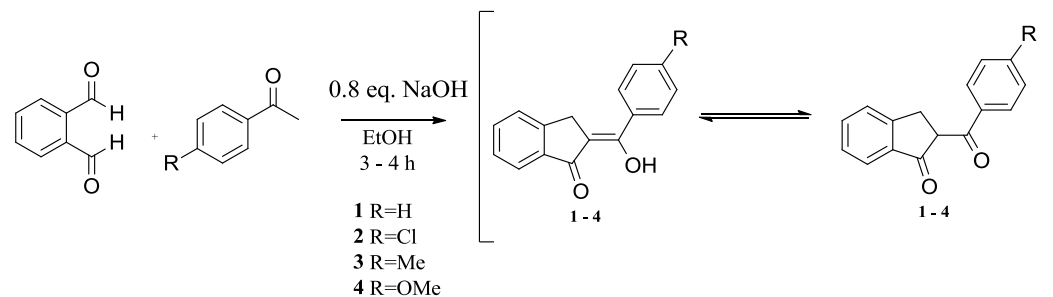


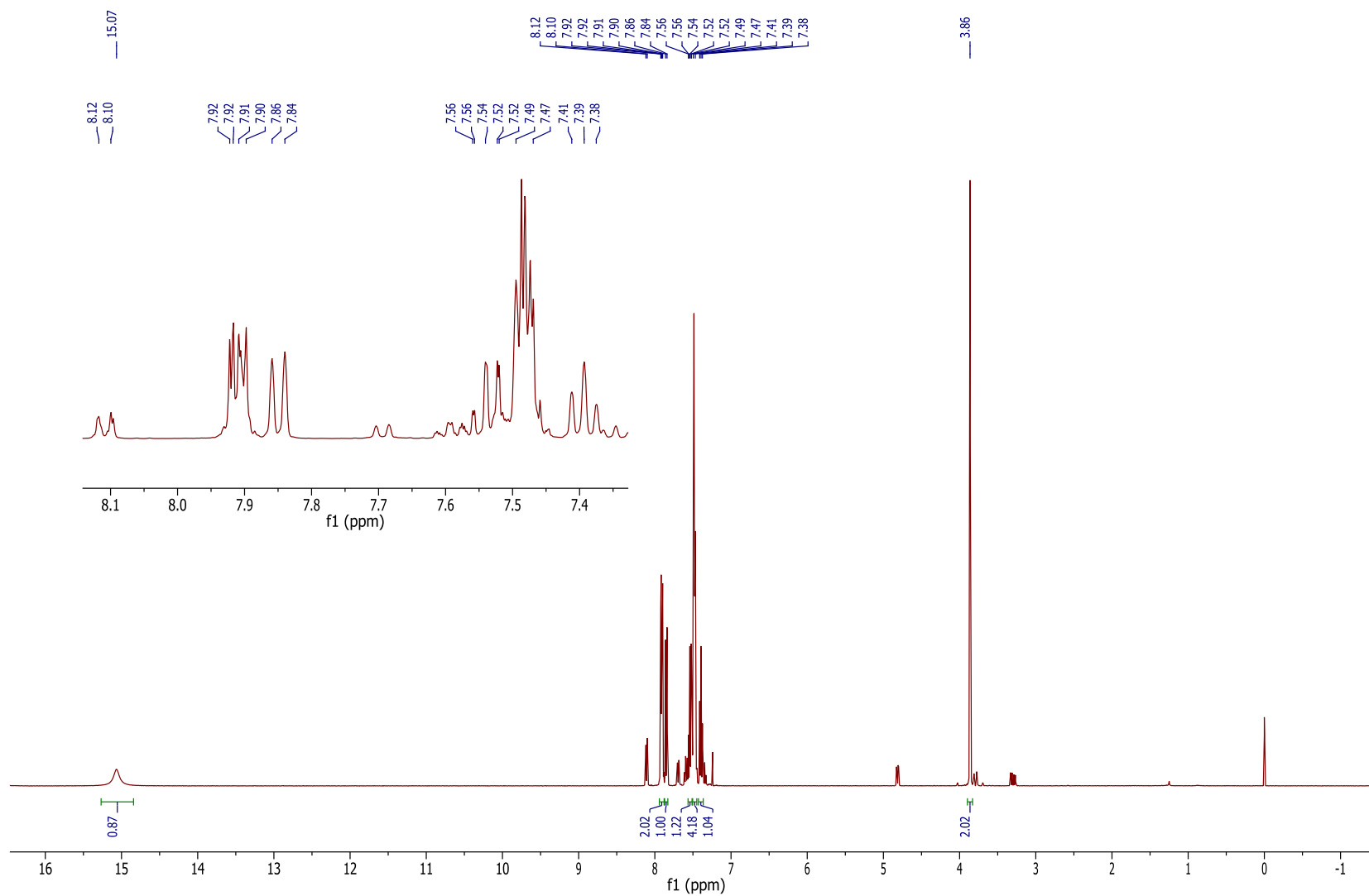
SUPPORTING INFORMATION

NMR Spectrum

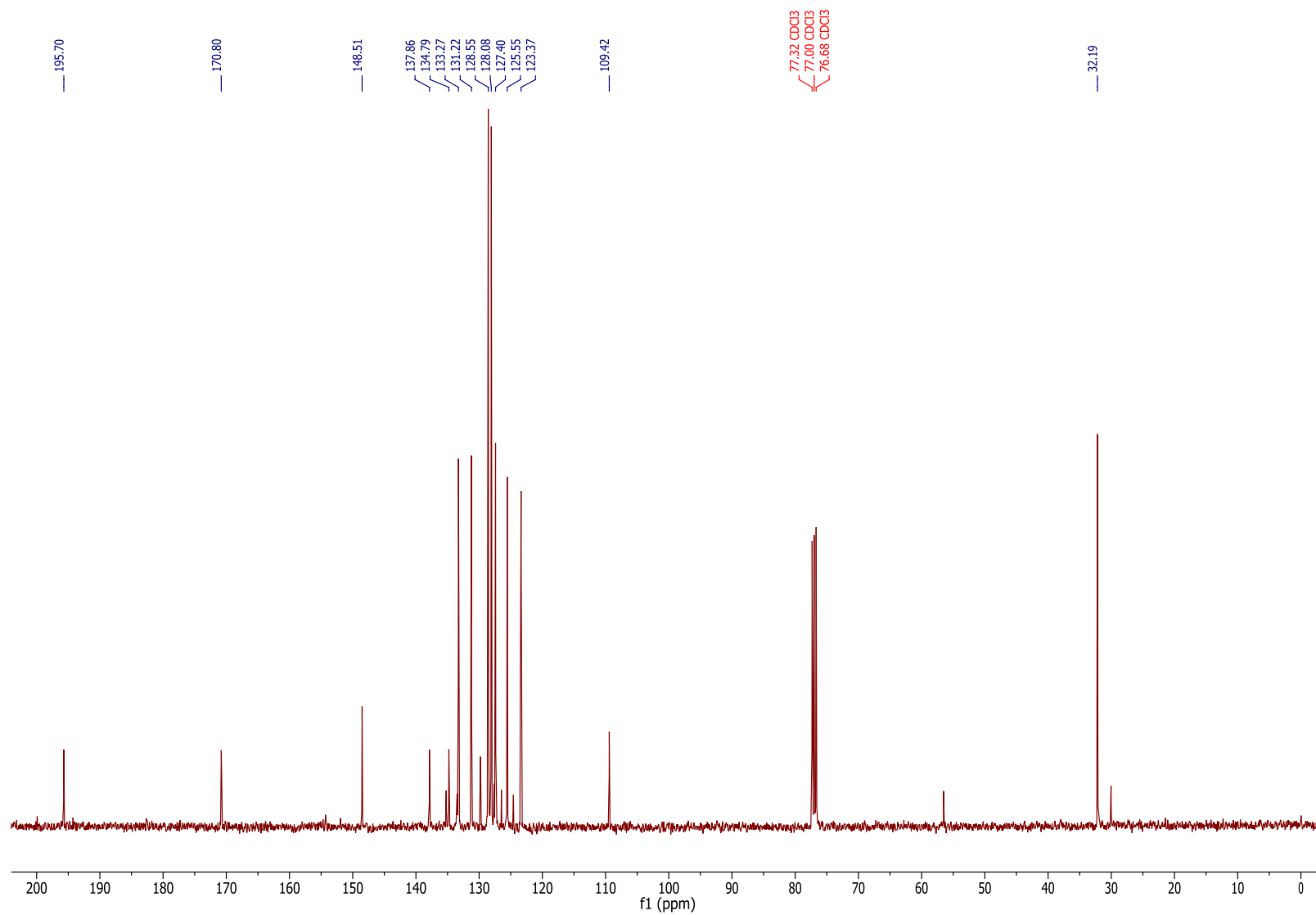


Exist an equilibrium ceto-enolic

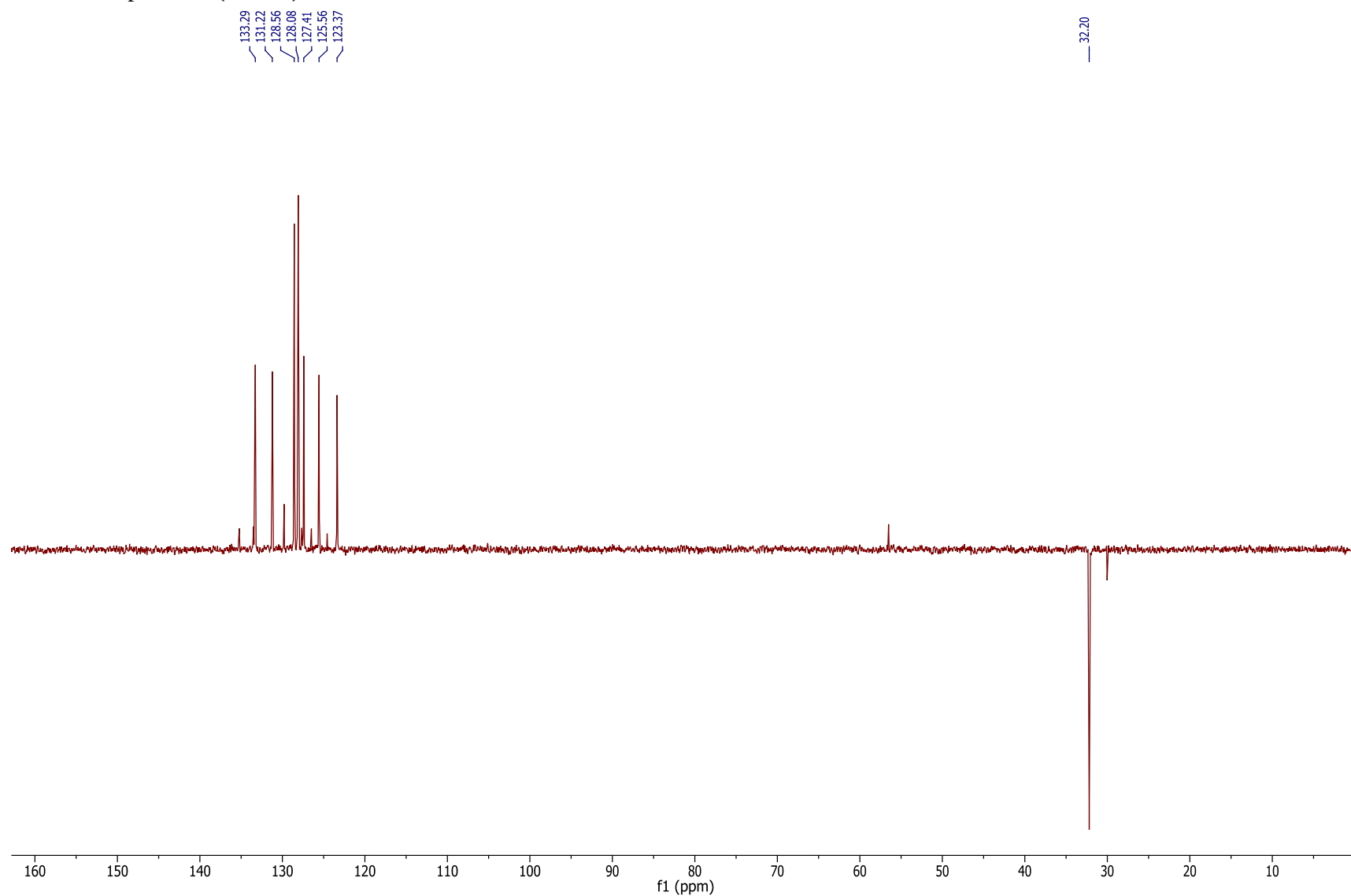
^1H NMR /Compound **1** (CDCl_3) 400MHz



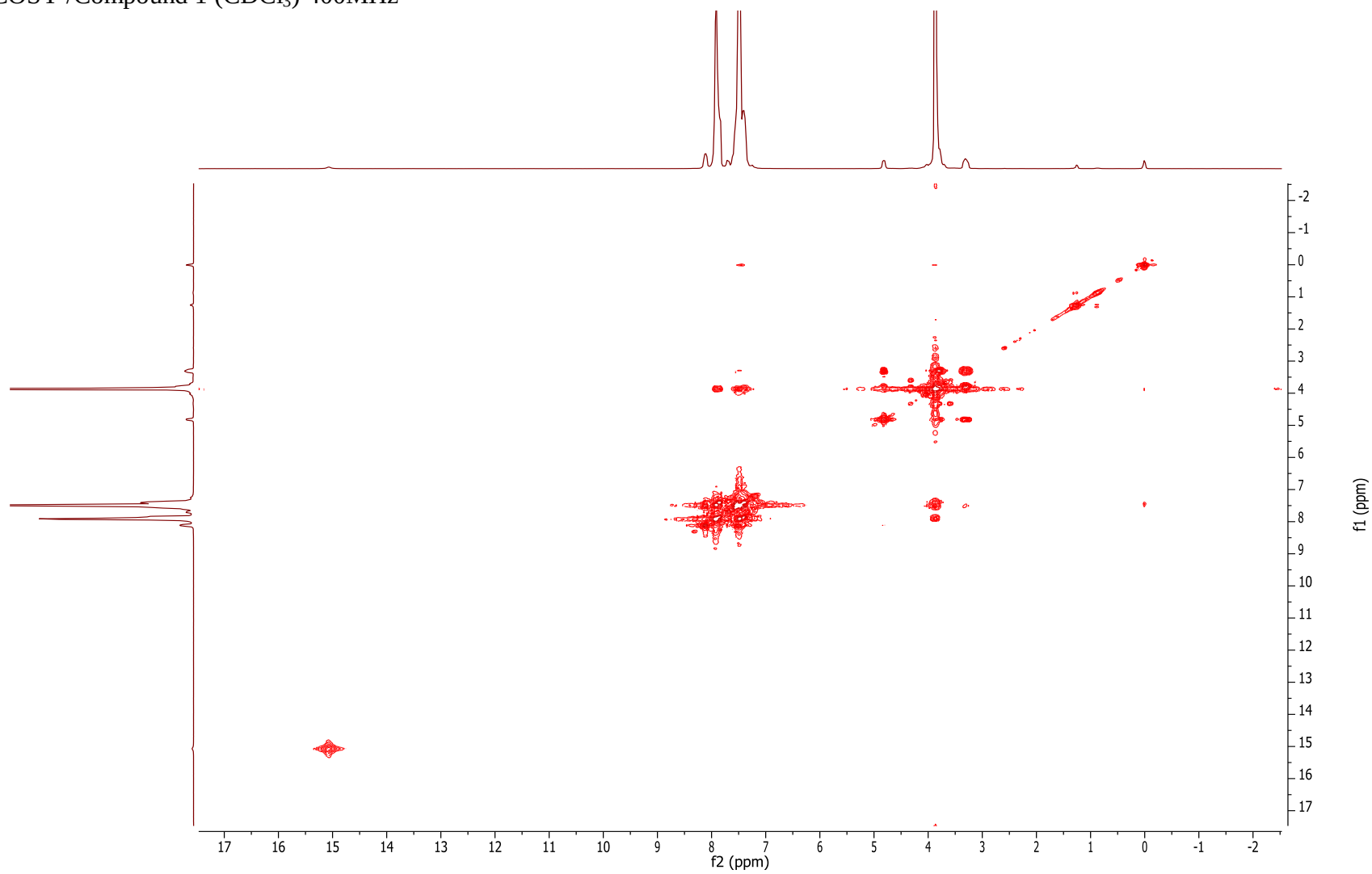
^{13}C NMR /Compound **1** (CDCl_3) 100MHz



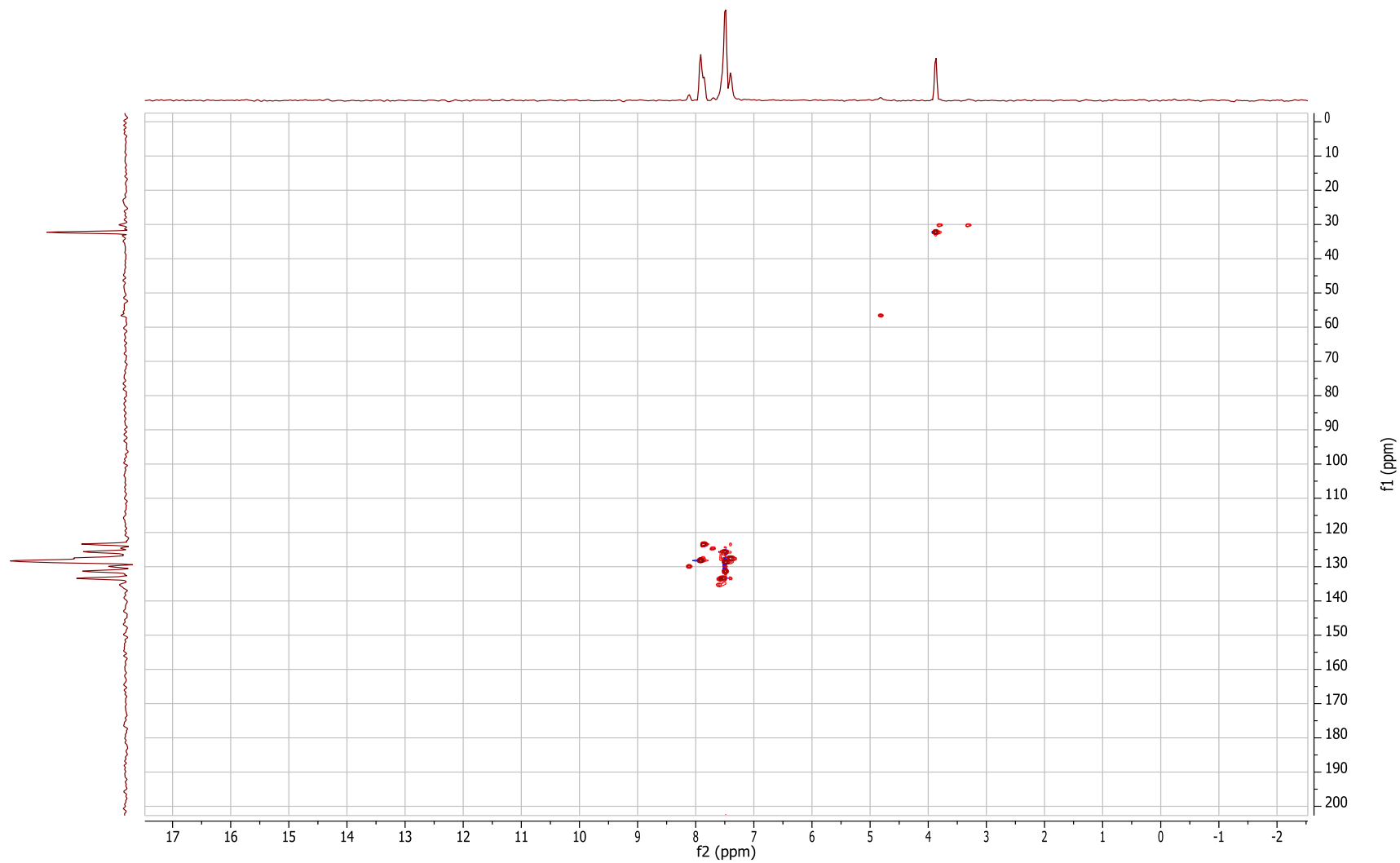
DEPT /Compound 1 (CDCl₃) 100MHz



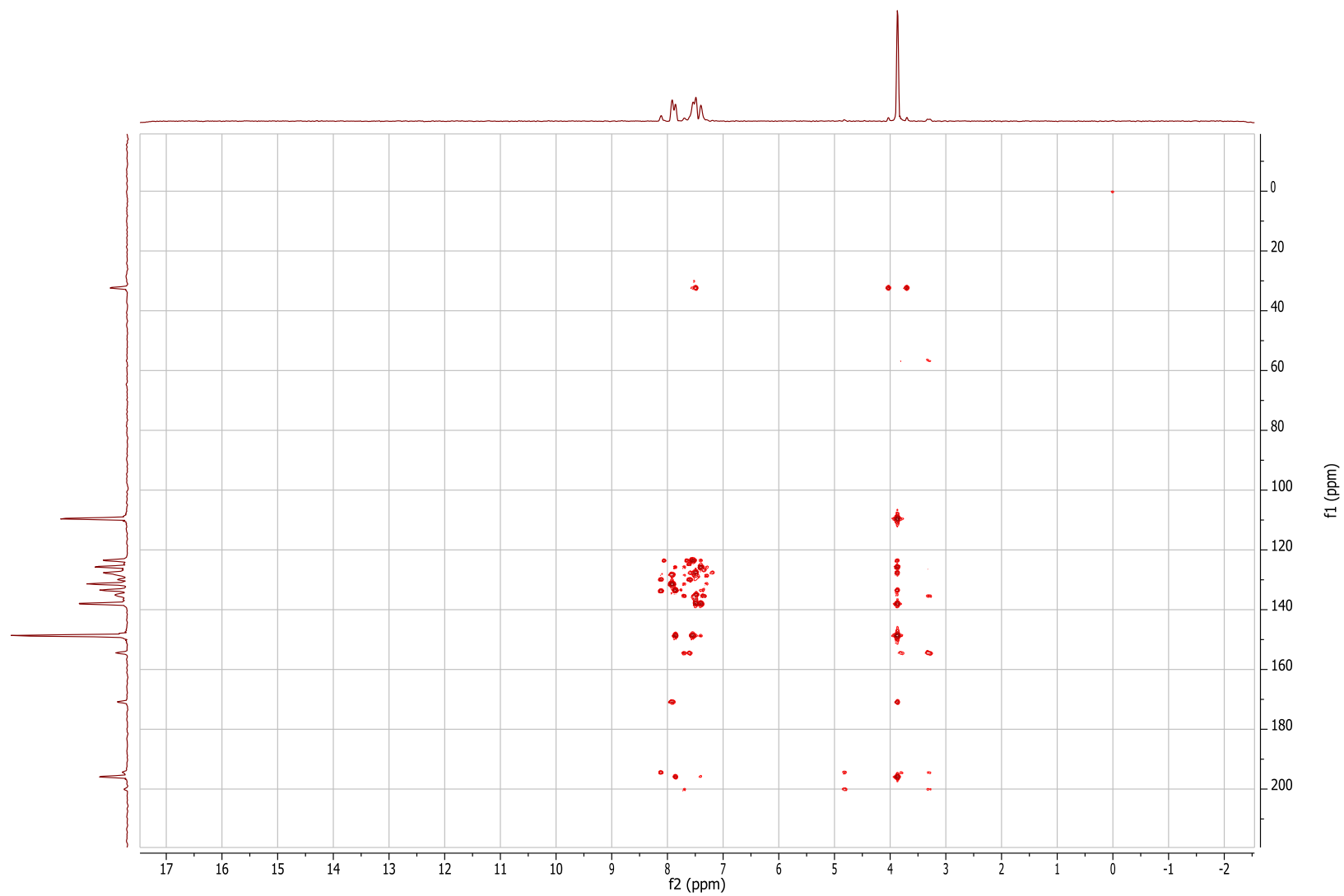
COSY /Compound 1 (CDCl₃) 400MHz



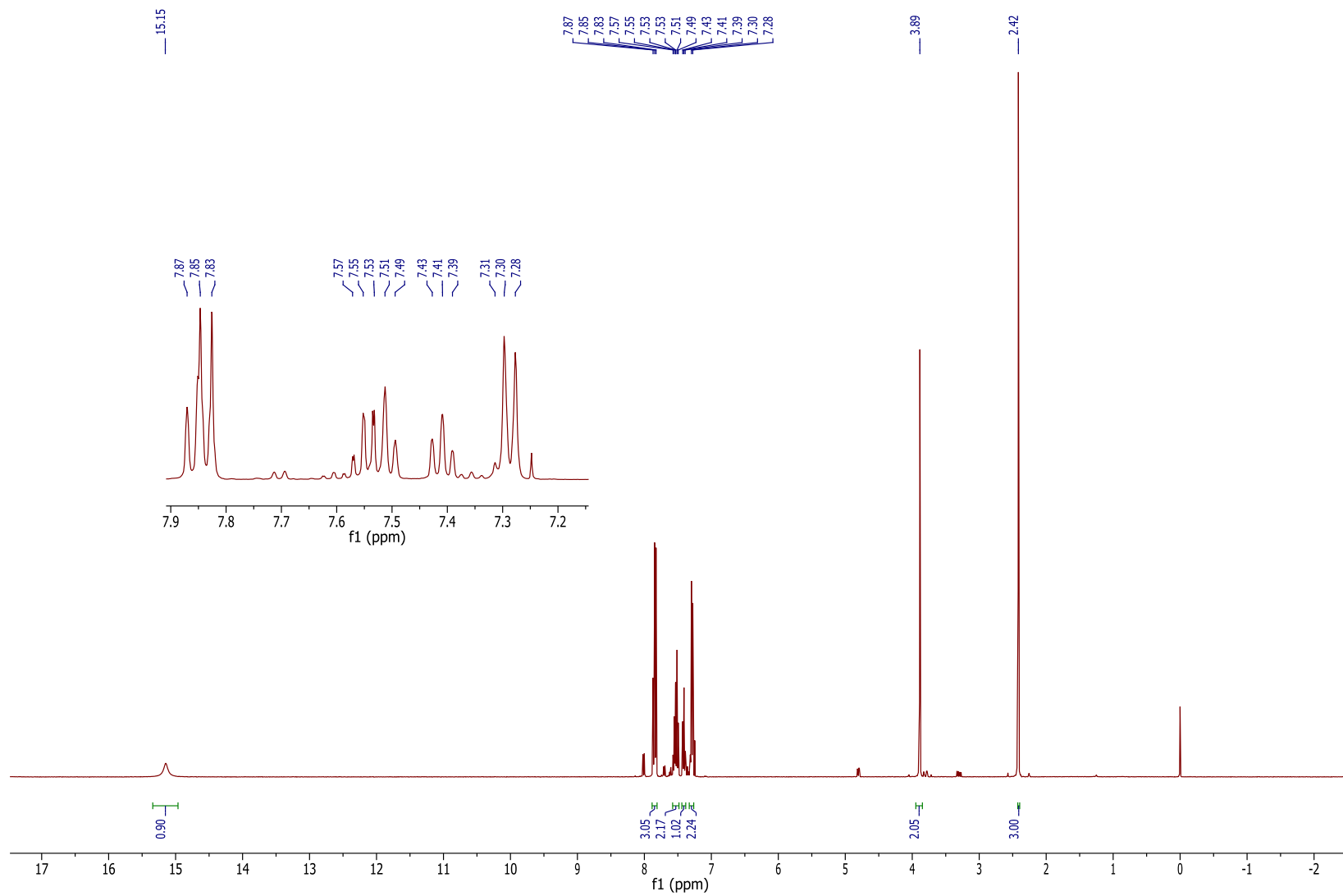
HSQC /Compound **1** (CDCl₃) 400MHz



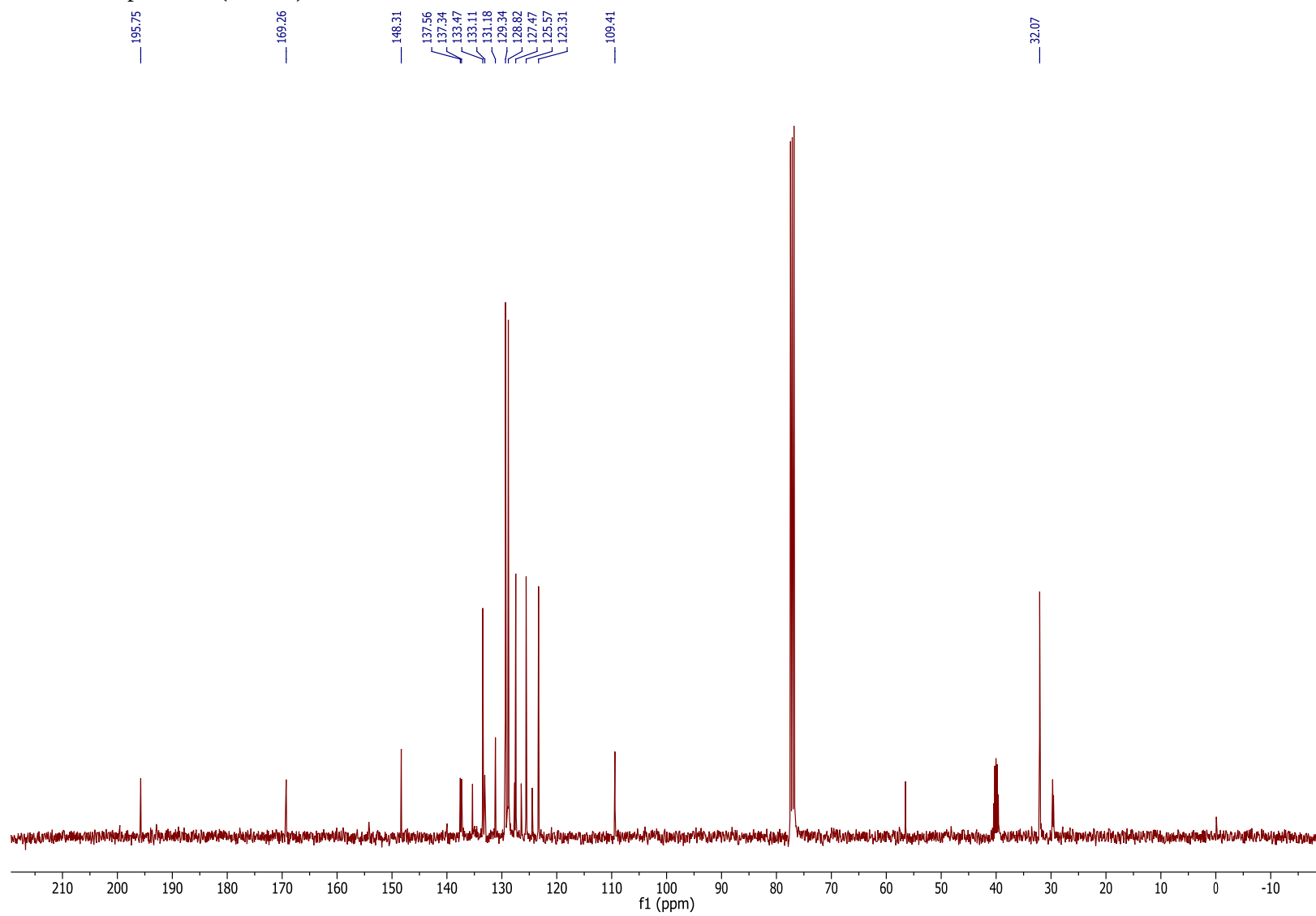
HMBC /Compound **1** (CDCl₃) 400MHz



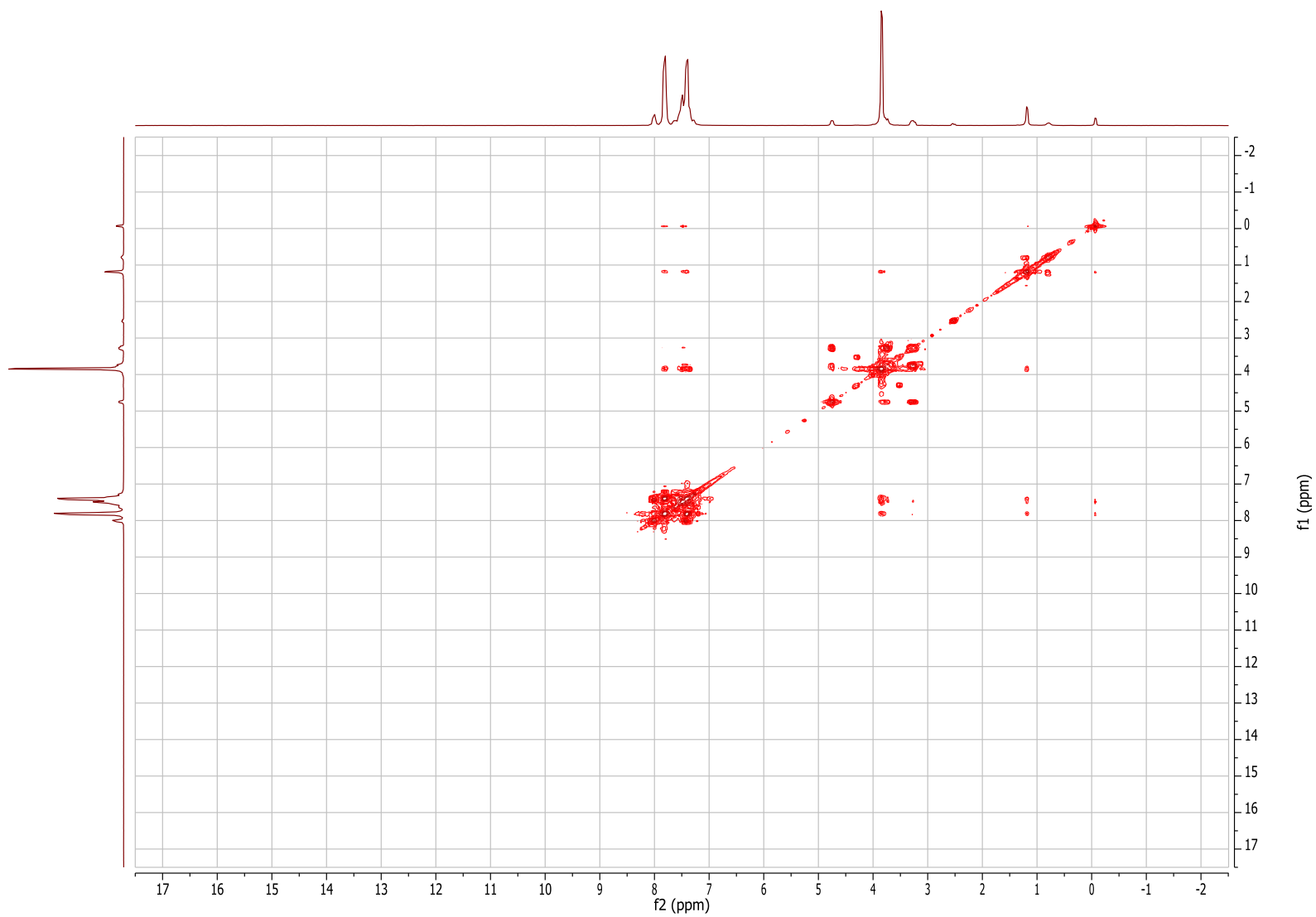
^1H NMR /Compound 2 (CDCl_3) 400MHz



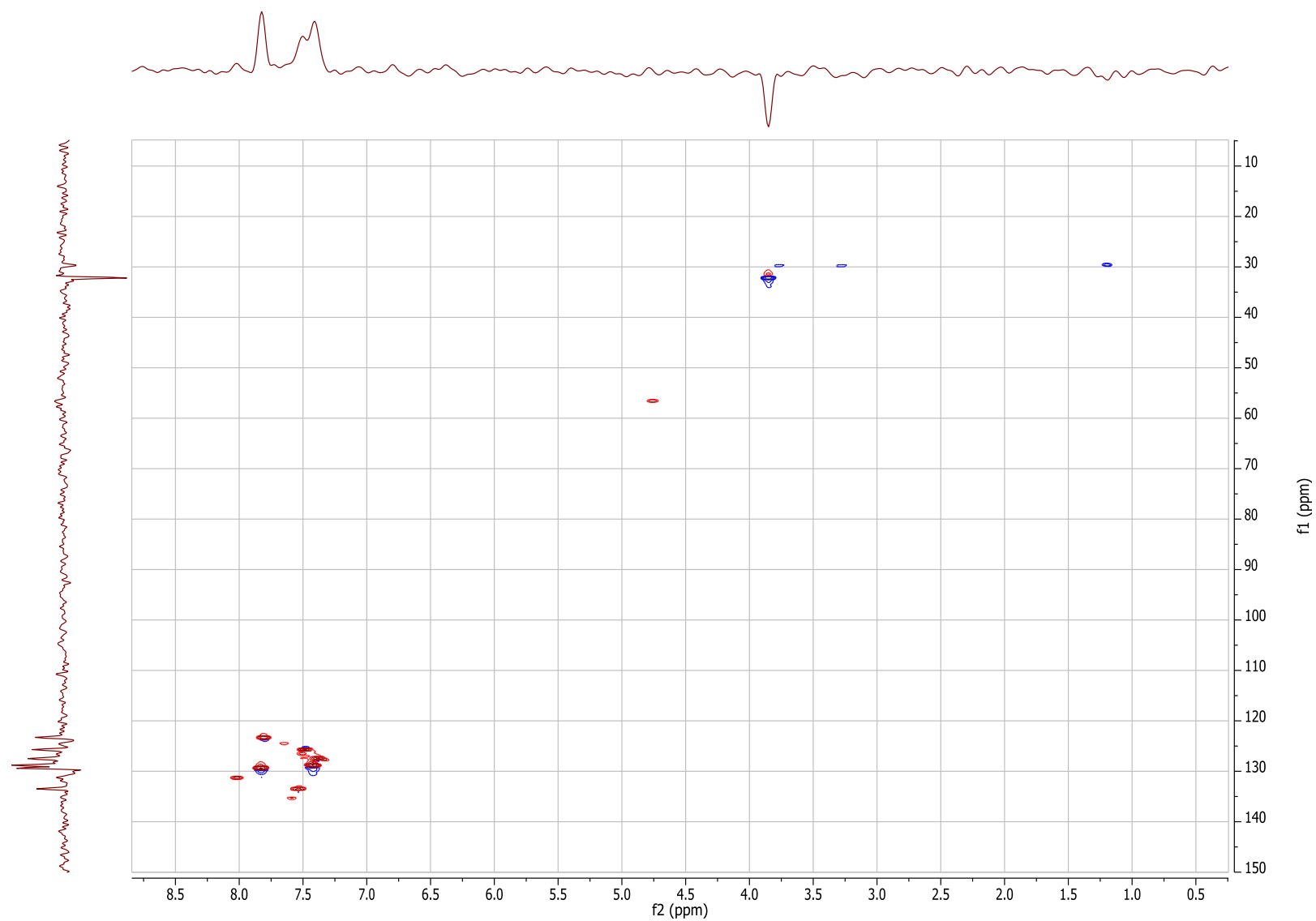
^{13}C NMR /Compound 2 (CDCl_3) 100MHz



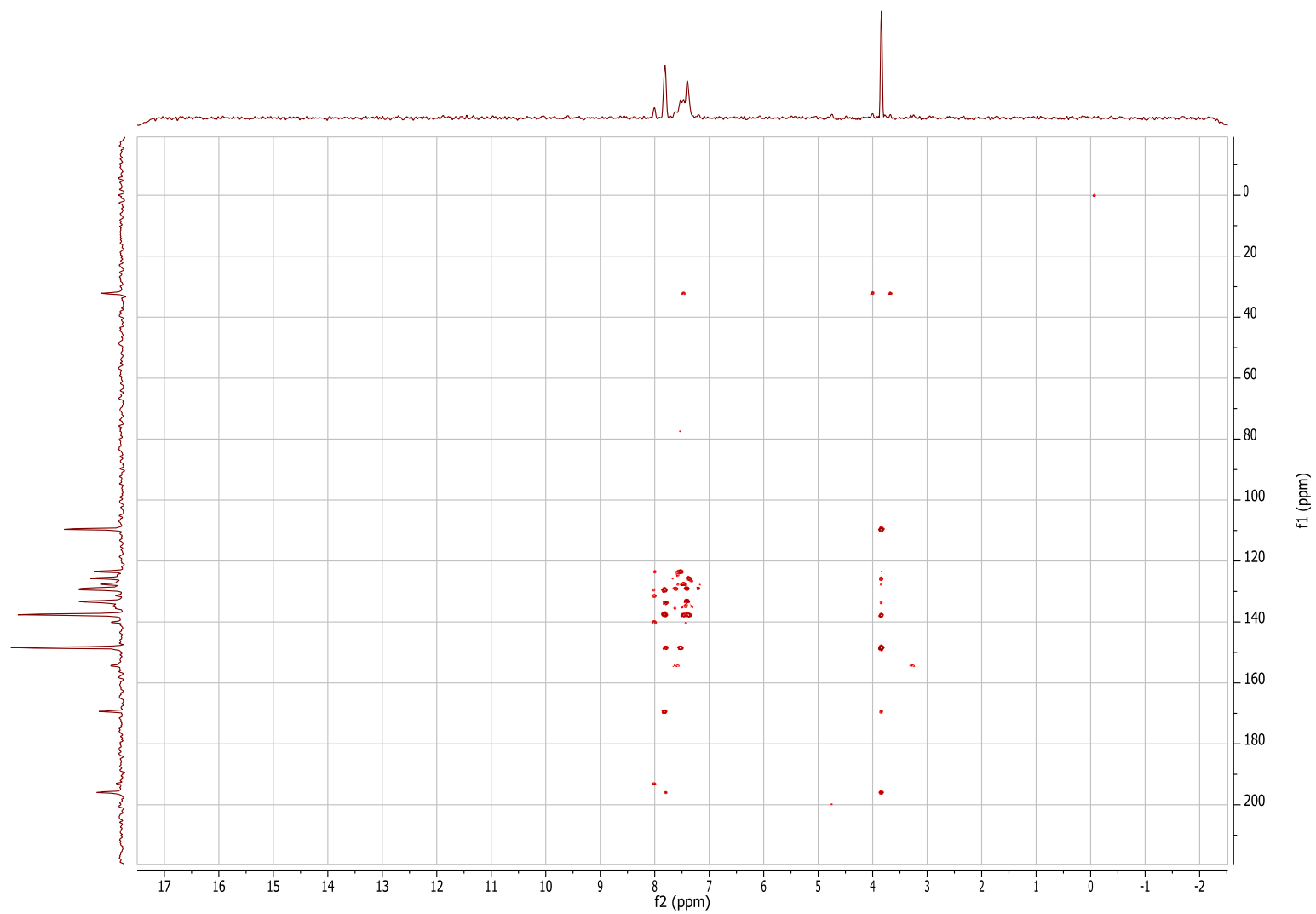
COSY /Compound 2 (CDCl₃) 400MHz



HSQC/Compound 2 (CDCl₃) 400MHz



HMBC/Compound 2 (CDCl₃) 400MHz



Elemental Composition Compound 2

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez139

Date : 29-Oct-2013 17:35

Sample: 2013 LC1-ME

Note : -luis-velasco

Inlet : Direct

Ion Mode : FAB+

RT : 5.53 min

Scan#: 14

Elements : C 40/0, H 58/0, O 6/1, Cl 3/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : 0.0 - 25.0

Observed m/z	Int%
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271.0522	100.0
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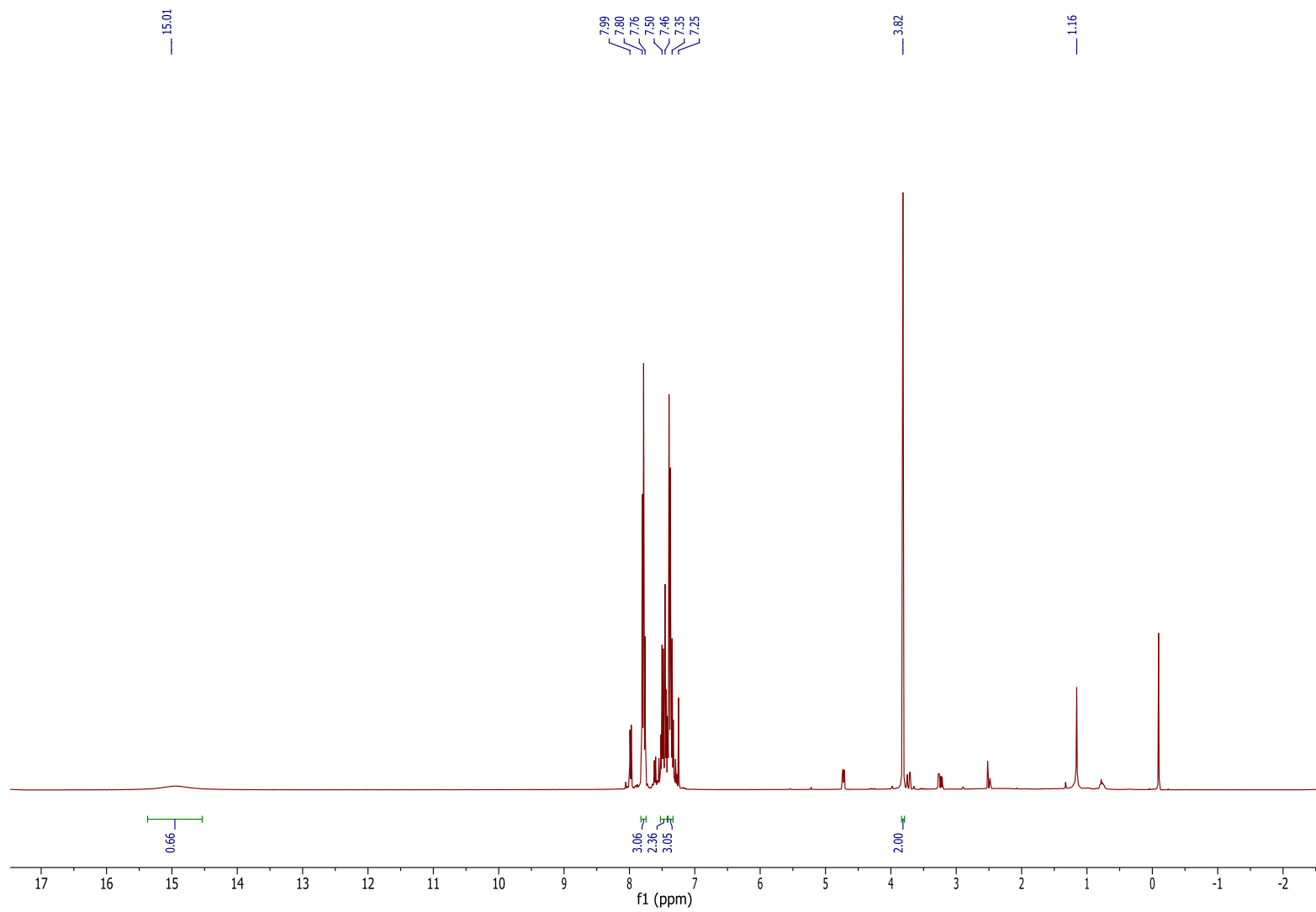
Estimated m/z	Error[ppm]
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271.0526	-1.2
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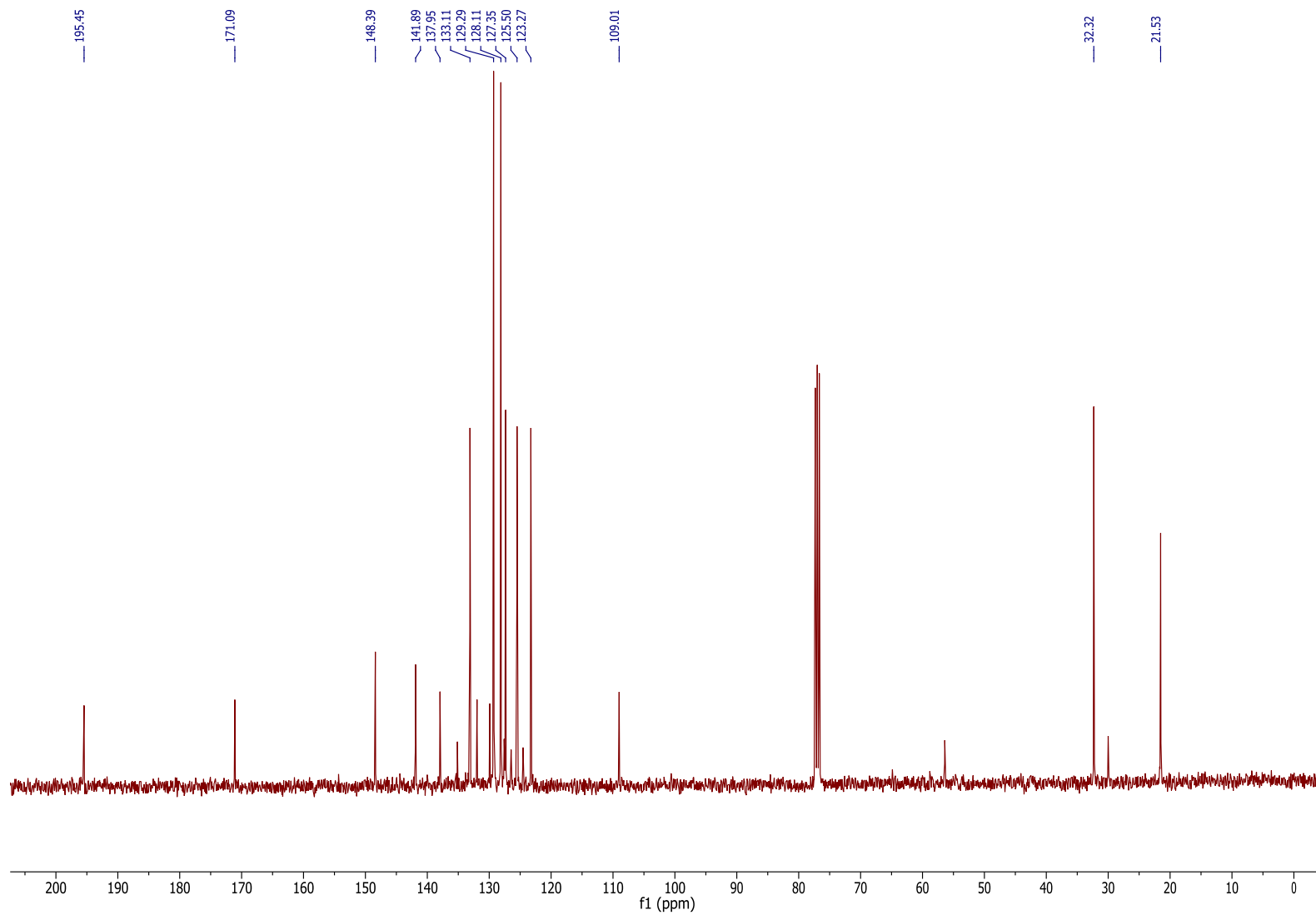
U.S.	C	H	O	Cl
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10.5	16	12	2	1
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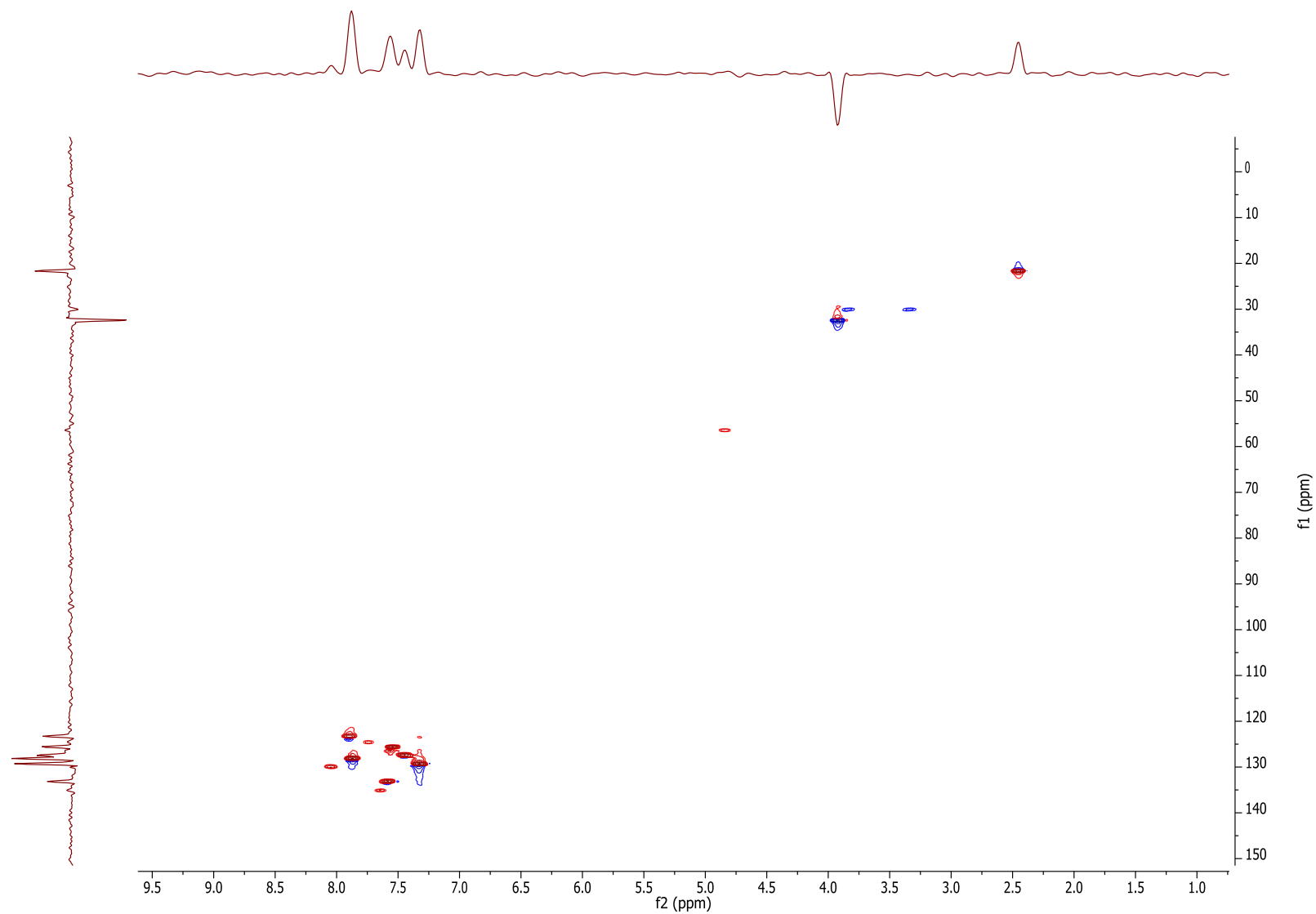
^1H NMR /Compound **3** (CDCl_3) 400MHz



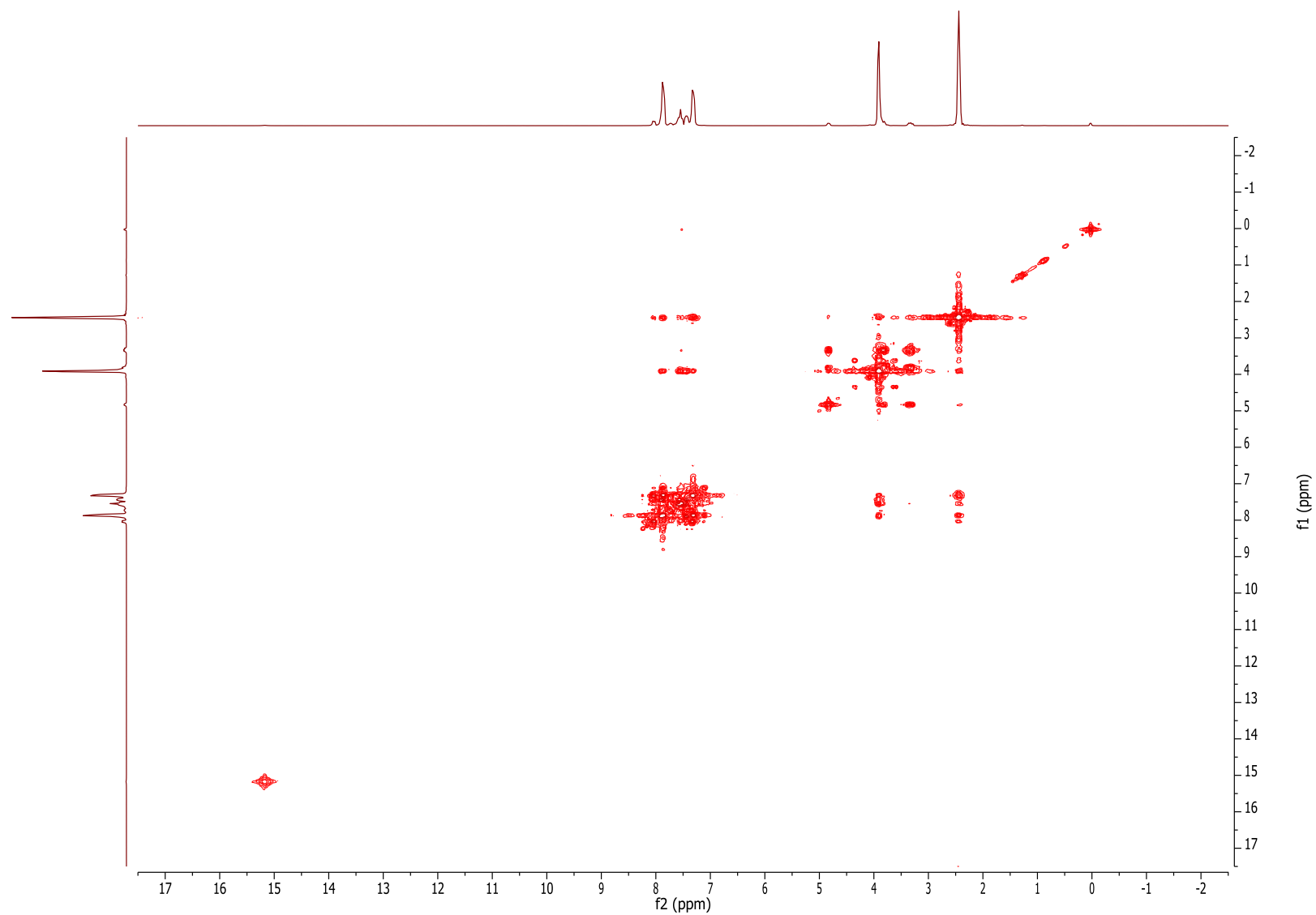
^{13}C NMR /Compound **3** (CDCl_3) 100MHz



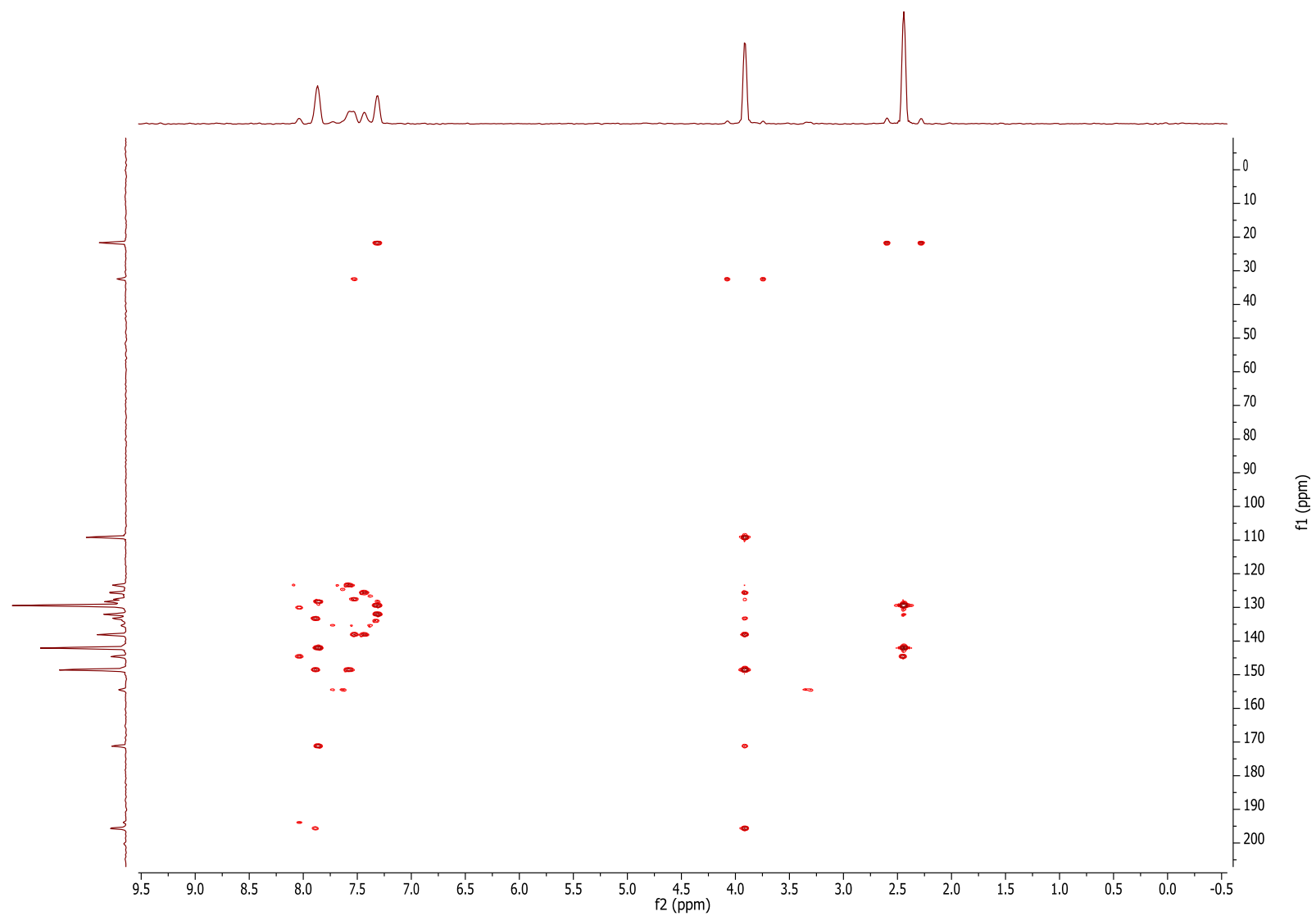
HSQC /Compound **3** (CDCl₃) 400MHz



COSY /Compound **3** (CDCl₃) 400MHz



HMBC /Compound 3 CDCl₃ 400MHz



Elemental Composition Compound 3

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez062

Date : 14-Jun-2013 14:27

Sample: 1407 C3Me

Note : -luis-velasco

Inlet : Direct

Ion Mode : FAB+

RT : 5.78 min

Scan#: (14,16)

Elements : C 40/0, H 49/0, O 9/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : 4.0 - 12.0

Observed m/z

Int%

251.1079

100.0

Estimated m/z

Error[ppm]

U.S.

C

H

O

251.1072

+2.7

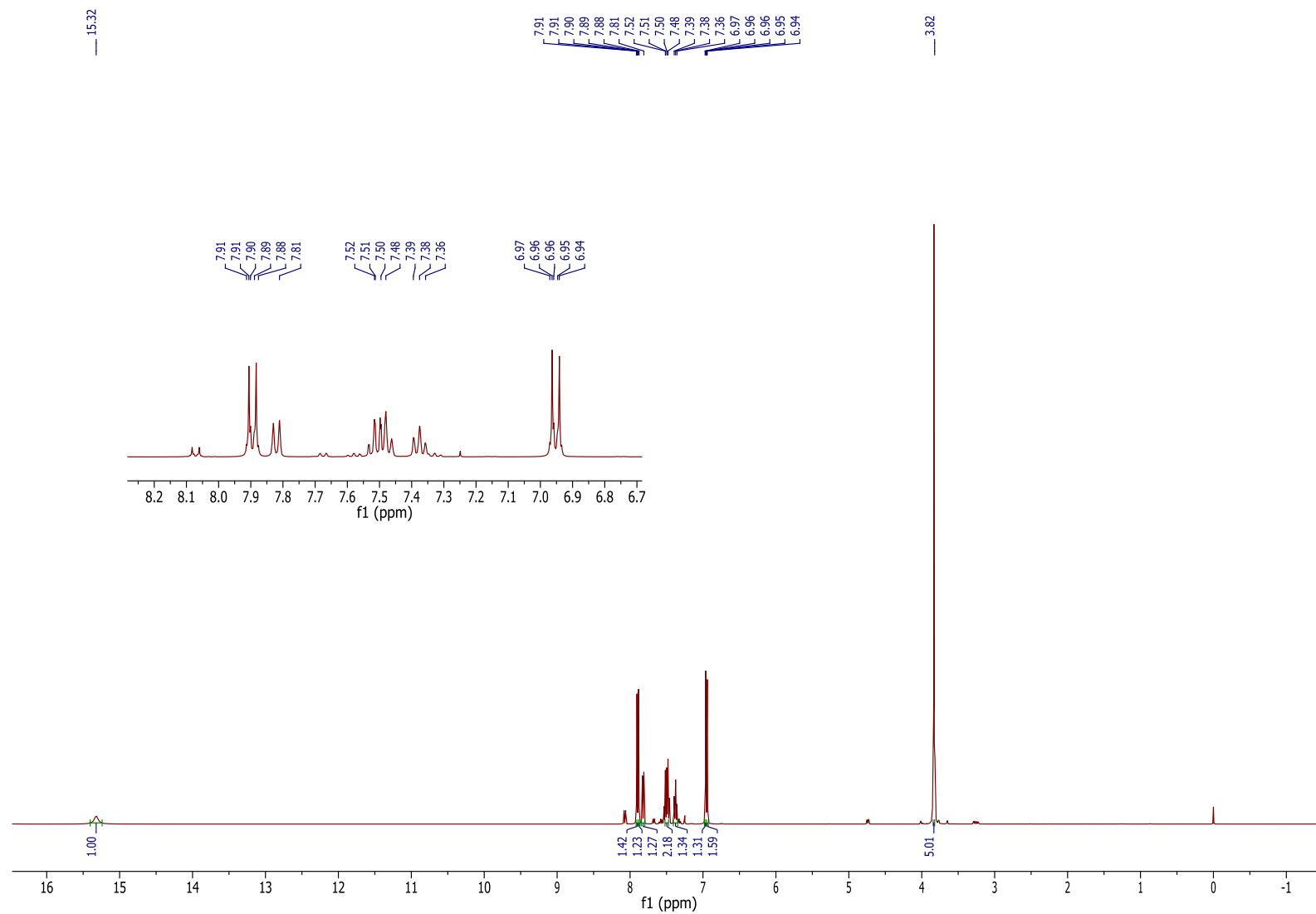
10.5

17

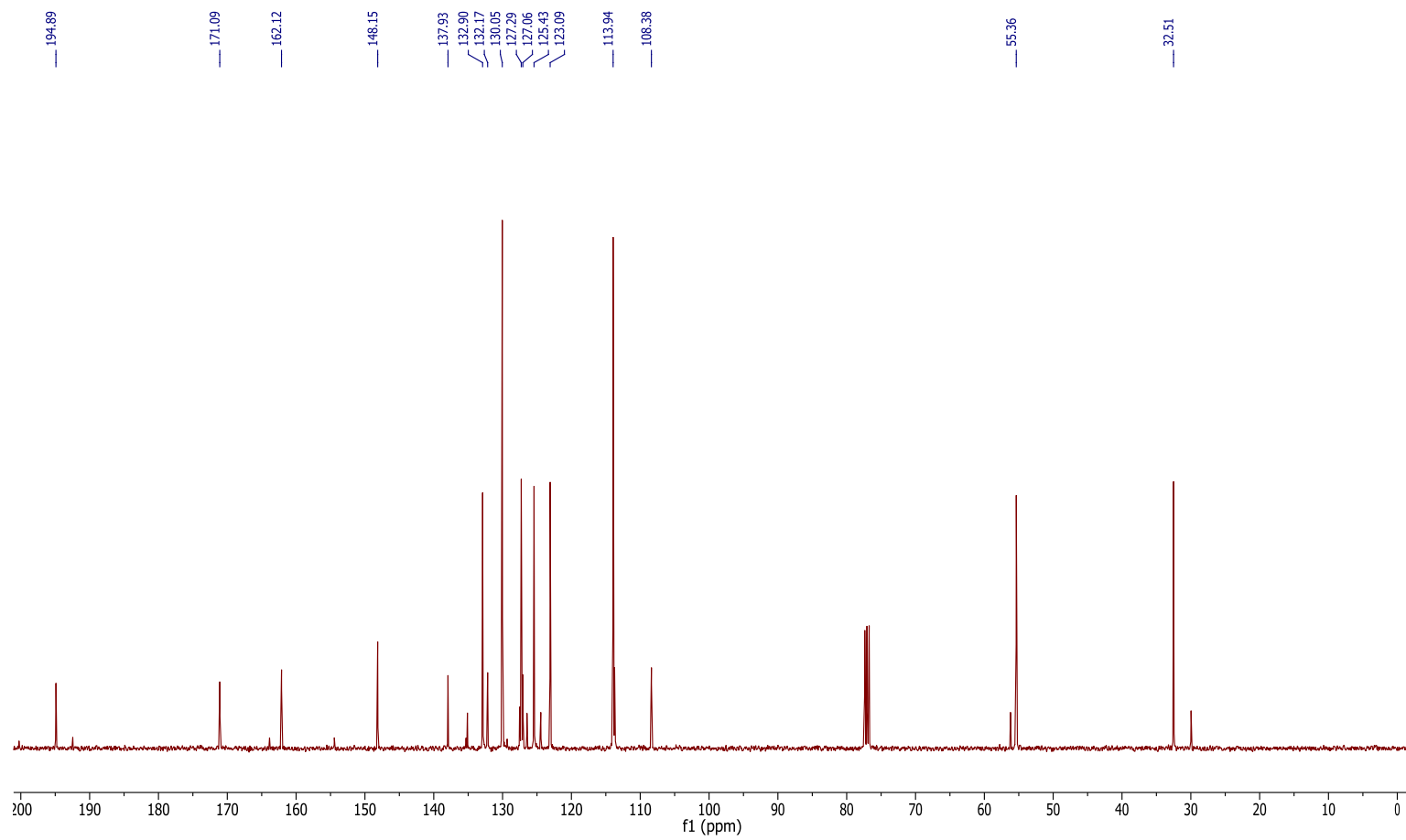
15

2

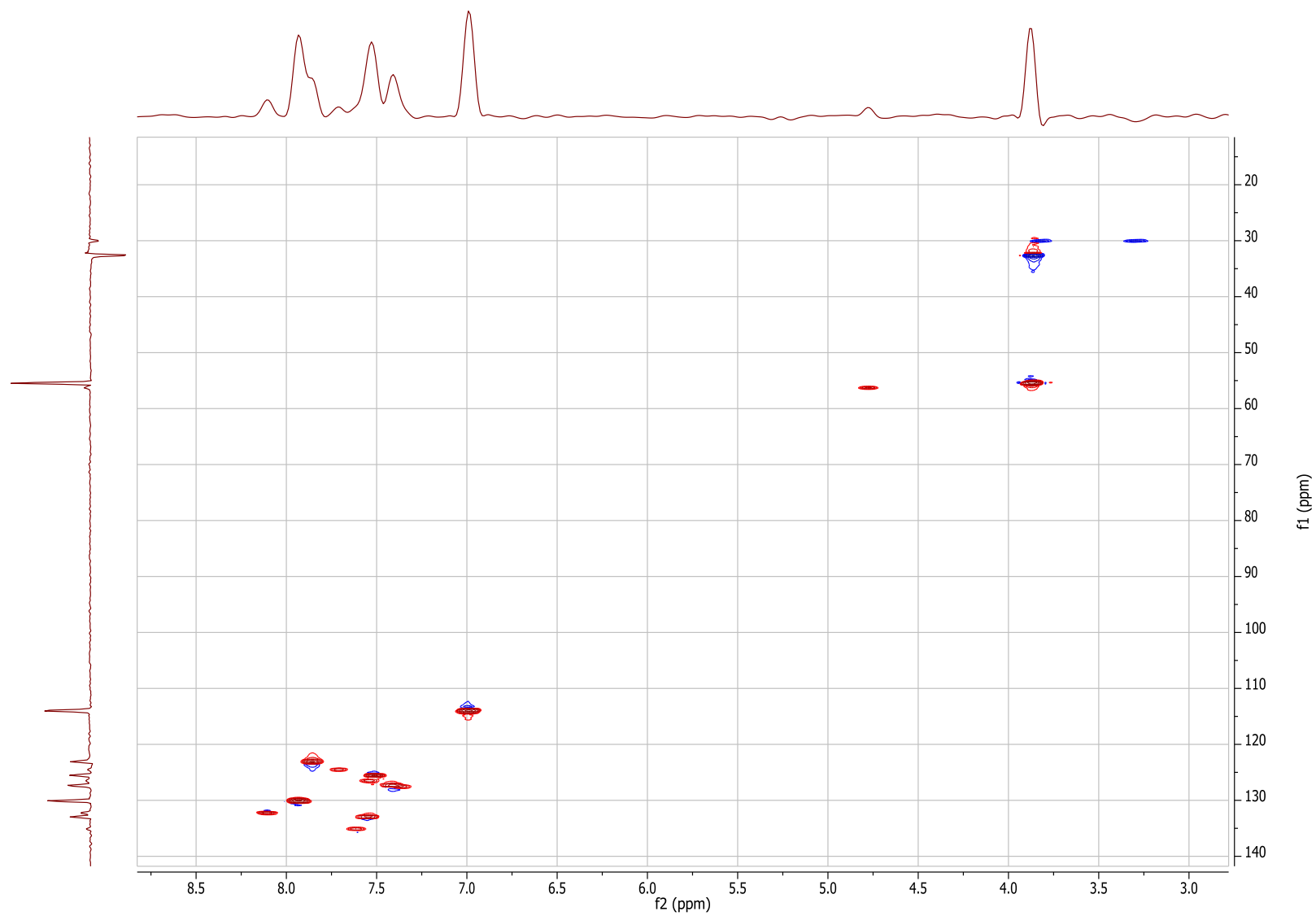
^1H NMR /Compound **4** (CDCl_3) 400MHz



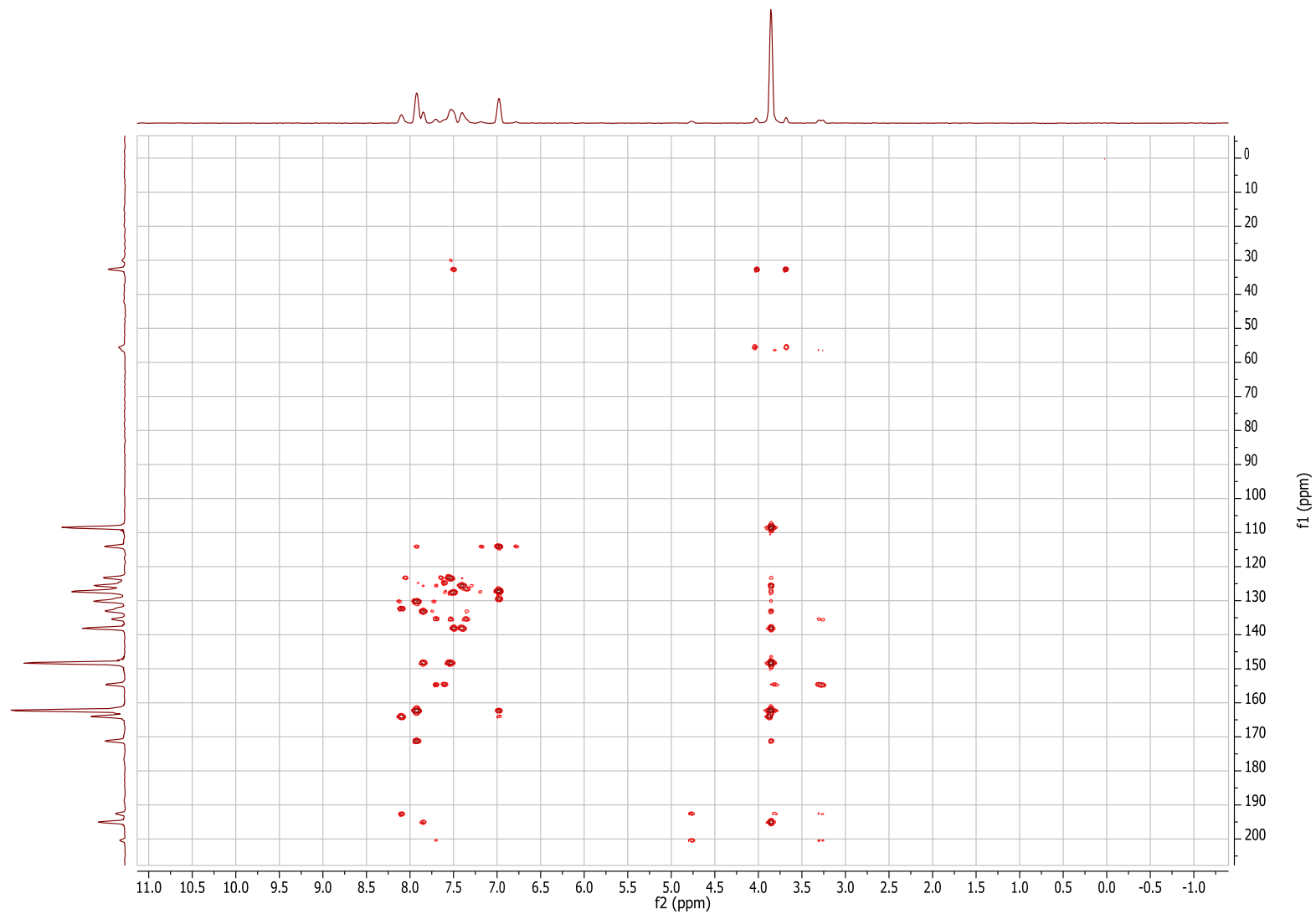
^{13}C NMR /Compound **4** (CDCl_3) 100MHz



HSQC /Compound 4 (CDCl₃) 400MHz



HMBC /Compound **4** (CDCl₃) 400MHz



Elemental Composition Compound 4

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez061

Date : 14-Jun-2013 14:12

Sample: 1408 C4OMe

Note : -luis-velasco

Inlet : Direct

Ion Mode : FAB+

RT : 2.89 min

Scan#: 8

Elements : C 40/0, H 49/0, O 9/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : 4.0 - 12.0

Observed m/z	Int%
267.1022	100.0

Estimated m/z	Error[ppm]	U.S.	C	H	O
267.1021	+0.3	10.5	17	15	3

Elemental Composition of fragment C₃₂H₂₂O₄Fe [M⁺] Compound 1a

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez047

Date : 27-Aug-2012 17:07

Sample: 2017 LC8NFe

Note : Luis-Velasco

Inlet : Direct

Ion Mode : FAB+

RT : 5.30 min

Scan#: (17,31)

Elements : C 40/0, H 49/0, O 10/1, Fe 5/1

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : -0.5 - 35.0

Observed m/z	Int%
526.0877	100.0

Estimated m/z	Error[ppm]	U.S.	C	H	O	Fe
526.0867	+1.8	22.5	32	22	4	1

Elemental Composition of fragment $C_{32}H_{20}O_4ClFe$ [M^+] Compound **2a**

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez131 Date : 29-Oct-2013 15:52
 Sample: 2009 FeLC8Cl-ME
 Note : -luis-velasco
 Inlet : Direct Ion Mode : FAB+
 RT : 0.75 min Scan#: (3,6)
 Elements : C 40/0, H 58/0, O 6/1, Cl 3/0, Fe 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1
 Unsaturation (U.S.) : 13.0 - 25.0

Observed m/z	Int%						
594.0092	100.0						
Estimated m/z	Error[ppm]	U.S.	C	H	O	Cl	Fe
594.0088	+0.6	22.5	32	20	4	2	1

Elemental Composition of fragment $C_{34}H_{26}O_4Fe$ [M^+] Compound **3a**

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez133 Date : 29-Oct-2013 16:17
 Sample: 2010 FeLC8Me-ME
 Note : -luis-velasco
 Inlet : Direct Ion Mode : FAB+
 RT : 0.43 min Scan#: 3
 Elements : C 40/0, H 58/0, O 6/1, Fe 3/0
 Mass Tolerance : 1000ppm, 1mmu if m/z > 1
 Unsaturation (U.S.) : 13.0 - 25.0

Observed m/z	Int%					
554.1187	100.0					
Estimated m/z	Error[ppm]	U.S.	C	H	O	Fe
554.1180	+1.1	22.5	34	26	4	1

Elemental Composition of fragment C₃₄H₂₆O₆Fe [M⁺] Compound **4a**

[Elemental Composition]

Page: 1

Data : Dr-Cecilio-Alvarez061

Date : 14-Jun-2013 14:12

Sample: 1408 C4OMe

Note : -luis-velasco

Inlet : Direct

Ion Mode : FAB+

RT : 2.89 min

Scan#: 8

Elements : C 40/0, H 49/0, O 9/0

Mass Tolerance : 1000ppm, 1mmu if m/z > 1

Unsaturation (U.S.) : 4.0 - 12.0

Observed m/z

Int%

267.1022 100.0

Estimated m/z

Error[ppm]

U.S.

C

H

O

267.1021 +0.3

10.5

17

15

3