

New amide alkaloids from *Piper longum* fruits

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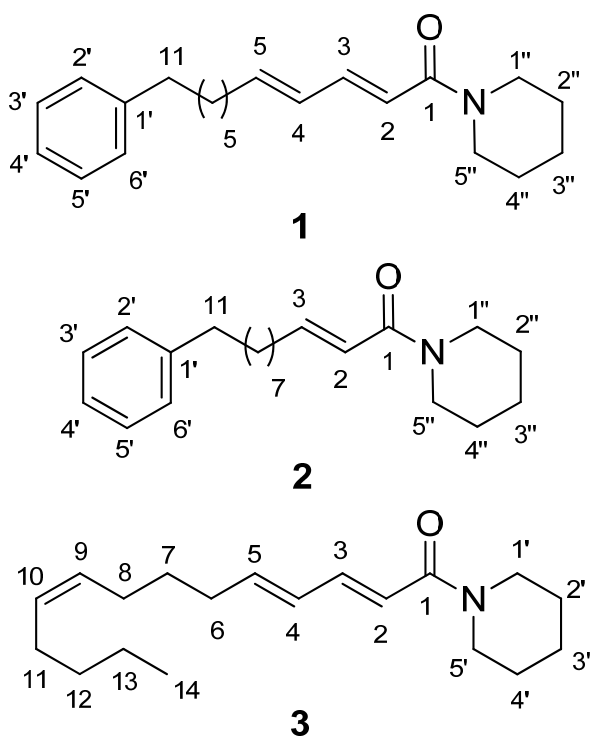
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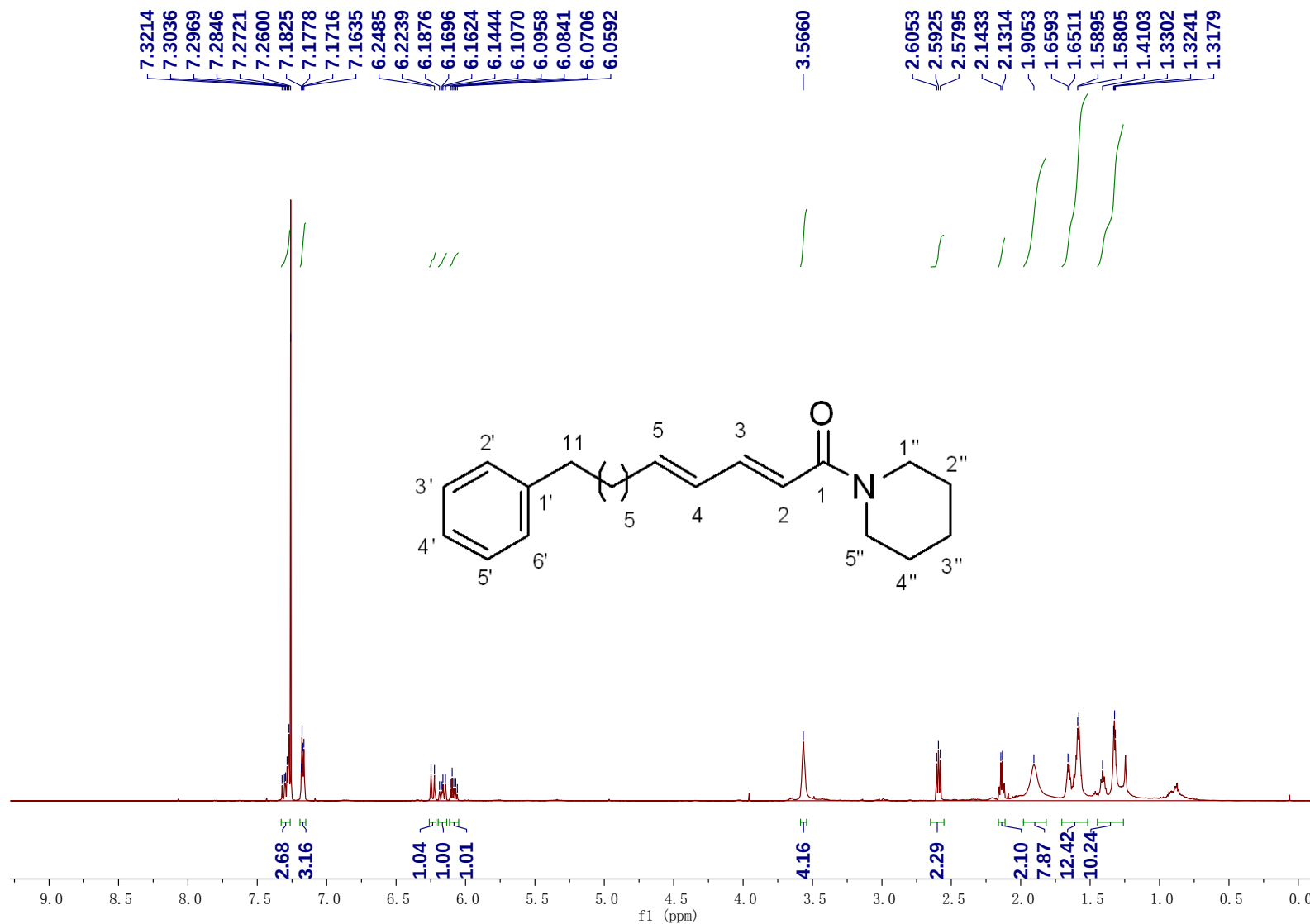
Structures of compounds 1–3

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S1 ^1H NMR (CDCl_3 , 600 MHz) spectrum of 1

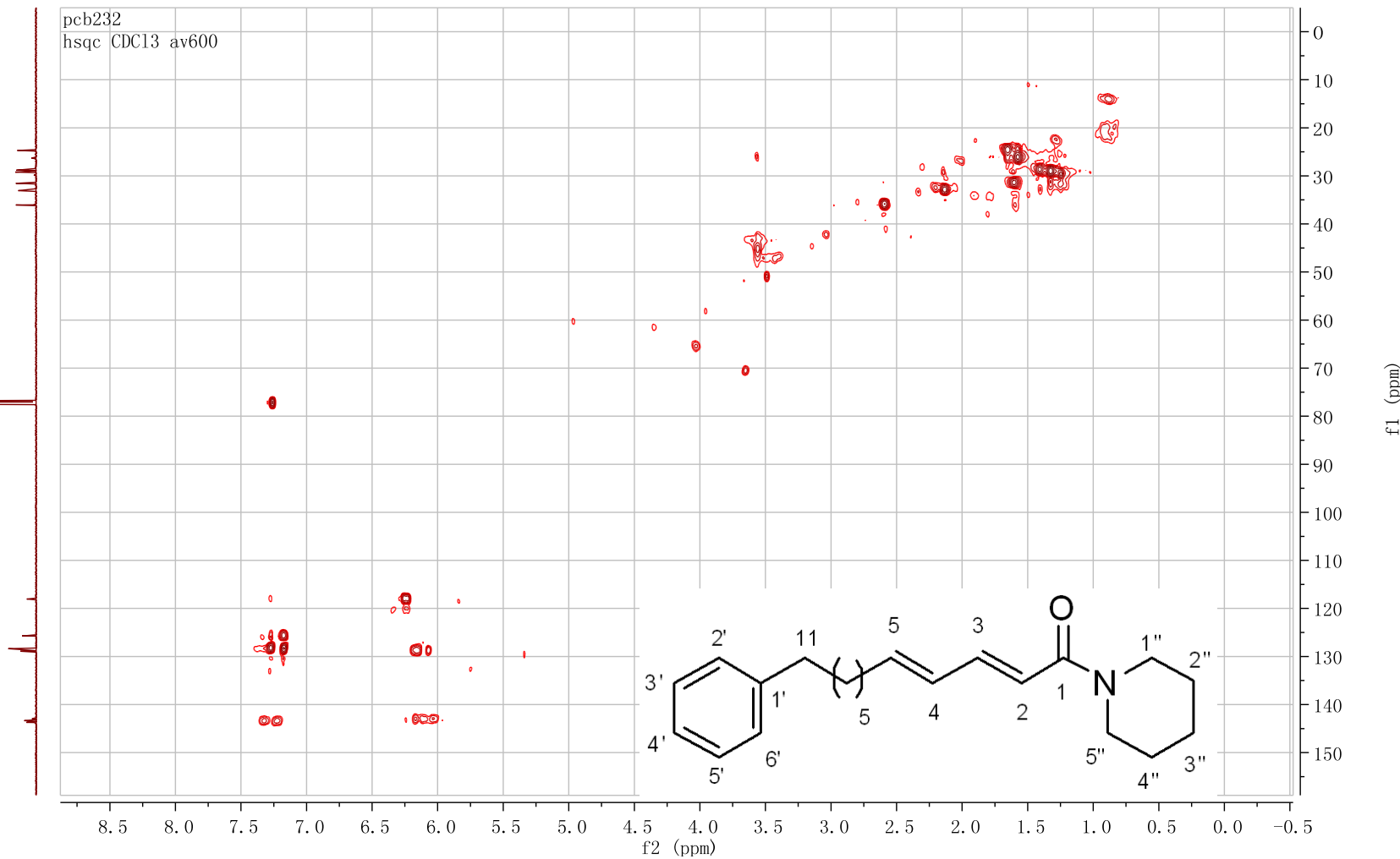


S2 ^{13}C NMR (CDCl_3 , 150 MHz) spectrum of 1

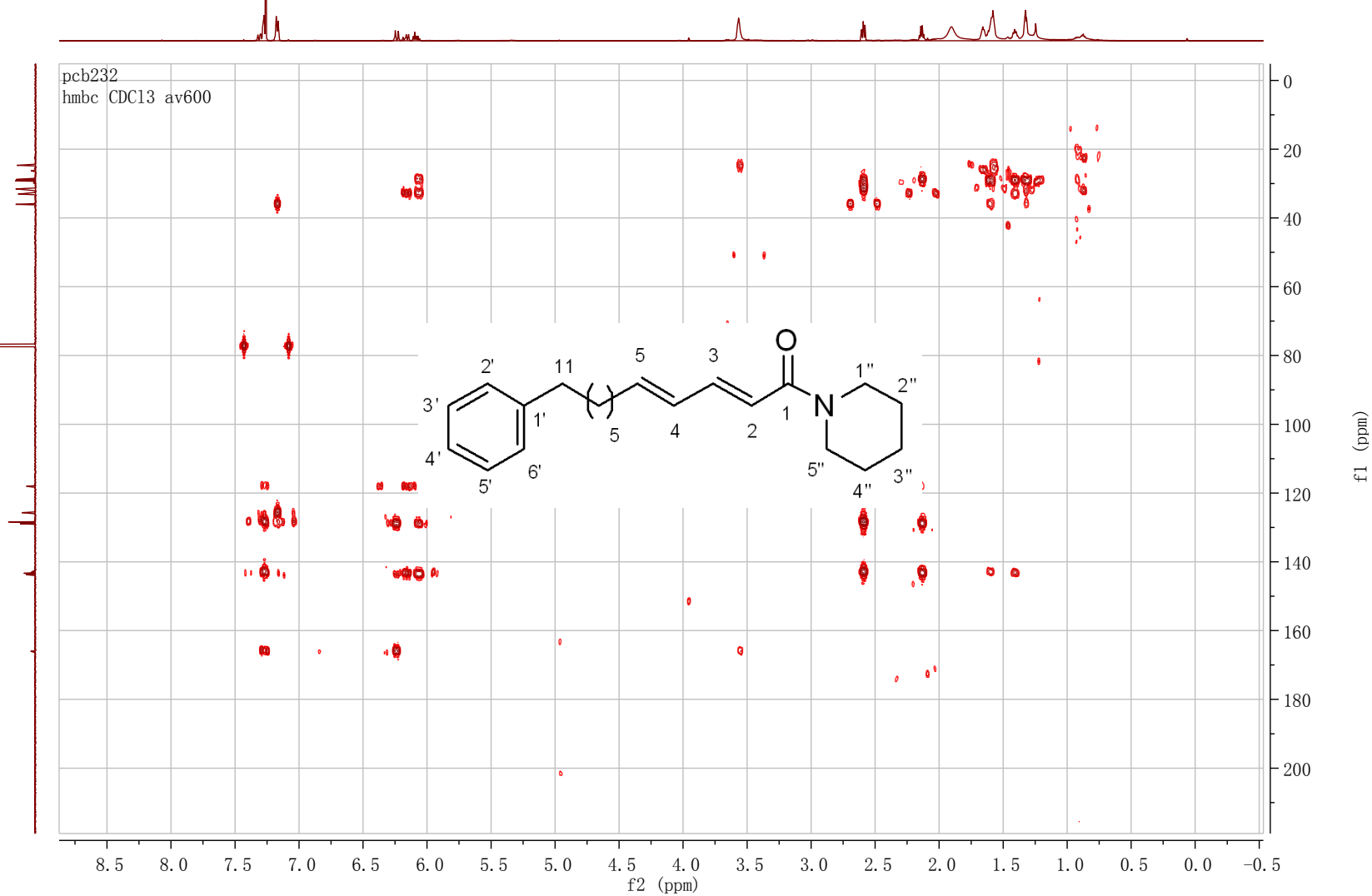


S3 HSQC spectrum of 1

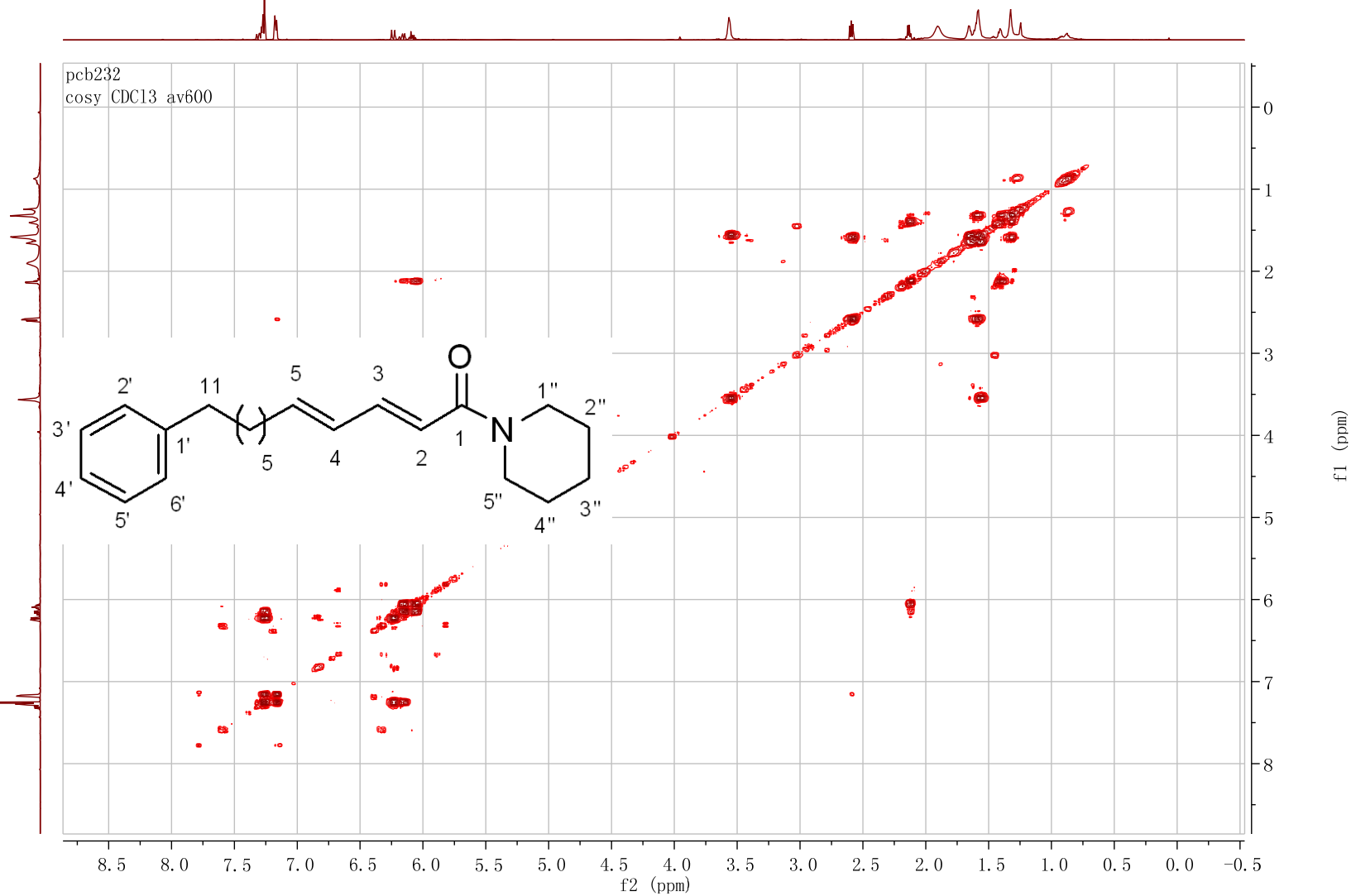
pcb232
hsqc CDC13 av600



S4 HMBC spectrum of 1



S5 ^1H - ^1H COSY spectrum of 1



Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

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

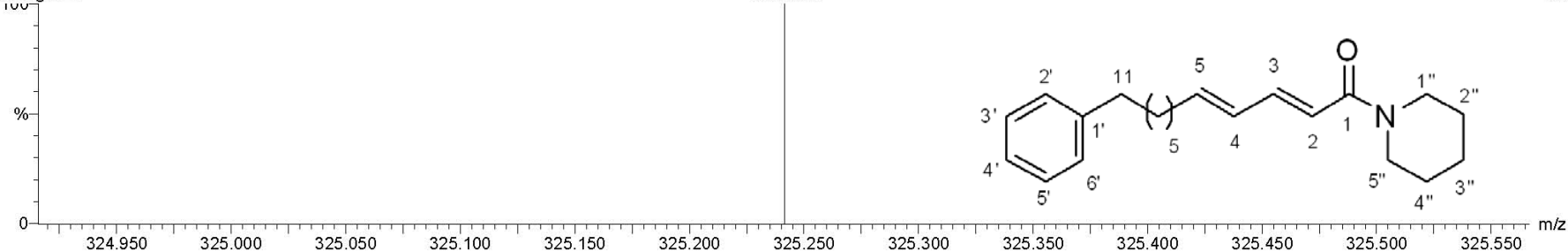
Elements Used:

C: 0-200 H: 0-400 N: 1-1 O: 0-2

pcb232

16:18:55 12-Nov-2012

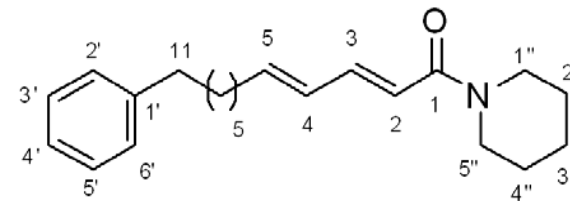
Voltage EI+



Autospec Premier

P776

199



Minimum: -10.0
Maximum: 100.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
325.2413	325.2406	0.7	2.2	8.0	5546114.0	C22 H31 N O

Display Report

Analysis Info

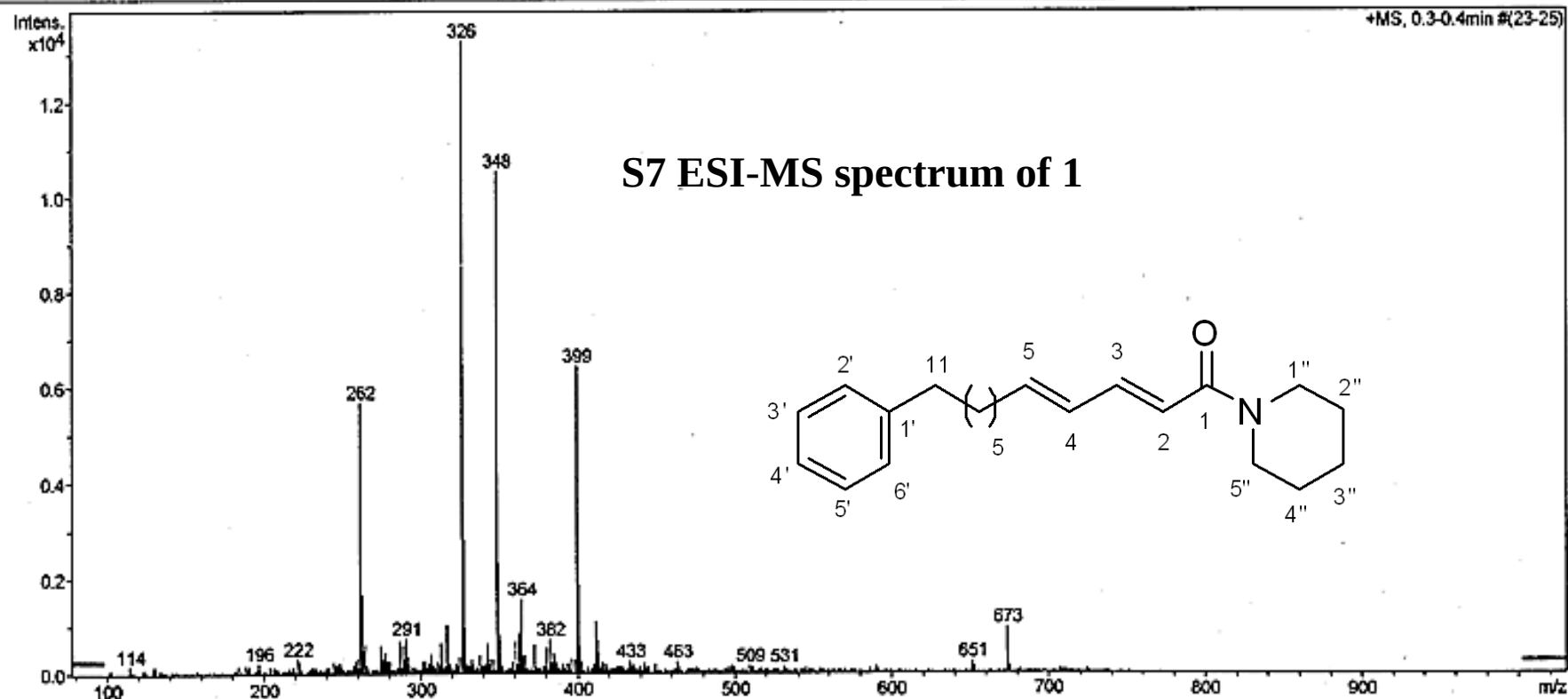
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Method ms_plservice.m
Sample Name pcb23-2
Comment

Acquisition Date 10/24/2012 4:26:39 PM

Operator
Instrument Bruker
HCT

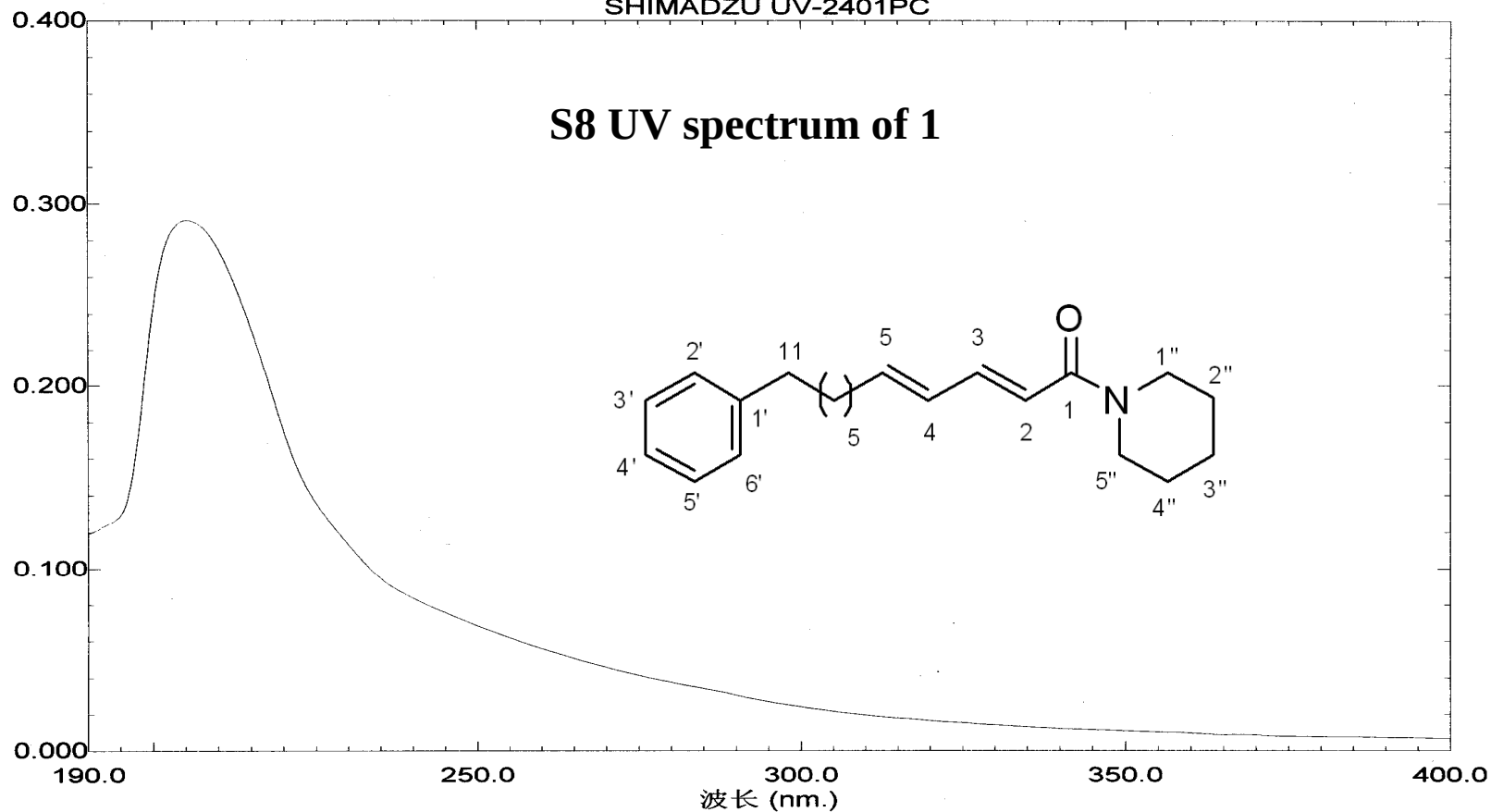
Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
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Capillary Exit	10.0 Volt	Skimmer	40.0 Volt	Trap Drive	34.4
Accumulation Time	100000 μ s	Averages	5 Spectra	Auto MS/MS	off



S8 UV spectrum of 1

Abs



文件名: 13100904

样品名称: PCB232

创建于: 15:57 13-10-09

数据: 原始

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.2

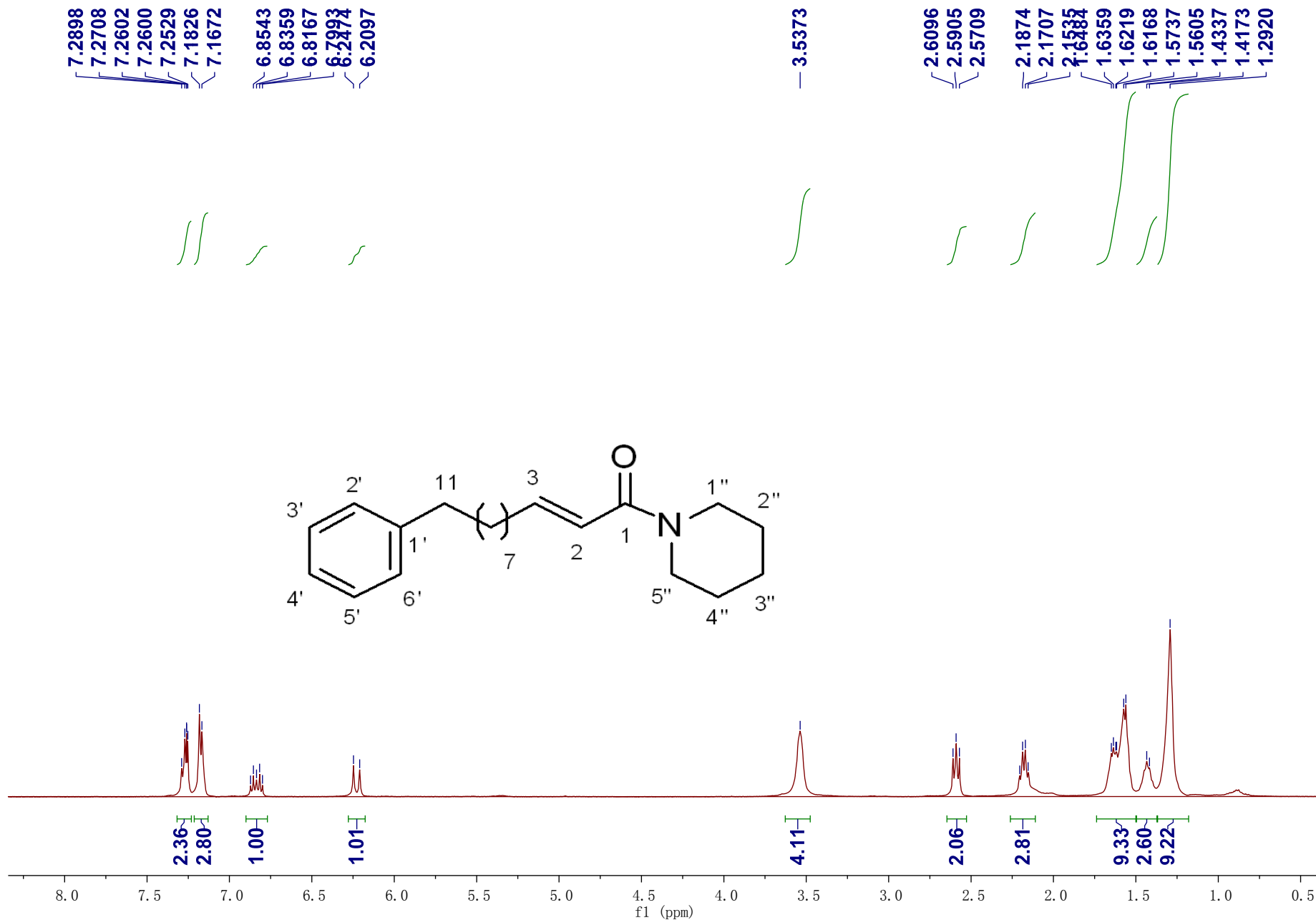
13100904

样品浓度: 0.0320毫克/毫升

溶剂: 甲醇

否.	波长 (nm.)	Abs.
1	205.40	0.2908

S9 ¹H NMR (CDCl₃, 400 MHz) spectrum of 2



S10 ^{13}C NMR (CDCl_3 , 100 MHz) spectrum of 2

— 165.85

— 146.55

— 143.02

— 128.52

— 128.34

— 125.68

— 120.16

— 77.48

— 77.16

— 76.84

— 36.09

— 32.72

— 31.64

— 29.54

— 29.48

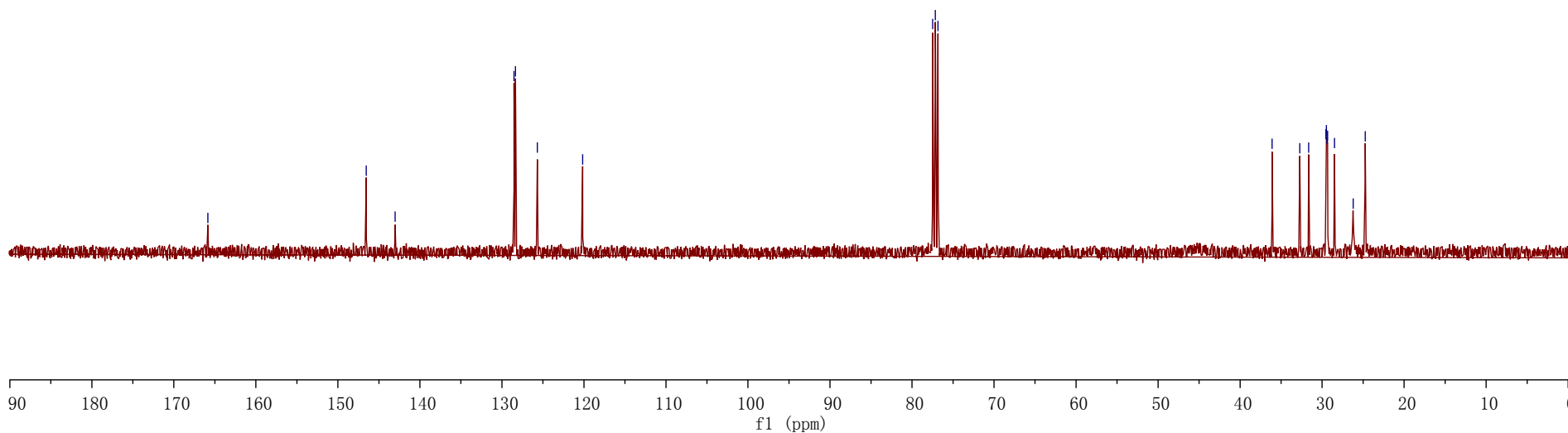
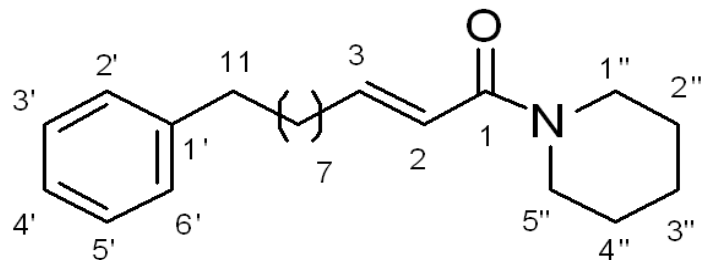
— 29.42

— 29.33

— 28.49

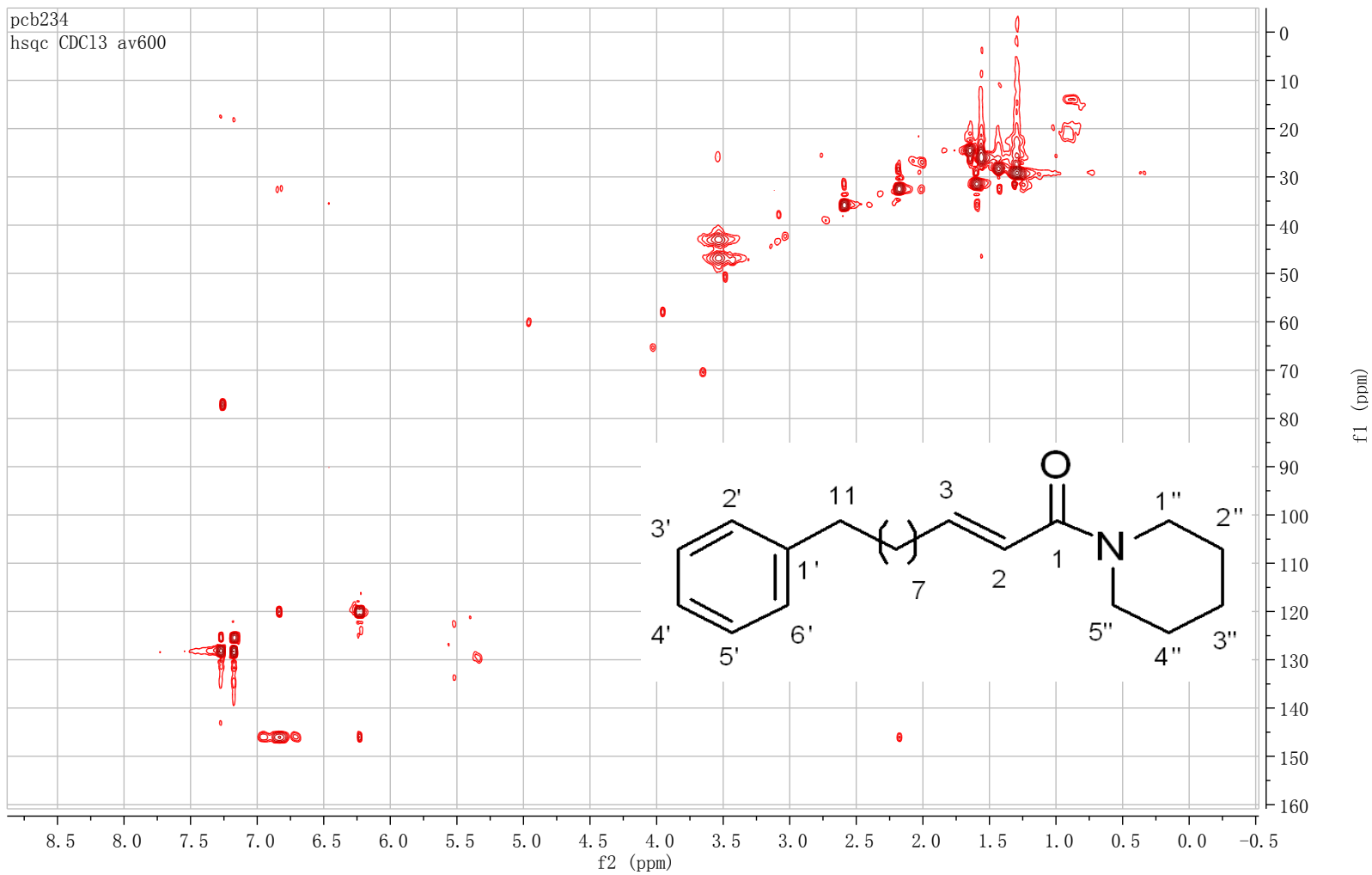
— 26.22

— 24.75

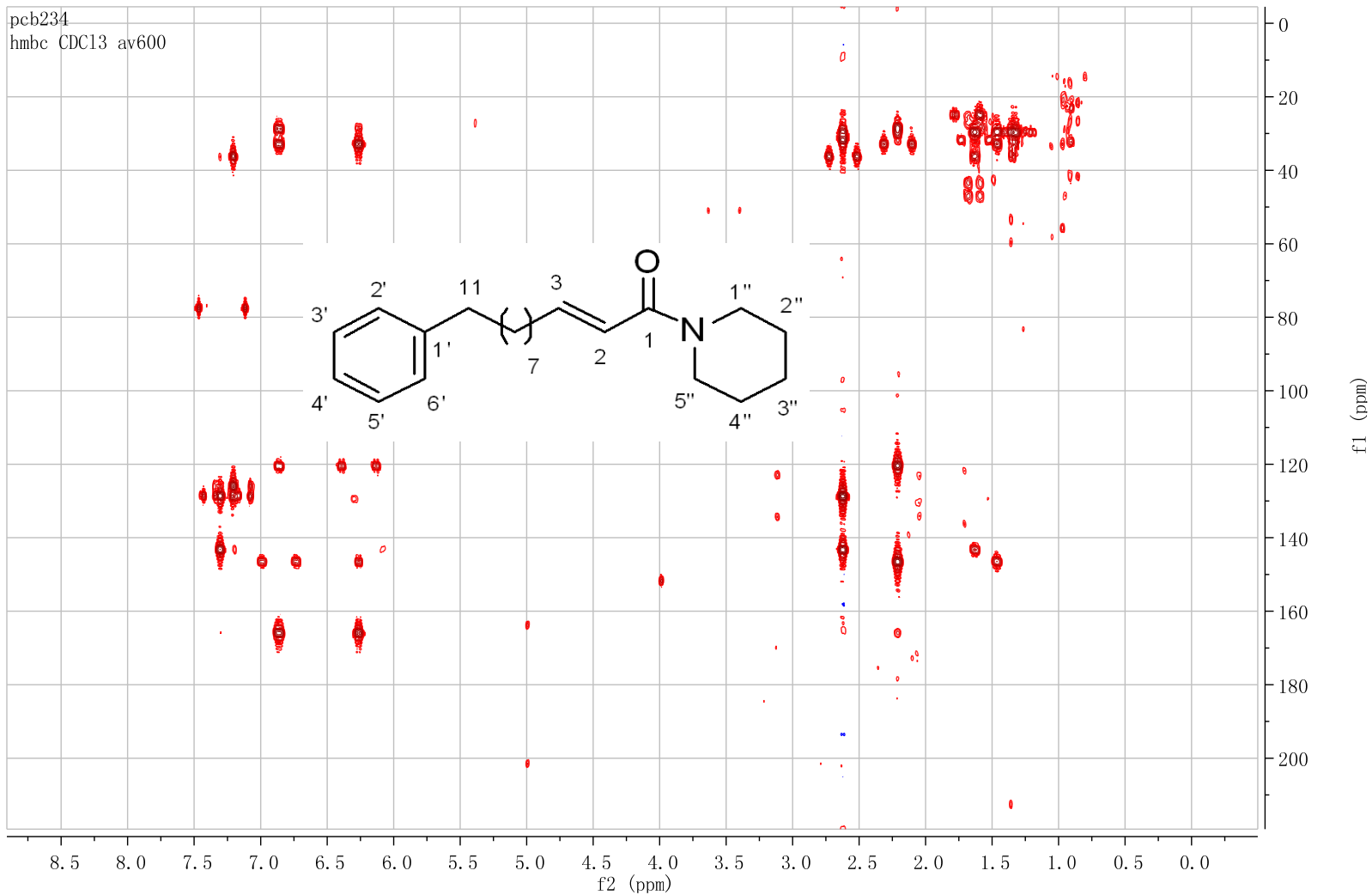


S11 HSQC spectrum of 2

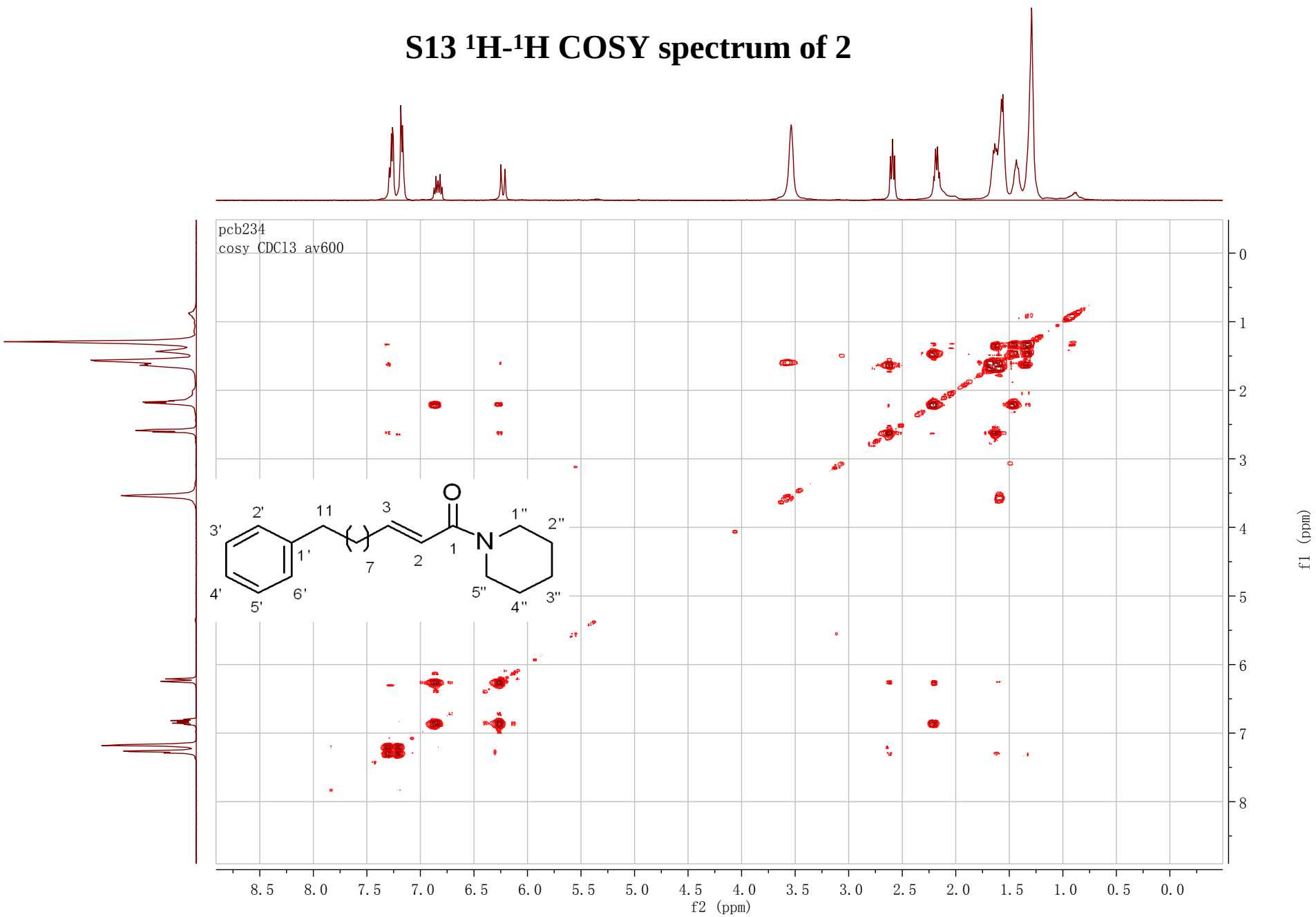
pcb234
hsqc CDC13 av600



S12 HMBC spectrum of 2



S13 ^1H - ^1H COSY spectrum of 2



Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, 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)

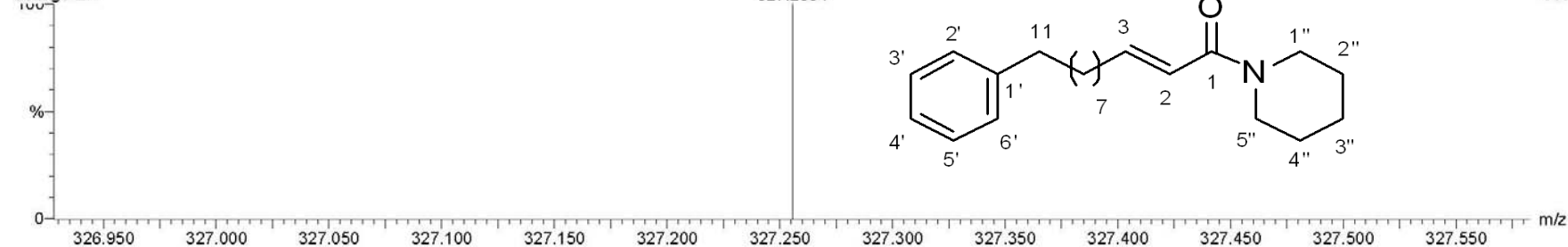
Elements Used:

C: 0-200 H: 0-400 N: 1-1 O: 0-2

pcb234

15:50:43 12-Nov-2012

Voltage E1+



Minimum: -10.0
Maximum: 100.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
327.2554	327.2562	-0.8	-2.4	7.0	5546293.5	C22 H33 N O

Display Report

Analysis Info

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Method ms_ptservice.m
Sample Name pcb23-4
Comment

Acquisition Date

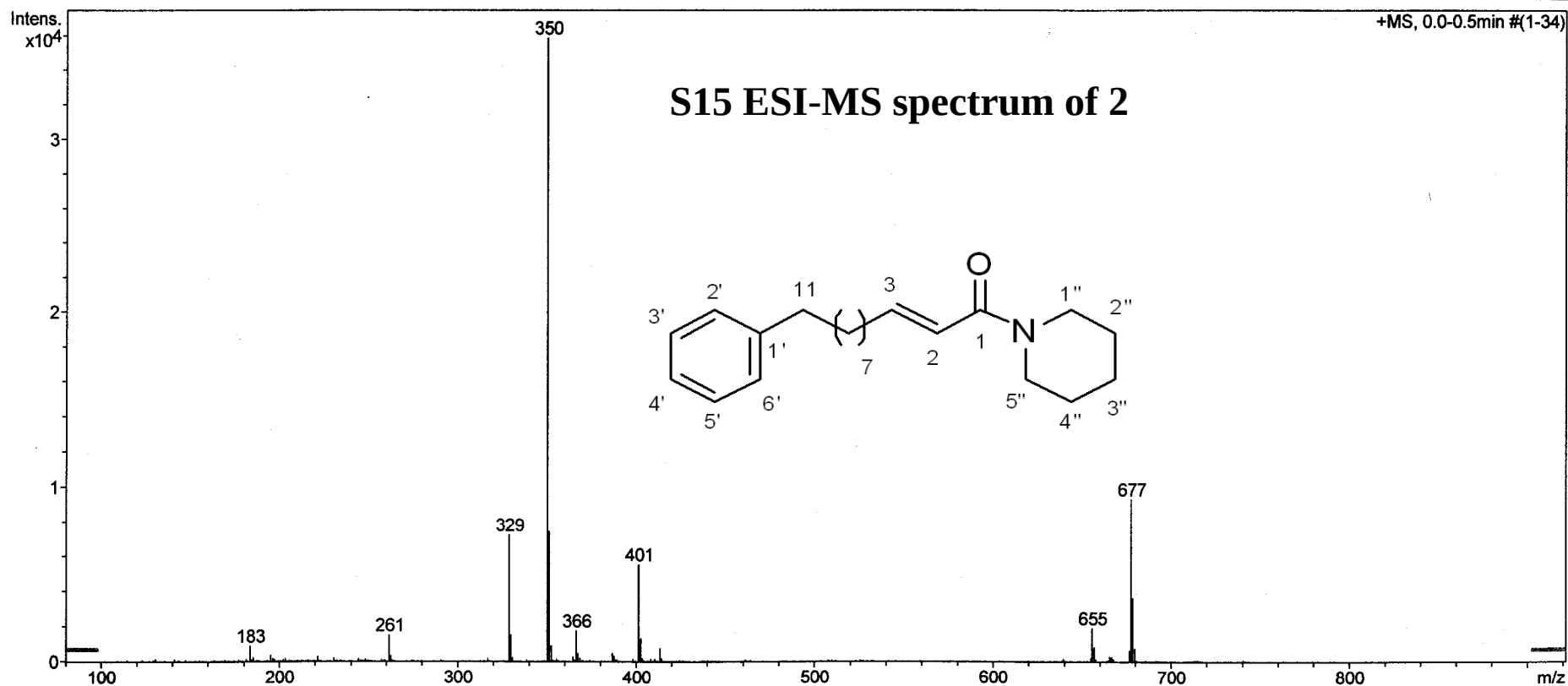
10/24/2012 4:07:23 PM

Operator
Instrument

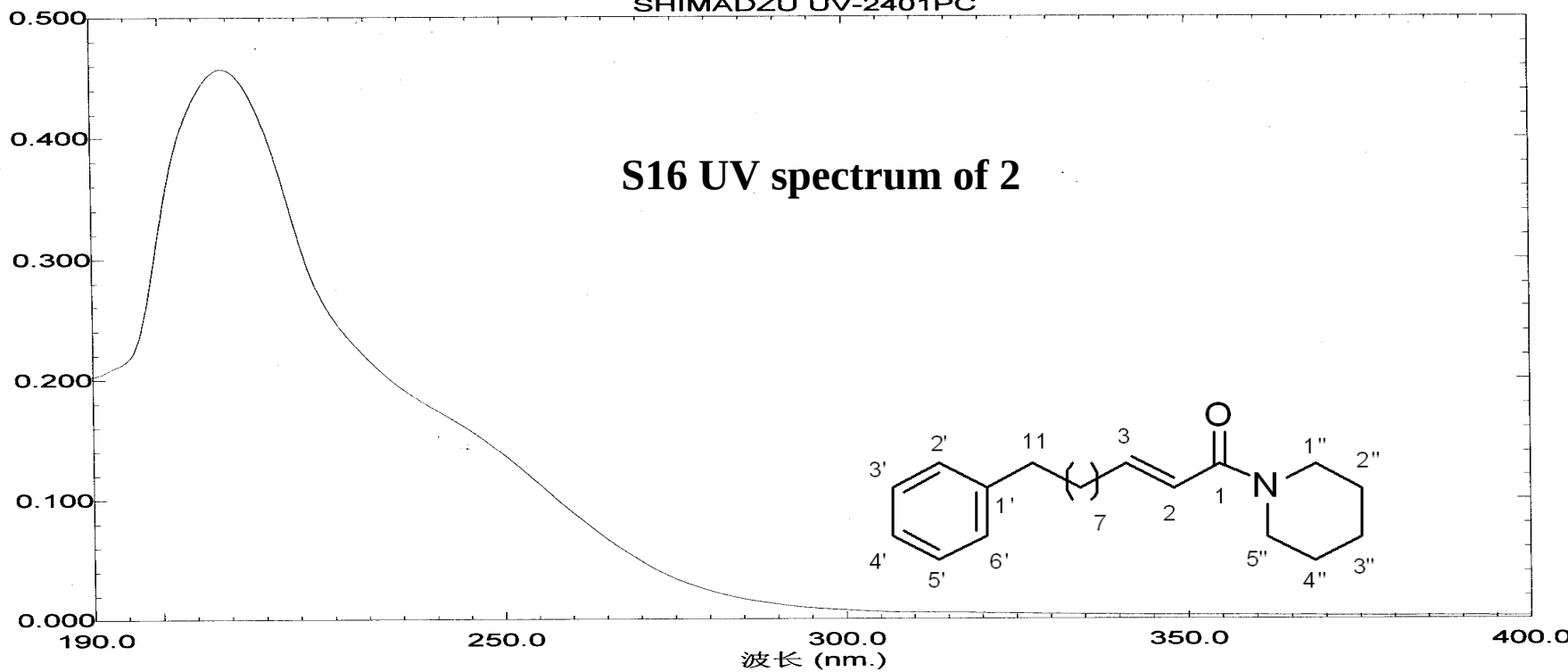
Bruker
HCT

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	900 m/z
Capillary Exit	16.0 Volt	Skimmer	40.0 Volt	Trap Drive	34.4
Accumulation Time	100000 μ s	Averages	5 Spectra	Auto MS/MS	off



S16 UV spectrum of 2



文件名: 13100906

样品名称: PCB234

创建于: 16:13 13-10-09

数据: 原始

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.2

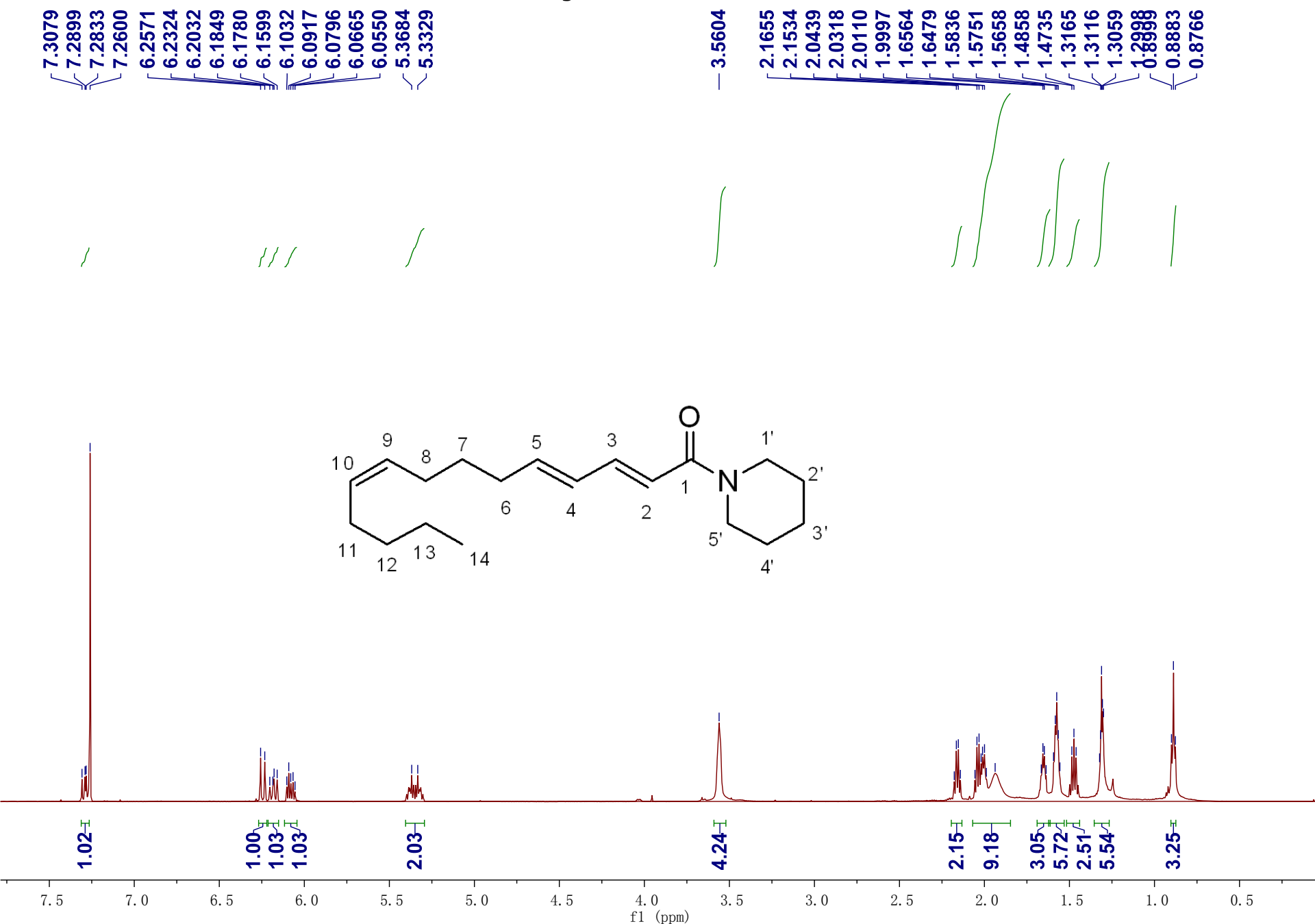
13100906

样品浓度: 0.0344毫克/毫升

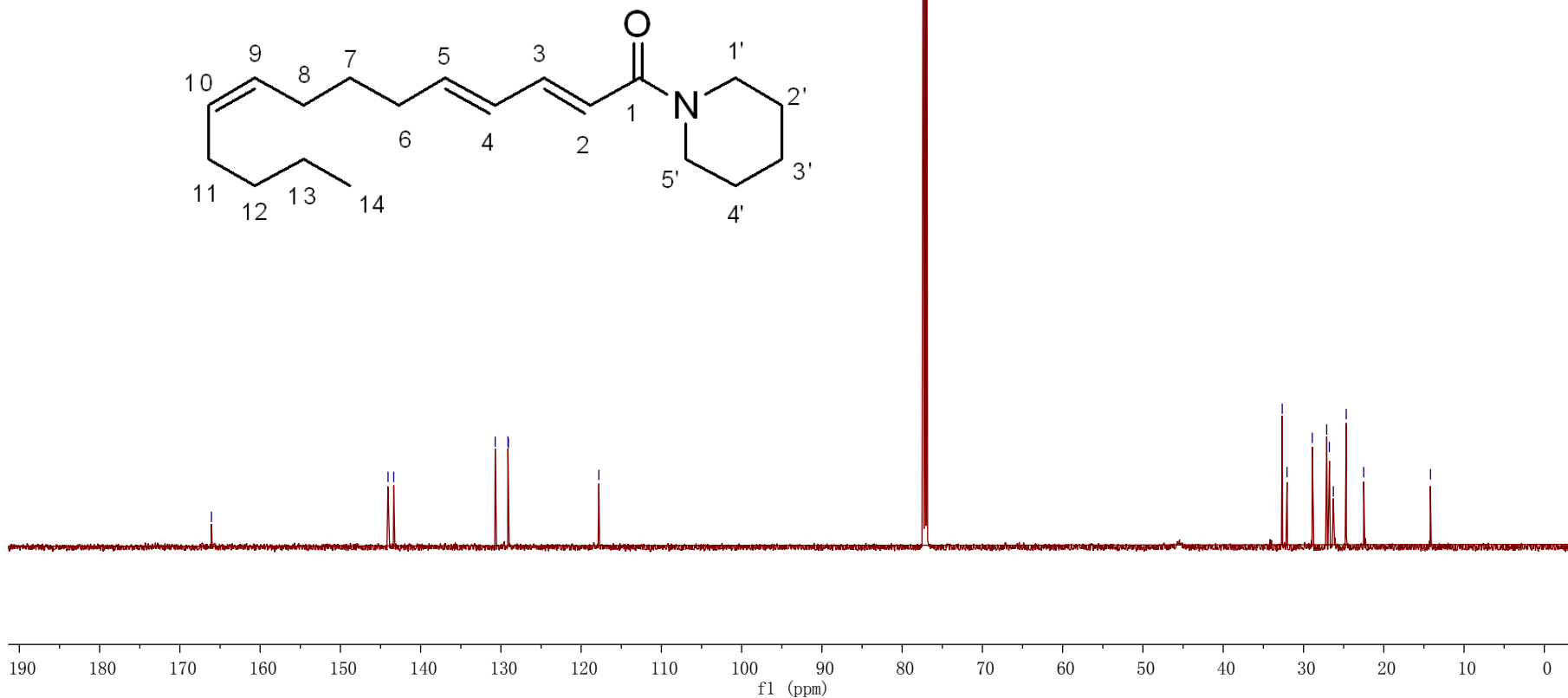
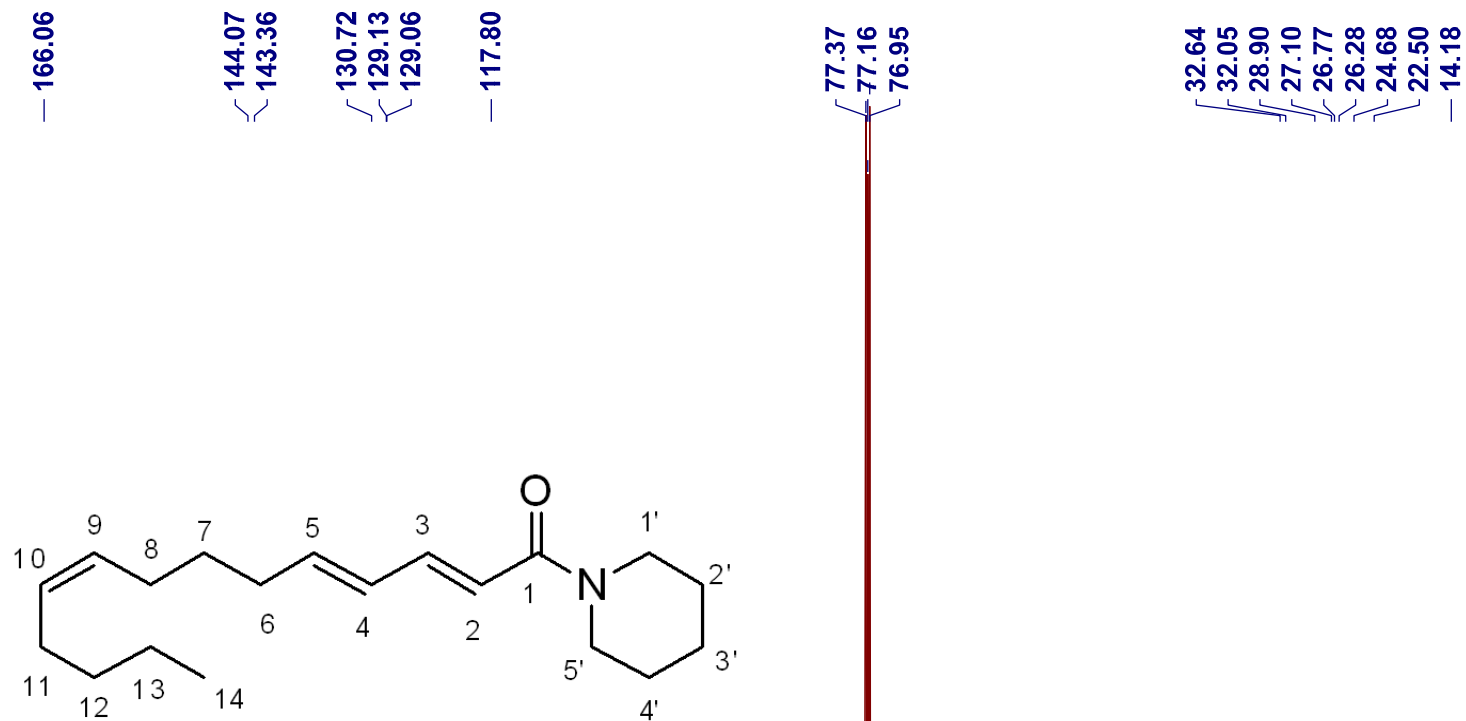
溶剂: 甲醇

否.	波长 (nm.)	Abs.
1	209.20	0.4571

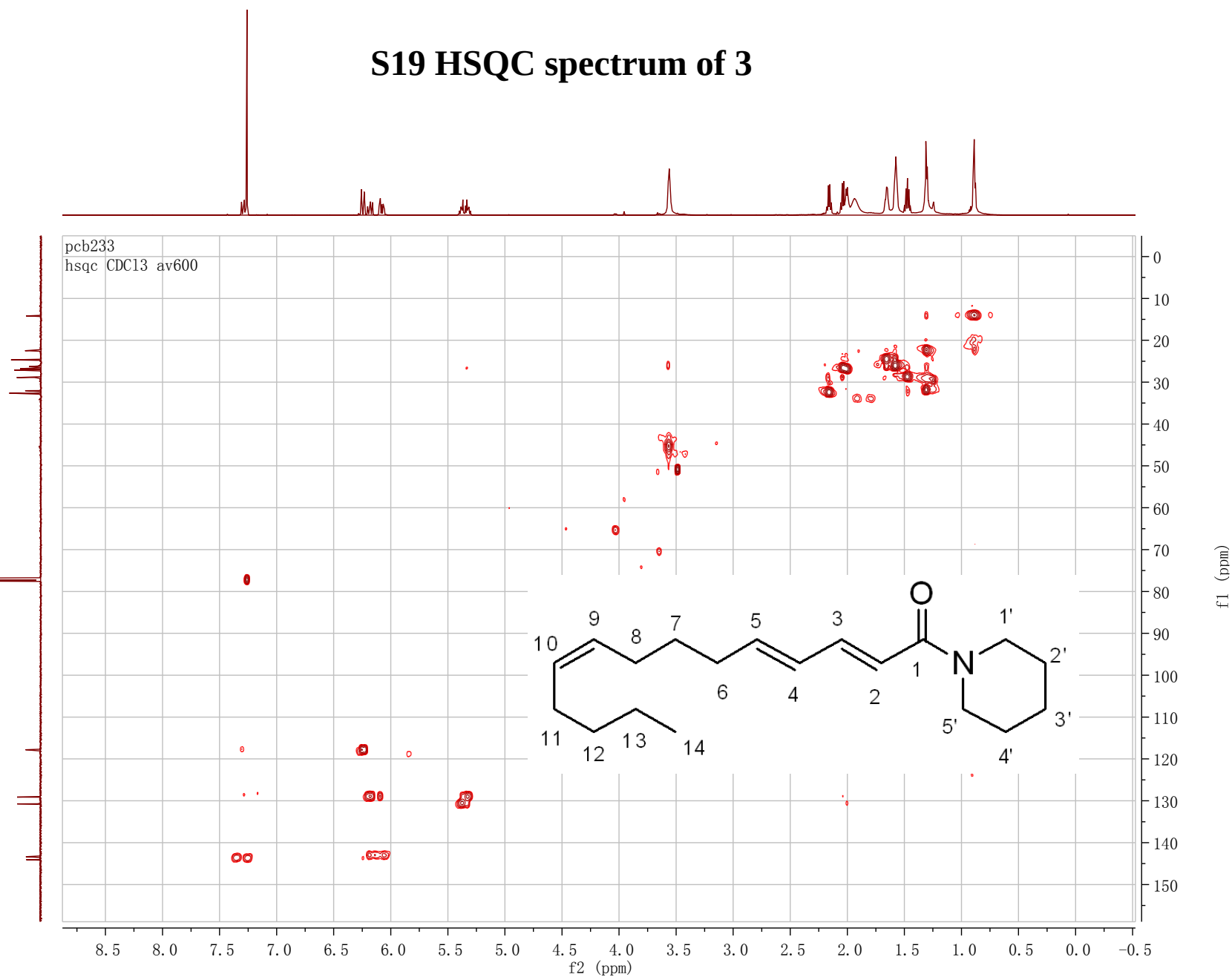
S17 ¹H NMR (CDCl₃, 600 MHz) spectrum of 3



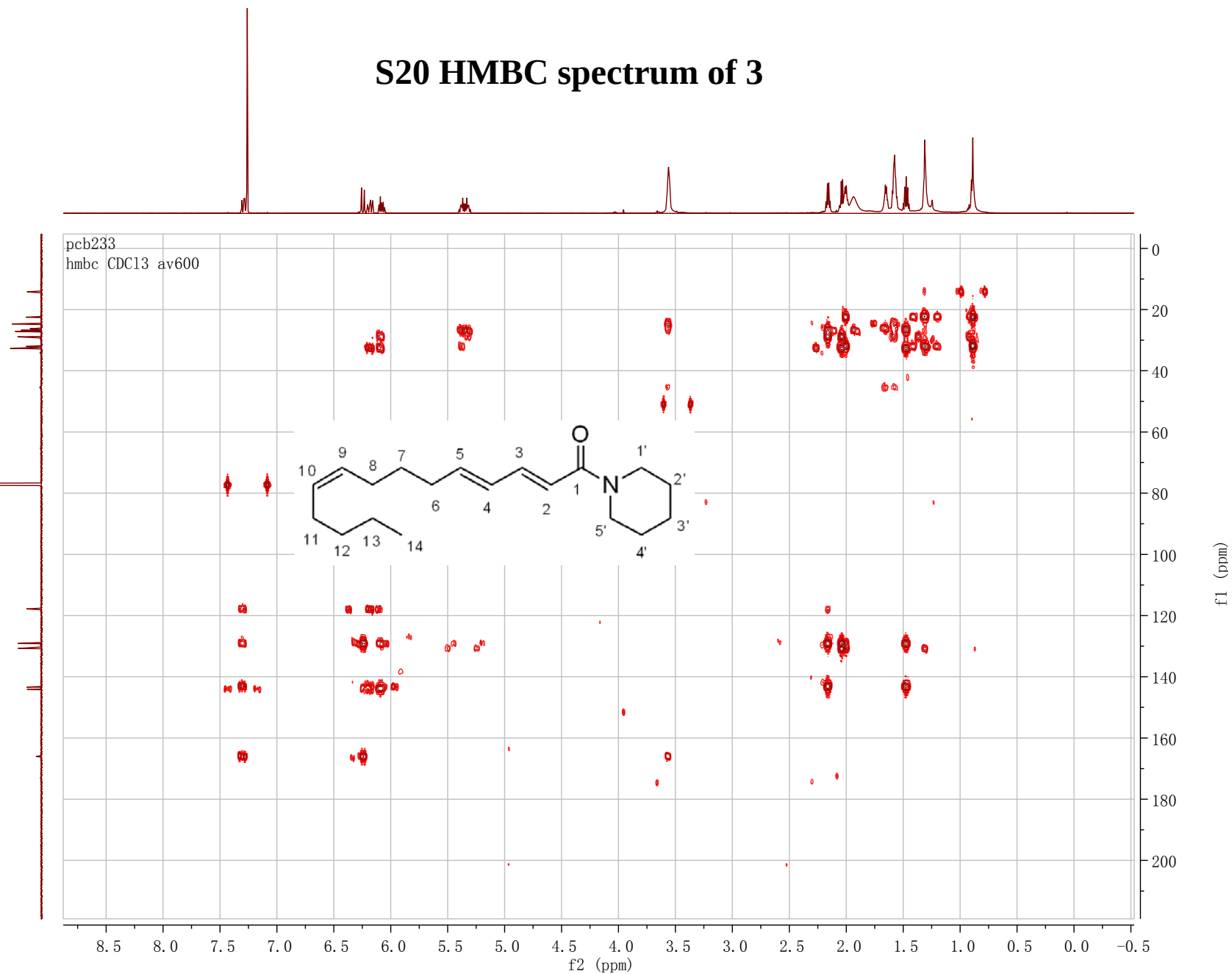
S18 ^{13}C NMR (CDCl_3 , 150 MHz) spectrum of 3



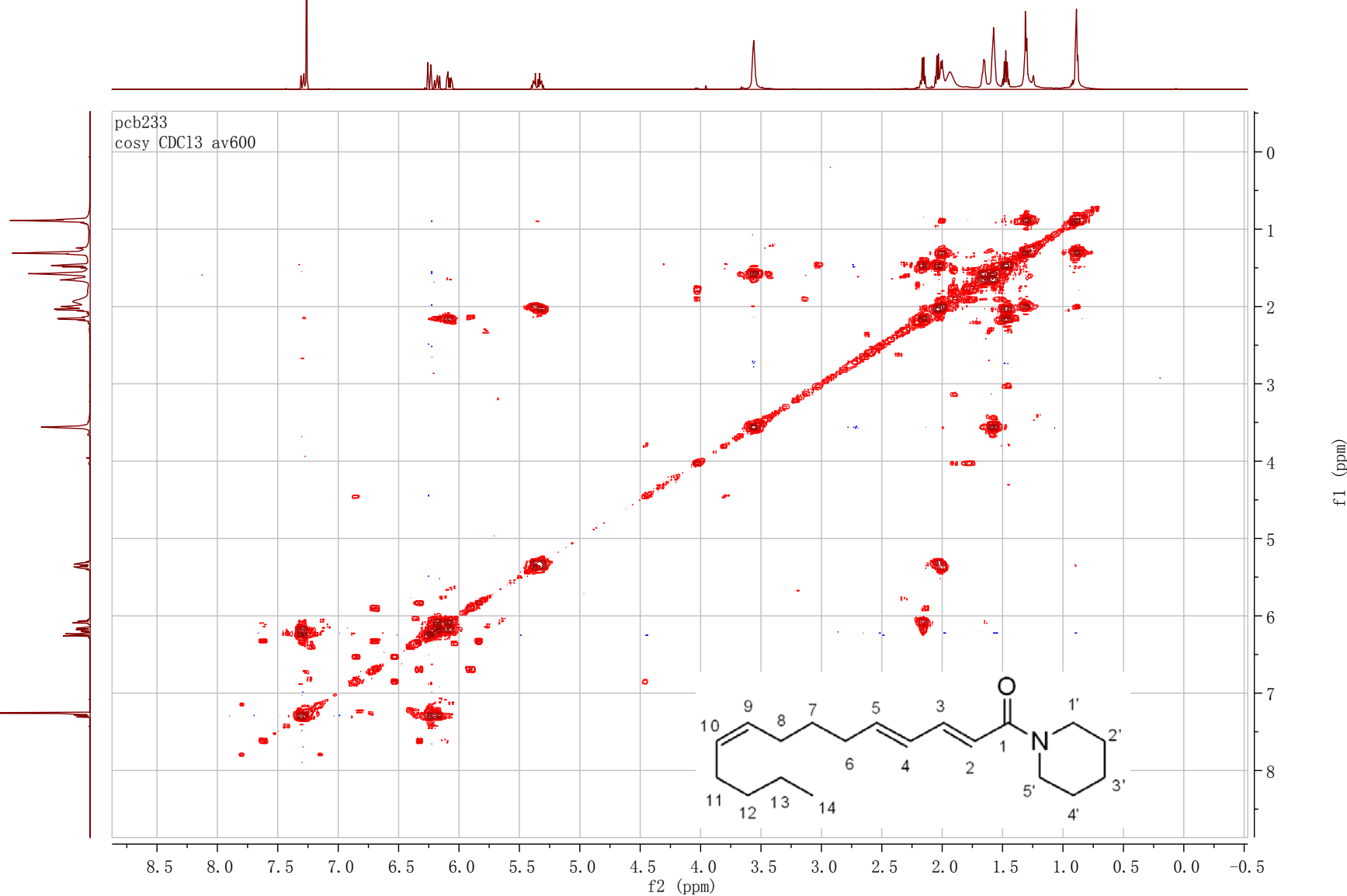
S19 HSQC spectrum of 3



S20 HMBC spectrum of 3



S21 ^1H - ^1H COSY spectrum of 3



Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

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

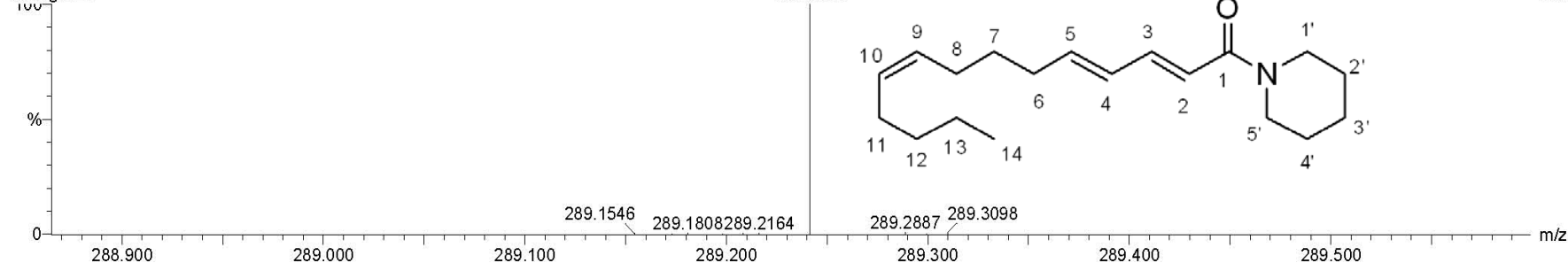
Elements Used:

C: 0-200 H: 0-400 N: 1-1 O: 0-2

pcb233

16:00:08 12-Nov-2012

Voltage EI+



Minimum: -10.0
Maximum: 100.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
289.2414	289.2406	0.8	2.8	5.0	5546192.0	C19 H31 N O

Display Report

Analysis Info

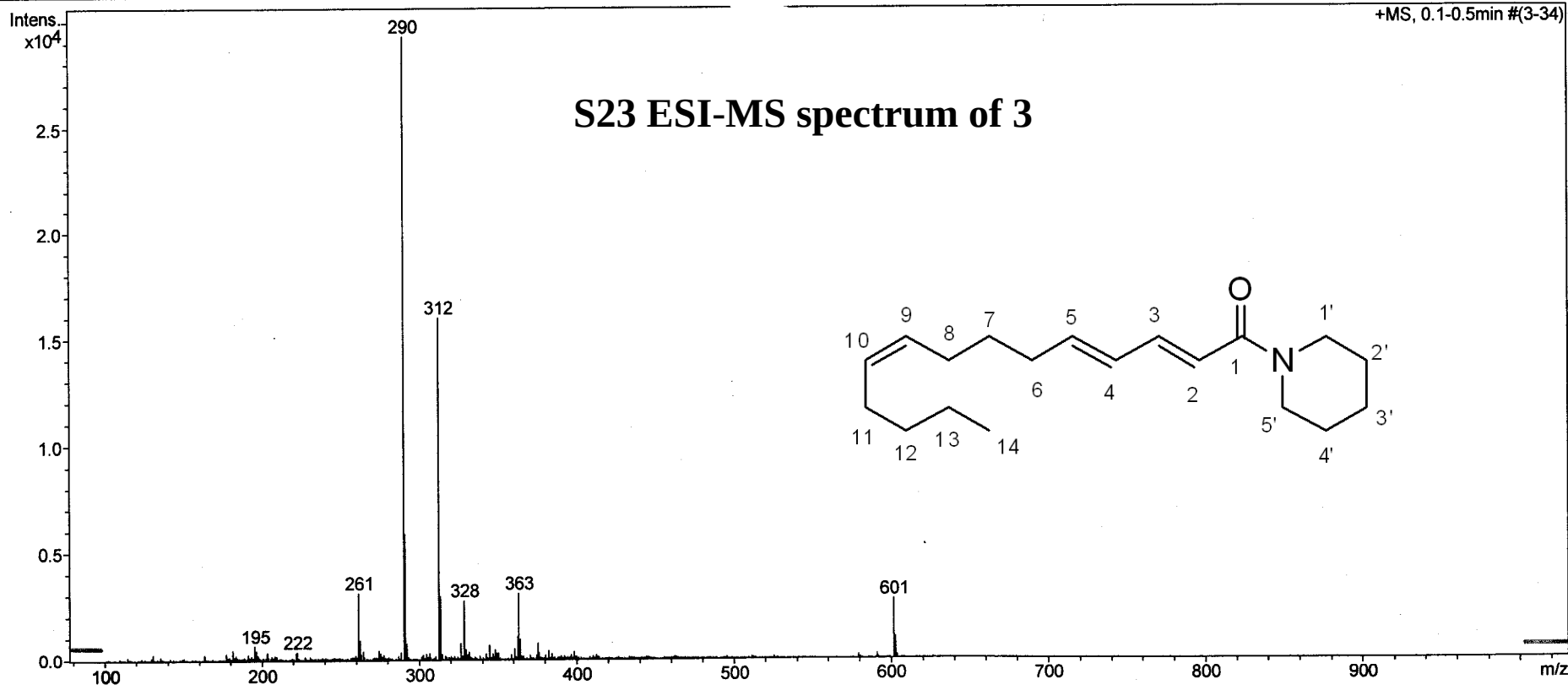
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Sample Name pcb23-3
Comment

Acquisition Date 10/24/2012 4:30:33 PM

Operator
Instrument Bruker
HCT

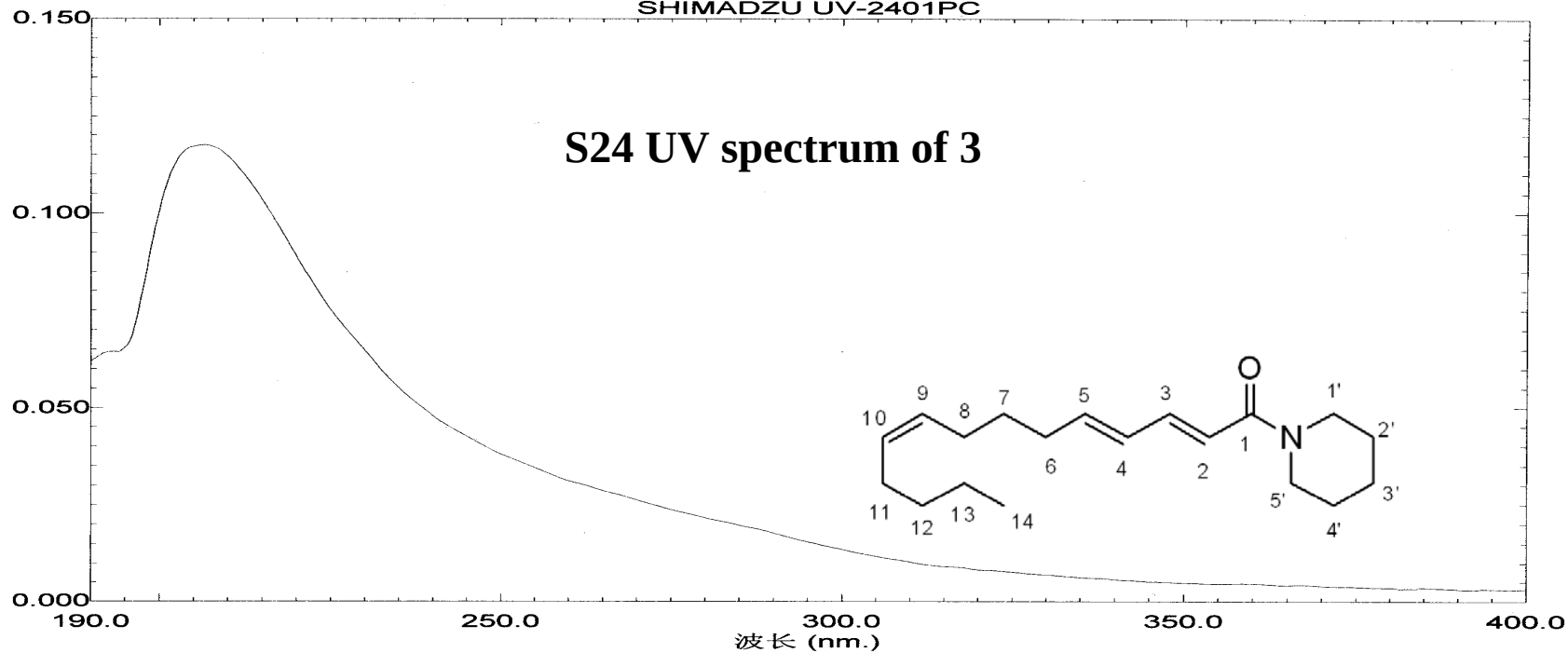
Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	1000 m/z
Capillary Exit	10.0 Volt	Skimmer	40.0 Volt	Trap Drive	30.4
Accumulation Time	100000 μ s	Averages	5 Spectra	Auto MS/MS	off



S24 UV spectrum of 3

Abs



文件名: 13100905
样品名称: PCB233

创建于: 16:06 13-10-09
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

13100905

样品浓度: 0.0320毫克/毫升
溶剂: 甲醇

否.	波长 (nm.)	Abs.
1	206.80	0.1174