Supporting Information for

Triterpenoids and their glycosides from *Glinus oppositifolius* with antifungal activities against *Microsporum gypseum* and *Trichophyton rubrum*

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3.1. General Experimental Procedures

Optical rotations were recorded using a JASCO P-1020 Polarimeter (Jasco Corp., Tokyo, Japan). UV spectra were recorded on a Shimadzu UV-2401 PC spectrophotometer (Shimadzu, Kyoto, Japan). Electronic circular dichroism (ECD) spectra were recorded on a Chirascan CD spectrometer (Applied Photophysics Ltd., Leatherhead, UK). IR spectra were measured on a Bruker Tensor 27 FTIR Spectrometer (Bruker Corp., Ettlingen, Germany) with KBr disks. ^{1}H and ^{13}C NMR spectra were collected on Bruker DRX-500, Avance III-600, and Ascend™ 800 MHz NMR spectrometers (Bruker Corporation, Karlsruhe, Germany), with TMS as an internal standard. ESIMS and HRESIMS analyses were performed on an API QSTAR Pulsar 1 spectrometer (Applied Biosystems/MDS Sciex, Foster City, CA, USA). Silica gel G (80–100 and 300–400 mesh, Qingdao Meigao Chemical Co., Ltd., Qingdao, China), C_{18} silica gel (40–75 μm, Fuji Silysia Chemical Ltd., Aichi, Japan), and Sephadex LH-20 (GE Healthcare Bio-Sciences AB, Uppsala, Sweden) were used for column chromatography. Thin-layer chromatography (TLC) spots were visualized under UV light at 254 nm and by dipping in 5% H_2SO_4 in alcohol followed by heating. Semipreparative high-performance liquid chromatography (HPLC) was performed on an Agilent 1200 series pump (Agilent Technologies, Santa Clara, USA) equipped with a diode array detector and a Welch Ultimate AQ-C_{18} column (5 μm, ϕ 4.6 × 300 mm, Welch Materials Inc., Shanghai, China), an Agilent Eclipse XDB-C_{18} column (5.0 μm, ϕ 4.6 × 150 mm), and an Agilent Zorbax SB-C_{18} column (5.0 μm, ϕ 9.4 × 250 mm).

Table S1. ^{1}H and ^{13}C NMR Data of 26 in Methanol-d_4 (δ in ppm, J in Hz)

no.	δ_H (500 MHz)	δ_C (126 MHz)
1	1.60, m	39.7
	0.96, m	
2	1.78, m	27.0
	1.66, m	
3	3.14, dd (11.6, 4.5)	91.1
4		40.2
5	0.78, overlapped	57.0
6	1.54, m	19.3
	1.39, m	
7	1.49, m	34.0
	1.30, m	
8		40.5
9	1.58, m	49.0
10		37.9
11	1.89, m	24.5
12	5.29, br t (3.4)	124.2
13		144.7
14		42.8
15	1.74, m	28.9
	1.07, m	
16	1.99, m	24.2
	1.64, m	
17		47.0
18	2.69, dd (13.7, 3.5)	44.0
19	1.92, m	43.3
	1.65, dd (13.7, 13.7)	
20		45.0
21	1.98, m	31.3
	1.35, m	
22	1.60, m	35.0
	1.56, m	
23	1.04, s	28.5
24	0.84, s	16.9
25	0.94, s	15.9
26	0.79, s	17.7
27	1.16, s	26.3
28		181.2
29	1.13, s	28.7
30		178.8
30-OMe	3.69, s	52.3
1′	4.38, d (7.8)	107.0
2′	3.22, dd (9.1, 7.8)	75.3

3′	3.35, dd (9.1, 9.1)	77.5
4′	3.50, dd (9.8, 9.1)	73.2
5′	3.82, d (9.8)	76.6
6′		171.4
6′-OMe	3.76, s	52.8

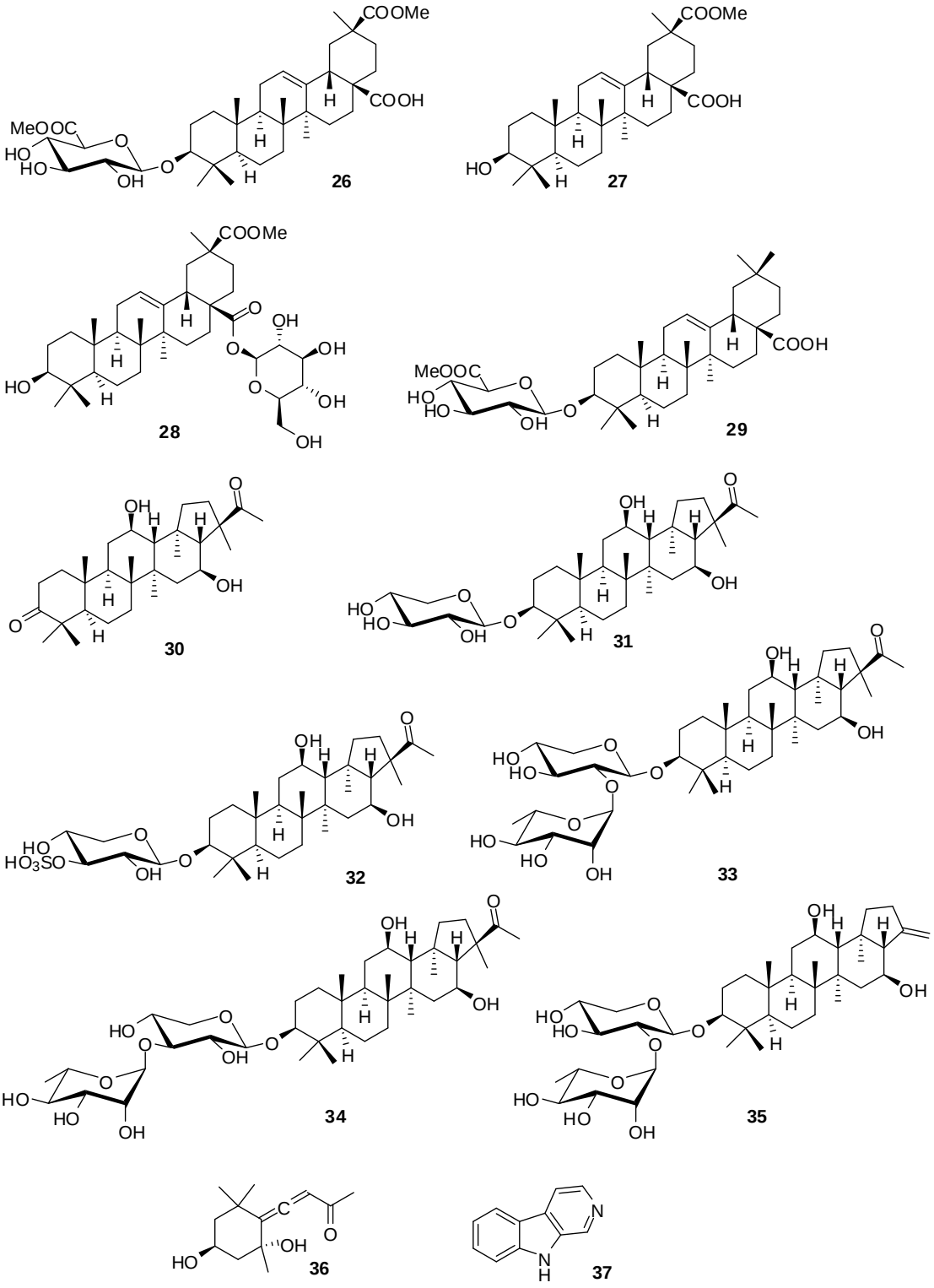


Figure S1. Structures of known compounds (**26**–**37**) from *Glinus oppositifolius*.

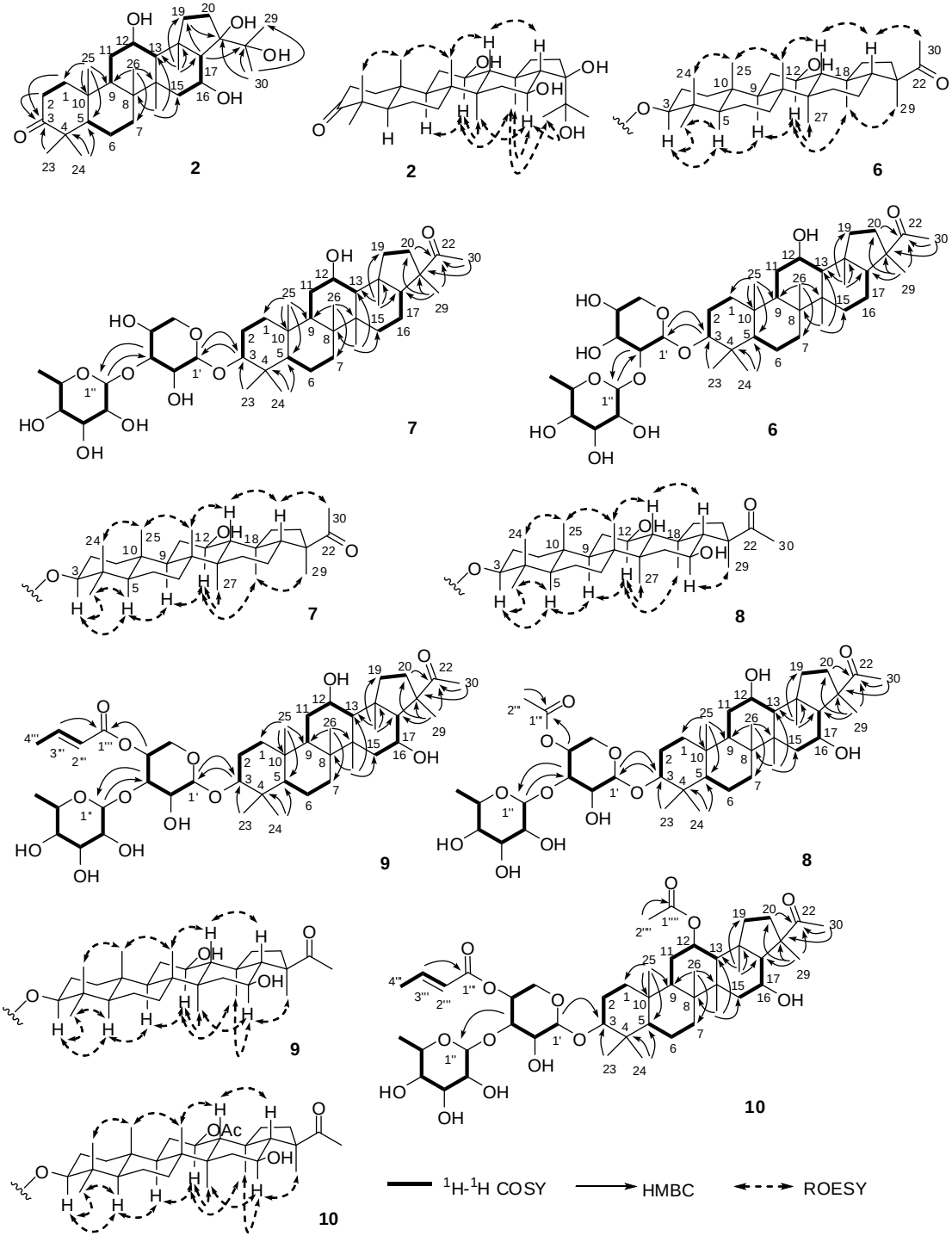


Figure S2. Key 2D NMR correlations of **2** and **6–10**.

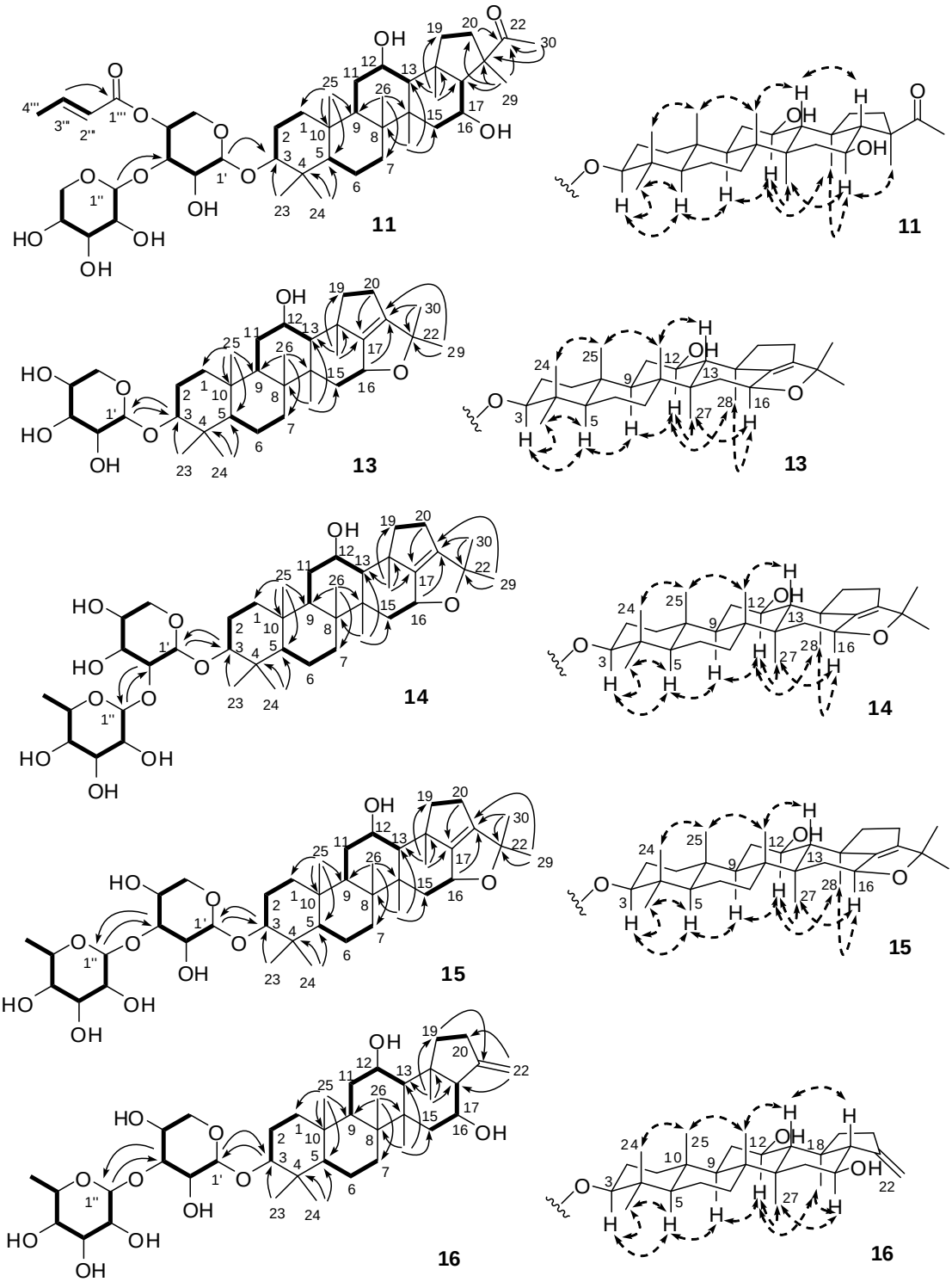


Figure S3. Key 2D NMR correlations of **11** and **13–16**.

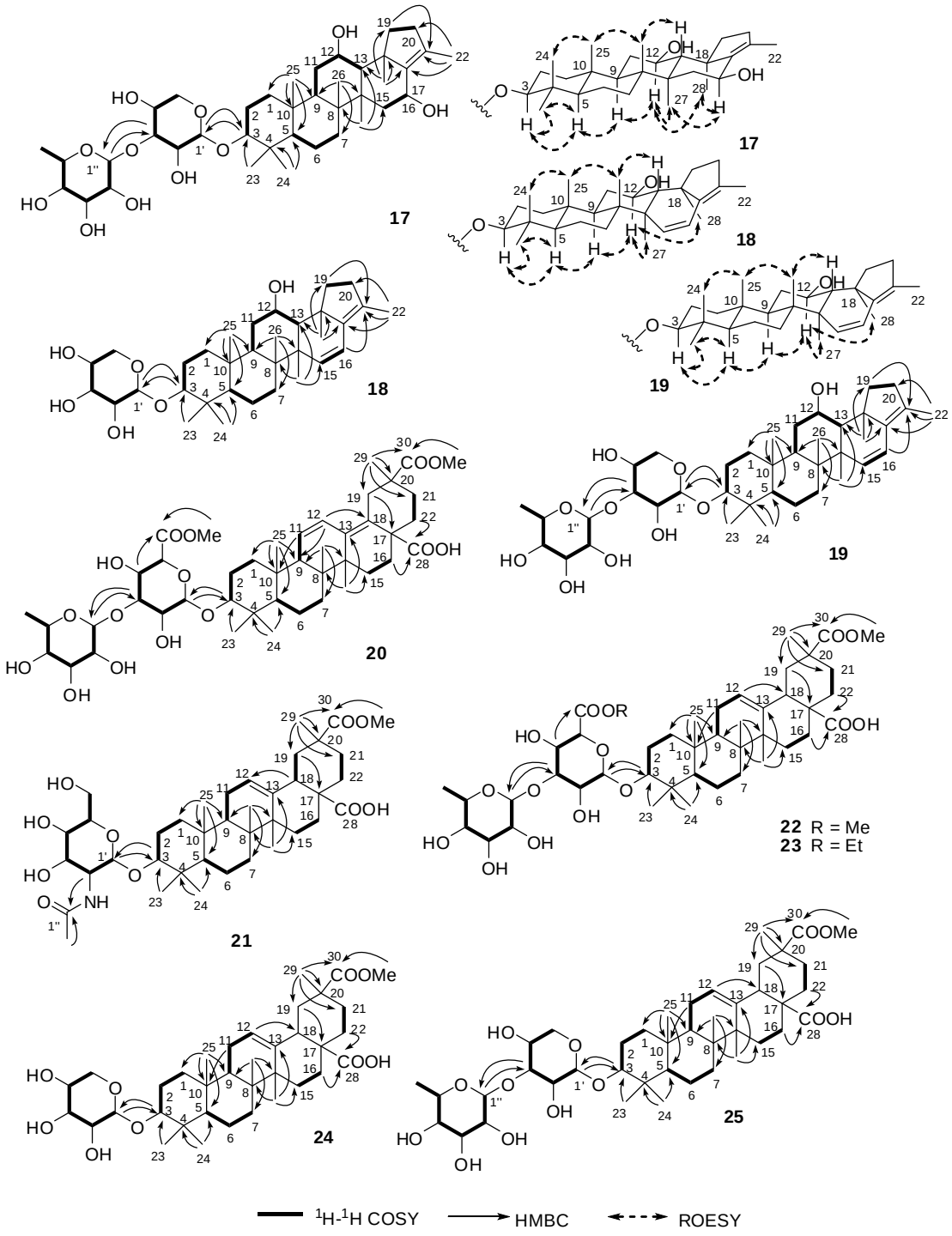


Figure S4. Key 2D NMR correlations of **17–25**.

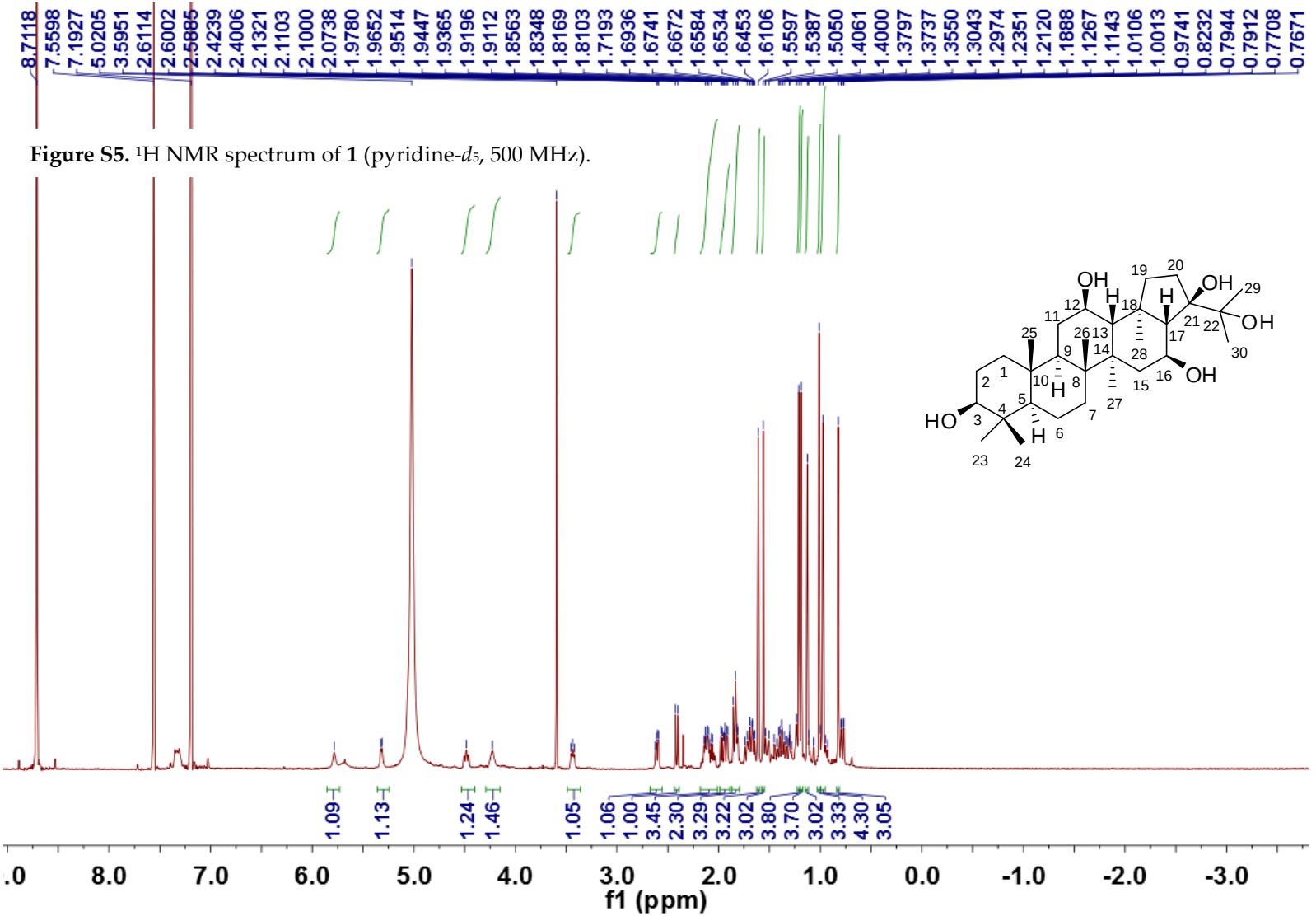


Figure S5. ^{1}H NMR spectrum of **1** (pyridine-d_5, 500 MHz).

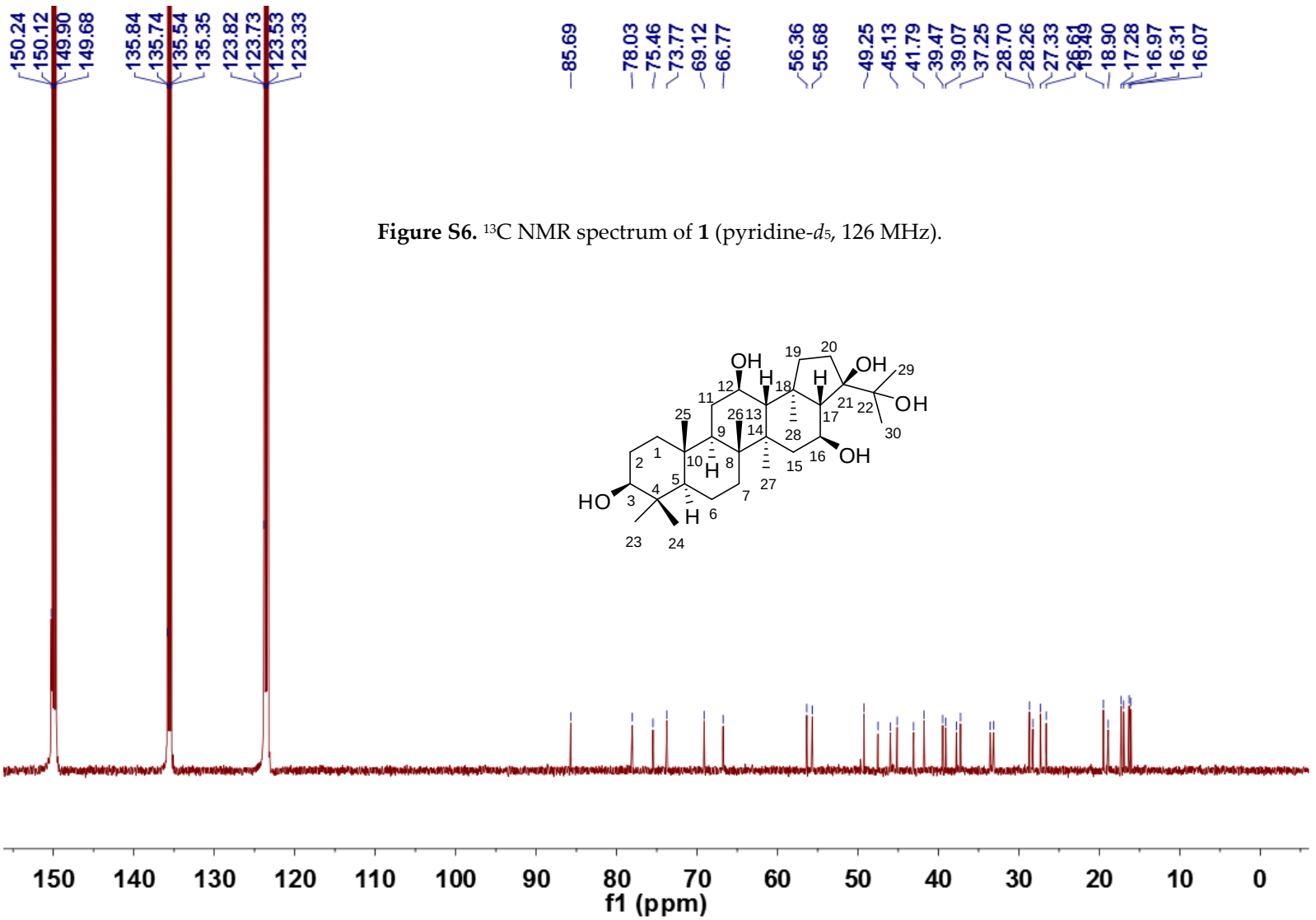


Figure S6. ^{13}C NMR spectrum of **1** (pyridine-d_5, 126 MHz).

Figure S7. HSQC spectrum of **1**.

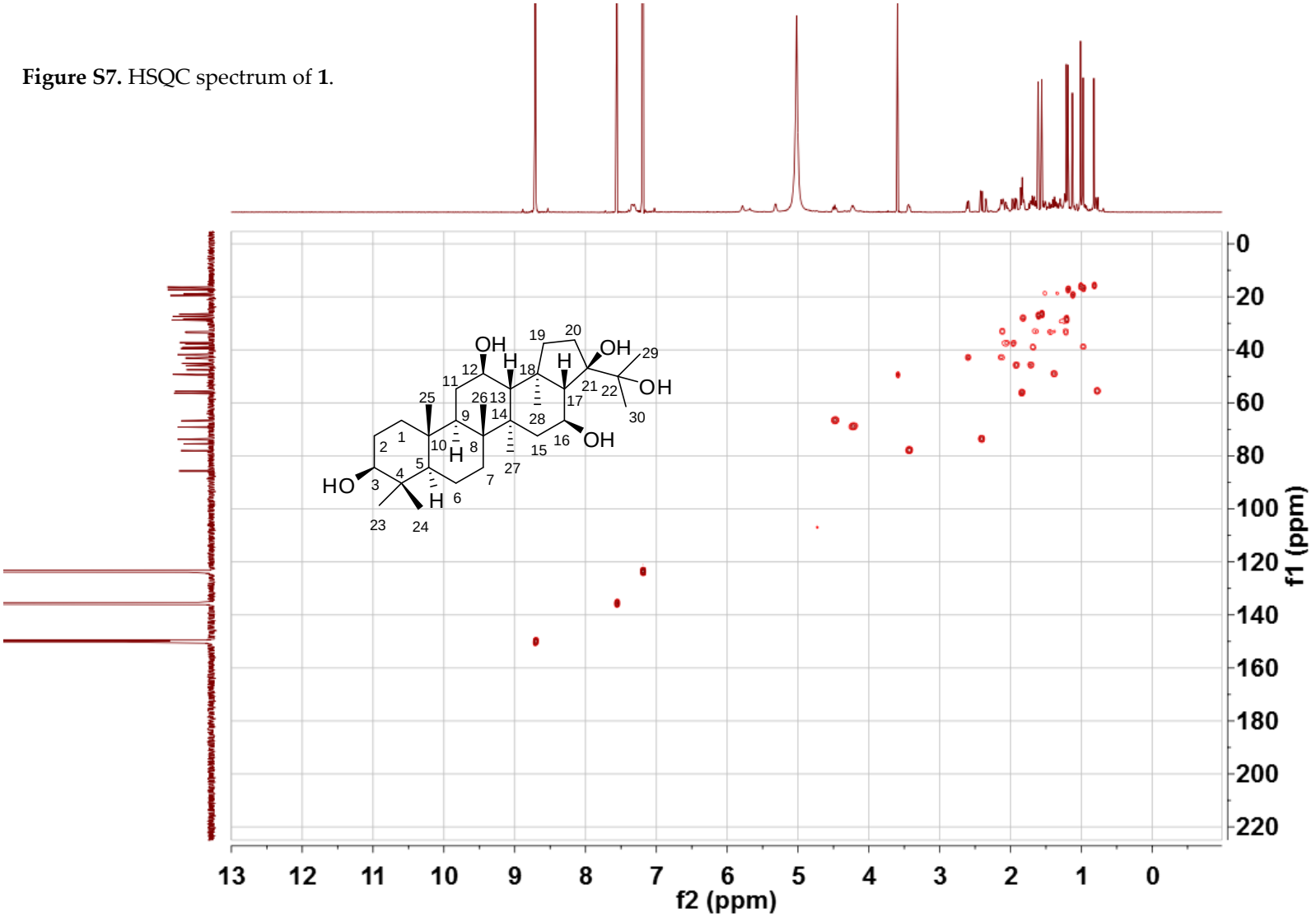
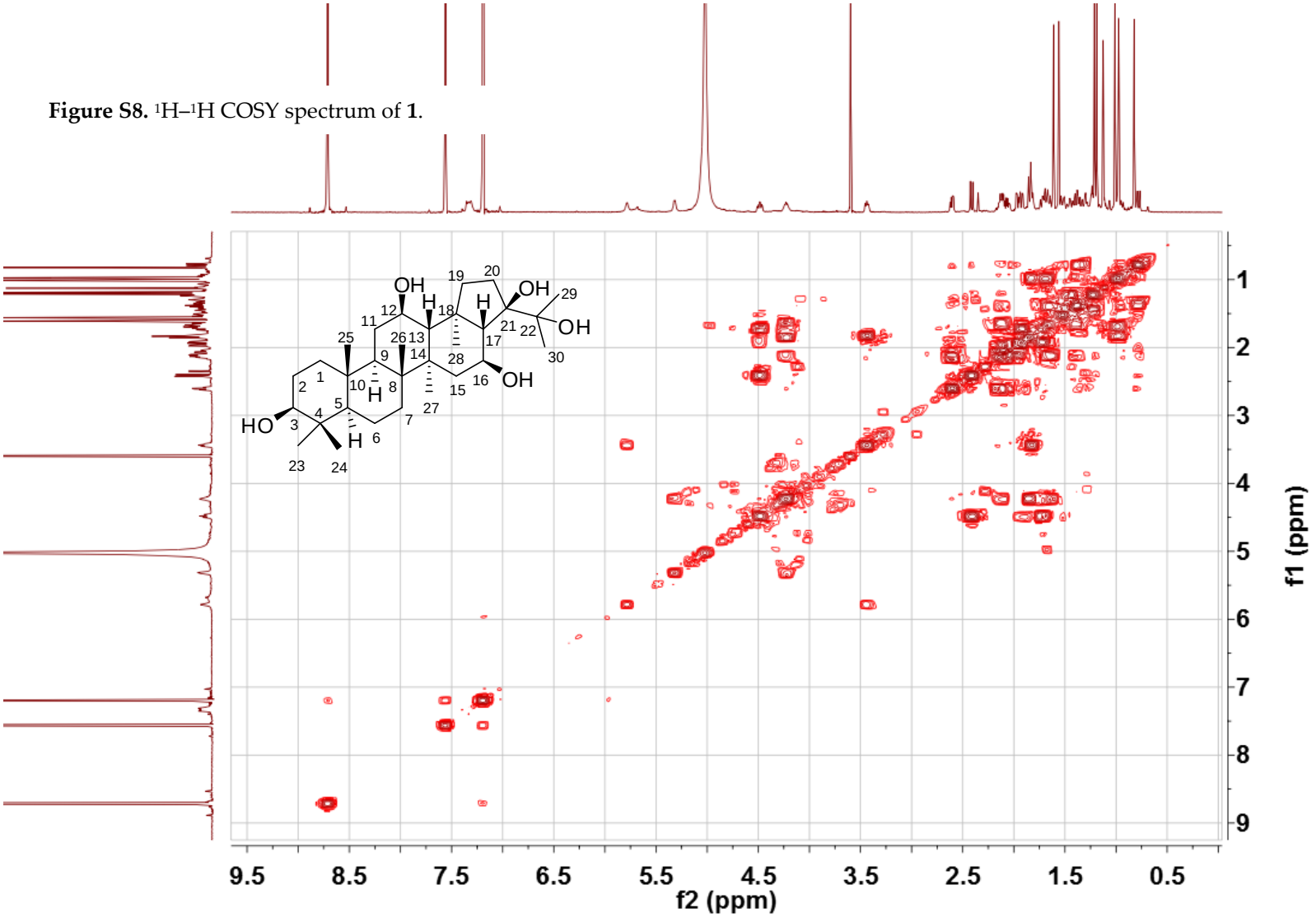


Figure S8. ^{1}H–^{1}H COSY spectrum of **1**.



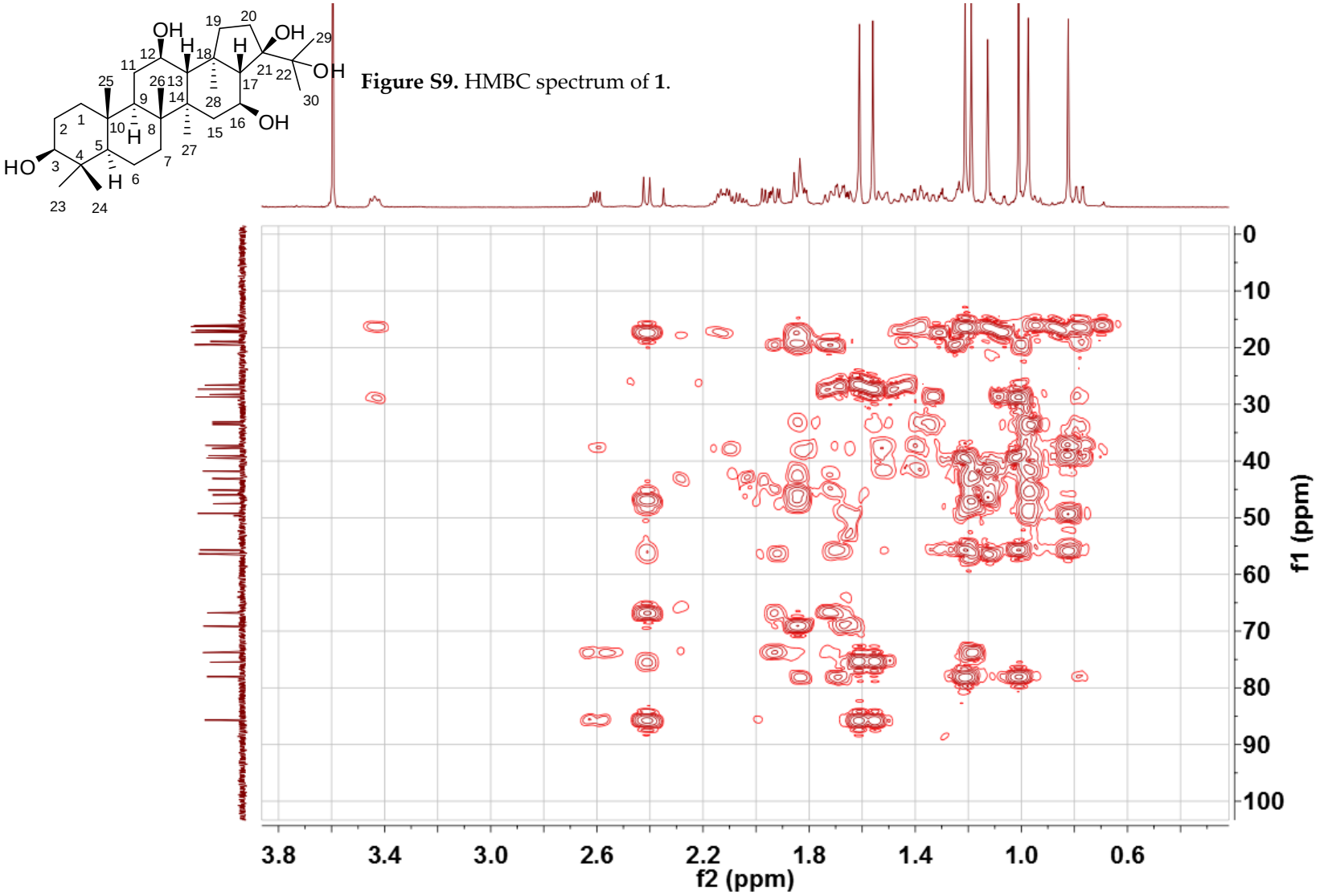


Figure S9. HMBC spectrum of **1**.

Figure S10. ROESY spectrum of **1**.

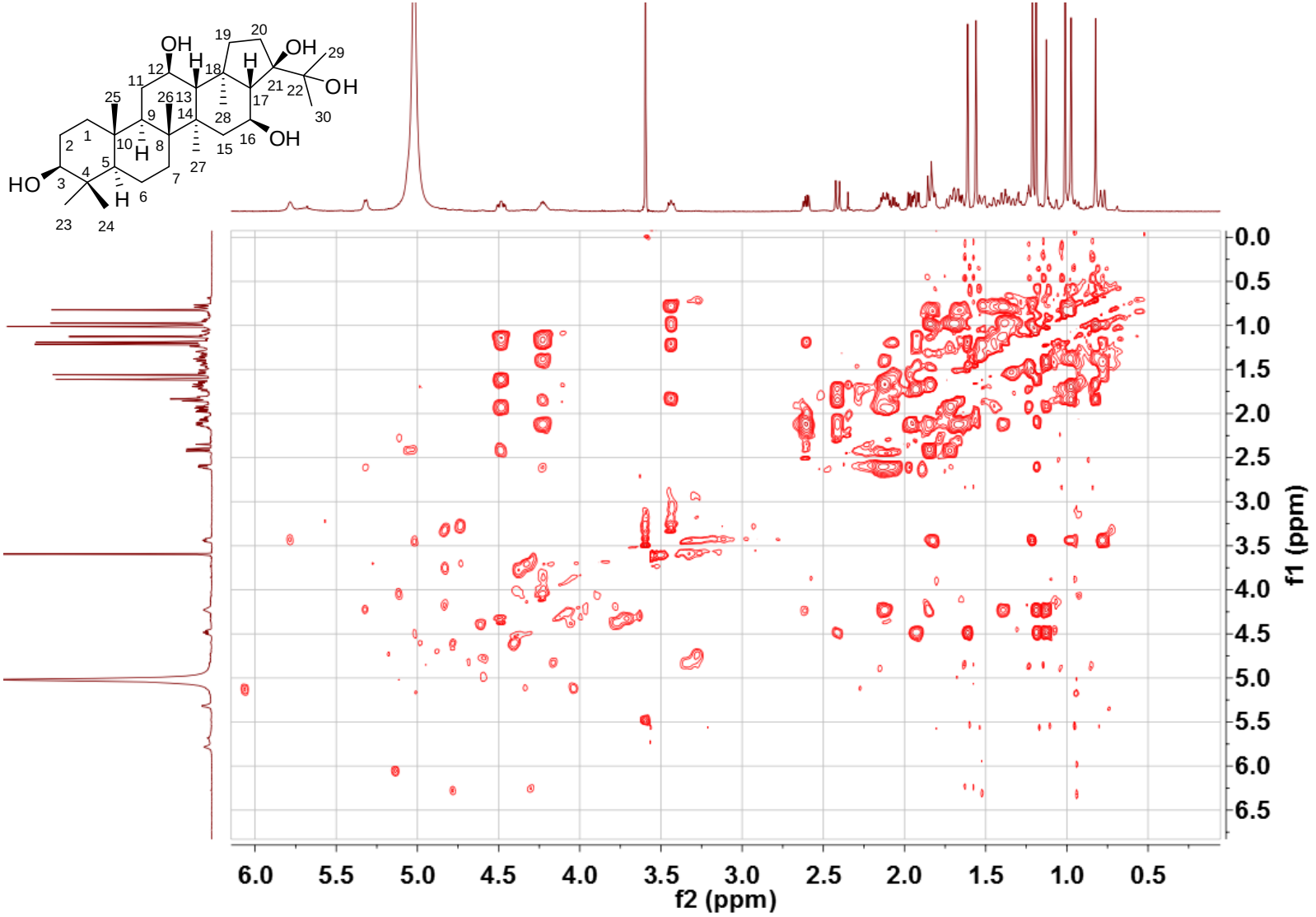


Figure S11. HRESIMS spectrum of **1**.

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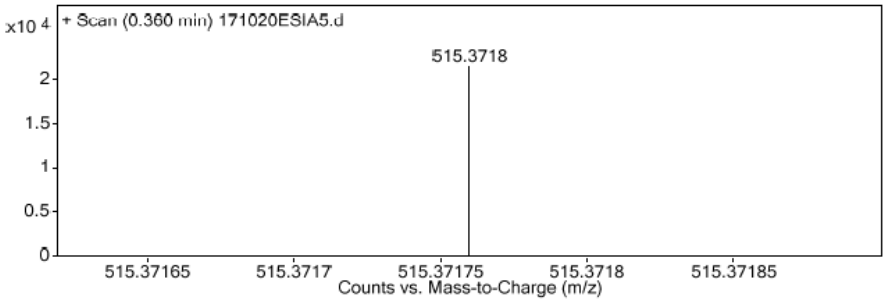
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	10/23/2017 10:45:31 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
230	0	ESI



Peak List

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100.1114		7040.62		
121.0509		7712.63		
125.1122	1	12984.43		
142.1592	1	30774.7		
186.2219	1	23846.48		
242.2848	1	104219.18		
243.2875	1	13899.02		
274.2739	1	6901.11		
515.3718	1	21392.95	C30 H52 Na O5	M+
922.0098	1	8991.66		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C30 H52 Na O5	515.3712	515.3718	-0.6	1.1	4.5

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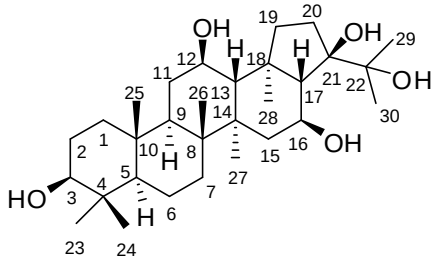

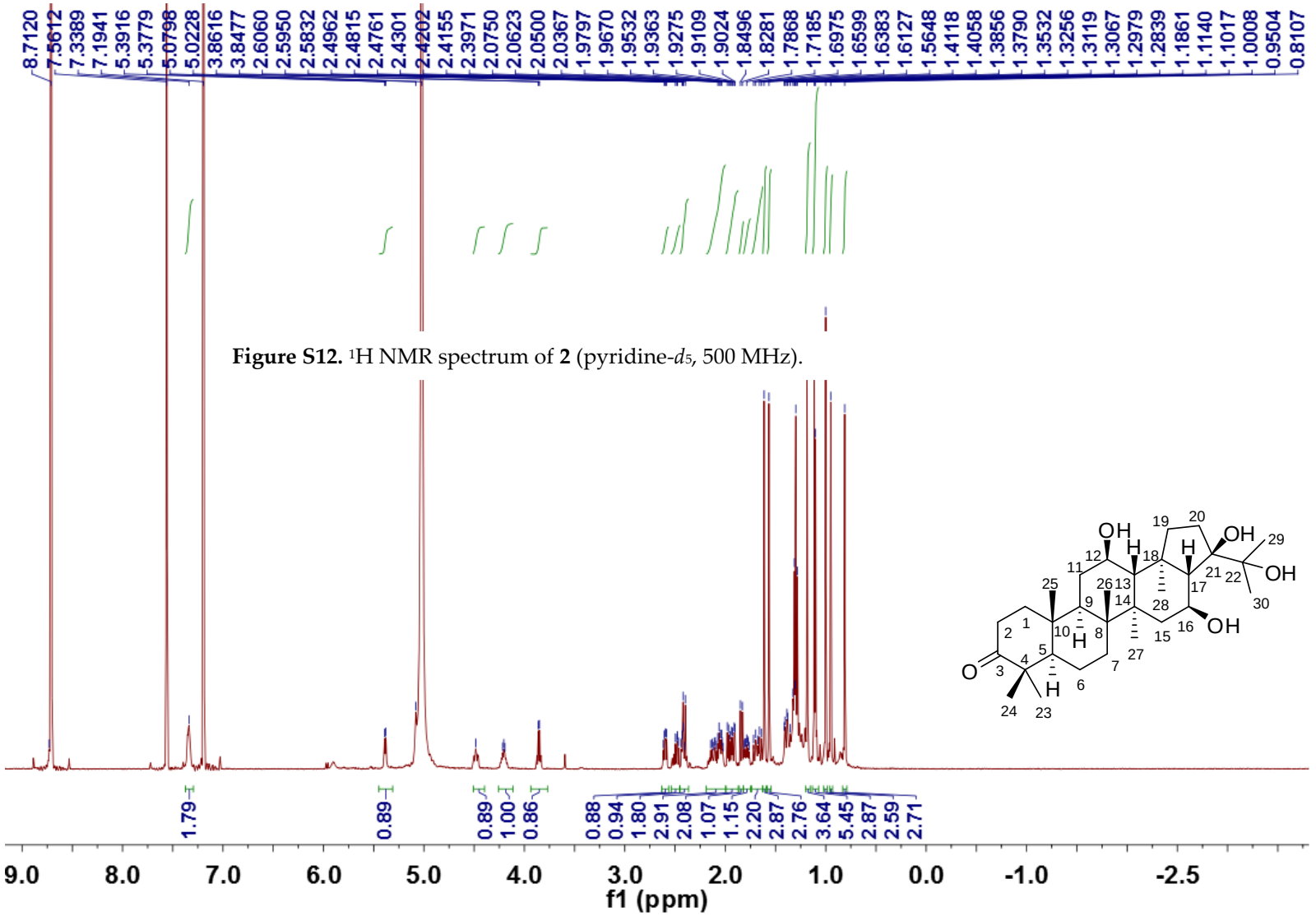

Figure S12. ^{1}H NMR spectrum of **2** (pyridine-d_5, 500 MHz).

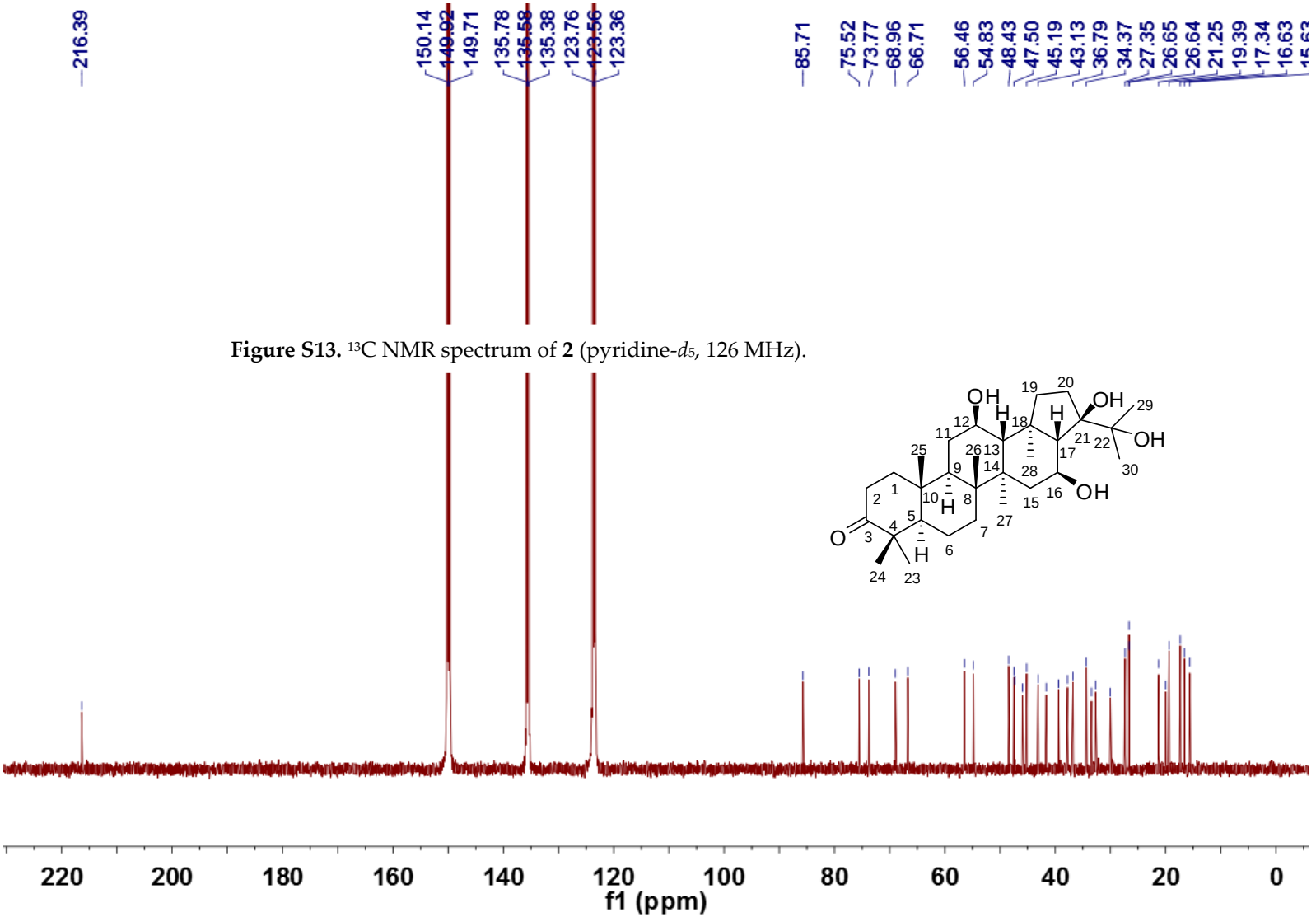

Figure S13. ^{13}C NMR spectrum of **2** (pyridine-d_5, 126 MHz).

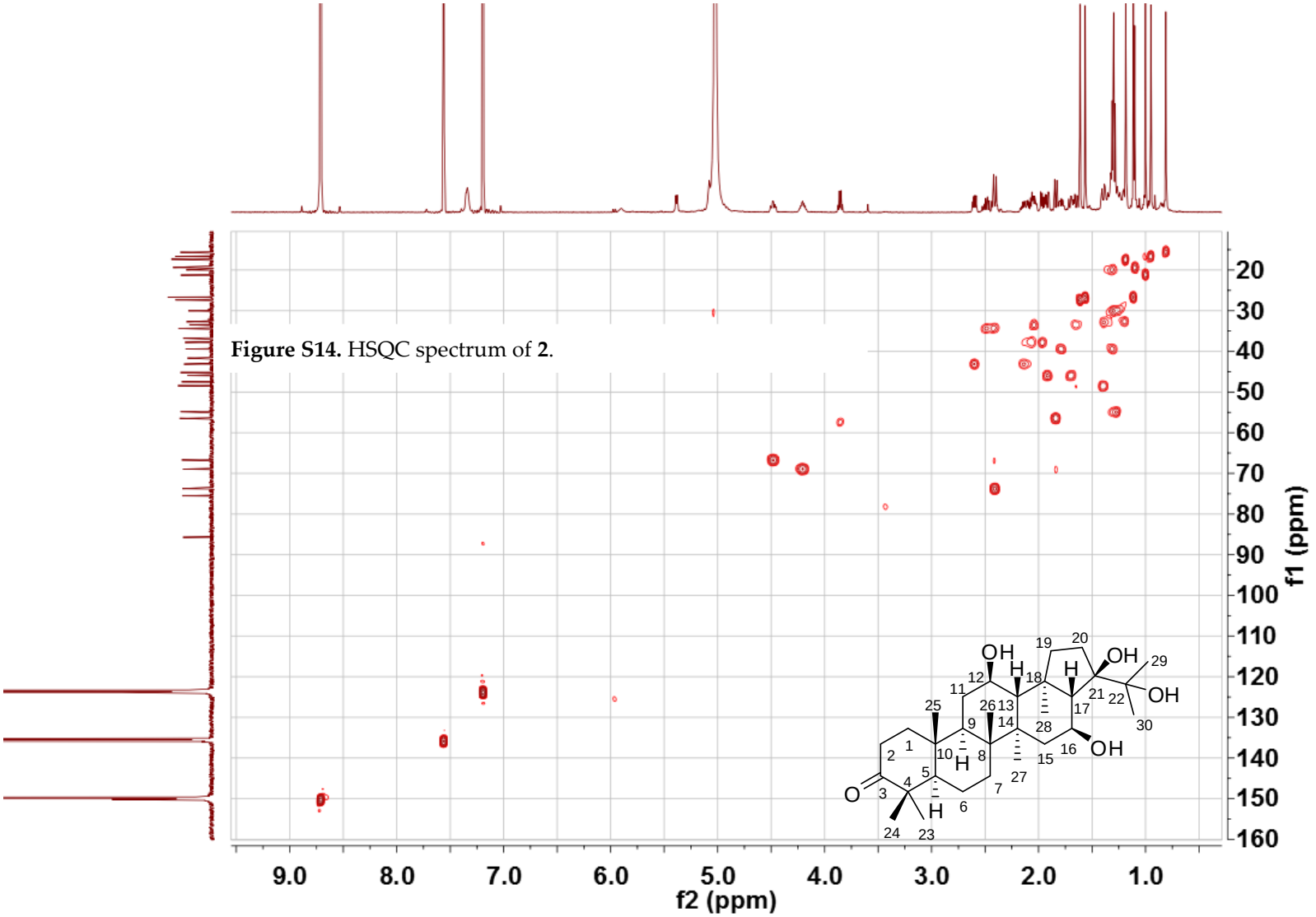

Figure S14. HSQC spectrum of **2**.

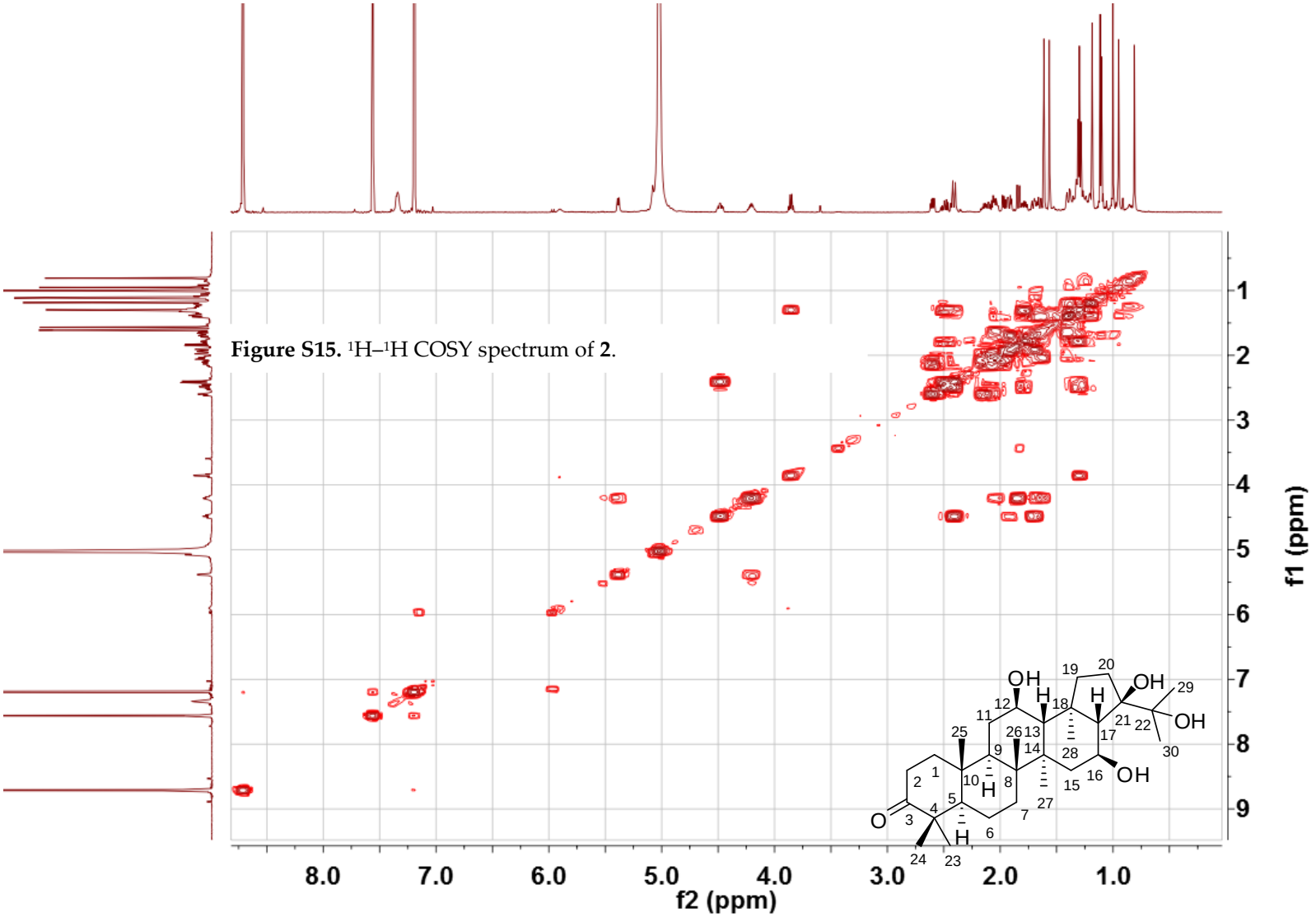

Figure S15. ^{1}H–^{1}H COSY spectrum of **2**.

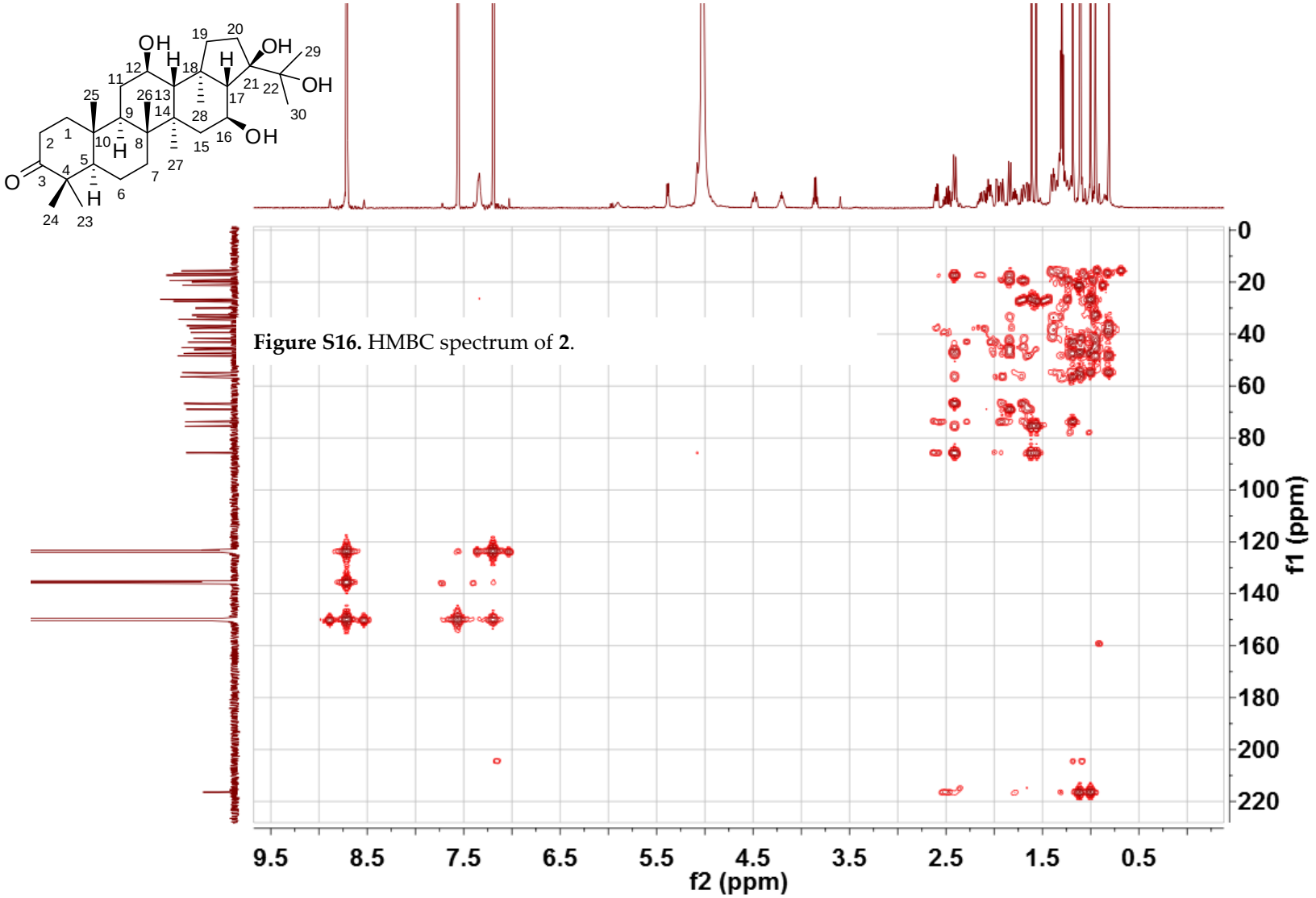

Figure S16. HMBC spectrum of **2**.

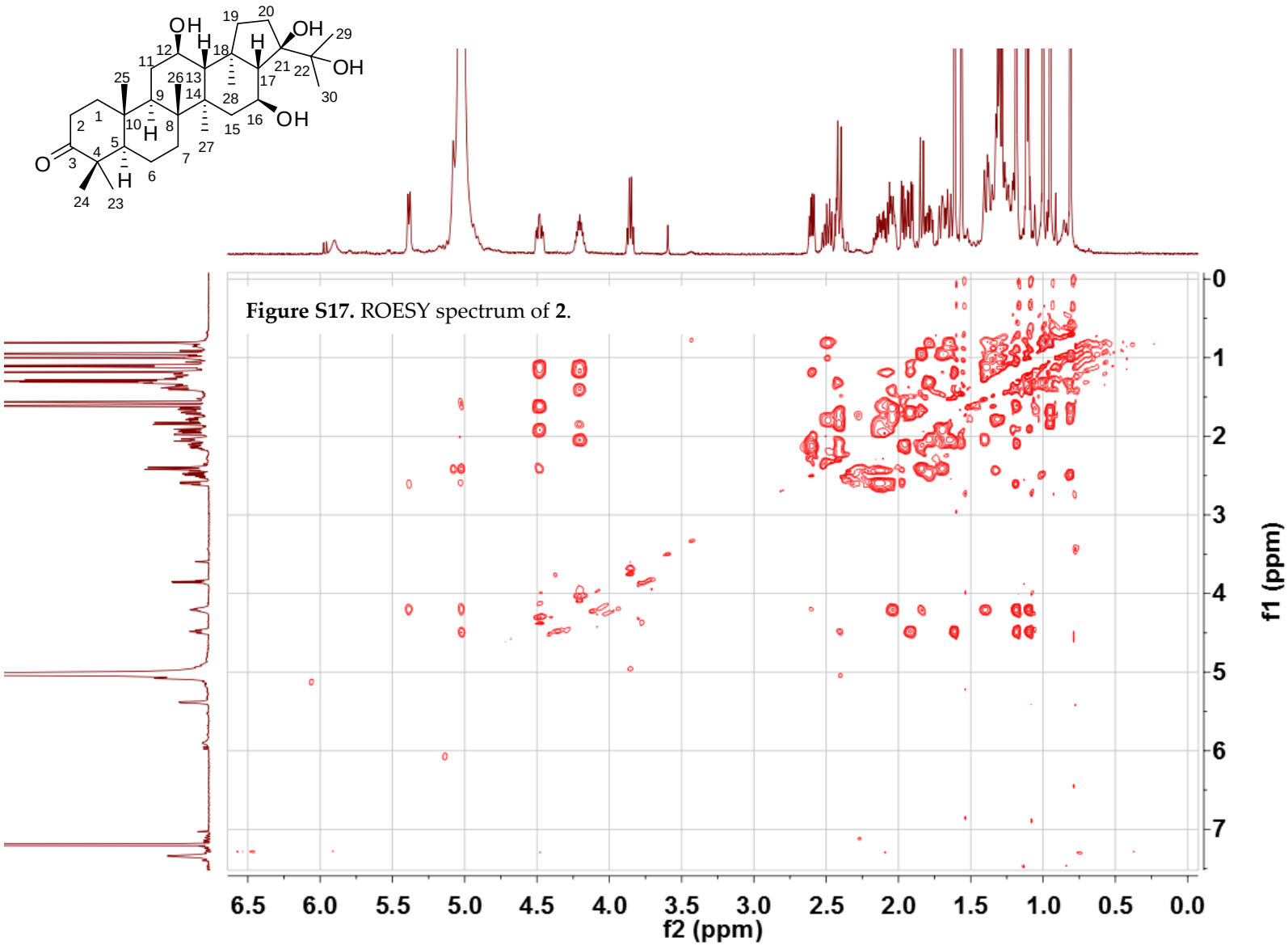

Figure S17. ROESY spectrum of **2**.

Figure S18. HRESIMS spectrum of **2**.

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Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
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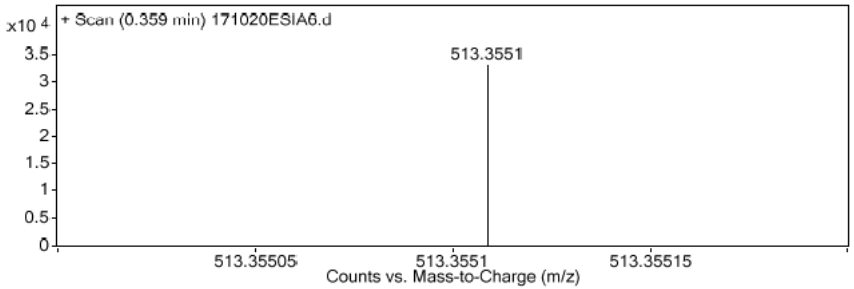
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
230	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
121.0509	1	12467.49		
142.1588	1	9737.21		
242.284	1	25951.61		
513.3551	1	33099.68	C30 H50 Na O5	M+
514.3579	1	8436.8	C30 H50 Na O5	M+
701.4931	1	15047.89		
814.5779	1	7262.12		
922.0098	1	23822.68		
1003.7204	1	17353.7		
1004.7223	1	10234.4		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

截图(Alt + A)

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C30 H50 Na O5	513.3556	513.3551	0.5	1.0	5.5

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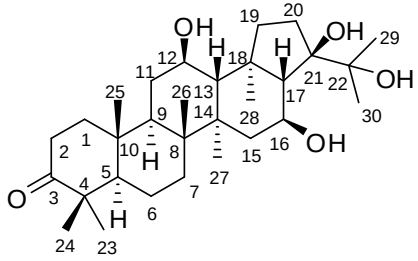


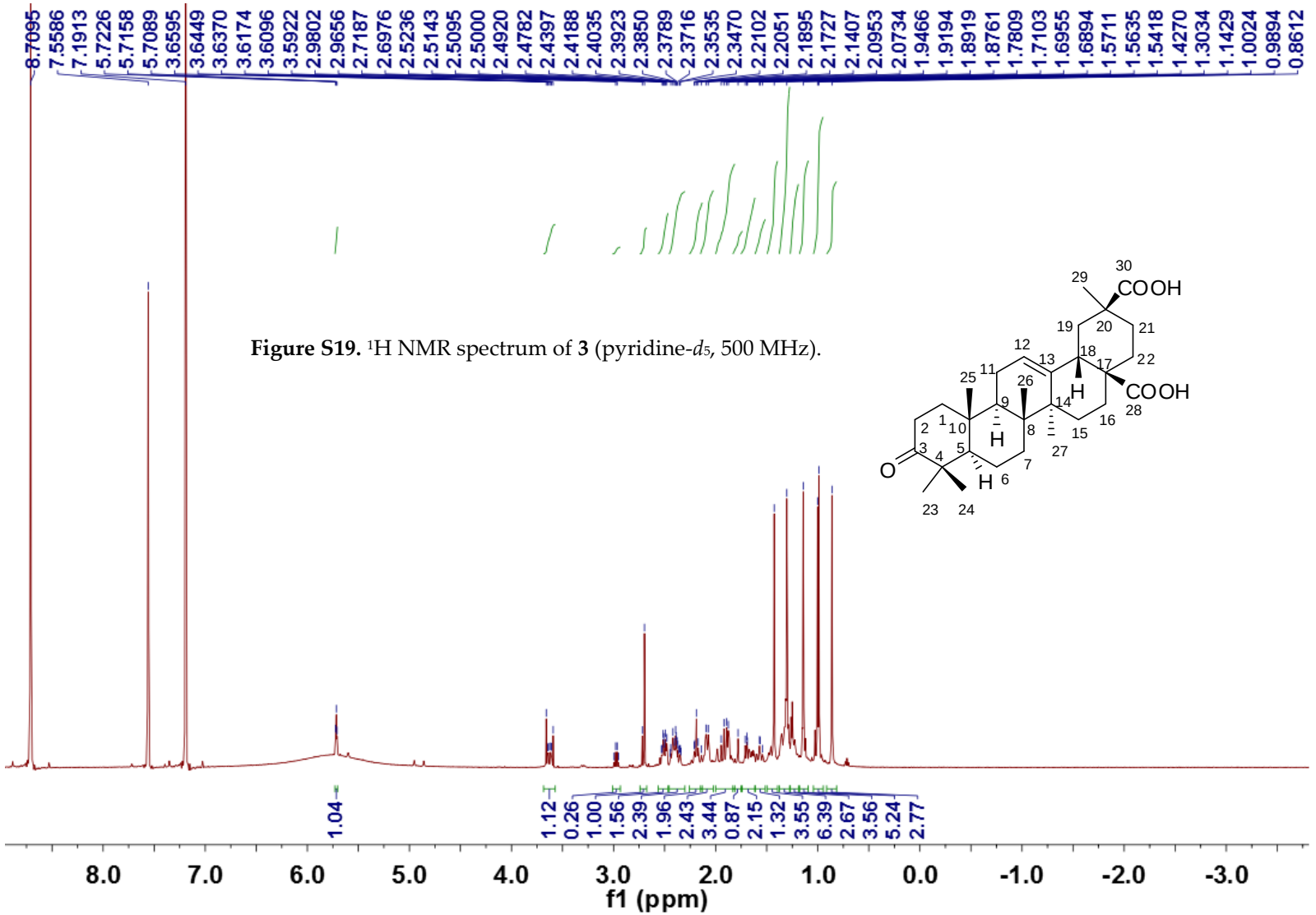


Figure S19. [1]H NMR spectrum of **3** (pyridine-d_5, 500 MHz).

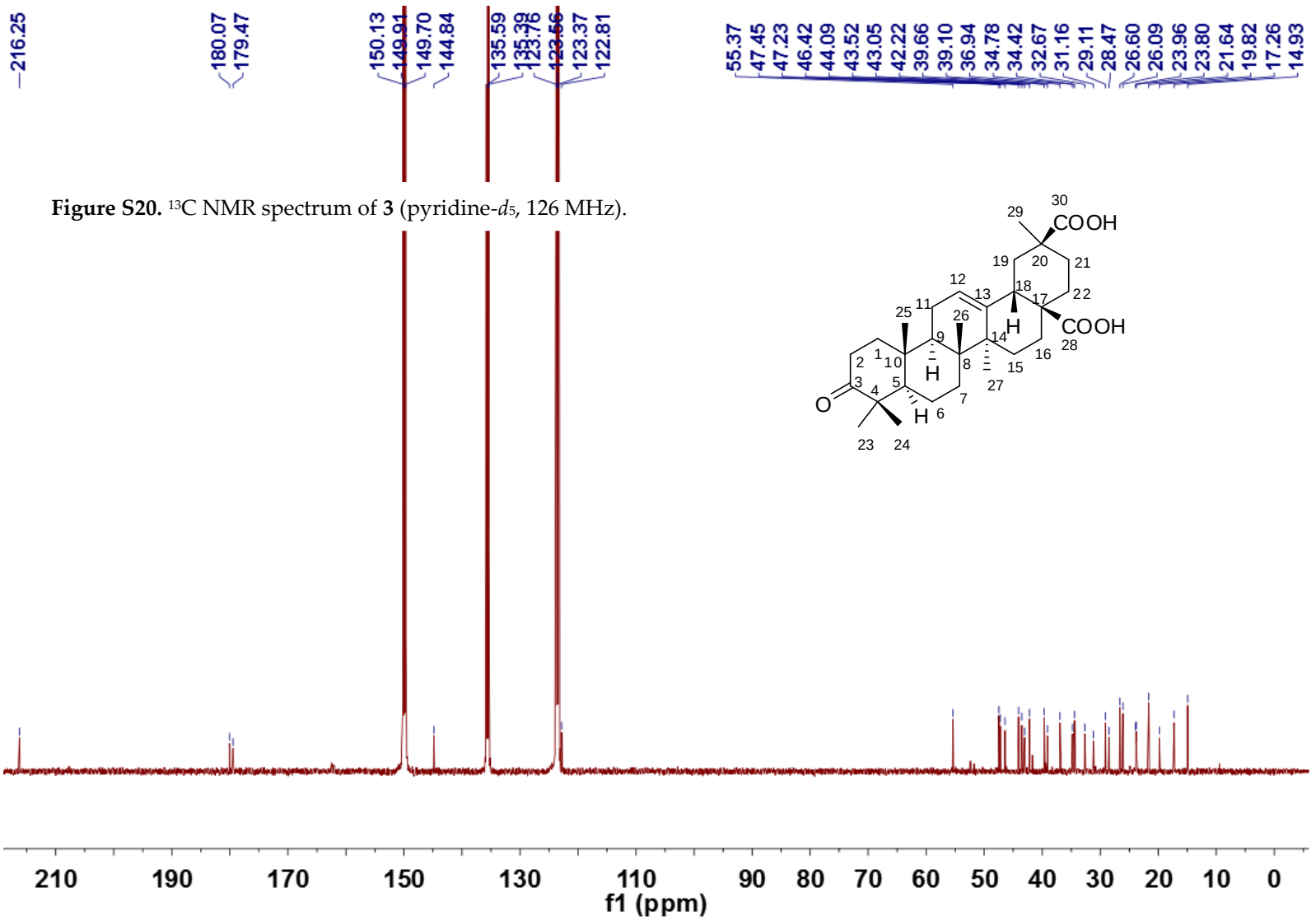


Figure S20. ^{13}C NMR spectrum of **3** (pyridine-d_5, 126 MHz).

Figure S21. HSQC spectrum of **3**.

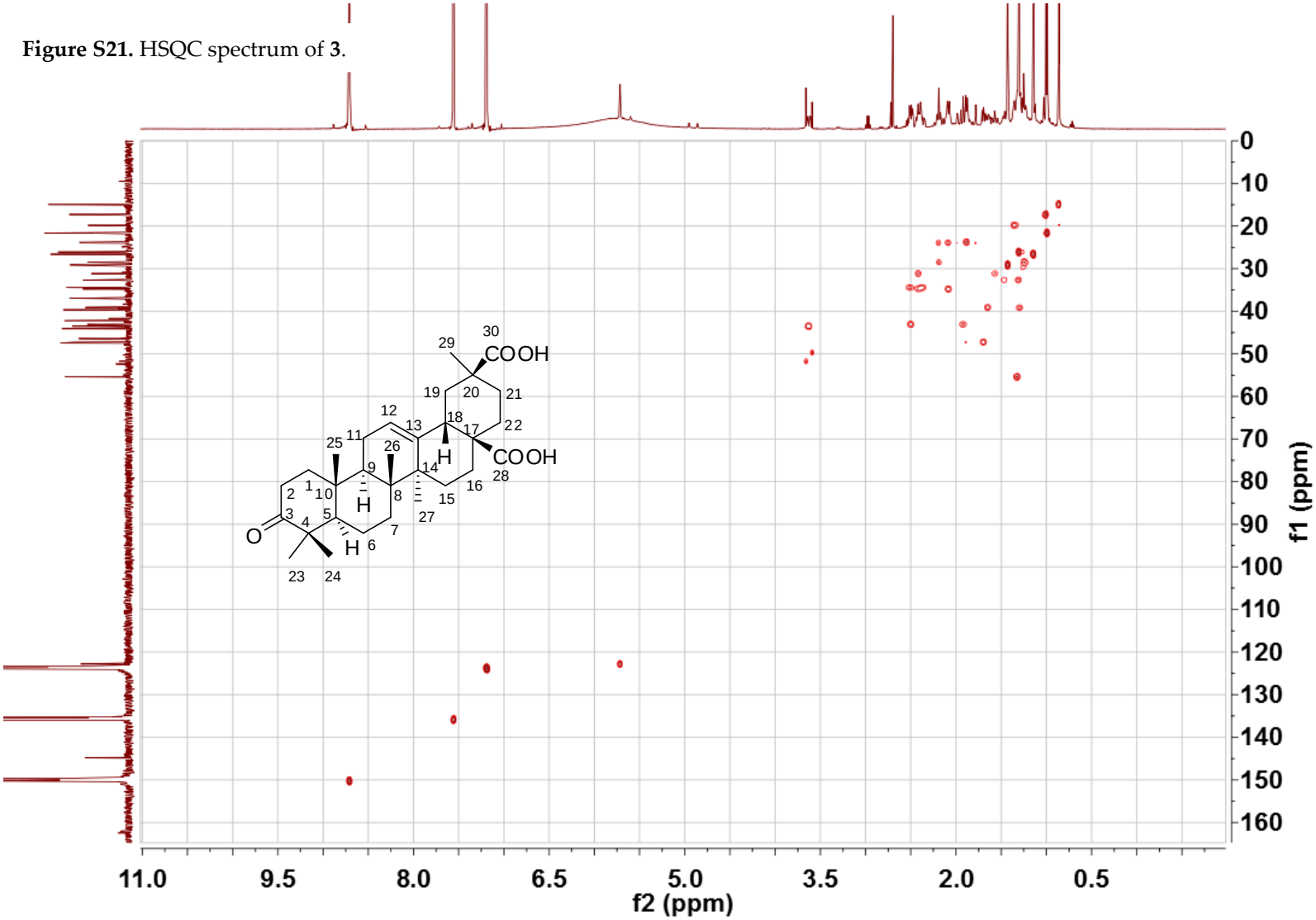


Figure S22. ^{1}H–^{1}H COSY spectrum of **3**.

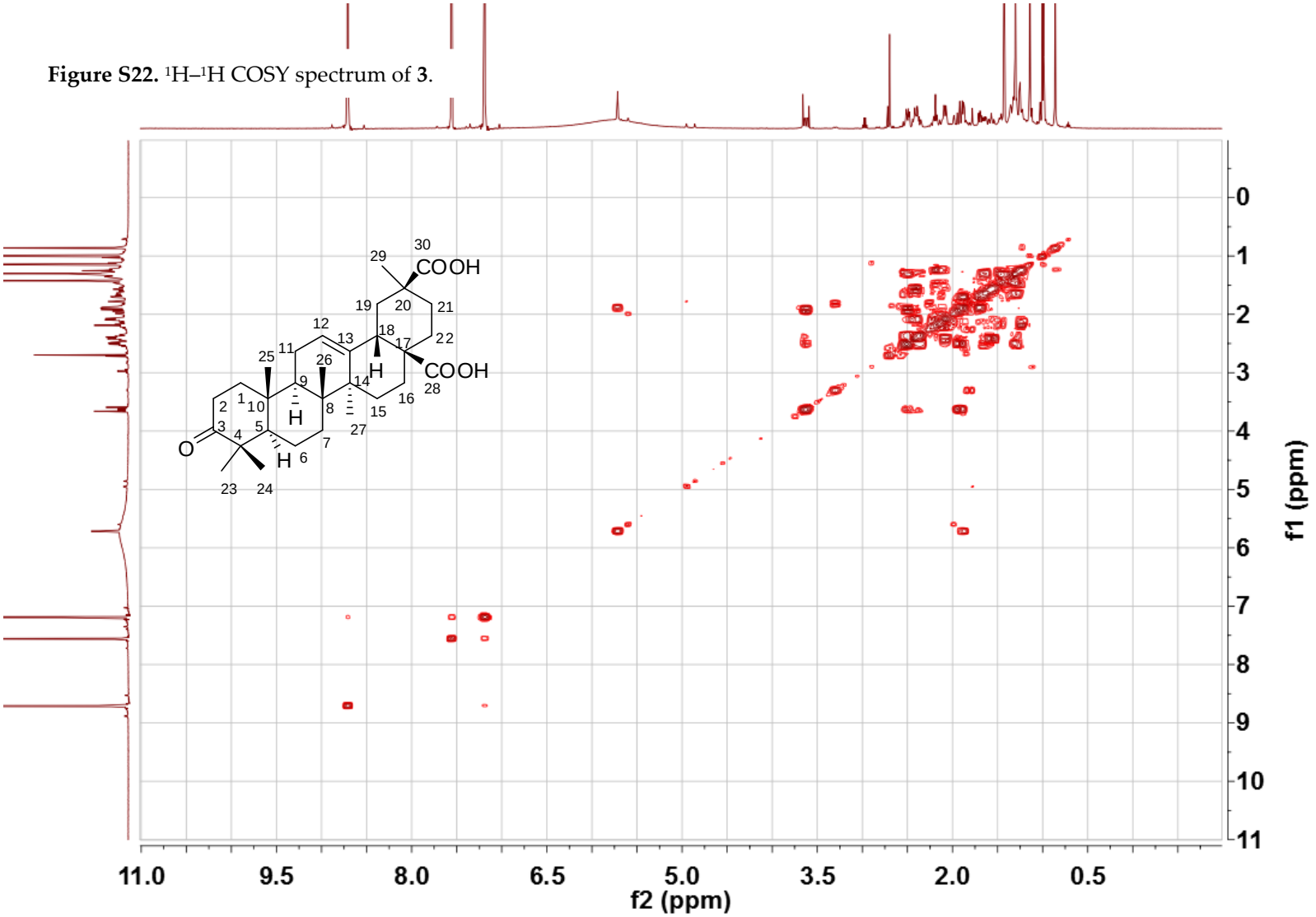


Figure S23. HMBC spectrum of **3**.

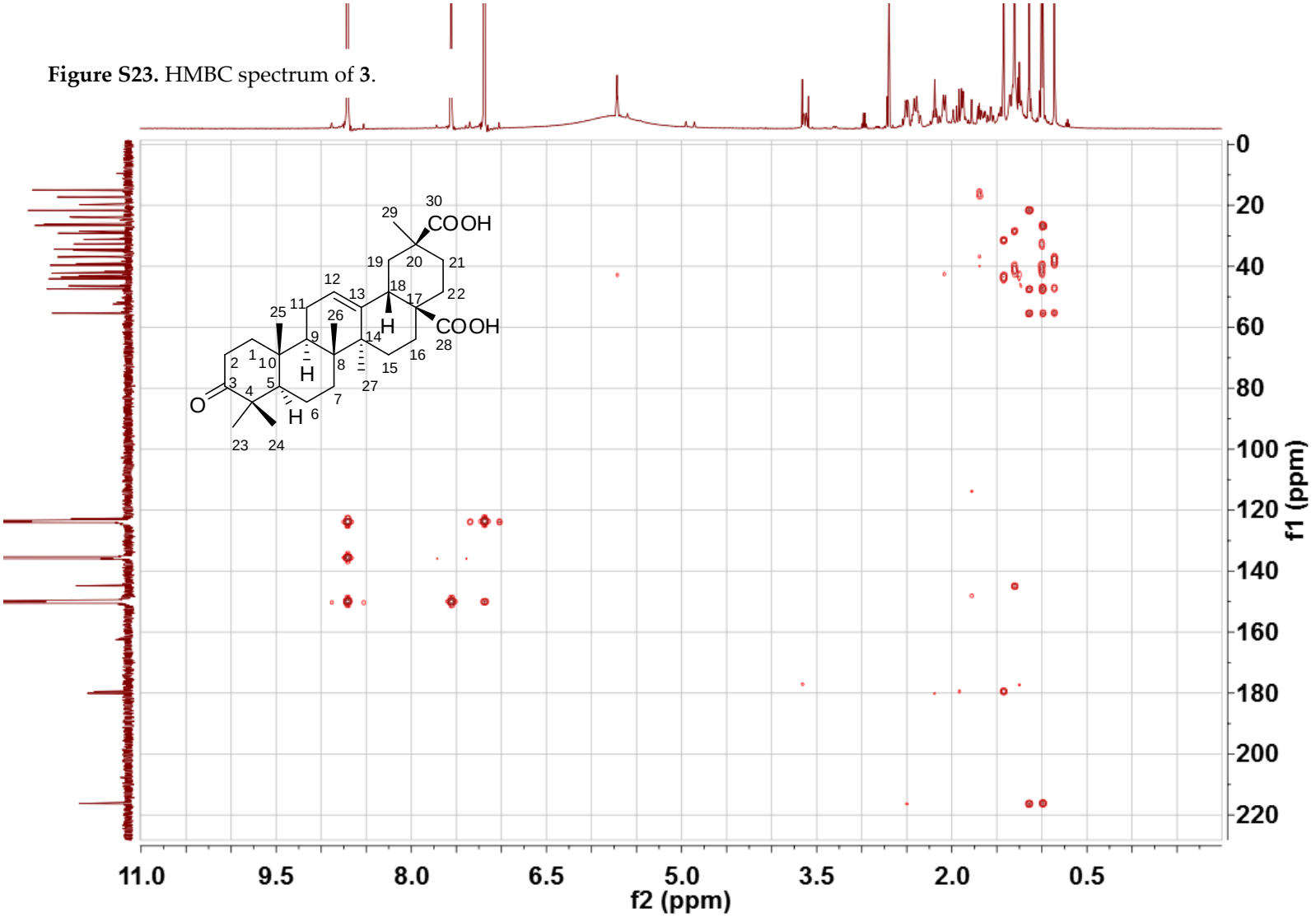
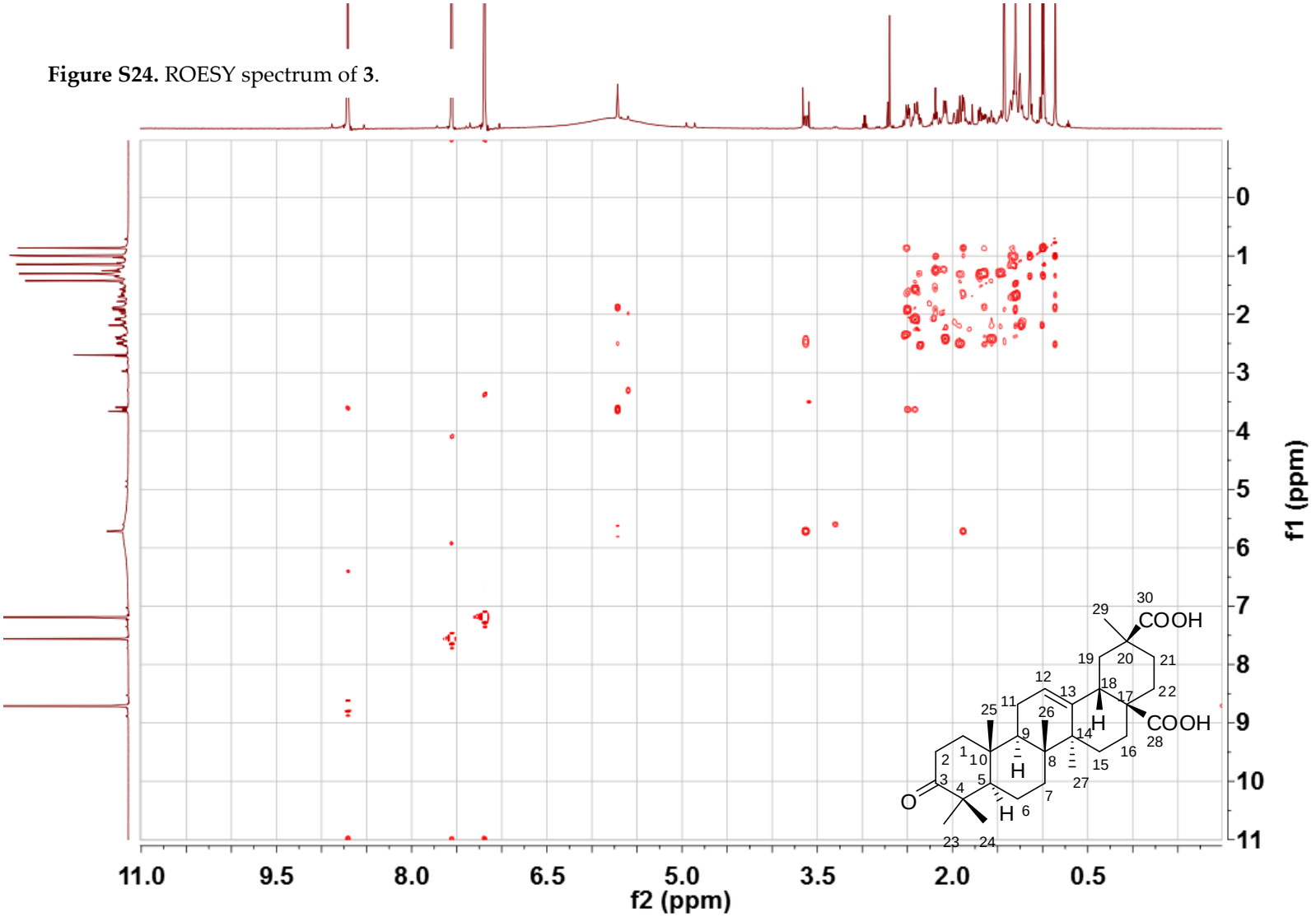


Figure S24. ROESY spectrum of **3**.



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IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group	**Info.**
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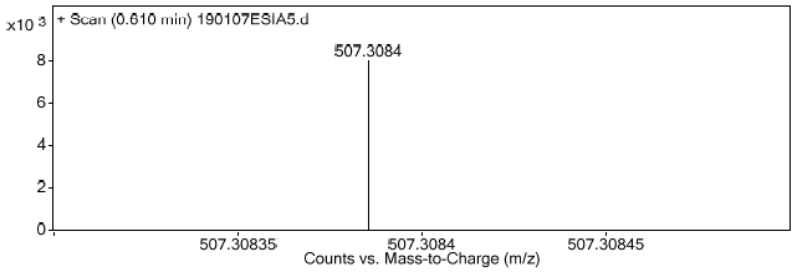
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
320	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
105.0435		6260.53		
112.1882		7240.67		
166.063	1	12333.17		
182.0406	1	60230.32		
218.9738		9341.78		
507.3084	1	7971.67	C30 H44 Na O5	M+
523.2797	1	10704.83		
537.3184	1	7292.68		
548.3337	1	6272.26		
553.2923	1	5397.99		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C30 H44 Na O5	507.3086	507.3084	0.2	0.5	8.5

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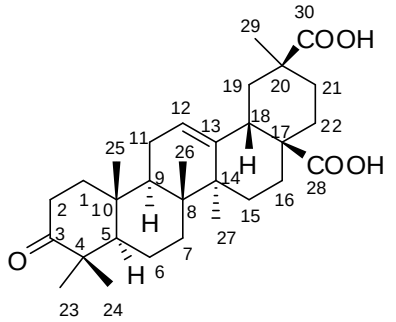
Figure S25. HRESIMS spectrum of **3**.



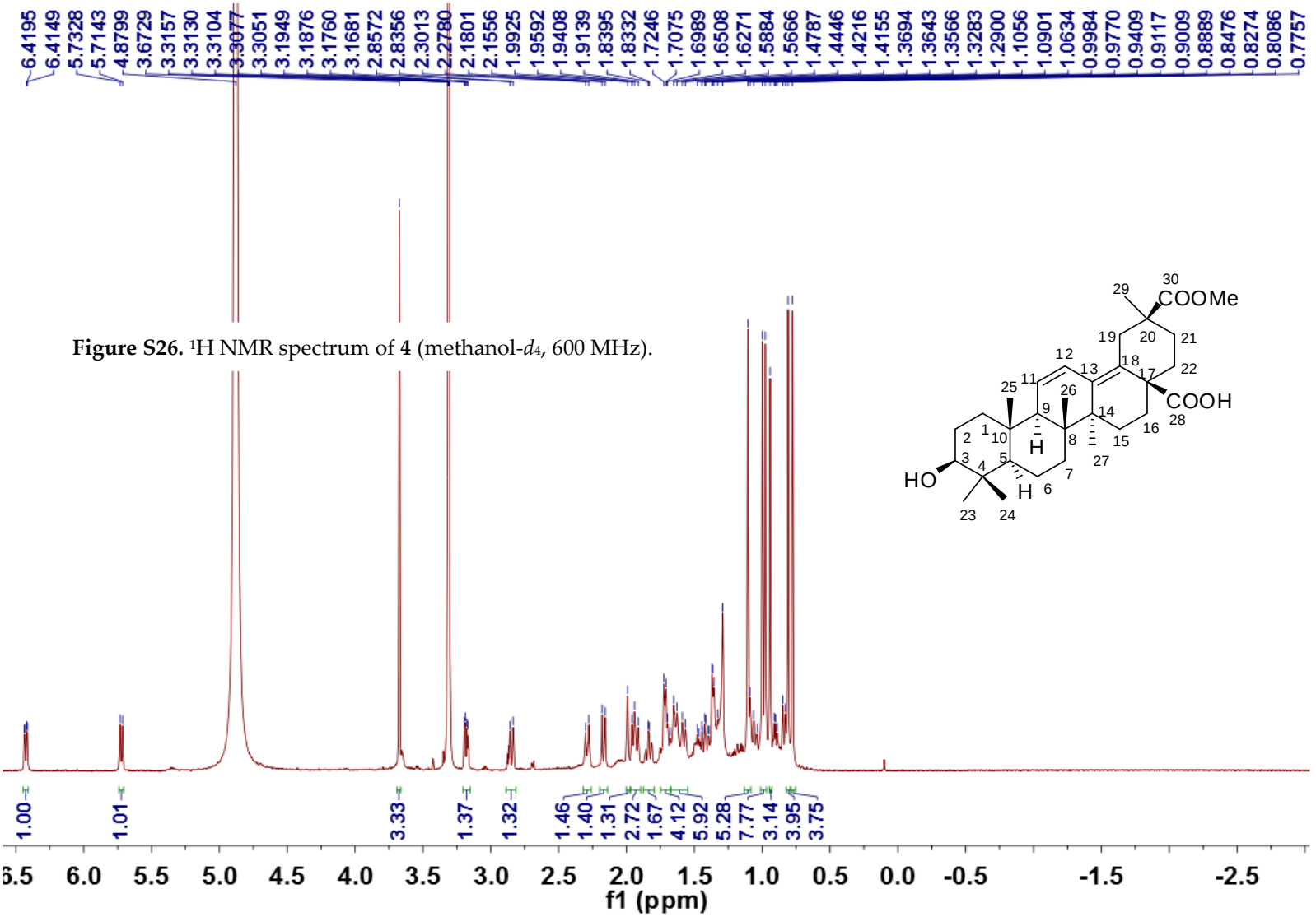


Figure S26. ^{1}H NMR spectrum of **4** (methanol-d_4, 600 MHz).

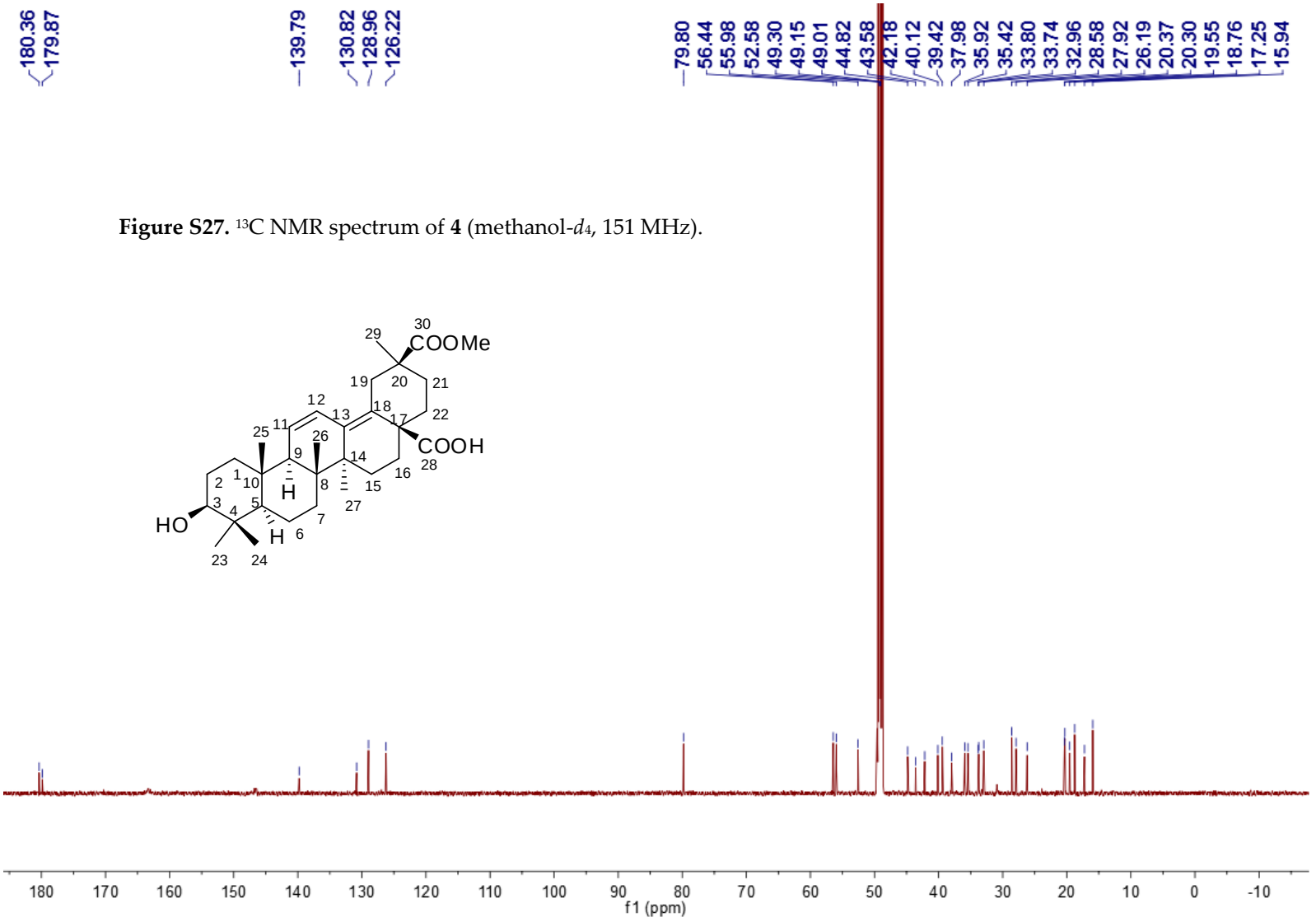


Figure S27. ^{13}C NMR spectrum of **4** (methanol-d_4, 151 MHz).

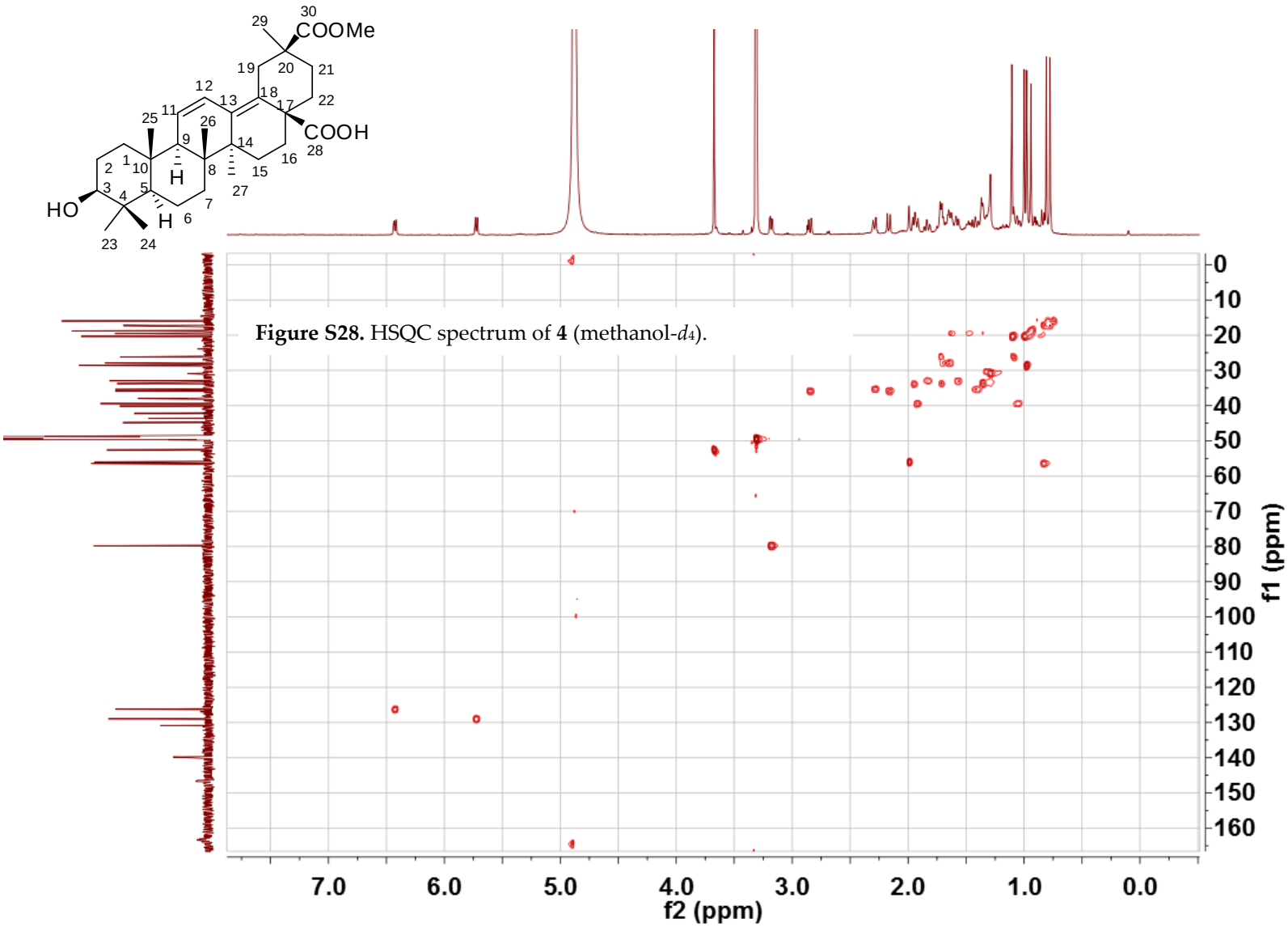


Figure S28. HSQC spectrum of **4** (methanol-d_4).

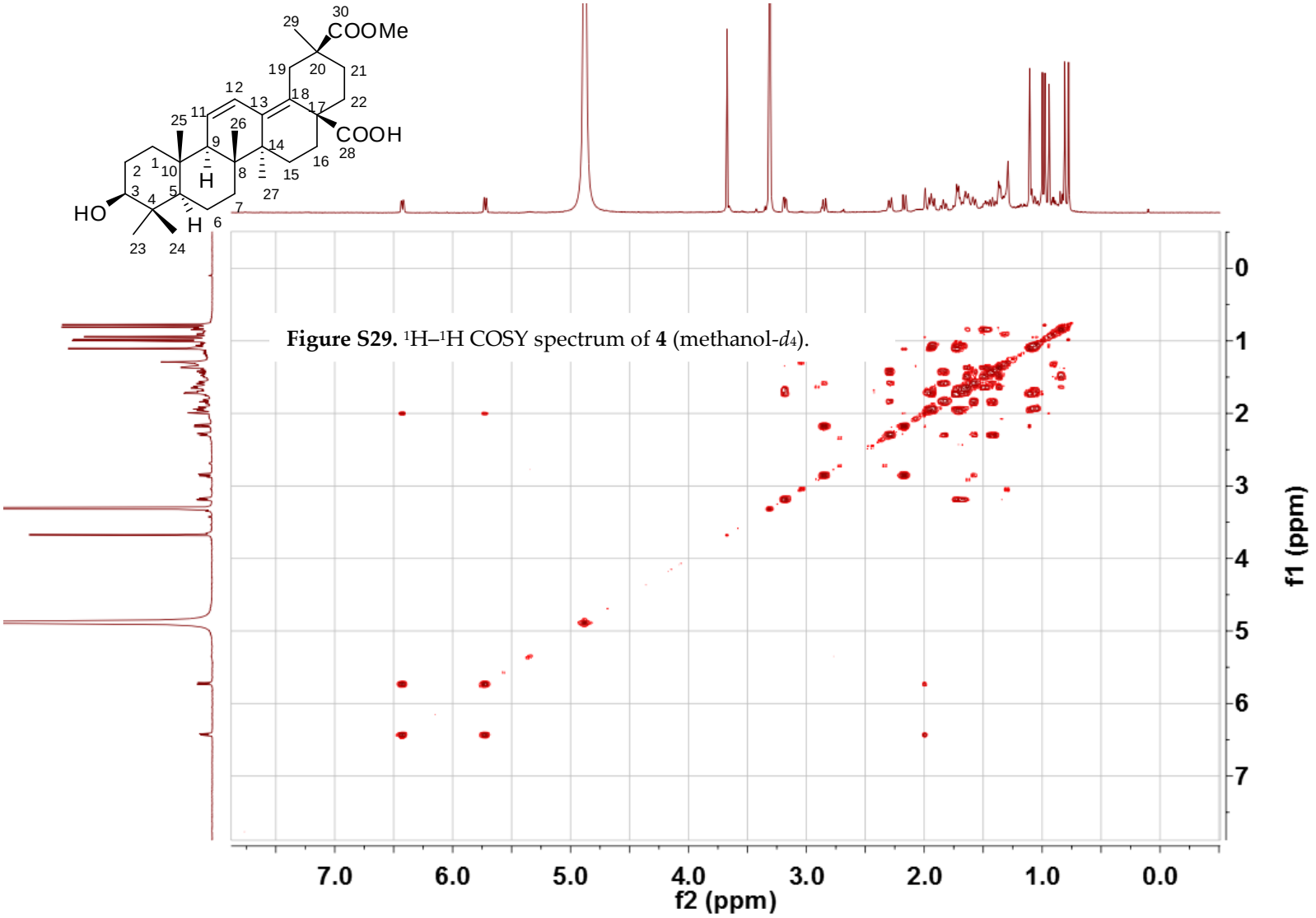


Figure S29. ^{1}H–^{1}H COSY spectrum of **4** (methanol-d_4).

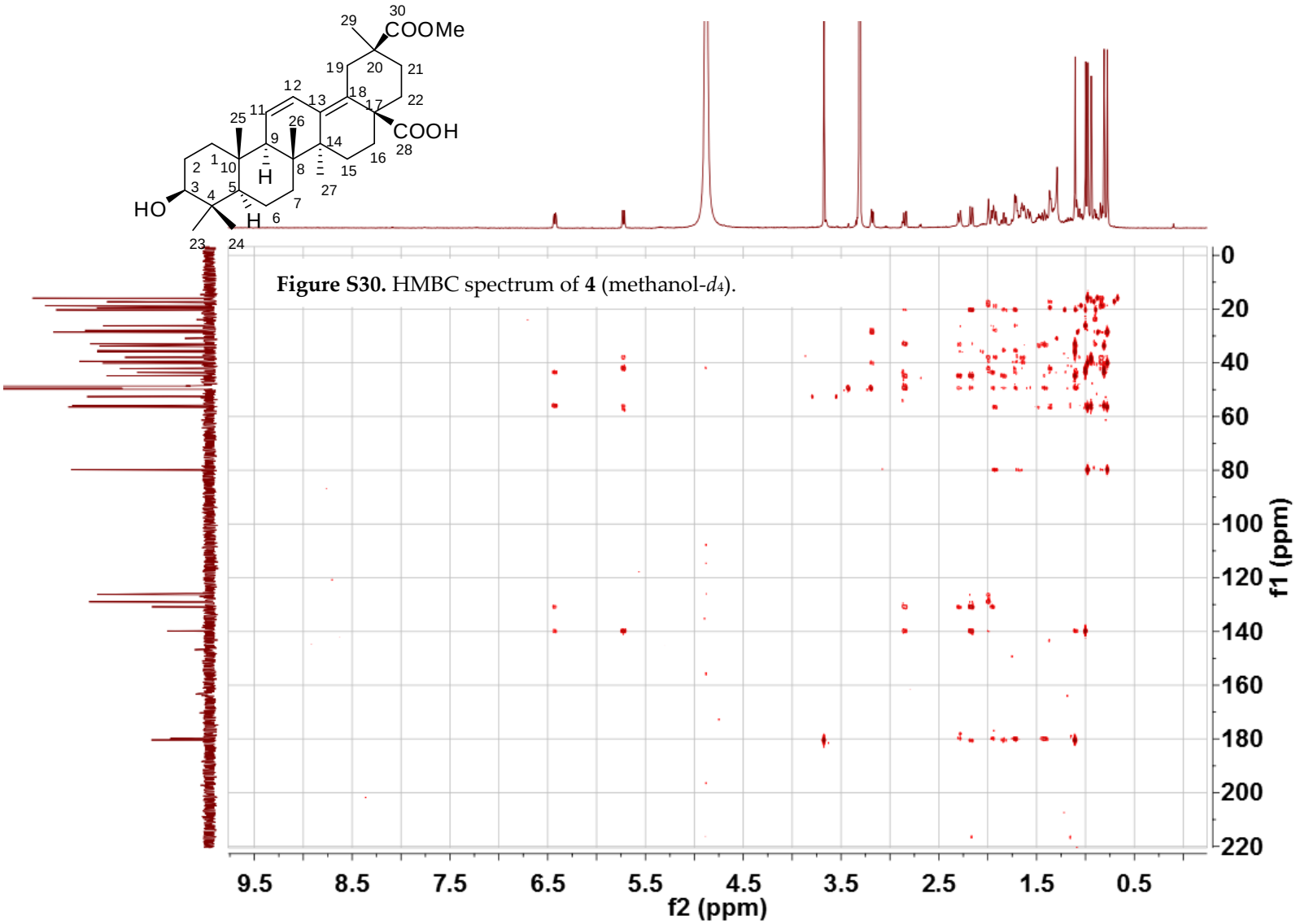


Figure S30. HMBC spectrum of **4** (methanol-d_4).

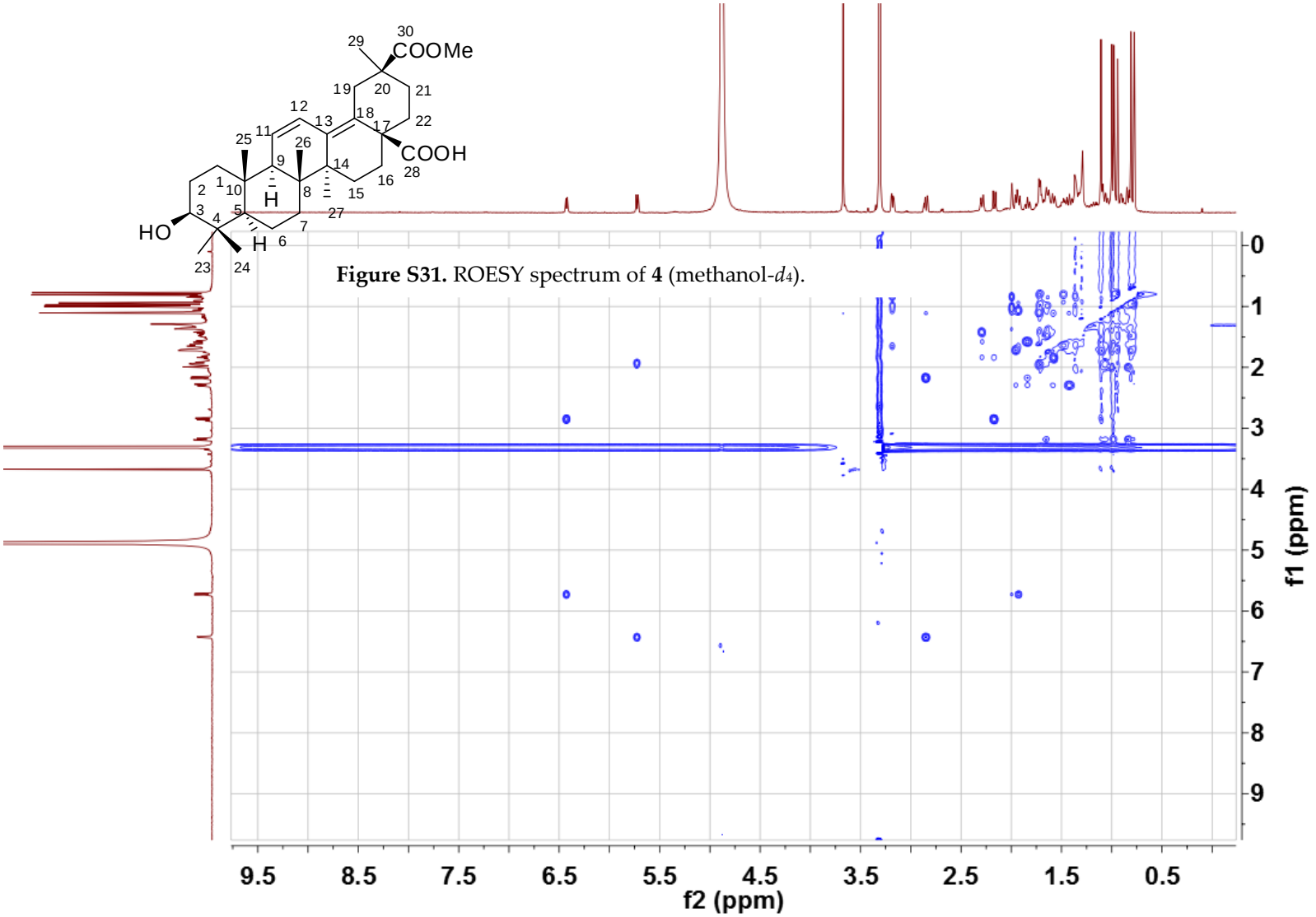


Figure S31. ROESY spectrum of **4** (methanol-d_4).

Formula Predictor Report - PDT32.lcd

Data File: E:\DATA\2018\0626\PDT32.lcd

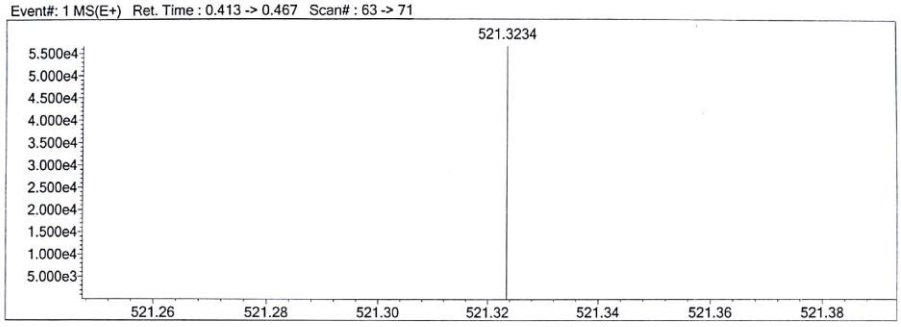
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	50	O	2	0	20	Si	4	0	0	Br	1	0	0	Na
C	4	10	50	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	0	Na	1	0	0	Cl	1	0	10					

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

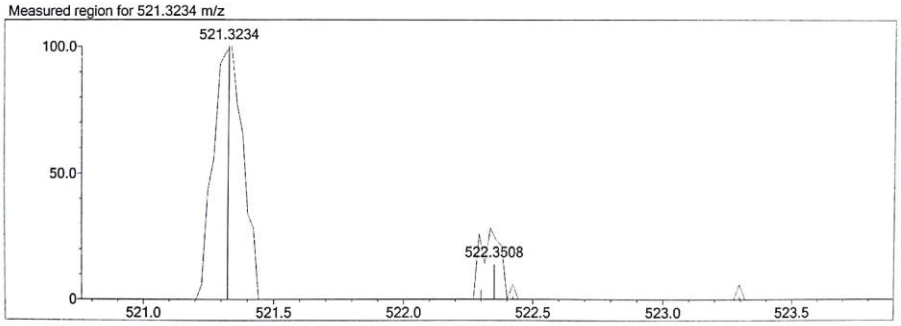
DBE Range: -2.0 - 100.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 10

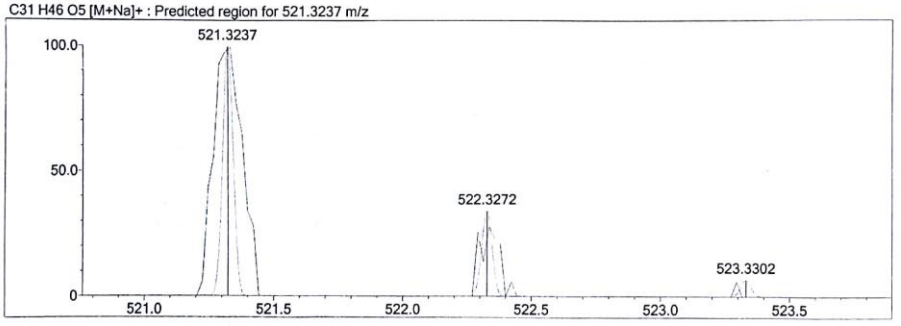
Event#: 1 MS(E+) Ret. Time : 0.413 -> 0.467 Scan# : 63 -> 71



Measured region for 521.3234 m/z



C31 H46 O5 [M+Na]+ : Predicted region for 521.3237 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C31 H46 O5	[M+Na]+	521.3234	521.3237	-0.3	-0.58	9.0

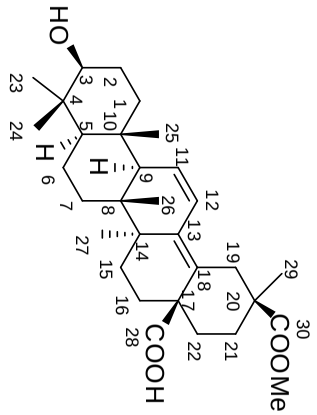


Figure S32. HRESIMS spectrum of **4**.

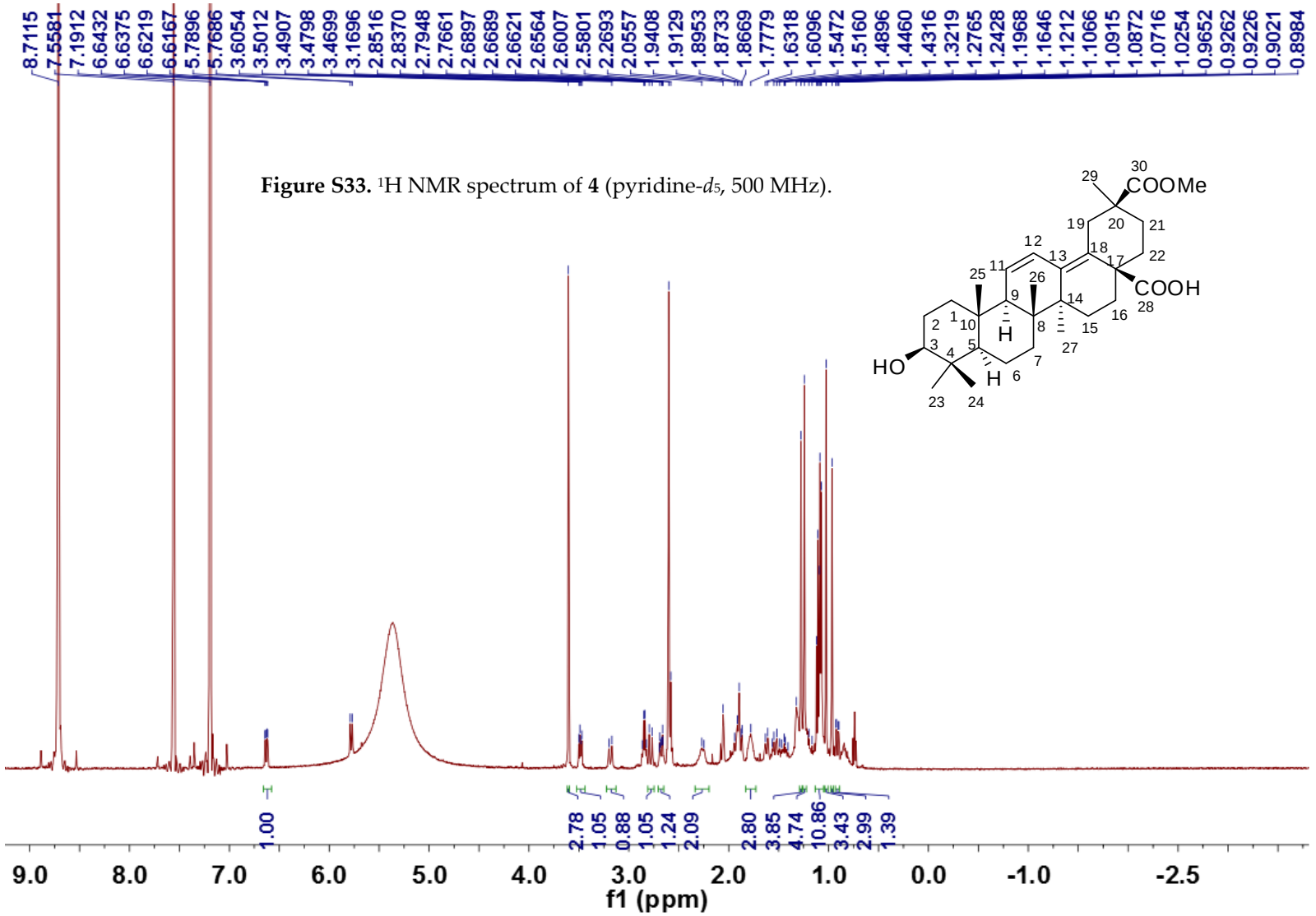


Figure S33. ^{1}H NMR spectrum of **4** (pyridine-d_5, 500 MHz).

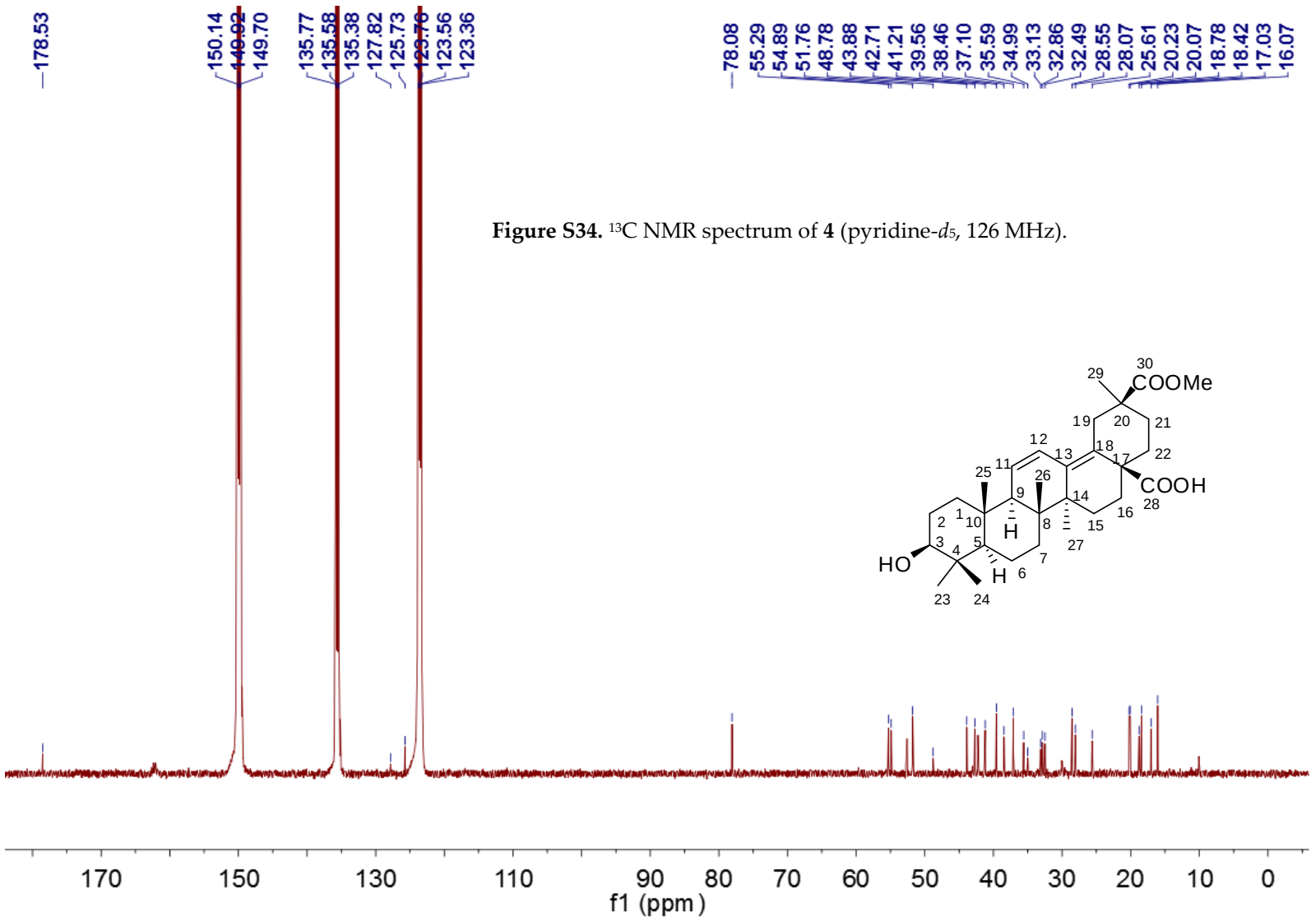
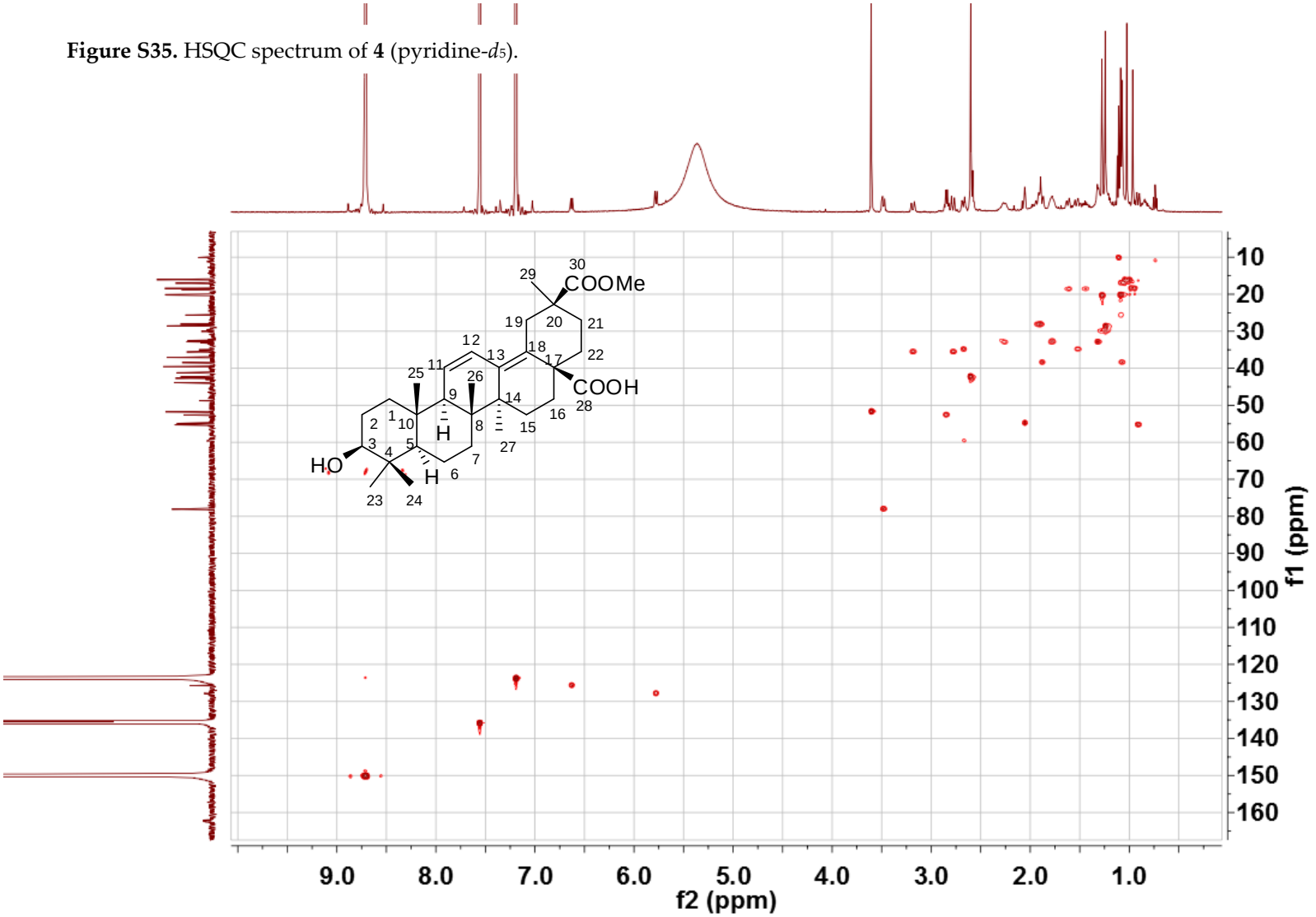


Figure S34. ^{13}C NMR spectrum of **4** (pyridine-d_5, 126 MHz).

Figure S35. HSQC spectrum of **4** (pyridine-d_5).



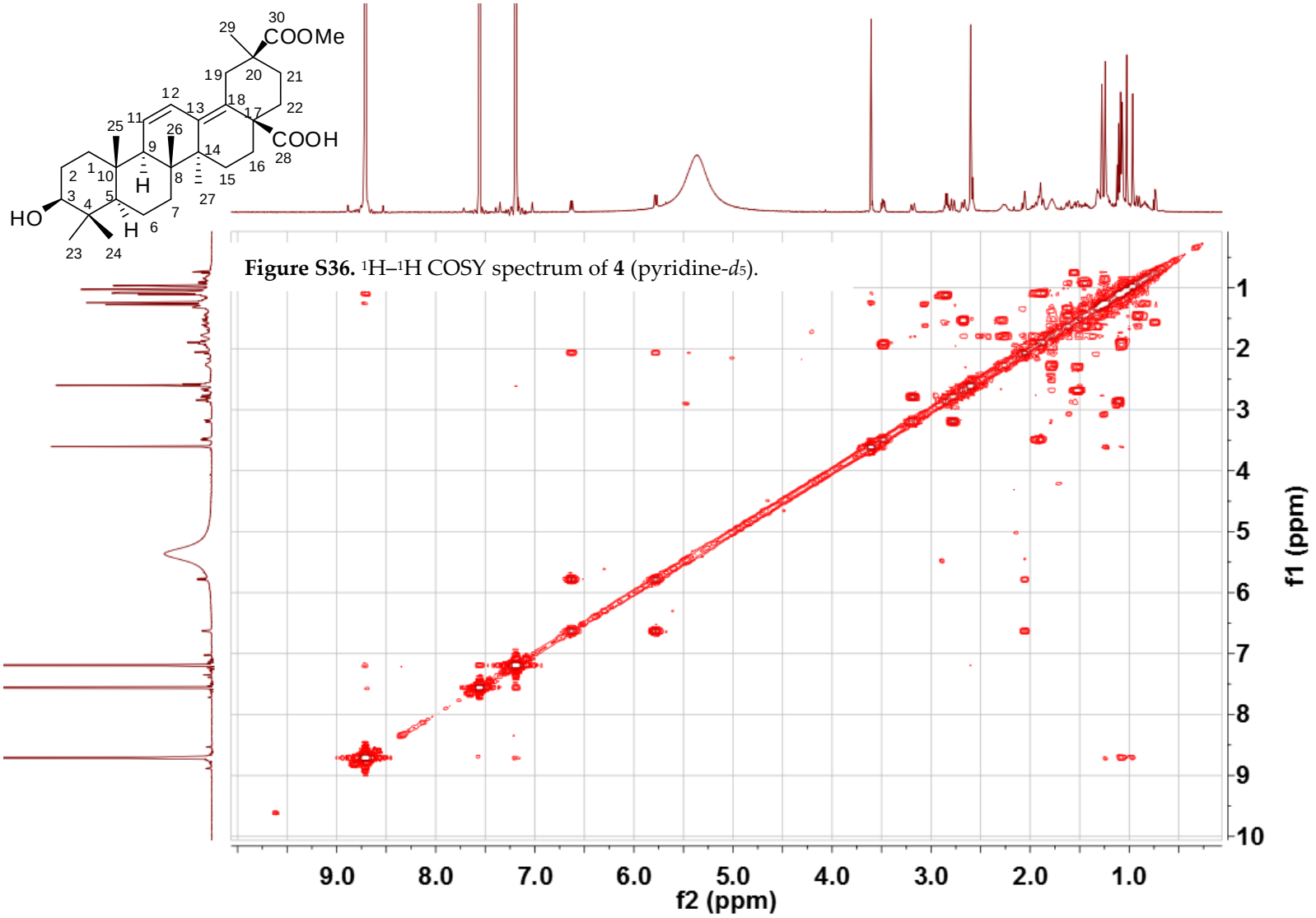


Figure S36. ^{1}H–^{1}H COSY spectrum of **4** (pyridine-d_5).

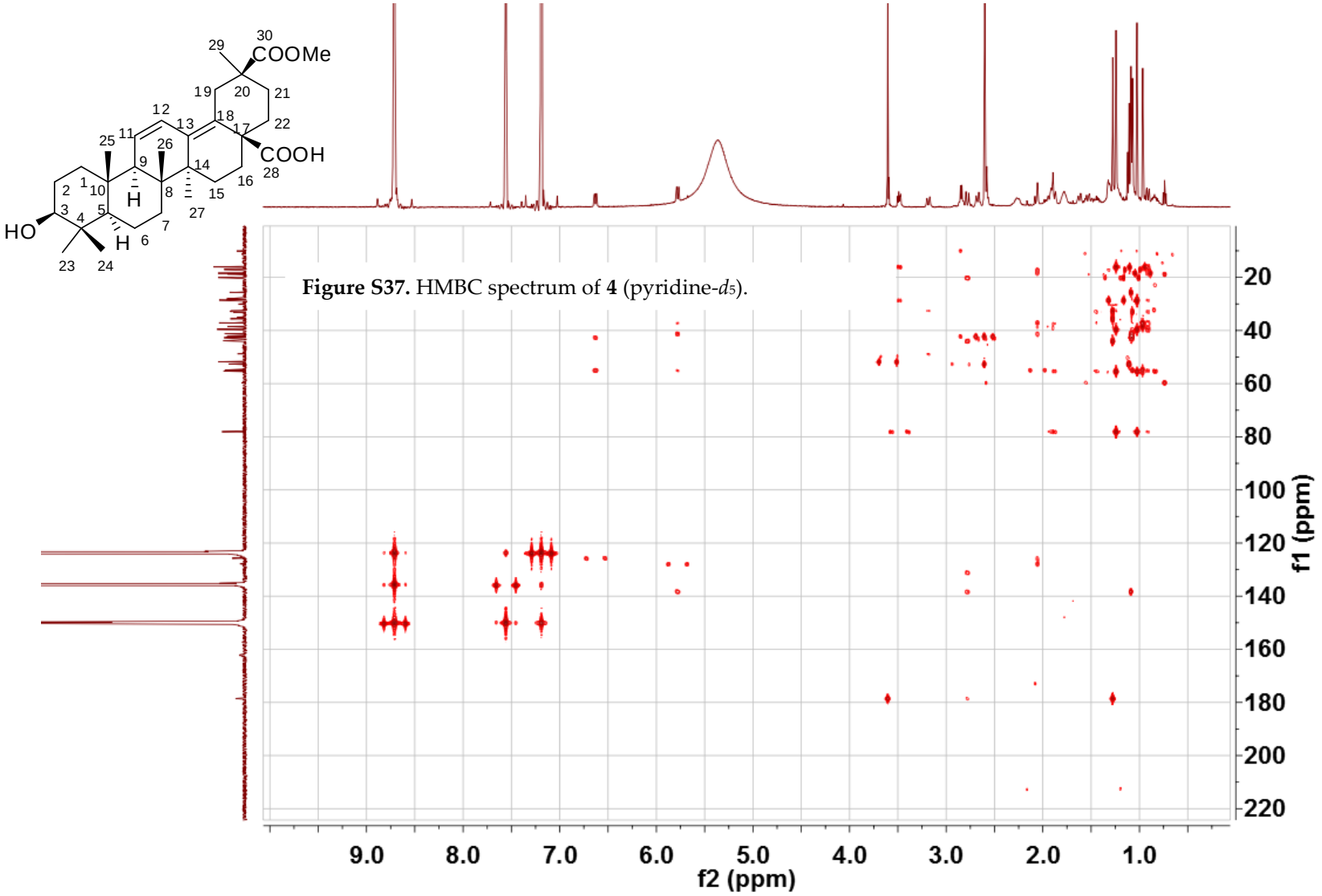


Figure S37. HMBC spectrum of **4** (pyridine-d_5).

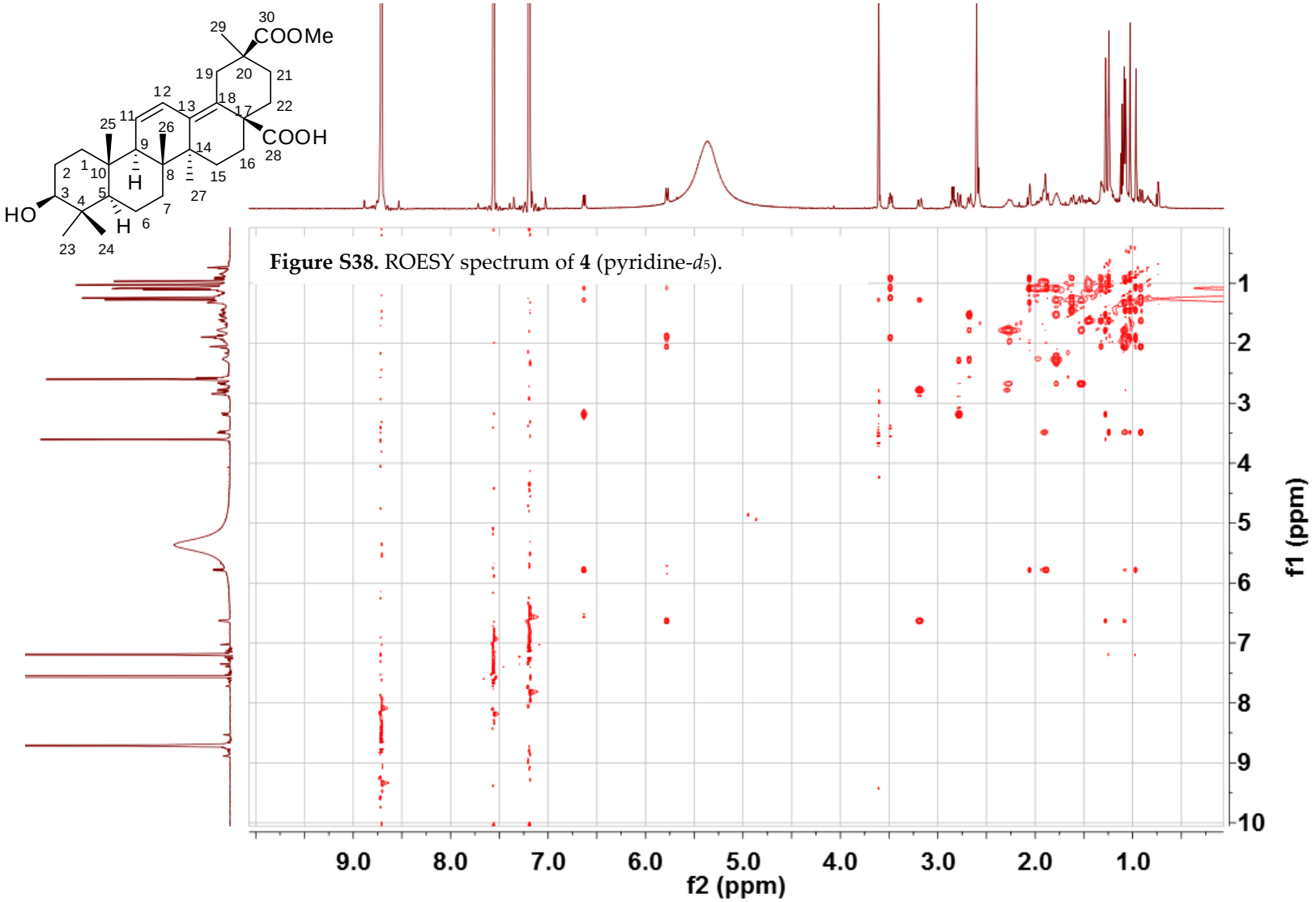


Figure S38. ROESY spectrum of **4** (pyridine-d_5).

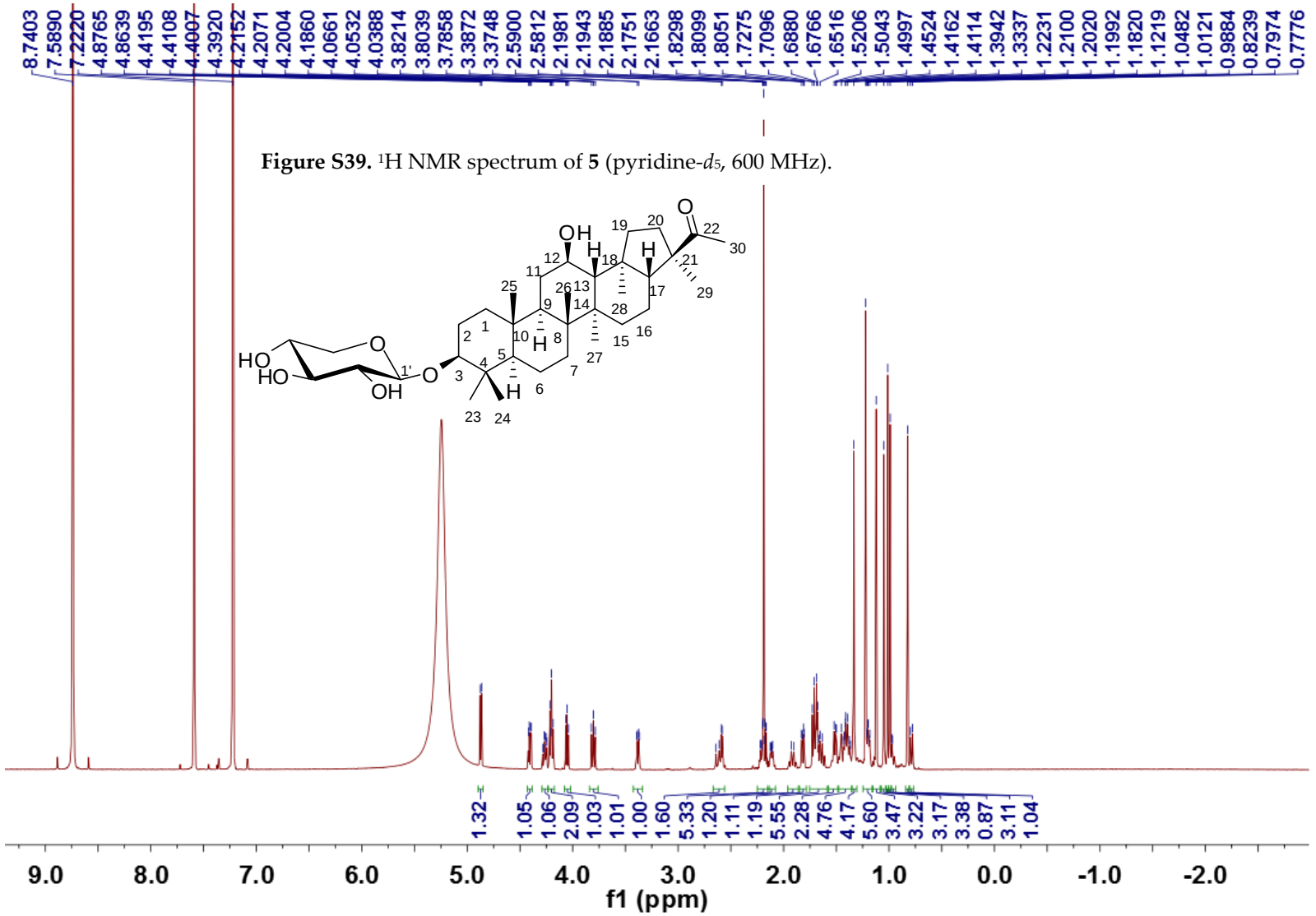


Figure S39. ^{1}H NMR spectrum of **5** (pyridine-d_5, 600 MHz).

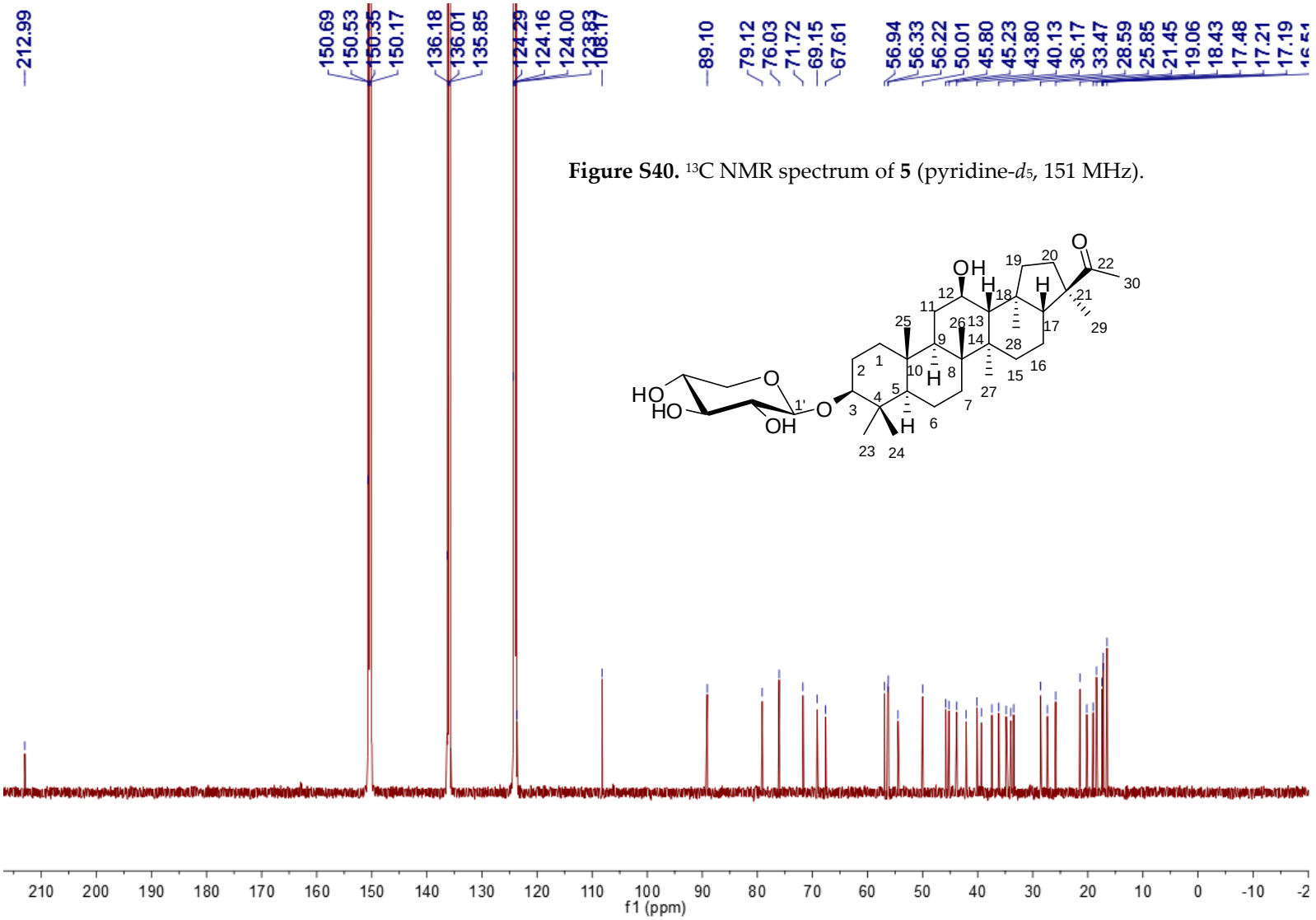
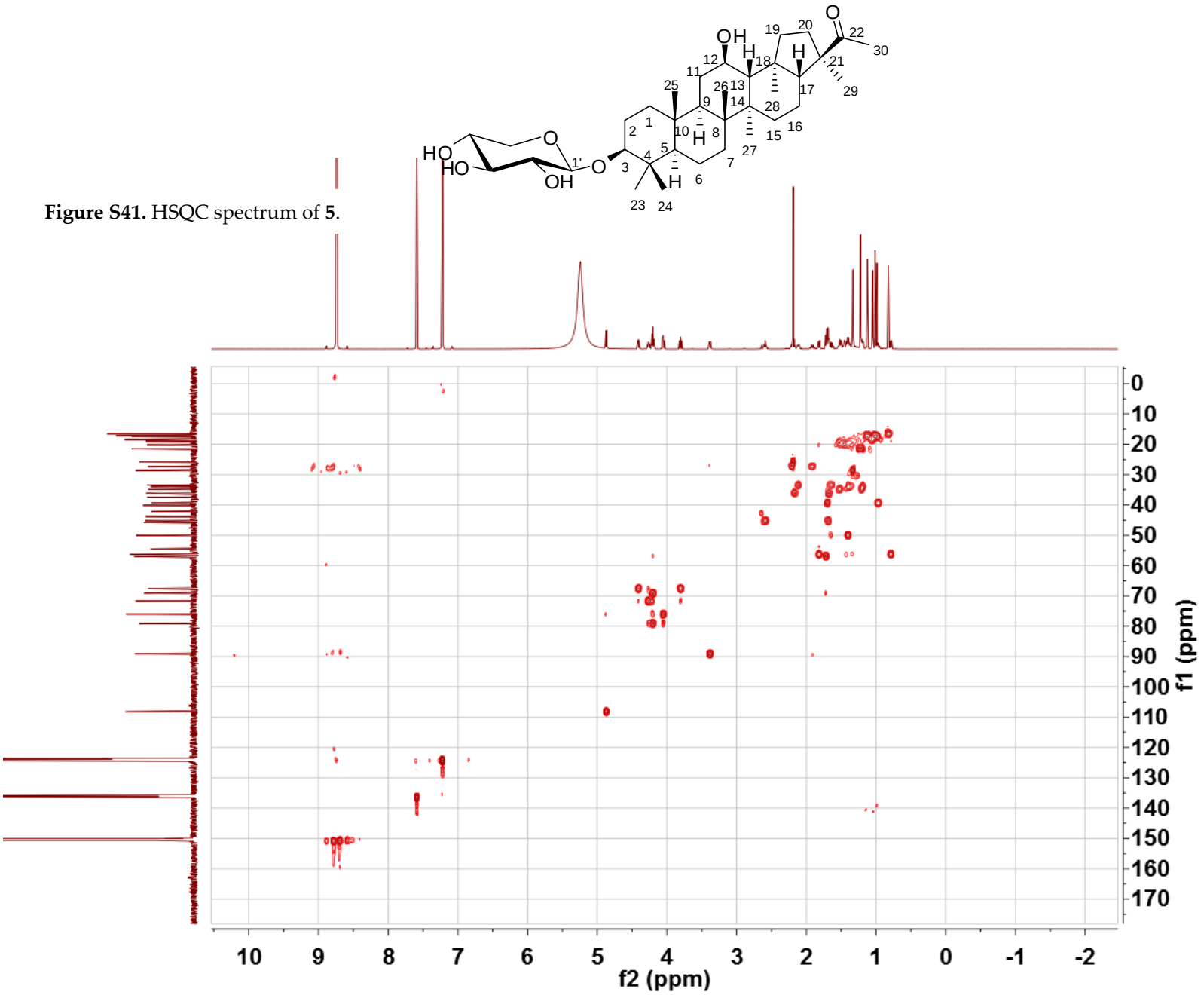


Figure S40. ^{13}C NMR spectrum of **5** (pyridine-d_5, 151 MHz).

Figure S41. HSQC spectrum of **5**.



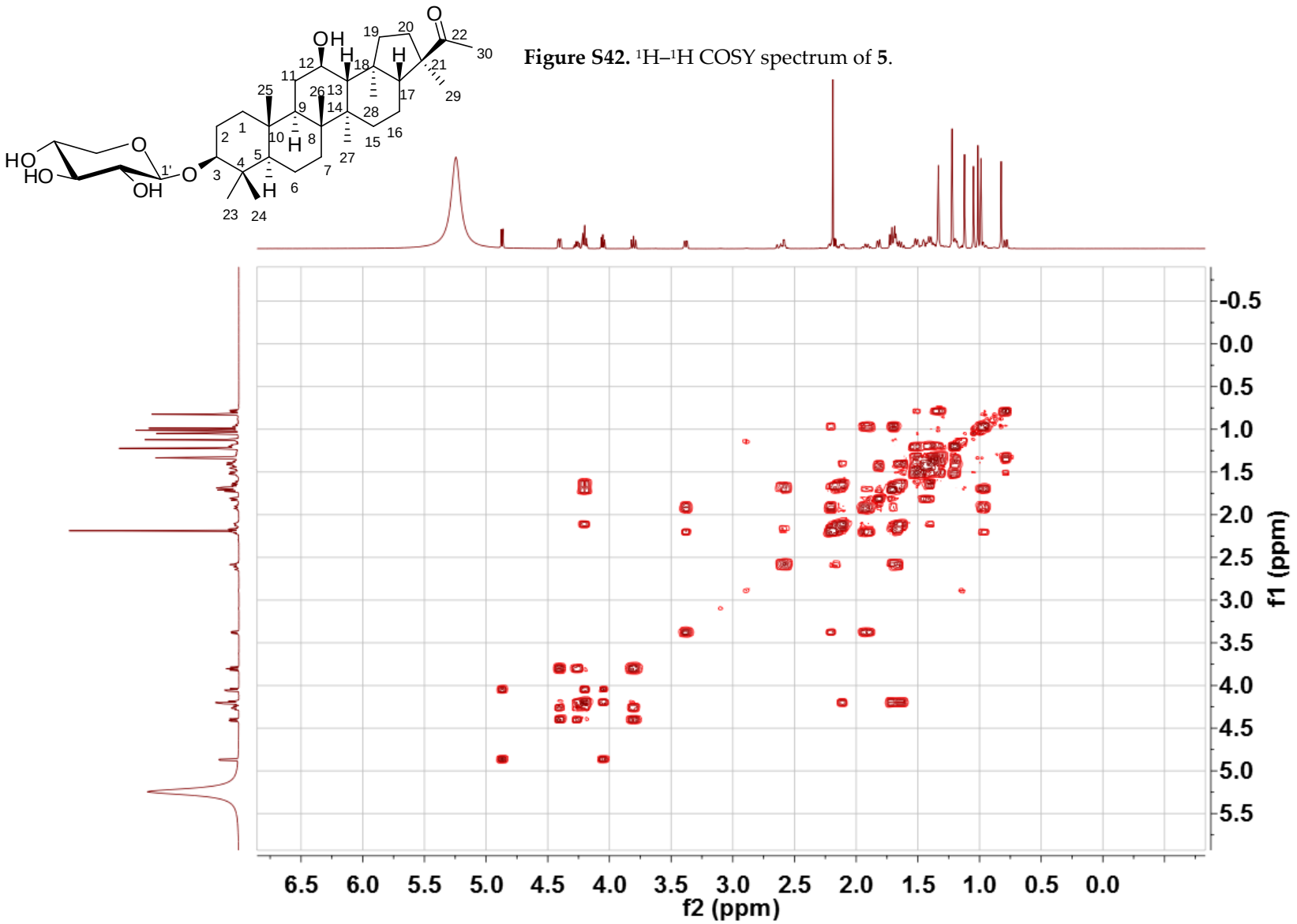


Figure S42. ^{1}H–^{1}H COSY spectrum of **5**.

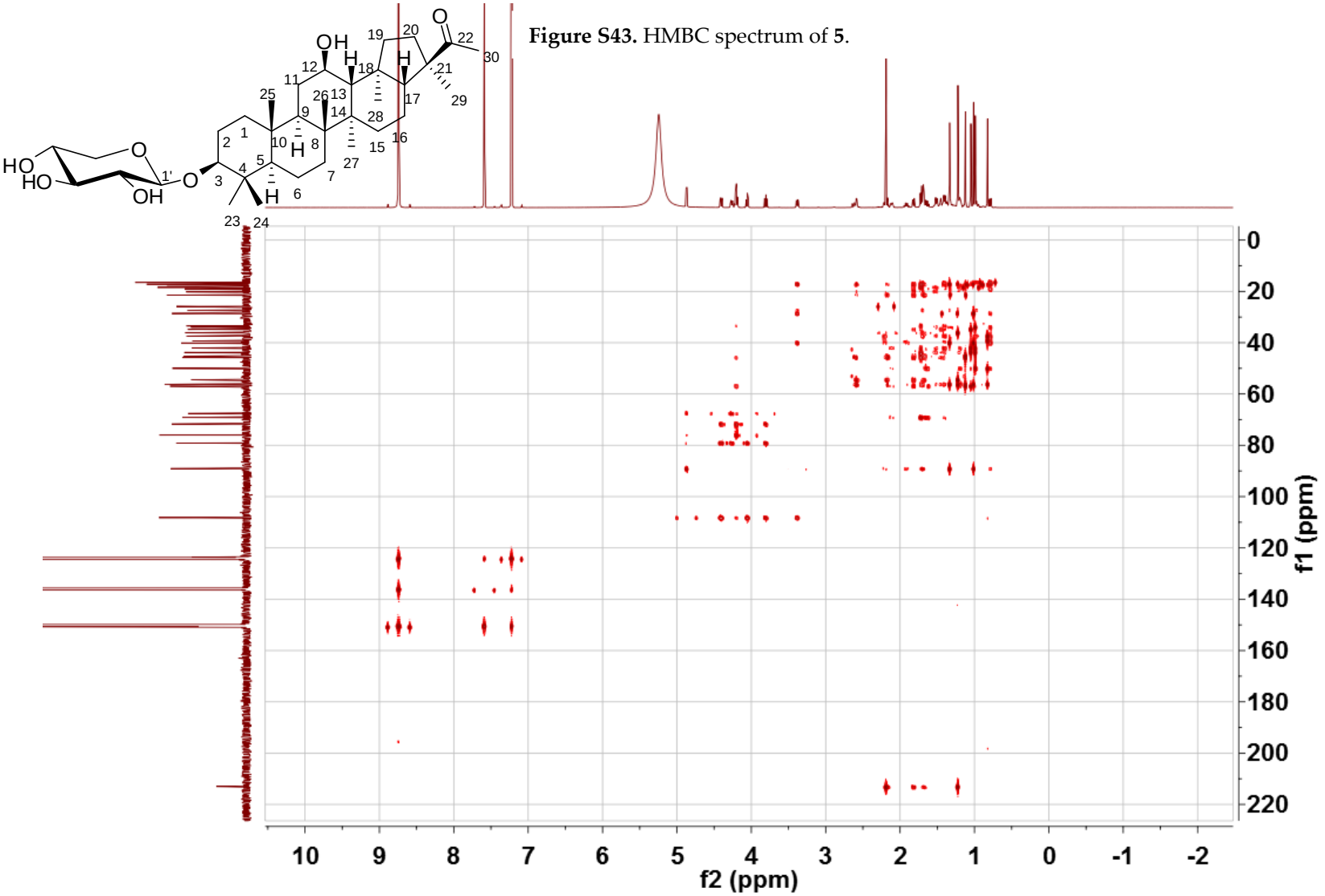


Figure S43. HMBC spectrum of **5**.

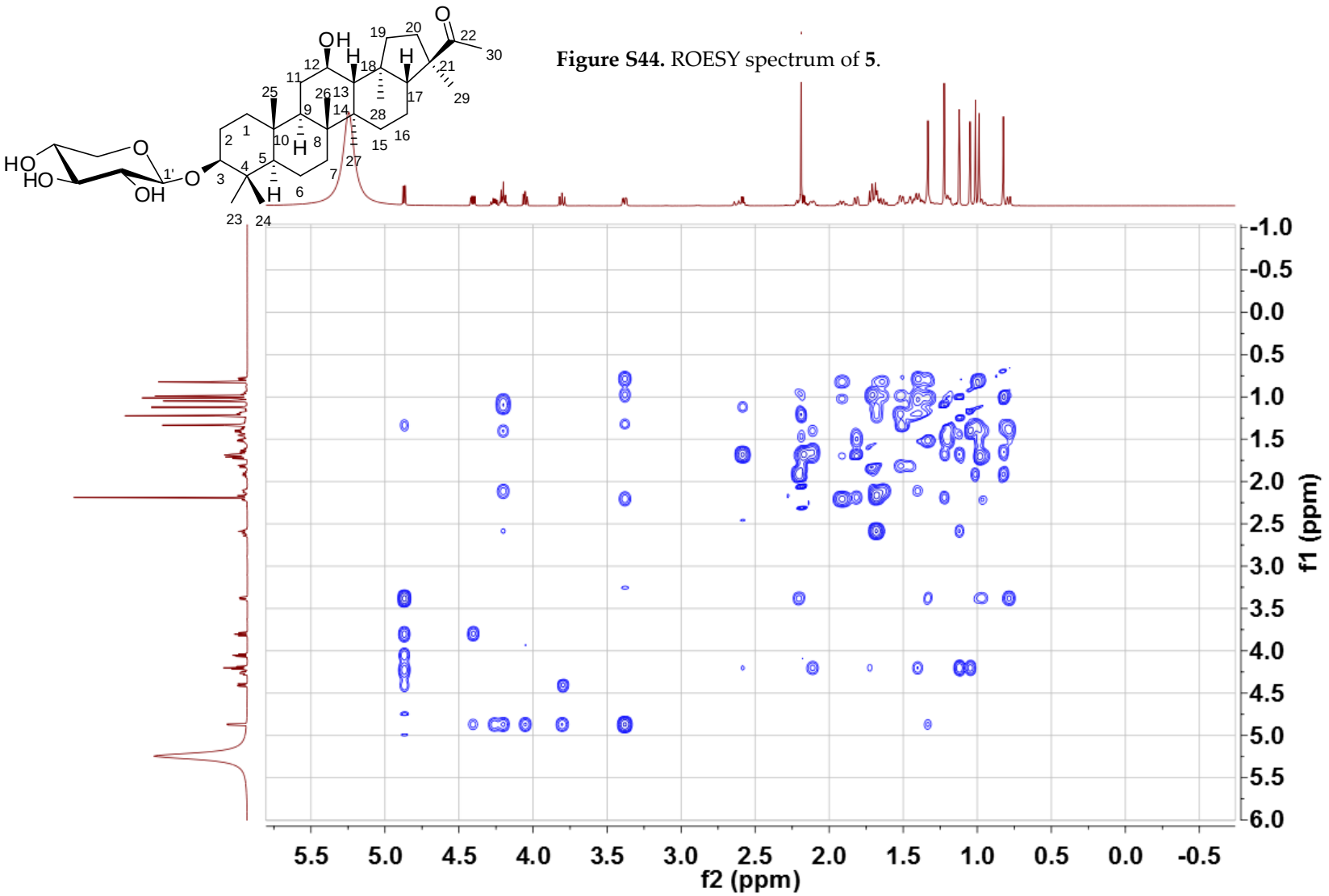


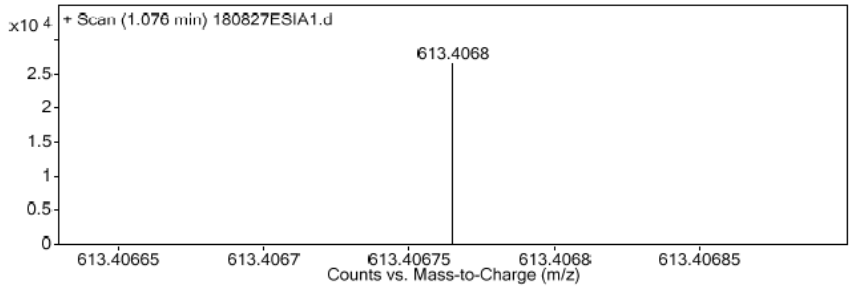
Figure S44. ROESY spectrum of **5**.

Data Filename	180827ESIA1.d	**Sample Name**	pdt54b
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/28/2018 9:54:22 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1278	1	67271.03		
111.1809		41545.32		
112.1872	1	204281.06		
144.2428		42565.64		
145.2492	1	218638.56		
146.2522	1	19284.63		
152.2175	1	23178.26		
368.4239	1	23795.48		
458.4712	1	25047.8		
613.4068	1	26485.34	C35 H58 Na O7	M+

Formula Calculator Element Limits

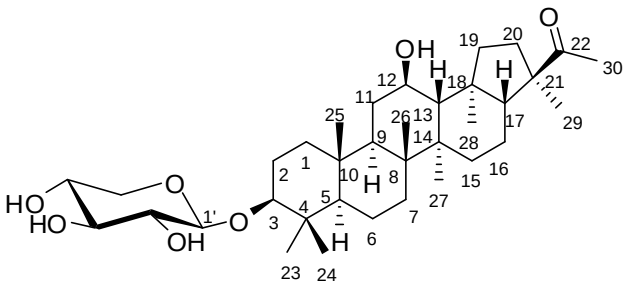
Element	Min	Max
C	0	200
H	0	400
O	3	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C35 H58 Na O7	613.4080	613.4068	1.2	2.0	6.5

--- End Of Report ---

Figure S45. HRESIMS spectrum of **5**.



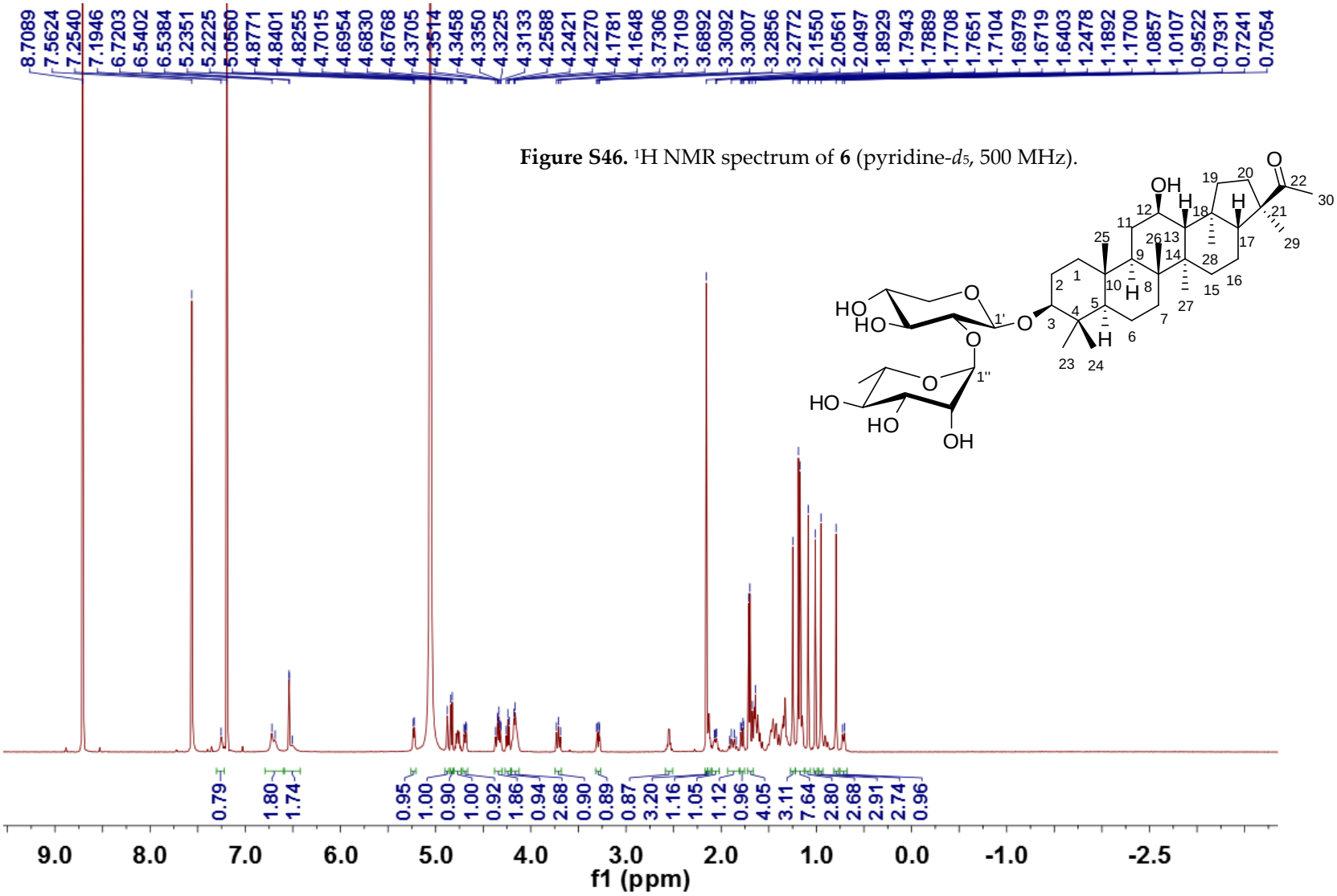


Figure S46. ^{1}H NMR spectrum of **6** (pyridine-d_5, 500 MHz).

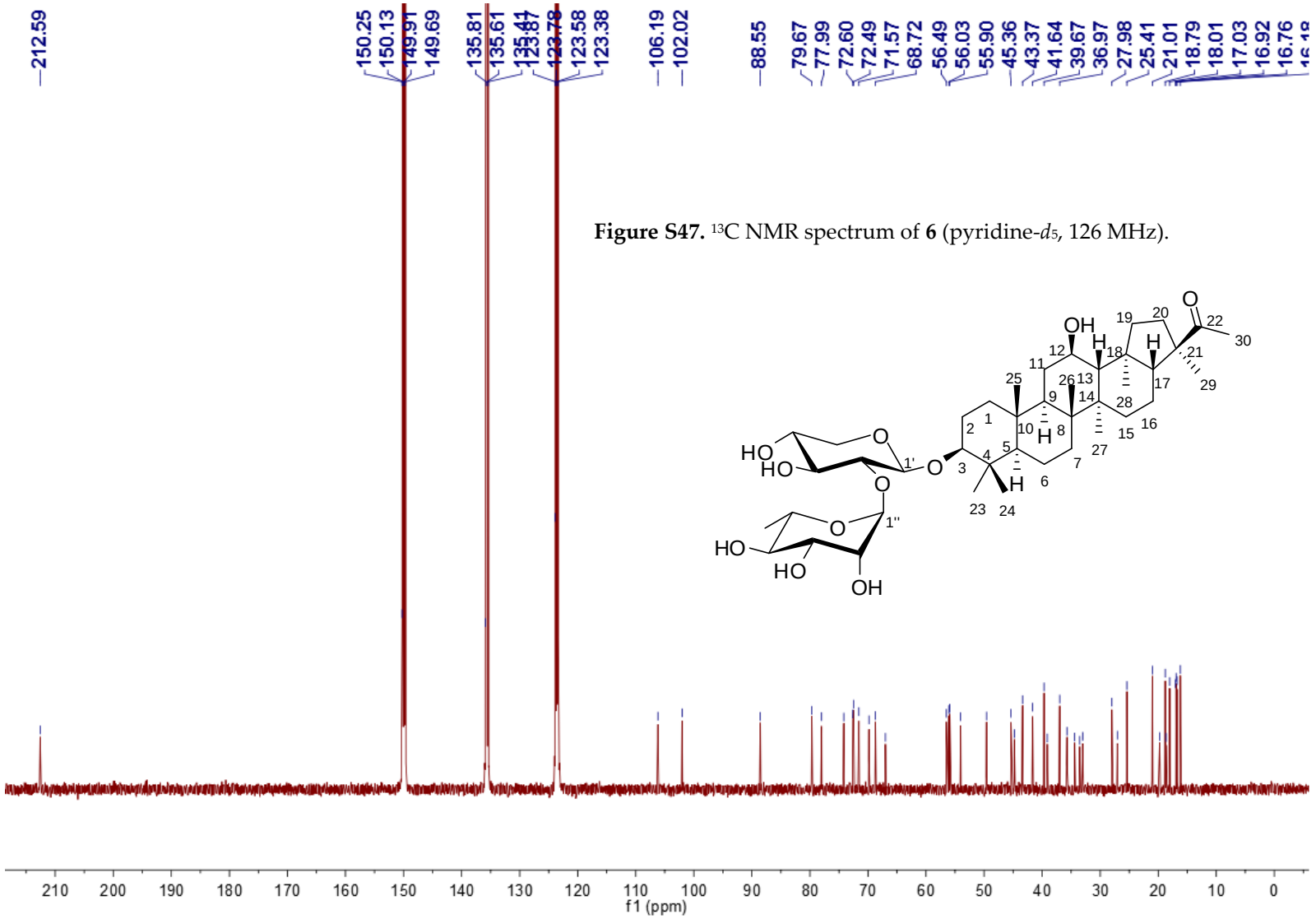


Figure S47. ^{13}C NMR spectrum of **6** (pyridine-d_5, 126 MHz).

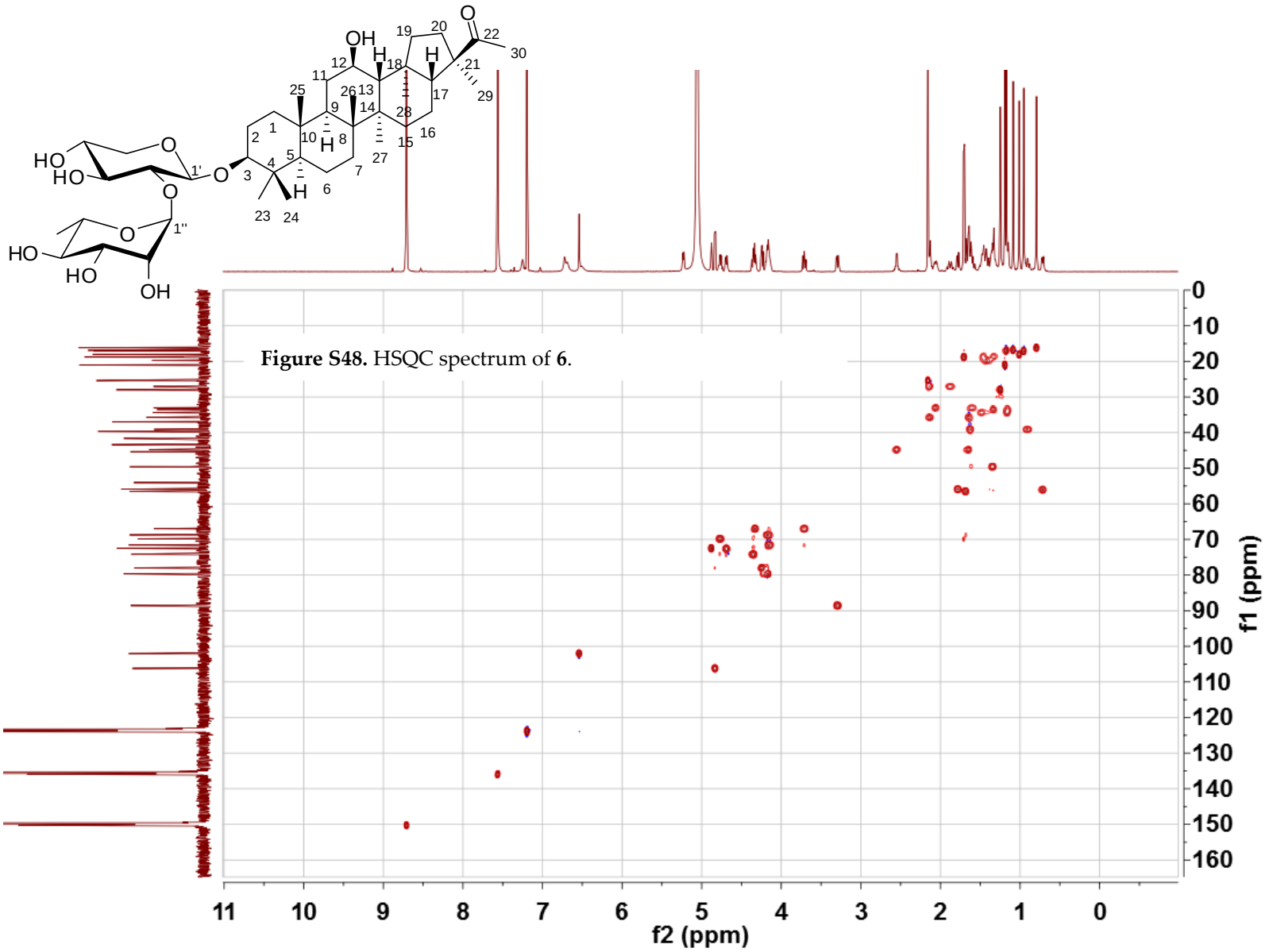


Figure S48. HSQC spectrum of **6**.

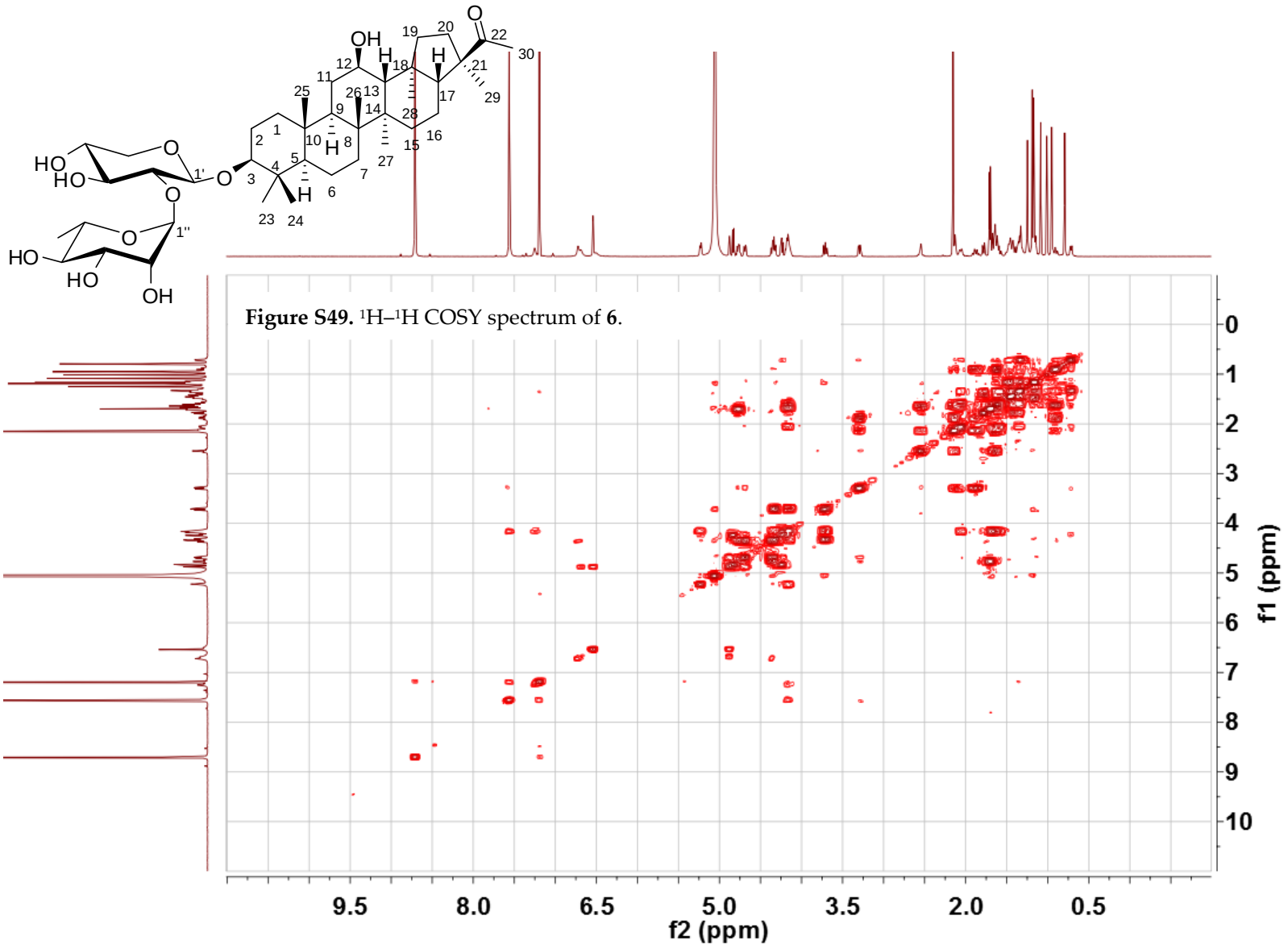


Figure S49. ^{1}H–^{1}H COSY spectrum of **6**.

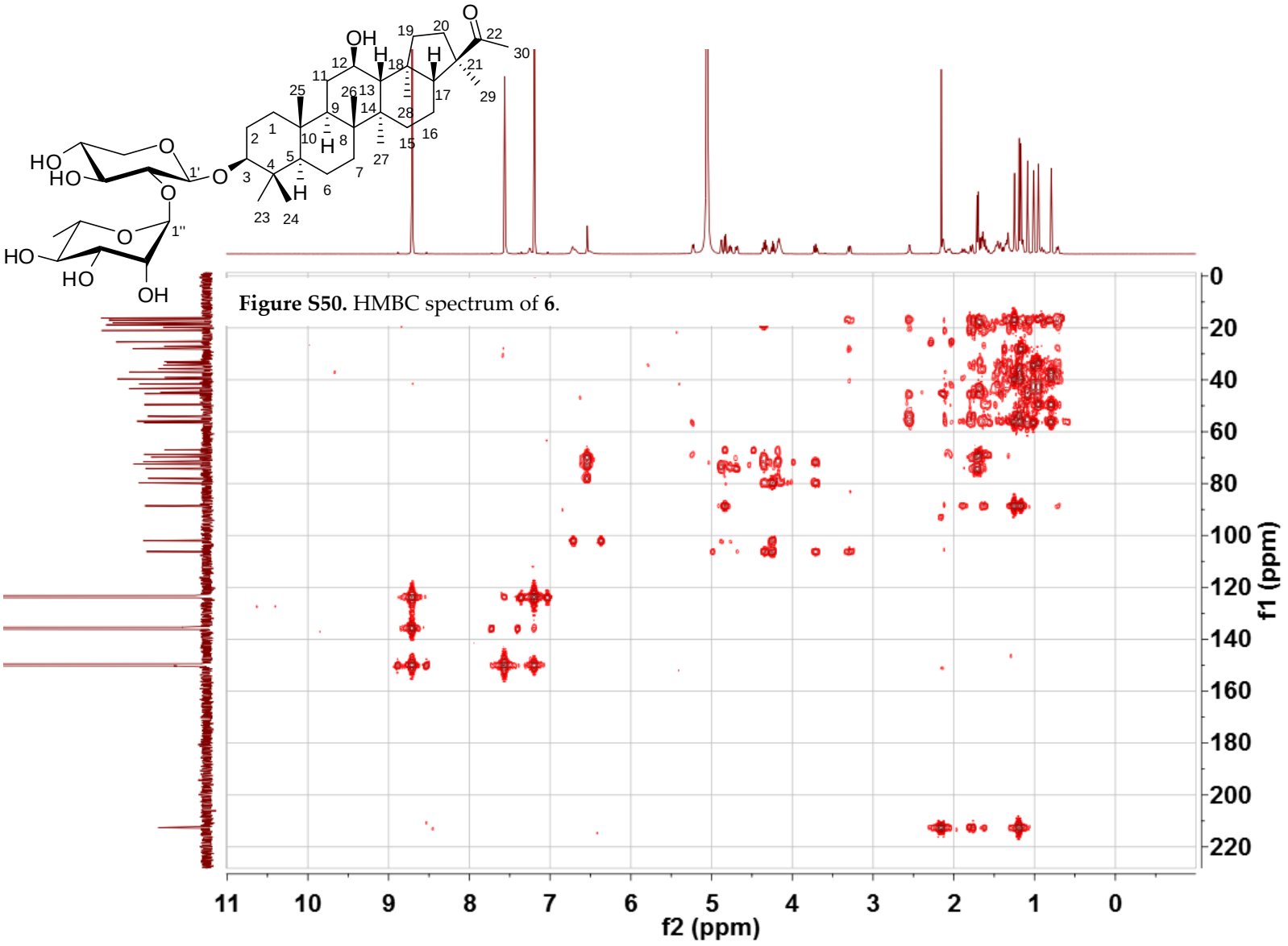


Figure S50. HMBC spectrum of **6**.

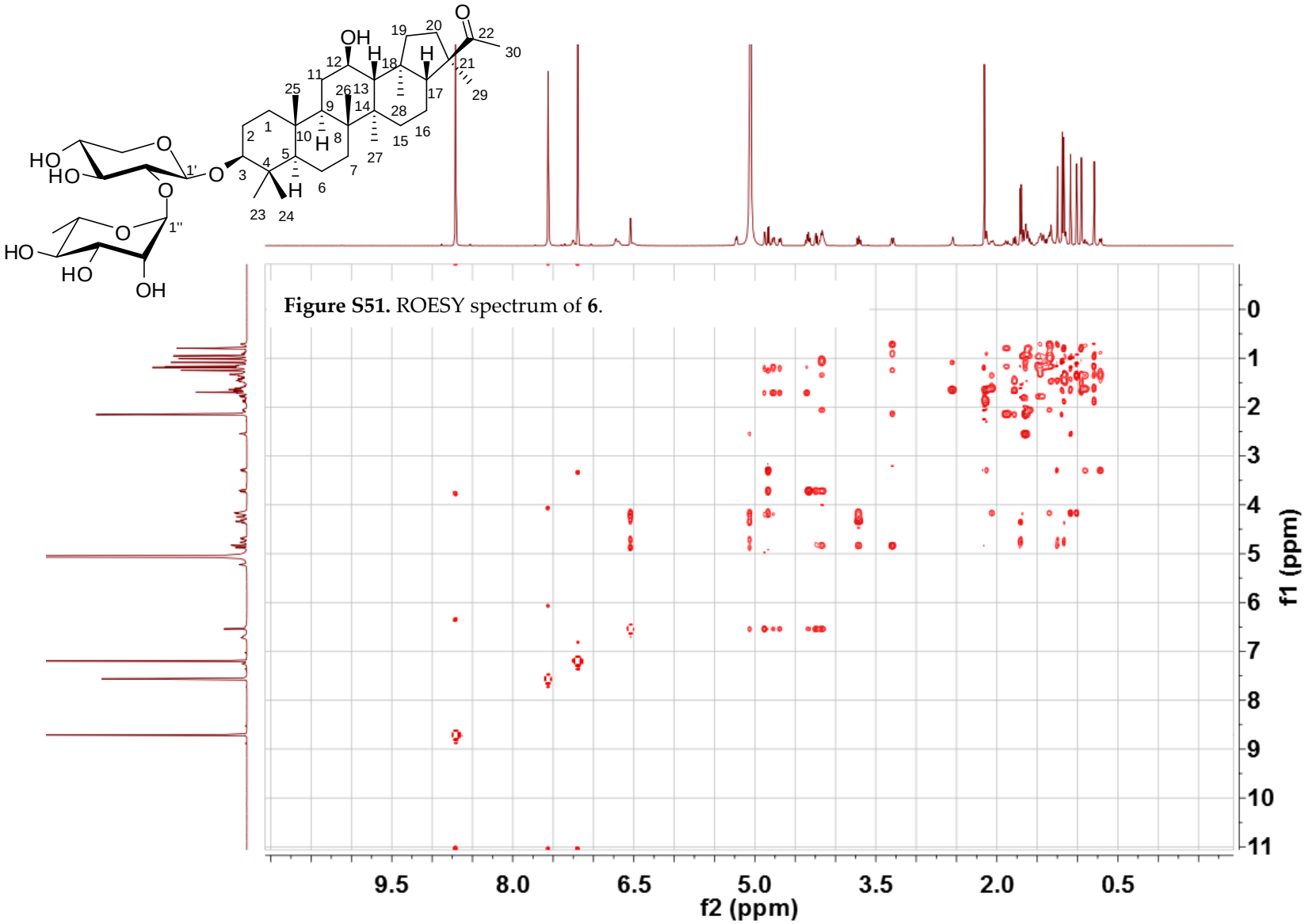


Figure S51. ROESY spectrum of **6**.

Data Filename	180828ESIA4.d	**Sample Name**	pdt52
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/28/2018 9:57:33 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

Figure S52. HRESIMS spectrum of **6**.

Peak List

m/z	z	Abund	Formula	Ion
274.2733	1	108594.22		
318.2996	1	104633.04		
340.2813	1	47140.76		
362.3255	1	30291.13		
384.3068	1	25858.5		
759.465	1	267465.66	C41 H68 Na O11	M+
760.4678	1	114278.83	C41 H68 Na O11	M+
761.4691	1	27402.06	C41 H68 Na O11	M+
775.438	1	42564.01		
1496.9424	2	24183.79		

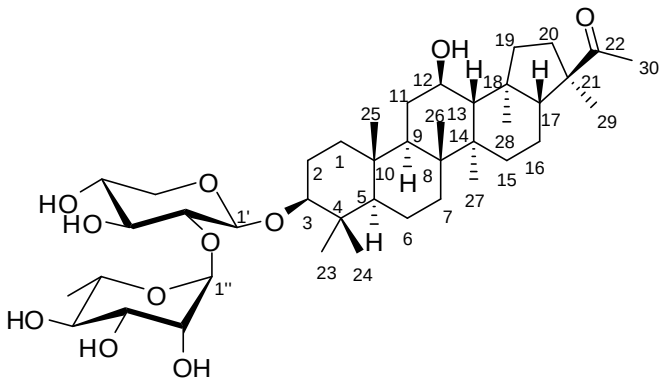
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C41 H68 Na O11	759.4659	759.4650	0.9	1.2	7.5

--- End Of Report ---



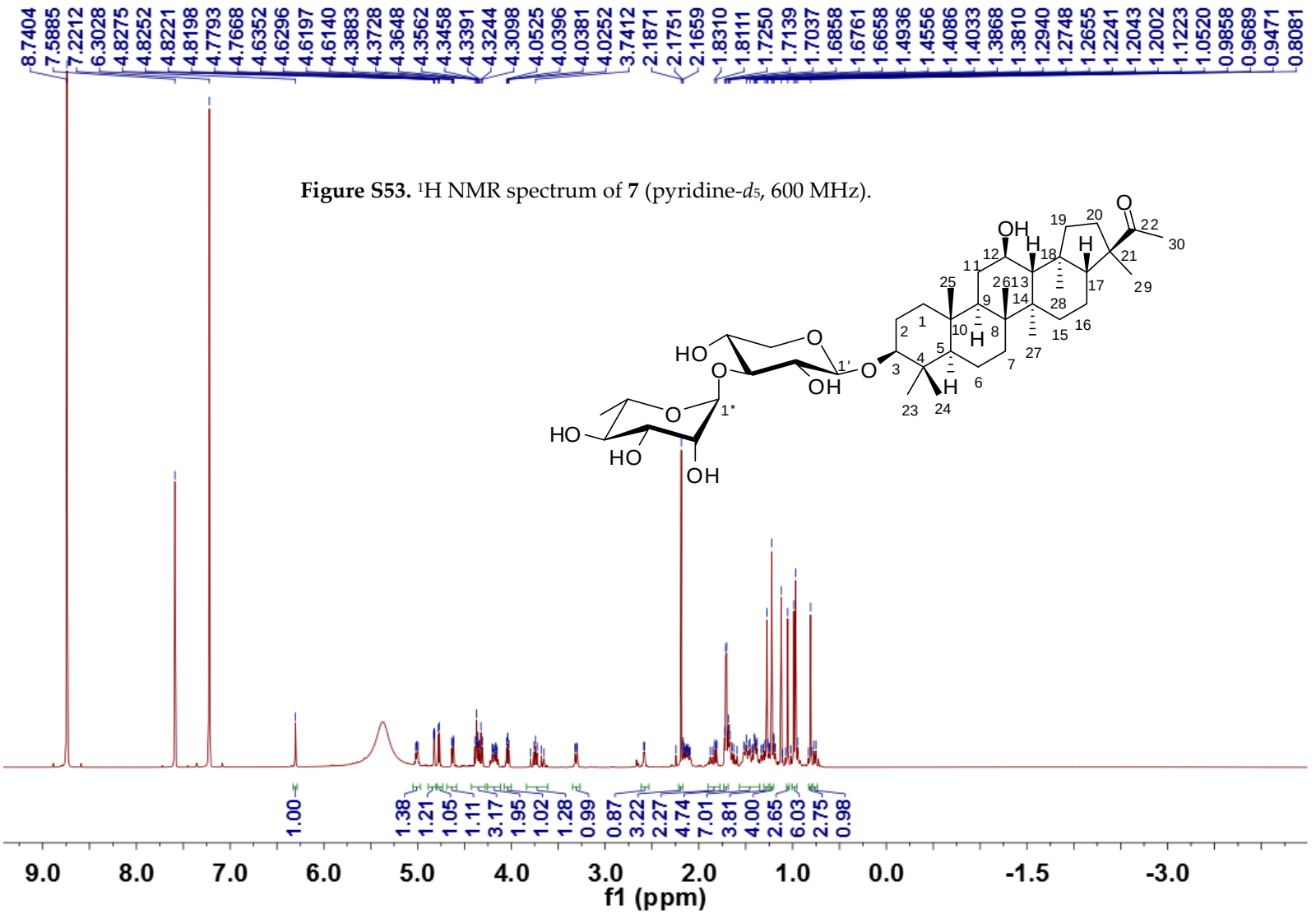


Figure S53. ^{1}H NMR spectrum of **7** (pyridine-d_5, 600 MHz).

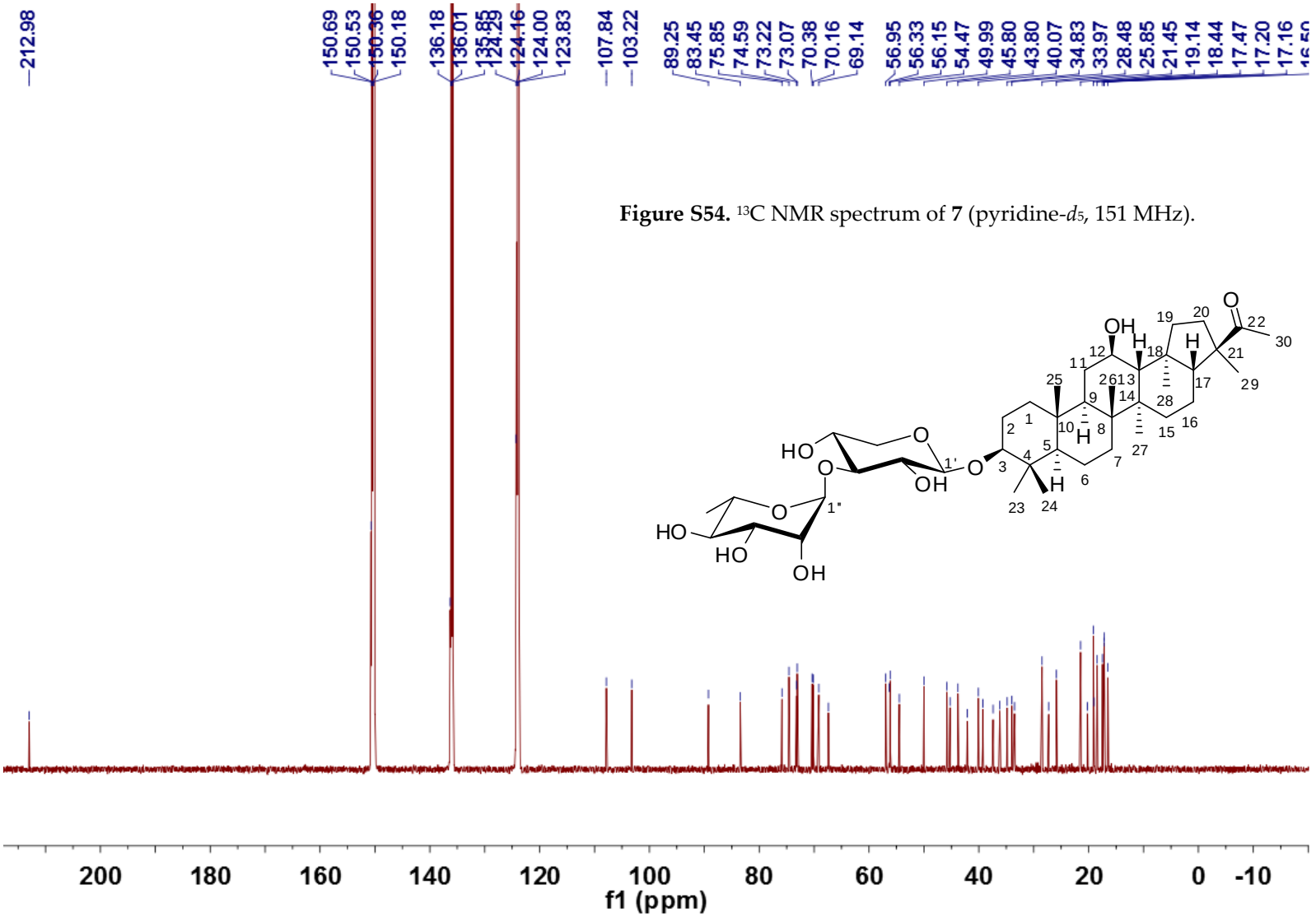


Figure S54. ^{13}C NMR spectrum of **7** (pyridine-d_5, 151 MHz).

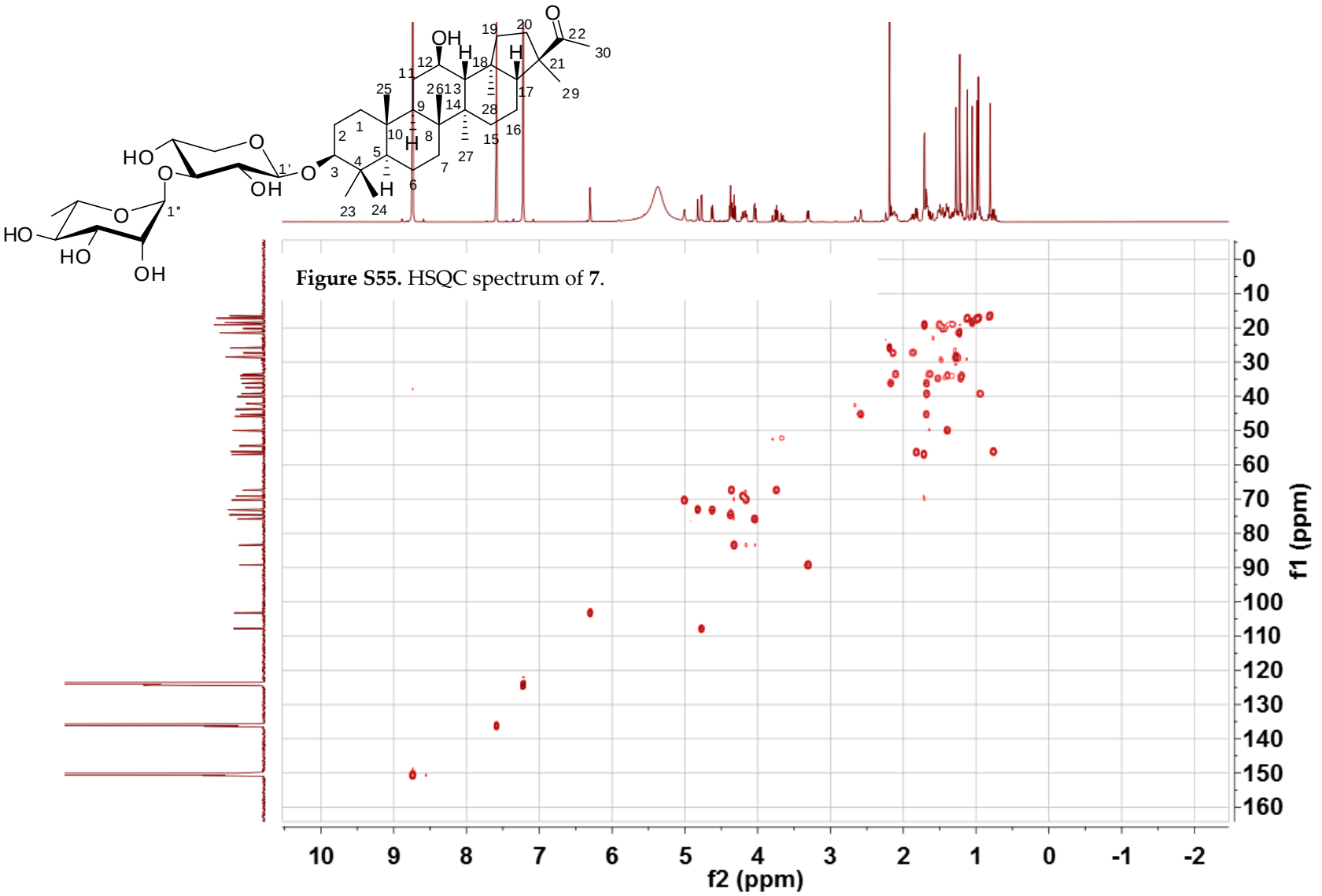


Figure S55. HSQC spectrum of **7**.

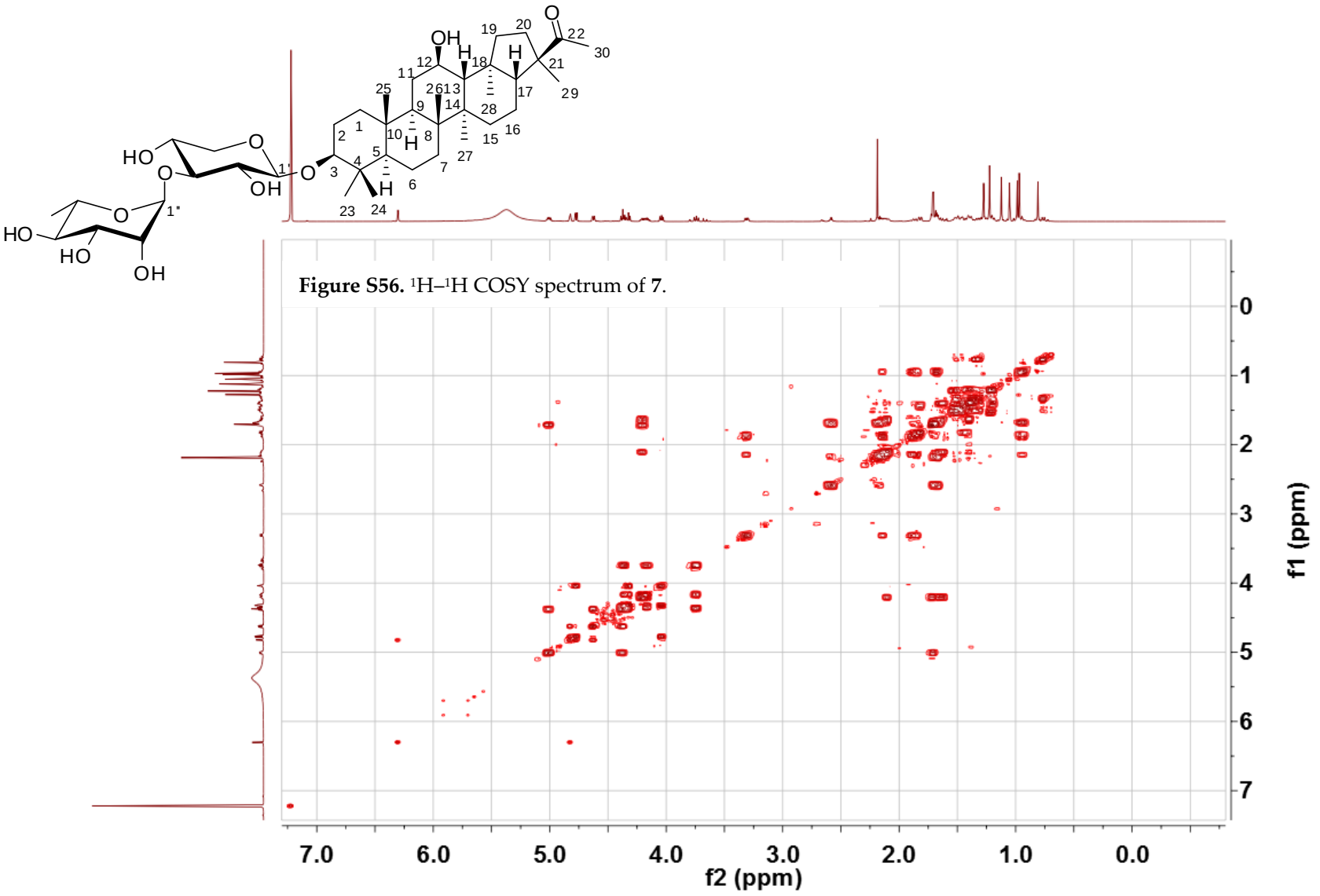


Figure S56. ^{1}H–^{1}H COSY spectrum of **7**.

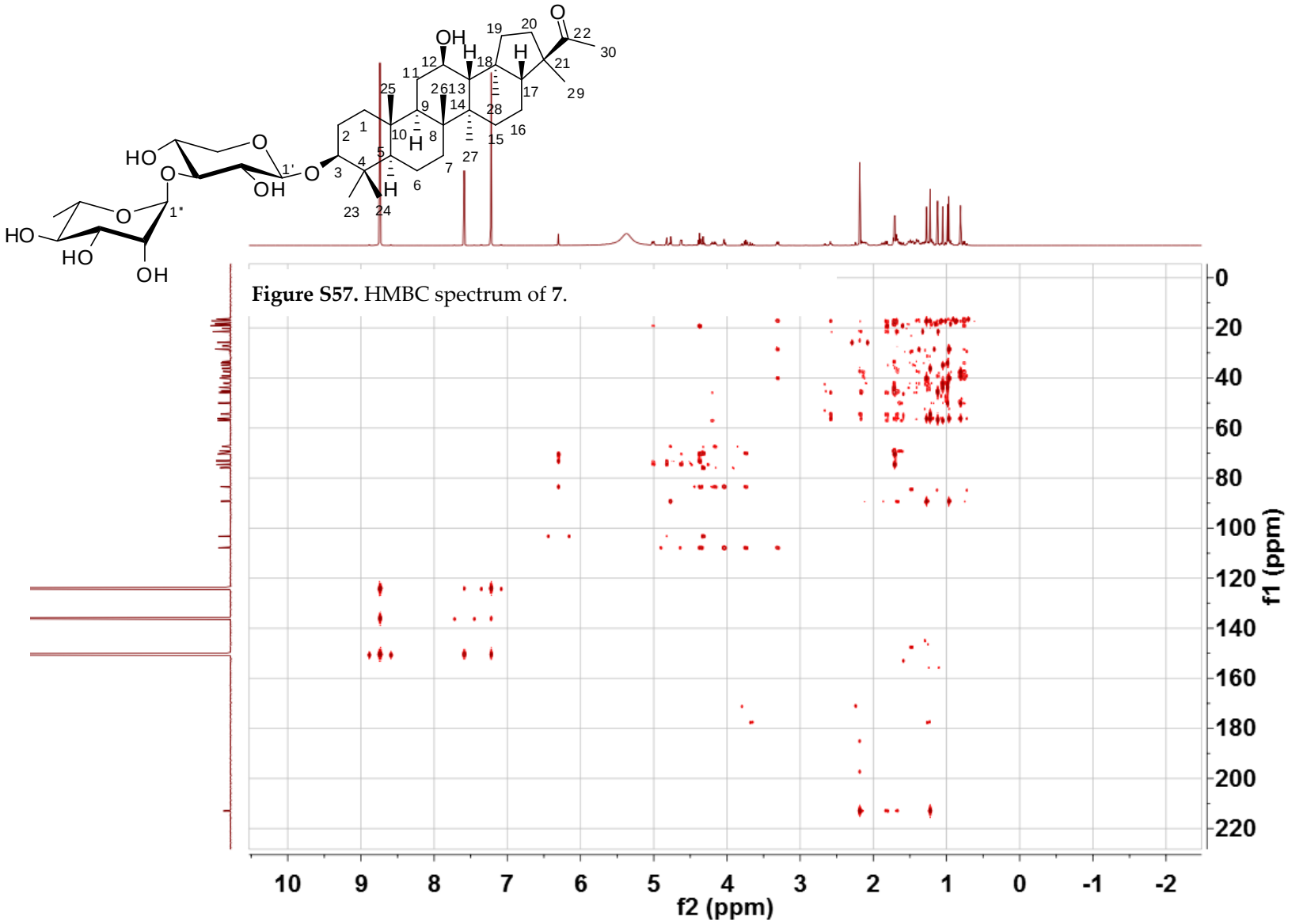


Figure S57. HMBC spectrum of **7**.

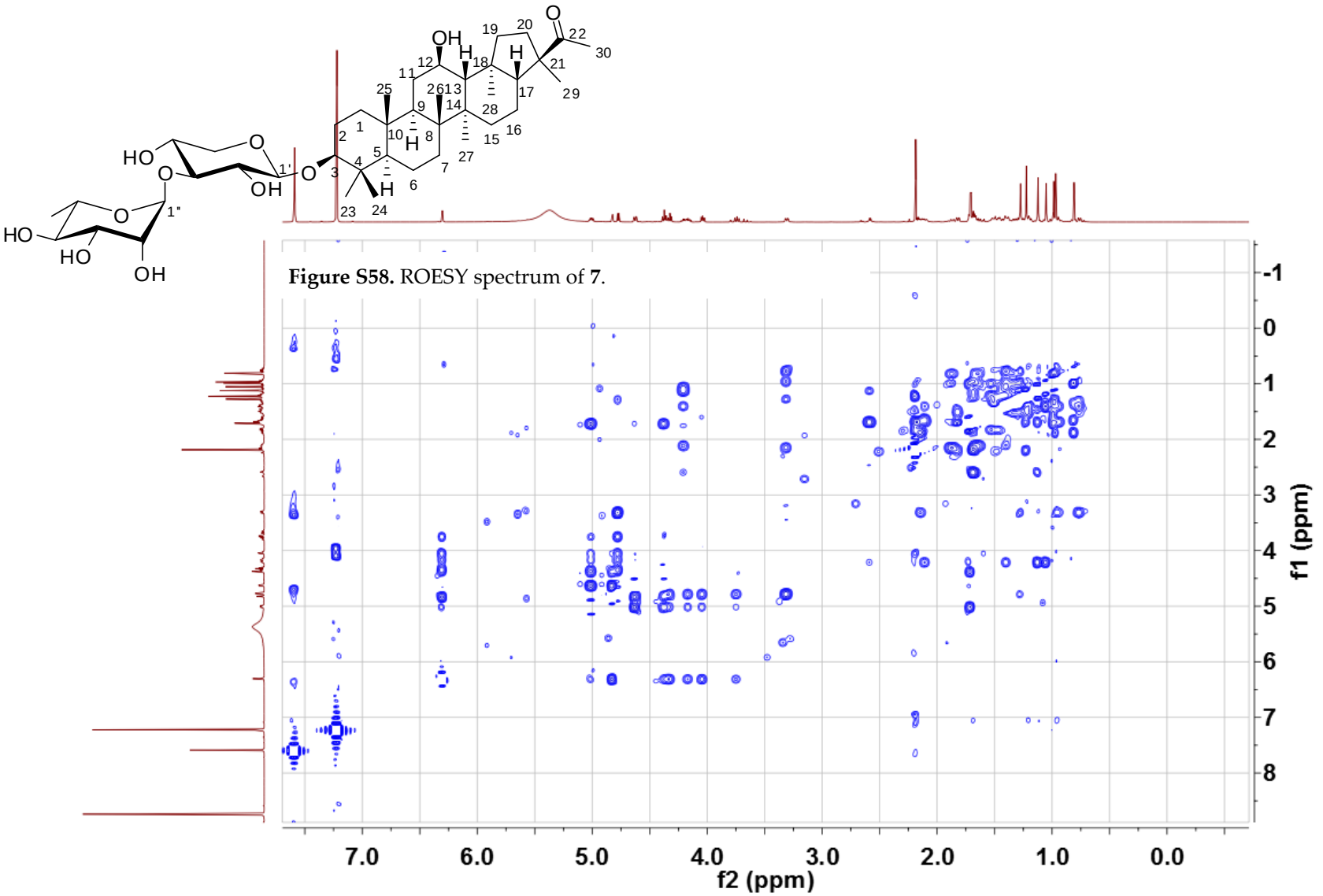


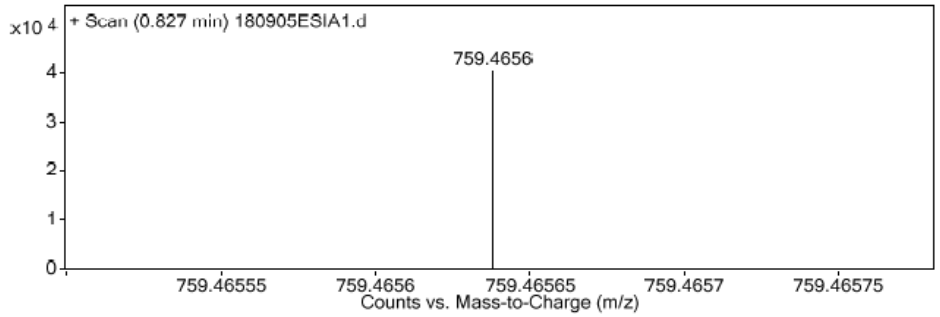
Figure S58. ROESY spectrum of **7**.

Data Filename	180905ESIA1.d	**Sample Name**	pdt55a
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	9/5/2018 9:29:38 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
105.0429	1	33201.03		
112.1875	1	32109.09		
118.1227		15357.97		
121.0509		187790.47		
759.4656	1	40396.77	C41 H68 Na O11	M+
760.4691	1	18545.26	C41 H68 Na O11	M+
922.0098	1	81067		
923.012	1	15091.32		
1495.9385	1	16909.07		
1496.9434	1	14735.45		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C41 H68 Na O11	759.4659	759.4656	0.3	0.4	7.5

--- End Of Report ---

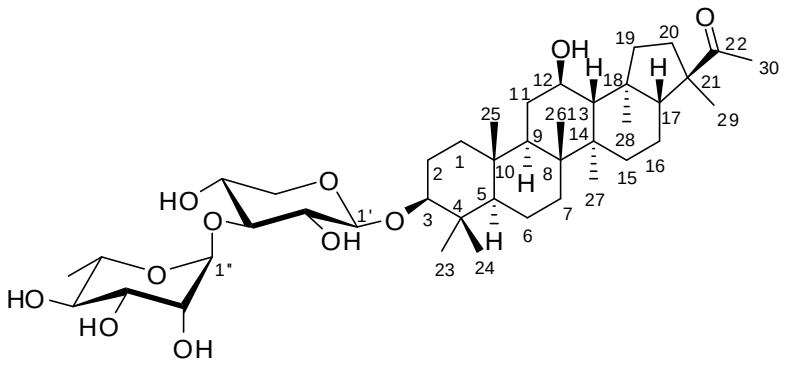


Figure S59. HRESIMS spectrum of **7**.

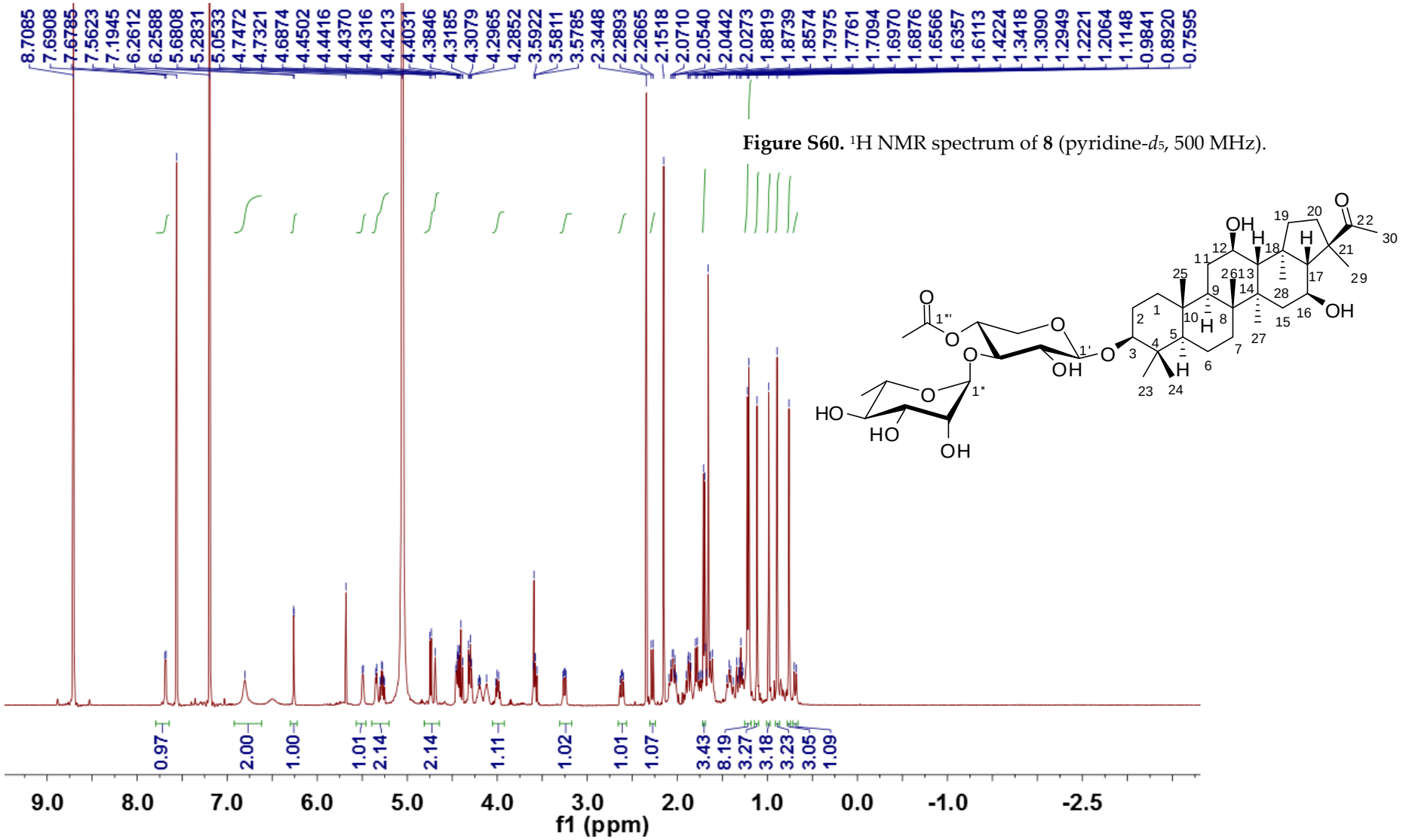


Figure S60. ^{1}H NMR spectrum of **8** (pyridine-d_5, 500 MHz).

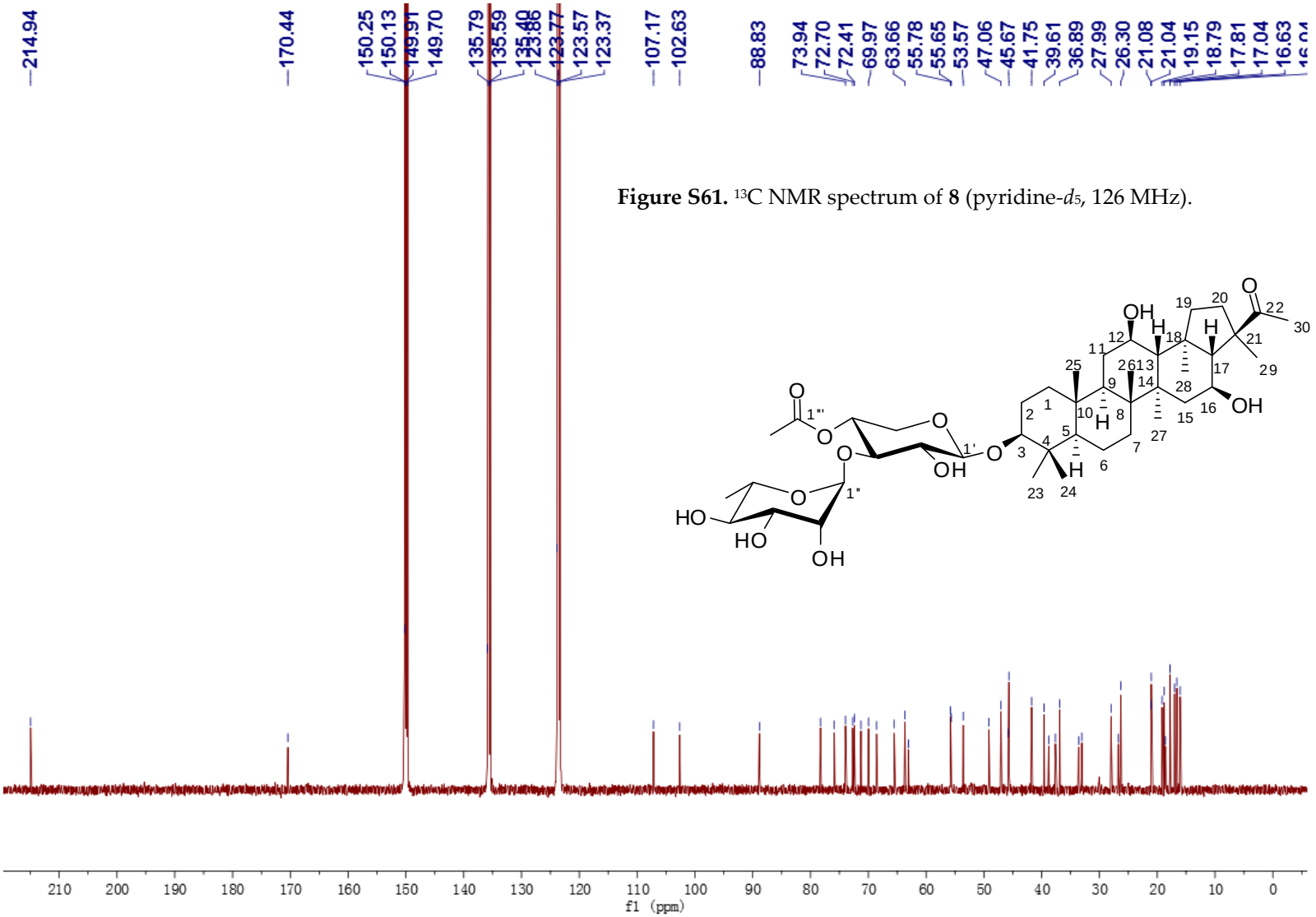


Figure S61. ^{13}C NMR spectrum of **8** (pyridine-d_5, 126 MHz).

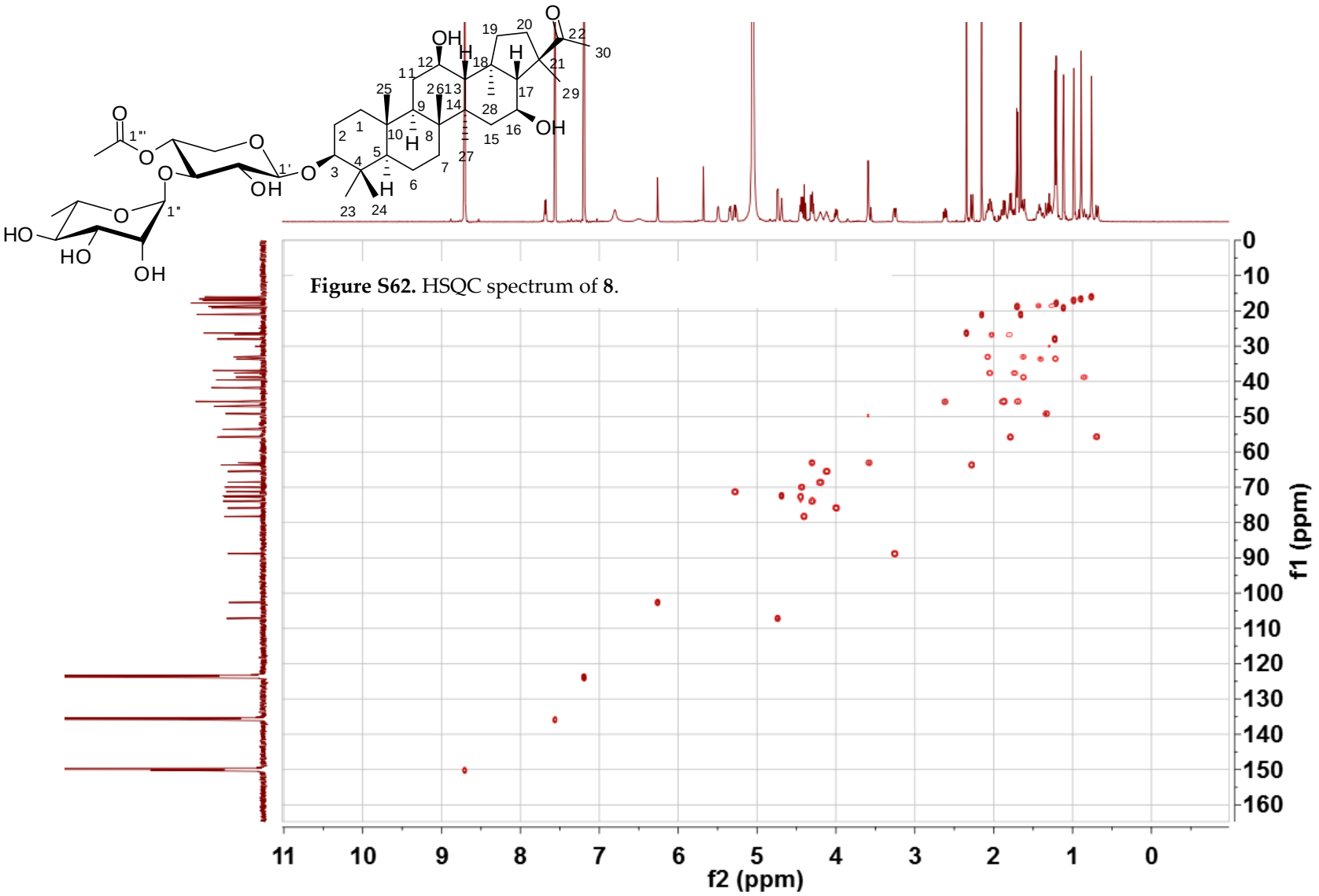


Figure S62. HSQC spectrum of **8**.

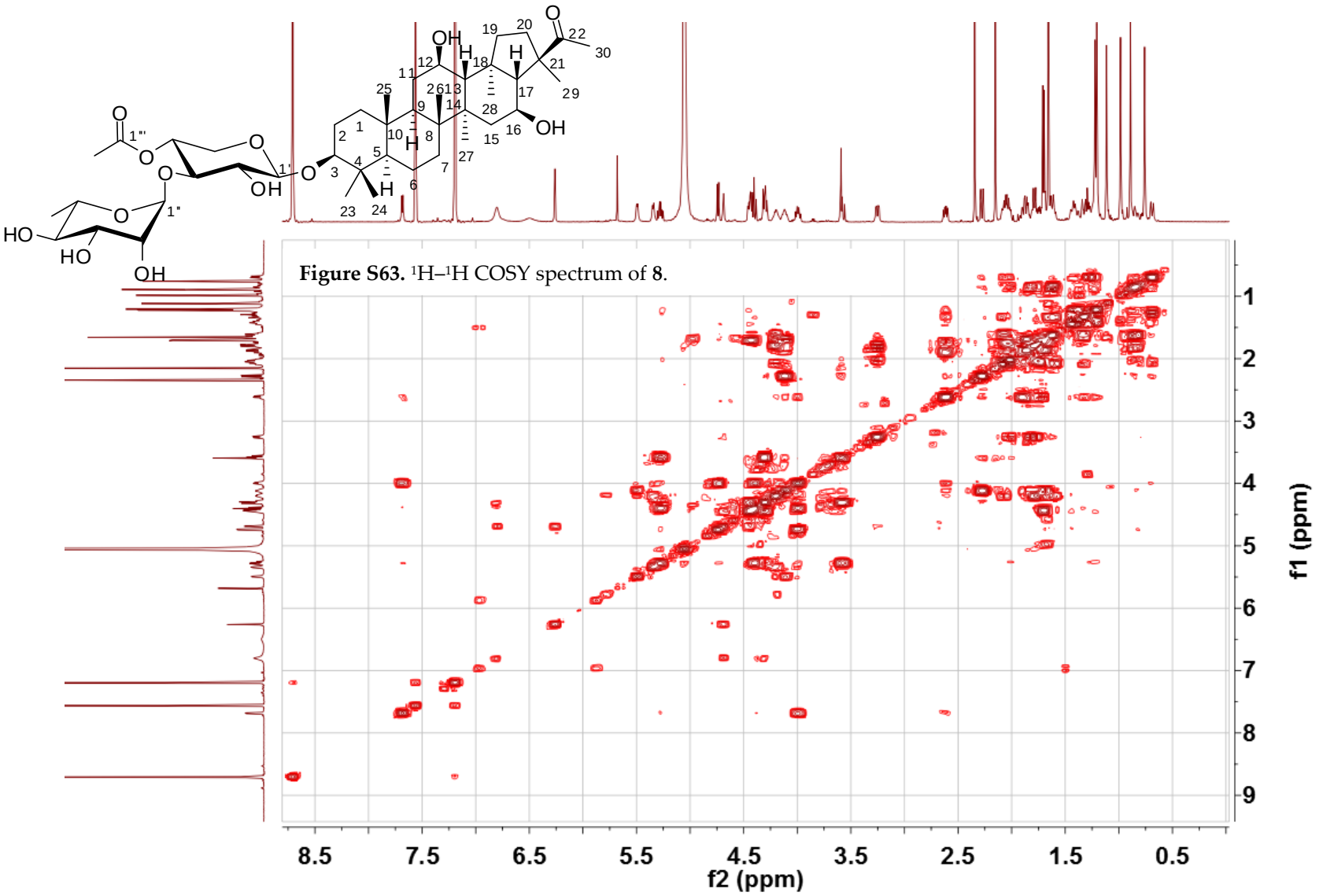


Figure S63. ^{1}H–^{1}H COSY spectrum of **8**.

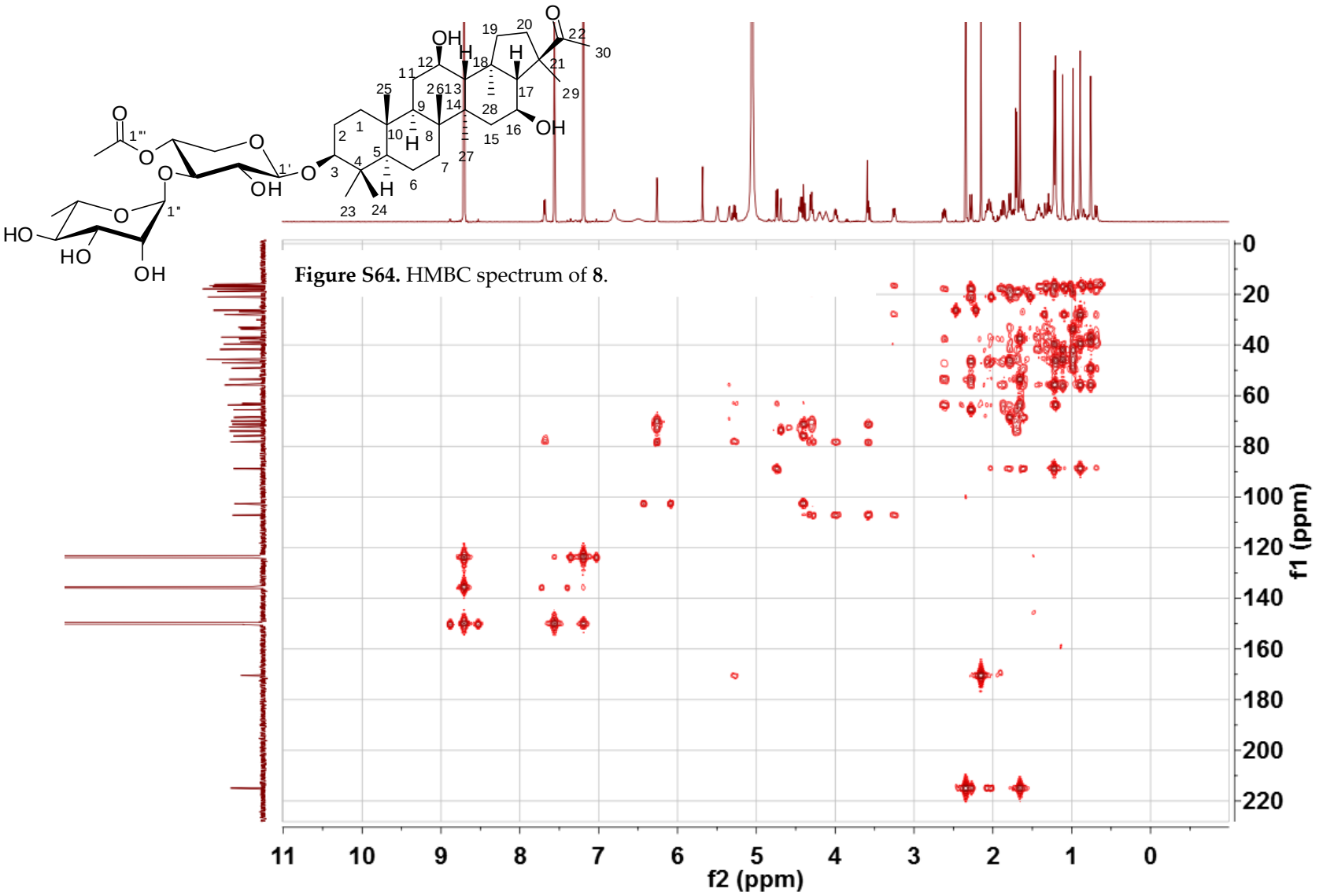


Figure S64. HMBC spectrum of **8**.

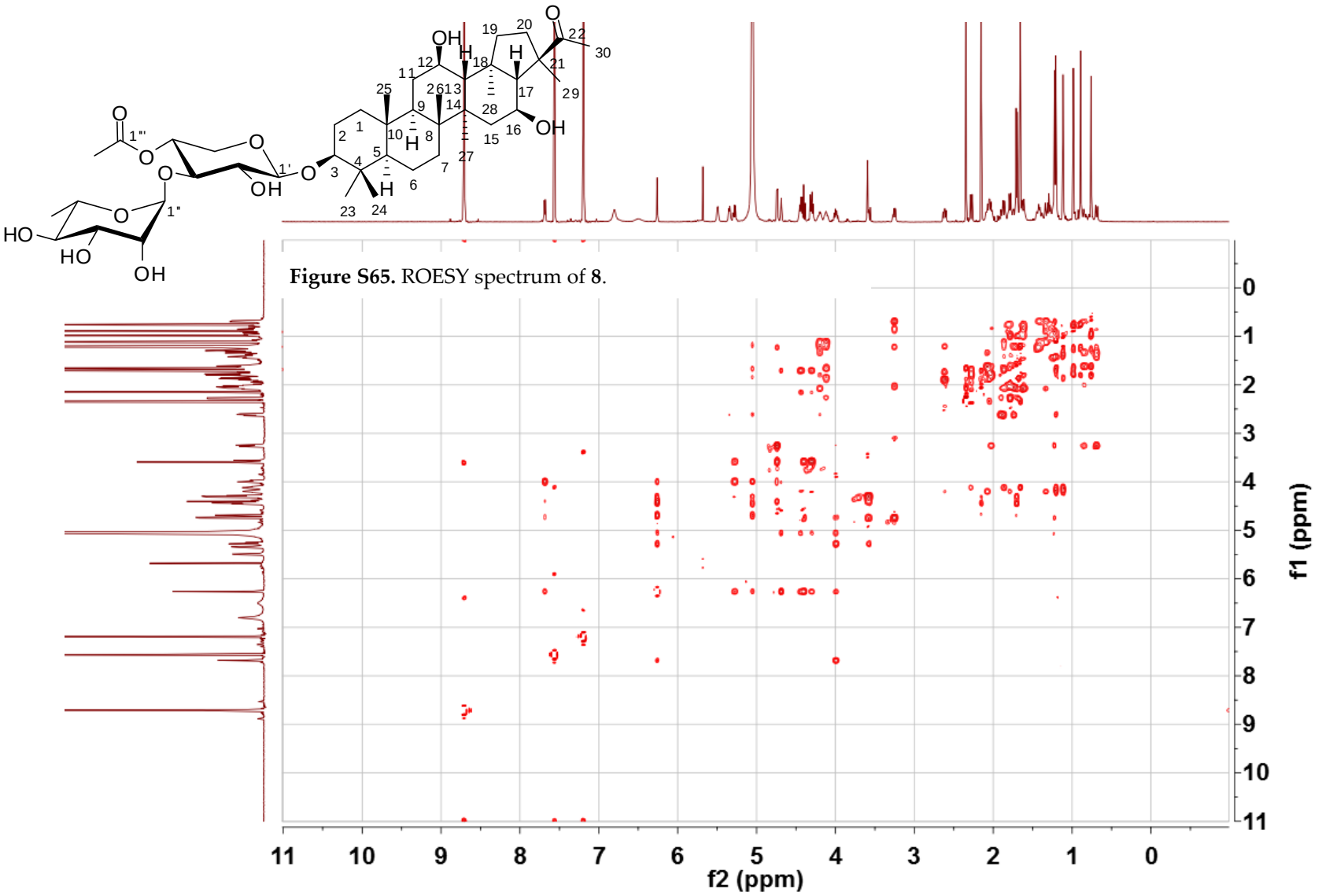


Figure S65. ROESY spectrum of **8**.

Data Filename	180409ESIA1.d	**Sample Name**	pdt 25
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	4/9/2018 10:11:10 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
280	0	ESI

Figure S66. HRESIMS spectrum of **8**.

Peak List

m/z	z	Abund	Formula	Ion
105.04381	1	7861.56		
107.0607	1	9758.46		
121.05087		10394.14		
437.21141	1	4743.33		
619.5291	1	6658.52		
817.47093	1	22933.7	C43 H70 Na O13	M+
818.47367	1	11609.89	C43 H70 Na O13	M+
922.00983	1	182465.73		
923.01244	1	33655.16		
924.01361	1	4635.13		

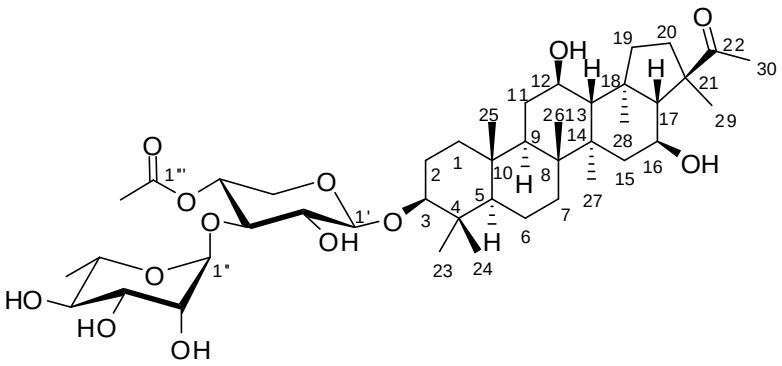
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	10	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C43 H70 Na O13	817.4714	817.4709	0.5	0.6	8.5

--- End Of Report ---



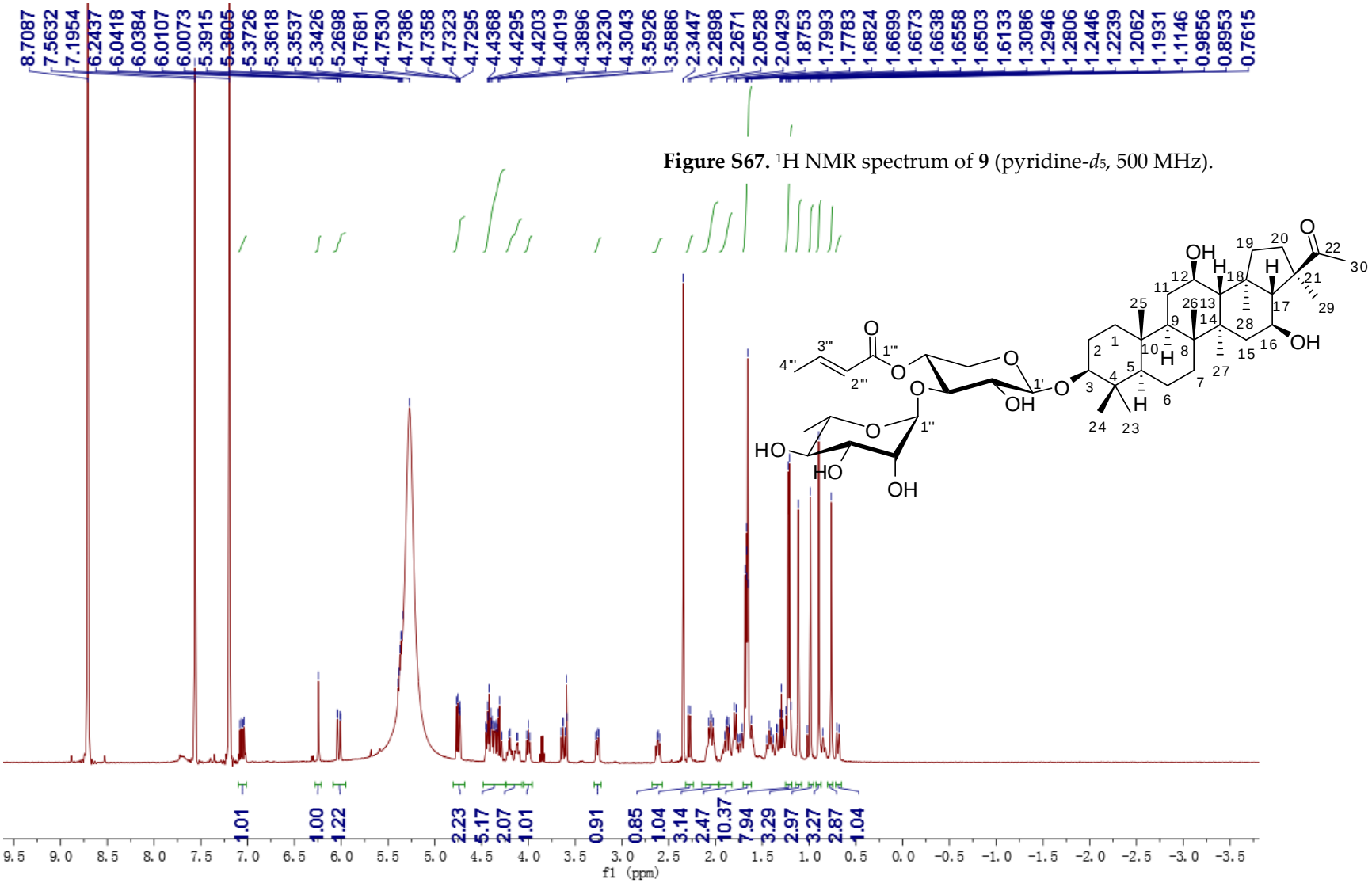


Figure S67. ^{1}H NMR spectrum of **9** (pyridine-d_5, 500 MHz).

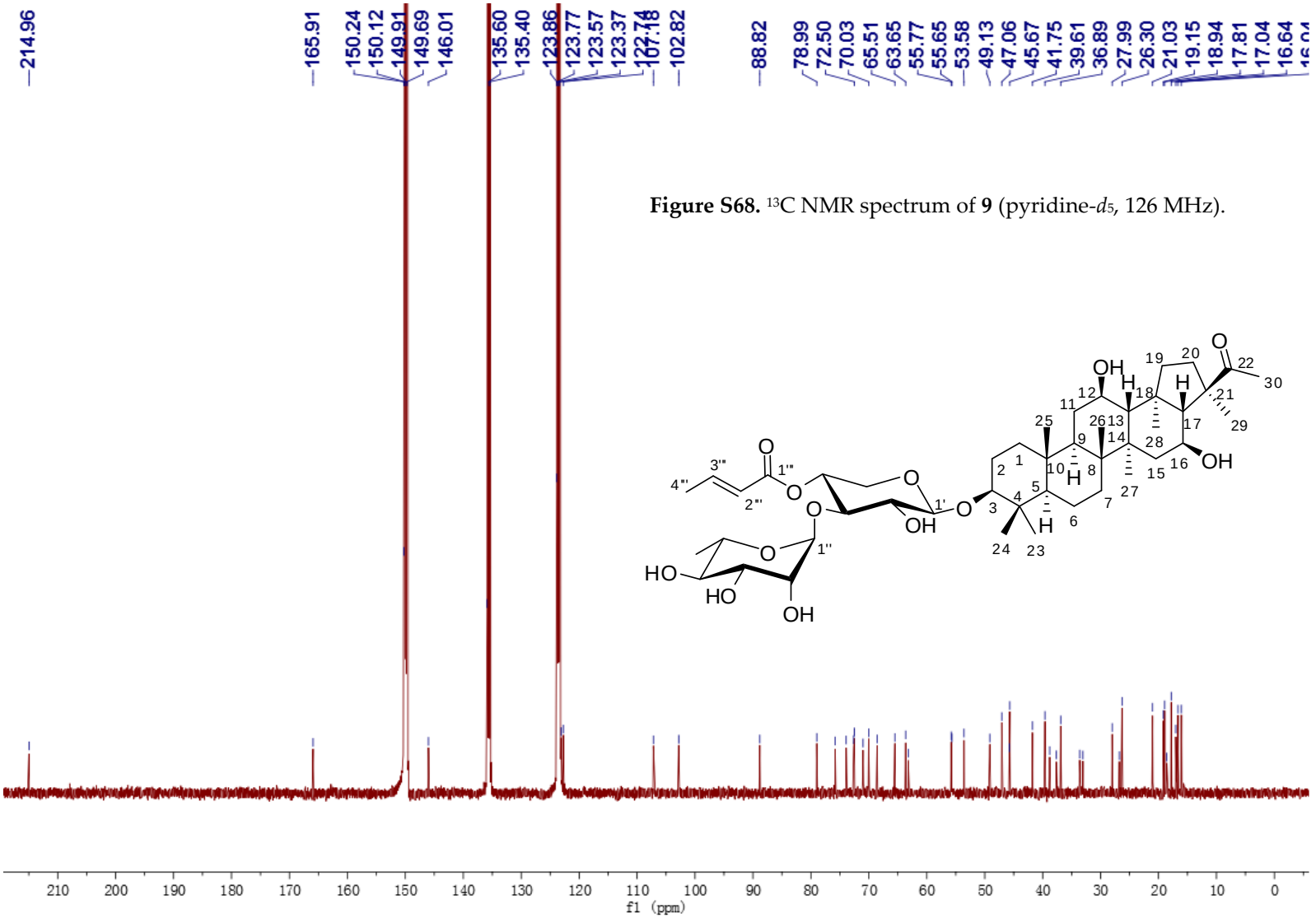


Figure S68. ^{13}C NMR spectrum of **9** (pyridine-d_5, 126 MHz).

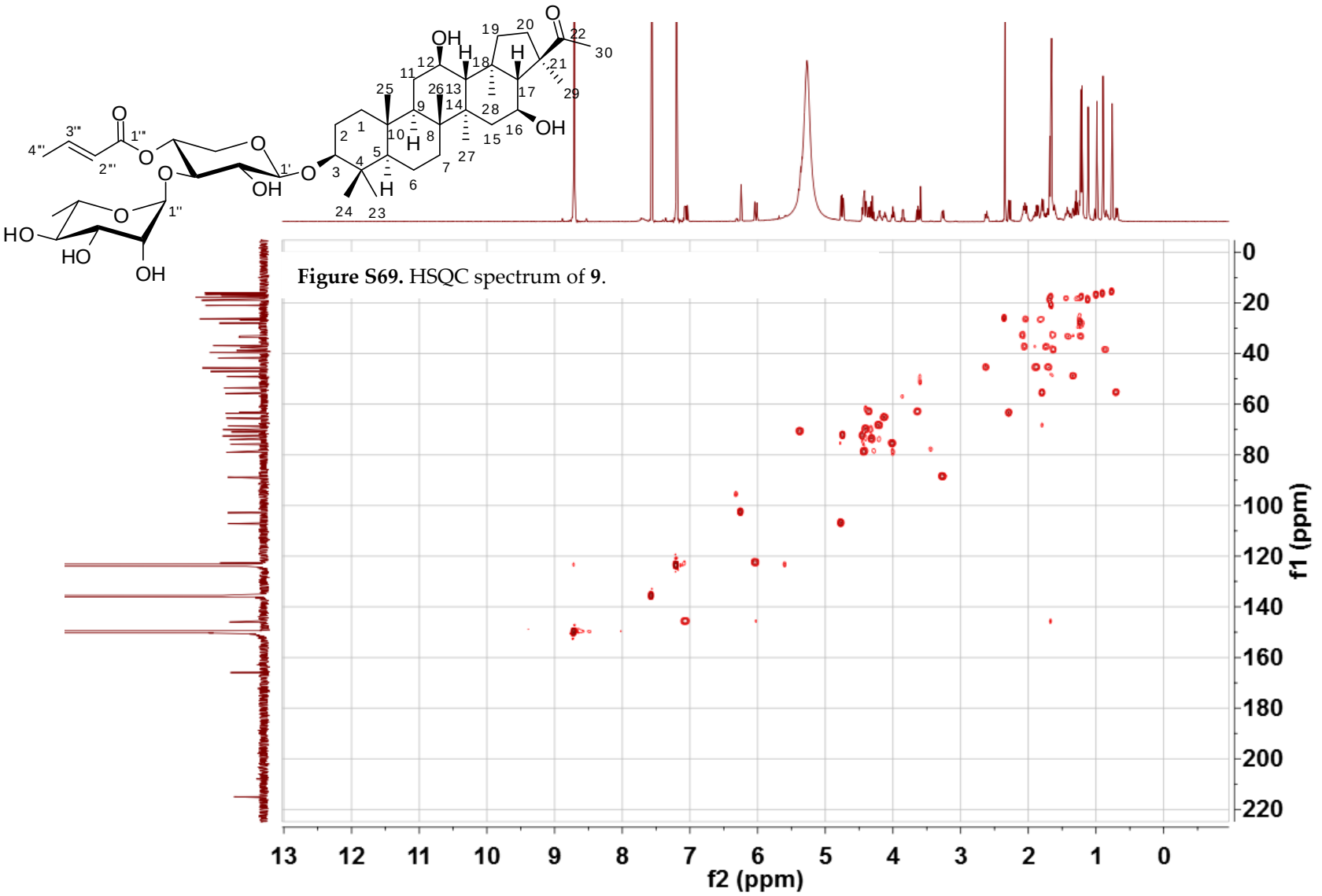


Figure S69. HSQC spectrum of **9**.

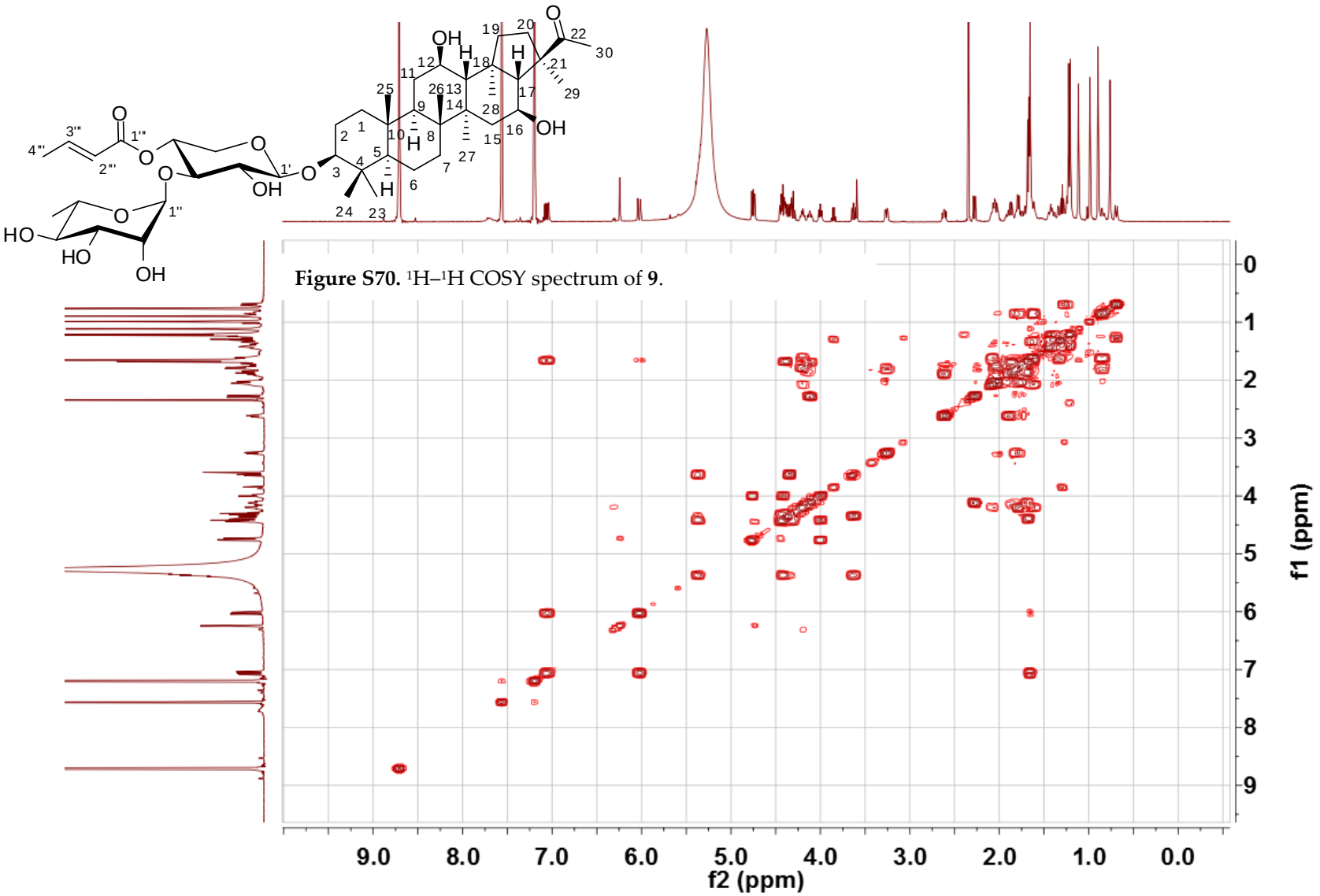


Figure S70. ^{1}H–^{1}H COSY spectrum of **9**.

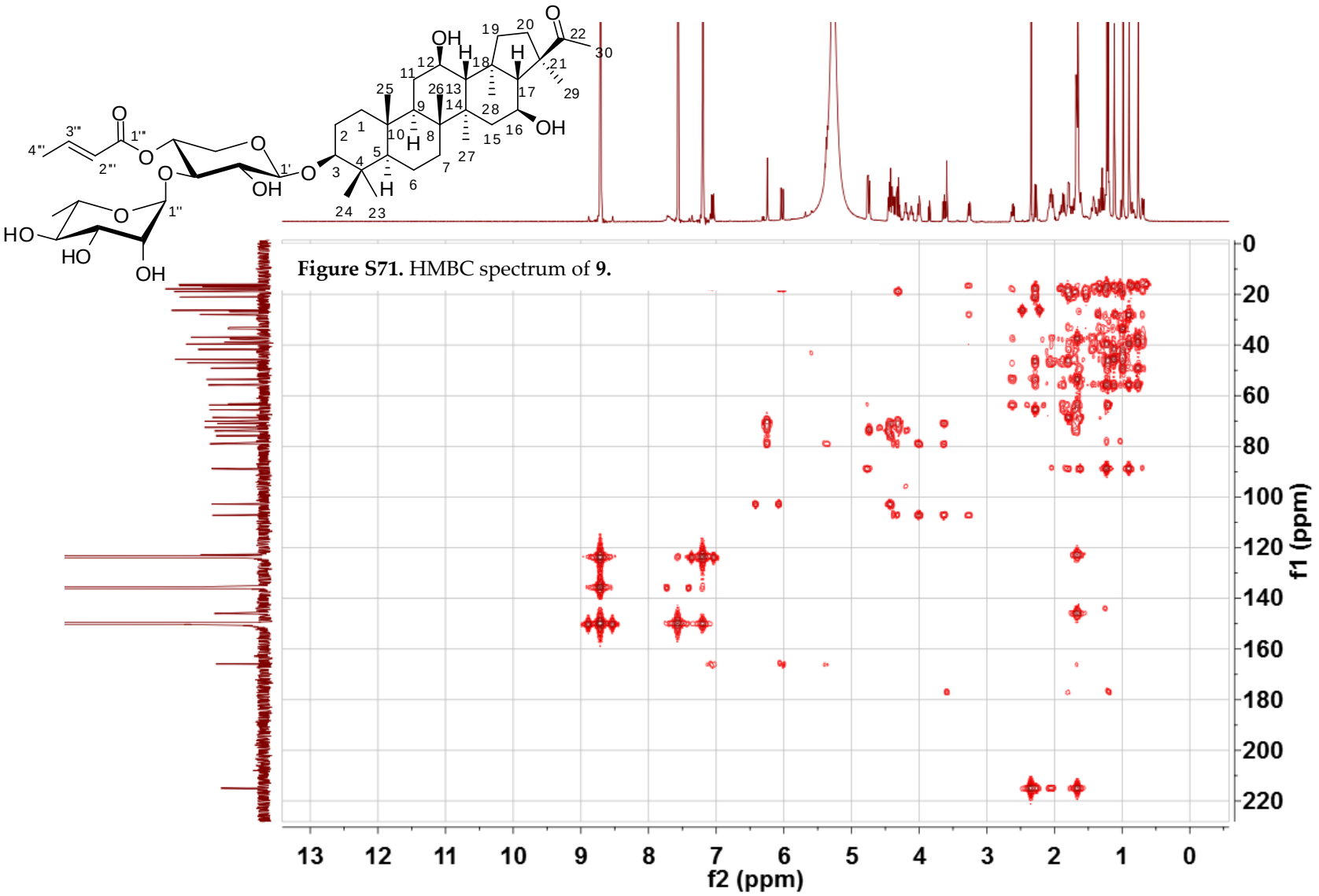


Figure S71. HMBC spectrum of **9**.

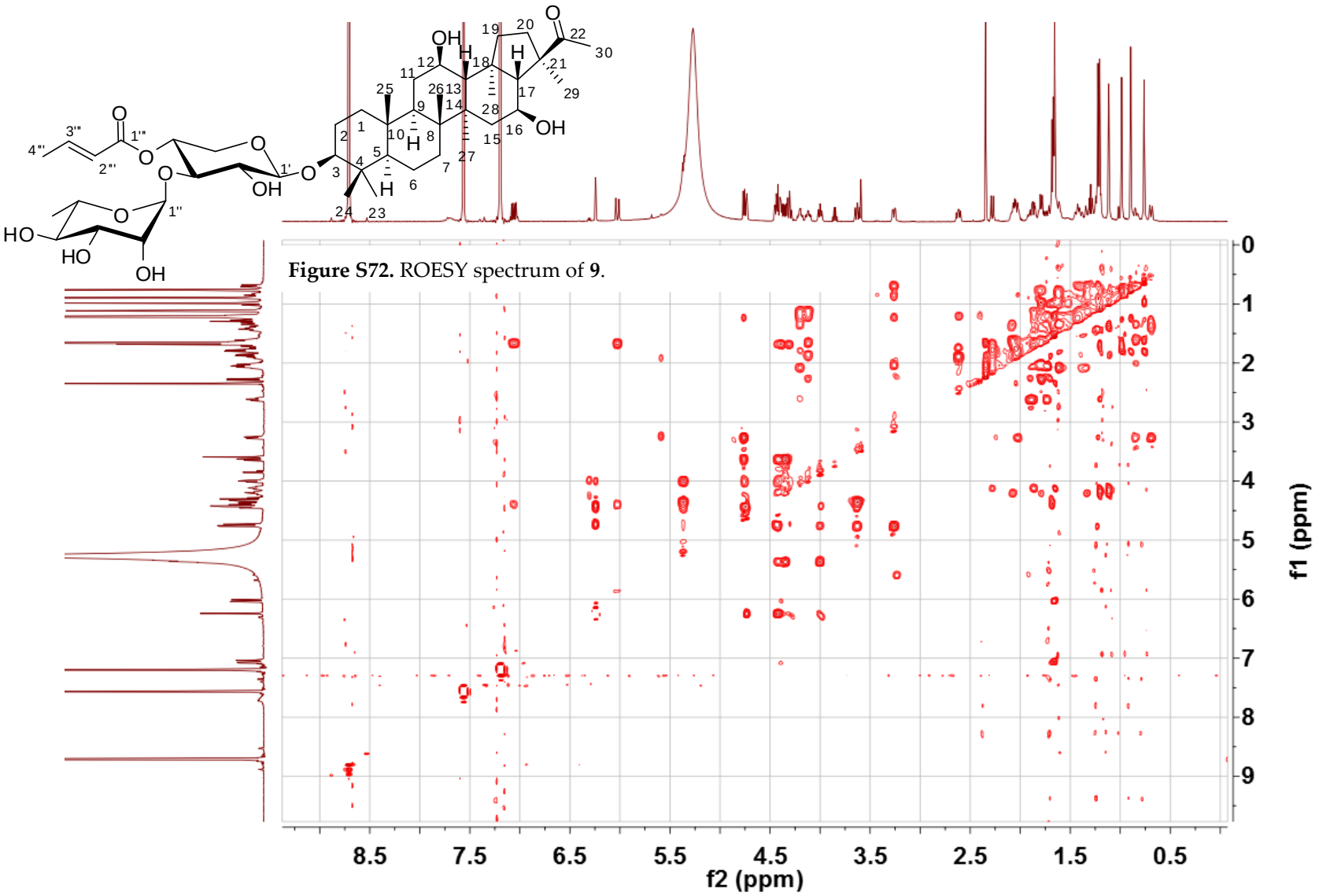


Figure S72. ROESY spectrum of **9**.

Data Filename	171023ESIA2.d	**Sample Name**	pdt21
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	10/23/2017 10:50:53 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
250	0	ESI

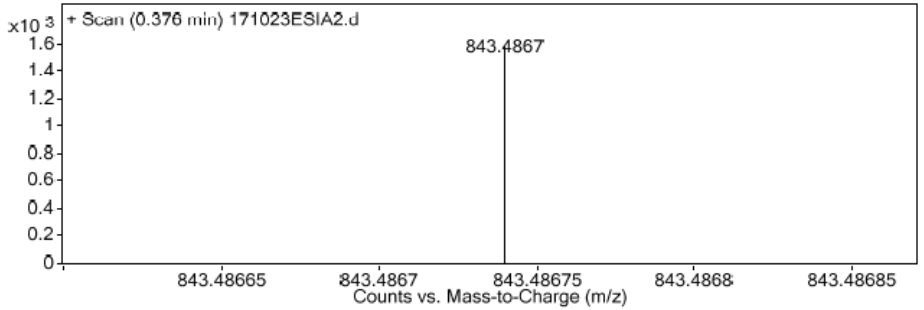


Figure S73. HRESIMS spectrum of **9**.

Peak List

m/z	z	Abund
112.1874	1	10026.1
141.0132	1	30683.75
166.0626	1	5483.01
182.0396	1	20365.15
218.9723		2794.6
289.4064		3495.92
290.4138	1	5943.82
406.9446	1	2901.76
973.4422	2	4264.08
1014.4671	1	2768.69

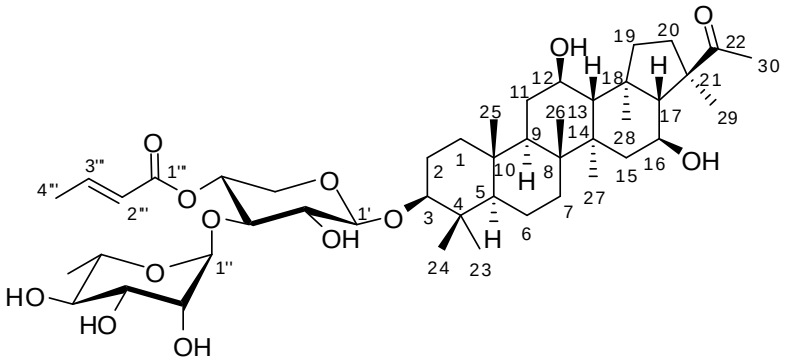
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	9	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C45 H72 Na O13	843.4871	843.4867	0.4	0.4	9.5

--- End Of Report ---



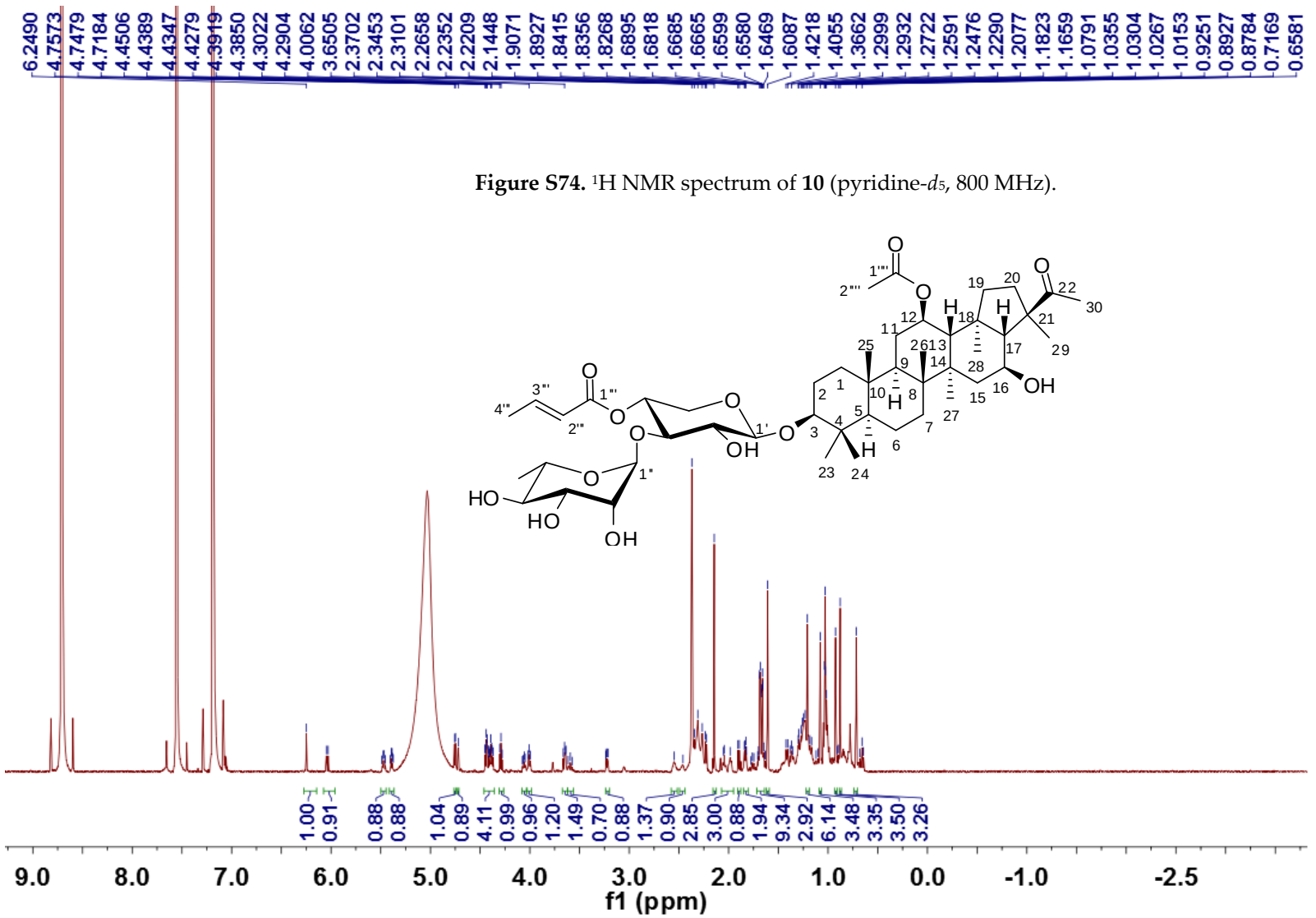


Figure S74. ^{1}H NMR spectrum of **10** (pyridine-d_5, 800 MHz).

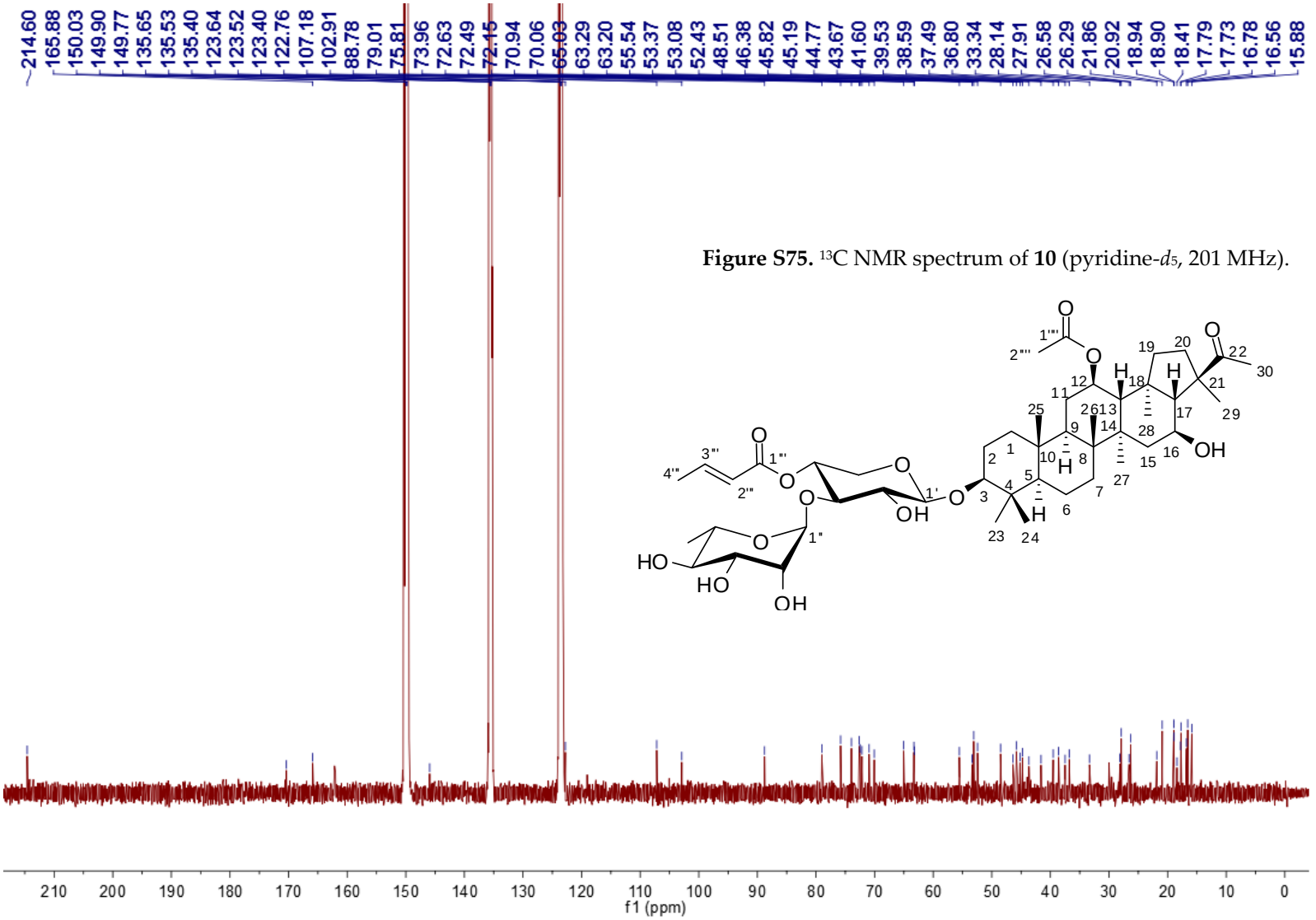


Figure S75. ^{13}C NMR spectrum of **10** (pyridine-d_5, 201 MHz).

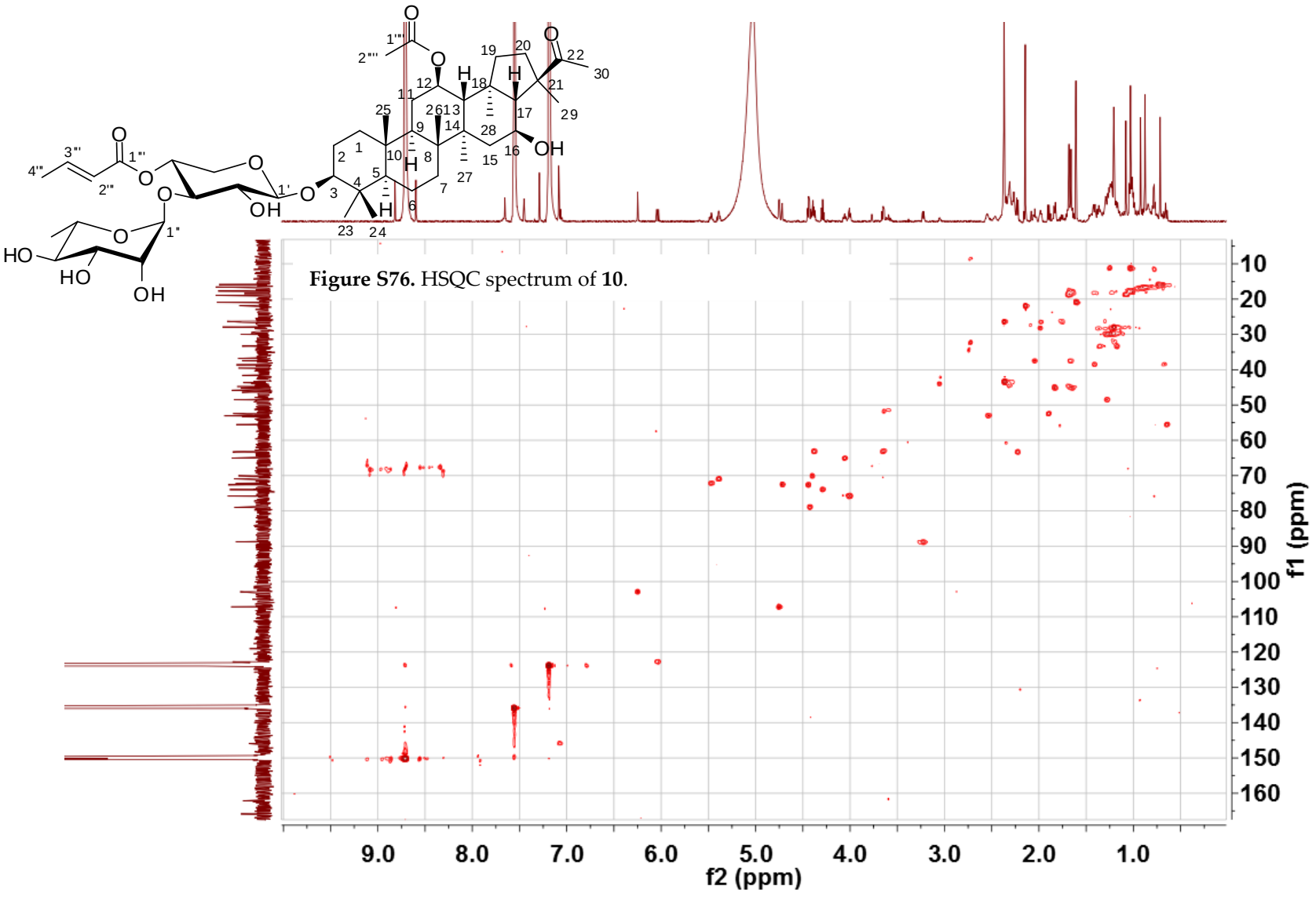


Figure S76. HSQC spectrum of **10**.

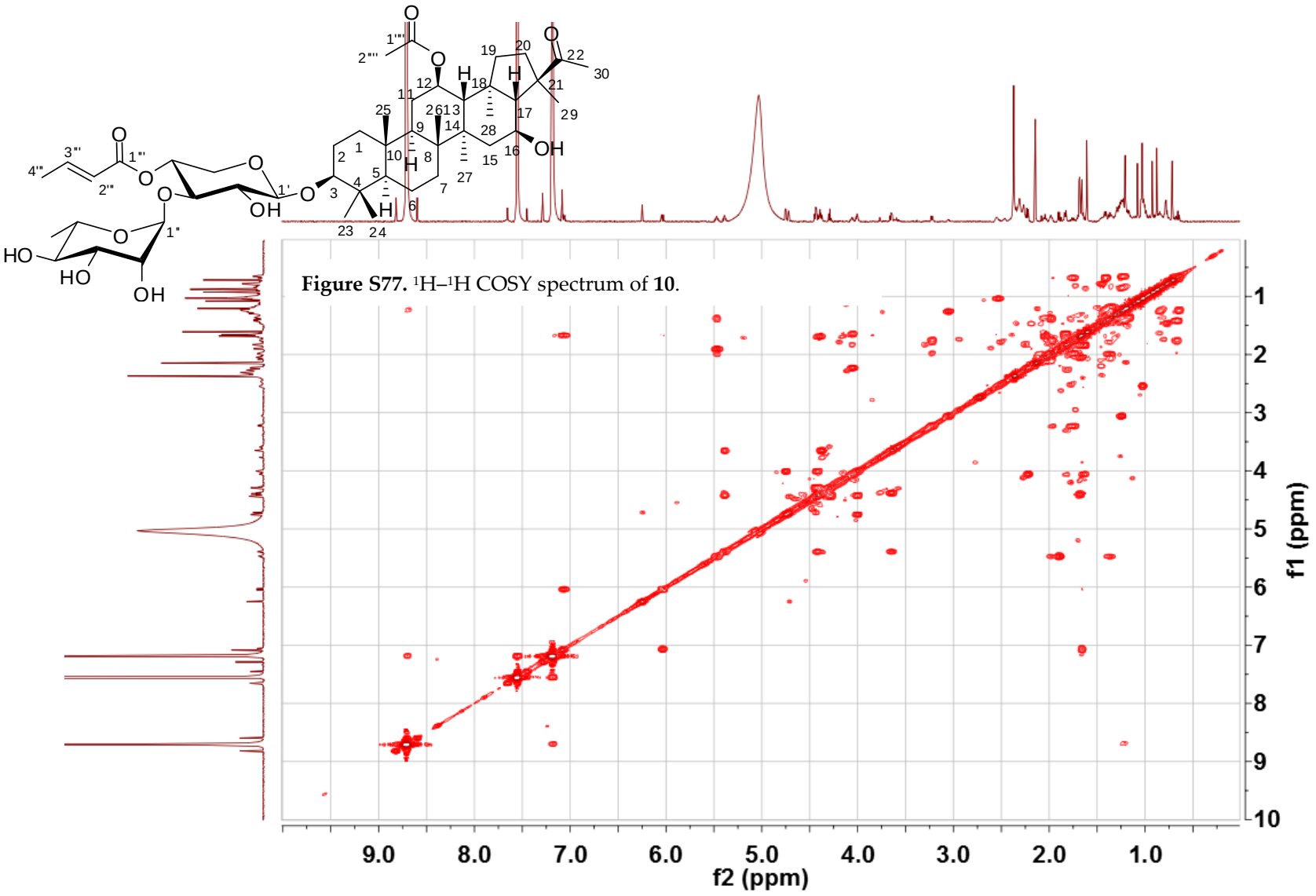


Figure S77. ^{1}H–^{1}H COSY spectrum of **10**.

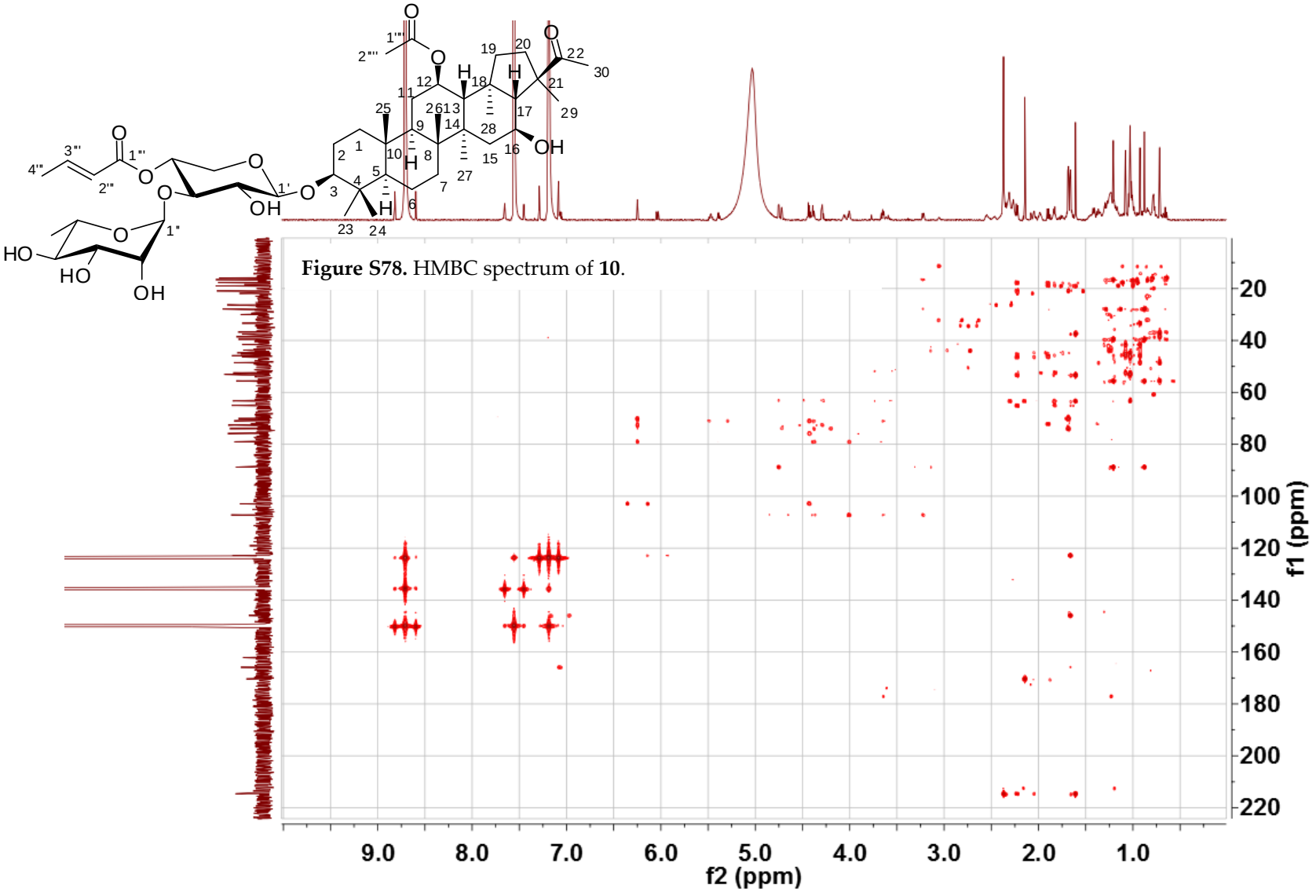


Figure S78. HMBC spectrum of **10**.

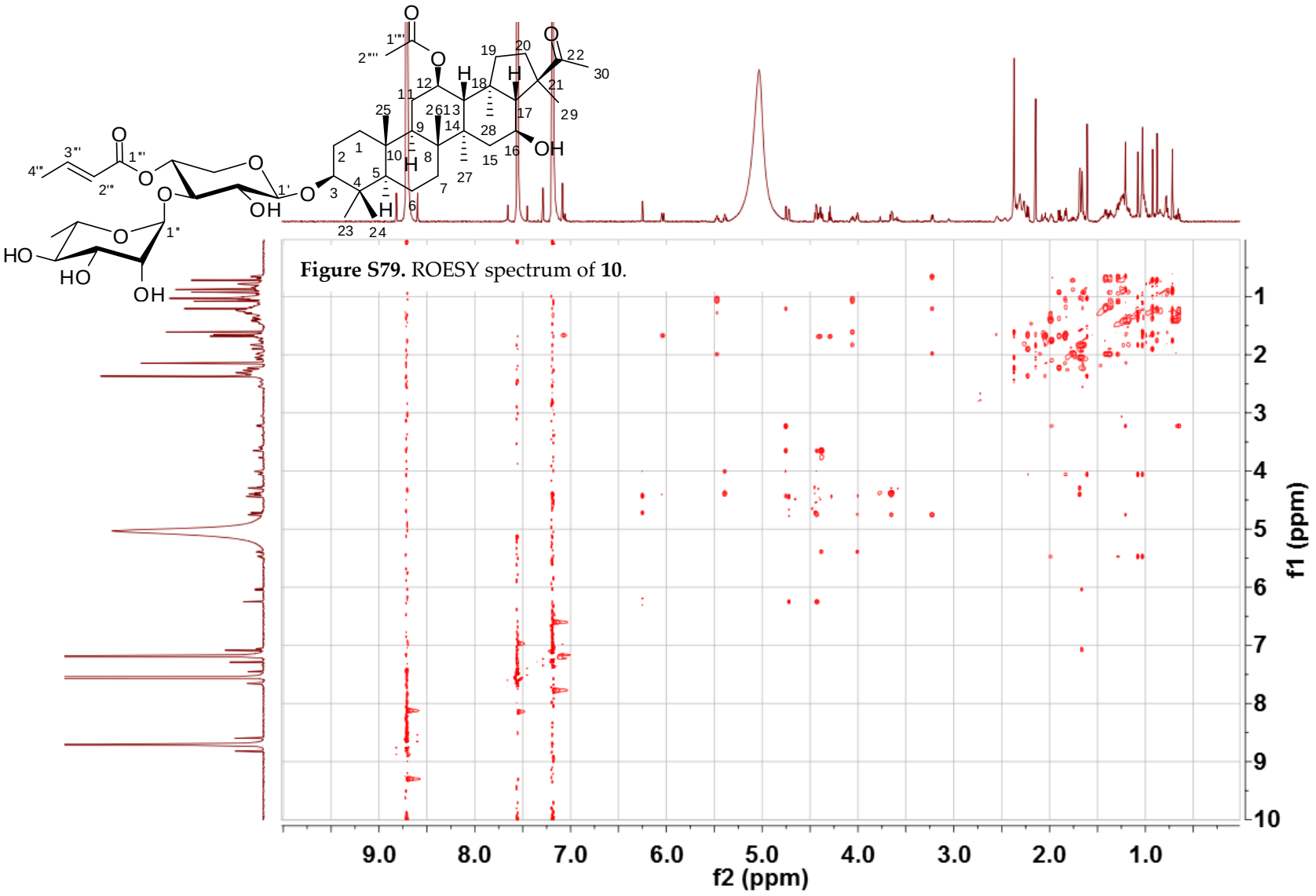


Figure S79. ROESY spectrum of **10**.

Data Filename	180824ESIA5.d	**Sample Name**	pdt 36a
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/24/2018 2:21:16 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
340	0	ESI

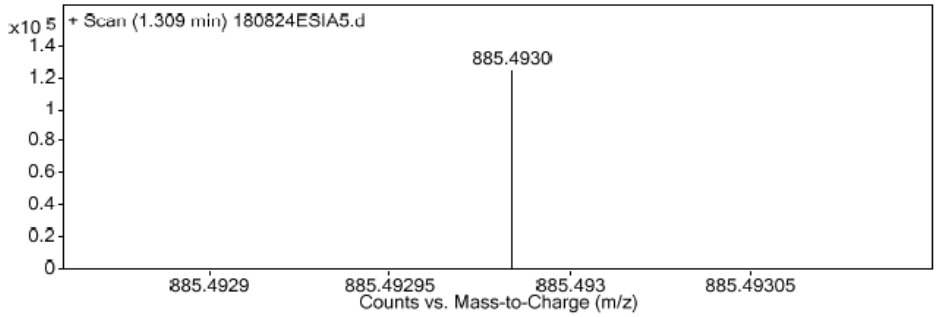


Figure S80. HRESIMS spectrum of **10**.

Peak List

m/z	z	Abund	Formula	Ion
112.1865	1	57330.41		
885.493	1	124318	C47 H74 Na O14	M+
886.4952	1	59689.01	C47 H74 Na O14	M+
887.4997	1	19585.49	C47 H74 Na O14	M+
901.4633	1	46731.28		
902.4662	1	23420.69		
947.5848	1	506711.25		
948.5882	1	291532.06		
949.5898	1	87454.73		
950.5916	1	20514.56		

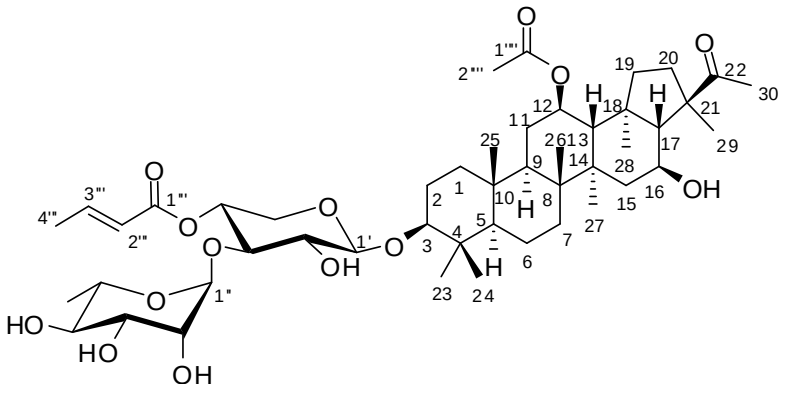
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	10	20
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C47 H74 Na O14	885.4976	885.4930	4.6	5.2	10.5

--- End Of Report ---



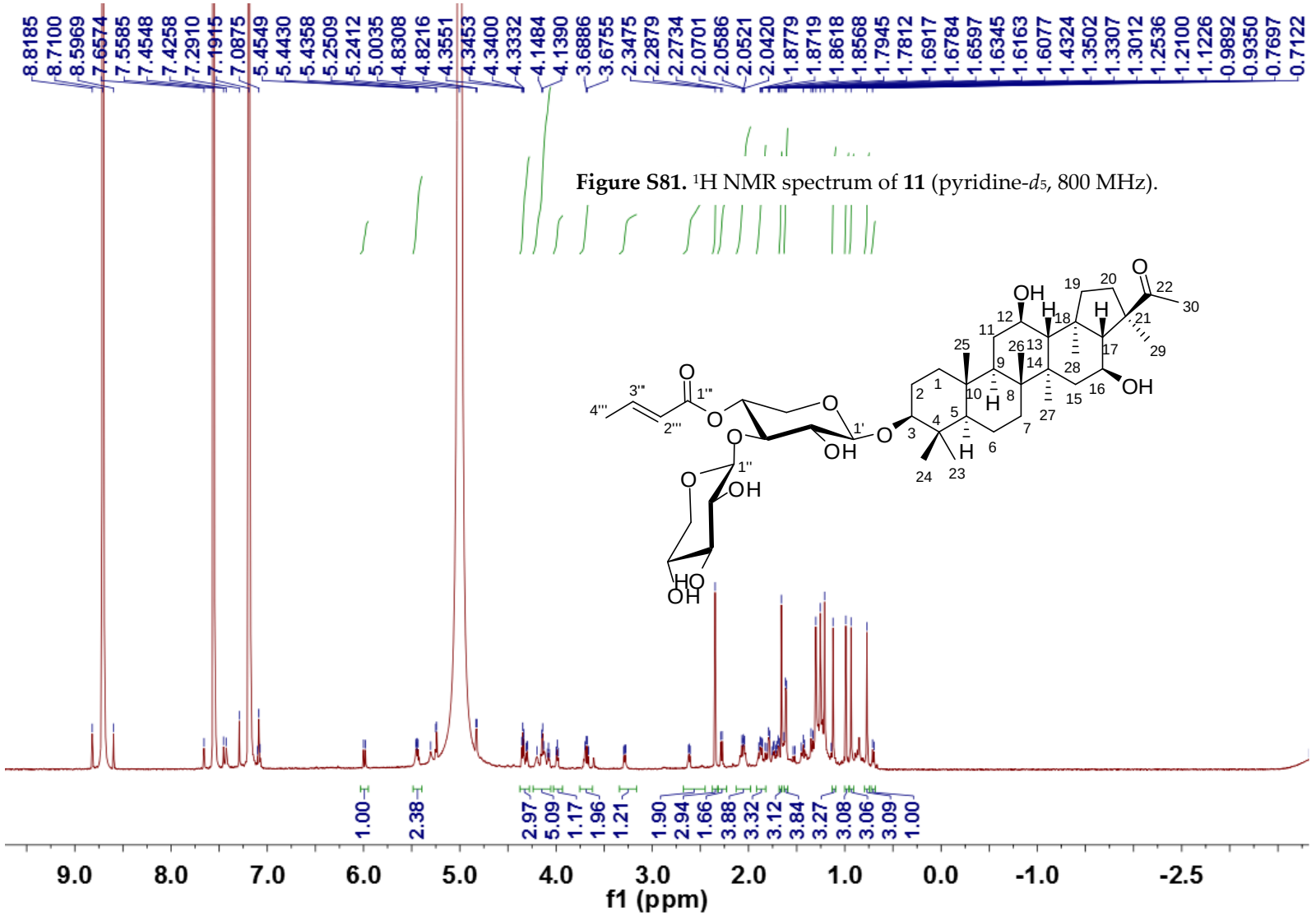


Figure S81. ^{1}H NMR spectrum of **11** (pyridine-d_5, 800 MHz).

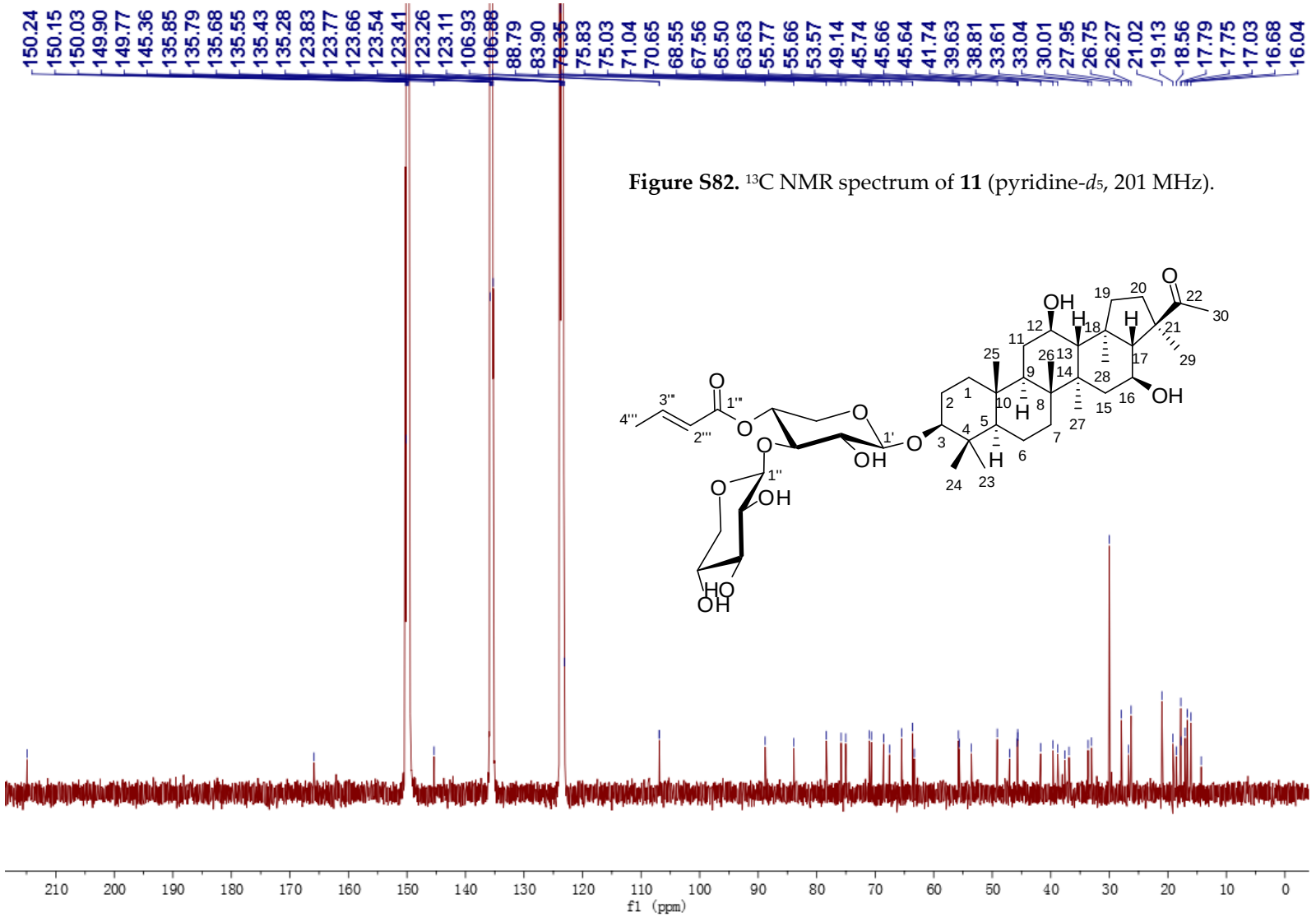


Figure S82. ^{13}C NMR spectrum of **11** (pyridine-d_5, 201 MHz).

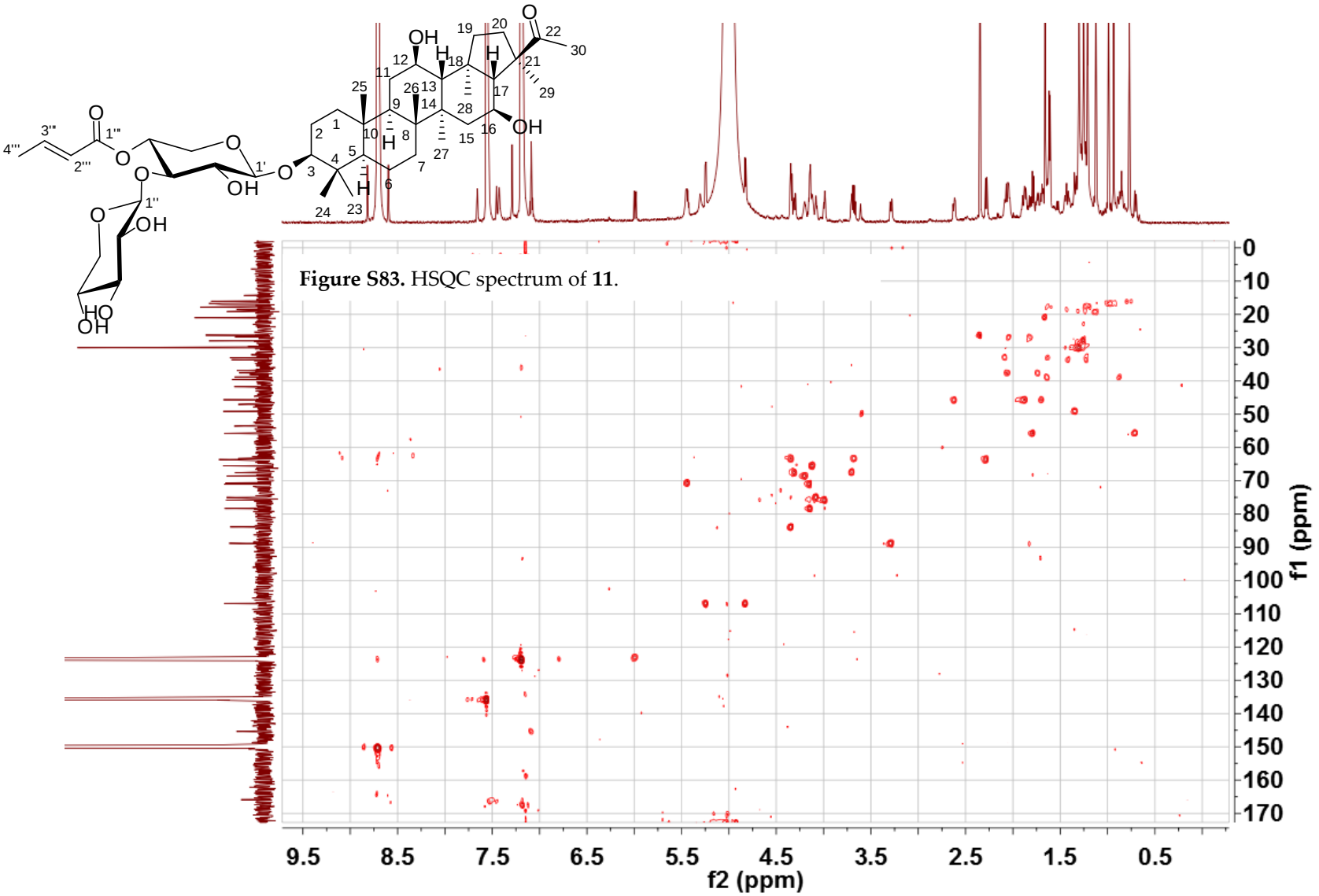


Figure S83. HSQC spectrum of **11**.

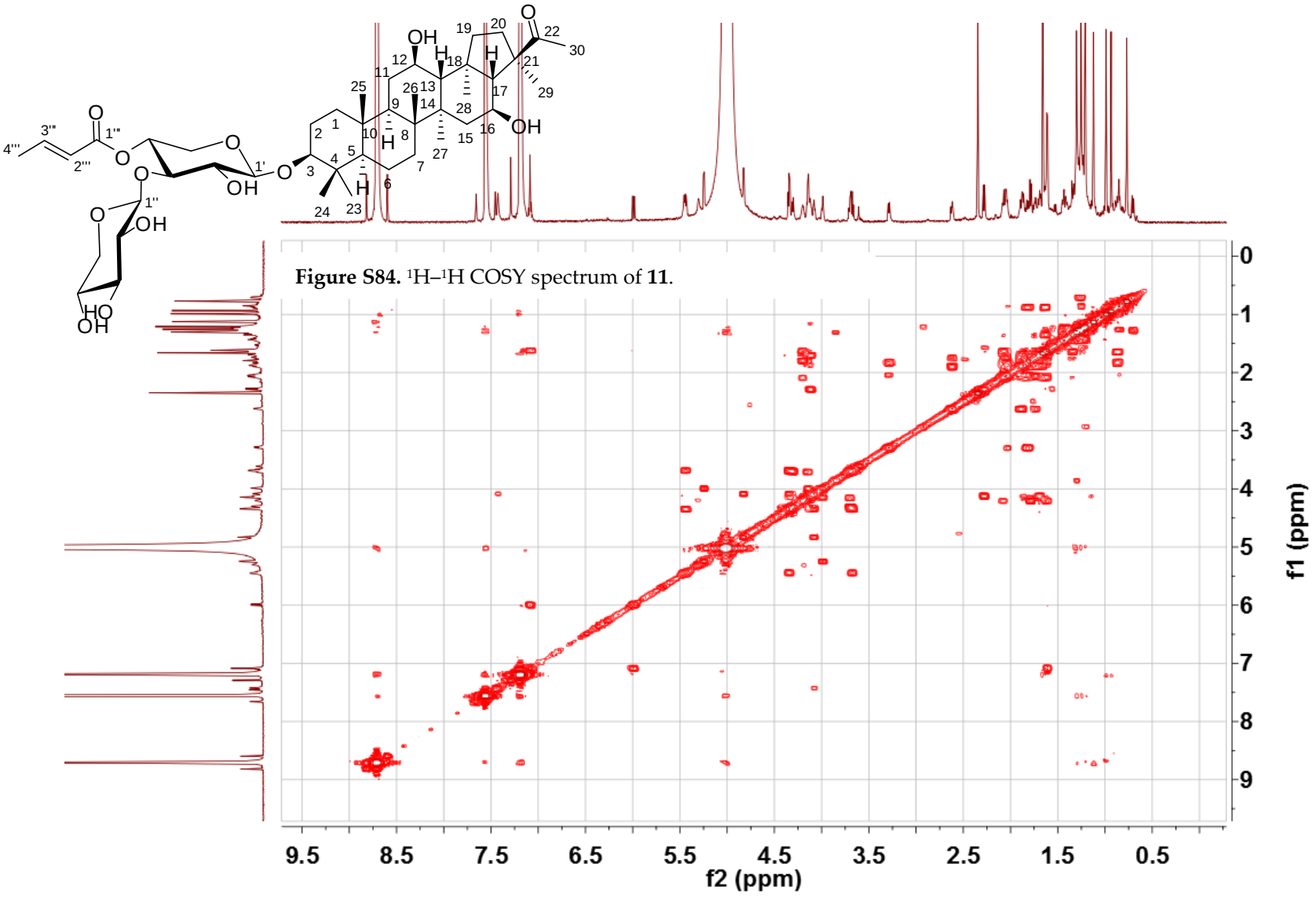


Figure S84. ^{1}H–^{1}H COSY spectrum of **11**.

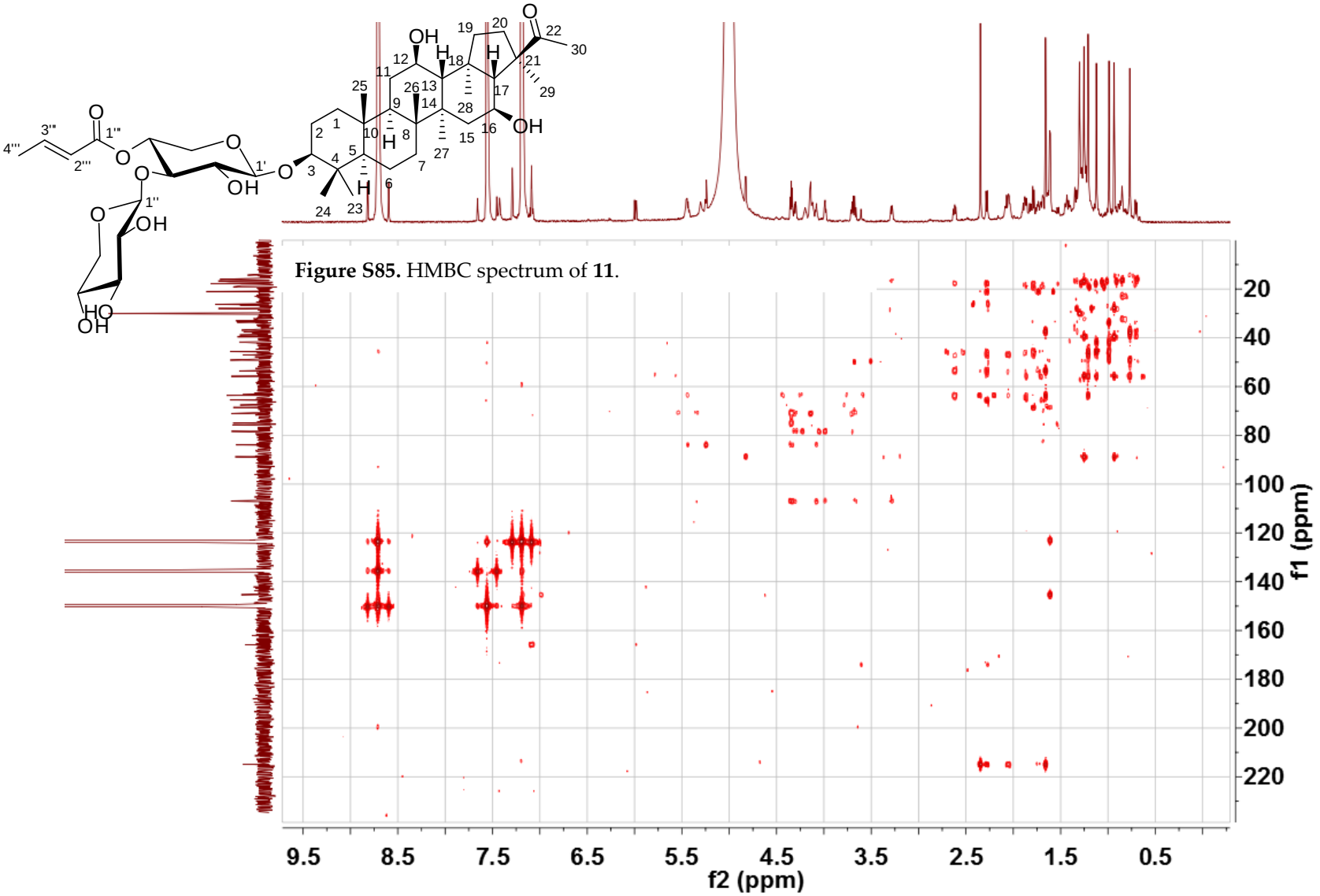


Figure S85. HMBC spectrum of **11**.

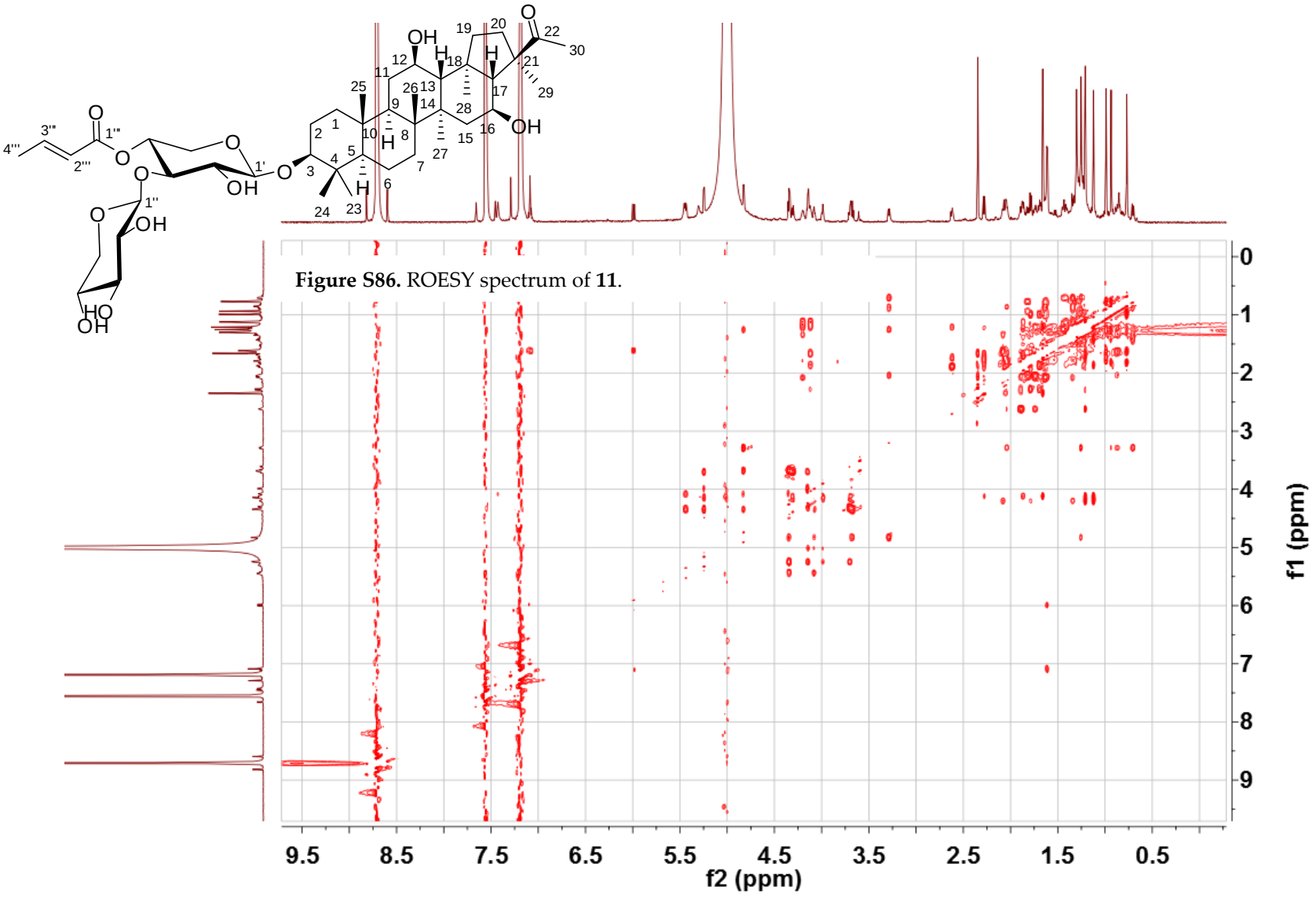


Figure S86. ROESY spectrum of **11**.

Data Filename	180409ESIA2.d	**Sample Name**	pdt 24
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	4/9/2018 10:13:33 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
300	0	ESI

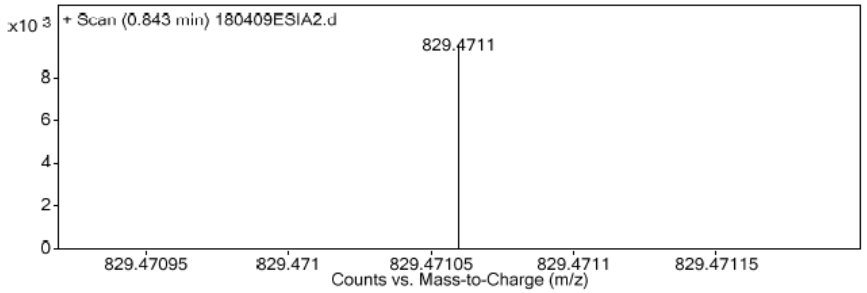


Figure S87. HRESIMS spectrum of **11**.

Peak List

m/z	z	Abund	Formula	Ion
106.086	1	5518.7		
437.1971	1	20021.2		
591.4976	1	6450.84		
619.5286		20222.86		
620.5325	2	8158.89		
647.5596	1	14319.98		
648.5633	1	6012.22		
829.4711	1	9490.67	C44 H70 Na O13	M+
922.0098	1	134531.05		
923.0134	1	23301.78		

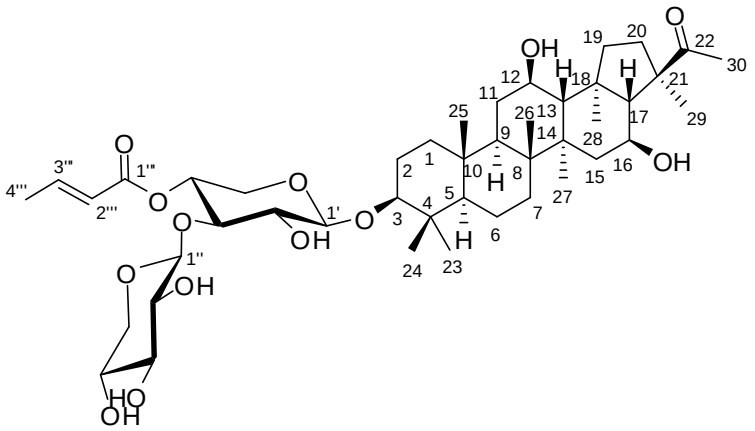
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	10	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C44 H70 Na O13	829.4714	829.4711	0.3	0.4	9.5

--- End Of Report ---



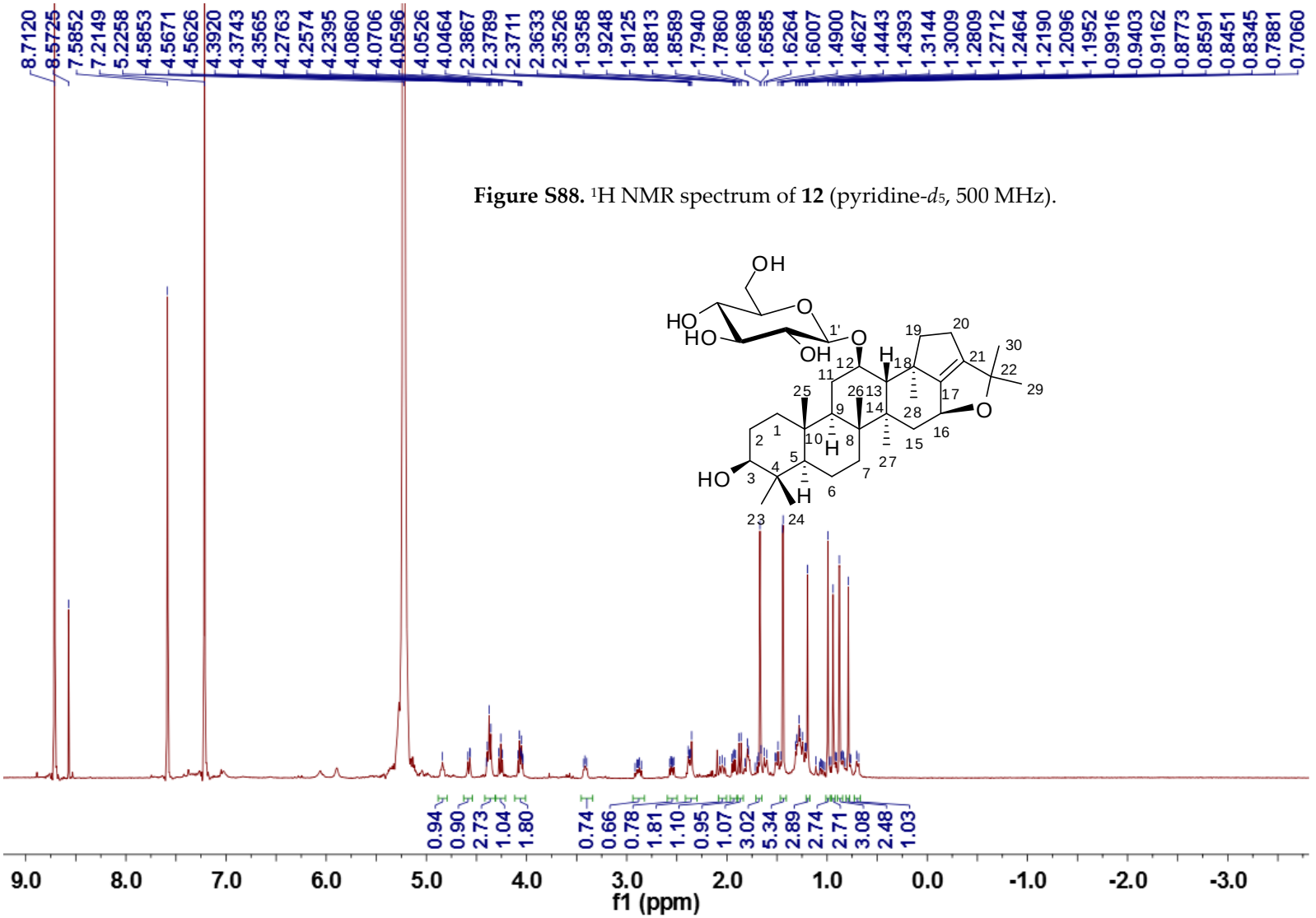


Figure S88. ^{1}H NMR spectrum of **12** (pyridine-d_5, 500 MHz).

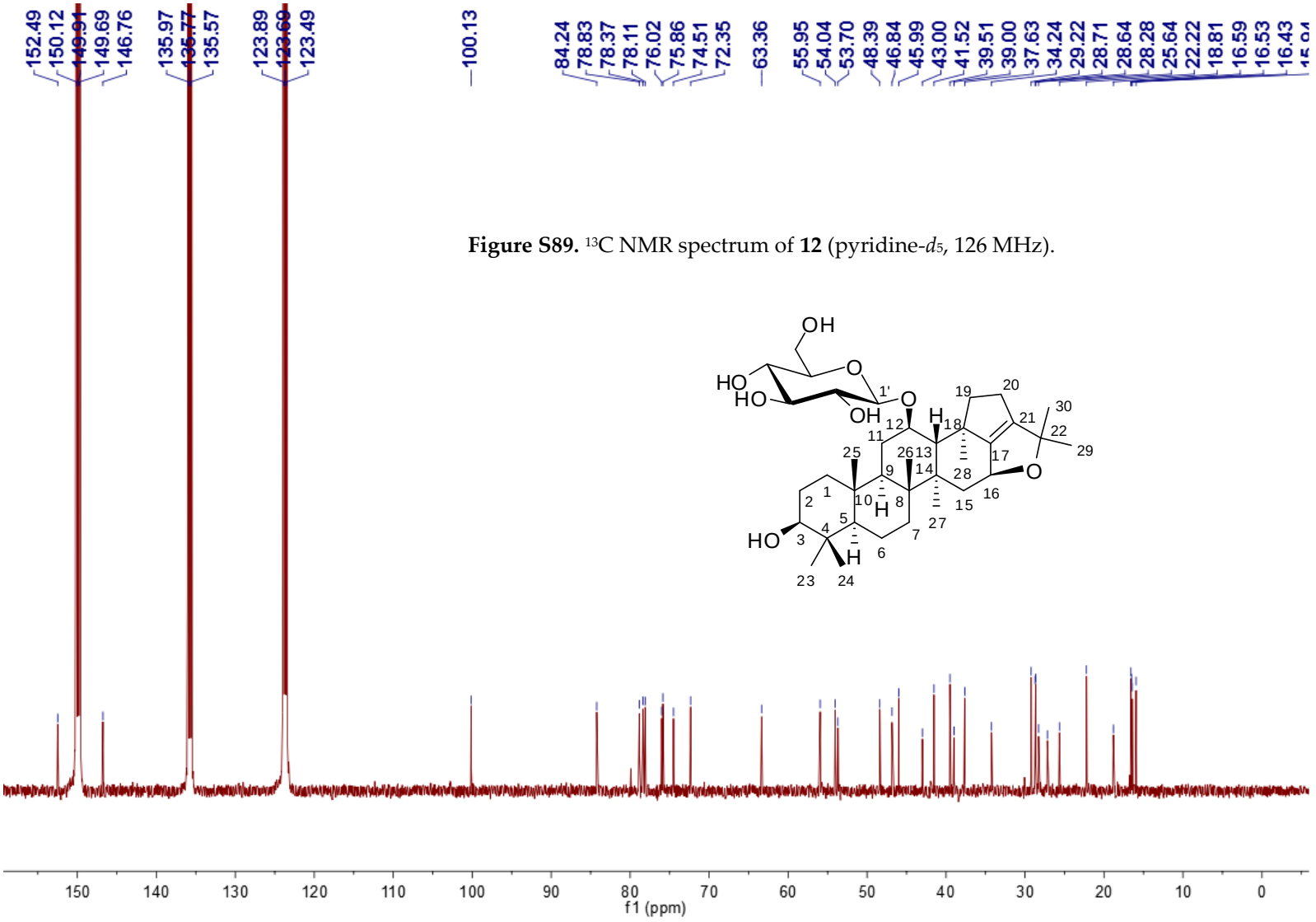


Figure S89. ^{13}C NMR spectrum of **12** (pyridine-d_5, 126 MHz).

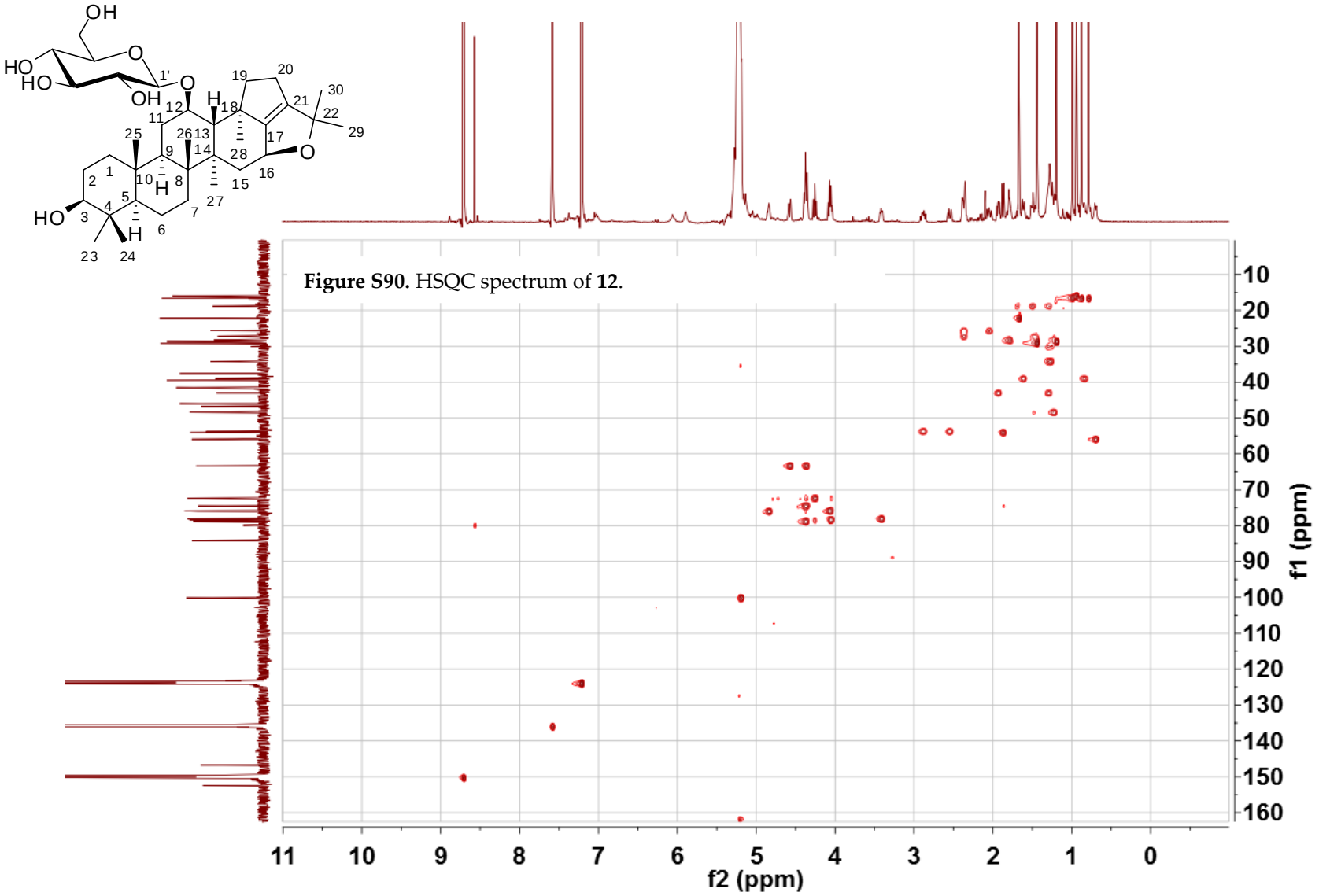


Figure S90. HSQC spectrum of **12**.

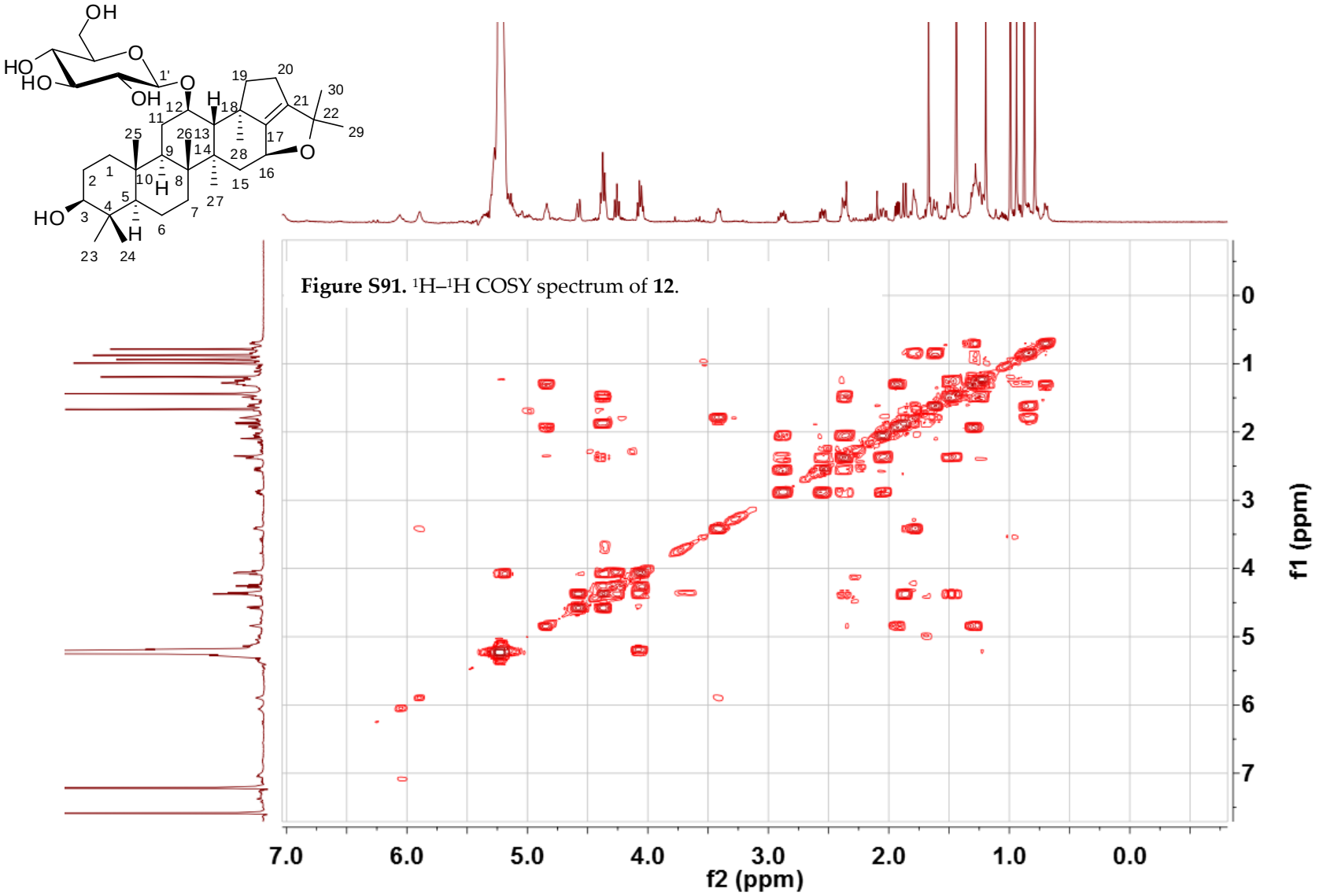


Figure S91. ^{1}H–^{1}H COSY spectrum of **12**.

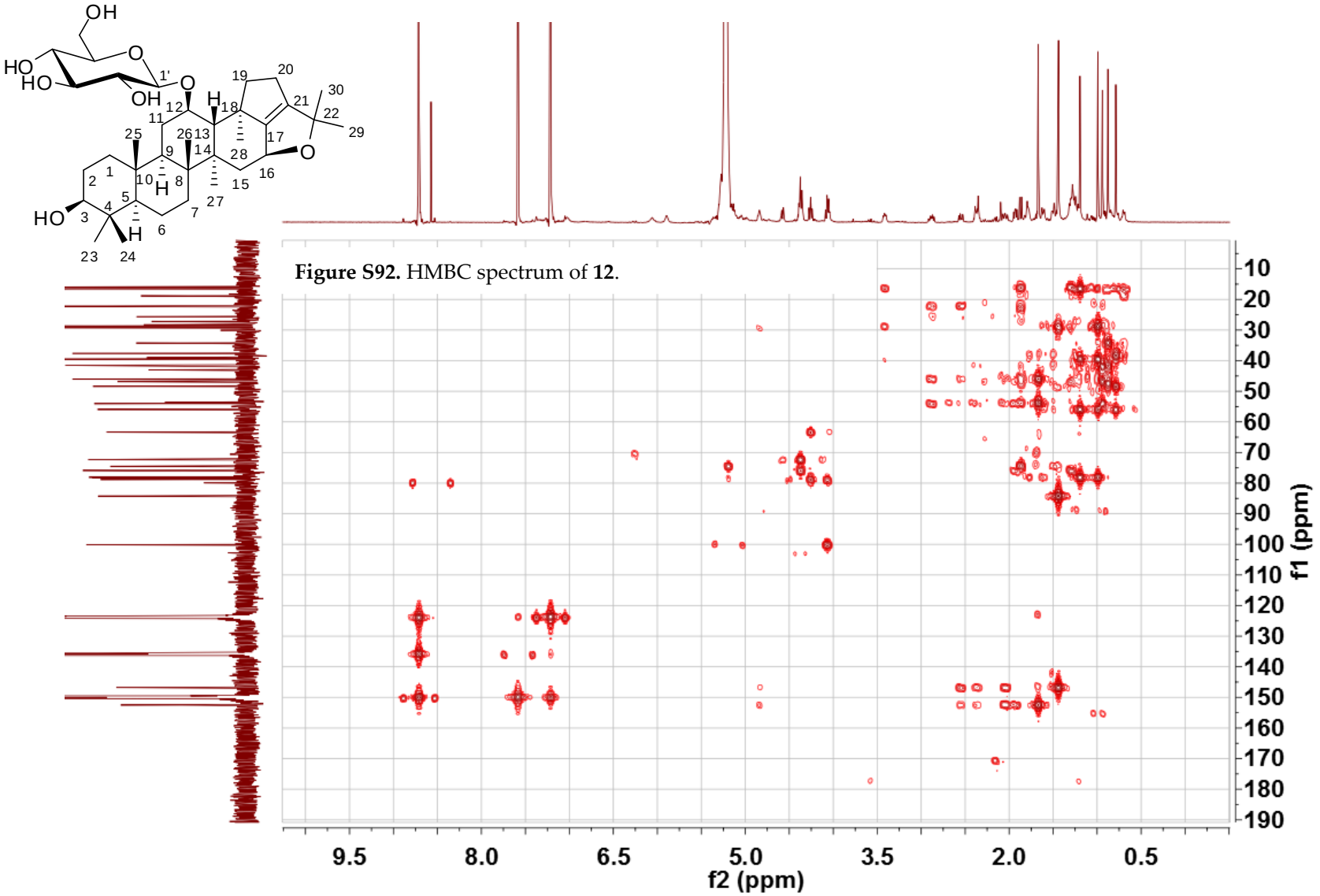


Figure S92. HMBC spectrum of **12**.

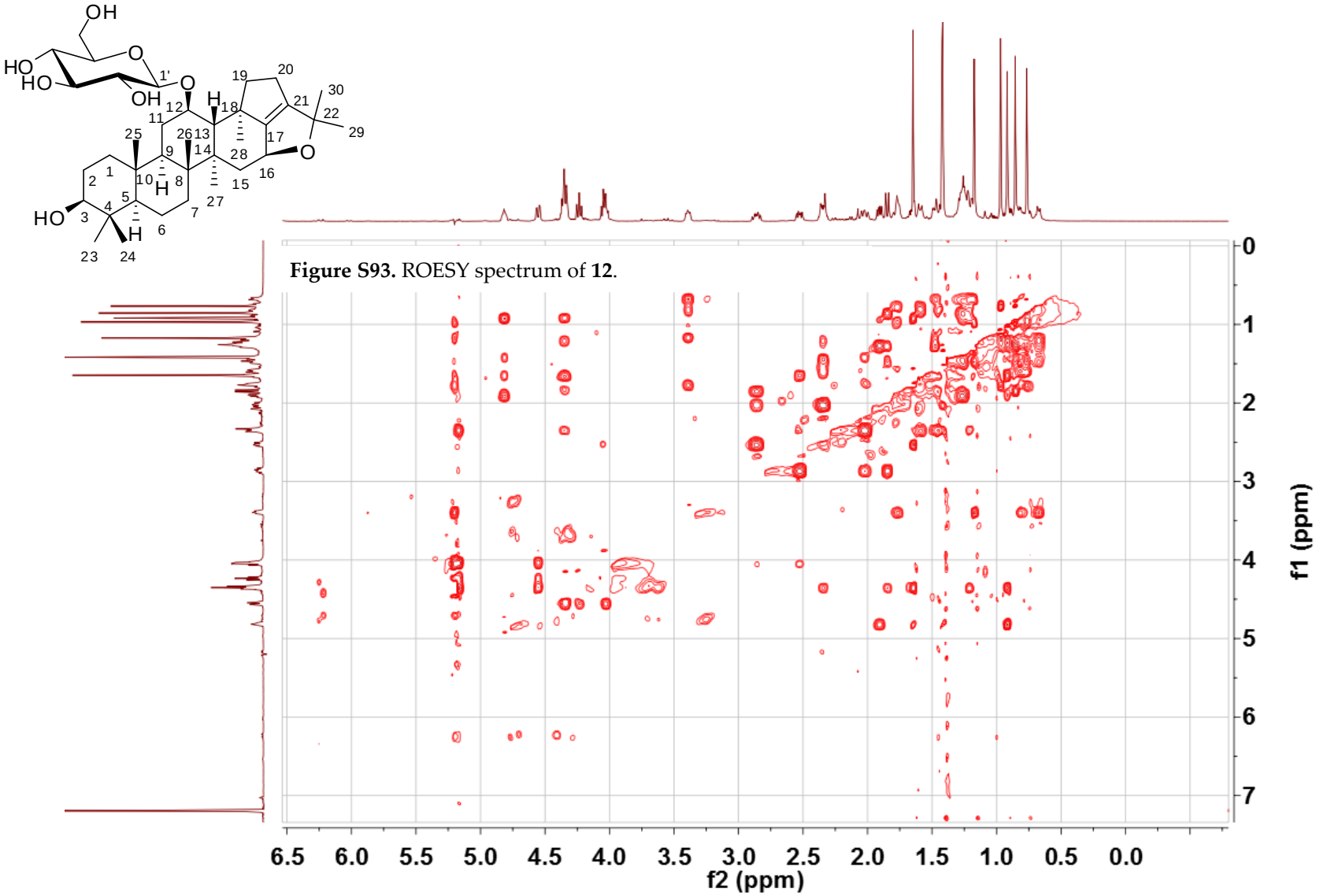


Figure S93. ROESY spectrum of **12**.

Formula Predictor Report - pdt41.lcd

Data File: E:\DATA\2018\0801\pdt41.lcd

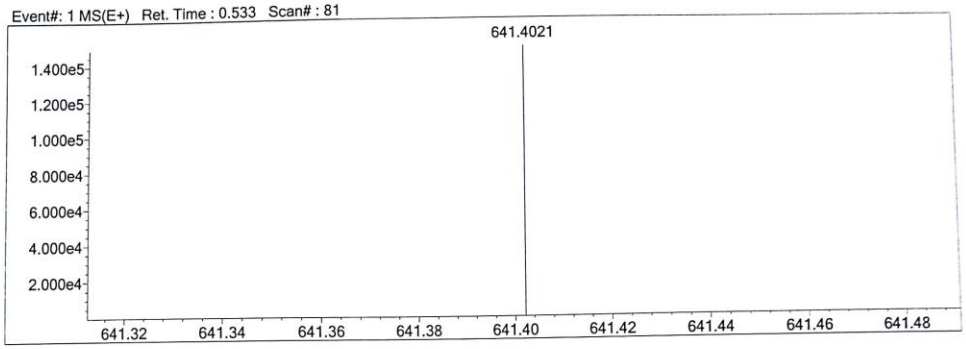
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	1	100	O	2	0	20	Si	4	0	0	Br	1	0	0	Na
C	4	10	50	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	0	Na	1	0	0	Cl	1	0	0					

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

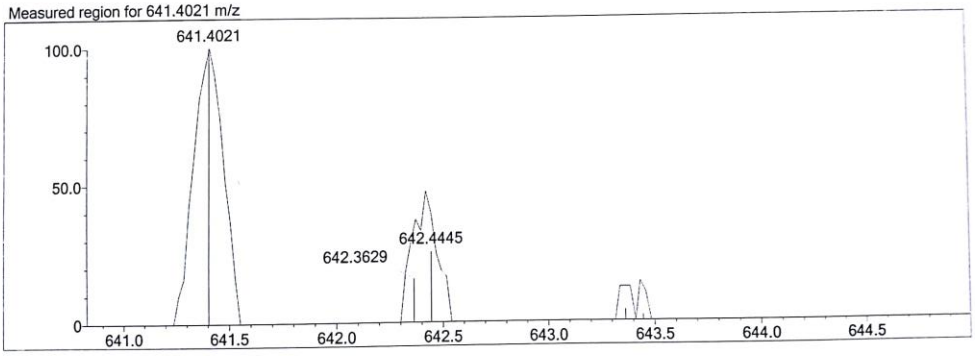
DBE Range: -2.0 - 100.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 10

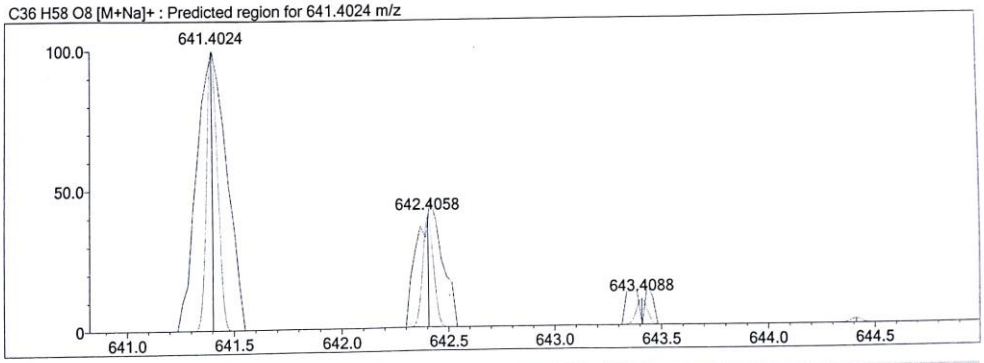
Event#: 1 MS(E+) Ret. Time : 0.533 Scan# : 81



Measured region for 641.4021 m/z



C36 H58 O8 [M+Na]+ : Predicted region for 641.4024 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C36 H58 O8	[M+Na]+	641.4021	641.4024	-0.3	-0.47	8.0

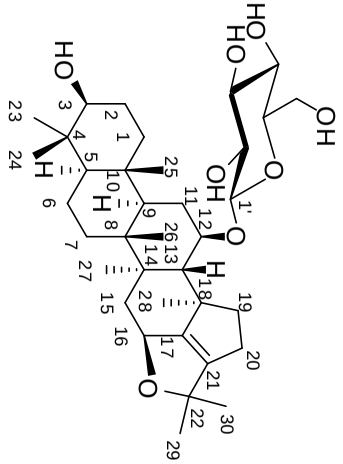


Figure S94. HRESIMS spectrum of **12**.

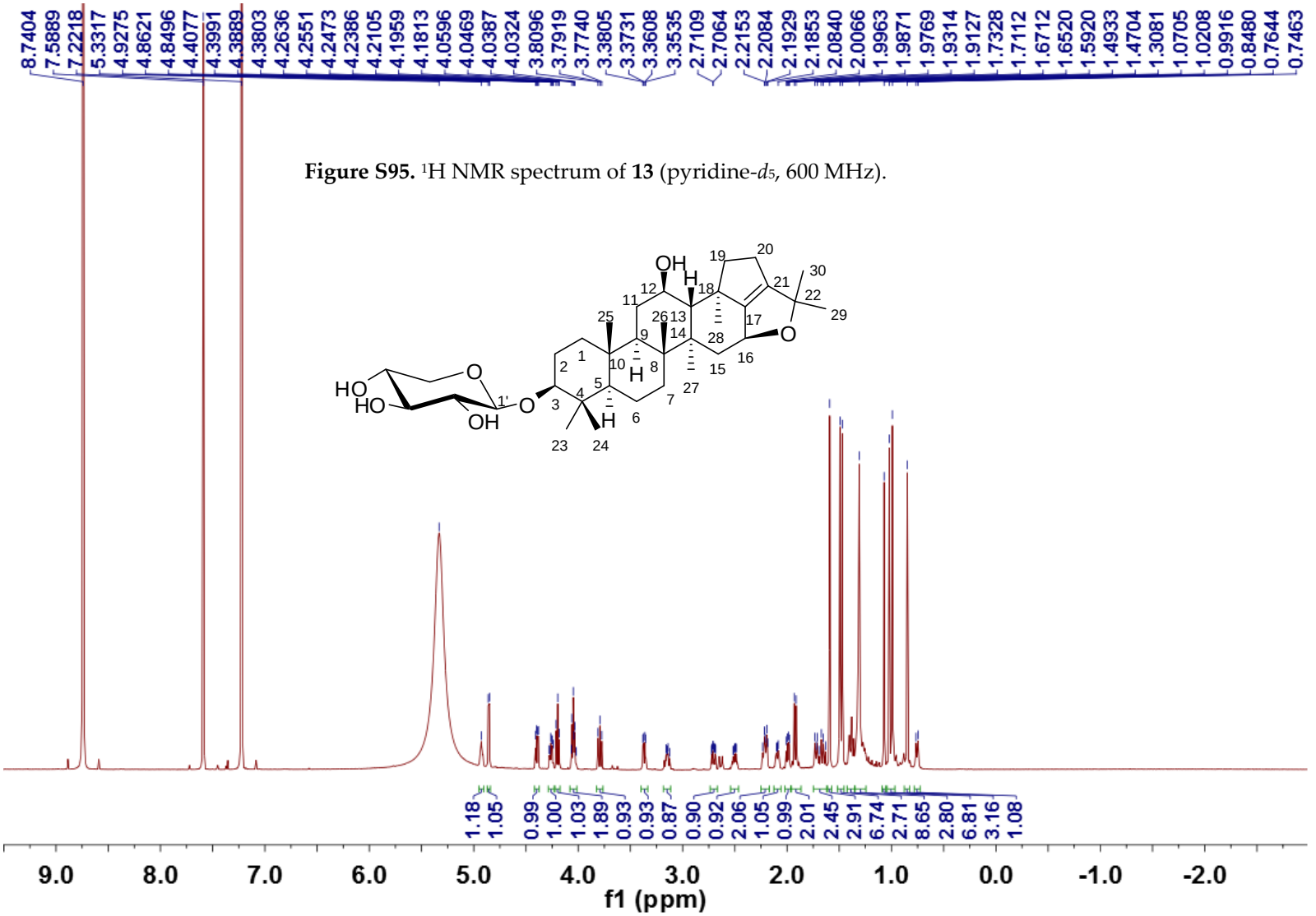


Figure S95. ^{1}H NMR spectrum of **13** (pyridine-d_5, 600 MHz).

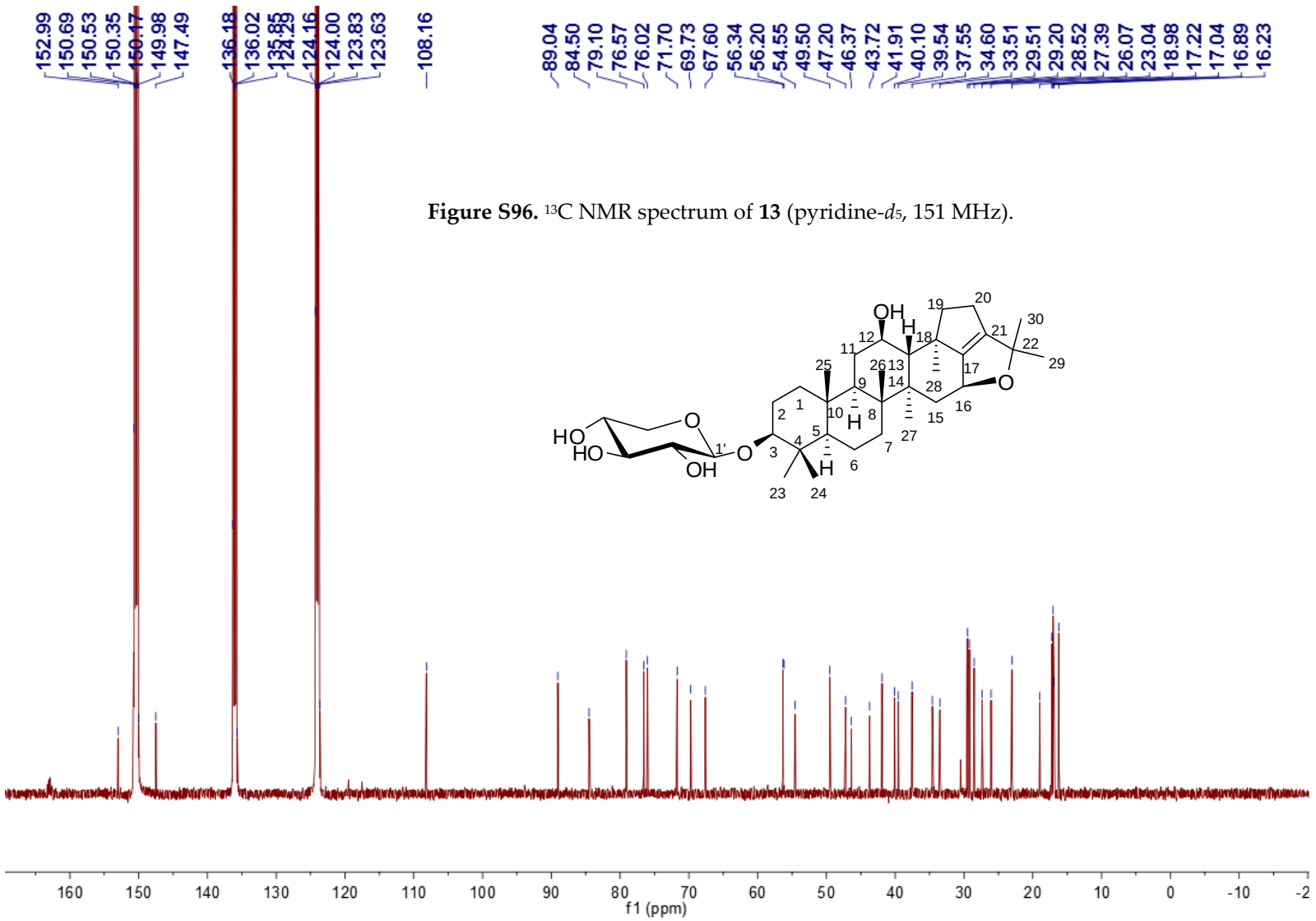


Figure S96. ^{13}C NMR spectrum of **13** (pyridine-d_5, 151 MHz).

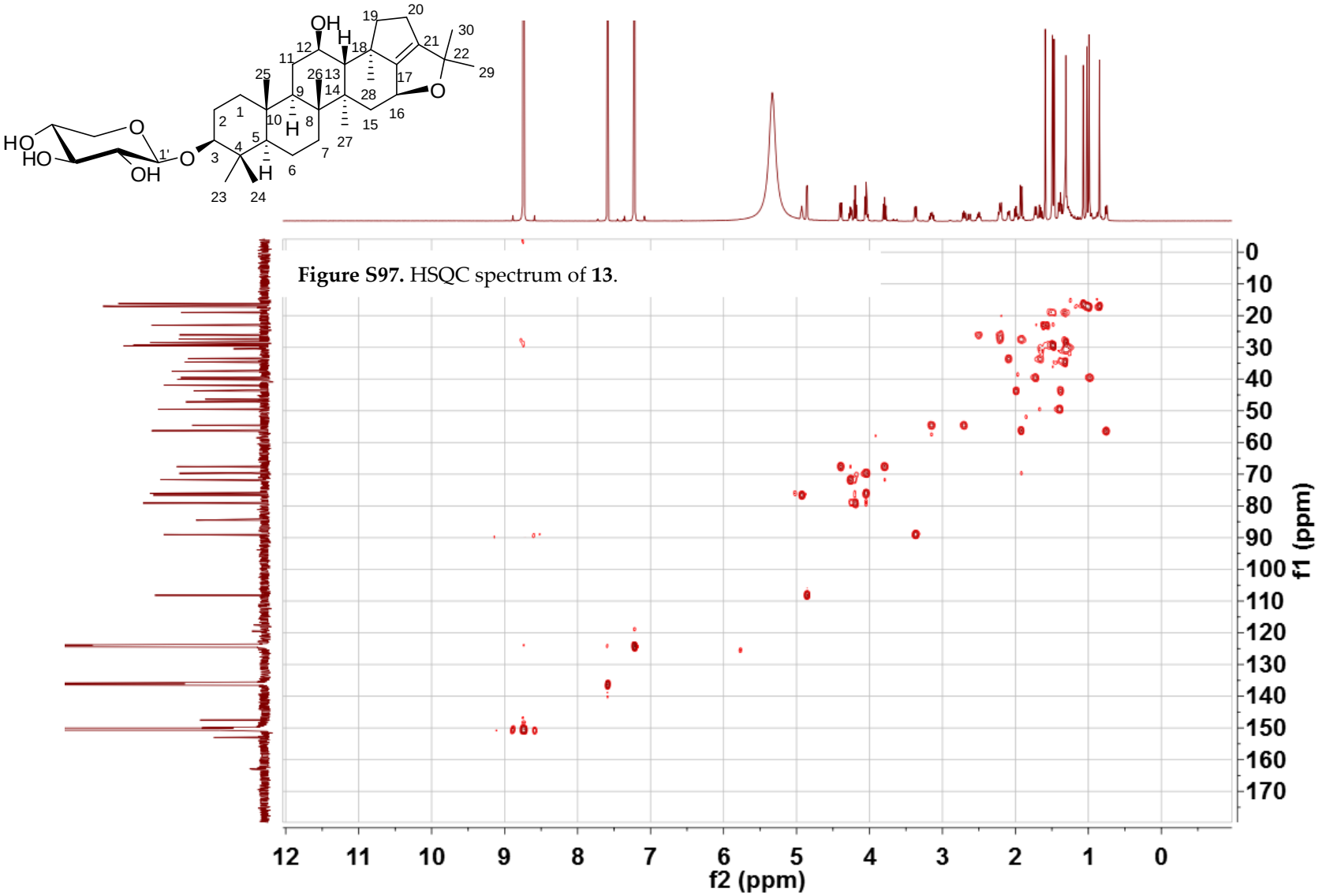


Figure S97. HSQC spectrum of **13**.

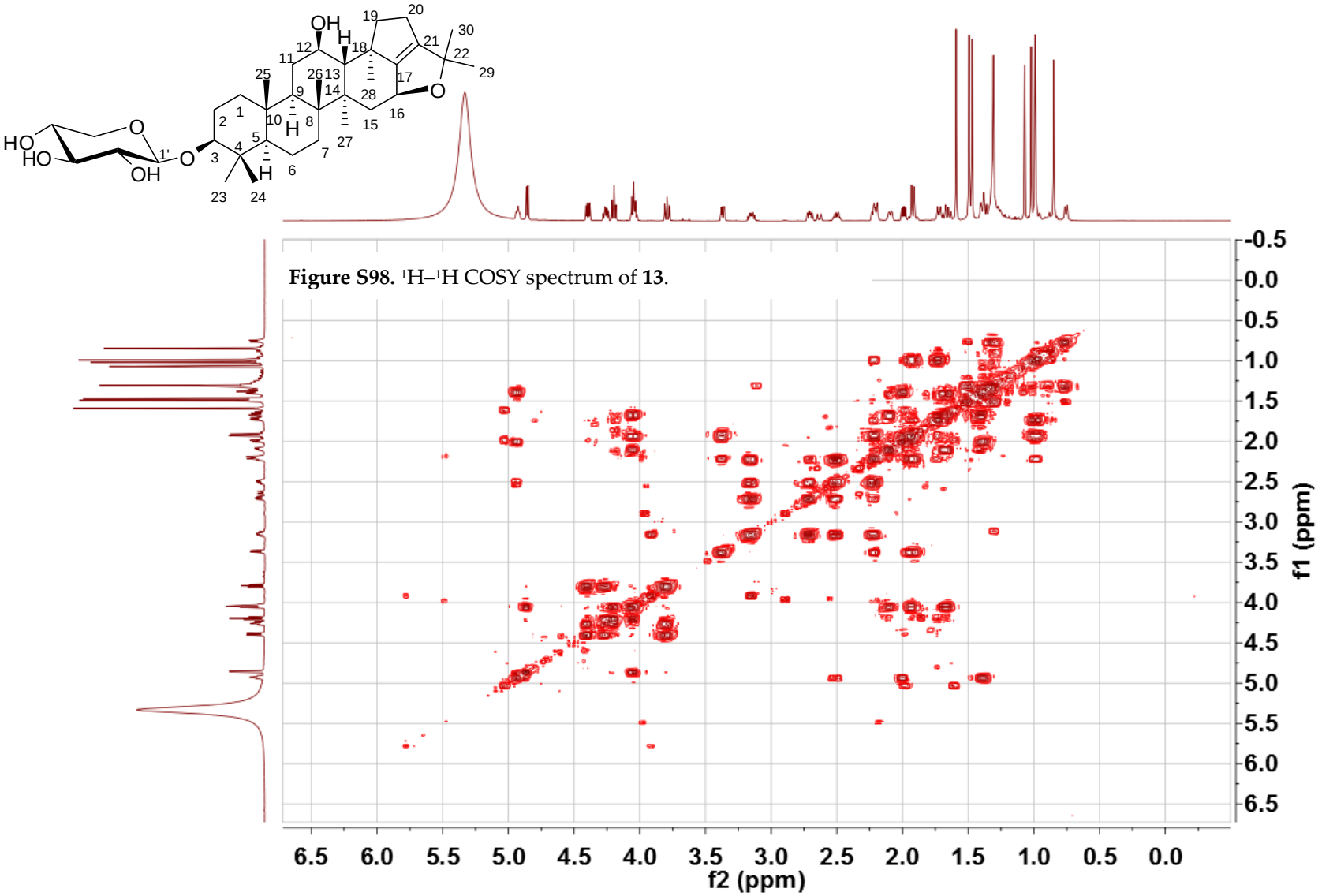


Figure S98. ^{1}H–^{1}H COSY spectrum of **13**.

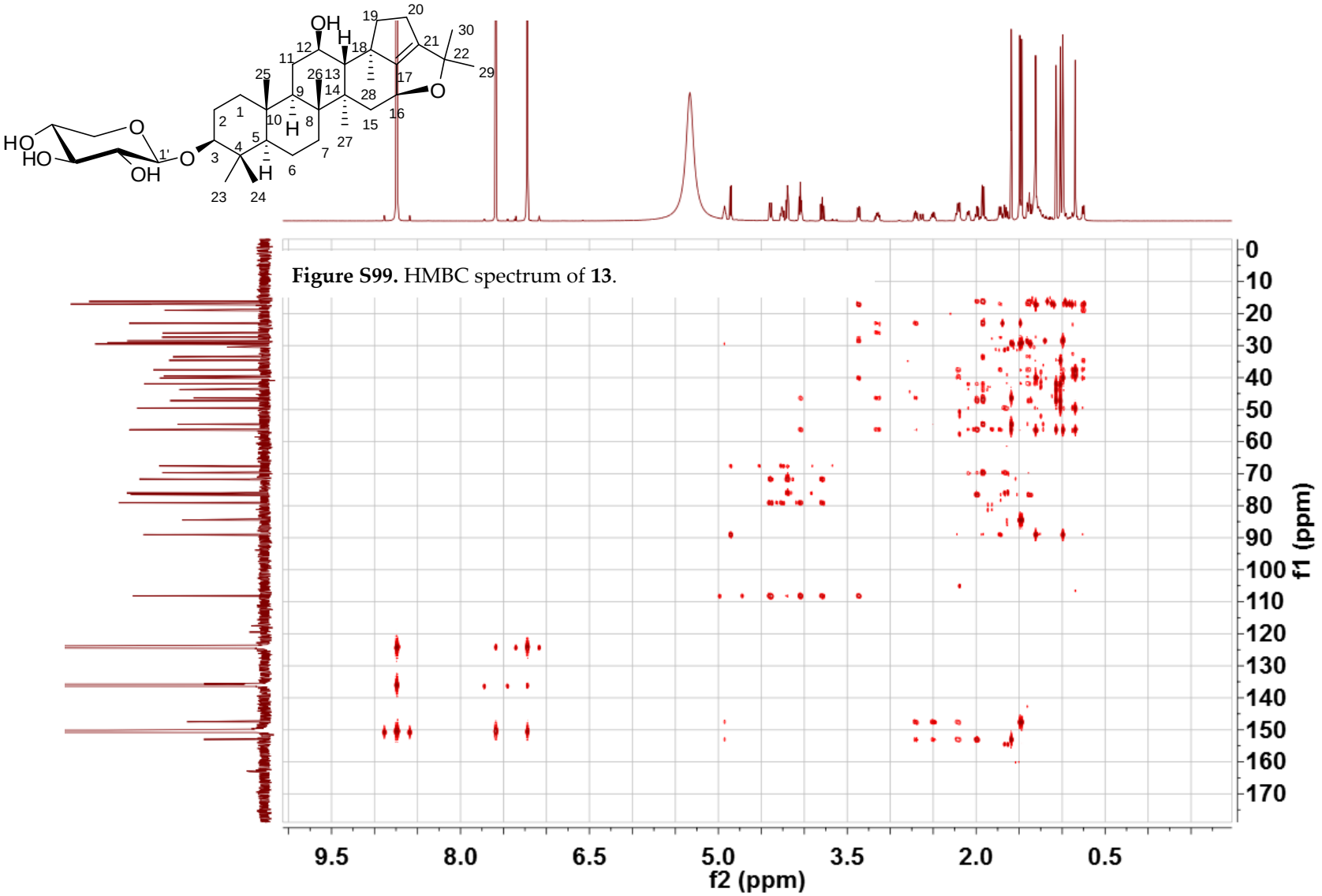


Figure S99. HMBC spectrum of **13**.

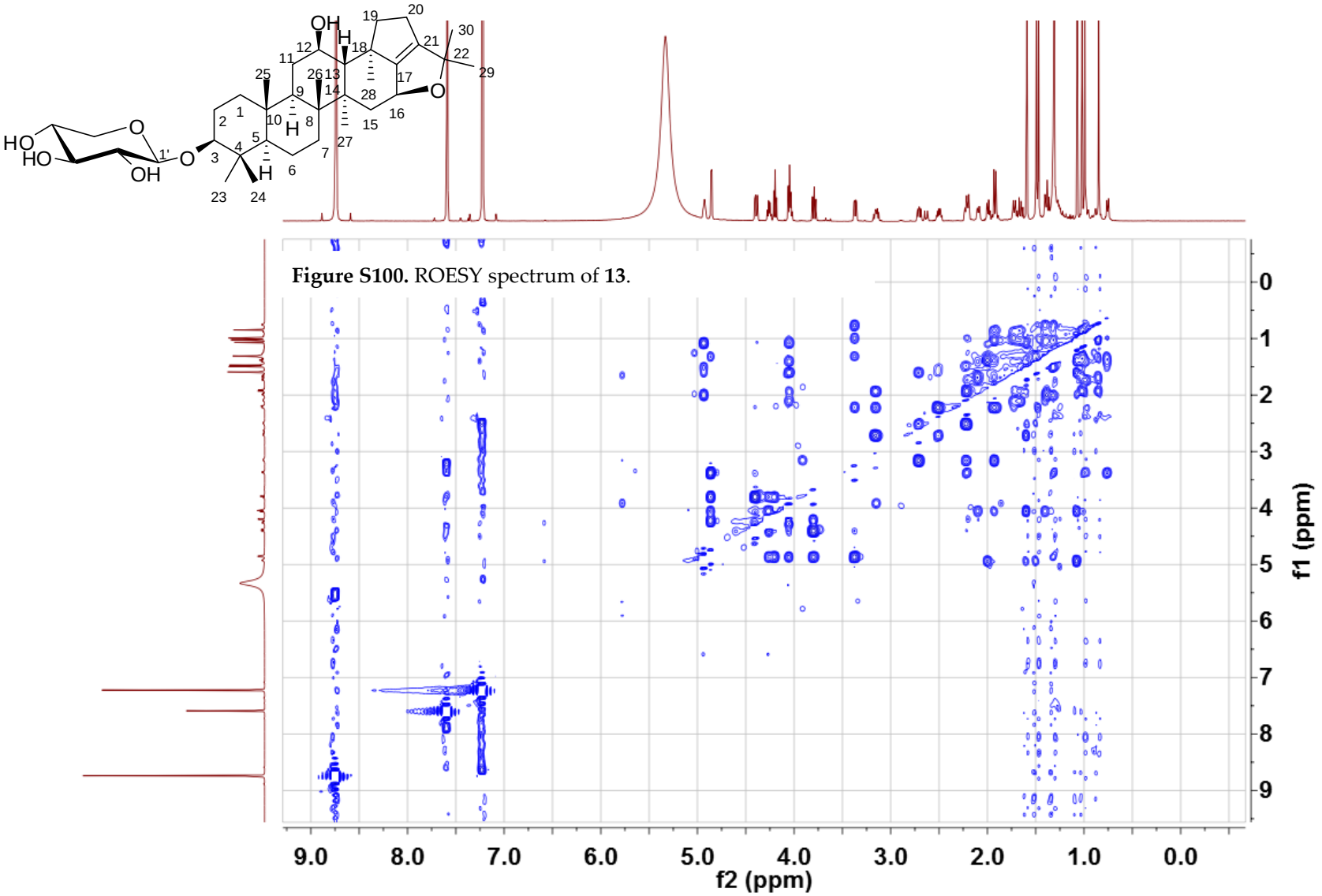


Figure S100. ROESY spectrum of **13**.

Data Filename	180824ESIA4.d	**Sample Name**	pdt 54a
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/24/2018 2:17:49 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
260	0	ESI

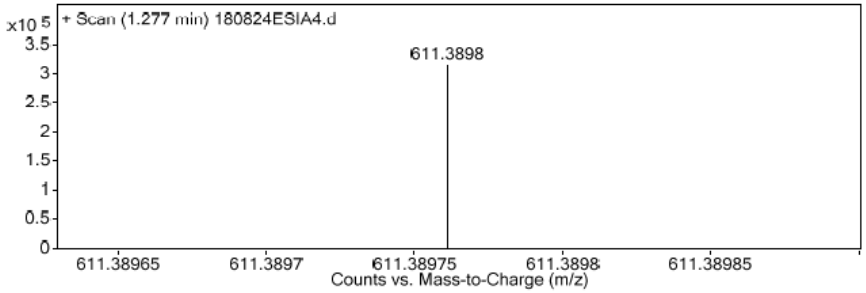


Figure S101. HRESIMS spectrum of **13**.

Peak List

m/z	z	Abund	Formula	Ion
136.9188		104846.75		
230.905		112693.76		
611.3898	1	314712.94	C35 H56 Na O7	M+
612.3924	1	113185.77	C35 H56 Na O7	M+
627.3625	1	84164.83		
687.3748	1	88003.44		
741.3473	1	410123.28		
742.3507	1	159524.27		
1329.7461	1	95505.48		
1330.7493	1	82139.52		

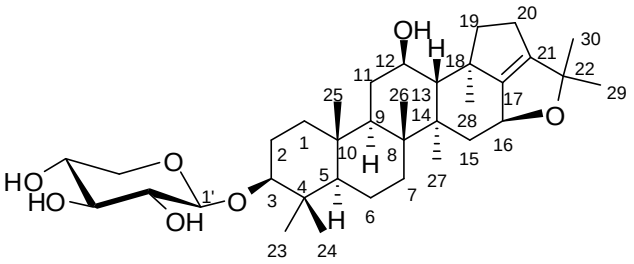
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	3	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C35 H56 Na O7	611.3924	611.3898	2.6	4.2	7.5

--- End Of Report ---



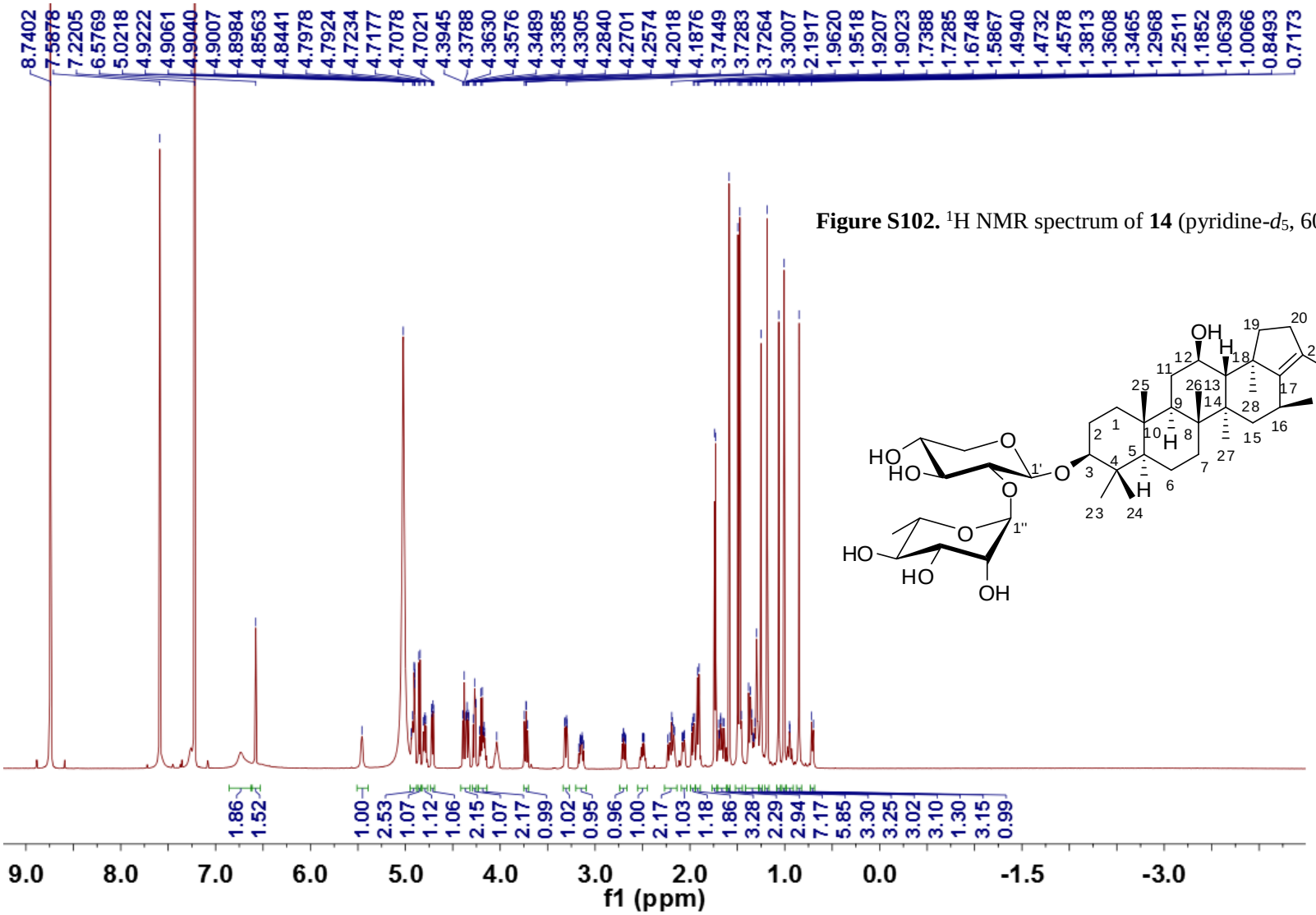


Figure S102. ^{1}H NMR spectrum of **14** (pyridine-d_5, 600 MHz).

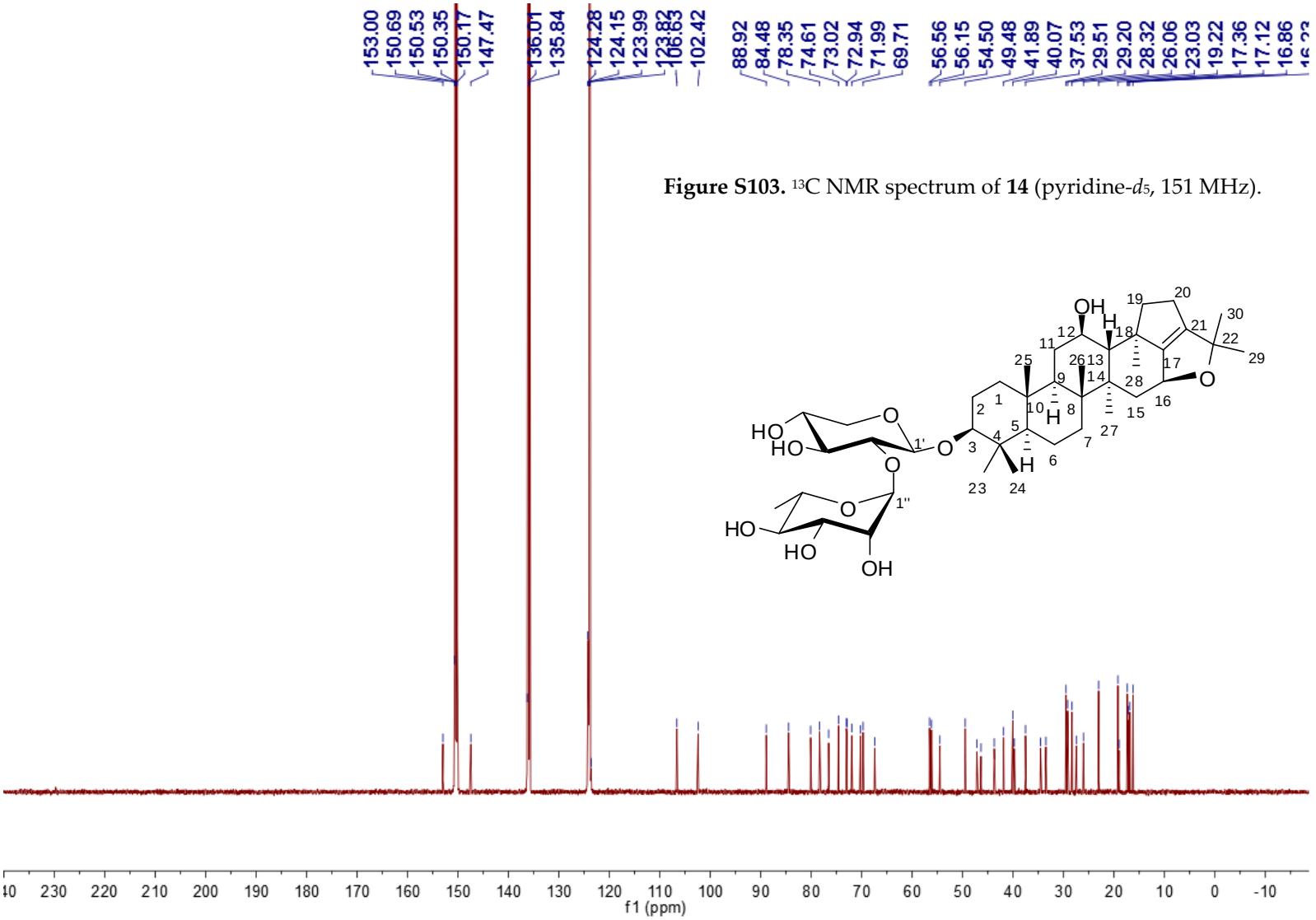


Figure S103. ^{13}C NMR spectrum of **14** (pyridine-d_5, 151 MHz).

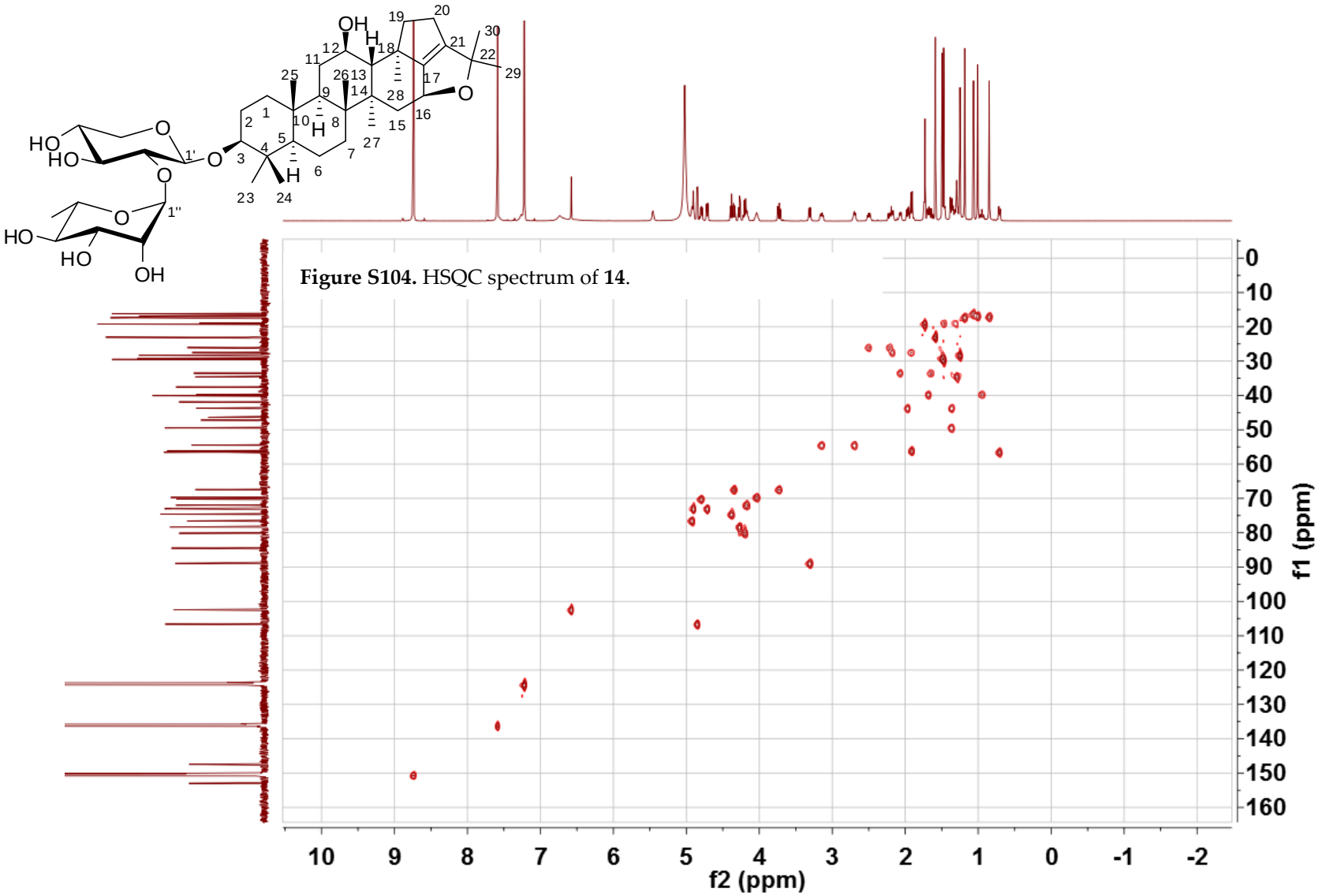


Figure S104. HSQC spectrum of **14**.

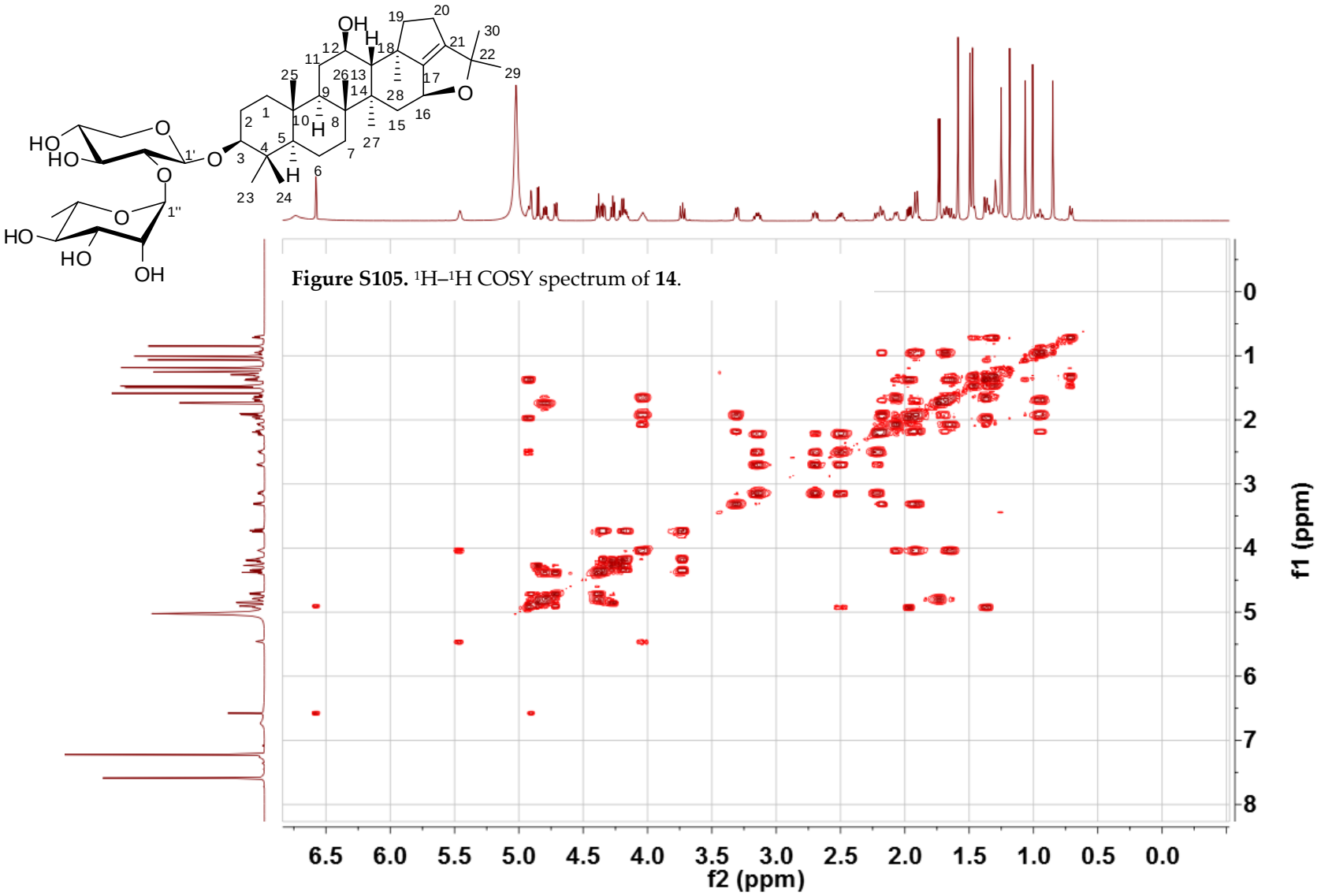


Figure S105. ^{1}H–^{1}H COSY spectrum of **14**.

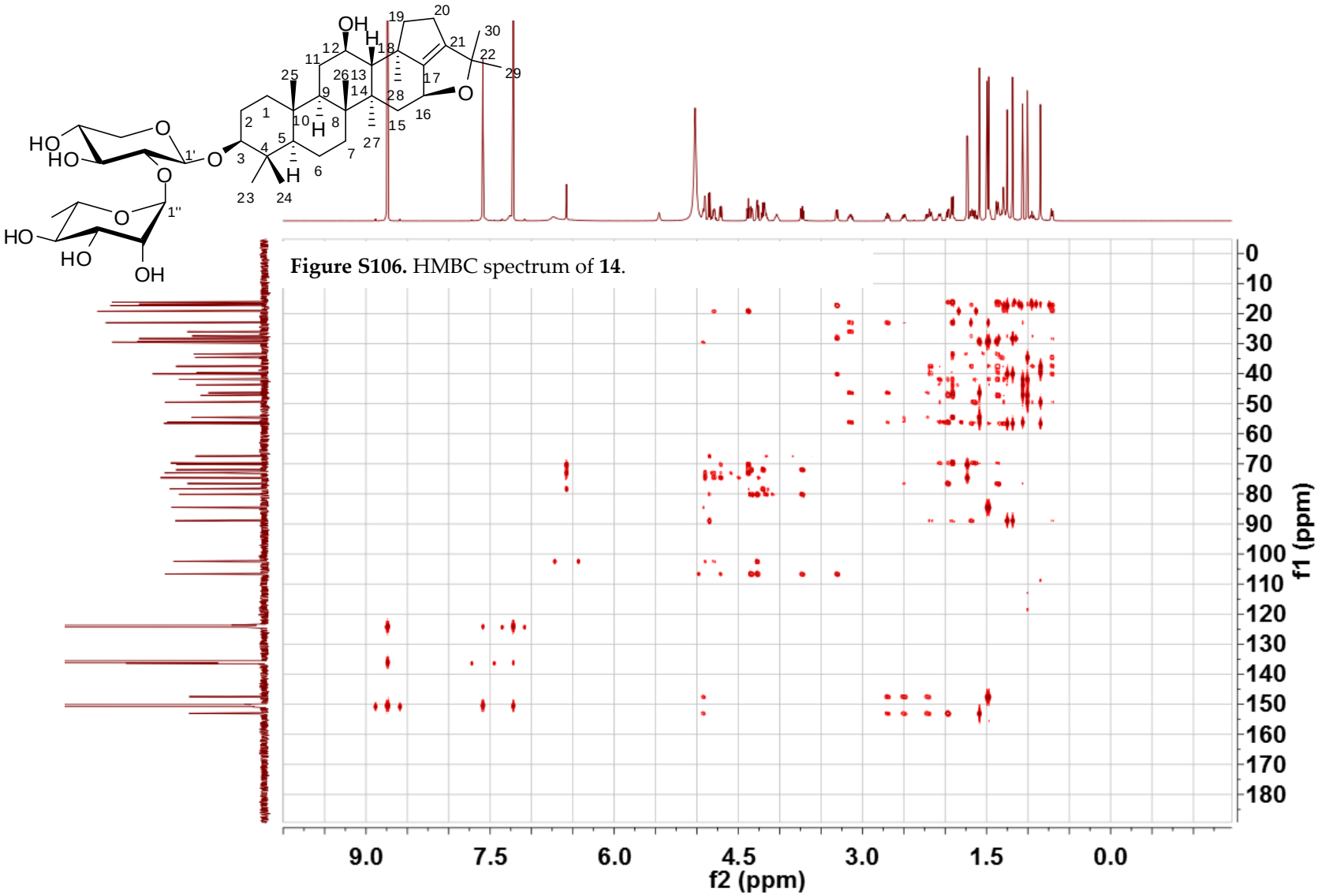


Figure S106. HMBC spectrum of **14**.

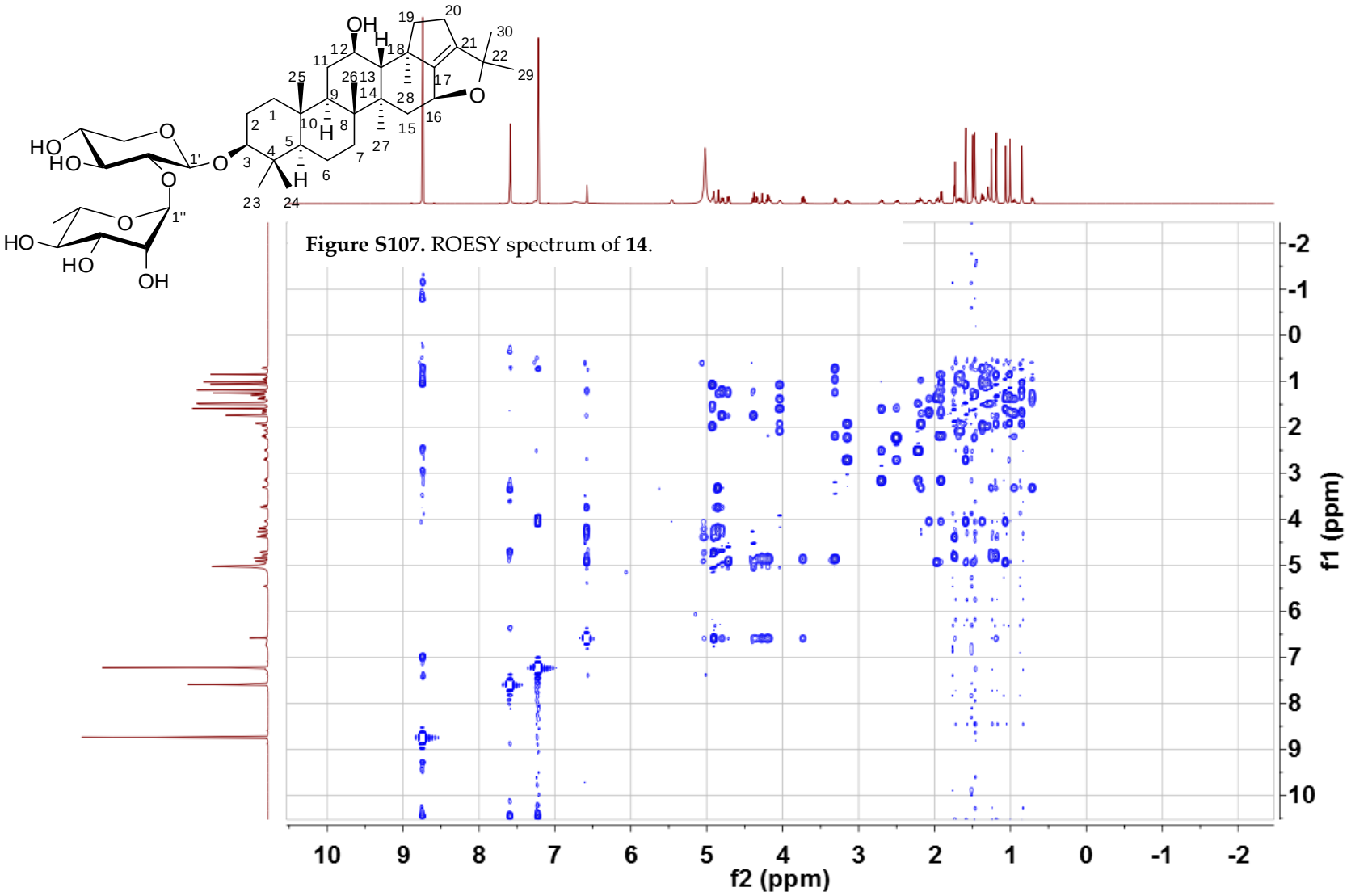


Figure S107. ROESY spectrum of **14**.

Data Filename	180828ESIA5.d	**Sample Name**	pdt53
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/28/2018 9:58:56 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

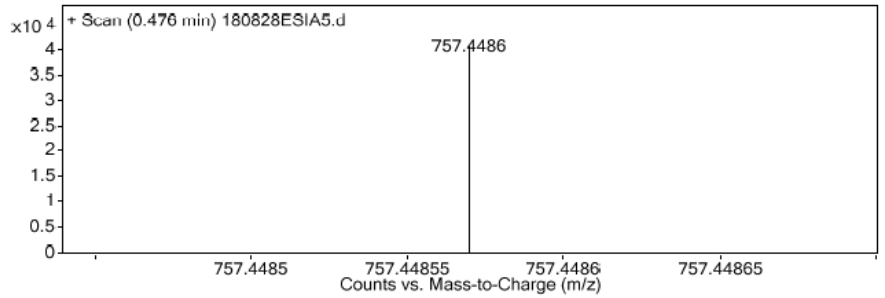


Figure S108. HRESIMS spectrum of **14**.

Peak List

m/z	z	Abund	Formula	Ion
112.1872	1	21524.53		
145.2493	1	27599.95		
274.2731	1	24295.63		
318.2995	1	25232.83		
619.5259	1	26303.13		
757.4486	1	40351.51	C41 H66 Na O11	M+
1188.0319	1	28121.41		
1189.0342	1	21680.37		
1216.0623	1	25862.58		
1217.066	1	21227.8		

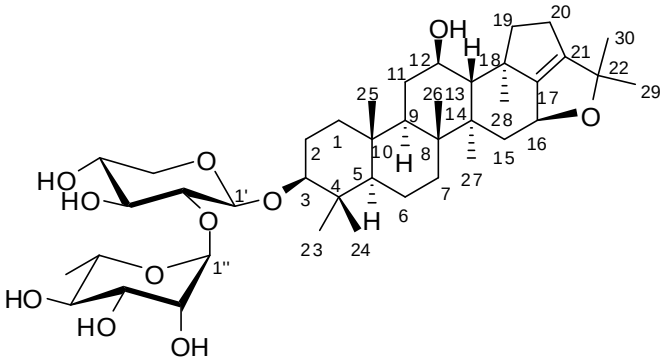
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C41 H66 Na O11	757.4503	757.4486	1.7	2.2	8.5

--- End Of Report ---



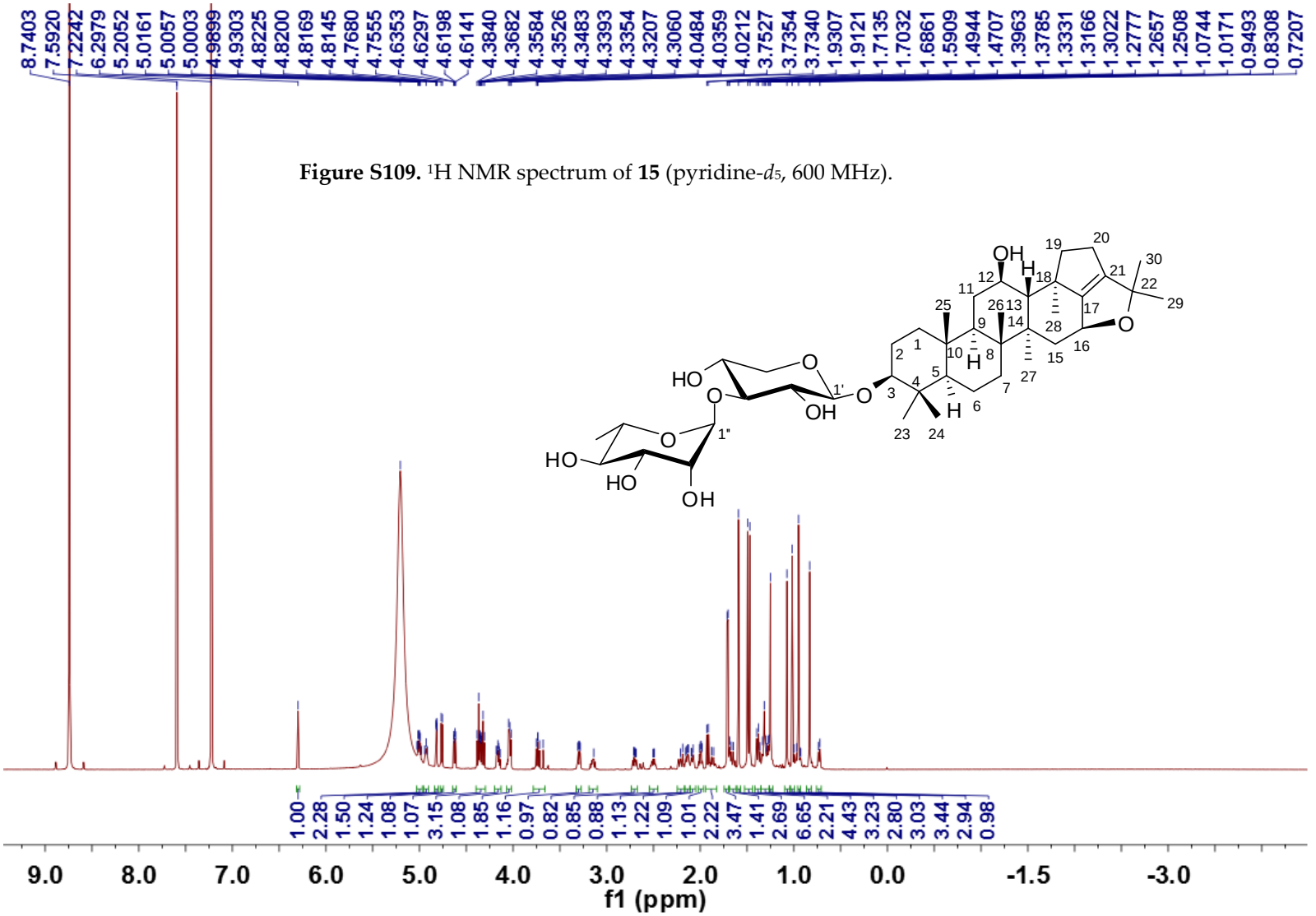


Figure S109. ^{1}H NMR spectrum of **15** (pyridine-d_5, 600 MHz).

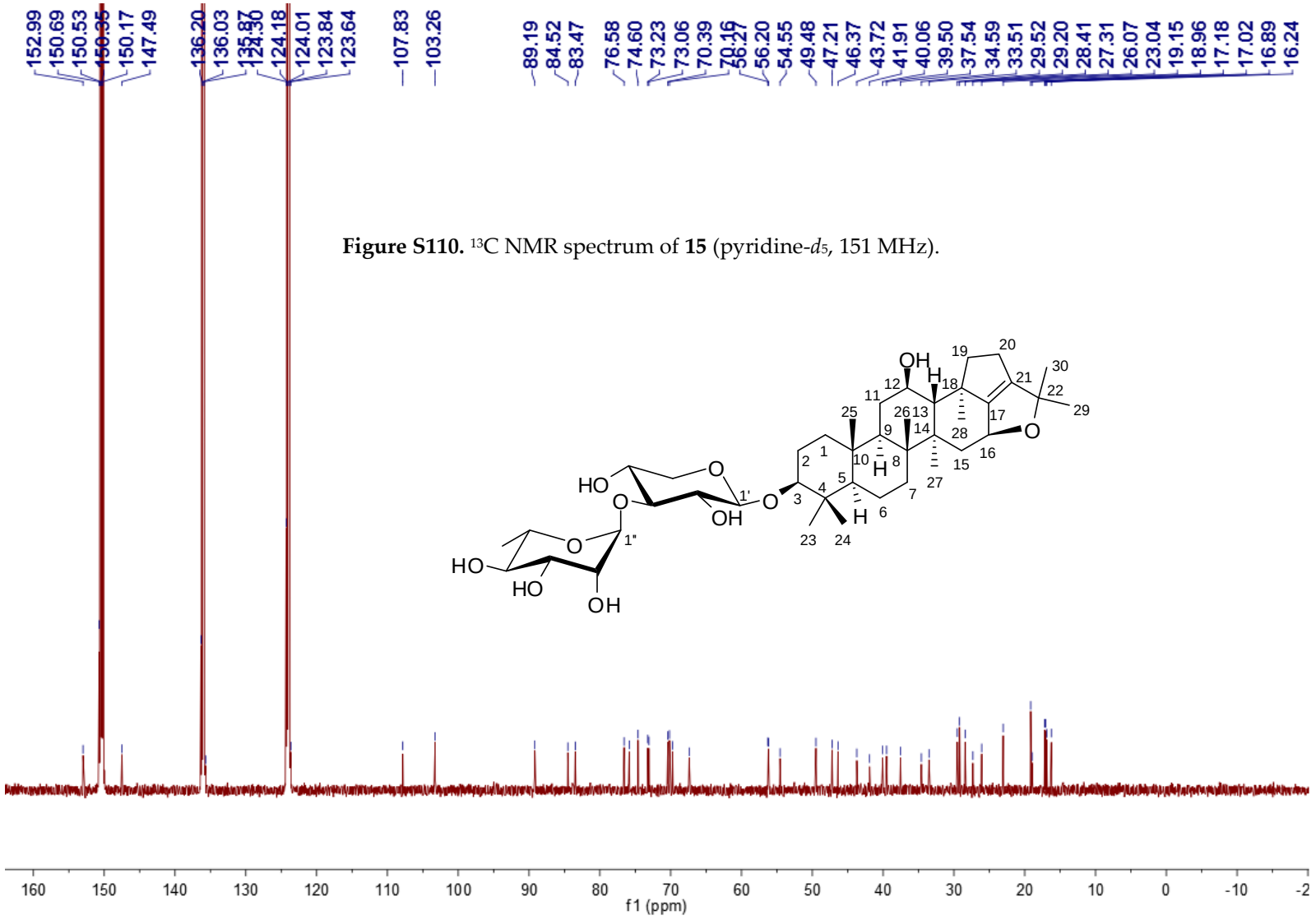


Figure S110. ^{13}C NMR spectrum of **15** (pyridine-d_5, 151 MHz).

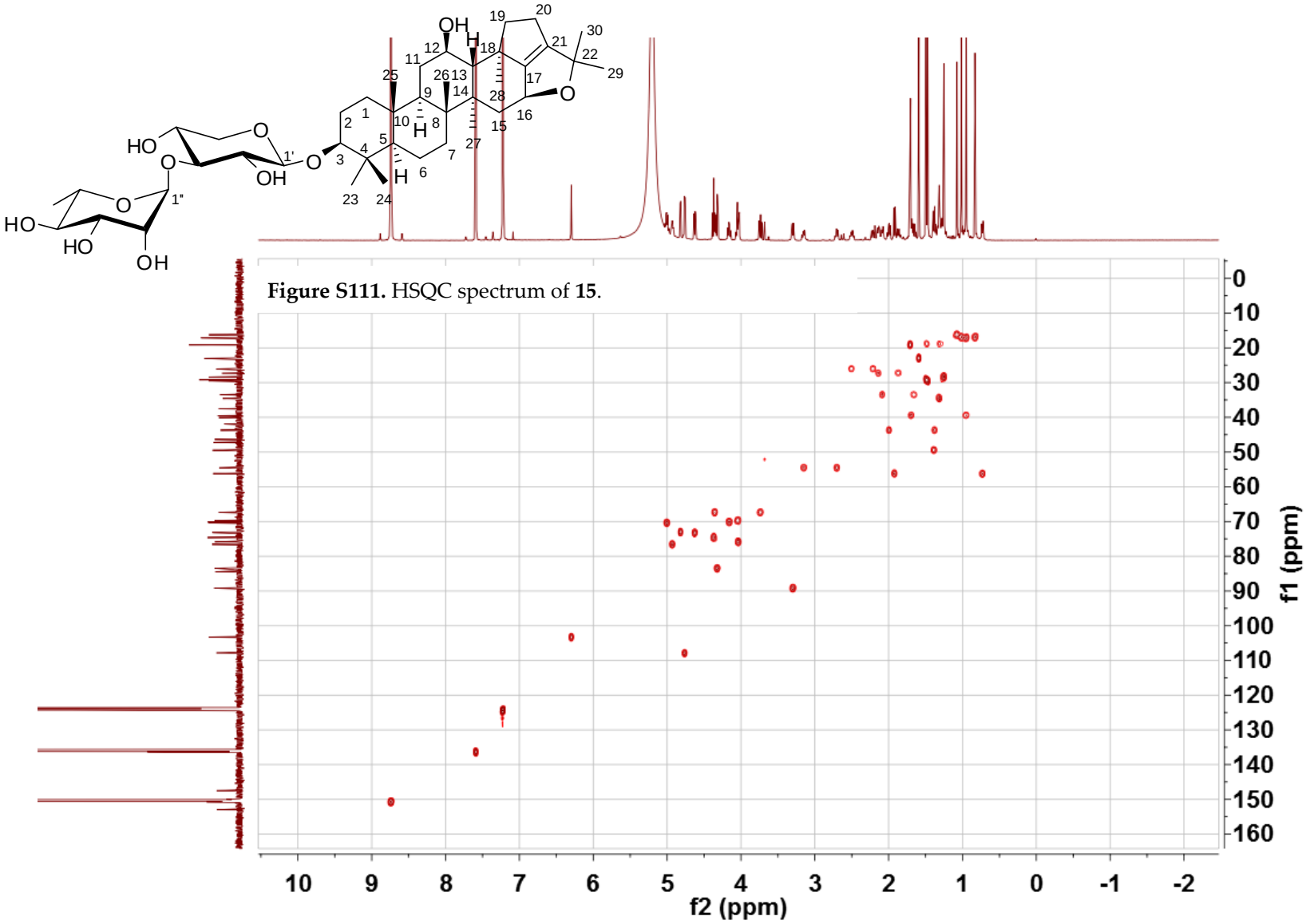


Figure S111. HSQC spectrum of **15**.

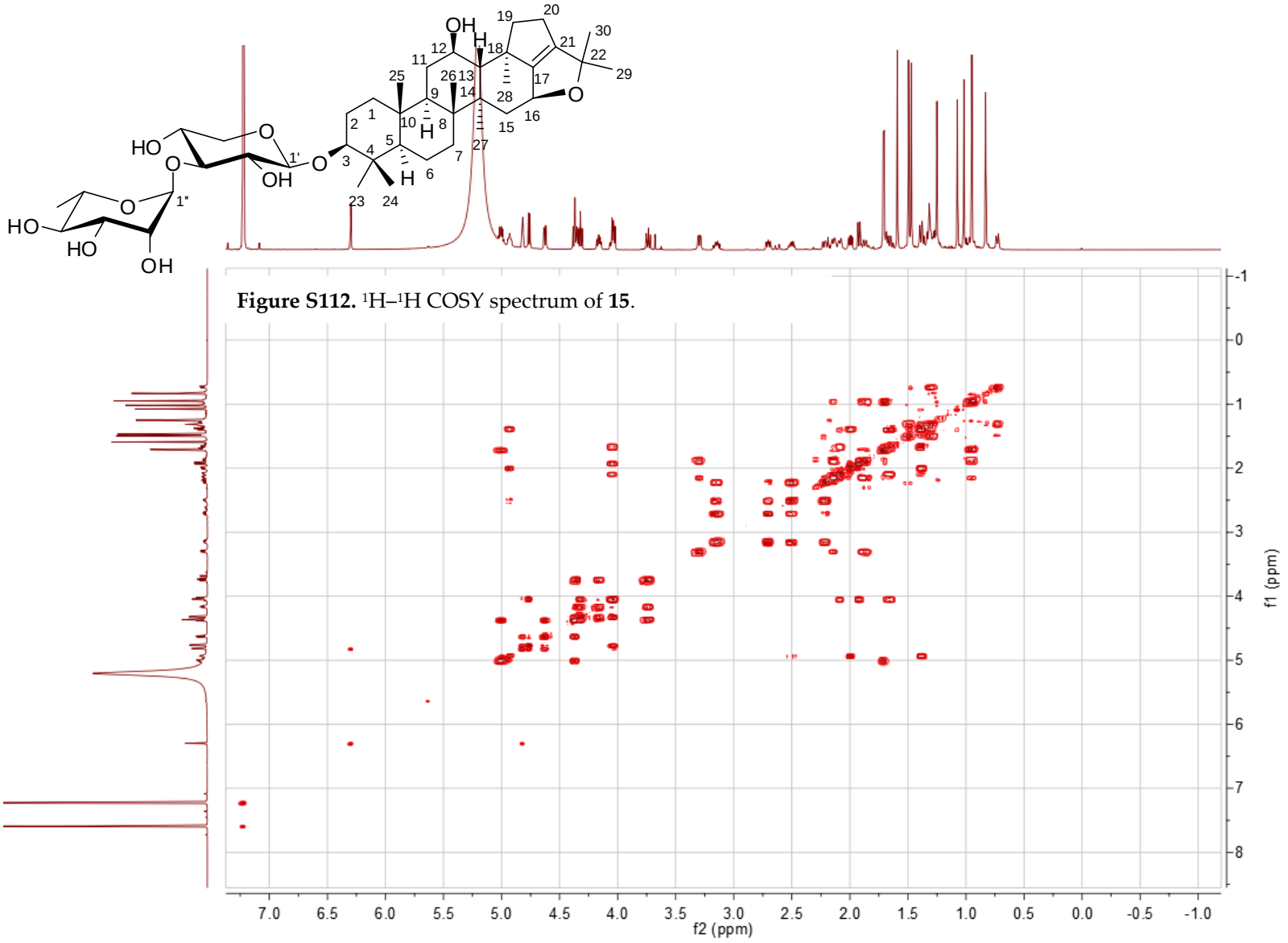


Figure S112. ^{1}H–^{1}H COSY spectrum of **15**.

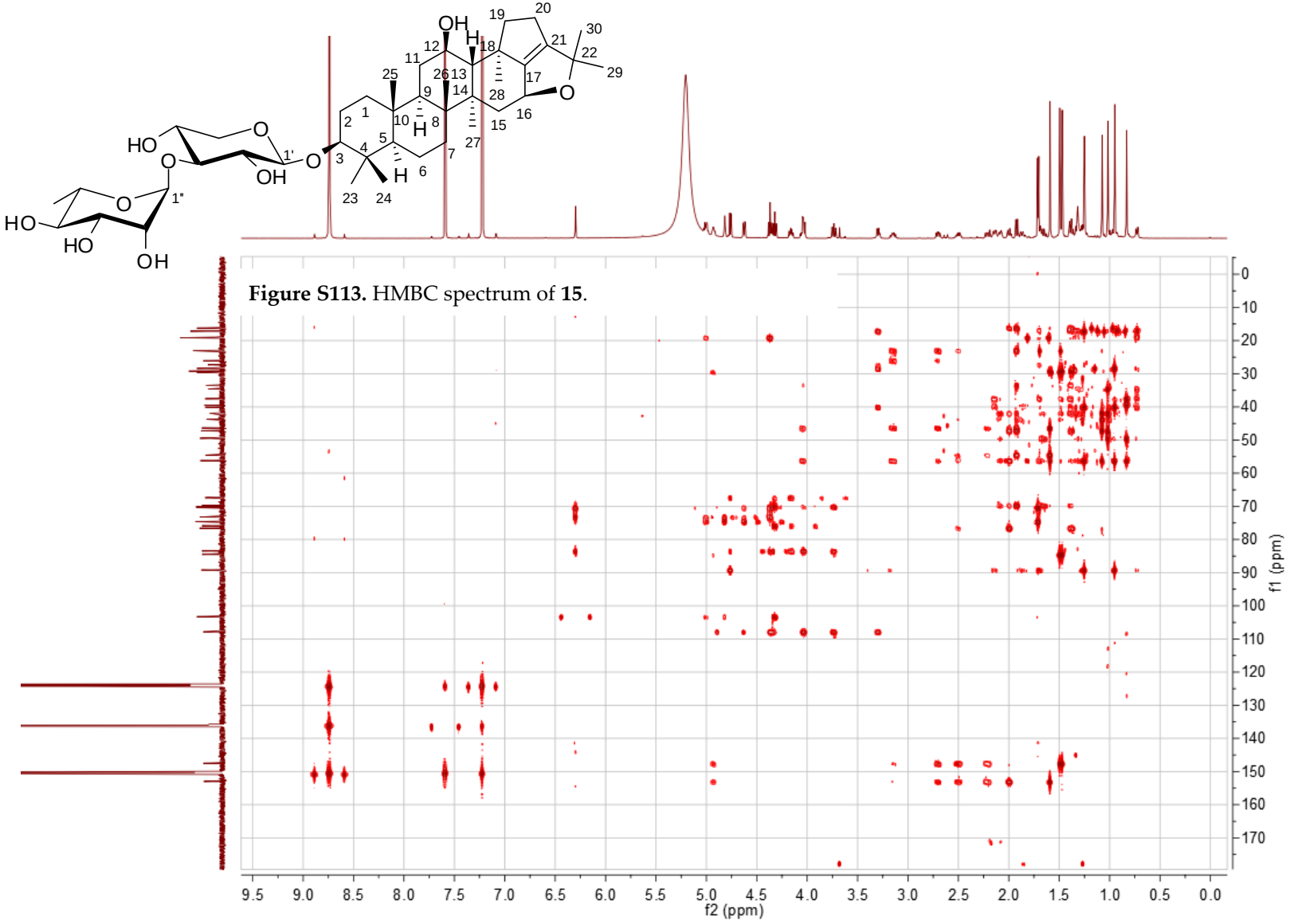


Figure S113. HMBC spectrum of **15**.

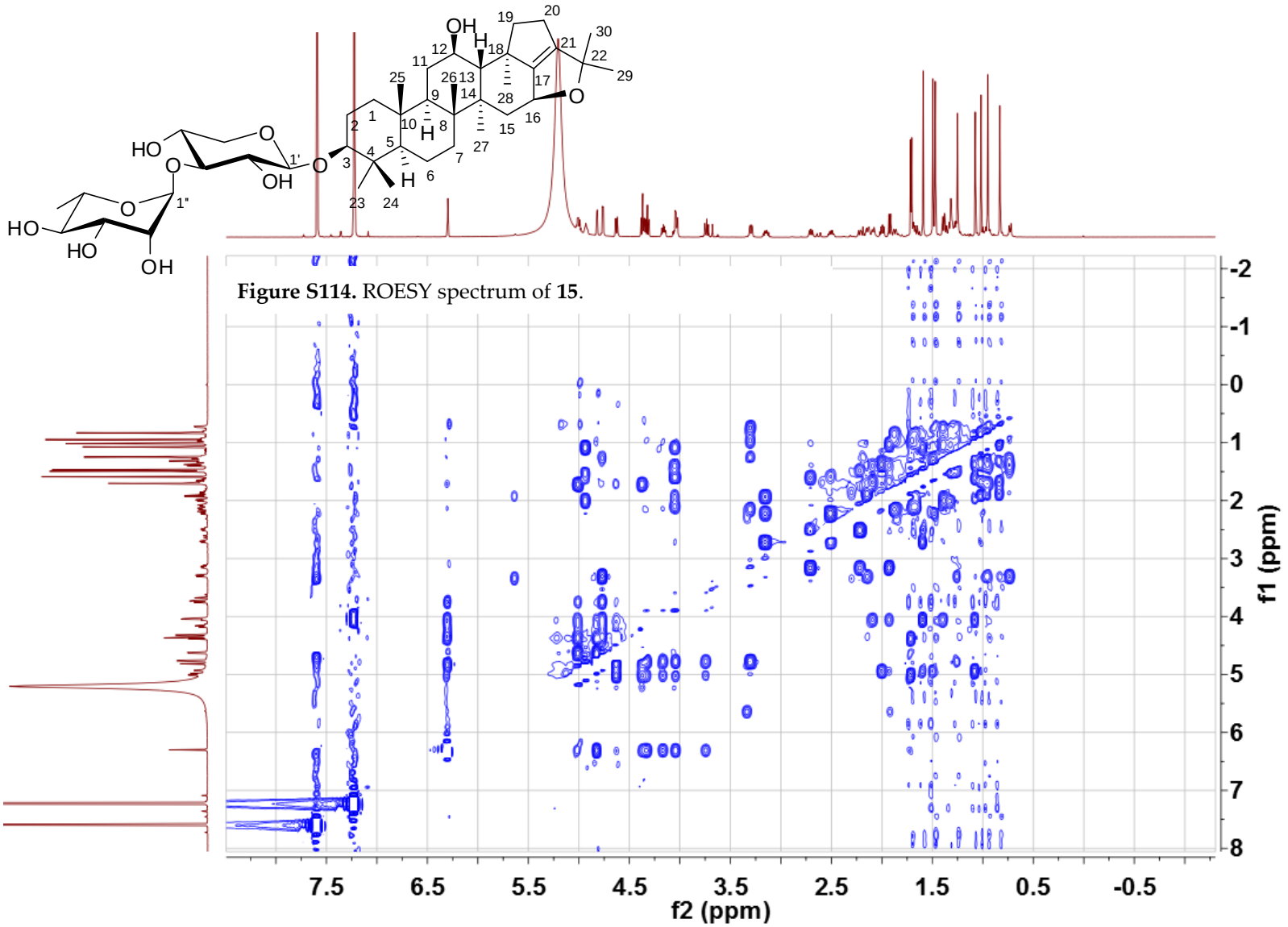


Figure S114. ROESY spectrum of **15**.

Data Filename	180829ESIA7.d	**Sample Name**	pdt56
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/29/2018 1:53:43 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

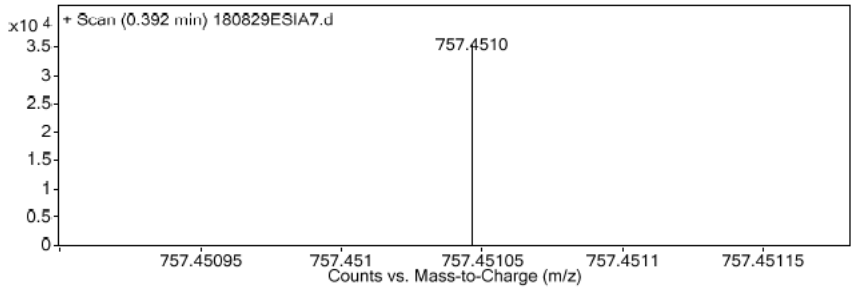


Figure S115. HRESIMS spectrum of **15**.

Peak List

m/z	z	Abund	Formula	Ion
107.0364	1	14841.42		
112.188	1	21820.84		
145.2501		9138.86		
152.9476		8863.32		
754.4438	2	10091.41		
754.9467	2	9362.35		
757.451	1	35198.19	C41 H66 Na O11	M+
758.455	1	17220.5	C41 H66 Na O11	M+
773.4255	1	9346.08		
887.409	1	13063.82		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C41 H66 Na O11	757.4503	757.4510	-0.7	1.0	8.5

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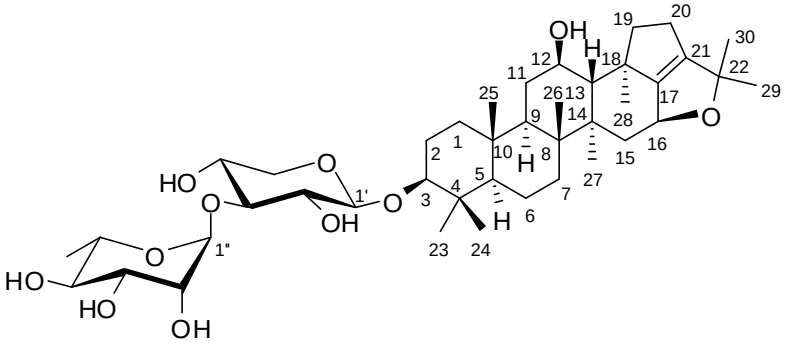

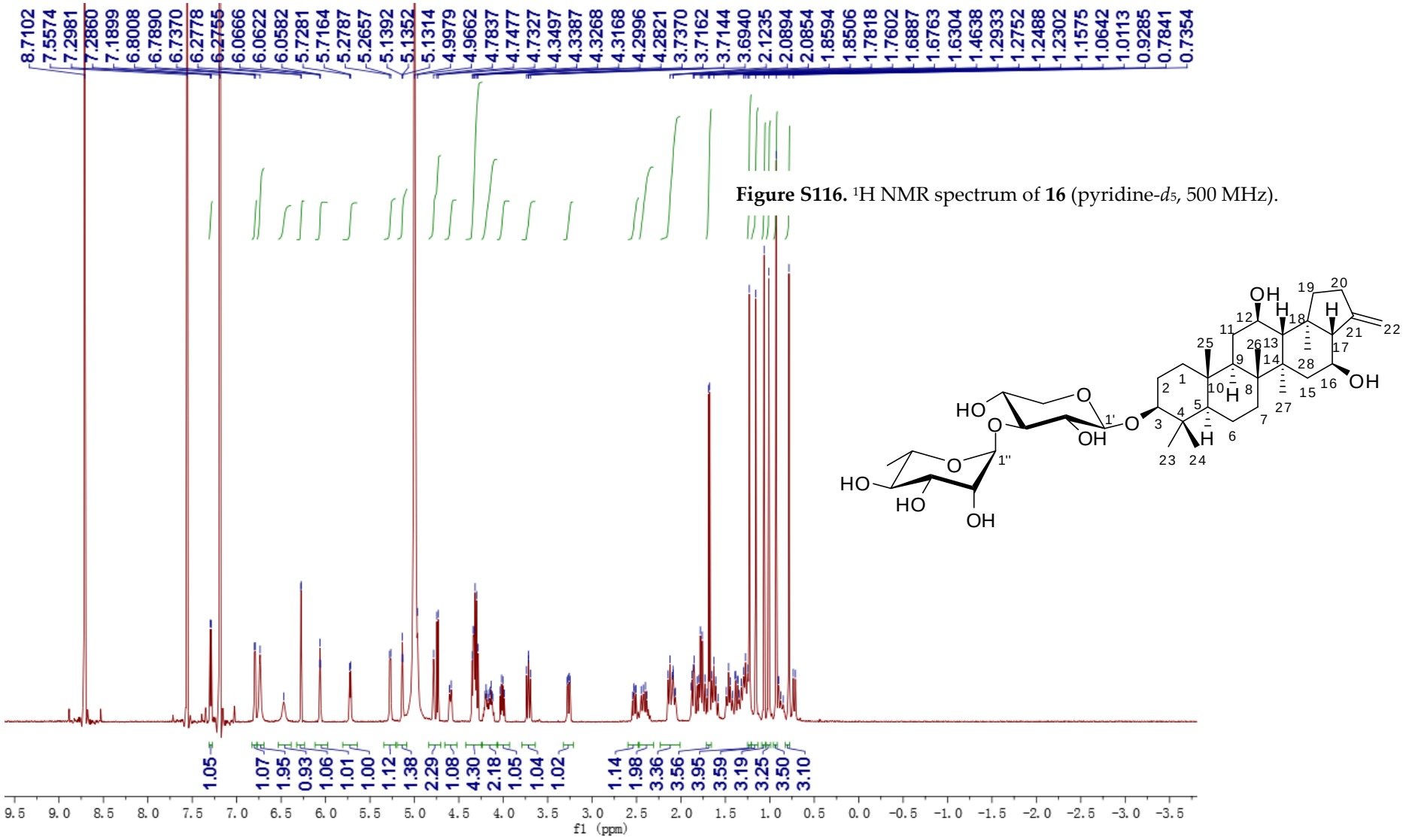

Figure S116. ^{1}H NMR spectrum of **16** (pyridine-d_5, 500 MHz).

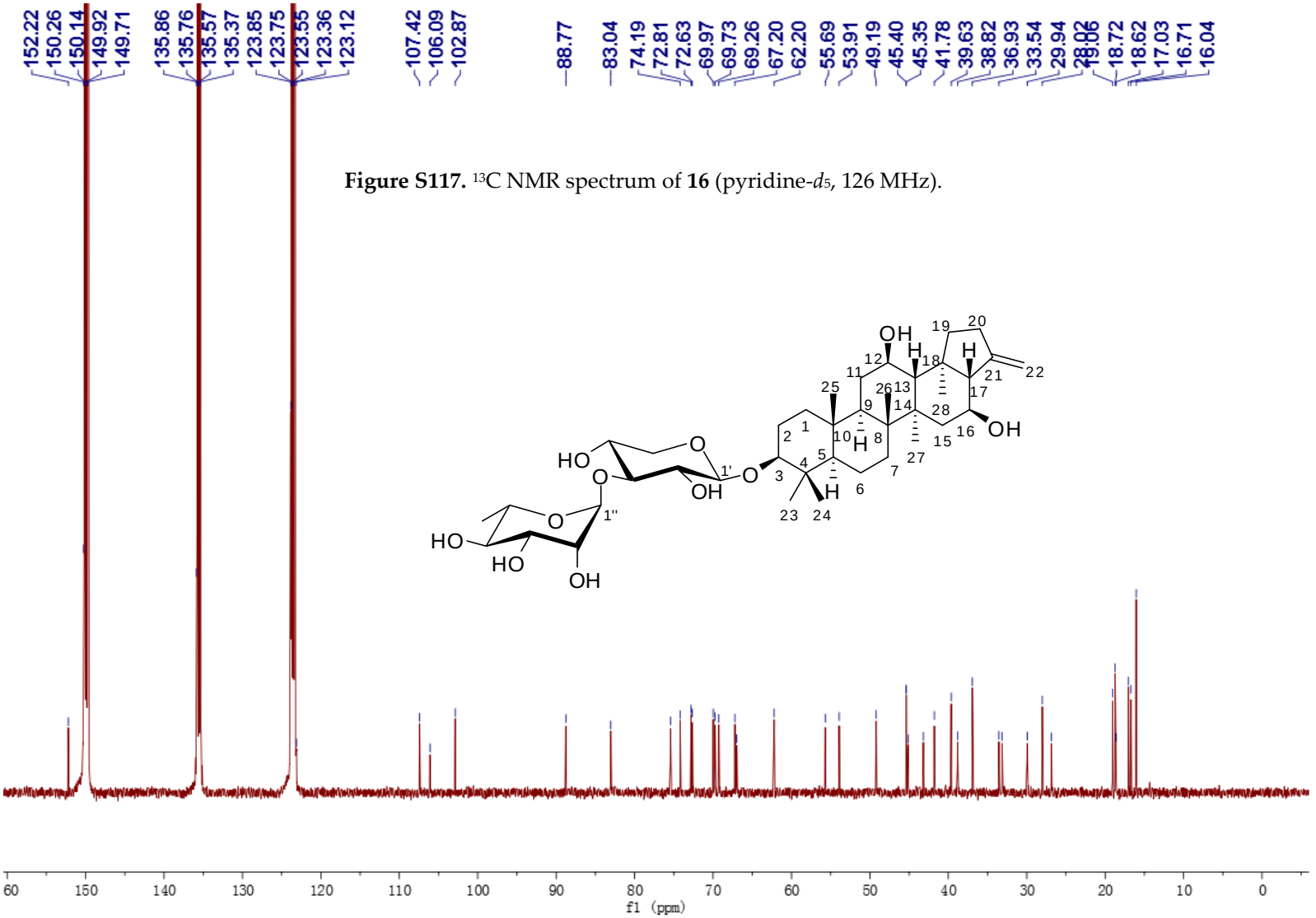

Figure S117. ^{13}C NMR spectrum of **16** (pyridine-d_5, 126 MHz).

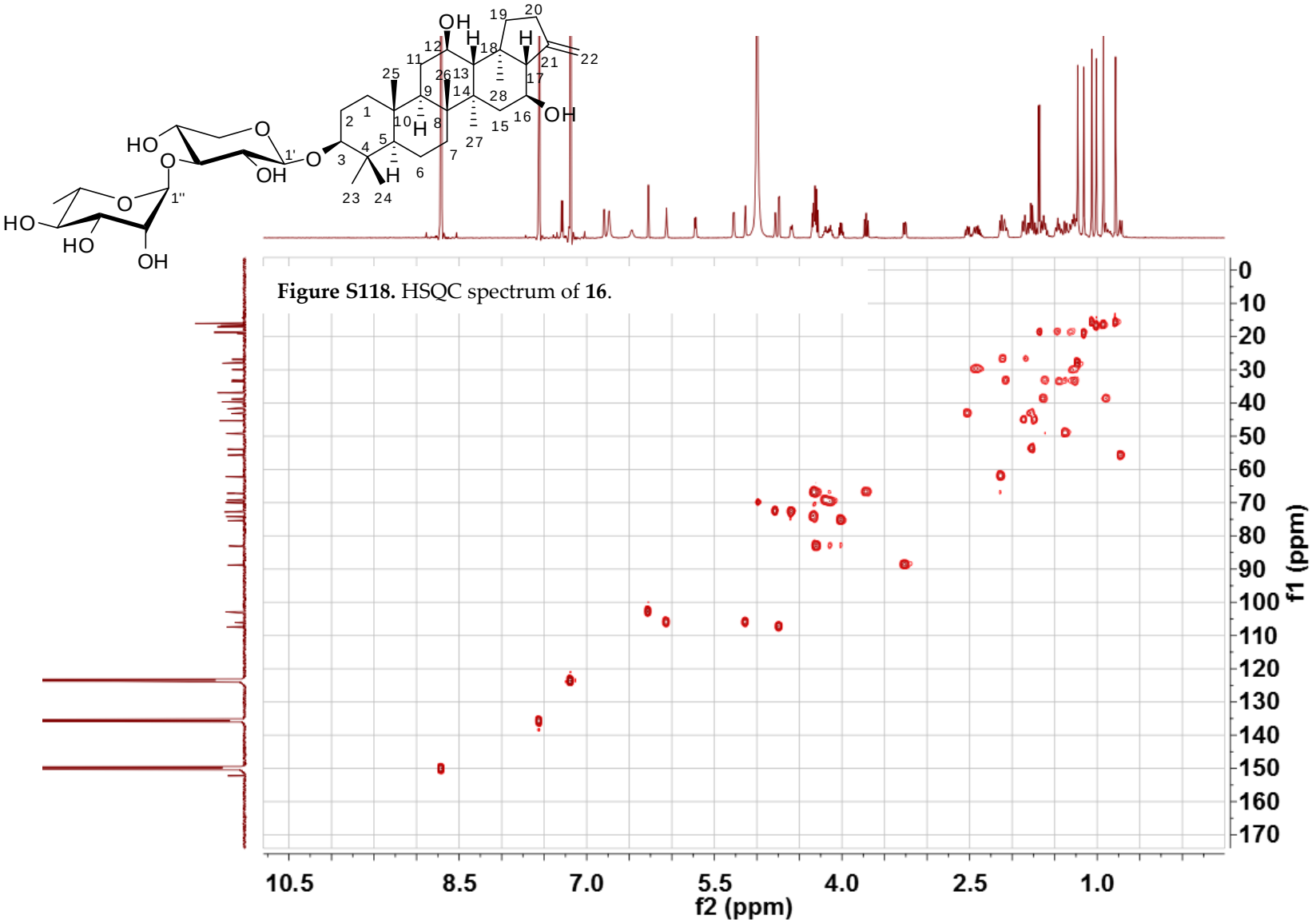

Figure S118. HSQC spectrum of **16**.

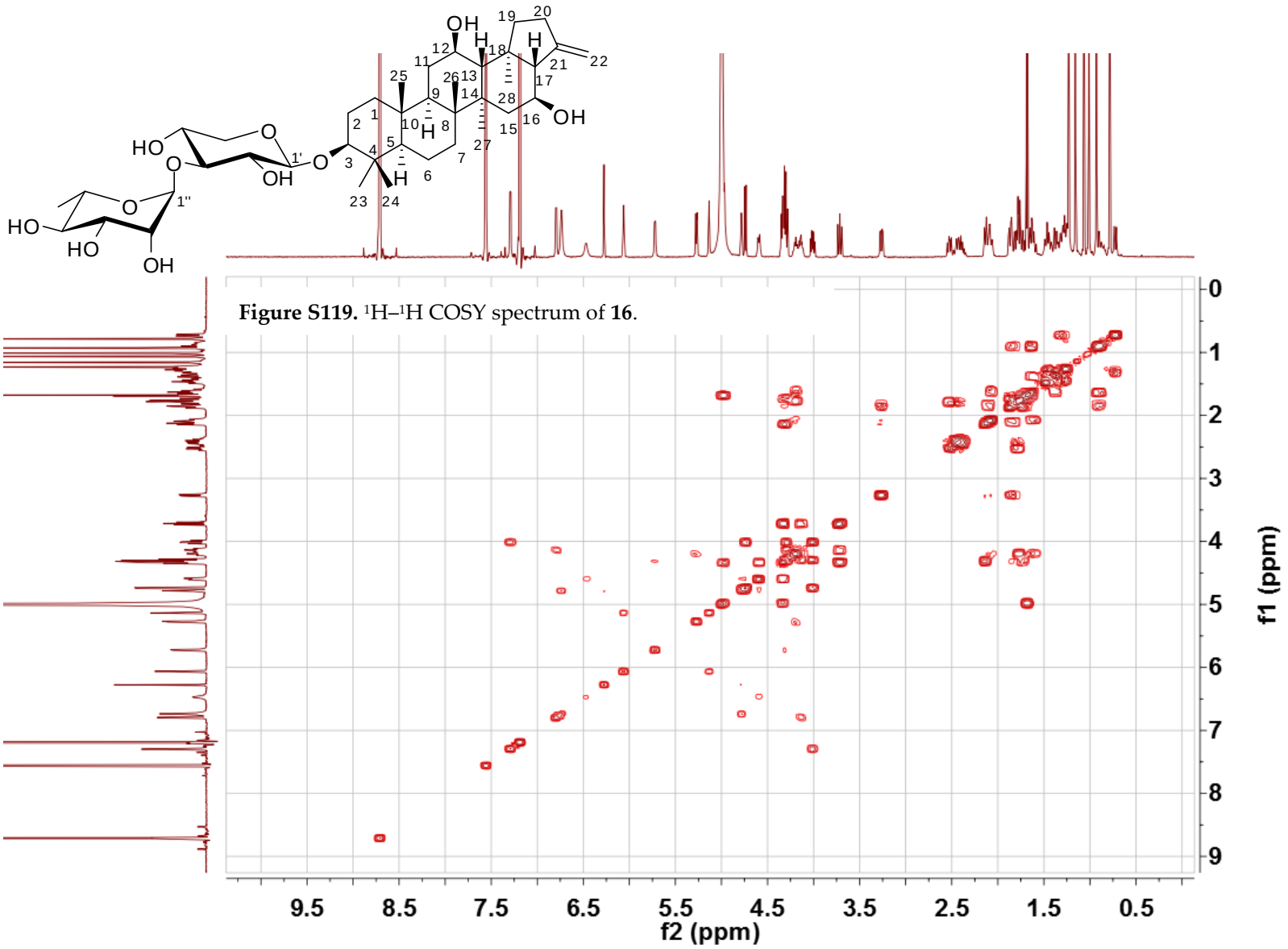

Figure S119. ^{1}H–^{1}H COSY spectrum of **16**.

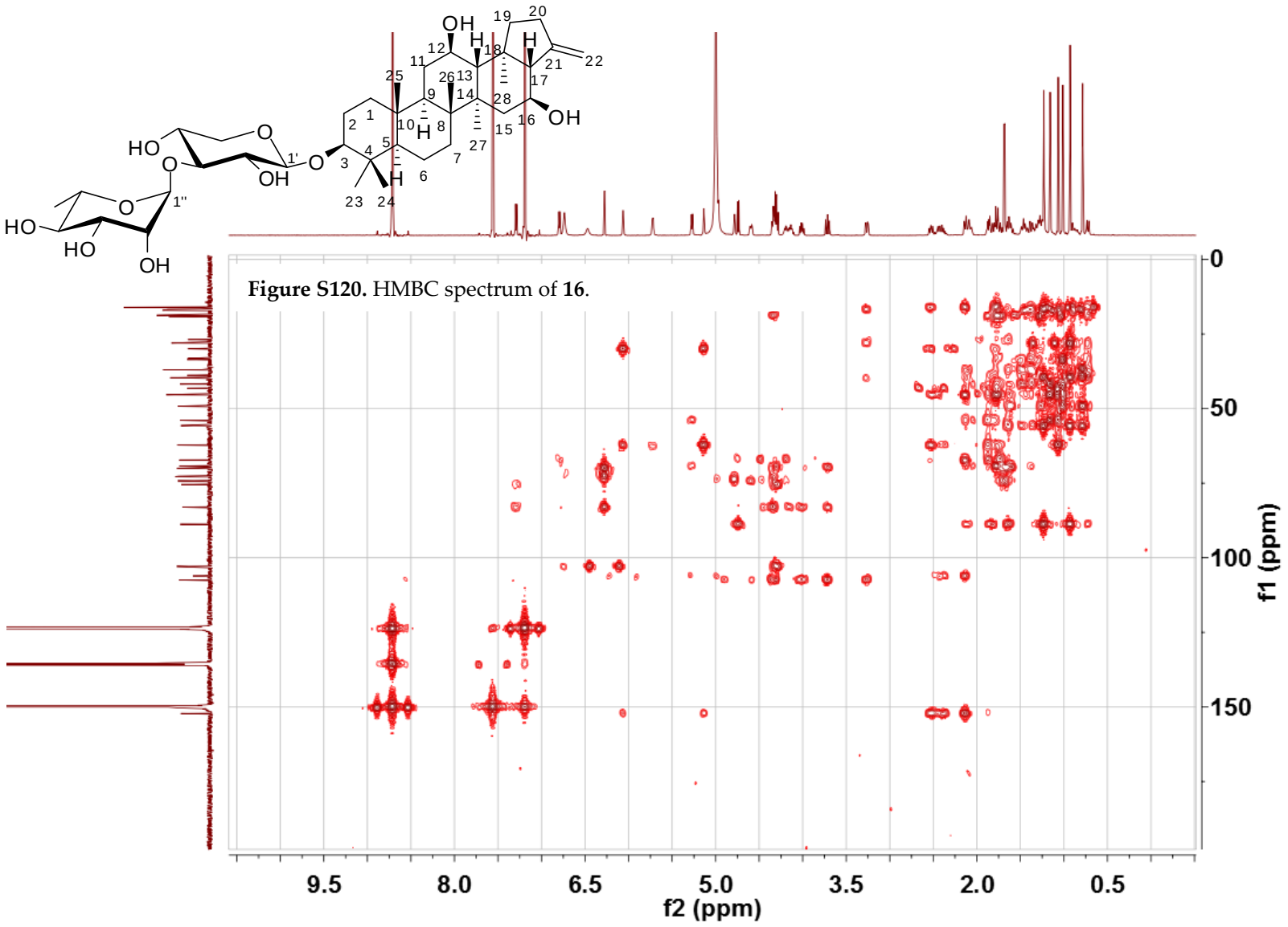

Figure S120. HMBC spectrum of **16**.

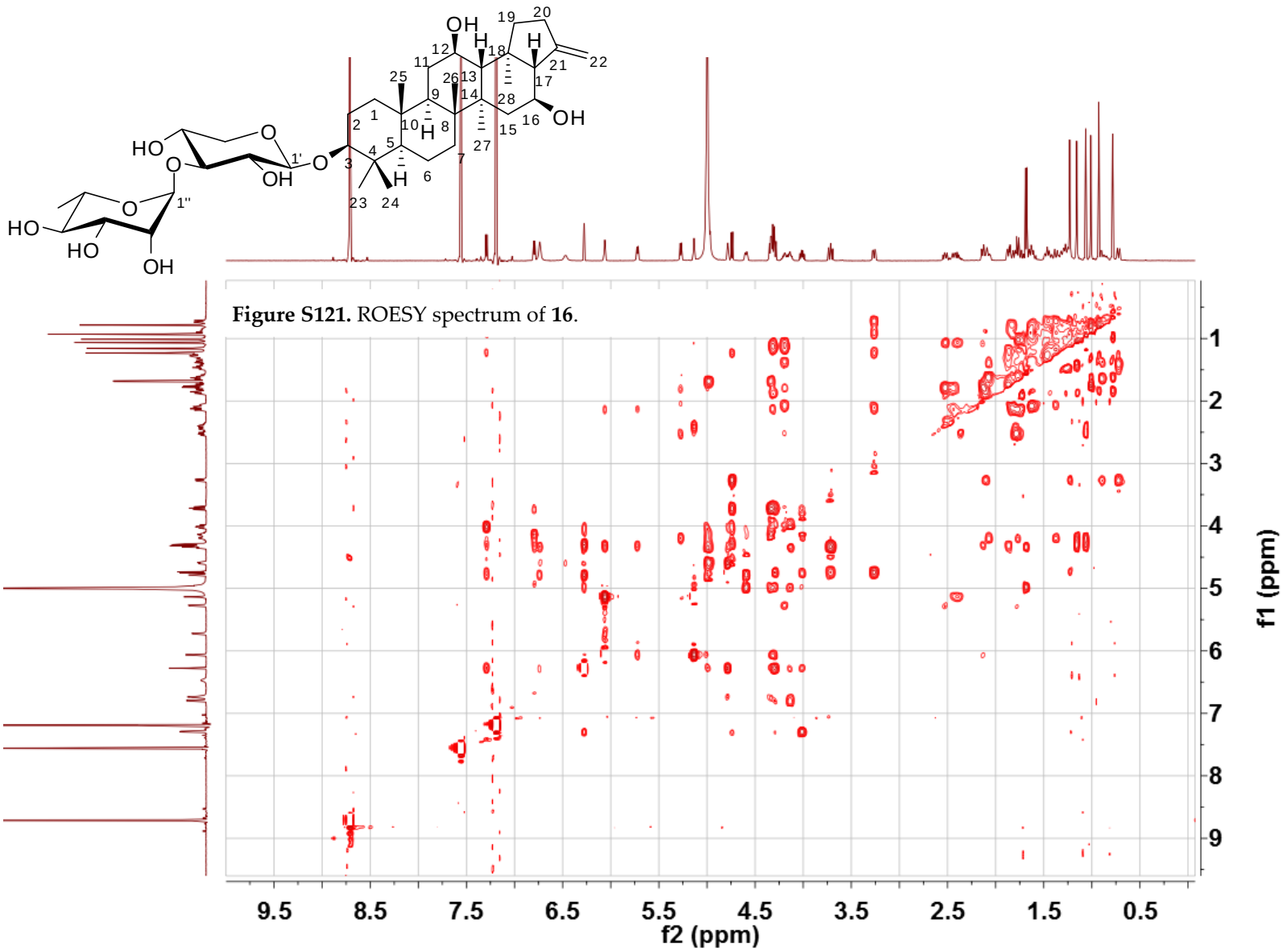

Figure S121. ROESY spectrum of **16**.

Data Filename	171020ESIA4.d	**Sample Name**	pdt4
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	10/23/2017 10:43:40 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
230	0	ESI

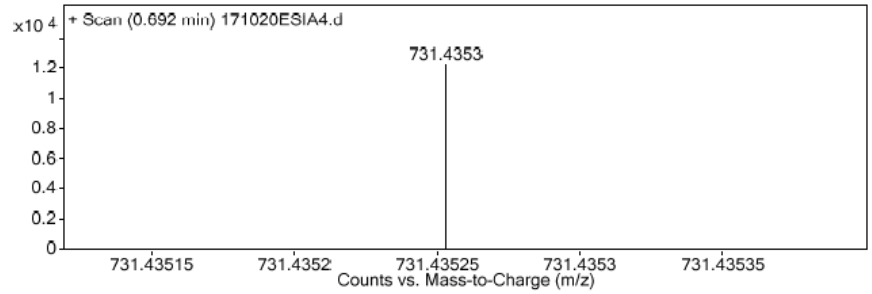

Figure S122. HRESIMS spectrum of **16**.

Peak List

m/z	z	Abund	Formula	Ion
142.1588		6618.62		
230.2478		3655.01		
242.284	1	24682.75		
243.2871	1	3987.93		
340.2823	1	4079.48		
384.309	1	3931.27		
437.2179	1	3262.22		
731.4353	1	12223.29	C39 H64 Na O11	M+
732.4388	1	4466.36	C39 H64 Na O11	M+
733.4218	1	3921.16	C39 H64 Na O11	M+

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	13
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C39 H64 Na O11	731.4346	731.4353	-0.7	0.9	7.5

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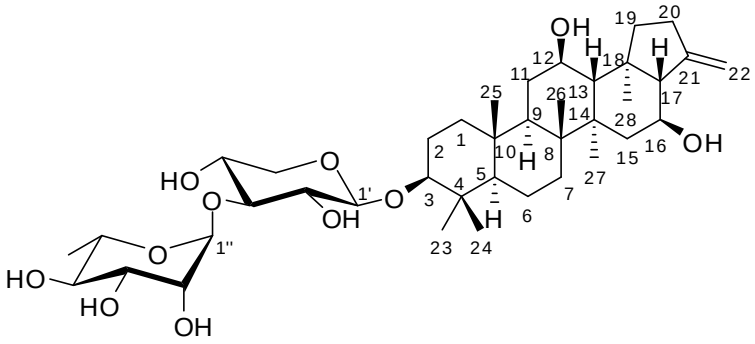

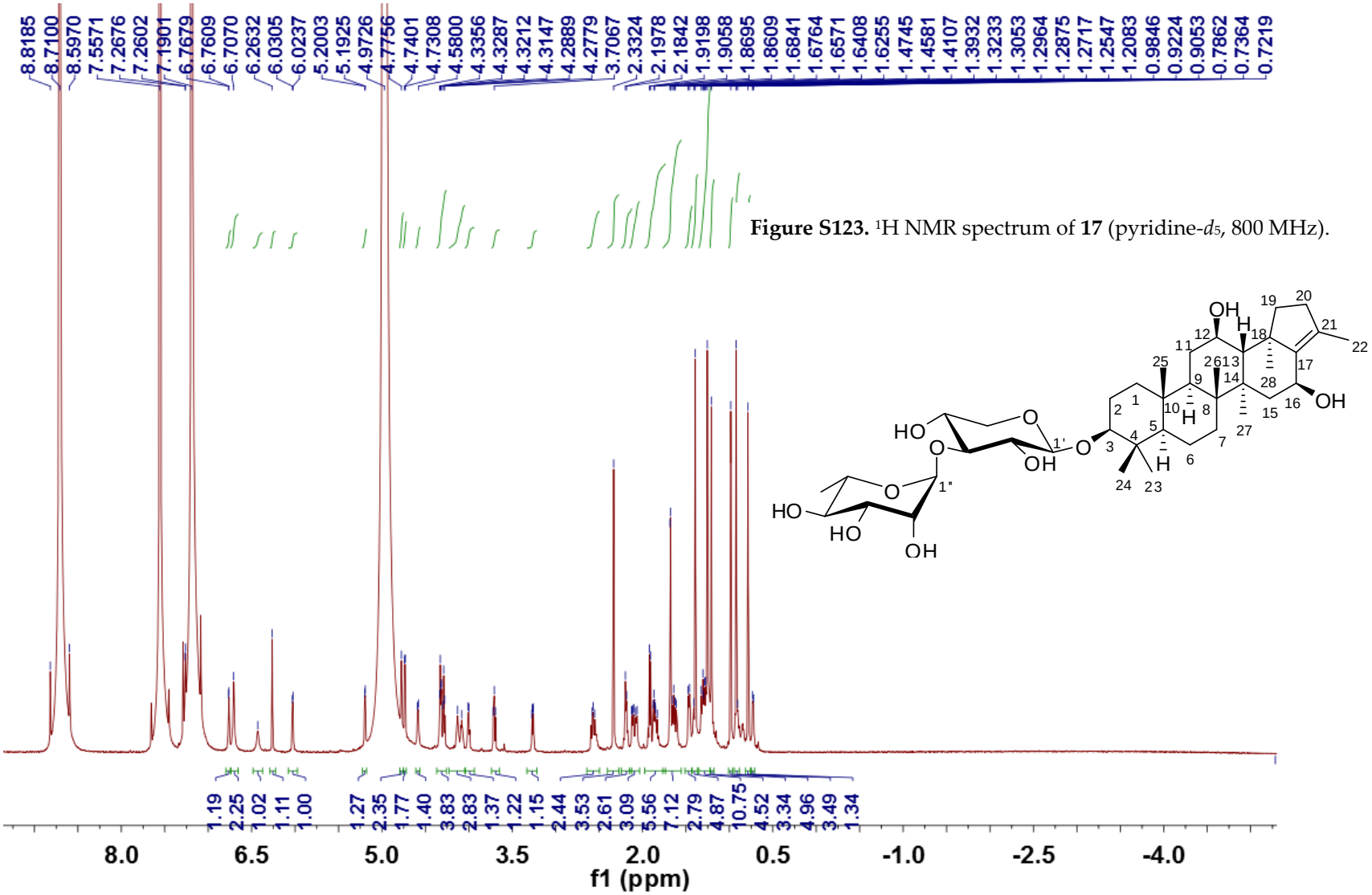

Figure S123. ^{1}H NMR spectrum of **17** (pyridine-d_5, 800 MHz).

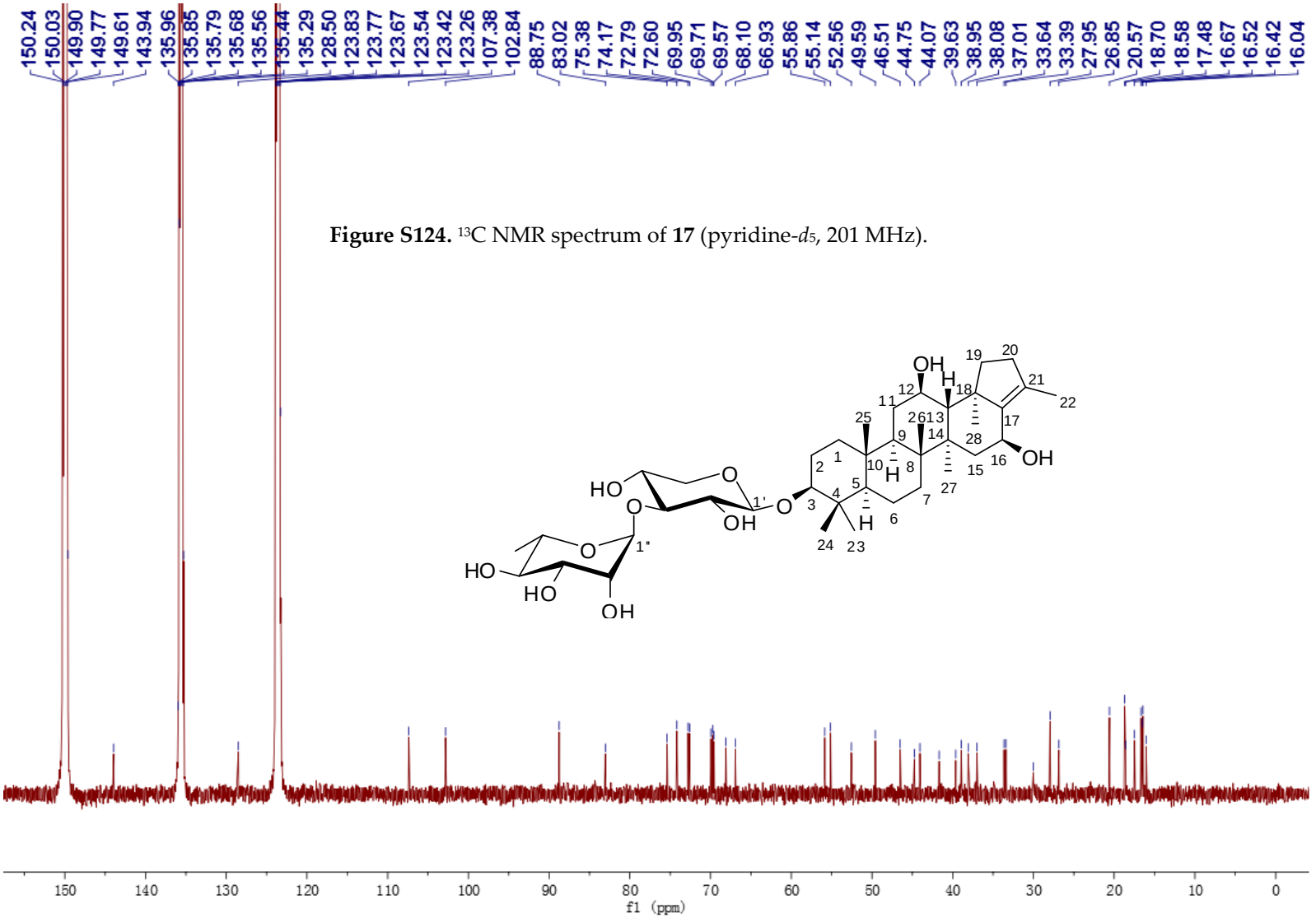

Figure S124. ^{13}C NMR spectrum of **17** (pyridine-d_5, 201 MHz).

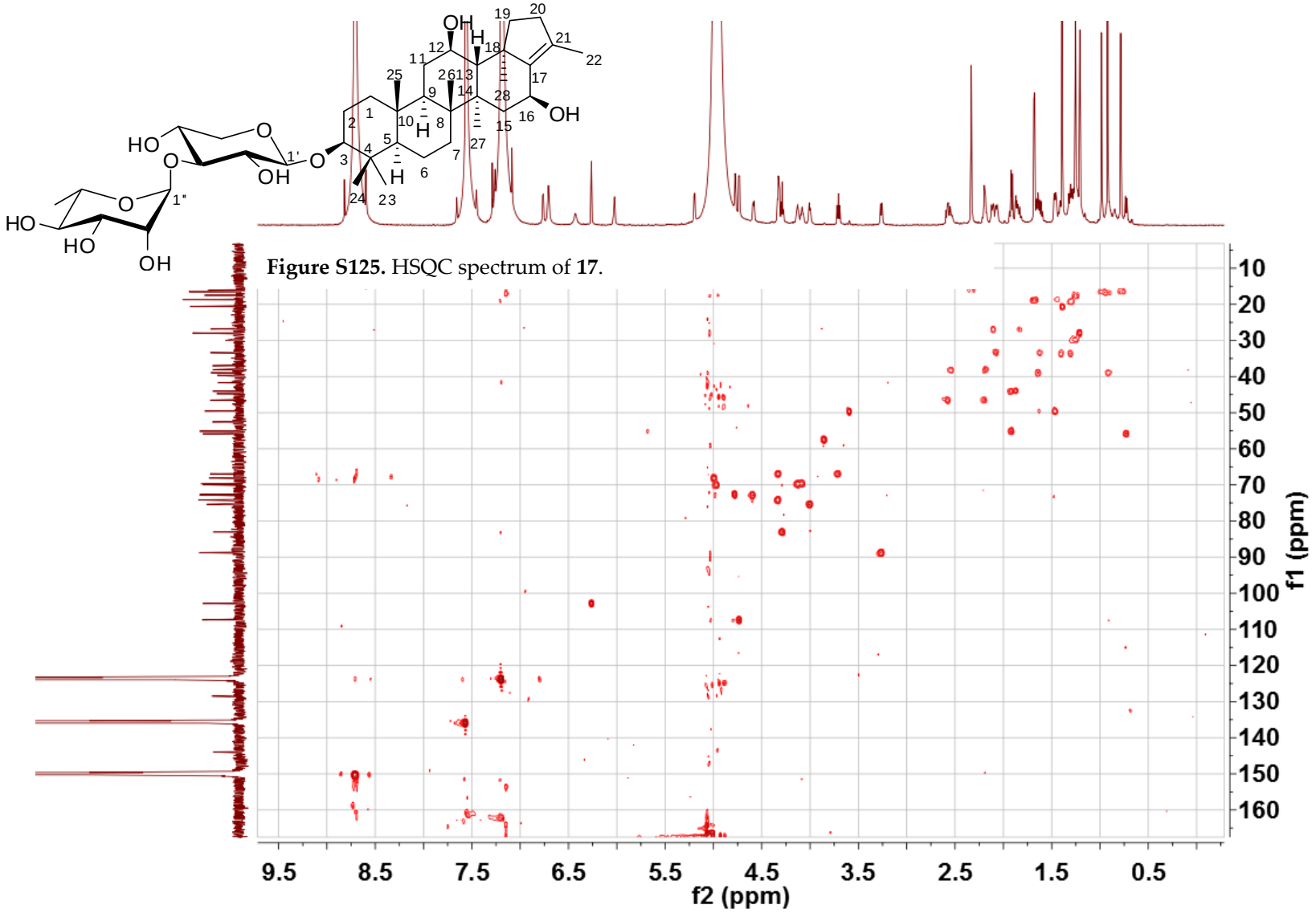

Figure S125. HSQC spectrum of **17**.

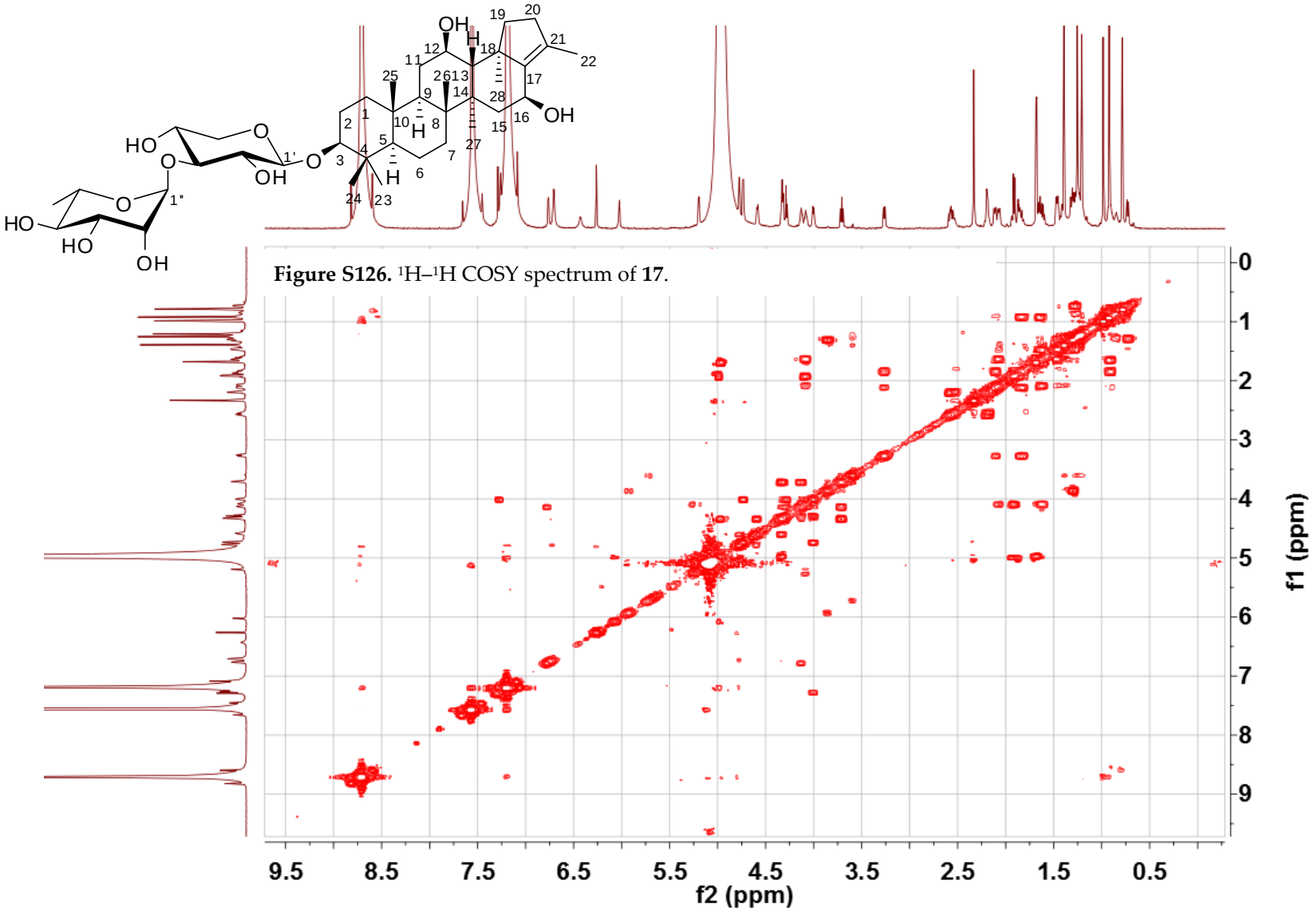

Figure S126. ^{1}H–^{1}H COSY spectrum of **17**.

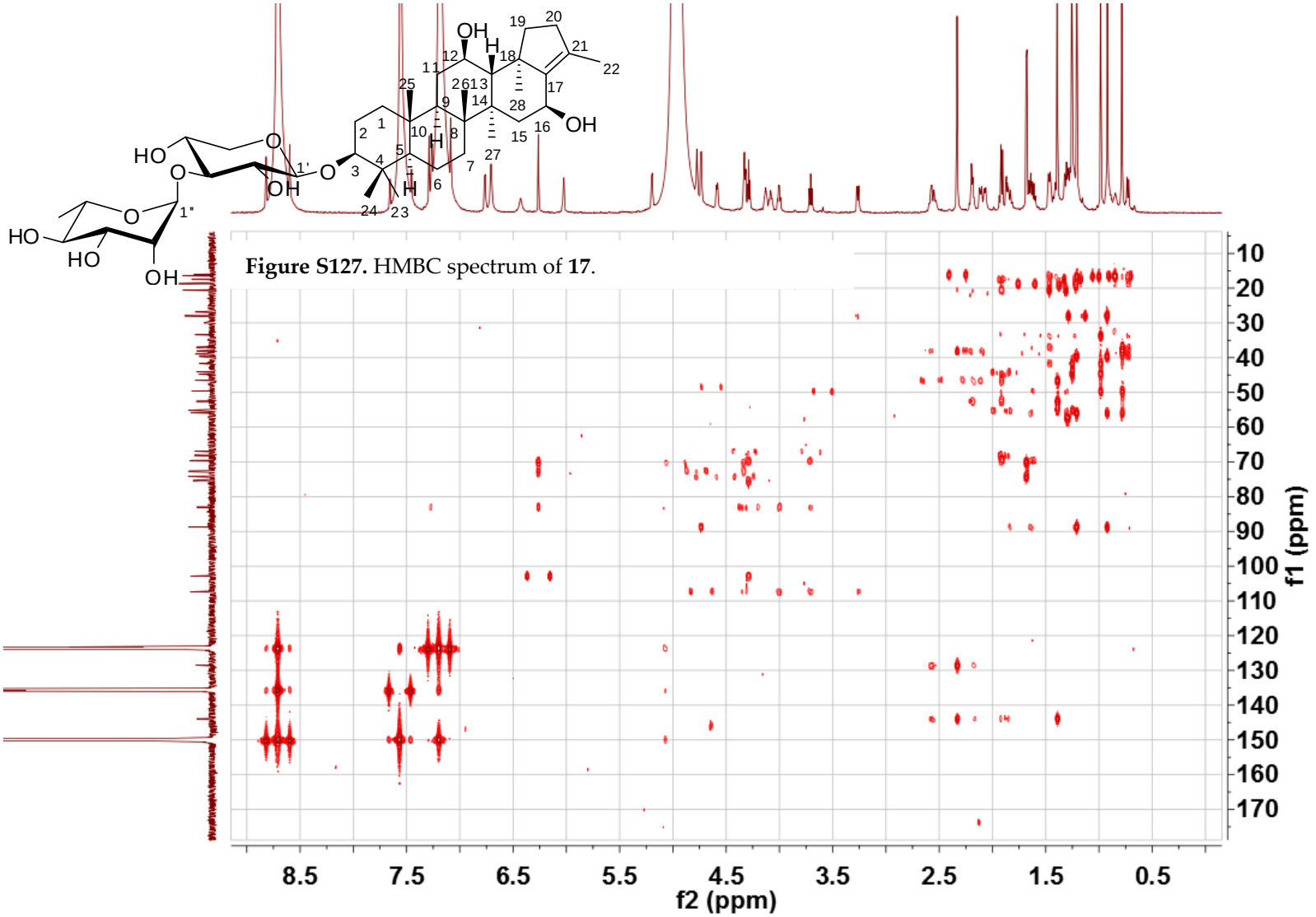

Figure S127. HMBC spectrum of **17**.

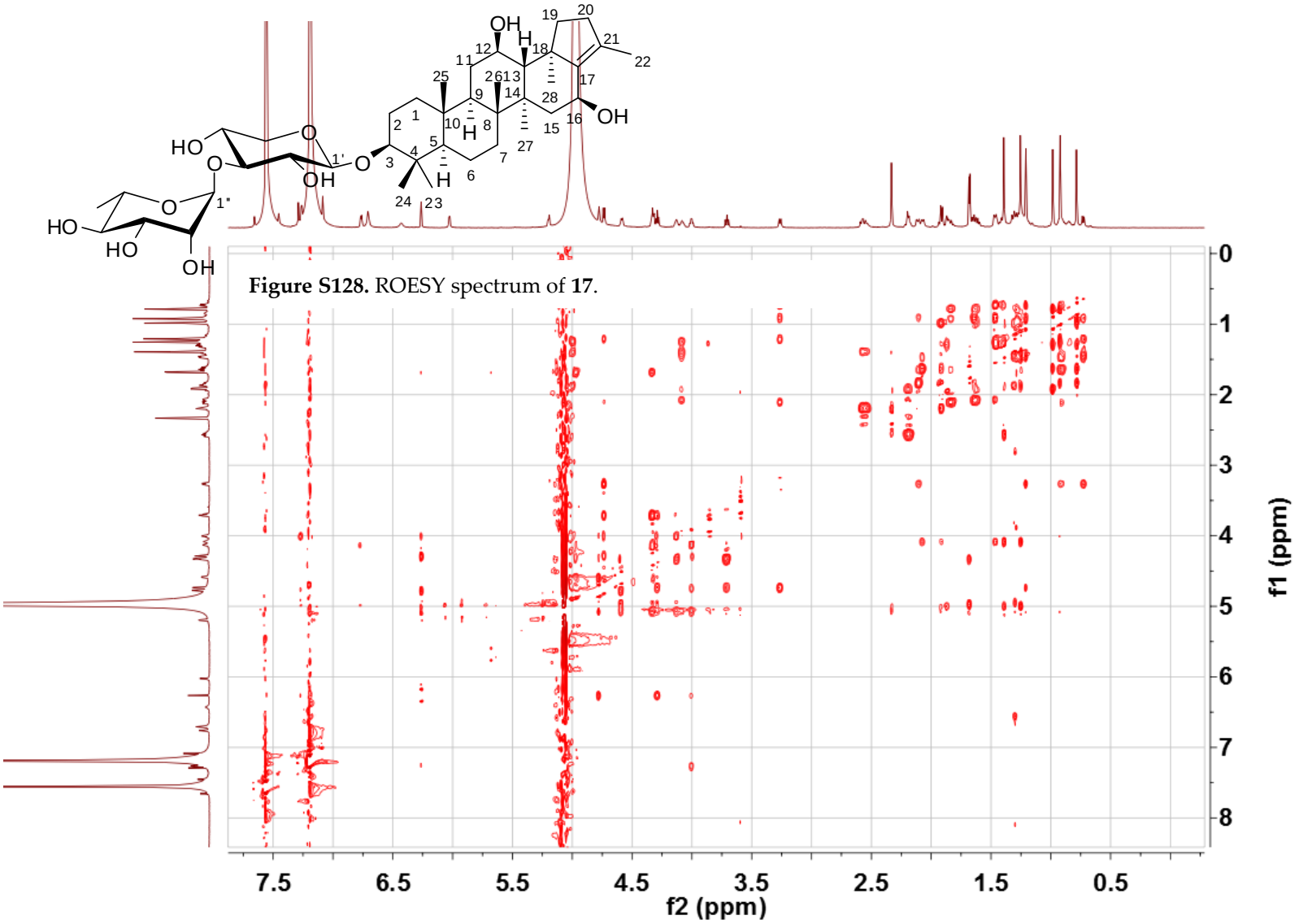

Figure S128. ROESY spectrum of **17**.

Data Filename	171023ESIA1.d	**Sample Name**	pdt18
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	10/23/2017 10:48:38 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
260	0	ESI

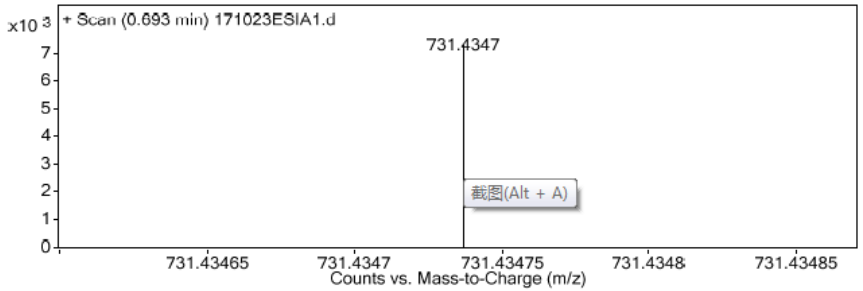

Figure S129. HRESIMS spectrum of **17**.

Peak List

m/z	z	Abund
112.1874	1	15398.25
178.2277	1	17871.92
182.256	1	21448.32
273.3796		10947.24
274.3865	1	32553.89
287.3954		11728.15
288.4024		48627.63
289.4091		195593.86
290.4155	1	464535.06
291.4184	1	66284.01

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	13
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C39 H64 Na O11	731.4346	731.4347	-0.1	0.1	7.5

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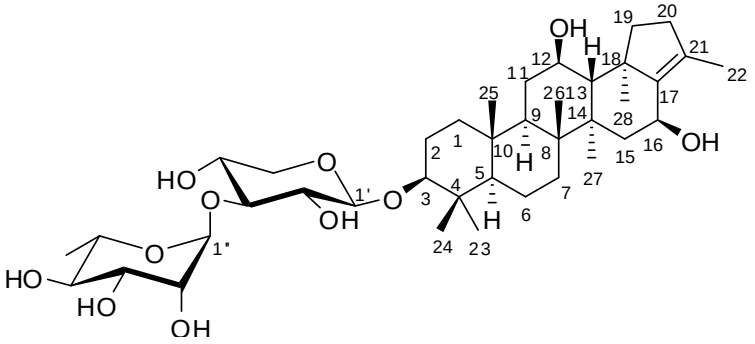


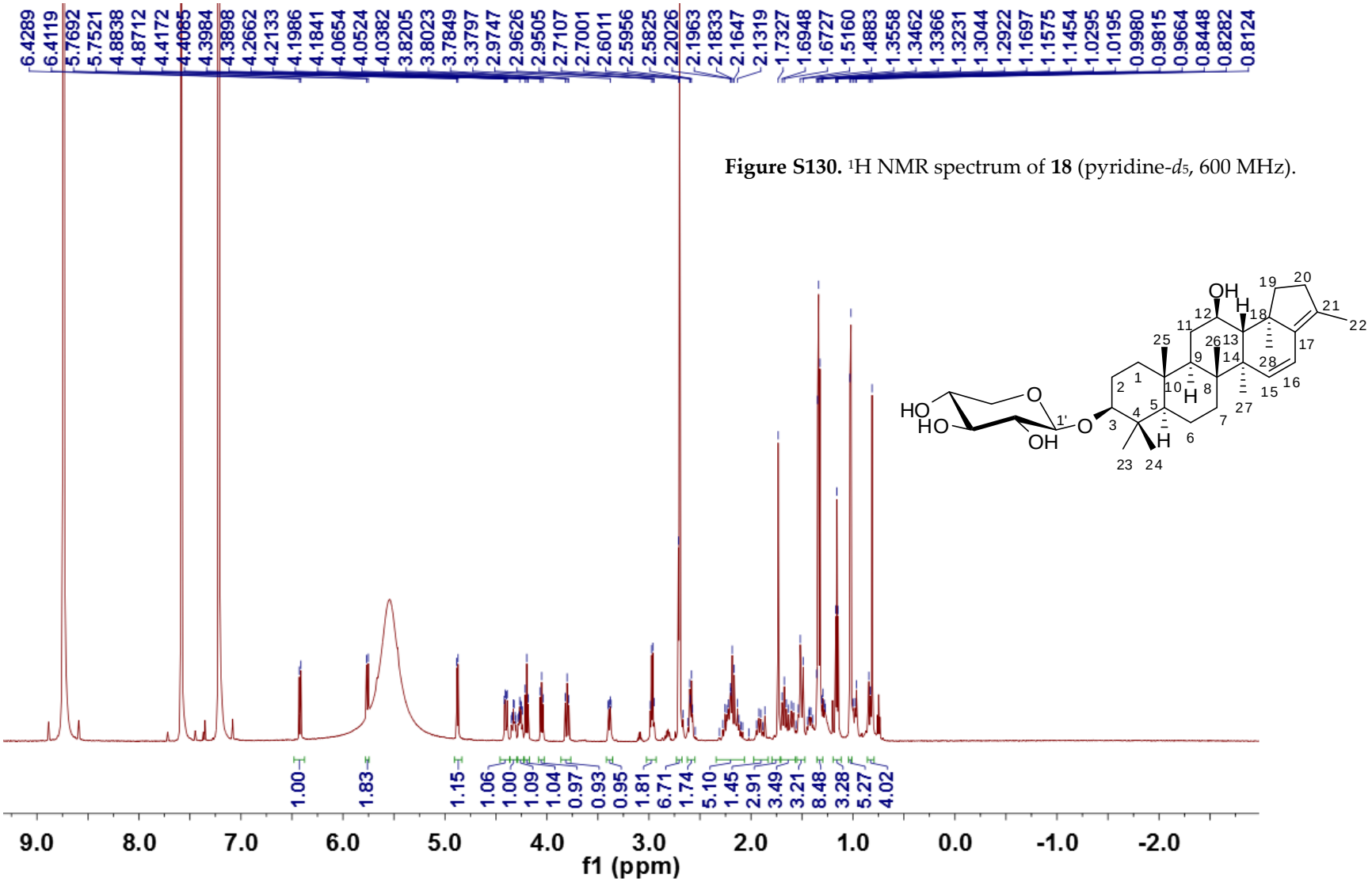


Figure S130. ^{1}H NMR spectrum of **18** (pyridine-d_5, 600 MHz).

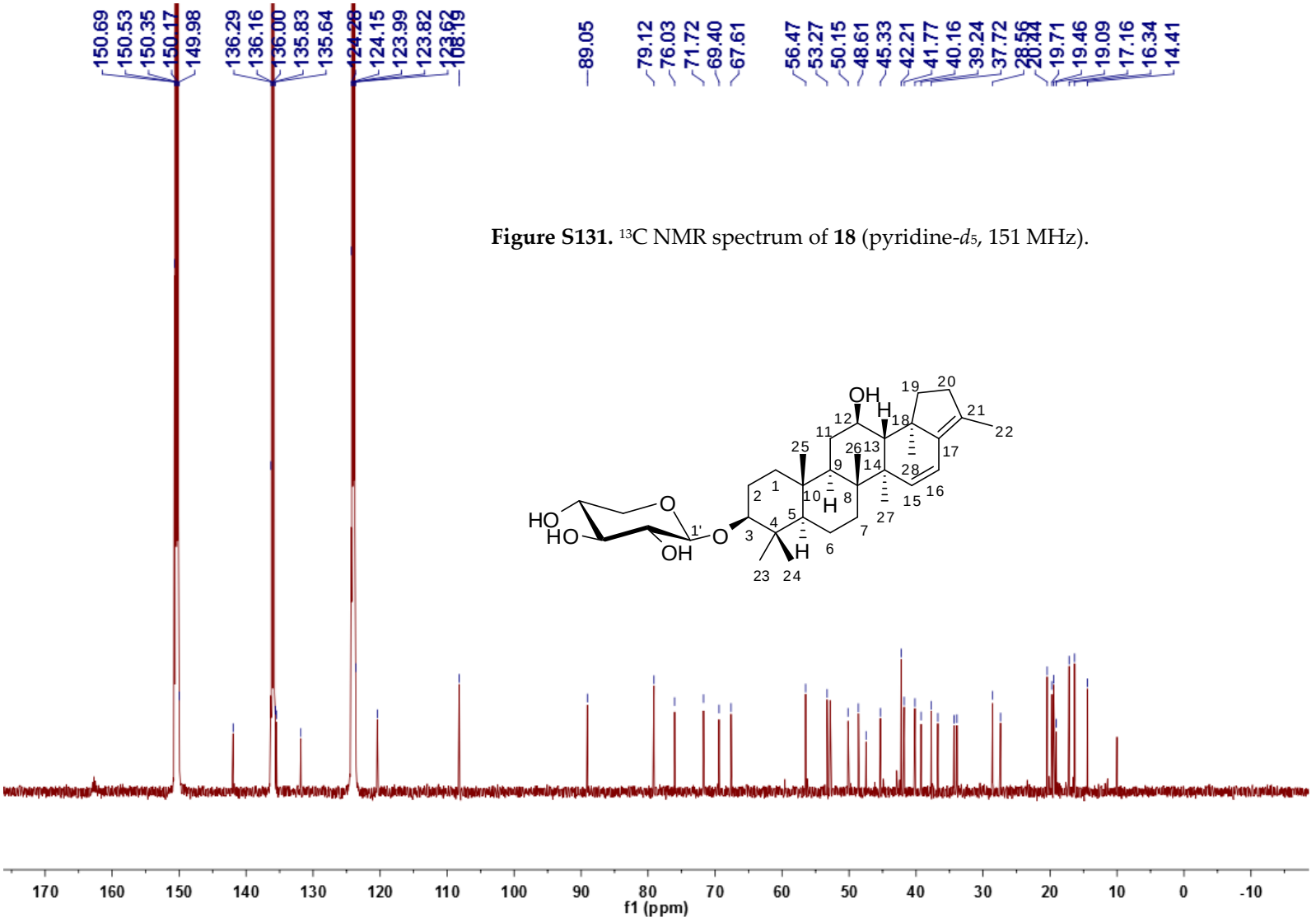


Figure S131. ^{13}C NMR spectrum of **18** (pyridine-d_5, 151 MHz).

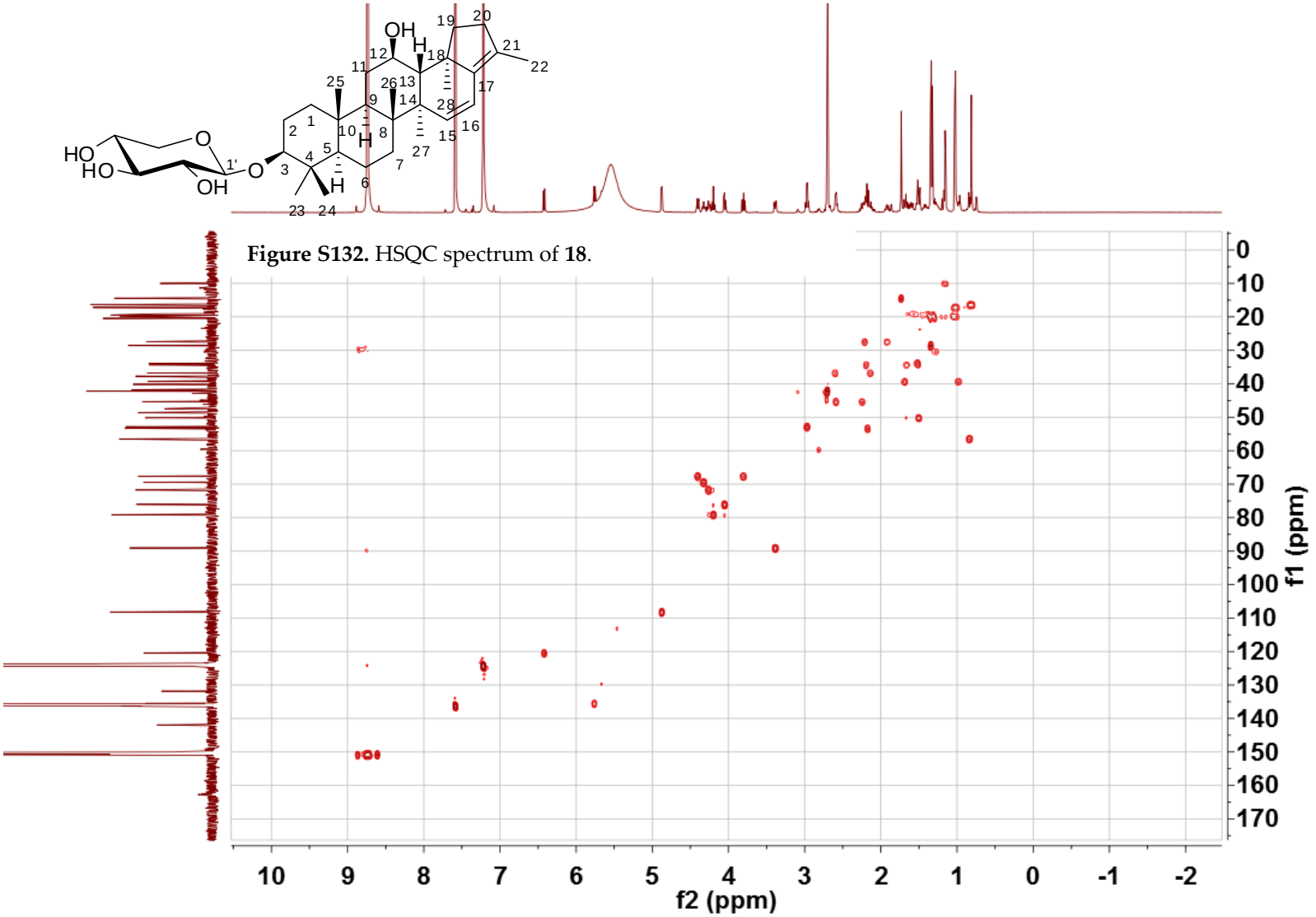


Figure S132. HSQC spectrum of **18**.

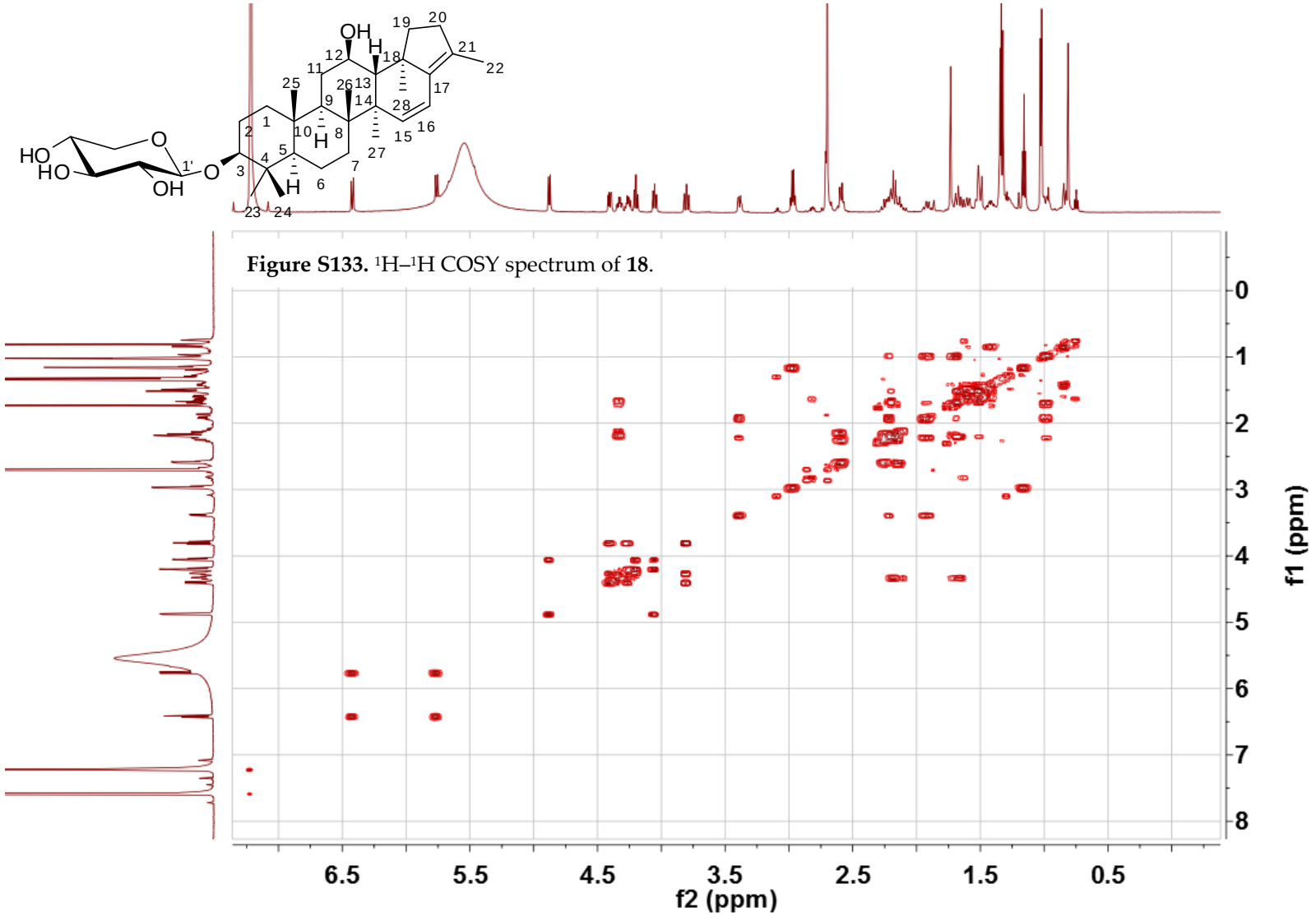


Figure S133. ^{1}H–^{1}H COSY spectrum of **18**.

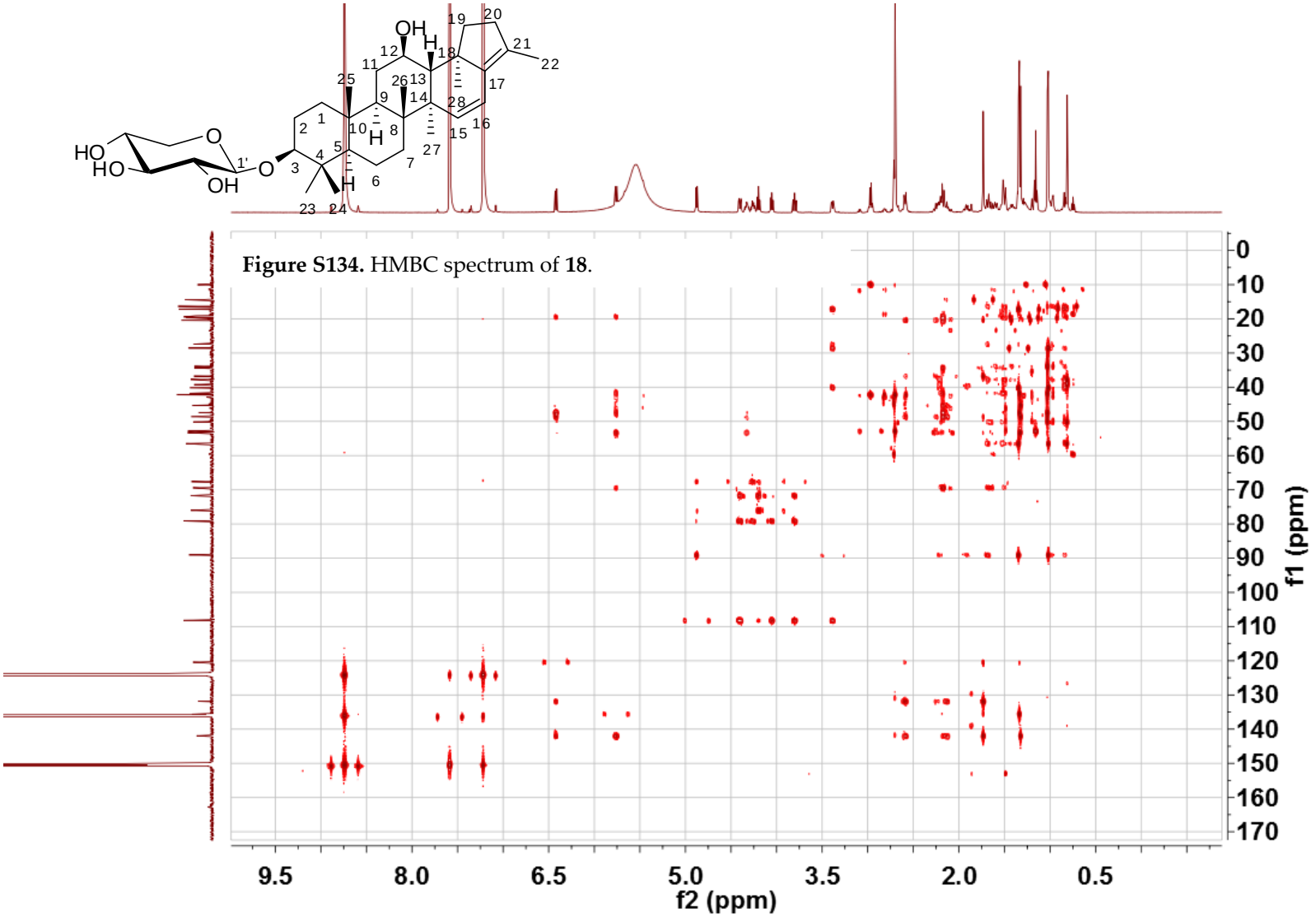


Figure S134. HMBC spectrum of **18**.

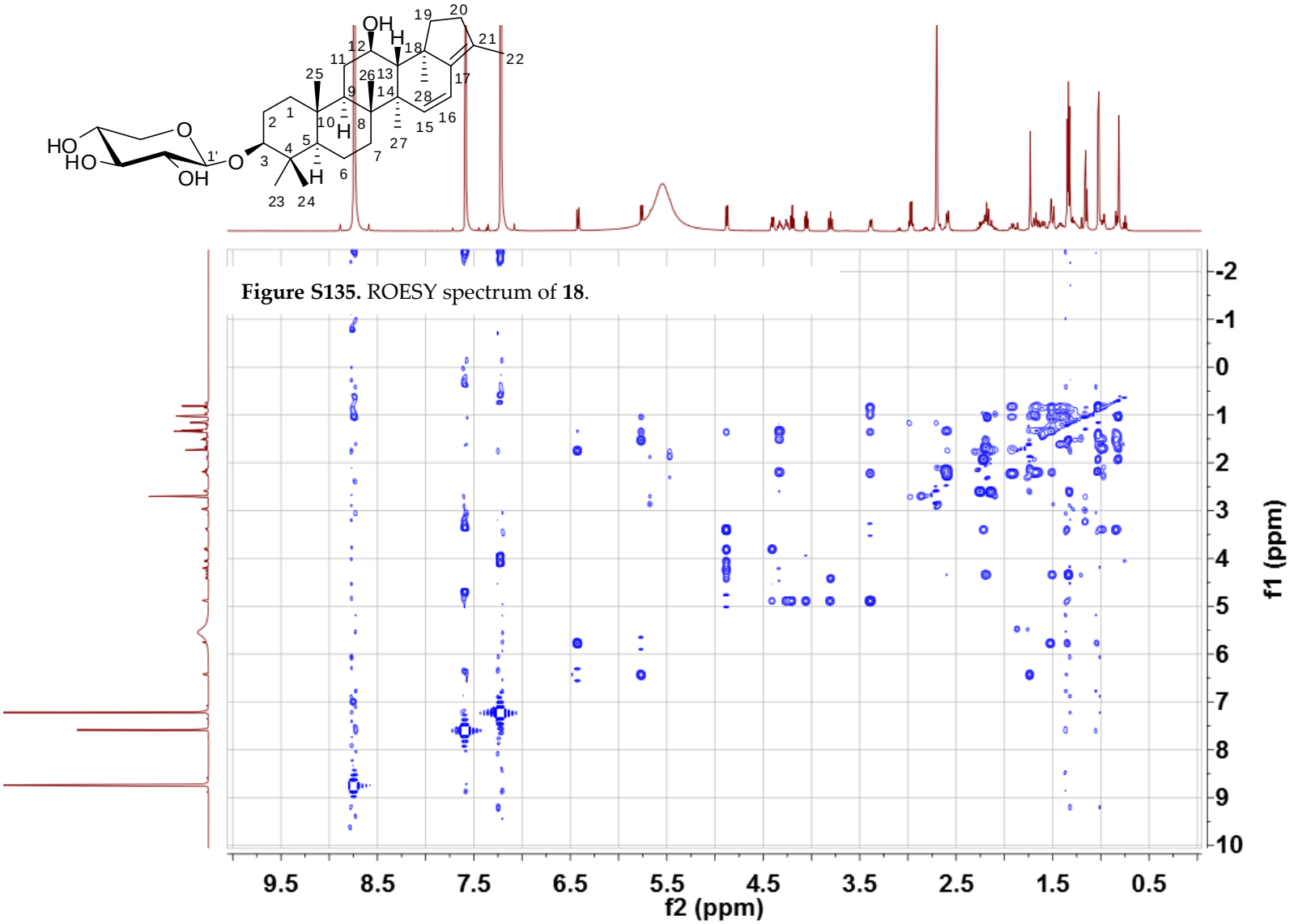


Figure S135. ROESY spectrum of **18**.

Data File: E:\DATA\2018\0719\pdt39c.lcd

Elmt	Val.	Min	Max
H	1	10	100
C	4	10	50
N	3	0	0

Elmt	Val.	Min	Max
O	2	0	20
F	1	0	0
Na	1	0	0

Elmt	Val.	Min	Max
Si	4	0	0
S	2	0	0
Cl	1	0	0

Elmt	Val.	Min	Max
Br	1	0	0
I	3	0	0

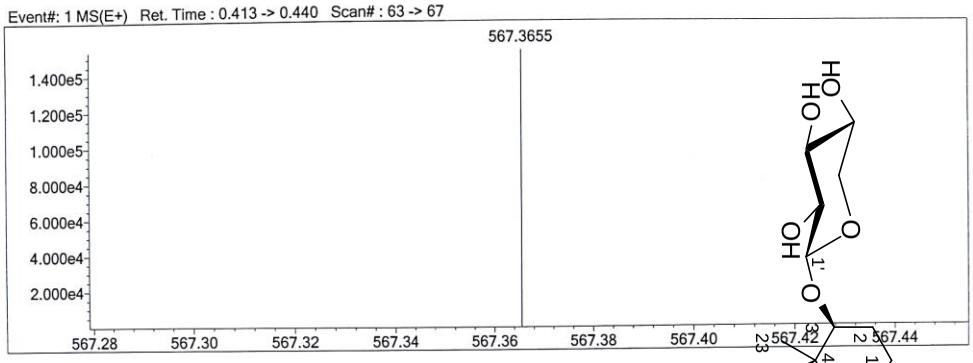
Use Adduct
Na

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

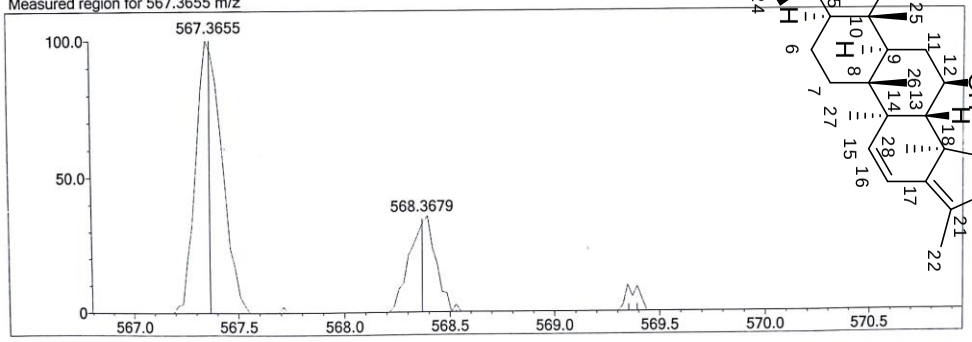
DBE Range: -2.0 - 100.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 10

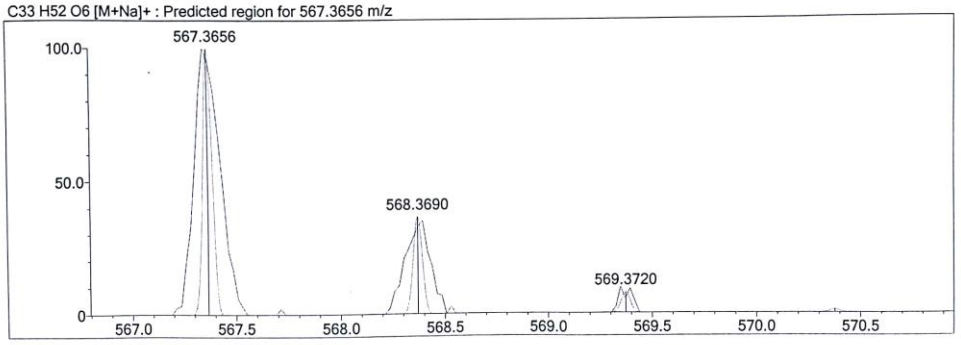
Event#: 1 MS(E+) Ret. Time : 0.413 -> 0.440 Scan# : 63 -> 67



Measured region for 567.3655 m/z



C33 H52 O6 [M+Na]+ : Predicted region for 567.3656 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C33 H52 O6	[M+Na]+	567.3655	567.3656	-0.1	-0.18	8.0

Figure S136. HRESIMS spectrum of **18**.

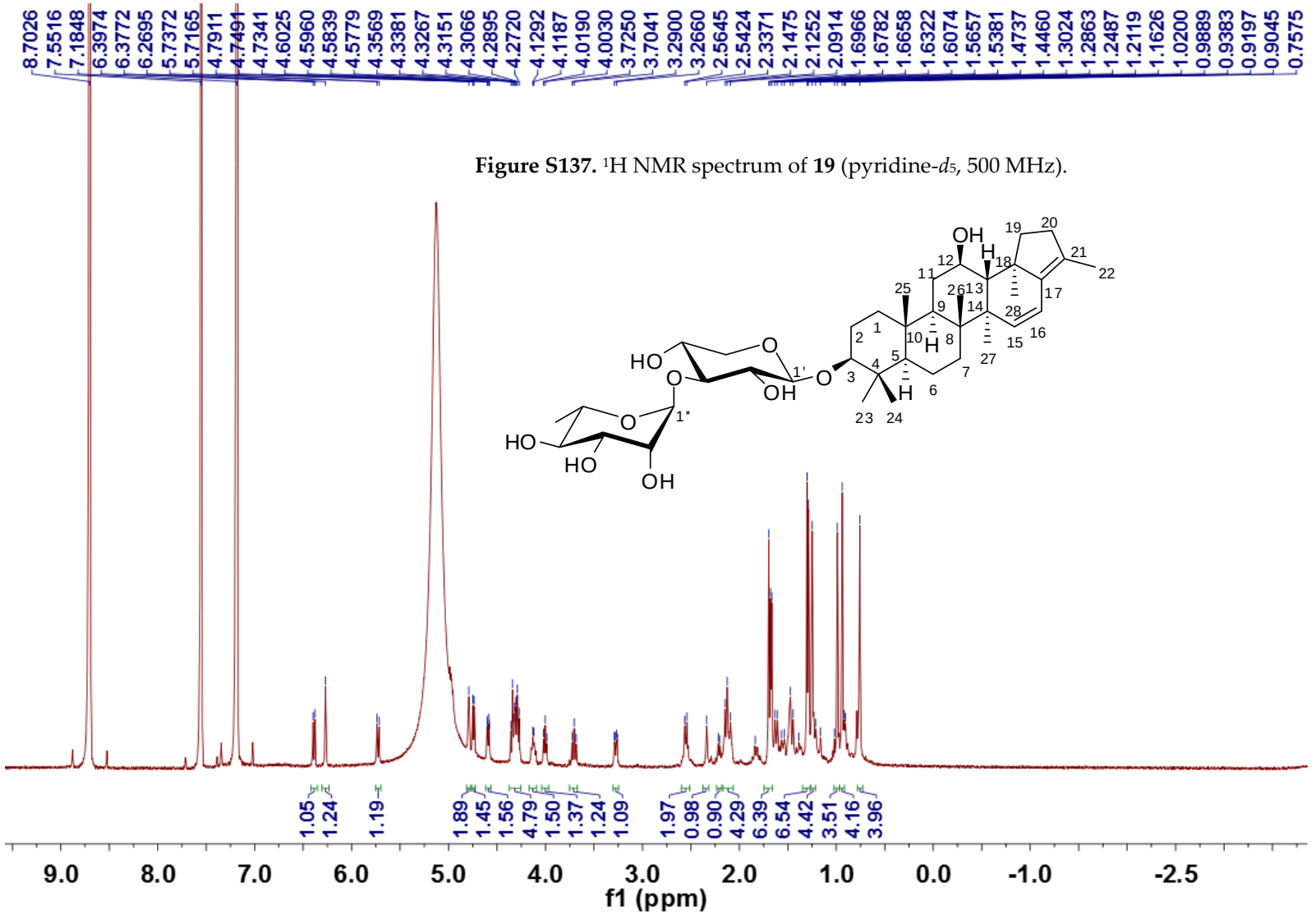


Figure S137. ^{1}H NMR spectrum of **19** (pyridine-d_5, 500 MHz).

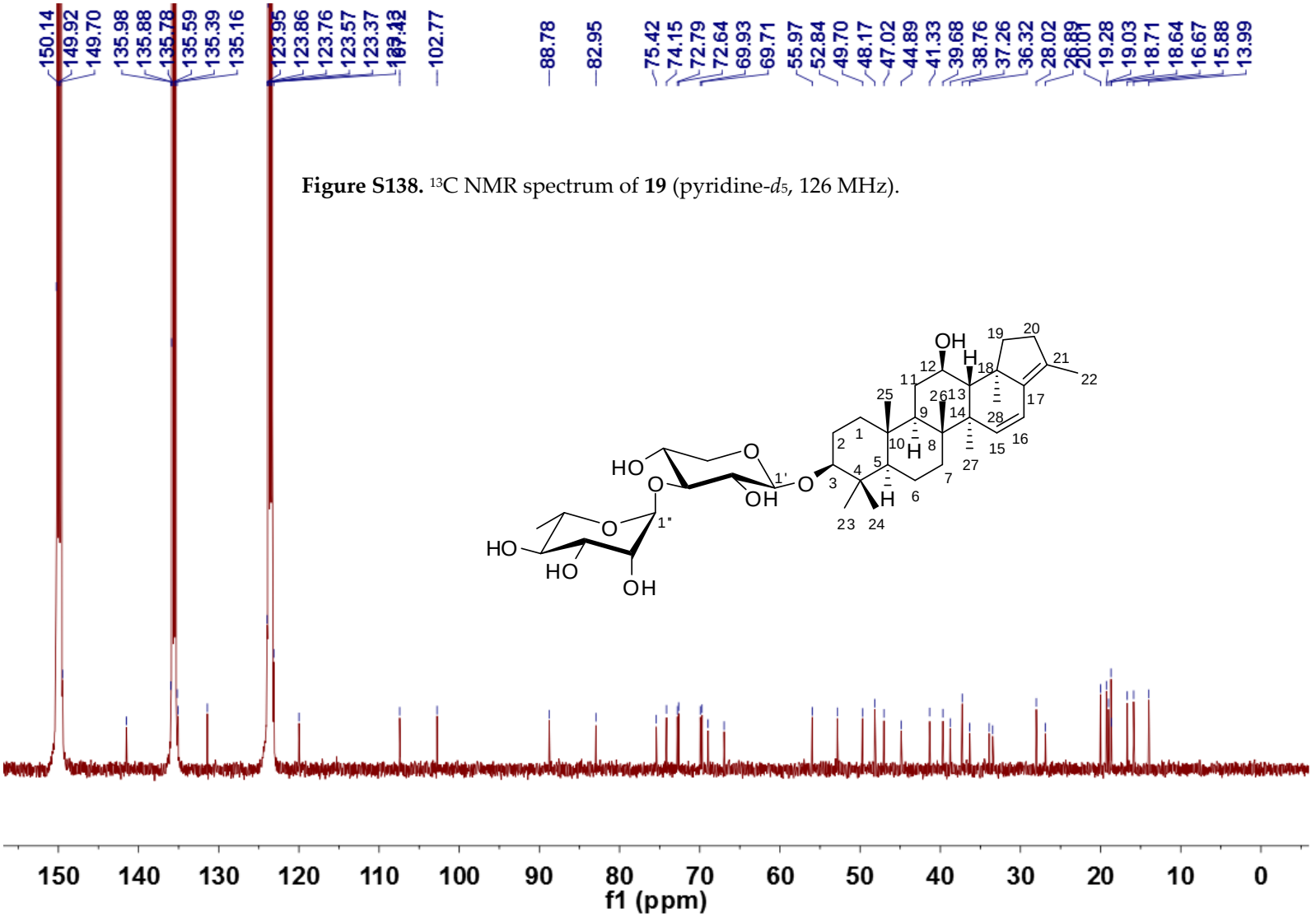


Figure S138. ^{13}C NMR spectrum of **19** (pyridine-d_5, 126 MHz).

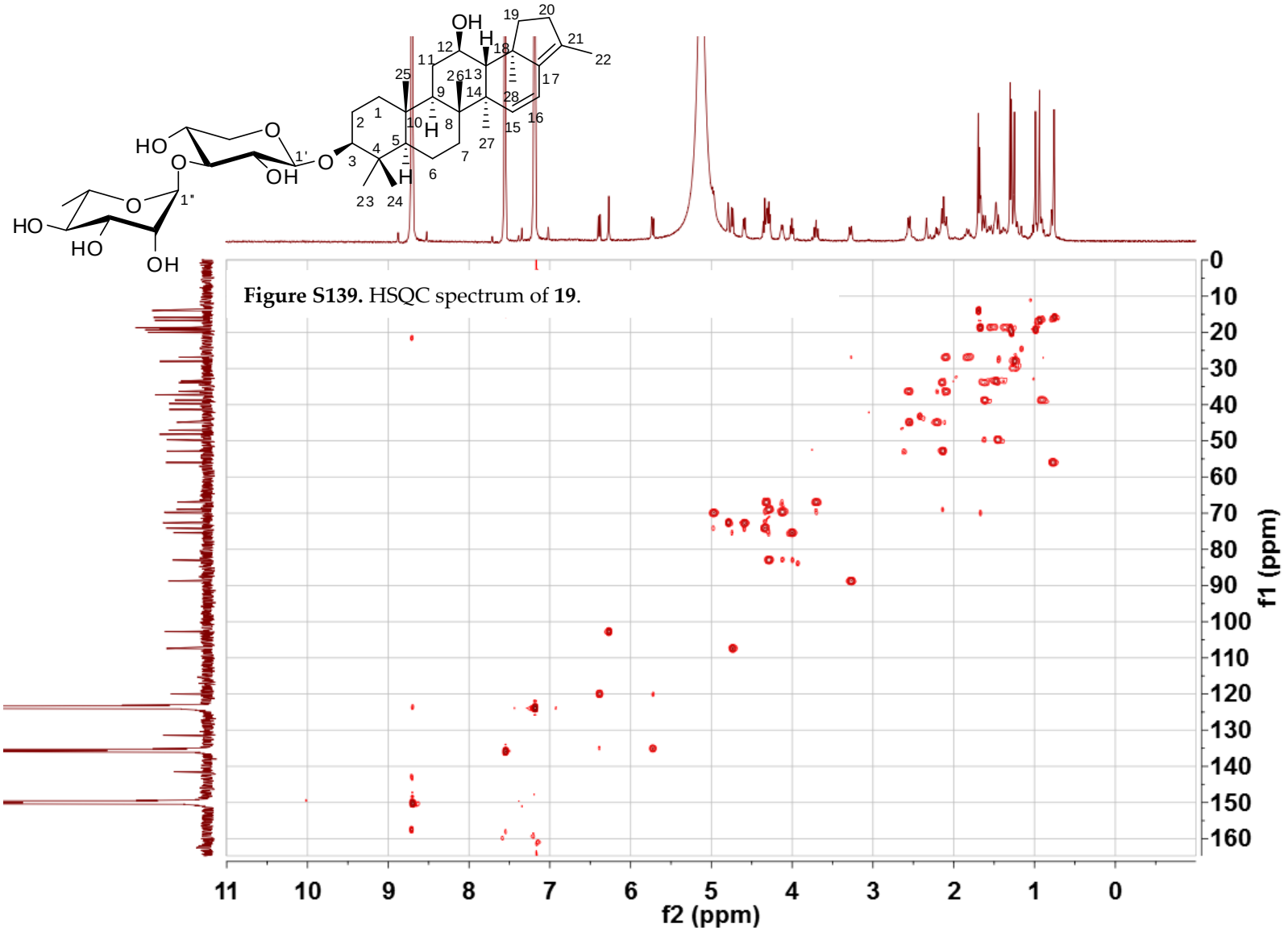


Figure S139. HSQC spectrum of **19**.

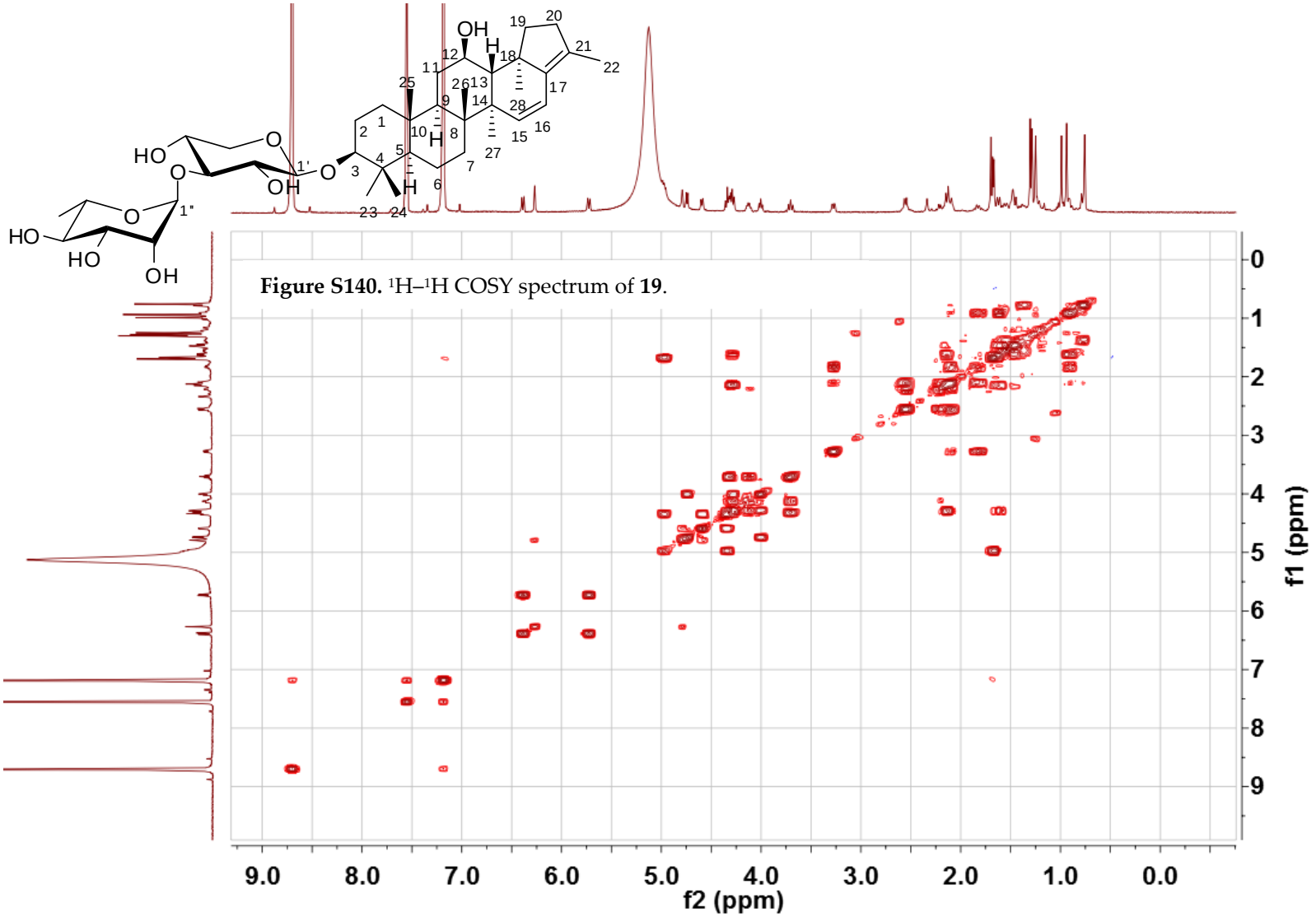


Figure S140. ^{1}H–^{1}H COSY spectrum of **19**.

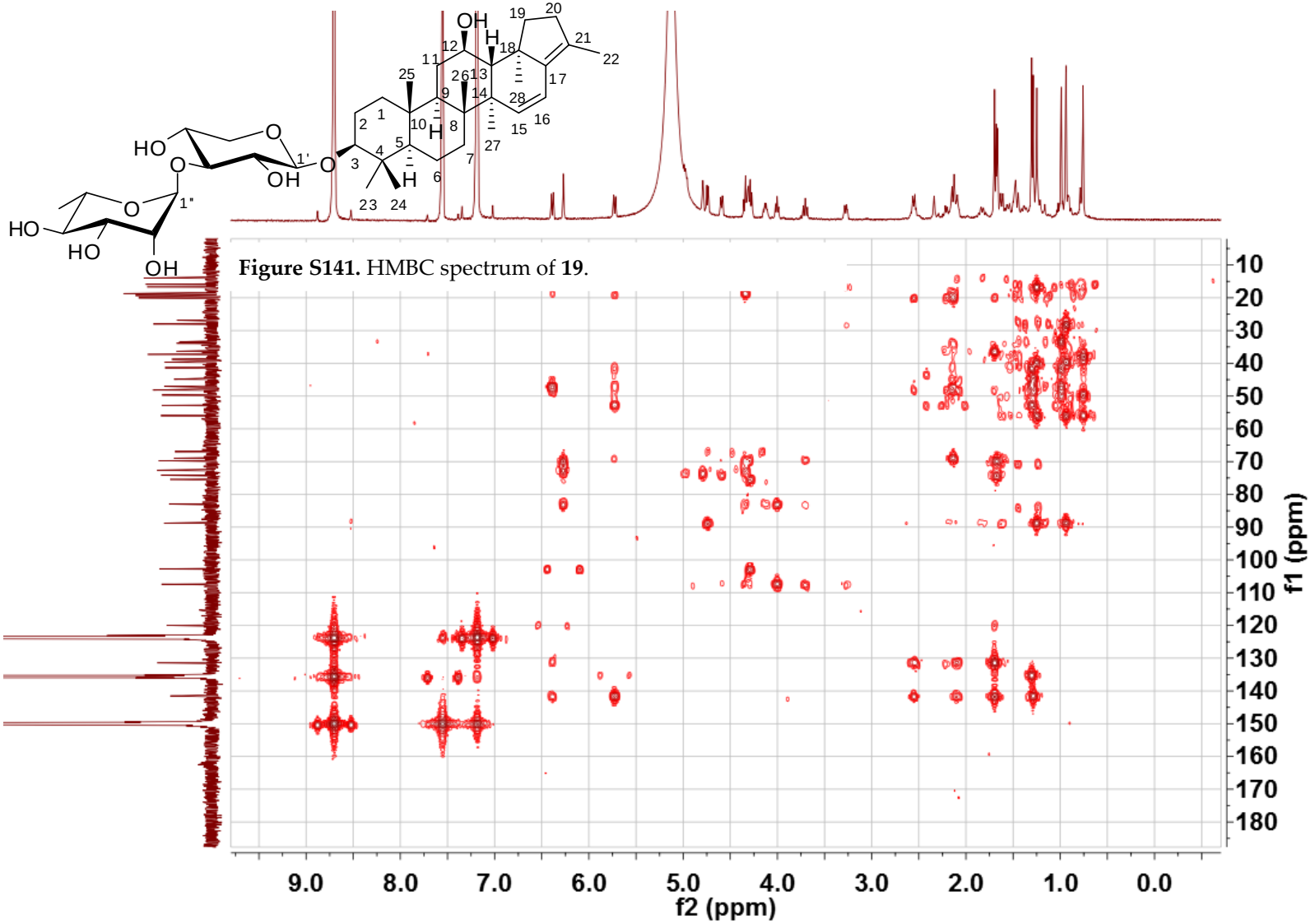


Figure S141. HMBC spectrum of **19**.

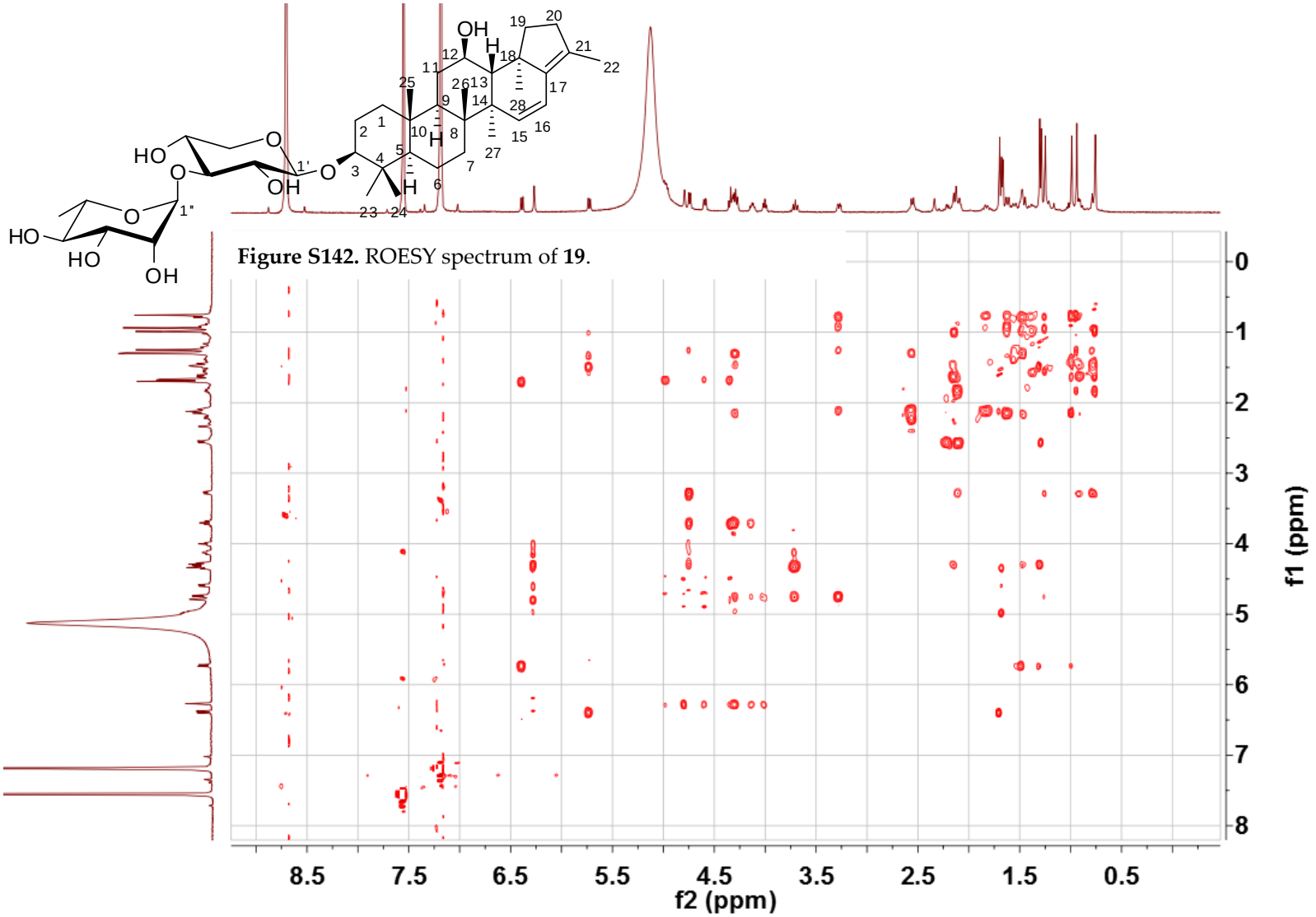


Figure S142. ROESY spectrum of **19**.

Data Filename	180824ESIA6.d	**Sample Name**	pdt46
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/24/2018 2:26:56 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
300	0	ESI

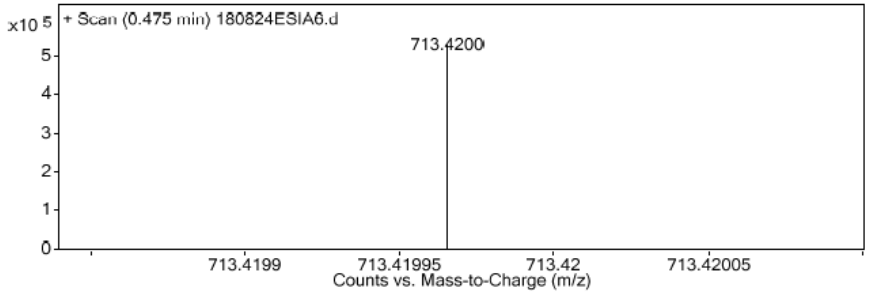


Figure S143. HRESIMS spectrum of **19**.

Peak List

m/z	z	Abund	Formula	Ion
112.1867	1	127159.51		
713.42	1	525814.06	C39 H62 Na O10	M+
714.4231	1	214905.25	C39 H62 Na O10	M+
729.3914	1	94761.45		
843.3773	1	502550.69		
844.3808	1	215964.44		
845.3827	1	57689.6		
1403.8481	1	57332.28		
1533.8059	1	88705.18		
1534.8091	1	78950.48		

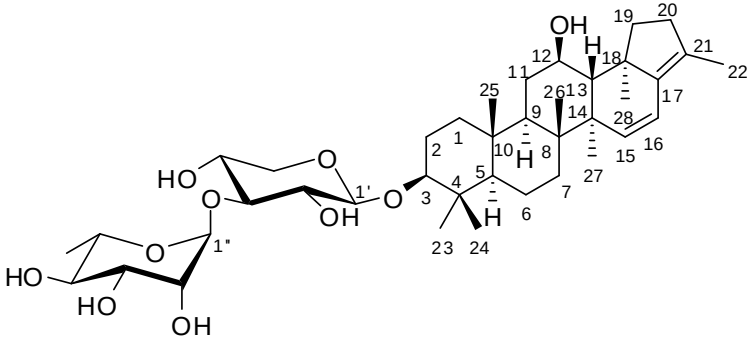
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C39 H62 Na O10	713.4241	713.4200	4.1	5.7	8.5

--- End Of Report ---



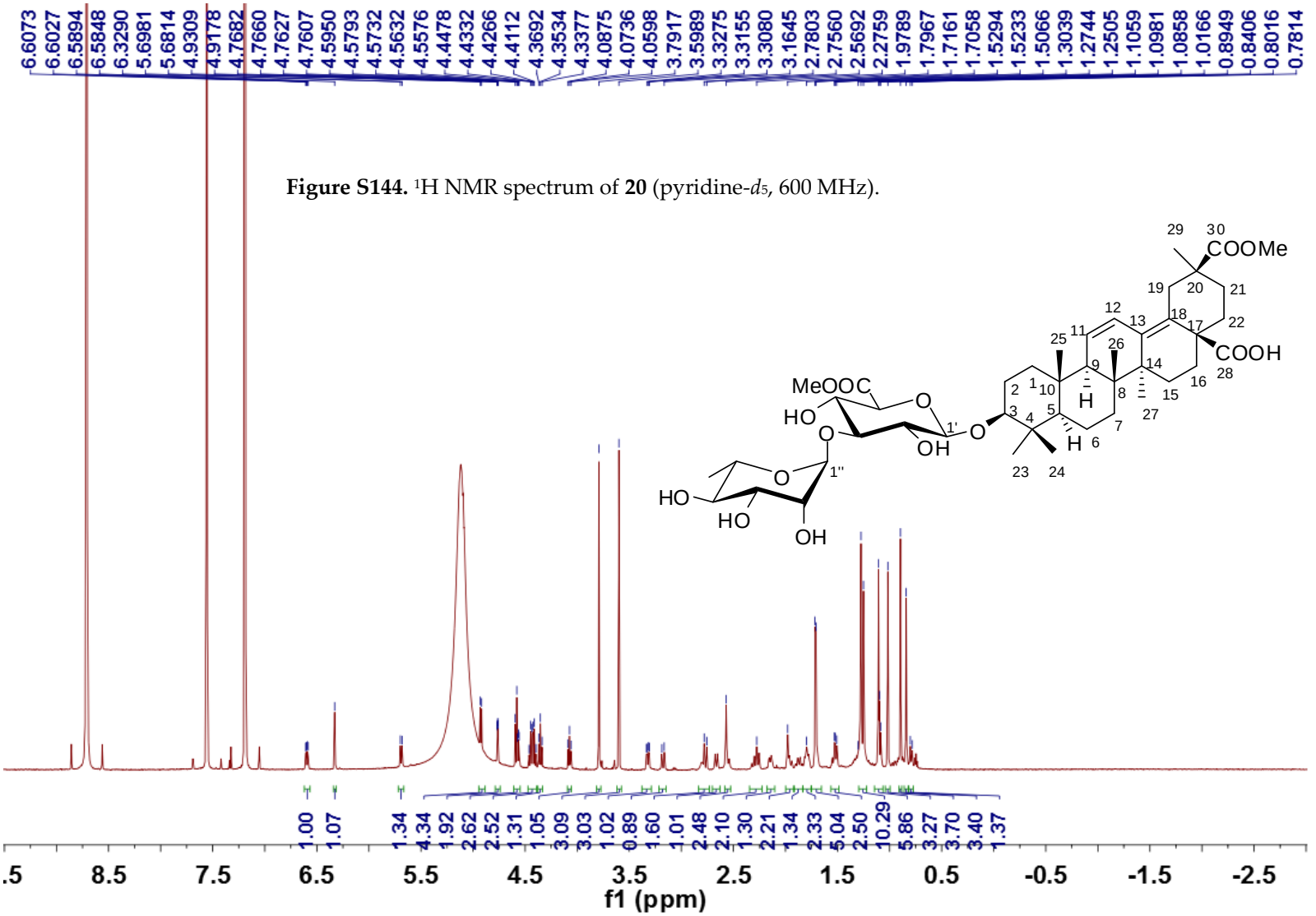


Figure S144. ^{1}H NMR spectrum of **20** (pyridine-d_5, 600 MHz).

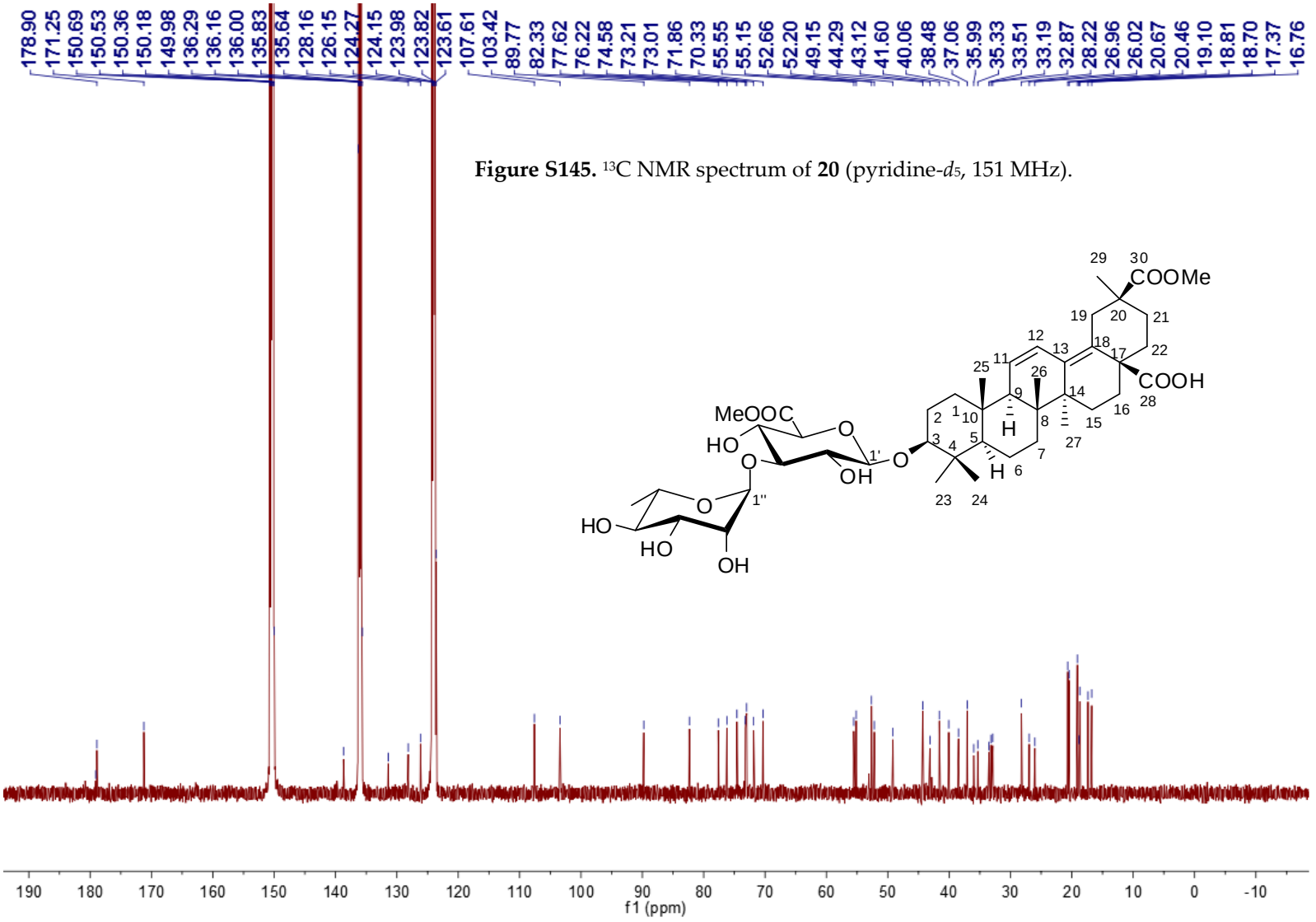


Figure S145. ^{13}C NMR spectrum of **20** (pyridine-d_5, 151 MHz).

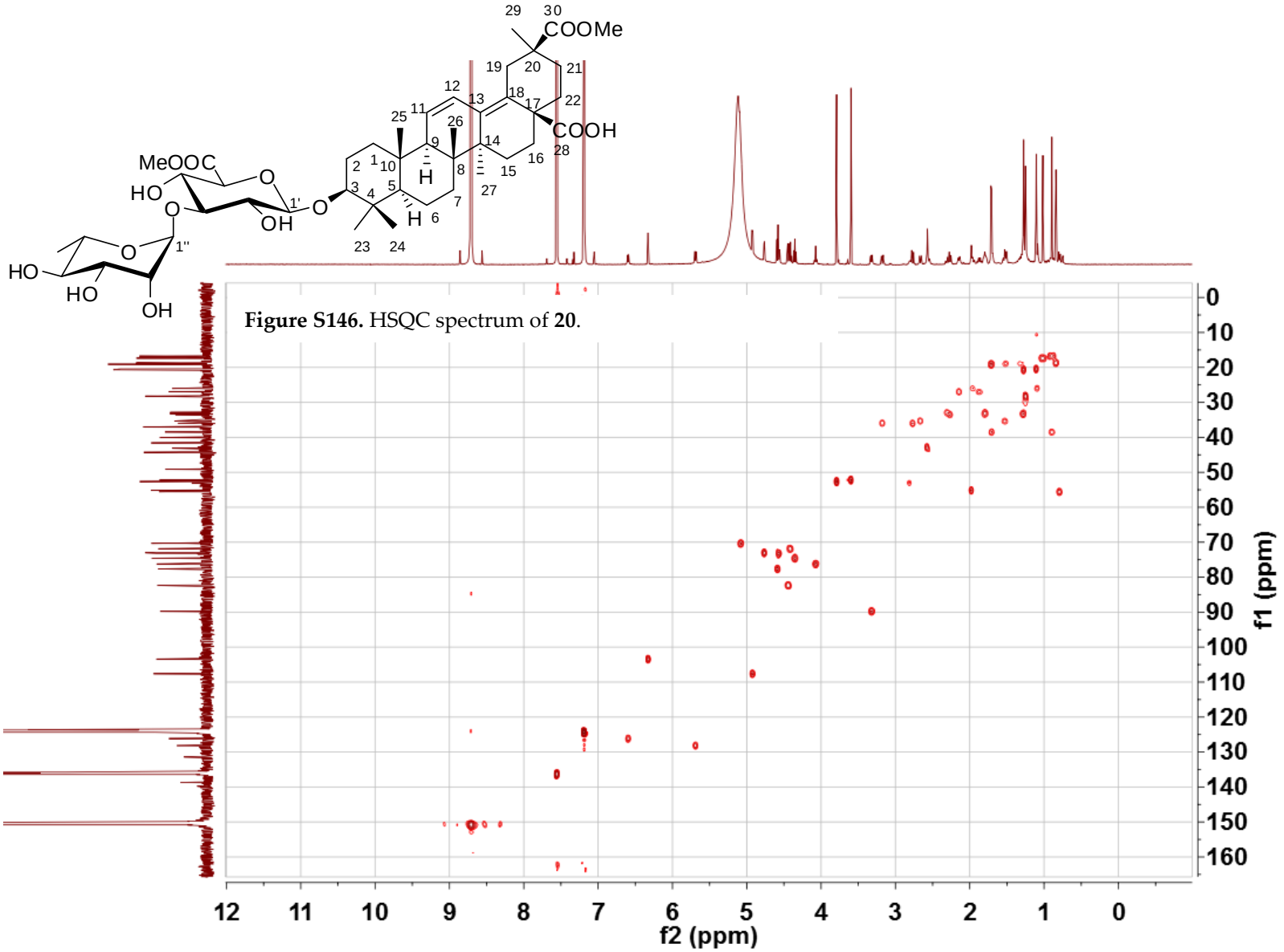


Figure S146. HSQC spectrum of **20**.

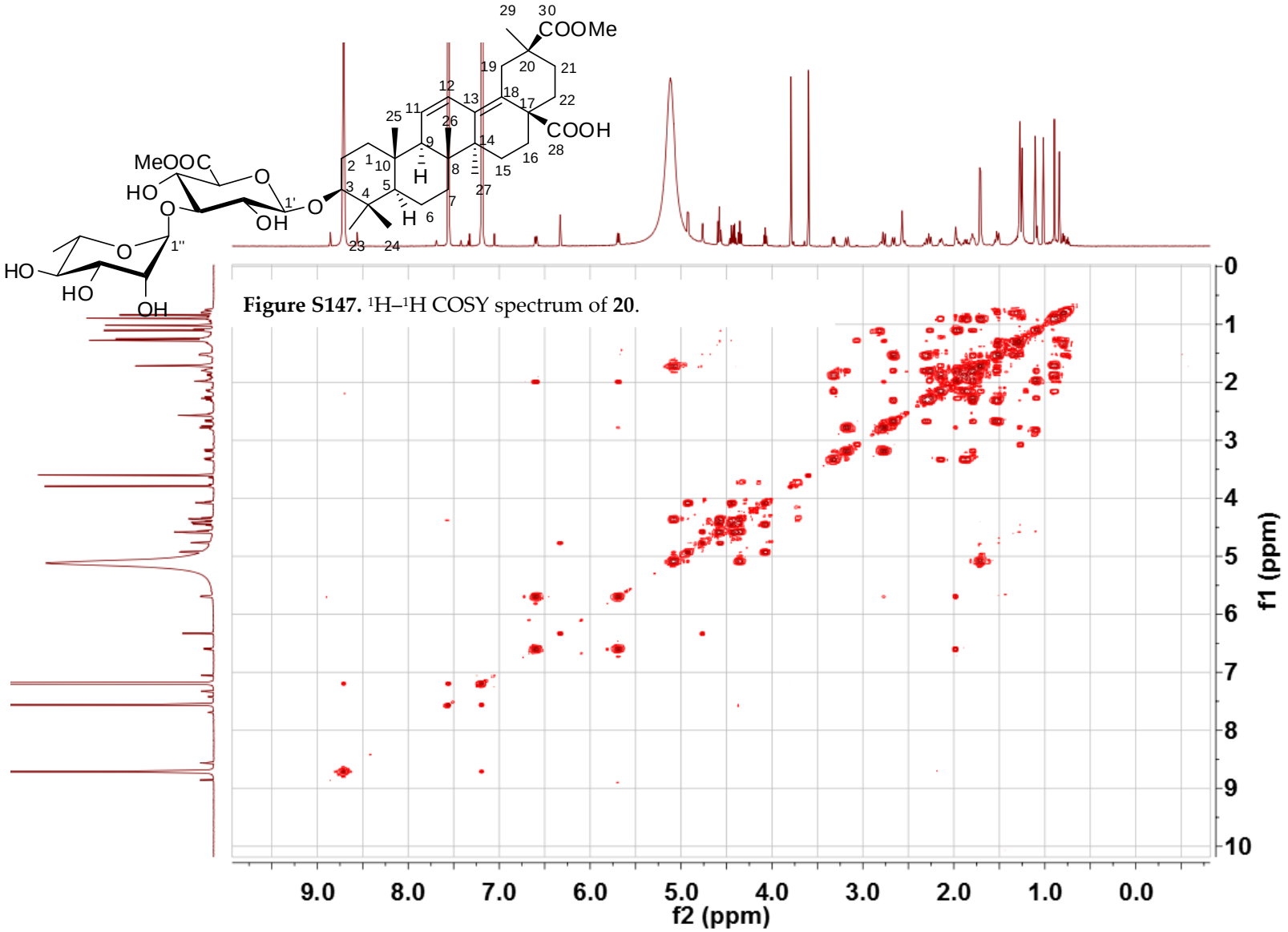


Figure S147. ^{1}H–^{1}H COSY spectrum of **20**.

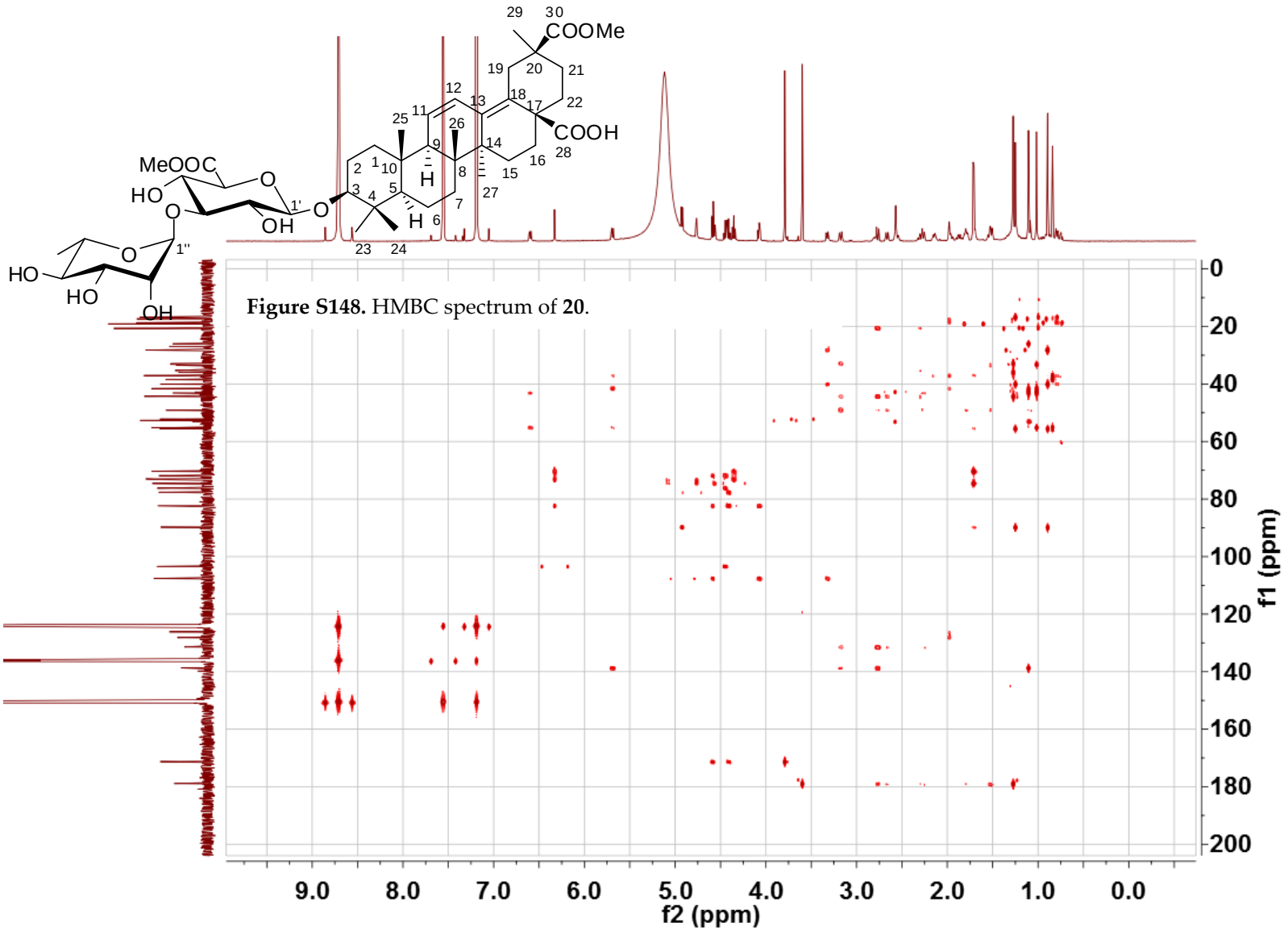


Figure S148. HMBC spectrum of **20**.

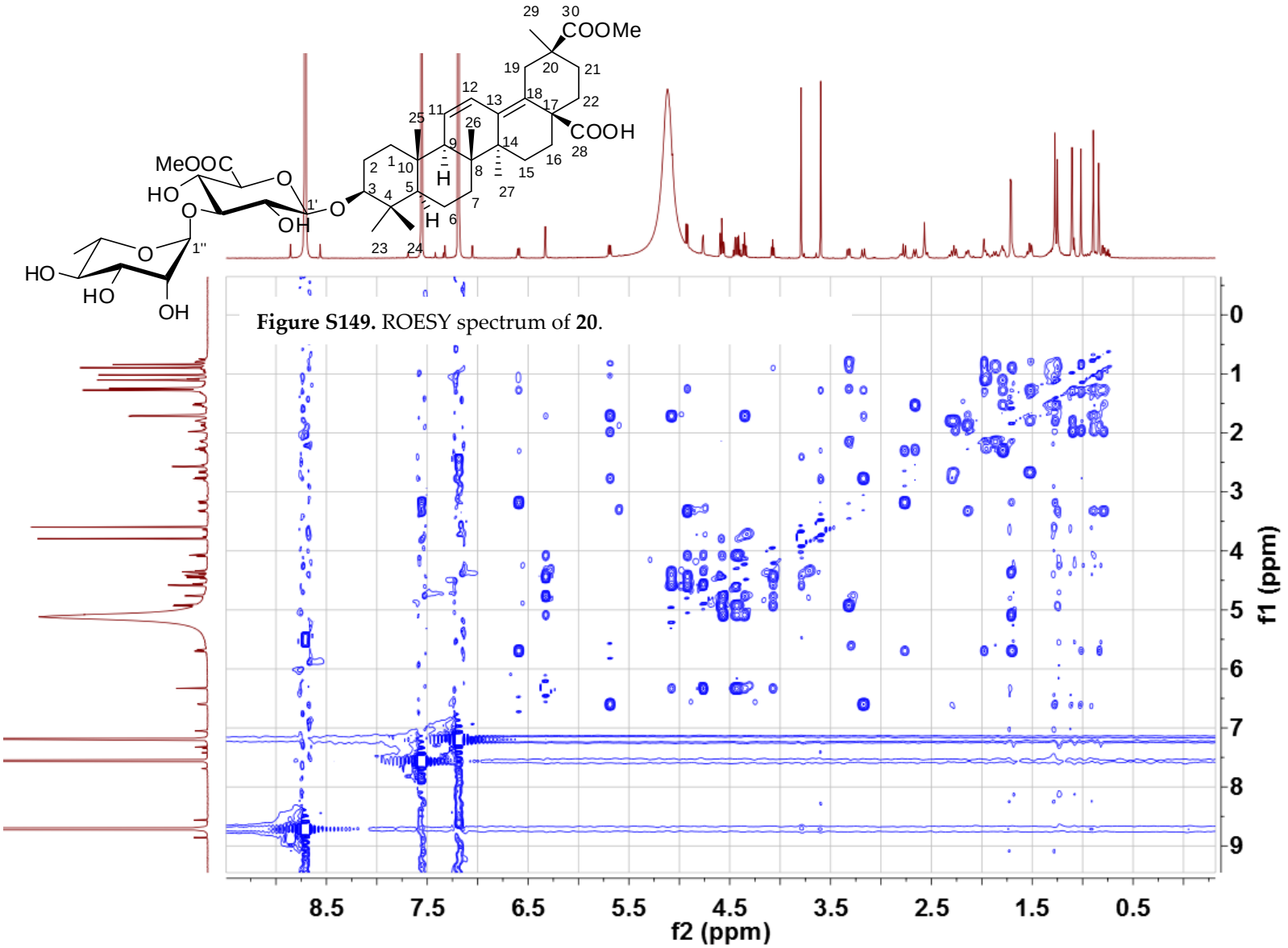


Figure S149. ROESY spectrum of **20**.

Data Filename	180828ESIA3.d	**Sample Name**	pdt47
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/28/2018 9:56:07 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

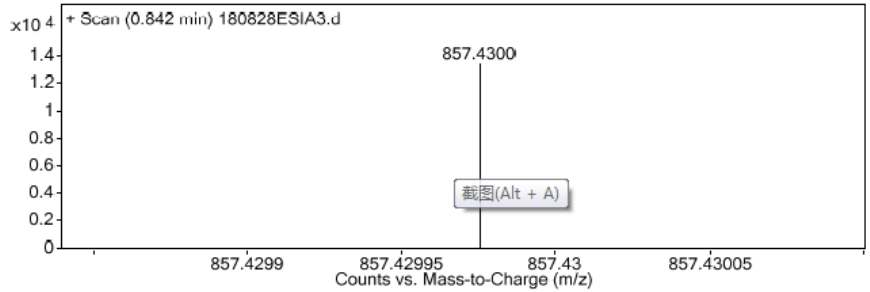


Figure S150. HRESIMS spectrum of **20**.

Peak List

m/z	z	Abund	Formula	Ion
102.1279	1	62256.19		
111.1809		17327.26		
112.1872	1	70639.46		
123.0914	1	13701.84		
144.0801	1	14600.05		
144.2429		35668.02		
145.2495	1	173775.77		
146.2524	1	14833.91		
152.2178	1	24149.91		
857.43	1	13353.48	C44 H66 Na O15	M+

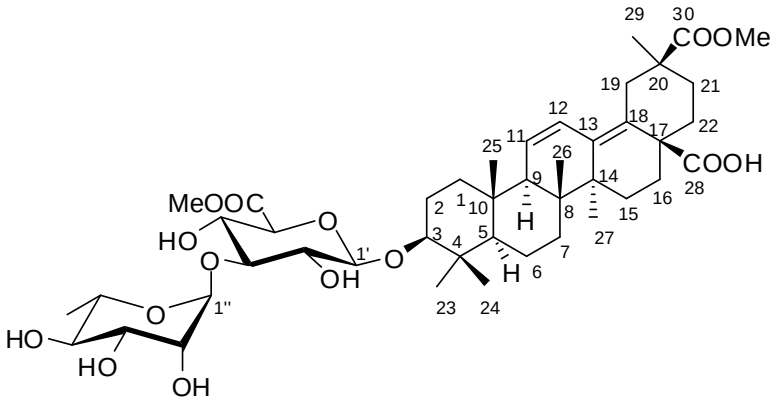
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	11	19
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C44 H66 Na O15	857.4299	857.4300	-0.1	0.1	11.5

--- End Of Report ---



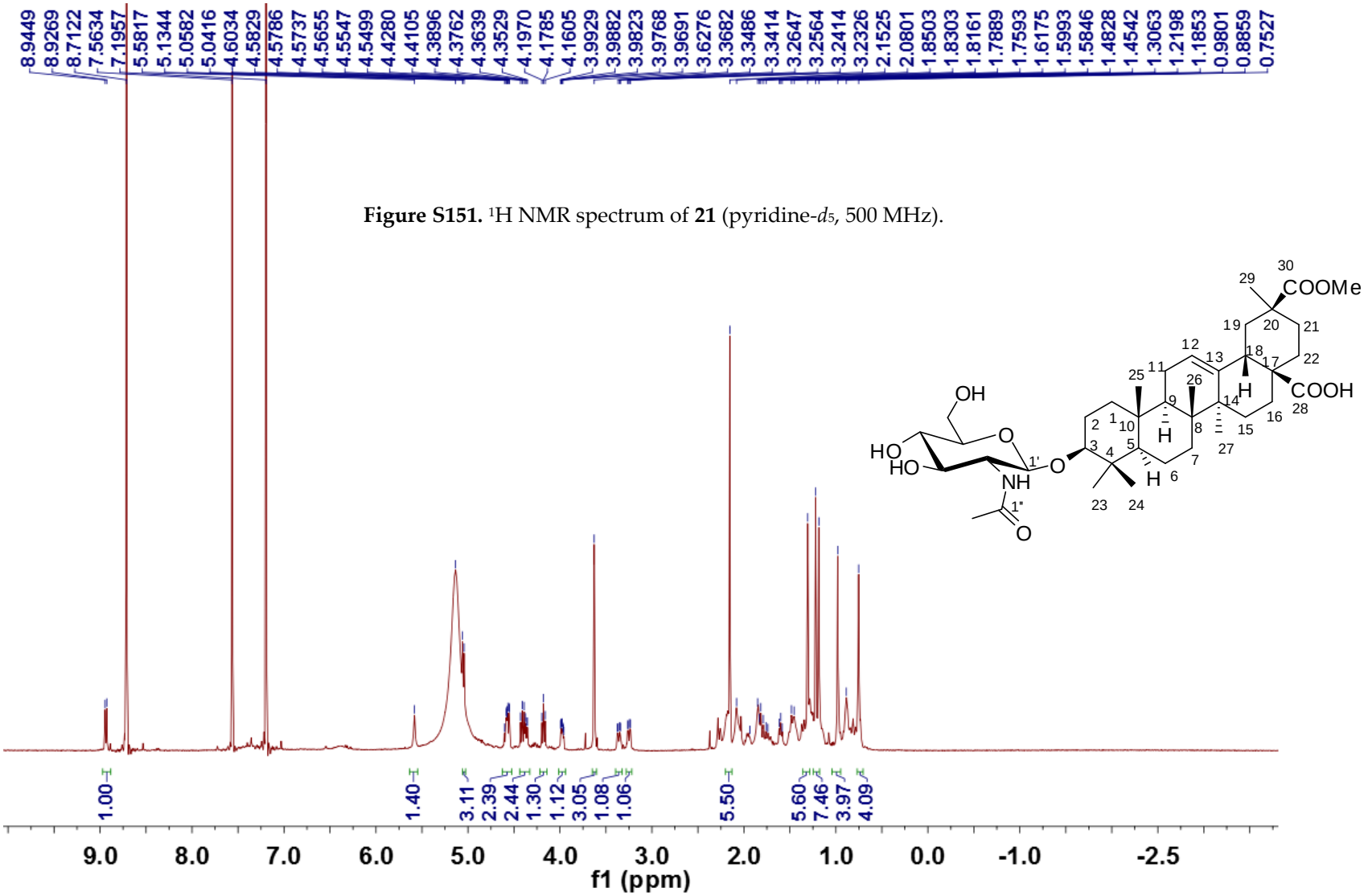


Figure S151. ^{1}H NMR spectrum of **21** (pyridine-d_5, 500 MHz).

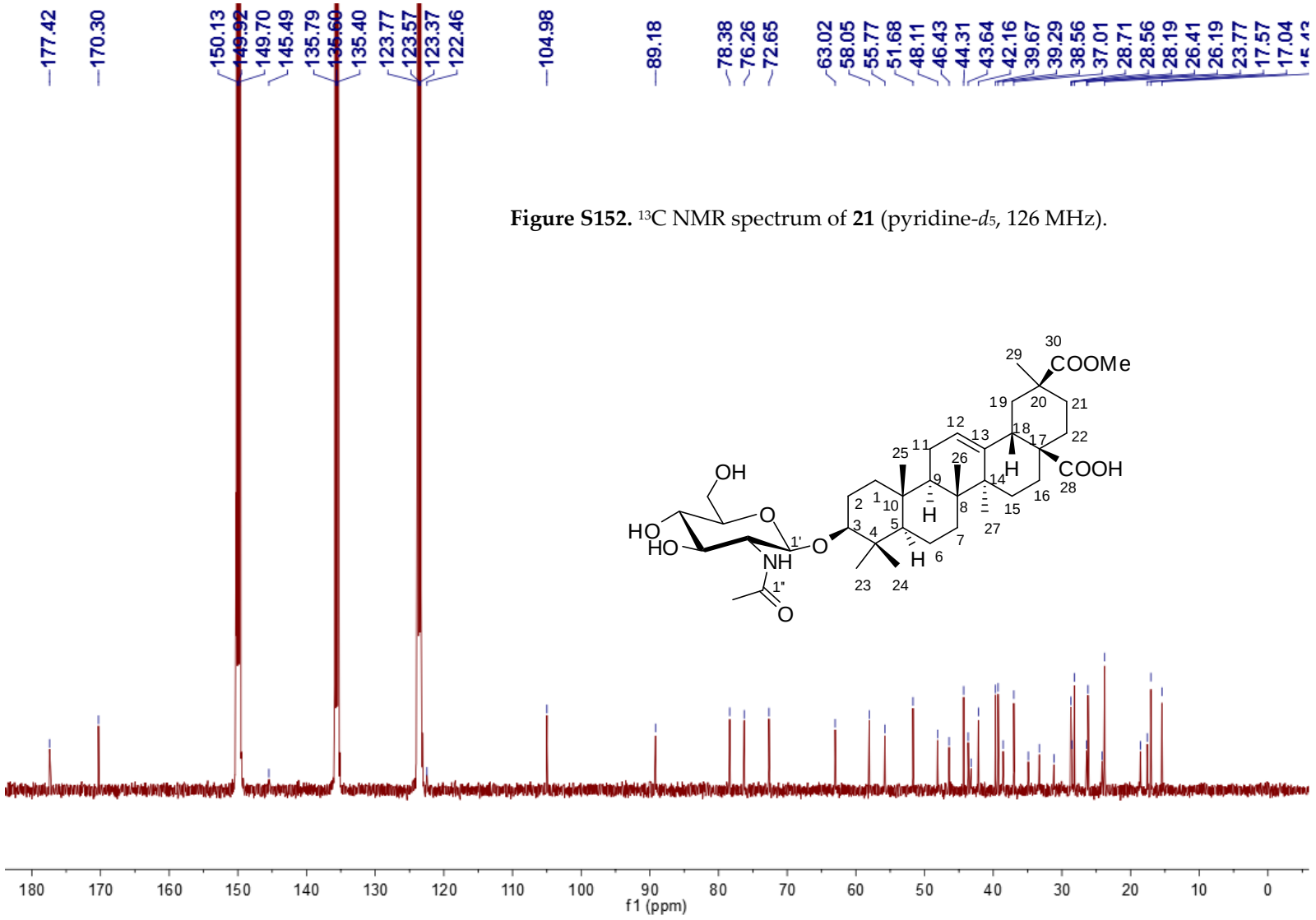


Figure S152. ^{13}C NMR spectrum of **21** (pyridine-d_5, 126 MHz).

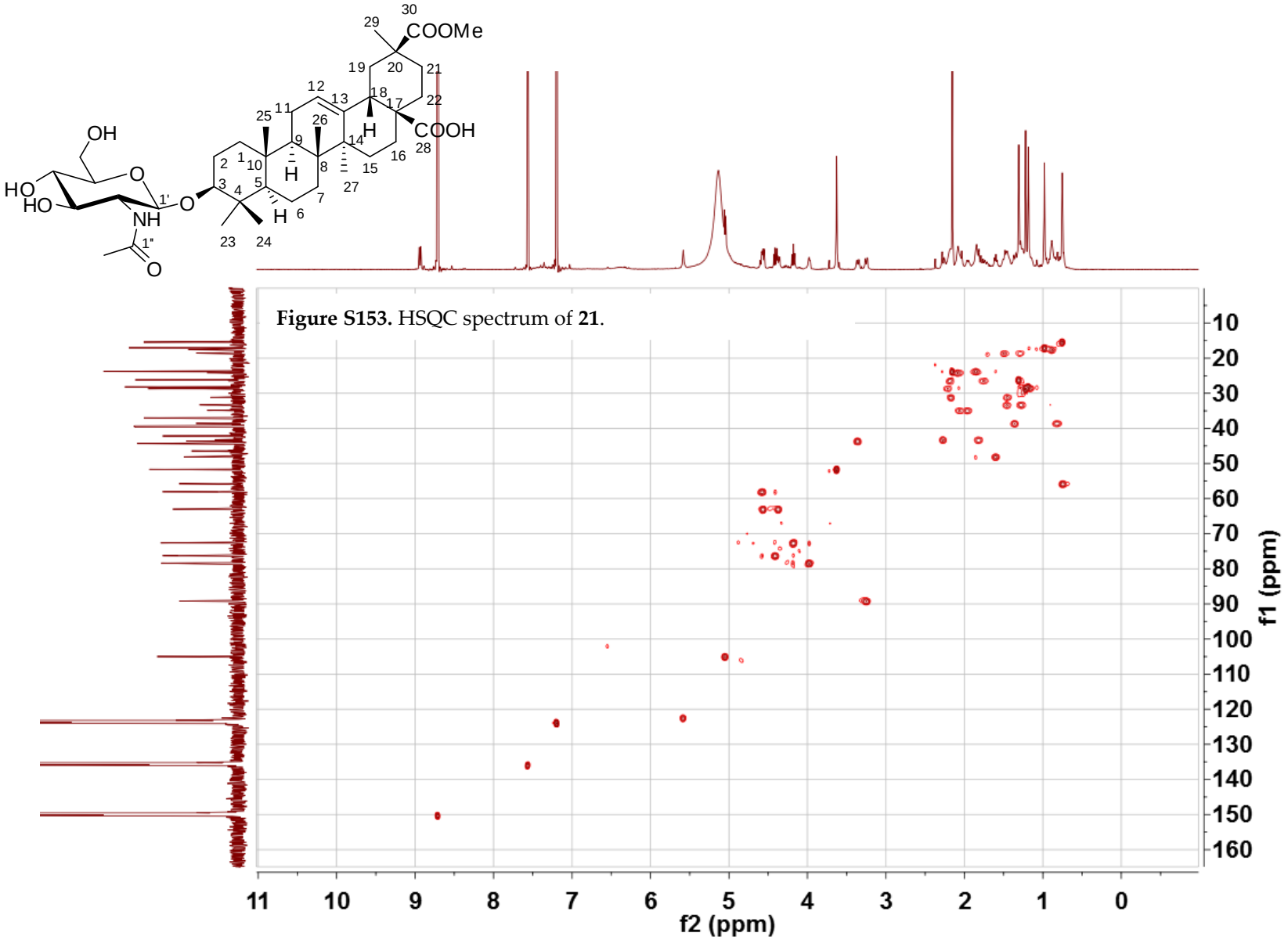


Figure S153. HSQC spectrum of **21**.

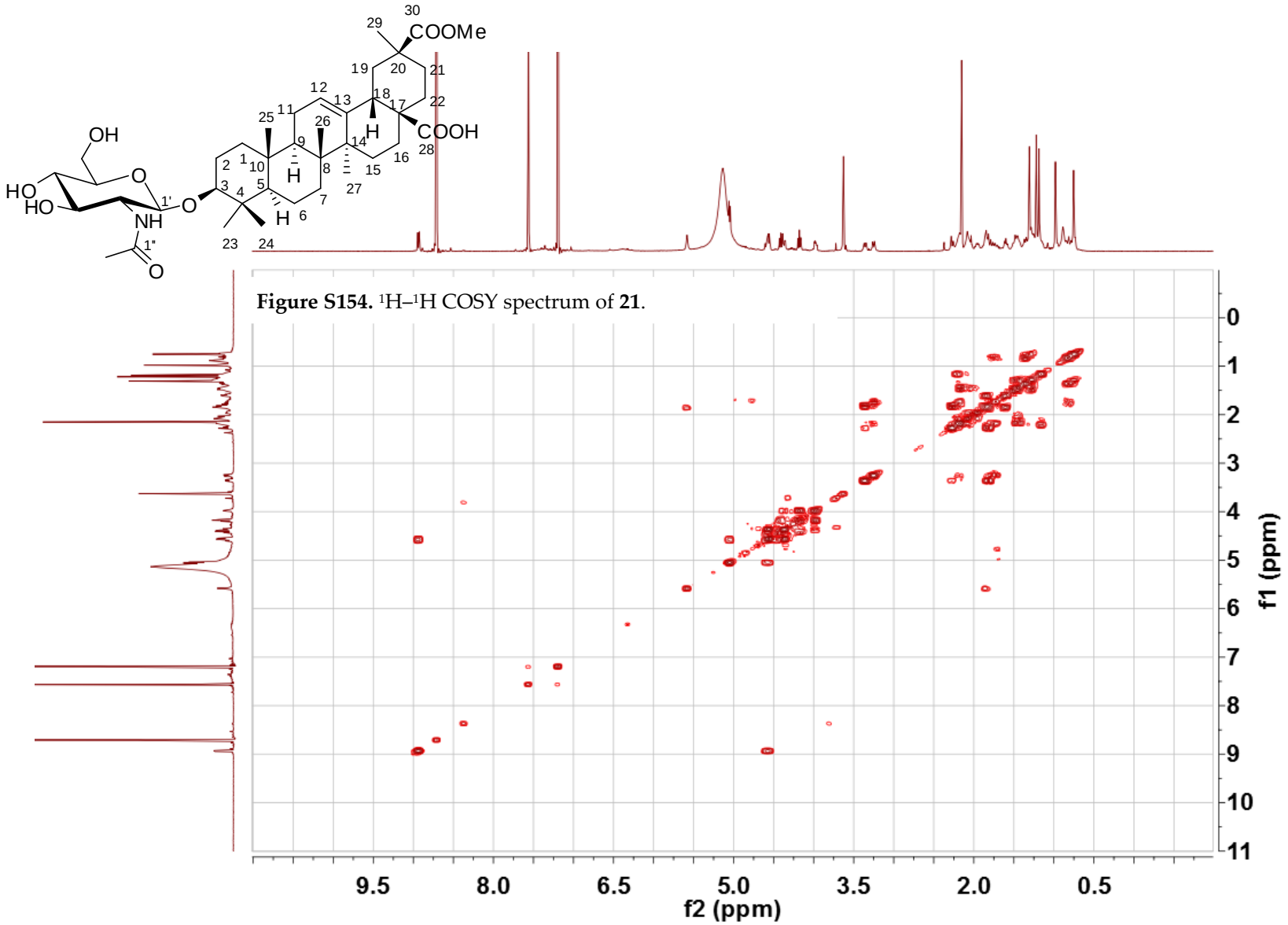


Figure S154. ^{1}H–^{1}H COSY spectrum of **21**.

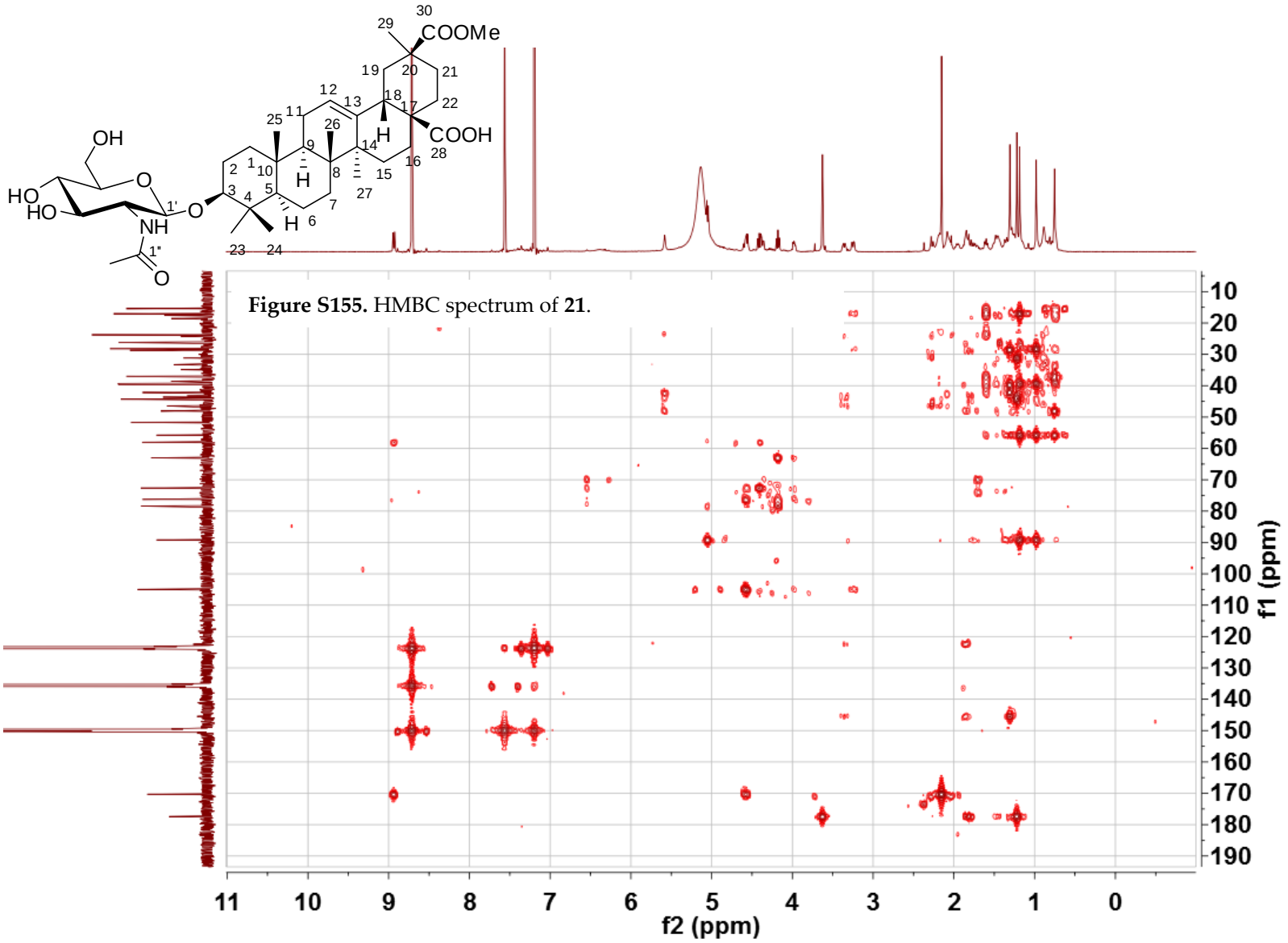


Figure S155. HMBC spectrum of **21**.

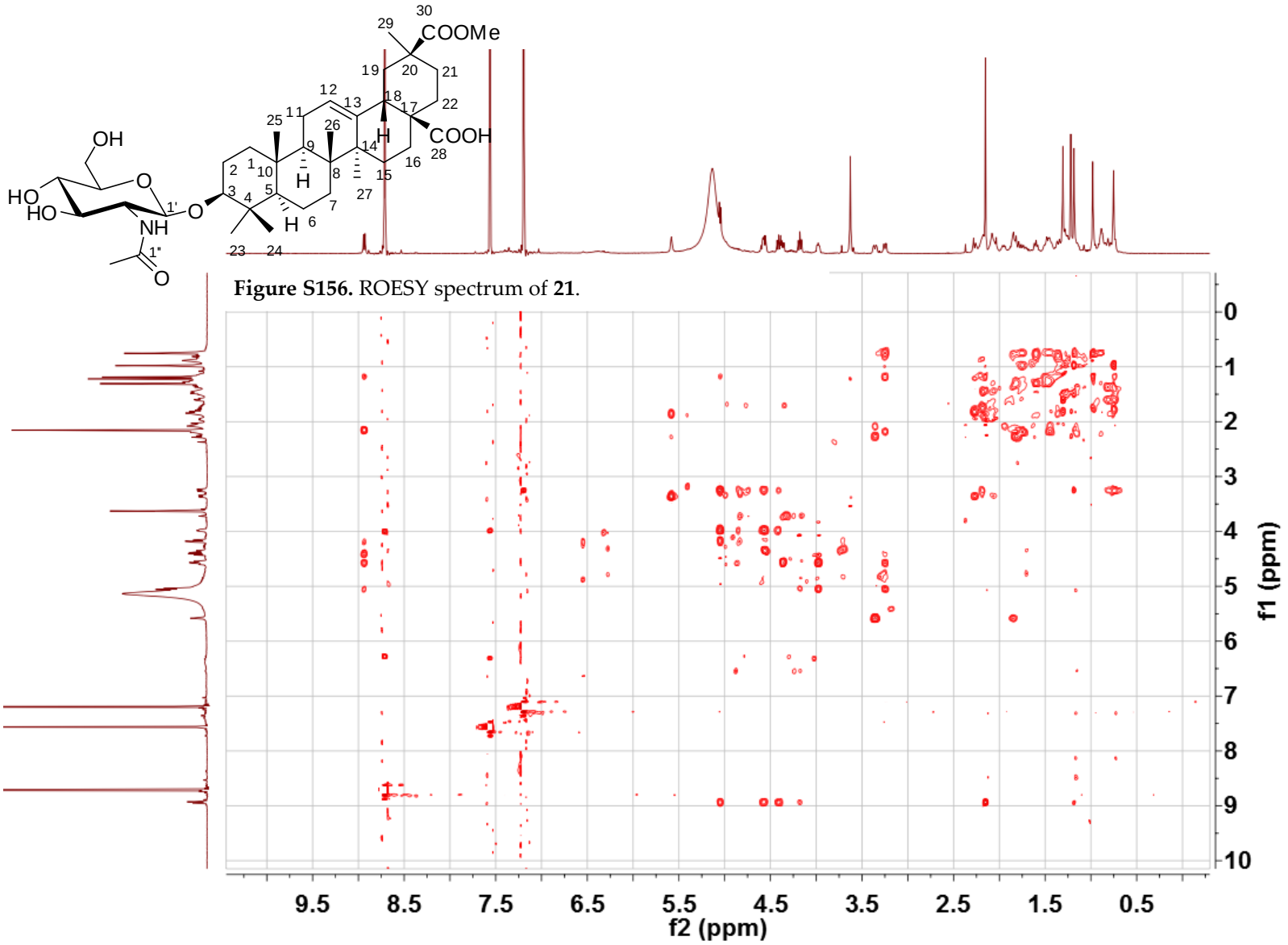


Figure S156. ROESY spectrum of **21**.

Data Filename	180829ESIA8.d	**Sample Name**	pdt51
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	8/29/2018 1:55:15 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

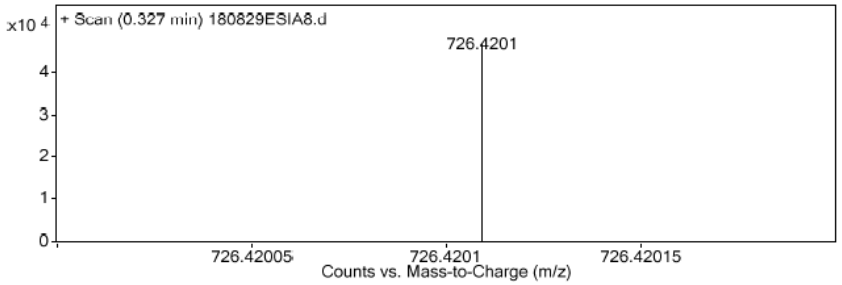


Figure S157. HRESIMS spectrum of **21**.

Peak List

m/z	z	Abund	Formula	Ion
103.0077		5729.59		
107.037	1	5492.39		
111.1819		4861.88		
112.1882	1	26780.22		
145.2506	1	10904.01		
726.4201	1	46460.01	C39 H61 N Na O10	M+
727.4231	1	20077.11	C39 H61 N Na O10	M+
742.3912	2	8471.38		
759.4663	1	7527.42		
856.3787	1	5568.69		

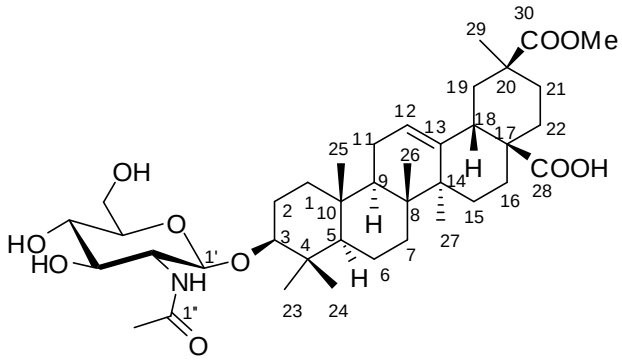
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	14
Na	1	1
N	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C39 H61 N Na O10	726.4193	726.4201	-0.8	1.1	9.5

--- End Of Report ---



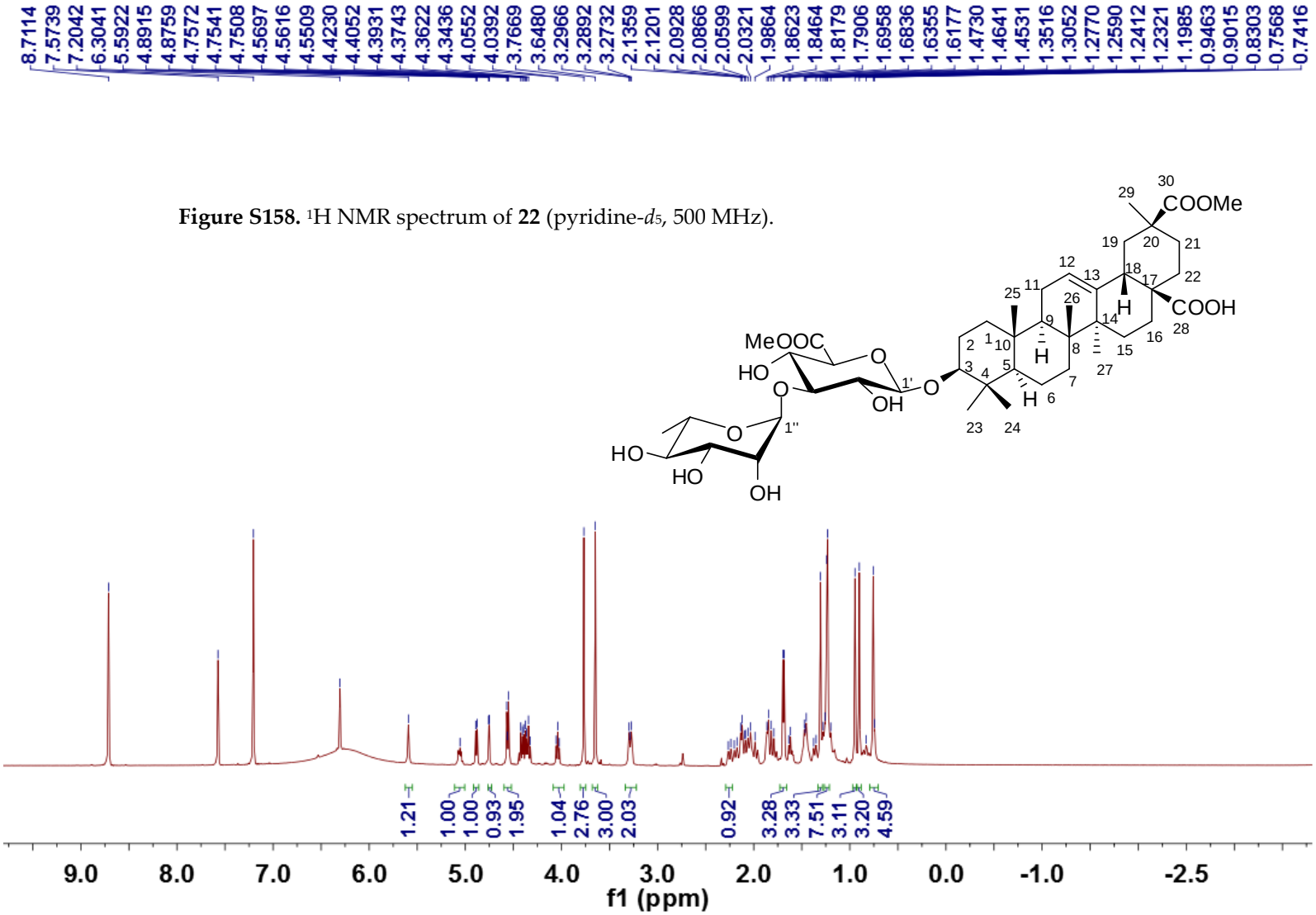


Figure S158. ^{1}H NMR spectrum of **22** (pyridine-d_5, 500 MHz).

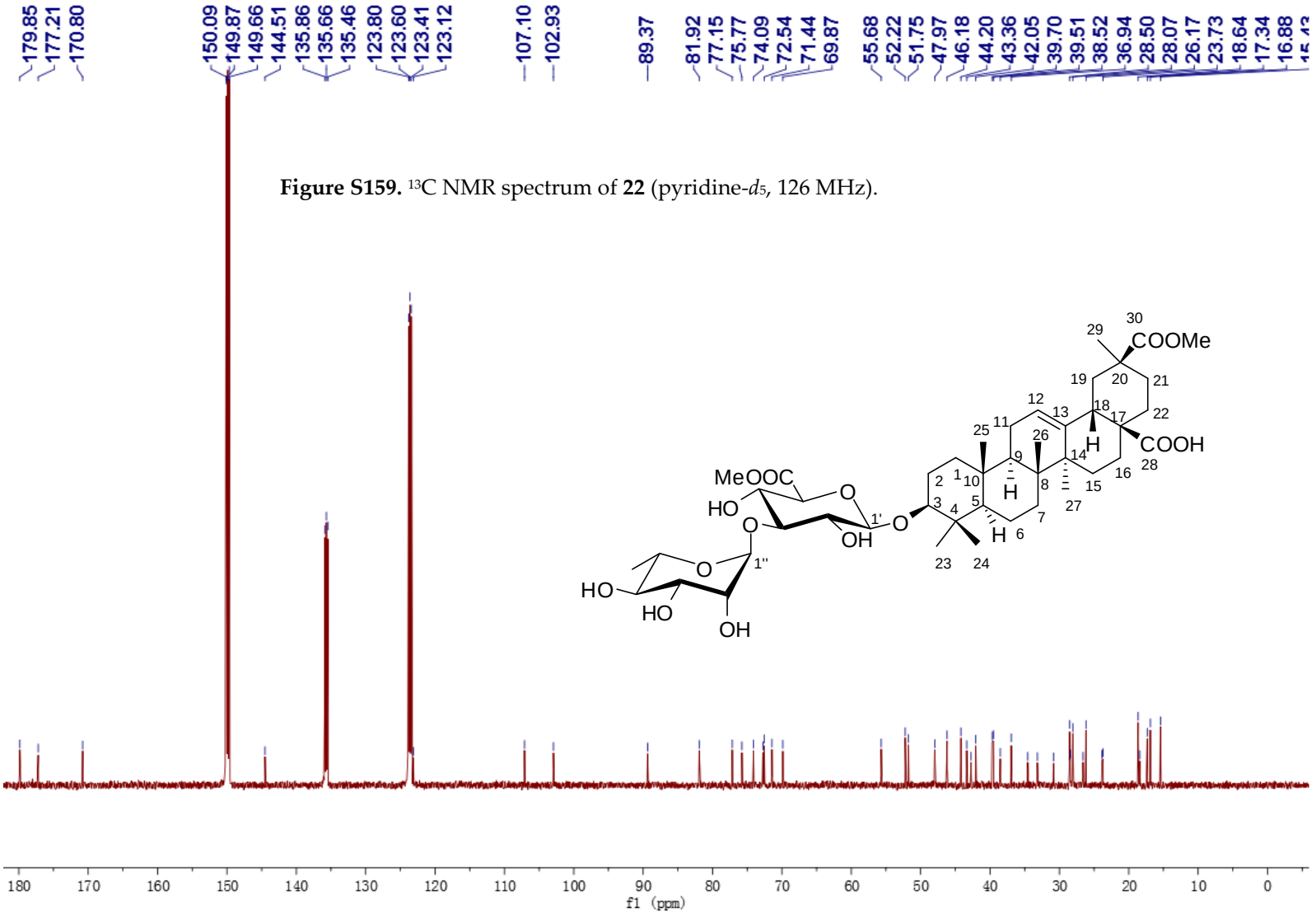


Figure S159. ^{13}C NMR spectrum of **22** (pyridine-d_5, 126 MHz).

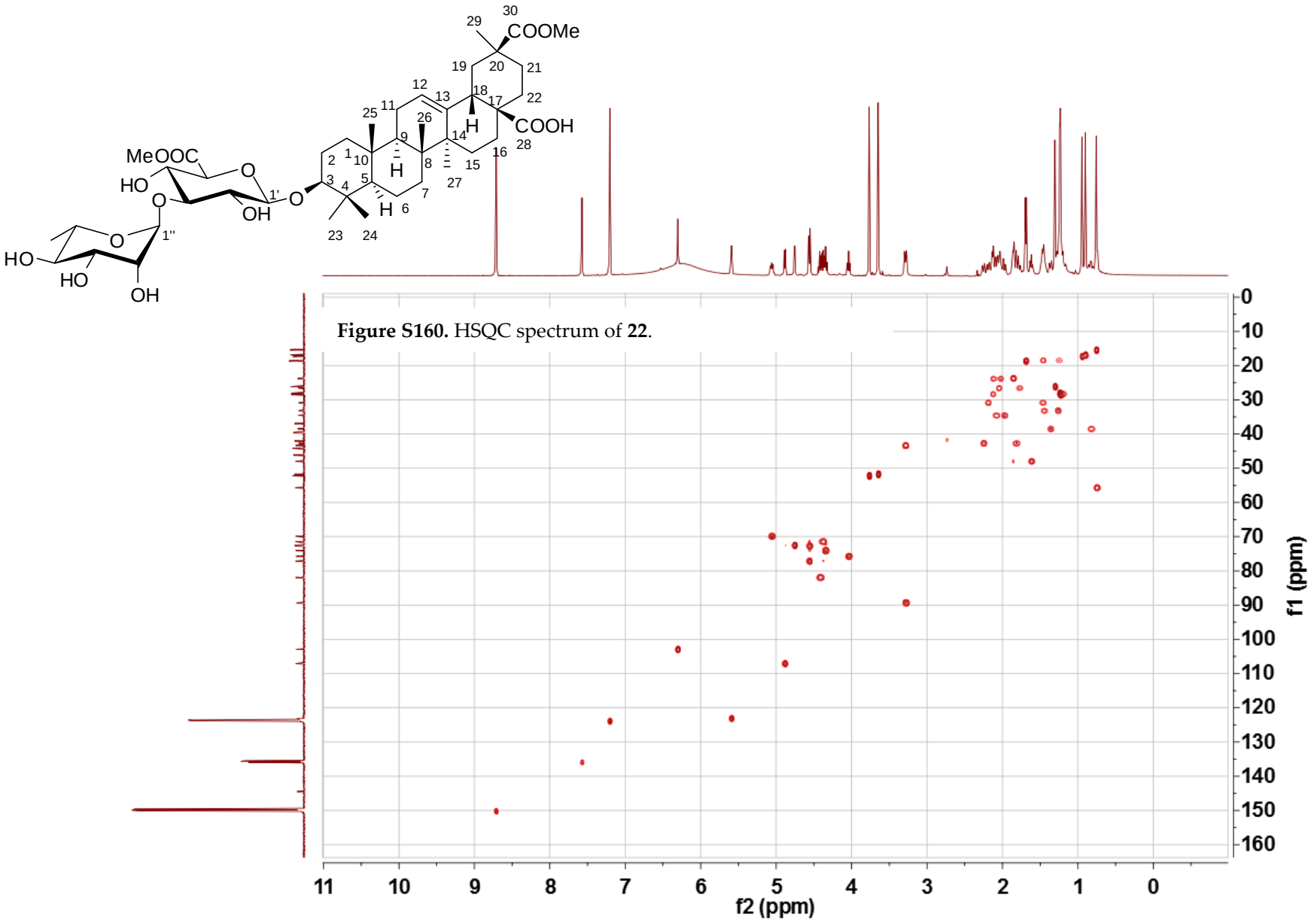


Figure S160. HSQC spectrum of **22**.

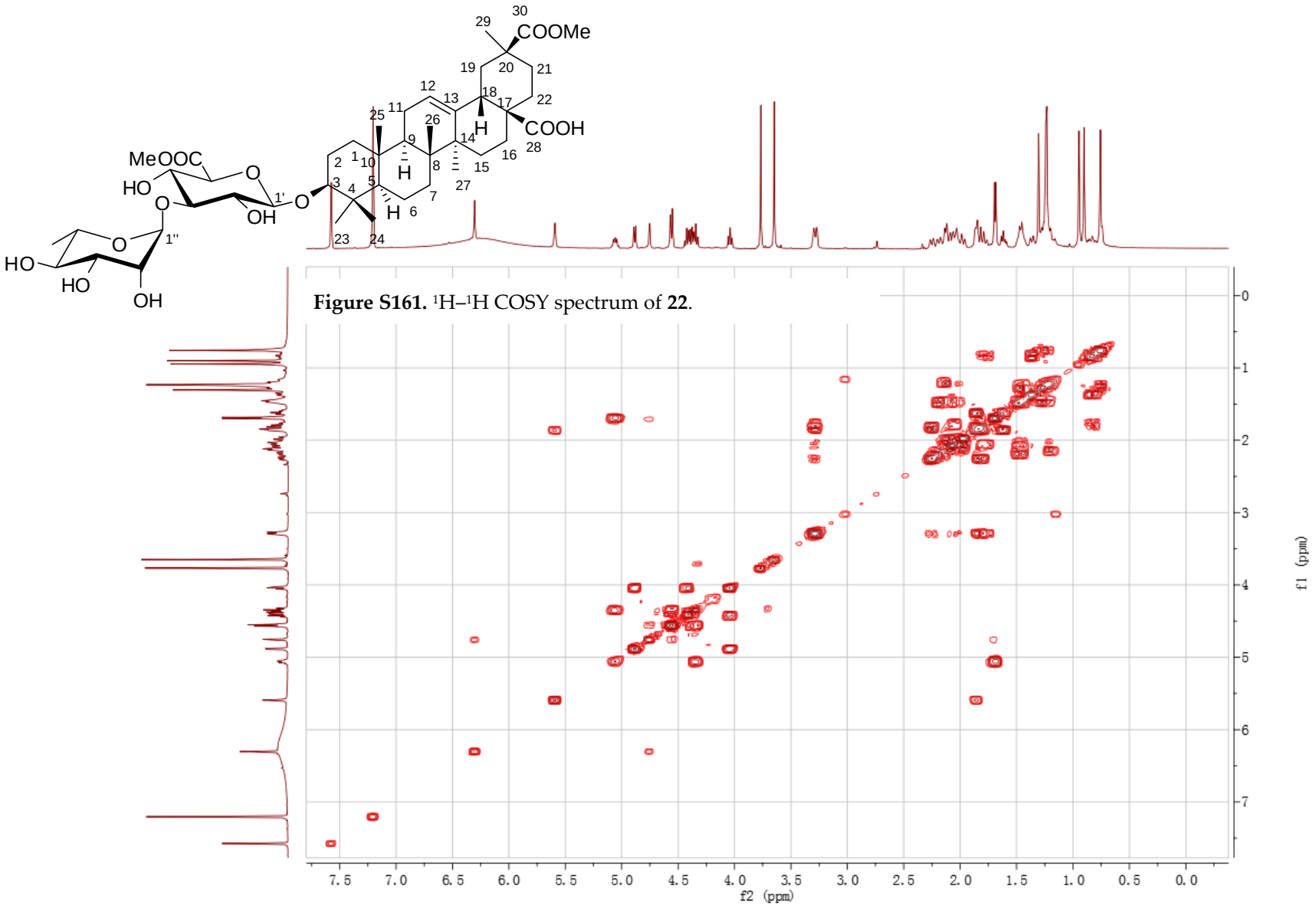


Figure S161. ^{1}H–^{1}H COSY spectrum of **22**.

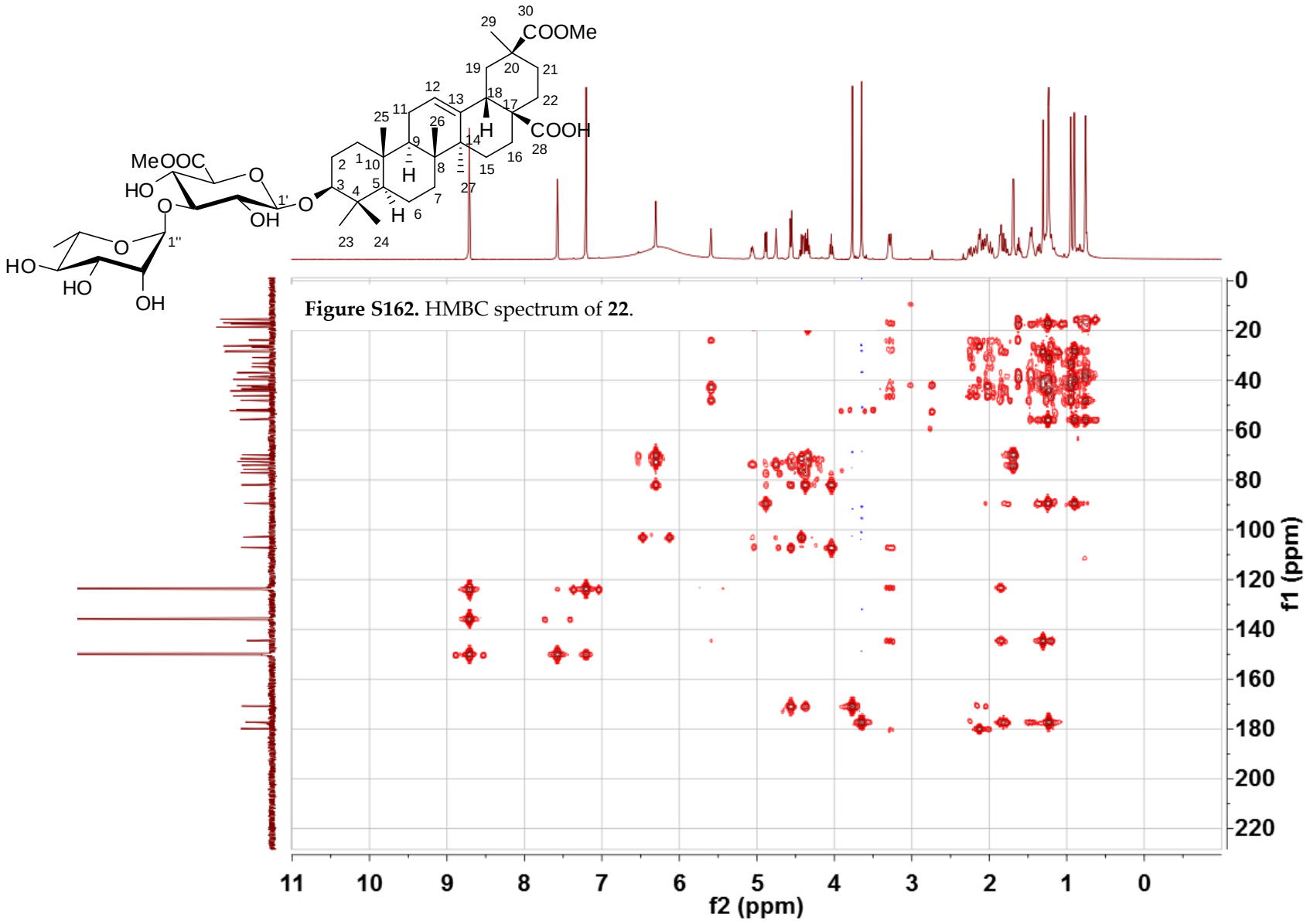


Figure S162. HMBC spectrum of **22**.

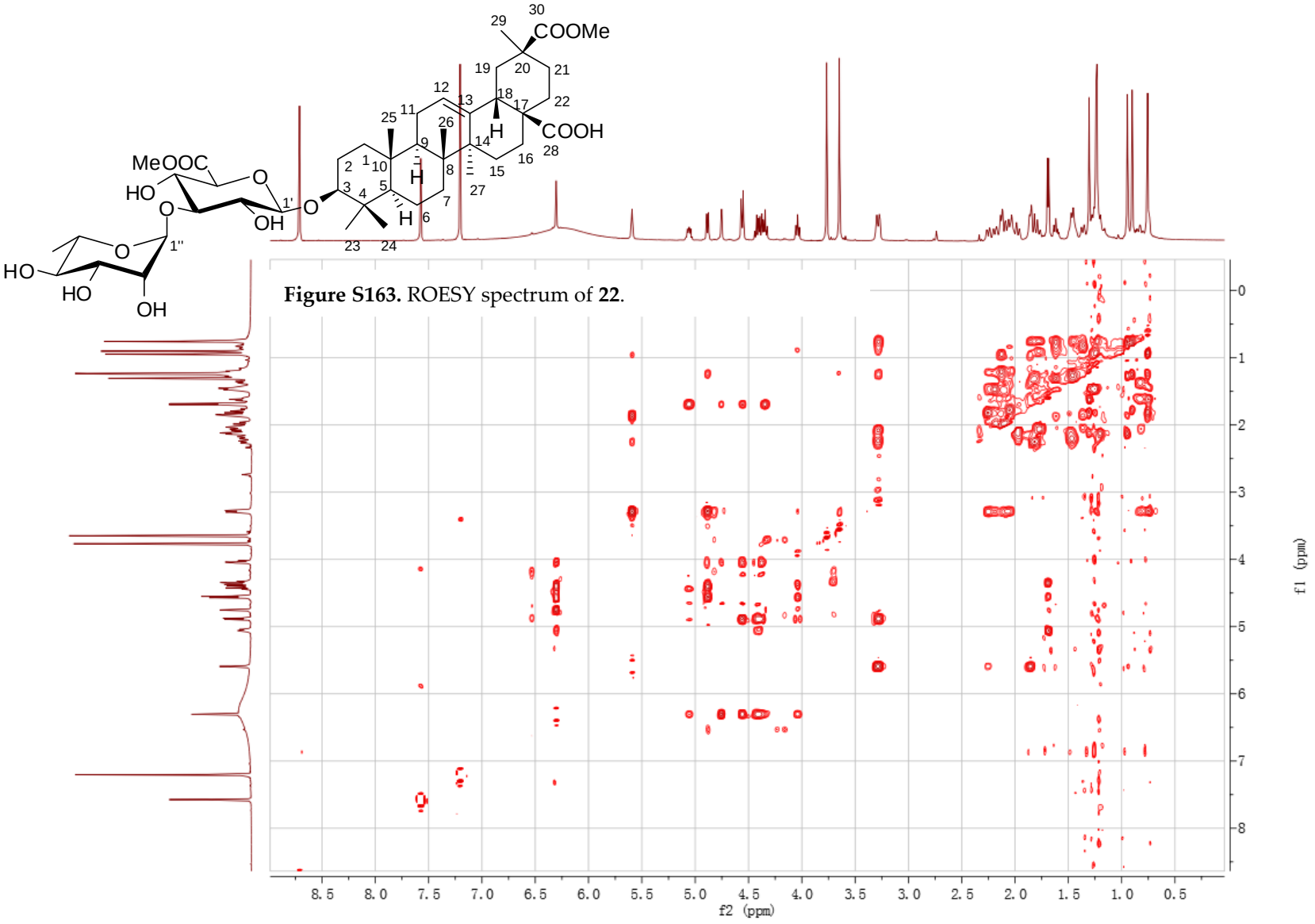


Figure S163. ROESY spectrum of **22**.

Formula Predictor Report - pdt34b.lcd

Data File: E:\DATA\2018\0702\pdt34b.lcd

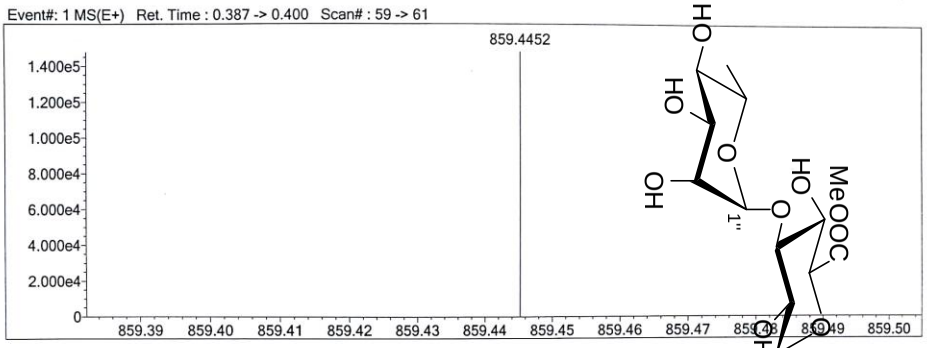
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	O	2	0	20	Si	4	0	0	Br	1	0	0	Na
C	4	10	50	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	0	Na	1	0	0	Cl	1	0	0					

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

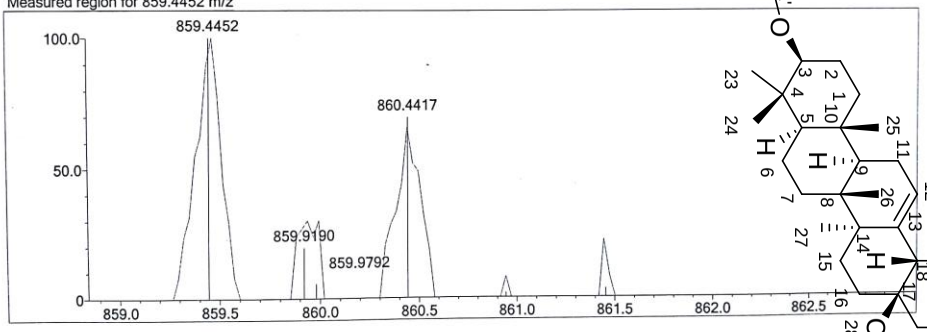
DBE Range: -2.0 - 100.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 10

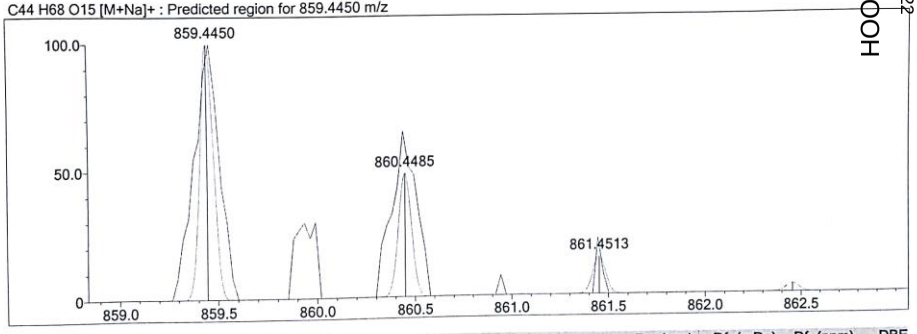
Event#: 1 MS(E+) Ret. Time : 0.387 -> 0.400 Scan# : 59 -> 61



Measured region for 859.4452 m/z



C44 H68 O15 [M+Na]+ : Predicted region for 859.4450 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C44 H68 O15	[M+Na]+	859.4452	859.4450	0.2	0.23	11.0

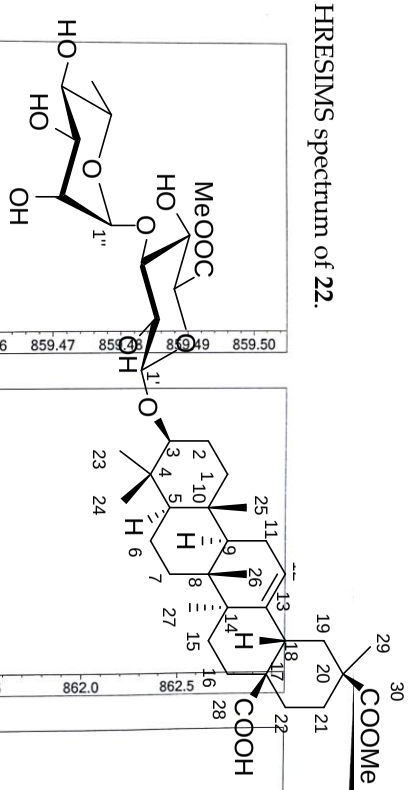


Figure S164. HRESIMS spectrum of **22**.

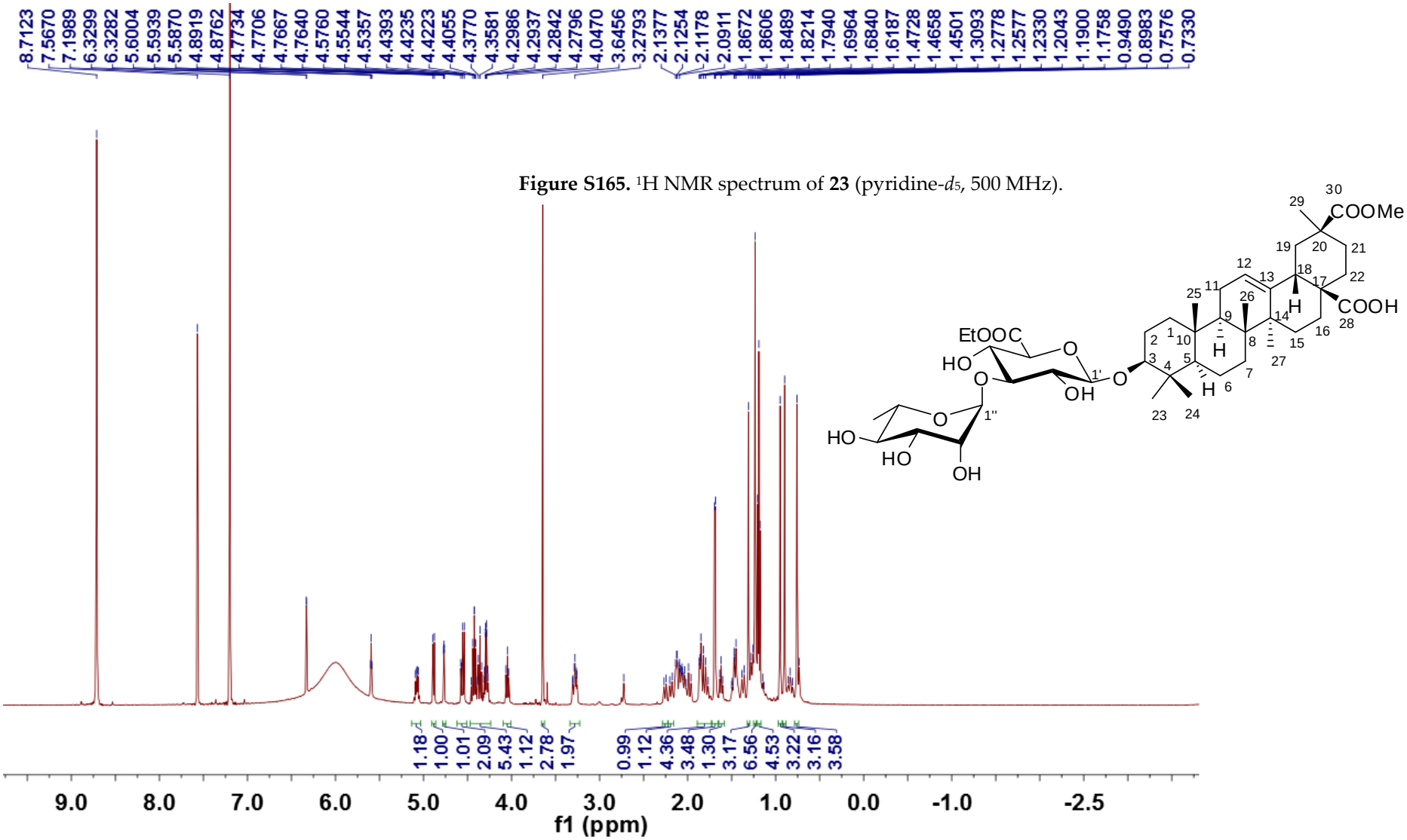


Figure S165. ^{1}H NMR spectrum of **23** (pyridine-d_5, 500 MHz).

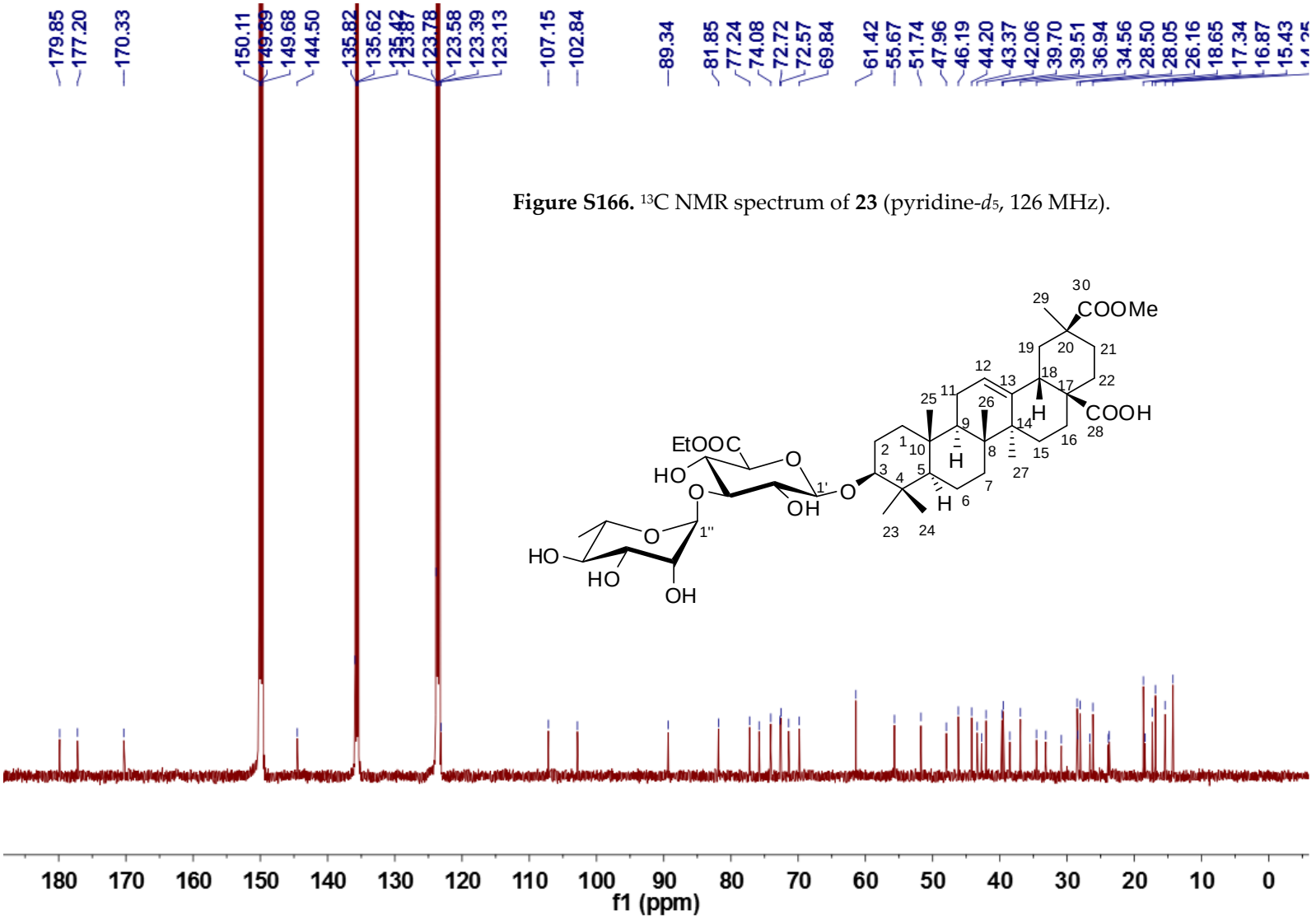


Figure S166. ^{13}C NMR spectrum of **23** (pyridine-d_5, 126 MHz).

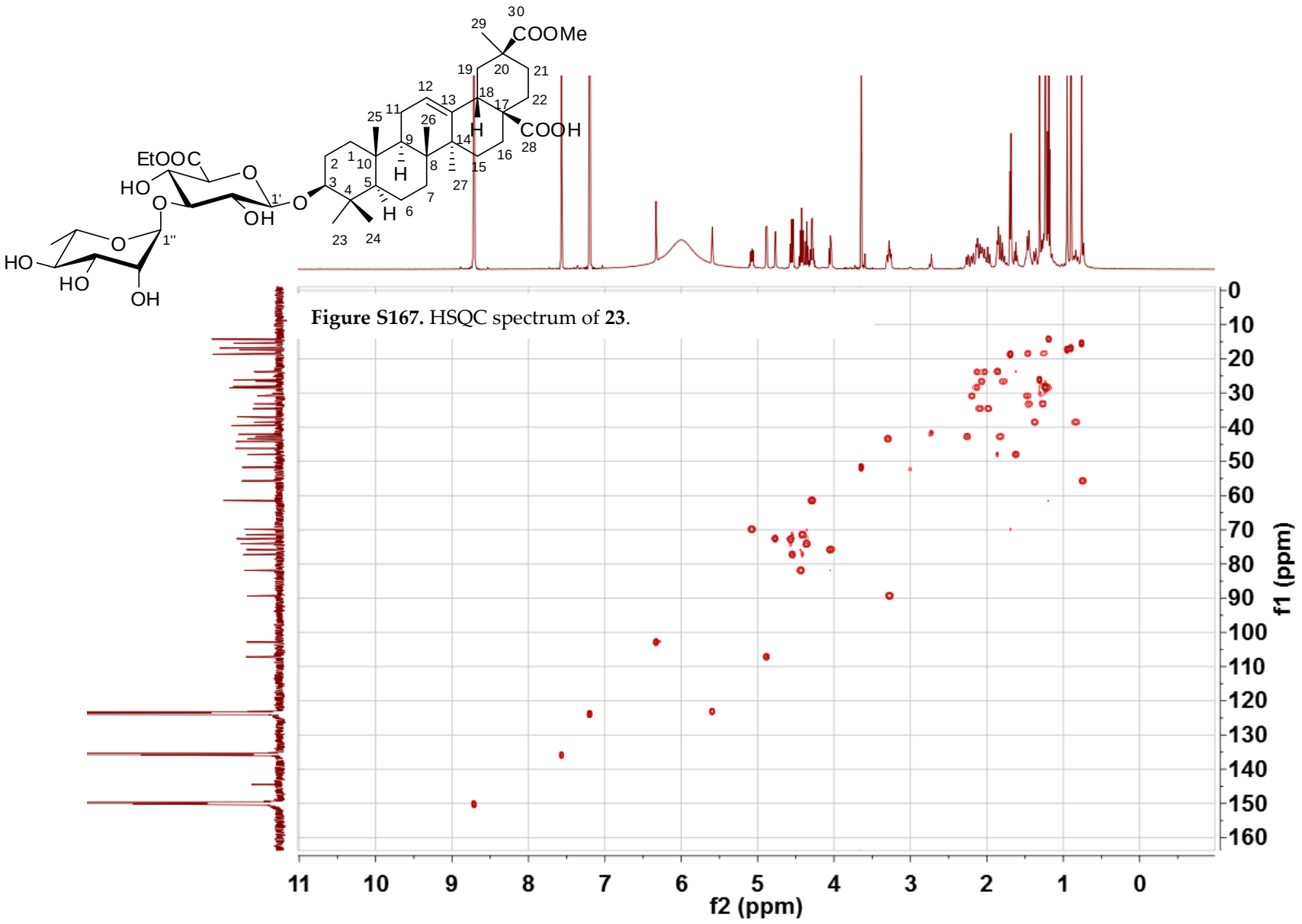


Figure S167. HSQC spectrum of **23**.

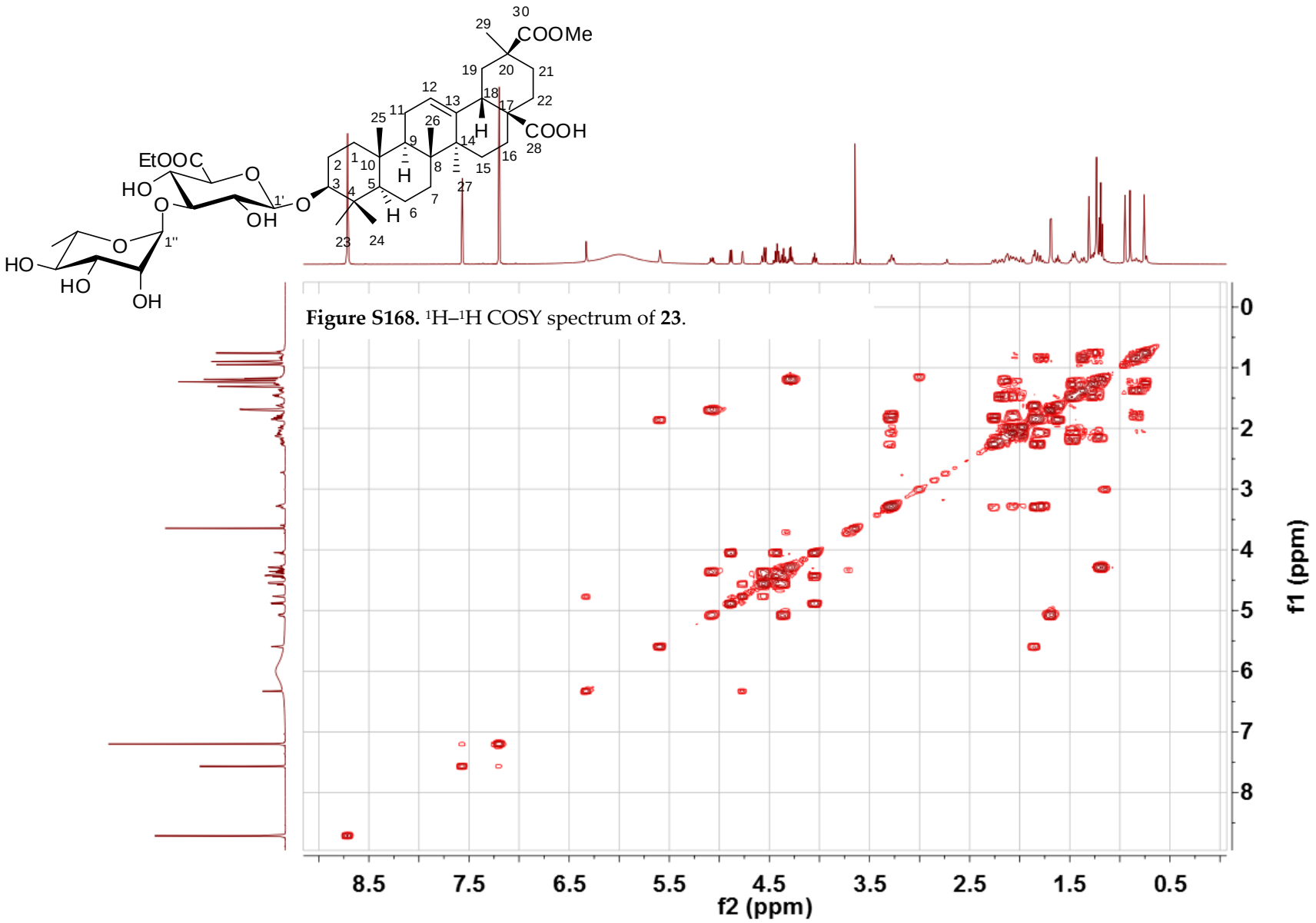


Figure S168. ^{1}H–^{1}H COSY spectrum of **23**.

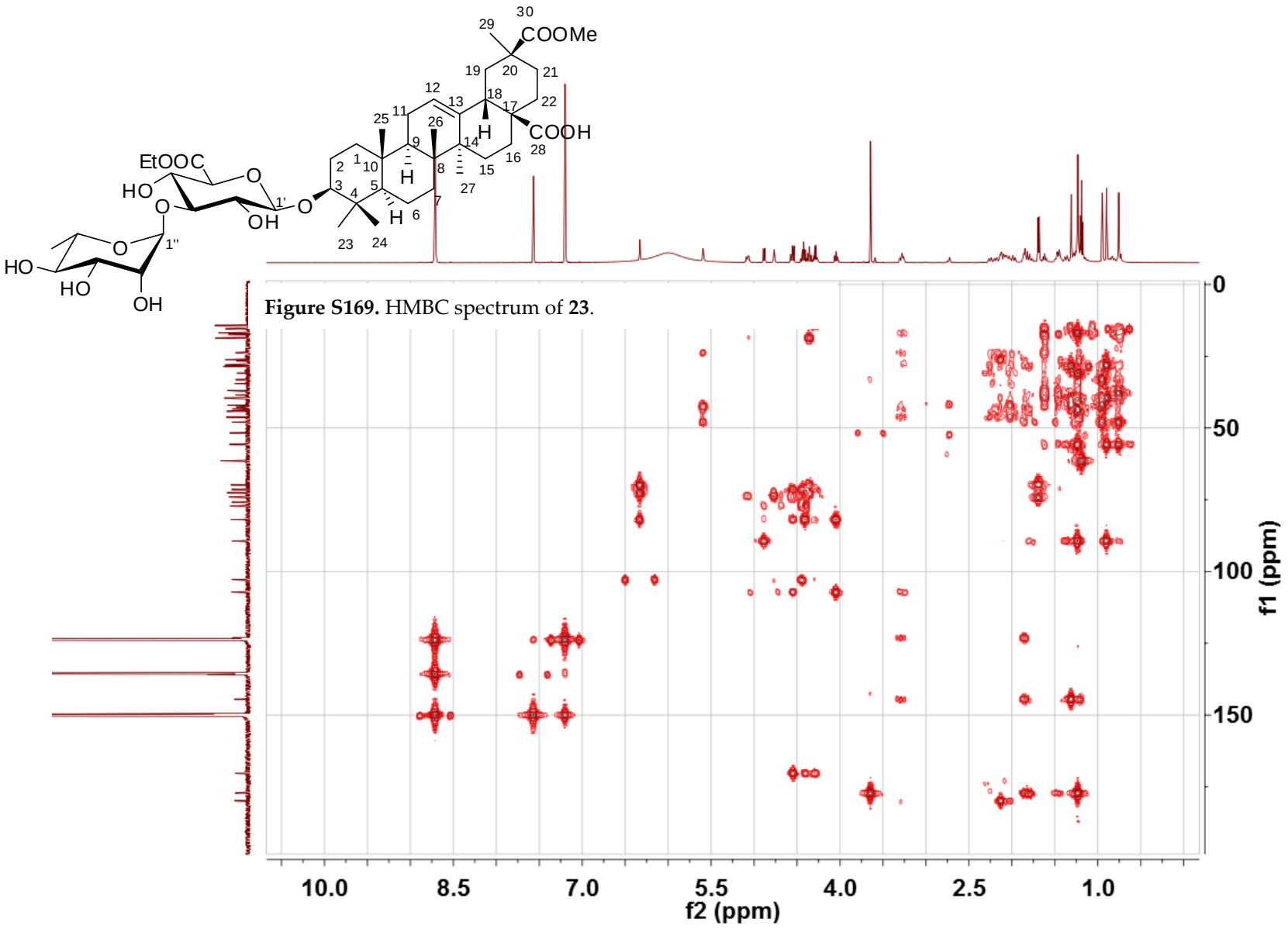


Figure S169. HMBC spectrum of **23**.

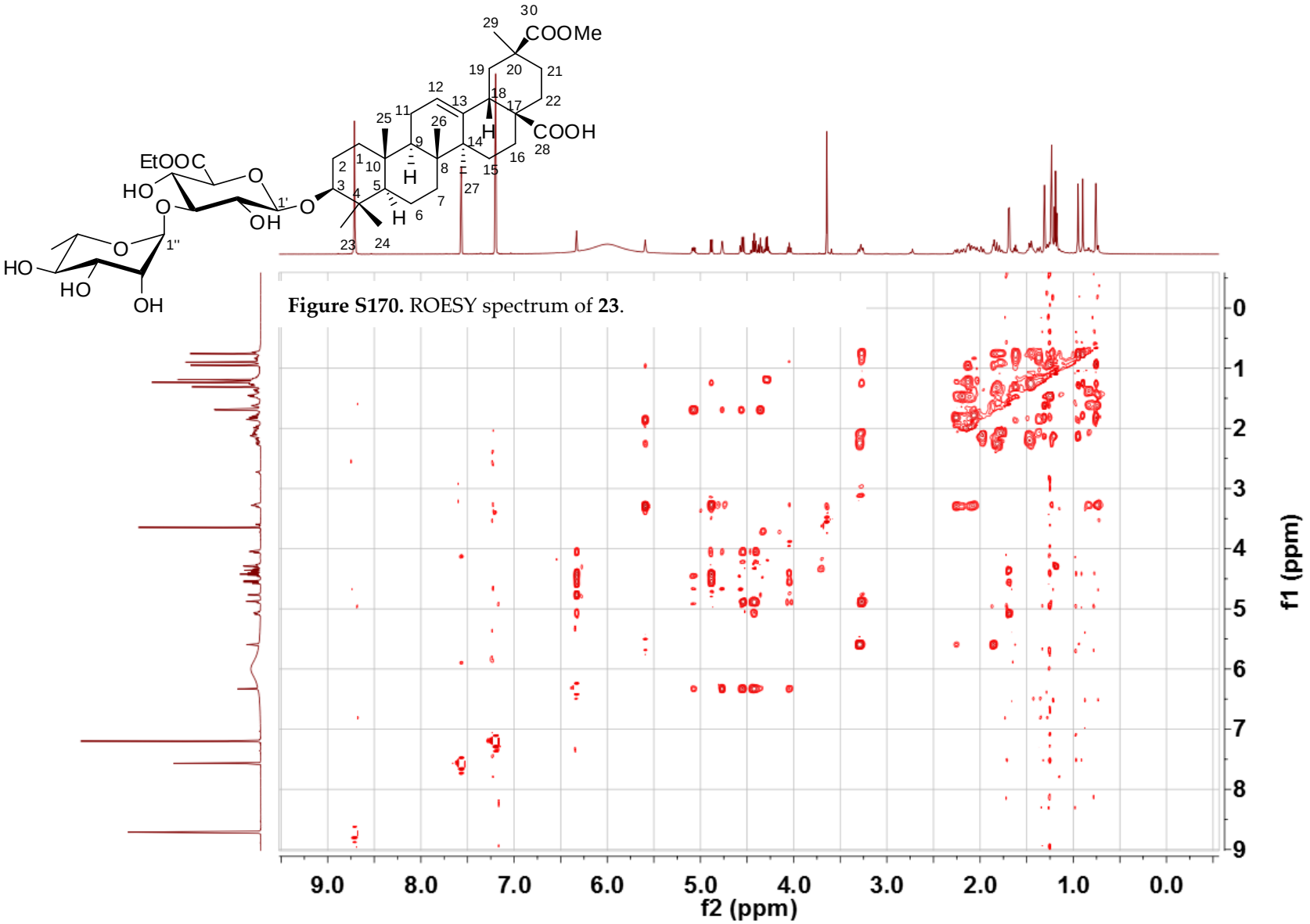


Figure S170. ROESY spectrum of **23**.

Figure S171. HRESIMS spectrum of **23**.

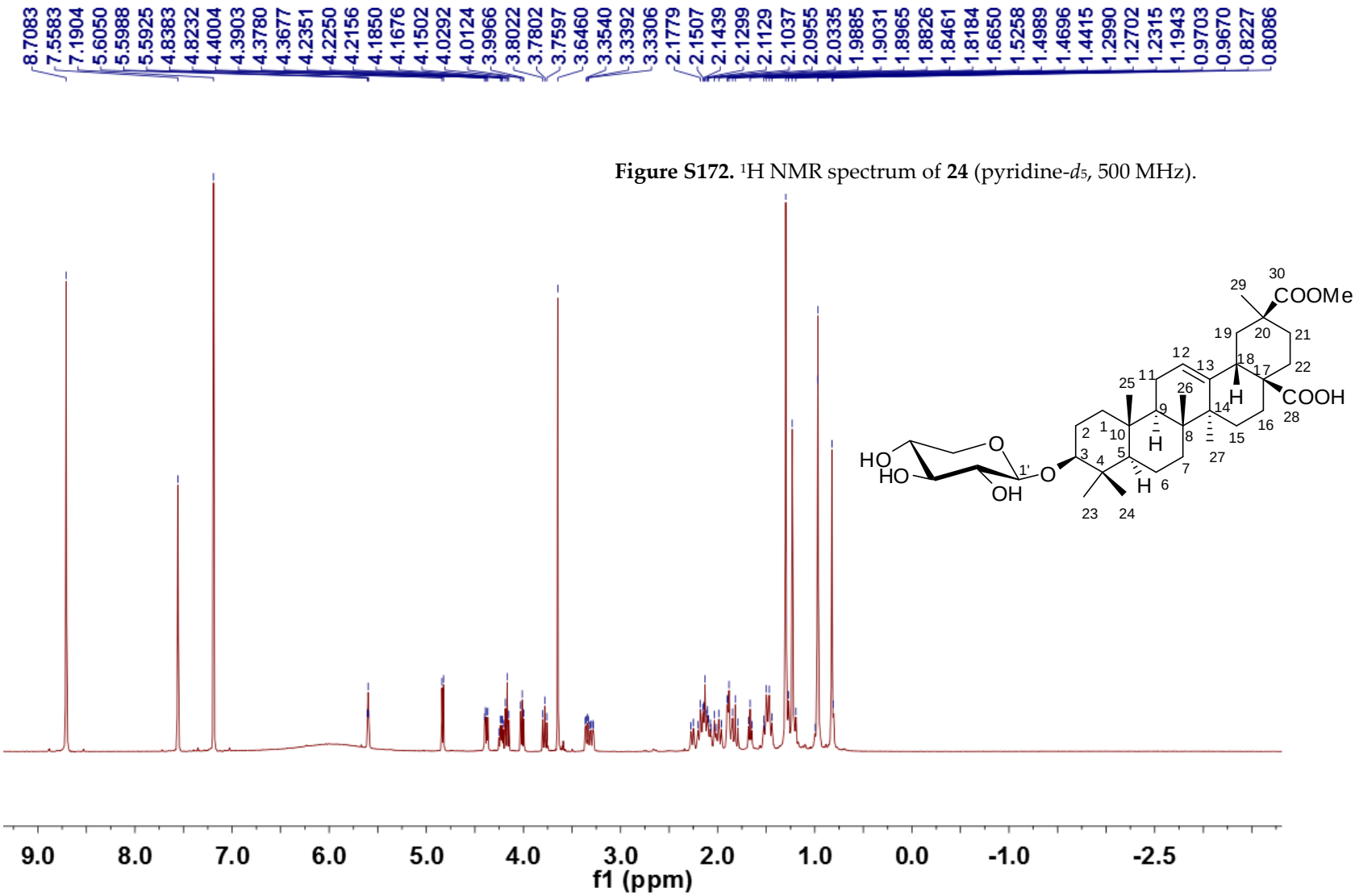


Figure S172. ^{1}H NMR spectrum of **24** (pyridine-d_5, 500 MHz).

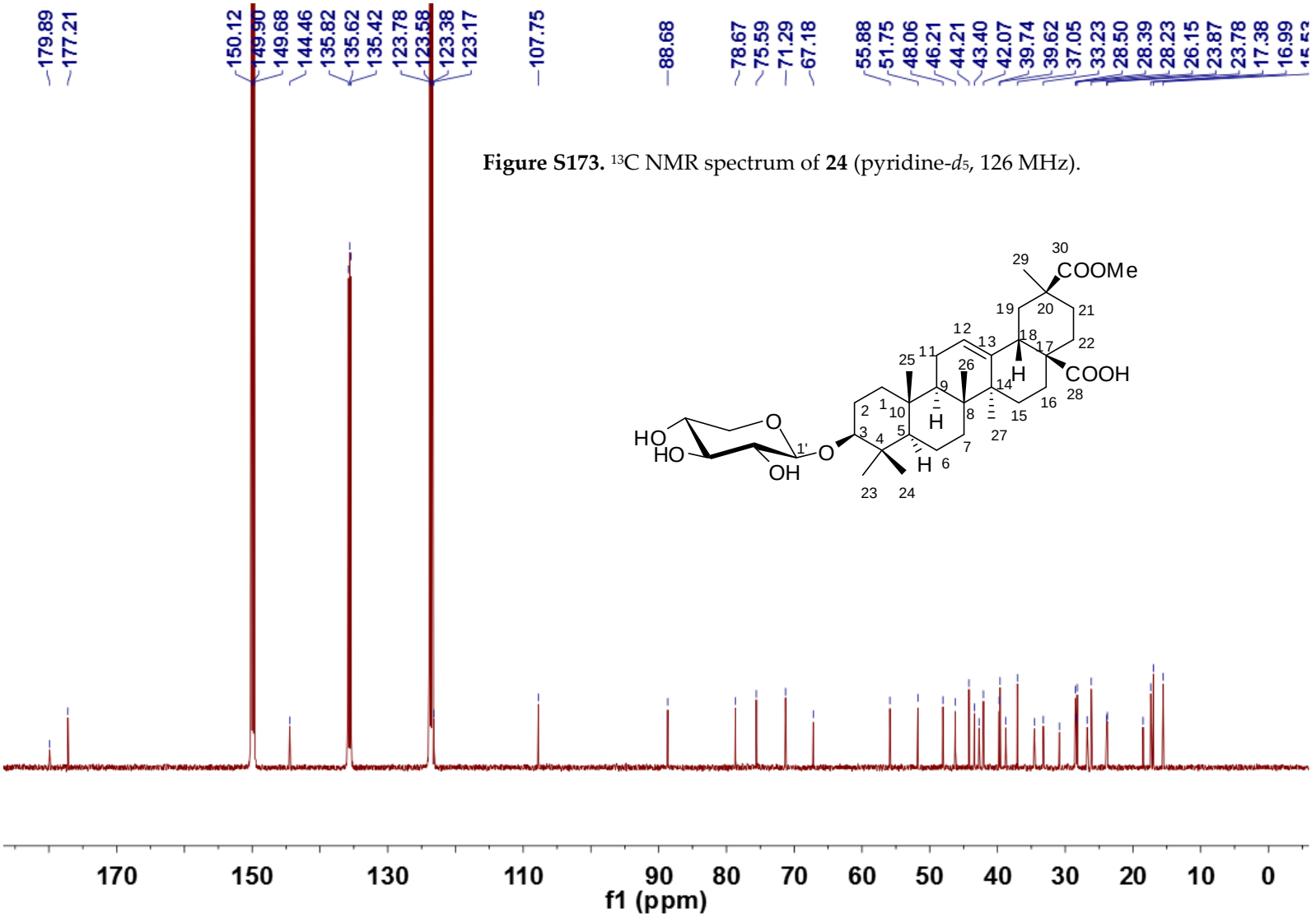


Figure S173. ^{13}C NMR spectrum of **24** (pyridine-d_5, 126 MHz).

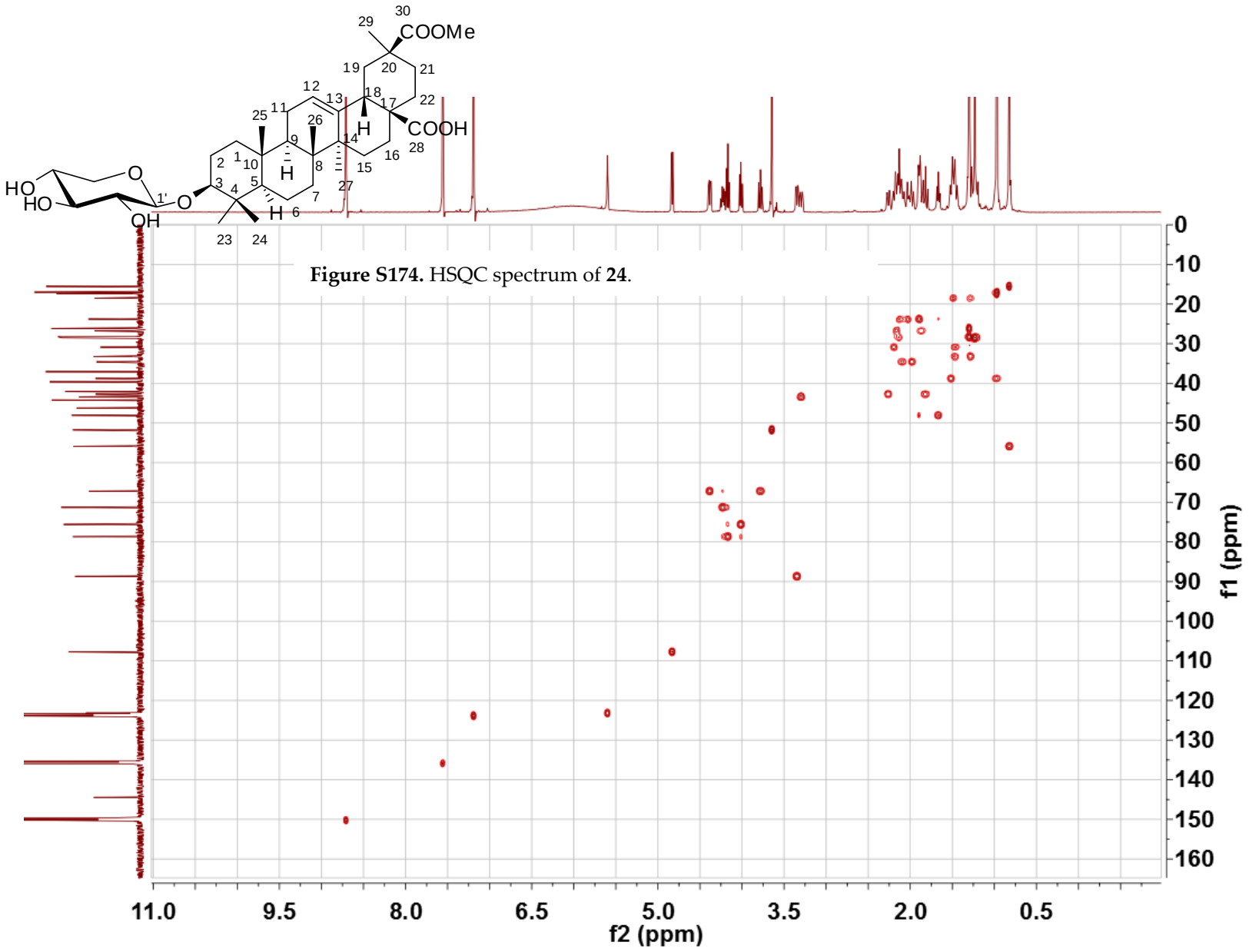


Figure S174. HSQC spectrum of **24**.

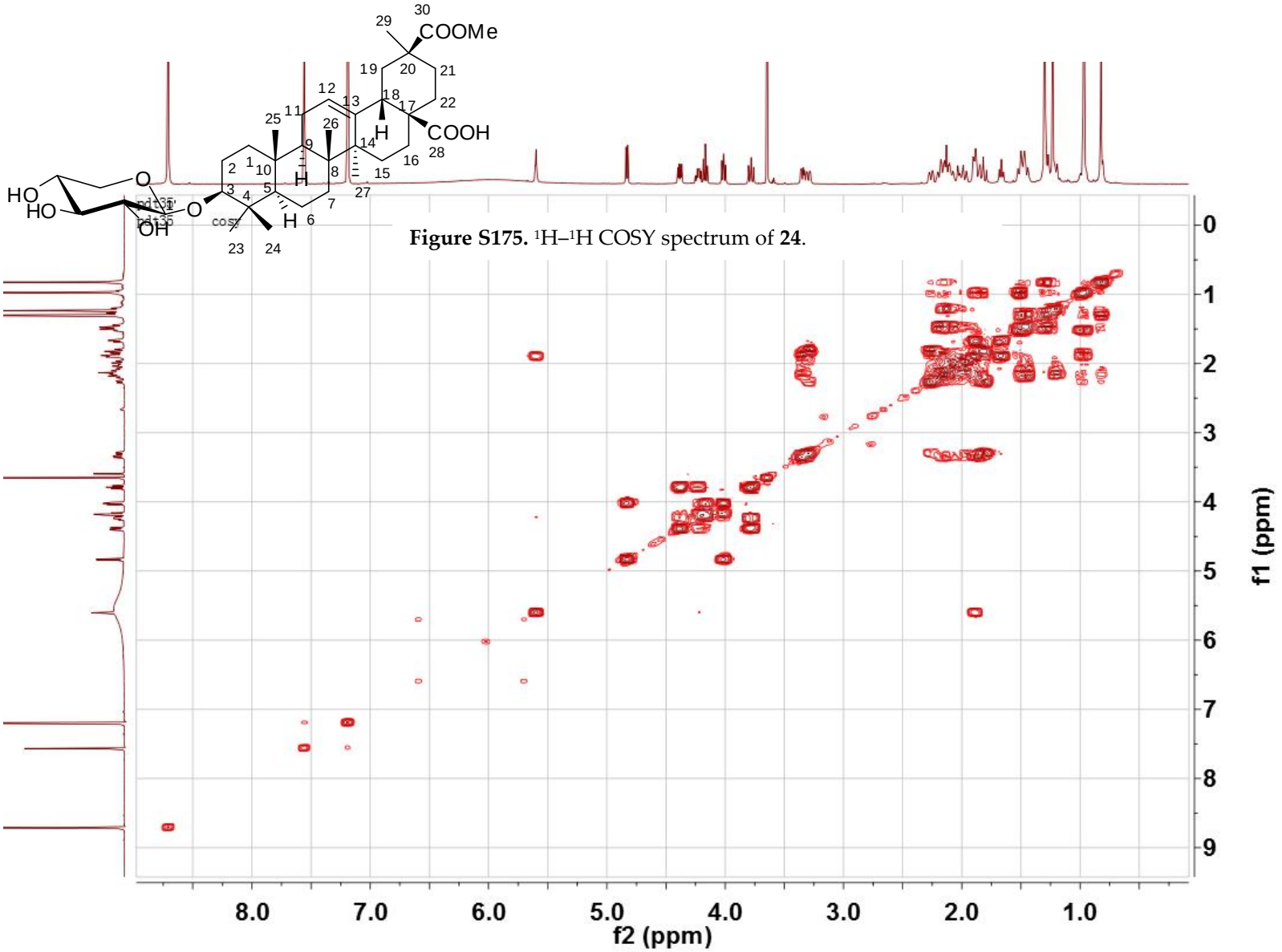


Figure S175. ^{1}H–^{1}H COSY spectrum of **24**.

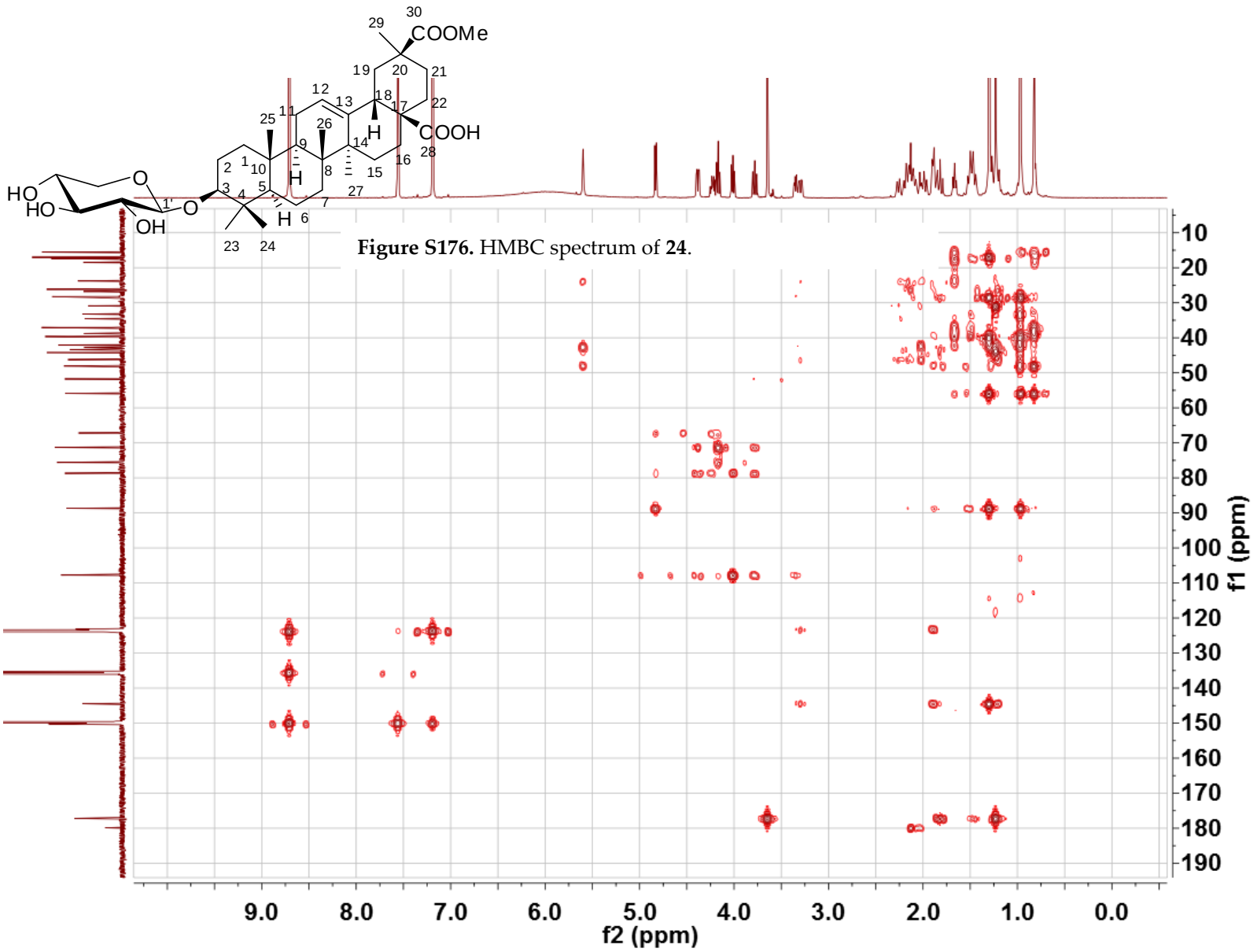


Figure S176. HMBC spectrum of **24**.

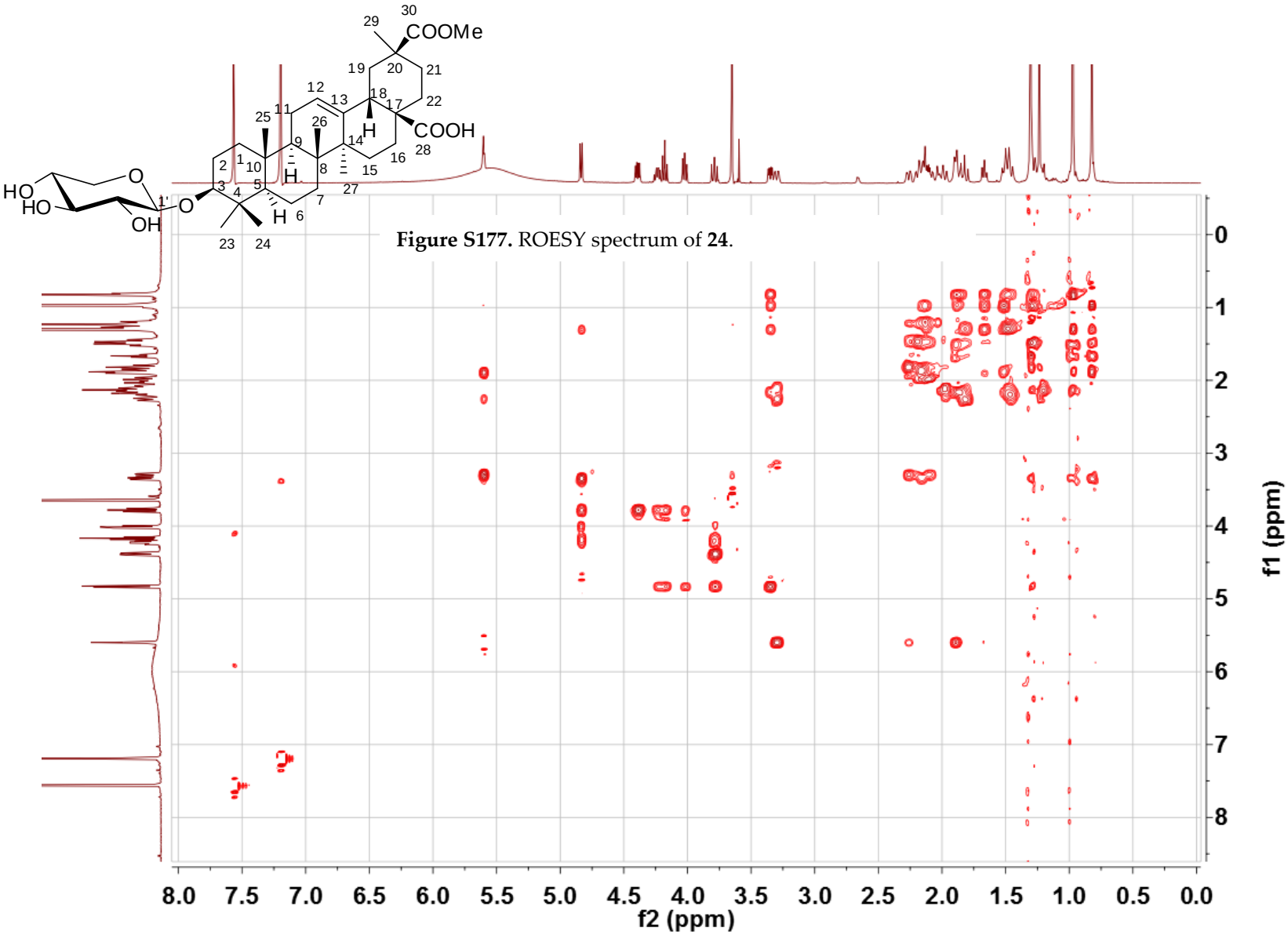


Figure S177. ROESY spectrum of **24**.

Data Filename	190107ESIA6.d	**Sample Name**	pdt35
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	1/7/2019 3:11:02 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
320	0	ESI

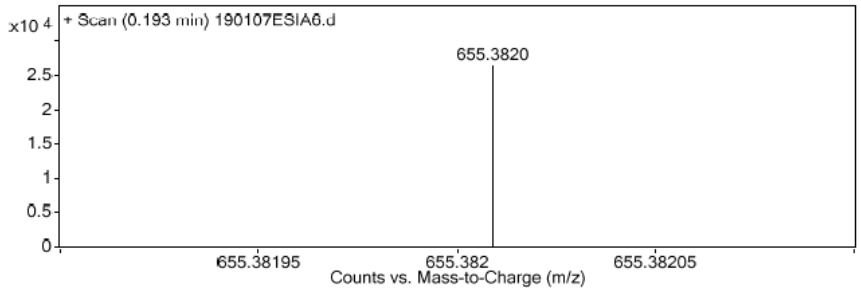


Figure S178. HRESIMS spectrum of **24**.

Peak List

m/z	z	Abund	Formula	Ion
106.0392	1	12415.93		
122.5483	2	27243.45		
166.0629	1	26196.08		
182.0404	1	78880.84		
194.0606	1	14238.85		
655.382	1	26472.7	C36 H56 Na O9	M+
671.3535	1	13972.36		
696.4058	1	16606.49		
826.3661	1	11042.4		
1287.7718	1	11313.11		

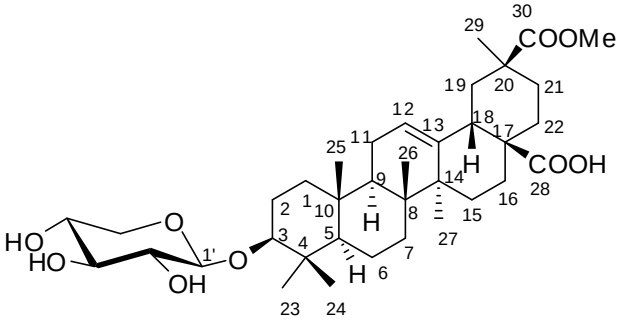
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	5	12
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C36 H56 Na O9	655.3822	655.3820	0.2	0.3	8.5

--- End Of Report ---



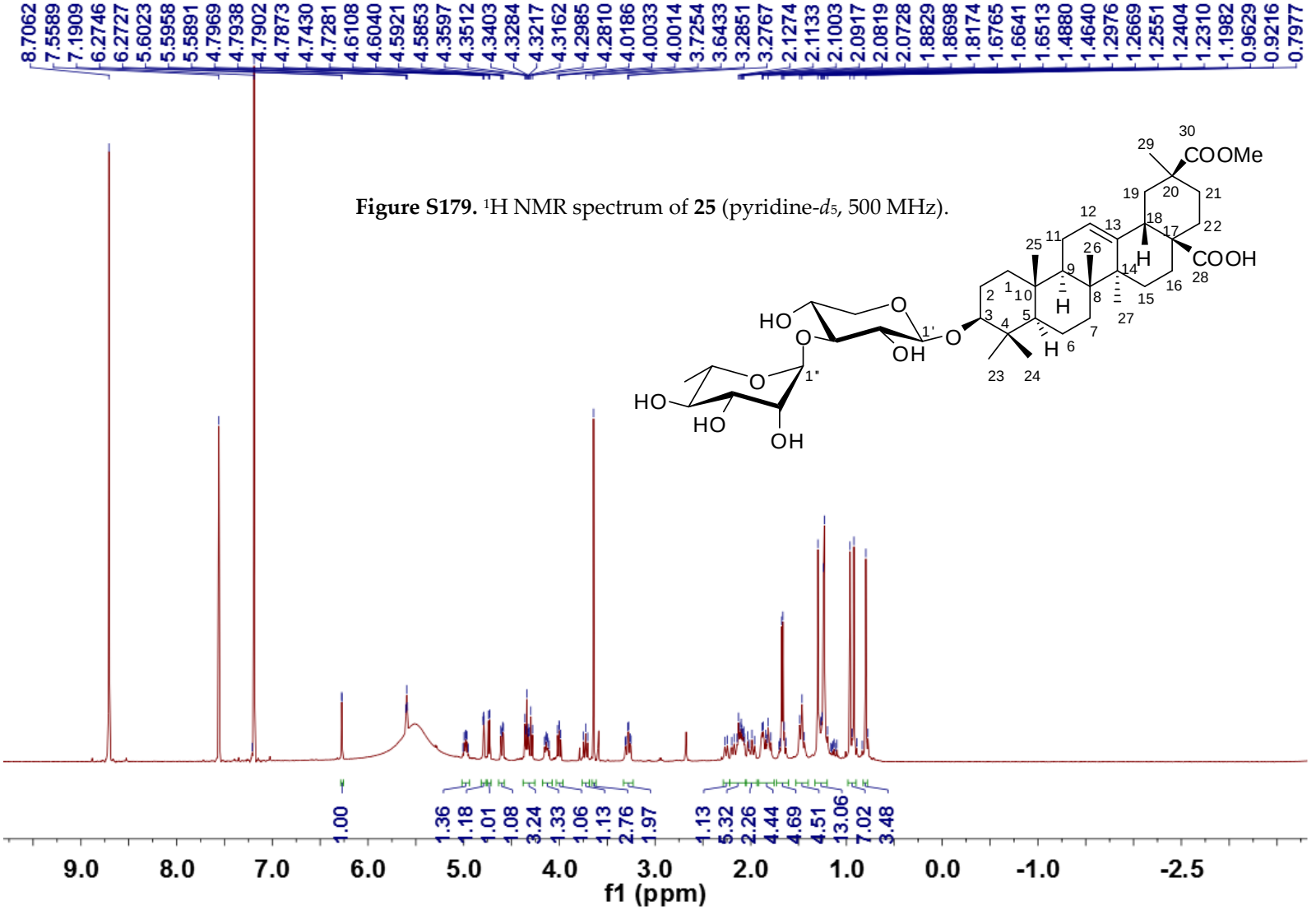


Figure S179. ^{1}H NMR spectrum of **25** (pyridine-d_5, 500 MHz).

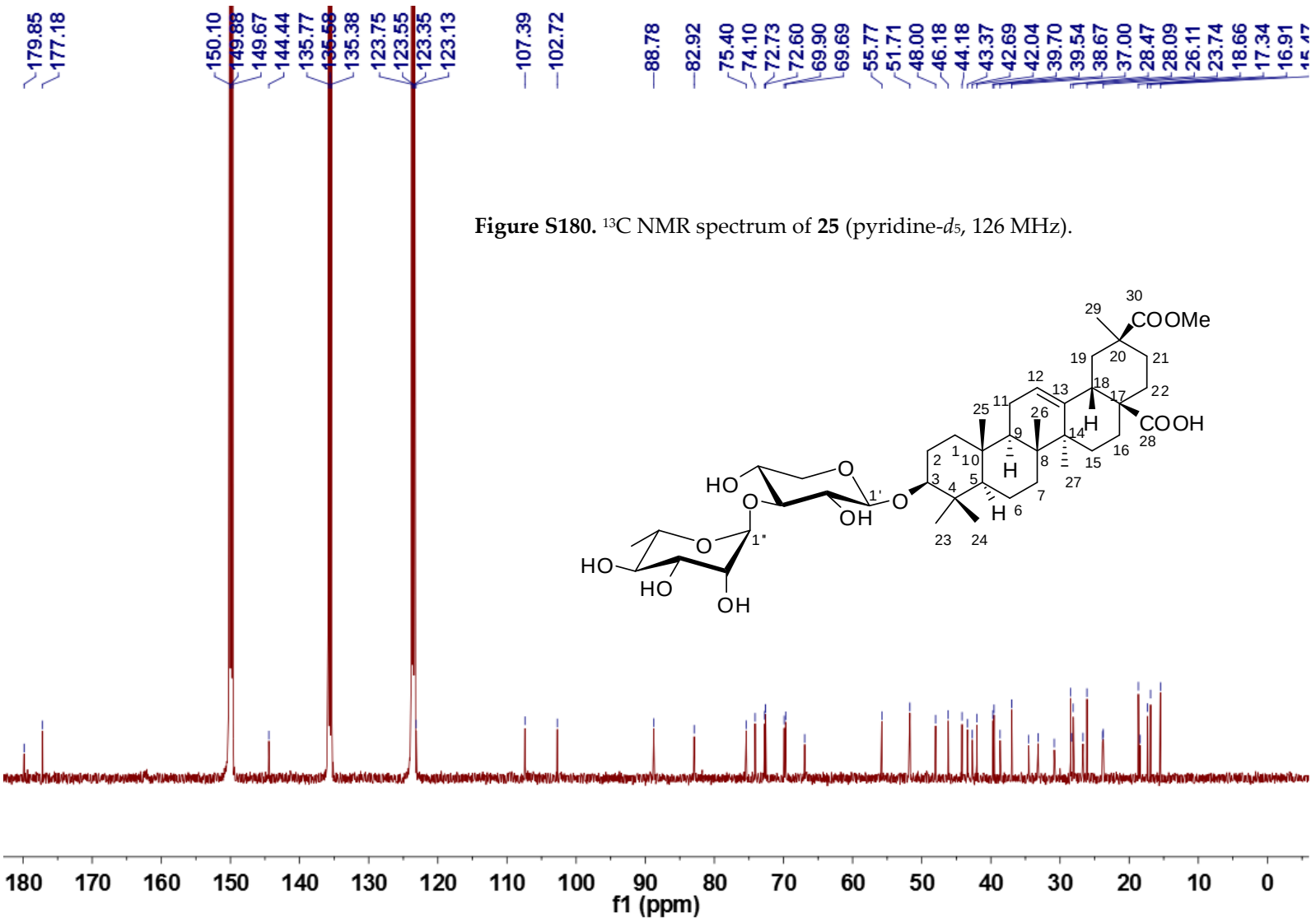


Figure S180. ^{13}C NMR spectrum of **25** (pyridine-d_5, 126 MHz).

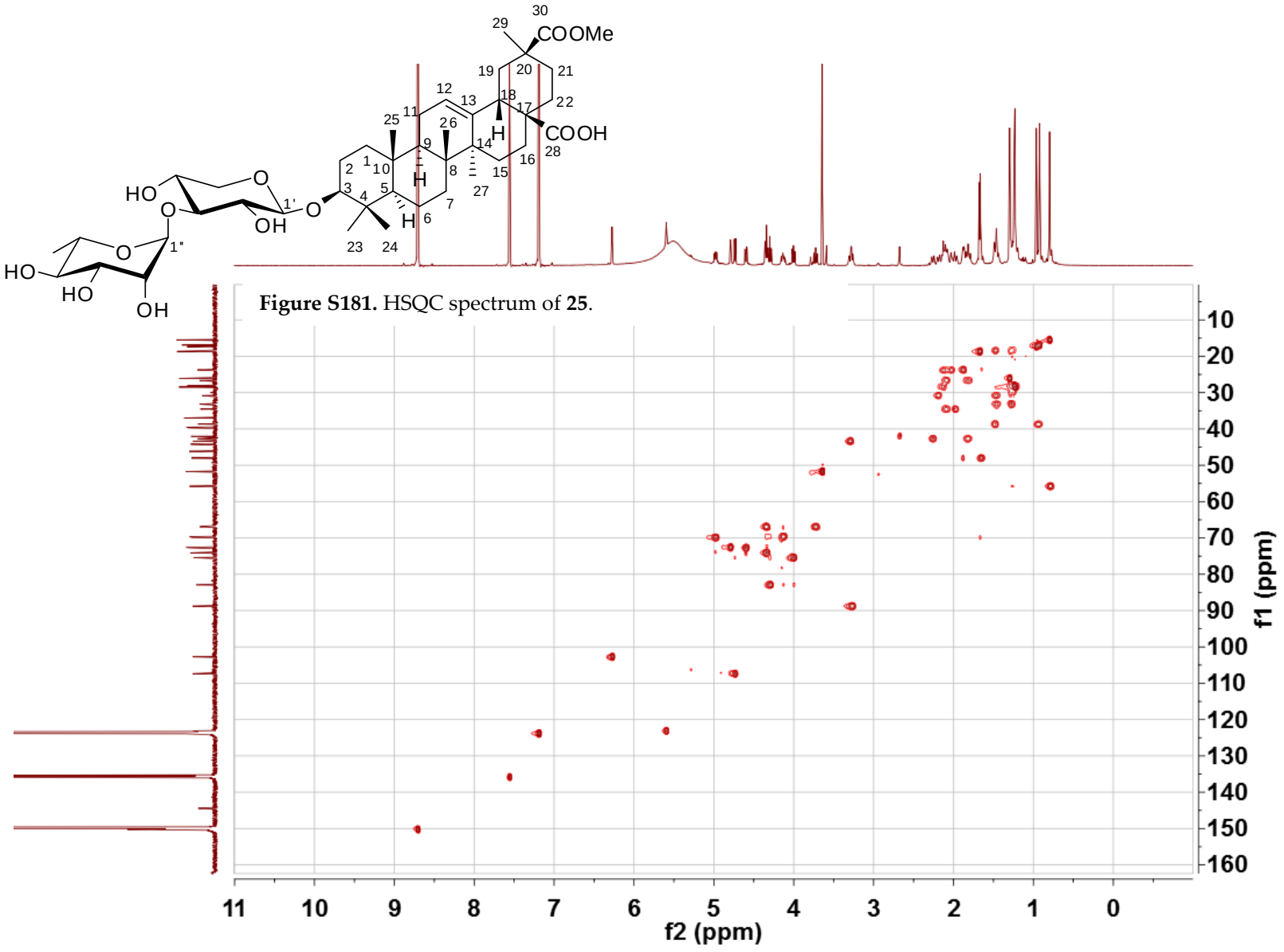


Figure S181. HSQC spectrum of **25**.

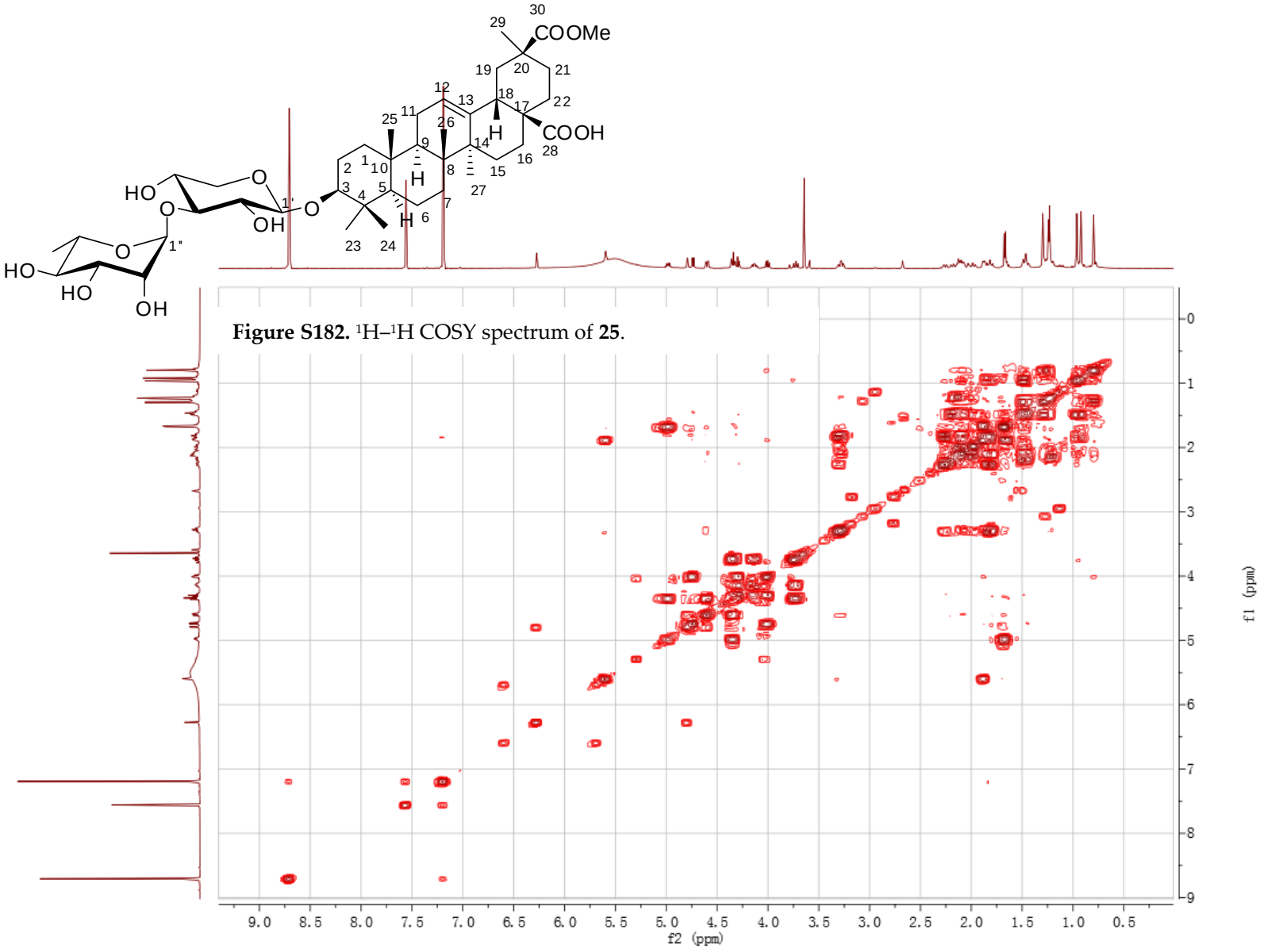


Figure S182. ^{1}H–^{1}H COSY spectrum of **25**.

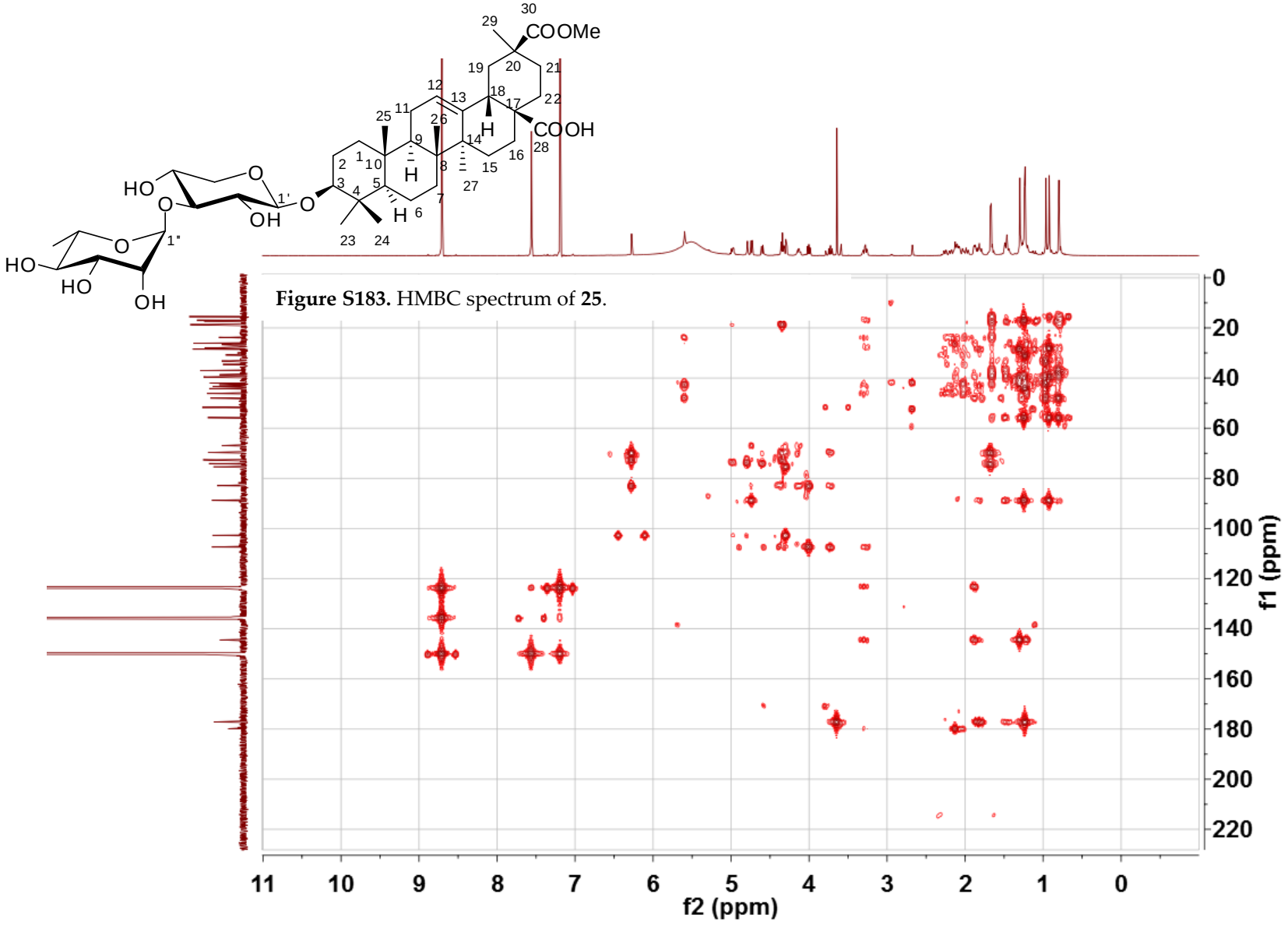


Figure S183. HMBC spectrum of **25**.

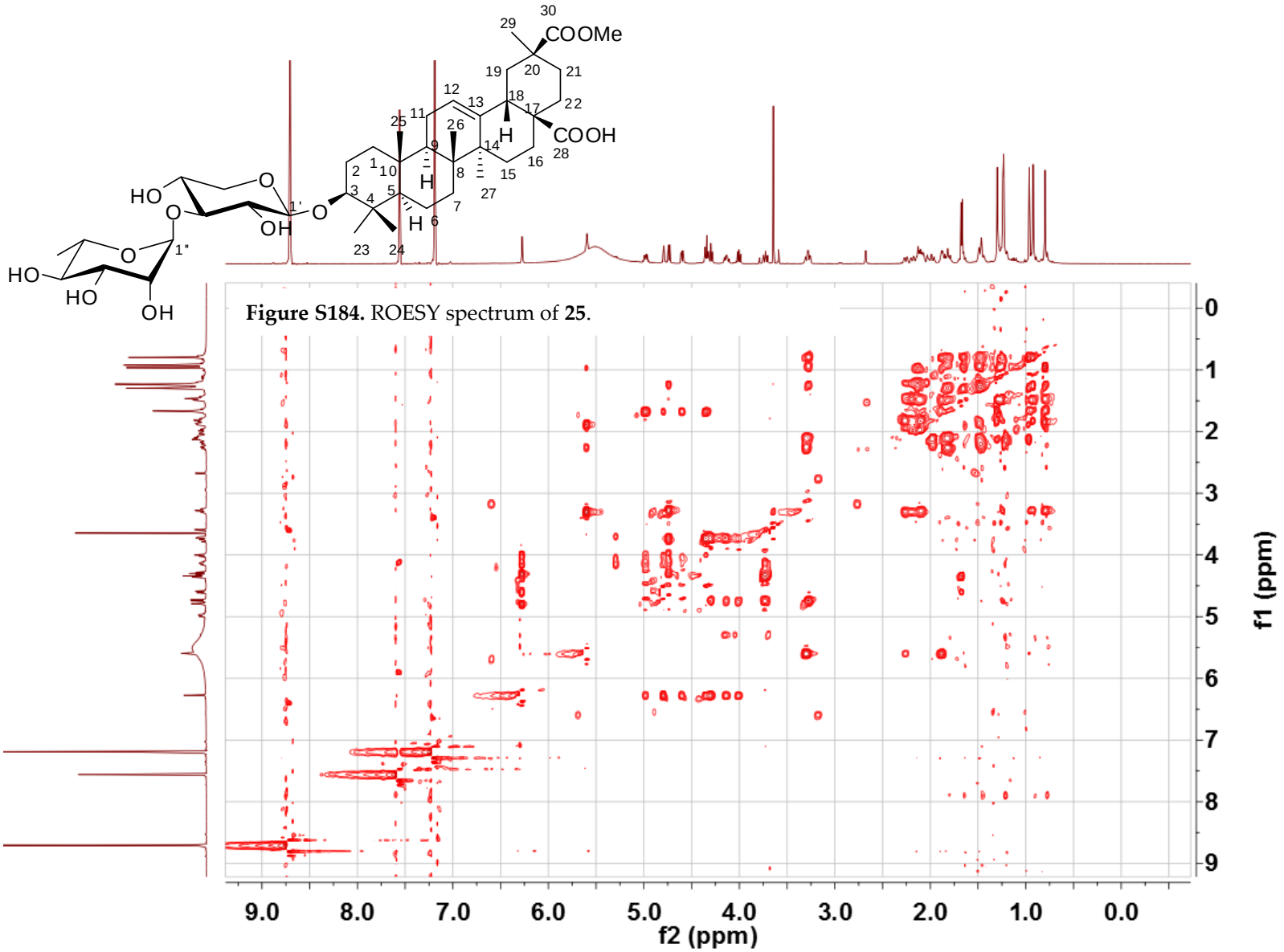


Figure S184. ROESY spectrum of **25**.

Formula Predictor Report - pdt34a.lcd

Data File: E:\DATA\2018\0702\pdt34a.lcd

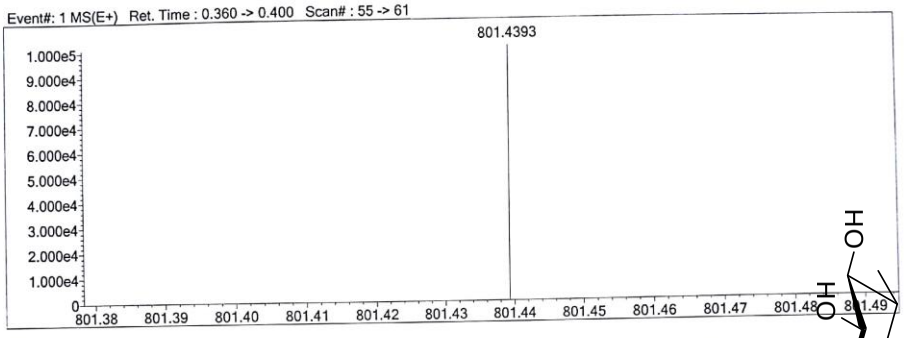
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	O	2	0	20	Si	4	0	0	Br	1	0	0	Na
C	4	10	50	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	0	Na	1	0	0	Cl	1	0	0					

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

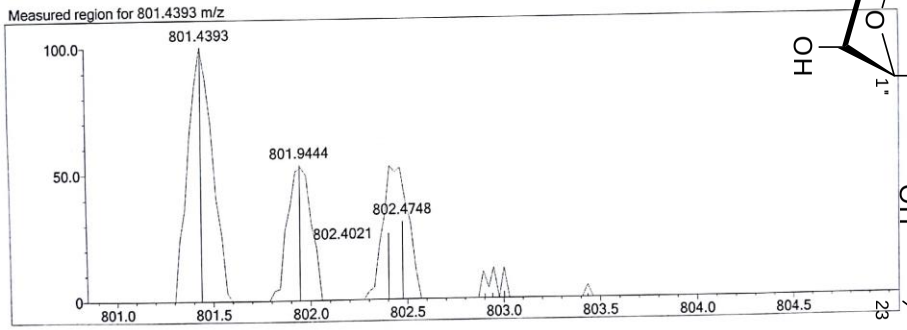
DBE Range: -2.0 - 100.0
Apply N Rule: yes
Isotope RI (%): 1.00
MSn Logic Mode: AND

Electron Ions: both
Use MSn Info: yes
Isotope Res: 10000
Max Results: 10

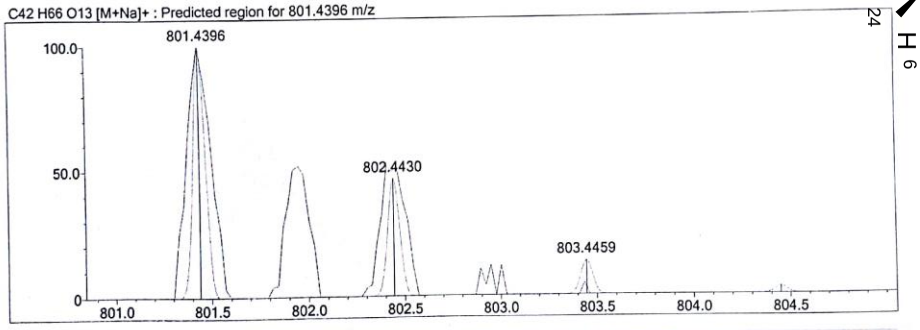
Event#: 1 MS(E+) Ret. Time : 0.360 -> 0.400 Scan# : 55 -> 61



Measured region for 801.4393 m/z



C42 H66 O13 [M+Na]+ : Predicted region for 801.4396 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C42 H66 O13	[M+Na]+	801.4393	801.4396	-0.3	-0.37	10.0

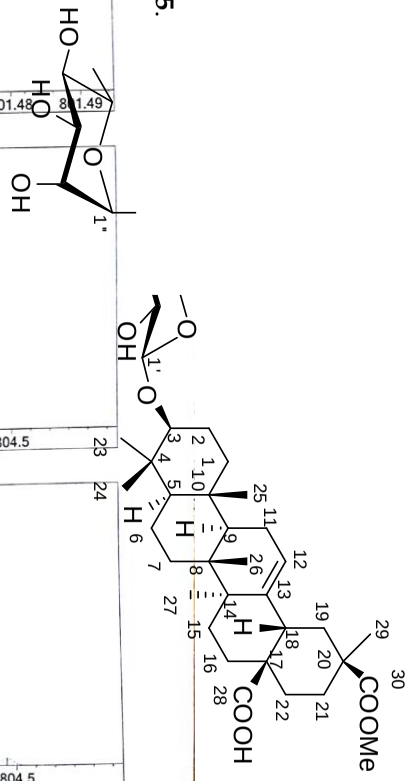


Figure S185. HRESIMS spectrum of **25**.

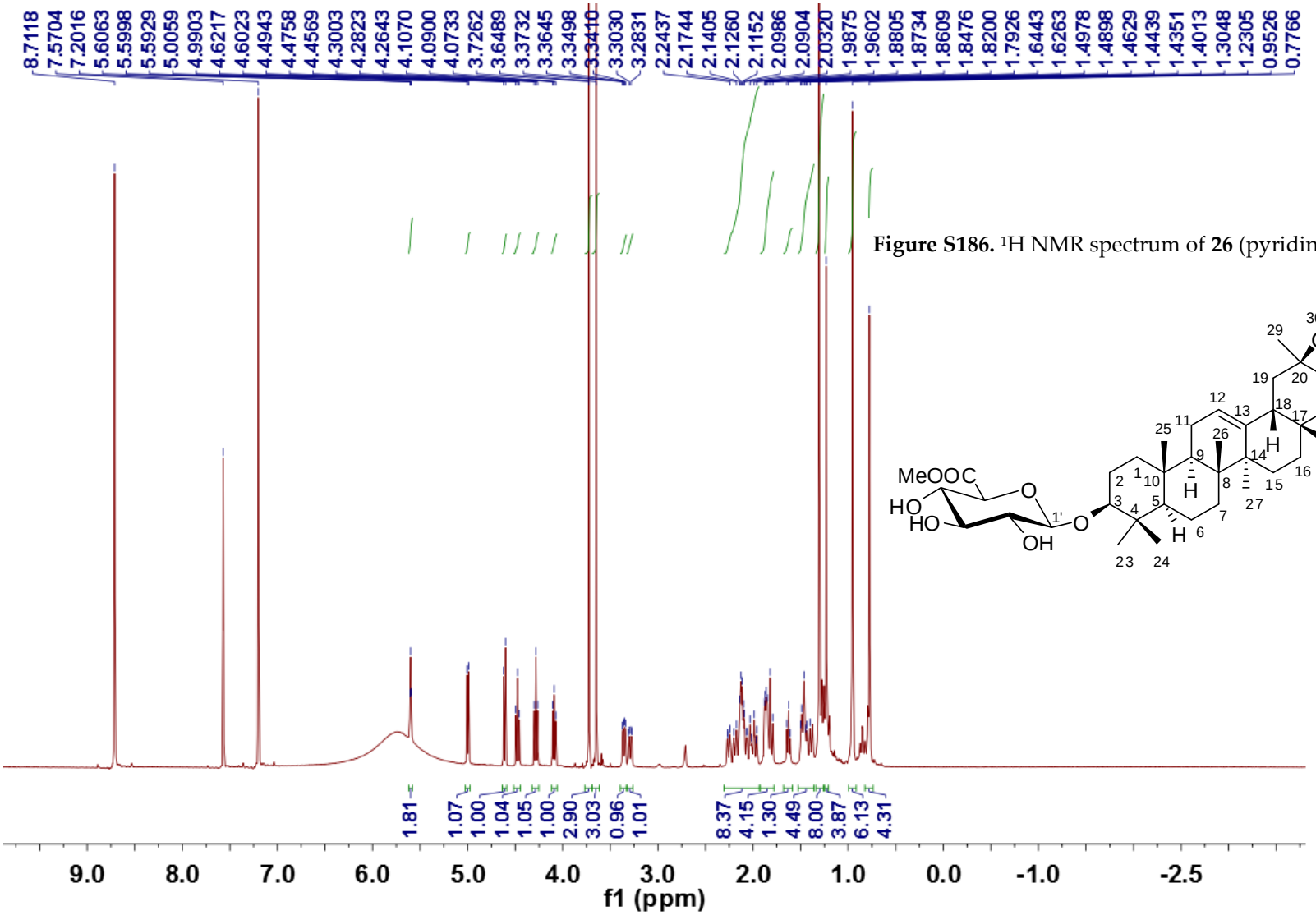


Figure S186. ^{1}H NMR spectrum of **26** (pyridine-d_5, 500 MHz).

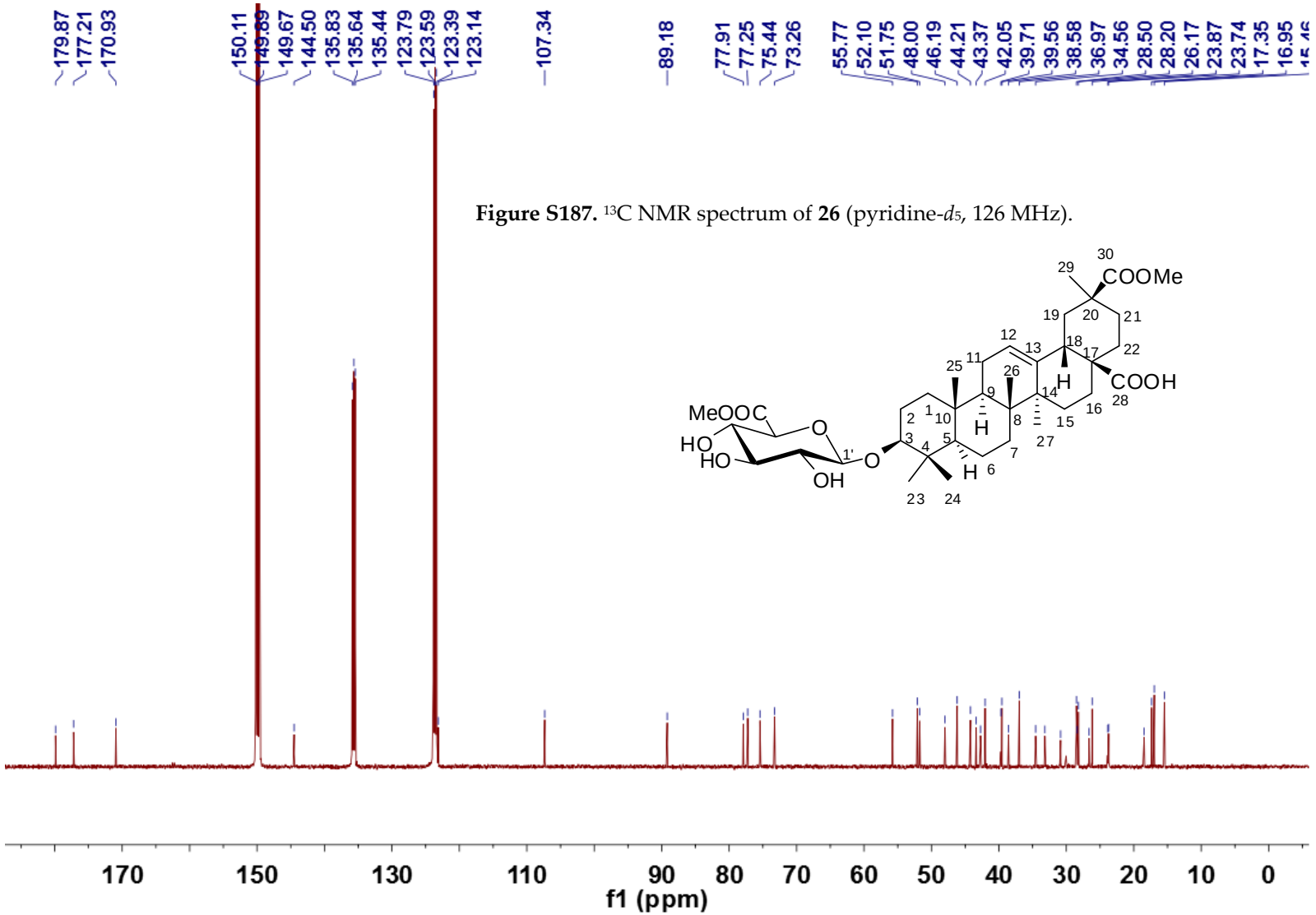


Figure S187. ^{13}C NMR spectrum of **26** (pyridine-d_5, 126 MHz).

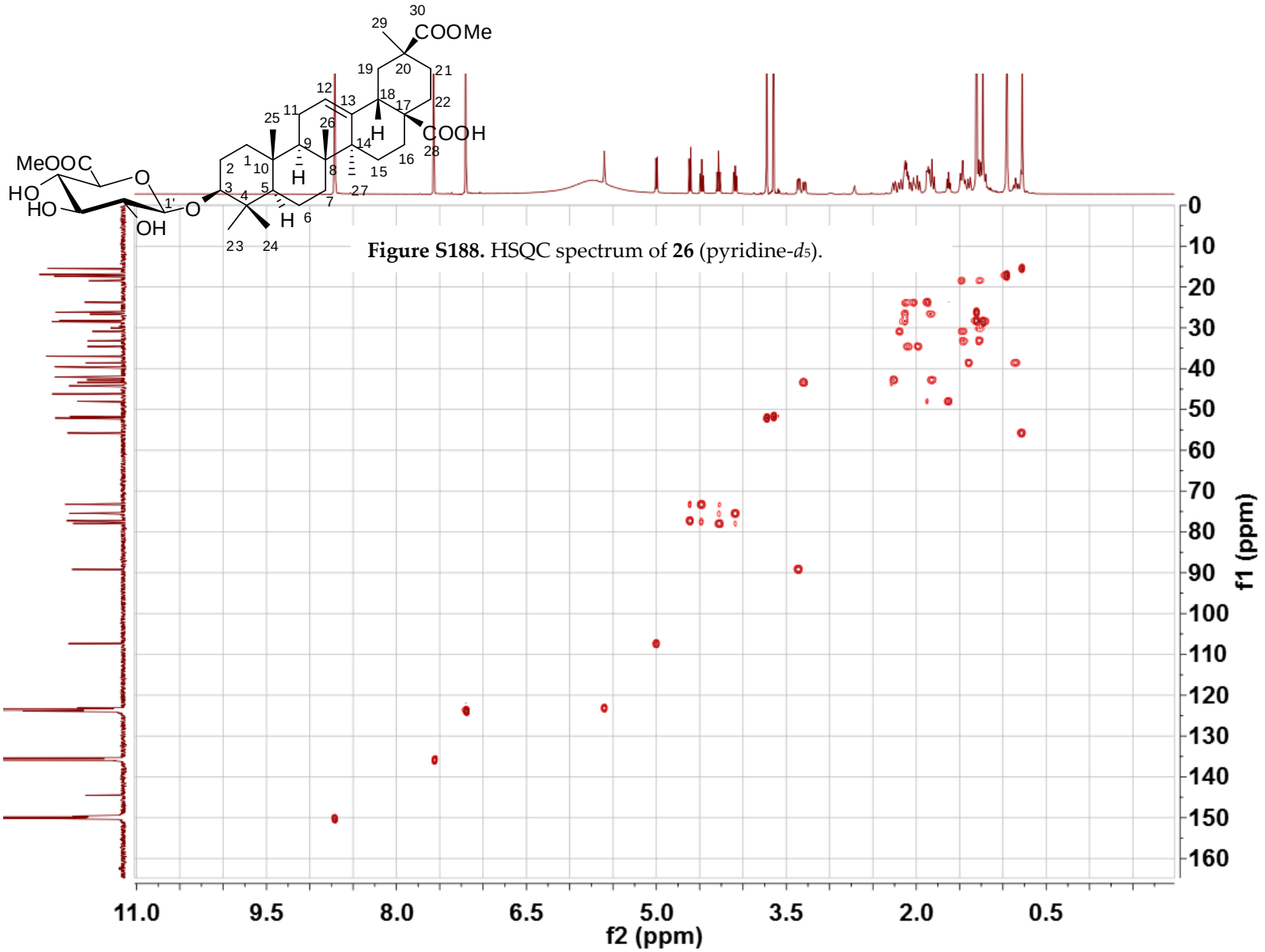


Figure S188. HSQC spectrum of **26** (pyridine-d_5).

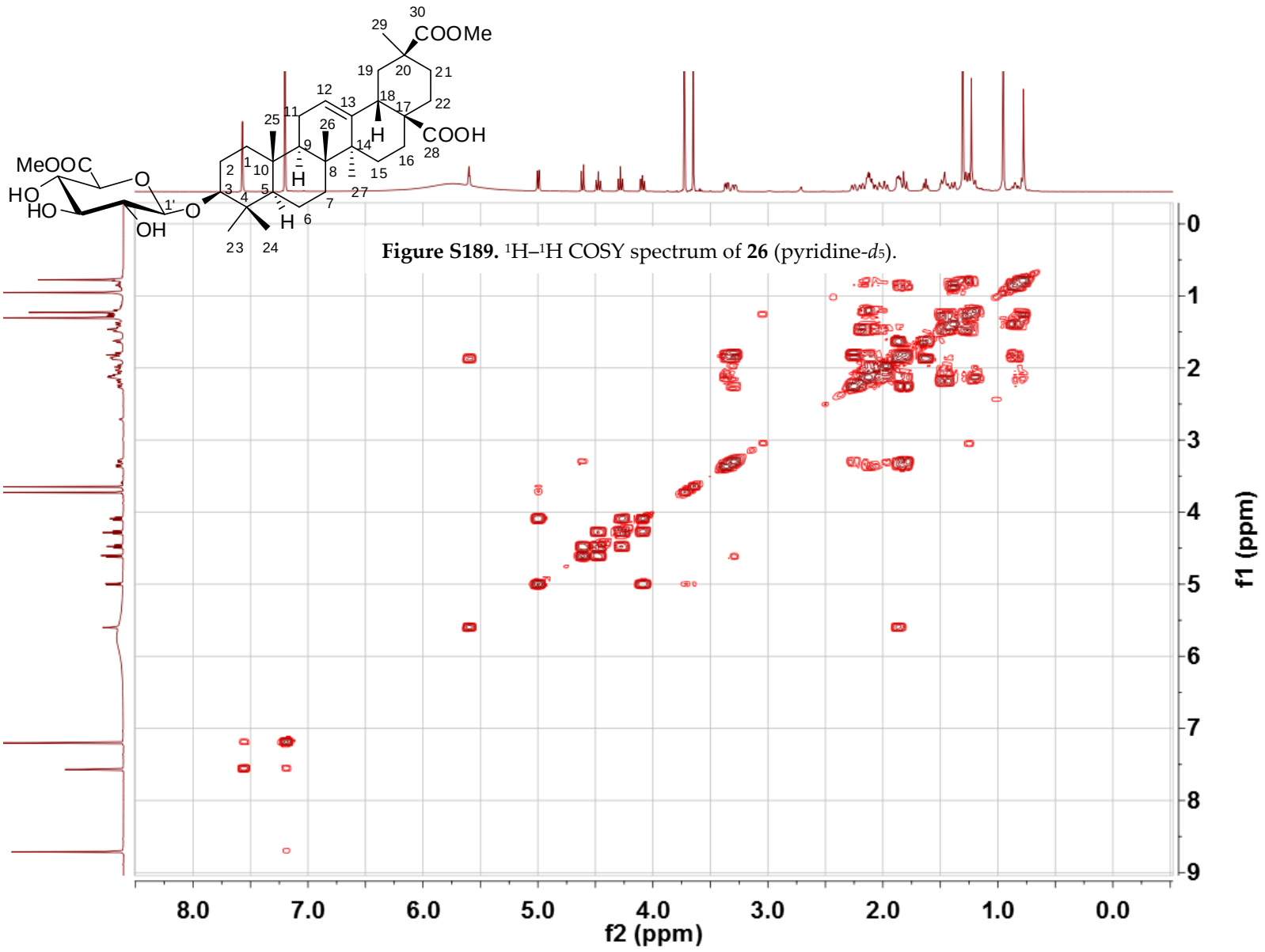


Figure S189. ^{1}H–^{1}H COSY spectrum of **26** (pyridine-d_5).

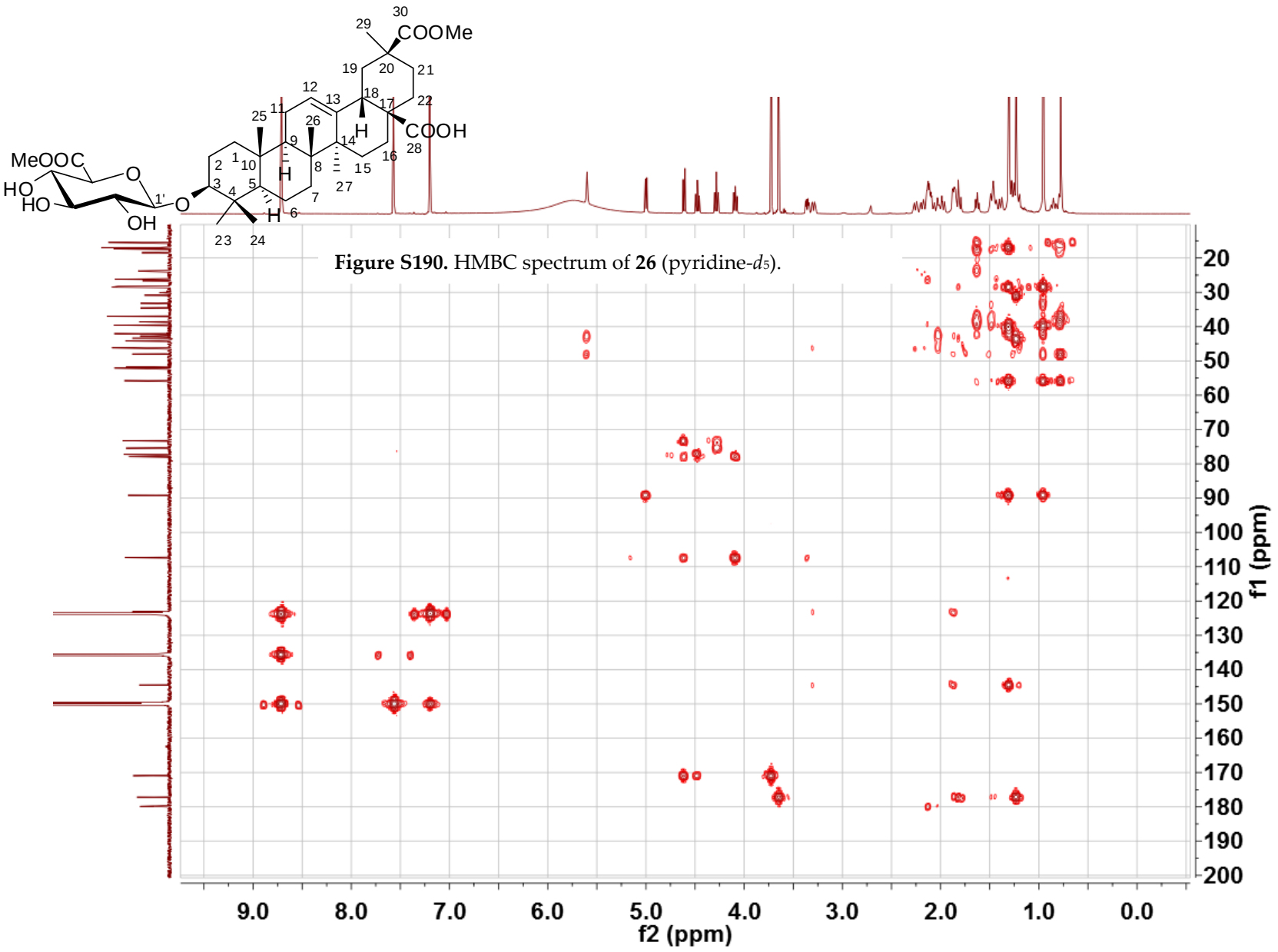


Figure S190. HMBC spectrum of **26** (pyridine-d_5).

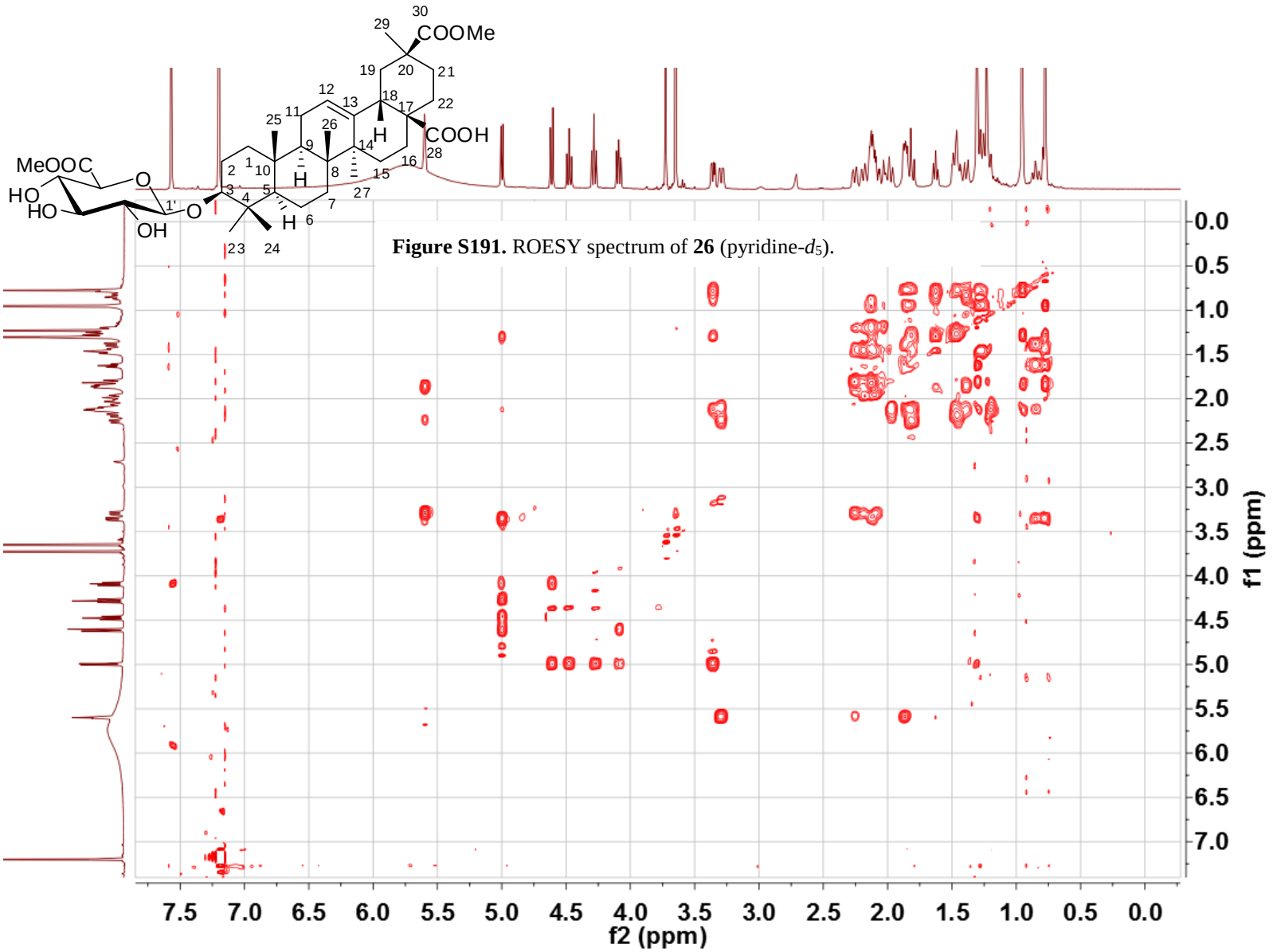


Figure S191. ROESY spectrum of **26** (pyridine-d_5).

Data Filename	190107ESIA7.d	**Sample Name**	pdt36
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	1/7/2019 3:12:16 PM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
320	0	ESI

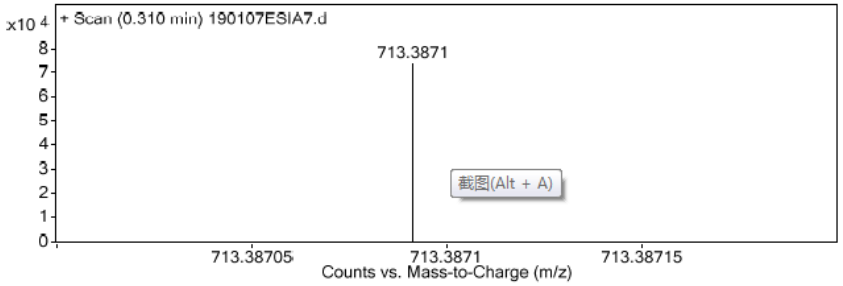


Figure S192. HRESIMS spectrum of **26**.

Peak List

m/z	z	Abund	Formula	Ion
122.5492	2	70062.16		
141.0137		49665.91		
182.0401	1	85748.97		
713.3871	1	73789.83	C38 H58 Na O11	M+
729.3569	1	105981.48		
730.36	1	43108.97		
922.0098	1	129708.32		
1403.7801	1	37441.74		
1419.7523	1	36564.46		
1420.7547	1	32141.41		

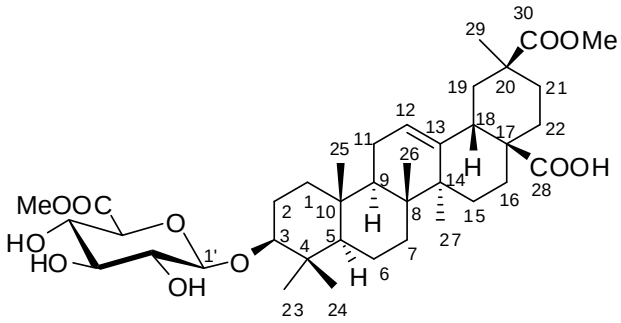
Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	7	15
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C38 H58 Na O11	713.3877	713.3871	0.6	0.8	9.5

--- End Of Report ---



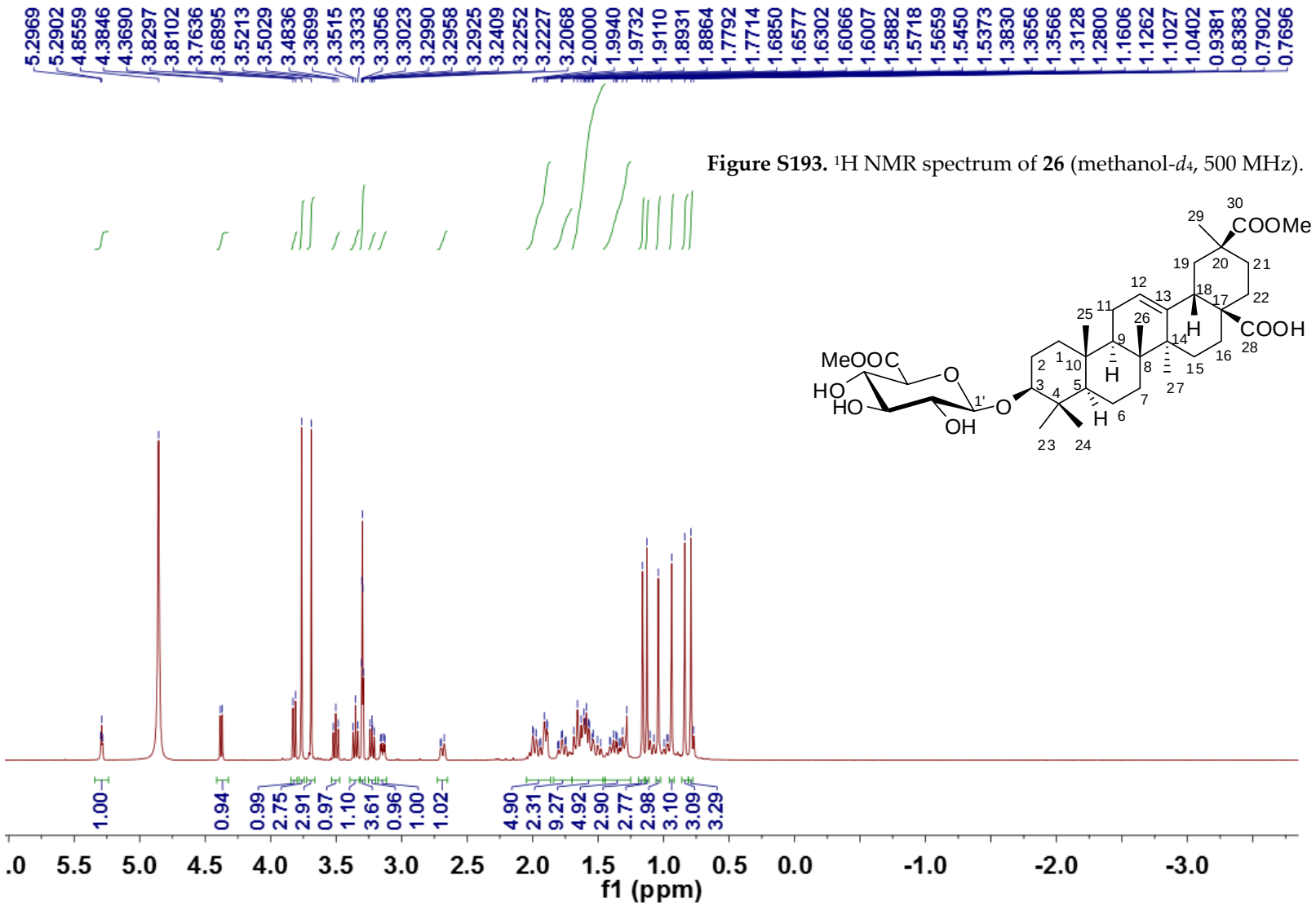


Figure S193. ^{1}H NMR spectrum of **26** (methanol-d_4, 500 MHz).

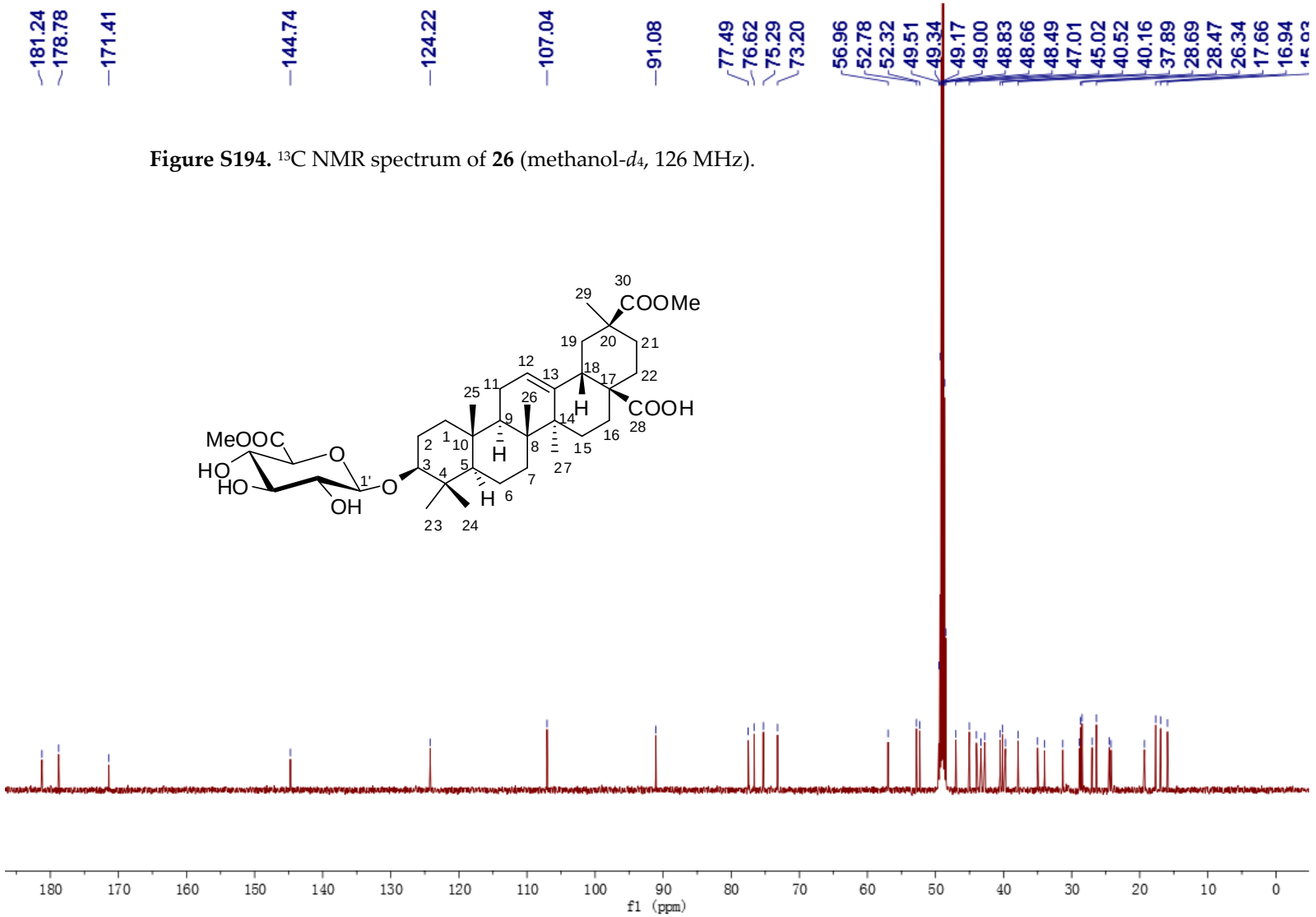


Figure S194. ^{13}C NMR spectrum of **26** (methanol-d_4, 126 MHz).

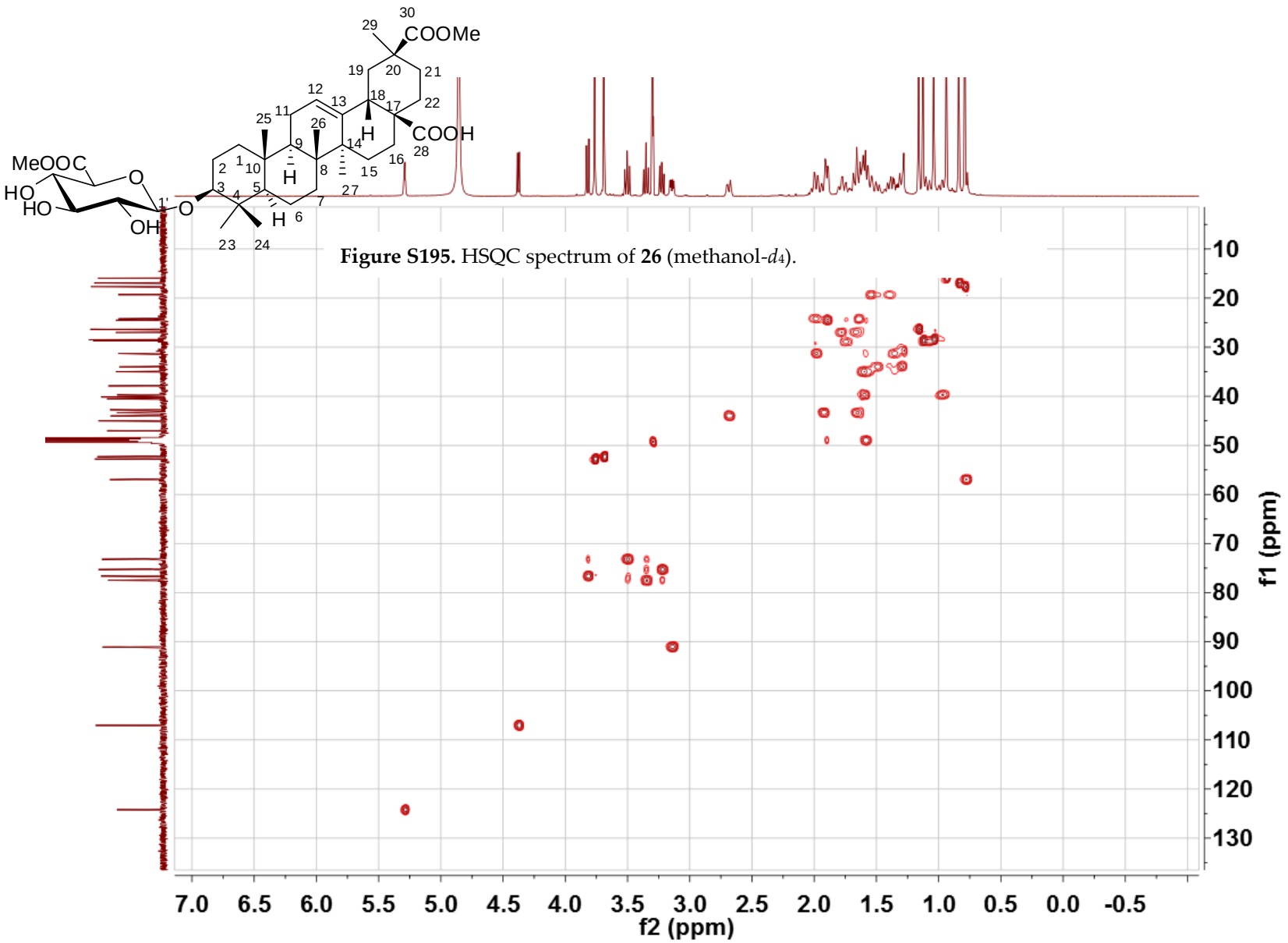


Figure S195. HSQC spectrum of **26** (methanol-d_4).

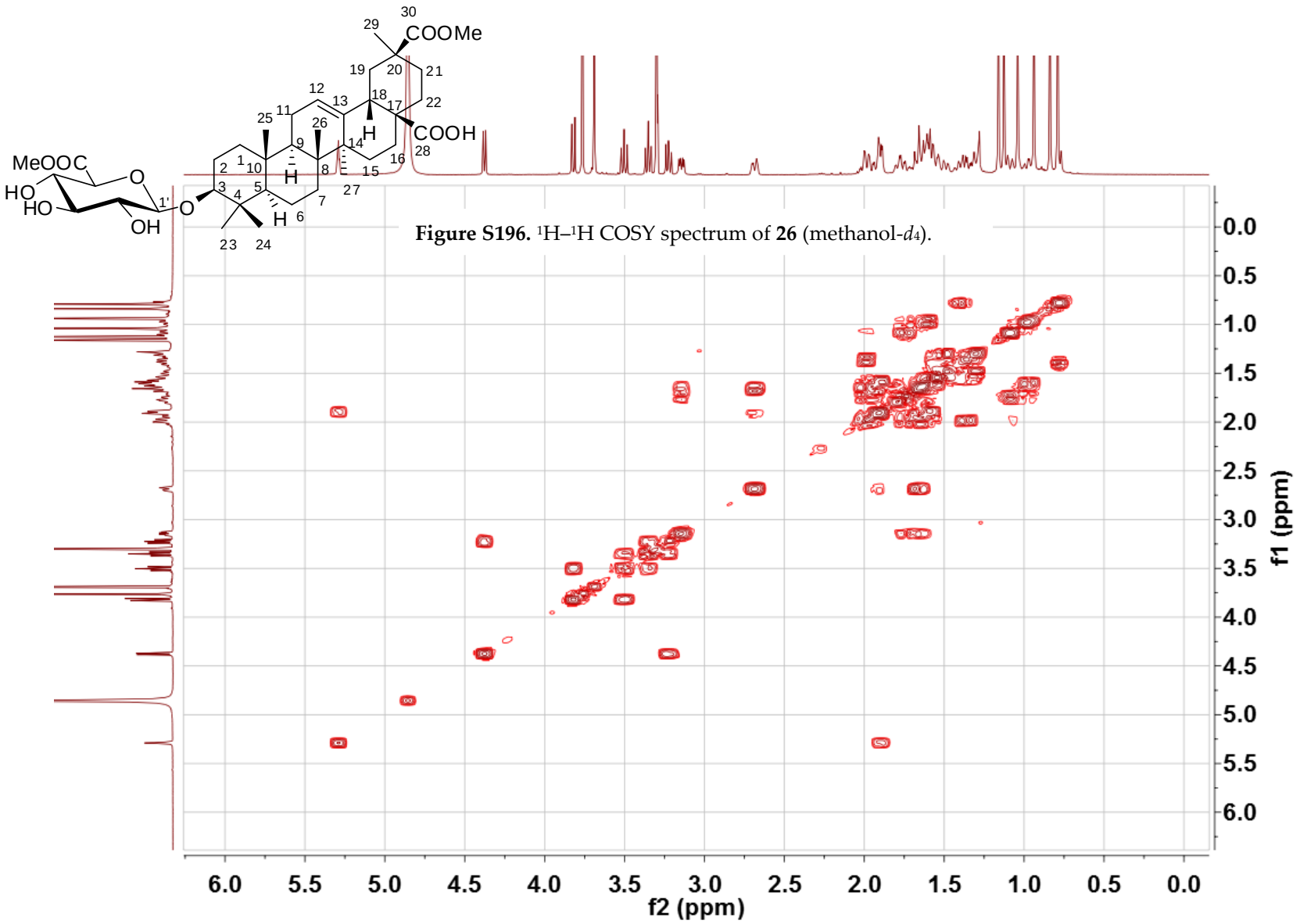


Figure S196. ^{1}H–^{1}H COSY spectrum of **26** (methanol-d_4).

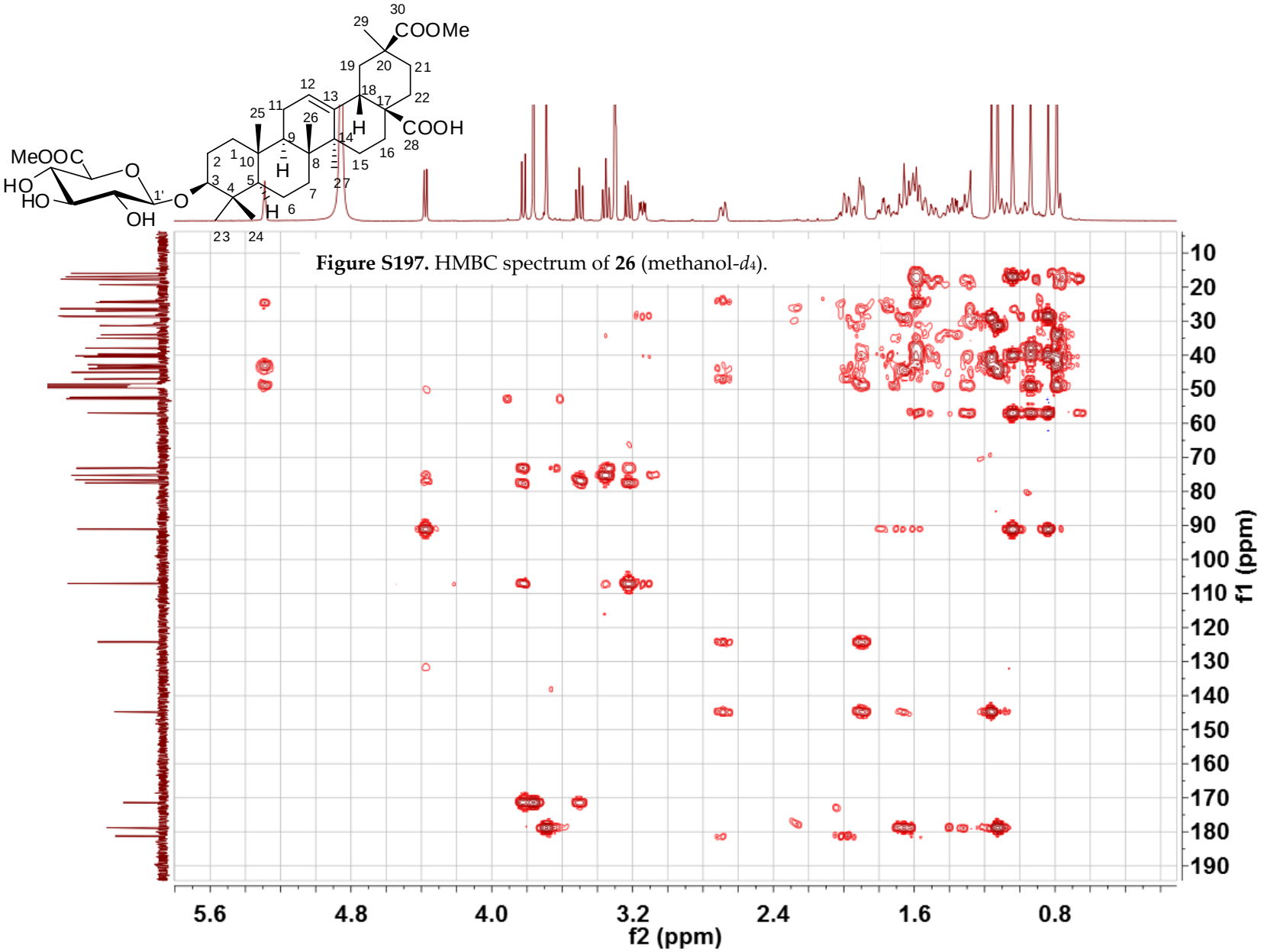


Figure S197. HMBC spectrum of **26** (methanol-d_4).

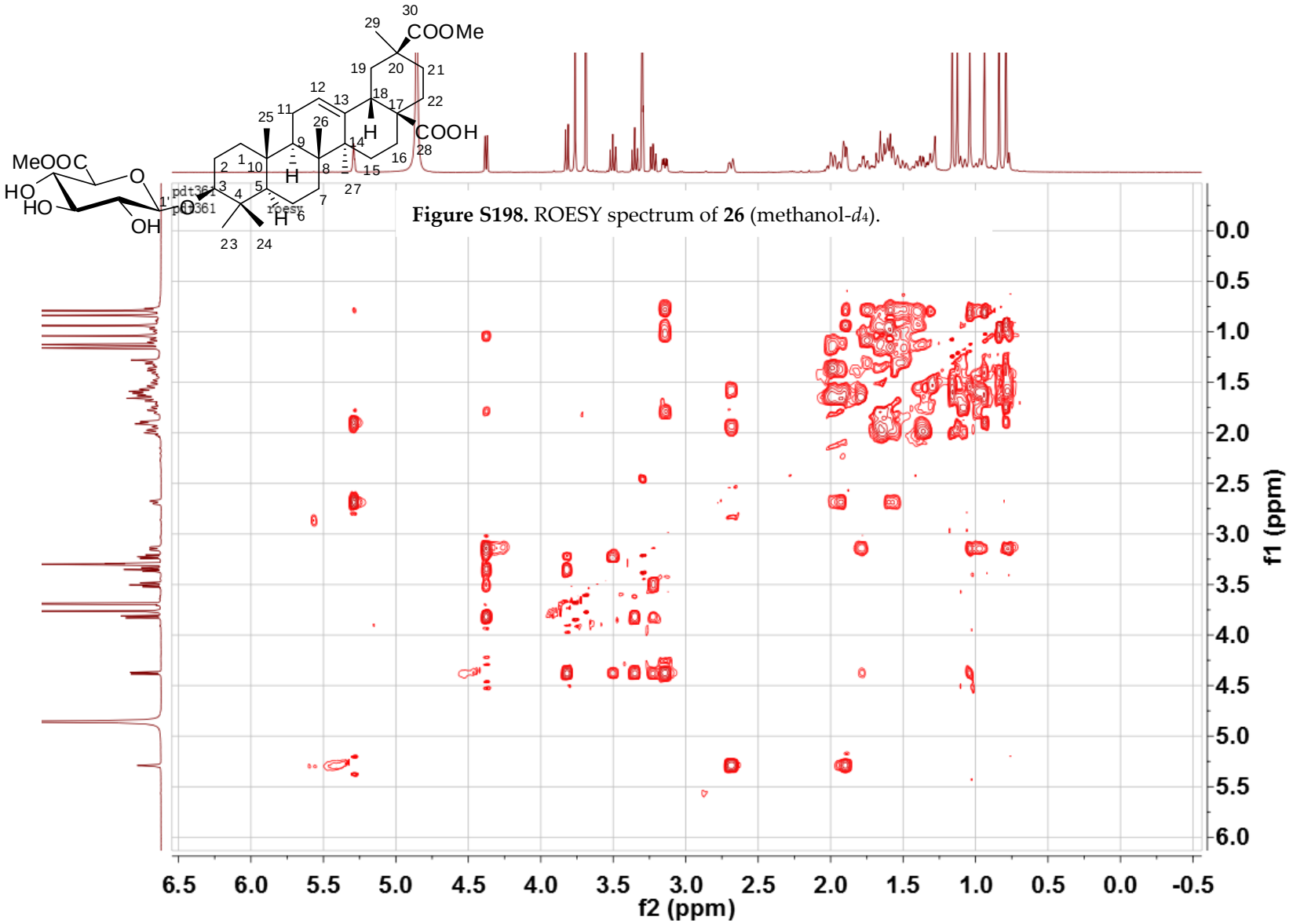


Figure S198. ROESY spectrum of **26** (methanol-d_4).