

**Palladium Mediated Intramolecular Multiple C-X/C-H Cross Coupling & C-H Activation:
Synthesis of Carbazole Alkaloids Calothrixin B & Murrayaquinone A**

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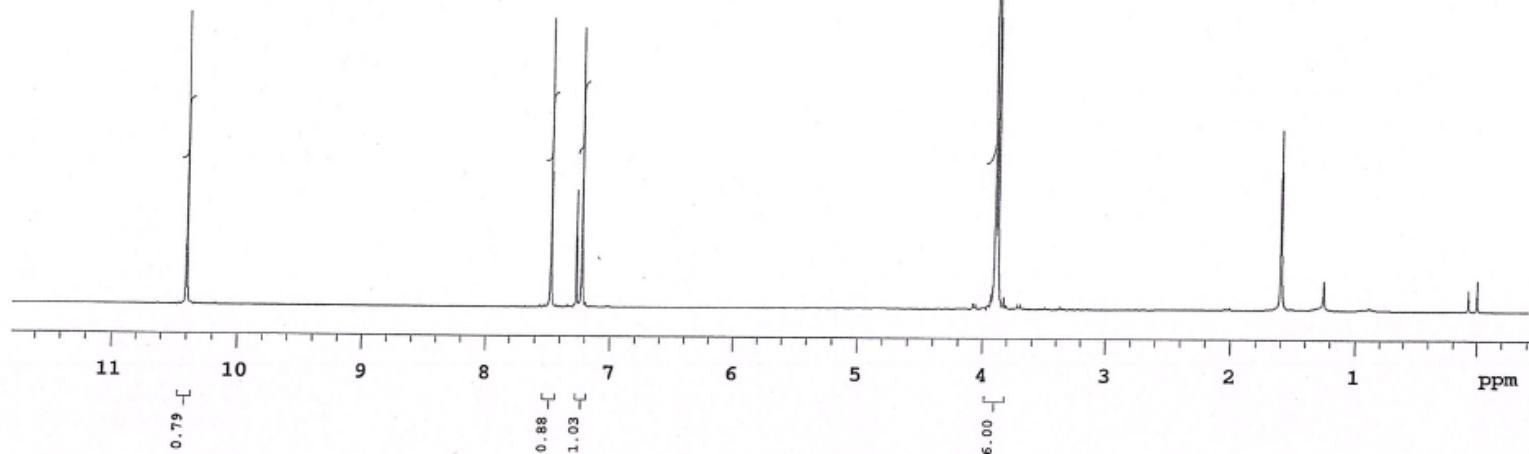
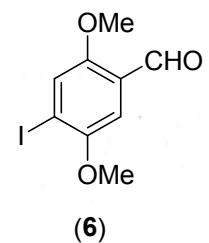
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¹H NMR of 4-iodo-2,5-dimethoxybenzaldehyde (6)

TDC-110 Iodo aldehyde in CDCl₃
NMR-400MHz
AR.No:ME1012/2734
Analyst: Haribabu
Date: 29th Oct. 2012

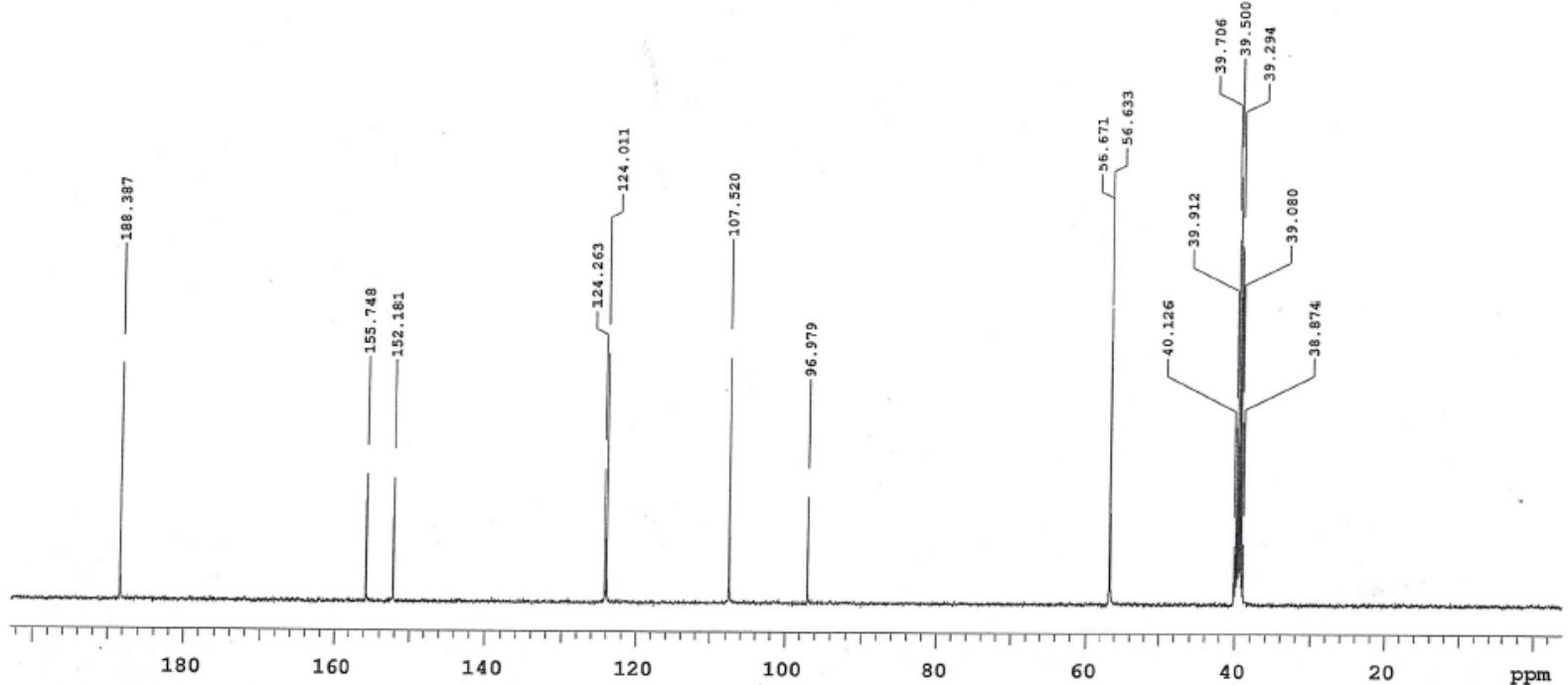
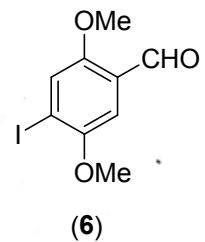
NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul



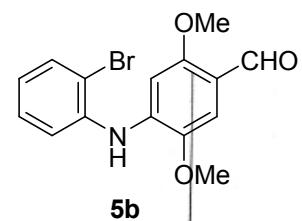
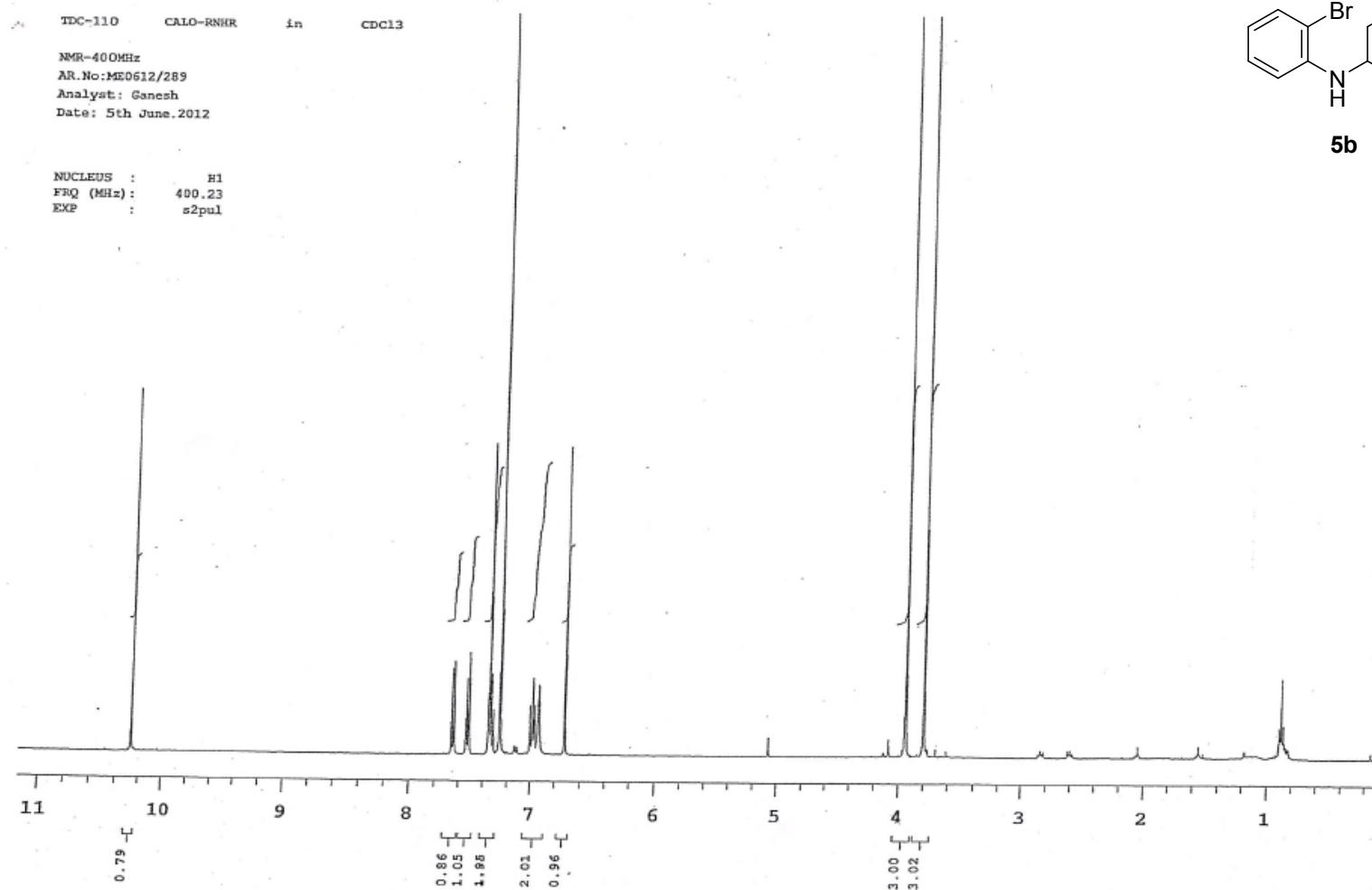
¹³C NMR of 4-iodo-2,5-dimethoxybenzaldehyde (6)

TDC-110 Iodo Aldehyde in DMSO
NMR-400MHz
AR.No:ME0813/1481
Analyst: Ganesh
Date: 16th Aug. 2013

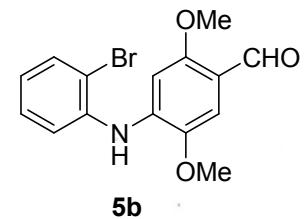
NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul



¹H NMR of 4 4-((2-bromophenyl)amino)-2,5-dimethoxybenzaldehyde (5b)



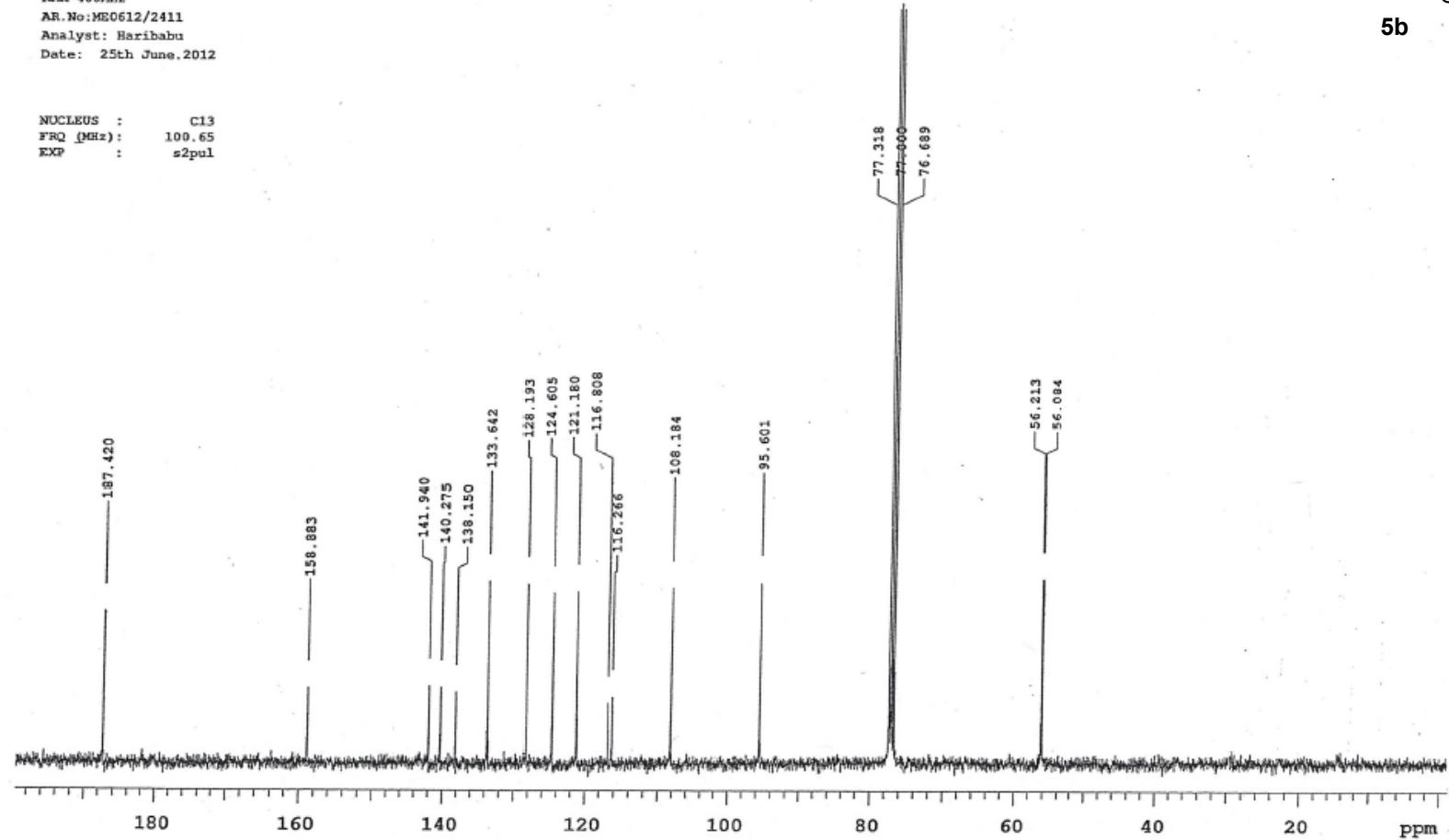
¹³C NMR of 4-((2-bromophenyl)amino)-2,5-dimethoxybenzaldehyde (5b)



TDC-110 Galo/RNHR/001 in CDCl₃

NMR-400MHz
AR.No:ME0612/2411
Analyst: Haribabu
Date: 25th June, 2012

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : z2pul

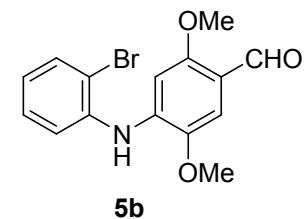


Mass Spectrum of 4-((2-bromophenyl)amino)-2,5-dimethoxybenzaldehyde (5b)

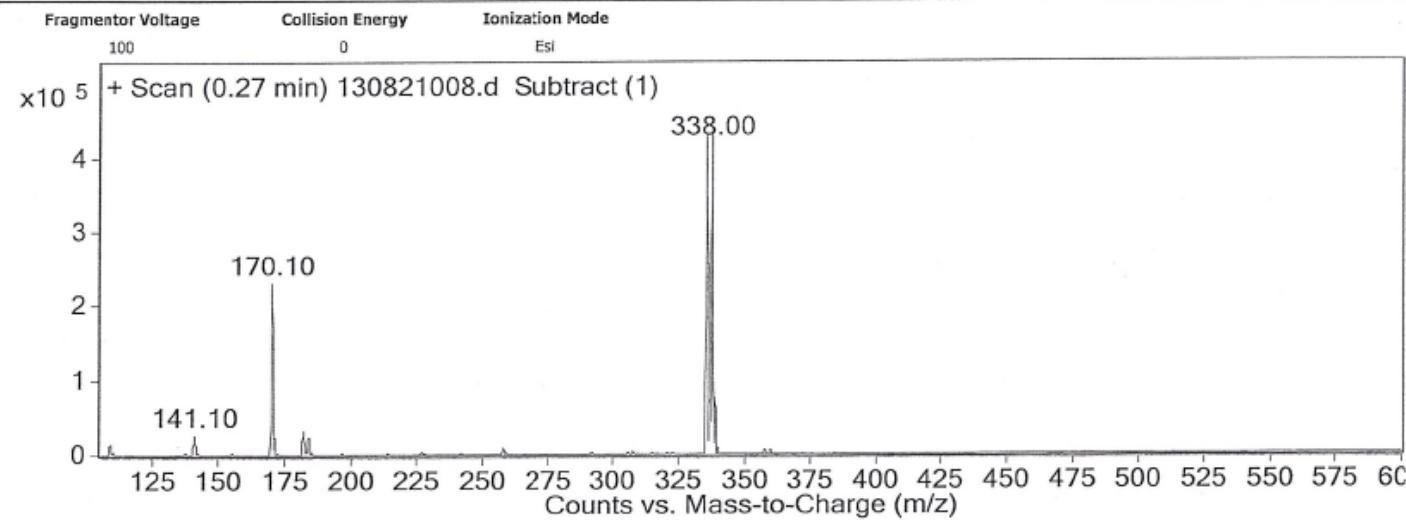
CPS, MIYAPUR

Mass Analysis Report

Data Filename	130821008.d	Sample Name	RNHR
Sample Type	Sample	Position	Vial 28
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	



User Spectra



--- End Of Report ---

HRMS of 4-((2-bromophenyl)amino)-2,5-dimethoxybenzaldehyde (5b)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

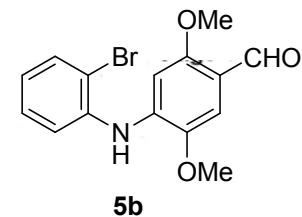
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

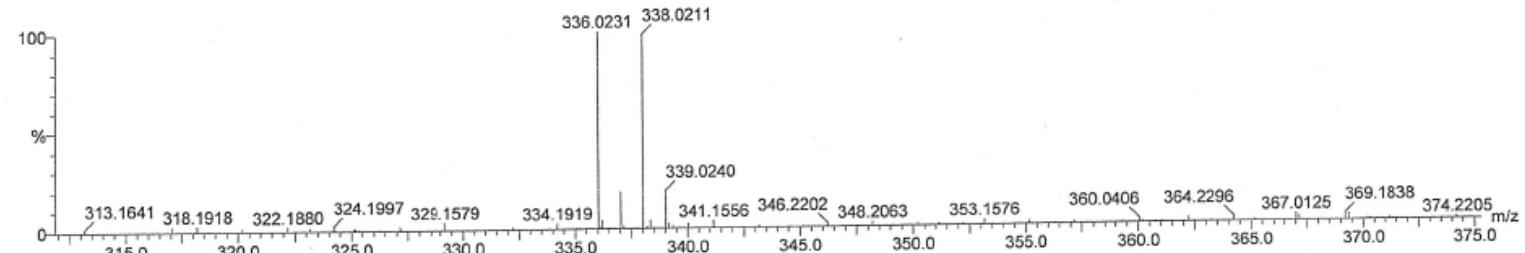
36 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

C: 0-20 H: 0-20 N: 0-2 O: 0-4 Br: 0-1

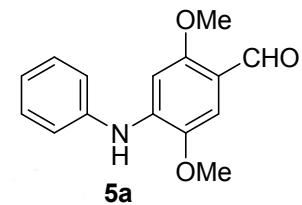


R-NHR
130926012 13 (0.478) Cm (13:15-1:2) 1: TOF MS ES+
1.04e+004



Minimum:	5.0	5.0	-5.0
Maximum:	80.0		
<hr/>			
Mass	Calc. Mass	mDa	PPM
336.0231	336.0235	-0.4	-1.2
			8.5
			i-FIT
			C15 H15 N O3 Br

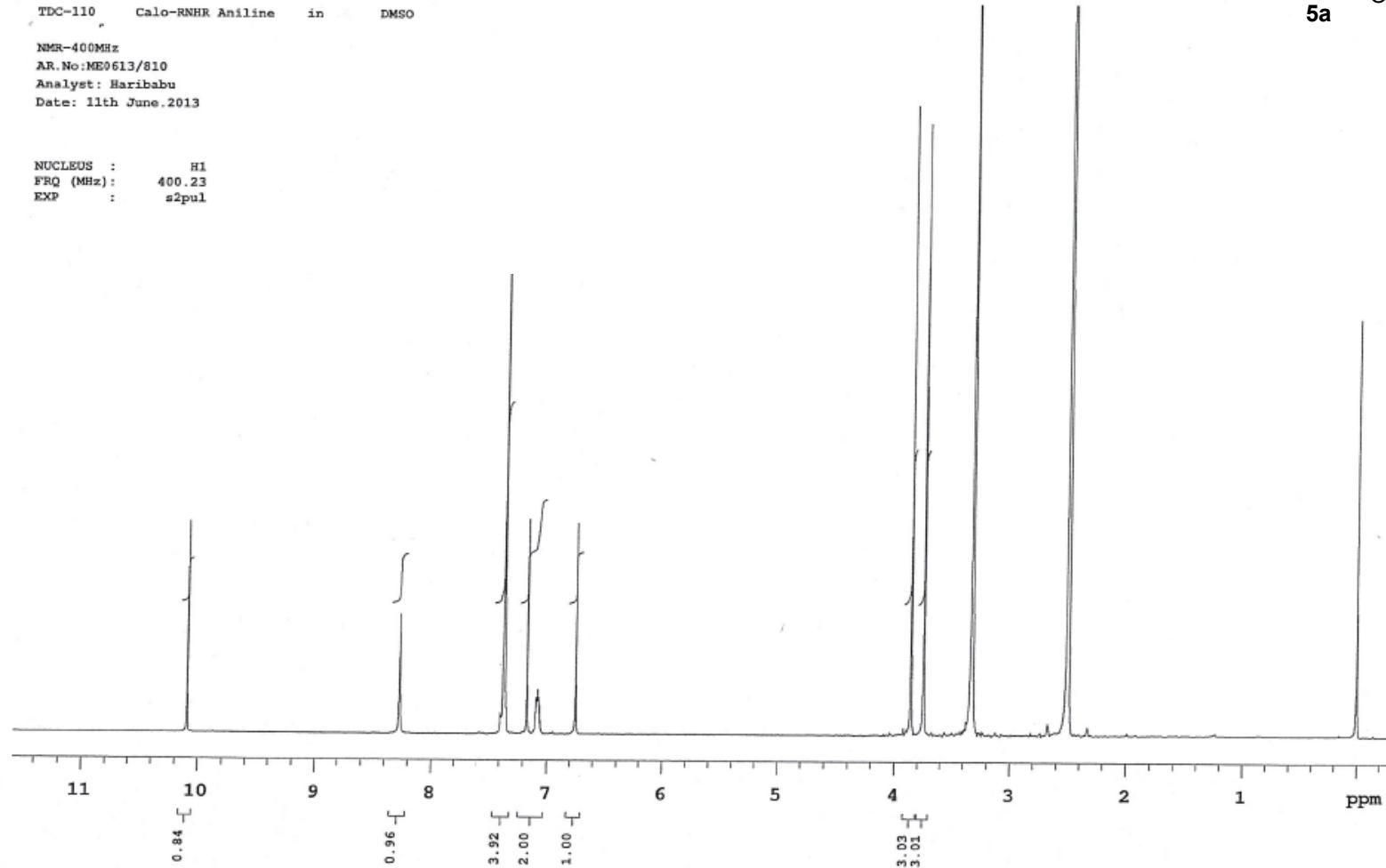
¹H NMR of 2,5-dimethoxy-4-(phenylamino)benzaldehyde (5a)



TDC-110 Calo-RNHR Aniline in DMSO

NMR-400MHz
AR. No:ME0613/810
Analyst: Haribabu
Date: 11th June, 2013

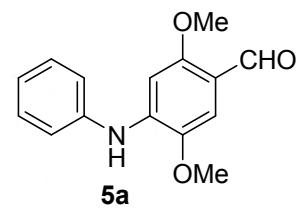
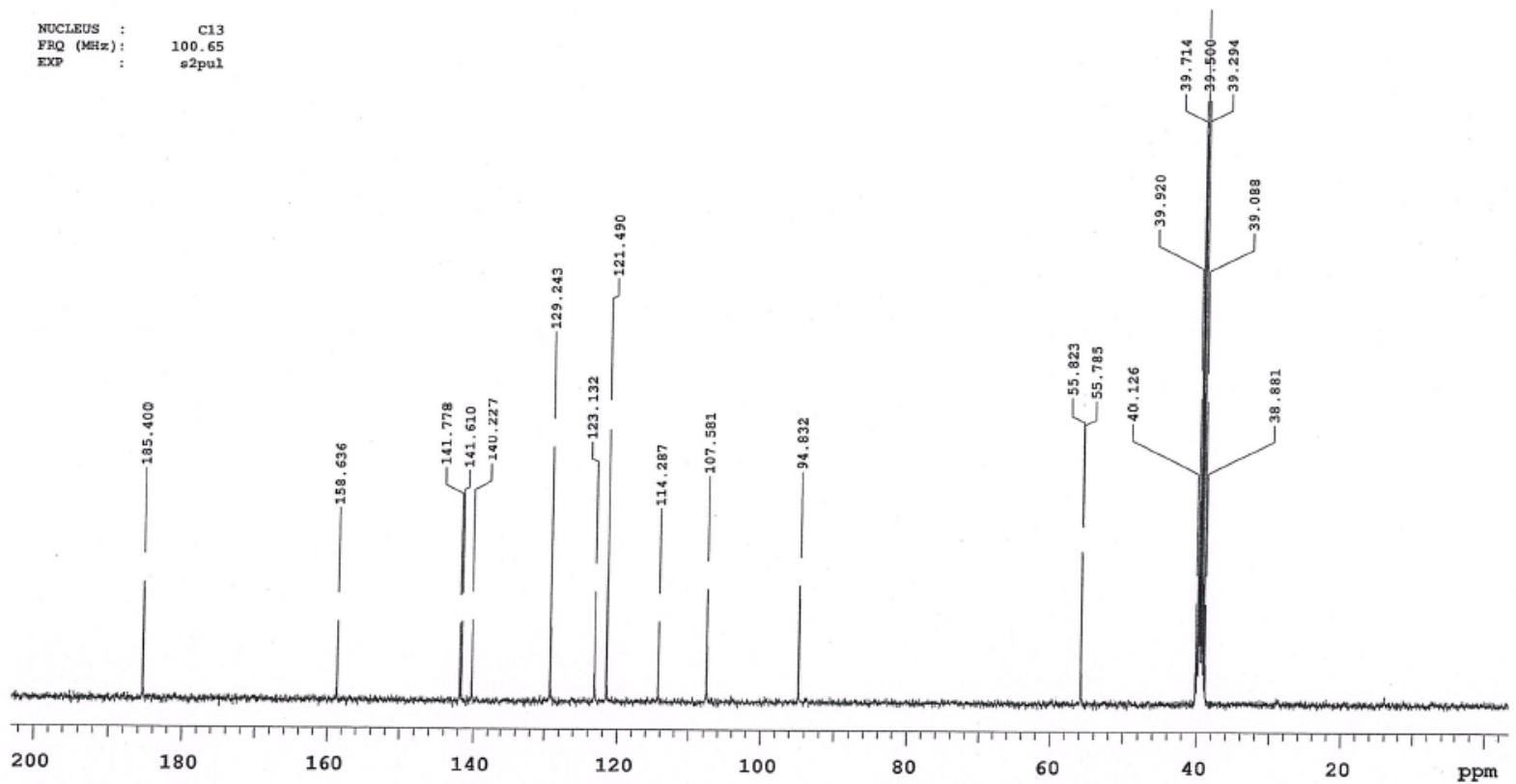
NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul



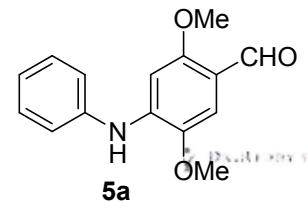
¹³C NMR of 2,5-dimethoxy-4-(phenylamino)benzaldehyde (5a)

TDC-110 R NMR Aniline in DMSO
NMR-400MHz
AR.No:ME0813/1483
Analyst: Ganesh
Date: 16th Aug. 2013

NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul



Mass Spectrum of 2,5-dimethoxy-4-(phenylamino)benzaldehyde (5a)

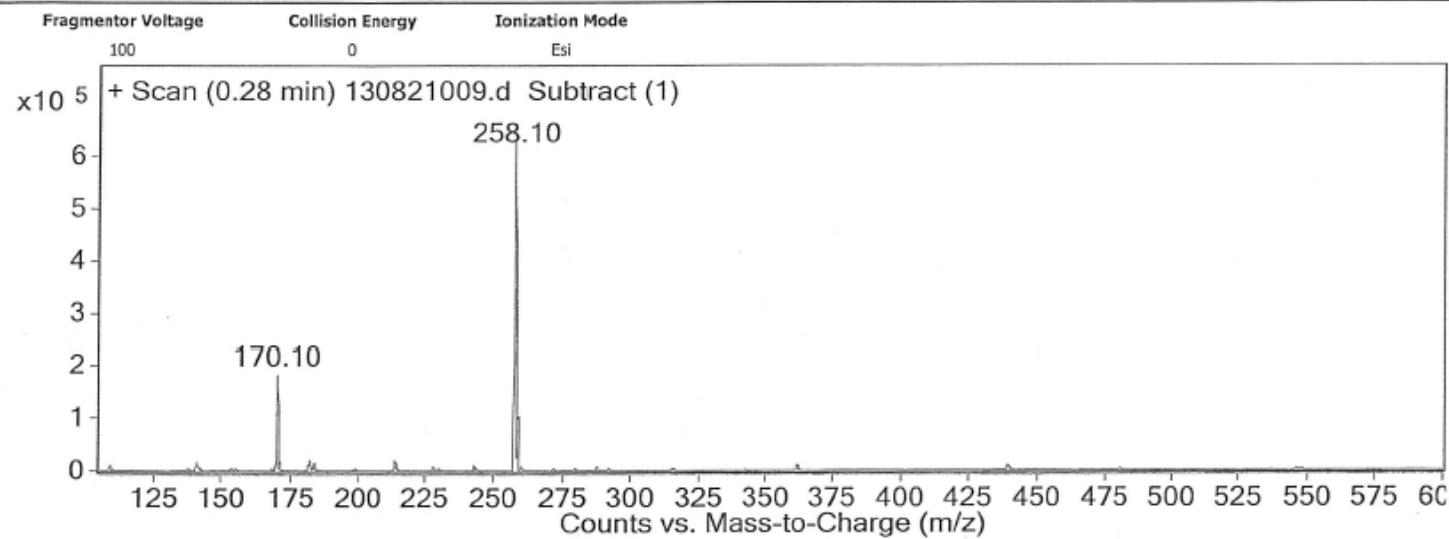


CPS,MIYAPUR

Mass Analysis Report

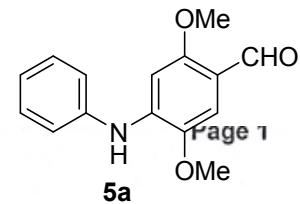
Data Filename	130821009.d	Sample Name	RNHR Aniline
Sample Type	Sample	Position	Vial 29
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

User Spectra



--- End Of Report ---

HRMS of 2,5-dimethoxy-4-(phenylamino)benzaldehyde (5a)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

53 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

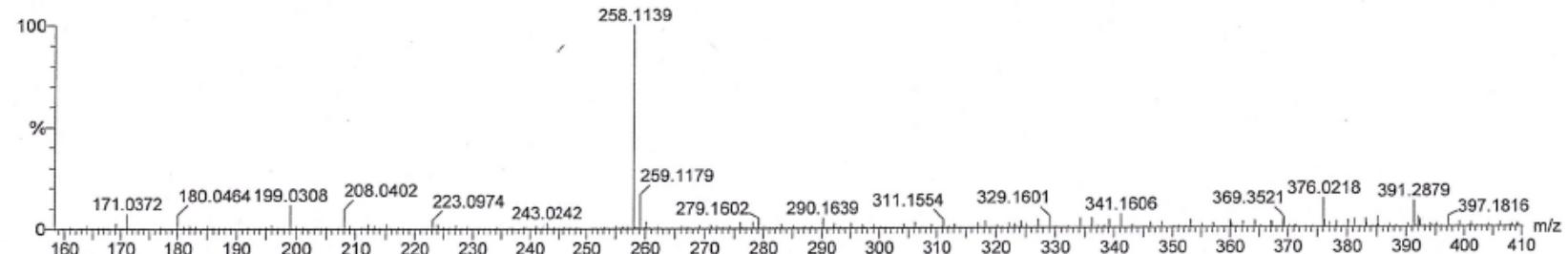
Elements Used:

C: 0-30 H: 0-40 N: 0-2 O: 0-4

R-NHR Aniline

130926010-1 13 (0.479) Cm (13:15-1:2)

1: TOF MS ES+
5.03e+003



Minimum: -5.0
Maximum: 5.0 5.0 80.0

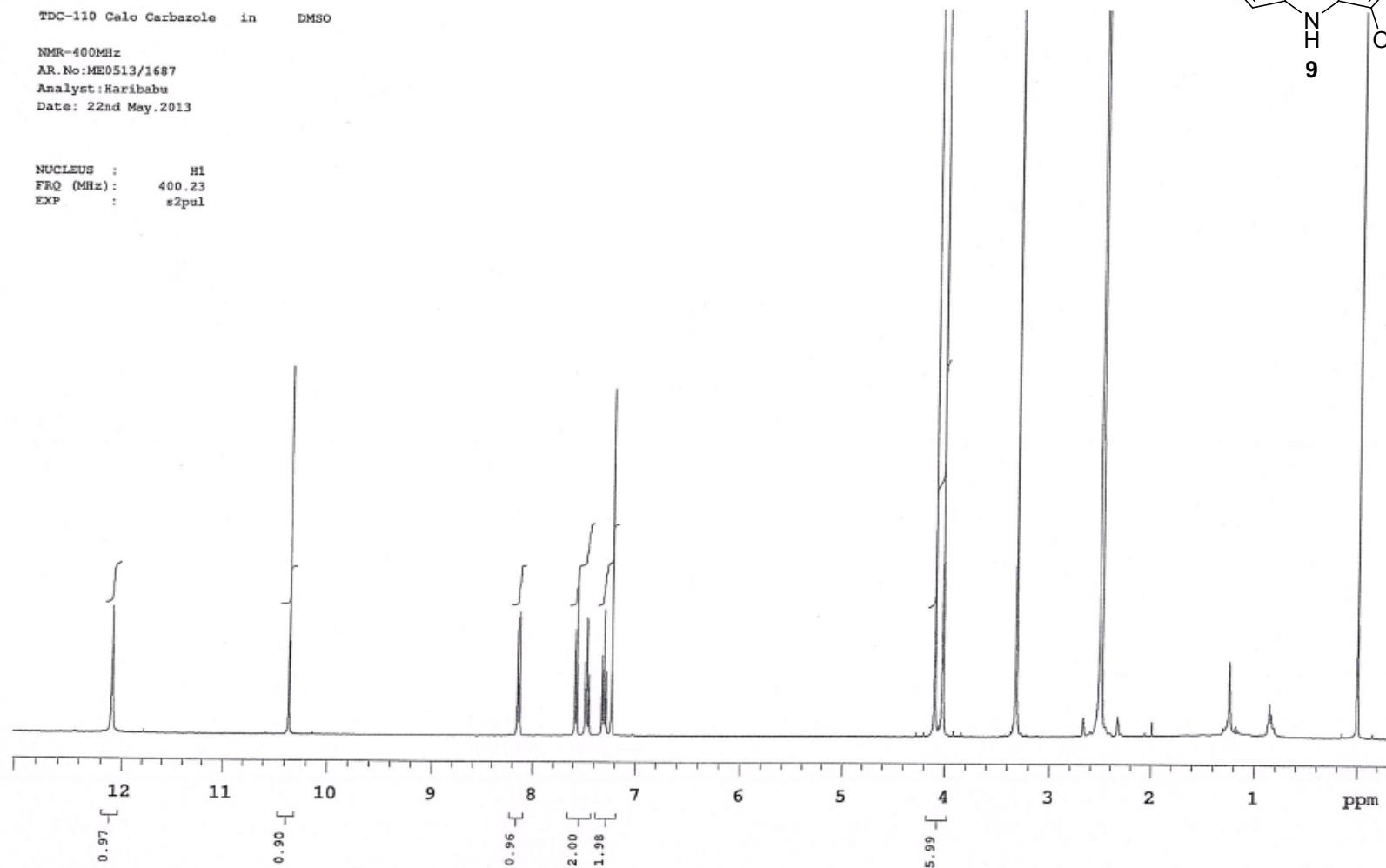
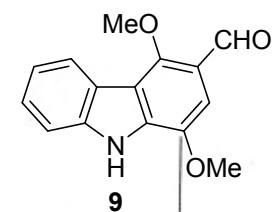
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
258.1139	258.1130	0.9	3.5	8.5	n/a	C15 H16 N O3

¹H NMR of 1,4-dimethoxy-9H-carbazole-3-carbaldehyde (9)

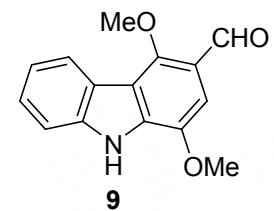
TDC-110 Calo Carbazole in DMSO

NMR-400MHz
AR.No:ME0513/1687
Analyst:Haribabu
Date: 22nd May. 2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul



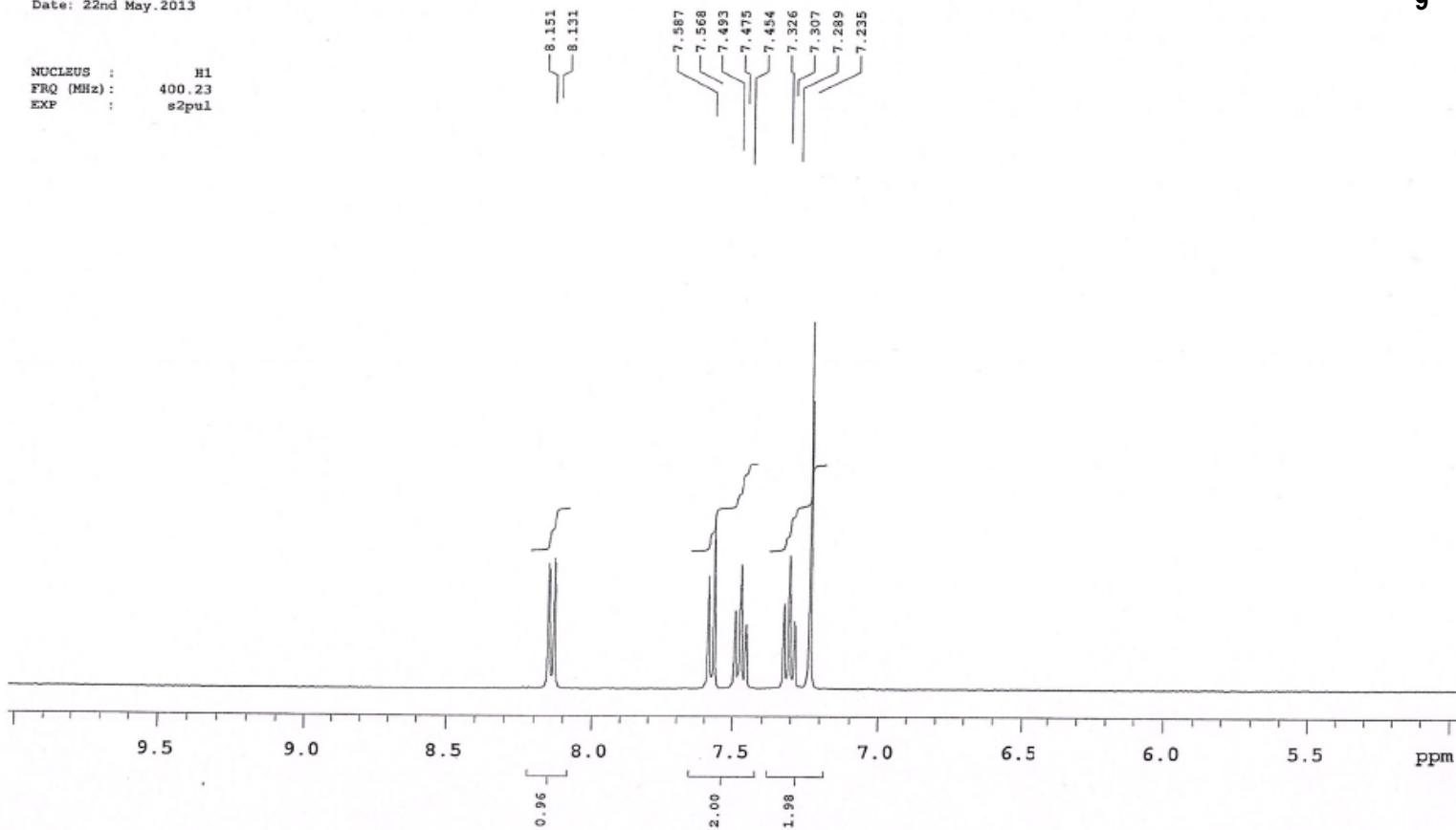
Expansion of ^1H NMR of 1,4-dimethoxy-9*H*-carbazole-3-carbaldehyde (9)



TDC-110 Calo Carbazole in DMSO

NMR-400MHz
AR.No:ME0513/1687
Analyst:Haribabu
Date: 22nd May.2013

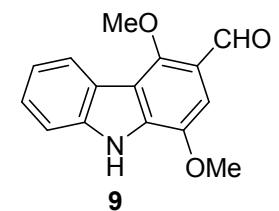
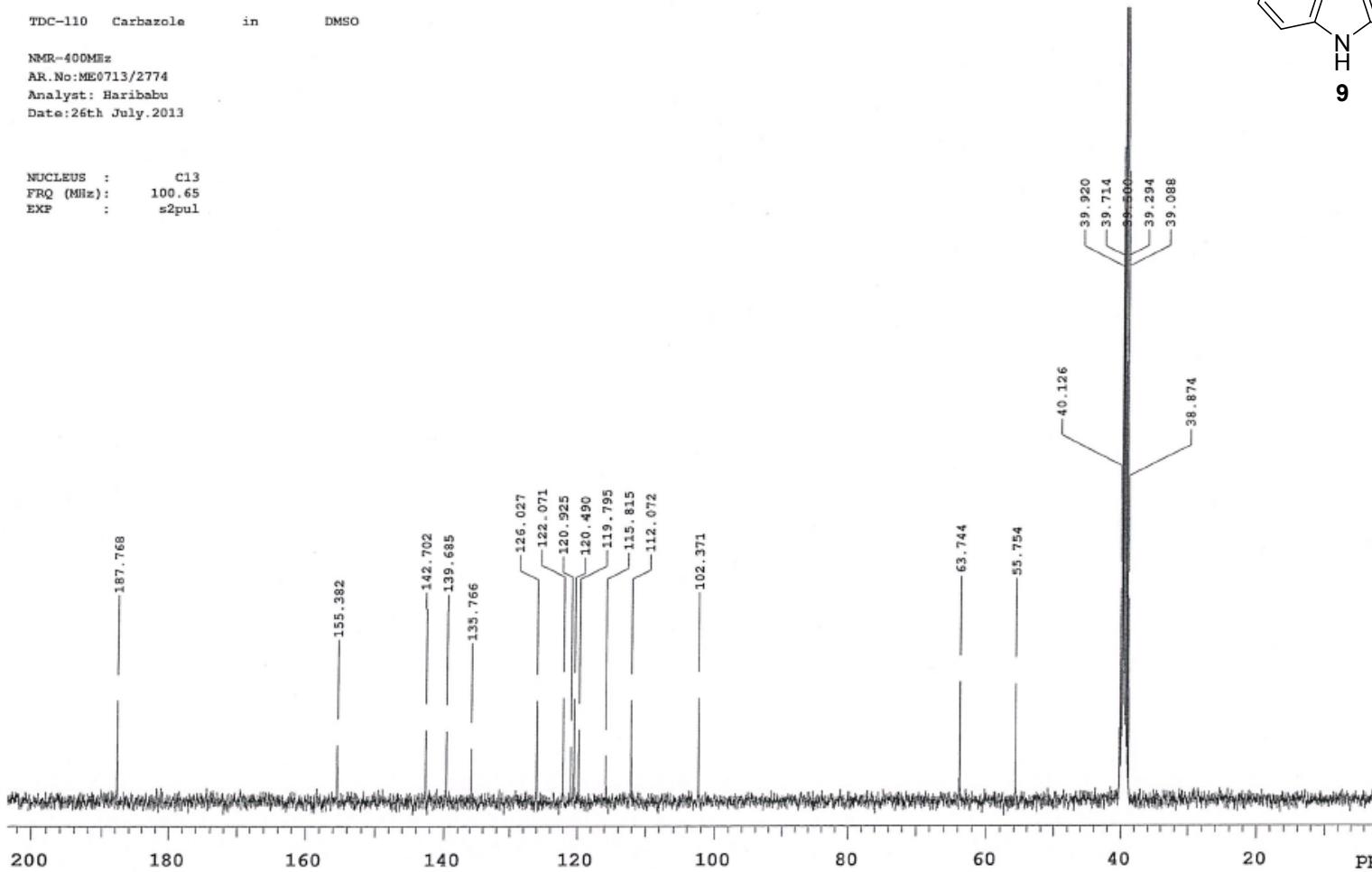
NUCLEUS : H1
FRQ [MHz] : 400.23
EXP : s2pul



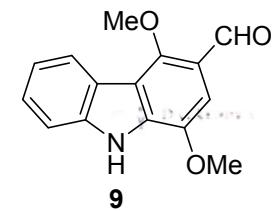
¹³C NMR of 1,4-dimethoxy-9H-carbazole-3-carbaldehyde (9)

TDC-110 Carbazole in DMSO
NMR-400MHz
AR.No:ME0713/2774
Analyst: Haribabu
Date:26th July,2013

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul



Mass Spectrum of 1,4-dimethoxy-9H-carbazole-3-carbaldehyde (9)

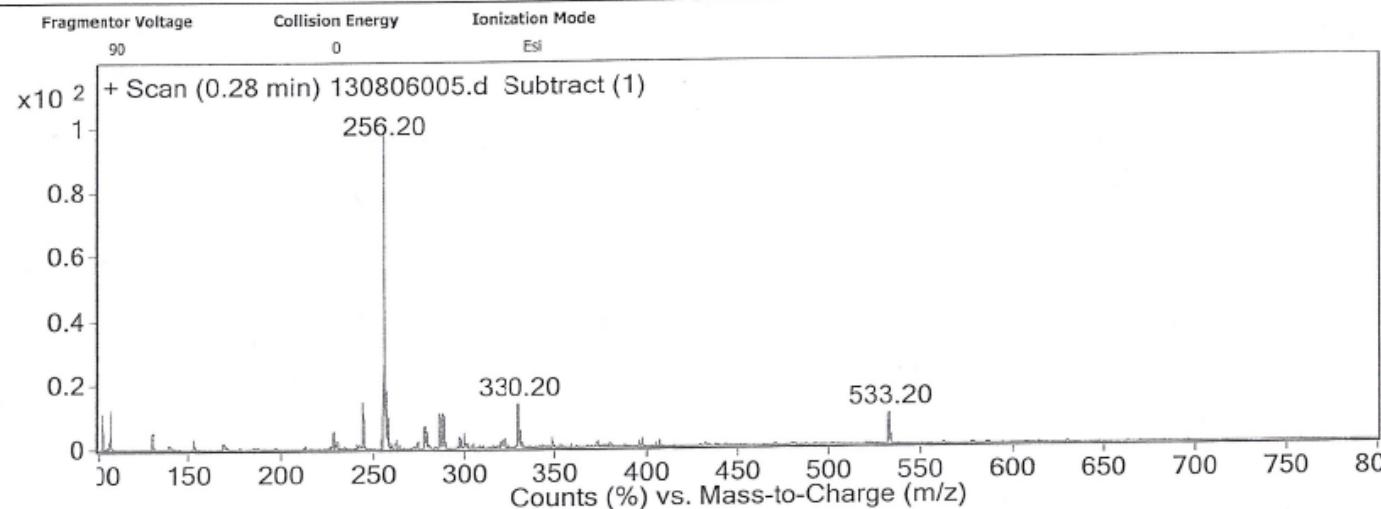


CPS, MIYAPUR

Mass Analysis Report

Data Filename	130806005.d	Sample Name	Carbazole
Sample Type	Sample	Position	Vial 96
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

User Spectra



--- End Of Report ---

HRMS of 1,4-dimethoxy-9H-carbazole-3-carbaldehyde (9)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

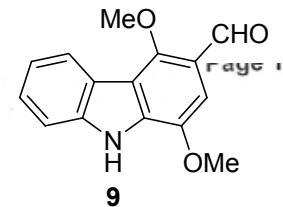
23 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

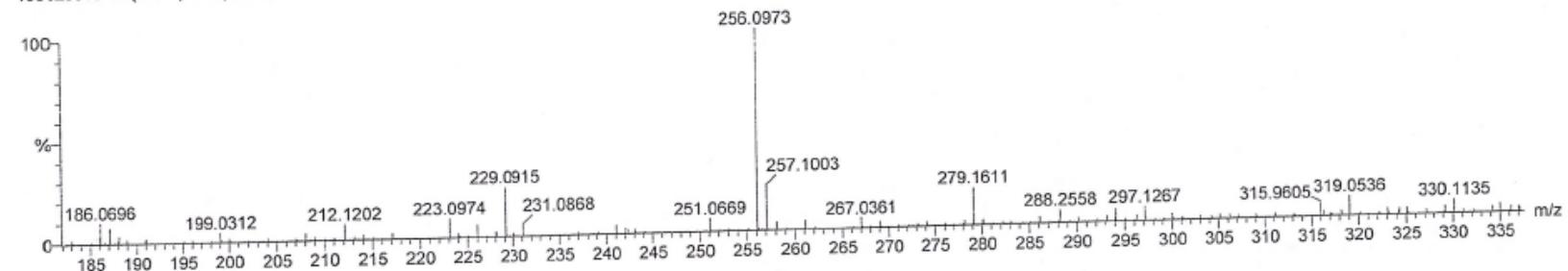
C: 0-25 H: 0-20 N: 0-2 O: 0-3

Carbazole

130925016 13 (0.478) Cm (13:17)



1: TOF MS ES+
1.13e+004



Mass Spectrum Parameters					
Minimum:	Maximum:	mDa	PPM	DBE	i-FIT
				-5.0	80.0
Mass	Calc. Mass				Formula
256.0973	256.0974	-0.1	-0.4	9.5	C15 H14 N O3

¹H NMR of *N*-(*(1,4-dimethoxy-9H-carbazol-3-yl)methyl*)-2-iodoaniline (**11**).

TDC-110 Carbazole Iodo Amine in DMSO

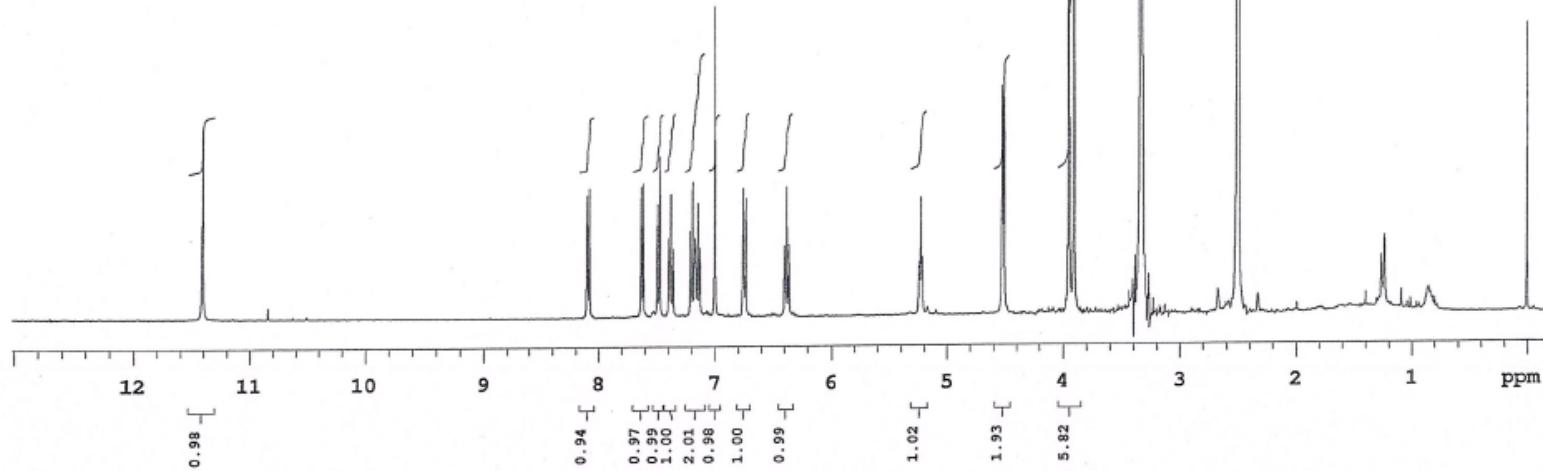
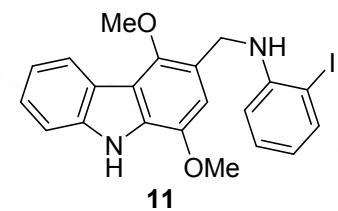
NMR-400MHz

AR.No:ME0613/1597

Analyst: Haribabu

Date:20th June, 2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul

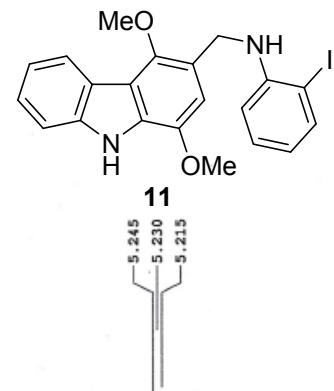
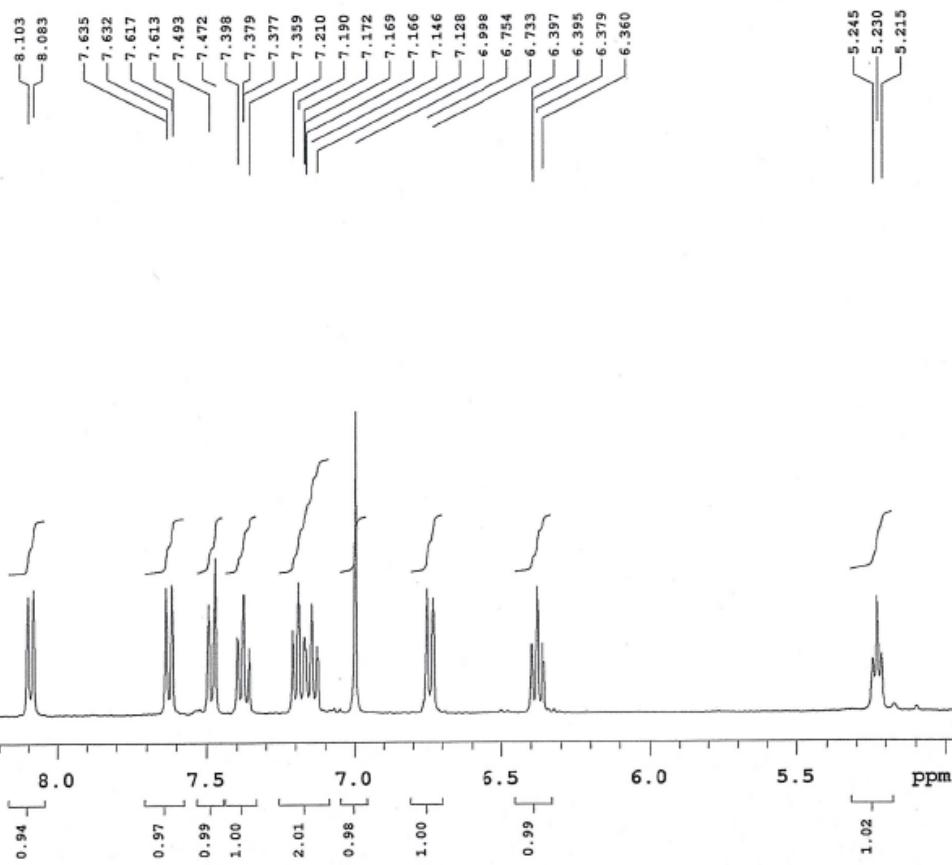


Expansion of ^1H NMR of *N*-(*(1,4-dimethoxy-9*H*-carbazol-3-yl)methyl*)-2-iodoaniline (11**).**

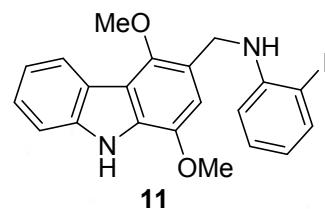
TDC-110 Carbazole Iodo Amine in DMSO

NMR-400MHz
AR.No:ME0613/1597
Analyst: Haribabu
Date:20th June.2013

NUCLEUS : H1
FREQ (MHz) : 400.23
EXP : s2pul



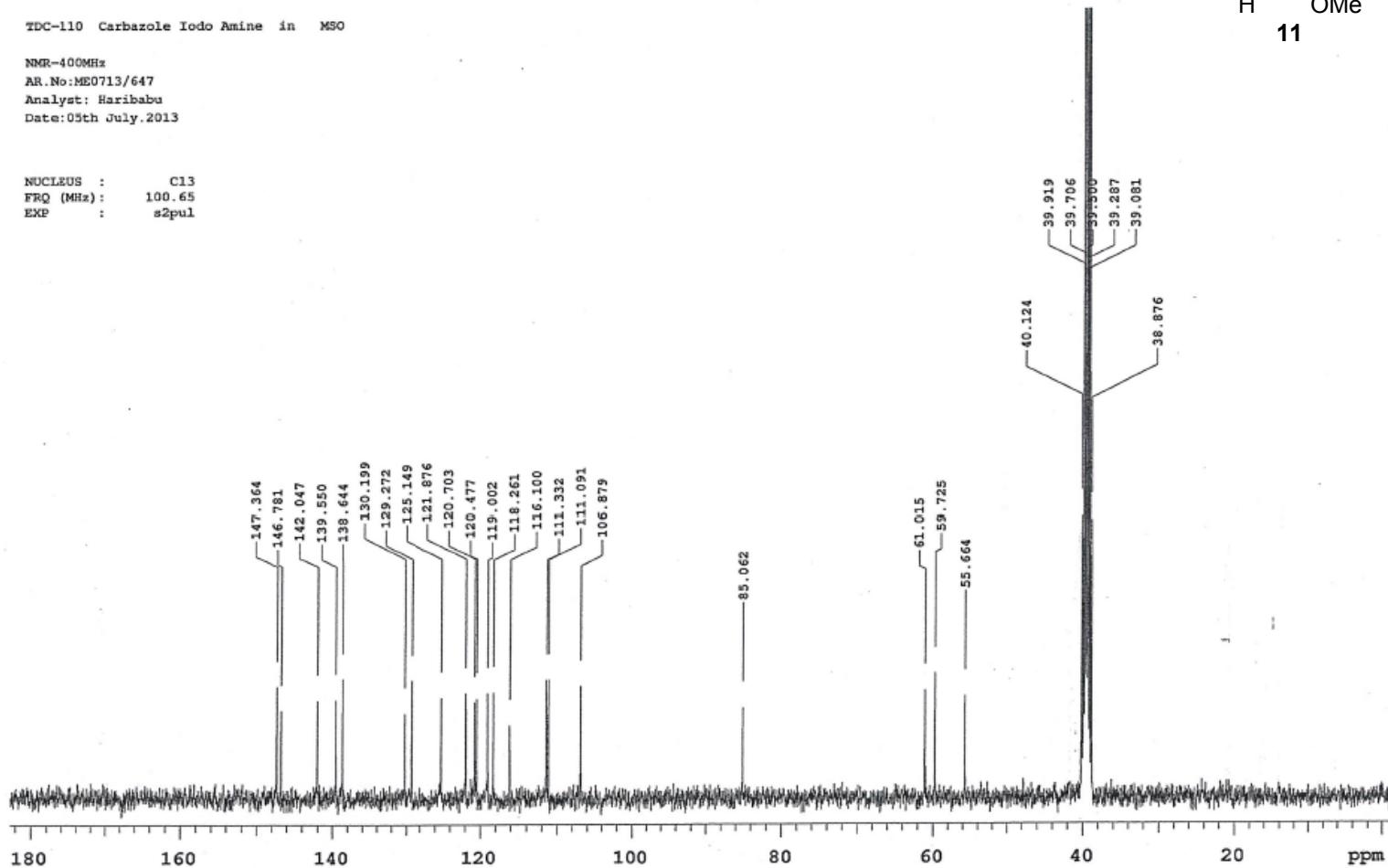
¹³C NMR of *N*-(1,4-dimethoxy-9*H*-carbazol-3-yl)methyl)-2-iodoaniline (11).



TDC-110 Carbazole Iodo Amine in MeO

NMR-400MHz
AR.No:ME0713/647
Analyst: Haribabu
Date:05th July.2013

NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul

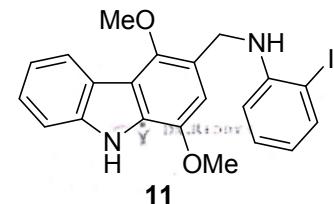


Mass Spectrum of *N*-(*1,4*-dimethoxy-*9H*-carbazol-*3*-yl)methyl)-*2*-iodoaniline (11**).**

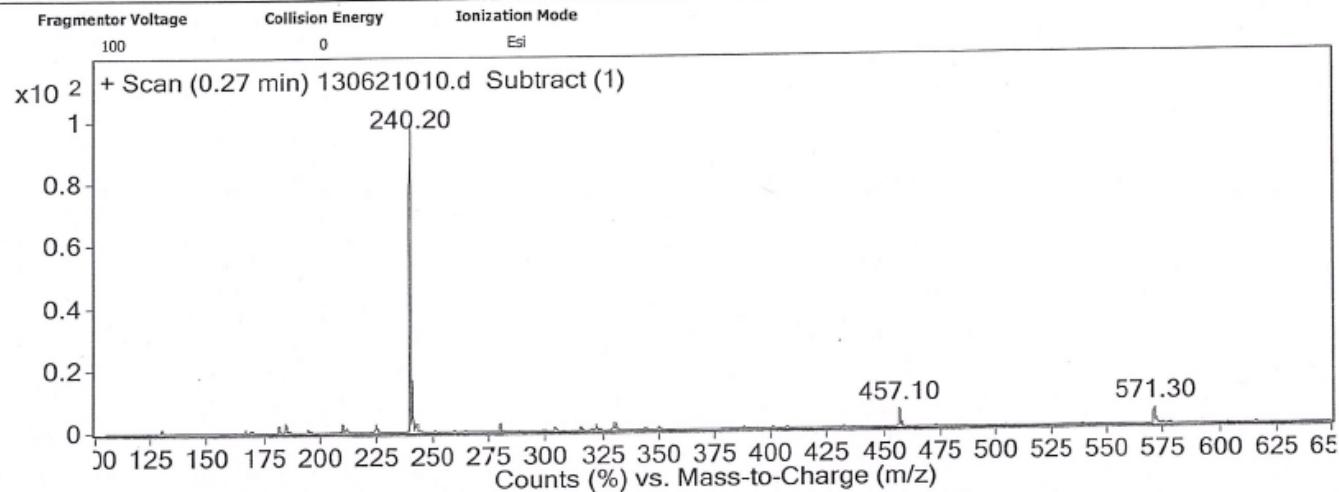
CPS,MIYAPUR

Mass Analysis Report

Data Filename	130621010.d	Sample Name	Carbazole iodo Amine
Sample Type	Sample	Position	Vial 89
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

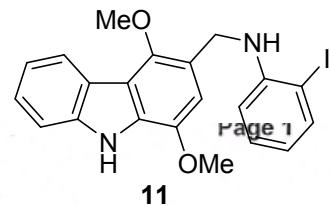


User Spectra



--- End Of Report ---

HRMS of *N*-(*(1,4-dimethoxy-9H-carbazol-3-yl)methyl*)-2-iodoaniline (11).



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

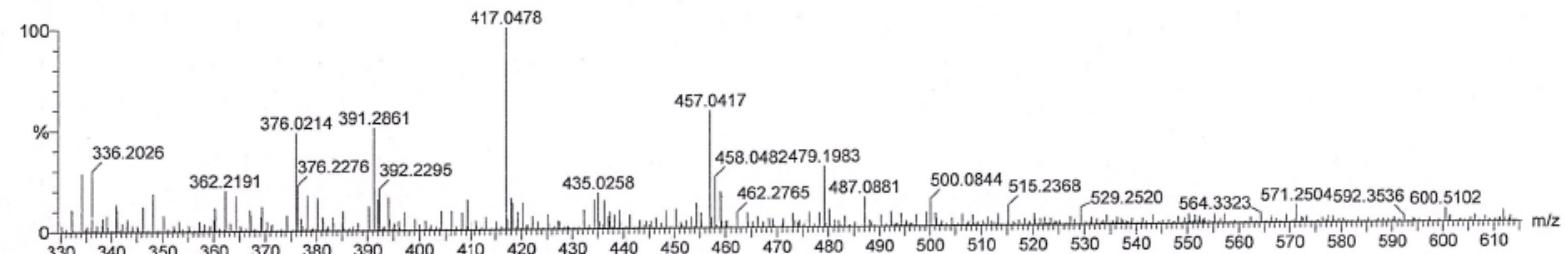
Monoisotopic Mass, Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

C: 0-25 H: 0-20 N: 0-2 O: 0-2 I: 0-1

Carbazole iodamine
130926011 9 (0.338) Cm (4:14)

1: TOF MS ES+
1.60e+004



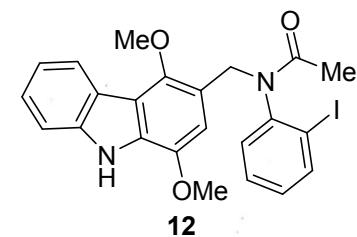
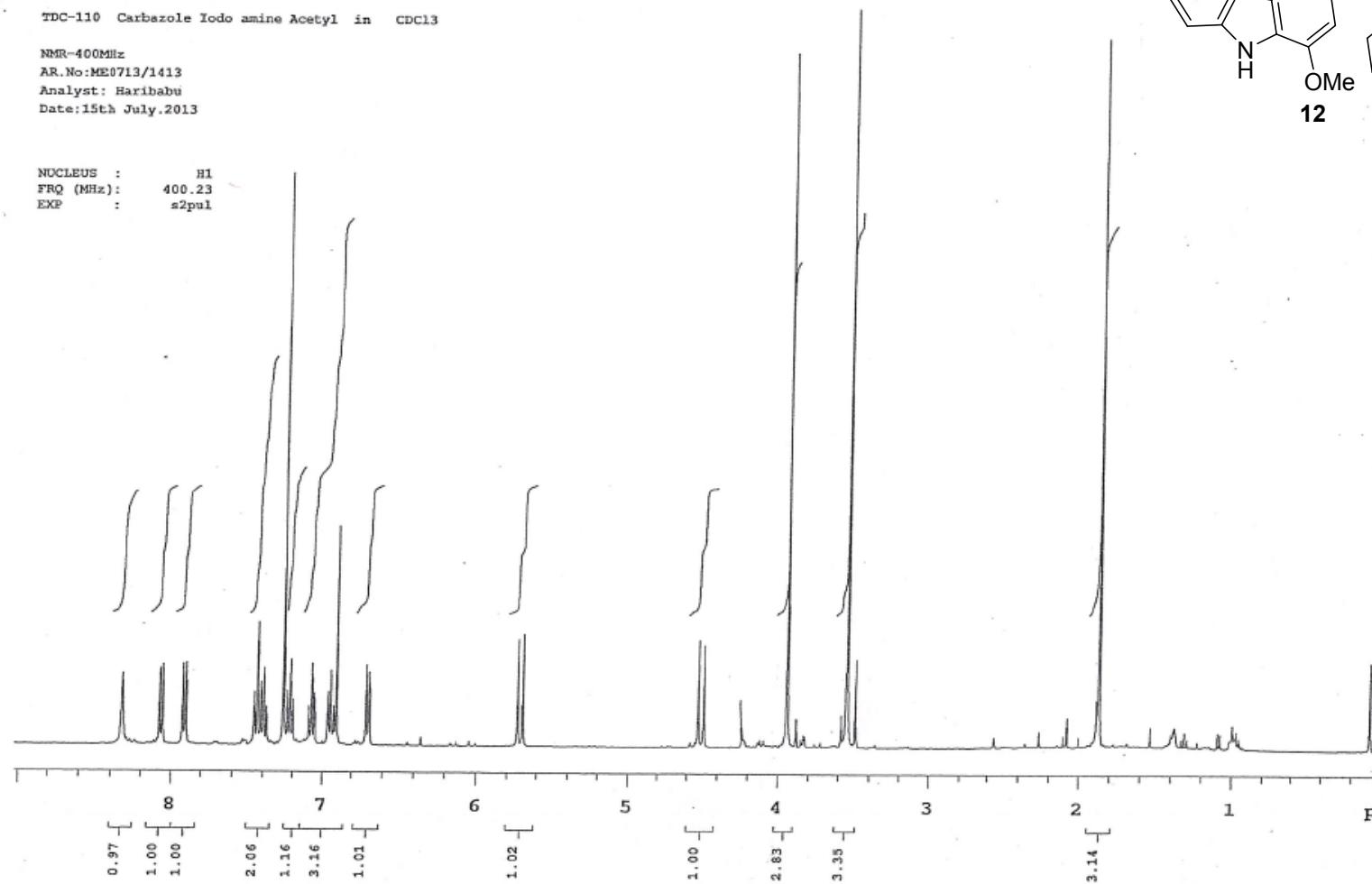
Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
457.0417	457.0413	0.4	0.9	13.5	1686.9	C21 H18 N2 O2 I

¹H NMR of *N*-(*(1,4-dimethoxy-9H-carbazol-3-yl)methyl*)-*N*-(2-iodophenyl)acetamide (**12**).

TDC-110 Carbazole Iodo amine Acetyl in CDCl₃
NMR-400MHz
AR.No:ME0713/1413
Analyst: Haribabu
Date:15th July.2013

NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul

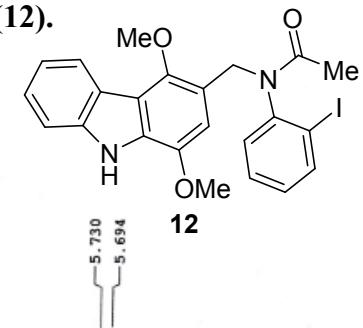
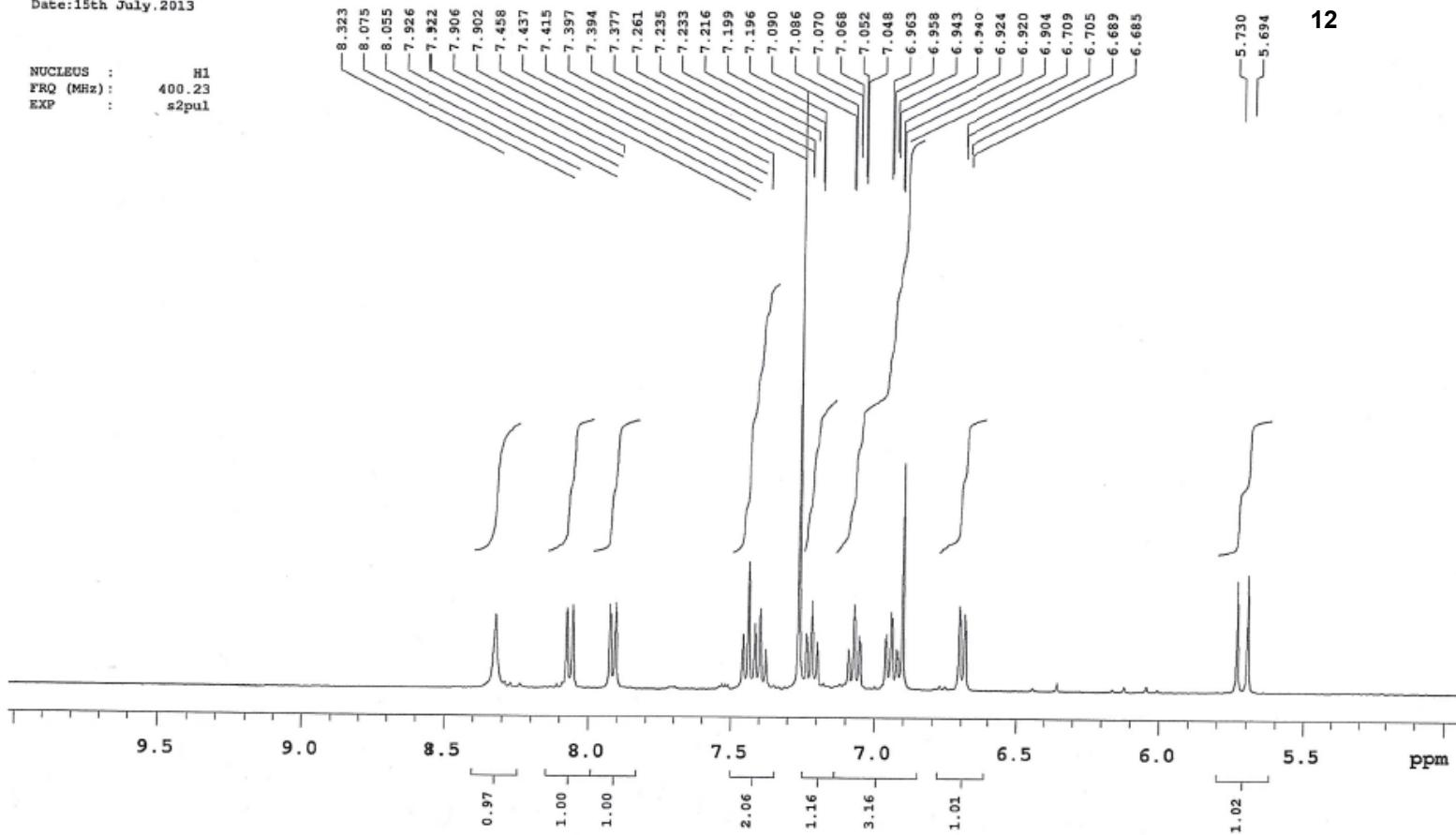


Expansion of ^1H NMR of *N*-(*(1,4-dimethoxy-9*H*-carbazol-3-yl)methyl*)-*N*-(2-iodophenyl)acetamide (12).

TDC-110 Carbazole Iodo amine Acetyl in CDCl₃

NMR-400MHz
AR.No:ME0713/1413
Analyst: Haribabu
Date:15th July,2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul



¹³C NMR of *N*-(1,4-dimethoxy-9*H*-carbazol-3-yl)methyl)-*N*-(2-iodophenyl)acetamide (12).

TDC-110 Carbazole Iodo amine acetyl in CDCl₃

NMR-400MHz

AR.No:ME0713/1960

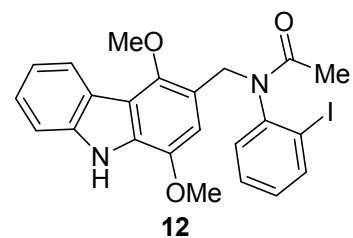
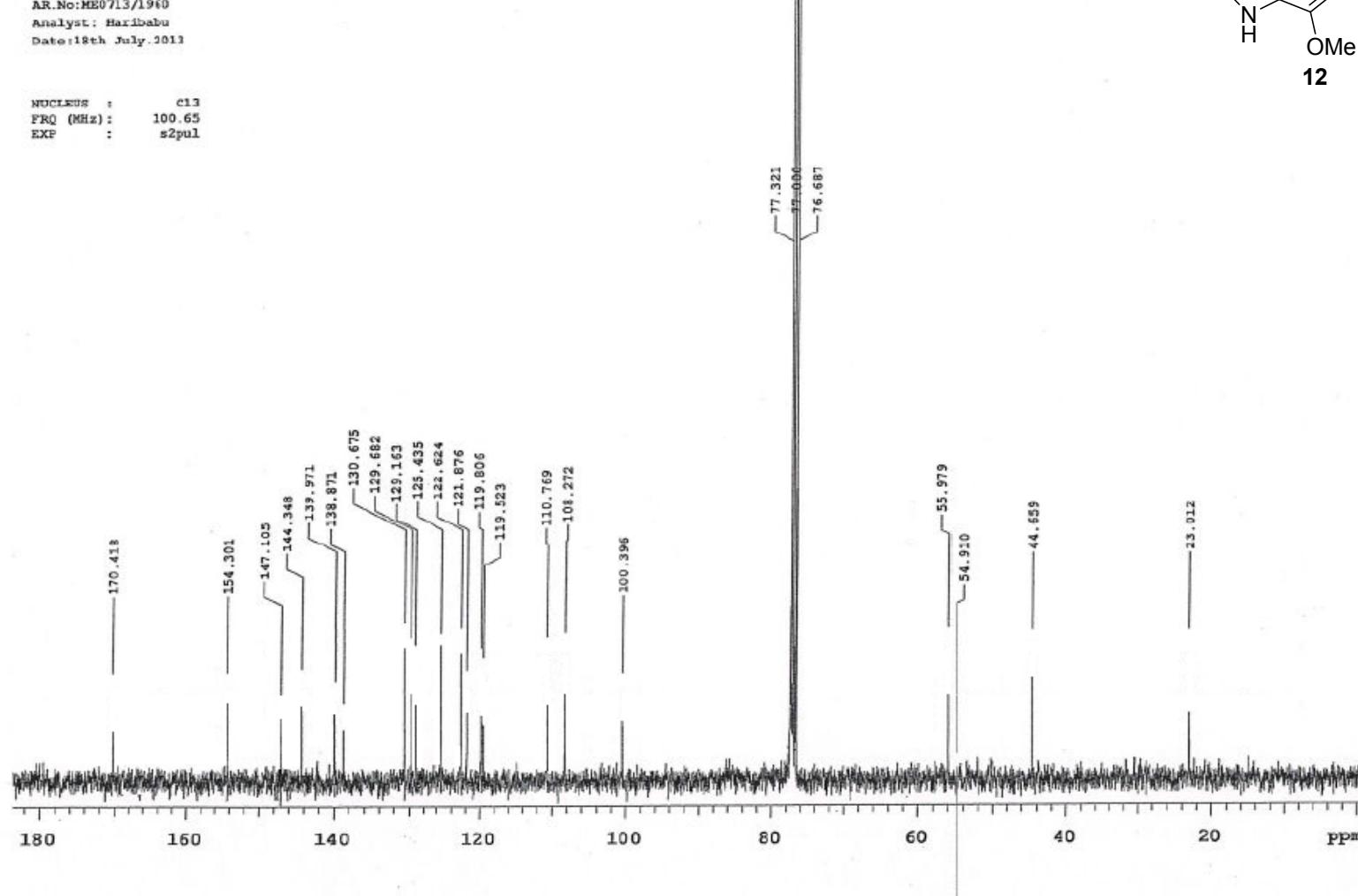
Analyst: Haribabu

Date: 18th July 2013

NUCLEUS : C13

FRQ (MHz): 100.65

EXP : s2pul

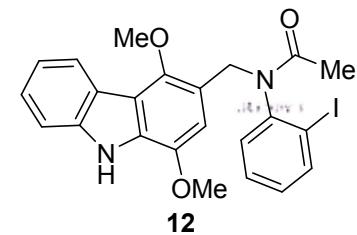


Mass Spectrum of *N*-((1,4-dimethoxy-9*H*-carbazol-3-yl)methyl)-*N*-(2-iodophenyl)acetamide (12).

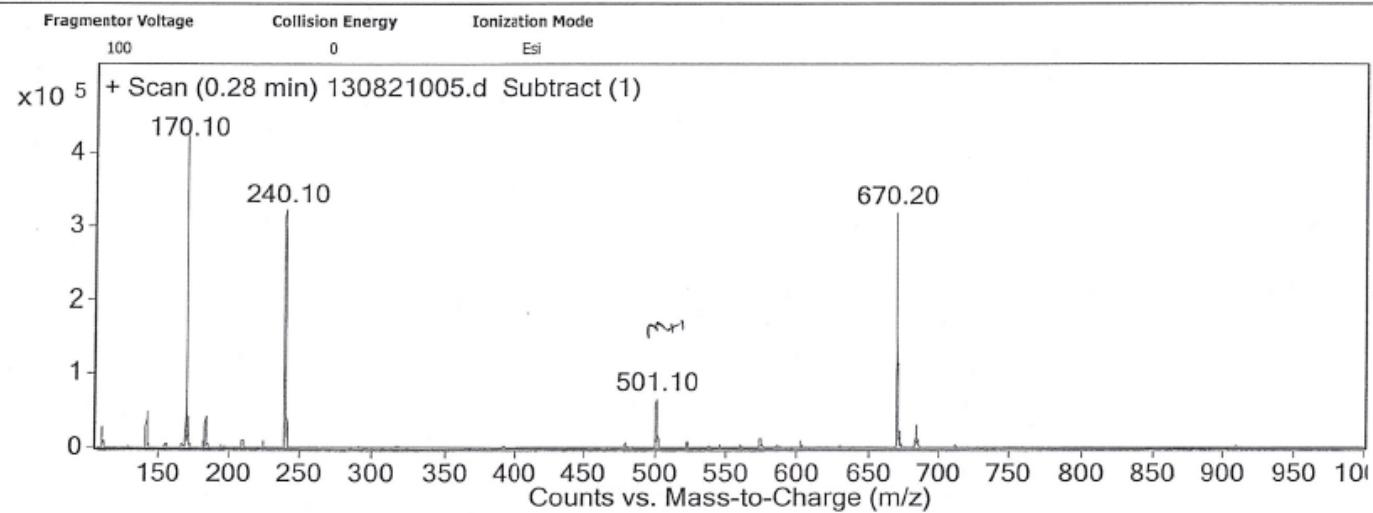
CPS,MIYAPUR

Mass Analysis Report

Data Filename	130821005.d	Sample Name	Carbazole Iodo amine Acetyl
Sample Type	Sample	Position	Vial 25
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

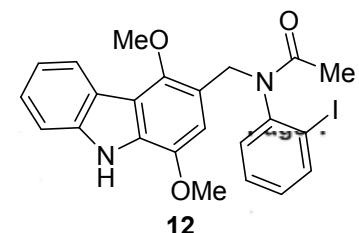


User Spectra



--- End Of Report ---

HRMS of *N*-(*(1,4-dimethoxy-9H-carbazol-3-yl)methyl*)-*N*-(2-iodophenyl)acetamide (12**).**



Elemental Composition Report

Single Mass Analysis

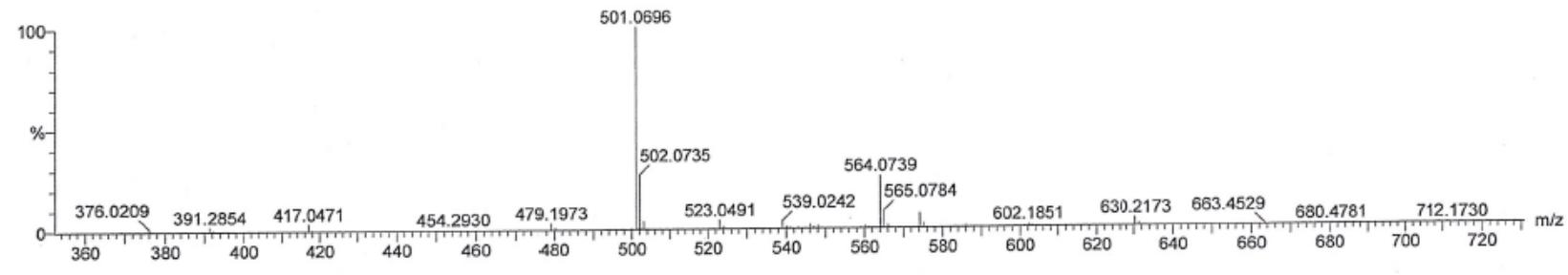
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
 27 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:
 C: 0-25 H: 0-25 N: 0-2 O: 0-4 I: 0-1

Carbazole Iodo amine Acetyl
 130926020 13 (0.479) Cm (13:16-1:2)

1: TOF MS ES+
 1.24e+005



Minimum: -5.0
 Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
501.0696	501.0675	2.1	4.2	13.5	41.2	C23 H22 N2 O3 I

¹H NMR of *N*-(2-bromophenyl)-4-(((2-iodophenyl) amino)methyl)-2,5-dimethoxyaniline (14)

TDC-110 Iodo Bromo Diamine in DMSO

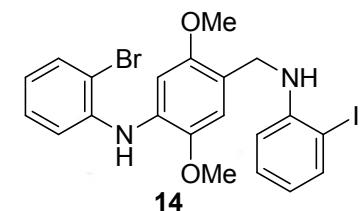
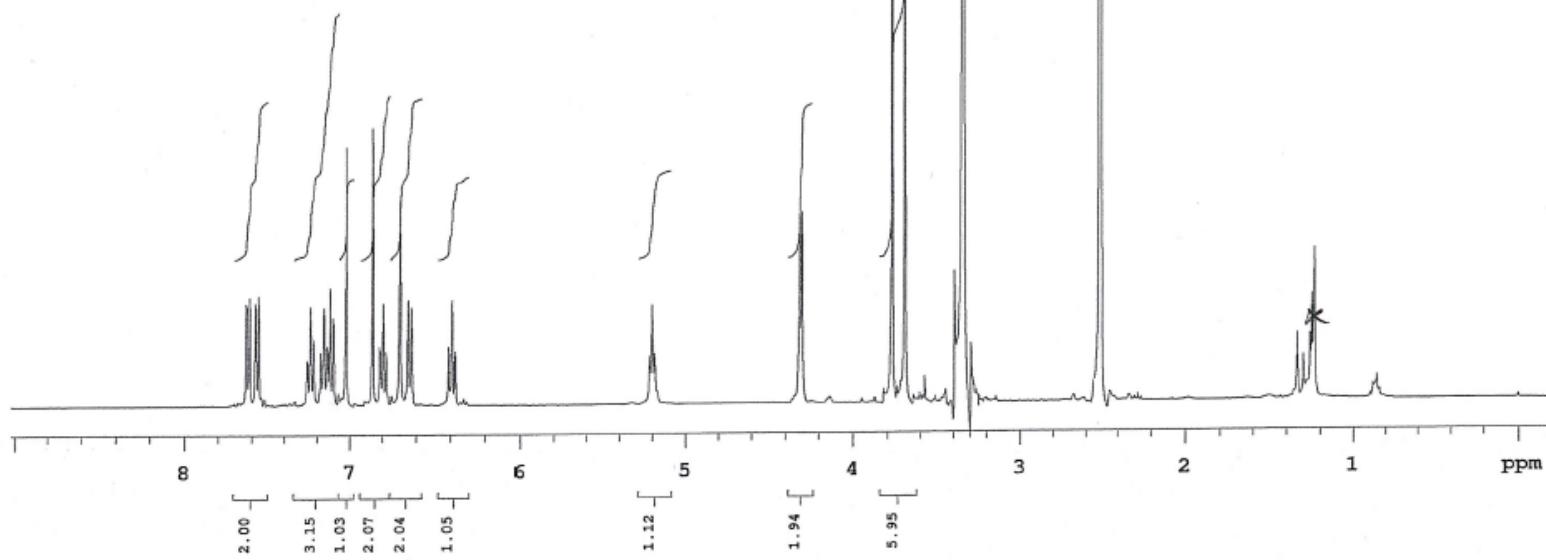
NMR-400MHz

AR.No:MR0913/1194

Analyst: Haribabu

Date:12th Sept.2013

NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul

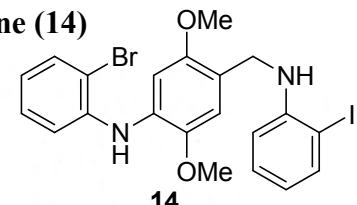
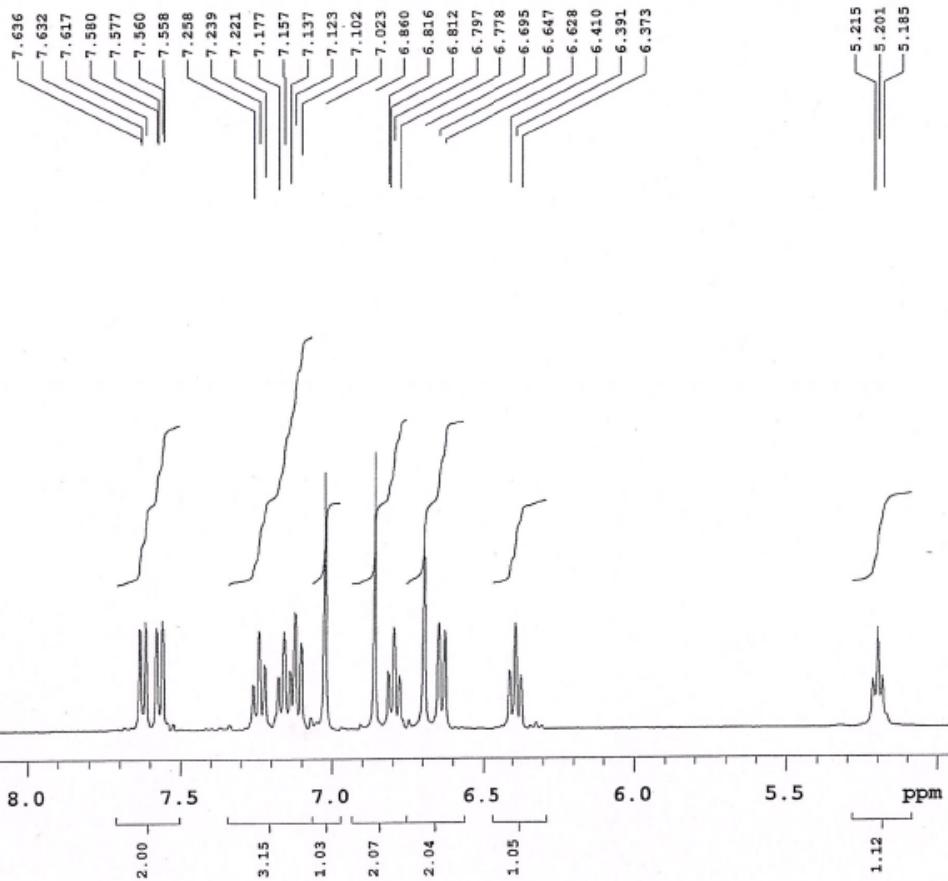


Expansion of ^1H NMR of *N*-(2-bromophenyl)-4-((2-iodophenyl) amino)methyl)-2,5-dimethoxyaniline (14)

TDC-110 Iodo Bromo Diamine in DMSO

NMR-400MHz
AR.No:ME0913/1194
Analyst: Haribabu
Date: 12th Sept. 2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul

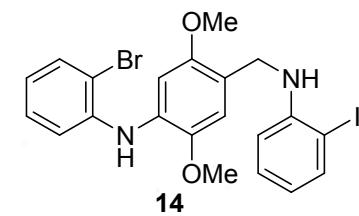
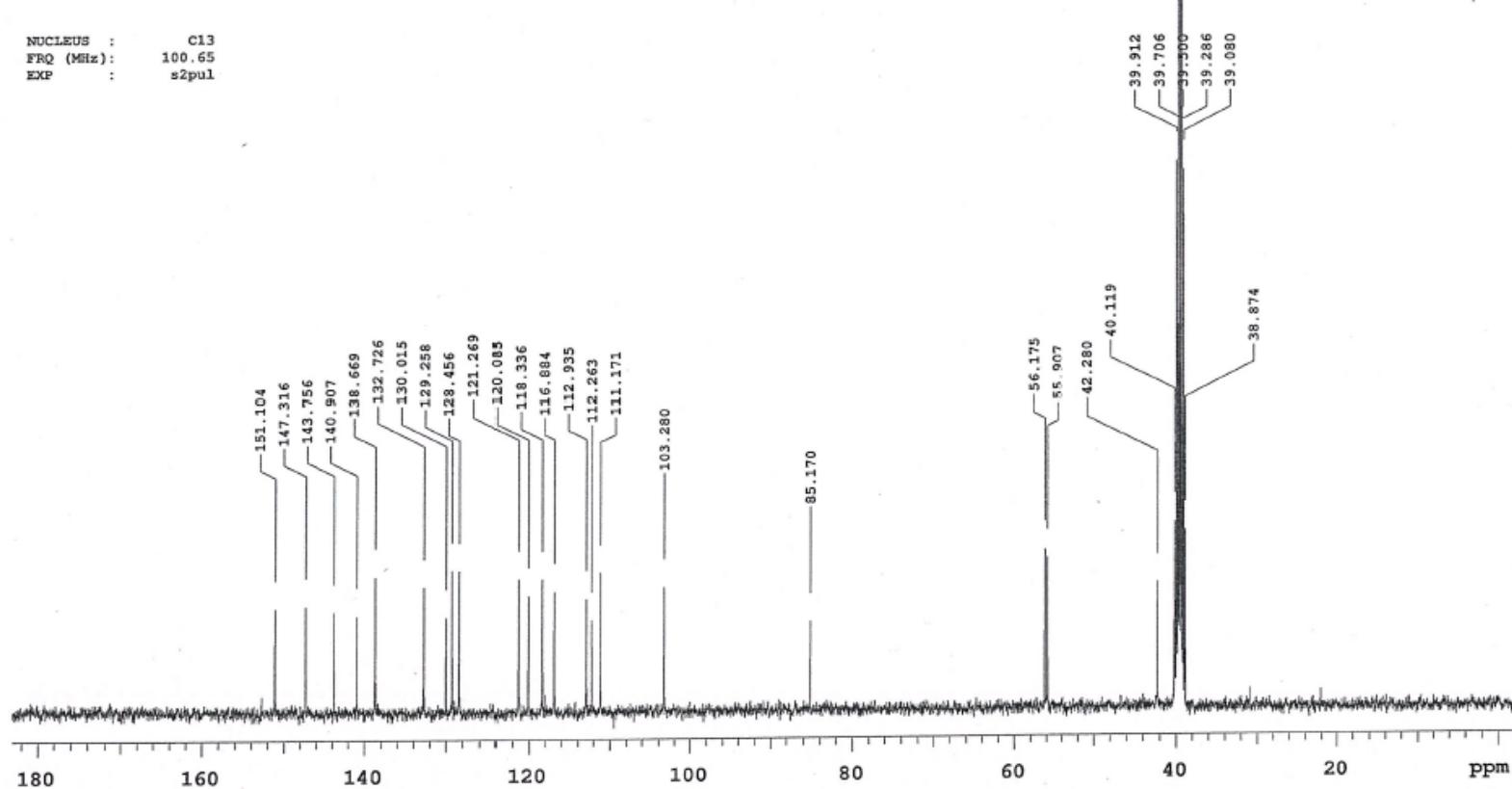


¹³C NMR of *N*-(2-bromophenyl)-4-((2-iodophenyl) amino)methyl)-2,5-dimethoxyaniline (14)

TDC-110 Iodo Bromo dicine in DMSO

NMR-400MHz
AR.No:ME0813/1484
Analyst: Ganesh
Date: 16th Aug. 2013

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul

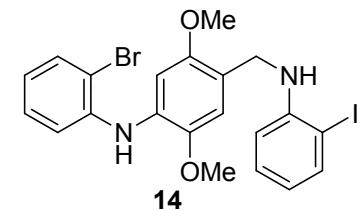


Mass Spectrum of *N*-(2-bromophenyl)-4-(((2-iodophenyl) amino)methyl)-2,5-dimethoxyaniline (14)

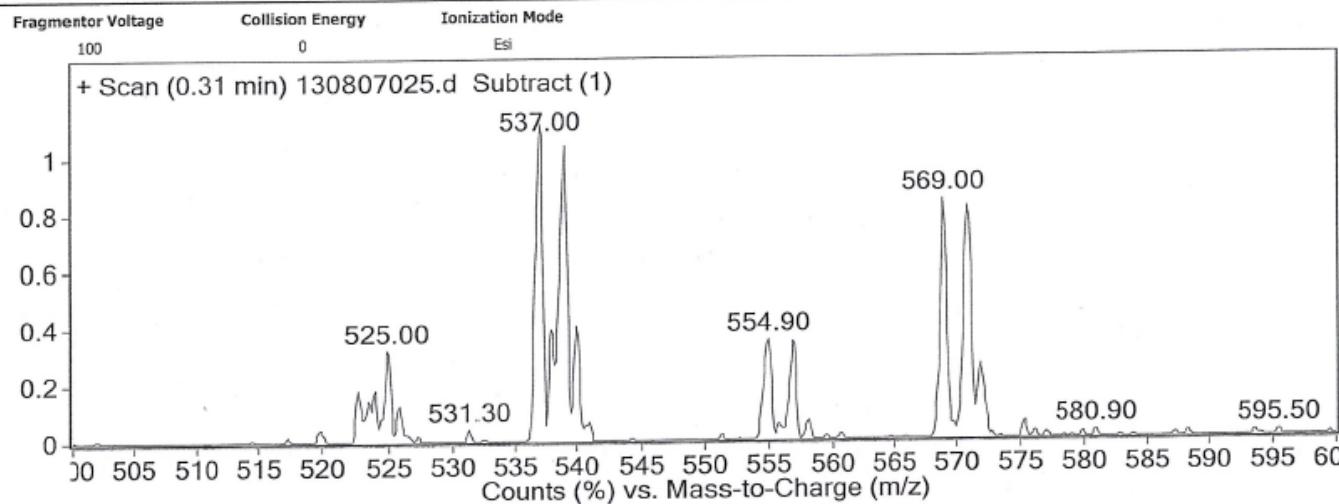
CPS, MIYAPUR

Mass Analysis Report

Data Filename	130807025.d	Sample Name	ODO BROMO DIAMINE
Sample Type	Sample	Position	Vial 45
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

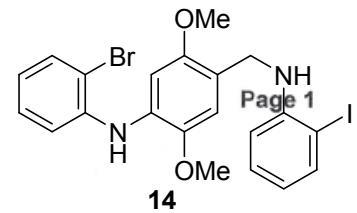


User Spectra



--- End Of Report ---

HRMS of *N*-(2-bromophenyl)-4-((2-iodophenyl) amino)methyl)-2,5-dimethoxyaniline (14)



Elemental Composition Report

Single Mass Analysis

Tolerance = 12.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

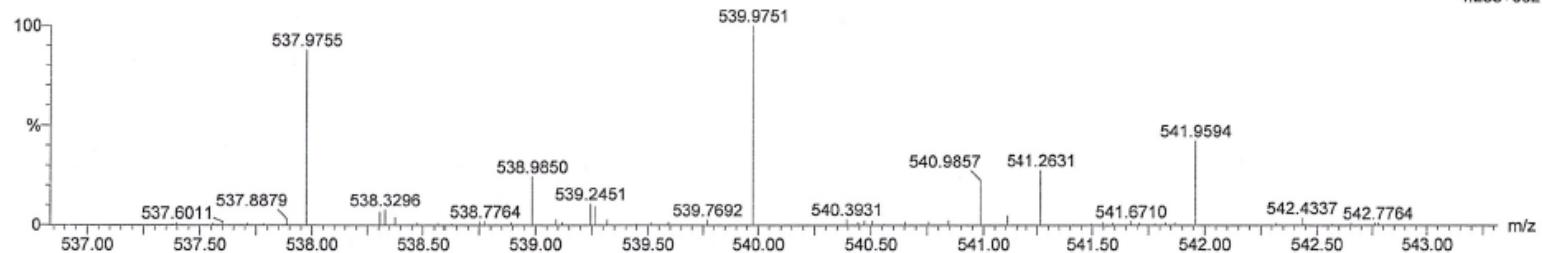
42 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-21 H: 0-21 N: 0-3 O: 0-2 Br: 0-1 I: 0-1

IODO BROMO DIAMINE
131008003 7 (0.251) Cm (6:7:1)

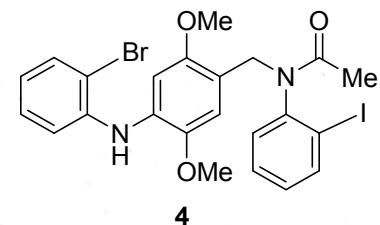
1: TOF MS ES+
4.23e+002



Minimum: -5.0
Maximum: 5.0 12.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
538.9850	538.9831	1.9	3.5	11.5	187.5	C21 H21 N2 O2 Br I

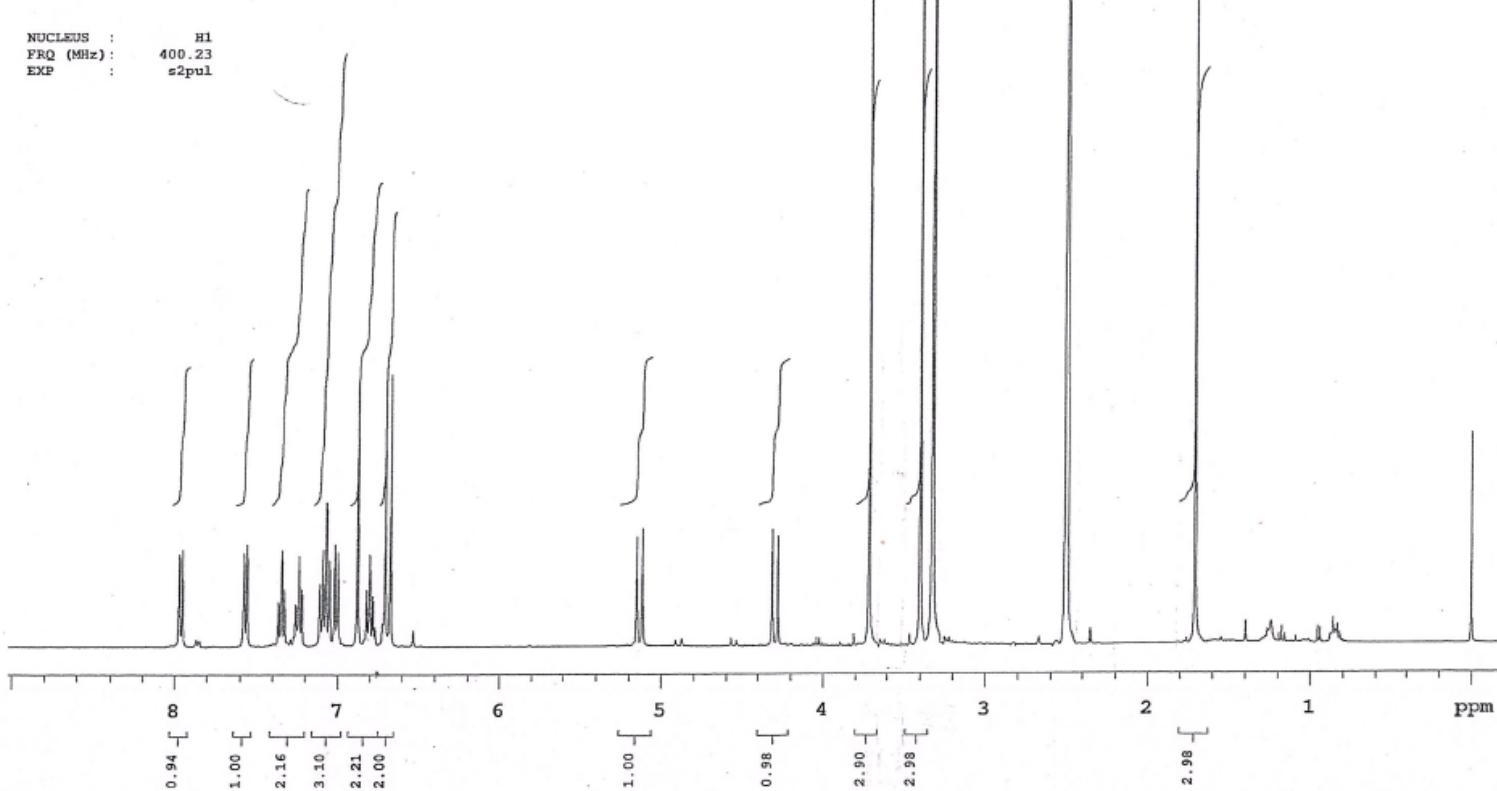
¹H NMR of *N*-(4-((2-bromophenyl)amino)-2,5-dimethoxybenzyl)-*N*-(2-iodophenyl)acetamide (4)



TDC-110 Iodo bromo diamine acetyl F-II in DMSO

NMR-400MHz
AR.No:ME0813/640
Analyst: Haribabu
Date:07th Aug.2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul

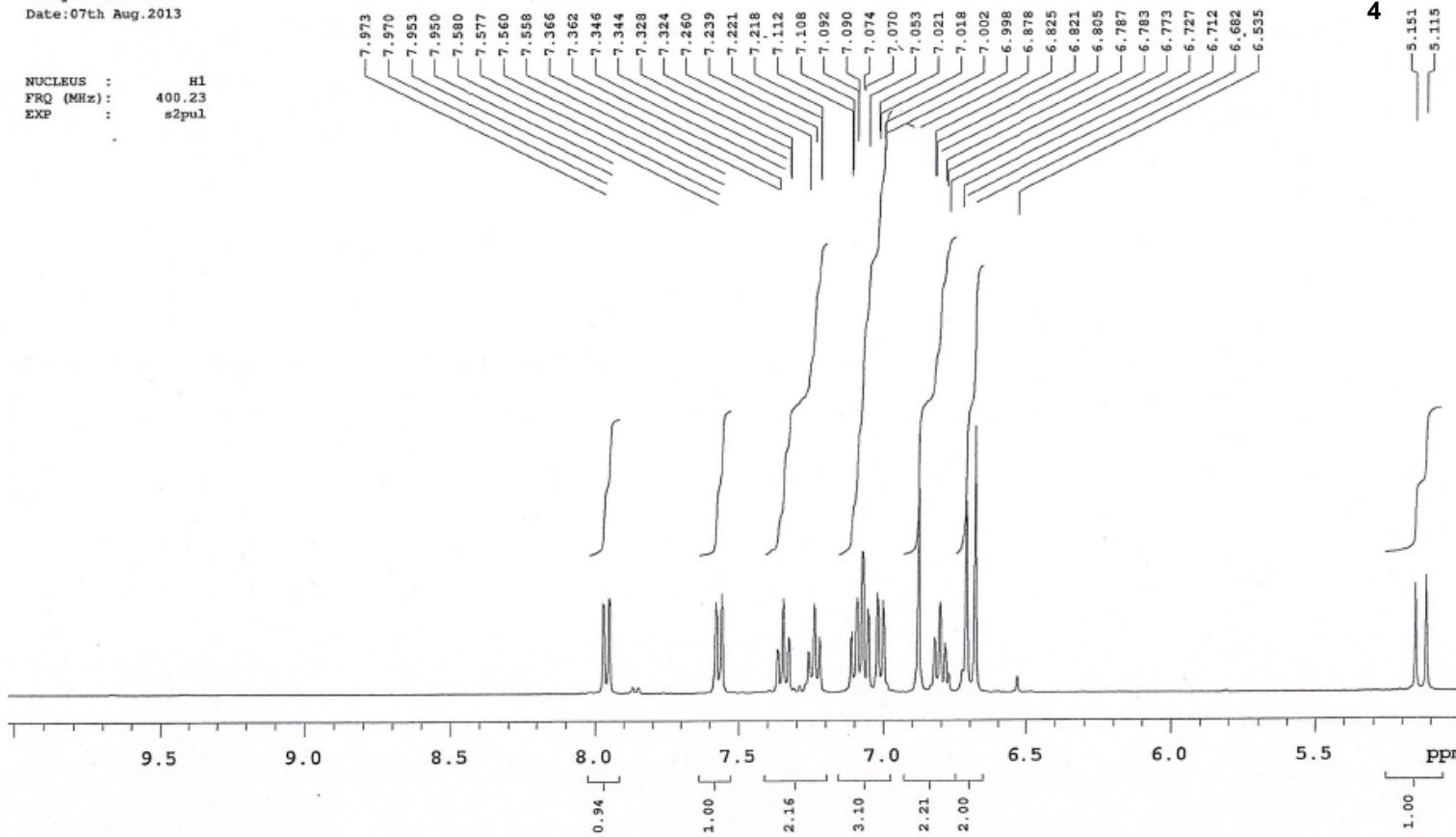


Expansion of ^1H NMR of *N*-(4-((2-bromophenyl)amino)-2,5-dimethoxybenzyl)-*N*-(2-iodophenyl)acetamide (4)

TDC-110 Iodo bromo diamine acetyl F-II in DMSO

NMR-400MHz
AR.No:ME0813/640
Analyst: Haribabu
Date:07th Aug.2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul

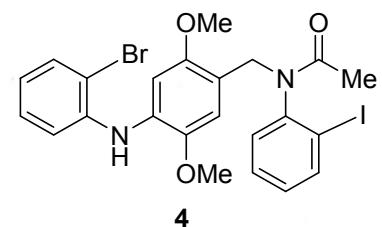
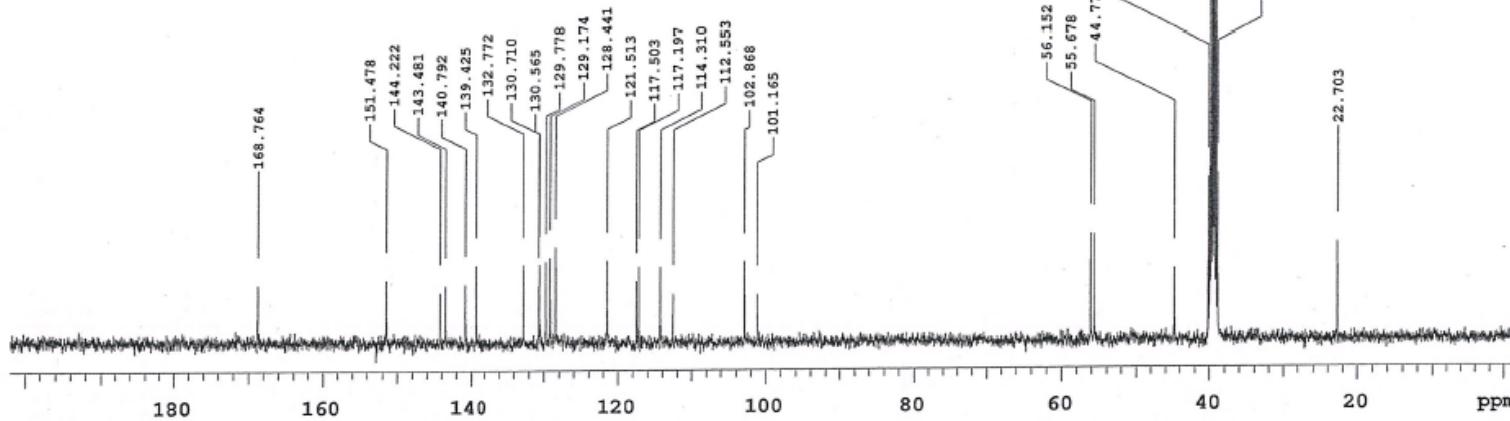


¹³C NMR of *N*-(4-((2-bromophenyl)amino)-2,5-dimethoxybenzyl)-*N*-(2-iodophenyl)acetamide (**4**)

TDC-110 Iodo Bromo diamine acetyl in DMSO

NMR-400MHz
AR. No:ME0813/1482
Analyst: Ganesh
Date: 16th Aug. 2013

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul

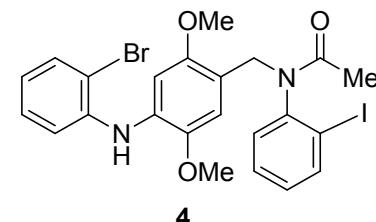


Mass Spectrum of *N*-(4-((2-bromophenyl)amino)-2,5-dimethoxybenzyl)-*N*-(2-iodophenyl)acetamide (4)

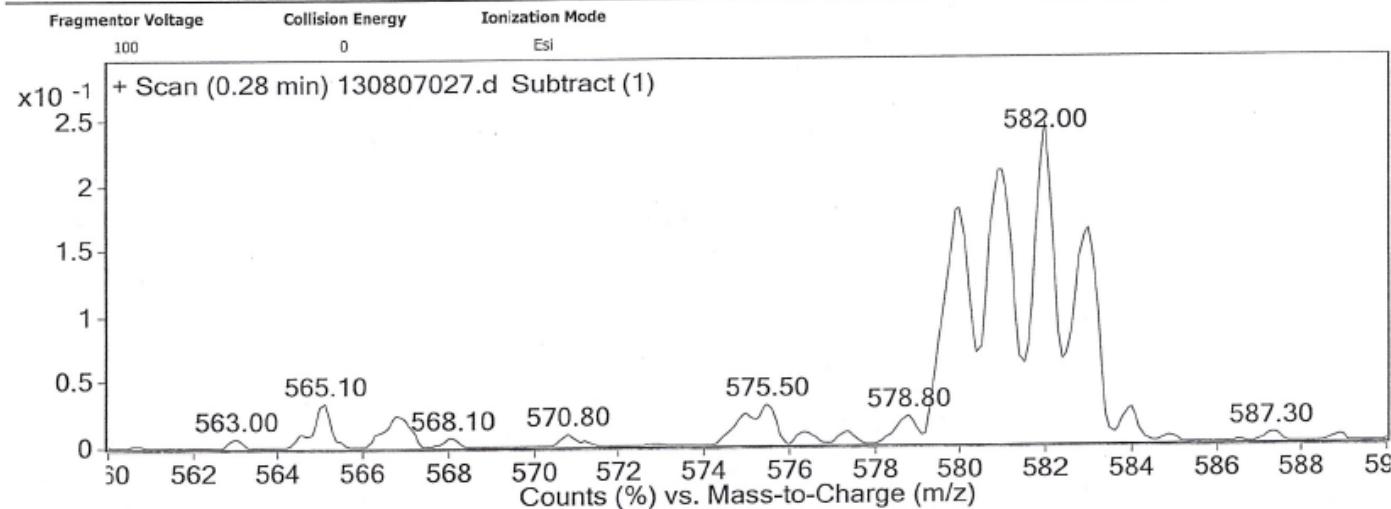
CPS, MIYAPUR

Mass Analysis Report

Data Filename	130807027.d	Sample Name	IODO BROMO ACETYL F-II
Sample Type	Sample	Position	Vial 47
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	



User Spectra



--- End Of Report ---

HRMS of *N*-(4-((2-bromophenyl)amino)-2,5-dimethoxybenzyl)-*N*-(2-iodophenyl)acetamide (4)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

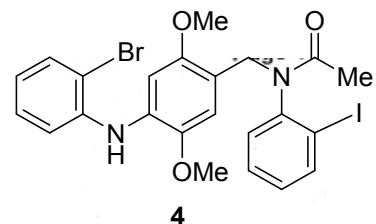
Monoisotopic Mass, Even Electron Ions

57 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

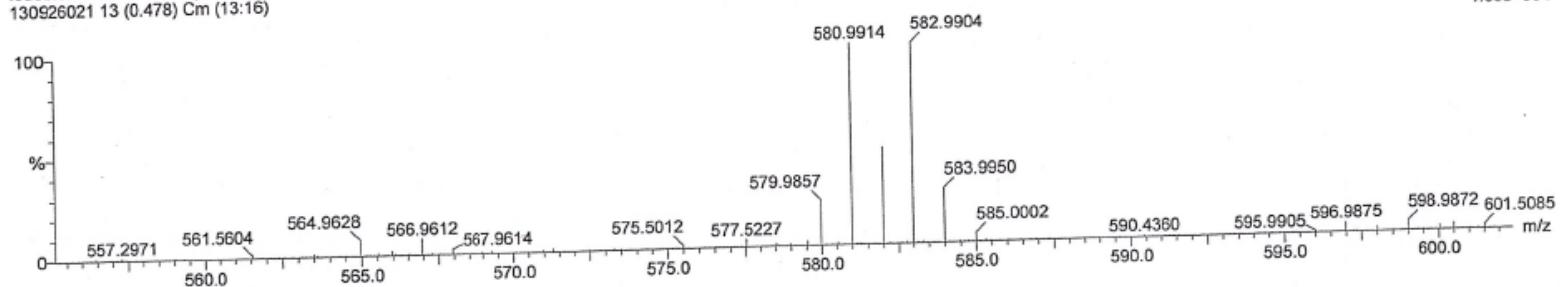
Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-4 Br: 0-1 I: 0-1

Iodobromo diamine acetyl
130926021 13 (0.478) Cm (13:16)

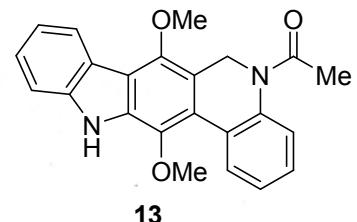


1: TOF MS ES+
1.39e+004



Minimum:	-5.0					
Maximum:	5.0	5.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
580.9914	580.9937	-2.3	-4.0	12.5	631.5	C23 H23 N2 O3 Br I

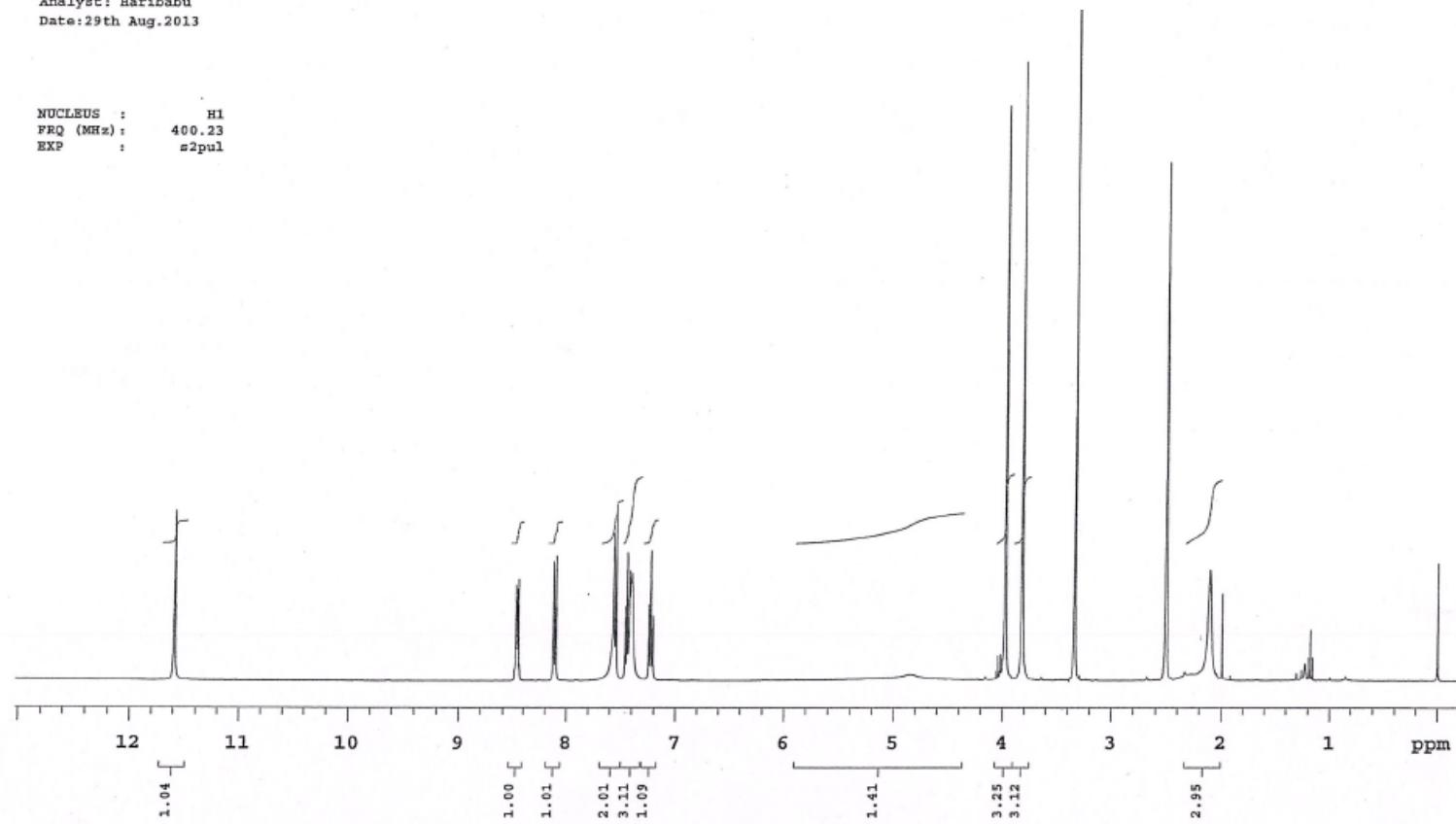
¹H NMR of 1-(7,13-dimethoxy-6,12-dihydro-5H-indolo[3,2-*j*]phenanthridin-5-yl)ethanone (13)



TDC-110 Phenanthridine acetyl CH in DMSO

NMR-400MHz
AR.No:ME0813/2734
Analyst: Haribabu
Date:29th Aug.2013

NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : zg2pul

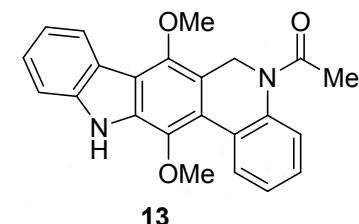
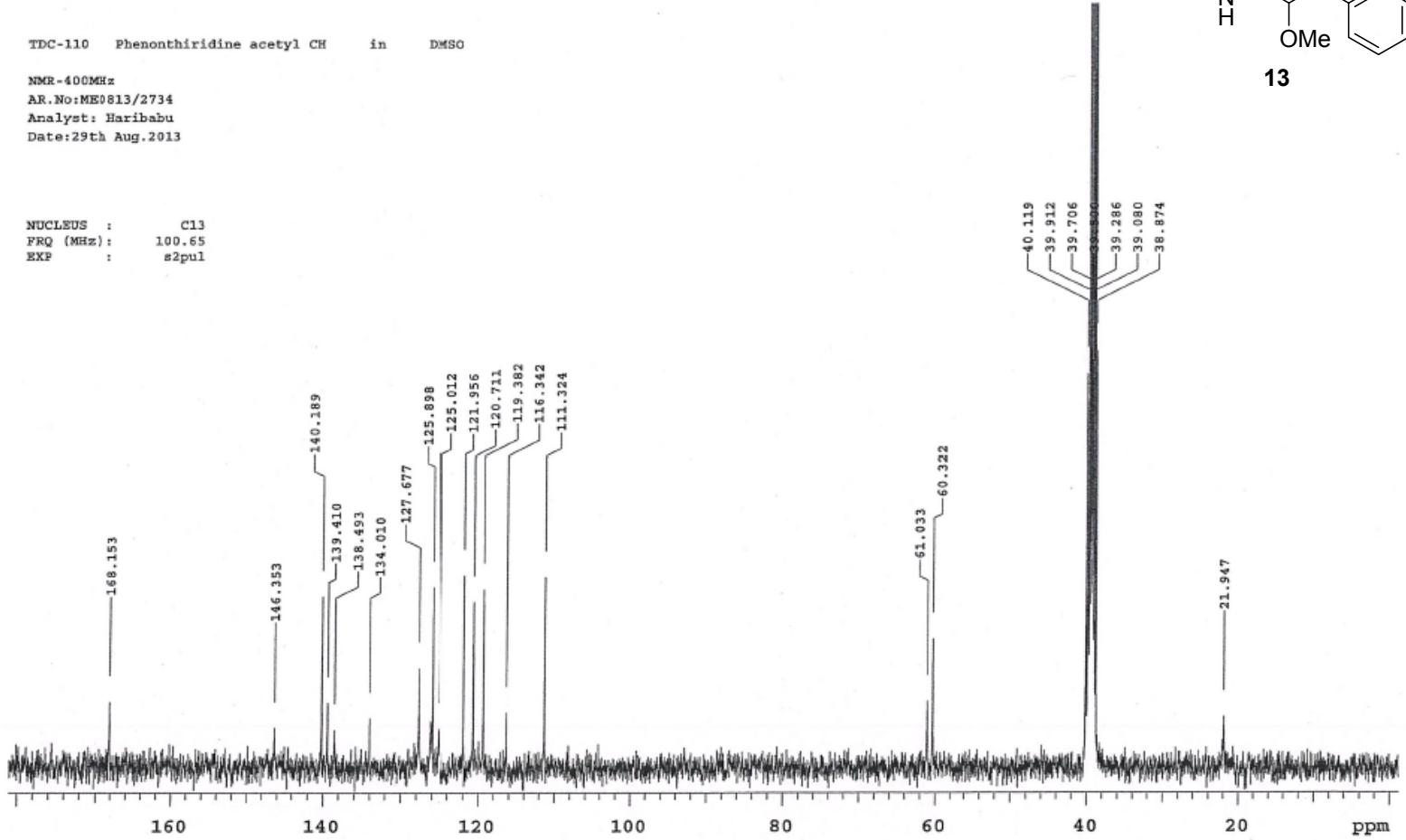


¹³C NMR of 1-(7,13-dimethoxy-6,12-dihydro-5H-indolo[3,2-*j*]phenanthridin-5-yl)ethanone (**13**)

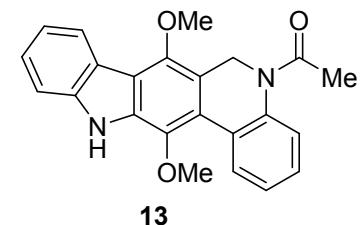
TDC-110 Phenanthridine acetyl CH in DMSO

NMR-400MHz
AR.No:ME0813/2734
Analyst: Haribabu
Date:29th Aug. 2013

NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul

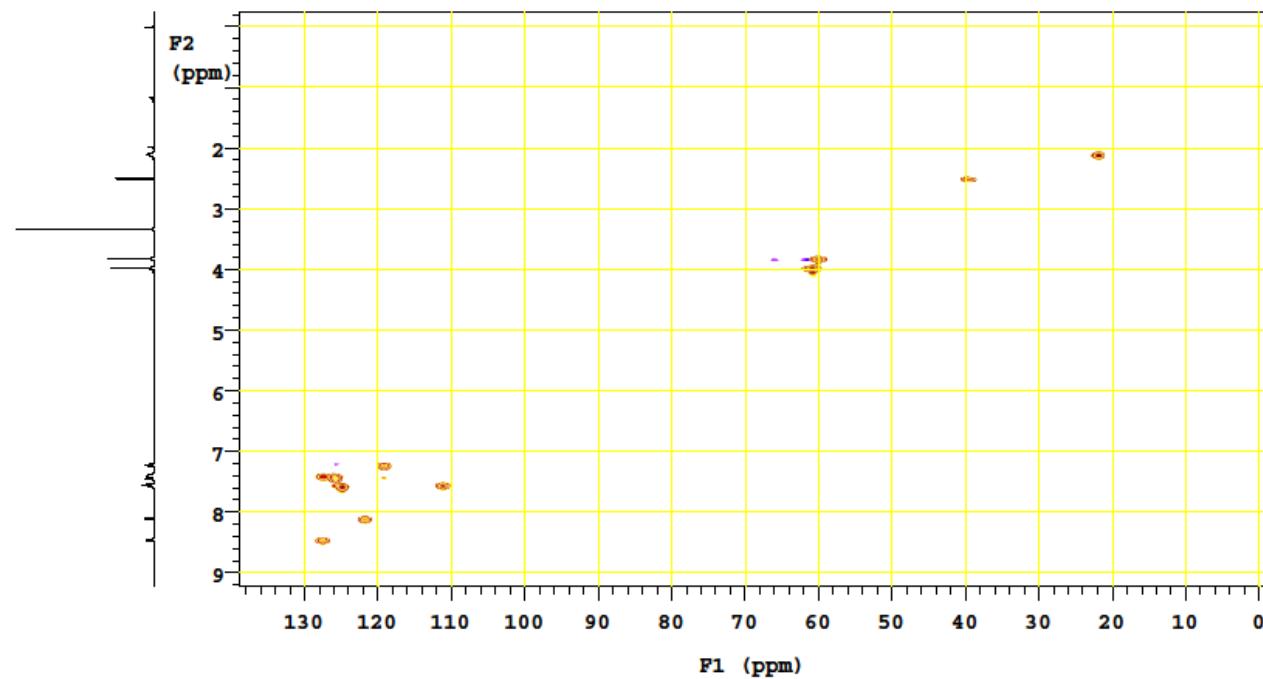


HSQC of 1-(7,13-dimethoxy-6,12-dihydro-5*H*-indolo[3,2-*j*]phenanthridin-5-yl)ethanone (13)



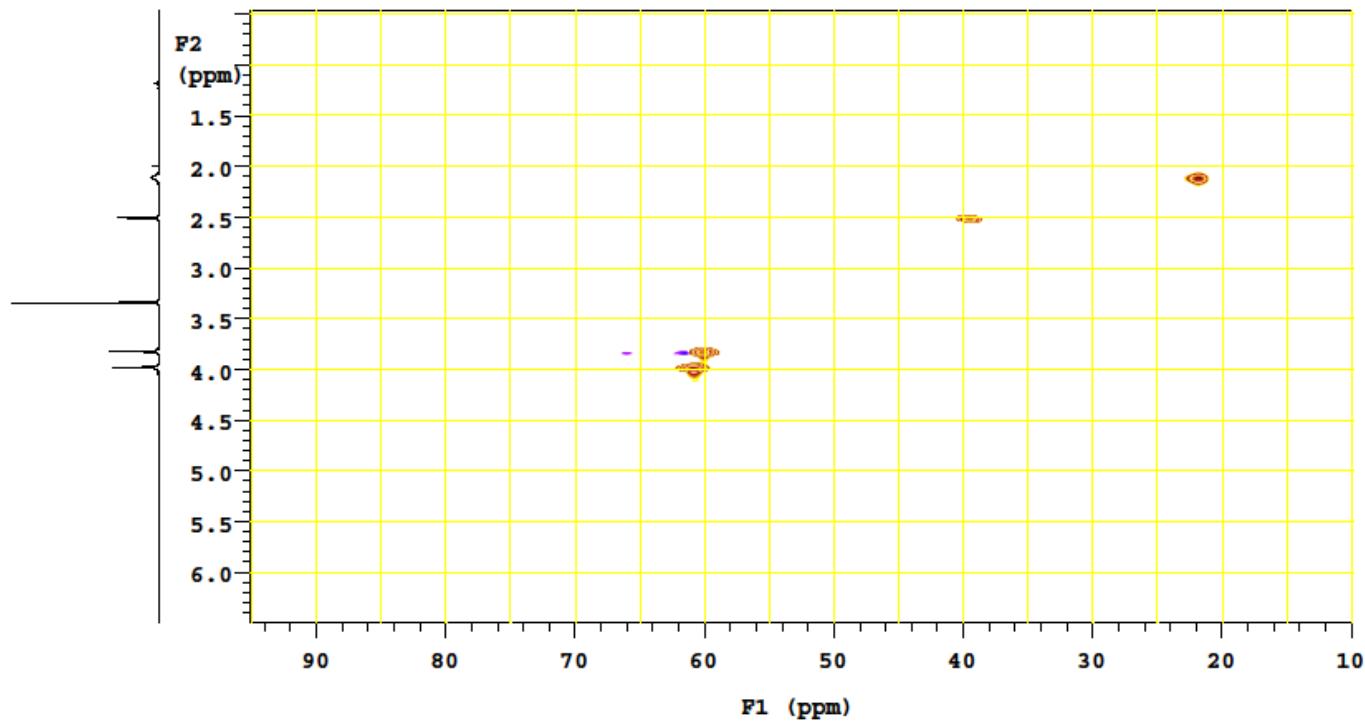
TDC-110 Phenanthridine acetyl CH in DMSO

NMR-400MHz
AR.No:ME0813/2734
Analyst: Haribabu
Date:29th Aug.2013



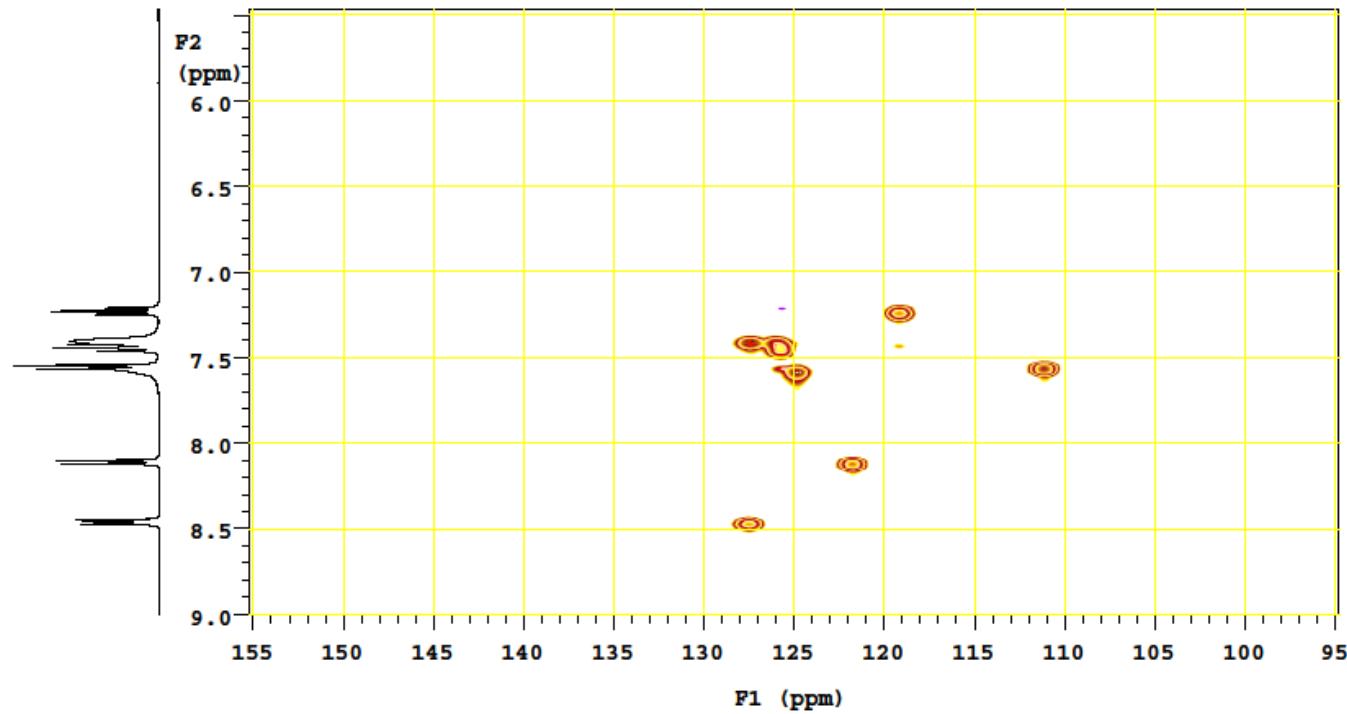
TDC-110 Phenanthridine acetyl CH in DMSO

NMR-400MHz
AR.No:MR0013/2734
Analyst: Haribabu
Date:29th Aug.2013



TDC-110 Phenanthridine acetyl CH in DMSO

NMR-400MHz
AR.No :ME0813/2734
Analyst: Haribabu
Date: 29th Aug. 2013

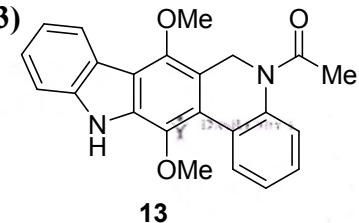


Mass Spectrum of 1-(7,13-dimethoxy-6,12-dihydro-5H-indolo[3,2-j]phenanthridin-5-yl)ethanone (13)

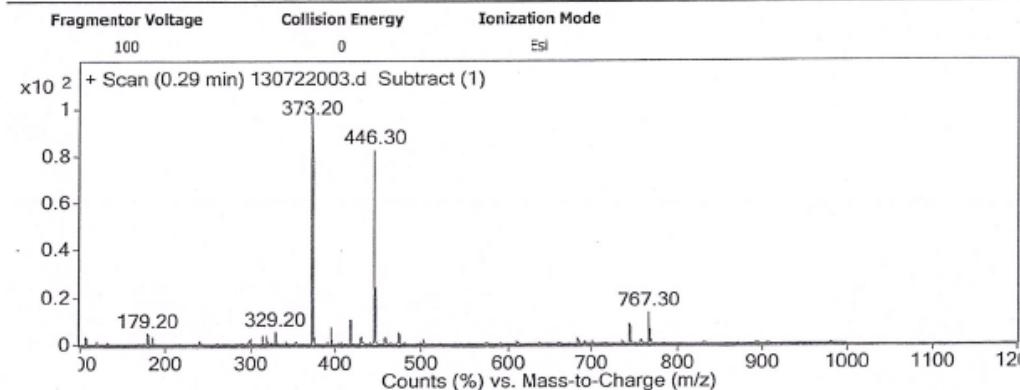
CPS,MIYAPUR

LCMS Analysis Report

Data Filename	130722003.d	Sample Name	Phenanthracin acid
Sample Type	Sample	Position	Vial 87
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

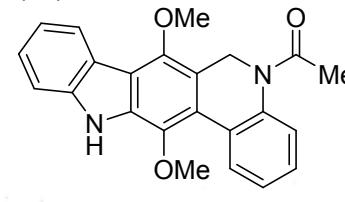


User Spectra



--- End Of Report ---

HRMS of 1-(7,13-dimethoxy-6,12-dihydro-5H-indolo[3,2-j]phenanthridin-5-yl)ethanone (13)



Page 1

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

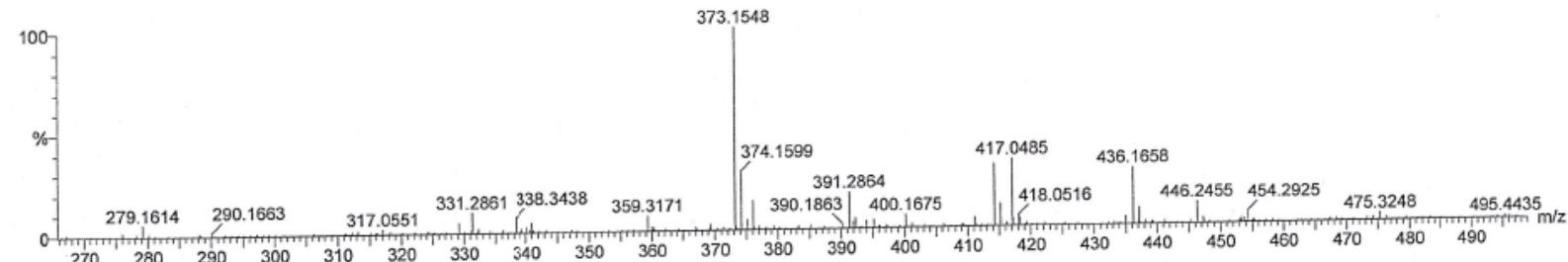
46 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

C: 0-25 H: 0-25 N: 0-2 O: 0-4 Br: 0-1

Phenanthidine acetyl
130926013 12 (0.419) Cm (12:17-1:2)

1: TOF MS ES+
3.48e+004



Minimum:	- 5.0					
Maximum:	5.0	5.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
373.1548	373.1552	-0.4	-1.1	14.5	55.4	C23 H21 N2 O3

¹H NMR of Calothrixin B (2)

TDC-110 Calothrixin in DMSO

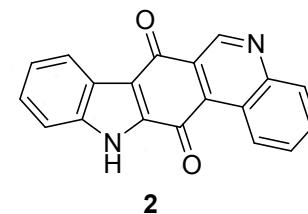
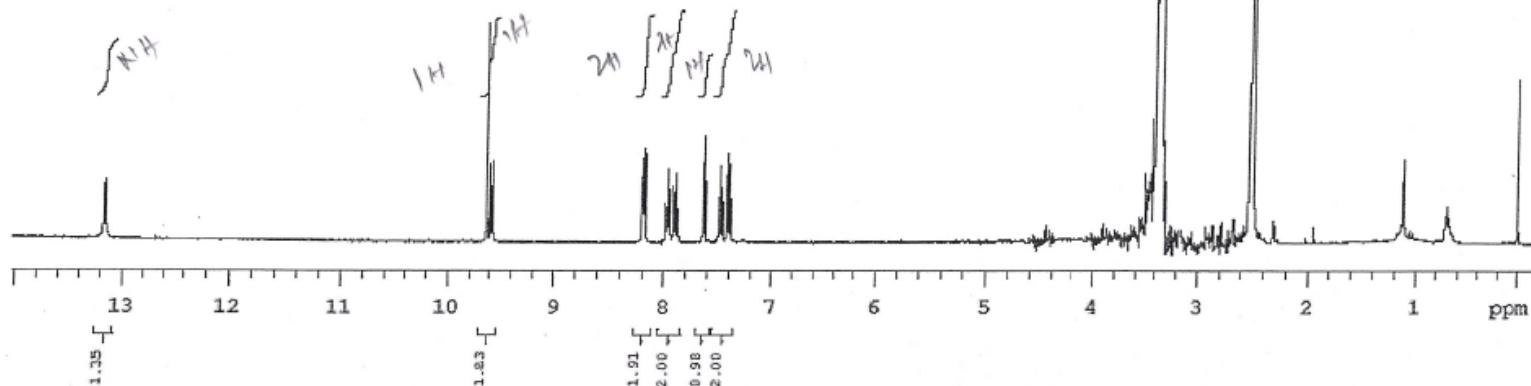
NMR-400MHz

AR.No:ME0313/26

Analyst: Haribabu

Date: 1st Aug.2013

NUCLEUS : H1
FRQ (MHz): 400.23
EXP : zgppul



Expansion of ^1H NMR of Calothrixin B (2)

TDC-110 Calothrixin in DMSO

NMR-400MHz

AR.No:ME0813/26

Analyst: Haribabu

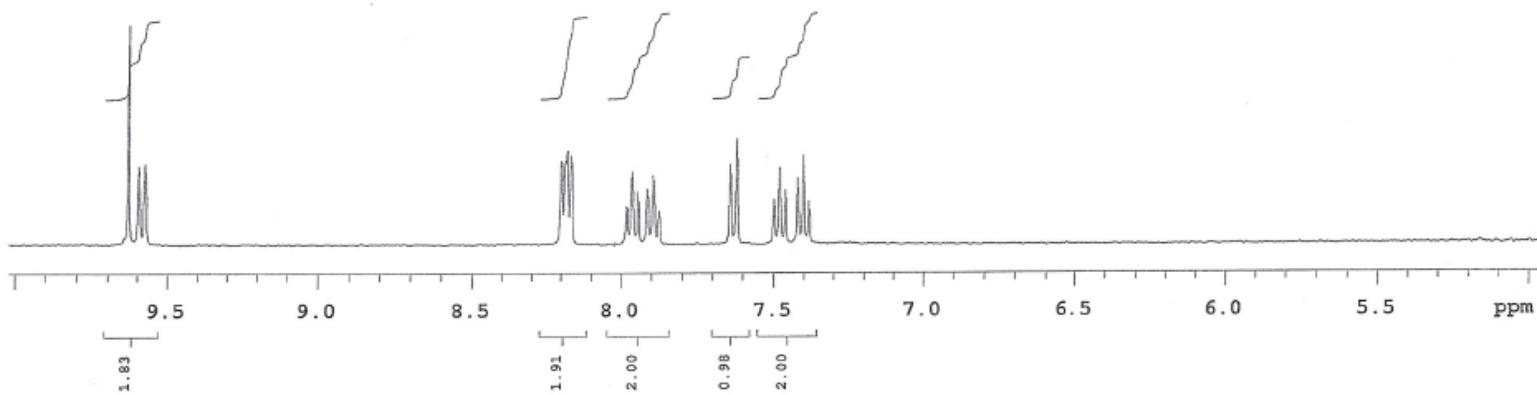
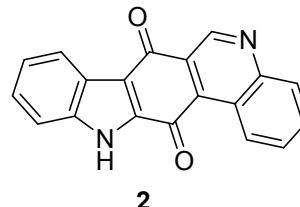
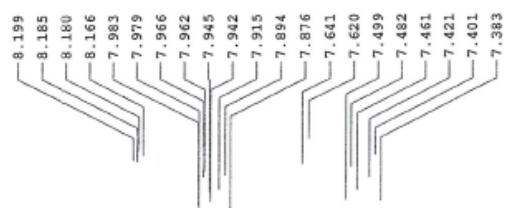
Date: 1st Aug 2013

9.62 9.59 9.51

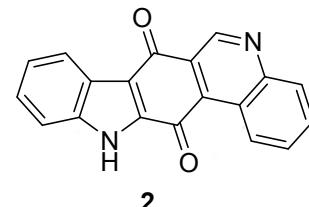
NUCLEUS : H1

FRQ (MHz) : 400.23

EXP : s2pul



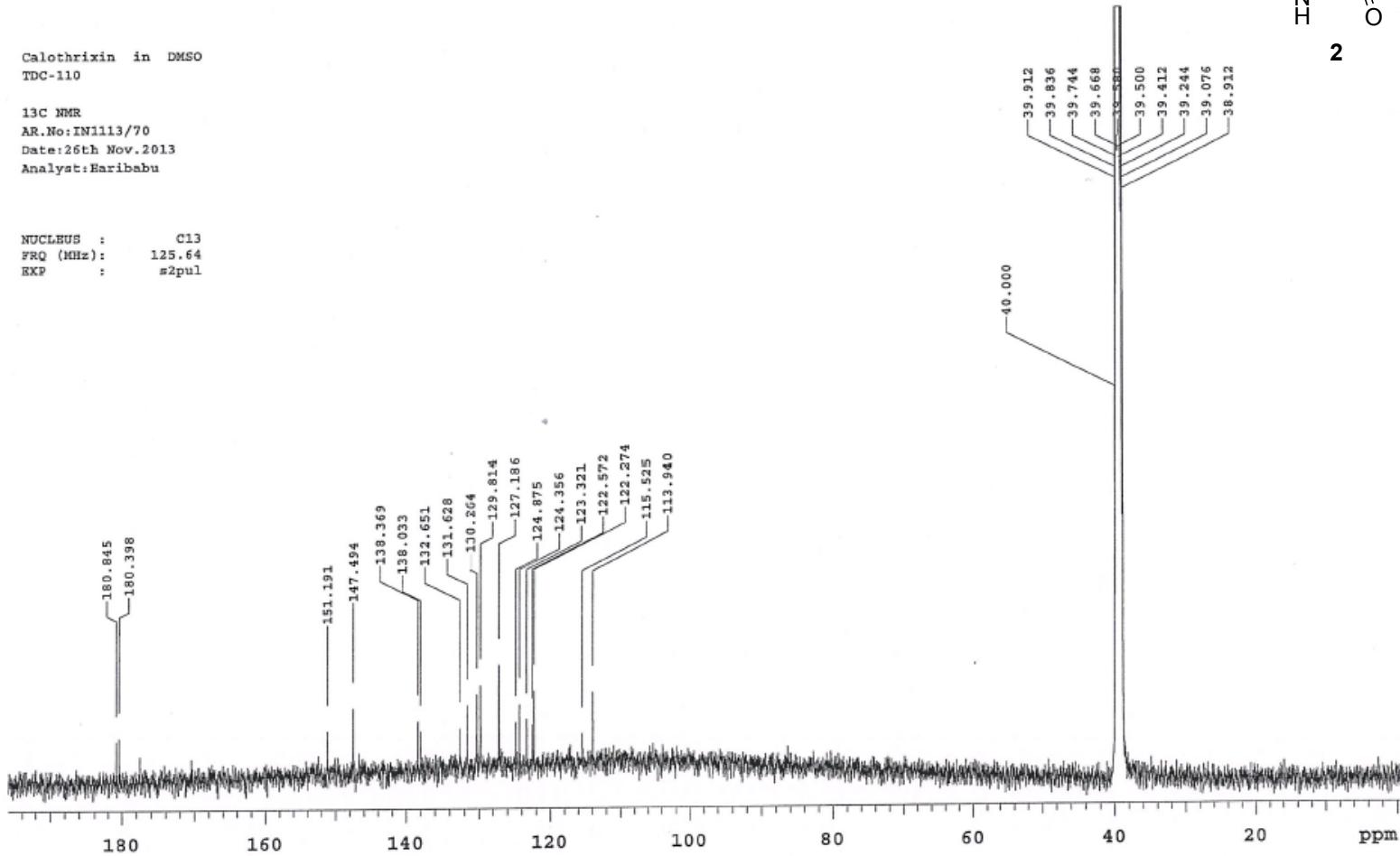
¹³C NMR of Calothrixin B (2)



Calothrixin in DMSO
TDC-110

¹³C NMR
AR.No:IN1113/70
Date:26th Nov.2013
Analyst:Haribabu

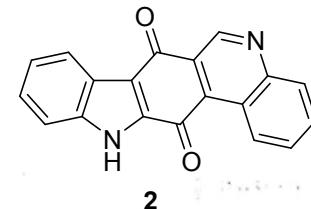
NUCLEUS : C13
FRQ (MHz): 125.64
EXP : s2pul



Mass Spectrum of Calothrixin B (2)

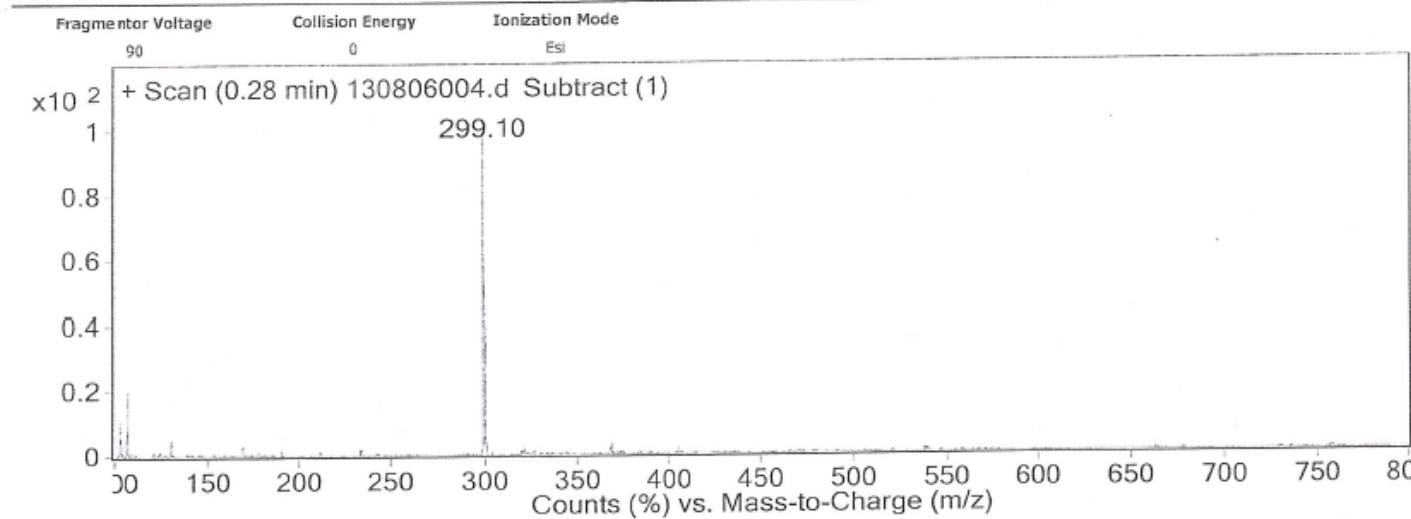
CPS,MIYAPUR

Mass Analysis Report



Data Filename	130806004.d	Sample Name	Calothrixin
Sample Type	Sample	Position	Vial 95
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	

User Spectra



--- End Of Report ---

HRMS of Calothrixin B (2)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

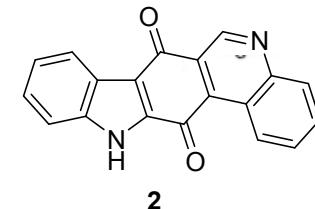
Monoisotopic Mass, Even Electron Ions

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

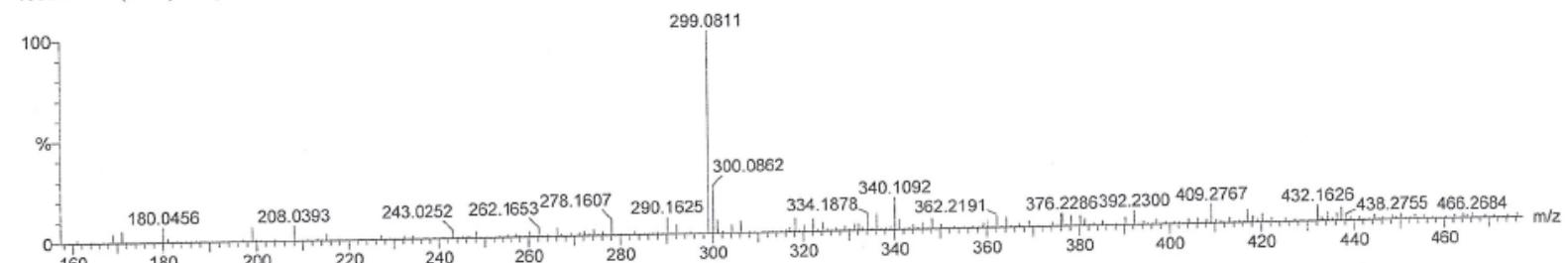
Elements Used:

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

Calothrixin
130926017 9 (0.338) Cm (9:12-1:4)



1: TOF MS ES+
1.55e+004

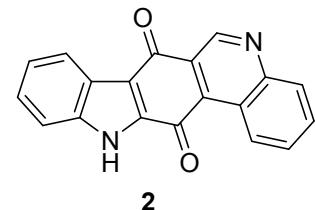


Minimum:	-5.0
Maximum:	5.0
Mass	Calc. Mass
299.0811	299.0821

mDa PPM DBE i-FIT Formula

-1.0 -3.3 15.5 226.3 C19 H11 N2 O2

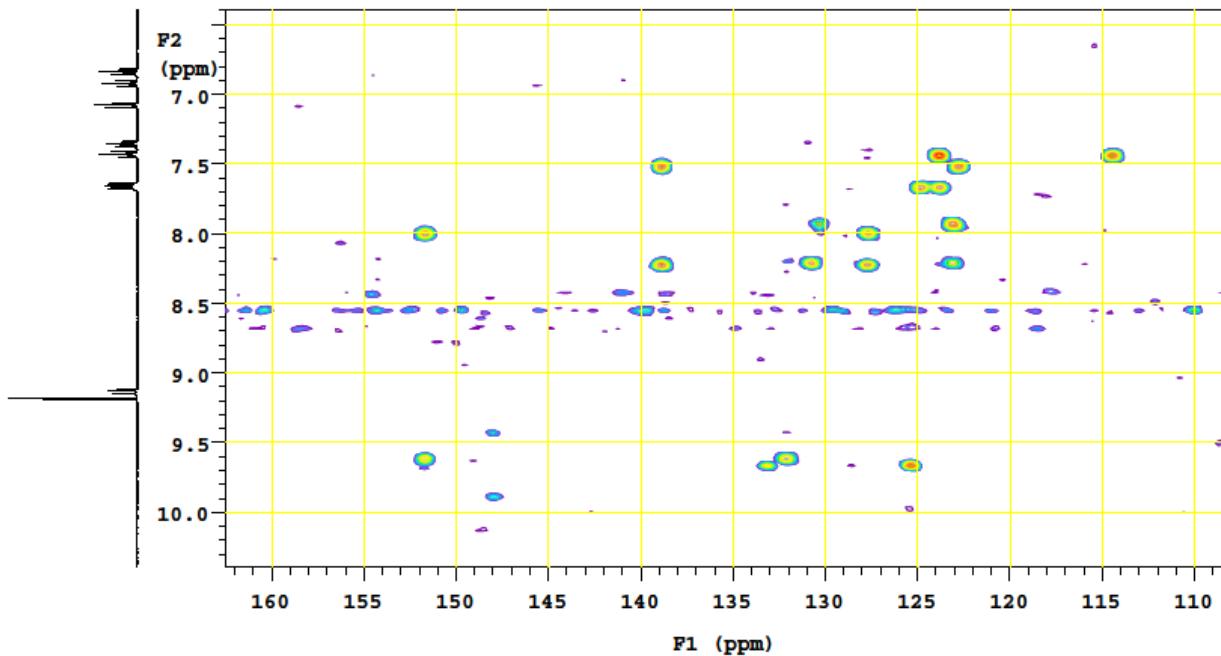
HMBC of Calothrixin B (2)



TDC-110 Calothrixin B in DMSO

NMR-400MHz
AR.No:ME1113/2106
Analyst: Haribabu
Date: 25th Nov.2013

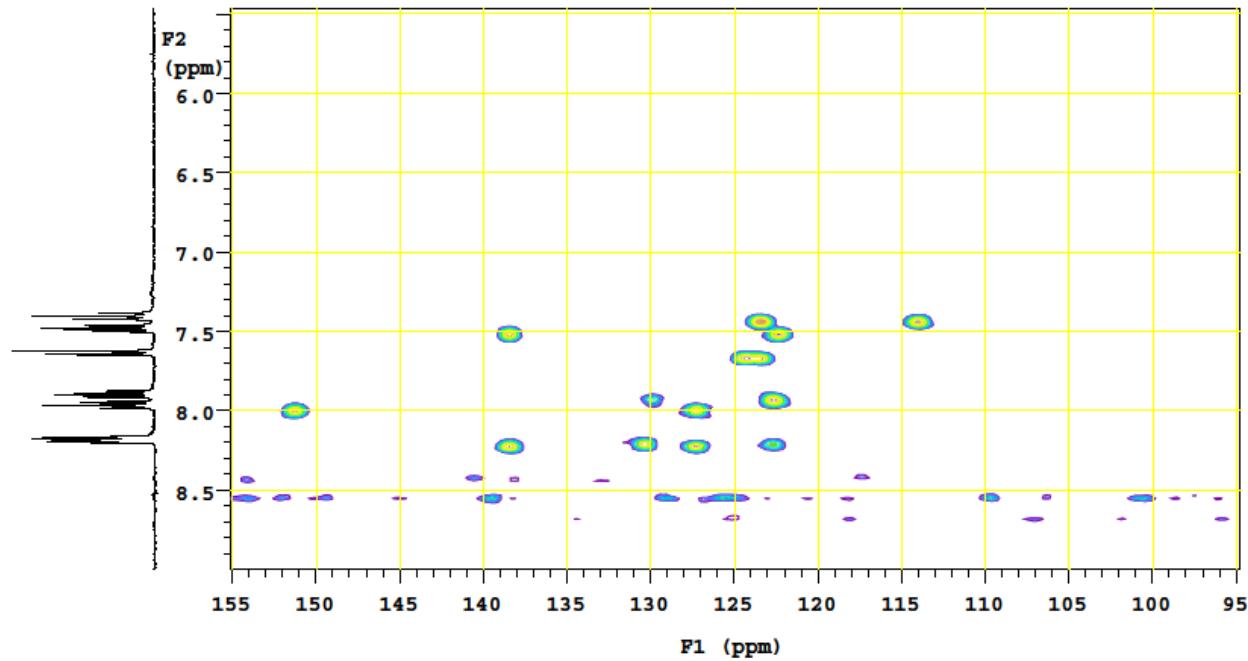
NUCLEUS : H1
FRQ (MHz) : 400.22
EXP : gHMBC



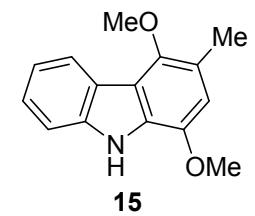
TDC-110 Calothrixin B in DMSO

NMR-400MHz
AR.No:ME1113/2106
Analyst: Haribabu
Date: 25th Nov.2013

NUCLEUS : H1
PRQ (MHz) : 400.22
EXP : gHMBC

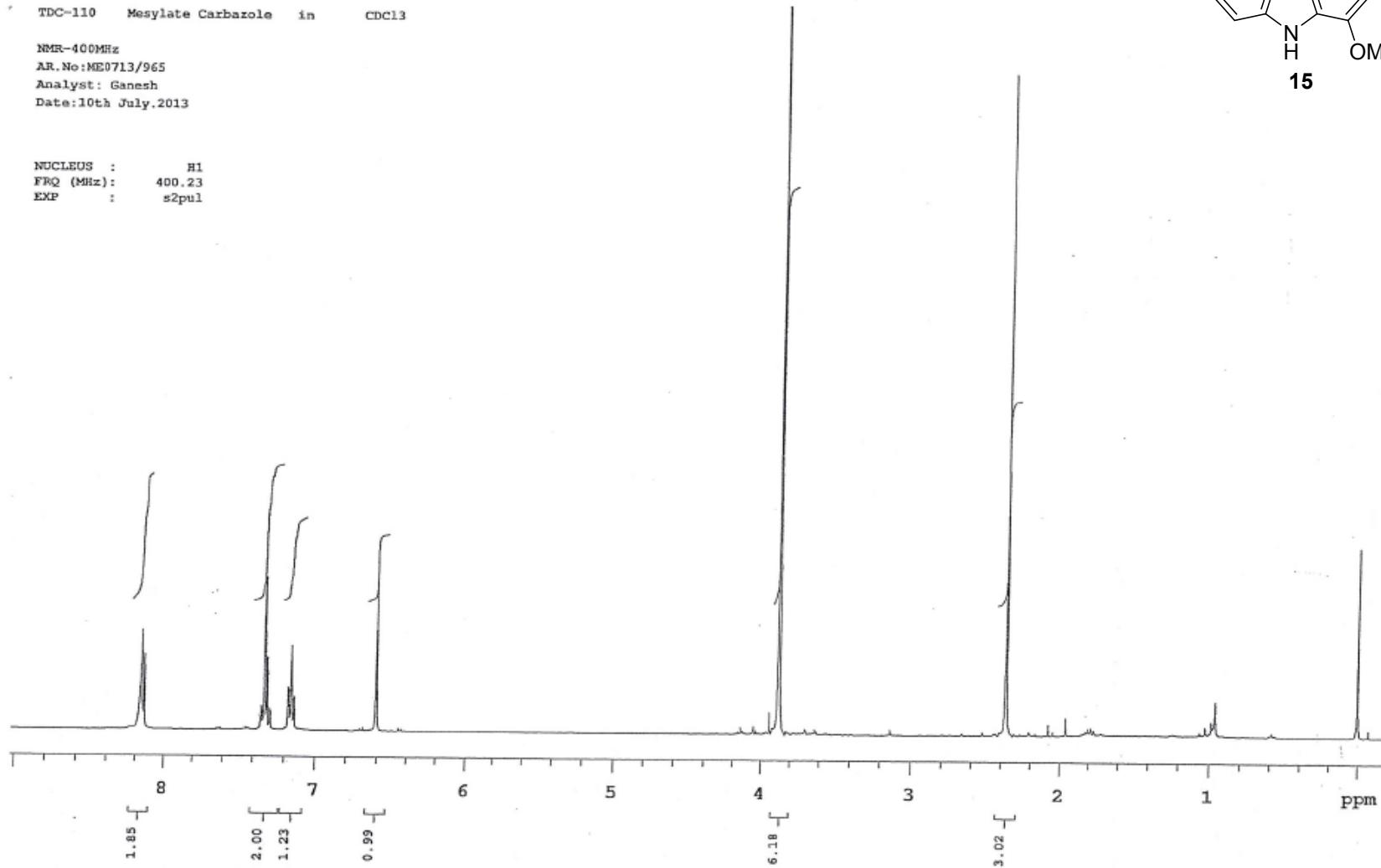


¹H NMR of 1,4-dimethoxy-3-methyl-9H-carbazole (15)



TDC-110 Mesylate Carbazole in CDCl₃
NMR-400MHz
AR.No:ME0713/965
Analyst: Ganesh
Date:10th July,2013

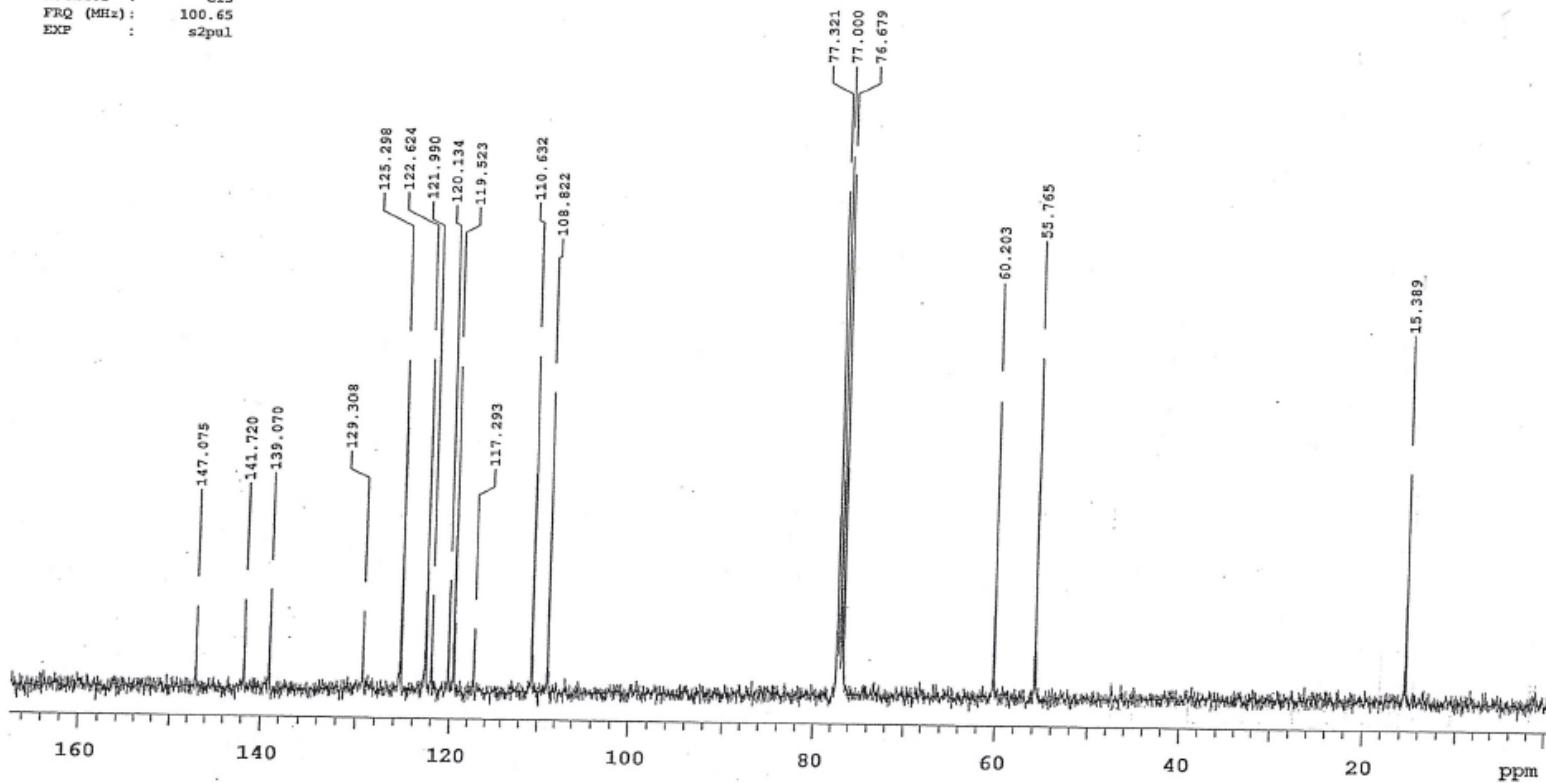
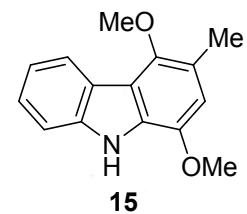
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul



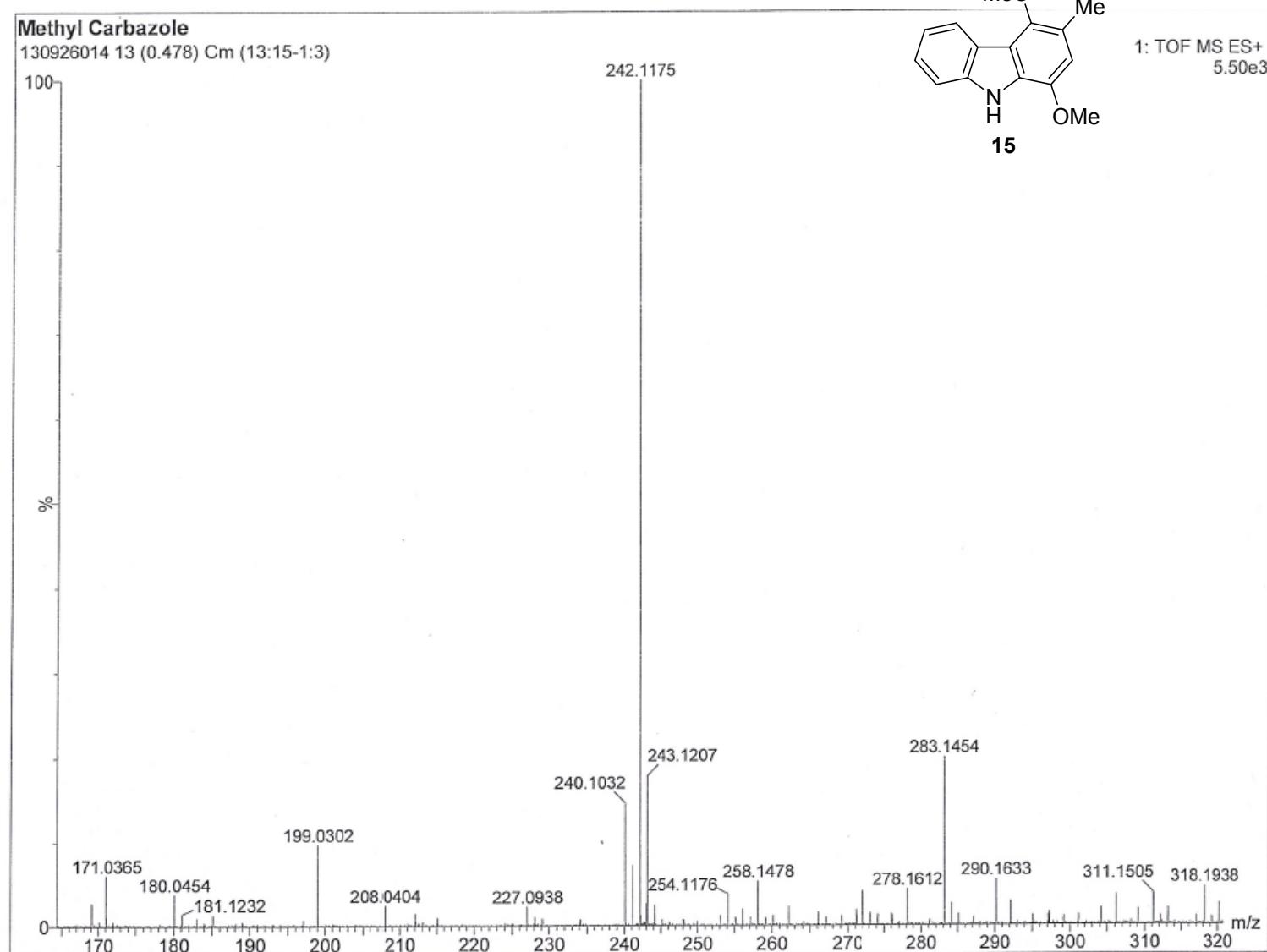
¹³C NMR of 1,4-dimethoxy-3-methyl-9H-carbazole (15)

TDC-110 Methyl Carbazole in CDCl₃
NMR-400MHz
AR.No:ME0713/1365
Analyst: Haribabu
Date:13th July.2013

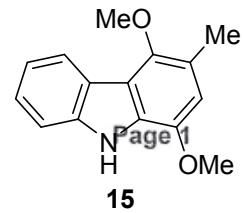
NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul



Mass Spectrum of 1,4-dimethoxy-3-methyl-9H-carbazole (15)



HRMS of 1,4-dimethoxy-3-methyl-9H-carbazole (15)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

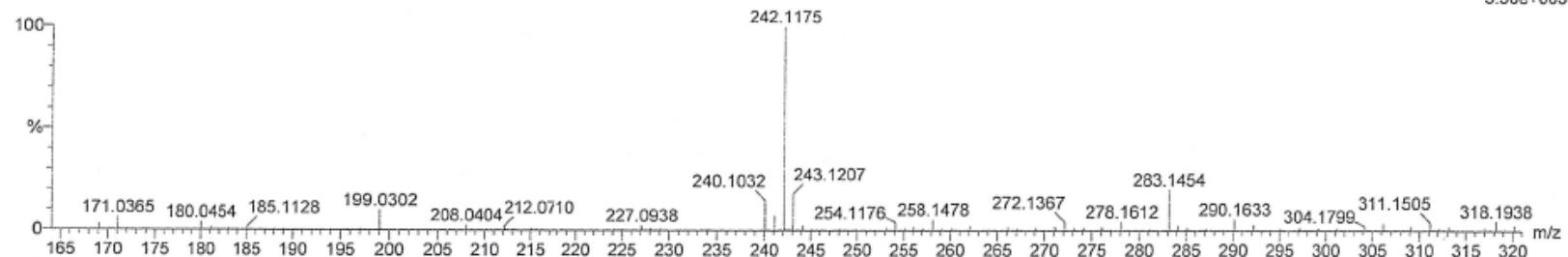
Elements Used:

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

Methyl Carbazole

130926014 13 (0.478) Cm (13:15:1:3)

1: TOF MS ES+
5.50e+003

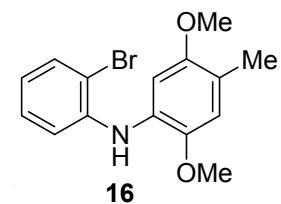


Minimum:

Maximum: 5.0 5.0 -5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
242.1175	242.1181	-0.6	-2.5	8.5	17.2	C15 H16 N O2

¹H NMR of *N*-(2-bromophenyl)-2, 5-dimethoxy-4-methylaniline (16)



TDC-110 Me adduct Fr-1 in DMSO

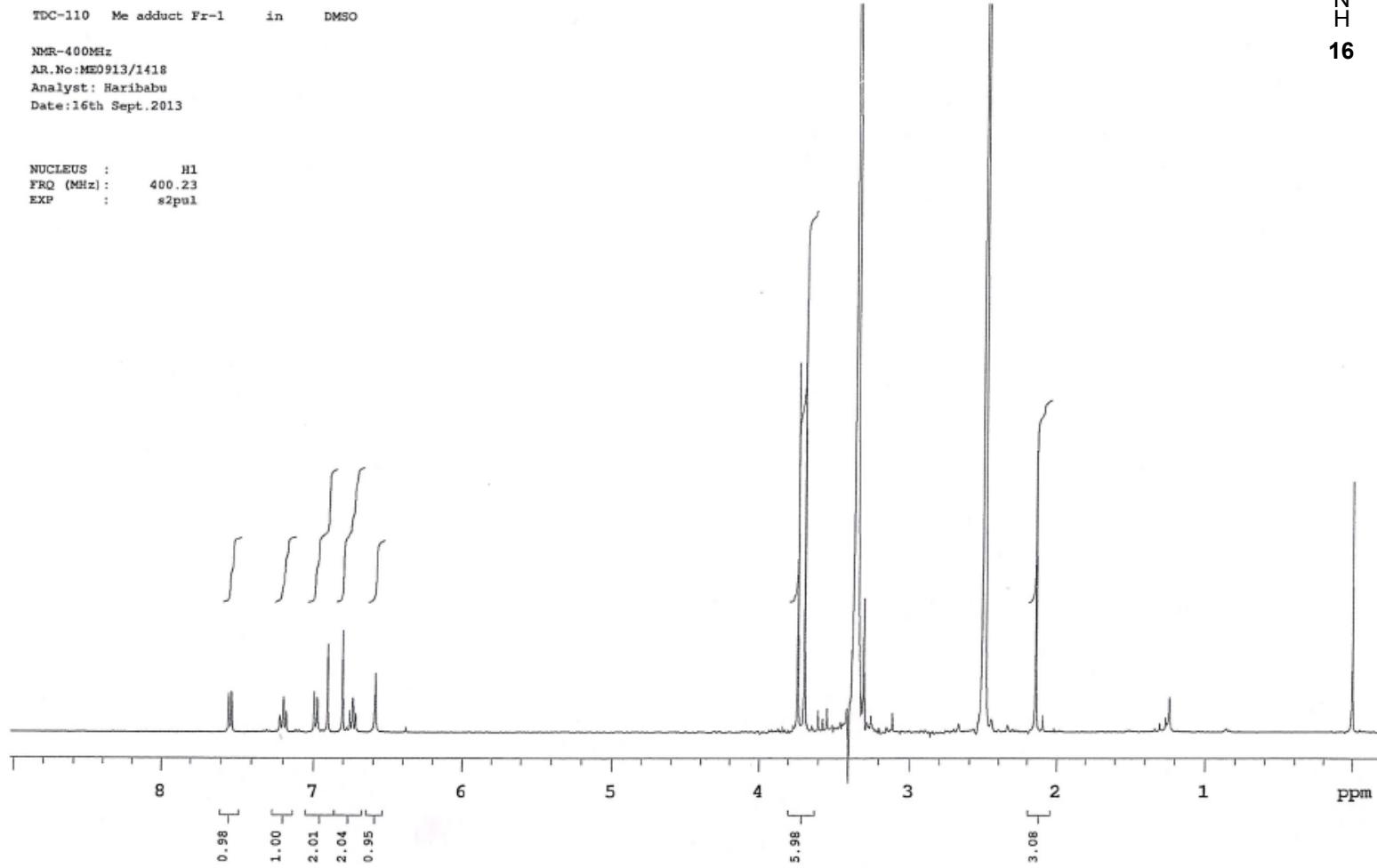
NMR-400MHz

AR.No:MED913/1418

Analyst: Haribabu

Date:16th Sept.2013

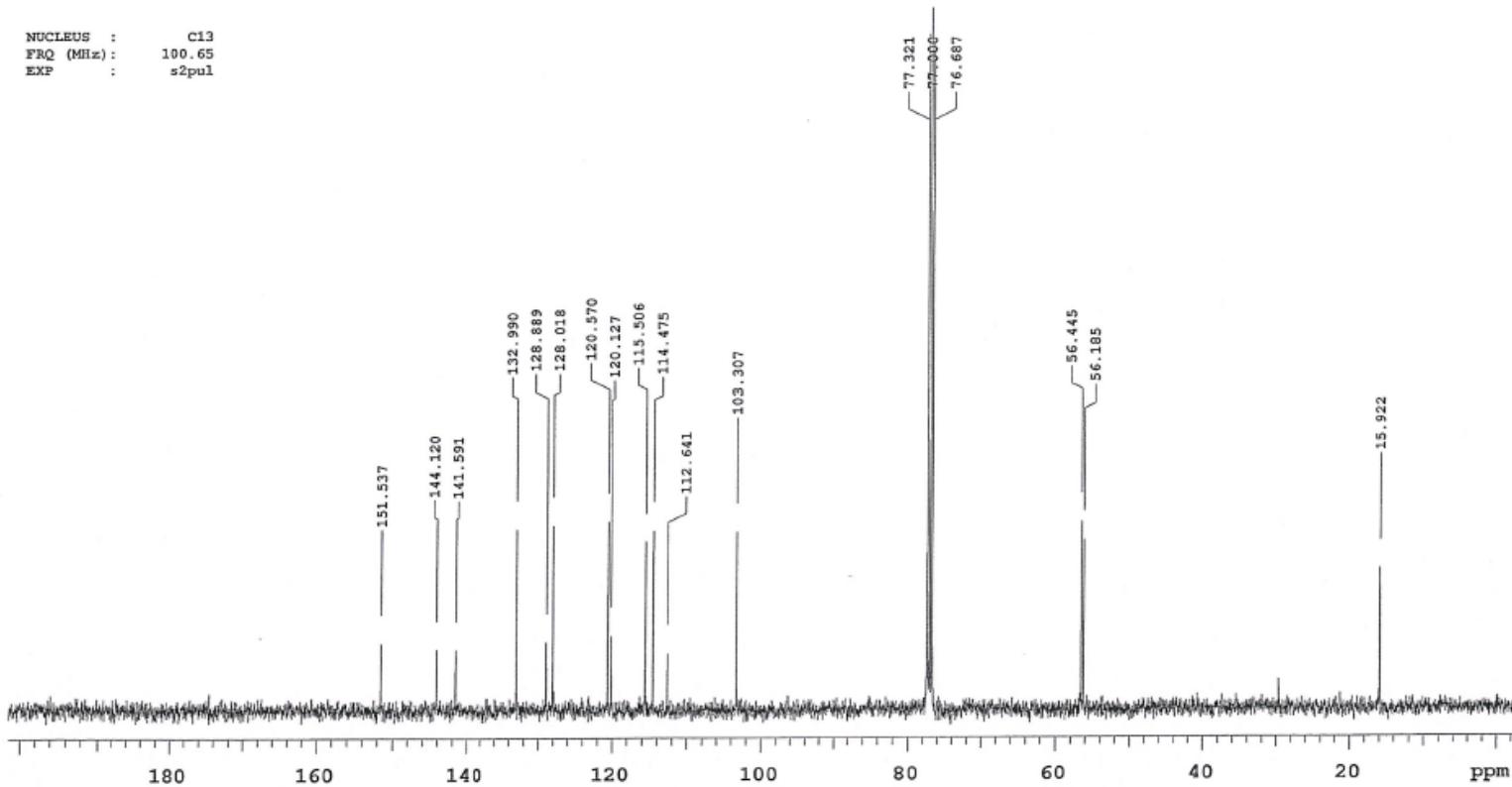
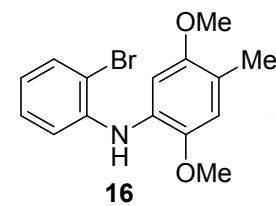
NUCLEUS : H1
FRQ (MHz) : 400.23
EXP : s2pul



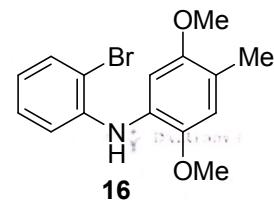
¹³C NMR of *N*-(2-bromophenyl)-2, 5-dimethoxy-4-methylaniline (16)

TDC-110 Me-adduct in CDCl₃
NMR-400MHz
AR. No:ME0913/2862
Analyst: Ganesh
Date: 27th Sept. 2013

NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul



Mass Spectrum of of *N*-(2-bromophenyl)-2, 5-dimethoxy-4-methylaniline (16)

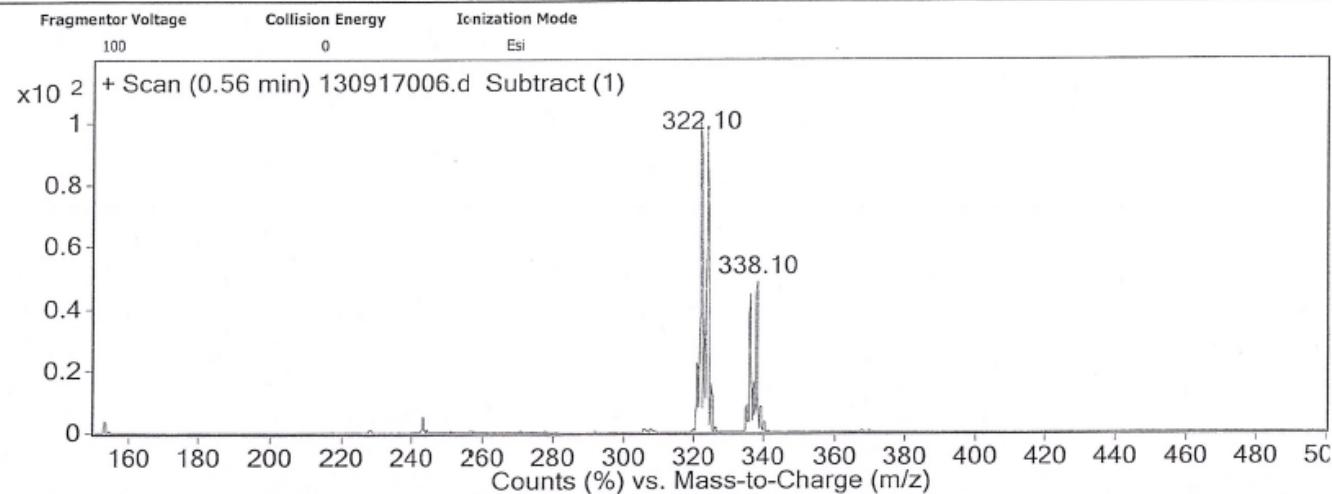


CPS, MIYAPUR

Mass Analysis Report

Data Filename	130917006.d	Sample Name	Me-adduct
Sample Type	Sample	Position	Vial 11
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	CUBI3.m	Comment	

User Spectra



--- End Of Report ---

HRMS of *N*-(2-bromophenyl)-2, 5-dimethoxy-4-methylaniline (16)

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

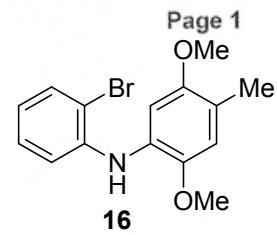
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

64 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

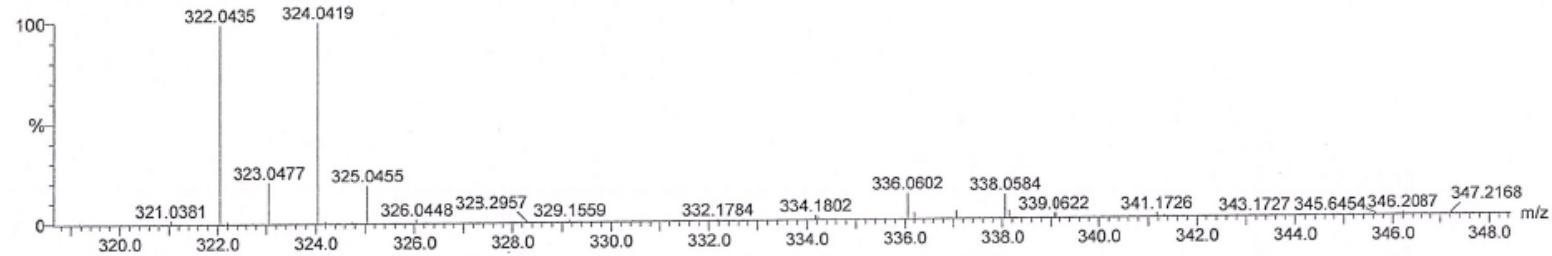
Elements Used:

C: 0-16 H: 0-18 N: 0-2 O: 0-3 Br: 0-3



1: TOF MS ES+
3.97e+003

ME ADDUCT
130920016 16 (0.560) Cm (16:19-26:33)



Minimum: -5.0
Maximum: 5.0 5.0 80.0

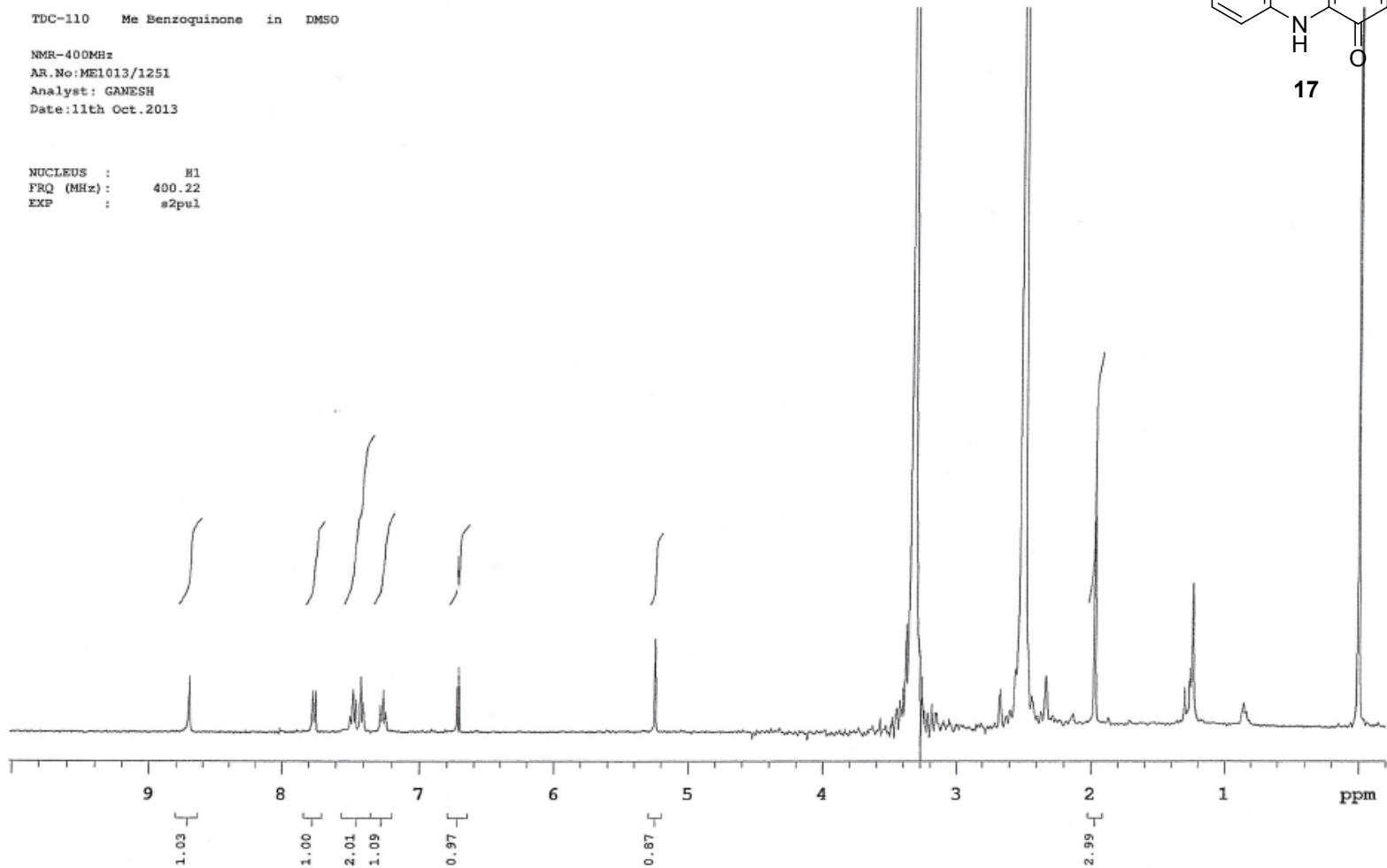
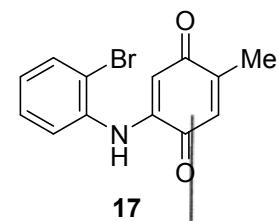
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
322.0435	322.0443	-0.8	-2.5	7.5	11.8	C15 H17 N O2 Br

¹H NMR of 2-((2-bromophenyl) amino)-5-methylcyclohexa-2,5-diene-1,4-dione (17)

TDC-110 Me Benzoguinone in DMSO

NMR-400MHz
AR.No:ME1013/1251
Analyst: GANESH
Date:11th Oct.2013

NUCLEUS : H1
FRQ (MHz) : 400.22
EXP : s2pul

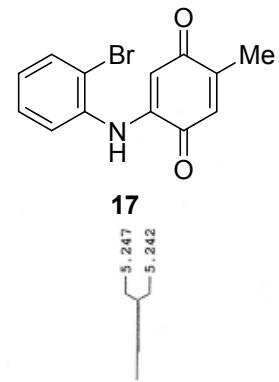
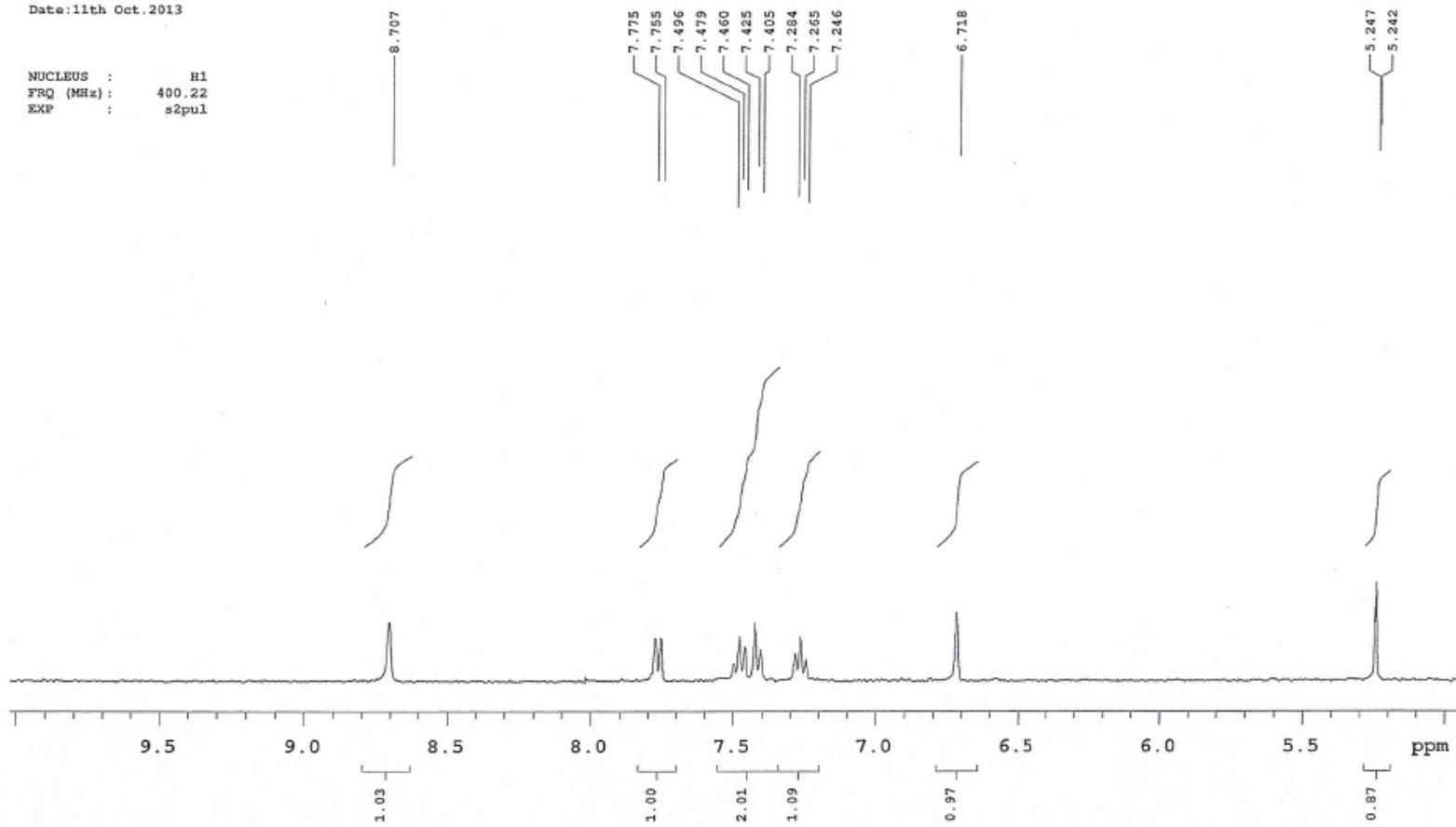


Expansion ^1H NMR of 2-((2-bromophenyl) amino)-5-methylcyclohexa-2,5-diene-1,4-dione (17)

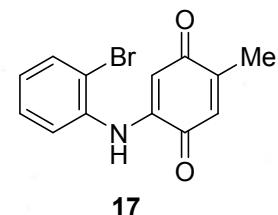
TDC-110 Me Benzoquinone in DMSO

NMR-400MHz
AR.No:ME1013/1251
Analyst: GANESH
Date:11th Oct.2013

NUCLEUS : H1
FRQ (MHz) : 400.22
EXP : s2pul

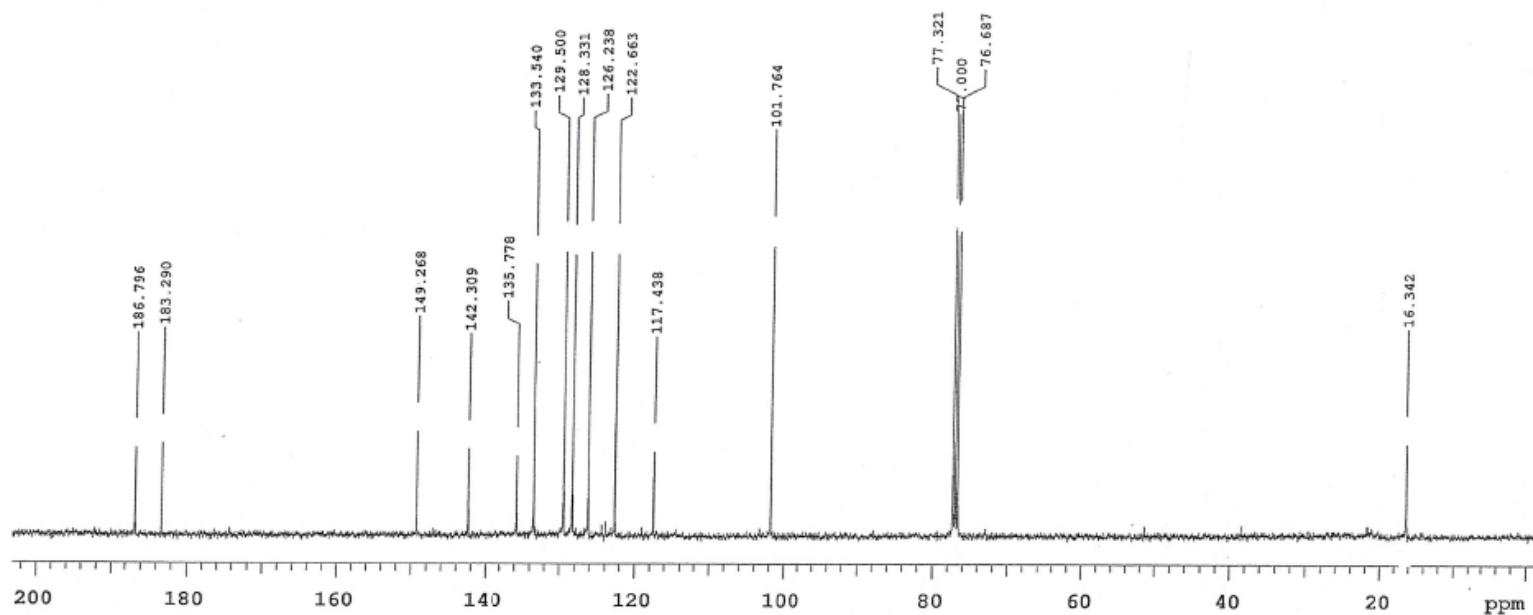


¹³C NMR of 2-((2-bromophenyl) amino)-5-methylcyclohexa-2,5-diene-1,4-dione (17)

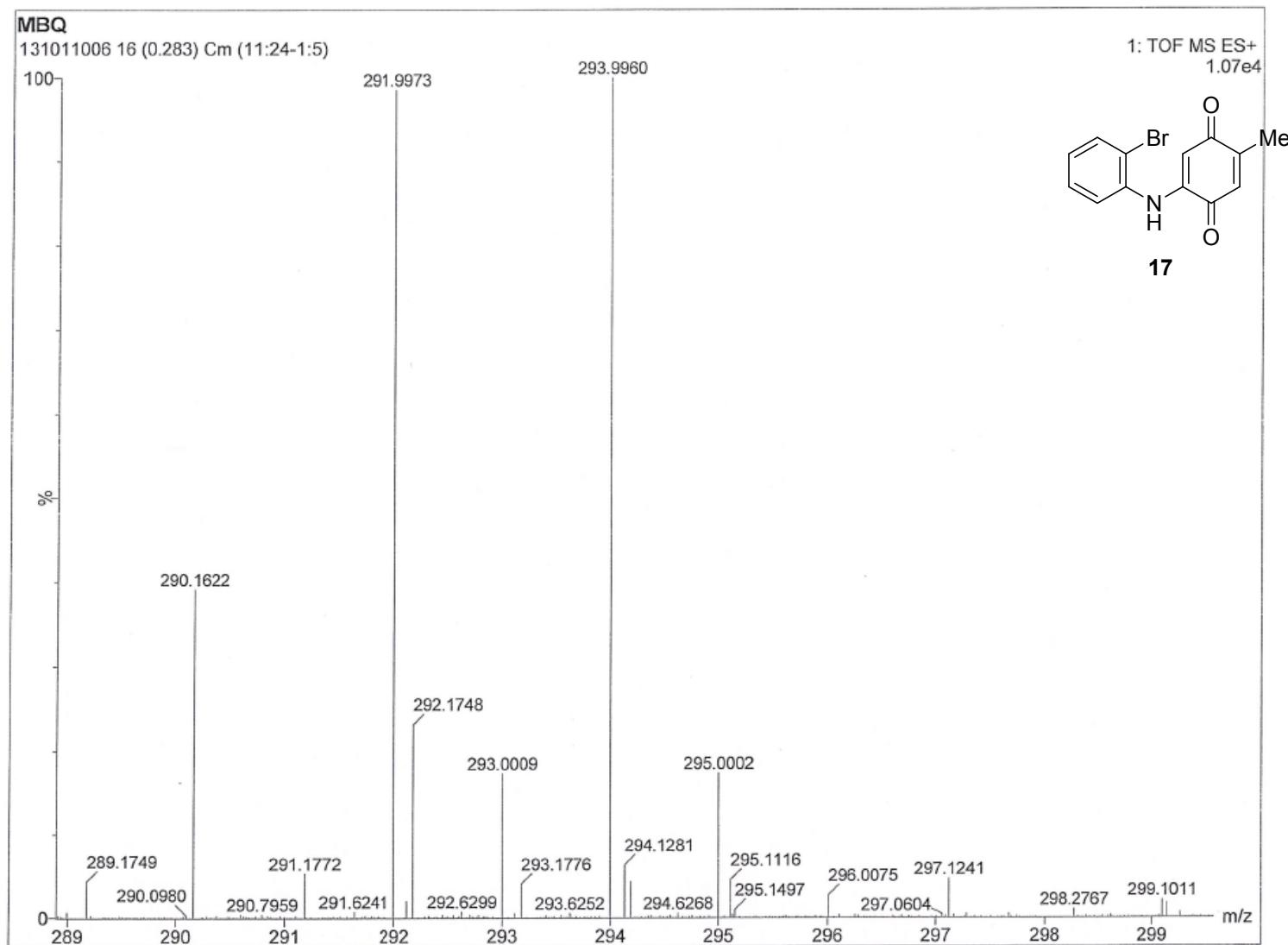


TDC-110 Me Bn Qn in DMSO
NMR=400MHz
AR.No:ME1013/1325
Analyst: Haribabu
Date: 11th Oct.2013.

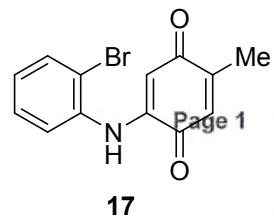
NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul



Mass Spectrum of 2-((2-bromophenyl) amino)-5-methylcyclohexa-2,5-diene-1,4-dione (17)



HRMS of 2-((2-bromophenyl) amino)-5-methylcyclohexa-2,5-diene-1,4-dione (17)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

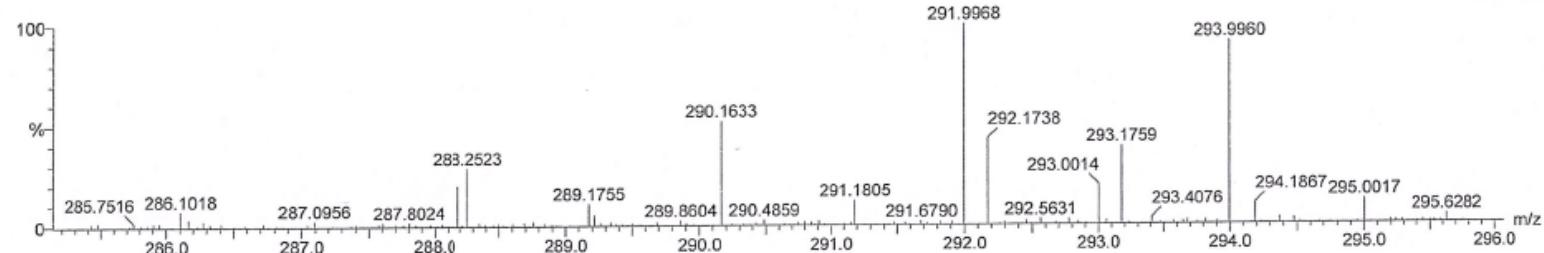
22 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

Elements Used:

C: 0-15 H: 0-13 N: 0-2 O: 0-3 Br: 0-1

MBQ
131011006 16 (0.283) Cm (15:24-5:11)

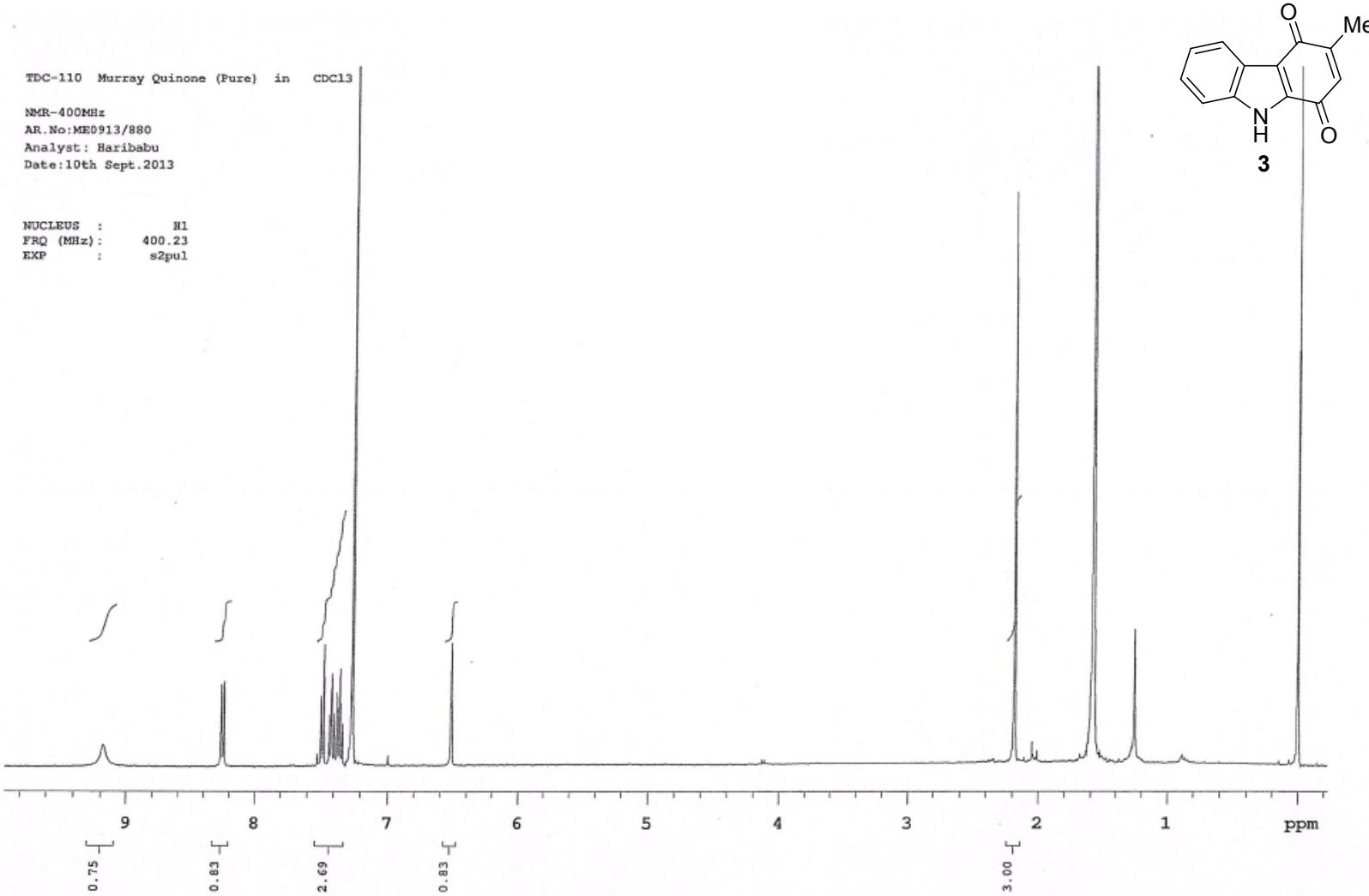
1: TOF MS ES+
1.01e+003



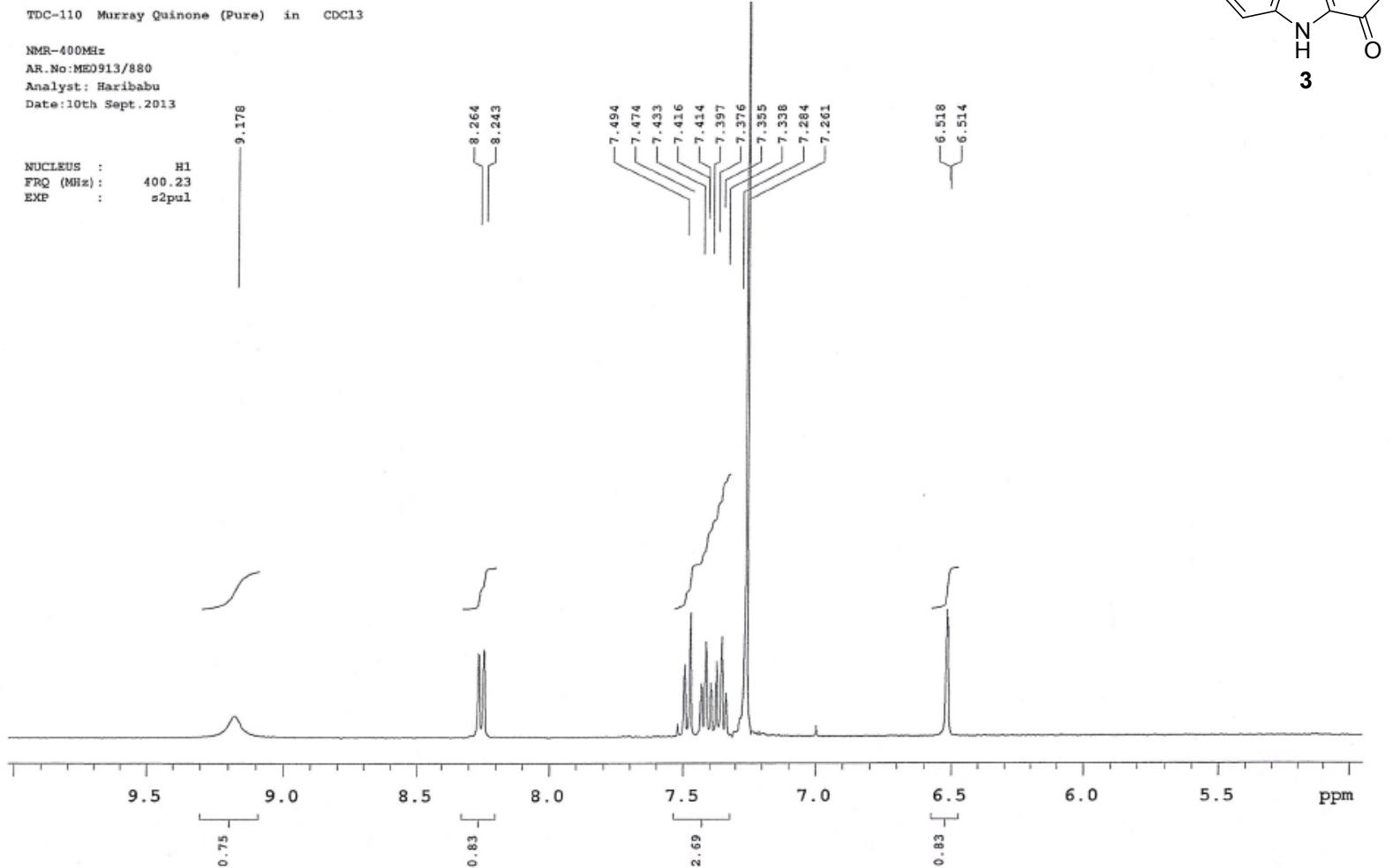
Minimum:				
Maximum:	5.0	5.0	-5.0	80.0
Mass	Calc. Mass	mDa	PPM	DBE
291.9968	291.9973	-0.5	-1.7	8.5

i-FIT Formula
C13 H11 N O2 Br

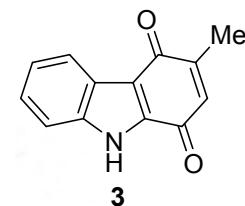
¹H NMR of Murrayquinone A (3)



Expansion ^1H NMR of Murrayquinone A (3)



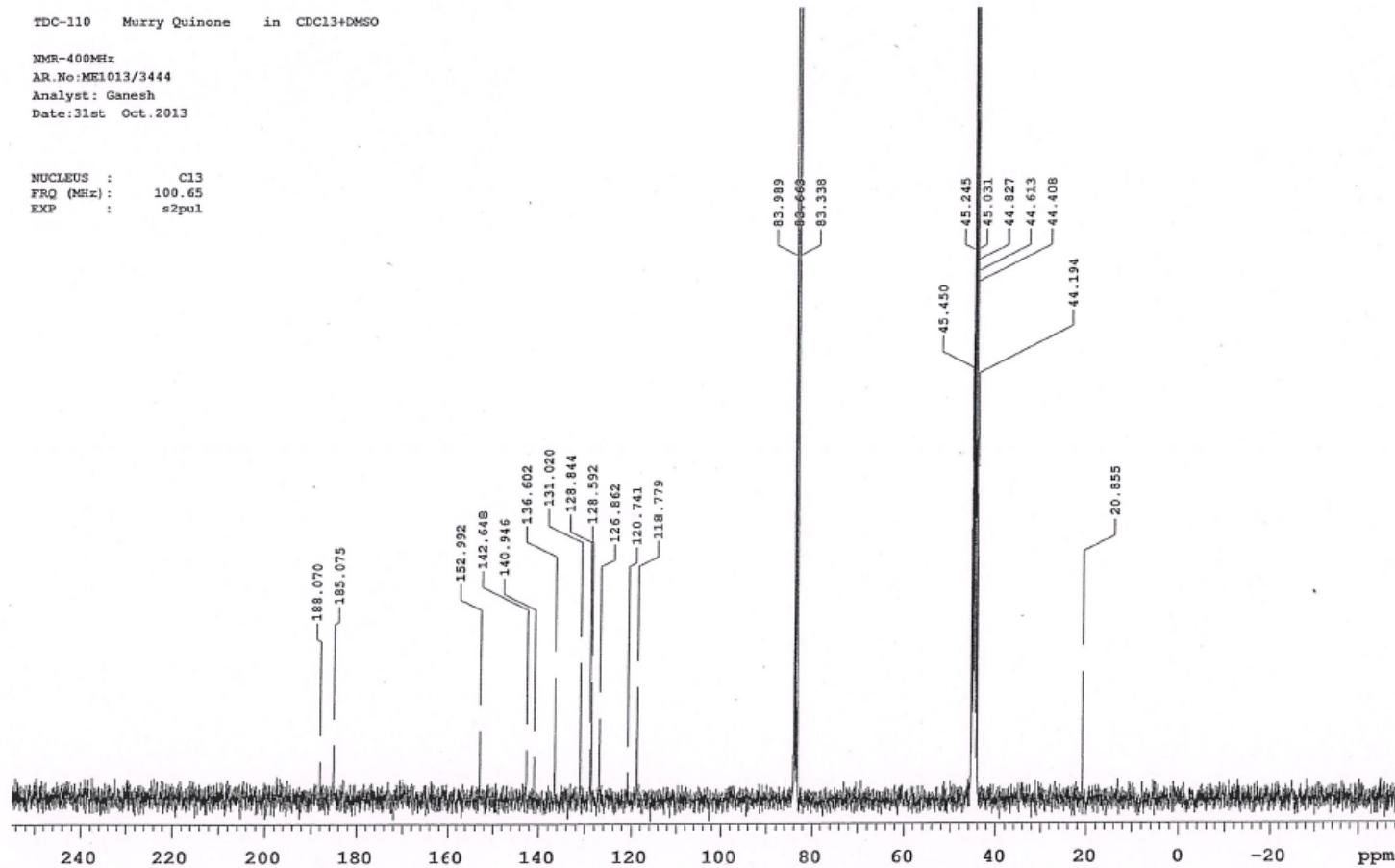
¹³C NMR of Murryaquinone A (3)



TDC-110 Murry Quinone in CDCl₃+DMSO

NMR-400MHz
AR.No:ME1013/3444
Analyst: Ganesh
Date:31st Oct.2013

NUCLEUS : C13
FRQ (MHz) : 100.65
EXP : s2pul

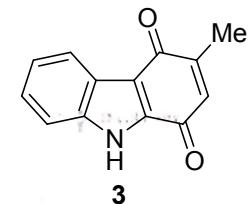


Mass Spectrum of Murrayquinone A (3)

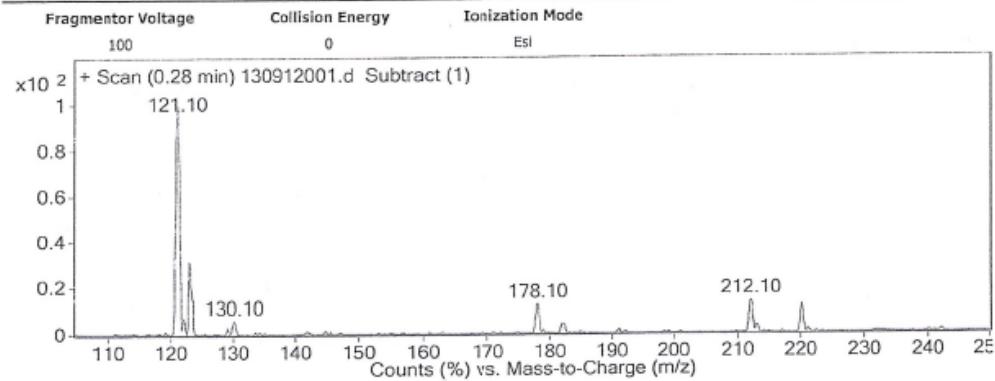
CPS,MIYAPUR

LCMS Analysis Report

Data Filename	130912001.d	Sample Name	Murrayquinone
Sample Type	Sample	Position	Vial 74
Instrument Name	Instrument 1	User Name	
Acq Method	ESI.m	IRM Calibration Status	Success
DA Method	Default.m	Comment	



User Spectra



--- End Of Report ---