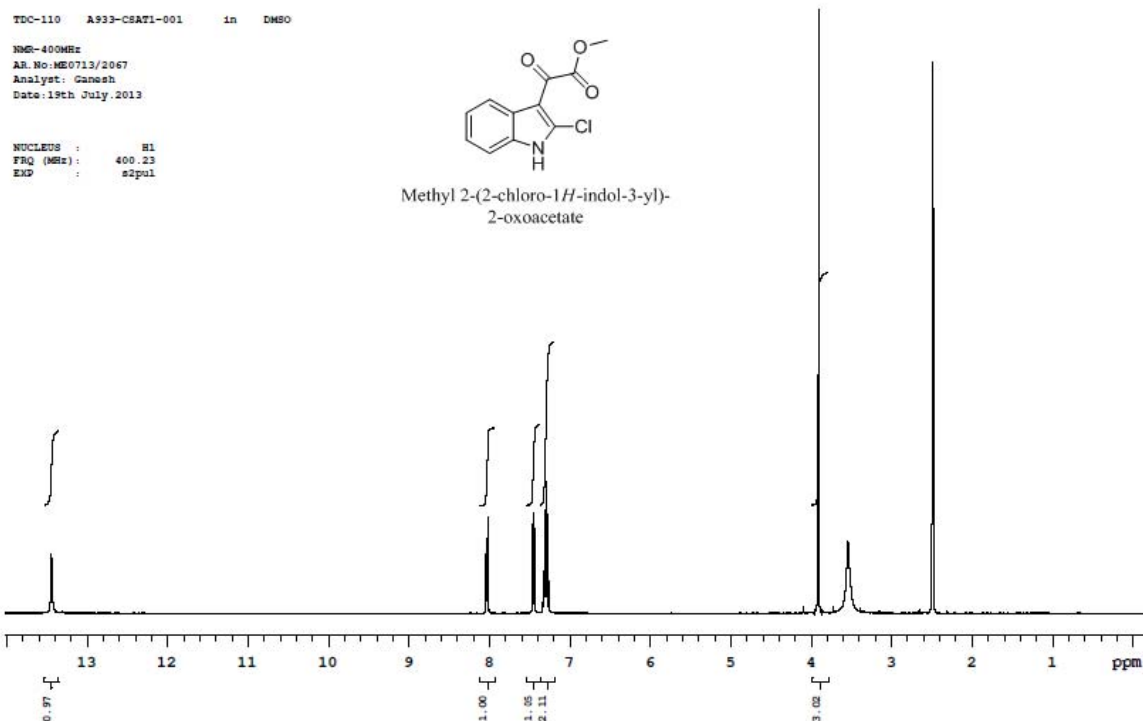


Copies of spectra



Elemental Composition Report

Page 1

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

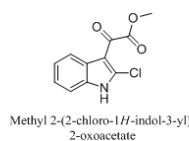
39 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

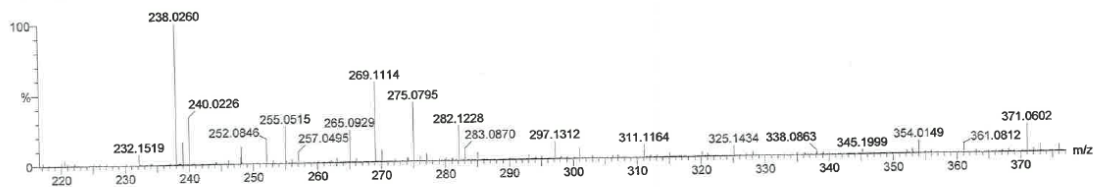
C: 0-15 H: 0-14 N: 0-2 O: 0-5 Cl: 0-1

C108/CSAT1/001

150521006 16 (0.293) Cm (16:17-37:46x0.500)



1: TOF MS ES+
1.25e+003



Minimum:

Maximum:

5.0

5.0

-1.5

80.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

Formula

238.0260

238.0271

-1.1

-4.6

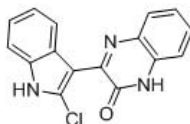
7.5

3.4

C11 H9 N O3 Cl

R. Nagaraju
21/07/2015

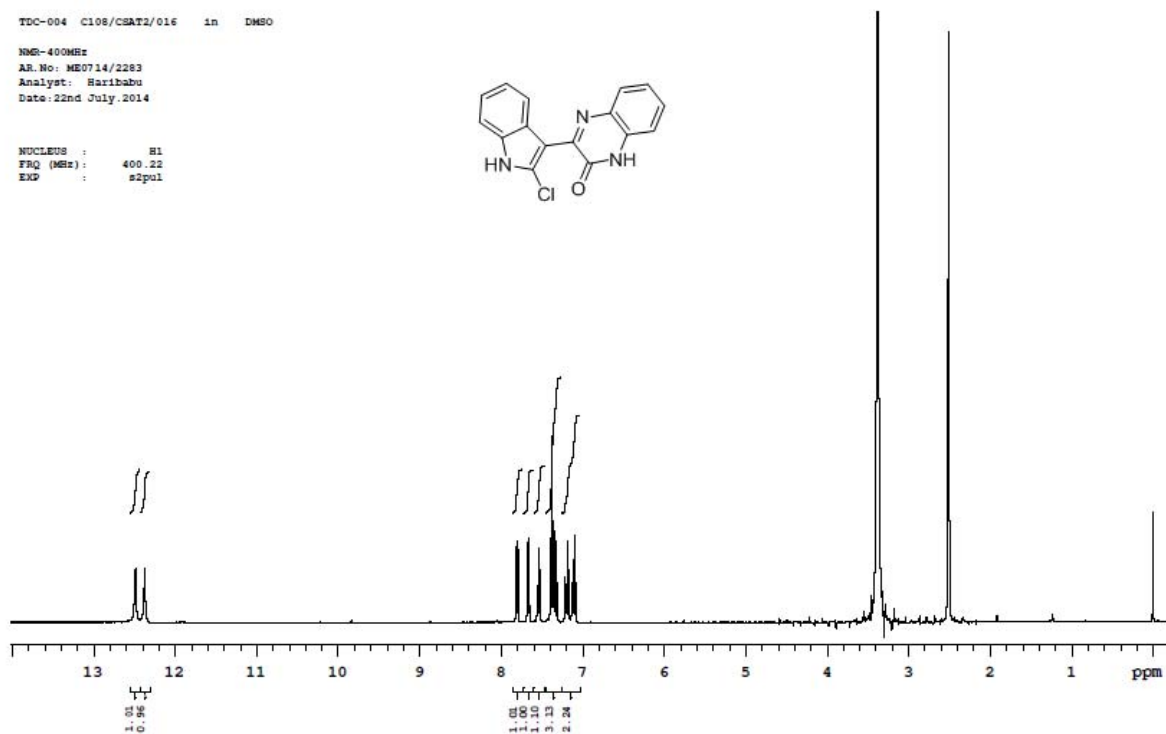
NMR-400MHz
AR.No: ME0714/2283
Analyst: Haribabu
Date: 22nd July, 2014



```

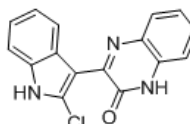
NUCLEUS   :      H1
FRQ (MHz) :    400.22
EXP       :    s2pul

```



TDC-004 C108/CSAT3/016 1n DMSO

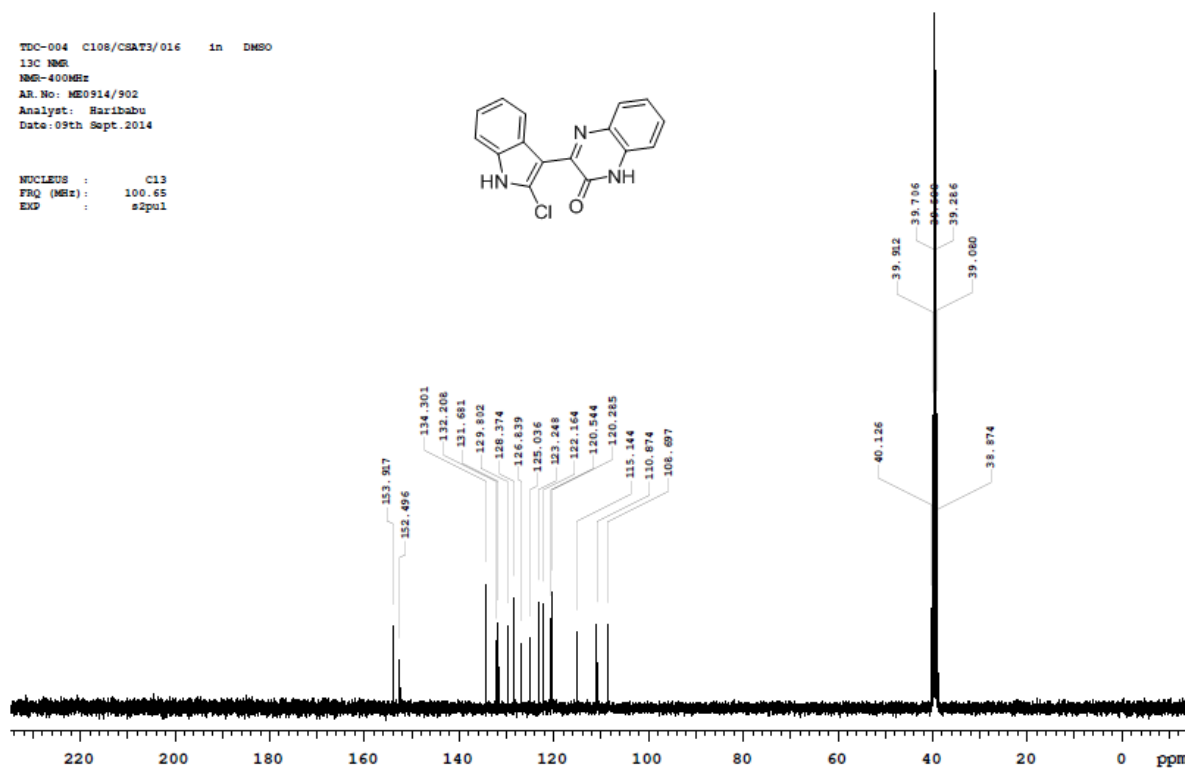
13C NMR
NMR-400MHz
AR.No: ME0914/902
Analyst: Haribabu
Date:09th Sept.2014



```

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

```



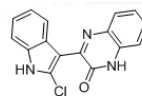
Elemental Composition Report

Page 1

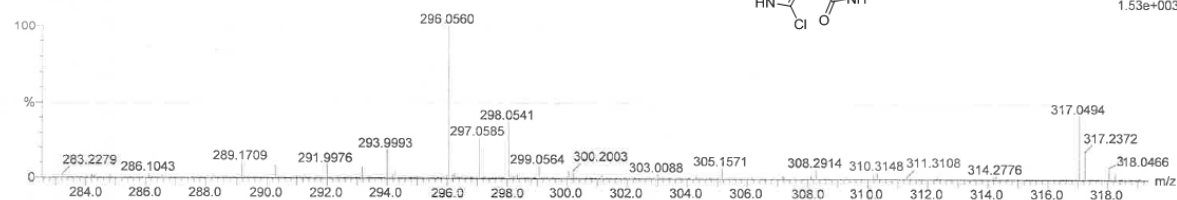
Single Mass Analysis

Tolerance = 11.0 PPM / DBE: min = -5.0, max = 30.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
 49 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
 Elements Used:
 C: 0-35 H: 0-35 N: 0-3 O: 0-1 Cl: 0-1
 C108/CSAT2/016
 140721005 58 (1.565) Cm (57.59)



1: TOF MS ES+
 1.53e+003

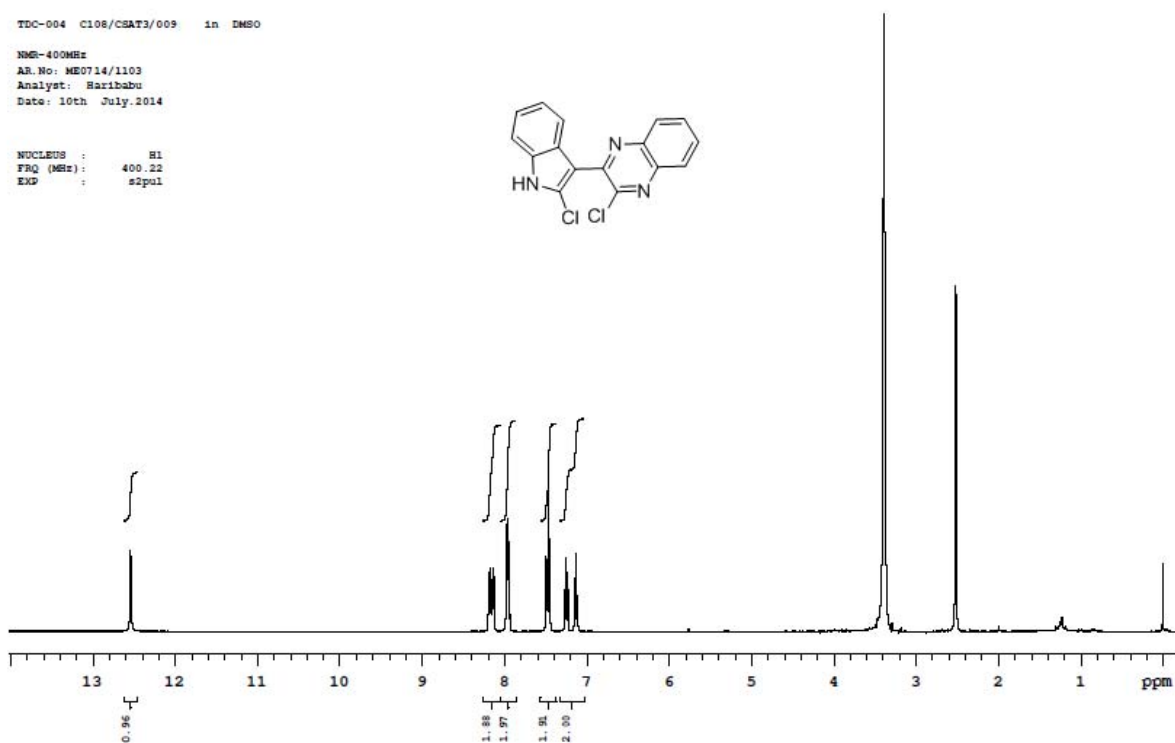
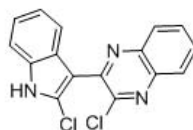


Minimum:						
Maximum:		5.0	11.0	-5.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0560	296.0591	-3.1	-10.5	12.5	18.2	C16 H11 N3 O Cl

TDC-004 C108/CSAT3/009 in DMSO

NMR-400MHz
 AR No: ME0714/1103
 Analyst: Waribabu
 Date: 10th July 2014

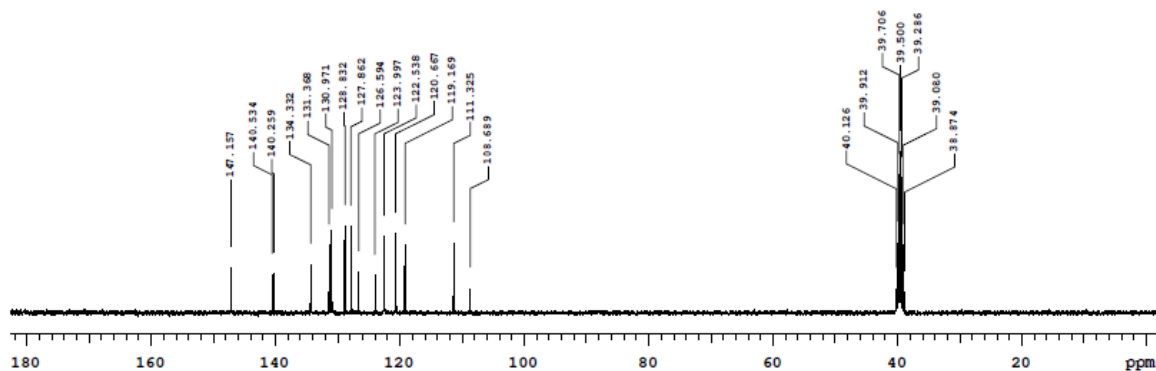
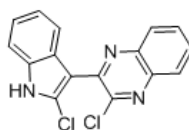
NUCLEUS : H1
 FREQ (MHz): 400.22
 EXP : zgpg30



TDC-004 C108-CSAT3-009 1n DMSO

NMR-400MHz
 AR. No: ME0714/1997
 Analyst: Haribabu
 Date: 14th July.2014

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



Single Mass Analysis

Tolerance = 19.0 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

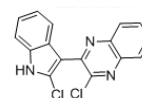
10 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

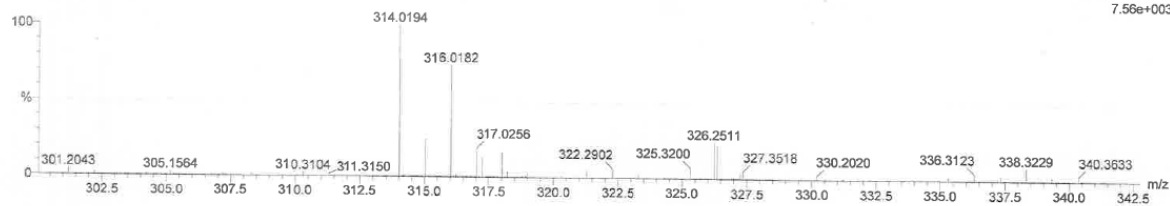
C: 0-20 H: 0-20 N: 0-3 Cl: 0-2

C108/CSAT3/009 (114070799)

140711005 17 (0.472) Cm (16:17)



1: TOF MS ES+
 7.56e+003



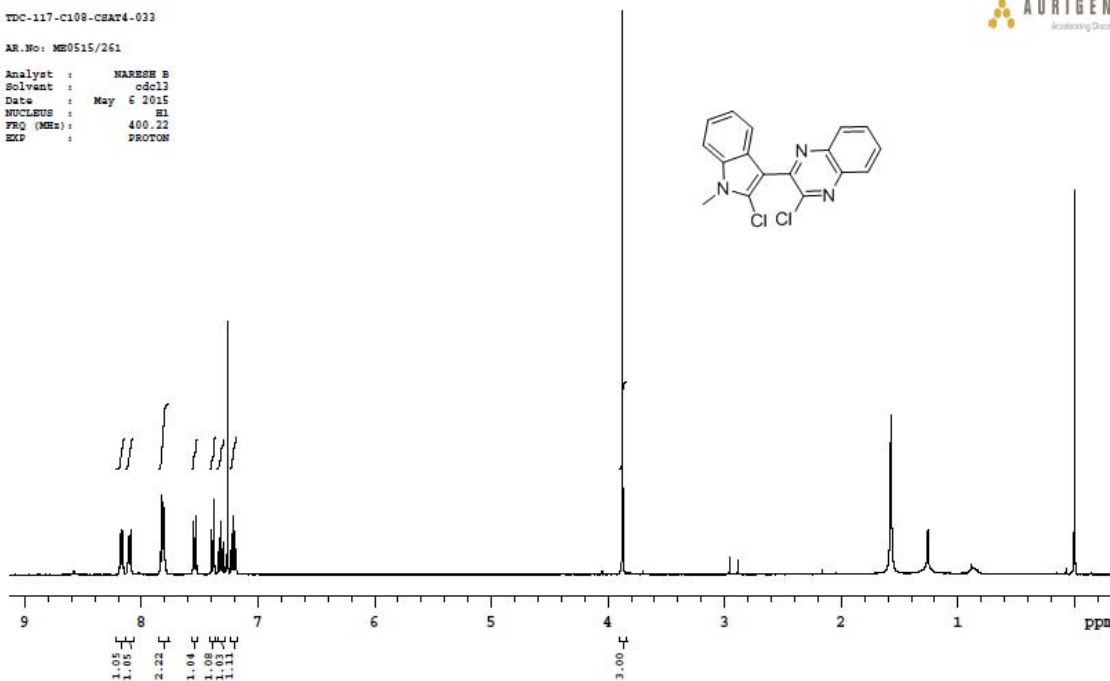
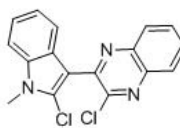
Minimum:				-5.0			
Maximum:		5.0	19.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
314.0194	314.0252	-5.8	2.5	12.5	121.1	C16 H10 N3 Cl2	

TDC-117-C108-CBAT4-033



AR.No: ME0515/261

Analyst : HARSH B
Solvent : cdcl3
Date : May 6 2015
NUCLEUS : H1
PFG (MHz): 400.22
EXP : PROTON

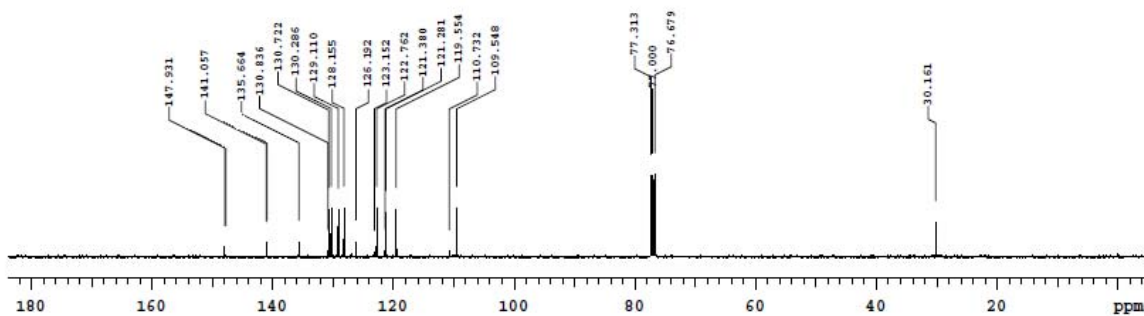
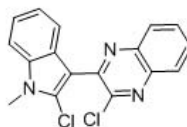


TDC-117 C108/CBAT4/033



AR.No: ME0515/525

Analyst : HARSH B
Solvent : cdcl3
Date : May 8 2015
NUCLEUS : C13
PFG (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

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

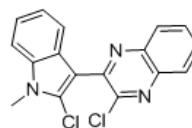
23 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

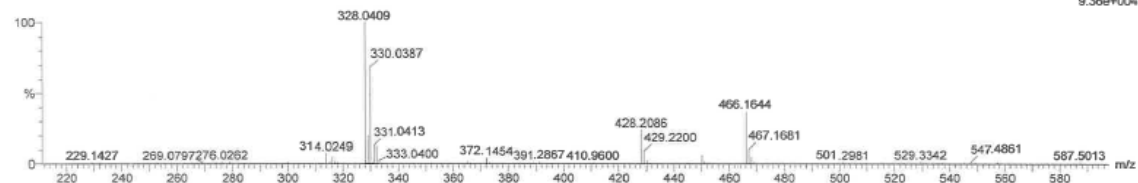
C: 0-20 H: 0-15 N: 0-5 Cl: 0-3

C108/CSAT4/033

150506003 12 (0.319) Cm (10:17:53:62x0.500)



1: TOF MS ES+
9.36e+004



Minimum:							
Maximum:							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
328.0409	328.0408	0.1	0.3	12.5	2.2	C17 H12 N3 Cl2	

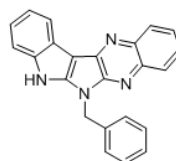
TDC-010 C108/CSAT2/011 in CDCl3+ DMSO

NMR-400MHz:

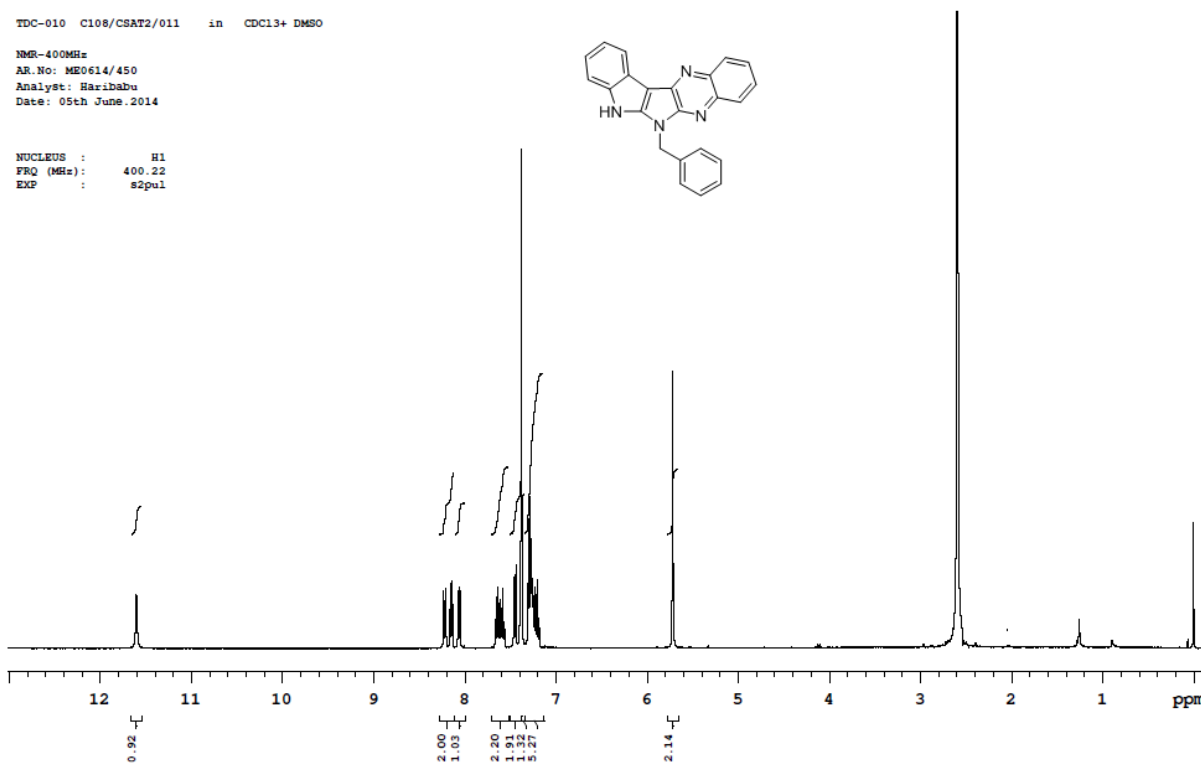
AR.No: ME0614/450

Analyst: Haribabu

Date: 05th June.2014



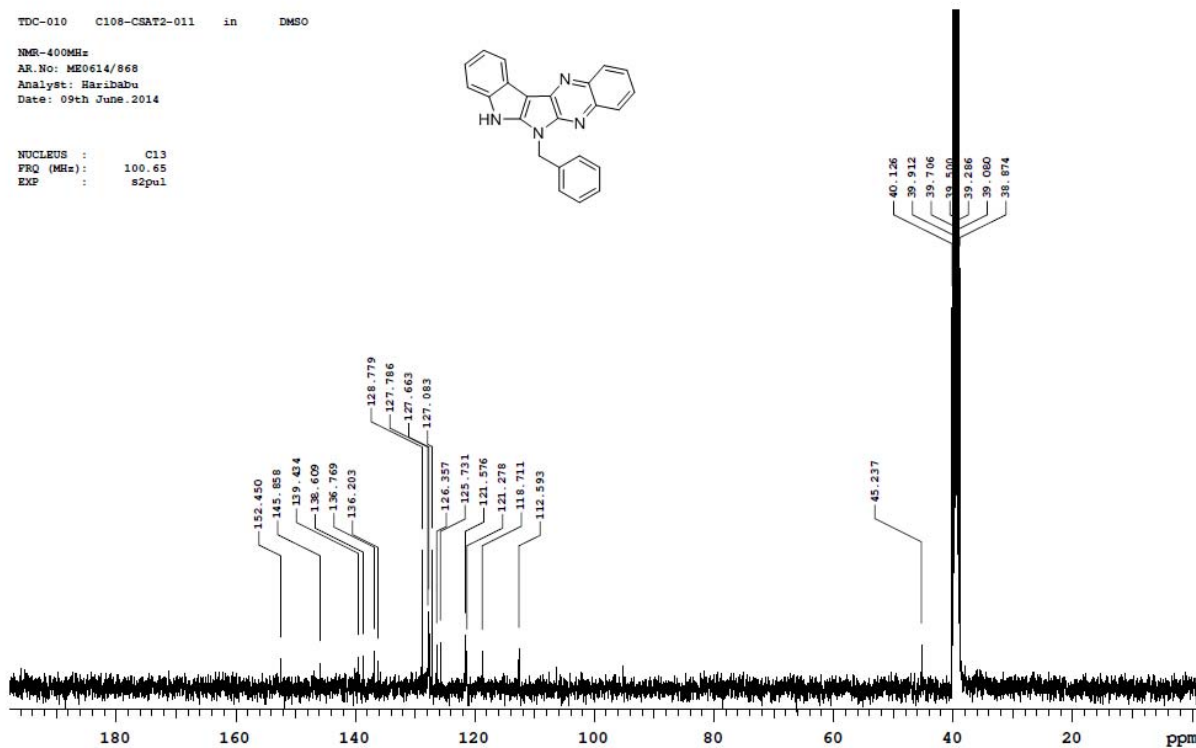
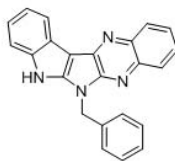
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-010 C108-CSAT2-011 in DMSO

NMR-400MHz
 Ac.No: ME0614/868
 Analyst: Haribabu
 Date: 09th June, 2014

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



Elemental Composition Report

Page 1

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 = 3

Monoisotopic Mass, Even Electron Ions

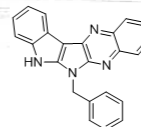
3 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

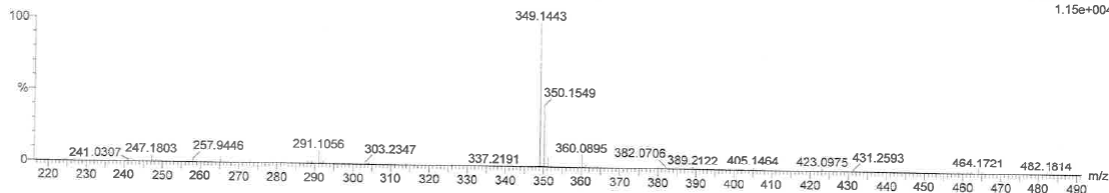
C: 0-24 H: 0-20 N: 0-4

C108/CSAT2/011

140610010 10 (0.278) Cm (9:11-(26:31+3:4))



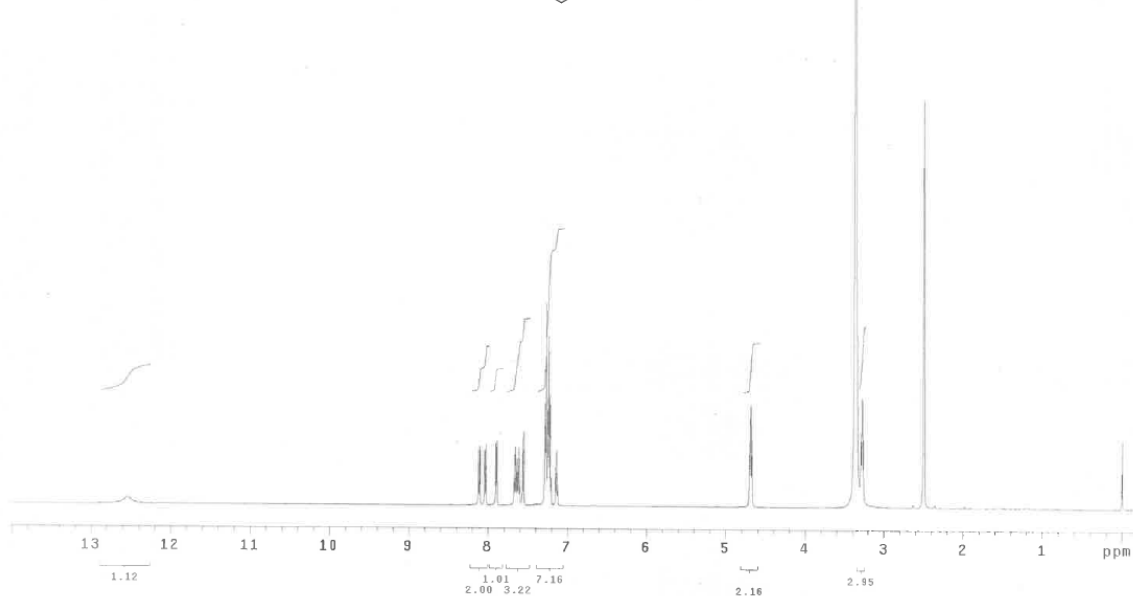
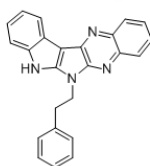
1: TOF MS ES+
 1.15e+004



Minimum:						
Maximum:		5.0	5.0	-5.0		
				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
349.1443	349.1453	-1.0	-2.9	17.5	343.8	C23 H17 N4

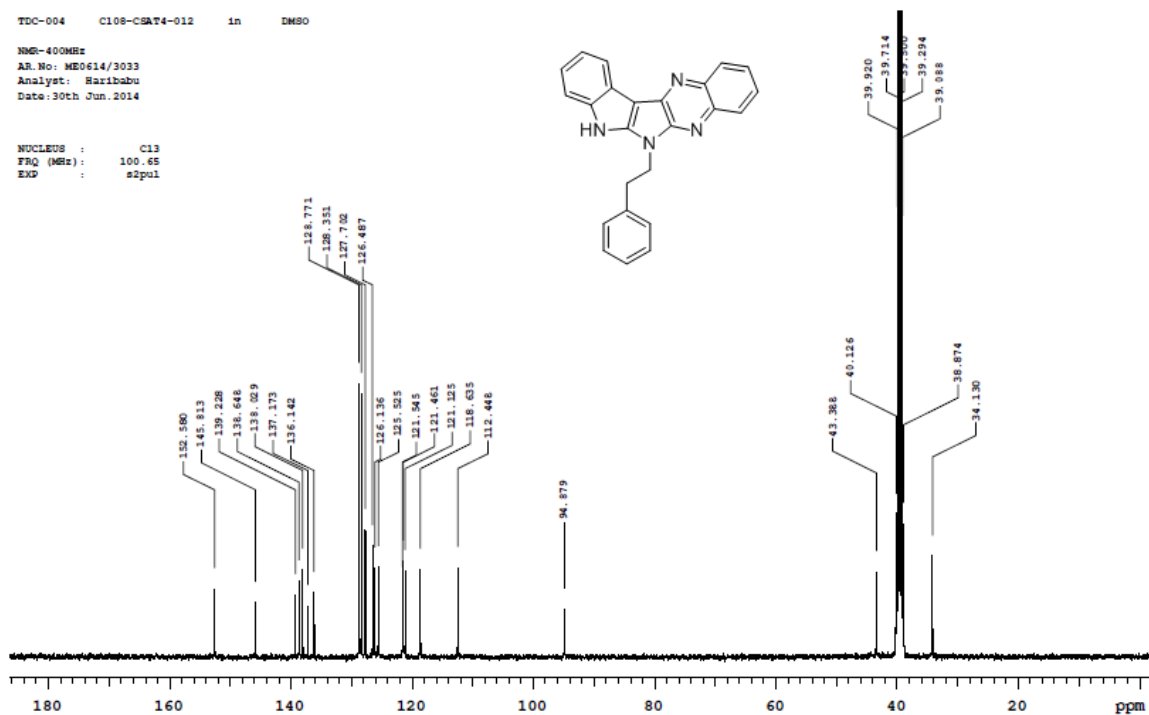
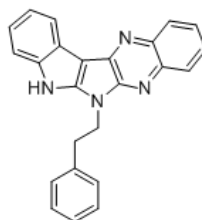
C108/CSAT4/012 in DMSO
TDC-004

AR.No:IN0614/190
Date:18th June,2014
Analyst: Haribabu.R



TDC-004 C108-CSAT4-012 in DMSO

NMR-400MHz
AR.No: ME0614/3033
Analyst: Haribabu
Date:30th Jun,2014



Elemental Composition Report

Page 1

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

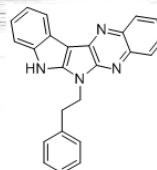
12 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

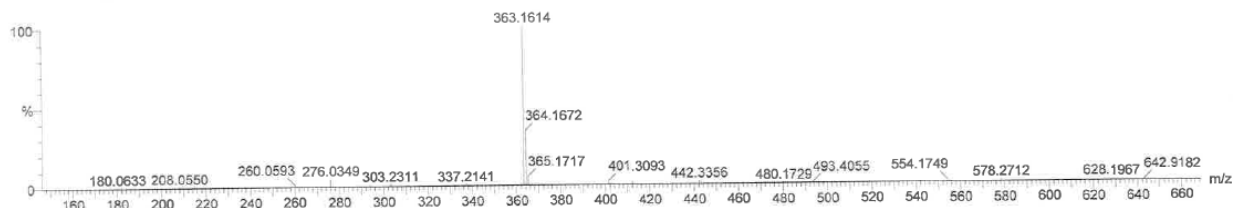
C: 0-26 H: 0-25 N: 0-4 O: 0-1

C108/CSAT4/012

140618013 13 (0.365) Cm (13:20-(2:6+26:29))



1: TOF MS ES+
1.44e+004



Minimum: -5.0
Maximum: 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
363.1614	363.1610	0.4	1.1	17.5	91.9	C24 H19 N4

TDC-004 C108/CSAT4/013-A in DMSO

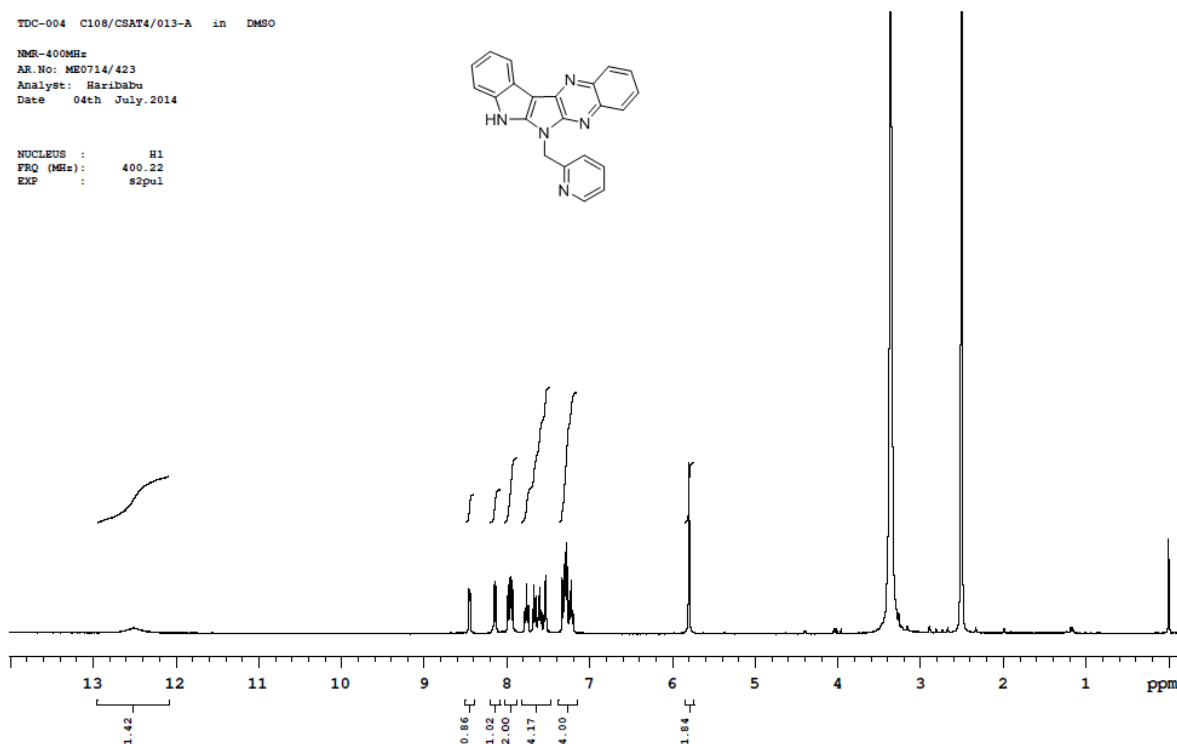
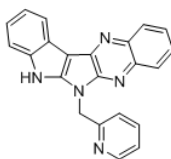
NMR-400MHz

AR.No: ME0714/423

Analyst: Haridabu

Date 04th July 2014

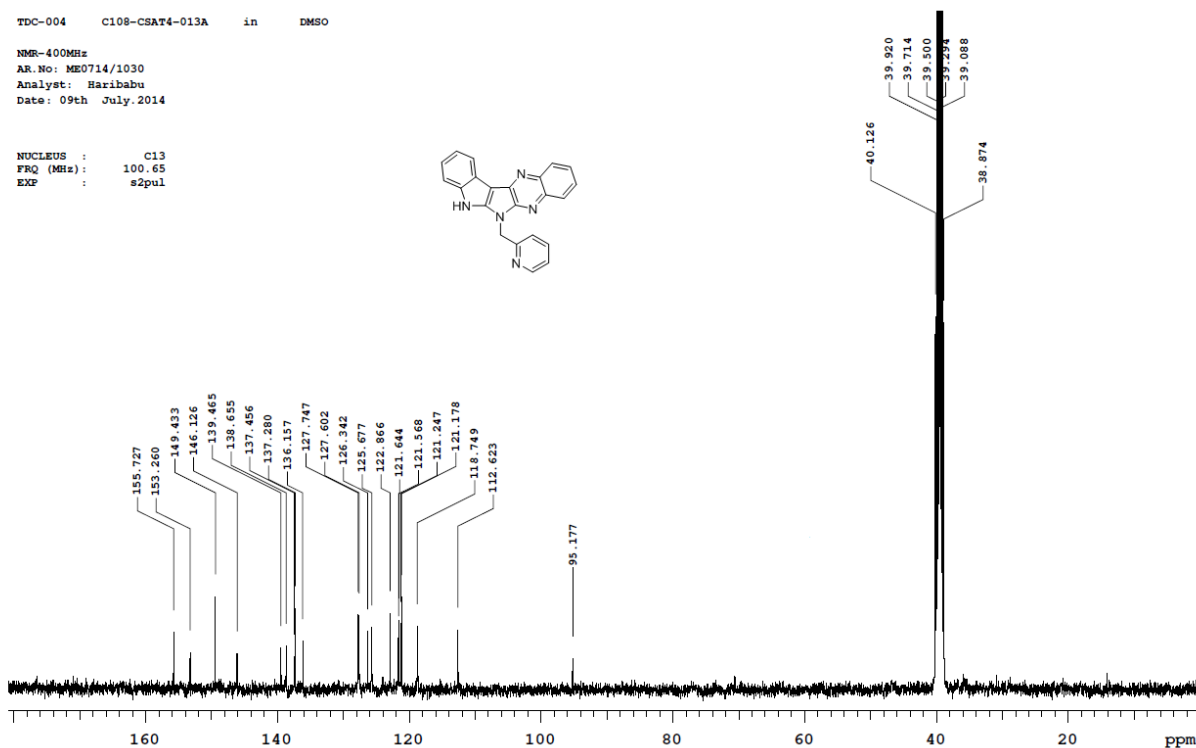
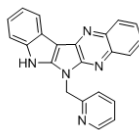
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108-CSAT4-013A in DMSO

NMR-400MHz
AR. No: ME0714/1030
Analyst: Haribabu
Date: 09th July. 2014

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



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = 3.0; max = 80.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions

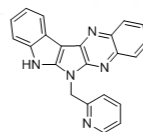
7 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

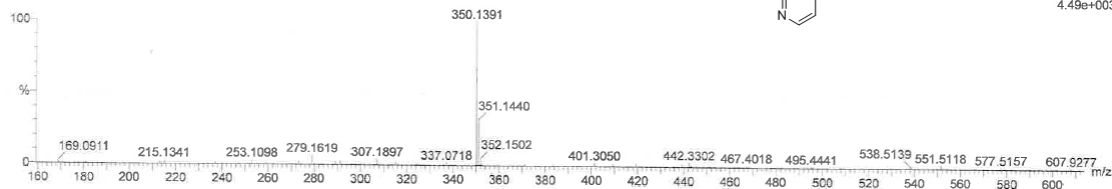
C: 0-25 H: 0-25 N: 0-5

C108/CSAT4/013A

140704004 29 (0.547) Cm (26:29-77:94)



1: TOF MS ES+
4.49e+003

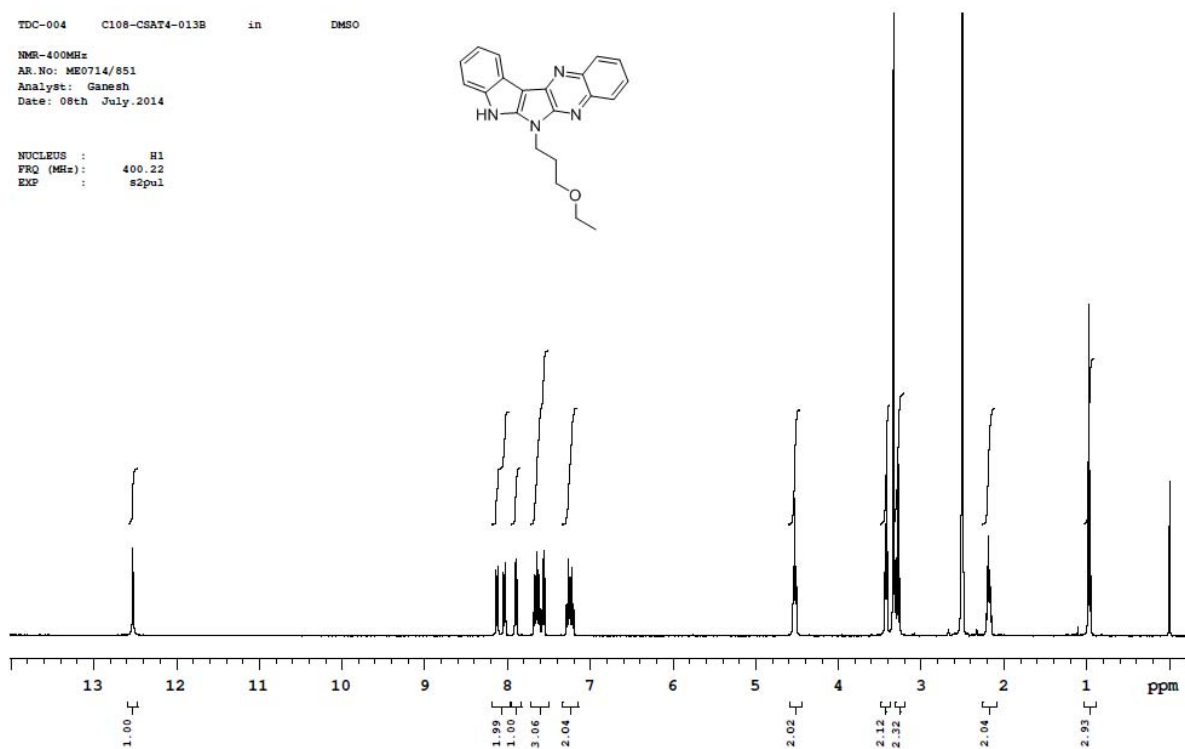
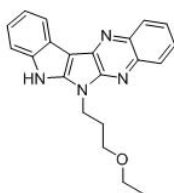


Minimum:						
Maximum:		5.0	5.0	-5.0		
				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
350.1391	350.1406	-1.5	-4.3	17.5	21.5	C22 H16 N5

TDC-004 C108-CSAT4-013B in DMSO

NMR-400MHz
AR.No: ME0714/851
Analyst: Ganesh
Date: 08th July 2014

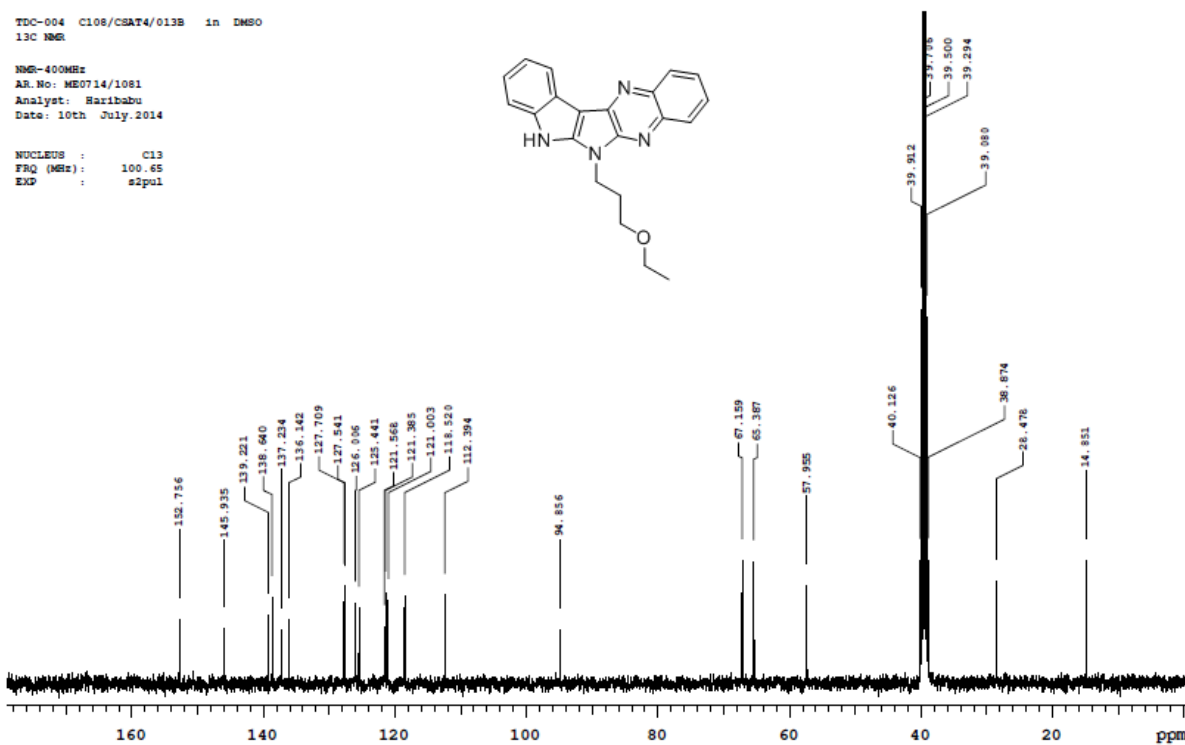
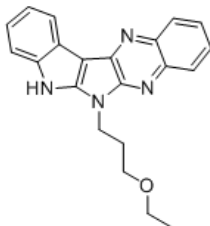
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT4/013B in DMSO
13C NMR

NMR-400MHz
AR.No: ME0714/1081
Analyst: Haribabu
Date: 10th July 2014

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



Elemental Composition Report

Page 1

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

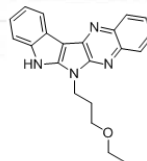
291 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

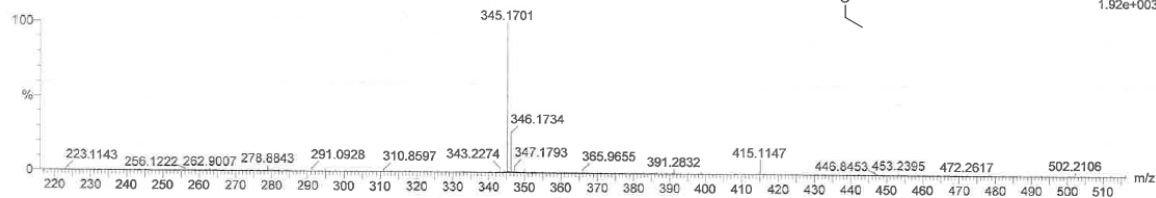
C: 0-25 H: 0-25 N: 0-5 O: 0-2 S: 0-1 Br: 0-3

C108/CSAT4/013B

140709007 30 (0.562) Cm (30.31-53.65)



1: TOF MS ES+
1.92e+003



Minimum:							
Maximum:		5.0	5.0	-5.0			
				80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
345.1701	345.1715	-1.4	-4.1	13.5	2.1	C21 H21 N4 O	

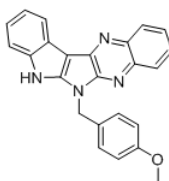
TDC-004 C108-CSAT4-013C in DMSO

NMR-400MHz

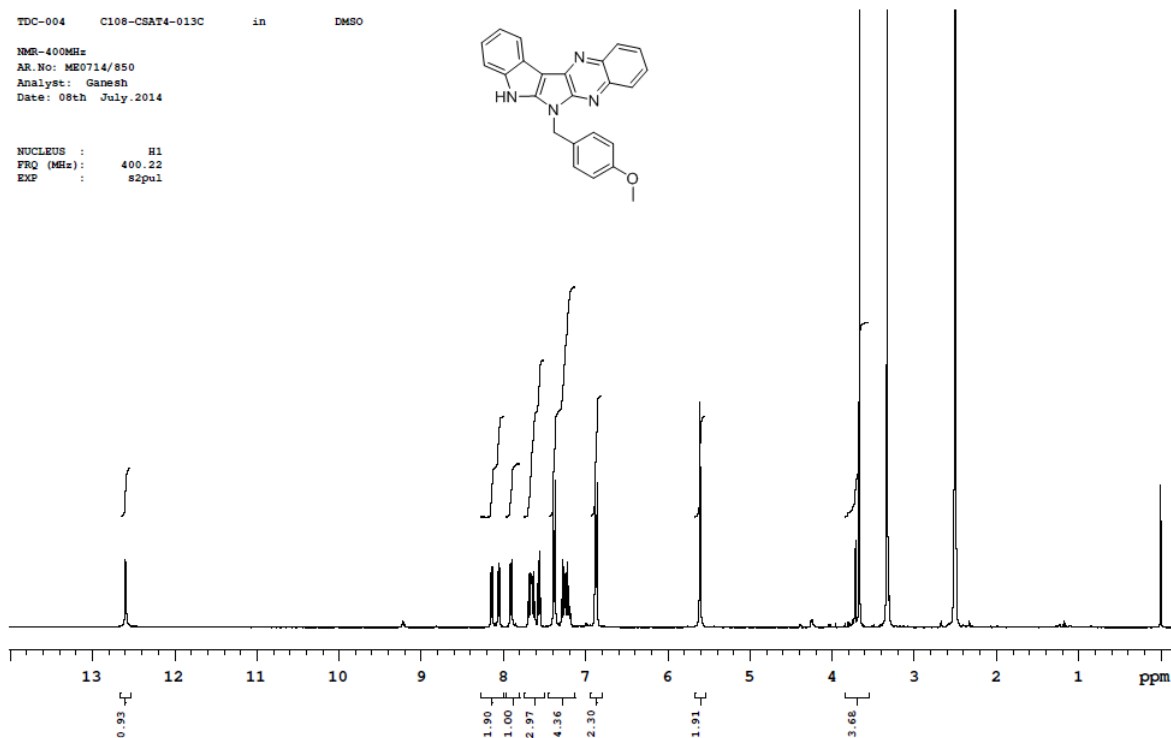
AR.No: ME0714/850

Analyst: Ganesh

Date: 08th July.2014



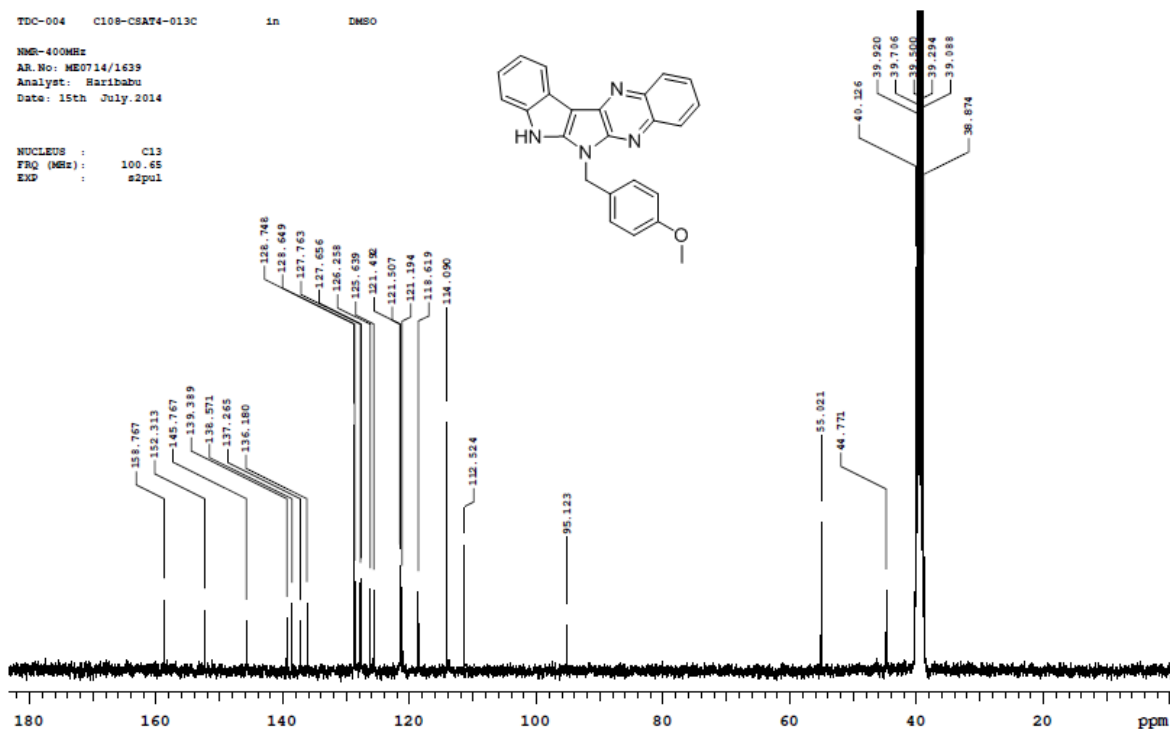
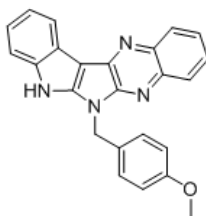
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108-CSAT4-013C in DMSO

NMR-400MHz
AR.No: ME0714/1639
Analyst: Haribabu
Date: 15th July 2014

NUCLEUS : C13
FREQ (MHz): 100.65
EXP : s2pol



Elemental Composition Report

Page 1

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

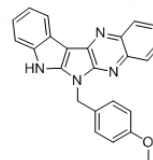
9 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

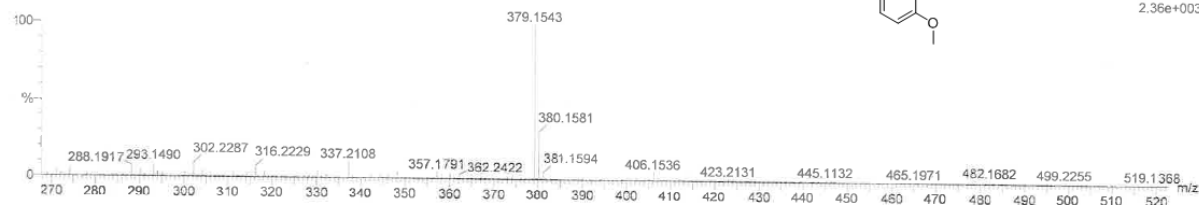
C: 0-25 H: 0-25 N: 0-5 O: 0-1

C108/CSAT4/013C

140715010.9 (0.257) Cm (6.9-35.41)



1: TOF MS ES+
2.36e+003

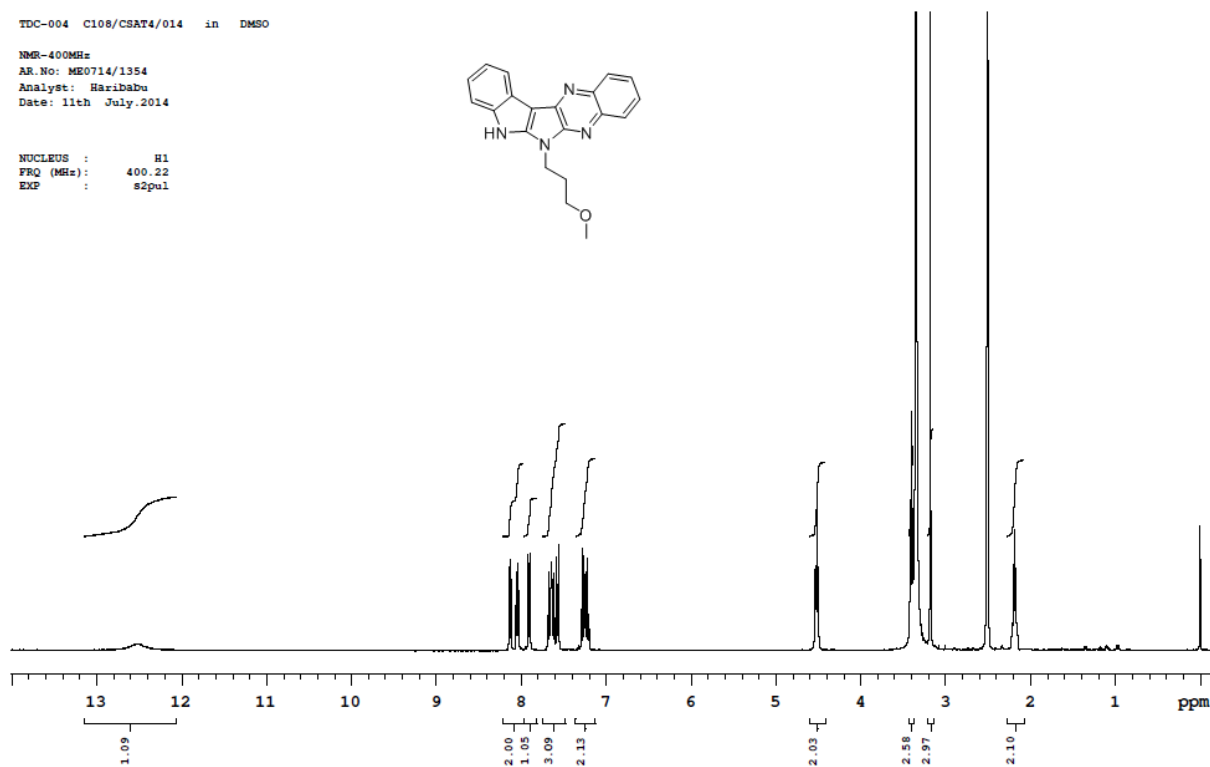
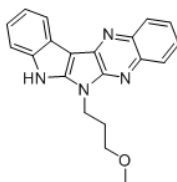


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.1543	379.1559	-1.6	-4.2	17.5	5.2	C24 H19 N4 O

TDC-004 C108/CSAT4/014 in DMSO

NMR-400MHz
AR.No: ME0714/1354
Analyst: Haribabu
Date: 11th July.2014

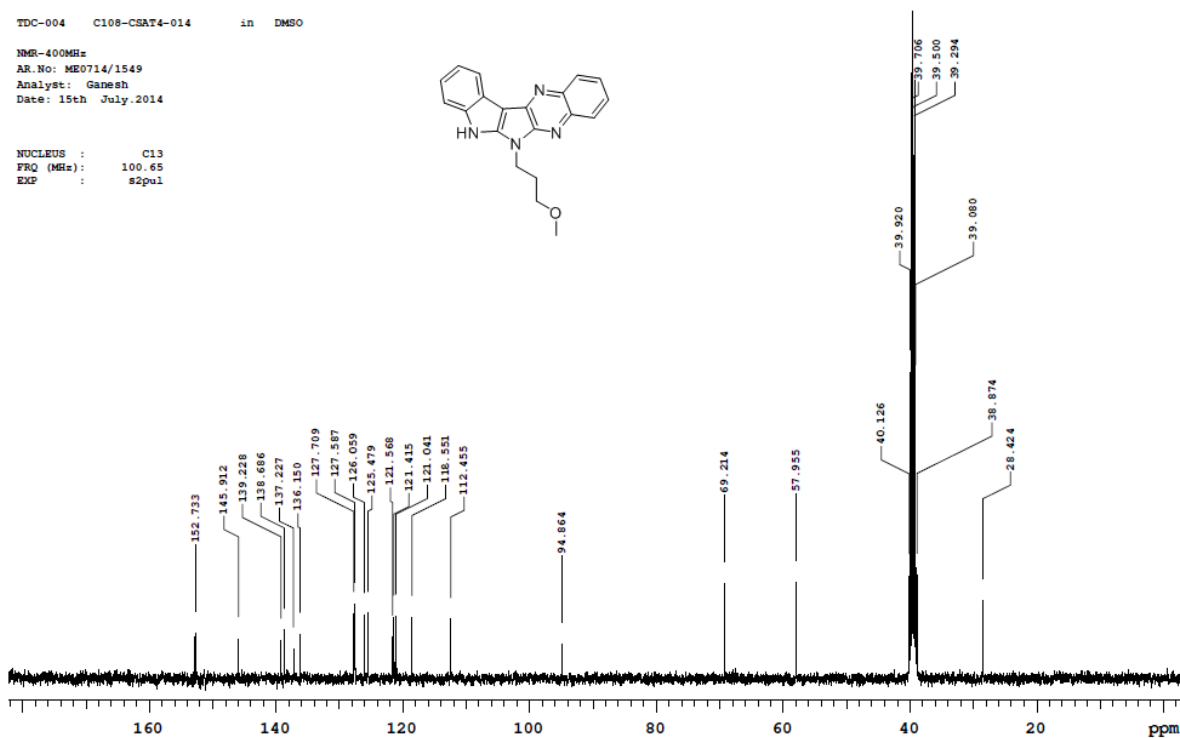
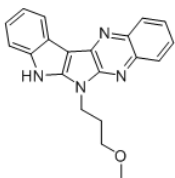
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108-CSAT4-014 in DMSO

NMR-400MHz
AR.No: ME0714/1549
Analyst: Ganesh
Date: 15th July.2014

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



Elemental Composition Report

Page 1

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

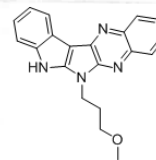
24 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

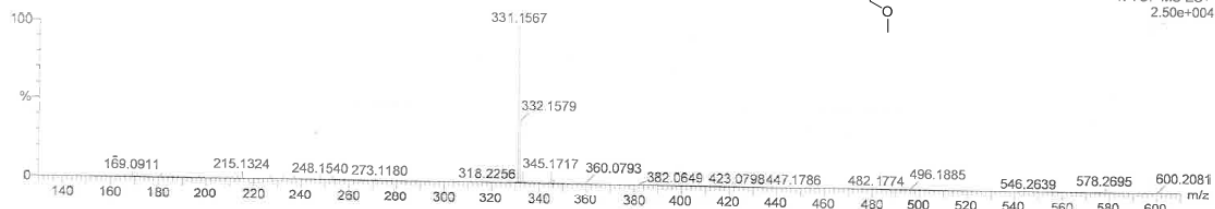
C: 0-25 H: 0-20 N: 0-4 O: 0-2

C108/CSAT4/014

140715009 10 (0.278) Cm (7:10-39:47)



1: TOF MS ES+
2.50e+004



Minimum:				-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
331.1567	331.1559	0.8	2.4	13.5	955.9	C20 H19 N4 O

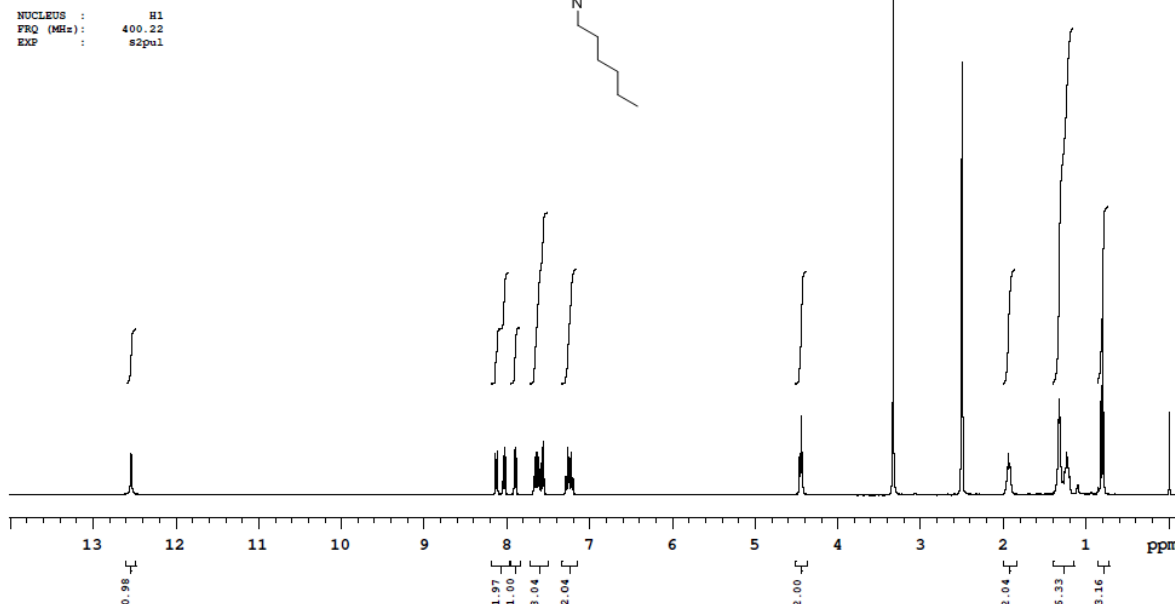
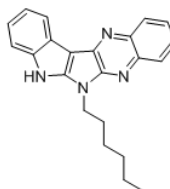
TDC-004 C108-CSAT4-015 in DMSO

NMR-400MHz

AR.No: ME0714/1822

Analyst: Ganesh

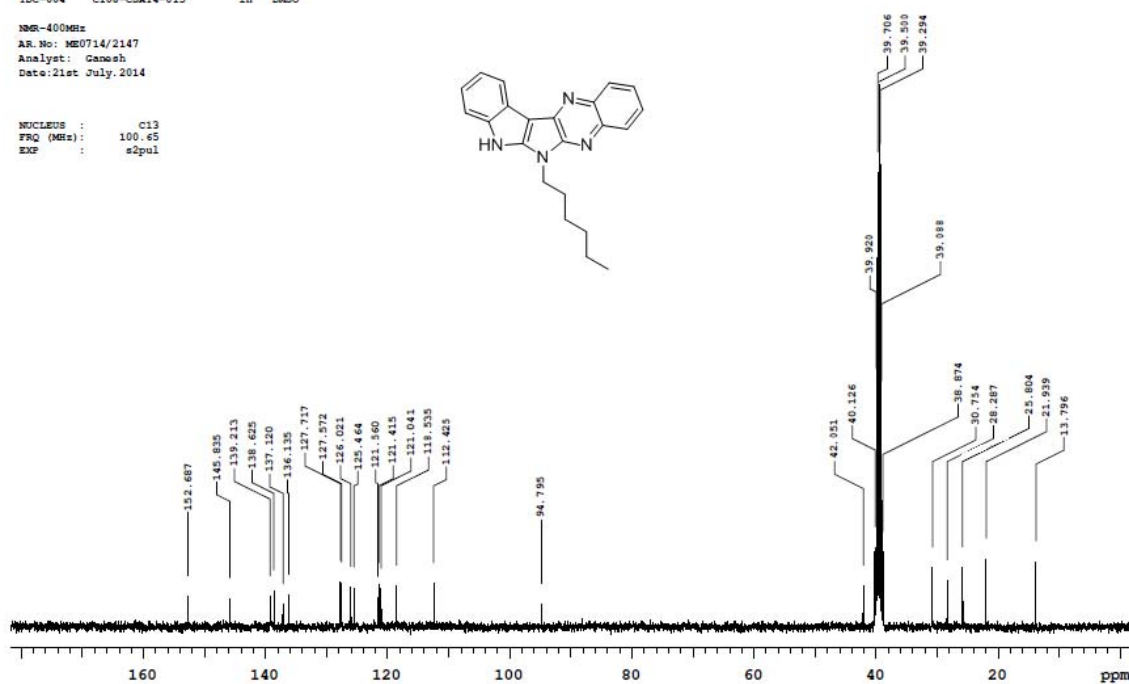
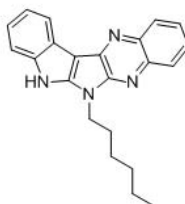
Date:17th July.2014



TDC-004 C109-CSAT4-015 in DMSO

MS-400MHz
AR No: MS0714/2147
Analyst: Ganesh
Date: 21st July, 2014

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



Elemental Composition Report

Page 1

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

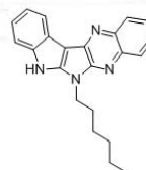
70 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

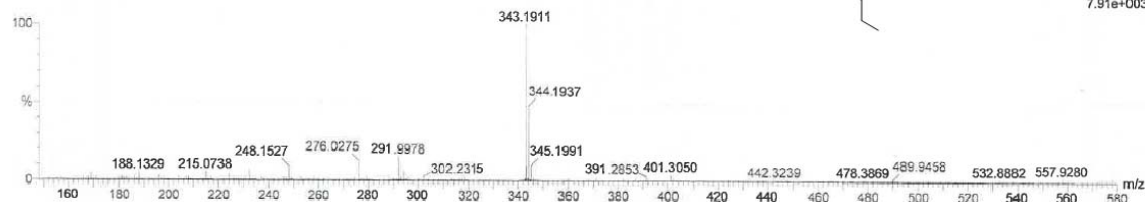
C: 0-25 H: 0-30 N: 0-4 O: 0-2 S: 0-1

C108/CSAT4/015

1407170111 12 (0.319) Cm (12)



1: TOF MS ES+
7.91e+003



Minimum:
Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.1911	343.1923	-1.2	-3.5	13.5	507.9	C22 H23 N4

Butes

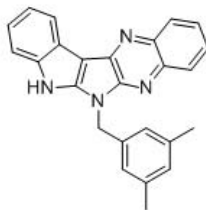
TDC-004 C108/CSAT4/017 in DMSO

MS-400MHz

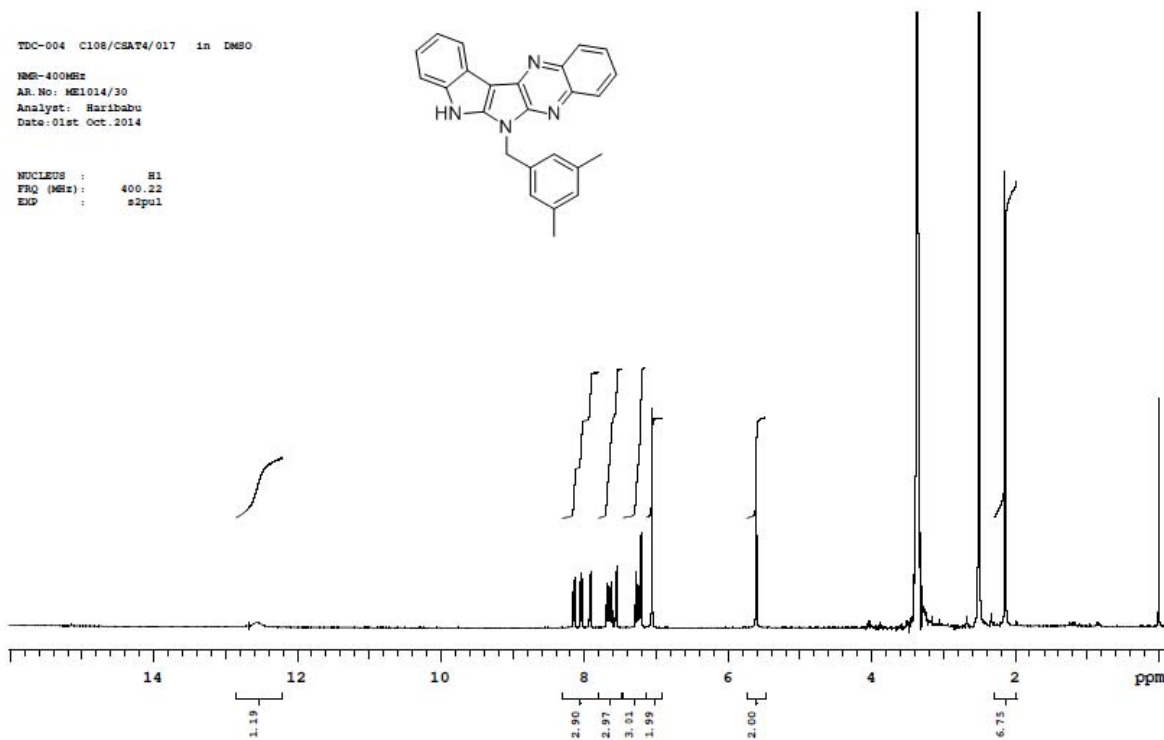
AR No: ME1014/30

Analyst: Haribabu

Date: 01st Oct. 2014



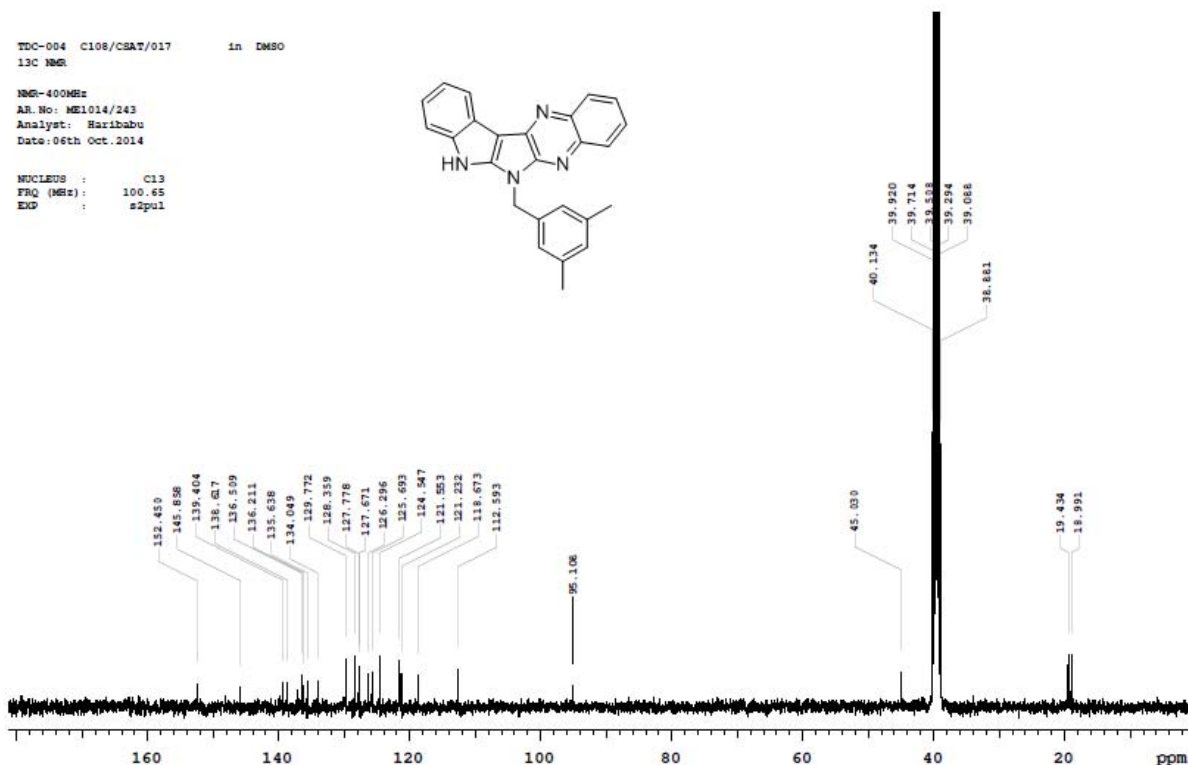
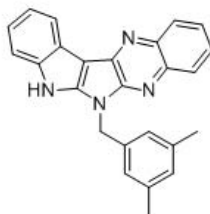
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT/017 in DMSO
13C NMR

NMR-400MHz
AR. No: ME1014/243
Analyst: Haribabu
Date: 06th Oct. 2014

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



Elemental Composition Report

Page 1

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 = 3

Monoisotopic Mass, Even Electron Ions

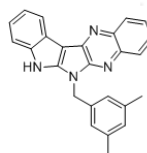
11 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

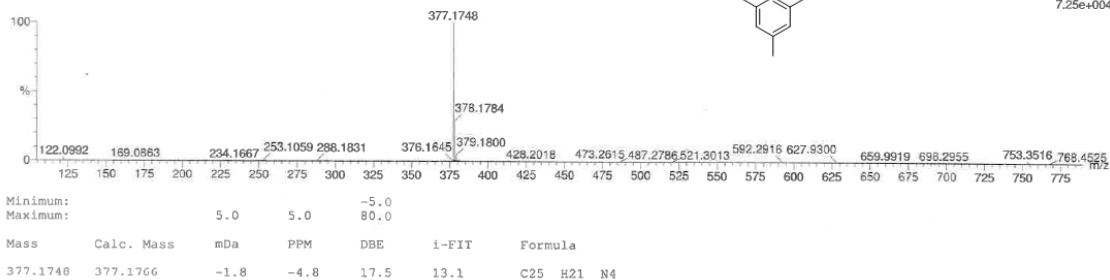
C: 0-30 H: 0-25 N: 0-4

C108/CSAT4/017

141001005 14 (0.385) Cm (12:14-44:54)



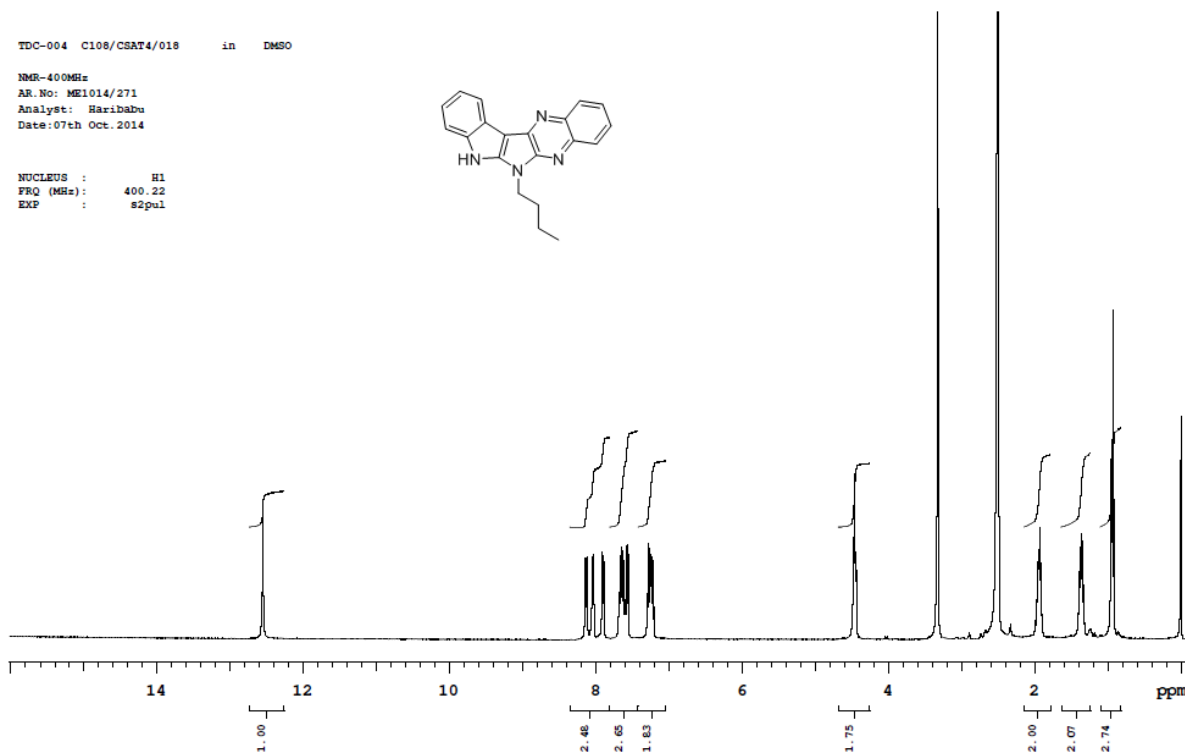
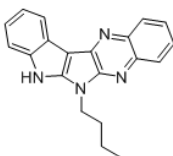
1: TOF MS ES+
7.25e+004



TDC-004 C108/CSAT4/018 in DMSO

NMR-400MHz
AR.No: ME1014/271
Analyst: Haribabu
Date:07th Oct. 2014

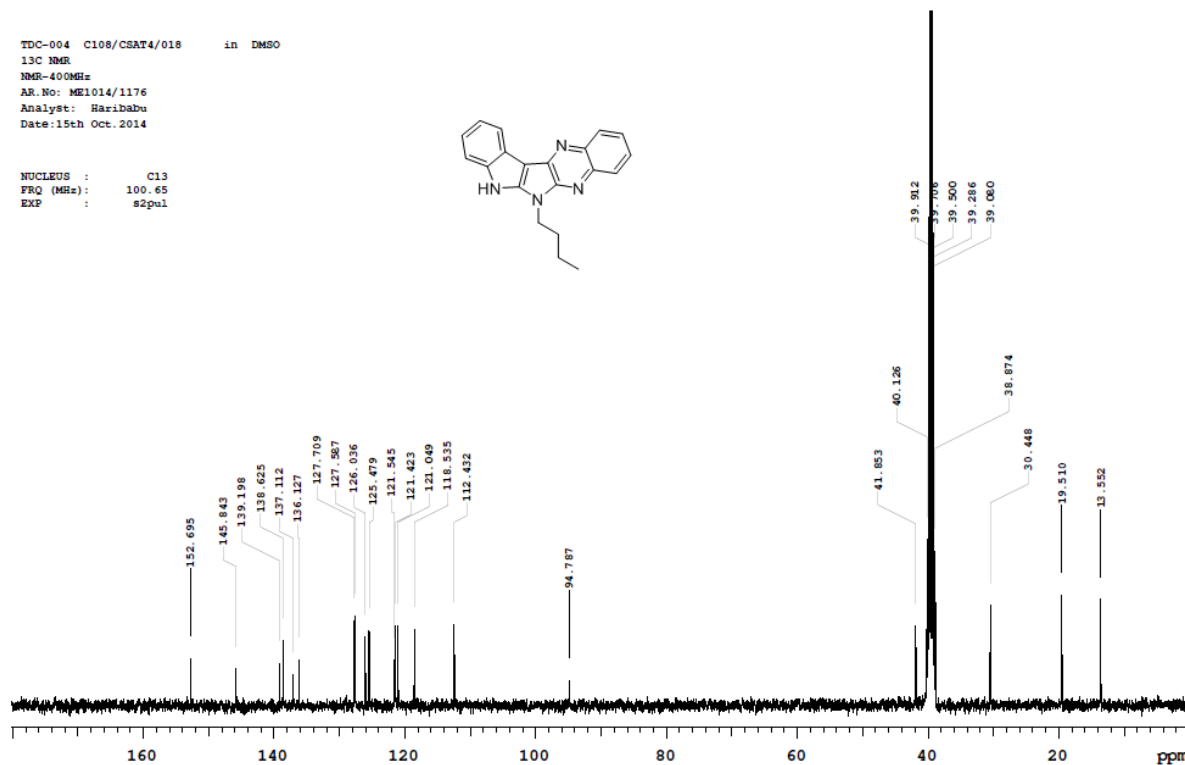
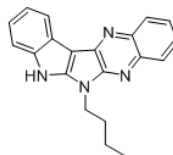
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT4/018 in DMSO

13C NMR
NMR-400MHz
AR.No: ME1014/1176
Analyst: Haribabu
Date:15th Oct. 2014

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



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

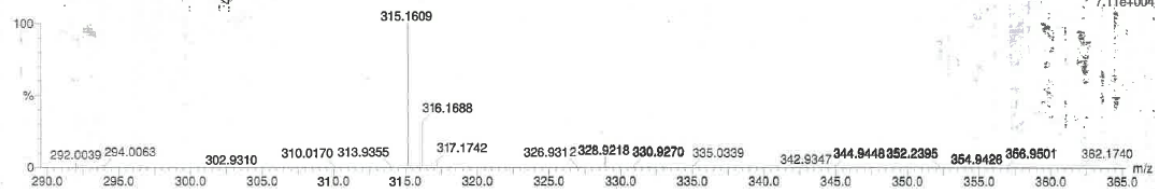
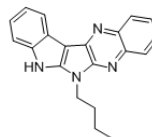
13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-28 H: 0-24 N: 0-5

C108/CSAT4/018

141205001 43 (0.405) Cm (41.53-110.132)



Minimum:				-1.5		
Maximum:	5.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
315.1609	315.1610	-0.1	-0.3	13.5	671.2	C20 H19 N4

ARD1426/ RNR1172
R. Nagarajan
05/12/2014

TDC-004 C108/CSAT4/020 in DMSO

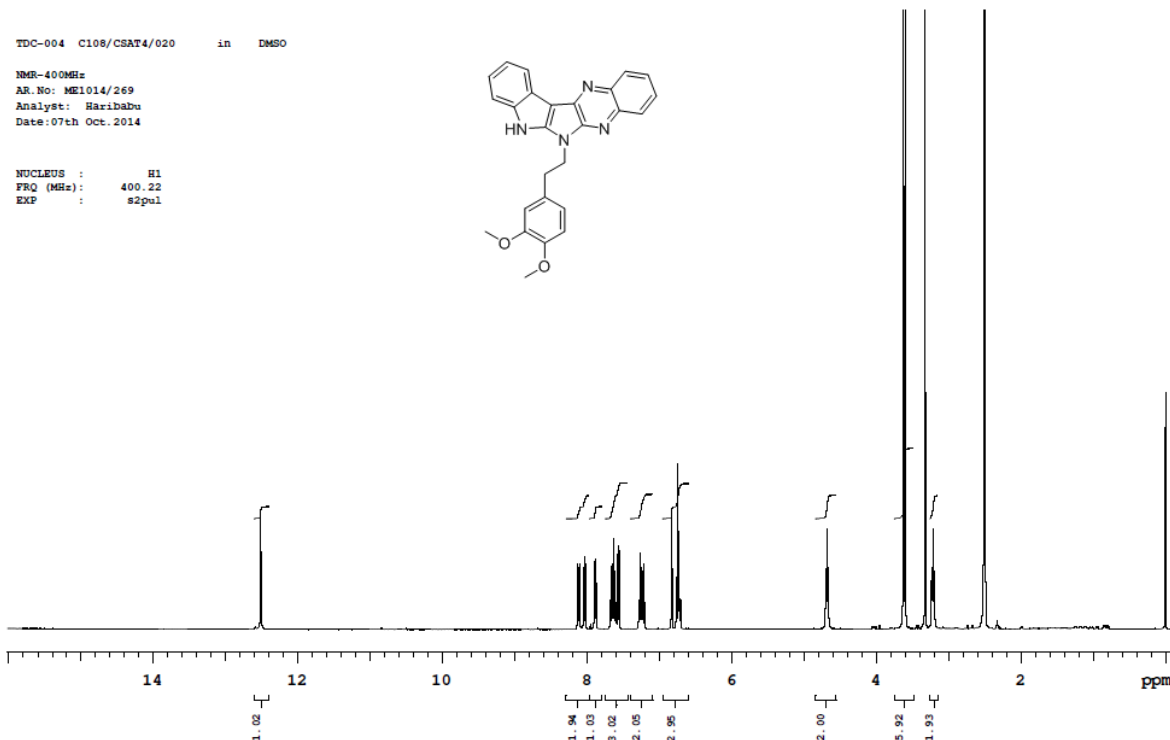
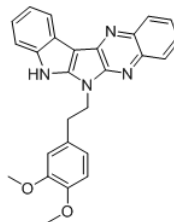
NMR-400MHz

AR. No: ME1014/269

Analyst: Haribabu

Date: 07th Oct. 2014

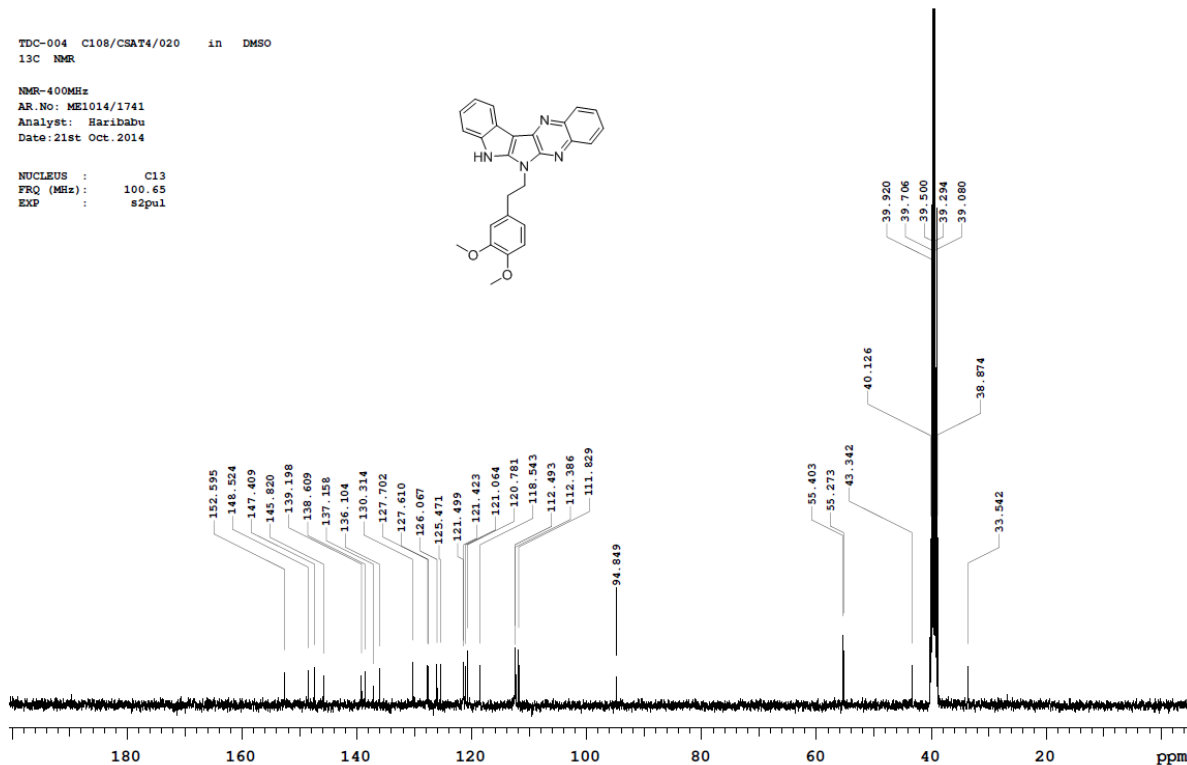
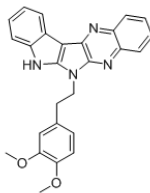
NUCLEUS : H1
PRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT4/020 in DMSO
13C NMR

NMR-400MHz
AR.No: ME1014/1741
Analyst: Haribabu
Date: 21st Oct. 2014

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



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

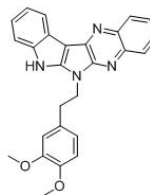
21 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-28 H: 0-24 N: 0-5 O: 0-3

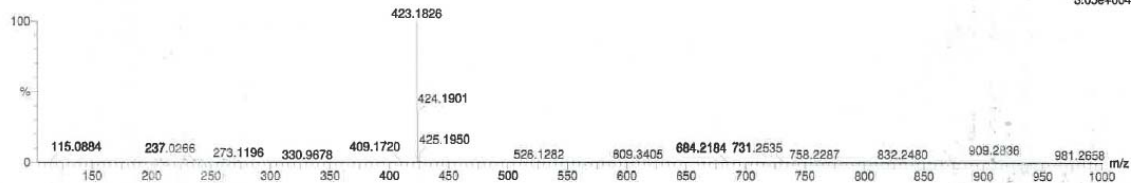
C108/CSAT4/020

141205002 52 (0.490) Cm (51:56-85:92)



Page 1

1: TOF MS ES+
3.05e+004



Minimum:	5.0	5.0	-1.5
Maximum:	5.0	5.0	50.0
Mass	Calc. Mass	mDa	PPM
423.1826	423.1821	0.5	1.2
			17.5
			88.9
			C26 H23 N4 O2

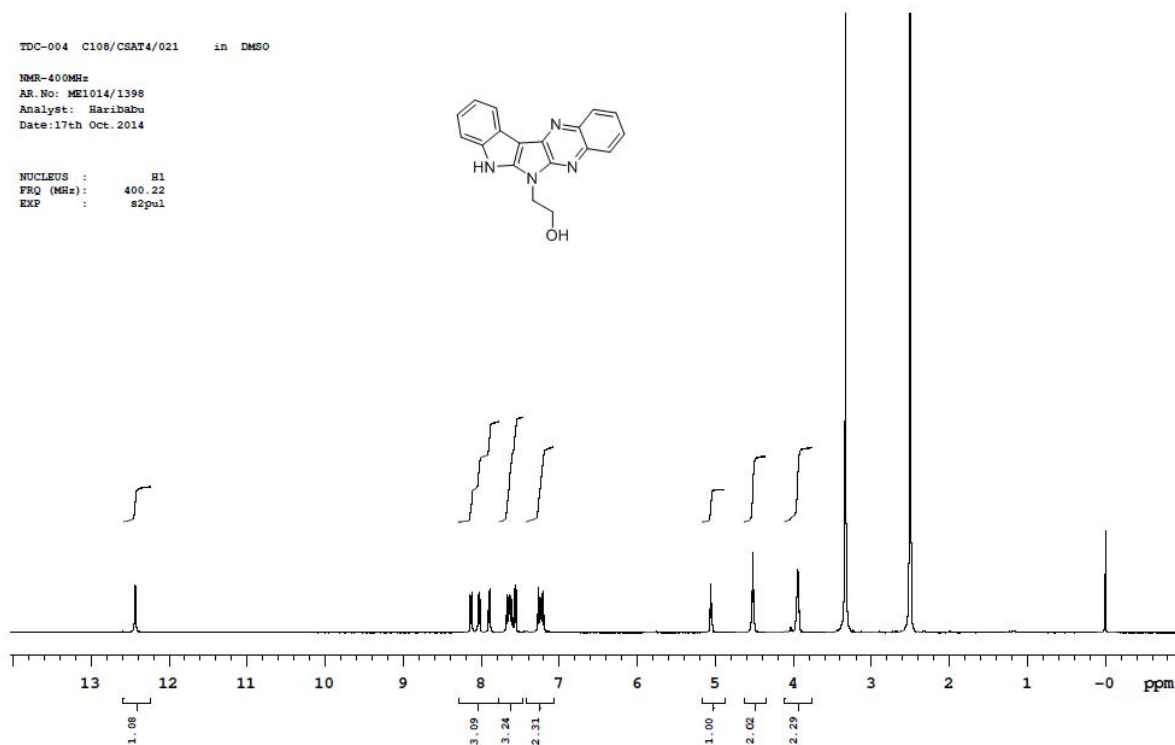
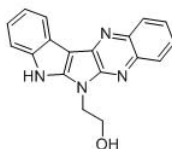
ARPA361/RN2172

R. Nagarajan
05/12/2014

TDC-004 C108/CSAT4/021 in DMSO

NMR-400MHz
AR.No: ME1014/1398
Analyst: Haribabu
Date:17th Oct.2014

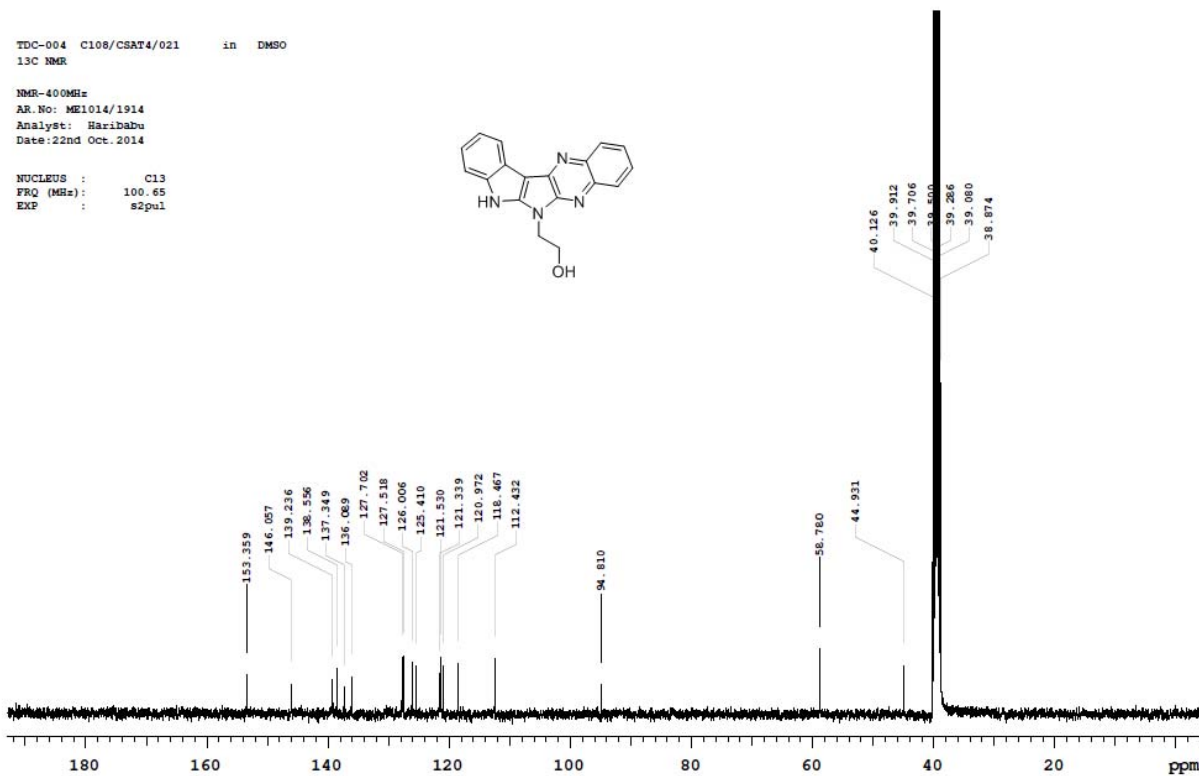
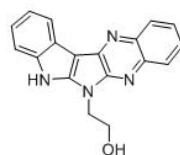
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT4/021 in DMSO
13C NMR

NMR-400MHz
AR.No: ME1014/1914
Analyst: Haribabu
Date:22nd Oct.2014

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



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

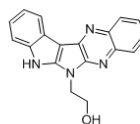
8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

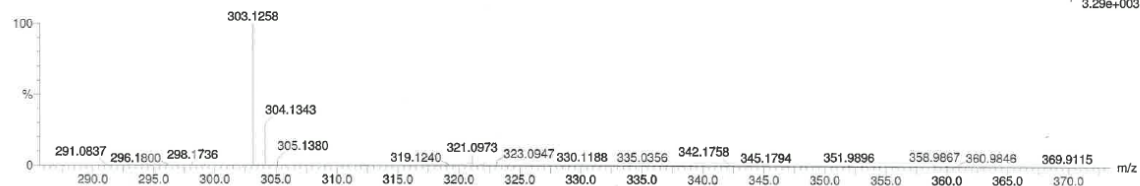
C: 0-20 H: 0-16 N: 0-5 O: 0-1

C108/CSAT4/021

141211033 16 (0.293) Cm (16-3:4)



1: TOF MS ES+
3.29e+003



Minimum:				-1.5		
Maximum:	5.0	5.0		50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
303.1258	303.1246	1.2	4.0	13.5	39.6	C18 H15 N4 O

ARD140361(RNF-1)82
R. Nagarajan 11/12/2014

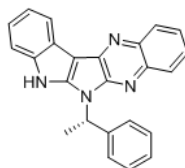
TDC-004 C108/CSAT4/022 1n DMSO

NMR-400MHz

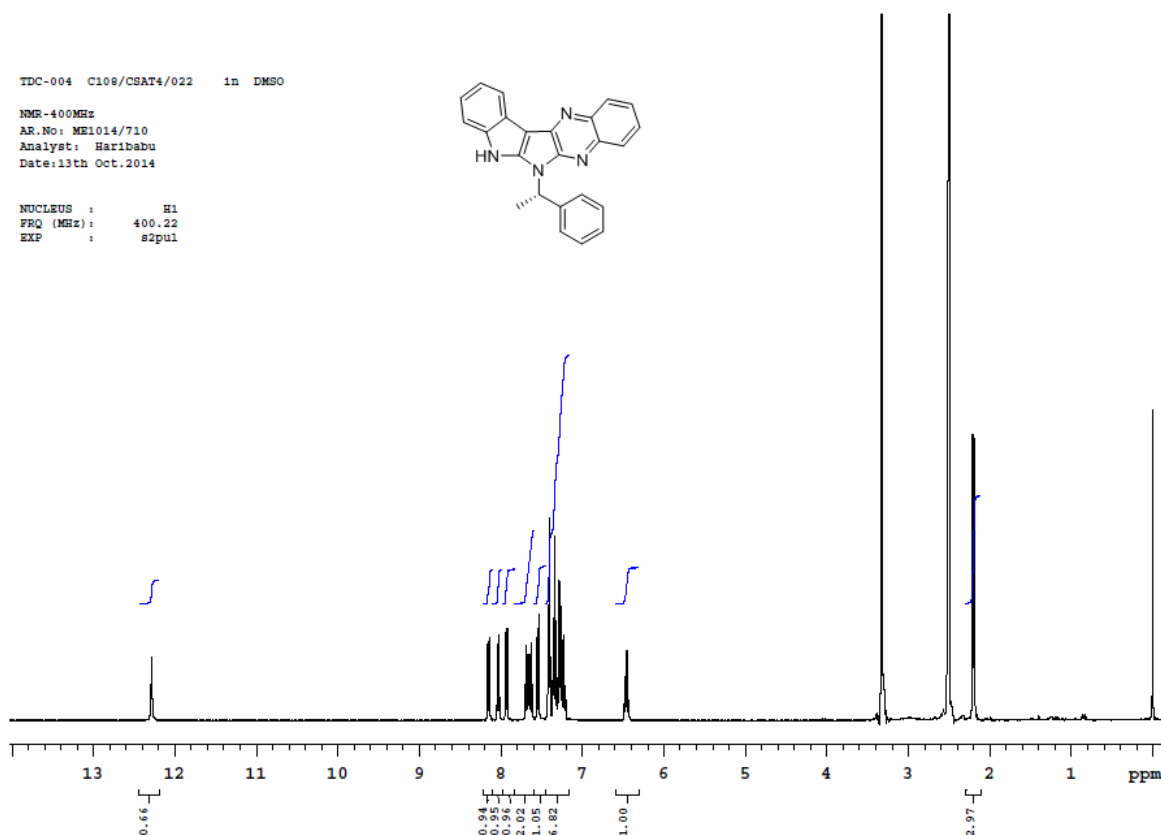
AR.No: ME1014/710

Analyst: Haribabu

Date:13th Oct.2014



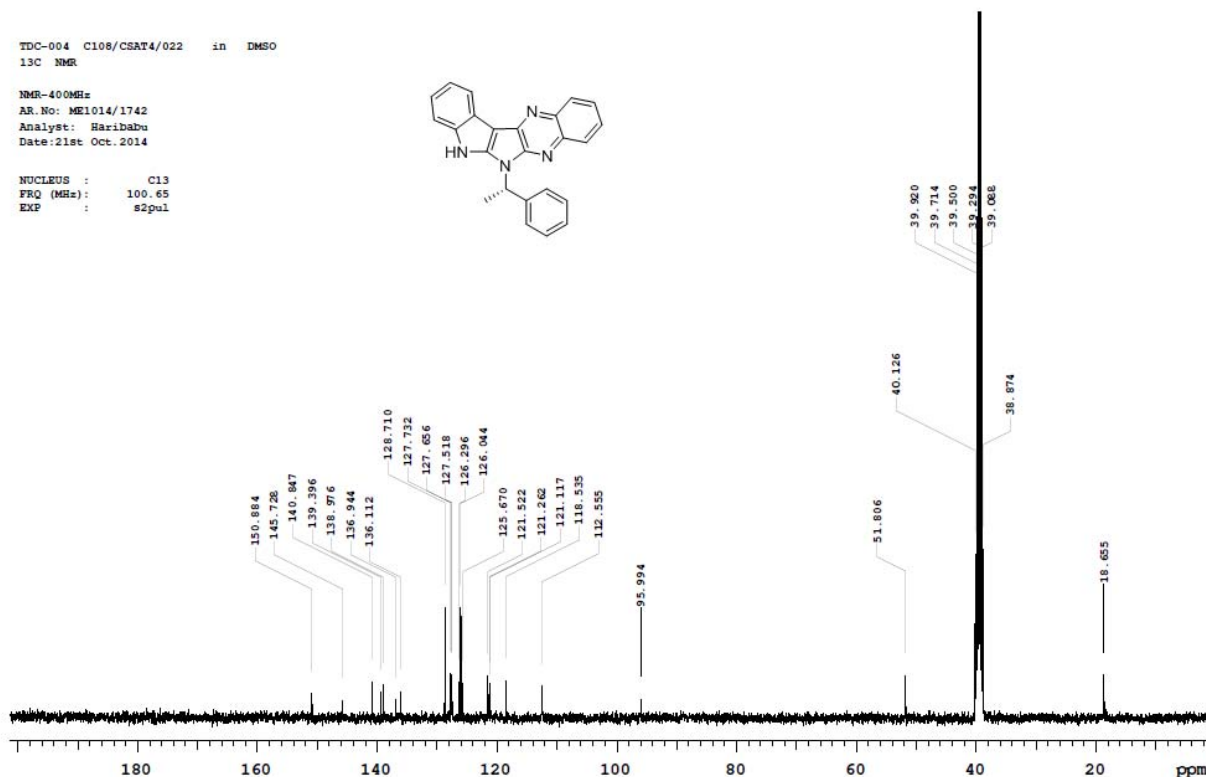
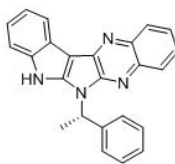
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT4/022 in DMSO
13C NMR

NMR-400MHz
AR. No: ME1014/1742
Analyst: Haridabu
Date: 21st Oct. 2014

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



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

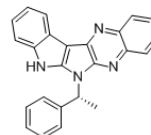
5 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

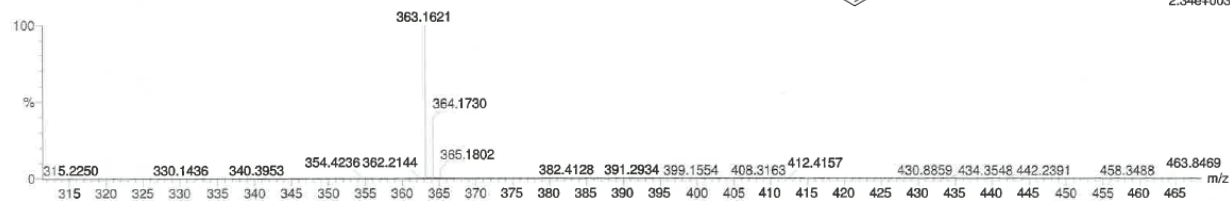
C: 0-26 H: 0-20 N: 0-5

C108/CSAT4/022

141211002 17 (0.325) Cm (17-4:5)



1: TOF MS ES+
2.34e+003



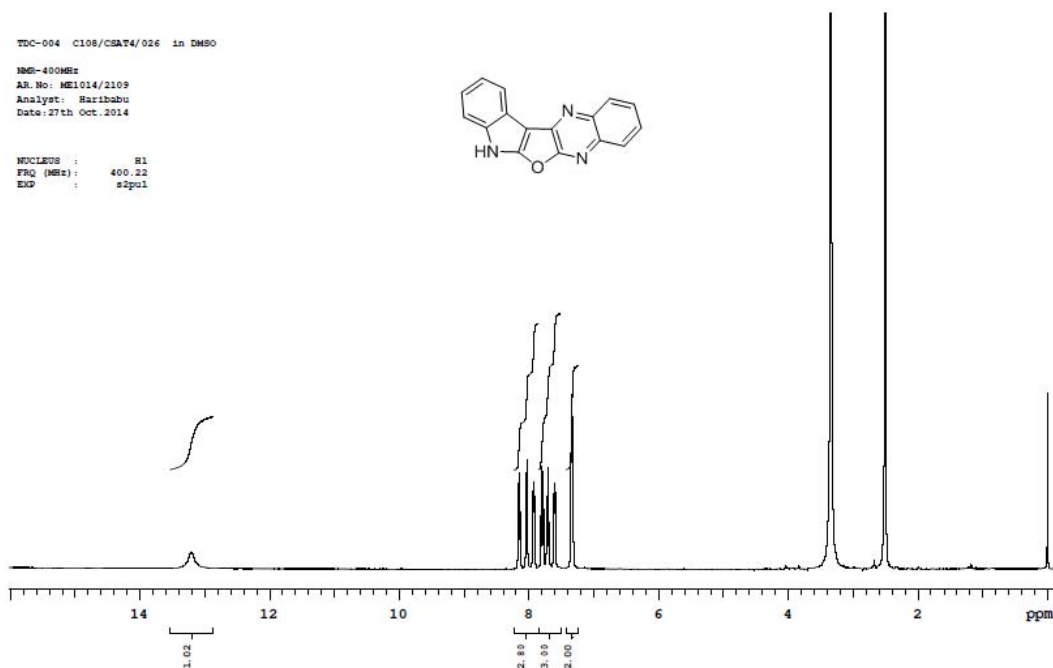
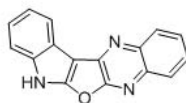
Minimum:				-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
363.1621	363.1610	1.1	3.0	17.5	34.7	C24 H19 N4

ARD40361 RNR/182
R. Nagarajan
11/12/2014

TDC-004 C108/CSAT4/026 in DMSO

NAME-400MHz
AR. No: ME1014/2109
Analyst: Haribabu
Date: 27th Oct. 2014

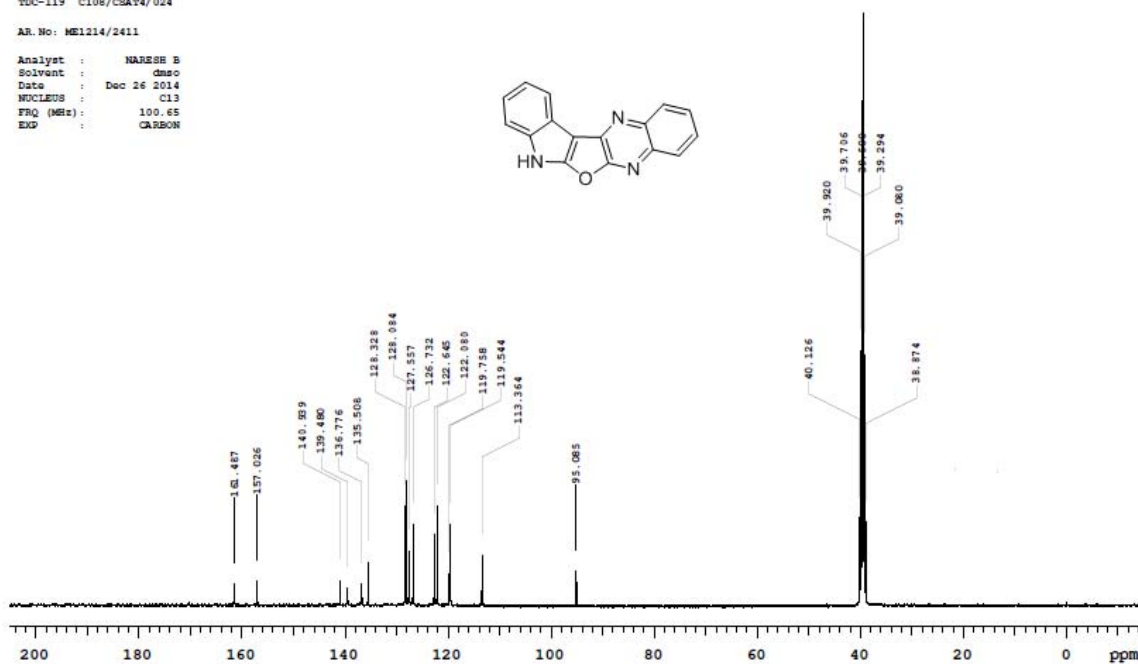
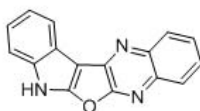
NUCLEUS : ¹H
PQ (MHz): 400.22
EXP : s2pul



TDC-119 C108/CSAT4/024

AR. No: ME1214/2411

Analyst : NARESH B
Solvent : dmsc
Date : Dec 26 2014
NUCLEUS : ¹³C
PQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

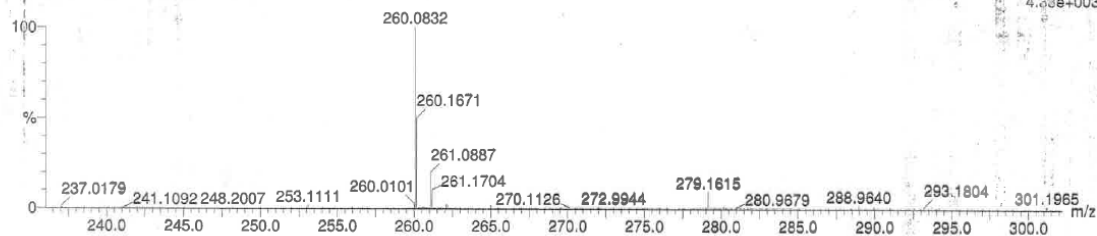
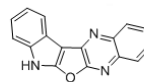
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-17 H: 0-12 N: 0-3 O: 0-1

C108/CSATY/025

141204014 32 (0.30) Cm (31:35-80:93)



1: TOF MS ES+
4.30e+003

Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
260.0832	260.0824	0.8	3.1	13.5	2.1	C16 H10 N3 O

TDC-004 C108-CSAT4-024 in DMSO

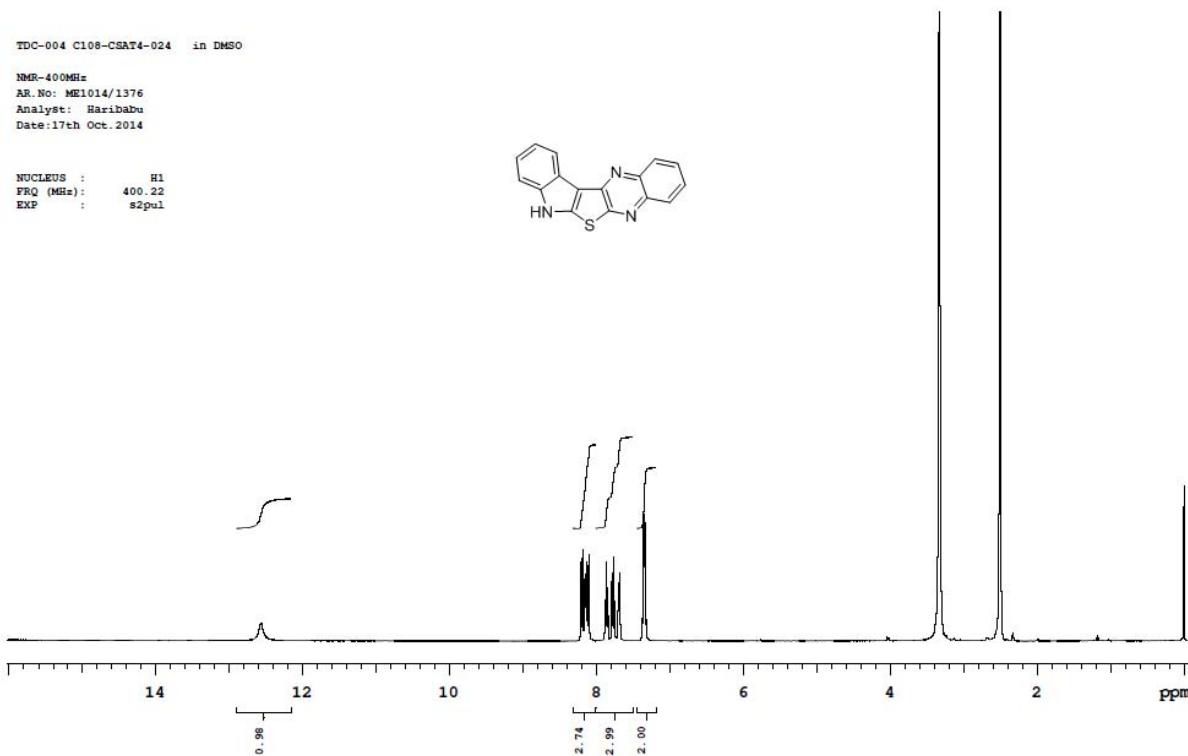
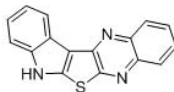
NMR-400MHz

AR.No: ME1014/1376

Analyst: Haribabu

Date: 17th Oct. 2014

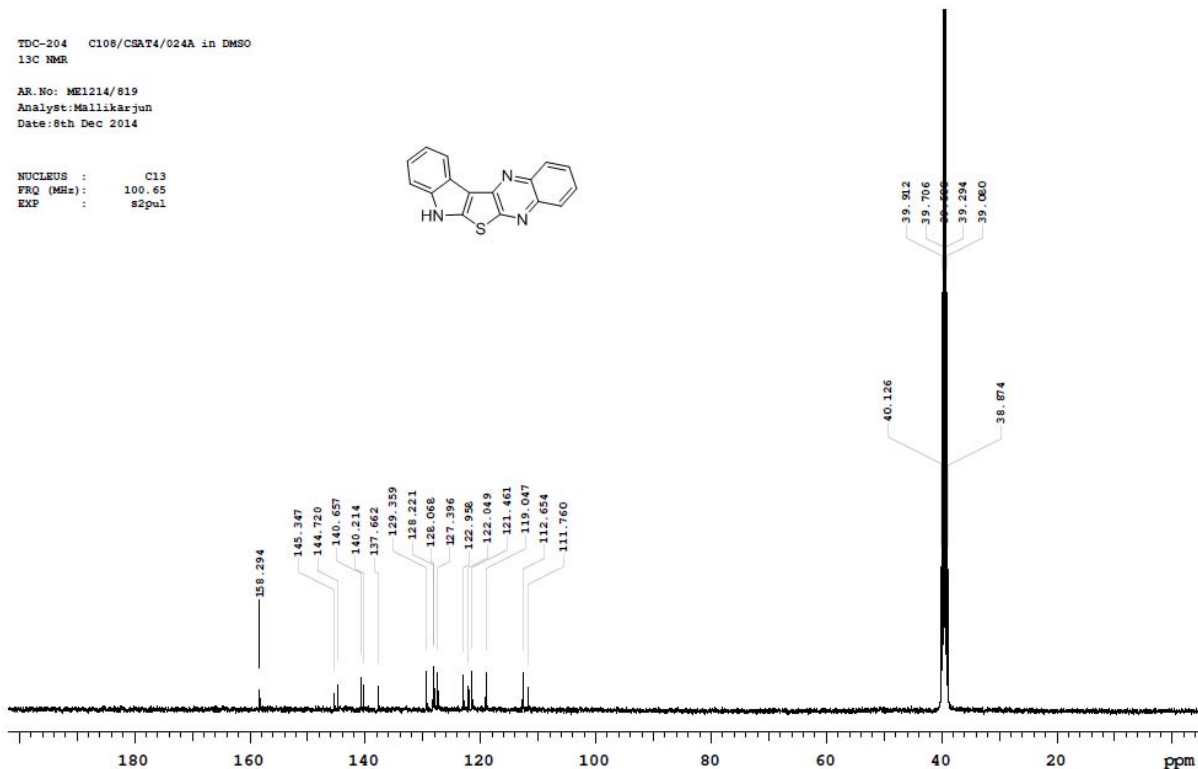
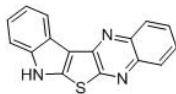
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : s2pul



TDC-204 C108/CSAT4/024A in DMSO
13C NMR

AR.No: ME1214/819
Analyst: Mallikarjun
Date: 8th Dec 2014

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



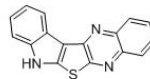
Elemental Composition Report

Page 1

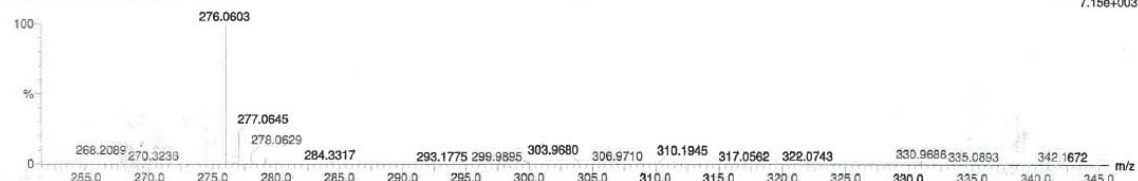
Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-18 H: 0-11 N: 0-3 S: 0-1
C108/CSATY/024
141204010 36 (0.339) Cm (36:44-77:91)



1: TOF MS ES+
7.15e+003

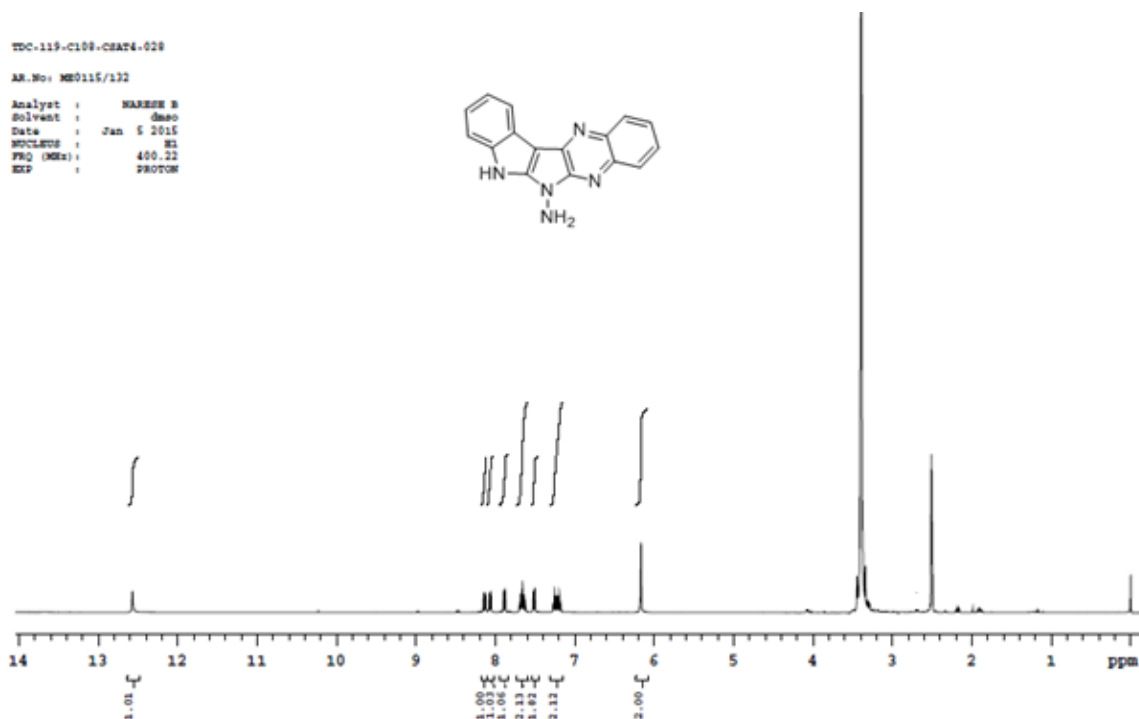
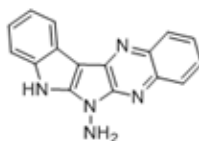


Minimum:					-1.5	
Maximum:		5.0	5.0		50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.0603	276.0595	0.8	2.9	13.5	13.3	C16 H10 N3 S

TDC-119-C108-CSAT4-028

AR.No: MD0115/132

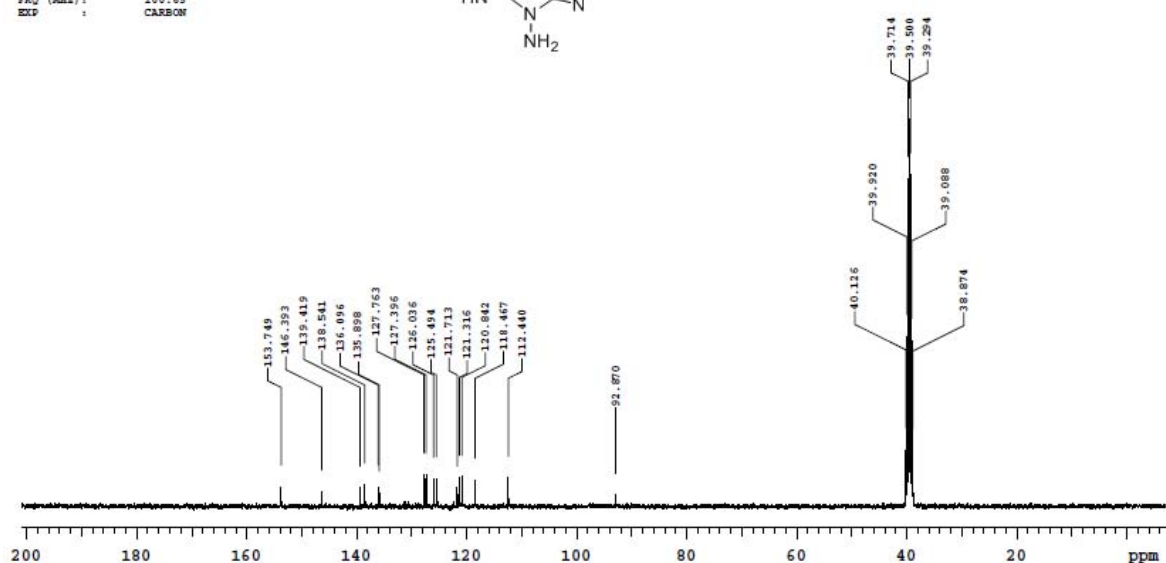
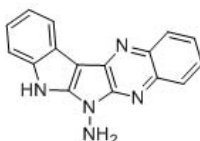
Analyst : NARESH B
Solvent : dmsc
Date : Jan 5 2015
NUCLEUS : H1
PQ (MHz) : 400.12
EXP : PROTON



TDC-117 C108/CSAT4/028

AR.No: MD0515/1083

Analyst : NARESH B
Solvent : dmsc
Date : May 14 2015
NUCLEUS : C13
PQ (MHz) : 100.65
EXP : CARBON



AURIGENE
Accelerating Discovery

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

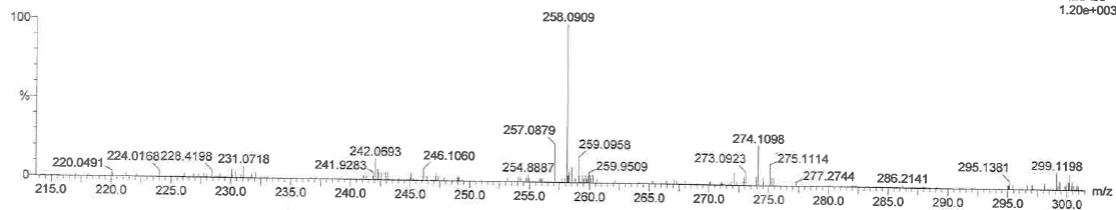
Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 0-20 H: 0-15 N: 0-9 I: 0-1

150106014 24 (0.542) Cm (24:28-45:55)

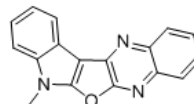
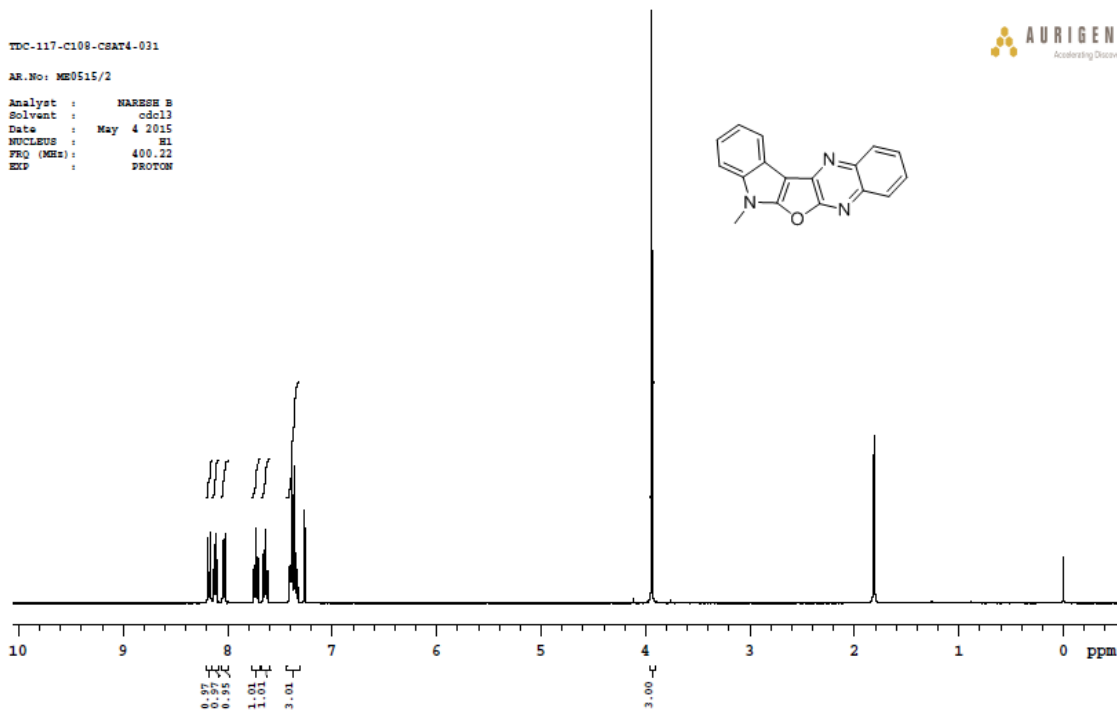
1: TOF MS ES+
1.20e+003

Minimum:						
Maximum:	5.0	10.0	-1.5			
			80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
274.1098	274.1093	0.5	1.8	13.5	n/a	C16 H12 N5

TDC-117-C108-CSAT4-031

AR.No: ME0515/2

Analyst : NARESH B
 Solvent : cdcl3
 Date : May 4 2015
 NUCLEUS : H1
 FREQ (MHz) : 400.22
 EXP : PROTON

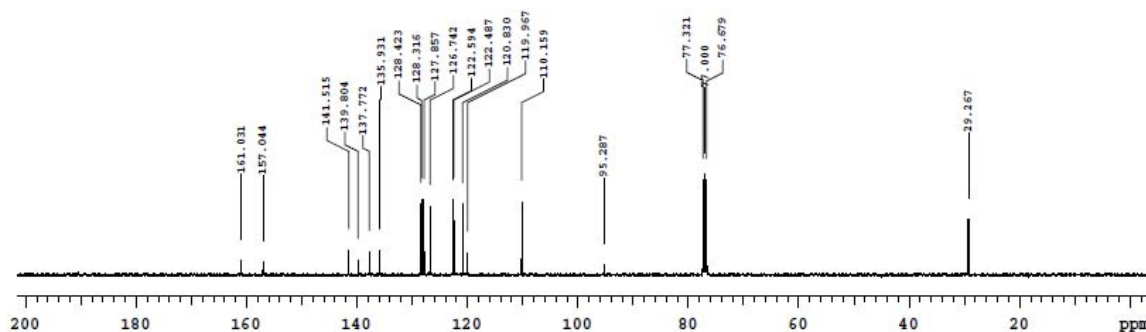
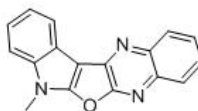

AURIGENE
 Accelerating Discovery


TDC-117 C108/CSAT4/031



AR.No: ME0515/381

Analyst : NARESH B
Solvent : cdcl3
Date : May 7 2015
NUCLEUS : C13
PFO (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

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

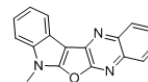
25 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)

Elements Used:

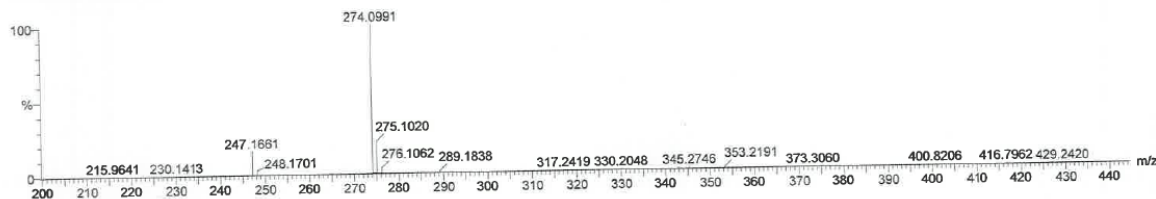
C: 0-21 H: 0-25 N: 0-3 O: 0-2

C108/CSAT4/031

150506002 21 (0.580) Cm (21:24-42:48x0.500)



1: TOF MS ES+
4.12e+004



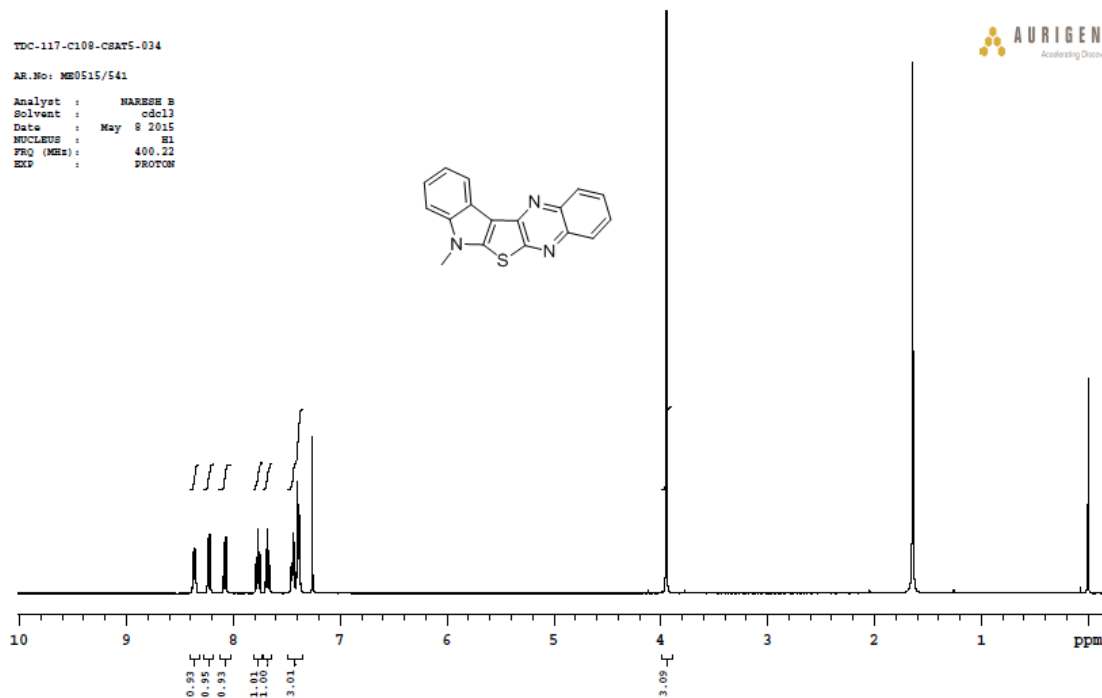
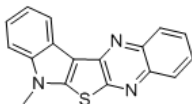
Minimum:					-1.5	
Maximum:		5.0	5.0		80.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
274.0991	274.0980	1.1	4.0	13.5	113.0	C17 H12 N3 O

R. Nagaraj
06/05/2015

TDC-117-C108-CSAT5-034

AR.No: ME0515/541

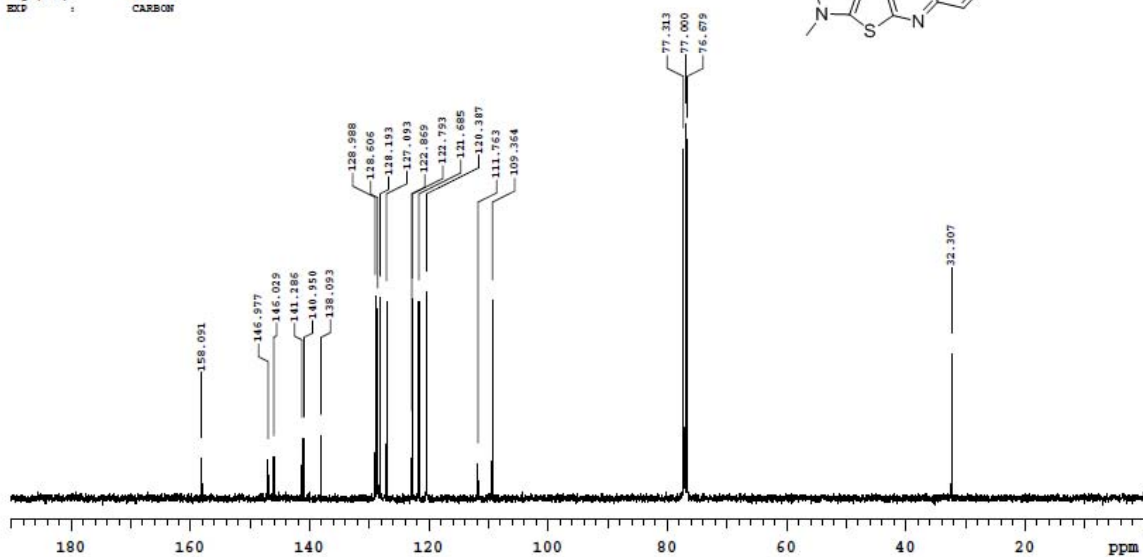
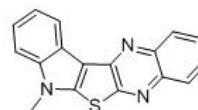
Analyst : HARESH B
Solvent : cdcl3
Date : May 8 2015
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON



TDC-117 C108/CSAT5/034

AR.No: ME0515/557

Analyst : Mallikarjun
Solvent : cdcl3
Date : May 9 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

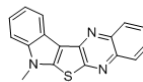
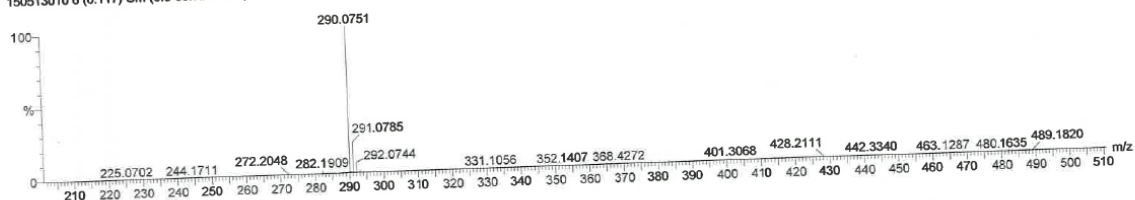
Monoisotopic Mass, Even Electron Ions
122 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

C: 0-21 H: 0-13 N: 0-5 O: 0-5 S: 0-2

C108/CSAT4/034

150513010 6 (0.117) Cm (6:8-63:72x0.500)

1: TOF MS ES+
1.69e+005

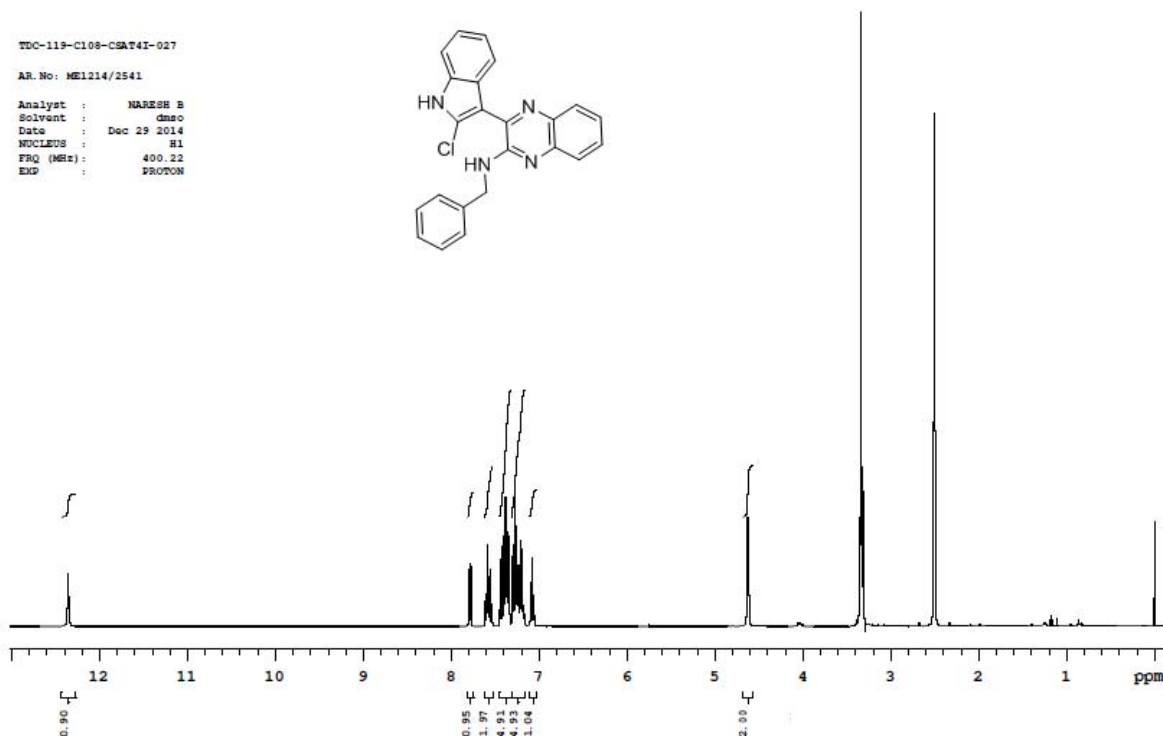
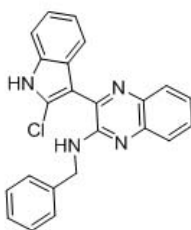
Minimum:				-1.5		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0751	290.0752	-0.1	-0.3	13.5	6.7	C17 H12 N3 S

R. Nagaraju
15/05/2015

TDC-119-C108-CSAT4I-027

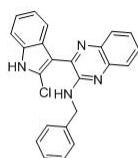
AR. No: ME1214/2541

Analyst : NARESH B
 Solvent : dmsc
 Date : Dec 29 2014
 NUCLEUS : H1
 PRQ (MHz): 400.22
 EXP : PROTON

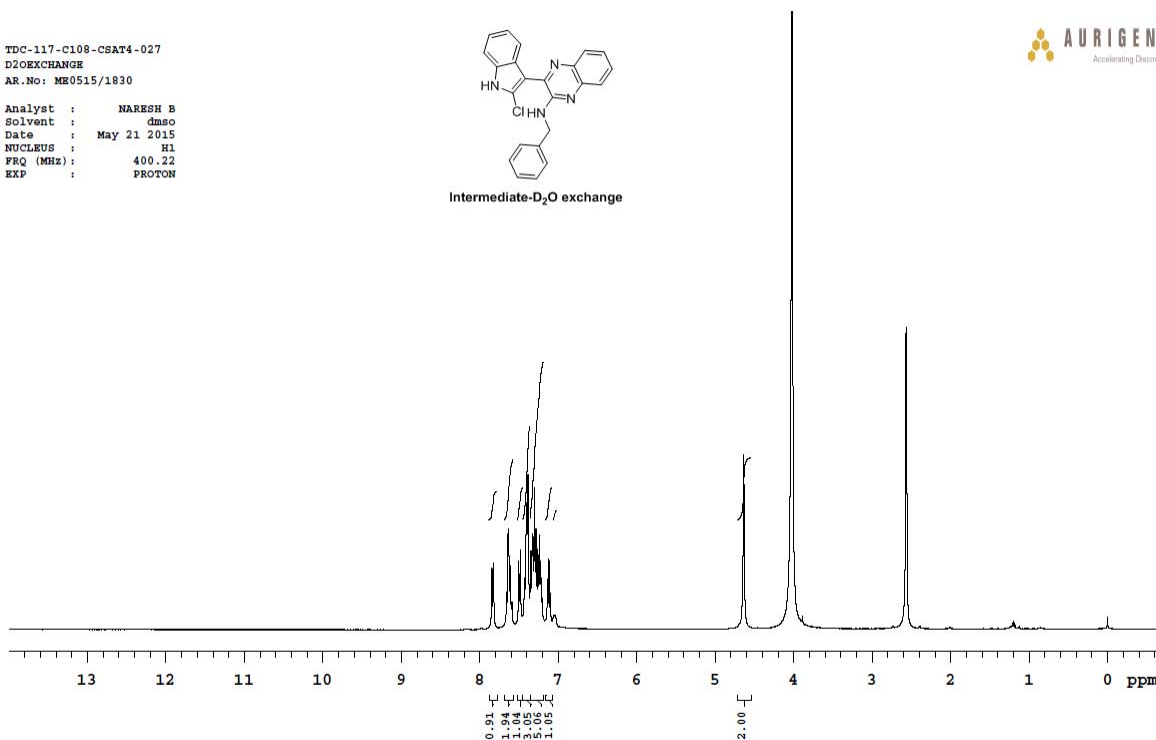


TDC-117-C108-CSAT4-027
D2OEXCHANGE
AR.No: ME0515/1830

Analyst : NARESH B
Solvent : dmsc
Date : May 21 2015
NUCLEUS : H1
FREQ (MHz) : 400.22
EXP : PROTON



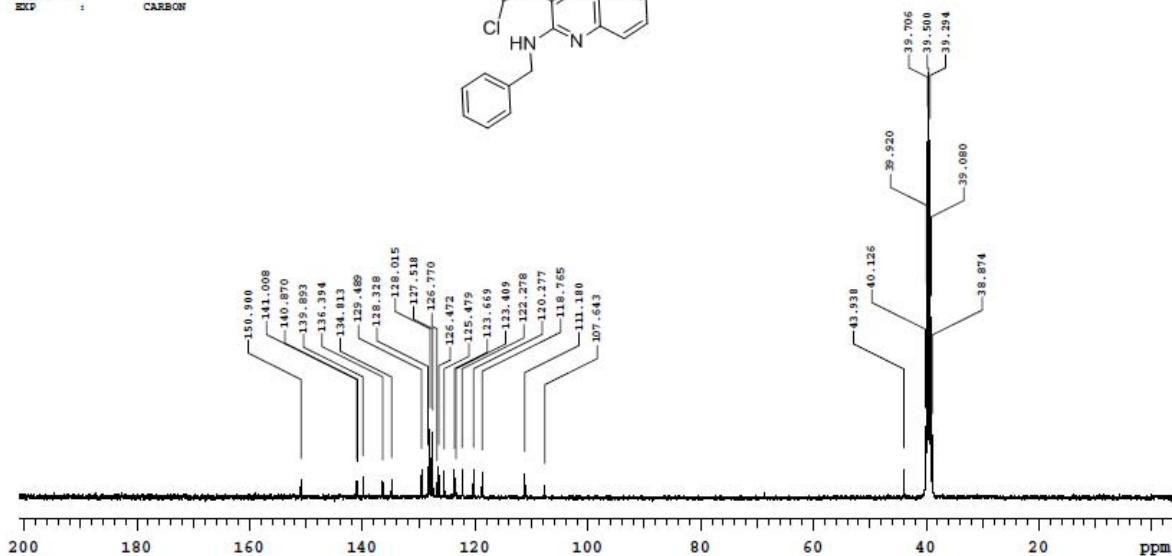
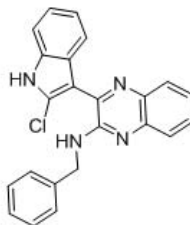
Intermediate-D₂O exchange



TDC-119 C108/CSAT41/027

AR.No: ME0115/561

Analyst : HARESH B
Solvent : dmso
Date : Jan 8 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

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

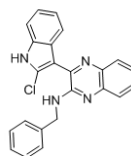
28 formula(e) evaluated with 1 results within limits (up to 5 best isotopic matches for each mass)

Elements Used:

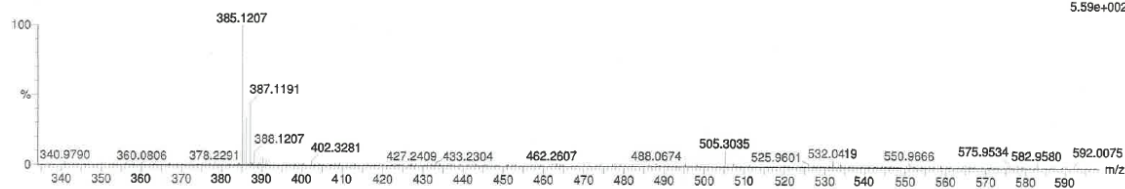
C: 0-24 H: 0-20 N: 0-5 Cl: 0-3

C108/CSAT41/027

141230002 72 (0.679) Cm (69:72-101:108)



1: TOF MS ES+
5.59e+002



Minimum:						
Maximum:	5.0	5.0		-1.5	80.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
385.1207	385.1220	-1.3	-3.4	16.5	2.9	C23 H18 N4 Cl

ARD14061 RNR/200

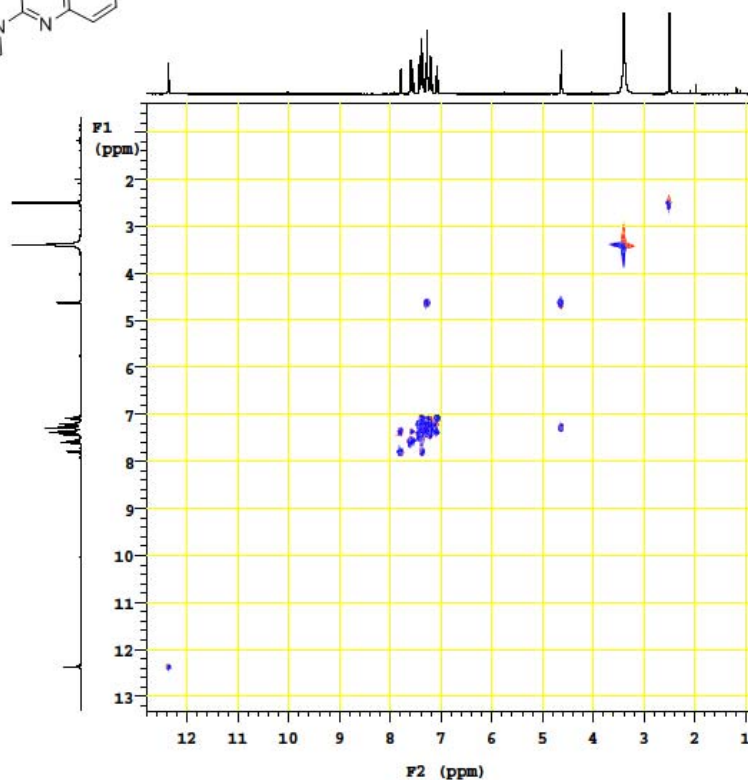
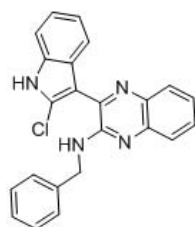
R. Nagarajan
30/12/2014

TDC-119-C108-CSAT41-027

AR.No: ME0115/1109

exp6 gDQCOBY

SAMPLE		FLAGS	
date	Jan 17 2015	hs	nn
solvent	dmsd	sepul	y
sample	TDC-119-C108	haglvl	1152
0-CSAT41-027_1109_		SPECIAL	
01	temp	25.0	
ACQUISITION		gain	18
sv	6410.3	spin	not used
at	0.150	F2 PROCESSING	
np	1918	sb	-0.125
fb	not used	sbs	-0.100
ss	32	lsfid	-10
dl	1.000	fn	2048
nt	15	F1 PROCESSING	
2D ACQUISITION		sb1	0.044
sw1	6410.3	sb1	-0.042
ni	200	procl	1p
PREGATURATION		fn1	2048
satmode	n	DISPLAY	
wet	n	sp	348.3
TRANSMITTER		wp	4776.4
tn	H1	sp1	154.2
sfrq	400.223	wp1	5170.8
tof	391.7	rf1	797.3
tpwr	52	rfp	0
pw	10.100	rf11	797.3
GRADIENTS		rfp1	0
gplvlb	771	PLOT	
gtE	0.001000	wc	139.3
gstab	0.000500	sc	10.0
DECOUPLER		wc2	139.3
dn	C13	sc2	0
ds	nnn	vs	359
	ai	th	4
		ph	



CI08/CSAT41/027 in DMSO
TDC-119

AR.No:IN1214/123
Date: 31st Dec.2014
Analyst: Mallikharjun

NUCLEUS : ¹H
FREQ (MHz): 499.63
EXP : NOESY1D

