

Supporting Information for

Cucurbitane Glucosides from the Crude Extract of *Siraitia grosvenorii* with Moderate Effects on PGC-1 α Promoter Activity

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Figure S1. ^1H NMR spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S2. ^{13}C NMR spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S3. HSQC spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S4. HMBC spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S5. ROESY spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S6. ^1H - ^1H COSY spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S7. TOCSY spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

Figure S8. IR spectrum of 11-oxomogroside III E (**1**)

Figure S9. HRESIMS spectrum of 11-oxomogroside III E (**1**)

Figure S10. ^1H NMR spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

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Figure S12. HSQC spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

Figure S13. HMBC spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

Figure S14. ROESY spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

Figure S15. ^1H - ^1H COSY spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

Figure S16. TOCSY spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

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Figure S18. HRESIMS spectrum of 11-oxomogroside IV (**2**)

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Figure S22. HMBC spectrum of 11-oxoisomogroside V (**3**) in $\text{C}_5\text{D}_5\text{N}$

Figure S23. ROESY spectrum of 11-oxoisomogroside V (**3**) in $\text{C}_5\text{D}_5\text{N}$

Figure S24. ^1H - ^1H COSY spectrum of 11-oxoisomogroside V (**3**) in $\text{C}_5\text{D}_5\text{N}$

Figure S25. TOCSY spectrum of 11-oxoisomogroside V (**3**) in $\text{C}_5\text{D}_5\text{N}$

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Figure S30. HSQC spectrum of 7-oxomogroside III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

Figure S31. HMBC spectrum of 7-oxomogroside III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

Figure S32. ROESY spectrum of 7-oxomogroside III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

Figure S33. ^1H - ^1H COSY spectrum of 7-oxomogroside III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

Figure S34. TOCSY spectrum of 7-oxomogrosid III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

Figure S35. IR spectrum of 7-oxomogroside III E (**4**)

Figure S36. HRESIMS spectrum of 7-oxomogroside III E (**4**)

Figure S37. ^1H NMR spectrum of 7-oxomogroside IV (**5**) in $\text{C}_5\text{D}_5\text{N}$

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Figure S39. HSQC spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

Figure S40. HMBC spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

Figure S41. ROESY spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

Figure S42. ¹H-¹H COSY spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

Figure S43. TOCSY spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

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Figure S45. HRESIMS spectrum of 7-oxomogroside IV (**5**)

Figure S46. ¹H NMR spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S47. ¹³C NMR spectrum of Mogroside VI A (**6**) in C₅D₅N

Figures S48. 1D TOCSY spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S49. Selective HSQC (C15-55) spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S50. Selective HSQC (C60-95) spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S51. Selective HSQC (C100-108) spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S52. Selective HMBC (C15-45) spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S53. Selective HMBC (C60-95) spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S54. Selective HMBC (C100-108) spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S55. COSY spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S56. ROESY spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S57. TOCSY spectrum of Mogroside VI A (**6**) in C₅D₅N

Figure S58. IR spectrum of Mogroside VI A (**6**)

Figure S59. HRESIMS spectrum of Mogroside VI A (**6**)

Figure S60. ^1H NMR spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S61. ^{13}C NMR spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figures S62. 1D TOCSY spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S63. Selective HSQC (C15-55) spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S64. Selective HSQC (C60-95) spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S65. Selective HSQC (C100-108) spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S66. Selective HMBC (C15-45) spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S67. Selective HMBC (C60-95) spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S68. Selective HMBC (C60-108) spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S69. COSY spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S70. ROESY spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S71. TOCSY spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

Figure S72. IR spectrum of Mogroside VI B (**7**)

Figure S73. HRESIMS spectrum of Mogroside VI B (**7**)

Figure S74. Crystallographic data of mogrol

Figure S75. The HPLC analysis of crude extract

Figure S76. The HPLC analysis of mogroside V

Figure S1. ^1H NMR spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

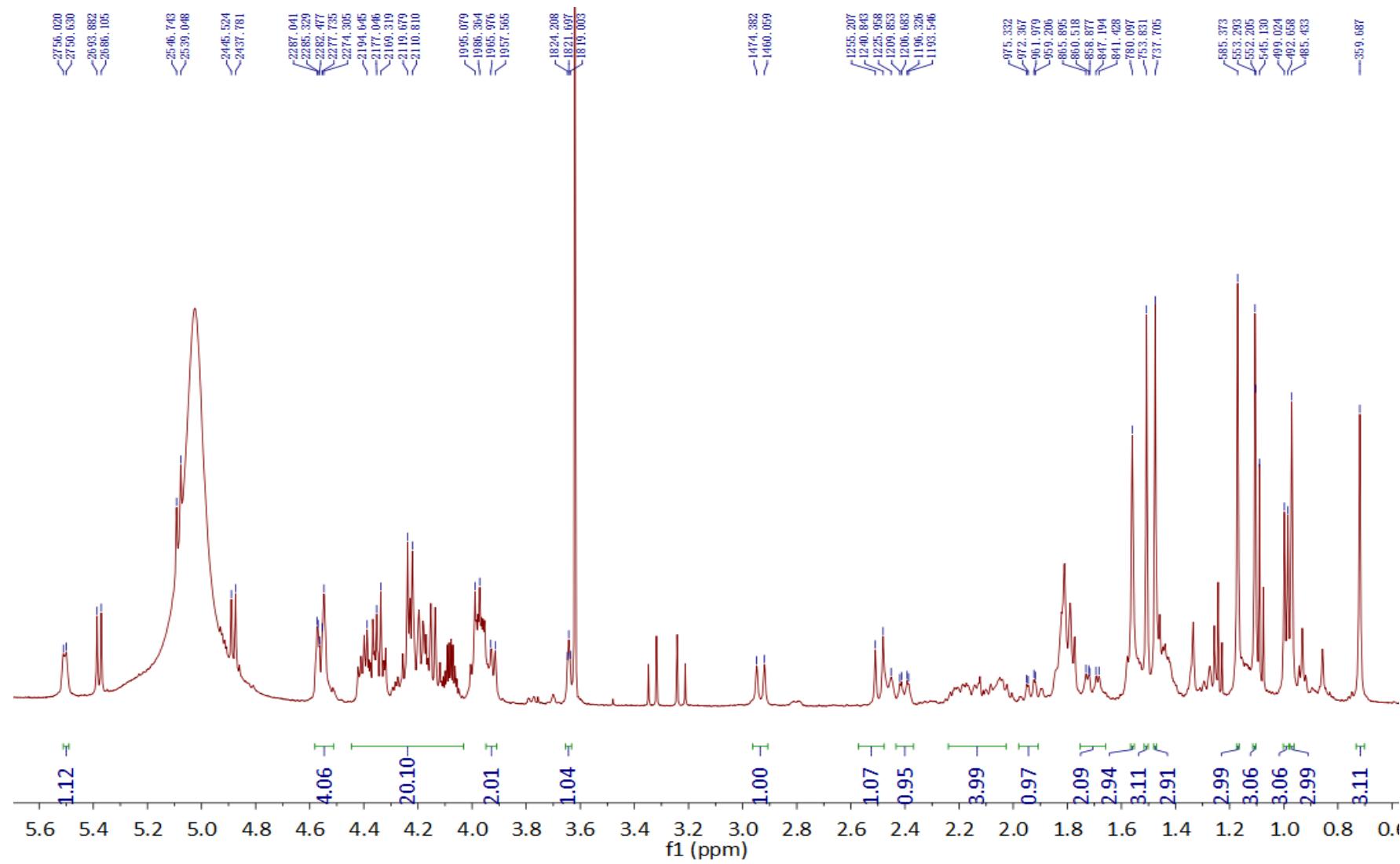


Figure S2. ^{13}C NMR spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

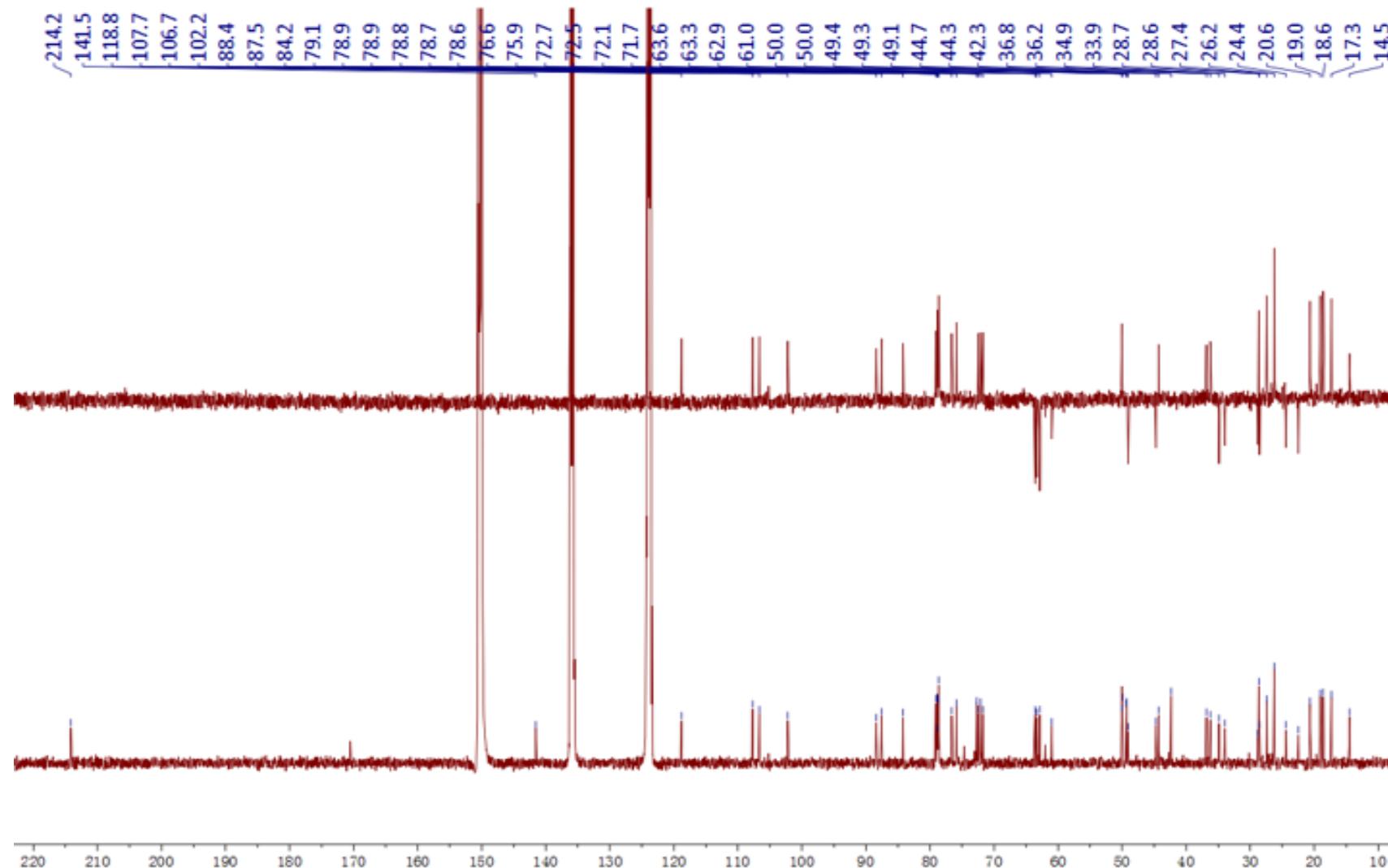


Figure S3. HSQC spectrum of 11-oxomogroside III E (**1**) in C₅D₅N

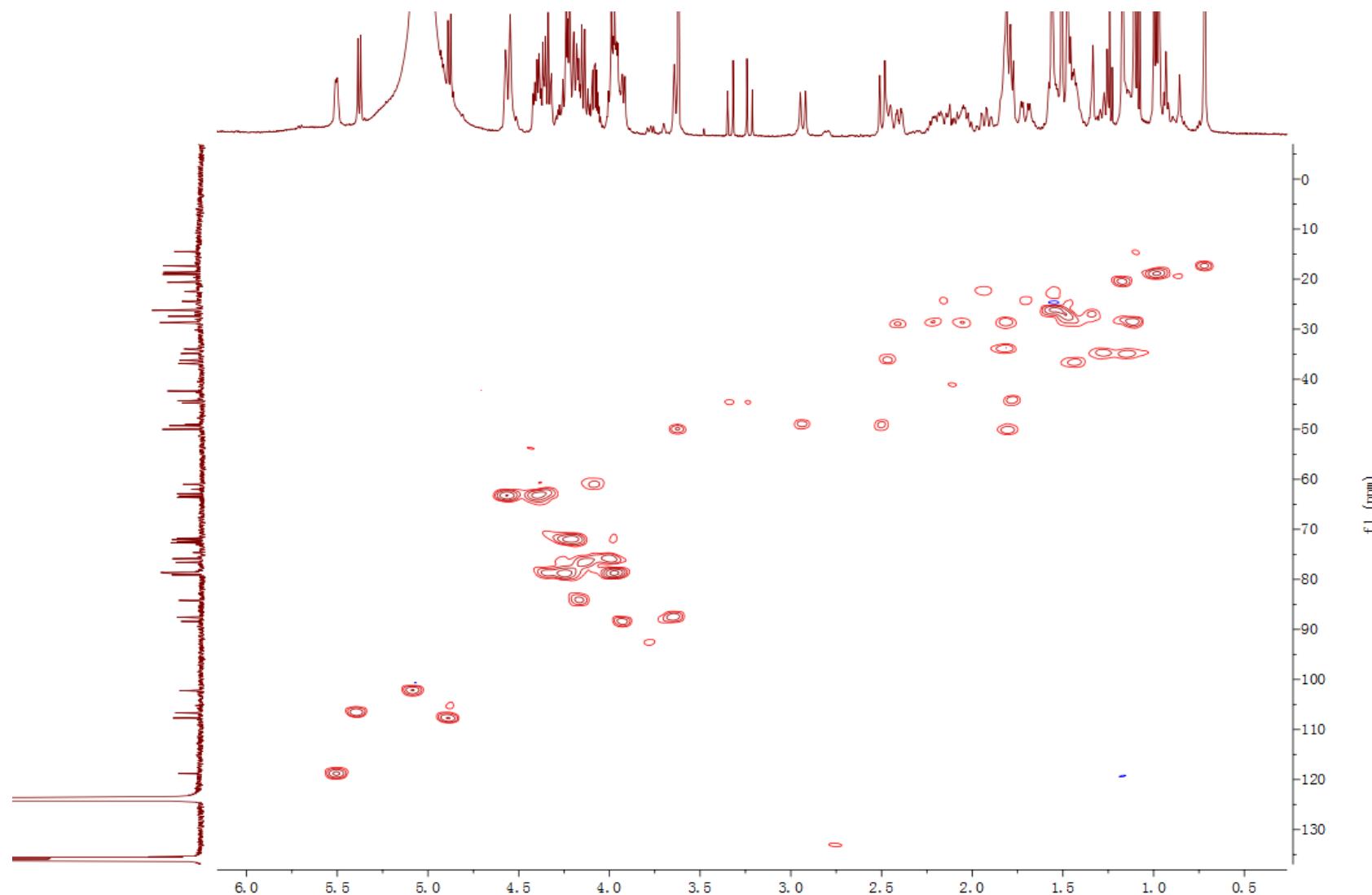


Figure S4. HMBC spectrum of 11-oxomogroside III E (**1**) in C₅D₅N

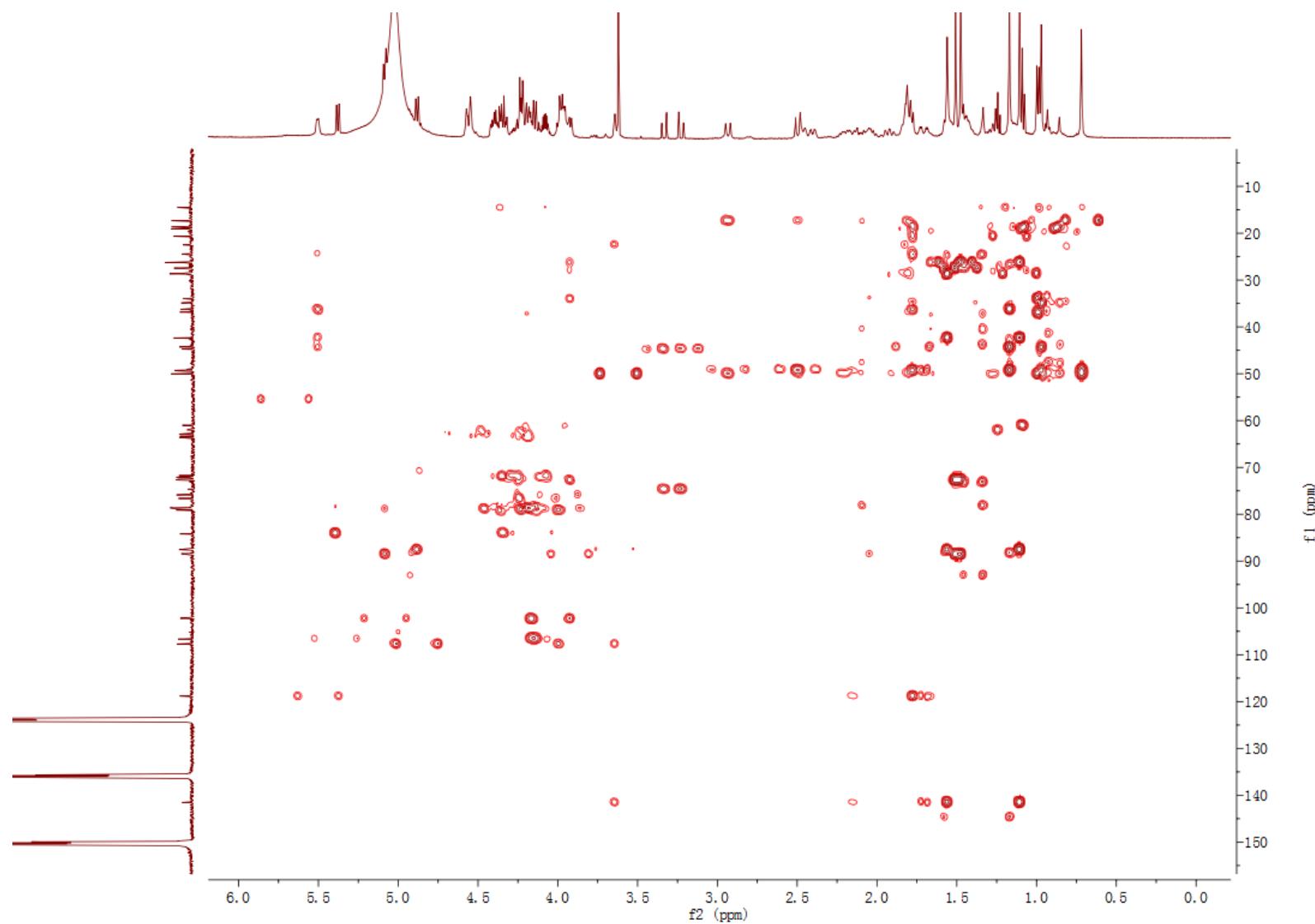


Figure S5. ROESY spectrum of 11-oxomogroside III E (**1**) in C₅D₅N

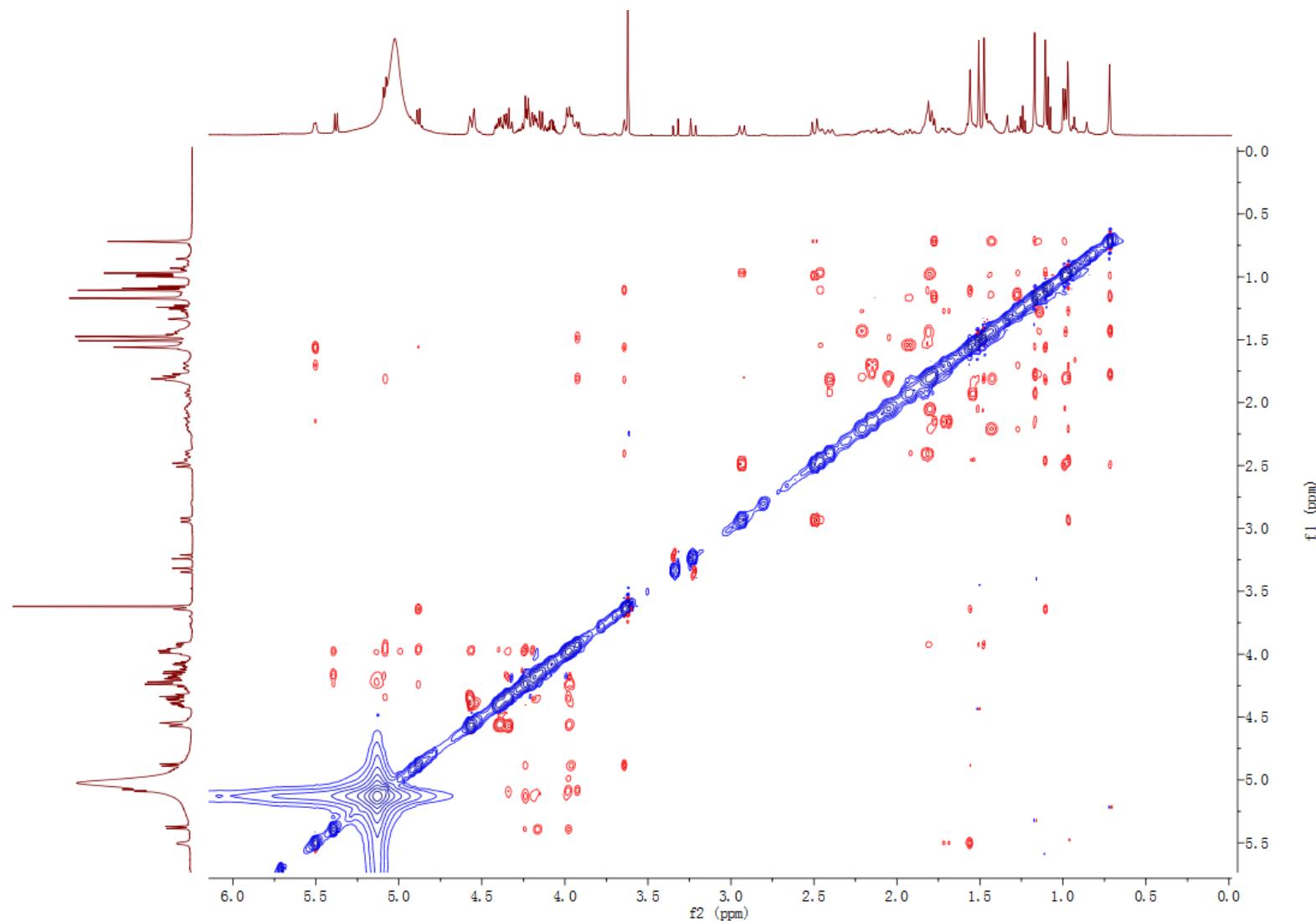


Figure S6. ^1H - ^1H COSY spectrum of 11-oxomogroside III E (**1**) in $\text{C}_5\text{D}_5\text{N}$

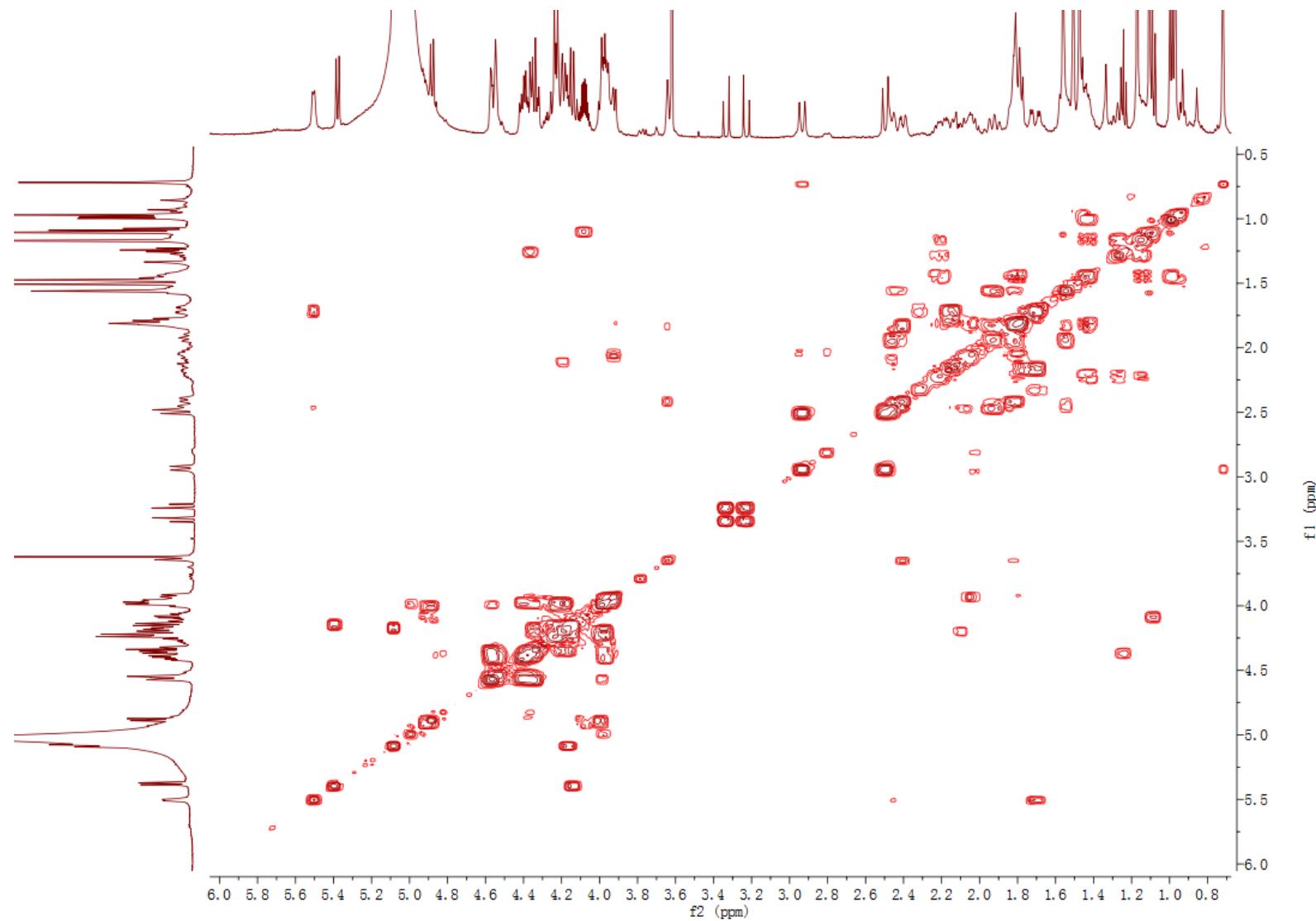


Figure S7. TOCSY spectrum of 11-oxomogroside III E (**1**) in C₅D₅N

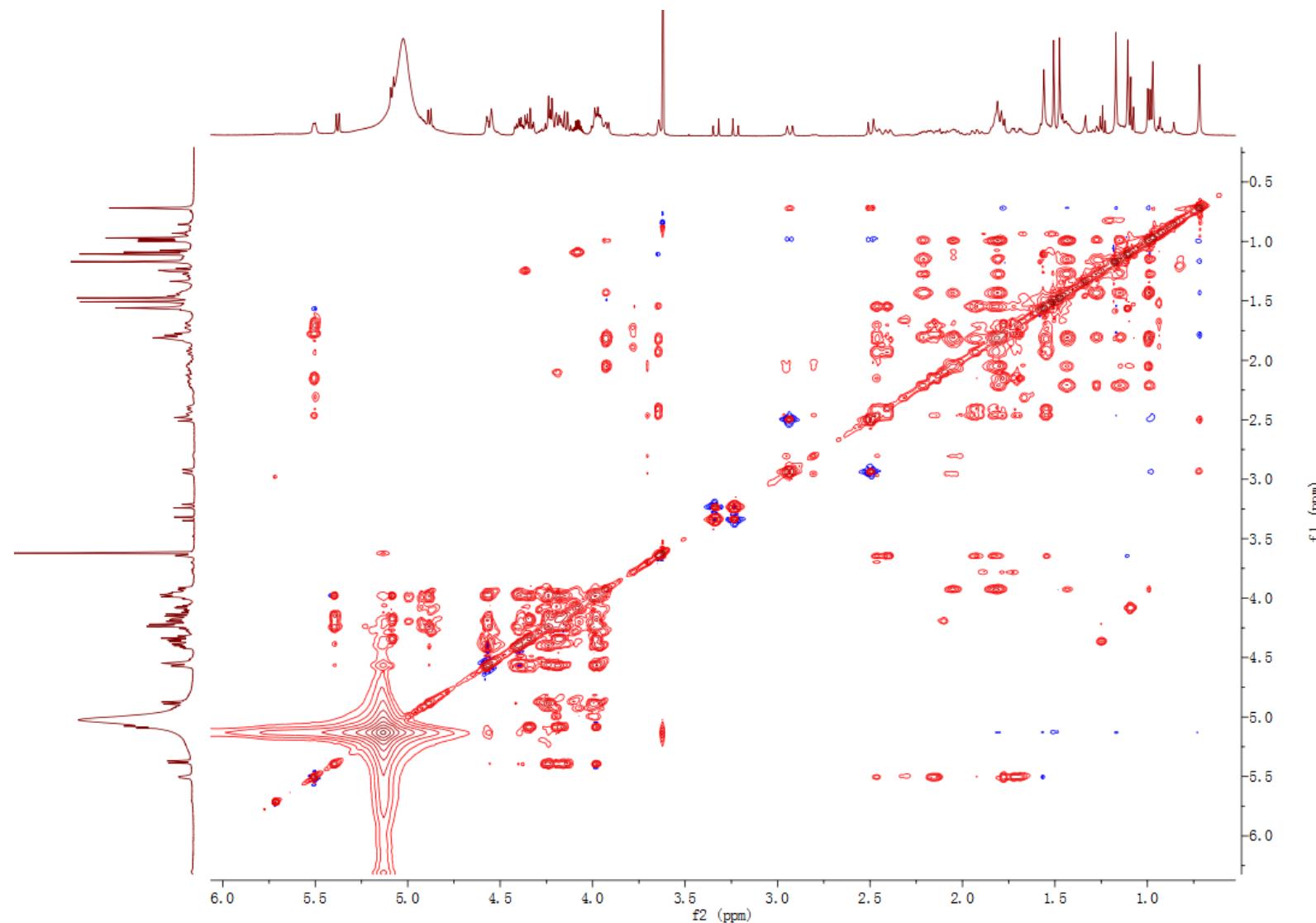


Figure S8. IR spectrum of 11-oxomogroside III E (**1**)

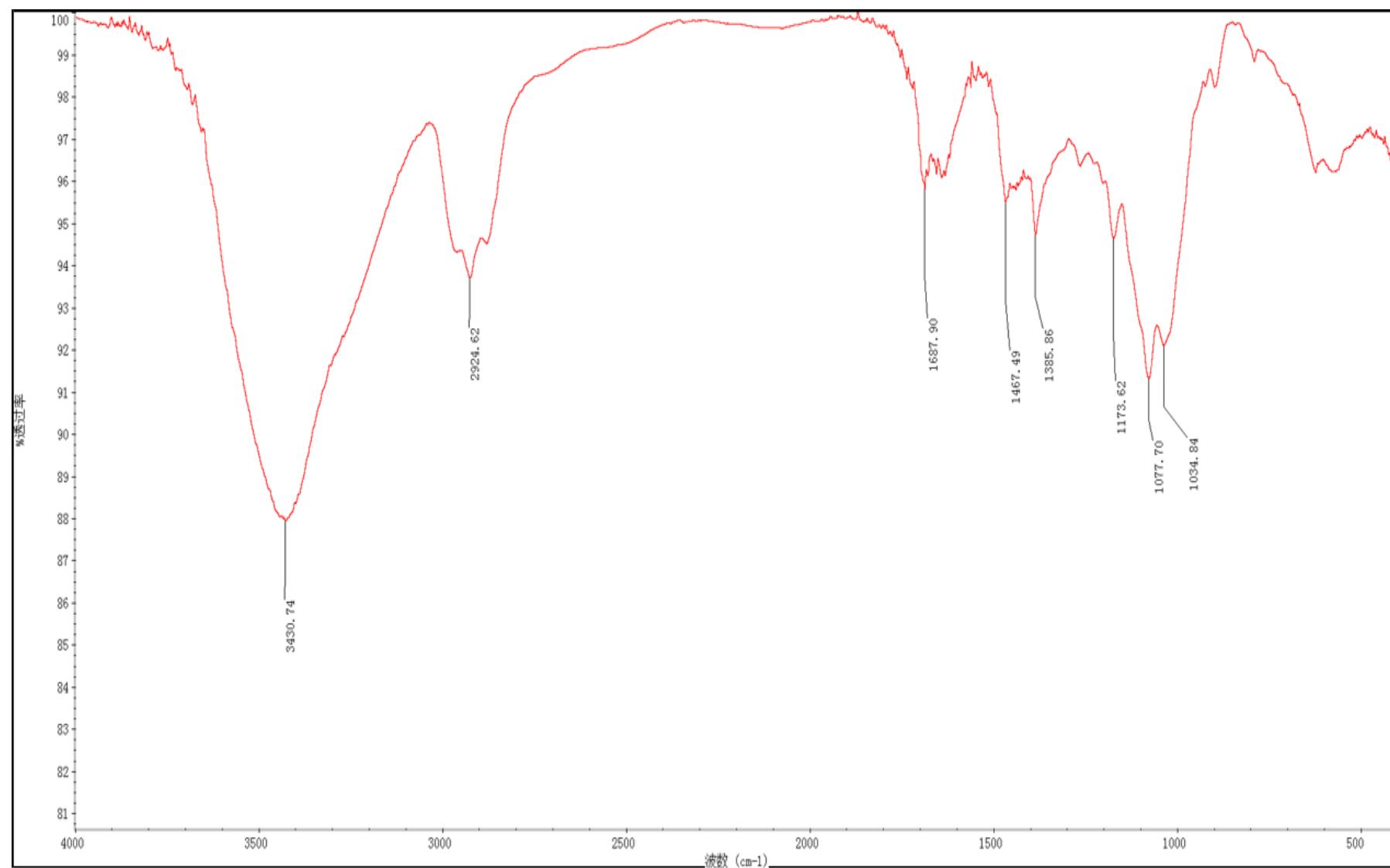


Figure S9. HRESIMS spectrum of 11-oxomogroside III E (**1**)

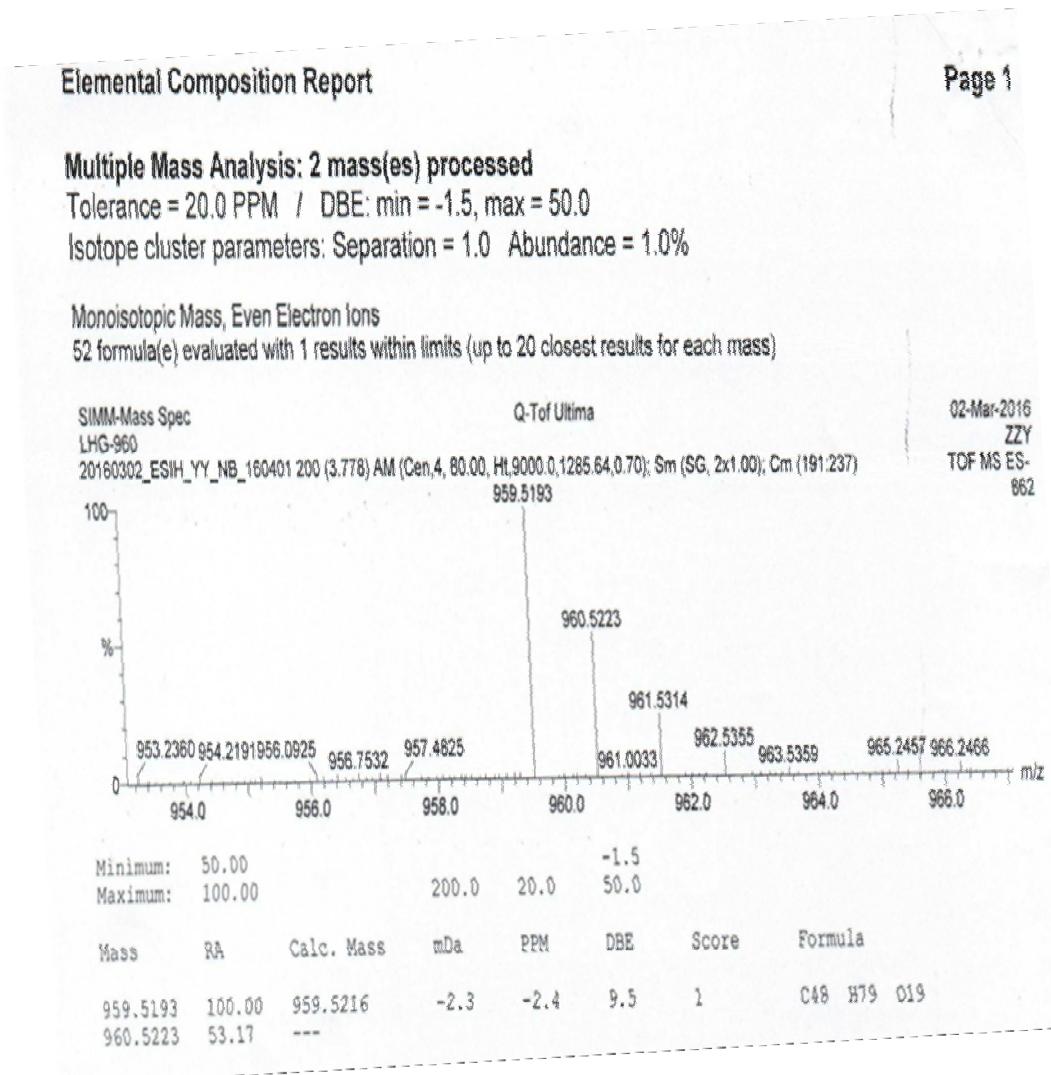


Figure S10. ^1H NMR spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

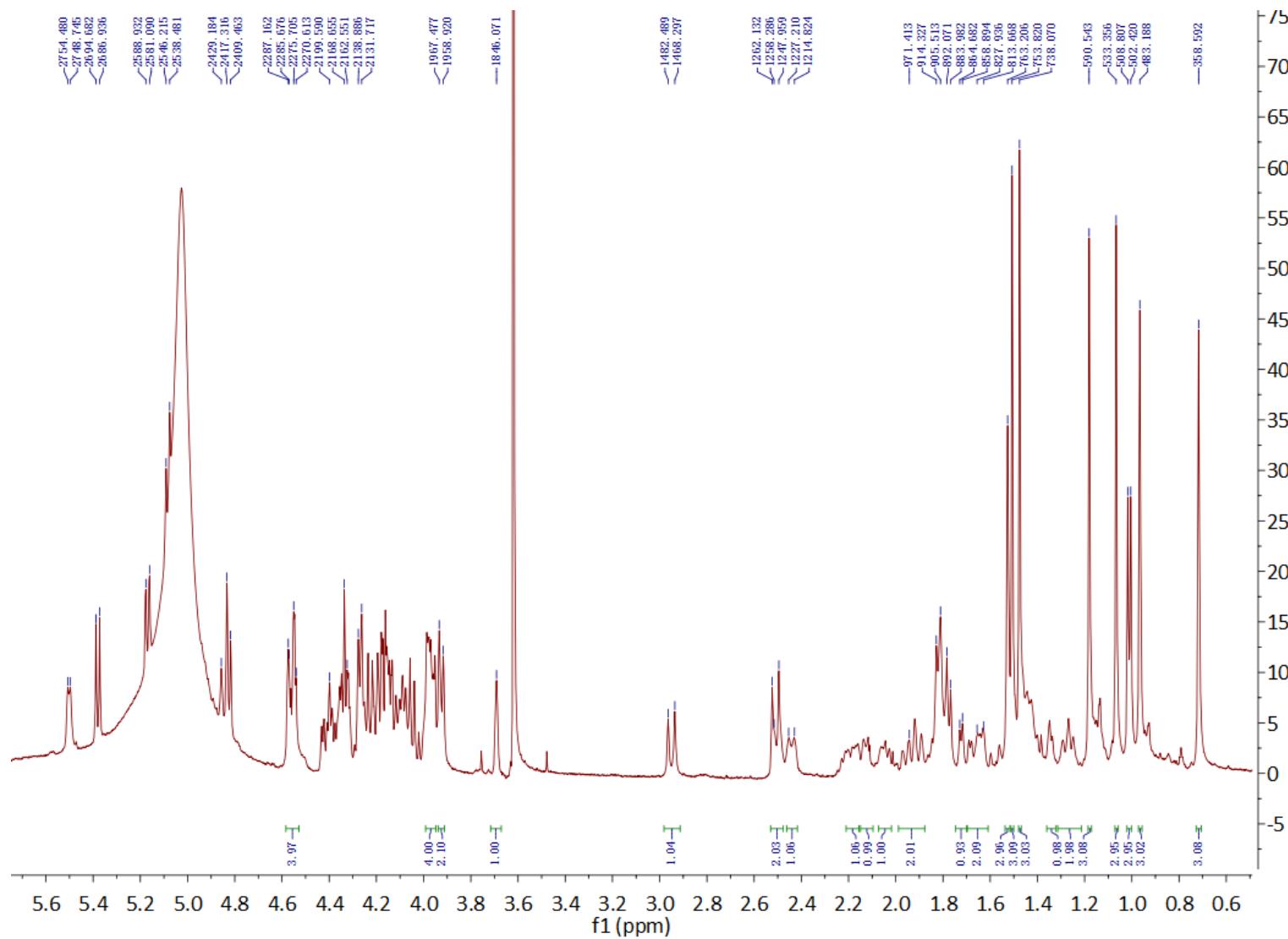


Figure S11. ^{13}C NMR spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

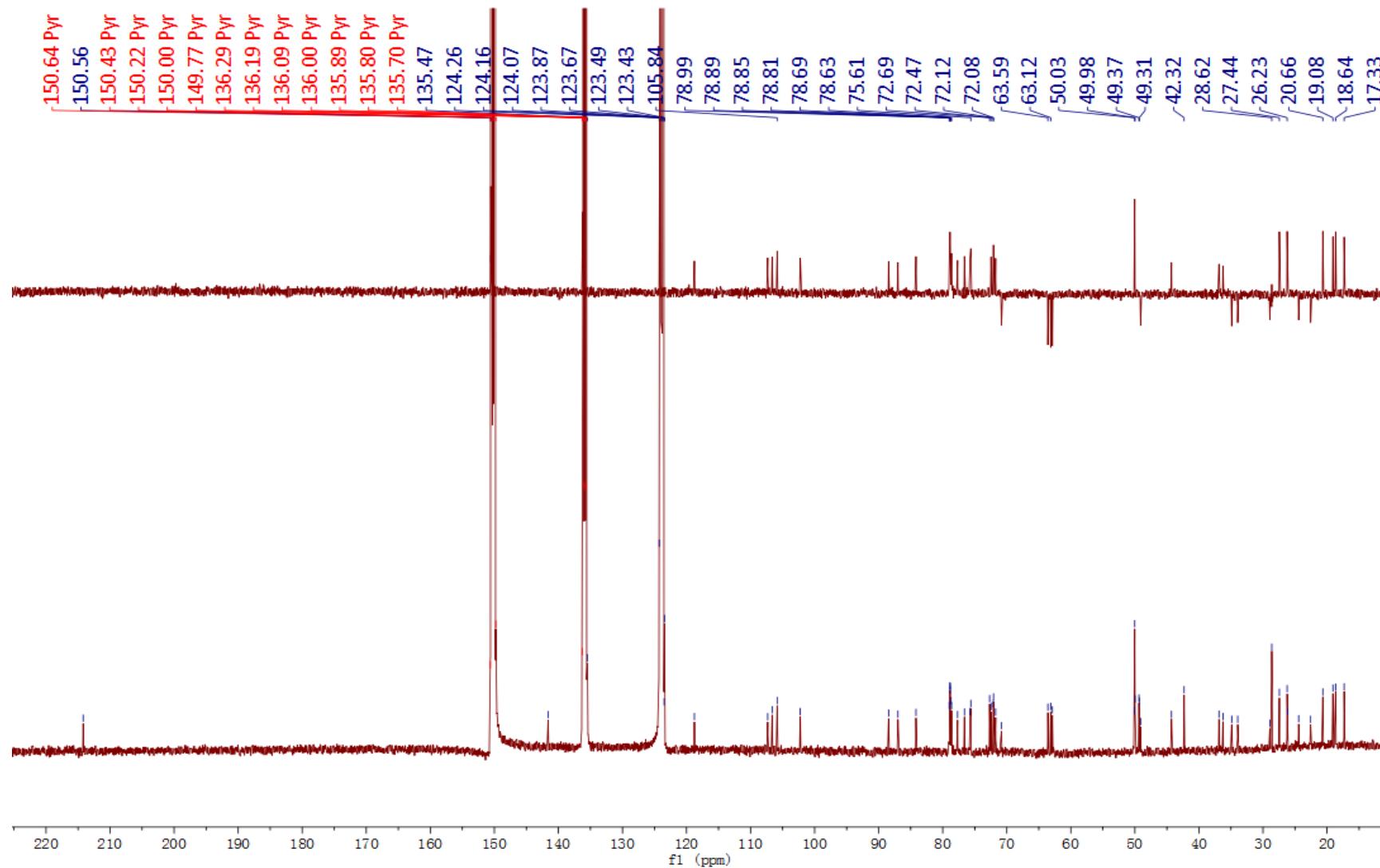


Figure S12. HSQC spectrum of 11-oxomogroside IV (**2**) in C₅D₅N

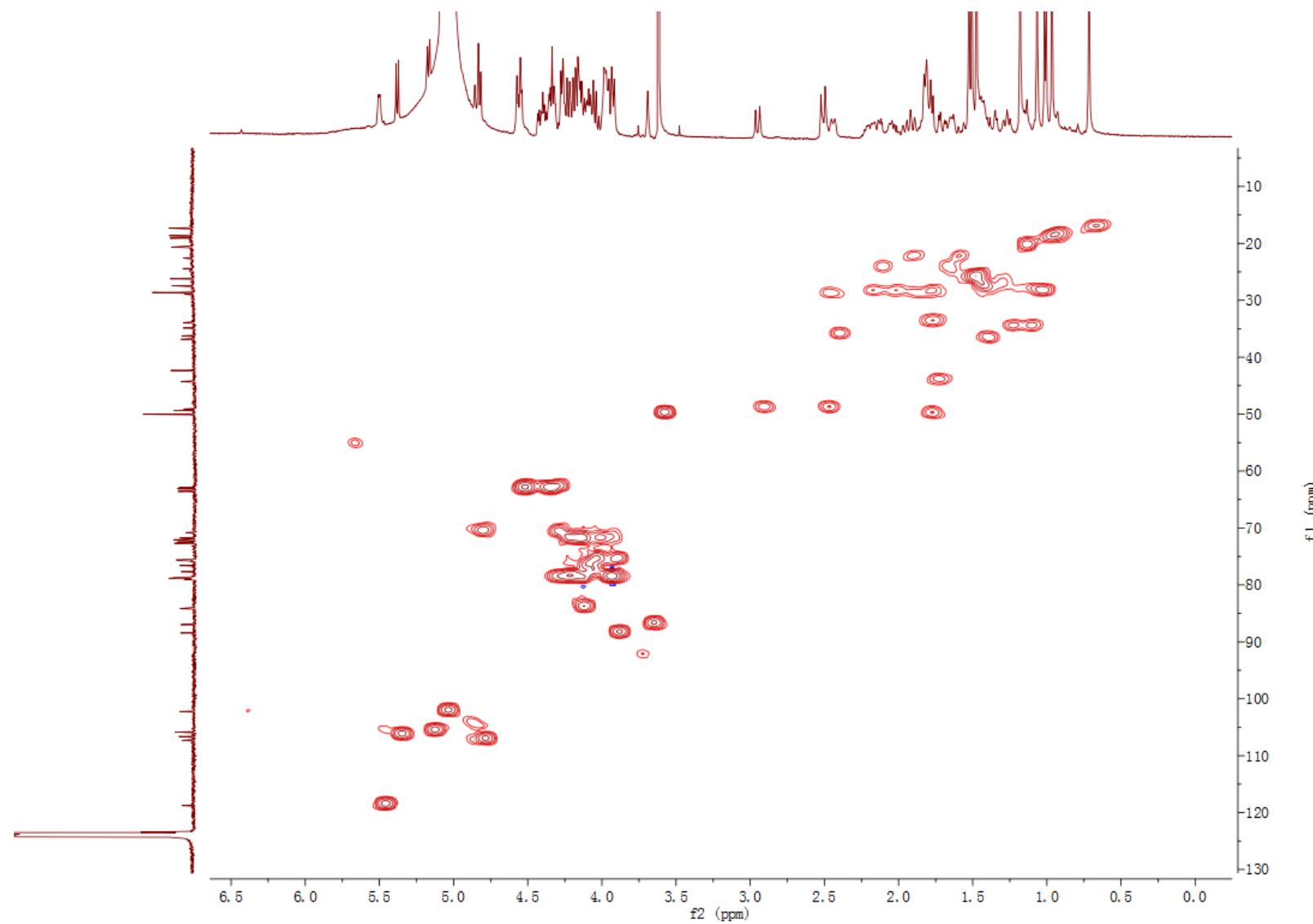


Figure S13. HMBC spectrum of 11-oxomogroside IV (**2**) in C₅D₅N

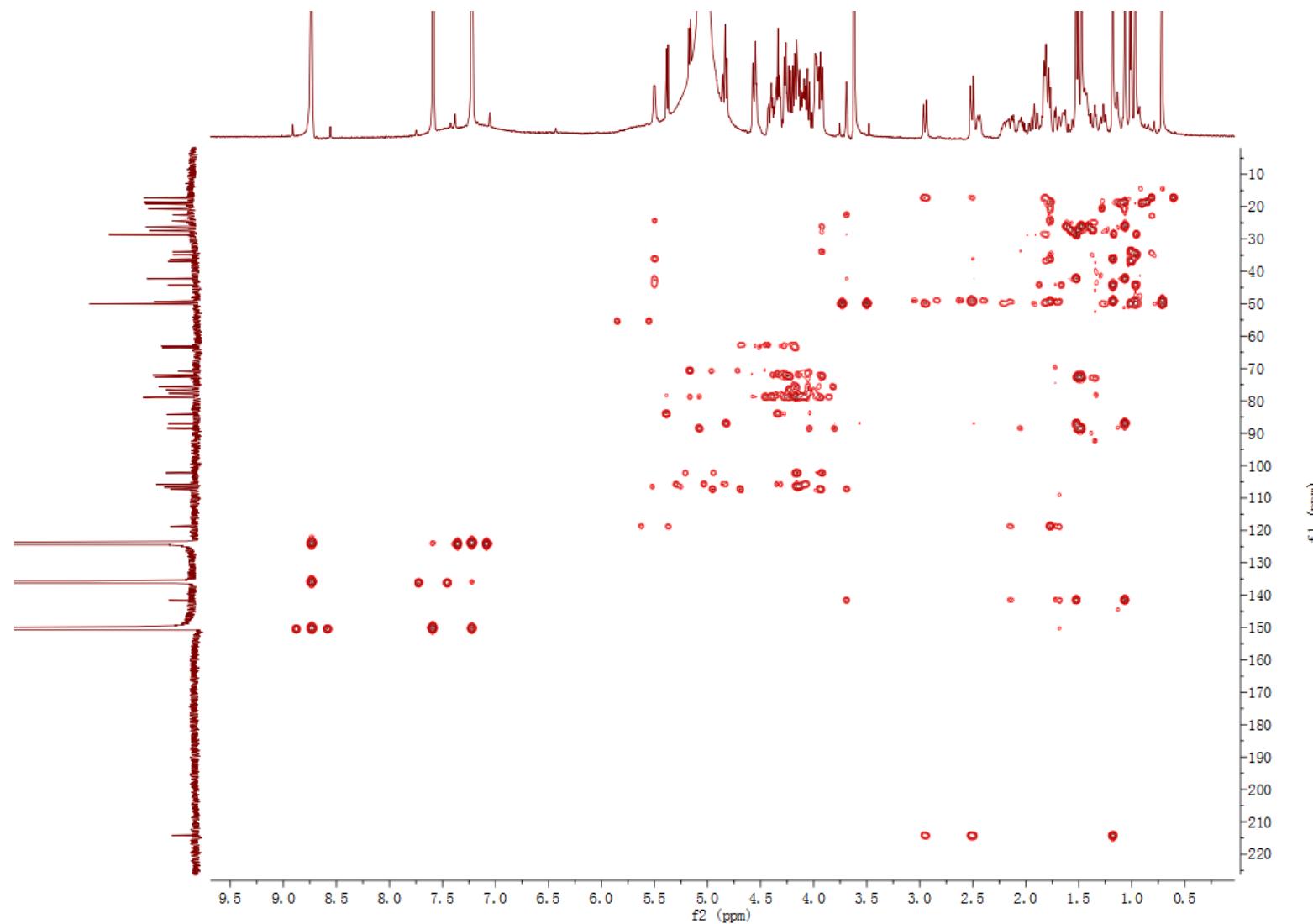


Figure S14. ROESY spectrum of 11-oxomogroside IV (**2**) in C₅D₅N

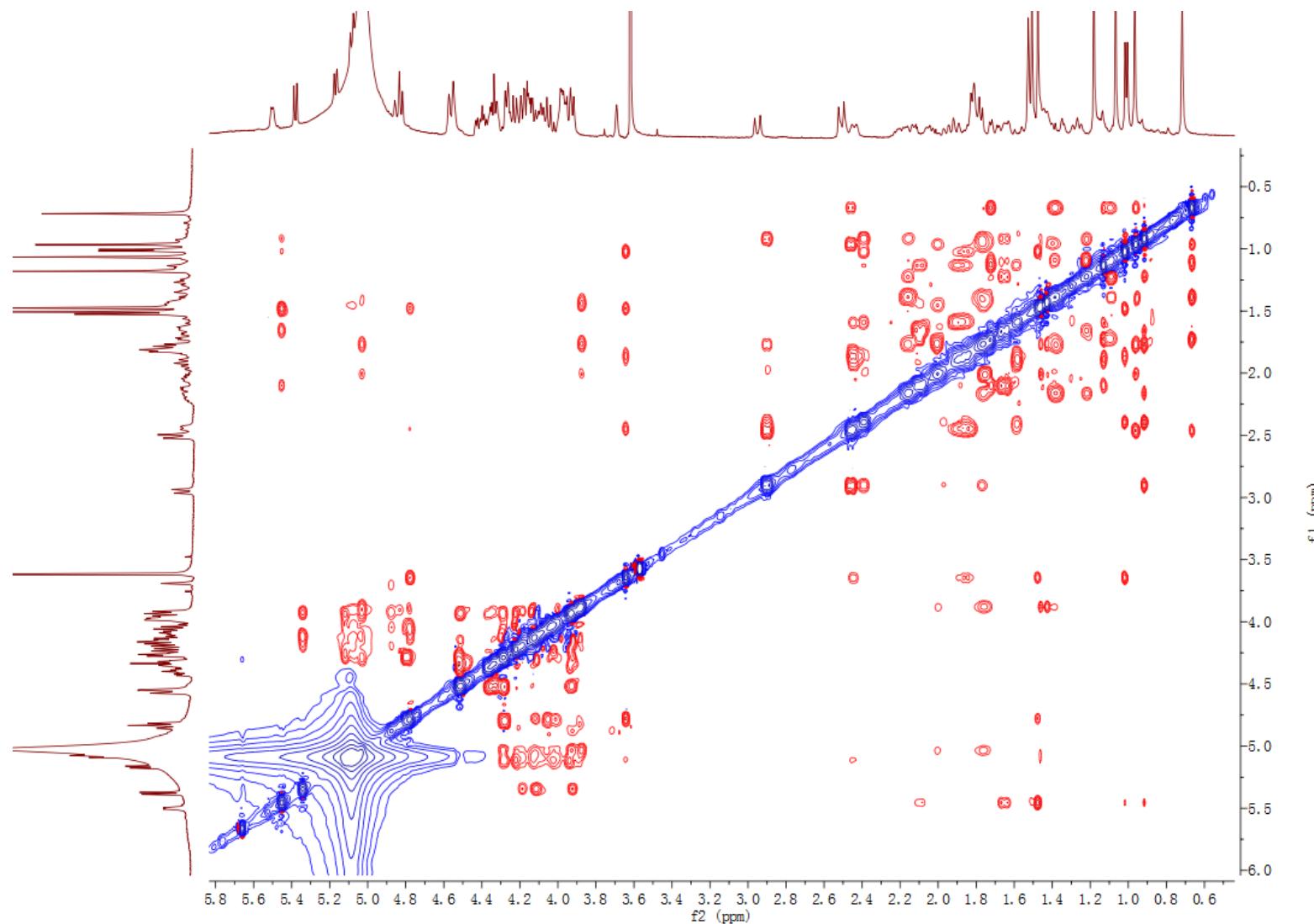


Figure S15. ^1H - ^1H COSY spectrum of 11-oxomogroside IV (**2**) in $\text{C}_5\text{D}_5\text{N}$

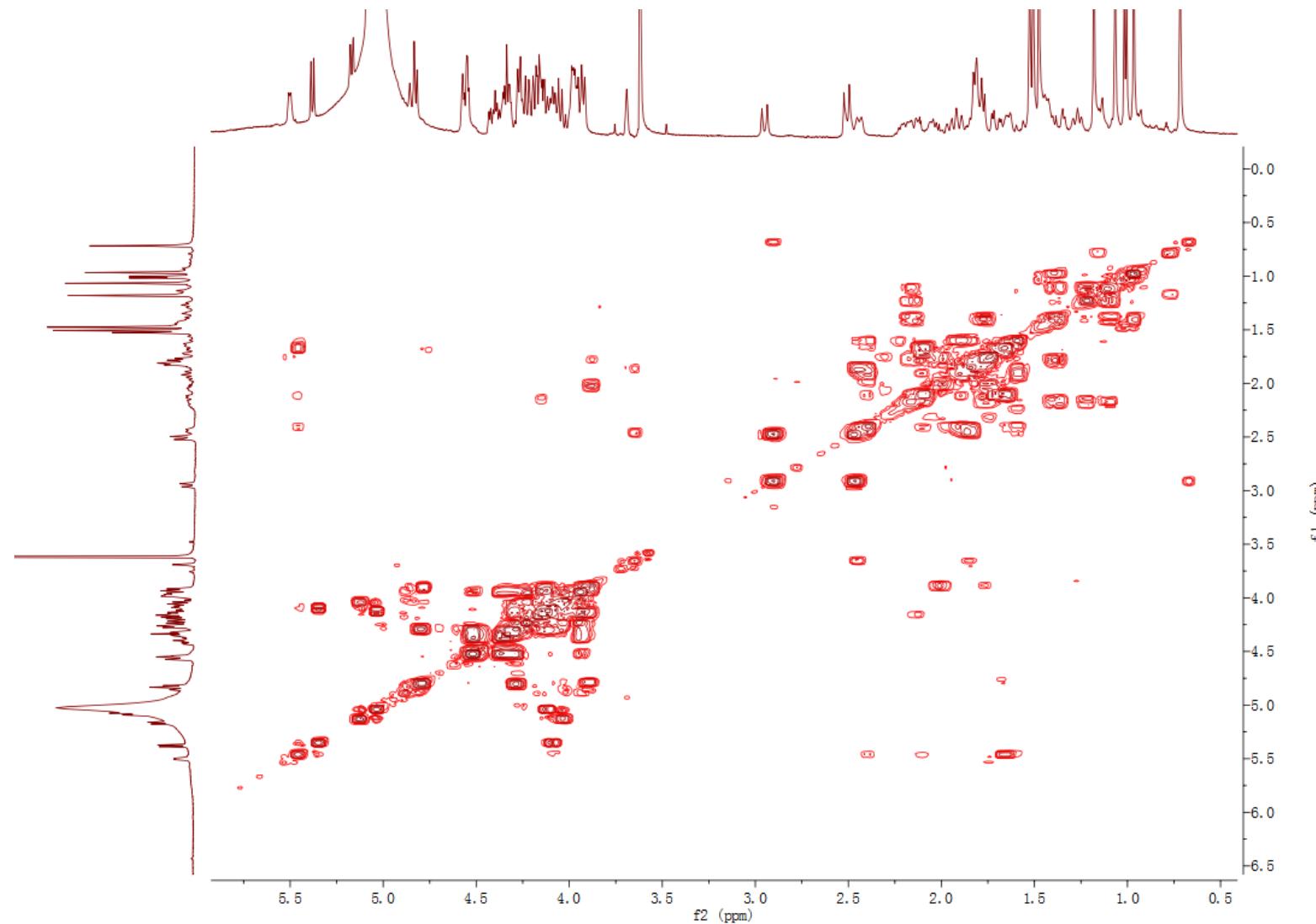


Figure S16. TOCSY spectrum of 11-oxomogroside IV (**2**) in C₅D₅N

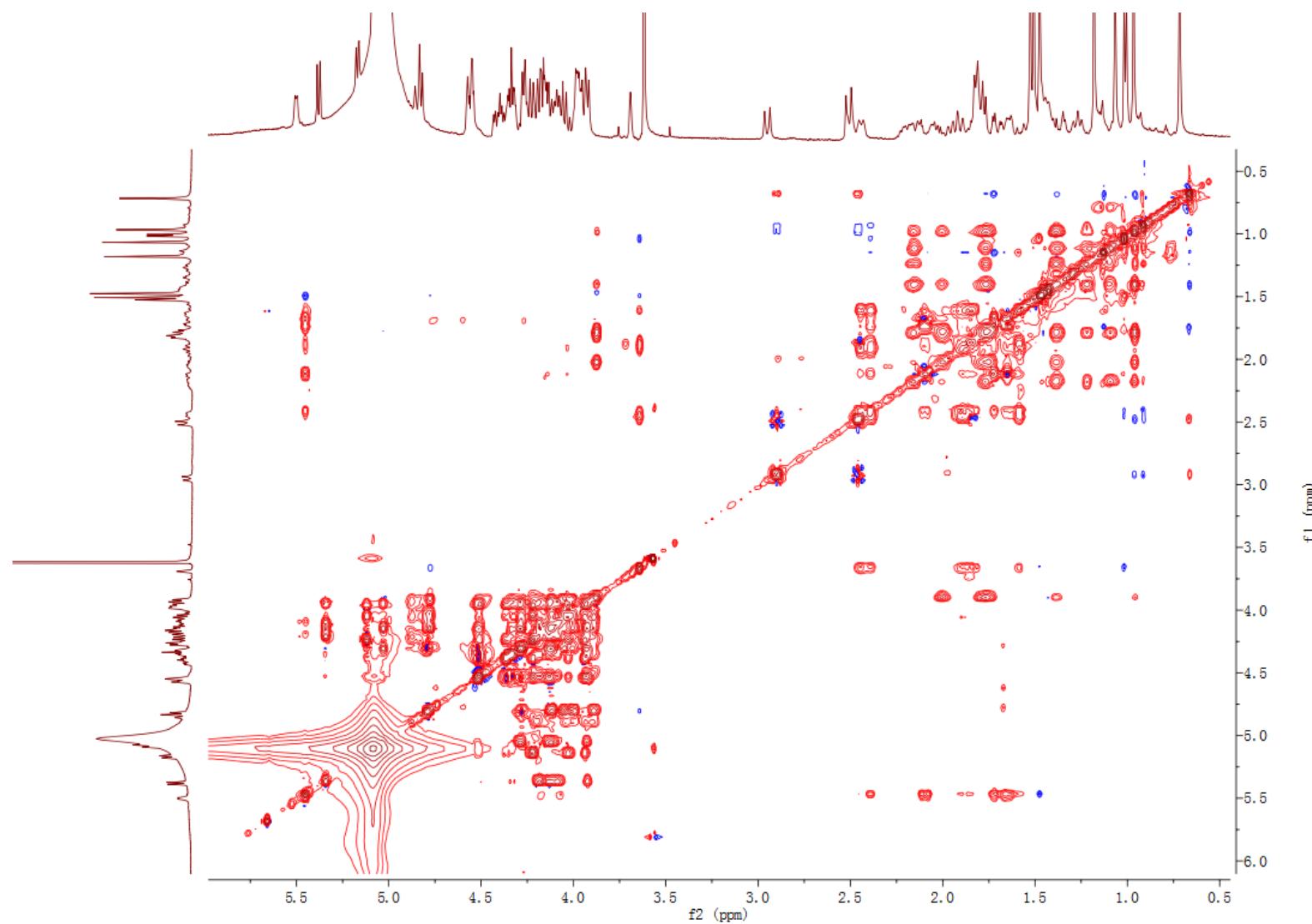


Figure S17. IR spectrum of 11-oxomogroside IV (2)

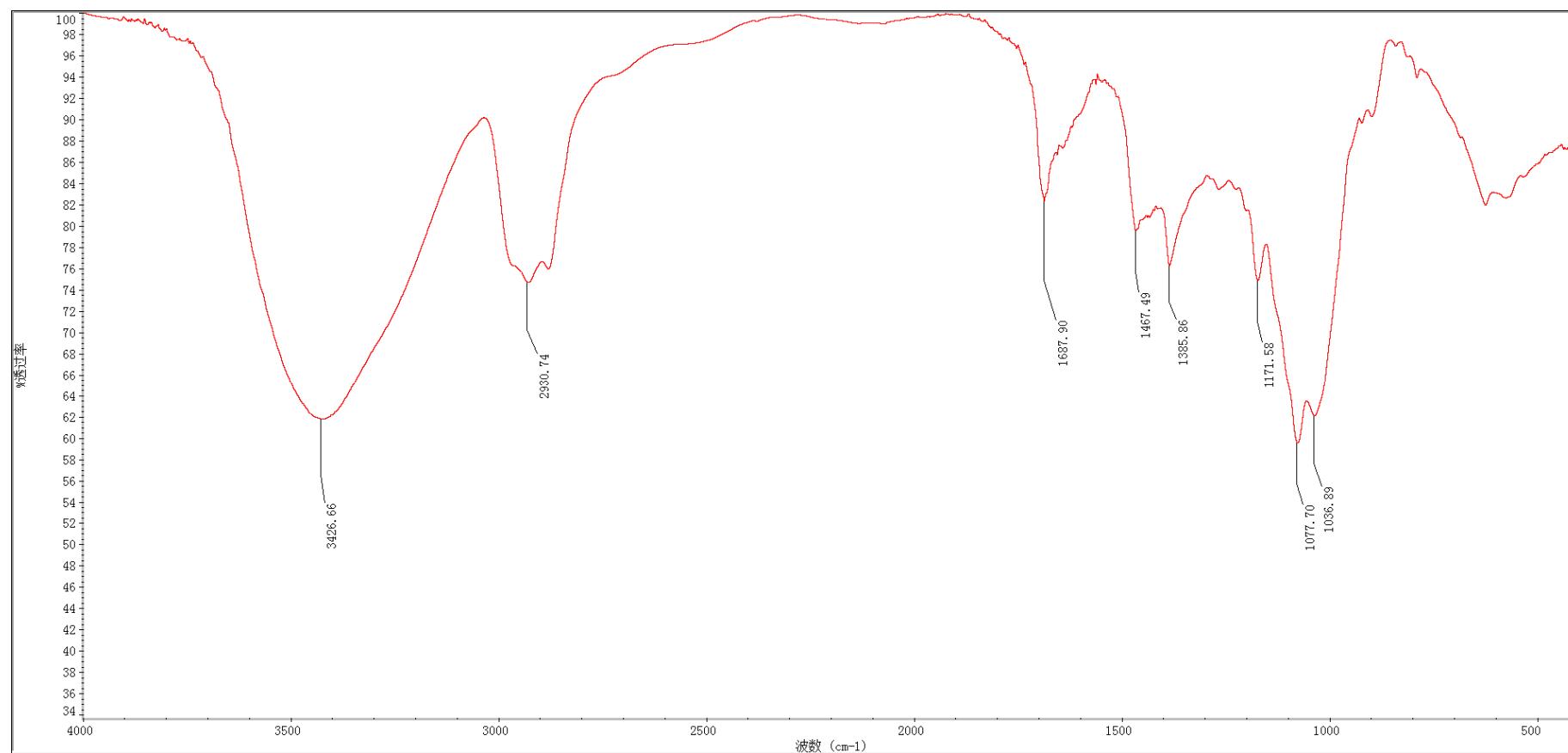


Figure S18. HRESIMS spectrum of 11-oxomogroside IV (**2**)

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

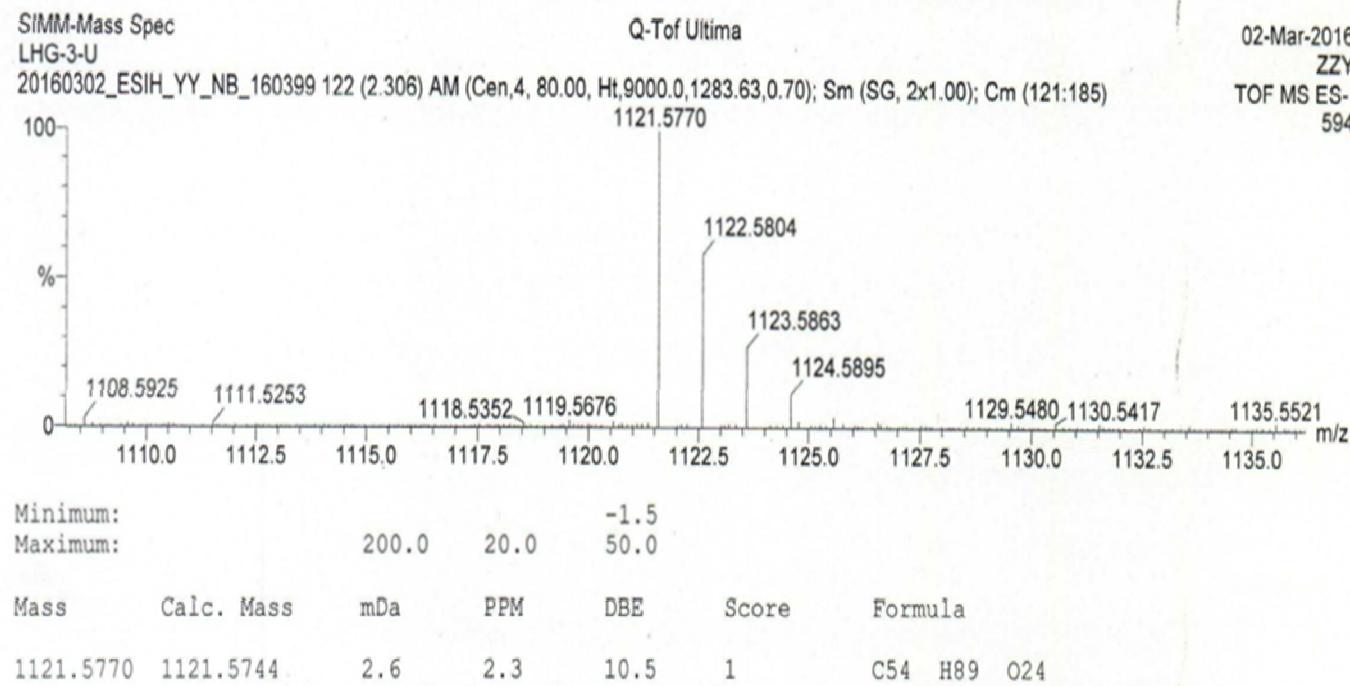


Figure S19. ^1H NMR spectrum of 11-oxoisomogroside V (**3**) in C₅D₅N

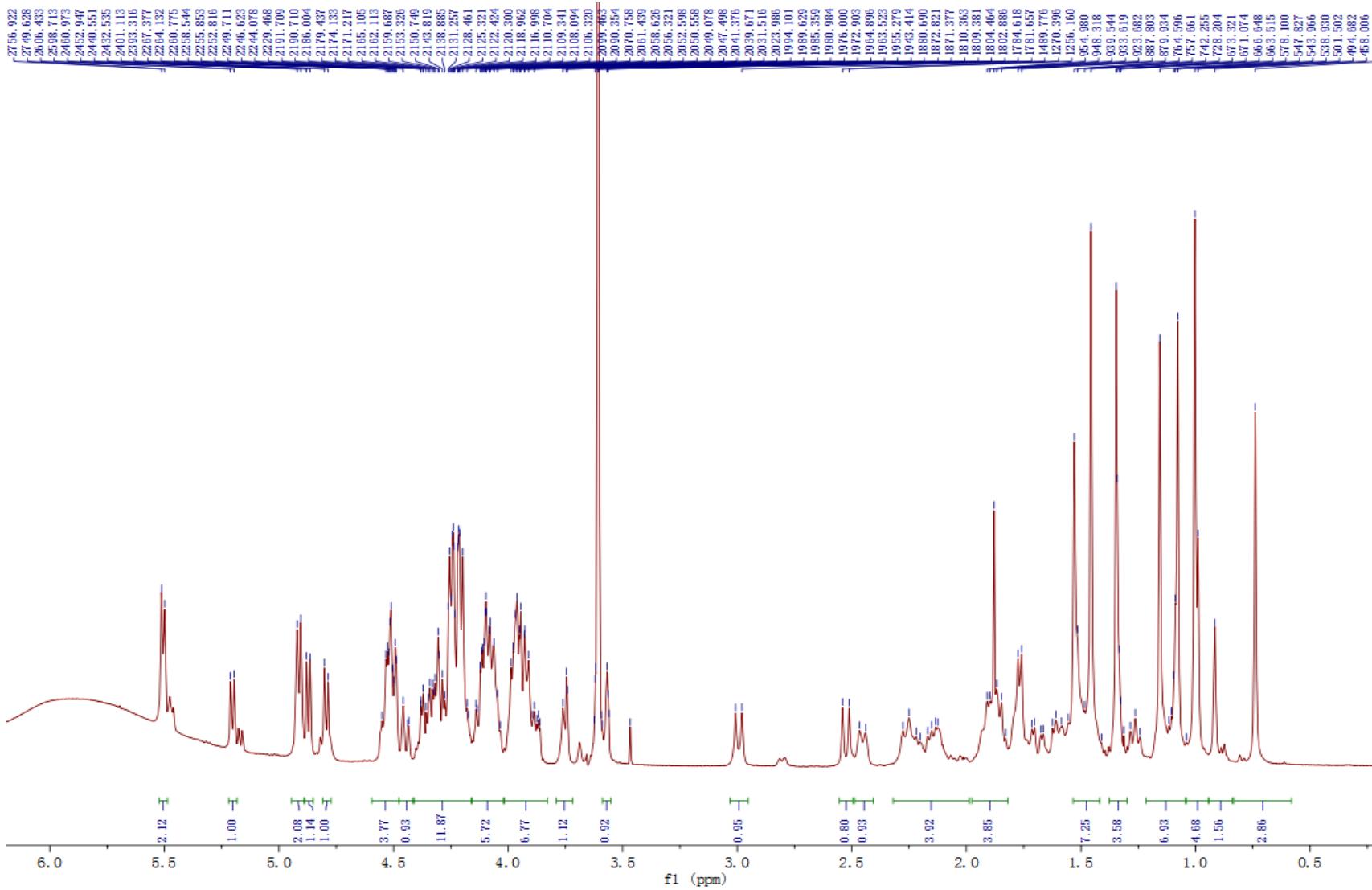


Figure S20. ^{13}C NMR spectrum of 11-oxoisomogroside V (**3**) in $\text{C}_5\text{D}_5\text{N}$

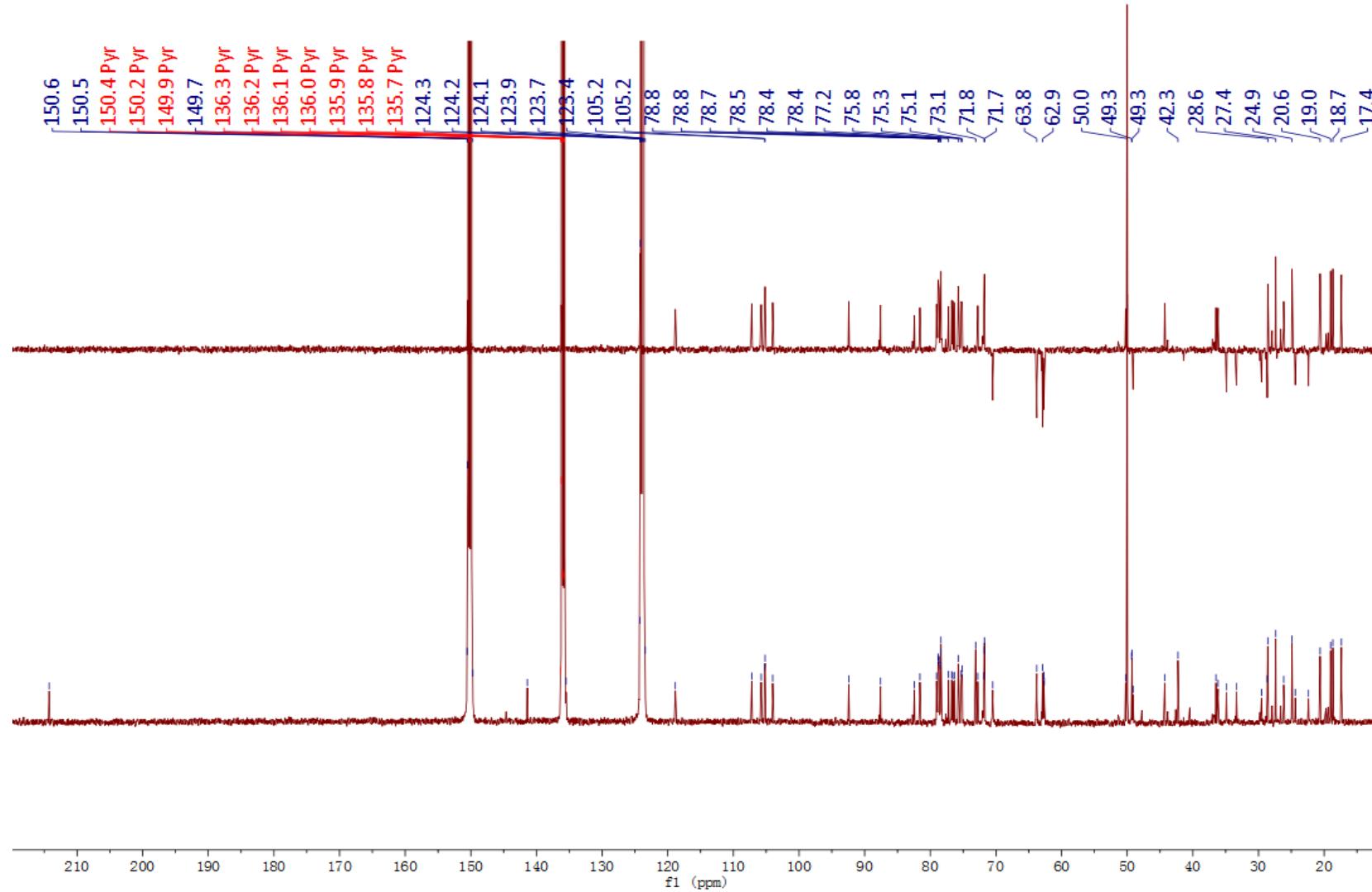


Figure S21. HSQC spectrum of 11-oxoisomogroside V (**3**) in C₅D₅N

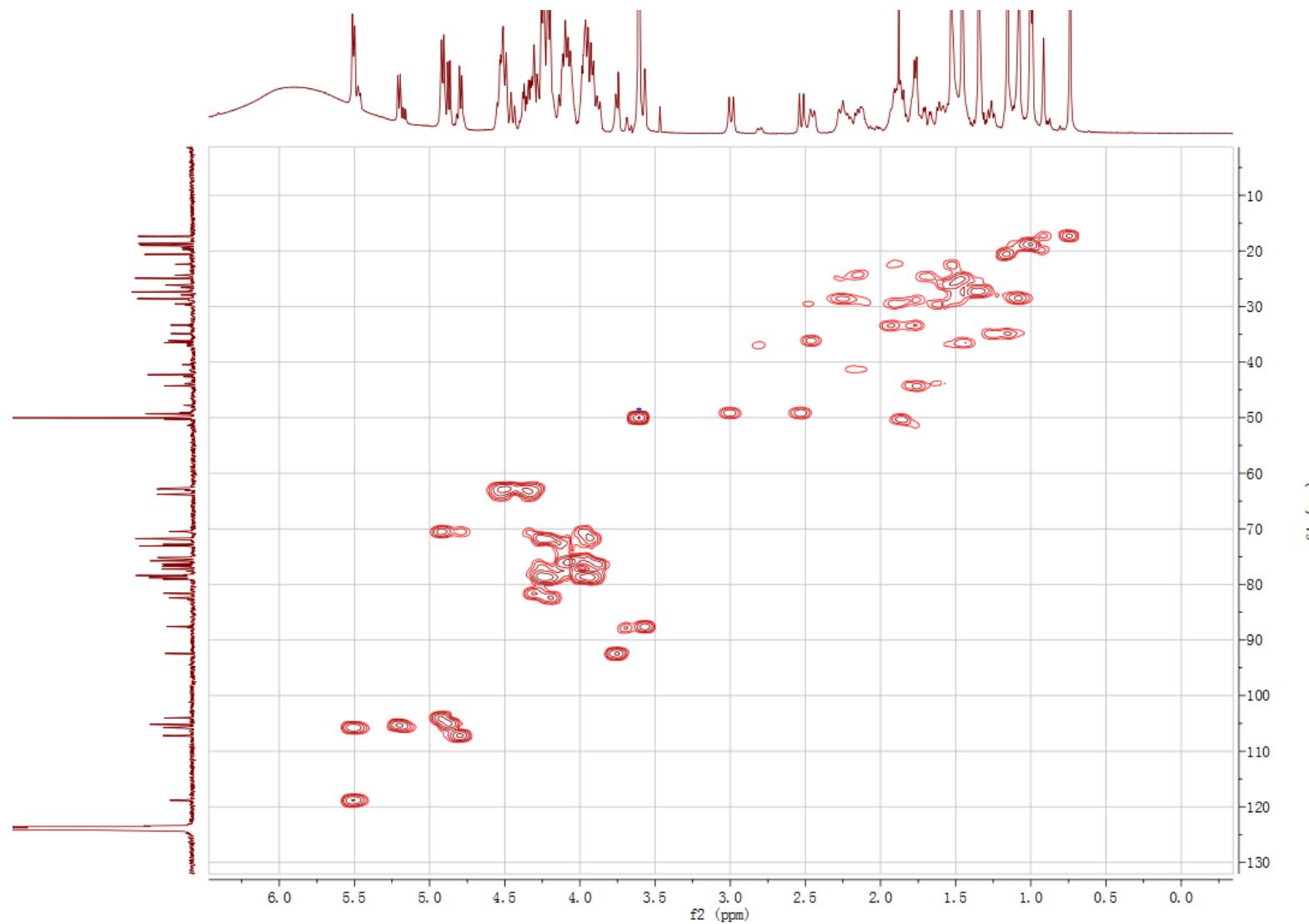


Figure S22. HMBC spectrum of 11-oxoisomogroside V (**3**) in C₅D₅N

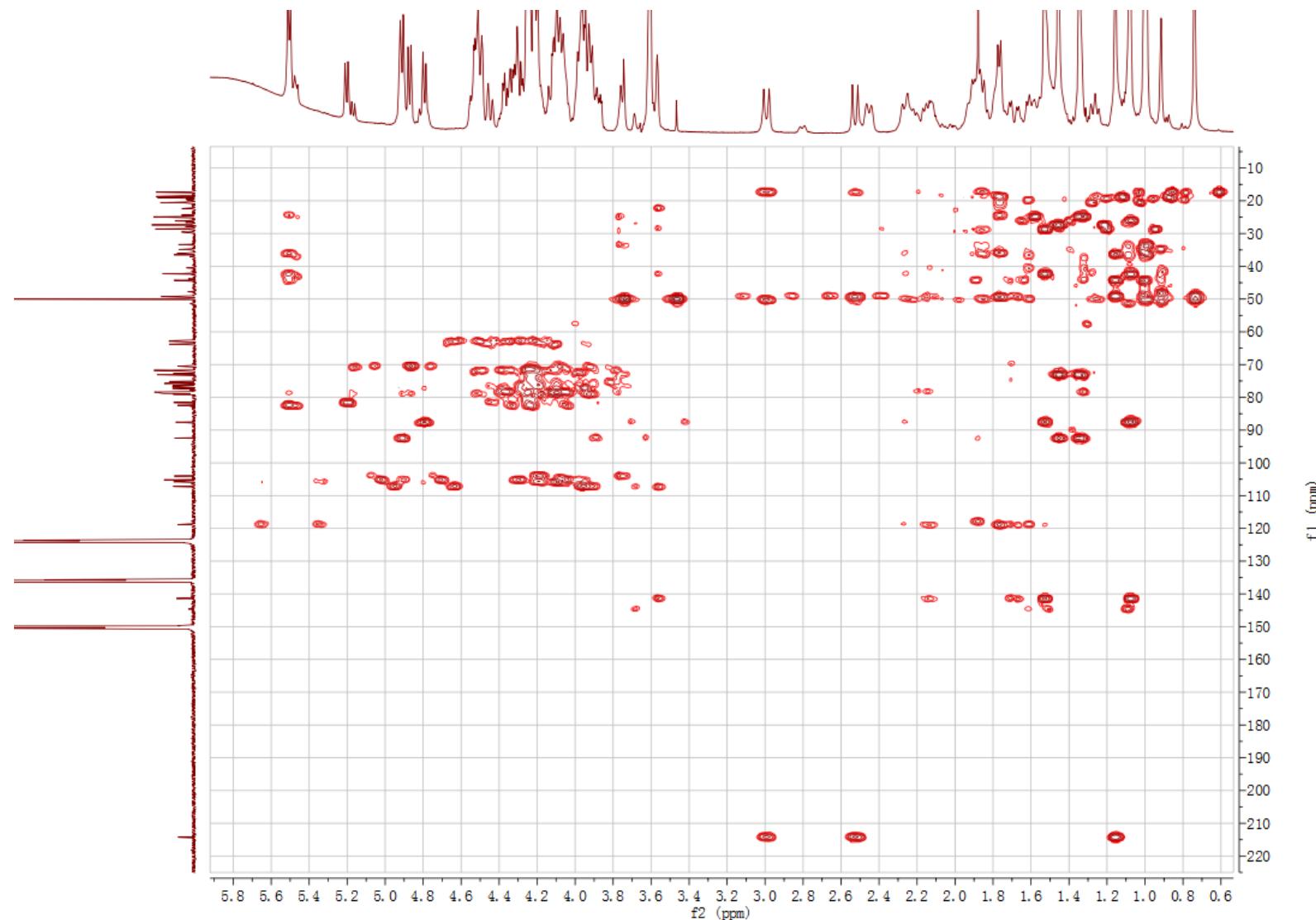


Figure S23. ROESY spectrum of 11-oxoisomogroside V (**3**) in C₅D₅N

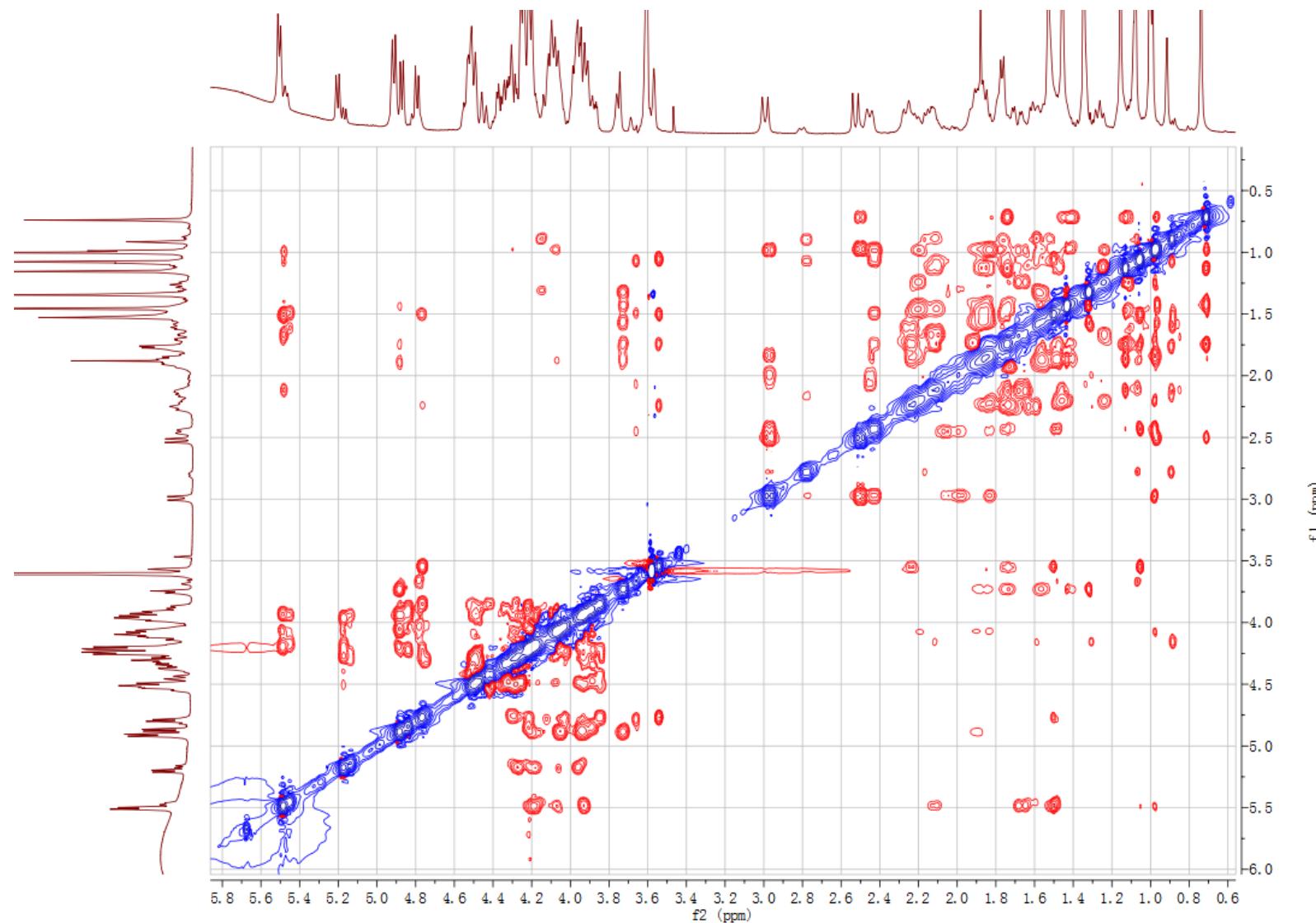


Figure S24. ^1H - ^1H COSY spectrum of 11-oxoisomogroside V (**3**) in $\text{C}_5\text{D}_5\text{N}$

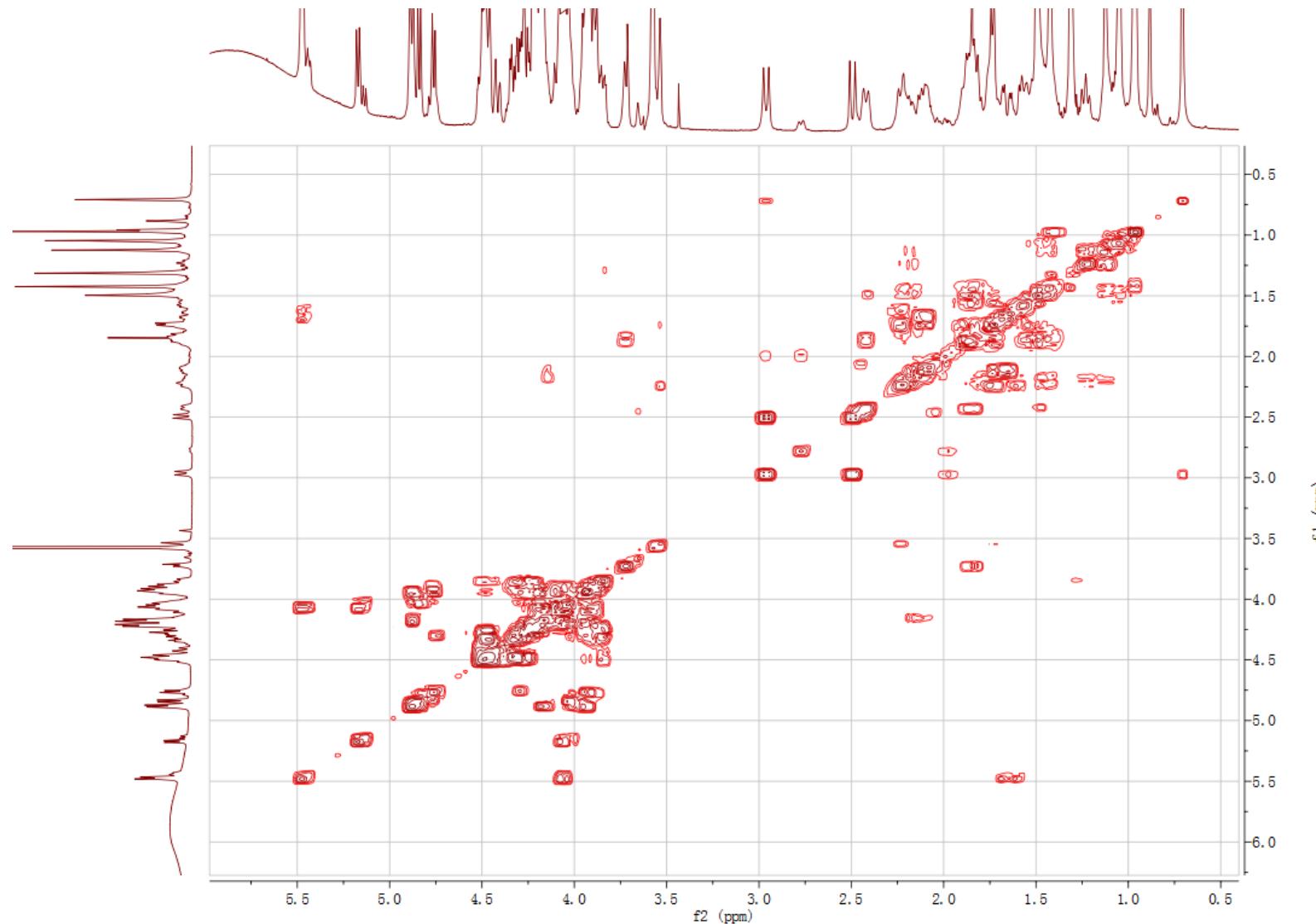


Figure S25. TOCSY spectrum of 11-oxoisomogroside V (**3**) in C₅D₅N

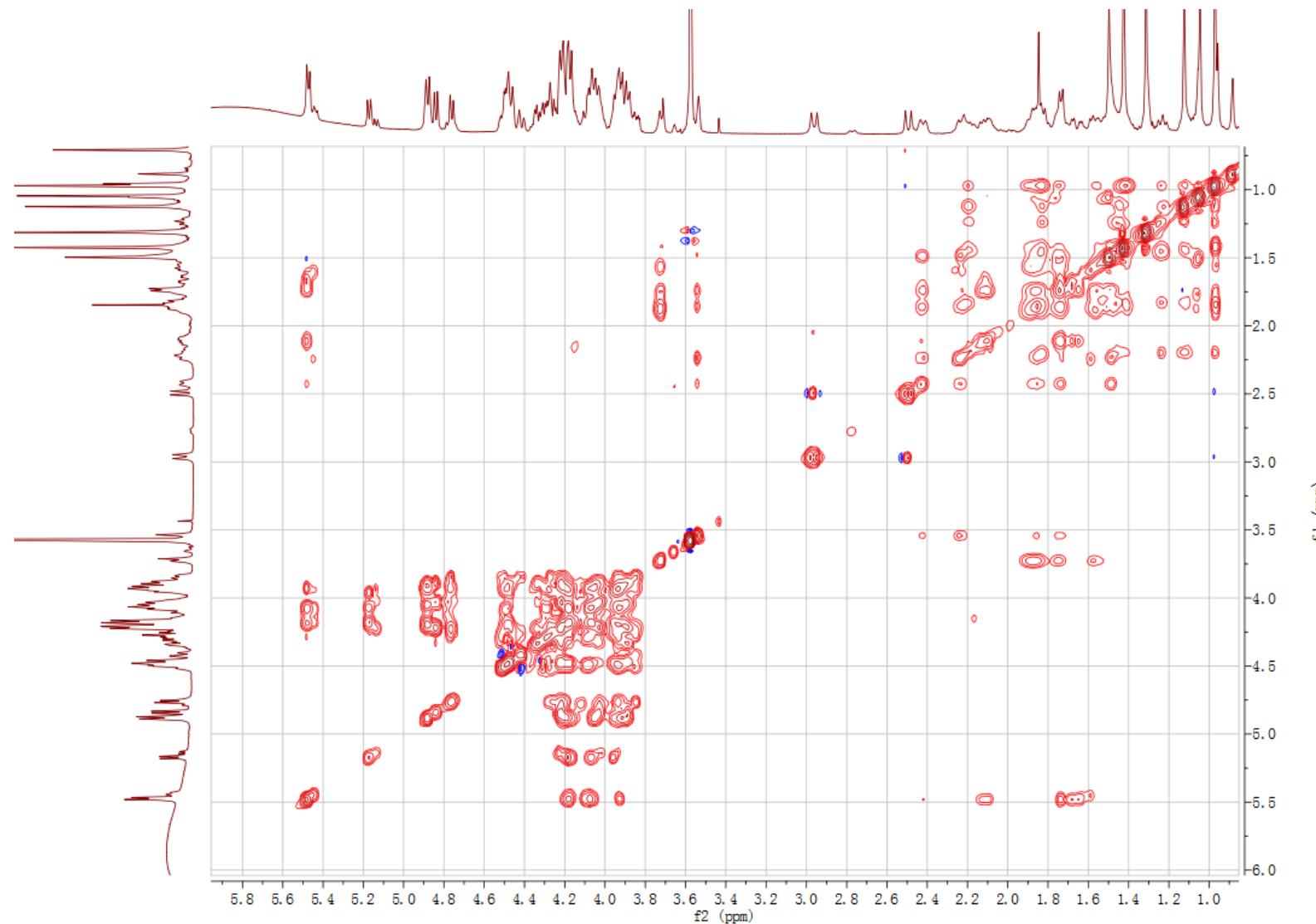


Figure S26. IR spectrum of 11-oxoisomogroside V (3)

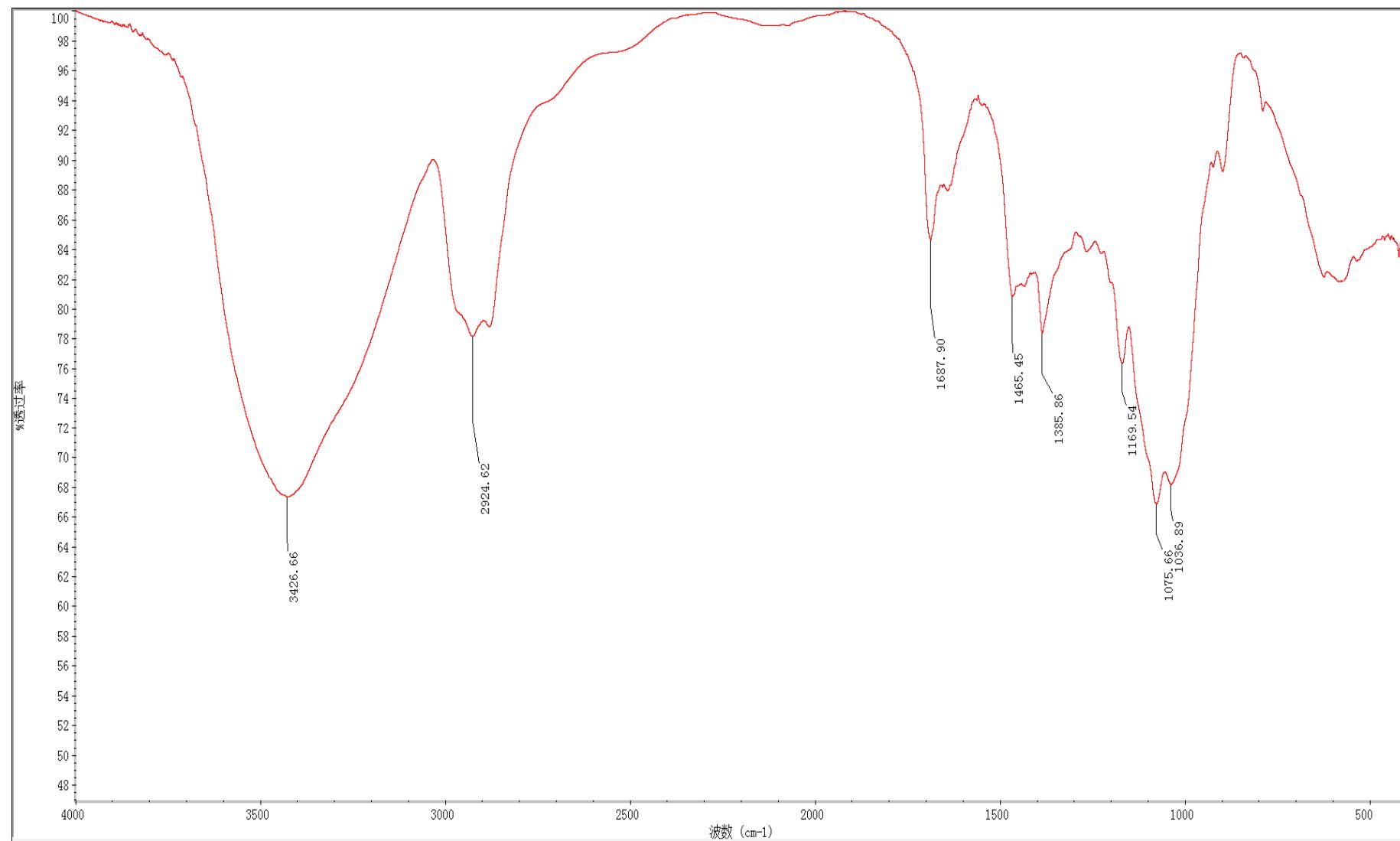


Figure S27. HRESIMS spectrum of 11-oxoisomogroside V (3)

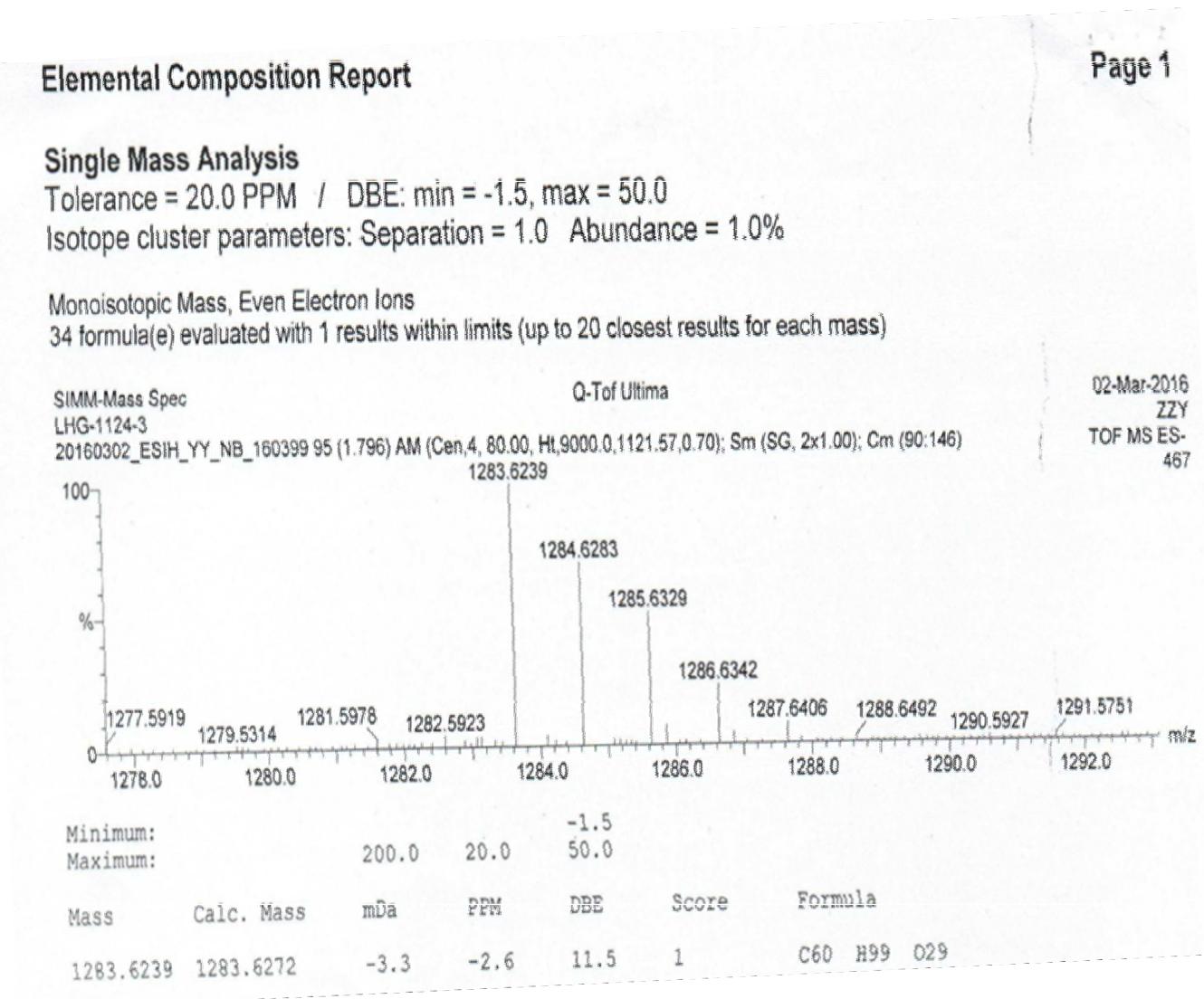


Figure S28. ^1H NMR spectrum of 7-oxomogroside III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

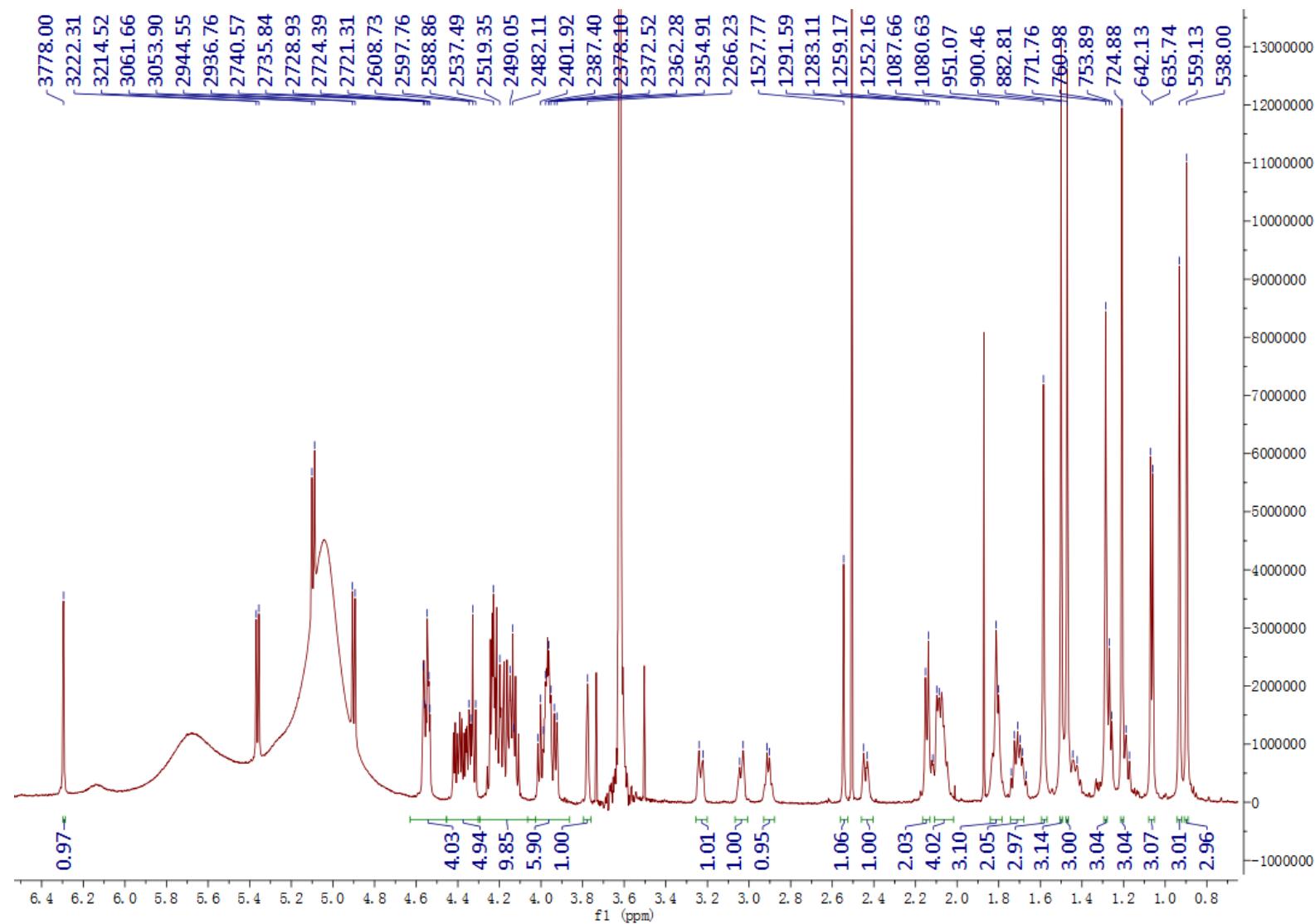


Figure S29. ^{13}C NMR spectrum of 7-oxomogroside III E (**4**) in CsD_5N

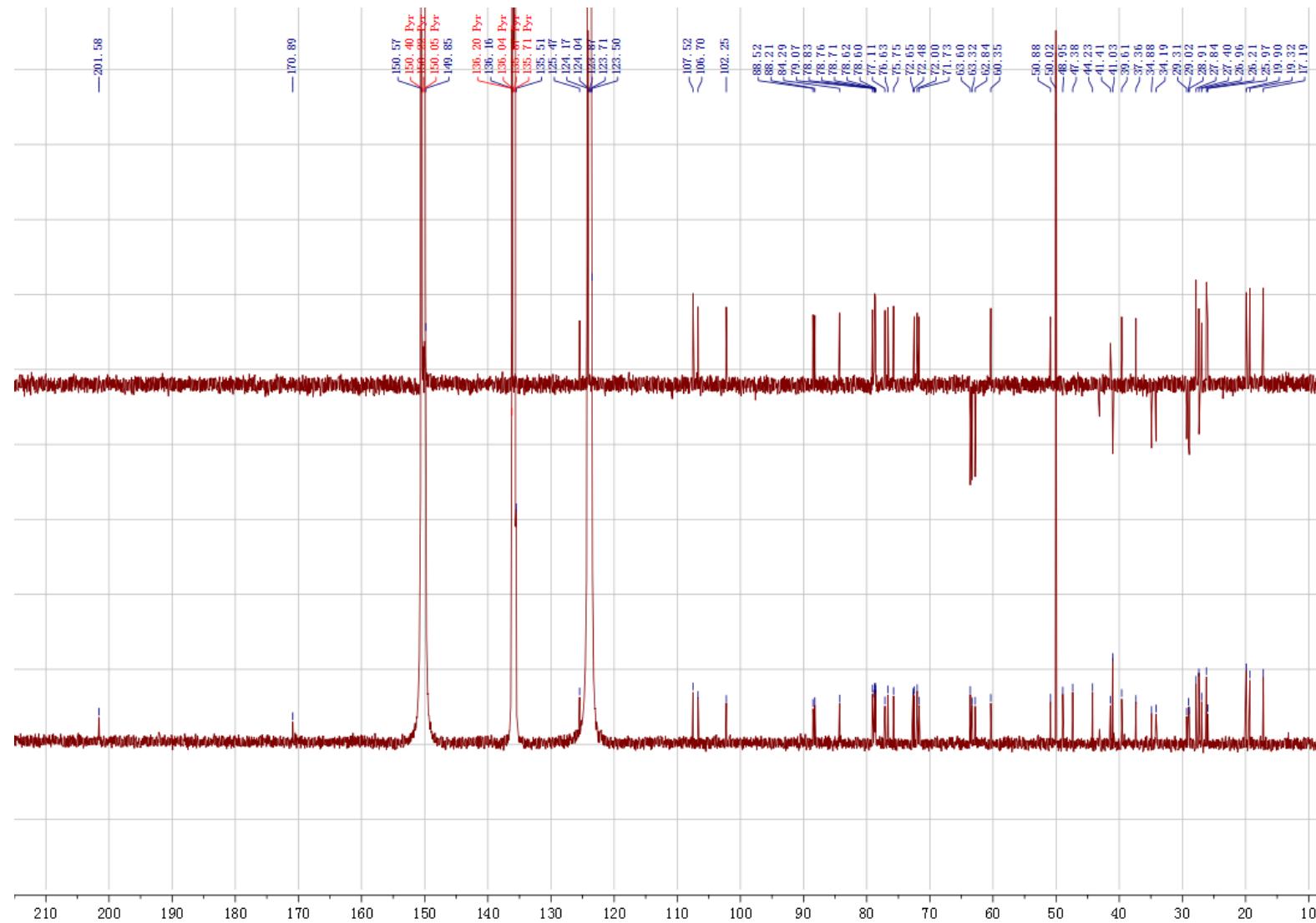


Figure S30. HSQC spectrum of 7-oxomogroside III E (**4**) in C₅D₅N

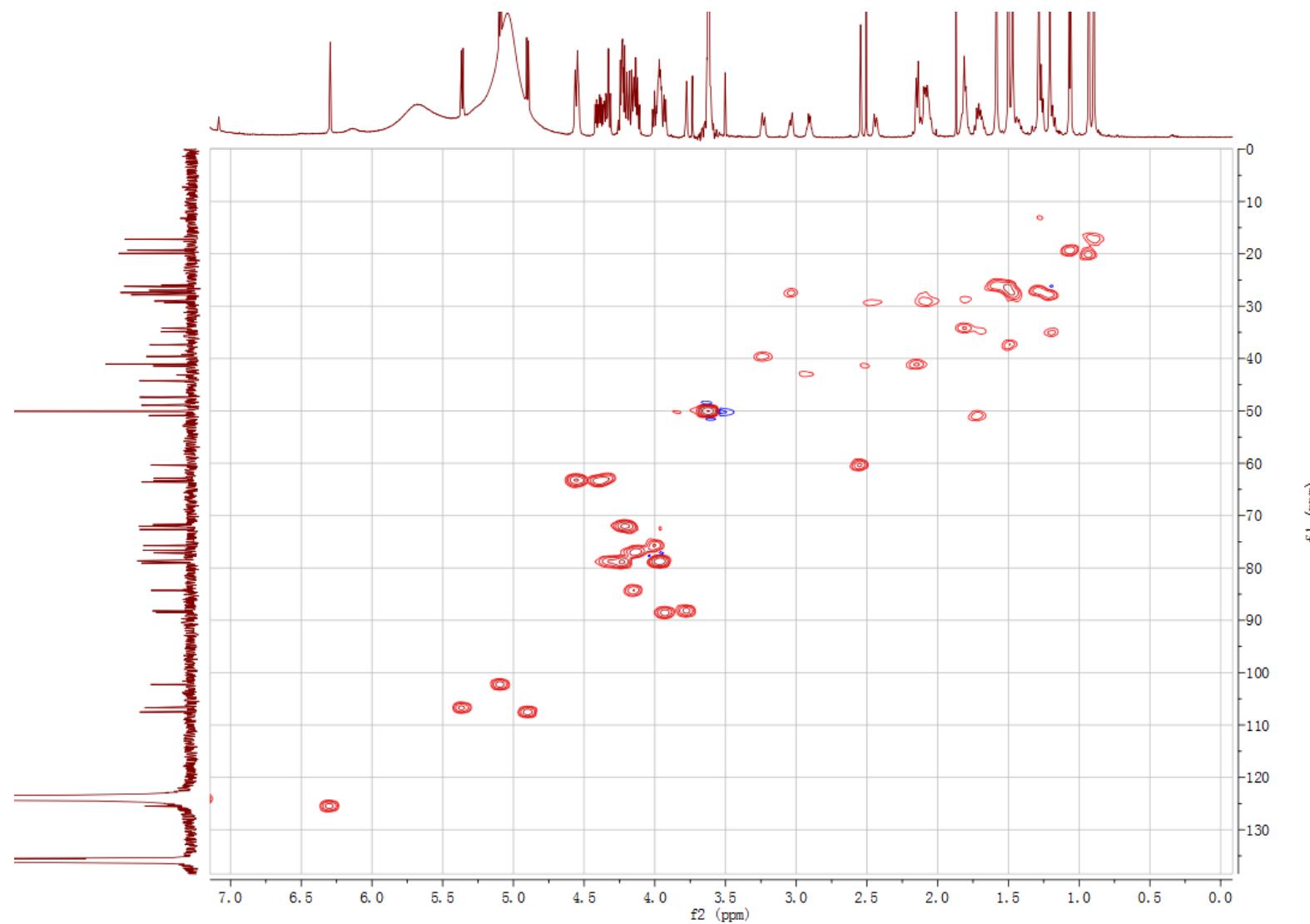


Figure S31. HMBC spectrum of 7-oxomogroside III E (**4**) in C₅D₅N

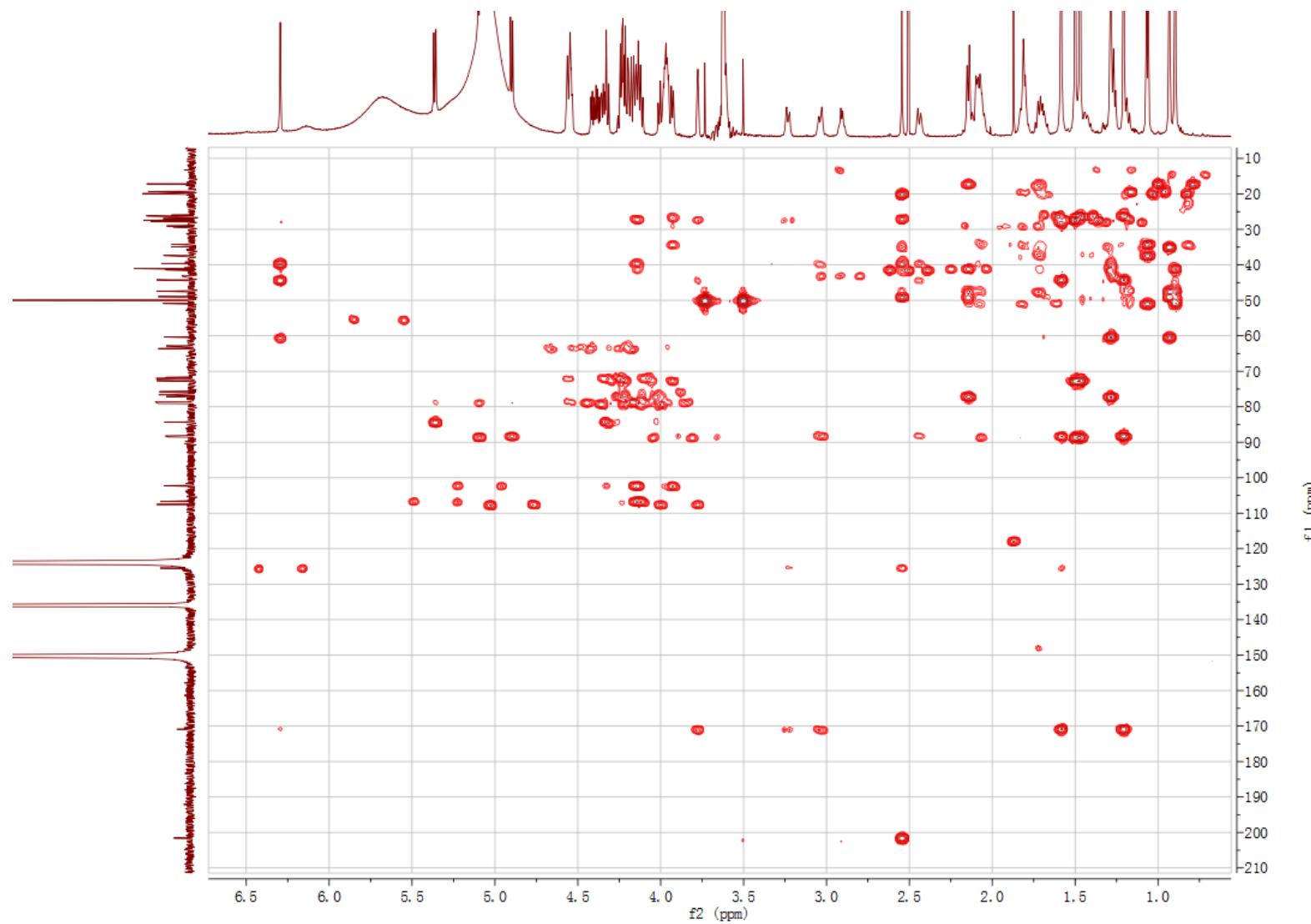


Figure S32. ROESY spectrum of 7-oxomogroside III E (**4**) in C₅D₅N

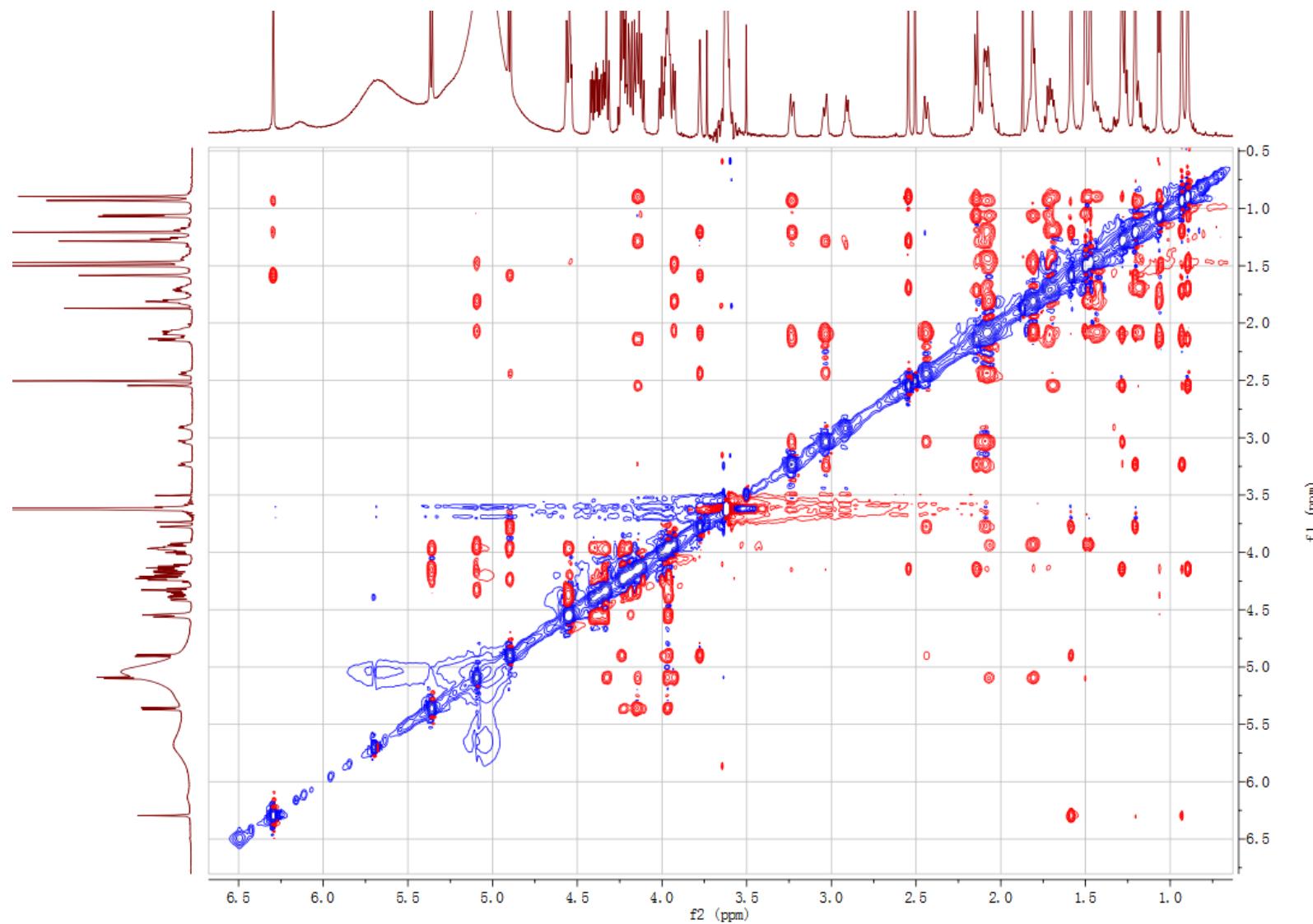


Figure S33. ^1H - ^1H COSY spectrum of 7-oxomogroside III E (**4**) in $\text{C}_5\text{D}_5\text{N}$

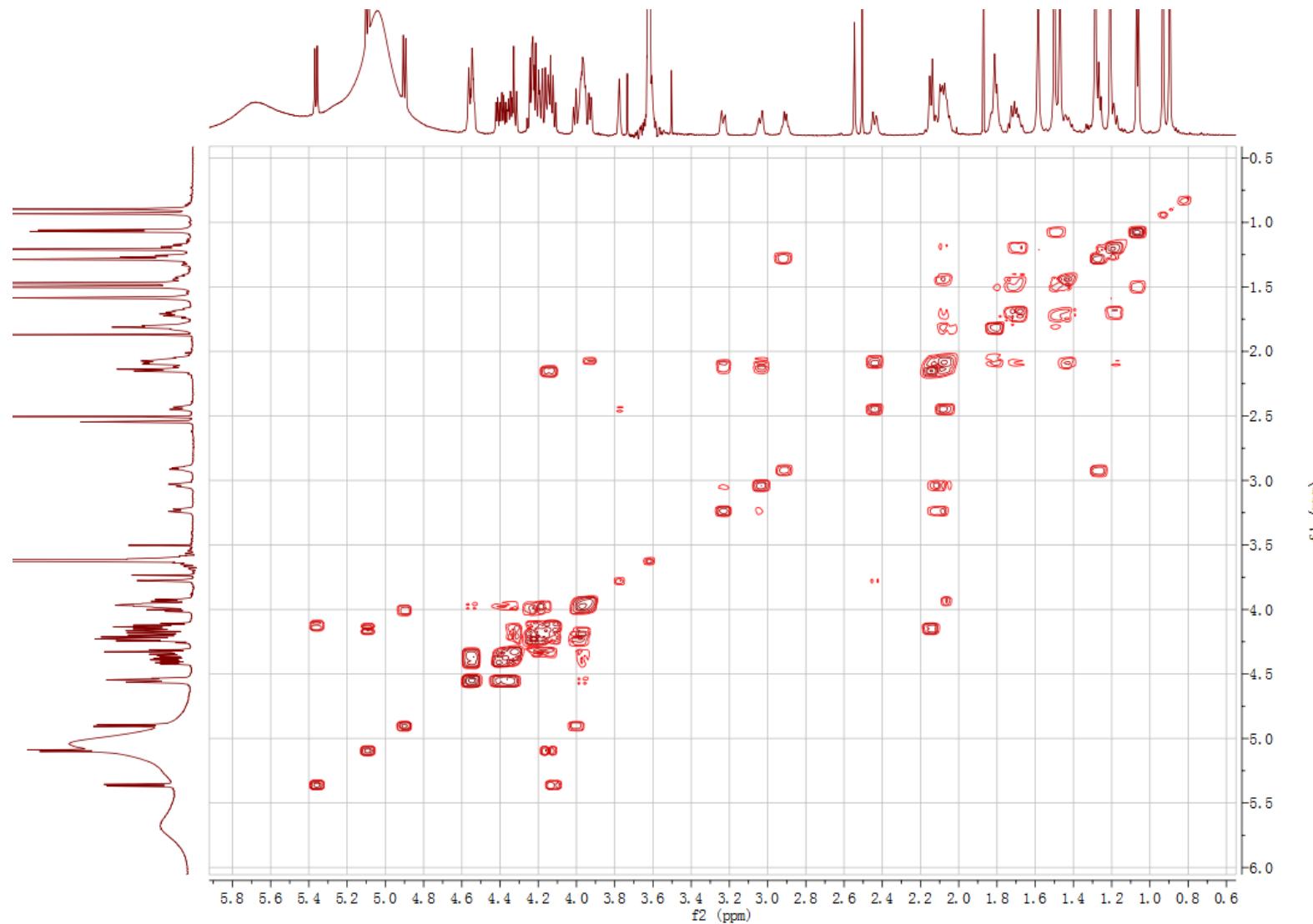


Figure S34. TOCSY spectrum of 7-oxomogrosid III E (**4**) in C₅D₅N

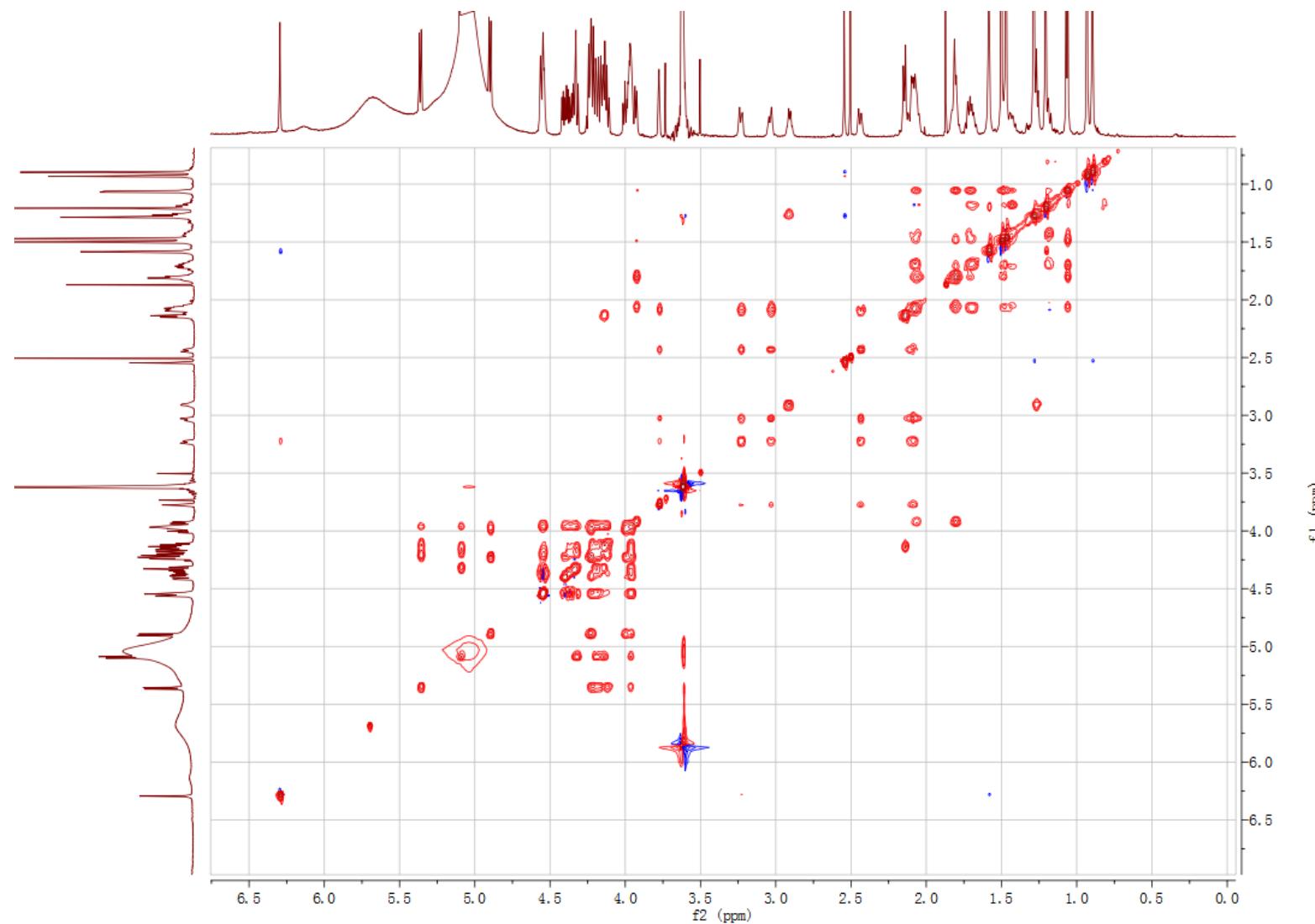


Figure S35. IR spectrum of 7-oxomogroside III E (4)

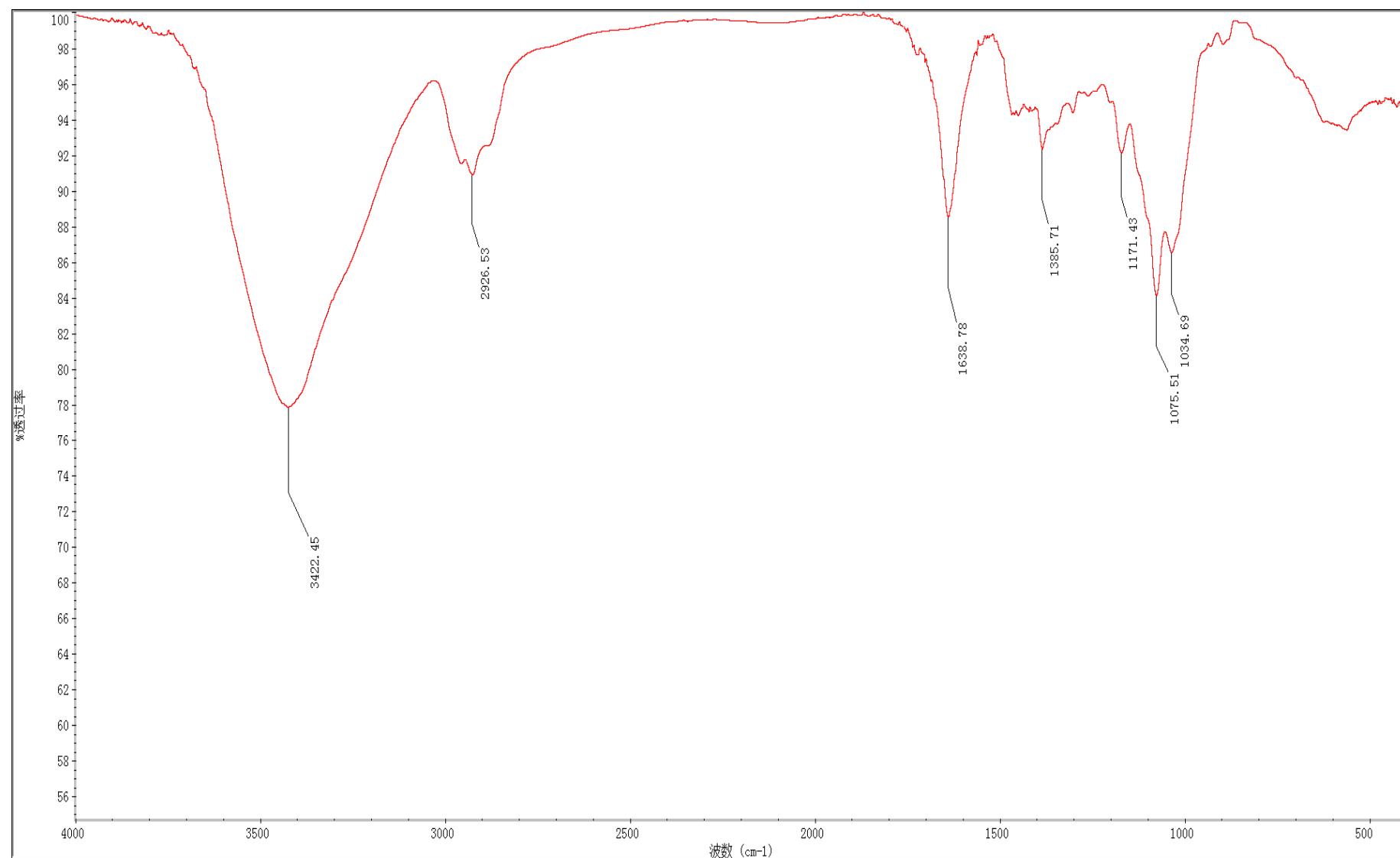


Figure S36. HRESIMS spectrum of 7-oxomogroside III E (**4**)

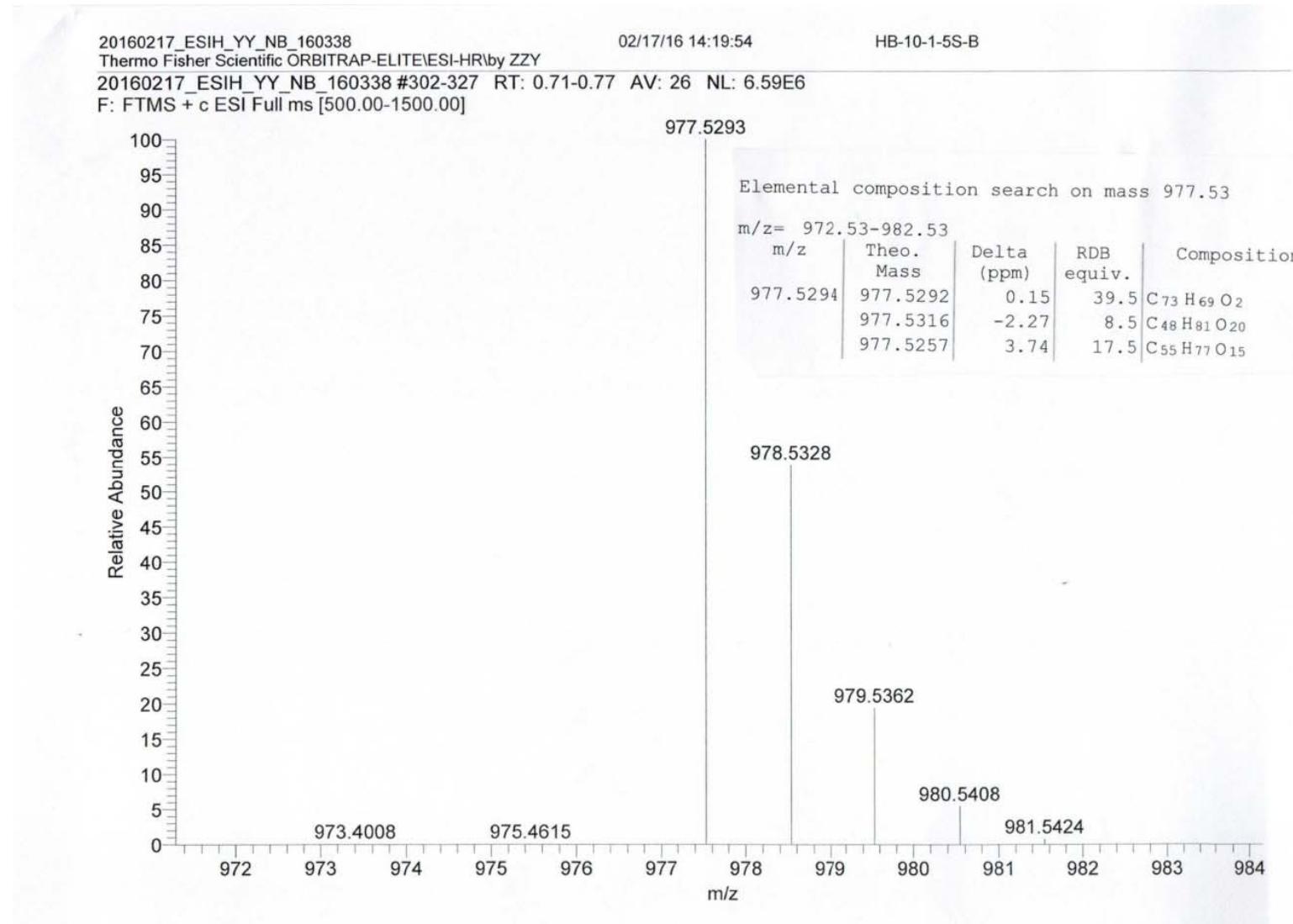


Figure S37. ^1H NMR spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

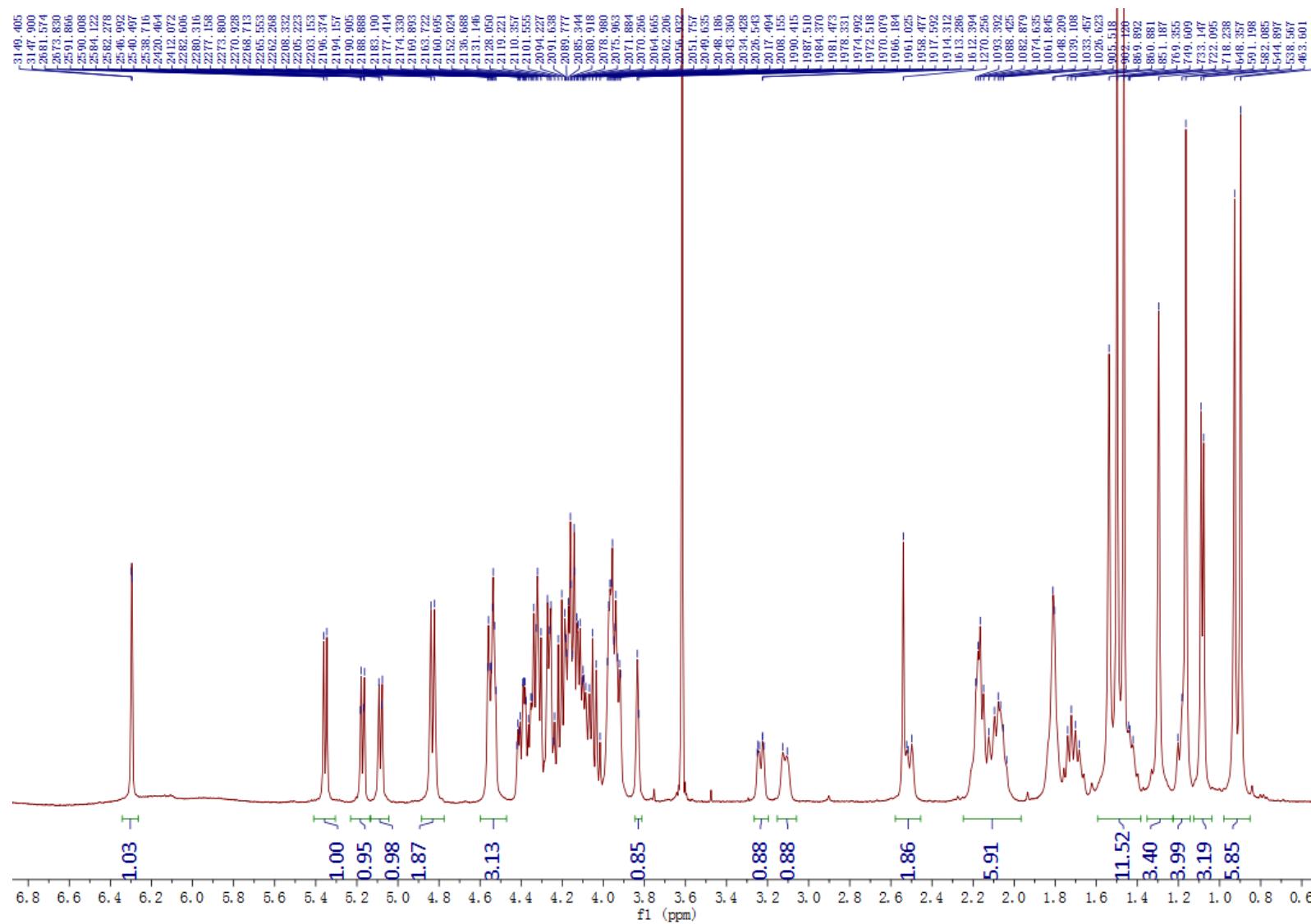


Figure S38. ^{13}C NMR spectrum of 7-oxomogroside IV (**5**) in $\text{C}_5\text{D}_5\text{N}$

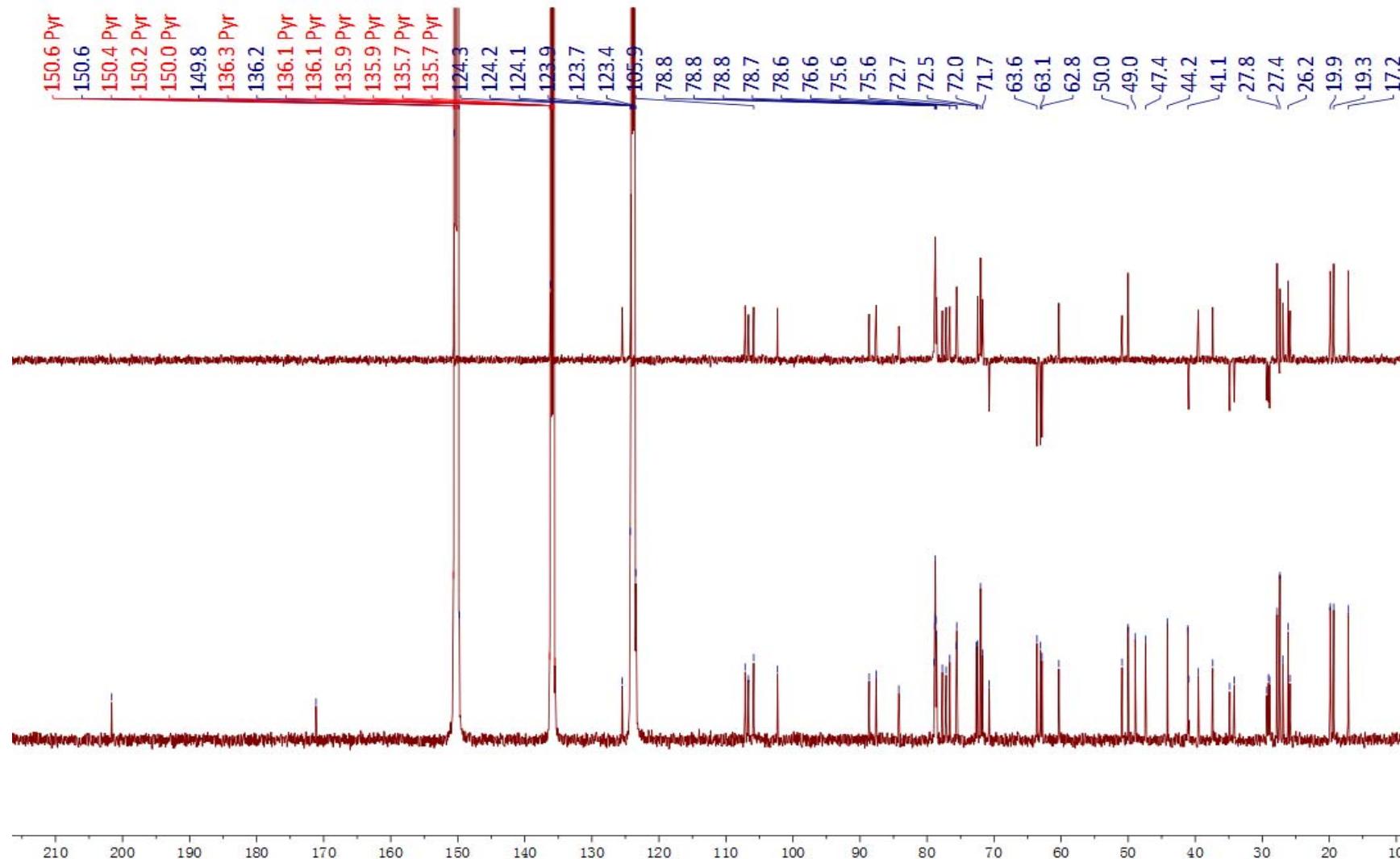


Figure S39. HSQC spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

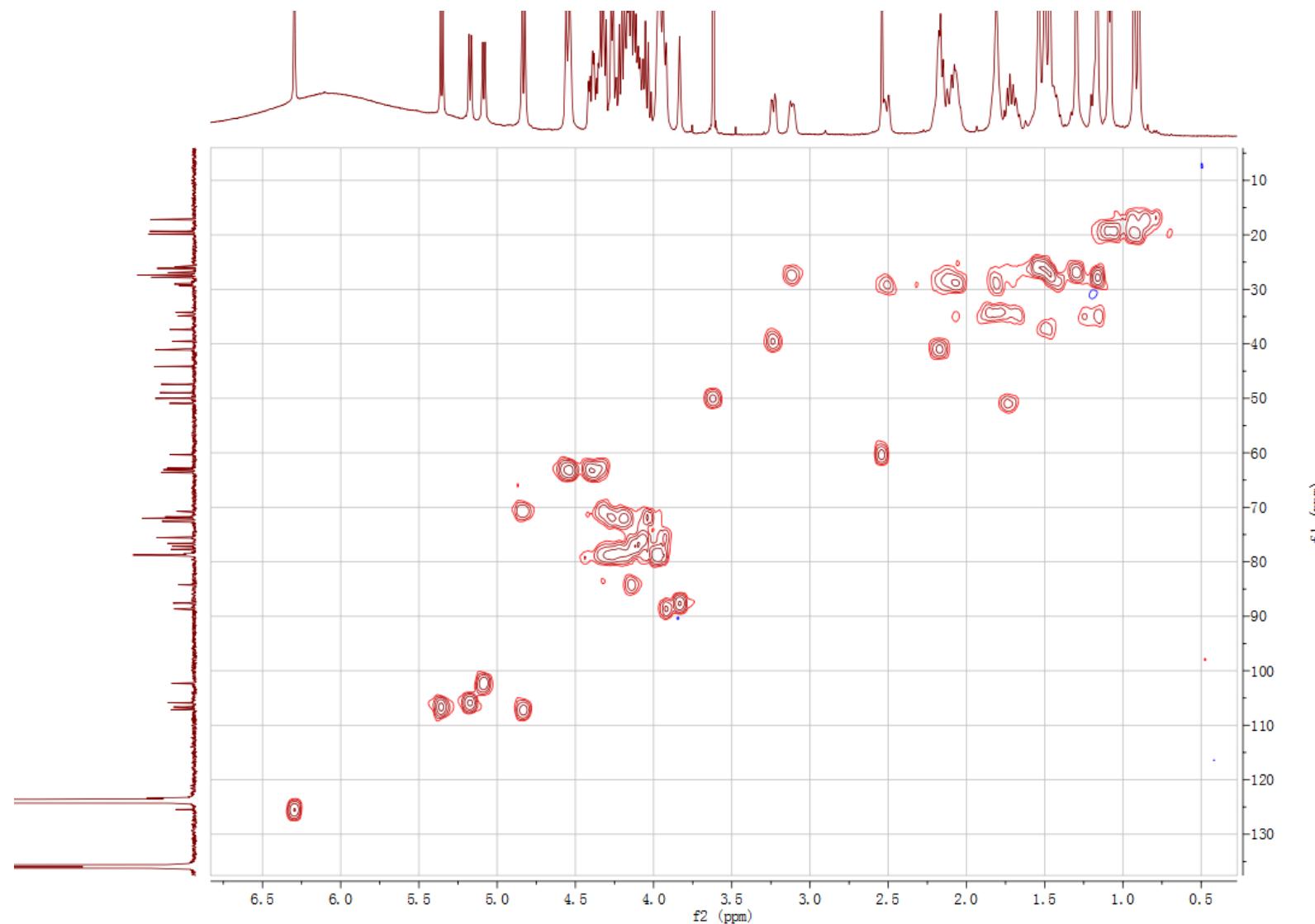


Figure S40. HMBC spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

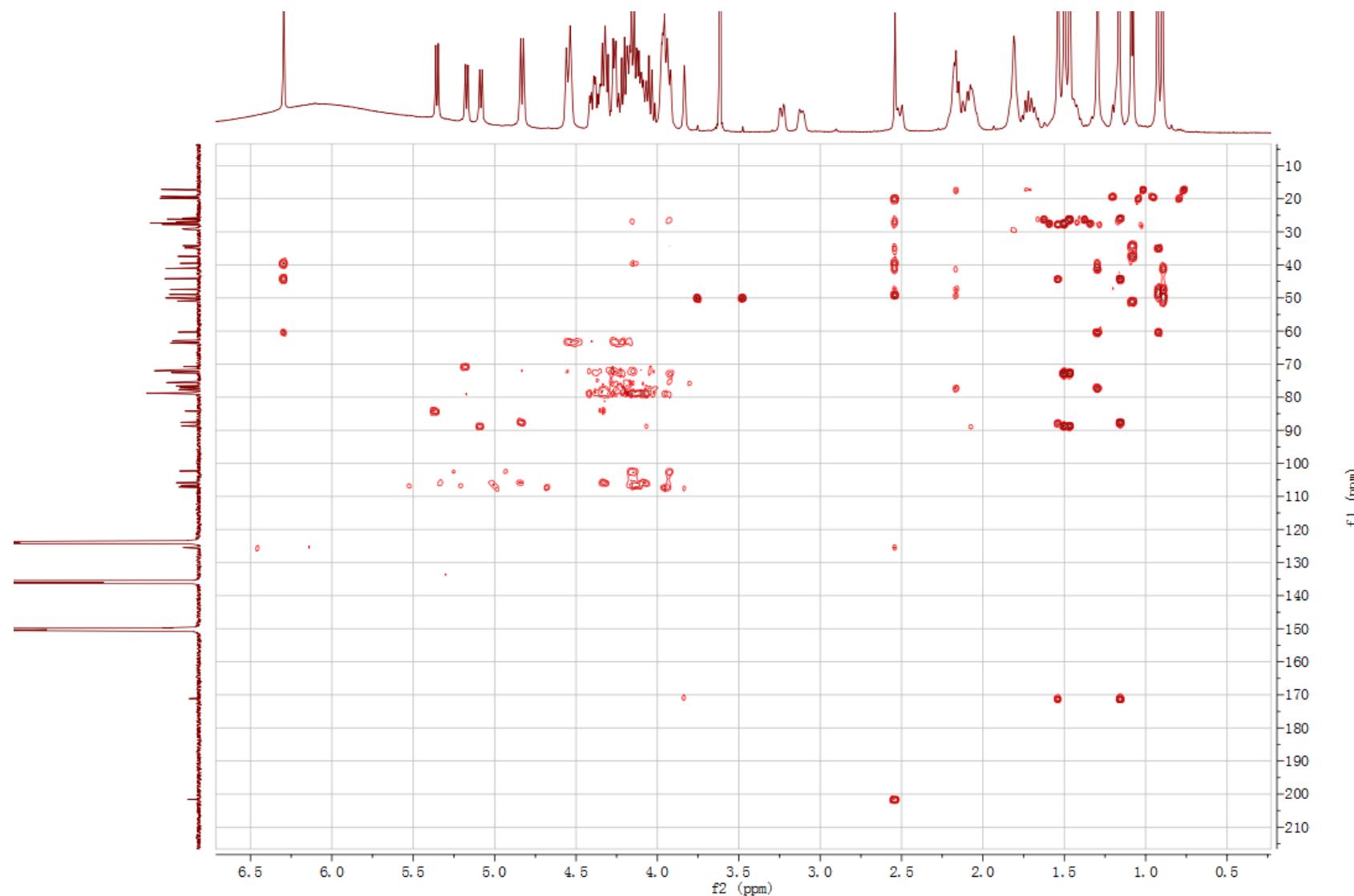


Figure S41. ROESY spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

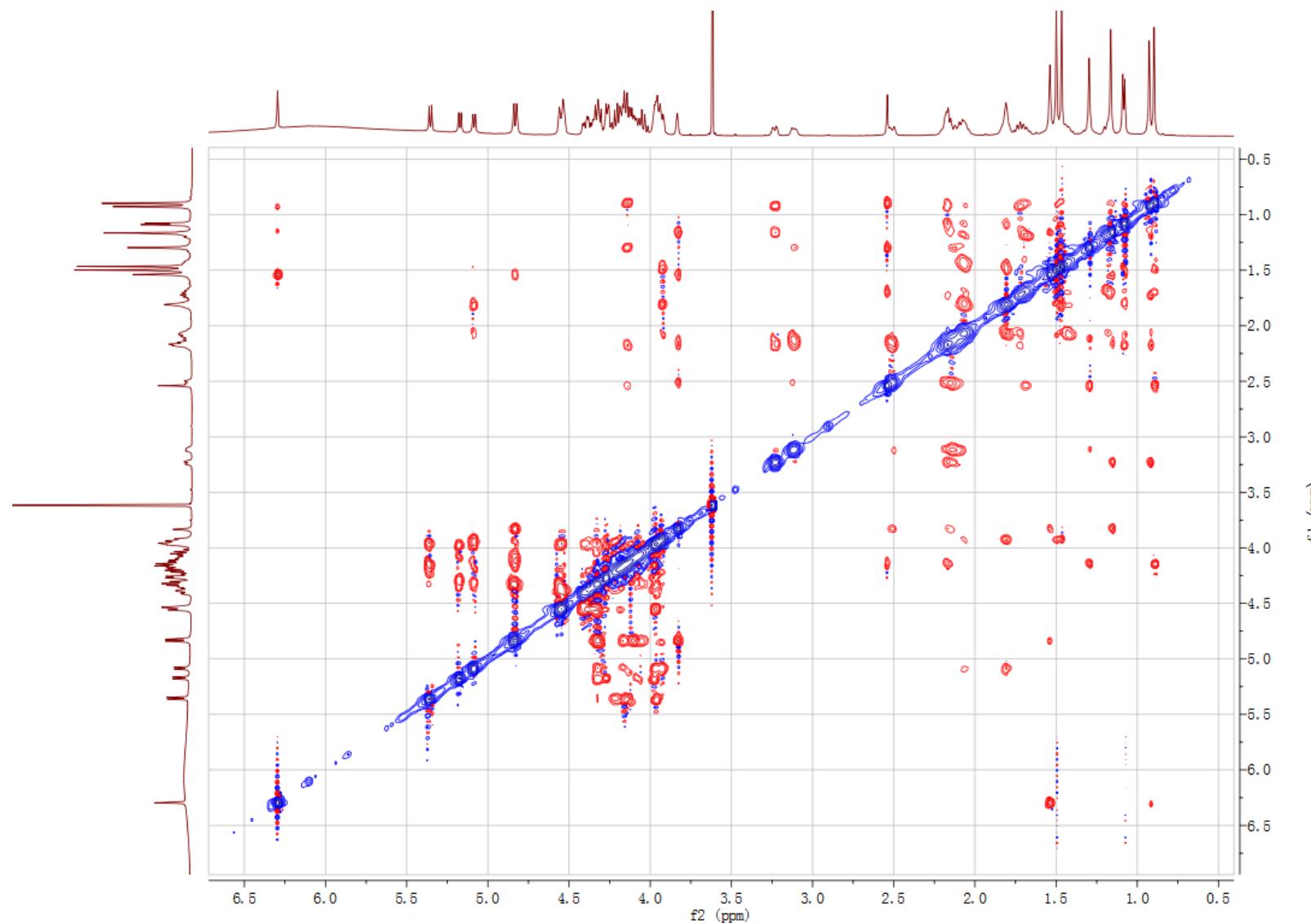


Figure S42. ^1H - ^1H COSY spectrum of 7-oxomogroside IV (**5**) in C₅D₅N

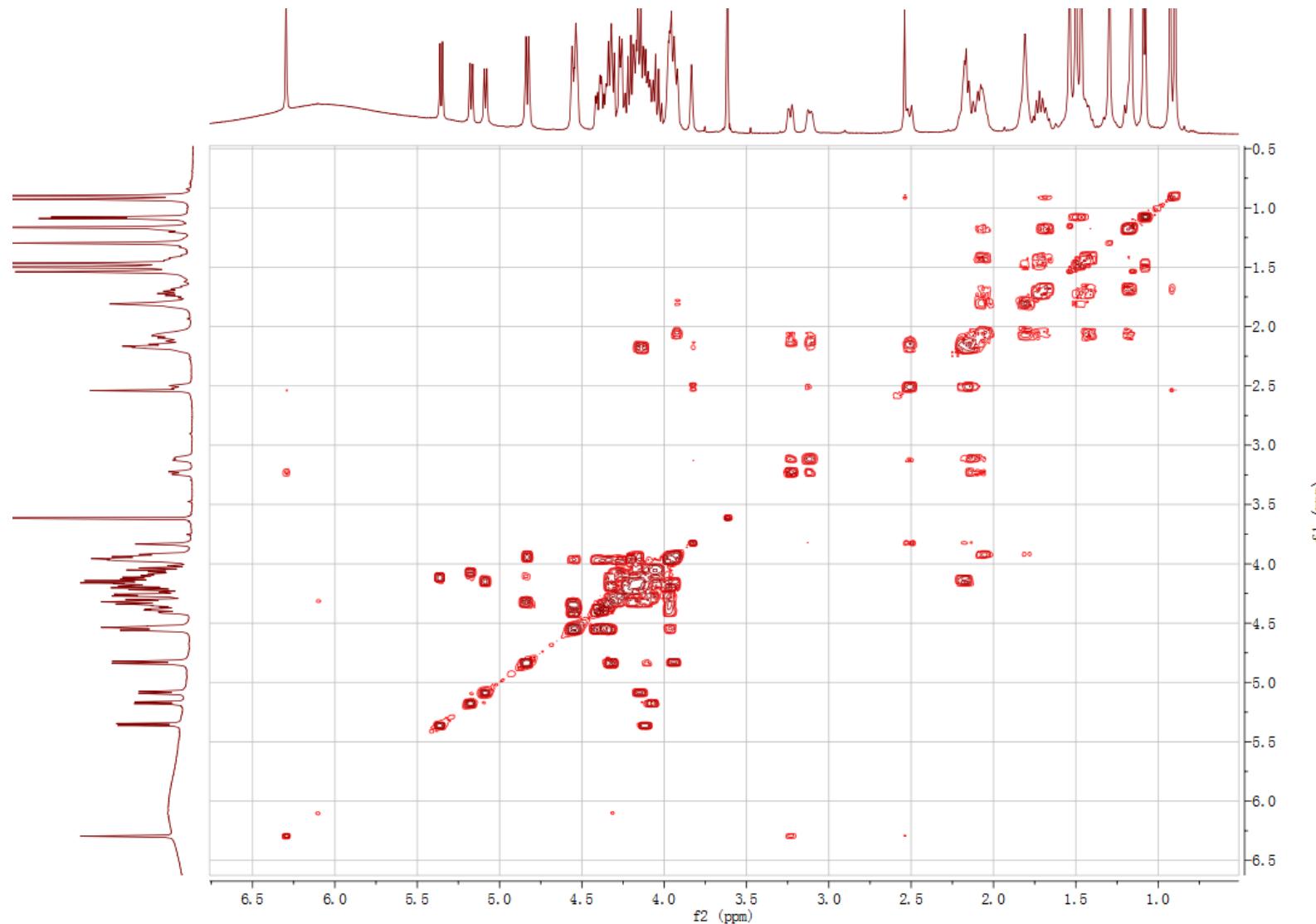


Figure S43. TOCSY spectrum of 7-oxomogroside IV (**5**) in C₅D₅N



Figure S44. IR spectrum of 7-oxomogroside IV (**5**)

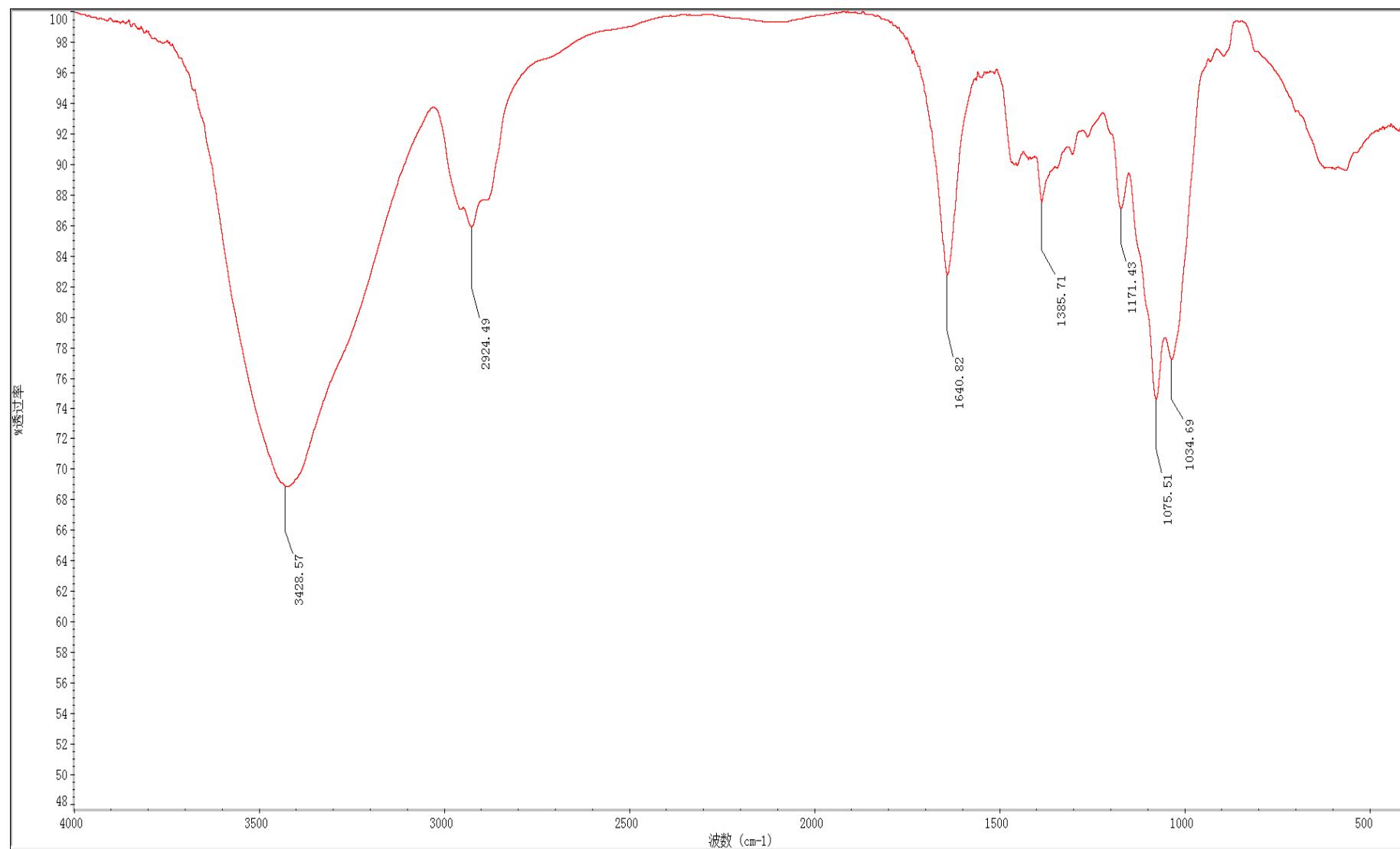


Figure S45. HRESIMS spectrum of 7-oxomogroside IV (**5**)

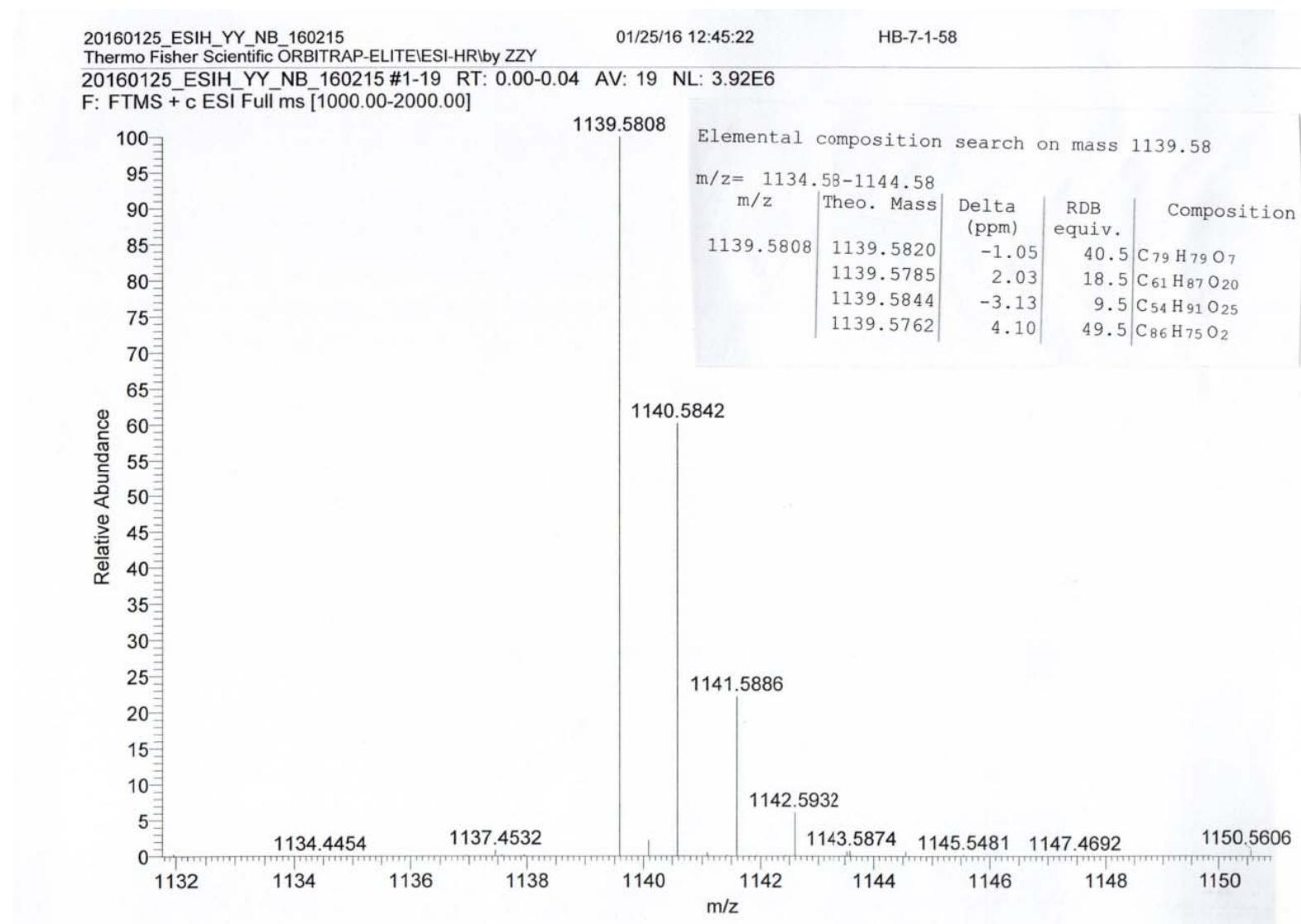


Figure S46. ^1H NMR spectrum of Mogroside VI A (**6**) in $\text{C}_5\text{D}_5\text{N}$

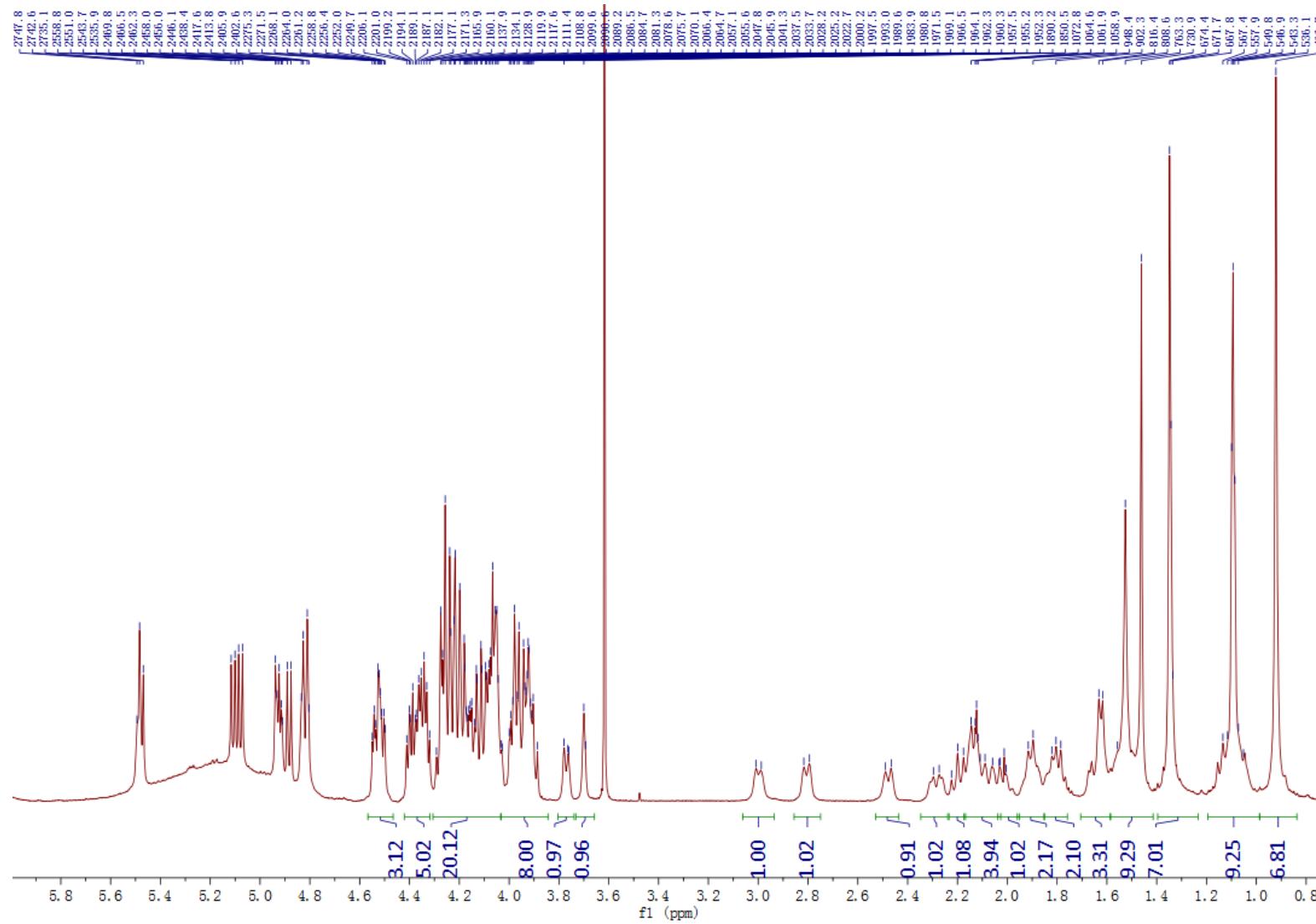
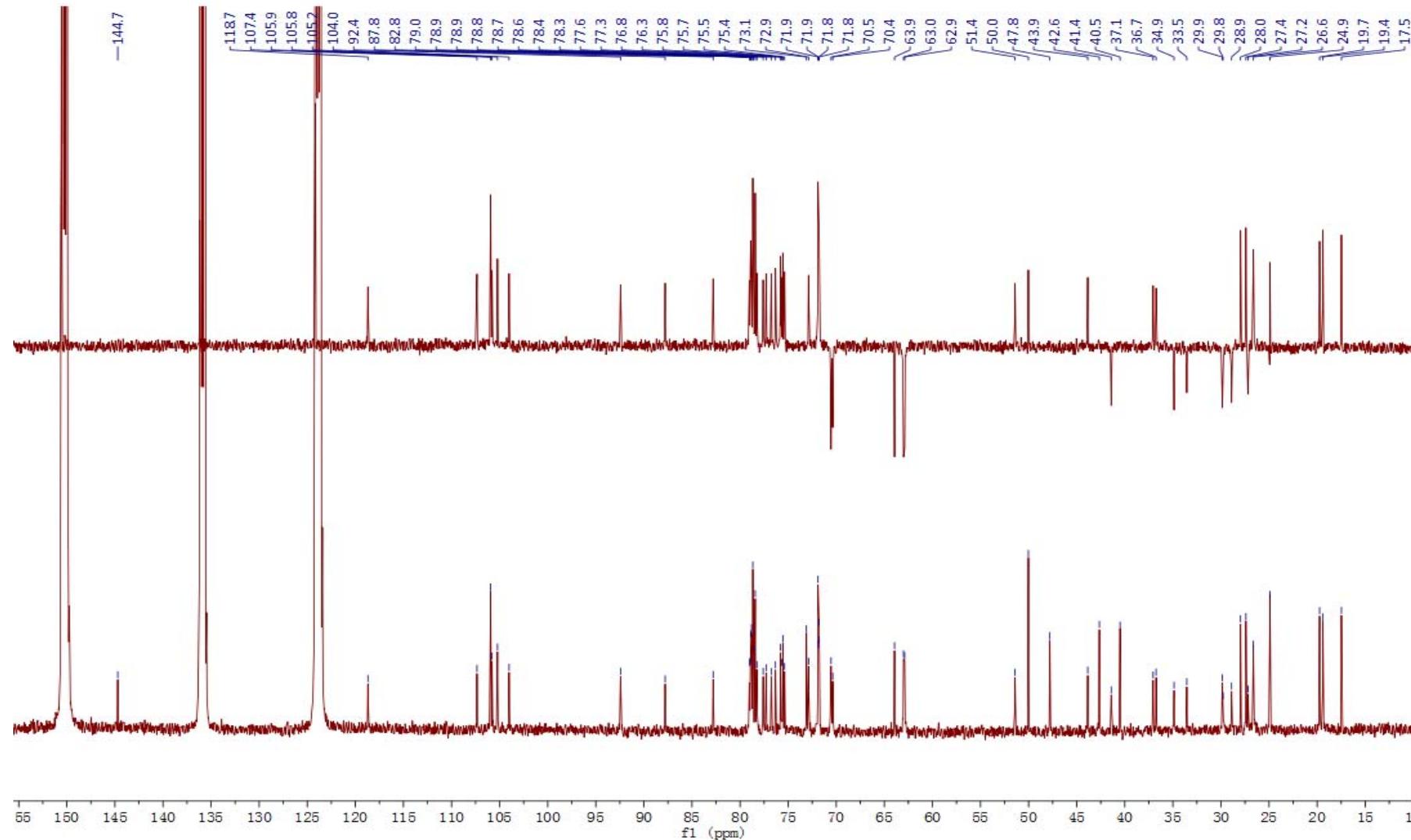
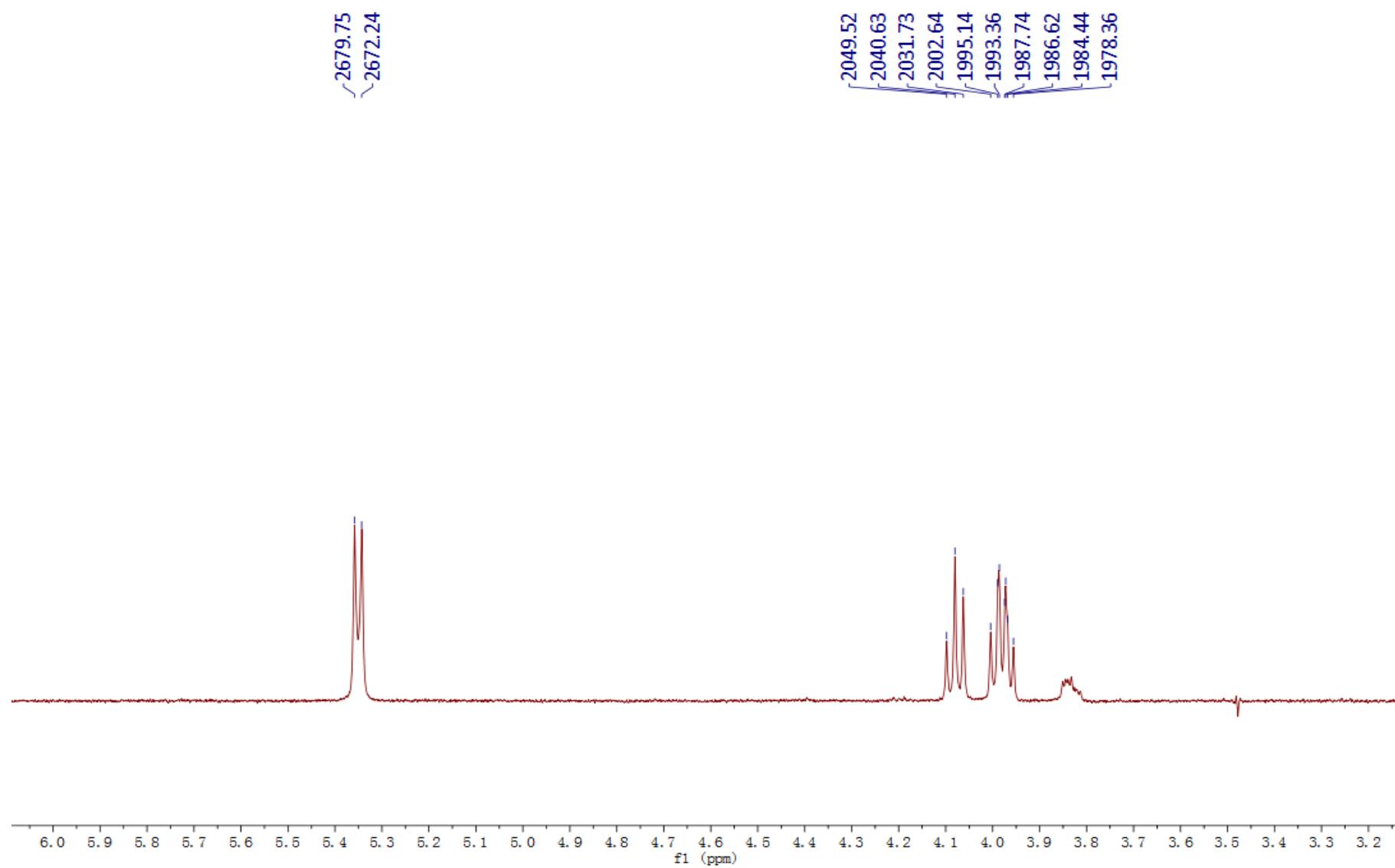
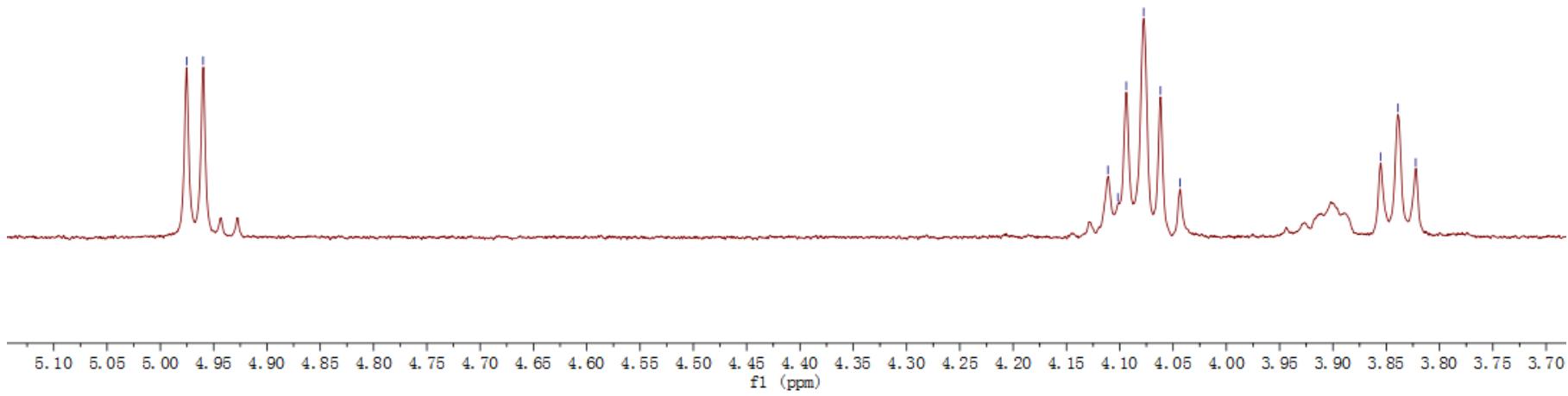


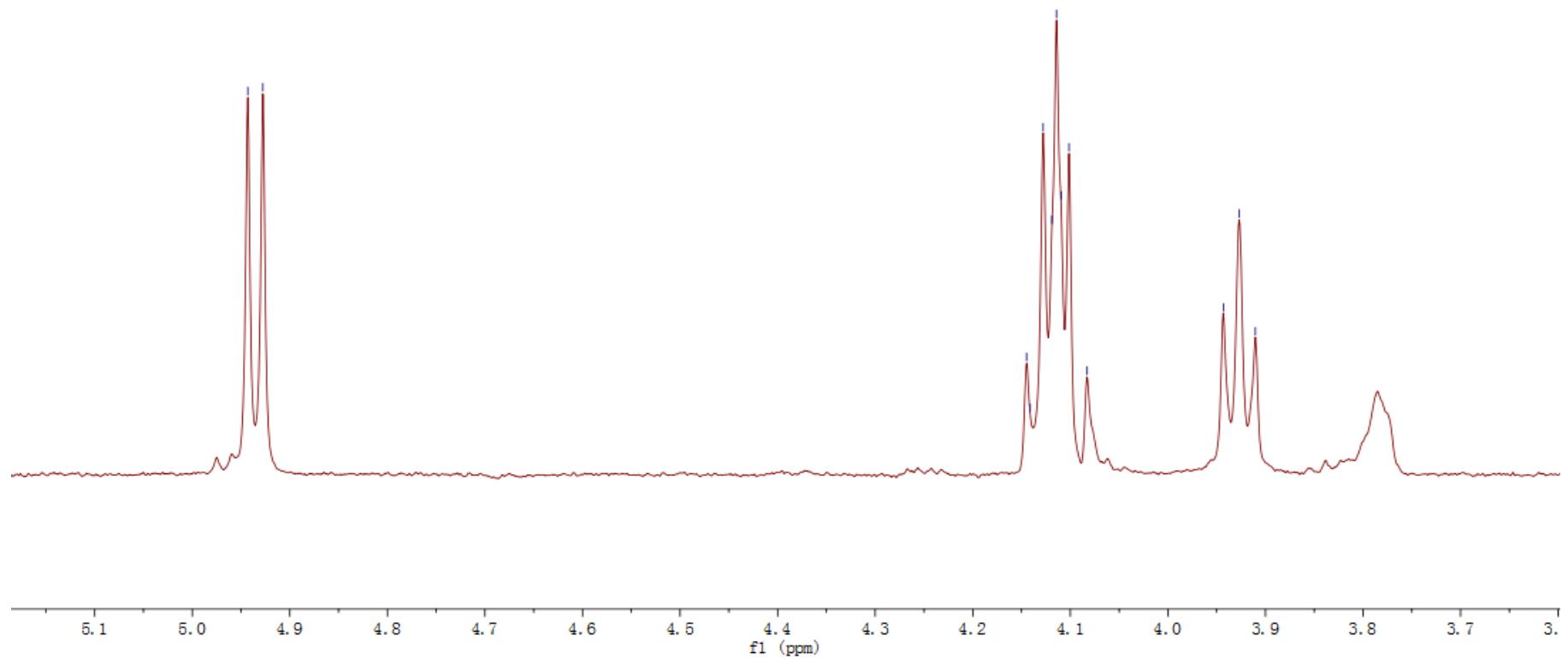
Figure S47. ^{13}C NMR spectrum of Mogroside VI A (**6**) in $\text{C}_5\text{D}_5\text{N}$

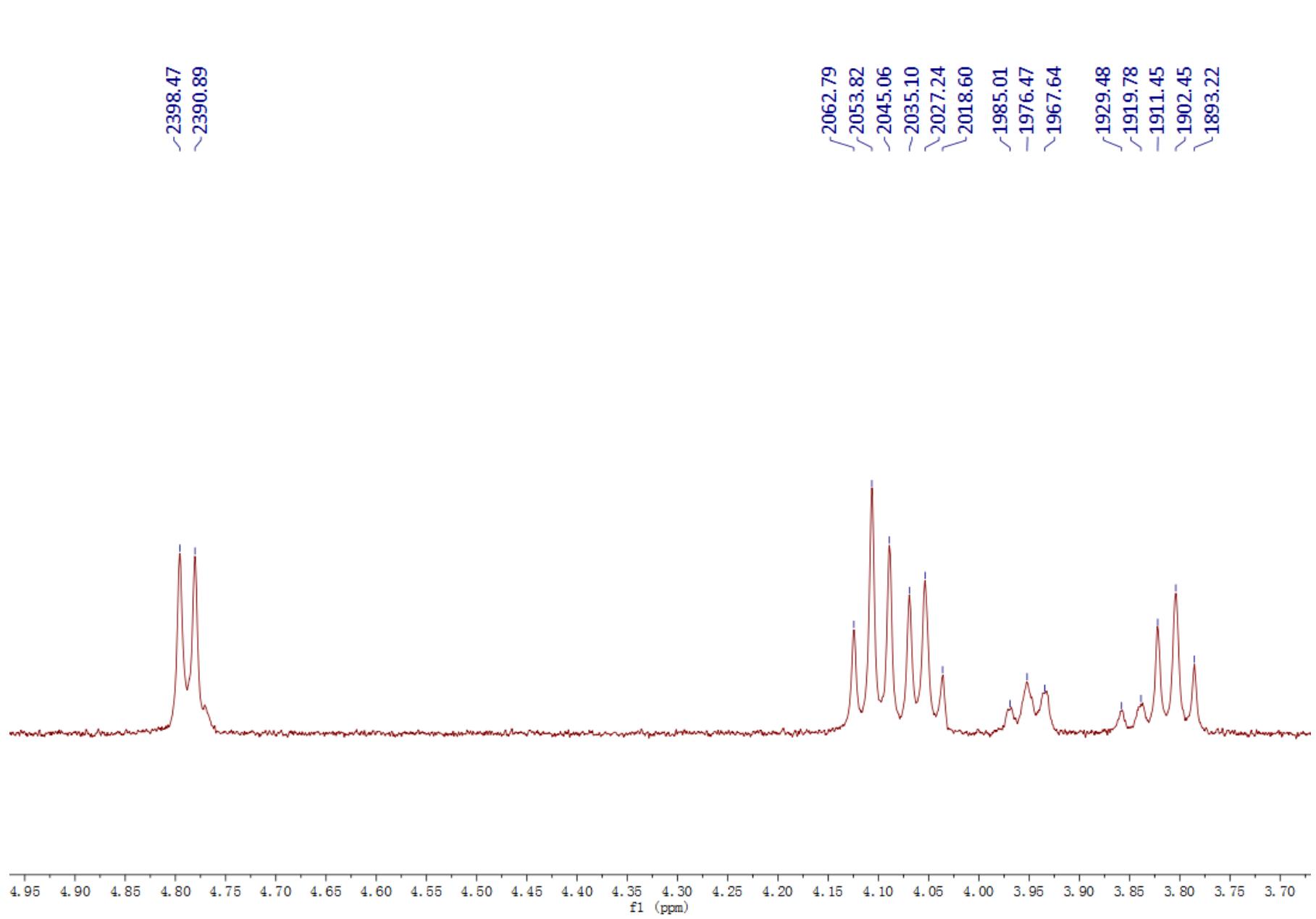


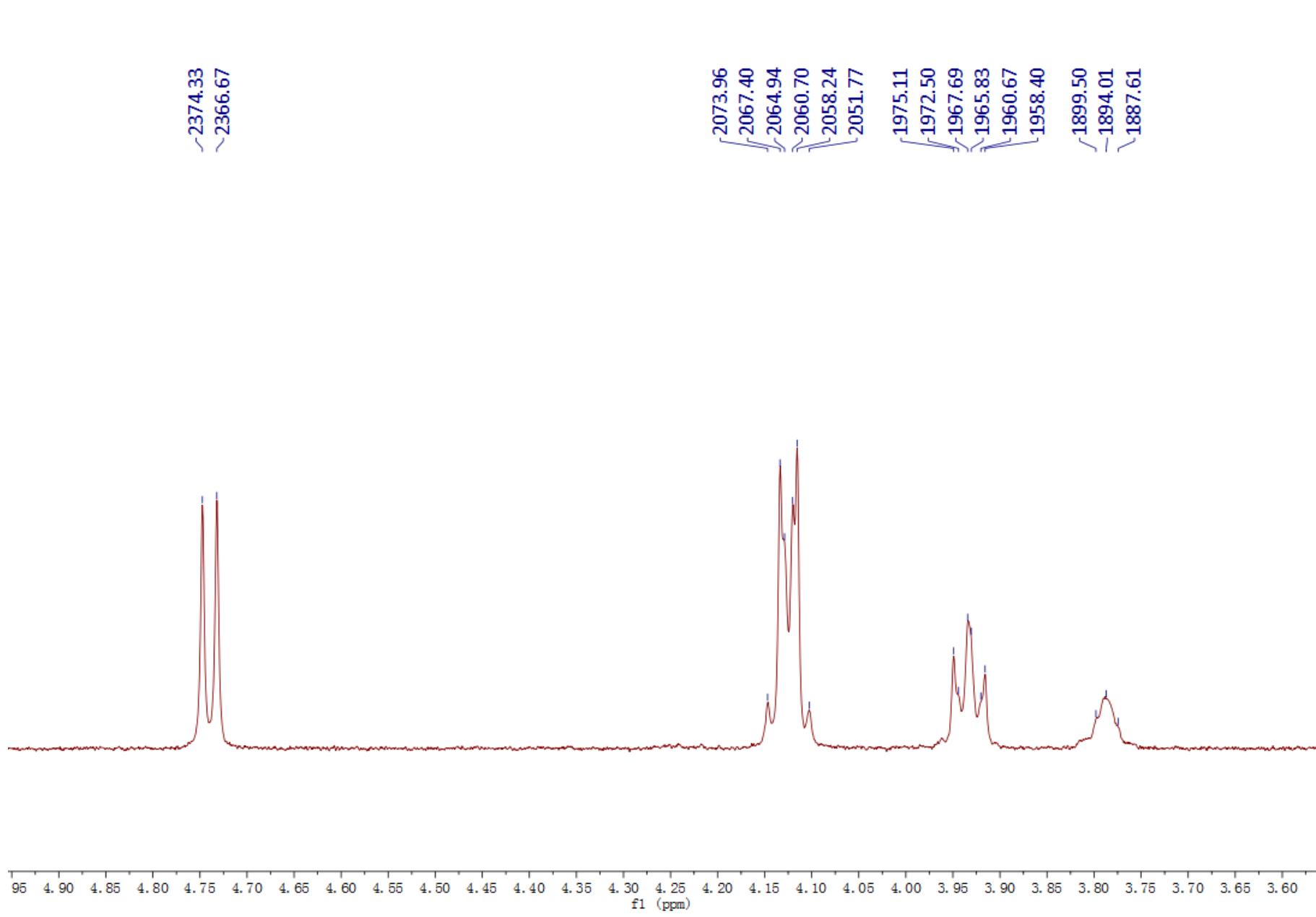
Figures S48. 1D TOCSY spectrum of Mogroside VI A (**6**) in C₅D₅N











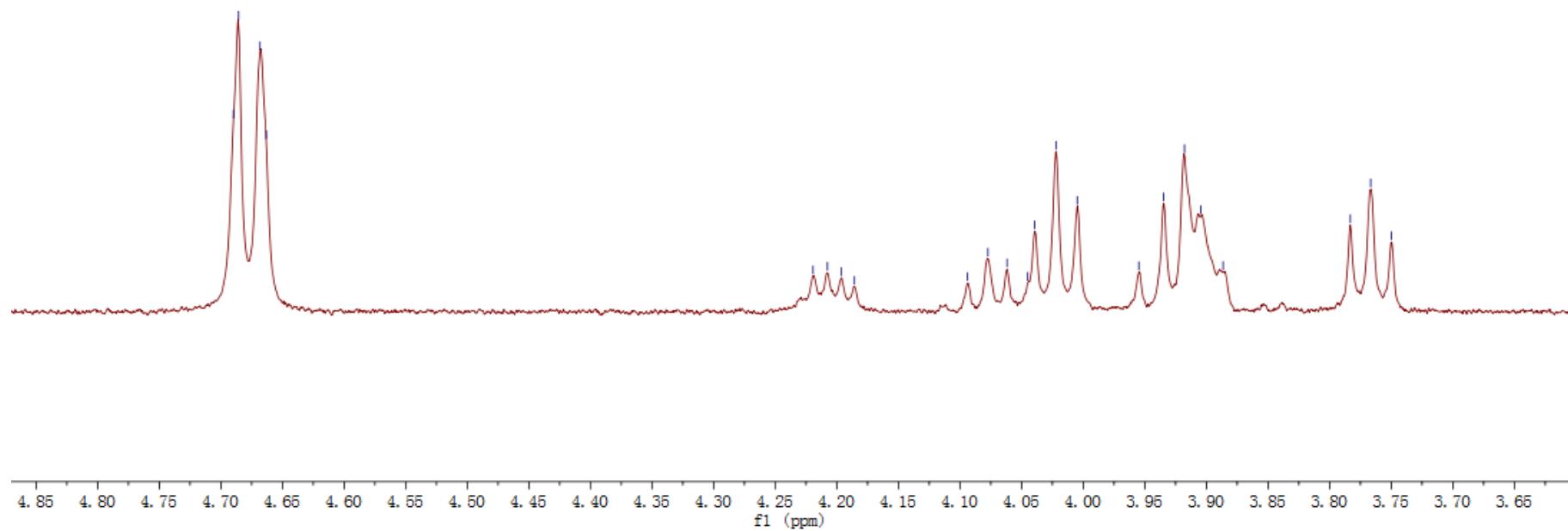


Figure S49. Selective HSQC (C15-55) spectrum of Mogroside VI A (**6**) in C₅D₅N

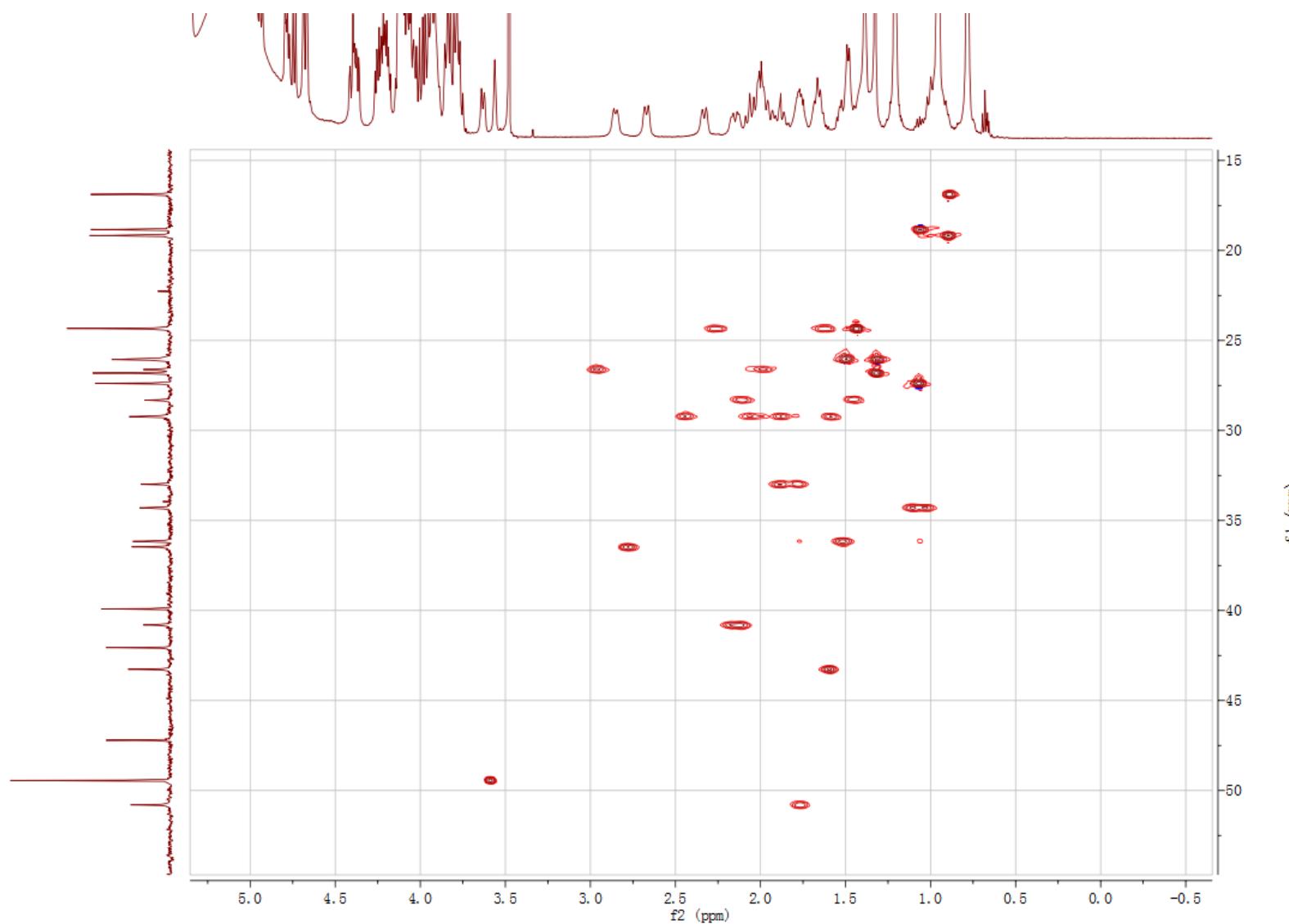


Figure S50. Selective HSQC (C60-95) spectrum of Mogroside VI A (**6**) in C₅D₅N

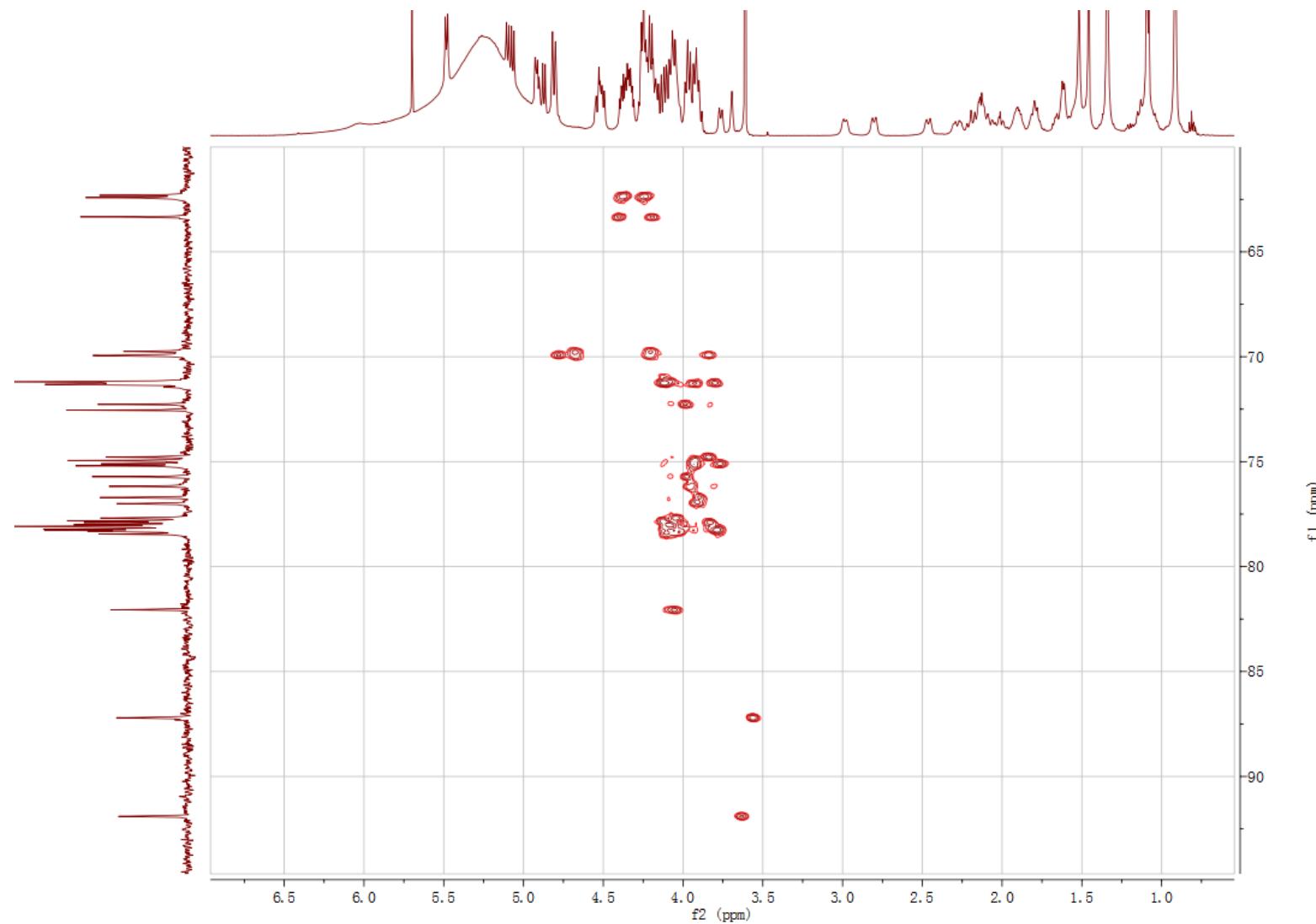


Figure S51. Selective HSQC (C100-108) spectrum of Mogroside VI A (**6**) in C₅D₅N

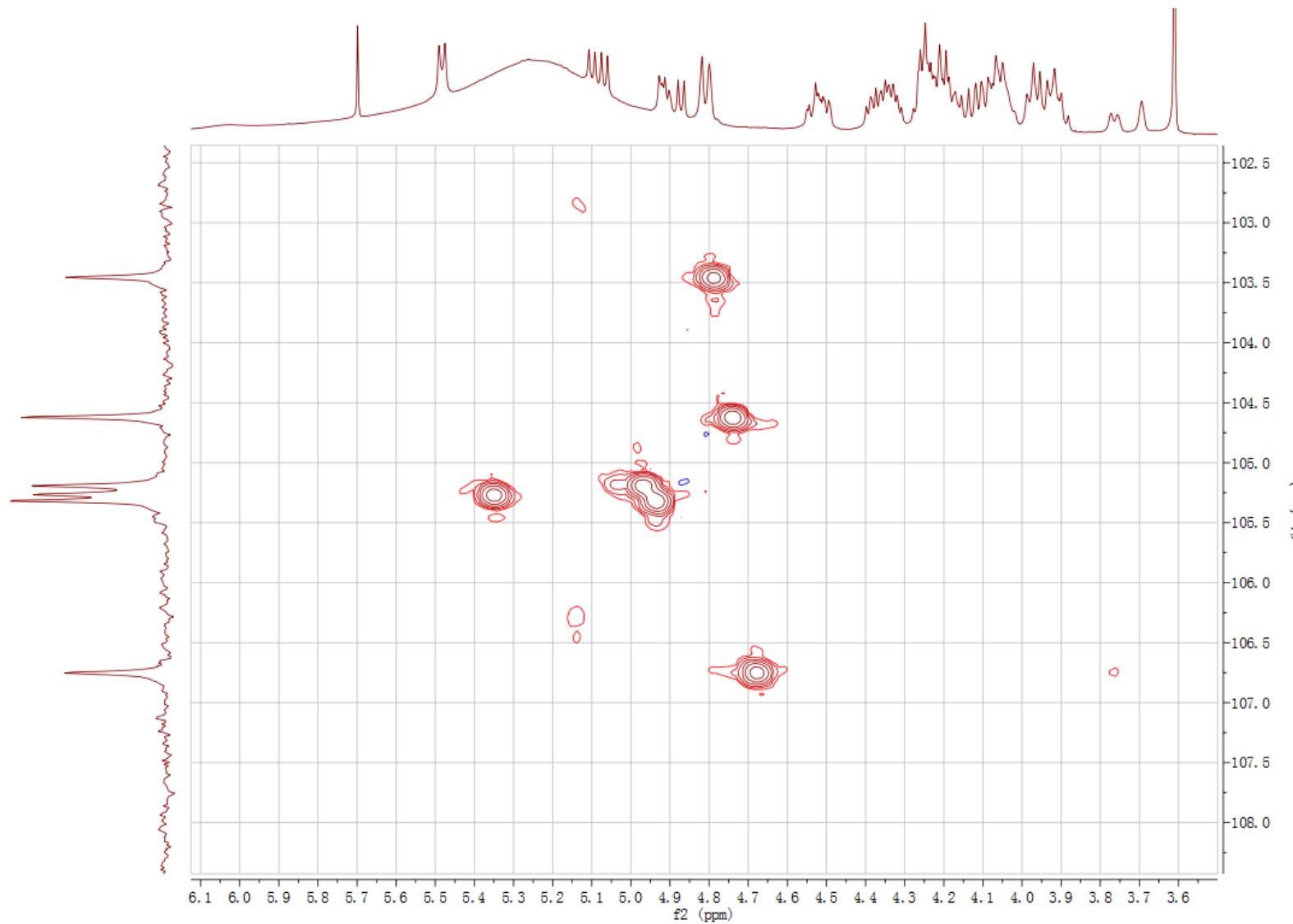


Figure S52. Selective HMBC (C15-45) spectrum of Mogroside VI A (**6**) in C₅D₅N

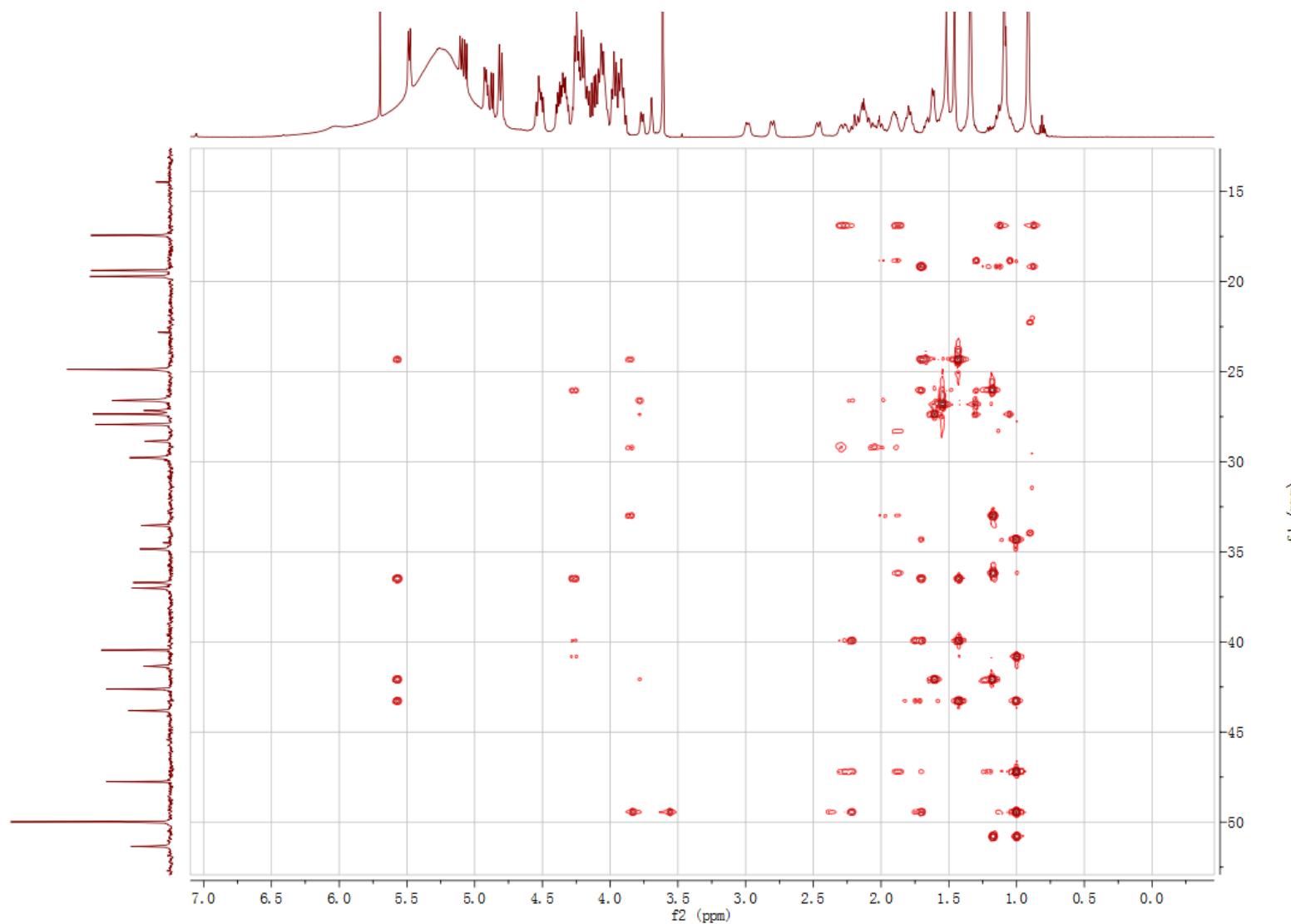


Figure S53. Selective HMBC (C60-95) spectrum of Mogroside VI A (**6**) in C₅D₅N

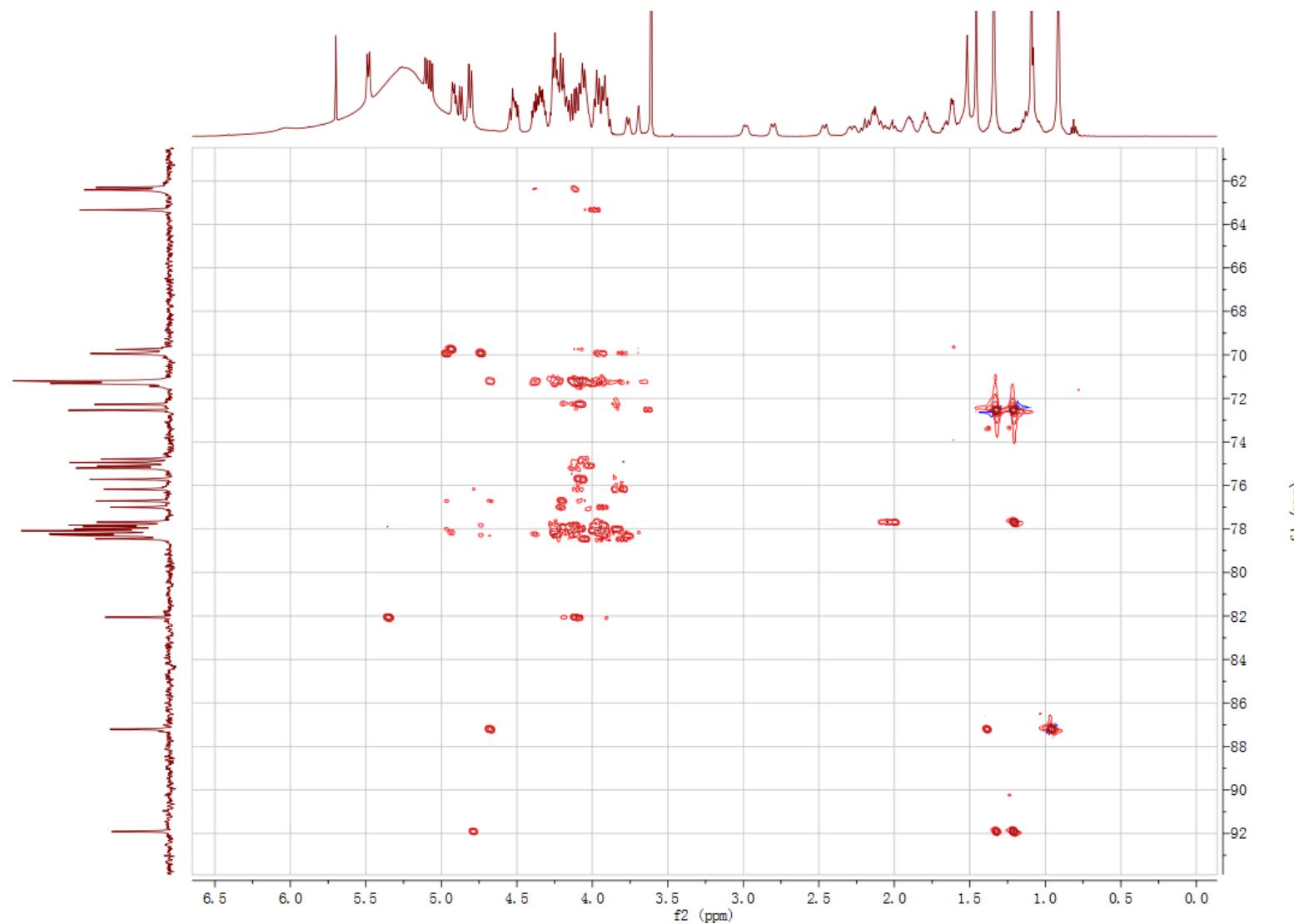


Figure S54. Selective HMBC (C100-108) spectrum of Mogroside VI A (**6**) in C₅D₅N

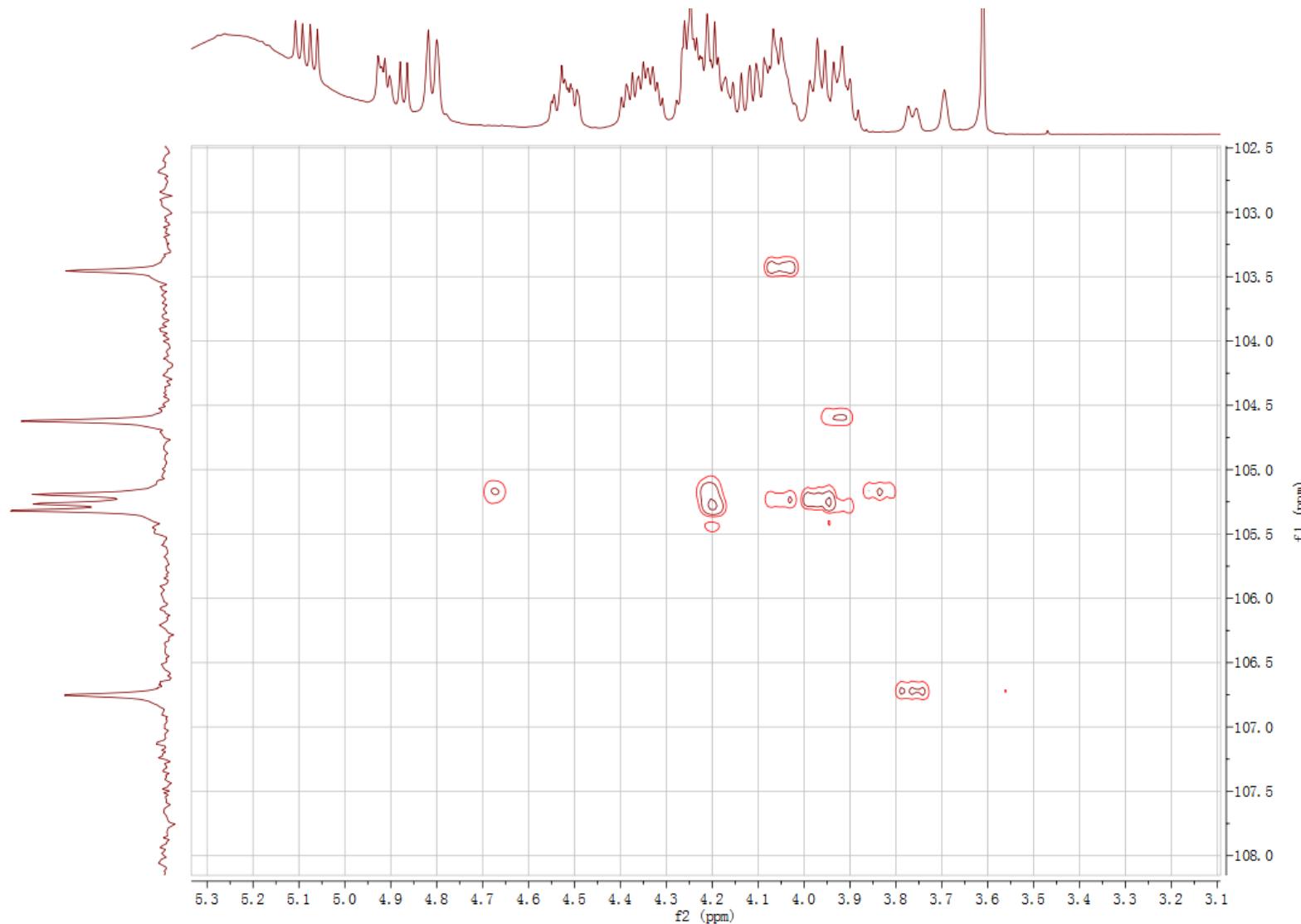


Figure S55. COSY spectrum of Mogroside VI A (**6**) in C₅D₅N

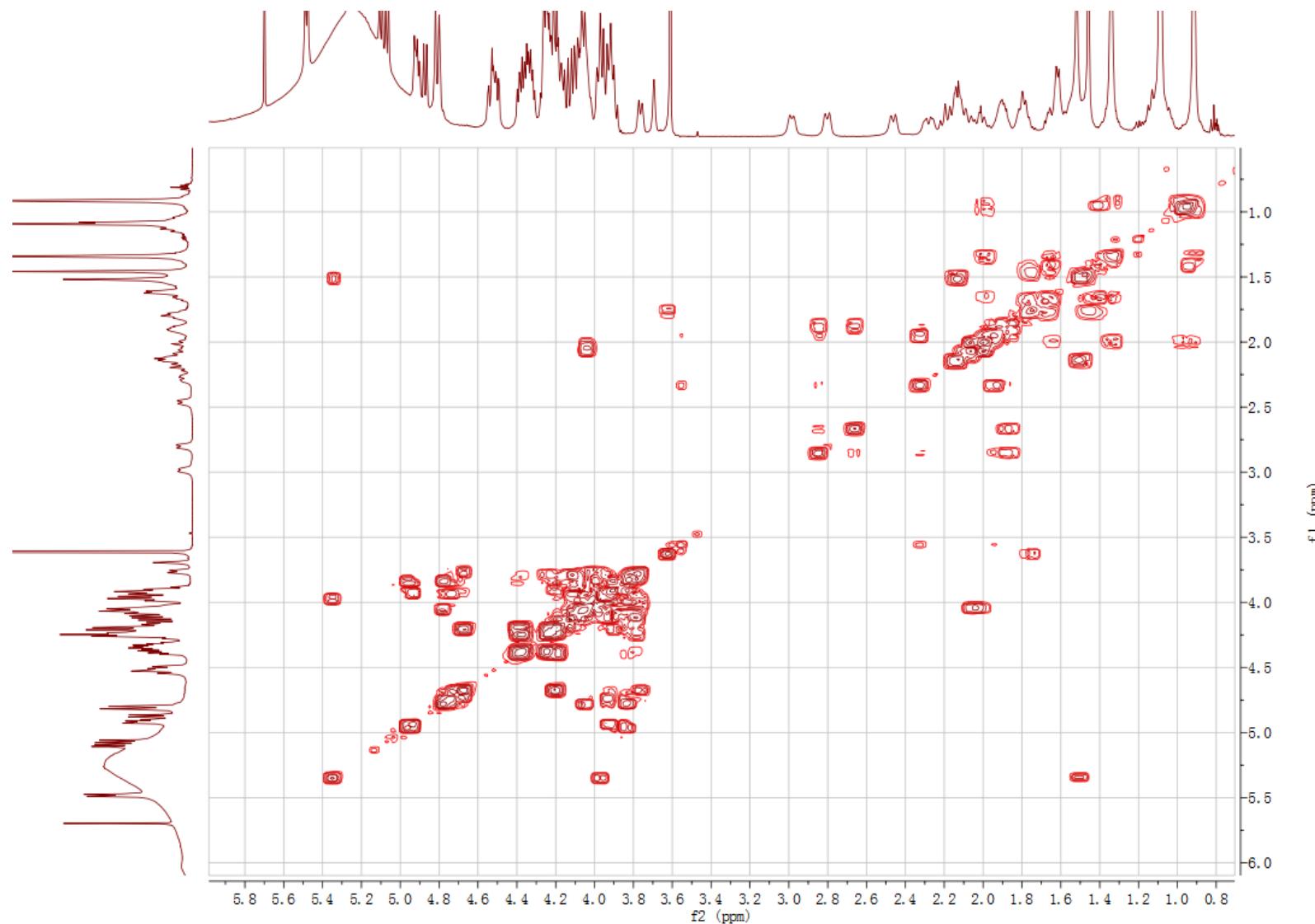


Figure S56. ROESY spectrum of Mogroside VI A (**6**) in C₅D₅N

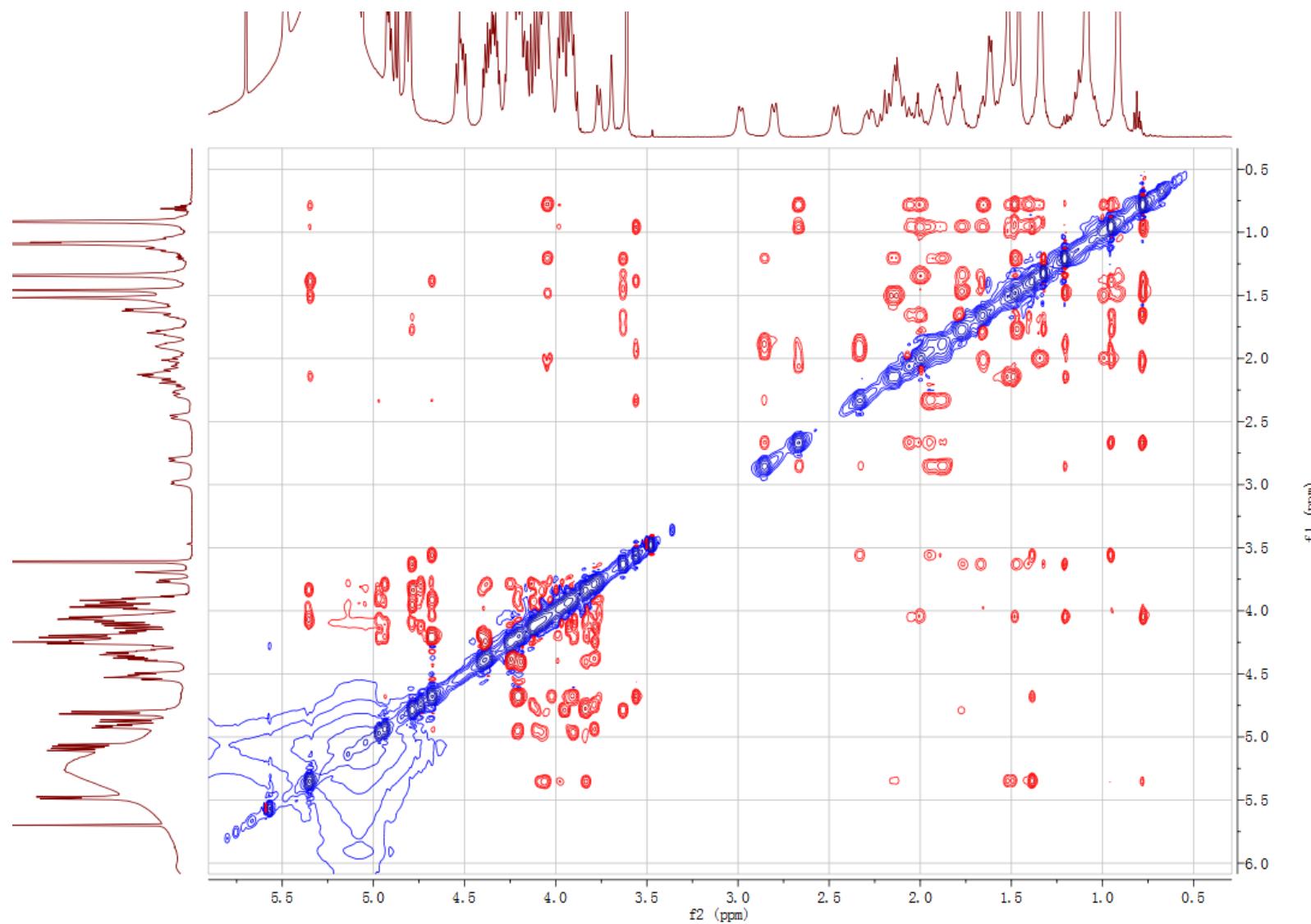


Figure S57. TOCSY spectrum of Mogroside VI A (**6**) in C₅D₅N

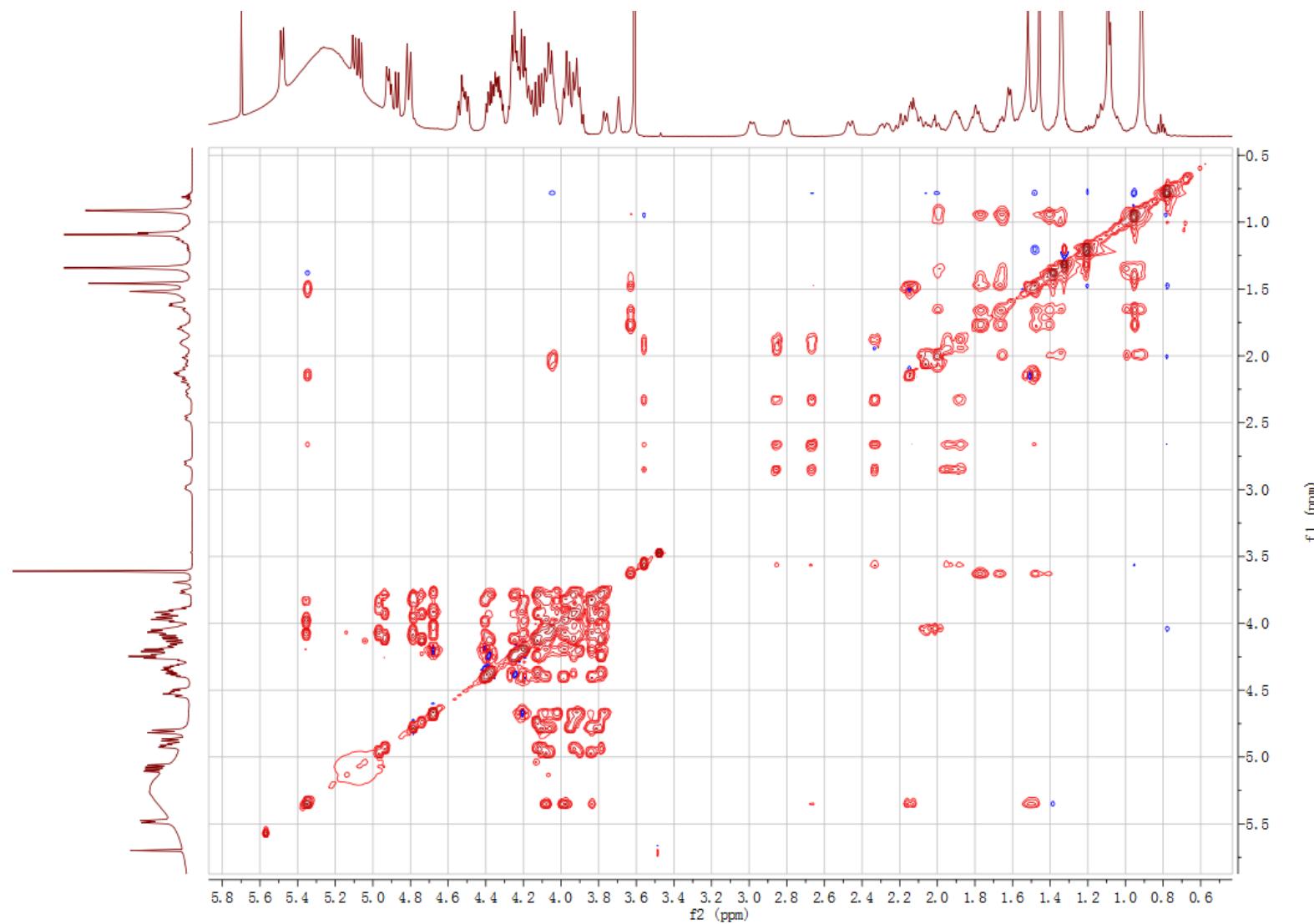


Figure S58. IR spectrum of Mogroside VI A (6)

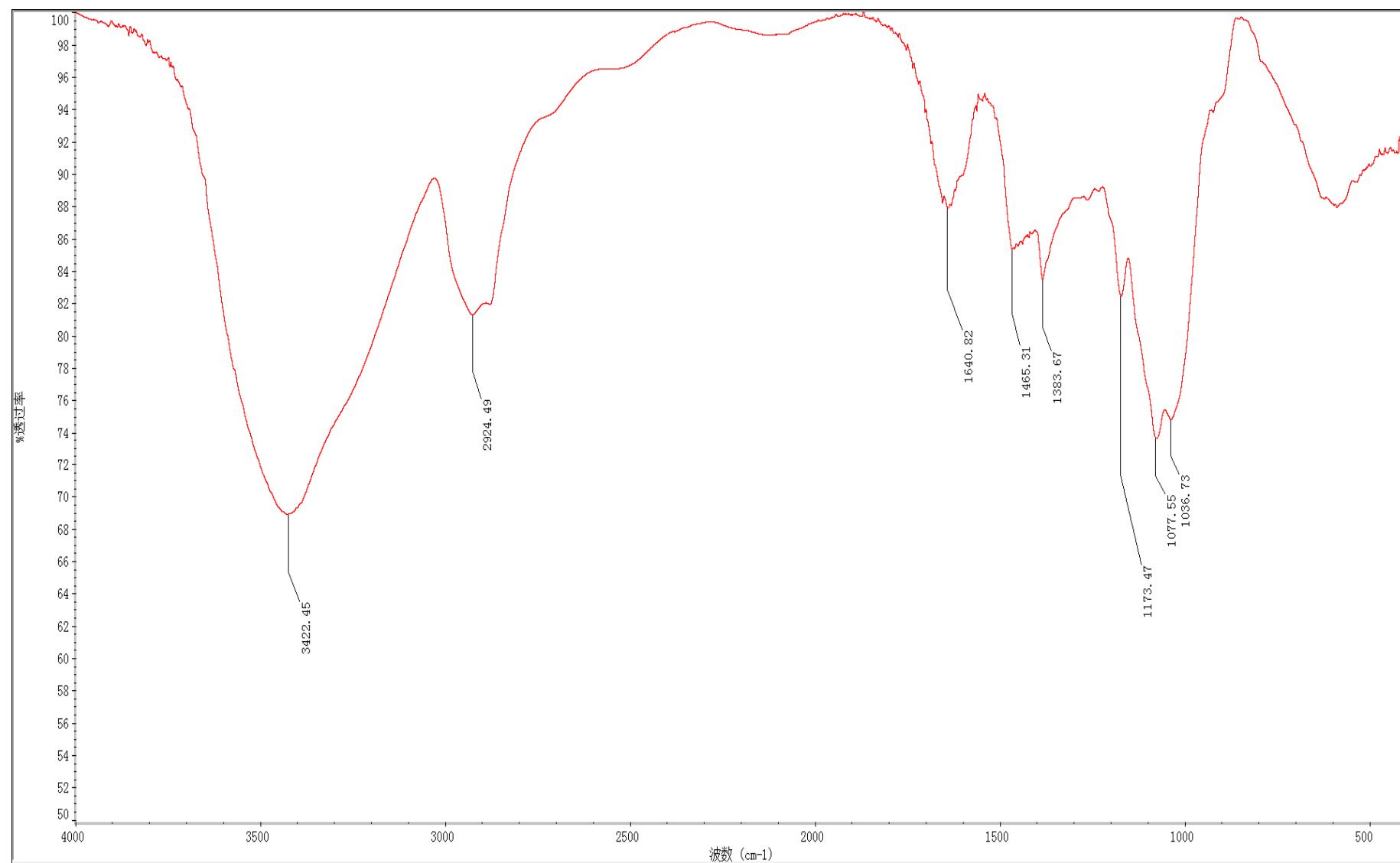
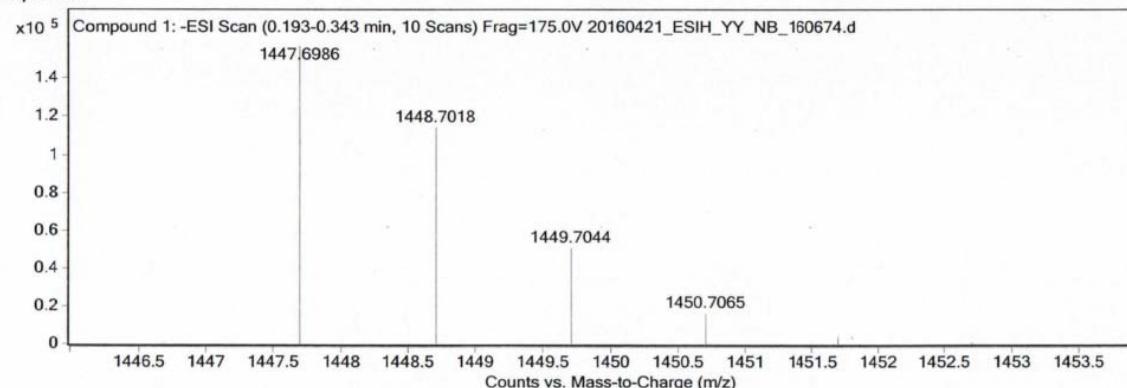


Figure S59. HRESIMS spectrum of Mogroside VI A (6)

Qualitative Compound Report

Data File	20160421_ESIH_YY_NB_160674.d	Sample Name	LHG-T-6-2
Sample Type	Sample	Position	P1-B1
Instrument Name	Agilent G6520 Q-TOF	Acq Method	20160322_MS_ESIH_NEG_1min_-2000.m
Acquired Time	4/21/2016 12:56:53 PM	IRM Calibration Status	Success
DA Method	small molecular data analysis method.m	Comment	ESIH

MS Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Formula	Ion
126.9047					
148.9524			1		
746.3505			2		
1447.6986	1447.6962	-1.67	1	C66 H112 O34	(M-H)-

Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Abund %	Calc Abund %
1	1447.6986	1447.6962	100	100
2	1448.7018	1448.6996	72.93	73.96
3	1449.7044	1449.7025	32.67	33.95
4	1450.7065	1450.7053	10.42	11.62
5	1451.708	1451.708	2.62	3.26



Agilent Technologies

Figure S60. ^1H NMR spectrum of Mogroside VI B (7) in C₅D₅N

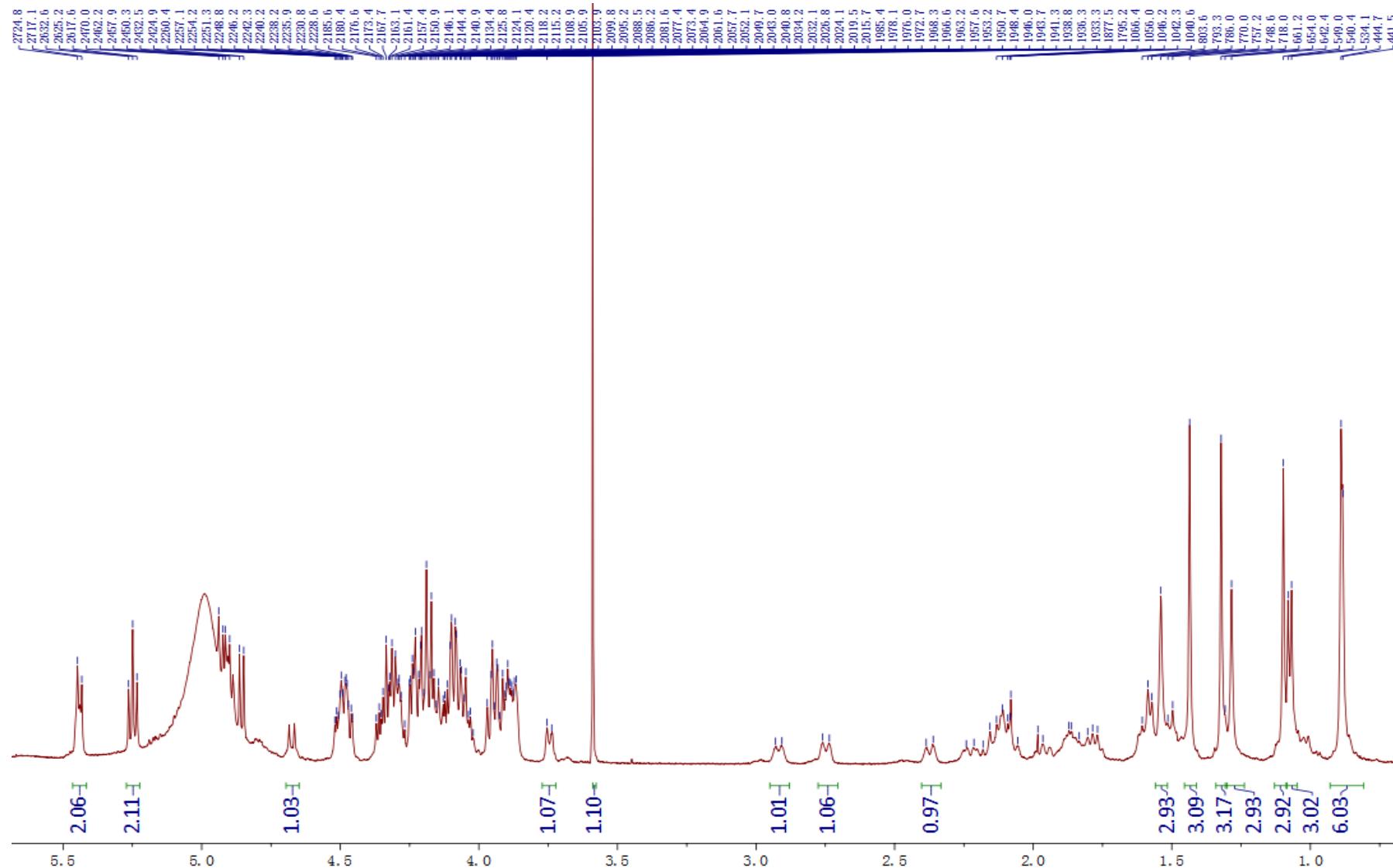
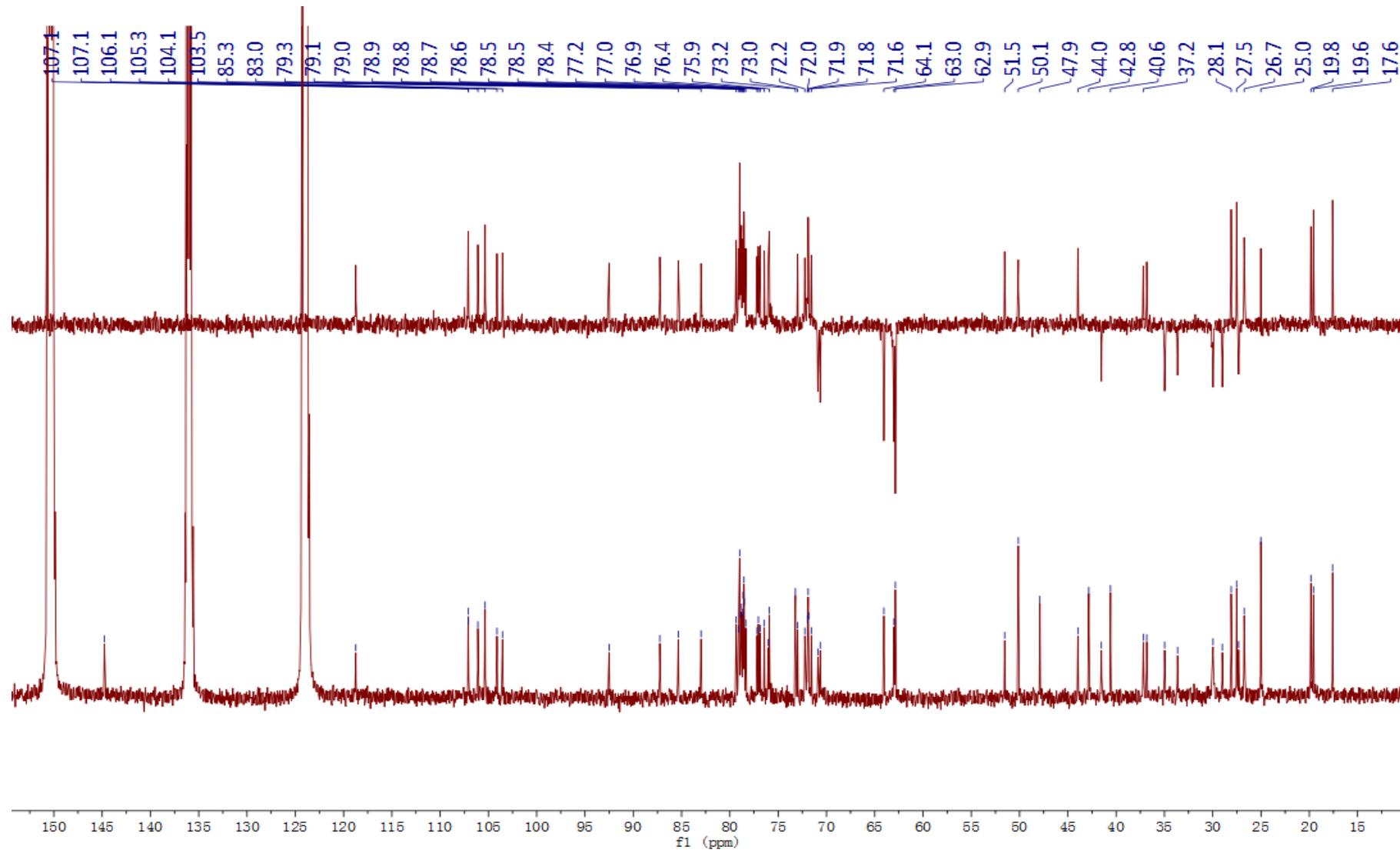
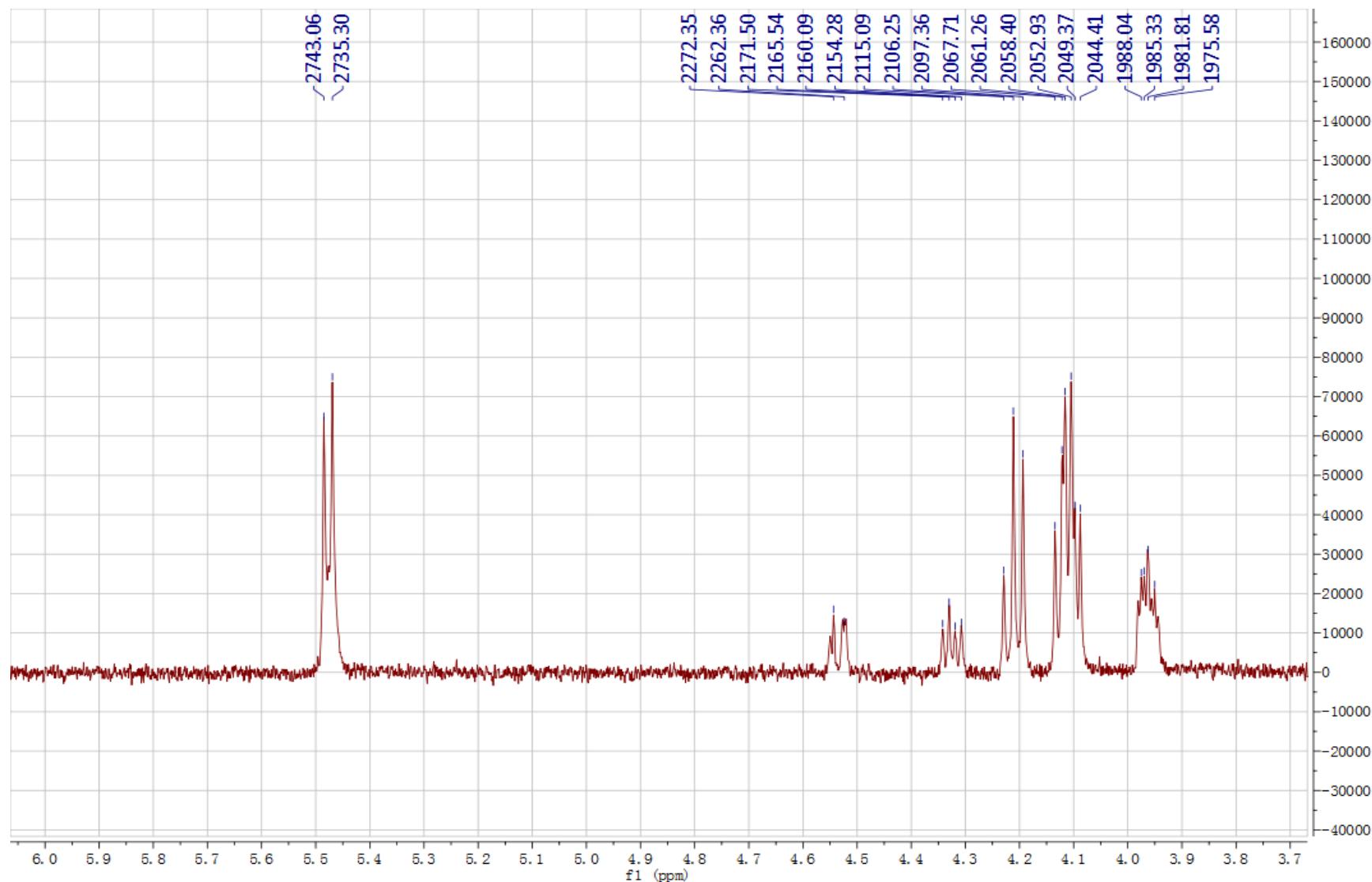
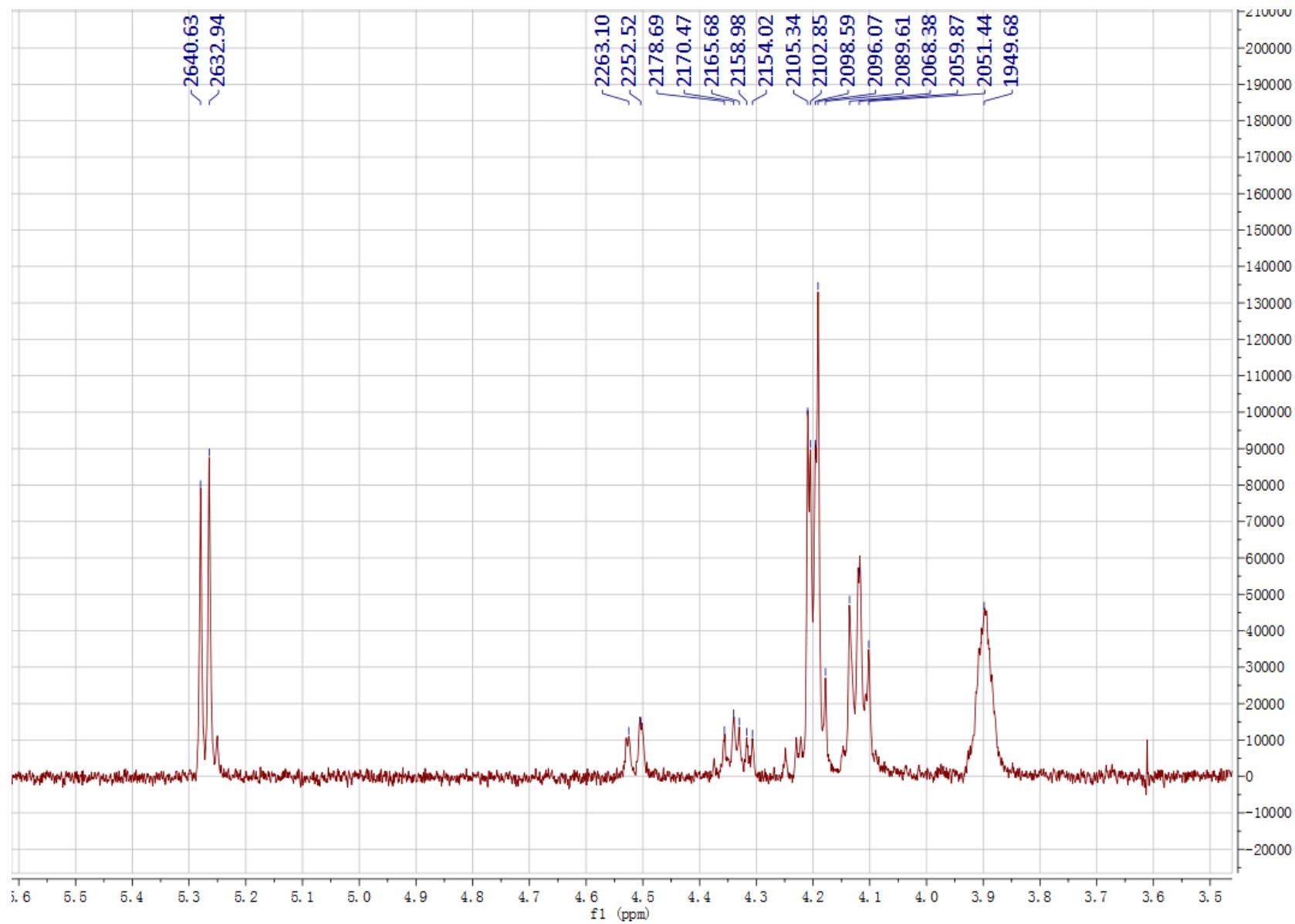


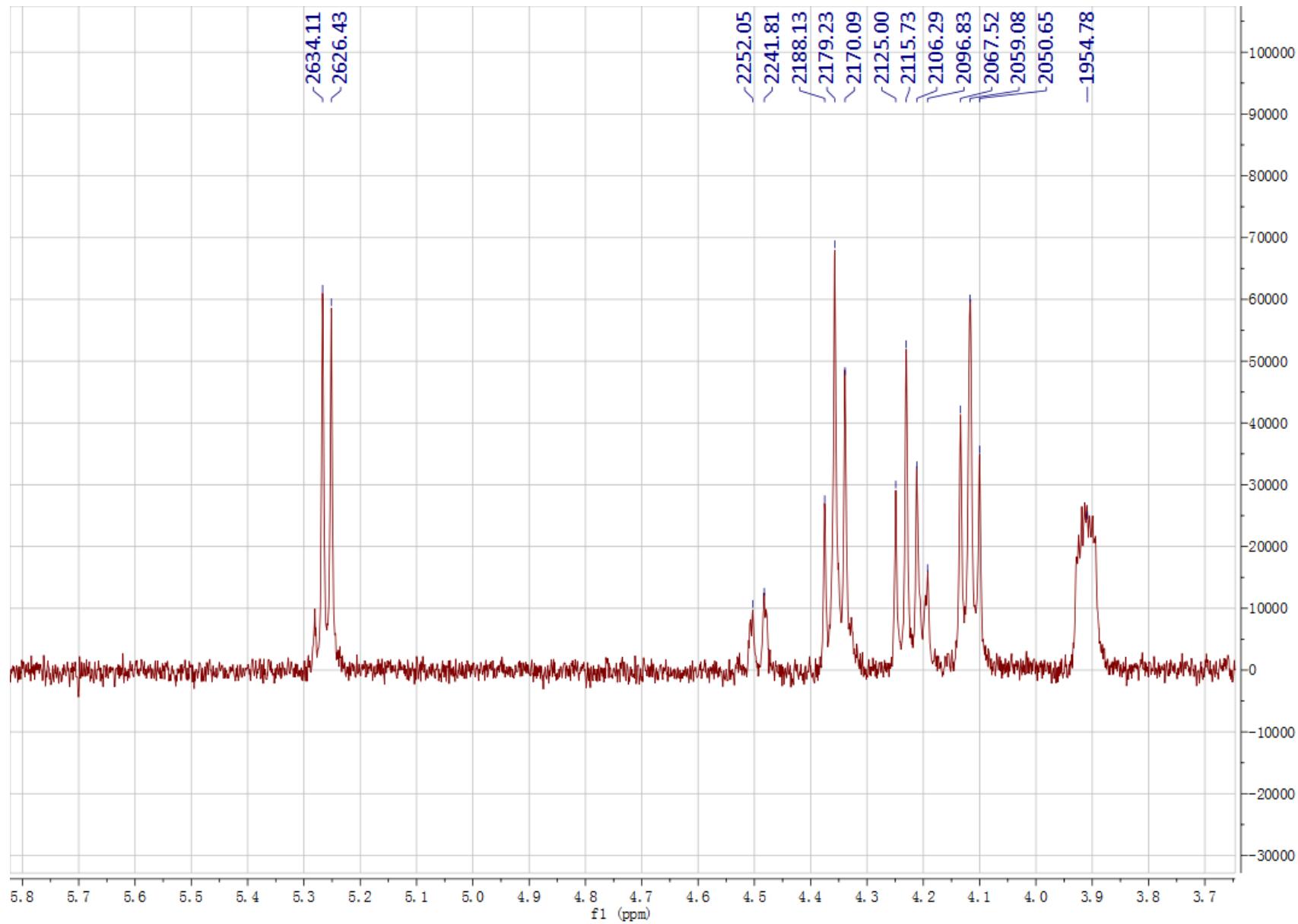
Figure S61. ^{13}C NMR spectrum of Mogroside VI B (**7**) in $\text{C}_5\text{D}_5\text{N}$

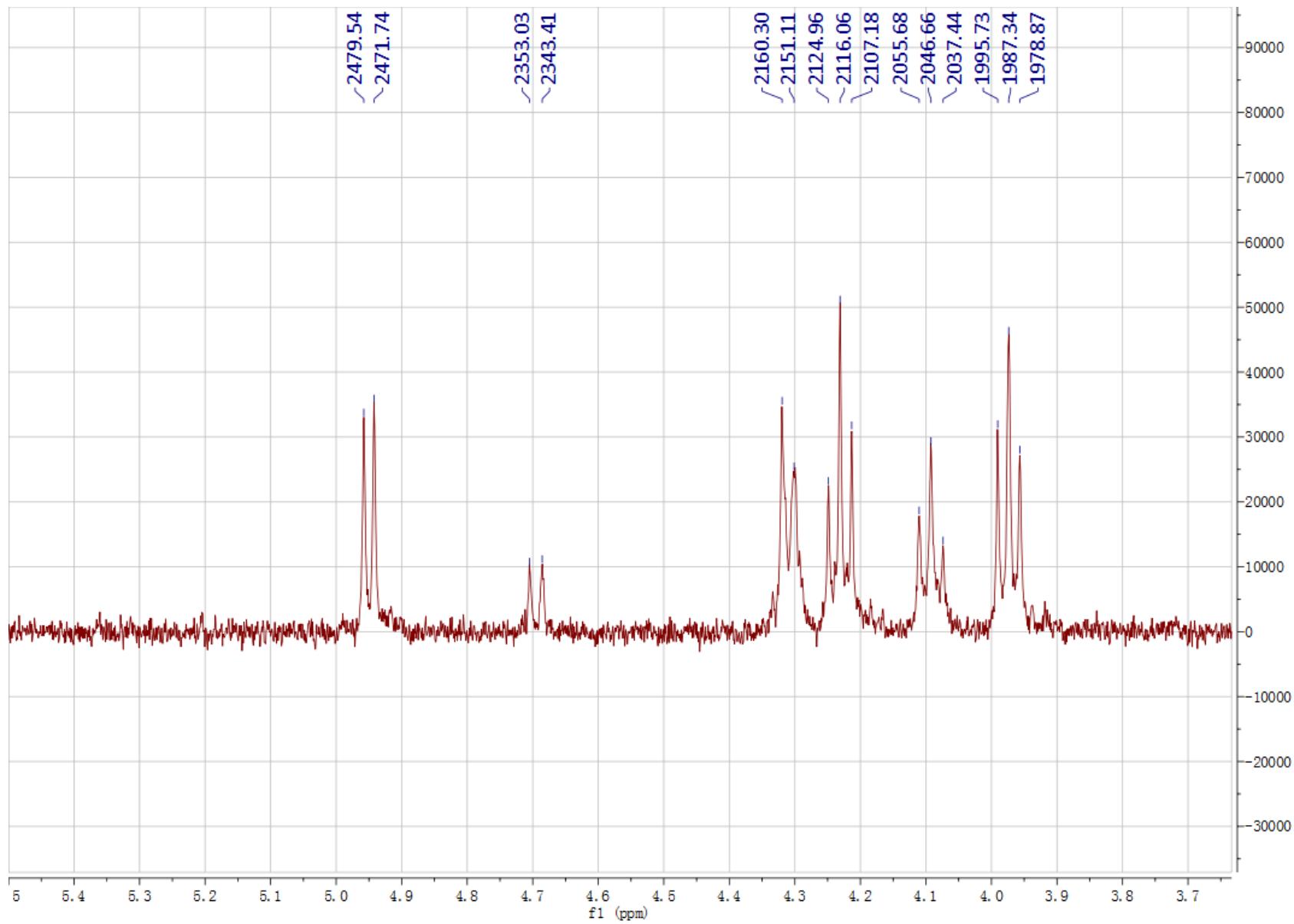


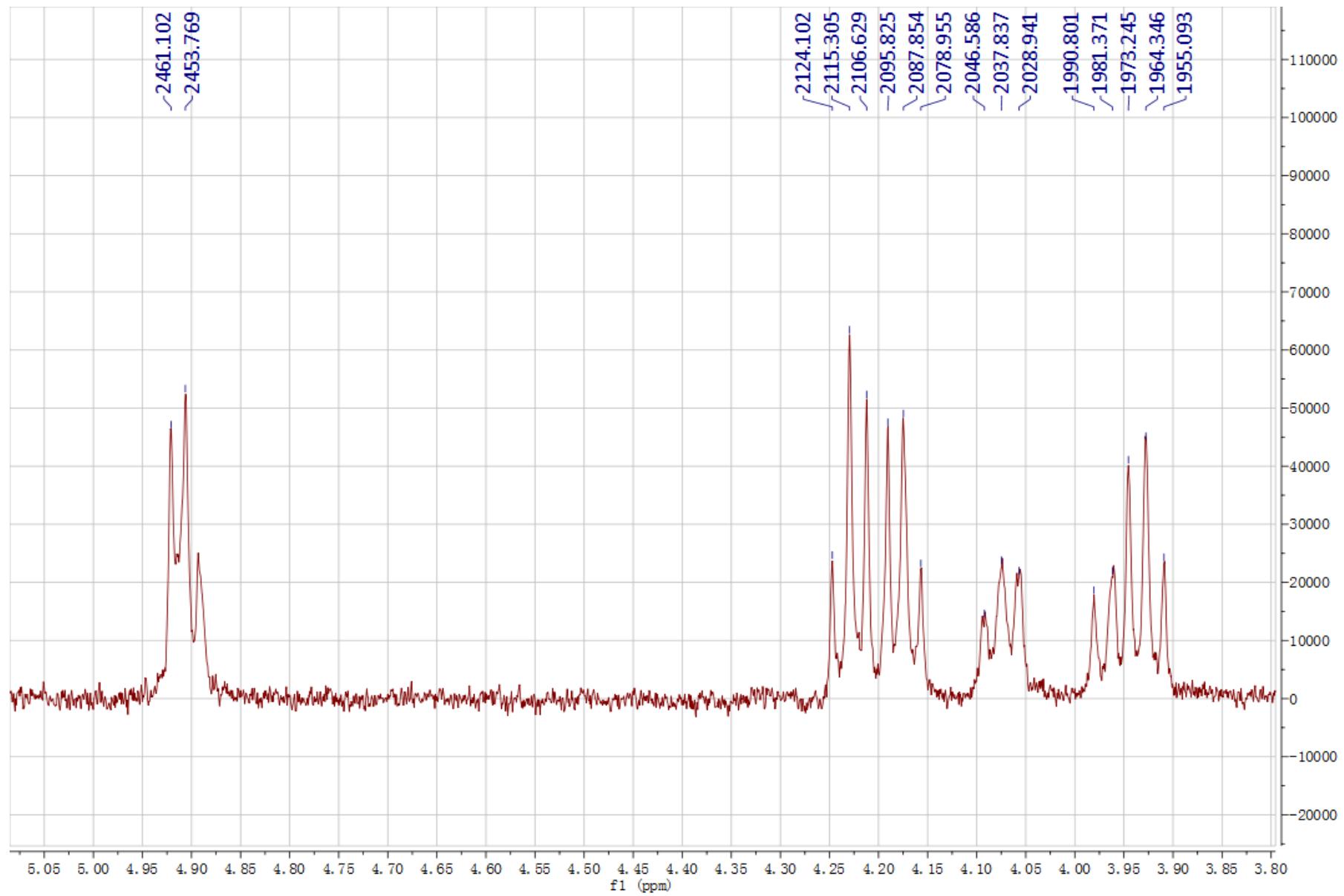
Figures S62. 1D TOCSY spectrum of Mogroside VI B (7) in C₅D₅N











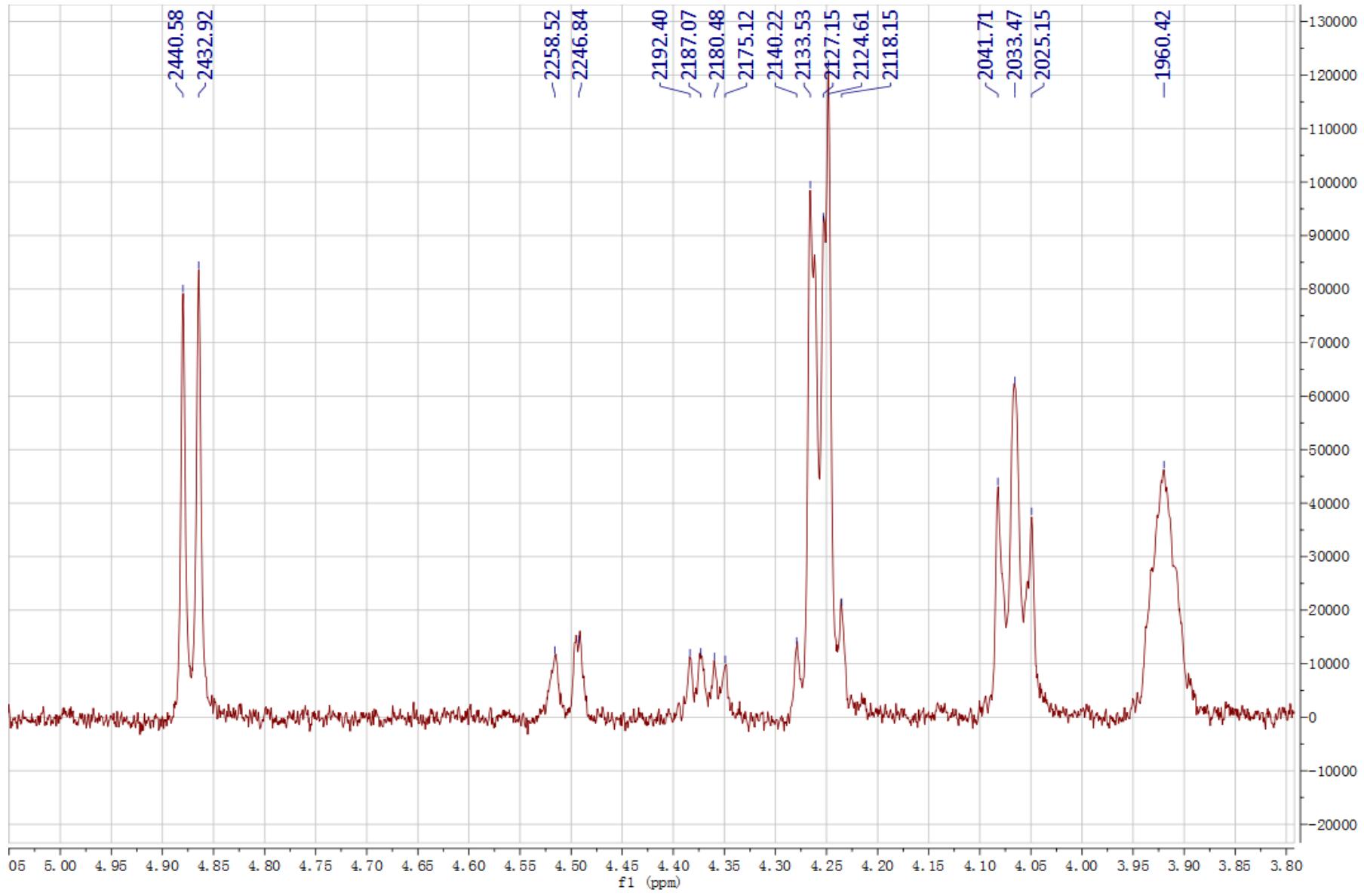


Figure S63. Selective HSQC (C15-55) spectrum of Mogroside VI B (7) in C₅D₅N

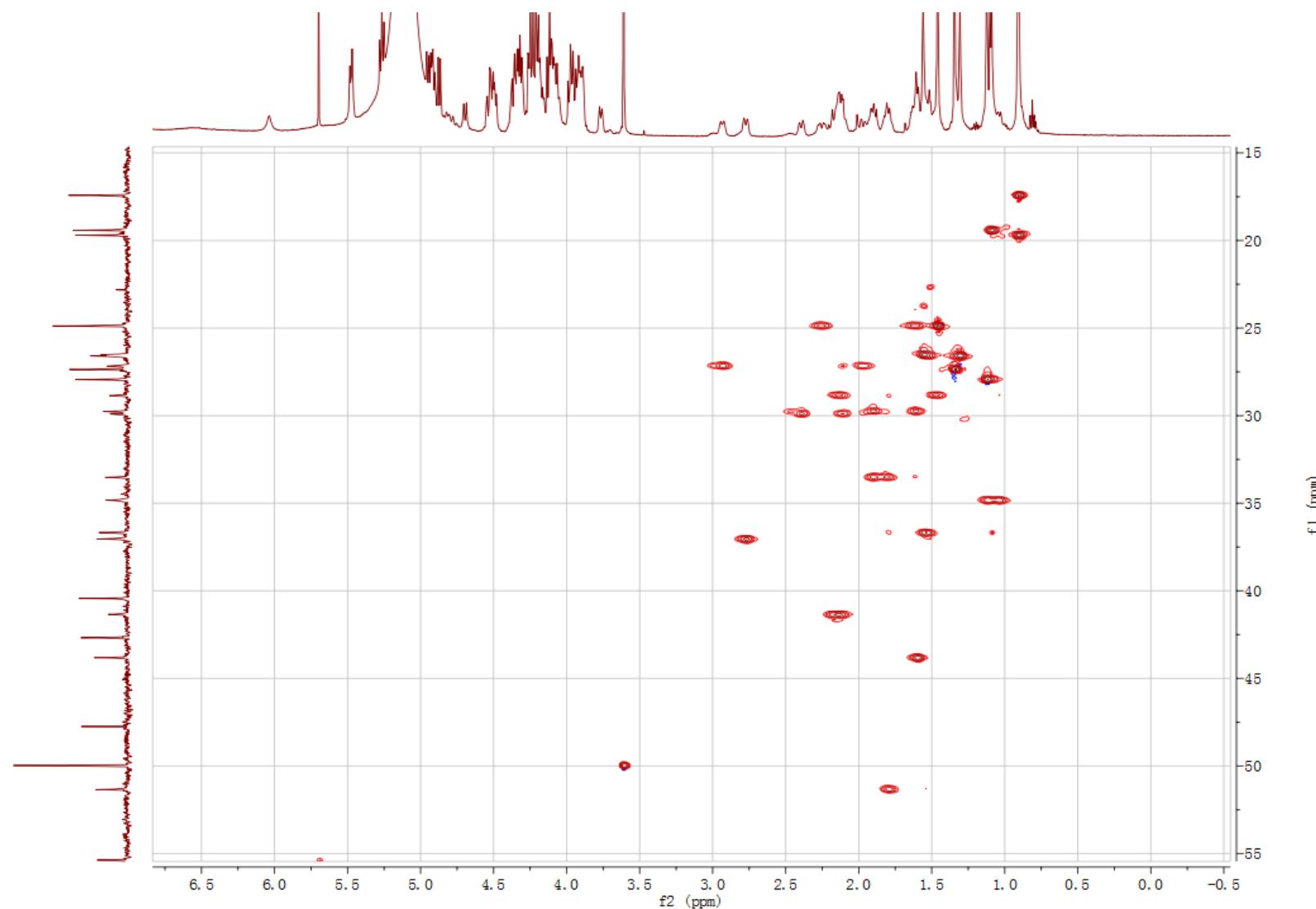


Figure S64. Selective HSQC (C60-95) spectrum of Mogroside VI B (7) in C₅D₅N

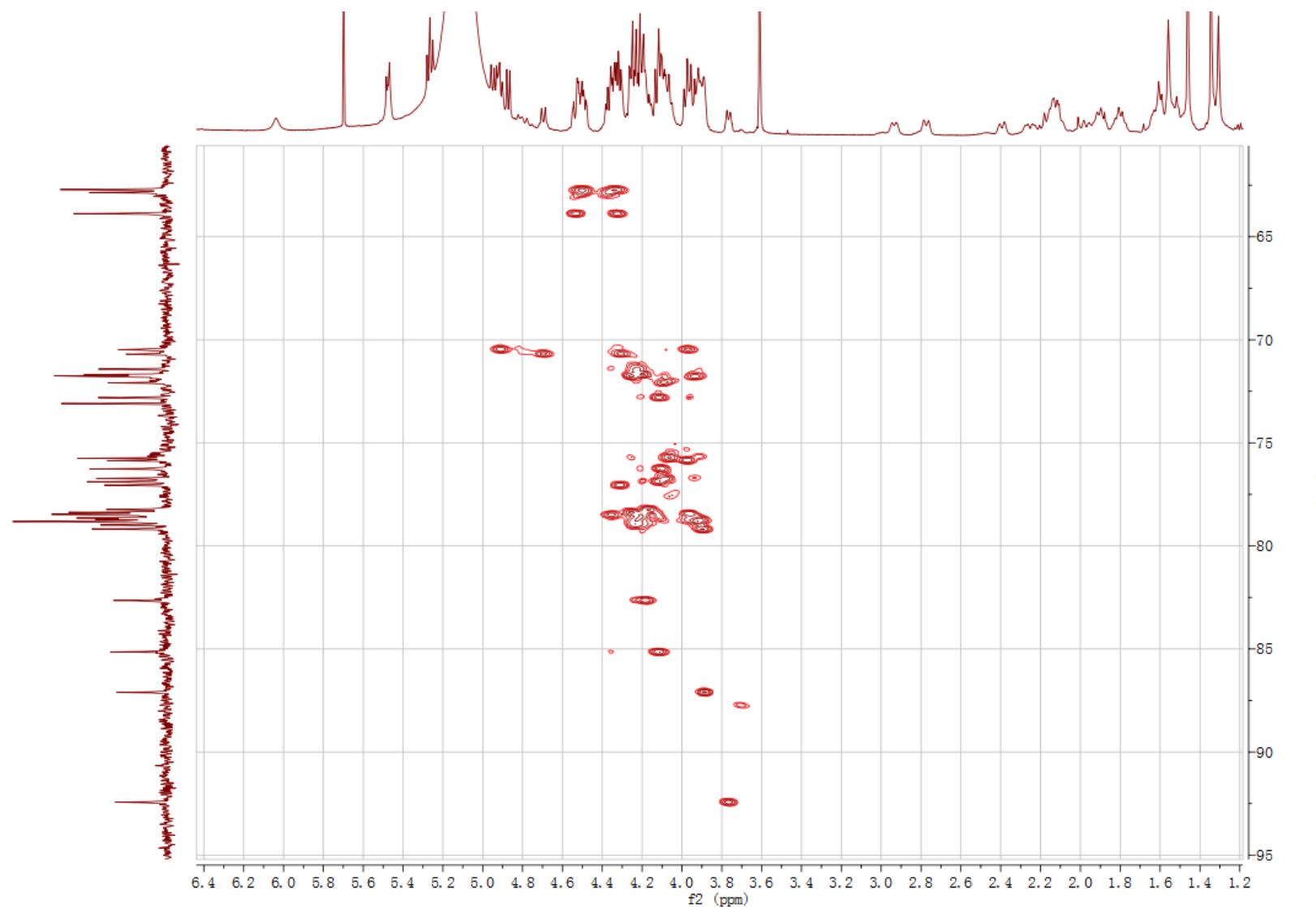


Figure S65. Selective HSQC (C100-108) spectrum of Mogroside VI B (**7**) in C₅D₅N

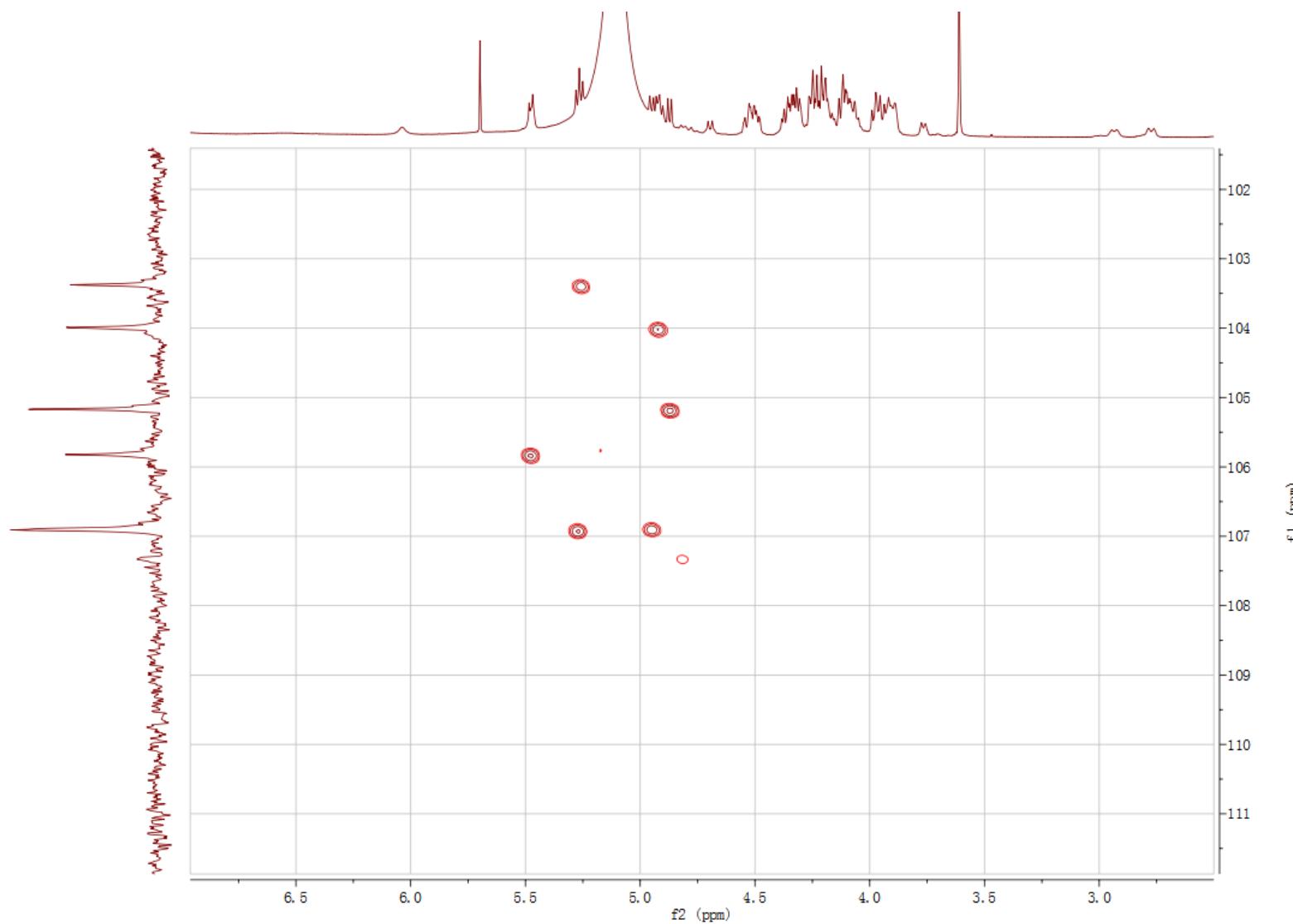


Figure S66. Selective HMBC (C15-45) spectrum of Mogroside VI B (7) in C₅D₅N

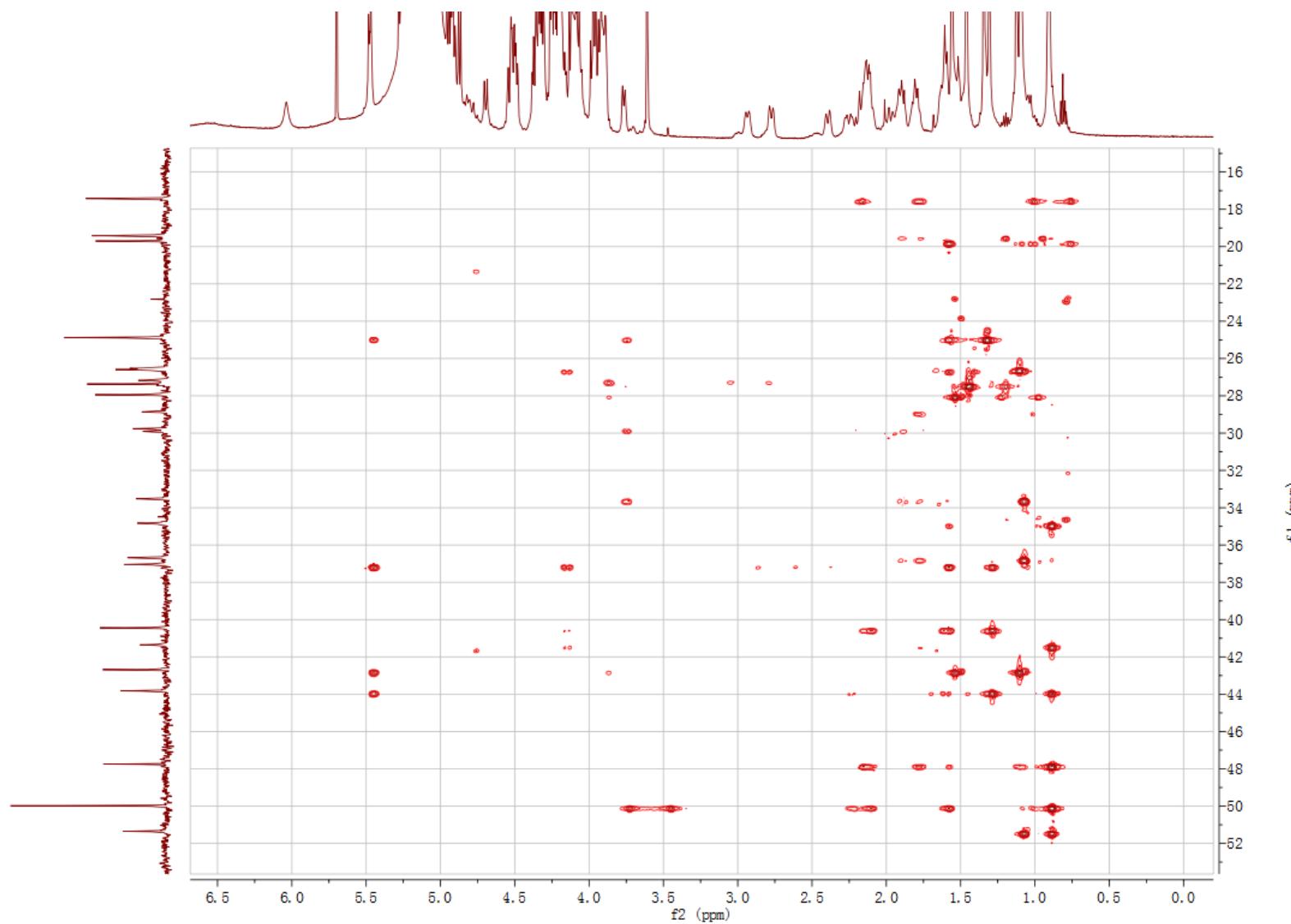


Figure S67. Selective HMBC (C60-95) spectrum of Mogroside VI B (**7**) in C₅D₅N

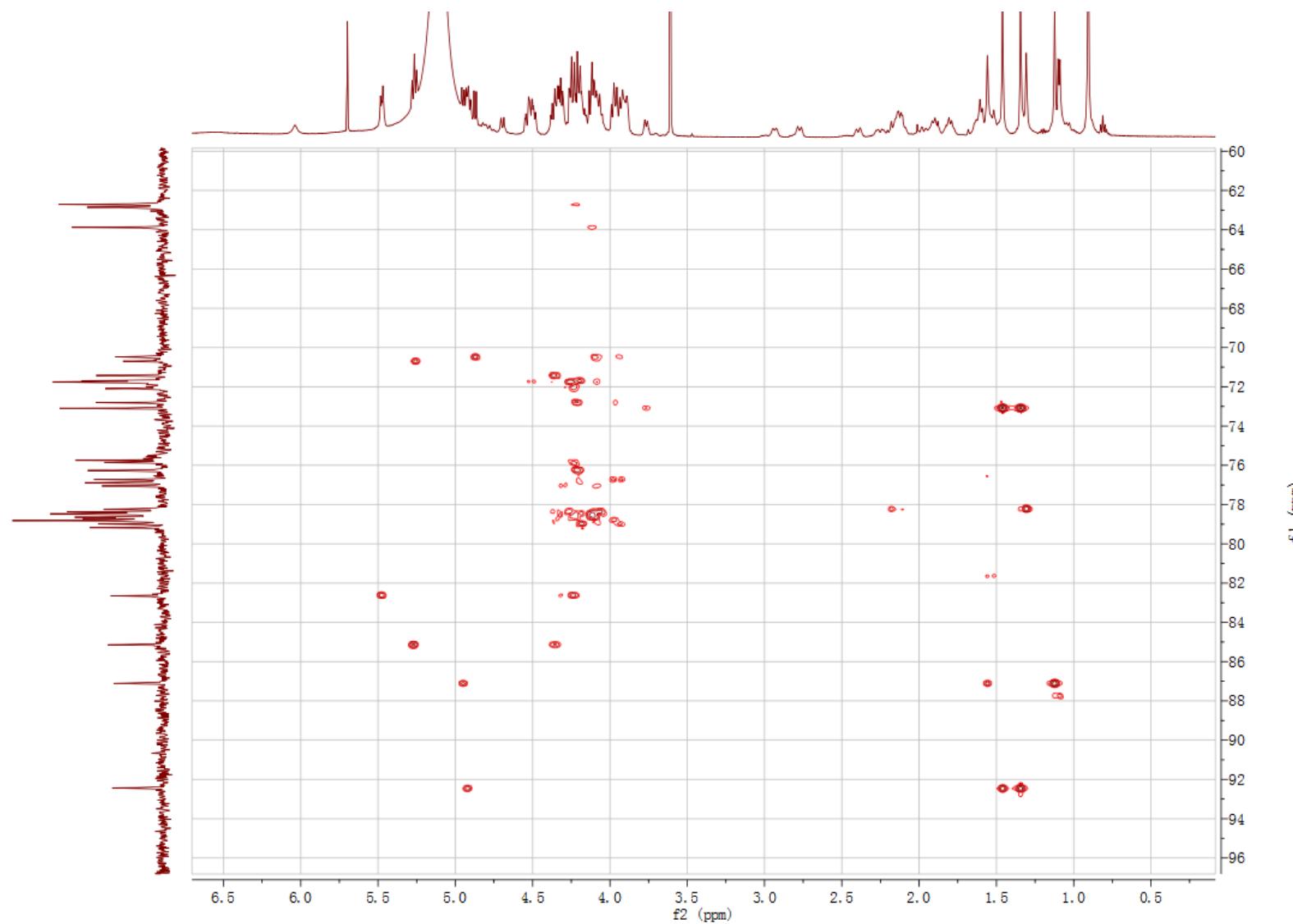


Figure S68. Selective HMBC (C60-108) spectrum of Mogroside VI B (**7**) in C₅D₅N

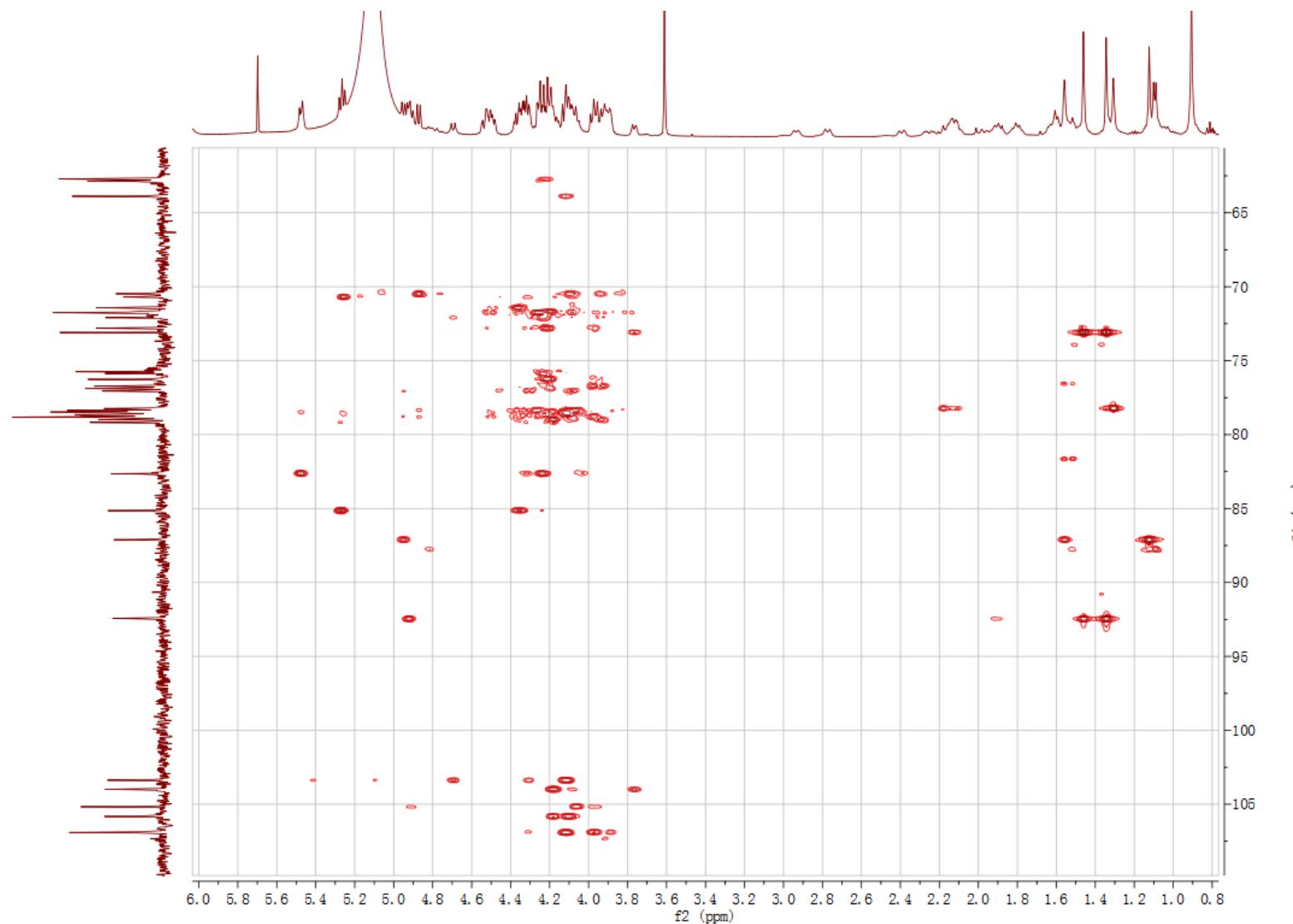


Figure S69. COSY spectrum of Mogroside VI B (7) in C₅D₅N

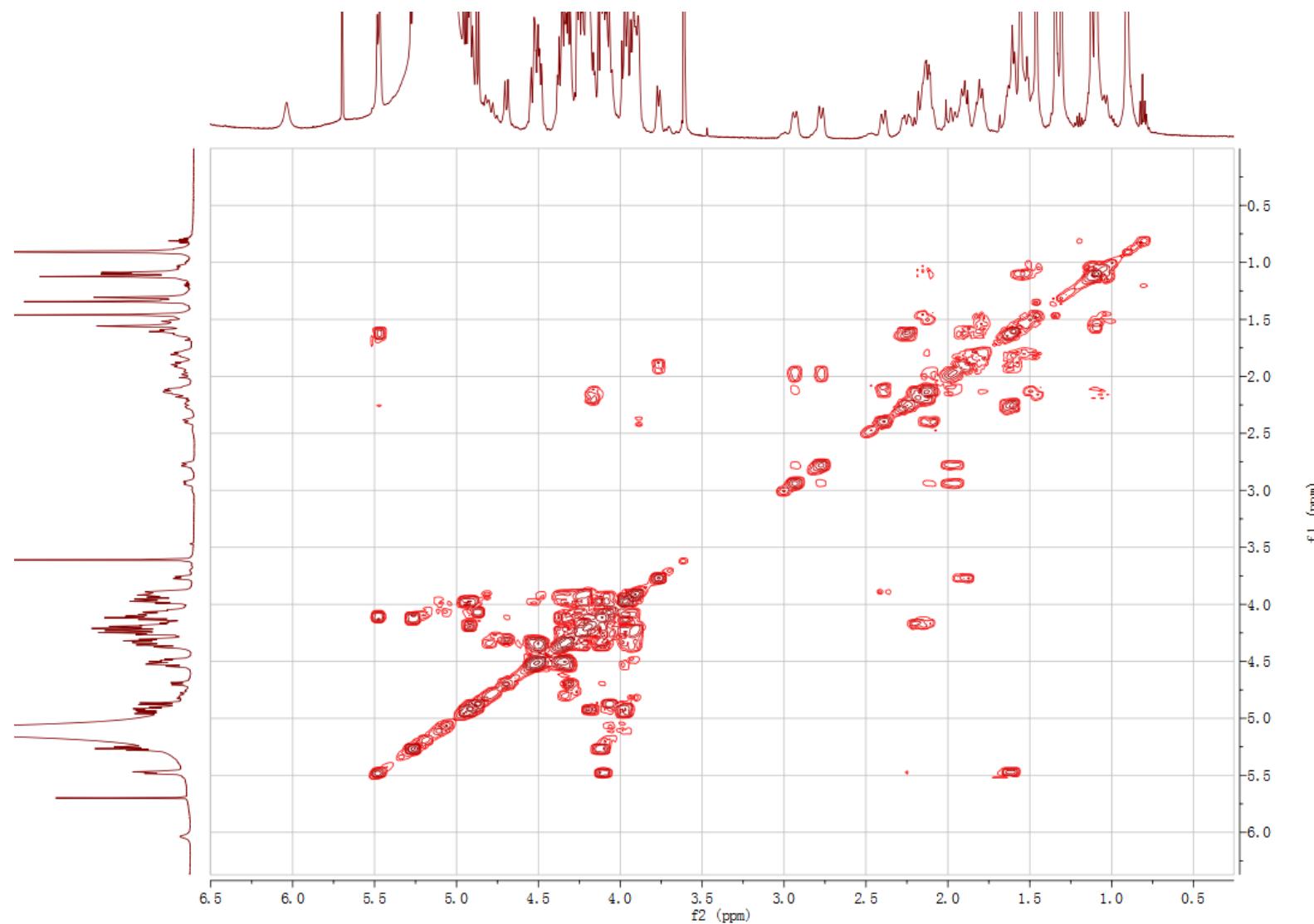


Figure S70. ROESY spectrum of Mogroside VI B (**7**) in C₅D₅N

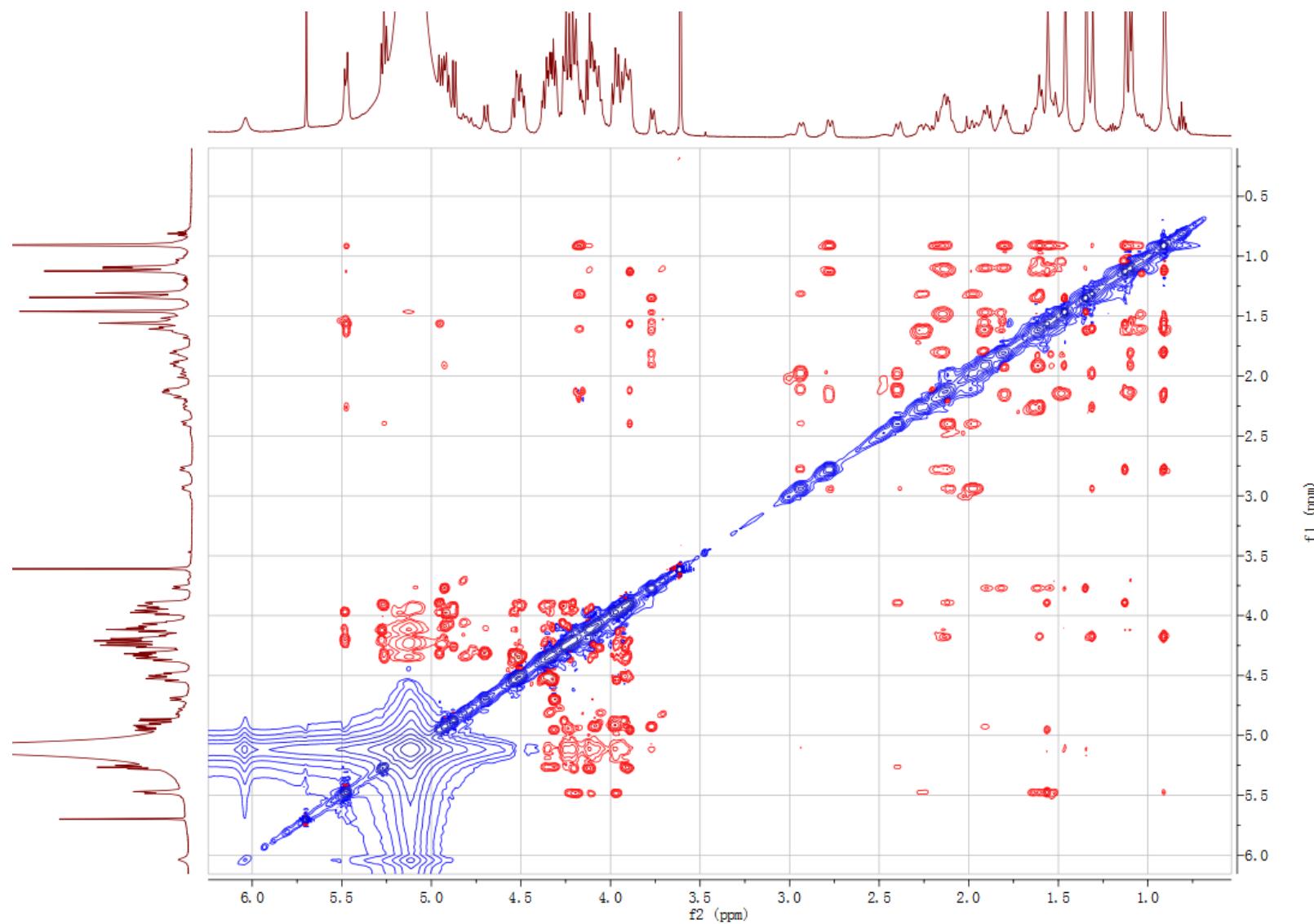


Figure S71. TOCSY spectrum of Mogroside VI B (**7**) in C₅D₅N

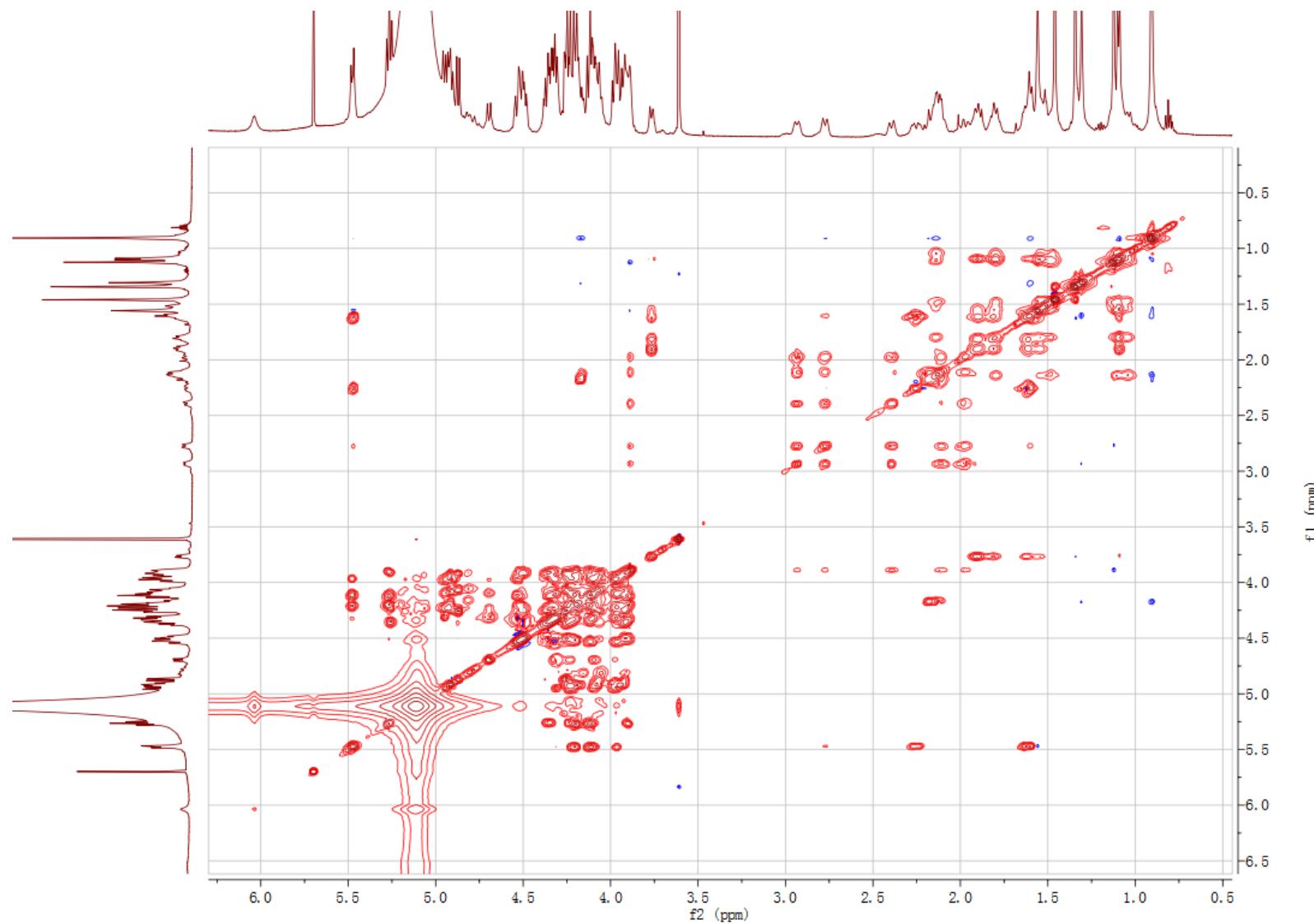


Figure S72. IR spectrum of Mogroside VI B (7)

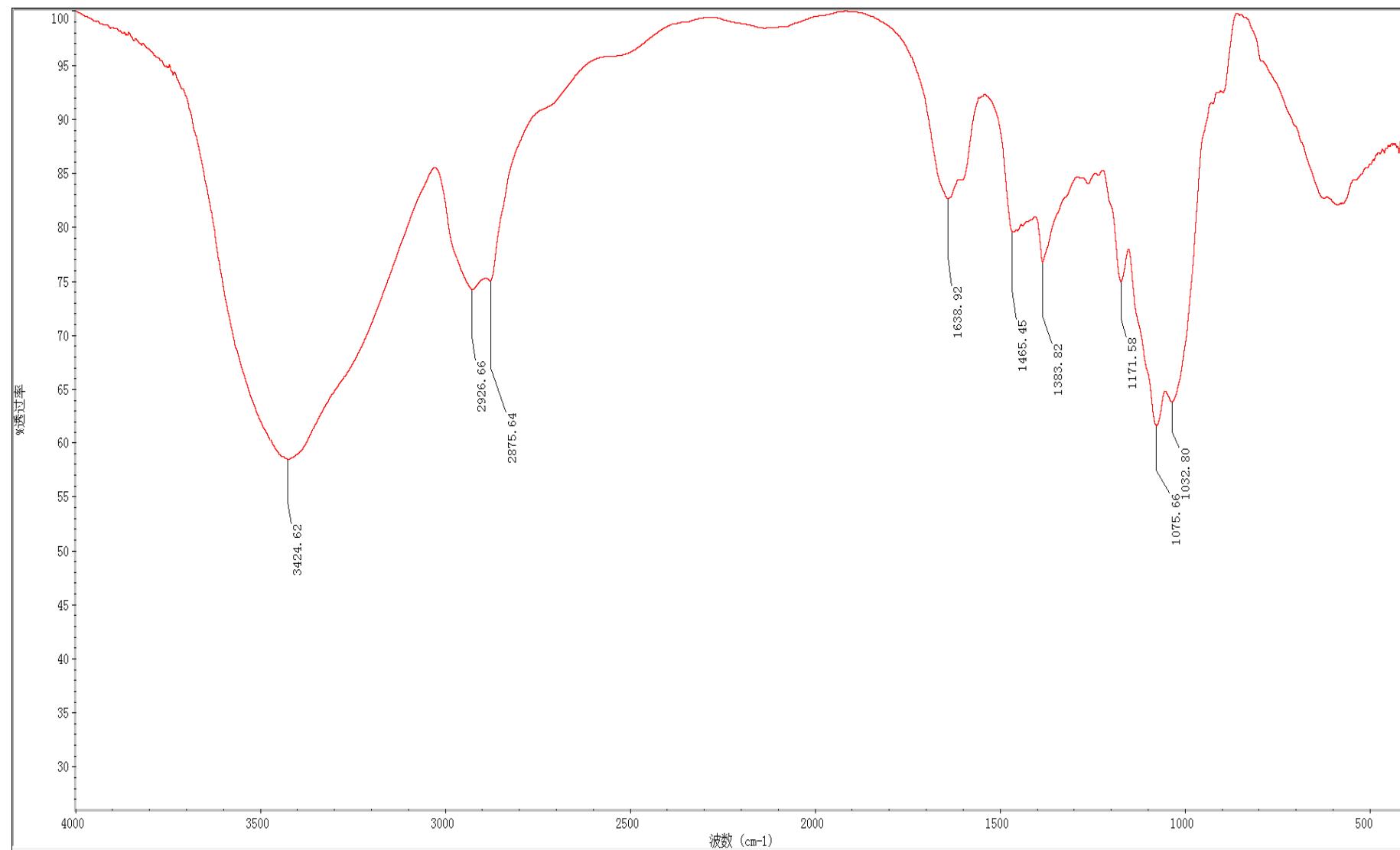
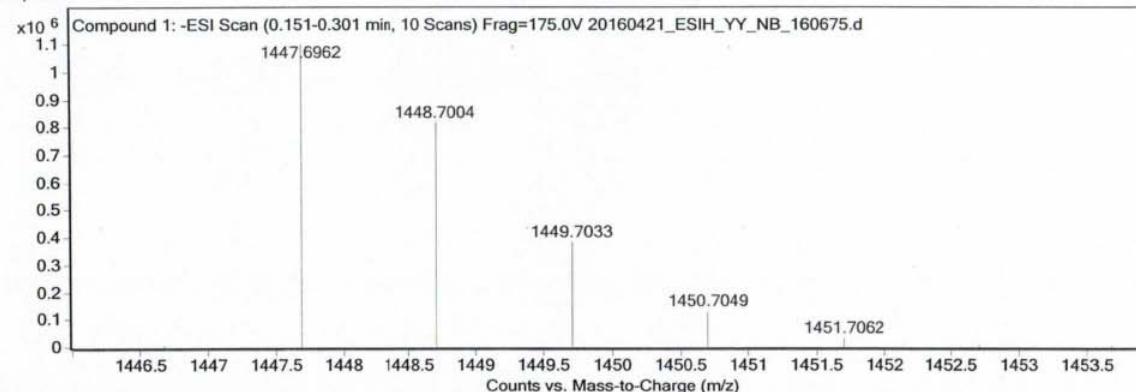


Figure S73. HRESIMS spectrum of Mogroside VI B (7)

Qualitative Compound Report

Data File 20160421_ESIH_YY_NB_160675.d
Sample Type Sample
Instrument Name Agilent G6520 Q-TOF
Acquired Time 4/21/2016 12:58:49 PM
DA Method small molecular data analysis method.m
MS Spectrum

Sample Name LHG-T-6-3
Position P1-B2
Acq Method 20160322_MS_ESIH_NEG_1min_-2000.m
IRM Calibration Status Success
Comment ESIH



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Abund %	Calc Abund %
1	1447.6962	1447.6962	100	100
2	1448.7004	1448.6996	74.04	73.96
3	1449.7033	1449.7025	34.72	33.95
4	1450.7049	1450.7053	11.76	11.62
5	1451.7062	1451.708	2.87	3.26

Figure S74. Crystallographic data of mogrol

Crystal data

$5(\text{C}_{30}\text{H}_{52}\text{O}_4) \cdot \text{C}_{31}\text{H}_{54}\text{O}_3 \cdot 8(\text{O}) \cdot 3(\text{CH}_4\text{O})$	$Z = 1$
$M_r = 3082.43$	$F(000) = 1702$
Triclinic, $P\bar{1}$	$D_x = 1.123 \text{ Mg m}^{-3}$
$a = 14.9136 (6) \text{ \AA}$	$\text{Cu } K\alpha \text{ radiation, } \lambda = 1.54178 \text{ \AA}$
$b = 14.9888 (6) \text{ \AA}$	Cell parameters from 9890 reflections
$c = 22.7918 (9) \text{ \AA}$	$\theta = 3.3\text{--}68.3^\circ$
$\alpha = 97.926 (2)^\circ$	$\mu = 0.59 \text{ mm}^{-1}$
$\beta = 93.125 (2)^\circ$	$T = 170 \text{ K}$
$\gamma = 114.454 (2)^\circ$	Block, colourless
$V = 4558.1 (3) \text{ \AA}^3$	$0.25 \times 0.18 \times 0.12 \text{ mm}$

Data collection

Bruker APEX-II CCD diffractometer	25315 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.035$
Absorption correction: multi-scan <i>SADABS2014/5</i> (Bruker,2014/5) was used for absorption correction. $wR2(\text{int})$ was 0.0808 before and 0.0611 after correction. The Ratio of minimum to maximum transmission is 0.0828. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 64.0^\circ, \theta_{\text{min}} = 3.3^\circ$
$T_{\text{min}} = 0.005, T_{\text{max}} = 0.065$	$h = -17 \rightarrow 17$
83600 measured reflections	$k = -17 \rightarrow 17$
29290 independent reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.082$	$w = 1/[\sigma^2(F_o^2) + (0.1554P)^2 + 0.4496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.220$	$(\Delta/\sigma)_{\text{max}} = 0.055$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.59 \text{ e \AA}^{-3}$
29290 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$
2080 parameters	Absolute structure: Flack x determined using 10316 quotients $[(I+)-(I-)]/[(I+)+(I-)]$ (Parsons, Flack and Wagner, <i>Acta Cryst. B</i> 69 (2013) 249-259).
2012 restraints	Flack parameter: 0.02 (5)

Figure S75. The HPLC analysis of crude extract.

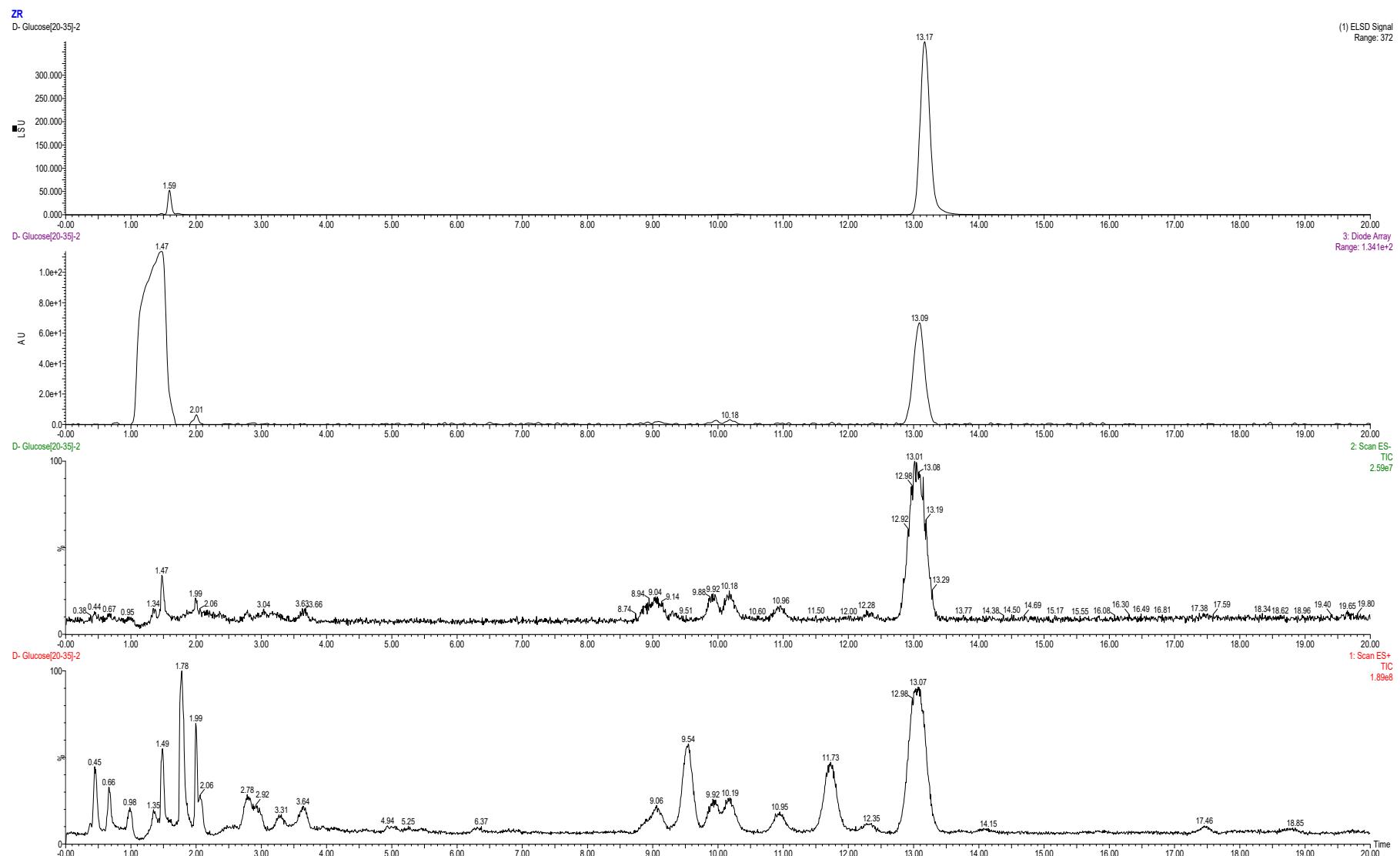


Figure S76. The retention time of L-glucose in HPLC

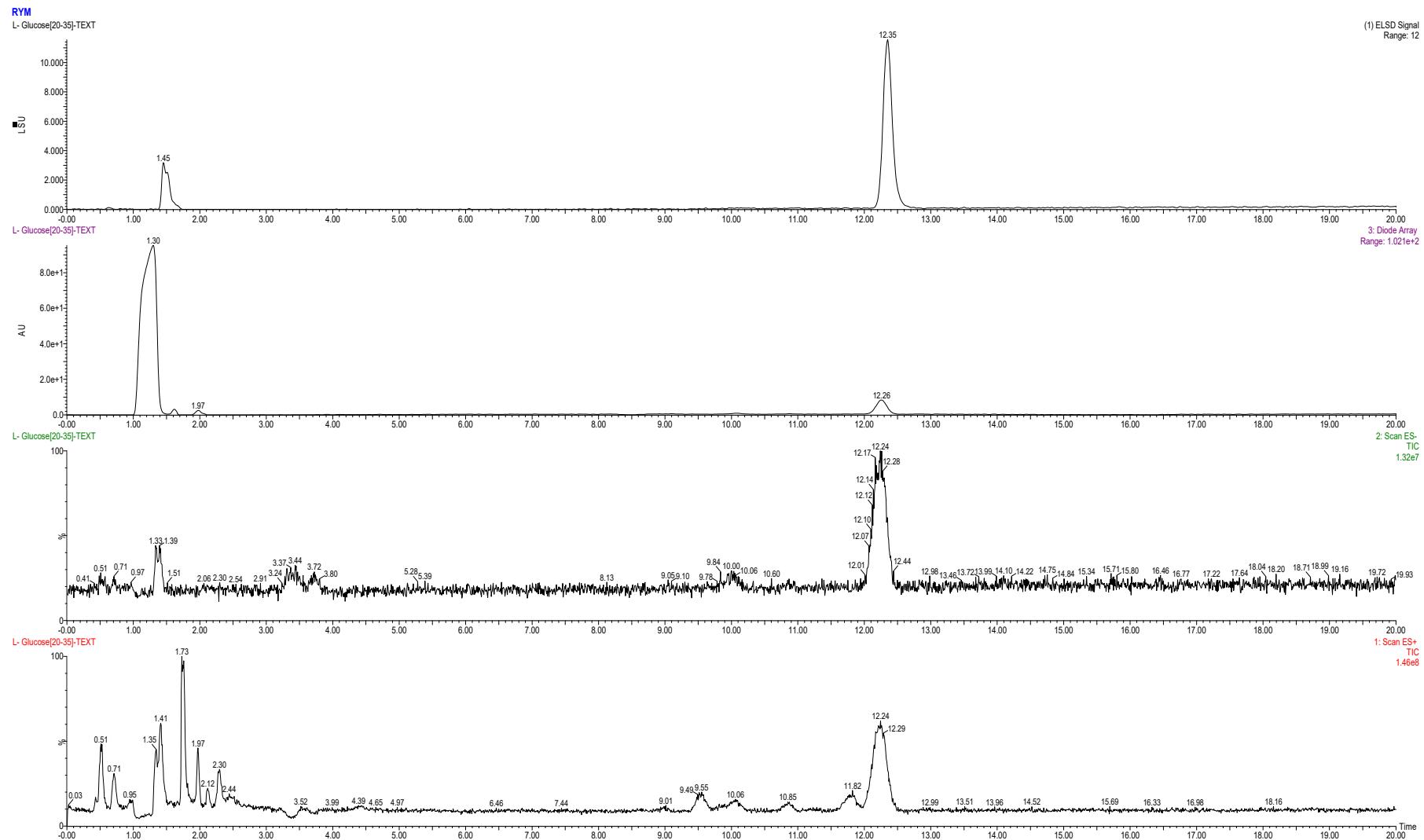


Figure S77. The retention time of glucose of compounds **1-7** in HPLC

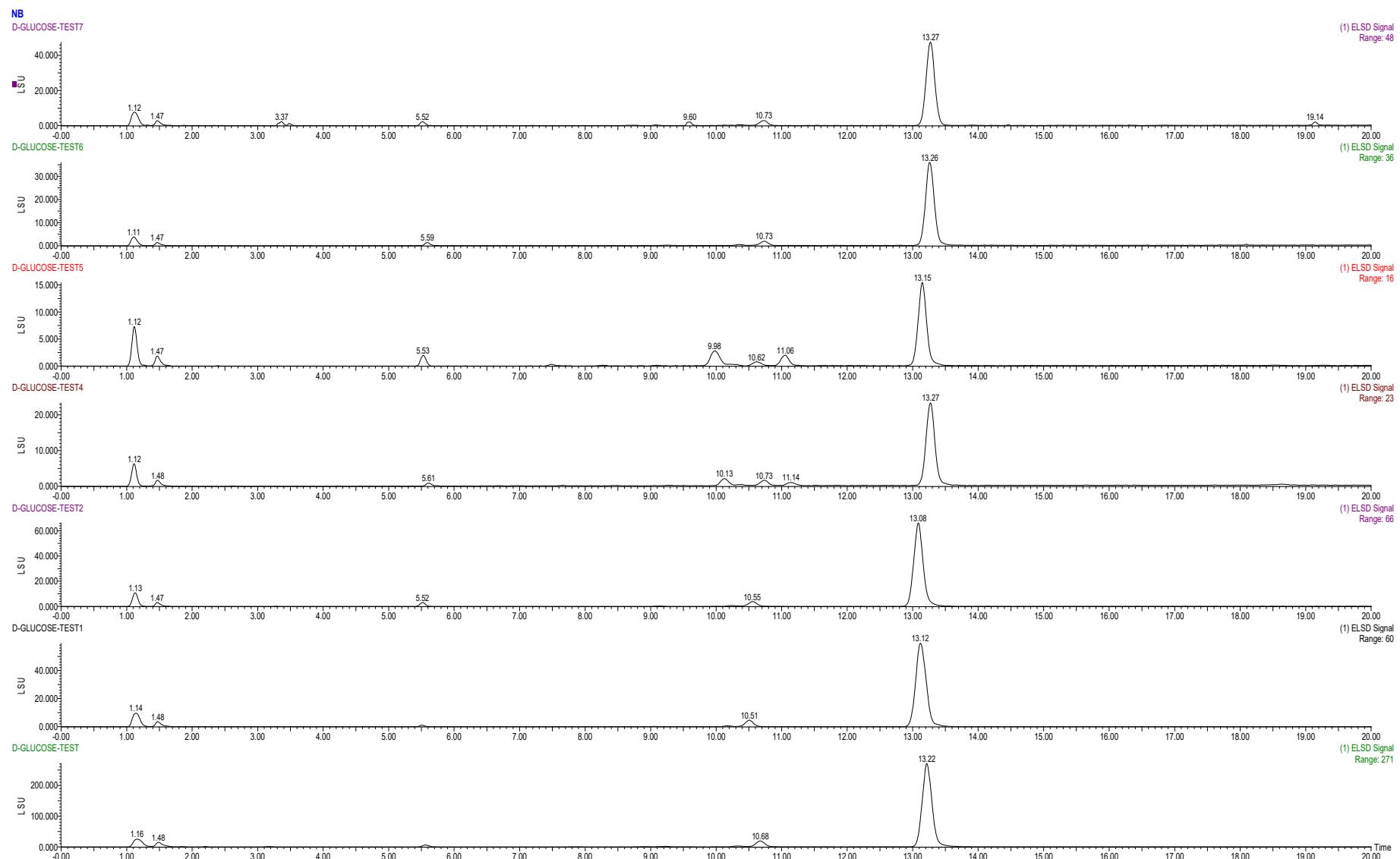
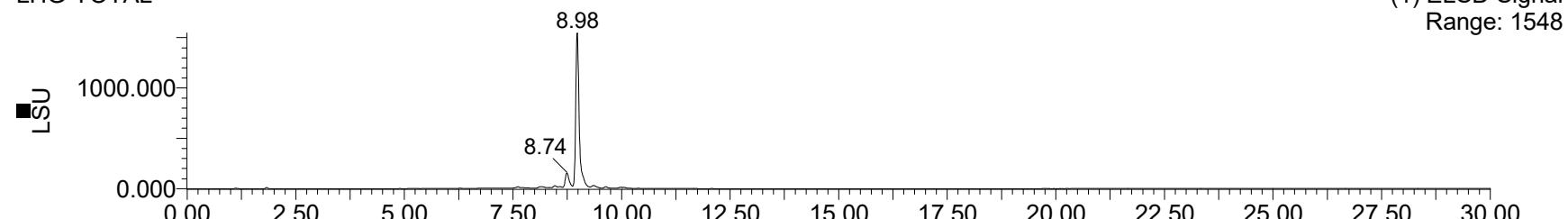


Figure S75. The HPLC analysis of crude extract.

13:47:09

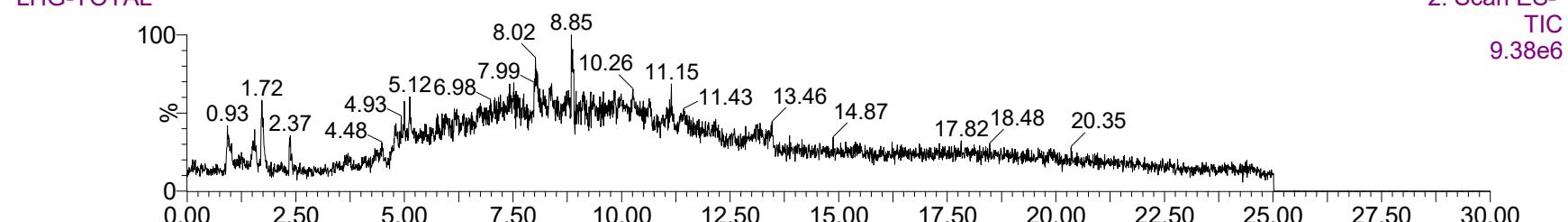
LHG-TOTAL

(1) ELSD Signal
Range: 1548



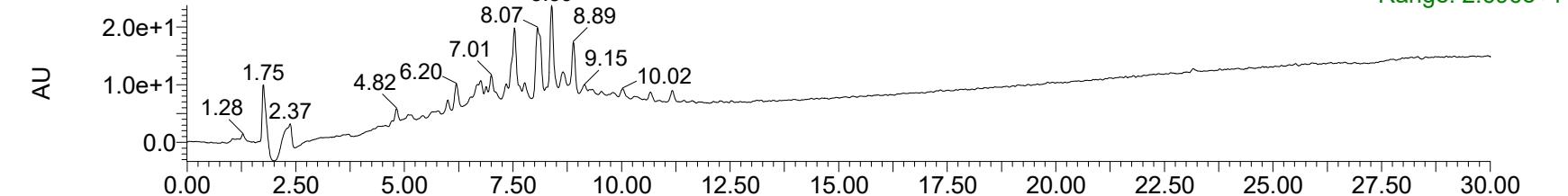
LHG-TOTAL

2: Scan ES-
TIC
9.38e6



LHG-TOTAL

3: Diode Array
Range: 2.696e+1



LHG-TOTAL

1: Scan ES+
TIC
2.69e8

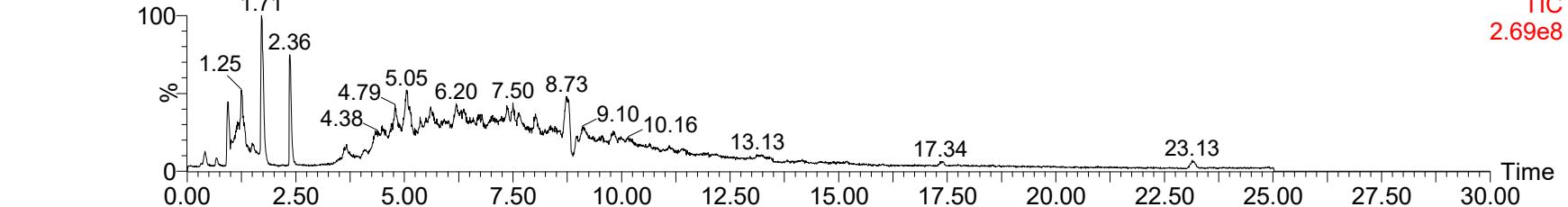
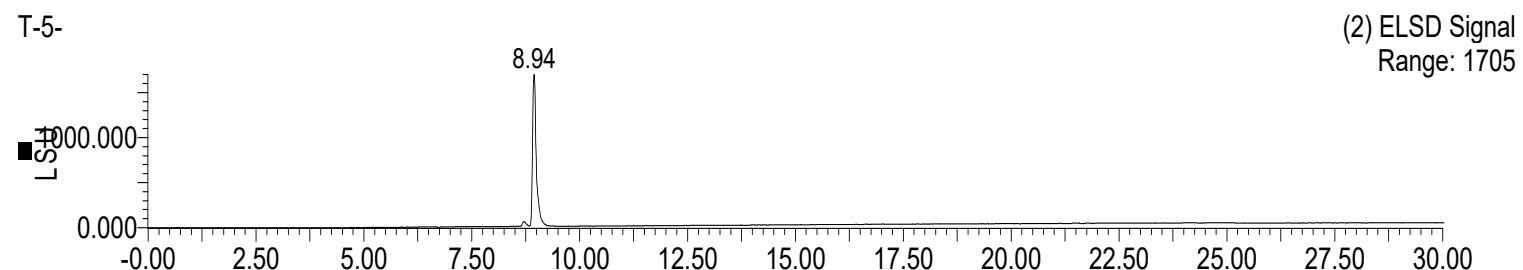


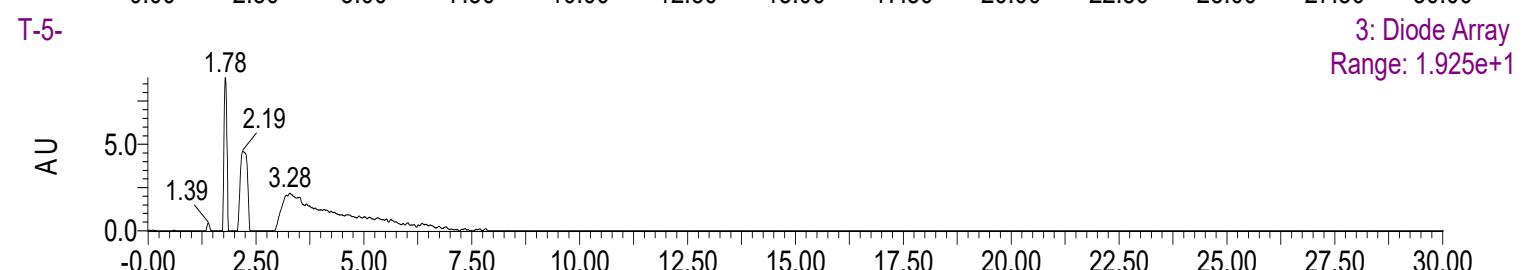
Figure S76. The HPLC analysis of mogroside V.

NB

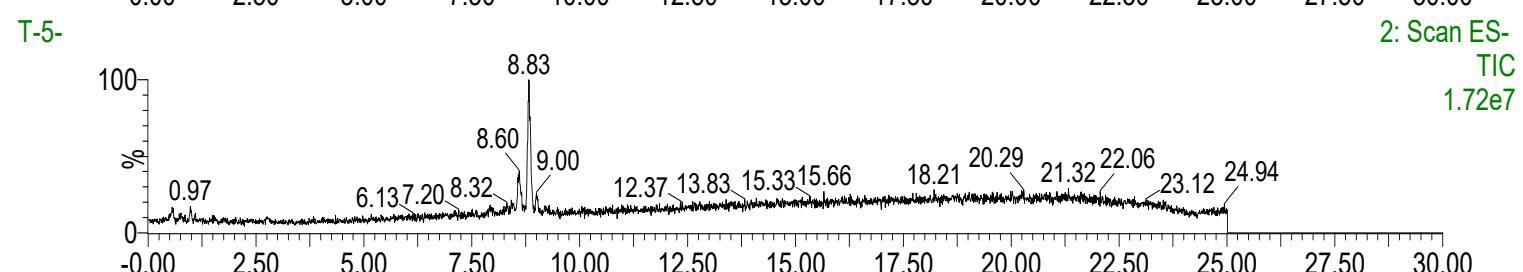
T-5-



T-5-



T-5-



T-5-

