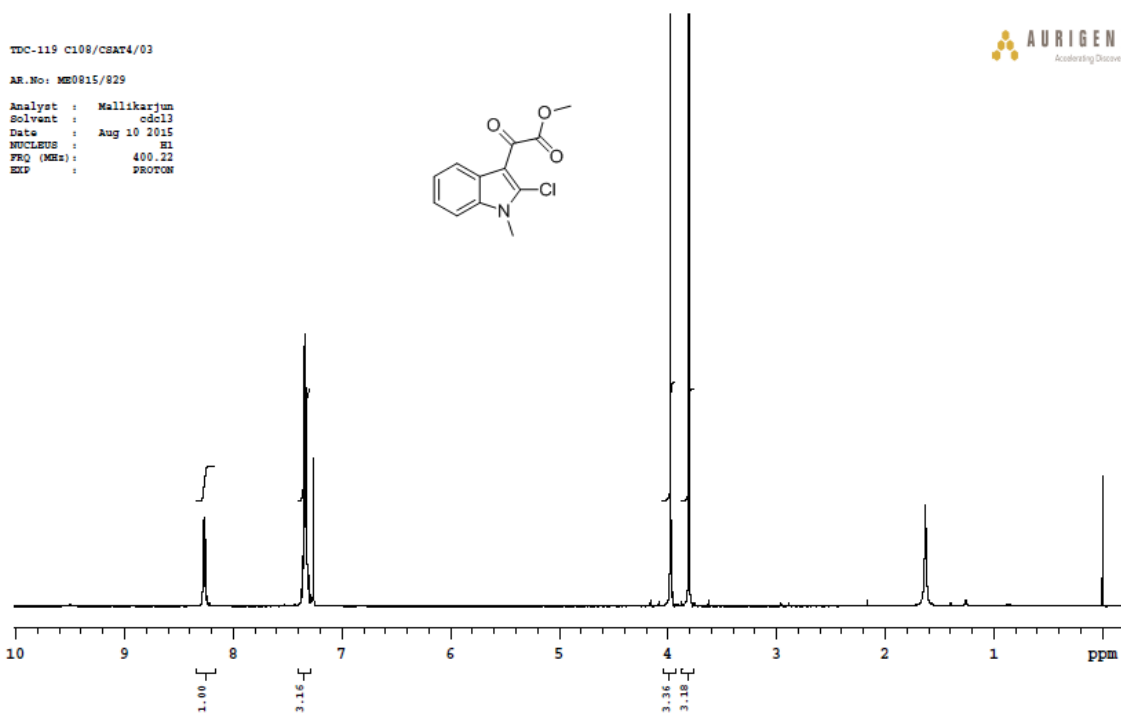


Copies of spectra

N-substituted- 2-(2-chloro-1H-indol-3-yl)-2-oxoacetate (1a-h)



AURIGENE
Accelerating Discovery

TDC-119 C108/CSAT4/031

AR.No: ME0815/1448

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 15 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON

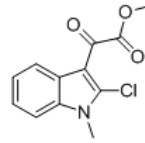
AURIGENE
Accelerating Discovery

Elemental Composition Report

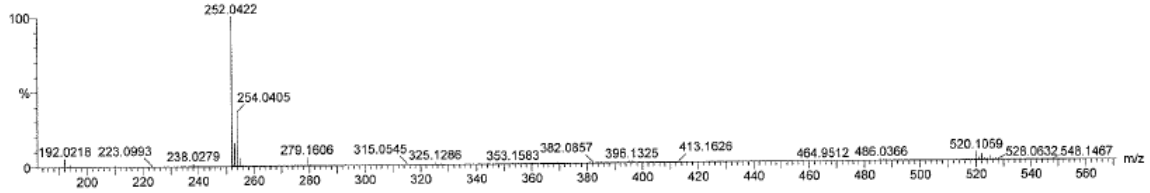
Single Mass Analysis

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
 56 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)
 Elements Used:
 C: 0-25 H: 0-25 N: 0-2 O: 0-3 Cl: 0-1
 C108/CSAT4/031
 150811009 9 (0.178) Cm (9-10)



1: TOF MS ES+
 4.20e+004

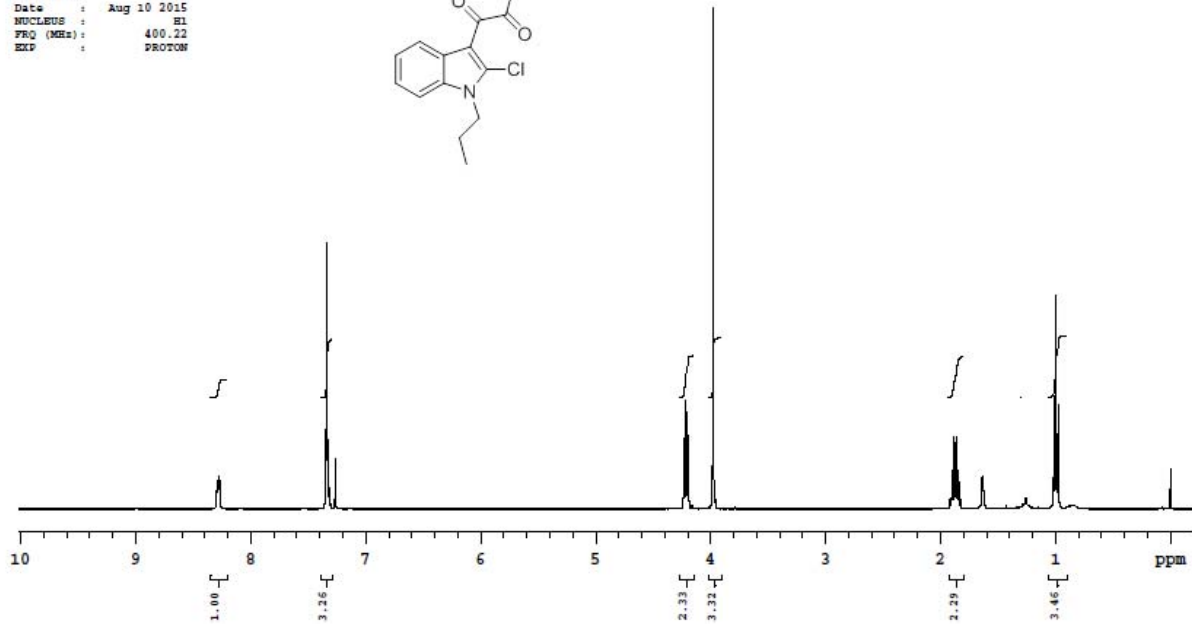
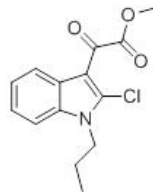


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.0422	252.0427	-0.5	-2.0	7.5	24.0	C12 H11 N O3 Cl

TIC-119 C108/CSAT4/033

AR.No: ME0815/830

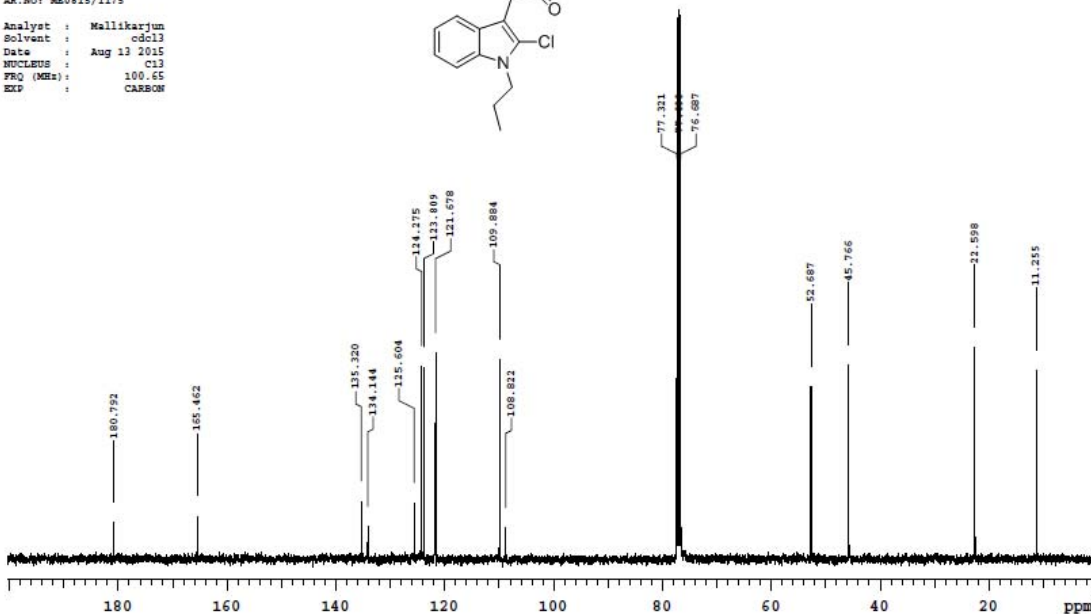
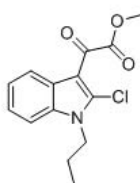
Analyst : Mallikarjun
 Solvent : cdcl3
 Date : Aug 10 2015
 NUCLEUS : H1
 PRQ (MHz): 400.22
 EXP : PROTON



TDC-119 C08/CSAT4/033

AR.No: ME0815/1175

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 13 2015
NUCLEUS : C13
PQ2 (MHz) : 100.62
EXP : CARBON



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 7.0 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

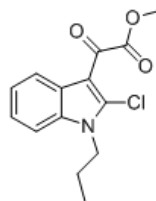
36 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)

Elements Used:

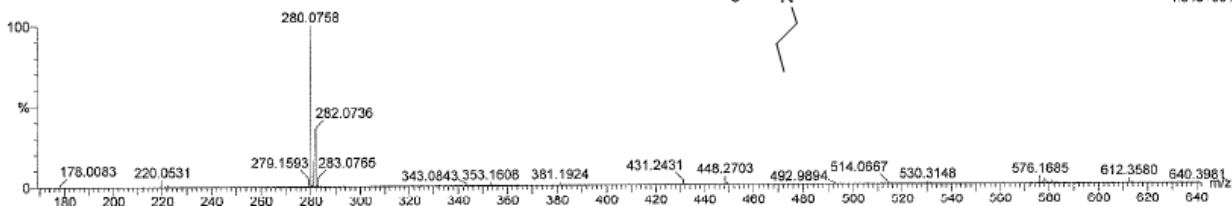
C: 0-18 H: 0-25 N: 0-2 O: 0-3 Cl: 0-1

C108/CSAT4/033

150811010.8 (0.145) Cm (8:9)



1: TOF MS ES+
4.84e+004



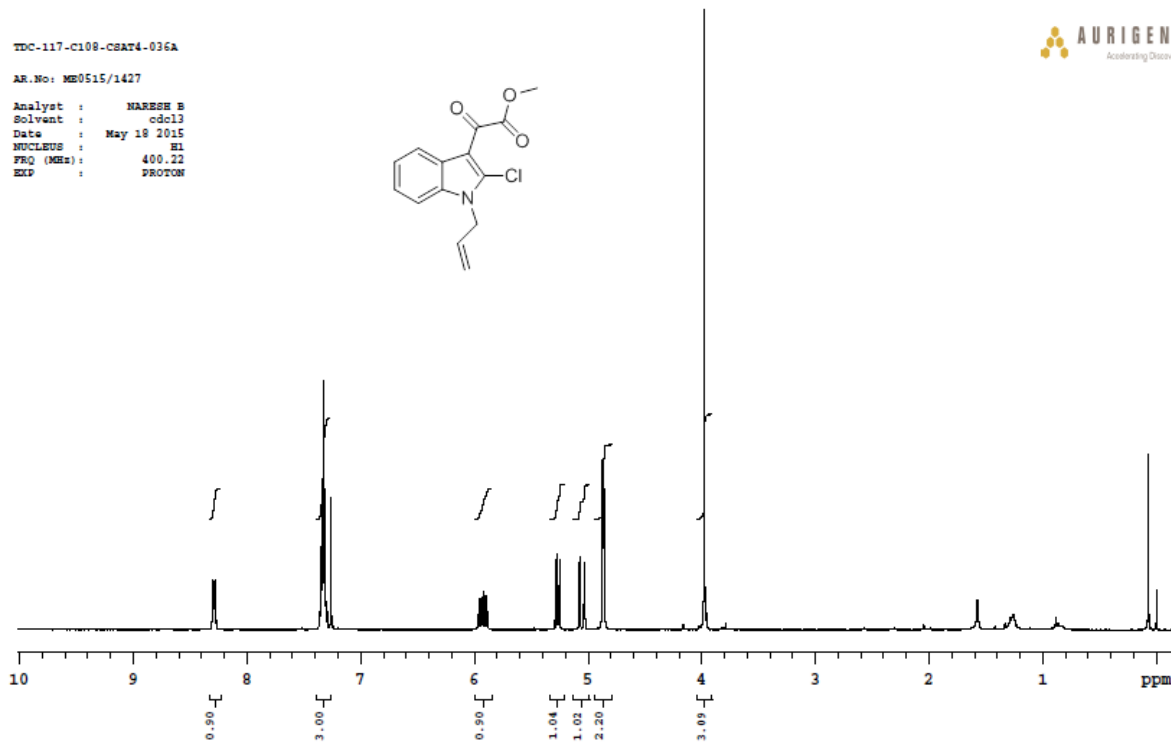
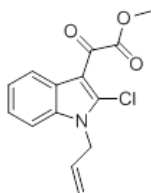
Minimum: -1.5
Maximum: 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
280.0758	280.0740	1.8	6.4	7.5	7.8	C14 H15 N O3 Cl

TDC-117-C108-CSAT4-036A

AR.No: MB0515/1427

Analyst : NARESH B
Solvent : cdcl3
Date : May 18 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

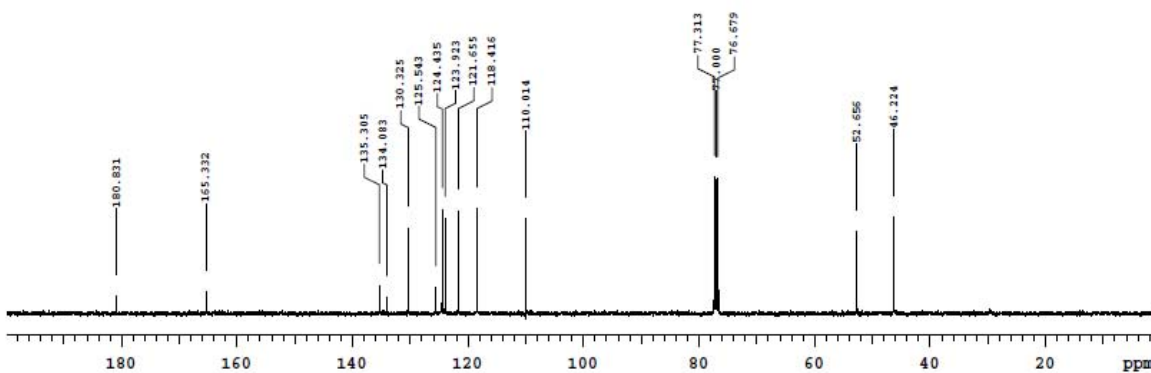
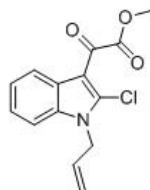


AURIGENE
Accelerating Discovery

TDC-117 C108/CSAT4/036A

AR.No: MB0515/2035

Analyst : Mallikarjun
Solvent : cdcl3
Date : May 23 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



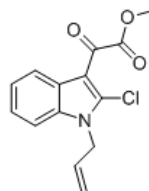
AURIGENE
Accelerating Discovery

Elemental Composition Report

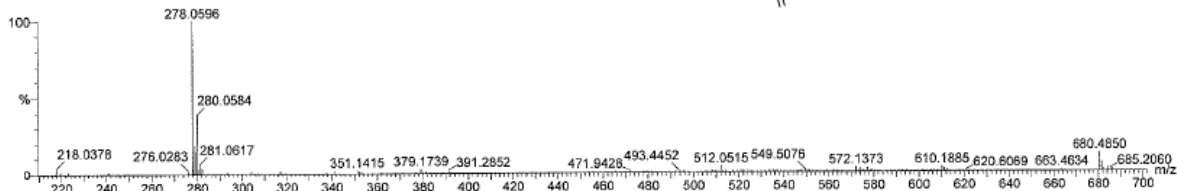
Single Mass Analysis

Tolerance = 7.0 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
 36 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)
 Elements Used:
 C: 0-18 H: 0-25 N: 0-2 O: 0-3 Cl: 0-1
 C108/CSAT4/036
 150811011 22 (0.413) Cm (22:24)



1: TOF MS ES+
 3.48e+004



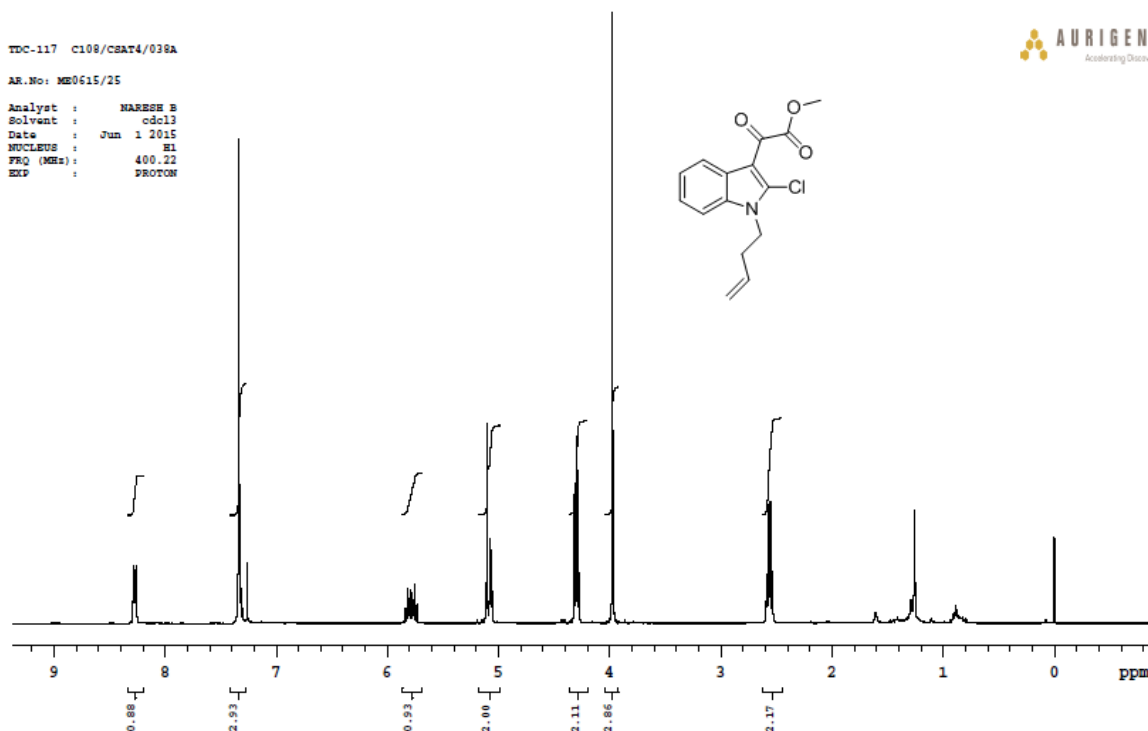
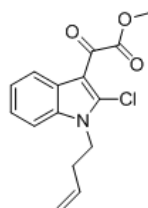
Minimum: -1.5
 Maximum: 5.0 7.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
278.0596	278.0584	1.2	4.3	8.5	60.5	C14 H13 N O3 Cl

TDC-117 C108/CSAT4/038A

AR.No: ME0615/25

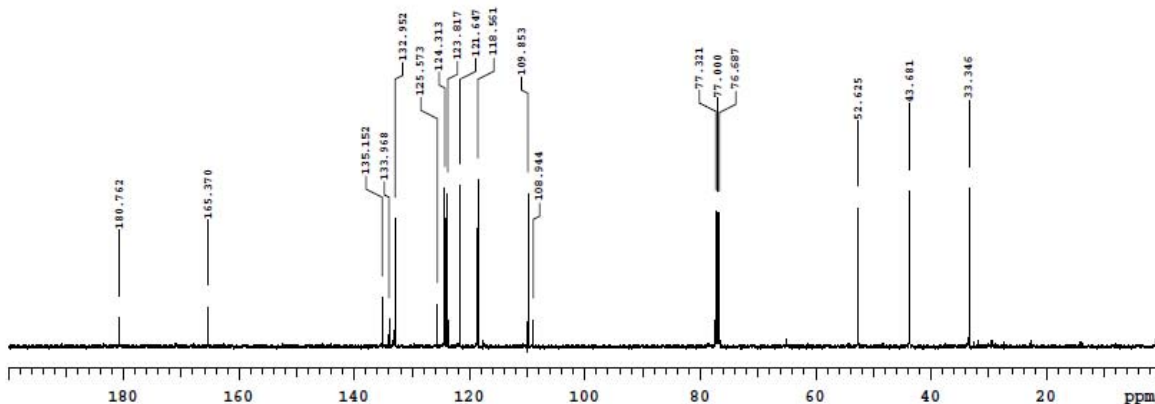
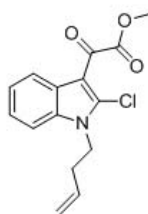
Analyst : HARSH B
 Solvent : cdcl3
 Date : Jun 1 2015
 NUCLEUS : H1
 FREQ (MHz): 400.22
 EXP : PROTON



TDC-117 C108/CSAT4/038A

AR.No: ME0515/477

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jun 5 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON

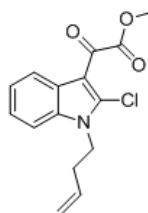


Elemental Composition Report

Page 1

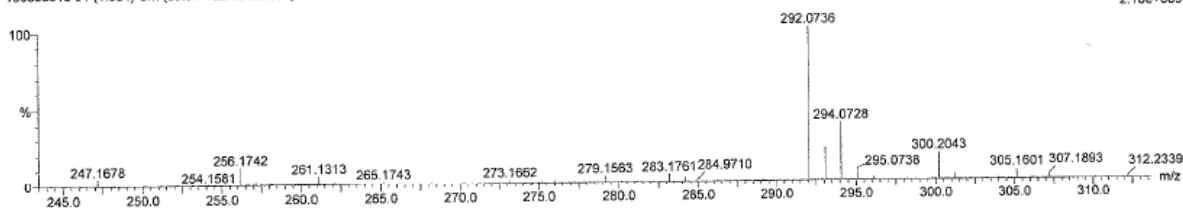
Single Mass Analysis

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
55 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
Elements Used:
C: 0-18 H: 0-19 N: 0-2 O: 0-4 Cl: 0-2
C108/CSAT4/038
150603013 91 (1.684) Cm (89.91-102:104x0.500)

1: TOF MS ES+
2.18e+003



Minimum: -1.5
Maximum: 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.0736	292.0740	-0.4	-1.4	8.5	6.4	C15 H15 N O3 Cl

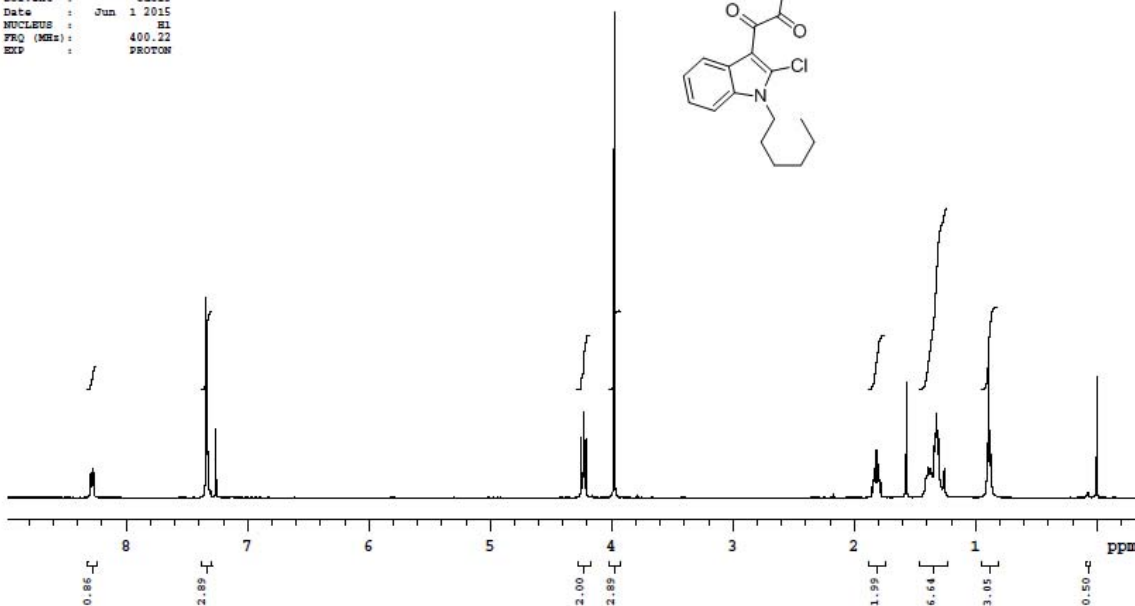
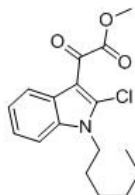
R. Nagarajan 03/06/2015

TDC-117 C108/CSAT4/035



AR.No: MB0615/24

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jun 1 2015
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON

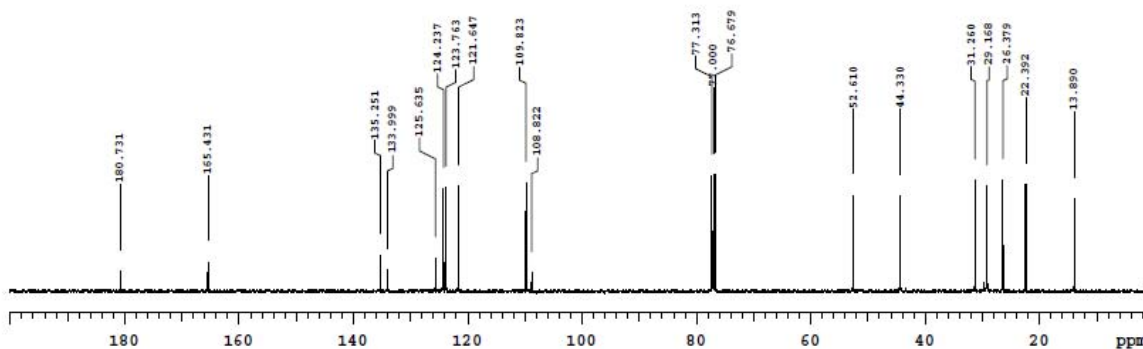
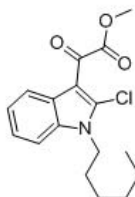


TDC-117 C108/CSAT4/035A



AR.No: MB0615/359

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jun 5 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON

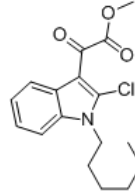


Elemental Composition Report

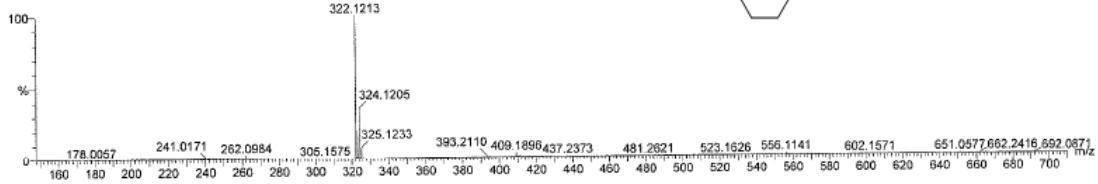
Single Mass Analysis

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
 163 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
 Elements Used:
 C: 0-21 H: 0-25 N: 0-3 O: 0-6 Cl: 0-2
 C108/CSAT4/035
 150603009 39 (0.723) Cm (39.44-93:104x0.500)



1: TOF MS ES+
 1.28e+005



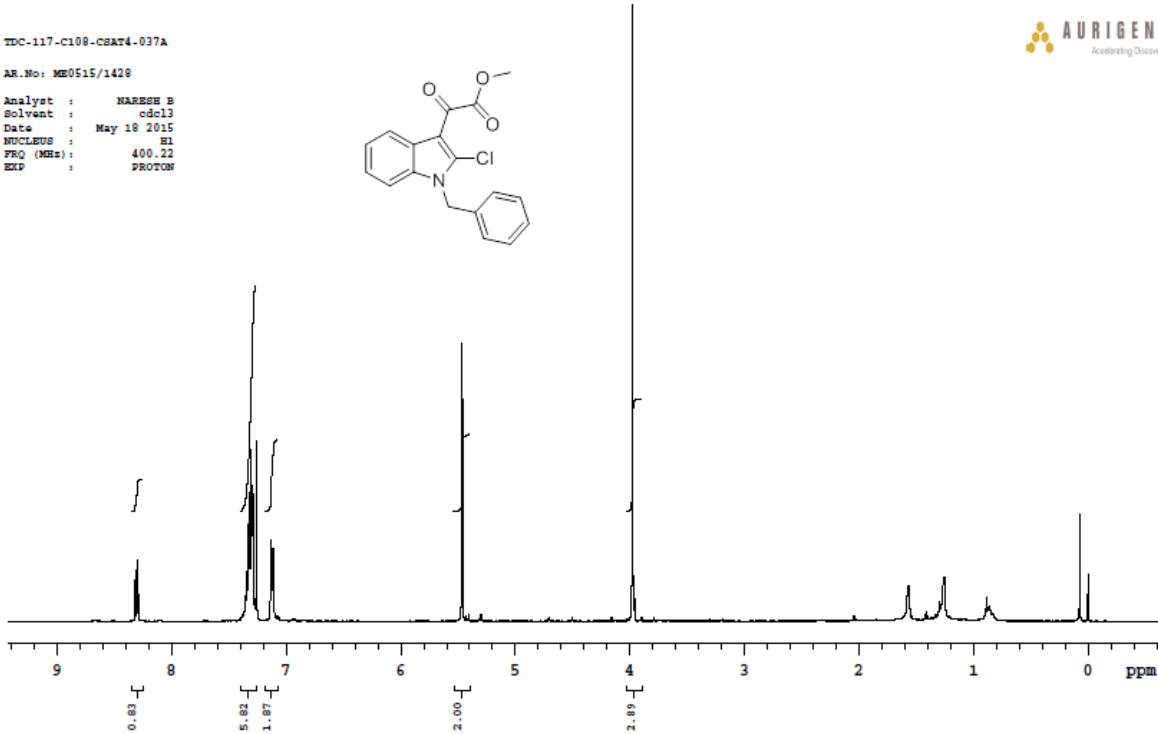
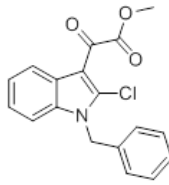
Mass	Calc. Mass	mDa	PPM	DBE	I-FIT	Formula
322.1213	322.1210	0.3	0.9	7.5	3.5	C17 H21 N O3 Cl

R. Nagarajan
 03/06/2015

TDC-117-C108-CSAT4-037A

AR.No: ME0515/1428

Analyst : NARSH B
 Solvent : cdcl3
 Date : May 18 2015
 NUCLEUS : H1
 FREQ (MHz): 400.22
 EXC : PROTON

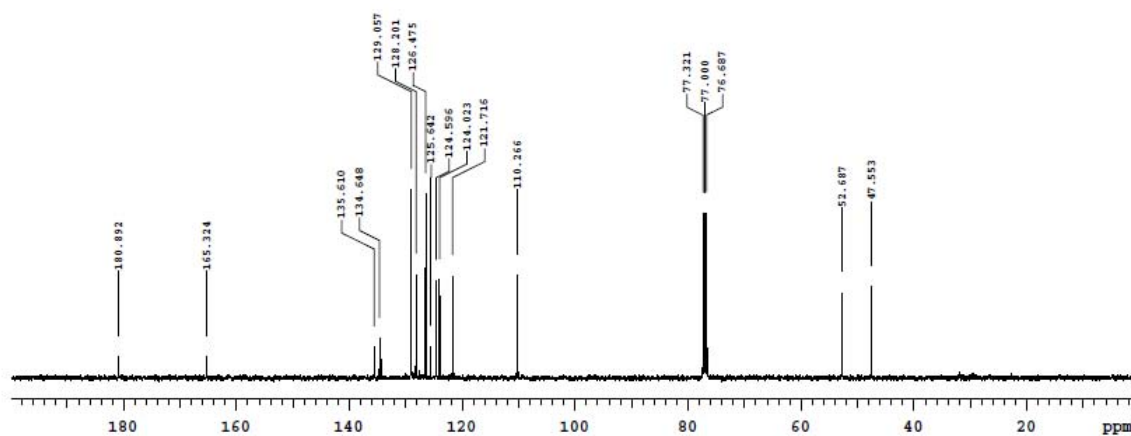
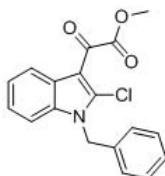


TDC-117 C108/CSAT4/037A



AR.No: ME0515/2036

Analyt : Mallikarjun
Solvent : cdcl3
Date : May 23 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

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

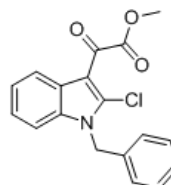
19 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)

Elements Used:

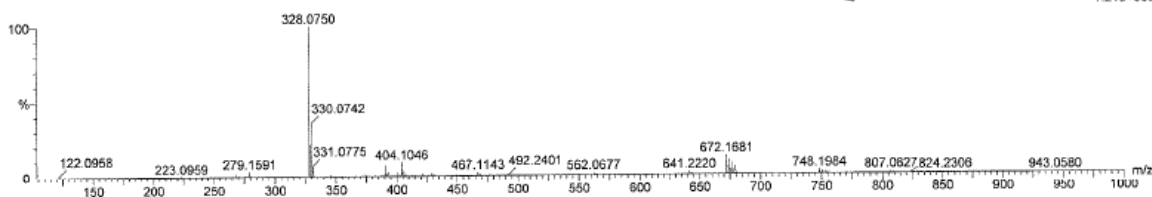
C: 0-18 H: 0-25 N: 0-2 O: 0-3 Cl: 0-1

C108/CSAT4/037

150811013 17 (0.326) Cm (16:18)



1: TOF MS ES+
1.21e+005



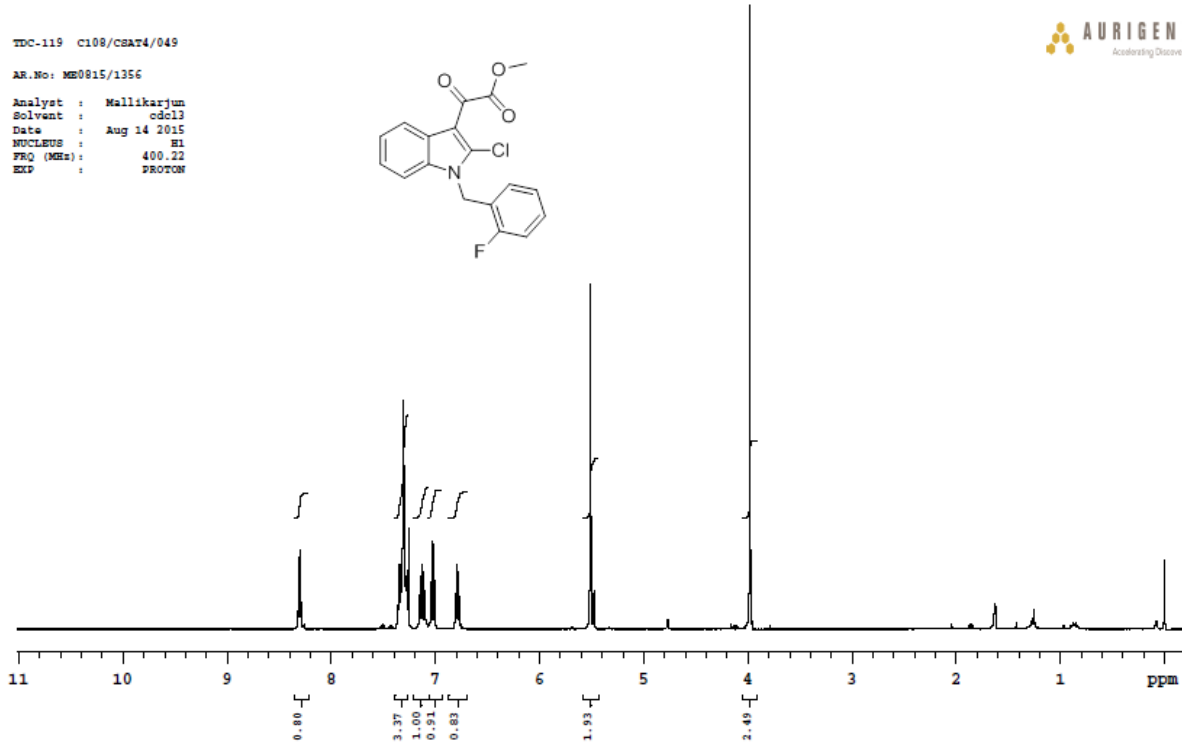
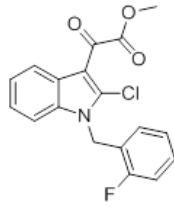
Minimum: 80.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.0750	100.00	328.0740	1.0	3.0	11.5	30.4	C18 H15 N O3 Cl

TDC-119 C108/CSA74/049

AR.No: ME0815/1356

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 14 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

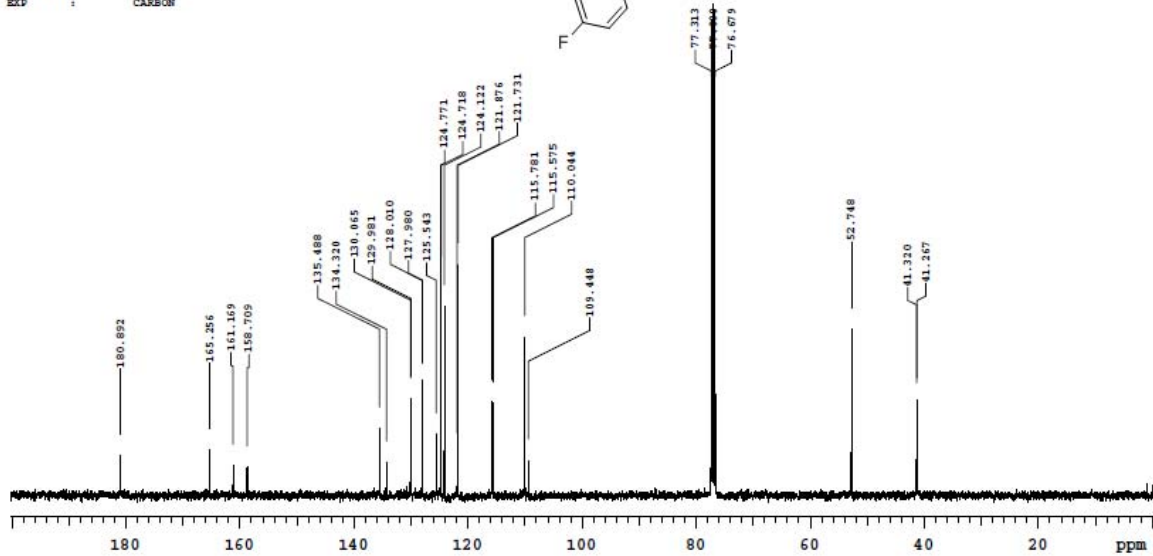
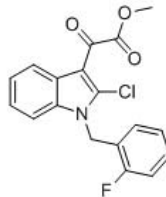


AURIGENE
Accelerating Discovery

TDC-119 C108/CSA74/049

AR.No: ME0815/1450

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 15 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON

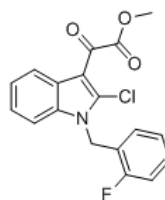


AURIGENE
Accelerating Discovery

Elemental Composition Report

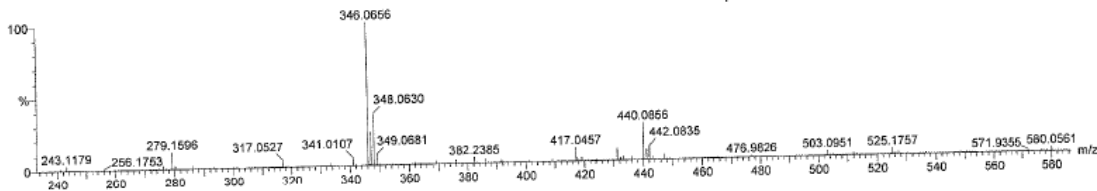
Single Mass Analysis

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
 327 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
 Elements Used:
 C: 0-23 H: 0-35 N: 0-2 O: 0-4 F: 0-1 Cl: 0-3
 C108/CSAT4/049
 150826002 28 (0.515) Cm (28.31)

1: TOF MS ES+
 2.79e+004



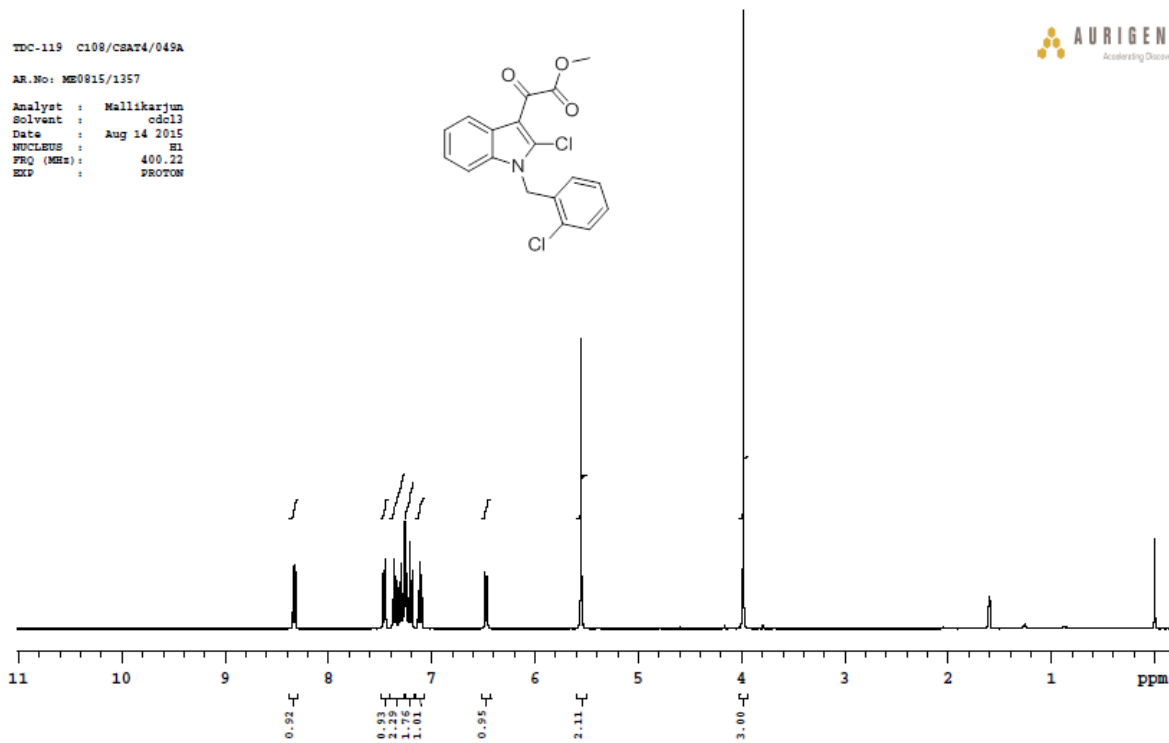
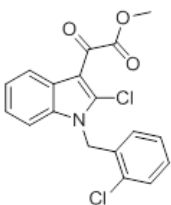
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
346.0656	346.0646	1.0	2.9	11.5	38.6	C18 H14 N O3 F Cl

B. Smit
 29/08/2015

TIC-119 C108/CSAT4/049A

AR.No: MB0815/1357

Analyst : Mallikarjun
 Solvent : cdcl3
 Date : Aug 14 2015
 NUCLEUS : H1
 PRQ (MHz): 400.22
 EXP : PROTON

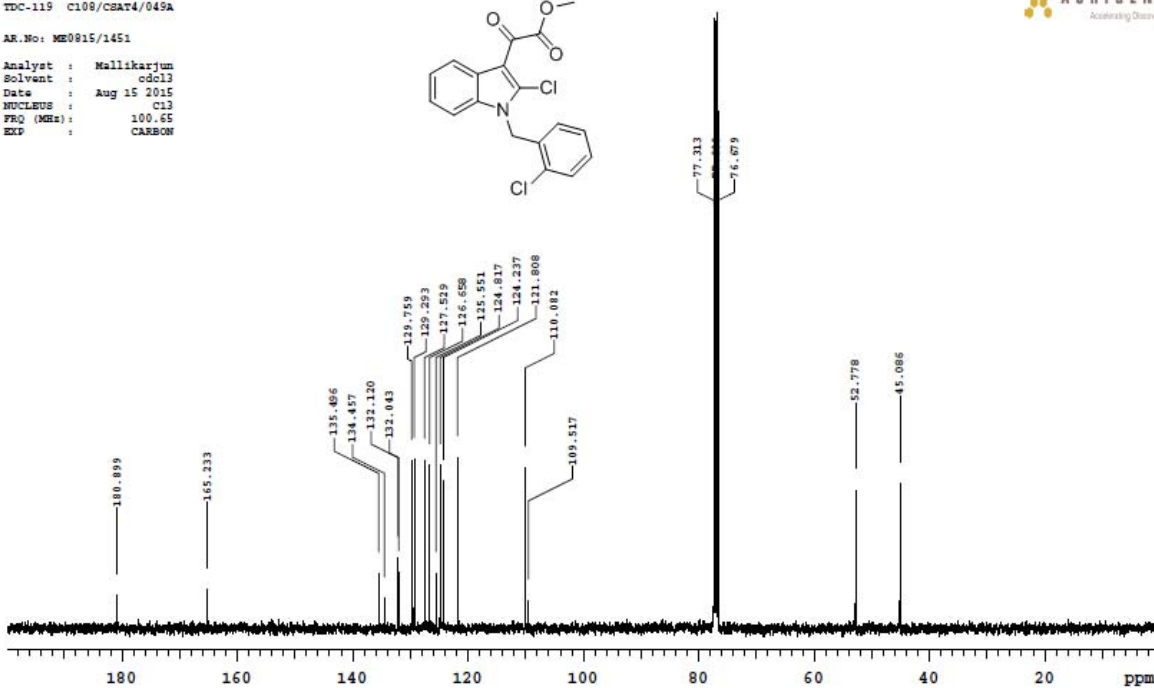
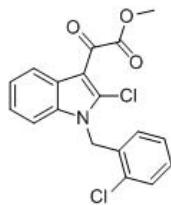


TDC-119 C108/CSAT4/049A



AR. No: ME0915/1451

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 15 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON

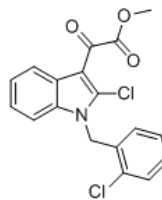


Elemental Composition Report

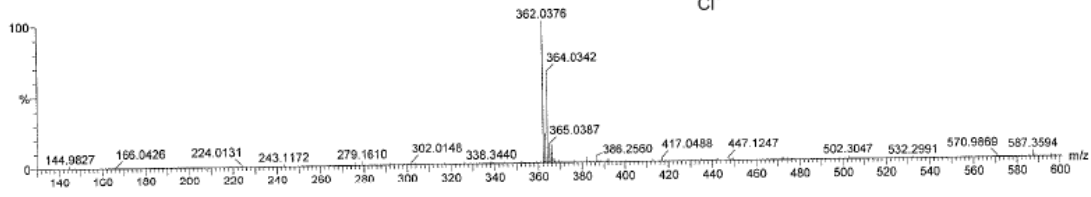
Single Mass Analysis

Tolerance = 8.0 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
142 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 0-23 H: 0-35 N: 0-2 O: 0-4 Cl: 0-3
C108/CSAT4/049 A
150826001 18 (0.339) Cm (18:19)



1: TOF MS ES+
7.21e+004



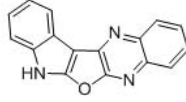
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
362.0376	362.0351	2.5	6.9	11.5	15.6	C18 H14 N O3 Cl2

B. Smigat
27 Aug 2015

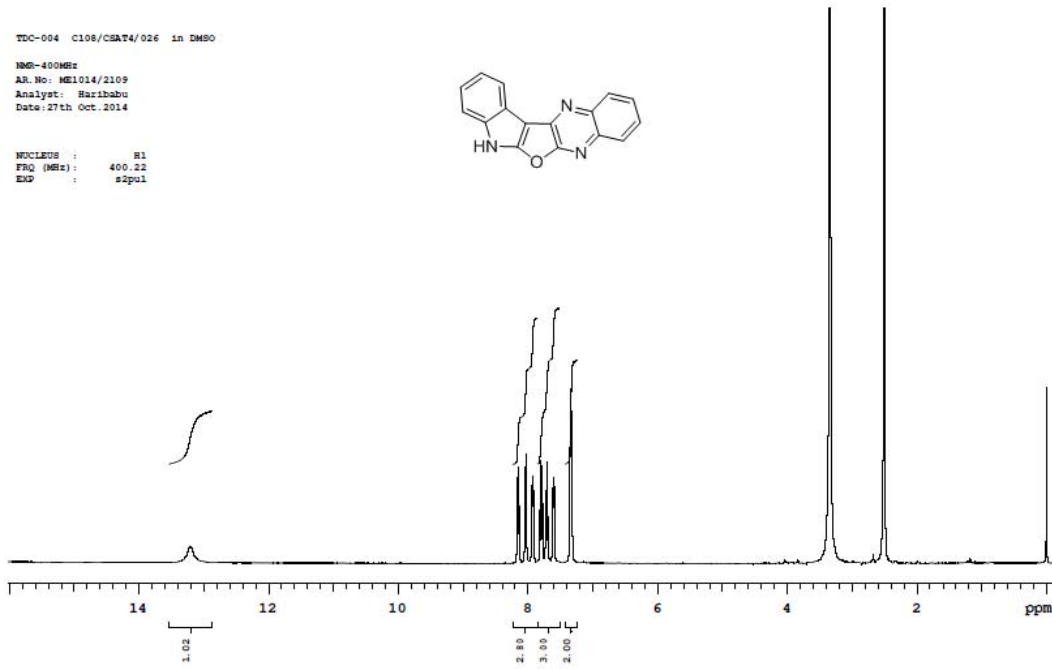
Indole fused- furo[2,3-*b*]quinoxalines(3)

TDC-004 C108/CSAT4/026 in DMSO

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



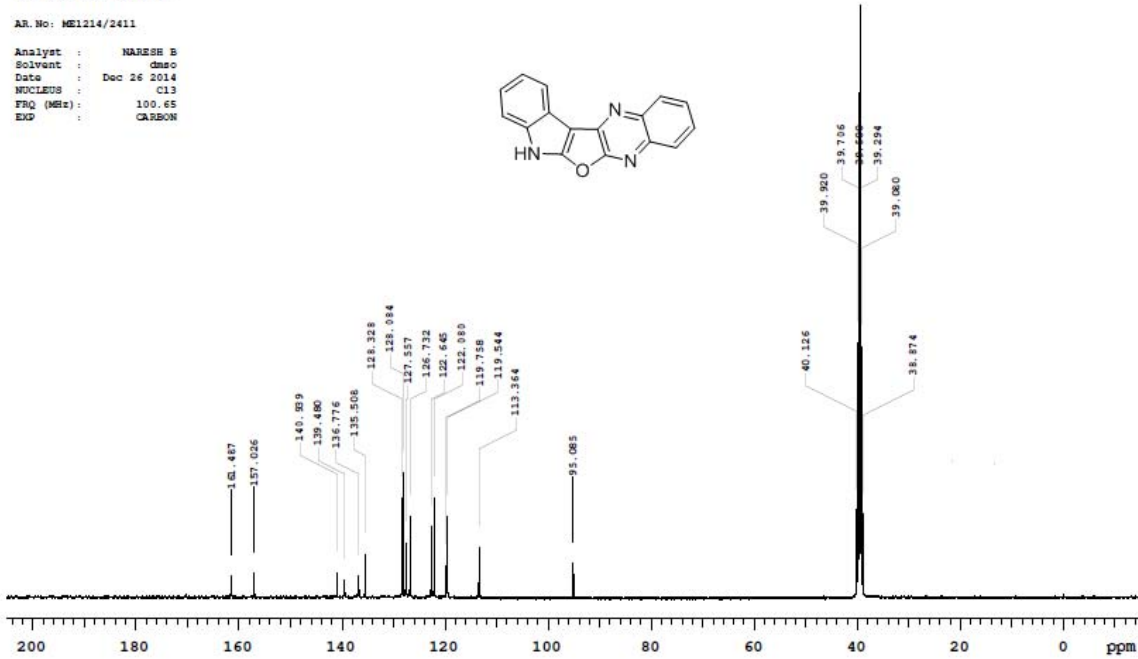
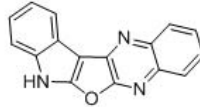
NUCLEUS : B1
FRQ (MHz) : 400.22
EXP : s2pul



TDC-119 C108/CSAT4/024

AR. No: ME1214/2411

Analyst : NARESH B
Solvent : DMSO
Date : Dec 26 2014
NUCLEUS : C13
FRQ (MHz) : 100.65
EXP :



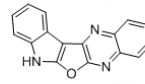
Elemental Composition Report

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

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

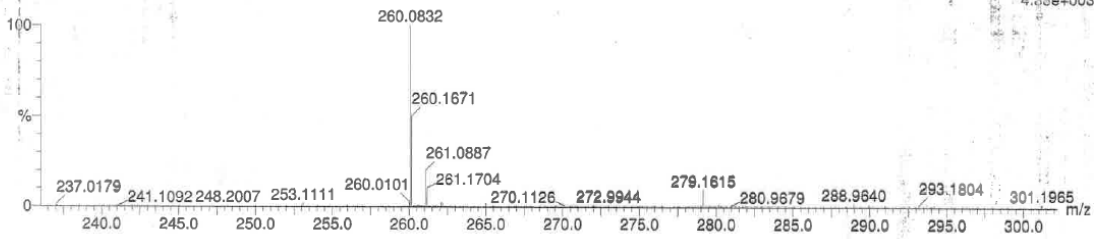
Elements Used:

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

C109/CSATY/025

141204014 32 (0.301) Cm (31:35-80:93)

1: TOF MS ES+
4.30e+003



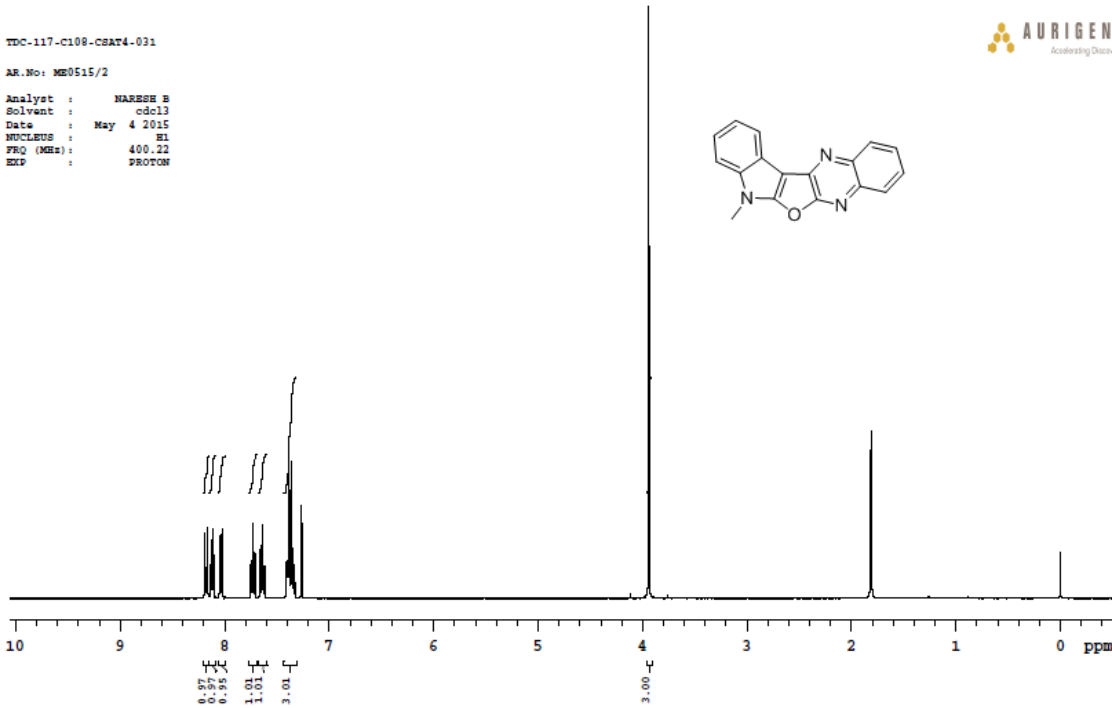
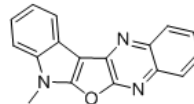
Minimum: -1.5
Maximum: 5.0 5.0 50.0

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-117-C108-CSAT4-031

AR.No: ME0515/2

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

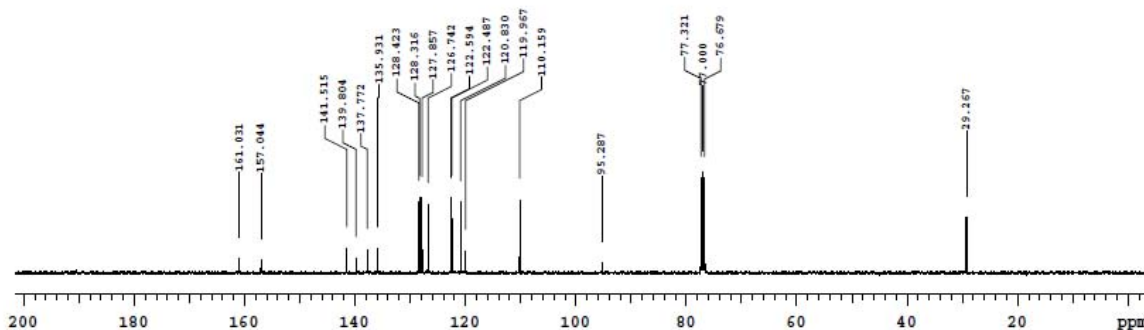
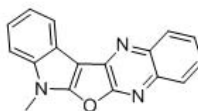


TDC-117 C108/CSAT4/031



AR.No: ME0515/381

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



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

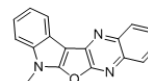
25 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)

Elements Used:

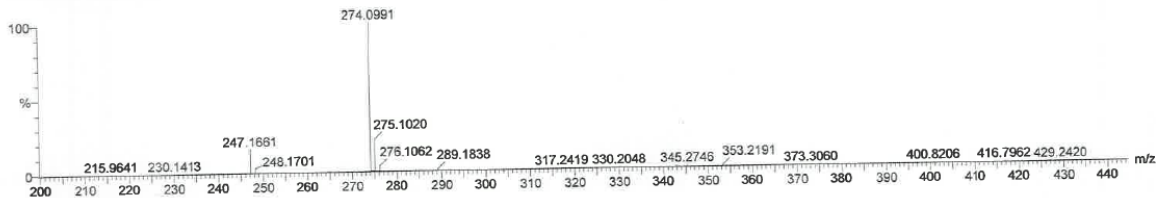
C: 0-21 H: 0-25 N: 0-3 O: 0-2

C108/CSAT4/031

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



1: TOF MS ES+
4.12e+004



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

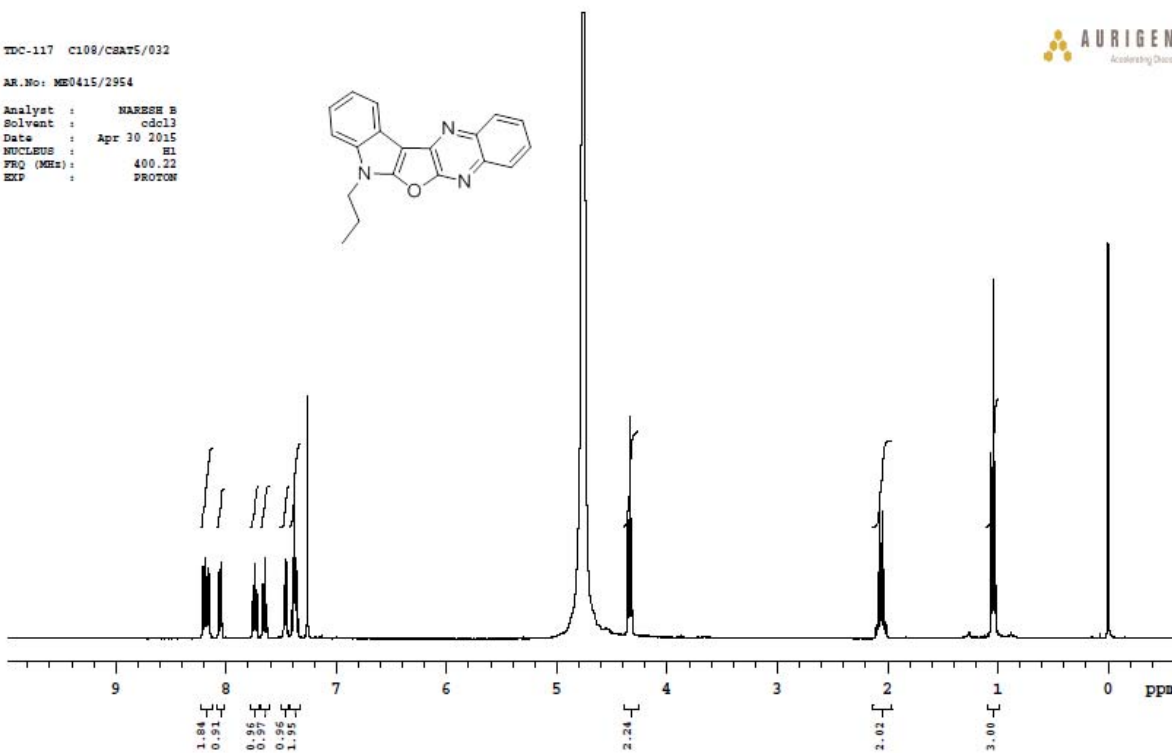
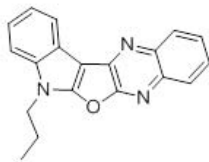
R-Nage Redy 06/05/2015

TDC-117 C108/CSAT5/032



AR.No: ME0415/2954

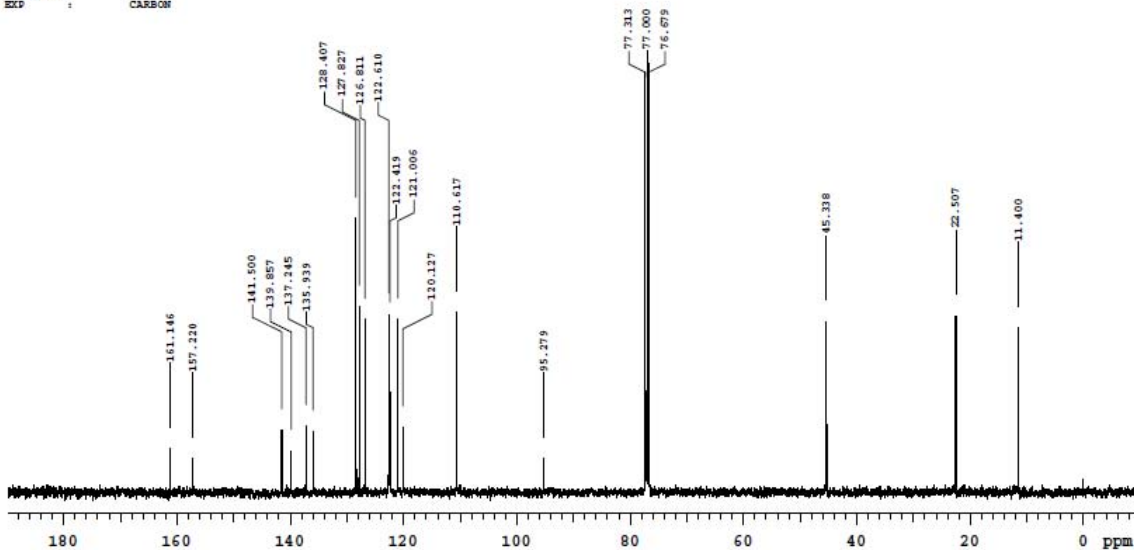
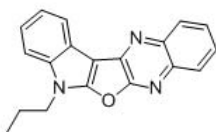
Analyst : NARESH B
Solvent : cdcl3
Date : Apr 30 2015
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON



TDC-117 C108/CSAT5/032

AR.No: ME0415/3064

Analyst : Mallikarjun
Solvent : cdcl3
Date : May 2 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON

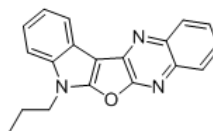


Elemental Composition Report

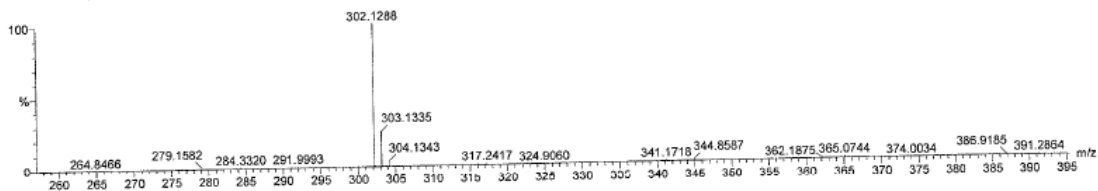
Single Mass Analysis

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
 16 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/CSATS/032
 150506001 15 (0.406) Cm (15:19-37:39x0.500)



1: TOF MS ES+
 1.01e+005



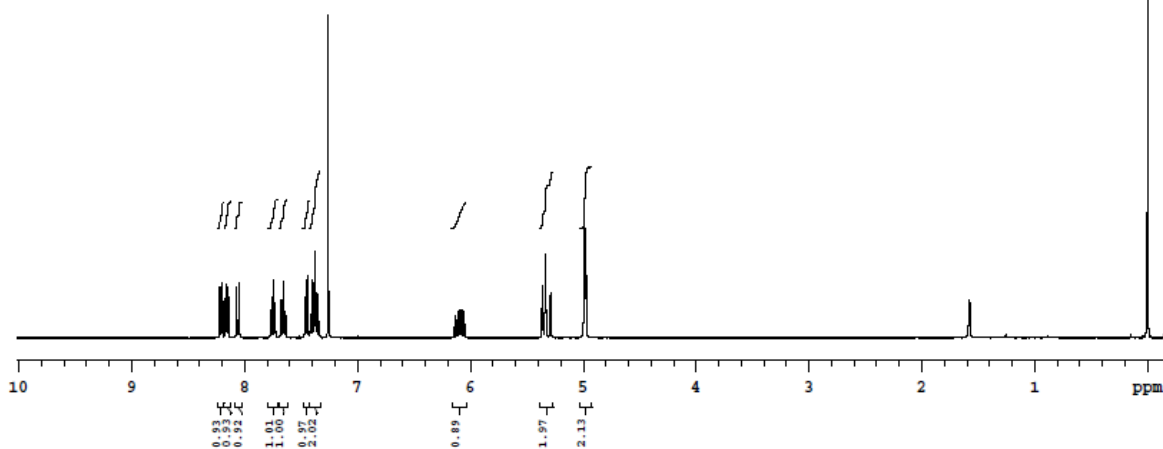
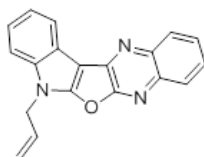
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
302.1288	302.1293	-0.5	-1.7	13.5	82.4	C19 H16 N3 O

R. Narayana Reddy
06/09/2015

TDC-117-C108-CSATS-036

AR.No: ME0515/1392

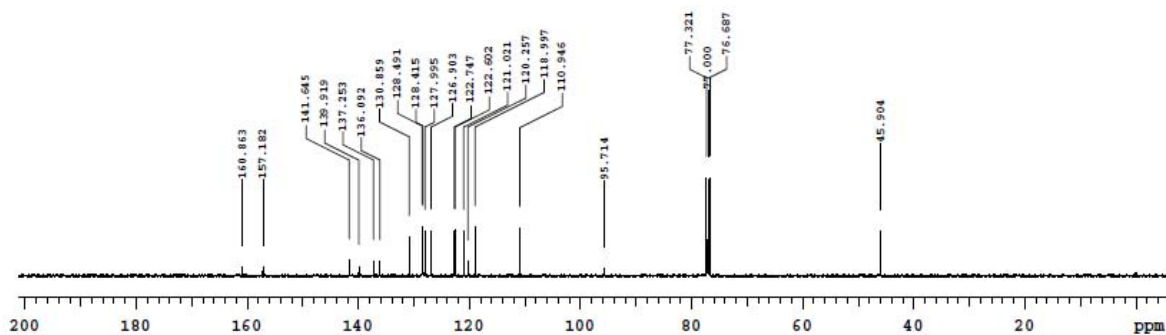
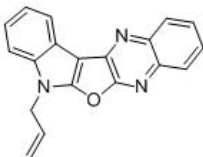
Analyst : NARESH B
 Solvent : cdcl3
 Date : May 18 2015
 NUCLEUS : H1
 FREQ (MHz): 400.22
 EXP : PROTON



TDC-117 C108/CSAT5/036

AR.No: ME0515/1480

Analyst : NARESH B
Solvent : cdcl3
Date : May 18 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

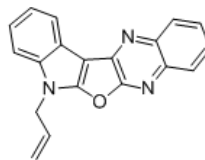
34 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)

Elements Used:

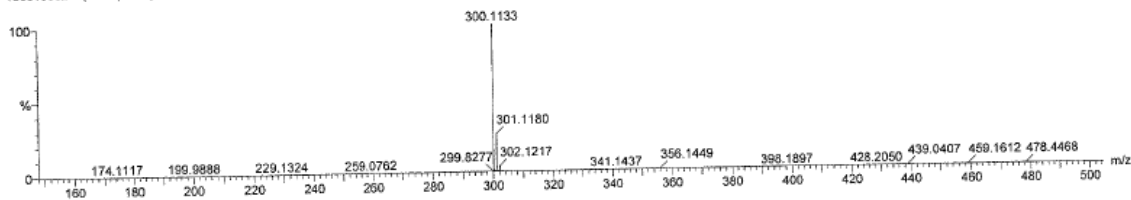
C: 0-23 H: 0-17 N: 0-5 O: 0-3

C108/CSAT5/036

150518002 7 (0.131) Cm (6.8-63.75x0.500)



1: TOF MS ES+
1.77e+005



Minimum:				-1.5			
Maximum:		5.0	5.0	80.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
300.1133	300.1137	-0.4	-1.3	14.5	230.9	C19 H14 N3 O	

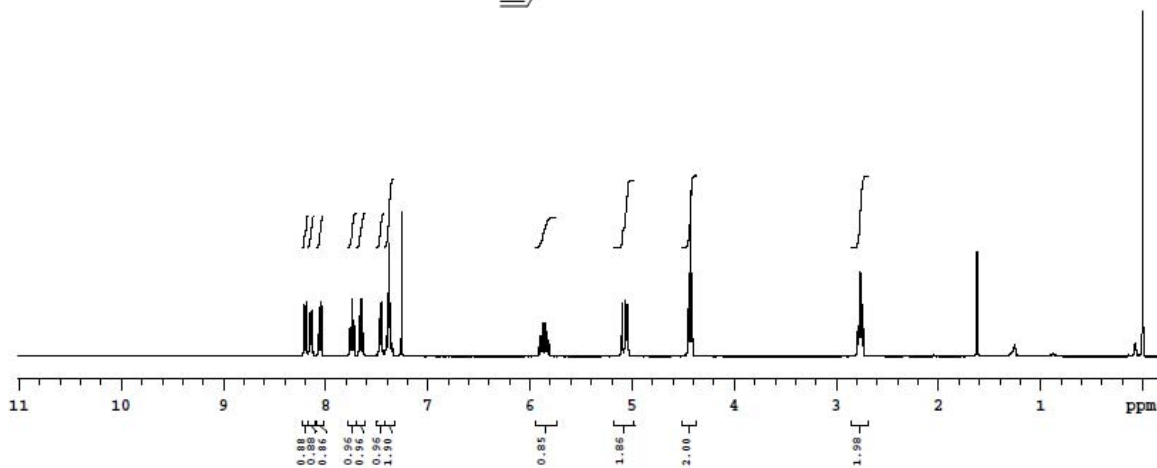
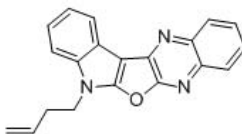
R. Nagarajan
18/05/2015

TDC-117 C108/CSAT5/038



AR.No: ME0615/189

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jun 3 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

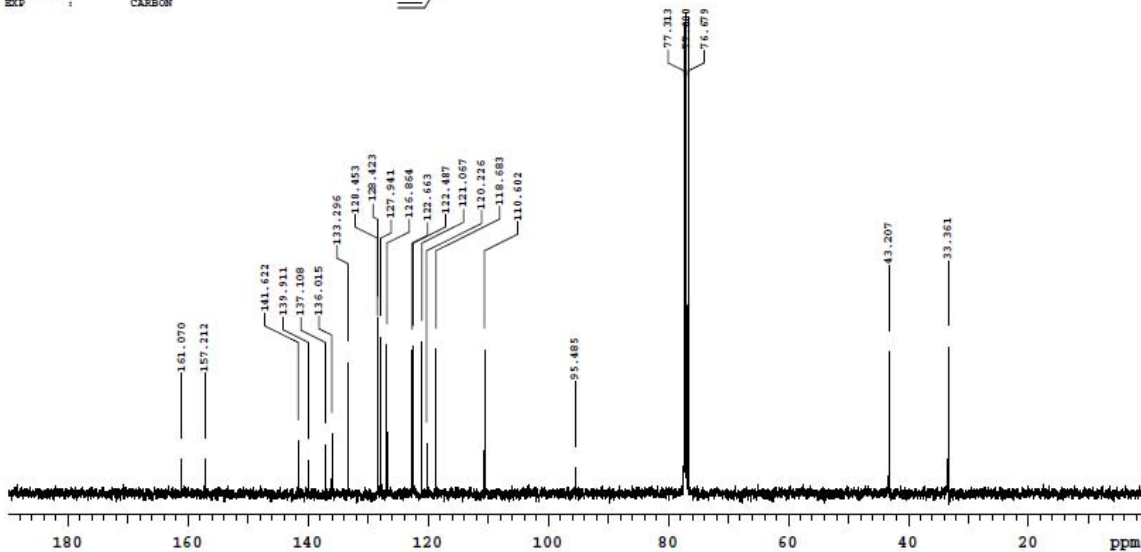
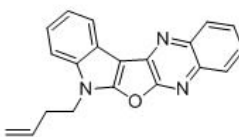


TDC-119 C108/CSAT5/038



AR.No: ME0815/547

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 7 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON

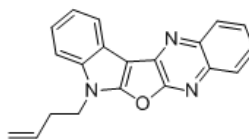


Elemental Composition Report

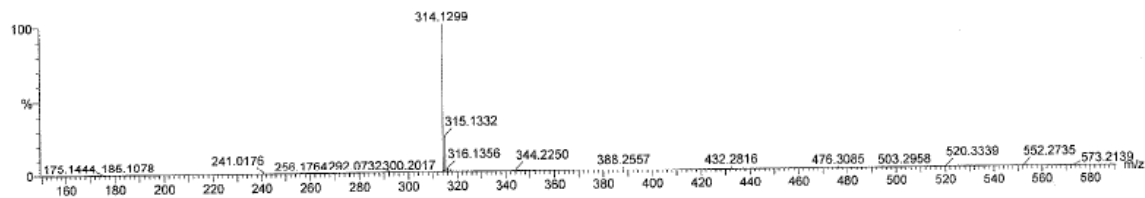
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
 39 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)
 Elements Used:
 C: 0-25 H: 0-18 N: 0-5 O: 0-3
 C108/CSAT5/038
 150603014 25 (0.473) Cm (25.28-65.68x0.500)



1: TOF MS ES+
 1.31e+005



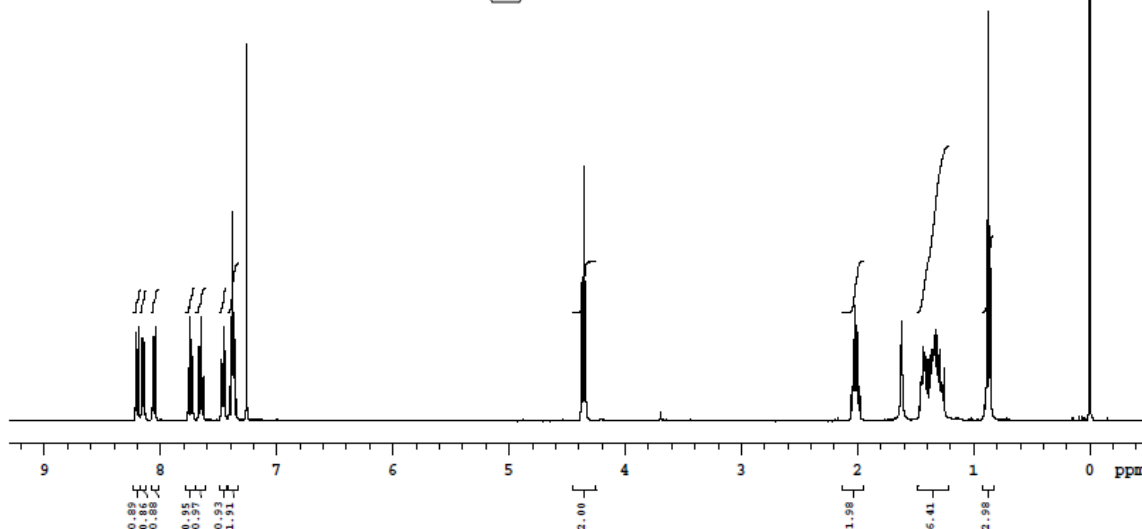
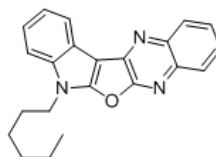
Minimum:				-1.5		
Maximum:	5.0	5.0		80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.1299	314.1293	0.6	1.9	14.5	47.0	C20 H16 N3 O

R. No. = 117-117-038 (2015)

TDC-117-C108-CSAT5-035

AR.No: MS0615/57

Analyst : Mallikarjun
 Solvent : cdCl3
 Date : Jun 1 2015
 NUCLEUS : H1
 FREQ (MHz): 400.22
 EXP : PROTON

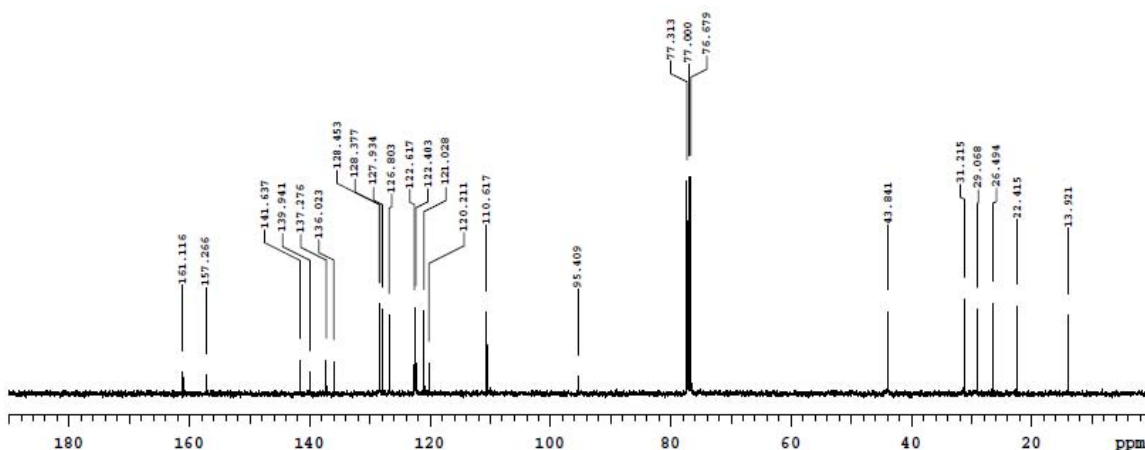
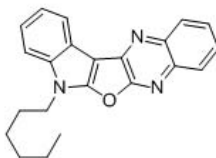


TDC-117 C108/CSAT5/035



AR.No: MB0615/251

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jun 3 2015
NUCLEUS : C13
PFG (MHz) : 100.65
EXP :



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

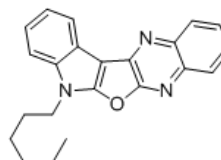
82 formula(e) evaluated with 1 results within limits (up to 5 closest results for each mass)

Elements Used:

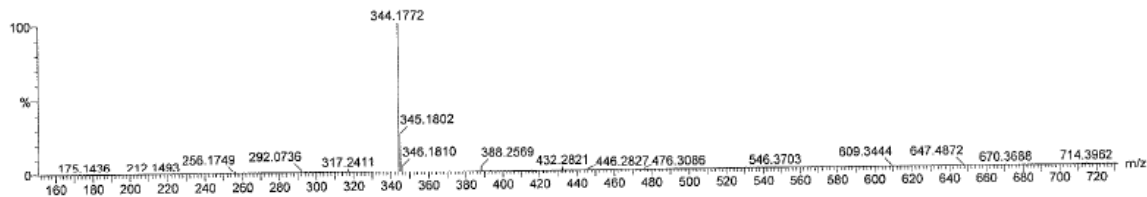
C: 0-25 H: 0-25 N: 0-5 O: 0-6

C108/CSAT5/035

150603011 68 (1.255) Cm (68.71-68.88x0.500)



1: TOF MS ES+
1.54e+005



Minimum:				-1.5		
Maximum:	5.0	5.0		80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
344.1772	344.1763	0.9	2.6	13.5	3.9	C22 H22 N3 O

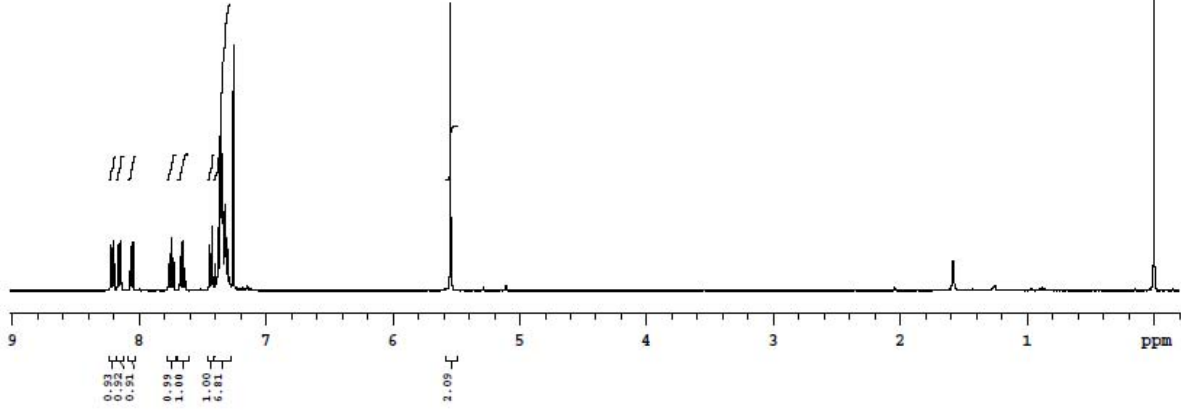
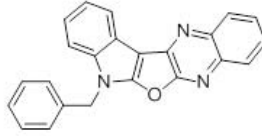
R. Narayana
03/06/2015

TDC-117-C108-CSAT5-037



AR.No: MB0515/1391

Analyst : NARESH B
Solvent : cdcl3
Date : May 18 2015
NUCLEUS : H1
FREQ (MHz): 400.12
EXP : PROTON

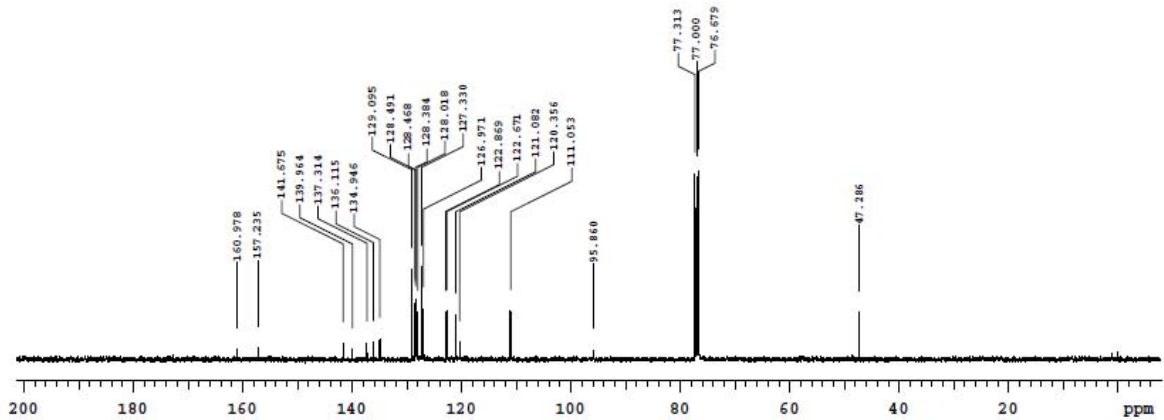
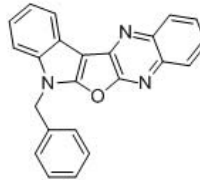


TDC-117 C108/CSAT5/037



AR.No: MB0515/1481

Analyst : NARESH B
Solvent : cdcl3
Date : May 19 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON

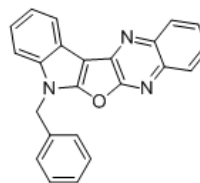


Elemental Composition Report

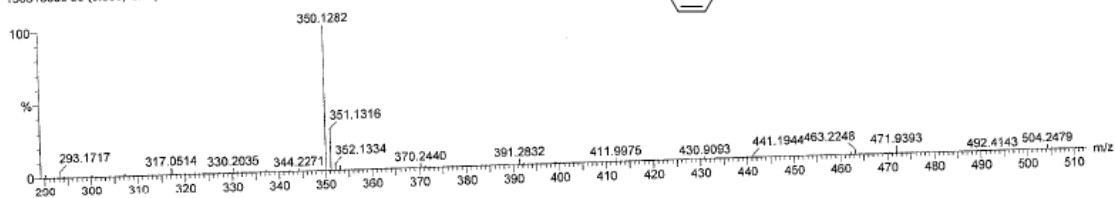
Single Mass Analysis

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
 32 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
 Elements Used:
 C: 0-25 H: 0-19 N: 0-5 O: 0-3
 C108/CSAT5/037
 150518003 50 (0.930) Cm (49:54-83:88x0.500)



1: TOF MS ES+
 1.38e+004



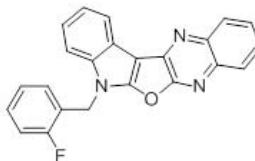
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
350.1282	350.1293	-1.1	-3.1	17.5	4.6	C23 H16 N3 O

*12. Nagendra
 12/05/2015*

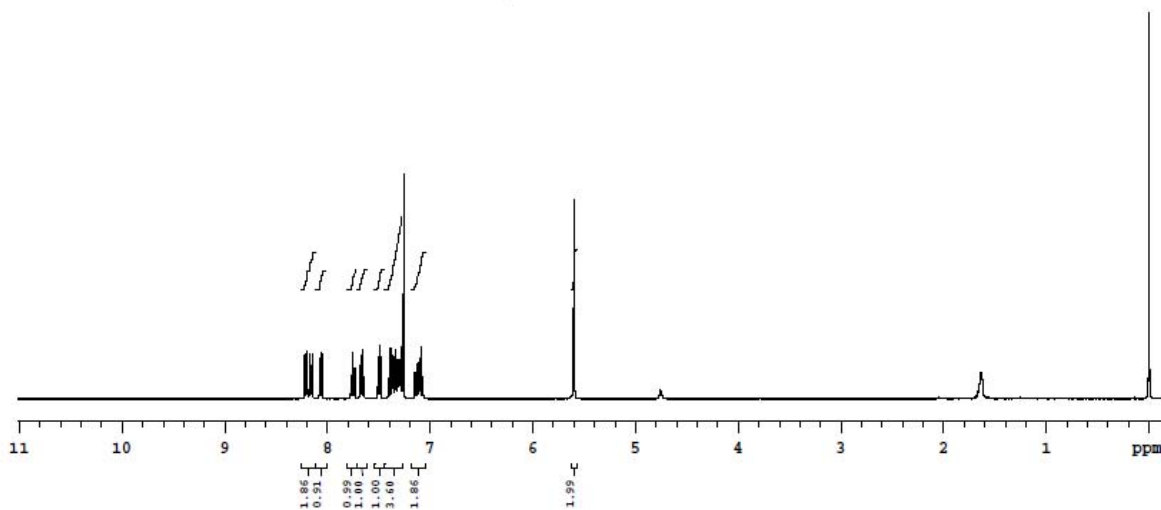
TDC-119 C108/CSAT5/048

AR.No: MB0715/2555

Analyst : Mallikarjun
 Solvent : cdcl3
 Date : Jul 27 2015
 NUCLEUS : H1
 FREQ (MHz) : 400.22
 EXP : PROTON



AURIGENE
 Accelerating Discovery

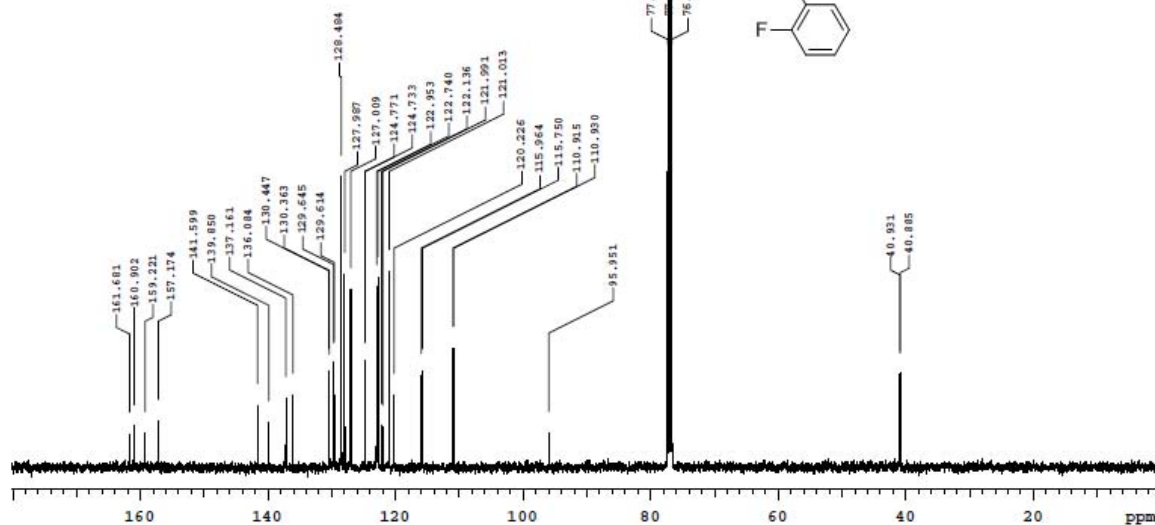
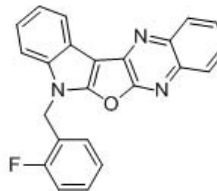


TDC-119 C108/CSAT5/048



AR.No: ME0815/716

Analyst : Mallikarjun
Solvent : CDCl3
Date : Aug 8 2015
NUCLBUS : 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

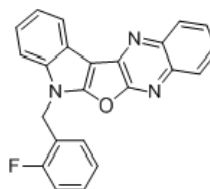
39 formula(e) evaluated with 1 results within limits (up to 20 best isotopic matches for each mass)

Elements Used:

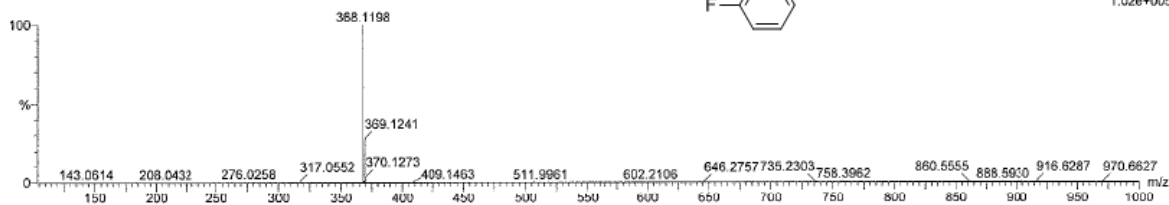
C: 0-25 H: 0-25 N: 0-4 O: 0-2 F: 0-1

C108/CSAT5/048

150811007 29 (0.547) Cm (29:33-95:105x0.500)



1: TOF MS ES+
1.02e+005



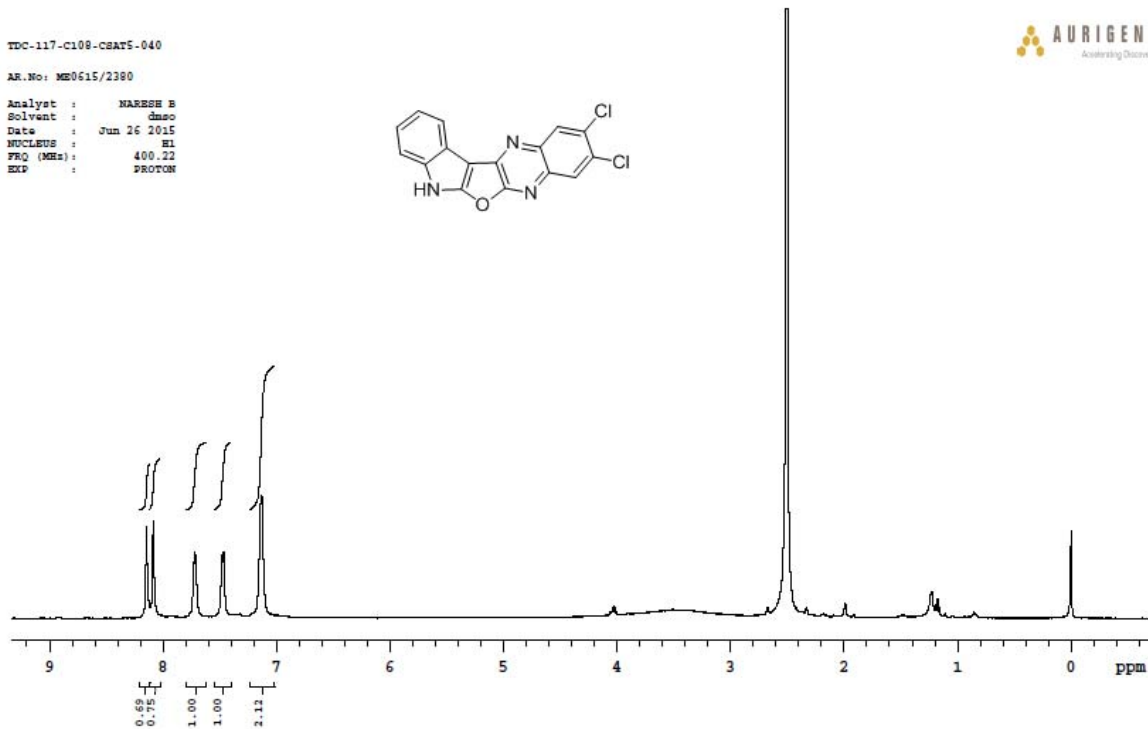
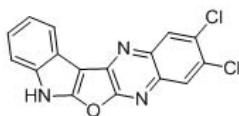
Minimum: -1.5
Maximum: 80.0

Mass	Calc. Mass	mDa	PPM	DBR	i-FIT	Formula
368.1198	368.1199	-0.1	-0.3	17.5	7.2	C23 H15 N3 O F

TDC-117-C108-CBATS-040

AR.No: MB0615/2380

Analyst : NARSH B
Solvent : dmso
Date : Jun 26 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

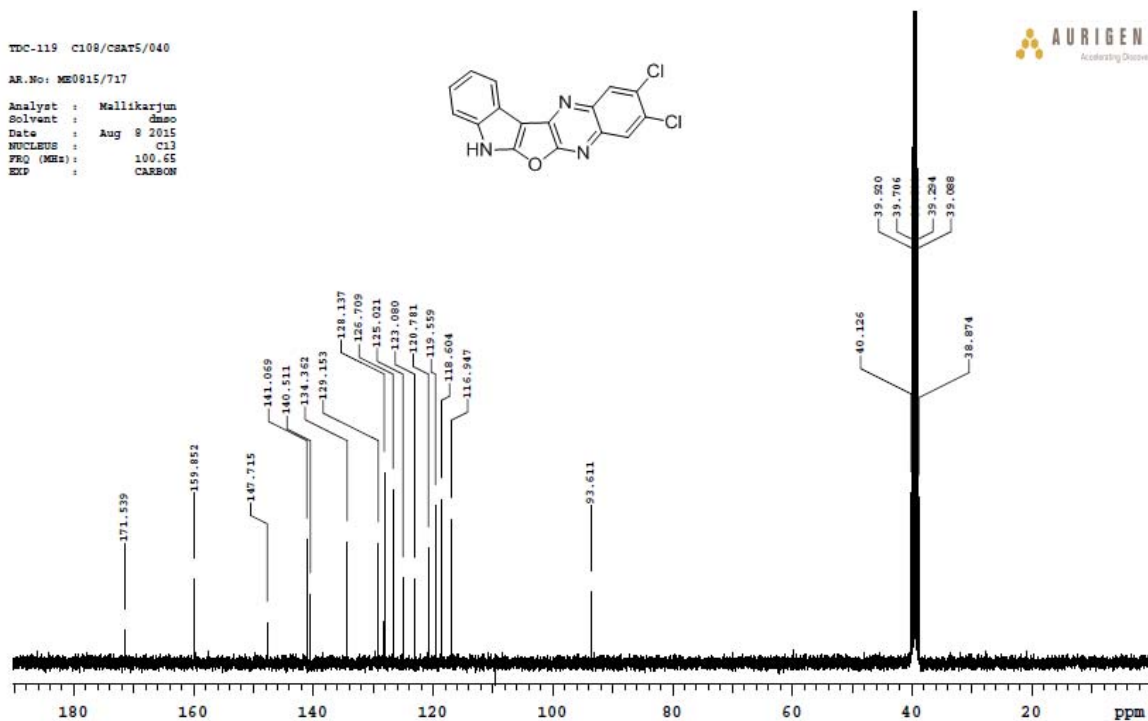
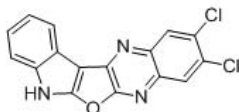


AURIGENE
Accelerating Discovery

TDC-119 C108/CBATS/040

AR.No: MB0915/717

Analyst : Mallikarjun
Solvent : dmso
Date : Aug 9 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



AURIGENE
Accelerating Discovery

Elemental Composition Report

Single Mass Analysis

Tolerance = 6.5 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

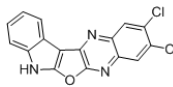
211 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

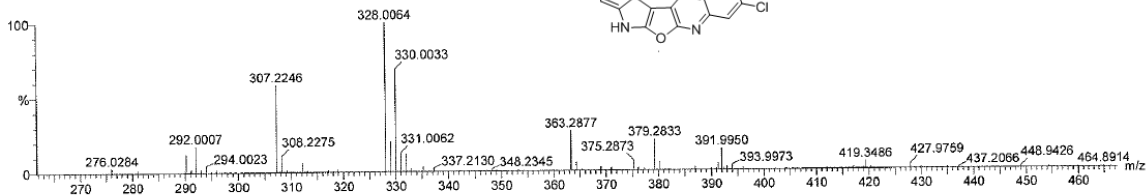
C: 0-25 H: 0-27 N: 0-5 O: 0-4 Cl: 0-2

C108/CSAT5/040

150829001 21 (0.400) Cm (21:29-(1:6+52:69)x0.500)



1: TOF MS ES+
2.67e+004

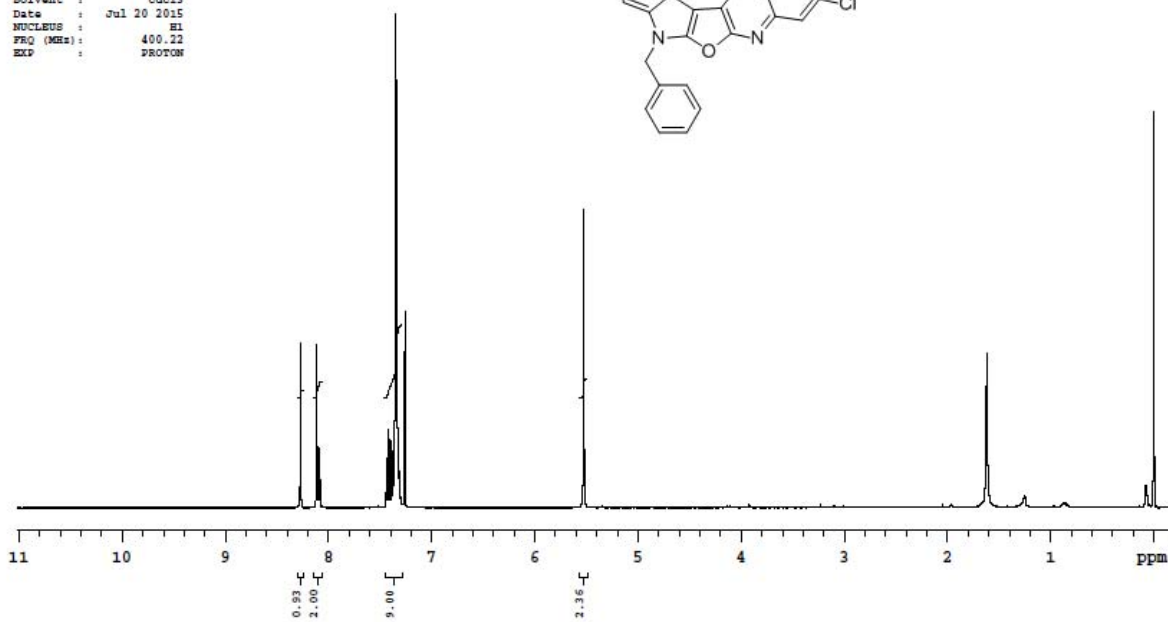
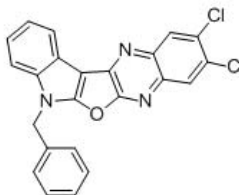


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
328.0064	328.0044	2.0	6.1	13.5	13.0	C16 H8 N3 O Cl2

TDC-117 C108/CSAT5/046

AR.No: ME0715/1985

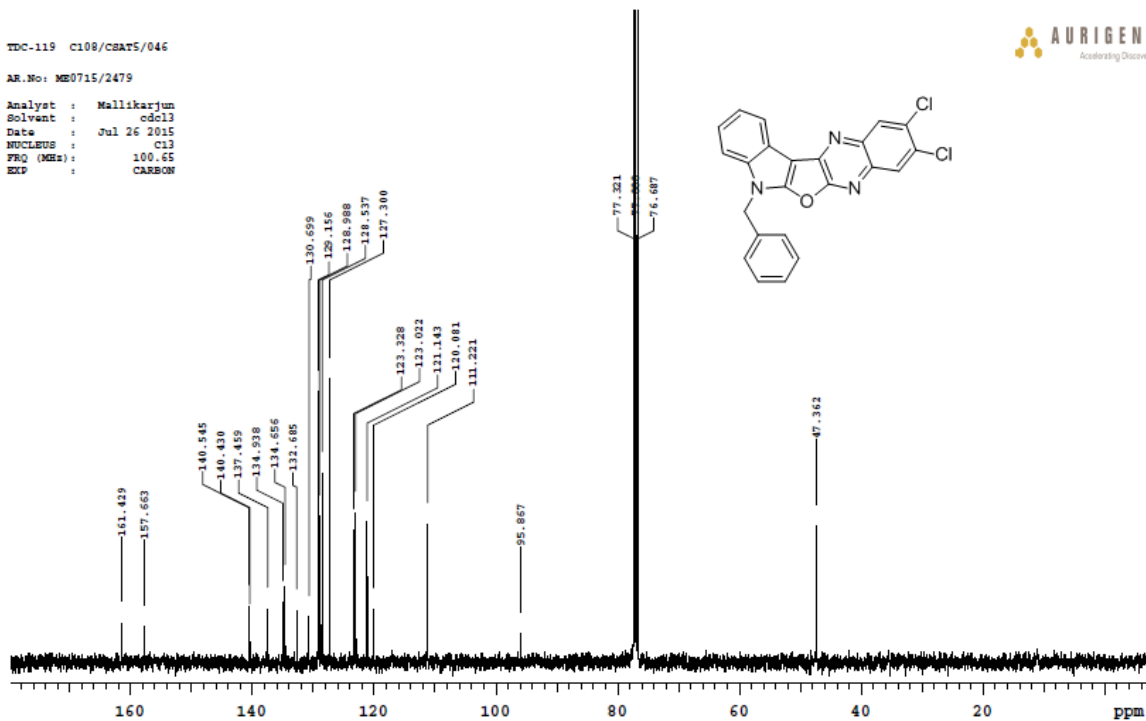
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jul 20 2015
NUCLEUS : EI
PFG (MHz) : 400.22
EXP : PROTON



TDC-119 C108/CSAT5/046

AR.No: MB0715/2479

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jul 26 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 7.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions

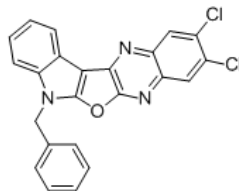
56 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

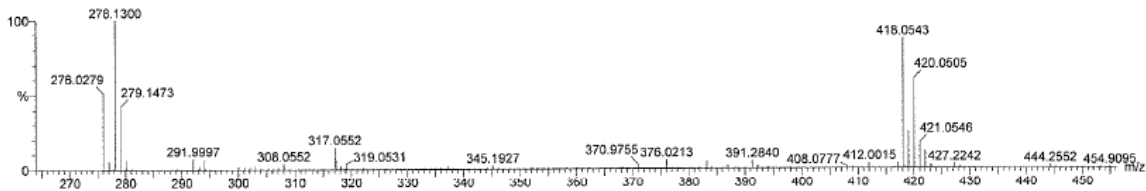
C: 0-25 H: 0-25 N: 0-5 O: 0-2 Cl: 0-2

C108/CSAT5/046

150720004 12 (0.319) Cm (11:12)



1: TOF MS ES+
9.49e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
418.0543	418.0514	2.9	6.9	17.5	3.9	C23 H14 N3 O Cl2

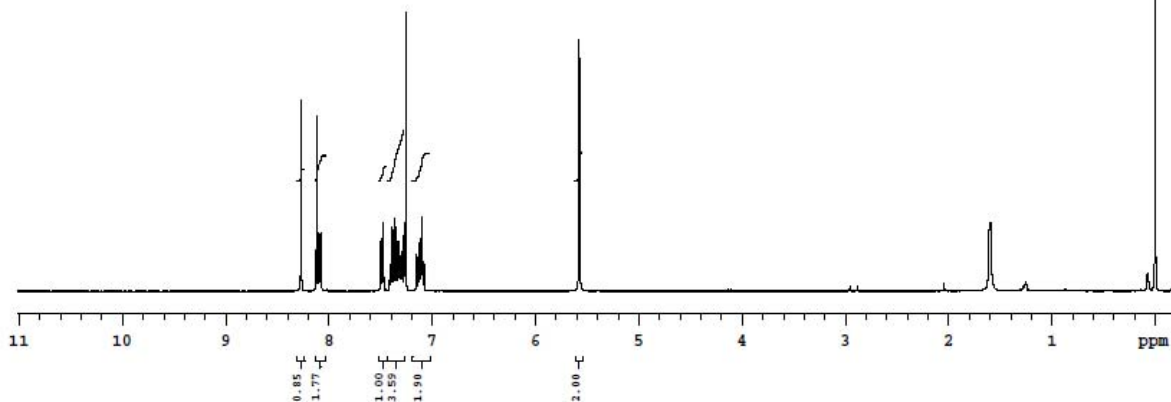
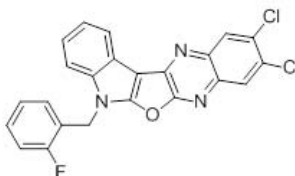
B-Singh

TDC-119 C108/CSAT5/047



AR.No: ME0715/2206

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jul 22 2015
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON

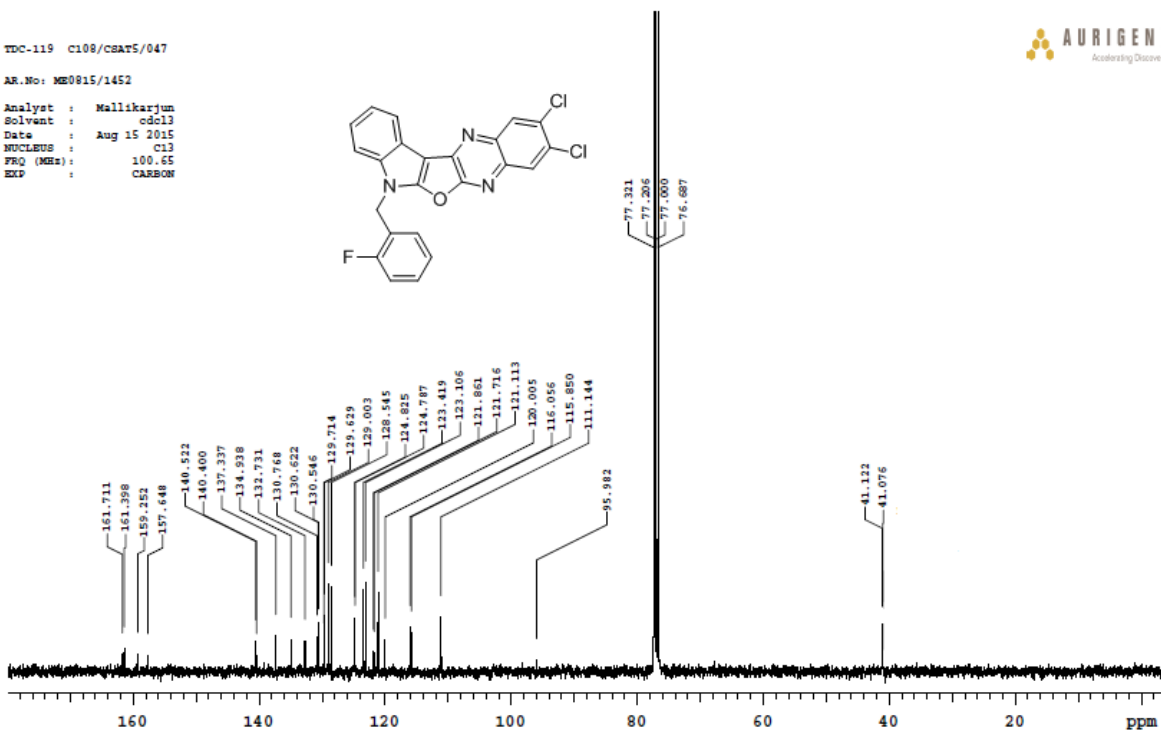
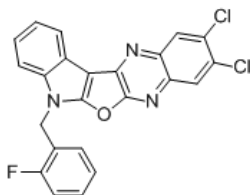


TDC-119 C108/CSAT5/047



AR.No: ME0815/1452

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 15 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON

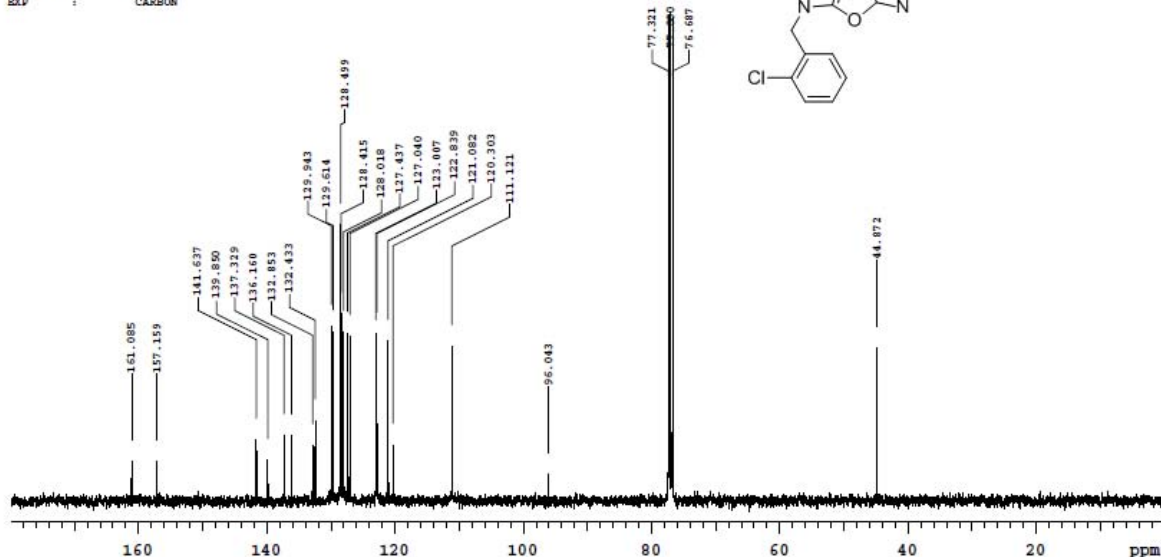


TDC-119 C108/CSAT5/049



AR.No: ME0815/2826

Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 28 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

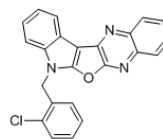
64 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

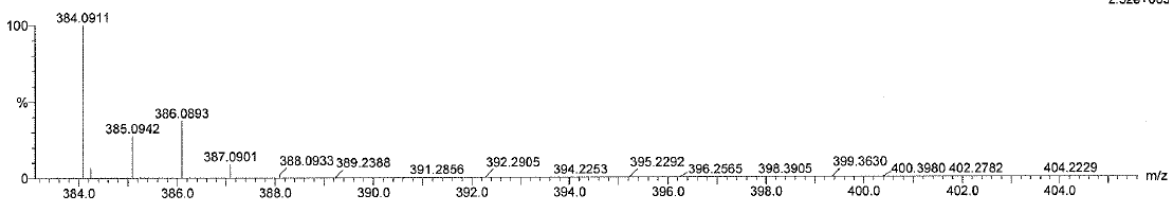
C: 0-25 H: 0-16 N: 0-4 O: 0-2 Cl: 0-3

C108/CSAT5/049

150818012 27 (0.501) Cm (27:31)



1: TOF MS ES+
2.52e+005



Minimum:

Maximum:

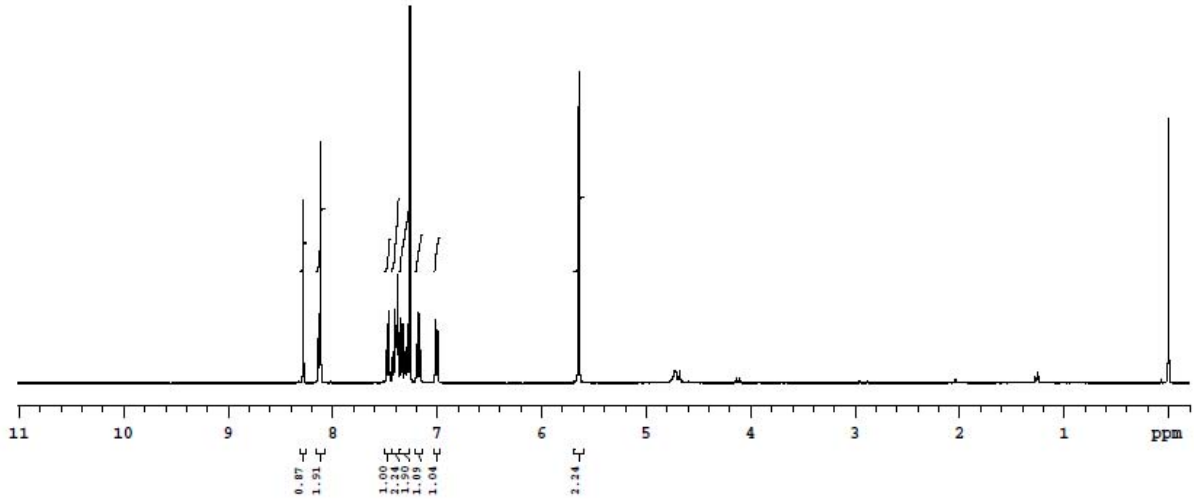
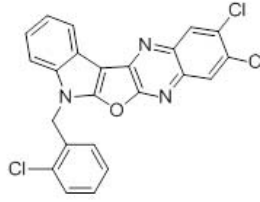
5.0 5.0 -1.5
80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
384.0911	384.0904	0.7	1.8	17.5	19.0	C23 H15 N3 O Cl

TDC-119 C108/CSAT5/050

AR.No: MR0815/1636

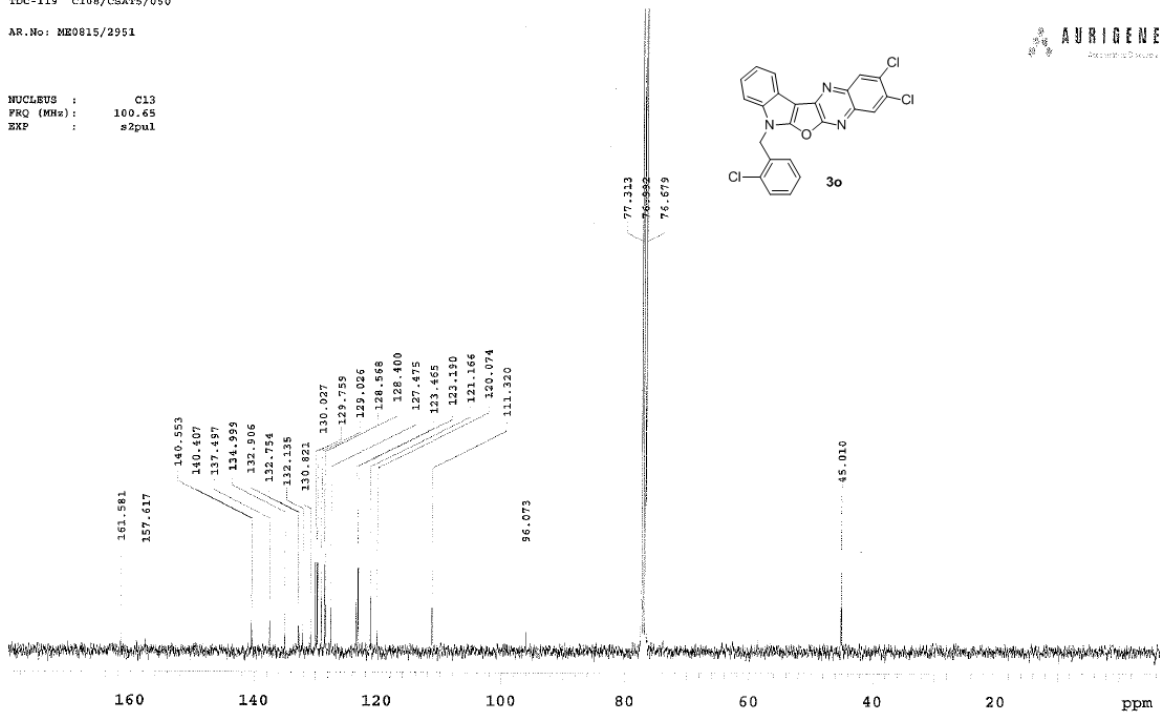
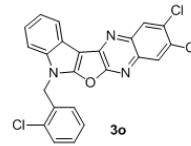
Analyst : Mallikarjun
Solvent : cdcl3
Date : Aug 18 2015
NUCLEUS : 1H
FREQ (MHz): 400.22
EXP : PROTON



TDC-119 C108/CSAT5/050

AR.No: MR0815/2951

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

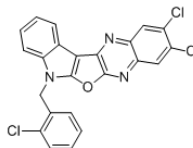


Elemental Composition Report

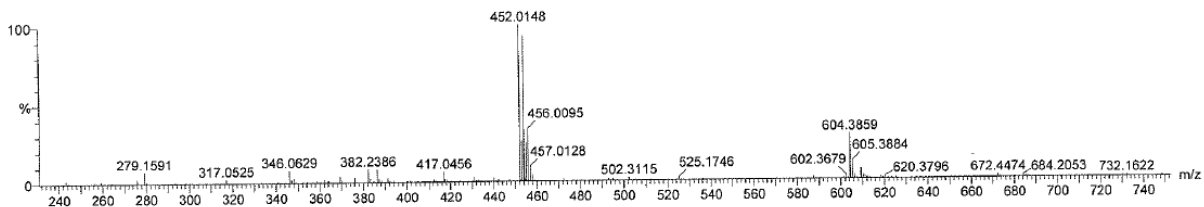
Single Mass Analysis

Tolerance = 6.5 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
 153 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)
 Elements Used:
 C: 0-25 H: 0-27 N: 0-5 O: 0-4 Cl: 0-3
 C108/CSATS050
 150826003 20 (0.368) Cm (20:22)



1: TOF MS ES+
 4.19e+004

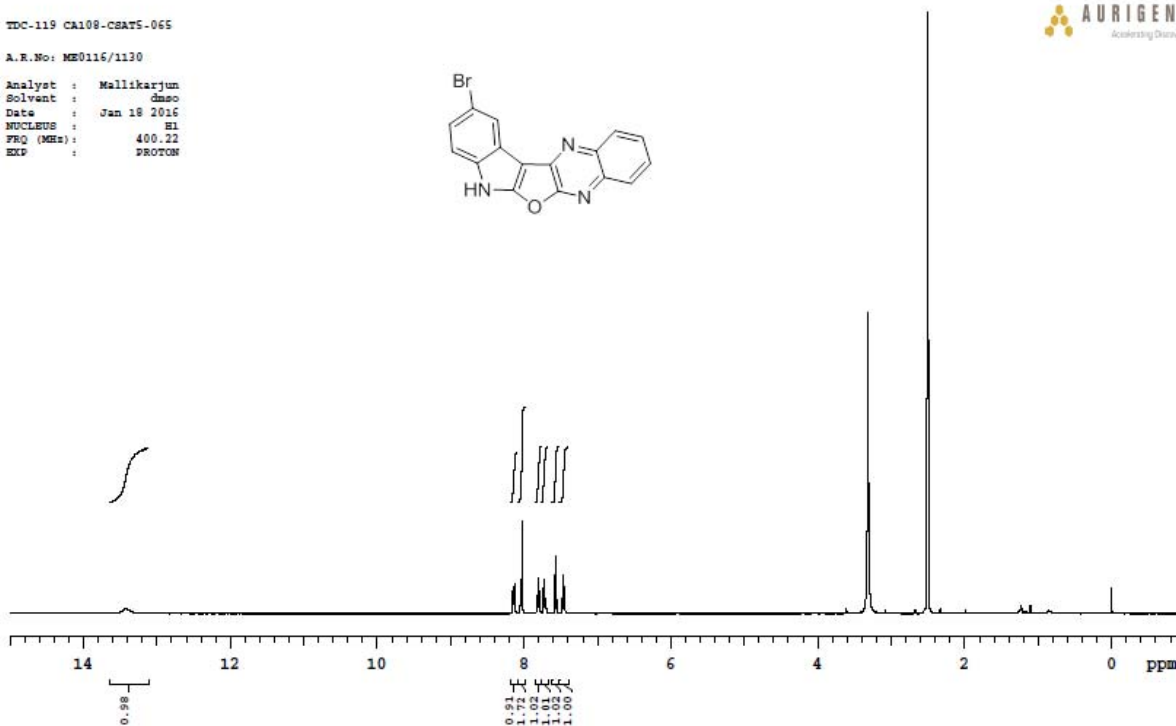
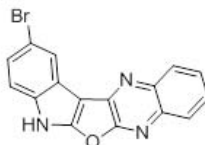


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
452.0148	452.0124	2.4	5.3	17.5	14.0	C23 H13 N3 O Cl3

TDC-119 CA108-CSATS-065

A.R.No: ME0116/1130

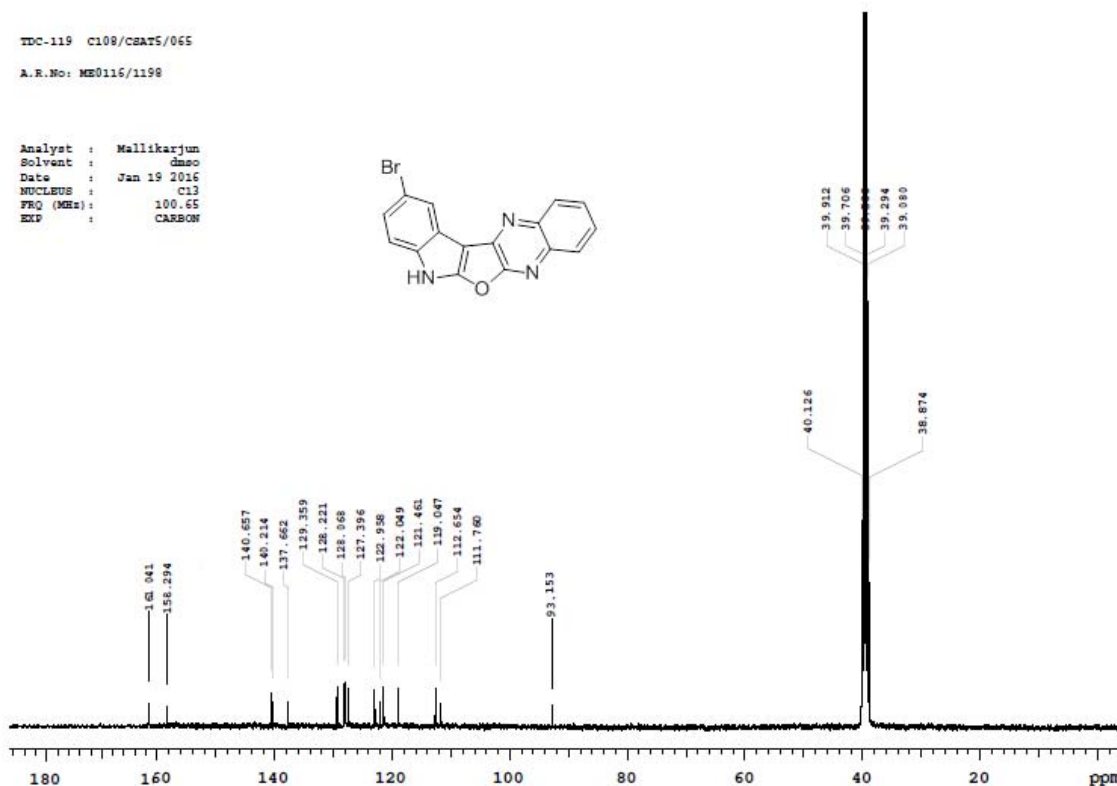
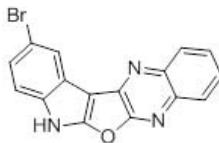
Analyst : Mallikarjun
 Solvent : dmsc
 Date : Jan 18 2016
 NUCLEUS : EI
 FREQ (MHz): 400.22
 EXP : PROTON



TDC-119 C108/CSATS/065

A.R.No: ME0116/1198

Analyst : Mallikarjun
Solvent : dmso
Date : Jan 19 2016
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

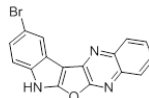
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

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

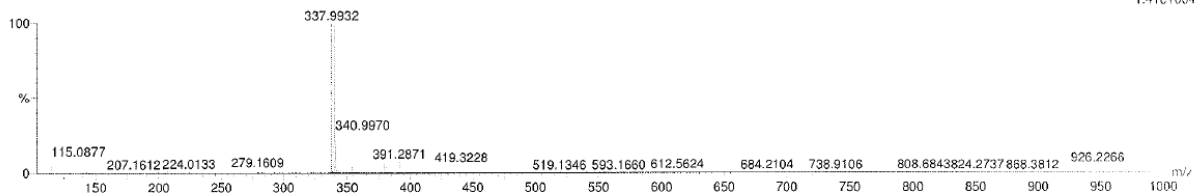
Elements Used:

C: 0-30 H: 0-22 N: 0-5 O: 0-1 Br: 0-1



C108/CSATS/065
160122001 18 (0.339) Cm (17.20)

1: TOF MS ES+
1.41e+04

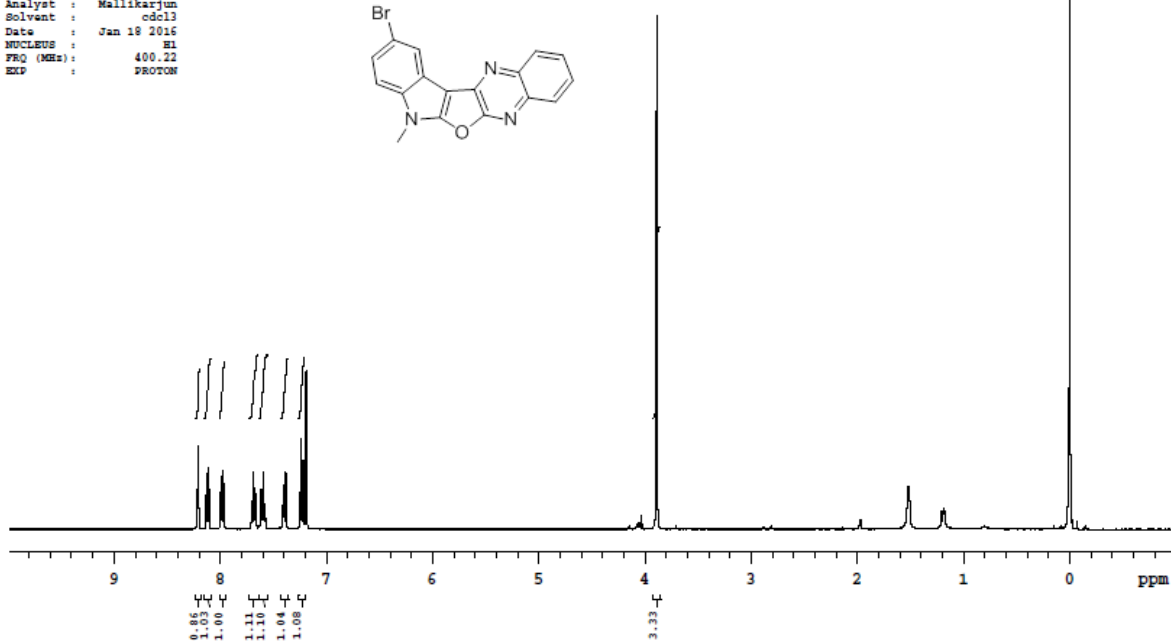
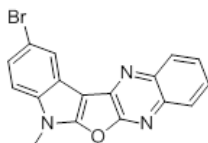


Minimum:	Maximum:	Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
-1.5	5.0	337.9932	337.9929	0.3	0.9	13.5	12.2	C16 H9 N3 O Br

TDC-119 C108-CSATS-066

A.R.No: MB0116/1122

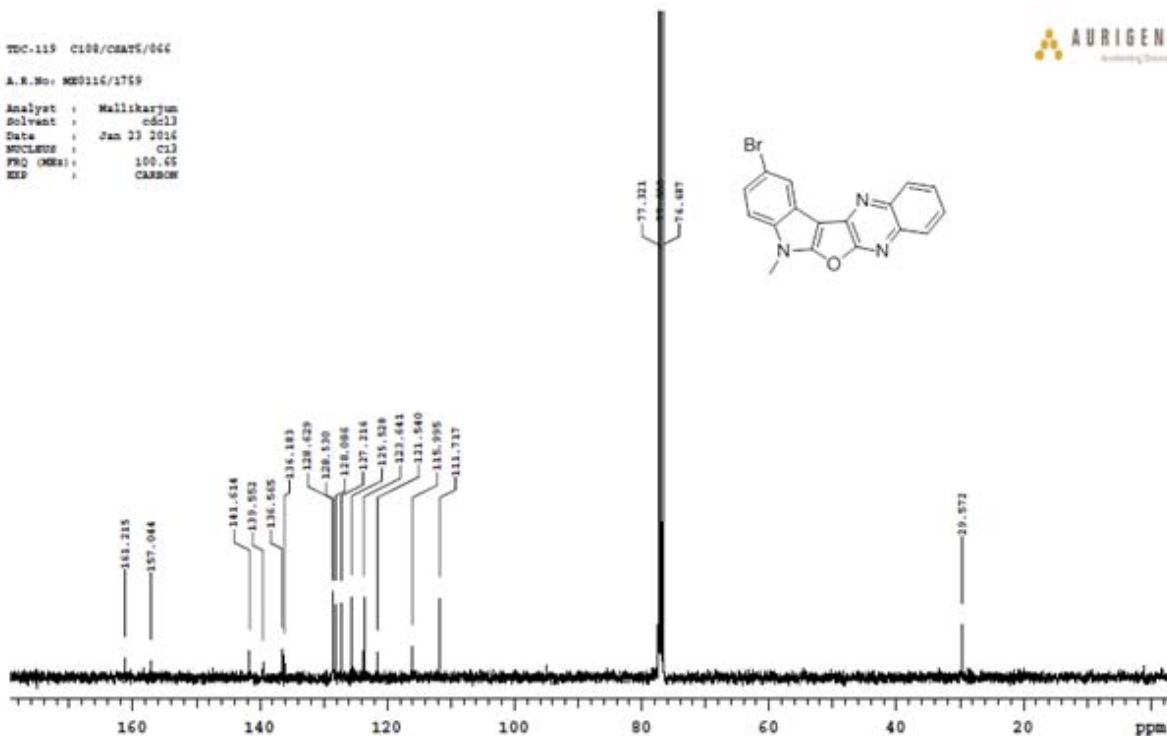
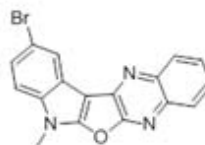
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 19 2016
NUCLEUS : H1
FREQ (MHz): 400.22
EXP : PROTON



TDC-119 C108/CSATS/066

A.R.No: MB0116/1759

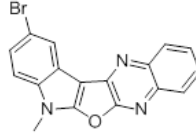
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 23 2016
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



Single Mass Analysis

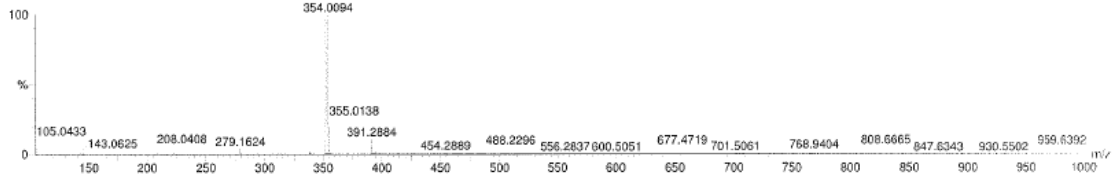
Tolerance = 6.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)
Elements Used:
C: 0-30 H: 0-22 N: 0-5 O: 0-1 Br: 0-1



C108/CSAT51068
160122002.22 (0.413) Cm (21:22)

1: TOF MS 1-S
4.42e+003



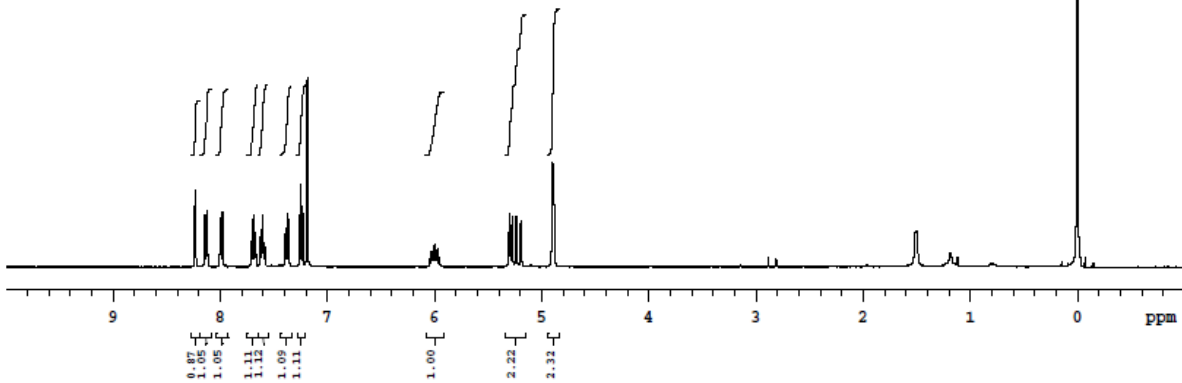
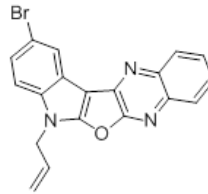
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
352.0104	352.0085	1.9	5.4	13.5	1.3	C17 H11 N3 O Br

BSM at 25/01/2016

TDC-119 C108-CSAT5-067

A.R.No: MS0116/1133

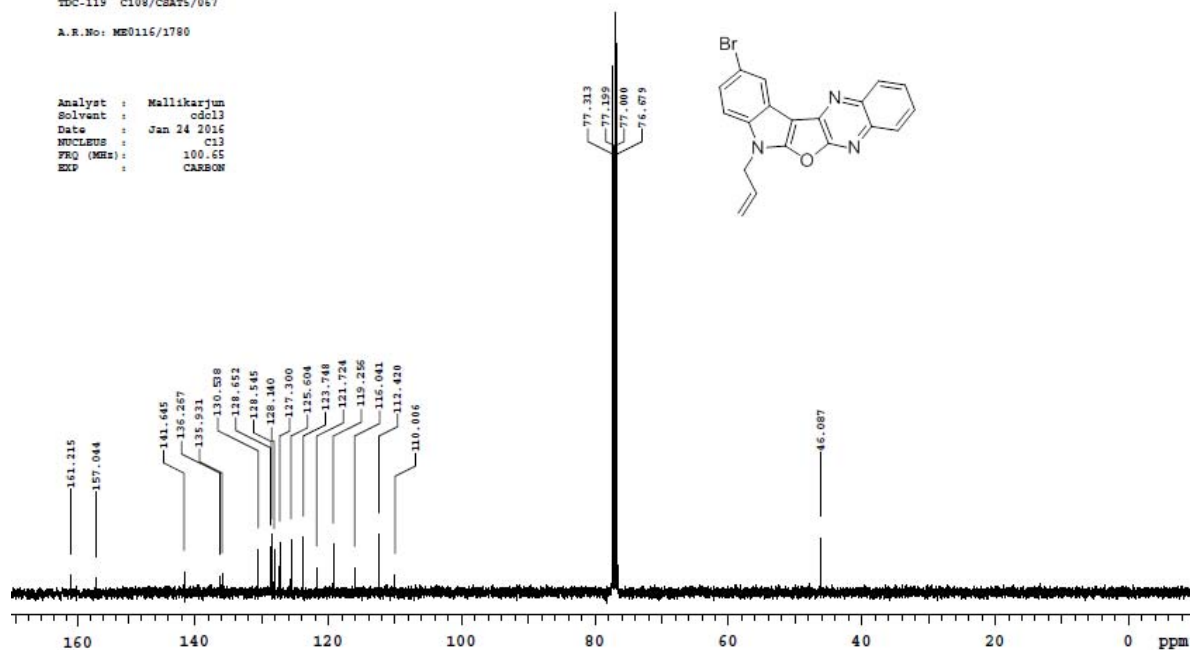
Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 18 2016
NUCLEUS : H1
PRQ (MHz): 400.22
EXP : PROTON



TDC-119 C108/CSATS/067

A.R.No: ME0116/1760

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jan 24 2016
NUCLEUS : C13
FREQ (MHz) : 100.62
EXP : CARBON



Elemental Composition report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

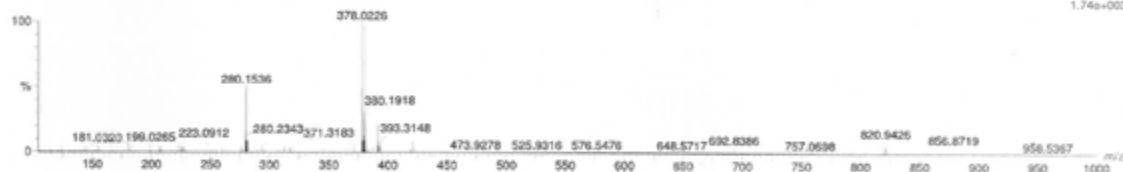
49 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-25 H: 0-20 N: 0-5 O: 0-2 Br: 0-1

C108/CSATS/067

160129001 33 (0.620) Cm (33:38)



1: TOF MS ES+
1.74e+003

Minimum:

Maximum: 5.0 5.0 -1.5 100.0

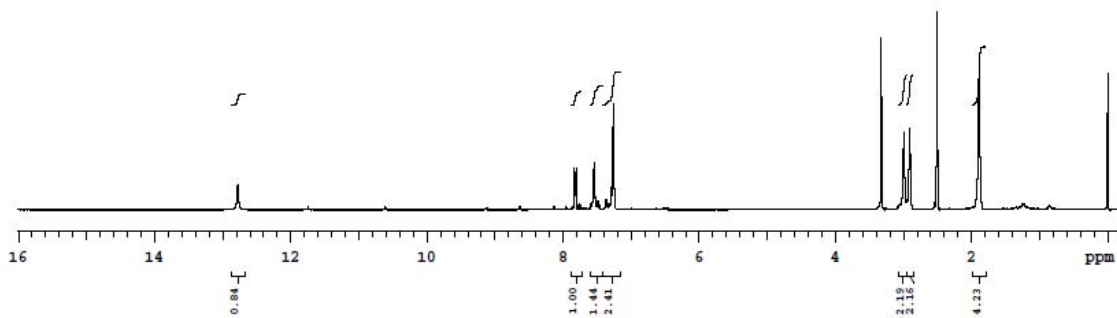
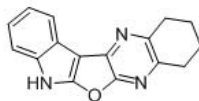
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
378.0226	378.0242	-1.6	-4.2	14.5	11.8	C19 H13 N3 O Br

TDC-117 C108/CSAT5/043



AR.No: ME0715/270

Analyt : Mallikarjun
Solvent : dmsc
Date : Jul 2 2015
NUCLEUS : H1
FRQ (MHz): 400.22
EXP : PROTON

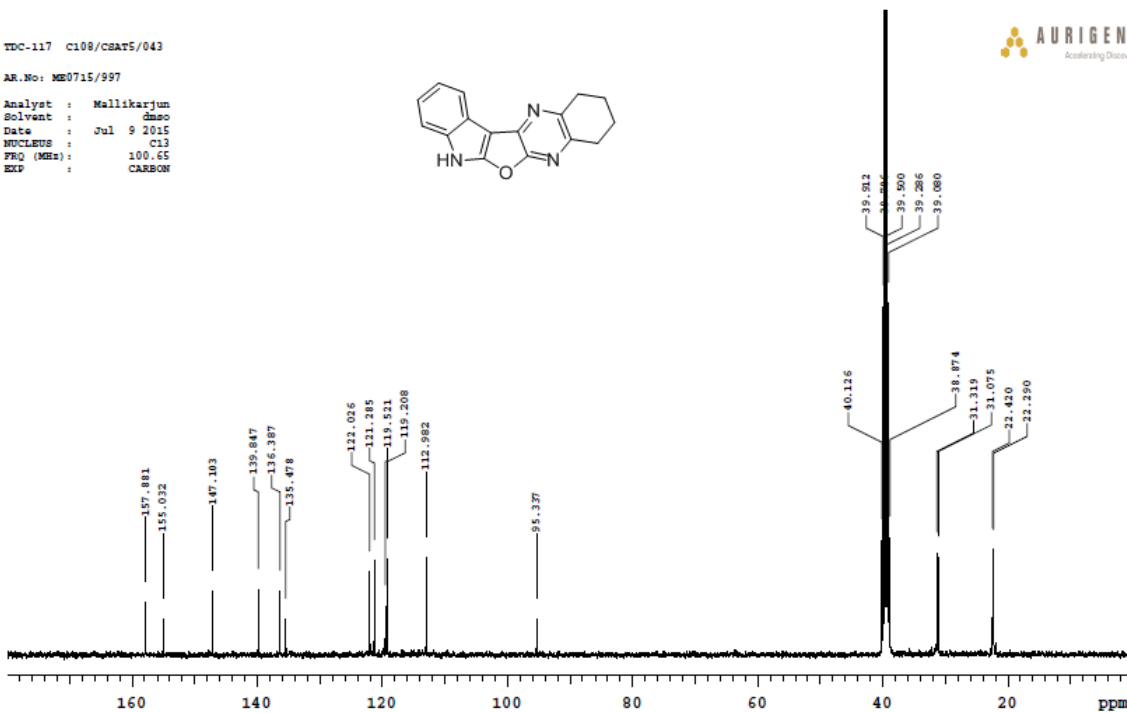
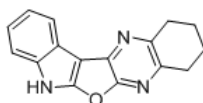


TDC-117 C108/CSAT5/043



AR.No: ME0715/997

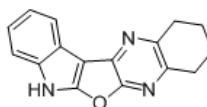
Analyt : Mallikarjun
Solvent : dmsc
Date : Jul 9 2015
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : CARBON



Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 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
40 formula(e) evaluated with 1 results within limits (up to 10 closest results for each mass)

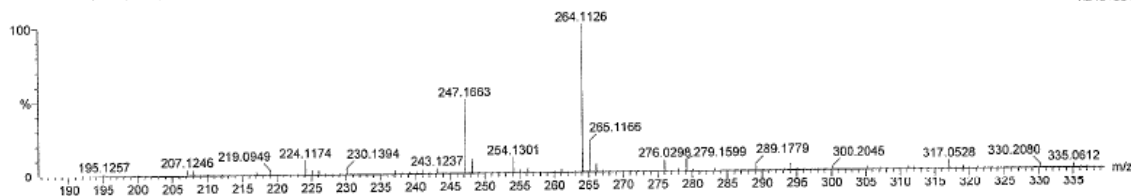
Elements Used:

C: 0-22 H: 0-30 N: 0-4 O: 0-2

C108/CSAT5/043

150702011 18 (0.493) Cm (17:20)

1: TOF MS ES+
4.24e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
264.1126	264.1137	-1.1	-4.2	11.5	590.8	C16 H14 N3 O

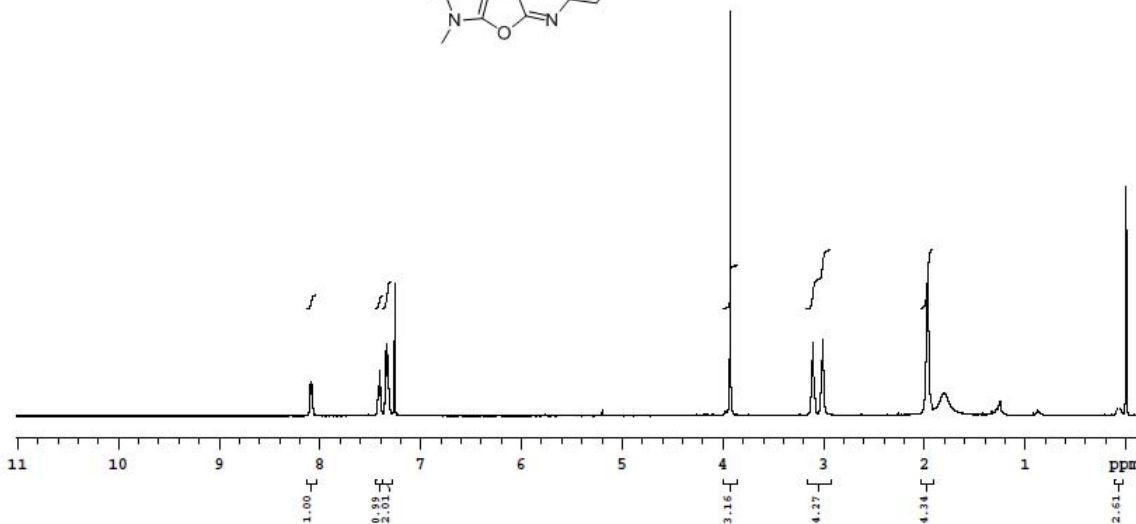
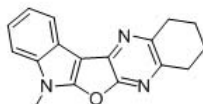
B. Sanyal
06/27/2015

TDC-117 C108/CSAT5/045



AR.No: MS0715/1986

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jul 20 2015
NUCLEUS : H1
P1 (MHz) : 400.22
EXP : PROTON

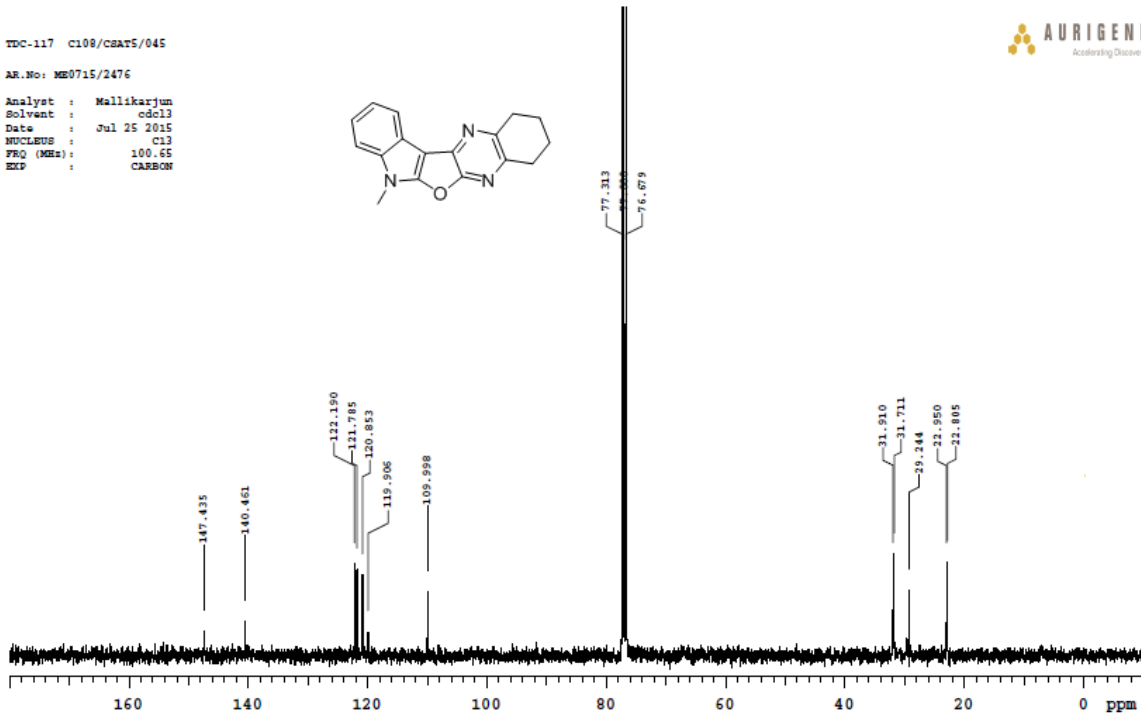
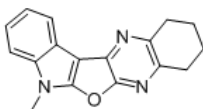


TDC-117 C108/CSAT5/045



AR.No: MB0715/2476

Analyst : Mallikarjun
Solvent : cdcl3
Date : Jul 25 2015
NUCLEUS : C13
FREQ (MHz): 100.65
EXP : CARBON



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 = 3

Monoisotopic Mass, Even Electron Ions

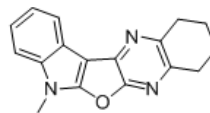
39 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

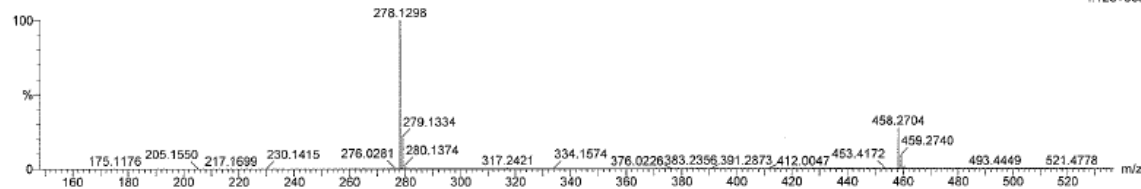
C: 0-25 H: 0-25 N: 0-5 O: 0-2

C108/CSAT5/045

150720003 13 (0.365) Cm (13:19)



1: TOF MS ES-
4.12e+005



Minimum: -1.5
Maximum: 5.0 10.0 80.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
278.1298	278.1293	0.5	1.8	11.5	562.6	C17 H16 N3 O

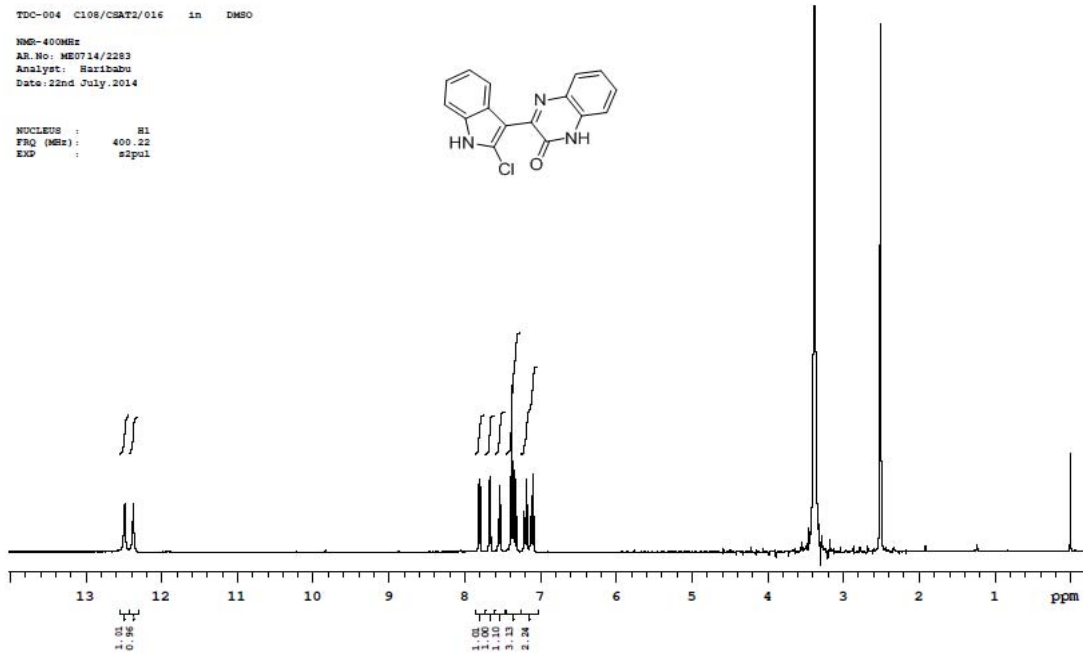
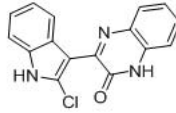
B. S. Mat
21/07/2015

Intermediate NMR

TDC-004 C108/CSAT2/016 in DMSO

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

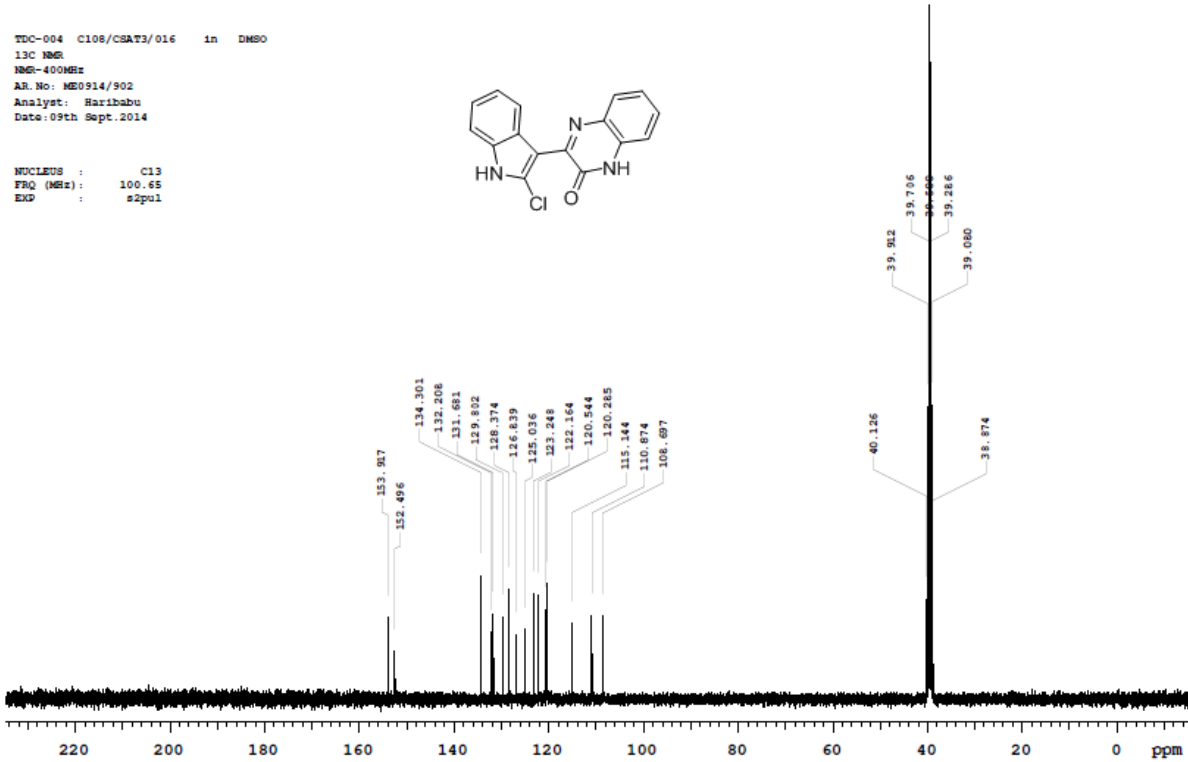
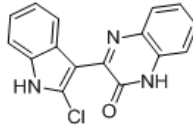
NUCLEUS : ¹H
FRQ (MHz): 400.22
EXP : s2pul



TDC-004 C108/CSAT3/016 in DMSO

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

NUCLEUS : ¹³C
FRQ (MHz): 100.65
EXP : s2pul



Elemental Composition Report

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

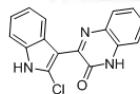
49 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)

Elements Used:

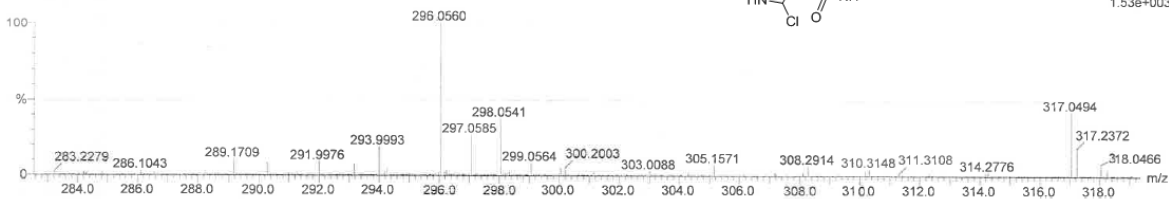
C: 0-35 H: 0-35 N: 0-3 O: 0-1 Cl: 0-1

C108/CSAT2/016

140721005 58 (1.565) Cm (57.59)



1: TOF MS ES+
1.53e+003



Minimum: -5.0
Maximum: 5.0 11.0 80.0

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