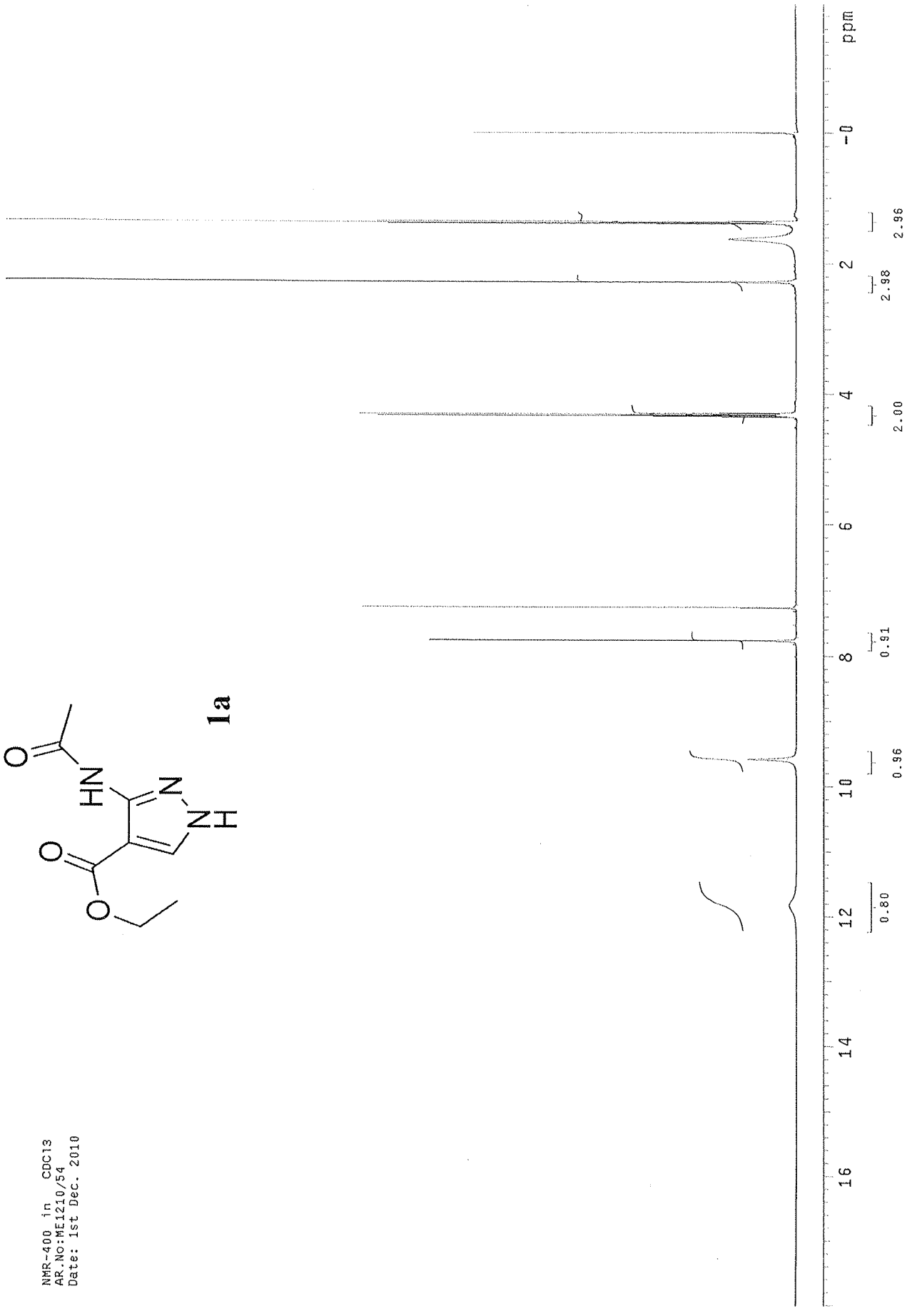
Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra



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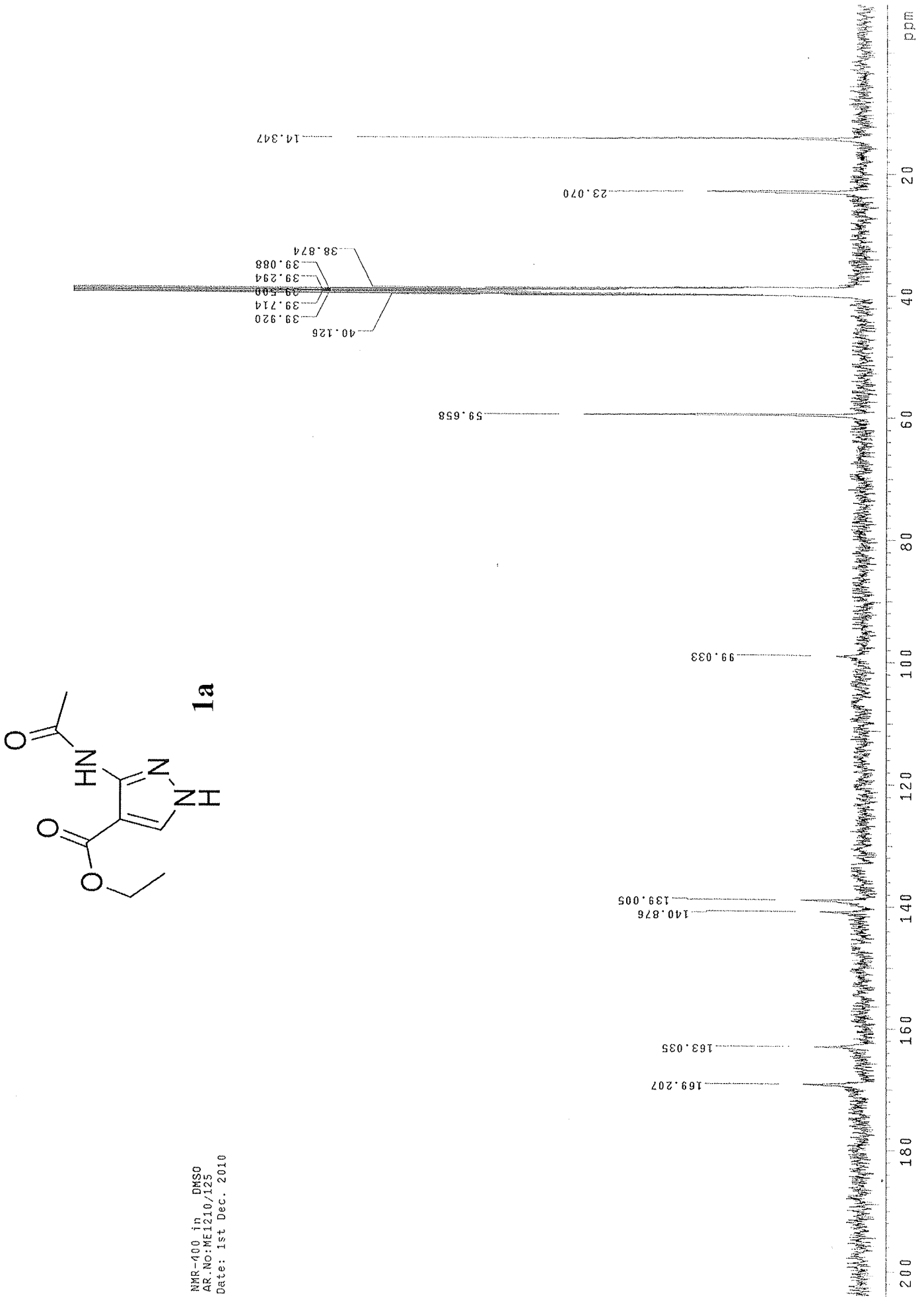
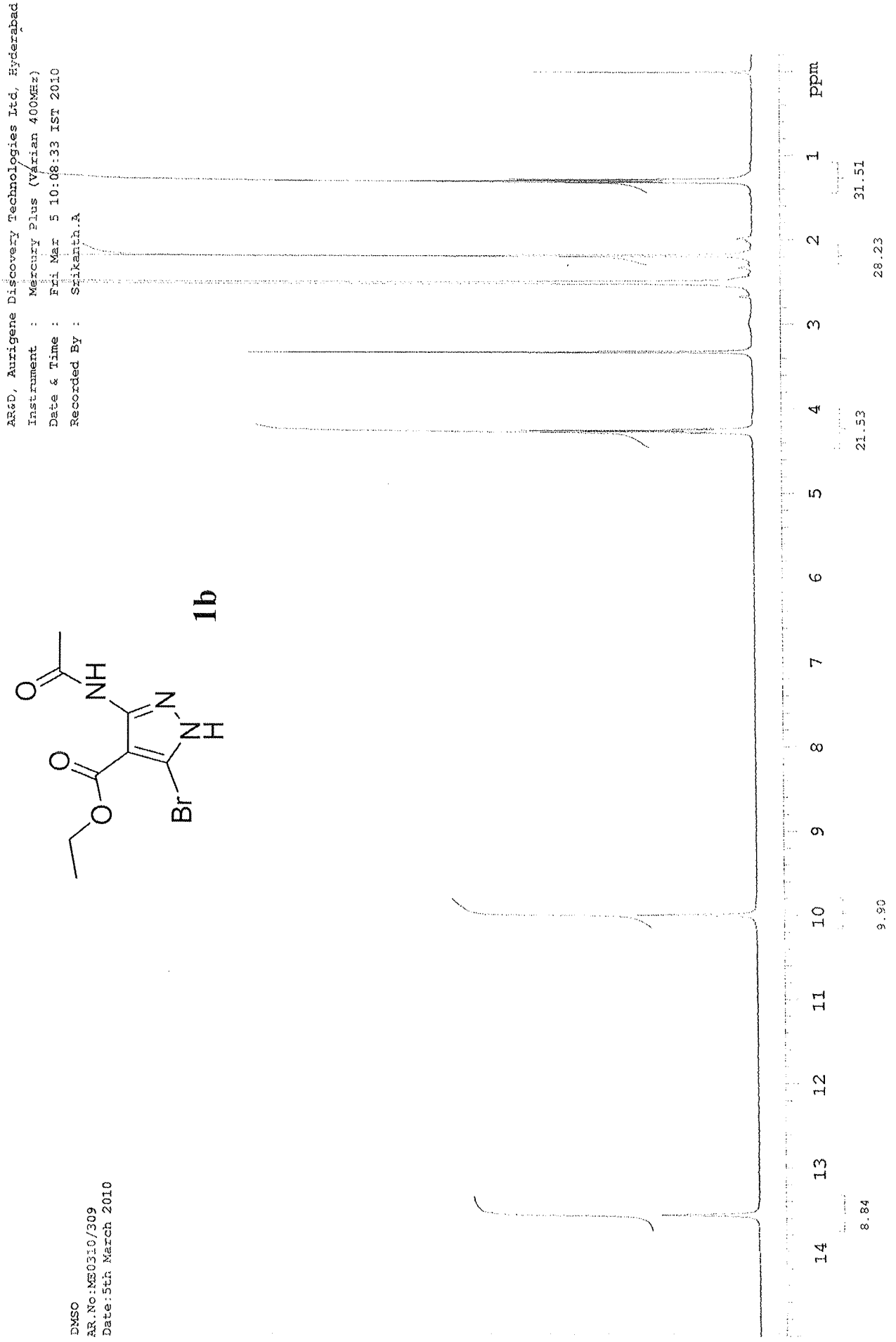


Copies of NMR spectra



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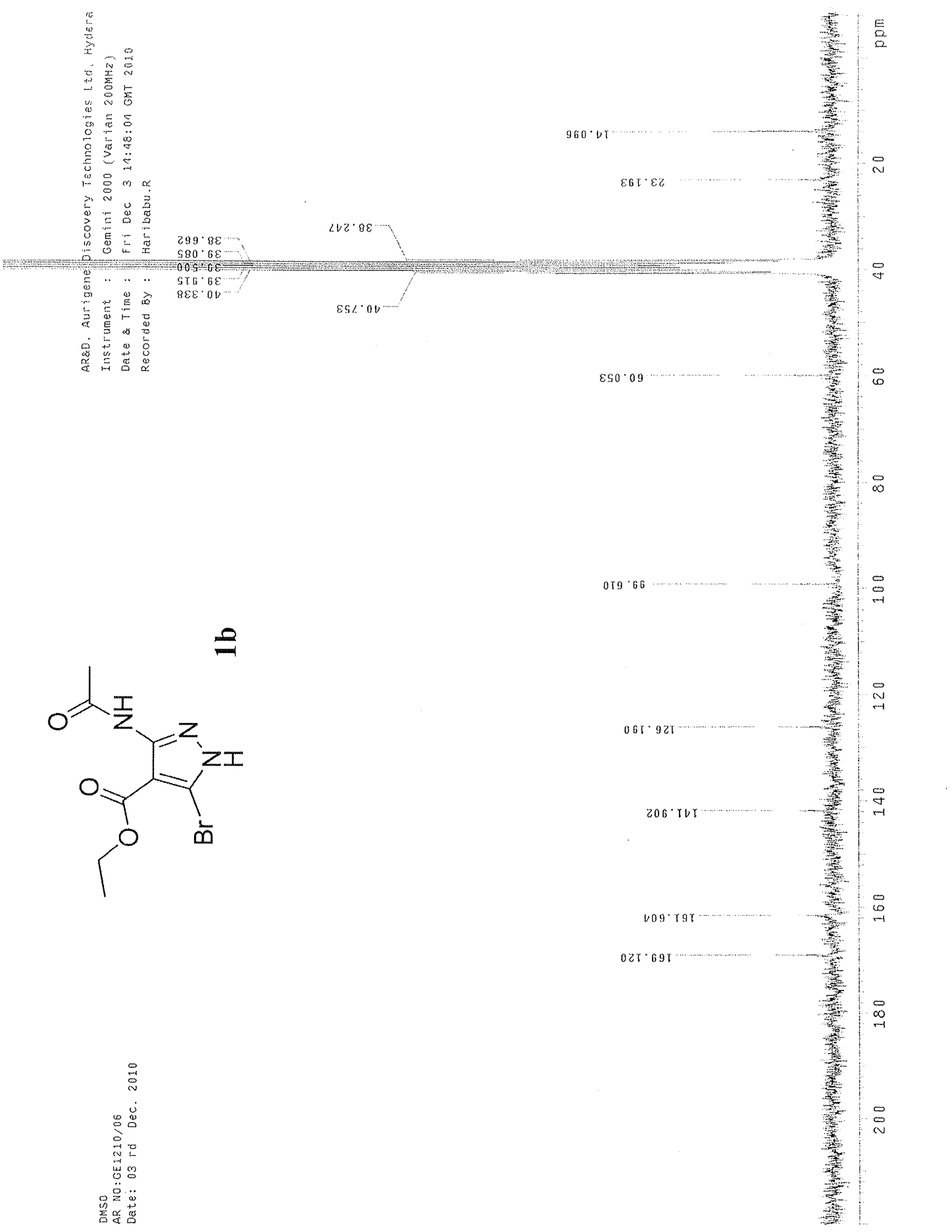

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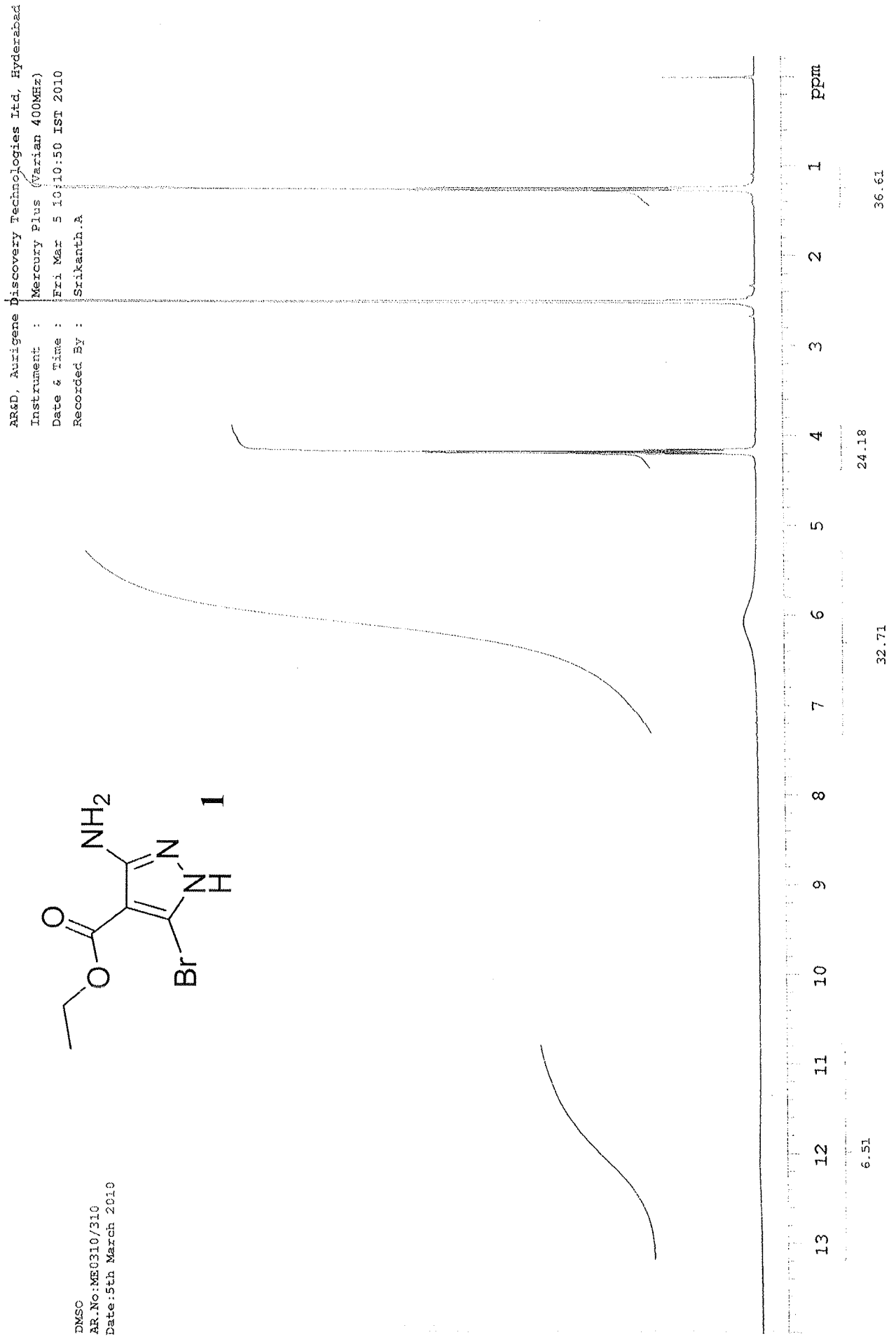

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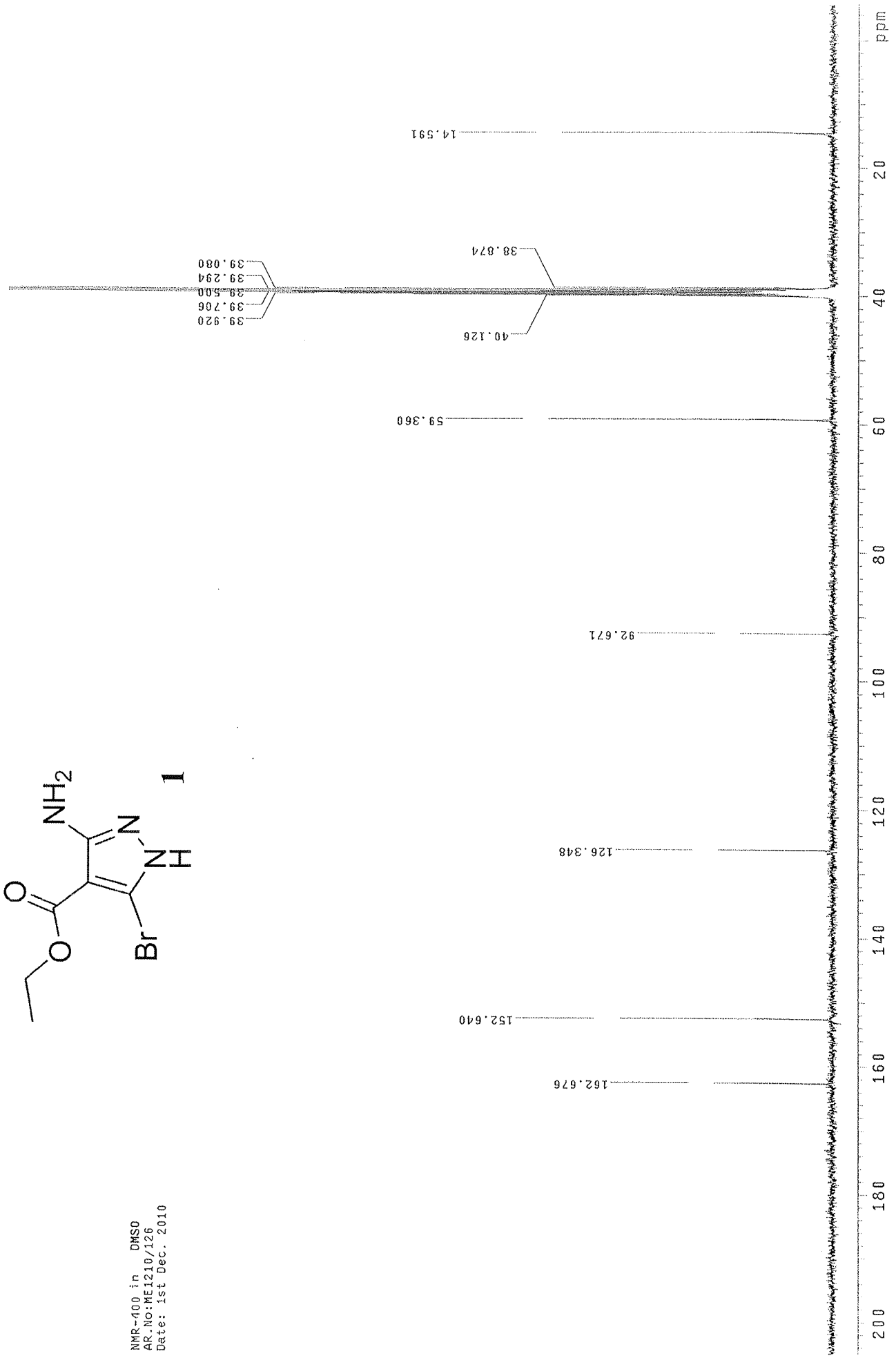

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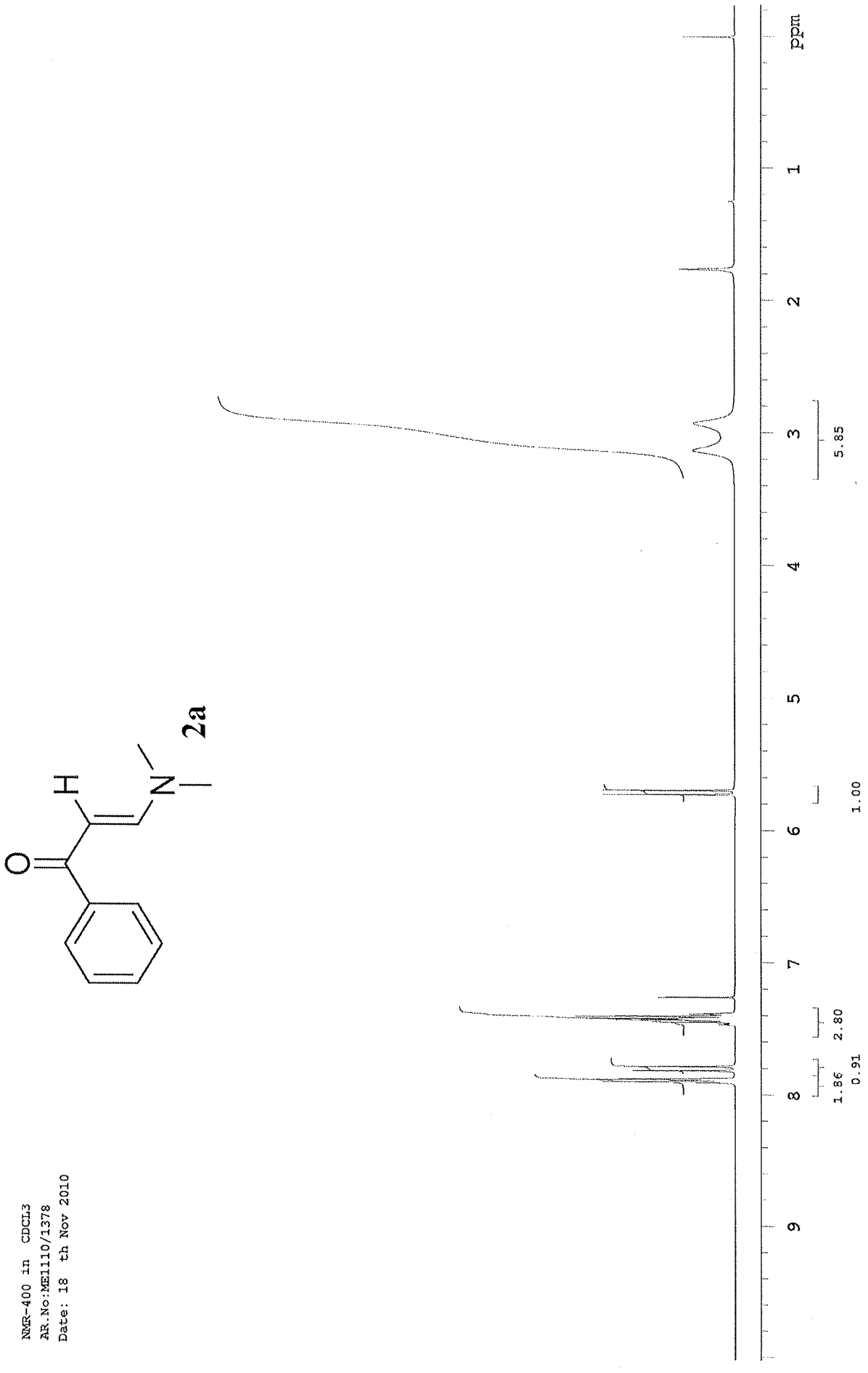

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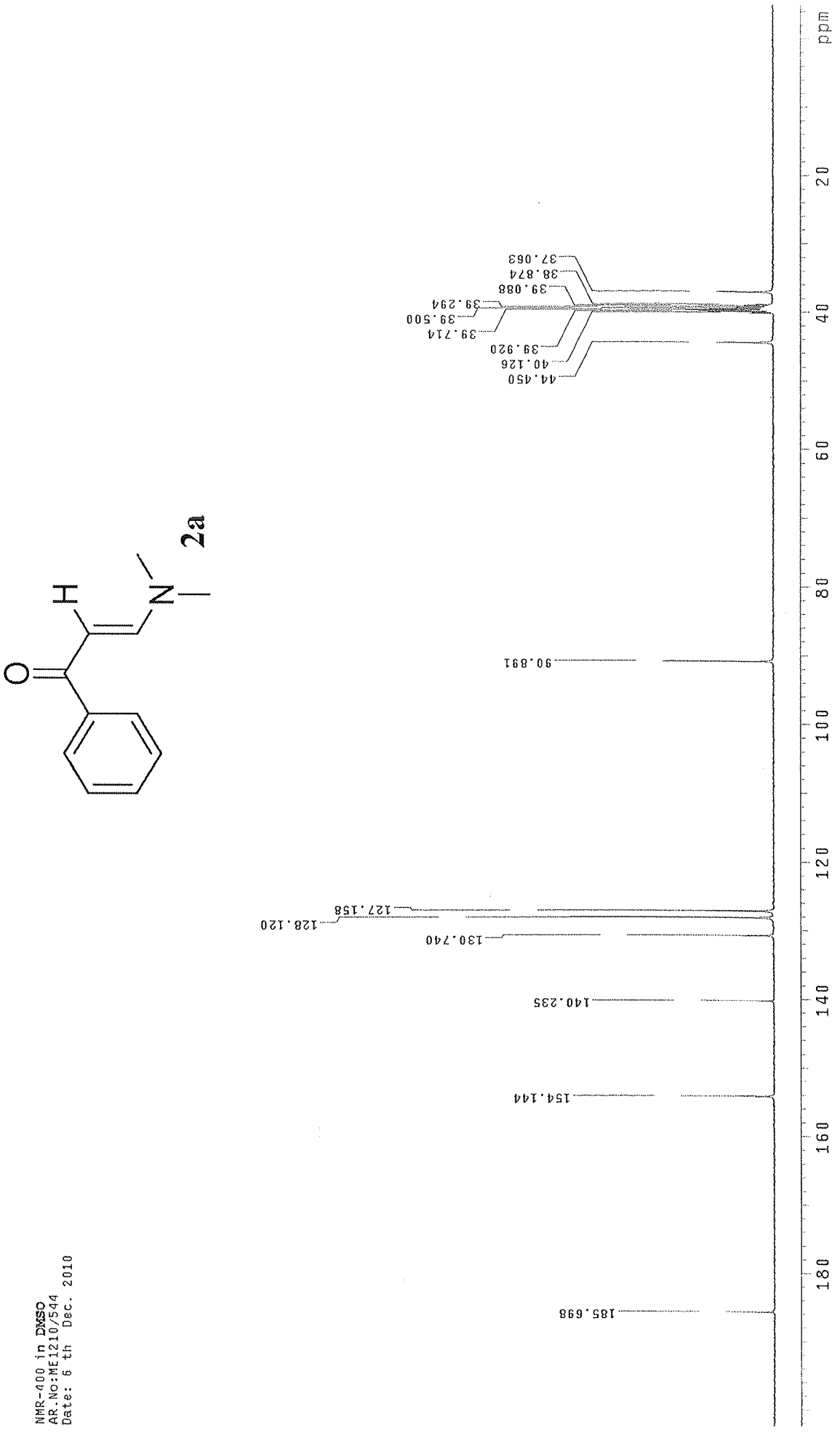

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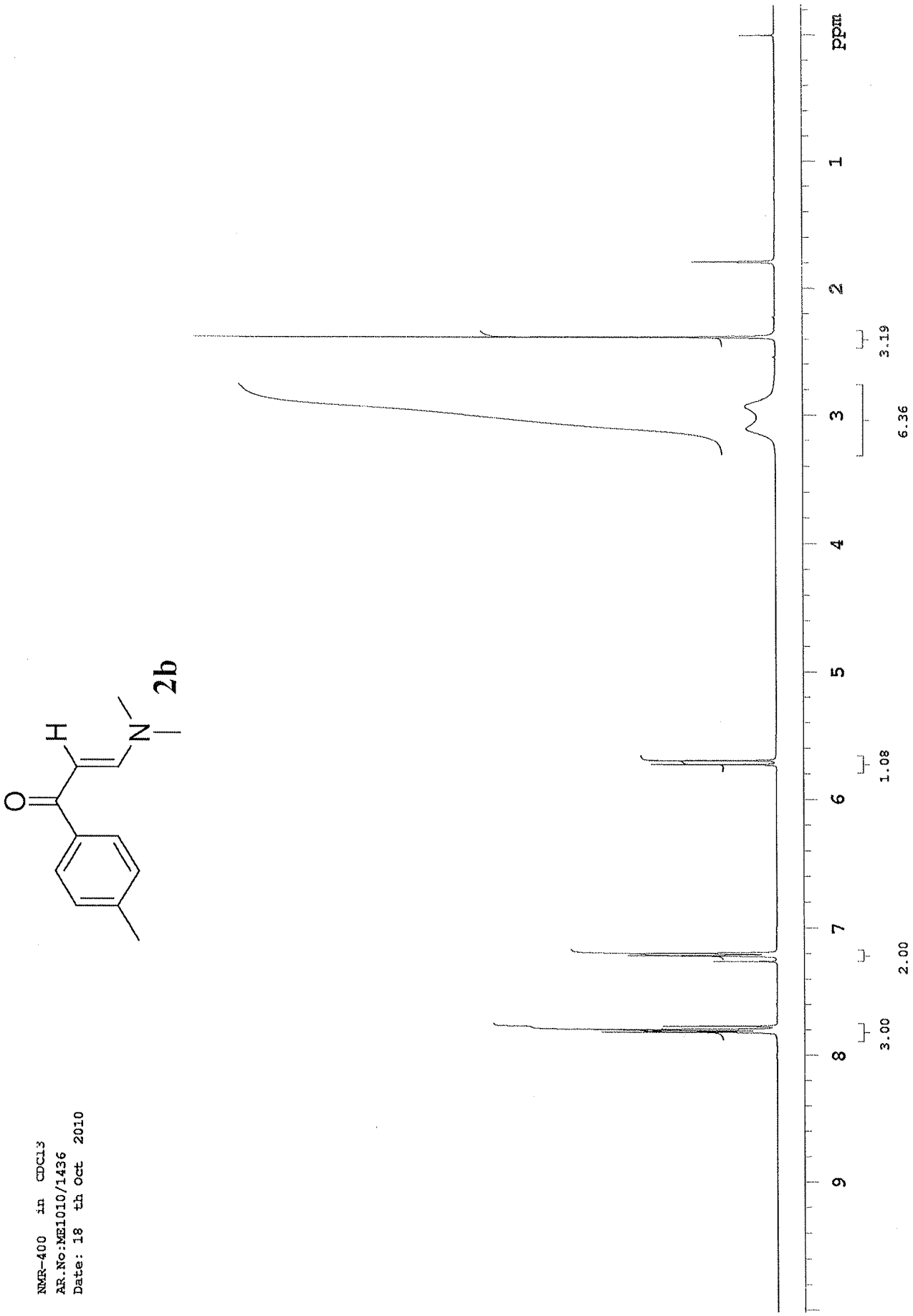

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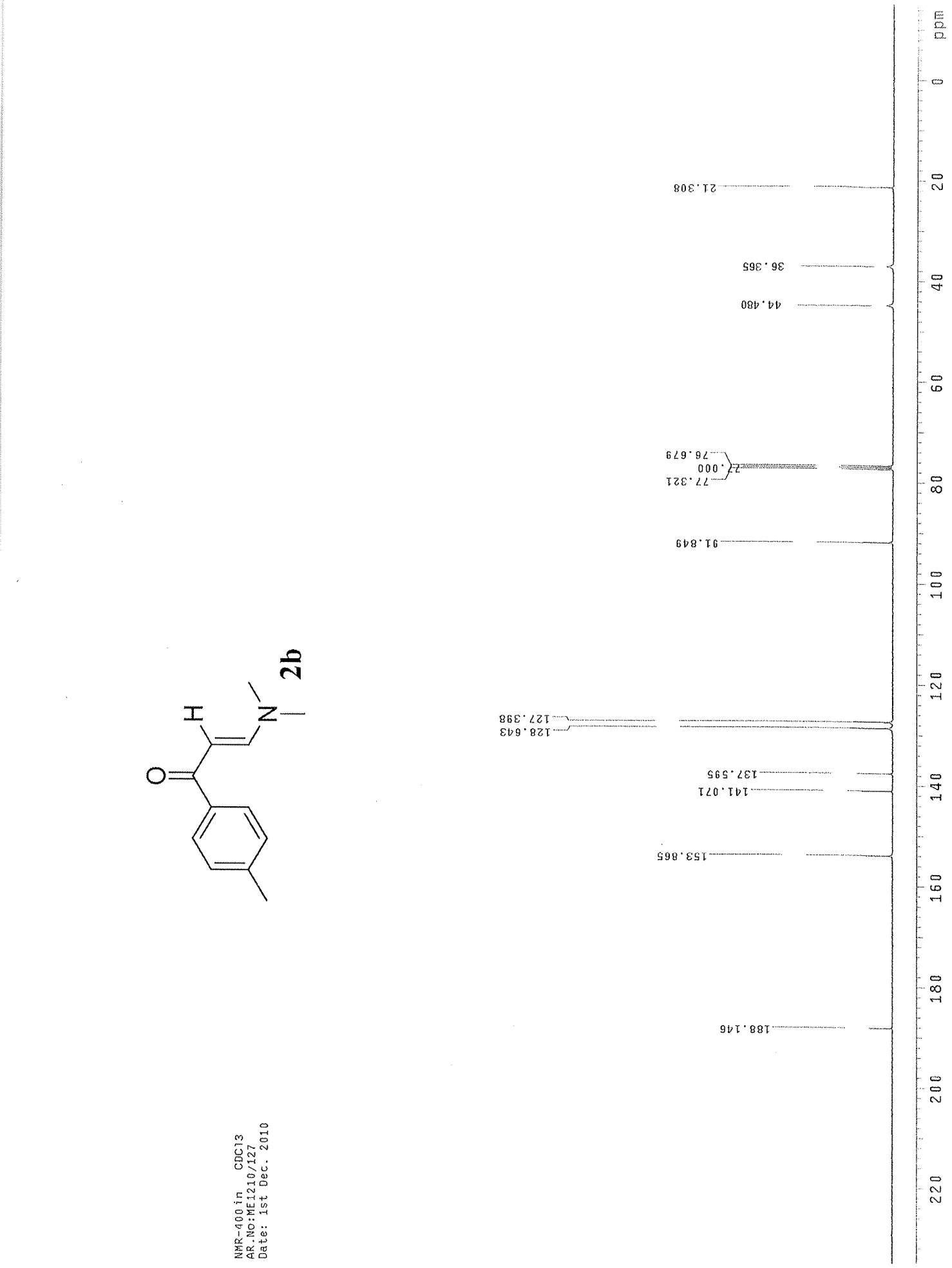

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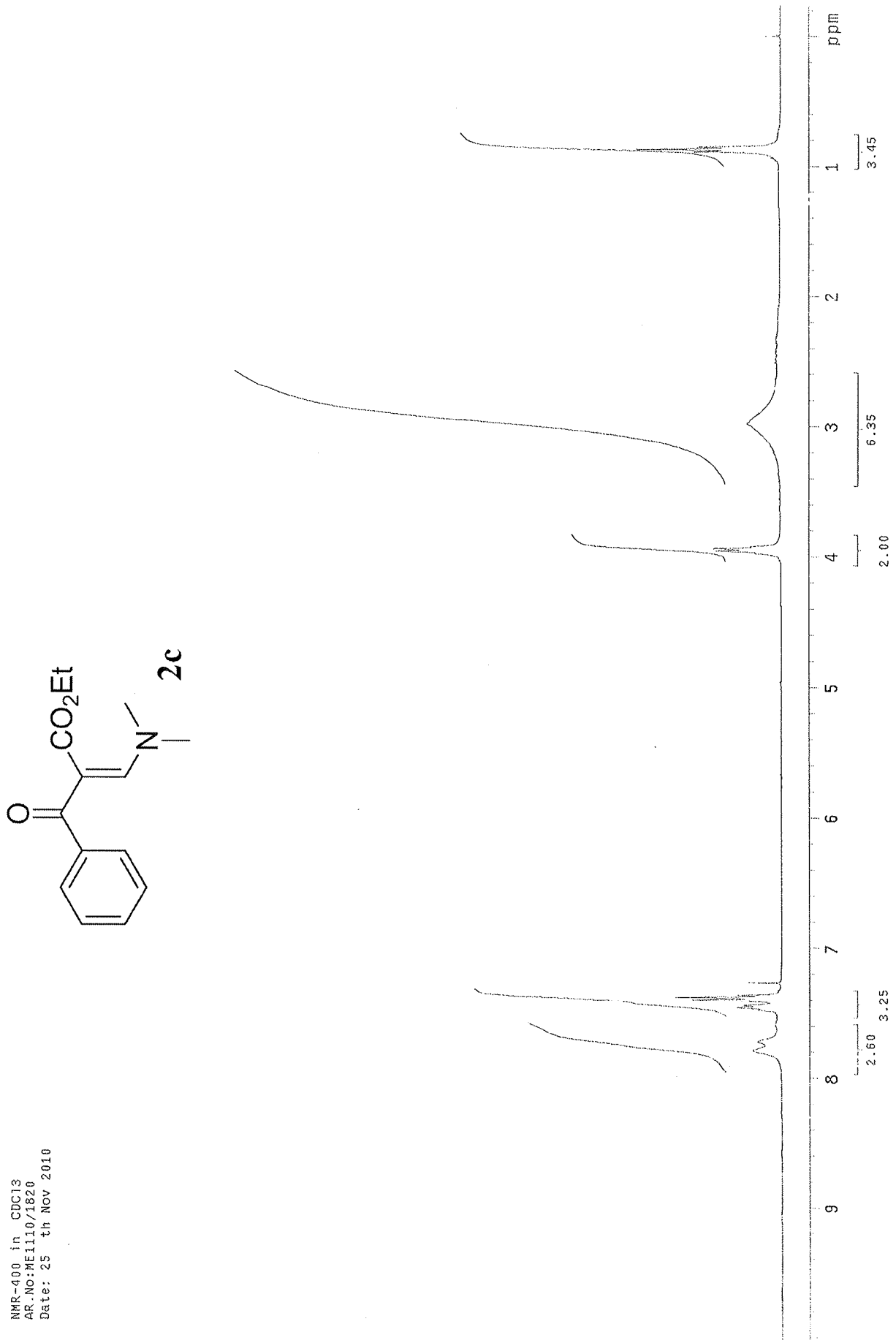

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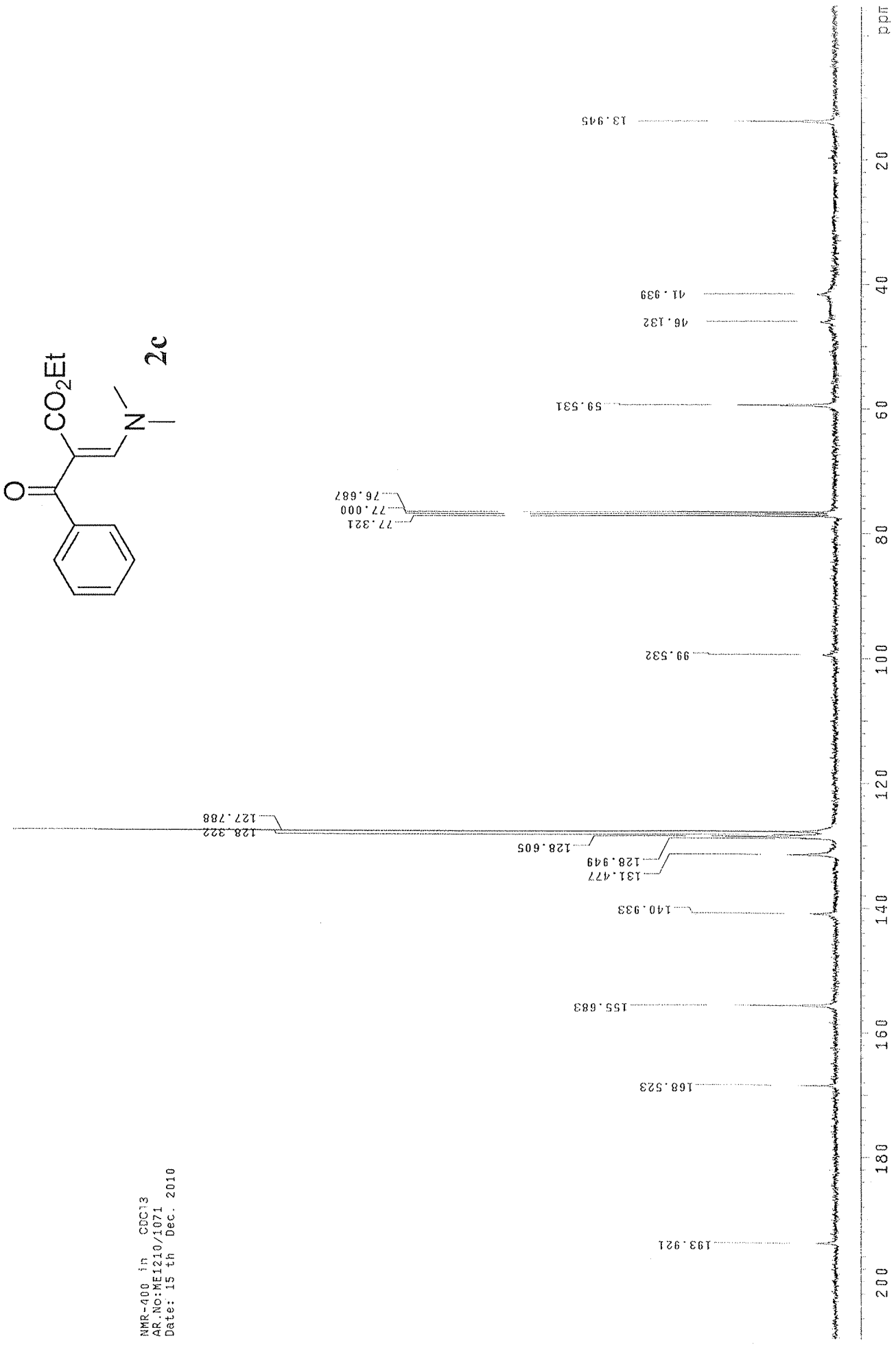

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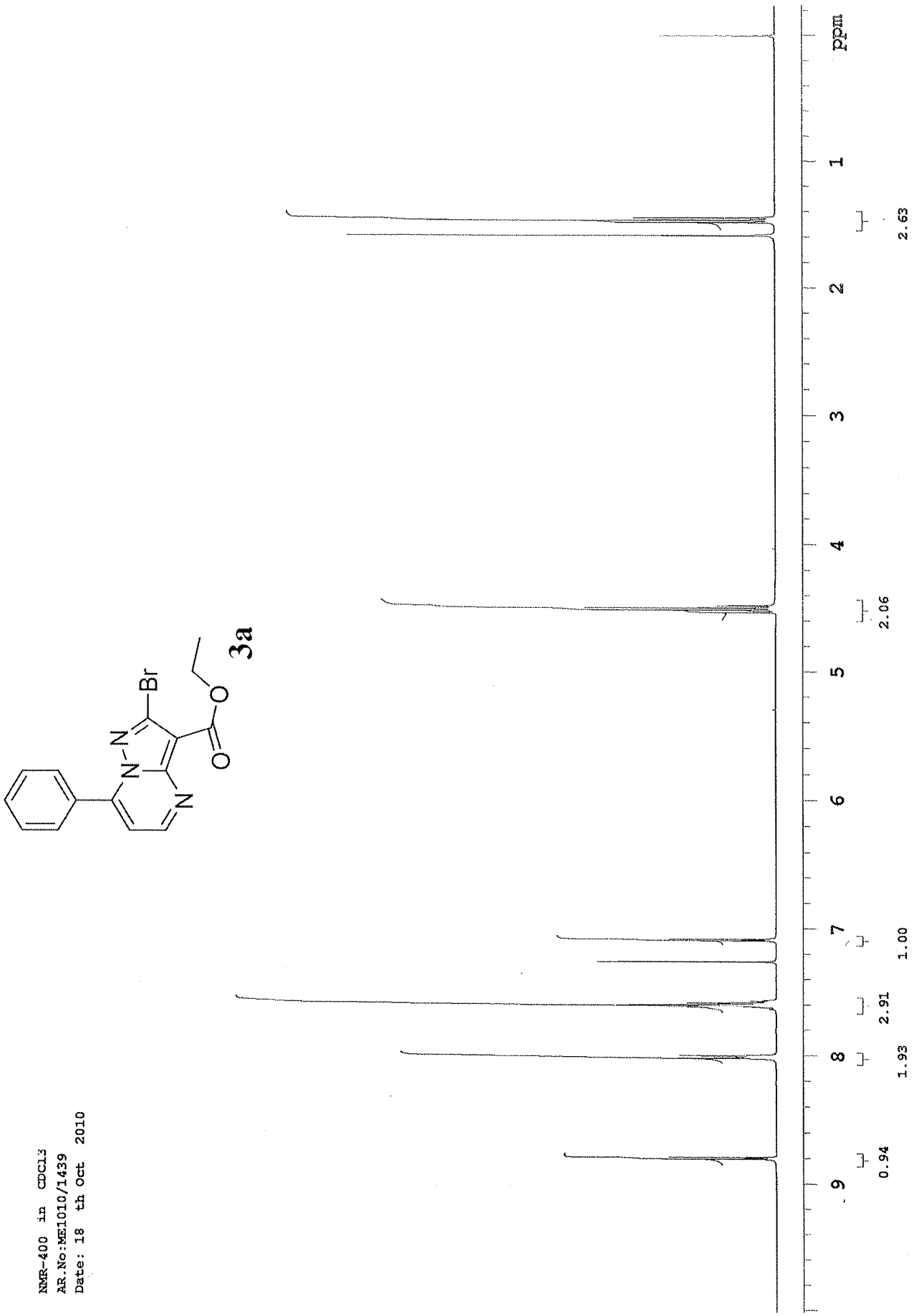

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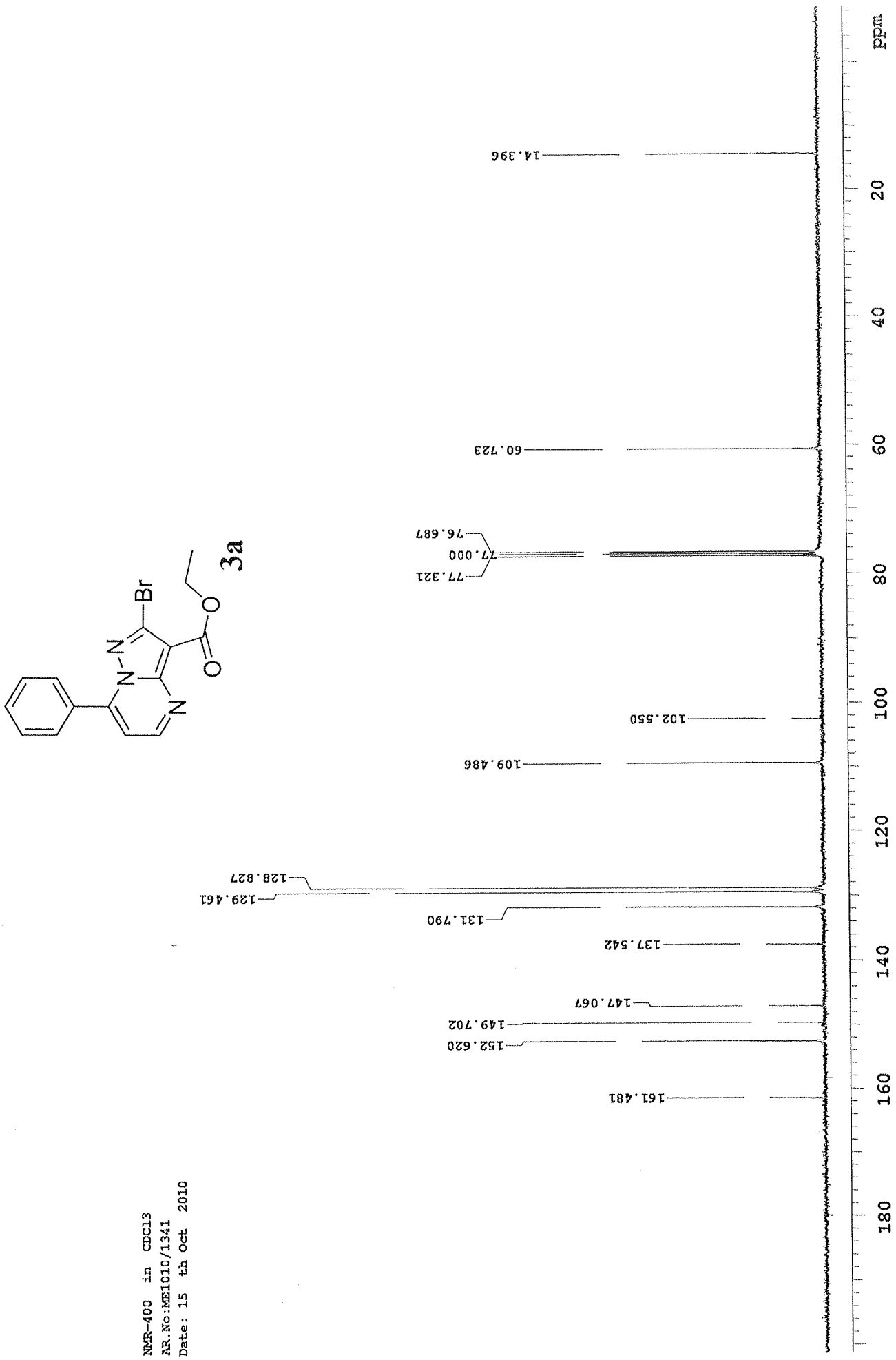

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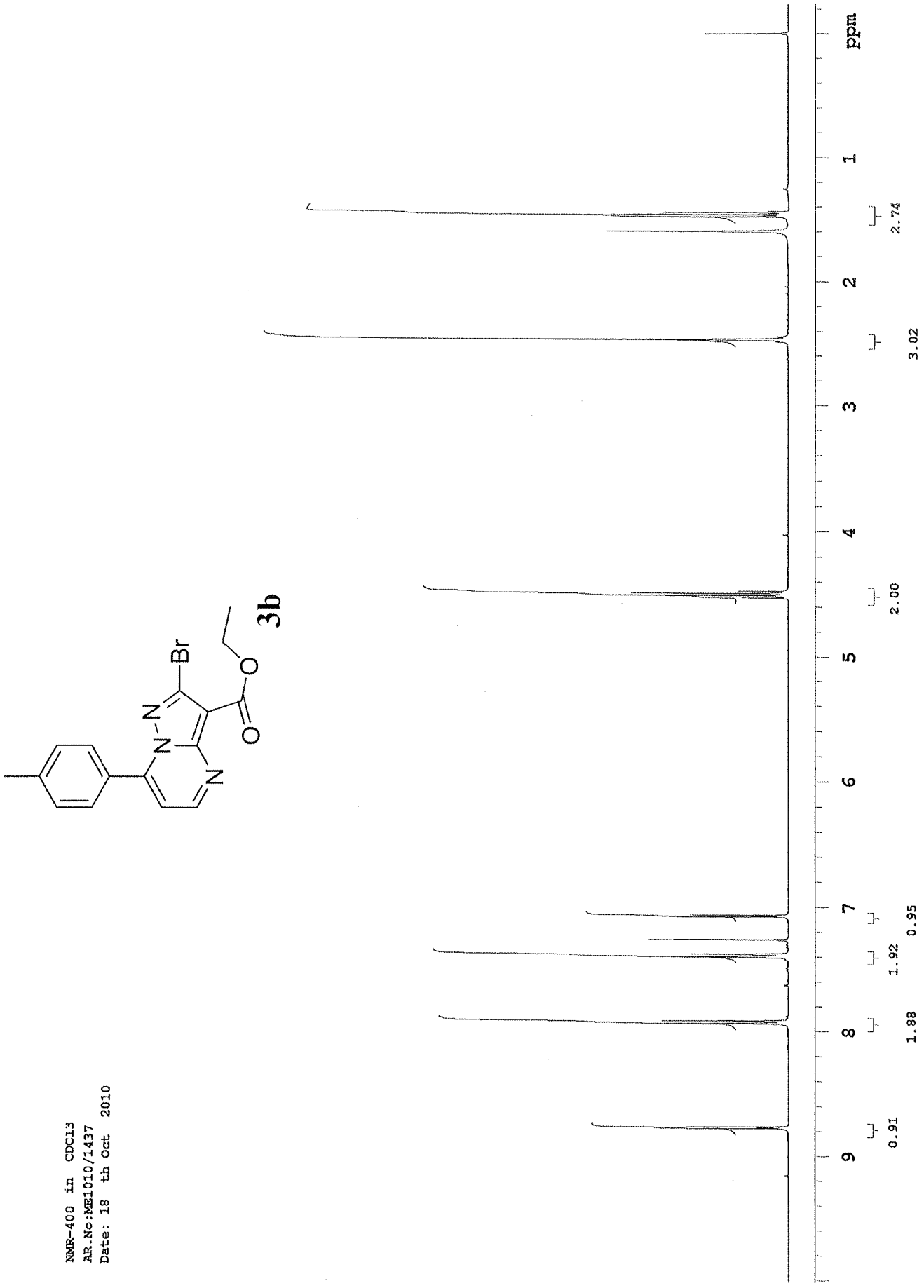

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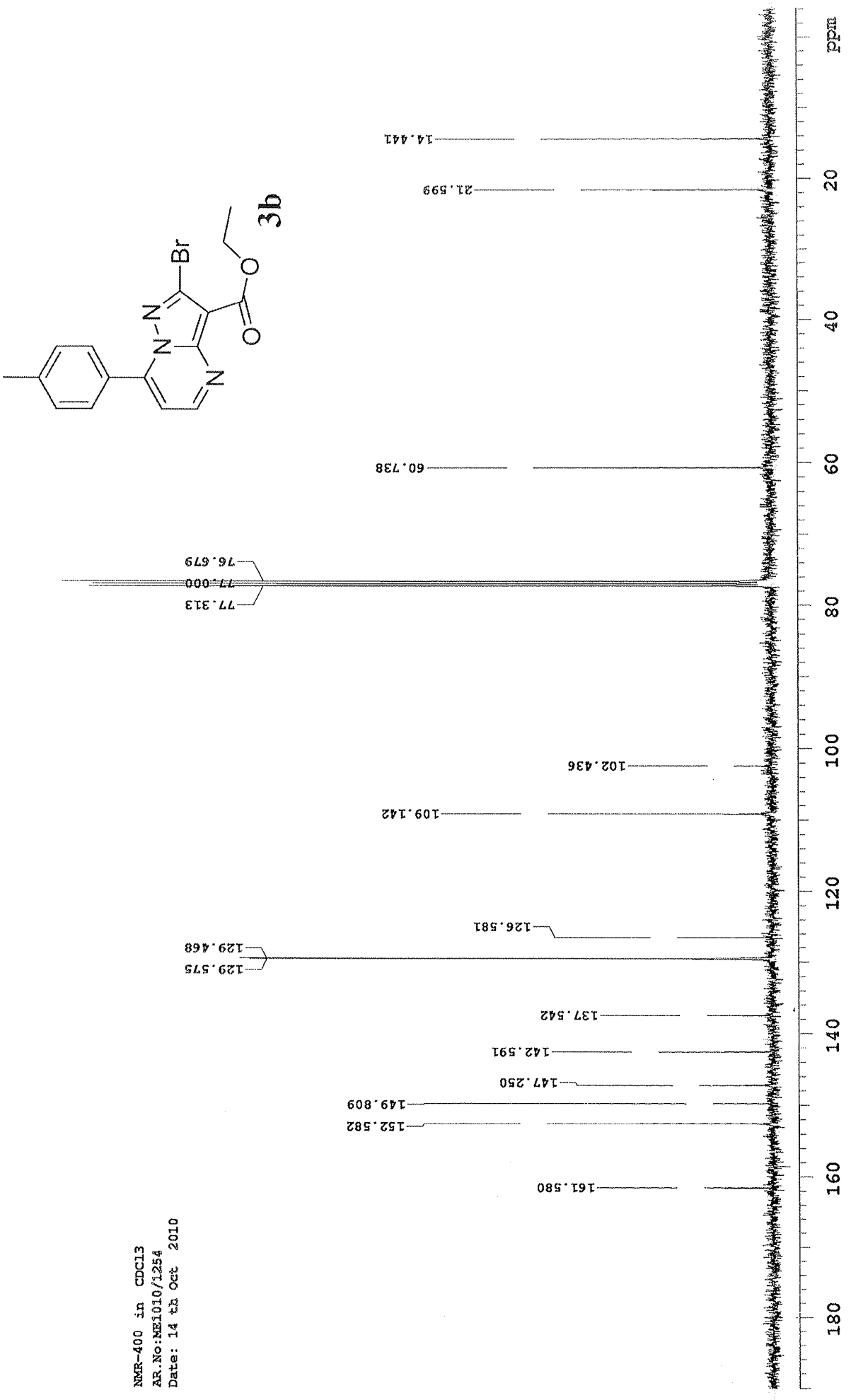

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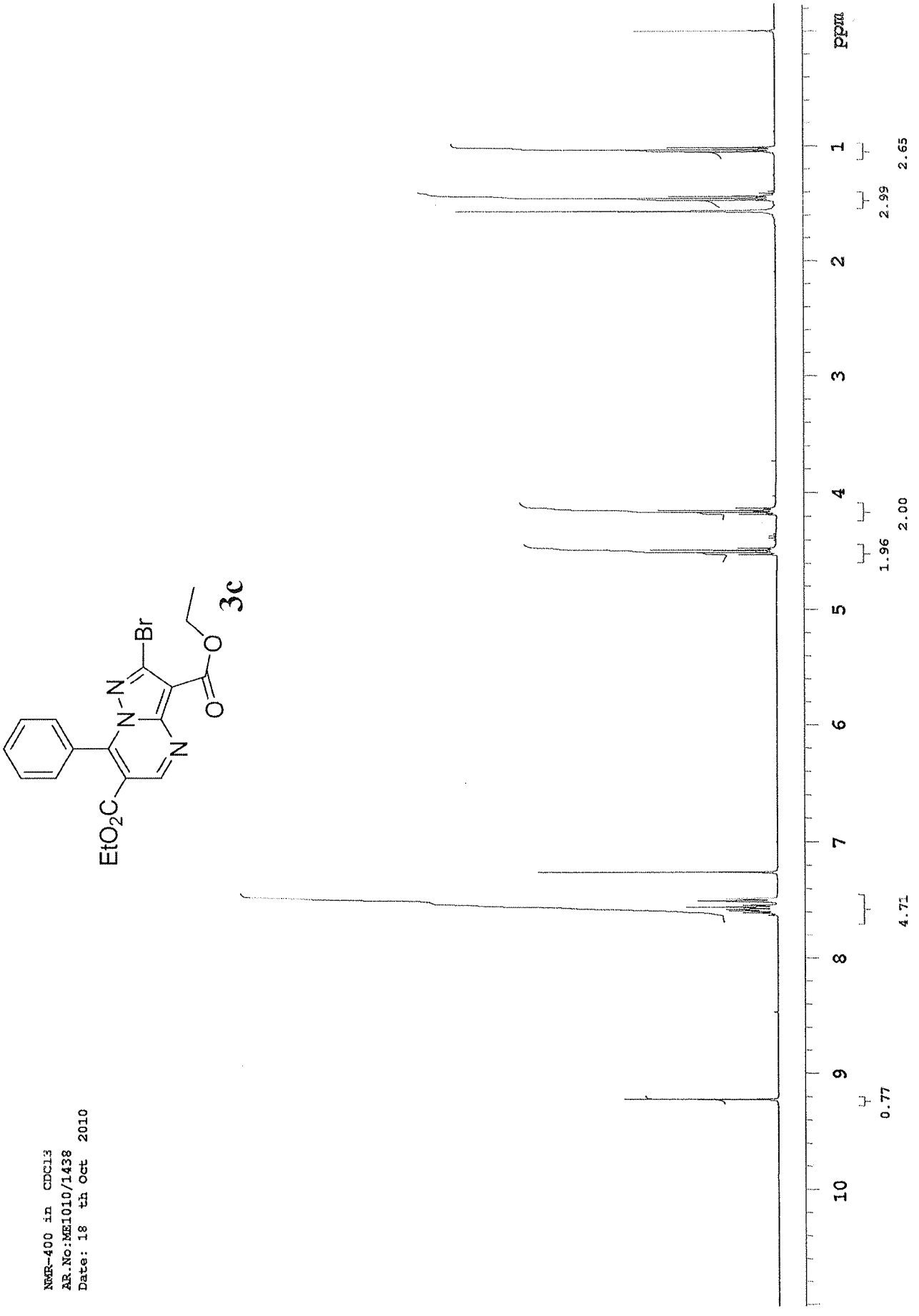

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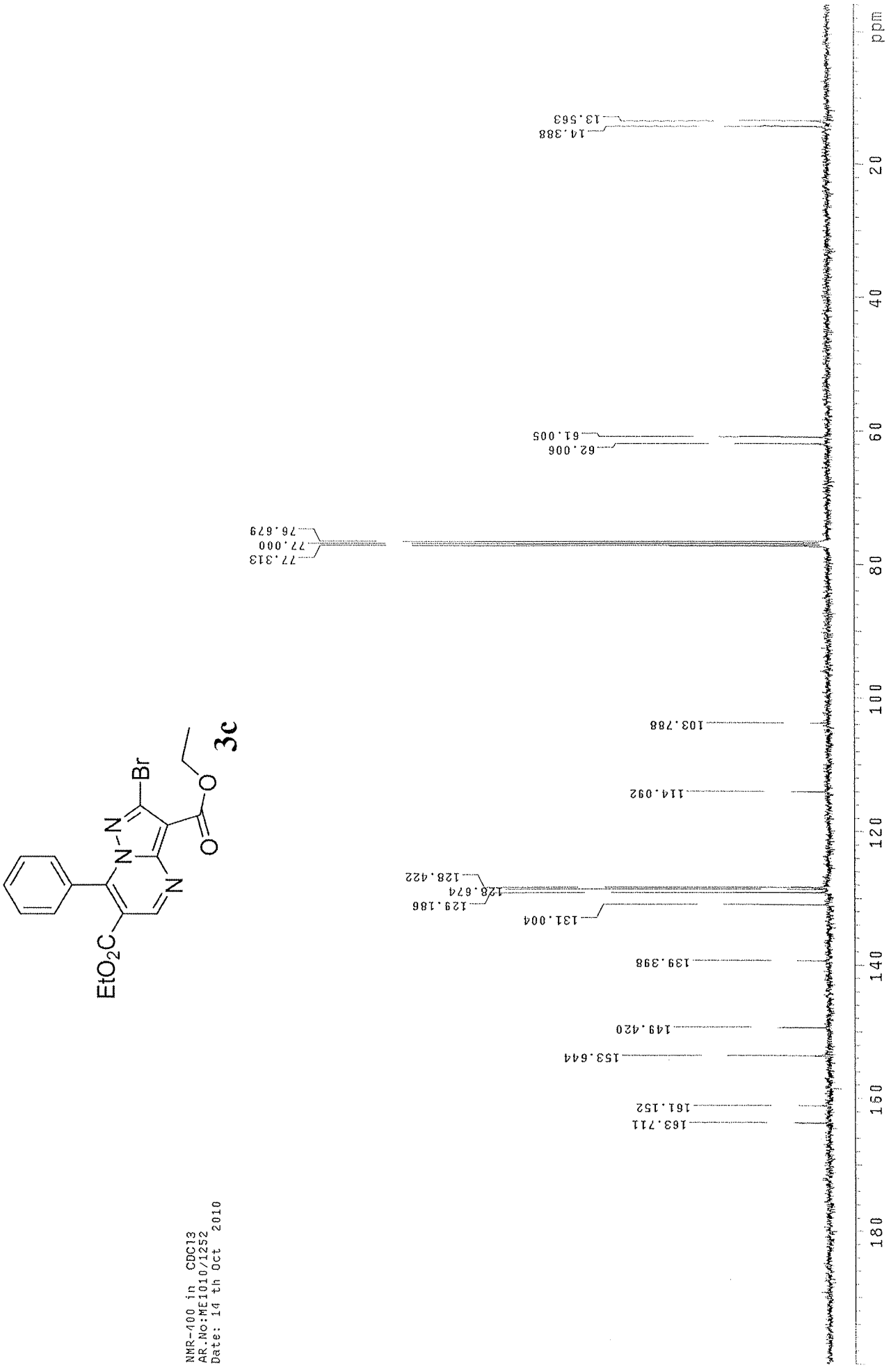

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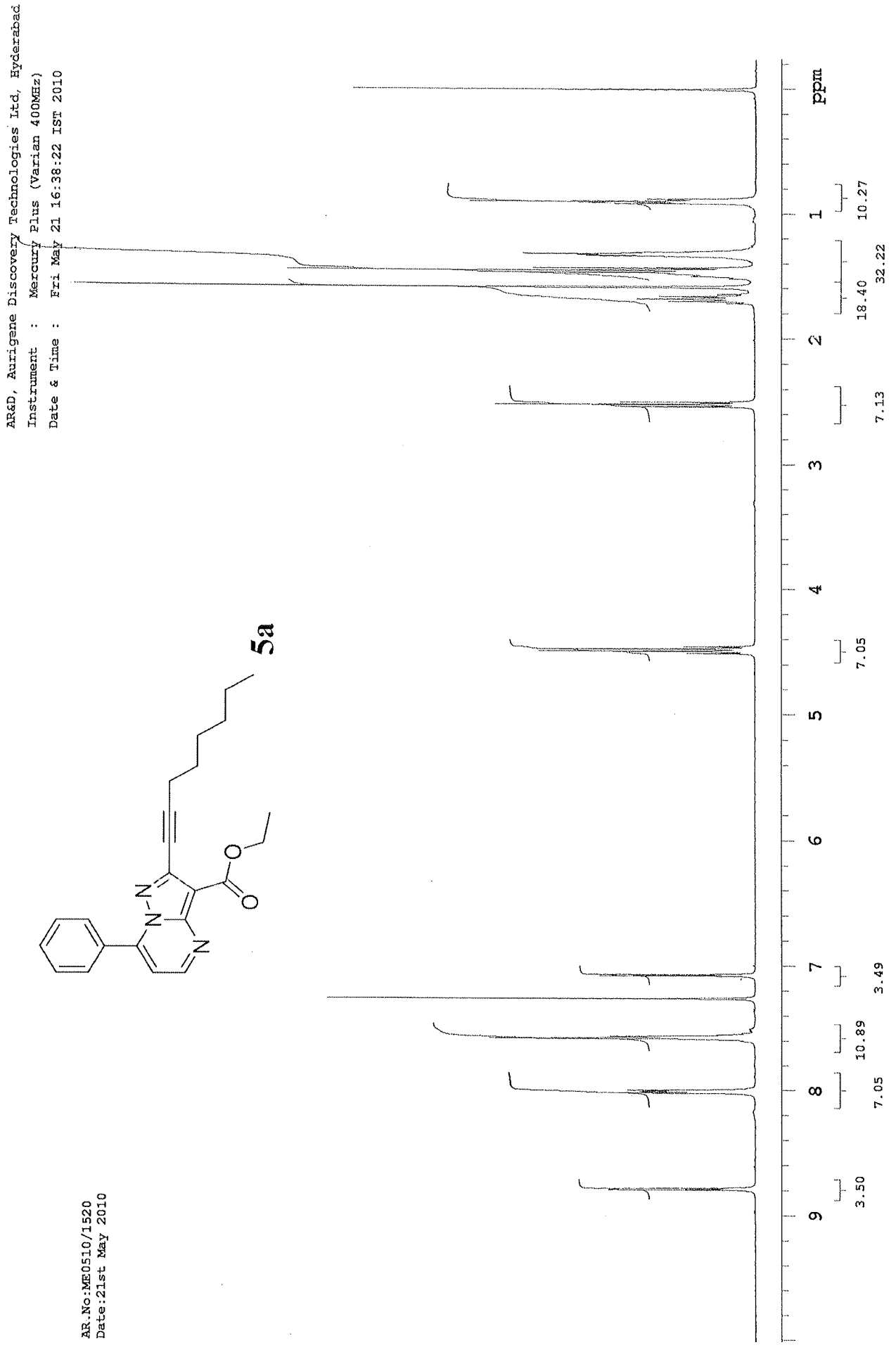

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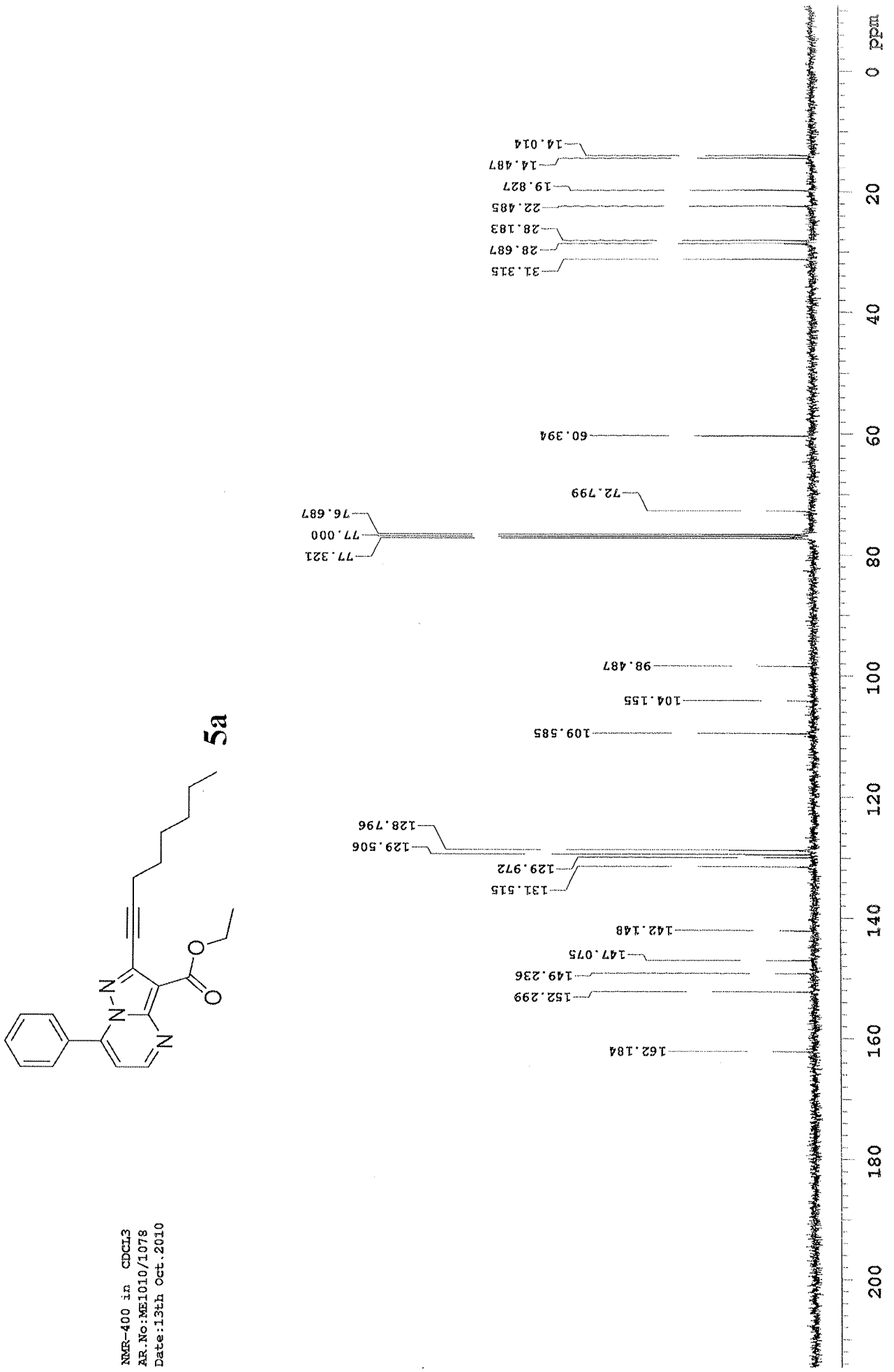

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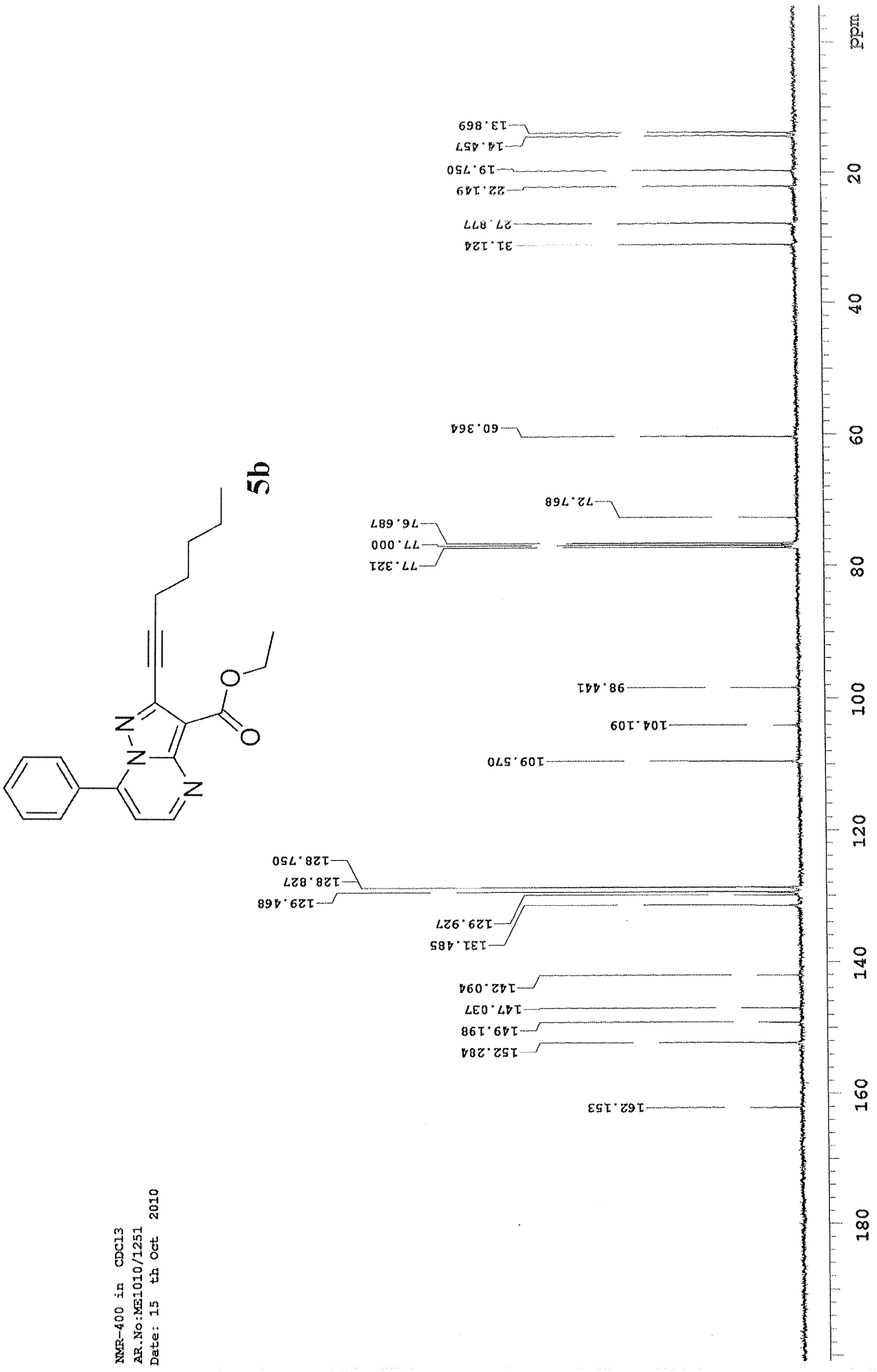

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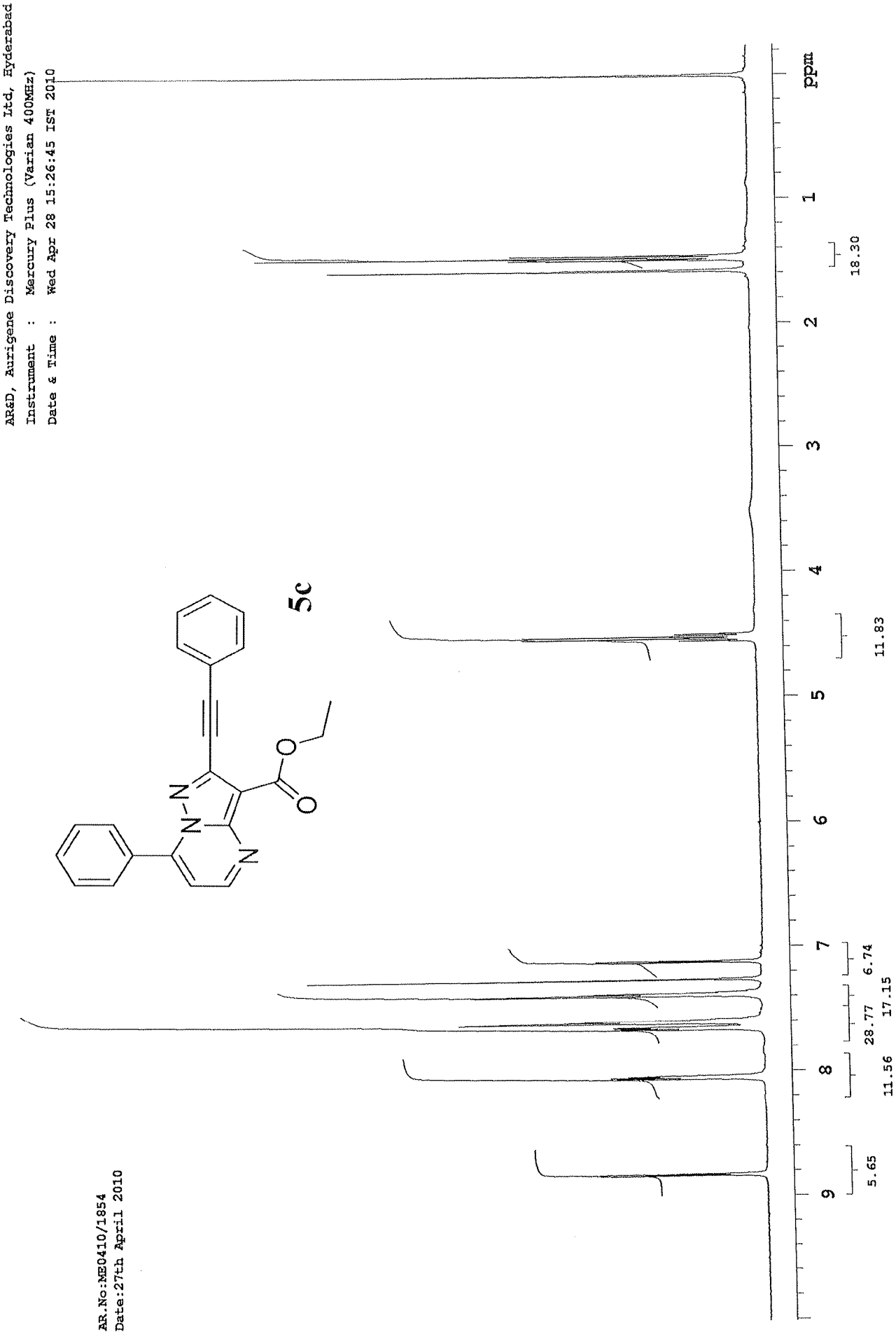

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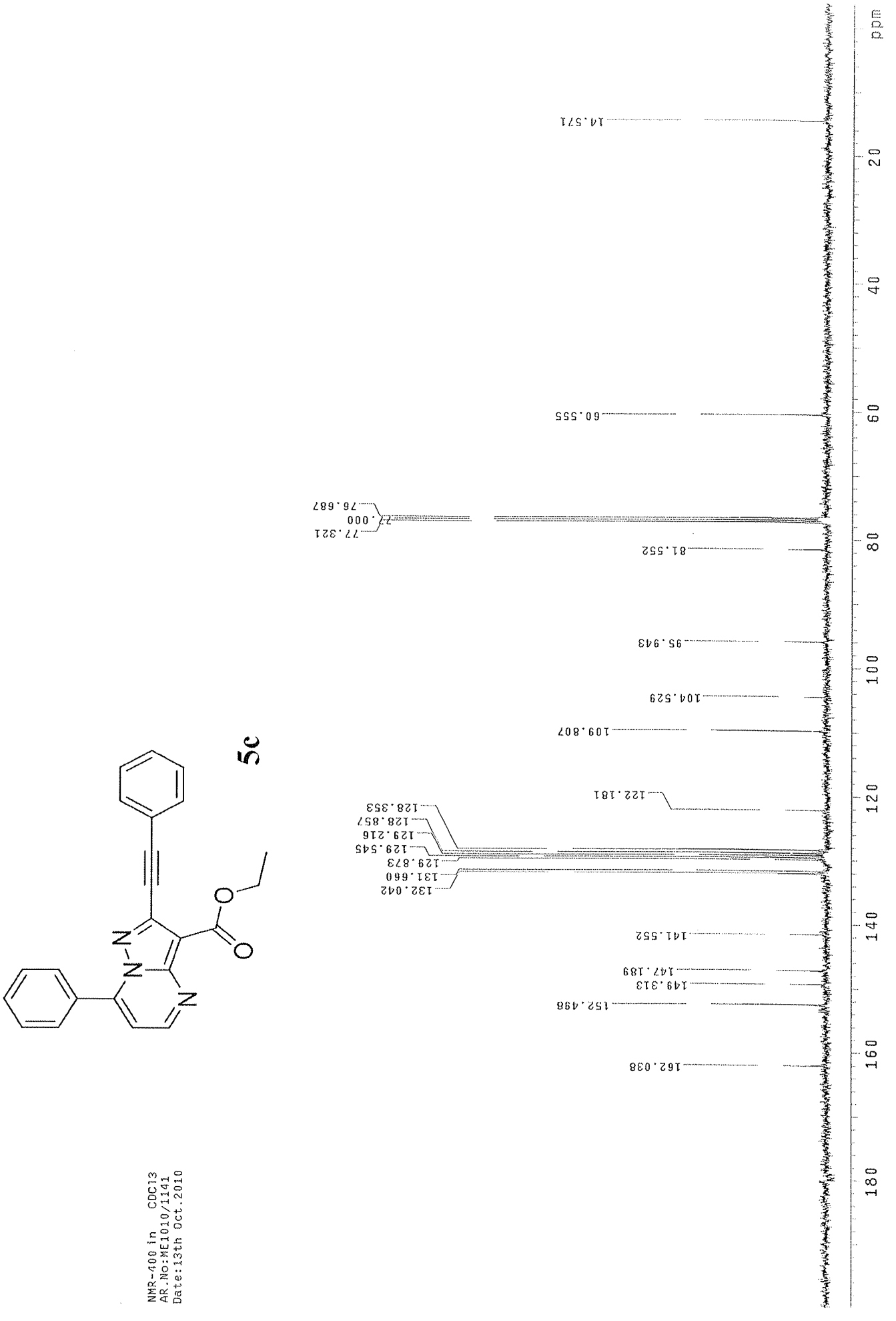

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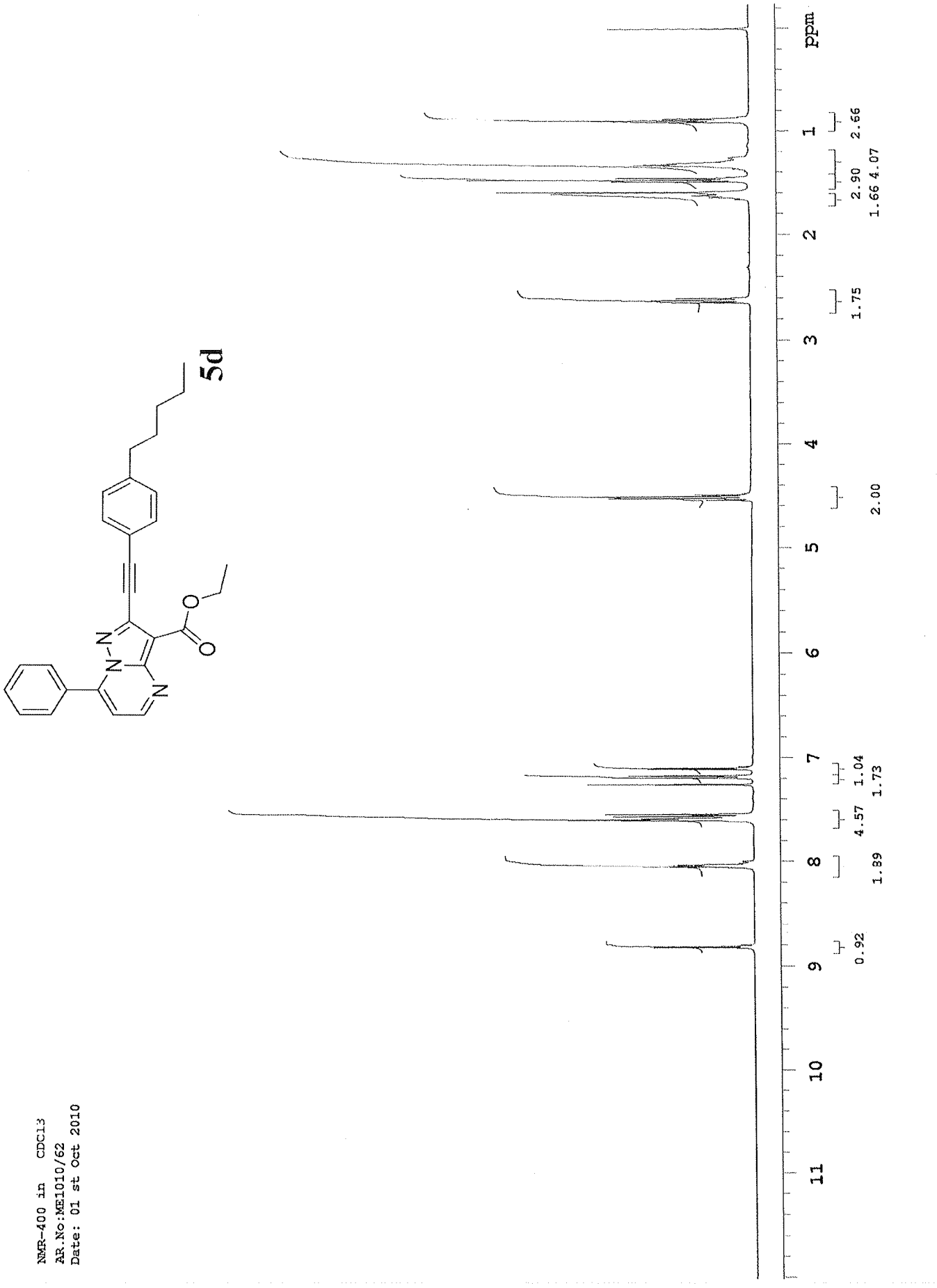

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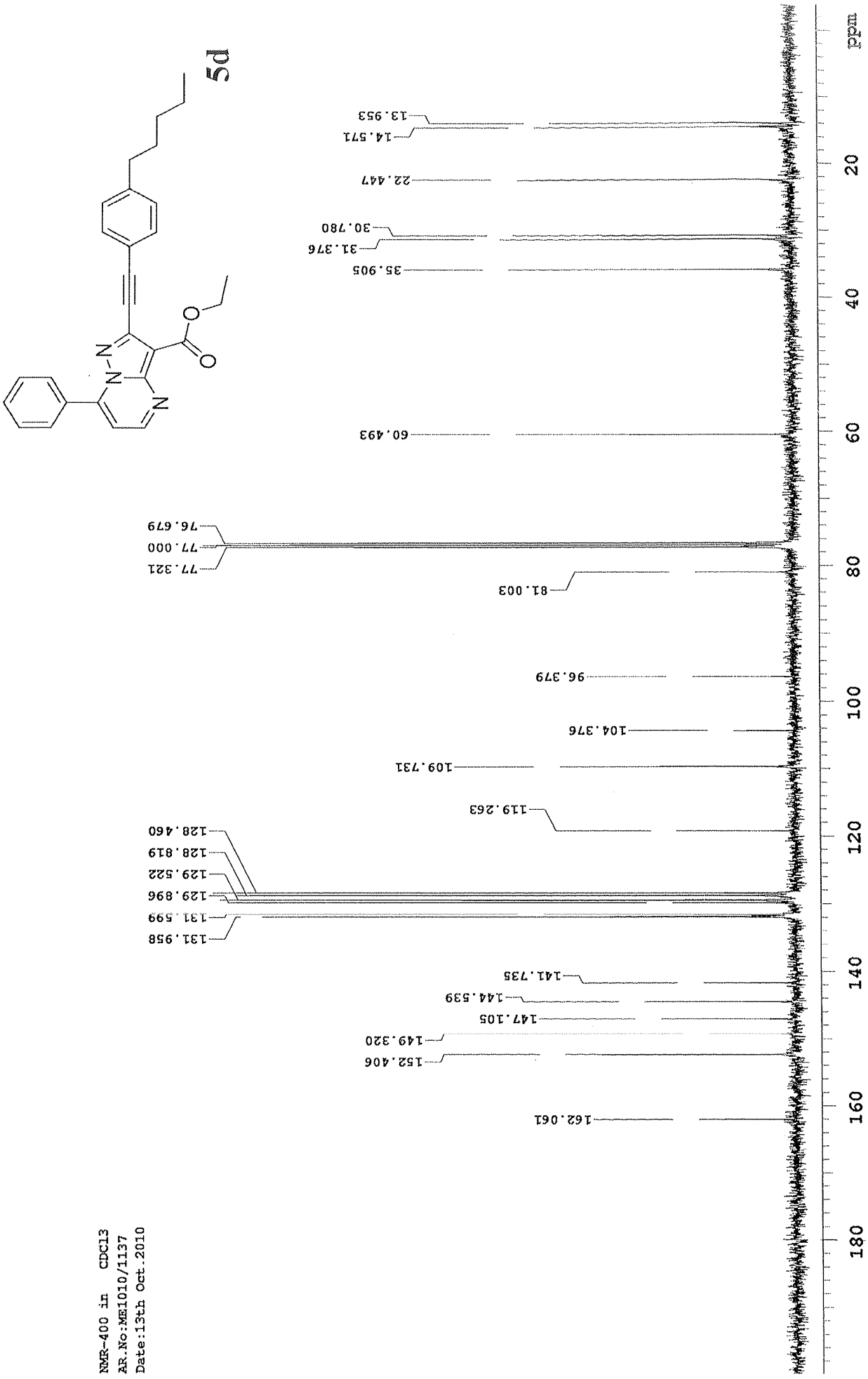

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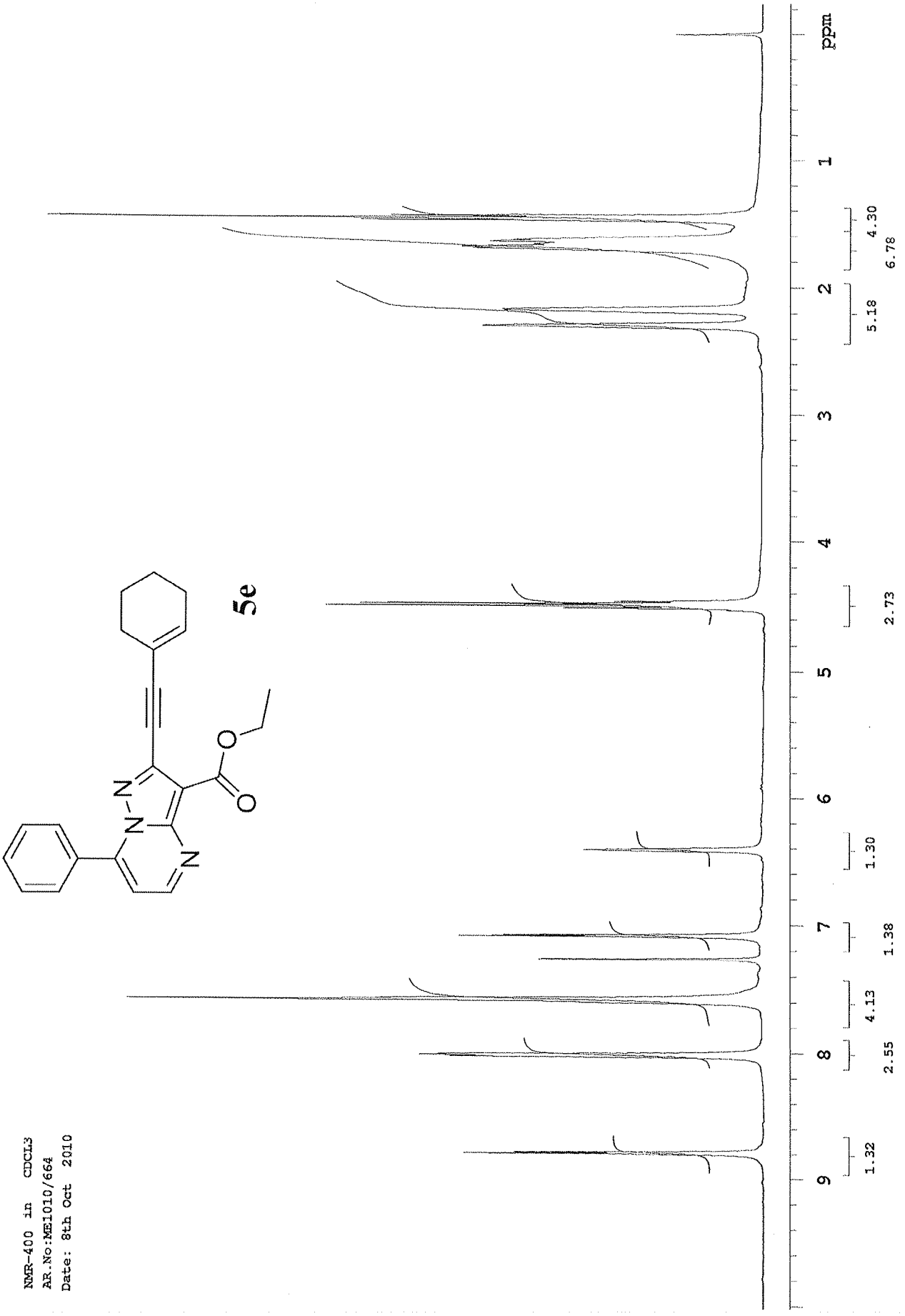

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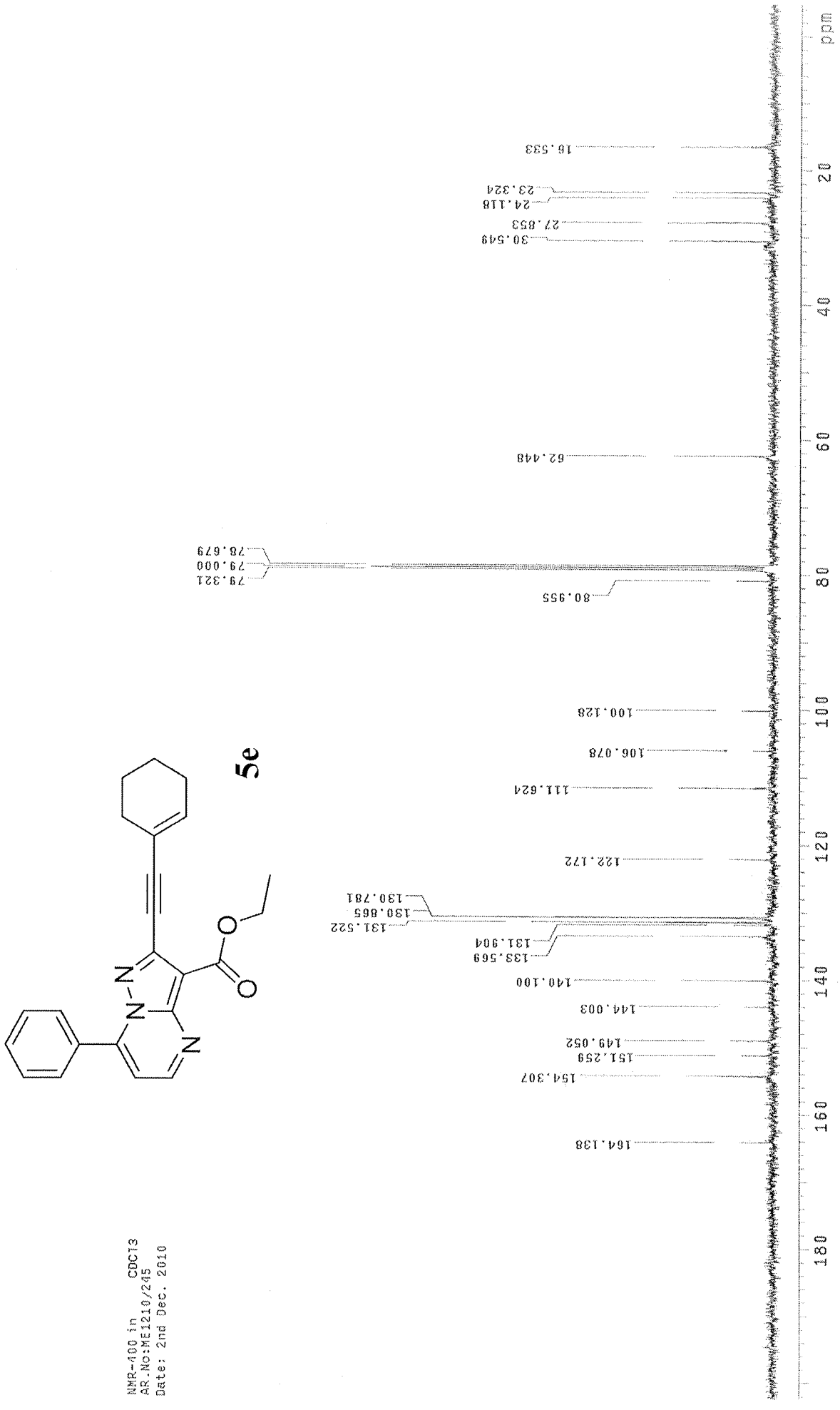

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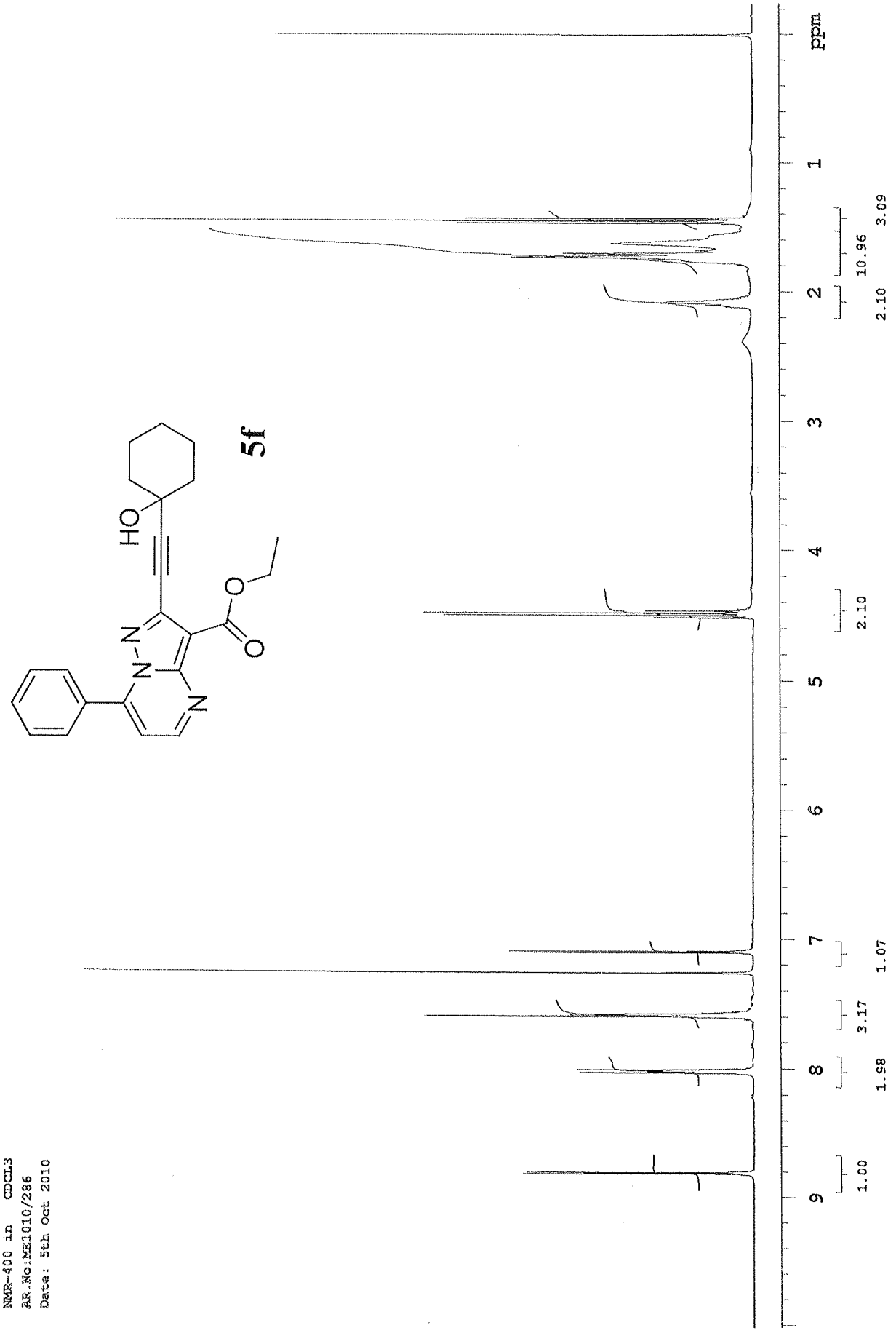

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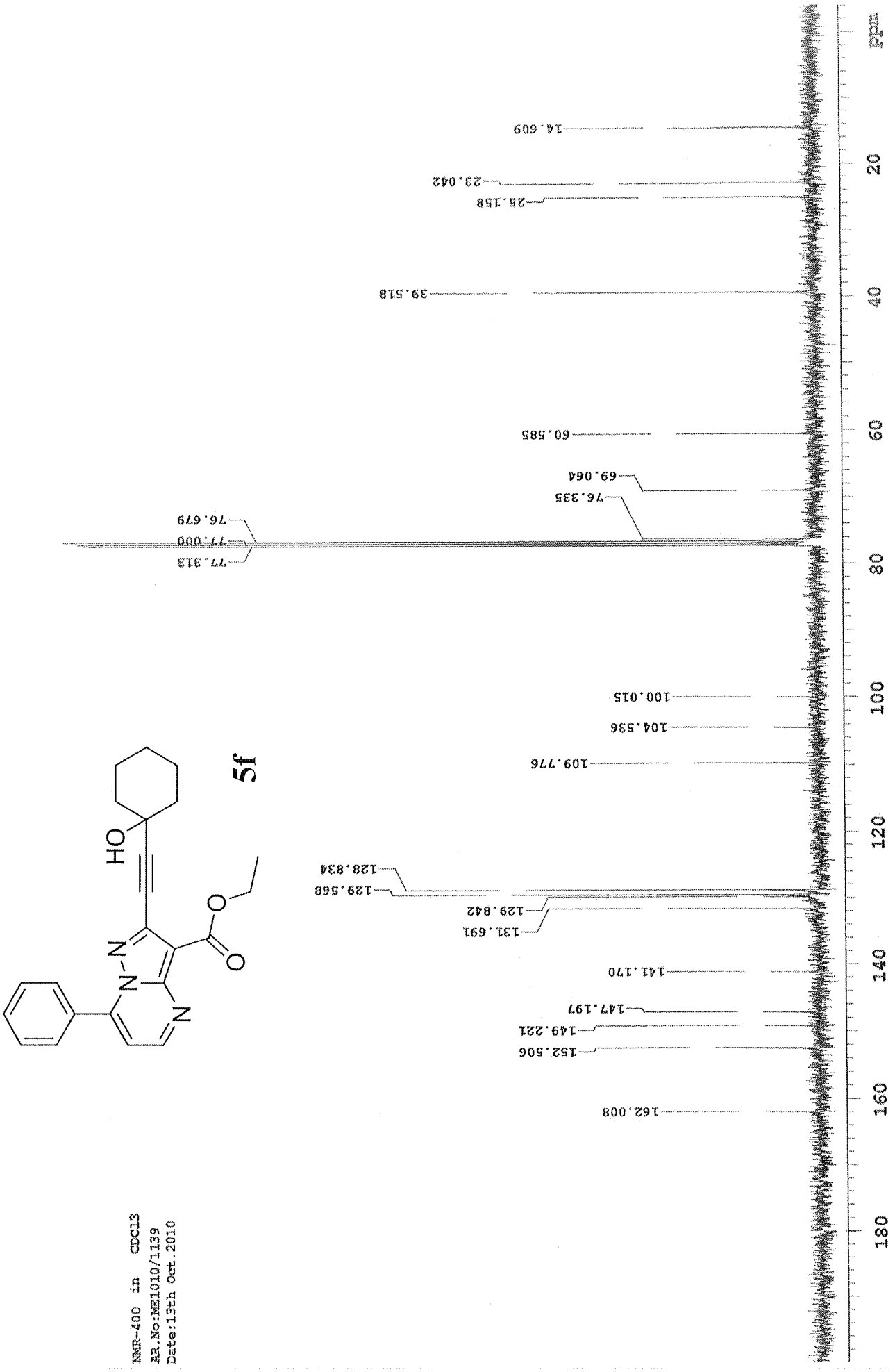

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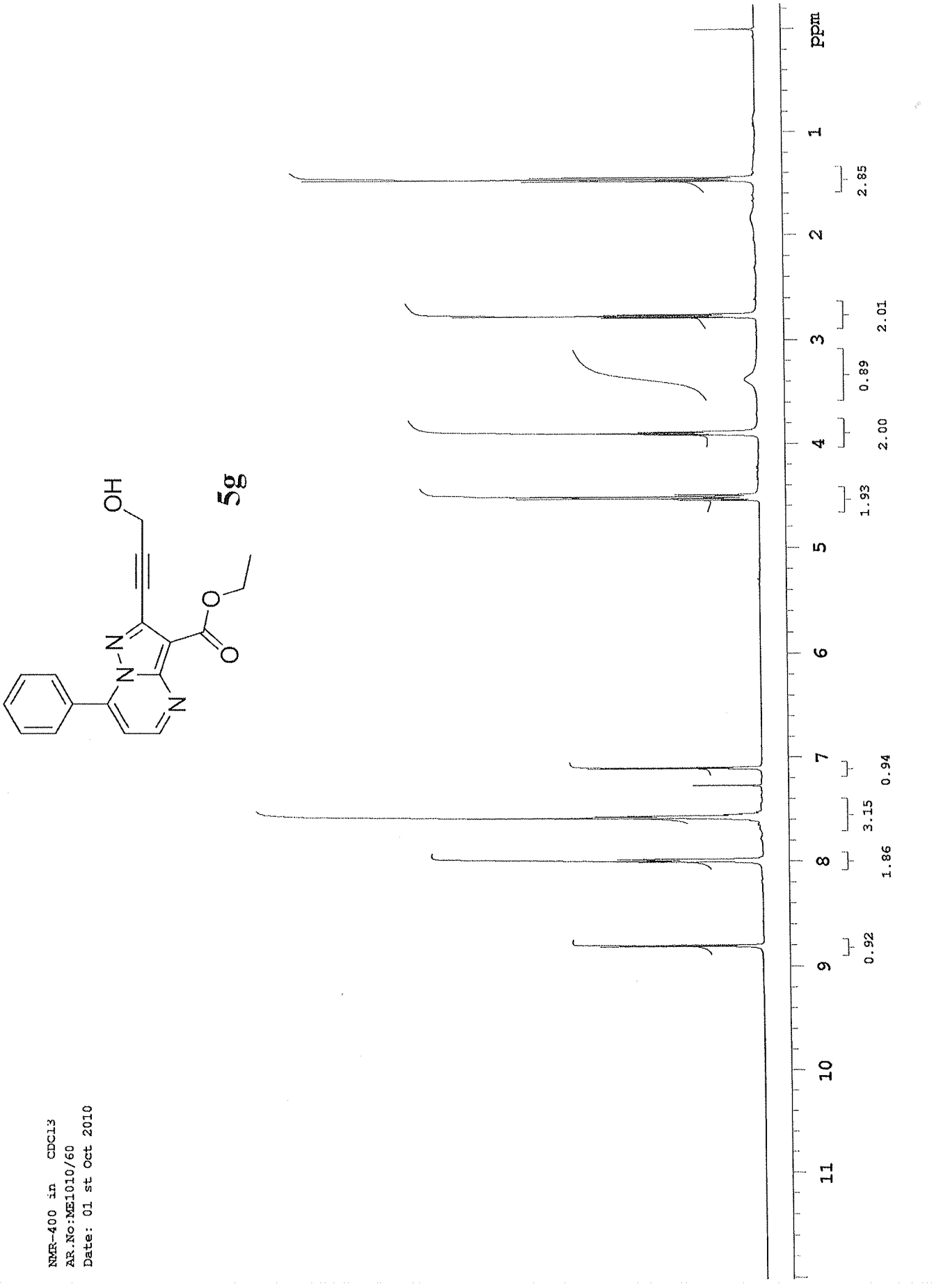

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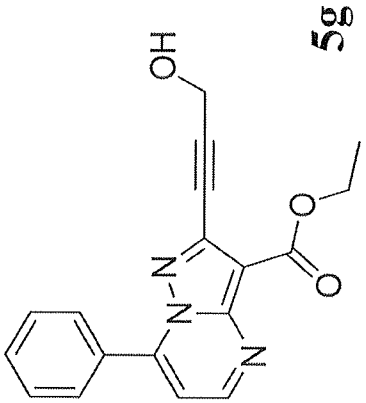

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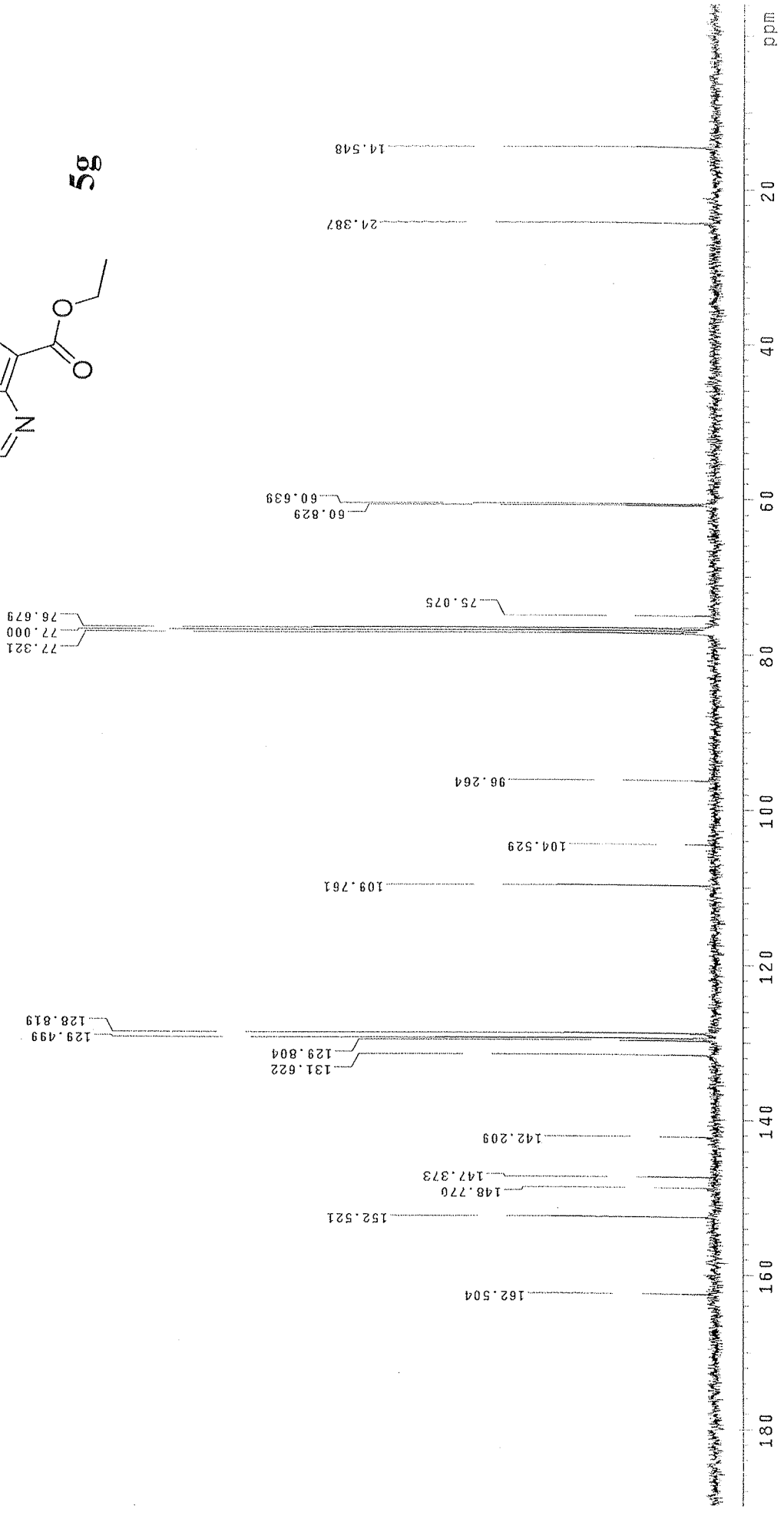

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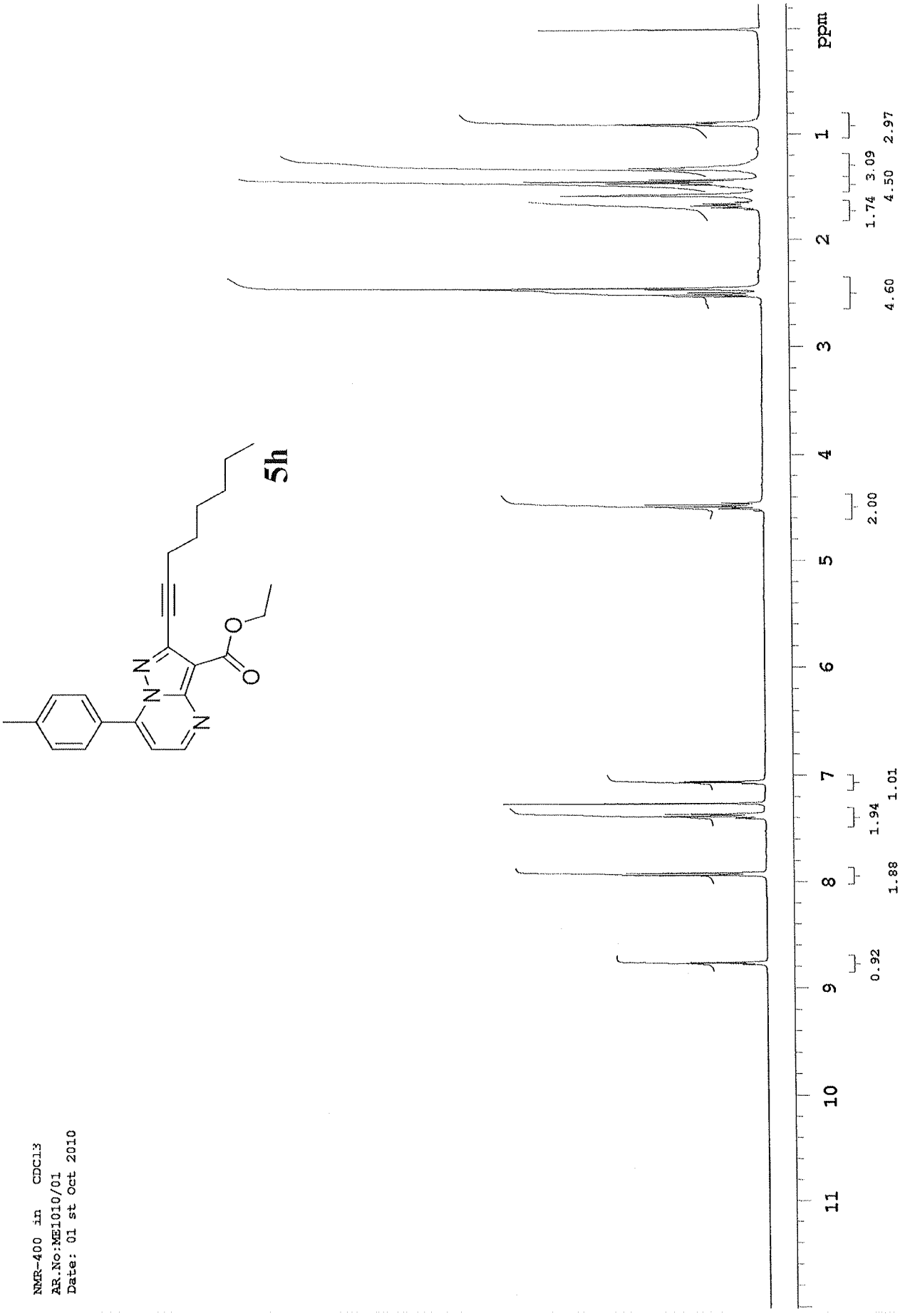

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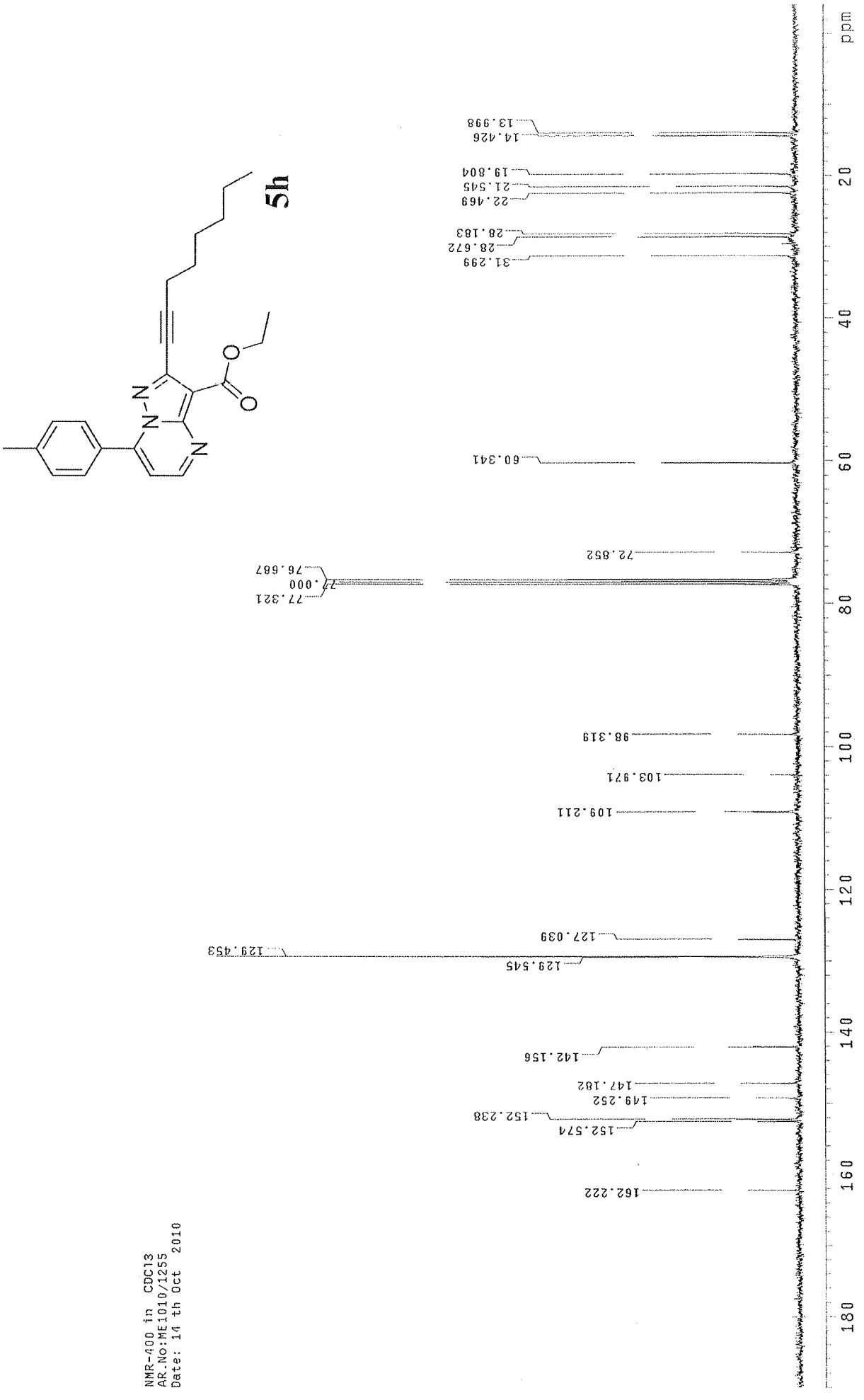

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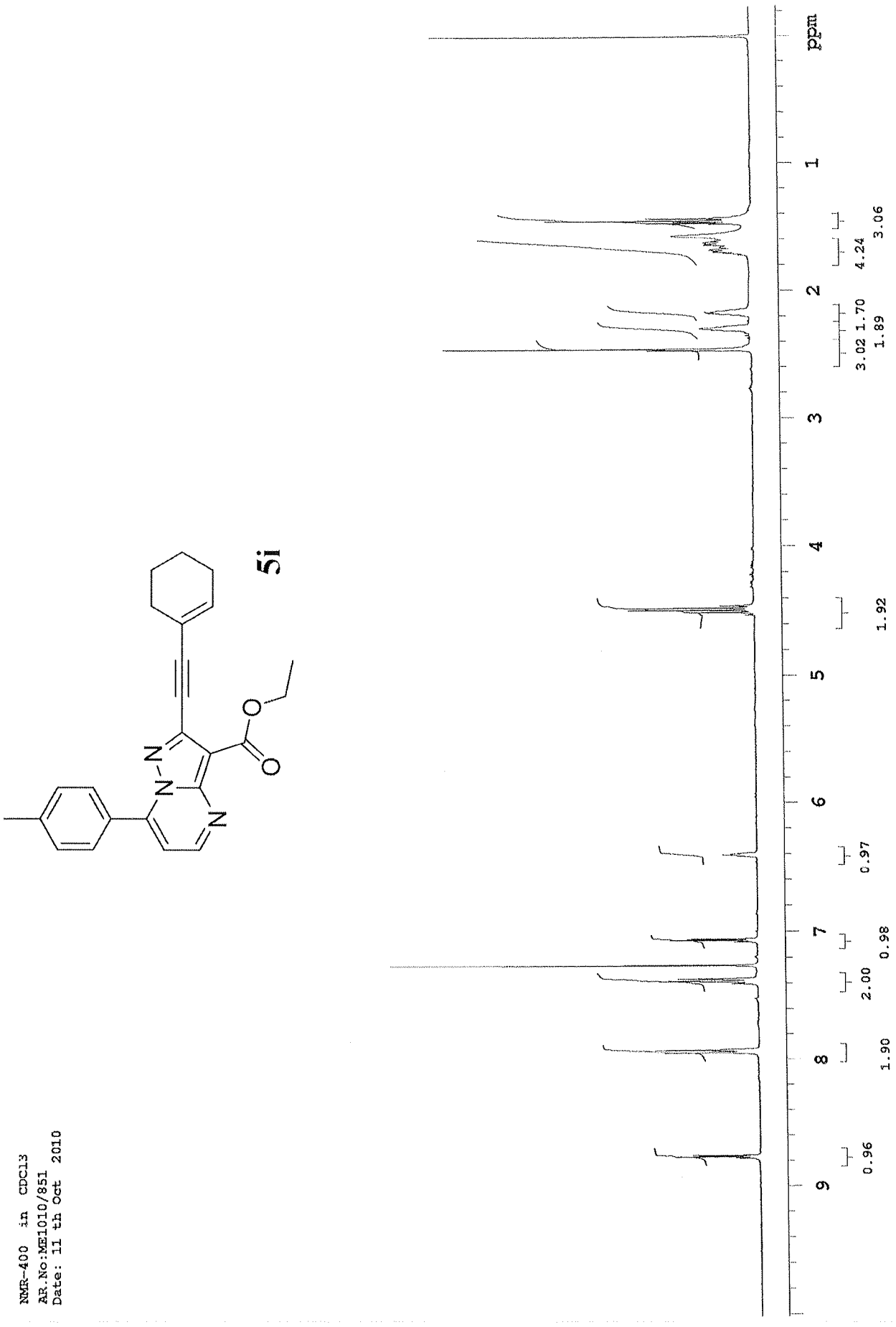

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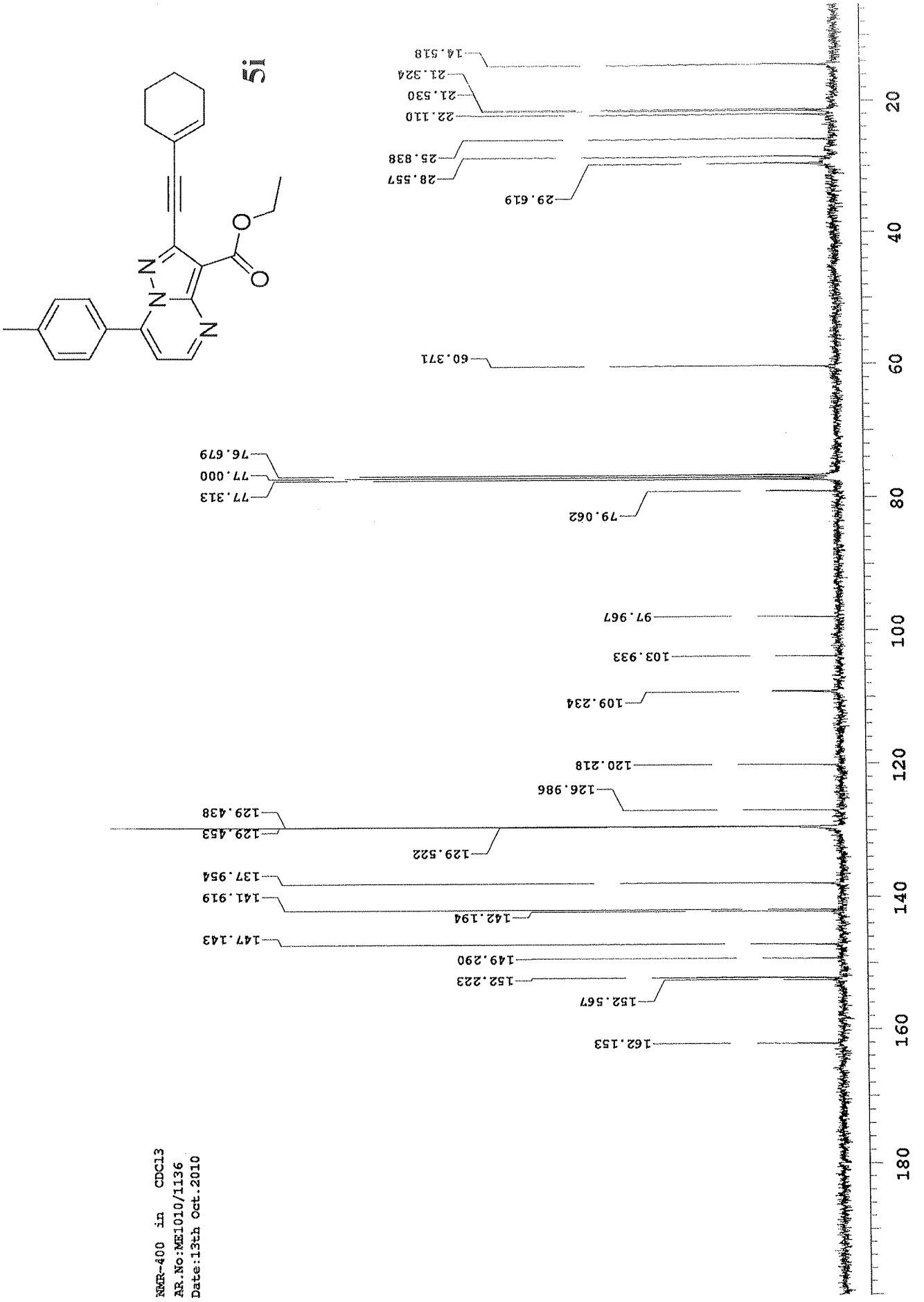

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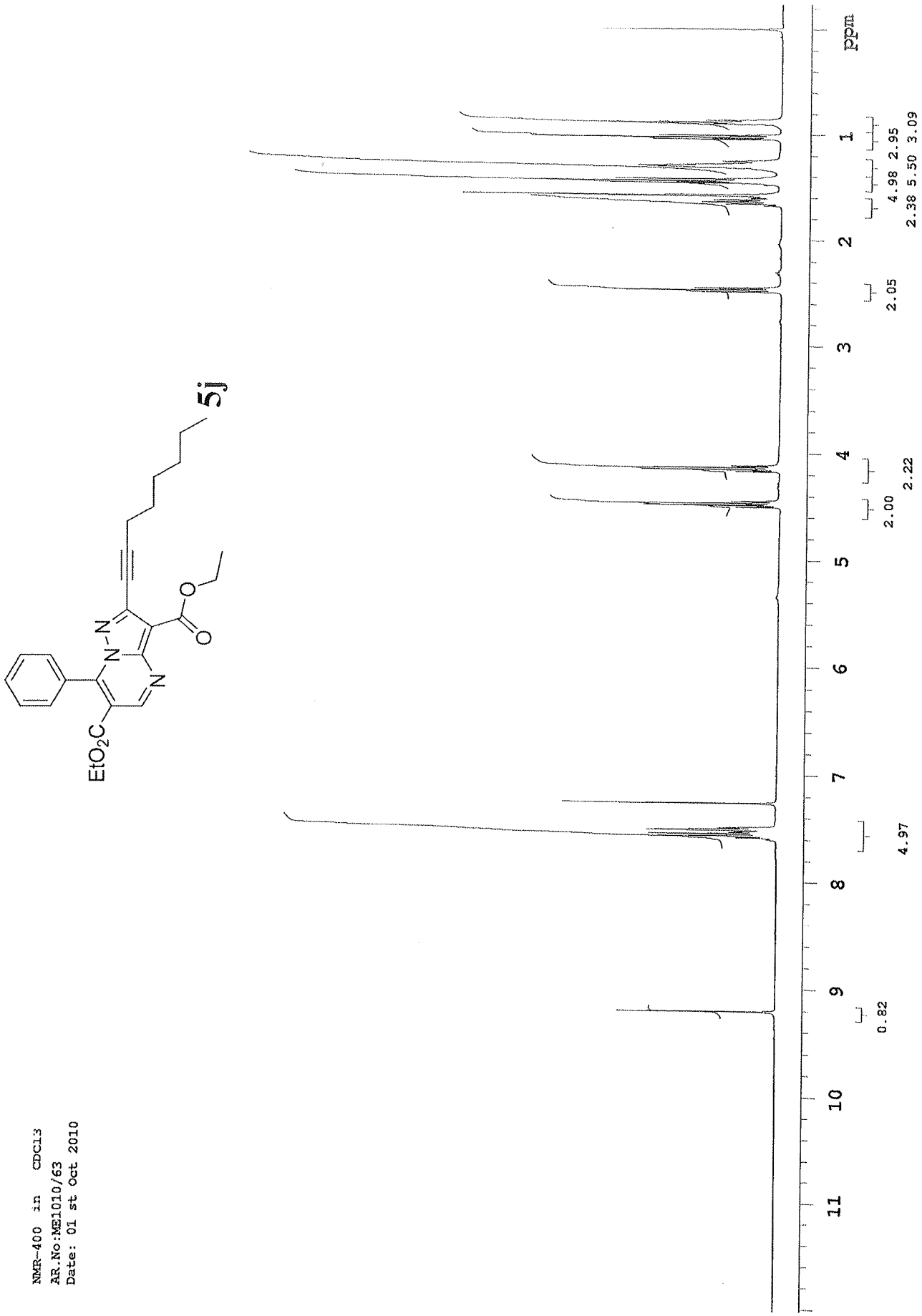

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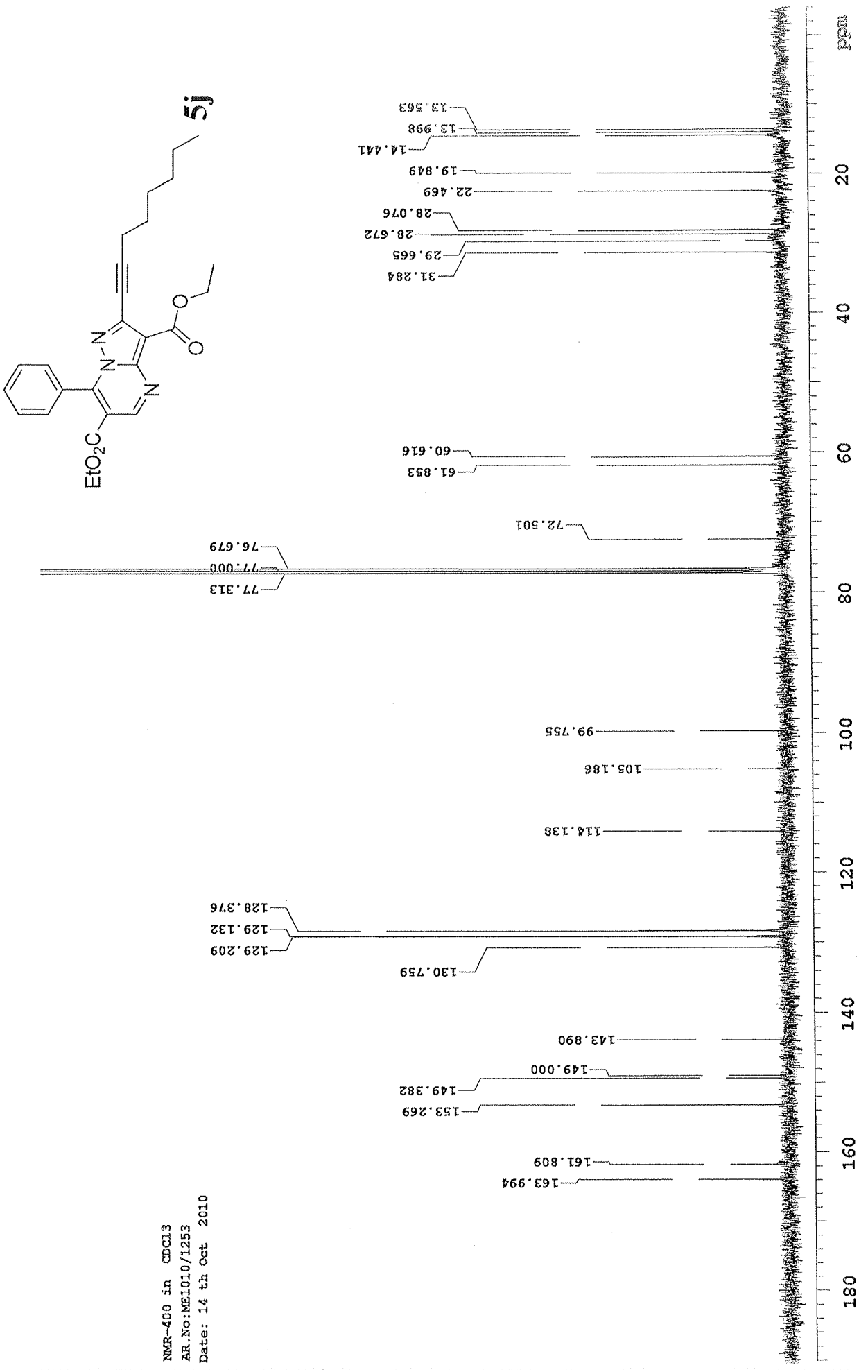

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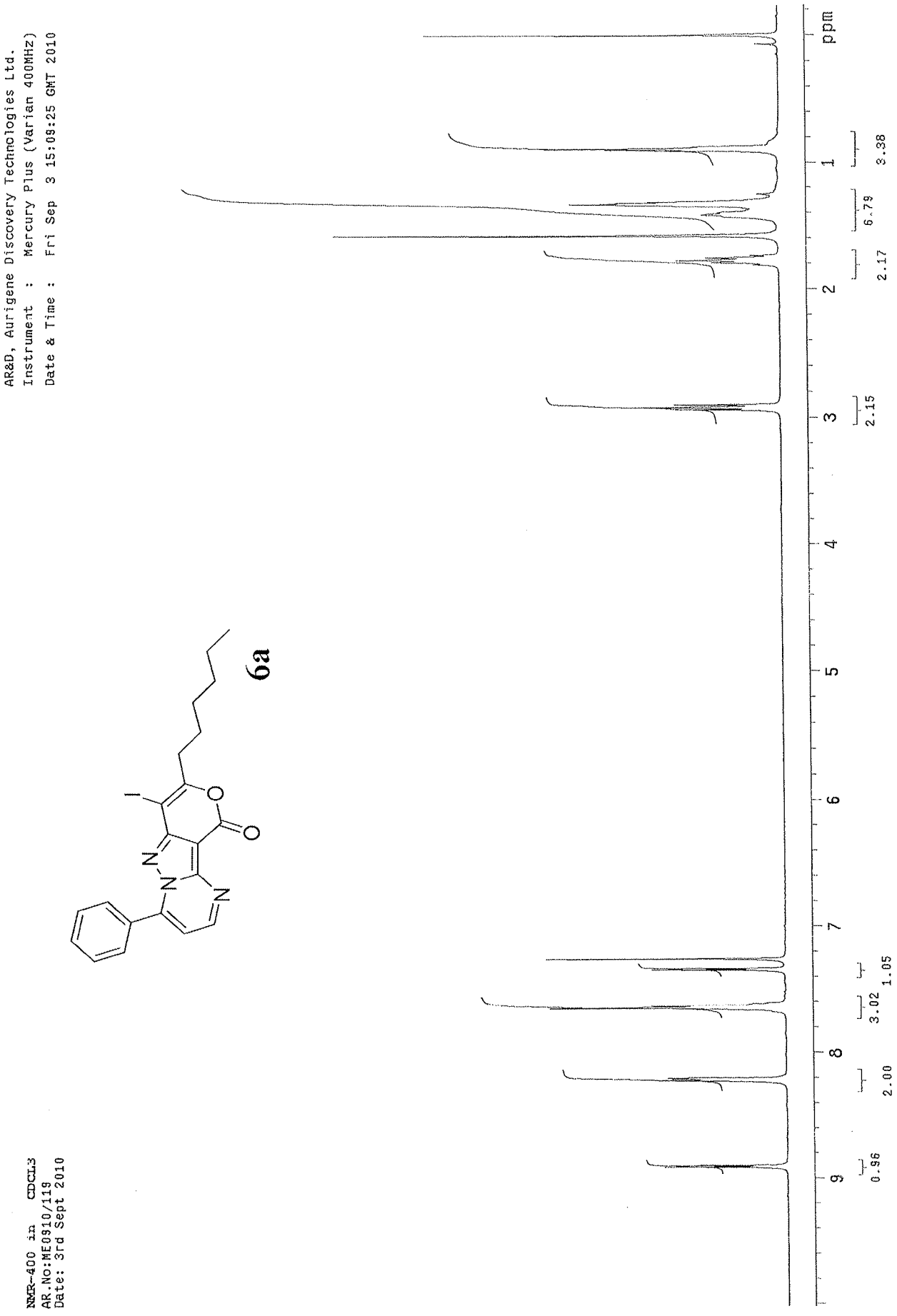

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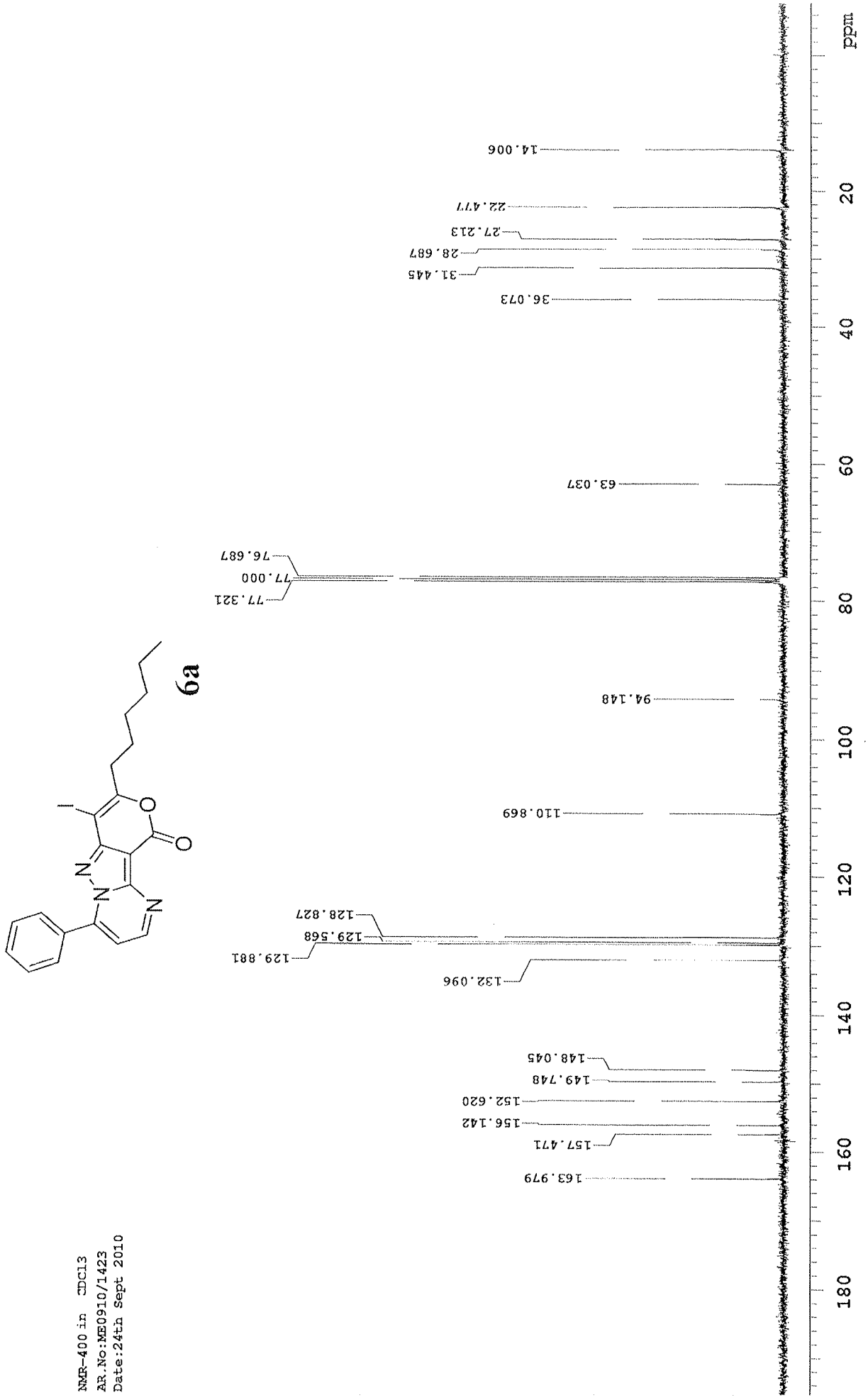

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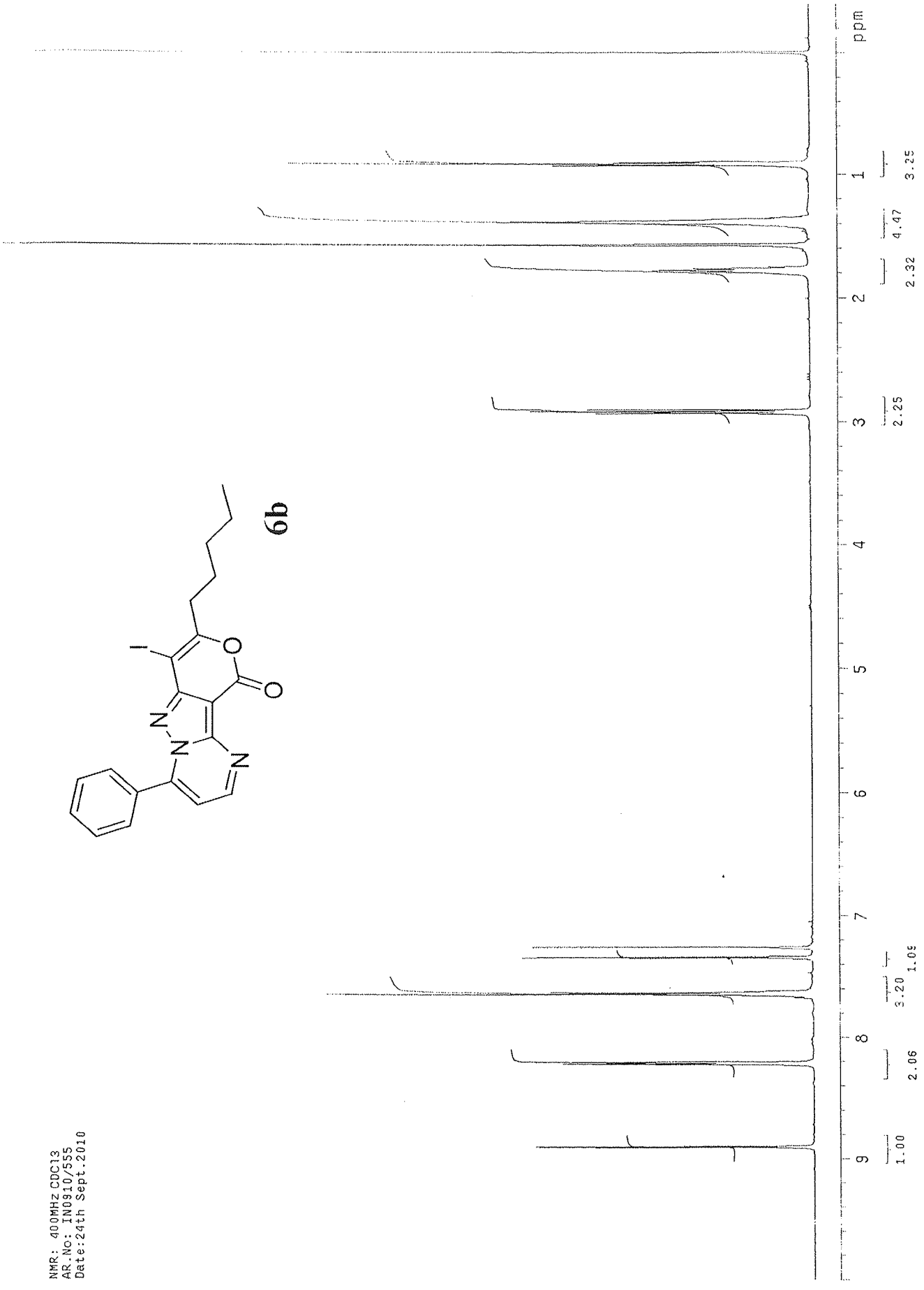

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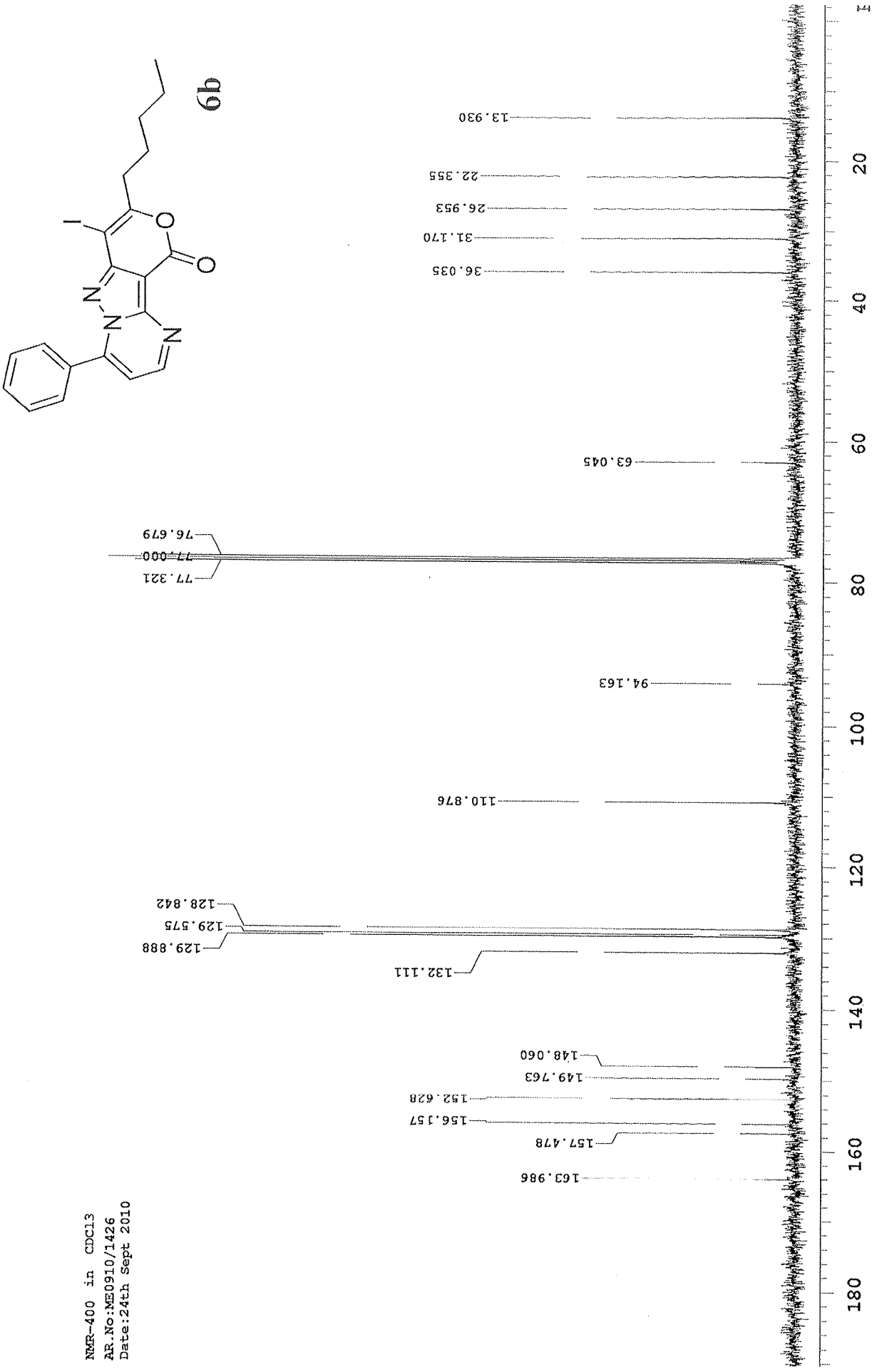

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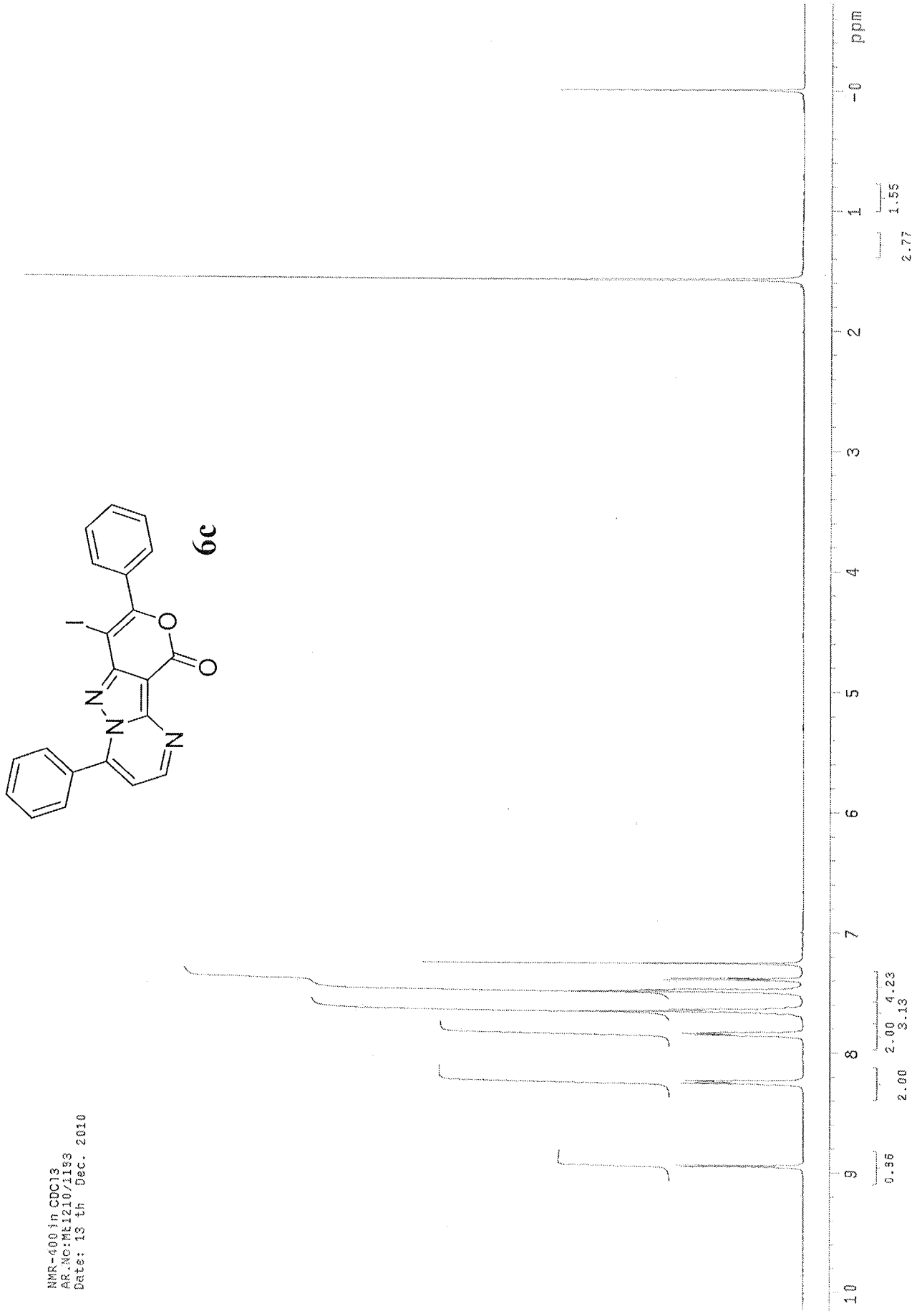

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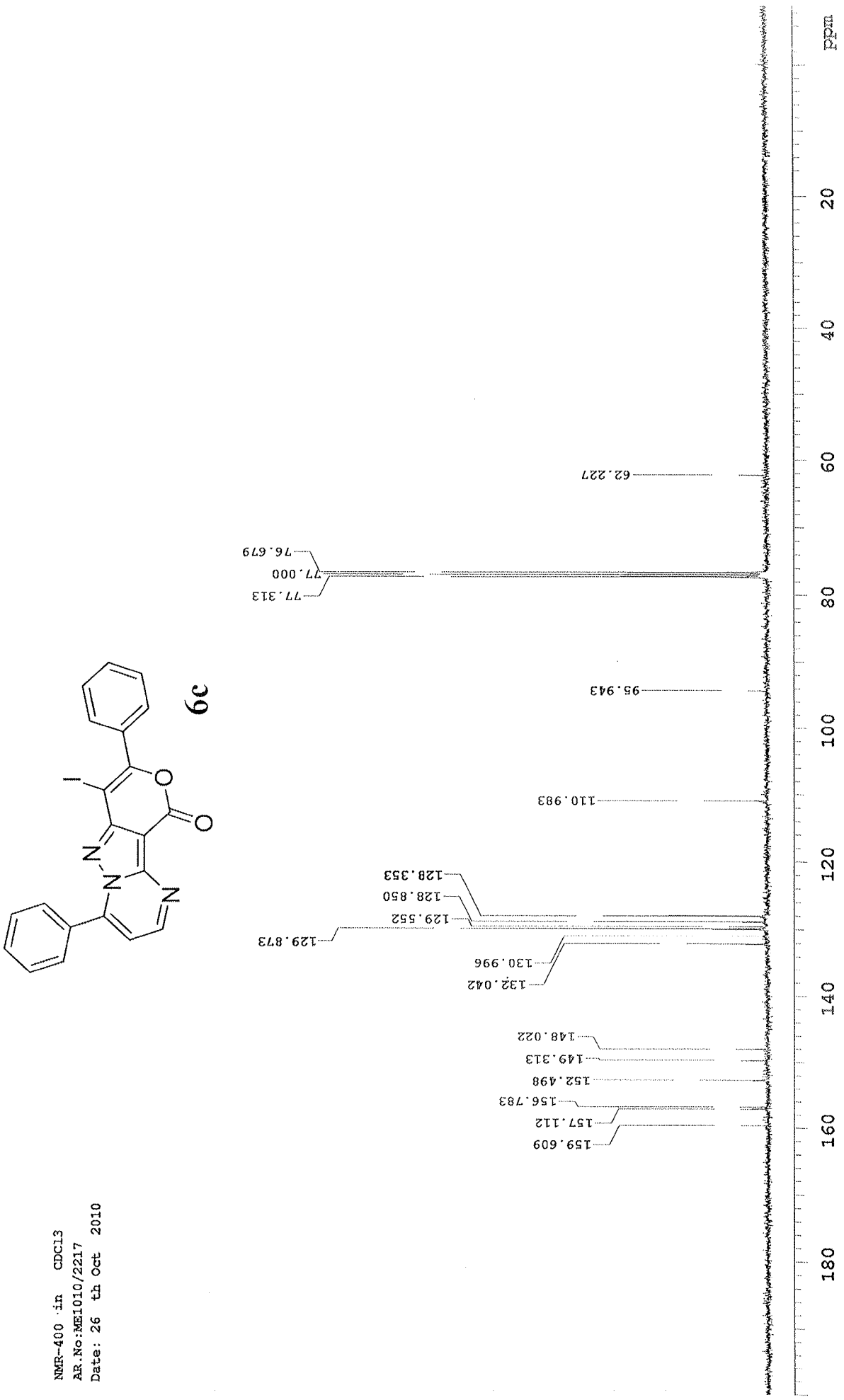

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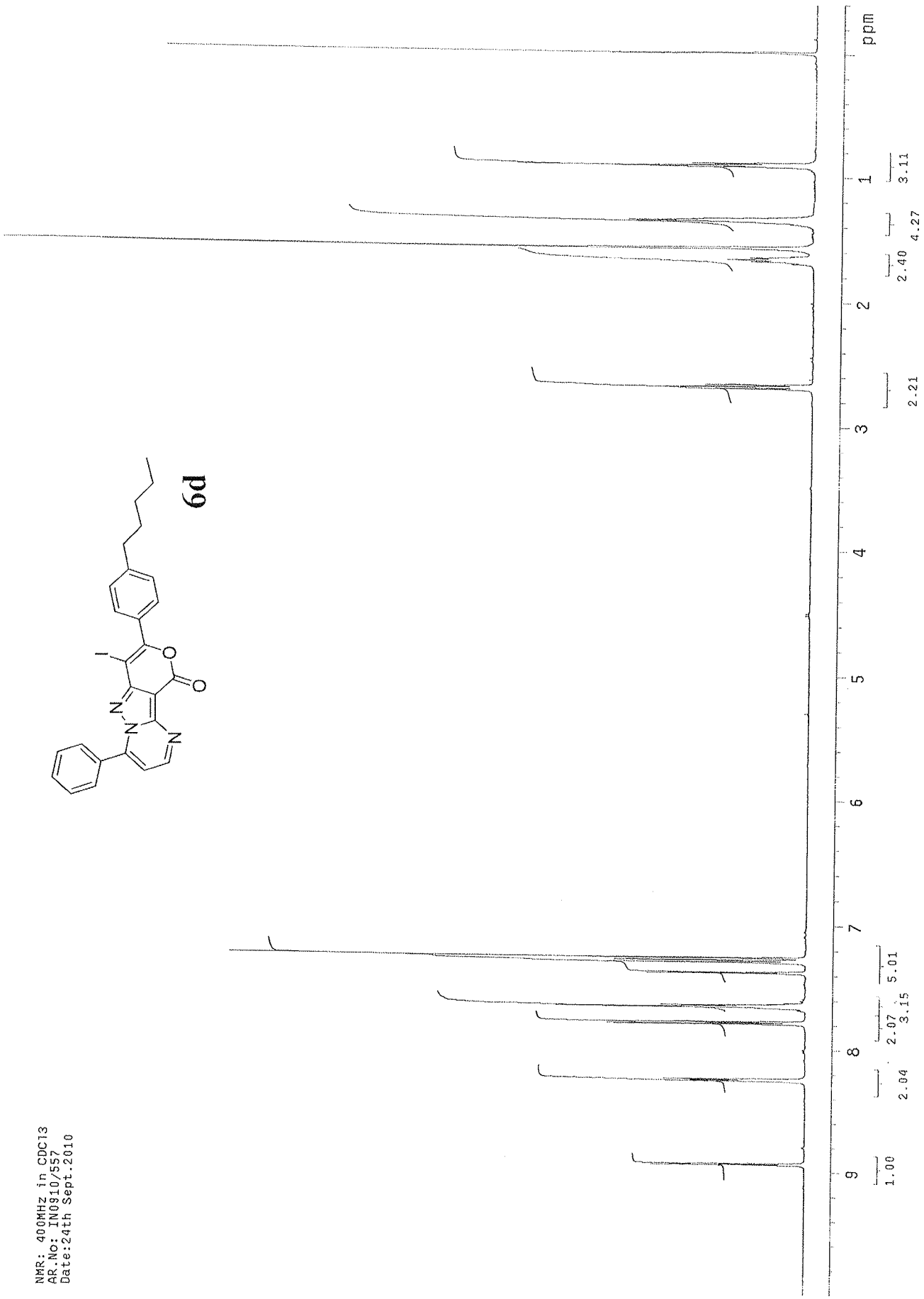

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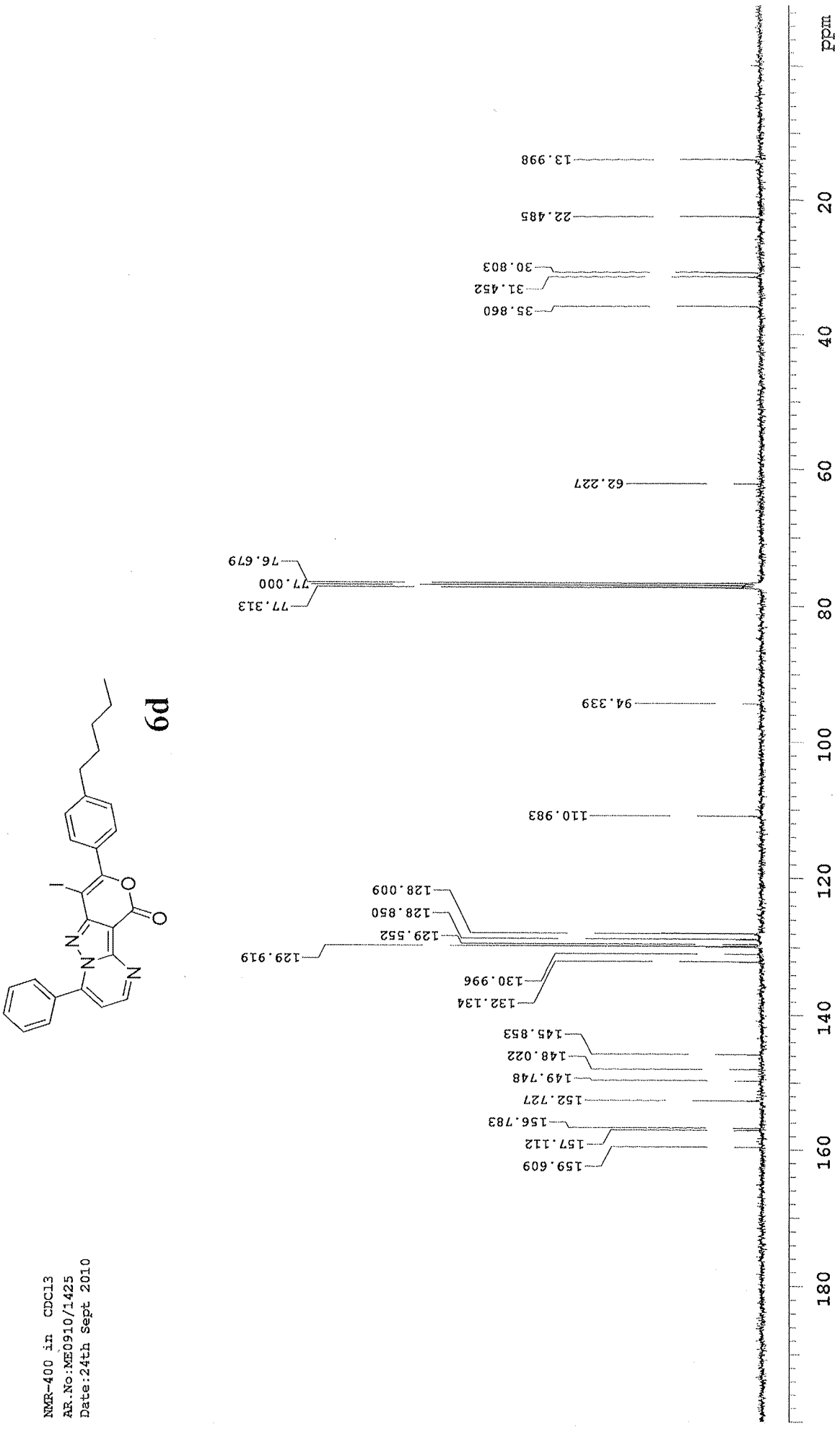

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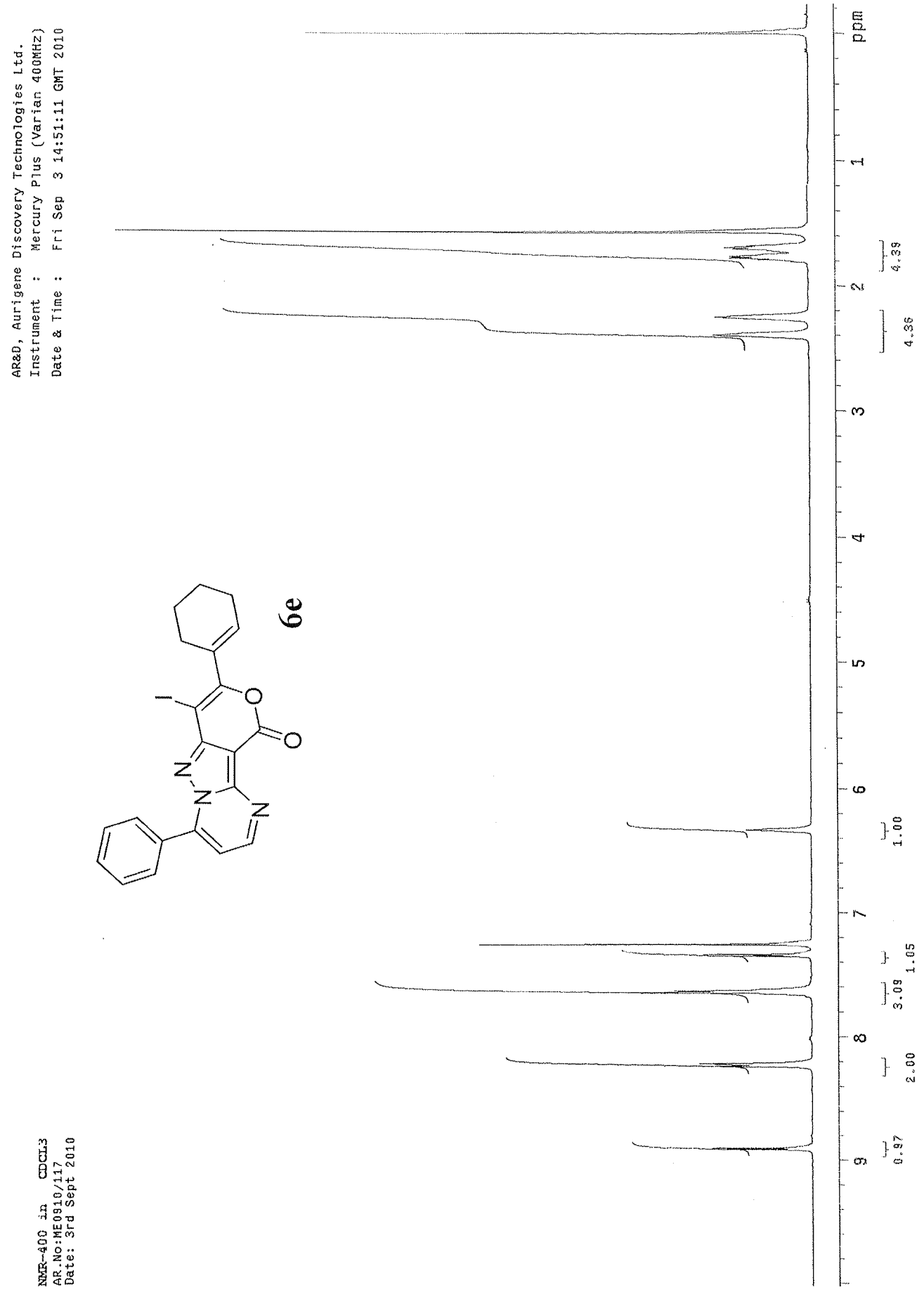

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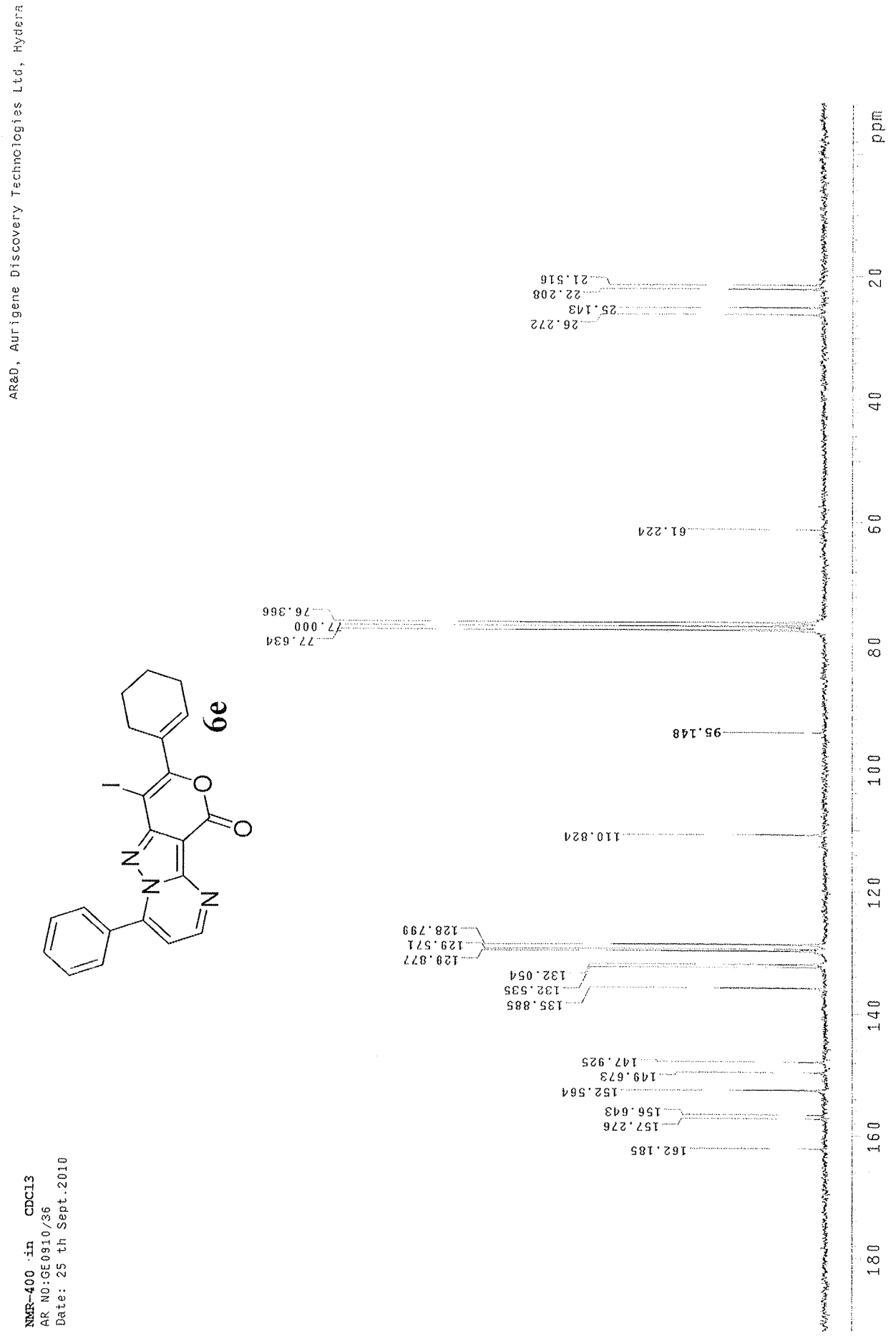

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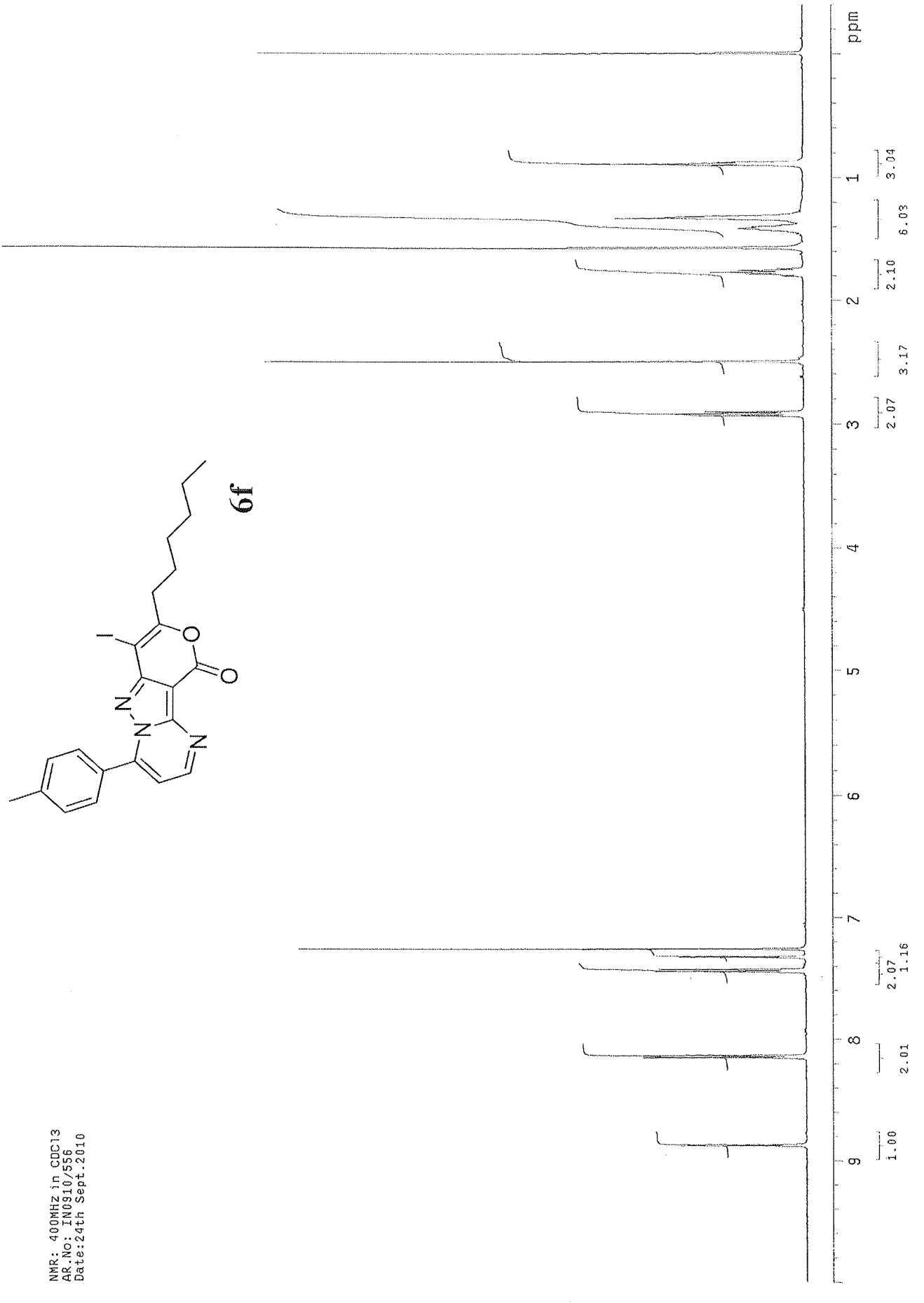

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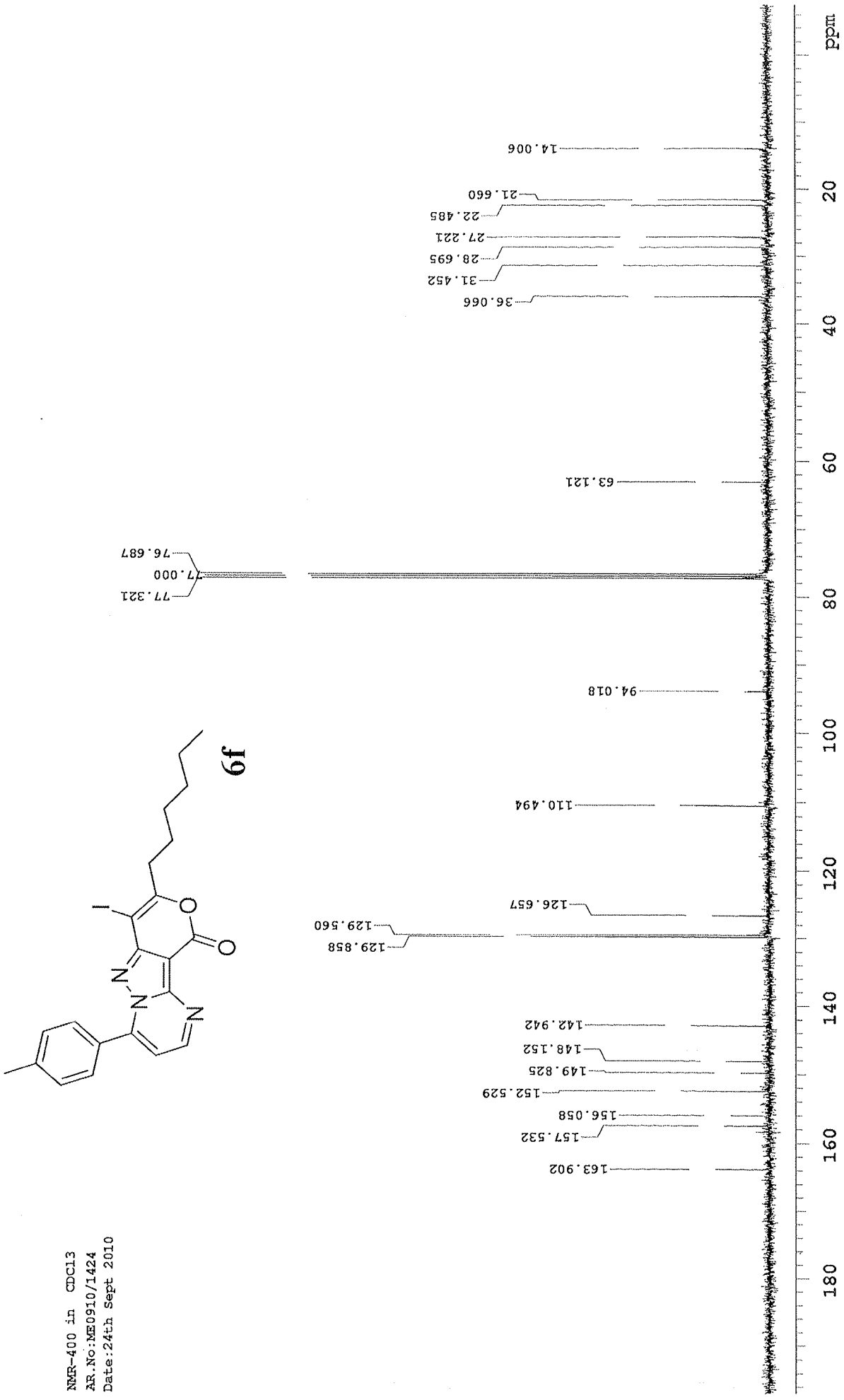

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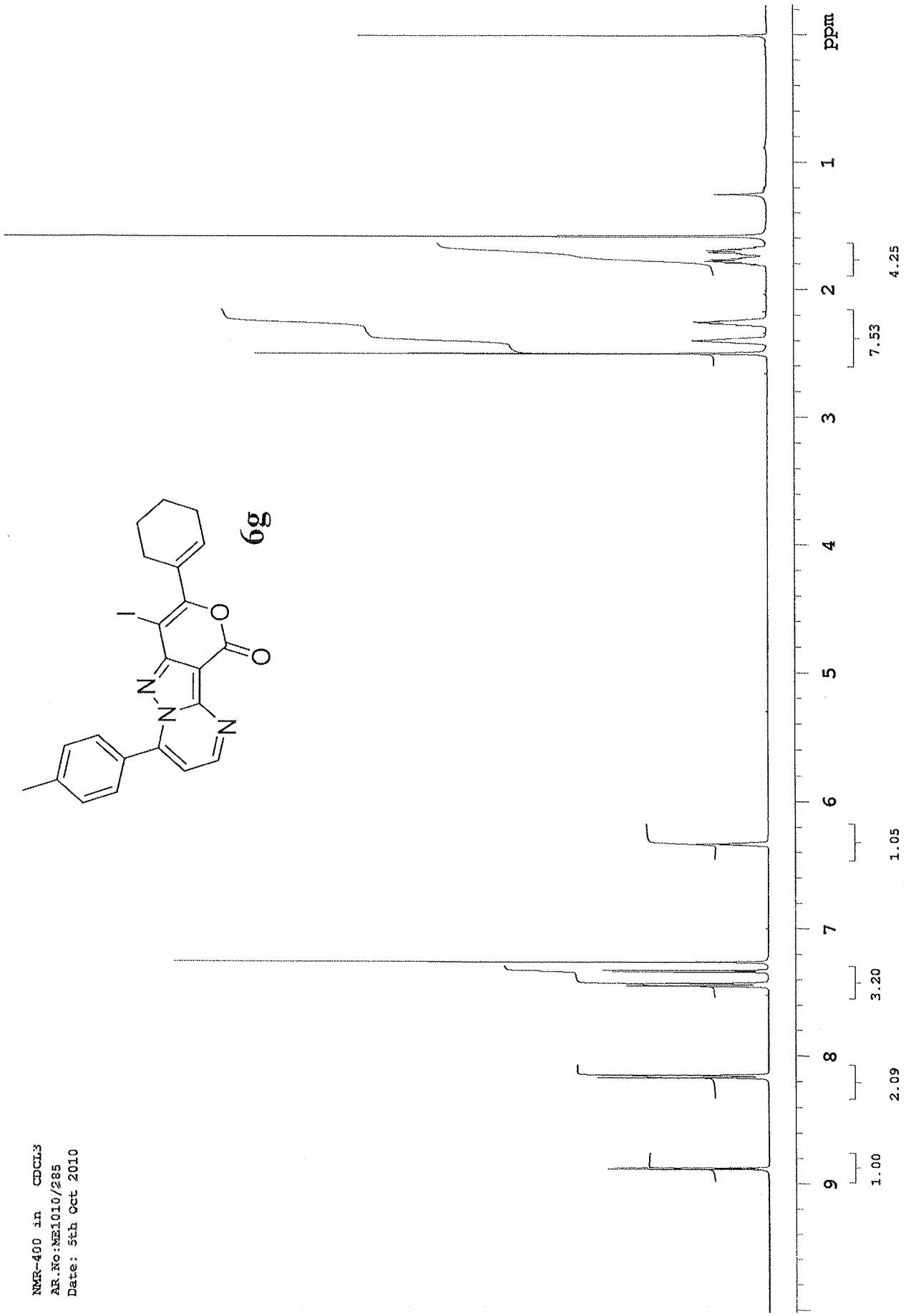

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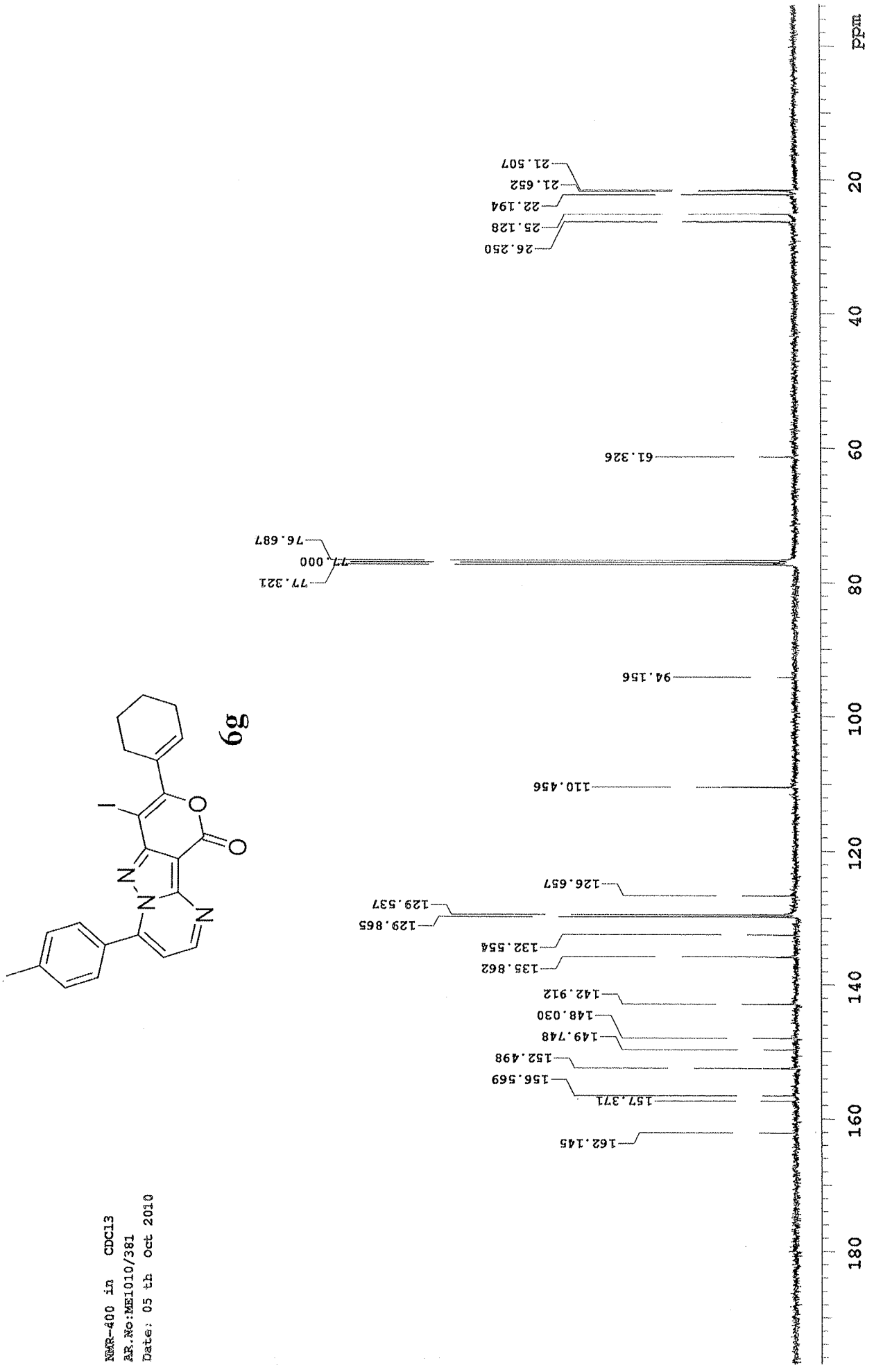

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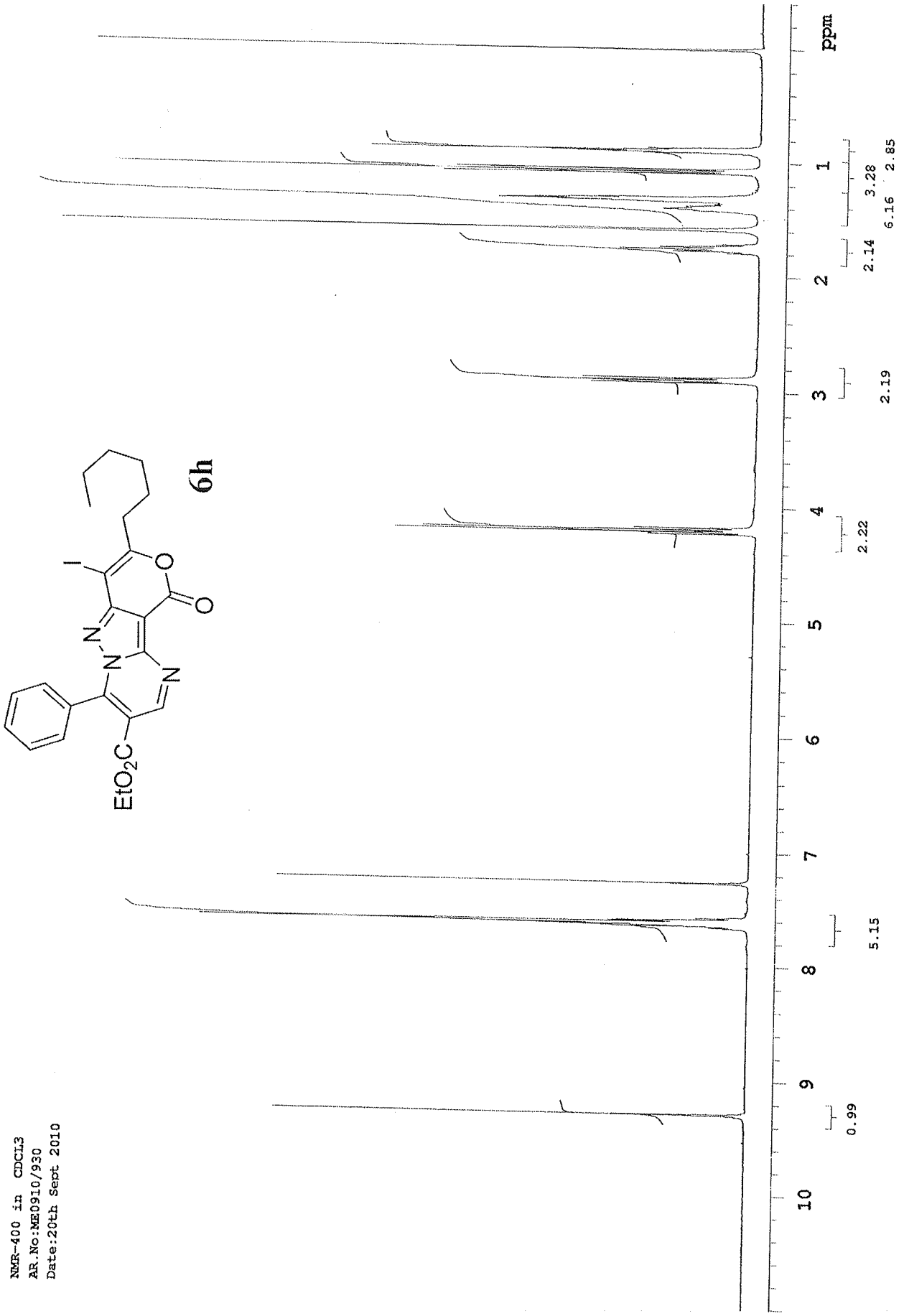

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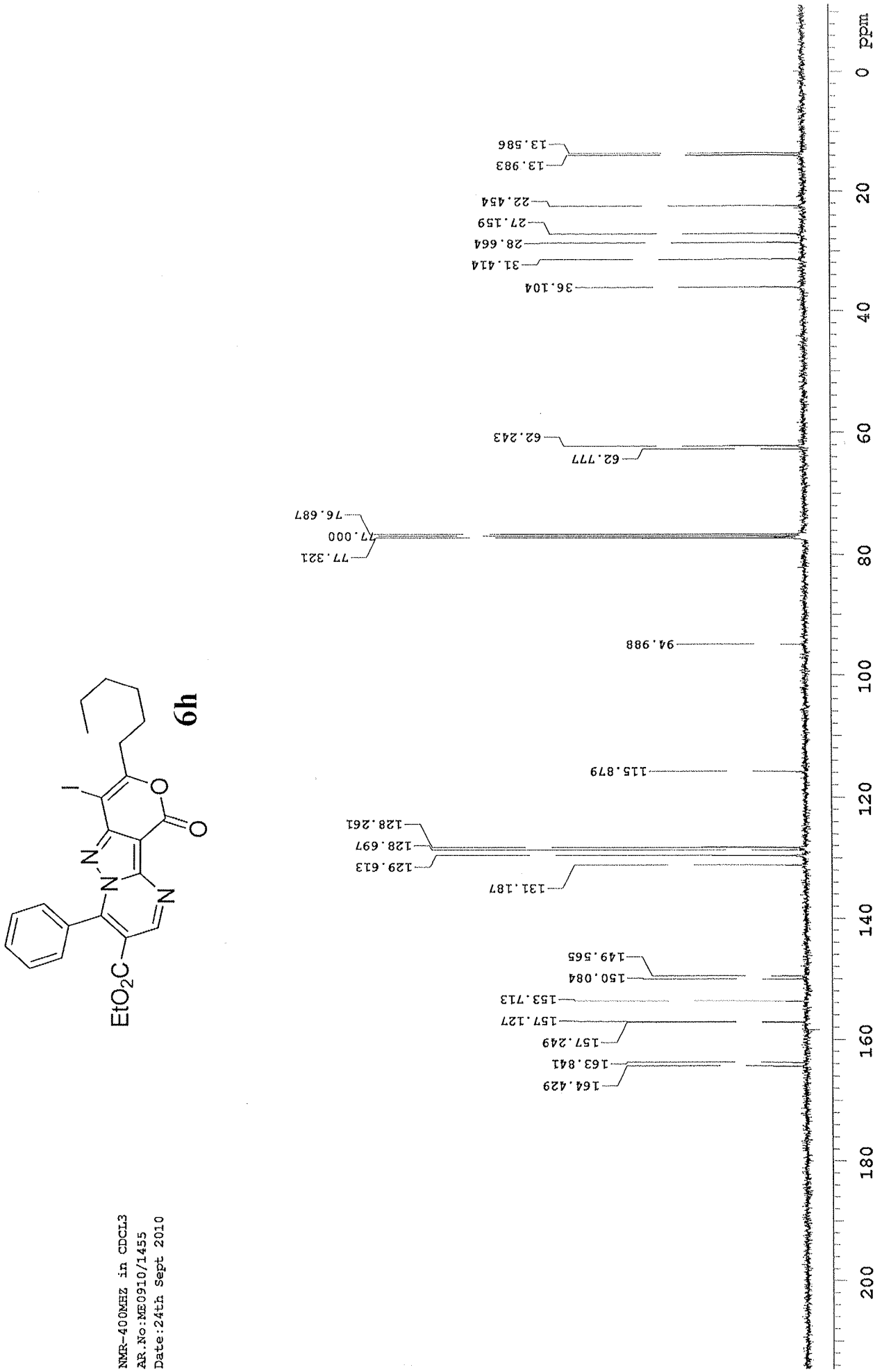

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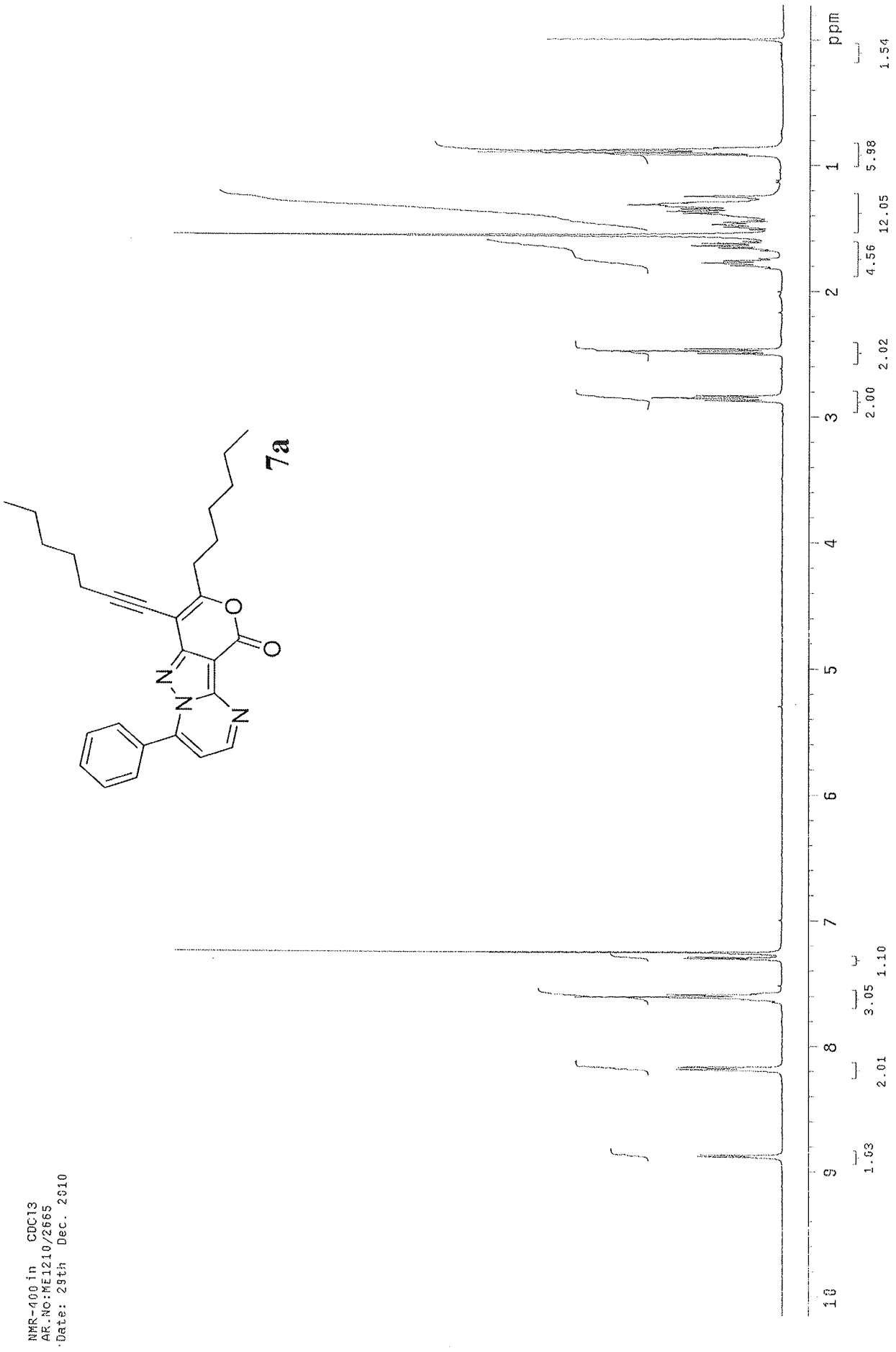

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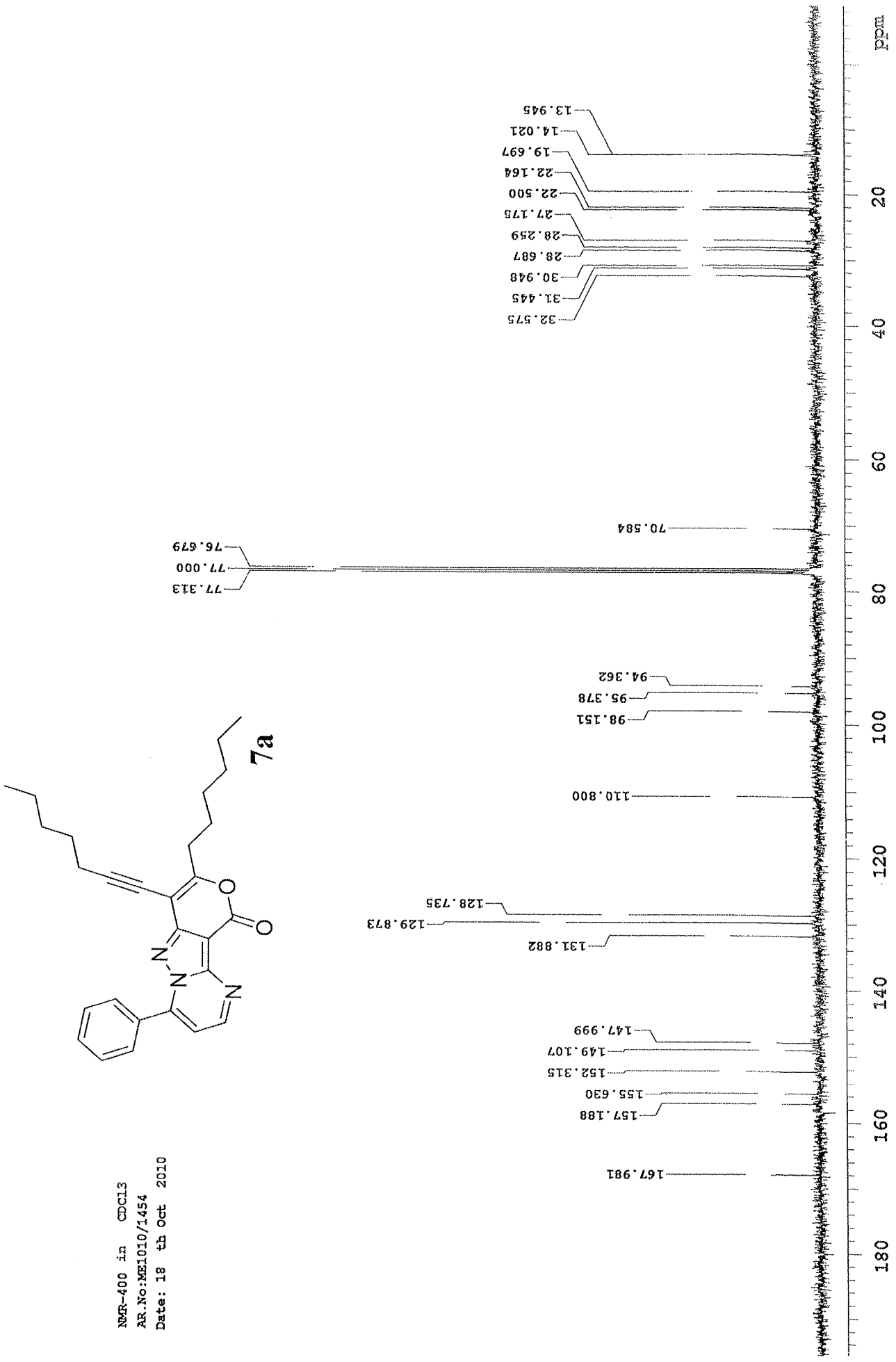

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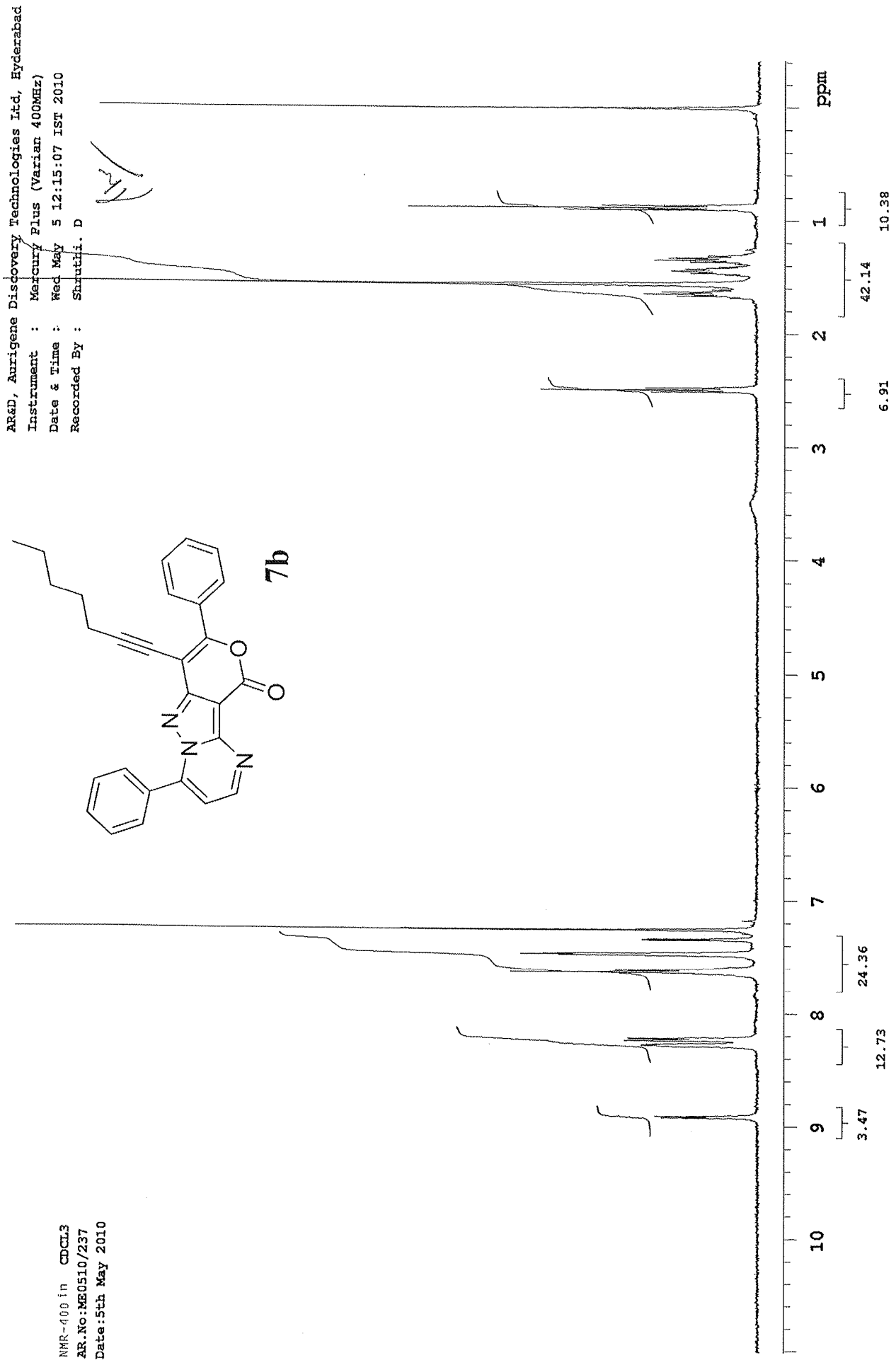

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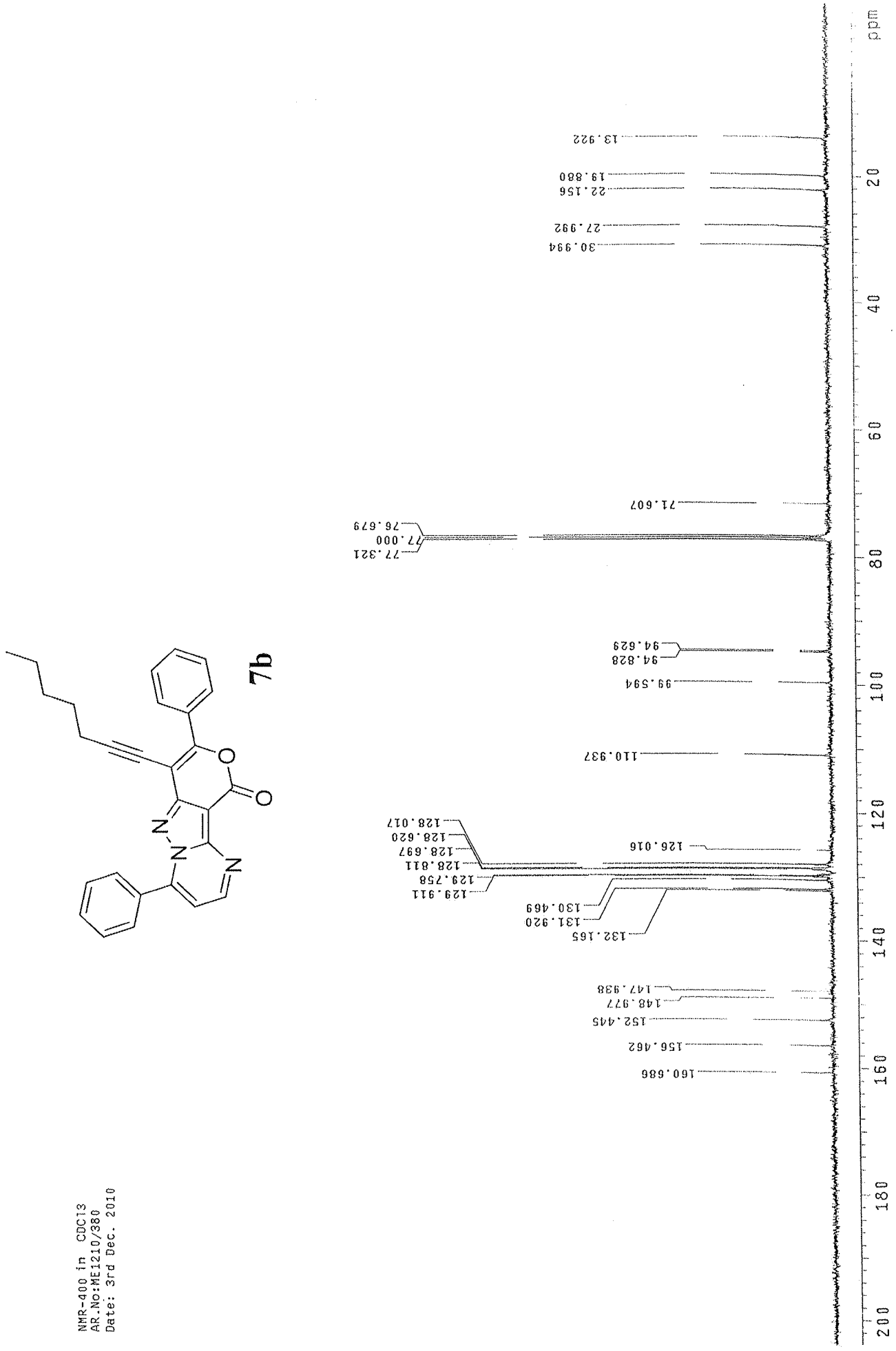
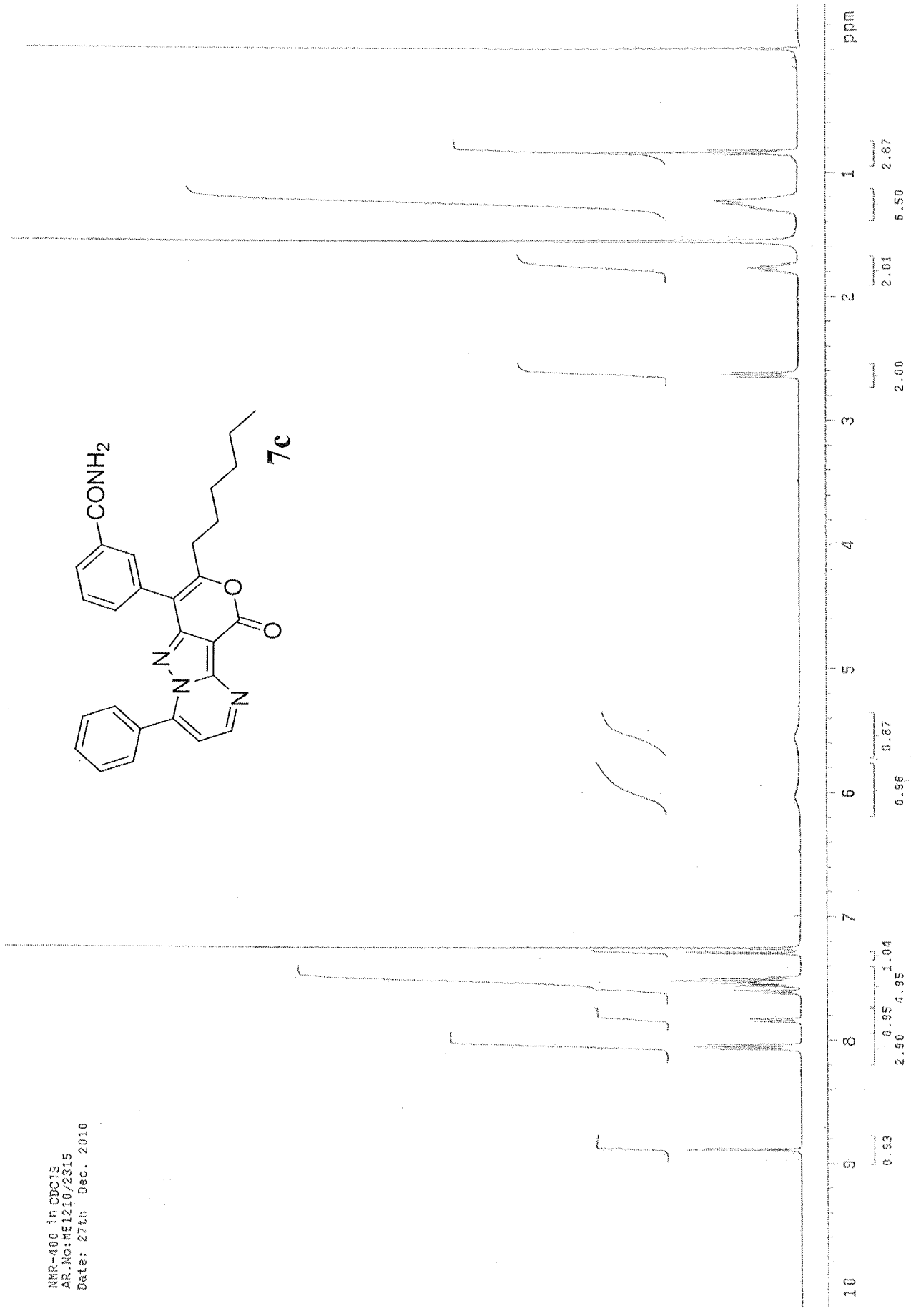
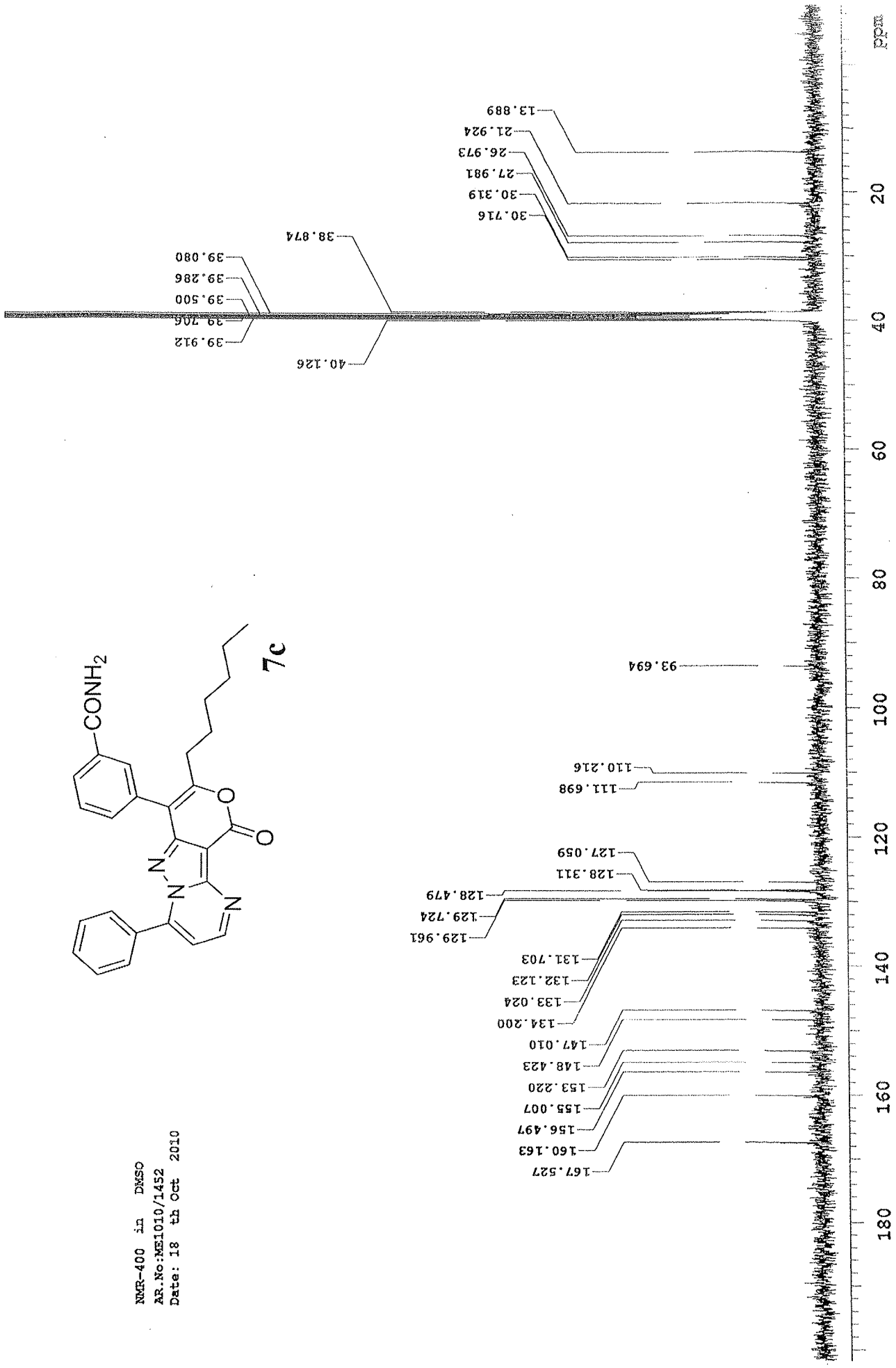


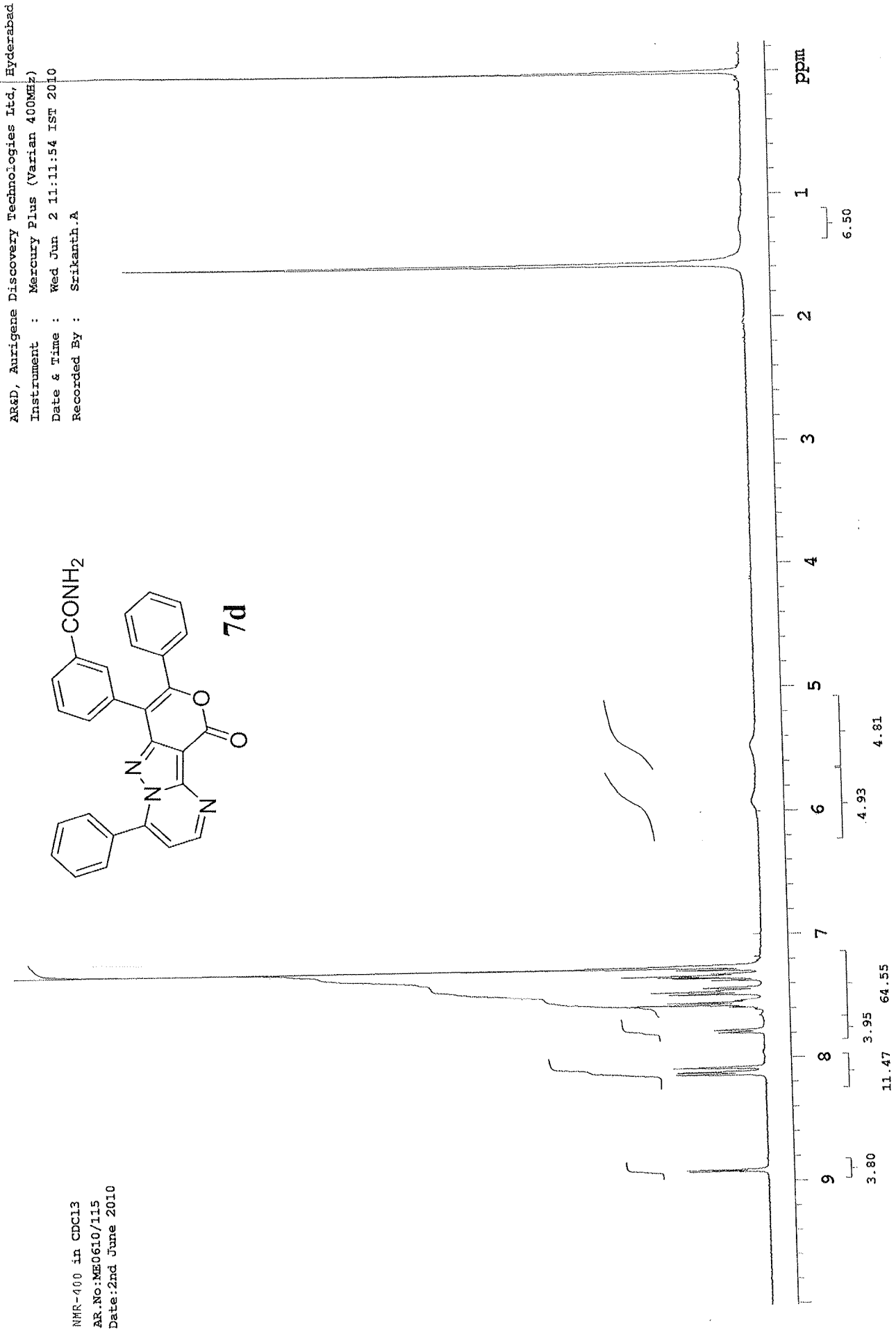
Copies of NMR spectra



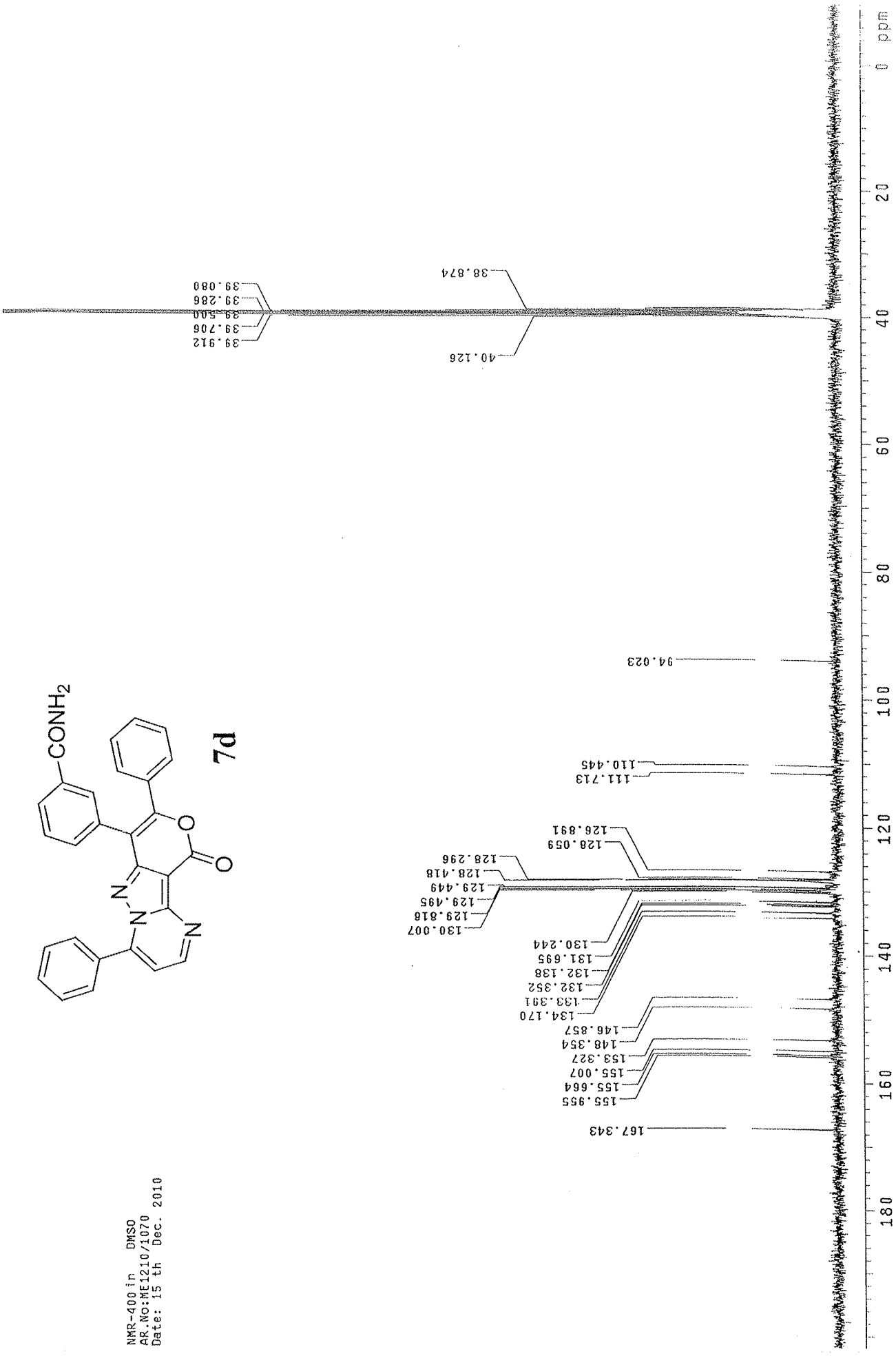
Copies of NMR spectra



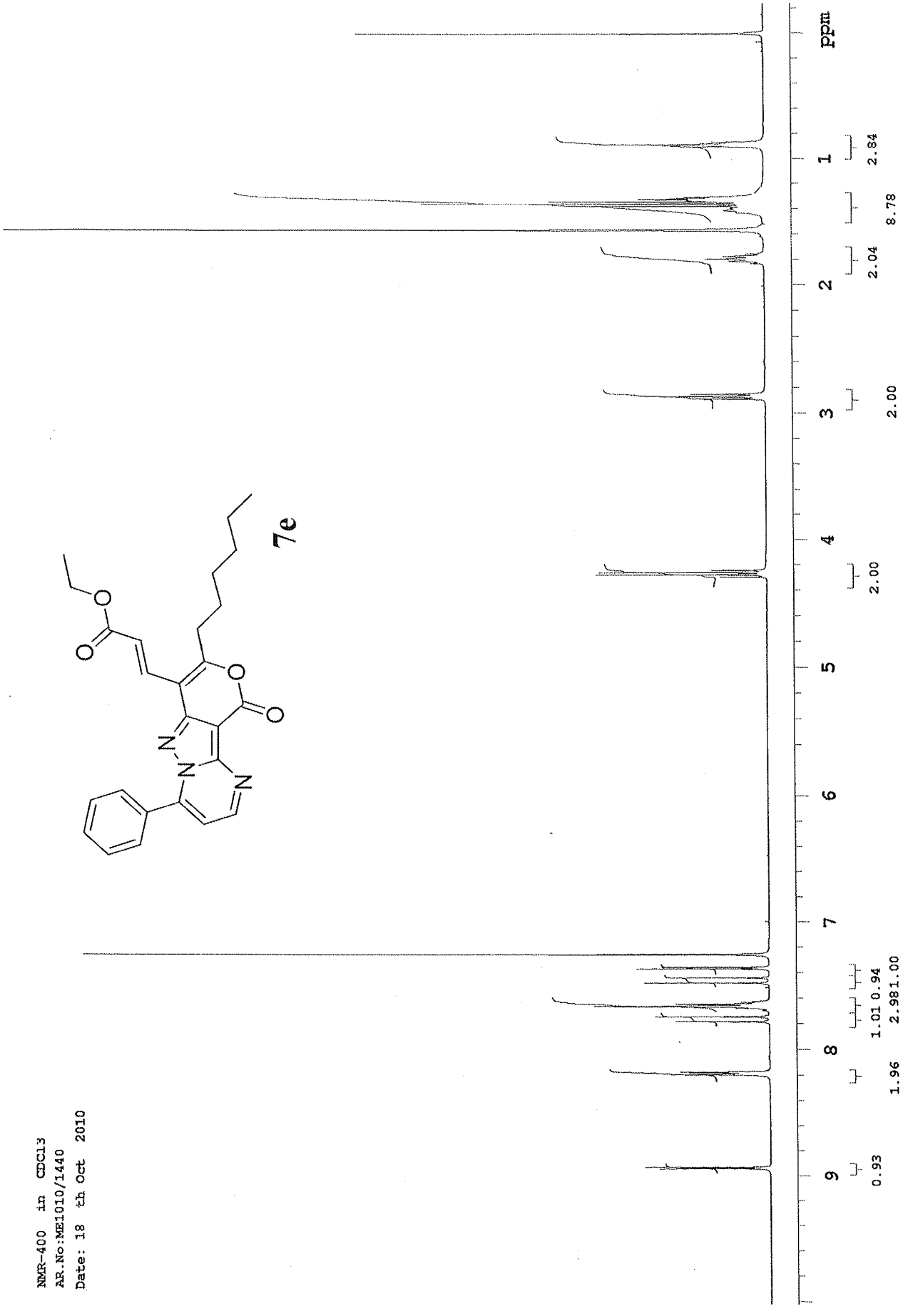
Copies of NMR spectra



Copies of NMR spectra

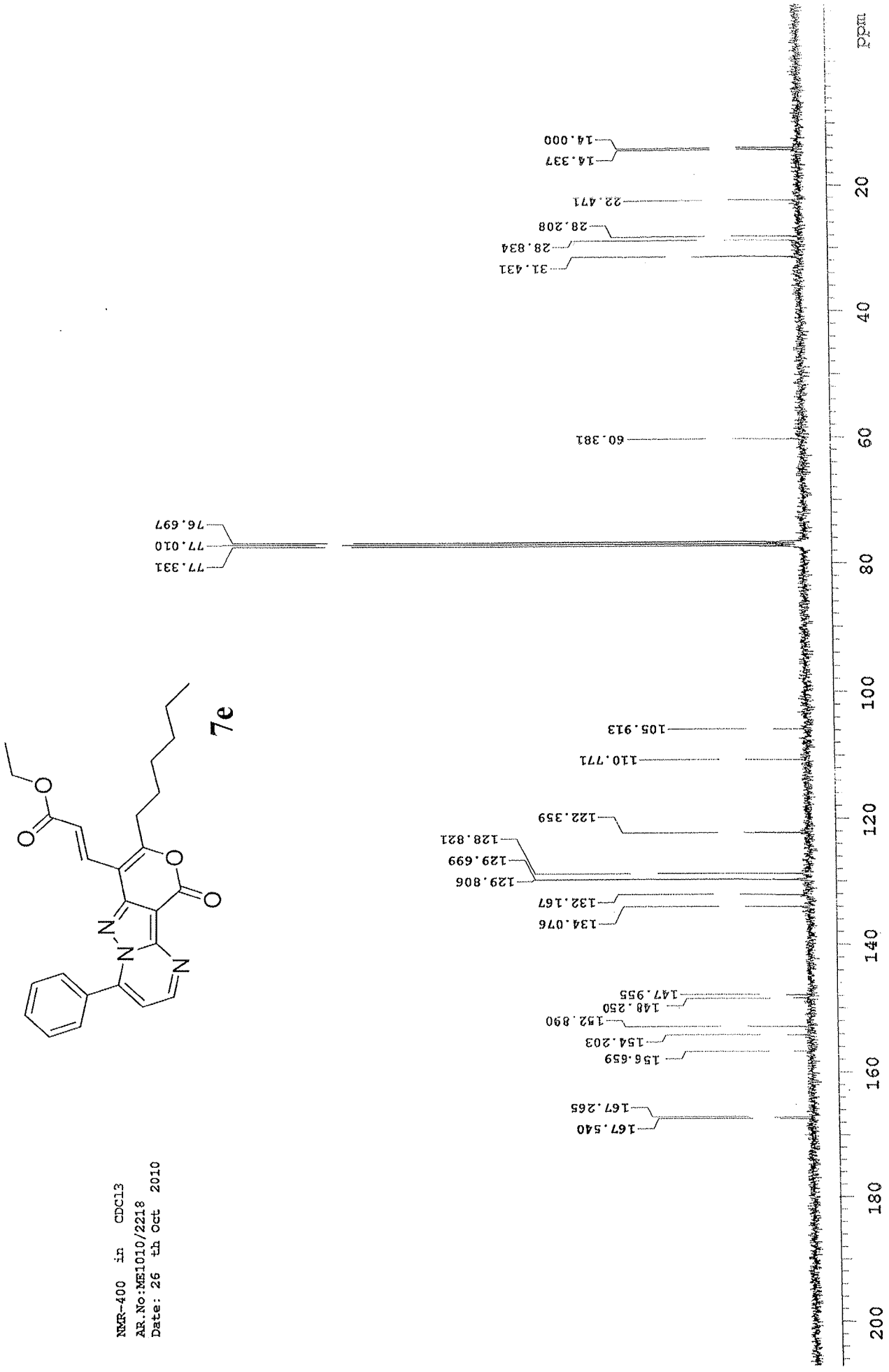


Copies of NMR spectra



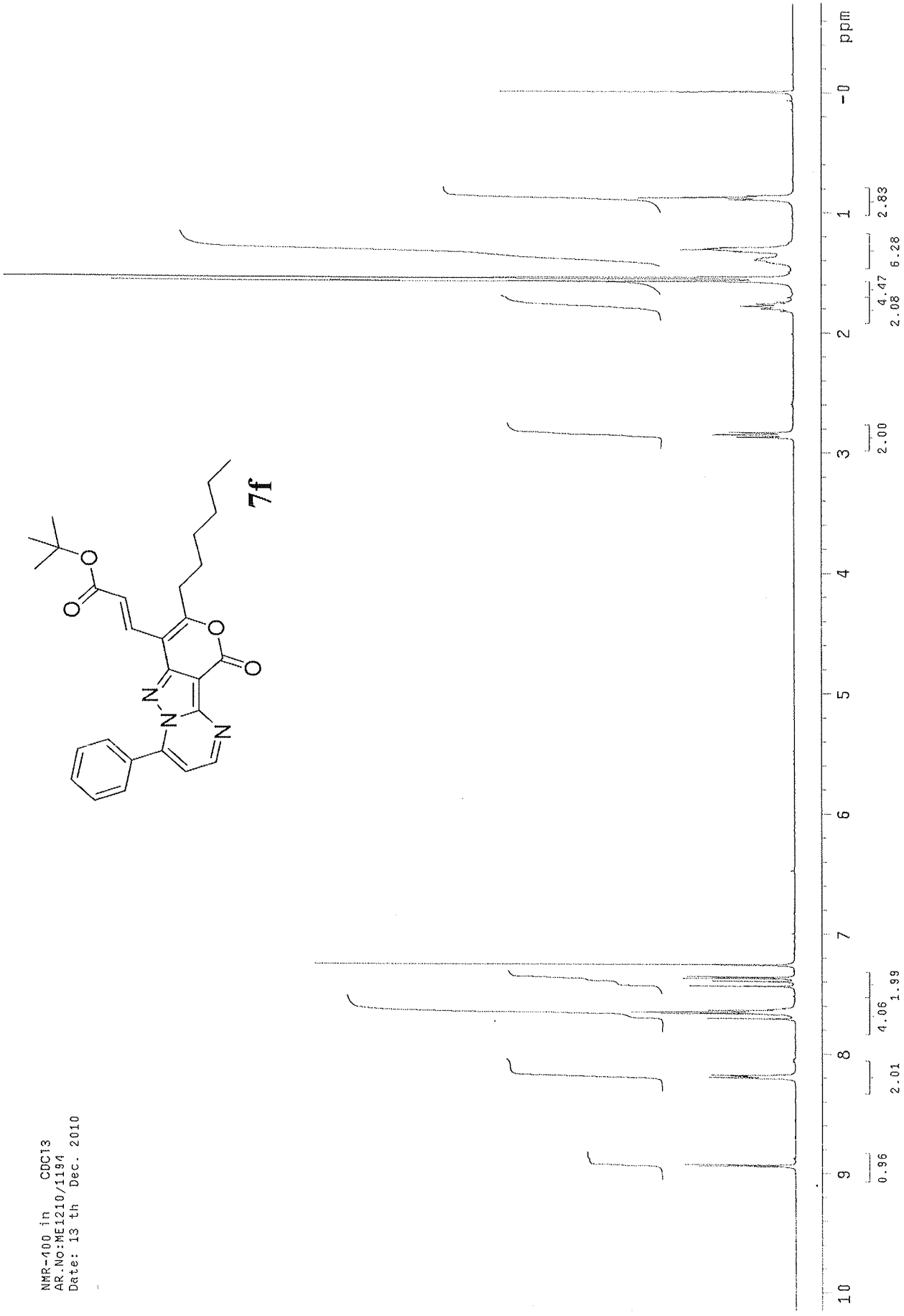
Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra

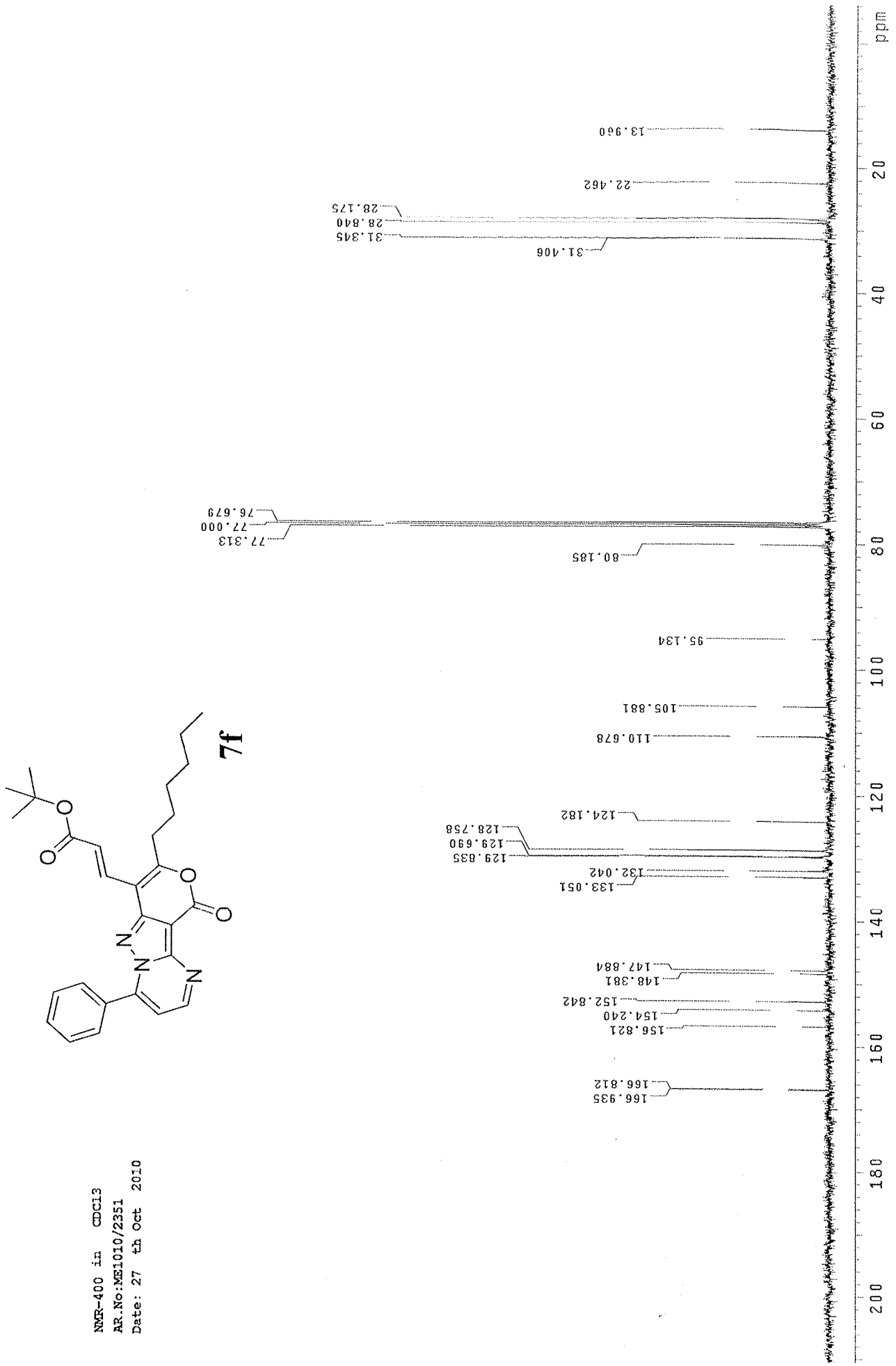


Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra

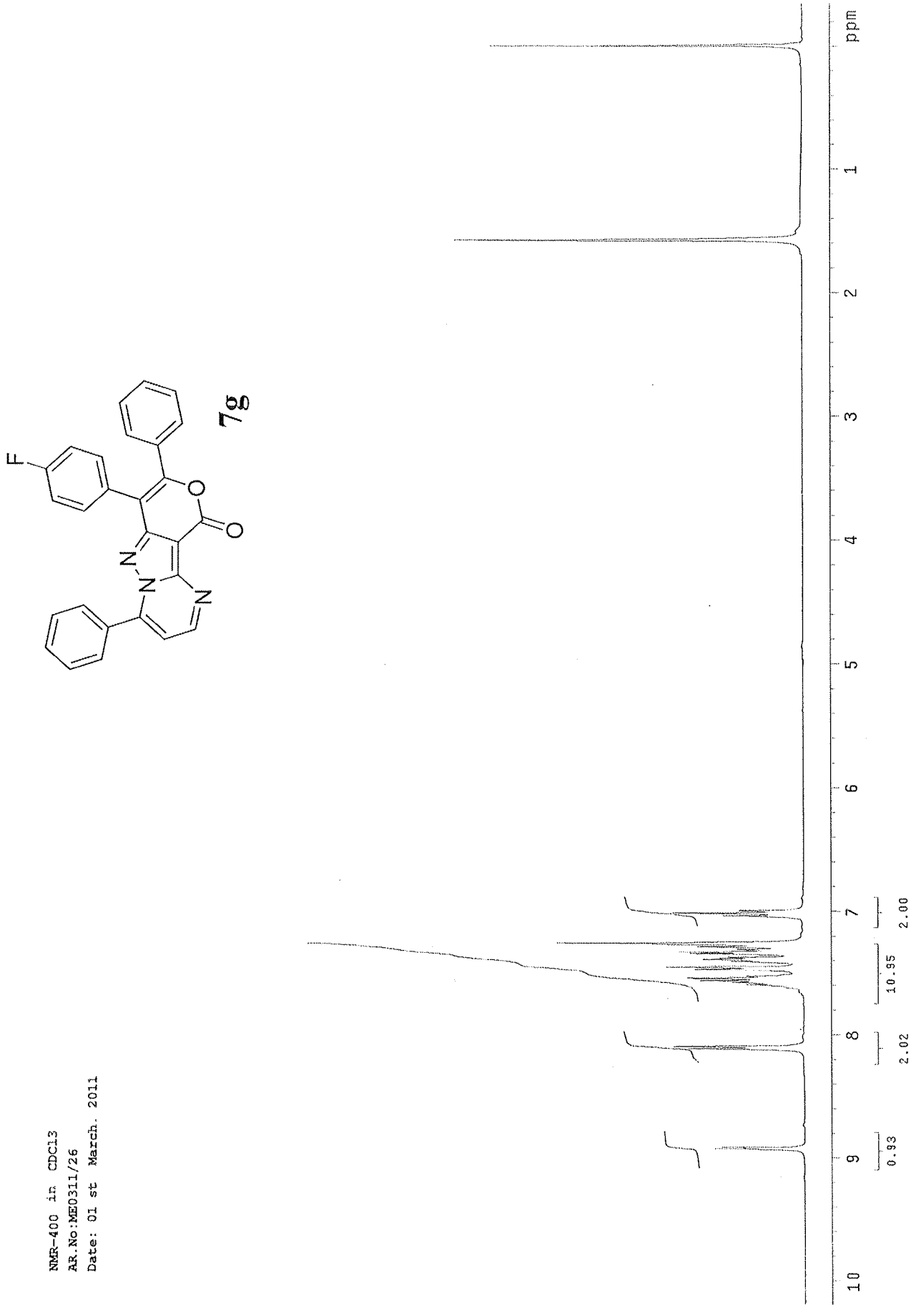


Copies of NMR spectra

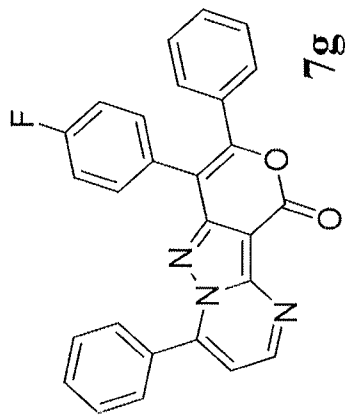


Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra

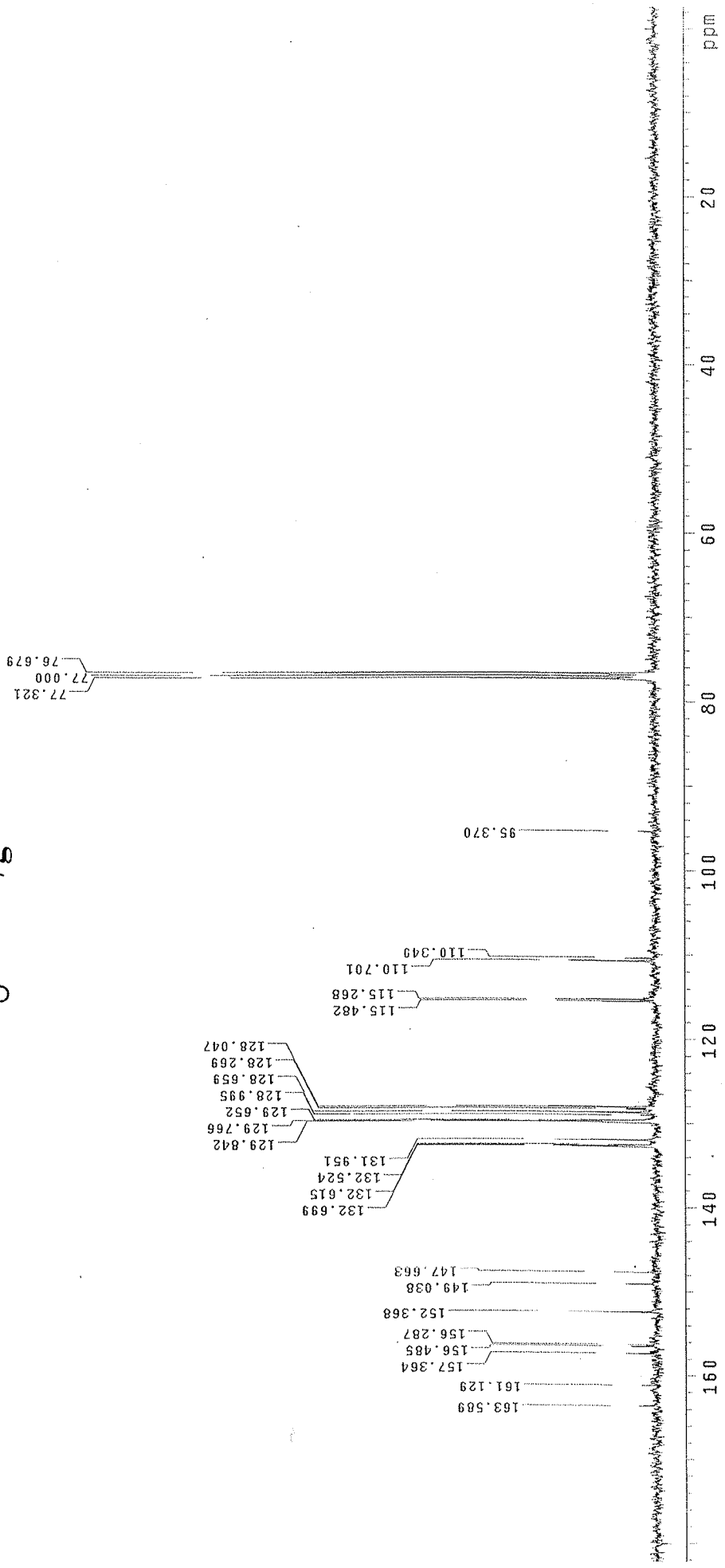


Copies of NMR spectra



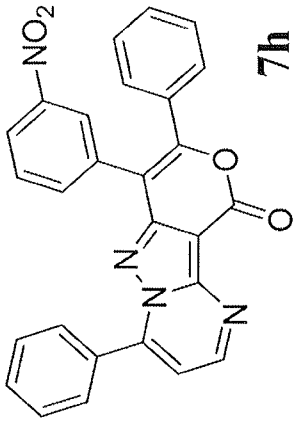
7g

NMR-400 in CDCl3
AR.No:ME0311/384
Date: 3rd March. 2011

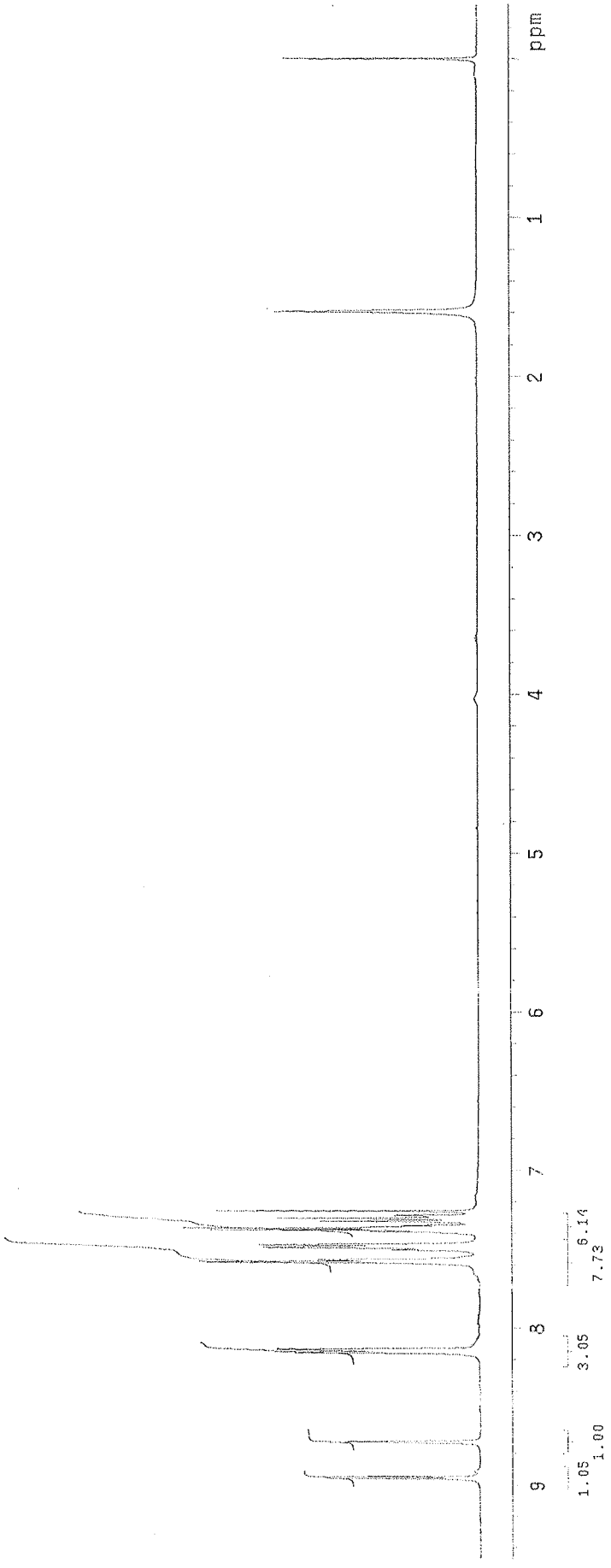


Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra

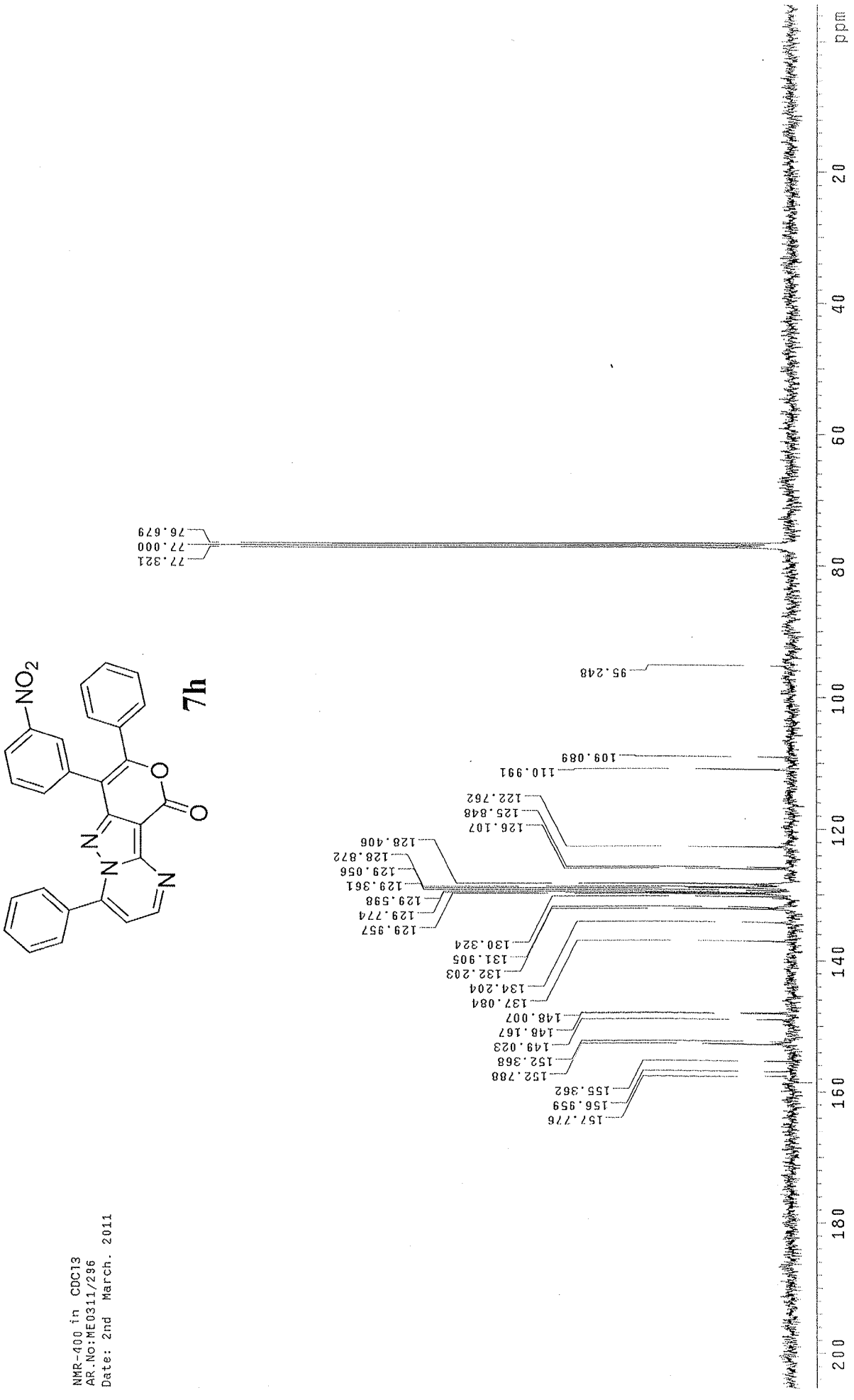


7h



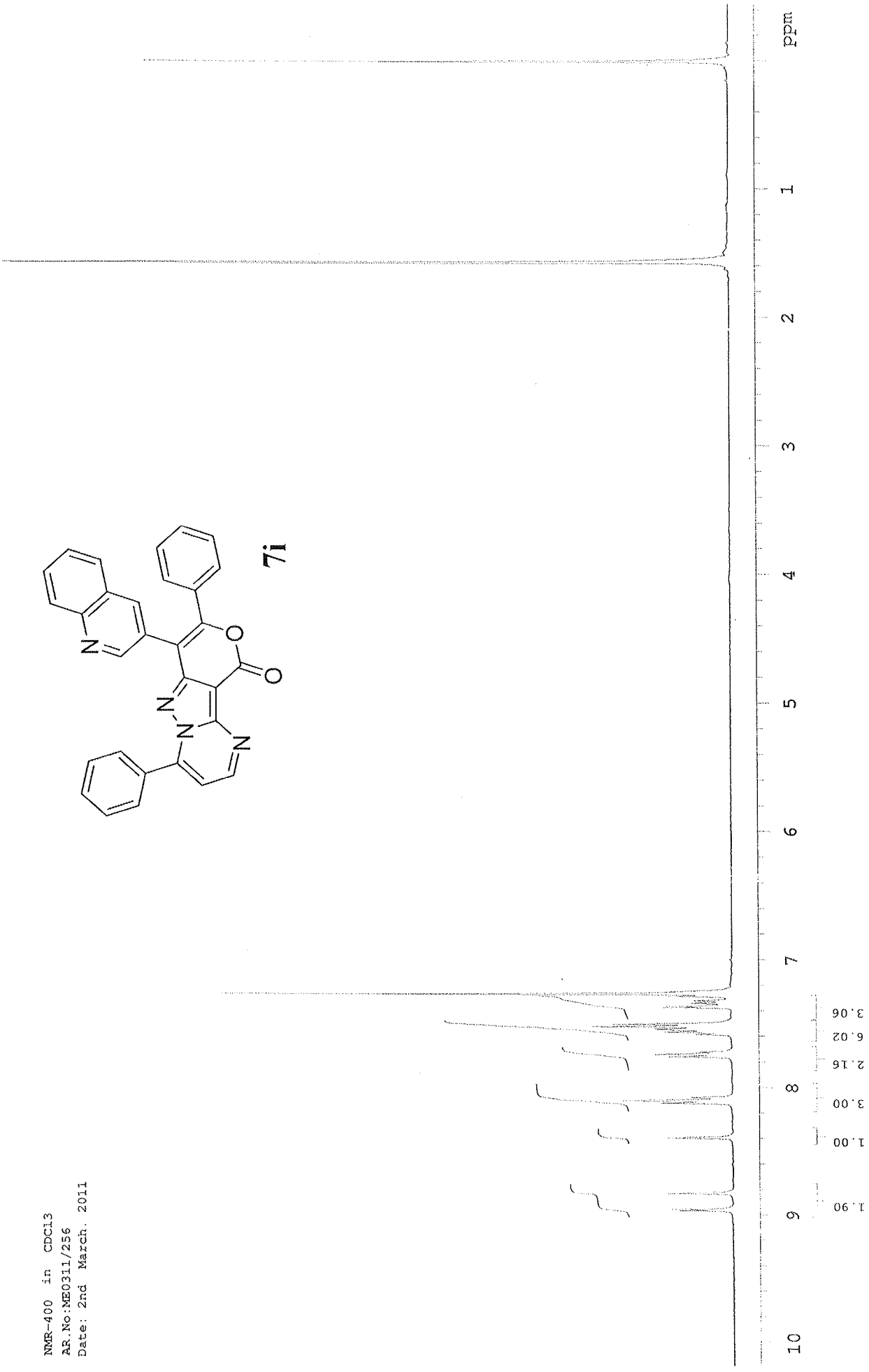
NMR-400 in CDCl3
AR.No:ME0311/376
Date: 3rd March. 2011

Copies of NMR spectra



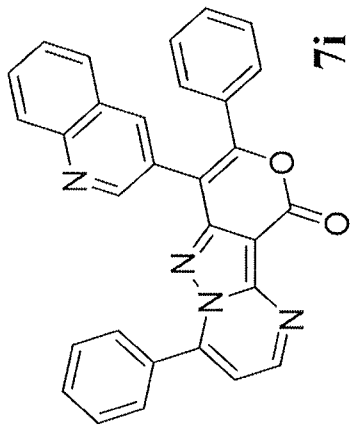
Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra

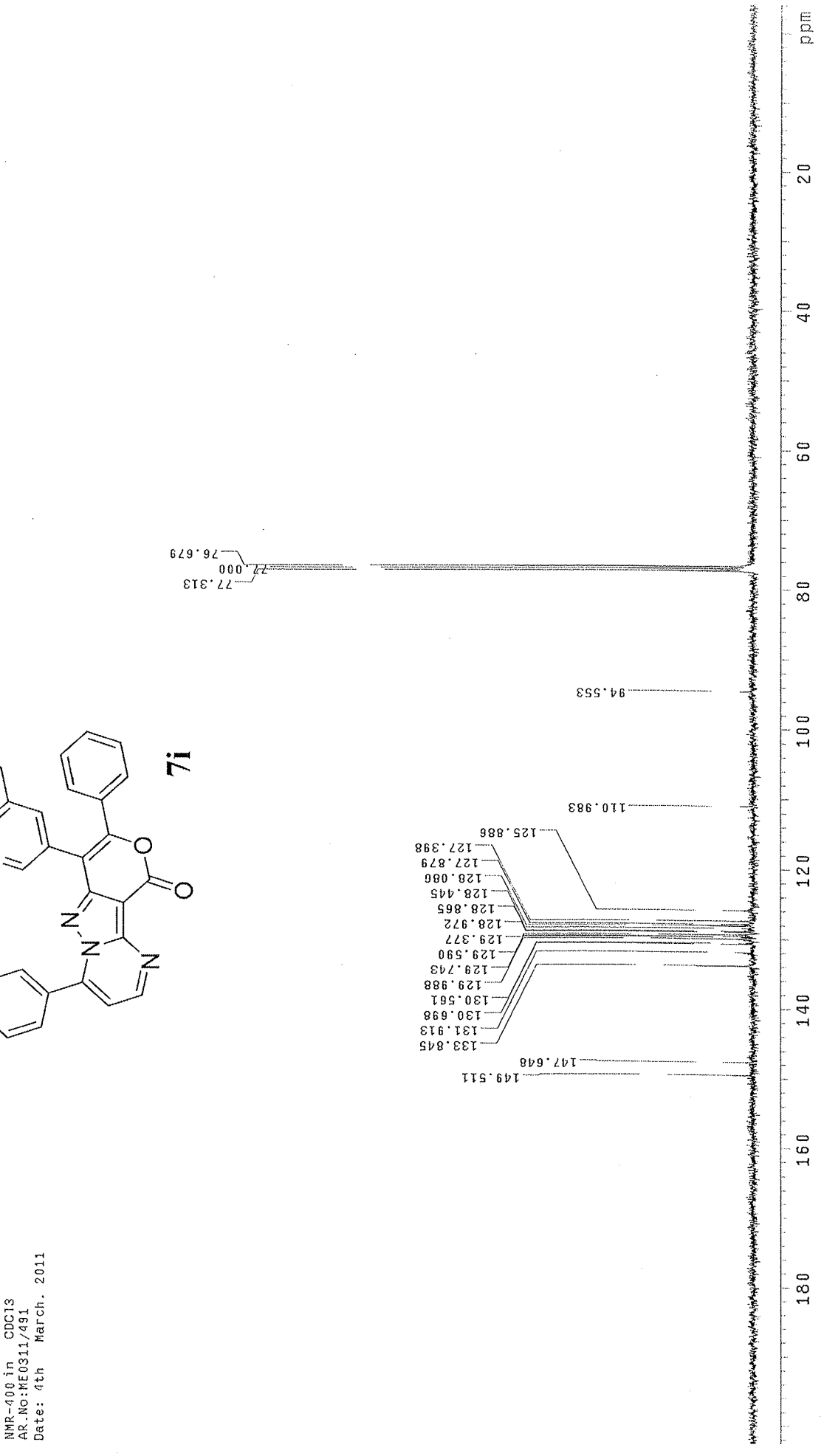


Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Copies of NMR spectra



7i

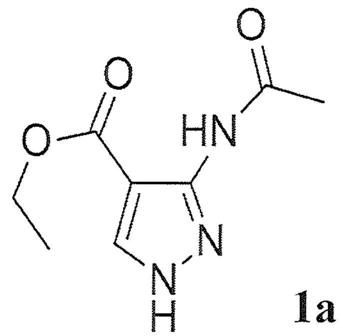


NMR-400.in CDCl3
AR.No:ME0311/491
Date: 4th March. 2011

Copies of HRMS spectra

CPS,MIYAPUR

Mass Analysis Report

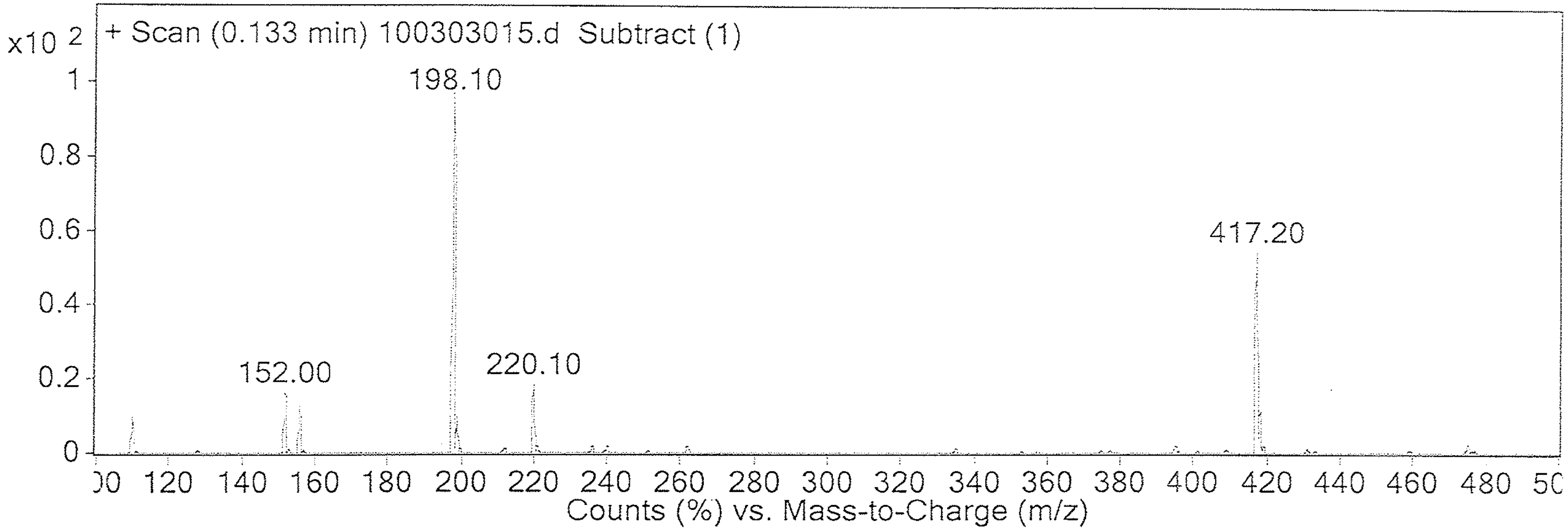


1a

Data Filename	100303015.d	Sample Name	APC-1
Sample Type	Sample	Position	Vial 76
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	default.m	Comment	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



--- End Of Report ---

Page 1 of 1

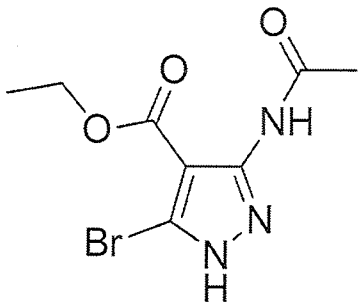
Printed at: 10:58 AM on:3/3/2010

6/12/10

Elemental Composition Report

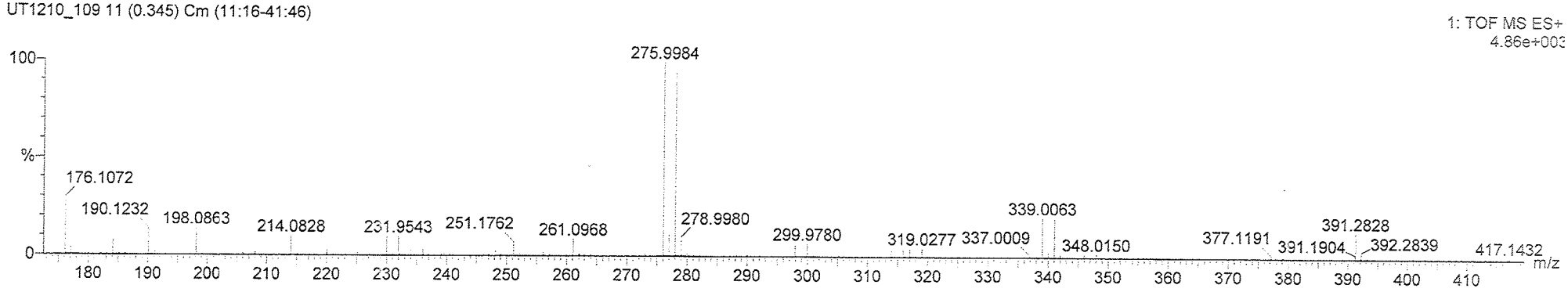
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



1b

Monoisotopic Mass, Even Electron Ions
281 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-6 O: 0-6 Br: 0-1
APC-2
UT1210_109 11 (0.345) Cm (11:16-41:46)



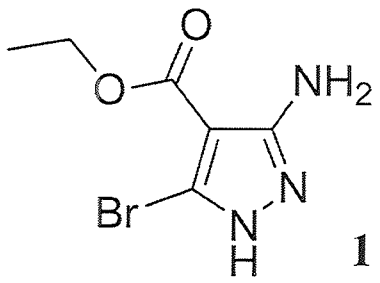
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
275.9984	275.9984	0.0	0.0	4.5	3.9	C8 H11 N3 O3 Br

Copies of HRMS spectra

Elemental Composition Report

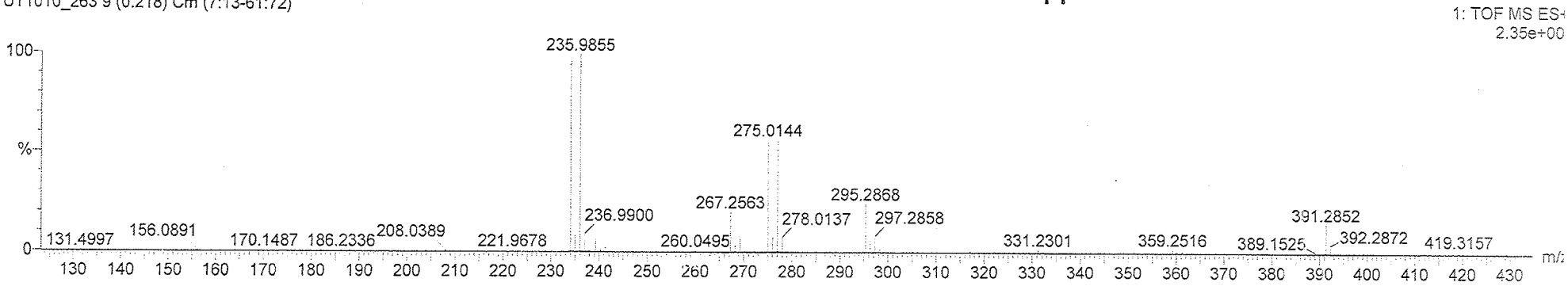
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



1

Monoisotopic Mass, Even Electron Ions
151 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4 Br: 0-1
APC-3
UT1010_263 9 (0.218) Cm (7:13-61:72)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
233.9874	233.9878	-0.4	-1.7	3.5	2.2	C6 H9 N3 O2 Br

Copies of HRMS spectra

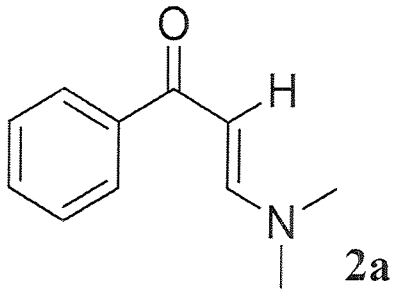
Copies of HRMS spectra

6/12/12

Elemental Composition Report

Single Mass Analysis

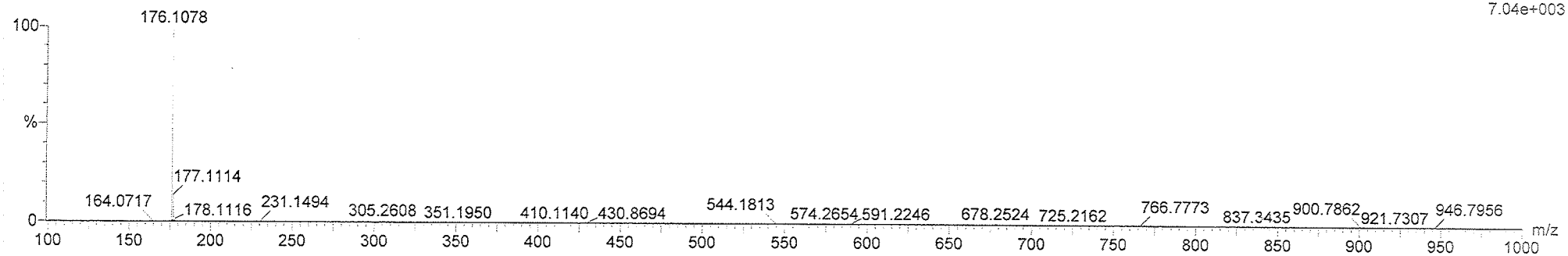
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



2a

Monoisotopic Mass, Even Electron Ions
103 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-6 O: 0-6
KSM-2A
UT1210_108 18 (0.569) Cm (18:20-47:50)

1: TOF MS ES+
7.04e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
176.1078	176.1075	0.3	1.7	5.5	1.1	C11 H14 N O

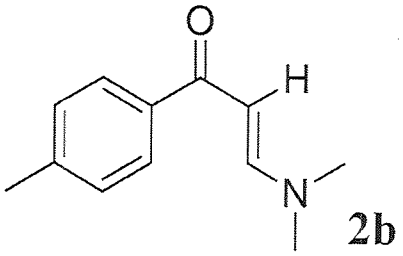
Copies of HRMS spectra

F 6/12/10

Elemental Composition Report

Single Mass Analysis

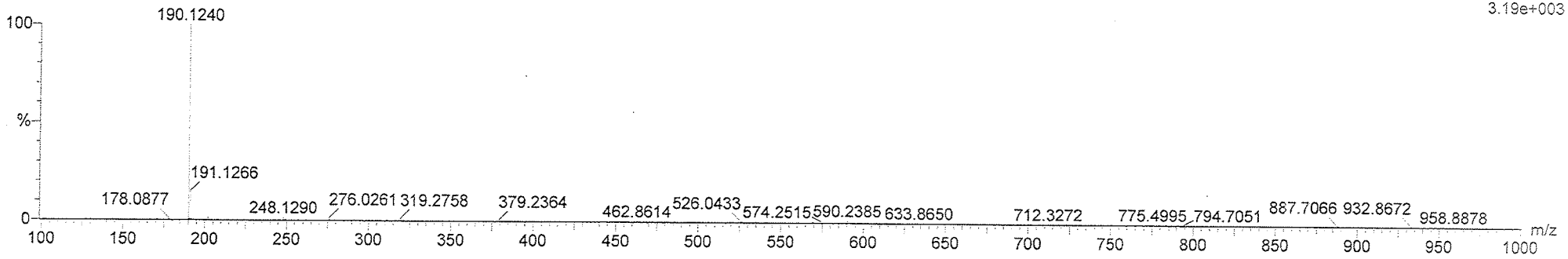
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



2b

Monoisotopic Mass, Even Electron Ions
111 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-6 O: 0-6
KSM-2B
UT1210_107 27 (0.841) Cm (24:27-57:61)

1: TOF MS ES+
3.19e+003

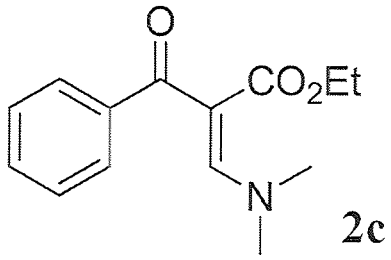


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
190.1240	190.1232	0.8	4.2	5.5	1.3	C12 H16 N O

Elemental Composition Report

Single Mass Analysis

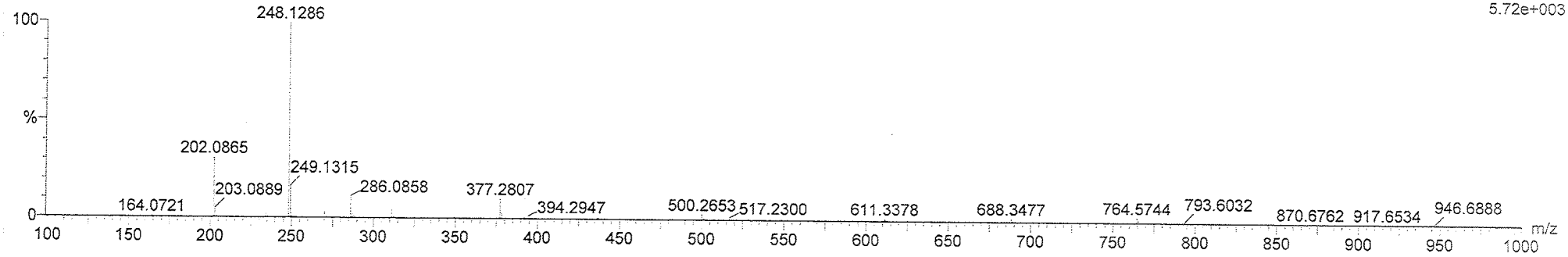
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



2c

Monoisotopic Mass, Even Electron Ions
244 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-6 O: 0-6 Br: 0-1
KSM-2C
UT1210_106 17 (0.547) Cm (17:20-49:56)

1: TOF MS ES+
5.72e+003



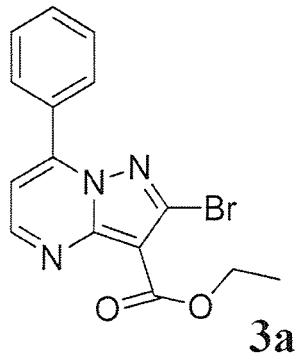
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
248.1286	248.1287	-0.1	-0.4	6.5	2.6	C14 H18 N O3

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

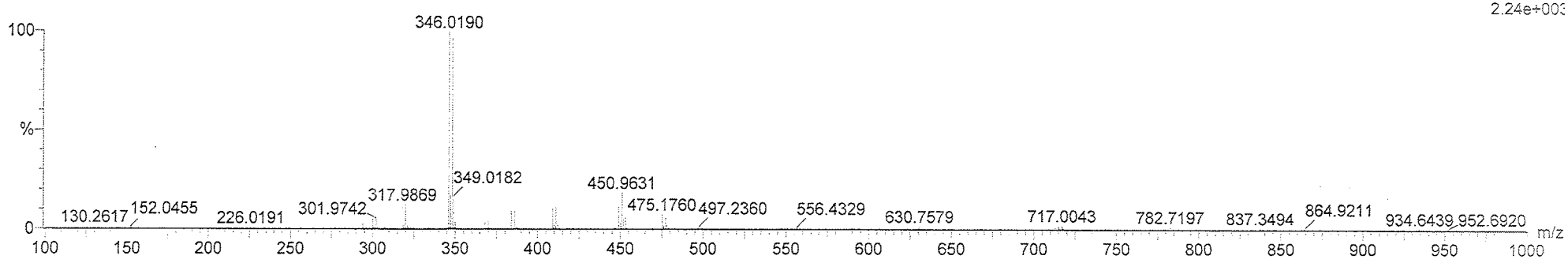
Monoisotopic Mass, Even Electron Ions
214 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25 H: 0-30 N: 0-5 O: 0-6 Br: 0-1



3a

BPPC-1
UT0910_102 27 (0.615) Cm (26:31-68:77)

1: TOF MS ES+
2.24e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
346.0190	346.0191	-0.1	-0.3	10.5	0.7	C15 H13 N3 O2 Br

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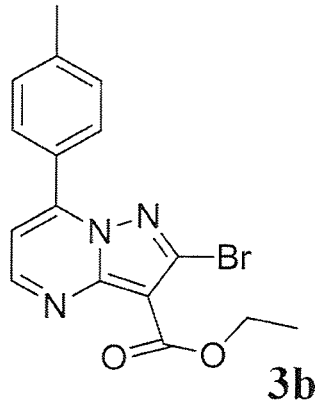
Copies of HRMS spectra

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

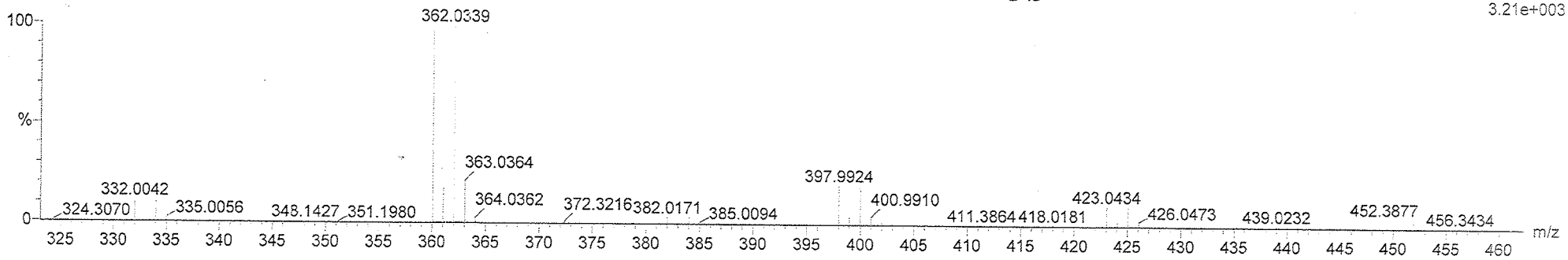
Monoisotopic Mass, Even Electron Ions
207 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25 H: 0-30 N: 0-5 O: 0-6 Br: 0-1



3b

MPPC-1
UT0910_103 21 (0.489) Cm (21:25-58:68)

1: TOF MS ES+
3.21e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
360.0358	360.0348	1.0	2.8	10.5	1.1	C16 H15 N3 O2 Br

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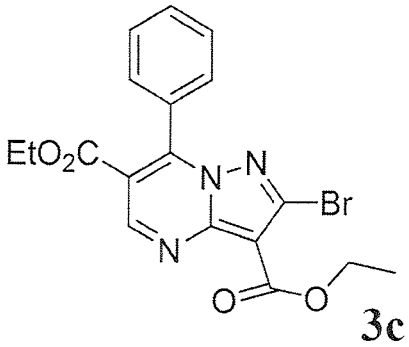
Elemental Composition Report

Single Mass Analysis

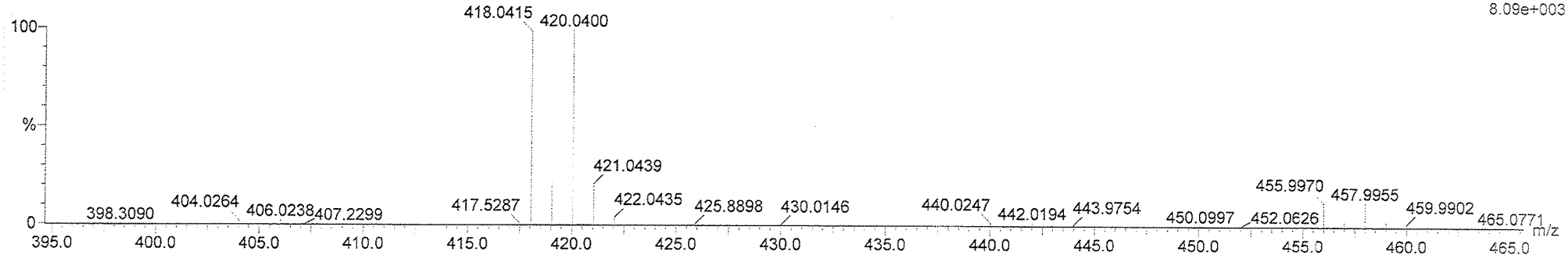
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



3c

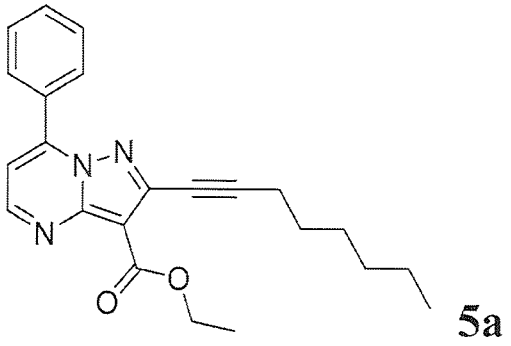
Monoisotopic Mass, Even Electron Ions
426 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-6 O: 0-6 Br: 0-1
BPPC-1C TDC-113
UT1210_105 13 (0.421) Cm (13:16-53:57)

1: TOF MS ES+
8.09e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
418.0415	418.0402	1.3	3.1	11.5	1.5	C18 H17 N3 O4 Br

Elemental Composition Report

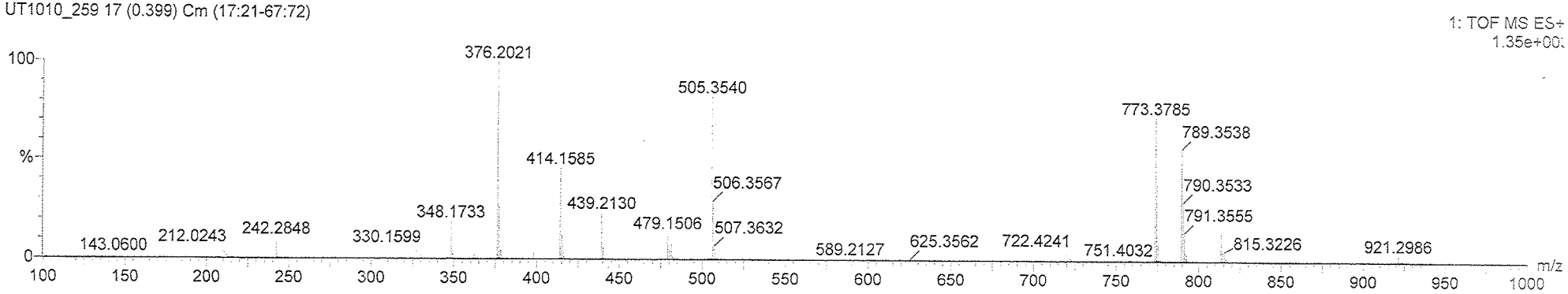


5a

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\001
UT1010_259 17 (0.399) Cm (17:21-67:72)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
376.2021	376.2025	-0.4	-1.1	12.5	0.3	C23 H26 N3 O2

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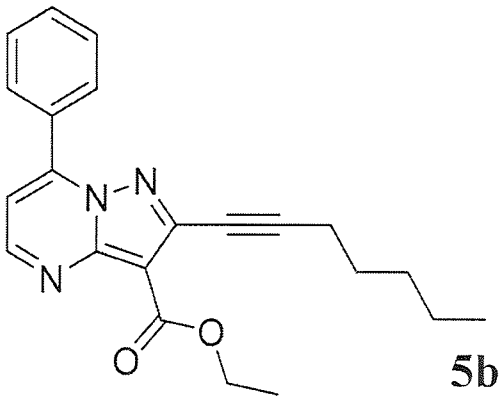
Elemental Composition Report



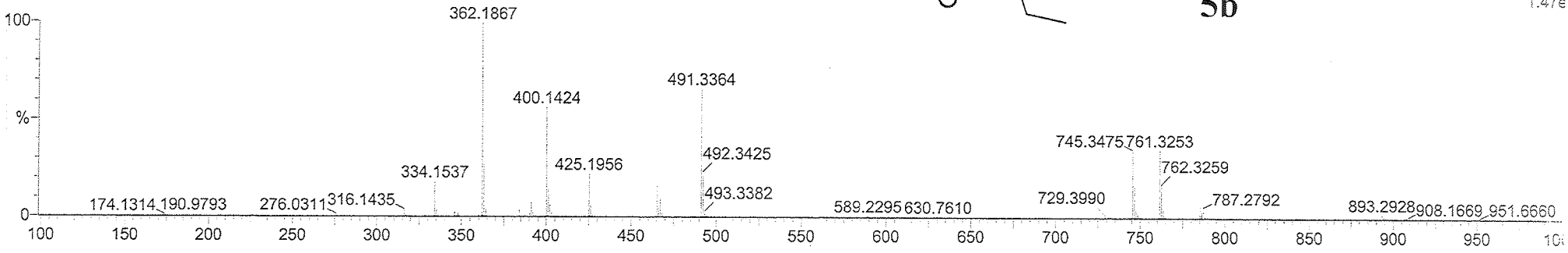
5b

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\006
UT1010_254 20 (0.450) Cm (20:24-65:78)

1: TOF MS
1.47e



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
362.1867	362.1869	-0.2	-0.6	12.5	0.3	C22 H24 N3 O2

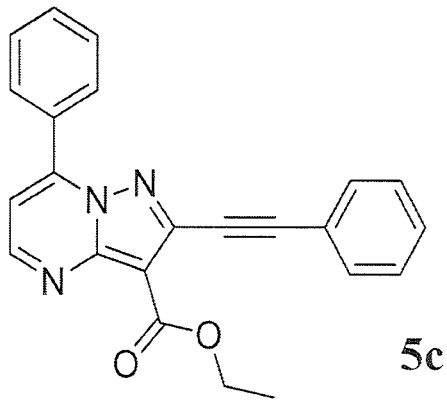
Copies of HRMS spectra

Elemental Composition Report

Single Mass Analysis

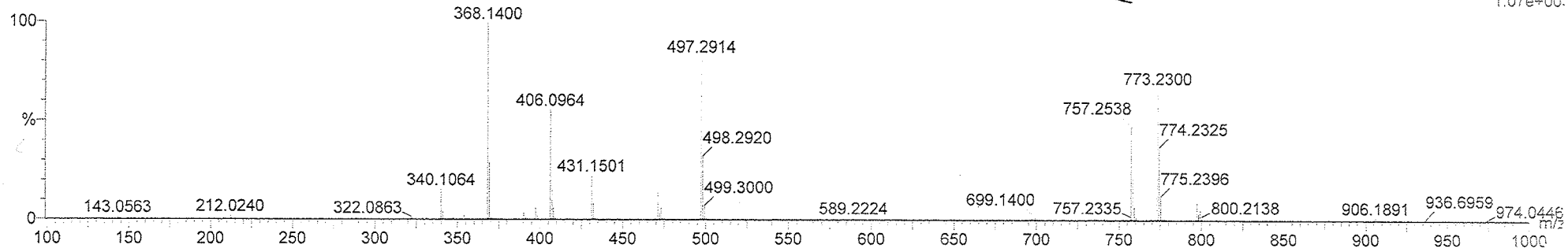
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\002
UT1010_258 17 (0.398) Cm (17:22-65:74)



5c

1: TOF MS ES+
1.07e+00



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.1400	368.1399	0.1	0.3	16.5	20.1	C23 H18 N3 O2

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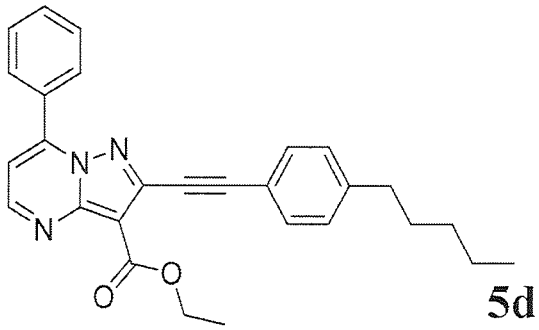
Elemental Composition Report

Single Mass Analysis

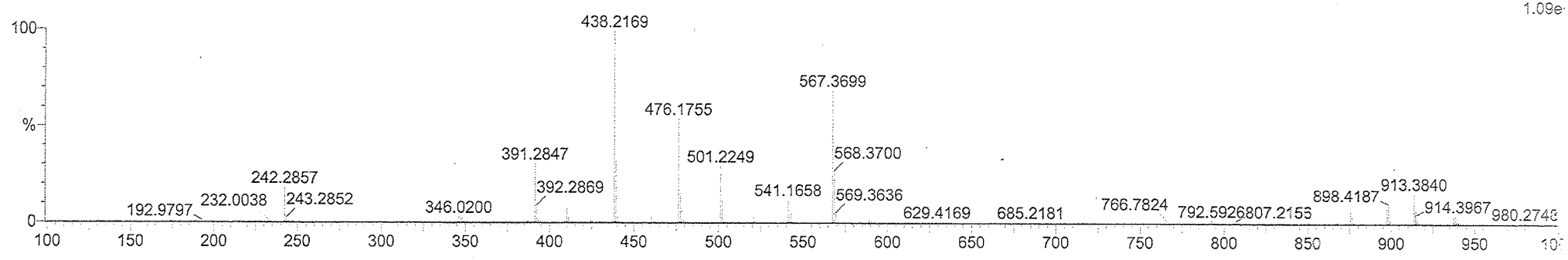
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
59 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\007
UT1010_253 17 (0.399) Cm (17:23-61:70)



5d

1: TOF MS
1.09e



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
438.2169	438.2182	-1.3	-3.0	16.5	17.4	C28 H28 N3 O2

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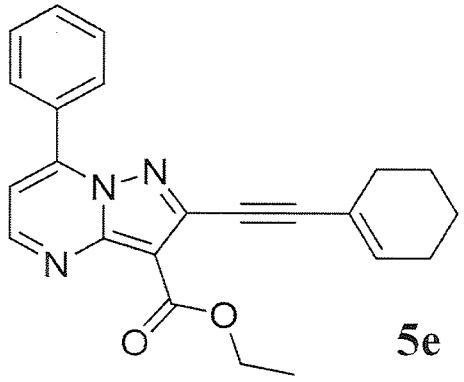
Elemental Composition Report

3/11/10

Single Mass Analysis

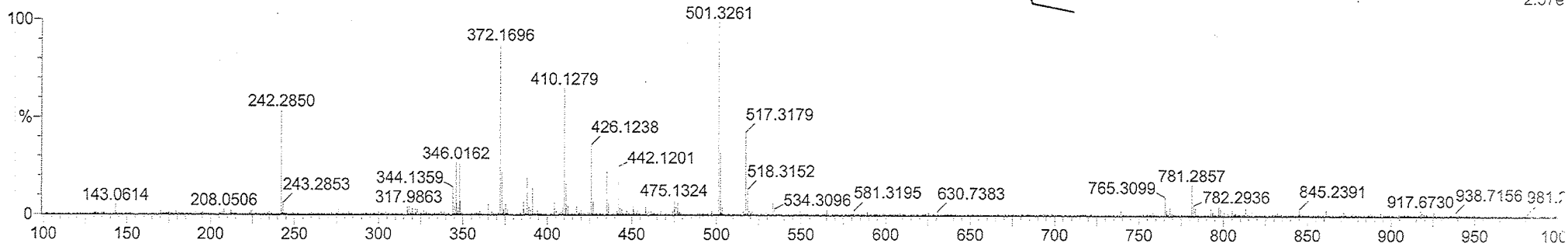
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\003
UT1010_257 20 (0.450) Cm (20:24-66:72)



5e

1: TOF MS
2.57e



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
372.1696	372.1712	-1.6	-4.3	14.5	1.4	C23 H22 N3 O2

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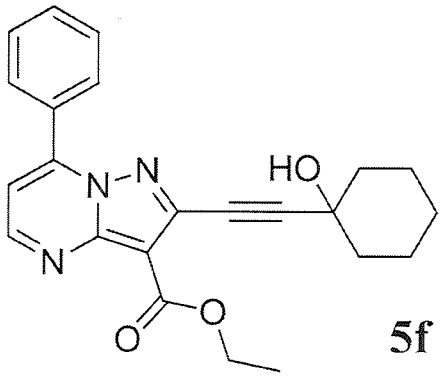
Elemental Composition Report

Single Mass Analysis

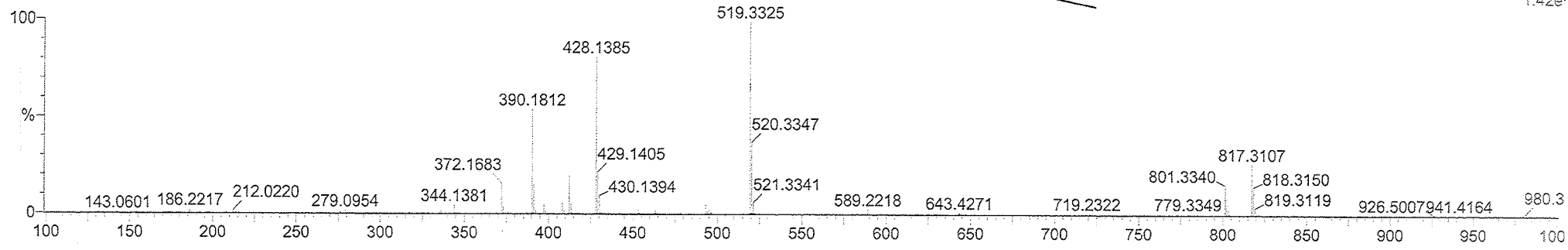
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
86 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\004
UT1010_256 17 (0.399) Cm (17:23-66:74)



5f

1: TOF MS :
1.42e

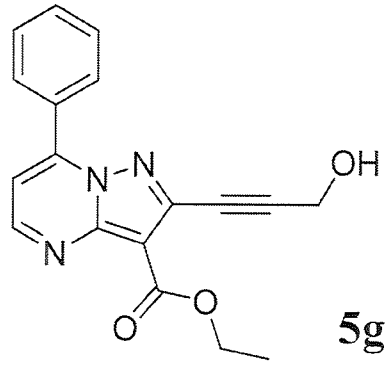


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
390.1812	390.1818	-0.6	-1.5	13.5	2.2	C23 H24 N3 O3

Single Mass Analysis

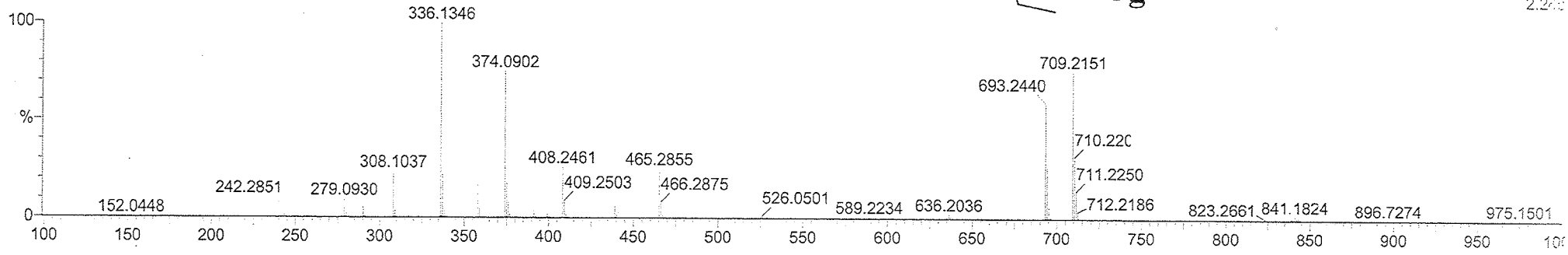
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
90 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
BPPC2\005
UT1010_255 18 (0.416) Cm (18:22-68:76)



5g

TOF MS



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
336.1346	336.1348	-0.2	-0.6	12.5	1.4	C19 H18 N3 O3

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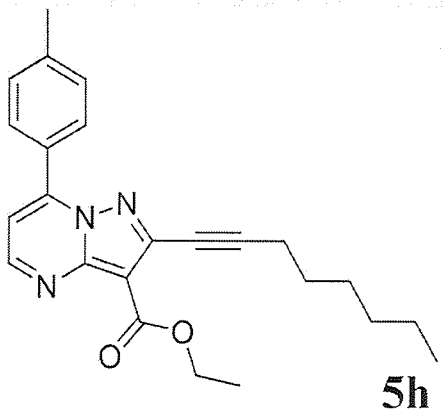
Elemental Composition Report

Single Mass Analysis

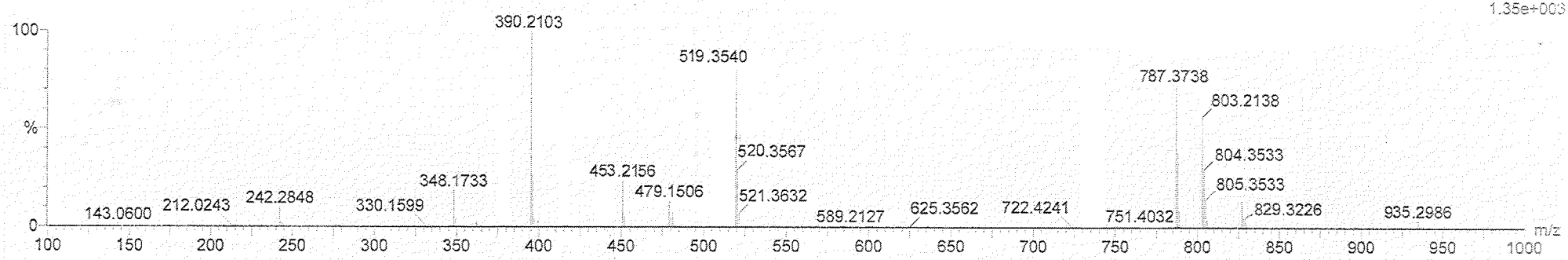
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
89 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4
MPPC2\001
UT1010_259 17 (0.399) Cm (17:21-67:72)



5h

1: TOF MS ES+
1.35e+003



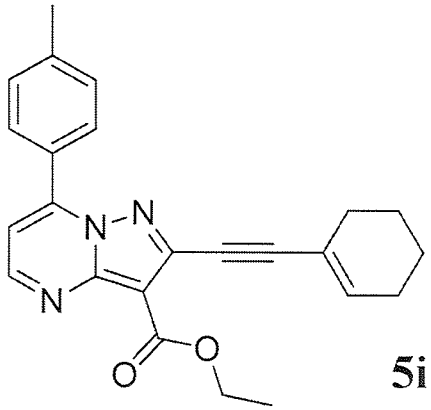
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
390.2103	390.2102	-0.4	-1.1	12.5	0.3	C24 H28 N3 O2

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

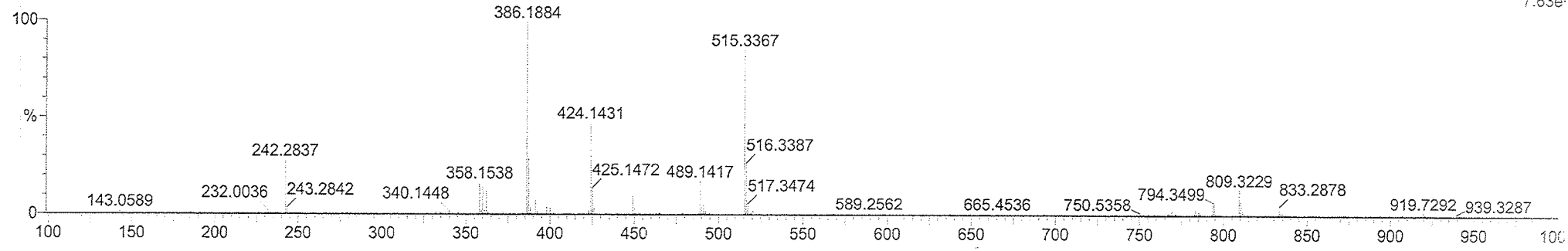
Monoisotopic Mass, Even Electron Ions
178 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4 I: 0-1



5i

MPPC2\002
UT1010_251 21 (0.489) Cm (21:28-61:72)

1: TOF MS
7.63e



Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
386.1884	386.1869	1.5	3.9	14.5	1.1	C24 H24 N3 O2

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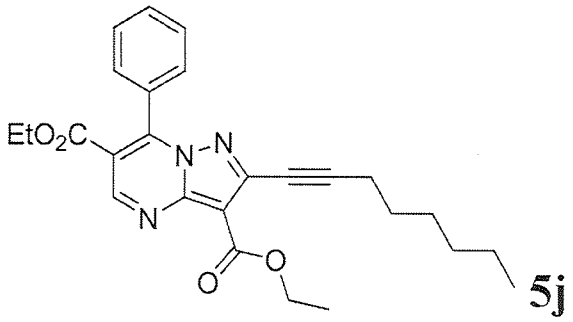
Elemental Composition Report

3/11/10

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

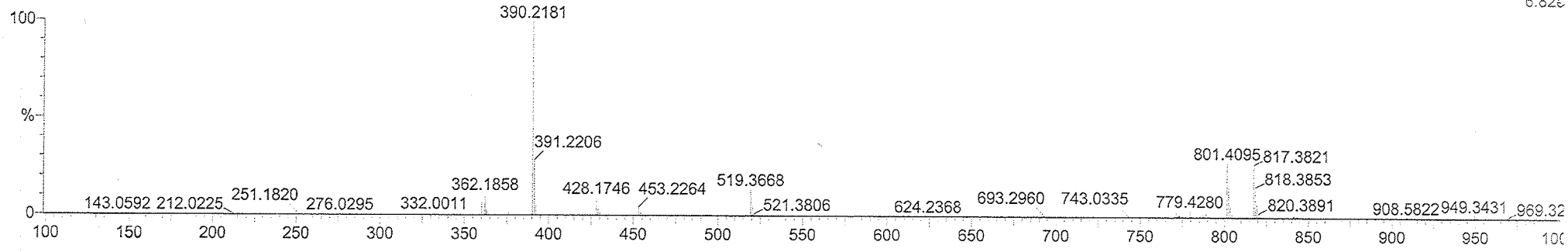
Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4 I: 0-1



5j

BPPC2C\001
UT1010_250 17 (0.398) Cm (17:20-62:71)

1: TOF MS
6.82e



Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
390.2181	390.2182	-0.1	-0.3	12.5	1.8	C24 H28 N3 O2

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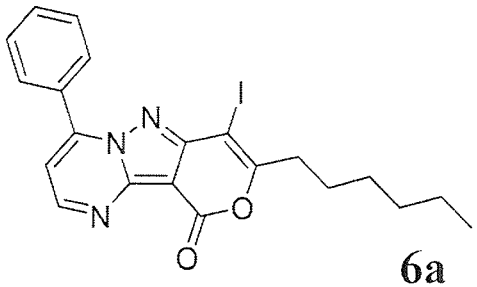
Elemental Composition Report

Single Mass Analysis

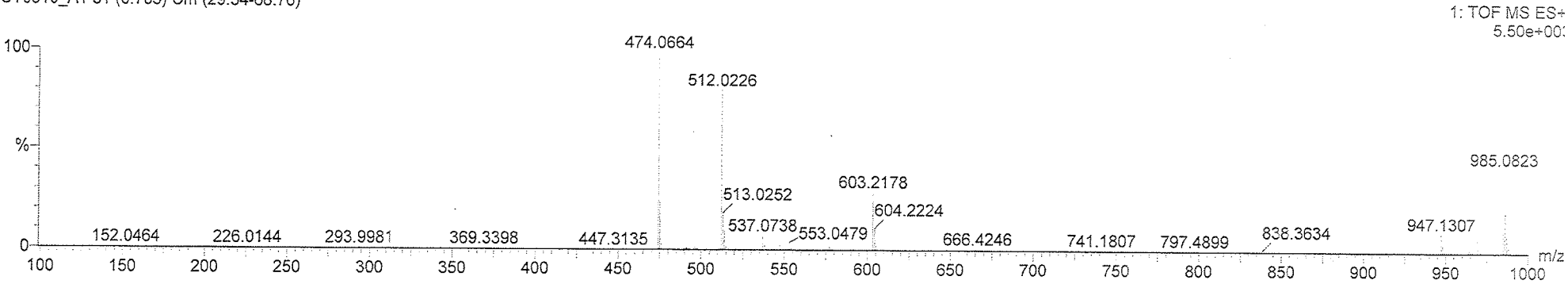
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
138 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-25 H: 0-30 N: 0-5 O: 0-6 I: 0-1



6a

BPPC3-001
UT0910_A1 31 (0.705) Cm (29:34-68:76)



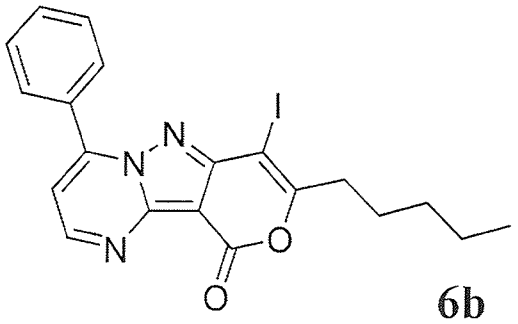
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
474.0664	474.0679	-1.5	-3.2	12.5	1.1	C21 H21 N3 O2 I

Elemental Composition Report

Single Mass Analysis

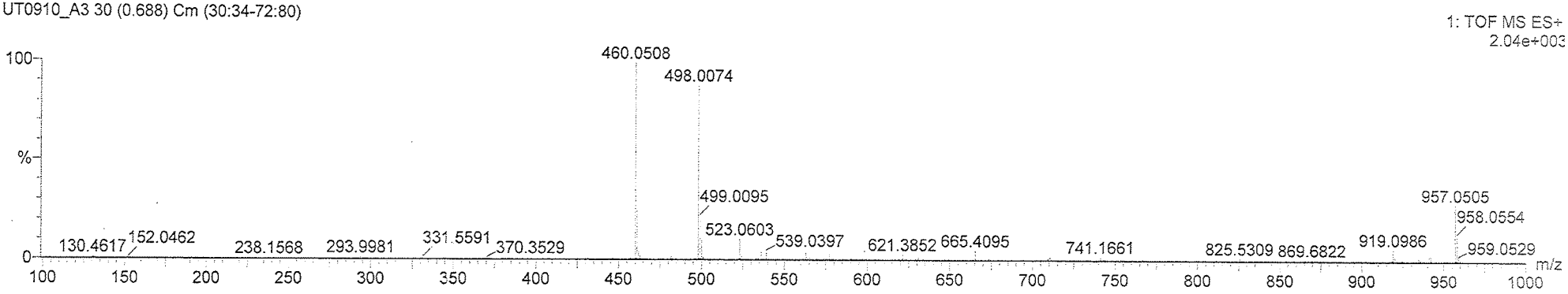
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
175 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-5 O: 0-6 I: 0-1



6b

BPPC3-006
UT0910_A3 30 (0.688) Cm (30:34-72:80)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
460.0508	460.0522	-1.4	-3.0	12.5	0.4	C20 H19 N3 O2 I

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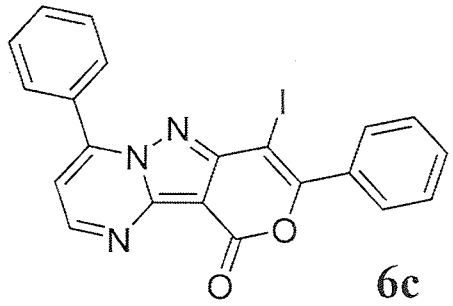
Elemental Composition Report

Single Mass Analysis

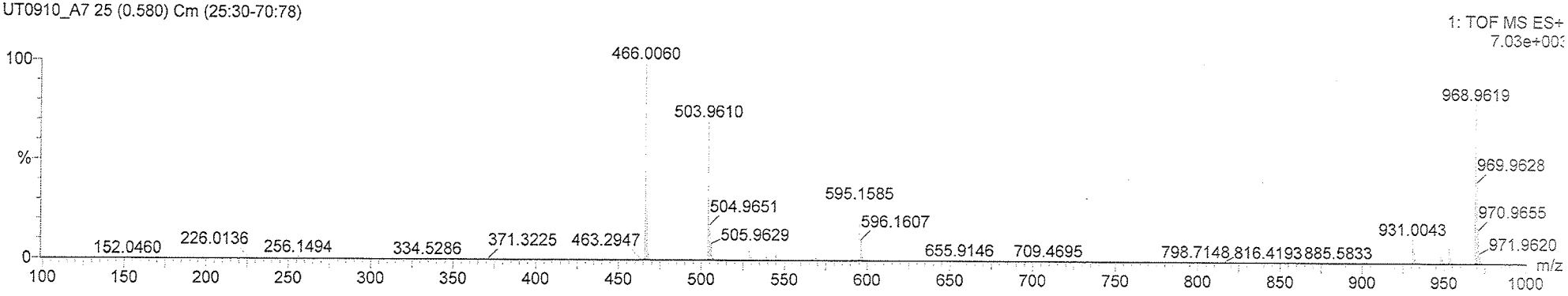
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
172 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-5 O: 0-6 I: 0-1



6c

BPPC3-002
UT0910_A7 25 (0.580) Cm (25:30-70:78)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
466.0060	466.0053	0.7	1.5	16.5	0.1	C21 H13 N3 O2 I

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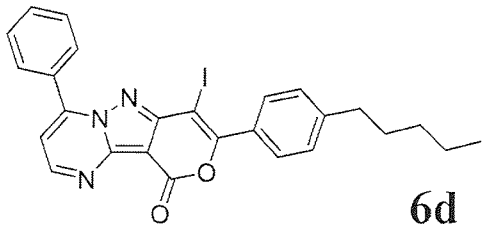
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

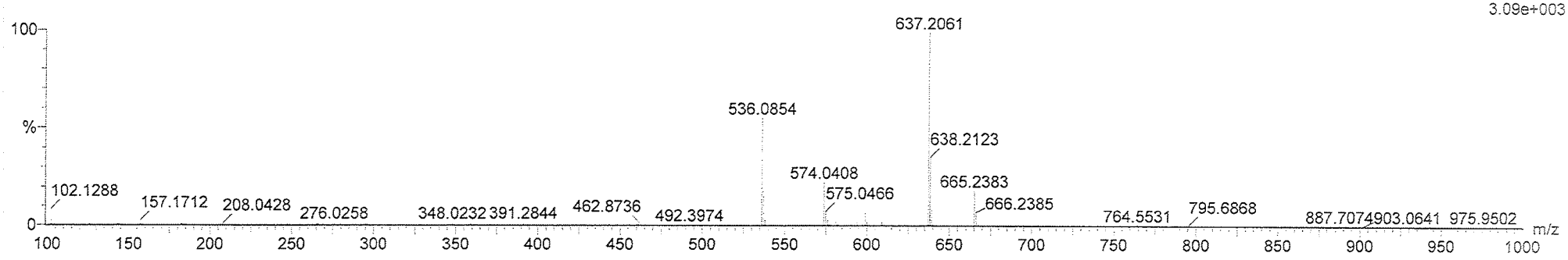
Monoisotopic Mass, Even Electron Ions
266 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-40 H: 0-55 N: 0-4 O: 0-5 I: 0-1



6d

BPPC3-007 TDC-113
UT1210_103 15 (0.469) Cm (15:20-49:56)

1: TOF MS ES+
3.09e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
536.0854	536.0835	1.9	3.5	16.5	1.2	C26 H23 N3 O2 I

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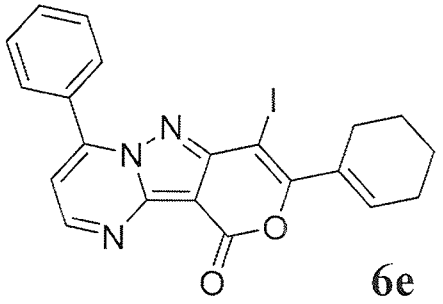
Elemental Composition Report

Single Mass Analysis

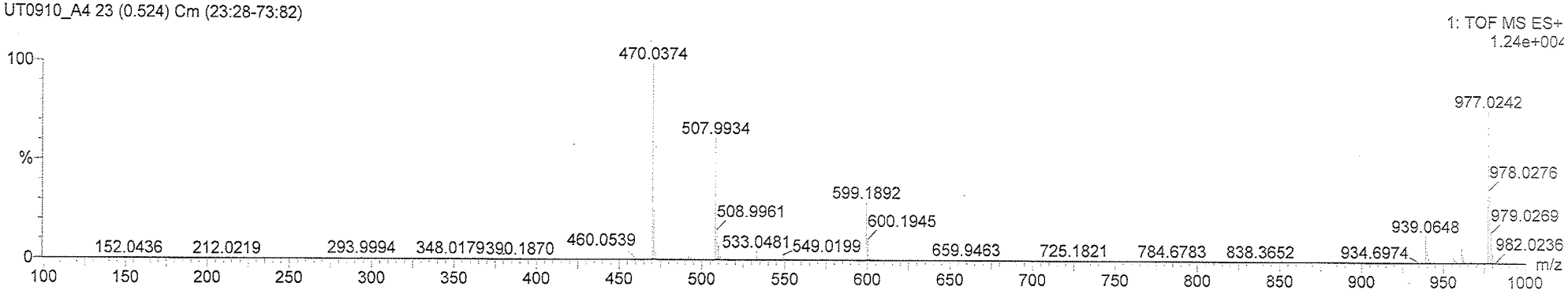
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
168 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-5 O: 0-6 I: 0-1



6e

BPPC3-003
UT0910_A4 23 (0.524) Cm (23:28-73:82)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
470.0374	470.0366	0.8	1.7	14.5	0.2	C21 H17 N3 O2 I

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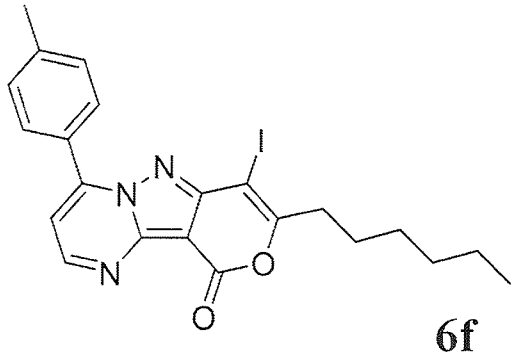
Elemental Composition Report

Single Mass Analysis

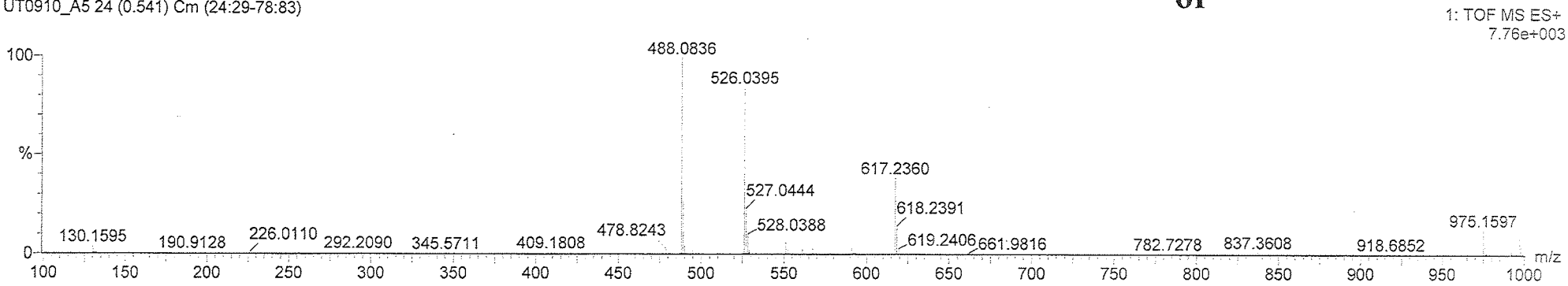
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
155 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-5 O: 0-6 I: 0-1



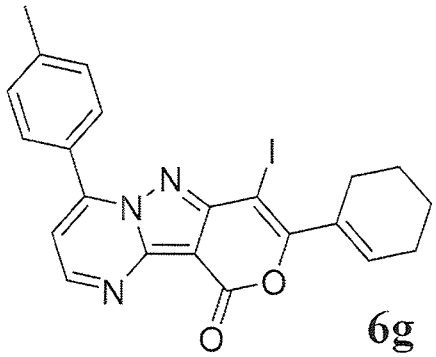
6f

MPPC3-001
UT0910_A5 24 (0.541) Cm (24:29-78:83)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
488.0836	488.0835	0.1	0.2	12.5	4.8	C22 H23 N3 O2 I

Elemental Composition Report



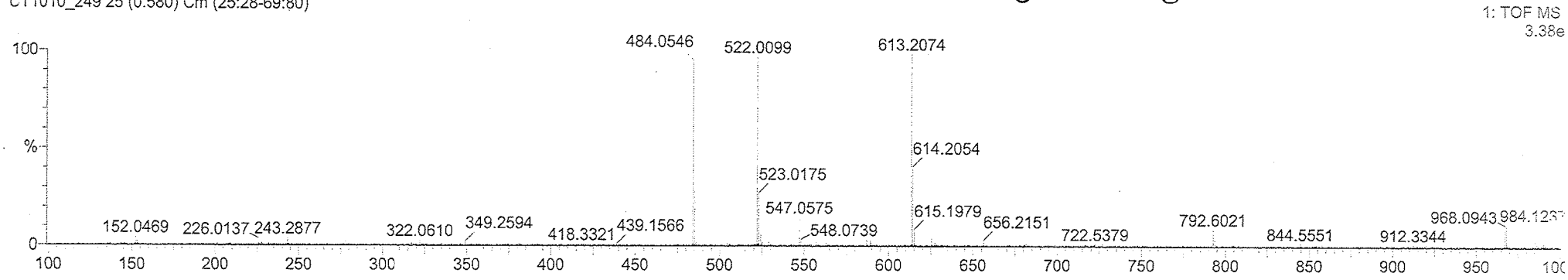
6g

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
122 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 N: 0-5 O: 0-4 I: 0-1

MPPC3\002
UT1010_249 25 (0.580) Cm (25:28-69:80)



Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
484.0546	484.0522	2.4	5.0	14.5	1.6	C22 H19 N3 O2 I

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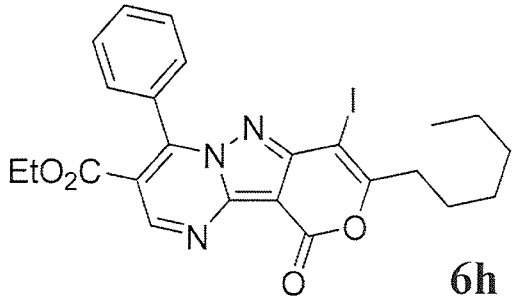
Elemental Composition Report

Single Mass Analysis

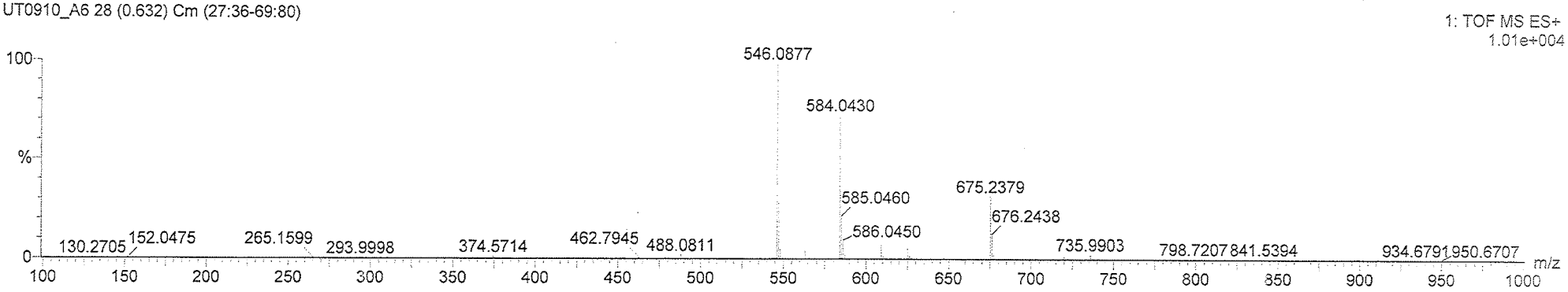
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
128 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-5 O: 0-6 I: 0-1



6h

BPPC3C-001
UT0910_A6 28 (0.632) Cm (27:36-69:80)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
546.0877	546.0890	-1.3	-2.4	13.5	0.6	C24 H25 N3 O4 I

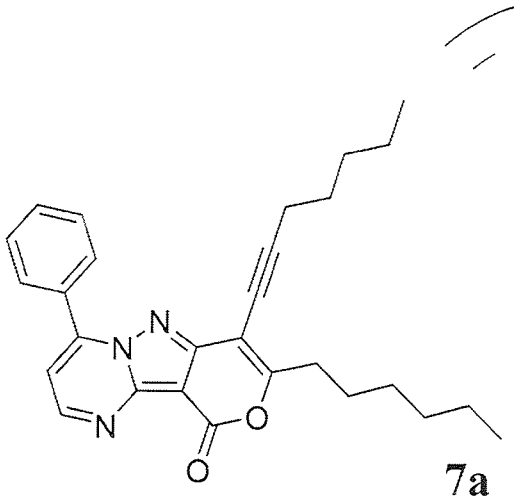
Elemental Composition Report

Single Mass Analysis

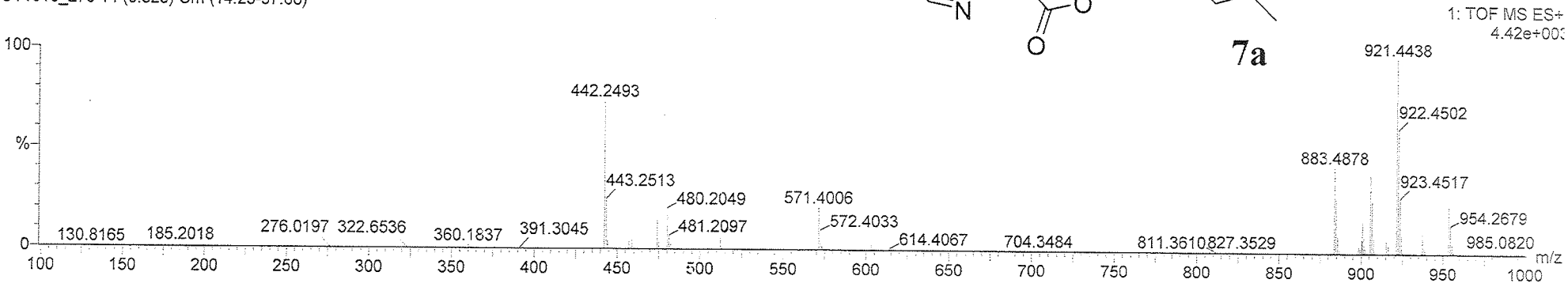
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
185 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-6 O: 0-6

BPPC4-SOG-001
UT1010_270 14 (0.325) Cm (14:25-57:68)



7a



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
442.2493	442.2495	-0.2	-0.5	14.5	0.3	C28 H32 N3 O2

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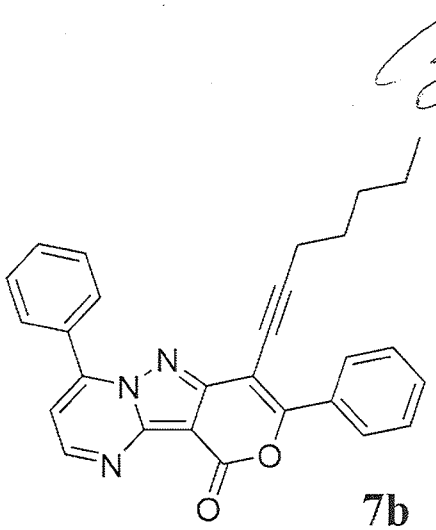
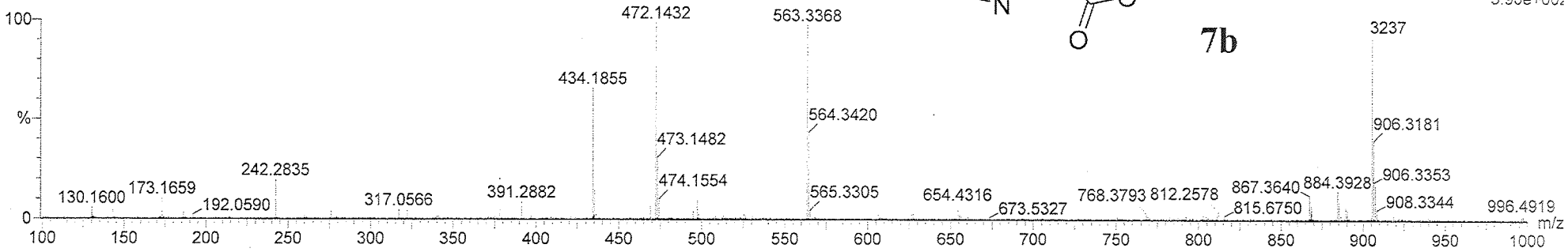
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
186 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-6 O: 0-6
BPPC4-SOG-002
UT1010_269 18 (0.416) Cm (17:26-57:67)





Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
434.1855	434.1869	-1.4	-3.2	18.5	5.2	C28 H24 N3 O2

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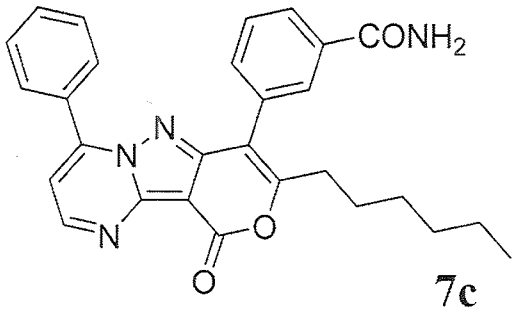
Elemental Composition Report

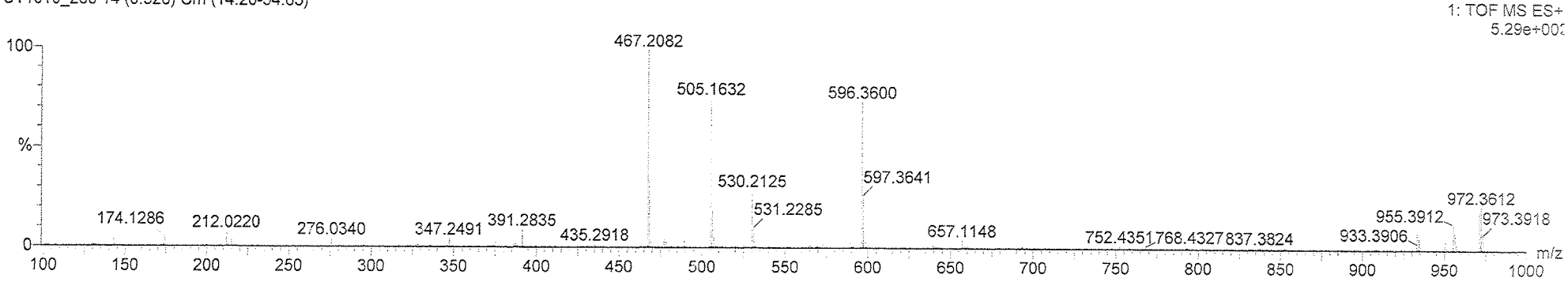


7c

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
185 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-6 O: 0-6
BPPC4-SU-001
UT1010_268 14 (0.326) Cm (14:20-54:63)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
467.2082	467.2083	-0.1	-0.2	17.5	7.9	C28 H27 N4 O3

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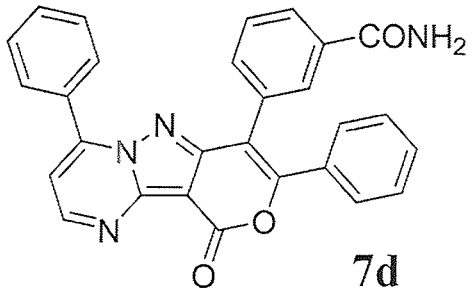
Elemental Composition Report

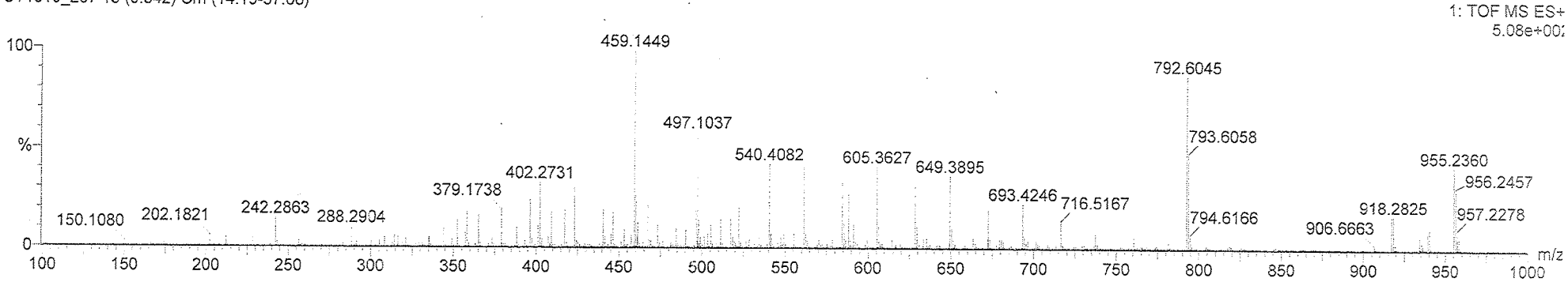
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
188 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-6 O: 0-6
BPPC4-SU-002
UT1010_267 15 (0.342) Cm (14:19-57:68)



7d



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
459.1449	459.1457	-0.8	-1.7	21.5	2.9	C28 H19 N4 O3

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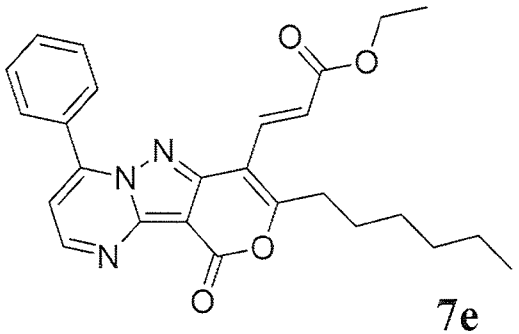
Elemental Composition Report

Single Mass Analysis

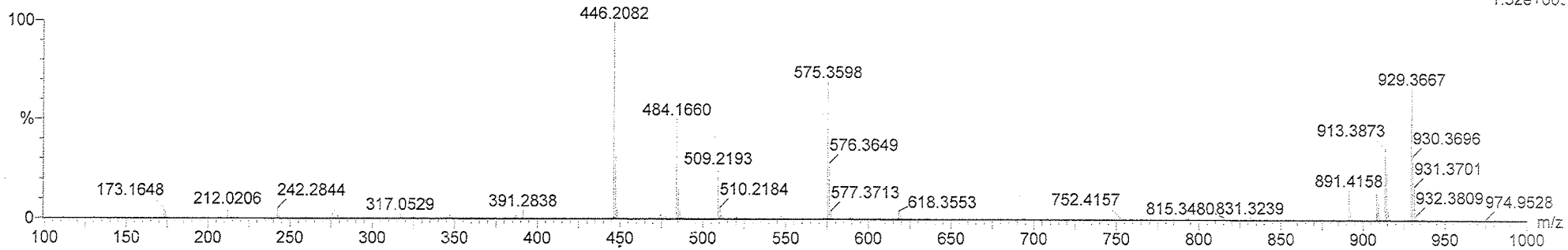
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
112 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-5 O: 0-4
BPPC4-HE-001
UT1010_265 16 (0.360) Cm (13:20-56:65)



7e

1: TOF MS ES+
1.32e+00



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
446.2082	446.2080	0.2	0.4	14.5	0.9	C26 H28 N3 O4

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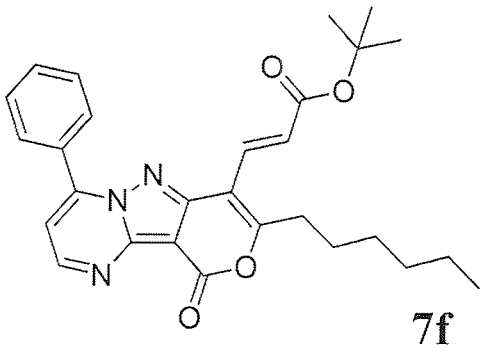
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
99 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-45 N: 0-5 O: 0-4
BPPC4-HE-002
UT1010_264 16 (0.360) Cm (16:20-58:64)



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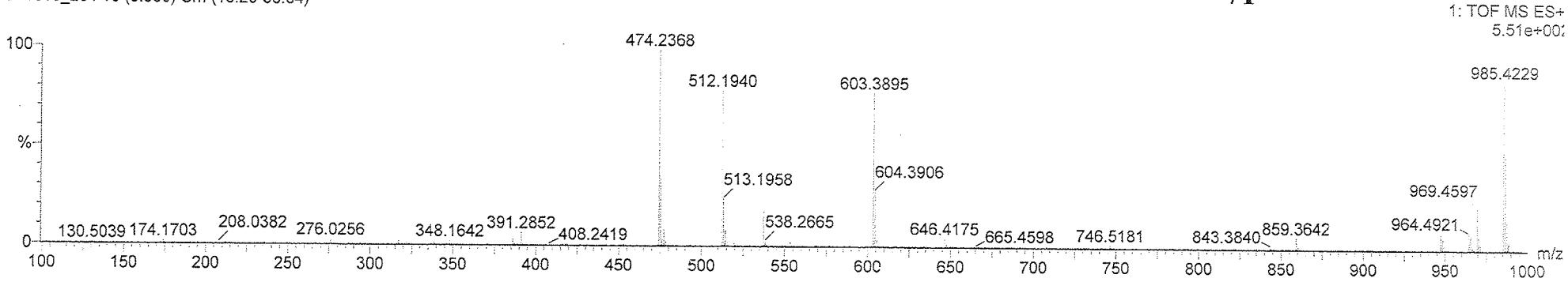
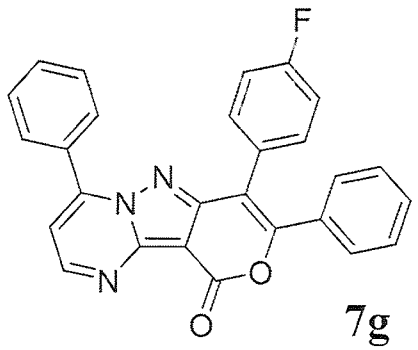


Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
474.2368	474.2393	-2.5	-5.3	14.5	6.0	C28 H32 N3 O4

CPS,MIYAPUR

Mass Analysis Report

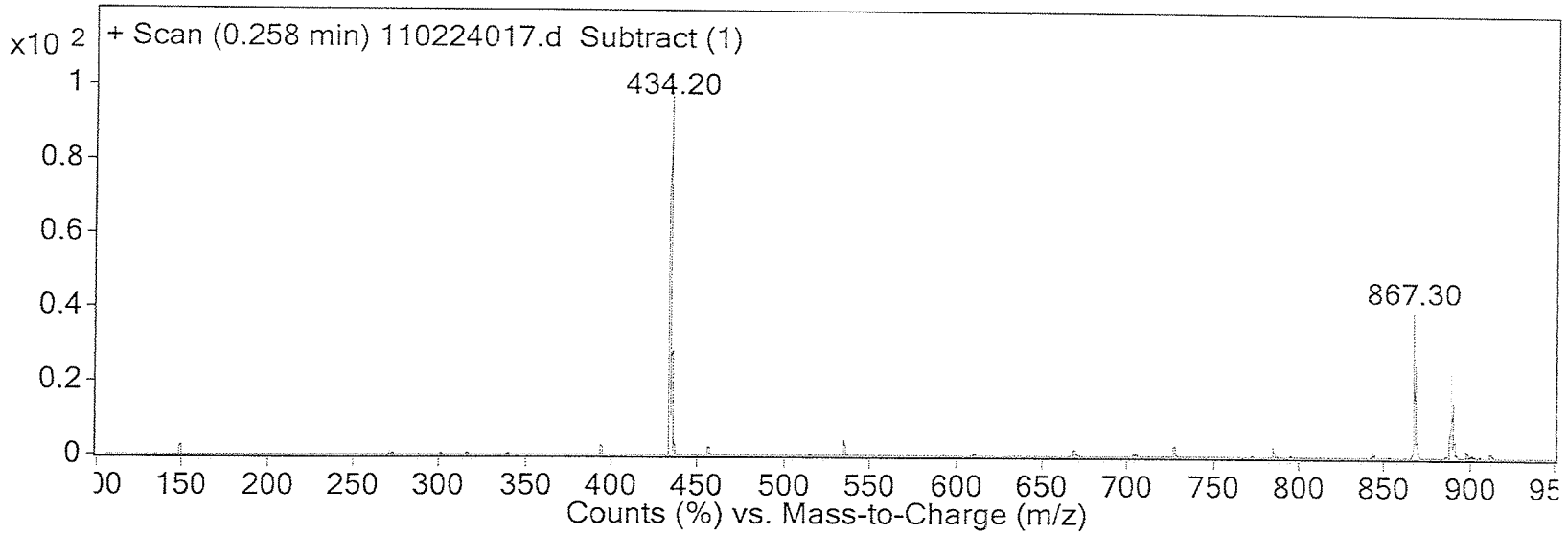


7g

Data Filename	110224017.d	**Sample Name**	BPPC4/SU/003
Sample Type	Sample	**Position**	Vial 61
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	CDD-MRM.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	Esi



--- End Of Report ---

24/02/20

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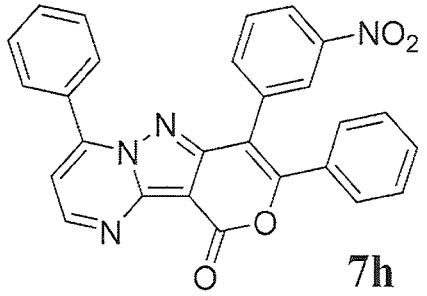
Mass Analysis Report

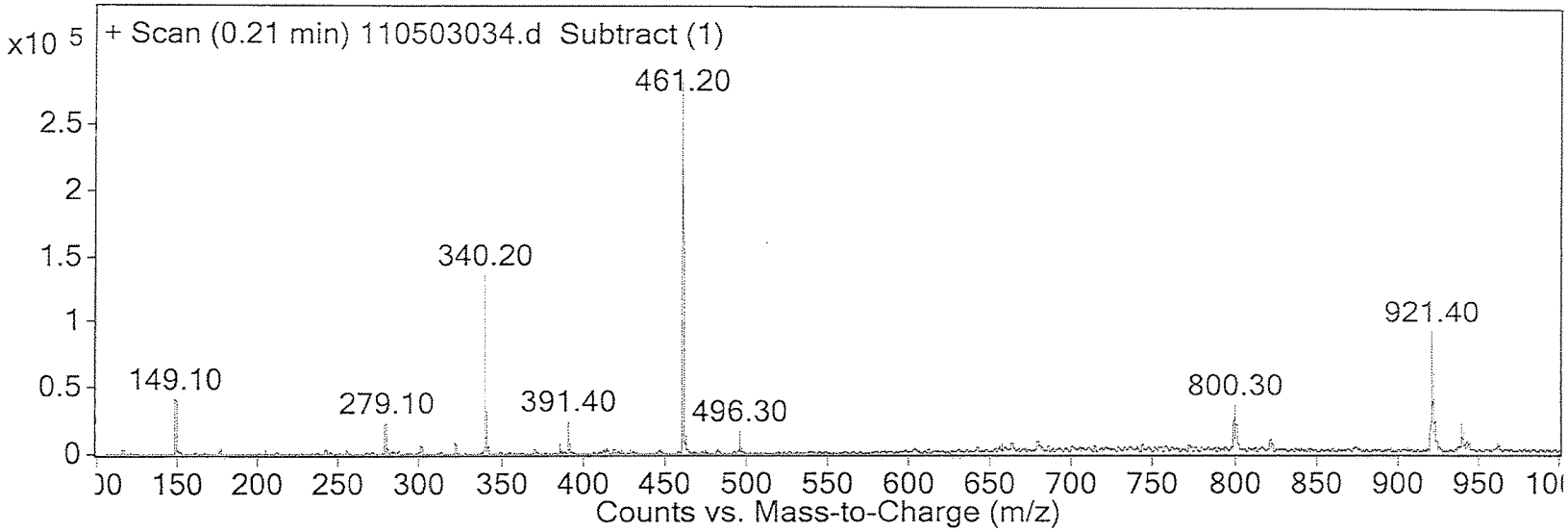


7h

Data Filename	110503034.d	**Sample Name**	BPPC/SU/004
Sample Type	Sample	**Position**	Vial 60
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	Default.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
110	0	Esi



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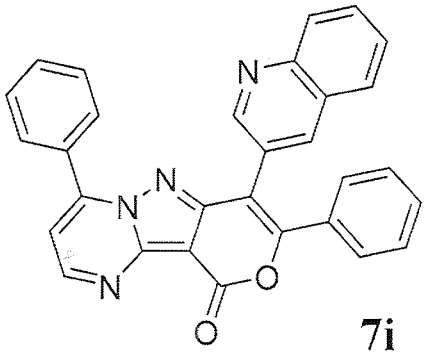
CPS,MIYAPUR

Mass Analysis Report

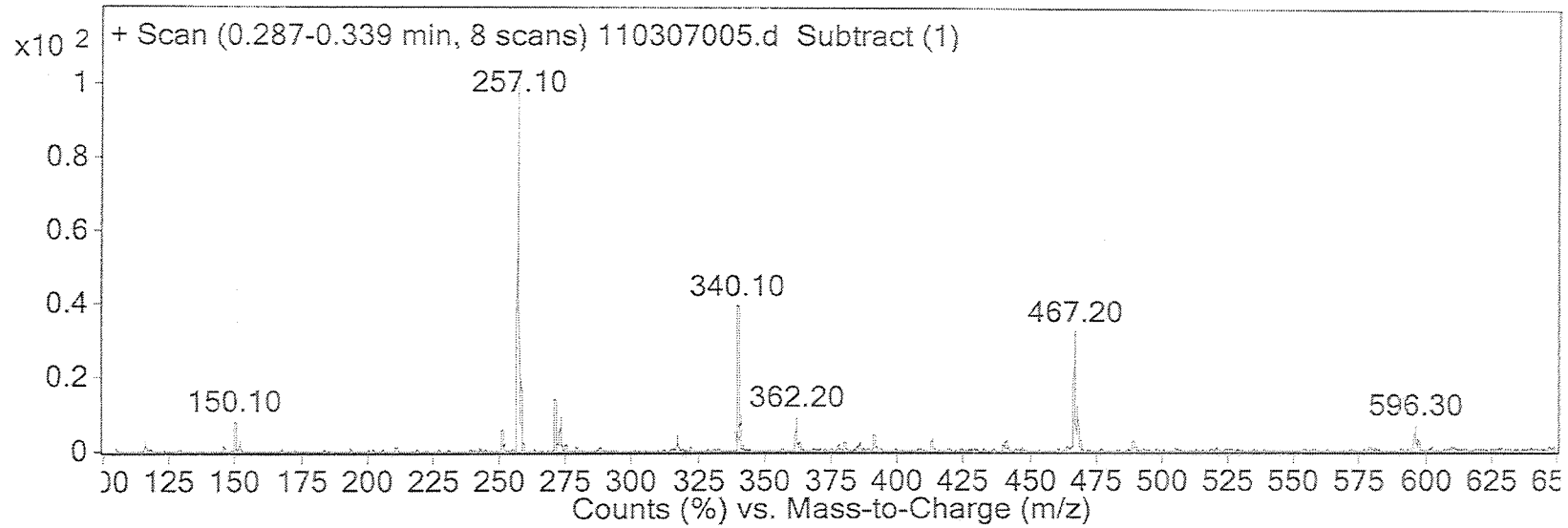
Data Filename	110307005.d	**Sample Name**	BPPC/SU/005
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	CDD-MRM.m	**Comment**	



7i

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



--- End Of Report ---

07/03/2011

Printed at: 10:09 AM on:3/7/2011

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