Electronic Supplementary Information (ESI)

N-heterocyclic carbene-mediated hydroacylation-Sonogashira / Heck / Suzuki coupling in a single pot: A new cascade reaction

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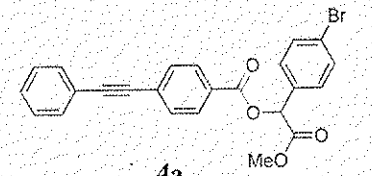
^{1}H and ^{13}C NMR, MS and HRMS data

TDC-213 BINASI in DMSO

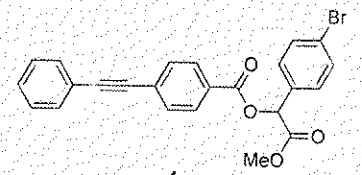
NMR-400
AR.No:ME1119/1987
Analyst:Haribabu.R
Date: 26 th Nov 2010



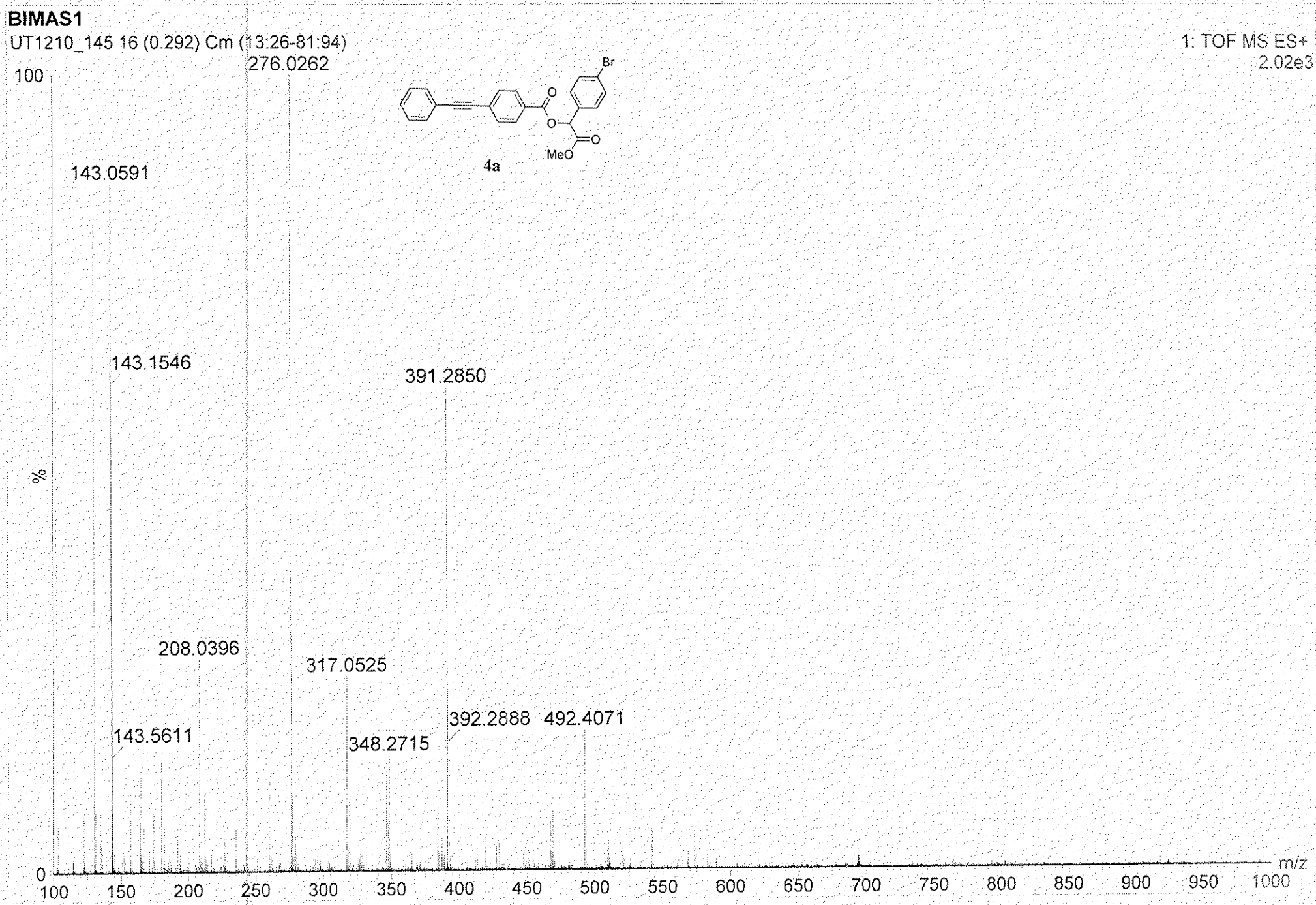
4a

TOC-213 BIMAS1 in DMSO

NMR-400
AR.No:ME1210/1671
Analyst:Haribabu.R
Date: 17 th Dec. 2010



4a



Elemental Composition Report

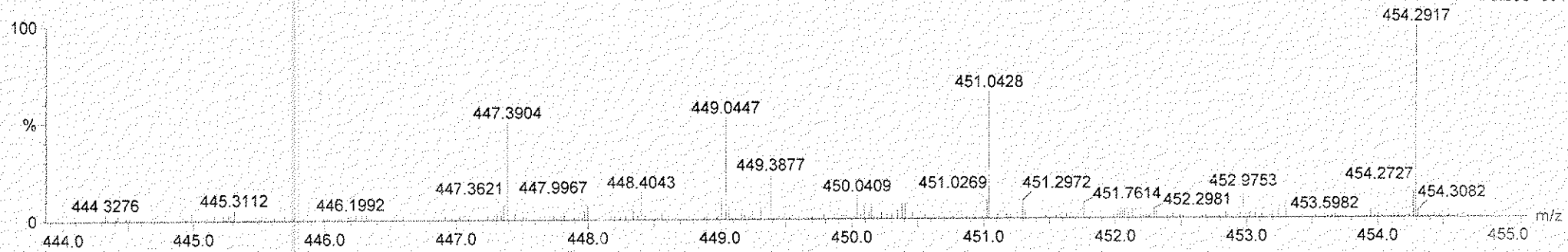
Single Mass Analysis

Tolerance = 20.0 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
58 formula(e) evaluated with 3 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-50 H: 0-60 O: 0-5 Br: 0-1

BIMAS1
UT1210_145 16 (0.292) Cm (13:26-81:94)

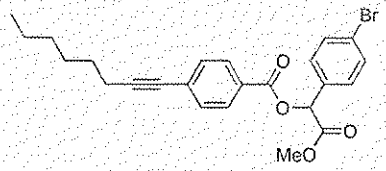
1: TOF MS ES+
9.25e+001



Minimum:				-1.0		
Maximum:		5.0	20.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
449.0447	449.0388	5.9	13.1	15.5	1.1	C24 H18 O4 Br
	449.0450	-0.3	-0.7	26.5	28.5	C30 H9 O5
	449.0391	5.6	12.5	35.5	29.3	C37 H5

TDC-213 BIMAS2 in DMSO

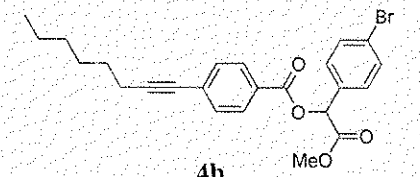
NMR-400
AR.No:ME1210/1236
Analyst:Haribabu.R
Date: 13 th Dec. 2010



4b

TDC-213 BIMAS2 in DMSO

NMR-400
AR.No:ME1210/1672
Analyst:Haribabu.R
Date: 17 th Dec. 2010



4b

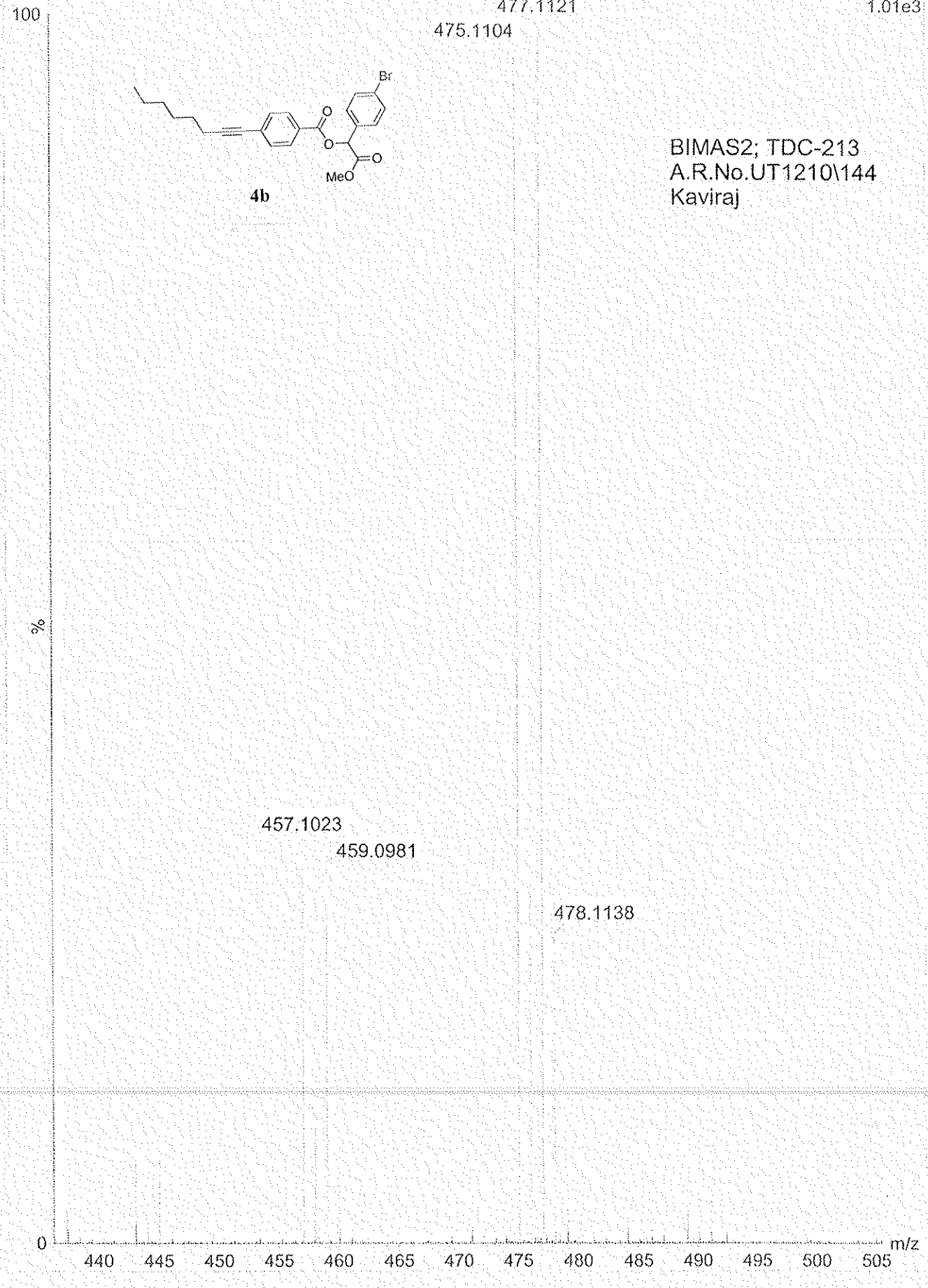
BIMAS2

UT1210_144 20 (0.367) Cm (20:23-83:88)

23/12/10

1: TOF MS ES+

1.01e3



BIMAS2; TDC-213
A.R.No.UT1210\144
Kaviraj

13/12/10

Elemental Composition Report

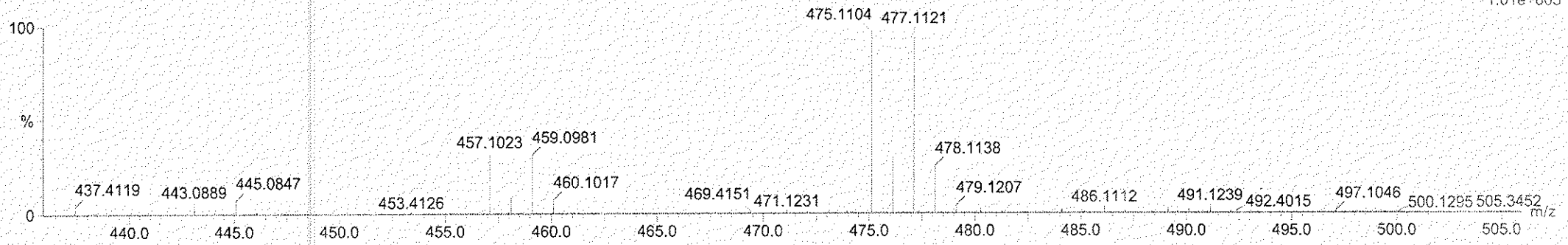
Single Mass Analysis

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
81 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 O: 0-8 Br: 0-1

BIMAS2
UT1210_144 20 (0.367) Cm (20:23-83:88)

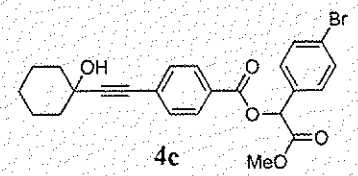
1: TOF MS ES+
1.01e+003



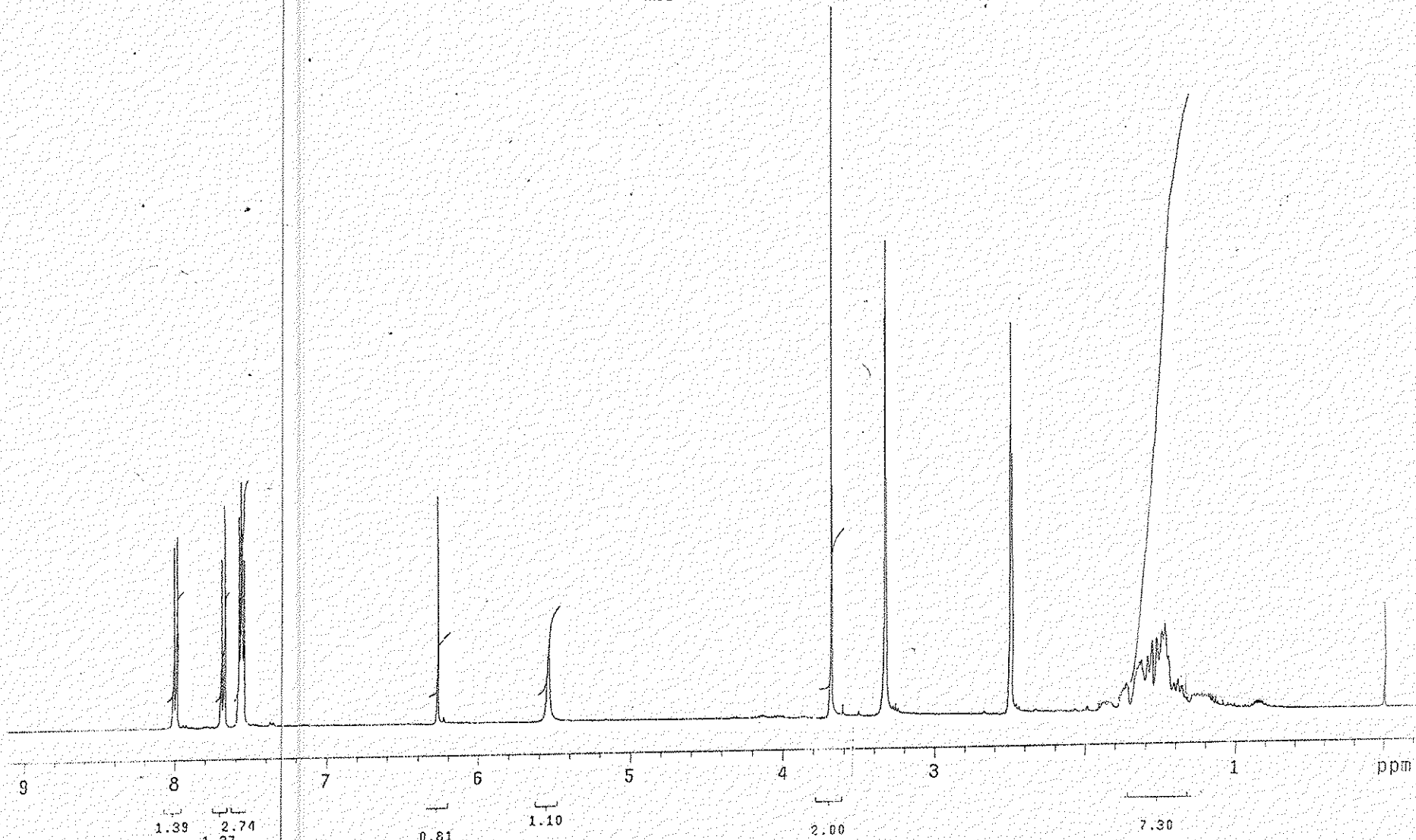
Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
457.1023	457.1014	0.9	2.0	11.5	1.3	C24 H26 O4 Br
	457.1017	0.6	1.3	31.5	136.8	C37 H13

TDC-213 BIMAS3 in DMSO

NMR-400
AR.No:ME1210/678
Analyst:Haribabu.R
Date: 8 th Dec. 201

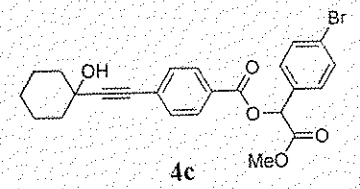


4c



TDC-213 BIMAS3 in DMSO

NMR-400
AR.No:ME1210/1673
Analyst:Haribabu.R
Date: 17 th Dec. 2010



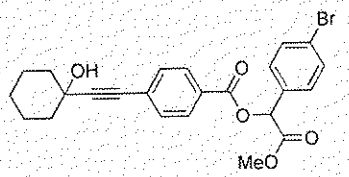
4c

BIMAS3

UT1210_143 17 (0.325) Cm (17:23-86:95)

13/12/10

1: TOF MS ES+
1.79e3



4c

BIMAS3; TDC-213
A.R.No.UT1210\143
Kaviraj

Elemental Composition Report

13/12/10

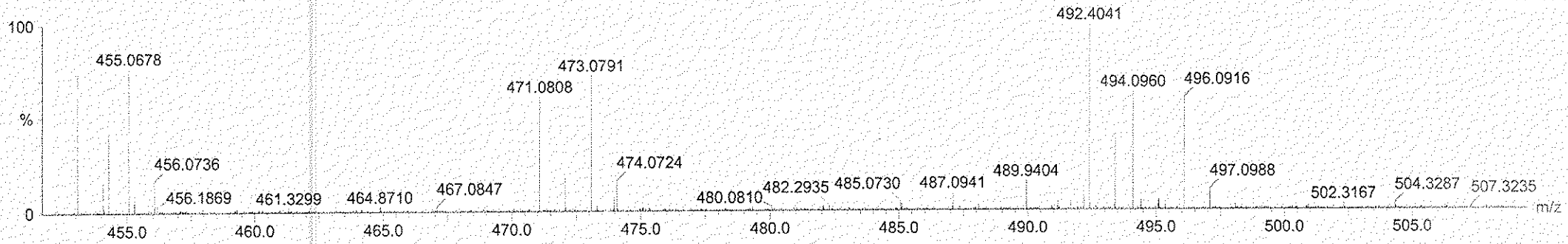
Single Mass Analysis

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
85 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 O: 0-8 Br: 0-1

BIMAS3
UT1210_143 17 (0.325) Cm (17:23-86:95)

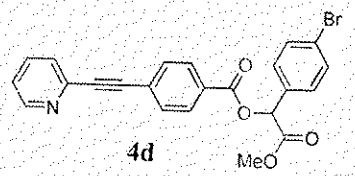
1: TOF MS ES+
3.43e+002



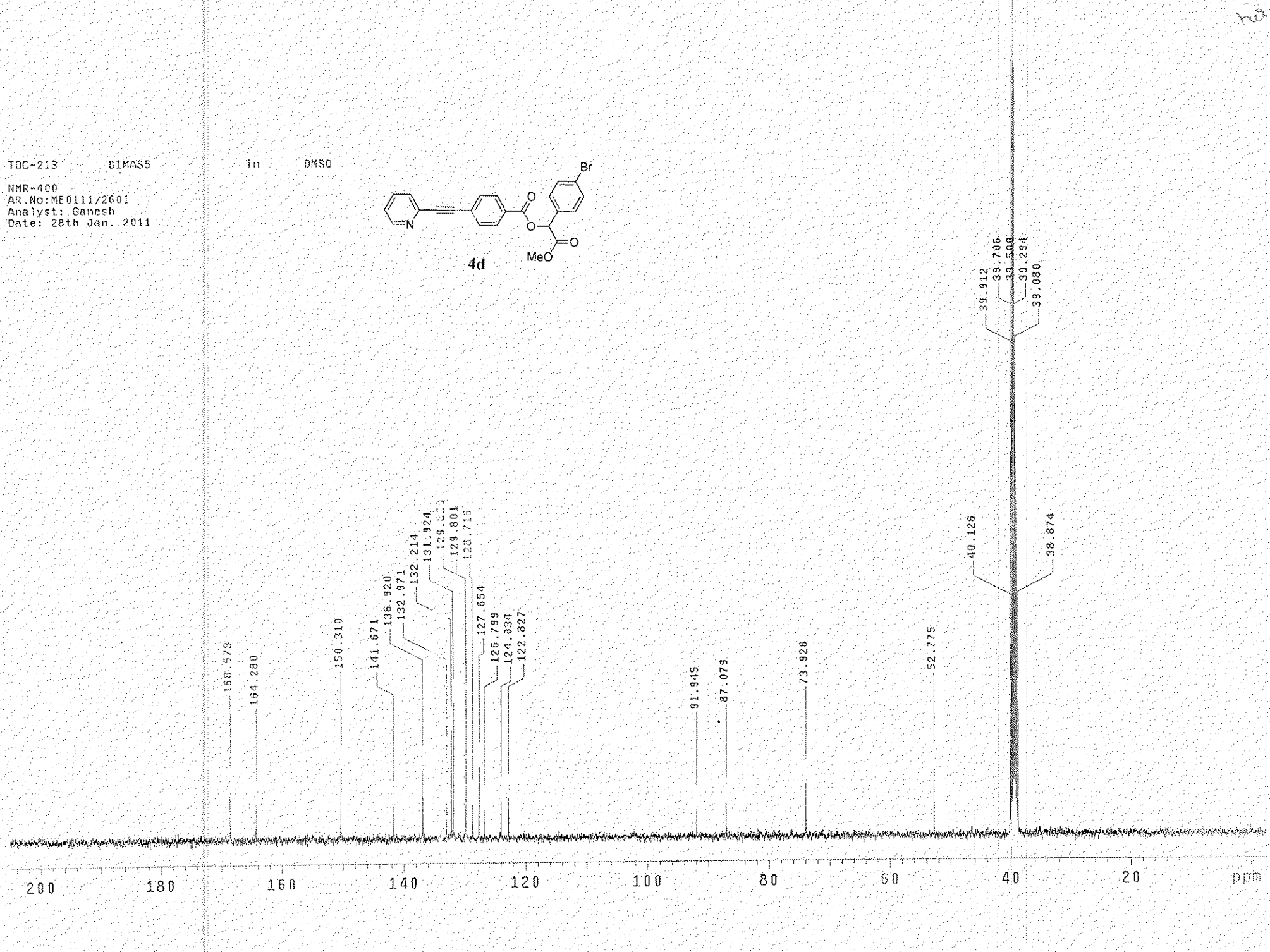
Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
471.0808	471.0807	0.1	0.2	12.5	1.3	C24 H24 O5 Br
	471.0810	-0.2	-0.4	32.5	113.3	C37 H11 O

TDC-213 ABIMAS5 in DMSO

NMR-400
AR.No:ME0111/1093
Analyst:Haribabu.R
Date: 12 th Jan. 2011



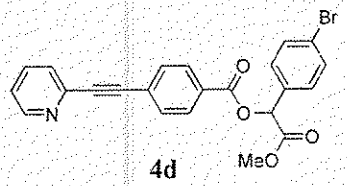
4d



BIMAS5

UT0111_197 44 (0.815) Cm (44:52-82:103)

1: TOF MS ES+
3.10e4



4d

BIMAS5 TDC-213
A.R.No.UT0111\196
Kaviraj

28/01/11

Elemental Composition Report

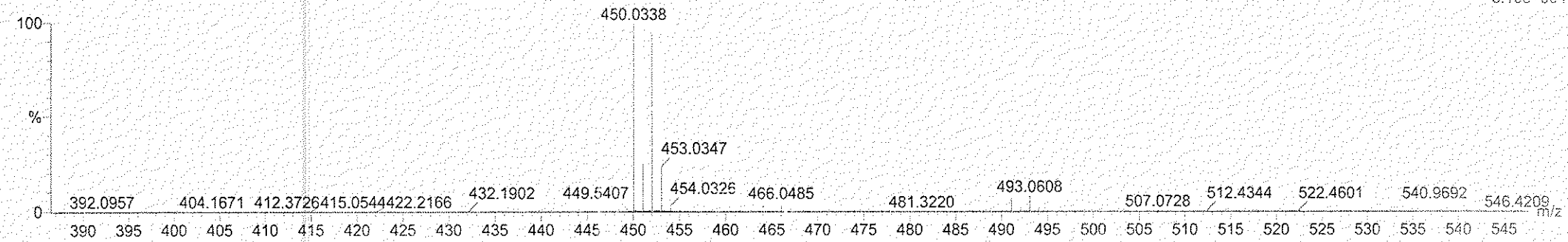
Single Mass Analysis

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
236 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-30 N: 0-4 O: 0-8 Br: 0-1

BIMAS5
UT0111_197 44 (0.815) Cm (44:52-82:103)

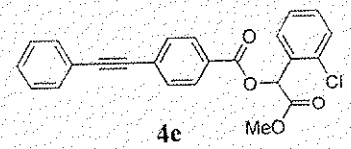
1: TOF MS ES+
3.10e+004



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
450.0338	450.0341	-0.3	-0.7	15.5	27.5	C23 H17 N O4 Br

TDC-213 BAS1 in DMSO

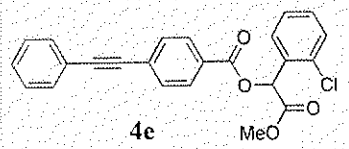
NMR-400
AR.No:ME0910/1539
Analyst:Haribabu.R
Date:27th Sept 2010



4e

BAS1 in DMSO
TDC-213

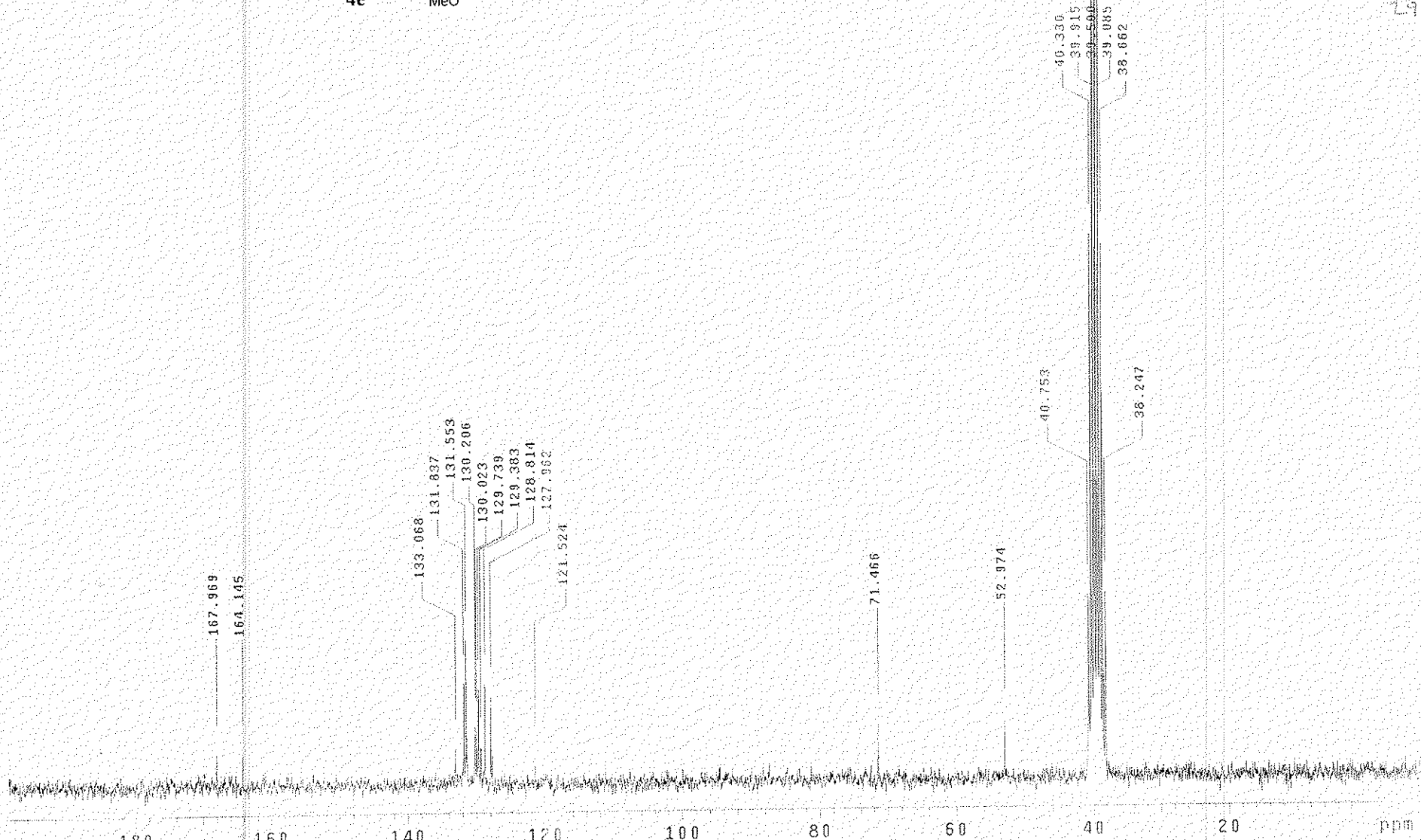
AR NO:GE0910/50
Analyst:Haribabu.R
Date: 29th Sept.2010



4e

AR&D, Aurigene Discovery Technologies ltd, Hydera
Instrument : Gemini 2000 (Varian 200MHz)
Date & Time : Wed Sep 29 19:37:45 GMT 2010
Recorded By : Haribabu.R

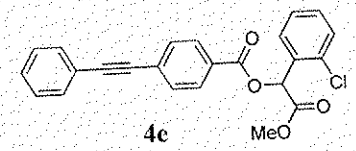
h
2/9



E 29/10/10

BAS1
UT1010_198 7 (0.131) Cm (5:20-81:92)

1: TOF MS ES+
1.32e3



4c

29/10/10

Elemental Composition Report

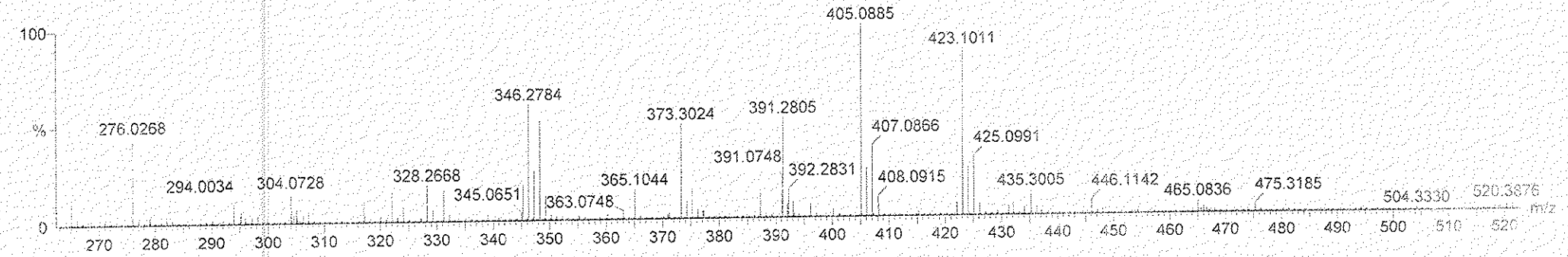
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
120 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-1 O: 0-5 Cl: 0-1

BAS1
UT1010_198 7 (0.131) Cm (5:20-81:92)

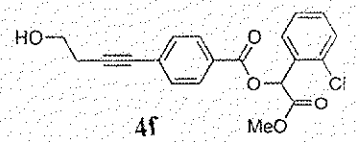
1: TOF MS ES+
1.32e+003



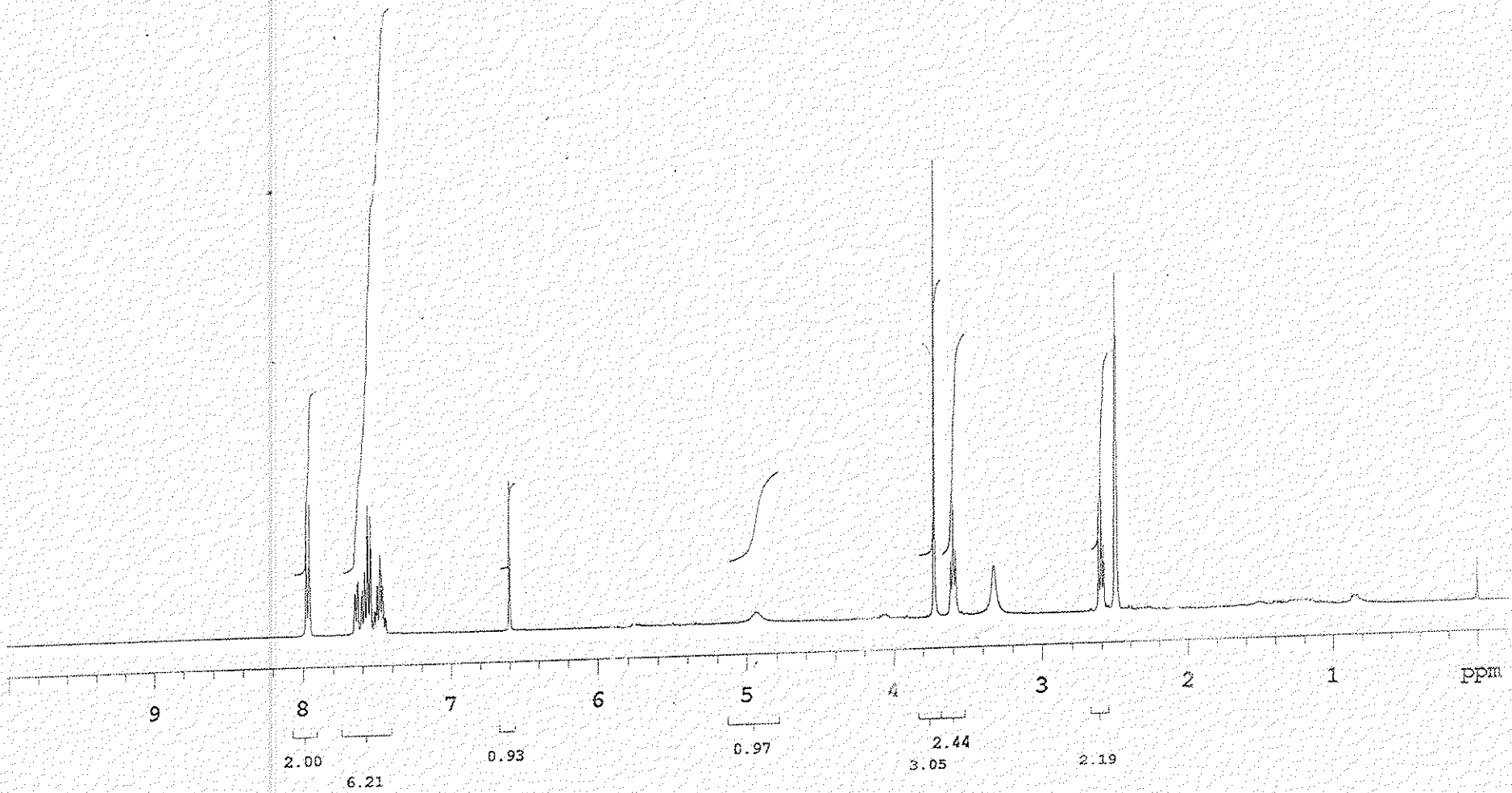
Minimum:		5.0	5.0	-1.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
405.0885	405.0894	-0.9	-2.2	15.5	1.3	C24 H18 O4 Cl

SDC-213 BAS2 in DMSO

NMR-400
AR.No:ME1010/209
Analyst:Haribabu.R
Date: 04 th Oct 2010

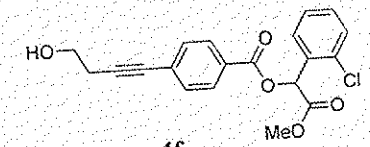


4f



TDC-213 BDS2 in DMSO

NMR-400
AR.No:ME1010/770
Analyst:Haribabu.R
Date: 8th Oct 2010

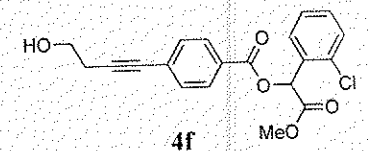


4f

BAS2
UT1010_199 8 (0.145) Cm (8:28-79:100)

29/10/10

1: TOF MS ES+
6.25e3



4f

CNYL BAS2 TDC-213
A.R.No.UT1010\199
Kaviraj

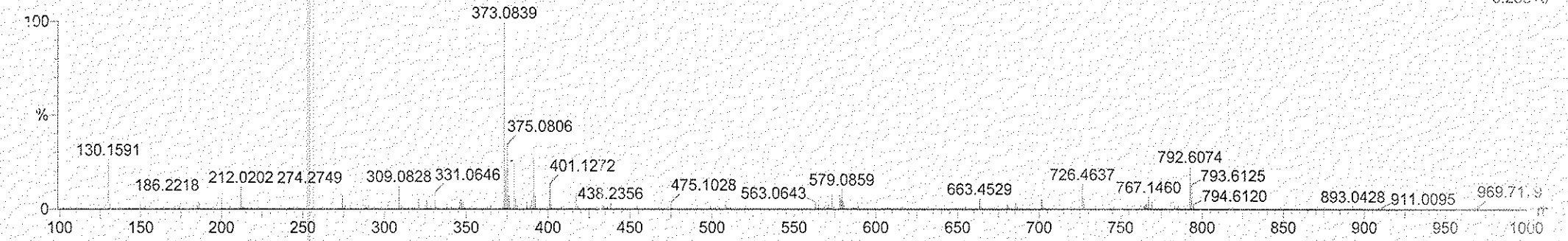
Elemental Composition Report

29/10/10

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
80 formula(e) evaluated with 1 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 O: 0-5 Cl: 0-2
BAS2
UT1010_199 8 (0.145) Cm (8:28-79:100)

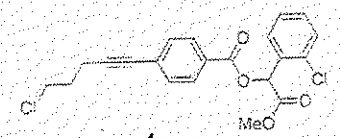
1: TOF MS ES+
6.25e+07



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
373.0839	373.0843	-0.4	-1.1	11.5	3.6	C20 H18 O5 Cl

TDC-213 SAS3 in DMSO

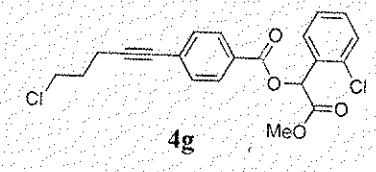
BKR-400
AR.No:MS1010/722
Analyst:Haribabu.R
Date: 8th Oct 2010



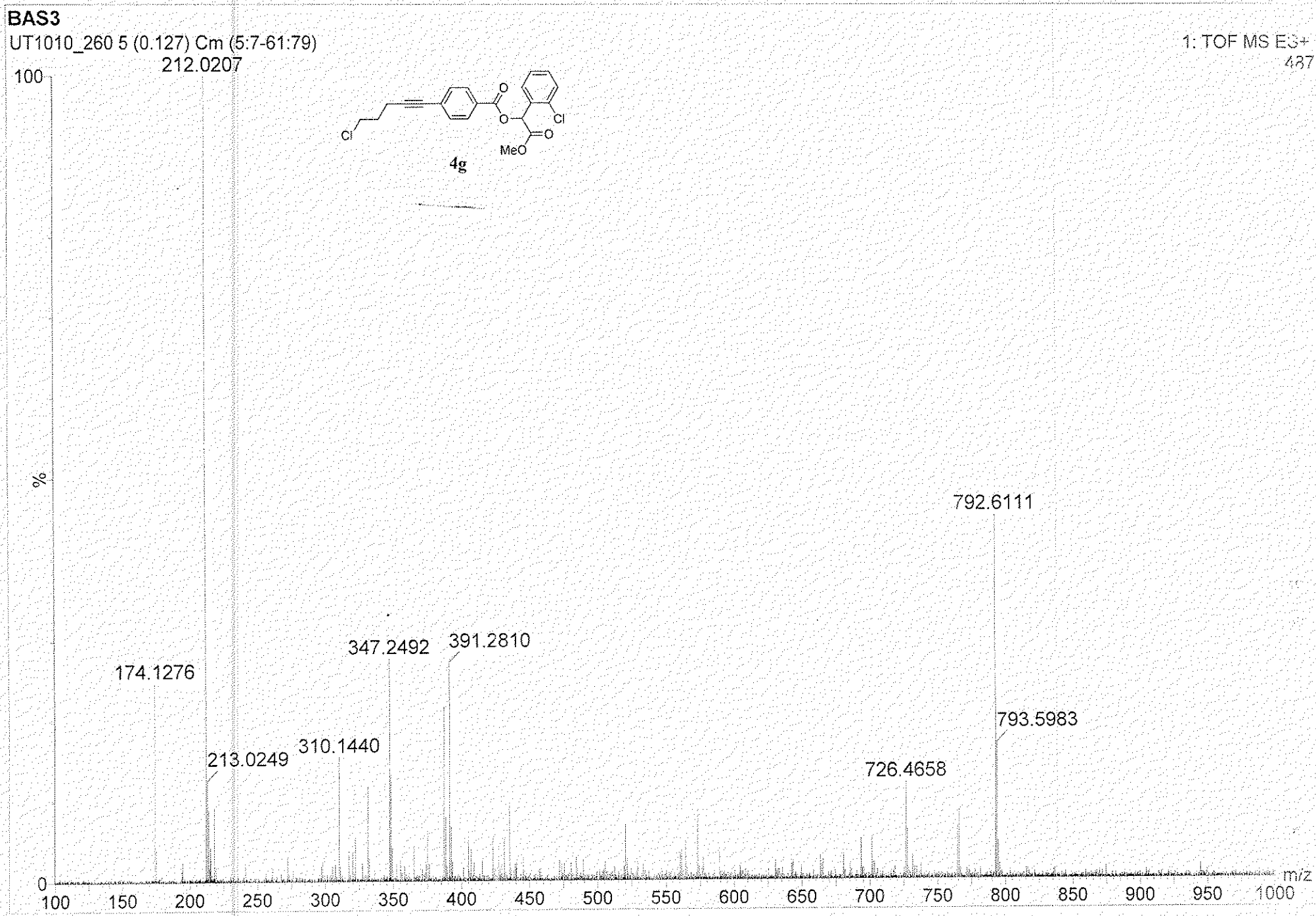
4g

TDC-213 BAS3 in DMSO

NMR-400
AR.No:ME1010/1048
Analyst:Shruthi
Date:12th Oct 2010



4g



4g

Elemental Composition Report

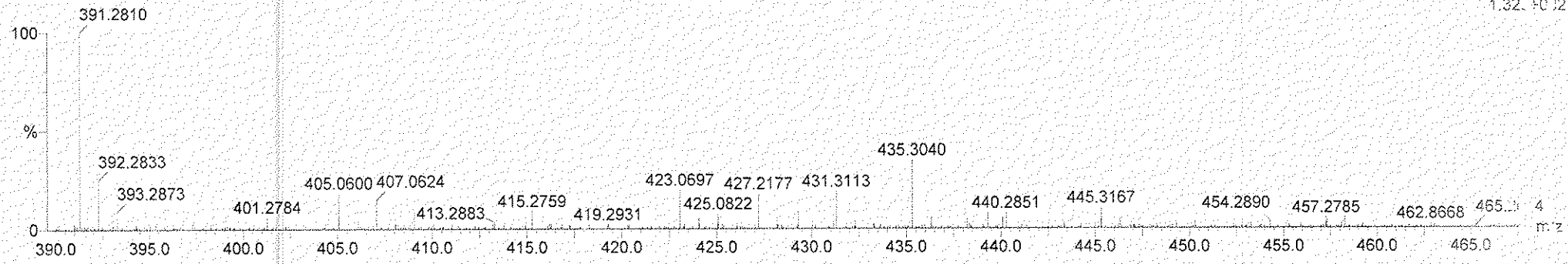
Single Mass Analysis

Tolerance = 20.0 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
78 formula(e) evaluated with 4 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-35 O: 0-8 Cl: 0-2

BAS3
UT1010_260 5 (0.127) Cm (5:7-61:79)

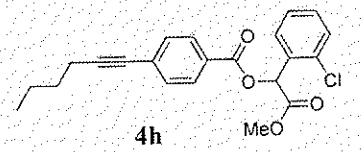
1: TOF MS ES+
1.32e+02



Minimum:				-1.0		
Maximum:		5.0	20.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
405.0600	405.0660	-6.0	-14.8	11.5	0.3	C21 H19 O4 Cl2
	405.0530	7.0	17.3	16.5	21.3	C23 H14 O5 Cl
	405.0610	-1.0	-2.5	16.5	21.4	C22 H13 O8
	405.0552	4.8	11.9	25.5	21.5	C29 H9 O3

TDC-213 BAS4 in DMSO

NMR-400
AR.No:ME1010/2365
Analyst:Shruthi
Date: 28 th Oct 2010



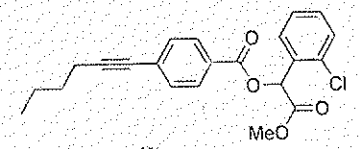
4h

TDC-213 BAS4 in DMSO

NMR-400
AR.No:ME1110/772
Analyst:Haribabu.R
Date: 12 th Nov 2010

Sample Name:
772-TDC-213_BAS4
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_12
Sample directory:
772-TDC-213_BAS4_20101113_01
FidFile: 772-TDC-213_BAS4_20101113_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 13 2010



4h

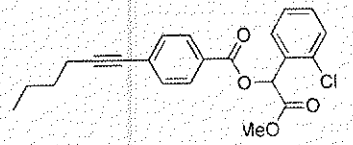
Plotname: 772-TDC-213_BAS4_20101113_01_plot01

BAS4

UT1010_200 7 (0.131) Cm (6:20-81:90)

29/10/10

1: TOF MS ES+
4.65e4



4h

CNYL BAS4 TDC-213
A.R.No.UT1010\200
Kaviraj

Elemental Composition Report

29/10/10

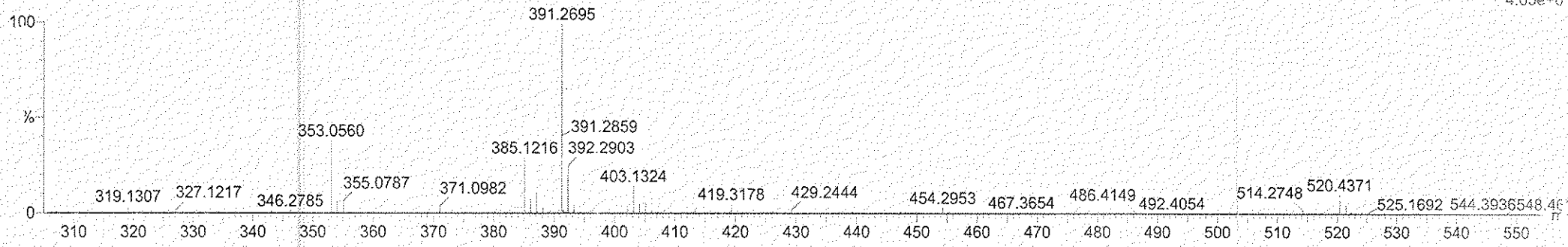
Single Mass Analysis

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
82 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 O: 0-5 Cl: 0-2

BAS4
UT1010_200 7 (0.131) Cm (6:20-81:90)

1: TOF MS ES
4.65e+0

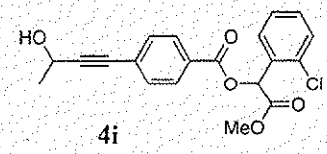


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.1216	385.1207	0.9	2.3	11.5	2.8	C22 H22 O4 Cl
	385.1229	-1.3	-3.4	20.5	1946.4	C28 H17 O2

TDC-213-A586-BAS-005 in DMSO

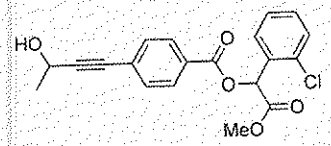
NMR-400
AR.No:ME1010/530
Analyst:Shruthi
Date: 7th Oct 2010



4i

BASS in CD3OD
TDC-213

AR NO:CE1010/64
Analyst:Haribabu.R
Date: 25 th Oct 2010



4i

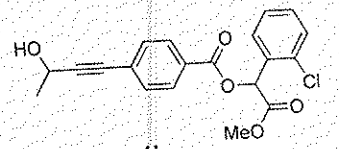
AR&D, Suriqeno Discovery Technologies Ltd, Hydera
Instrument : Gemini 2000 (Varian 200MHz)
Date & Time : Wed Oct 27 19:04:05 GMT 2010
Recorded By : Haribabu.R

BAS5

UT1010_201 7 (0.131) Cm (7:10-73:84)

29/10/10

1: TOF MS ES+
2.97e3



4i

CNYL BAS5 TDC-213
A.R.No.UT1010\201
Kaviraj

29/10/10

Elemental Composition Report

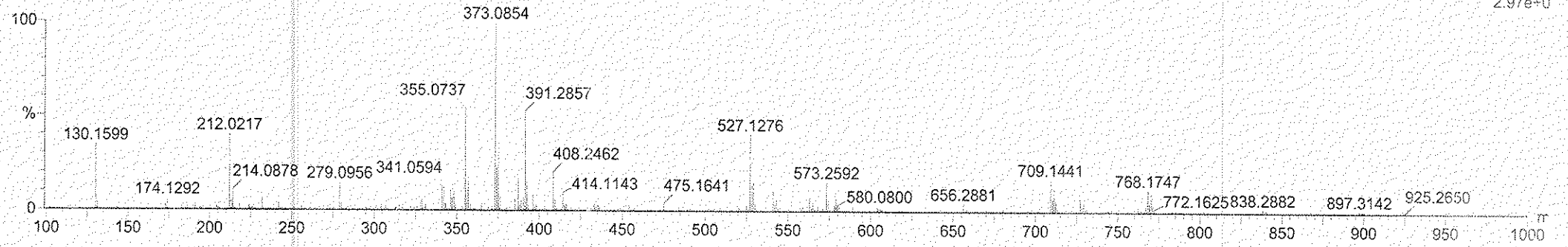
Single Mass Analysis

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

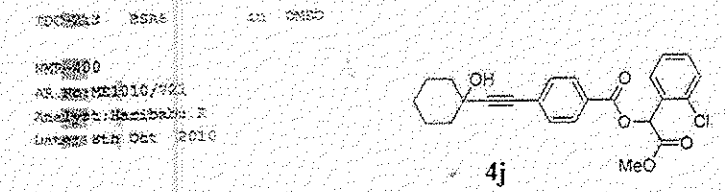
Monoisotopic Mass, Even Electron Ions
92 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 O: 0-6 Cl: 0-2

B\S5
UT1010_201 7 (0.131) Cm (7:10-73:84)

1: TOF MS ES
2.97e+0



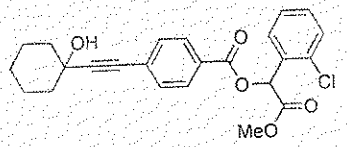
Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
373.0854	373.0843	1.1	2.9	11.5	0.1	C20 H18 O5 Cl
	373.0865	-1.1	-2.9	20.5	430.3	C26 H13 O3



4j

TDC-213 BAS6 in DMSO

NMR-400
AR.No:ME1010/2353
Analyst:Shruthi
Date: 27 th Oct 2010



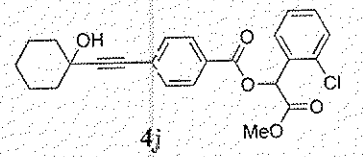
4j

BAS6

UT1010_202 22 (0.413) Cm (22:27-84:92)

29/10/10

1: TOF MS ES+
353



4j

CNYL BAS6 TDC-213
A.R.No.UT1010\202
Kaviraj

Elemental Composition Report

29/10/10

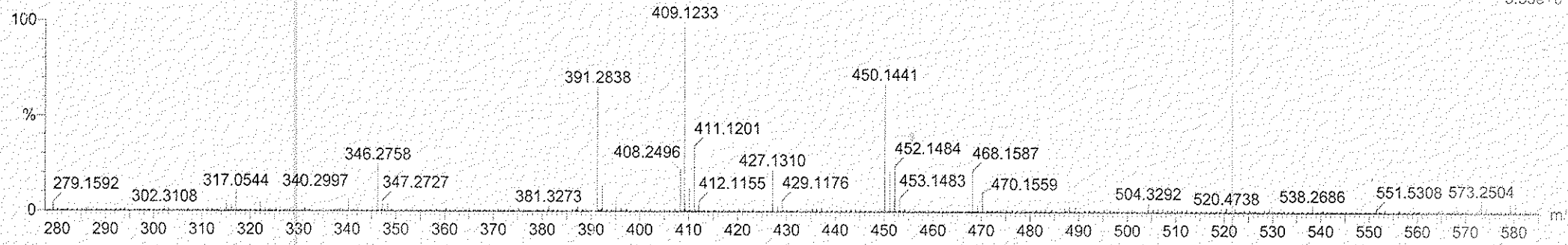
Single Mass Analysis

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

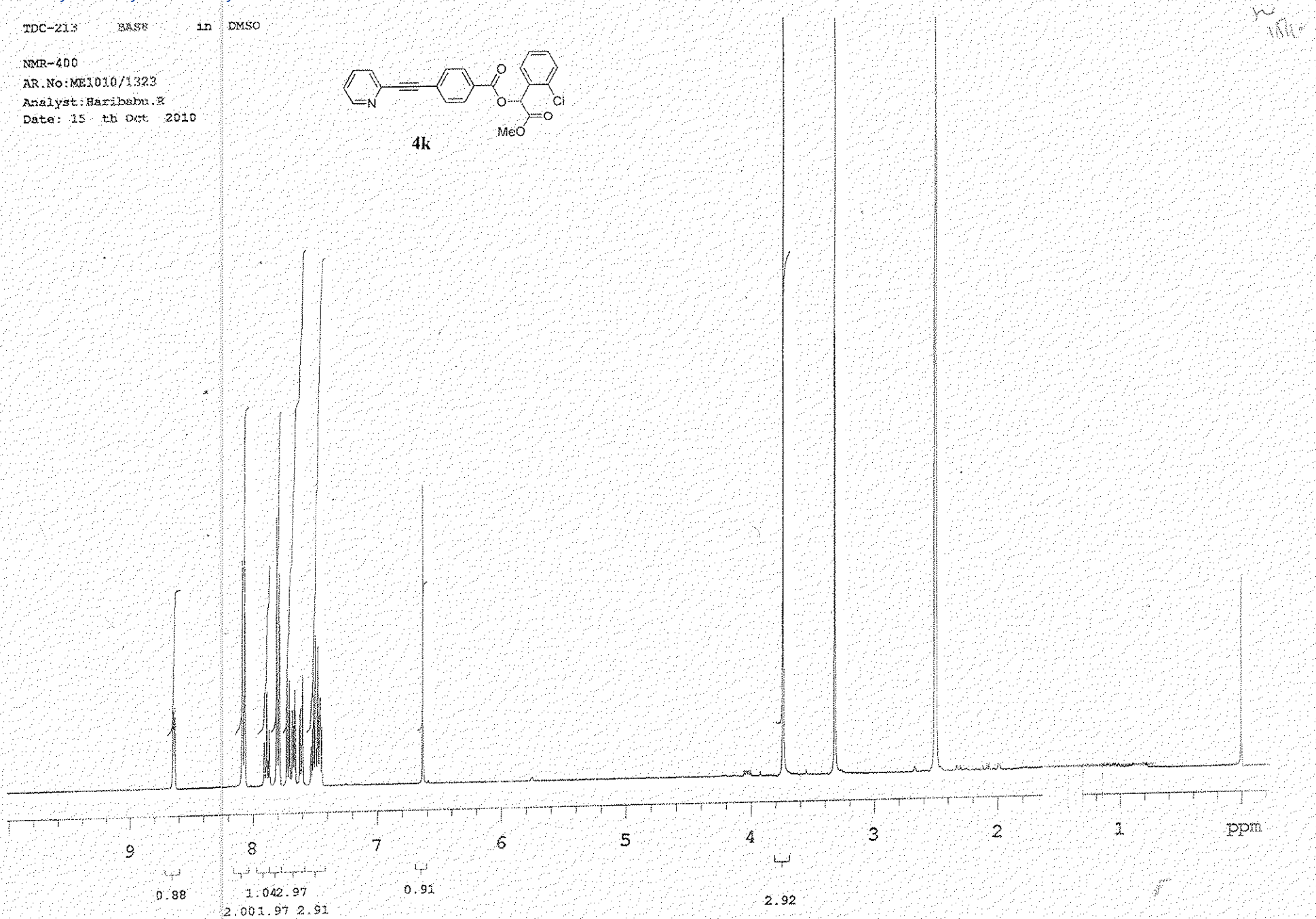
Monoisotopic Mass, Even Electron Ions
105 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 O: 0-6 Cl: 0-2

BAS6
UT1010_202 22 (0.413) Cm (22:27-84:92)

1: TOF MS ES
3.53e+0

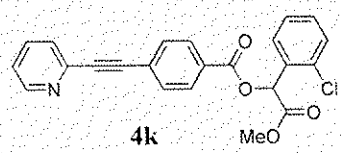


Minimum:				-1.0		
Maximum:		5.0	10.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
427.1310	427.1312	-0.2	-0.5	12.5	10.0	C24 H24 O5 Cl
	427.1334	-2.4	-5.6	21.5	18.9	C30 H19 O3

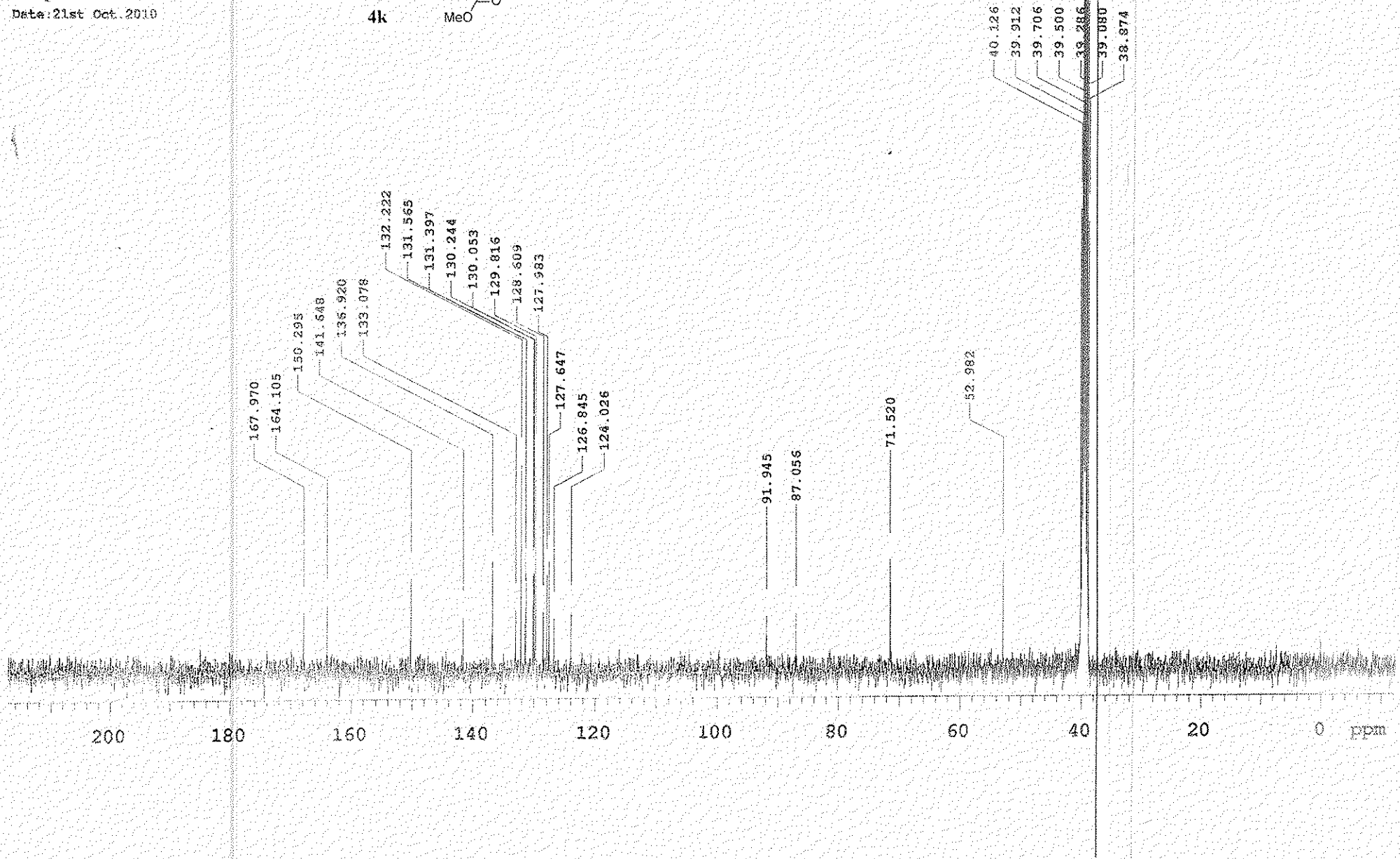


TDC-213 BASE in DMSO

NMR-400
AR.No:ME1010/1835
Analyst:Shruthi
Date:21st Oct.2010



4k

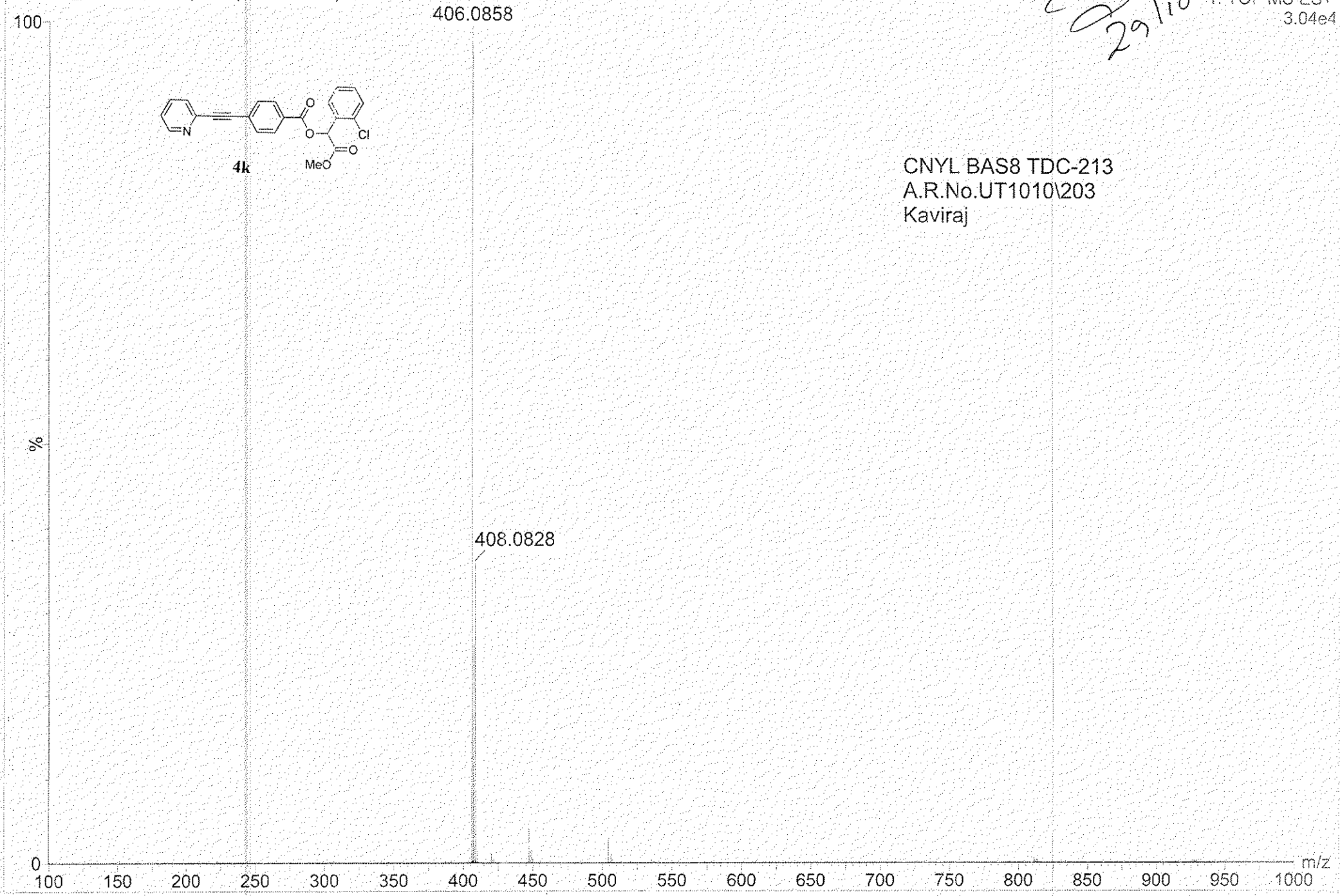


BAS8

UT1010_203 23 (0.427) Cm (22:29-81:92)

29/10/10

1: TOF MS ES+
3.04e4



4k

CNYL BAS8 TDC-213
A.R.No.UT1010\203
Kaviraj

29/10/10

Elemental Composition Report

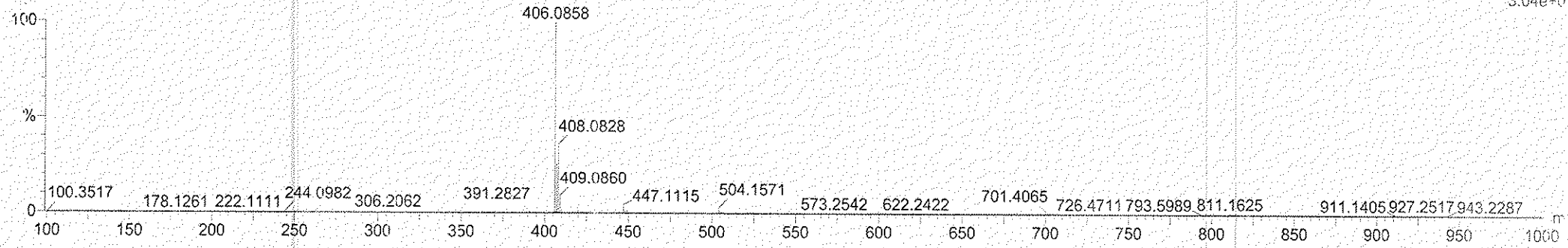
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
269 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 O: 0-6 Cl: 0-1

BAS8
UT1010_203 23 (0.427) Cm (22:29-81:92)

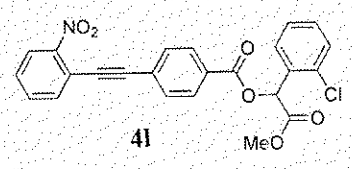
1: TOF MS ES
3.04e+0



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
406.0858	406.0846	1.2	3.0	15.5	1.0	C23 H17 N O4 Cl
	406.0868	-1.0	-2.5	24.5	4185.2	C29 H12 N O2

TDC-Z13 CNYL BASN in DMSO

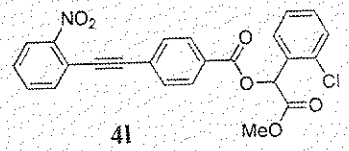
NMR-400
AR.No:ME1010/1556
Analyst:Haribabu.R
Date: 19 th Oct 2010



4l

TDC-213 BASN in DMSO

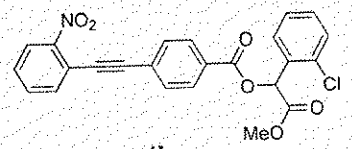
NMR-400
AR.NO:ME1210/1978
Analyst:Haribabu.R
Date: 21st Dec. 2010



41

BASN
UT1010_204 22 (0.413) Cm (21:24-85:92)

1: TOF MS ES+
188



4l

CNYL BASN TDC-213
A.R.No.UT1010\204
Kaviraj

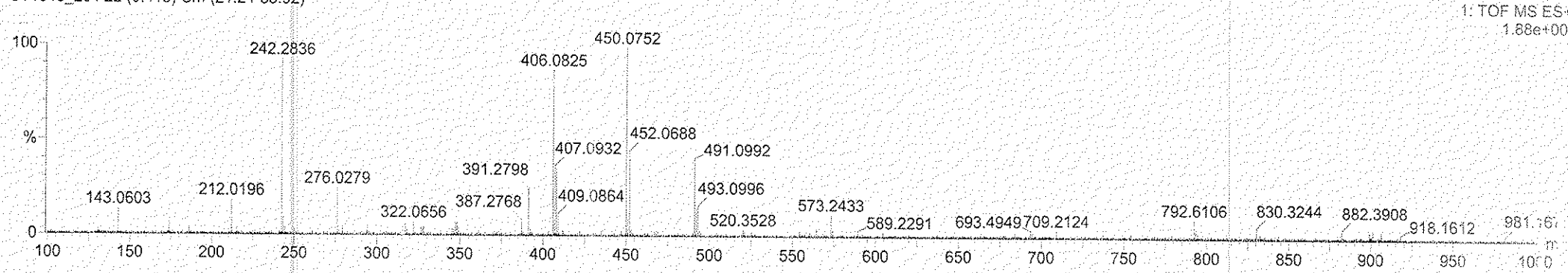
29/10/10

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

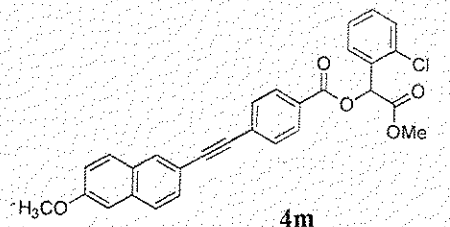
Monoisotopic Mass, Even Electron Ions
300 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 O: 0-6 Cl: 0-1
BASN
UT1010_204 22 (0.413) Cm (21:24-85:92)



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
450.0752	450.0744	0.8	1.8	16.5	25.8	C24 H17 N O6 Cl
	450.0766	-1.4	-3.1	25.5	63.9	C30 H12 N O4

YDC-213 BAST in DMSO

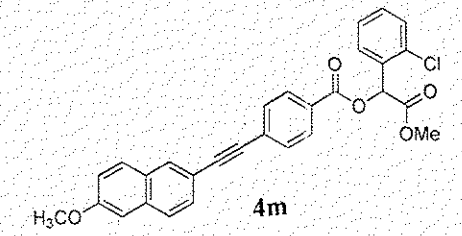
NMR-400
AR.No:ME1010/1877
Analyst:Haribabu.R
Date: 22 nd Oct 2010



4m

TDC-213 BAST in DMSO

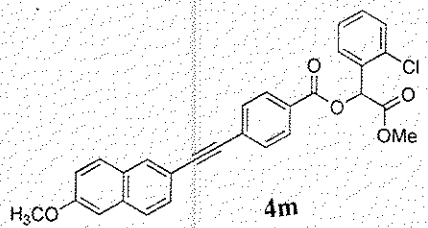
NMR-400
AR.No:ME1010/2352
Analyst:Shruthi
Date: 27 th Oct 2010



4m

BAST
IJT1010_205 17 (0.324) Cm (17:23-78:87)

1: TOF MS ES+
117



4m

CNYL BAST TDC-213
A.R.No.UT1010\205
Kaviraj

Elemental Composition Report

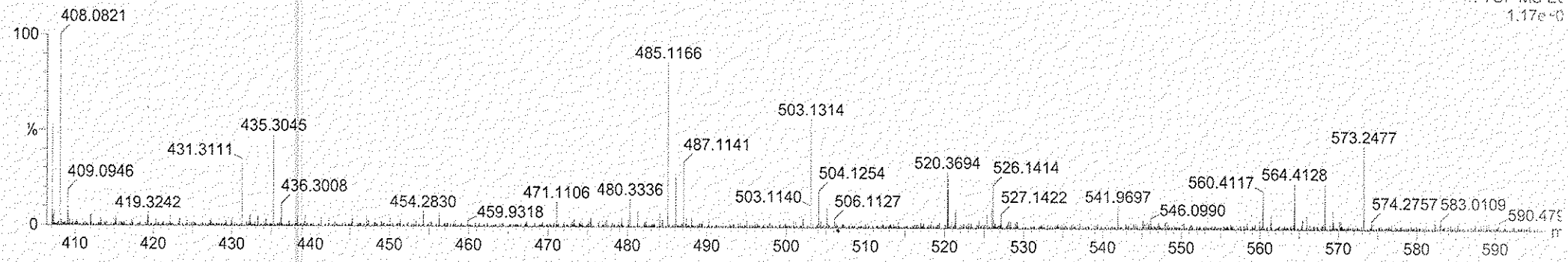
Single Mass Analysis

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
318 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 C: 0-6 Cl: 0-1

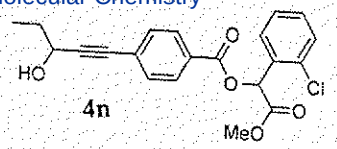
BAST
UT1010_205 17 (0.324) Cm (17:23-78:87)

1: TOF MS ES
1.17e+0

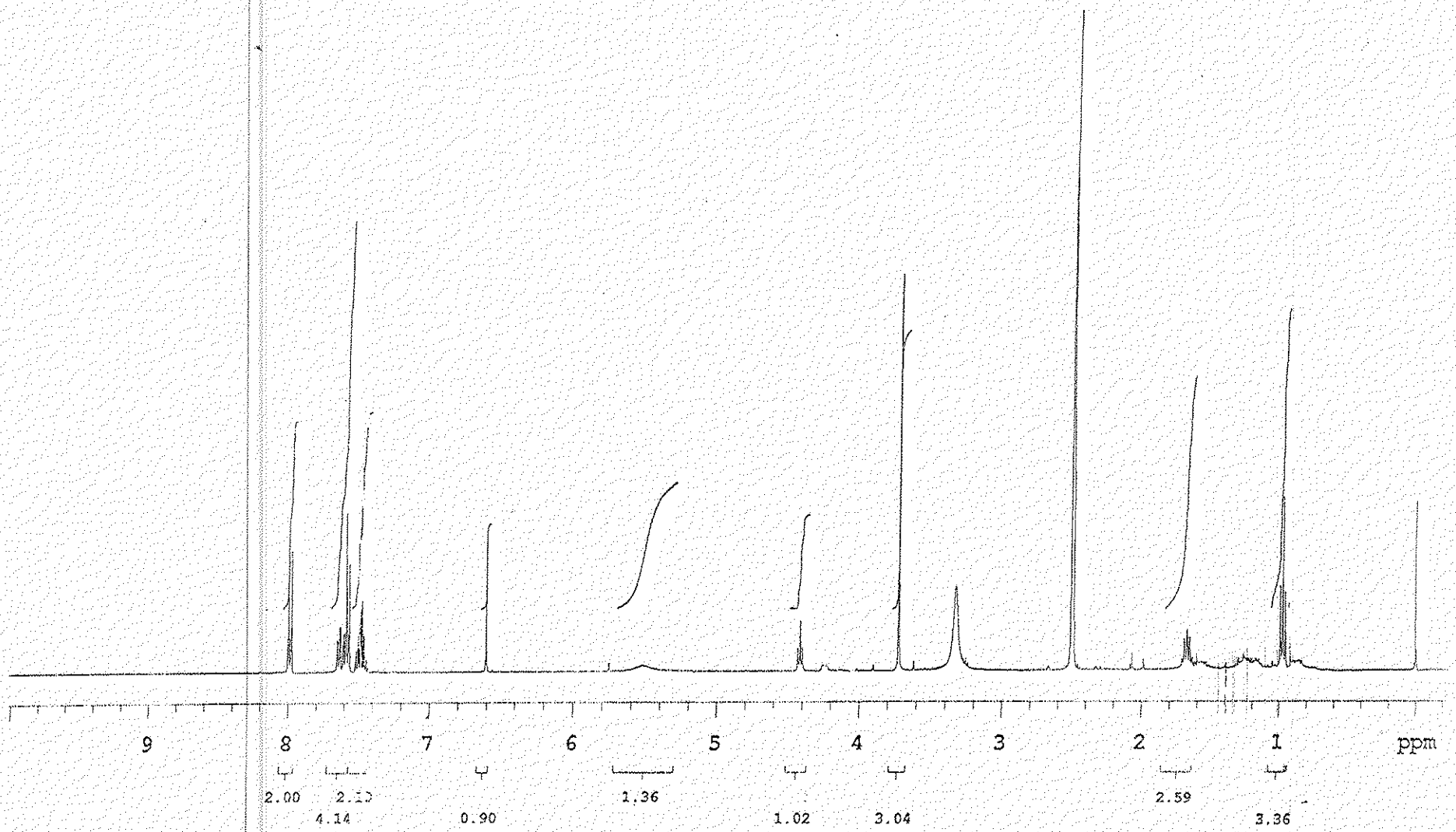


Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
485.1166	485.1156	1.0	2.1	18.5	0.1	C29 H22 O5 Cl
	485.1178	-1.2	-2.5	27.5	13.8	C35 H17 O3

TRC-218 BASF 14 CDCl3
NMR-400
AR.No:ME1010/1945
Analyst:Haribabu.R
Date: 22 th Oct 2010

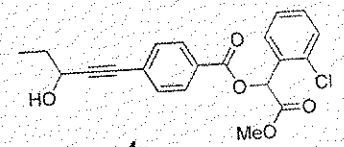


4n

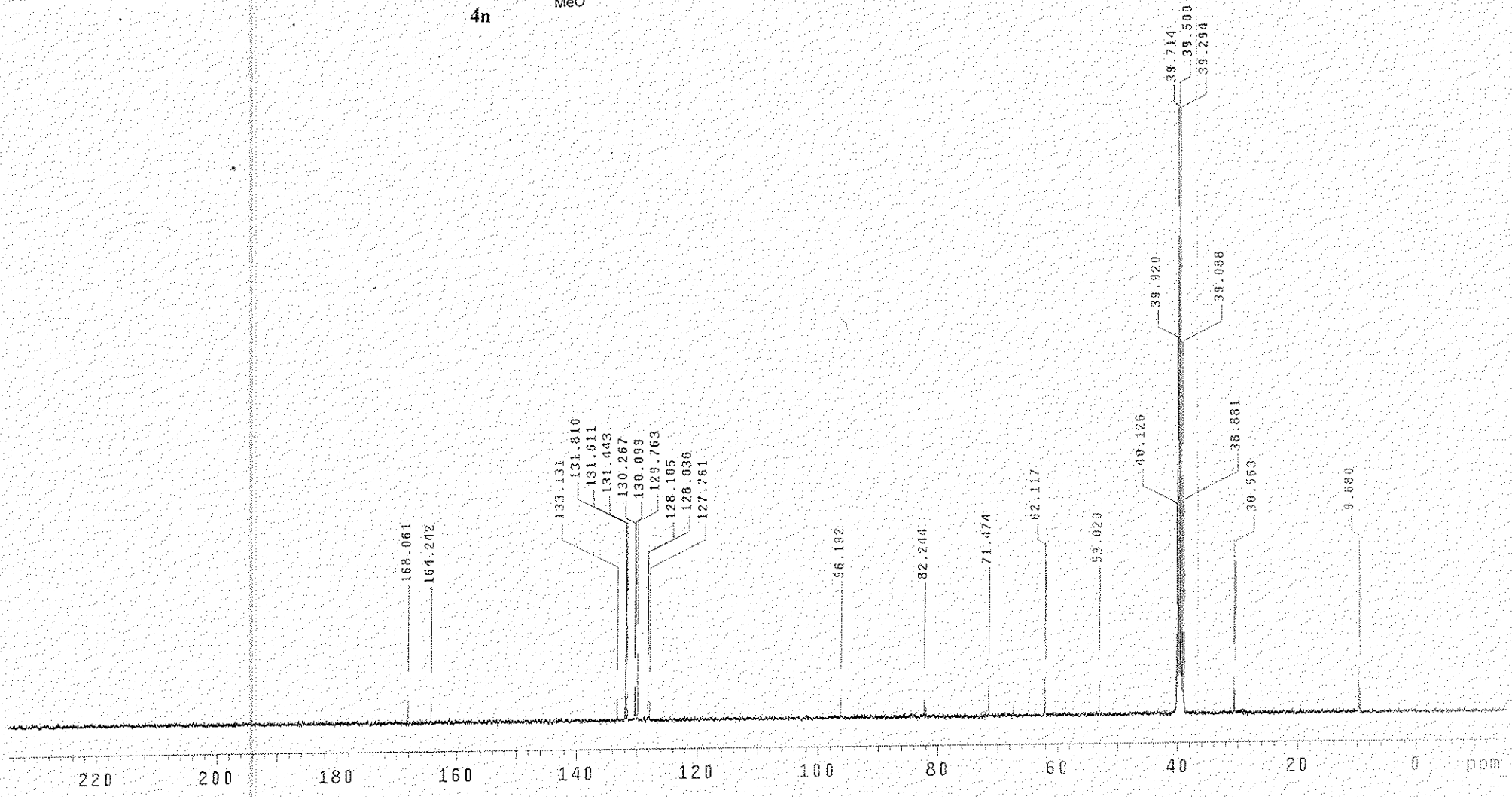


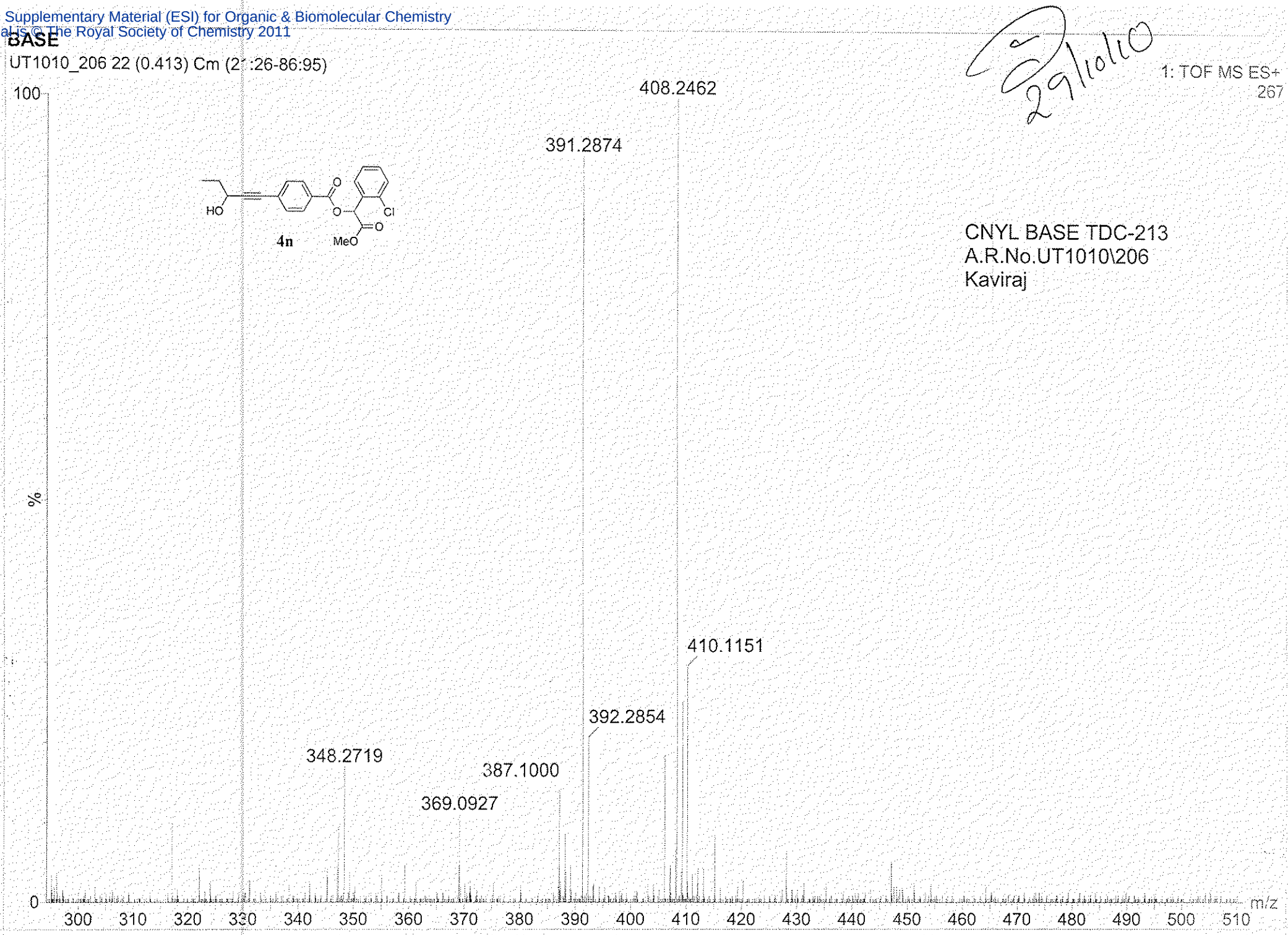
TDC-213 BASE in DMSO

NMR-400
AR.No:ME1210/992
Analyst:Haribabu.R
Date: 10 th Dec. 2010



4n





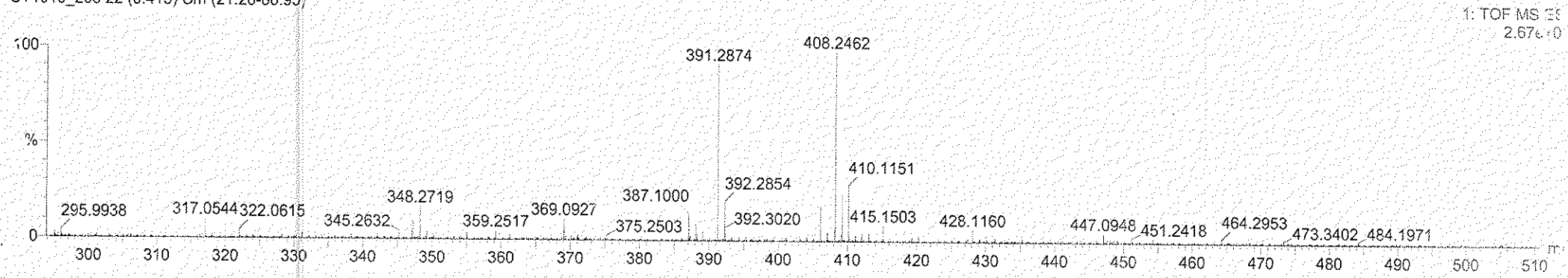
Elemental Composition Report

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
258 formula(e) evaluated with 2 results within limits (up to 4 closest results for each mass)
Elements Used:
C: 0-45 H: 0-70 N: 0-3 O: 0-6 Cl: 0-1

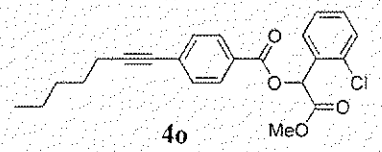
BASE
UT1010_206 22 (0.413) Cm (21:26-86:95)



	Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
Minimum:					-1.0		
Maximum:			5.0	5.0	80.0		
	387.1000	387.0999	0.1	0.3	11.5	4.2	C21 H20 O5 Cl
		387.0981	1.9	4.9	16.5	8.0	C22 H15 N2 O5

TDC-213 BASTW in DMSO

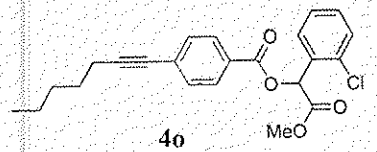
NMR-400MHz.
AR.No:ME1010/2186
Analyst:Shruthi
Date: 26 th Oct2010



4o

BASTW in DMSO
TDC-213

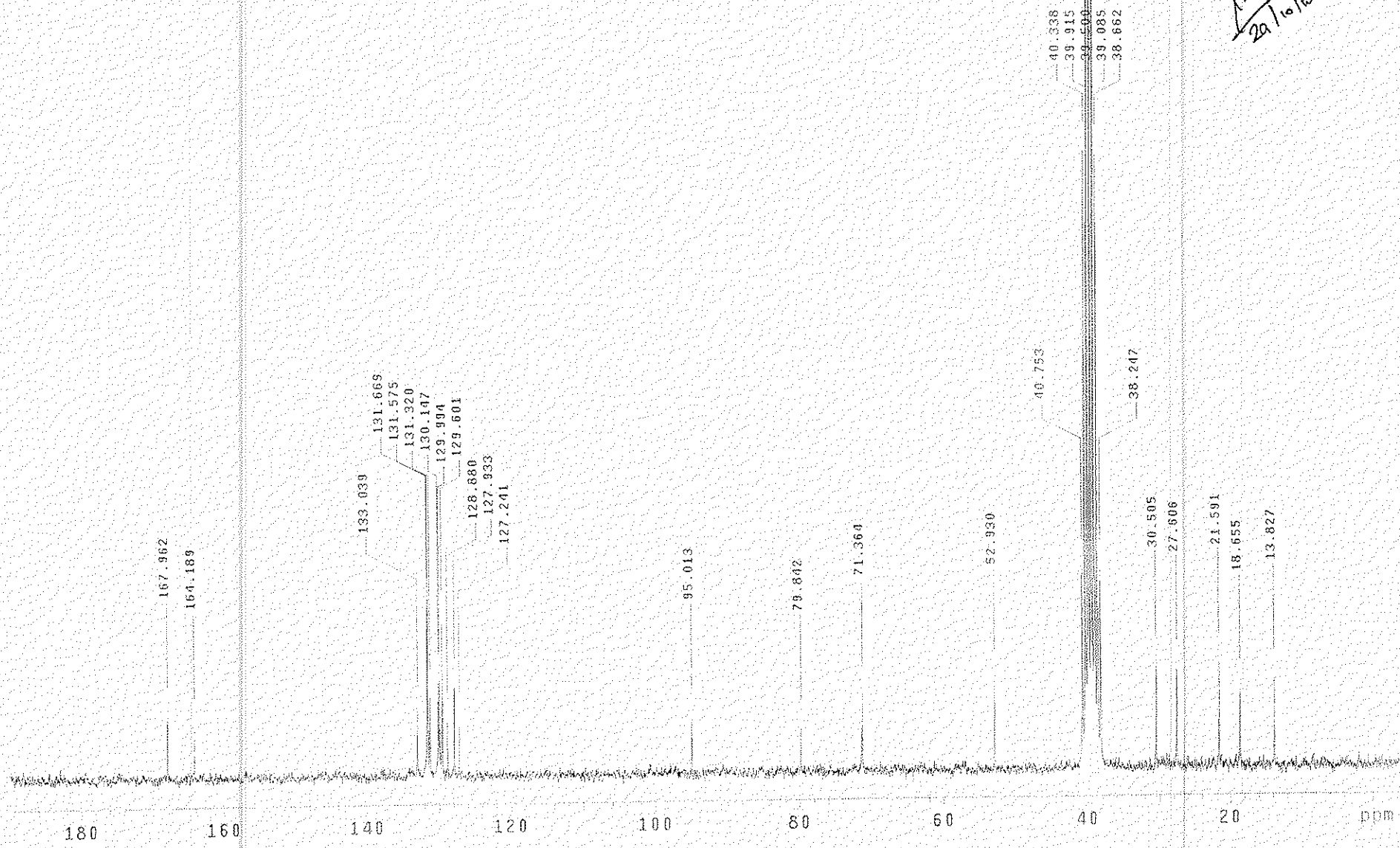
AR NO:GE1010/72
Analyst:Shruthi
Date: 29th Oct 2010



4o

AR&D, Aurigene Discovery Technologies Ltd, Hydera
Instrument : Gemini 2000 (Varian 200MHz)
Date & Time : Fri Oct 29 11:56:28 GMT 2010
Recorded By : Haribabu.R

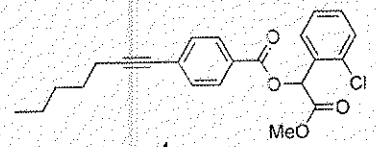
29/10/10



BASTW

UT1110_86 23 (0.426) Cm (23:33-79:88)

1: TOF MS ES+
3.05e3



4o

CNYL BASTW TDC-213
A.R.No.UT1110\86
Kaviraj

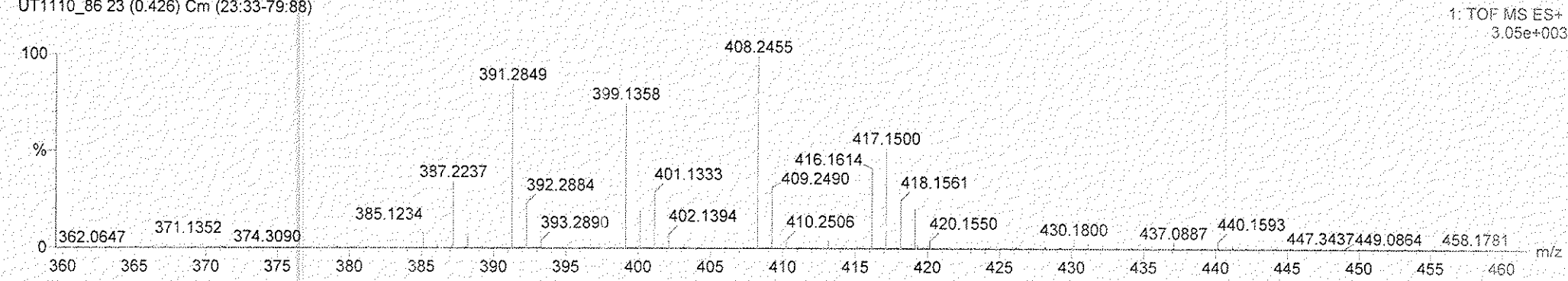
Elemental Composition Report

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
61 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-55 H: 0-65 O: 0-5 Cl: 0-1

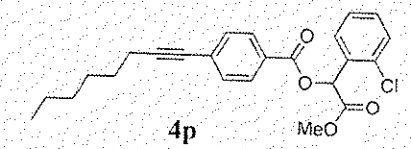
BASTW
UT1110_86 23 (0.426) Cm (23:33-79:88)



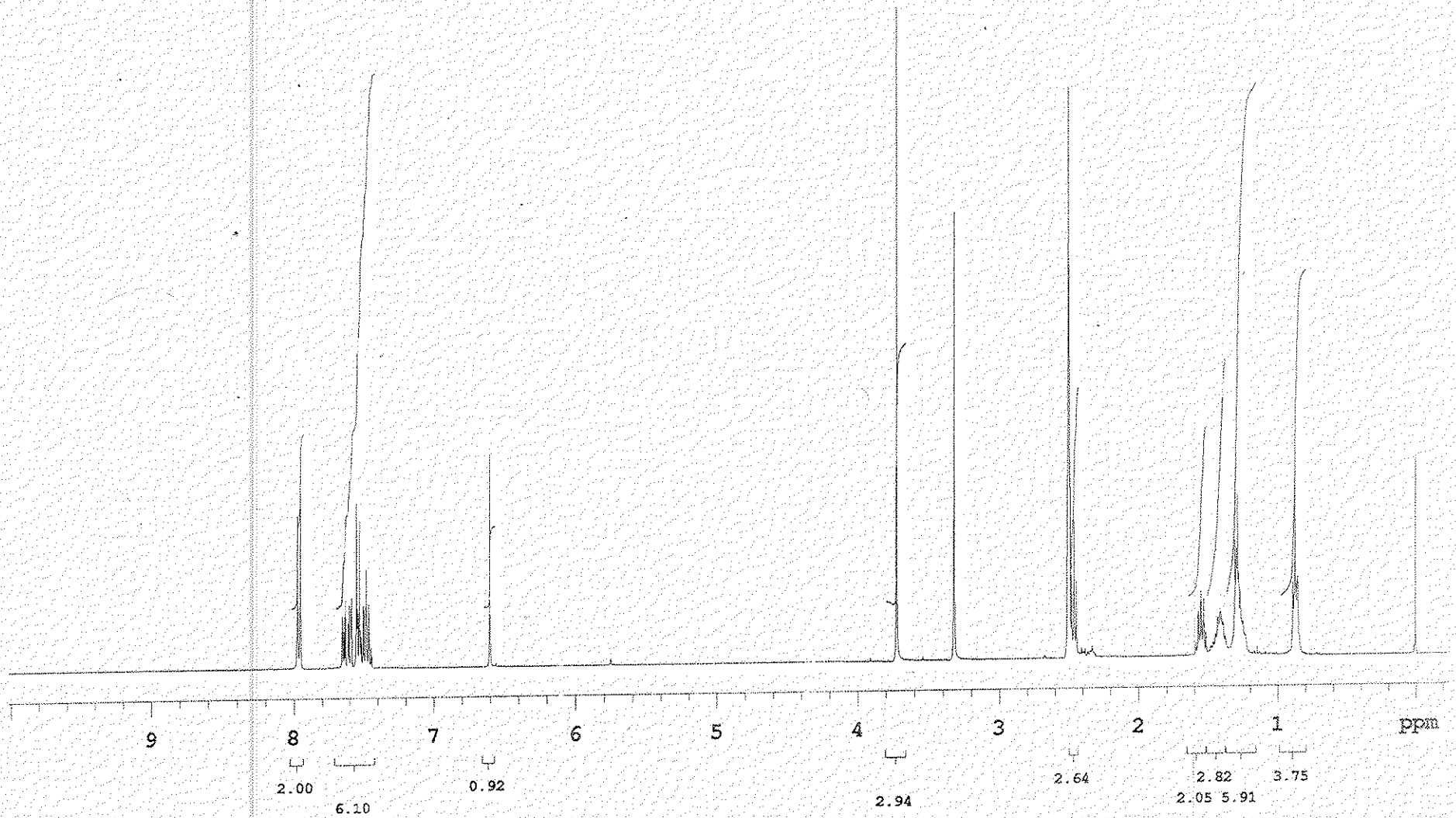
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
399.1358	399.1363	-0.5	-1.3	11.5	1.4	C23 H24 O4 Cl

TDC-213 BASTH in DMSO

NMR-400
AR.No:ME1010/2519
Analyst:Haribabu.R
Date: 29 th Oct 2010



4p

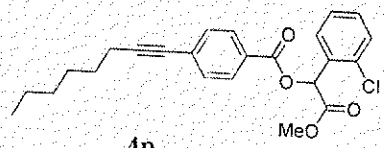


TDC-213 BAST4 in DMSO

NMR-400
AR.No:ME1110/773
Analyst:Haribabu.R
Date: 12 th Nov 2010

Sample Name:
773-TDC-213_BAST4
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_12
Sample directory:
773-TDC-213_BAST4_20101113_01
FidFile: 773-TDC-213_BAST4_20101113_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 13 2010



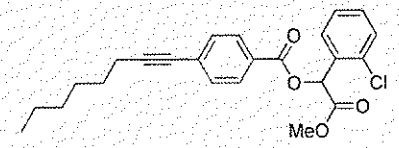
4p

Plotname: 773-TDC-213_BAST4_20101113_01_plot01

BASTH

UT1110_85 19 (0.353) Cm (19:29-73:81)

1: TOF MS ES+
4.44e3



4p

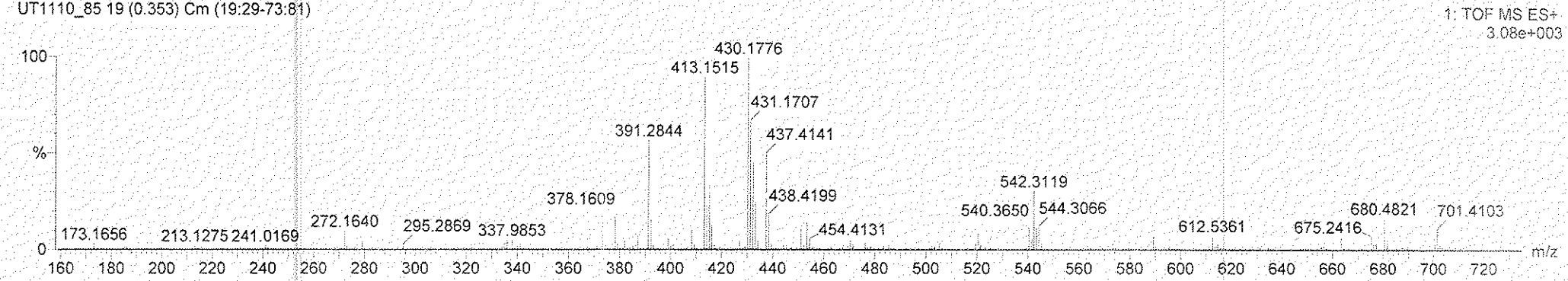
CNYL BASTH TDC-213
A.R.No.UT1110\85
Kaviraj

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

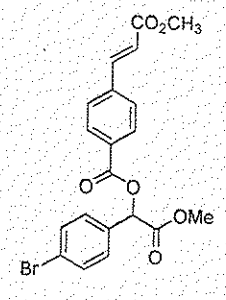
Monoisotopic Mass, Even Electron Ions
61 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-55 H: 0-65 O: 0-5 Cl: 0-1
BASTH
UT1110_85 19 (0.353) Cm (19:29-73:81)



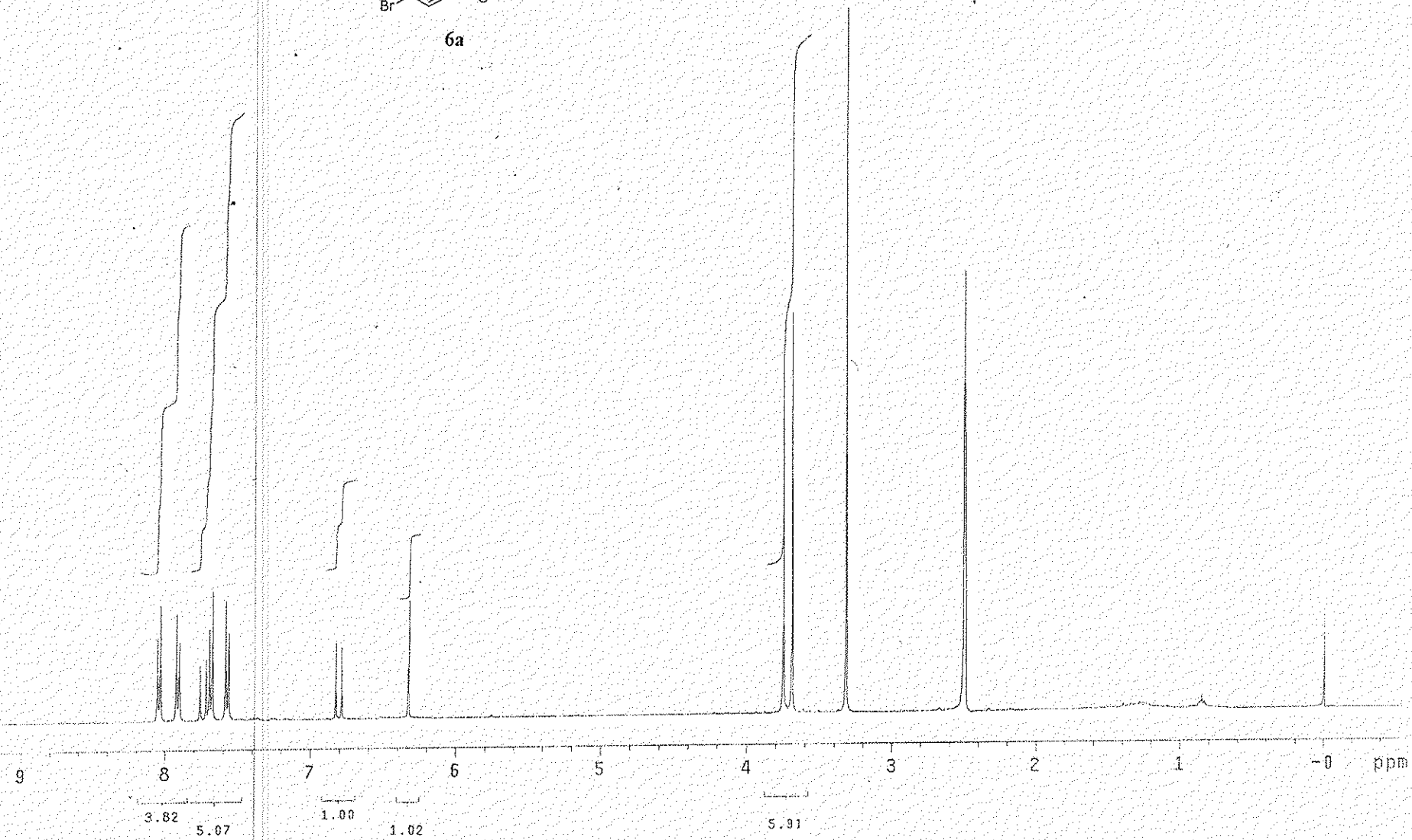
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
413.1515	413.1520	-0.5	-1.2	11.5	2.0	C24 H26 O4 Cl

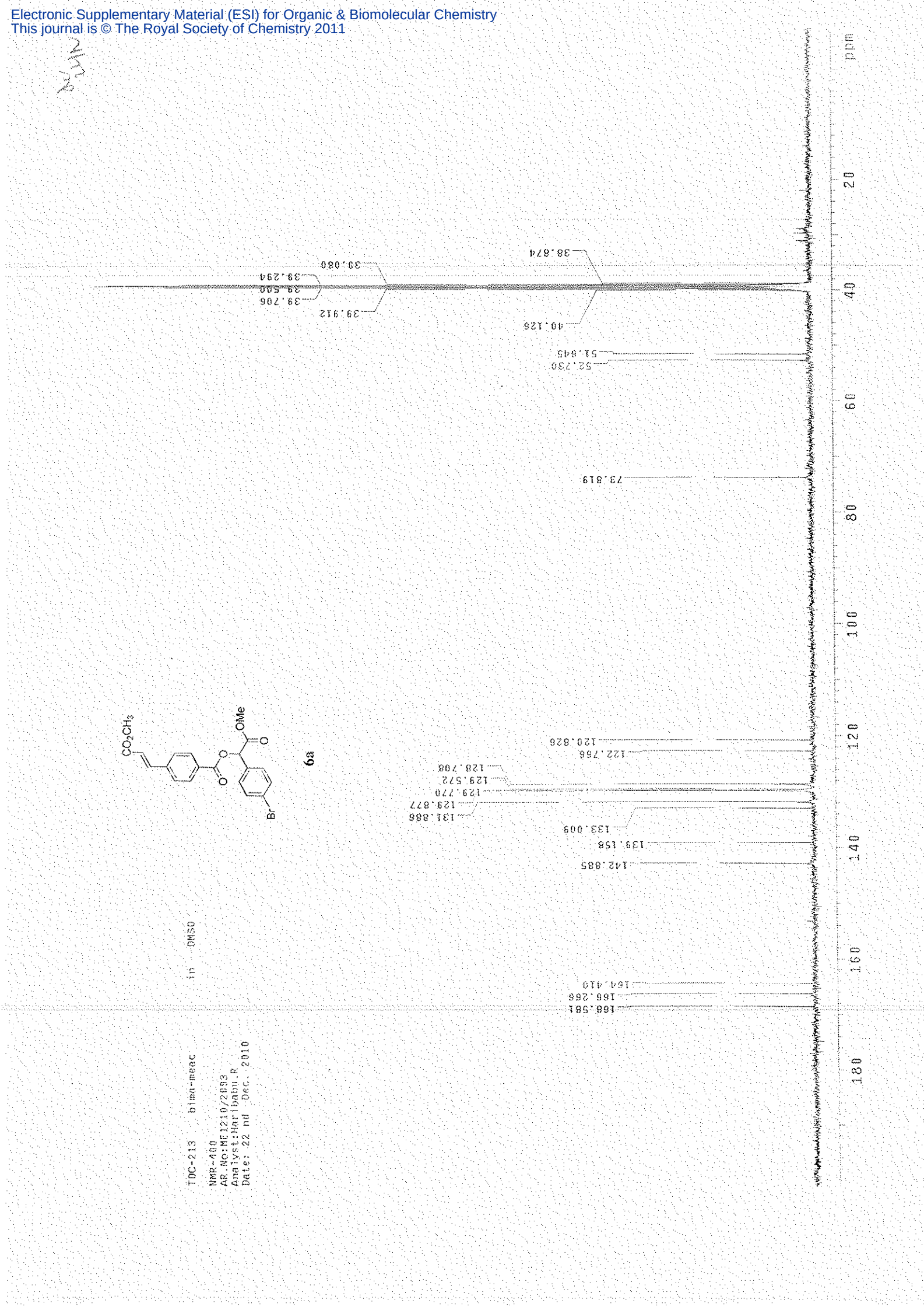
TDC-213 BIMA/MeAC in DMSO

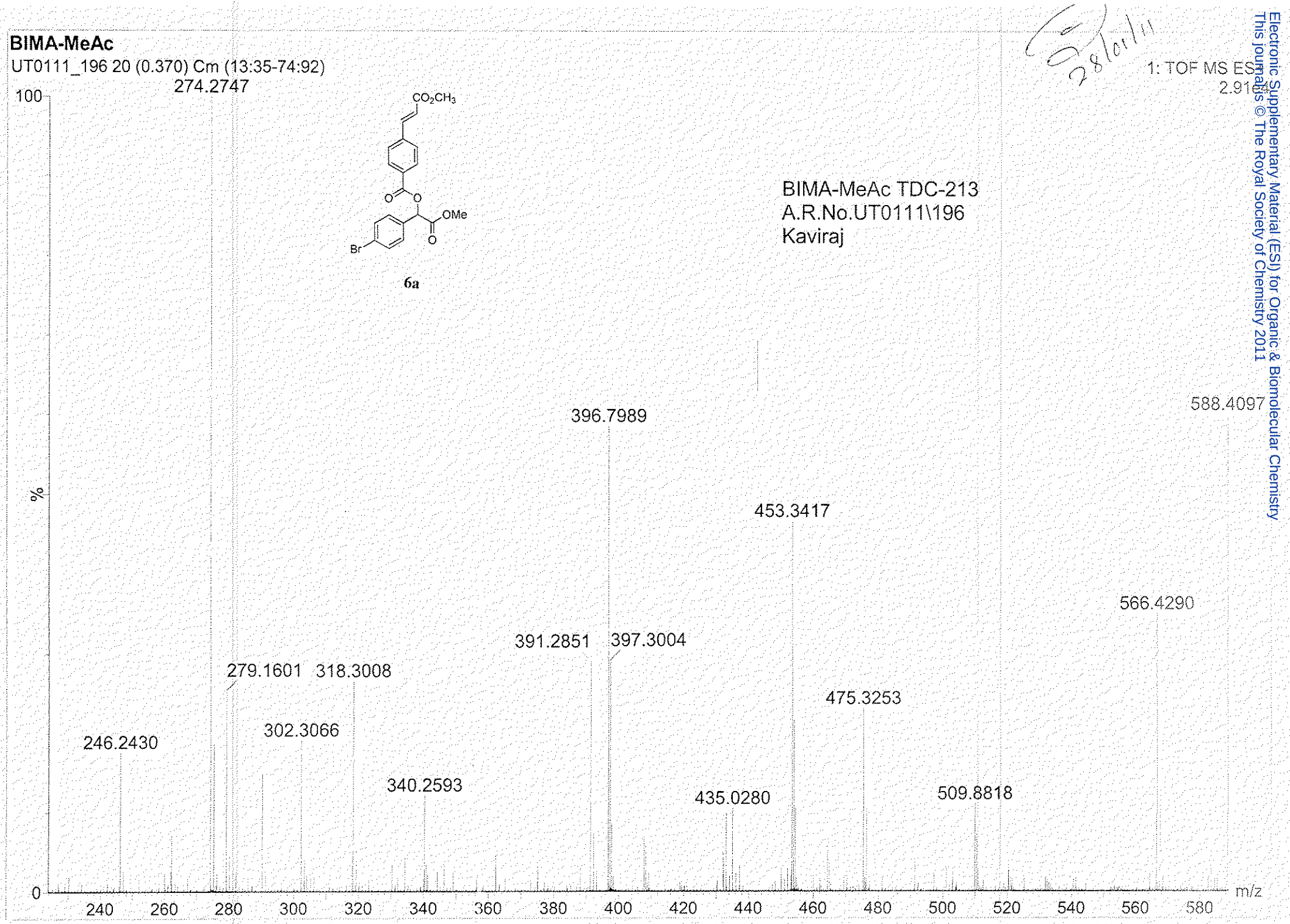
NMR-400
AR.No:ME1210/1237
Analyst:Haribabu.R
Date: 13 th Dec. 2010



6a







Elemental Composition Report

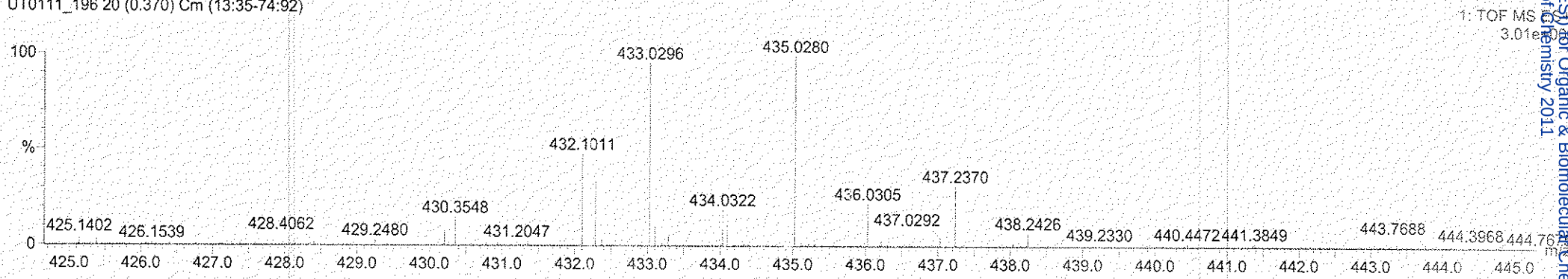
28/10/11

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
47 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-30 O: 0-8 Br: 0-1

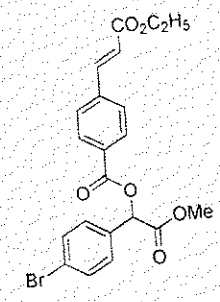
BIMA-MeAc
UT0111_196 20 (0.370) Cm (13:35-74:92)



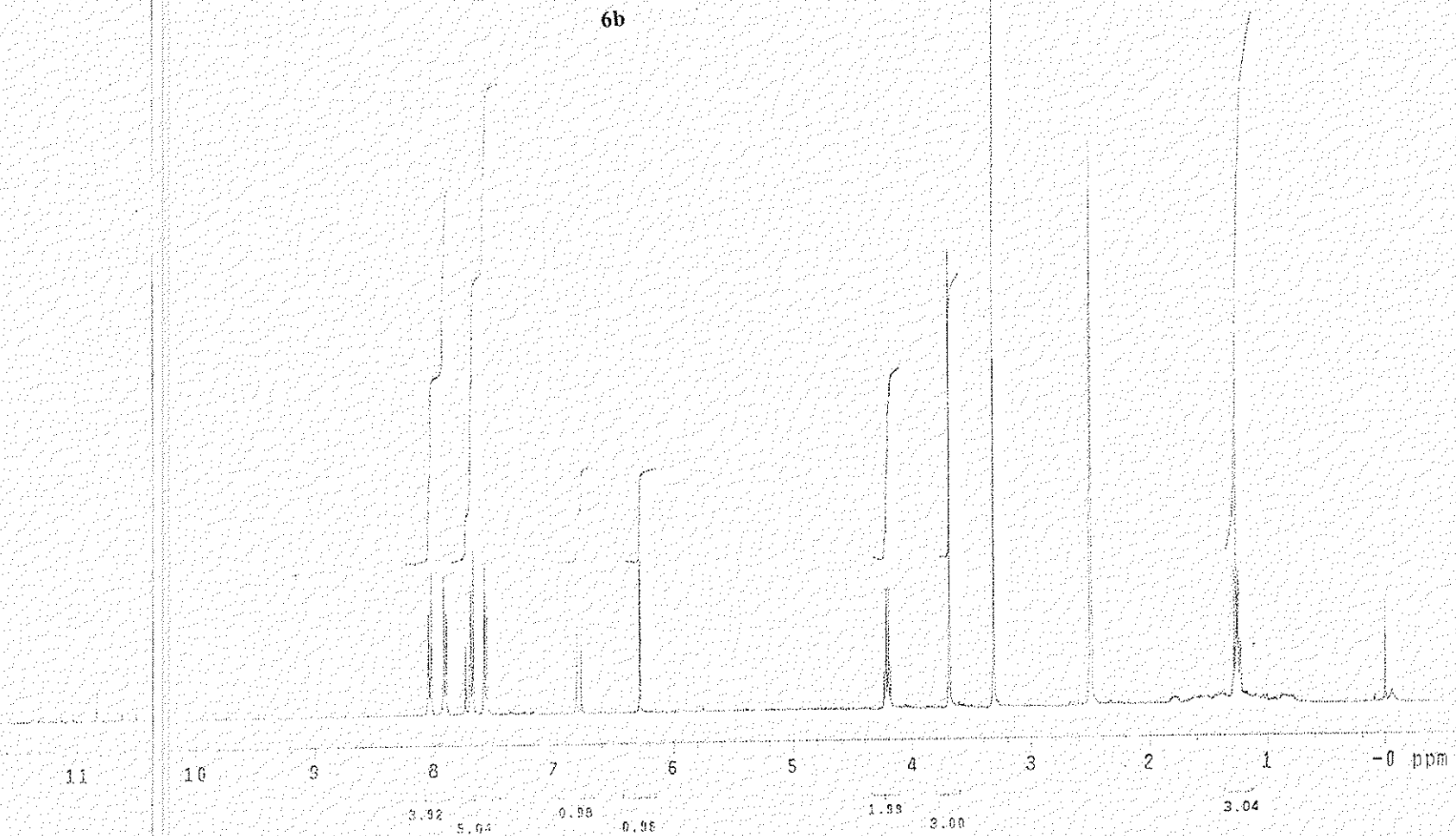
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
433.0296	433.0287	0.9	2.1	11.5	8.0	C20 H18 O6 Br
	433.0290	0.6	1.4	31.5	1468.1	C33 H5 O2

TDC-213 BIRA-ETAC in DMSO

NMR-400
AR.No:ME1210/1575
Analyst:Haribabu.R
Date: 17 th Dec. 2010

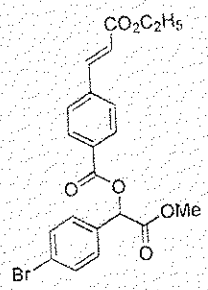


6b

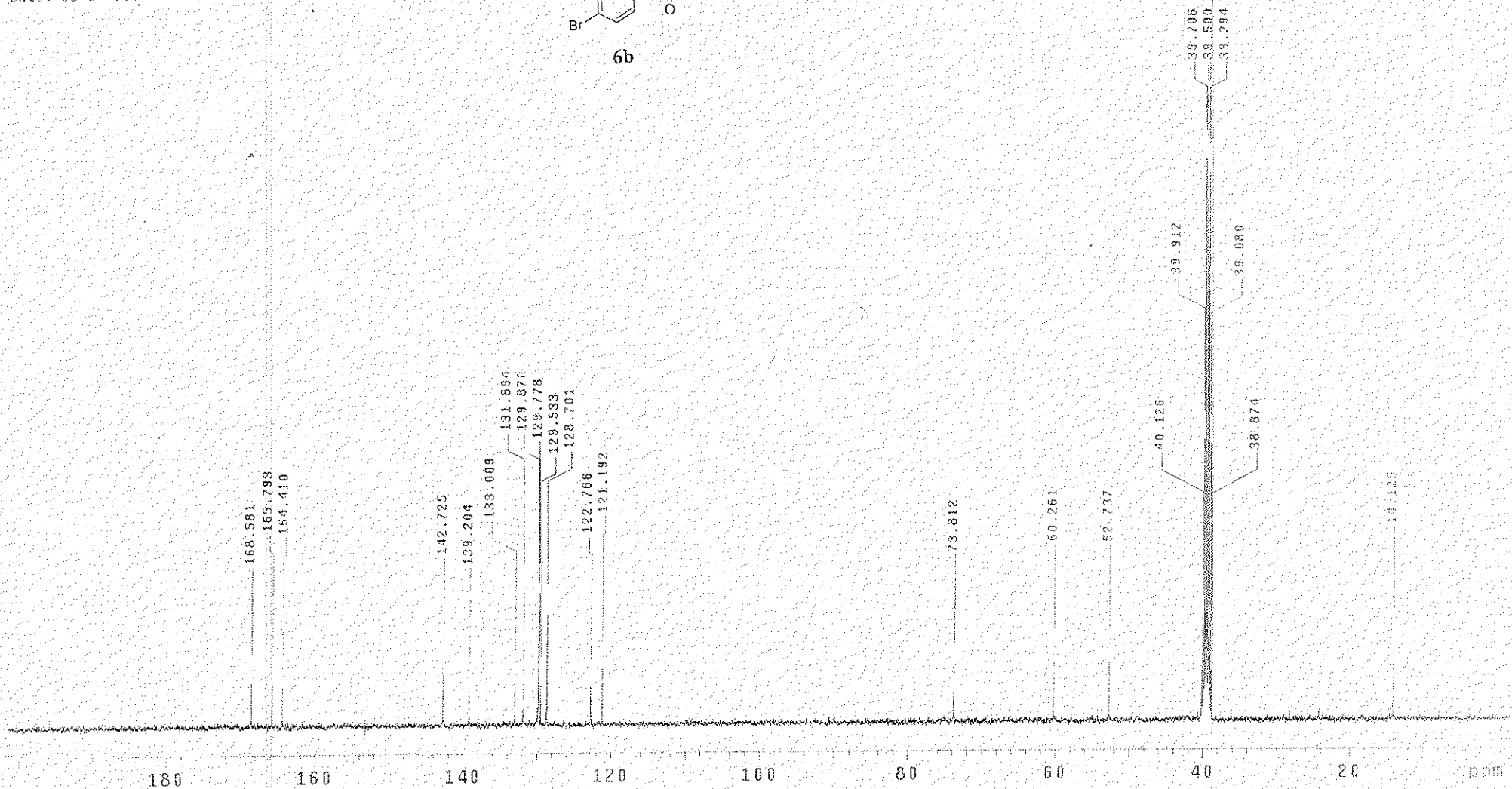


TDC-213 BIMA-ETAC in DMSO

NMR-400
AR.No:ME1210/2234
Analyst:Haribabu.R
Date: 23rd Dec. 2010



6b

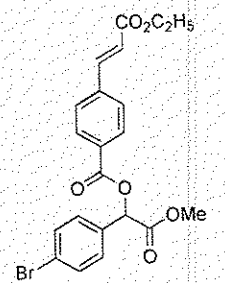


BIMA/ETAC

UT1210_208 19 (0.353) Cm (17:26-53:64)

21/12/10

1: TOF MS ES+
5.35e3



6b

BIMA/ETAC TDC-213
A.R.No.UT1210\208
Kaviraj

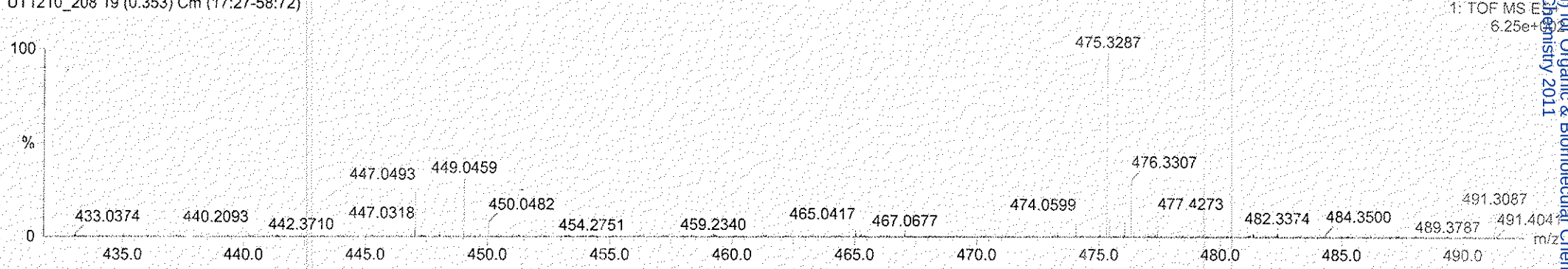
21/12/10

Single Mass Analysis

Tolerance = 19.0 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
57 formula(e) evaluated with 2 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-35 H: 0-50 O: 0-6 Br: 0-1

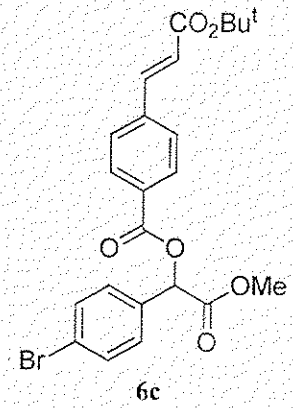
BIMA/ETAC
UT1210_208 19 (0.353) Cm (17:27-58:72)



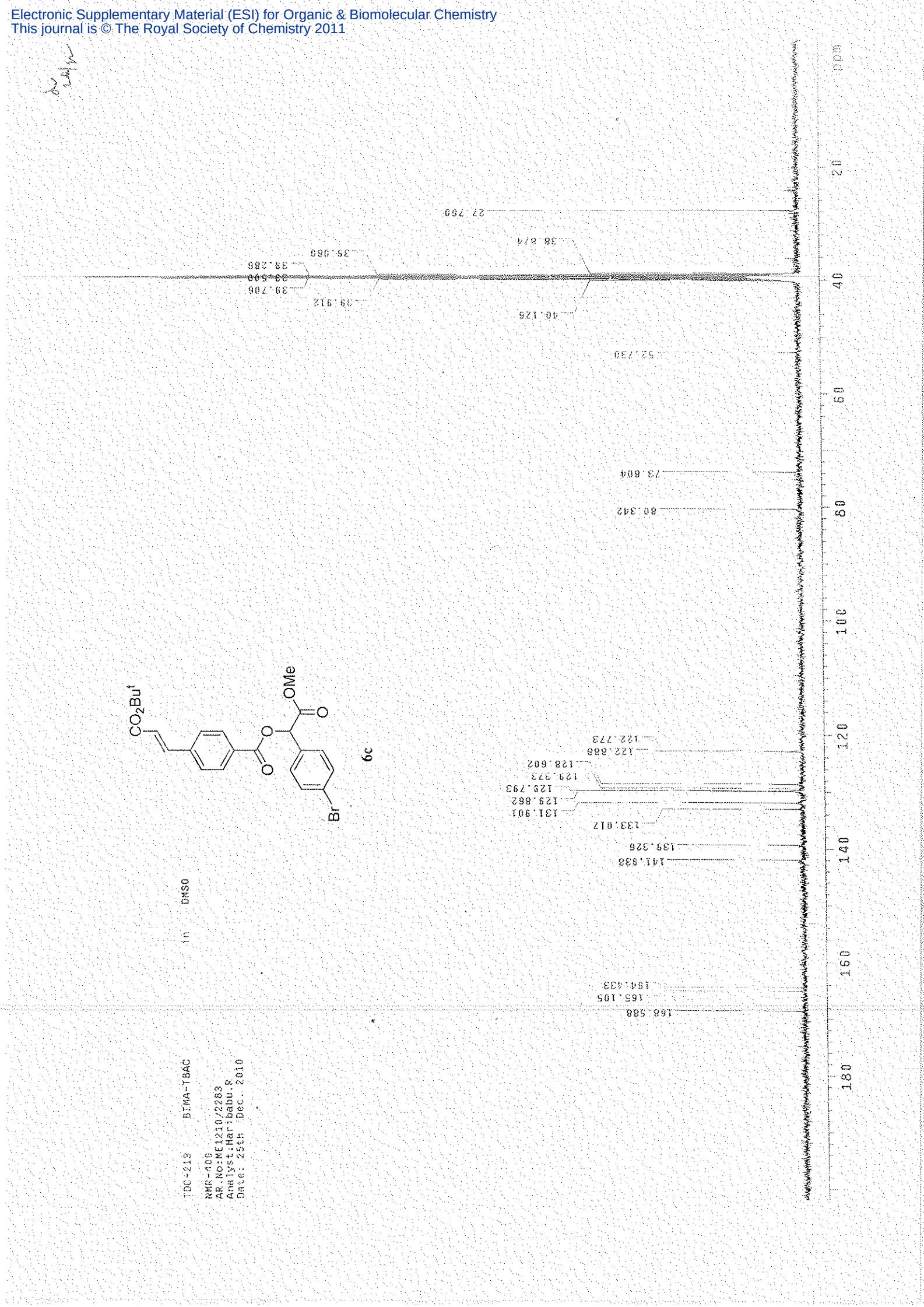
Minimum:				-1.0			
Maximum:		5.0	19.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
447.0493	447.0443	5.0	11.2	11.5	13.1	C21 H20 O6 Br	
	447.0446	4.7	10.5	31.5	110.2	C34 H7 O2	

TDC-213 BIMA-TBAC in DMSO

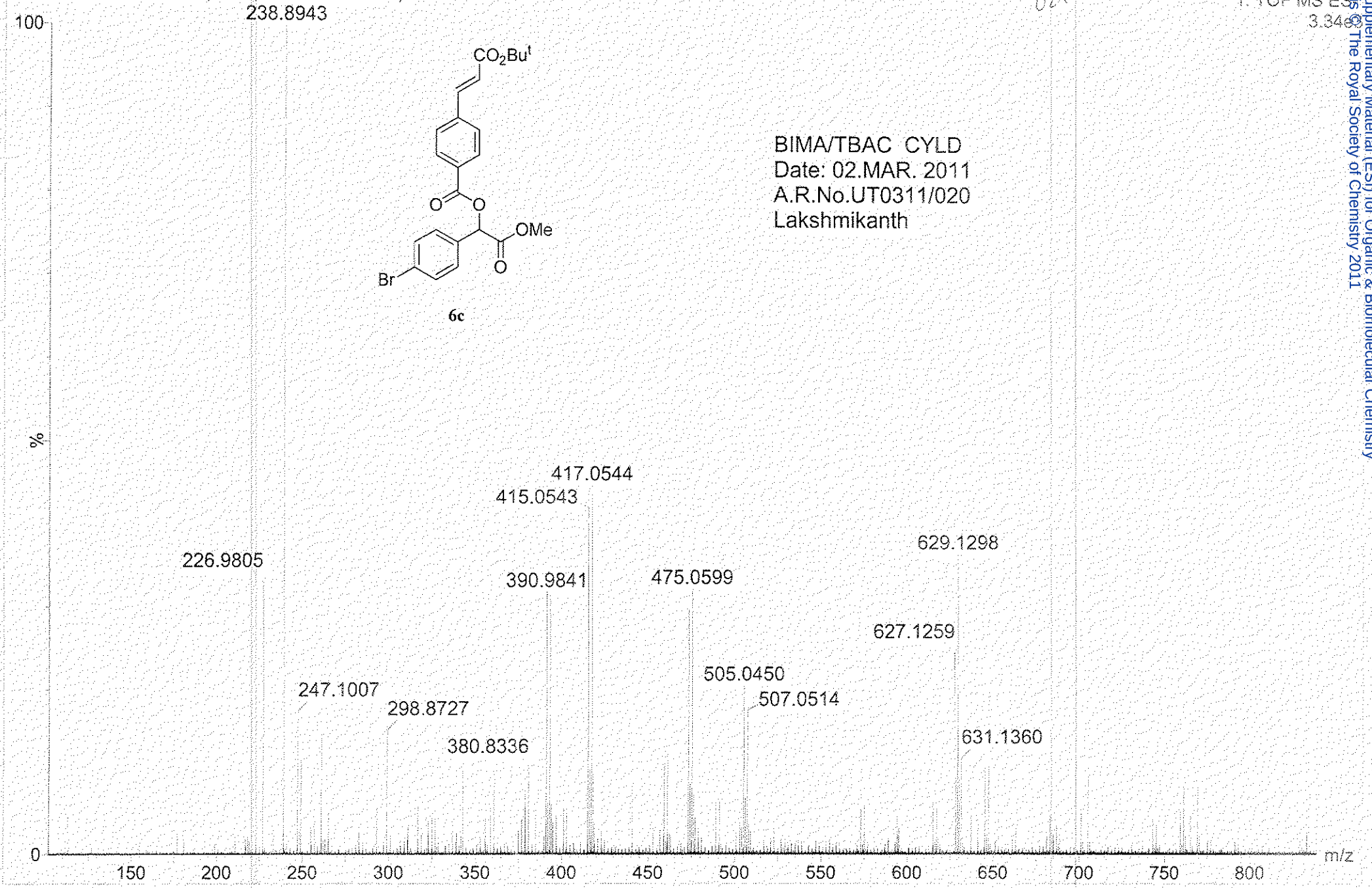
NMR-400
AR.No:ME1210/1578
Analyst:Haribabu.R
Date: 17 th Dec. 2010



6c



UT0311_020A 14 (0.251) Cm (6:14-72:80x0.010)



6c

BIMA/TBAC CYLD
Date: 02.MAR. 2011
A.R.No.UT0311/020
Lakshmikanth

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

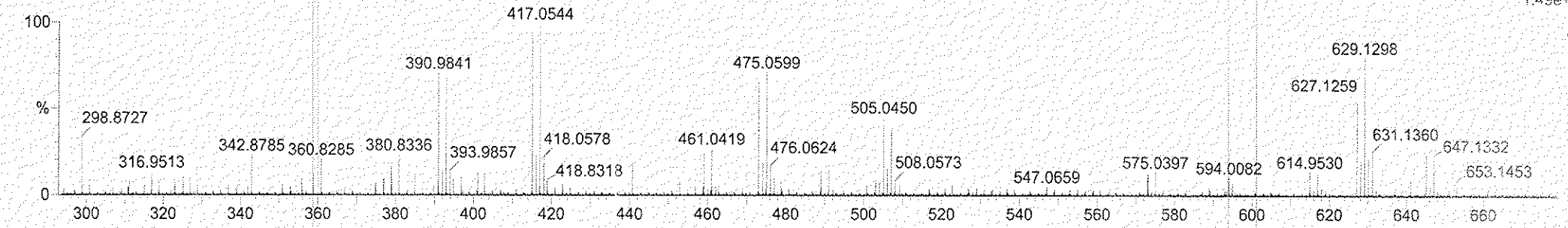
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-25 O: 0-7 Br: 0-1

BIMA/TBAC CYLD

Aurigene Discovery Technologies, Hyderabad

02-Mar-20
Lakshmikanth
1: TOF MS E
1.49e+003

UT0311_020A 14 (0.251) Cm (6:14-72:80x0.010)



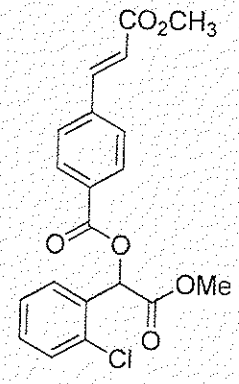
Minimum:				-1.0		
Maximum:		5.0	5.0	15.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
473.0619	473.0600	1.9	4.0	12.5	1.7	C23 H22 O6 Br

TDC-213 MEAC in DMSO

NMR-400
AR.No:ME1110/1283
Analyst:Haribabu.R
Date: 18 th Nov 2010

Sample Name:
1283-TDC-213_MEAC
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_18
Sample directory:
1283-TDC-213_MEAC_20101118_01
FidFile: 1283-TDC-213_MEAC_20101118_01

Pulse Sequence: PROTON {s2pul}
Solvent: dmso
Data collected on: Nov 18 2010



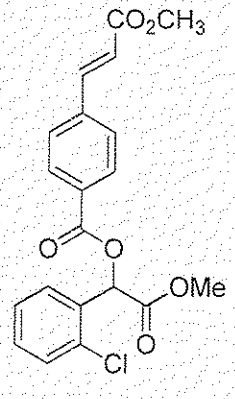
6d

VARIAN

Plotname: 1283-TDC-213_MEAC_20101118_01_plot01

MEAC in DMSO
TDC-213

AR NO:GE1210/04
Analyst:Haribabu.R
Date: 2nd Dec. 2010



6d

AR&D, Aurigene Discovery Technologies Ltd, Hydera
Instrument : Gemini 2000 (Varian 200MHz)
Date & Time : Thu Dec 2 14:17:36 GMT 2010
Recorded By : Haribabu.R

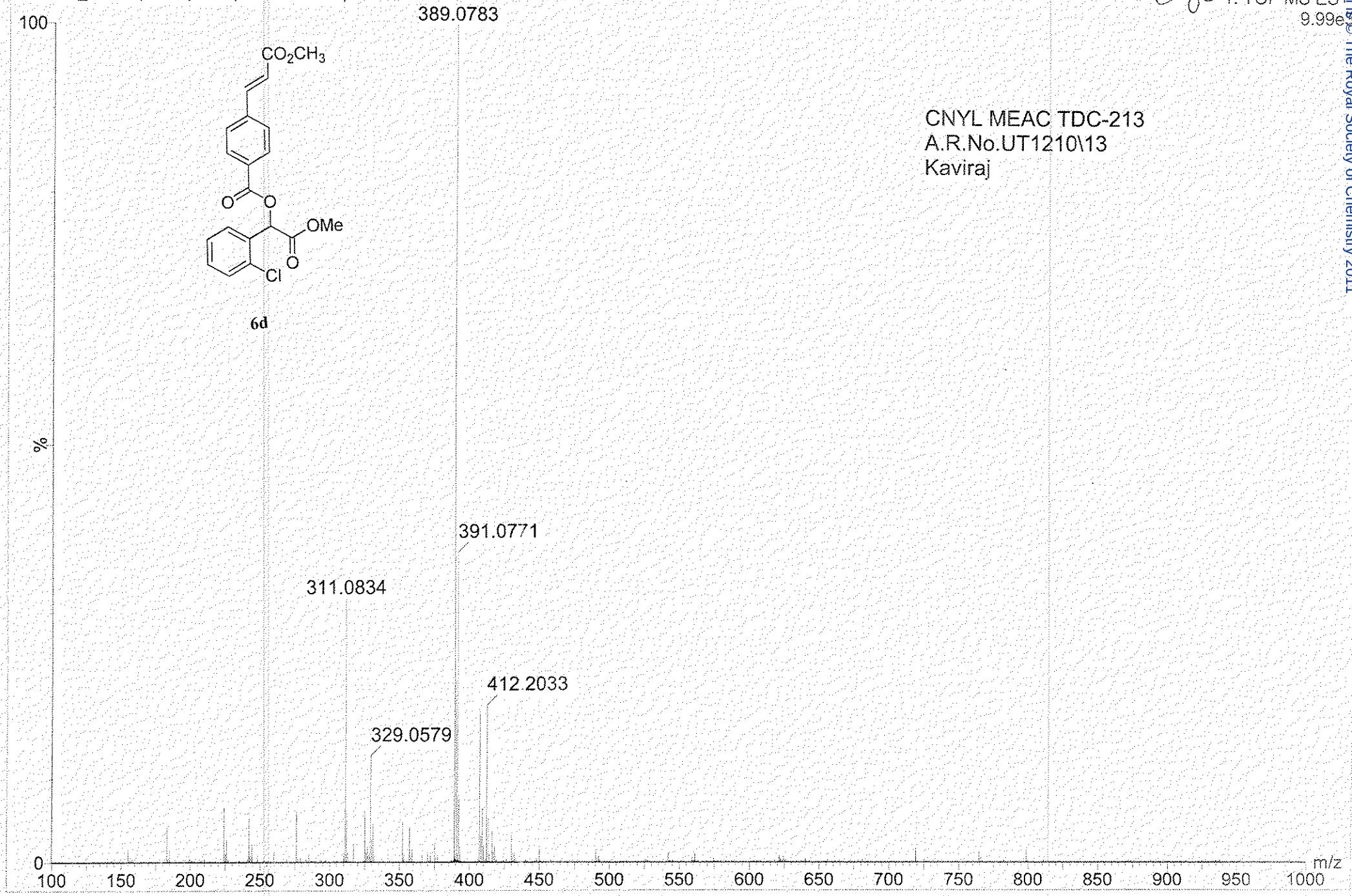
MEAC

UT1210_13 34 (0.634) Cm (33:40-93:103)

03/12/10

1: TOF MS ES+

9.99e3



6d

CNYL MEAC TDC-213
A.R.No.UT1210\13
Kaviraj

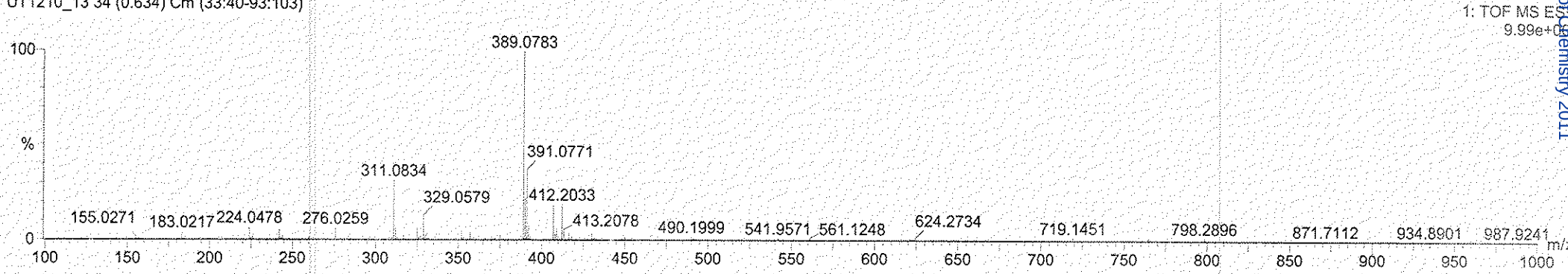
Elemental Composition Report

09/12/10

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
79 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 O: 0-8 Cl: 0-1
MEAC
UT1210_13 34 (0.634) Cm (33:40-93:103)



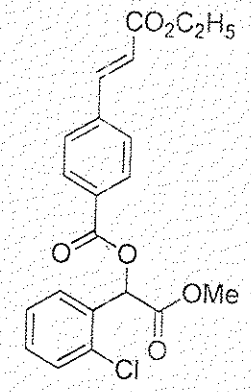
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
389.0783	389.0792	-0.9	-2.3	11.5	3.5	C20 H18 O6 Cl

TDC-213 ETAC in CDCl3

NMR-400
AR.No:ME1110/1408
Analyst:Haribabu.R
Date: 19 th Nov 2010

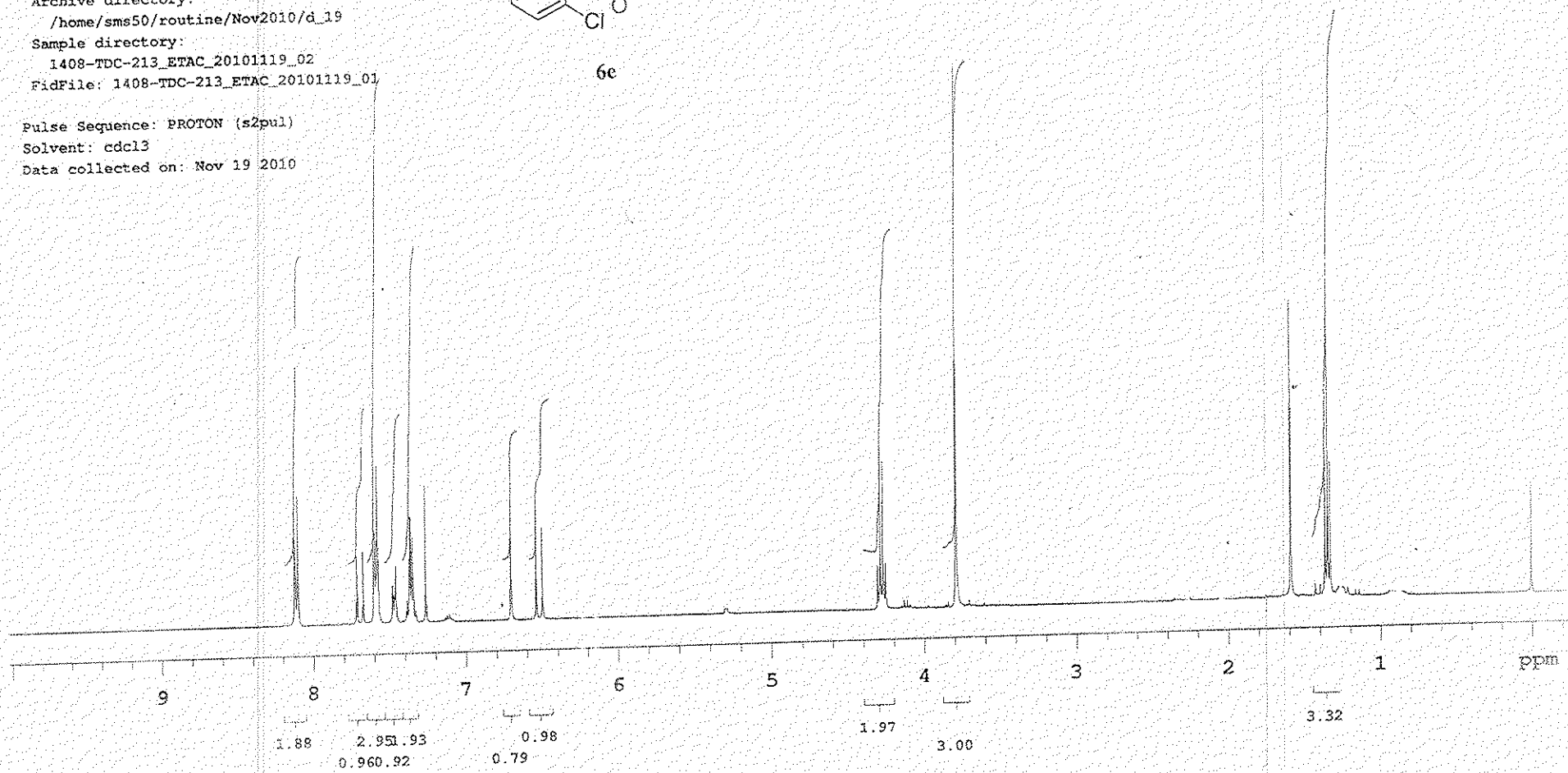
Sample Name:
1408-TDC-213_ETAC
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_19
Sample directory:
1408-TDC-213_ETAC_20101119_02
FidFile: 1408-TDC-213_ETAC_20101119_01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 19 2010



6e

VARIAN



Plotname: 1408-TDC-213_ETAC_20101119_01_plot01

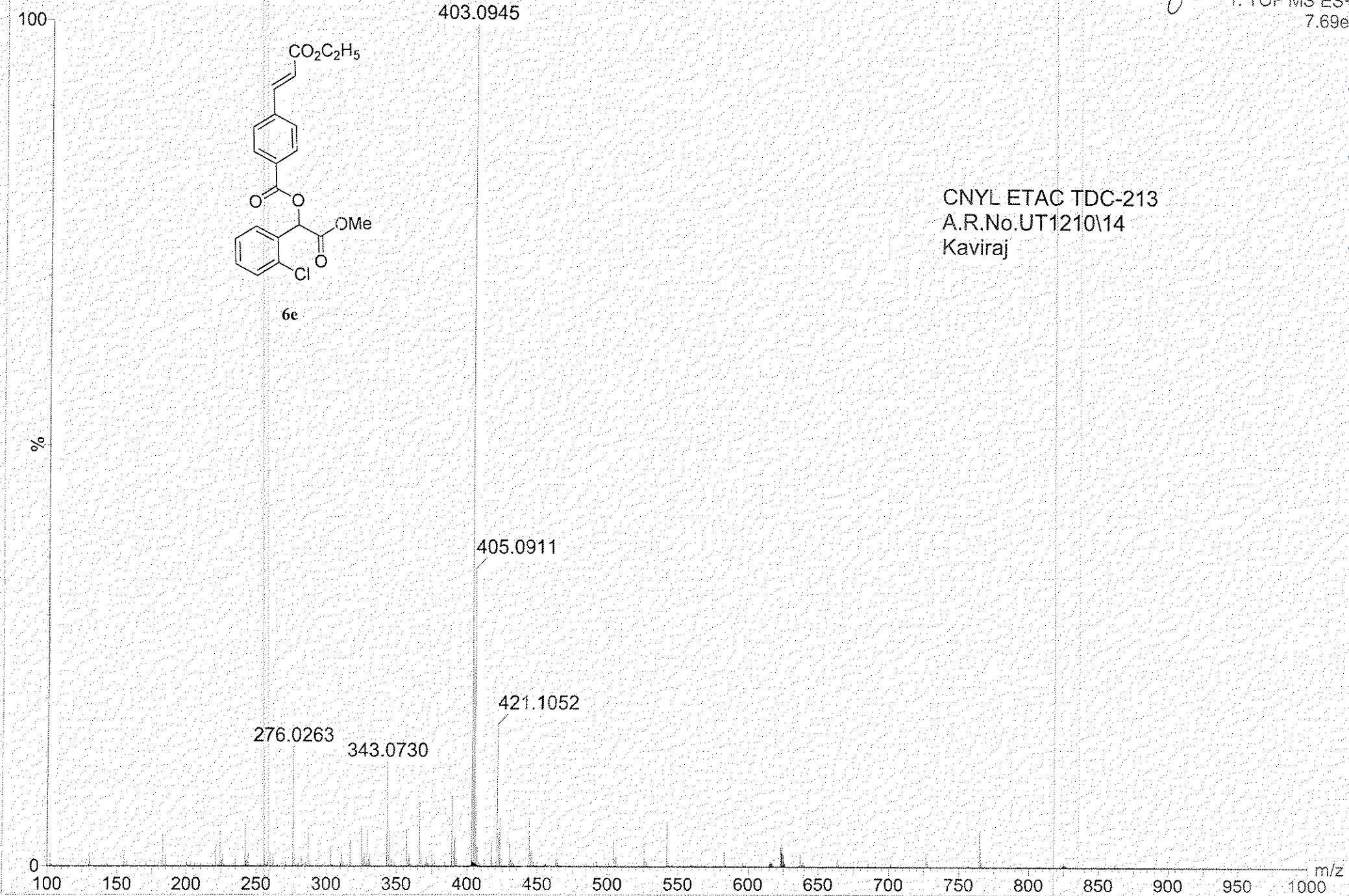
14.141
38.881
39.088
39.294
39.500
39.714
39.920
40.126
52.982
60.292
71.444
121.223
127.990
128.731
129.449
129.931
130.053
130.244
131.374
131.649
133.085
139.265
142.740
164.265
165.816
168.038
ppm
20
40
60
80
100
120
140
160
TDC-213 EtAc in DMSO
NMR-400
AR No:ME1110/2132
Analyst:Shruthi
Date: 30th Nov 2010
OMe
Cl
O
O
O
$CO_2C_2H_5$
6e

ETAC

UT1210_14 19 (0.352) Cm (18:28-80:89)

03/12/10

1: TOF MS ES+
7.69e4



Elemental Composition Report

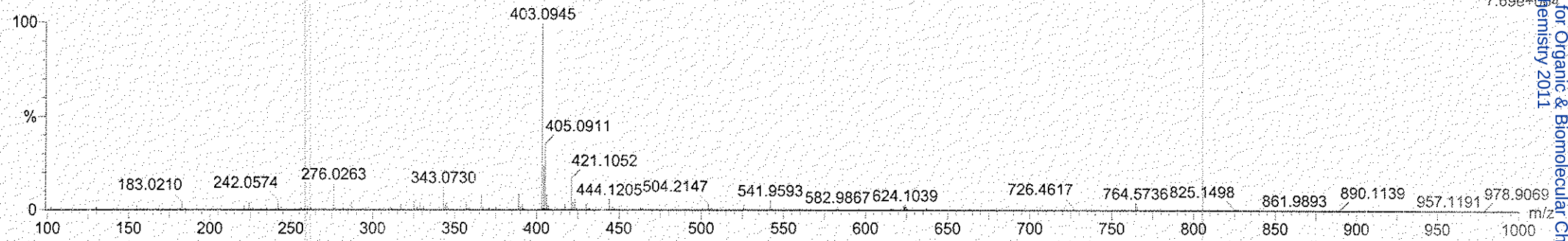
08/12/10

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
84 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 O: 0-8 Cl: 0-1
ETAC
UT1210_14 19 (0.352) Cm (18:28-80:89)

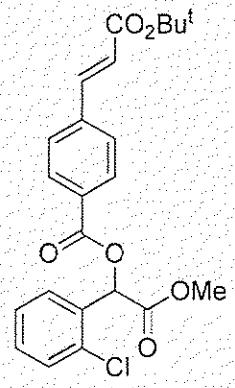
1: TOF MS ES+
7.69e+004



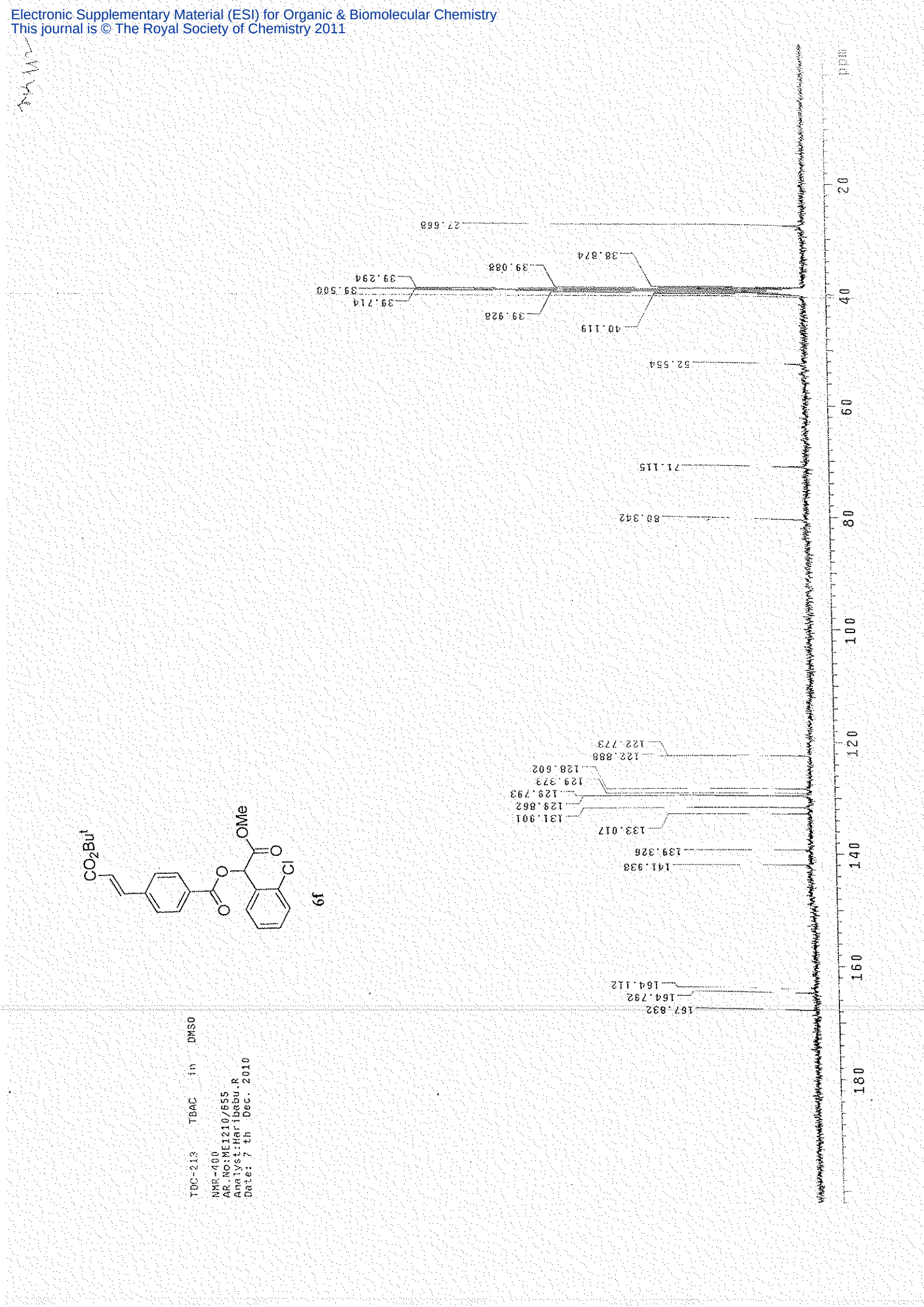
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
403.0945	403.0948	-0.3	-0.7	11.5	3.7	C21 H20 O6 Cl

TDC-213 TBAC in DMSO

NMR-400
AR.No:ME1110/1724
Analyst:Haribabu.R
Date: 23 th Nov 2010



6f

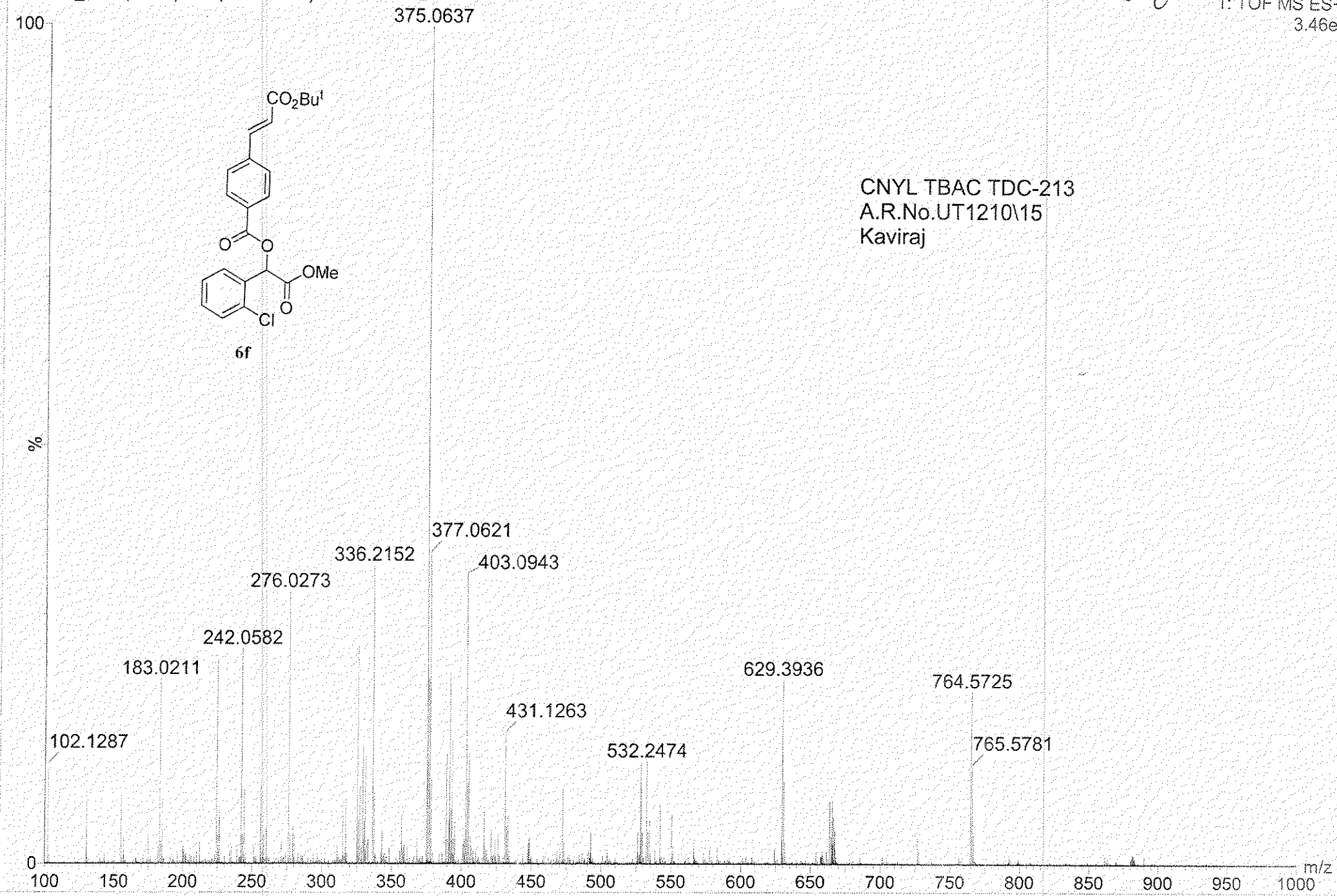


TBAC

UT1210_15 6 (0.117) Cm (5:22-79:87)

03/12/10

1: TOF MS ES+
3.46e4



6f

CNYL TBAC TDC-213
A.R.No.UT1210\15
Kaviraj

Elemental Composition Report

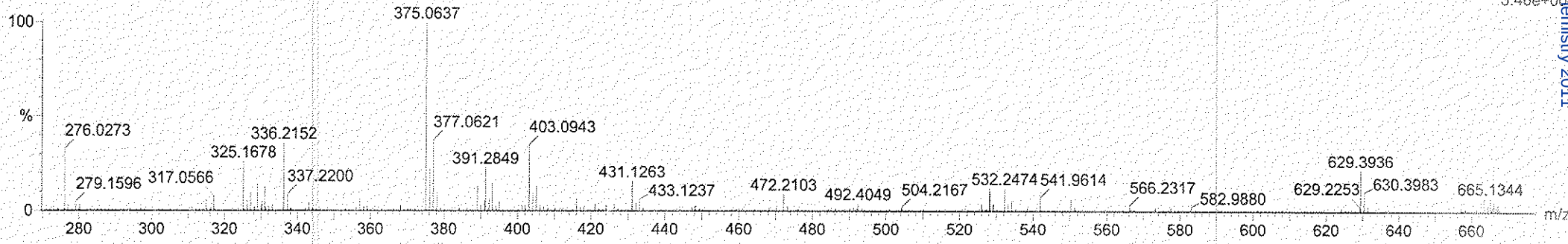
08/12/10

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
86 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 O: 0-8 Cl: 0-1
TBAC
UT1210_15 6 (0.117) Cm (5:22-79:87)

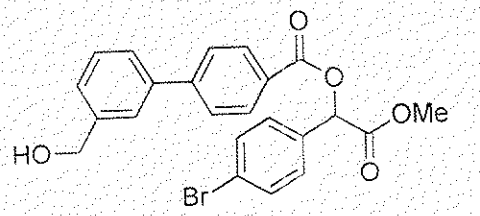
1: TOF MS ES+
3.46e+0



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
431.1263	431.1261	0.2	0.5	11.5	3.2	C23 H24 O6 Cl
	431.1283	-2.0	-4.6	20.5	745.7	C29 H19 O4

TDC-213 8IMA/PHBA in DMSO

NMR-400
AR.No:ME0111/702
Analyst:Haribabu.R
Date: 07 th Jan. 2011



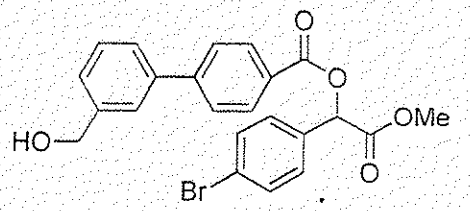
8a

TDC-213 BIMA-PHBA in DMSO

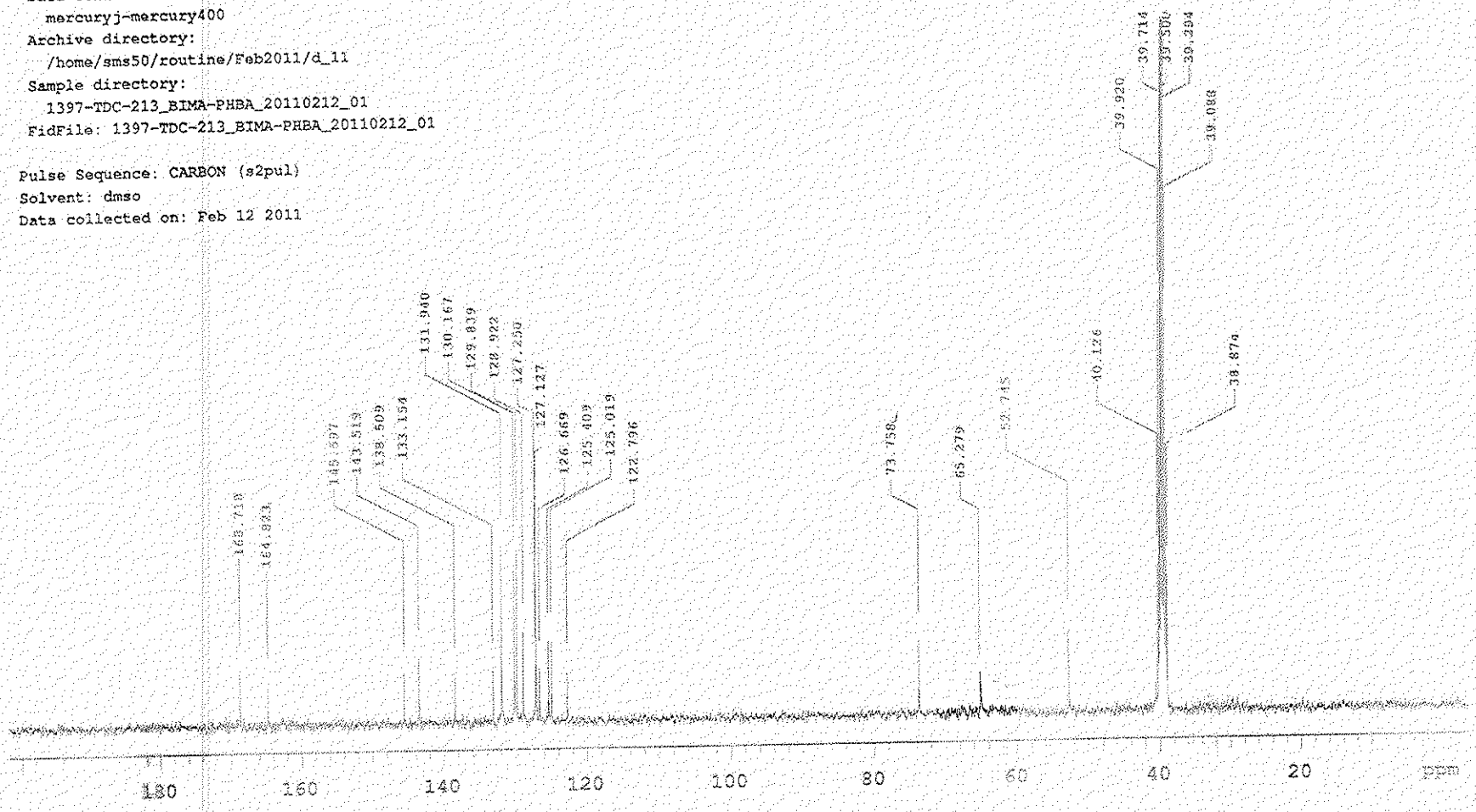
NMR-400
AR.No:ME0211/1397
Analyst:Haribabu.R
Date: 11 th Feb. 2011

Sample Name:
1397-TDC-213_BIMA-PHBA
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Feb2011/d_11
Sample directory:
1397-TDC-213_BIMA-PHBA_20110212_01
FidFile: 1397-TDC-213_BIMA-PHBA_20110212_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Feb 12 2011



8a



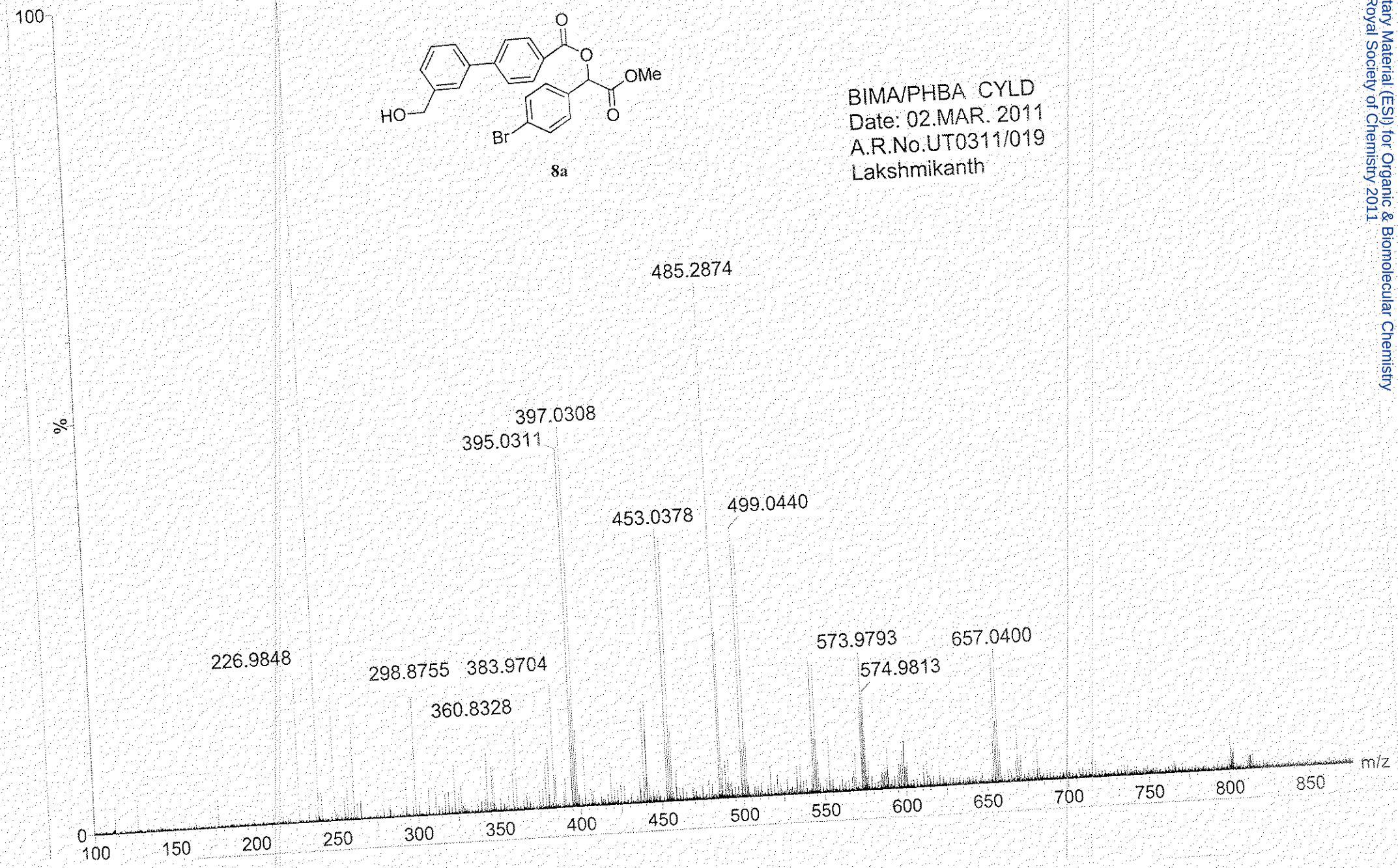
Plotname: 1397-TDC-213_BIMA-PHBA_20110212_01_plot01

Aurigene Discovery Technologies, Hyderabad

02-Mar-2011
Lakshmikanth
1: TOF MS ES-
1.10e3

BIMA/PHBA CYLD

UT0311_019A 9 (0.163) Cm (9:11-87:94x0.010)



8a

BIMA/PHBA CYLD
Date: 02.MAR. 2011
A.R.No.UT0311/019
Lakshmikanth

Elemental Composition Report

02/03/11

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.0, max = 15.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

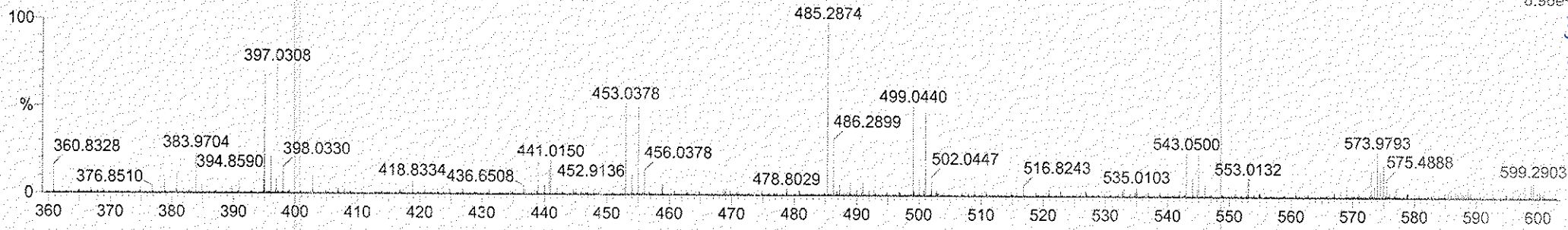
Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-25 O: 0-7 Br: 0-1

BIMA/PHBA CYLD

Aurigene Discovery Technologies, Hyderabad

02-Mar-2011
Lakshmikanth
1: TOF MS ES+
6.96e+002

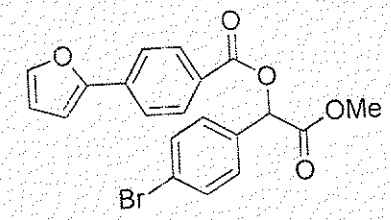
UT0311_019A 9 (0.163) Cm (9:11-87:94x0.010)



Minimum:				-1.0		
Maximum:		5.0	10.0	15.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
453.0378	453.0338	4.0	8.8	14.5	1.3	C23 H18 O5 Br

TDC-213 BIMA-FBA in DMSO

NMR-400
AR.No:ME0111/2255
Analyst: Ganesh
Date: 25th Jan. 2011



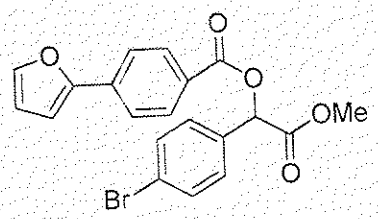
8b

TDC-213 BIMA-FBA in DMSO

NMR-400
AR.No:ME0211/1396
Analyst:Haribabu.R
Date: 11 th Feb. 2011

Sample Name:
1396-TDC-213_BIMA-FBA
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Feb2011/d_11
Sample directory:
1396-TDC-213_BIMA-FBA_20110211_01
FidFile: 1396-TDC-213_BIMA-FBA_20110212_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Feb 12 2011



8b

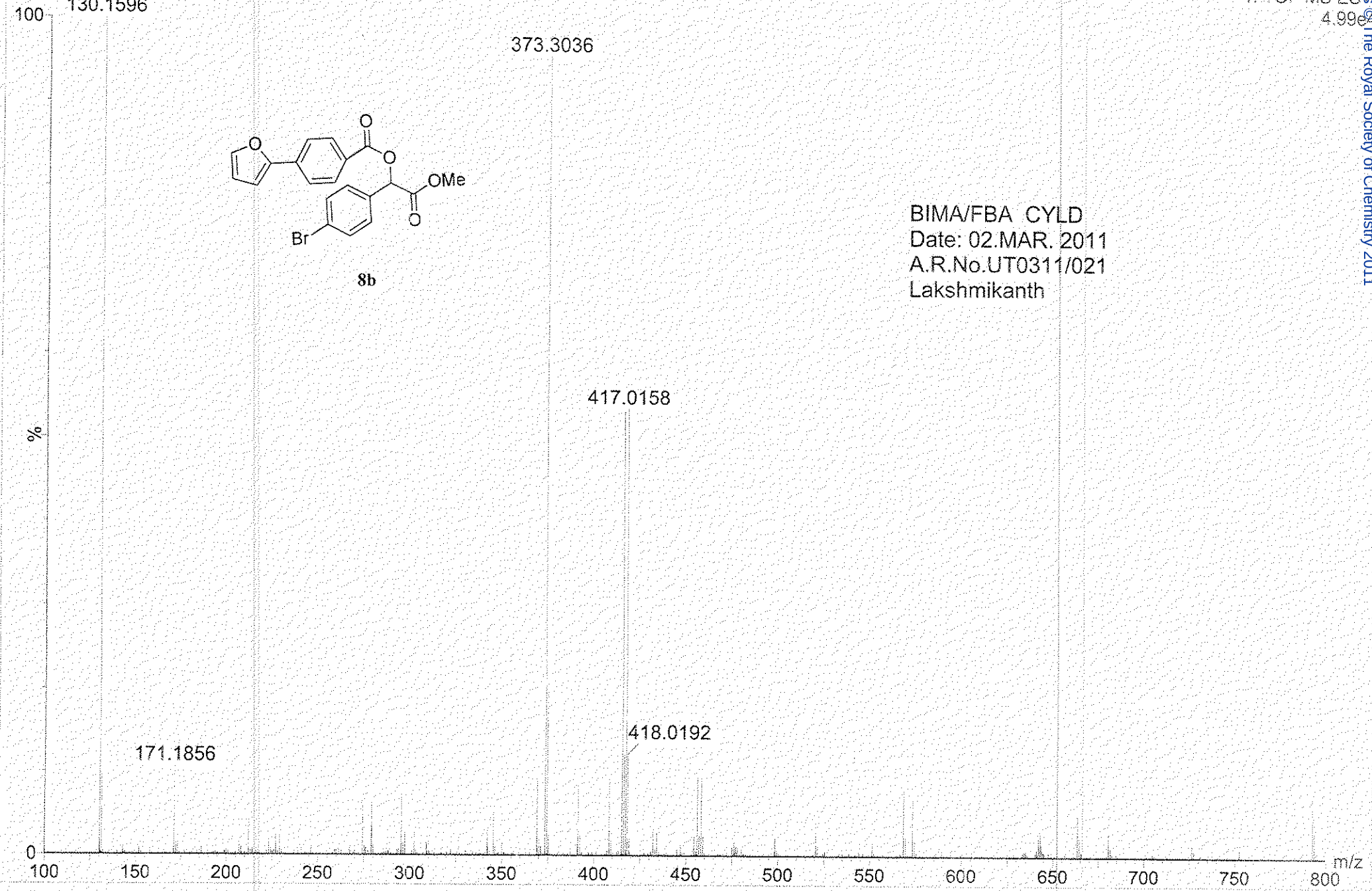
Plotname: 1396-TDC-213_BIMA-FBA_20110212_01_plot01

BIMA/FBA CYLD

Aurigene Discovery Technologies, Hyderabad

02-Mar-2011
Lakshmikanth
1. TOF MS ES+
4.99e3

UT0311_021 5 (0.103) Cm (5:20-87:93x0.010)



8b

BIMA/FBA CYLD
Date: 02.MAR. 2011
A.R.No.UT0311/021
Lakshmikanth

Elemental Composition Report

02/03/11

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.0, max = 15.0
Element prediction: Off
Number of isotope peaks usec for i-FIT = 3

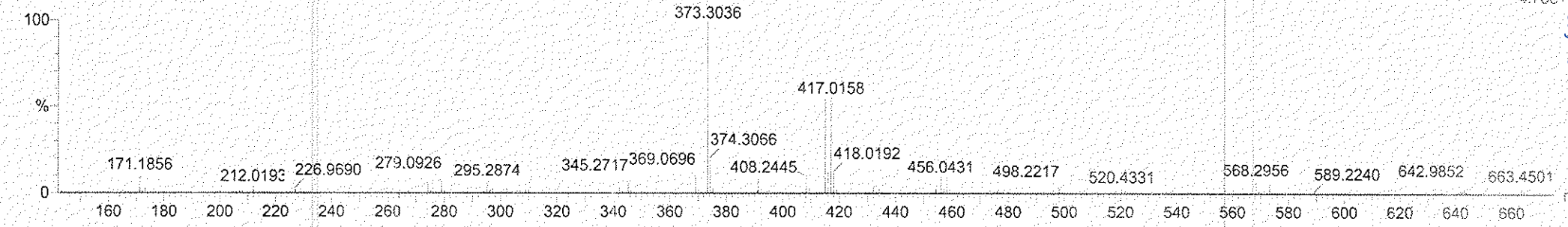
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-25 O: 0-7 Br: 0-1

BIMA/FBA CYLD

Aurigene Discovery Technologies, Hyderabad

02-Mar-2011
Lakshmikanth
1: TOF MS ES+
4.78e+00

UT0311_021 5 (0.103) Cm (5:20-87:93x0.010)

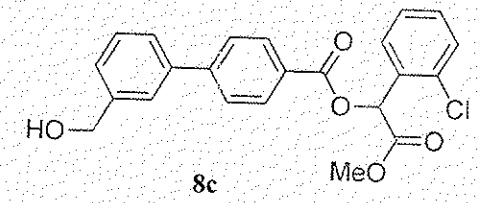


Minimum:				-1.0		
Maximum:		5.0	5.0	15.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
415.0173	415.0181	-0.8	-1.9	12.5	0.4	C20 H16 O5 Br

TDC-213 PHBA in DMSO

NMR-400
AR.No:ME1210/570

Analyst:Haribabu.R
Date: 7 th Dec. 2010



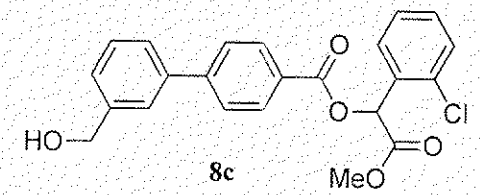
8c

TDC-213 PHBA in DMSO

NMR-400
AR.No:ME1110/1510
Analyst:Haribabu.R
Date: 19 th Nov 2010

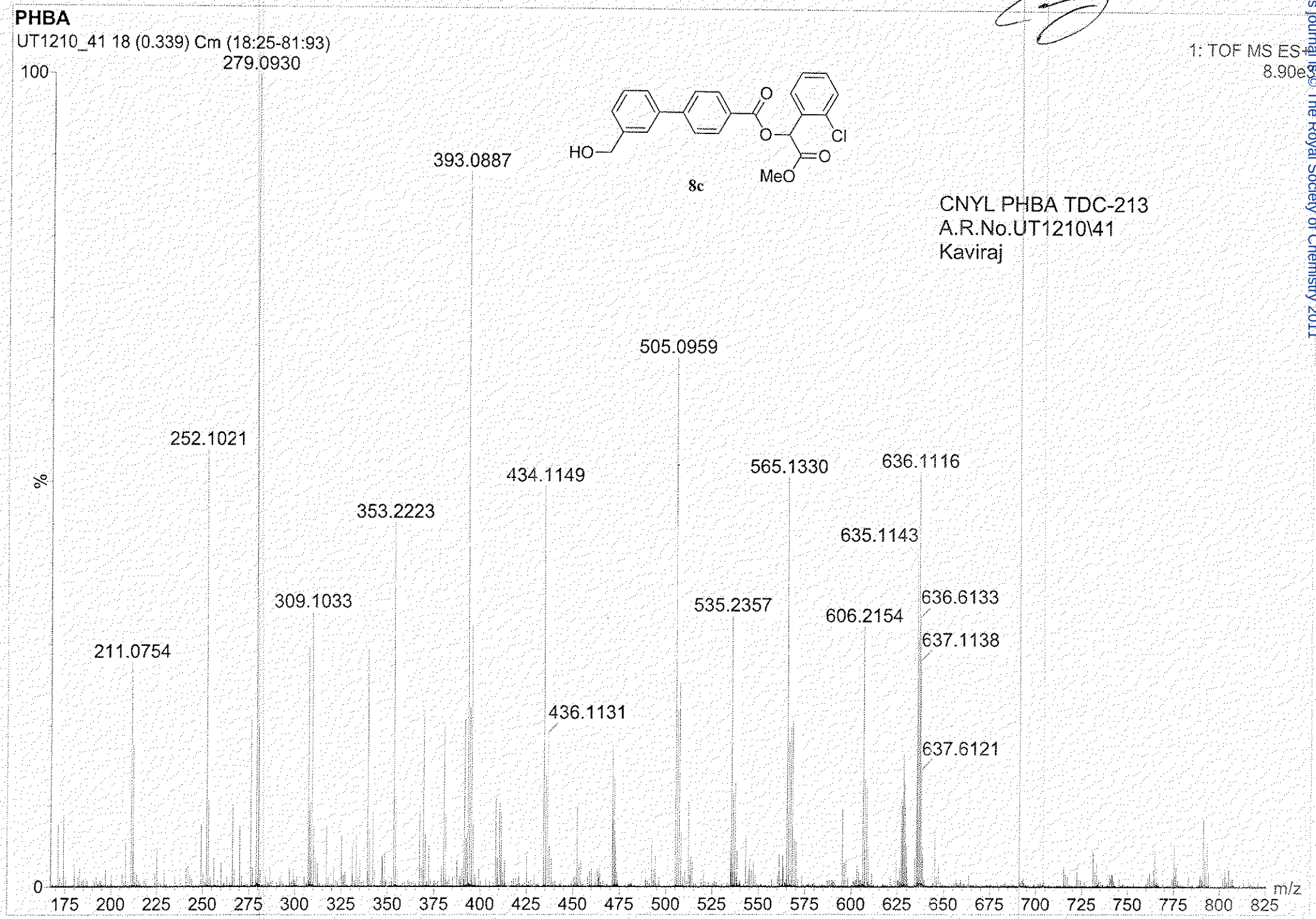
Sample Name:
1510-TDC-213_PHBA
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_19
Sample directory:
1510-TDC-213_PHBA_20101120_01
FidFile: 1510-TDC-213_PHBA_20101120_02

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 20 2010



8c

Plotname: 1510-TDC-213_PHBA_20101120_02_plot01

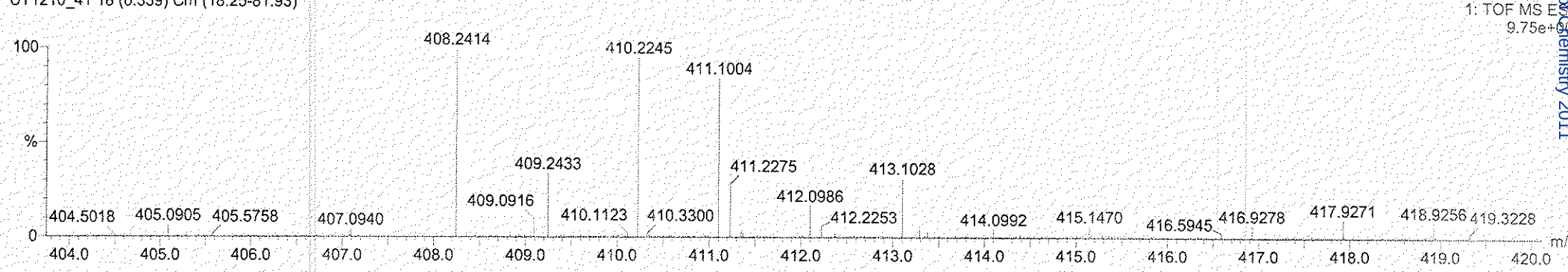


Elemental Composition Report

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
84 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 O: 0-8 Cl: 0-1
PHBA
UT1210_41 18 (0.339) Cm (18:25-81:93)



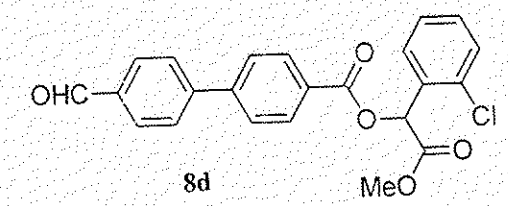
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
411.1004	411.0999	0.5	1.2	13.5	6.9	C23 H20 O5 Cl
	411.1021	-1.7	-4.1	22.5	137.1	C29 H15 O3

TDC-213 FPBA in DMSO

NMR-400
AR.No:ME1110/120
Analyst:Shruthi
Date: 2nd Nov 2010

Sample Name:
120_TDC-213_FPBA
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_02
Sample directory:
120_TDC-213_FPBA_20101102_01
FidFile: 120_TDC-213_FPBA_20101102_01

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Nov 2 2010



8d

VARIAN

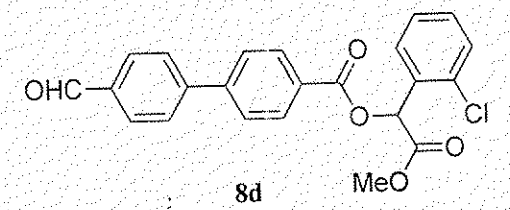
Plotname: 120_TDC-213_FPBA_20101102_01_plot01

TDC-213 FPBA in DMSO

NMR-400
AR.No:ME1110/1511
Analyst:Haribabu.R
Date: 19 th Nov 2010

Sample Name:
1511-TDC-213_FPBA
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_19
Sample directory:
1511-TDC-213_FPBA_20101120_01
FidFile: 1511-TDC-213_FPBA_20101120_01

Pulse Sequence: CARBON (s2pul)
Solvent: dmso
Data collected on: Nov 20 2010



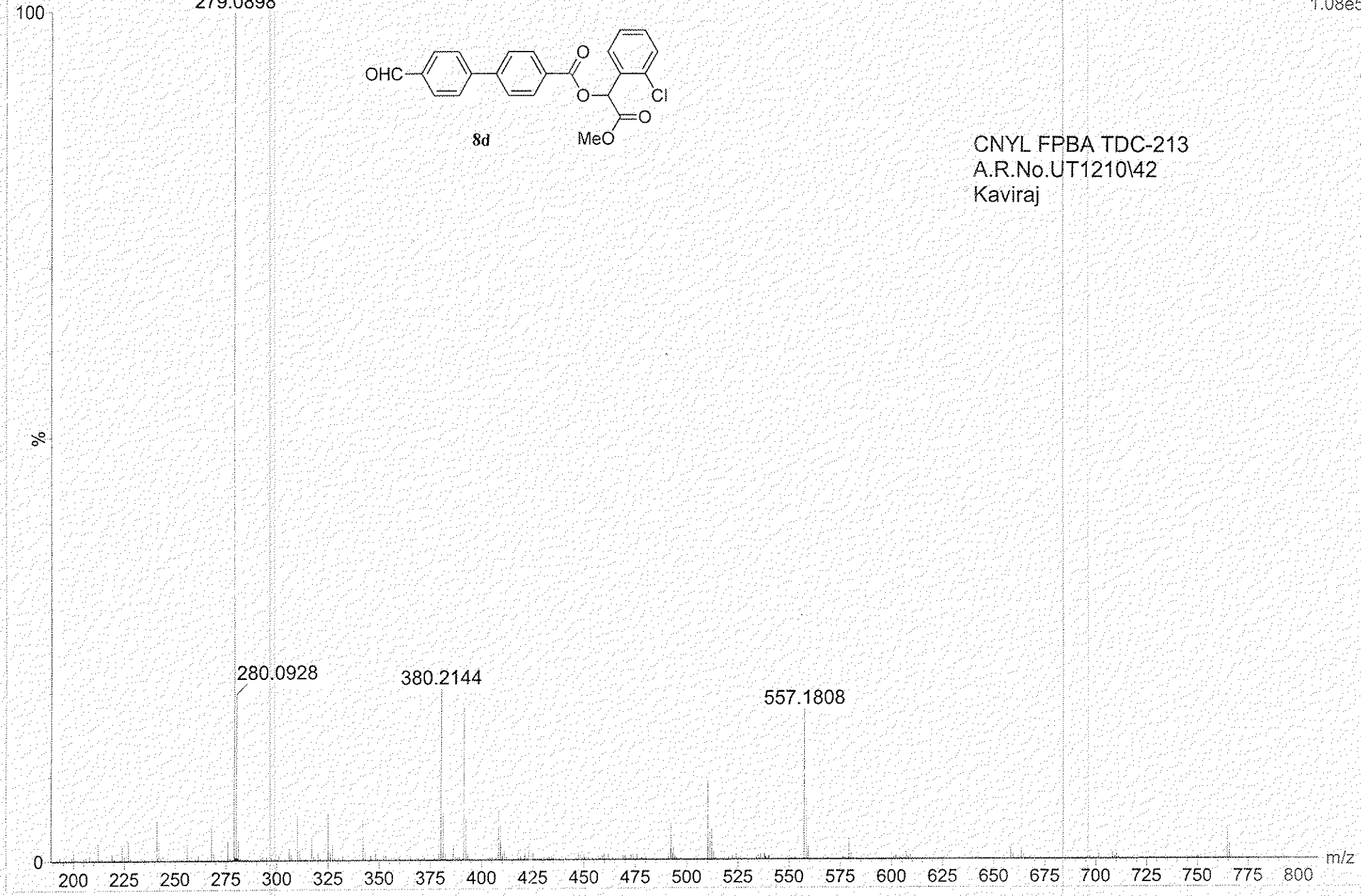
8d

Plotname: 1511-TDC-213_FPBA_20101120_01_plot01

FPBA

UT1210_42 17 (0.324) Cm (17:31-85:101)

1: TOF MS ES+
1.08e5



8d

CNYL FPBA TDC-213
A.R.No.UT1210\42
Kaviraj

Elemental Composition Report

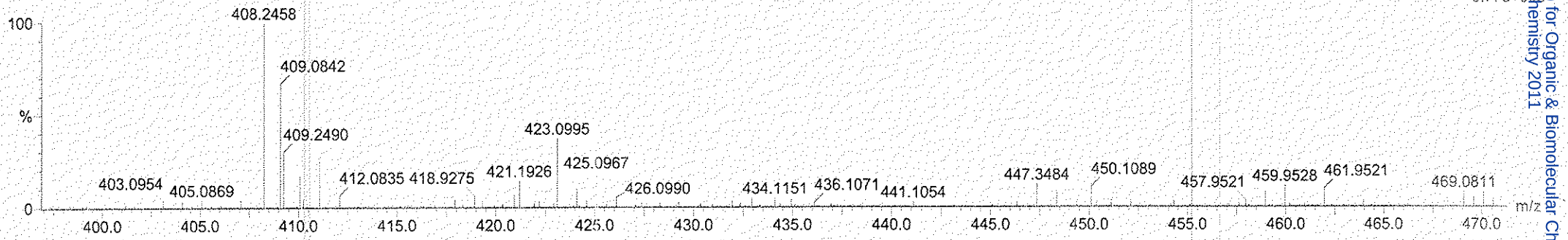
Single Mass Analysis

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
80 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 O: 0-8 Cl: 0-1

FPBA
UT1210_42 17 (0.324) Cm (17:31-85:101)

1: TOF MS ES+
6.77e+003



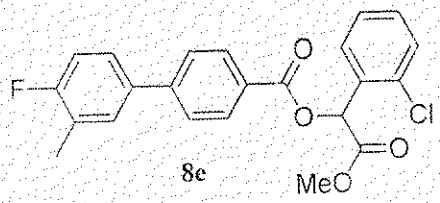
Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
409.0842	409.0843	-0.1	-0.2	14.5	1.6	C23 H18 O5 Cl

TDC-213 MFBA in DMSO

NMR-400
AR.No:ME1110/302
Analyst:Haribabu.R
Date: 8th Nov 2010

Sample Name:
302-TDC-213_MFBA
Data Collected on:
mercuryj-mercury400
Archive directory:
/home/sms50/routine/Nov2010/d_08
Sample directory:
302-TDC-213_MFBA_20101108_01
FidFile: 302-TDC-213_MFBA_20101108_01

Pulse Sequence: PROTON (s2pul)
Solvent: dmso
Data collected on: Nov 8 2010



8e

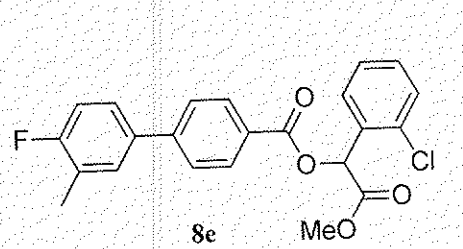
Plotname: 302-TDC-213_MFBA_20101108_01_plot01

VARIAN

MFBA

UT1110_89 8 (0.145) Cm (7:12-85:92)

1: TOF MS ES+
2.78e3



8e

CNYL MFBA TDC-213
A.R.No.UT1110\89
Kaviraj

Elemental Composition Report

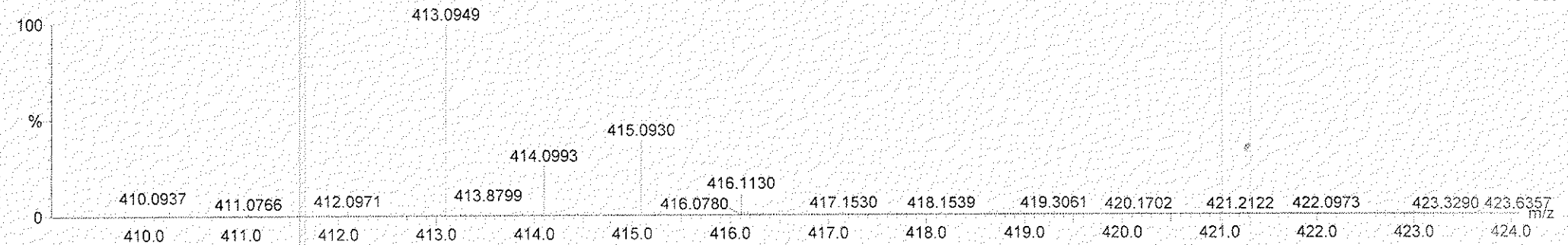
Single Mass Analysis

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

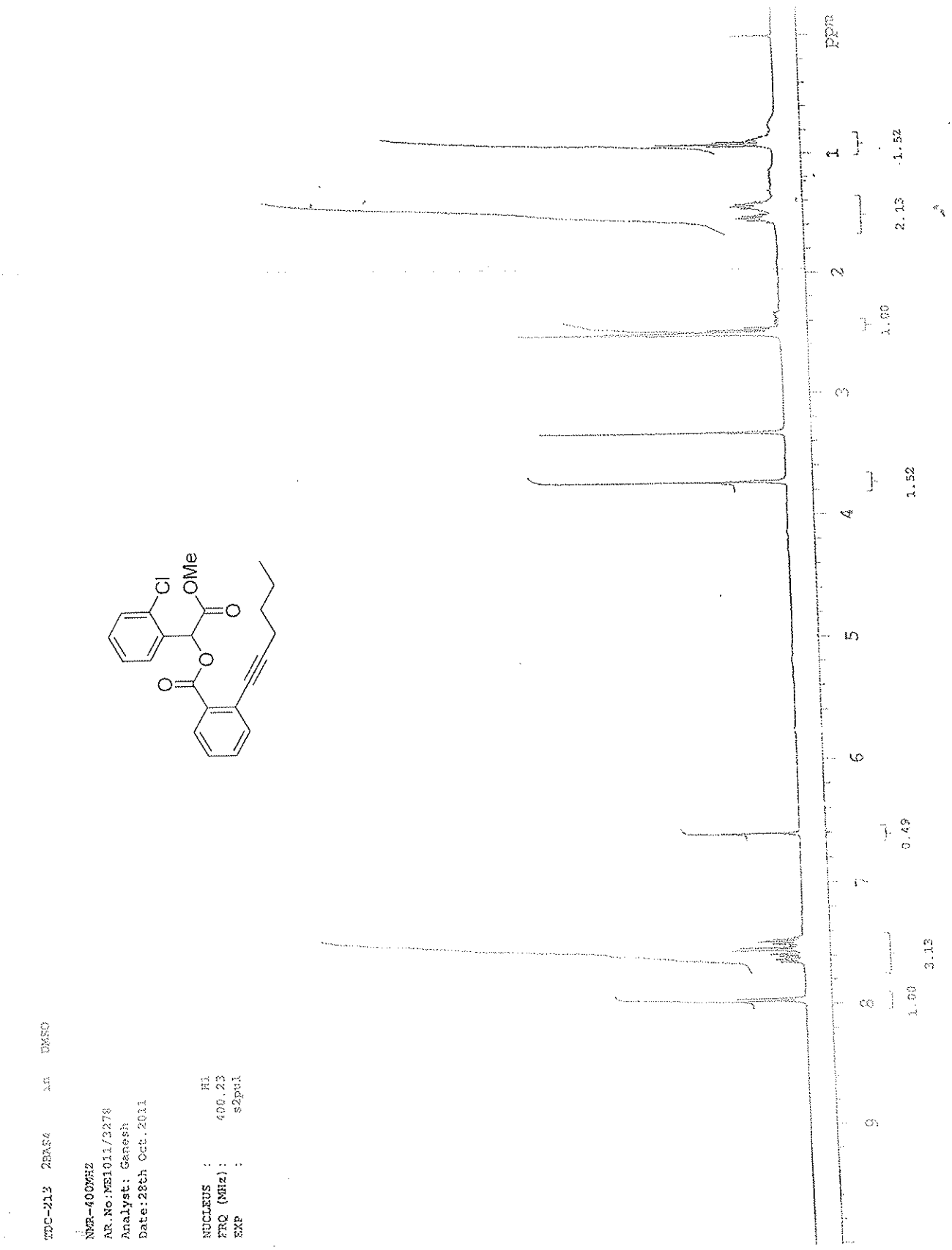
Monoisotopic Mass, Even Electron Ions
227 formula(e) evaluated with 4 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-55 H: 0-65 O: 0-5 F: 0-3 Cl: 0-1

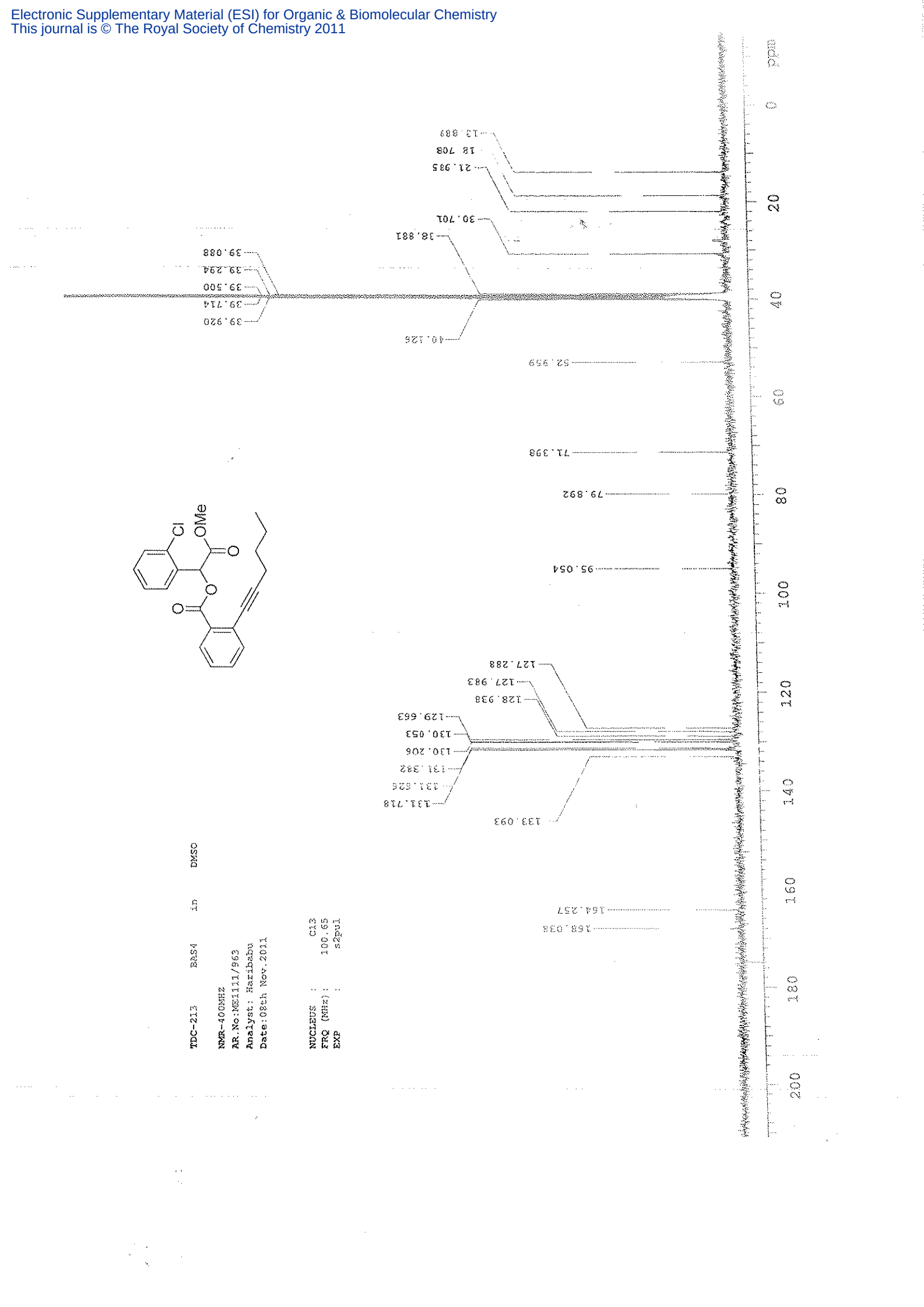
MFBA
UT1110_89 8 (0.145) Cm (7:12-85:92)

1: TOF MS ES+
1.41e+003



Minimum:				-1.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
413.0949	413.0956	-0.7	-1.7	13.5	1.6	C23 H19 O4 F Cl
	413.0967	-1.8	-4.4	9.5	4.0	C20 H20 O5 F2 Cl
	413.0944	0.5	1.2	17.5	4.1	C26 H18 O3 Cl
	413.0966	-1.7	-4.1	26.5	219.0	C32 H13 O

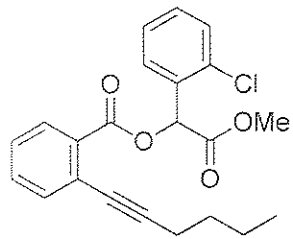




Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4



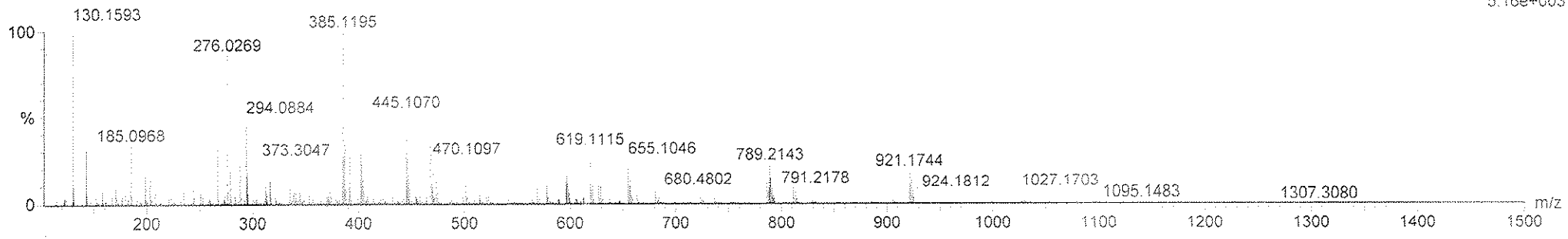
Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 O: 0-6 Cl: 0-1

BAS4

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

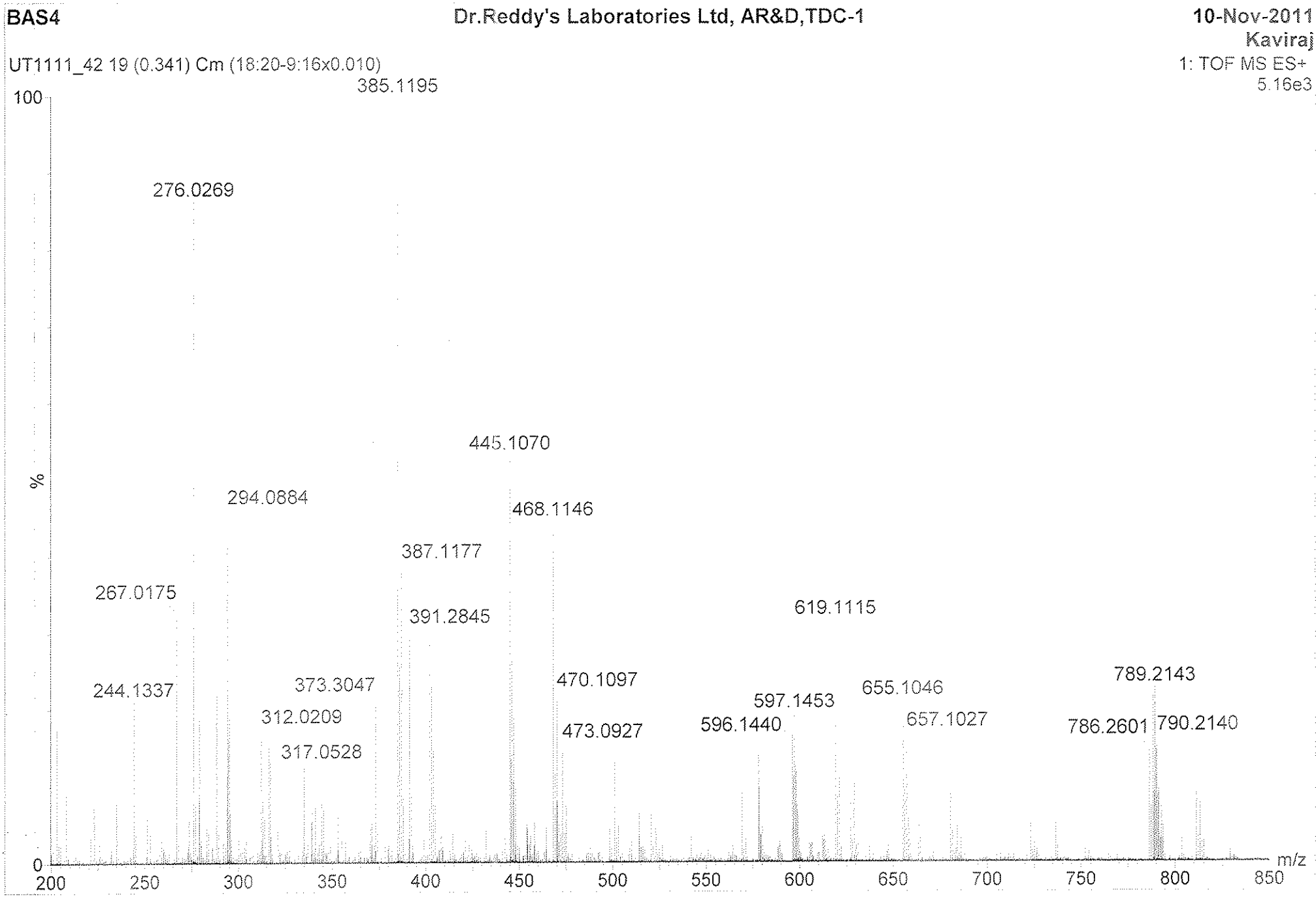
10-Nov-2011
Kaviraj
1: TOF MS ES+
5.16e+003

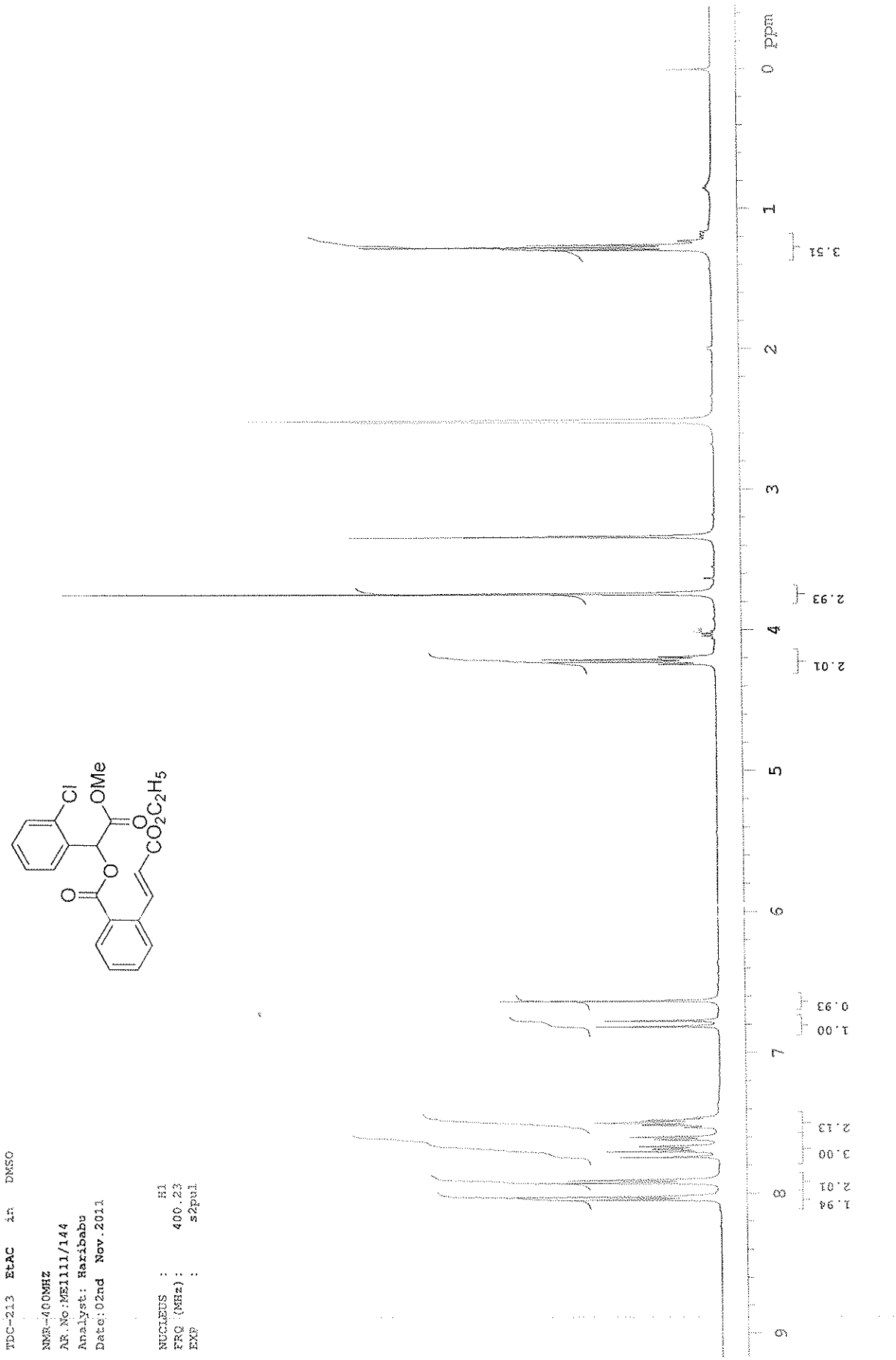
UT1111_42 19 (0.341) Cm (18:20-9:16x0.010)

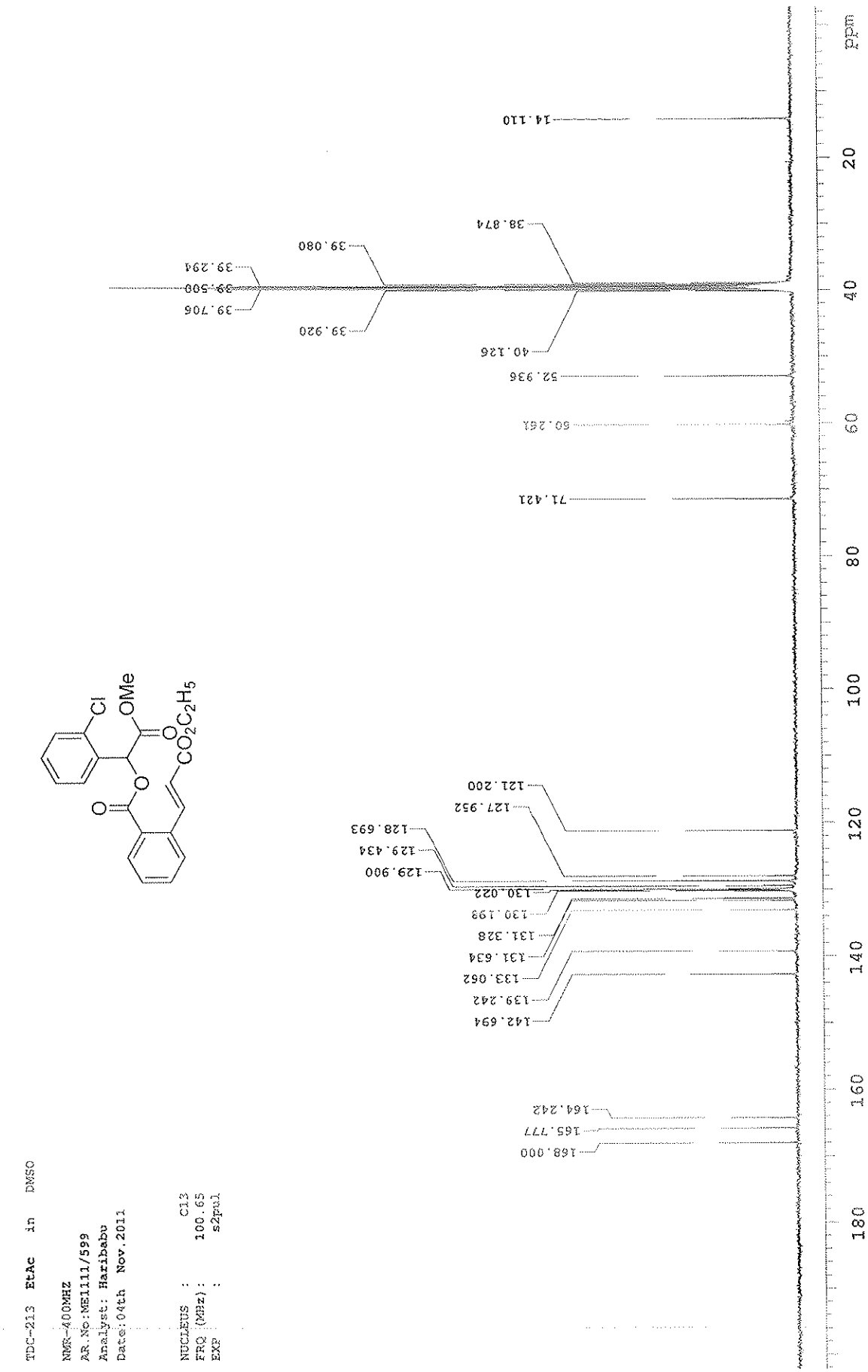


Minimum:				0.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.1195	385.1207	-1.2	-3.1	11.5	2.9	C22 H22 O4 Cl

BA1265
10/11/2011



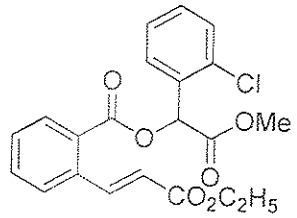




Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4



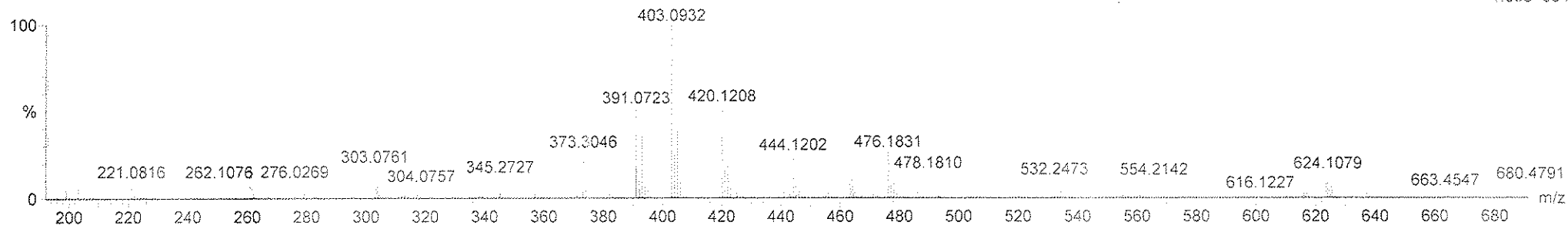
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 O: 0-6 Cl: 0-1

ETAC

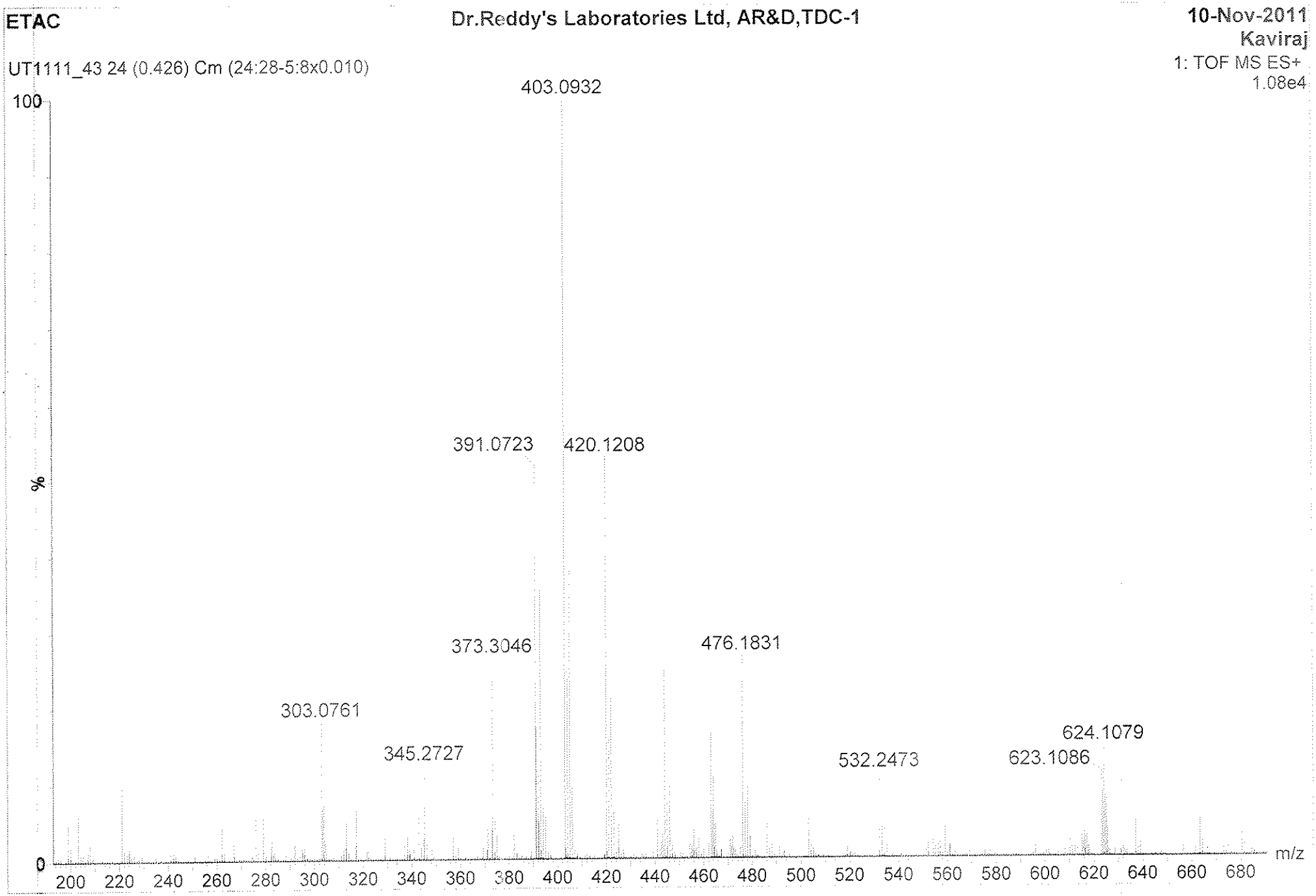
Dr.Reddy's Laboratories Ltd, ARD,TDC-1

10-Nov-2011
Kaviraj
1: TOF MS ES+
1.08e+004

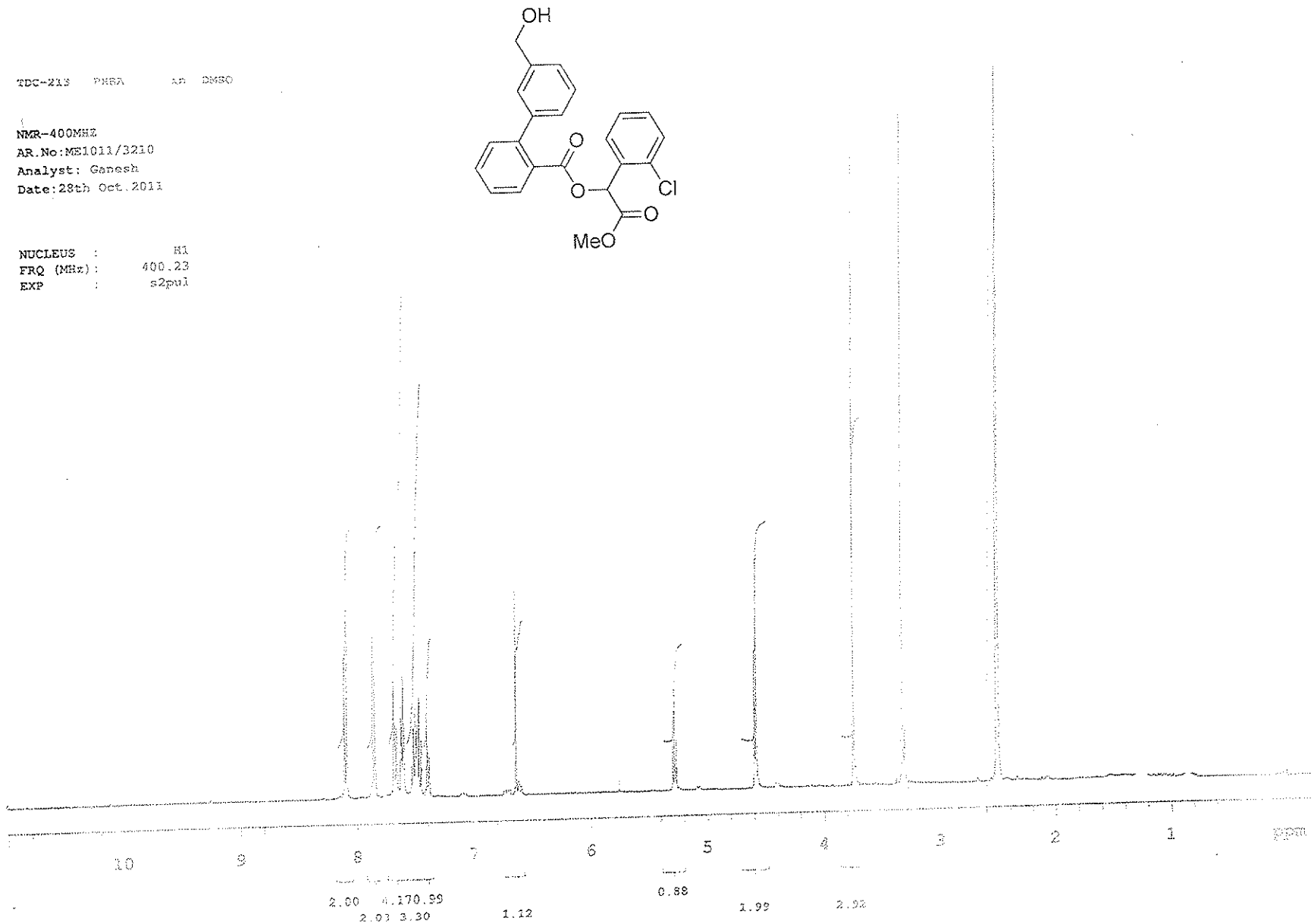
UT1111_43 24 (0.426) Cm (24:28-5:8x0.010)

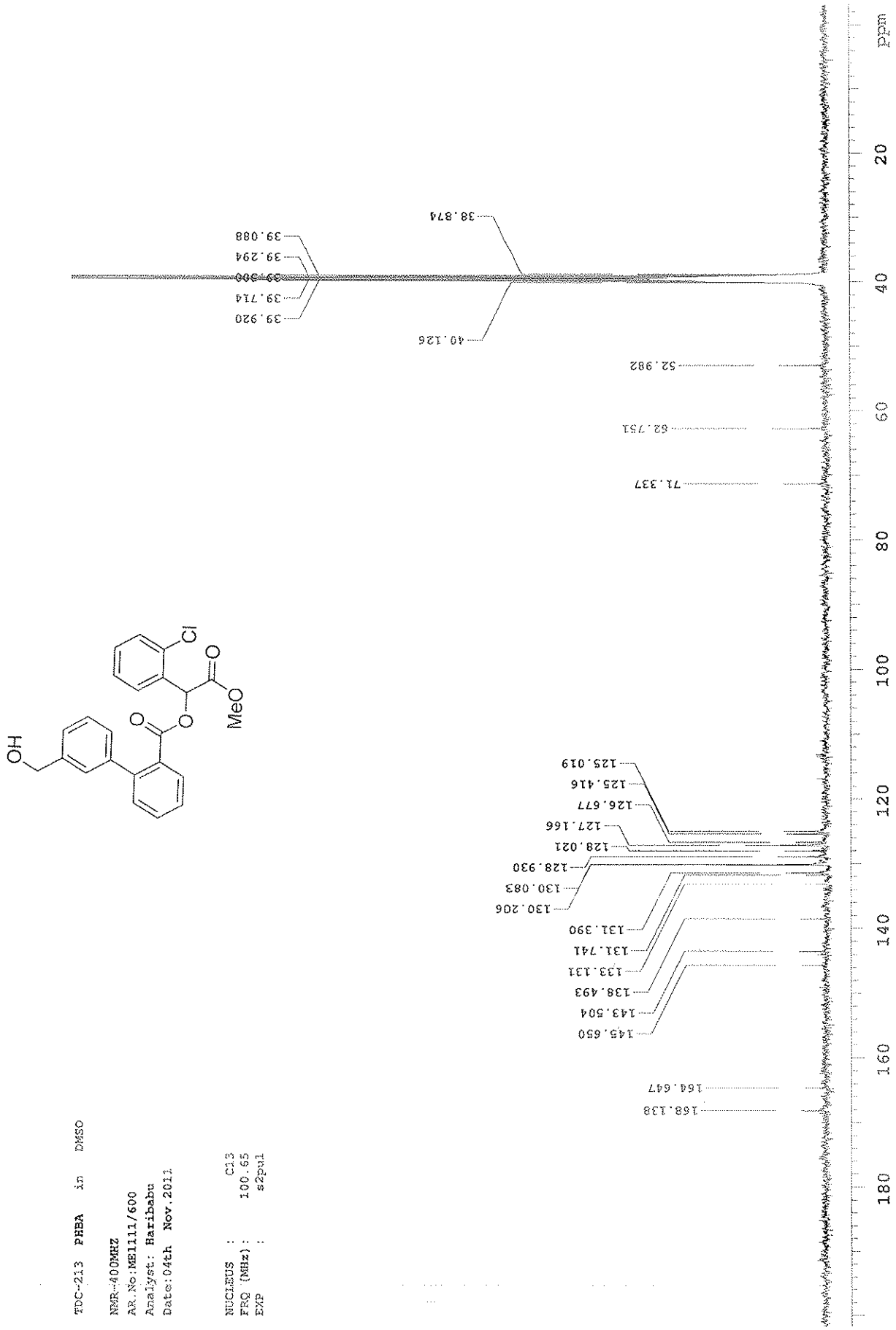


Minimum:				0.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
403.0932	403.0948	-1.6	-4.0	11.5	14.2	C21 H20 O6 Cl

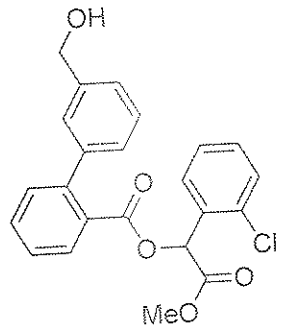


10/11/2011





Elemental Composition Report



Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

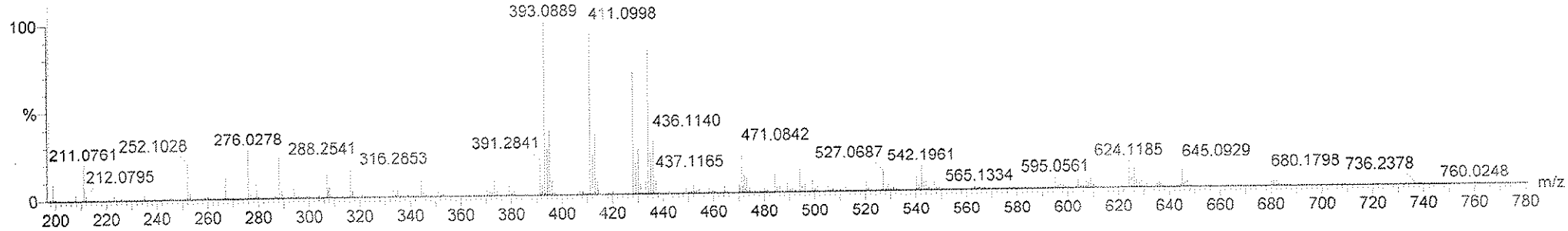
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 O: 0-6 Cl: 0-1

PHBA

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

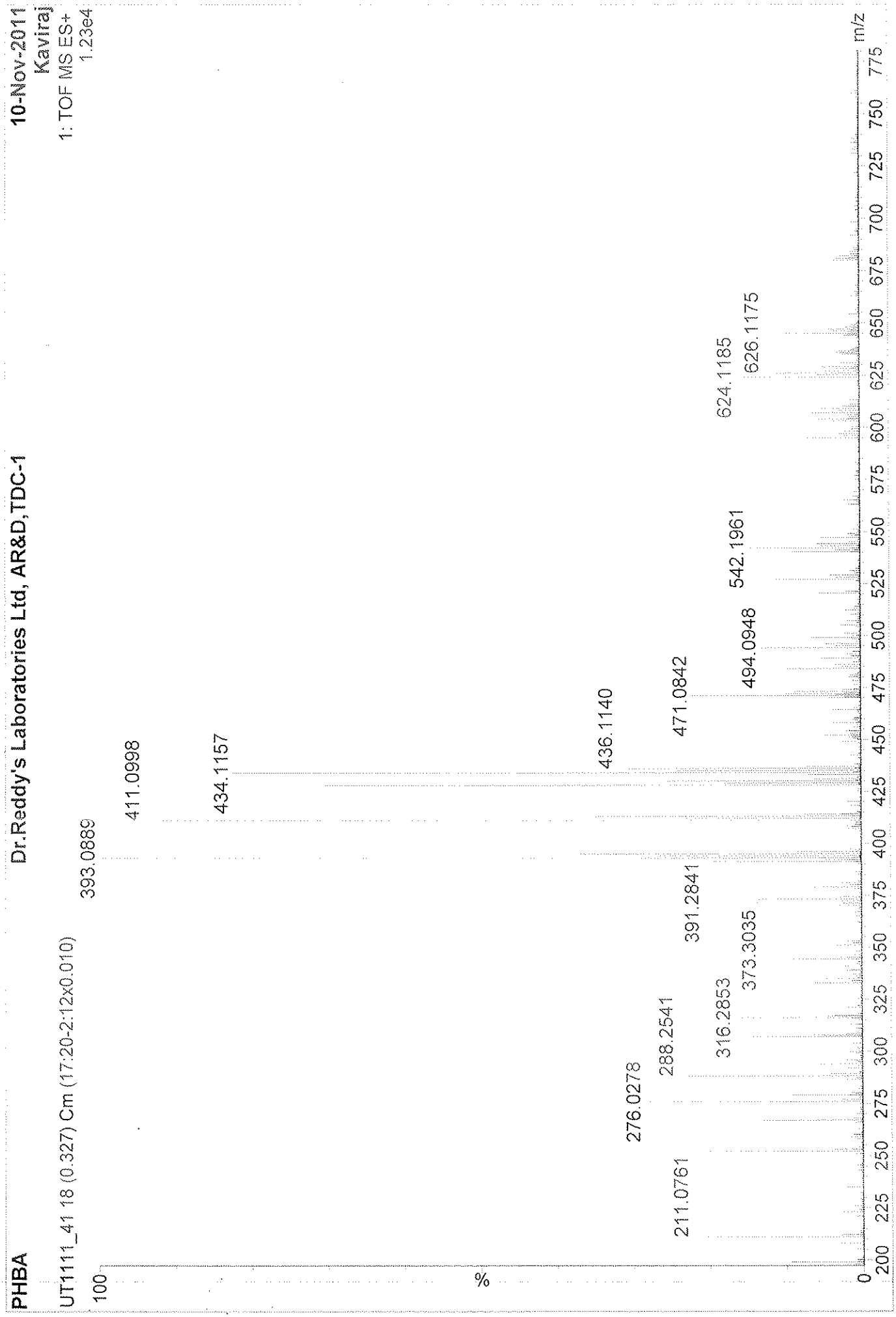
10-Nov-2011
Kaviraj
1: TOF MS ES+
1.23e+004

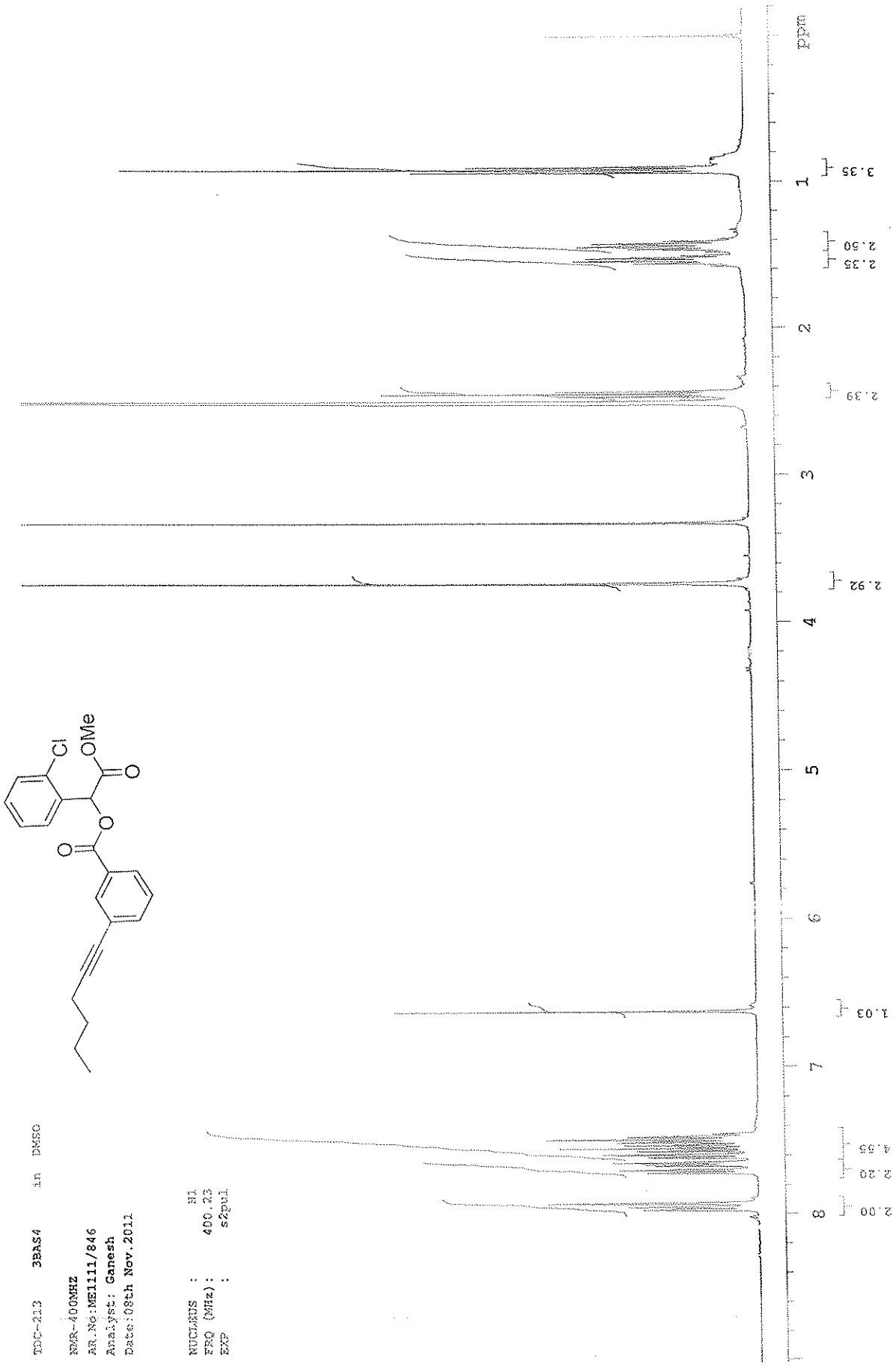
UT1111_41 18 (0.327) Cm (17:20-2:12x0.010)

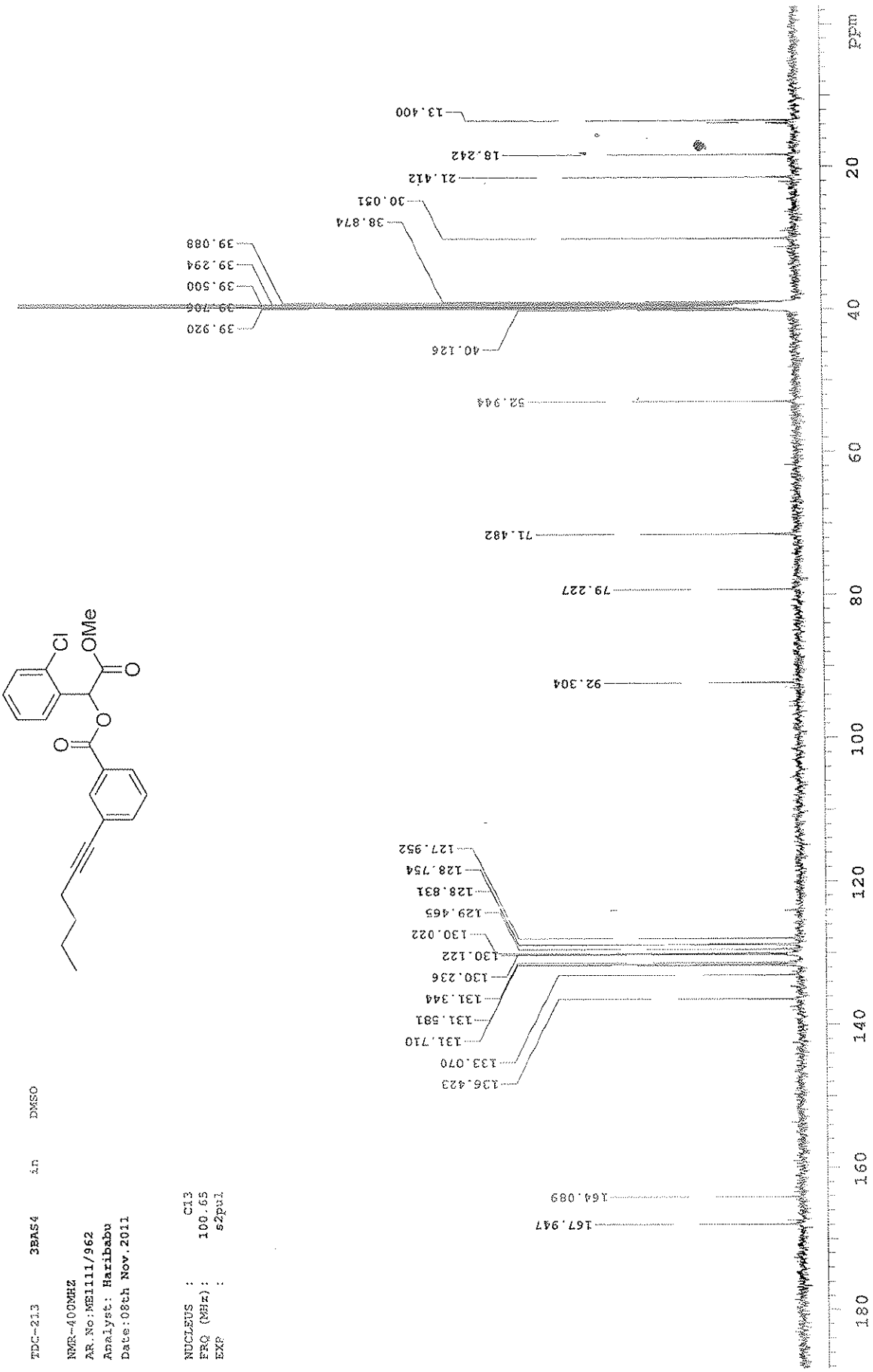


Minimum:				0.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
411.0998	411.0999	-0.1	-0.2	13.5	10.3	C23 H20 O5 Cl

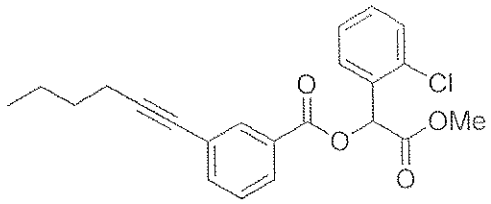
sotks
9/11/2011







Elemental Composition Report

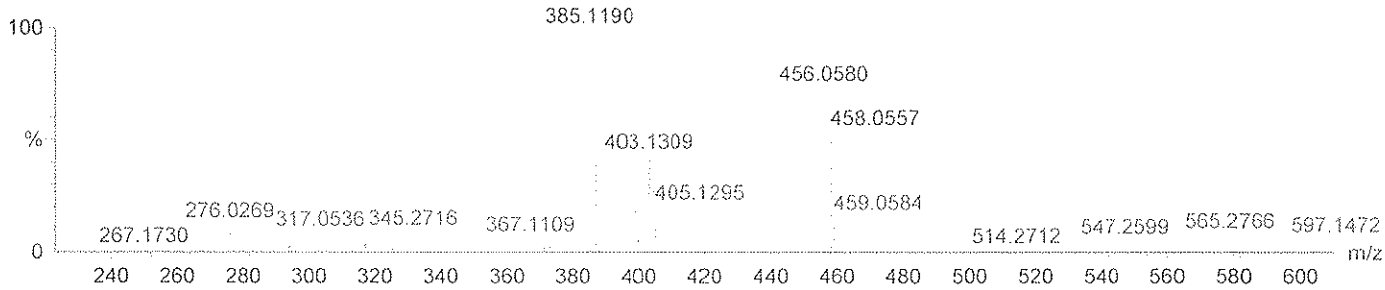


Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

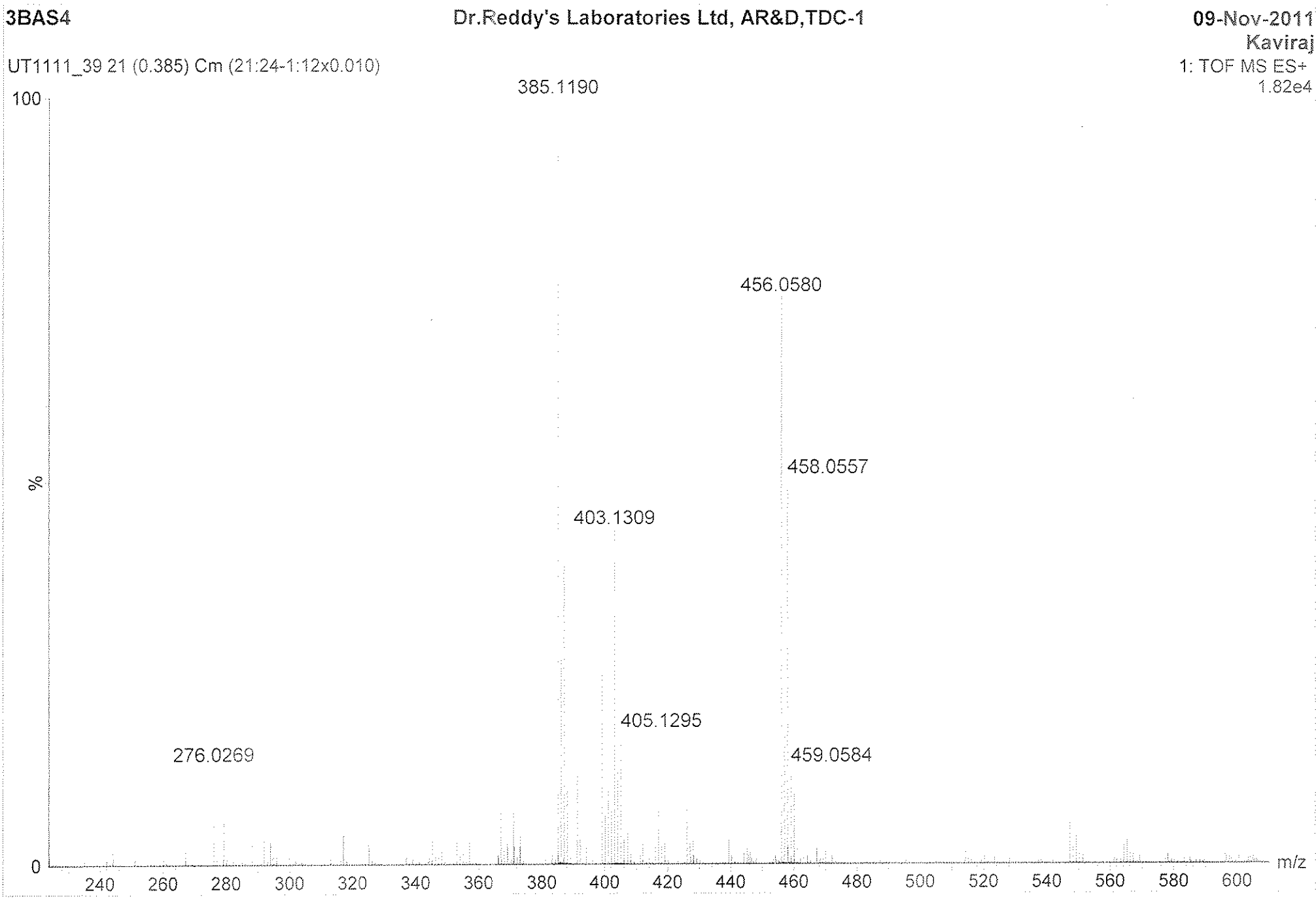
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 O: 0-4 Cl: 0-1

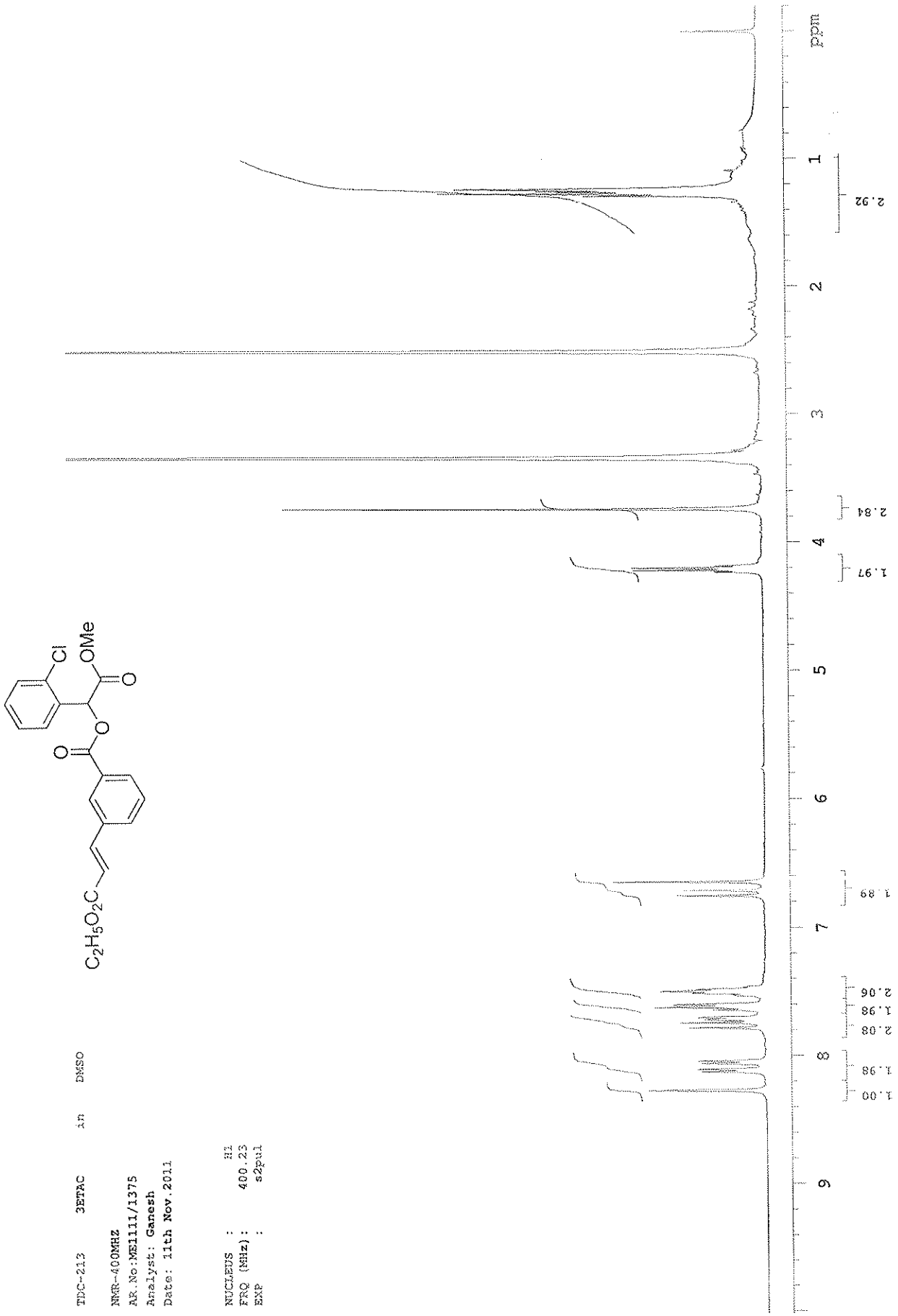
3BAS4 Dr.Reddy's Laboratories Ltd, ARD,TDC-1 09-Nov-2011
Kaviraj
UT1111_39 21 (0.385) Cm (21:24-1:12x0.010) 1: TOF MS ES+
1.82e+004

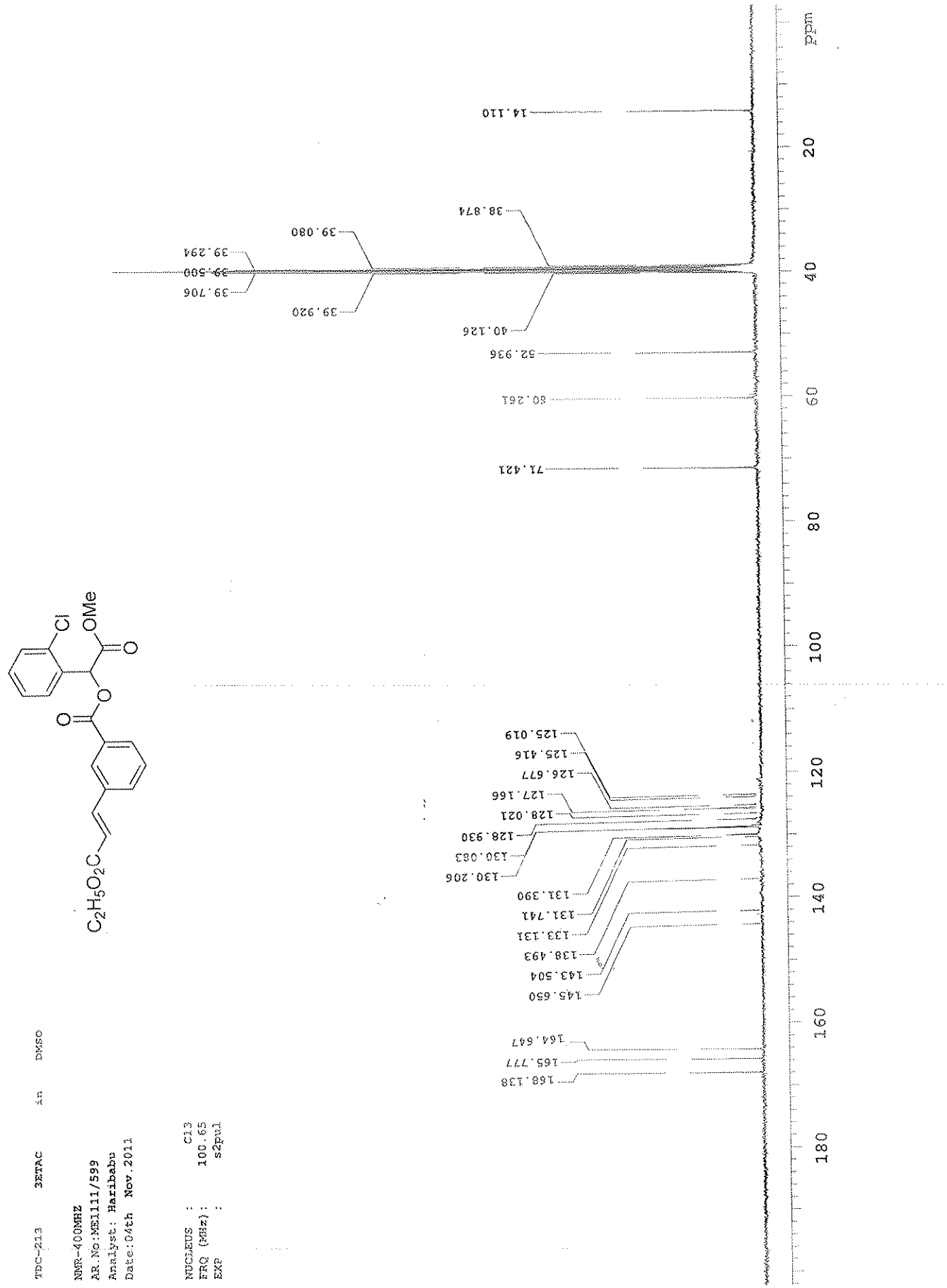


Minimum:		5.0	5.0	0.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.1190	385.1207	-1.7	-4.4	11.5	33.5	C22 H22 O4 Cl

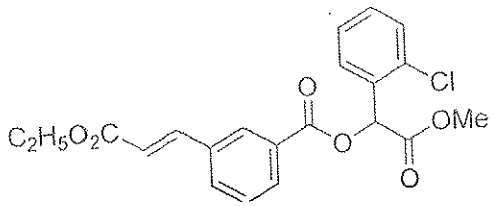
Bothra
03/11/2011







Elemental Composition Report

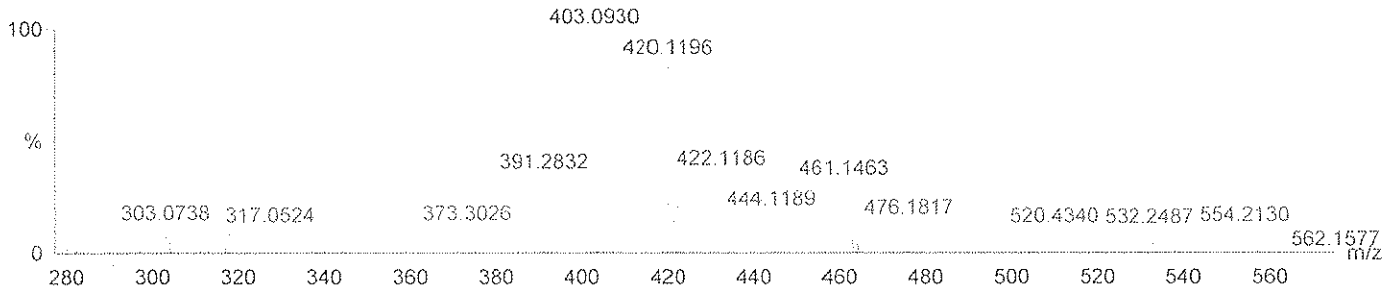


Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

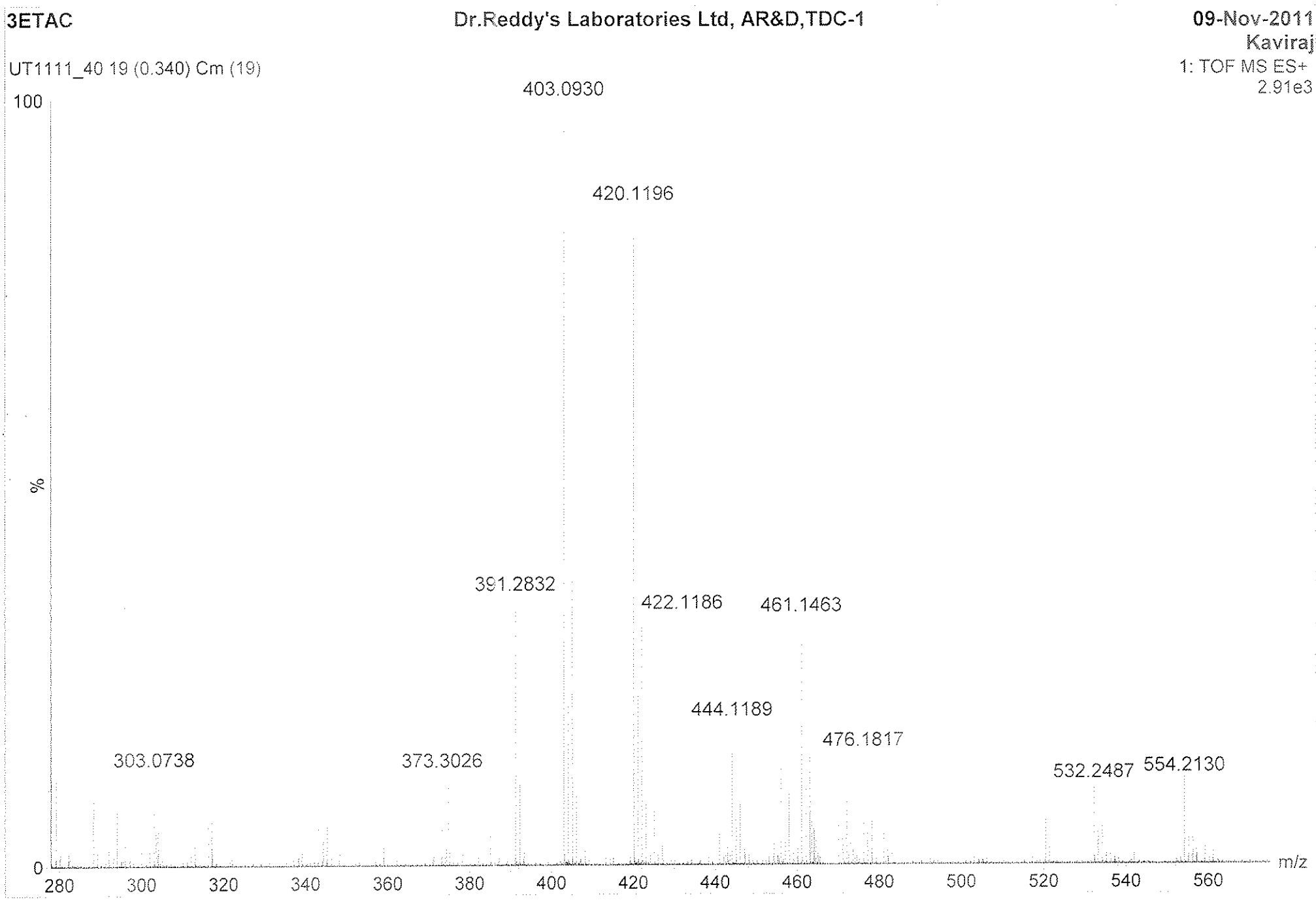
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 O: 0-6 Cl: 0-1

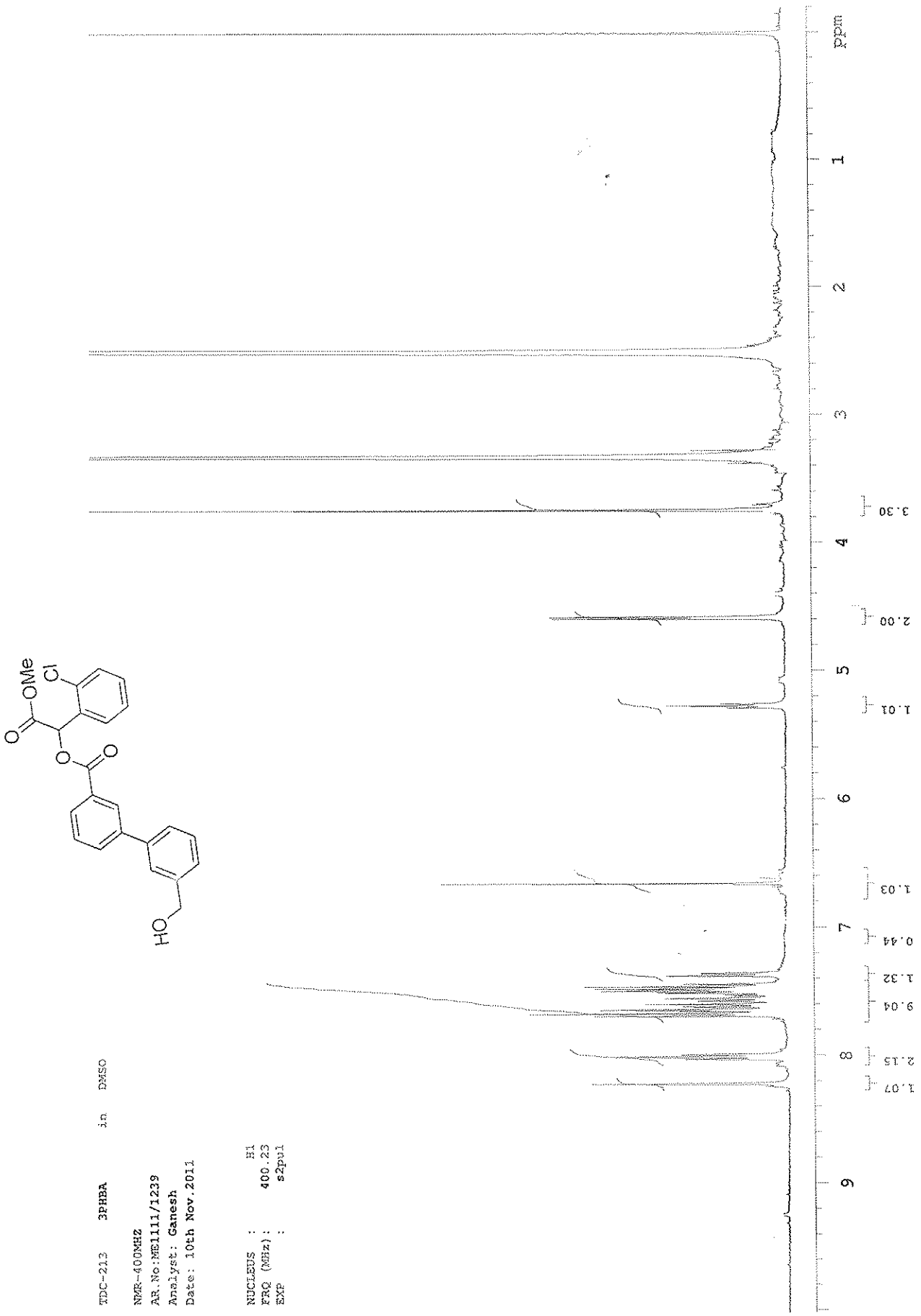
3ETAC — Dr.Reddy's Laboratories Ltd, ARD,TDC-1 — 09-Nov-2011
Kaviraj
UT1111_40 19 (0.340) Cm (19) — 1: TOF MS ES+
2.92e+003

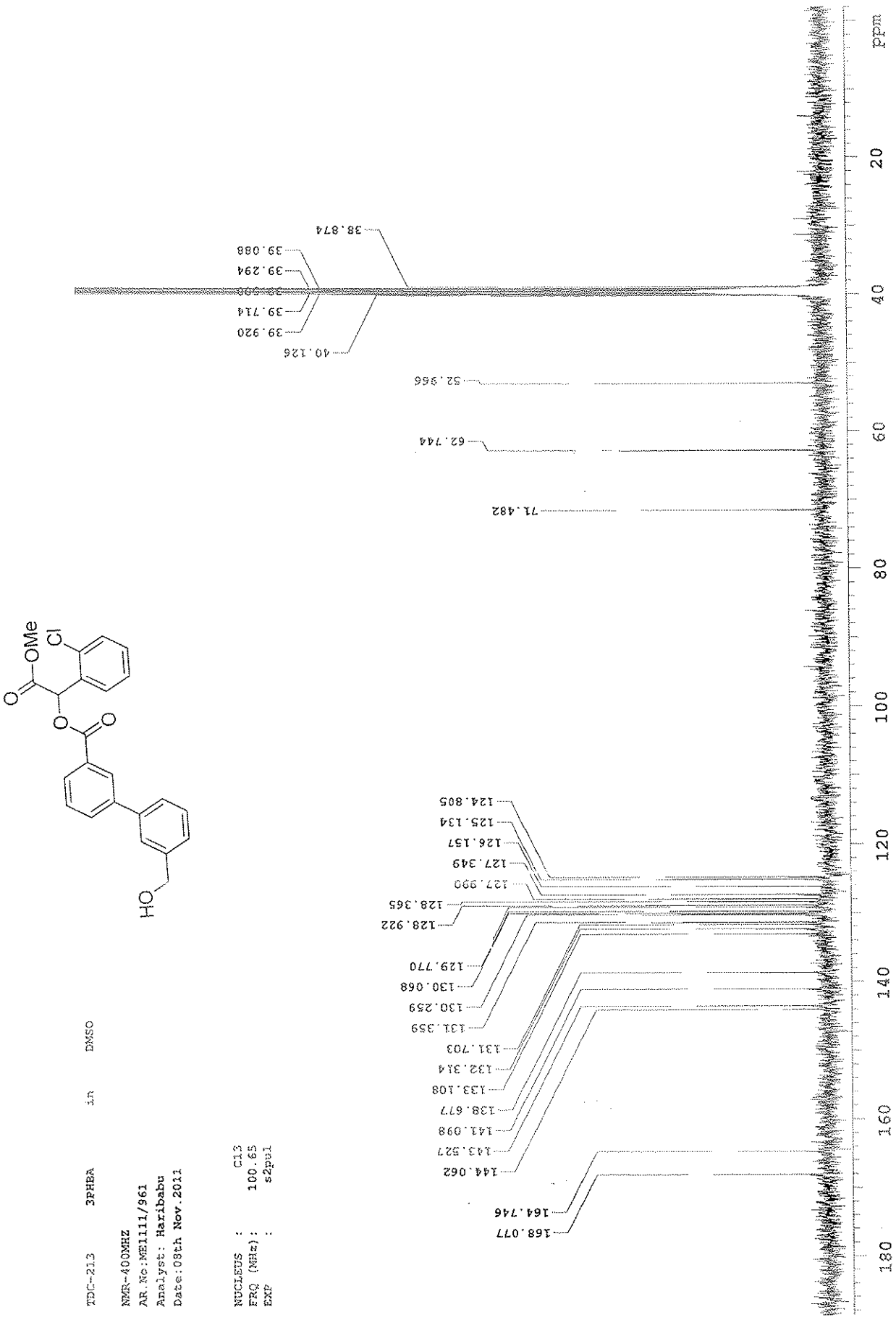


Minimum:				0.0		
Maximum:		5.0	10.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
403.0930	403.0948	-1.8	-4.5	11.5	3.5	C21 H20 O6 Cl

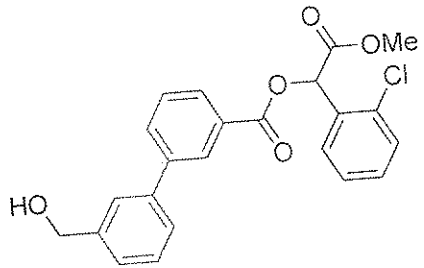
09/11/2011







Elemental Composition Report

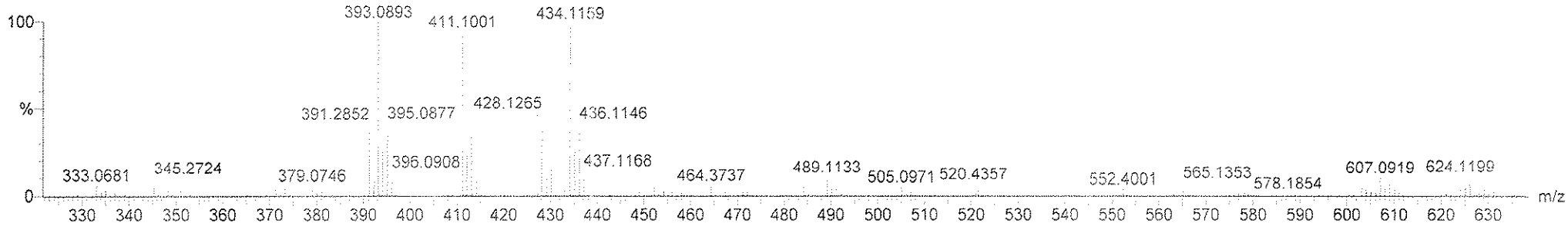


Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = 0.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 O: 0-6 Cl: 0-1

3PHBA Dr.Reddy's Laboratories Ltd, ARD,TDC-1 09-Nov-2011
Kaviraj
UT1111_38 18 (0.327) Cm (17:24-82:96x0.010) 1: TOF MS ES+
1.96e+004



Minimum:				0.0		
Maximum:		5.0	4.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
411.1001	411.0999	0.2	0.5	13.5	2.3	C23 H20 O5 Cl

Prathap
03/11/2011