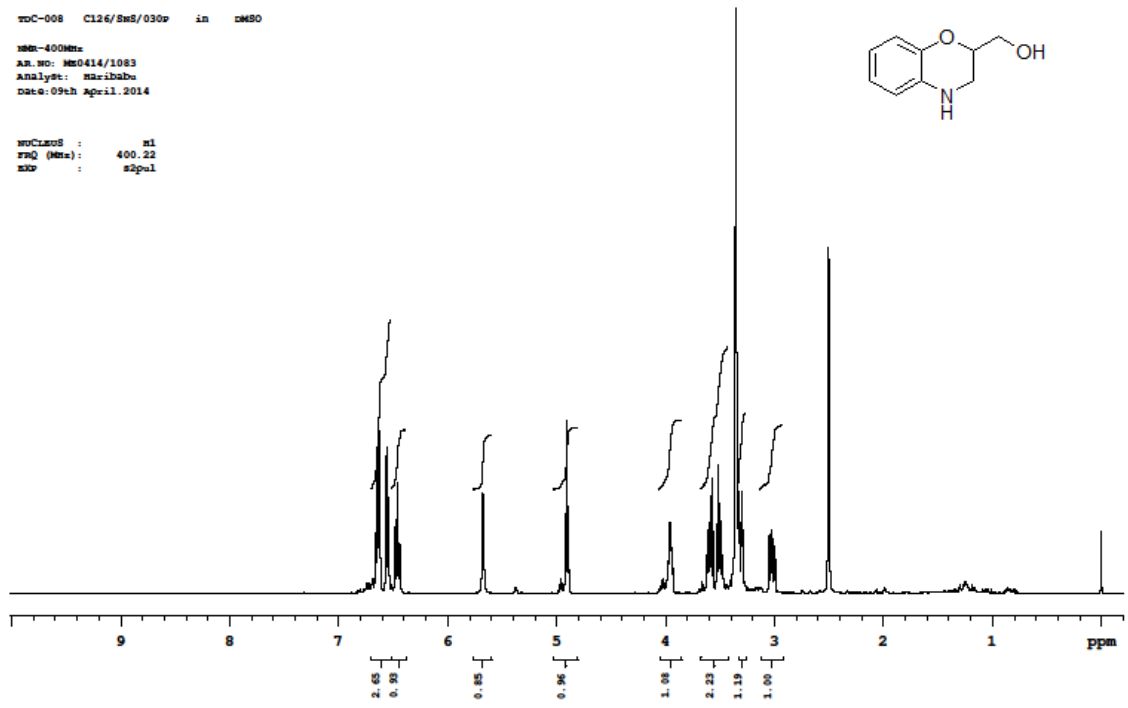
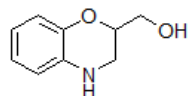


Copies of spectra

TDC-008 C126/SNS/030P in DMSO
NMR-400MHz
AN.No: ME0414/1083
Analyst: Haribabu
Date: 09th April, 2014

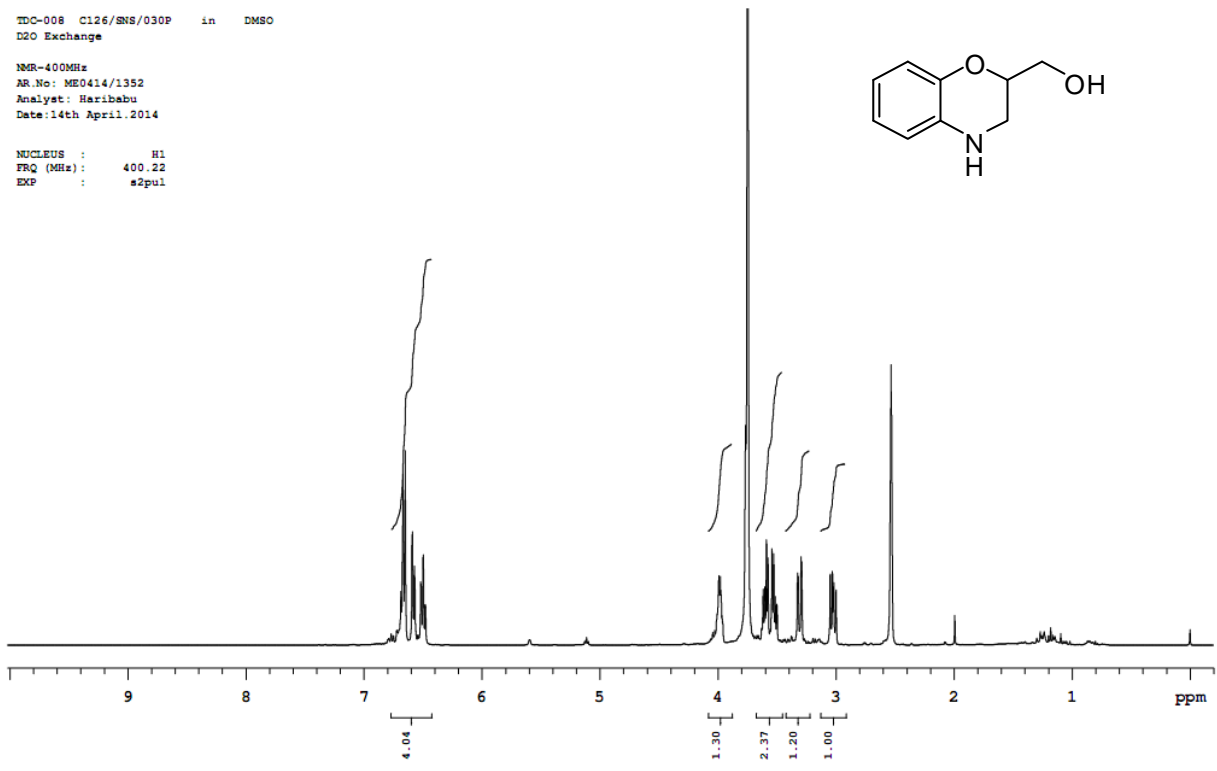
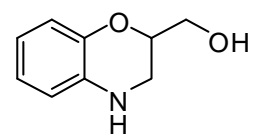
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



¹H NMR spectra in DMSO-d₆

TDC-008 C126/SNS/030P in DMSO
D2O Exchange
NMR-400MHz
AN.No: ME0414/1352
Analyst: Haribabu
Date: 14th April, 2014

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

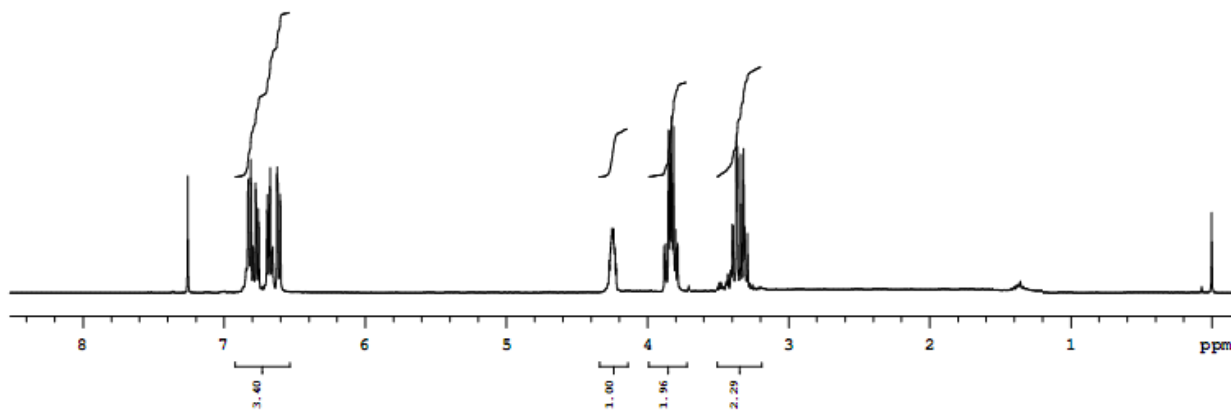
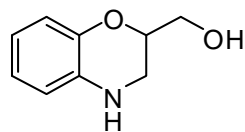


D₂O exchange spectra

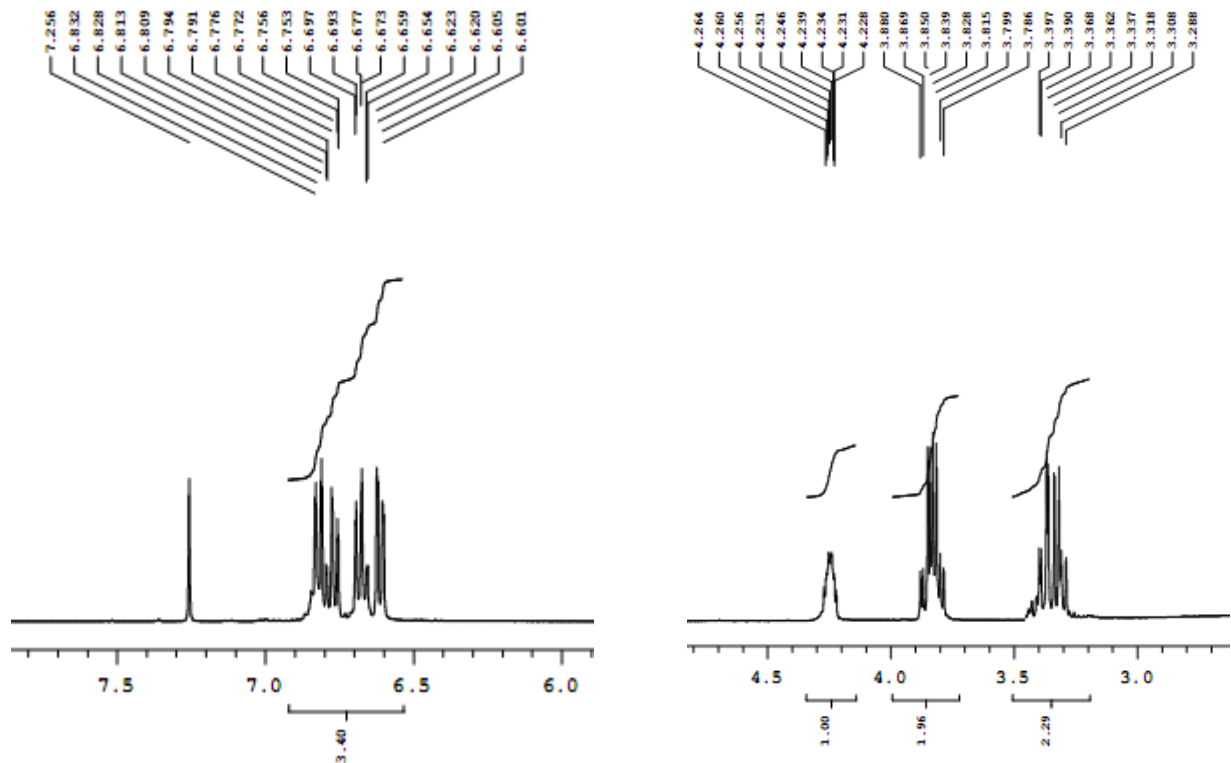
TDC-008 C126-BNS-030-P in CDCl3

MR=400MHz
AR.No: MS0414/1561
Analyt: Genesha
Date: 14th April, 2014

NUCLEUS : H1
FREQ (MHz): 400.22
EXP : zgpg1



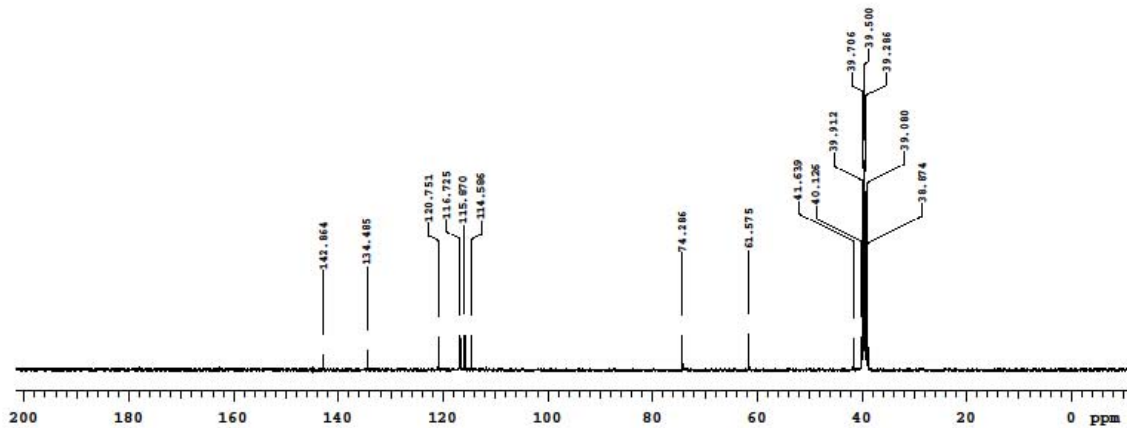
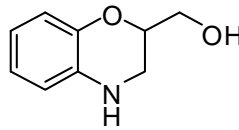
¹H NMR spectra in CDCl₃



TDC-110-Cl26-C8M3-030

AR.No: M20115/642

Analyst : NARESH B
Solvent : DMSO
Date : Jan 12 2015
NOCLABS : C13
FPO (MHz): 100.65
EXP : CARBON



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 = 2

Monoisotopic Mass, Even Electron Ions

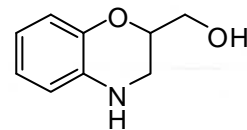
33 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

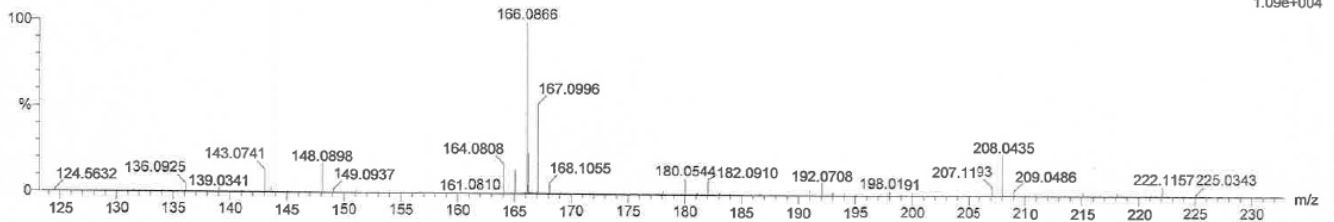
C: 0-20 H: 0-20 N: 0-2 O: 0-2 Cl: 0-1

C126/SNS/030P

140415013 19 (0.593) Cm (19:22-41:44)



Page 1

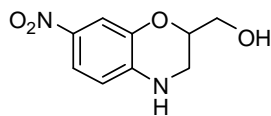


1: TOF MS ES+
1.09e+004

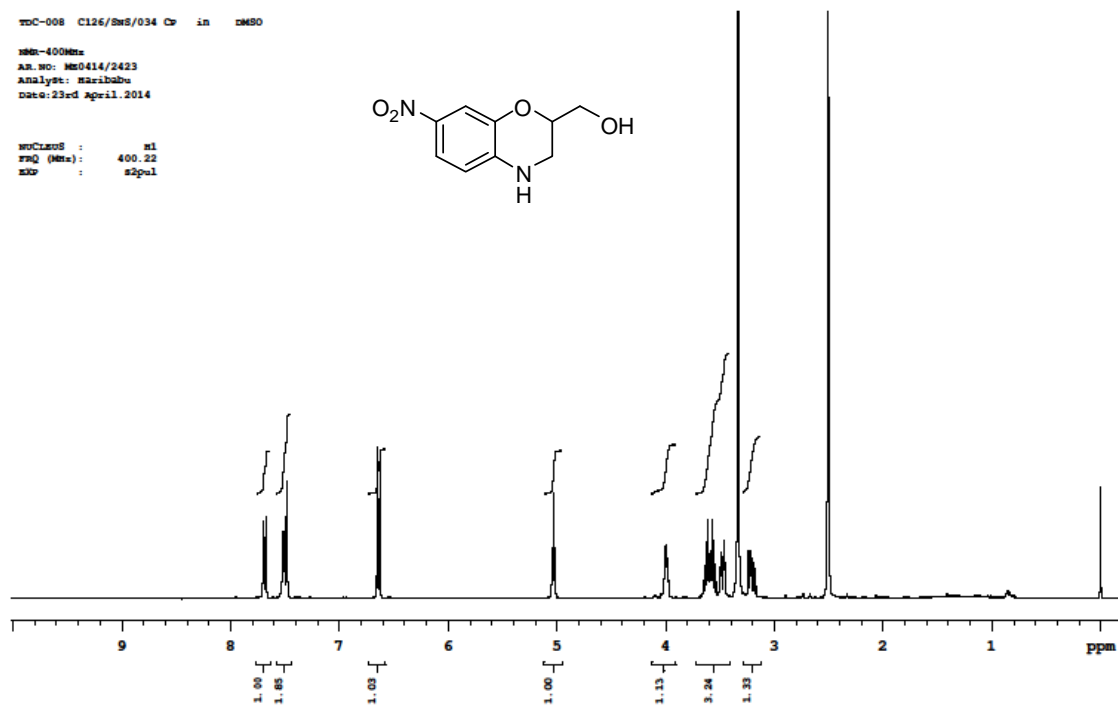
Minimum: -5.0
Maximum: 5.0 5.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
166.0866	166.0868	-0.2	-1.2	4.5	1820.3	C9 H12 N O2

IND-008 C126/SMS/034 Cr in CDCl₃
NMR-400MHz
AN. NO: MS0414/2423
ANALYST: Haribabu
DATE: 23rd April, 2014



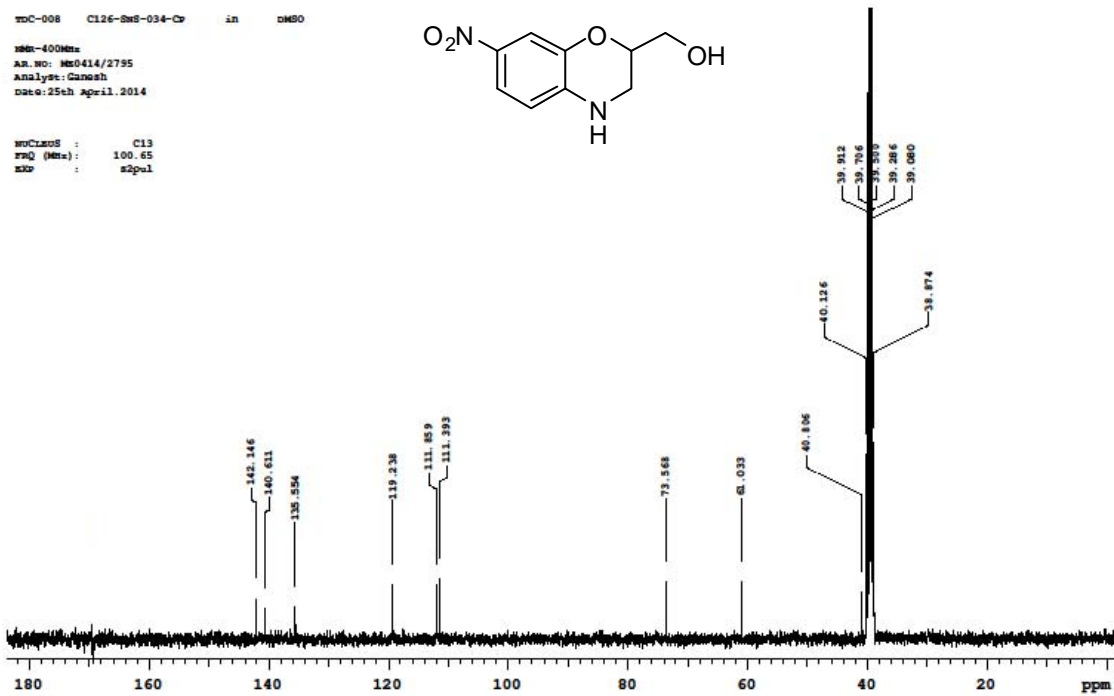
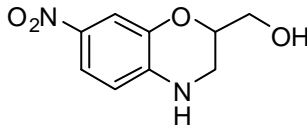
WUCLASS : M1
FREQ (MHz) : 400.22
NMR : s2pul



TOC-008 C126-SHS-034-CP in DMSO

HM-400MHz
Ac. No: MS0414/2795
Analyst: Ganesh
Date: 25th April, 2014

PROCLOS : C13
PFIQ (Hz): 100.65
SD : s2pol

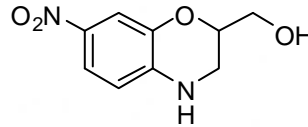


Elemental Composition Report

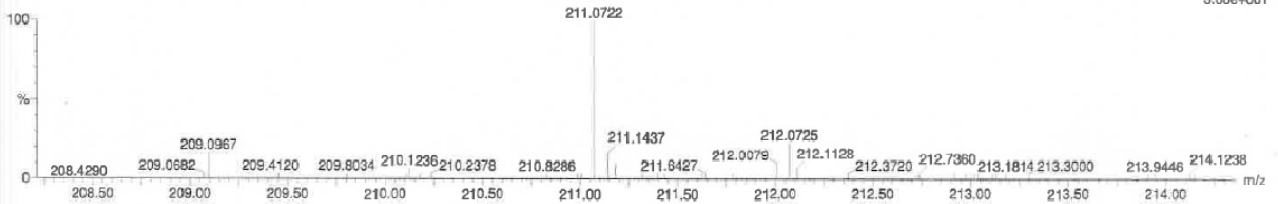
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
Elements Used:
C: 0-13 H: 0-14 N: 0-4 O: 0-6
C126/CSNS3/034-CP
141230006 35 (0.331) Cm (33:36-86:96)



Page 1



1: TOF MS ES+
3.08e+001

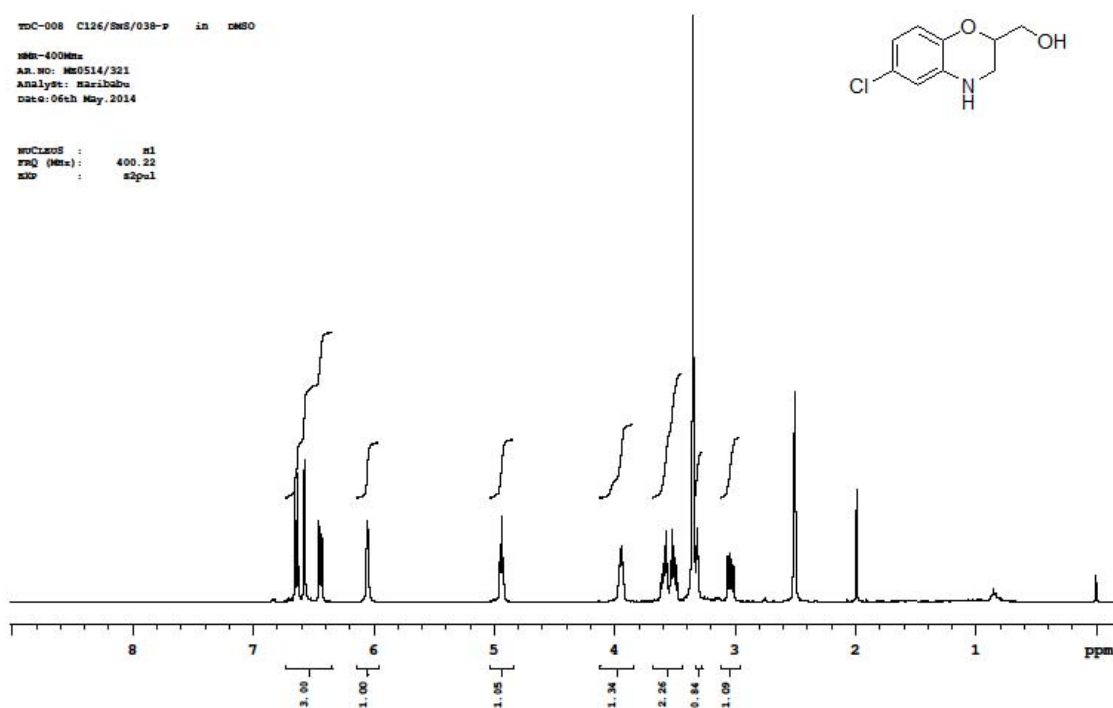
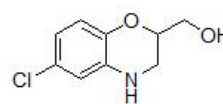
Minimum:							
Maximum:		5.0	5.0	-1.5	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
211.0722	211.0719	0.3	1.4	5.5	0.9	C9 H11 N2 O4	

ARDL08C1 RNR202
R. Nagarajan
20/12/2014

TOC-008 C126/SnS/038-p in DMSO

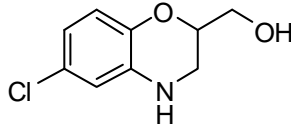
RMN-400MHz
AN. NO: MM0514/321
Analyte: Maribabu
Date: 06th May, 2014

NOCLMUS : n1
PFG (Hz): 400.22
SFO : s2p1

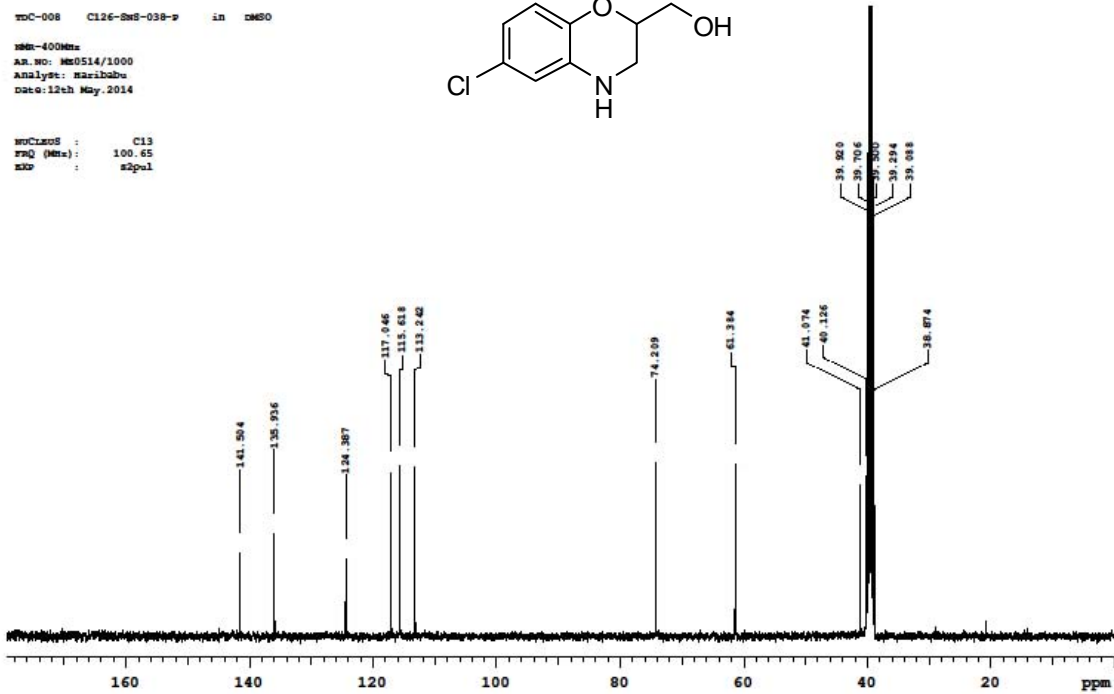


TOC-008 C126-SNS-038-P in DMSO

IRN-400MHz
 Ac. No: MS0514/1000
 Analyst: Haribabu
 Date: 12th May, 2014



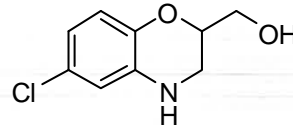
NOCLAS : C13
 FREQ (MHz): 100.65
 XDP : s2pol



Elemental Composition Report

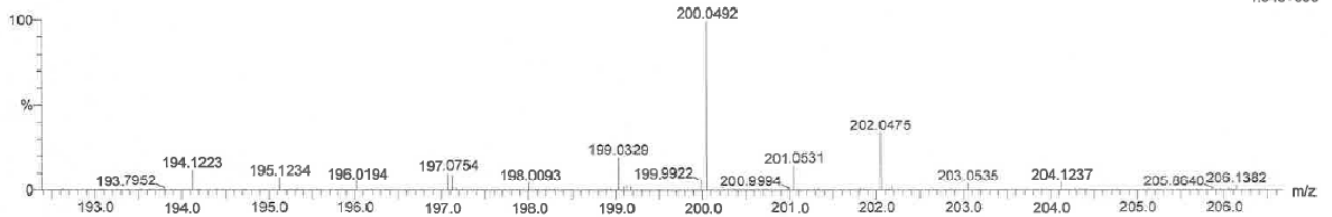
Single Mass Analysis

Tolerance = 8.0 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
 21 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
 Elements Used:
 C: 0-14 H: 0-14 N: 0-2 O: 0-2 Cl: 0-1
 C126/SNS/038 P
 140514002 16 (0.294) Cm (14:16-27)

1: TOF MS ES+
 1.34e+003

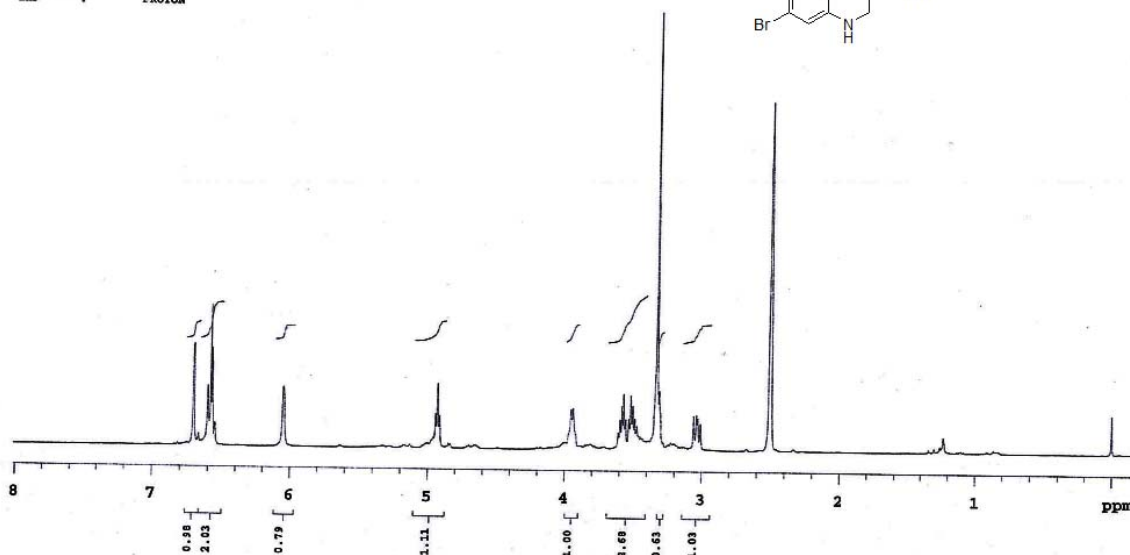
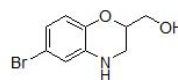


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
200.0492	200.0478	1.4	7.0	4.5	6.6	C9 H11 N O2 Cl

TDC-110 C126/CSMS3/059

AR.No: MH0115/630

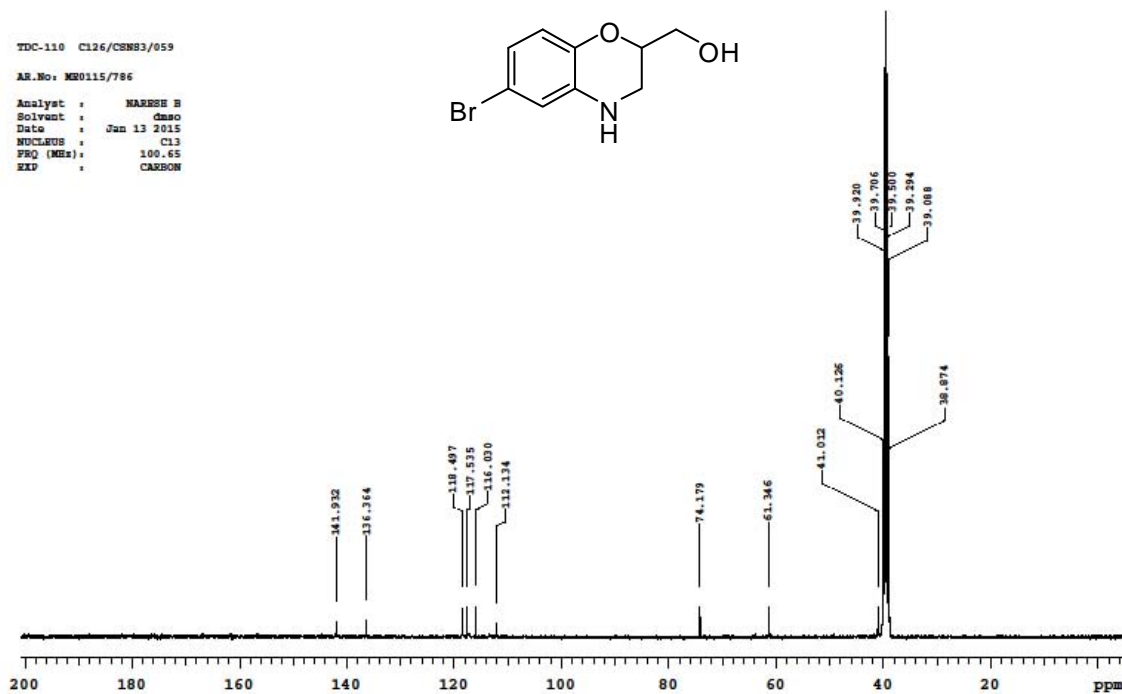
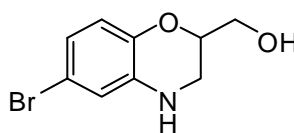
Analyst : Mallikarjun
Solvent : DMSO
Date : Jan 9 2015
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON



TDC-110 C126/CSMS3/059

AR.No: MH0115/786

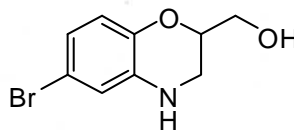
Analyst : HARSH B
Solvent : DMSO
Date : Jan 13 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 2

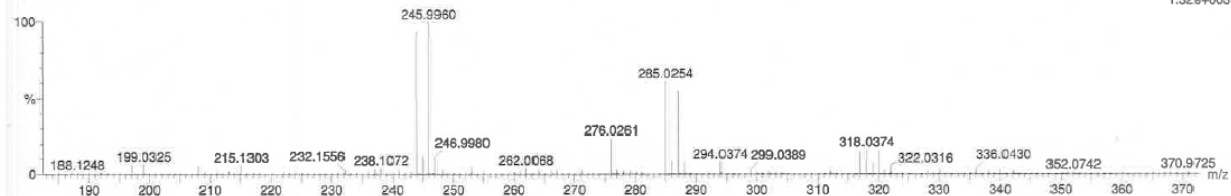


Monoisotopic Mass, Even Electron Ions
 111 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
 Elements Used:

C: 0-14 H: 0-15 N: 0-4 O: 0-6 Br: 0-3

C126/CSNS3/059 P
 141230009 23 (0.219) Cm (23:27-108:113)

1: TOF MS ES+
 1.32e+003



Minimum: -1.5
 Maximum: 5.0 5.0 80.0

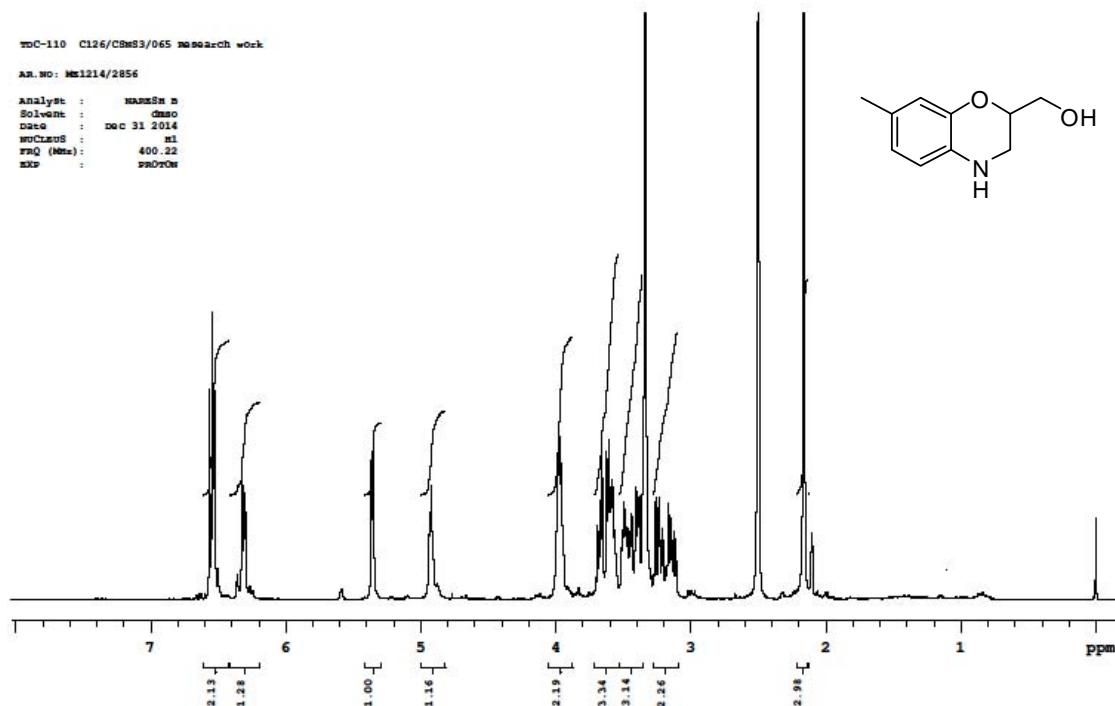
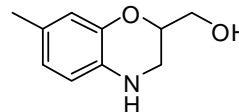
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
243.9978	243.9973	0.5	2.0	4.5	3.0	C9 H11 N O2 Br

*Andreas RNR/202
 R-Nager
 30/11/14*

msC-110 C126/CSNS3/065 research work

sr. no: MS1214/2856

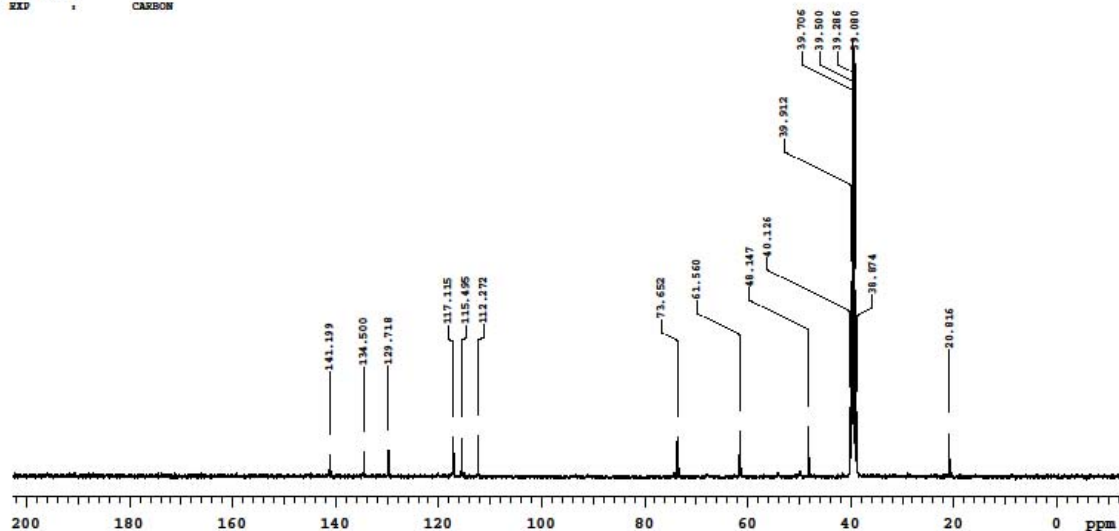
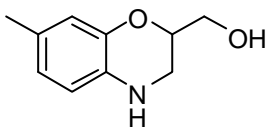
Analyst : NARSEN B
 Solvent : DMSO
 Date : Dec 31 2014
 mCubes : M1
 FWHM (MHz): 400.22
 EXP : PR0708



TDC-110 C126/CSNS3/065

AR.No: M20115/563

Analyst : NARESH B
Solvent : DMSO
Date : Jan 9 2015
NOCLASIS : C13
FREQ (MHz): 100.65
EXP : CARBON

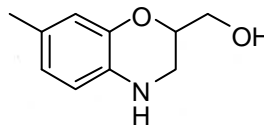


Elemental Composition Report

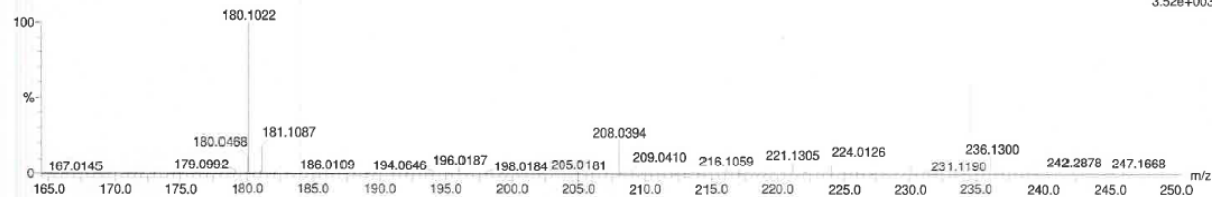
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, 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 4 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-17 N: 0-4 O: 0-6
C126/CSNS3/065
150122016 0 (0.171) Cm (5:10-49)



Page 1



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
180.1022	180.1025	-0.3	-1.7	4.5	40.6	C10 H14 N O2

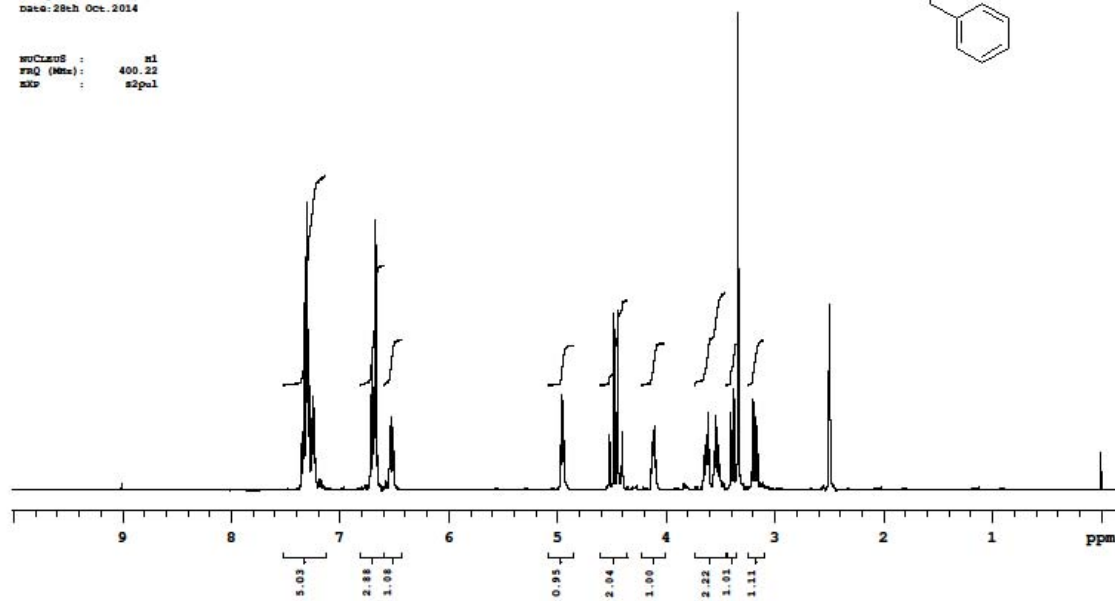
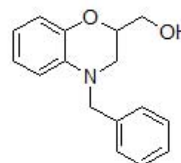
ARDISOOI/KNR/02
R. Nagarajan
23/01/2015
[Signature]
23/01/2015

1: TOF MS ES+
3.52e+003

TOC-008 C126/CSMS3/055 in DMSO

MR-400ms
AN. NO: MS1014/2248
ANALYST: Maribabo
DATE: 29th Oct. 2014

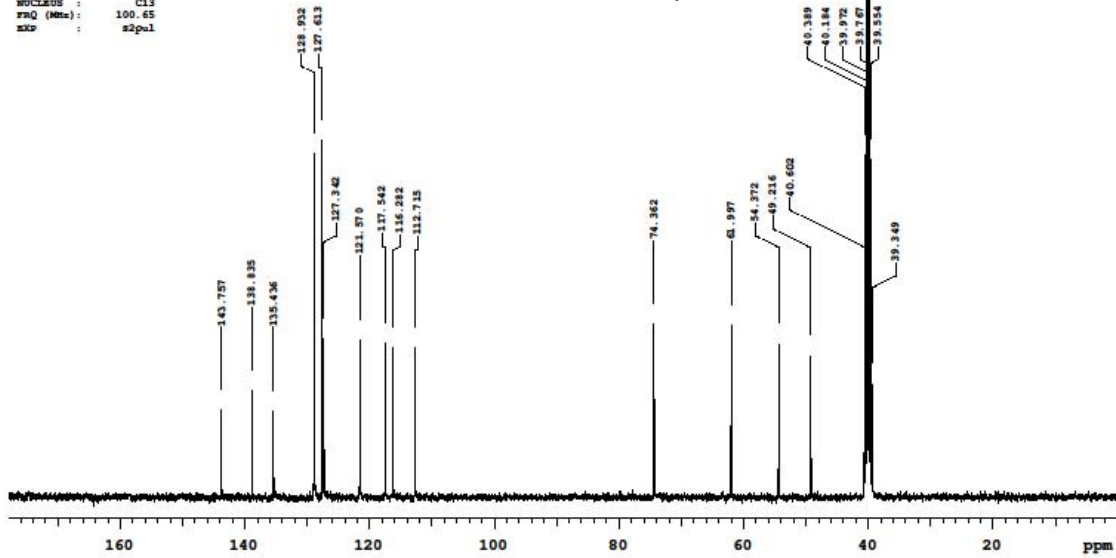
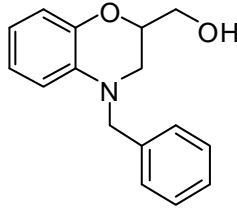
NO. OF SCANS : 1
PULPROG : zgpg30
FREQ (MHz) : 400.22
EXP : s2ps1



TOC-008 C126/CSNS3/055 in DMSO

MSM-400MHz
AN. NO: MS1014/2790
Analyst: Haribabu
Date: 31st Oct. 2014

NOCLASUS : C13
FREQ (MHz): 100.65
XDP : s2p.u1



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

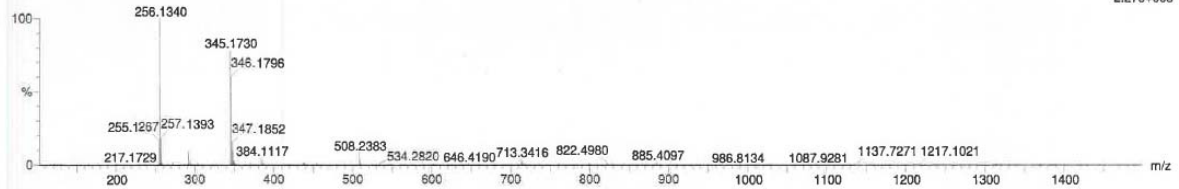
98 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-26 H: 0-25 N: 0-4 O: 0-8

C126/CSNS3/055-CP

141230011 52 (0.491) Cm (52:55-125:132)



Minimum:

Maximum:

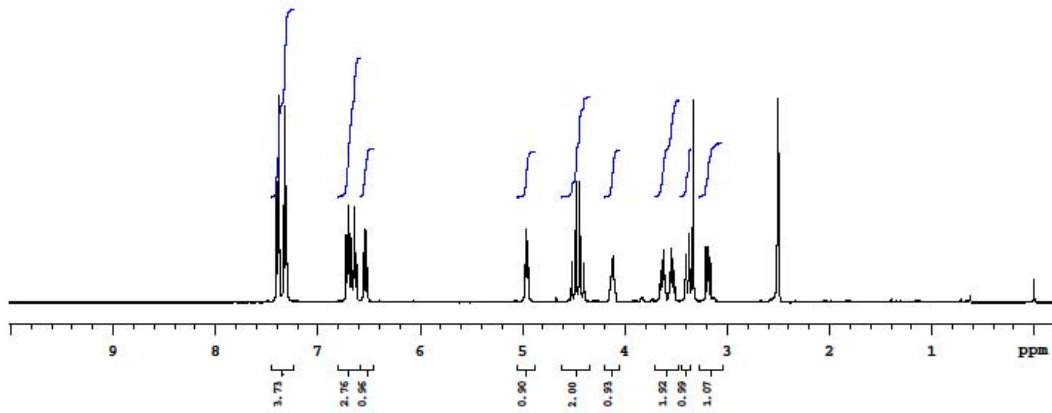
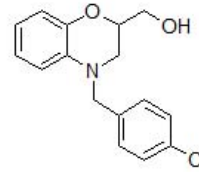
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.1340	256.1338	0.2	0.8	8.5	0.1	C16 H18 N O2

ADP/AS/RNR/202
R. Nagarajan
30/12/2014

TDC-008 C126/CEN3/060P in DMSO

NMR-400MHz
AR.No: MR1014/2214
Analyst: Haribabu
Date: 28th Oct. 2014

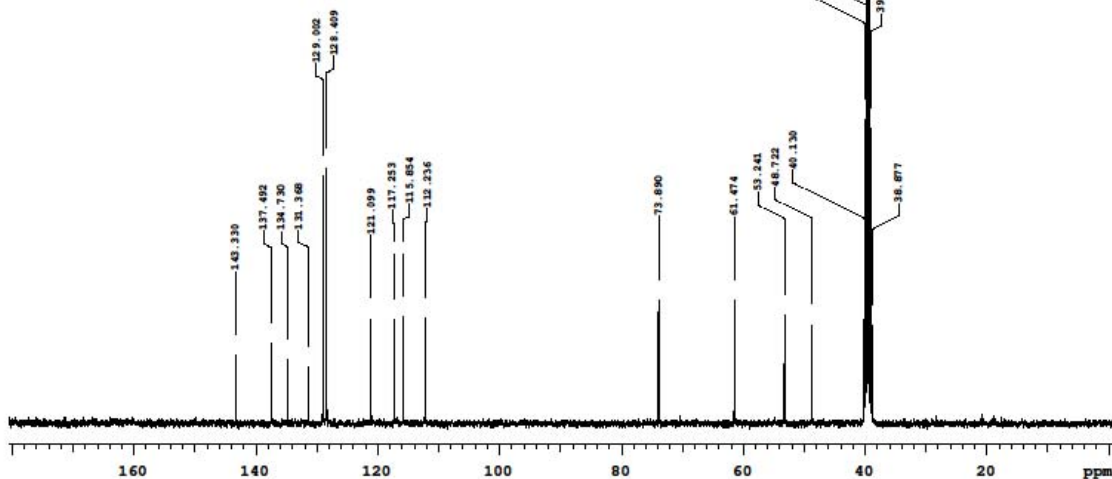
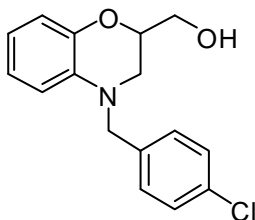
NUCLEUS : E1
FRQ (MHz): 400.22
EXP : s2pul



WC-008 C126/CSNS3/060 in DMSO

MS-400MHz
AN. NO: MS1014/2788
Analyst: Karibabu
Date: 31st Oct. 2014

NOCLUS : C13
PULP (Hz): 100.625
SFO : s2p=1



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

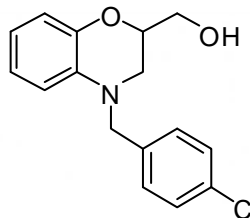
294 formula(a) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

C: 0-26 H: 0-25 N: 0-4 O: 0-3 Cl: 0-2

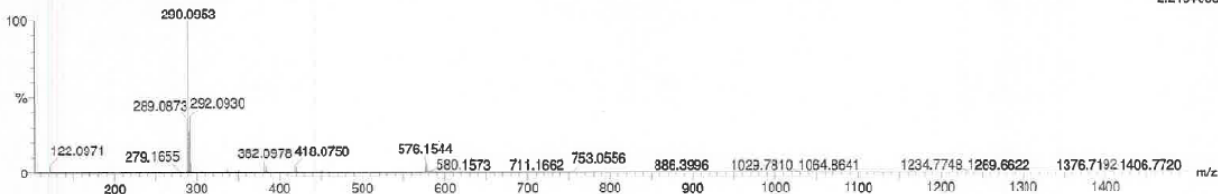
C126/CSNS3/060-CP

14123001232 (0.302) Cm (32:35-148:154)



Page 1

I: TOF MS ES+
2.21e+003



Minimum:

Maximum:

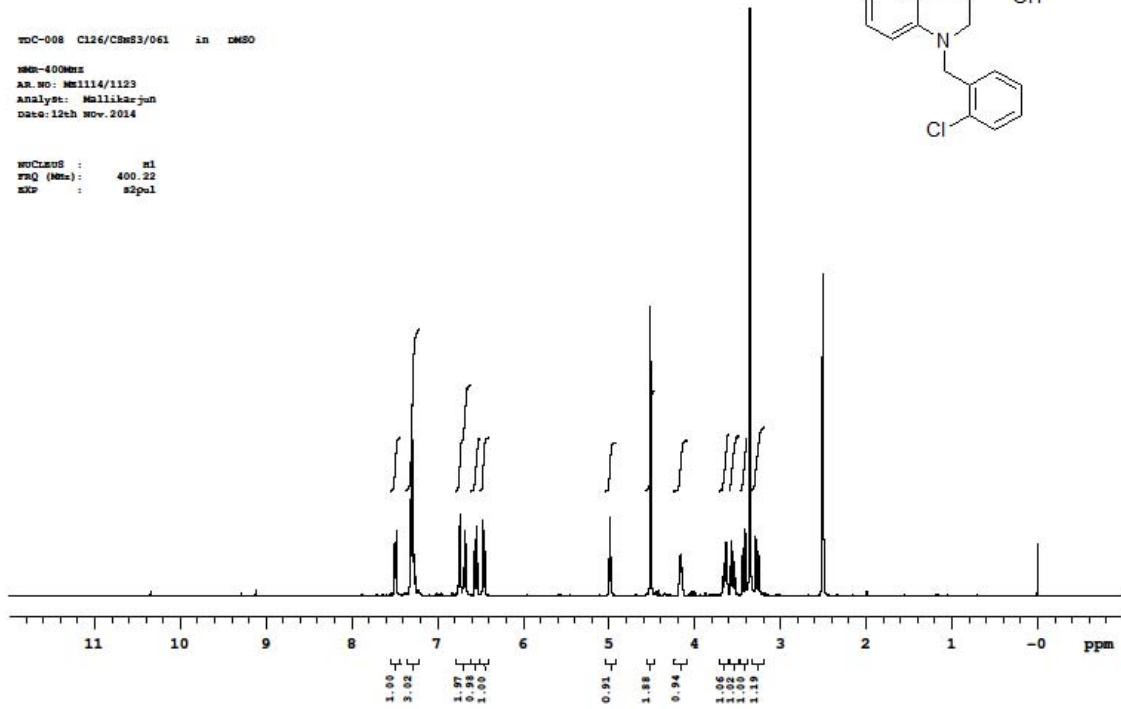
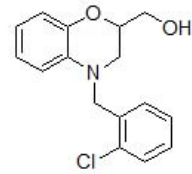
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0953	290.0948	0.5	1.7	8.5	33.2	C16 H17 N O2 Cl

ADDRESS KARIBABU
R. Nagaraj
30/12/2014

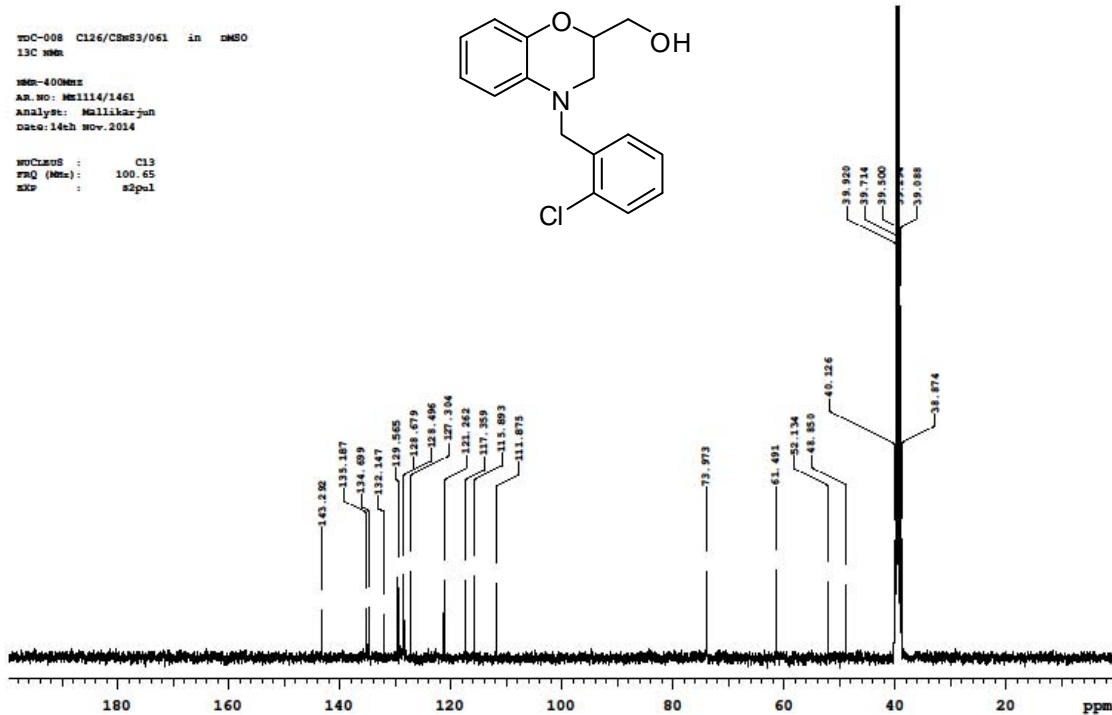
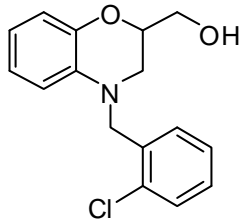
MO-C-008 C126/CSMS3/061 in DMSO

MSM-400MHz
AN. NO: MM1114/1123
ANALYST: Mallikarjun
DATE: 12th Nov. 2014

NUCLEUS : ¹H
PULP (MHz): 400.22
SOLV : DMSO



TOC-008 C126/CSMS3/061 in DMSO
 13C NMR
 MSN-400MHz
 AR. NO: MS1114/1461
 Analyst: Mallikarjun
 Date: 14th Nov. 2014
 NOCLXUS : C13
 FREQ (MHz): 100.65
 XPR : s2pol

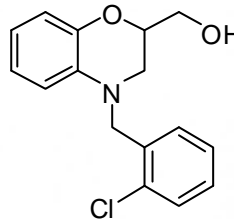


Elemental Composition Report

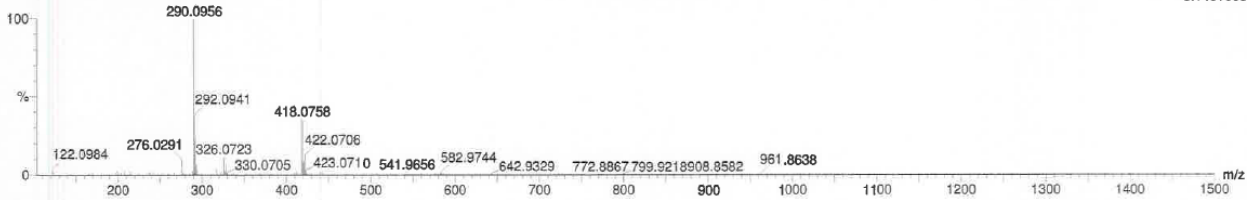
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
 247 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)
 Elements Used:
 C: 0-20 H: 0-20 N: 0-4 O: 0-6 Cl: 0-3
 C126/CSMS3/061 P
 141230007 24 (0.226) Cm (21:24-160:164)



Page 1



1: TOF MS ES+
3.14e+003

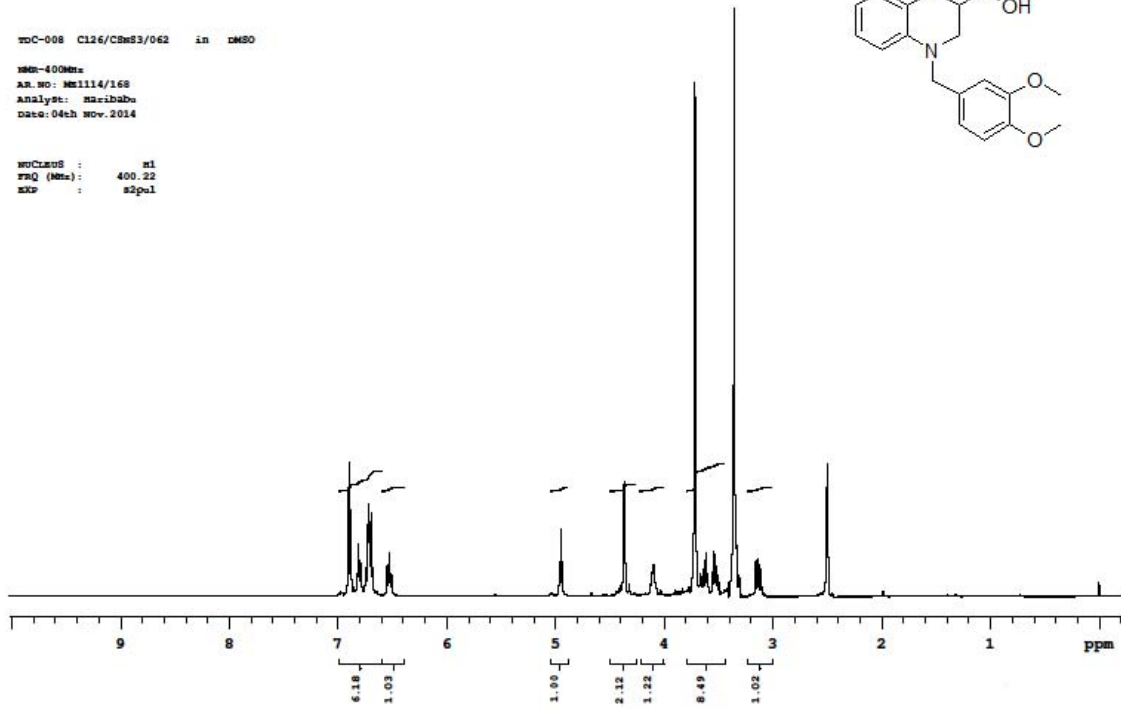
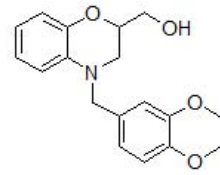
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0956	290.0948	0.8	2.8	8.5	7.6	C16 H17 N O2 Cl

AND KBC/RNR/202
 R. Nagaraja
 30/11/2014

MO-C-008 C126/CSMS3/062 in DMSO

MSM-400MHz
AN. NO: MM1114/168
ANALYST: Haribabu
DATE: 04th Nov. 2014

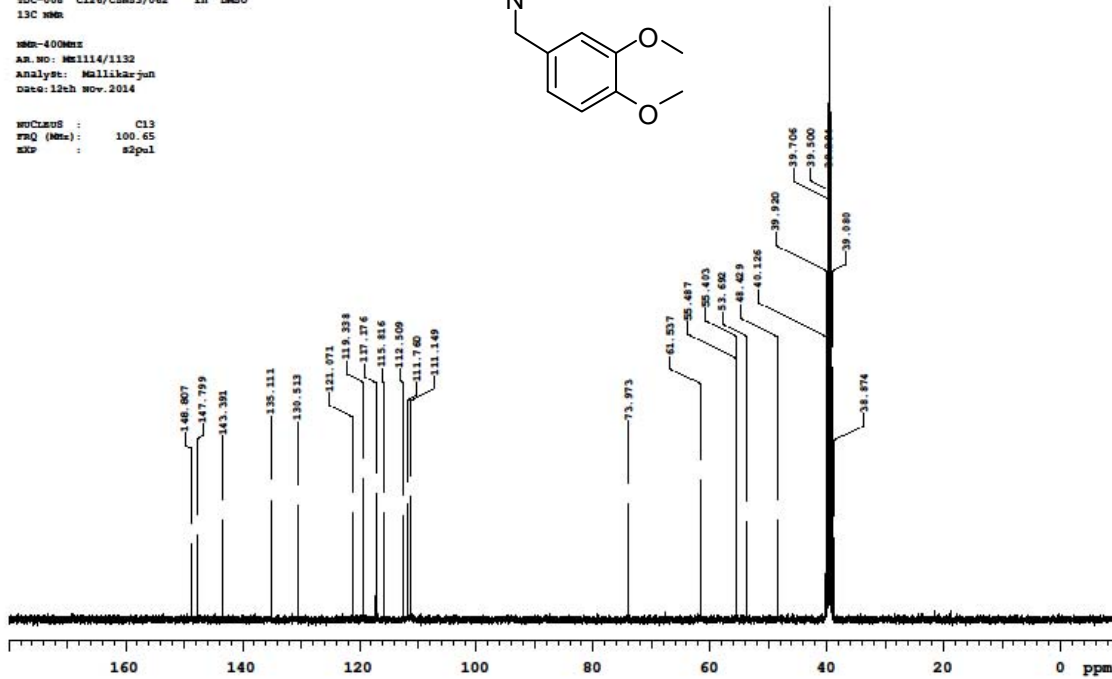
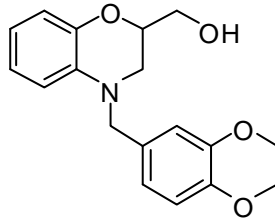
NUCLEUS : ¹H
PFG (MHz): 400.22
XPR : s2p1



TOC-008 C126/CSMS3/062 in DMSO
13C NMR

IR-4000Hz
AR. NO: M1114/1132
Analyst: Mallikarjun
Date: 12th Nov. 2014

WUCLEUS : C13
PFG (kHz): 100.65
XPR :

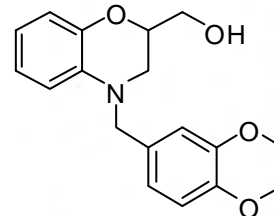


Elemental Composition Report

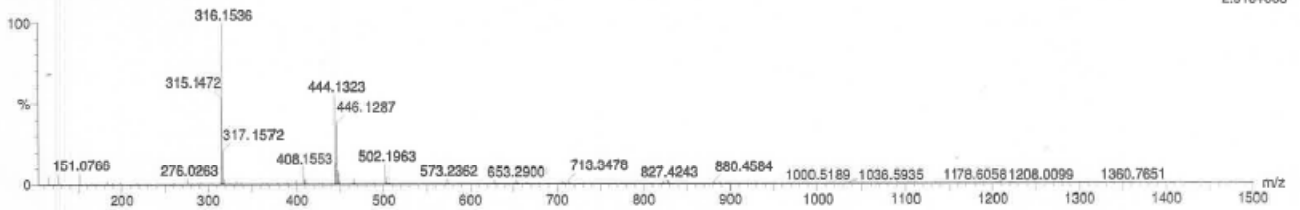
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
99 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 N: 0-4 O: 0-8
C126/CSMS3/062-P
141230010 51 (0.484) Cm (50:56-133:137)



1: TOF MS ES+
2.91e+003



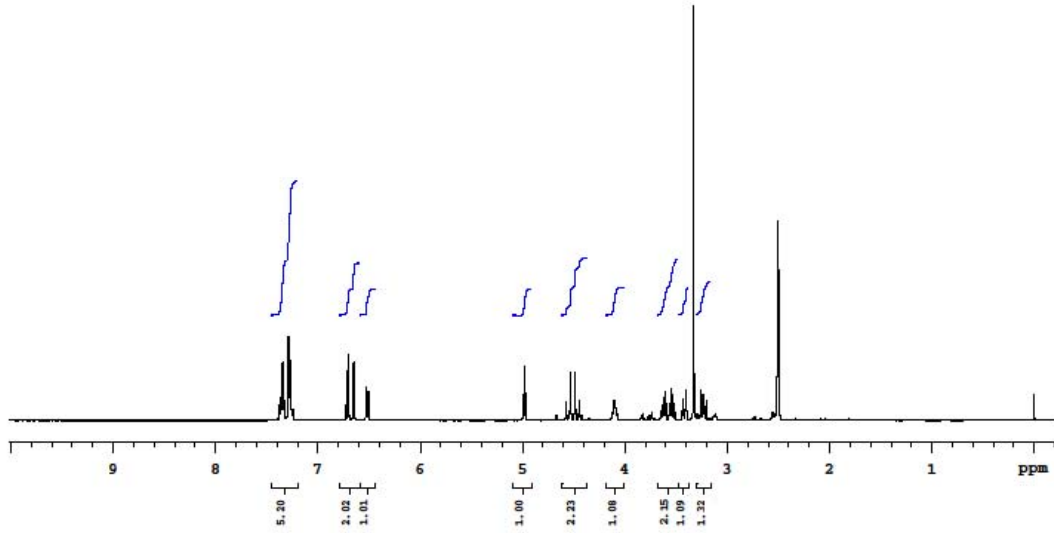
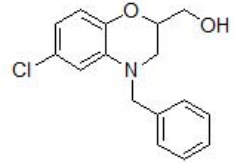
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
316.1536	316.1549	-1.3	-4.1	8.5	0.3	C18 H22 N O4

ARUNESH RNR/10.02
R. Nagarajan
30/11/2014

TDC-008 C126/C8883/056 in DMSO

NMR-400MHz
AR.No: MR1014/2213
Analyst: Haribabu
Date: 28th Oct. 2014

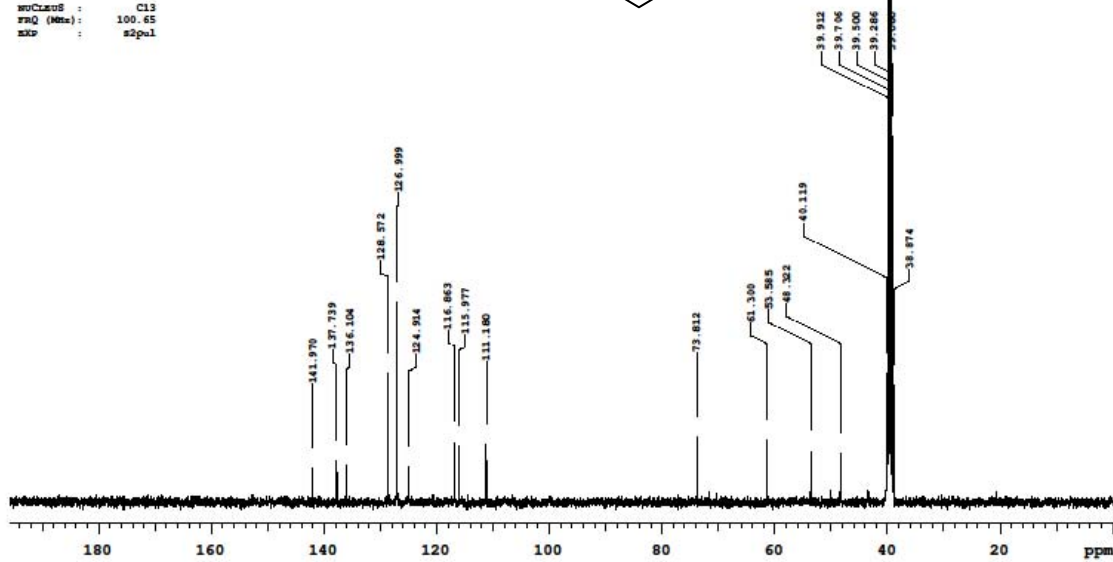
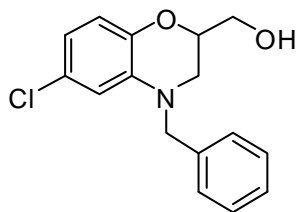
NUCLEUS : E1
FRQ (MHz): 400.22
EXP : s2pul



WOC-008 C126/CSMS3/056 in DMSO
13C NMR

MR=400MHz
AN. NO: M21114/277
ANALYST: Haridaba
Date: 04th Nov. 2014

NOCLBUS : C13
PULP (MHz): 100.625
SFO : s2pul



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

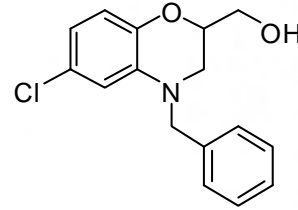
247 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

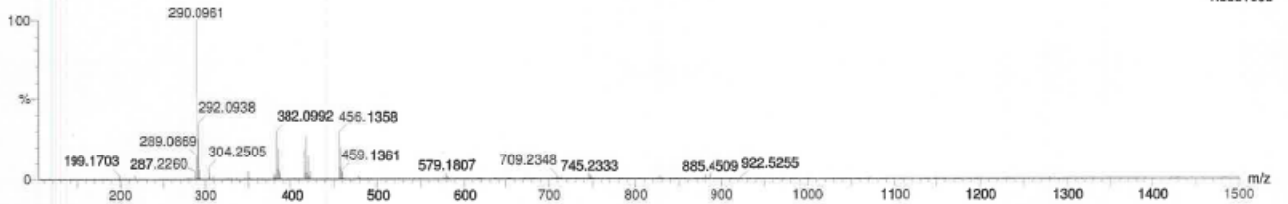
C: 0-20 H: 0-20 N: 0-4 O: 0-6 Cl: 0-3

C126/CSNS3/056 CP

14123000855 (0.520) Cm (54:56-119:124)



1: TOF MS ES+
1.55e+003



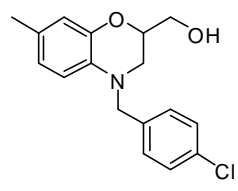
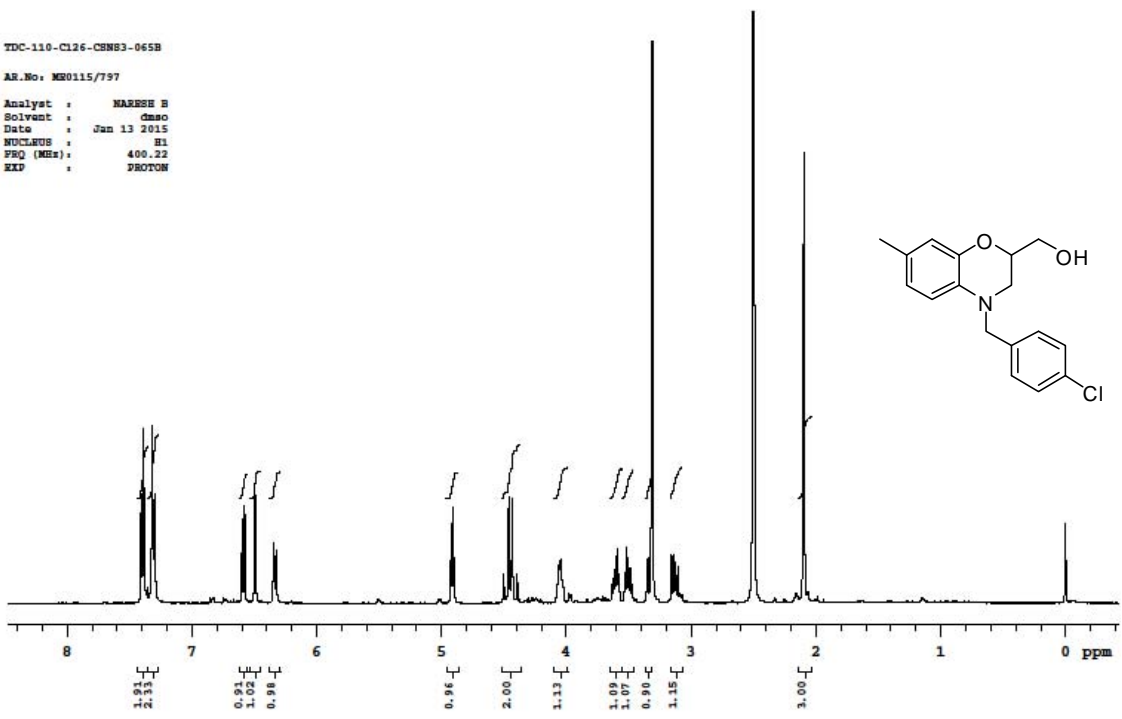
Minimum:						
Maximum:		5.0	5.0	-1.5		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0961	290.0948	1.3	4.5	8.5	11.8	C16 H17 N O2 Cl

ANDIA 06/12/2012
R. Nagarajan
30/12/2014

TDC-110-Cl26-C8M93-065B

AR.No: M20115/797

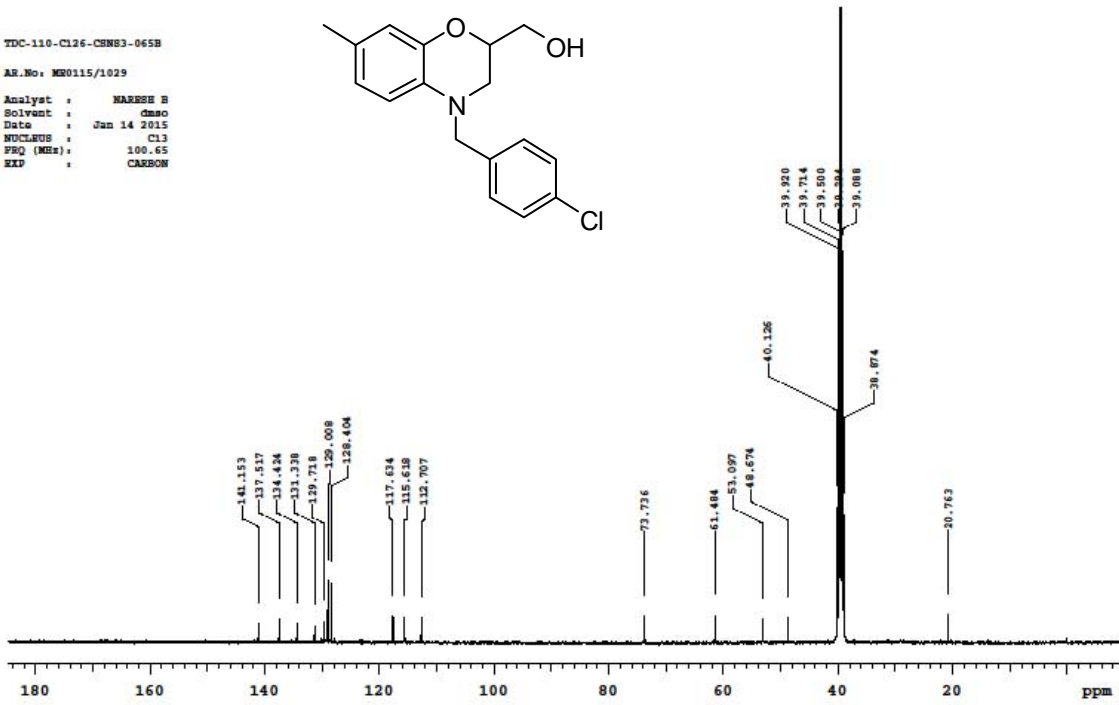
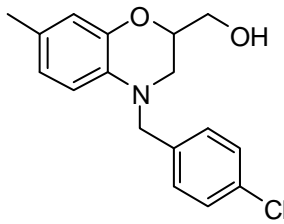
Analyst : NARESH B
Solvent : DMSO
Date : Jan 13 2015
NUCLEUS : ¹H
FREQ (MHz): 400.22
EXP : PROTON



TDC-110-Cl26-C8NS3-065B

AR.No: M20115/1029

Analyst : NARESH B
Solvent : dmso
Date : Jan 14 2015
Nucleus : C13
FREQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

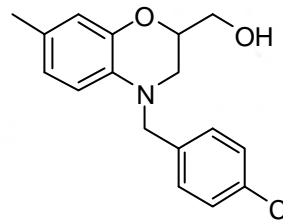
222 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

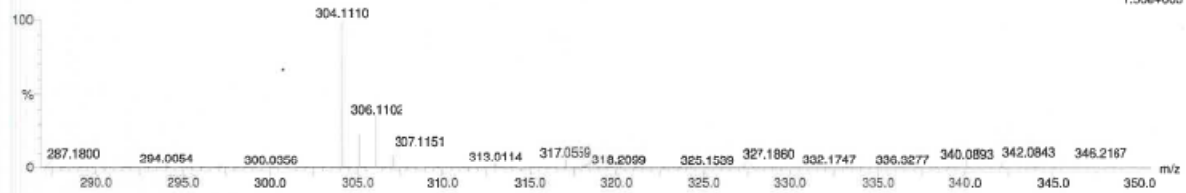
C: 0-21 H: 0-25 N: 0-4 O: 0-6 Cl: 0-2

C126/CSNS3/065 B

150122019 9 (0.258) Cm (9.10-36)



Page 1



1: TOF MS ES+
1.50e+003

Minimum:	Maximum:	Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
		304.1110	304.1104	0.6	2.0	8.5	6.6	C17 H19 N O2 Cl

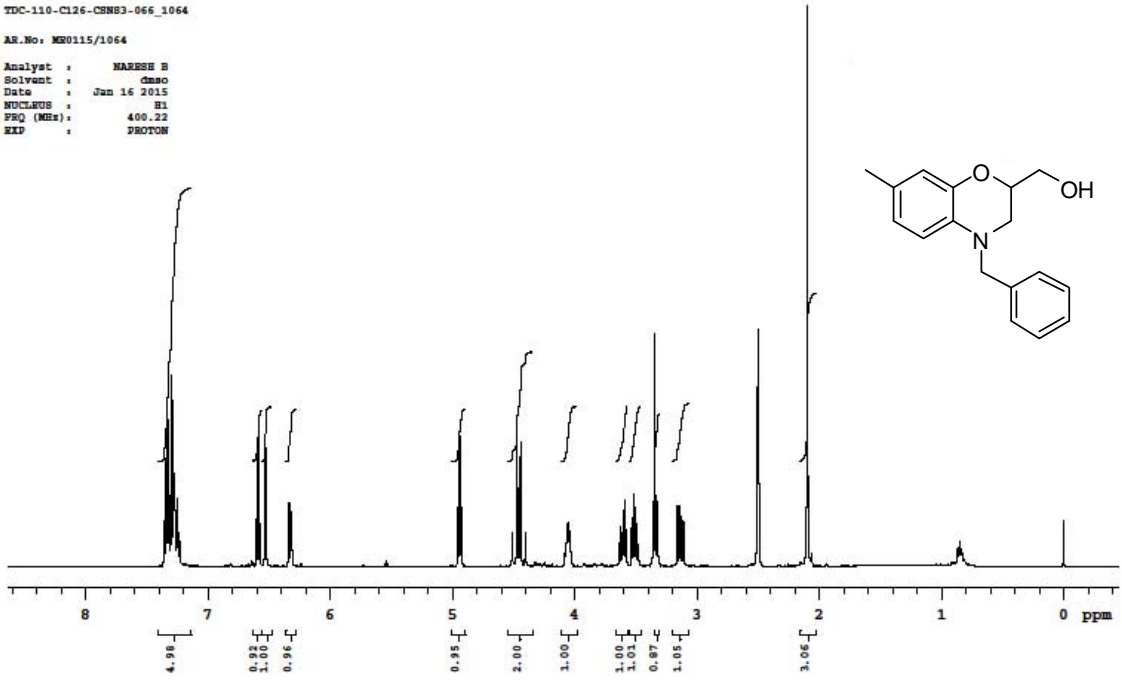
ARDISOOI / RNR/O 21
R. Nagarajan
23/01/2015

22/01/2015

TDC-110-CL26-CMS3-066_1064

AR.No: MS0115/1064

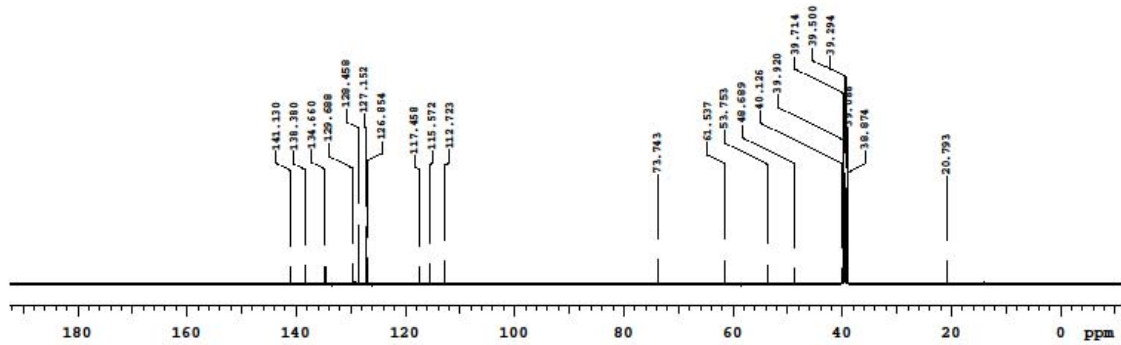
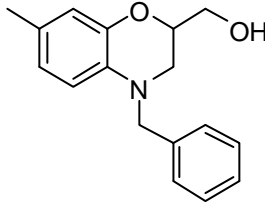
Analyst : NARESH B
Solvent : DMSO
Date : Jan 16 2015
NUCLEUS : 31
FREQ (MHz): 400.22
EXP : PROTON



TDC-110 C126/CSNS3/066

AR.No. MW0115/2212

Analyst : MARESE B
Solvent : DMSO
Date : Jan 30 2015
Wavelength : C13
FRQ (MHz) : 100.65
EXP : CARBON

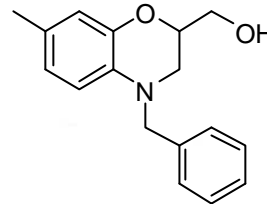


Elemental Composition Report

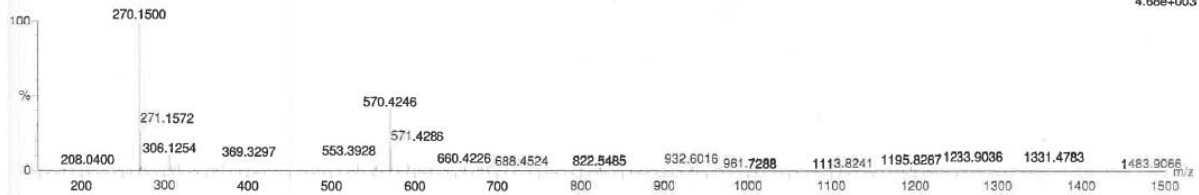
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
75 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-23 H: 0-25 N: 0-4 O: 0-6
C126/CSNS3/066
150122020 9 (0.258) Cm (9:12-46:48)



Page 1



1: TOF MS ES+
4.68e+003

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.1500	270.1494	0.6	2.2	8.5	35.2	C17 H20 N O2

ARDIS001/RNR/02

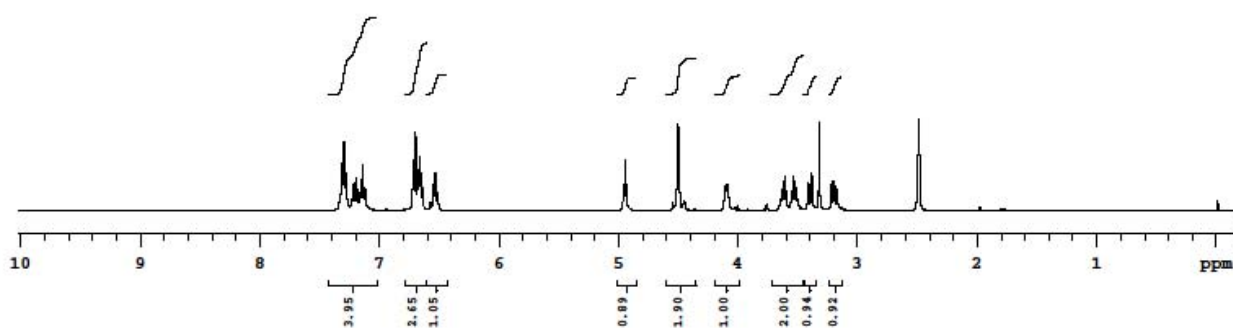
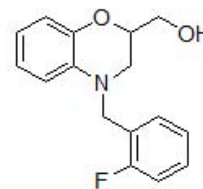
R. N. Nagarajan
22/01/2015

22/01/2015

TDC-110-C126-C8N83-067

AR.No: MR0215/1553

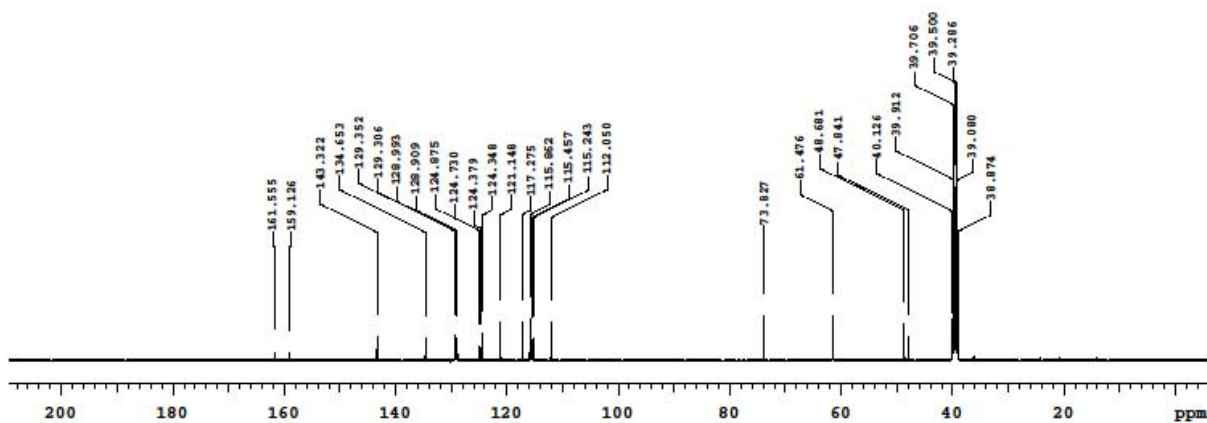
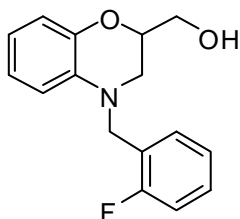
Analyst : Mallikarjun
Solvent : dmsd
Date : Feb 16 2015
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON



TDC-110 C126/CSNS3/067

AR.No: MR0215/1590

Analyst : NARRESE B
Solvent : DMSO
Date : Feb 20 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

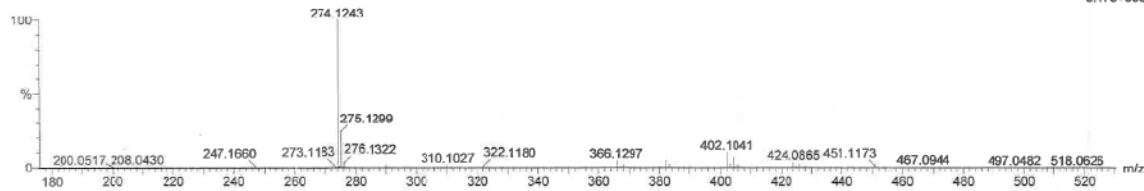
113 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-18 H: 0-25 N: 0-3 O: 0-3 F: 0-1 I: 0-1

C126/CSNS3/067

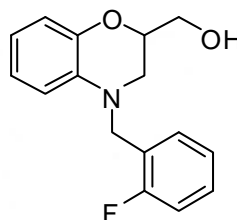
1502200C3 7 (0.192) Cm (6.8)



Minimum:

Maximum: 5.0 5.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
274.1243	274.1243	0.0	0.0	8.5	2241.9	C16 H17 N O2 F



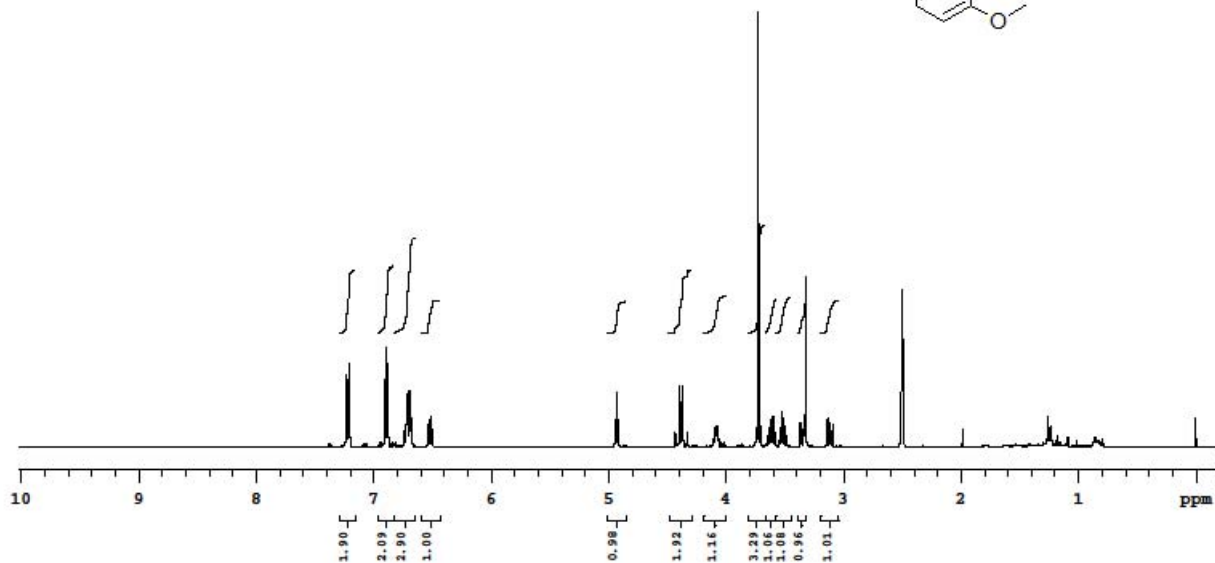
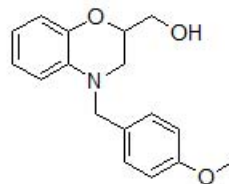
Page 1

1: TOF MS ES+
3.47e+005

TDC-110-Cl26-C88B3-068

AR.No: MR0215/1552

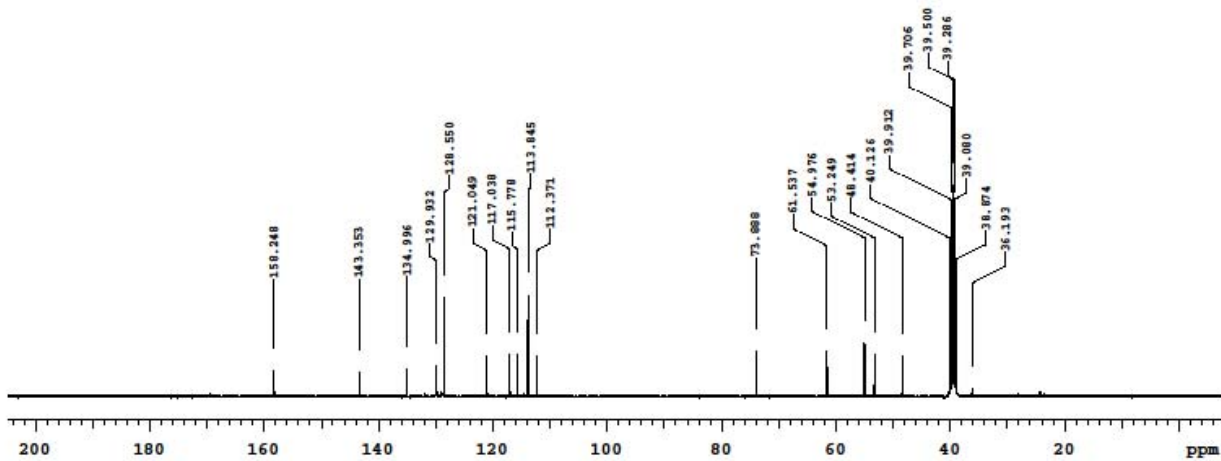
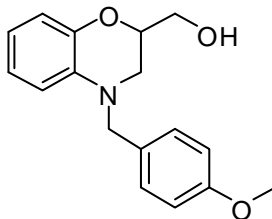
Analyst : Mallikarjun
Solvent : DMSO
Date : Feb 16 2015
NUCLEUS : ¹H
FRQ (MHz): 400.22
EXP : PROTON



TDC-110 C126/C8NS3/068P

AR.No: ME2015/2430

Analyst : NARESH B
Solvent : dmsd
Date : Feb 25 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



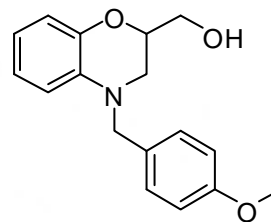
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4



Monoisotopic Mass, Even Electron Ions

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

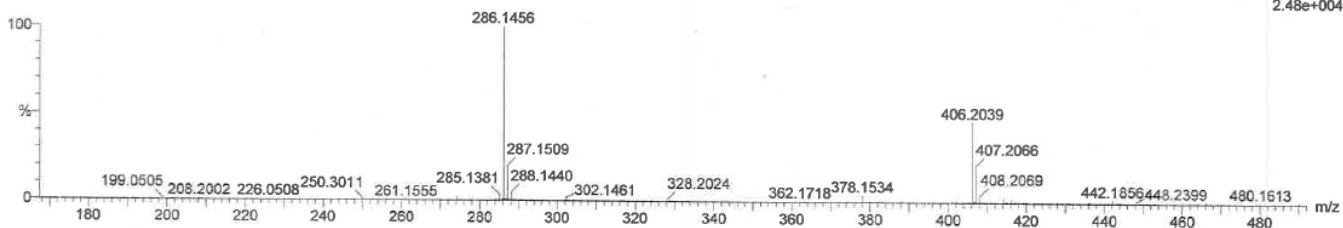
Elements Used:

C: 0-18 H: 0-25 N: 0-3 O: 0-3 F: 0-1 I: 0-1

C126/GSNS3/068

150220004 8 (0.212) Cm (8-57:60)

1: TOF MS ES+
2.48e+004

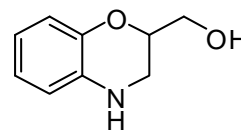


Minimum: -1.5
Maximum: 5.0 5.0 80.0

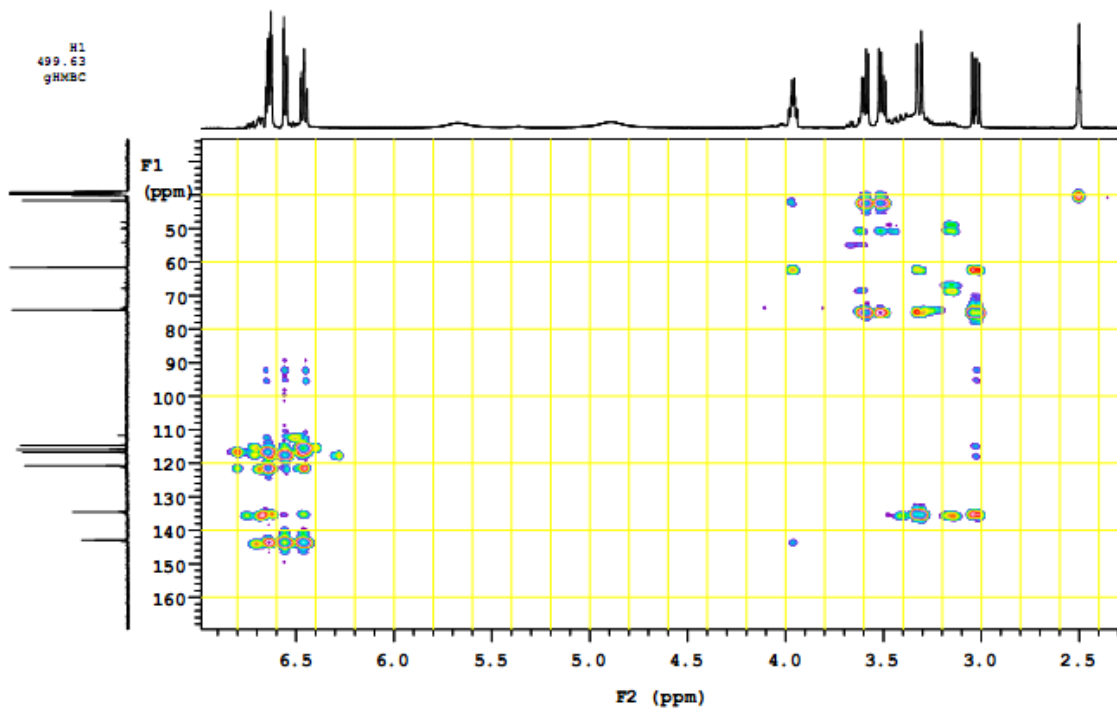
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
286.1456	286.1443	1.3	4.5	8.5	187.9	C17 H20 N O3

Fig. S-1. The results of HMBC study for *compound 3a*

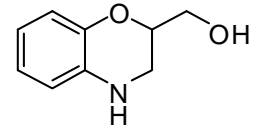
026/0583/030 in DMSO
CPS
EDC-110
MR No: IN0115/128
Date: 20th Jan 2015
Analyst: Mallikarjun



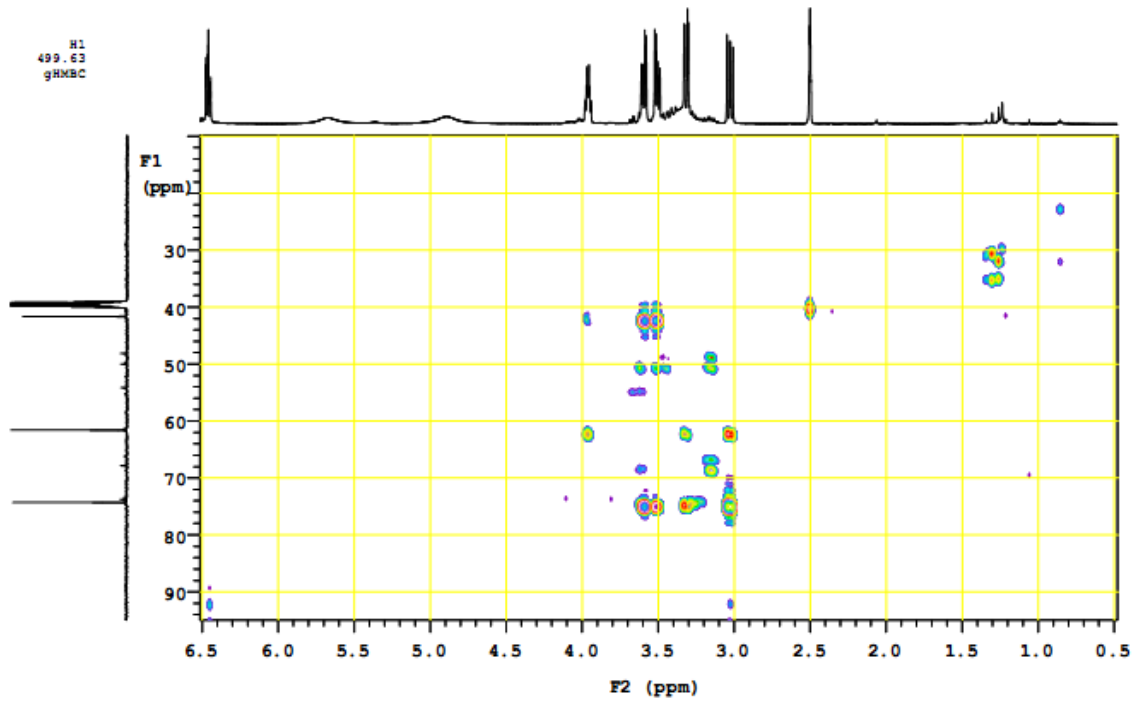
NUCLEUS : H1
PULP (MHz): 499.63
EXP : gHMBC



CL26/C8N83/030 in DMSO
CPS
EUC-110
RR No: IN0115/128
Date: 20th Jan 2015
Analyst: Mallikarjun

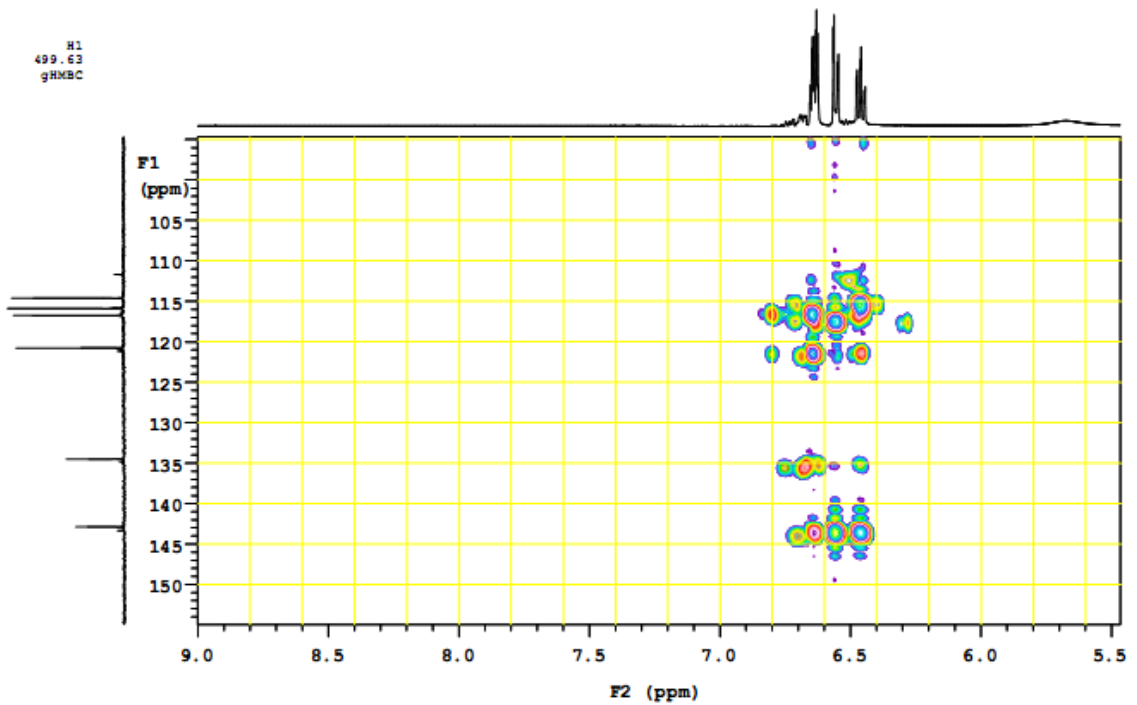


NUCLEUS : H1
PULP (MHz): 499.63
EXP : gHMBC



CL26/C8N83/030 in DMSO
CPS
EUC-110
RR No: IN0115/128
Date: 20th Jan 2015
Analyst: Mallikarjun

NUCLEUS : H1
PULP (MHz): 499.63
EXP : gHMBC



CL26/CSN83/030 in DMSO
CP8
EUC-110

MR No: IN0115/128
Date: 20th Jan 2015
Analyst: Mallikarjun

NUCLEUS : H1
PULP (MHz) : 499.63
EXP : gHMBC

