

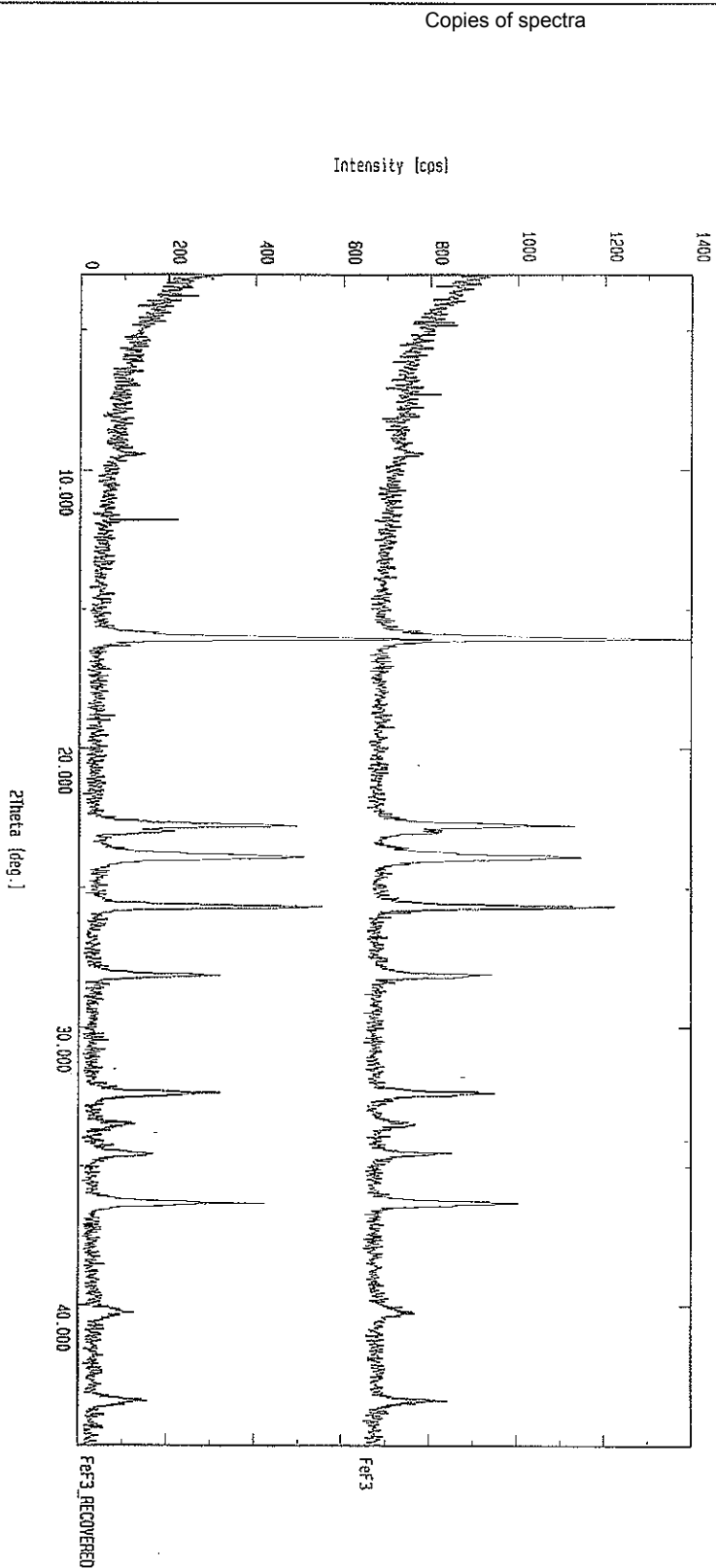
Multi-Recording

Sample : FeF₃_RECOVERED
File : PX-120330-092.1120
Comment : IDC-1/P138
Date : 30-Mar-12 16:22
Operator : S.V.Narasayya

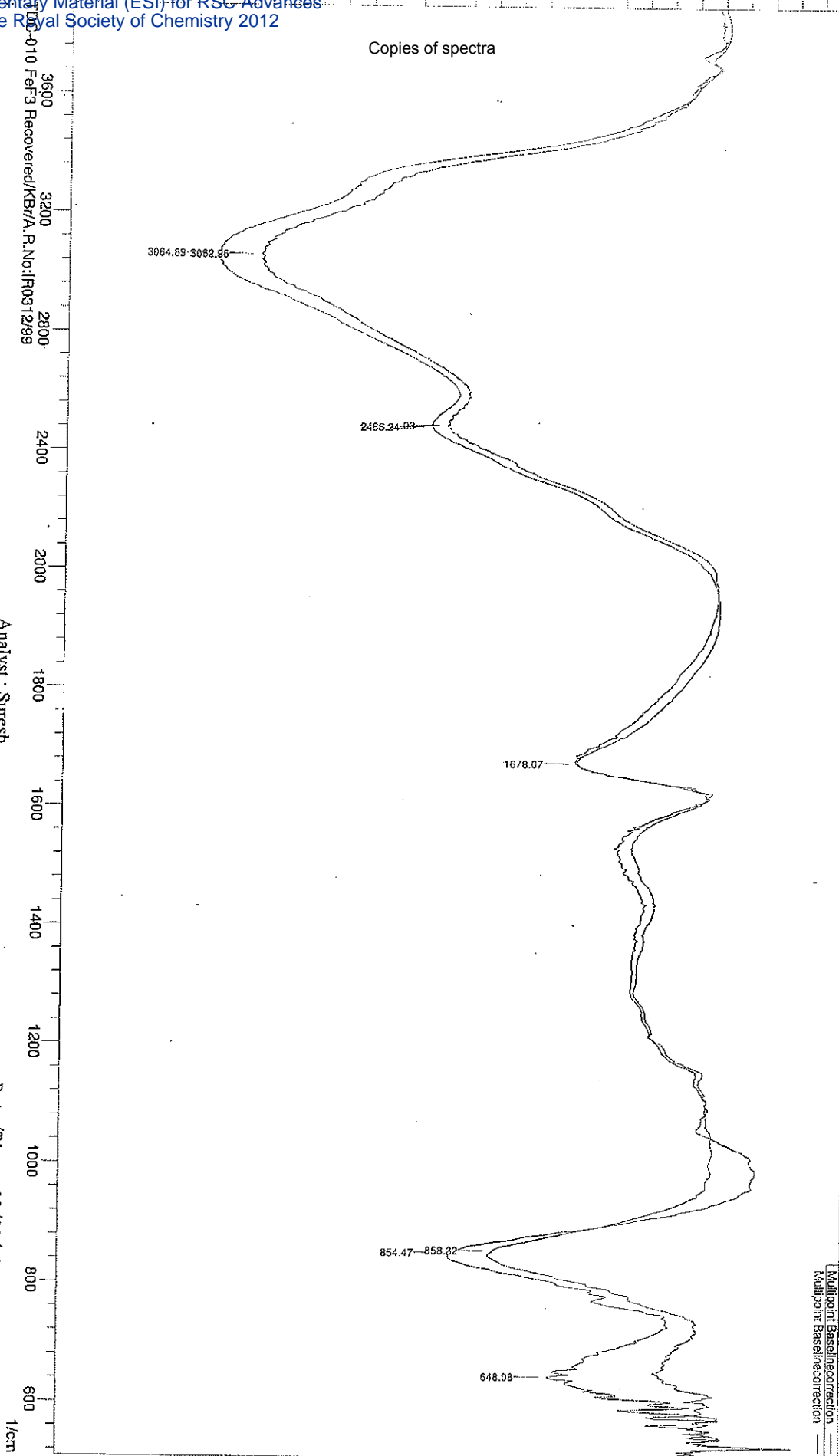
X-ray : Cu K-ALPHA1 / 50 kV / 34 mA
Gonio : RINT2000 Wide angle goniometer
Attachment : Standard Sample Holder
Filter : Not installed
I. Monochro :
C. Monochro : Automatic monochromator
Divergence slit : "1deg."
Scattering slit : "1deg."
Receiving slit : "0.15mm"

Counter : Scintillation counter
Scan mode : CONTINUOUS
Scan speed : 3 deg./min.
Scan step : 0.02 deg.
Scan axis : 2 Theta / Theta
Scan range : 3 -> 45 deg.
Theta offset: 0 deg.
Sample rotation: 0 deg.

SV
30/03/2012



Copies of spectra



3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
1/cm

Analyst: Suresh

03/30/12 08:04:44 PM

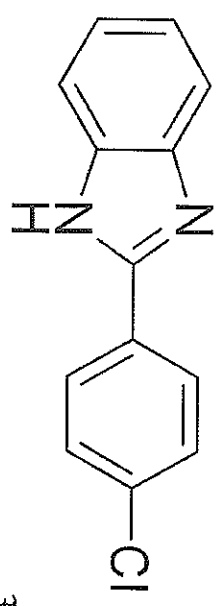
03/30/12 08:08:33 PM

03/30/12 08:08:33 PM

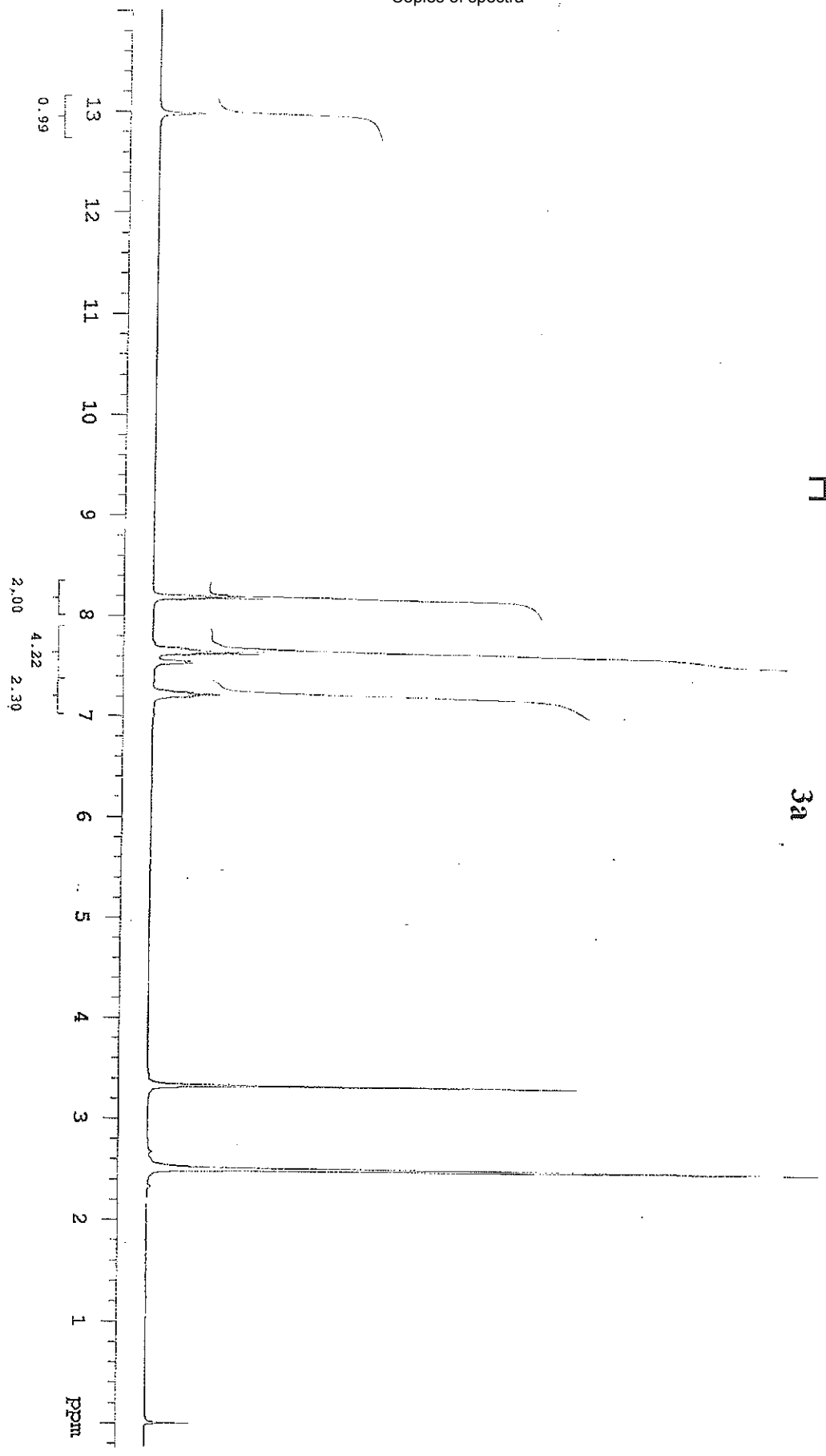
Date/Time: 03/30/12 08:04:44 PM
 03/30/12 08:08:33 PM
 User: lib-3

Copies of spectra

NMR-400MHz in DMSO
AR.No:ME0710/688
Date:9th July 2010

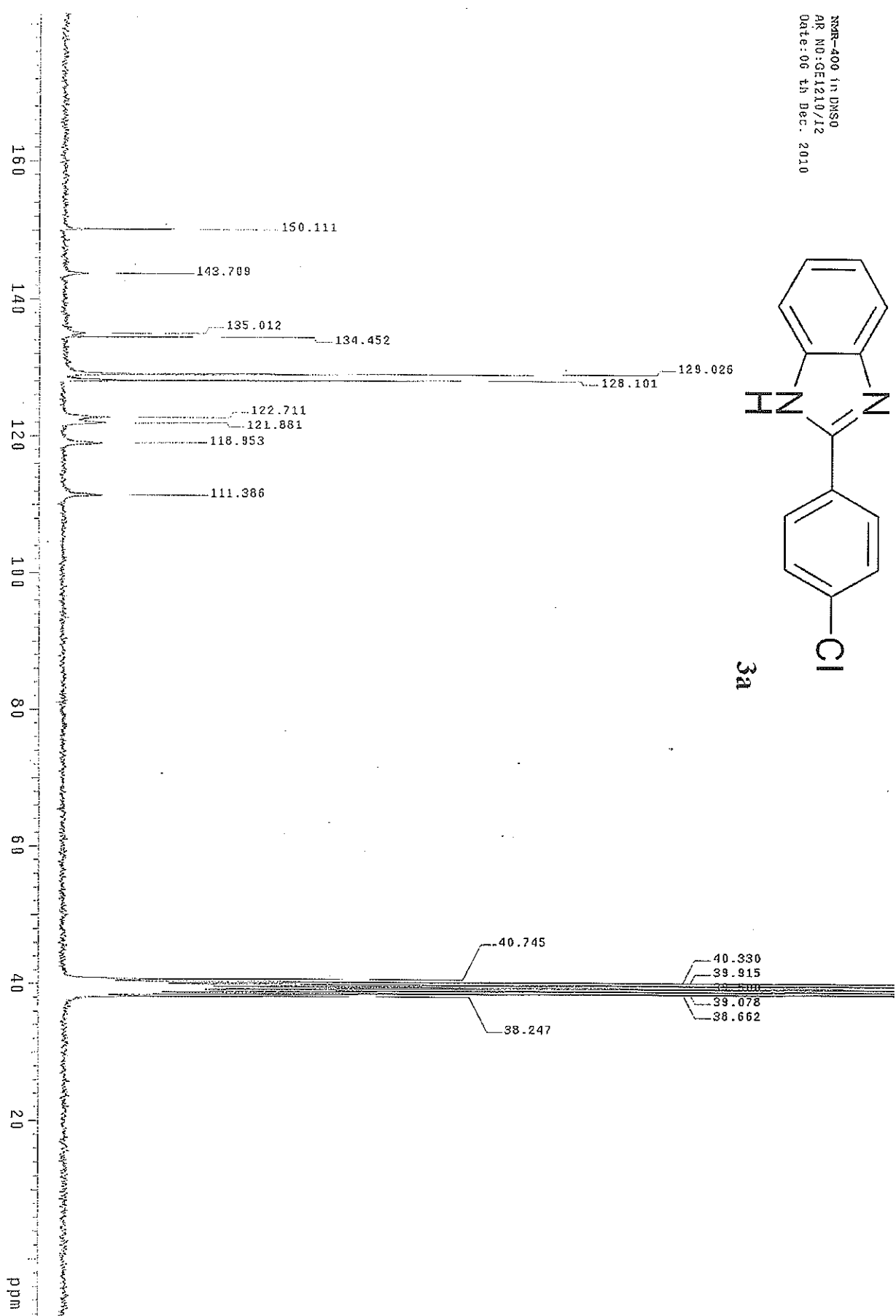


3a



Copies of spectra

MSR-400 in DMSO
AR NO:GE1210/12
Date:06 th Dec. 2010



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

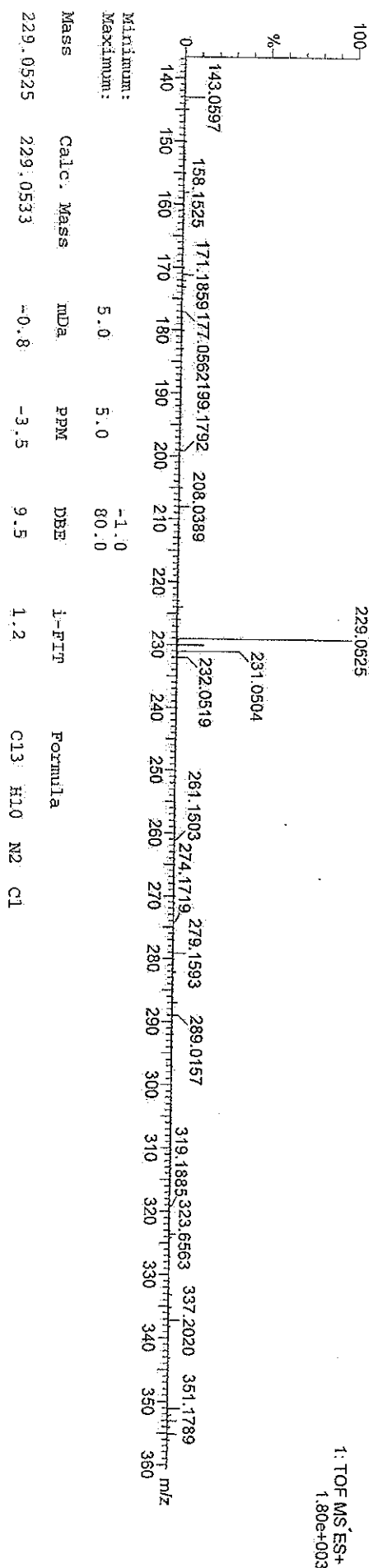
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-15 H: 0-10 N: 0-2 Cl: 0-1

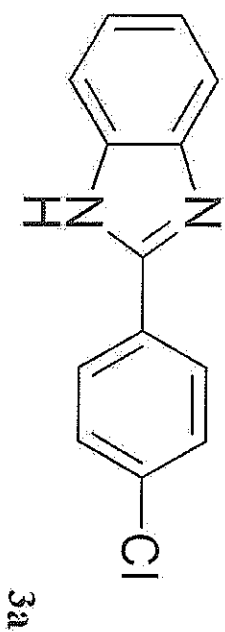
UT0312_1613 (0.251) Cm (13:15)

Dr.Reddy's Laboratories Ltd, ARD, TDC-1



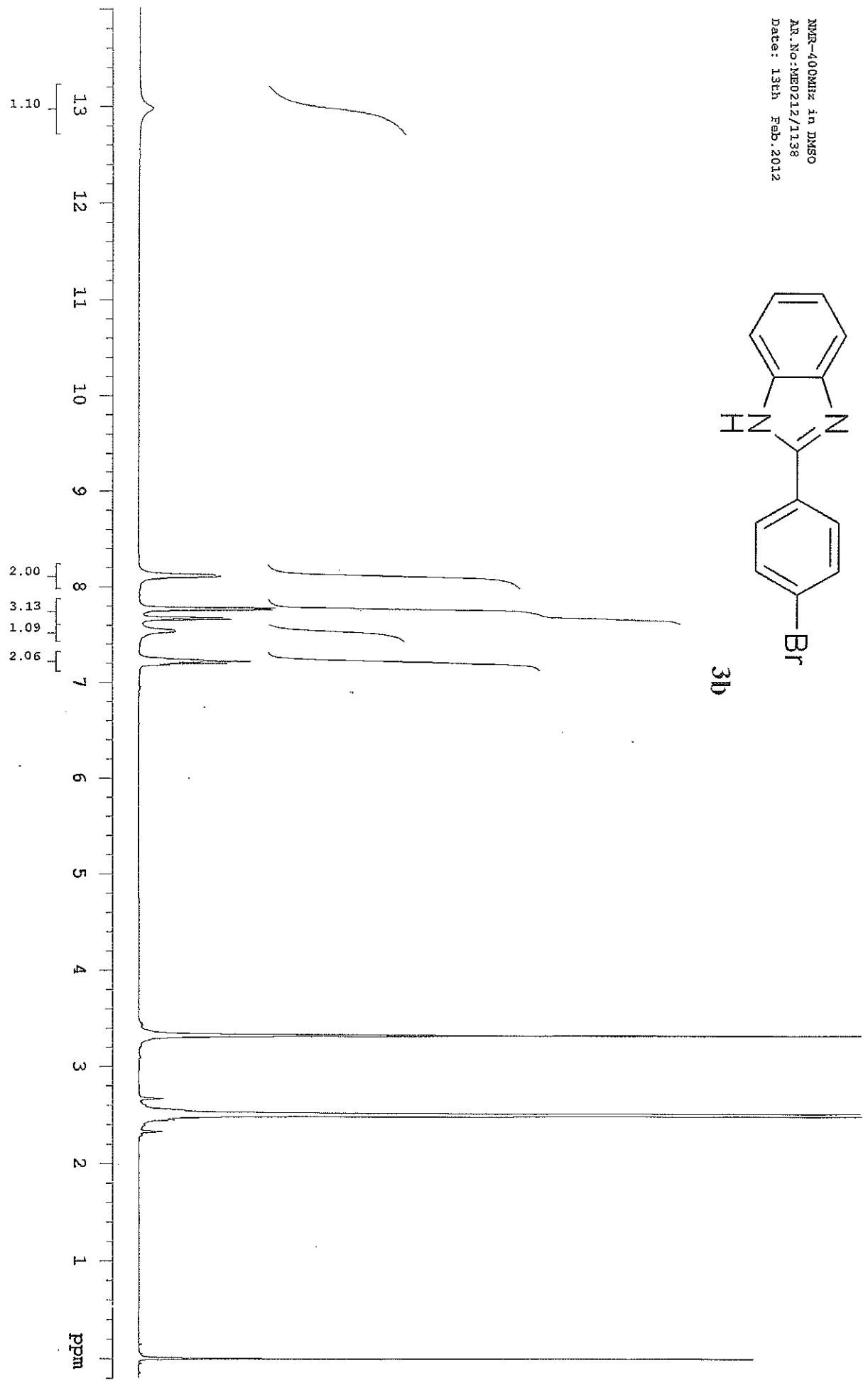
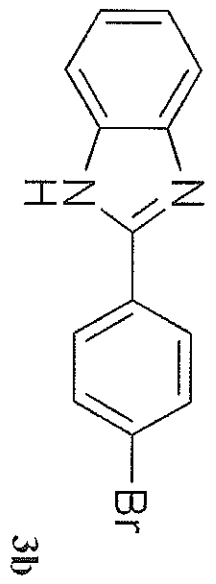
Minimum: 5.0
Maximum: 5.0
-1.0
80.0

Mass	Calc. Mass	MDA	PPM	DBE	I-FIT	Formula
229.0525	229.0533	-0.8	-3.5	9.5	1.2	C13 H10 N2 Cl

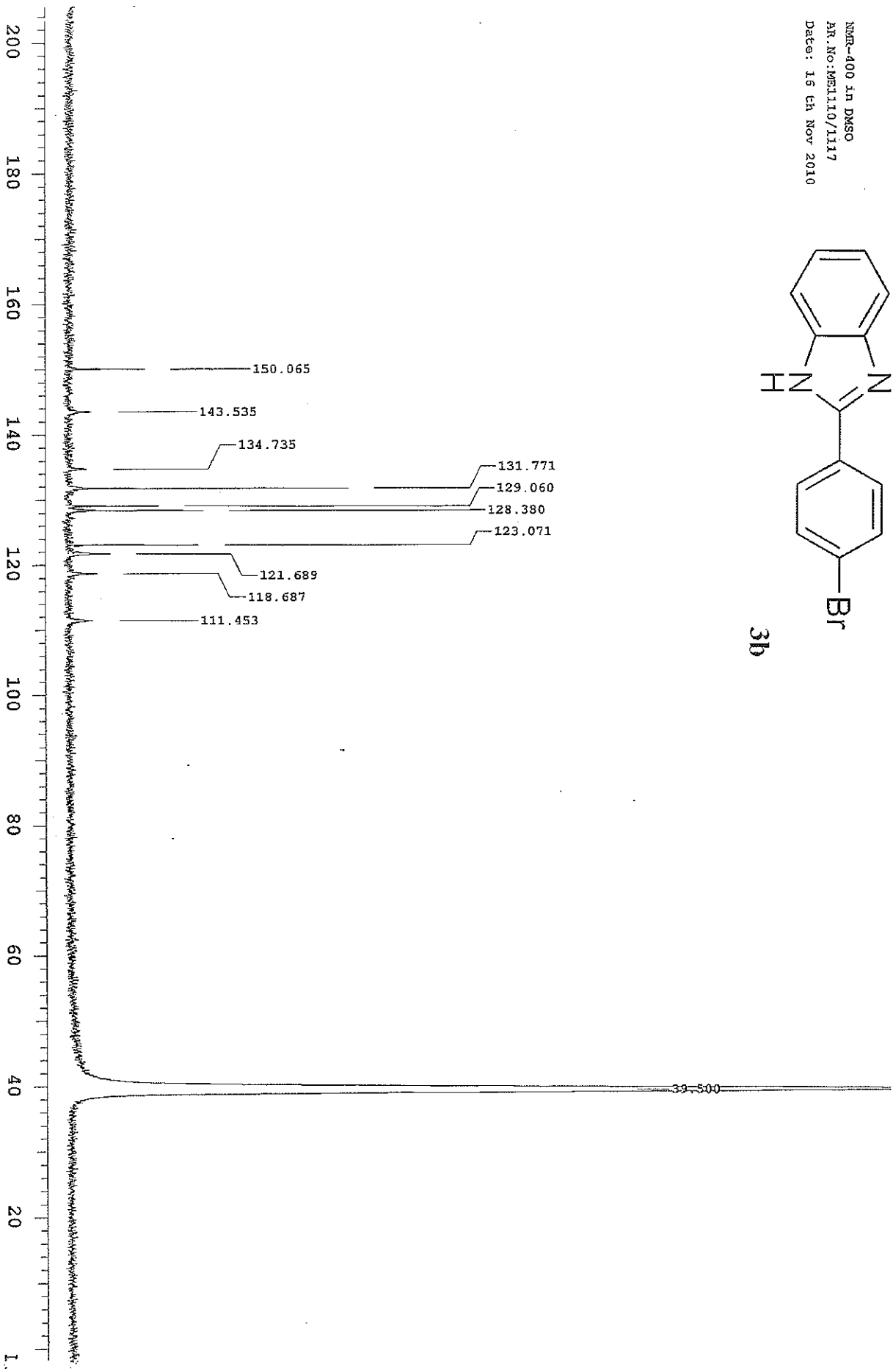
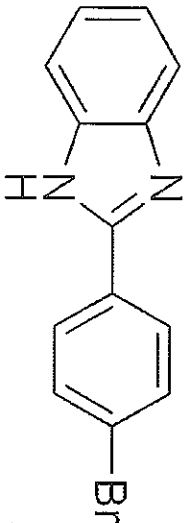


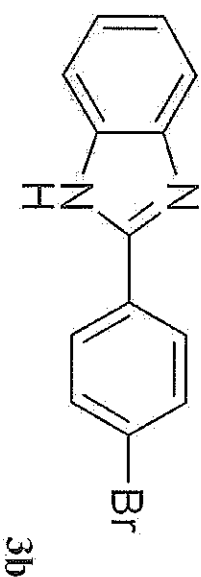
Copies of spectra

NMR-400MHz in DMSO
Ac.No:ME0212/1138
Date: 13th Feb.2012



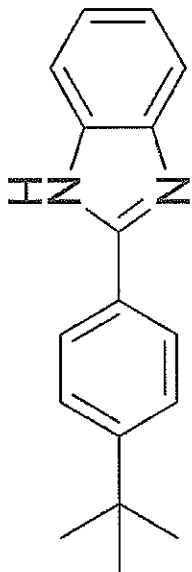
NMR-400 in DMSO
AR.No:ME1110/1117
Date: 16 th Nov 2010



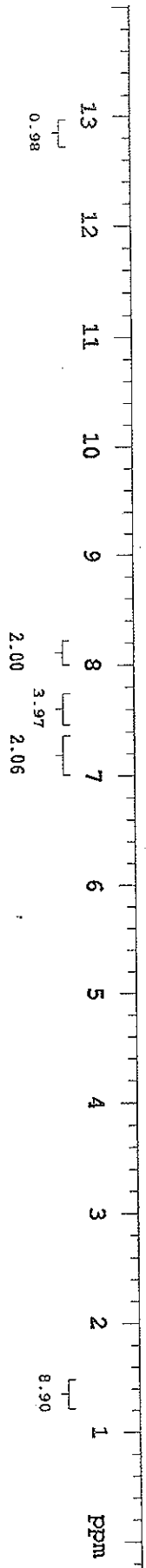


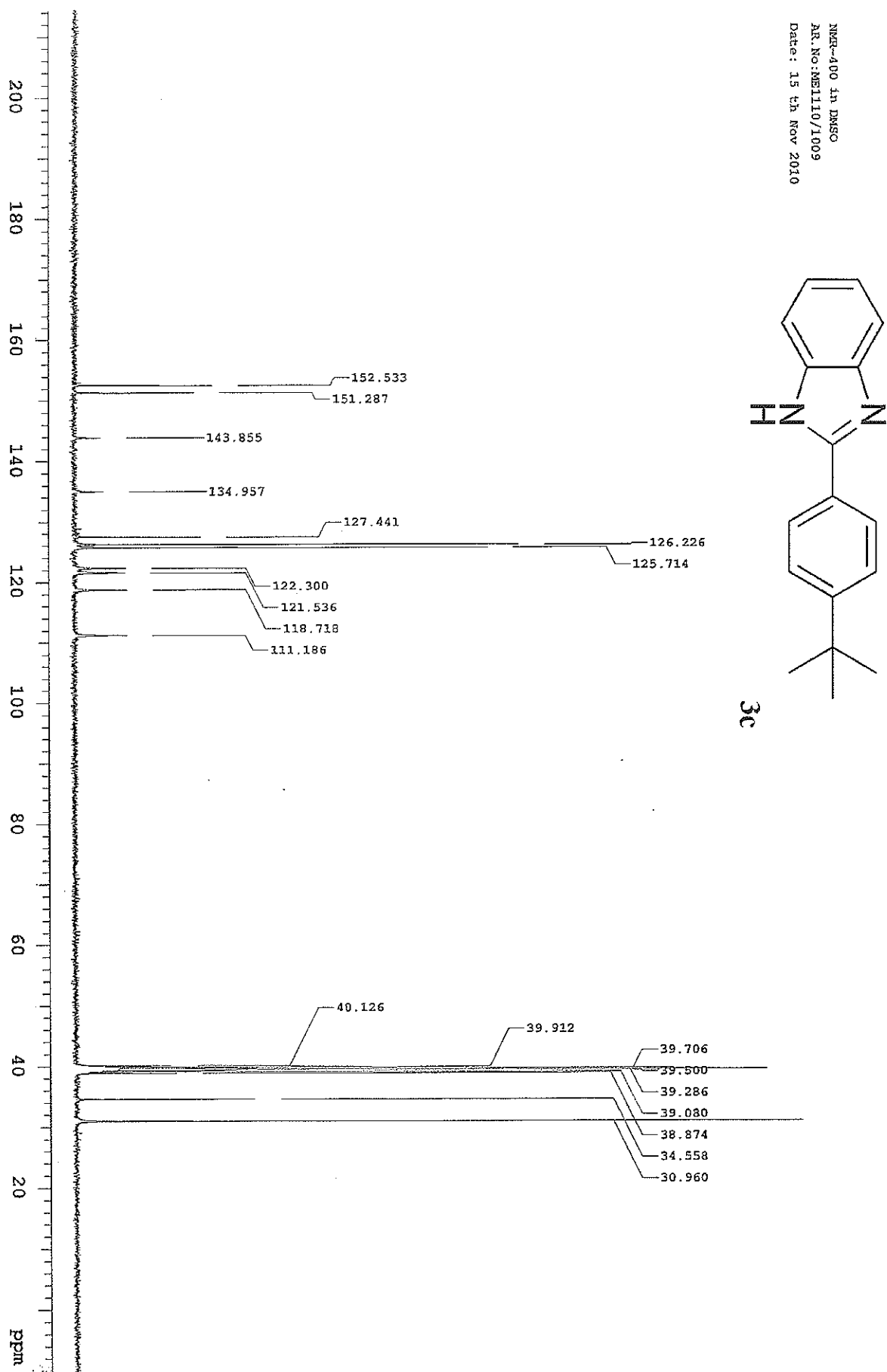
Copies of spectra

NMR-400 in DMSO
Ac.No: ME1010/41
Date: 01 st Oct 2010



3c





NMR-400 in DMSO
AR.No:ME110/1009
Date: 15 th Nov 2010

3c

Single Mass Analysis

Element prediction: Off

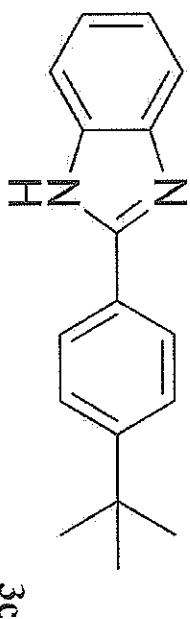
Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

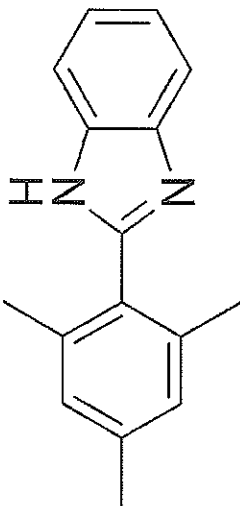
Elements Used:

C: 0-20 H: 0-20 N: 0-2

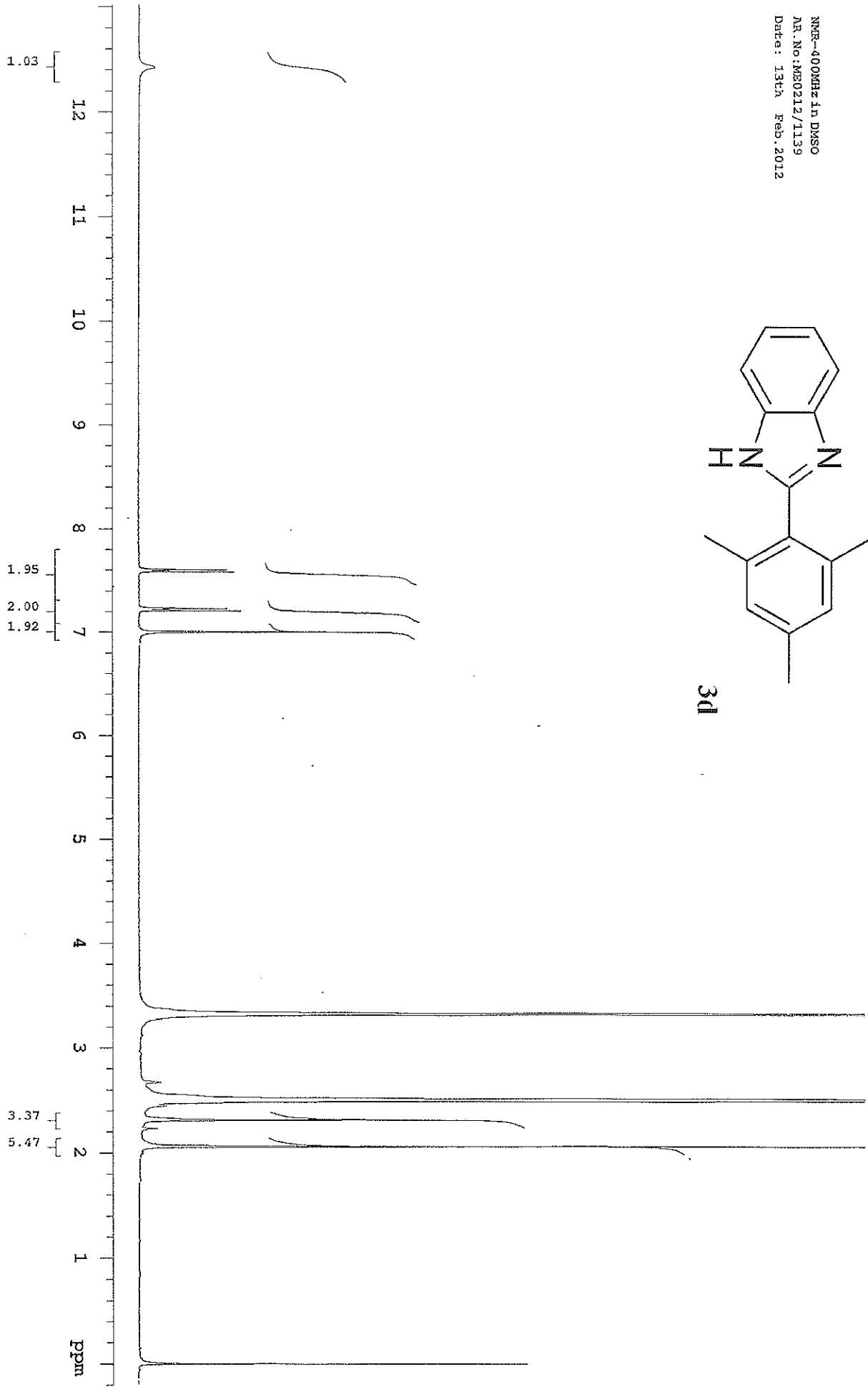
Dr.Reddy's Laboratories Ltd, ARD, TDC-1



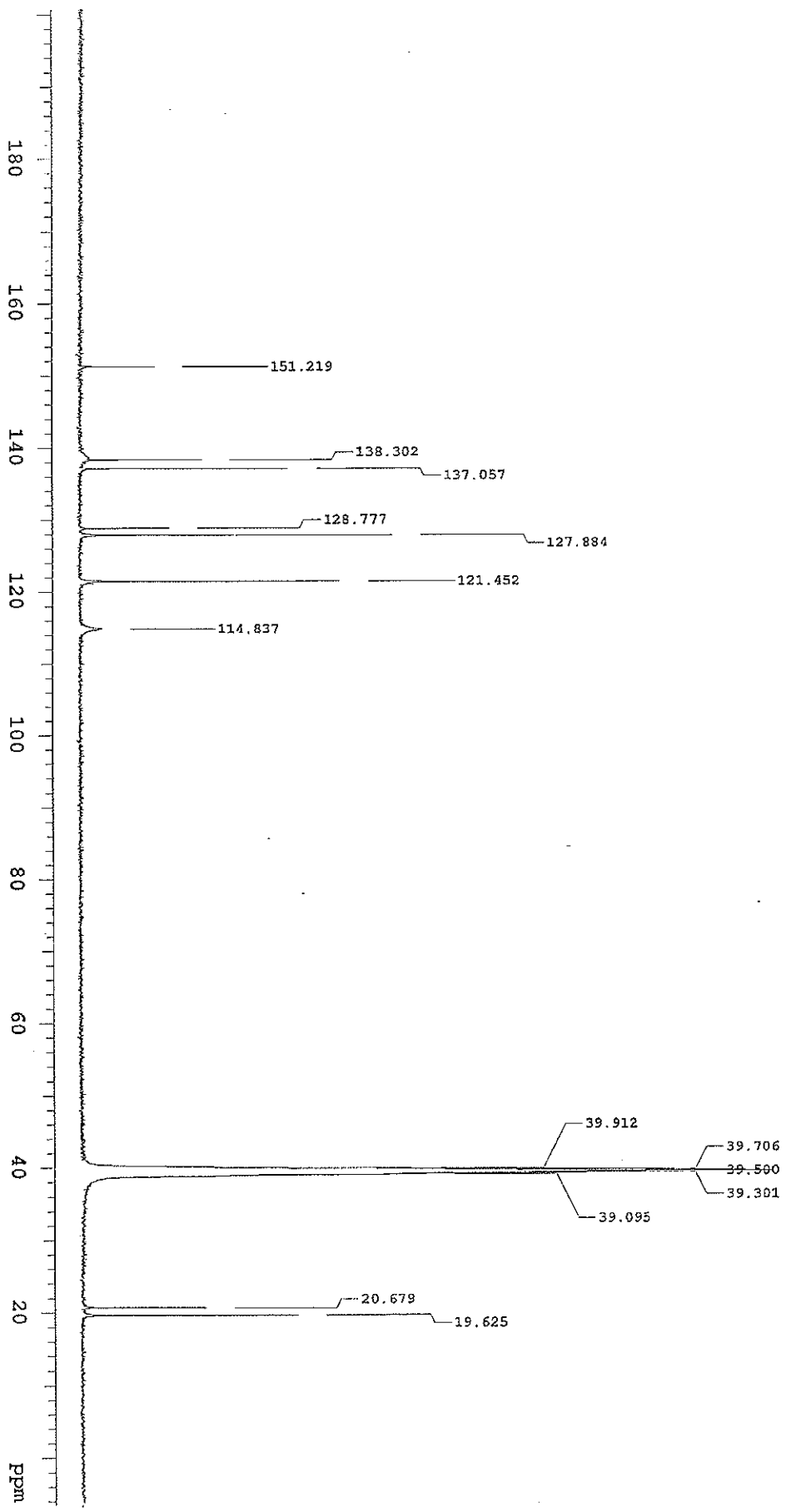
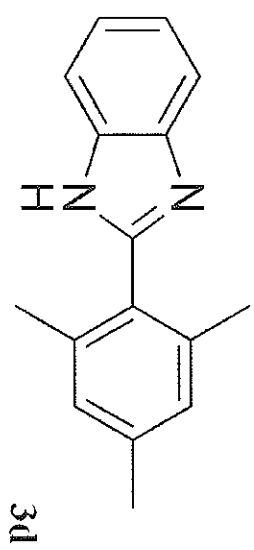
HNMR-400MHz in DMSO
Ac.No: MS0212/1139
Date: 13th Feb, 2012



3d



NR-400 1h DMSO
IR.No:ME110/1118
Date: 16 th Nov 2010



Copies of 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

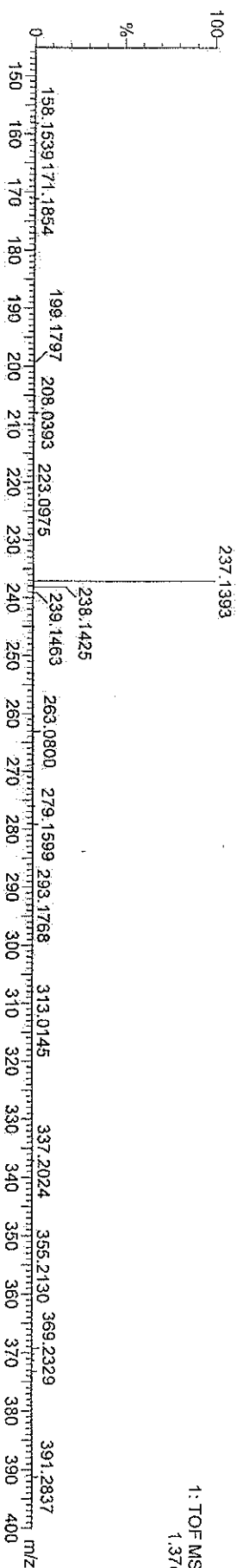
5 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-2

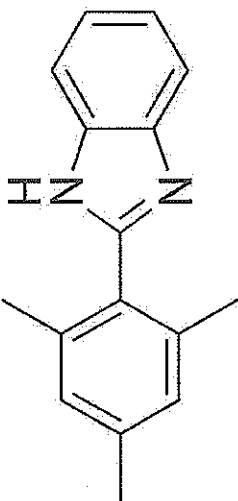
Dr. Reddy's Laboratories Ltd, ARD, TDC-1

UT0312_18 22 (0.413) Cm (21:24*(1:2+37:42)x0.010)



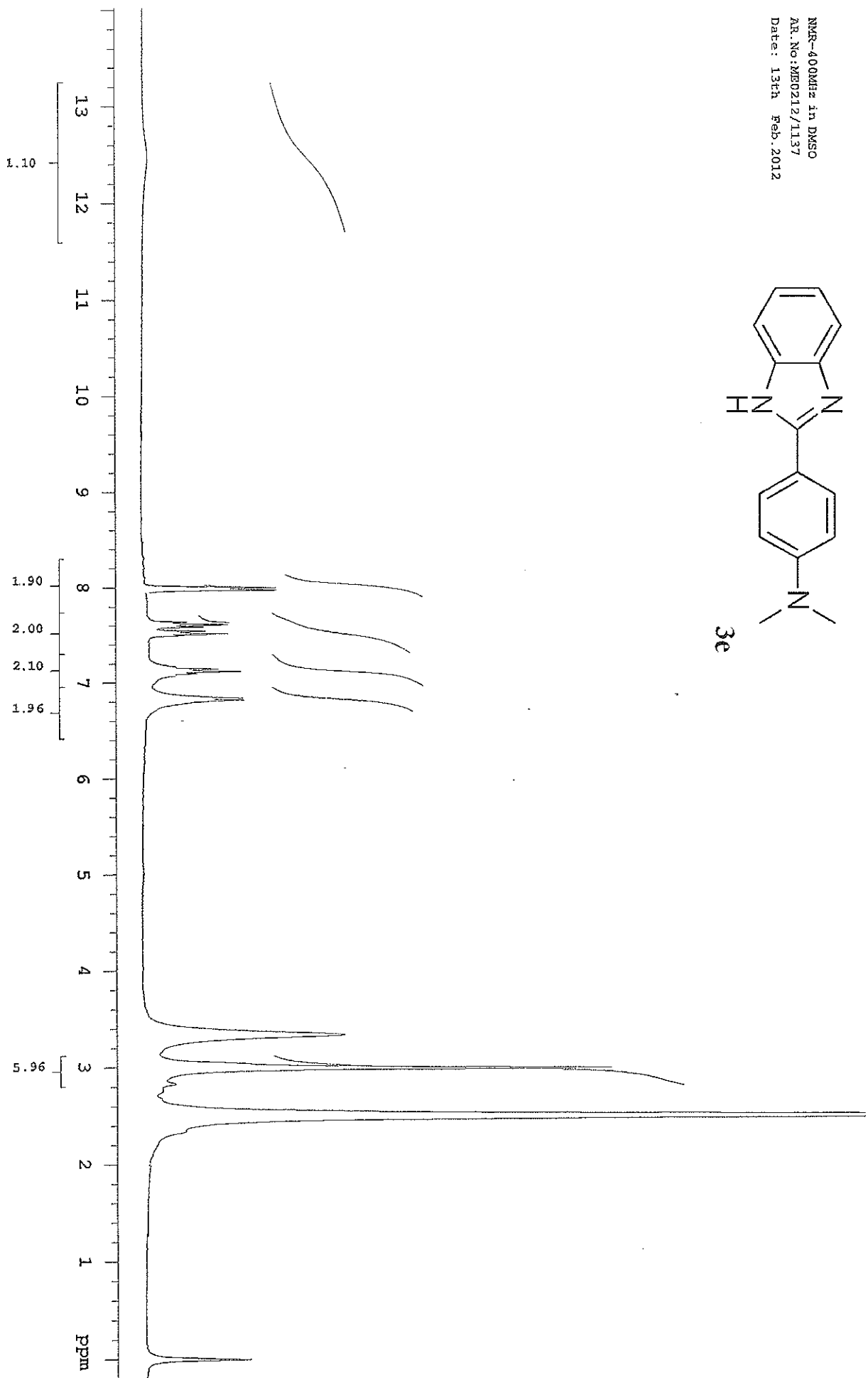
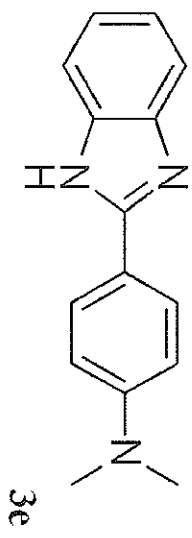
Minimum: 5.0
Maximum: 5.0
-1.0
80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
237.1393	237.1392	0.1	0.4	9.5	3.3	C16 H17 N2

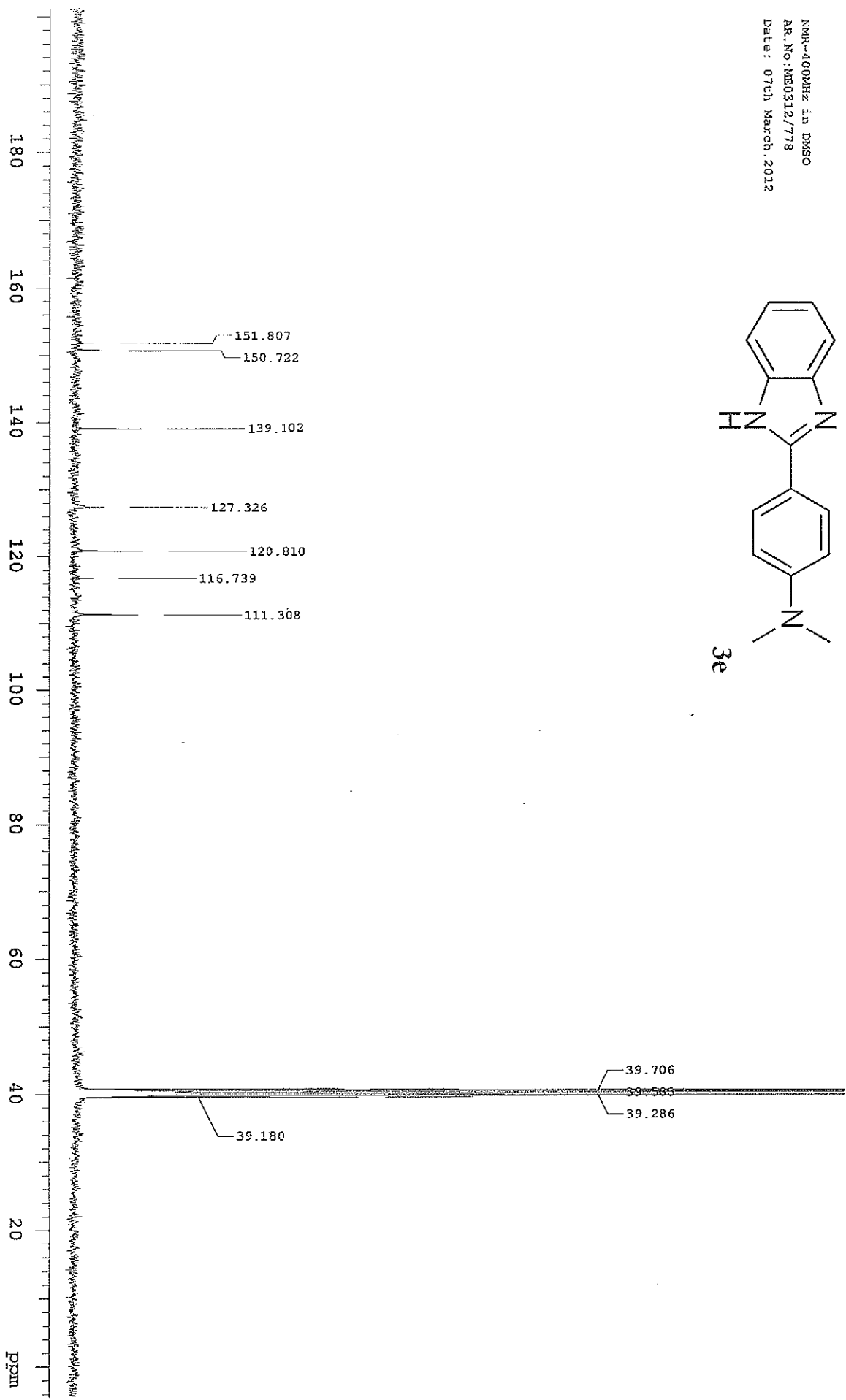
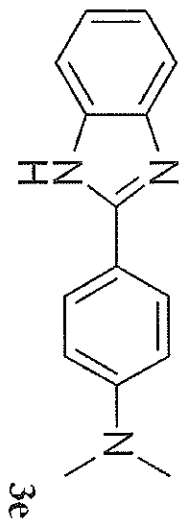


3d

NMR-400MHz in DMSO
AR.No:ME0212/1137
Date: 13th Feb. 2012



NMR-400MHz in DMSO
AR.No: ME0312/778
Date: 07th March, 2012



Elemental Composition Report

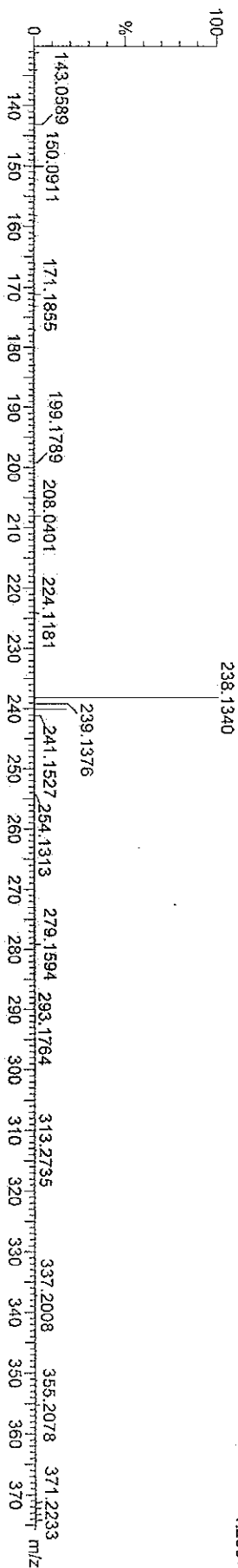
Single Mass Analysis

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
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-20 N: 0-3

Dr.Reddy's Laboratories Ltd, ARD,TDC-1

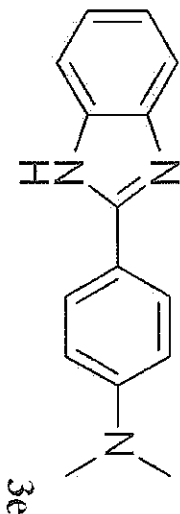
UT0312_07 15 (0.279) Cm (12.20-14x0.010)



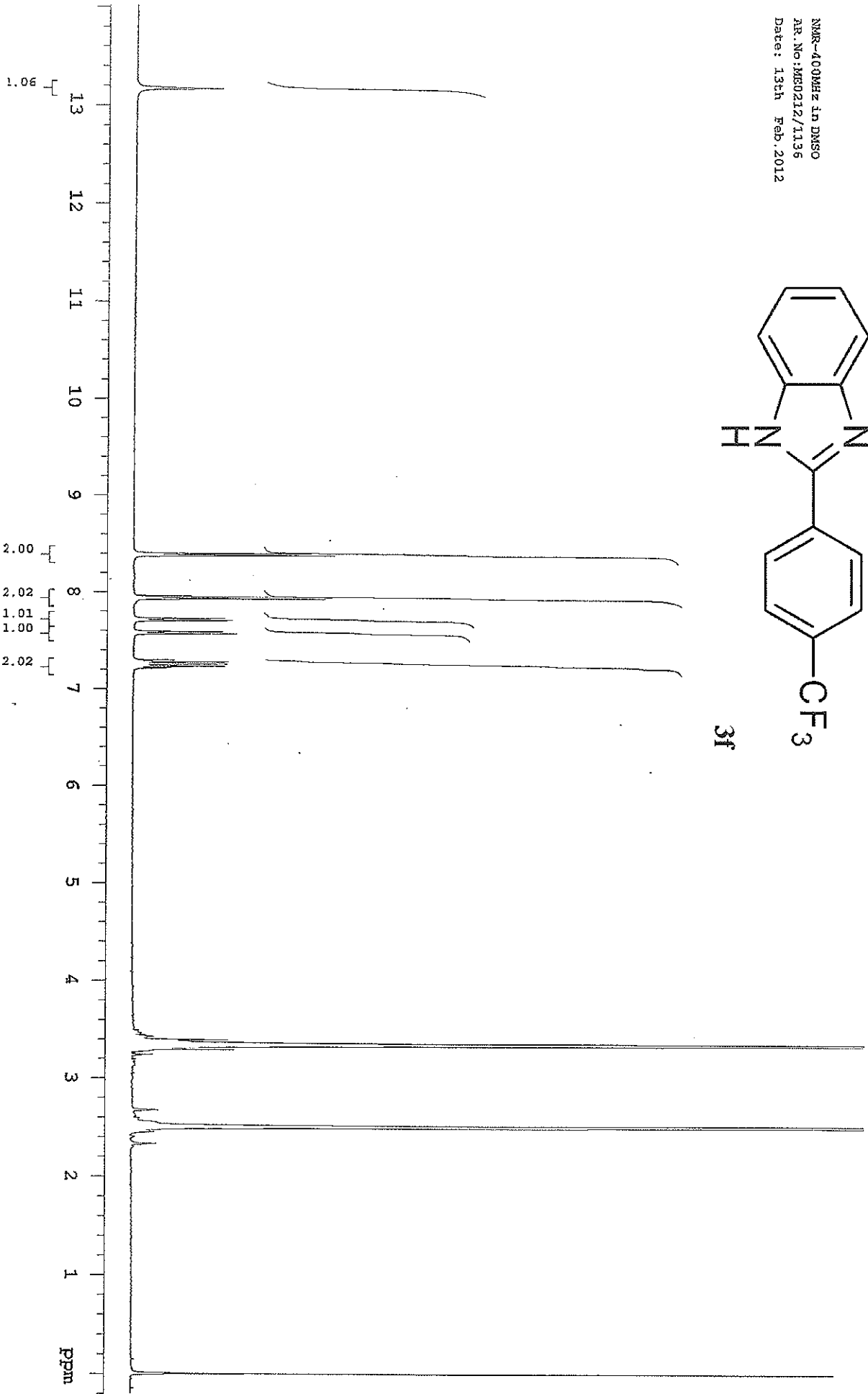
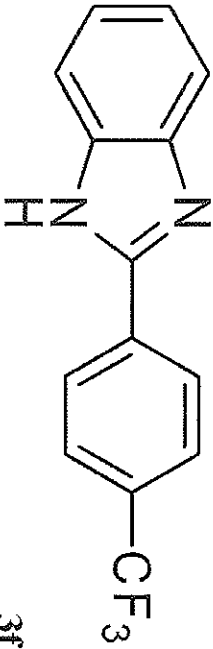
1: TOF MS ES+
1.28e+004

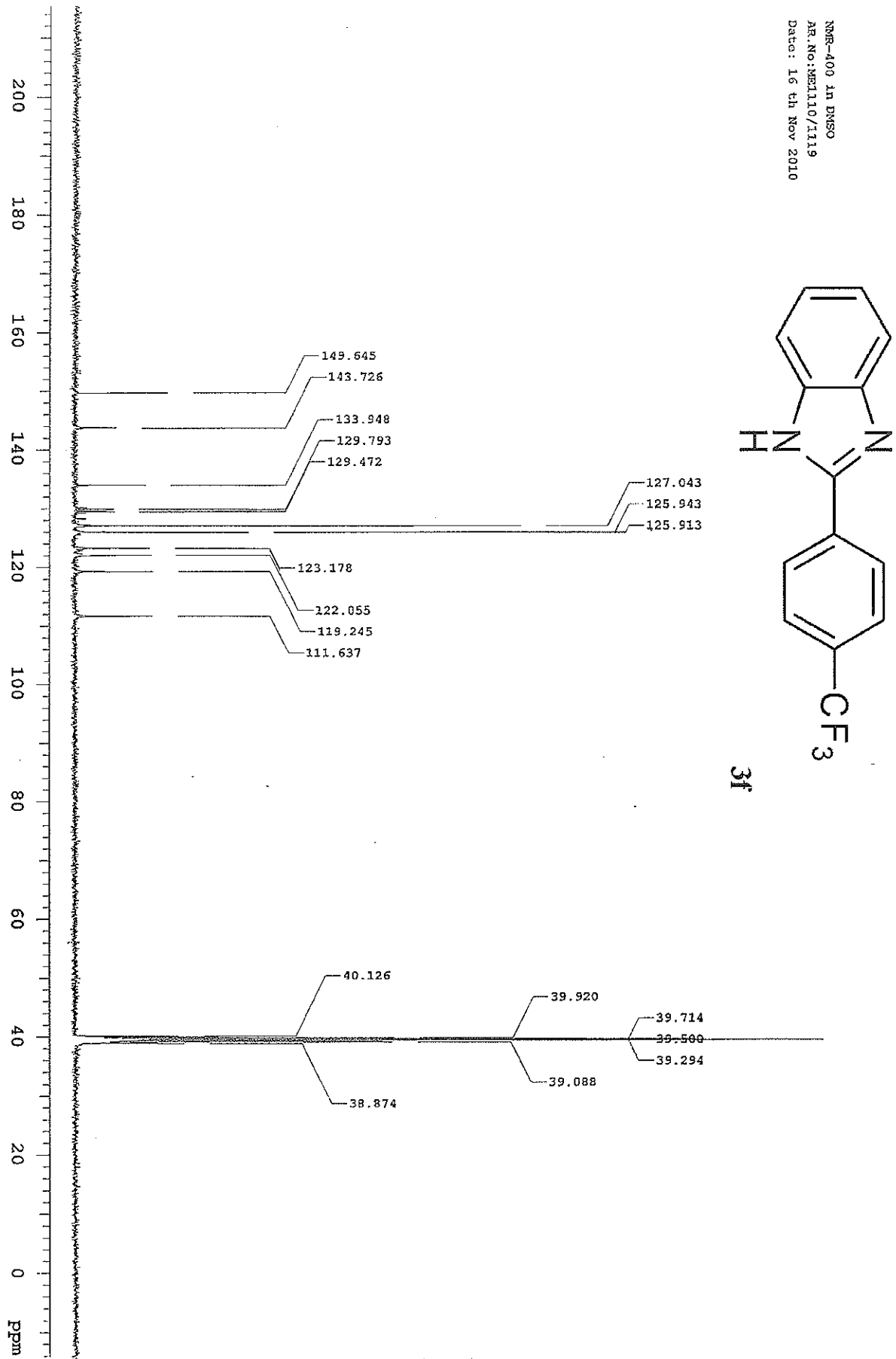
Copies of spectra

Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
238.1340	238.1344	-0.4	-1.7	9.5	935.6	C15 H16 N3



NMR-400MHz in DMSO
Ac.No:ME0212/1136
Date: 13th Feb. 2012





Single Mass Analysis

Element prediction: Off

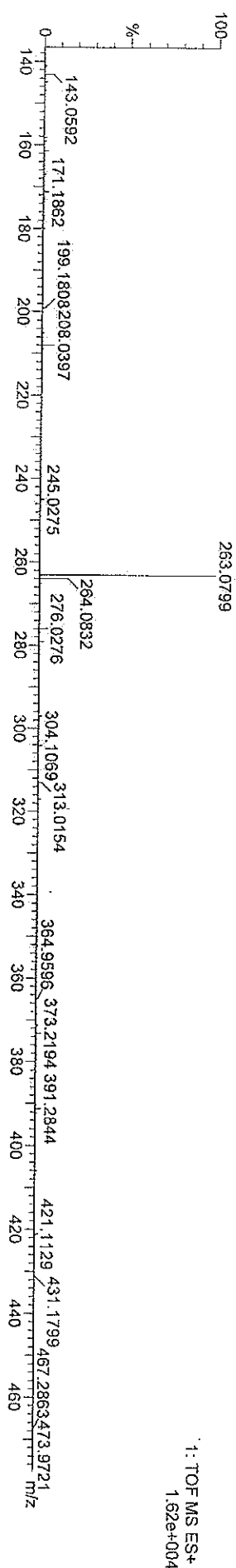
Monoisotopic Mass, Even Electron Ions

19 formula(e) evaluated with 1 result(s) within limits (up to 4 best isotopic matches for each mass)
Elements Used:

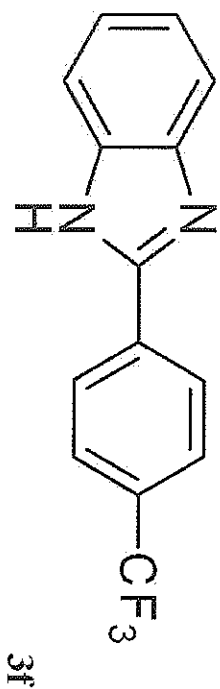
C: 0-20 H: 0-20 N: 0-2 F: 0-3

Dr.Reddy's Laboratories Ltd, ARD,TDC-1

UT0312_17 32 (0.588) Cm (30:34-45:46x0.010)

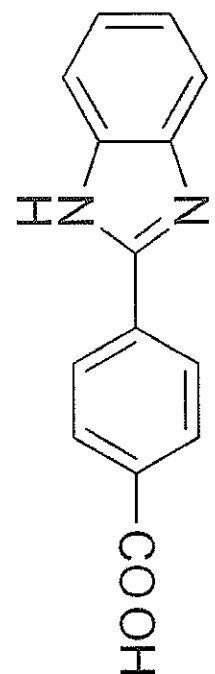


Minimum:									
Maximum:			5.0	5.0	-1.0				
					80.0				
Mass	Calc. Mass	mDa	PPM	DBE	1-Fit	Formula			
263.0799	263.0796	0.3	1.1	9.5	0.5	C14 H10 N2 F3			

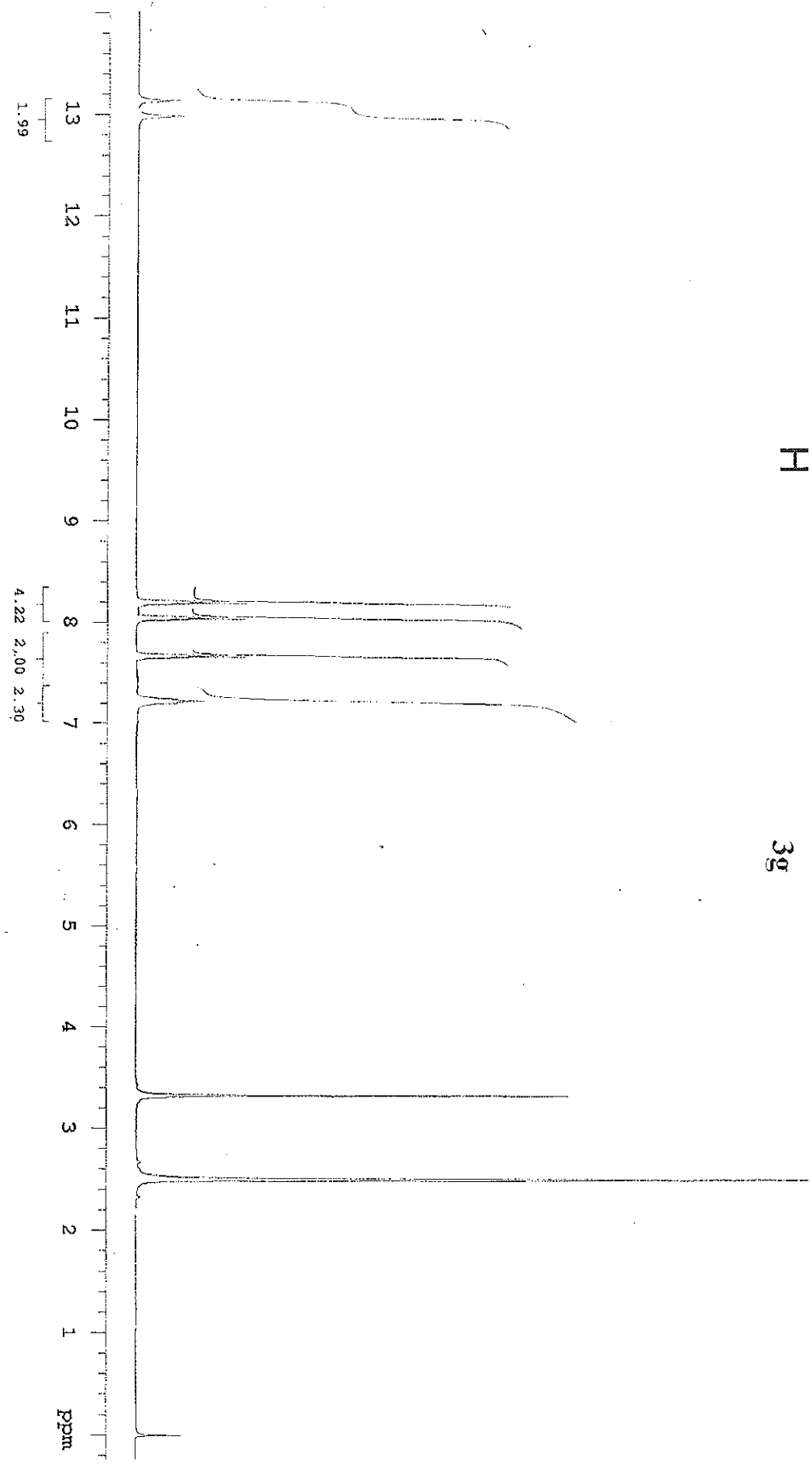


Copies of spectra

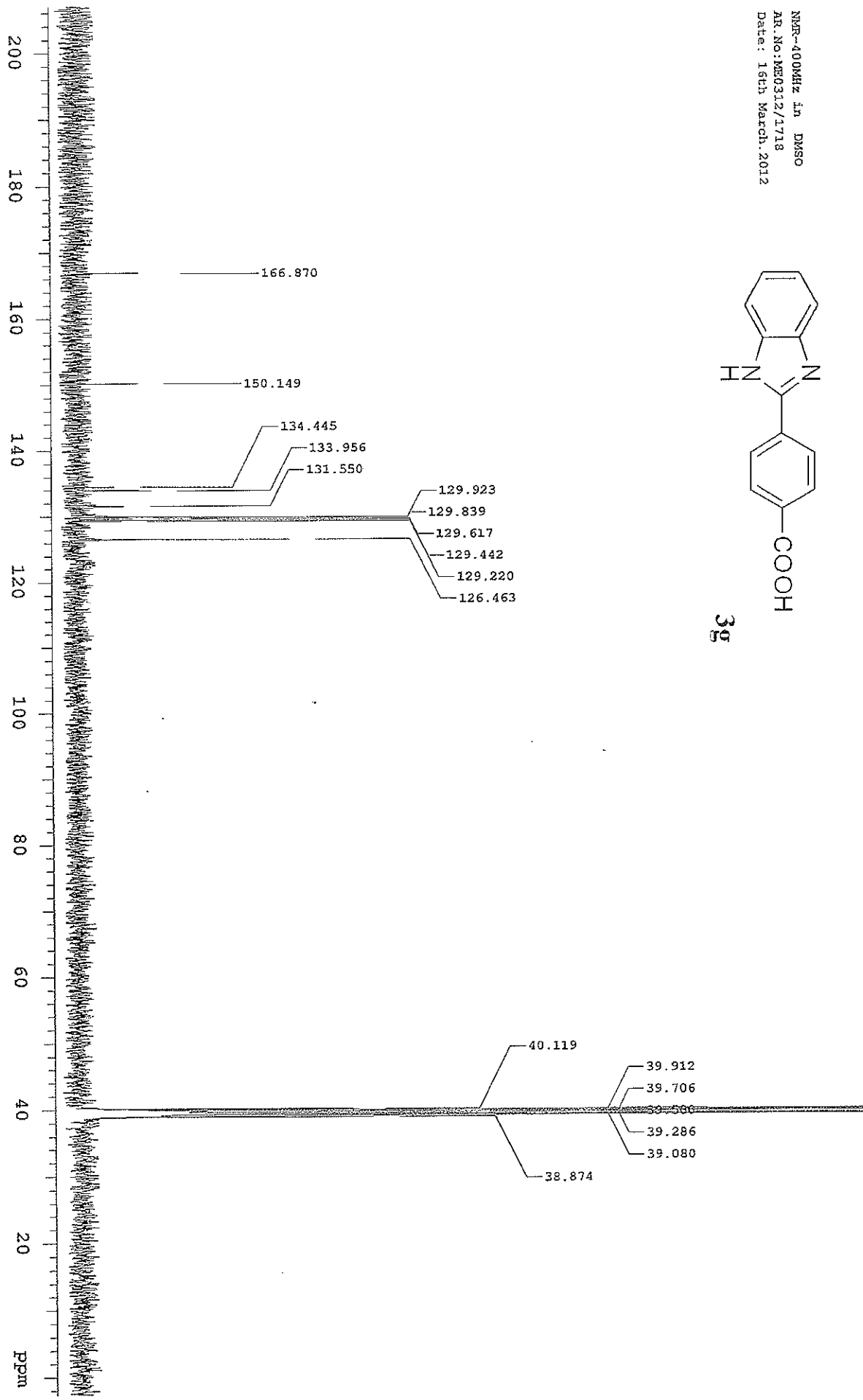
NMR-400MHz 4h DMSO
AR.No:ME0710/933
Date:13th July 2010



3g



Copies of spectra



NMR-400MHz in DMSO
AR.No:ME0312/1718
Date: 16th March, 2012

Copies of spectra

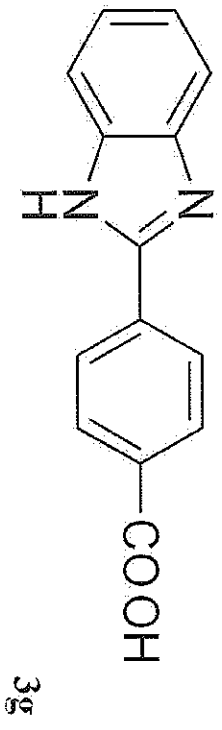
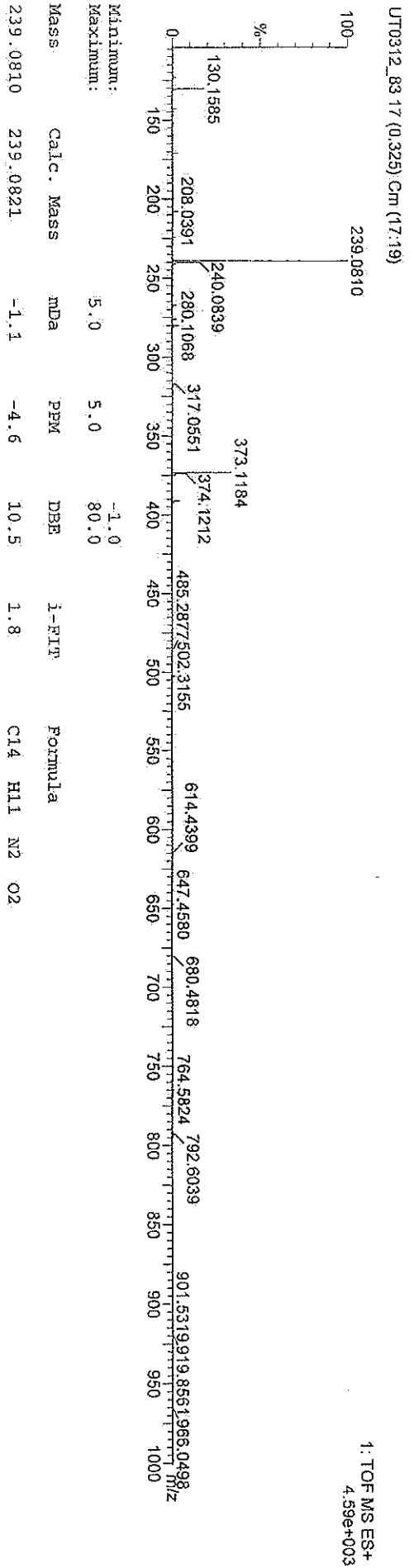
Elemental Composition Report

Single Mass Analysis

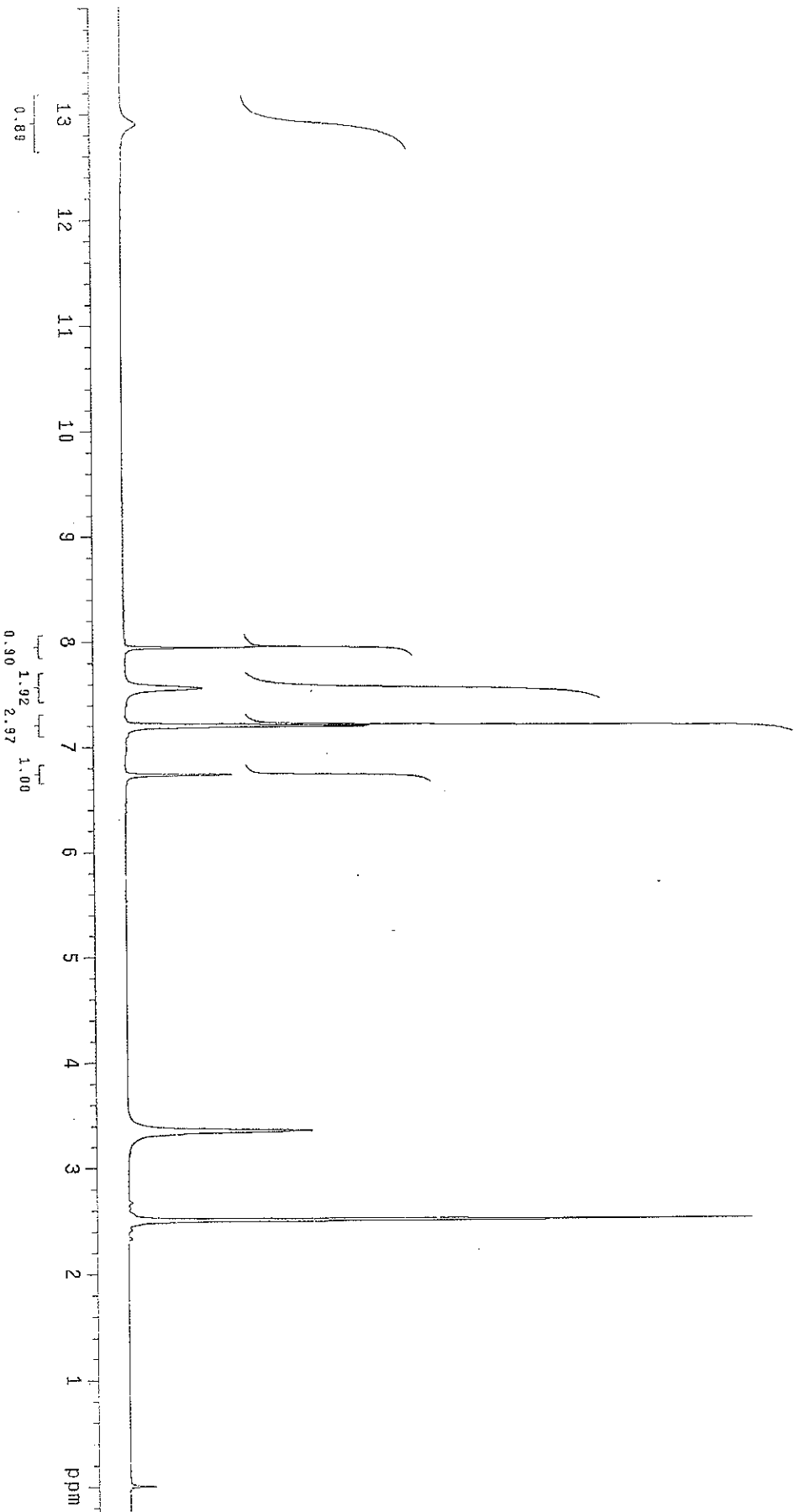
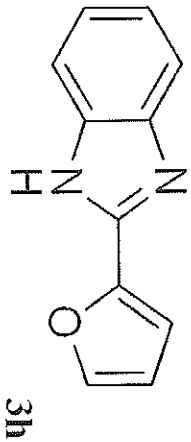
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

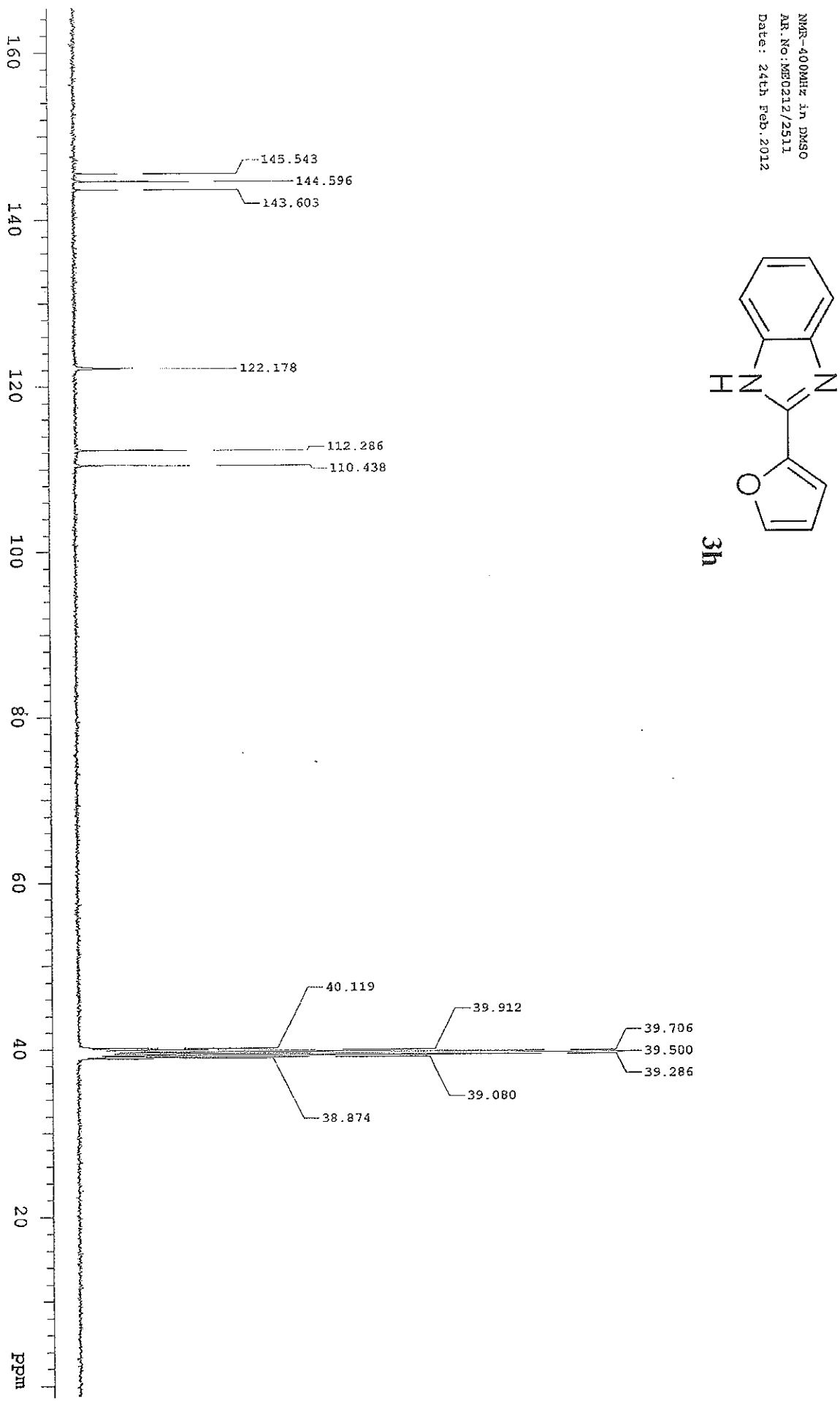
Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-2 O: 0-2

Dr. Reddy's Laboratories Ltd, ARD, TDC-1



1H NMR-400 in DMSO
AR.No:ME0411/2524
Date: 26 th April, 2011





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

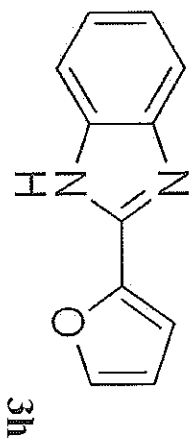
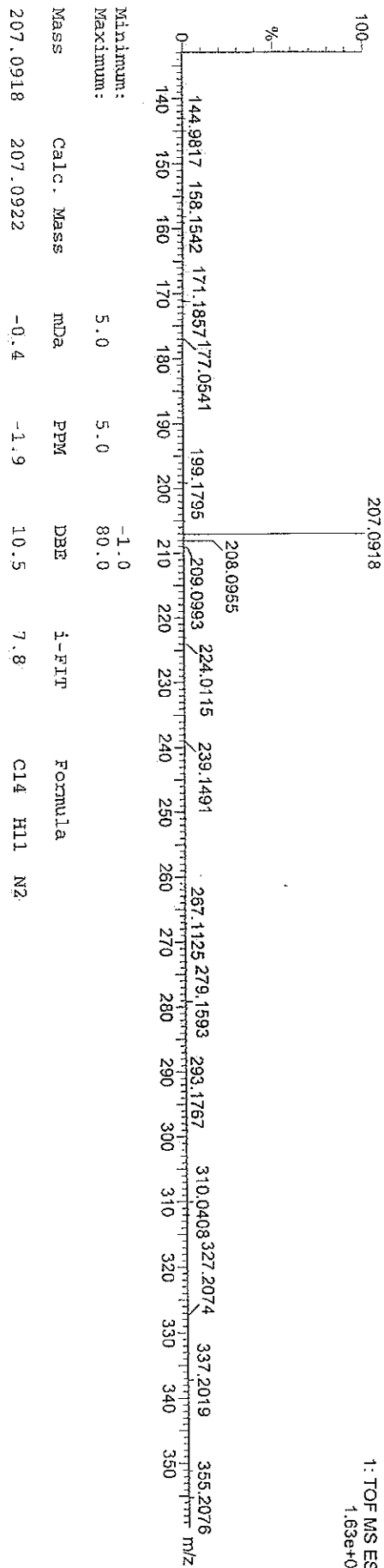
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

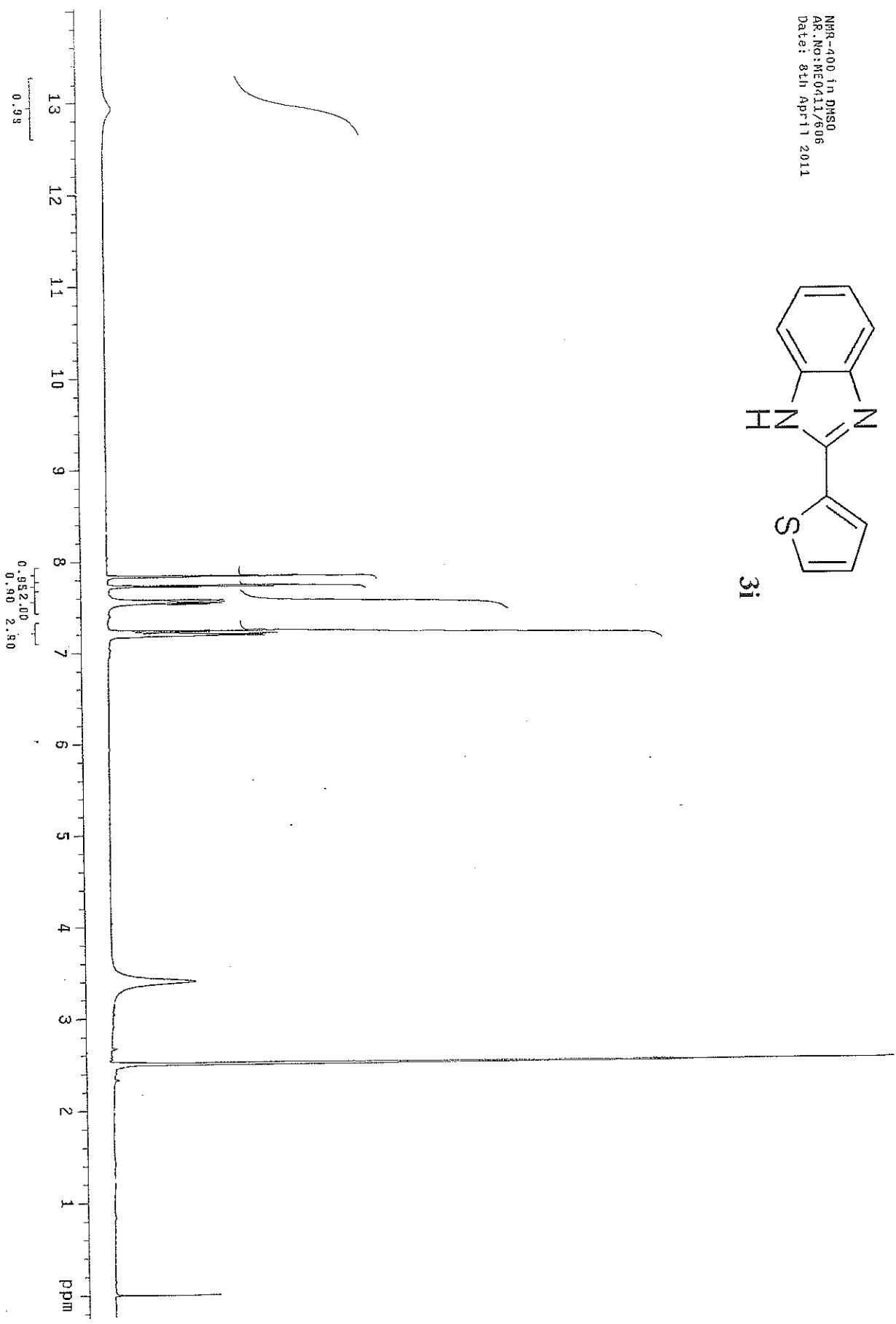
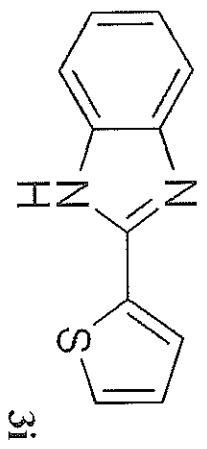
C: 0-15 H: 0-20 N: 0-2

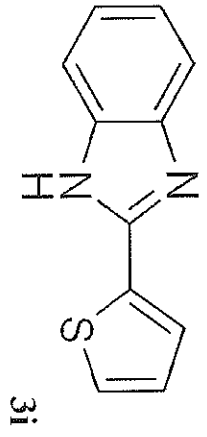
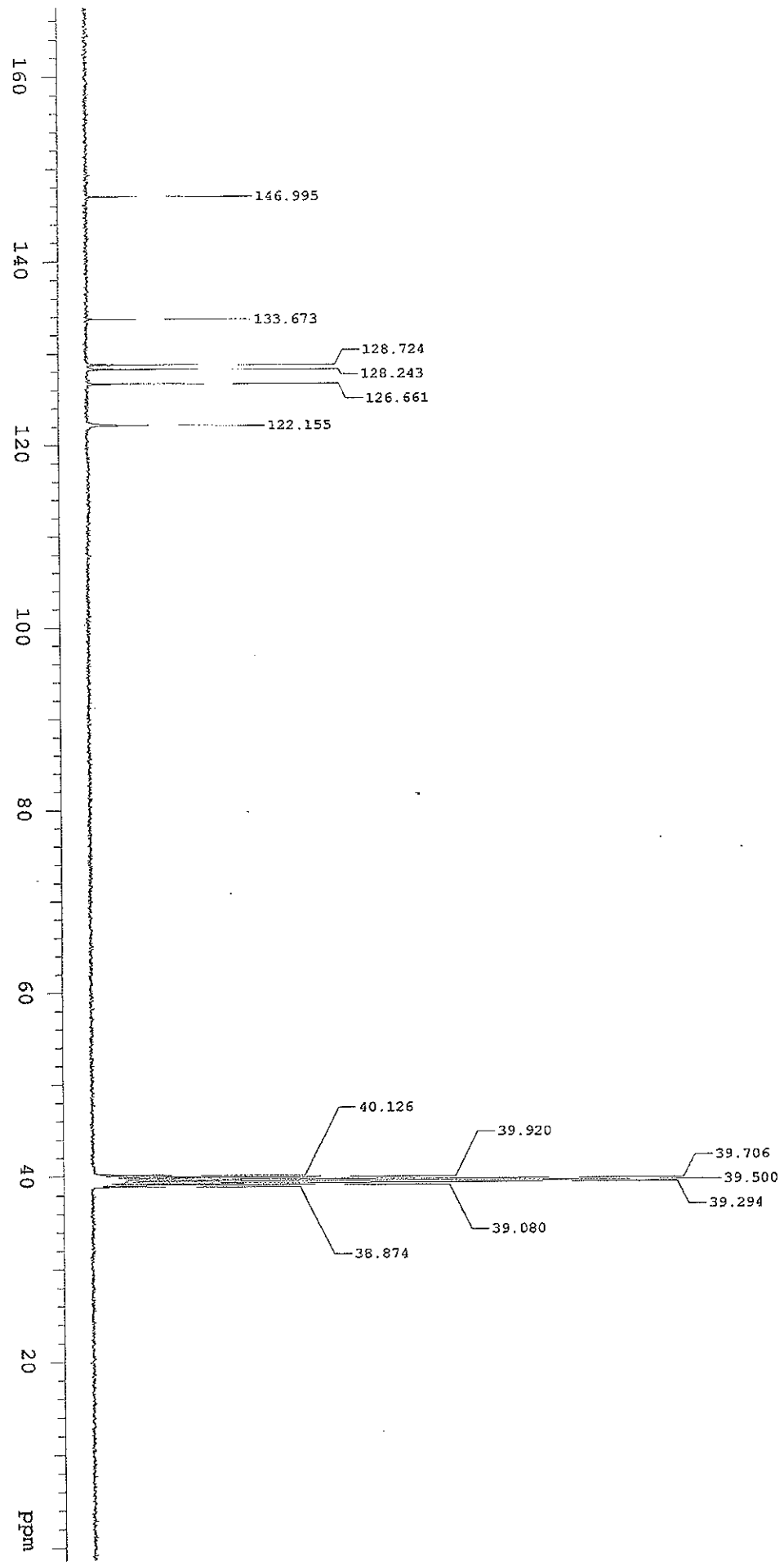
Dr.Reddy's Laboratories Ltd, ARD, TDC-1

UT0312_04 18 (0.339) Cm (18.28)



MR-400 in DMSO
AR No: ME041/606
Date: 8th April 2011



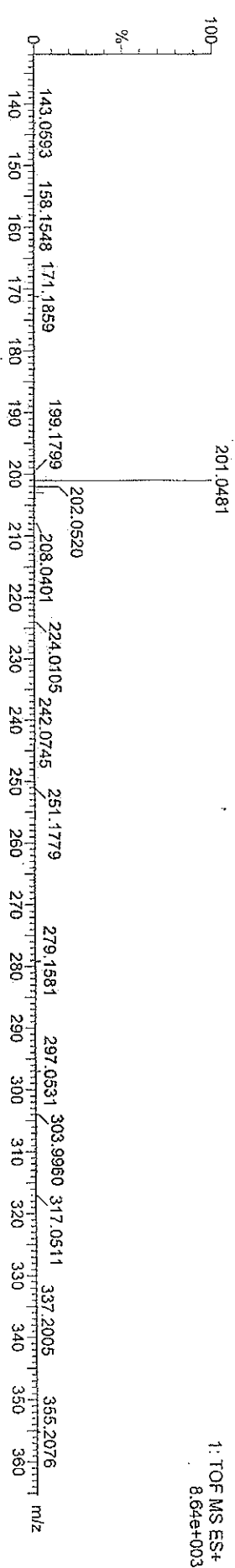


NMR-400MHz in DMSO
Ac.No:ME0212/2513
Date: 24th Feb. 2012

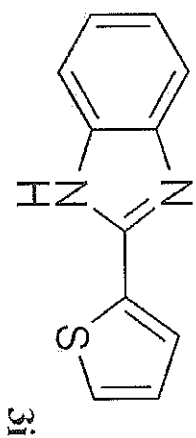
Single Mass Analysis

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-20 N: 0-2 S: 0-1

UT0312_05 18 (0.338) Cm (18:22-1:4x0.010)

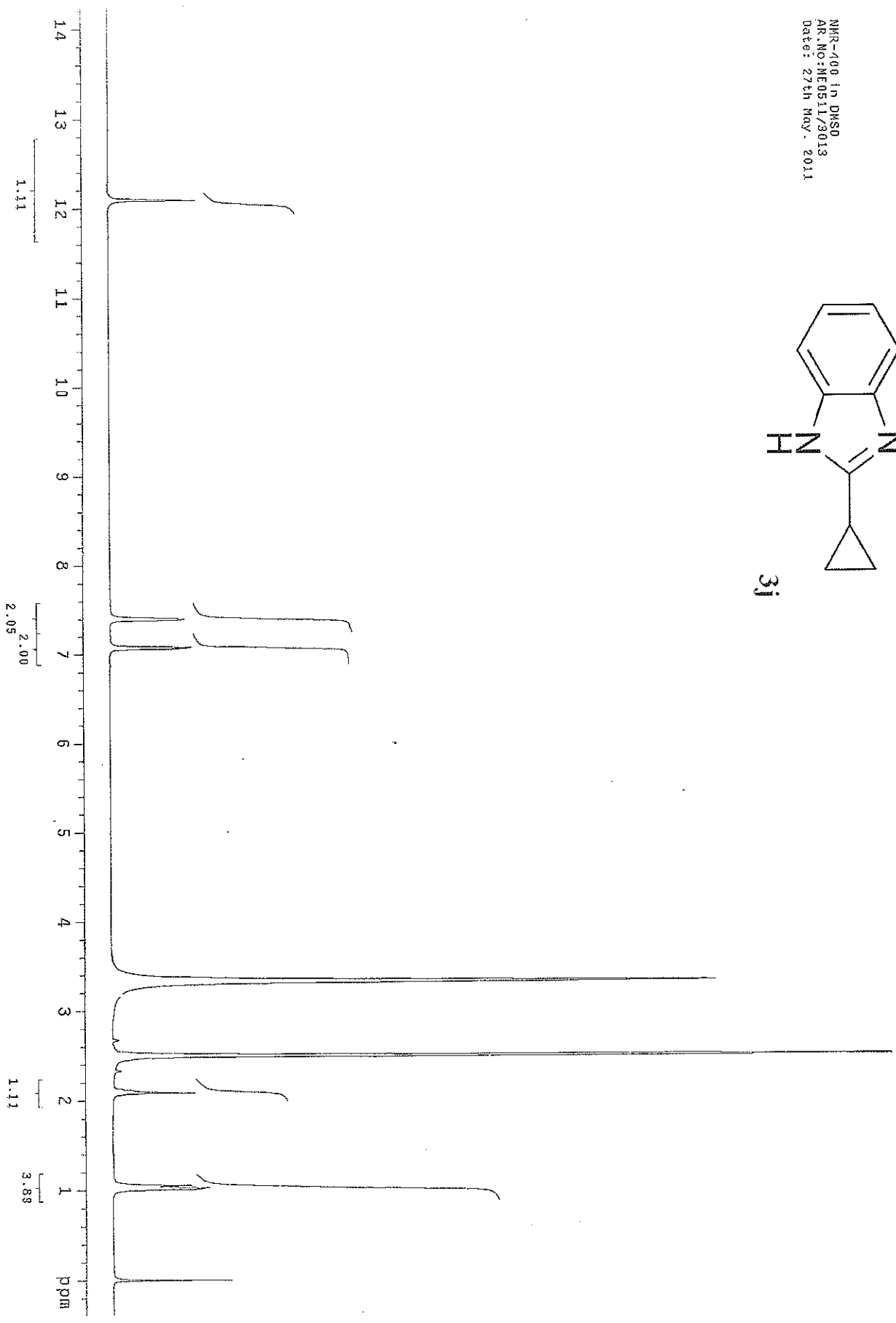
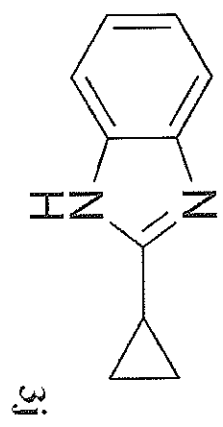


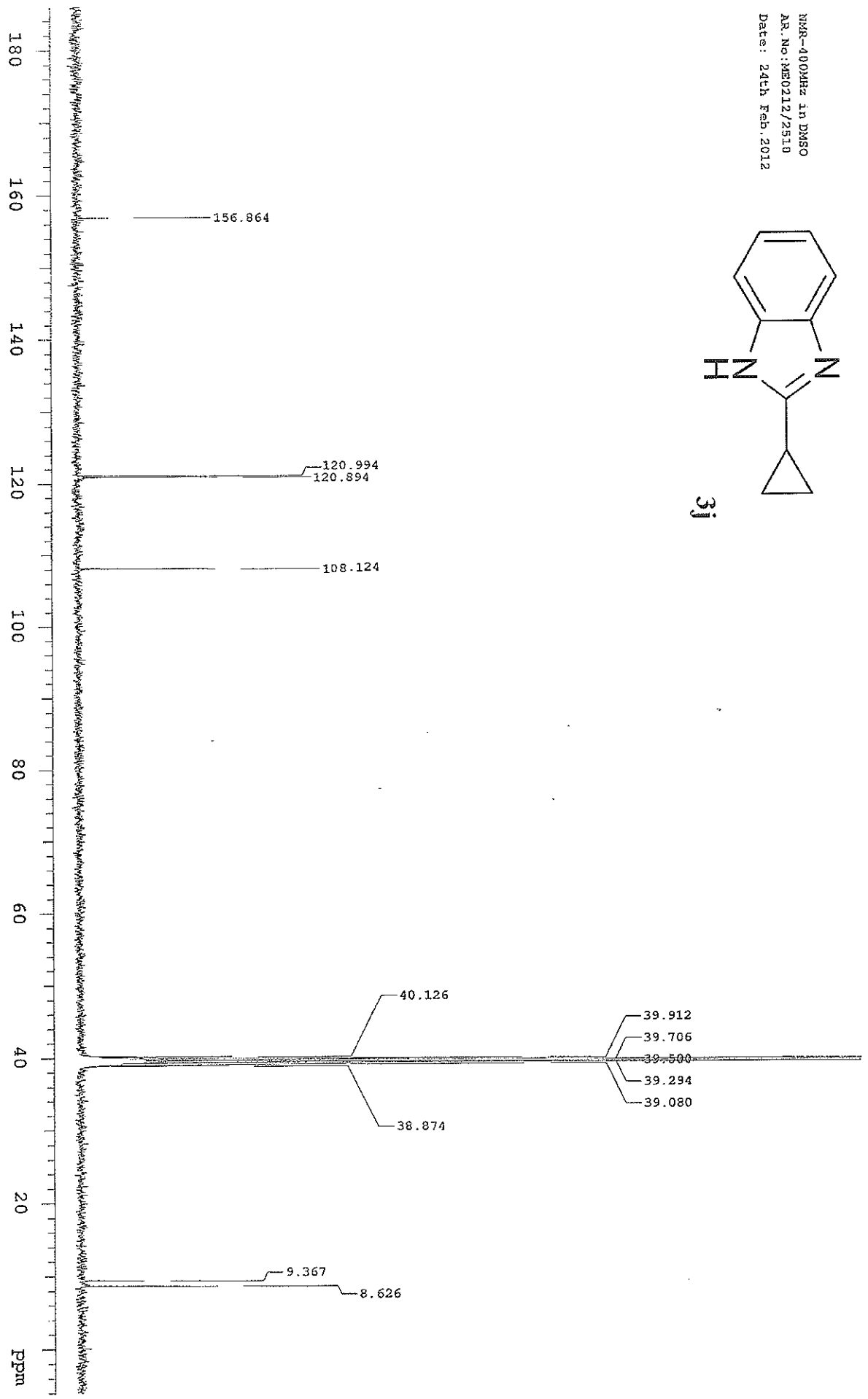
Minimum: Maximum:						
		5.0	5.0	-1.0 80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
201.0481	201.0486	-0.5	-2.5	8.5	0.7	C11 H9 N2 S



Copies of spectra

NMR-100 in DMSO
AR.No:ME0511/3013
Date: 27th May. 2011





NMR-400MHz in DMSO
AR.No:ME0212/2510
Date: 24th Feb.2012

Copies of spectra

Elemental Composition Report

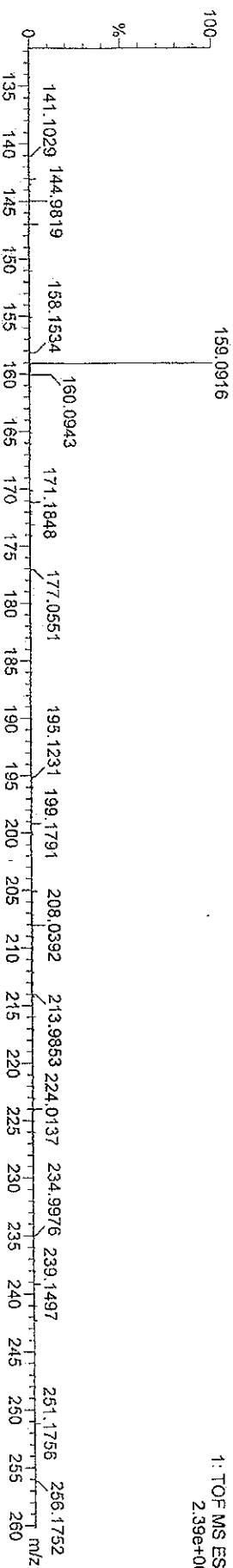
Single Mass Analysis

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

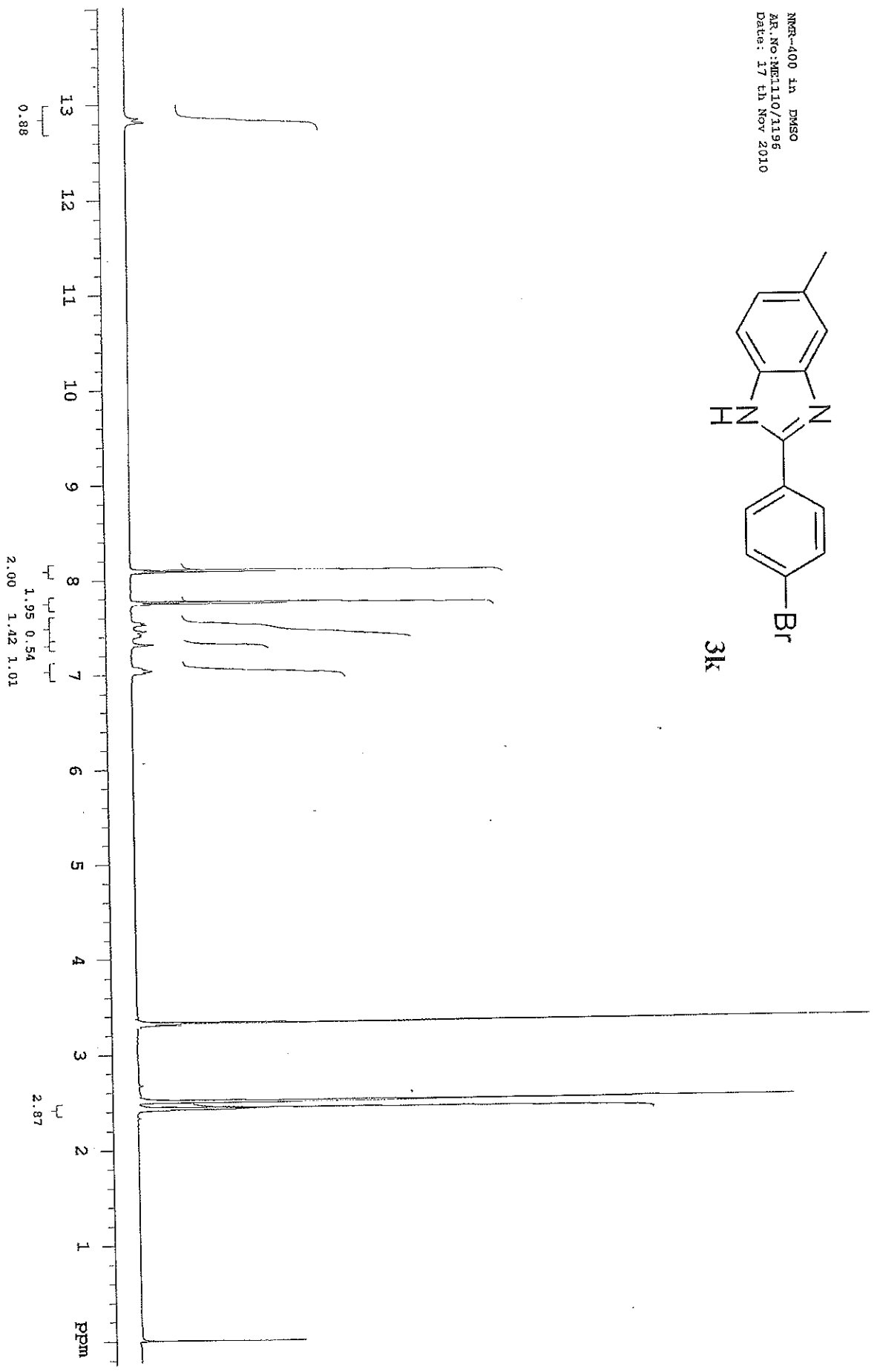
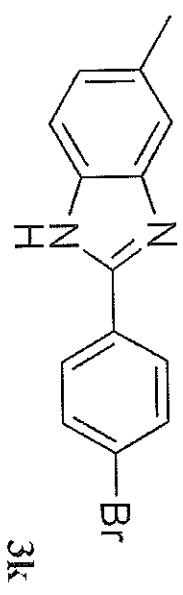
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-20 N: 0-2

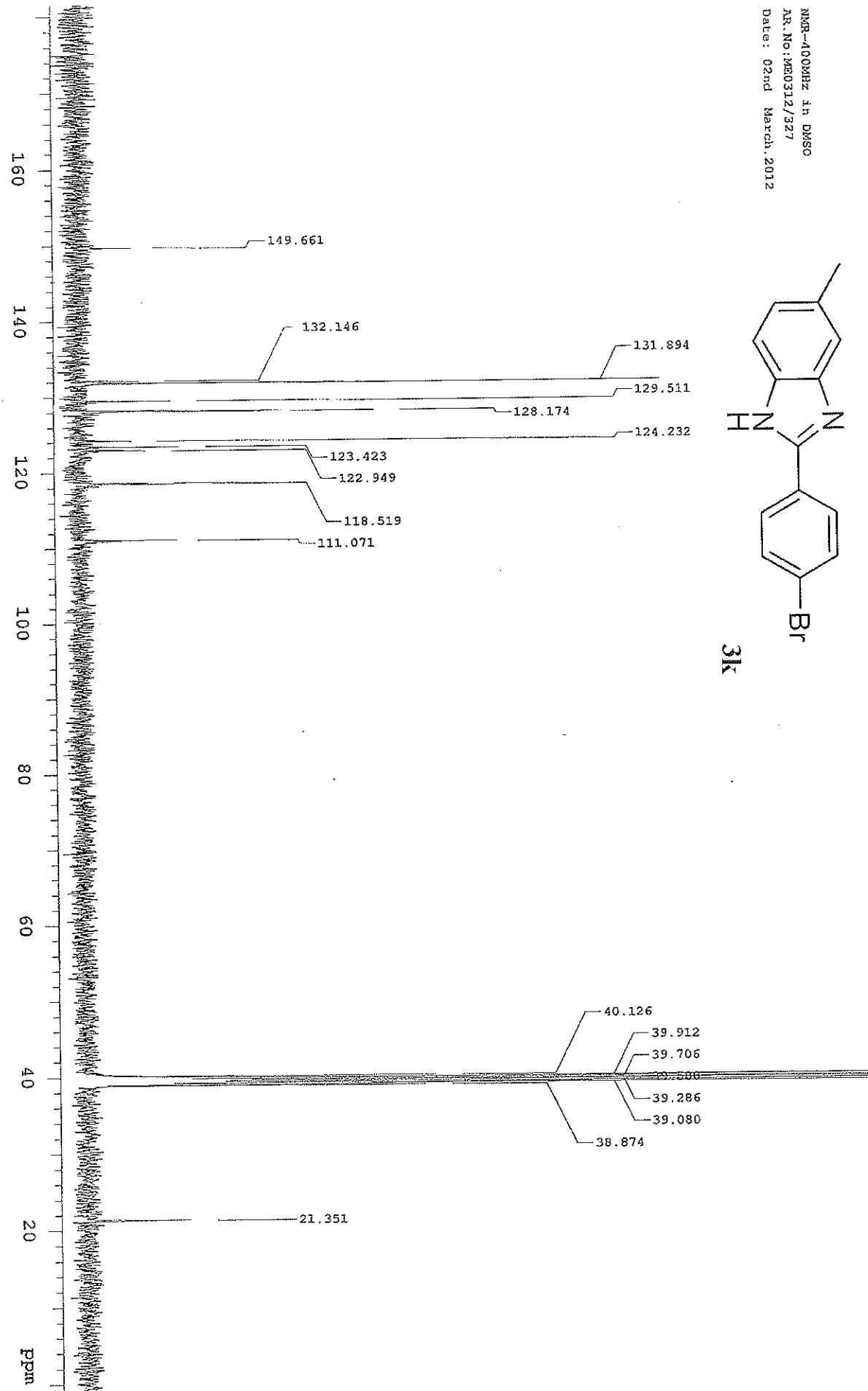
Dr.Reddy's Laboratories Ltd, ARD, TDC-1

UT0312_03 26 (0.486) Cm (25:31)



NMR-400 in DMSO
AR No: ME1110/1196
Date: 17 th Nov 2010





NMR-400MHz in DMSO
AR.No:ME0312/327
Date: 02nd March, 2012

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

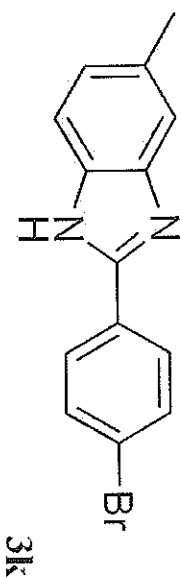
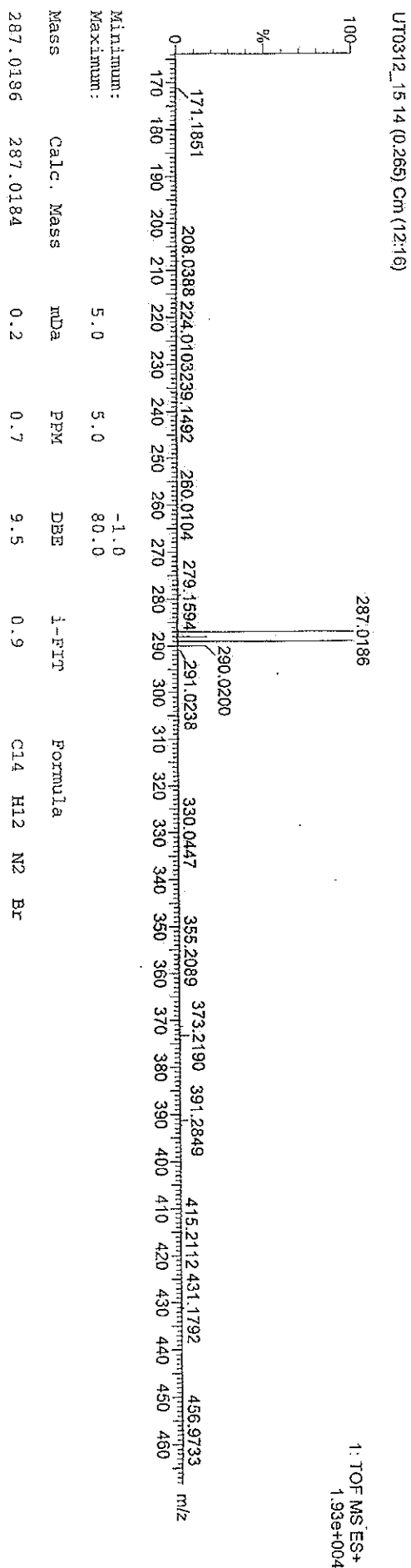
Monoisotopic Mass, Even Electron Ions

19 formula(e), evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

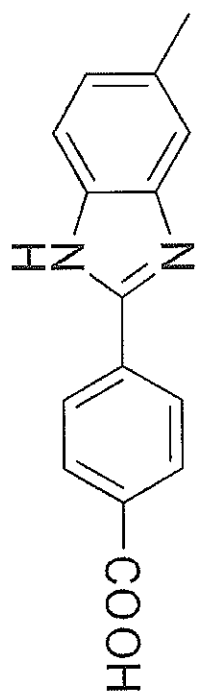
C: 0-30 H: 0-35 N: 0-2 Br: 0-1

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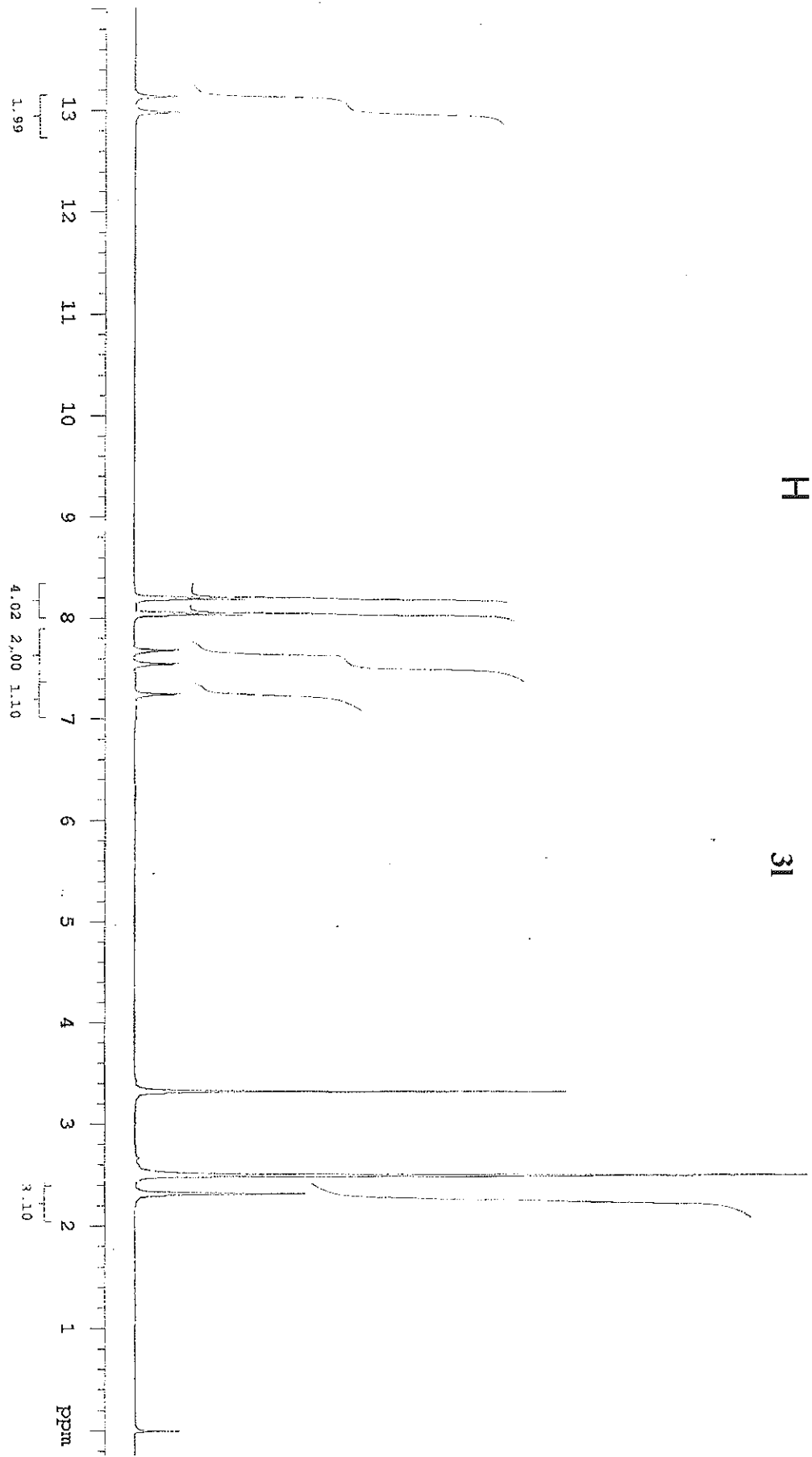


Copies of spectra

NMR-400MHz 1h DMSO
AR.No:ME0212/1374
Date: 14th Feb. 2012



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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-FT = 3

Monoisotopic Mass, Even Electron Ions

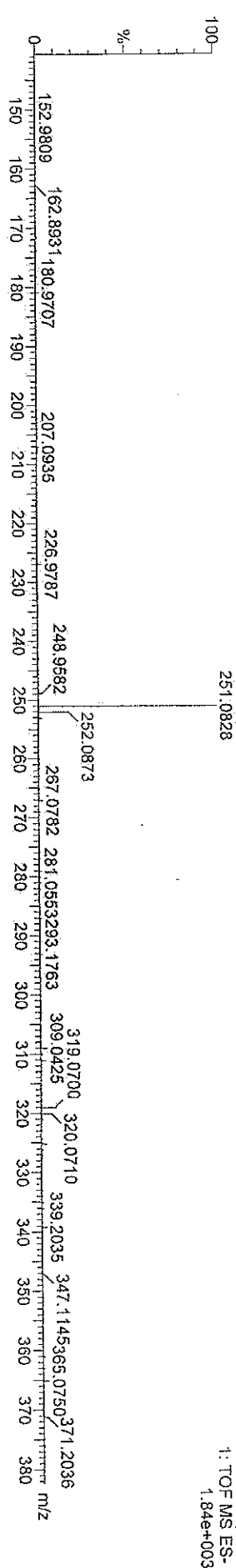
16 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

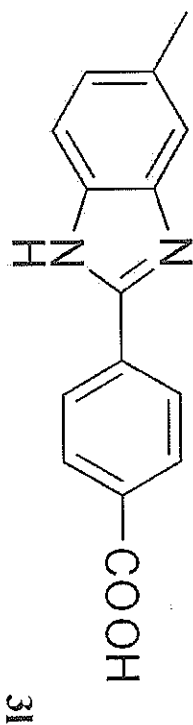
C: 0-20 H: 0-20 N: 0-2 O: 0-2

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

UT0312_87_11 (0.210) Cm (11:16)

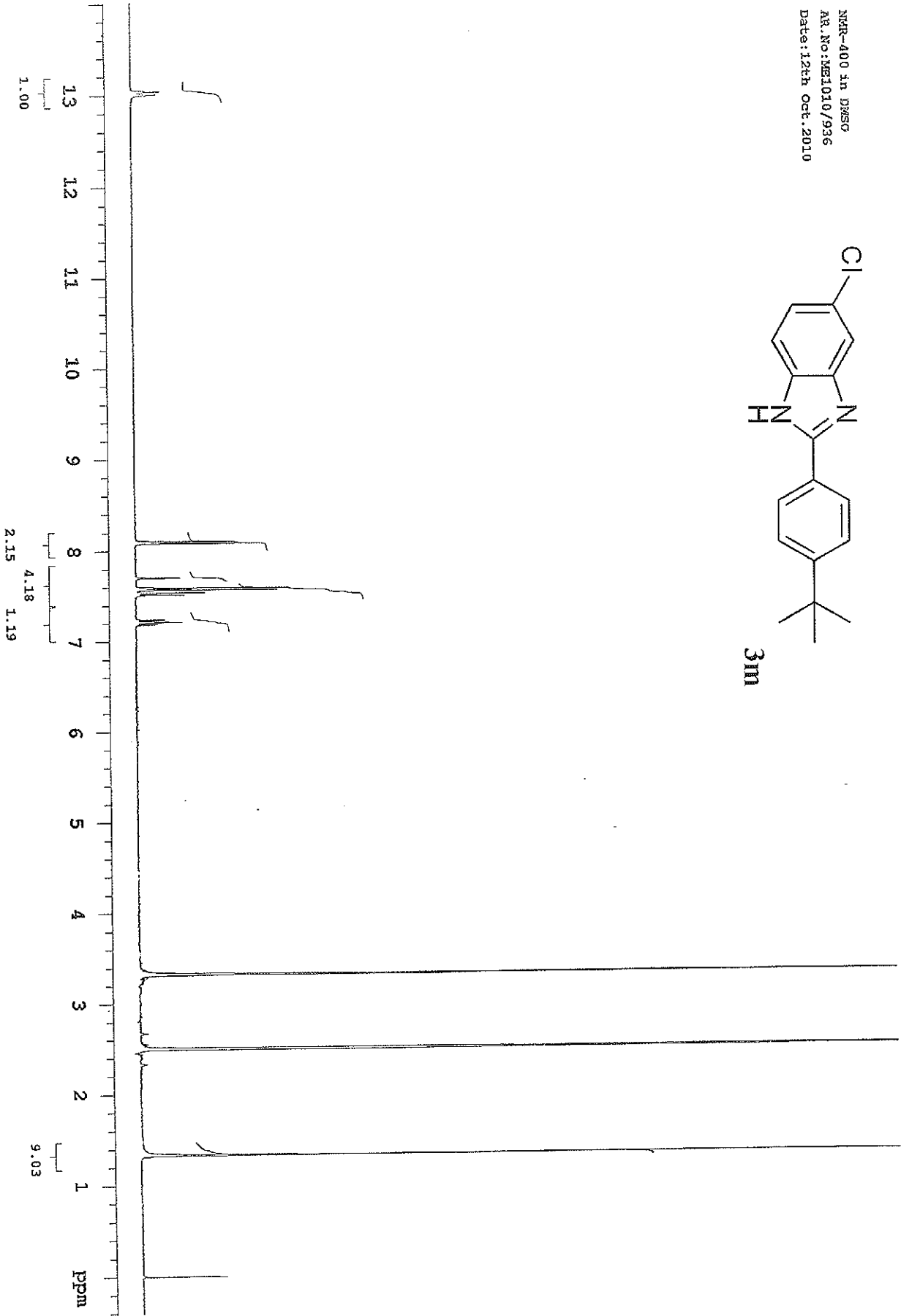
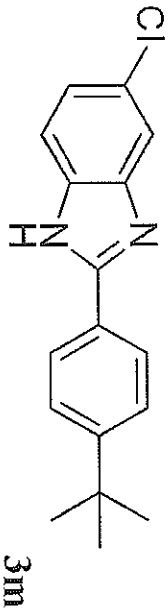


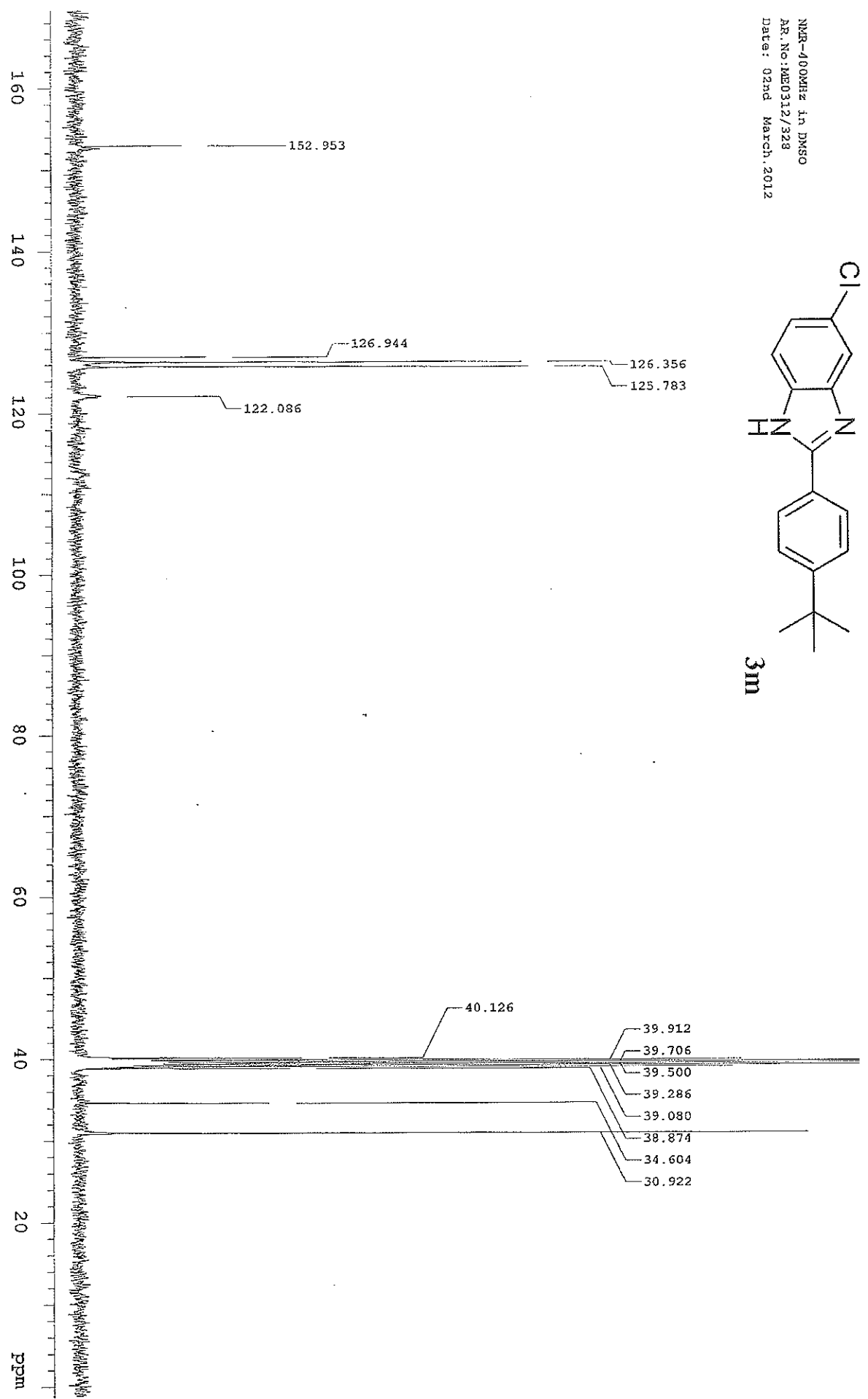
	Minimum:	Maximum:							
Mass	Calc.	Mass	mDa	PPM	DBE	i-FIT	Formula		
251.0828	251.0821	0.7	2.8	11.5	0.8	C15 H11 N2 O2			



Copies of spectra

NMR-400 in DMSO
AK.No:ME1010/936
Date:12th Oct.2010





NMR-400MHz in DMSO
AR.No:ME0312/328
Date: 02nd March, 2012

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

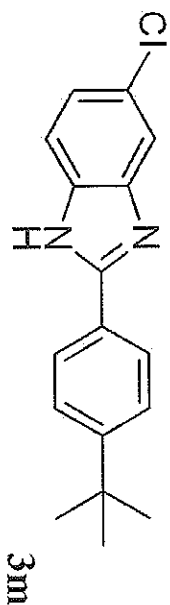
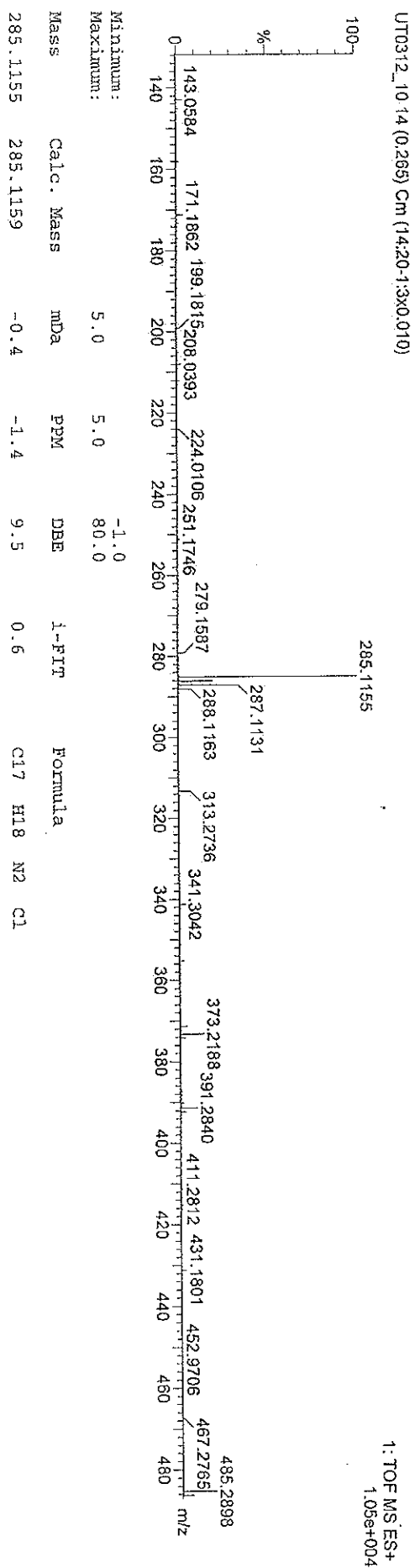
Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

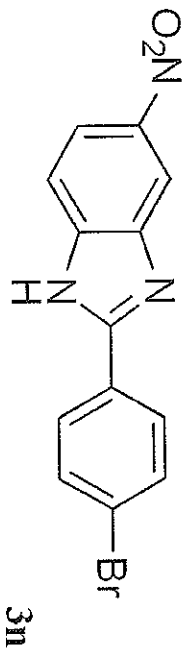
Elements Used:

C: 0-20 H: 0-20 N: 0-2 Cl: 0-1

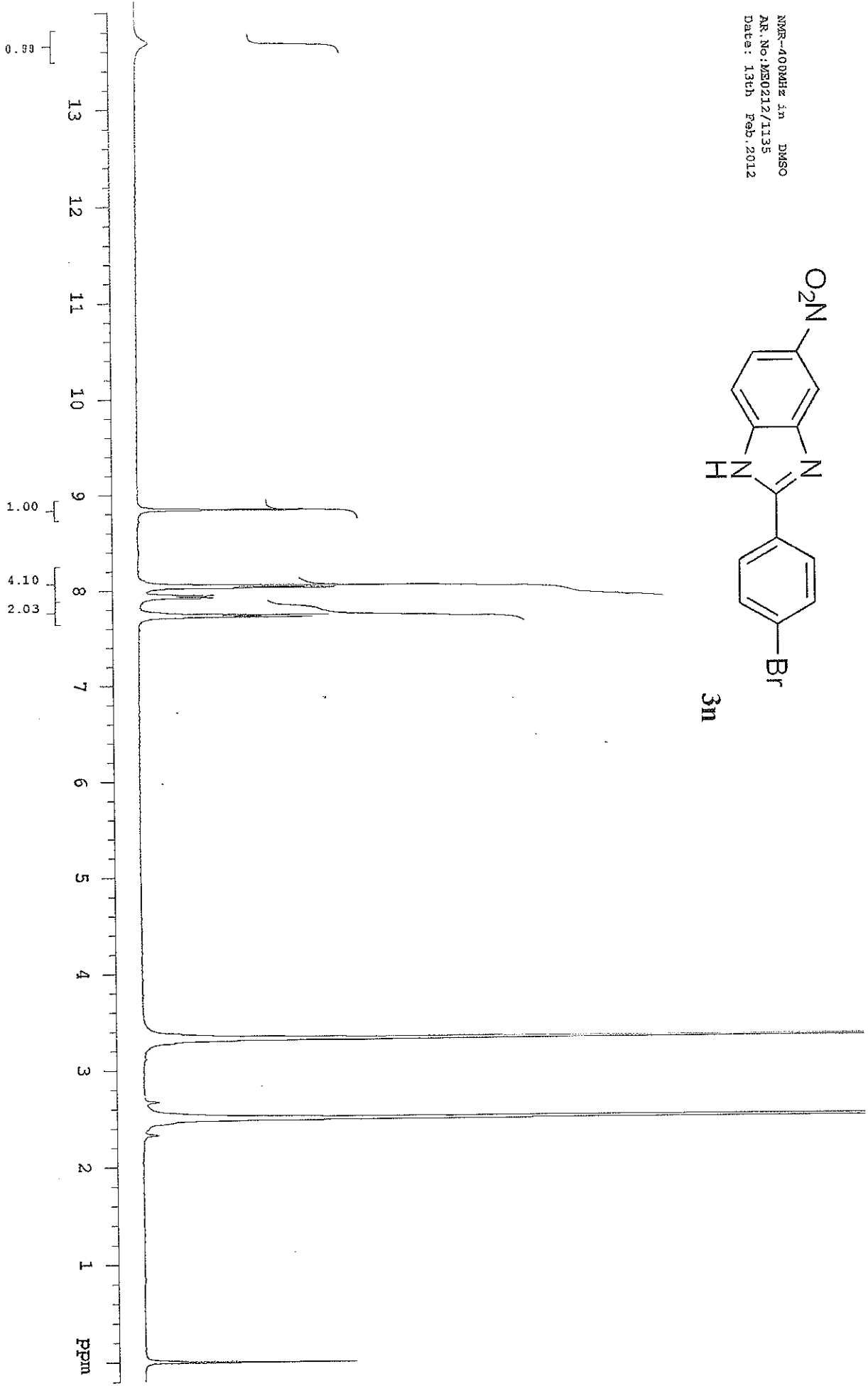
Dr. Reddy's Laboratories Ltd, ARD, TDC-1



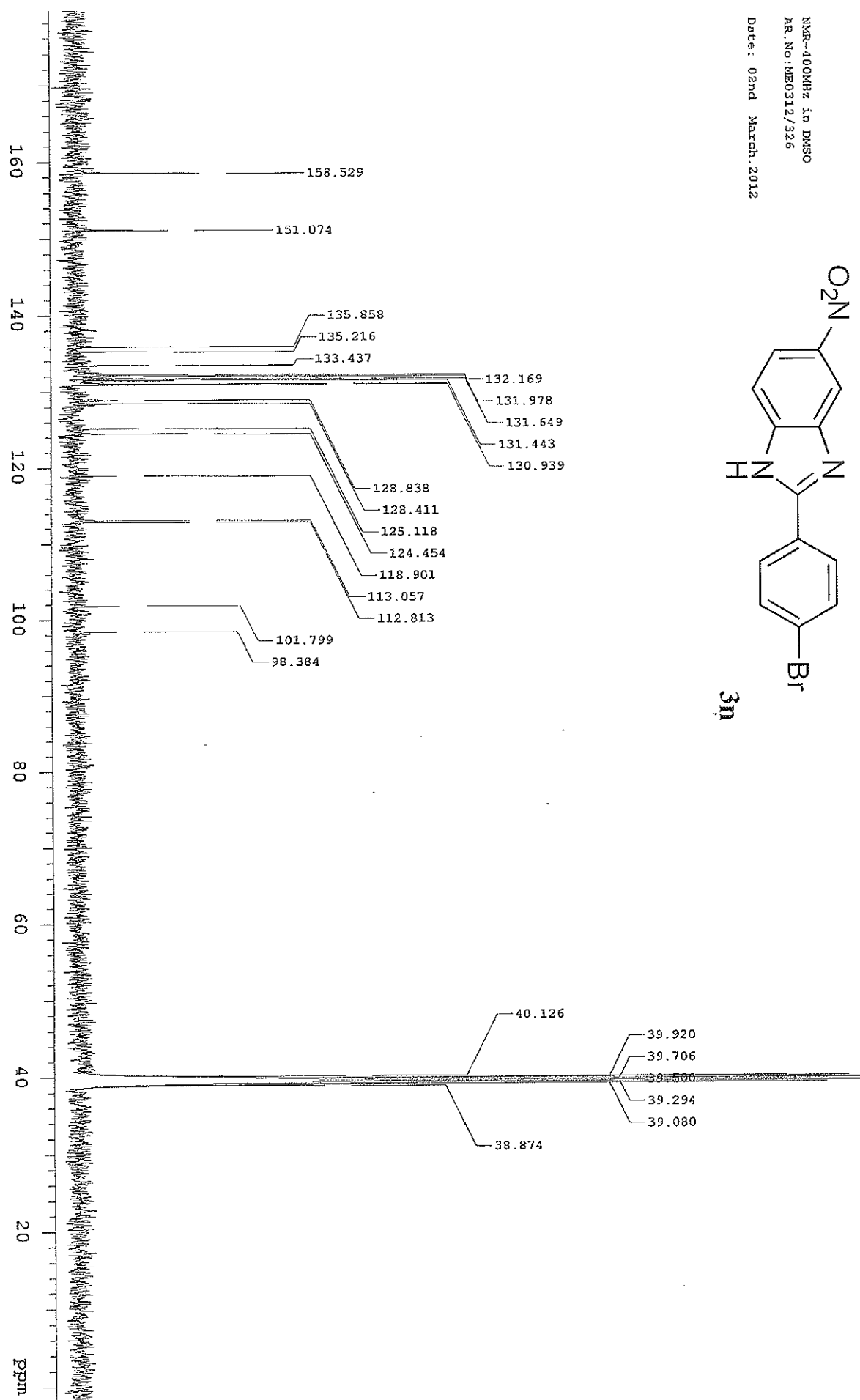
Copies of spectra



NMR-400MHz in DMSO
AR.No:ME0212/1135
Date: 13th Feb. 2012



Copies of spectra



NMR-400MHz in DMSO
AR. No: ME0312/326
Date: 02nd March. 2012

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

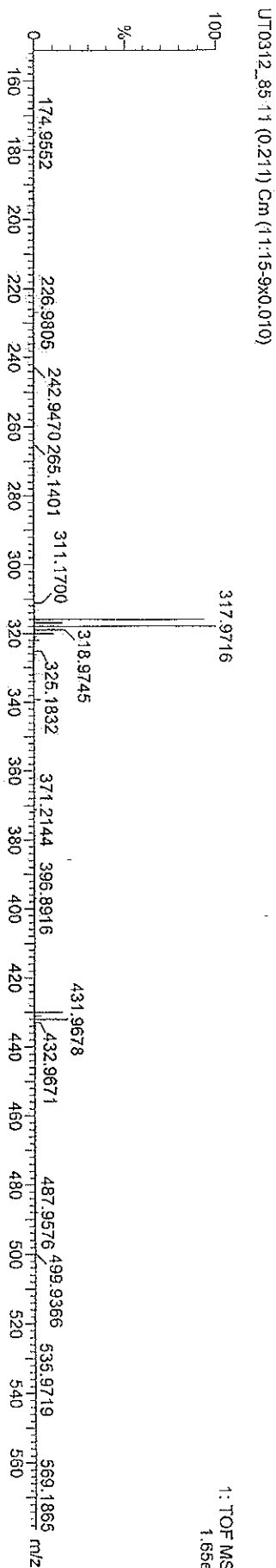
Monoisotopic Mass, Even Electron Ions

18 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

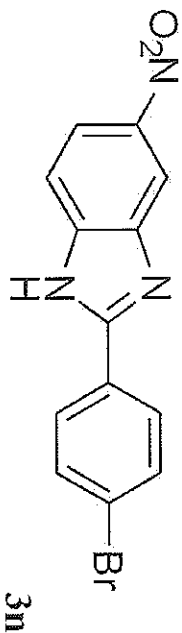
C: 0-15 H: 0-10 N: 0-3 O: 0-2 Br: 0-1

Dr. Reddy's Laboratories Ltd, ARD, TDC-1



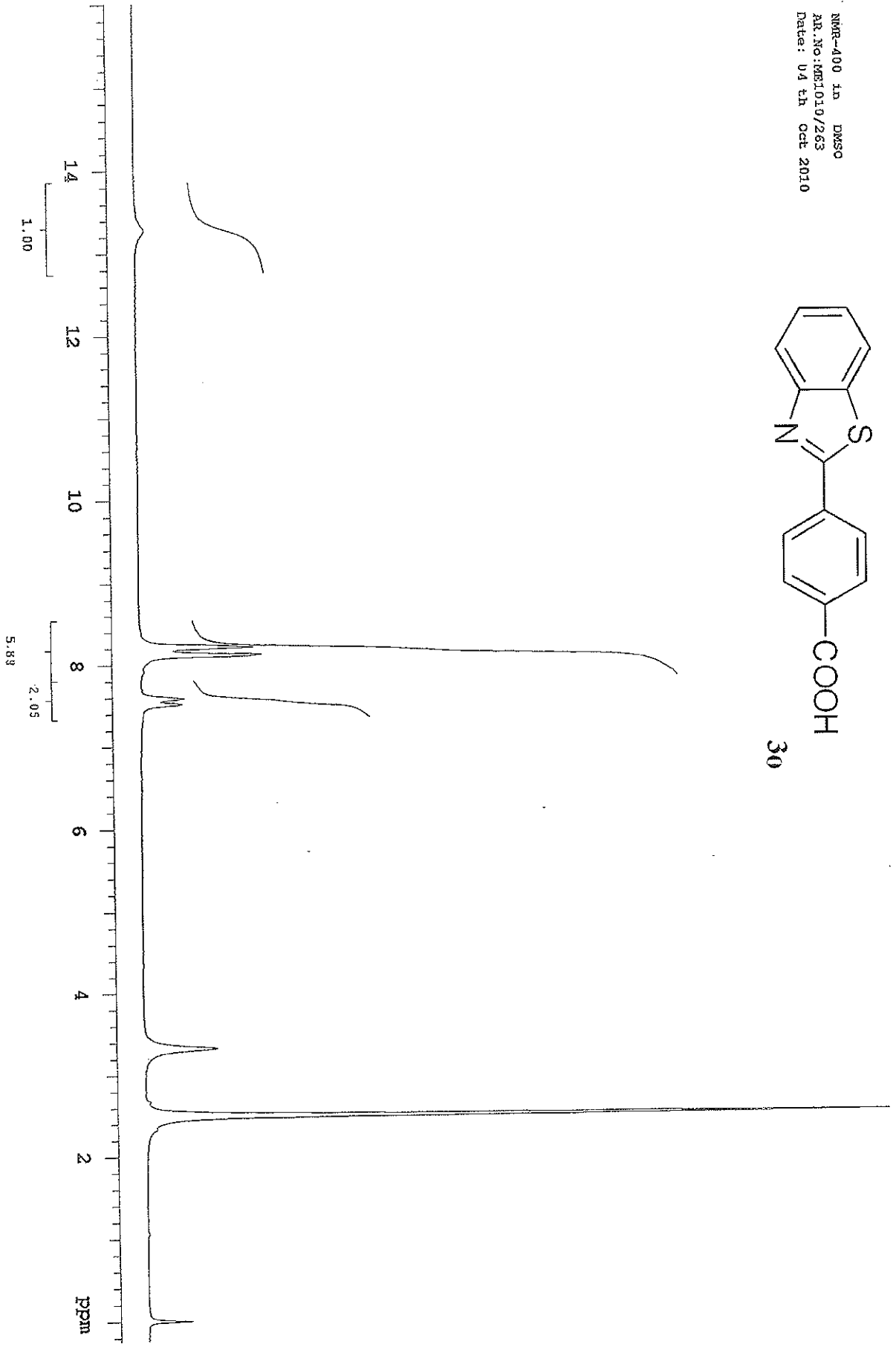
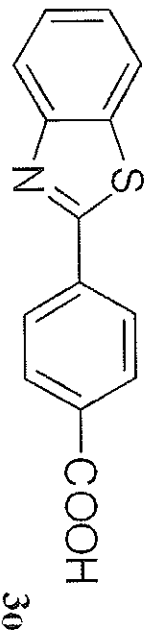
Copies of spectra

Minimum:		5.0	5.0	-1.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
315.9729	315.9722	0.7	2.2	11.5	2.8	C13 H7 N3 O2 Br

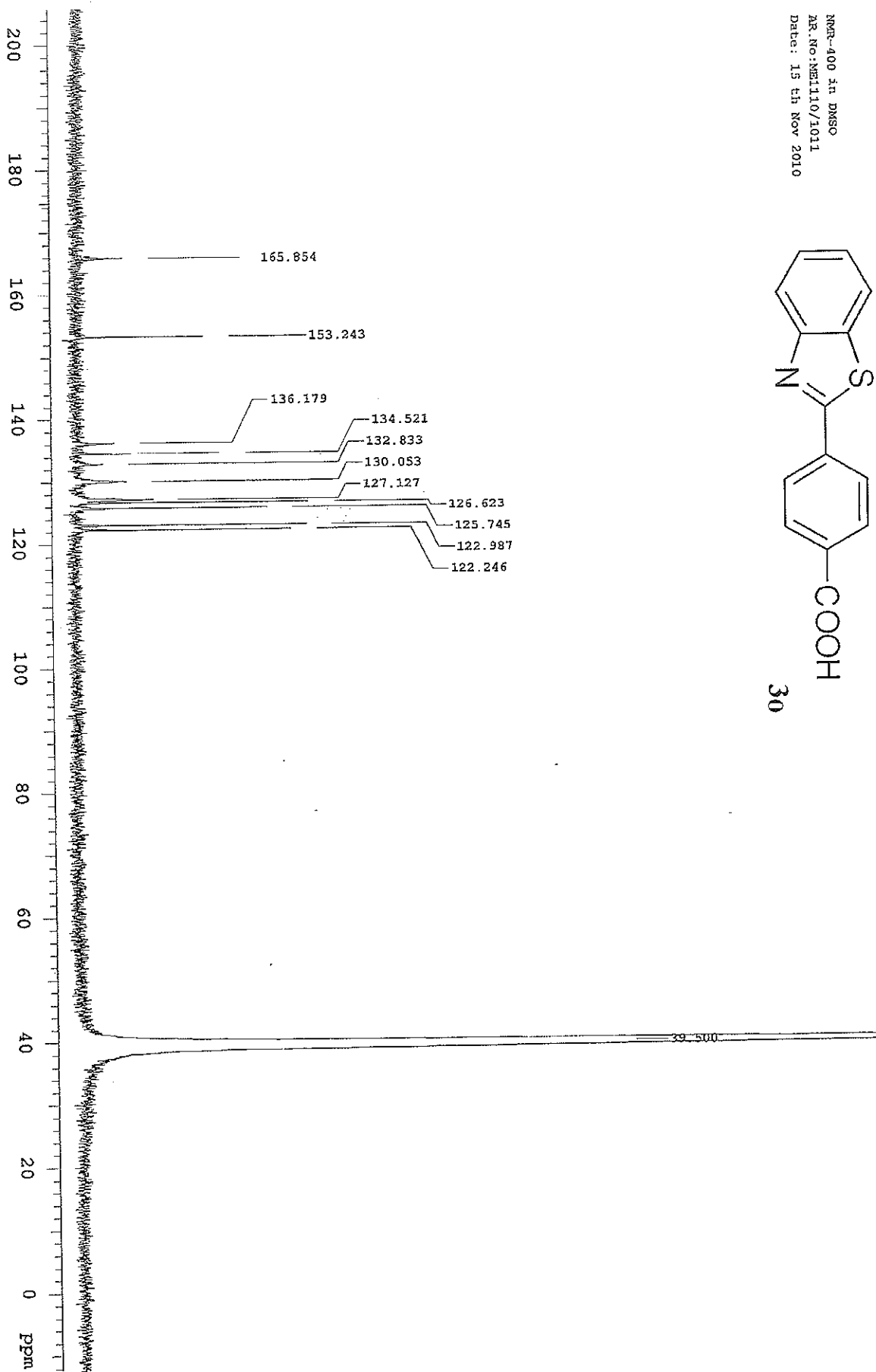
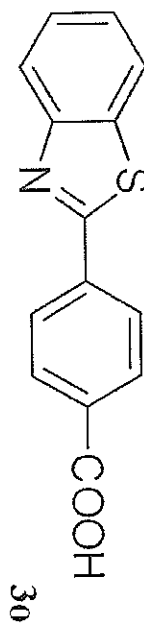


Copies of spectra

NMR-400 in DMSO
R.R.No:ME1010/263
Date: 04 th Oct 2010



NR-400 in DMSO
AR.No:ME110/1011
Date: 15 th Nov 2010



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

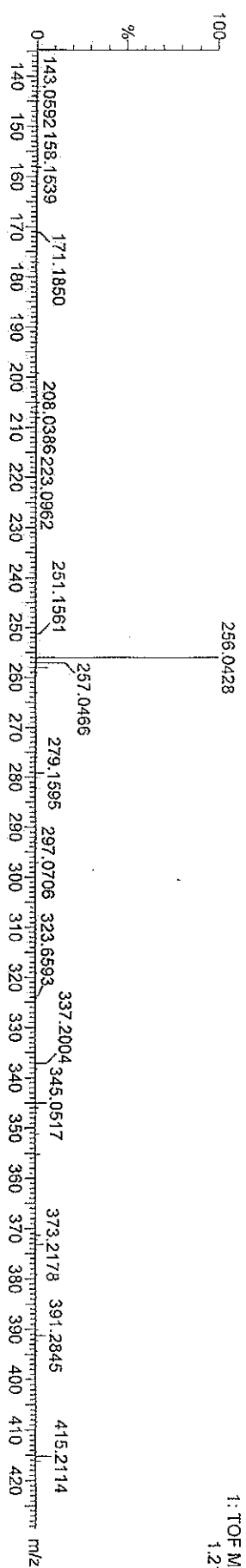
33 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-2 S: 0-1

Dr.Reddy's Laboratories Ltd, ARD, IDC-1

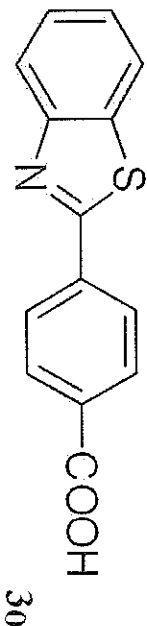
UT0312_24 14 (0.264) Cm (13:18)



1: TOF MS ES+
1.21e+004

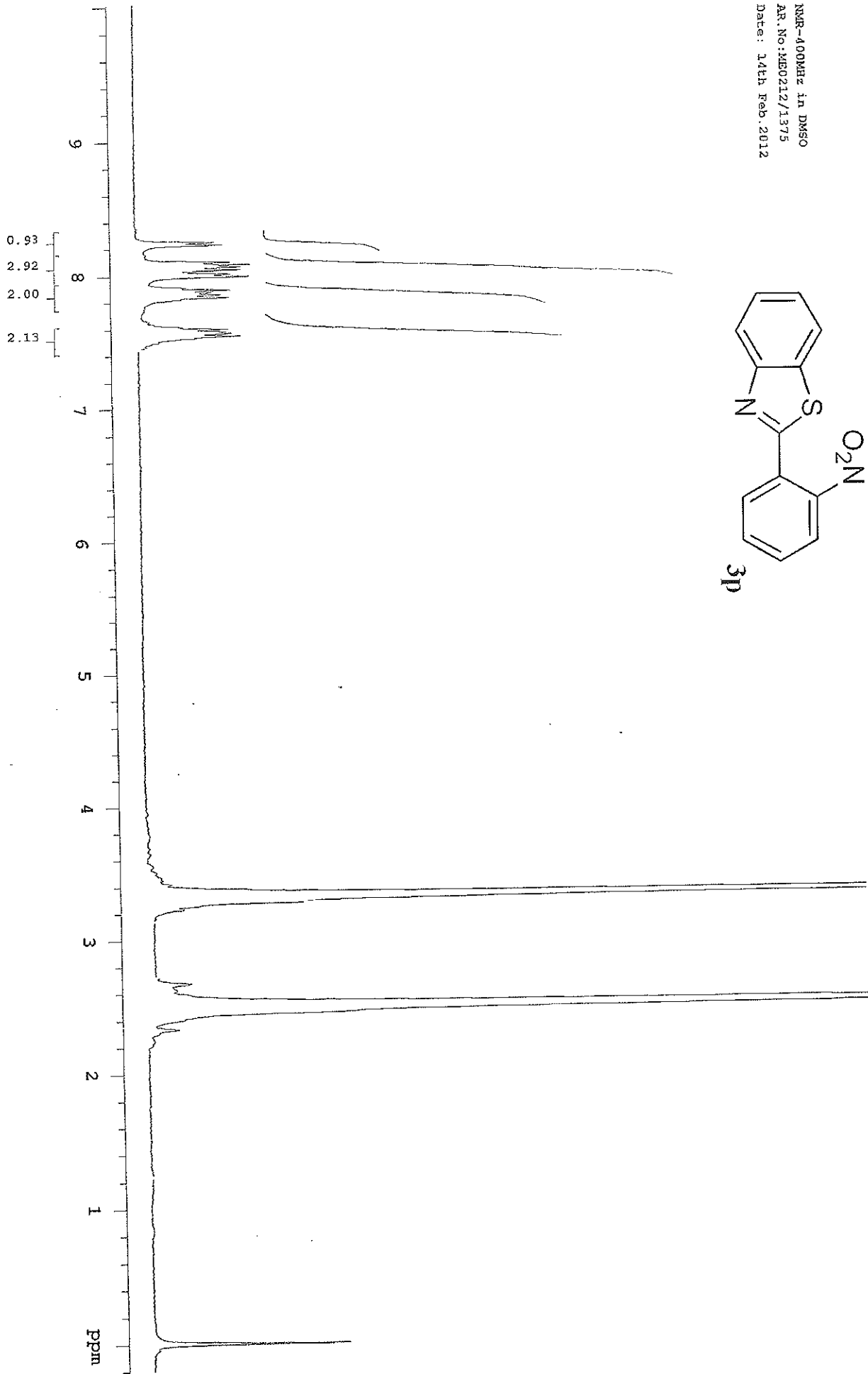
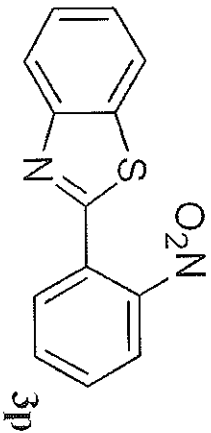
Copies of spectra

Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.0428	256.0432	-0.4	-1.6	10.5	5.5	C14 H10 N O2 S

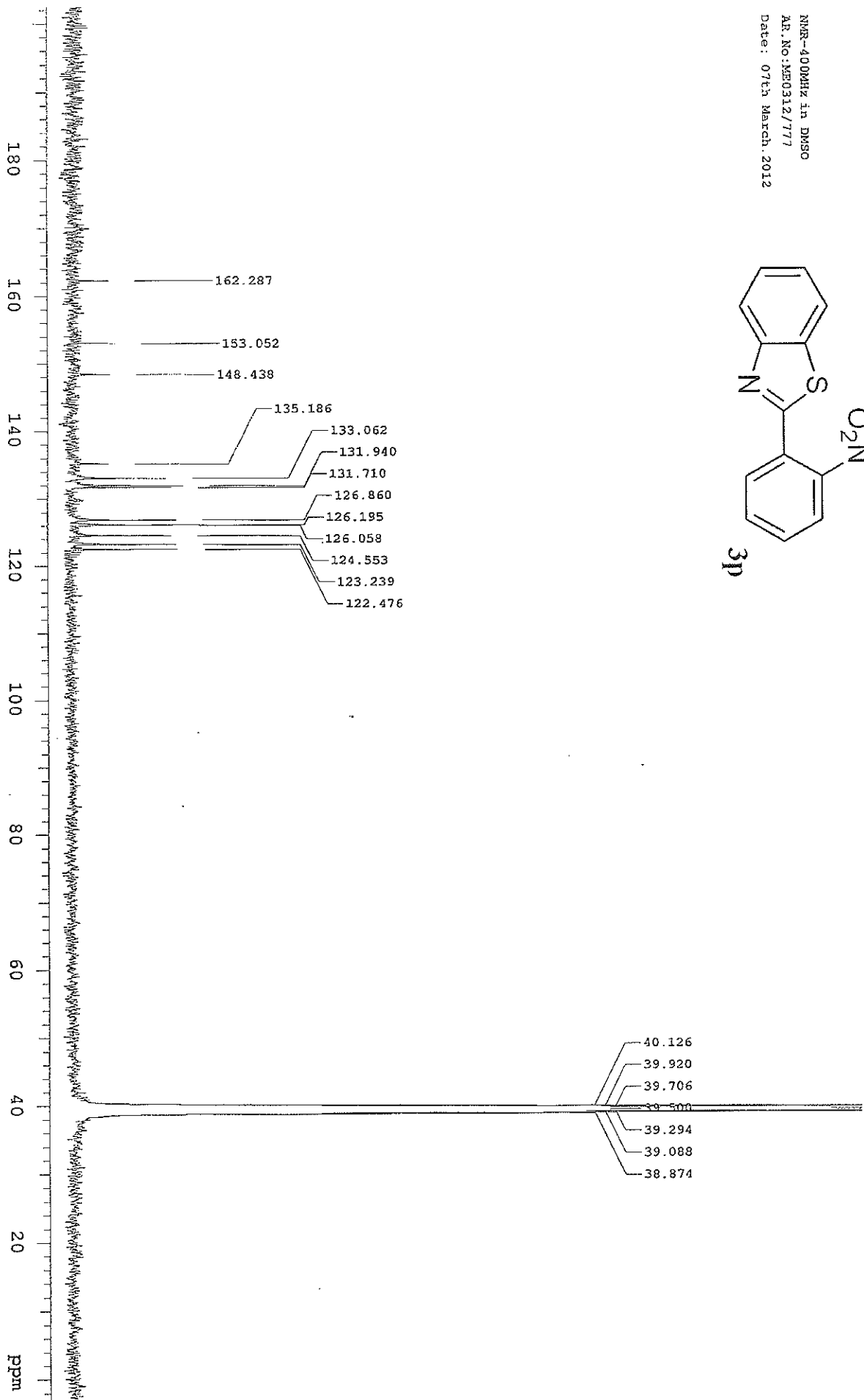
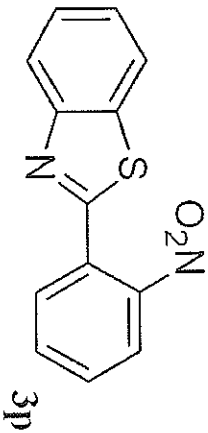


Copies of spectra

NMR-400MHz in DMSO
AR.No:ME0212/1375
Date: 14th Feb. 2012



nmr-400MHz in DMSO
Ac.No:ME0312/777
Date: 07th March, 2012



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

25 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

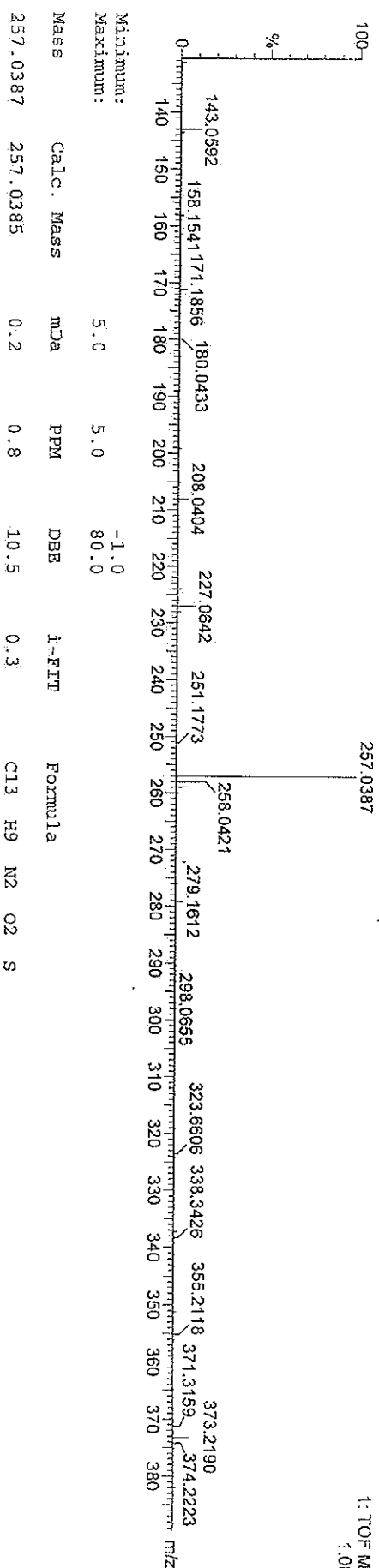
Elements Used:

C: 0-15 H: 0-20 N: 0-3 O: 0-2 S: 0-1

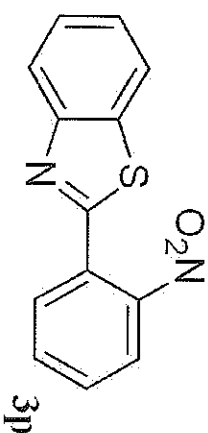
UT0312_08 15 (0.279) Cm (9:17-1x0.010)

Dr. Reddy's Laboratories Ltd, ARD, TDC-1

Copies of spectra

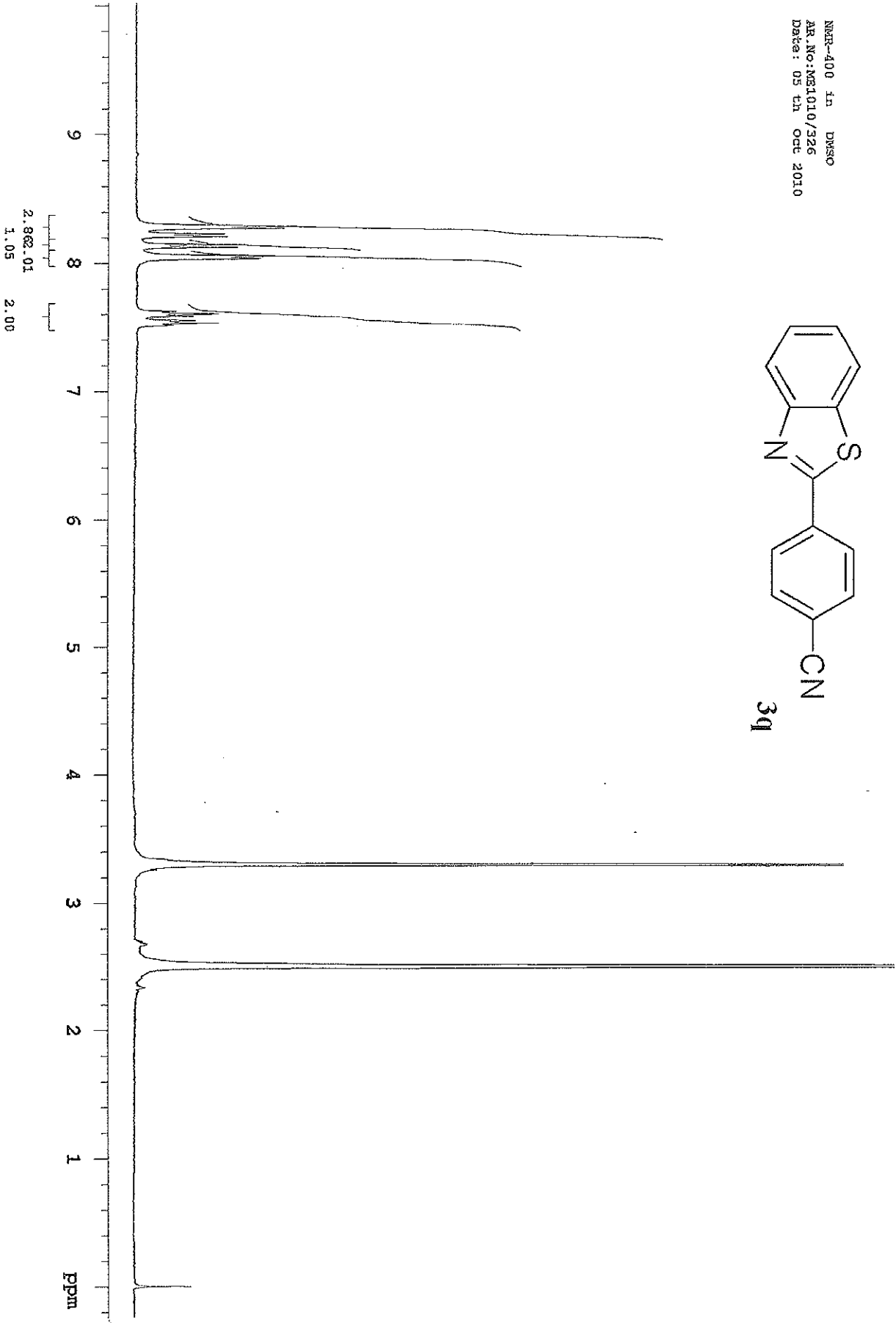
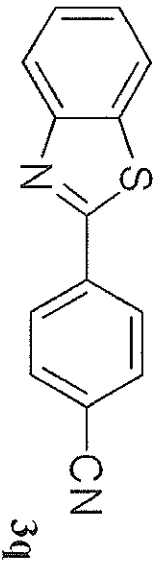


1: TOF MS ES+
1.08e+004

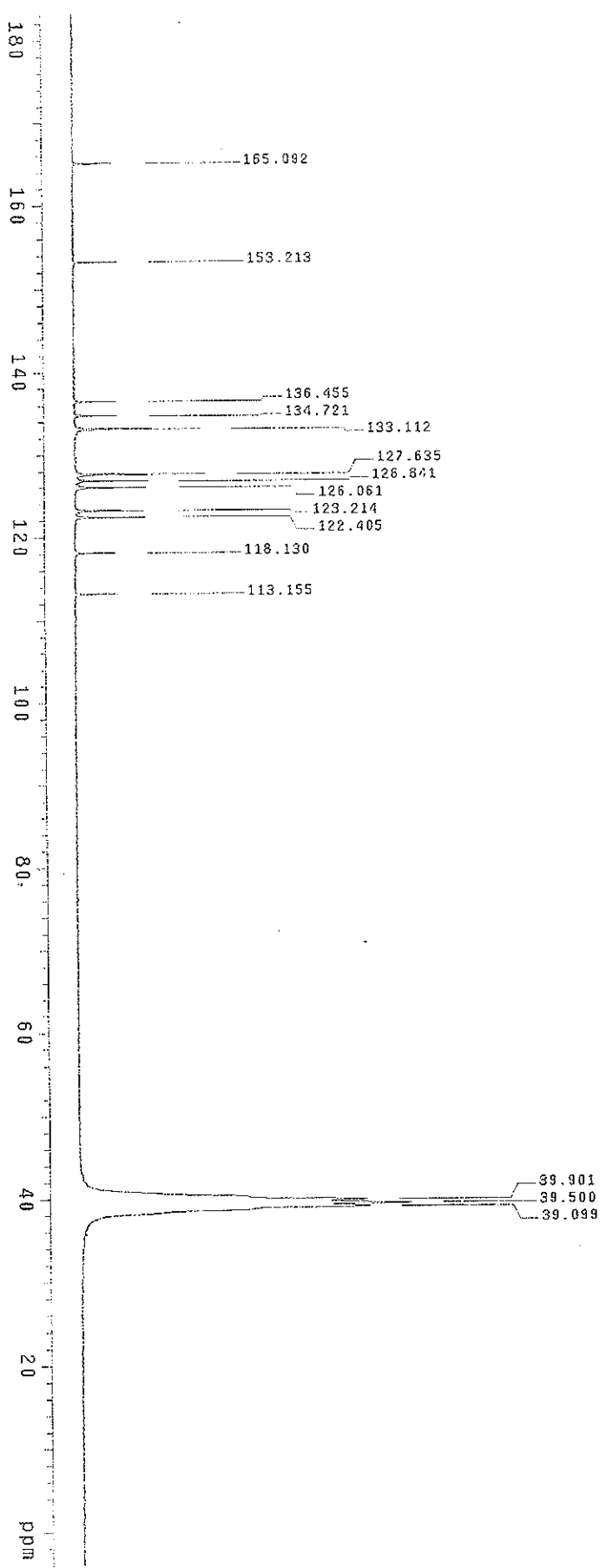
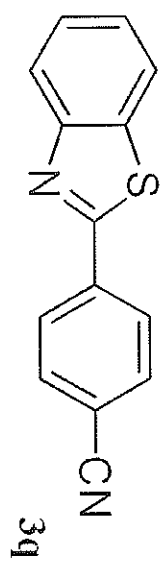


Copies of spectra

NMR-400 in DMSO
AR.No:ME1010/326
Date: 05 th Oct 2010



NMR-400 in DMSO
AR NO: GE1210/24
Date: 13 th Dec. 2010



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

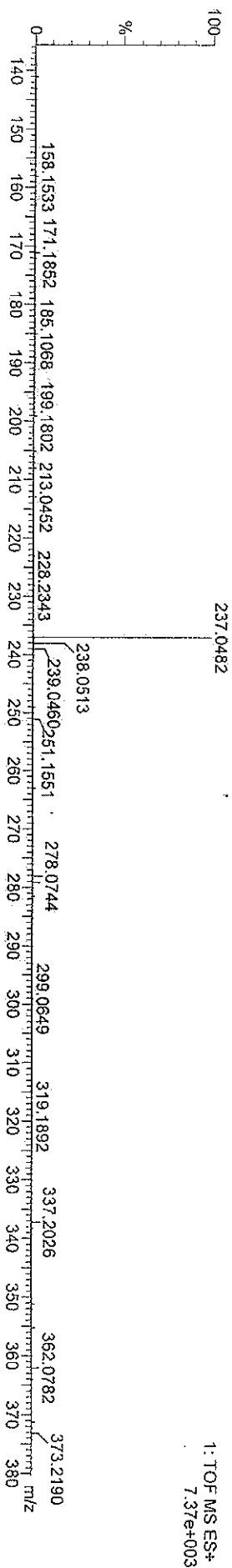
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-15 H: 0-10 N: 0-2 S: 0-1

Dr.Reddy's Laboratories Ltd, ARD,TDC-1

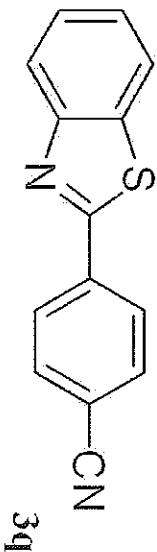
UT0312_237 (0.131) Cm (5:9)

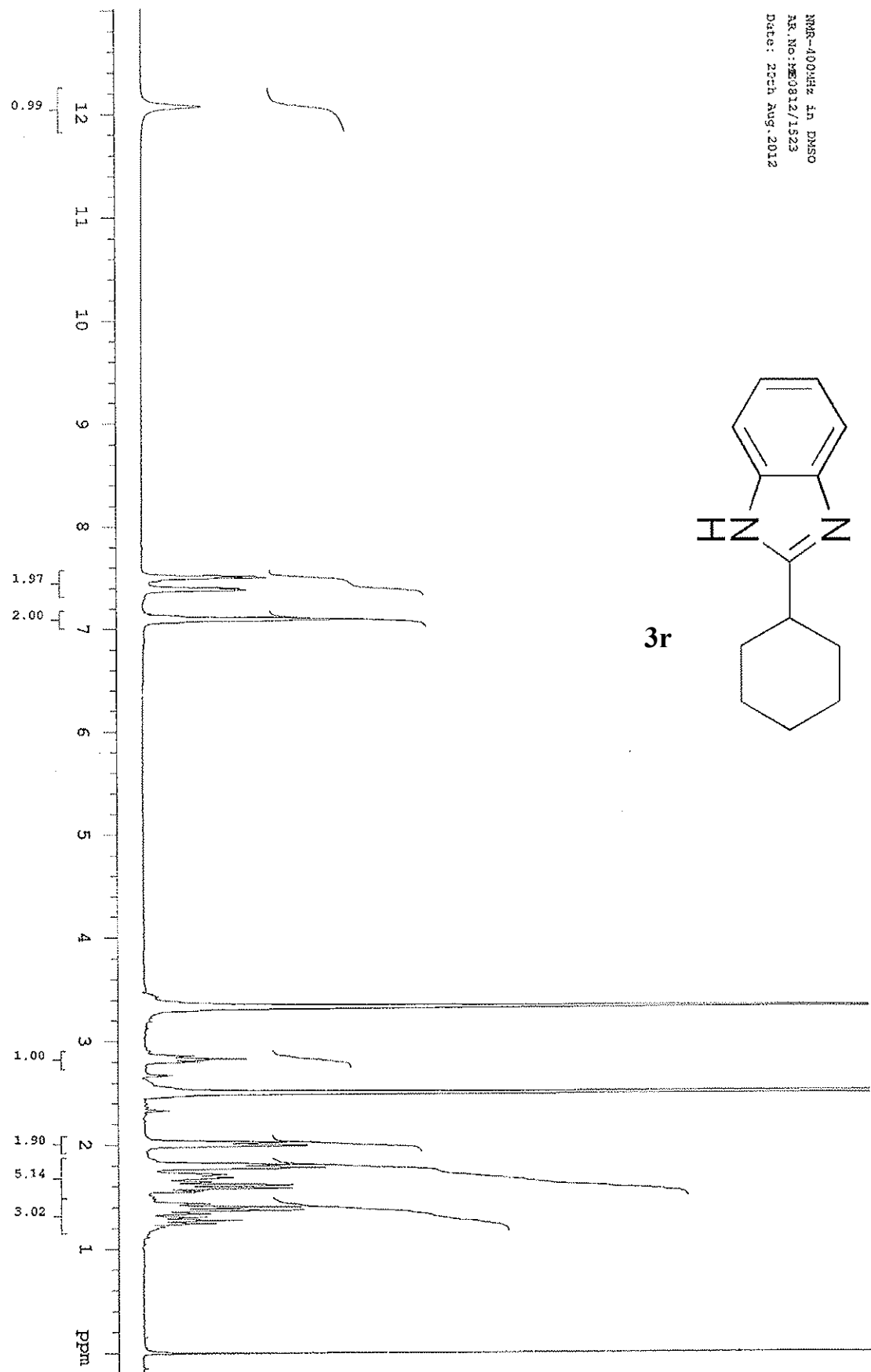


1: TOF MS ES+
7.37e+003

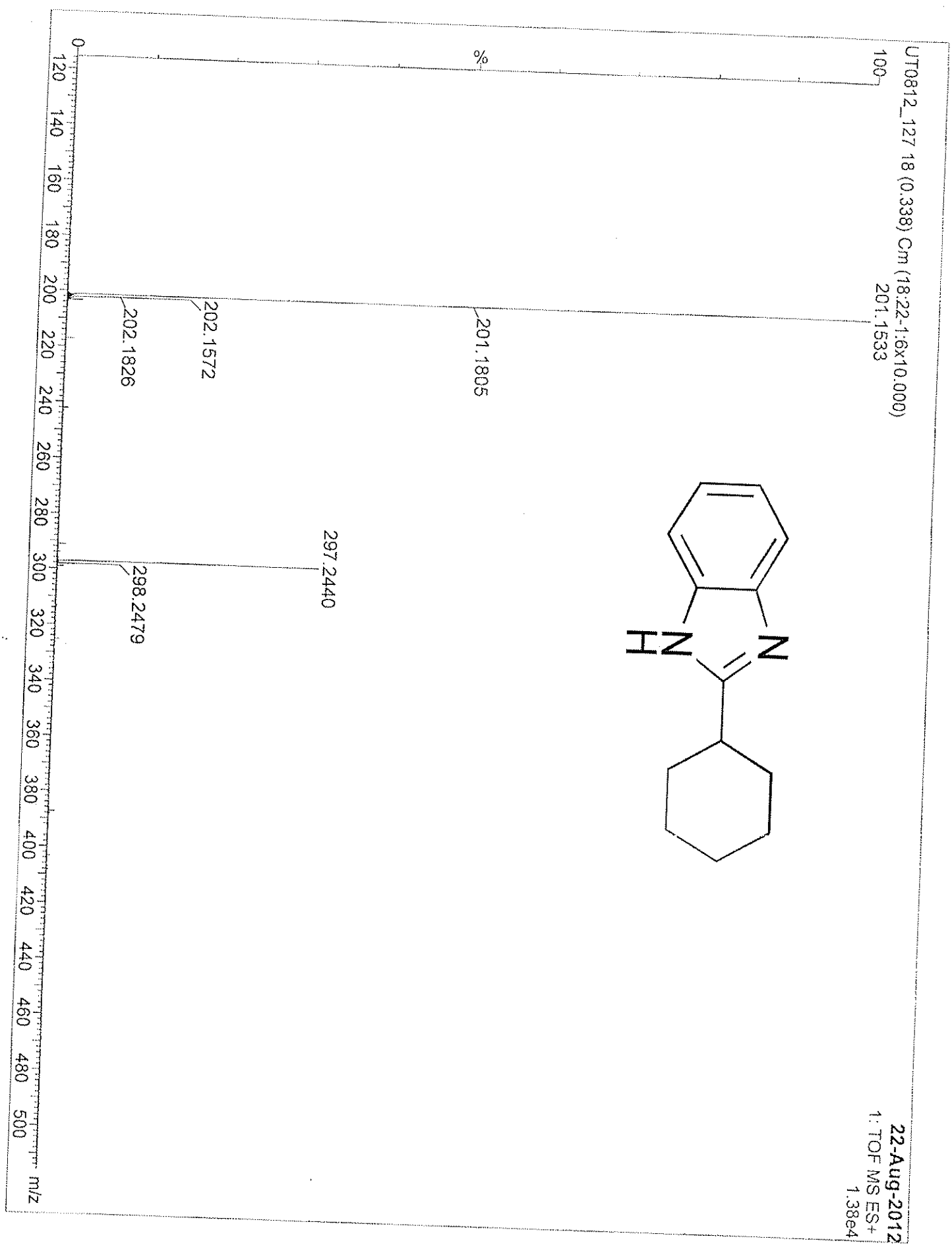
Copies of spectra

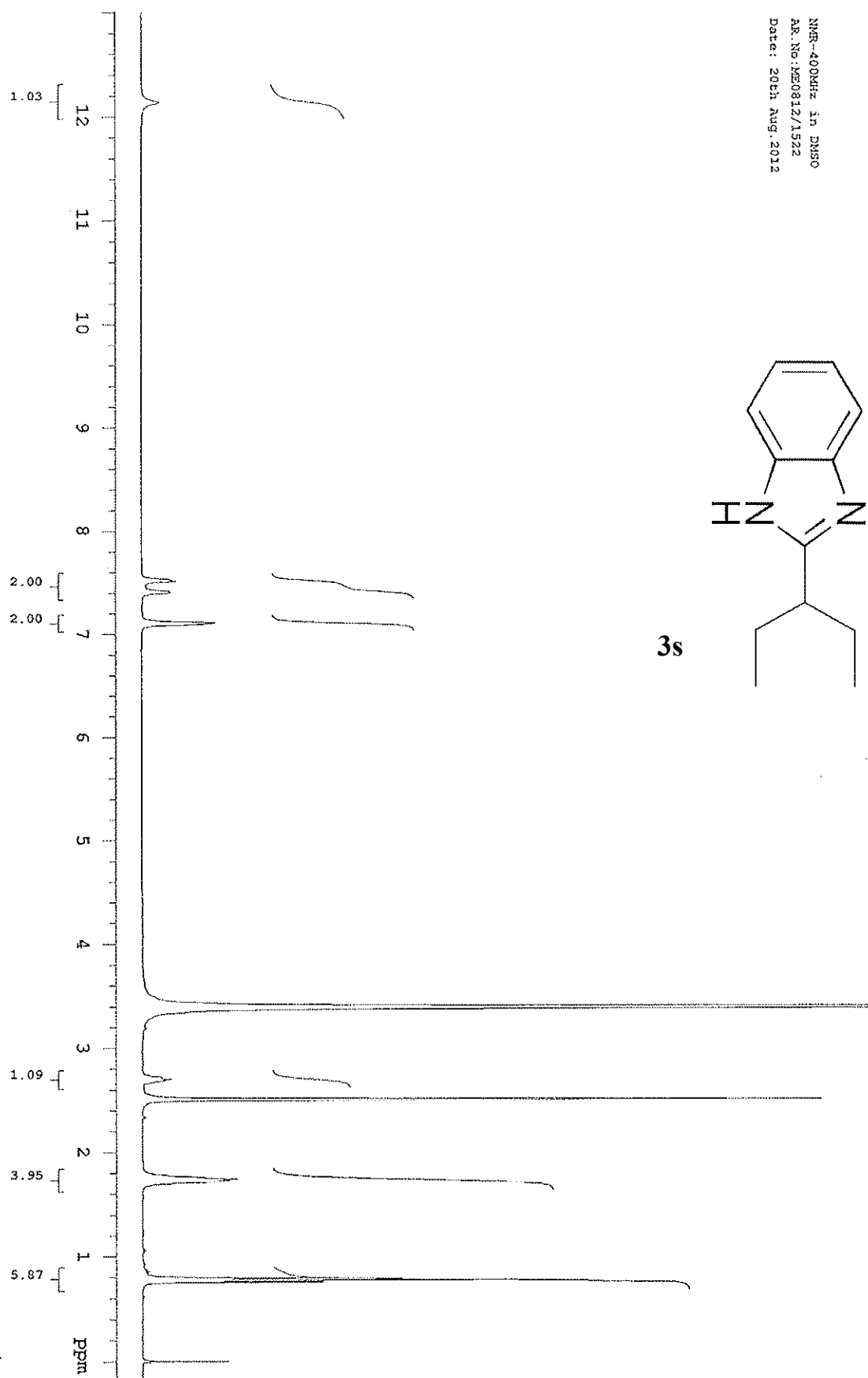
Minimum:							
Maximum:							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
237.0482	237.0486	-0.4	-1.7	11.5	1.0	C14 H9 N2 S	





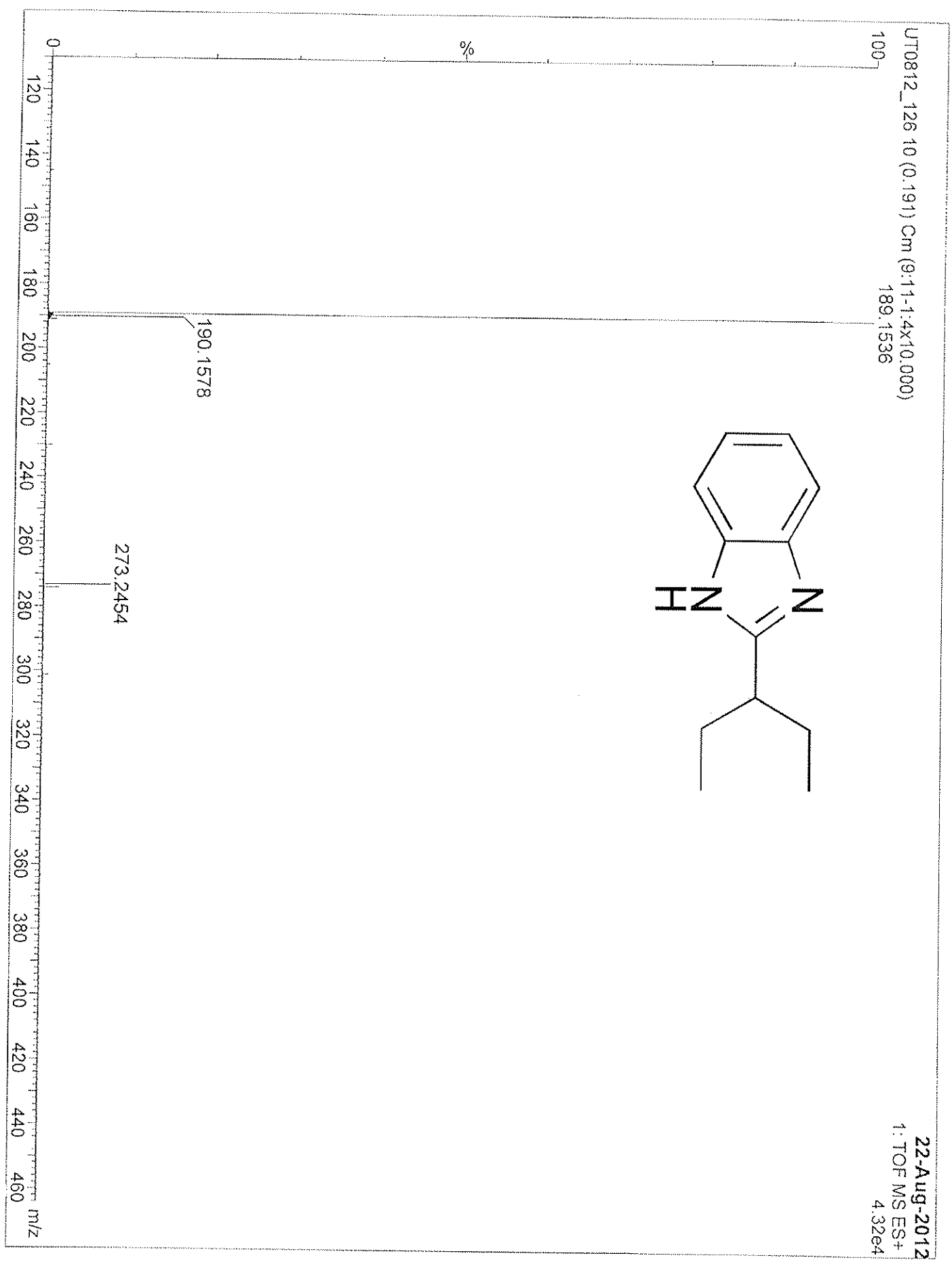
NMR-400MHz in DMSO
Ac.No:HE0812/1523
Date: 25th Aug.2012

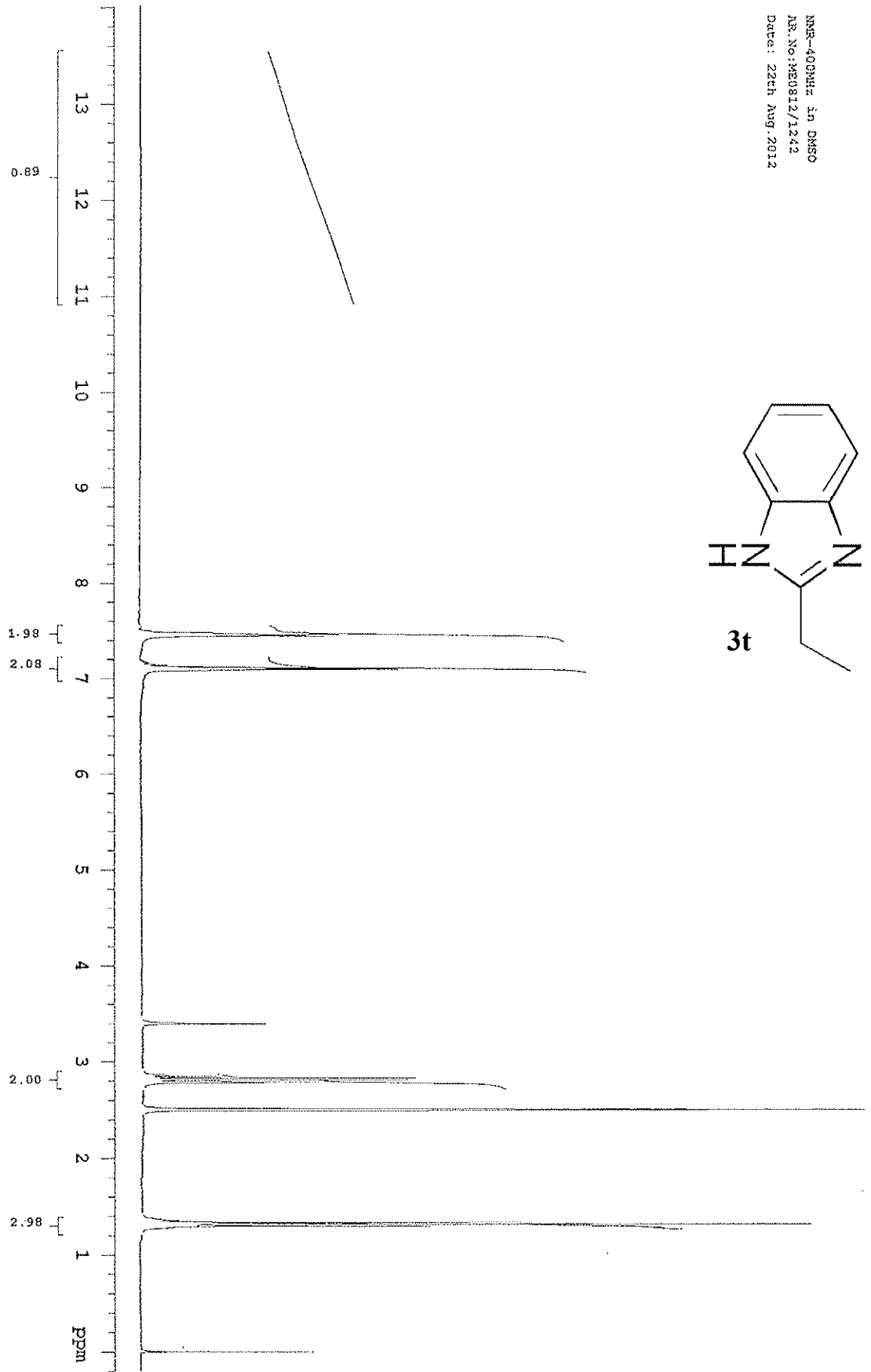




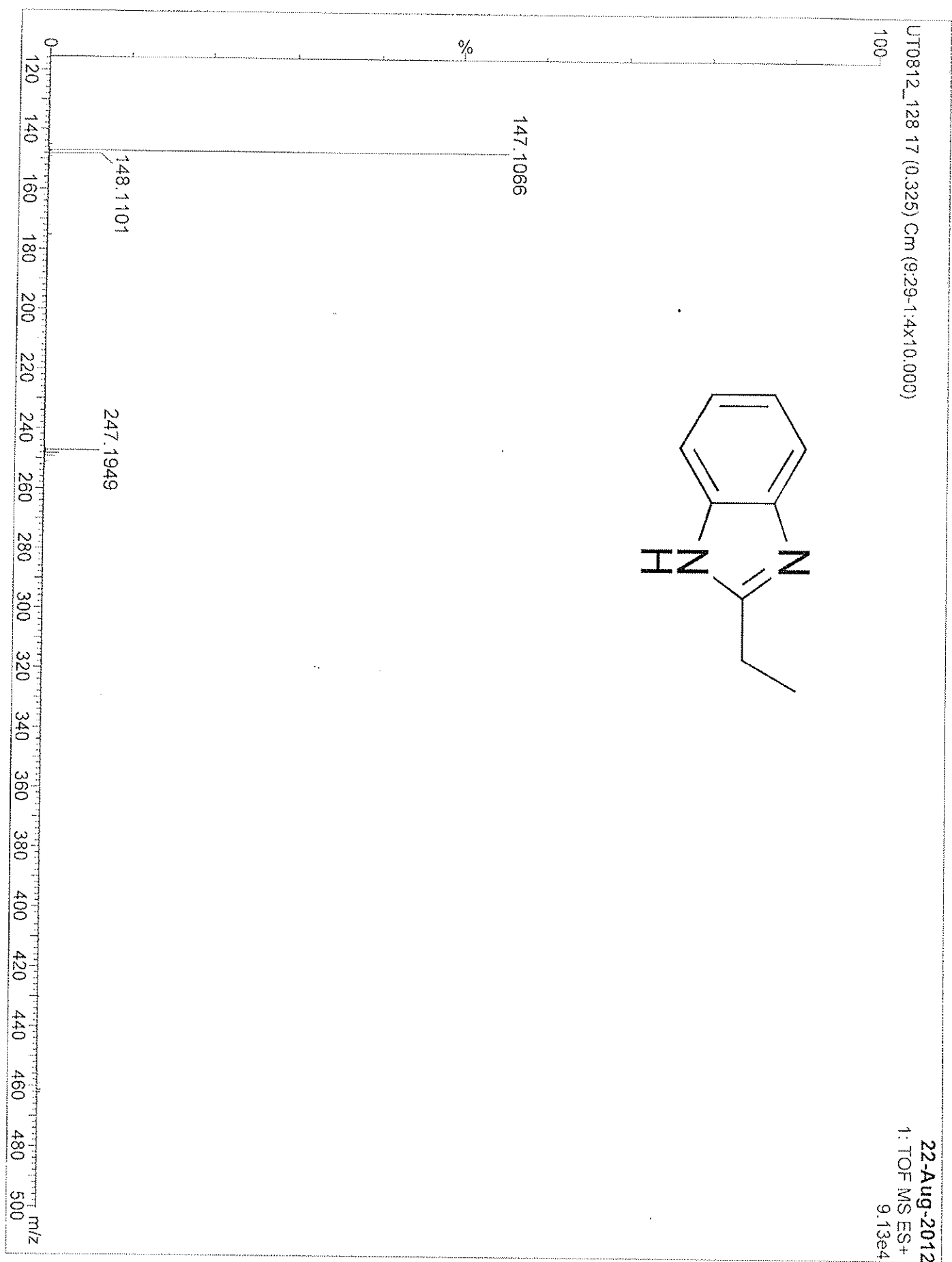
NMR-400MHz in DMSO
Ac. No: ME0812/1522
Date: 20th Aug. 2012

3s



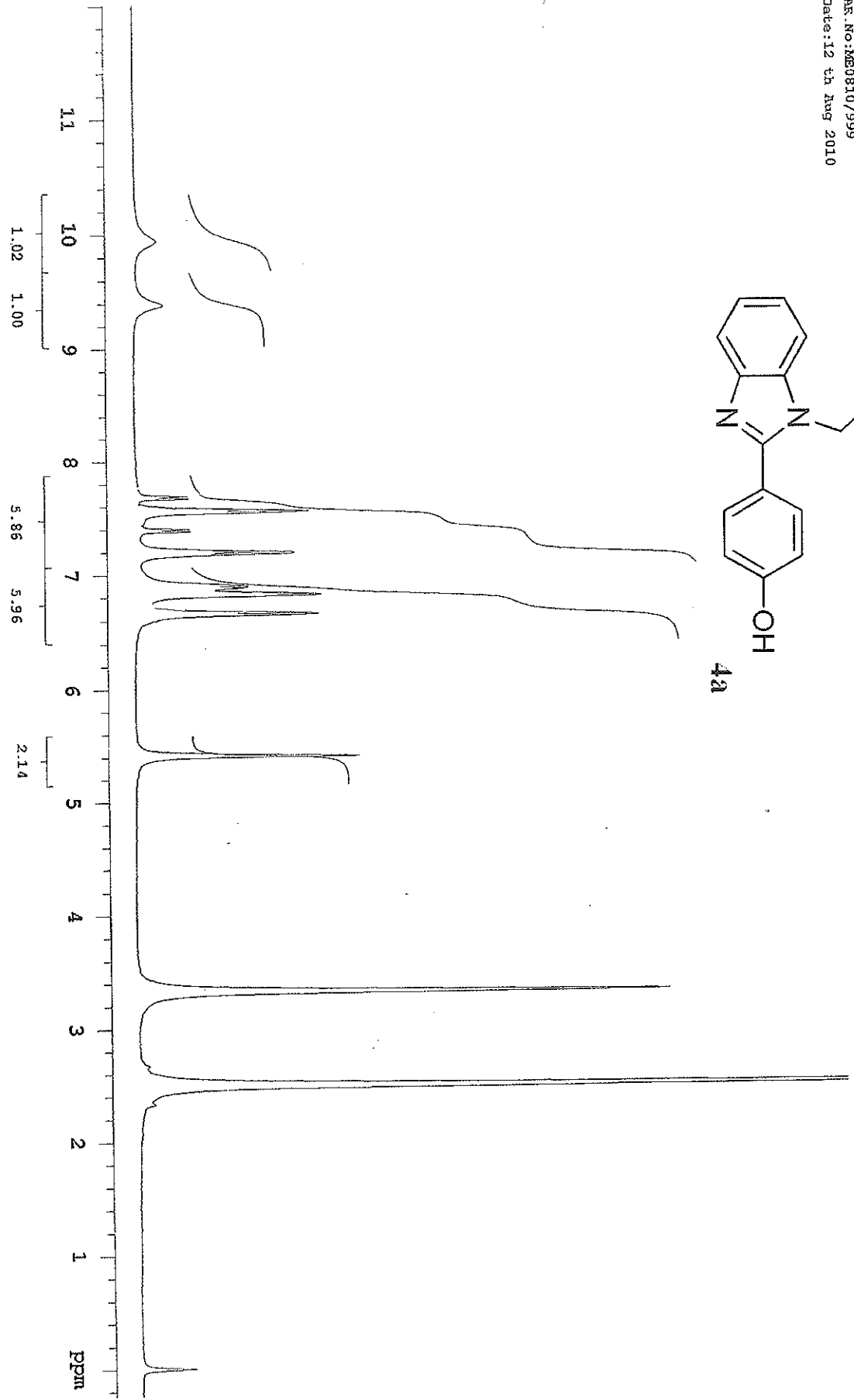
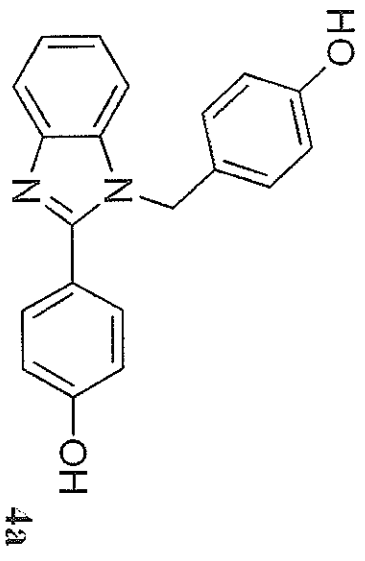


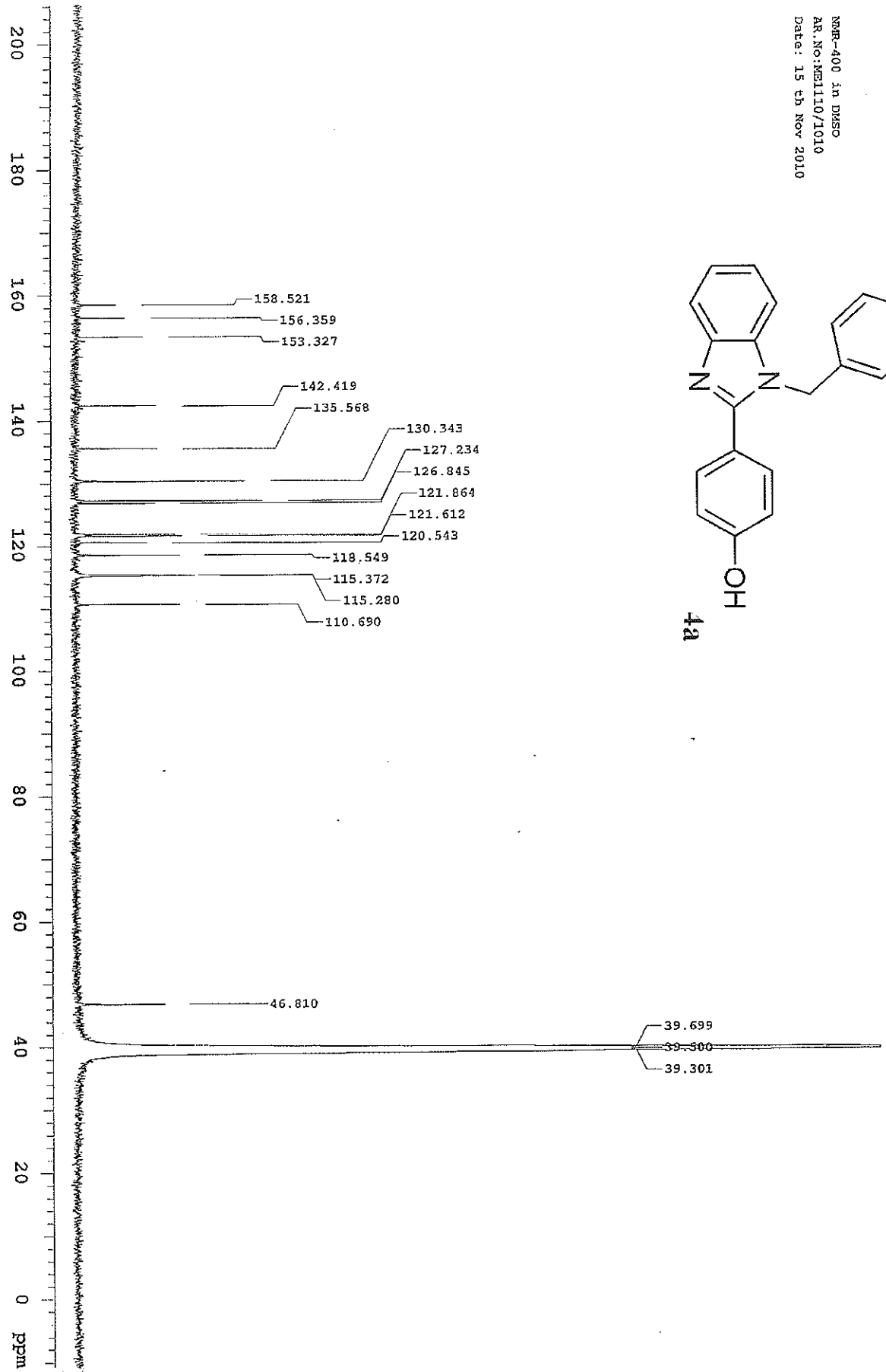
NR-400MHz in DMSO
AR.No:ME0812/1242
Date: 22th Aug.2012



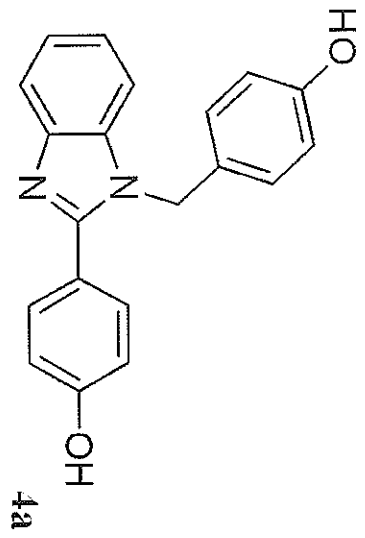
Copies of spectra

NMR-400 in DMSO
AS.No:ME0810/999
Date:12 th Aug 2010





NR-400 in DMSO
AR, No: ME110/1010
Date: 15 th Nov 2010



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

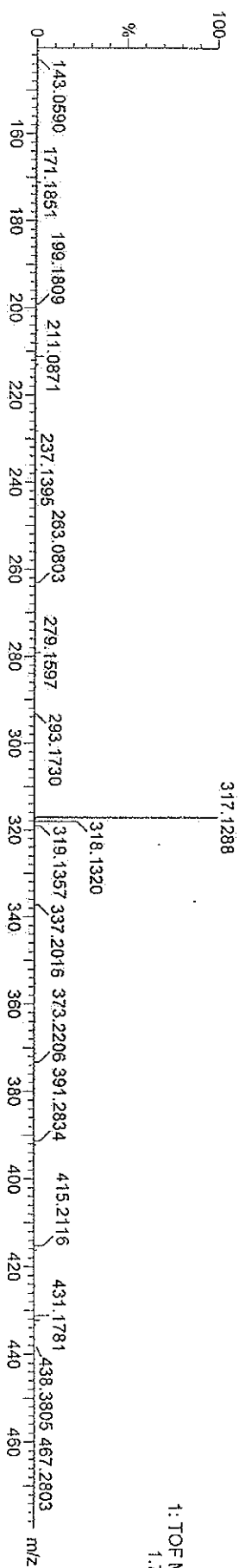
4 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-2

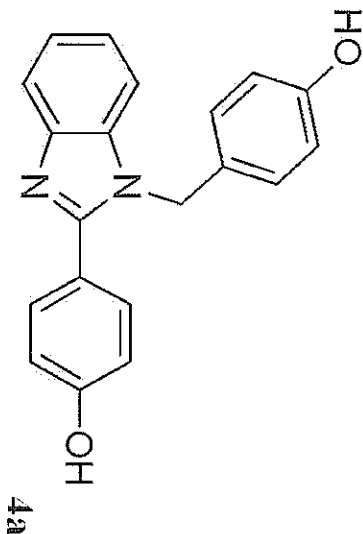
UT0312_19 5 (0.103) Cm (4:10)

Dr.Reddy's Laboratories Ltd, ARD, TDC-1



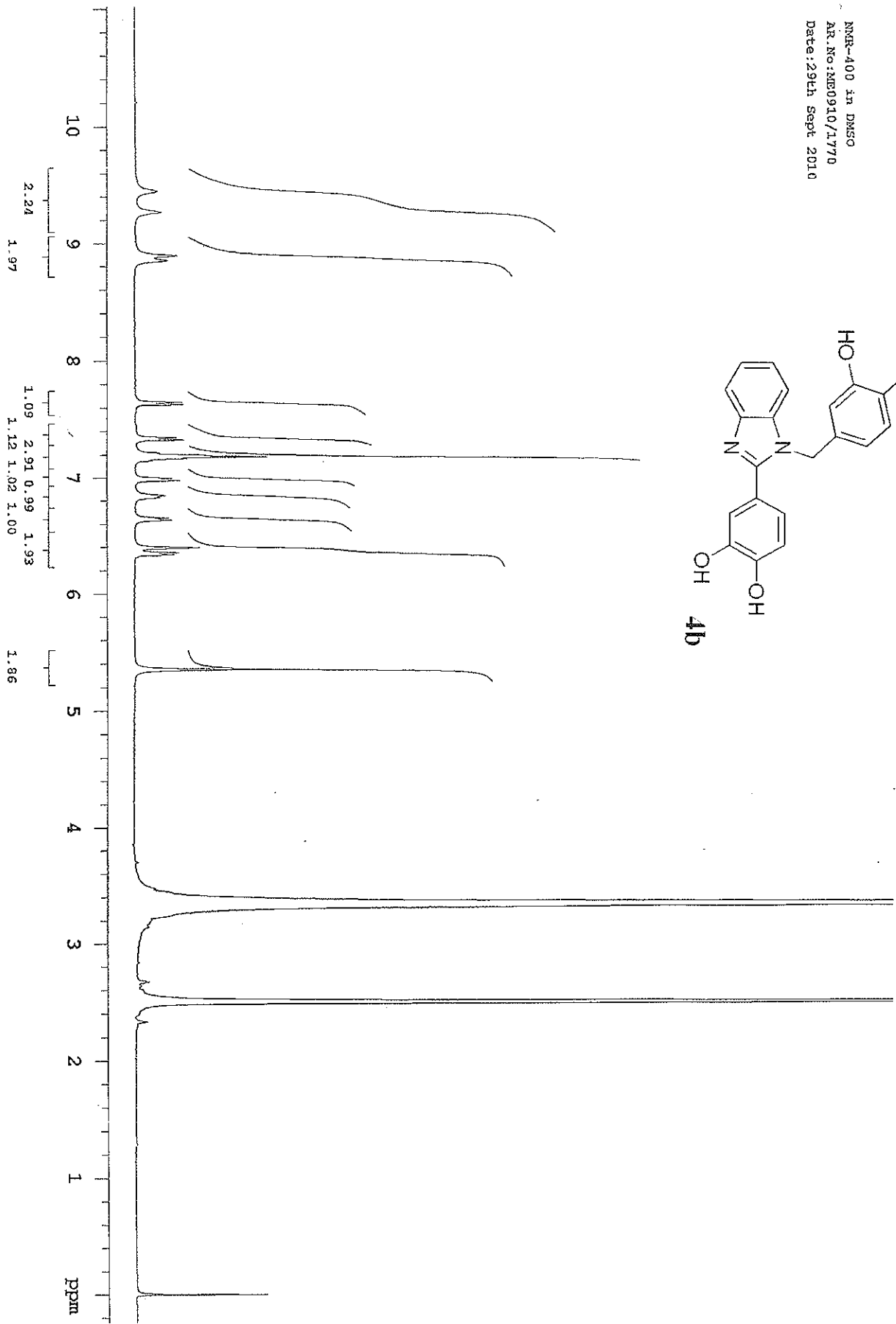
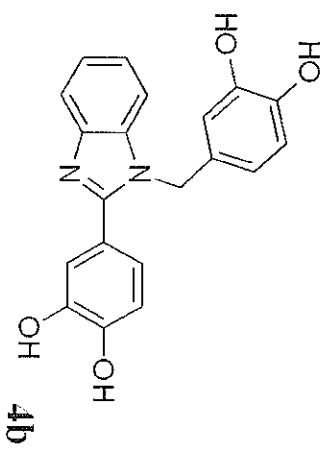
Copies of spectra

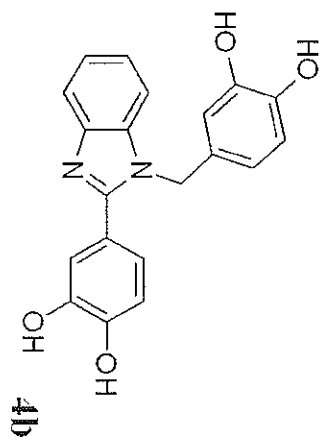
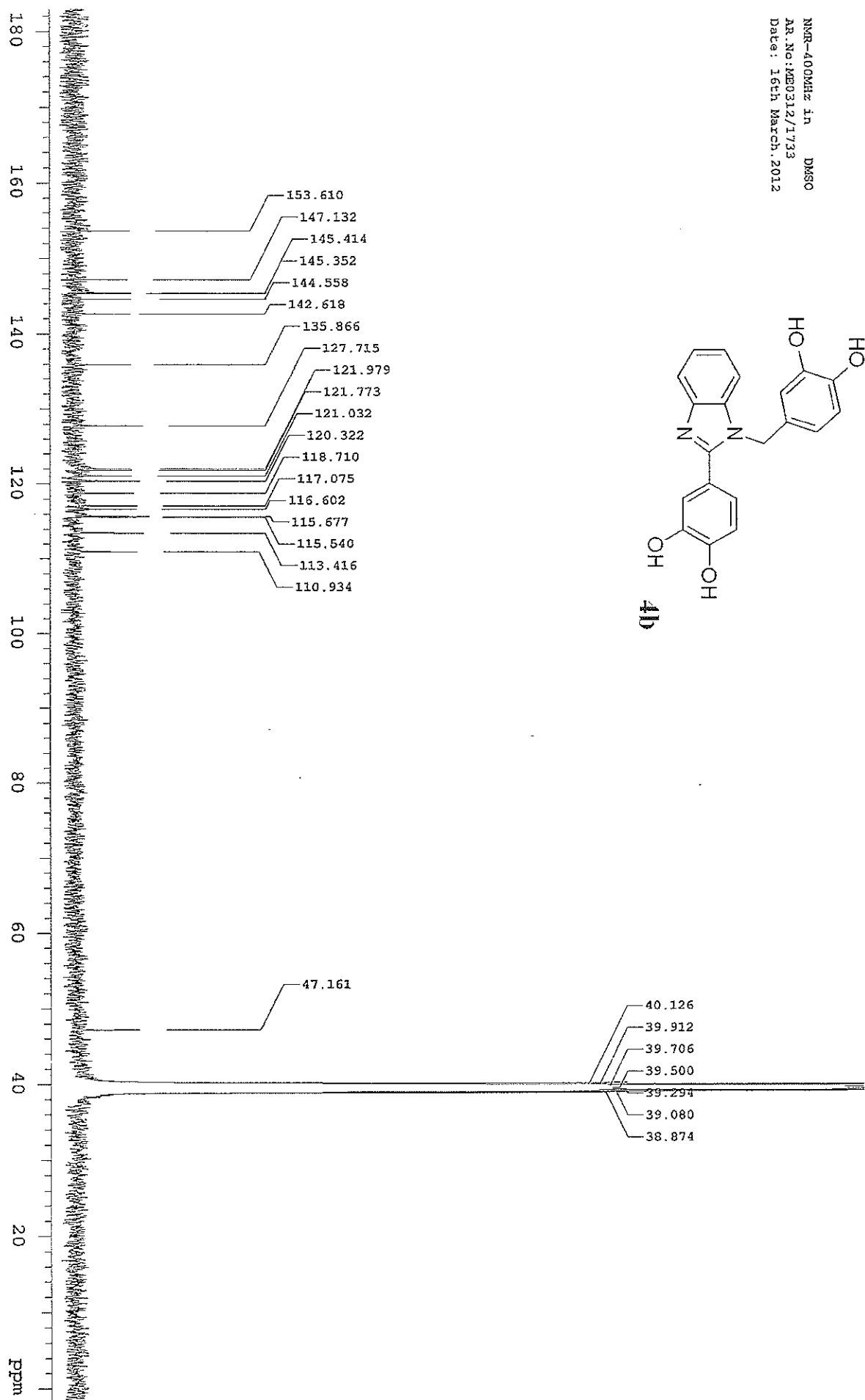
Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
317.1288	317.1290	-0.2	-0.6	13.5	0.4	C20 H17 N2 O2



Copies of spectra

nmr-400 in DMSO
AR.No:ME0910/1770
Date:29th Sept 2010





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

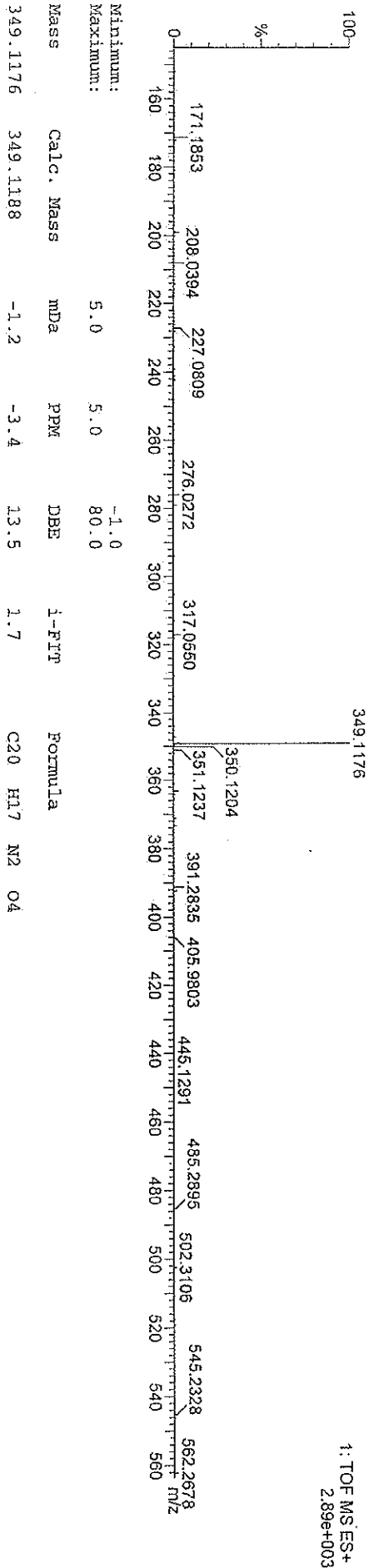
10 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

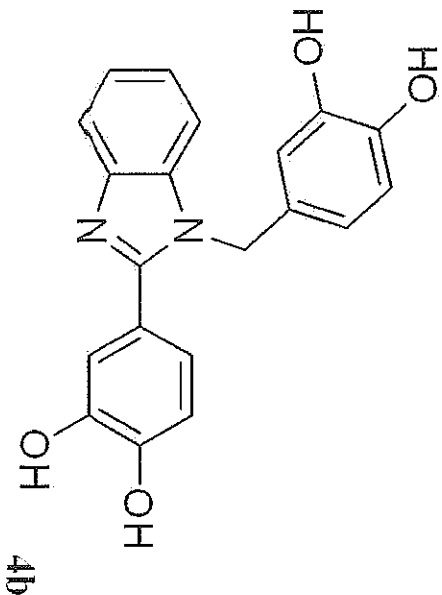
C: 0-20 H: 0-20 N: 0-2 O: 0-4

UT0312_89 31 (0.575) Cm (31.39)

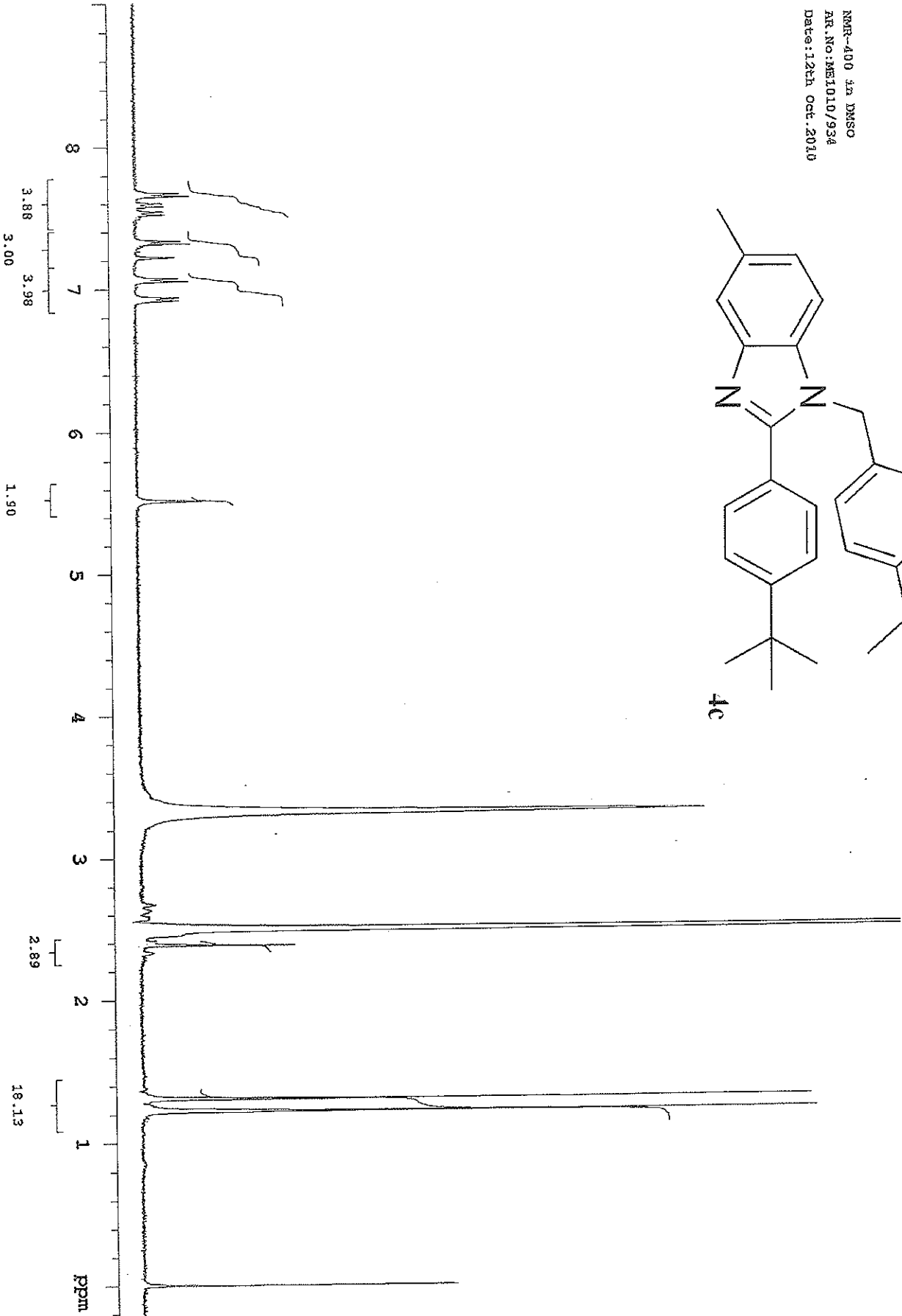
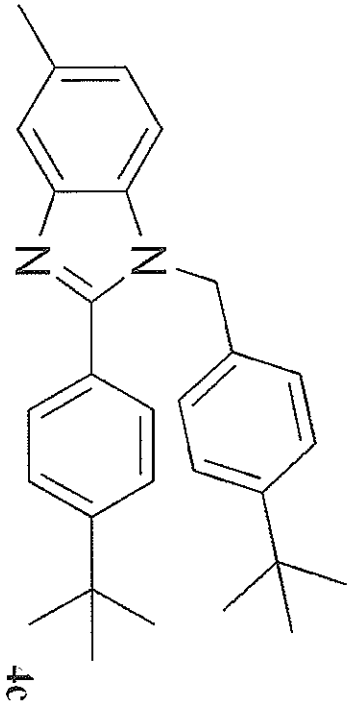
Dr.Reddy's Laboratories Ltd, ARD,TDC-1

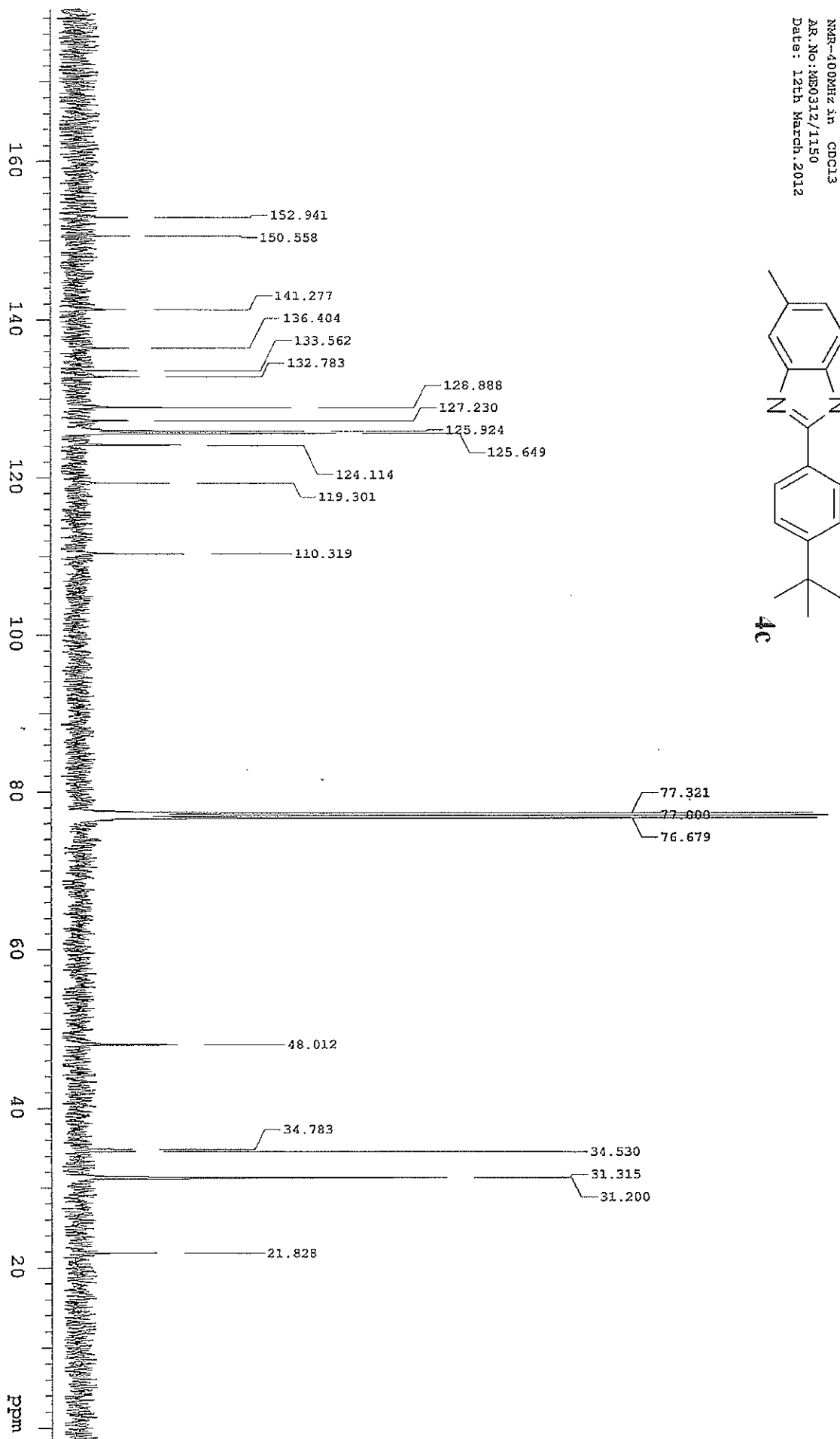


Copies of spectra



NMR-400 in DMSO
Ac.No: ME1010/934
Date: 12th Oct. 2010





Single Mass Analysis

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

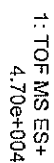
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

C: 0-30 H: 0-40 N: 0-2

UT0312.09 8(0.144) Cm (8:16)

Dr.Reddy's Laboratories Ltd, ARD,TDC-1

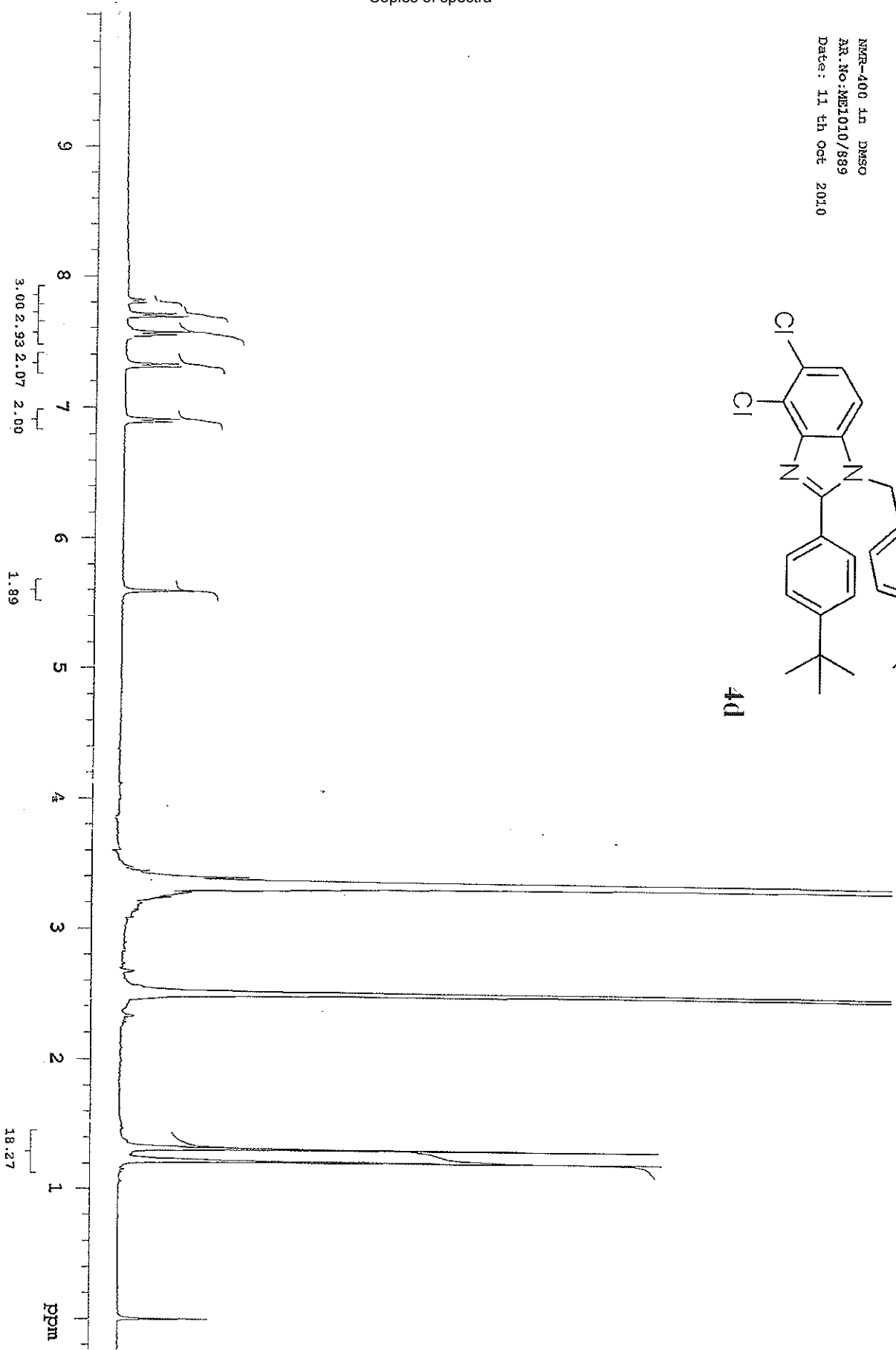
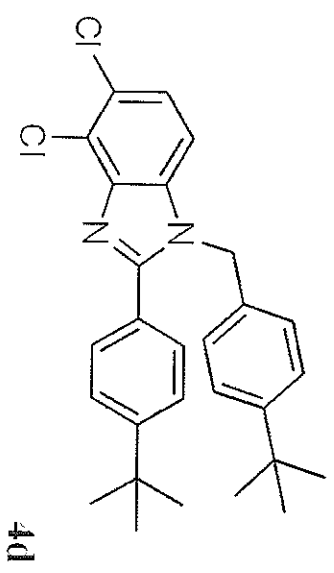


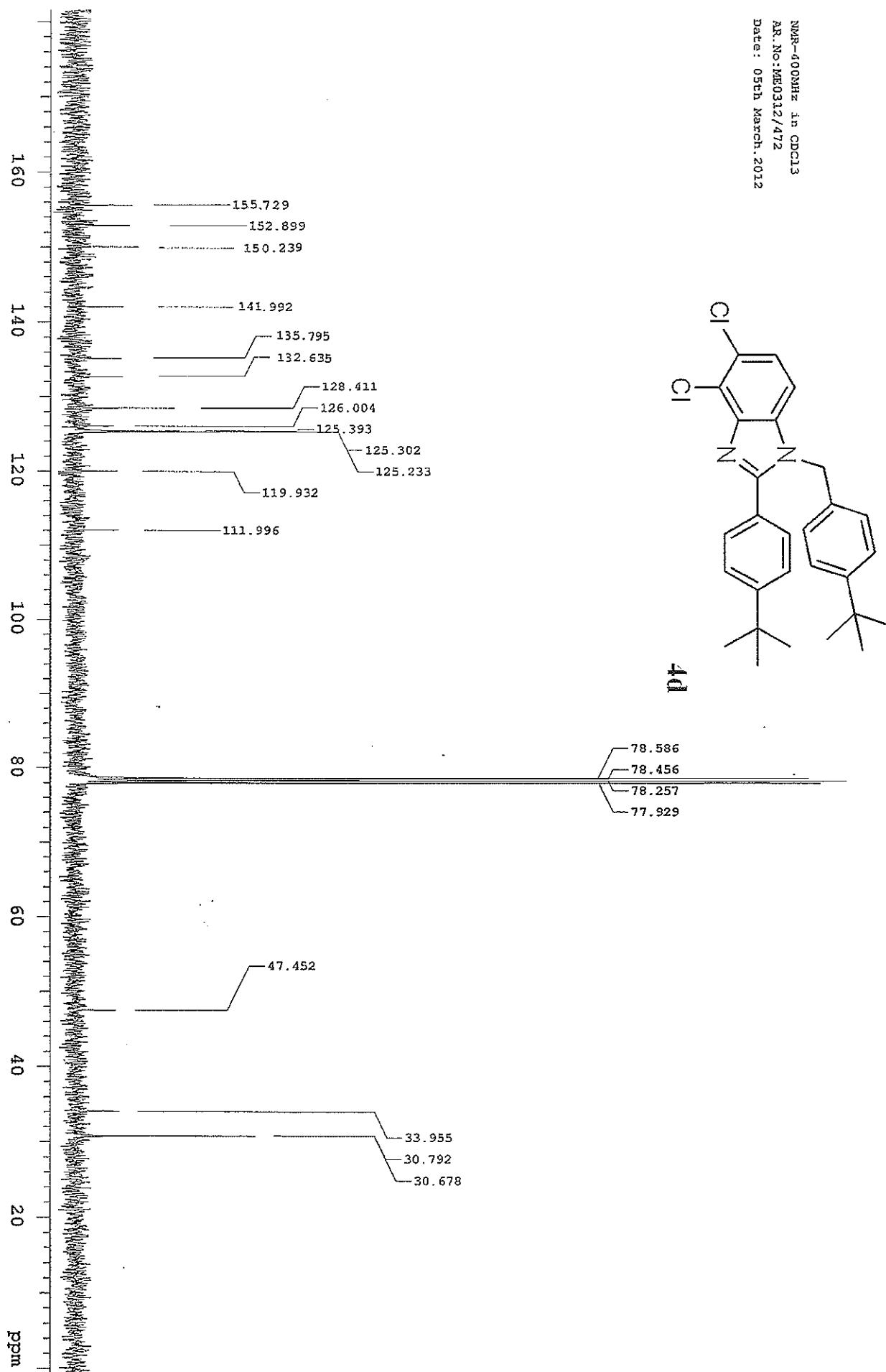
1-11-11



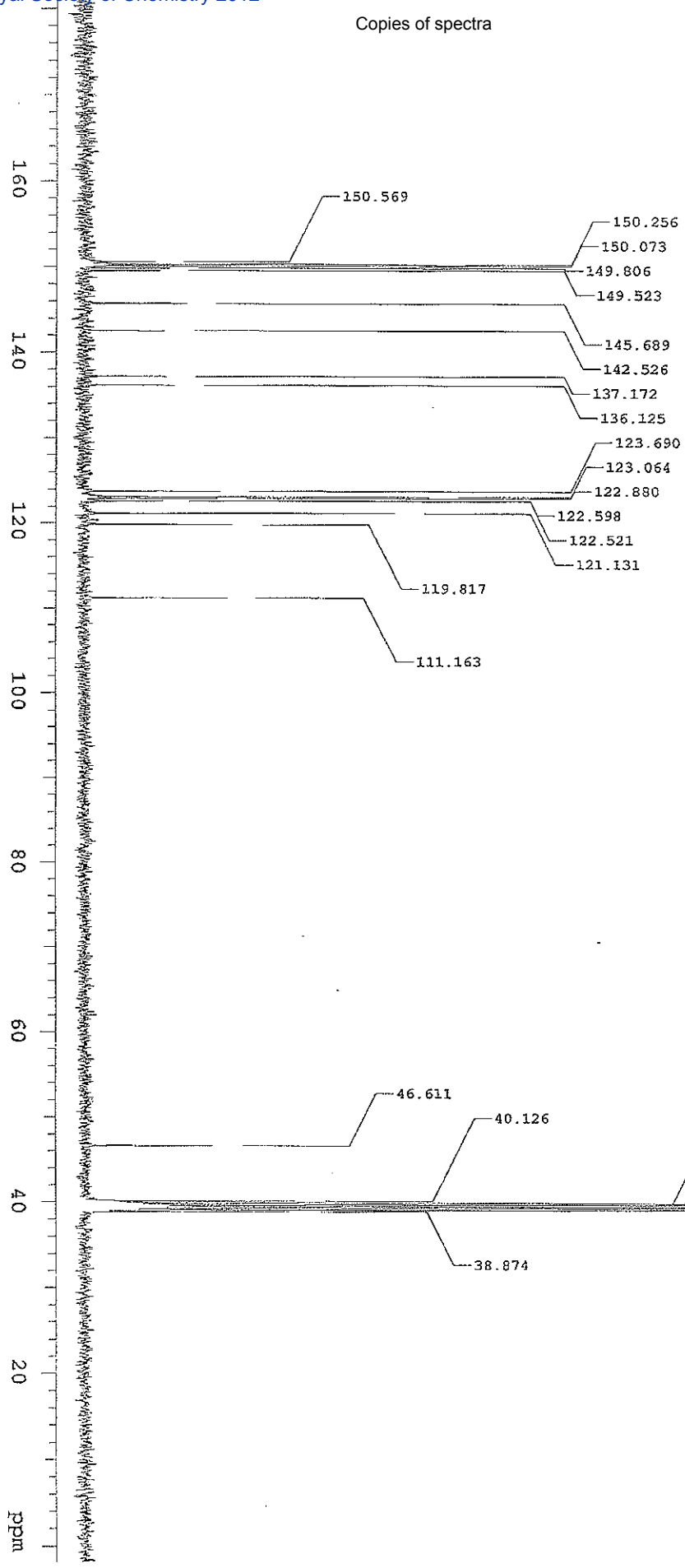
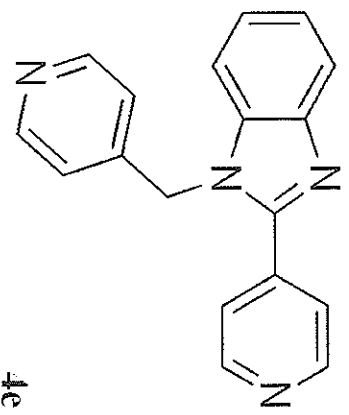
Copies of spectra

NMR-400 1H DMSO
Ac.No:ME1010/889
Date: 11 th Oct 2010





NMR-400MHz in DMSO
AR.No:ME0312/1717
Date: 16th March, 2012



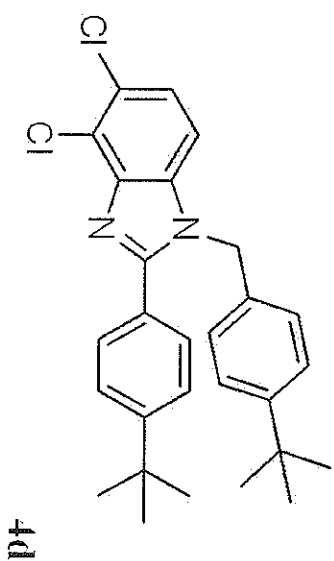
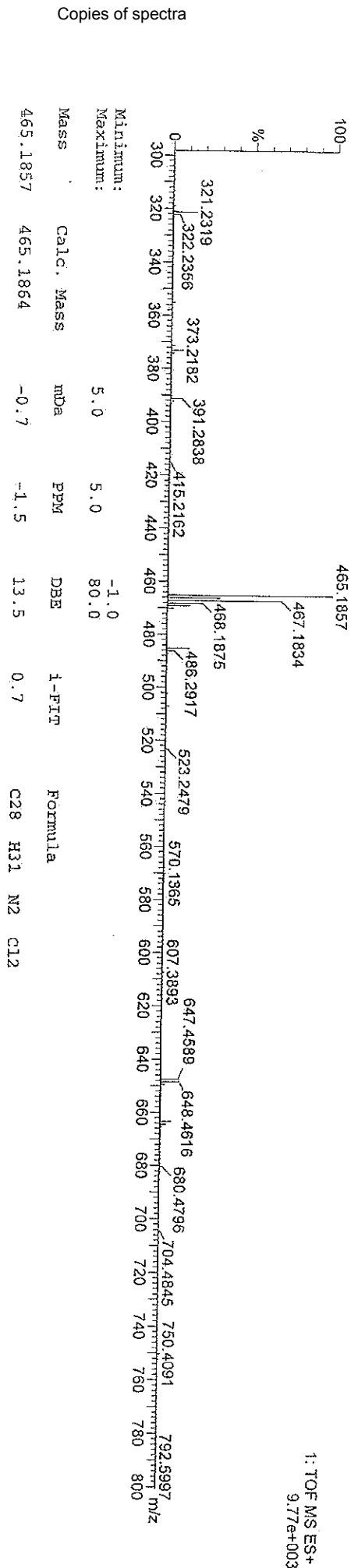
Elemental Composition Report

Single Mass Analysis

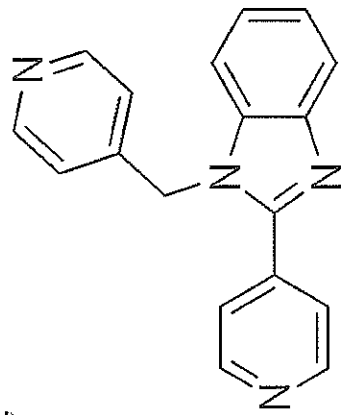
Tolerance = 5.0 PPM / DBE: min = -1.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9 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: 0-2 Cl: 0-2

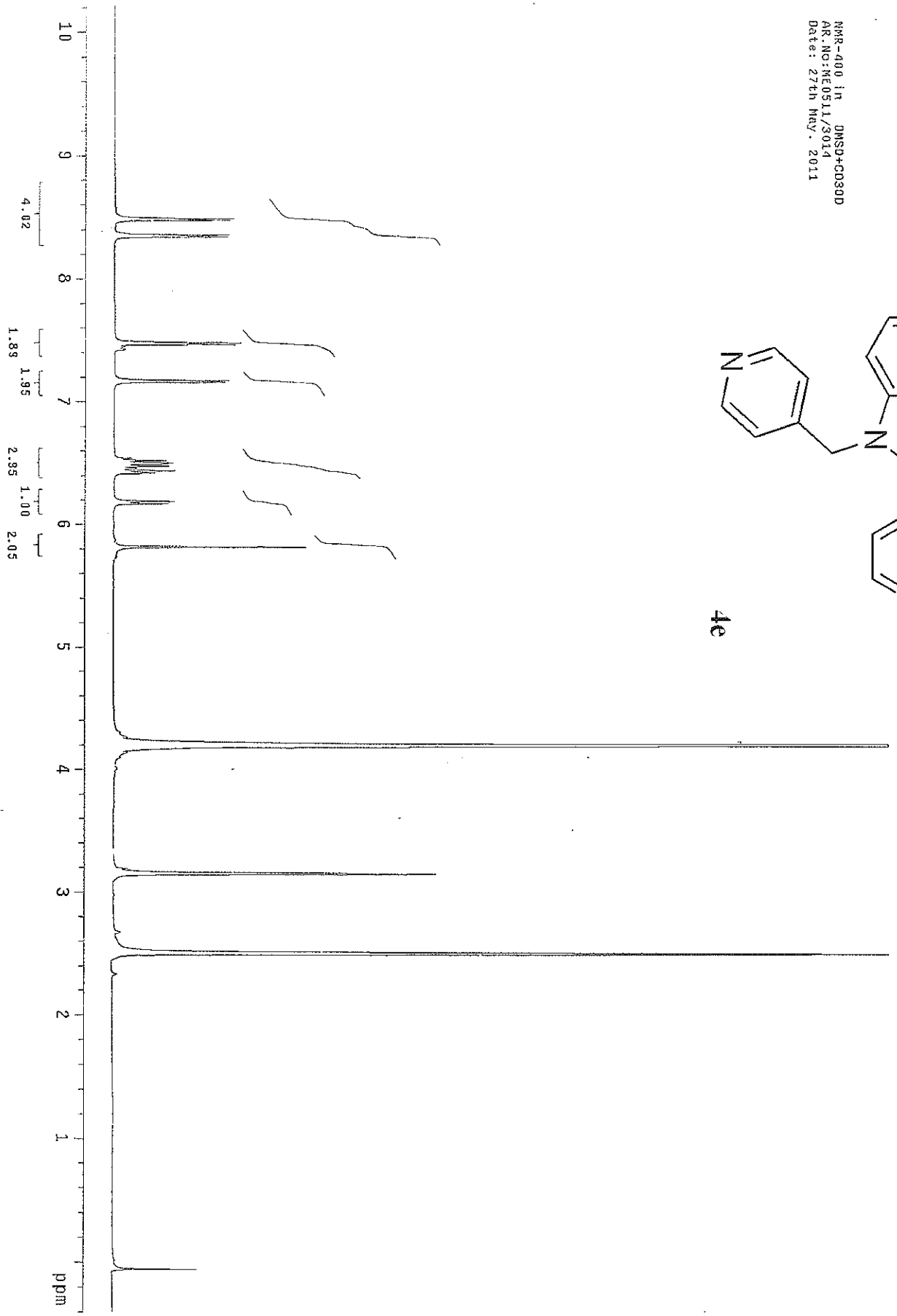
Dr. Reddy's Laboratories Ltd, ARD, TDC-1



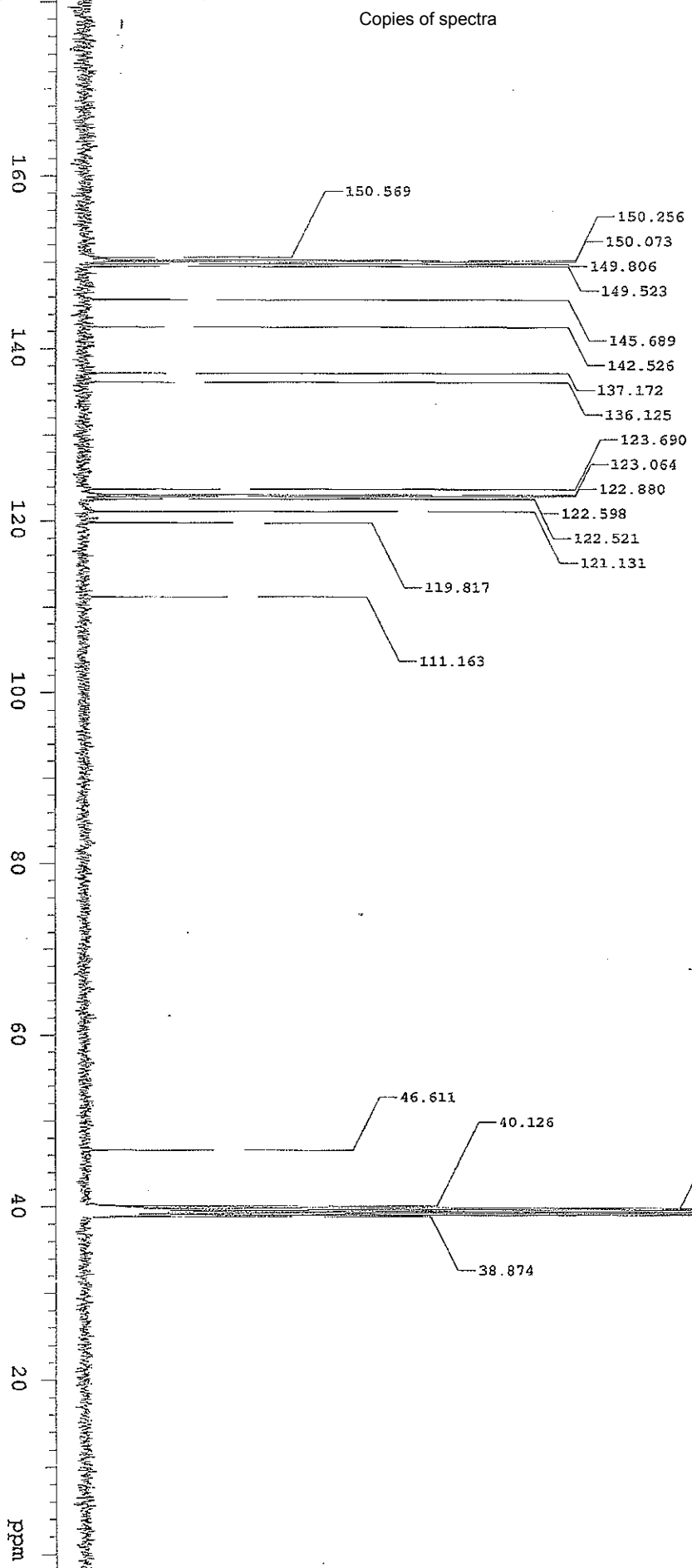
HNMR-400 in DMSO-d6
AK.NC:NE0311/3014
Date: 27th May, 2011



4c



4c
NMR-400MHz in DMSO
AR.No:ME0312/1717
Date: 16th March, 2012



Elemental Composition Report

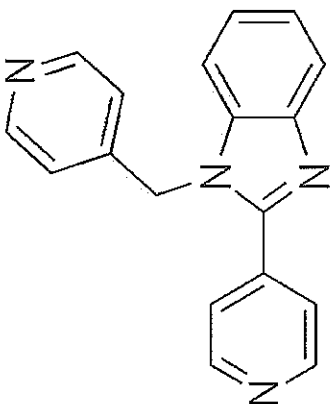
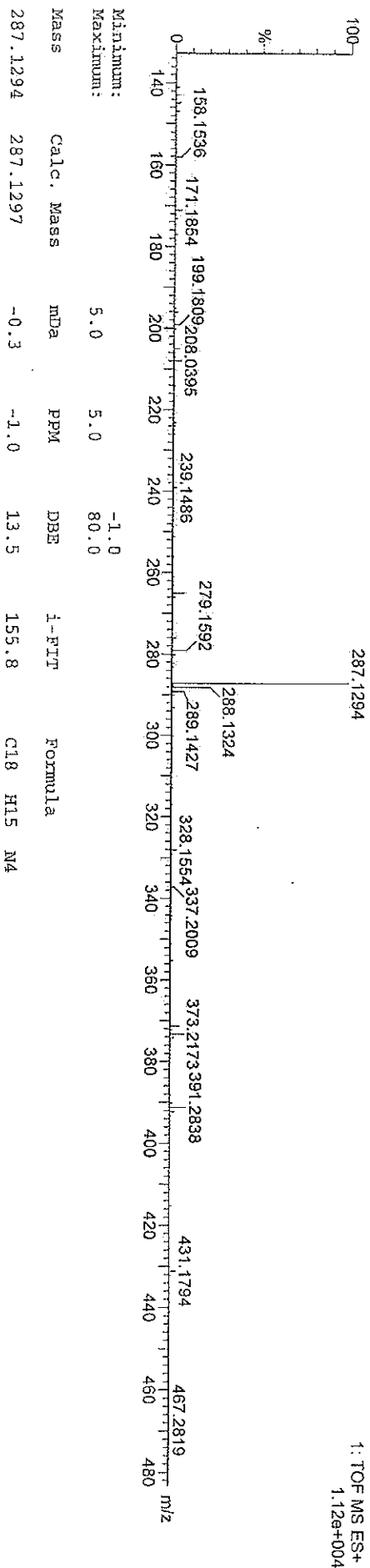
Single Mass Analysis

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
5 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-20 N: 0-4

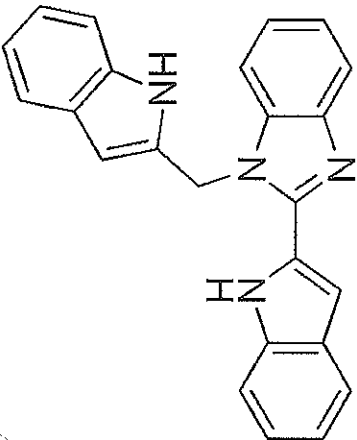
Dr.Reddy's Laboratories Ltd, ARD, TDC-1

UT0312_27 22 (0.414) Cm (22.30)

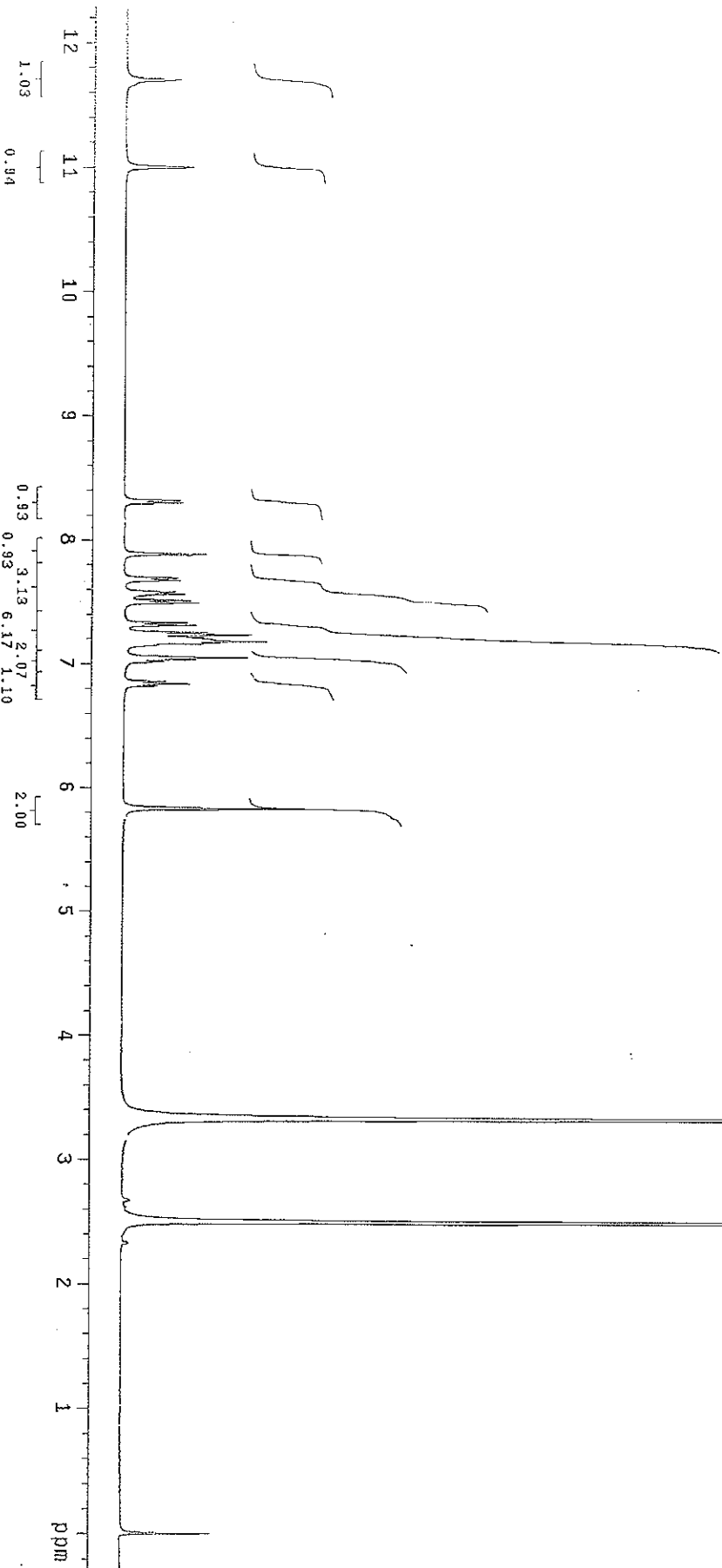


4c

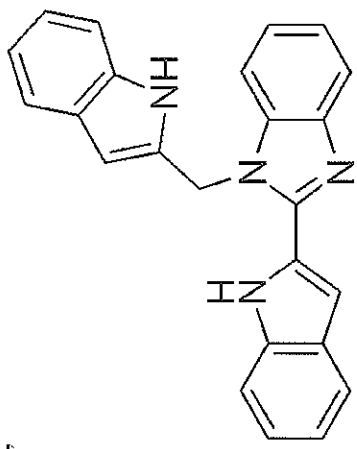
NMR-400 in DMSO
AR.No:HE0511/2992
Date: 27th May, 2011



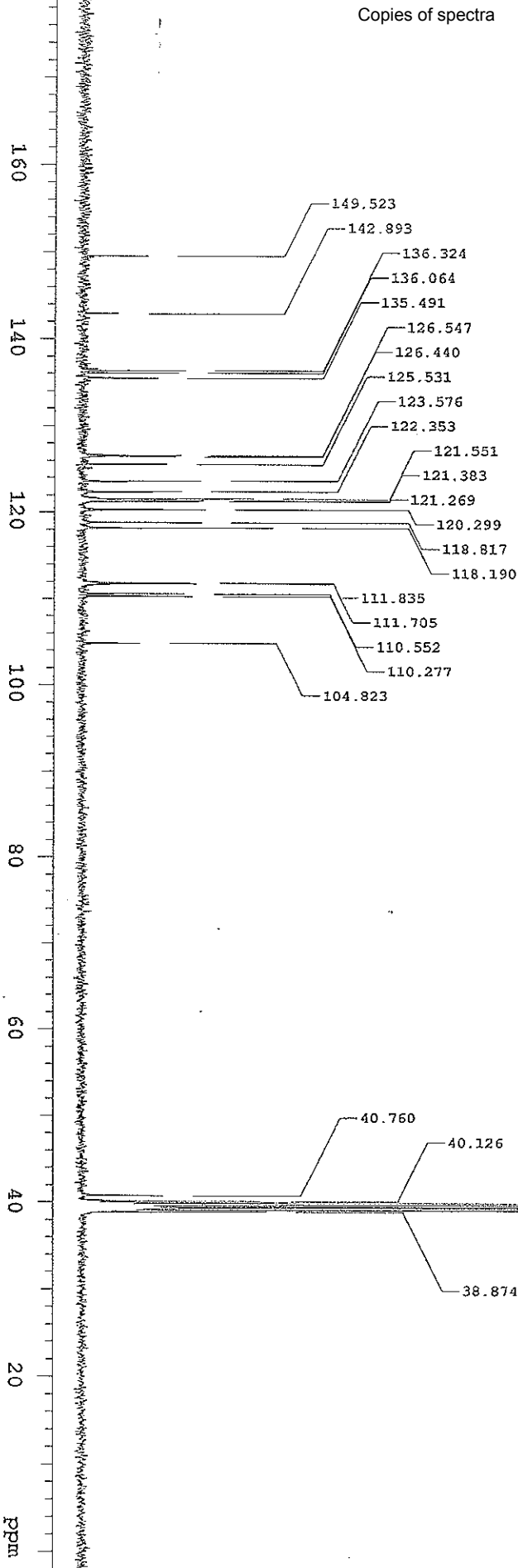
4f



NMR-400MHz in DMSO
AR.No:ME0312/1716
Date: 16th March, 2012



4



Elemental Composition Report

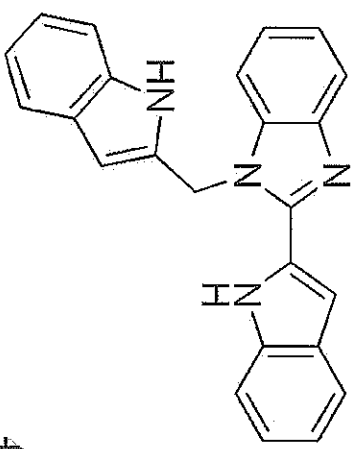
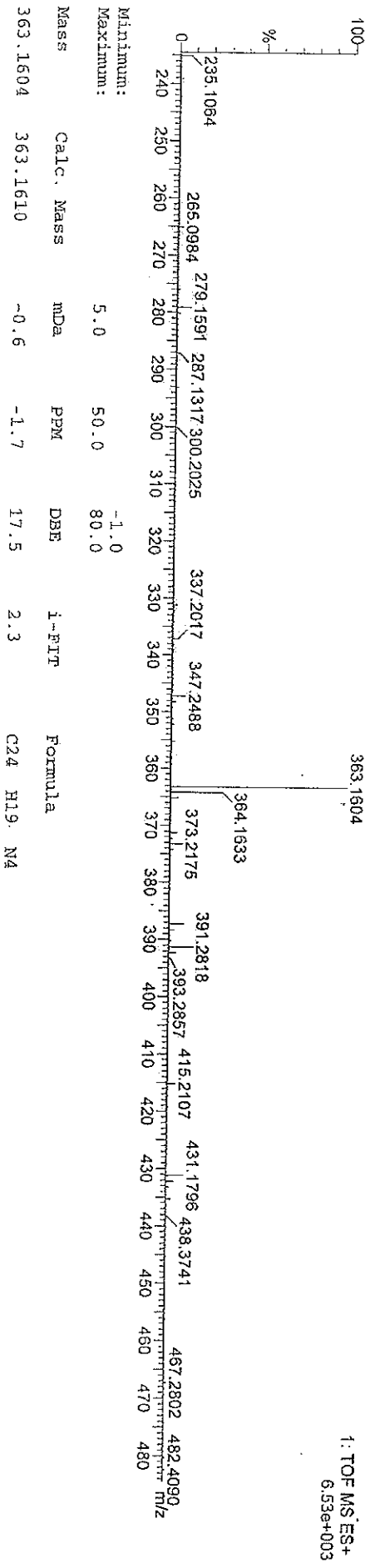
Single Mass Analysis

Tolerance = 50.0 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
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-4

Dr.Reddy's Laboratories Ltd, ARD, TDC-1

UT0312_28 22 (0.413) Cm (22.26)



4f