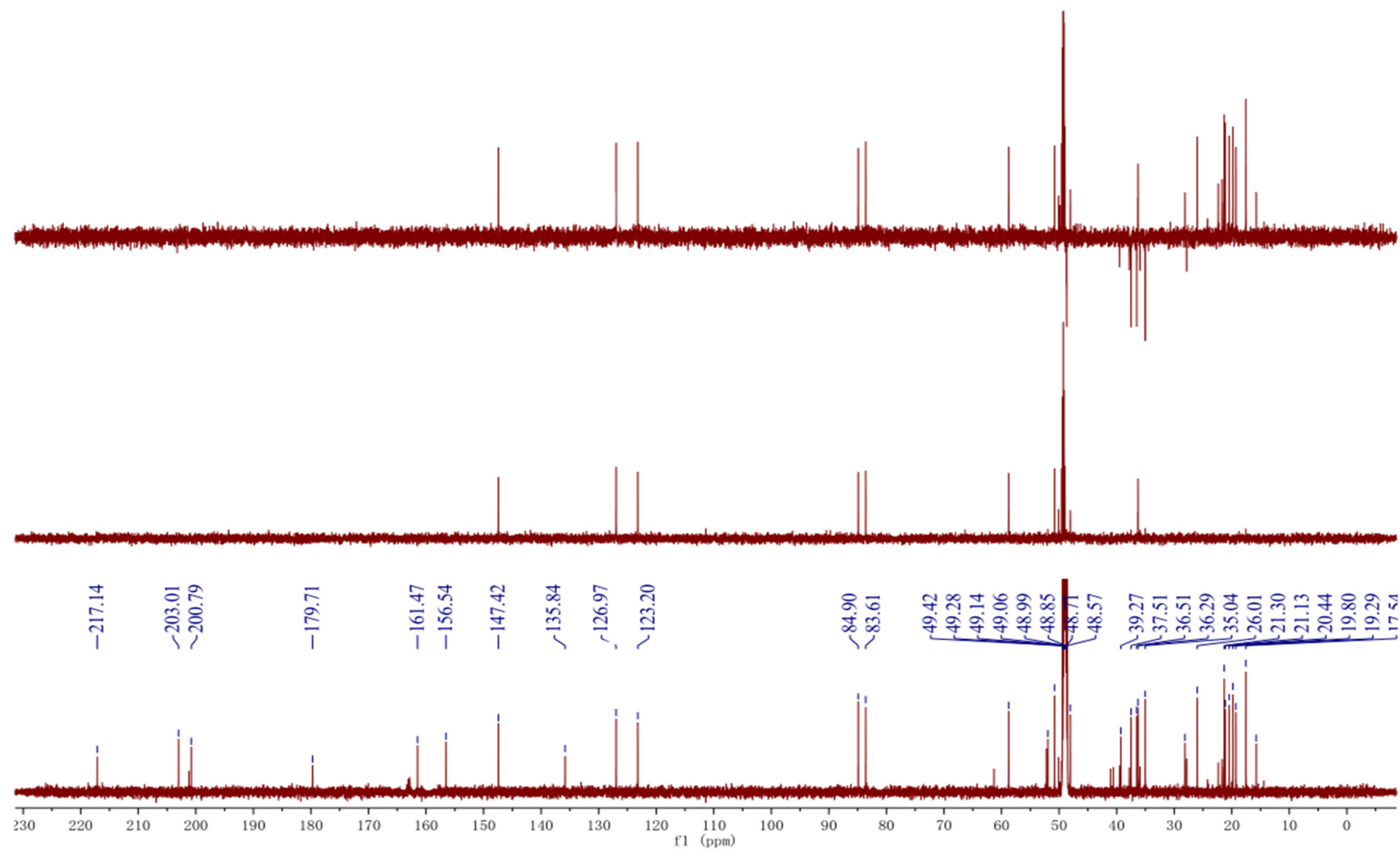


Figure S34.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 5.

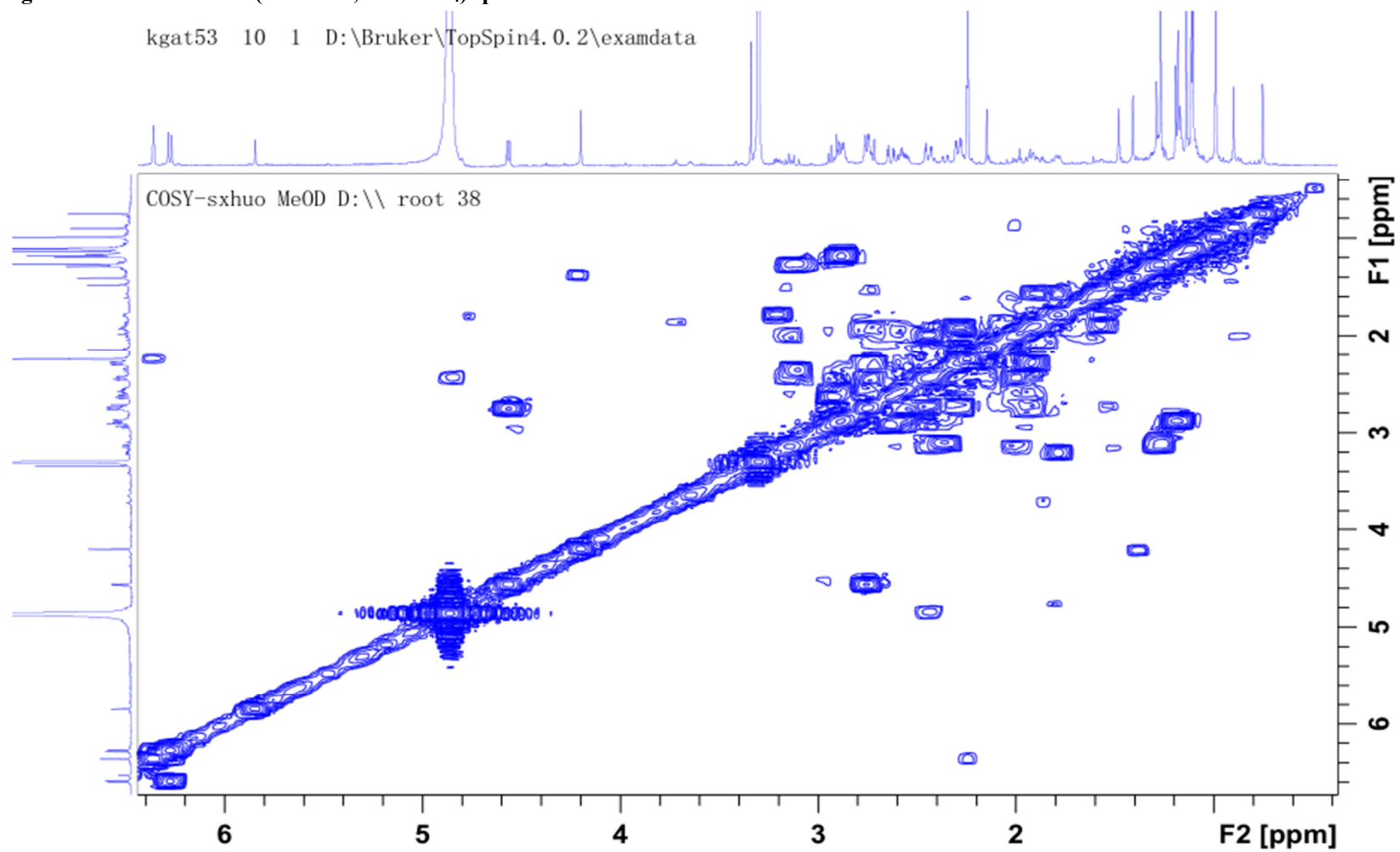


Figure S35. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 5.

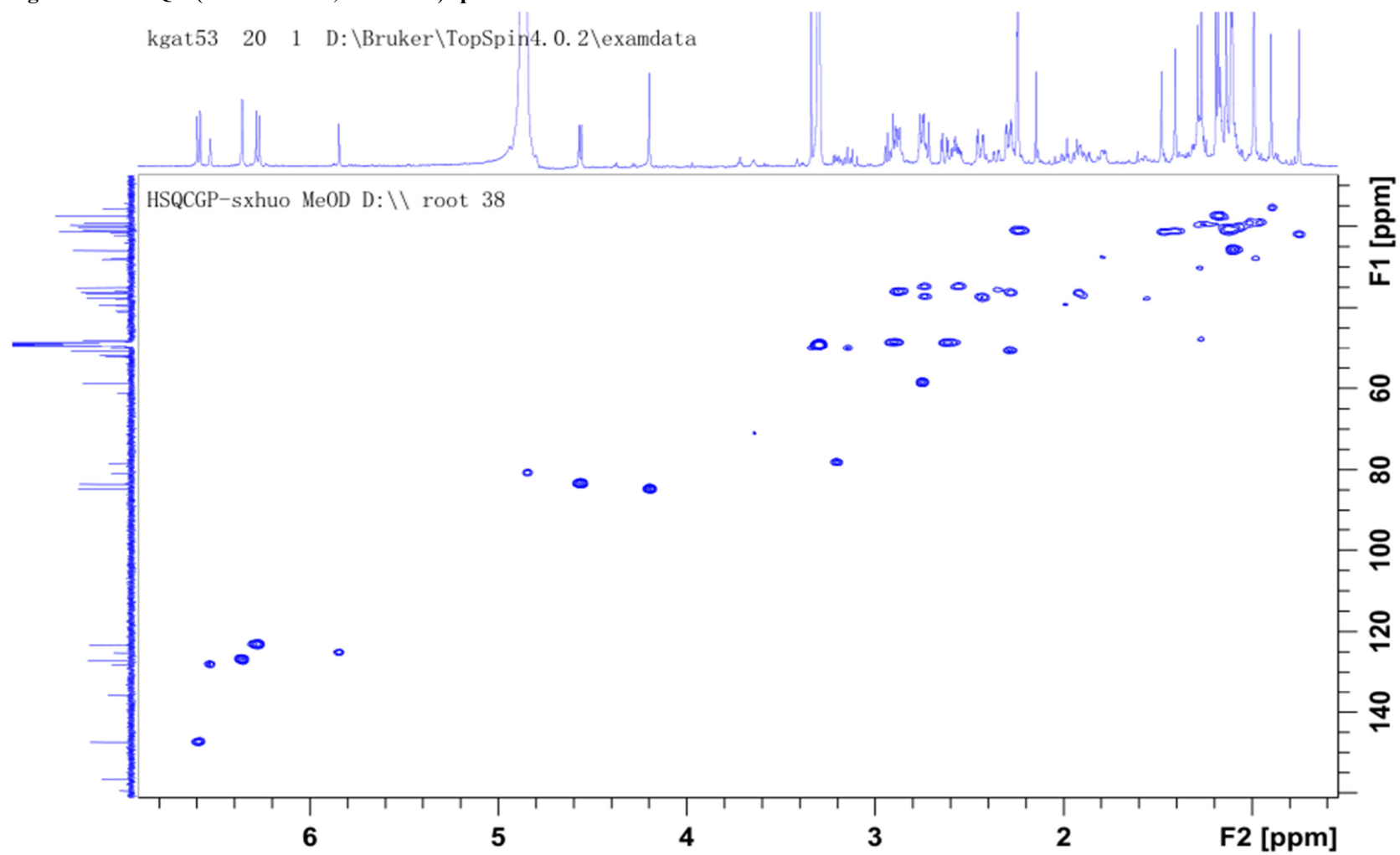




Figure S36. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 5.

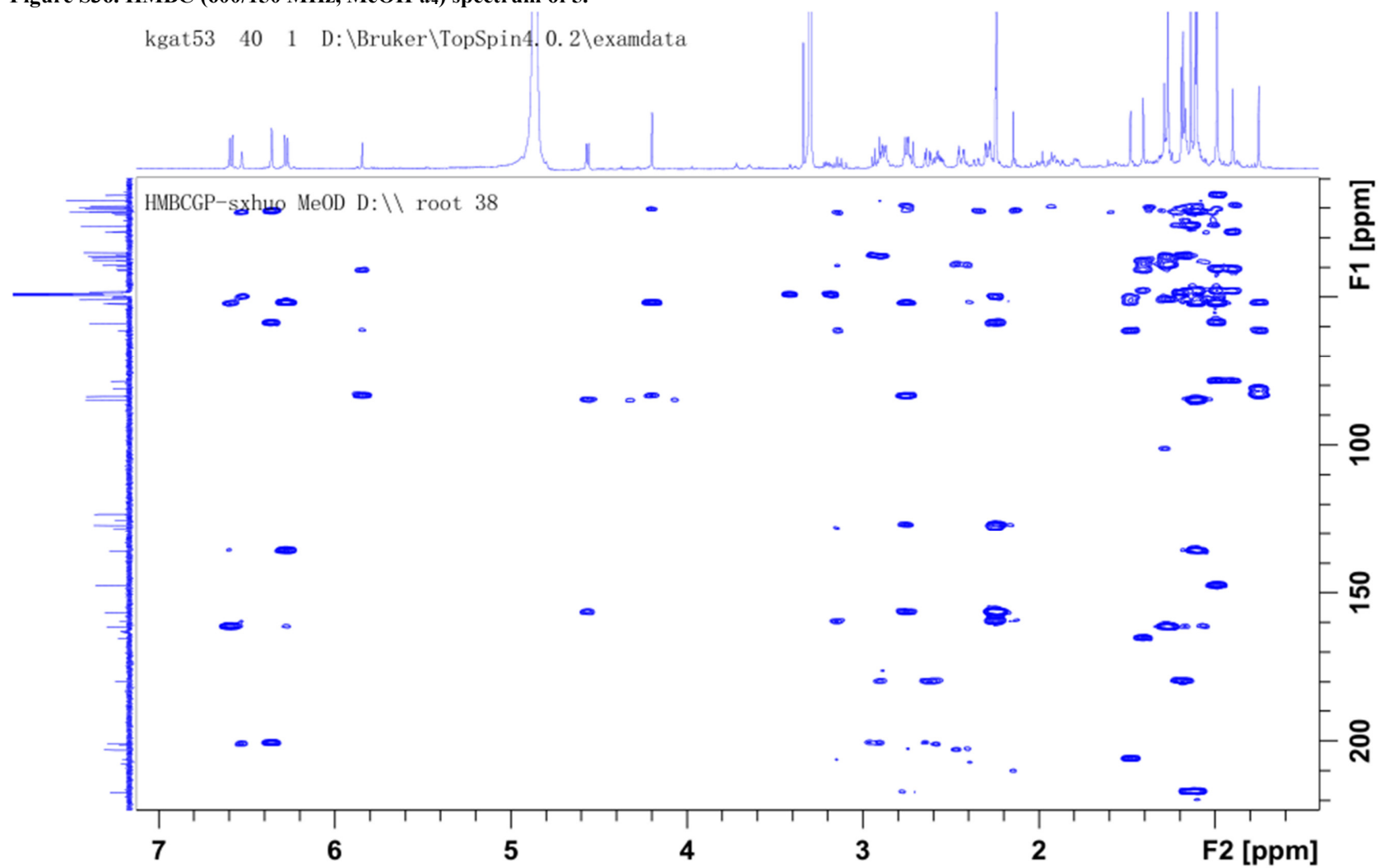
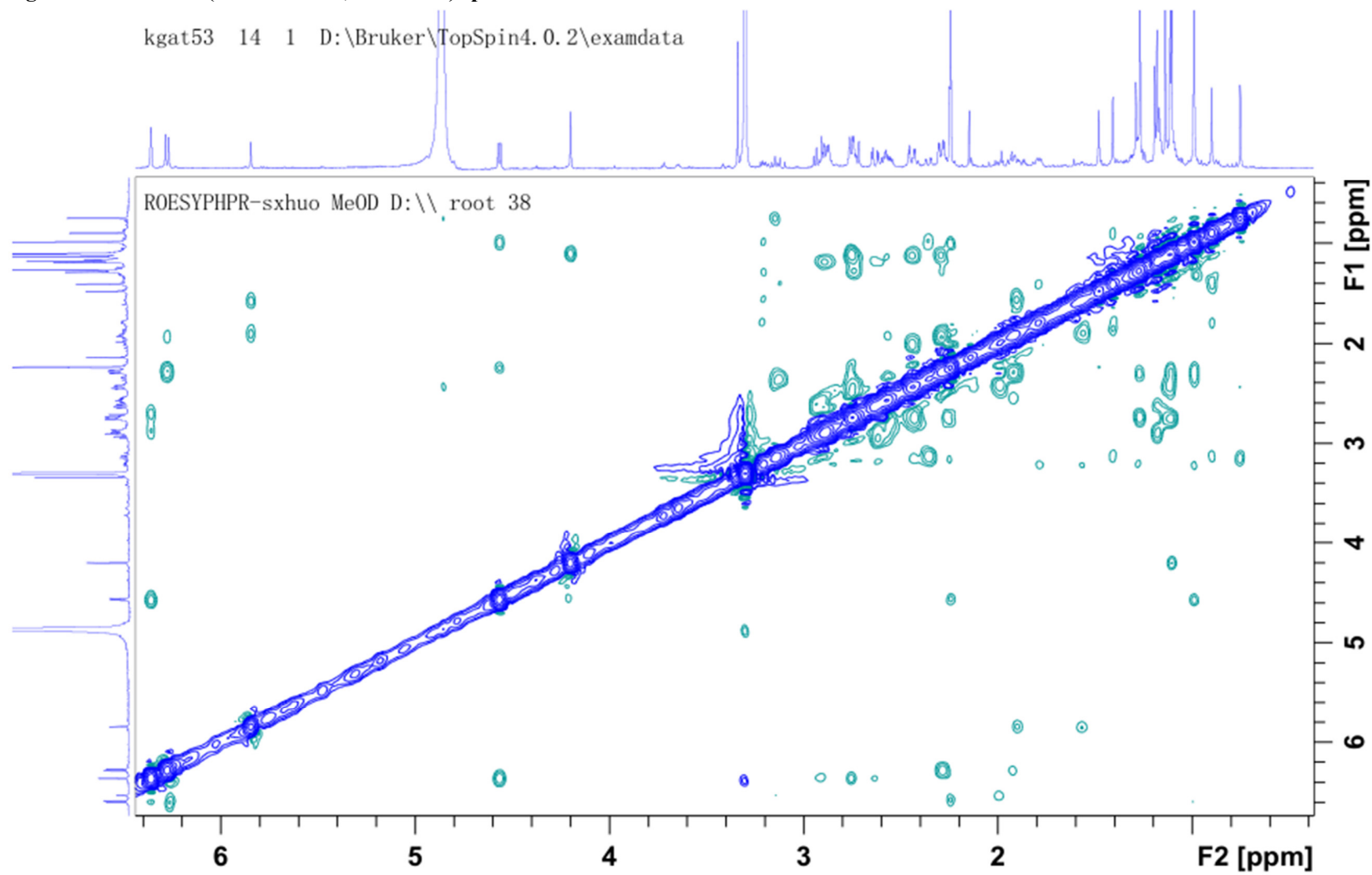


Figure S37. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 5.



## Section S12: HRESIMS spectrum of 5

Figure S38. HRESIMS spectrum of 5.

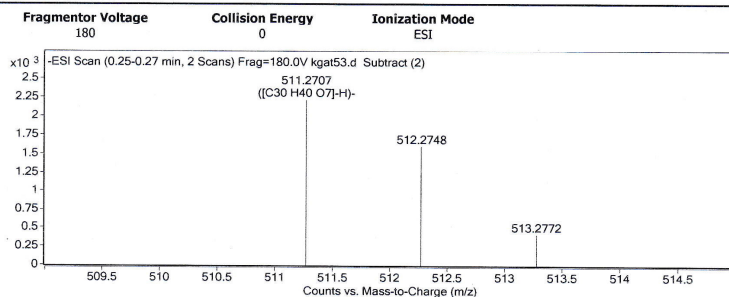
### Qualitative Analysis Report

<b>Data Filename</b>	kgat53.d	<b>Sample Name</b>	kgat53
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A2
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s-.m	<b>Acquired Time</b>	7/9/2021 2:52:30 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
113.9895		422.89		
511.2707		2213.88	C30 H40 O7	(M-H)-
512.2748	1	1590.76		
513.2772	1	409.76		
515.3022		448.46		
525.2506		447.94		
527.2635	1	789.87		
529.281		2487.08		
530.2848	1	1967.59		
551.2611		398.79		
579.2579	1	496.07		
643.2744	1	433.25		

### 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
C30 H40 O7	512.2774	511.2701	511.2707	-0.60	-1.17	11.0000

--- End Of Report ---

# Section S13: 1D and 2D NMR spectra of compound 6

Figure S39. <sup>1</sup>H NMR (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of 6.

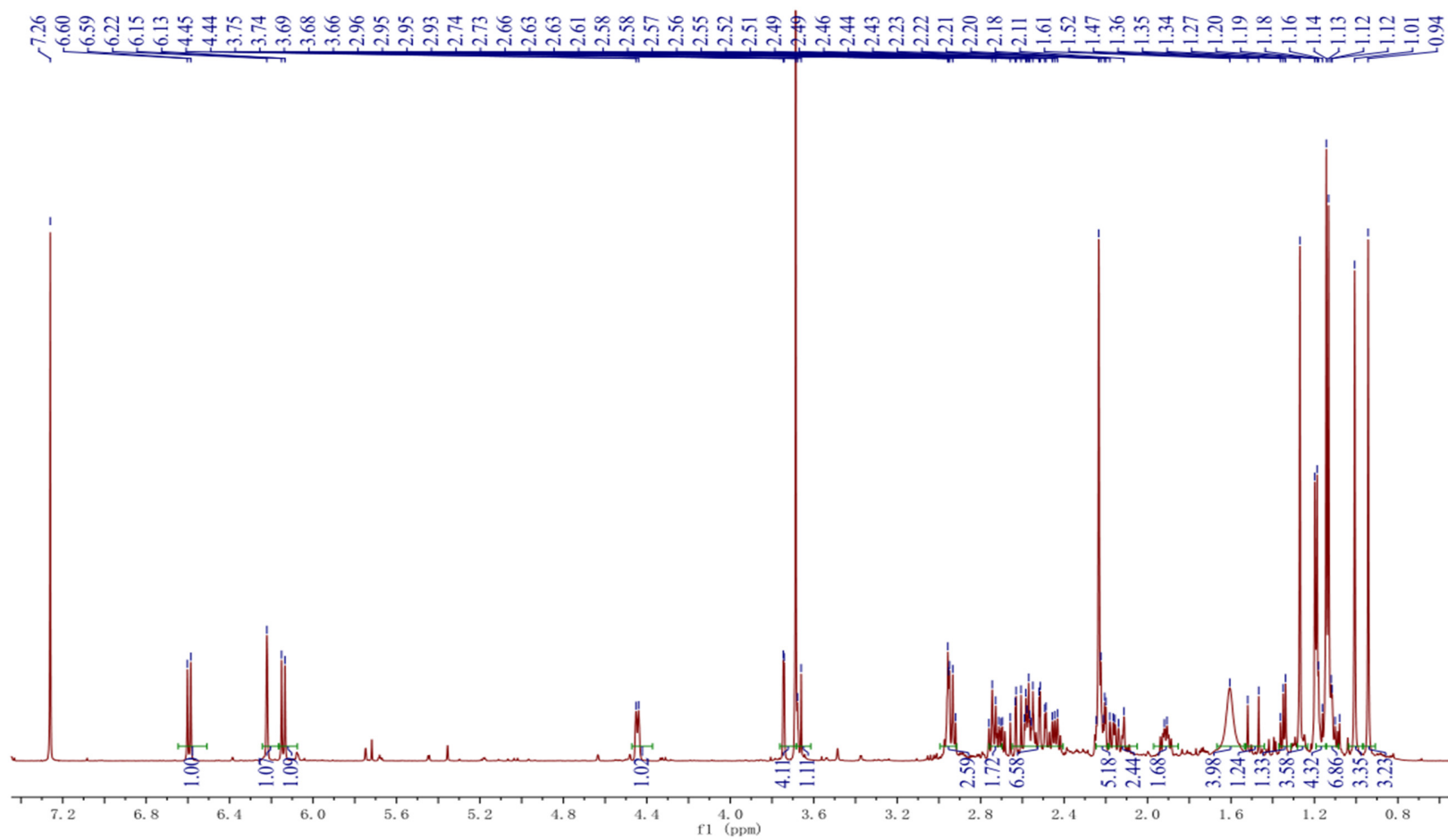


Figure S40.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 6.

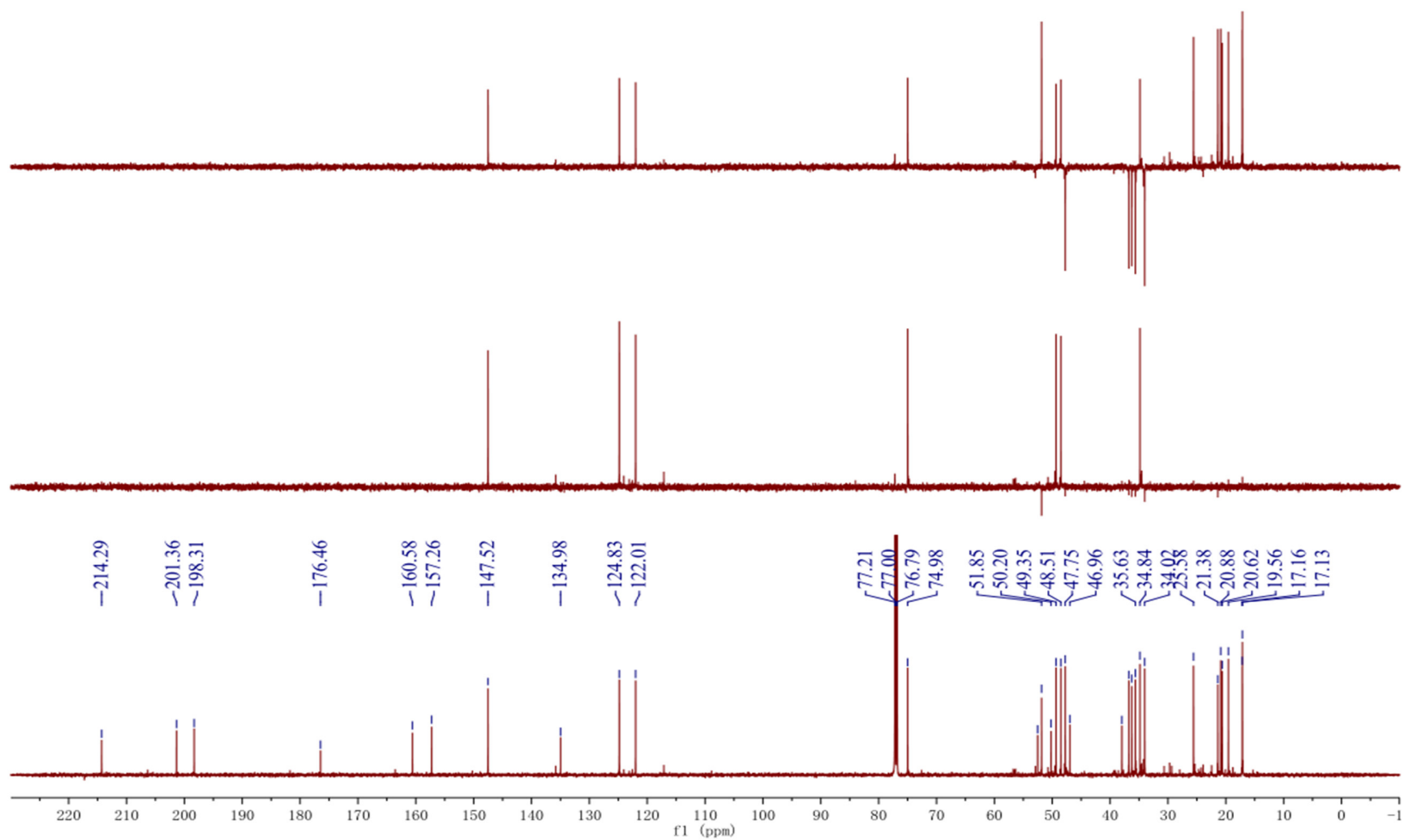


Figure S41.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 6.

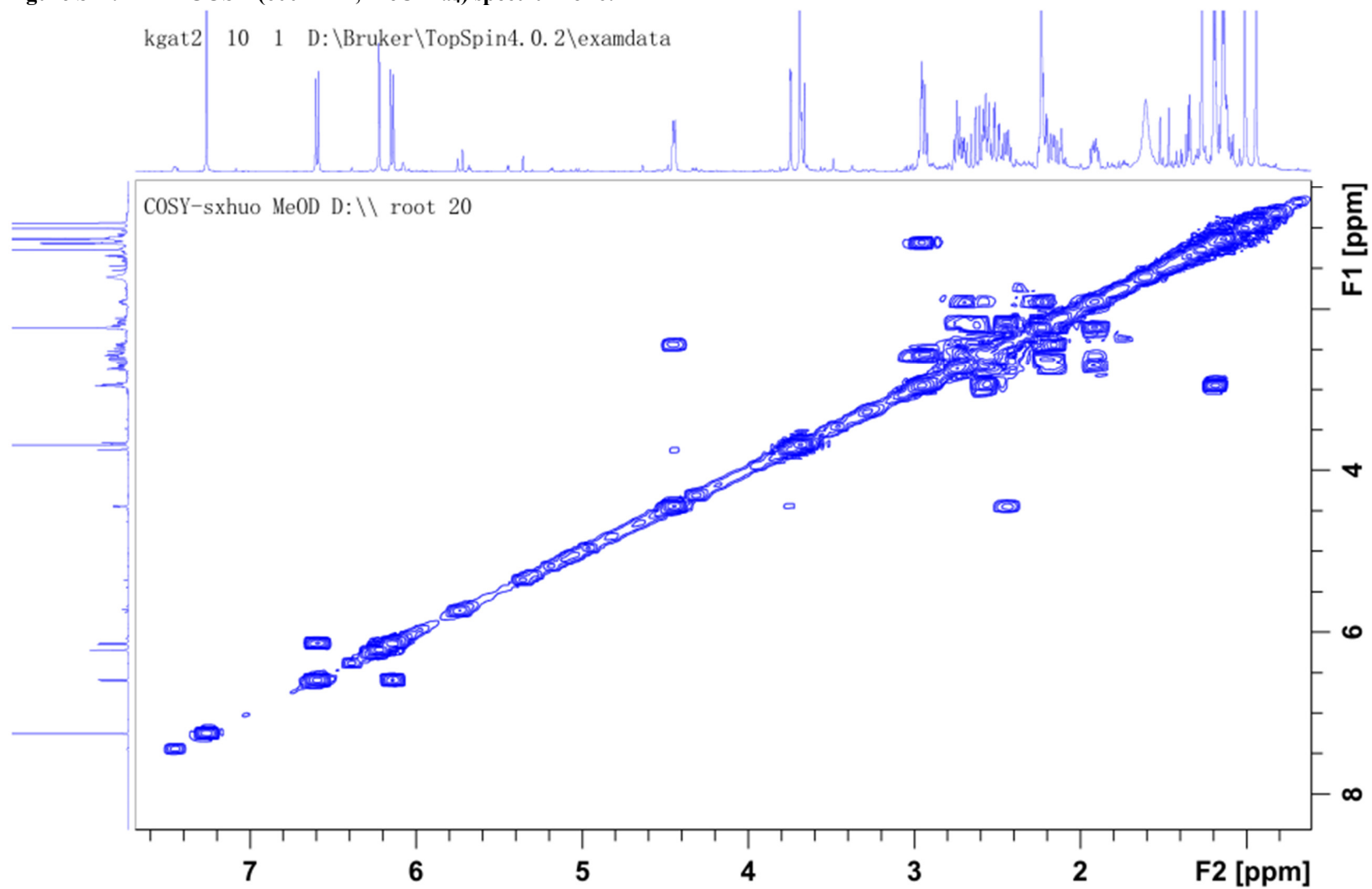


Figure S42. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 6.

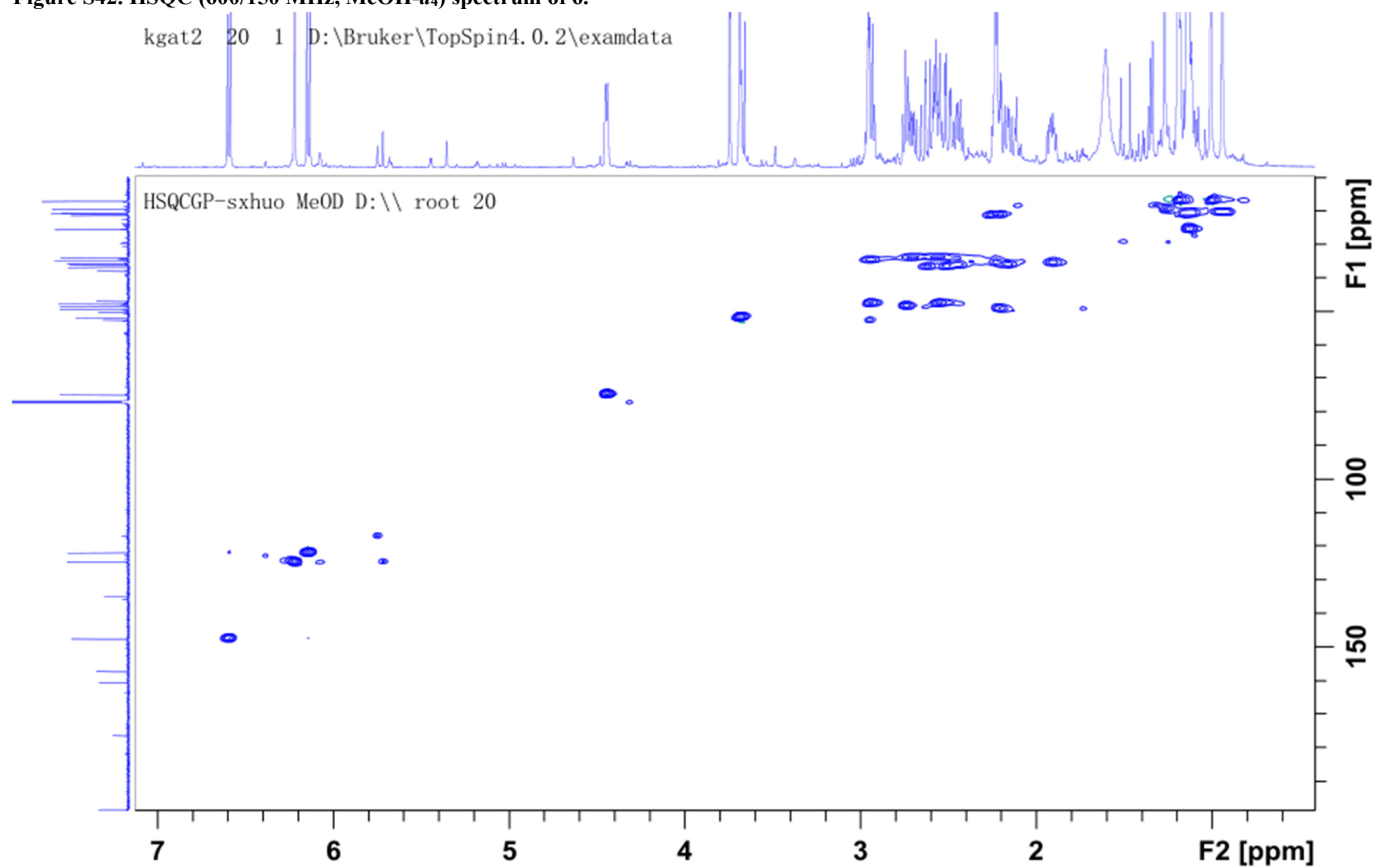


Figure S43. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 6.

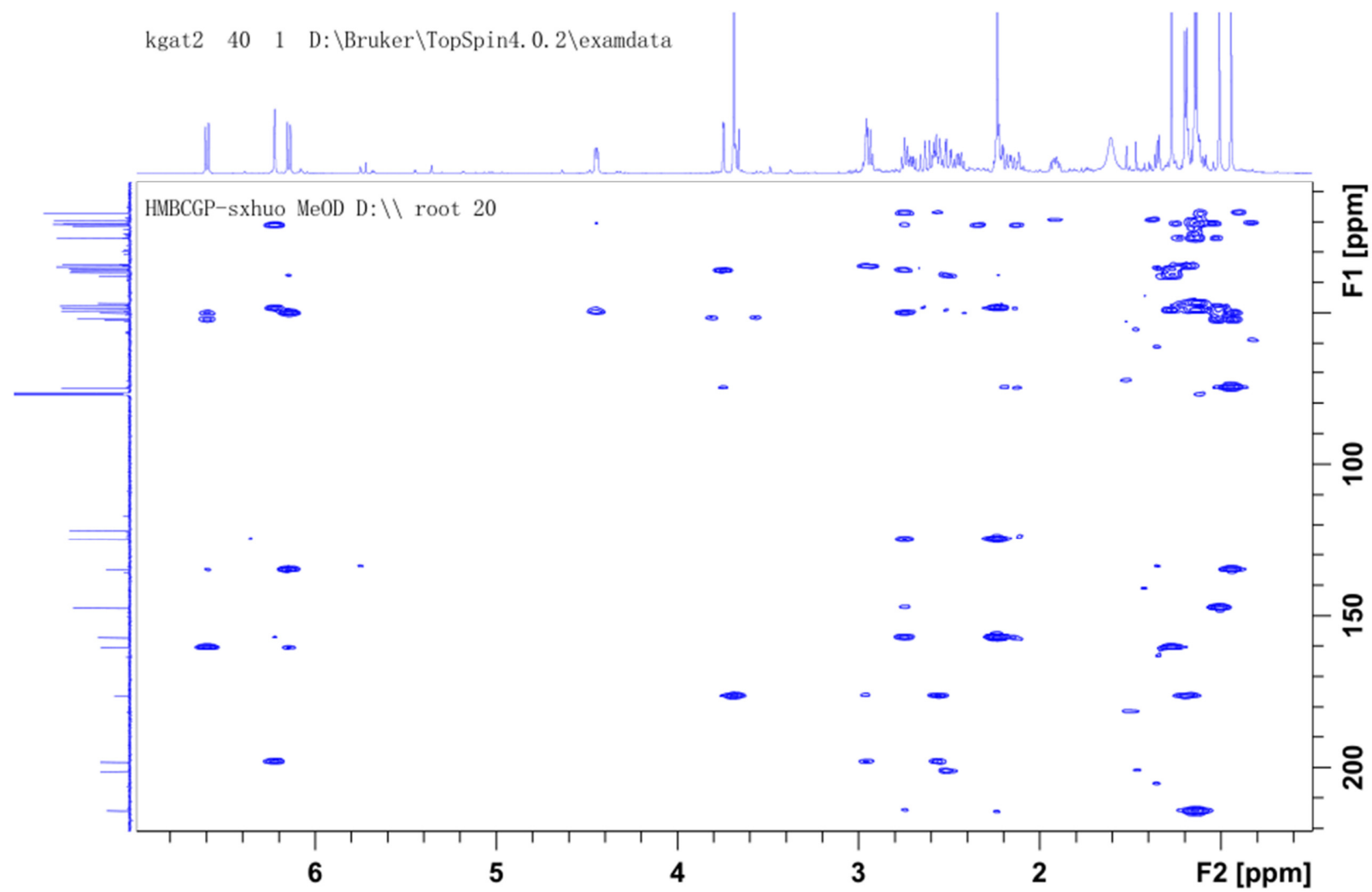
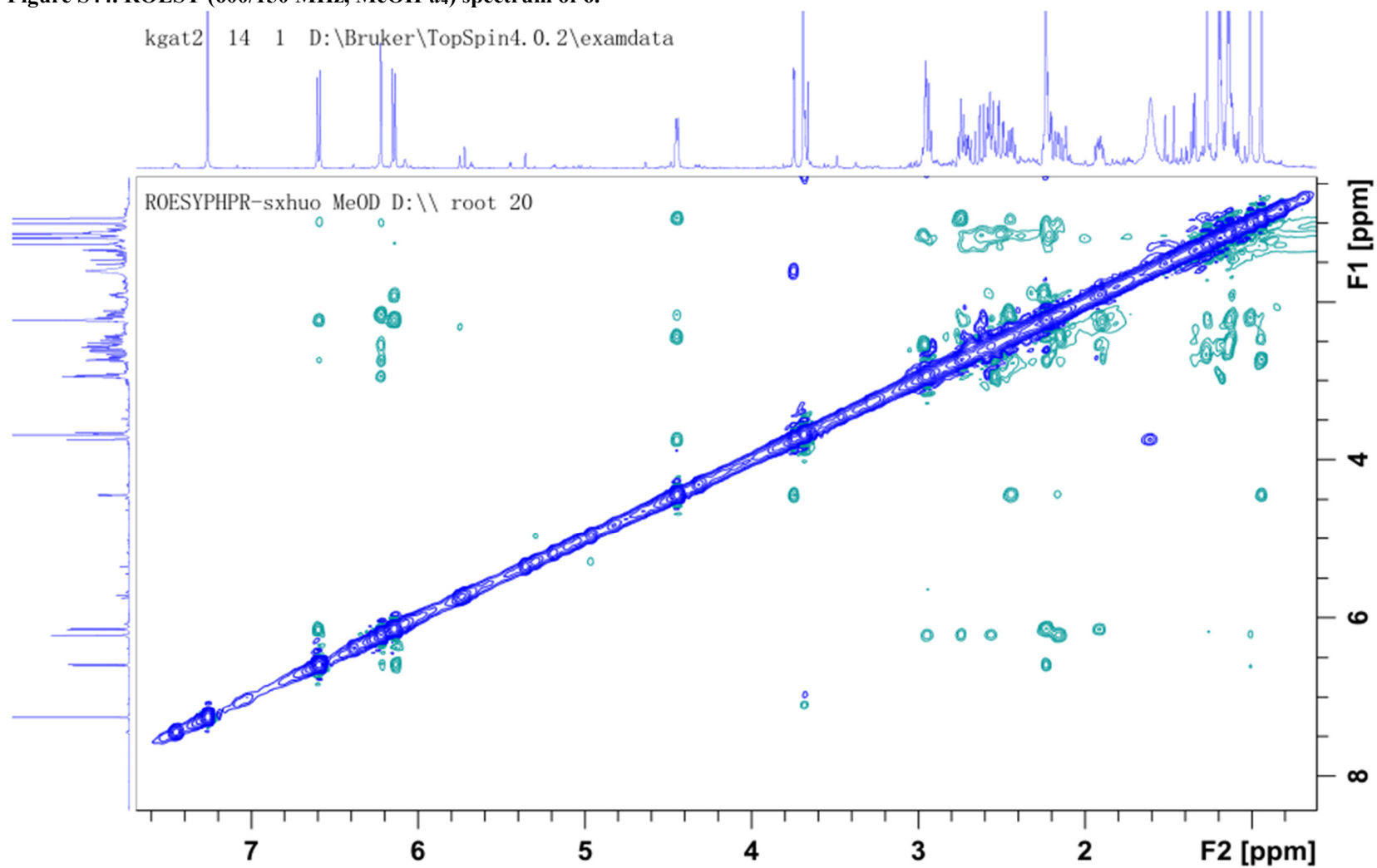




Figure S44. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 6.



## Section S14: HRESIMS spectrum of 6

Figure S45. HRESIMS spectrum of 6.

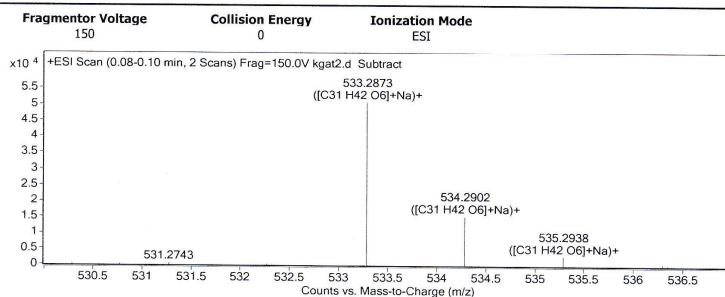
### Qualitative Analysis Report

<b>Data Filename</b>	kgat2.d	<b>Sample Name</b>	kgat2
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A3
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:39:22 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
102.1274	1	37320.11		
511.3058	1	14331.96		
533.2873	1	50725.95	C31 H42 O6	(M+Na)+
534.2902	1	15496.51	C31 H42 O6	(M+Na)+
547.2663	1	16946.77		
549.27	1	16798.7		
1043.5859	1	26370.52		
1044.5892	1	16678.78		
1057.5643	1	10931.84		
1059.5744	1	7625.36		

### 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
C31 H42 O6	510.2981	533.2874	533.2873	0.10	0.19	11.0000

--- End Of Report ---

# Section S15: 1D and 2D NMR spectra of compound 7

Figure S46. <sup>1</sup>H NMR (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of 7.

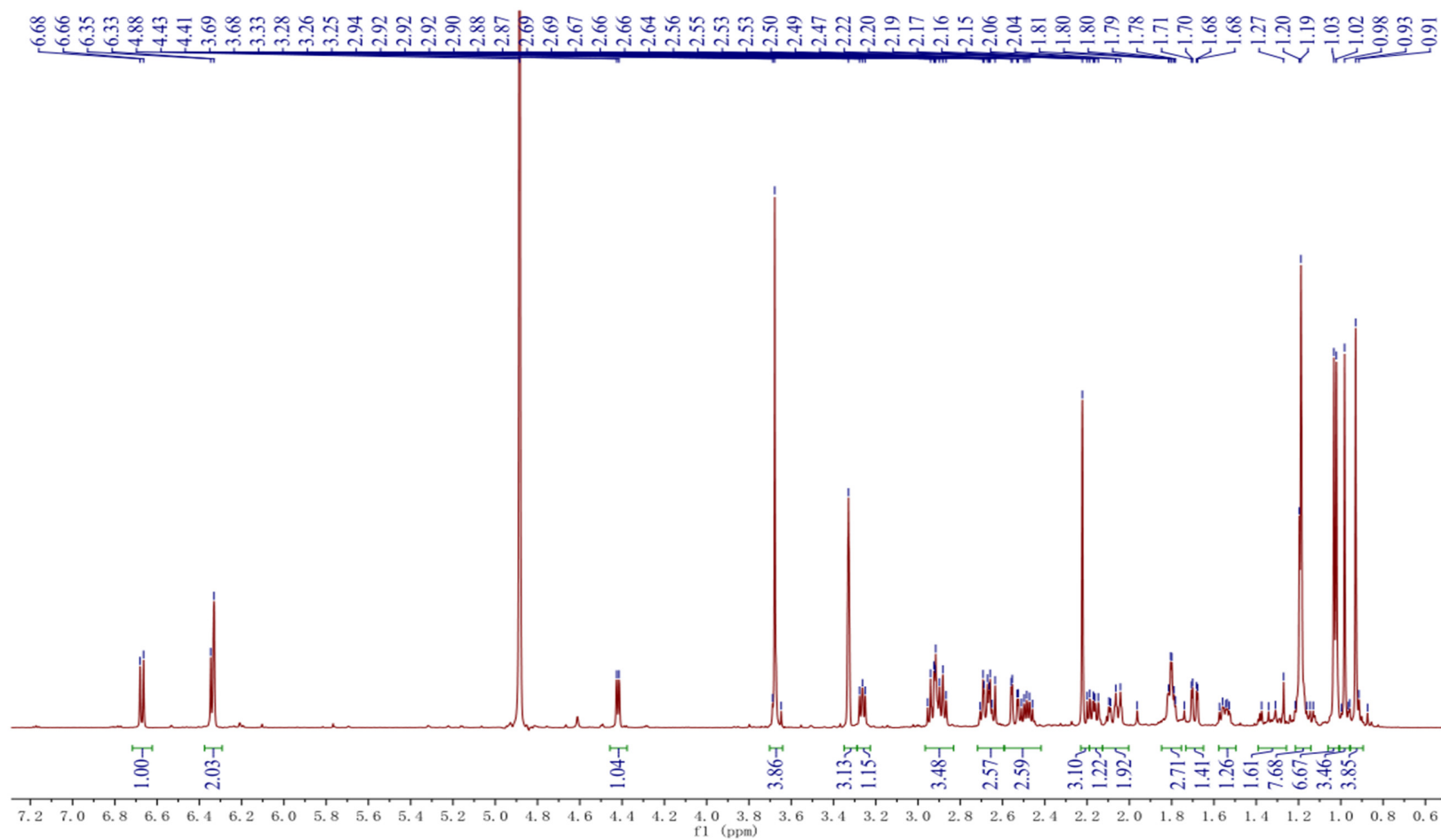


Figure S47.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 7.

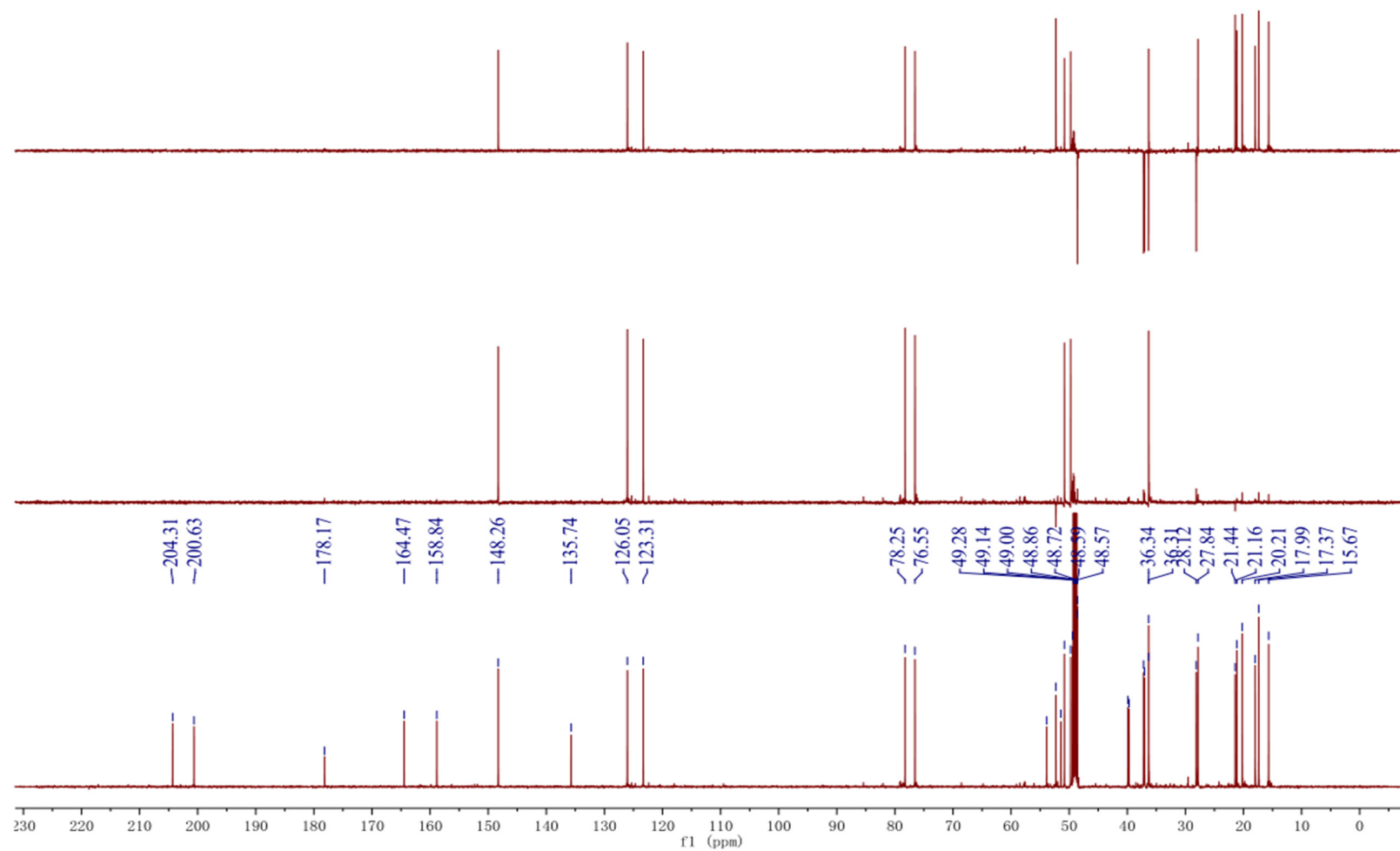


Figure S48.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 7.

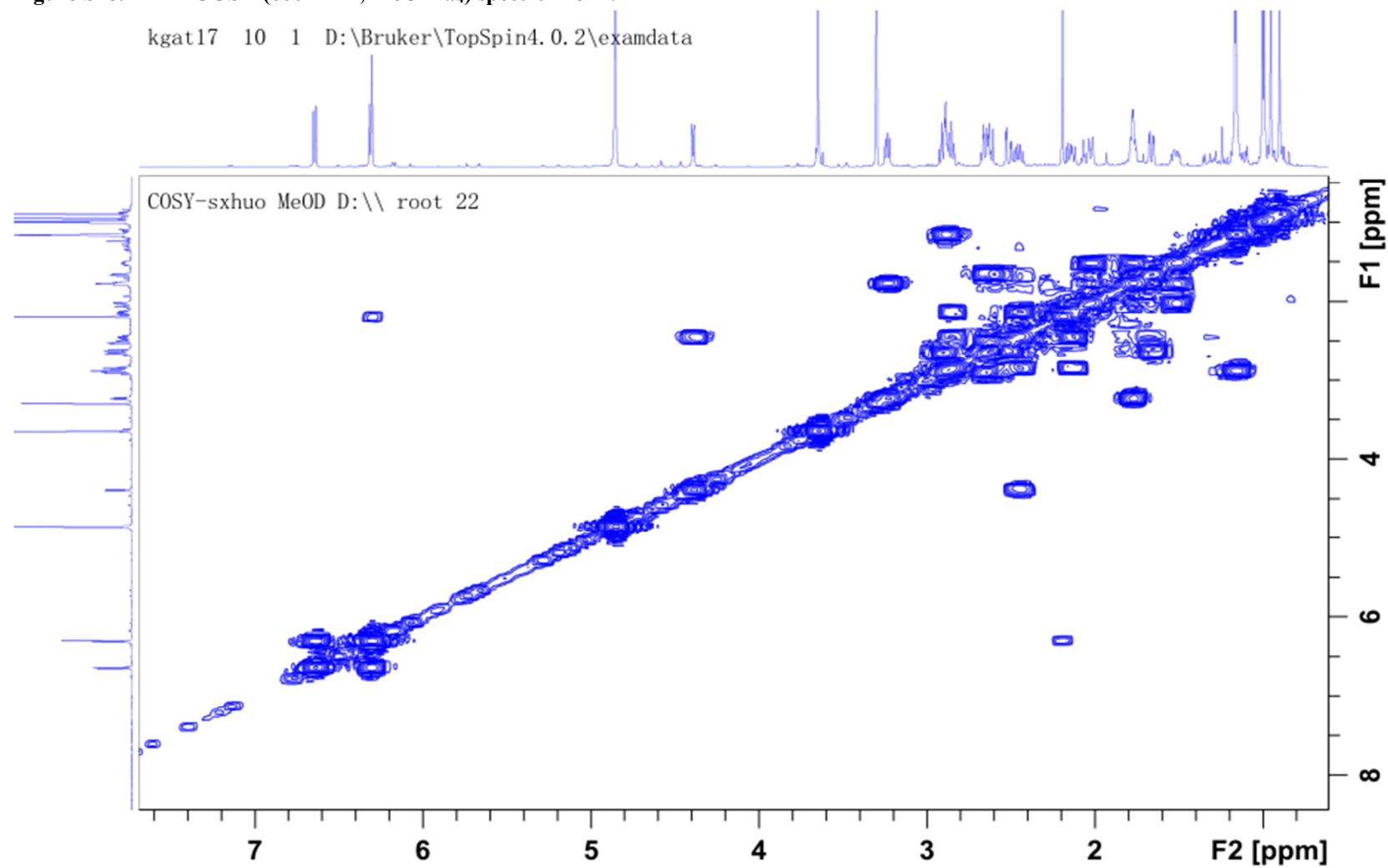


Figure S49. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 7.

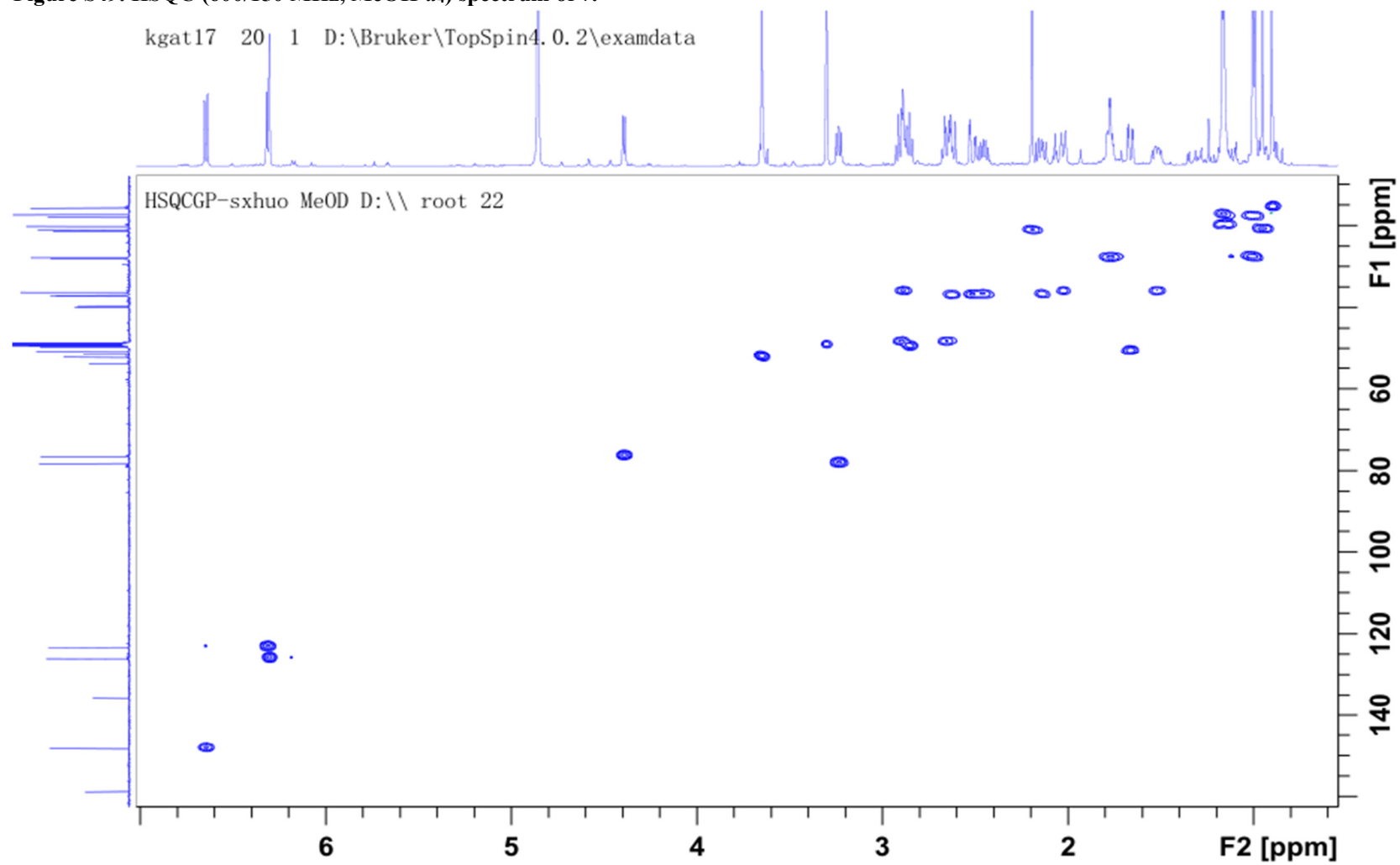


Figure S50. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 7.

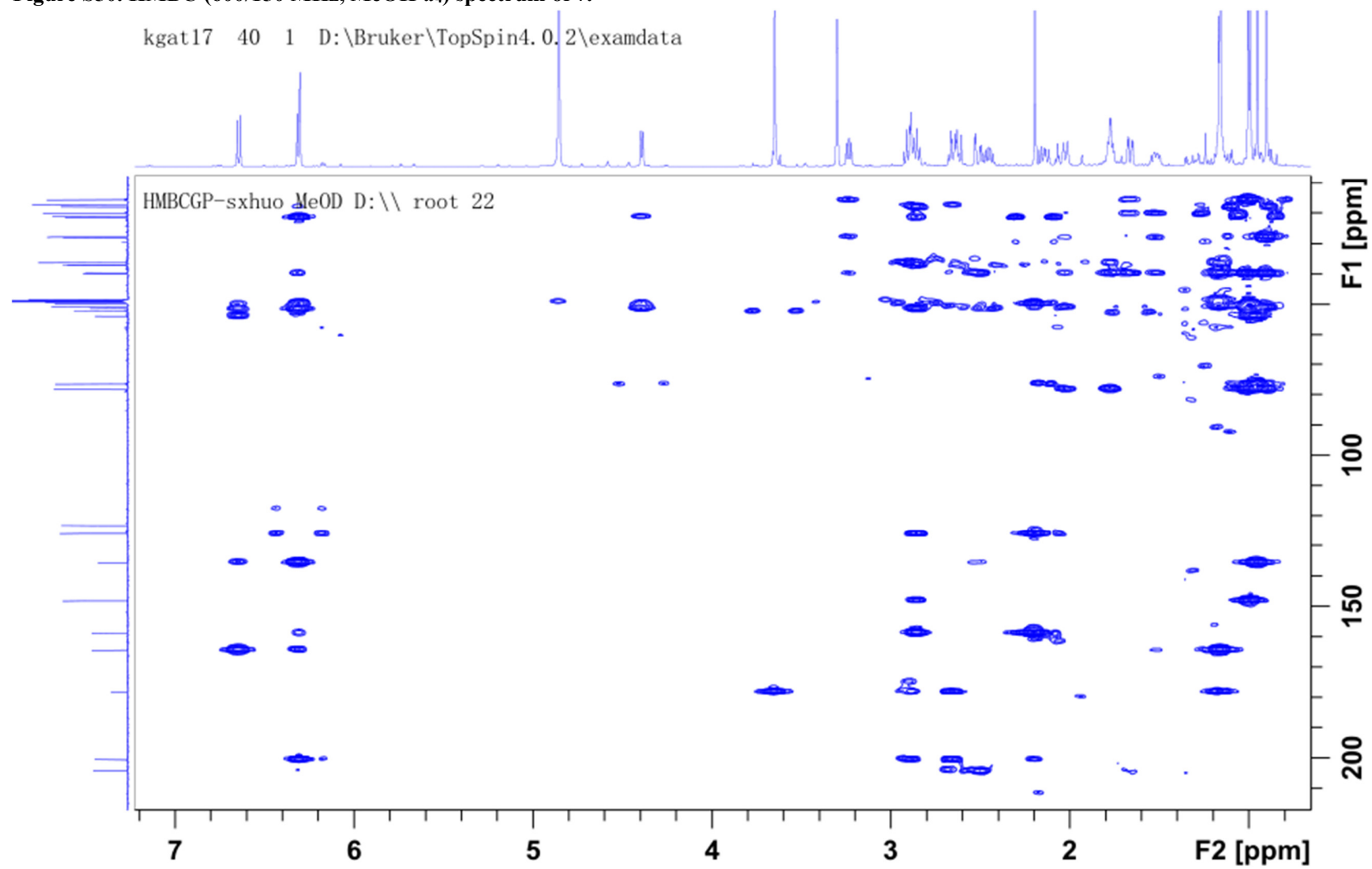
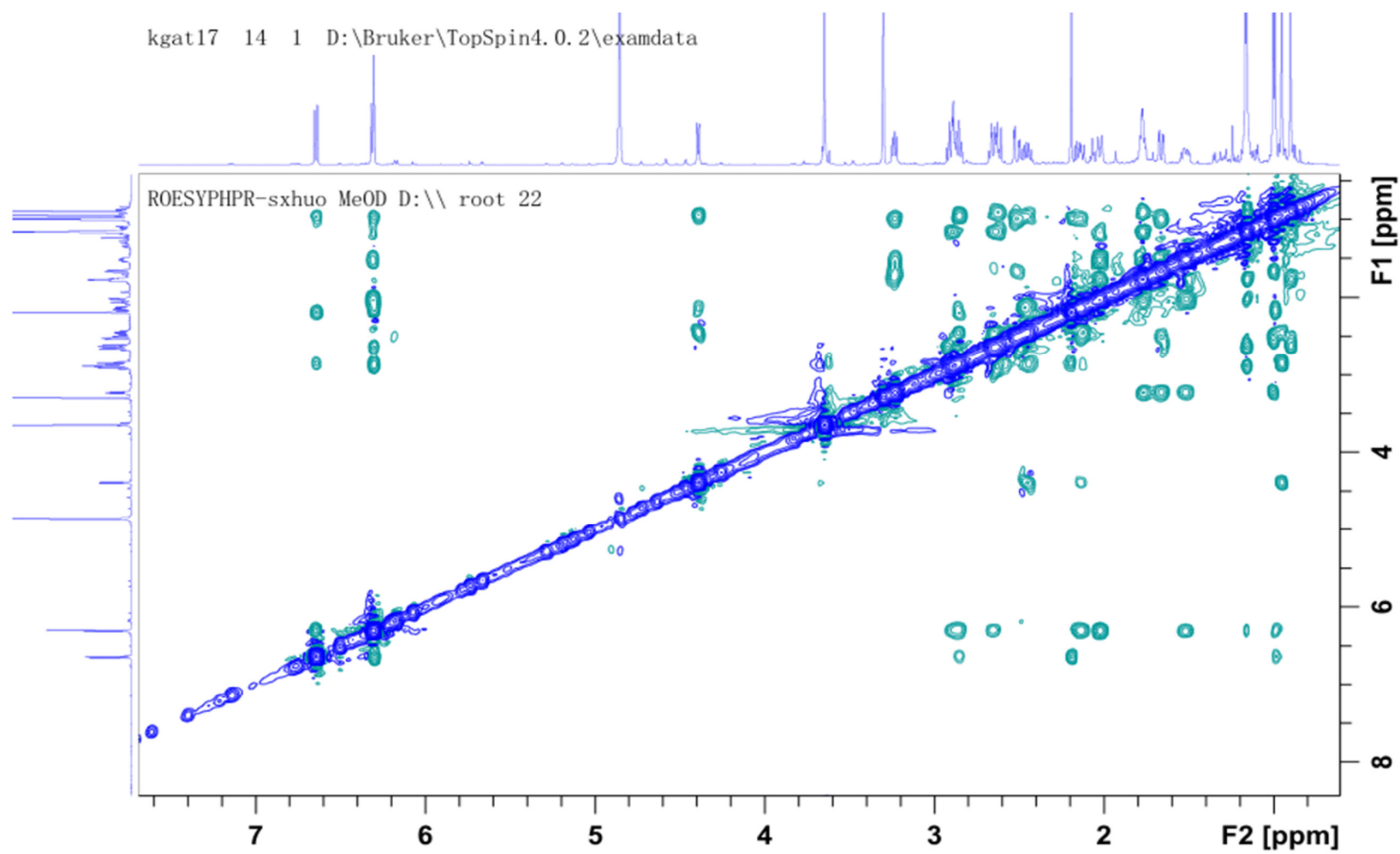


Figure S51. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 7.





## Section S16: HRESIMS spectrum of 7

Figure S52. HRESIMS spectrum of 7.

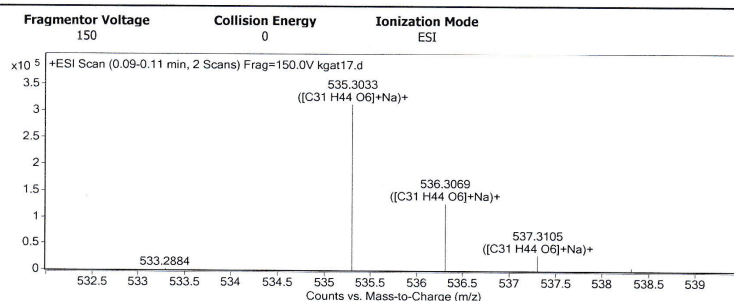
### Qualitative Analysis Report

<b>Data Filename</b>	kgat17.d	<b>Sample Name</b>	kgat17
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A6
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:42:54 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>	Info.
<b>Acquisition SW</b>	6200 series TOF/6500 series
<b>Version</b>	Q-TOF B.05.01 (B5125.2)

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
102.1274	1	86095.78		
146.0803	1	29545.42		
172.0936	1	51061.72		
513.3209	1	77645.1		
514.3248	1	33235.68		
535.3033	1	312486.22	C31 H44 O6	(M+Na)+
536.3069	1	127098.86	C31 H44 O6	(M+Na)+
1047.6183	1	225229.94		
1048.622	1	183508.3		
1049.625	1	76631.34		

### 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
C31 H44 O6	512.3138	535.3030	535.3033	-0.30	-0.56	10.0000

--- End Of Report ---

Section S17: 1D and 2D NMR spectra of compound 8

Figure S53.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 8.

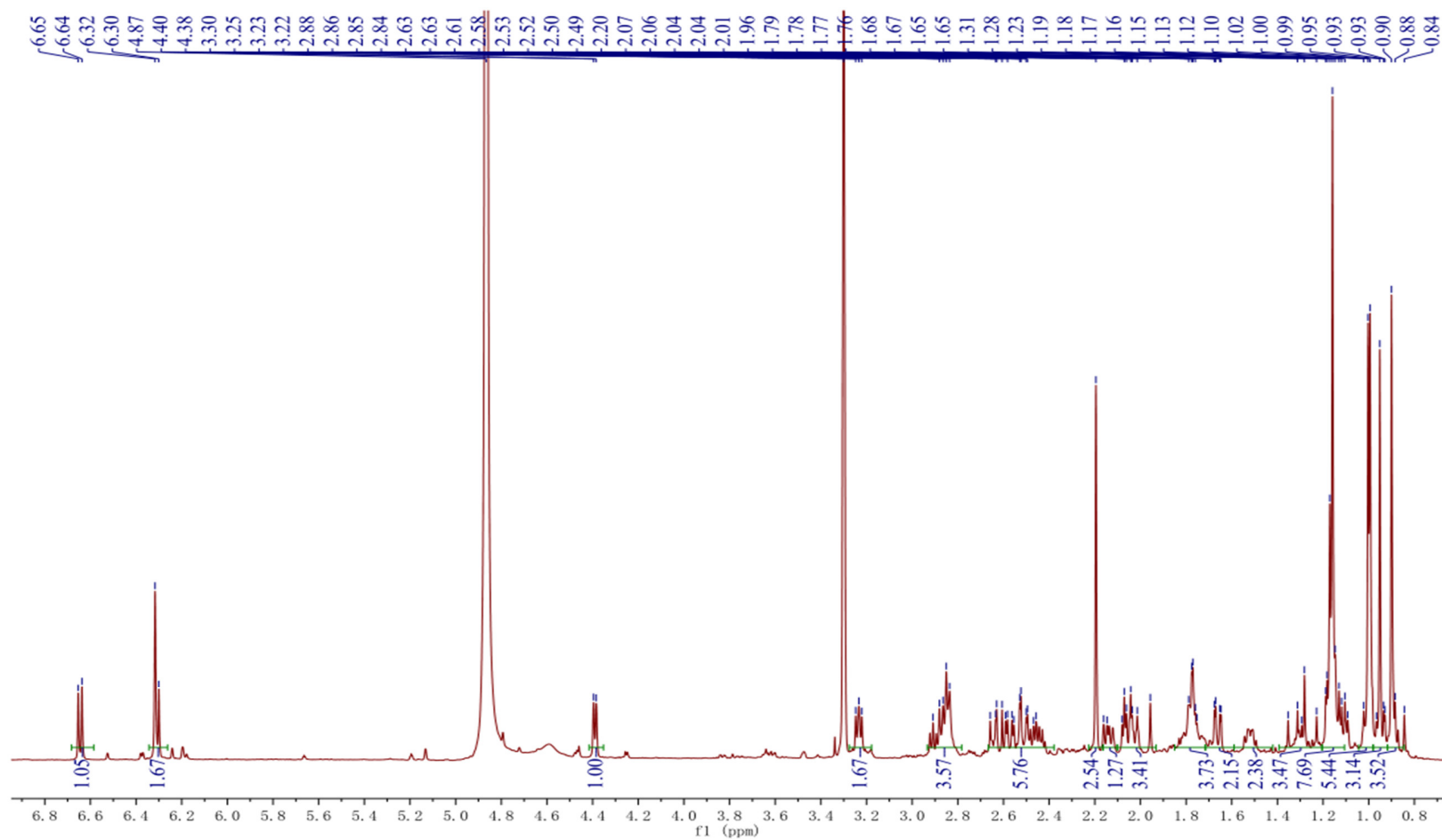


Figure S54.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 8.

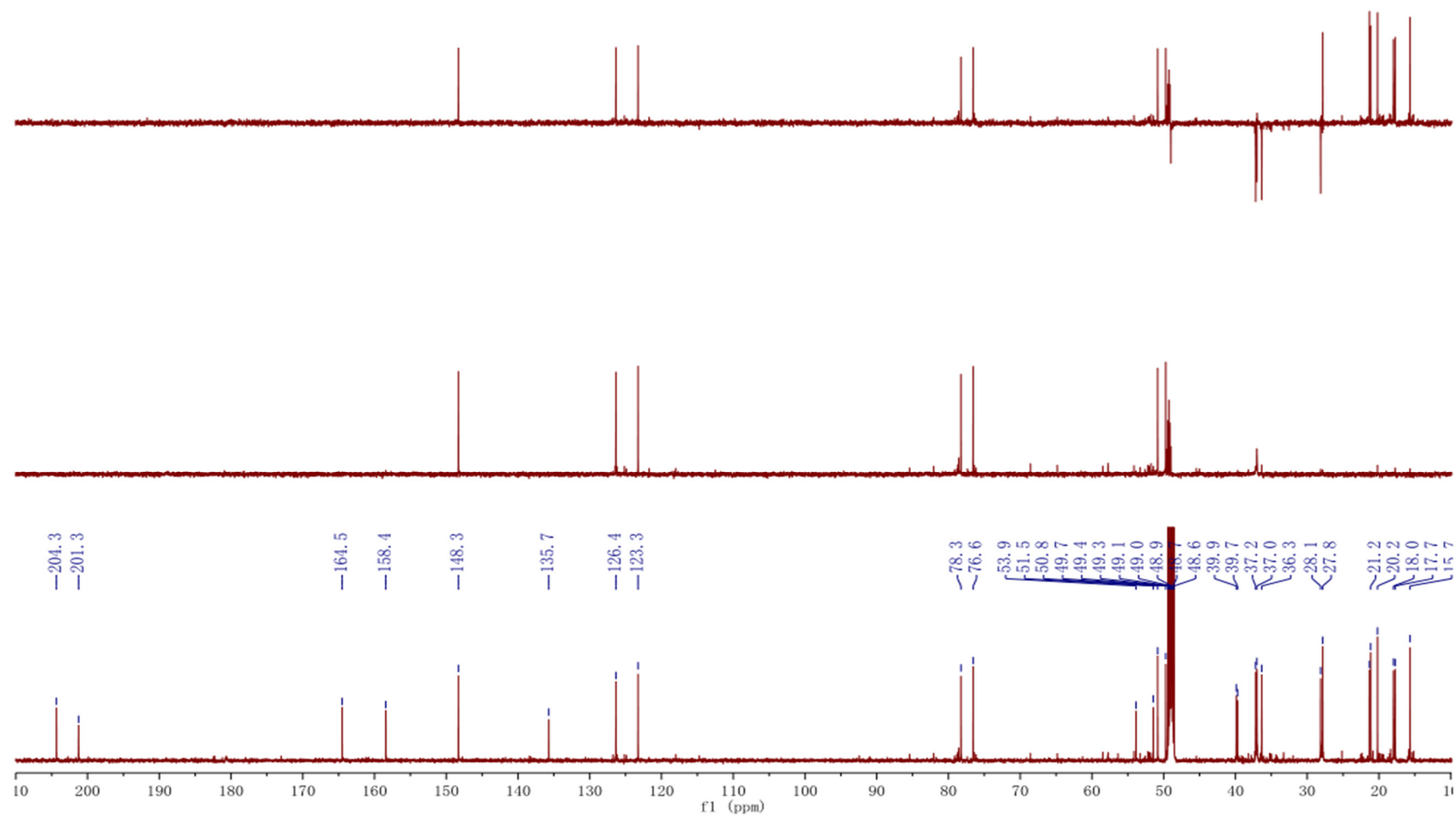


Figure S55.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 8.

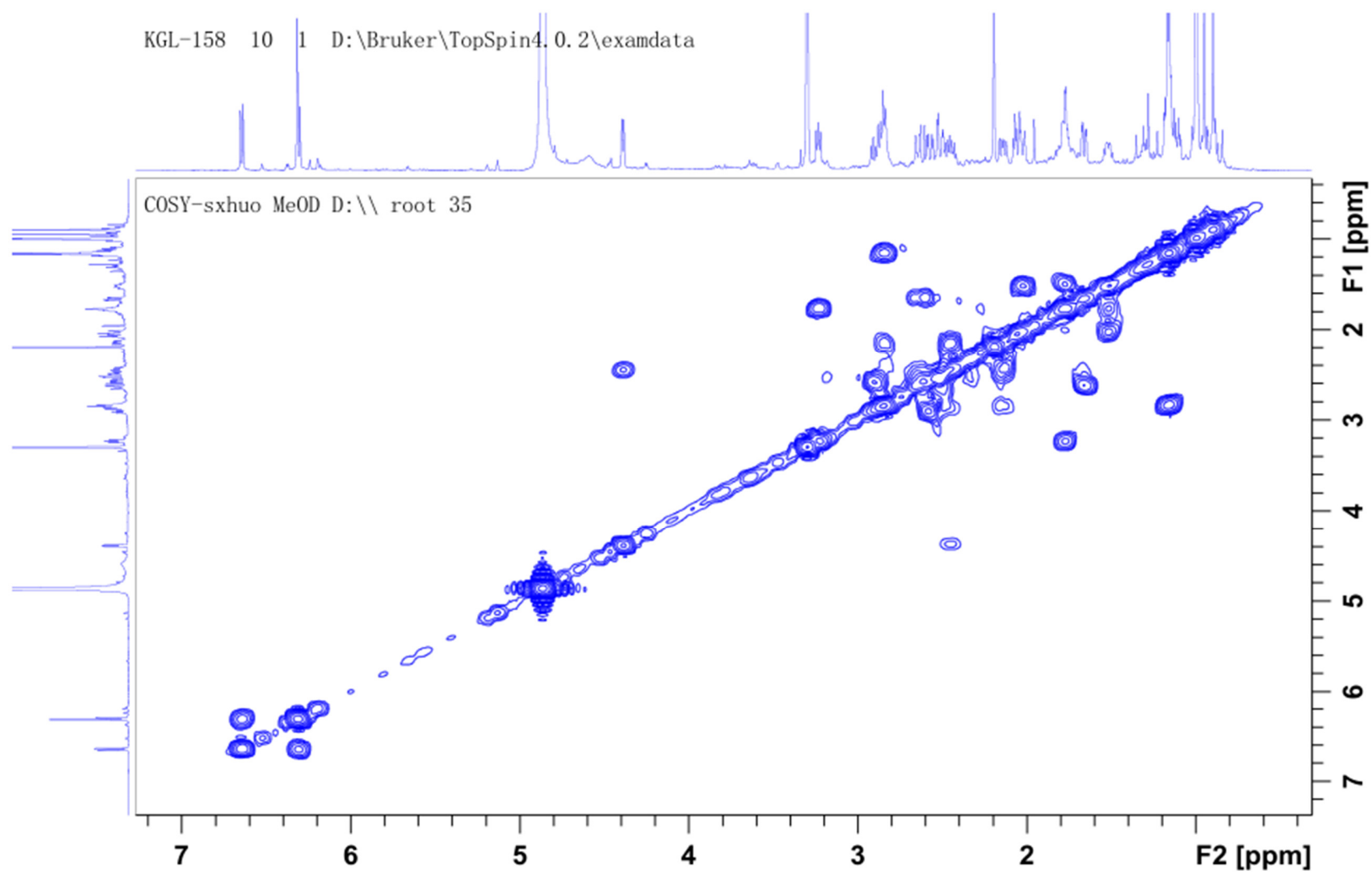


Figure S56. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 8.

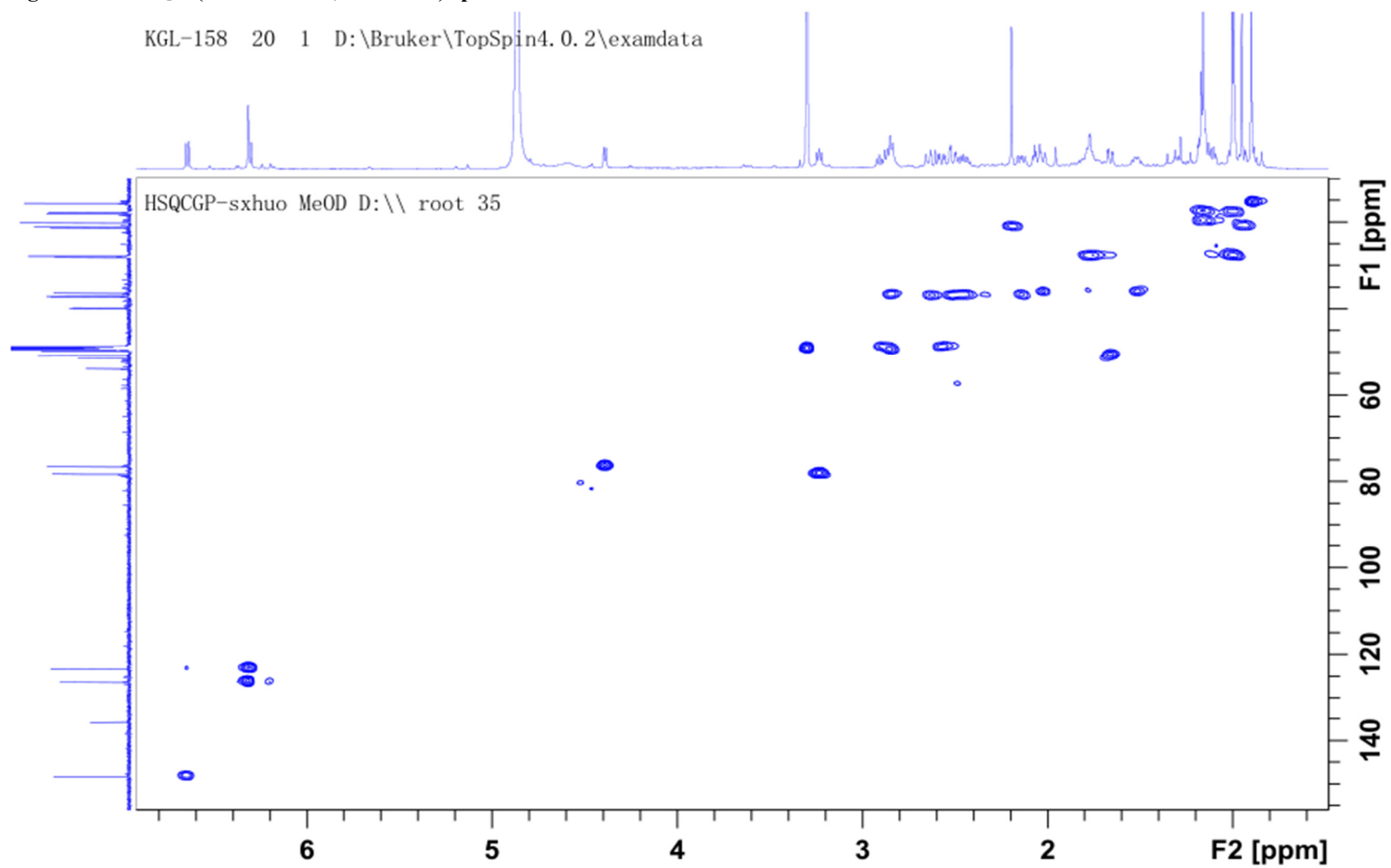


Figure S57. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 8.

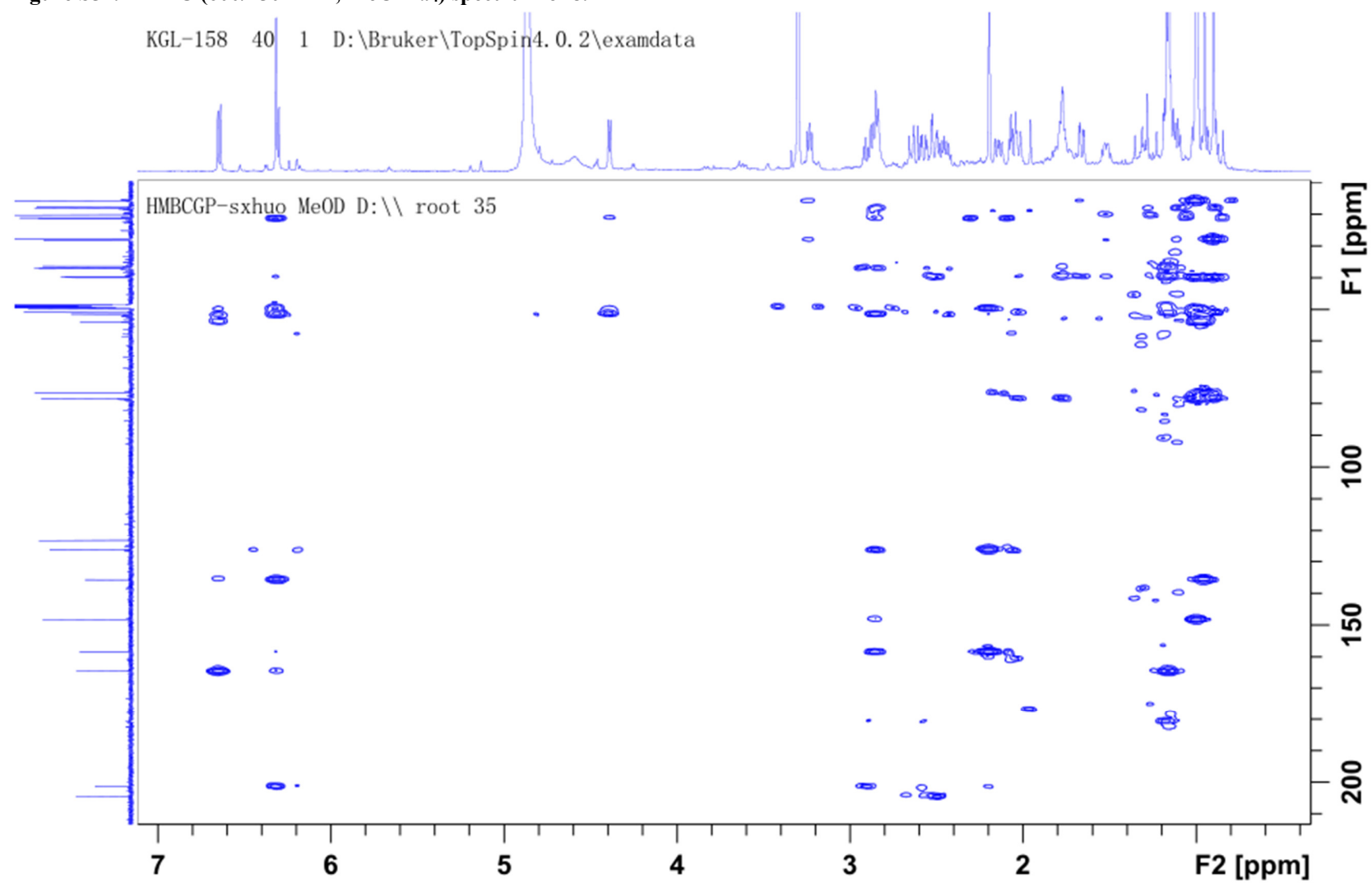
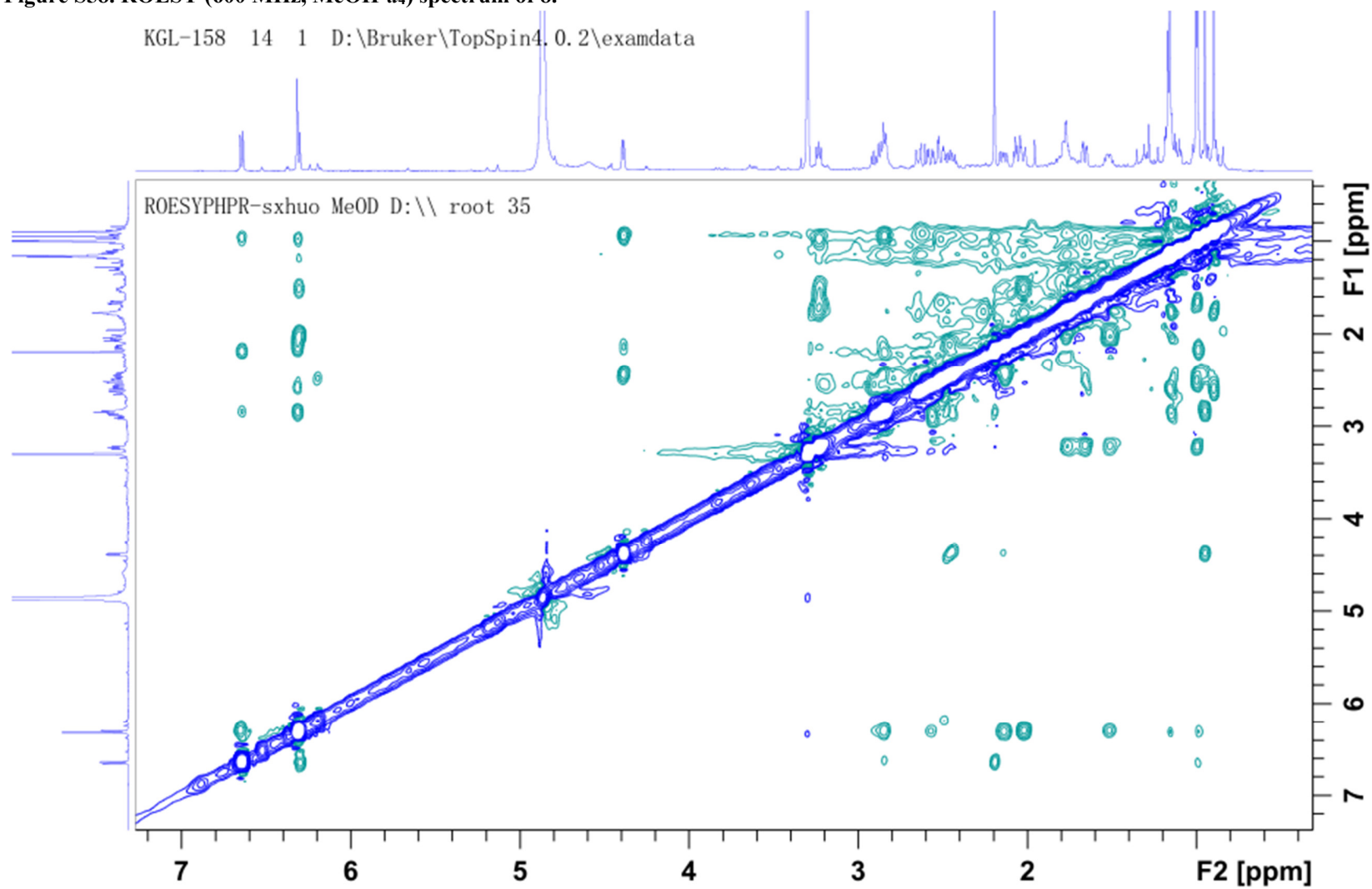


Figure S58. ROESY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of 8.



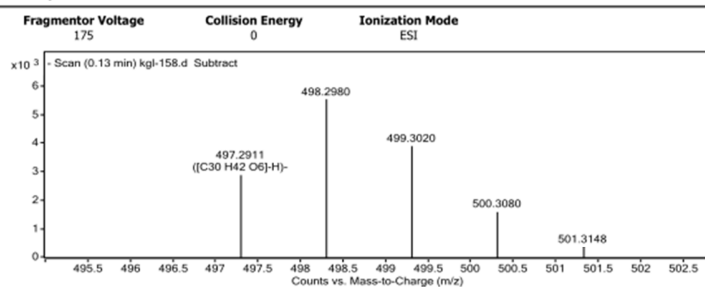
## Section S18: HRESIMS spectrum of 8

Figure S59. HRESIMS spectrum of 8.

### Qualitative Analysis Report

<b>Data Filename</b>	kg1-158.d	<b>Sample Name</b>	kg1-158
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A2
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s-m	<b>Acquired Time</b>	10/12/2020 11:08:38 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	ZRR3.m
<b>Comment</b>			
<b>Sample Group</b>	<b>Info.</b>		
<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
497.2911		2925.91	C30 H42 O6	(M-H)-
498.298		5542.1		
499.302	1	3925.09		
500.308	1	1642.42		
512.2784		921.76		
513.2855		1117.4		
514.292	1	1240.95		
515.3006	1	692.01		
566.2904	1	797.03		
1033.9881		1762.93		

### 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
C30 H42 O6	498.2981	497.2909	497.2911	-0.20	-0.40	10.0000

--- End Of Report ---



# Section S19: 1D and 2D NMR spectra of compound 9

Figure S60. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of 9.

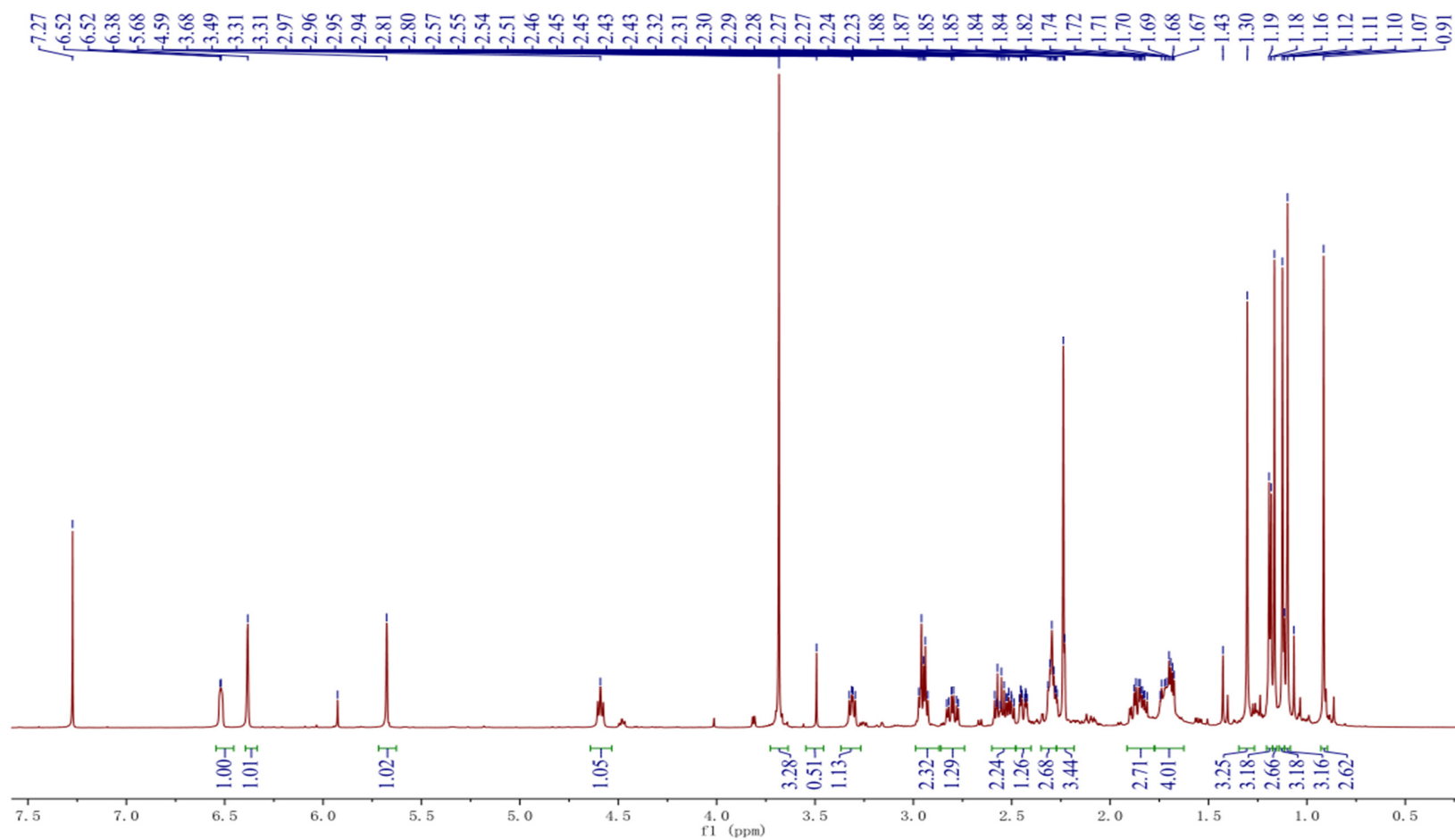


Figure S61.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of 9.

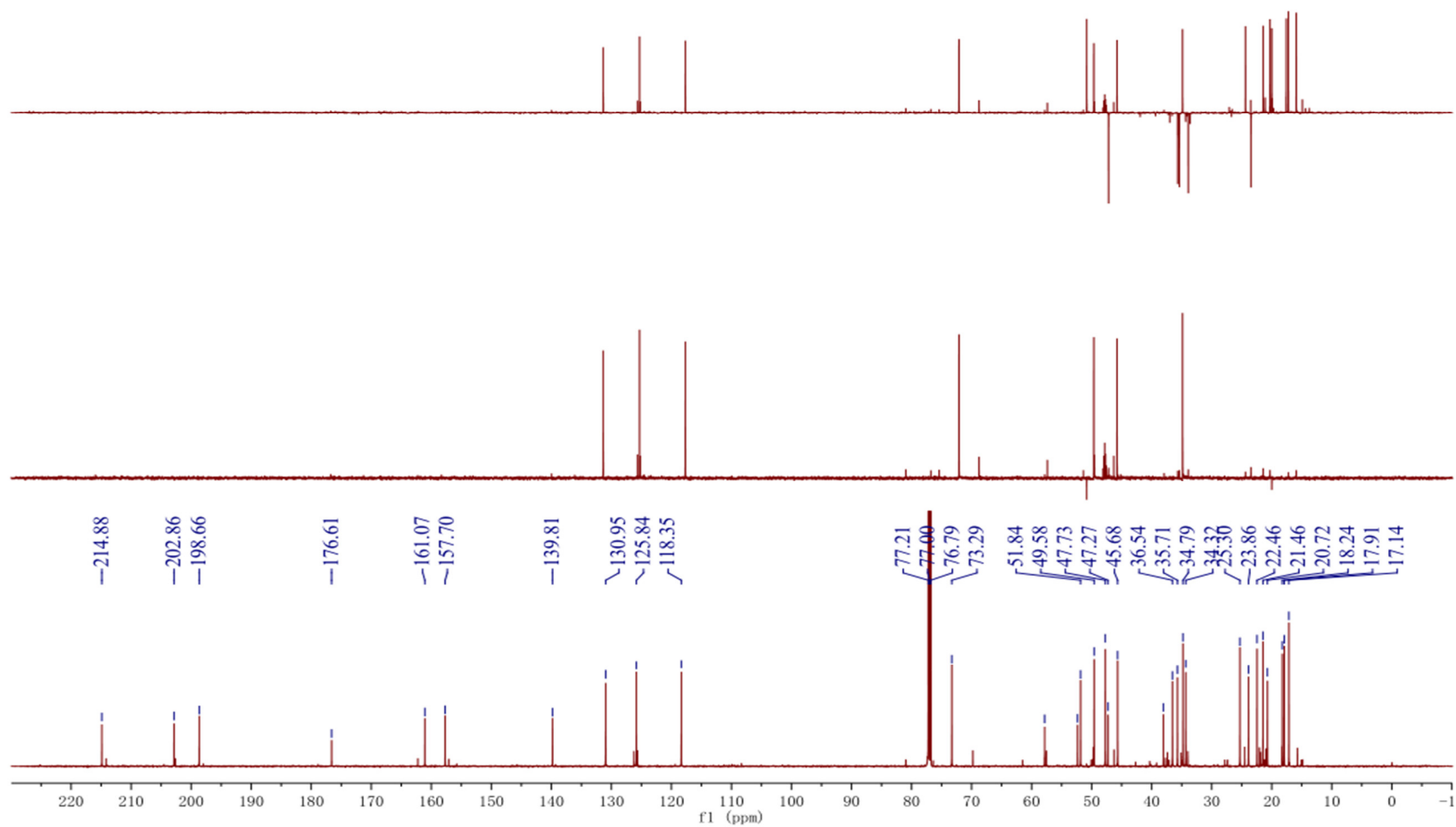


Figure S62.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{CDCl}_3$ ) spectrum of 9.

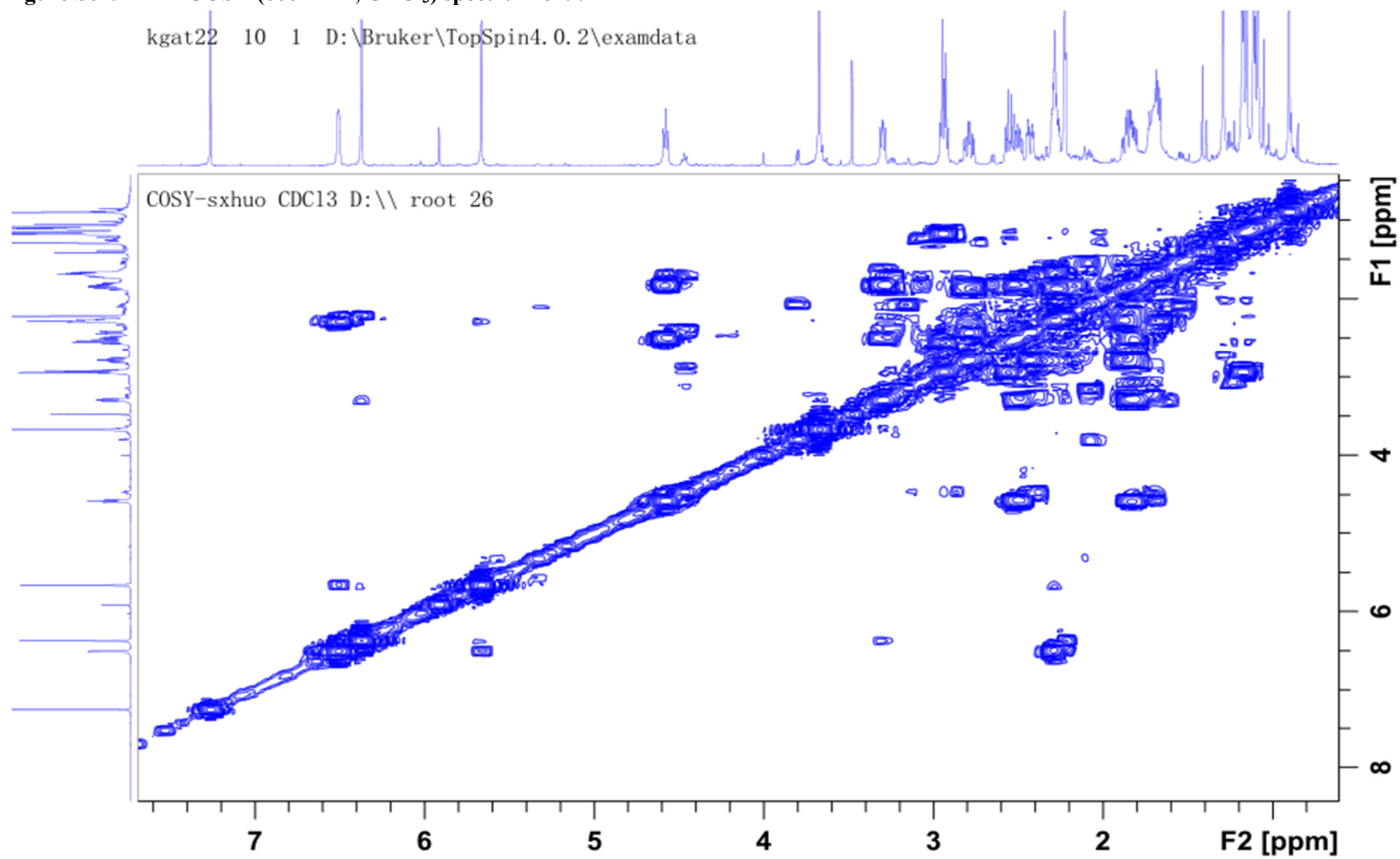


Figure S63. HSQC (600/150 MHz, CDCl<sub>3</sub>) spectrum of 9.

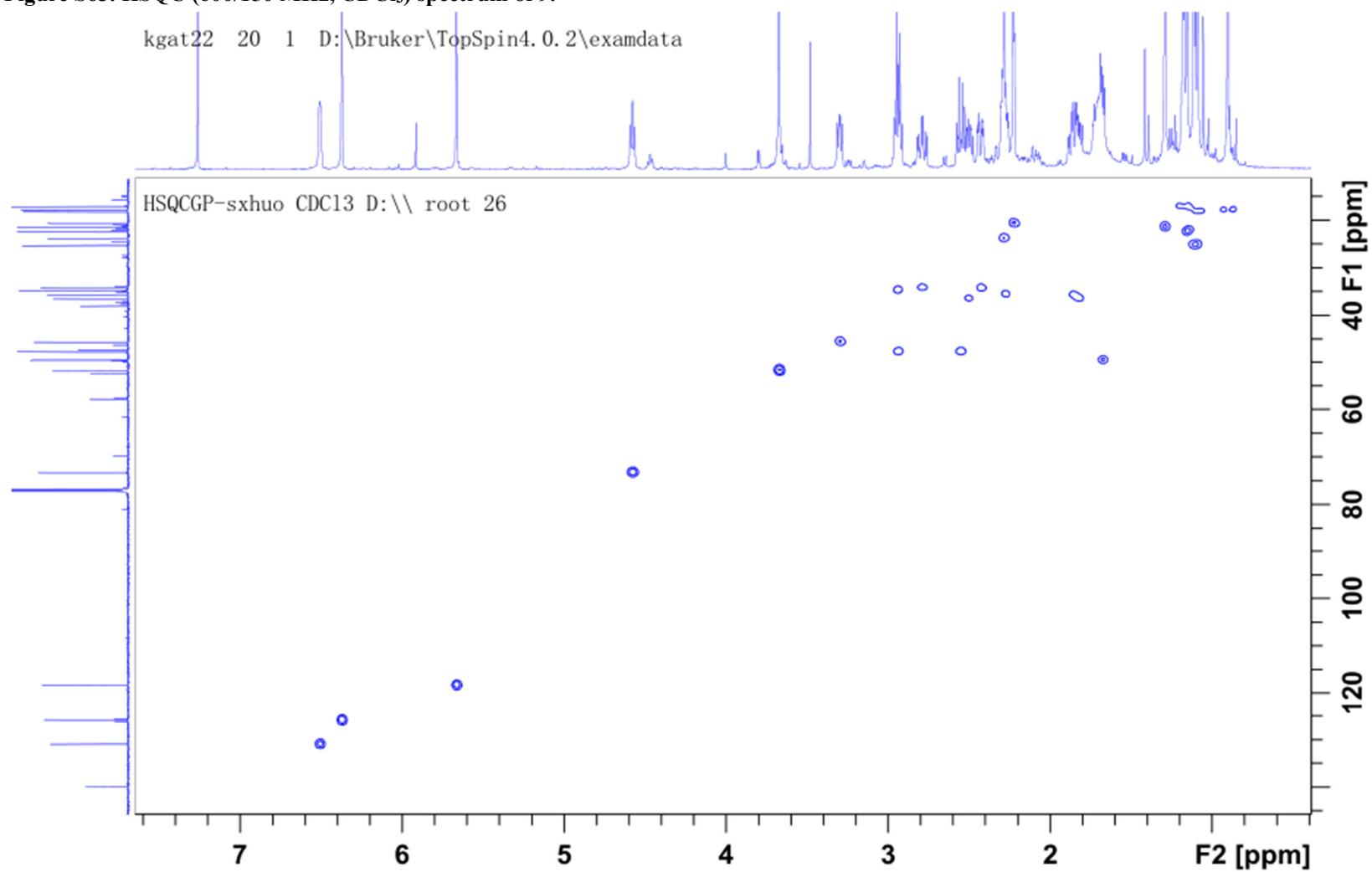


Figure S64. HMBC (600/150 MHz, CDCl<sub>3</sub>) spectrum of 9.

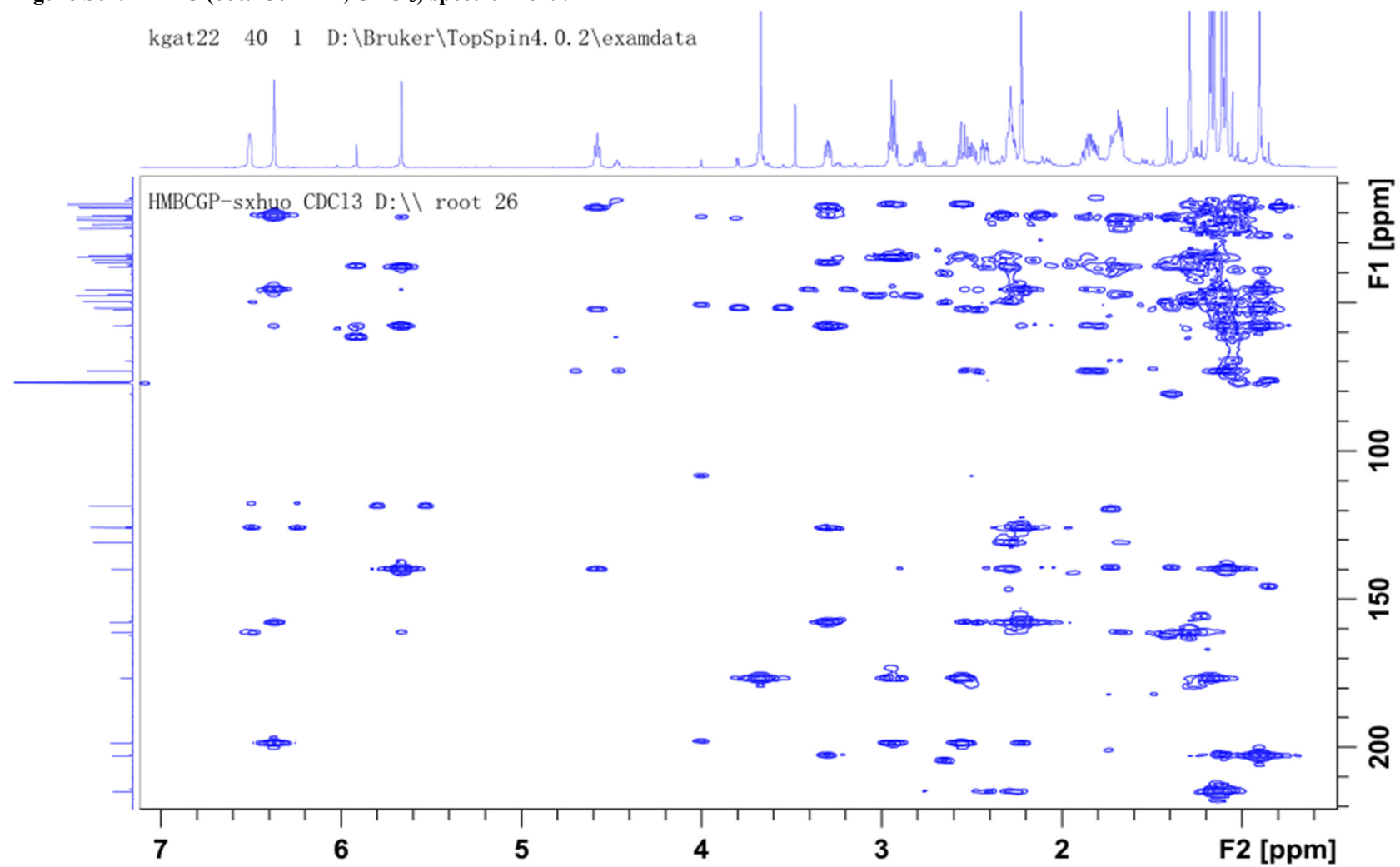
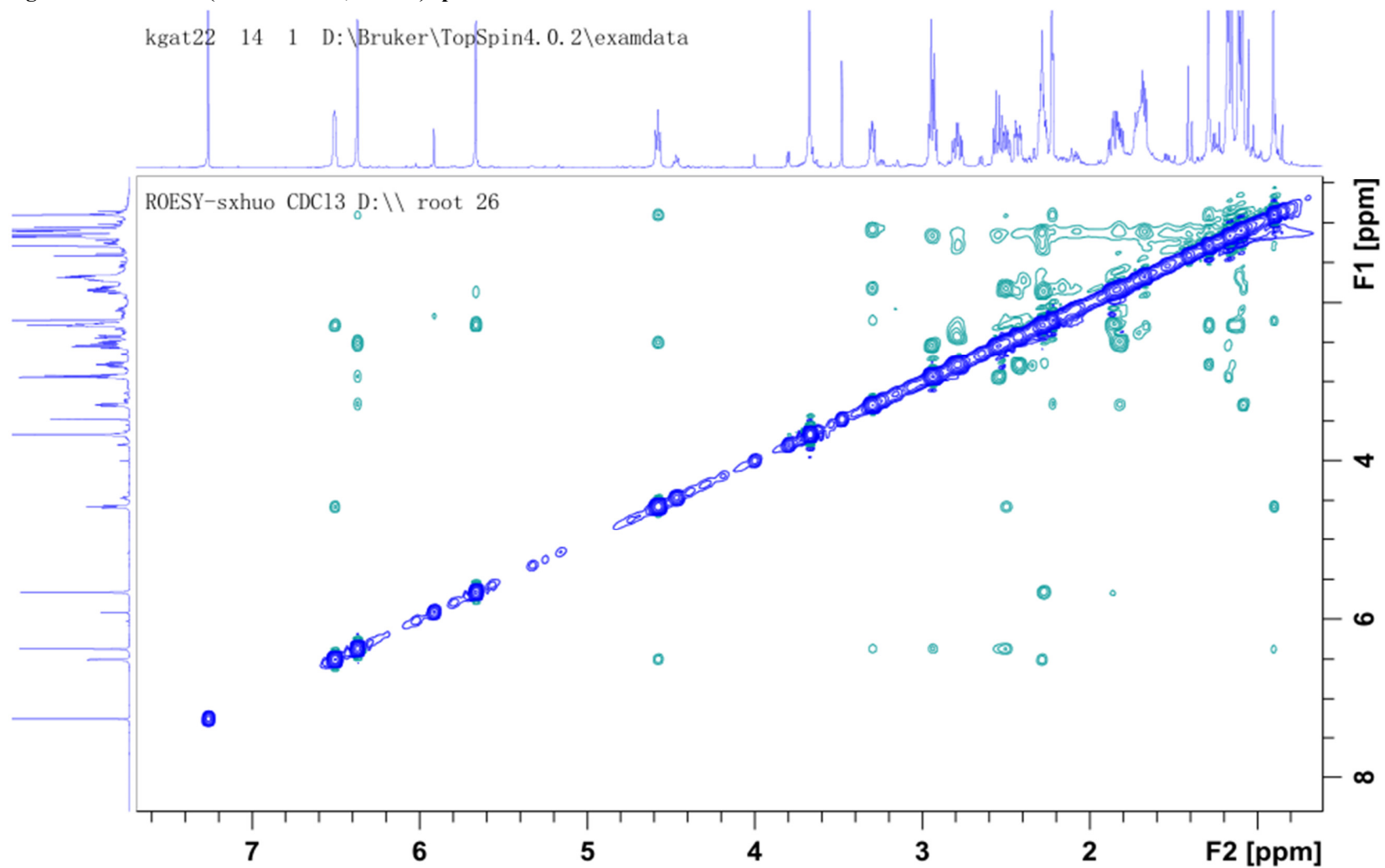


Figure S65. ROESY (600/150 MHz, CDCl<sub>3</sub>) spectrum of 9.



**Section S20: HRESIMS spectrum of 9**

**Figure S66. HRESIMS spectrum of 9.**

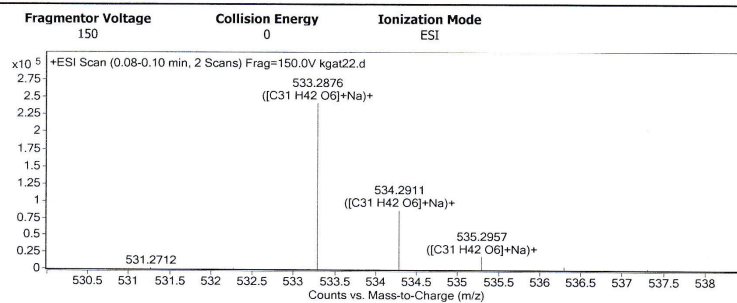
### Qualitative Analysis Report

<b>Data Filename</b>	kgat22.d	<b>Sample Name</b>	kgat22
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A9
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:46:27 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>	<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series
<b>Version</b>	Q-TOF B.05.01 (B5125.2)

#### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
102.1274	1	24207.48		
172.0936	1	56103.34		
511.3051	1	46827.01		
533.2876	1	242101.48	C31 H42 O6	(M+Na)+
534.2911	1	87653.3	C31 H42 O6	(M+Na)+
549.2734	1	36785.6		
1043.5863	1	125190.95		
1044.5899	1	93311.35		
1045.5928	1	41897.05		
1059.5807	1	31313.65		

#### 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
C31 H42 O6	510.2981	533.2874	533.2876	-0.20	-0.38	11.0000

--- End Of Report ---

# Section S21: 1D and 2D NMR spectra of compound 10

Figure S67. <sup>1</sup>H NMR (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of 10.

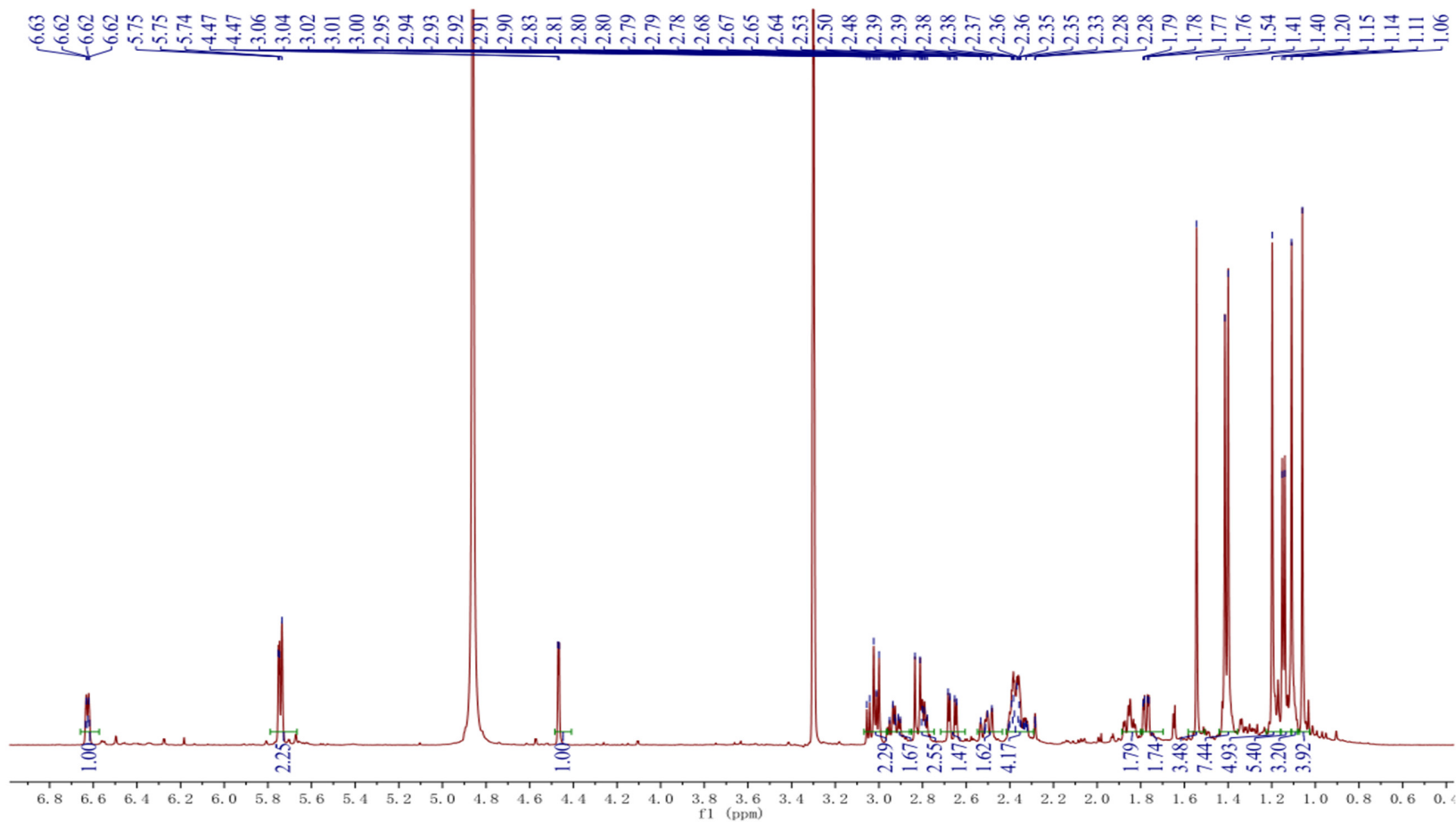




Figure S68.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 10.

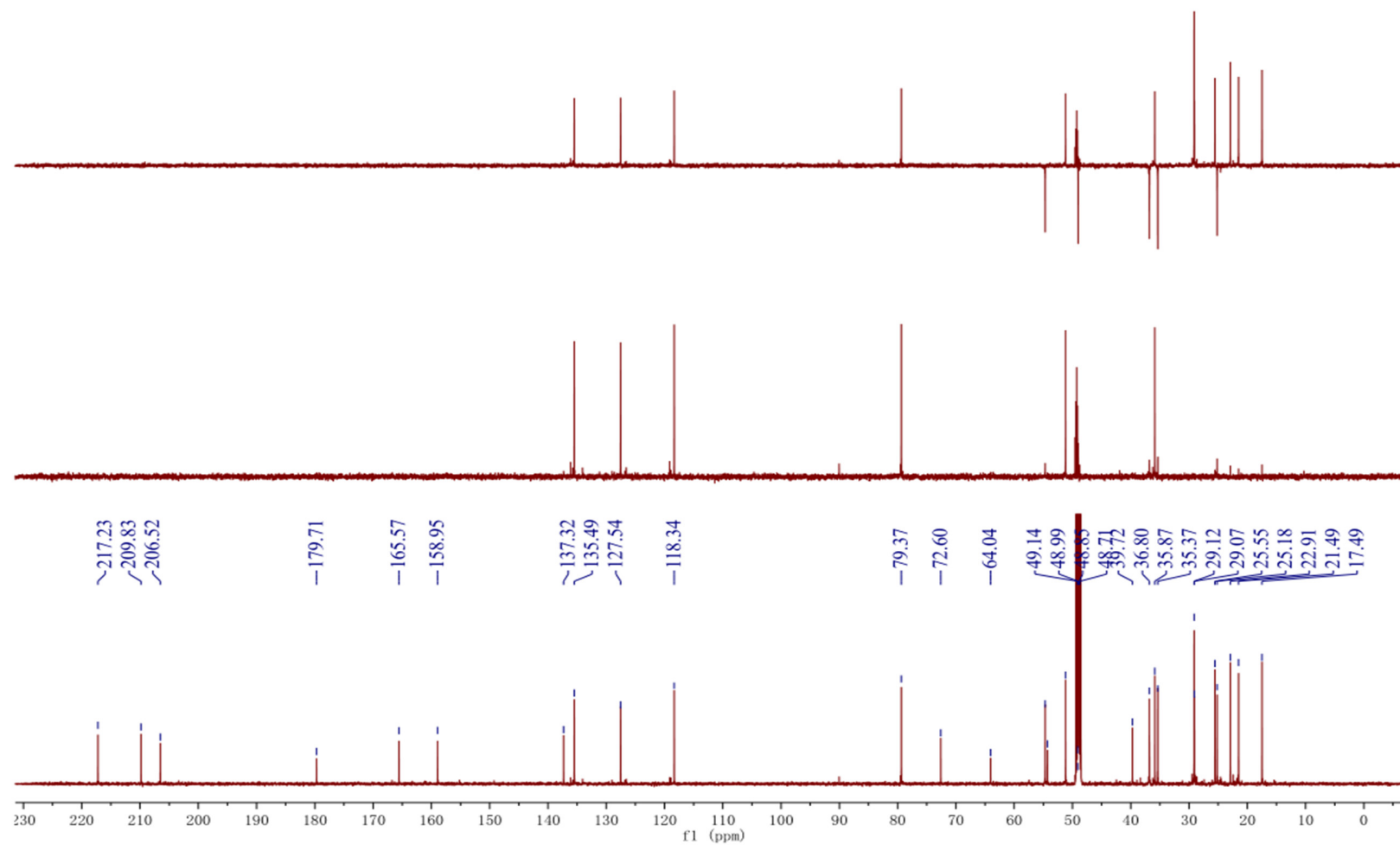


Figure S69.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 10.

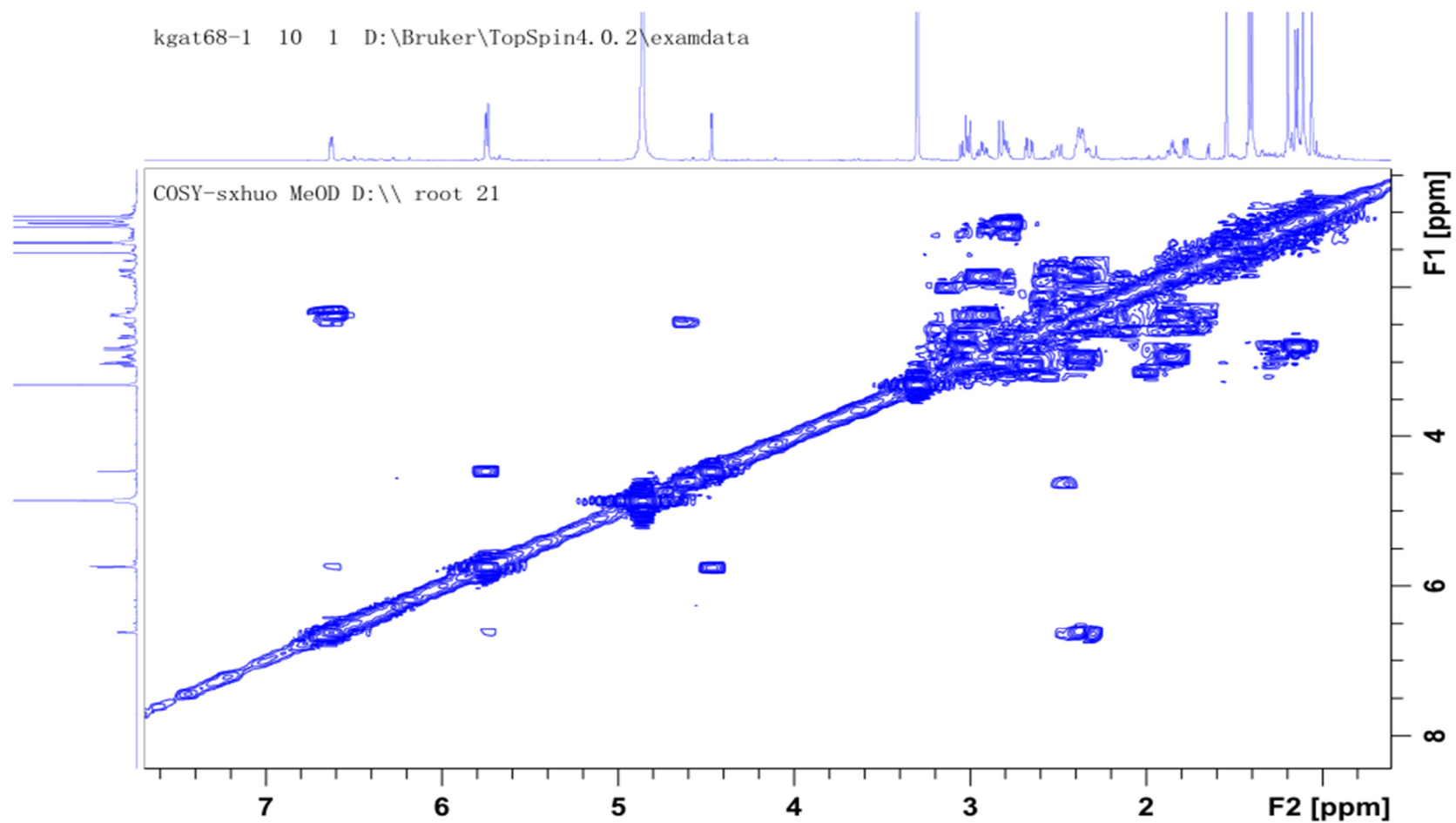


Figure S70. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 10.

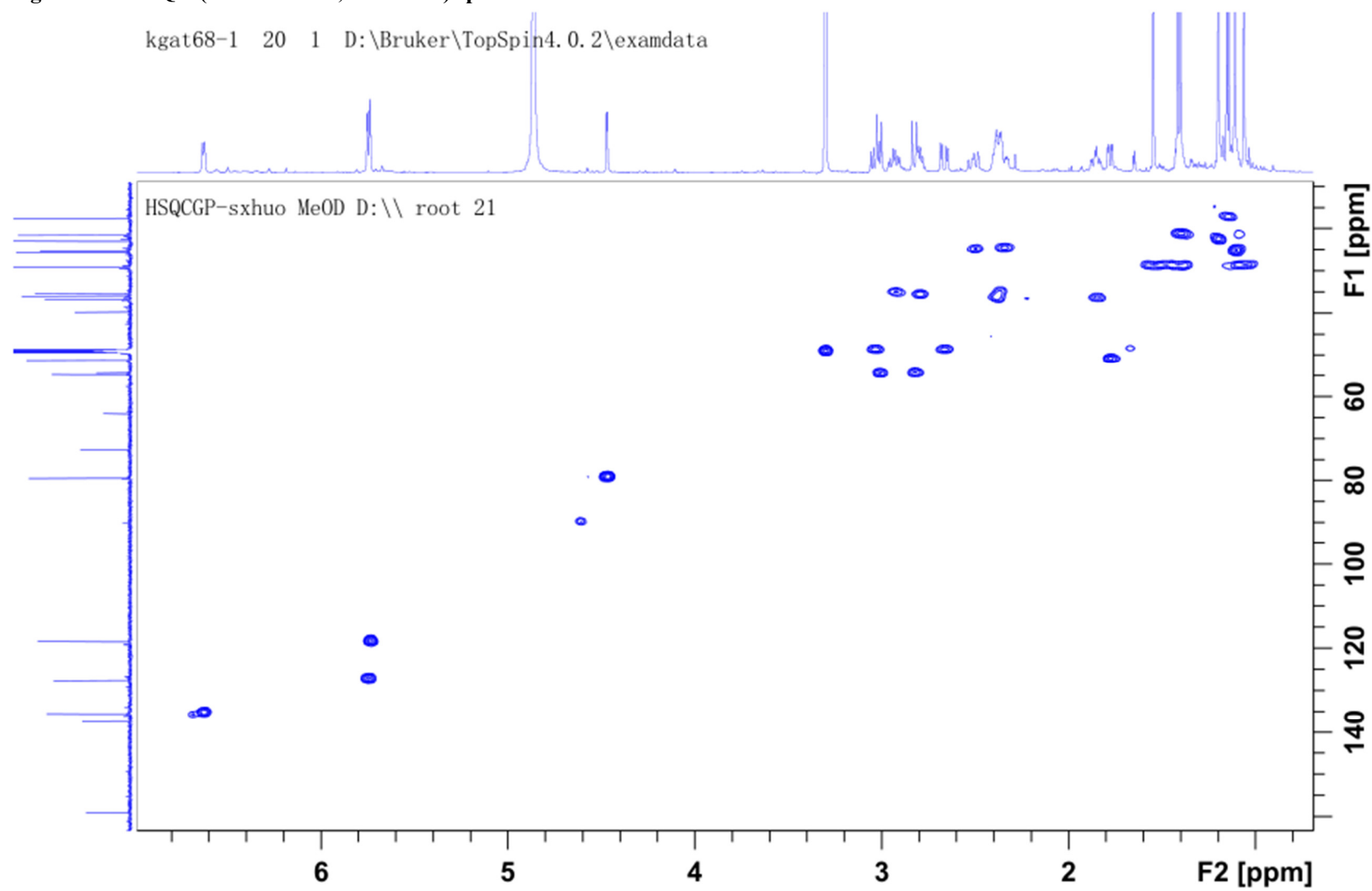


Figure S71. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 10.

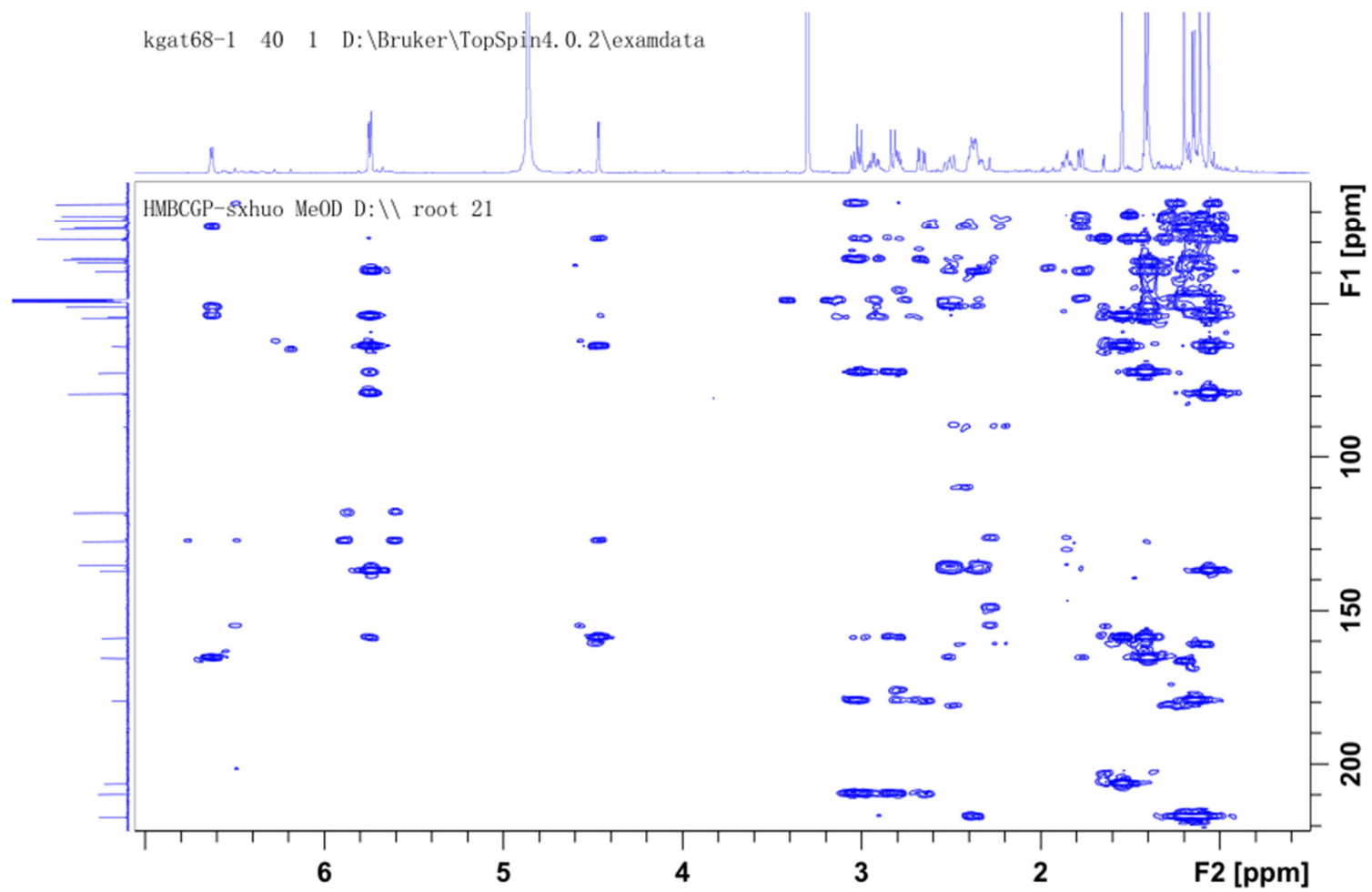
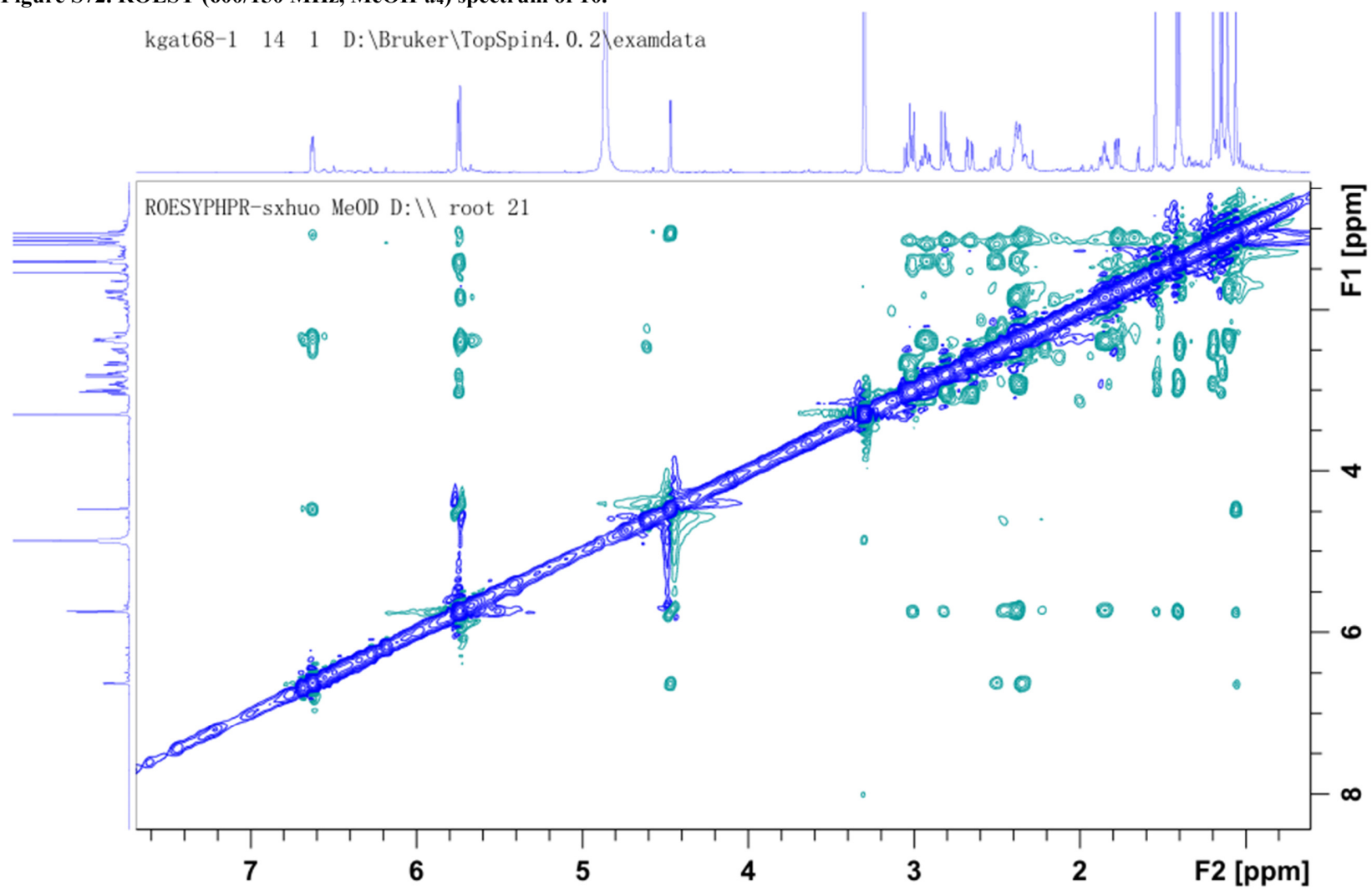


Figure S72. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 10.



## Section S22: HRESIMS spectrum of 10

Figure S73. HRESIMS spectrum of 10.

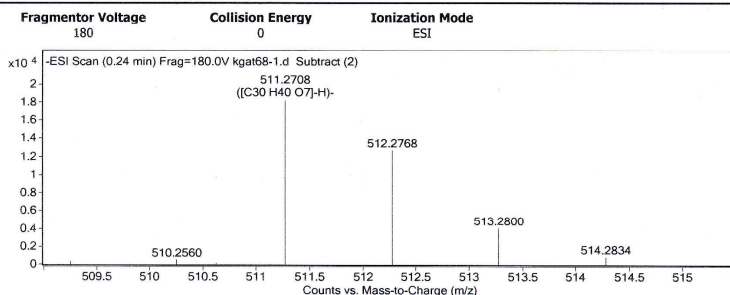
### Qualitative Analysis Report

<b>Data Filename</b>	kgat68-1.d	<b>Sample Name</b>	kgat68-1
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A6
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s-.m	<b>Acquired Time</b>	7/9/2021 3:17:33 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
129.0554		2320		
493.2601		1402.9		
494.2642	1	1299.74		
511.2708		18227.04	C30 H40 O7	(M-H)-
512.2768	1	12667.26		
513.28	1	4049.29		
527.2673		3307.64		
528.2705	1	2243.17		
528.3024	1	1029.55		
529.2735	1	1051.21		
579.2585	1	2825.05		
580.2648	1	1943.69		

### 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
C30 H40 O7	512.2774	511.2701	511.2708	-0.70	-1.37	11.0000

--- End Of Report ---

Section S23: 1D and 2D NMR spectra of compound 11

Figure S74.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 11.

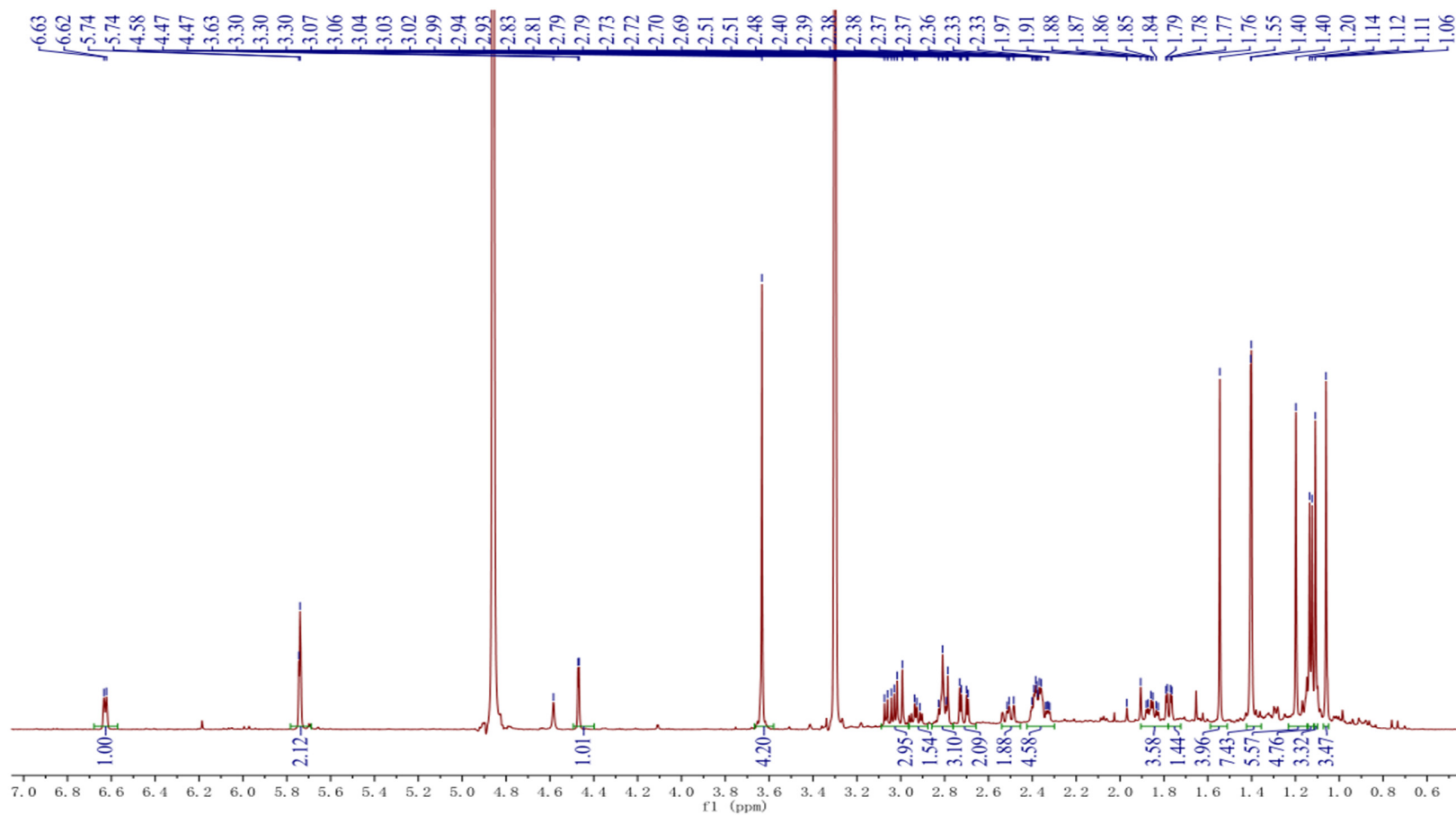


Figure S75.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 11.

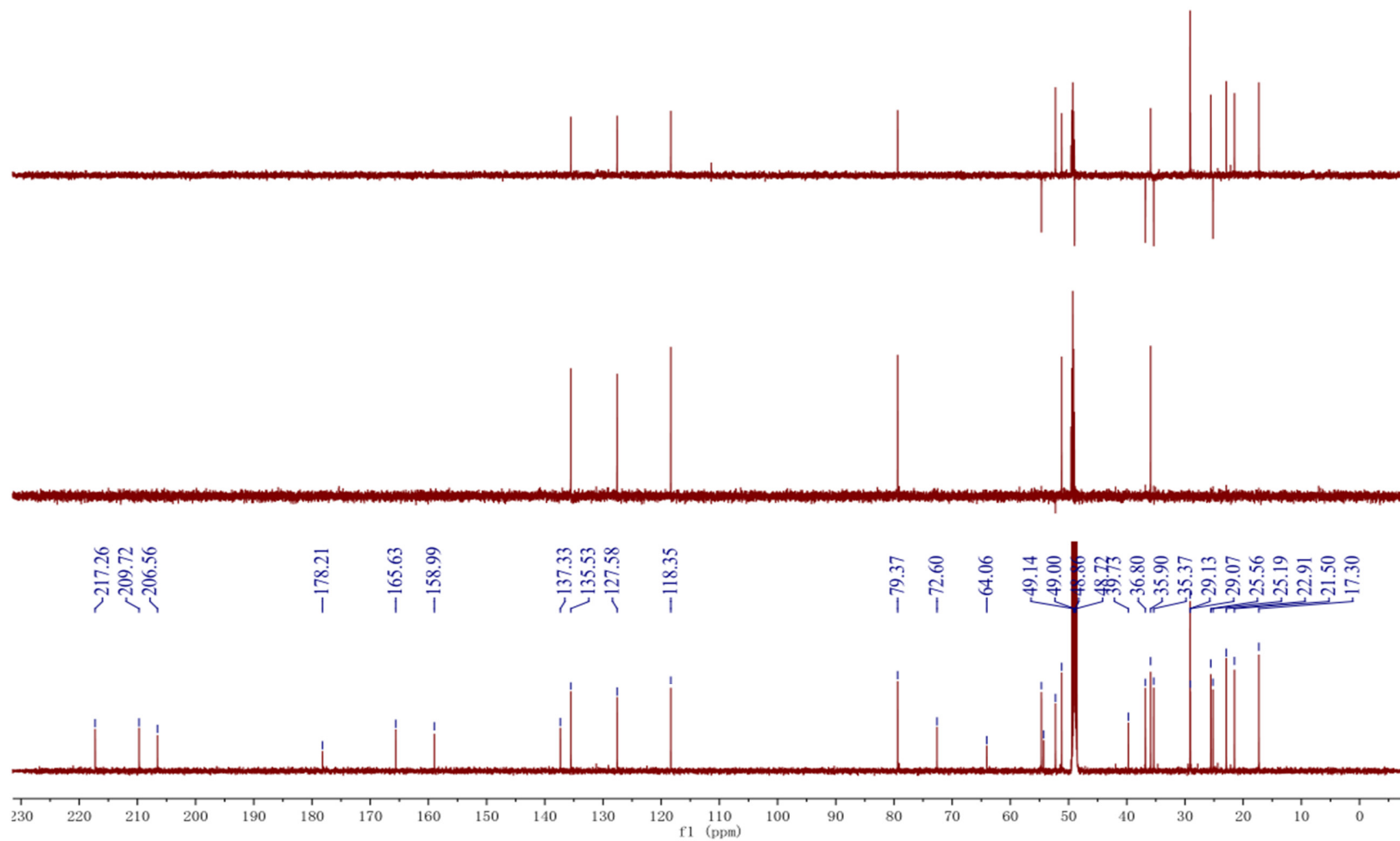




Figure S76.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 11.

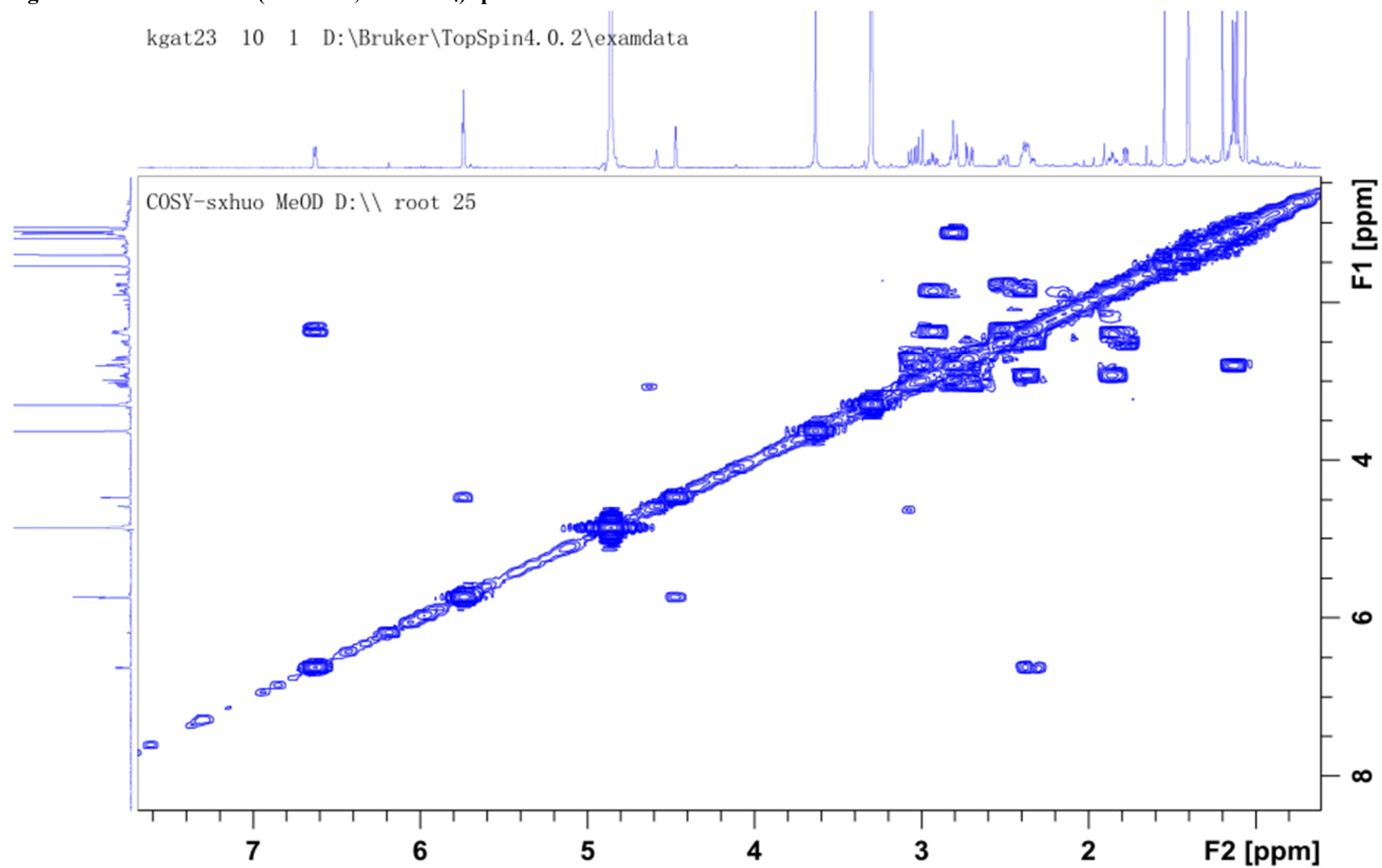


Figure S77. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 11.

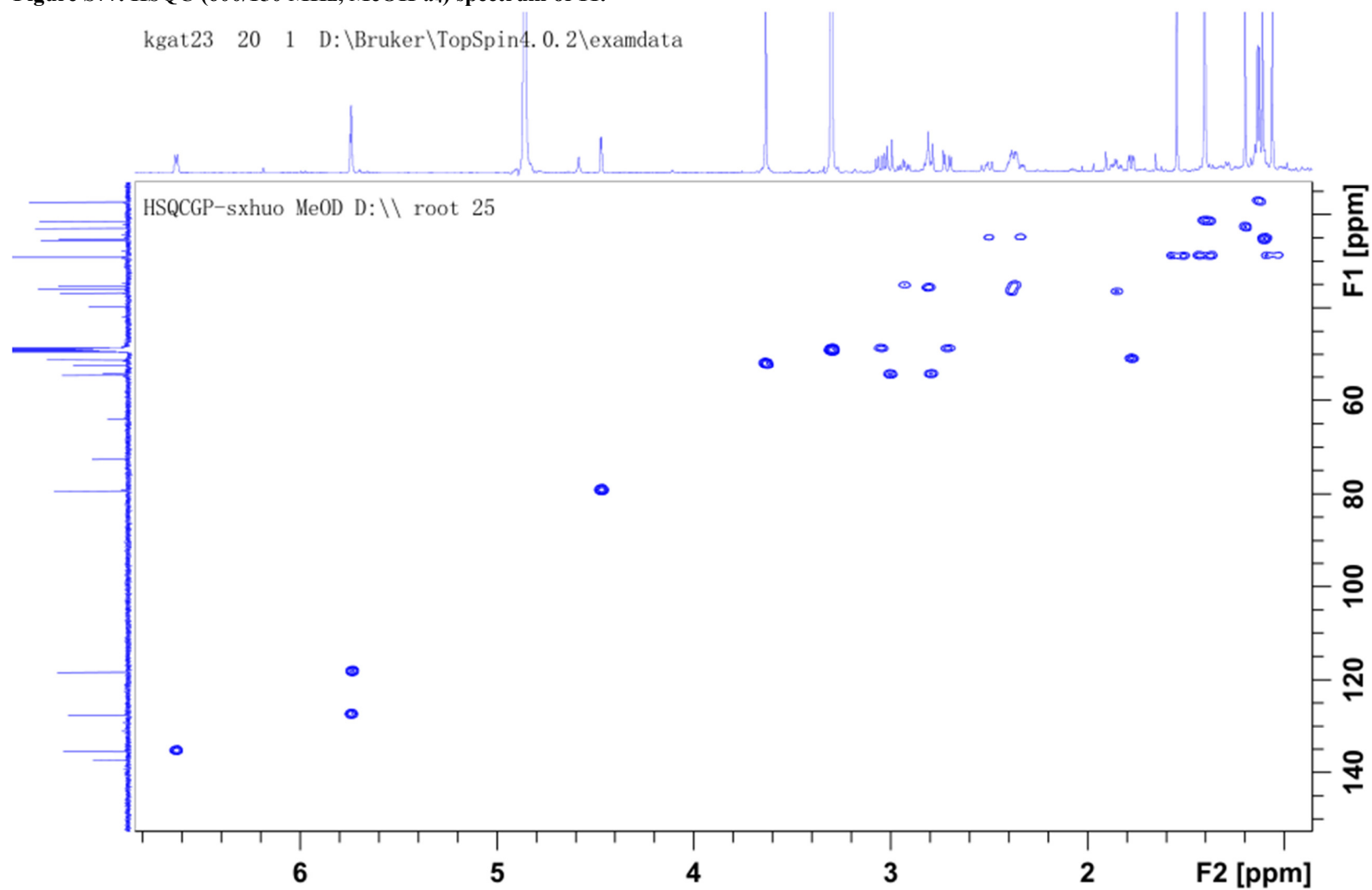


Figure S78. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 11.

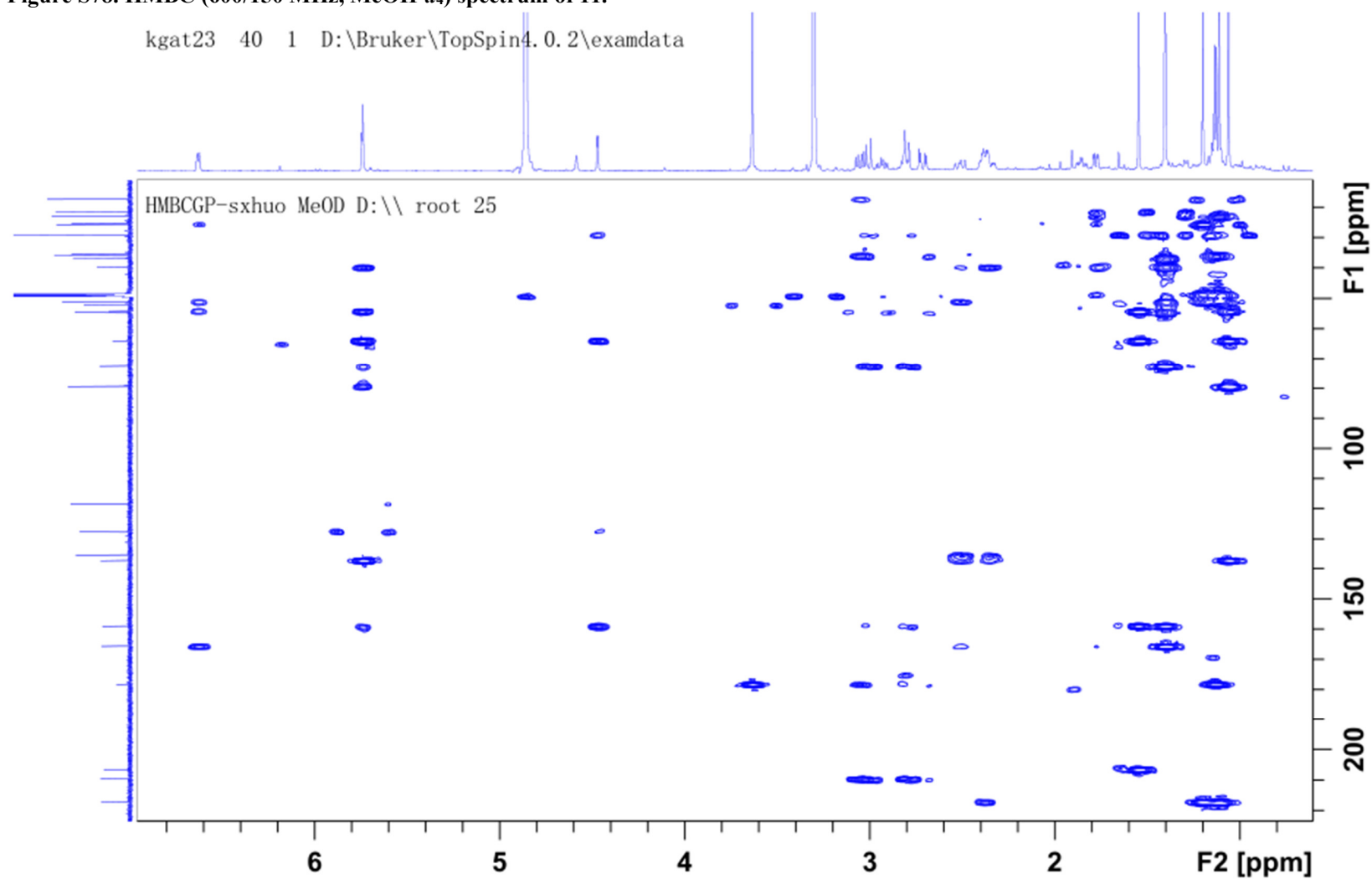
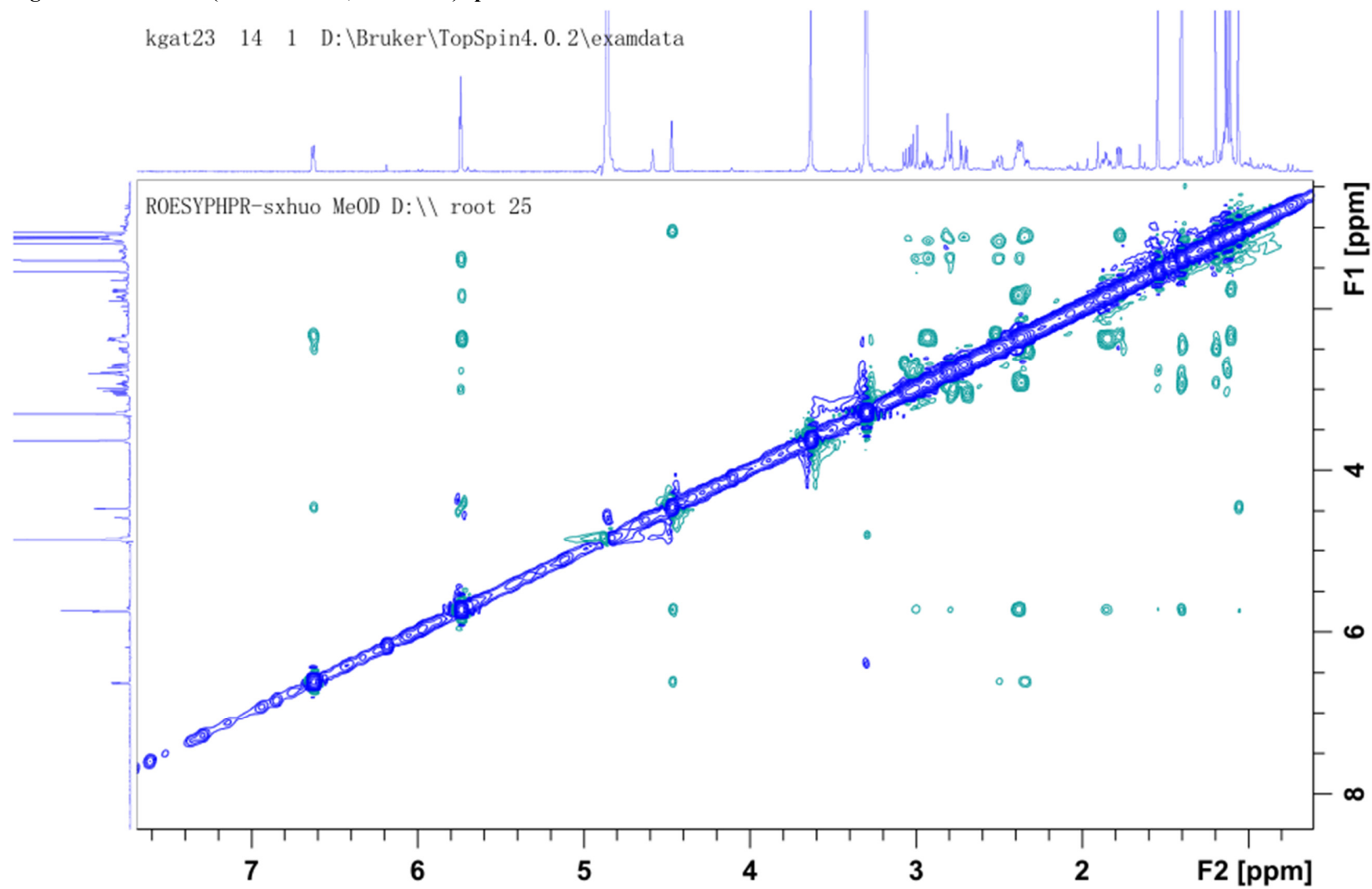


Figure S79. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 11.



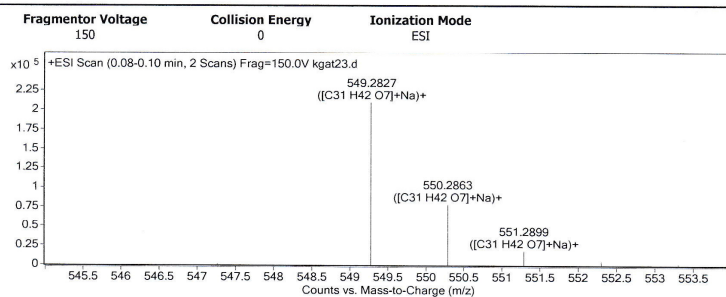
## Section S24: HRESIMS spectrum of 11

Figure S80. HRESIMS spectrum of 11.

### Qualitative Analysis Report

<b>Data Filename</b>	kgat23.d	<b>Sample Name</b>	kgat23
<b>Sample Type</b>	Sample	<b>Position</b>	P1-B1
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:47:38 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			
<b>Sample Group</b>	Info.		
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125.2)		

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
146.0803	1	25692.33		
172.0937	1	58315.53		
527.3001	1	35446.52		
533.2871	1	34701.41		
549.2827	1	209133.06	C31 H42 O7	(M+Na)+
550.2863	1	78684.9	C31 H42 O7	(M+Na)+
698.3877	1	23987.68		
1075.577	1	124756.34		
1076.5805	1	99580.17		
1077.5836	1	41677.77		

### 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
C31 H42 O7	526.2931	549.2823	549.2827	-0.40	-0.73	11.0000

--- End Of Report ---

# Section S25: 1D and 2D NMR spectra of compound 12

Figure S81.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 12.

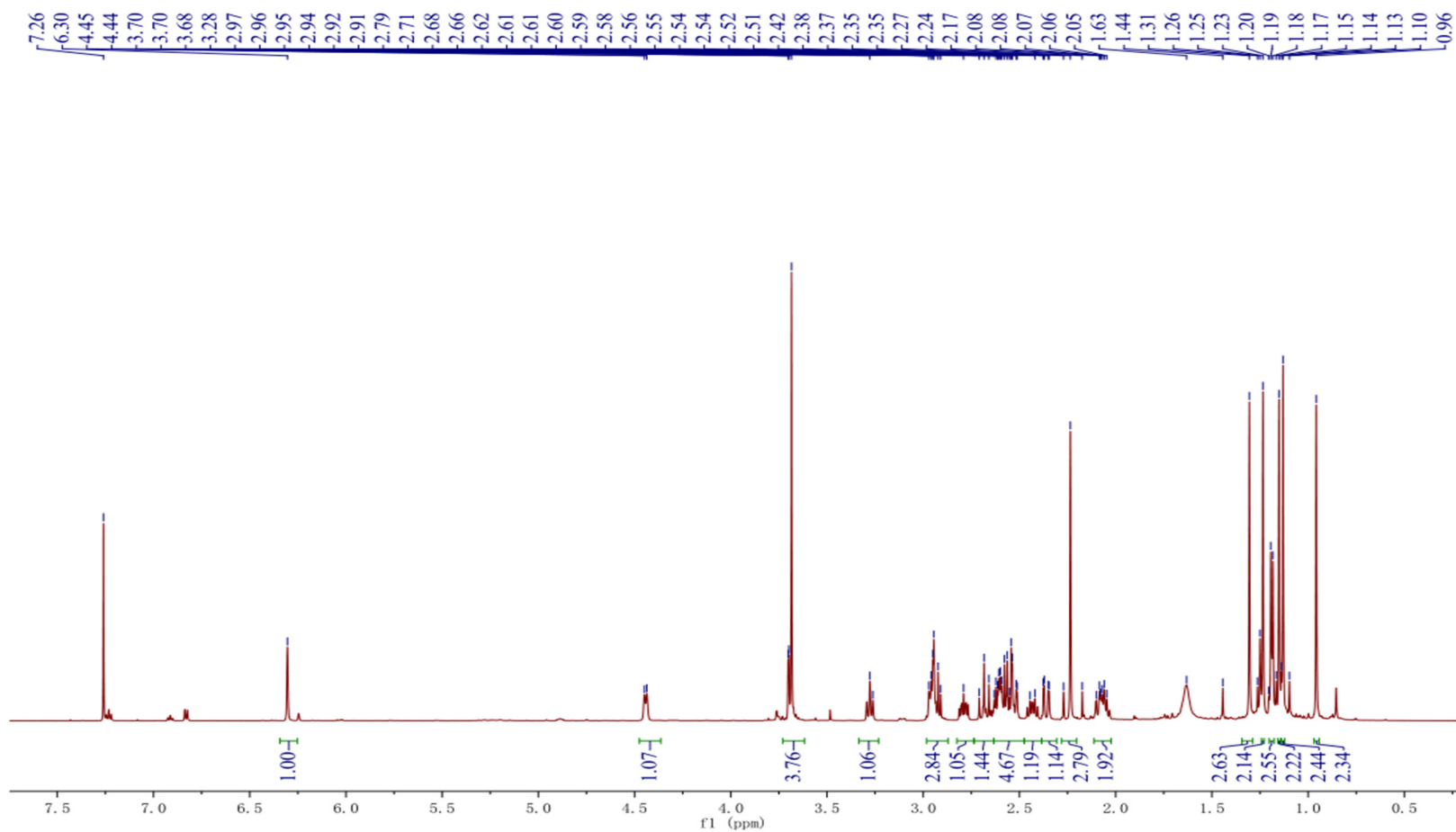


Figure S82.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 12.

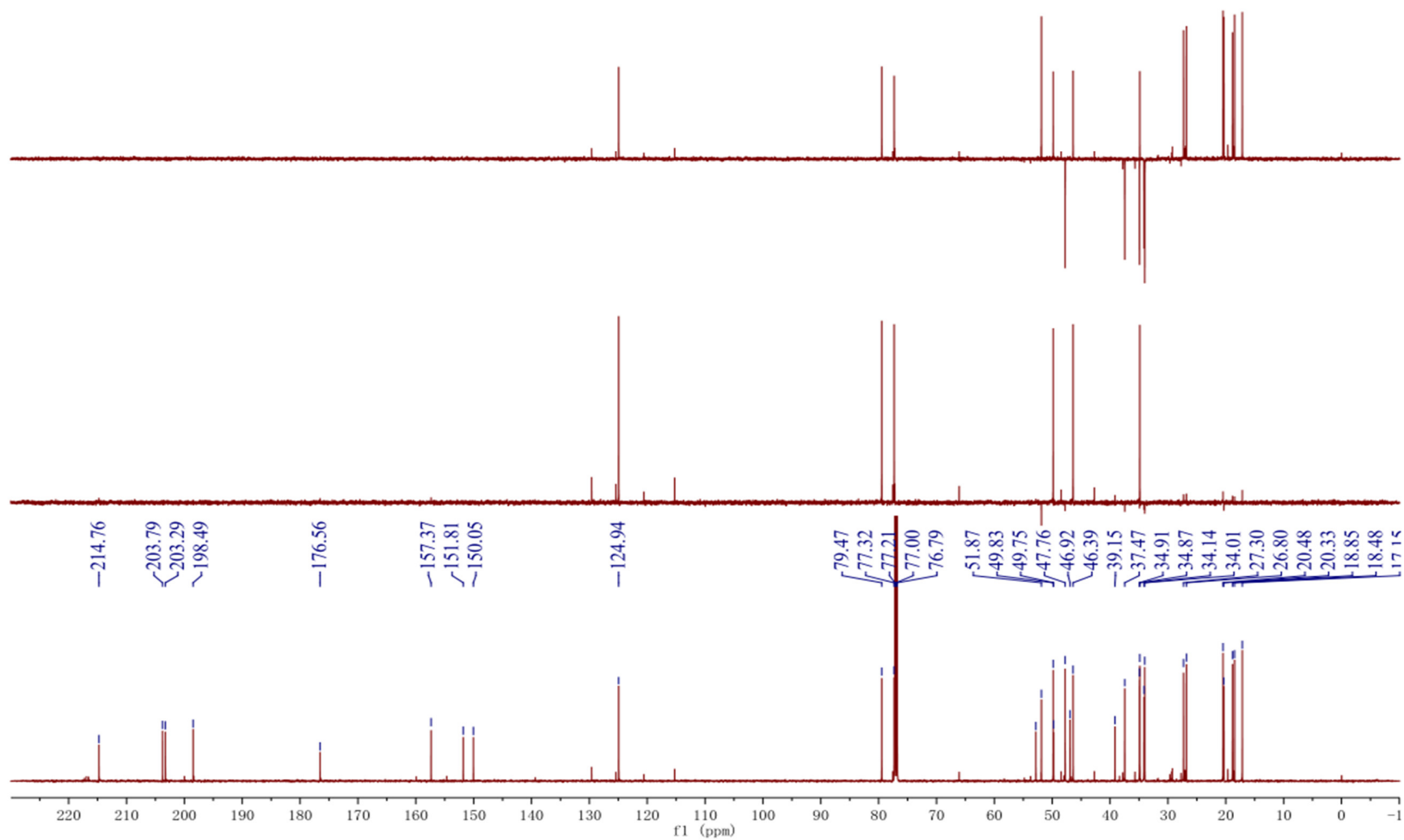


Figure S83.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 12.

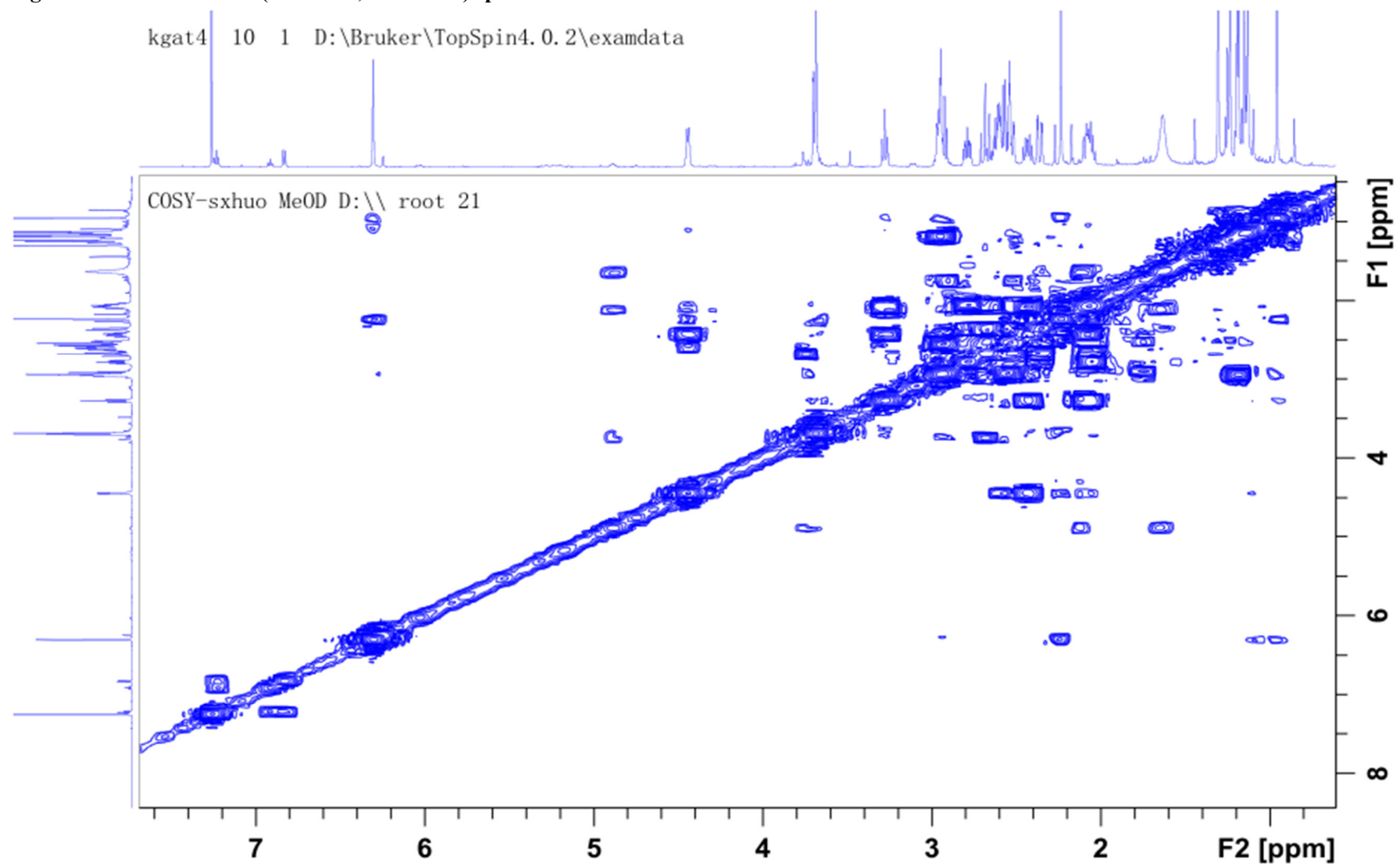




Figure S84. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 12.

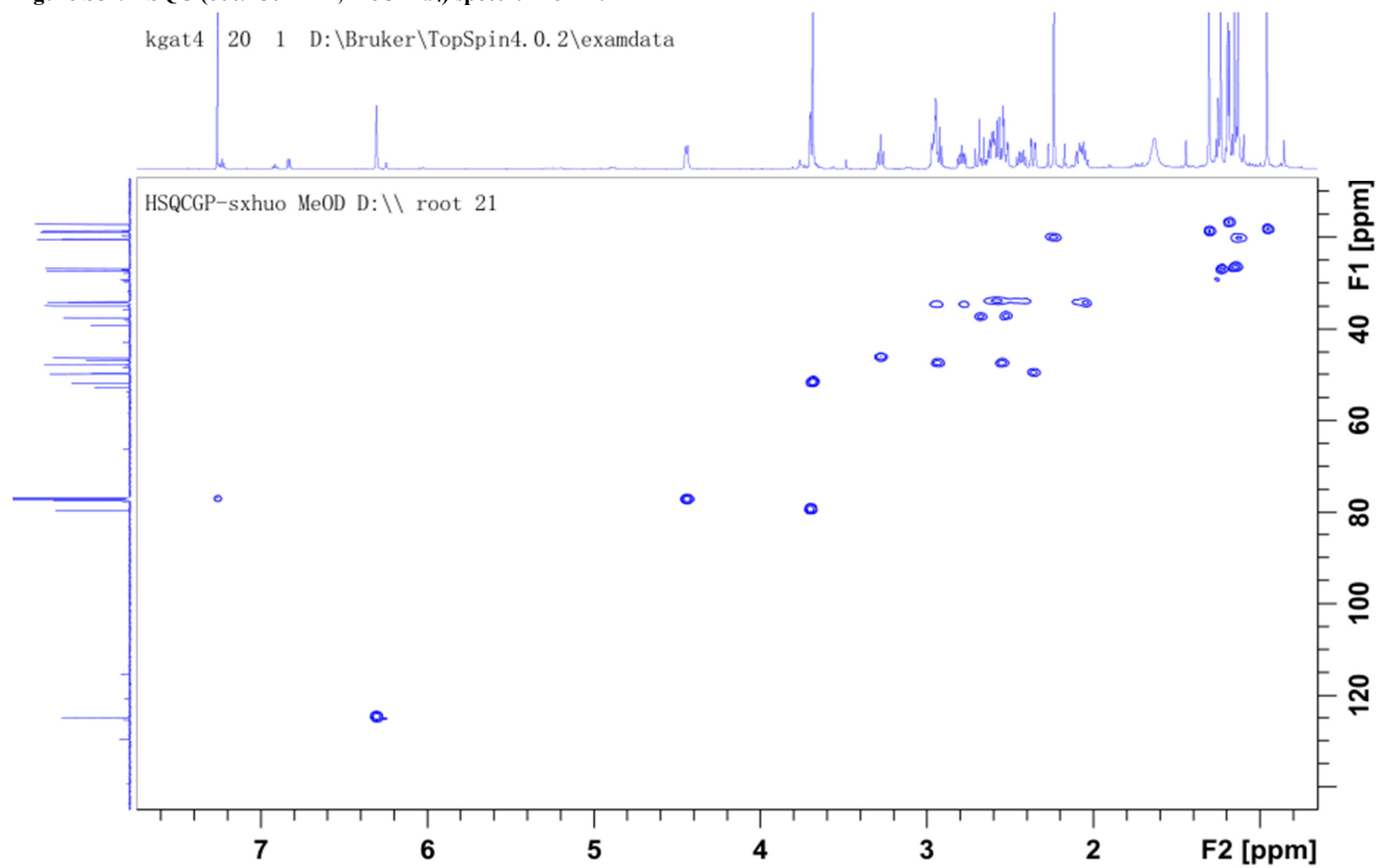


Figure S85. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 12.

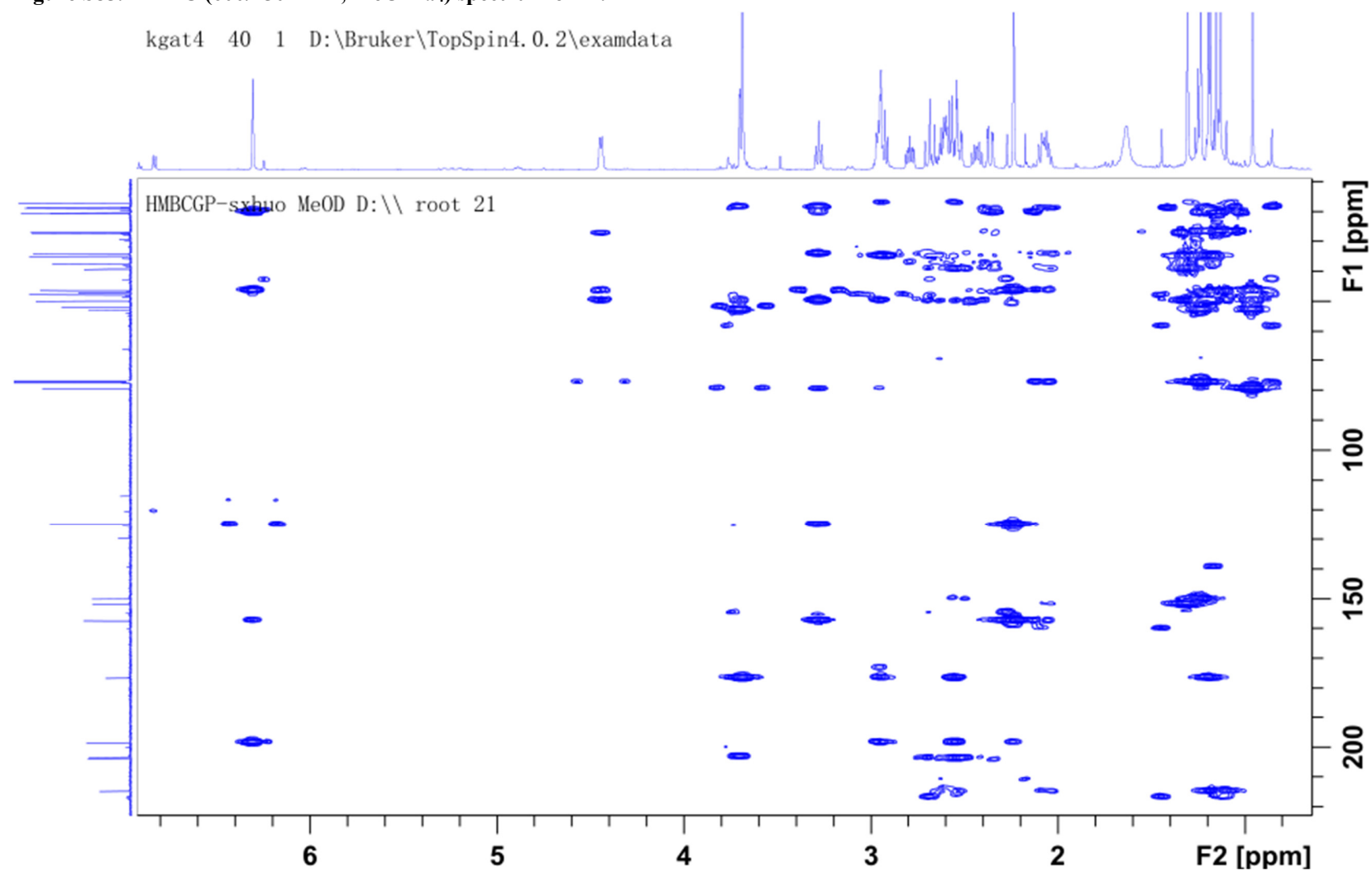
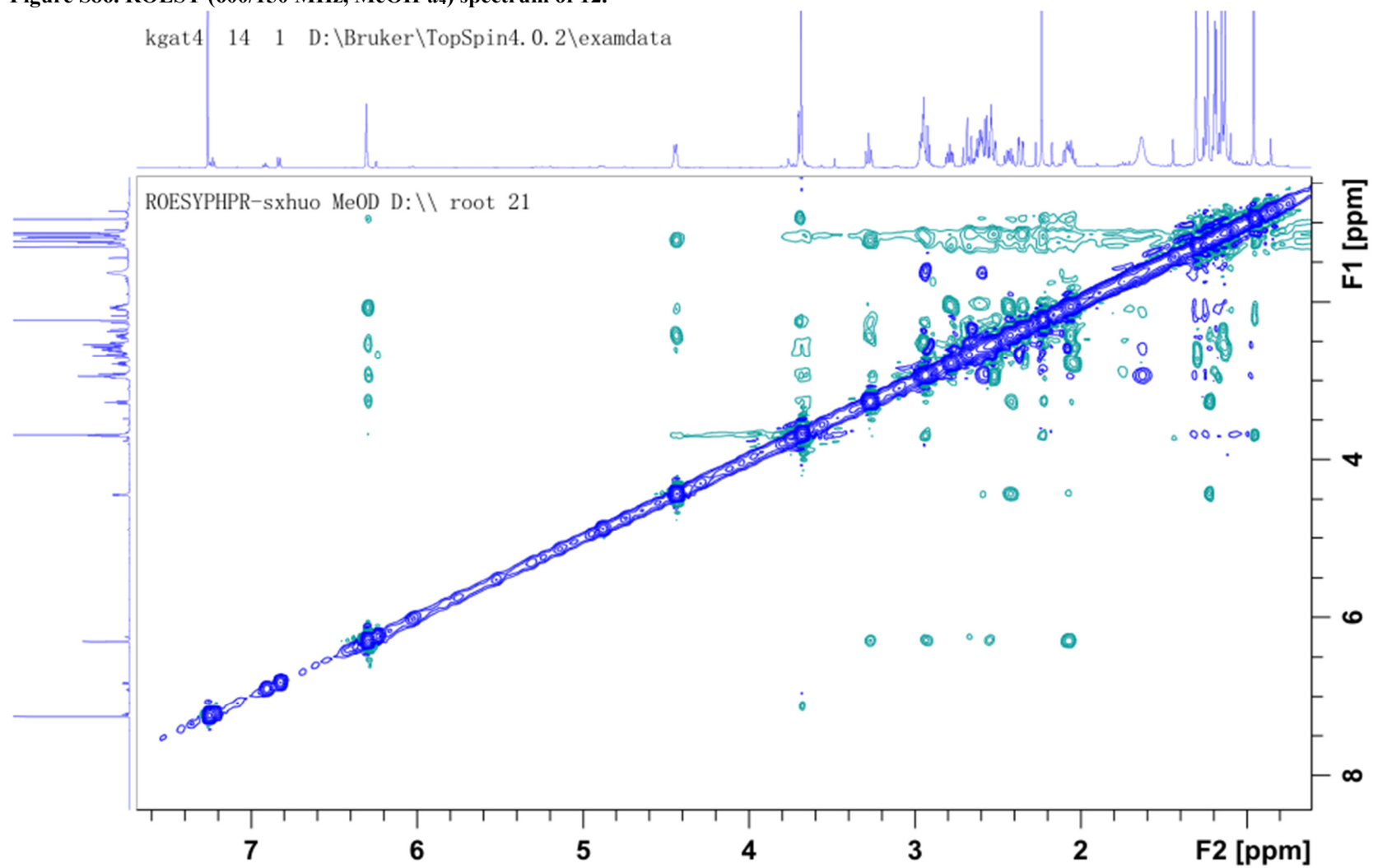


Figure S86. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 12.



Section S26: HRESIMS spectrum of 12  
Figure S87. HRESIMS spectrum of 12.

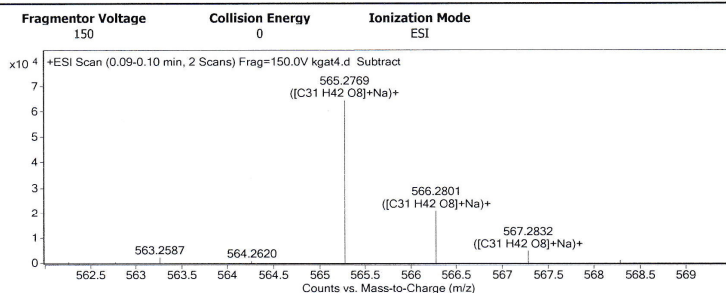
### Qualitative Analysis Report

<b>Data Filename</b>	kgat4.d	<b>Sample Name</b>	kgat4
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:40:32 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125.2)		

#### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
102.1274	1	16389.11		
533.2869	1	4995.39		
543.2943	1	9074.71		
565.2769	1	64496.13	C31 H42 O8	(M+Na)+
566.2801	1	20900.9	C31 H42 O8	(M+Na)+
581.2508	1	13391.67		
582.2538	1	5103.63		
1107.5652	1	44161.14		
1108.5683	1	28777.86		
1109.5723	1	10624.63		

#### 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
C31 H42 O8	542.2880	565.2772	565.2769	0.30	0.53	11.0000

--- End Of Report ---

# Section S27: 1D and 2D NMR spectra of compound 13

Figure S88.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 13.

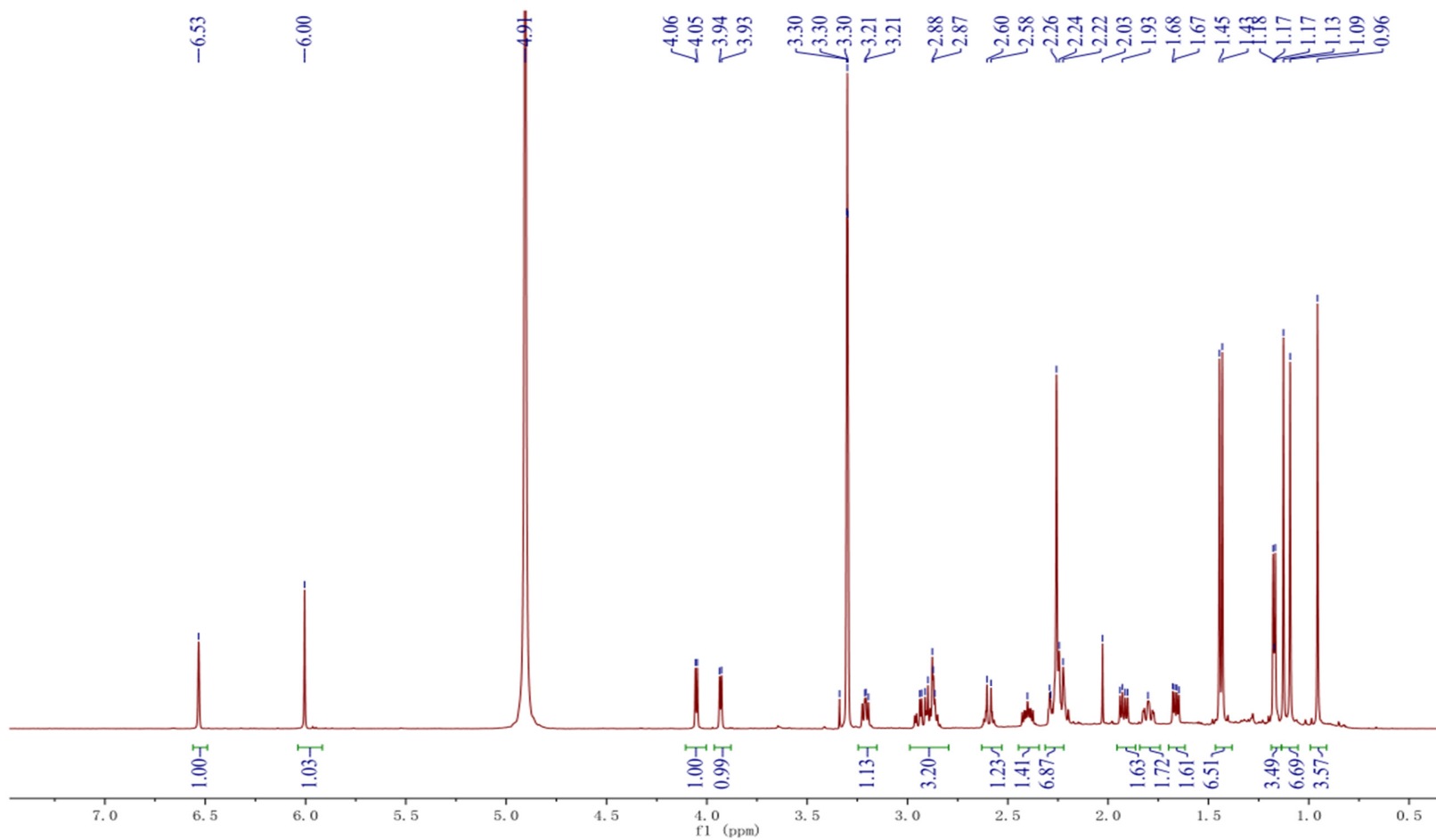


Figure S89.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 13.

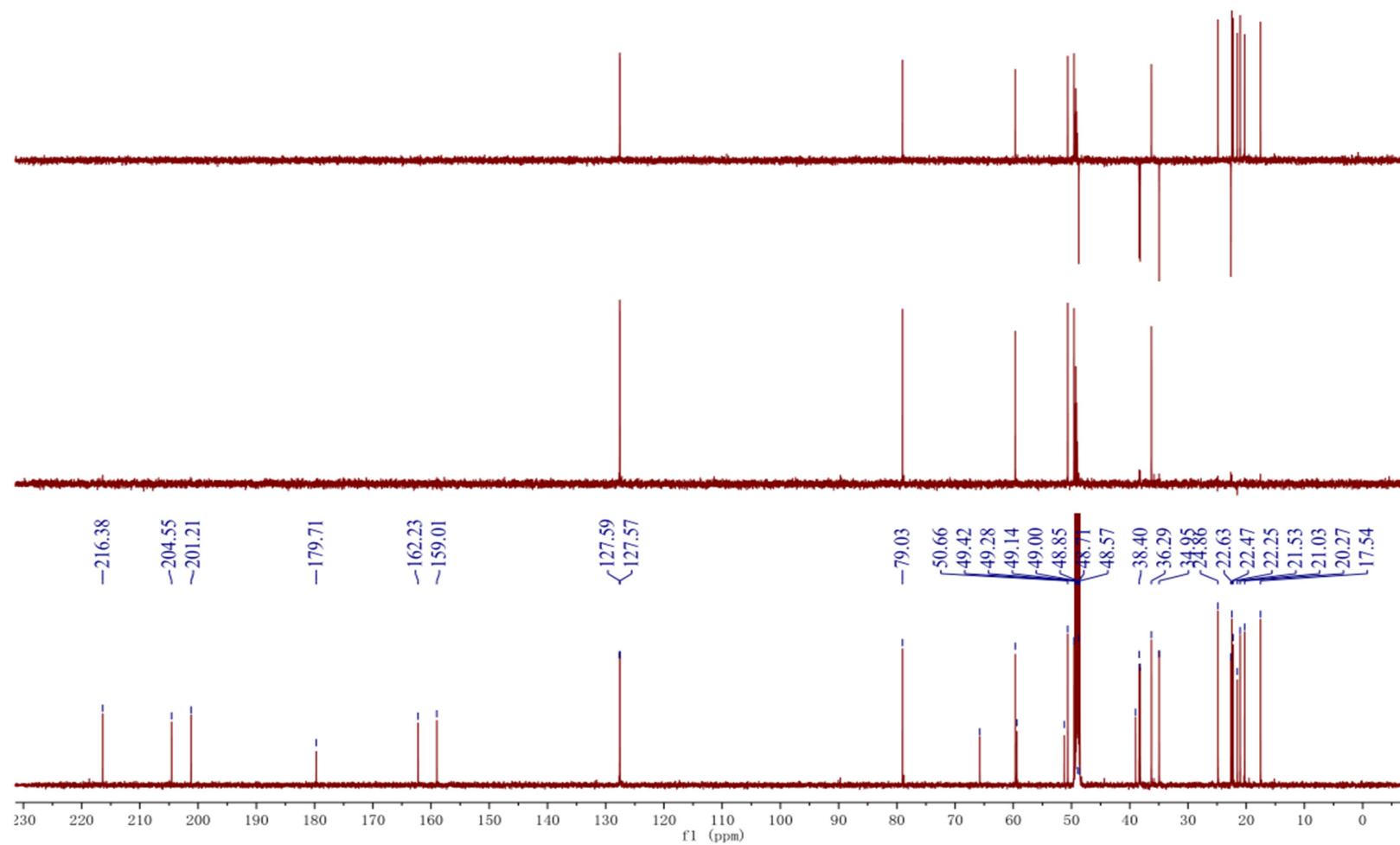


Figure S90.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 13.

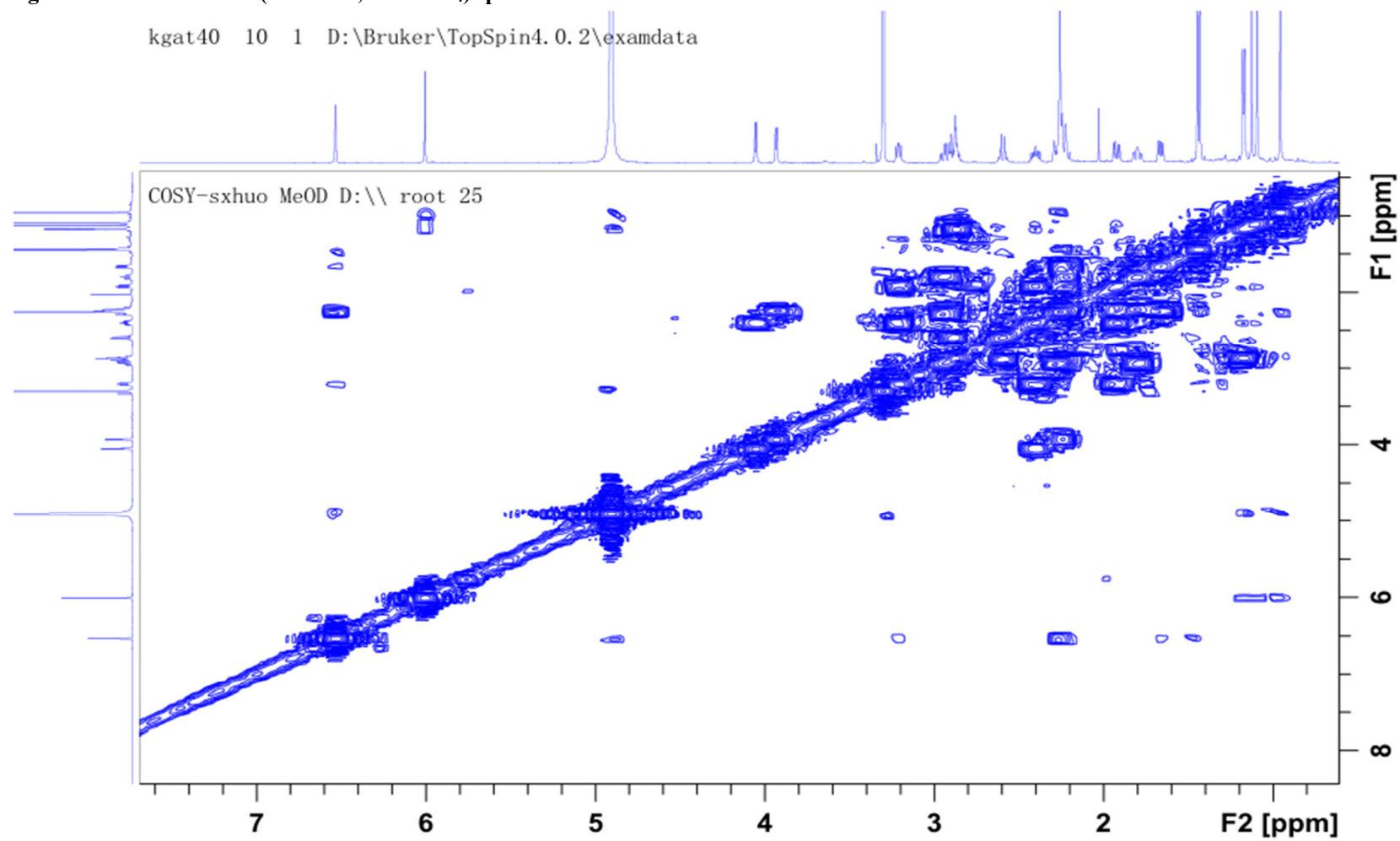


Figure S91. HSQC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 13.

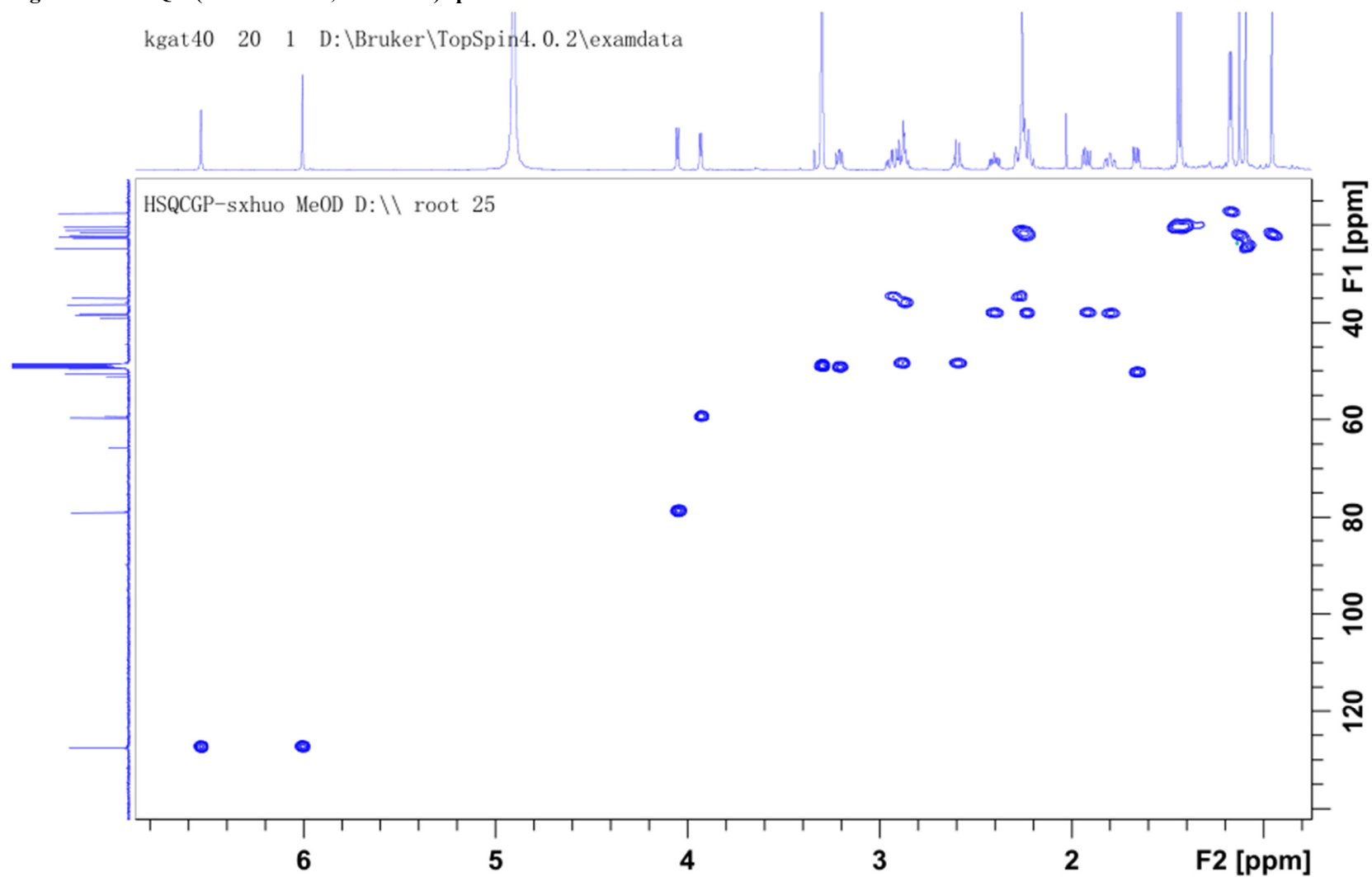




Figure S92. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 13.

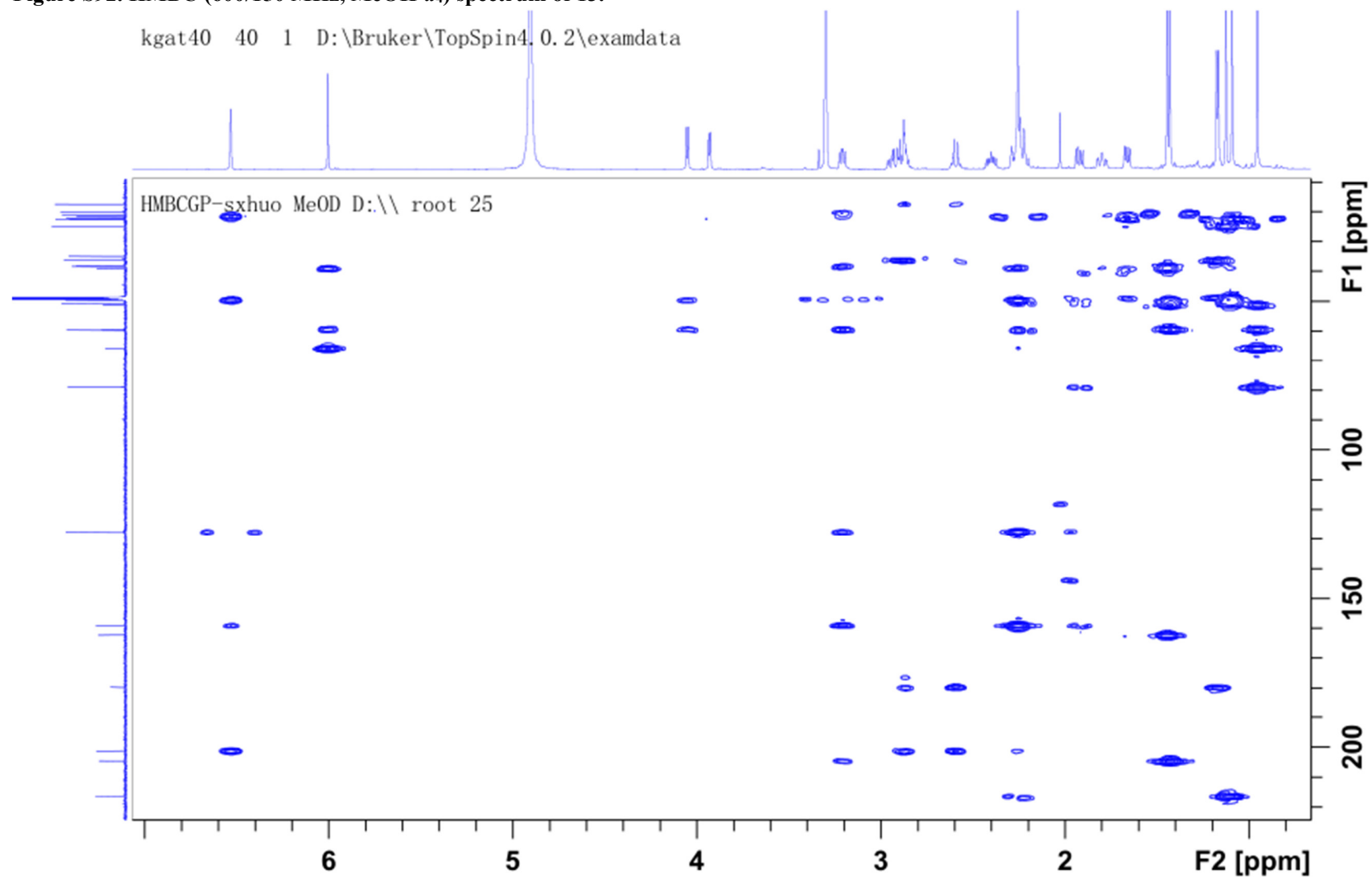
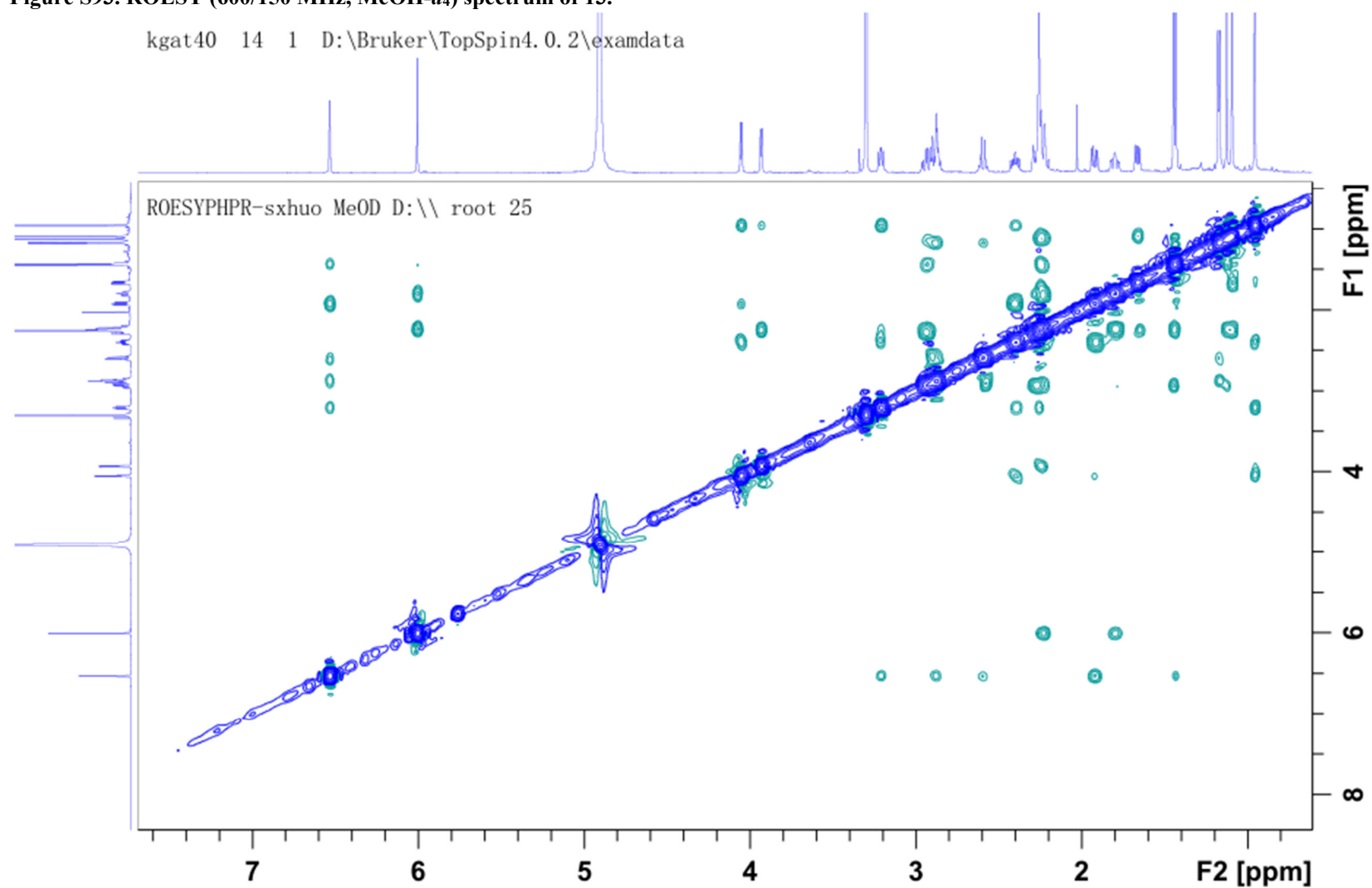


Figure S93. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 13.



Section S28: HRESIMS spectrum of 13  
Figure S94. HRESIMS spectrum of 13.

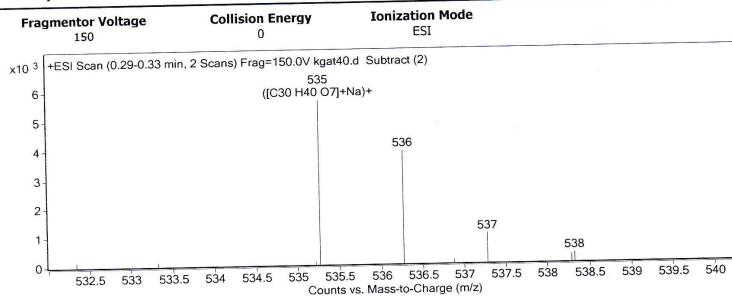
### Qualitative Analysis Report

<b>Data Filename</b>	kgat40.d	<b>Sample Name</b>	kgat40
<b>Sample Type</b>	Sample	<b>Position</b>	P1-B4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 2:06:00 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Acquisition SW</b>	6200 series TOF/6500 series		
<b>Version</b>	Q-TOF B.05.01 (B5125.2)		

#### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
535		5665.46	C30 H40 O7	(M+Na)+
536	1	3920.02		
552	1	19353.48		
553	1	11162.89		
554	1	3792.42		
557	1	2477.68		
568	1	7182.2		
569	1	3411.75		
701	1	4822.14		
702	1	3227.21		

#### 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
C30 H40 O7	512.2774	535.0000	535.0000	0.00	0.00	11.0000

--- End Of Report ---

## Section S29: 1D and 2D NMR spectra of compound 14

Figure S95.  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of 14.

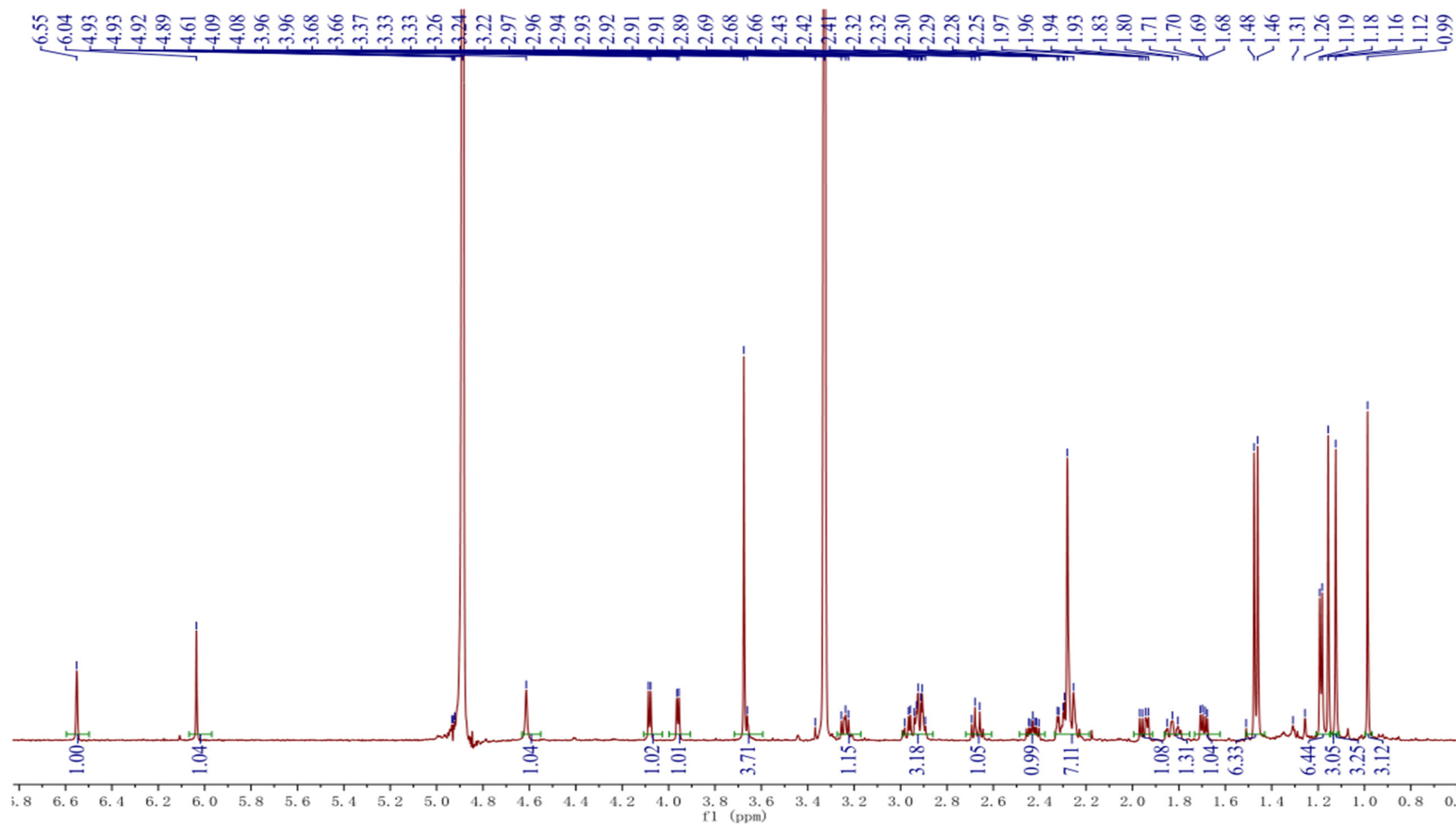
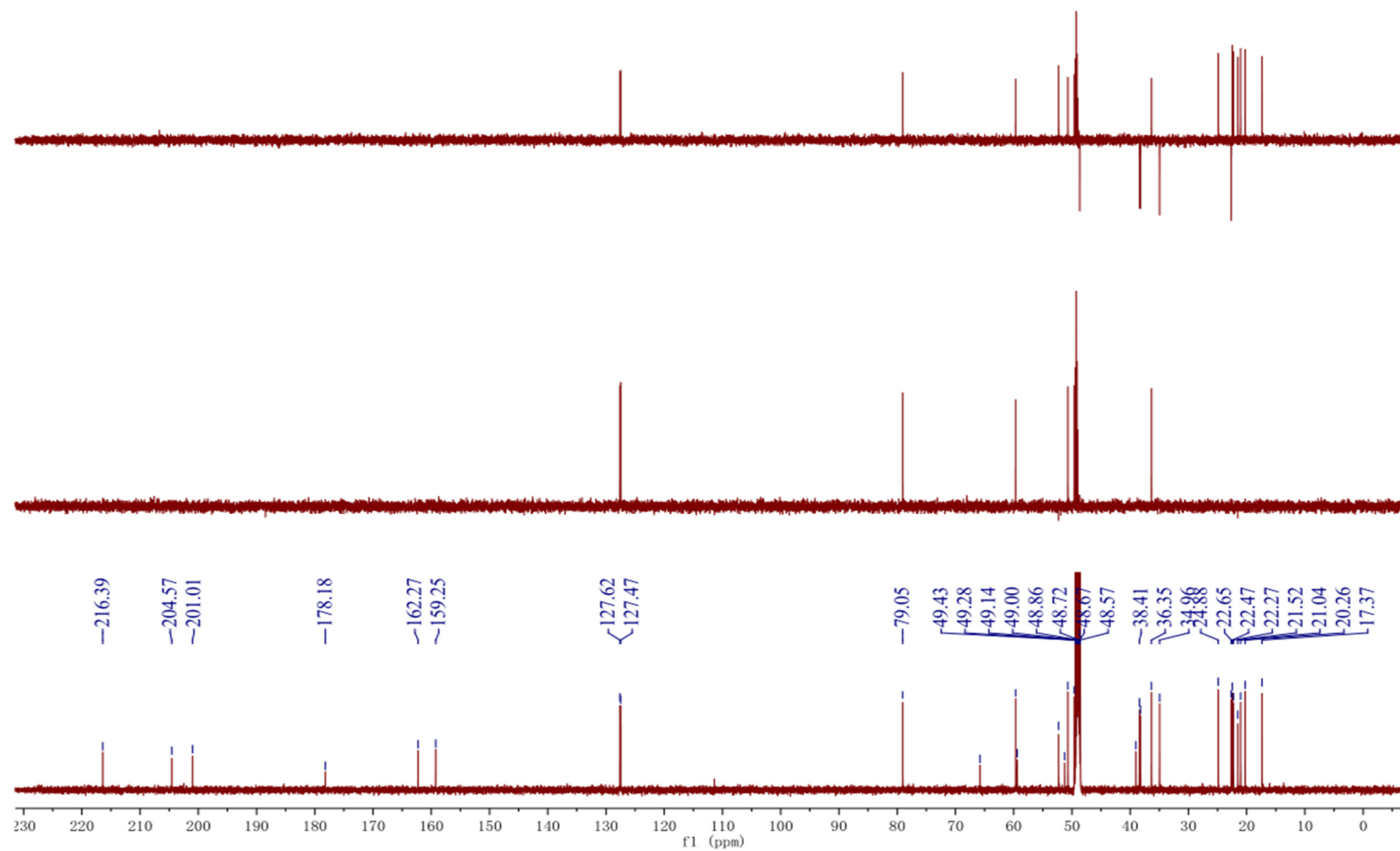


Figure S96.  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of 14.



2D COSY NMR spectrum of compound 23 in MeOD. The plot shows correlations between protons, with a diagonal of 1D <sup>1</sup>H NMR peaks. Significant cross-peaks are observed, particularly in the aromatic region (6-7 ppm) and the aliphatic region (2-4 ppm). The x-axis is labeled F2 [ppm] and the y-axis is labeled F1 [ppm].



Figure S99. HMBC (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 14.

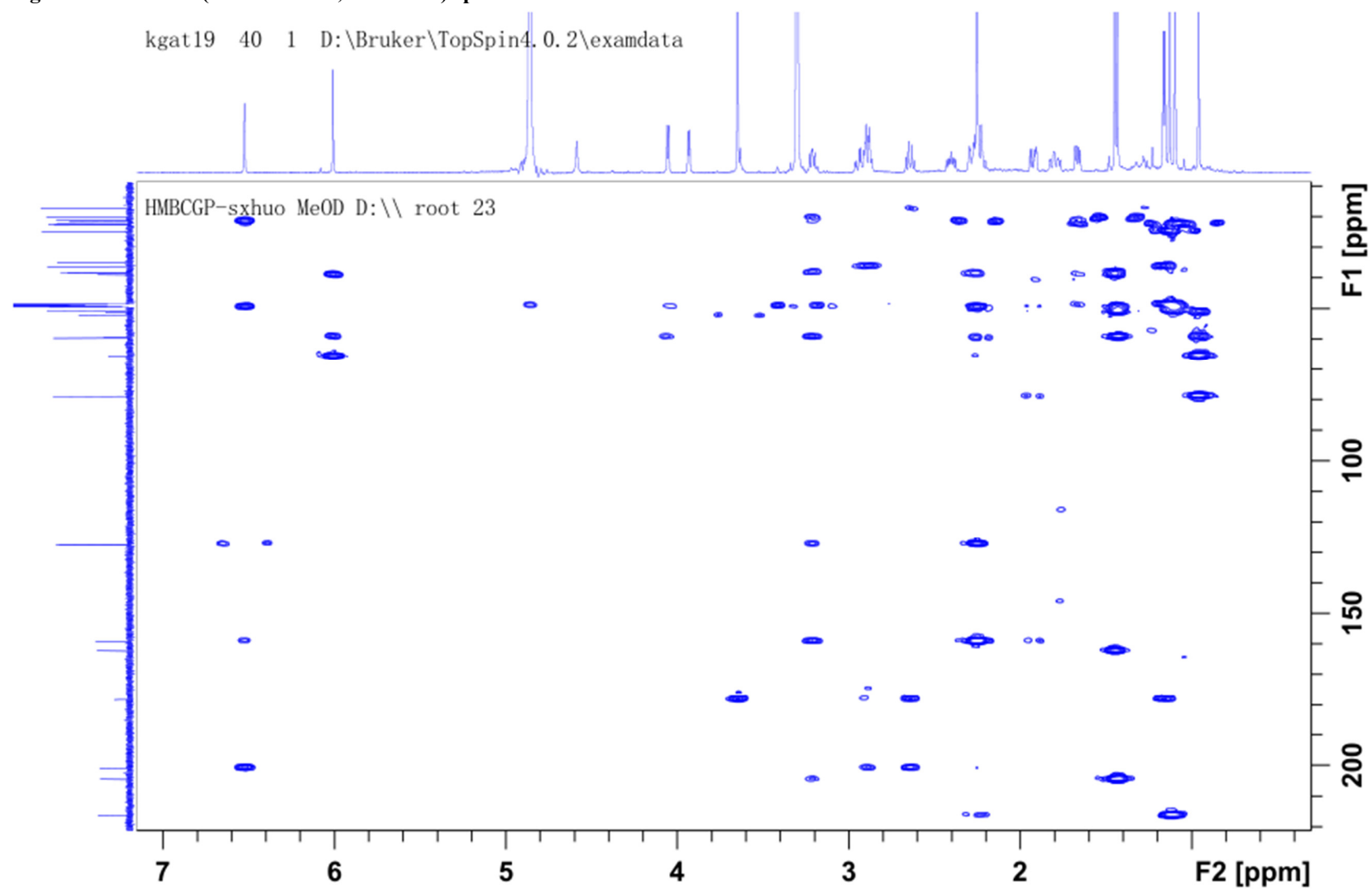
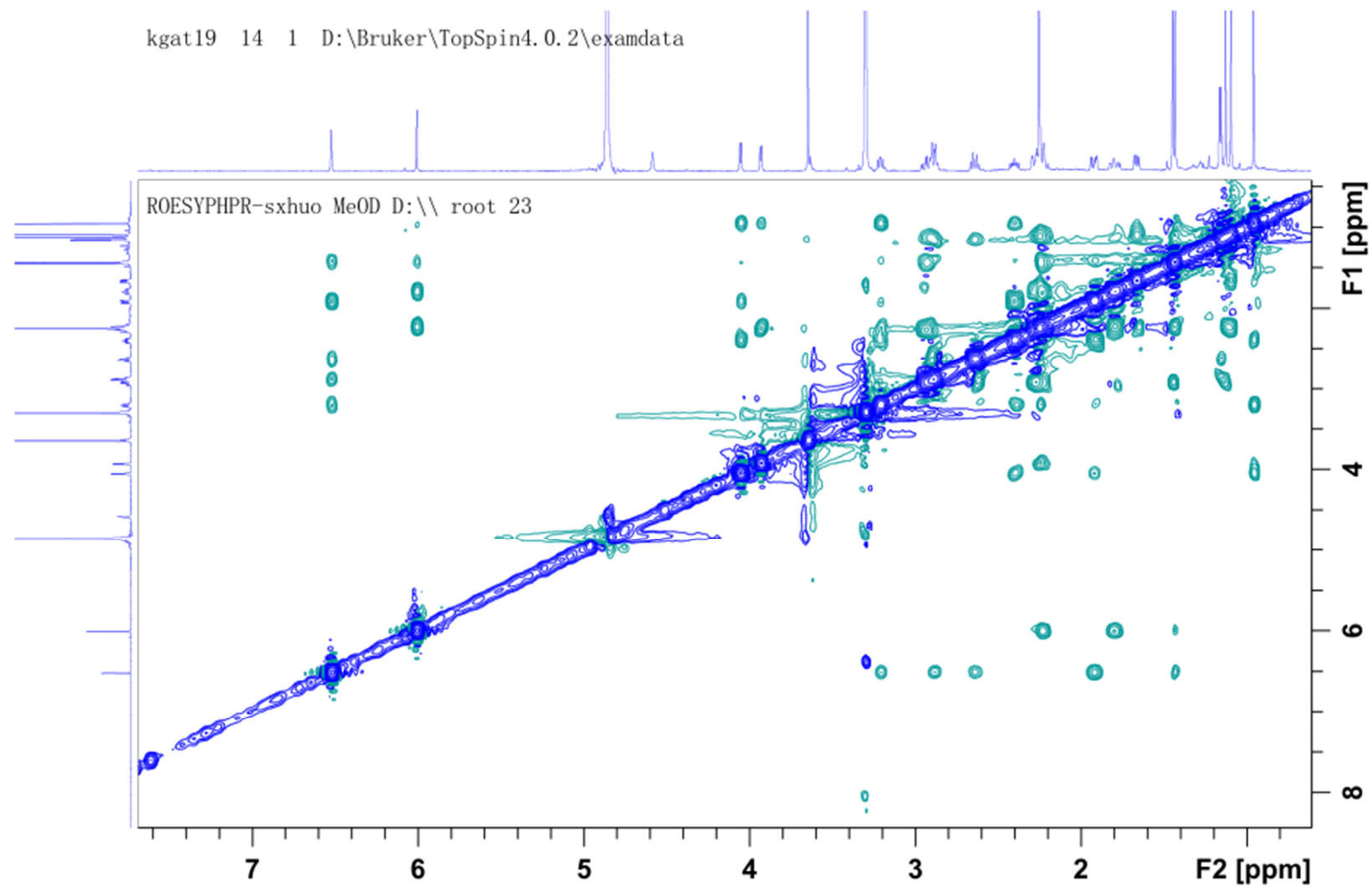




Figure S100. ROESY (600/150 MHz, MeOH-*d*<sub>4</sub>) spectrum of 14.



## Section S30: HRESIMS spectrum of 14

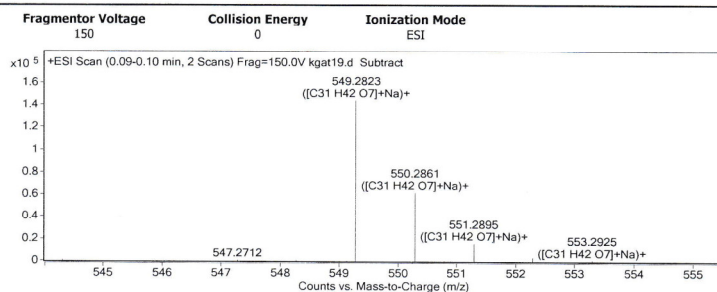
Figure S101. HRESIMS spectrum of 14.

### Qualitative Analysis Report

<b>Data Filename</b>	kgat19.d	<b>Sample Name</b>	kgat19
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A8
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:45:17 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

#### User Spectra



#### Peak List

m/z	z	Abund	Formula	Ion
535.3027	1	41472.34		
536.3062	1	16993.7		
549.2823	1	144187.16	C31 H42 O7	(M+Na)+
550.2861	1	61901.48	C31 H42 O7	(M+Na)+
551.2895	1	15919.39	C31 H42 O7	(M+Na)+
565.2684	1	22792.32		
698.3868	1	20275.38		
1061.5959	1	17146.34		
1075.5751	1	36301.75		
1076.5791	1	32261.56		

#### Formula Calculator Element Limits

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

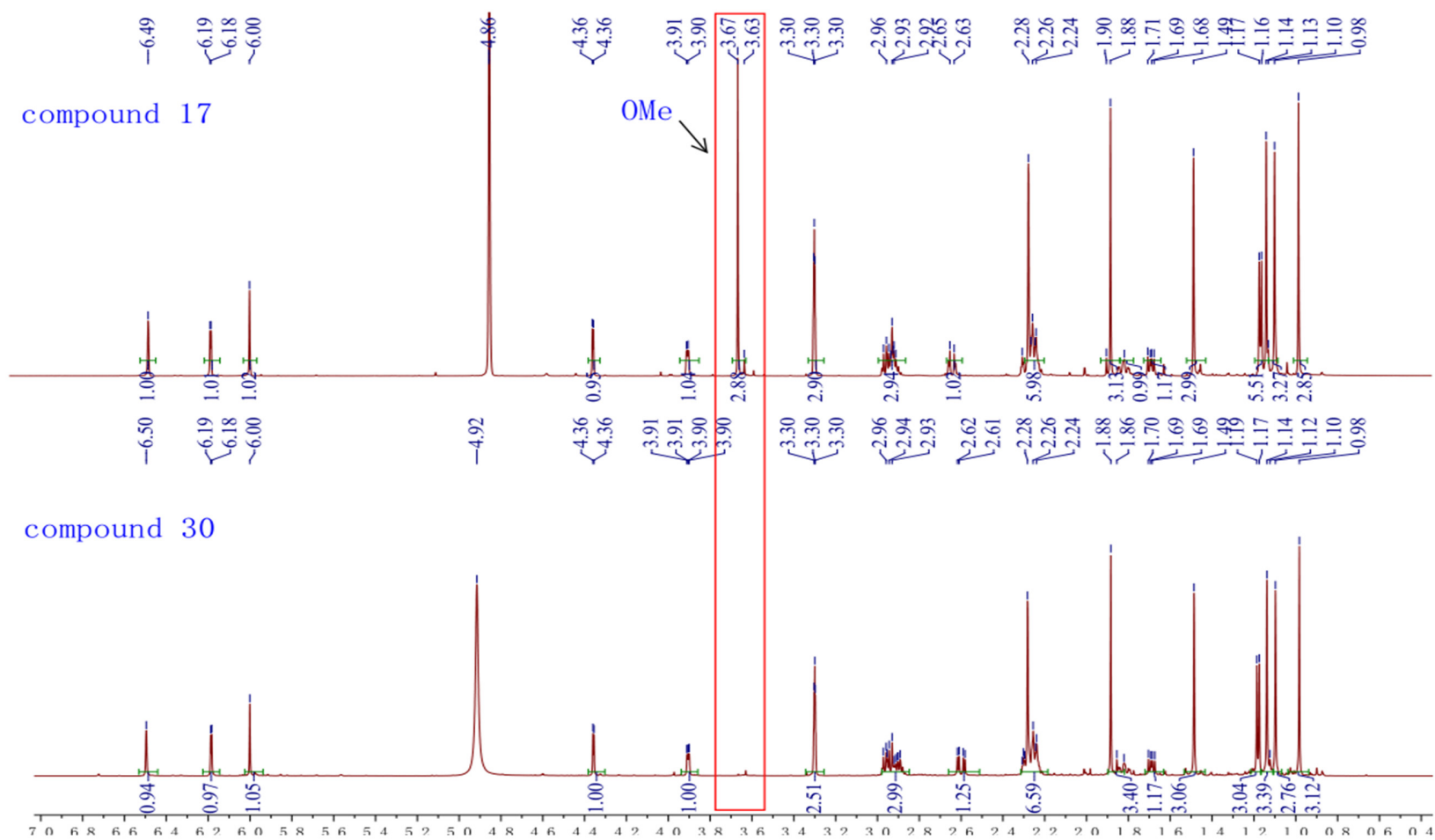
#### Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C31 H42 O7	526.2931	549.2823	549.2823	0.00	0.00	11.0000

--- End Of Report ---

# Section S31: 1D and 2D NMR spectra of compound 15

Figure S102. Comparison of the  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectra of 15 and 28.



## Section S32: HRESIMS spectrum of 15

Figure S103. HRESIMS spectrum of 15.

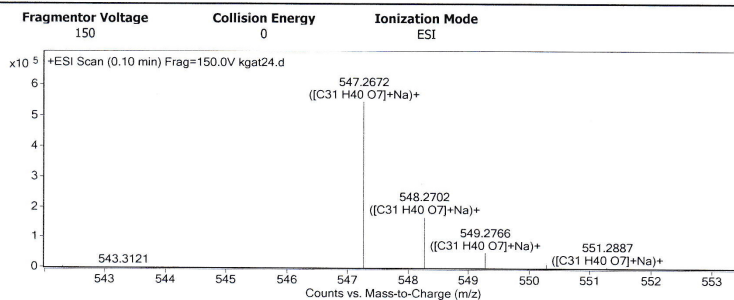
### Qualitative Analysis Report

<b>Data Filename</b>	kgat24.d	<b>Sample Name</b>	kgat24
<b>Sample Type</b>	Sample	<b>Position</b>	P1-B2
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:48:49 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

### User Spectra



### Peak List

m/z	z	Abund	Formula	Ion
172.0937	1	58406.09		
507.2738	1	47417.16		
547.2672	1	545135.31	C31 H40 O7	(M+Na)+
548.2702	1	169740.53	C31 H40 O7	(M+Na)+
549.2766	1	49009.27	C31 H40 O7	(M+Na)+
563.2411	1	65920.91		
696.372	1	58927.06		
1071.5453	1	236543.08		
1072.5485	1	156751.8		
1073.5541	1	76835.13		

### 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
C31 H40 O7	524.2774	547.2666	547.2672	-0.60	-1.10	12.0000

--- End Of Report ---

# Section S33: 1D and 2D NMR spectra of compound 16

Figure S104.  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of 16.

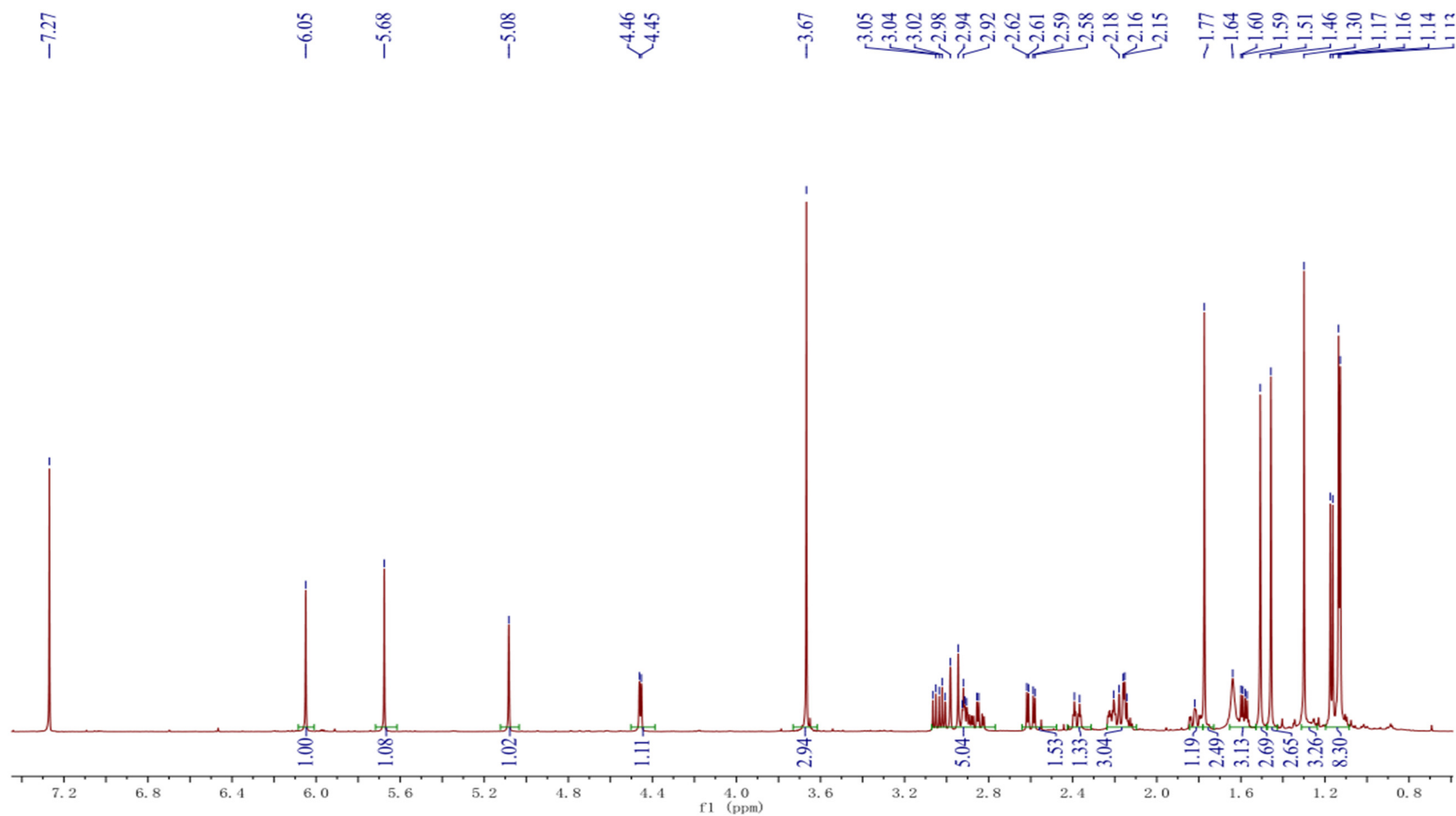


Figure S105.  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of 16.

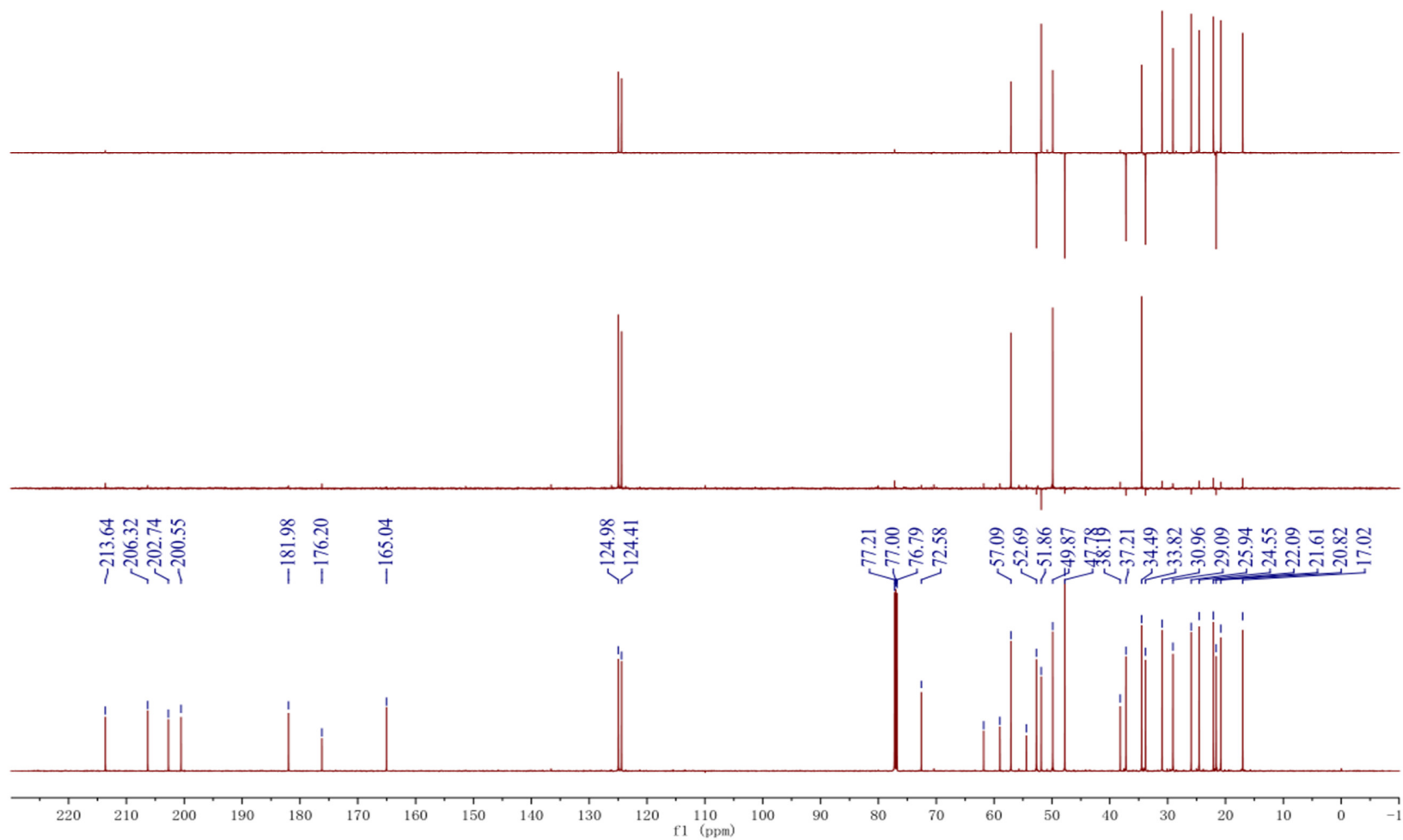


Figure S106.  $^1\text{H}$ - $^1\text{H}$  COSY (600 MHz,  $\text{CDCl}_3$ ) spectrum of 16.

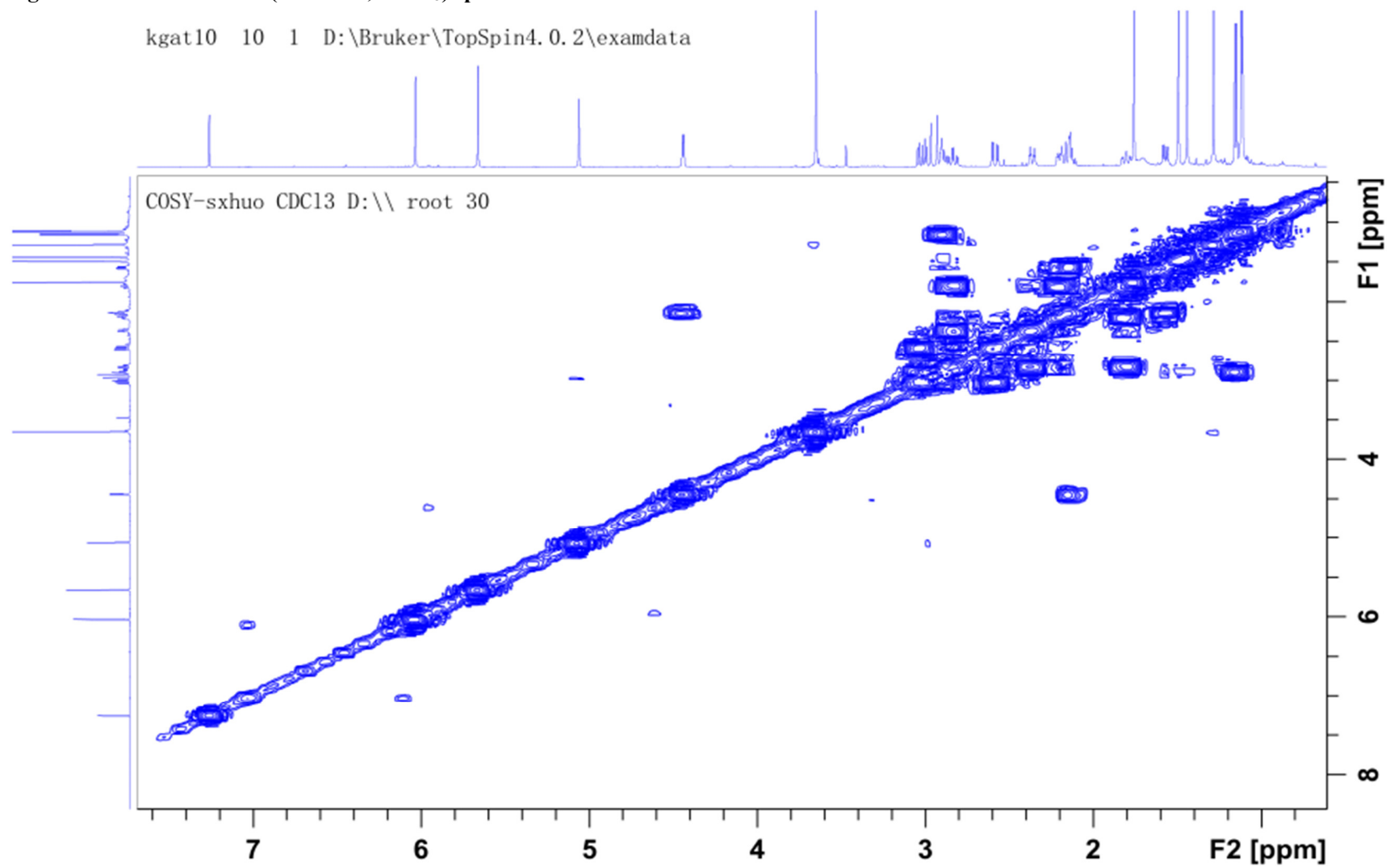


Figure S107. HSQC (600/150 MHz, CDCl<sub>3</sub>) spectrum of 16.

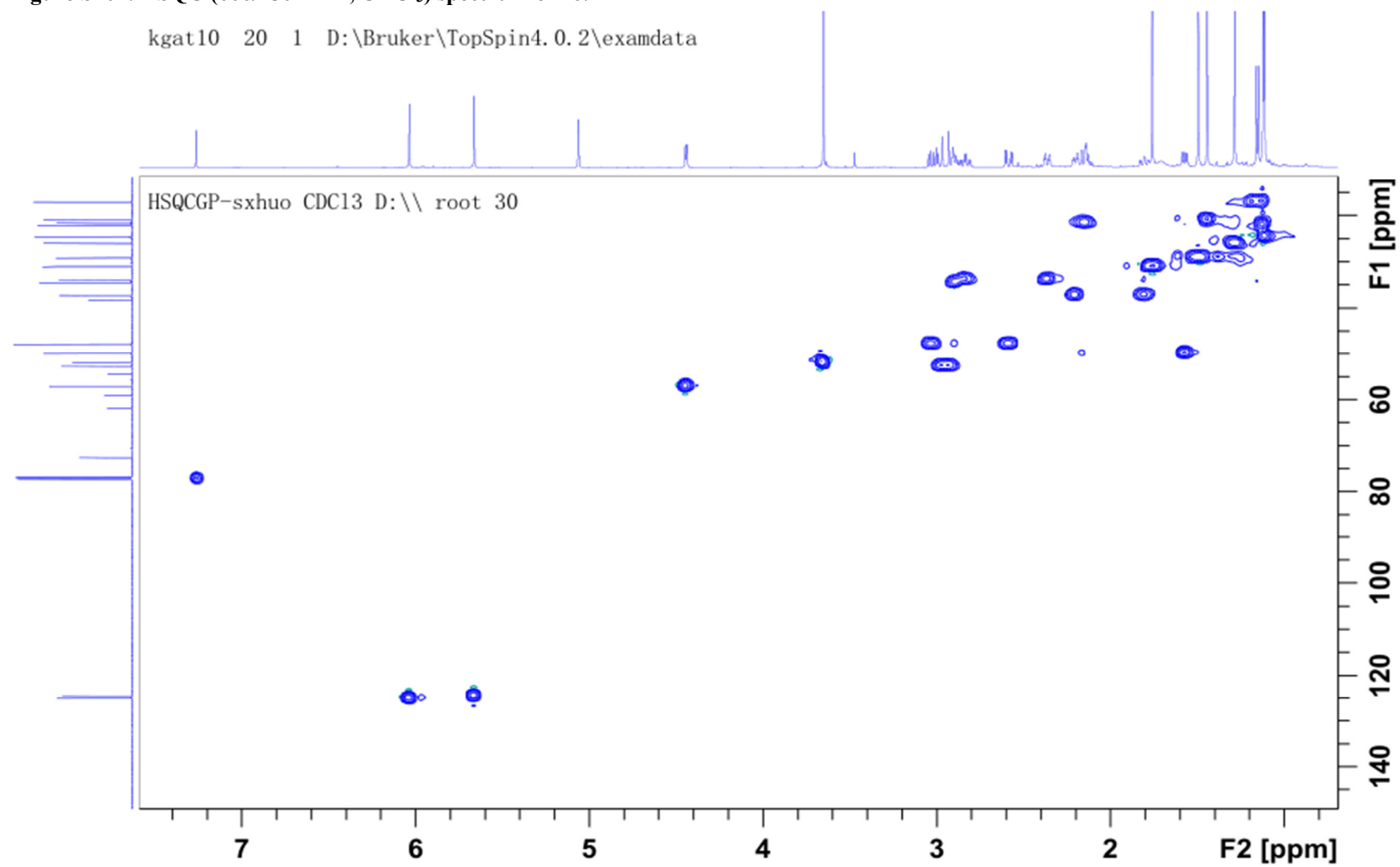
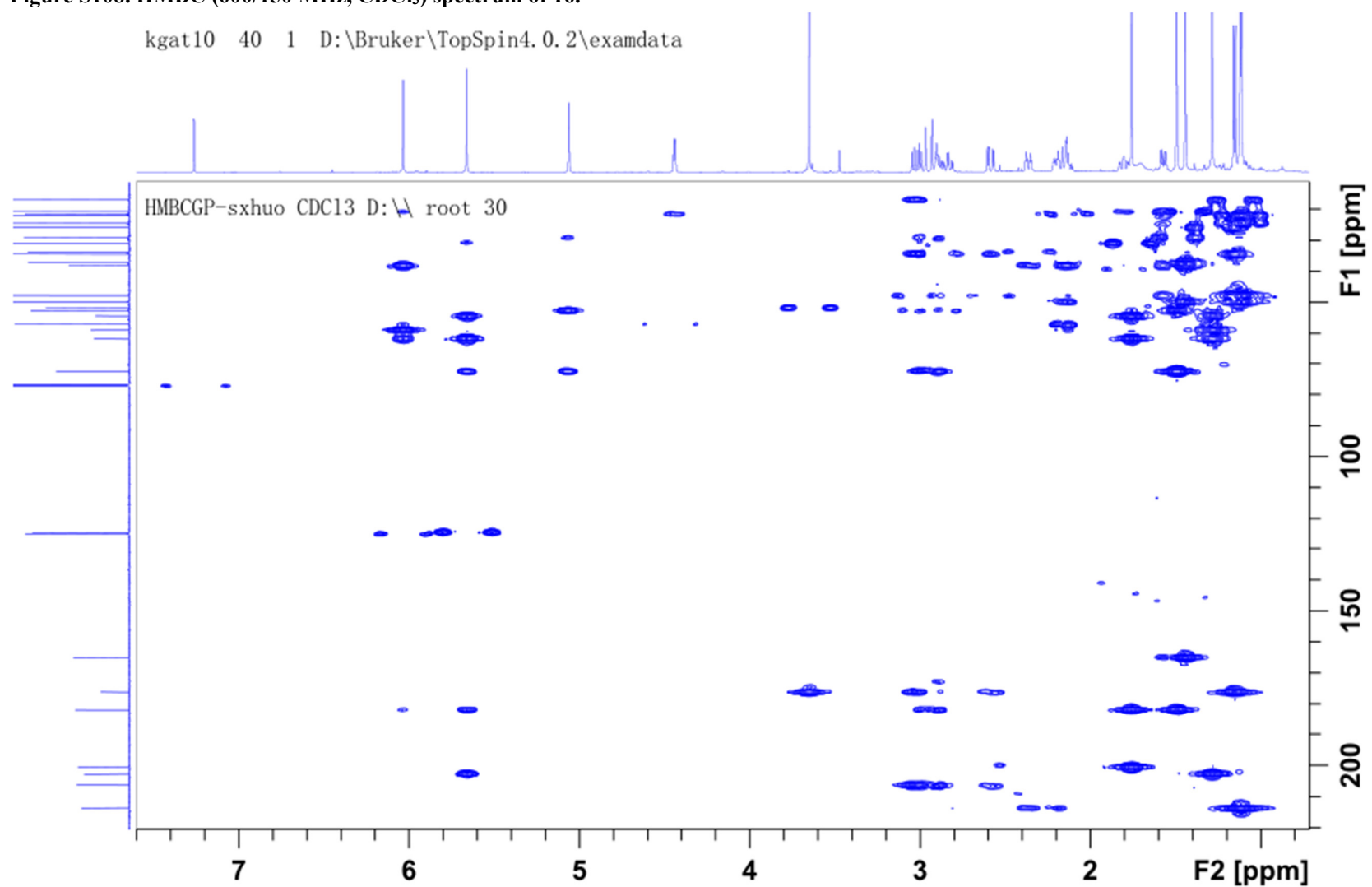




Figure S108. HMBC (600/150 MHz, CDCl<sub>3</sub>) spectrum of 16.



ROESY-sxhuo CDC13 D:\\ root 30

**Section S34: HRESIMS spectrum of 16**  
**Figure S110. HRESIMS spectrum of 16.**

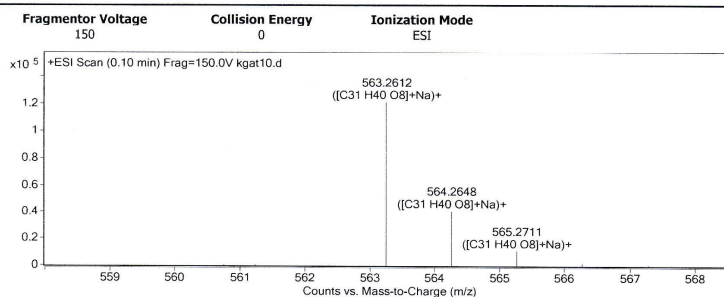
### Qualitative Analysis Report

<b>Data Filename</b>	kgat10.d	<b>Sample Name</b>	kgat10
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A5
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	s.m	<b>Acquired Time</b>	2/25/2021 11:41:44 AM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125.2)	

#### User Spectra



#### Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
102.1273	1	84281.93		
118.0856	1	18442.87		
134.0802	1	26488.62		
146.0803	1	39095.93		
150.1117	1	18621.35		
172.0936	1	38768.34		
563.2612	1	121532.69	C31 H40 O8	(M+Na)+
564.2648	1	41008.18	C31 H40 O8	(M+Na)+
579.2346	1	14703.55		
1103.5336	1	16689.55		

#### 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
C31 H40 O8	540.2723	563.2615	563.2612	0.30	0.53	12.0000

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