

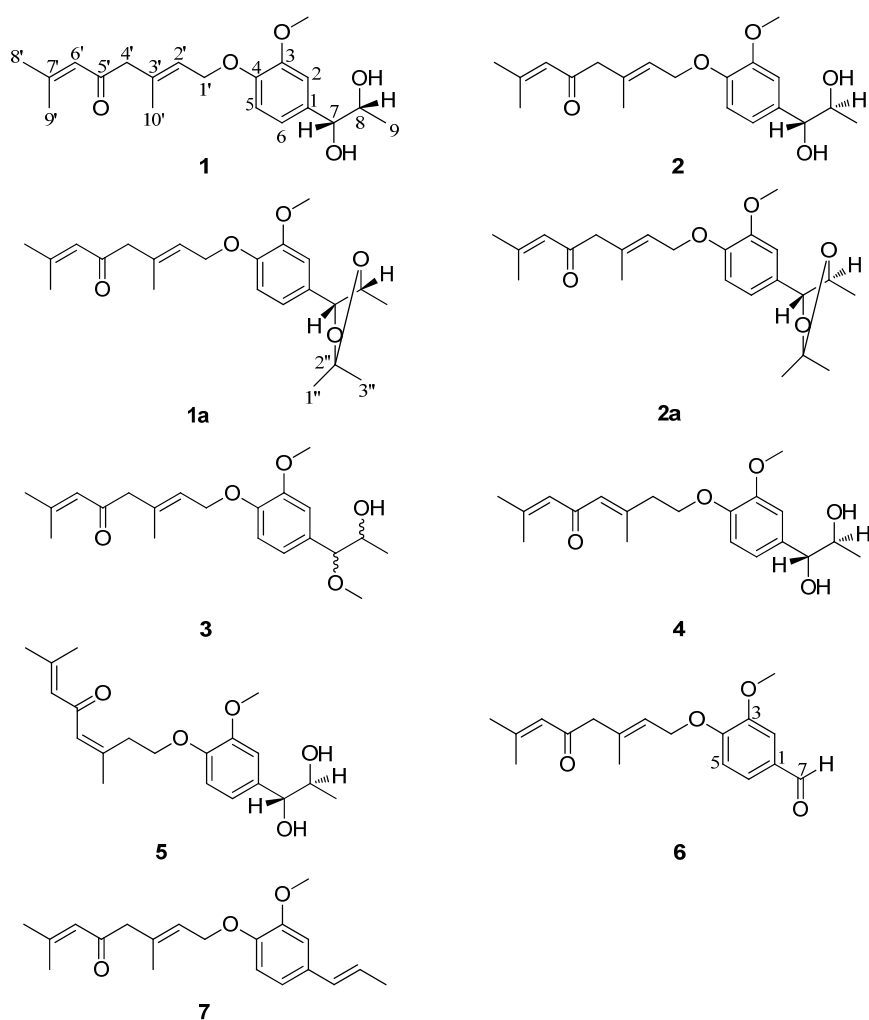
New monoterpene phenyl ethers from *Illicium micranthum*

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Structures of compounds 1–7, 1a and 2a

Figure 1S-7S. NMR and MS spectra of compound **1**

Figure 8S-14S. NMR and MS spectra of compound **2**

Figure 15S-17S. NMR spectra of compound **1a**

Figure 18S-20S. NMR spectra of compound **2a**

Figure 21S-27S. NMR and MS spectra of compound **3**

Figure 28S-34S. NMR and MS spectra of compound **4**

Figure 35S-41S. NMR and MS spectra of compound **5**

Figure 42S-48S. NMR and MS spectra of compound **6**

Figure 49S-55S. NMR and MS spectra of compound **7**

Figure 1S. ¹H NMR of compound 1.

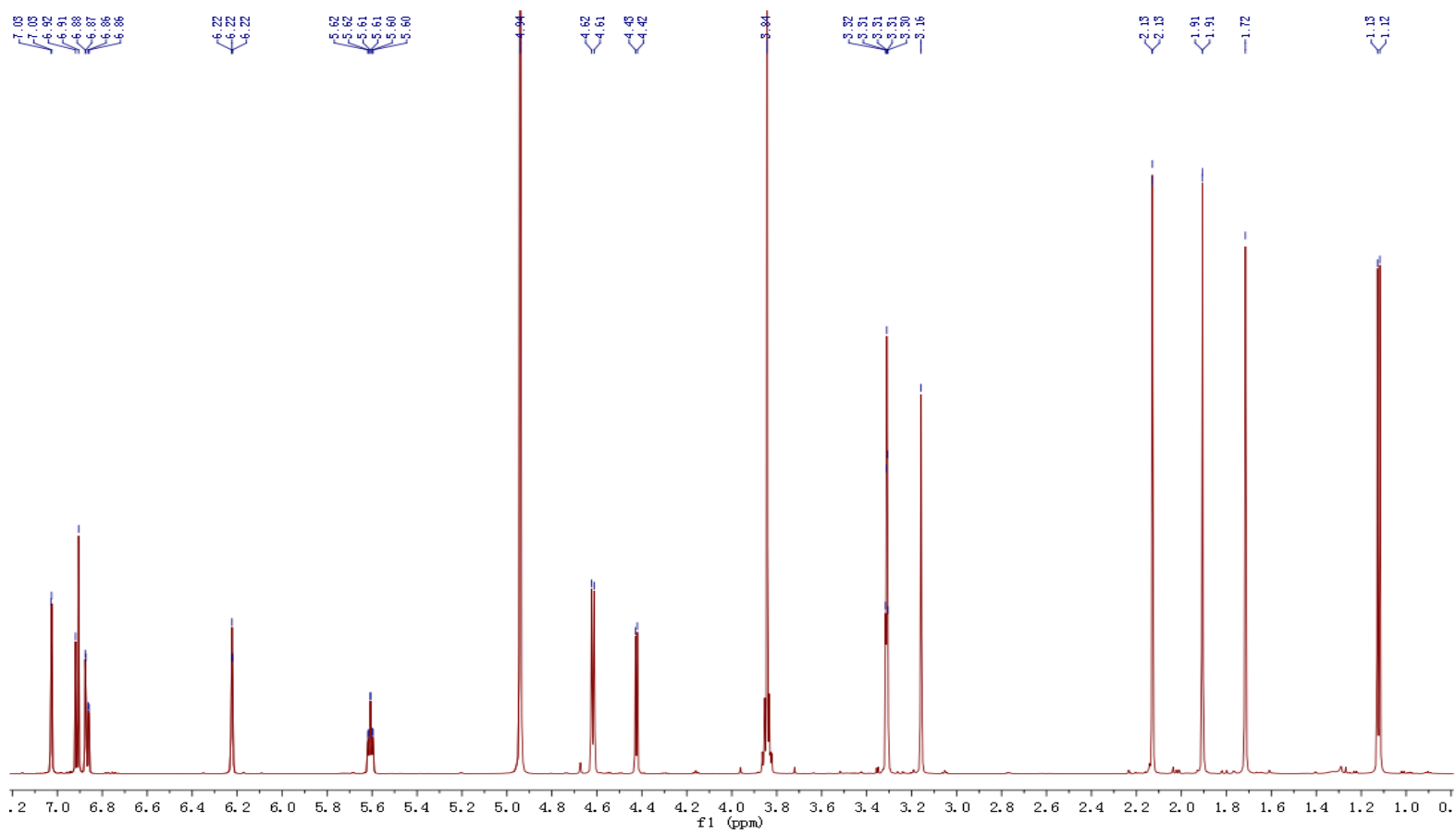


Figure 2S. ^{13}C NMR and DEPT of compound **1**.

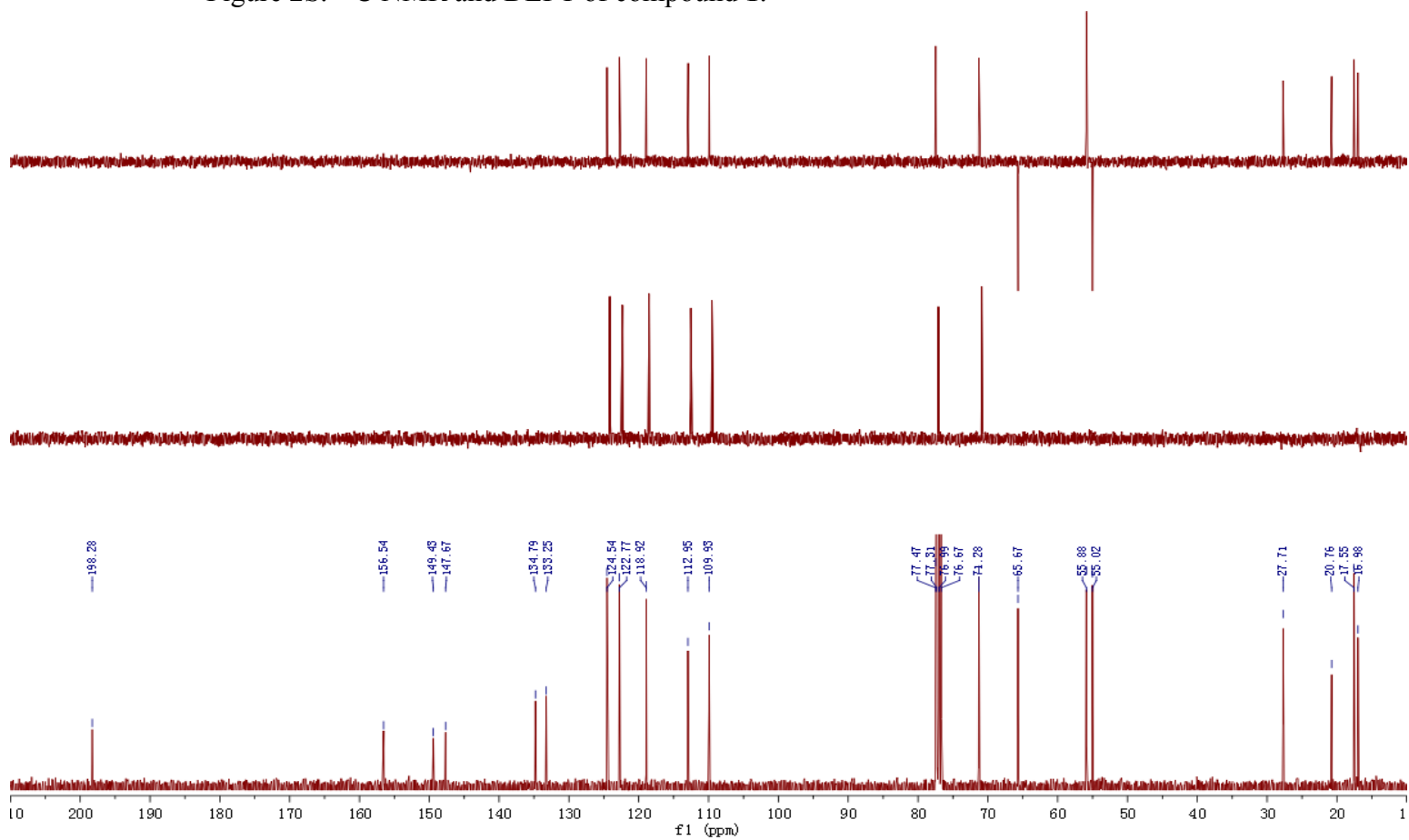


Figure 3S. HSQC of compound 1

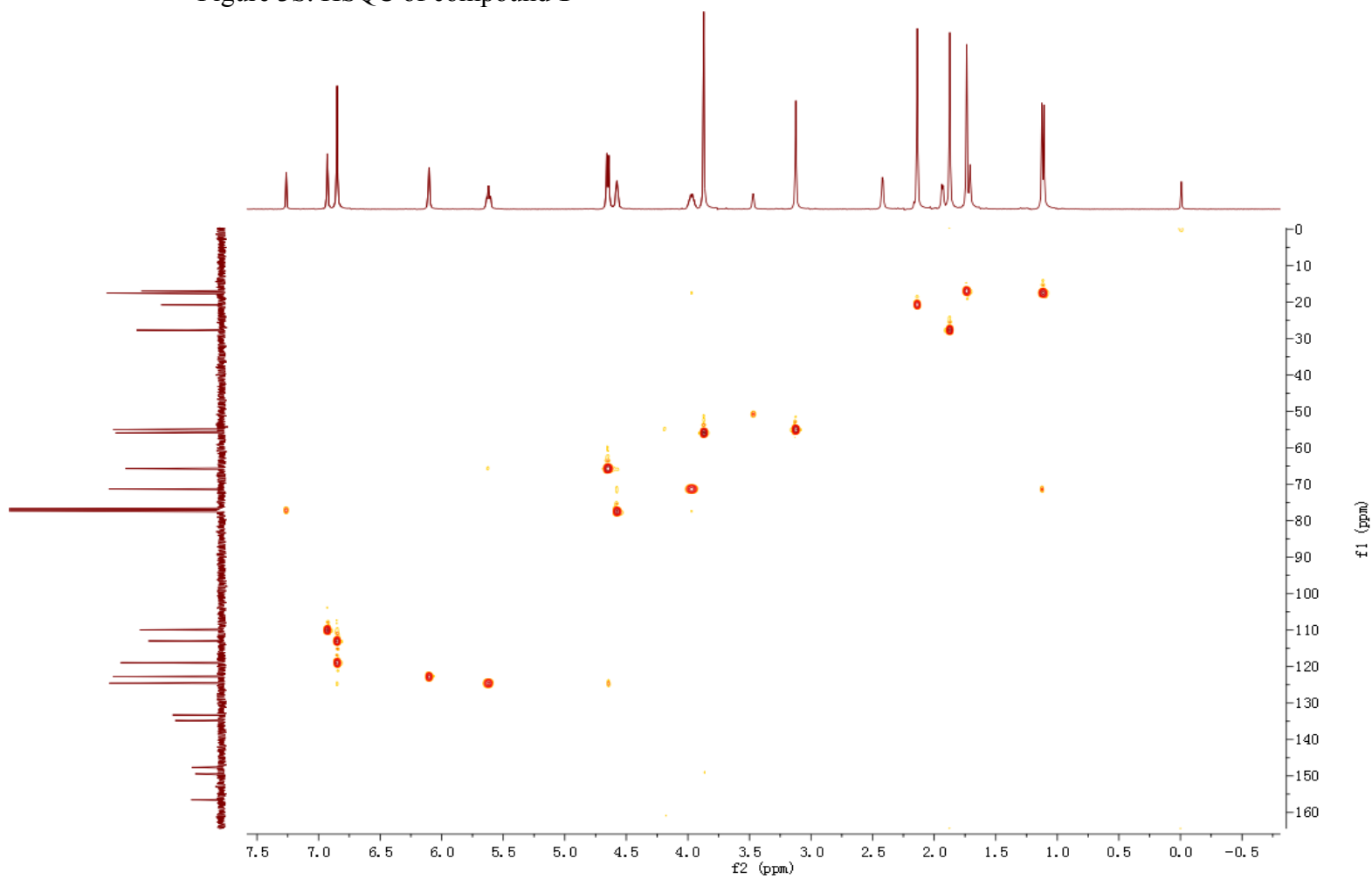


Figure 4S. HMBC of compound 1.

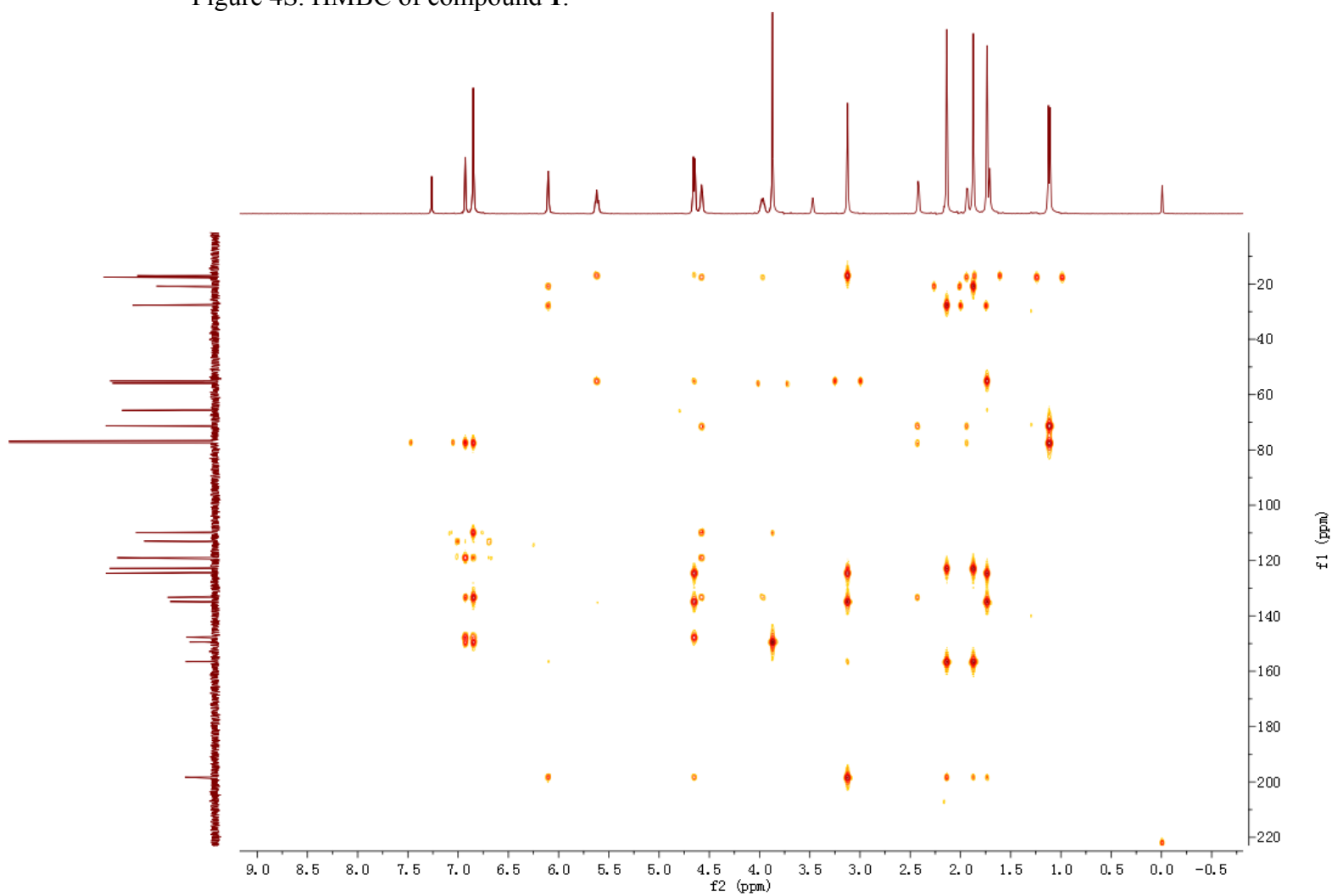


Figure 5S. H-H COSY of compound 1.

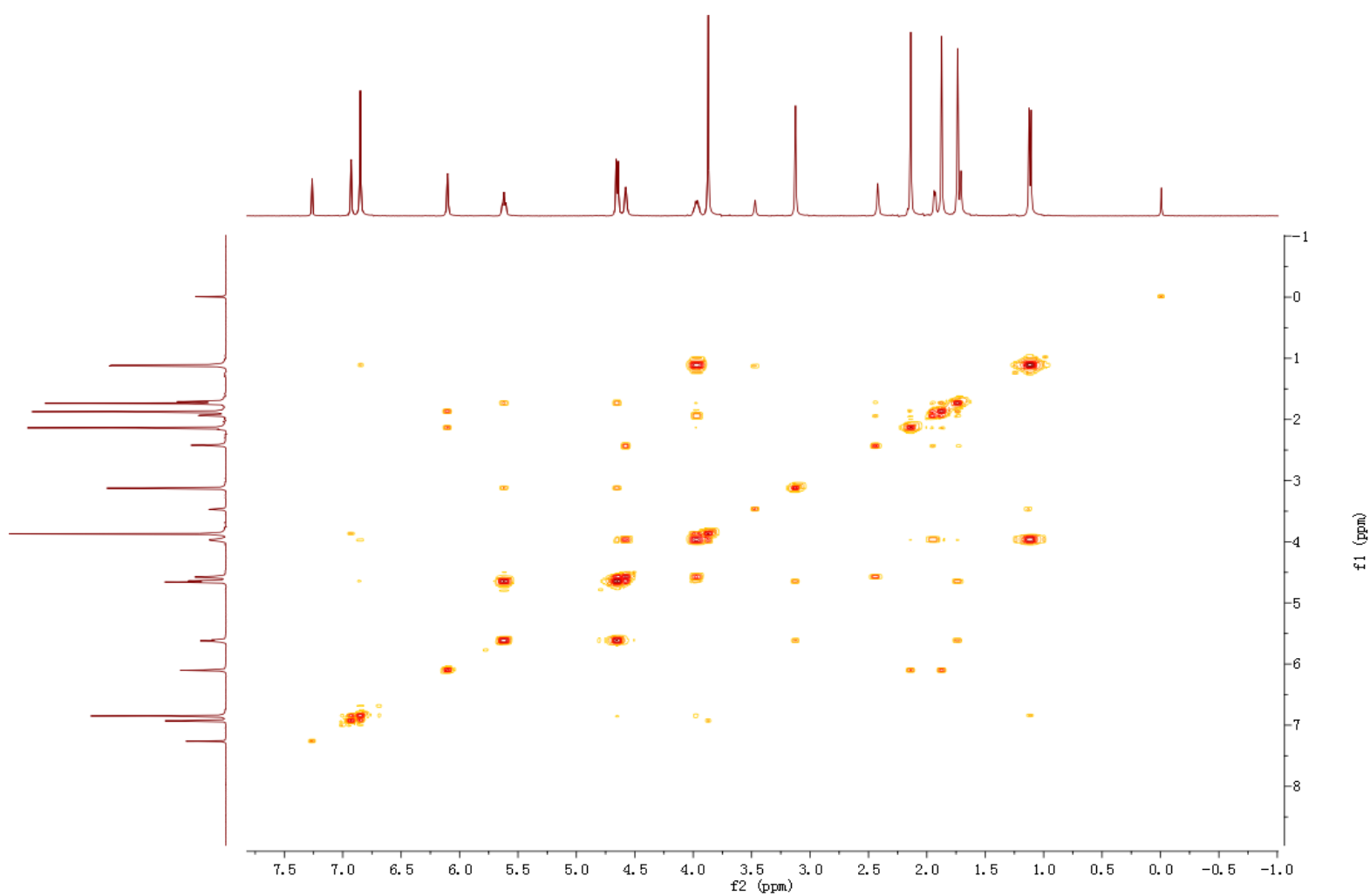


Figure 6S. ROESY of compound 1.

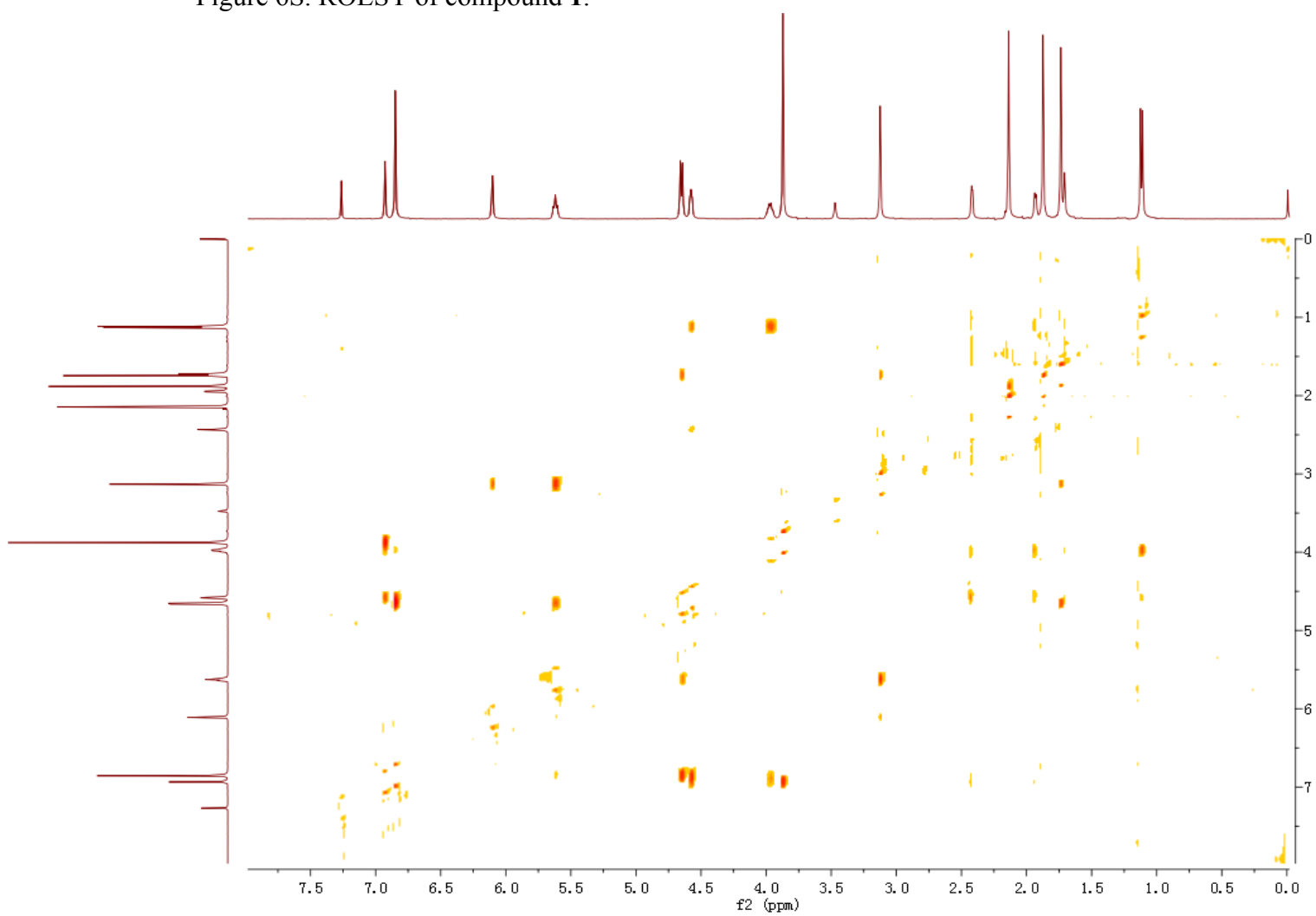


Figure 7S. HRESIMS of compound 1.

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 60.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

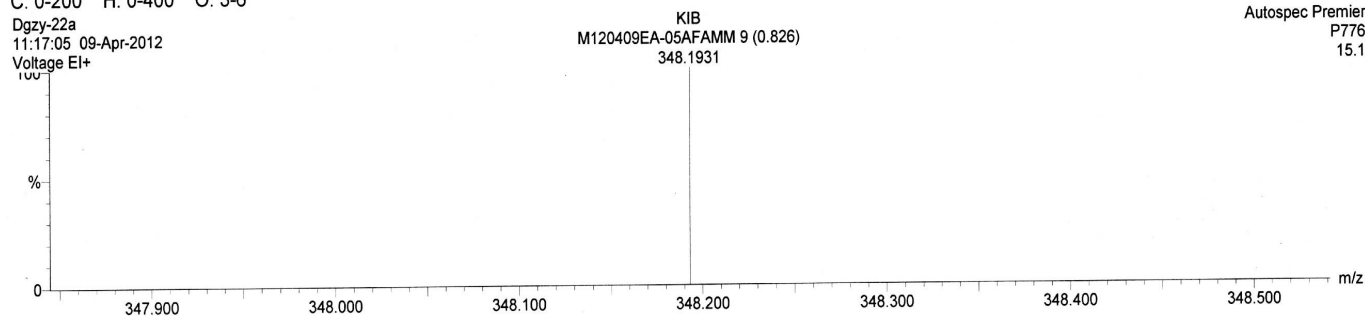
C: 0-200 H: 0-400 O: 3-6

Dgzy-22a

11:17:05 09-Apr-2012

Voltage EI+

Autospec Premier
P776
15.1



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.1931	348.1937	-0.6	-1.7	7.0	5546027.0	C20 H28 O5

Figure 8S. ^1H NMR of compound **2**.

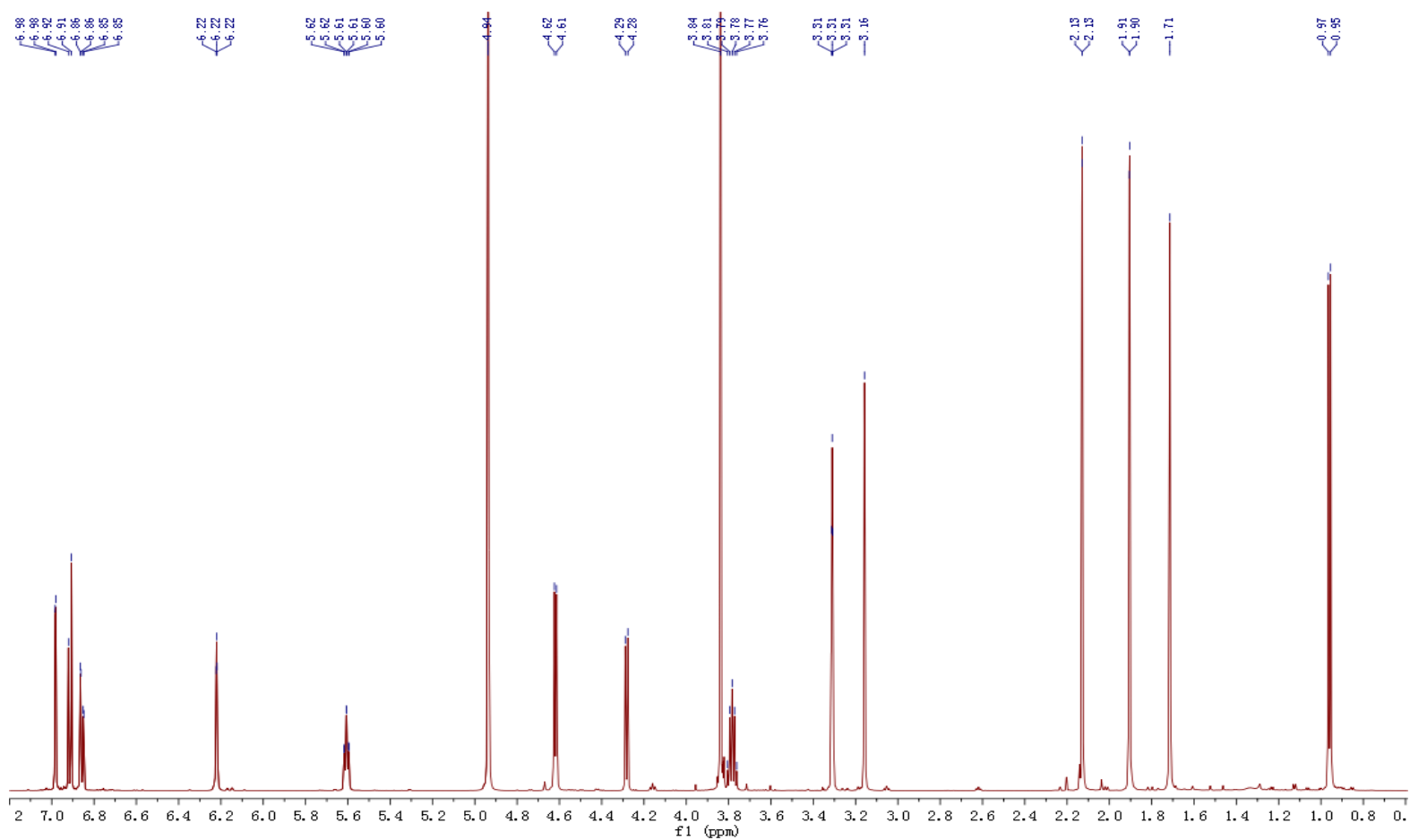


Figure 9S. ^{13}C NMR and DEPT of compound **2**.

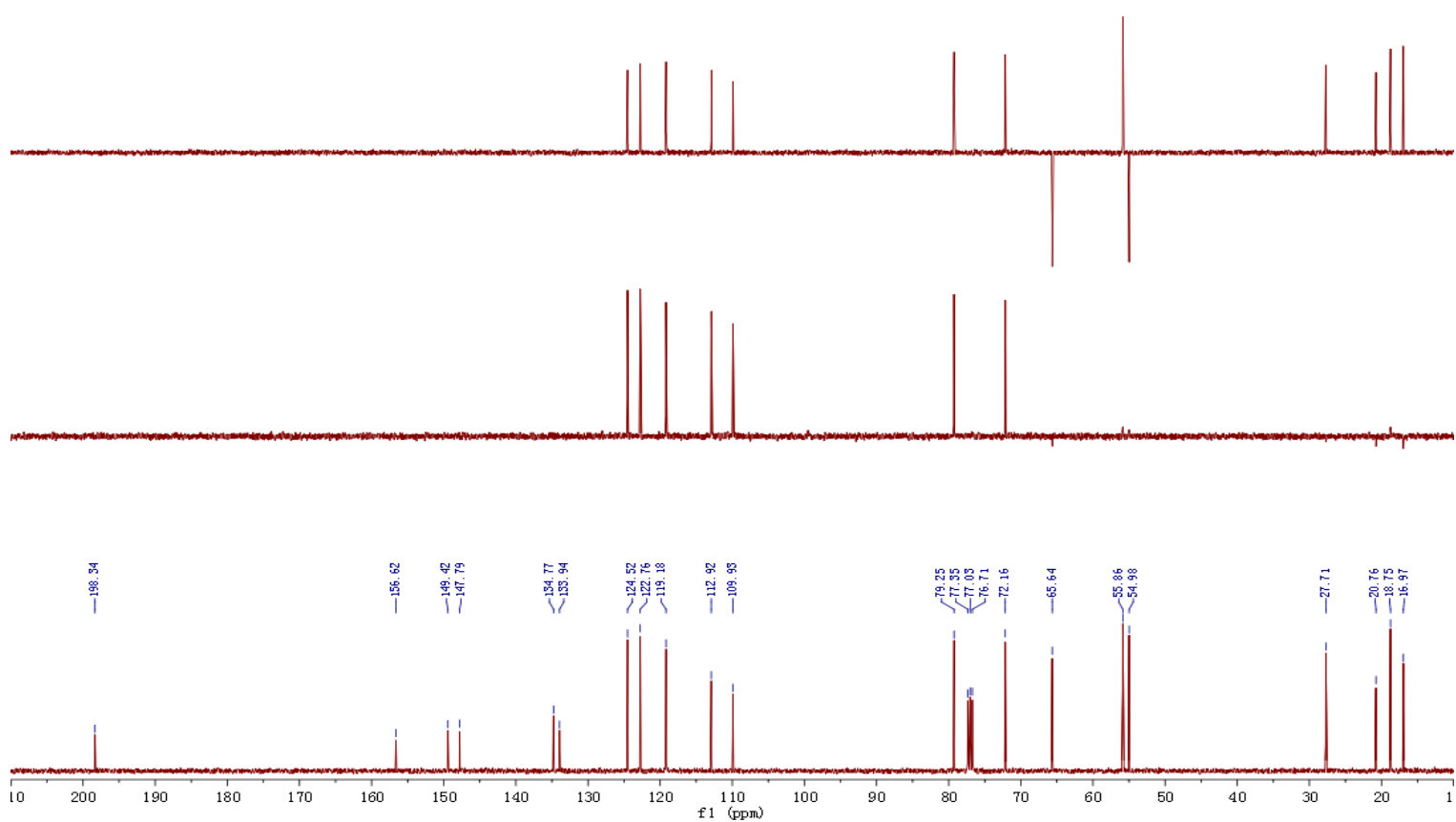


Figure 10S. HSQC of compound 2.

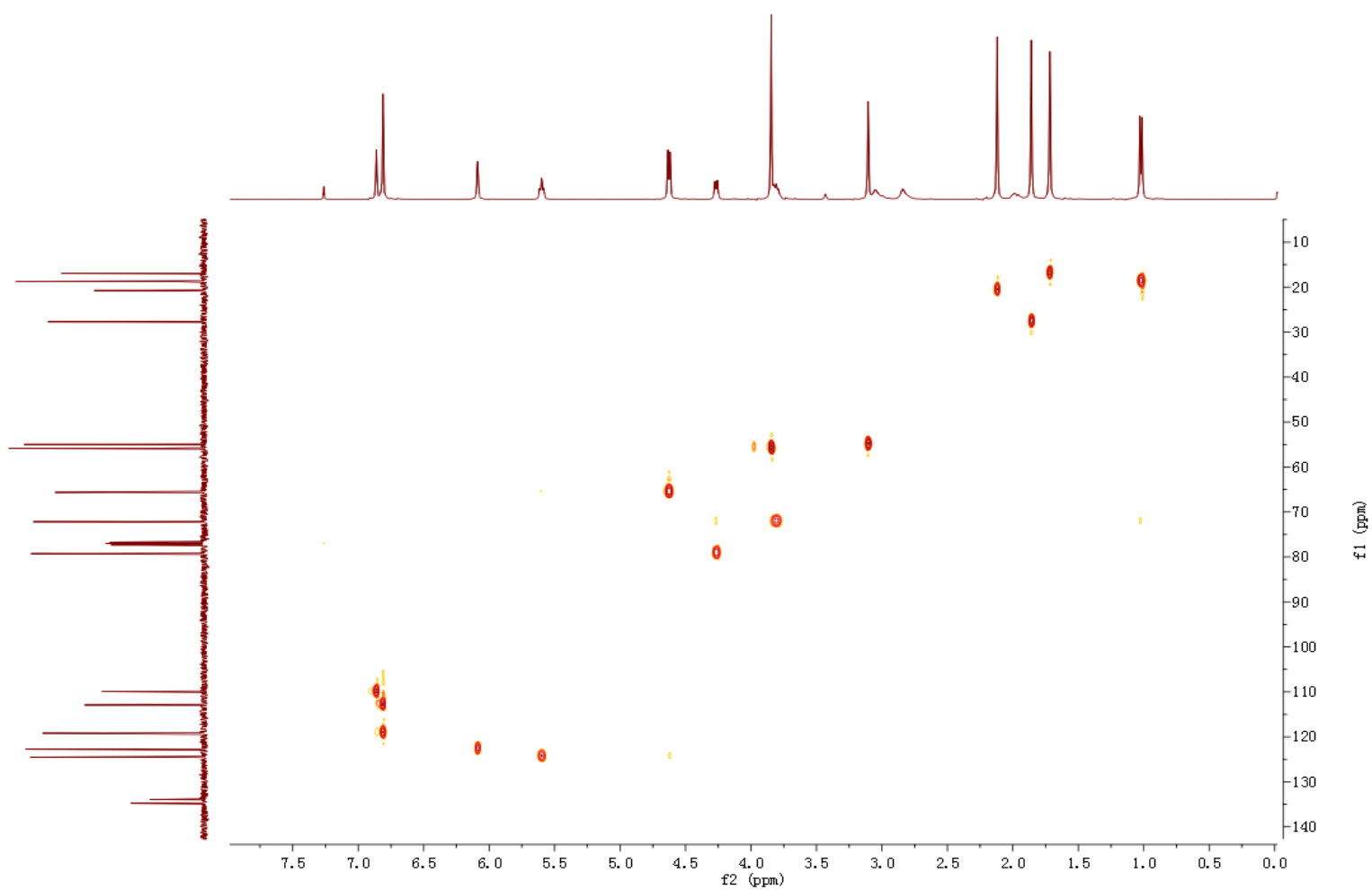


Figure 11S. HMBC of compound 2.

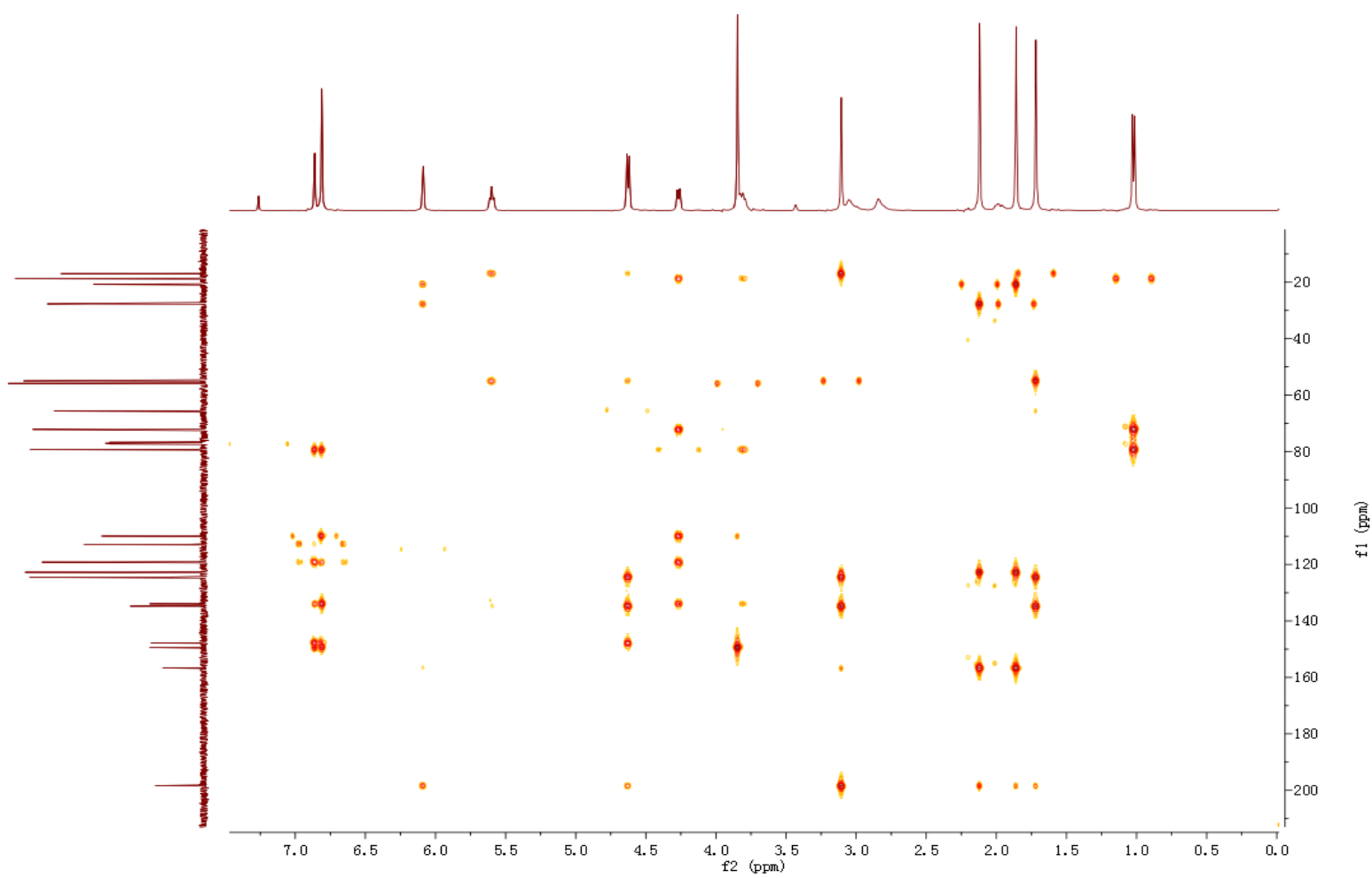


Figure 12S. ^1H - ^1H COSY of compound 2.

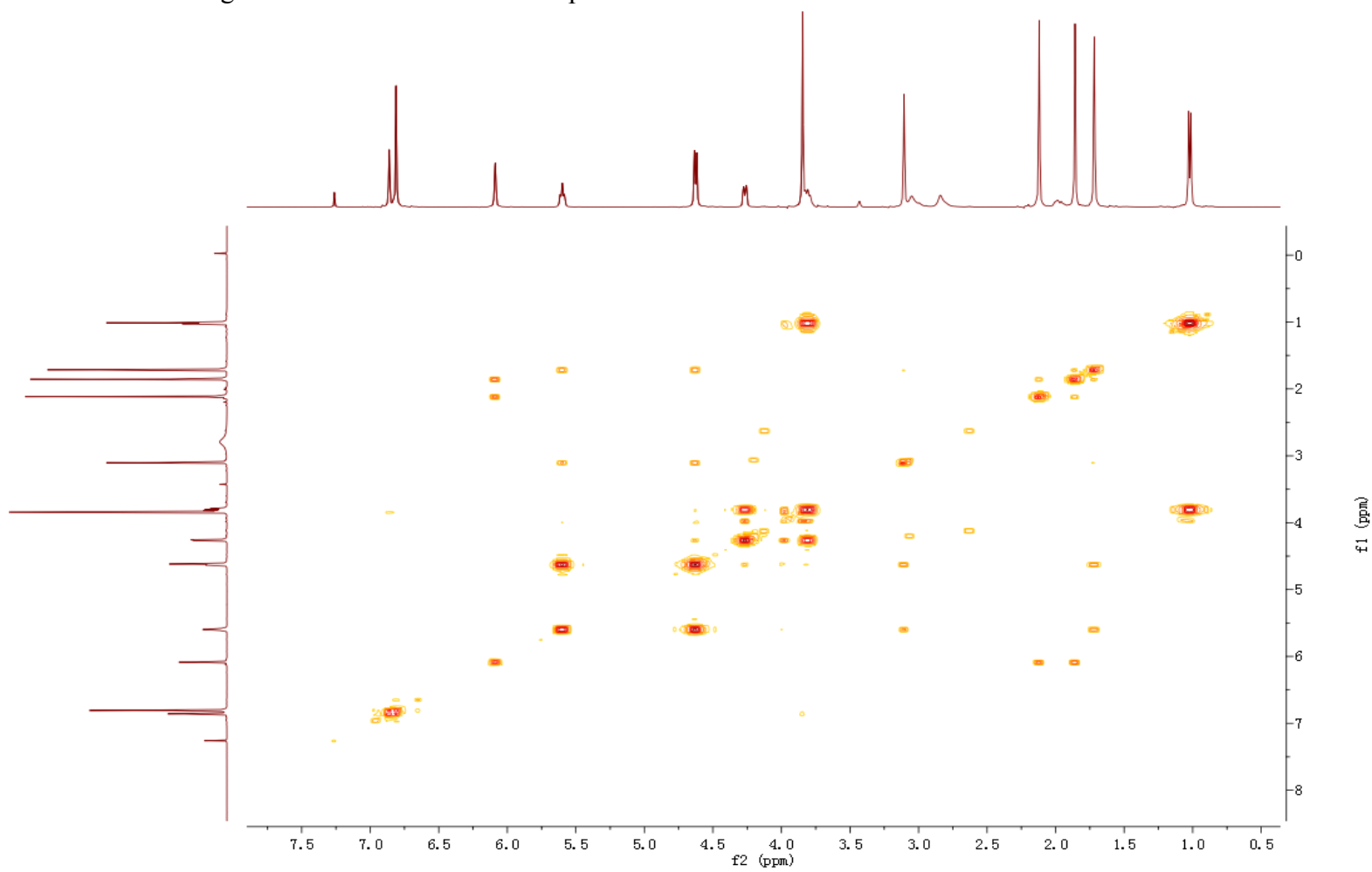


Figure 13S. ROESY of compound 2.

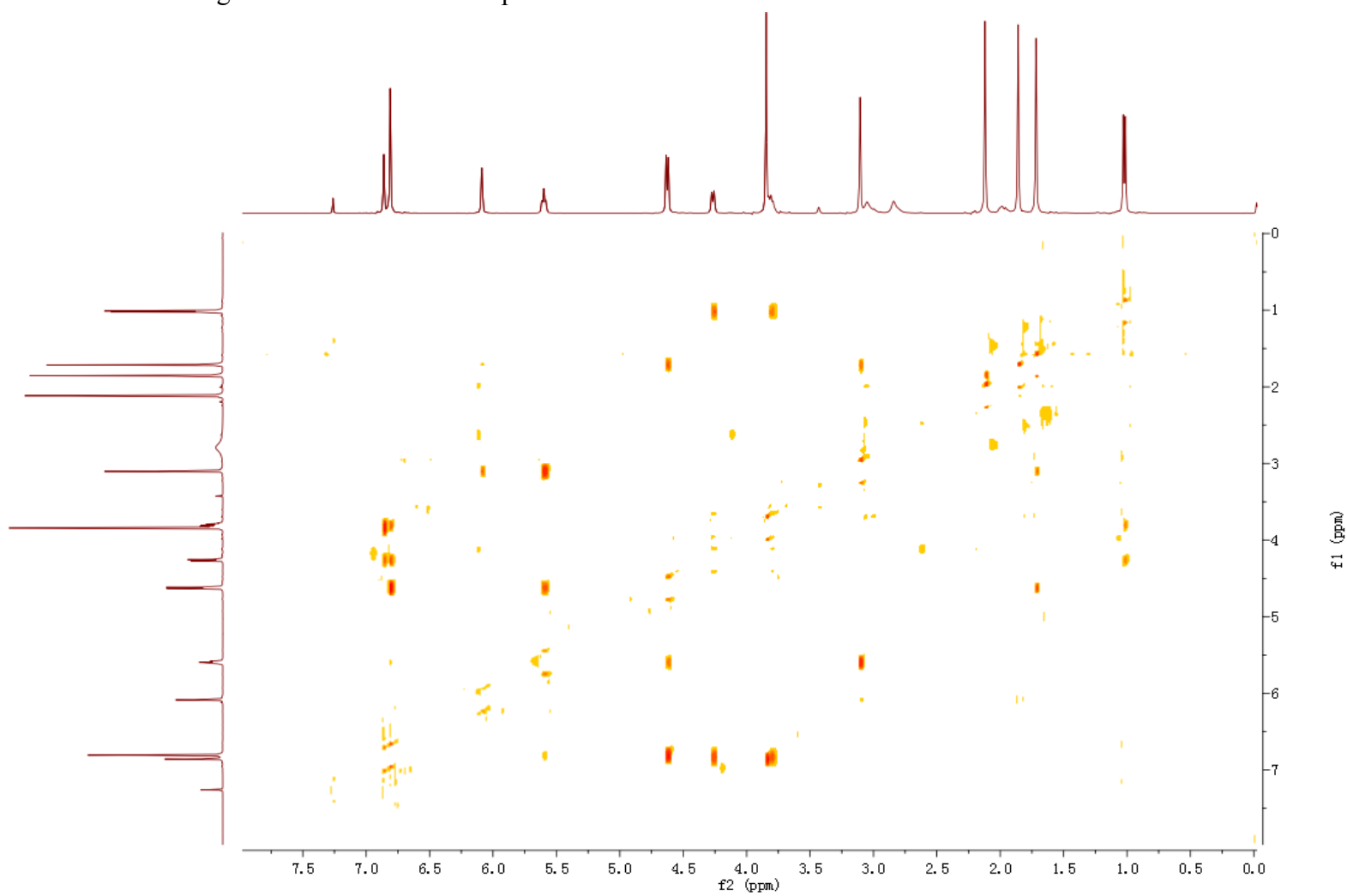


Figure14S. HRESIMS of compound 2.

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 60.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 3-6

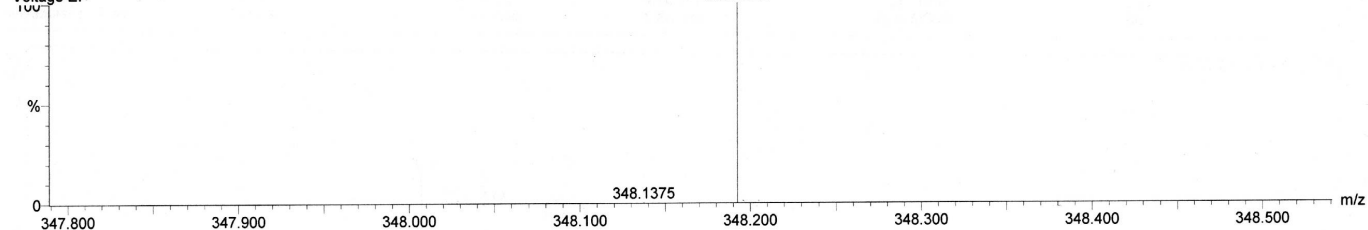
Dgzy-22b

11:20:53 09-Apr-2012

Voltage EI+

KIB
M120409EA-06AFAMM 12 (1.102)
348.1925

Autospec Premier
P776
1.73e3



Minimum: 0.5
Maximum: 73.0 10.0 60.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.1925	348.1937	-1.2	-3.4	7.0	5546874.5	C20 H28 O5

Figure 15S. ^1H NMR of compound **1a**.

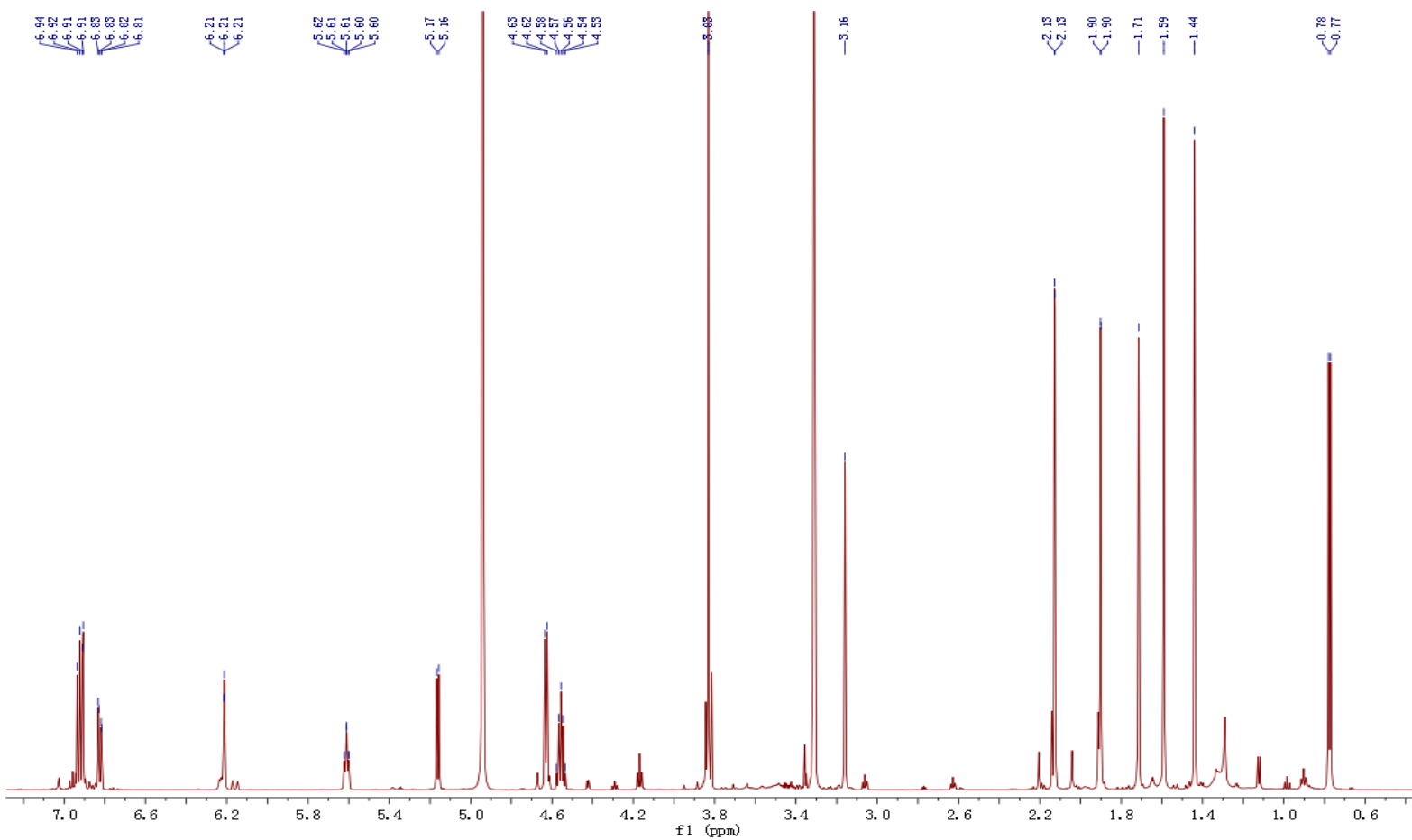


Figure 16S. ^{13}C NMR and DEPT of compound **1a**.

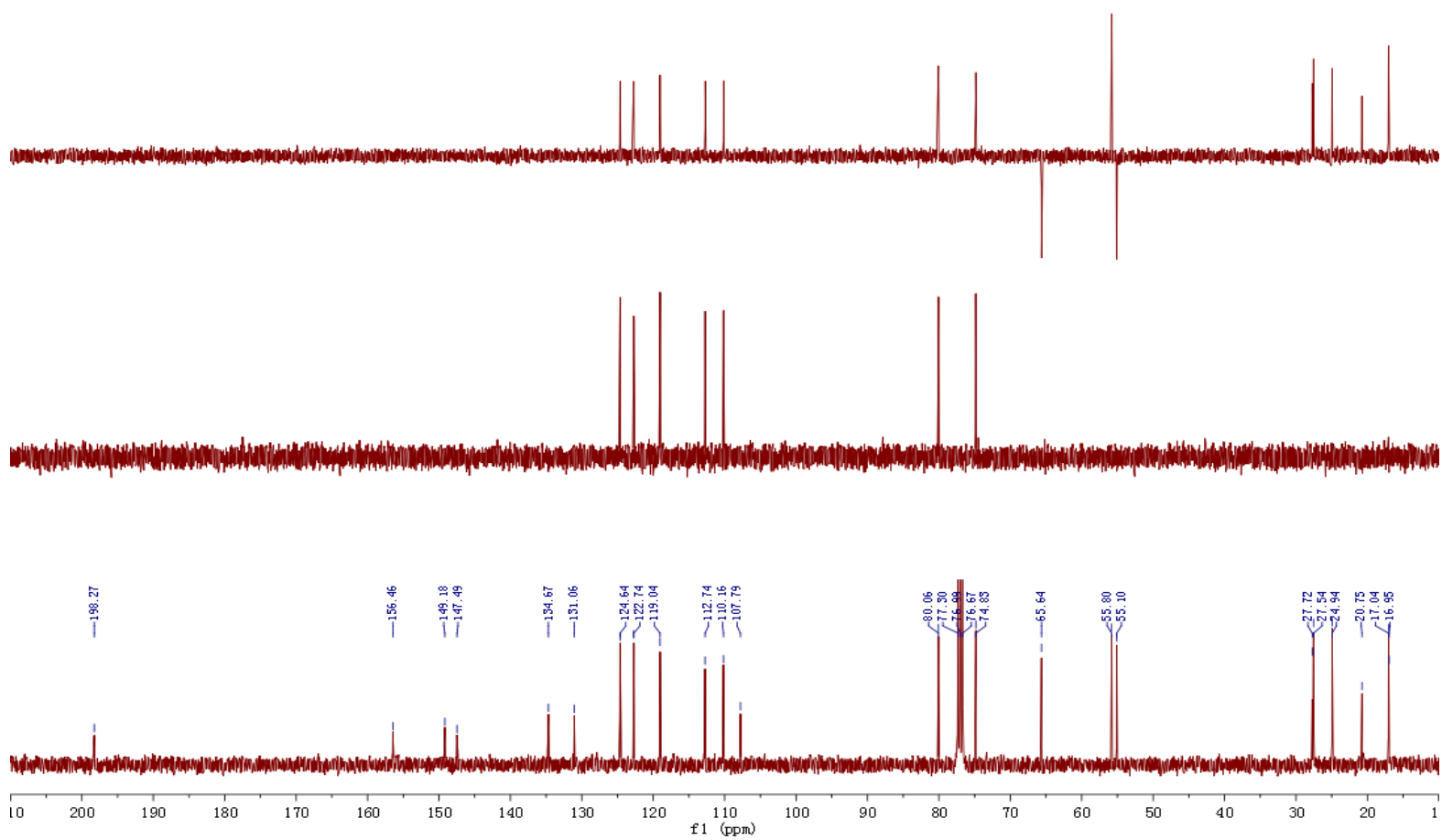


Figure 17S. ROESY of compound **1a**.

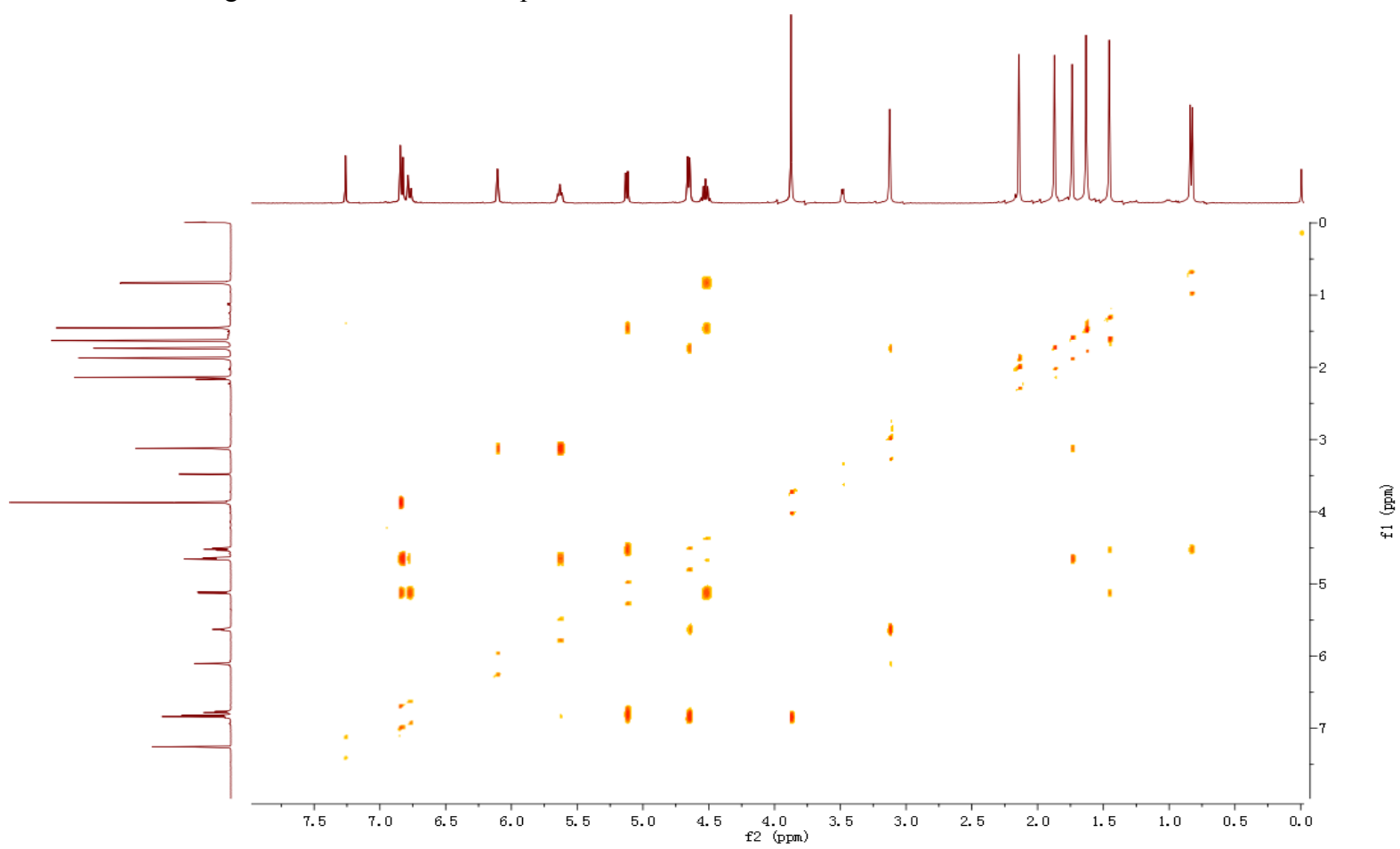


Figure 18S. ^1H NMR of compound **2a**.

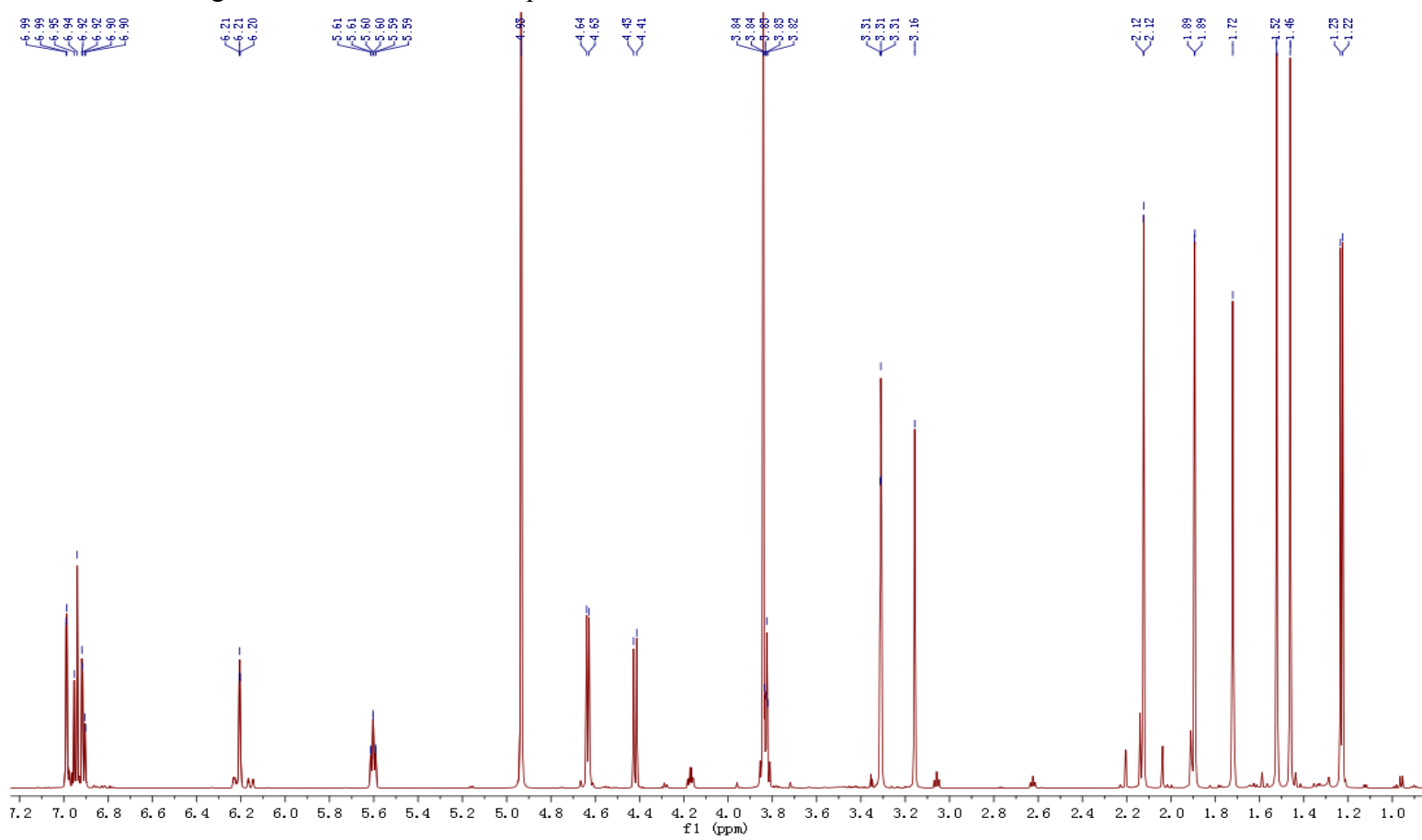


Figure 19S. ^{13}C NMR and DEPT of compound **2a**.

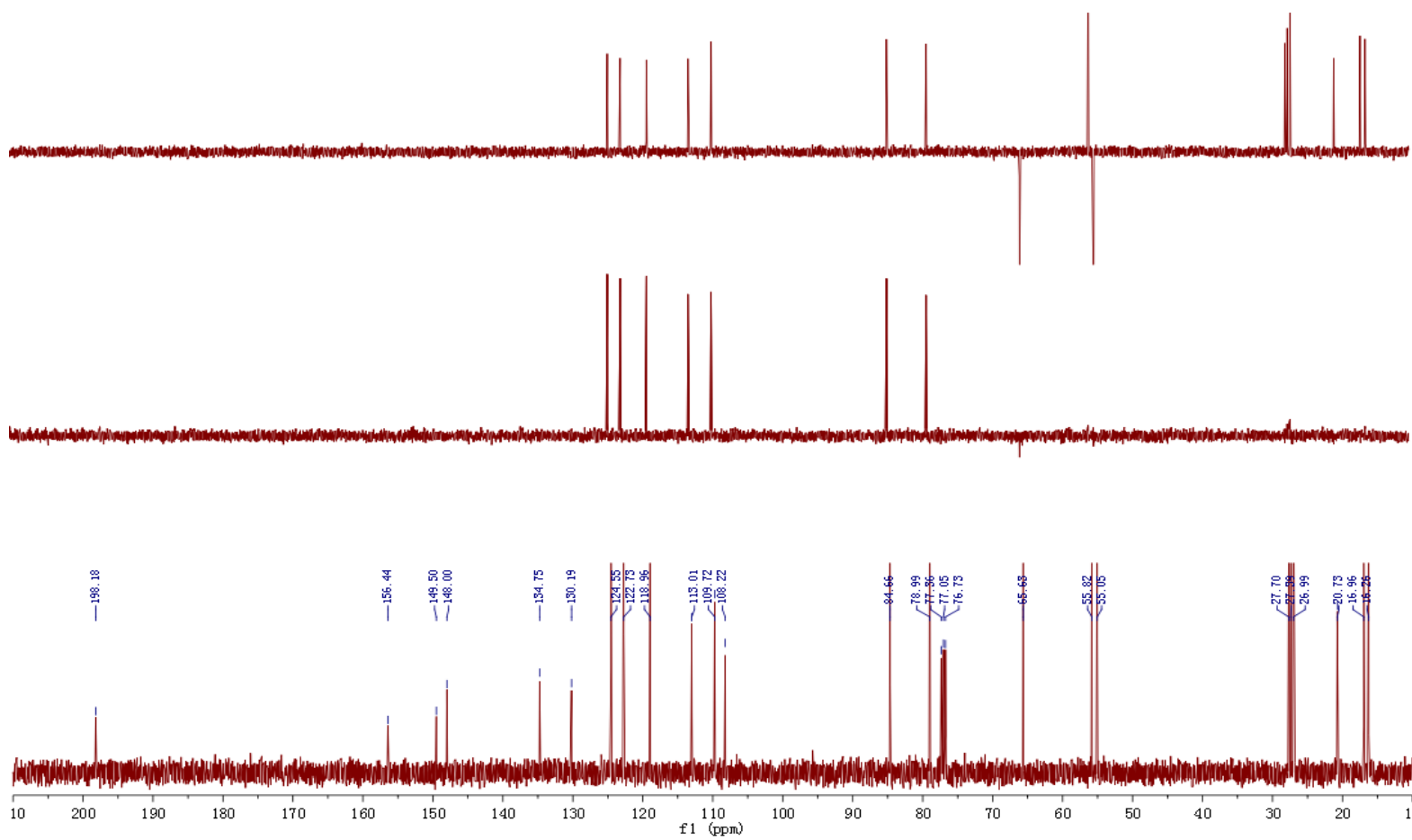


Figure 20S. ROESY of compound **2a**.

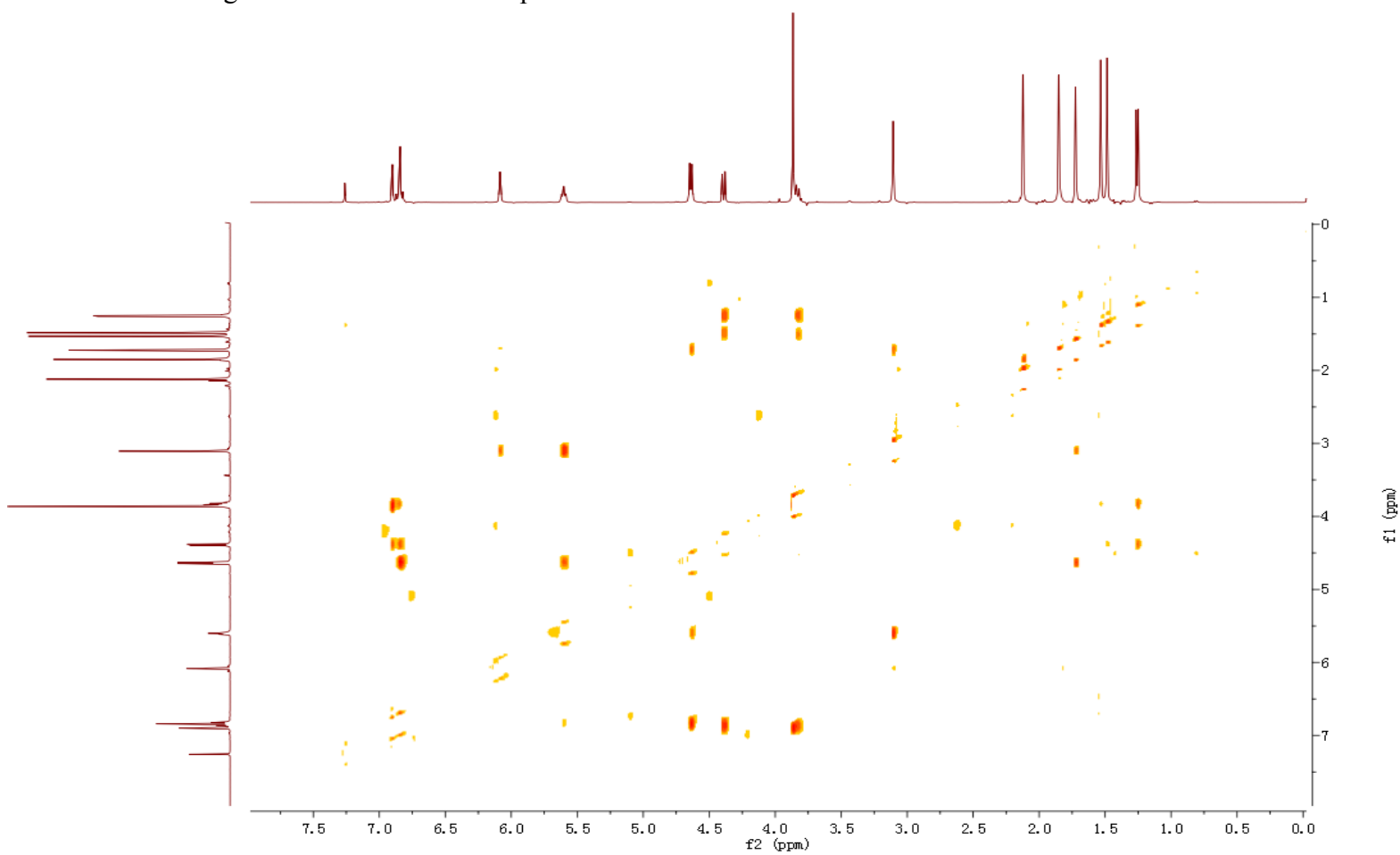


Figure 21S. ^1H NMR of compound **3**.

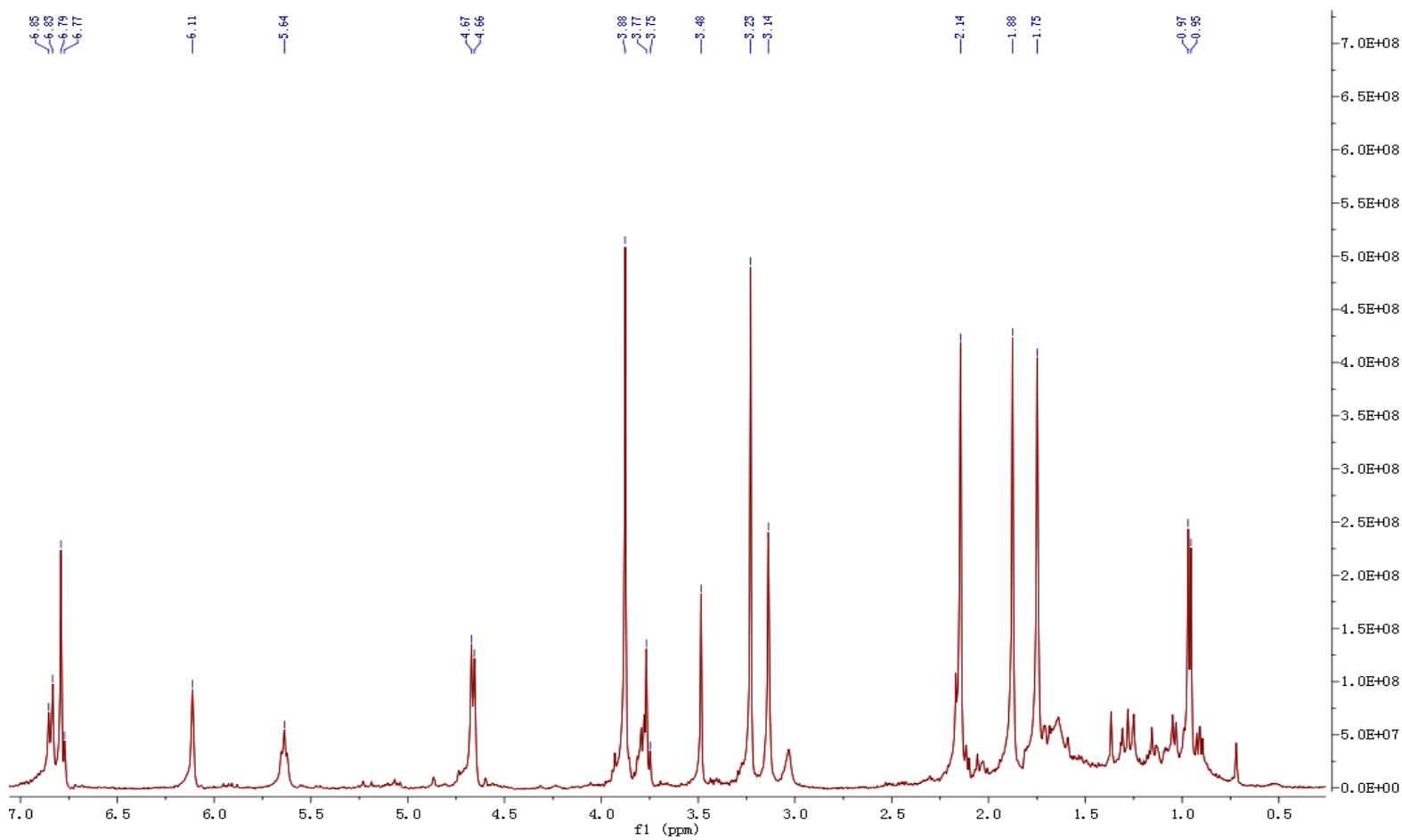


Figure 22S. ^{13}C NMR and DEPT of compound **3**.

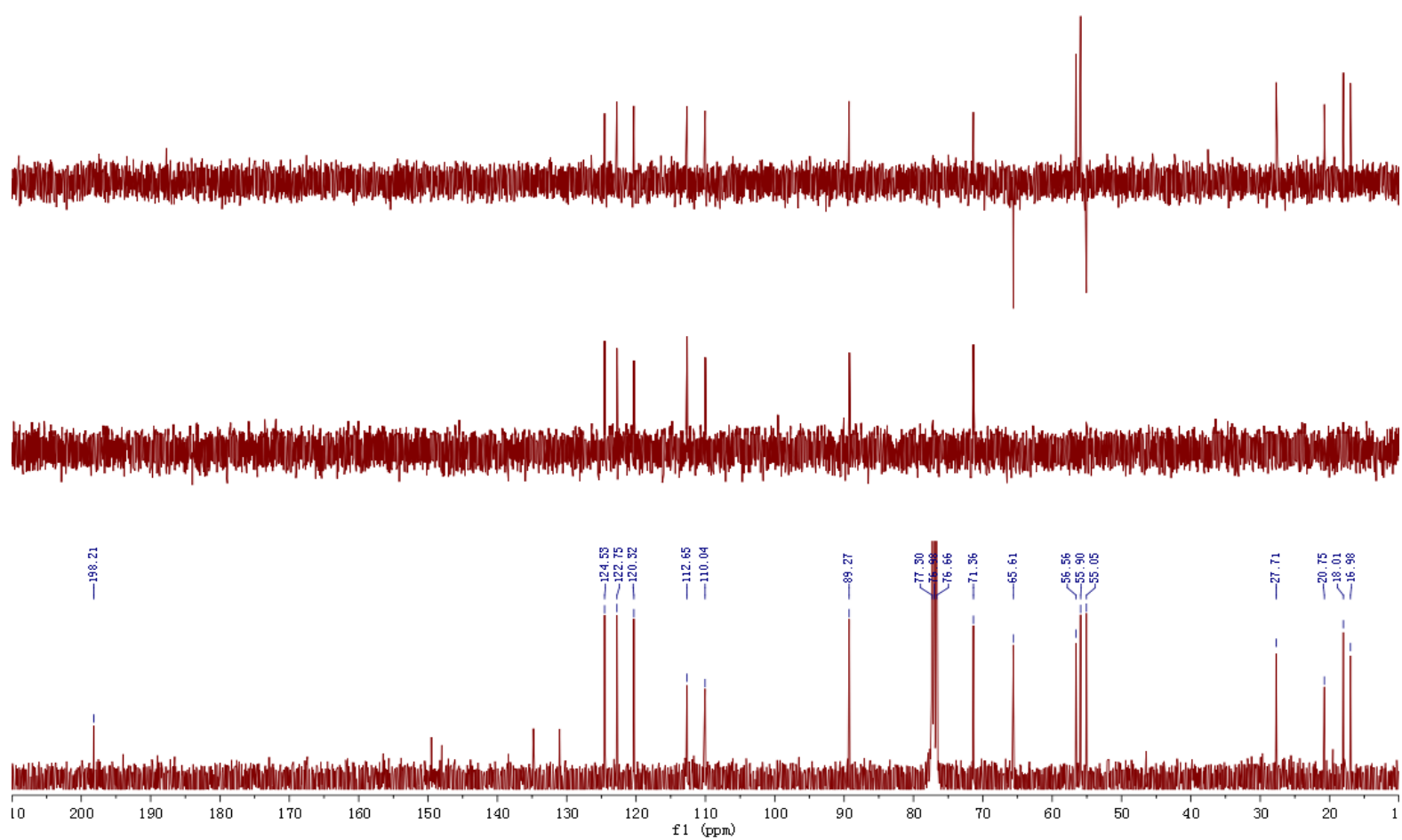


Figure 23S. HSQC of compound 3.

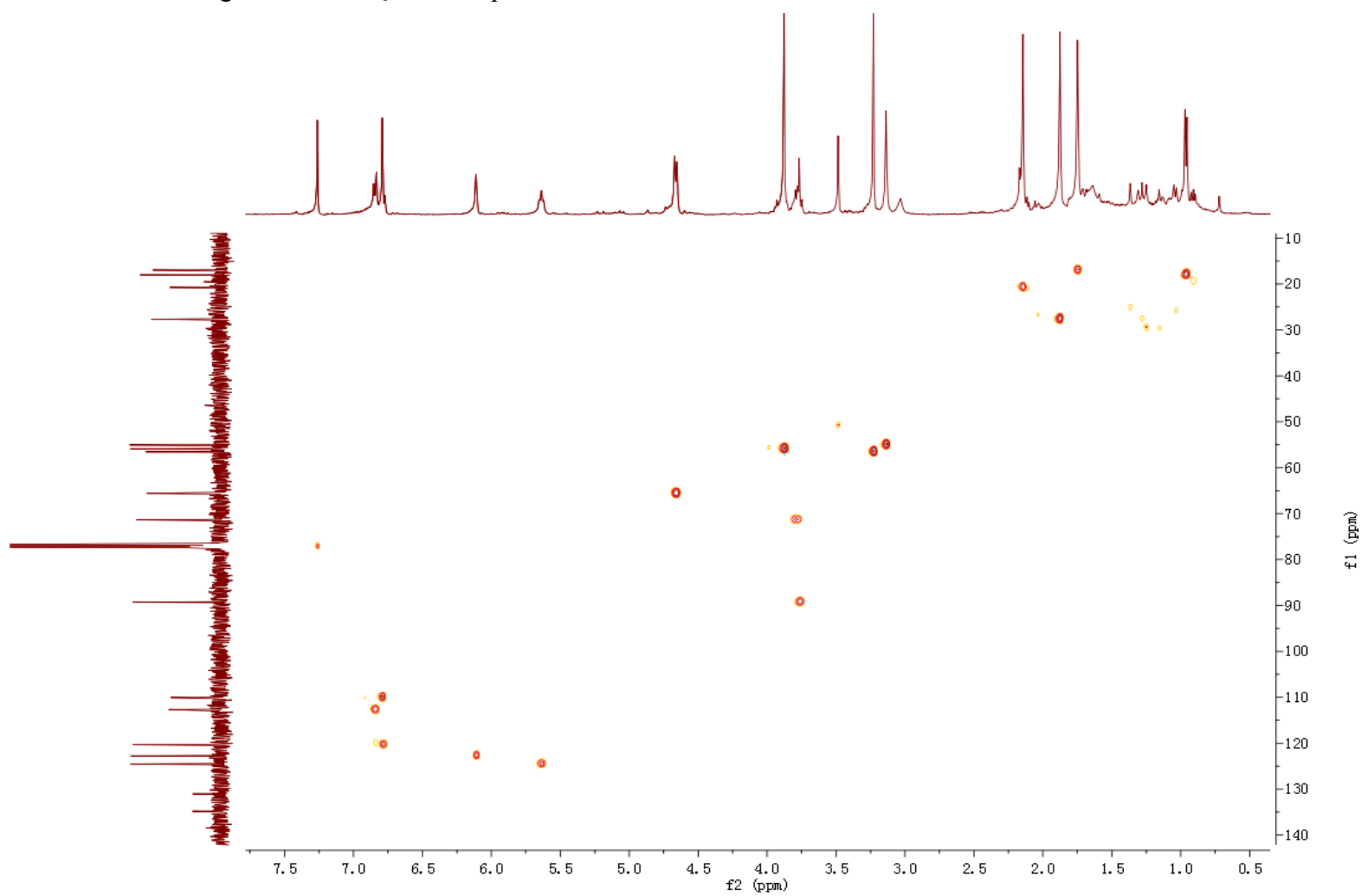


Figure 24S. HMBC of compound **3**.

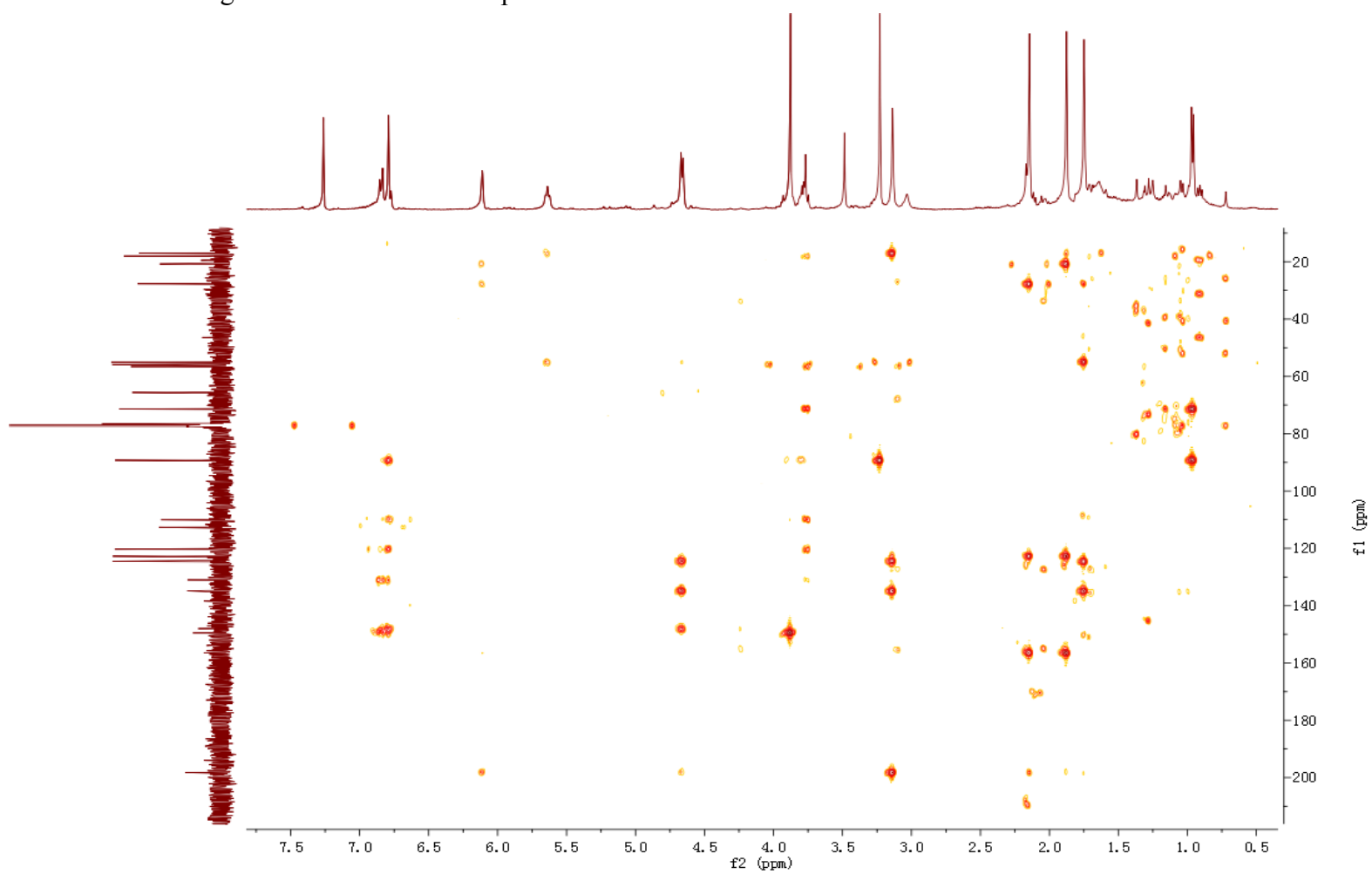


Figure 25S. ^1H - ^1H COSY of compound **3**.

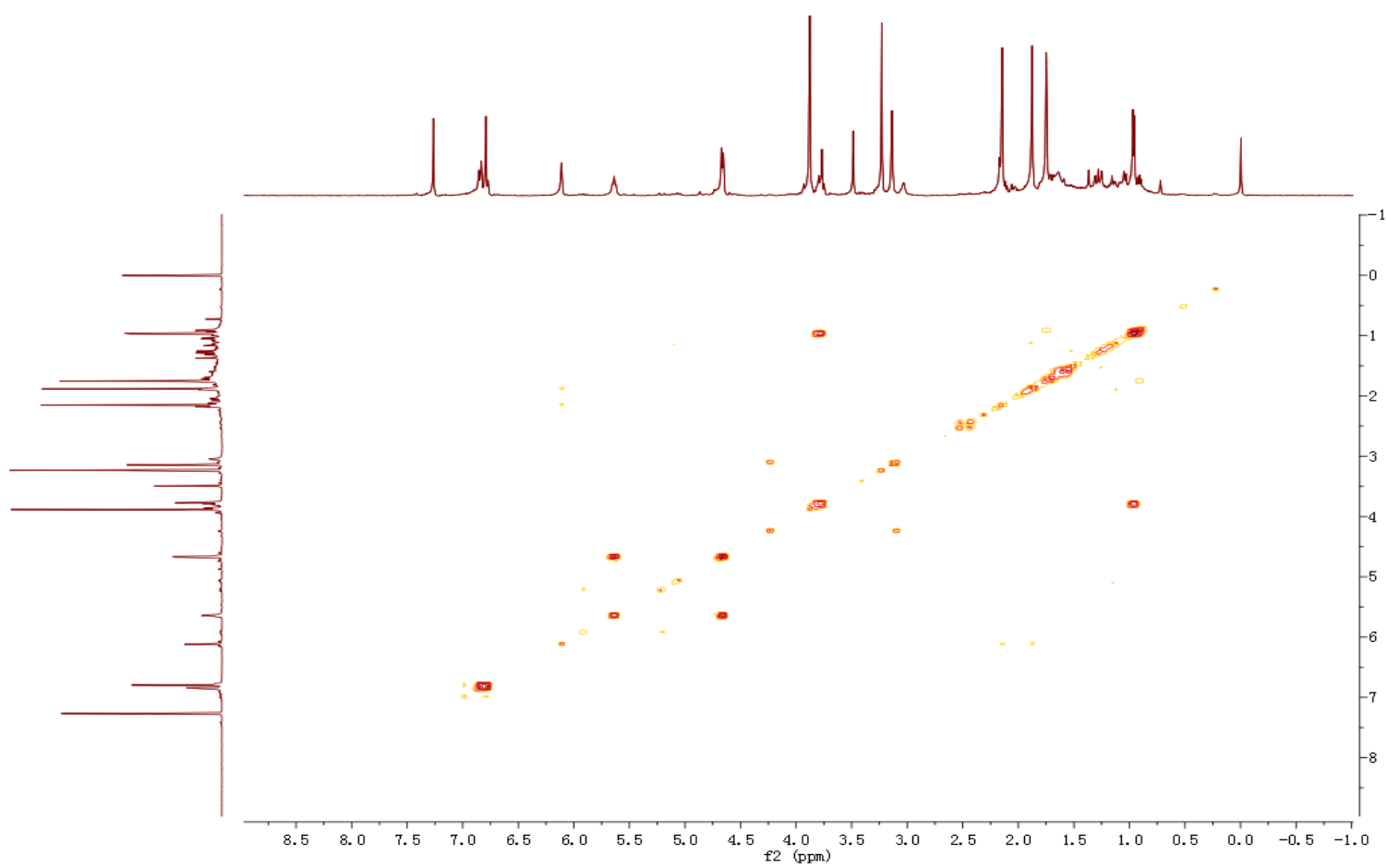


Figure 26S. ROESY of compound **3**.

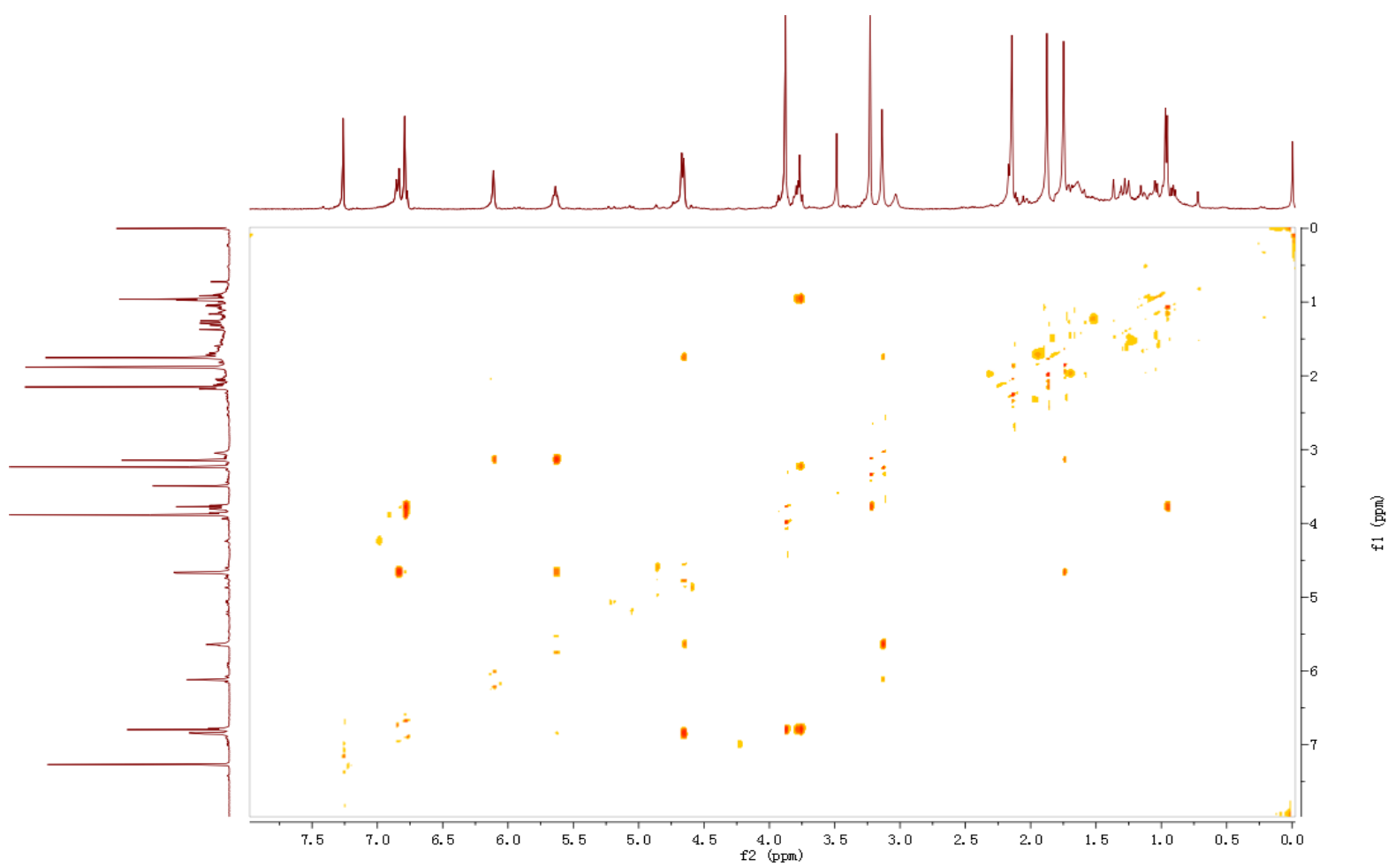


Figure27S. HRESIMS of compound 3.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

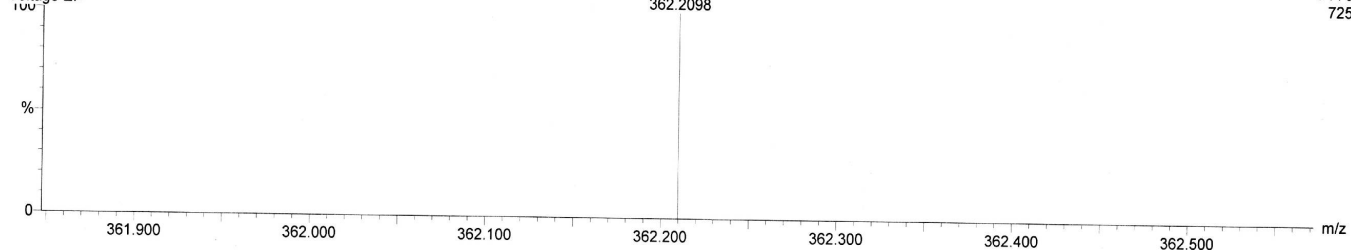
Elements Used:

C: 0-200 H: 0-400 O: 3-6

Dgzy-28c

12:03:06 18-Apr-2012

Voltage EI+



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
362.2098	362.2093	0.5	1.4	7.0	5546375.0	C21 H30 O5

Figure 28S. ^1H NMR of compound 4.

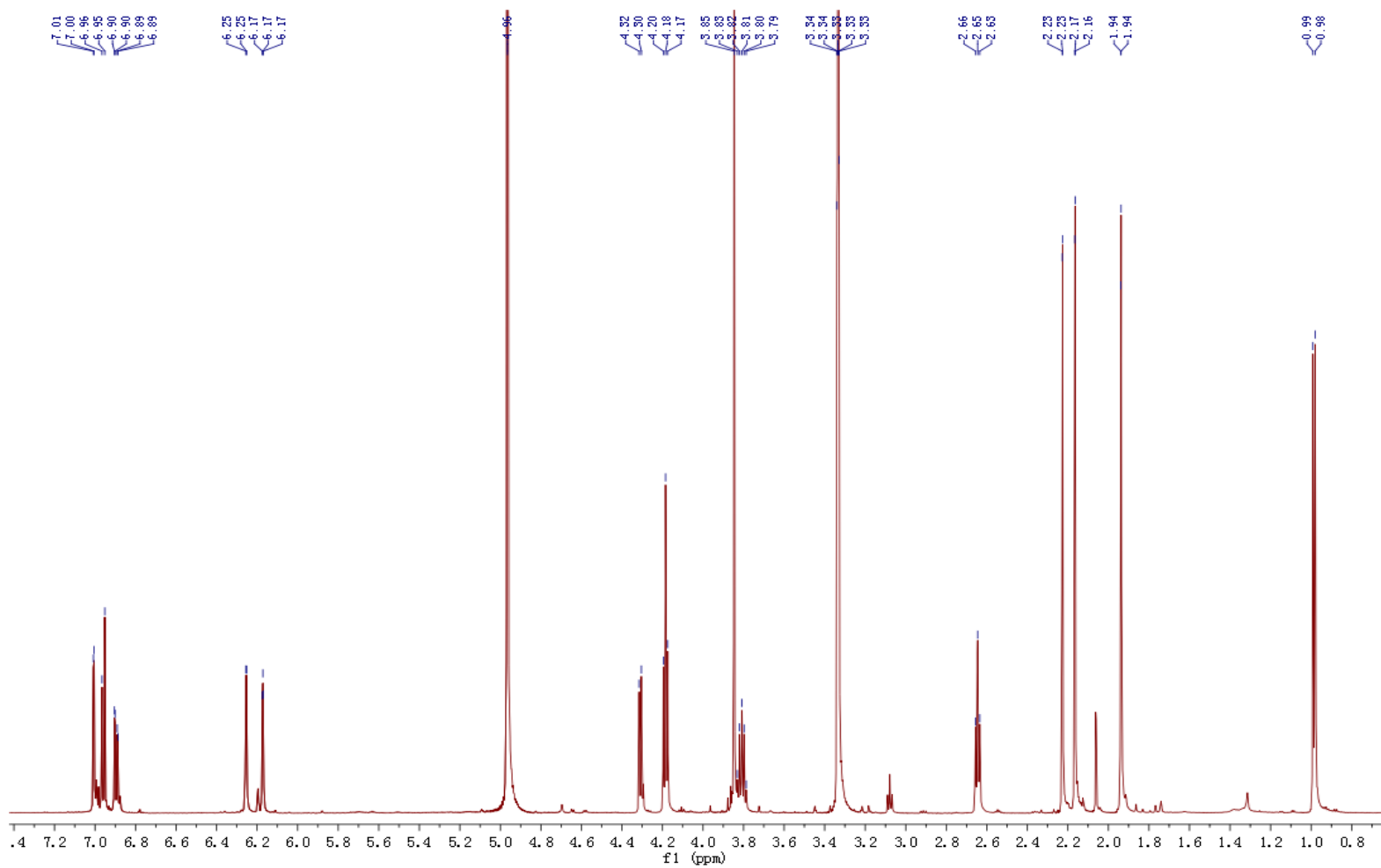


Figure 29S. ^{13}C NMR and DEPT of compound 4.

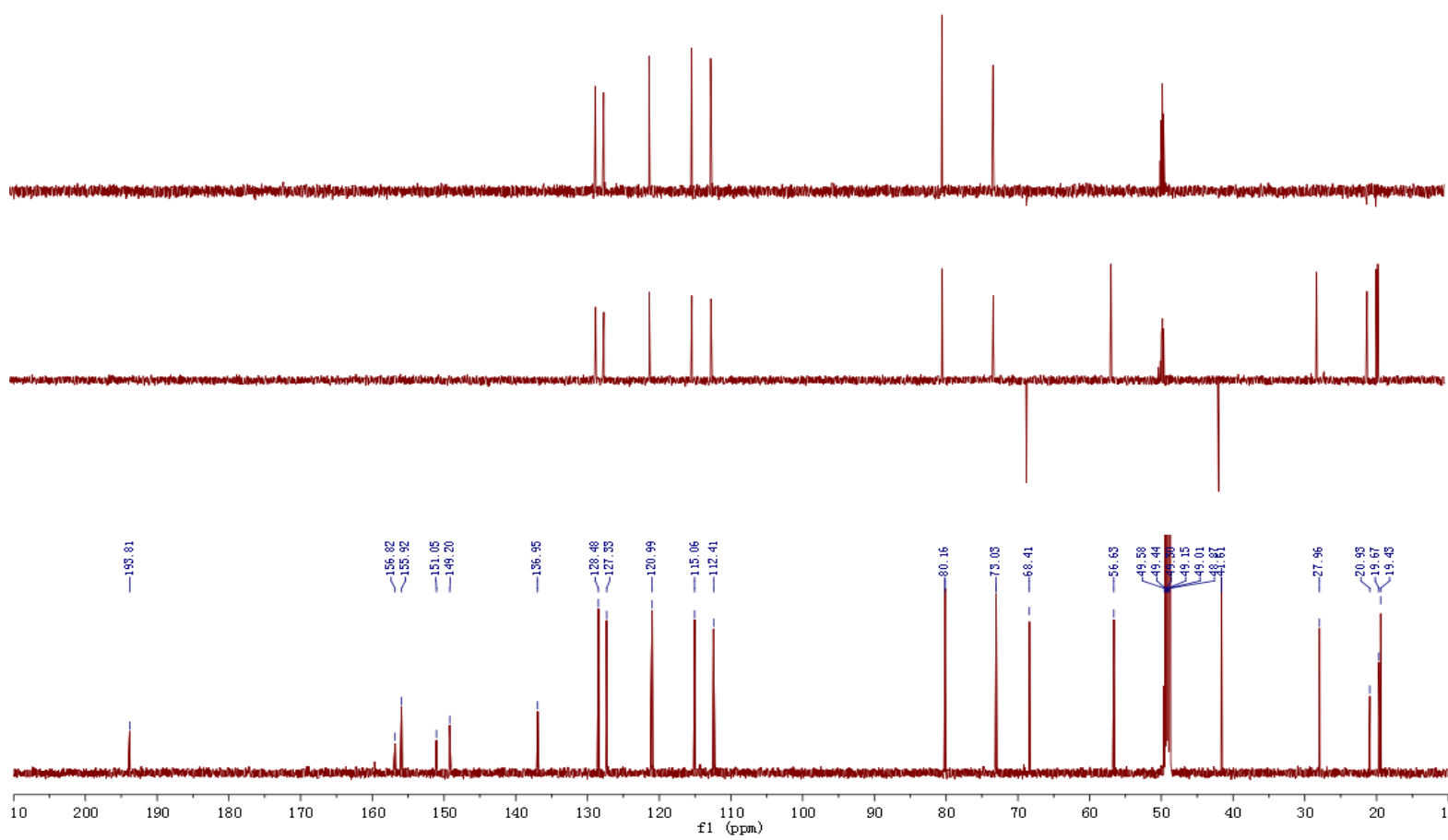


Figure 30S. HSQC of compound 4.

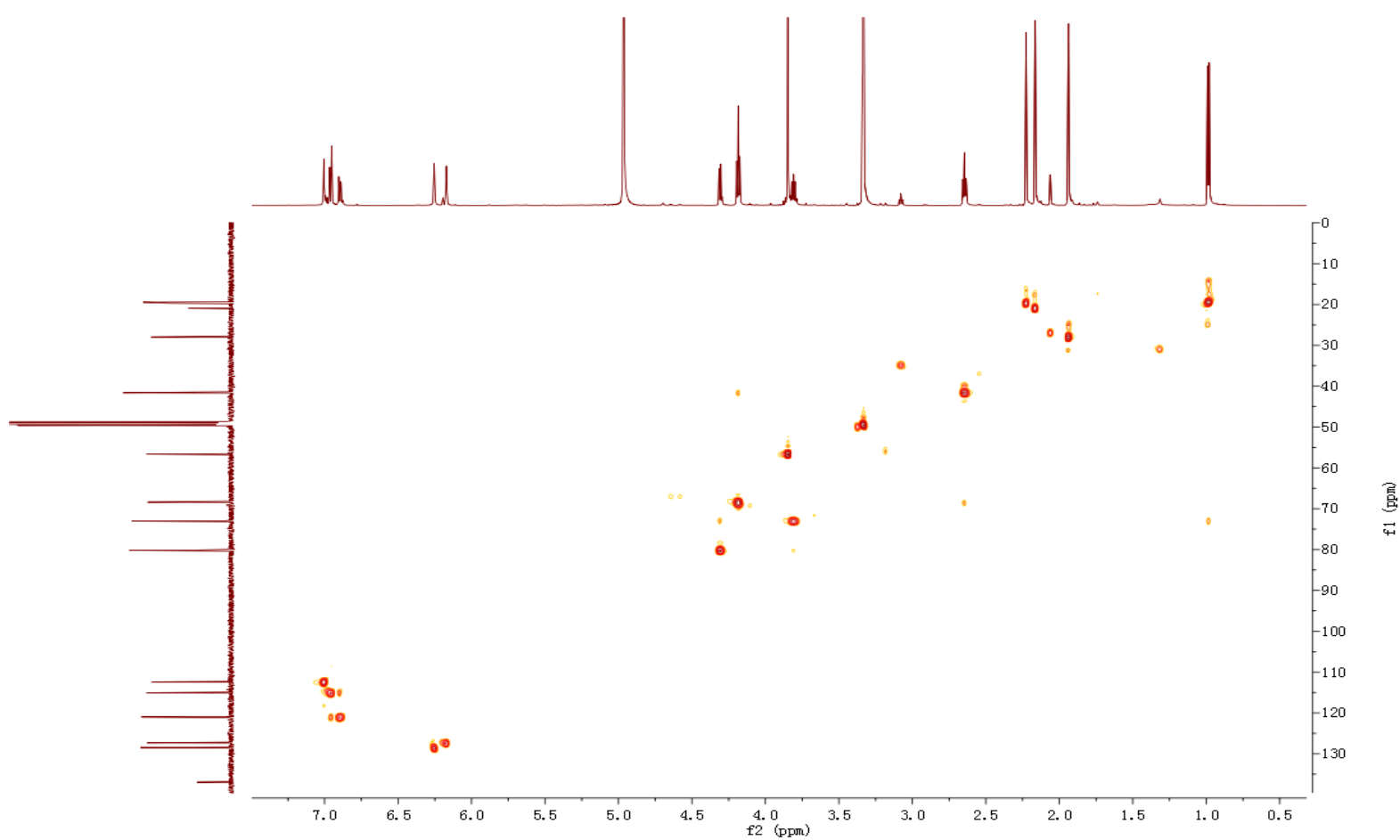


Figure 31S. HMBC of compound 4.

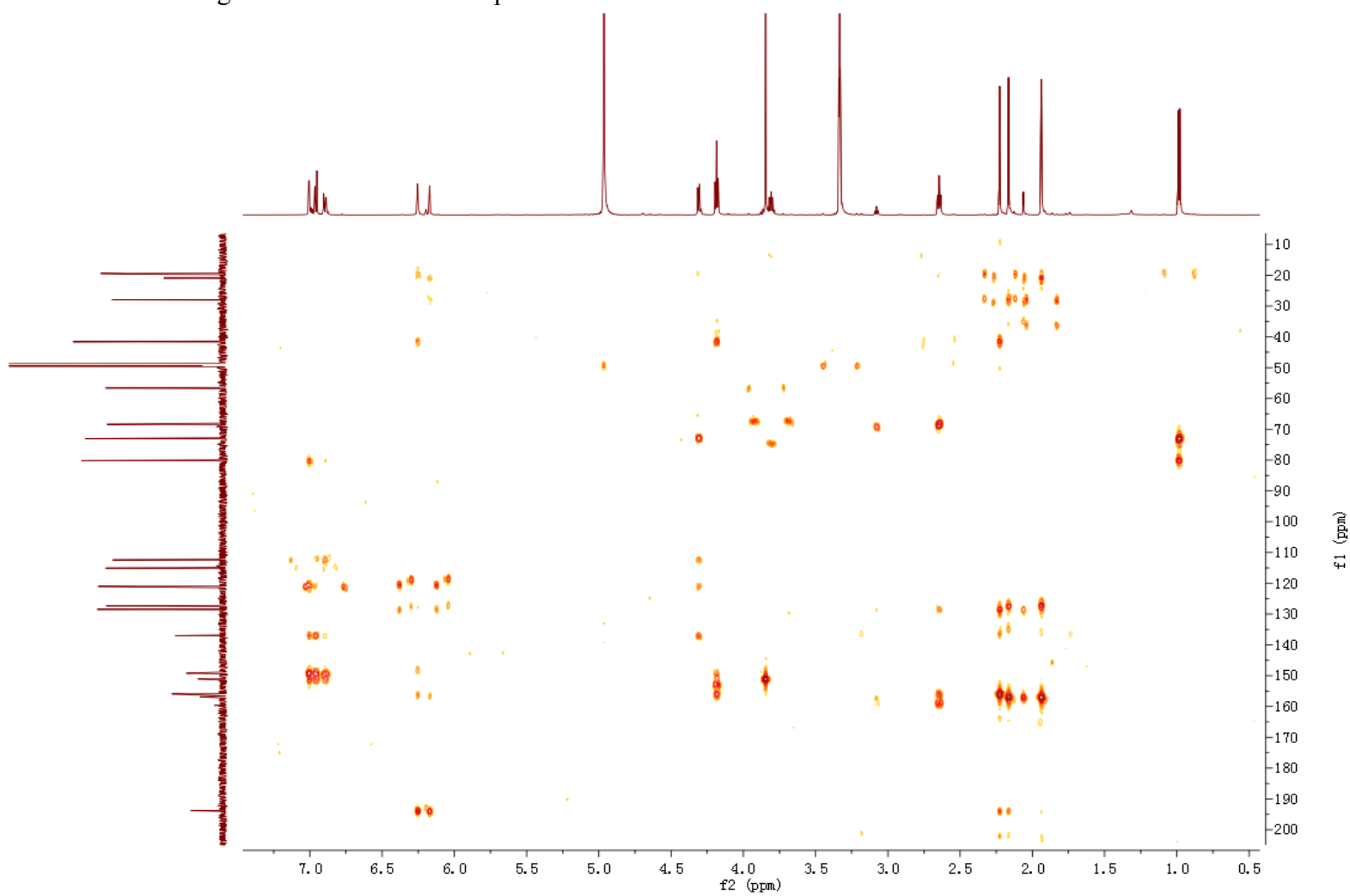


Figure 32S. ^1H - ^1H COSY of compound 4.

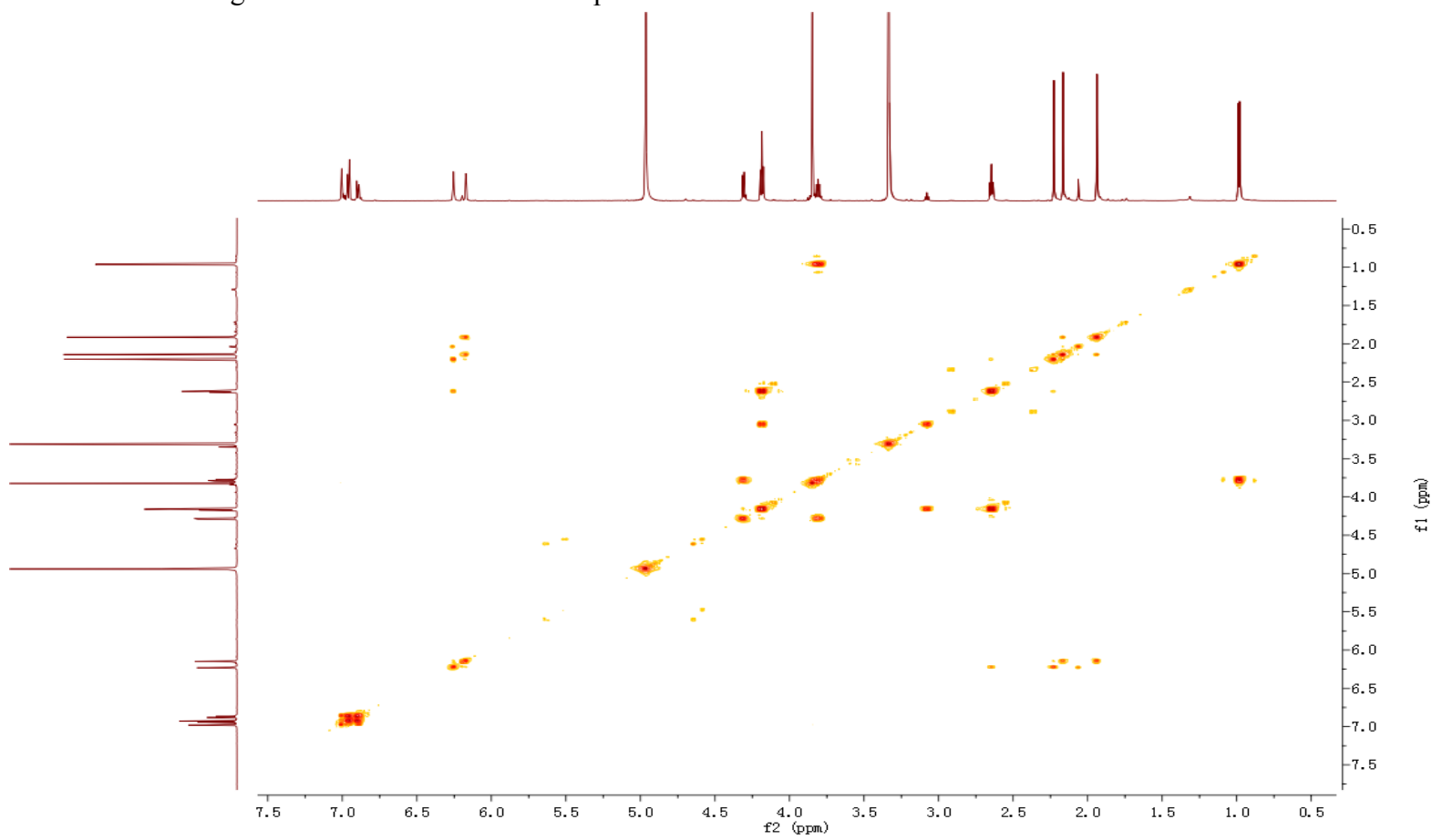


Figure 33S. ROESY of compound 4.

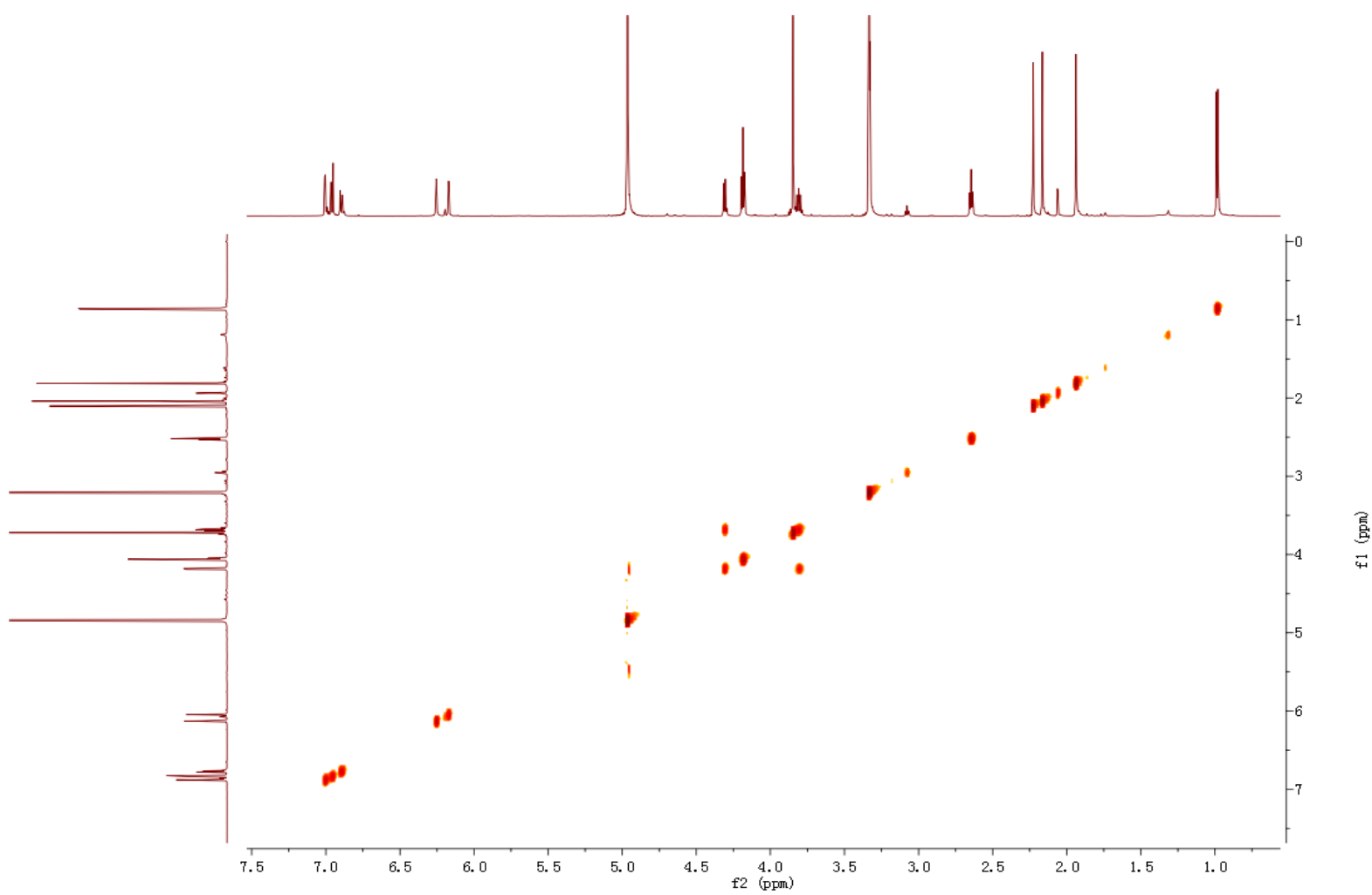


Figure34S. HRESIMS of compound 4.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 3-6

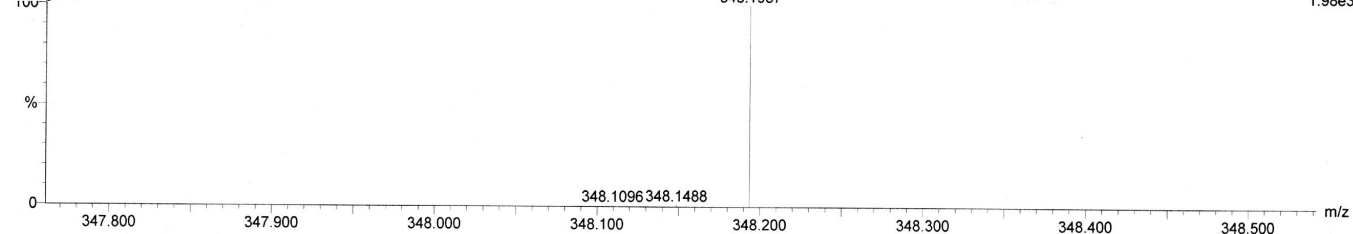
Dgzy-25c

11:54:27 18-Apr-2012

Voltage EI+

KIB
M120418EA-10AFAMM 12 (1.102)
348.1937

Autospec Premier
P776
1.98e3



Minimum: 0.5
Maximum: 40.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.1937	348.1937	0.0	0.0	7.0	5547000.5	C20 H28 O5

Figure 35S. ¹H NMR of compound **5**.

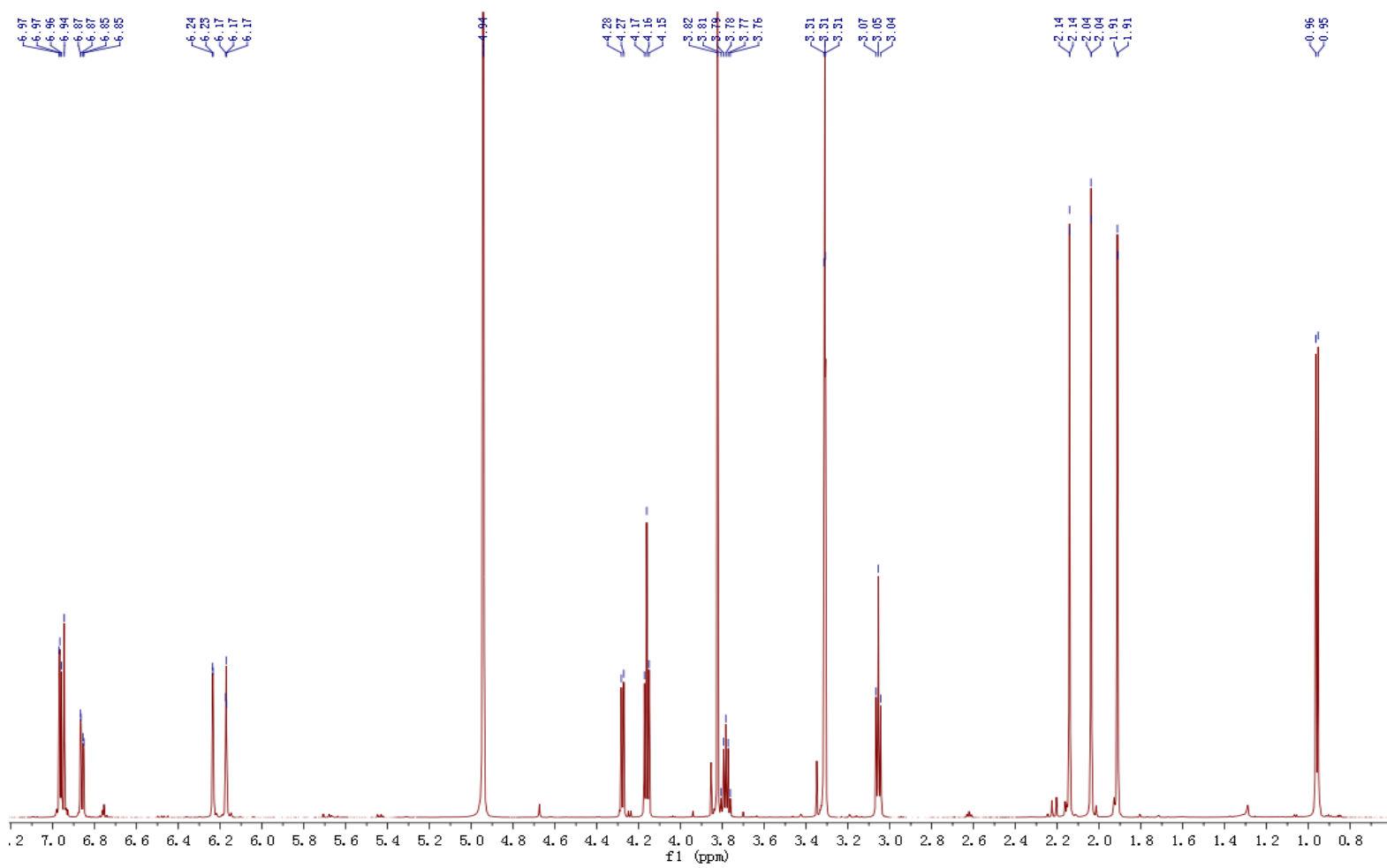


Figure 36S. ^{13}C NMR and DEPT of compound **5**.

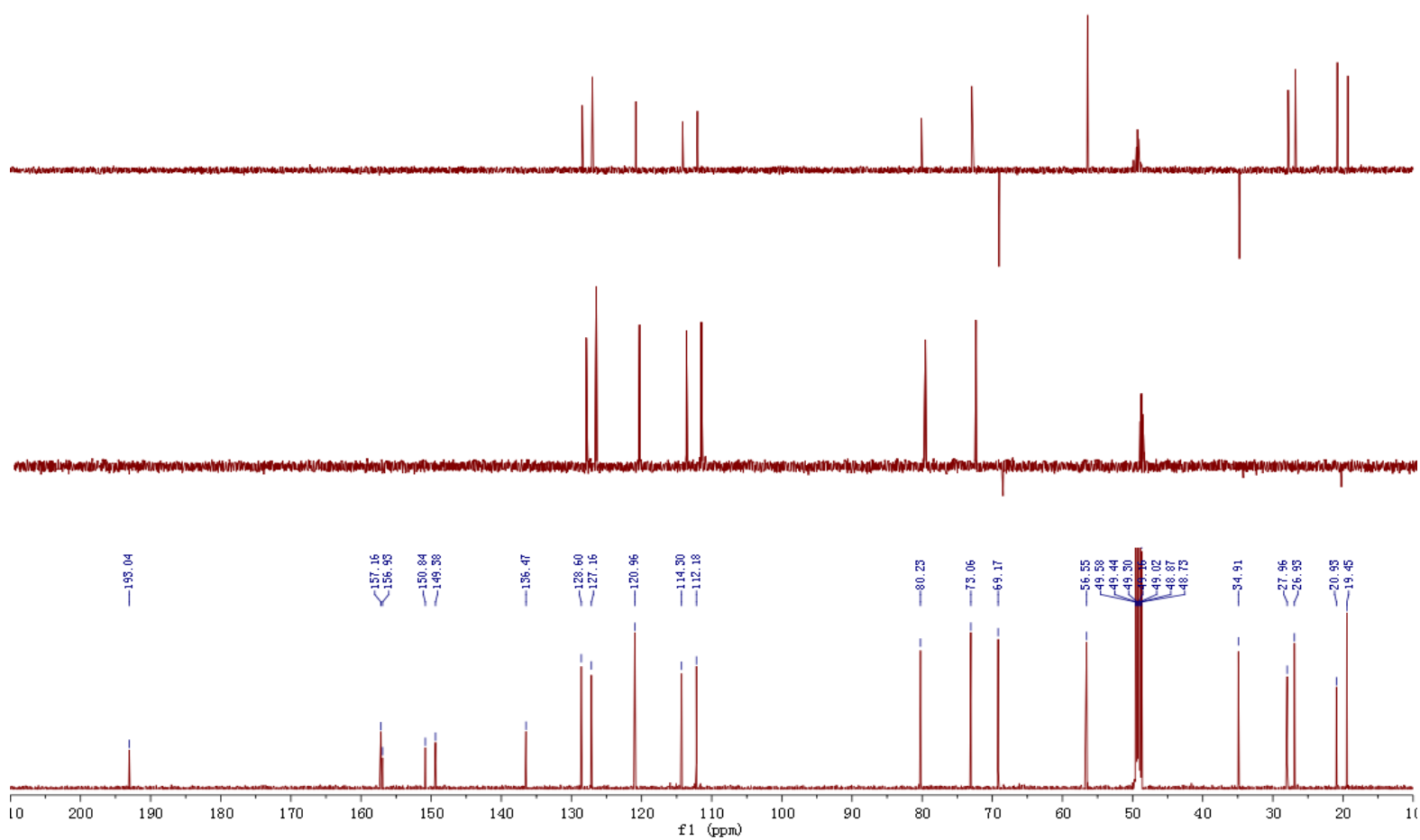


Figure 37S. HSQC of compound 5.

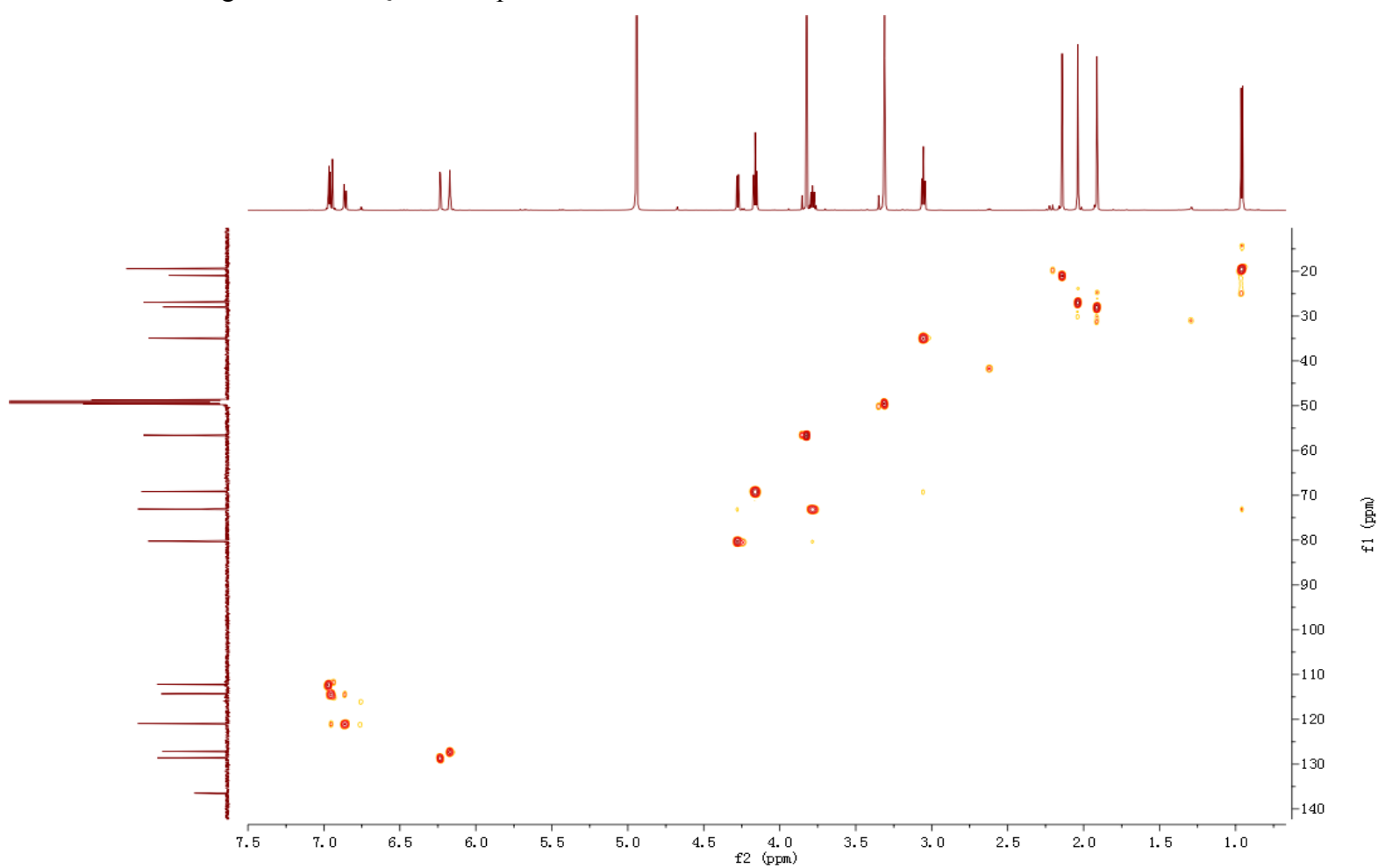


Figure 38S. HMBC of compound **5**.

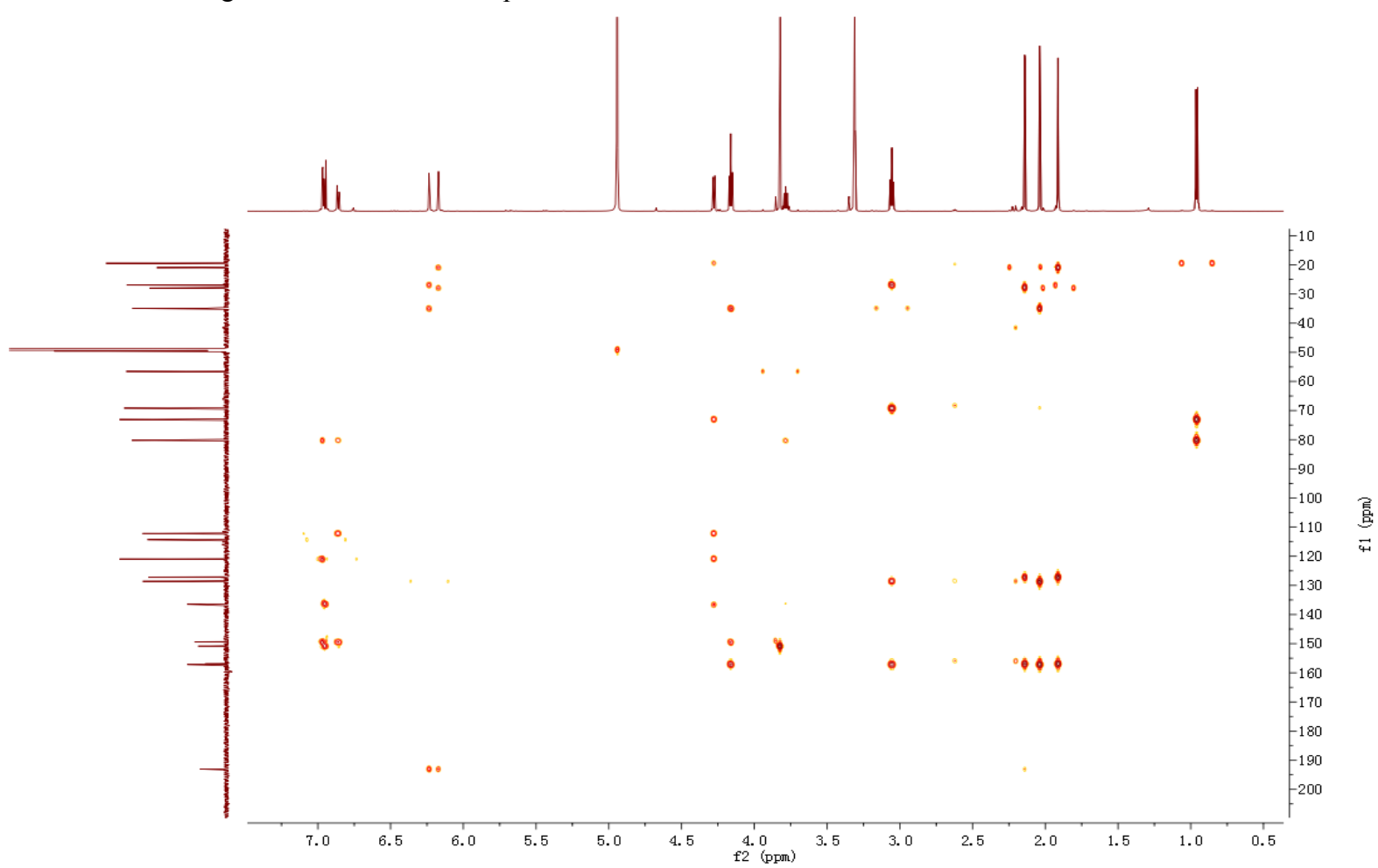


Figure 39S. COSY of compound **5**.

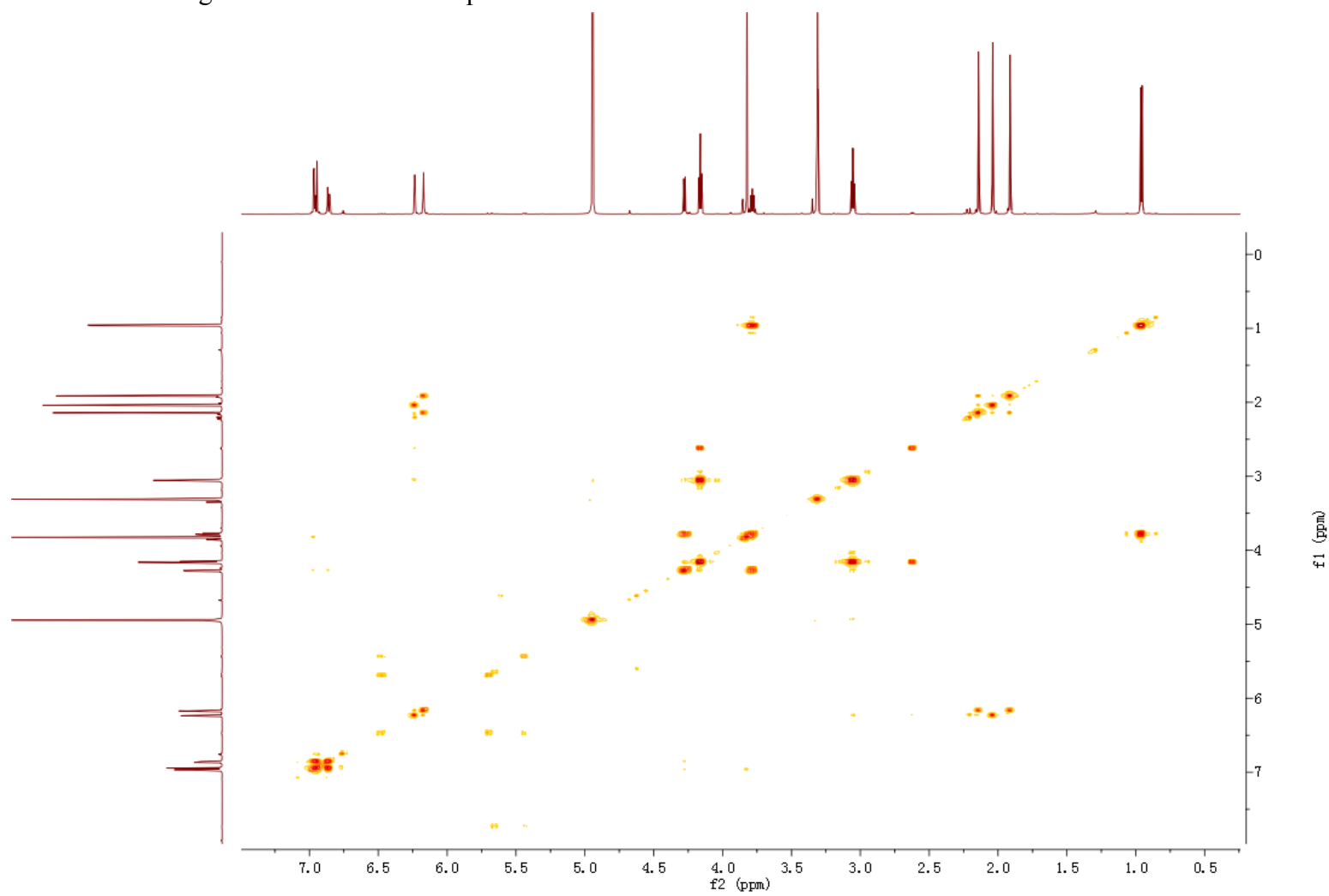


Figure 40S. ROESY of compound **5**.

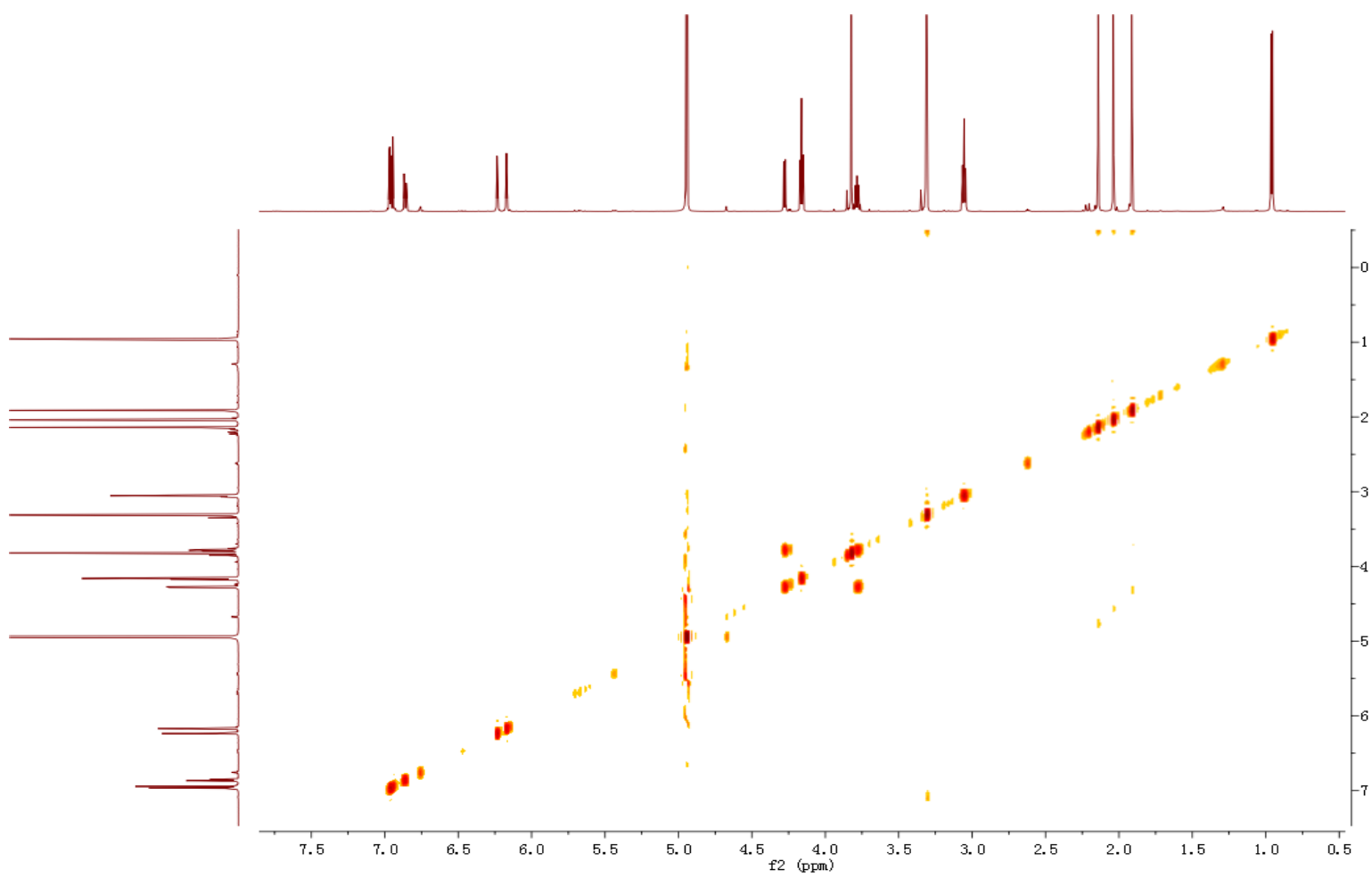


Figure41S. HRESIMS of compound 5.

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 120.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 3-6

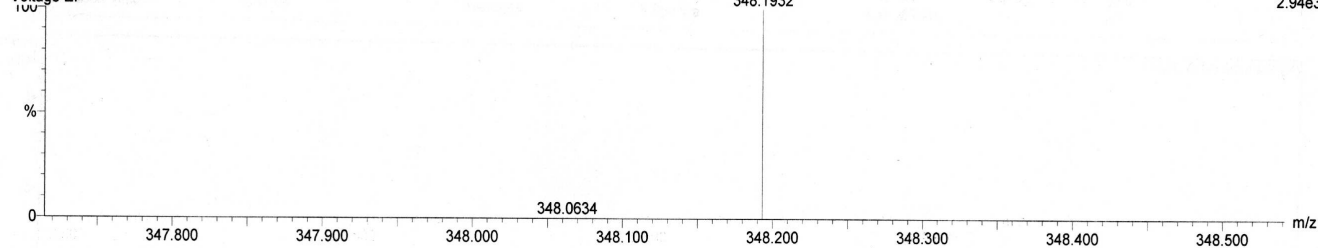
Dgzy-25d

11:58:35 18-Apr-2012

Voltage EI+

KIB
M120418EA-11AFAMM 15 (1.377)
348.1932

Autospec Premier
P776
2.94e3



Minimum: 0.5
Maximum: 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.1932	348.1937	-0.5	-1.4	7.0	5547479.0	C20 H28 O5

Figure 42S. ^1H NMR of compound **6**.

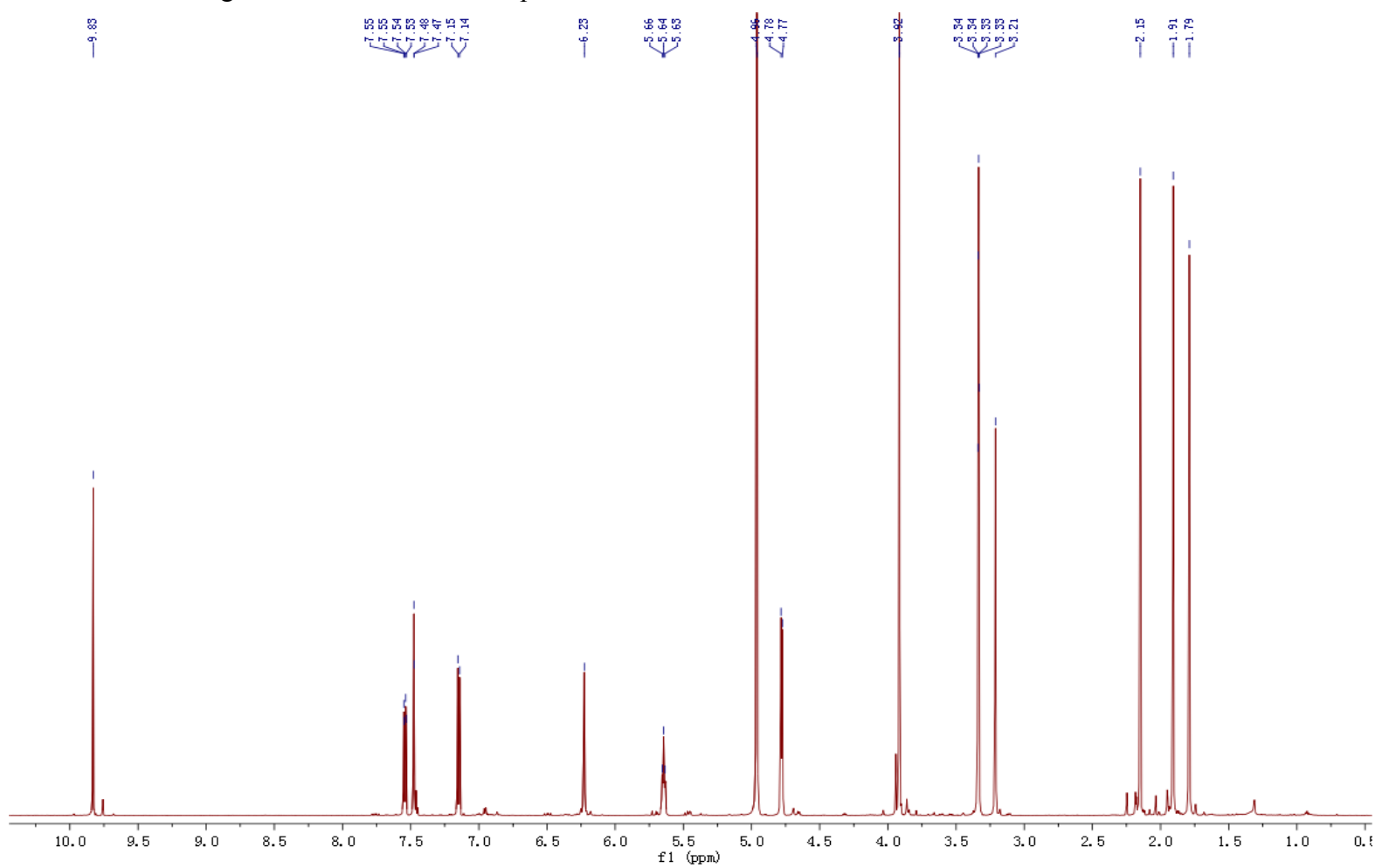


Figure 43S. ^{13}C NMR and DEPT of compound 6.

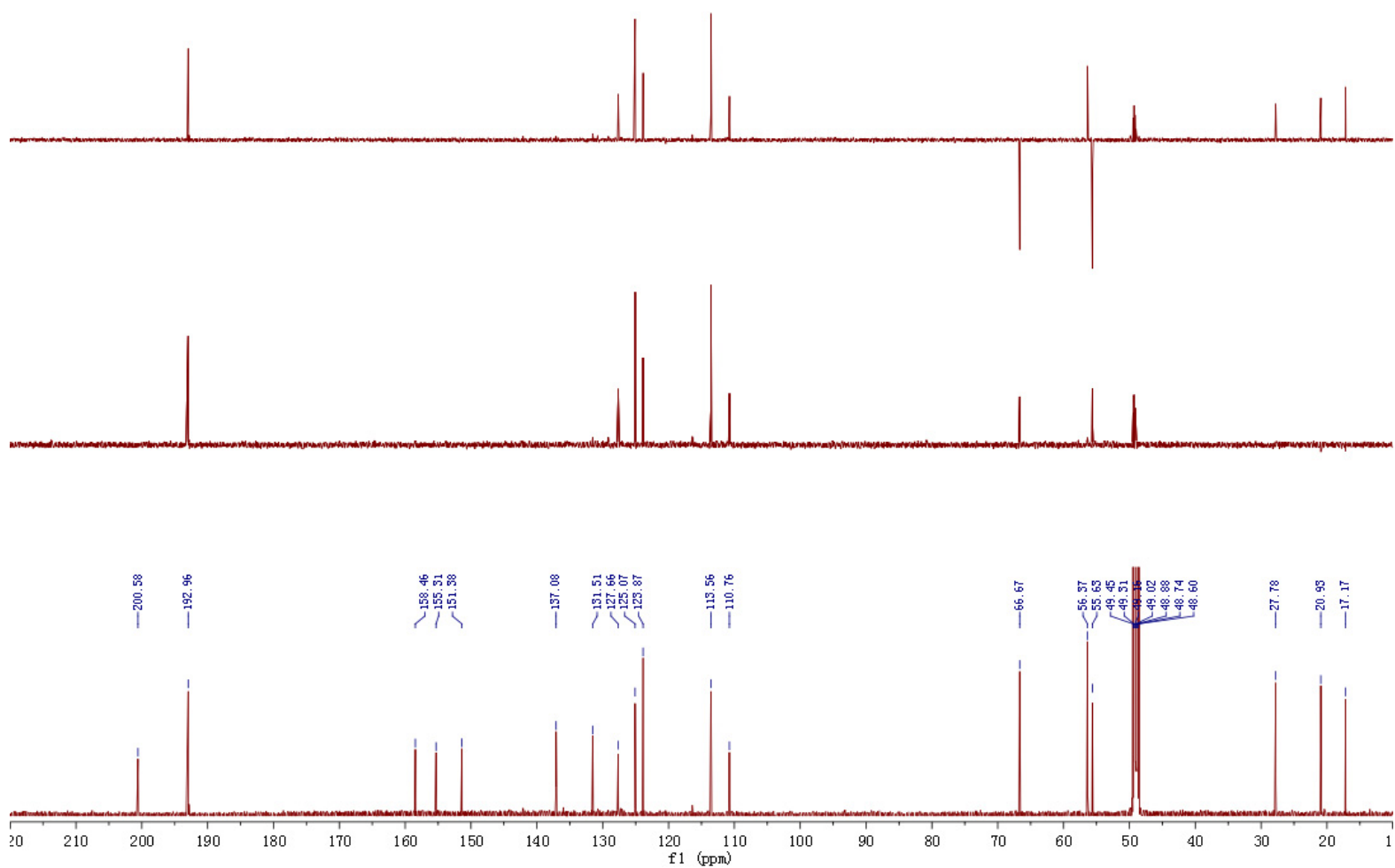


Figure 44S. HSQC of compound 6.

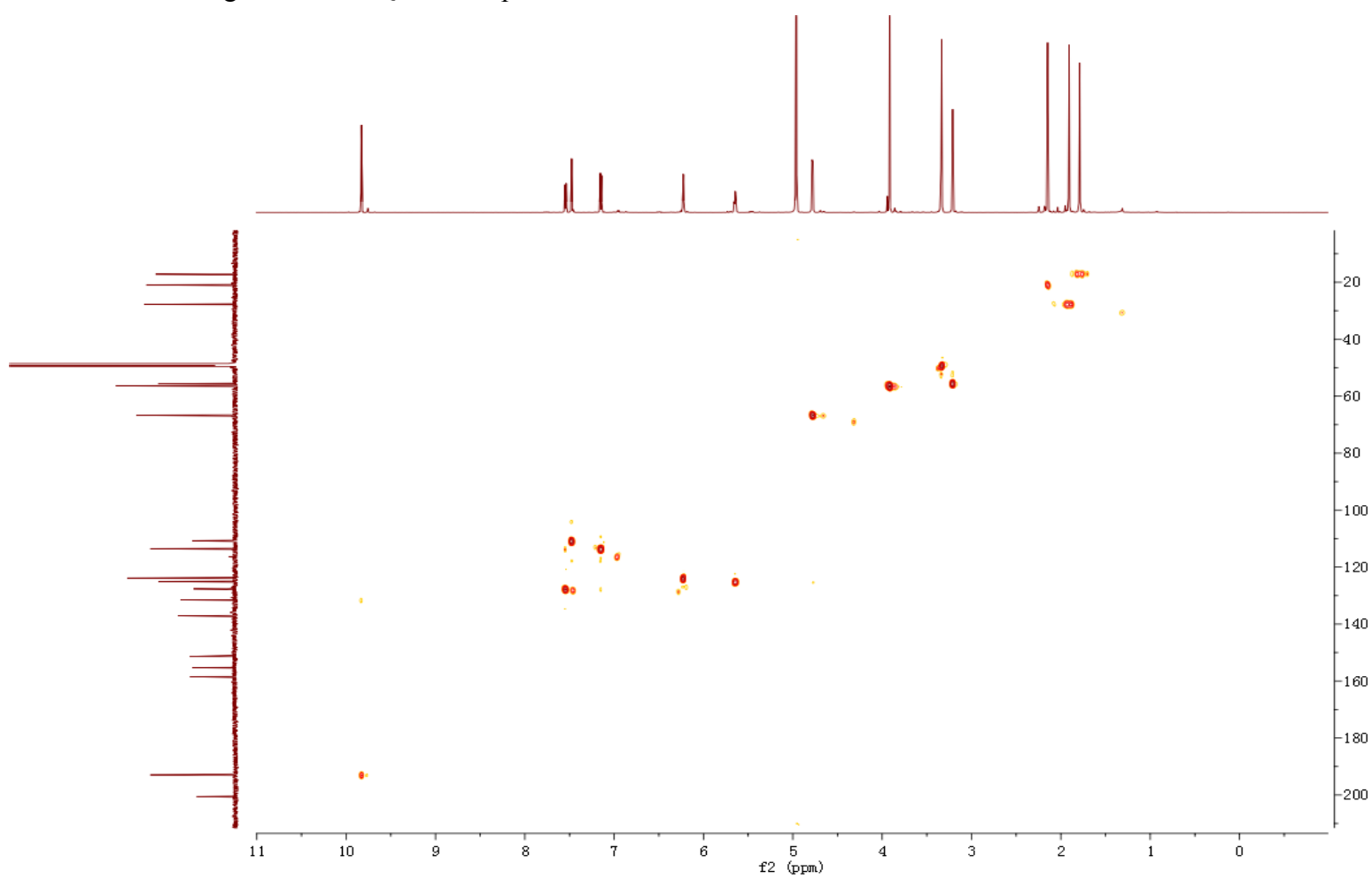


Figure 45S. HMBC of compound 6.

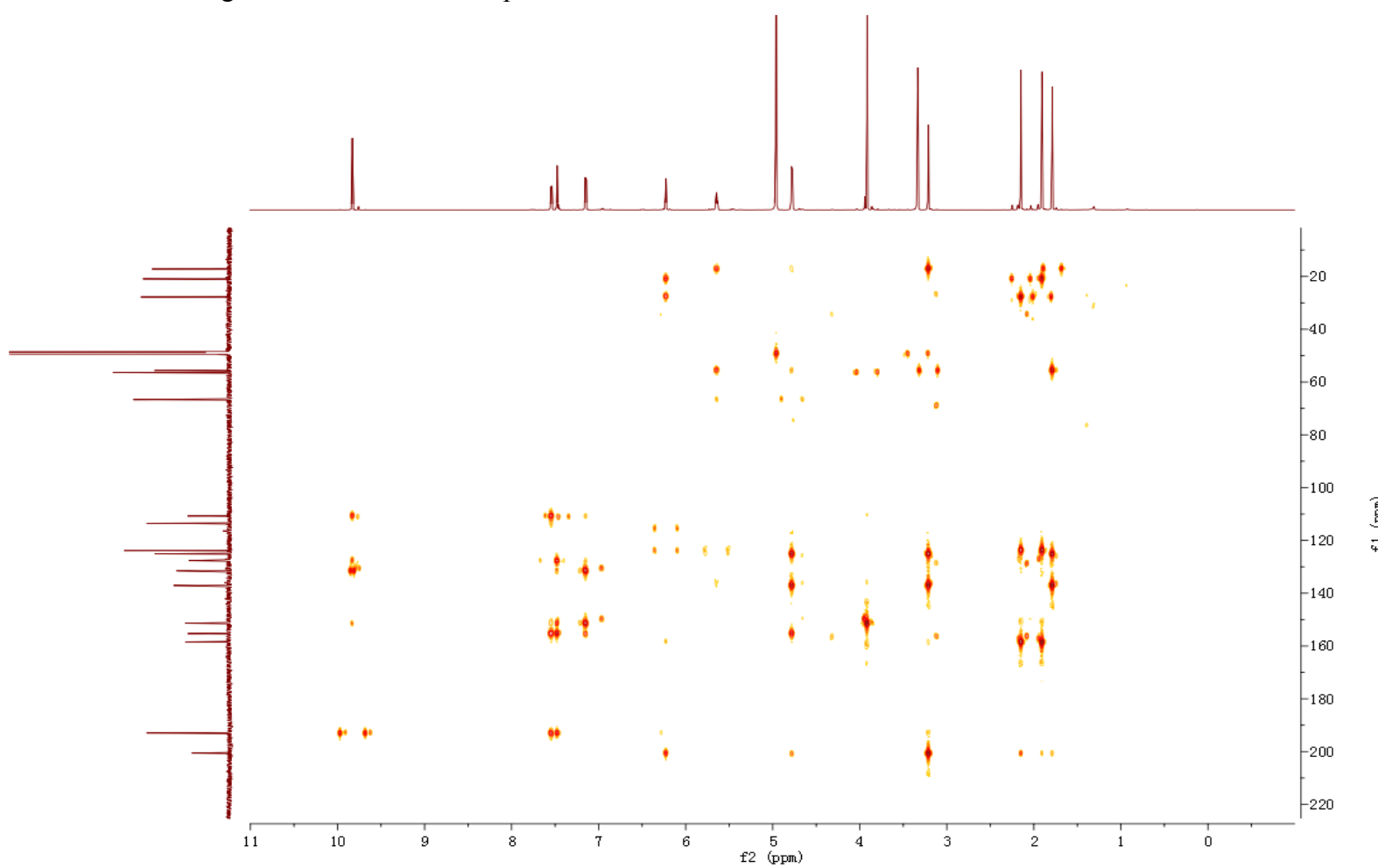


Figure 46S. ^1H - ^1H COSY of compound **6**.

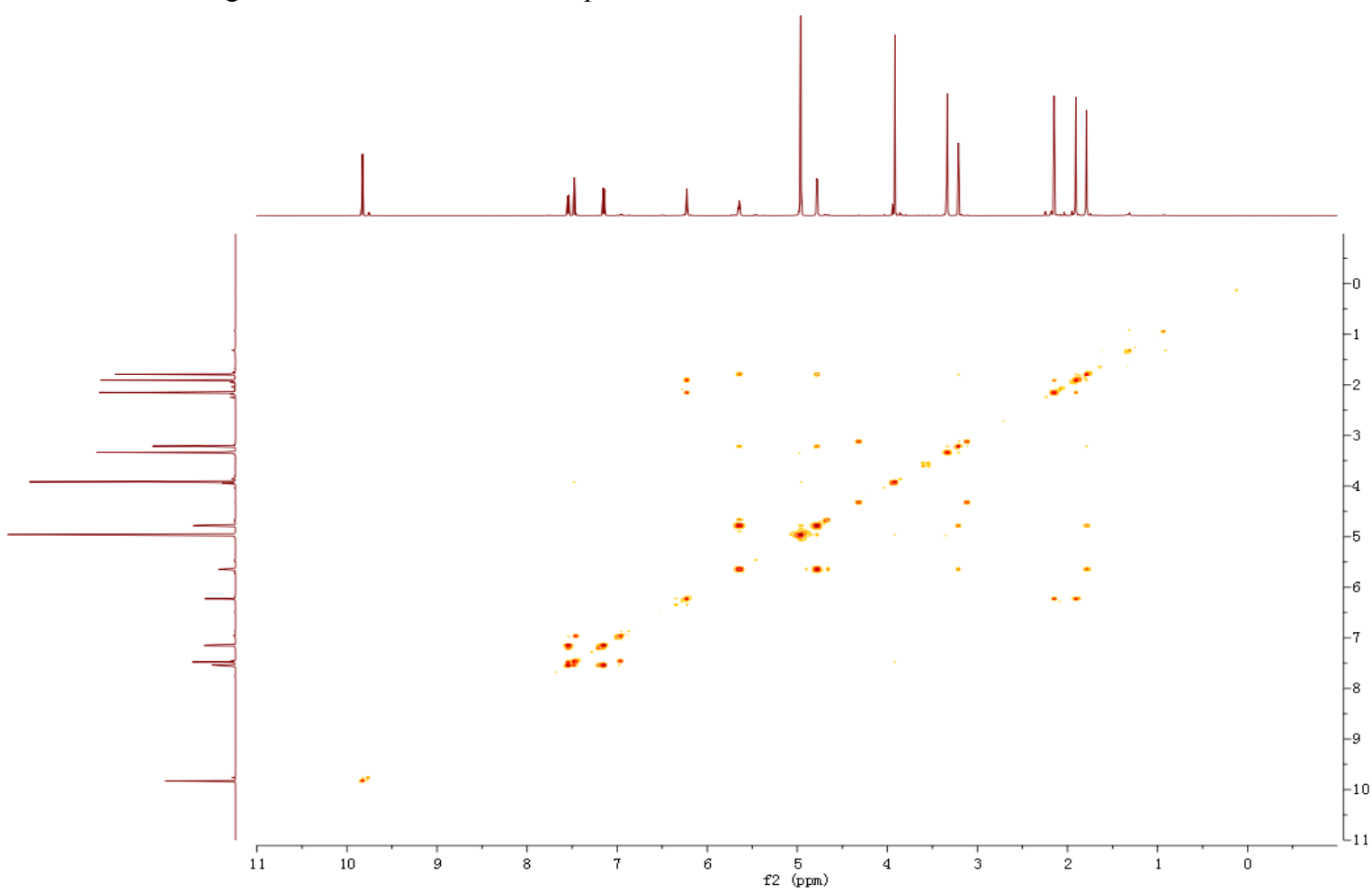


Figure 47S. ROESY of compound 6.

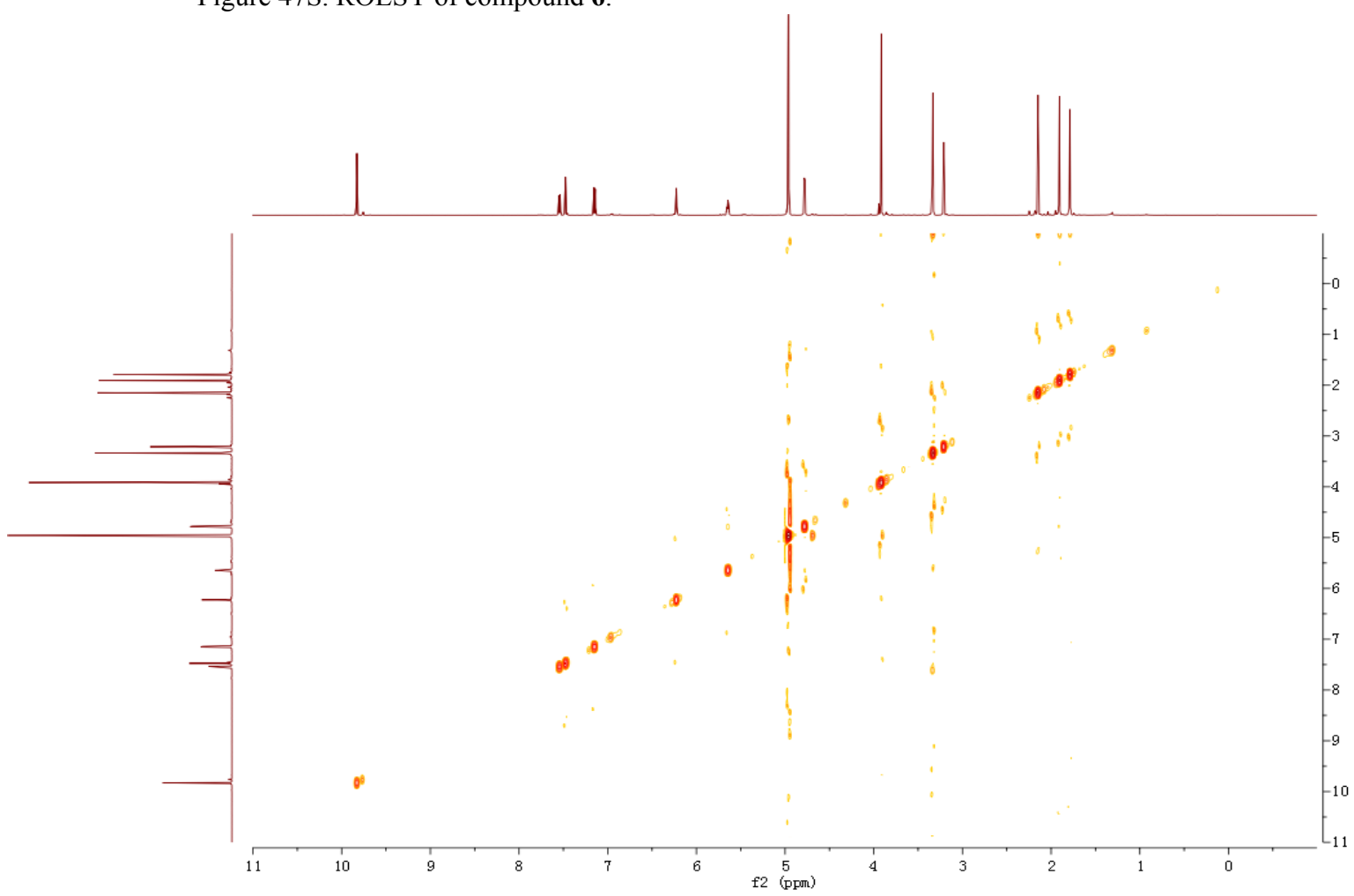


Figure 48S. HRESIMS of compound 6.

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 60.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 3-6

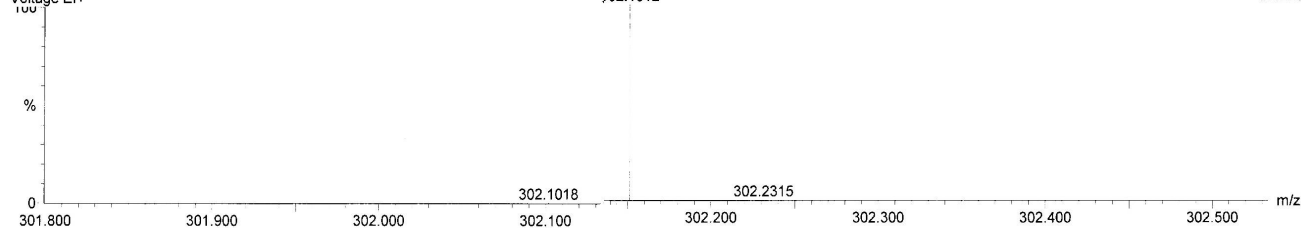
Dgzy-12

11:02:14 09-Apr-2012

Voltage EI+

KIB
M120405EA-01AFAMM 13 (1.194)
302.1512

Autospec Premier
P776
3.68e3



Minimum:

Maximum: 73.0 10.0 0.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
302.1512	302.1518	-0.6	-2.0	8.0	5547847.5	C18 H22 O4

Figure 50S. ^{13}C NMR and DEPT of compound 7.

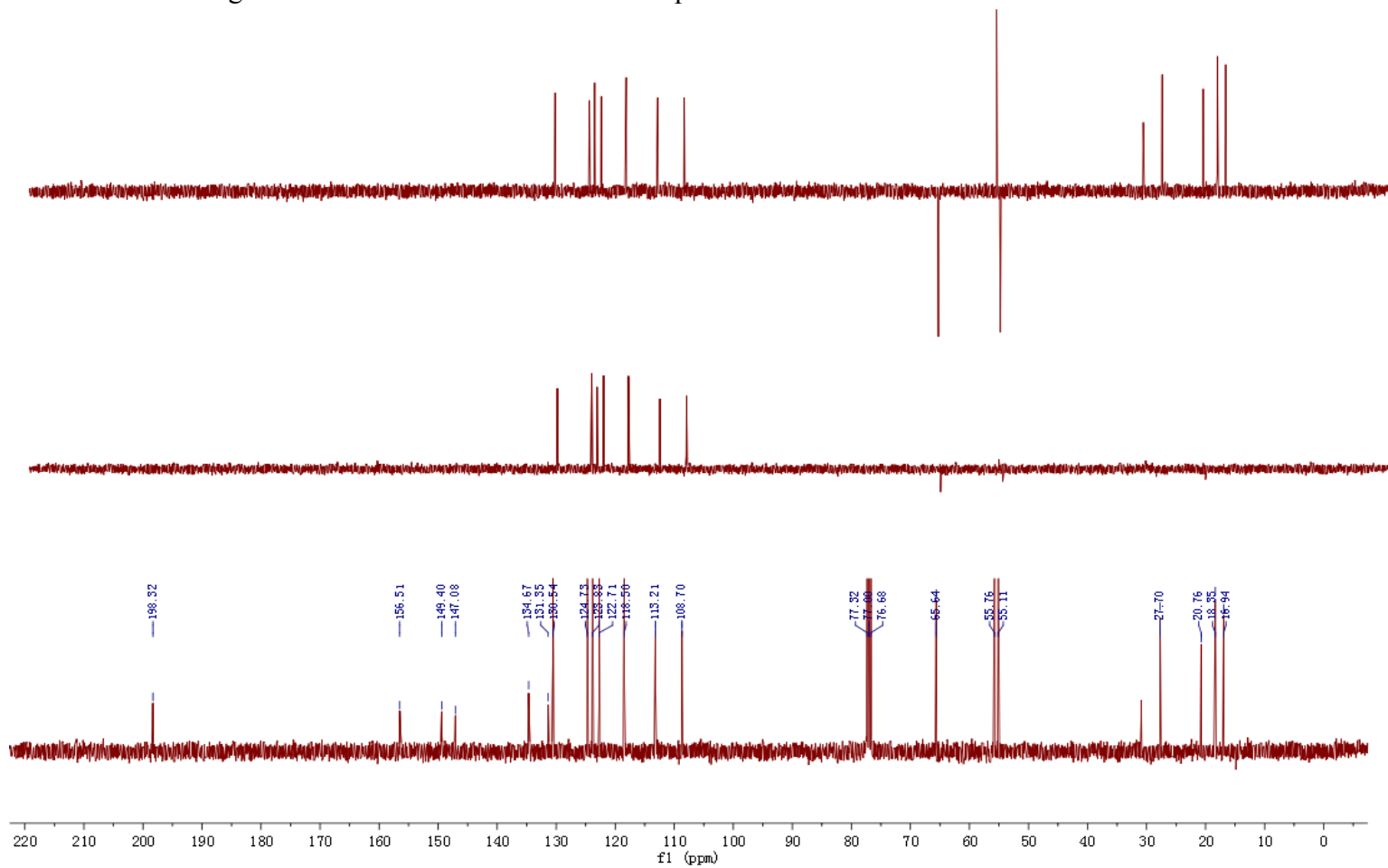


Figure 51S. HSQC of compound 7.

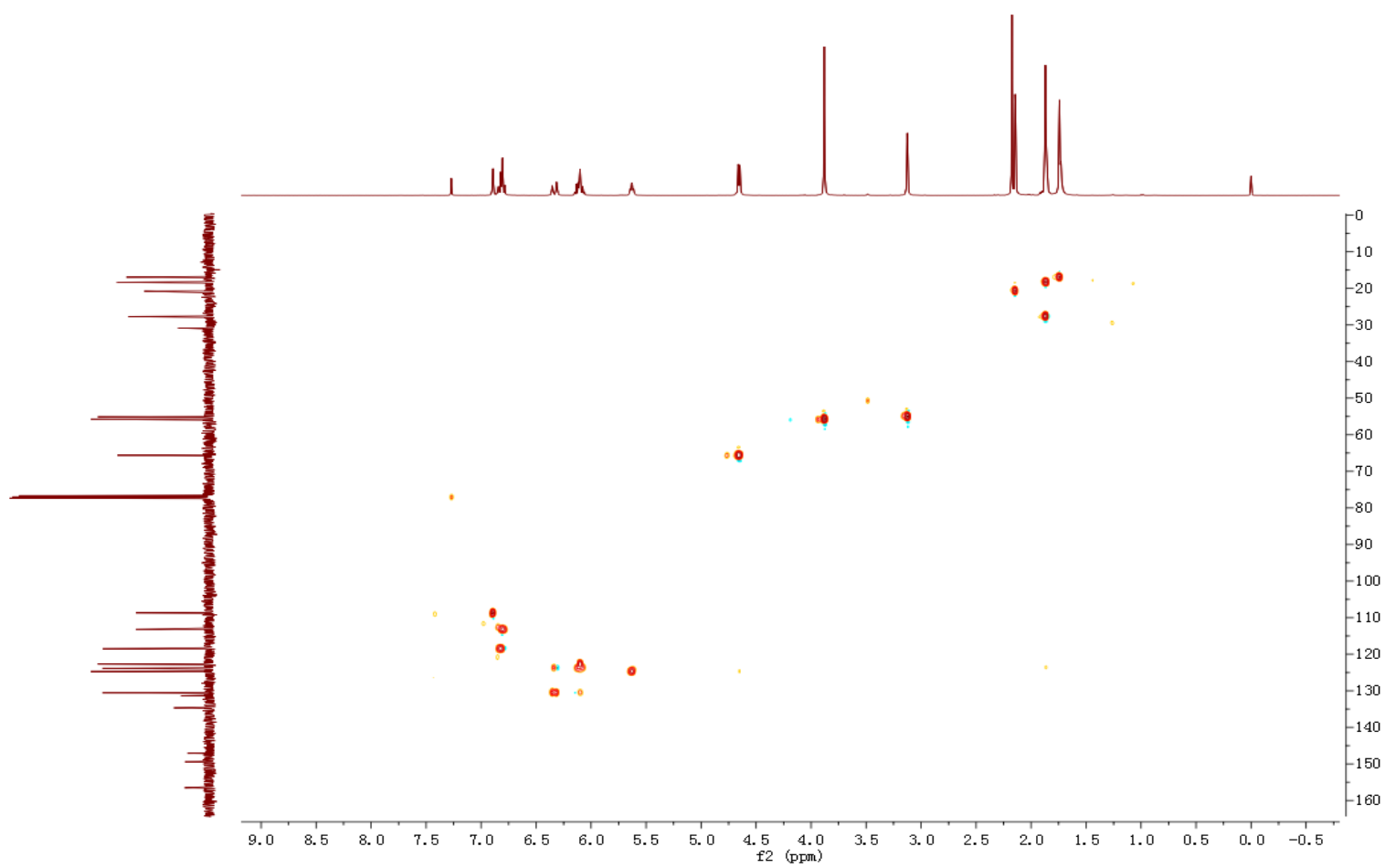


Figure 52S. HMBC of compound 7.

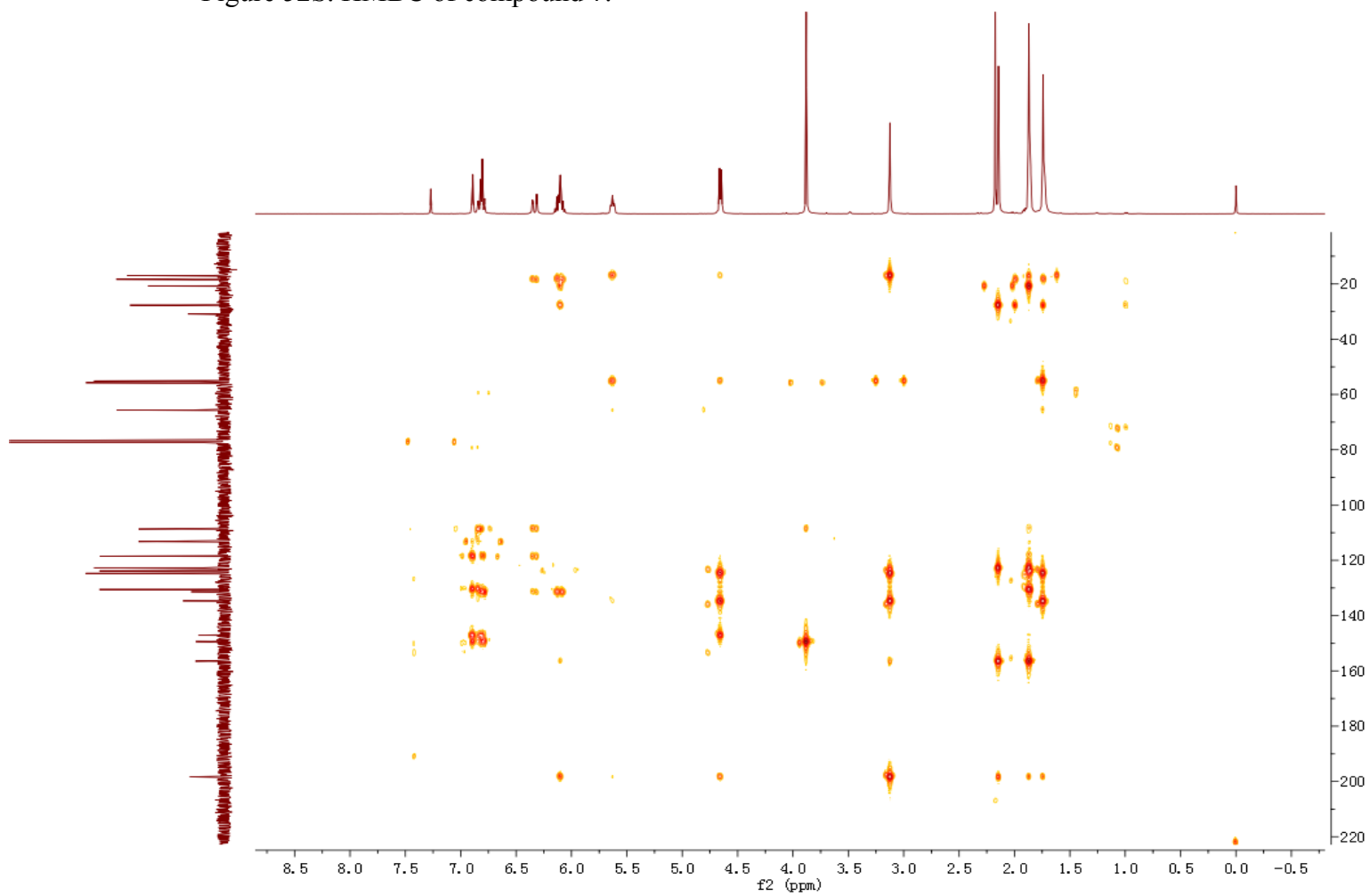


Figure 53S. ^1H - ^1H COSY of compound 7.

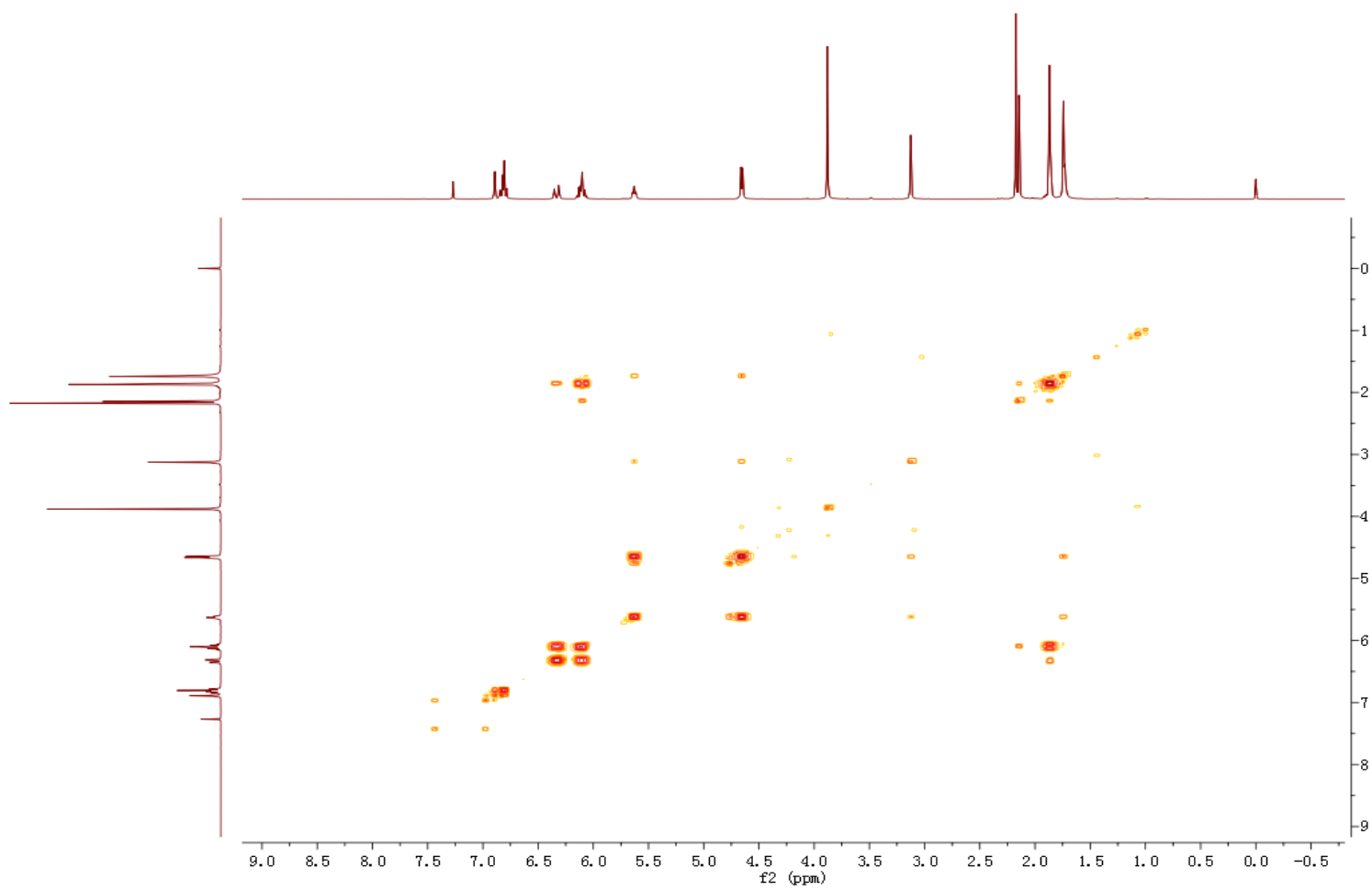


Figure 54S. ROESY of compound 7.

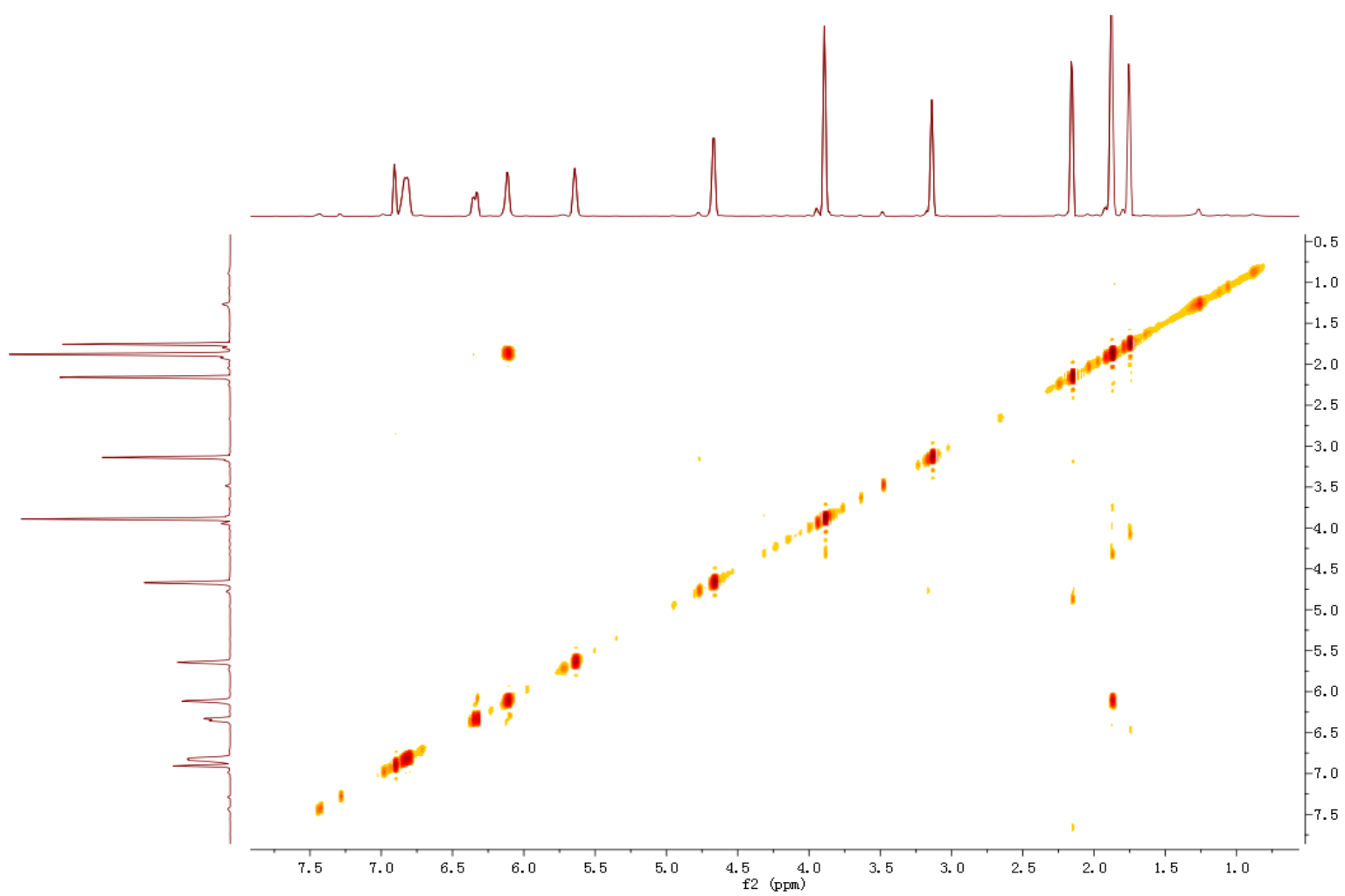


Figure 55S. HRESIMS of compound 7.

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 60.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

14 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 3-6

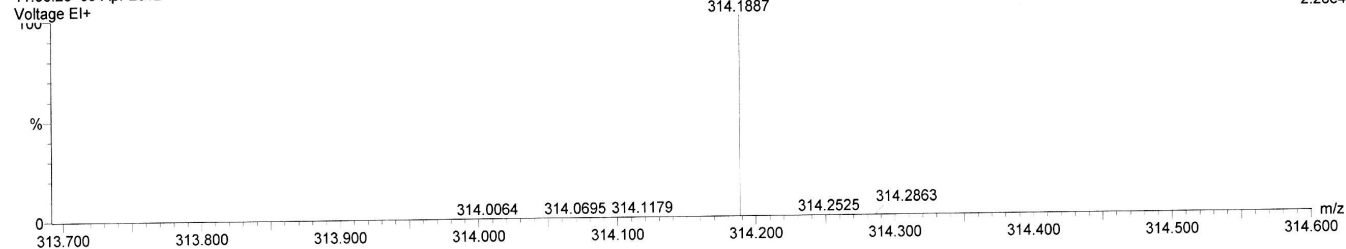
Dgzy-3

11:06:26 09-Apr-2012

Voltage E1+

KIB
M120409EA-02AFAMM 9 (0.826)
314.1887

Autospec Premier
P776
2.26e4



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.1887	314.1882	0.5	1.6	8.0	5557311.0	C20 H26 O3