

## *Supporting Information*

### **Cytotoxic Scalarane Sesterterpenoids from the South China**

#### **Sea Sponge *Carteriospongia foliascens***

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|| These authors contributed equally to this work.

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**Figure S55.** ESIMS spectrum of compound **7**

**Figure S56.** HRESIMS spectrum of compound **7**

**Figure S57.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **8**

**Figure S58.** <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound **8**

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**Figure S59.** HMQC (CDCl<sub>3</sub>) spectrum of compound **8**

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**Figure S79.** ESIMS spectrum of compound **10**

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**Figure S81.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **11**

**Figure S82.** <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound **11**

**Figure S83.** HMQC (CDCl<sub>3</sub>) spectrum of compound **11**

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**Figure S85.** HMBC (CDCl<sub>3</sub>) spectrum of compound **11**

**Figure S86.** NOESY (CDCl<sub>3</sub>) spectrum of compound **11**

**Figure S87.** EIMS spectrum of compound **11**

**Figure S88.** HREIMS spectrum of compound **11**

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**Figure S89.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3a**

**Figure S90.** ESIMS spectrum of compound **3a**

**Figure S91.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3ar**

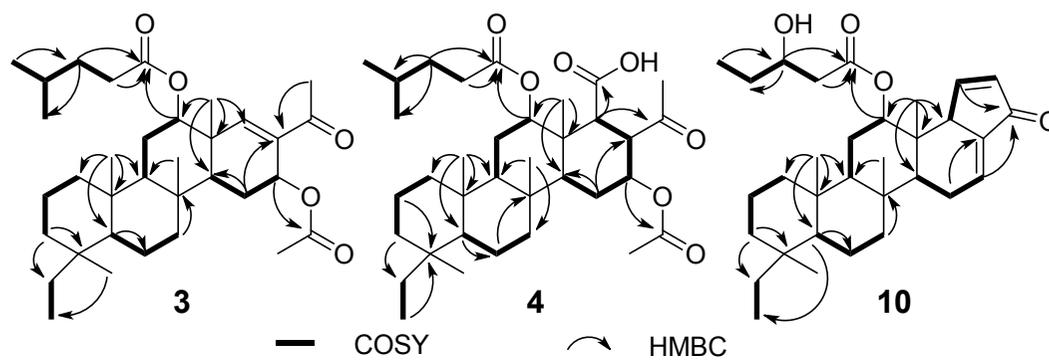
**Figure S92.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **3ar**

**Figure S93.** ESIMS spectrum of compound **3ar**

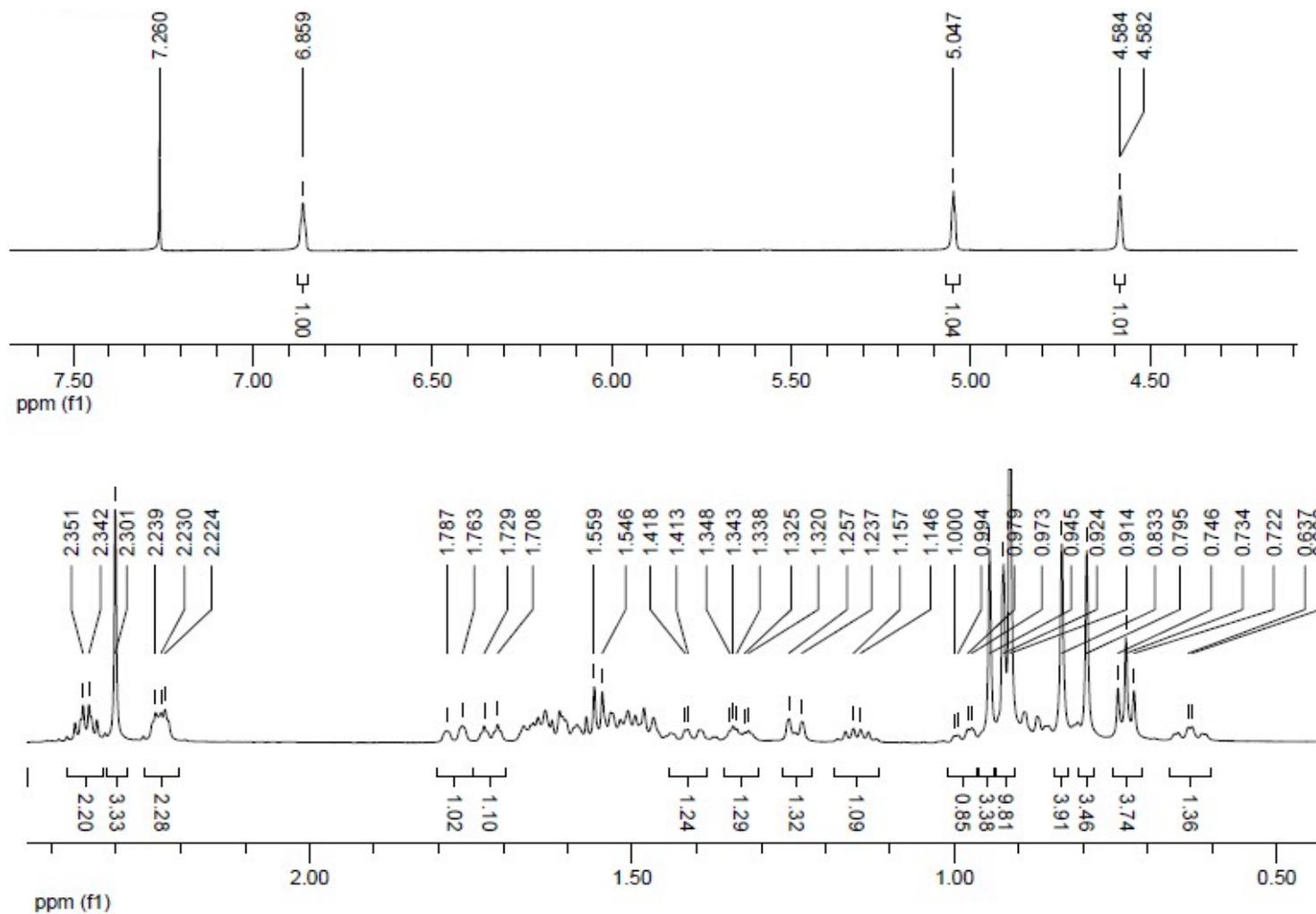
**Figure S94.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3as**

**Figure S95.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **3as**

**Figure S96.** ESIMS spectrum of compound **3as**



**Figure S1.** COSY and key HMBC correlations of **3**, **4** and **10**



**Figure S2.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**

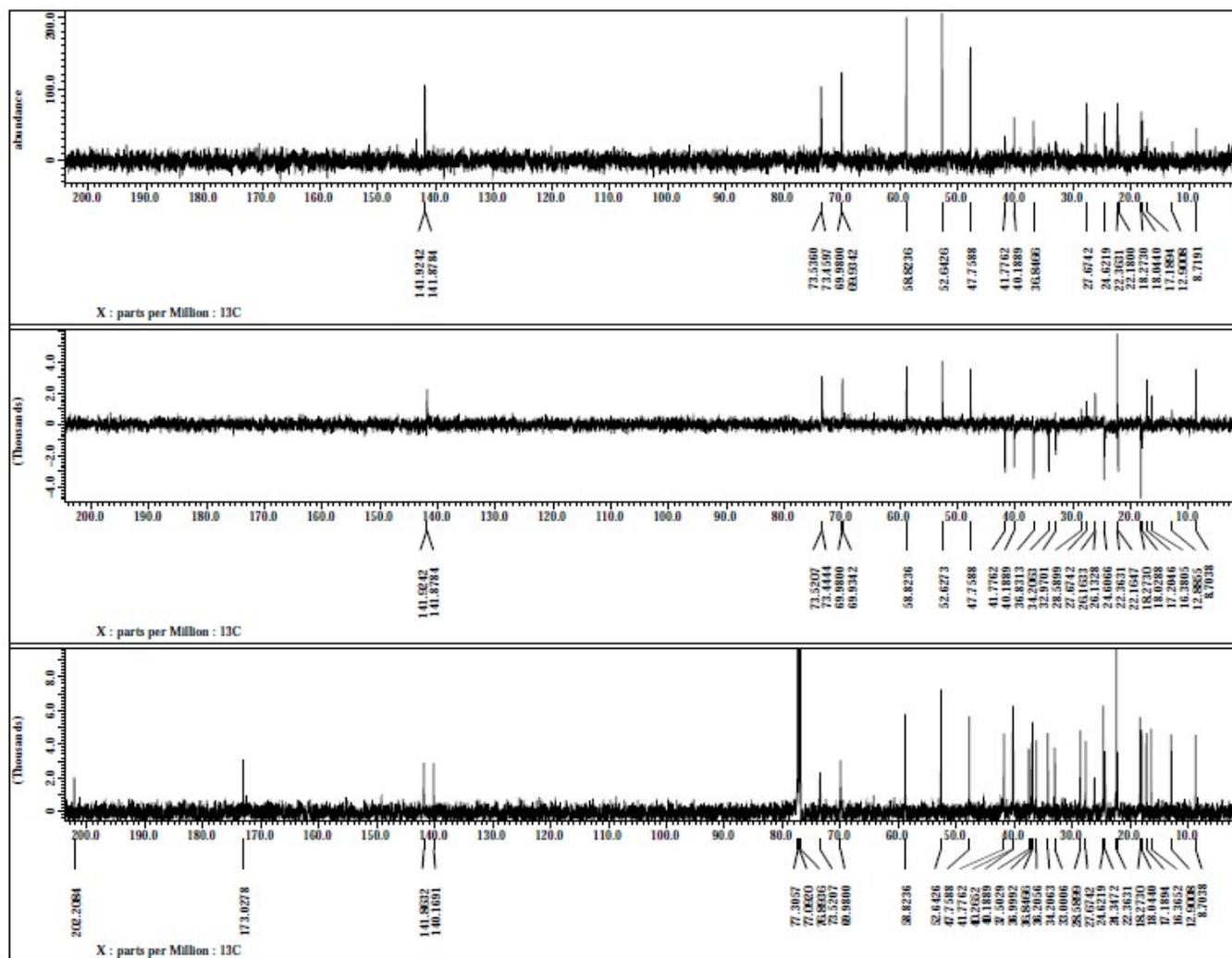


Figure S3. <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound 1

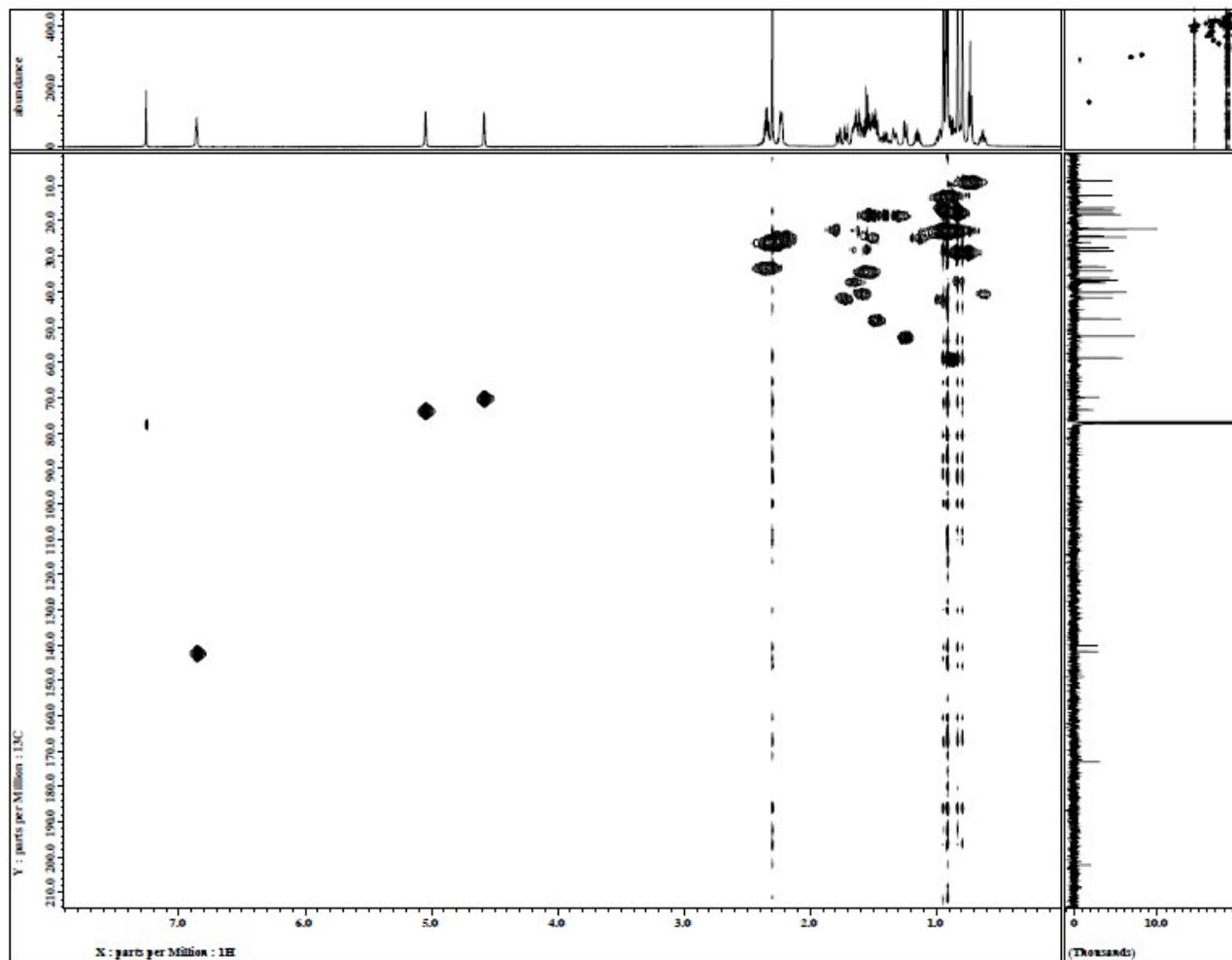


Figure S4. HMQC (CDCl<sub>3</sub>) spectrum of compound 1

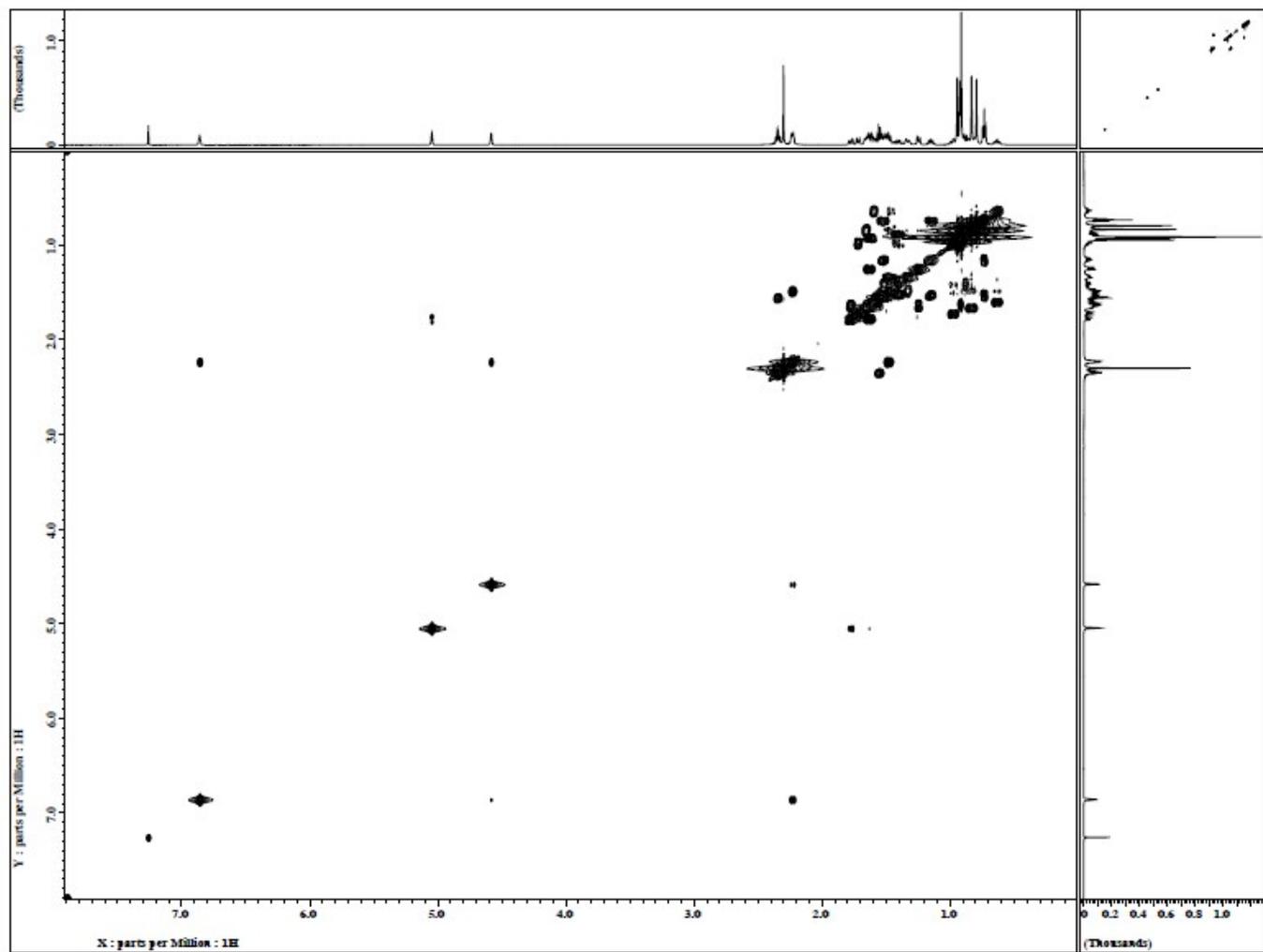


Figure S5. COSY ( $\text{CDCl}_3$ ) spectrum of compound 1

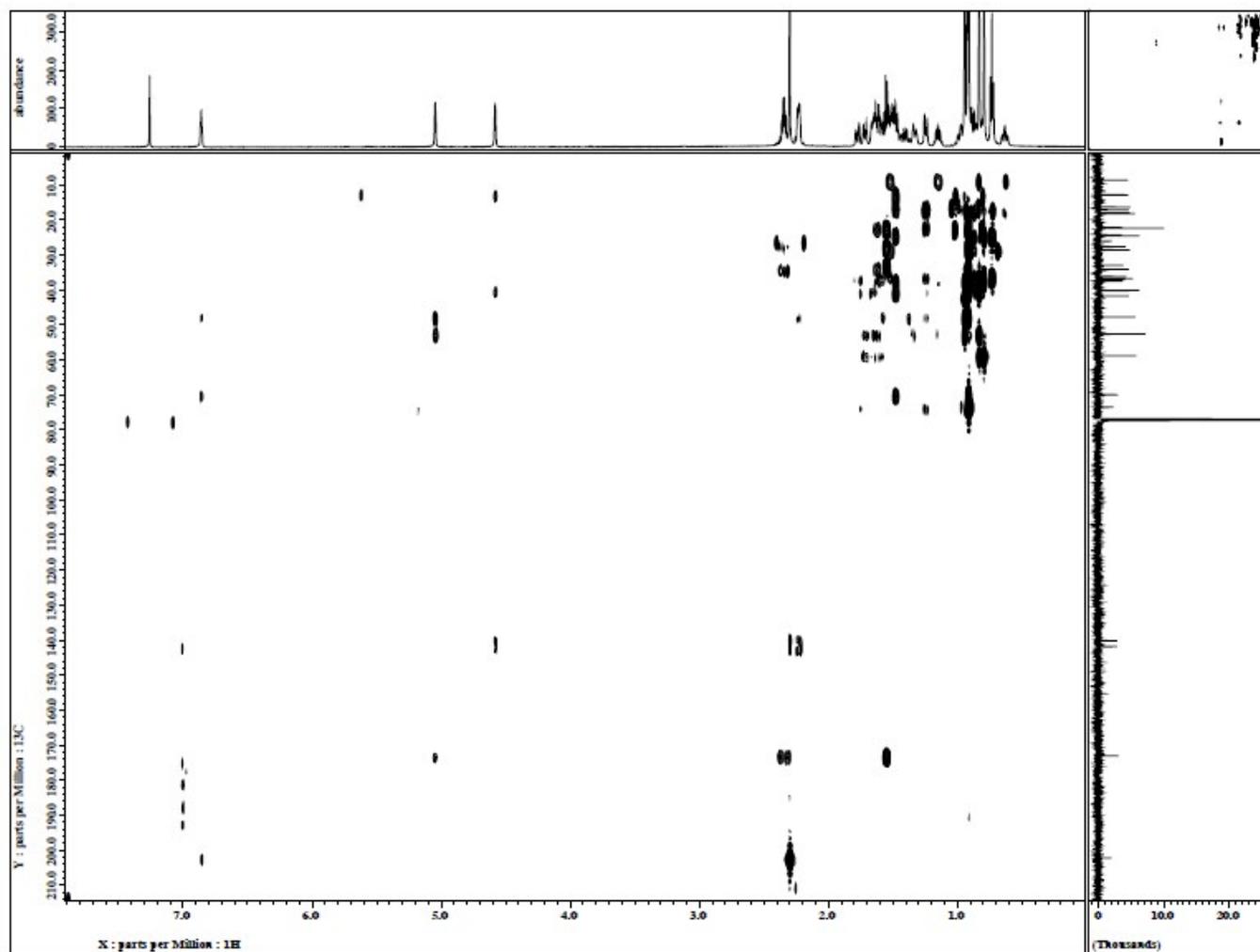
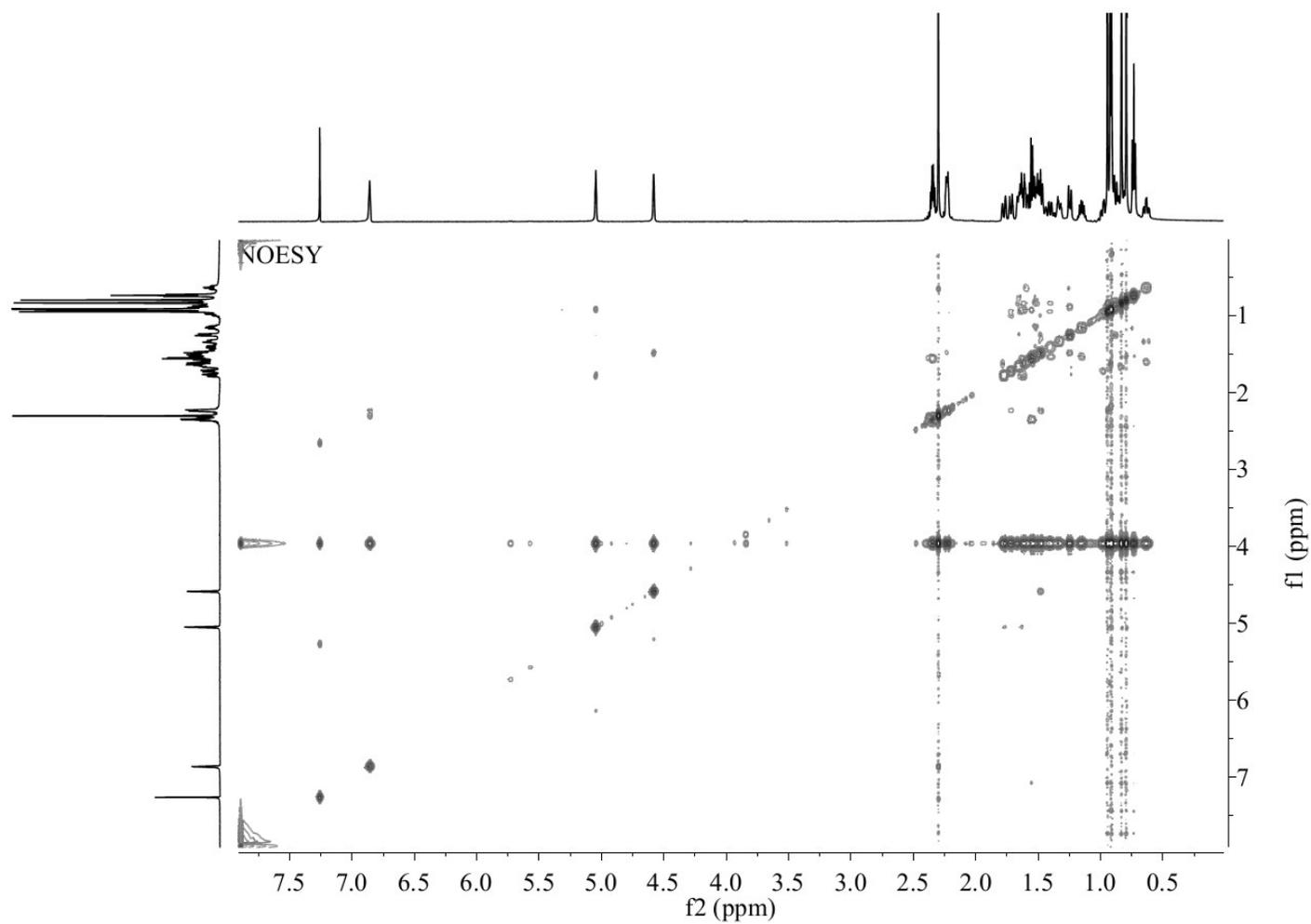
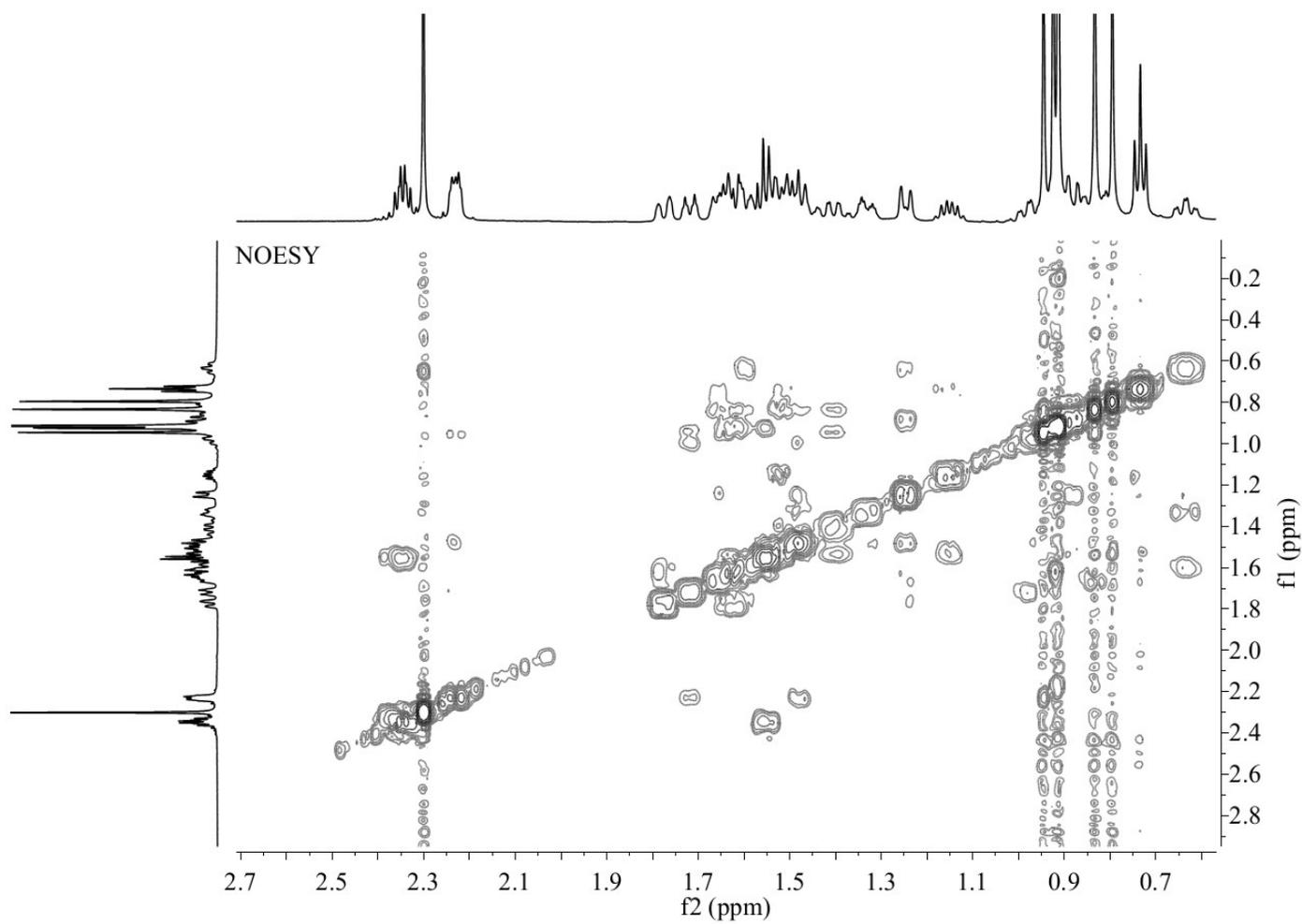


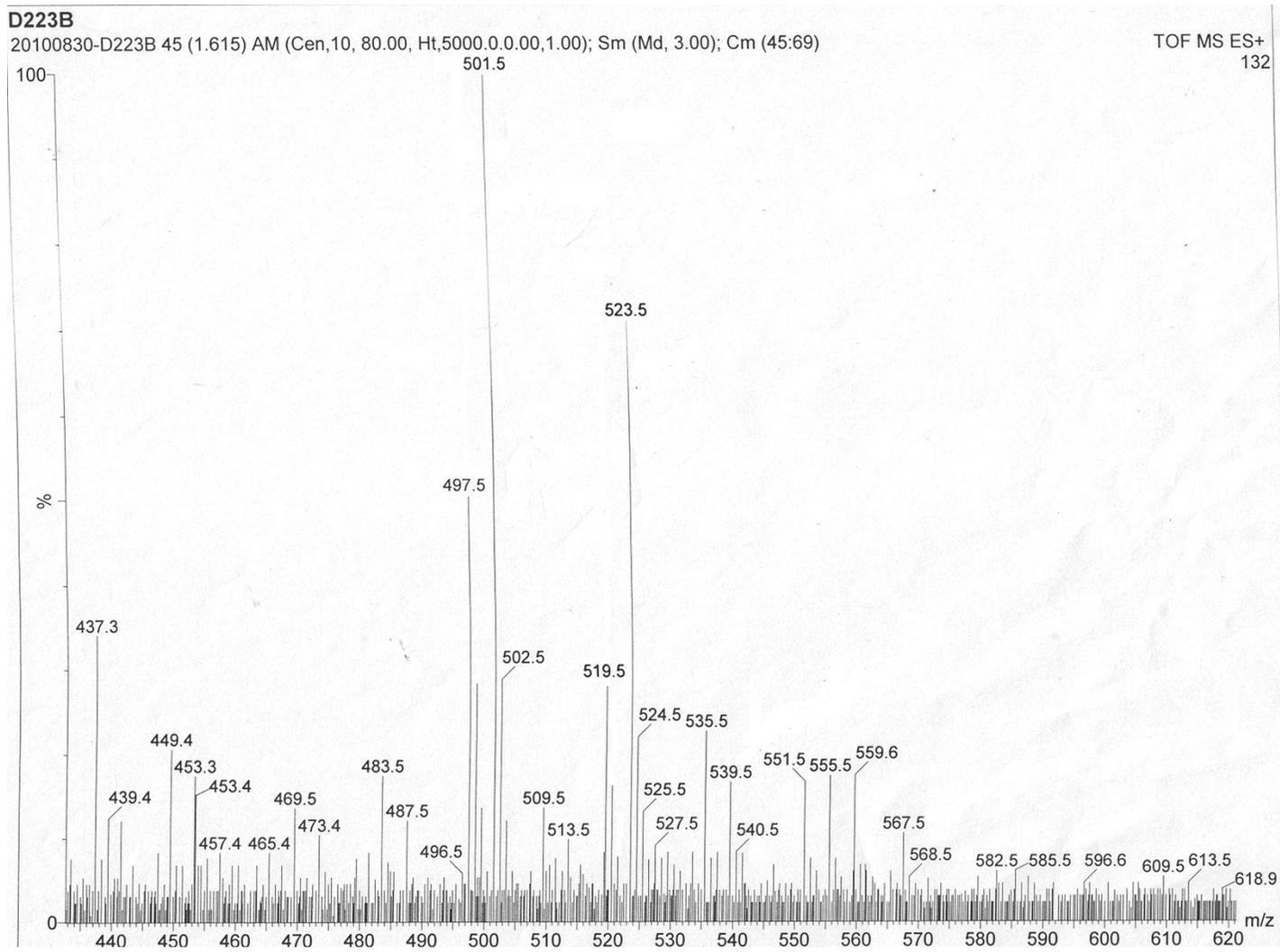
Figure S6. HMBC (CDCl<sub>3</sub>) spectrum of compound 1



**Figure S7.** NOESY (CDCl<sub>3</sub>) spectrum of compound **1**



**Figure S8.** Partial NOESY ( $\text{CDCl}_3$ ) spectrum of compound **1**



**Figure S9.** ESIMS spectrum of compound **1**

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

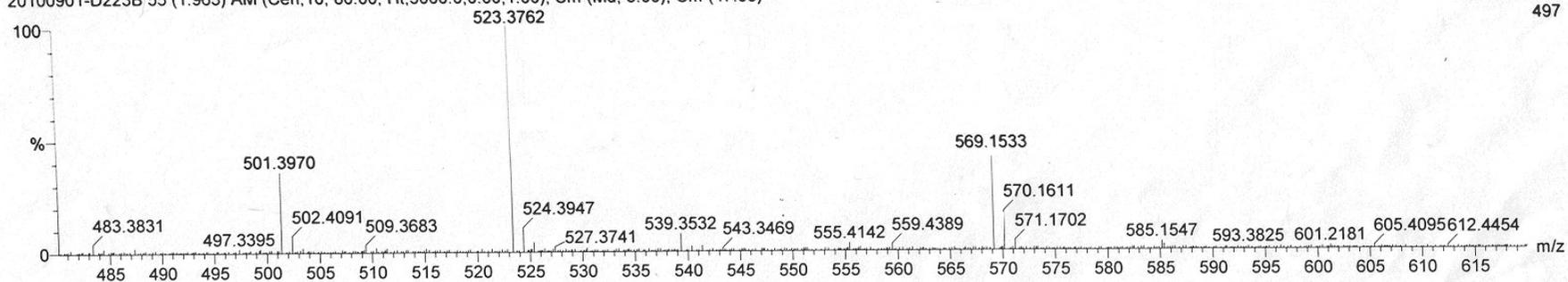
Monoisotopic Mass, Odd and Even Electron Ions

157 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

d223b

20100901-D223B 55 (1.963) AM (Cen, 10, 80.00, Ht, 5000.0, 0.00, 1.00); Sm (Md, 3.00); Cm (47:55)

TOF MS ES+  
497

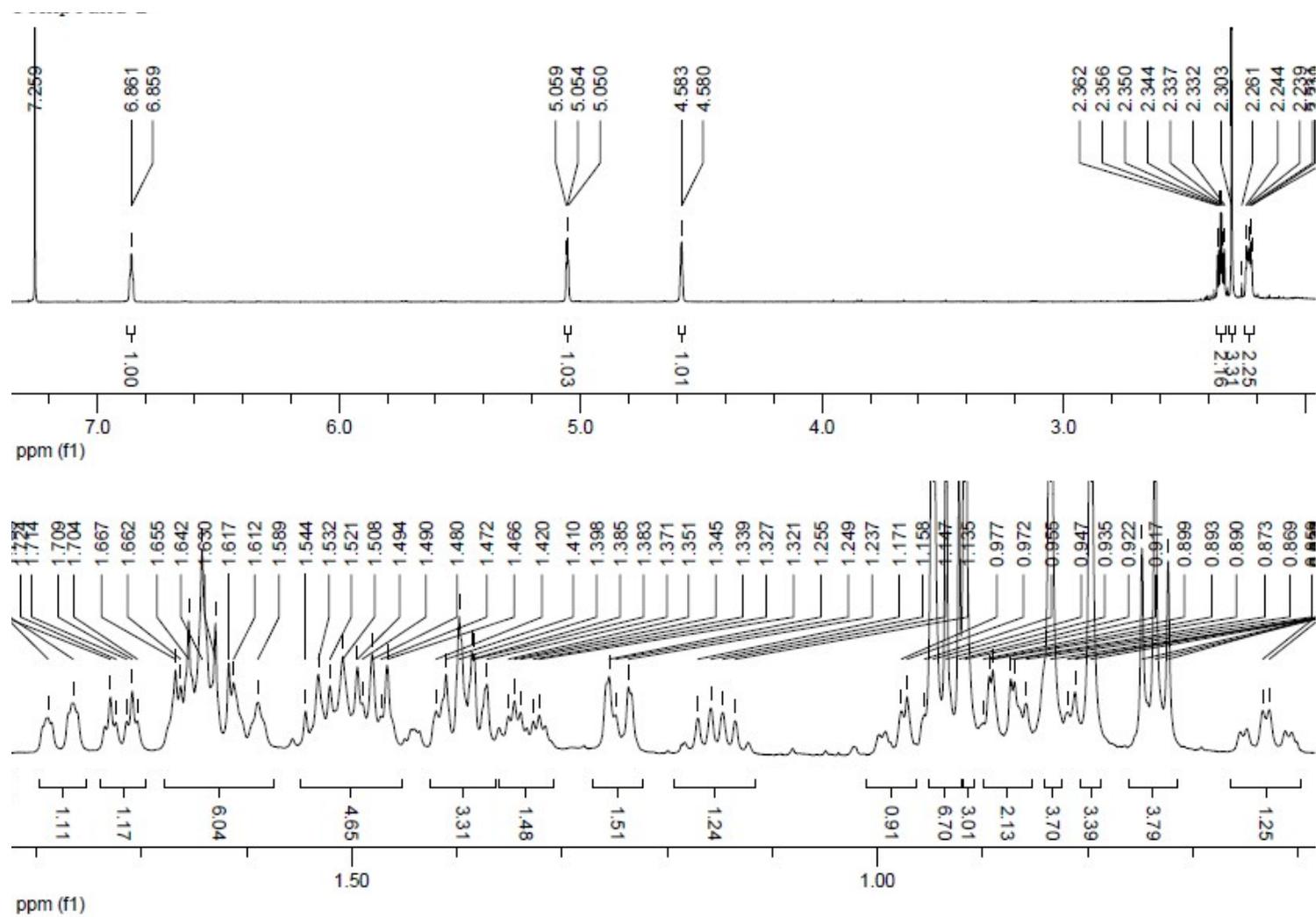


Minimum:

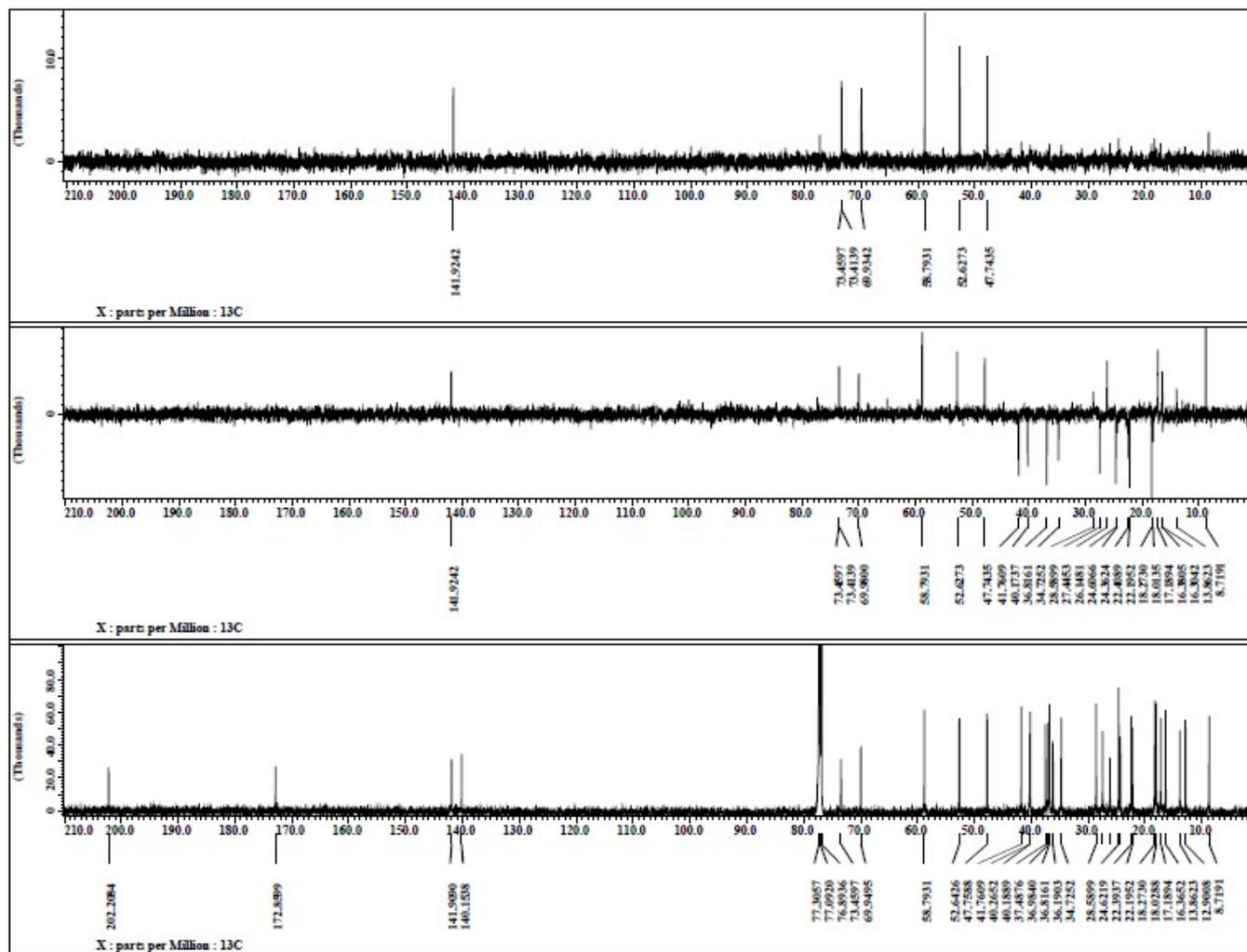
Maximum: 200.0 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
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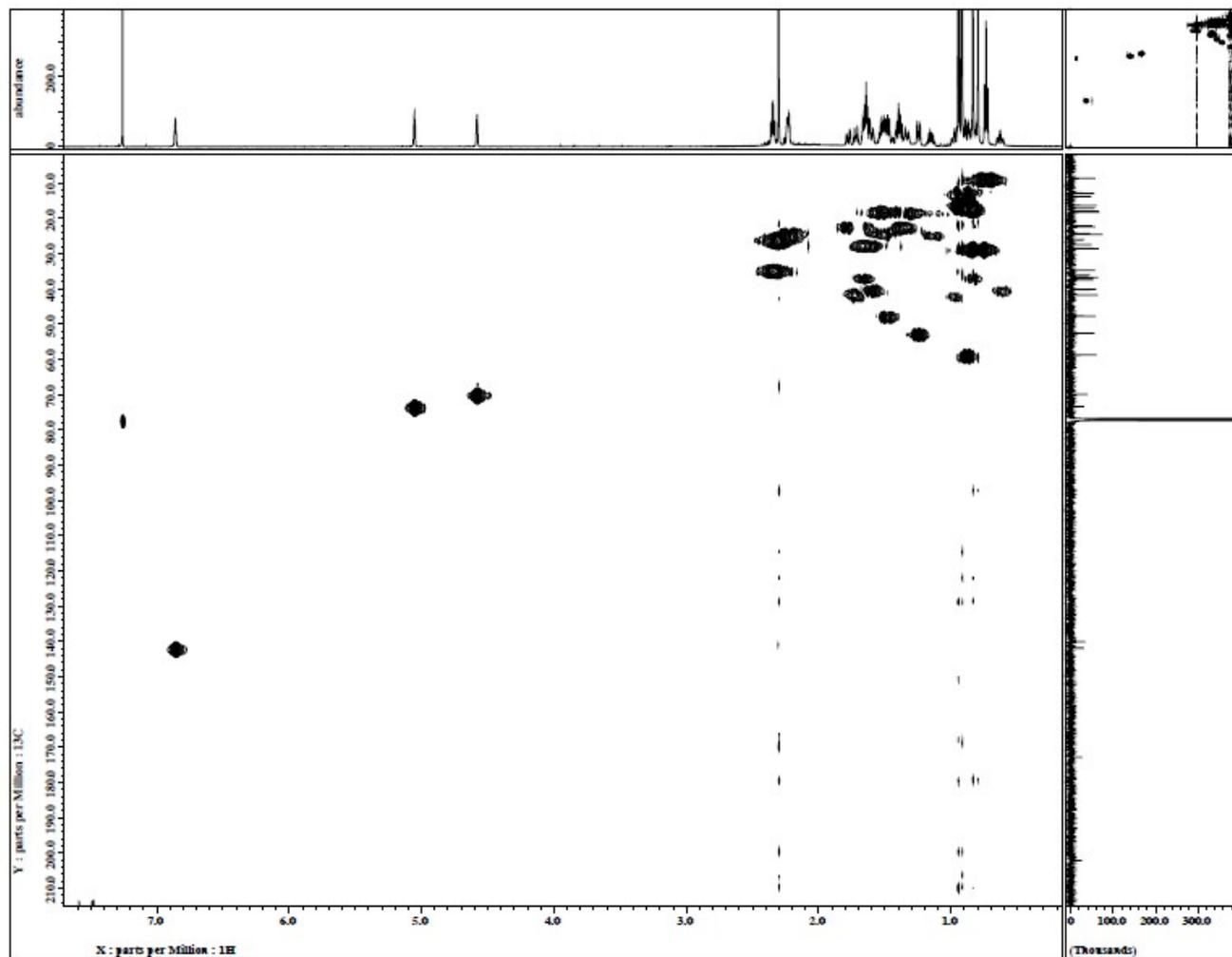
Figure S10. HRESIMS spectrum of compound 1



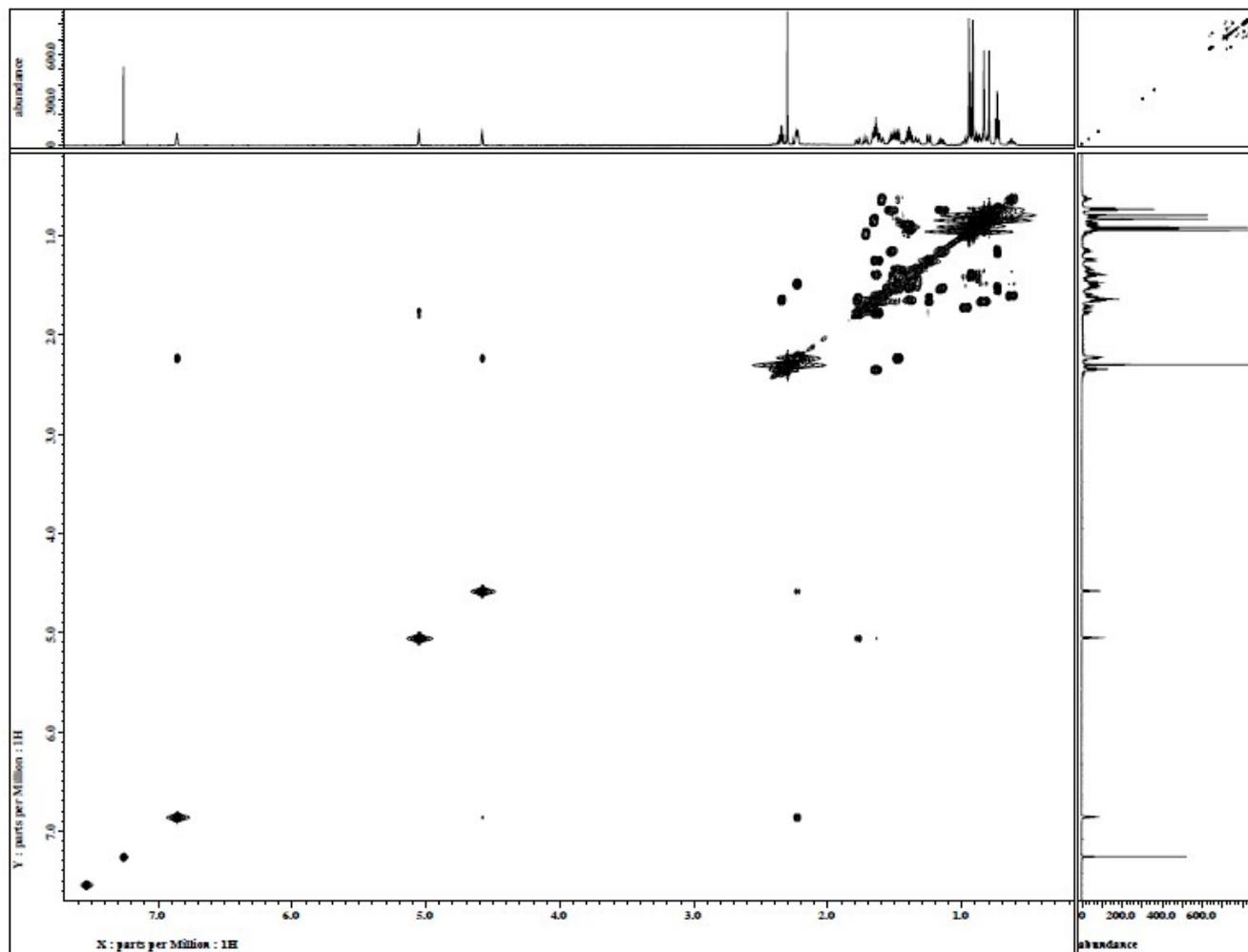
**Figure S11.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **2**



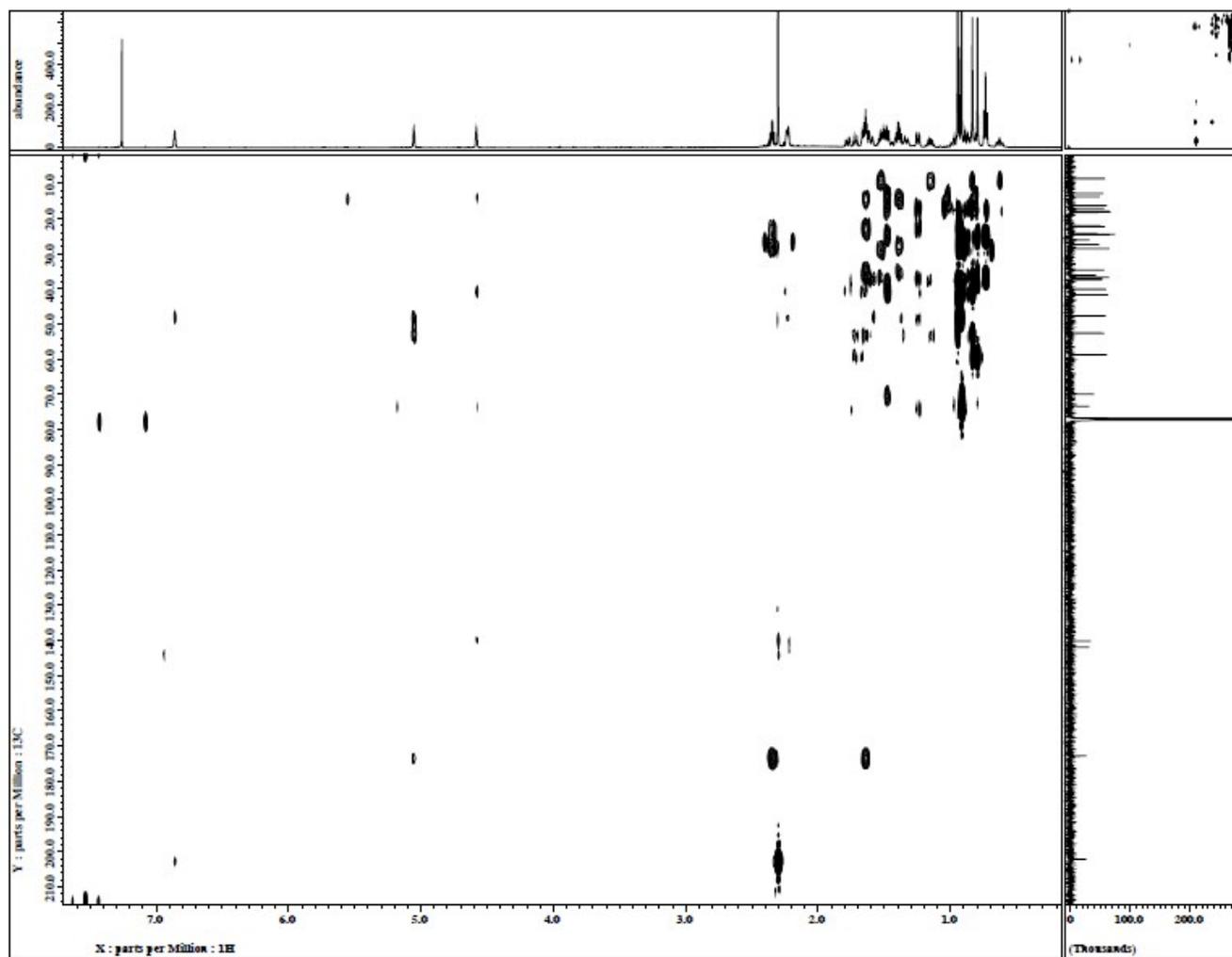
**Figure S12.**  $^{13}\text{C}$  and DEPT NMR (150 MHz,  $\text{CDCl}_3$ ) spectra of compound **2**



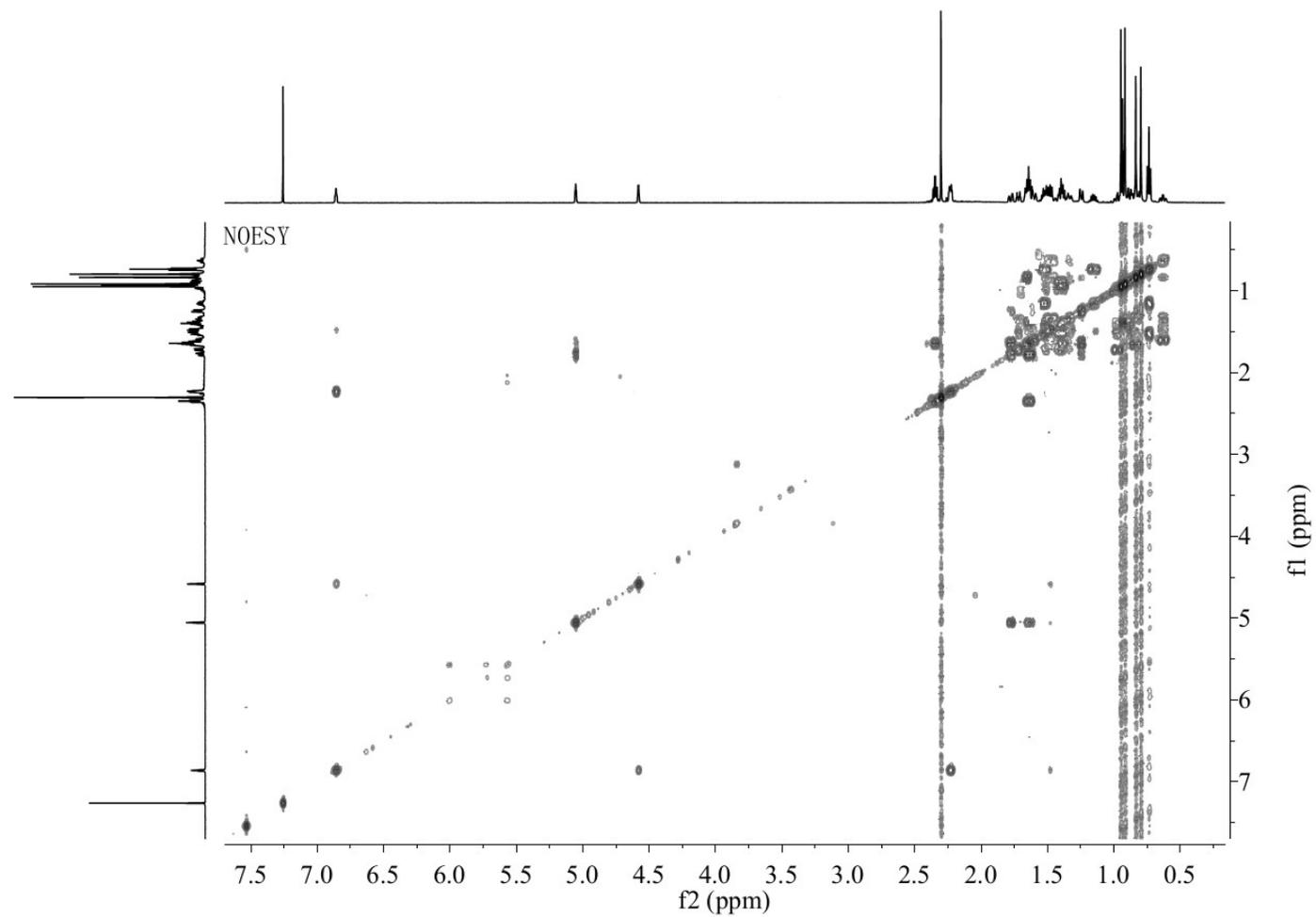
**Figure S13.** HMQC (CDCl<sub>3</sub>) spectrum of compound 2



**Figure S14.** COSY (CDCl<sub>3</sub>) spectrum of compound 2



**Figure S15.** HMBC (CDCl<sub>3</sub>) spectrum of compound 2



**Figure S16.** NOESY (CDCl<sub>3</sub>) spectrum of compound **2**

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

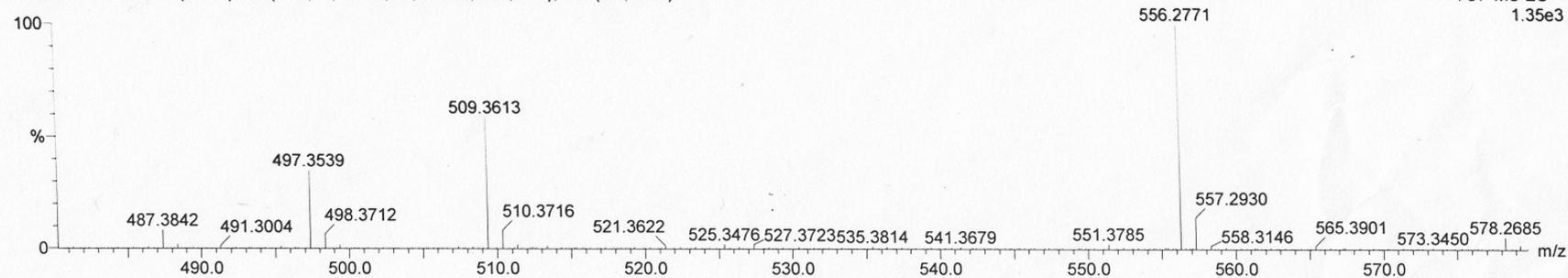
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

64 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

D-223A

20101018-D-223A 52 (1.855) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

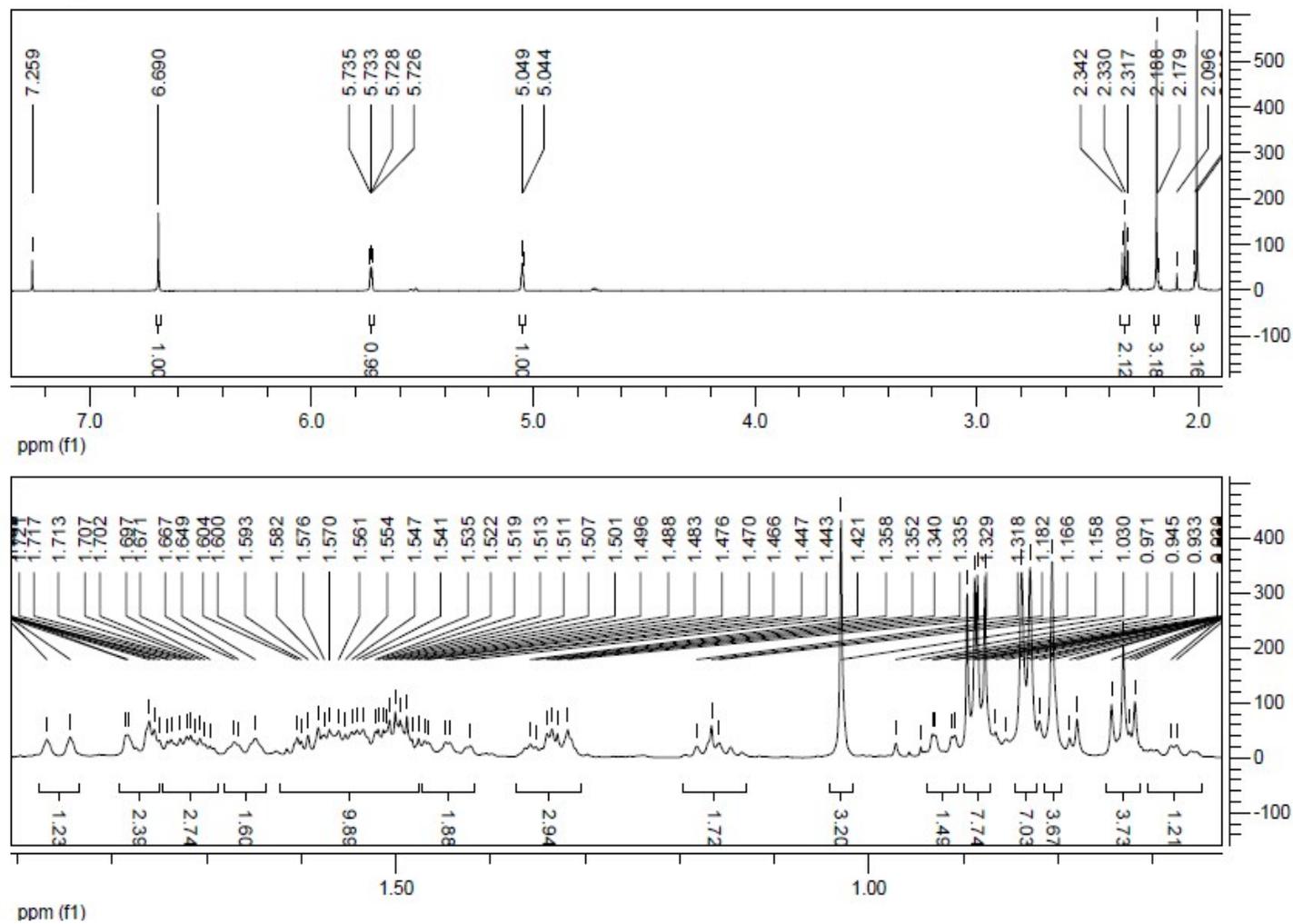


Minimum:

Maximum: 200.0 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
509.3613	509.3607	0.6	1.2	6.5	1	C31 H50 O4 Na

Figure S17. HRESIMS spectrum of compound 2



**Figure S18.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **3**

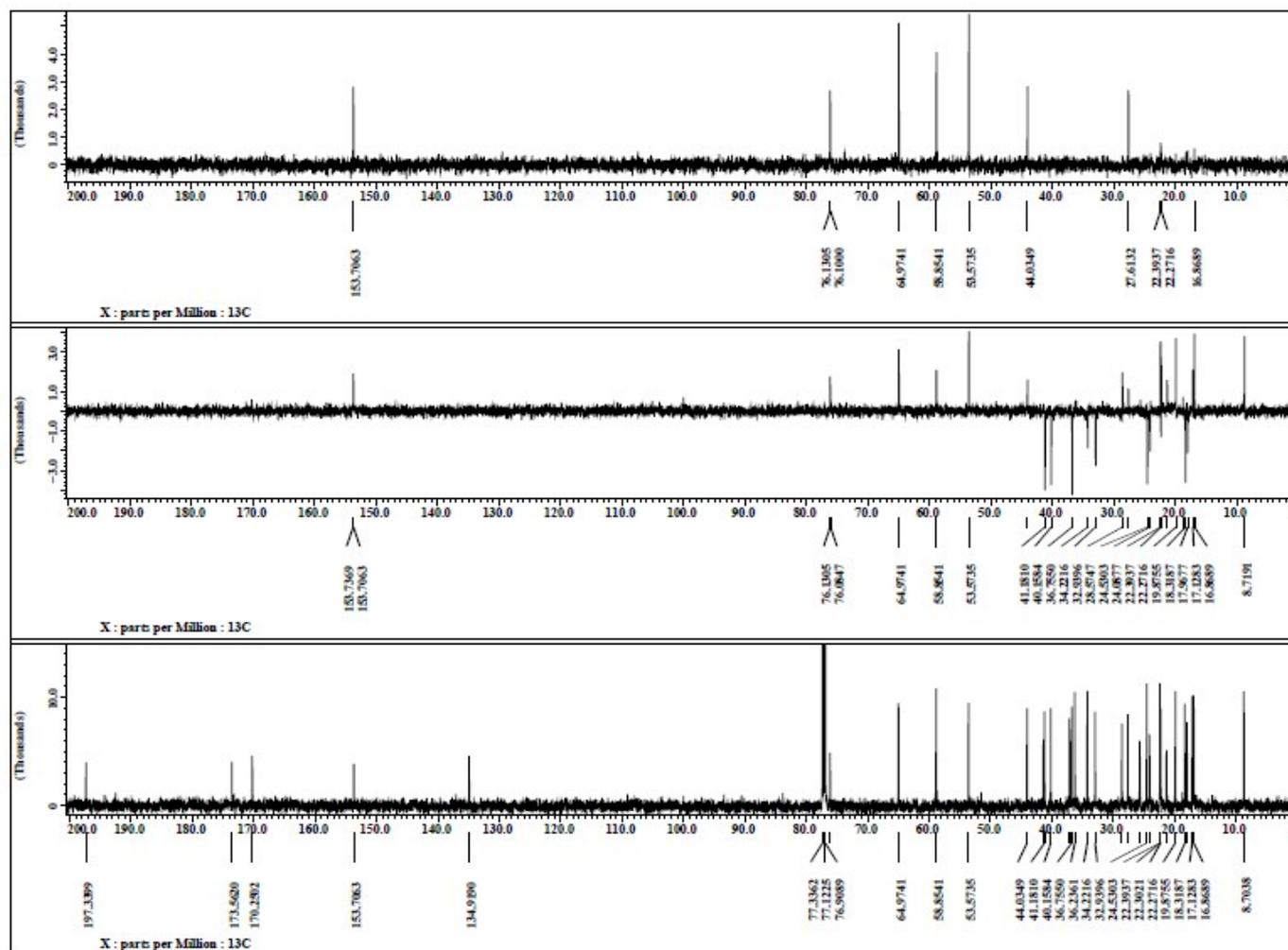


Figure S19. <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound 3

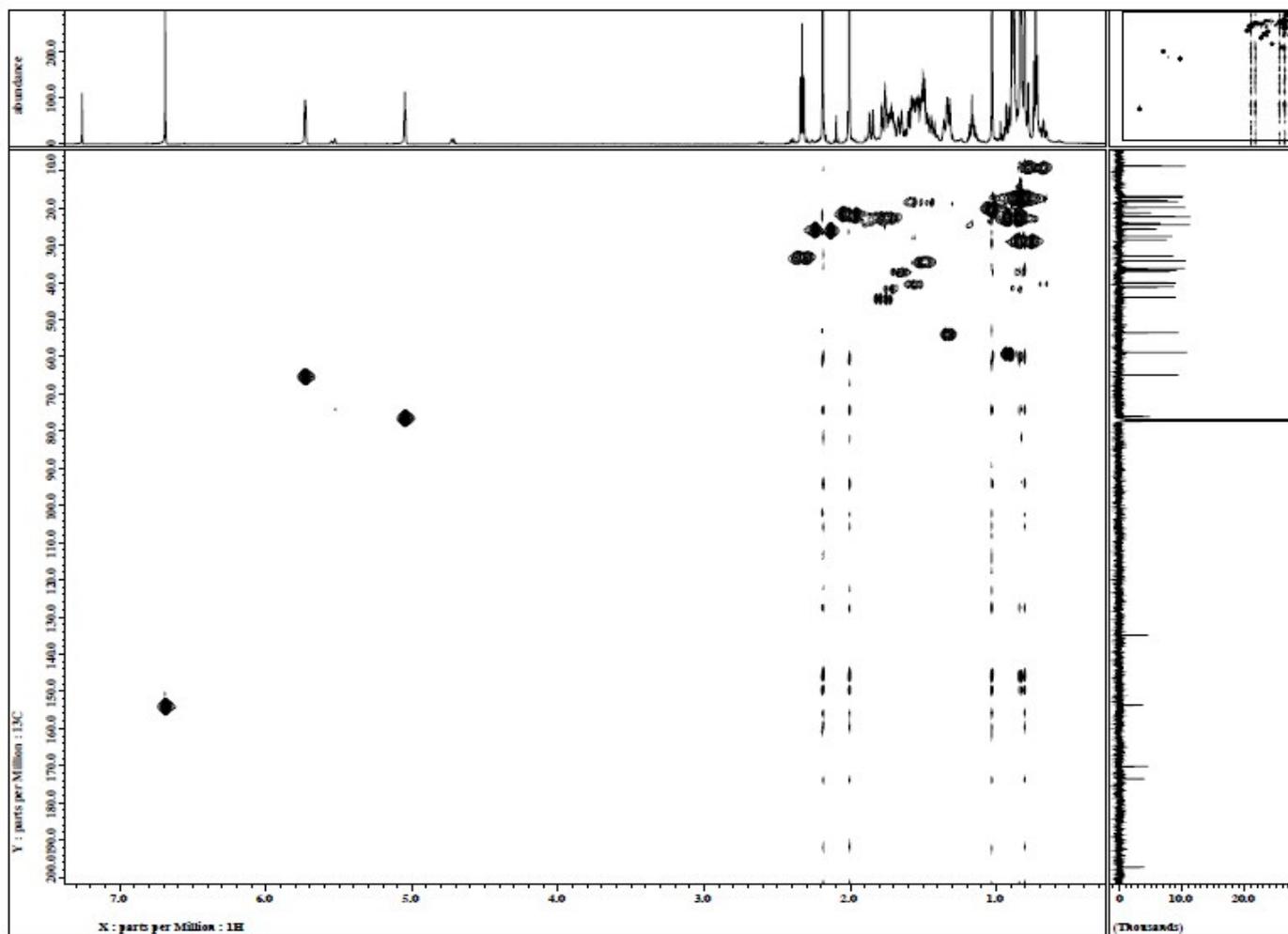
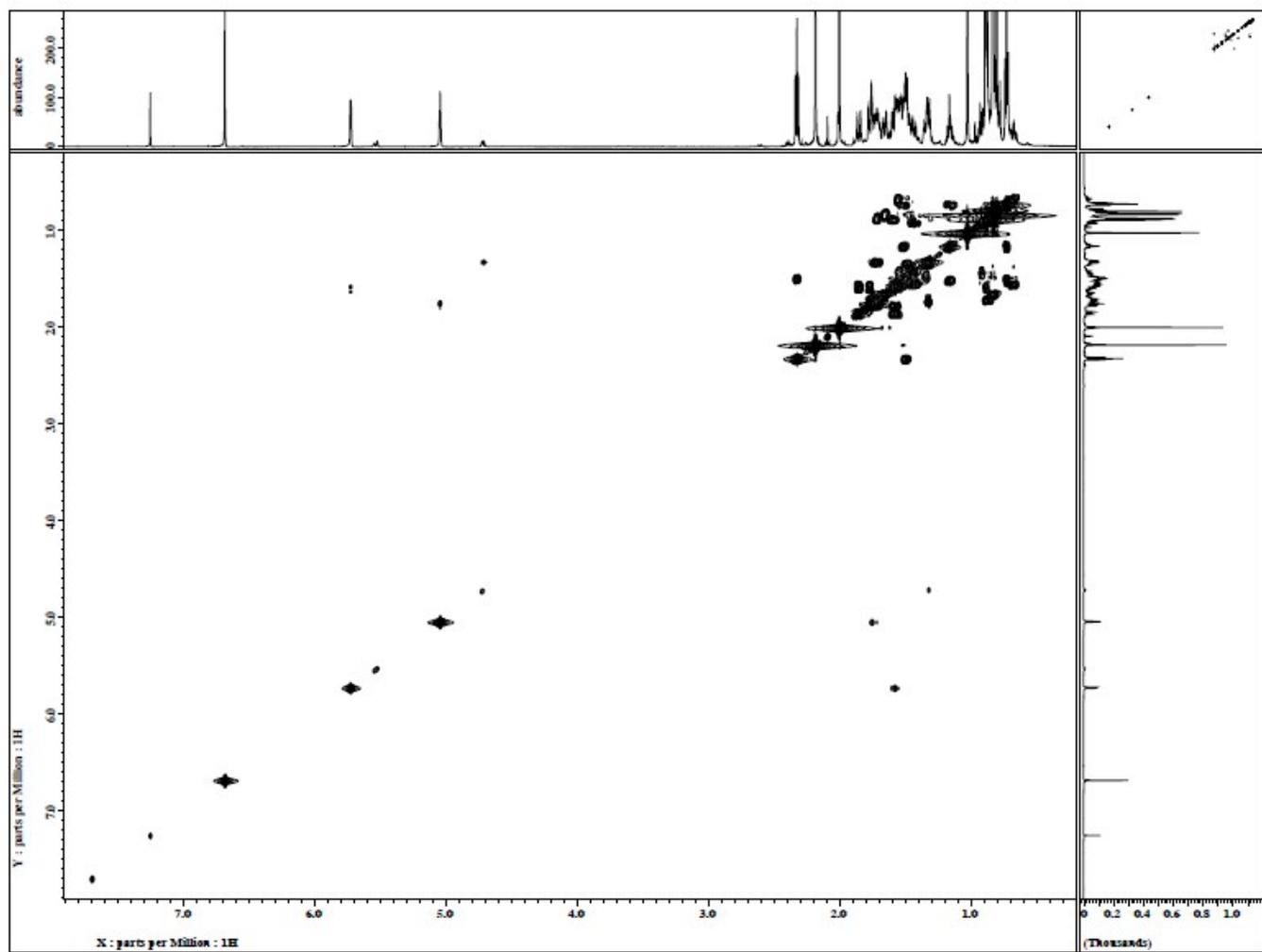
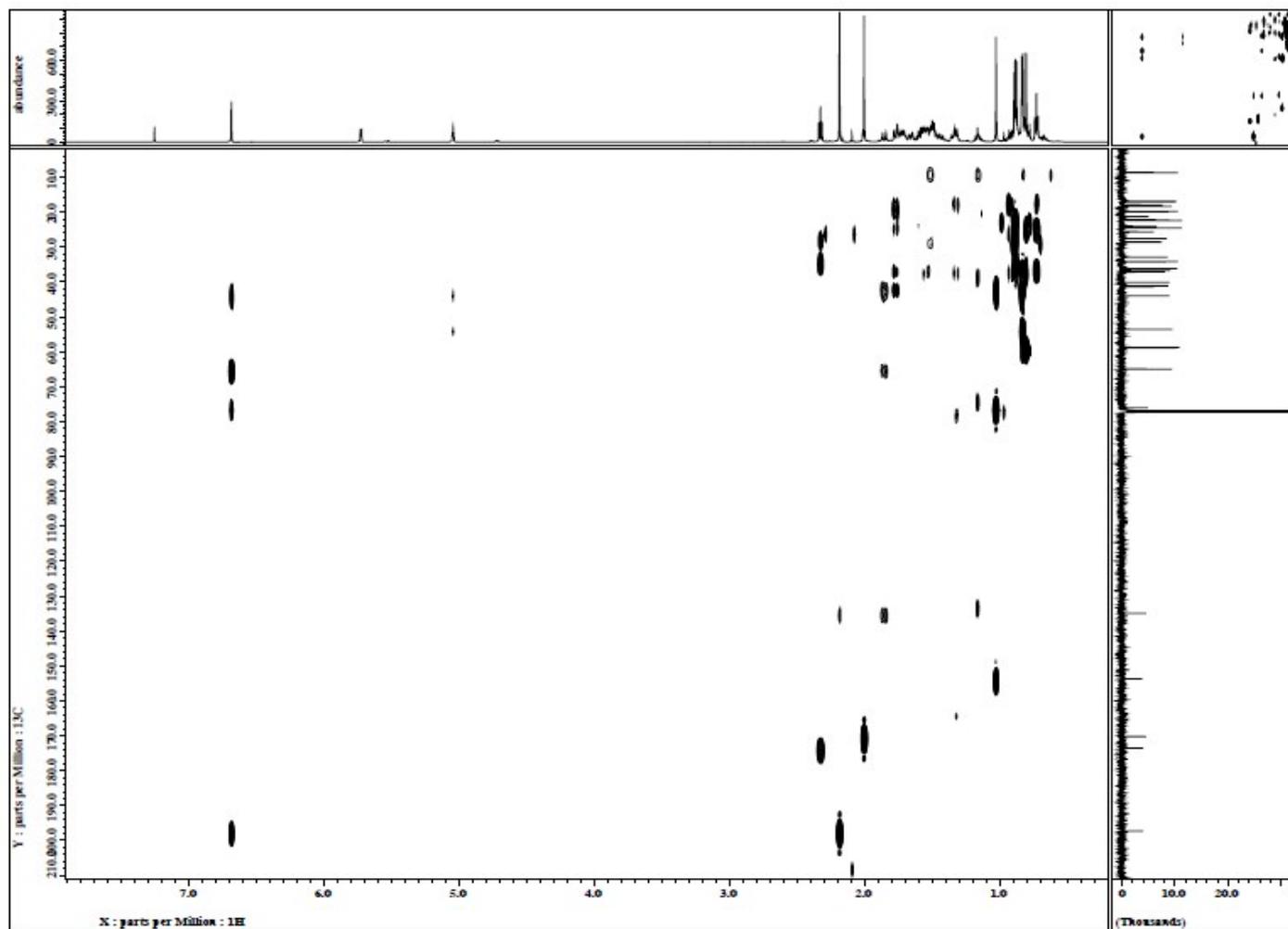


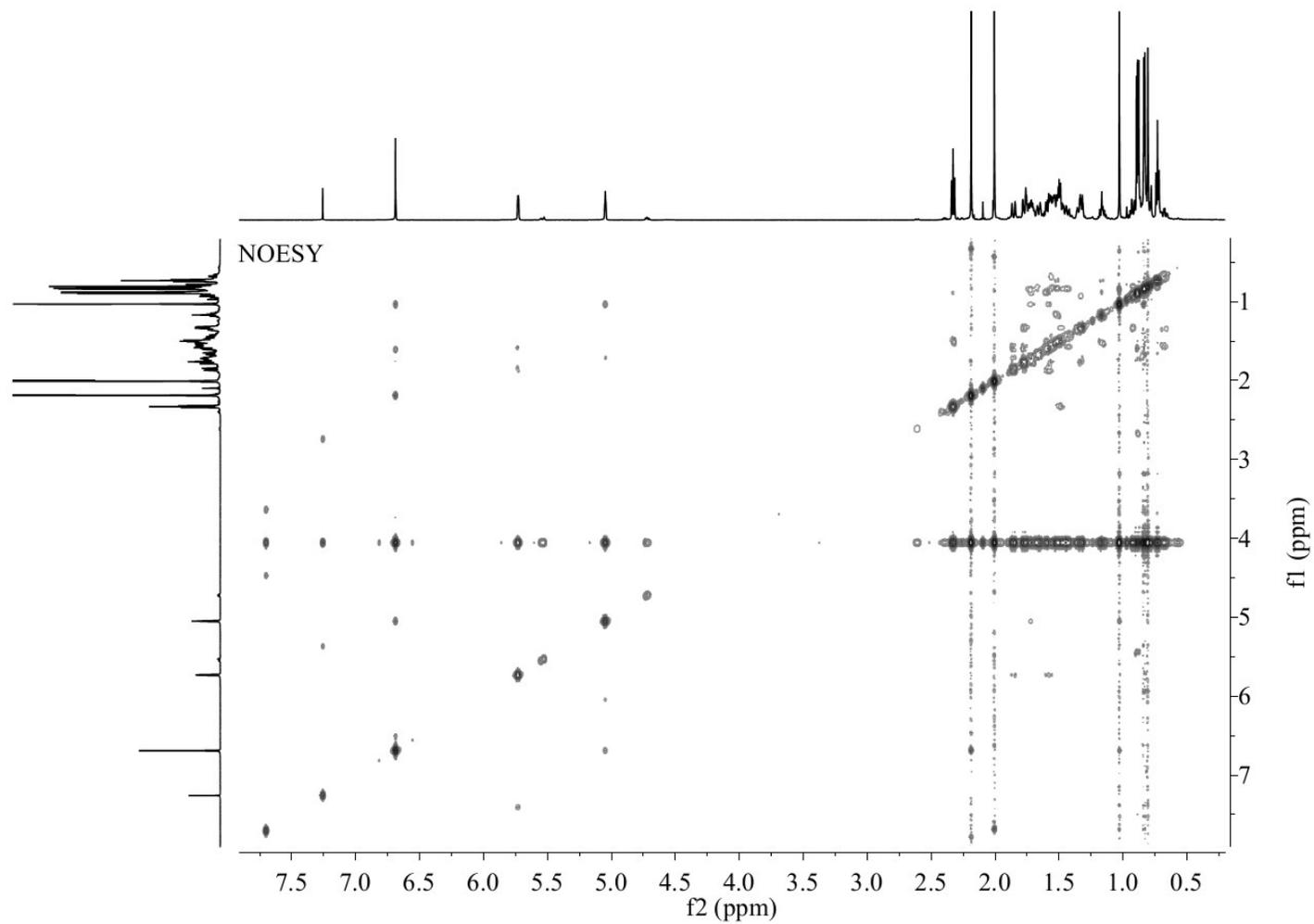
Figure S20. HMQC (CDCl<sub>3</sub>) spectrum of compound 3



**Figure S21.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **3**



**Figure S22.** HMBC (CDCl<sub>3</sub>) spectrum of compound **3**



**Figure S23.** NOESY (CDCl<sub>3</sub>) spectrum of compound **3**

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

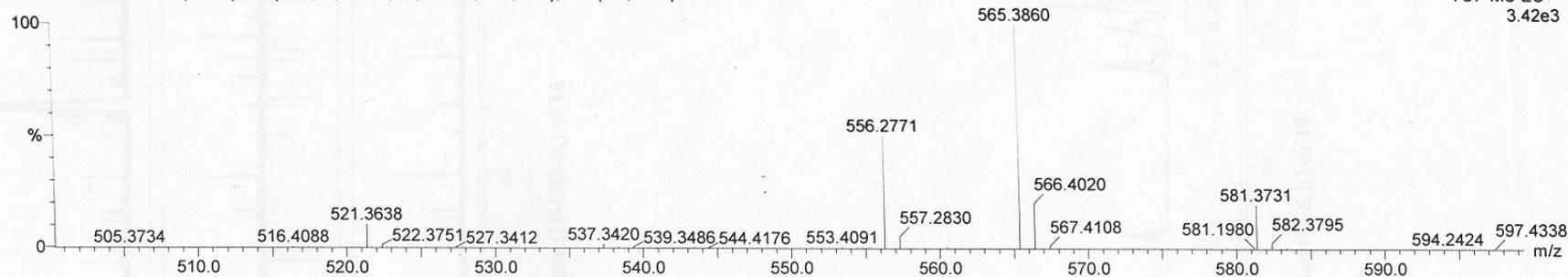
Monoisotopic Mass, Odd and Even Electron Ions

27 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

D-4-3B

20101018-D-4-3B 101 (3.601) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

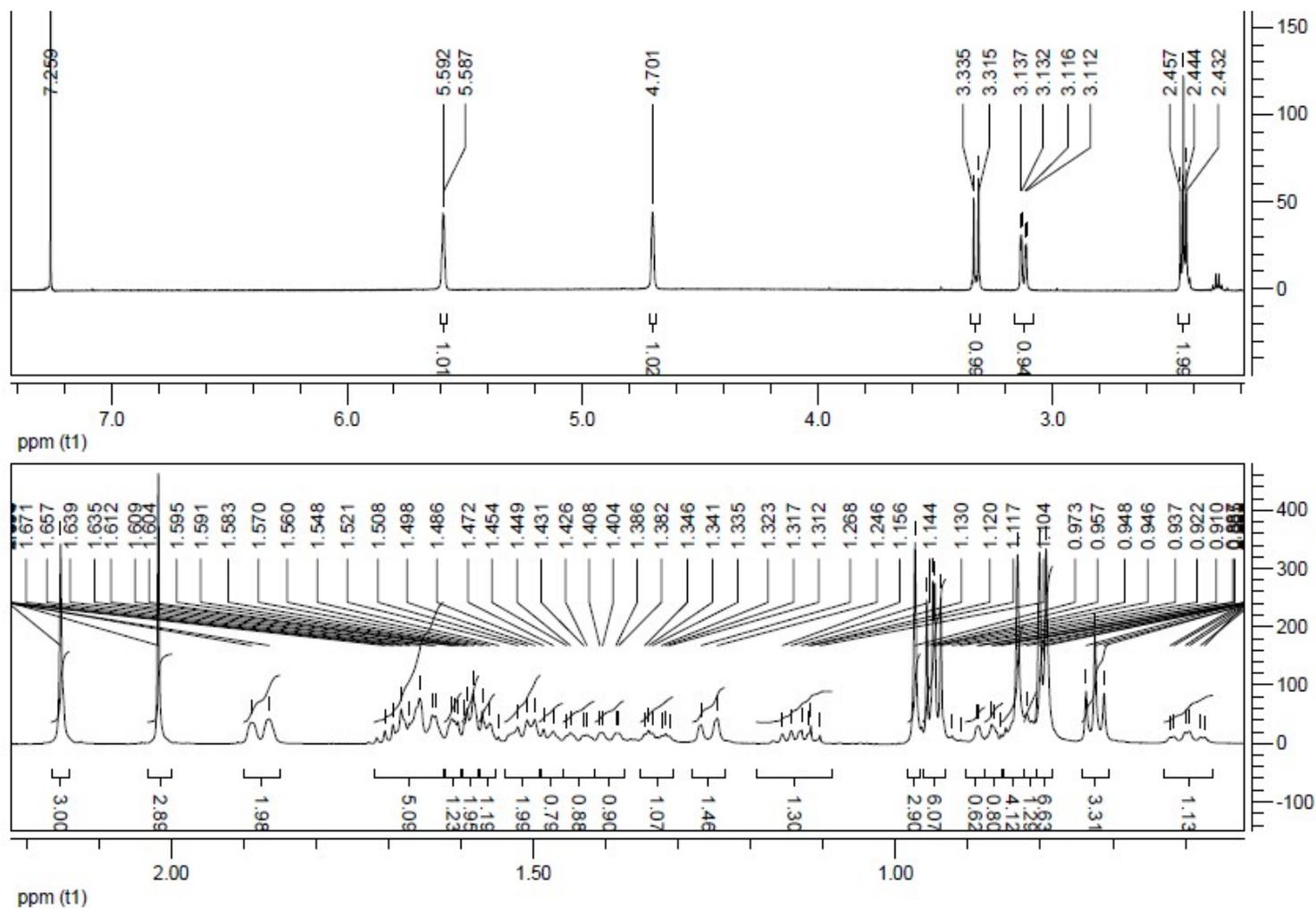
TOF MS ES+  
3.42e3



Minimum: -1.5  
Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
565.3860	565.3869	-0.9	-1.6	7.5	1	C34 H54 O5 Na

Figure S24. HRESIMS spectrum of compound 3



**Figure S25.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 4

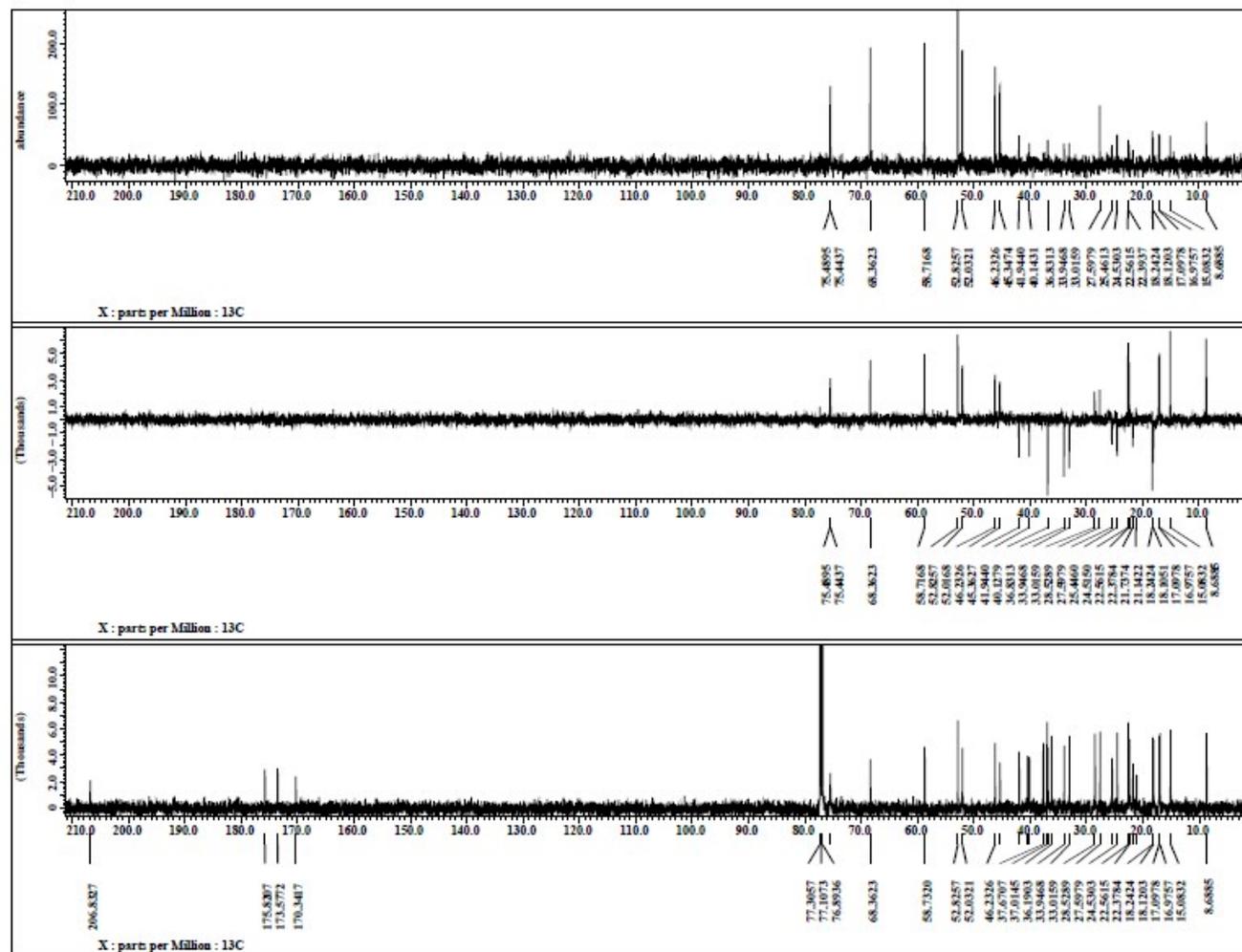
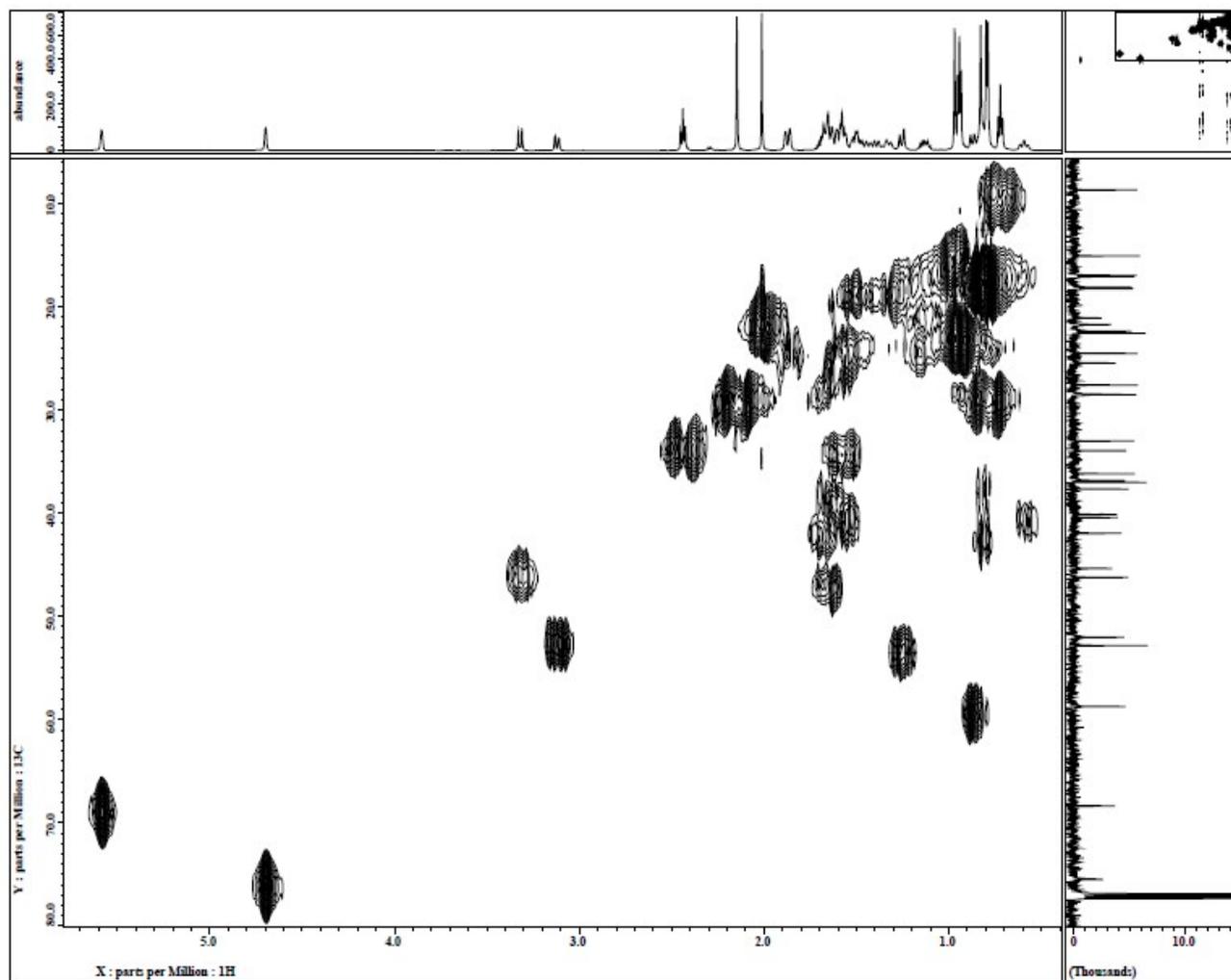
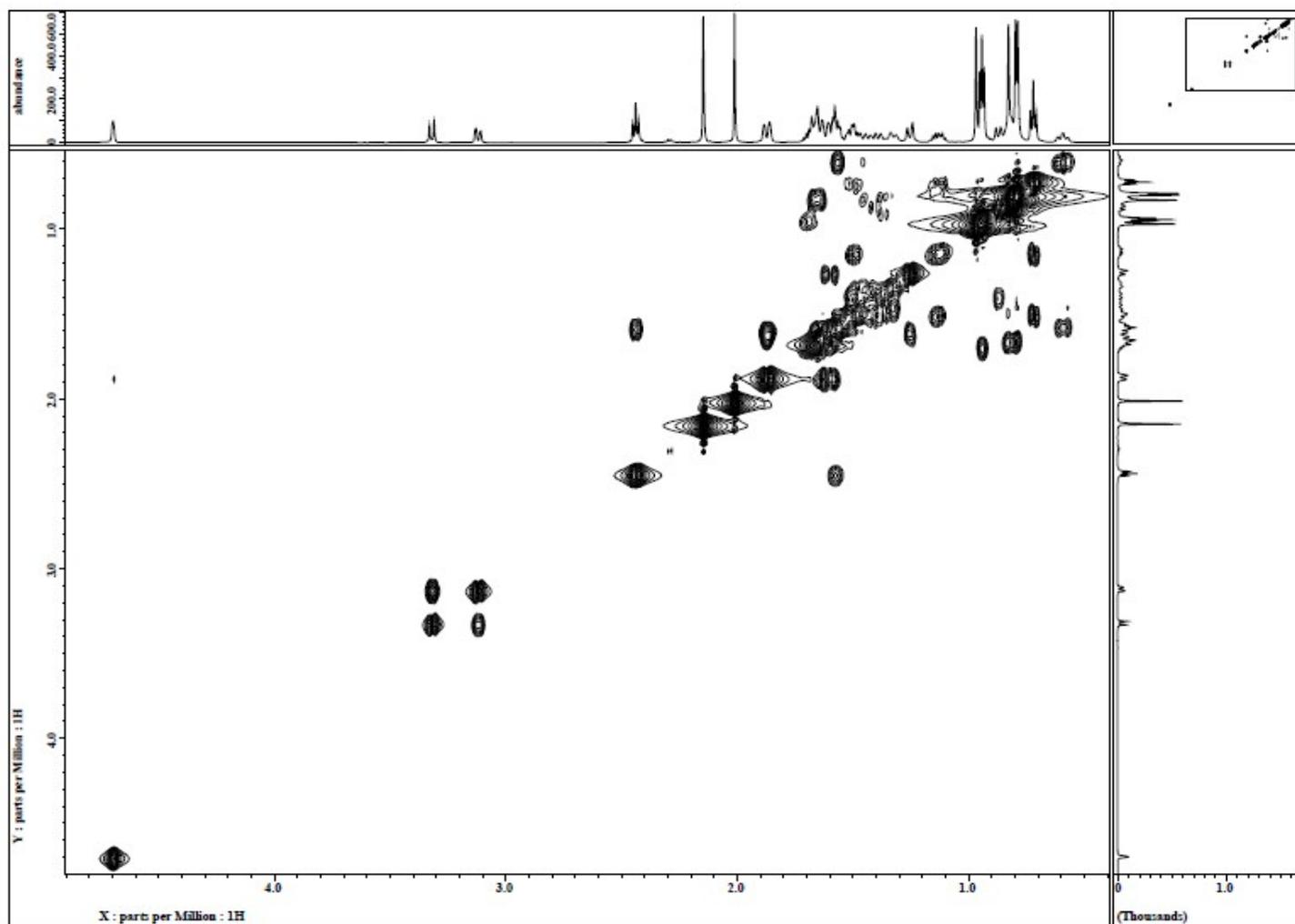


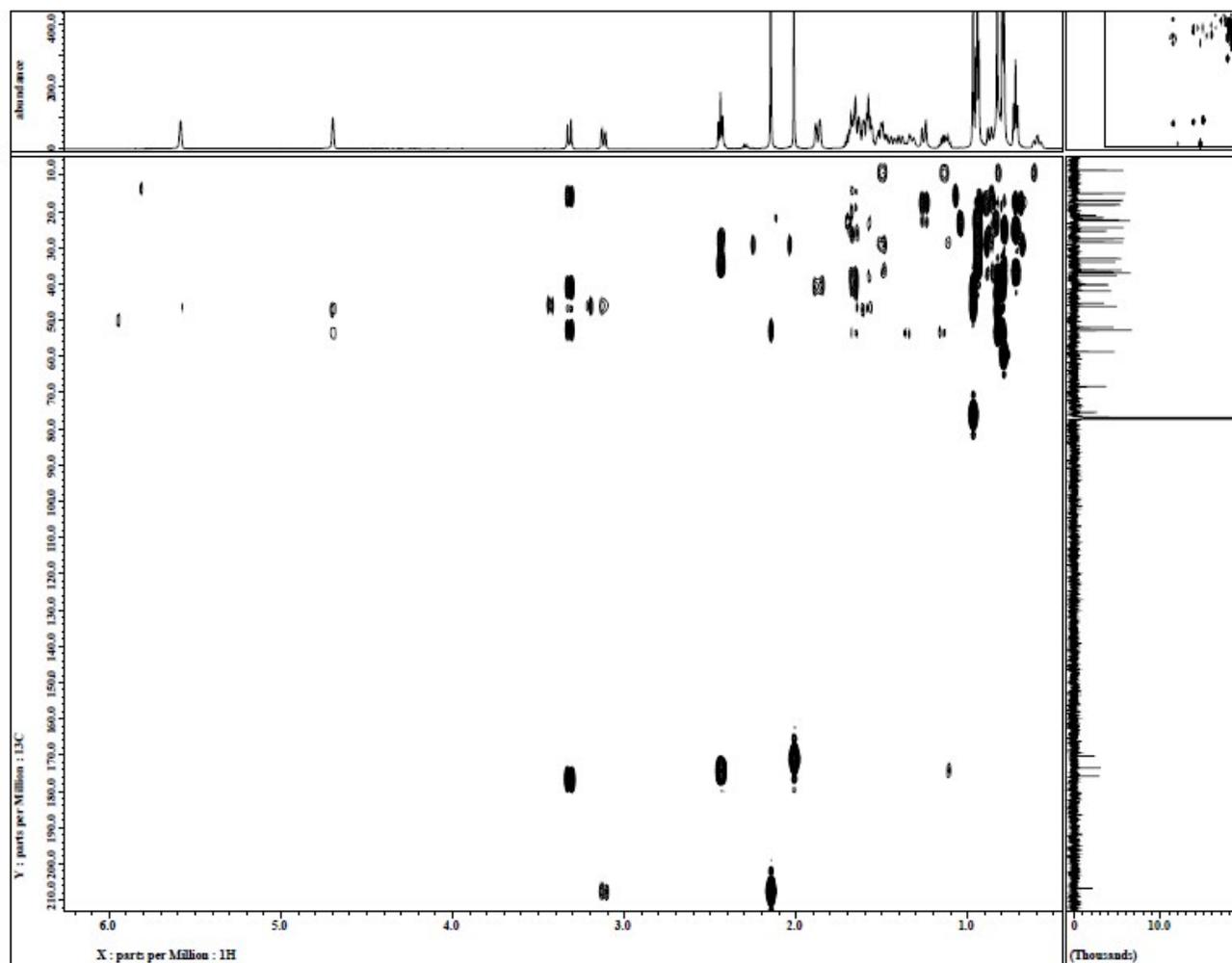
Figure S26. <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound 4



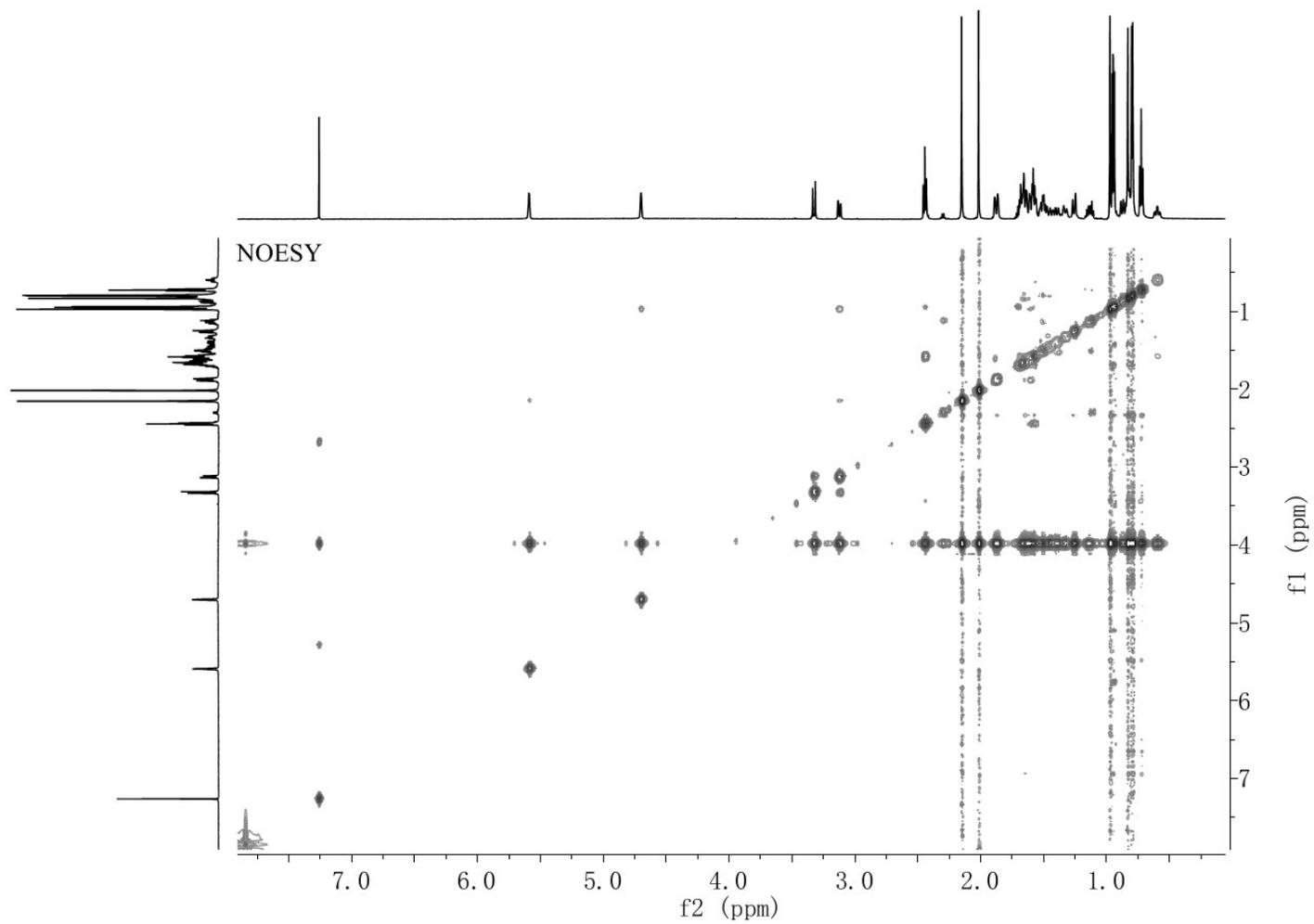
**Figure S27.** HMQC (CDCl<sub>3</sub>) spectrum of compound 4



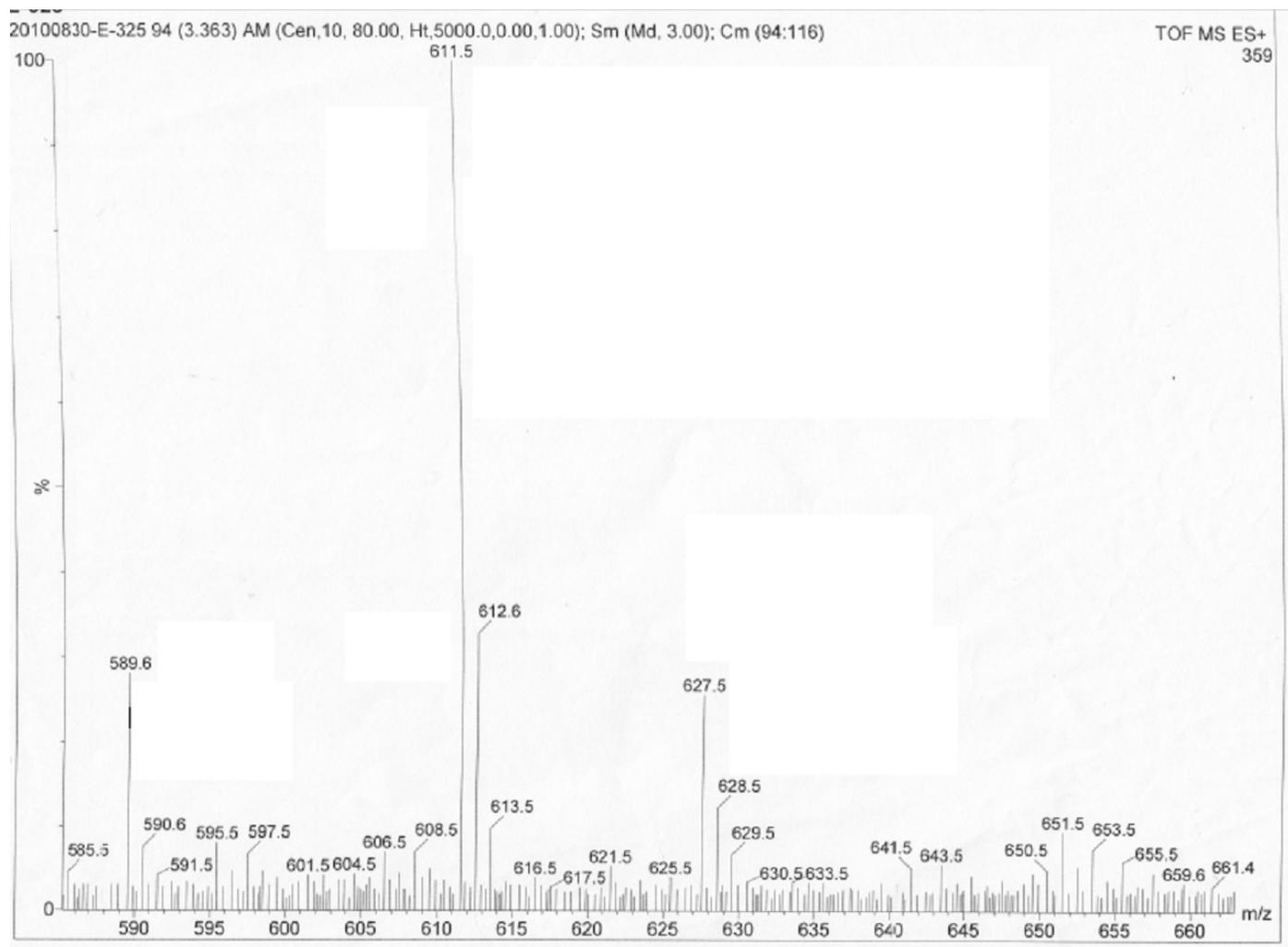
**Figure S28.** COSY ( $\text{CDCl}_3$ ) spectrum of compound 4



**Figure S29.** HMBC ( $\text{CDCl}_3$ ) spectrum of compound 4



**Figure S30.** NOESY (CDCl<sub>3</sub>) spectrum of compound **4**



**Figure S31.** ESIMS spectrum of compound **4**

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

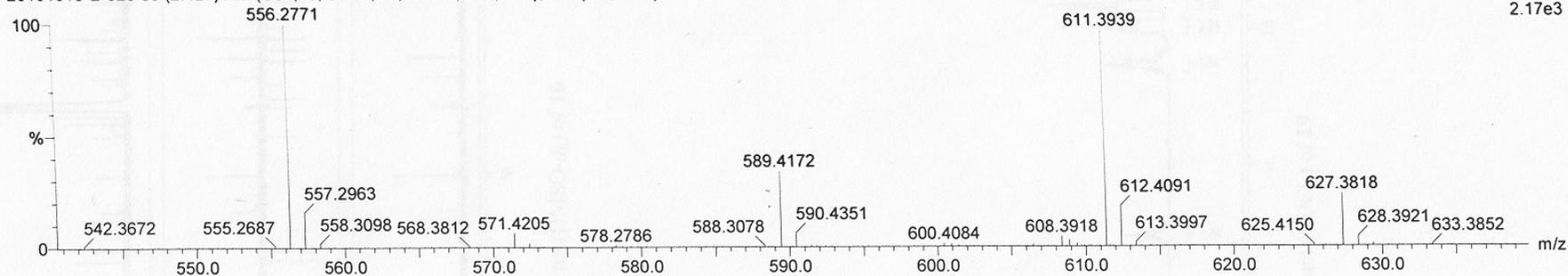
Monoisotopic Mass, Odd and Even Electron Ions

60 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

E-325

20101018-E-325 68 (2.427) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

TOF MS ES+  
2.17e3



Minimum: -1.5  
Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
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Figure S32. HRESIMS spectrum of compound 4

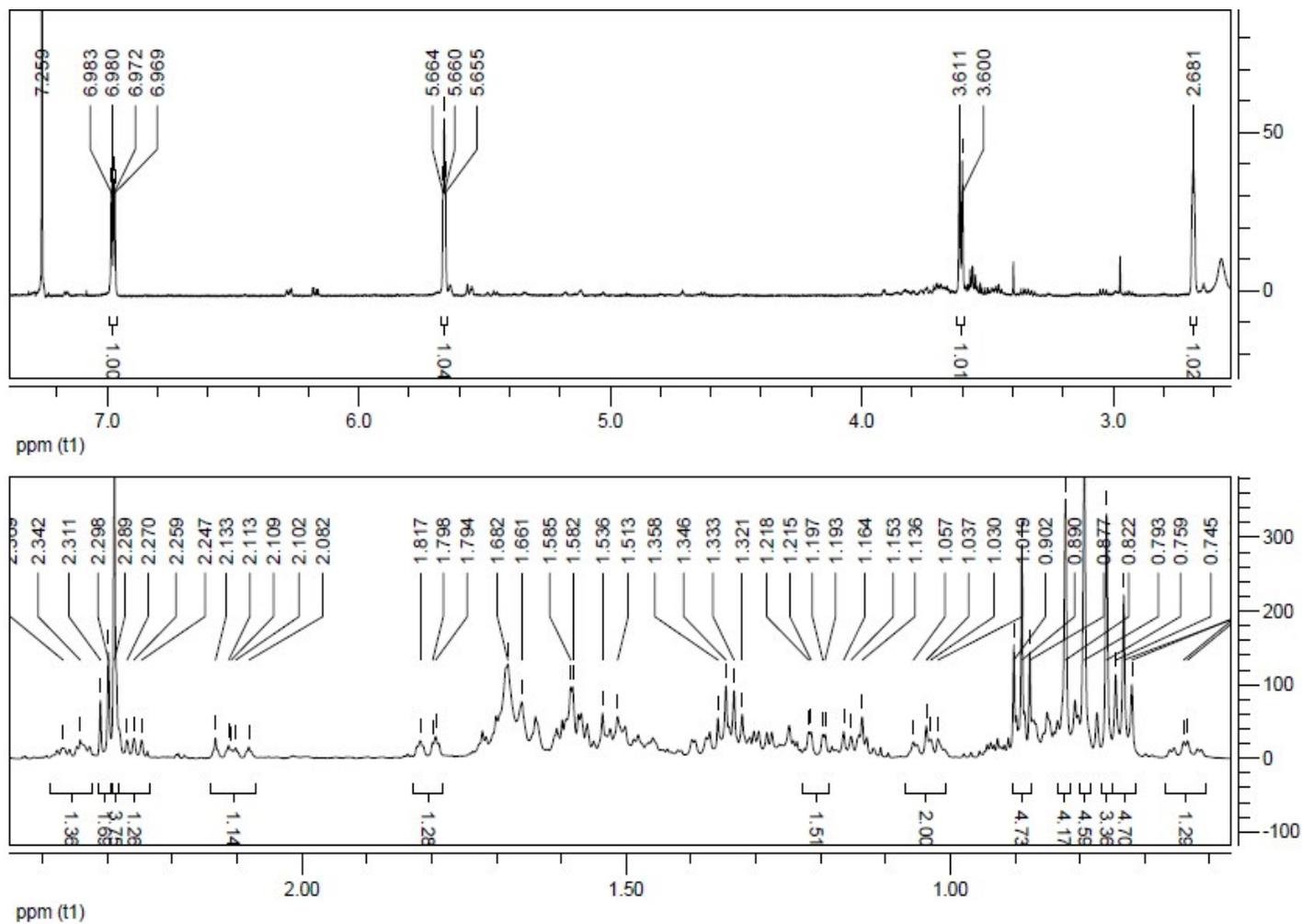


Figure S33. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 5

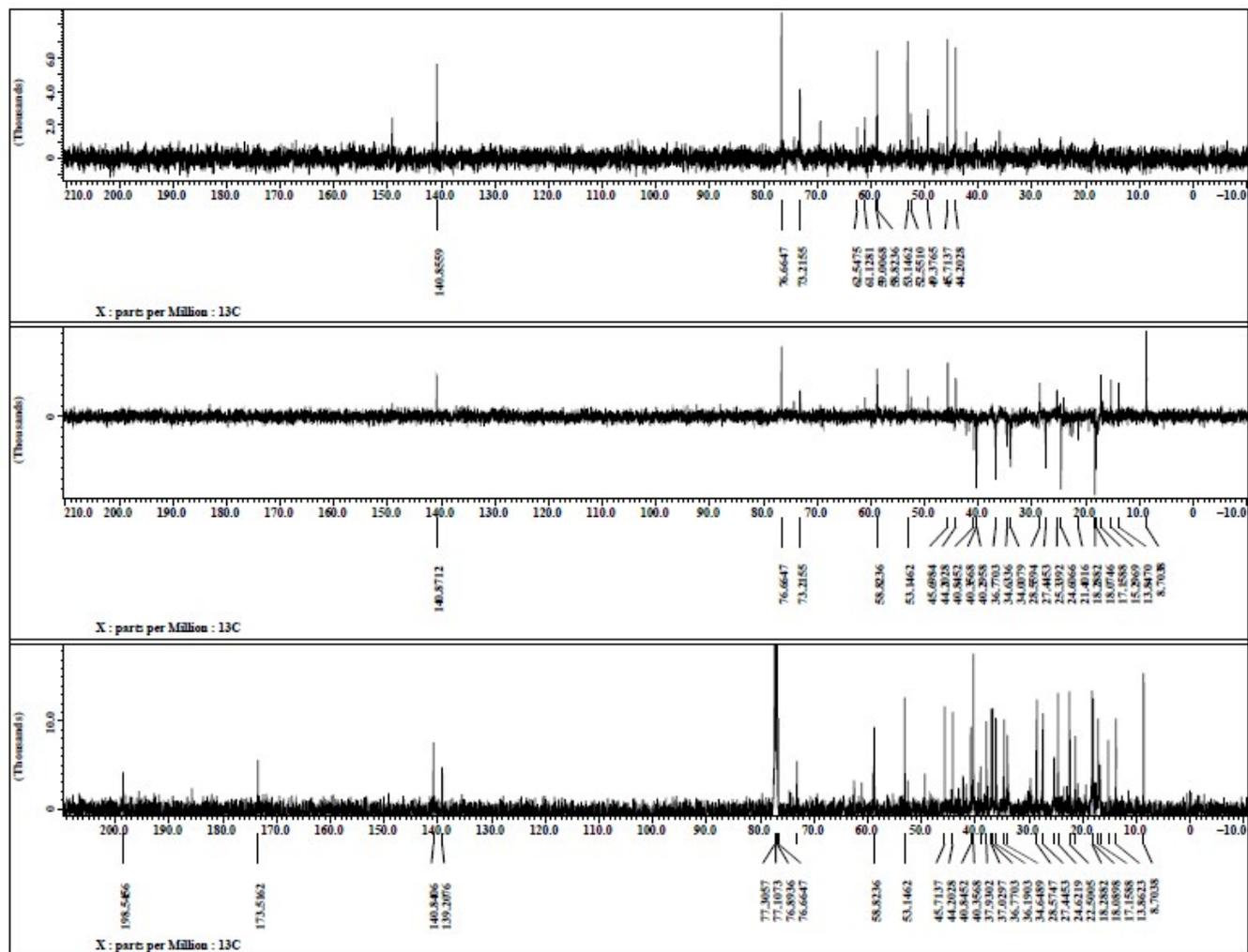


Figure S34. <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound 5

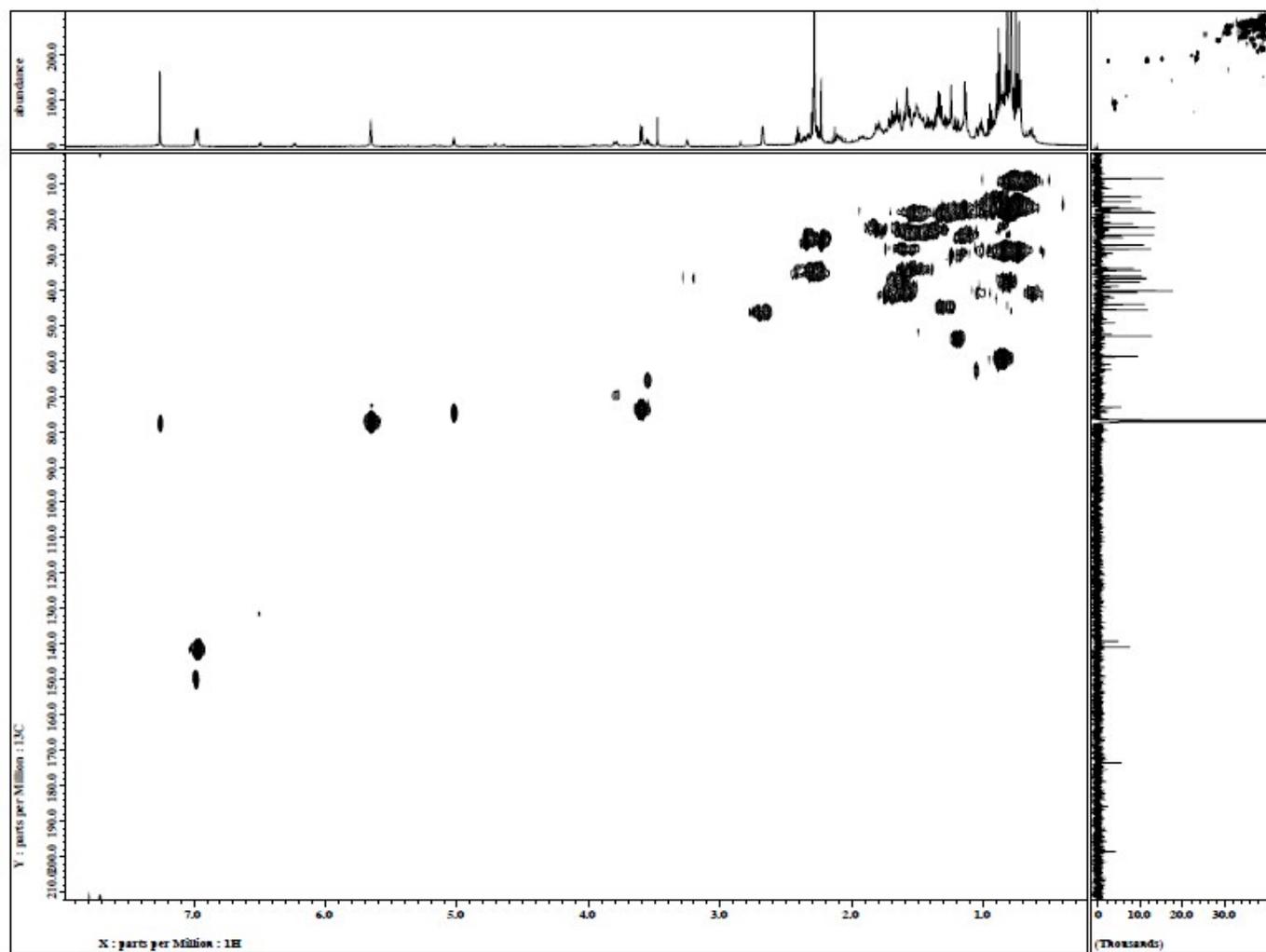
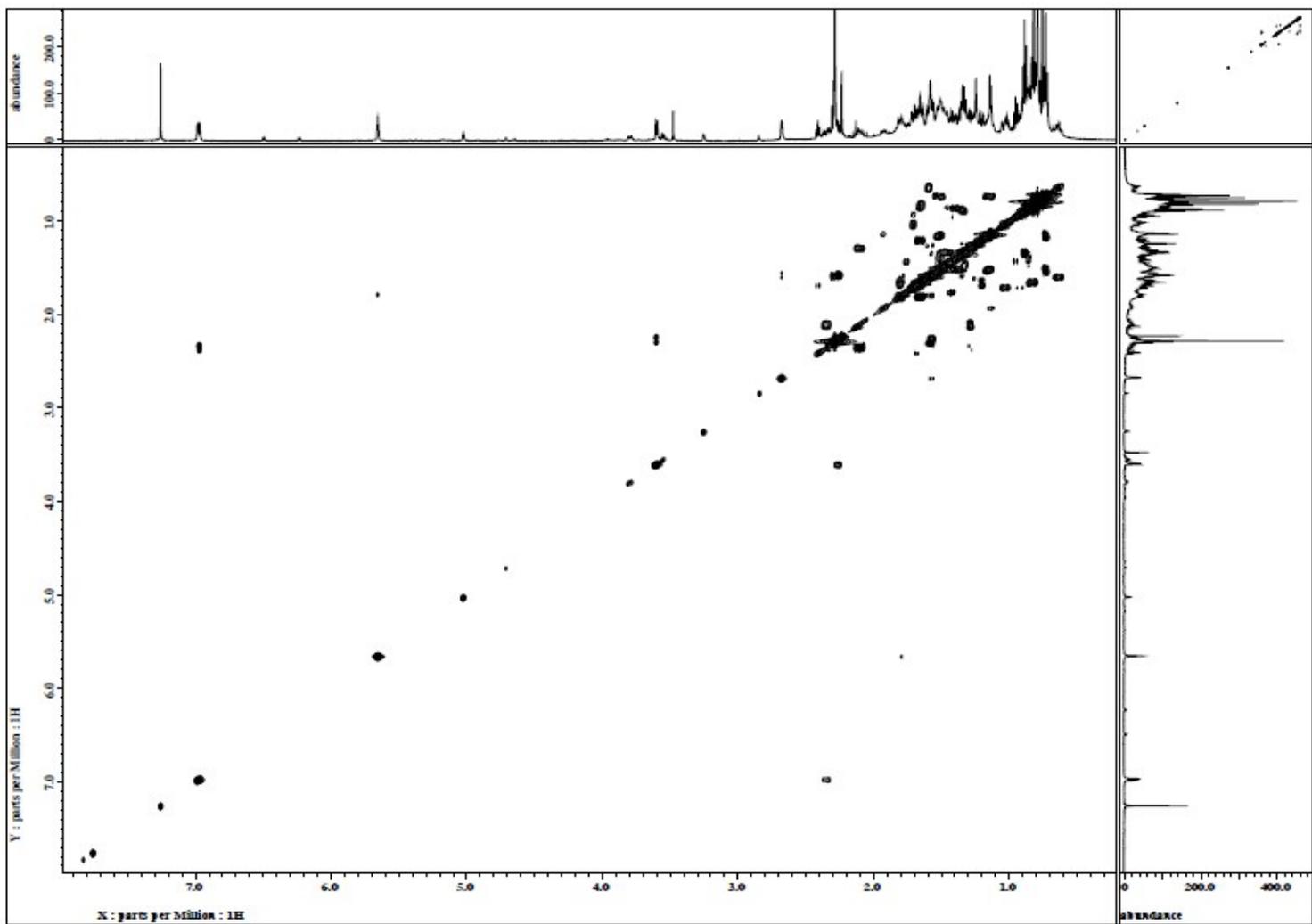


Figure S35. HMQC (CDCl<sub>3</sub>) spectrum of compound 5



**Figure S36.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **5**

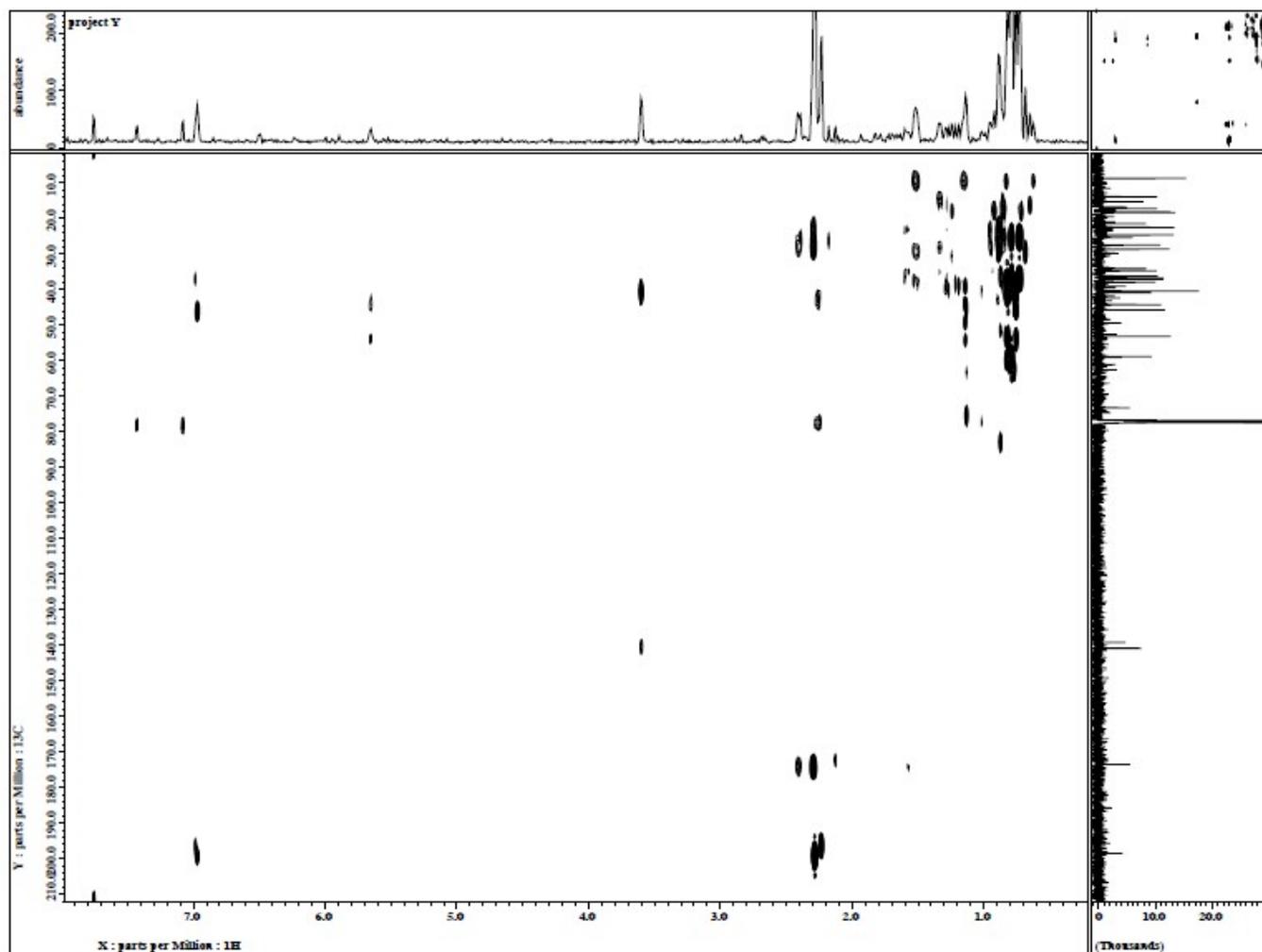
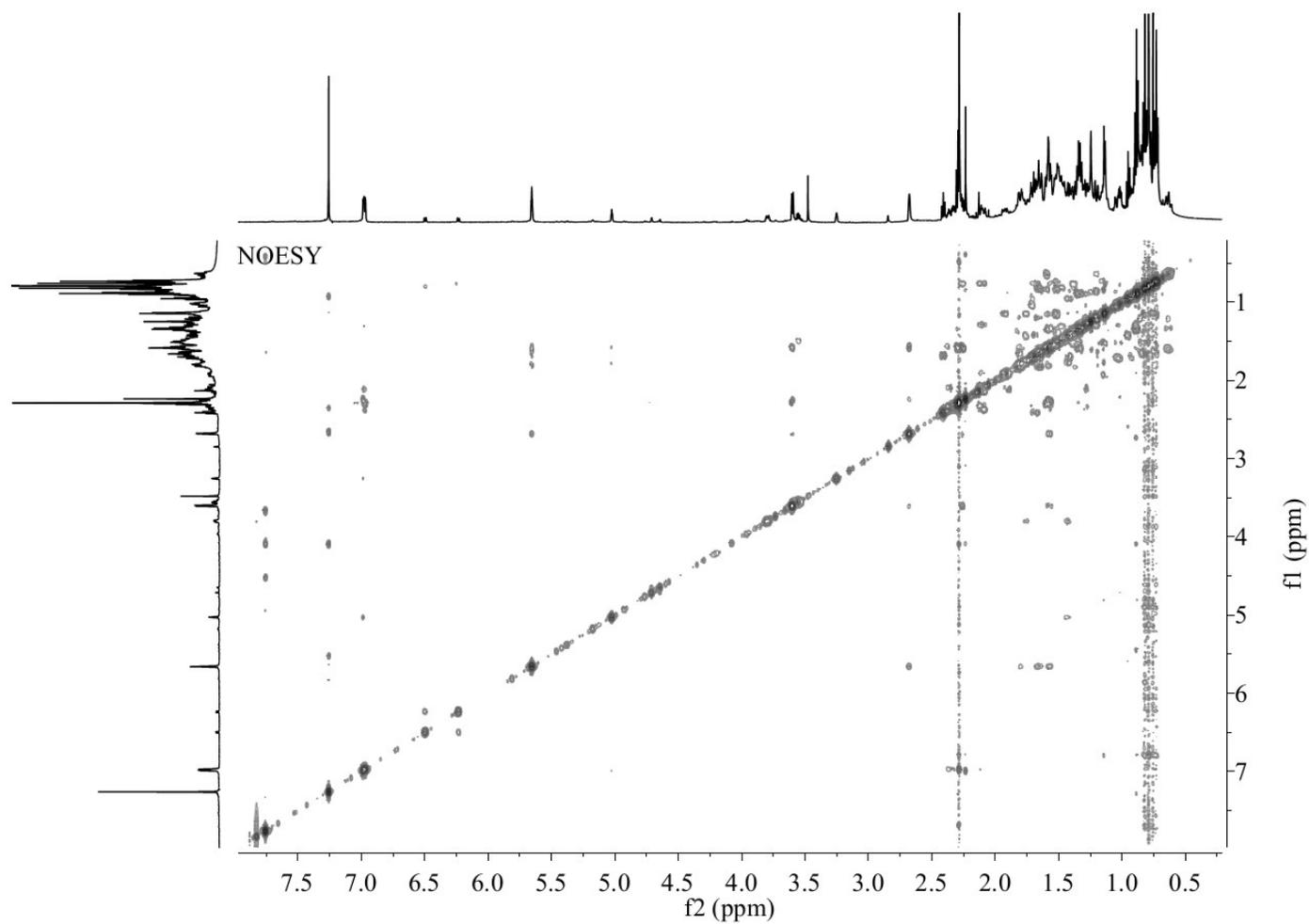
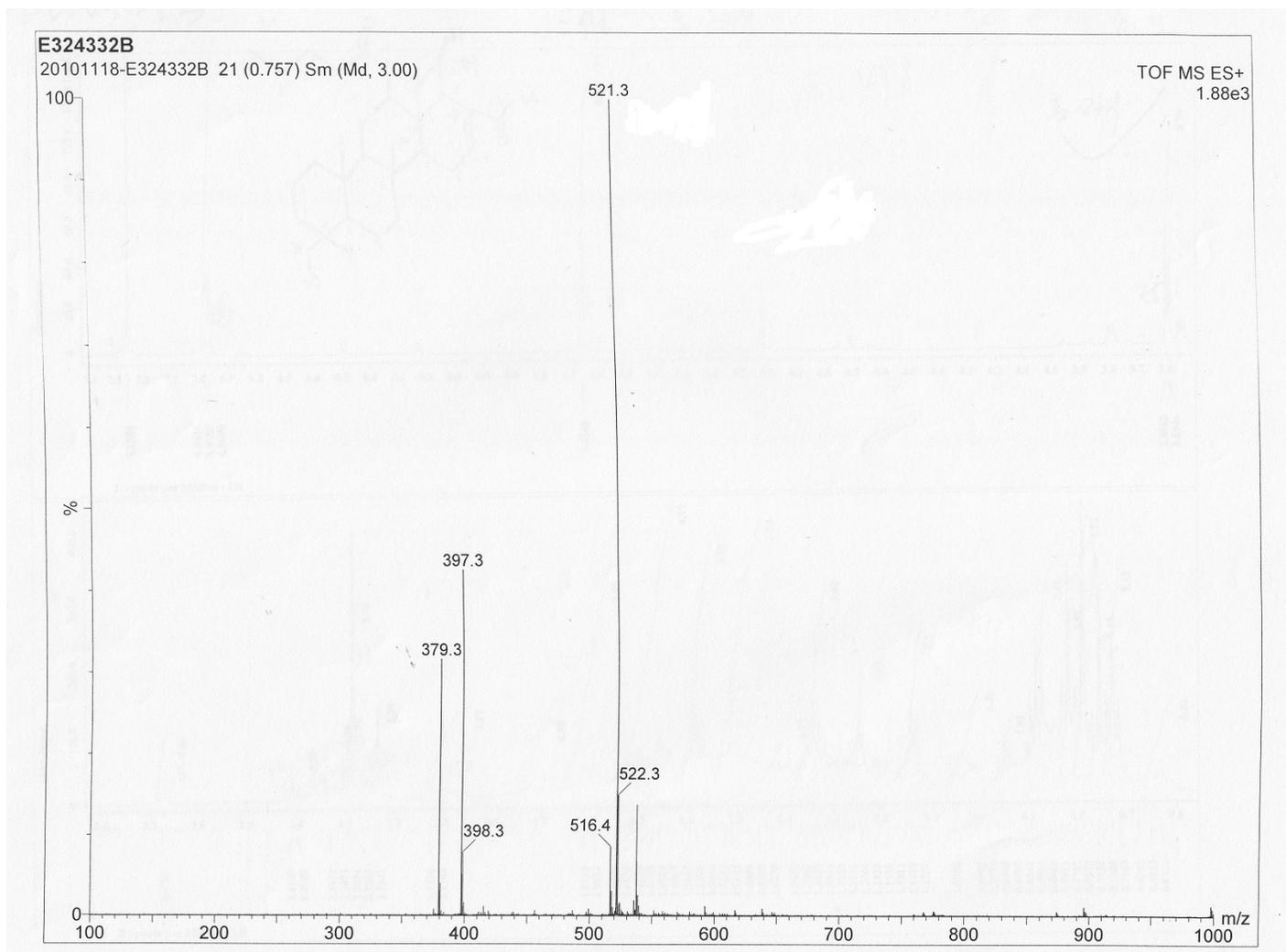


Figure S37. HMBC ( $\text{CDCl}_3$ ) spectrum of compound 5



**Figure S38.** NOESY (CDCl<sub>3</sub>) spectrum of compound **5**



**Figure S39.** ESIMS spectrum of compound **5**

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

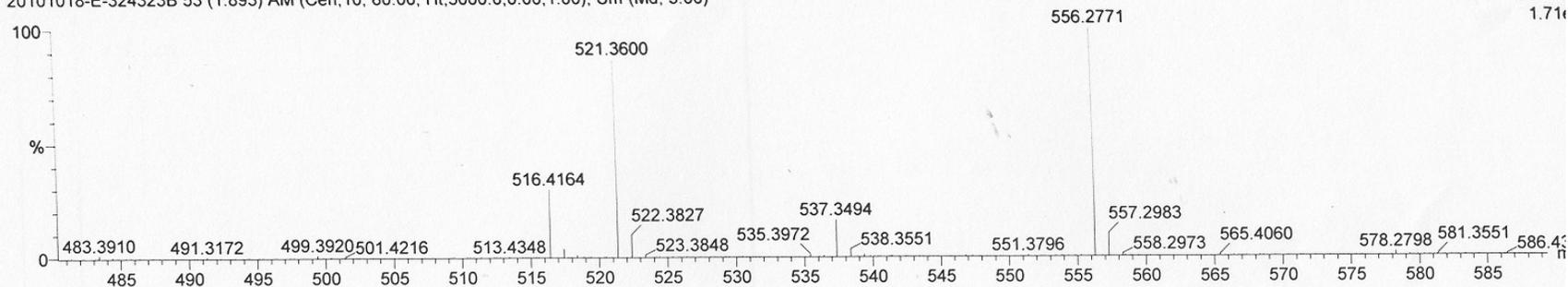
35 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

E-324323B

20101018-E-324323B 53 (1.893) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

TOF MS ES+

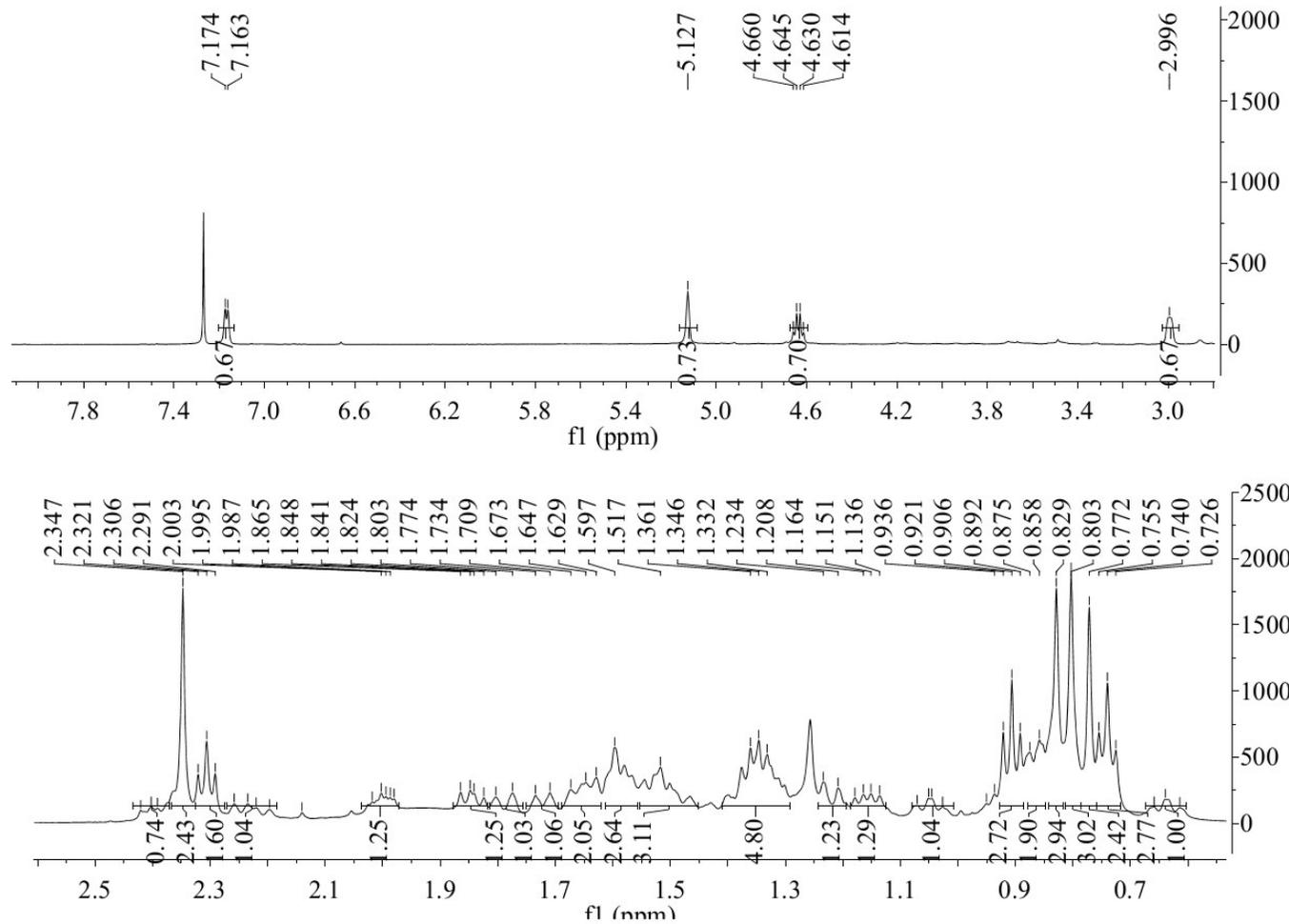
1.71e



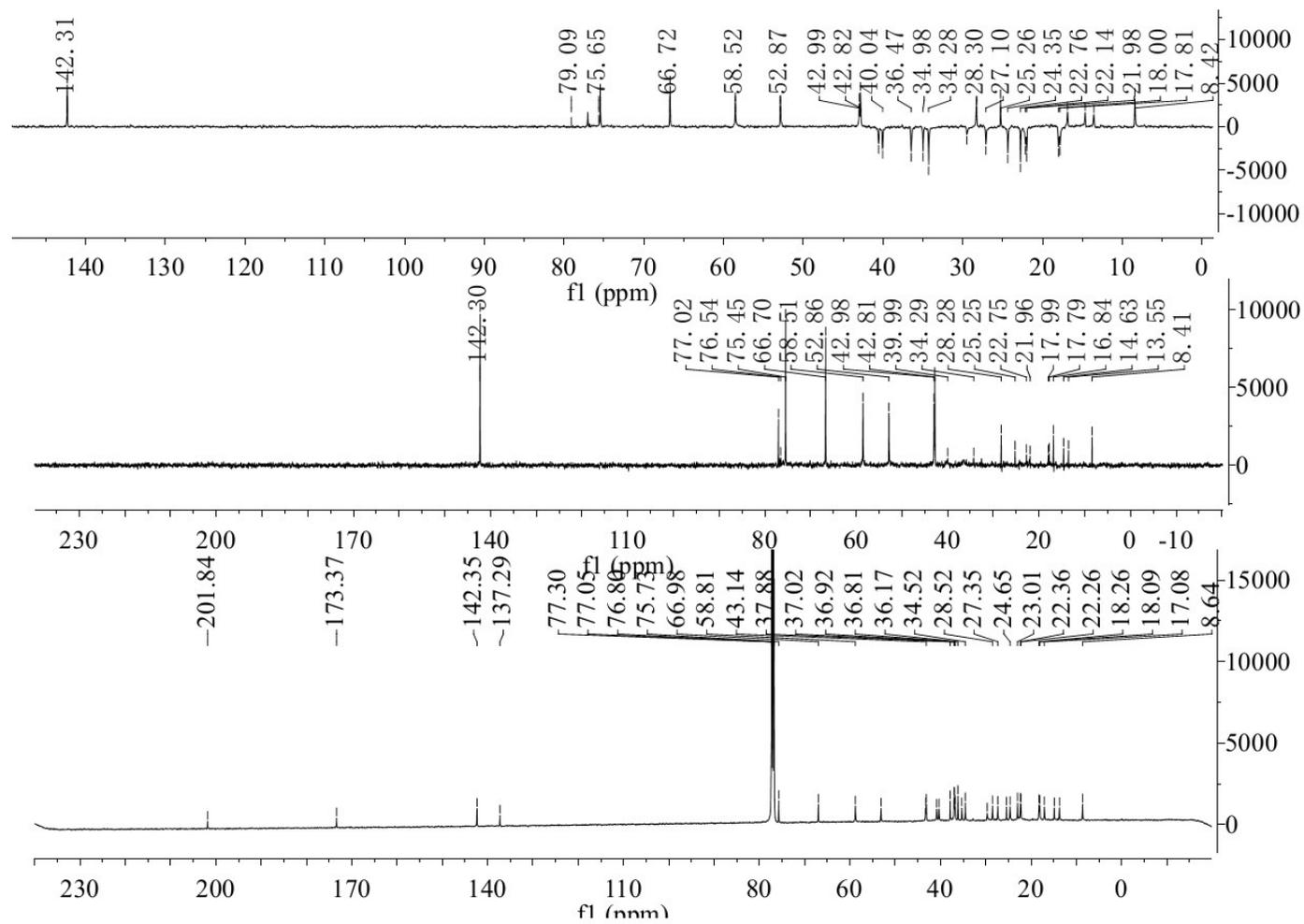
Minimum: -1.5  
Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
521.3600	521.3607	-0.7	-1.3	7.5	1	C32 H50 O4 Na

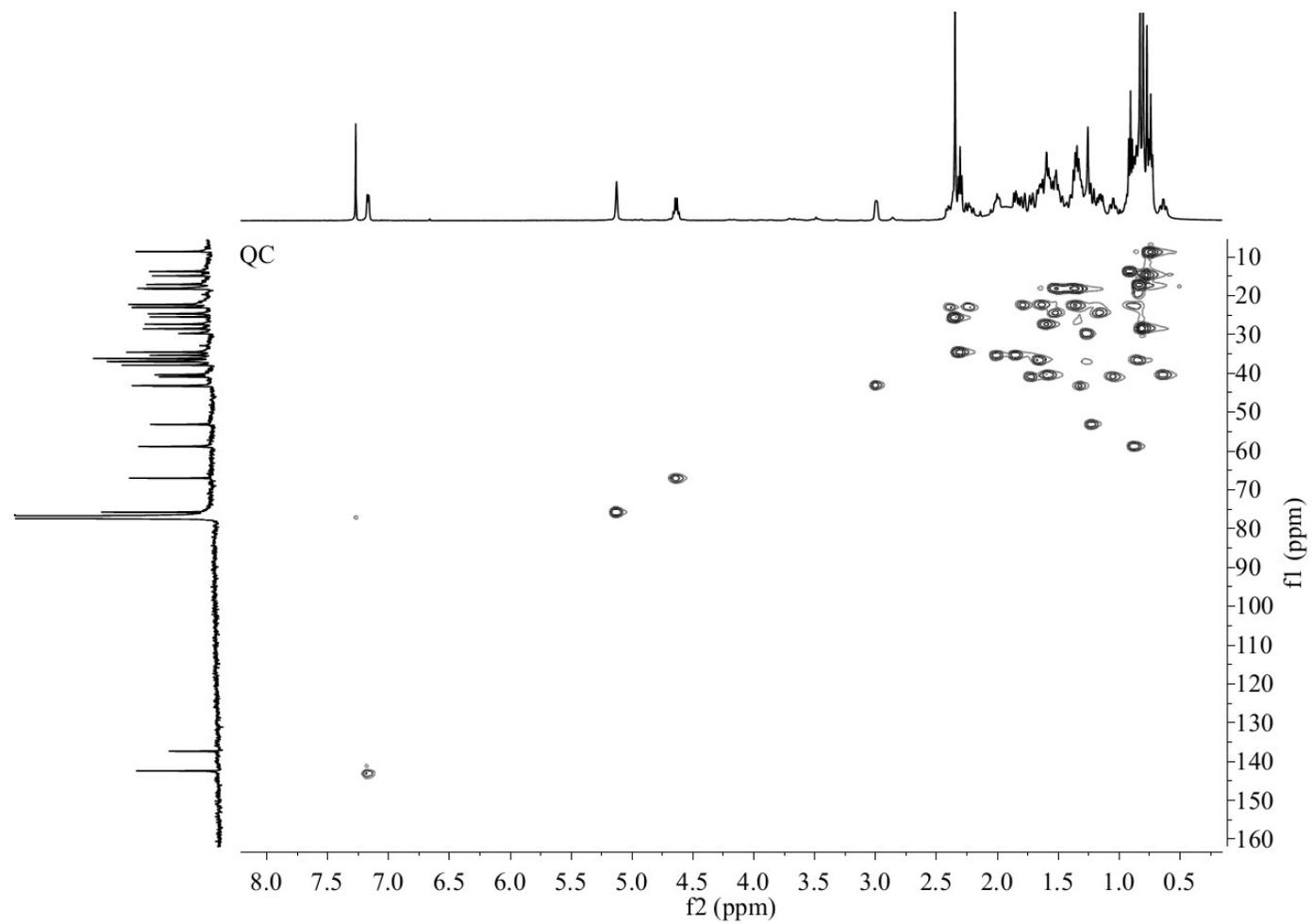
Figure S40. ESIMS spectrum of compound 5



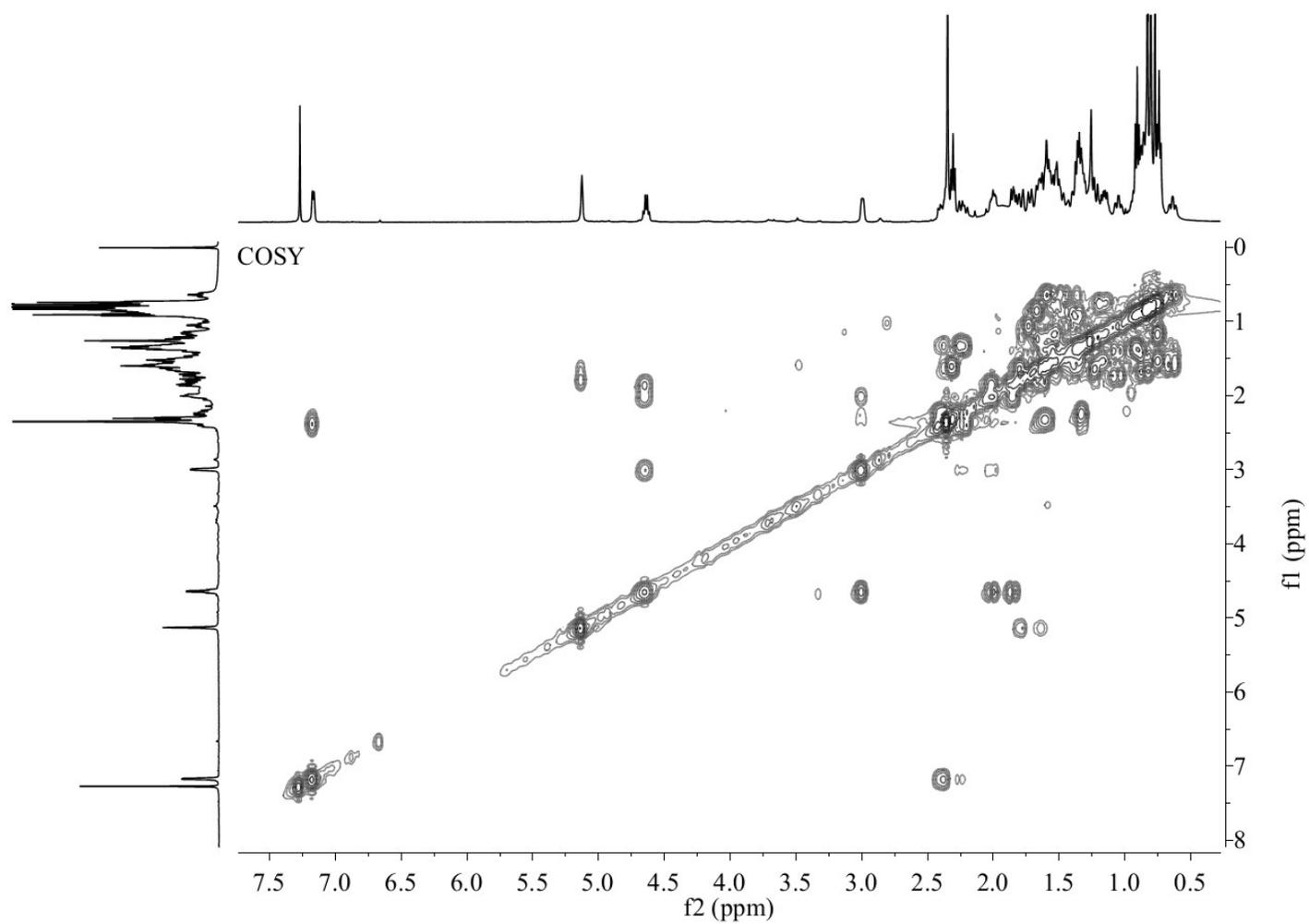
**Figure S41.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of compound **6**



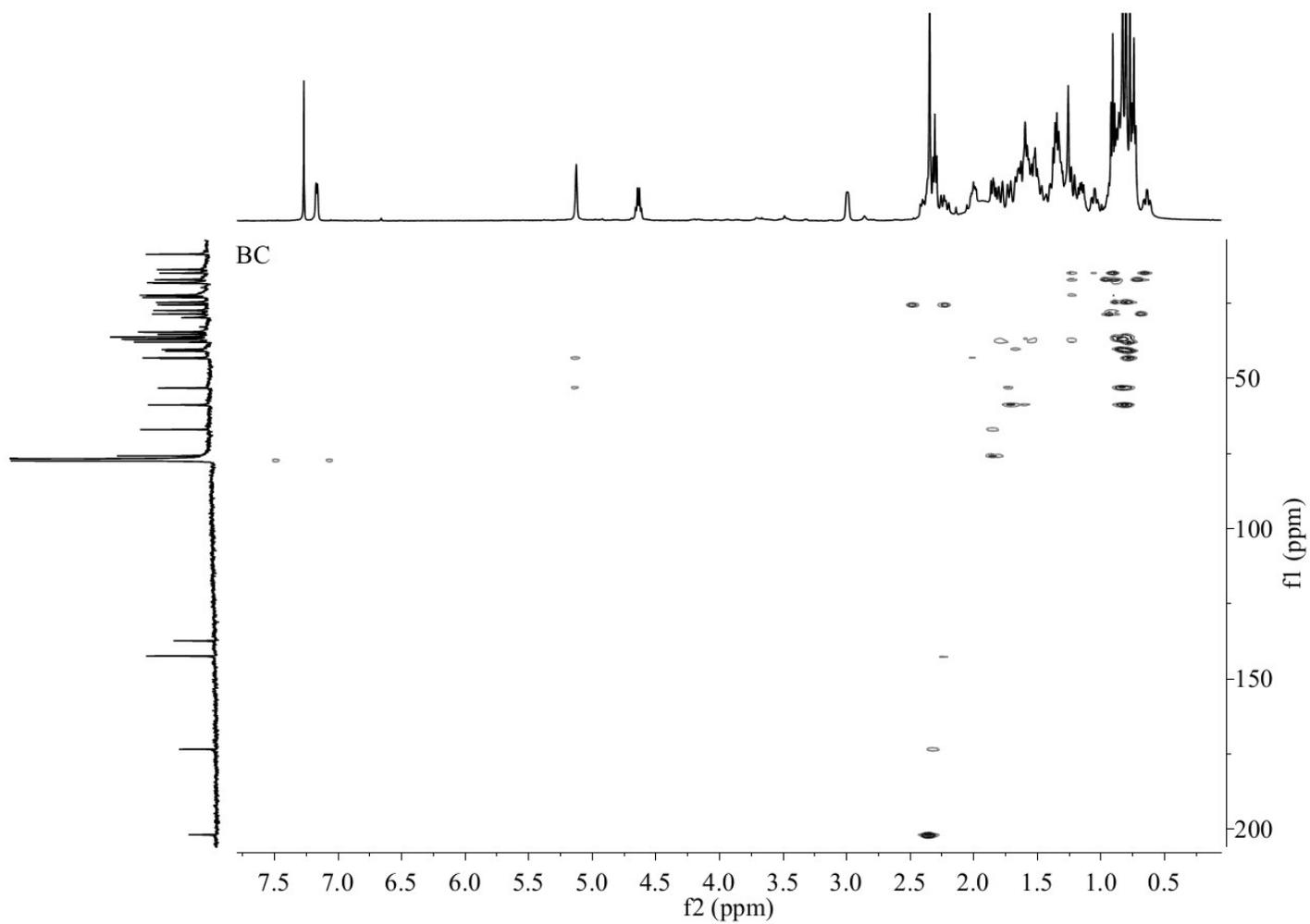
**Figure S42.** <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound **6**



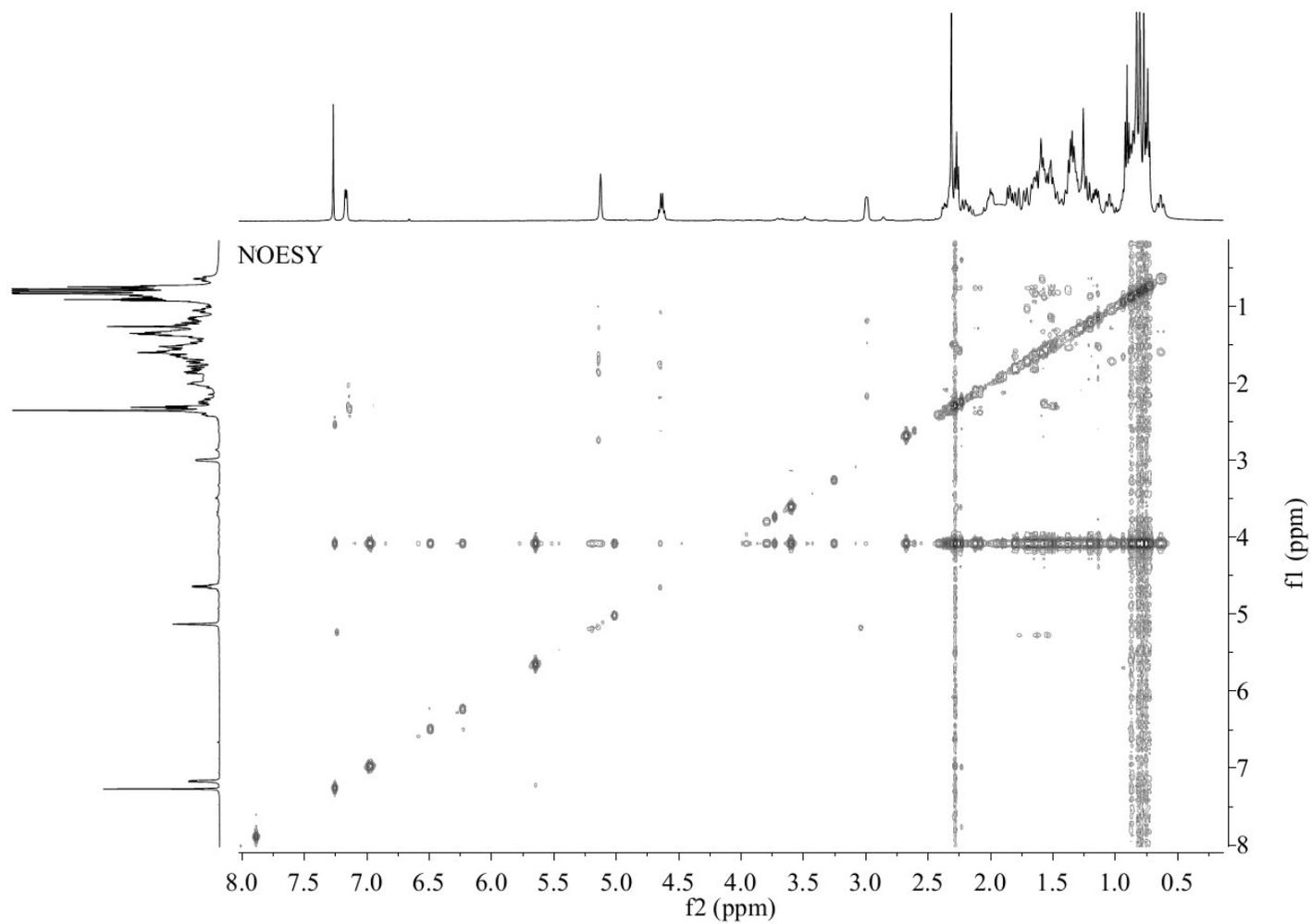
**Figure S43.** HMQC (CDCl<sub>3</sub>) spectrum of compound **6**



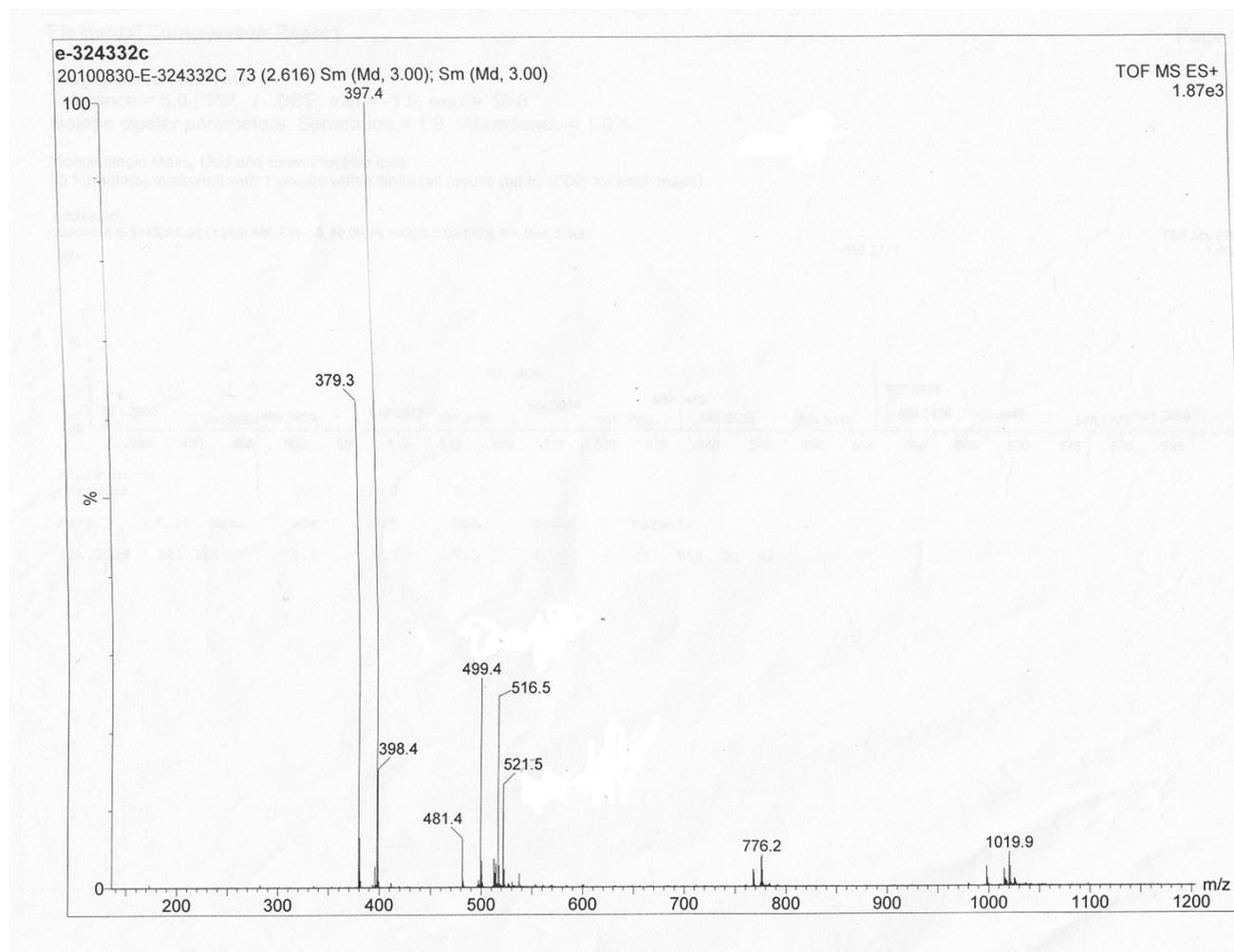
**Figure S44.** COSY (CDCl<sub>3</sub>) spectrum of compound **6**



**Figure S45.** HMBC (CDCl<sub>3</sub>) spectrum of compound **6**



**Figure S46.** NOESY (CDCl<sub>3</sub>) spectrum of compound **6**



**Figure S47.** ESIMS spectrum of compound **6**

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

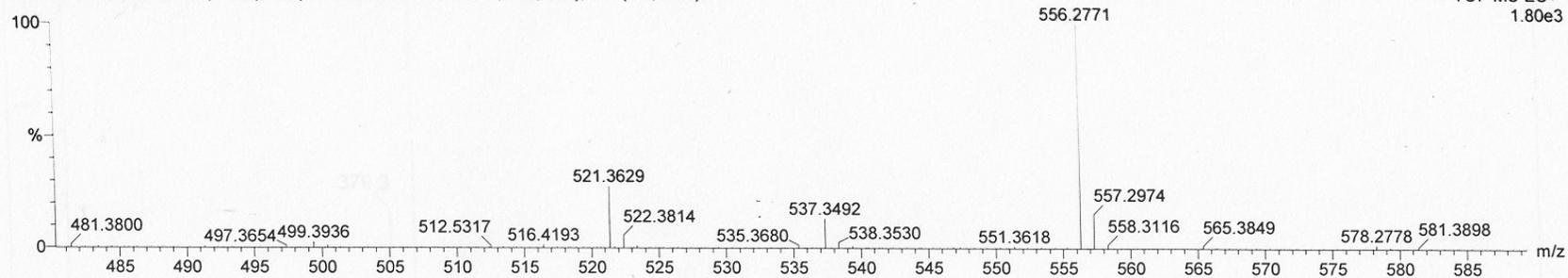
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

35 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

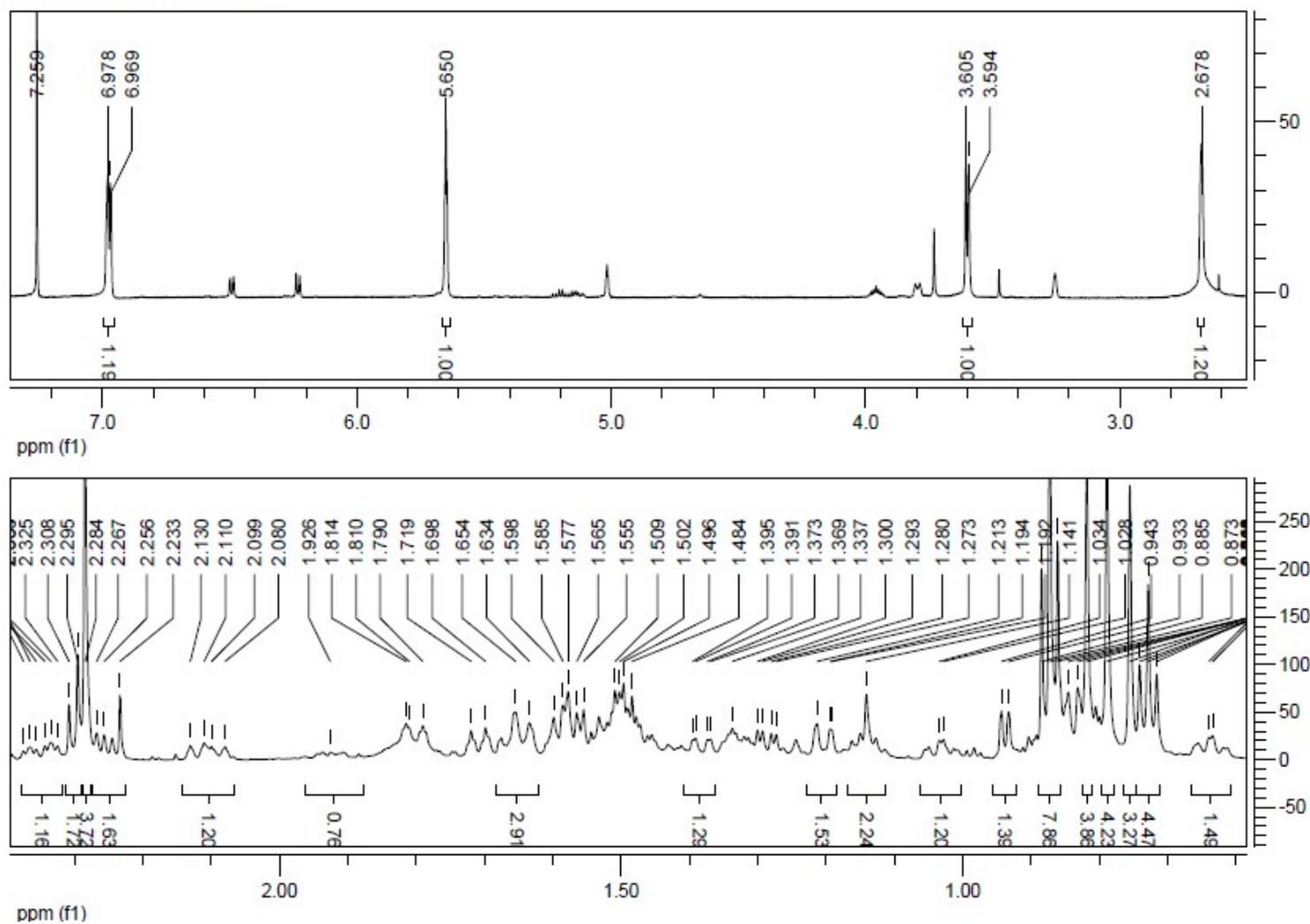
E-324332C

20101018-E-324332C 92 (3.280) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)



Minimum:				-1.5		
Maximum:	200.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
521.3629	521.3607	2.2	4.3	7.5	1	C32 H50 O4 Na

Figure S48. HRESIMS spectrum of compound 6



**Figure S49.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 7

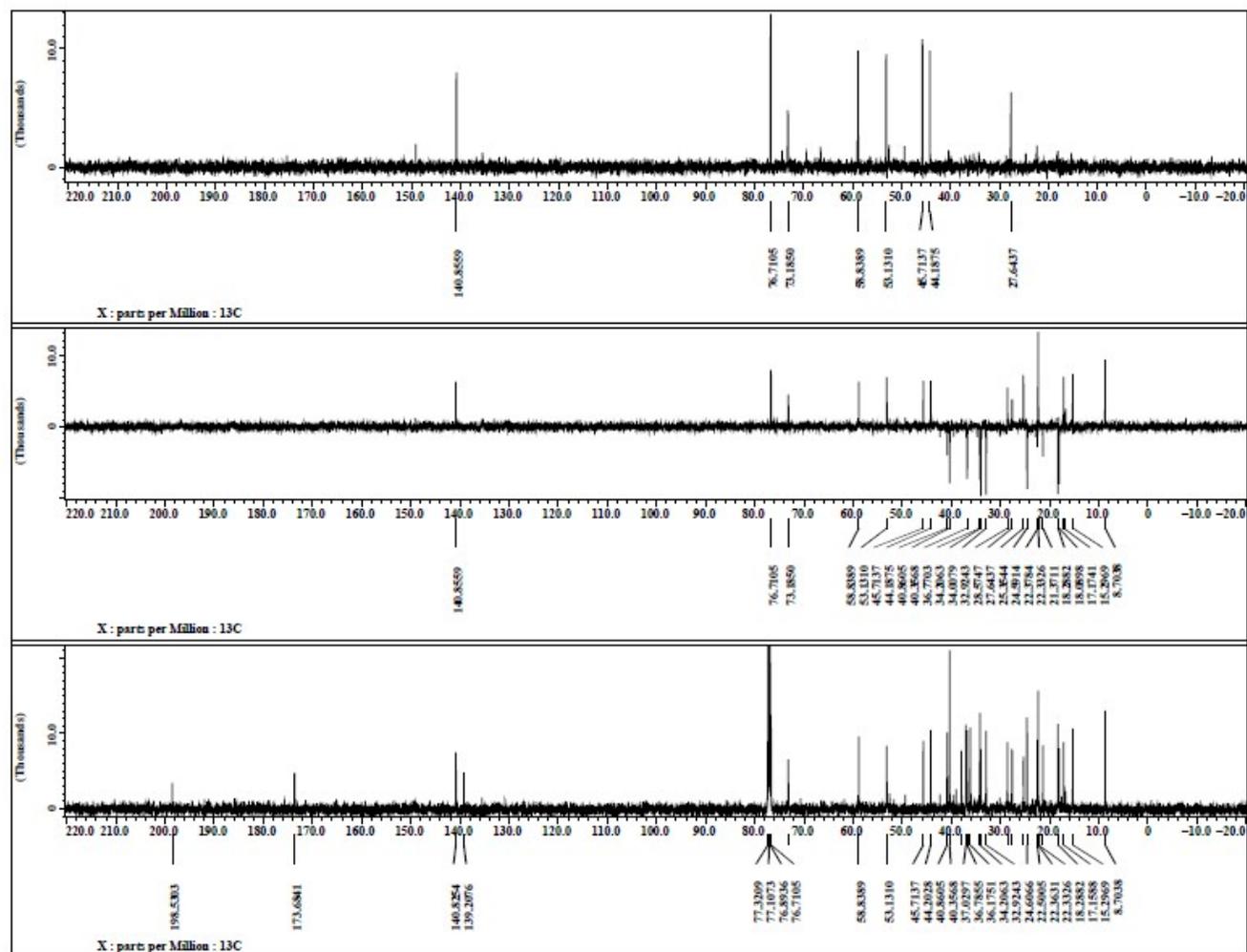


Figure S50.  $^{13}\text{C}$  and DEPT NMR (150 MHz,  $\text{CDCl}_3$ ) spectra of compound 7

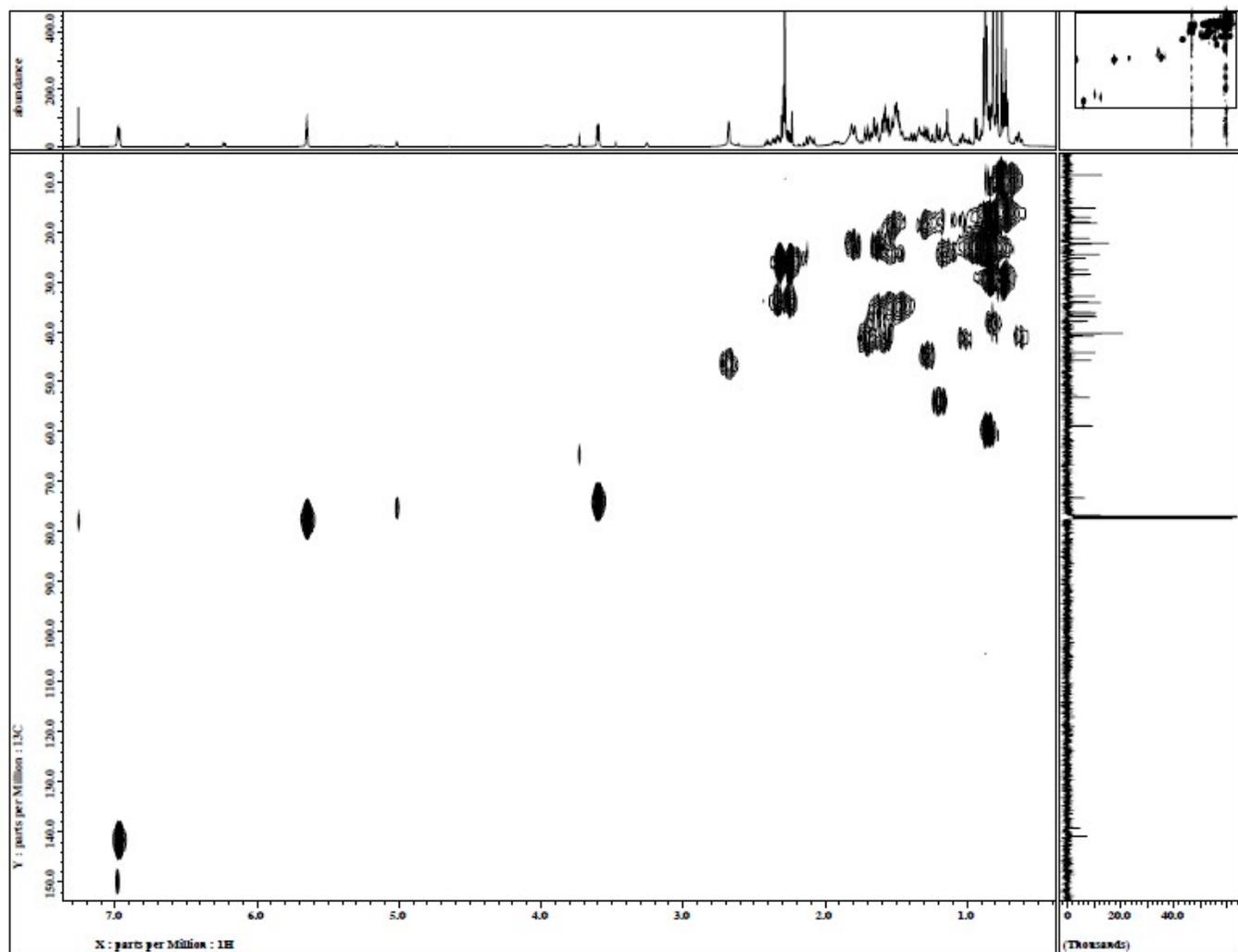


Figure S51. HMQC (CDCl<sub>3</sub>) spectrum of compound 7

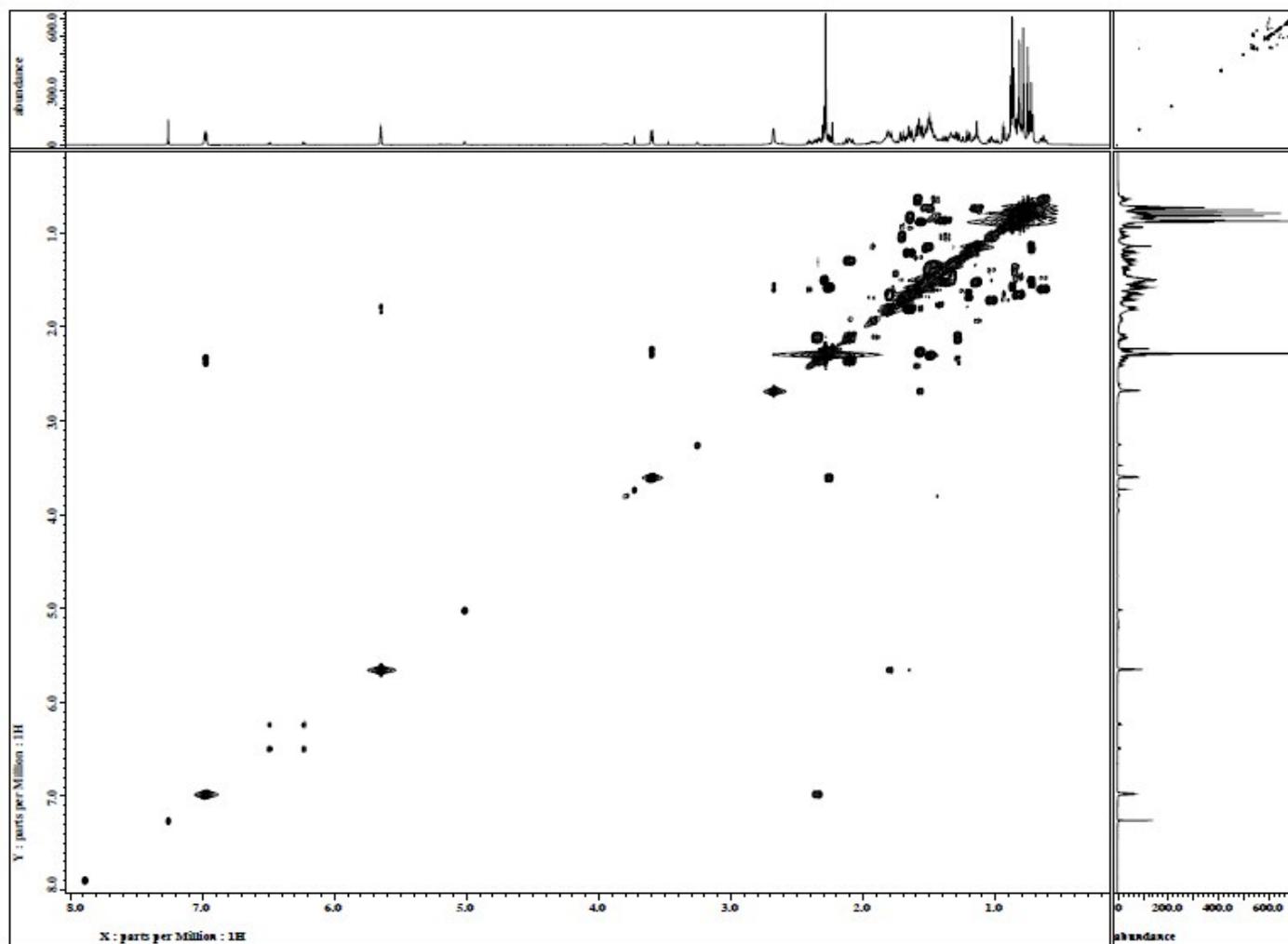


Figure S52. COSY ( $\text{CDCl}_3$ ) spectrum of compound 7

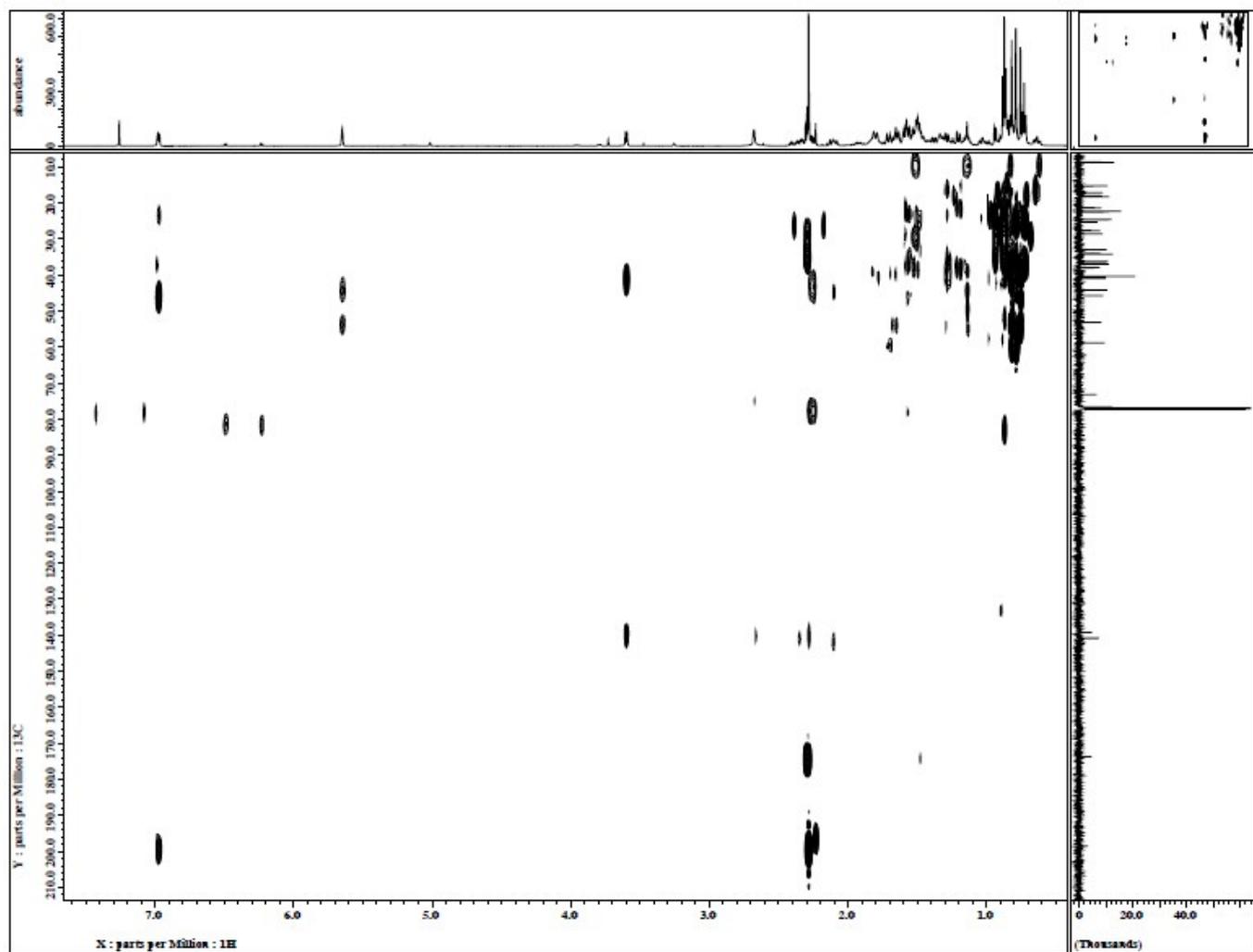
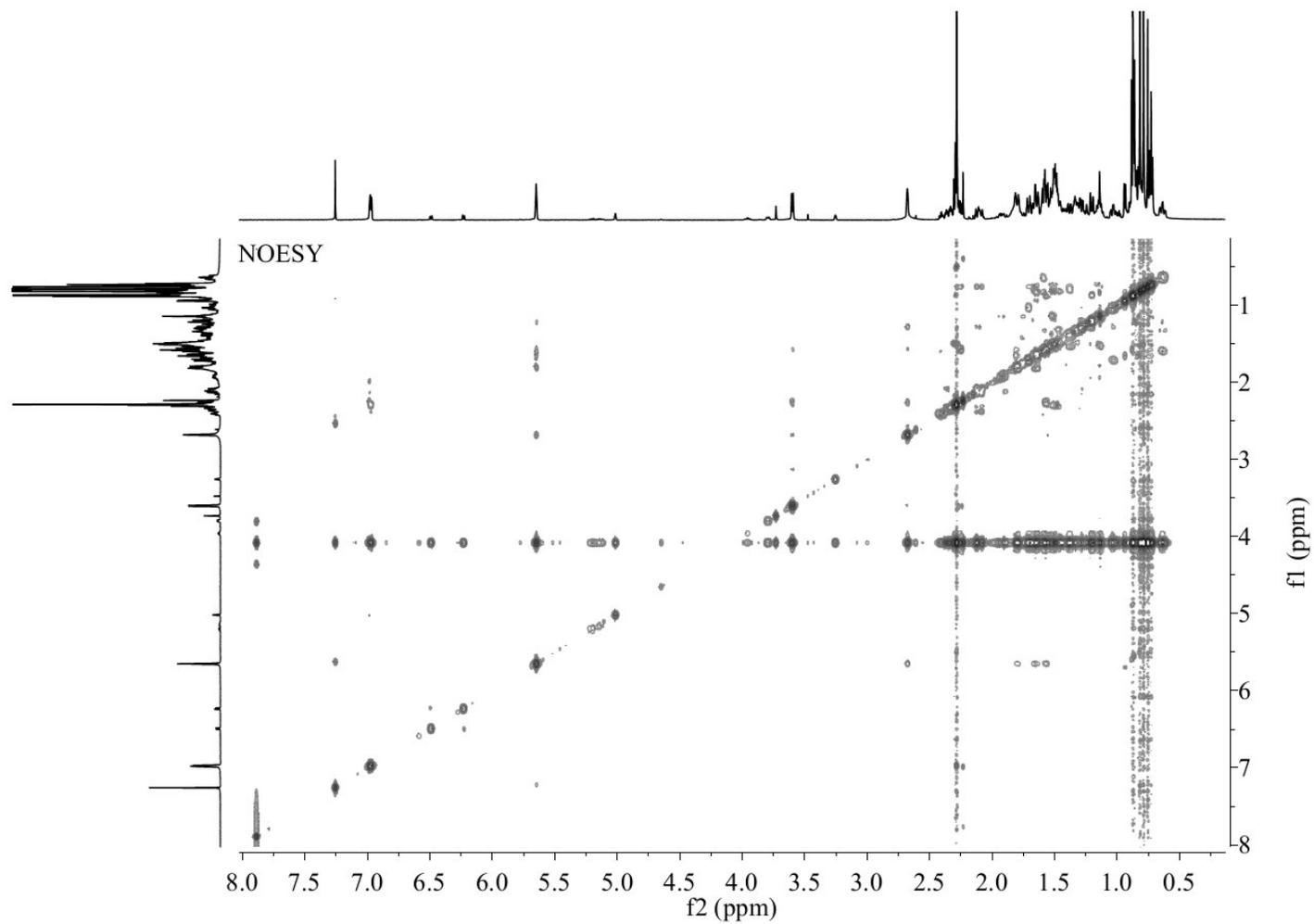
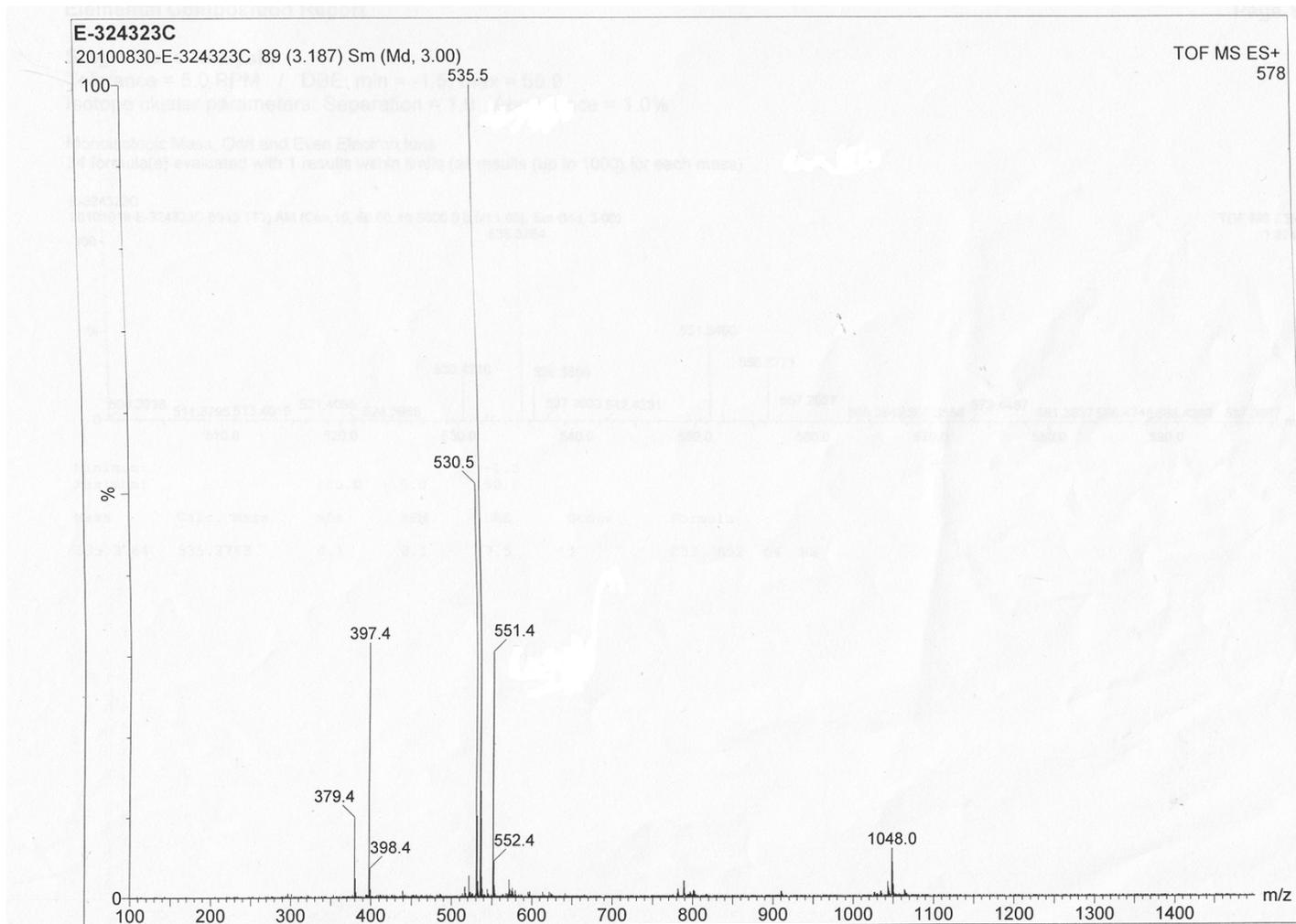


Figure S53. HMBC (CDCl<sub>3</sub>) spectrum of compound 7



**Figure S54.** NOESY (CDCl<sub>3</sub>) spectrum of compound **7**



**Figure S55.** ESIMS spectrum of compound **7**

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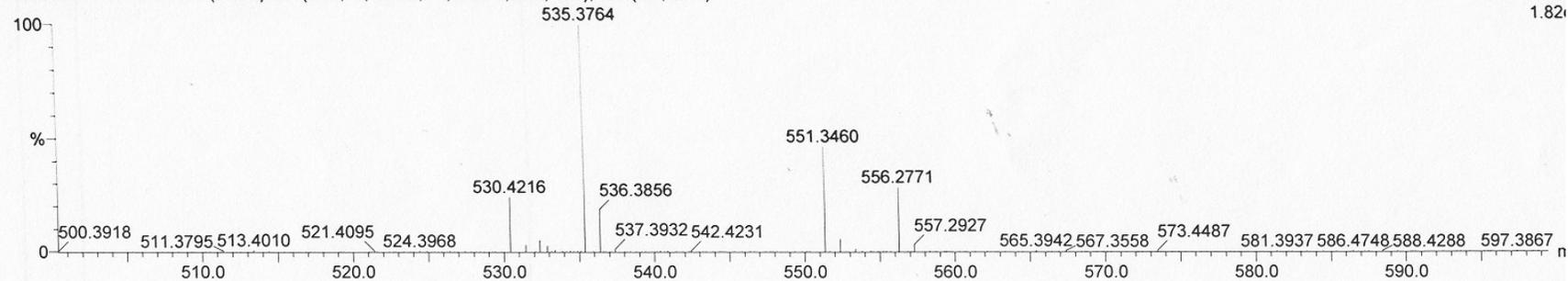
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
 34 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

E-324323C  
 20101018-E-324323C 89 (3.173) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

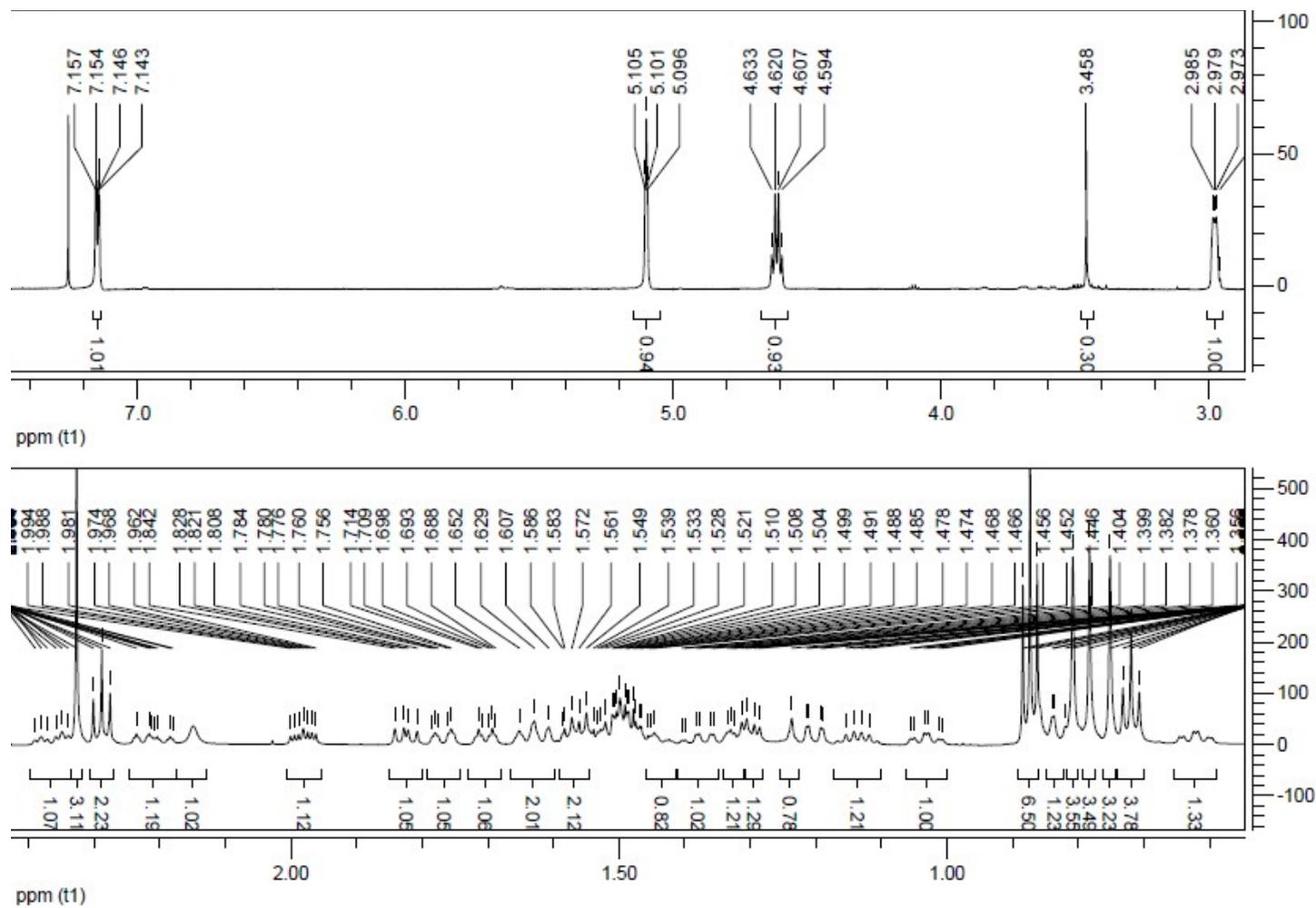
TOF MS ES-  
 1.82



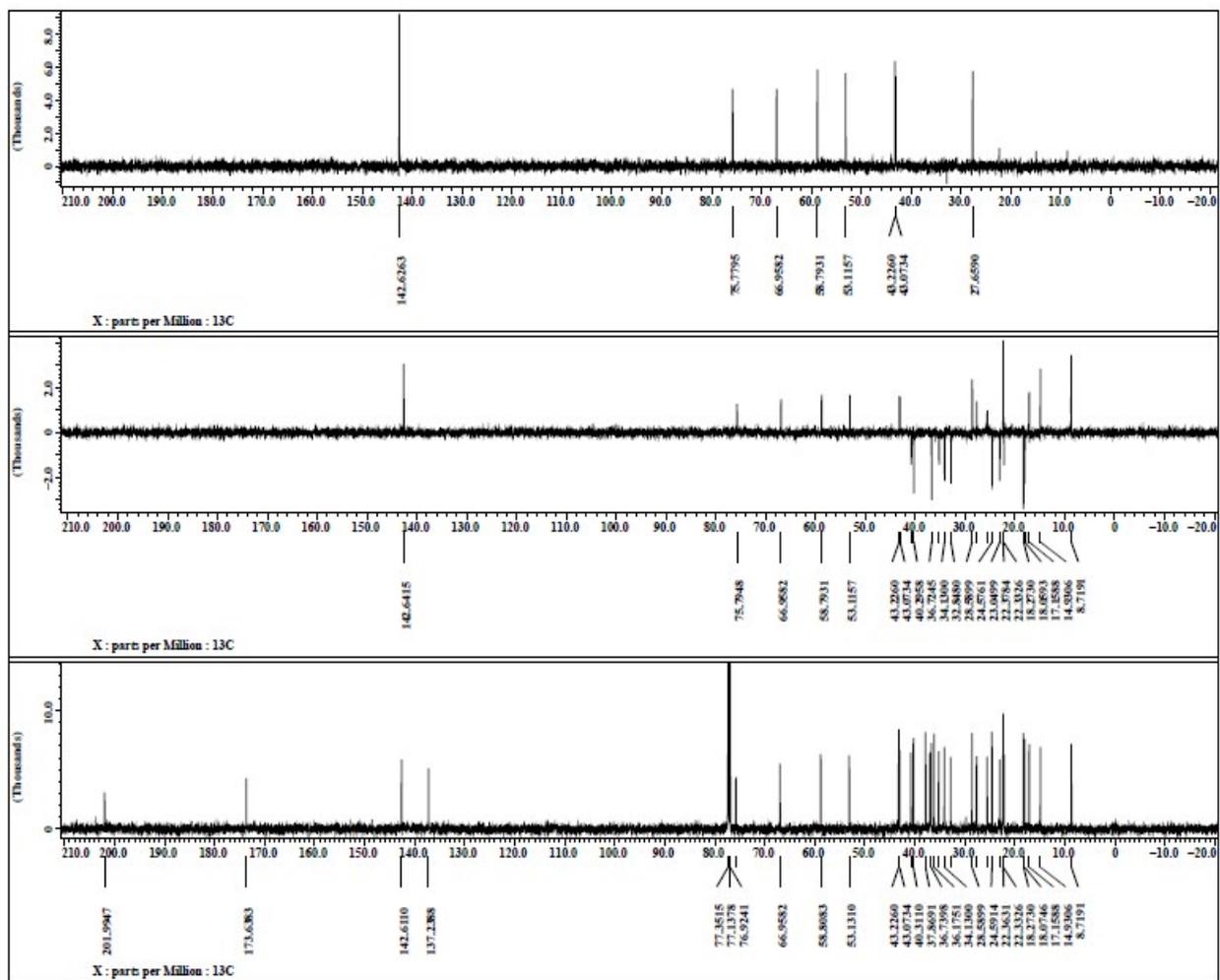
Minimum: -1.5  
 Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
535.3764	535.3763	0.1	0.1	7.5	1	C33 H52 O4 Na

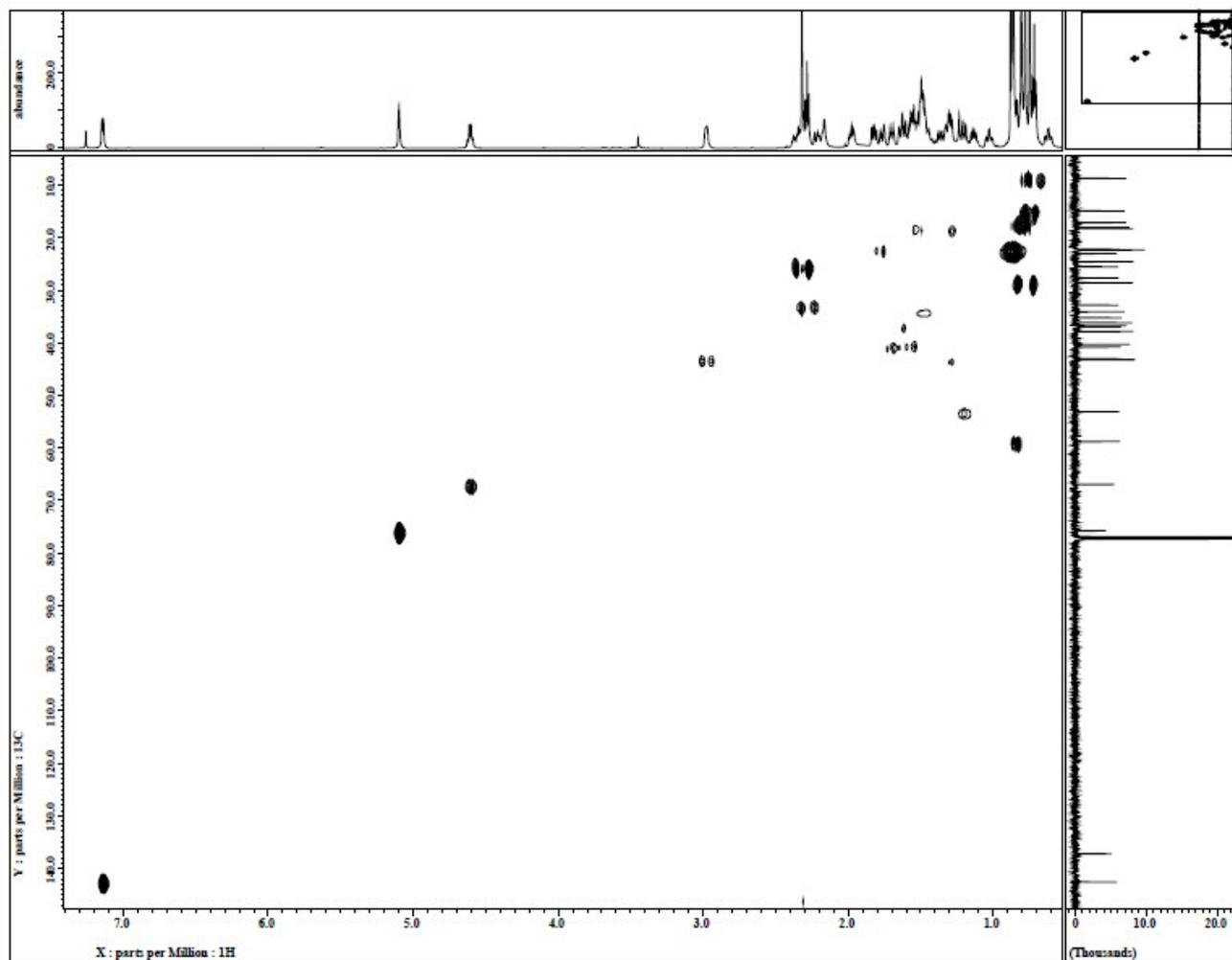
Figure S56. HRESIMS spectrum of compound 7



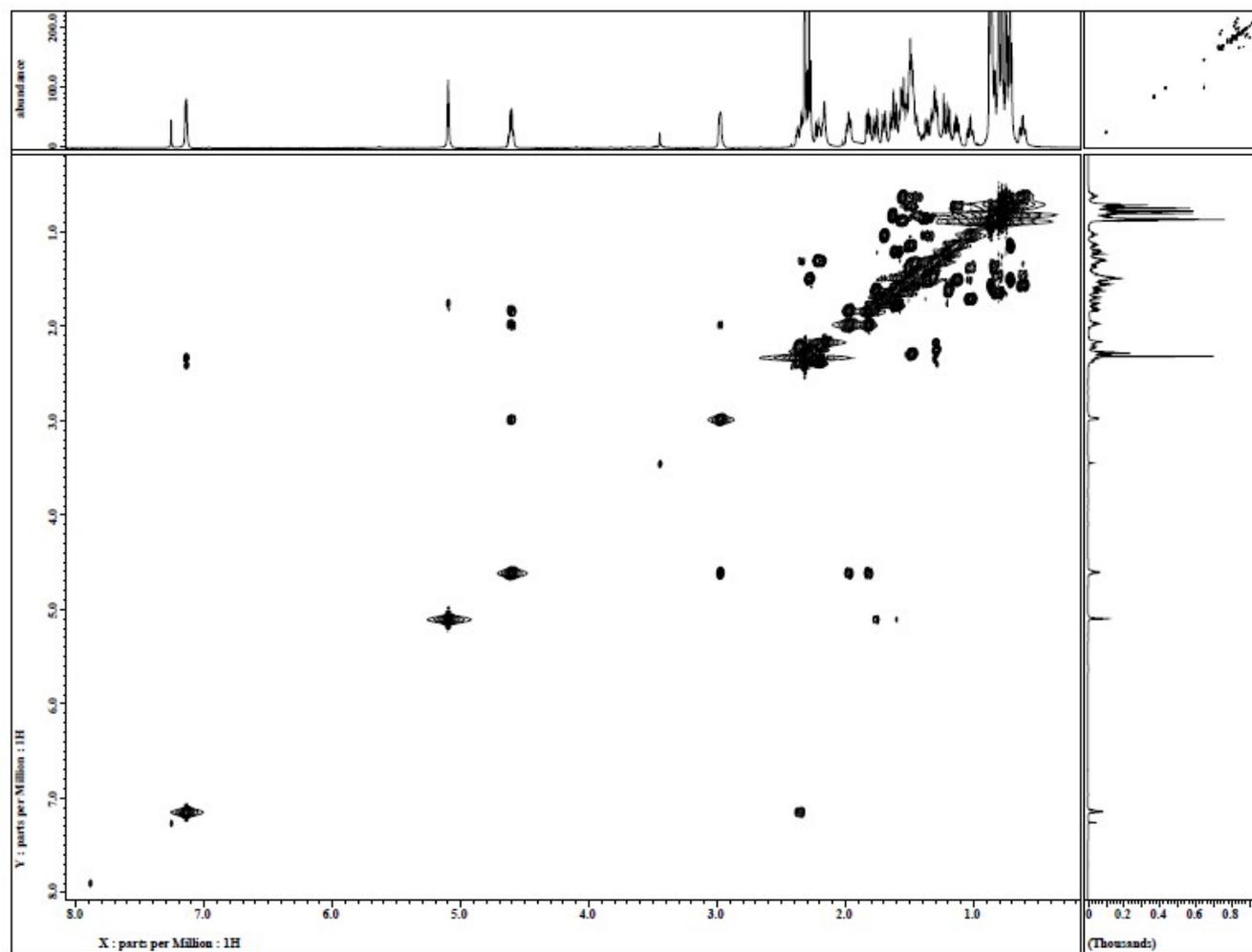
**Figure S57.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **8**



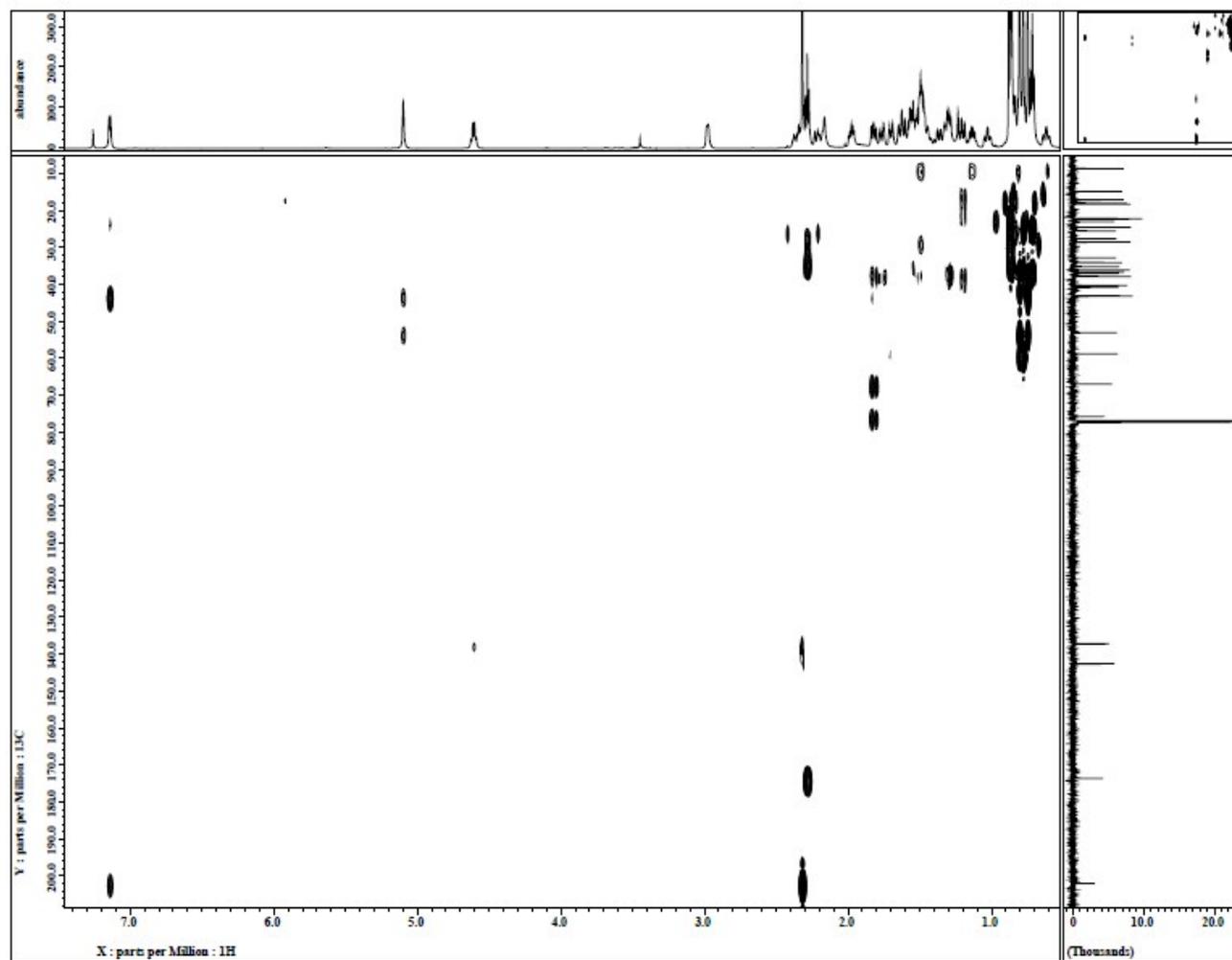
**Figure S58.**  $^{13}\text{C}$  and DEPT NMR (150 MHz,  $\text{CDCl}_3$ ) spectra of compound **8**



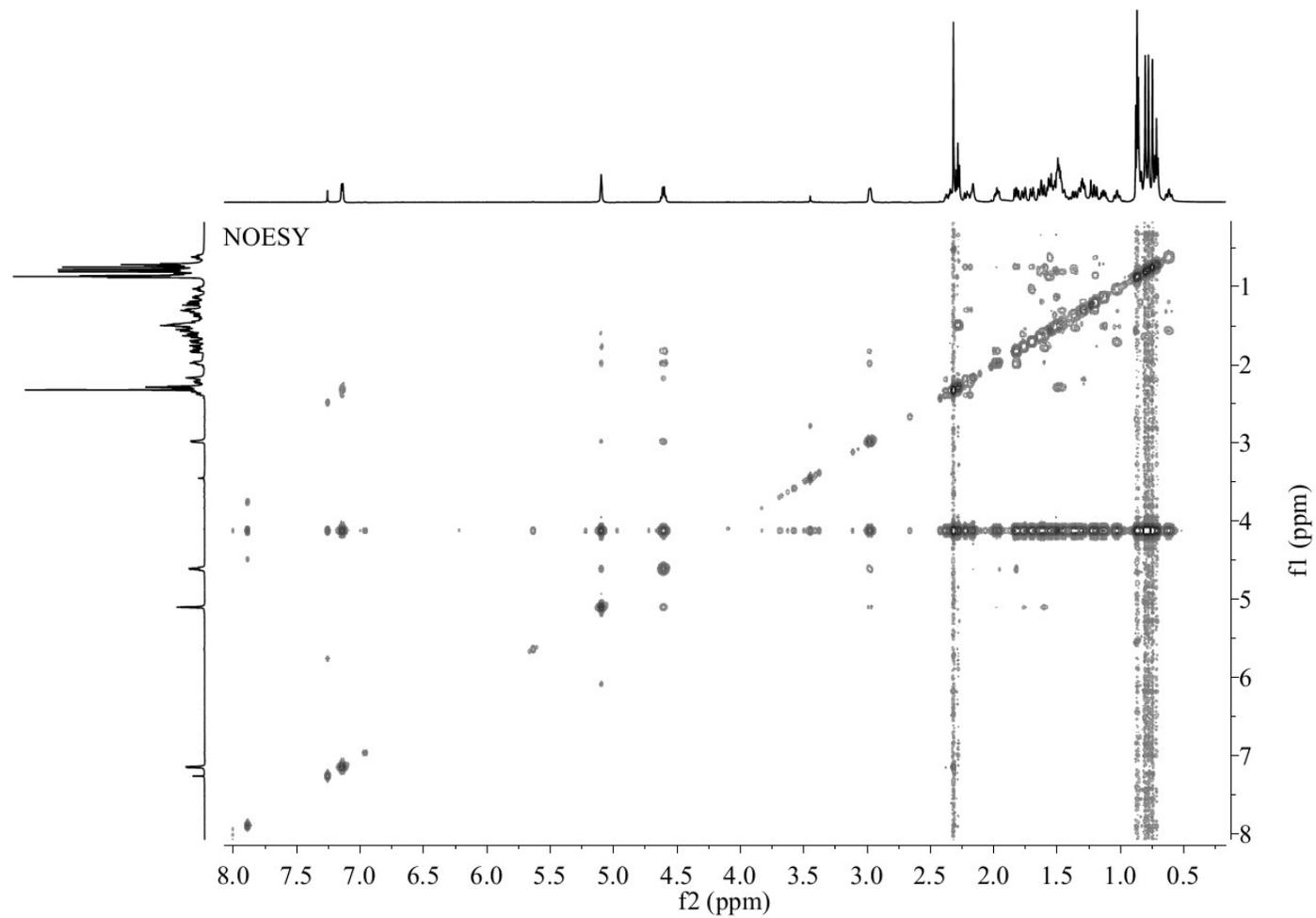
**Figure S59.** HMQC (CDCl<sub>3</sub>) spectrum of compound **8**



**Figure S60.** COSY (CDCl<sub>3</sub>) spectrum of compound **8**



**Figure S61.** HMBC ( $\text{CDCl}_3$ ) spectrum of compound **8**



**Figure S62.** NOESY (CDCl<sub>3</sub>) spectrum of compound **8**

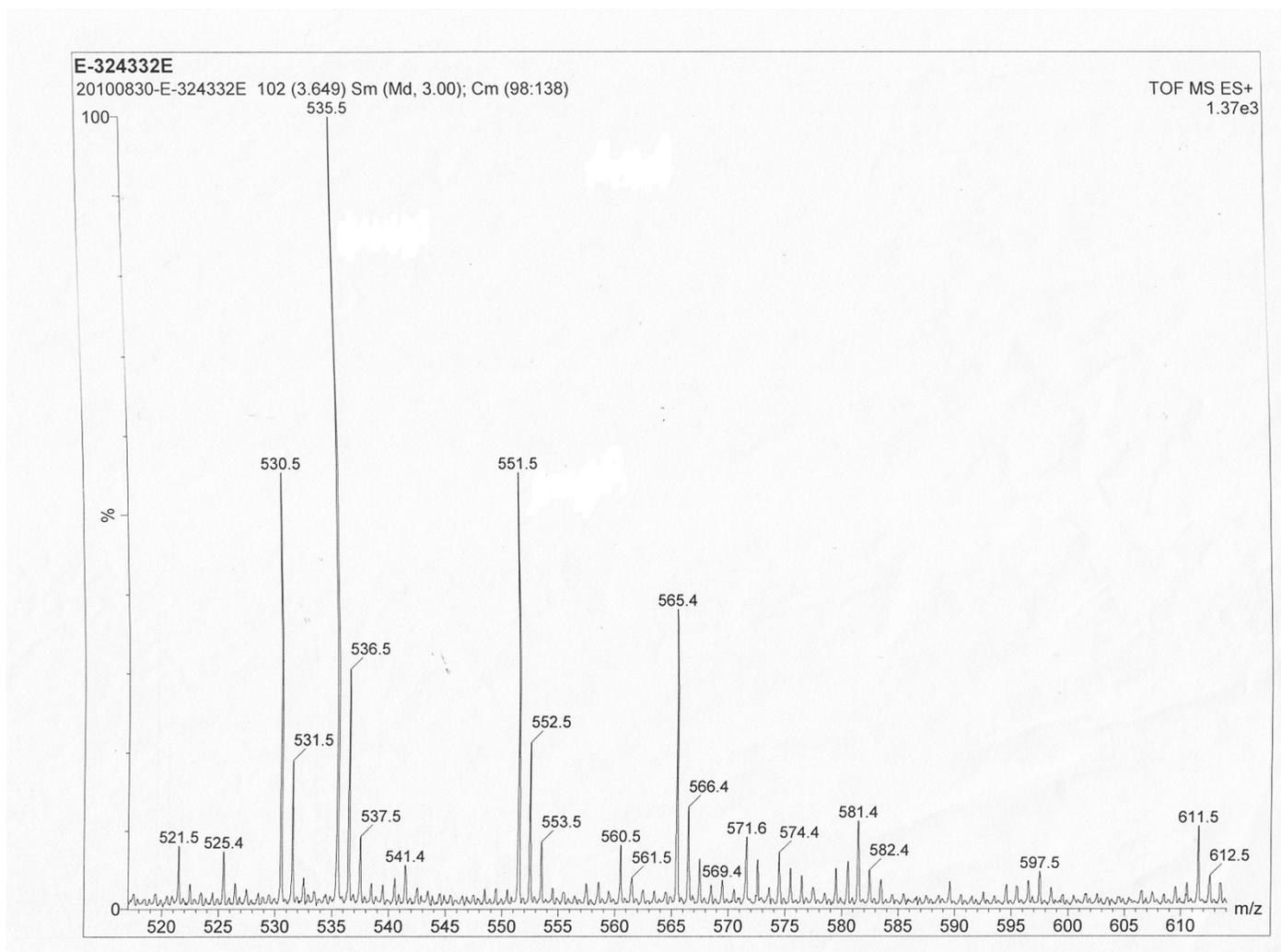


Figure S63. ESIMS spectrum of compound 8

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

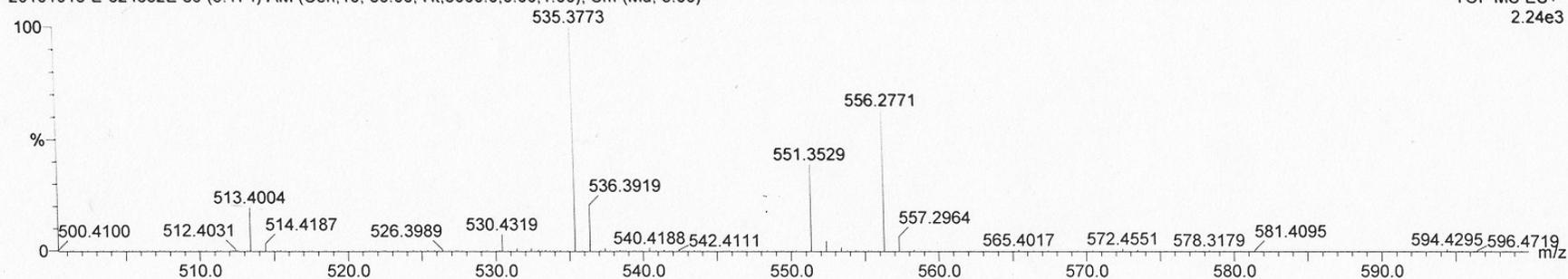
Monoisotopic Mass, Odd and Even Electron Ions

34 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

E-324332E

20101018-E-324332E 89 (3.174) AM (Cen, 10, 80.00, Ht, 5000.0, 0.00, 1.00); Sm (Md, 3.00)

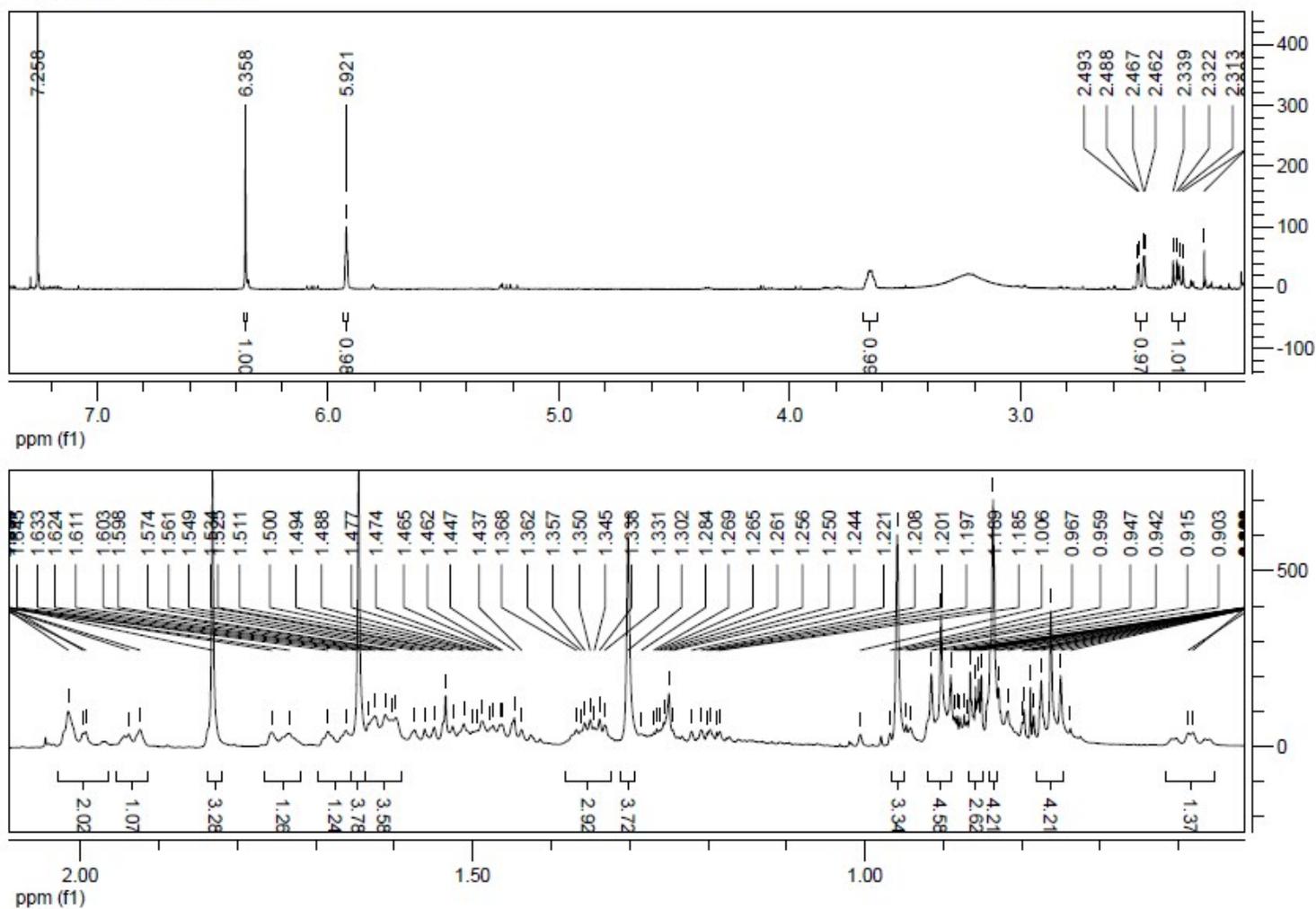
TOF MS ES+  
2.24e3



Minimum: -1.5  
Maximum: 200.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
535.3773	535.3763	1.0	1.8	7.5	1	C33 H52 O4 Na

Figure S64. HRESIMS spectrum of compound 8



**Figure S65.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **9**

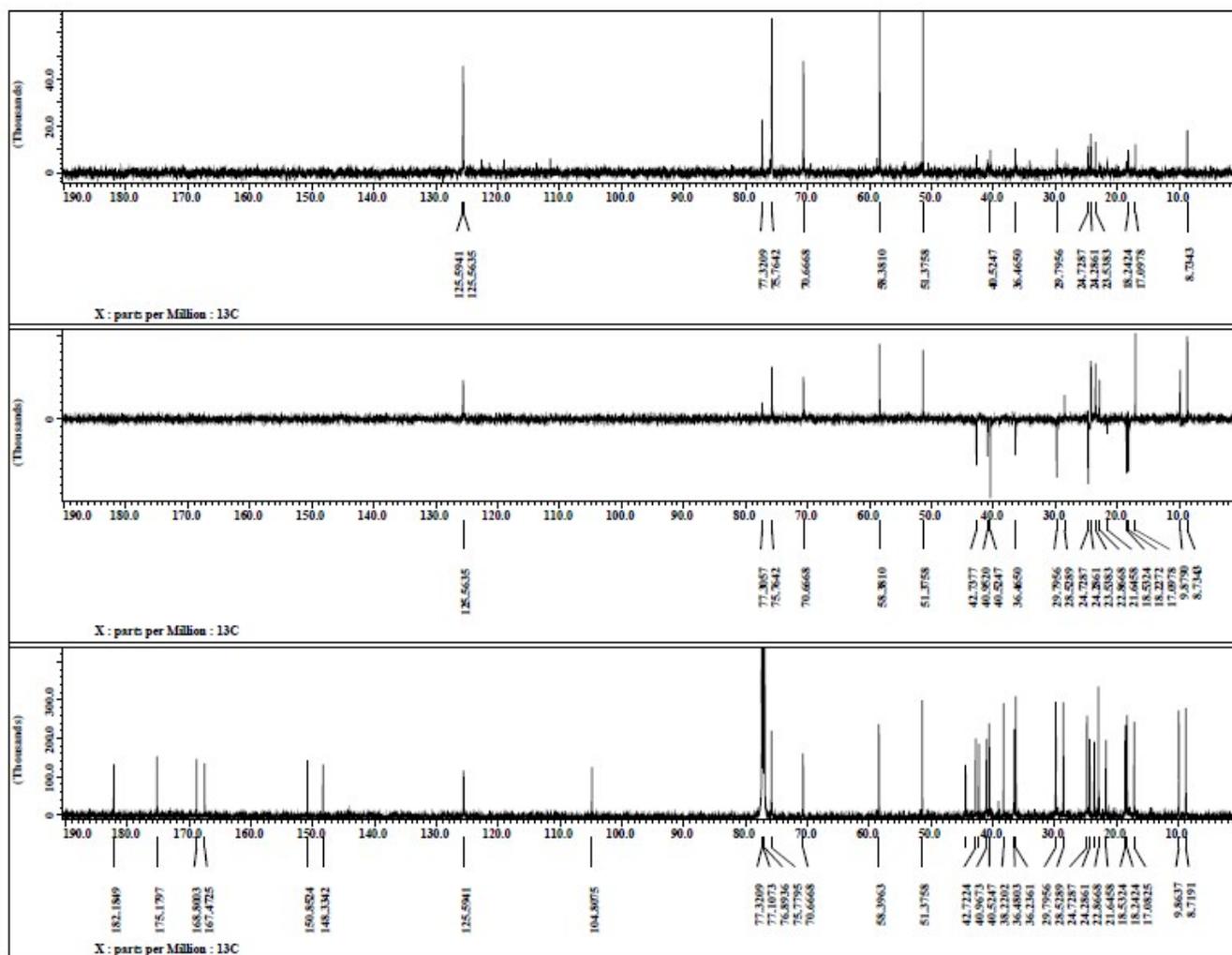


Figure S66.  $^{13}\text{C}$  and DEPT NMR (150 MHz,  $\text{CDCl}_3$ ) spectra of compound **9**

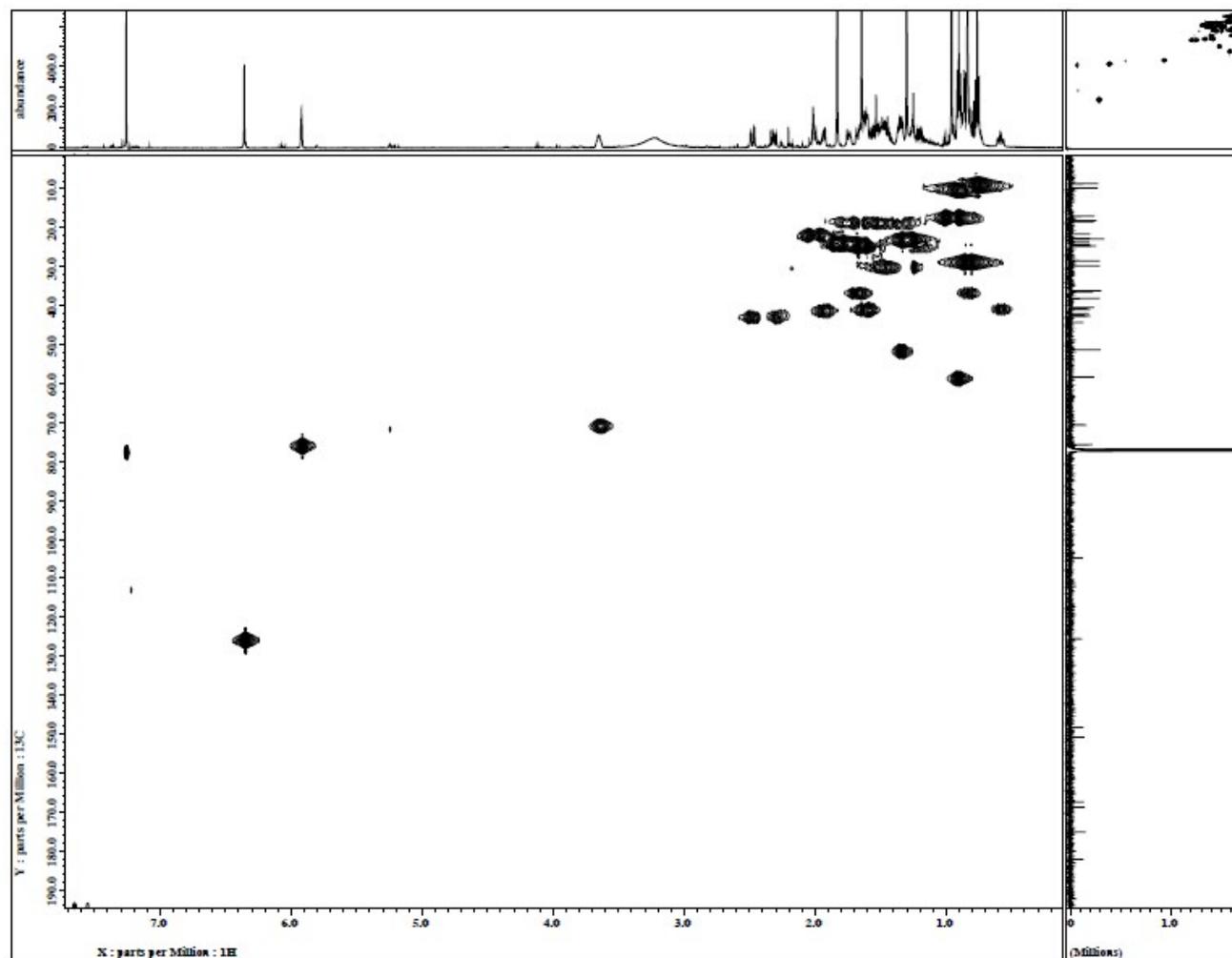
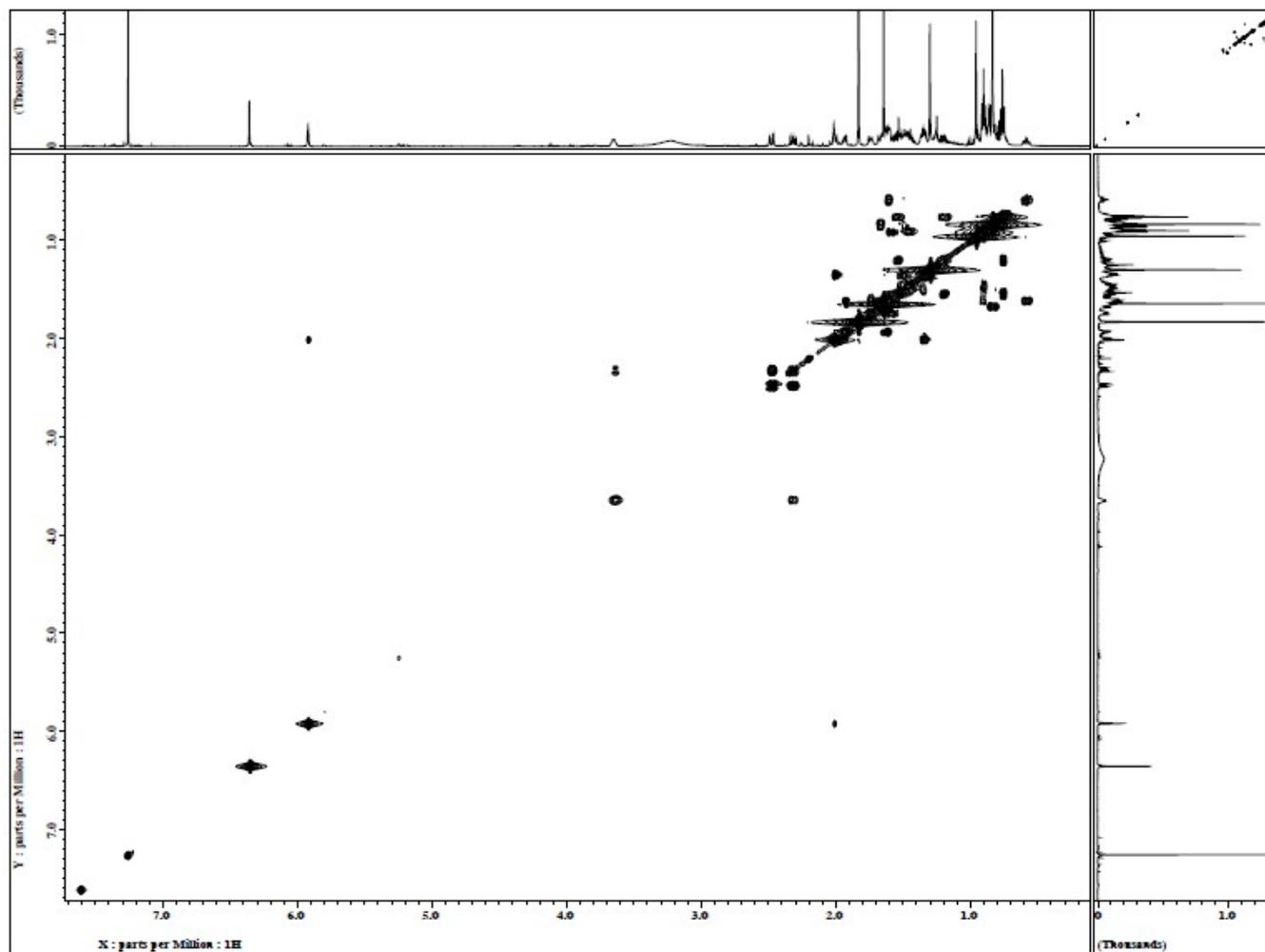
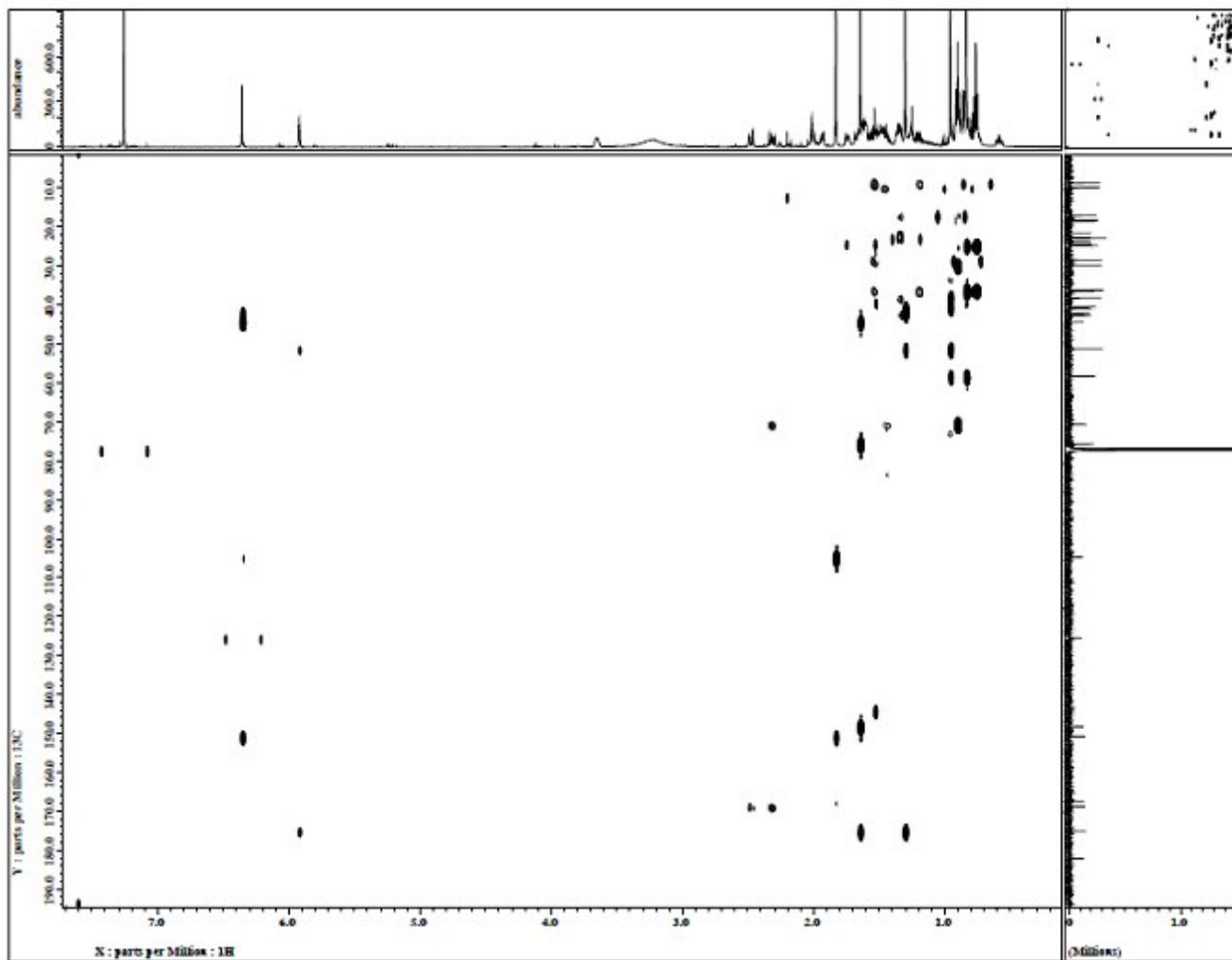


Figure S67. HMQC (CDCl<sub>3</sub>) spectrum of compound 9

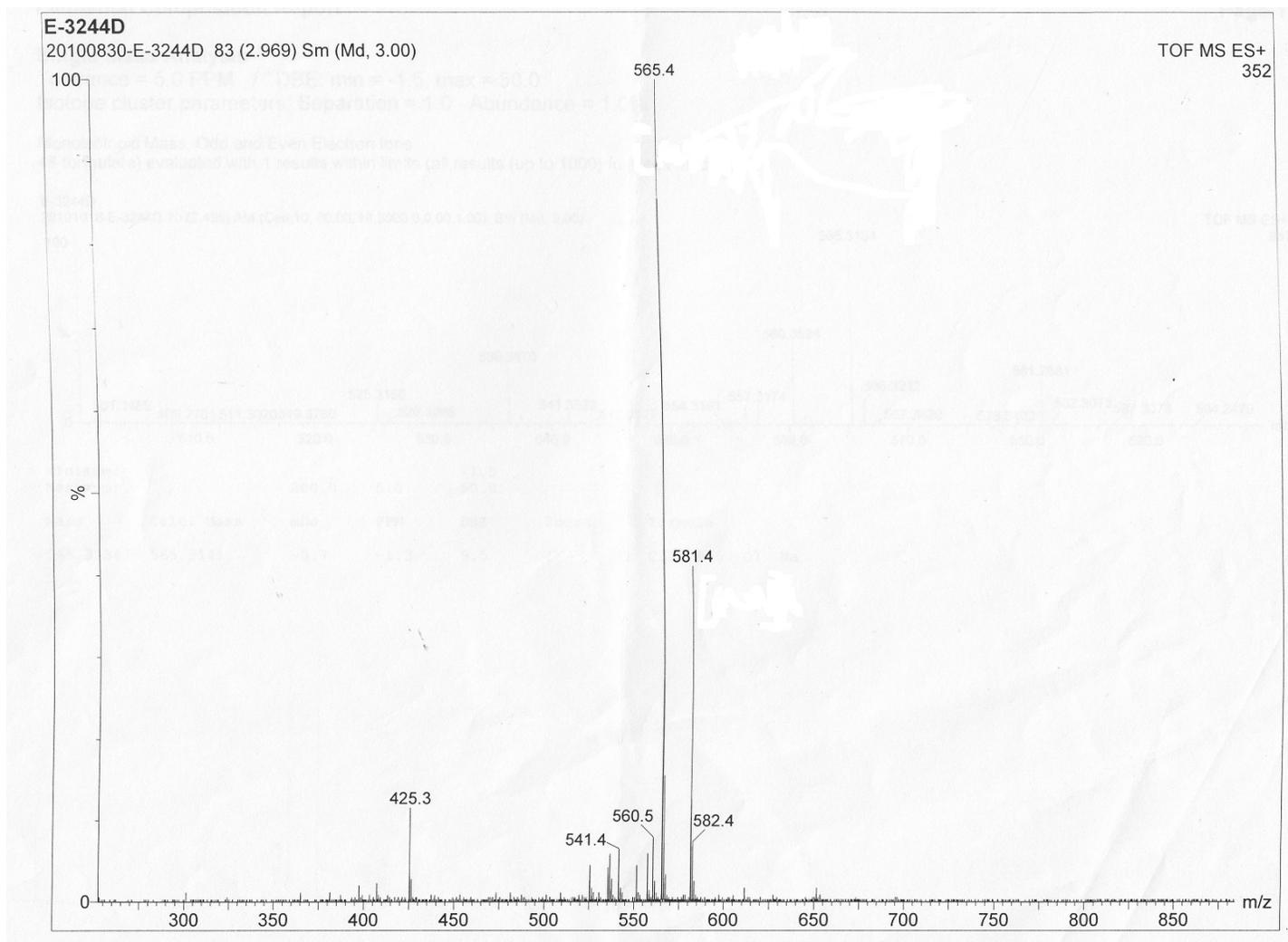


**Figure S68.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **9**



**Figure S69.** HMBC (CDCl<sub>3</sub>) spectrum of compound **9**





**Figure S71.** ESIMS spectrum of compound **9**

# Elemental Composition Report

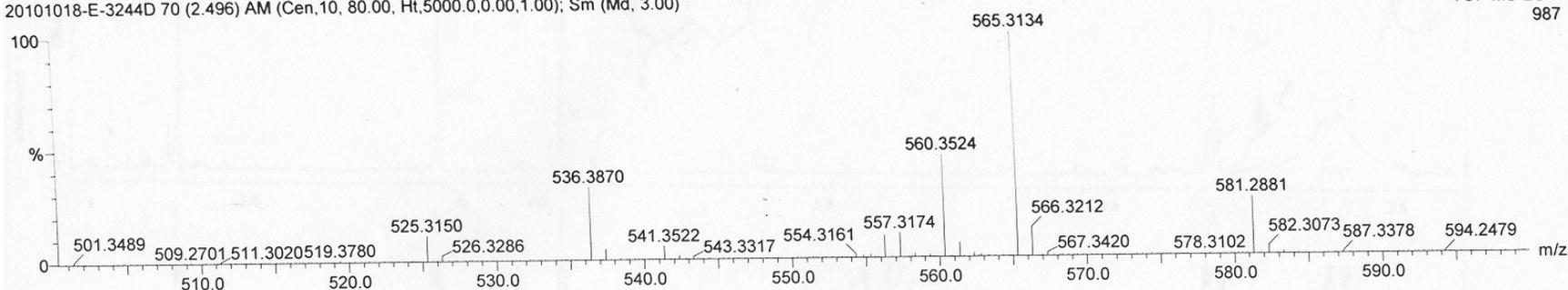
## Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions  
48 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

E-3244D  
20101018-E-3244D 70 (2.496) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

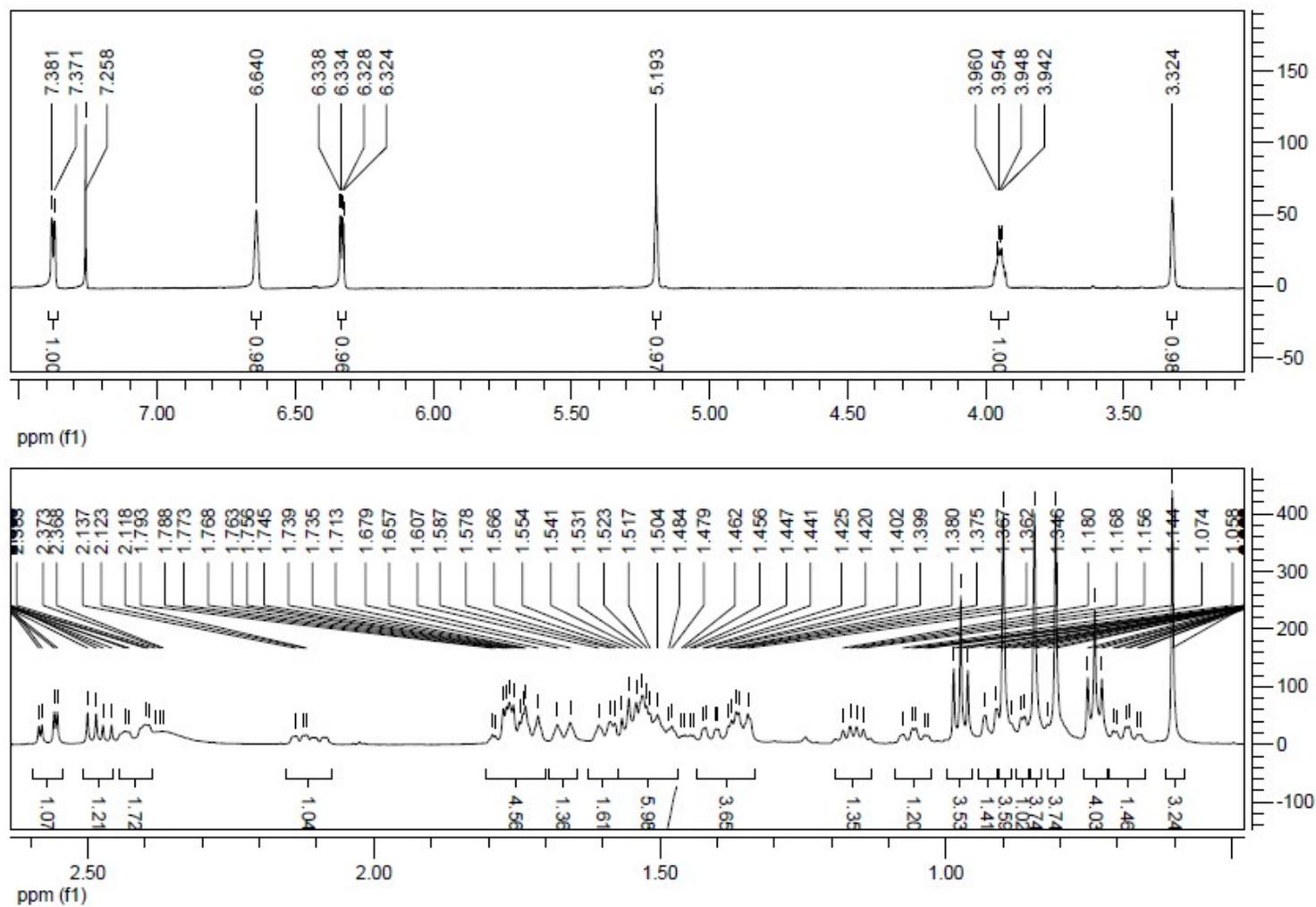
TOF MS ES+  
987



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
565.3134	565.3141	-0.7	-1.3	9.5	1	C32 H46 O7 Na

Figure S72. HRESIMS spectrum of compound 9



**Figure S73.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **10**

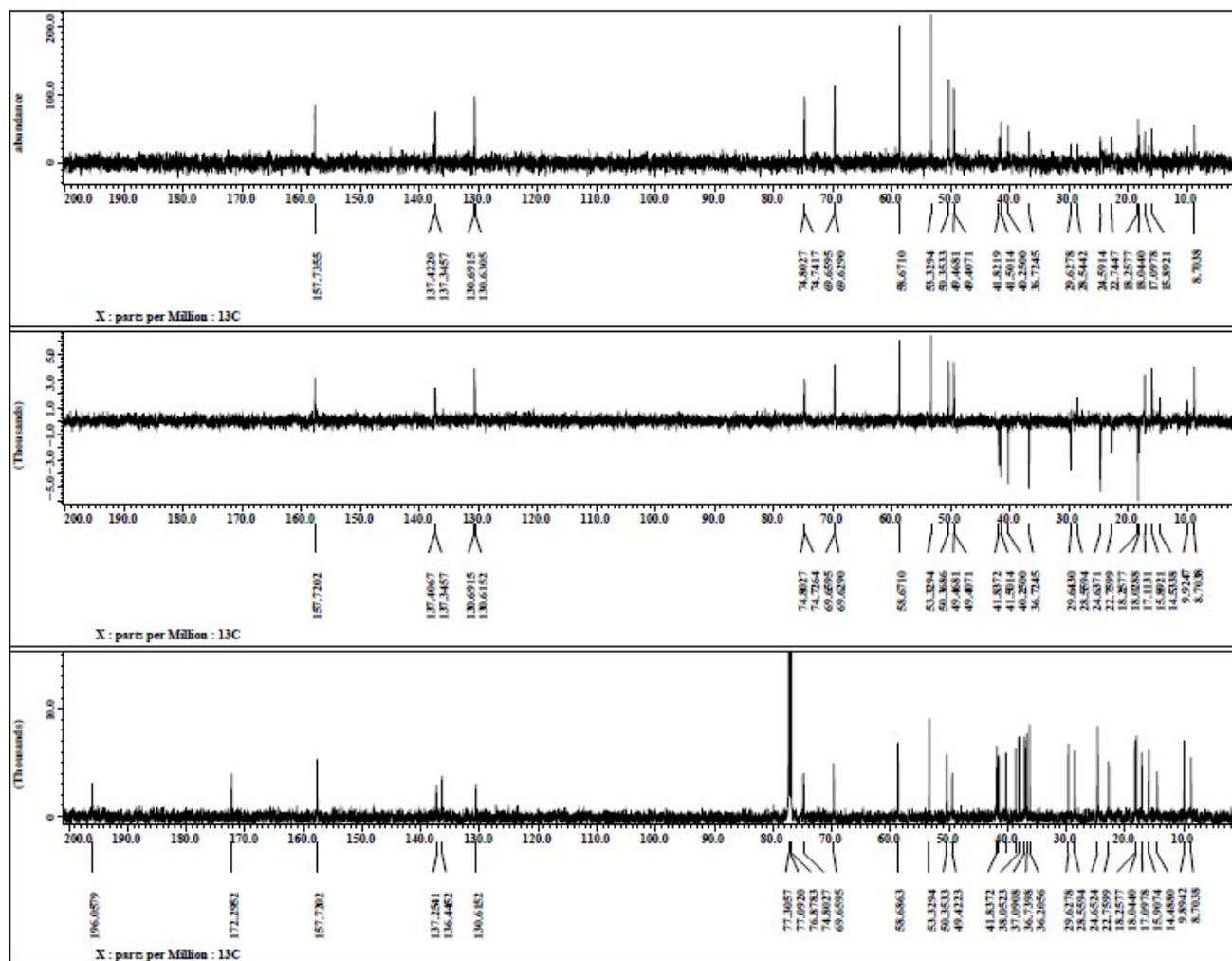


Figure S74.  $^{13}\text{C}$  and DEPT NMR (150 MHz,  $\text{CDCl}_3$ ) spectra of compound 10

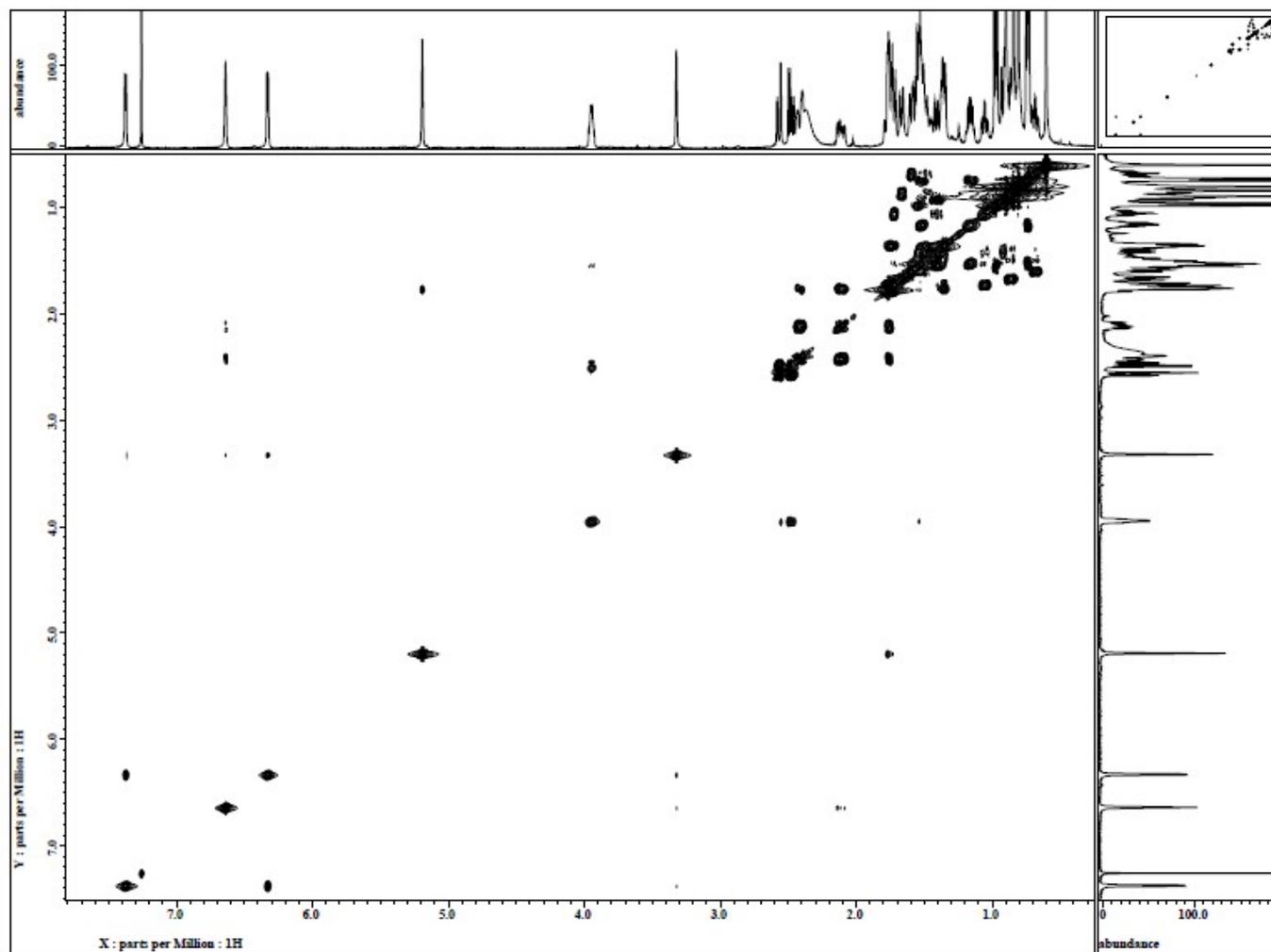


Figure S75. COSY ( $\text{CDCl}_3$ ) spectrum of compound 10

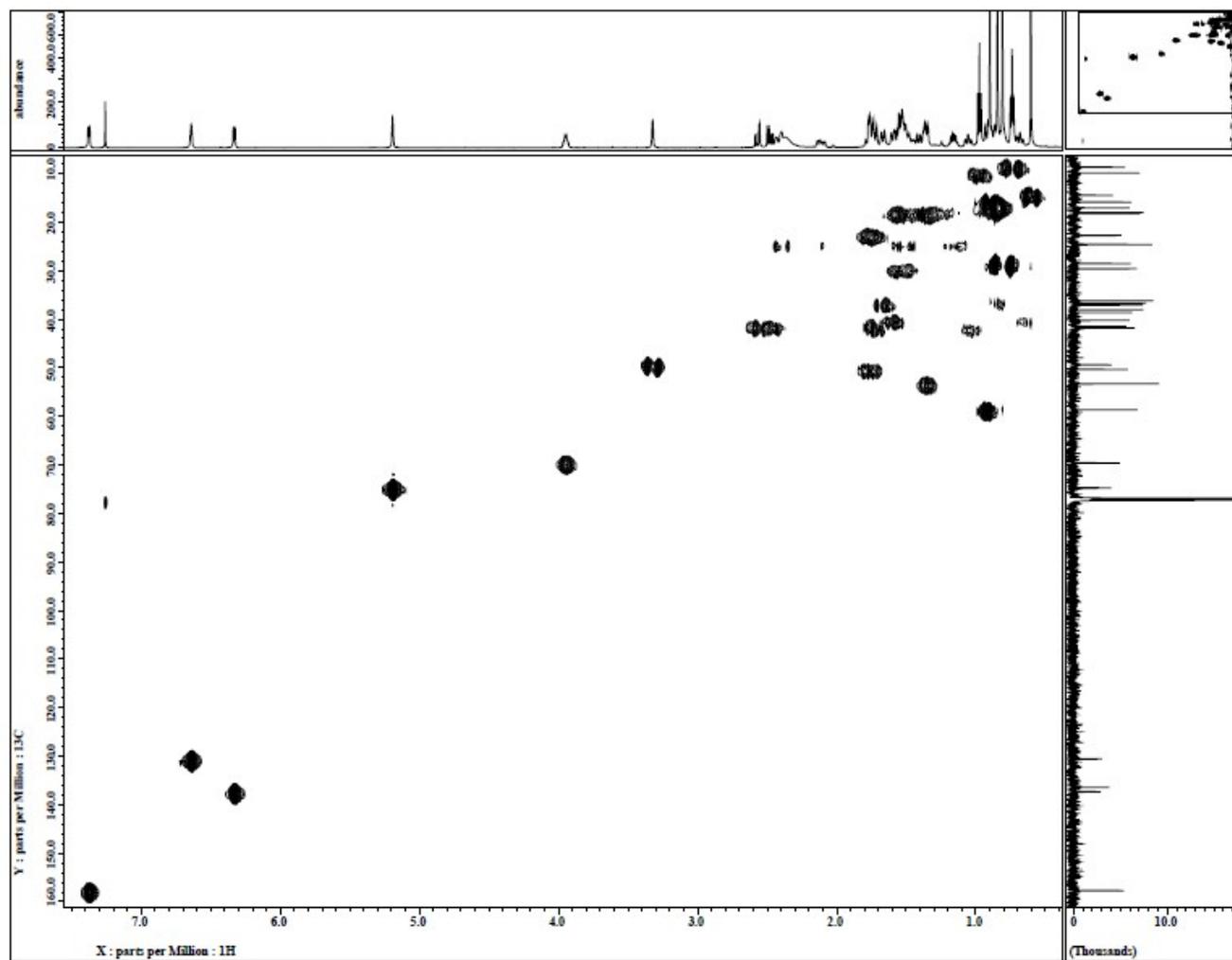


Figure S76. HMQC (CDCl<sub>3</sub>) spectrum of compound 10

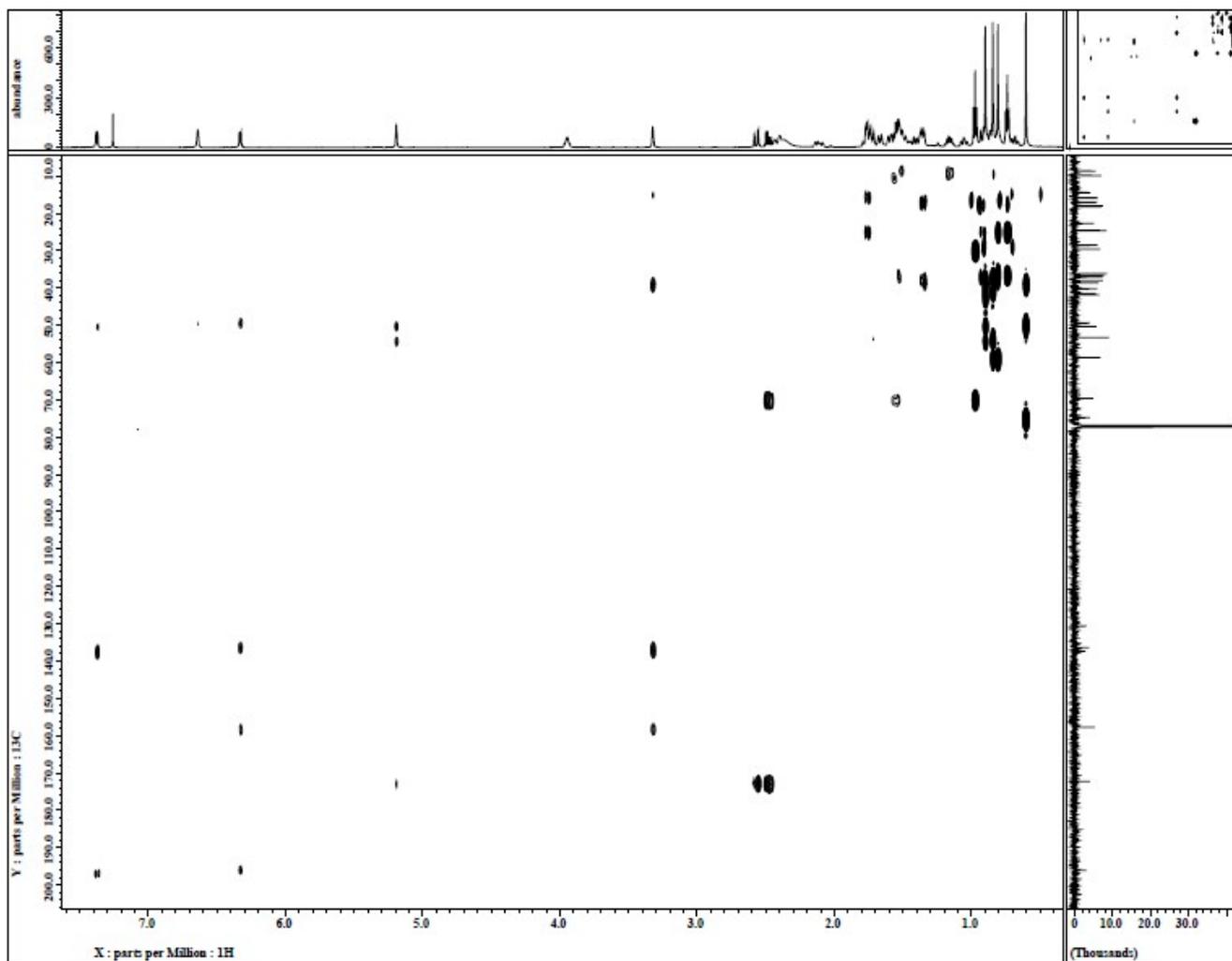
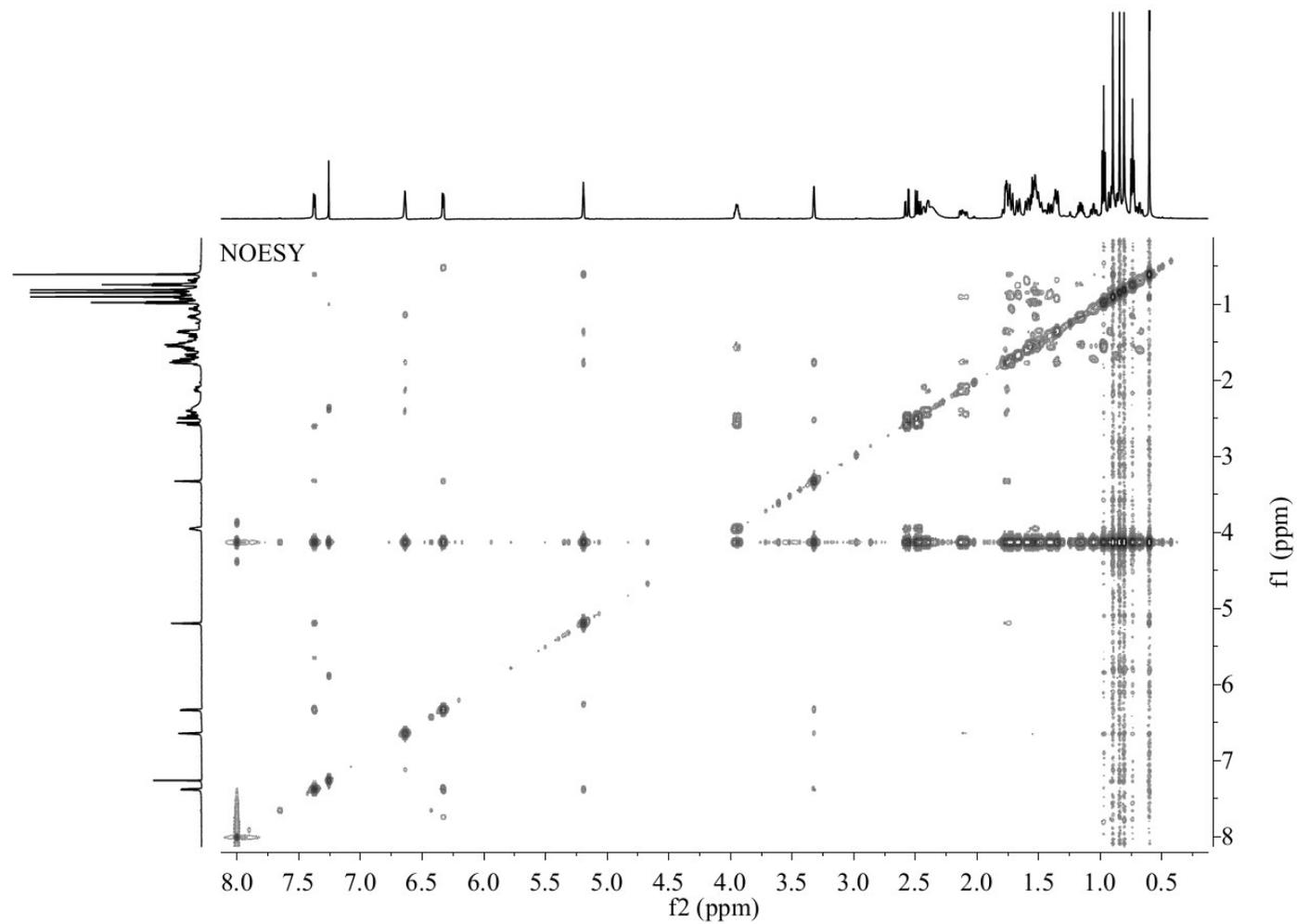


Figure S77. HMBC ( $\text{CDCl}_3$ ) spectrum of compound 10



**Figure S78.** NOESY (CDCl<sub>3</sub>) spectrum of compound **10**

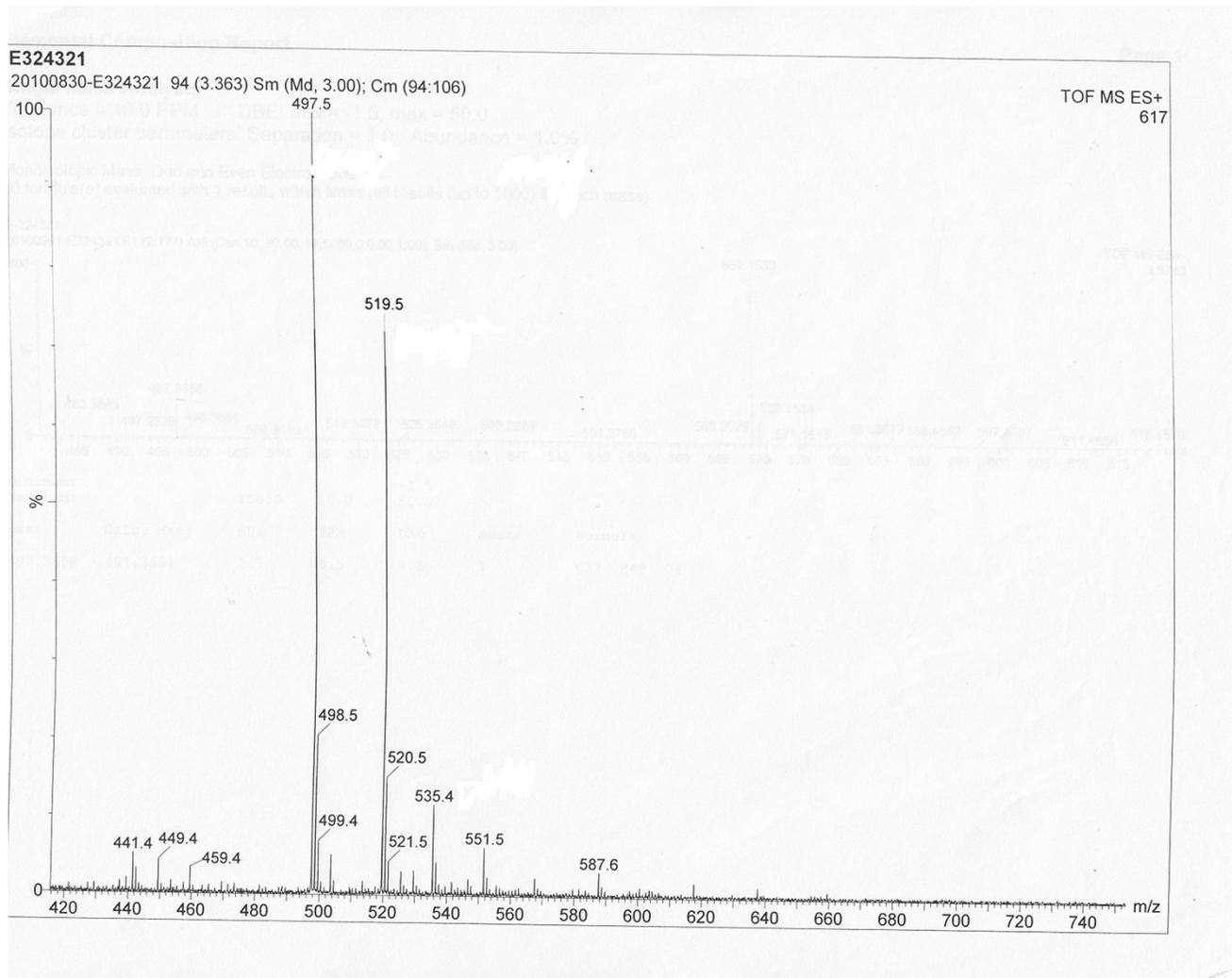


Figure S79. ESIMS spectrum of compound 10

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

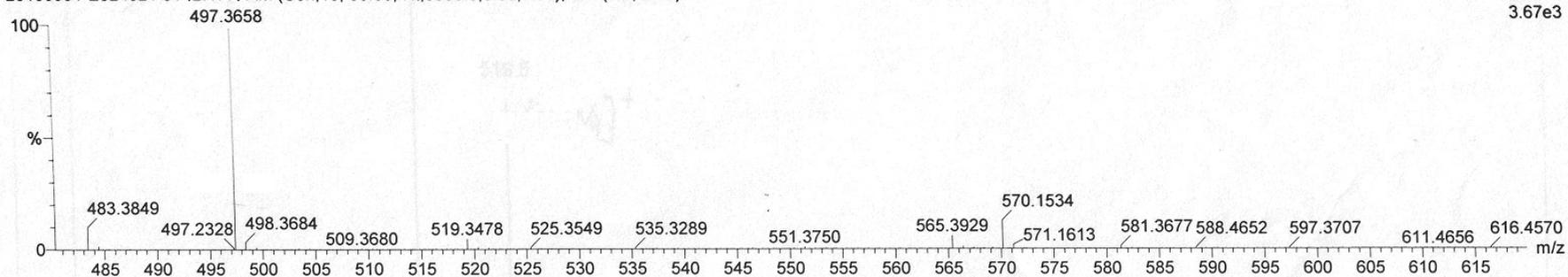
Monoisotopic Mass, Odd and Even Electron Ions

50 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

E-324321

20100901-E324321 61 (2.177) AM (Cen,10, 80.00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00)

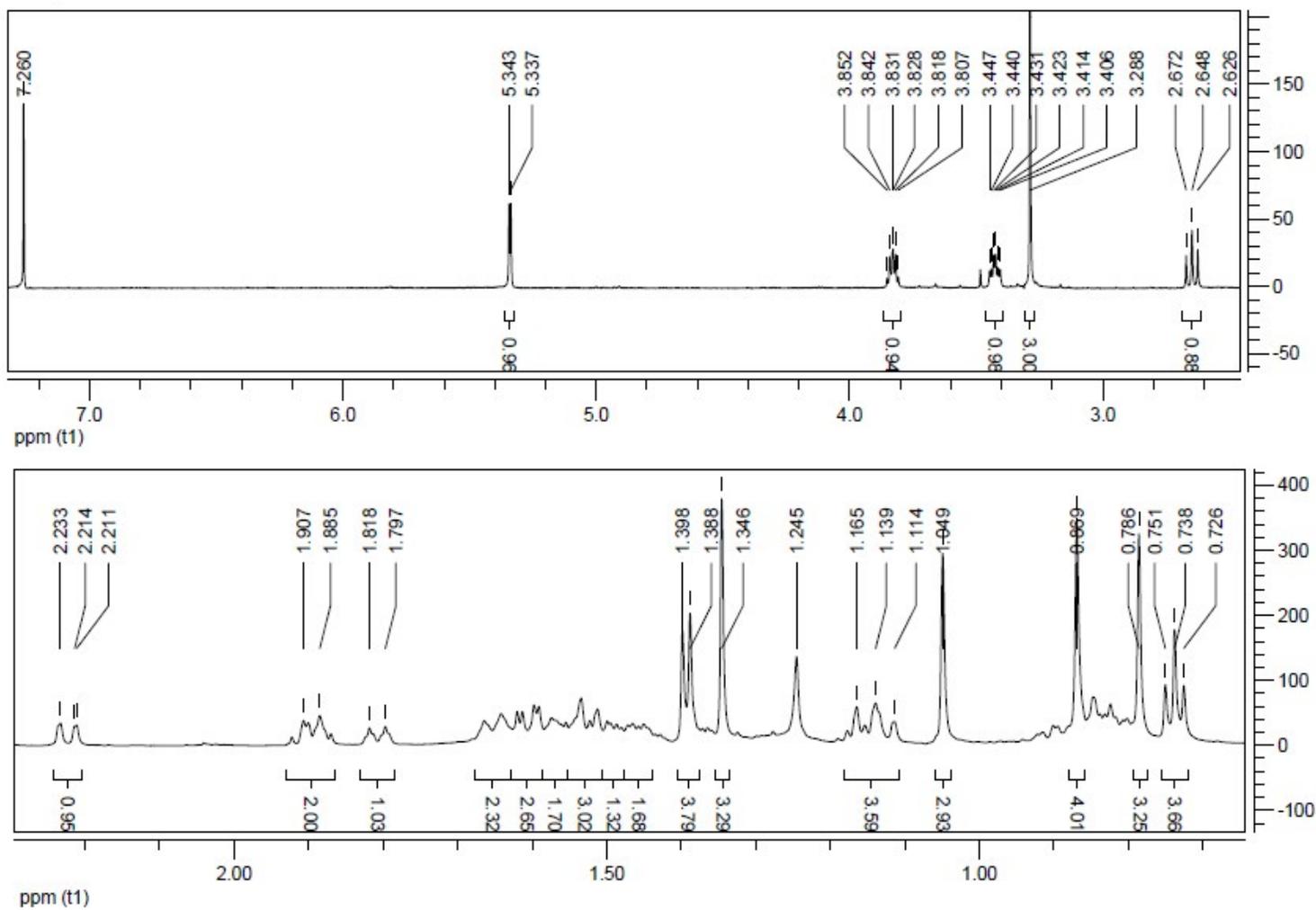
TOF MS ES+  
3.67e3



Minimum: -1.5  
Maximum: 200.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
497.3658	497.3631	2.7	5.5	8.5	1	C32 H49 O4

Figure S80. HRESIMS spectrum of compound 10



**Figure S81.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **11**

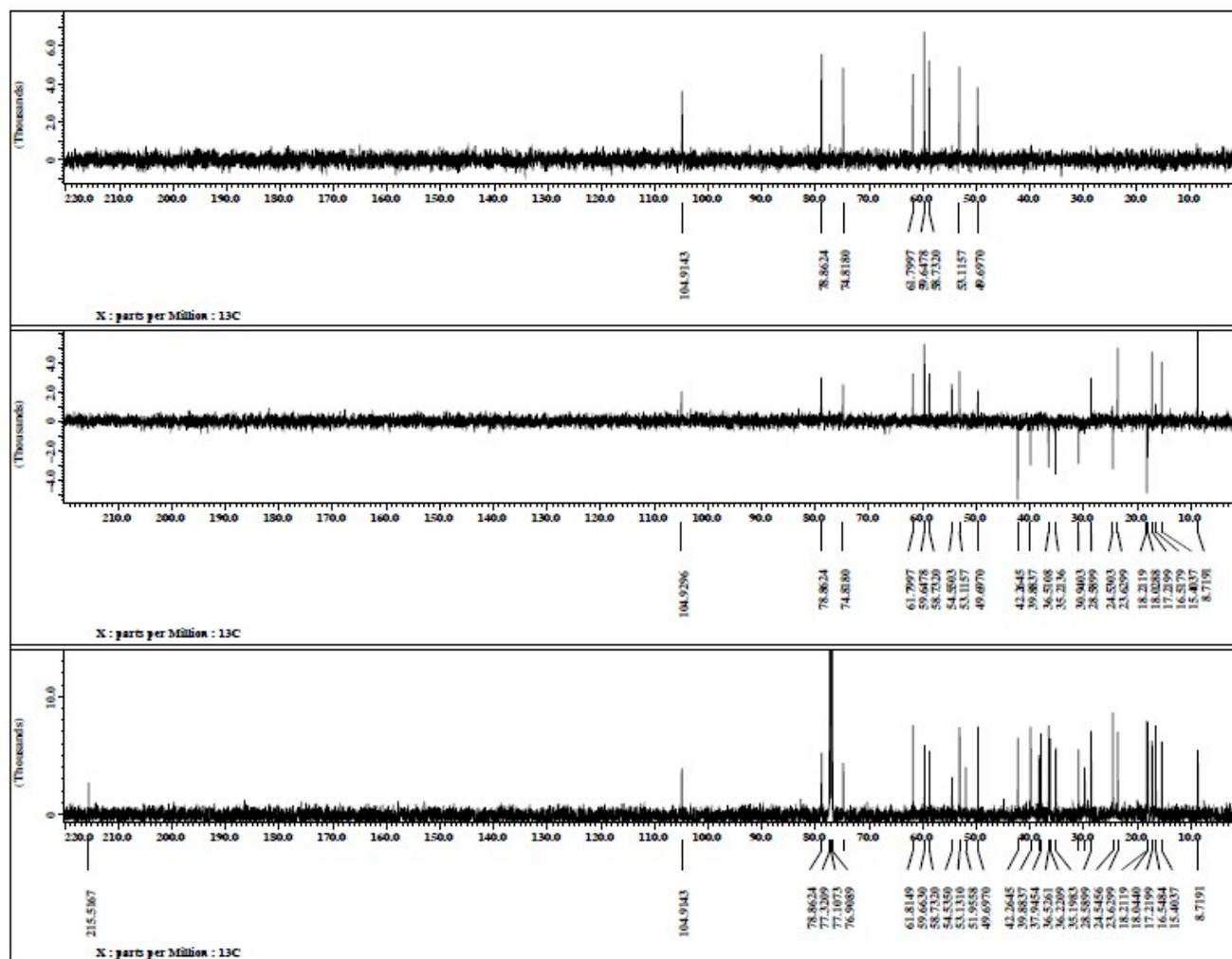
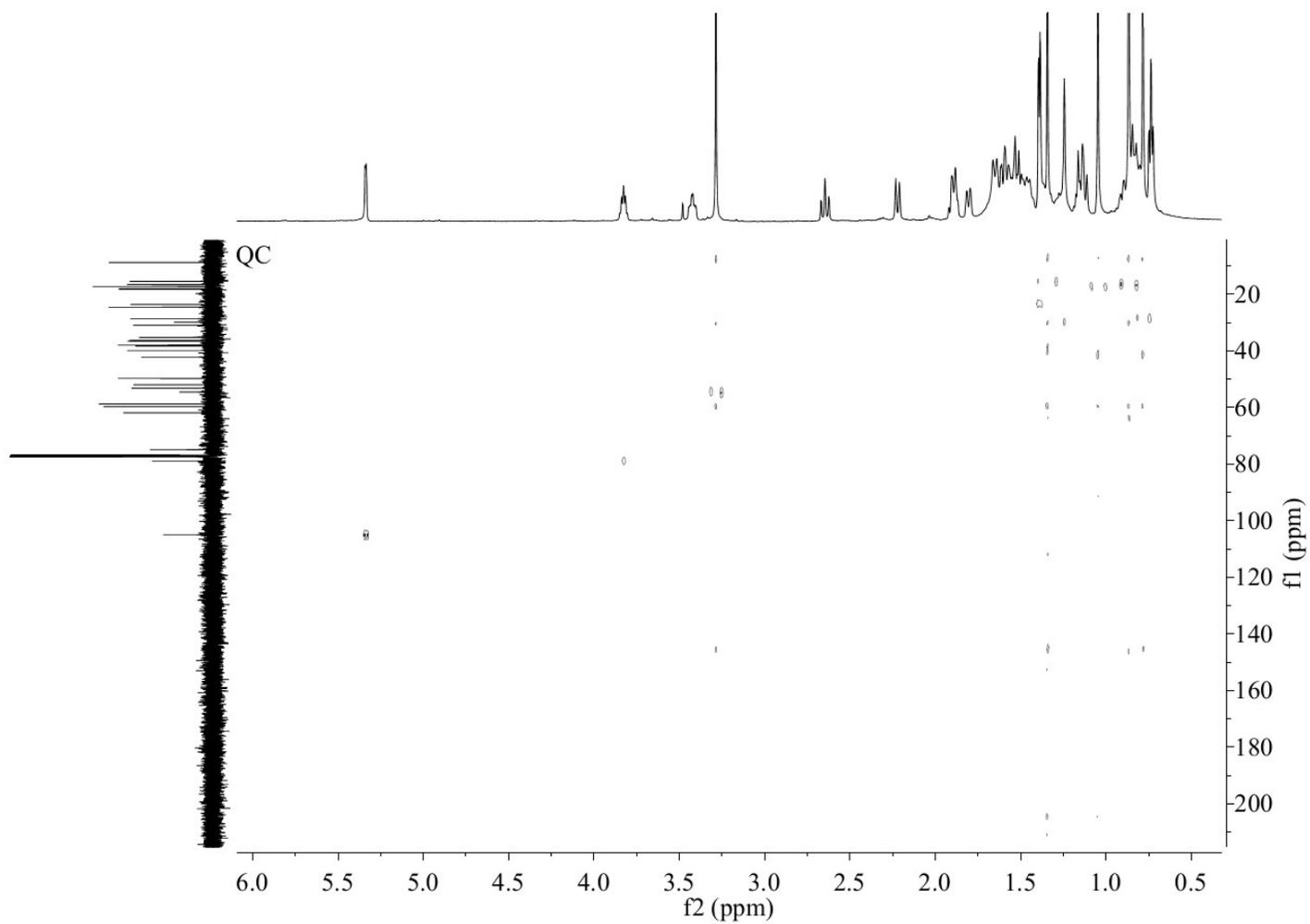
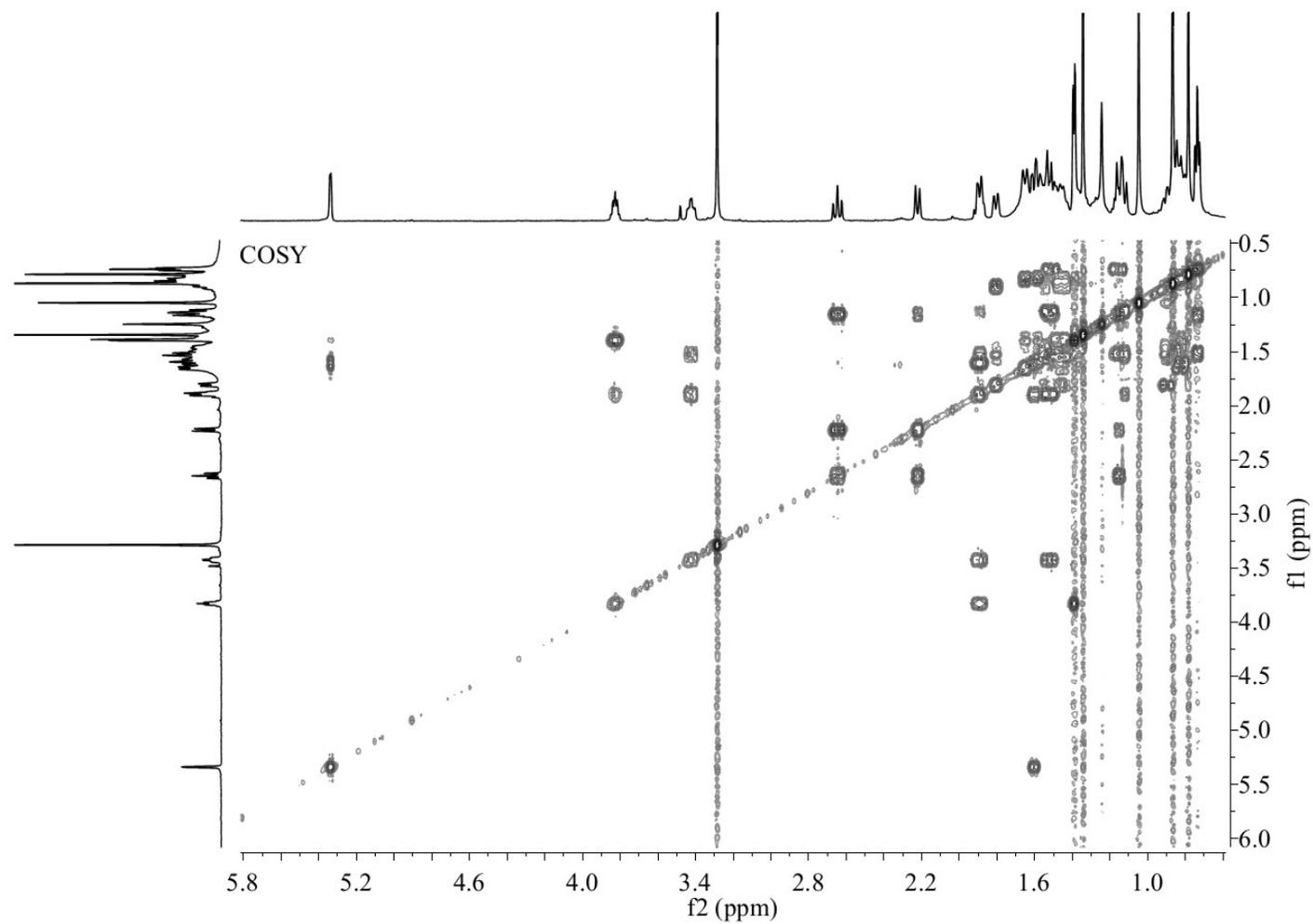


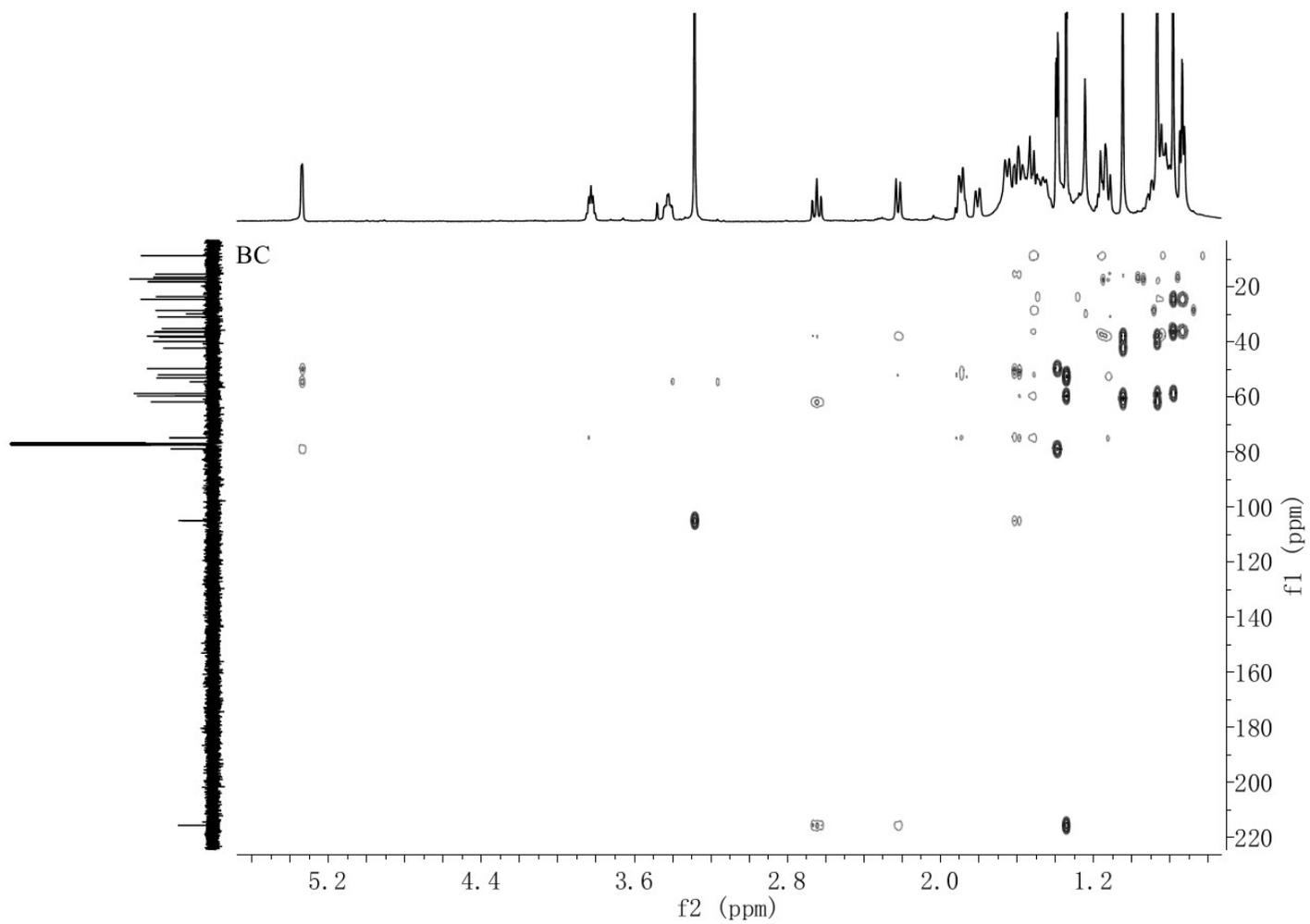
Figure S82. <sup>13</sup>C and DEPT NMR (150 MHz, CDCl<sub>3</sub>) spectra of compound 11



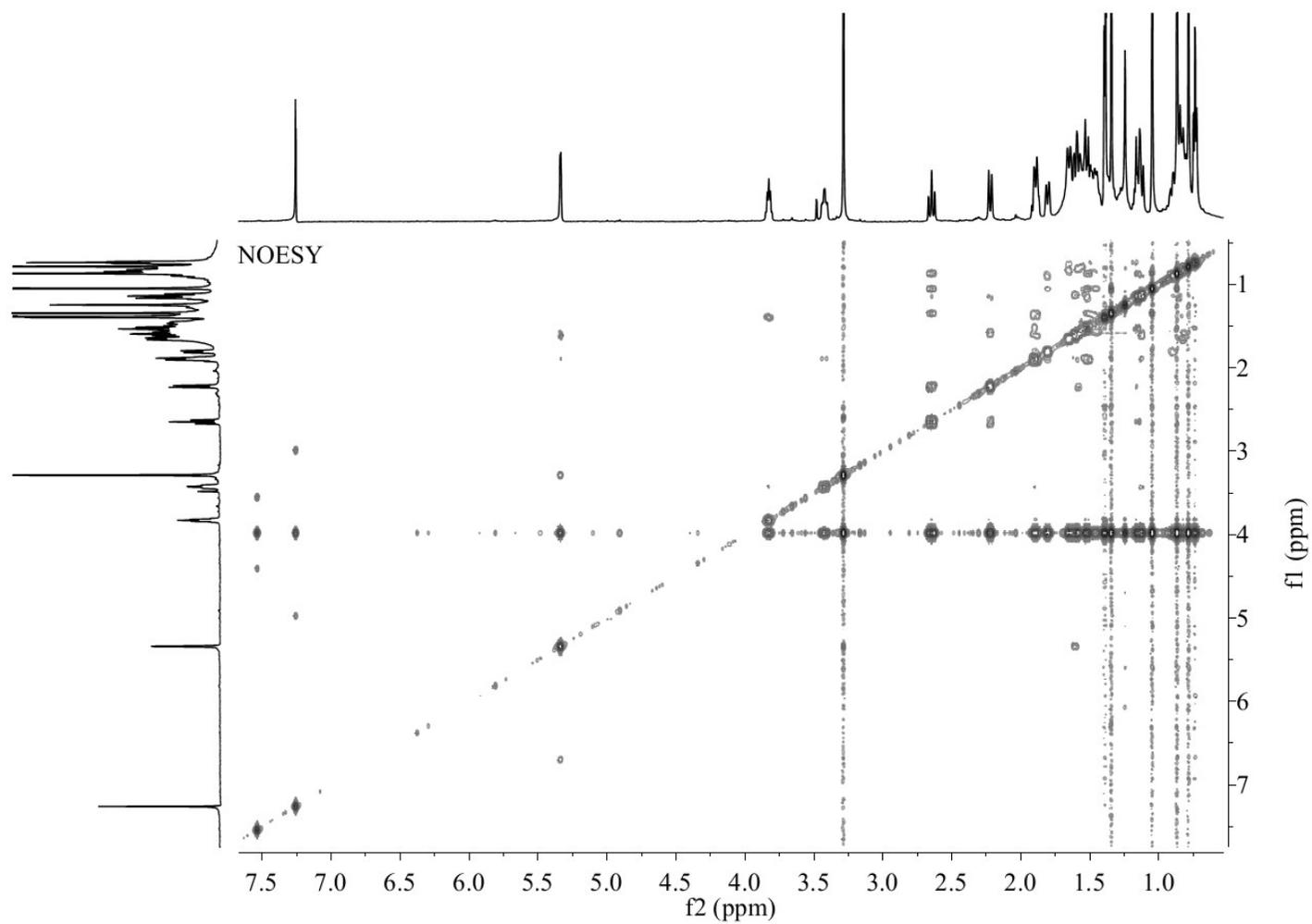
**Figure S83.** HMQC (CDCl<sub>3</sub>) spectrum of compound **11**



**Figure S84.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **11**



**Figure S85.** HMBC ( $\text{CDCl}_3$ ) spectrum of compound **11**



**Figure S86.** NOESY (CDCl<sub>3</sub>) spectrum of compound **11**

Instrument:DSQ(Thermo)  
Ionization Method:EI  
D:\DSQDATA-LR11\O50620  
O50620 #149 RT: 2.43 AV: 1 NL: 1.27E7  
T: + c Full ms [ 45.00-800.00]

5/6/2011 4:45:22 PM

F-2211

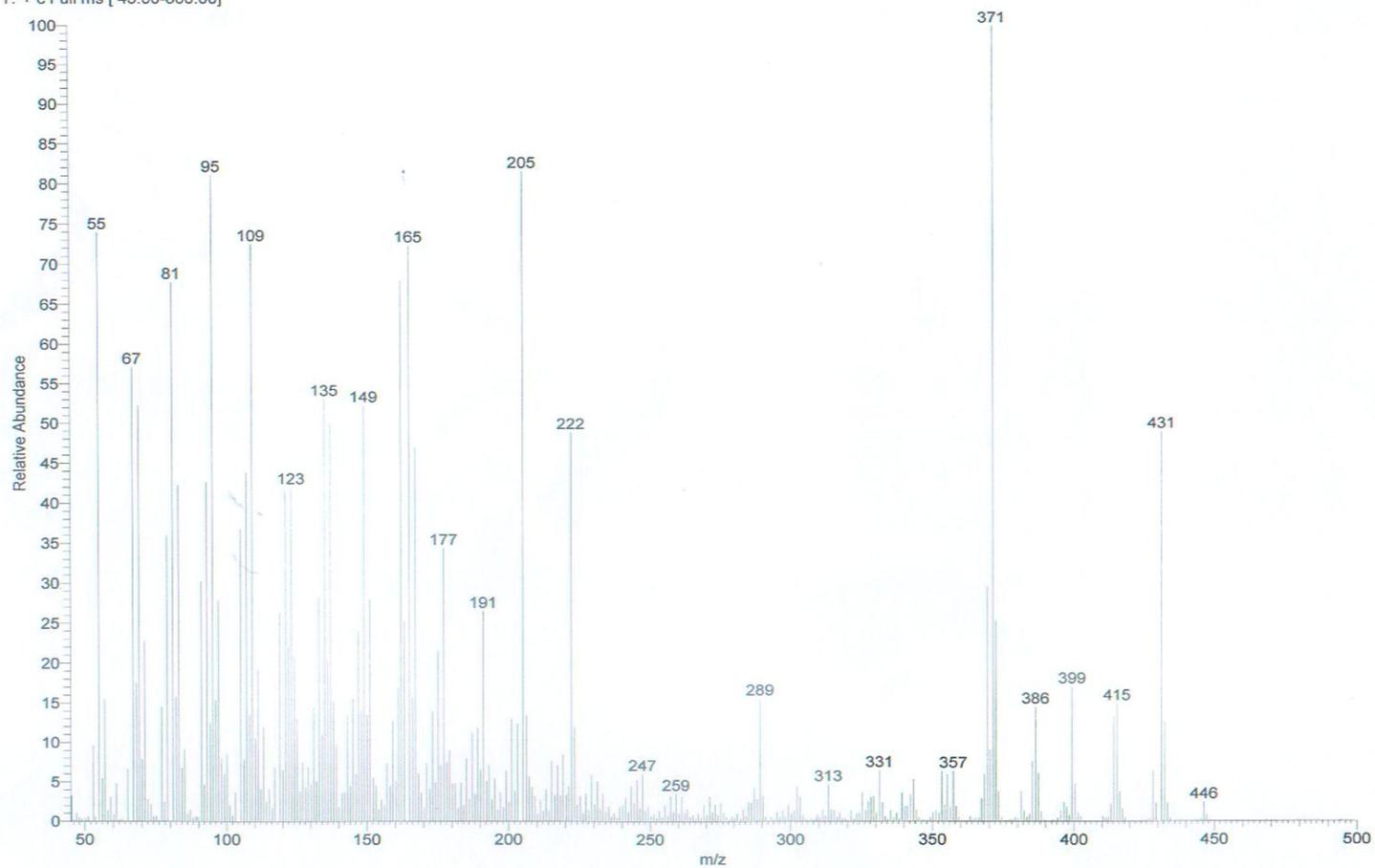


Figure S87. EIMS spectrum of compound 11

SPECTRUM - MS

File : D:\DATA-HR\11\051705-f-2211-c1.RAW

Full ms [442.100 - 450.500 ] - Range: 442.100 - 450.500

Scan No. 13 of 22

Scan #: 13

RT: 0.53

Data points: 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
446.3395	92.8	446.3391	1.0	0.4	6.0	C <sub>28</sub> H <sub>46</sub> O <sub>4</sub>

Instrument: MAT 95XP(Thermo)

D:\DATA-HR\11\051705-f-2211-c1

5/17/2011 3:36:03 PM

F-2211

051705-f-2211-c1 #13 RT: 0.53 AV: 1 NL: 1.45E5  
T: + c EI Full ms [ 442.10-450.50]

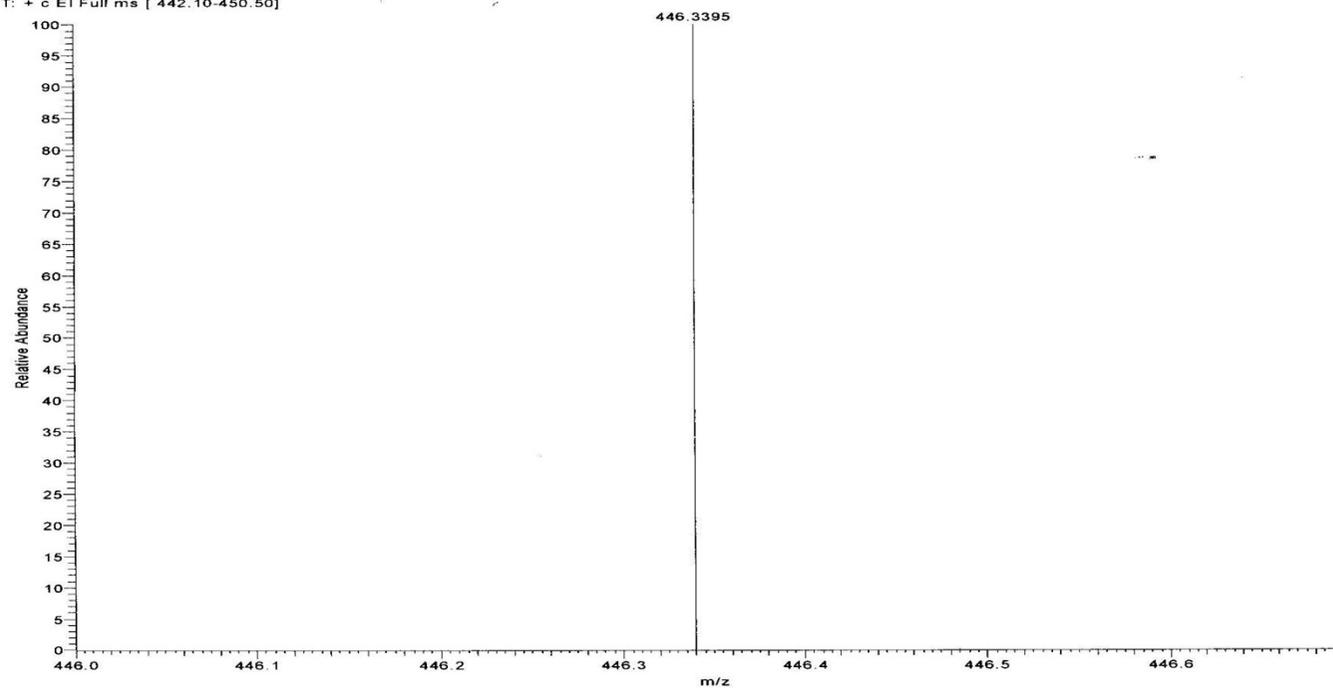
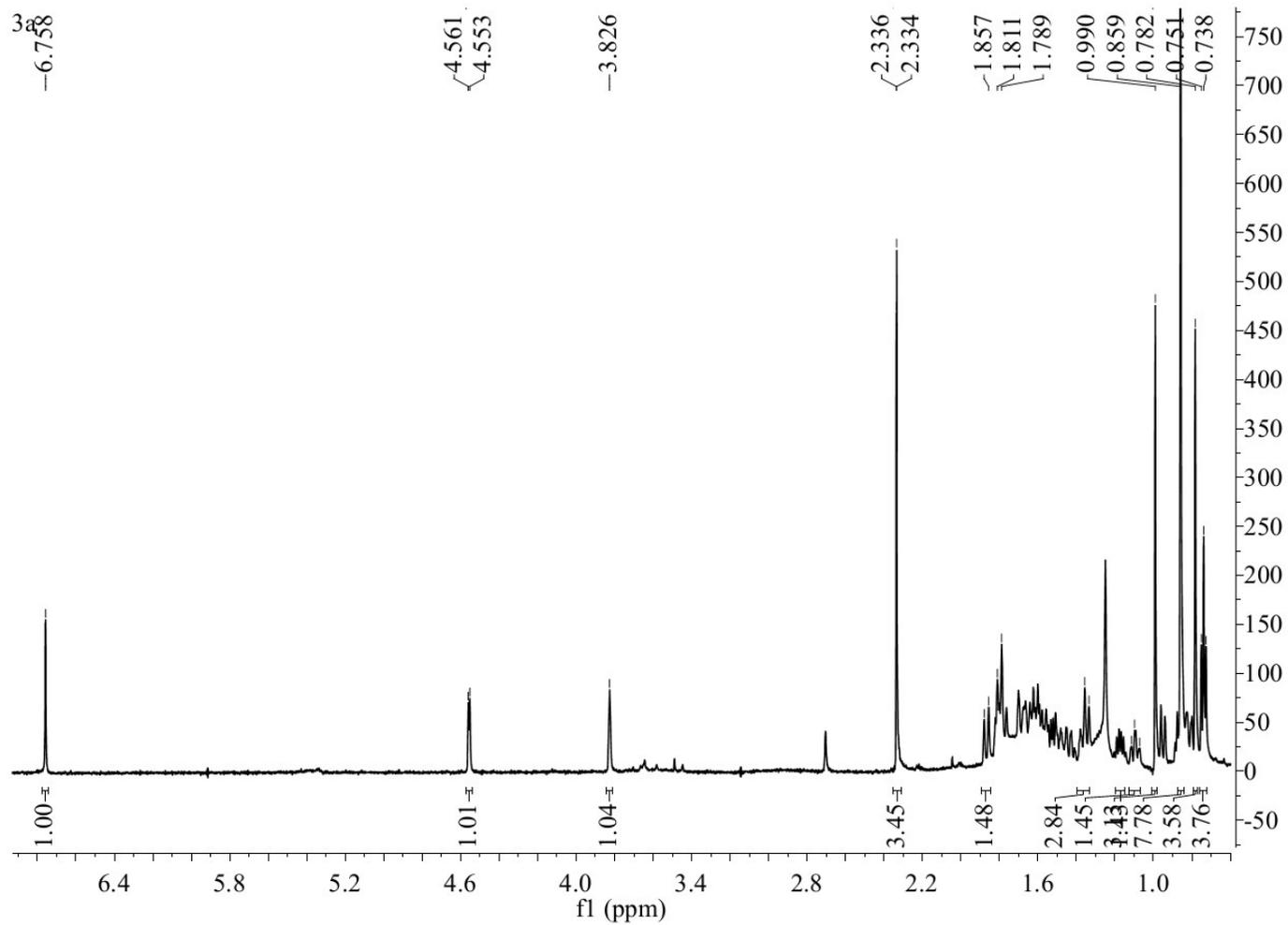
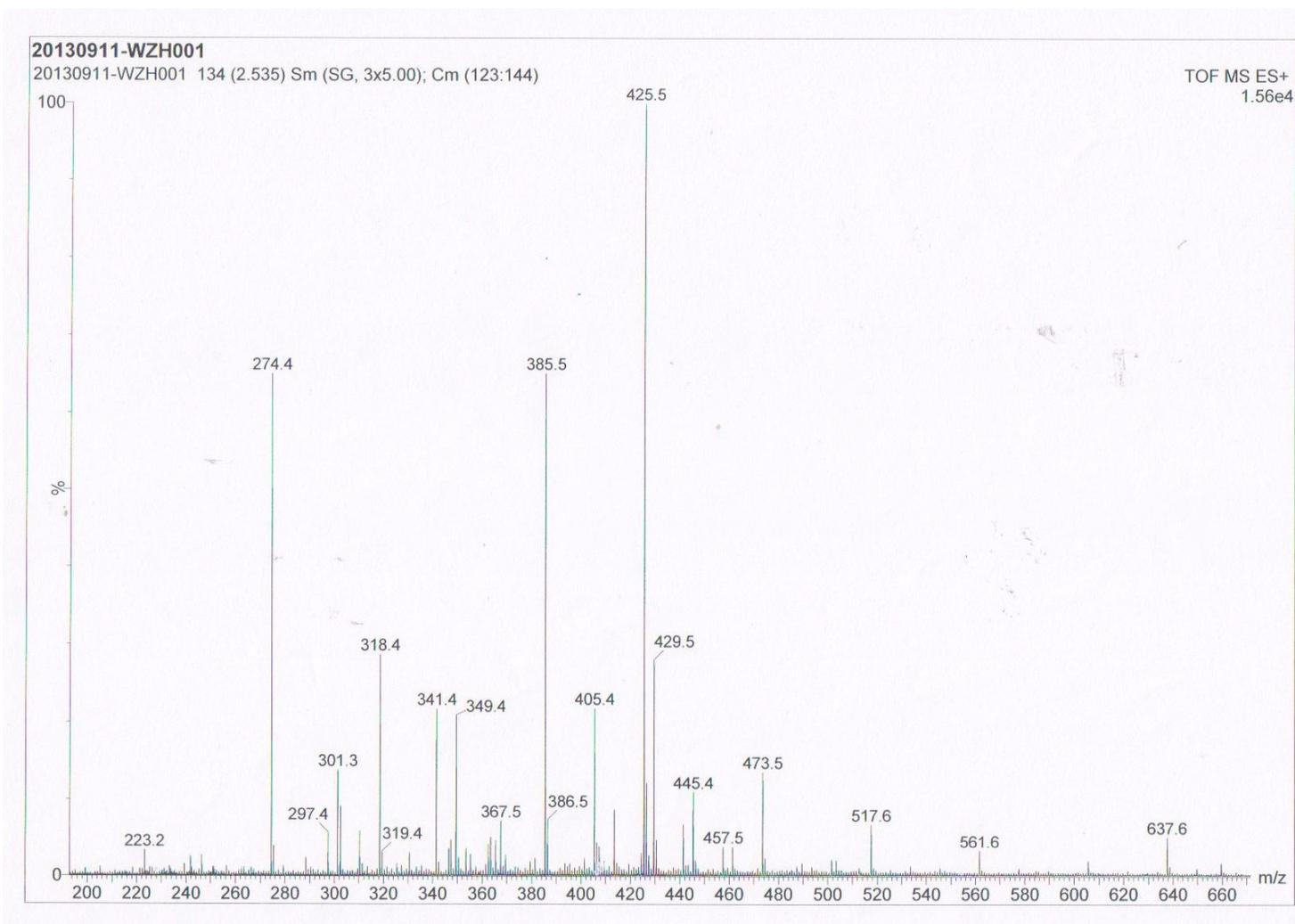


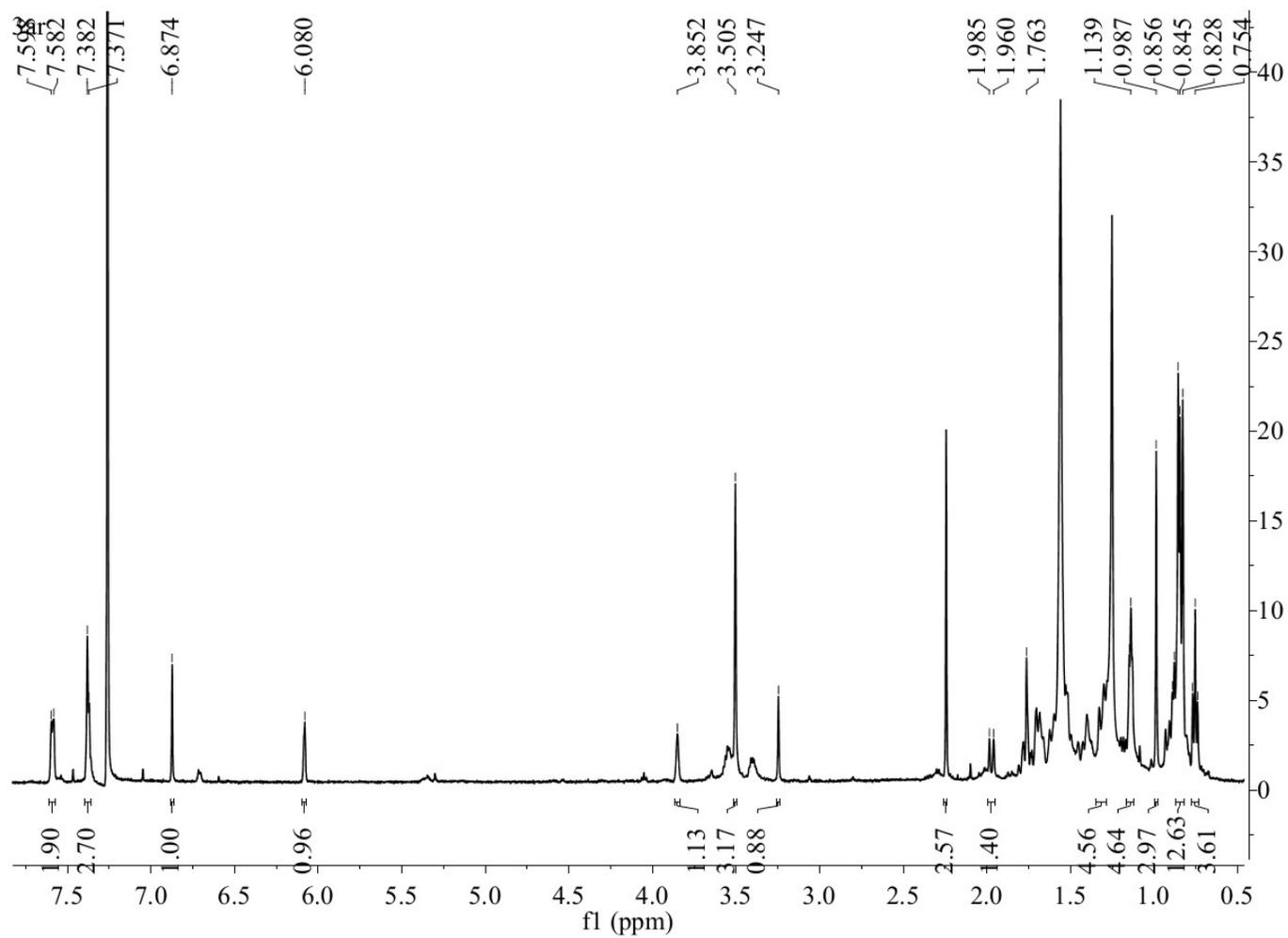
Figure S88. HREIMS spectrum of compound 11



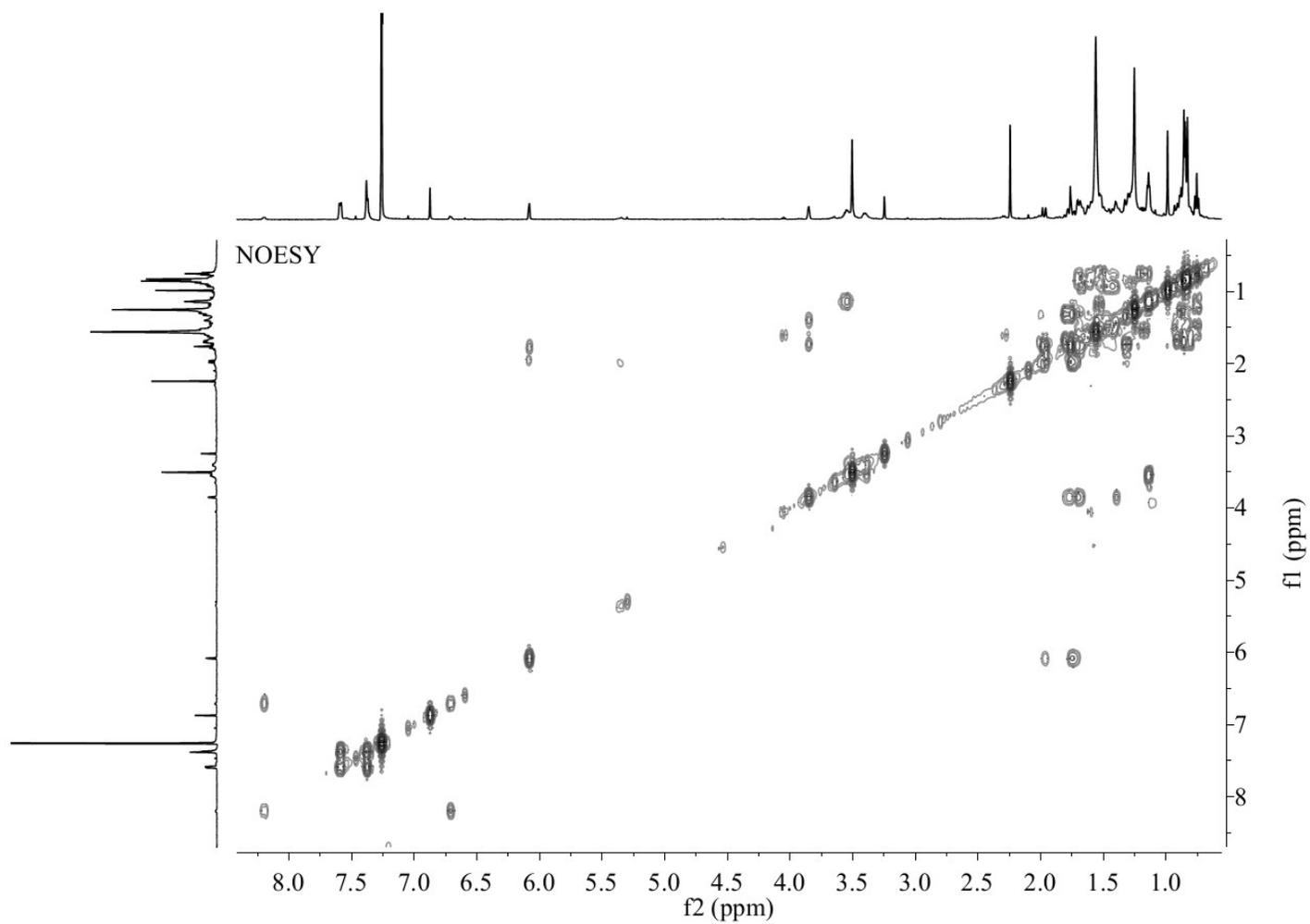
**Figure S89.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **3a**



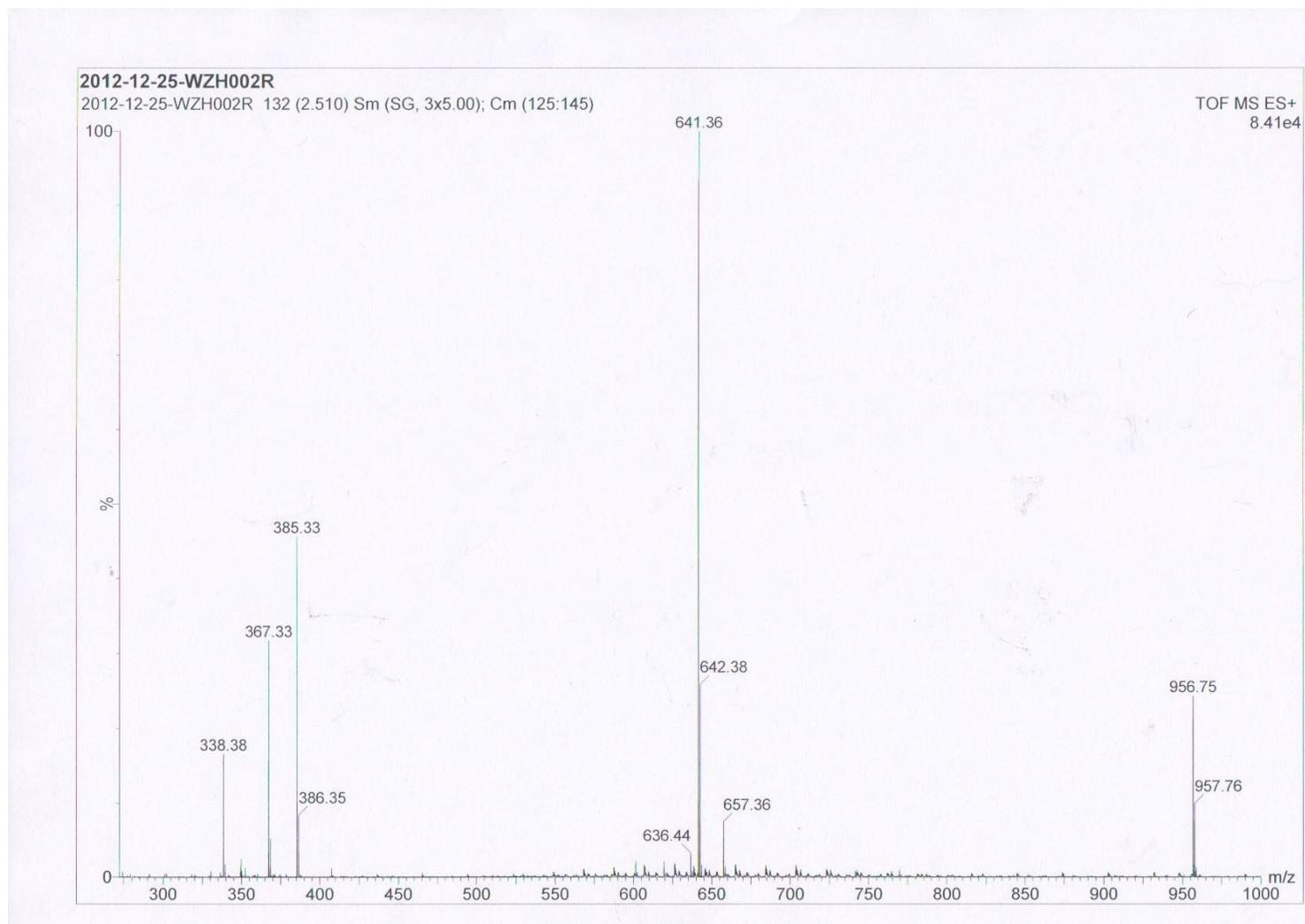
**Figure S90.** ESIMS spectrum of compound **3a**



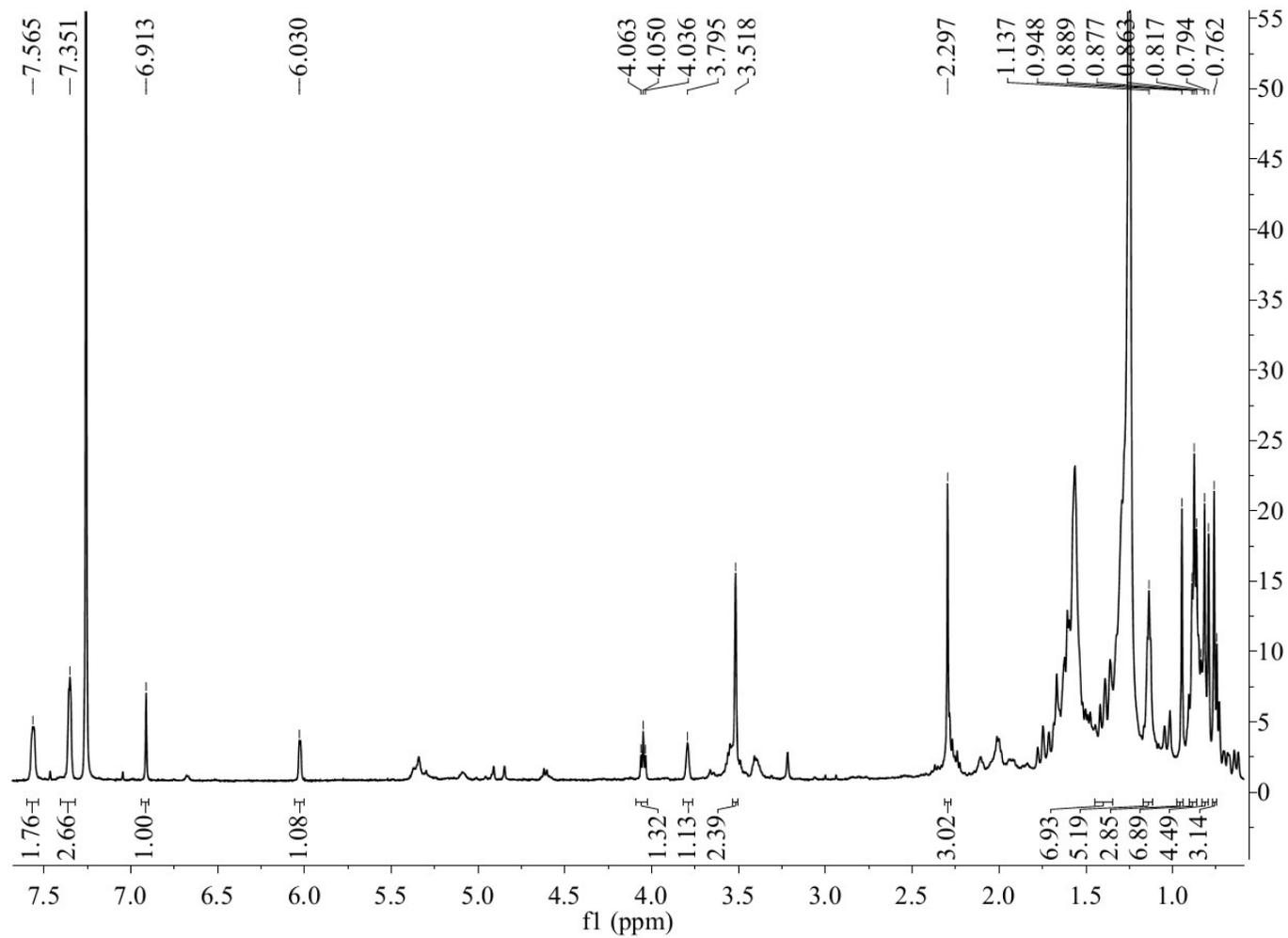
**Figure S91.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound **3ar**



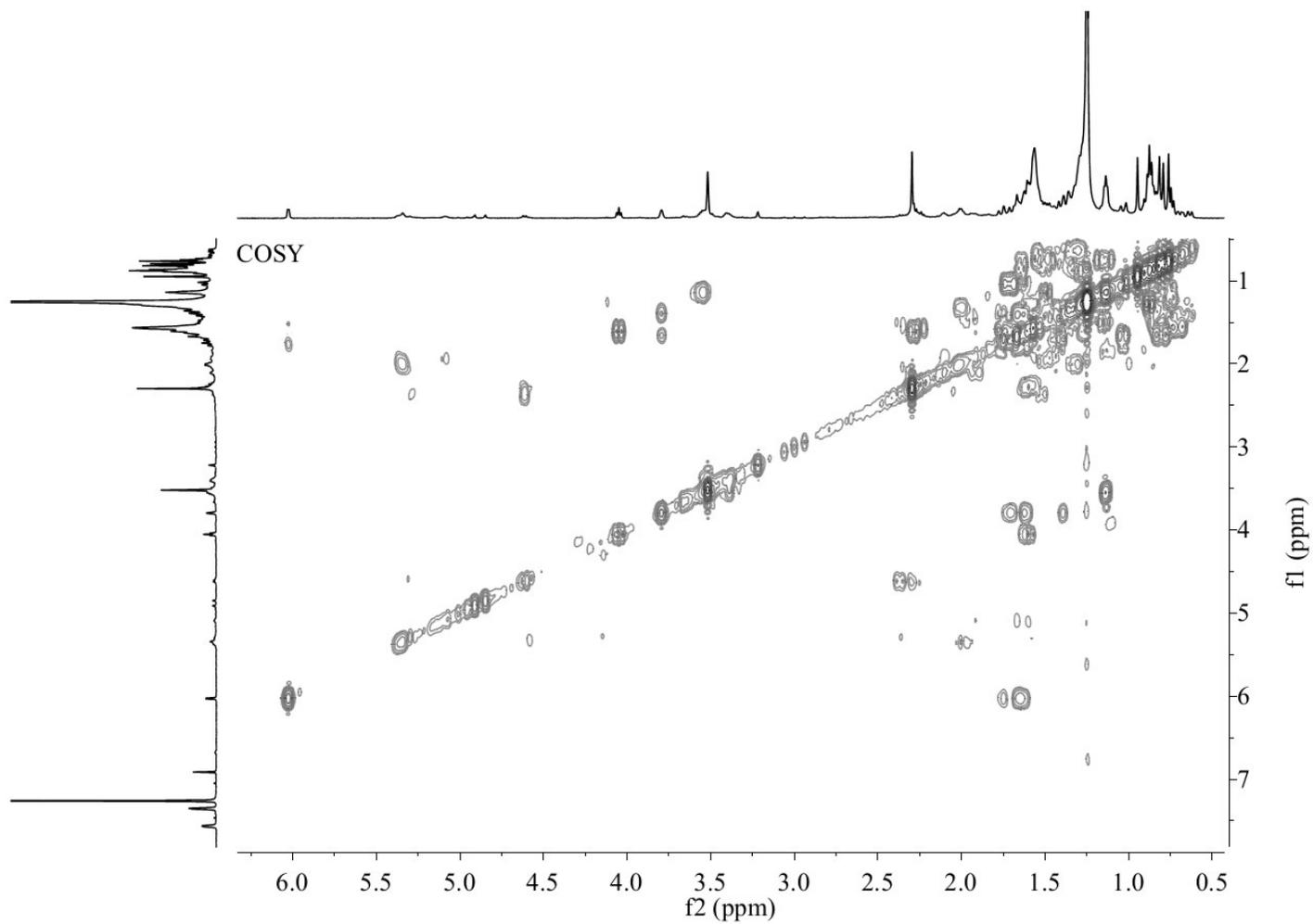
**Figure S92.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **3ar**



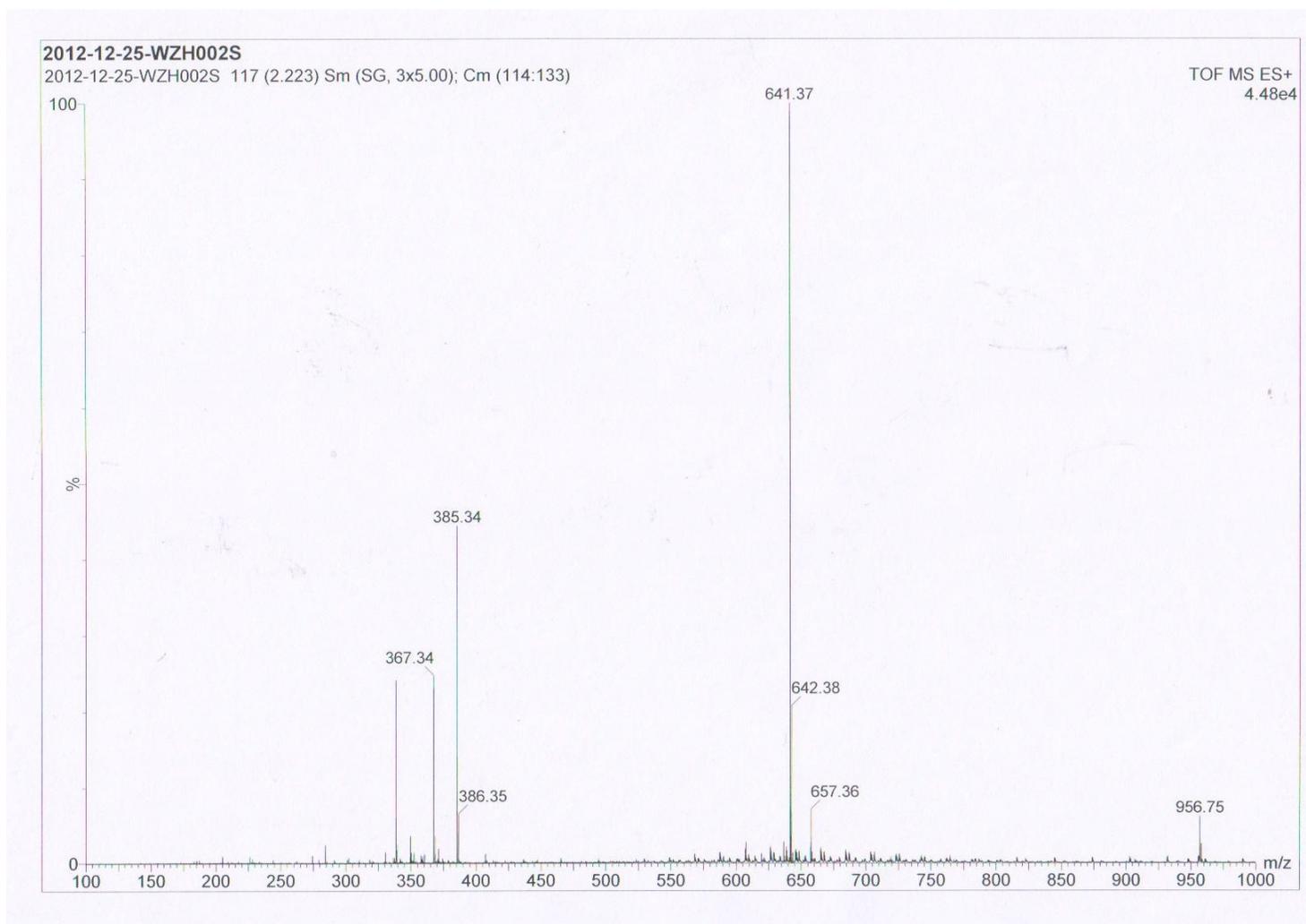
**Figure S93.** ESIMS spectrum of compound **3ar**



**Figure S94.** <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 3as



**Figure S95.** COSY ( $\text{CDCl}_3$ ) spectrum of compound **3as**



**Figure S96.** ESIMS spectrum of compound **3**