Electronic Supplementary Material (ESI) for RSC Advances.

An efficient and convenient protocol for the synthesis of Tetracyclic Isoindolo[1,2-a]quinazolines Derivatives.

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Supporting Informations

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Section C: **^{1}H, ^{13}C, Mass, ESMS and HRMS spectrum.....9**

Section A: General Information:

Reagent information.

Unless otherwise stated, all reactions were carried out in an oven-dried flask under a pure and dry nitrogen atmosphere. All lewis acids were purchased from Aldrich, SRL Co. and Merck.. Generally, Alkyne compound and alcohols were purchased from commercial sources (Aldrich, Acros, Alfa Aesar, Aladdin, Adamas) and purified when necessary. All the solvents were bought from Aldrich in sure seal bottle and were used as received. These solvents were transferred by syringe to the reaction flask. Analytical thin layer chromatography (TLC) was performed using Merck silica gel GF254 plates. For column chromatography, silica gel (60–120 mesh or 100–200 mesh) from SRL Co. was used.

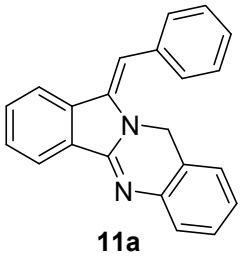
Analytical Information:

Melting points were determined either on DSC-60A, Schimadzu or on an electrothermal melting point apparatus and are uncorrected. Infrared spectra were recorded on a Perkin-Elmer 1650 Fourier transform spectrometer. NMR spectra were measured in CDCl3, DMSO-d6 (all with TMS as internal standard) on a Varian Gemini 400 MHz FT and 500 MHz FT magnetic resonance spectrometers. Chemical shifts (δ) are reported in ppm, and coupling constants (J) are in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, dd = doublet of doublets t = triplet, q = quartet, m = multiplet. Mass spectra were recorded on an HP-5989A quadrapole mass spectrometer.

Section B: Experimental Procedures:

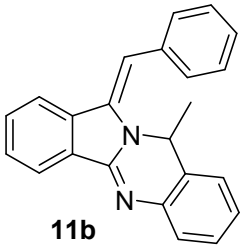
General Procedure for the synthesis ofIsoindolo[*1,2-b*]quinazolinederivatives: Boron trifluoride diethyl etherate (BF_3Et_2O, 48-50 % solution) (3.0 eq.) charged into a clean oven dried RB flask under nitrogen atmosphere. Charged a mixture of 2-Amino benzyl alcohol (1.0 eq.) and 2-(phenylethynyl)benzonitrile (1.0 eq.) and the mixture was warmed to70 °C for 10-14 h under nitrogen atmosphere. After completion of the reaction, the mixture was cooled to 0 °C and quenched into 10 % sodium carbonate solution (5.0 mL) and stirred for 1-2 h. The product was then extracted with DCM (2* 2.0 mL). The organic layer was washed with water (2.0 mL). Then dried over anhydrous sodium sulphate and concentrated the organic layer was under vaccum. Desired product was purified via column chromatography through silica gel and DCM as eluent.

***Section C*: Analytical data**



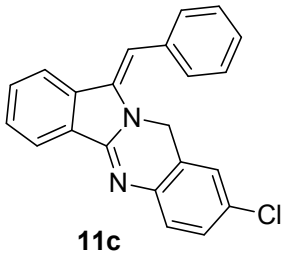
11a

(*Z*)-12-benzylidene-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11a): Off-white color solid; Yield: 68%, Melting point: 109-111 °C; IR (KBr): 693, 759, 1280, 1441, 1491, 1592, 1695, 1824, 1906, 2217, 3056, 3782; ^{1}H NMR (400 MHz, CD_3OD) δ: 4.58 (s, 2H, CH_2), 6.46 (d, *J* = 8.4 Hz, 1H, ArH), 6.75 (s, 1H, olefinic CH), 6.89 (t, *J* = 7.6 Hz, 1H, ArH), 7.09 (t, *J* = 7.6 Hz, 1H, ArH), 7.08 (d, *J* = 7.6 Hz, 1H, ArH), 7.32-7.43 (m, 4H, ArH), 7.53-7.57 (m, 4H, ArH), 8.19 (d, *J* = 8.4 Hz, 1H, ArH), ^{13}C NMR (100 MHz, DMSO d^6) δ: 48.6 (N-CH_2), 110.3(olefinic CH), 119.9, 124.6, 124.8, 125.5, 125.8, 126.2, 126.7, 126.9, 127.3, 127.3, 128.5 (2C), 128.7(2C), 131.0, 133.2, 136.2, 137.4, 139.2 (olefinic C), 151.3 (C=N); HRMS: m/z [M+H] calcd for $C_{22}H_{17}N_2$ [M+H]:309.1392; found: 309.1385 [M+H].



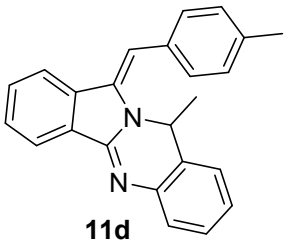
11b

(*Z*)-12-benzylidene-10-methyl-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11b): Light yellow color solid; Yield:72 %, Melting point: 105-107 °C; IR (KBr): 700, 758, 1233, 1311, 1383, 1476, 1591, 1622, 1691, 2968, 3411; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.93 (d, *J* = 6.4 Hz, 3H, CH_3), 5.29 (q, *J* = 6.4 Hz, 1H, NCH), 6.68 (s, 1H, olefinic CH), 6.86 (d, *J* = 7.2 Hz, 1H, ArH), 7.09 (t, *J* = 7.2 Hz, 1H, ArH), 7.25-7.30 (m, 2H, ArH), 7.35-7.45 (m, 5H, ArH), 7.51-7.59 (m, 2H, ArH), 7.77 (d, *J* = 7.6 Hz, 1H, ArH), 8.07 (d, *J* = 7.6 Hz, 1H, ArH),^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.8 (aliphaticCH_3), 51.3(N-CH), 103.7(olefinic CH), 119.5, 122.4, 125.3, 125.9, 127.2, 127.3, 128.0(2C), 128.3(2C), 128.9, 129.8 (2C), 130.9, 131.2, 135.3, 136.7, 138.1 (olefinic C), 141.4, 154.8 (C=N); MS: *m/z* (%) = 323.2[M+H]; HRMS: m/z [M+H] calcd for $C_{23}H_{19}N_2$[M+H]: 323.1548; found:323.1563[M+H].



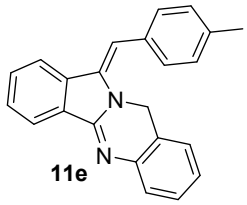
11c

(*Z*)-12-benzylidene-8-chloro-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11c): Light yellow color solid; Isolated yield:65% (141 mg), Melting point: 178-180 °C; IR (KBr): 1025, 1140, 1269, 1417, 1512, 1606, 2072, 2932, 3053, 3444, 3853; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.61 (s, 2H, CH_2), 6.77 (s, 1H, Olefinic CH), 6.81 (s, 1H), 7.19 (dd, *J* = 2.0, 8.4 Hz, 1H, ArH), 7.29-7.43 (m, 5H, ArH), 7.51-7.55 (m, 1H, ArH),7.59 (t, *J* = 8.0 Hz, 1H, ArH), 7.78 (d, *J* = 8.0 Hz, 1H, ArH), 8.04 (d, *J* =7.6 Hz, 1H, ArH), ^{13}C NMR (100 MHz, $CDCl_3$) δ: 46.2(N-CH_2), 104.1(Olefinic CH), 119.5, 122.4, 123.0, 126.1, 126.9, 127.3, 127.7, 128.4(2C), 128.6, 128.9, 129.6, 129.9, 130.1, 130.8, 131.1 (C-Cl), 134.8, 137.2, 137.5 (olefinic C), 140.5 (C=N); MS: *m/z* (%) = 343.1 [M+H];HRMS: m/z [M+ H] calcd for $C_{22}H_{16}N_2Cl$[M+H]: 343.1002; found: 343.0991[M+H].



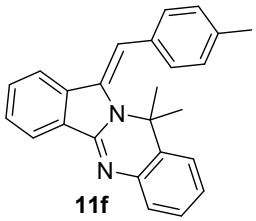
11d

(*Z*)-10-methyl-12-(4-methylbenzylidene)-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11d): Brown color solid; Yield: 71%, Melting point: 106-108 °C; IR (KBr): 760, 818, 1068, 1388, 1454, 1490, 1639, 1726, 2974, 3314; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.80 (d, *J* = 6.0 Hz, 3H,aliphaticCH_3), 2.37 (s, 3H, ArCH_3), 4.91-4.93 (m, 1H, aliphaticCH), 6.60 (d, *J* = 8.4 Hz, 1H, ArH),6.82 (s, 1H, olefinic CH), 6.92-6.97 (m, 1H, ArH), 7.17-77.20 (m, 3H, ArH), 7.28-7.31 (m, 1H, ArH), 7.34 (d, *J* = 7.4 Hz, 2H, ArH), 7.50-7.56 (m, 3H, ArH), 8.48 (d, *J* = 8.4 Hz, 1H, ArH),^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.2(aliphatic CH_3), 22.6 (Ar CH_3), 51.6(N-CH), 113.0 (olefinic CH),122.2, 125.0(2C), 125.4, 126.5(2C), 126.7, 126.8, 127.2(2C), 128.5, 129.6, 129.8(2C), 133.0(2C), 134.3, 139.2, 139.3(olefinic C), 153.3 (C=N); MS: *m/z* (%) = 337.2 [M+H]; HRMS: m/z [M+ H] calcd for $C_{24}H_{21}N_2$ [M+H]:337.1705; found:337.1706[M+H].



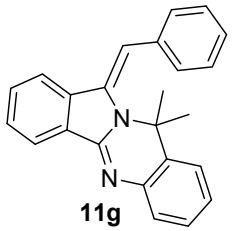
11e

(*Z*)-12-(4-methylbenzylidene)-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11e): Brown color solid; Yield: 69 %, Melting point: 108-110 °C; IR (KBr): 756, 875, 1031, 1151, 1255, 1381, 1507, 1600, 1735, 2223, 2963, 3425; ^{1}H NMR (400 MHz, CD_3OD) δ:2.37 (s, 3H, $ArCH_3$), 4.84 (s, 2H, CH_2), 6.85 (s, 1H, olefinic CH), 7.09 (t, *J* = 8.0 Hz, 1H, ArH), 7.25 (d, *J* = 8.4 Hz, 2H, ArH), 7.35 (t, *J* = 8.0 Hz, 1H, ArH), 7.46-7.51(m, 4H, ArH), 7.77-7.81 (m, 1H, ArH), 7.99 (d, *J* = 4.0 Hz, 2H, ArH), 8.42 (d, *J* = 8.4 Hz, 1H, ArH);^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.8($ArCH_3$), 51.2(N-CH_2), 110.2 (olefinic CH), 121.2, 123.3, 124.5, 125.6, 125.7, 125.9, 127.1(2C), 128.2(2C), 129.5(2C), 130.6, 133.6, 133.7, 134.4, 136.2, 138.2, 139.4(olefinic C), 149.6 (C=N); MS: *m/z* (%) = 323.2 [M+H]



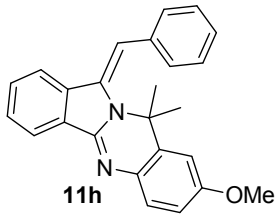
11f

(*Z*)-10,10-dimethyl-12-(4-methylbenzylidene)-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11f): Off white color solid; Yield:74%, Melting point: 169-171 °C; IR (KBr): 754, 810, 1136, 1280, 1308, 1366, 1480, 1629, 2970, 3434; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.71 (b, 6H, Aliphatic CH_3), 2.35 (s, 3H, $ArCH_3$), 6.46 (s, 1H, ArH), 6.47 (s, 1H, olefinic CH), 6.85 (t, *J* = 8.0 Hz, 1H, ArH), 7.07 (t, *J* = 7.6 Hz, 1H, ArH), 7.13 (d, *J* = 7.6 Hz, 2H, ArH), 7.28-7.37 (m, 5H, ArH), 7.44-7.47 (m, 1H, ArH), 8.33 (d, *J* = 8.0 Hz, 1H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.2($ArCH_3$), 28.0 (2C, aliphatic CH_3),54.7(NC-$(CH_3)_2$), 110.2 (olefinic CH), 121.1, 123.3, 124.5, 125.6, 125.7, 125.9, 127.1(2C), 128.2(2C), 129.4(2C), 130.5, 133.5, 133.7, 134.4, 136.2, 138.2, 139.4 (olefinic C), 149.6 (C=N); MS: *m/z* (%) = 351.3 [M+H]; HRMS: m/z [M+ H] calcd for $C_{25}H_{23}N_2$[M+H]: 351.1861; found: 351.1856[M+H].



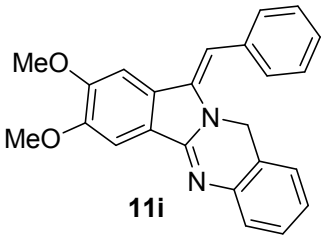
11g

(*Z*)-12-benzylidene-10,10-dimethyl-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11g): Light yellow color solid; Yield:75%, Melting point: 208-210 °C; IR (KBr): 1025, 1140, 1269, 1417, 1512, 1606, 2072, 2932, 3053, 3444, 3853; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.72 (s, 6H, alpiphatic CH_3), 6.43 (d, *J* = 8.0 Hz, 1H, ArH), 6.49 (s, 1H, olefinic CH), 6.84 (t, *J* = 7.2 Hz, 1H, ArH), 7.06 (t, *J* = 7.2 Hz, 1H, ArH), 7.29-7.36 (m, 6H, ArH), 7.39-7.46 (m, 3H, ArH), 8.34 (d, *J* = 7.6 Hz, 1H, ArH), ^{13}C NMR (100 MHz, $CDCl_3$) δ: 28.7 (2C, aliphatic CH_3), 54.7(NC-$(CH_3)_2$), 110.8 (olefinic CH), 121.1, 123.4, 124.6, 125.6, 125.7, 126.0, 127.1(2C), 127.2(2C), 128.2, 128.7(2C), 130.6, 133.4, 133.7, 136.0, 137.2, 139.3 (olefinc C), 149.5 (C=N); MS: *m/z* (%) = 383.20 [M+H];HRMS: m/z [M+ H] calcd for $C_{24}H_{21}N_2$[M+H]:337.1705; found:337.1718[M+H].



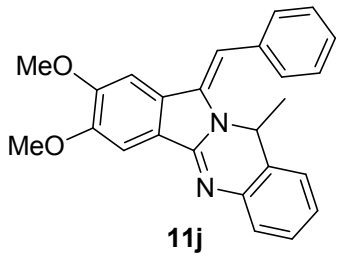
11h

(*Z*)-12-benzylidene-8-methoxy-10,10-dimethyl-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11h): Light yellow color solid; Yield: 69%, Melting point: 170-172 °C; IR (KBr): 695, 762, 1063, 1258, 1467, 1572, 1615, 2929, 3438; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.40 (s, 6H, aliphatic CH_3), 3.98 (s, 3H, OCH_3), 6.71 (s, 1H, olefinic CH), 6.75 (d, 1H, *J* = 8.0 Hz, ArH), 6.85 (d, *J* = 8.0 Hz, 1H, ArH), 7.07 (t, *J* = 7.2 Hz, 1H, ArH), 7.33 (t, *J* = 7.6 Hz, 1H, ArH), 7.38-7.54 (m, 7H, ArH), 7.69 (d, *J* = 7.6Hz, 1H, ArH), 8.15 (d, *J* = 7.2 Hz, 1H, ArH), ^{13}C NMR (100 MHz, $CDCl_3$) δ: 28.4 (2C, aliphatic CH3), 56.2(NC-$(CH_3)_2$), 60.4(OCH_3), 109.8 (olefinic CH), 121.1, 123.3, 124.5, 125.7, 125.9, 127.1 (2C), 128.3, 129.6 (2C), 130.0,133.2, 133.7, 134.4, 136.2, 138.2, 138.6 (olefinic C), 149.6, 152.8, 154.1 (C=N); HRMS: m/z [M+H] calcd for $C_{25}H_{23}N_2O$[M+H]: 367.1810; found: 367.1816[M+H].



11i

(*Z*)-12-benzylidene-2,3-dimethoxy-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11i): Light yellow color solid; yield: 67%, Melting point: 145-147 °C;IR (KBr): 730, 875, 1011, 1119, 1287, 1458, 1516, 1692, 2219, 2972, 3431; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.04 (s, 6H, OCH_3), 4.62 (s, 2H, CH2), 6.62 (s, 1H, olefinic CH), 6.86 (d, *J* = 8.0 Hz, 1H, ArH), 7.07 (t, *J* = 7.6 Hz, 1H, ArH), 7.26 (s, 2H, ArH), 7.28-7.43 (m, 6H, ArH), 7.52 (s, 1H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 43.5 (N-CH_2), 58.7 (2C, OCH3), 105.28 (olefinic CH), 122.7, 123.1, 124.5, 125.6, 125.7, 125.9, 126.9, 128.3 (2C), 129.2, 129.4, 130.2, 130.5, 131.1, 135.3, 136.5, 137.9, 140.1(olefinic C), 142.4, 154.8 (C=N); HRMS: m/z [M+ H] calcd for $C_{24}H_{21}N_2O_2$ [M+H]:369.1603; found:369.1621[M+H].

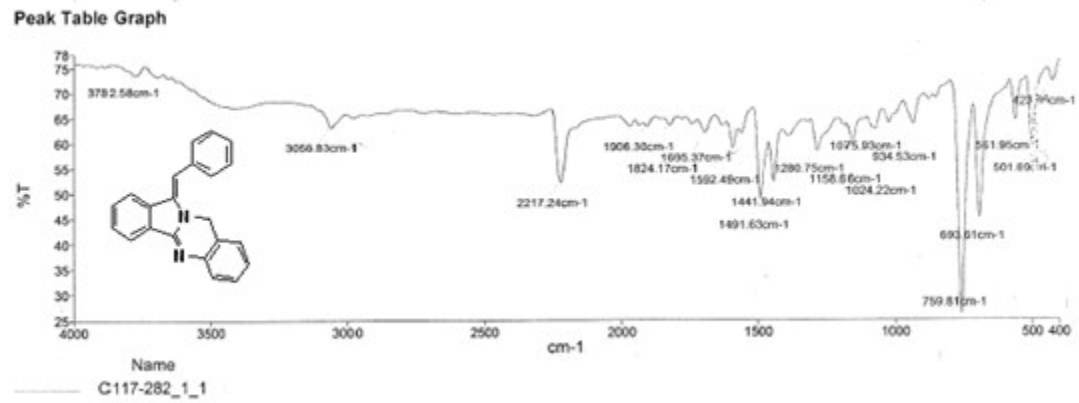


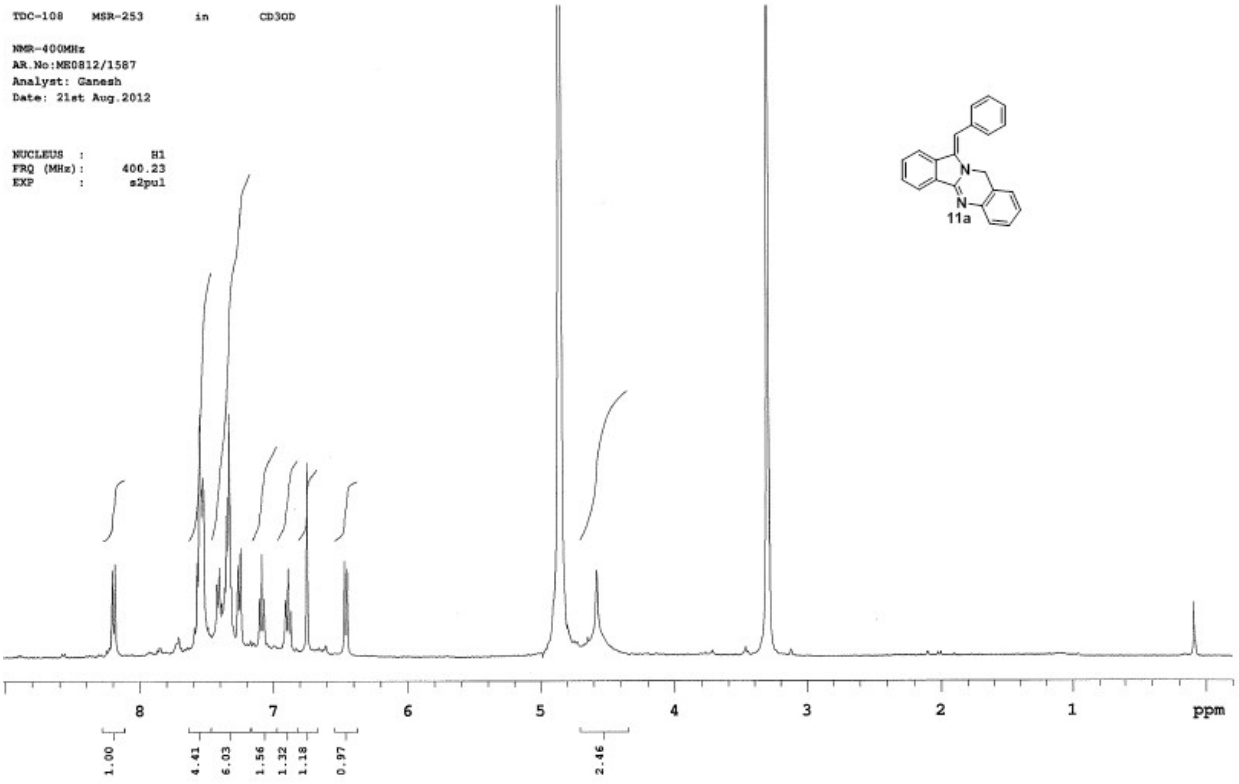
11j

(*Z*)-12-benzylidene-2,3-dimethoxy-10-methyl-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11j): Light yellow color solid; yield: 64%, Melting point: 163-165 °C; IR (KBr): 705, 772, 851, 1070, 1184, 1284, 1495, 1571, 1628, 2960, 3444 ; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.91 (d, *J* = 6.0 Hz, 3H, aliphatic CH_3), 4.03 (s, 6H, OCH_3), 5.22 (q, *J* = 6.4 Hz, 1H, NCH), 6.55 (s, 1H, olefinic CH), 6.85 (d, *J* = 7.2 Hz, 1H, ArH), 7.08 (t, *J* = 7.6 Hz, 1H, ArH), 7.18 (s, 1H, ArH),7.27-7.44 (m, 7H, ArH), 7.50 (s, 1H, ArH),^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.4 (aliphatic CH_3), 51.3 (NCH), 56.2 (O-CH3), 56.3 (OCH3), 101.4 (olefinic CH), 103.2, 103.6, 124.8, 125.1, 125.9, 127.1, 127.4 (2C), 128.0, 128.2, 128.4 (2C), 129.7 (olefinic C), 131.8, 135.3, 136.9, 141.3, 150.9, 152.5, 155.3 (C=N); HRMS: m/z [M+ H] calcd for $C_{25}H_{23}N_2O_2$[M+H]: 383.1760; found: 383.1774 [M+H].

Section D: **^{1}H, ^{13}C, Mass, ESMS and HRMS spectrum:**

1. **(*Z*)-12-benzylidene-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11a):**





NSR/253/P in DMSO
TDC-108

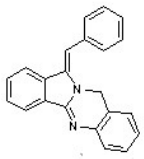
NMR: 500MHz
AR.No: IN0811/327
Date:30th Aug.2011;
Analyst:Haribabu

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

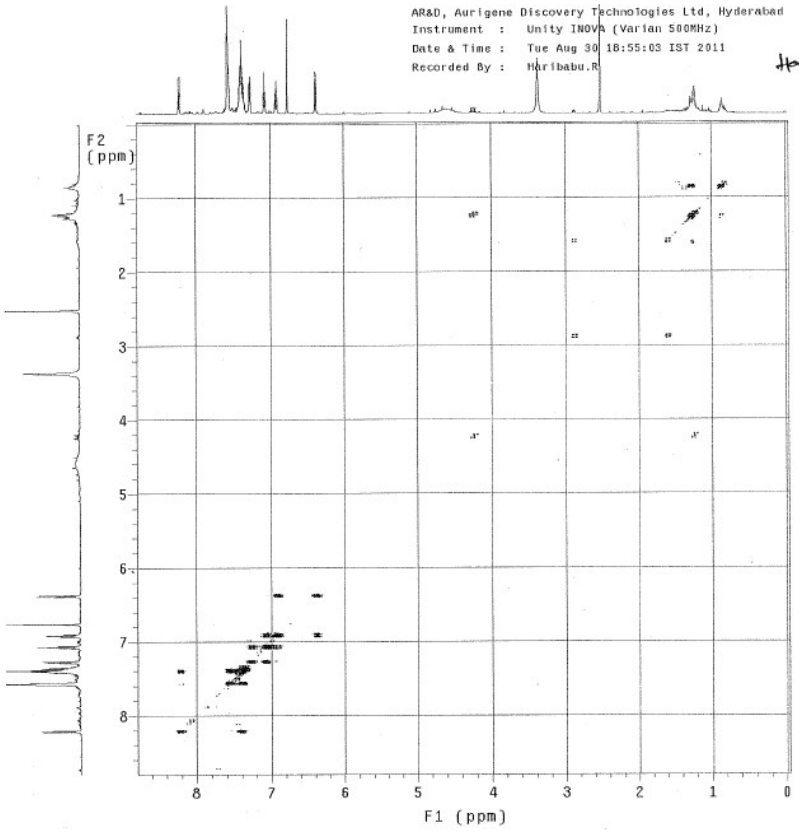
Pulse Sequence: gDQCOSY

Solvent: DMSO
Temp. 25.0 C / 298.1 K
Operator: vnmr1
INOVA-500 "dr-inovaj"

Relax. delay 1.000 sec
Acq. time 0.185 sec
Width 5526.4 Hz
2D Width 5526.4 Hz
8 repetitions
2 x 256 increments
OBSERVE H1, 499.6259205 MHz
DATA PROCESSING
Sq. sine bell 0.139 sec
Shifted by -0.093 sec
F1 DATA PROCESSING
Gauss apodization 0.052 sec
Sq. sine bell 0.037 sec
Shifted by -0.025 sec
FT size 2048 x 2048
Total time 1 hr, 24 min, 45 sec



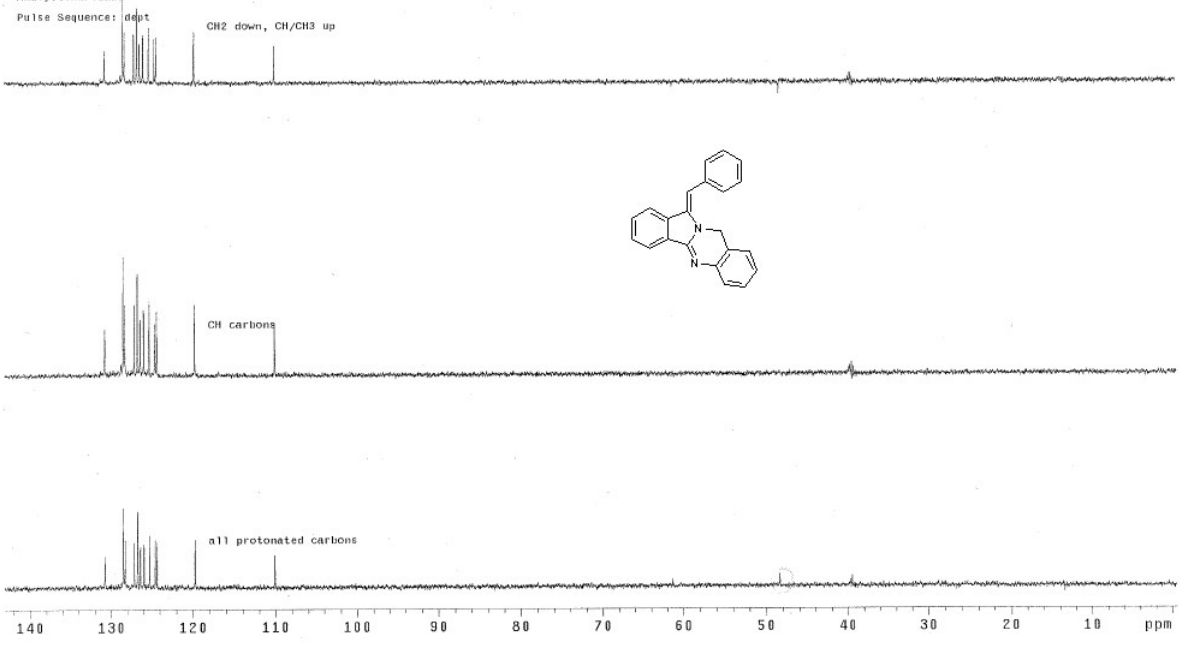
AR&D, Aurigene Discovery Technologies Ltd, Hyderabad
Instrument : Unity INOVA (Varian 500MHz)
Date & Time : Tue Aug 30 18:55:03 IST 2011
Recorded By : Haribabu.R



NSR/253/P in DMSO
TDC-108
not reffered
NMR: 500MHz
AR.No: IN0811/328
Date:30th Aug.2011;
Analyst:Haribabu

Pulse Sequence: dept

AR&D, Aurigene Discovery Technologies Ltd, Hyderabad
Instrument : Unity INOVA (Varian 500MHz)
Date & Time : Tue Aug 30 18:51:49 IST 2011
Recorded By : Haribabu.R



MSR/253/P in DMSO
TDC-108

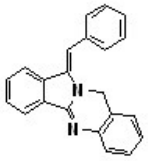
NMR: 500MHz
AR.No: IN0811/327
Date:30th Aug.2011;
Analyst:Haribabu

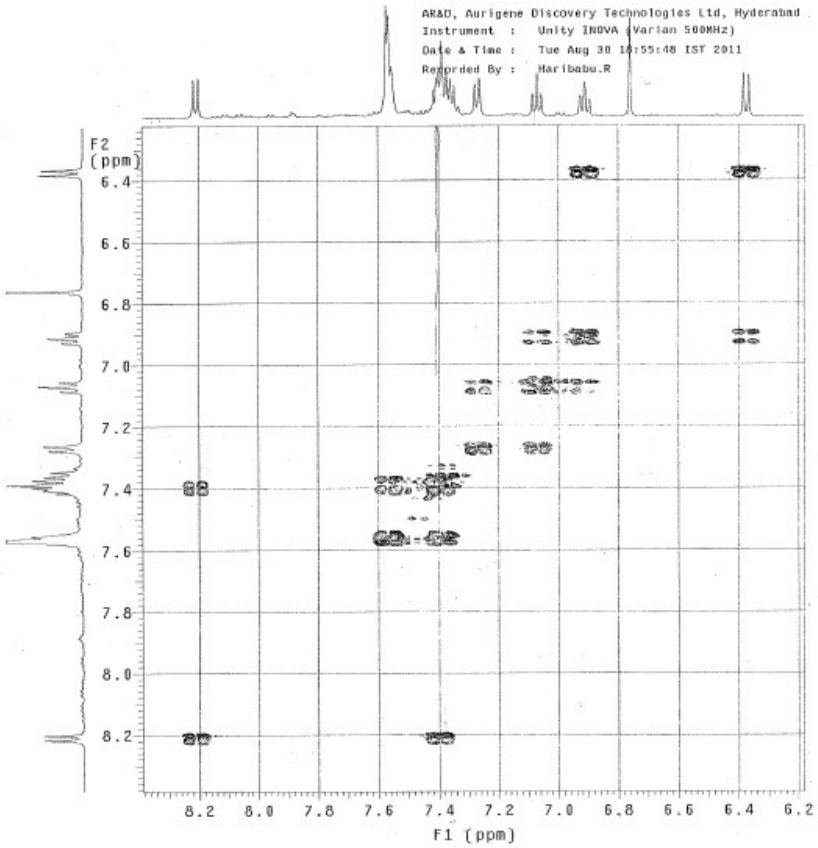
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: gDQCOSY

Solvent: DMSO
Temp. 25.0 C / 298.1 K
Operator: vnmr1
INOVA-500 "dr-inovaj"

Relax. delay 1.000 sec
Acq. time 0.185 sec
Width 5526.4 Hz
2D Width 5526.4 Hz
8 repetitions
2 x 256 increments
OBSERVE H1, 499.6259205 MHz
DATA PROCESSING
Sq. sine bell 0.139 sec
Shifted by -0.093 sec
F1 DATA PROCESSING
Gauss apodization 0.052 sec
Sq. sine bell 0.037 sec
Shifted by -0.025 sec
FT size 2048 x 2048
Total time 1 hr, 24 min, 45 sec

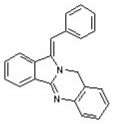


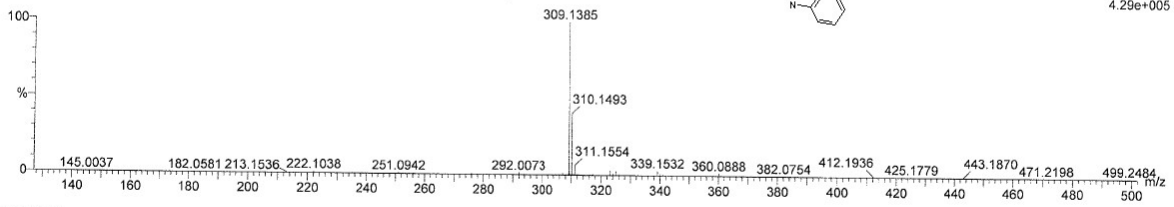


Elemental Composition Report

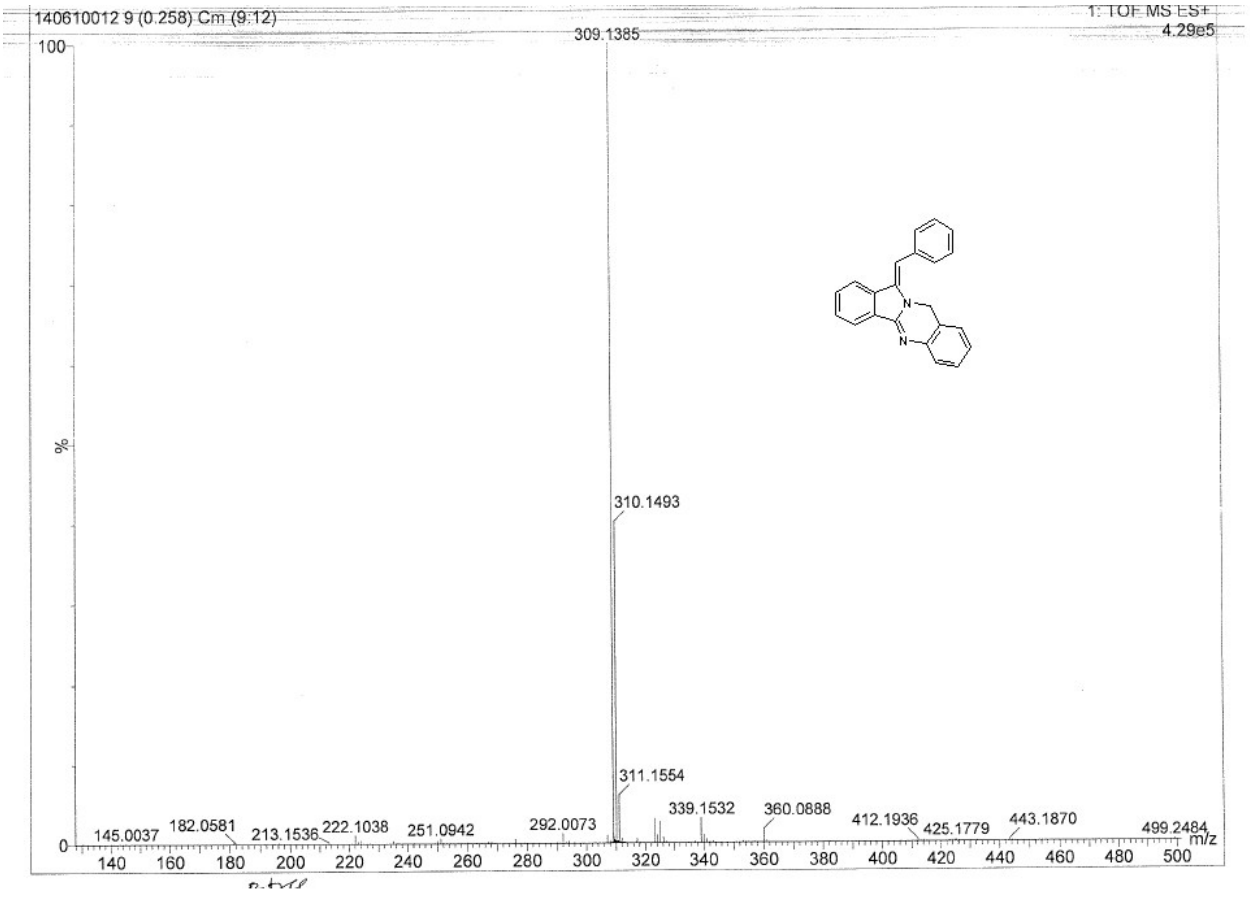
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-30 N: 0-4
MSR253
140610012 9 (0.258) Cm (9:12)

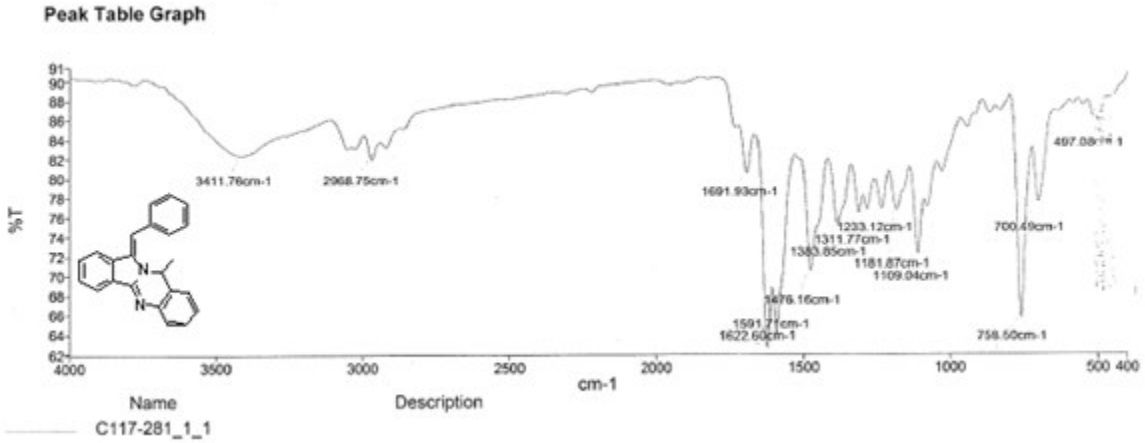




Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
309.1385	309.1392	-0.7	-2.3	15.5	12722.0	C22 H17 N2



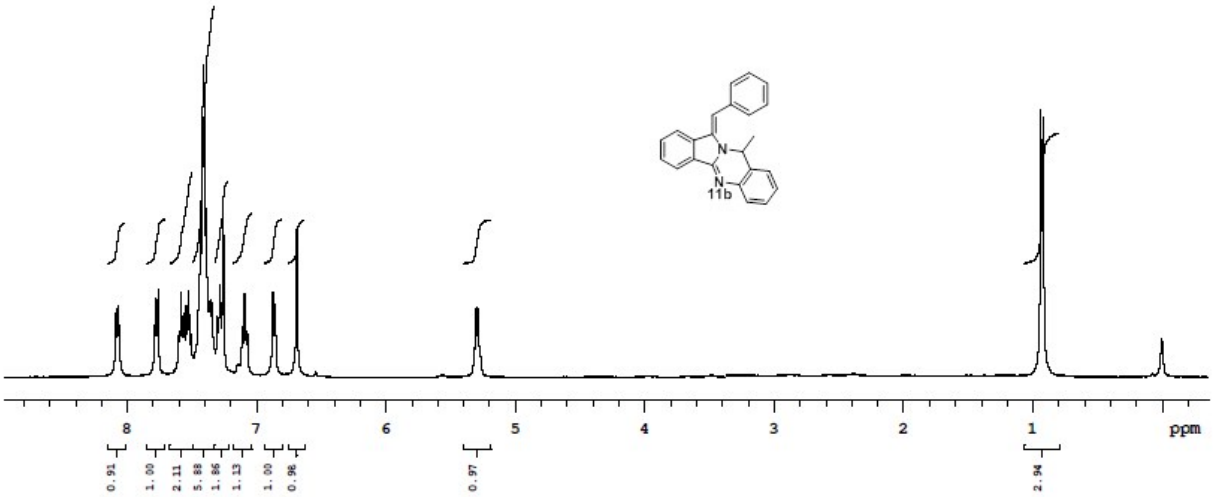
2. (*Z*)-12-benzylidene-10-methyl-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11b):



TDC-108 MSR/281 in CDCl3

NMR-400MHz
AR.No:ME0312/170
Analyst:Haribabu
Date: 02nd March.2012

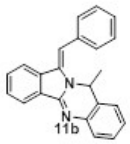
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul

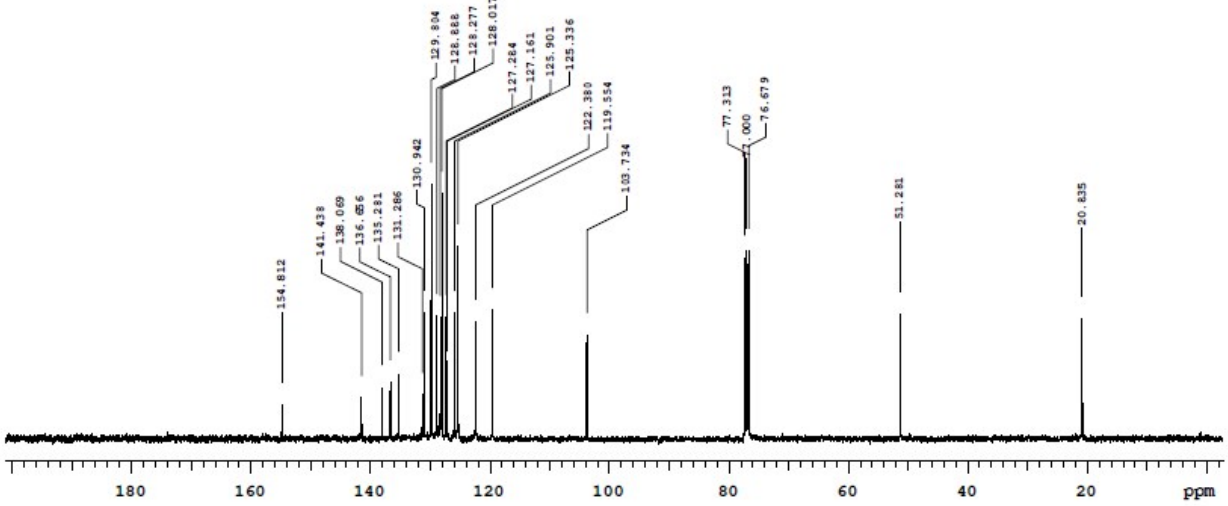


TDC-108 MSR-281 in CDCl3

NMR-400MHz
AR.No:ME0312/313
Analyst: Ganesh
Date: 02nd March.2012

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





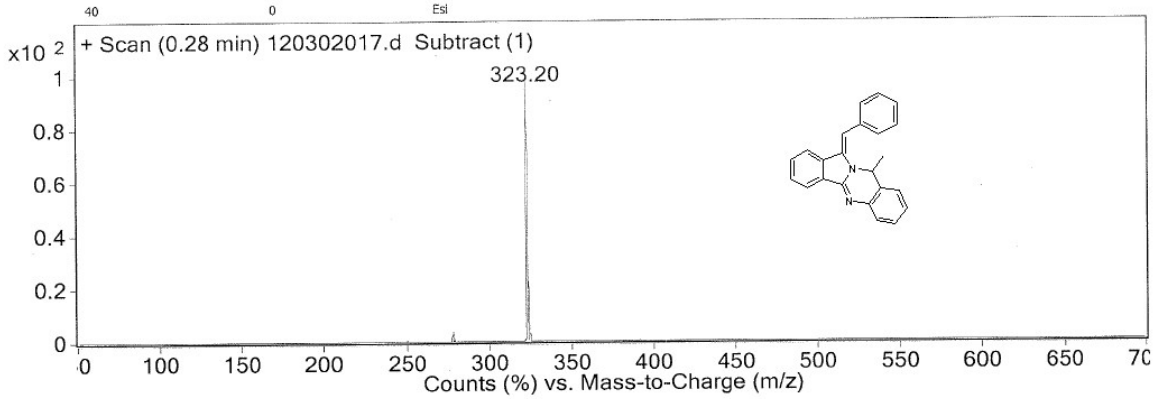
CPS,MIYAPUR

Mass Analysis Report

Data Filename	120302017.d	**Sample Name**	MSR/259
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	EDC-5.m	**Comment**	

User Spectra

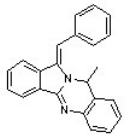
Fragmentor Voltage	Collision Energy	Ionization Mode
40	0	Esi



Elemental Composition Report

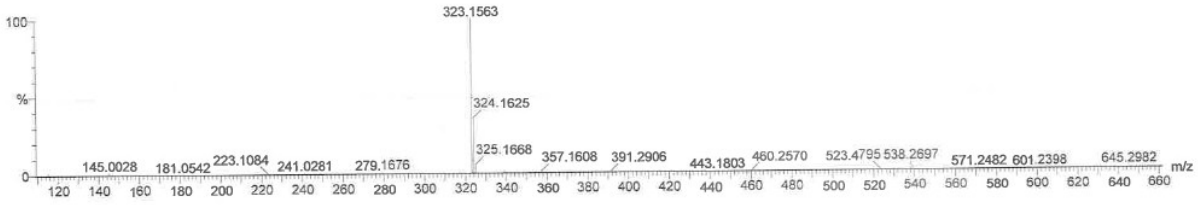
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
10 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



MSR281
140618005 23 (0.621) Cm (23:28-2:4)

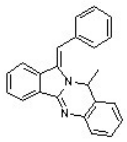
1: TOF MS ES+
9.15e+004



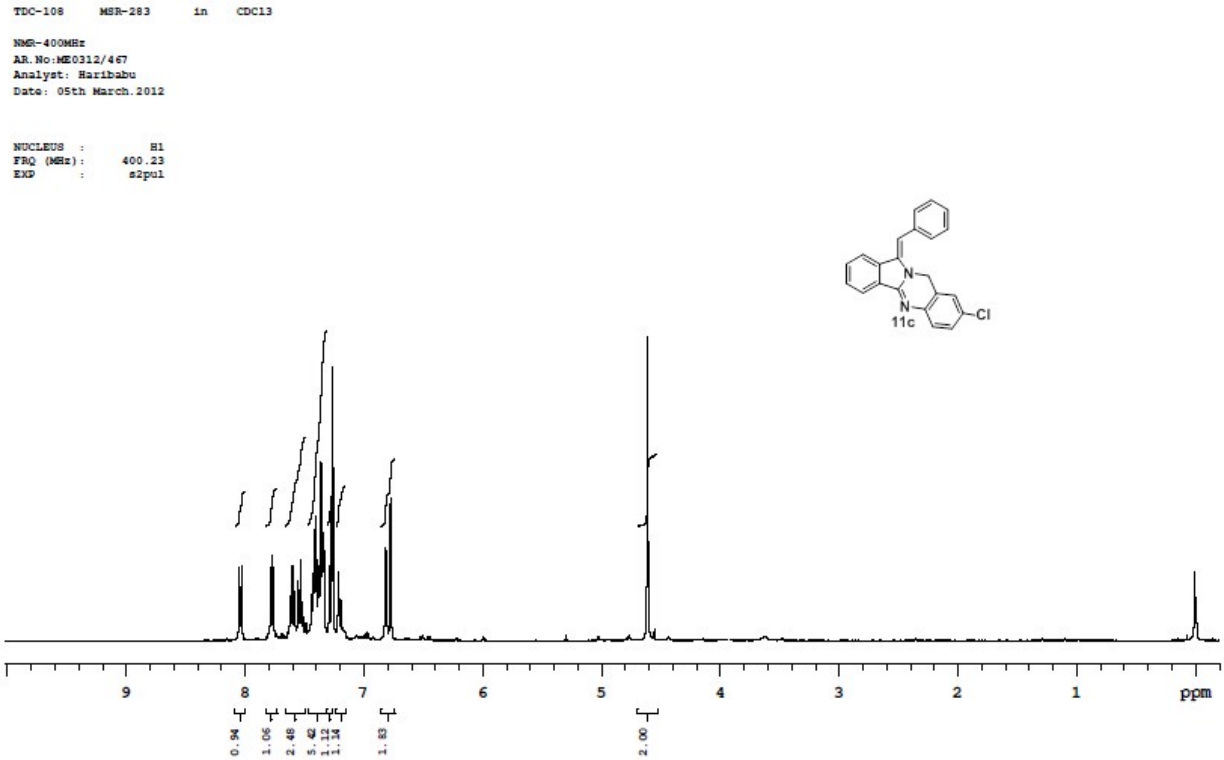
Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
323.1563	323.1548	1.5	4.6	15.5	1265.3	C23 H19 N2

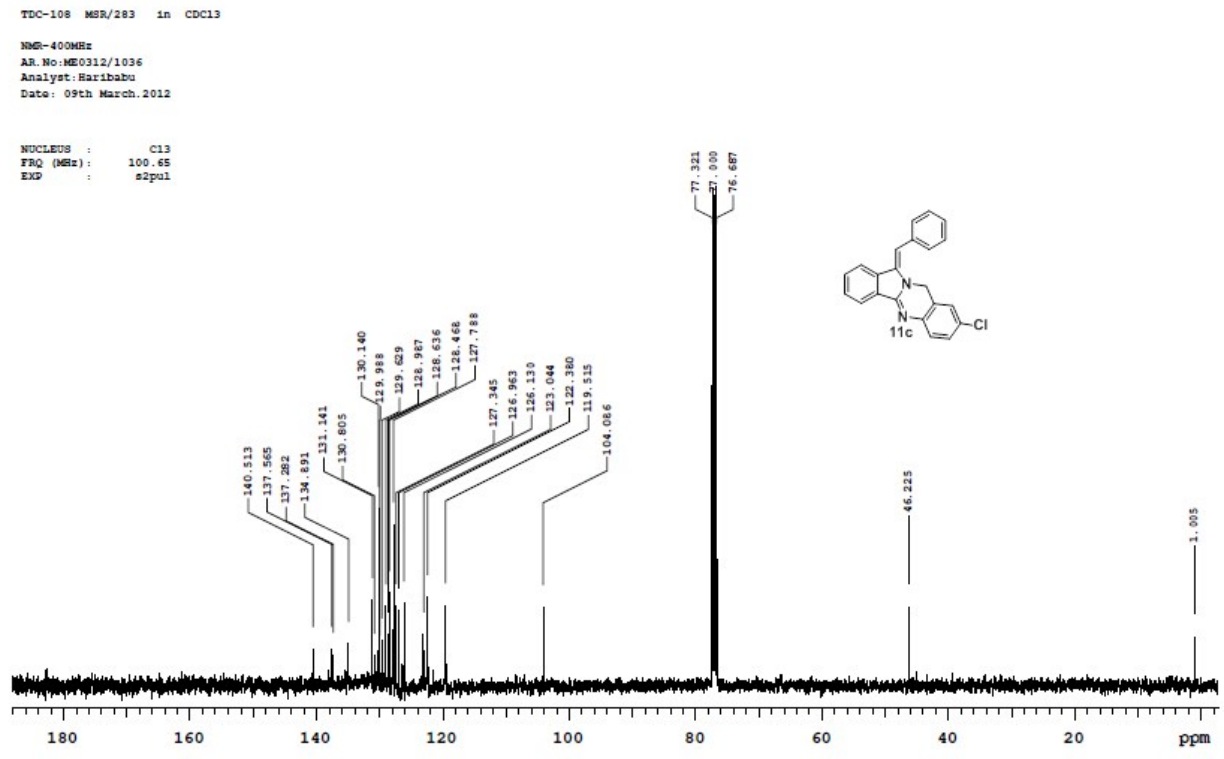
MSR281
140618005 23 (0.621) Cm (23:28-2:4)

1: TOF MS ES+
9.15e4



3. (*Z*)-12-benzylidene-8-chloro-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11c):





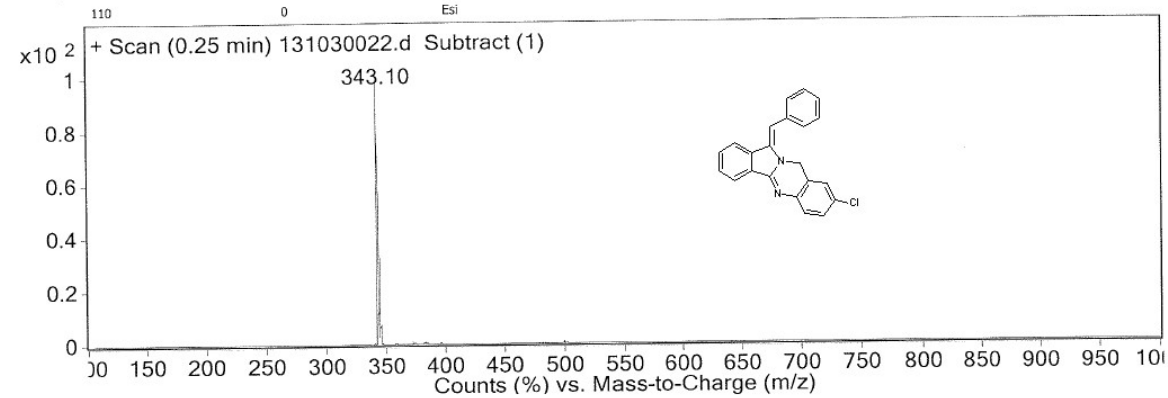
CPS,MIYAPUR

Mass Analysis Report

Data Filename	131030022.d	**Sample Name**	MSR283
Sample Type	Sample	**Position**	Vial 61
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.M	**IRM Calibration Status**	Success
DA Method	CACH8.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
110	0	Esi



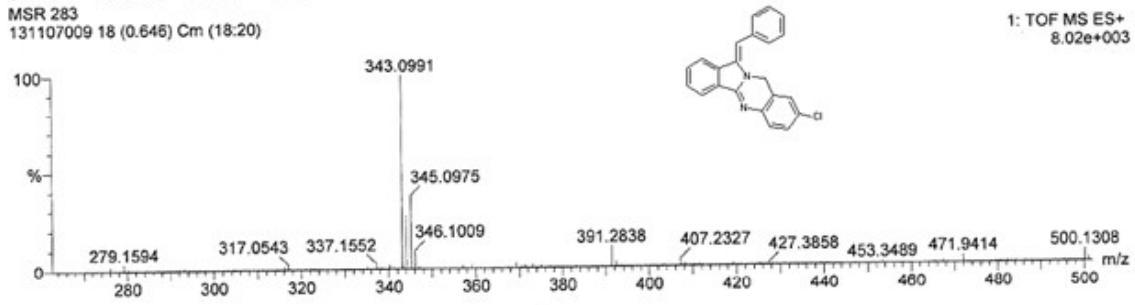
Elemental Composition Report

Single Mass Analysis

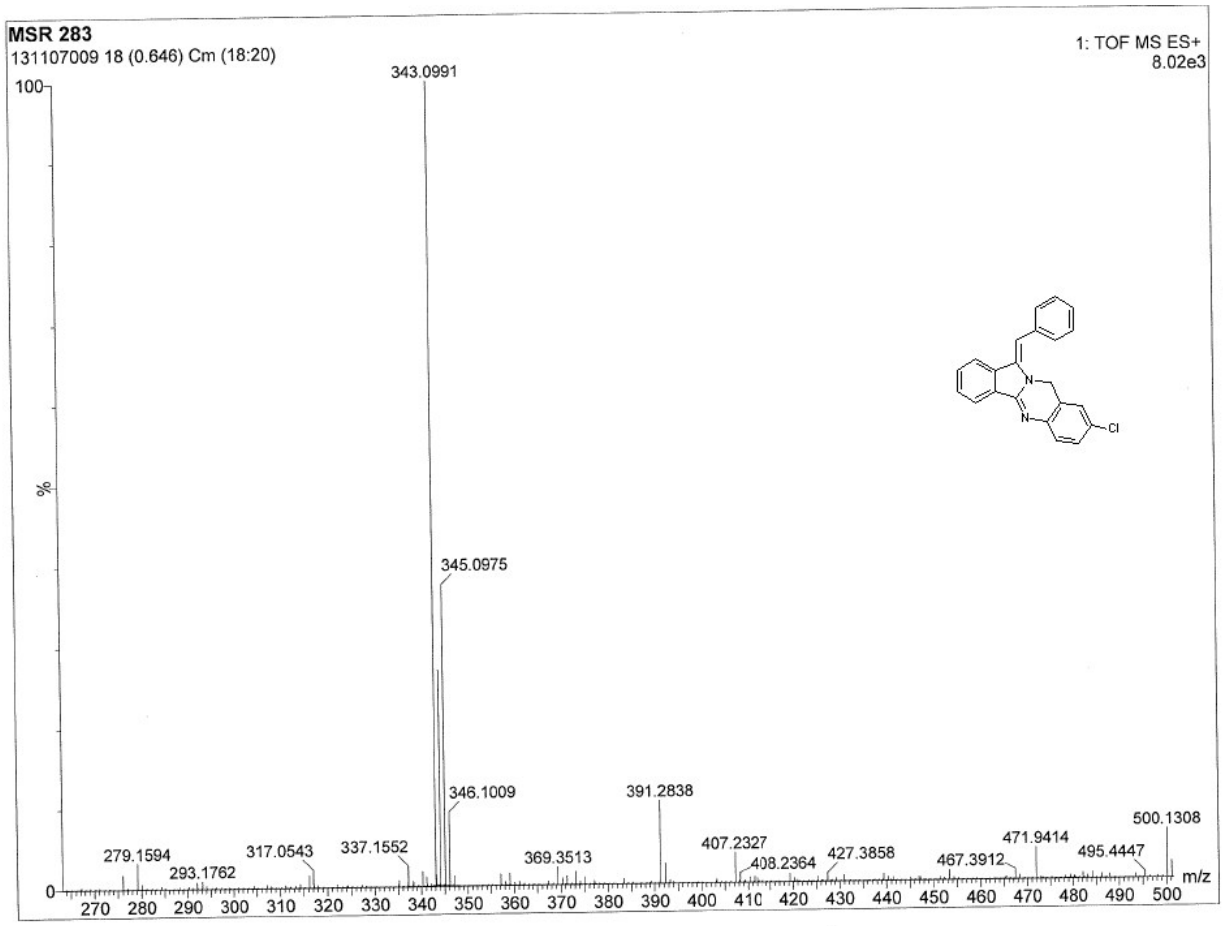
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

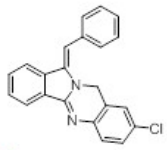
Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 10 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-25 N: 0-3 O: 0-2 Cl: 0-1

MSR 283
131107009 18 (0.646) Cm (18:20)

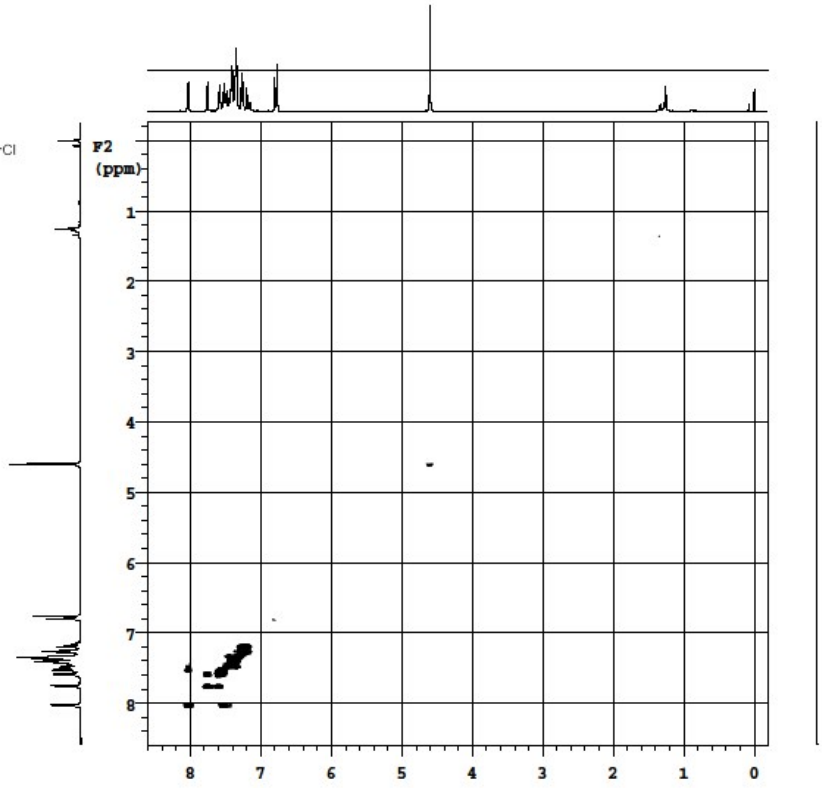


Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
343.0991	343.1002	-1.1	-3.2	15.5	8.0	C22 H16 N2 Cl





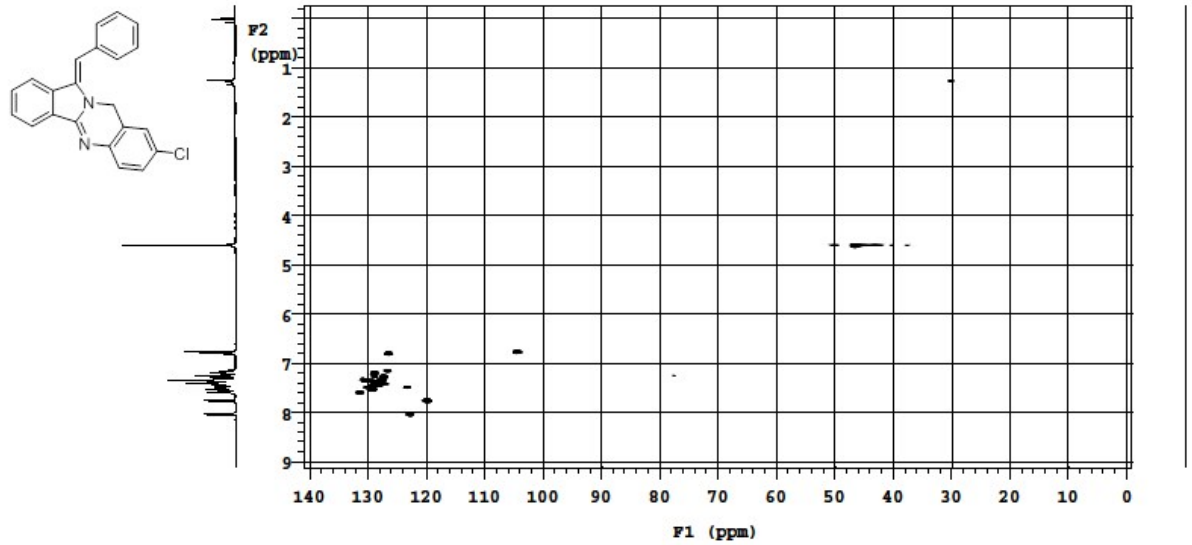

```
MSR283 in  CDCl3
TDC-108

AR.No:IN0514/127
Date:22nd May.2014
Analyst: Haribabu.R

exp2  gDQCOSY

      SAMPLE                FLAGS
date    May 22 2014  hs                 nn
solvent       CDCl3  sspul              y
sample              hsglvl          4255
   ACQUISITION           SPECIAL
sw           5629.0  temp            25.0
at             0.182 gain              18
np              2048 spin        not used
fb          not used   F2 PROCESSING
ss                32 sb            -0.136
d1             1.000 sbs           -0.091
nt                 8 lsfid            -17
  2D ACQUISITION     fn              2048
sw1          5629.0   F1 PROCESSING
ni              400 sb1           -0.069
   TRANSMITTER      sbs1          -0.025
tn               H1 gf1             0.025
sfrq       499.626  gfs1        not used
tof         -182.5  proc1             lp
tpwr            58  fn1             2048
pw            6.450       DISPLAY
    GRADIENTS       sp             -131.9
gzlvl1         3191 wp             4425.2
gt1        0.002500 sp1             -93.5
gzlvl2         6382 wp1            4392.2
gt2        0.002500 rf1             511.2
gstab      0.000500 rfp                0
    DECOUPLER       rfl1            511.2
dn               C13 rfp1               0
dm               nnn           PLOT
                     wc             138.9
                     sc              10.0
                     wc2            138.9
                     sc2                0
                     vs               714
                     th                 2
                     ai  cdc  ph
```



MSR283 in CDCl3
TDC-108

AR.No:IN0514/128
Date:22nd May.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : gHSQC

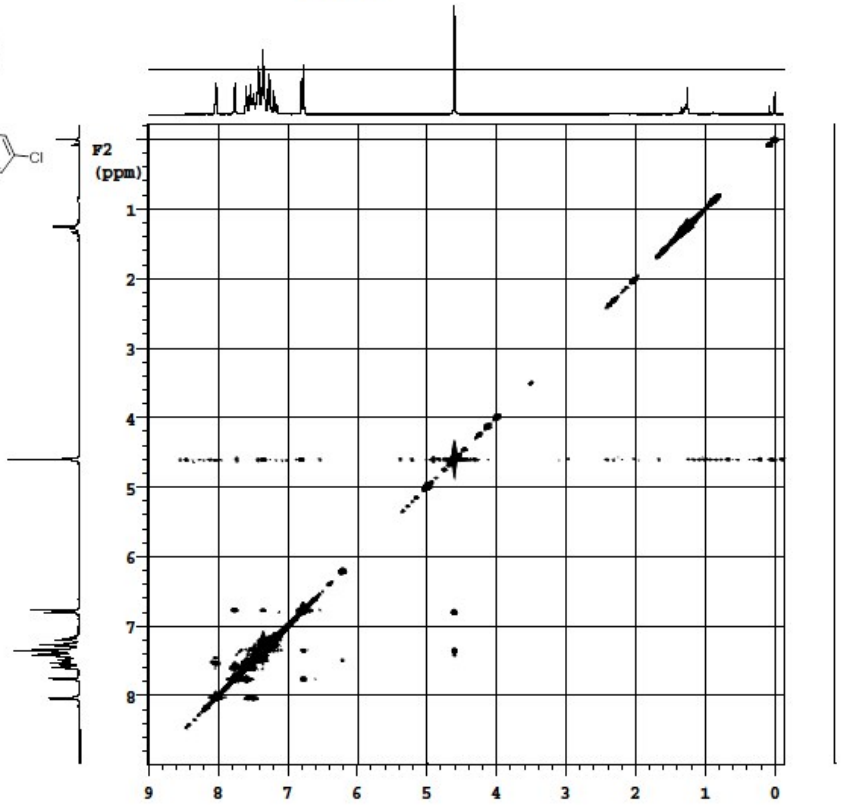


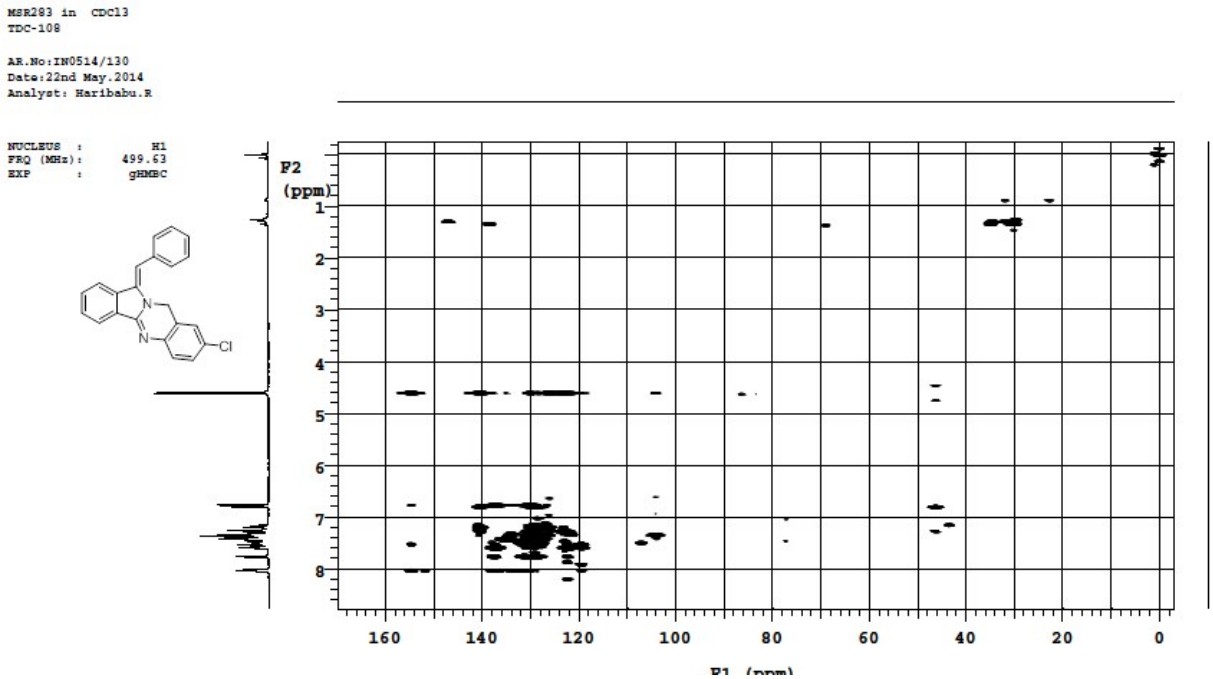
MSR283 in CDCl3
TDC-108

AR.No:IN0514/129
Date:22nd May.2014
Analyst: Haribabu.R

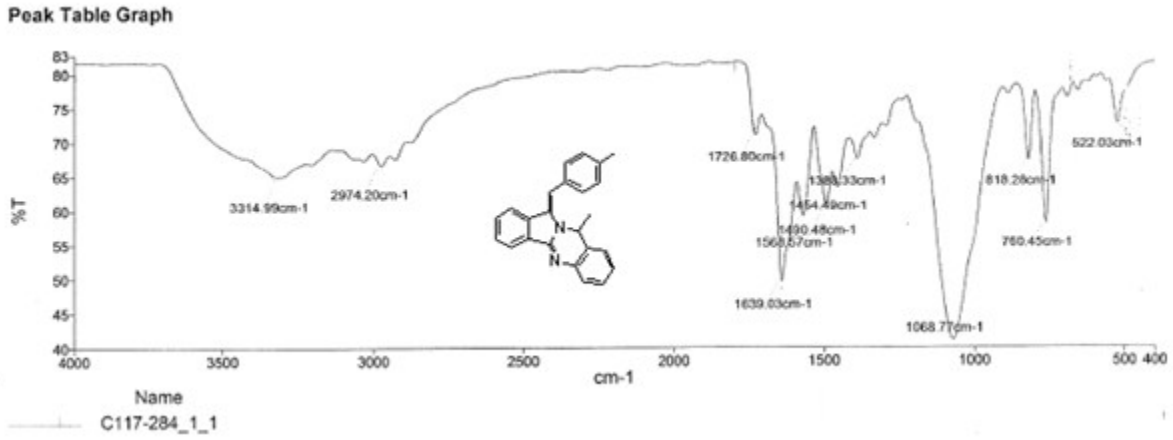
exp2 NOESY

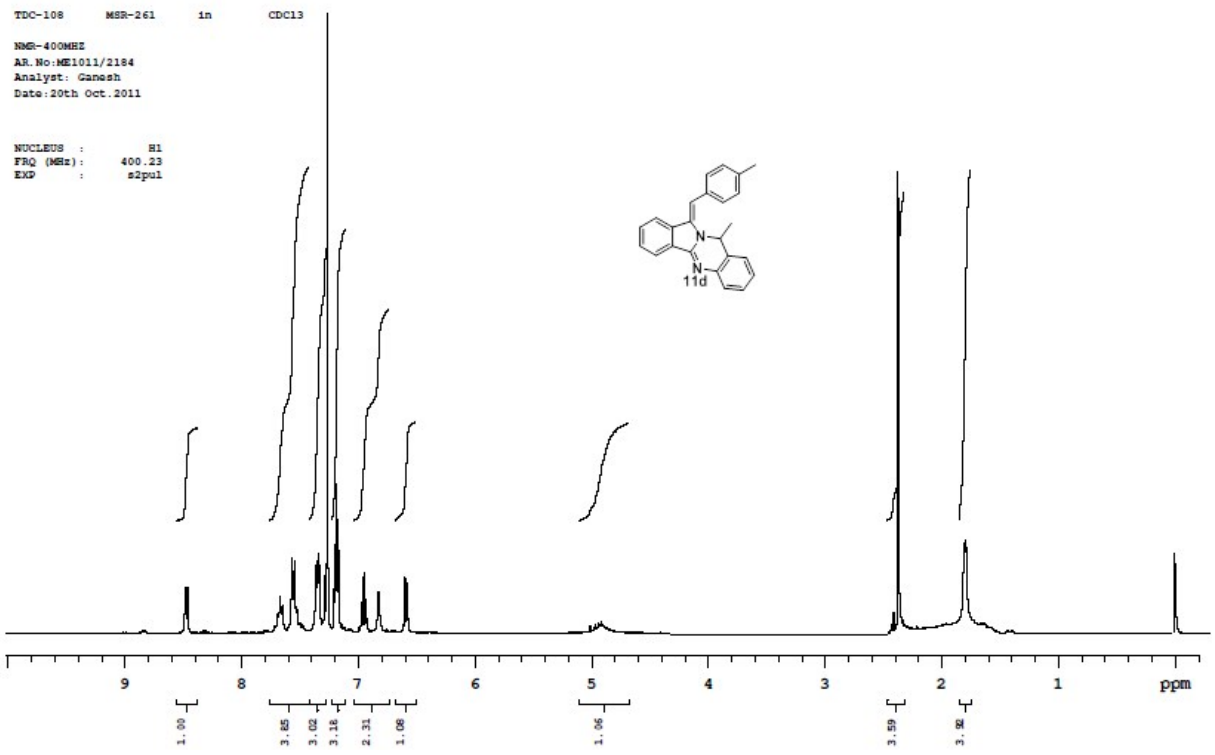
SAMPLE		FLAGs	
date	May 22 2014	hs	n
solvent	CDCl3	sspul	y
sample		PFGflg	y
ACQUISITION		hsglvl	4255
sw	5629.0	SPECIAL	
at	0.182	temp	25.0
np	2048	gain	38
fb	not used	spin	not used
ss	32	F2 PROCESSING	
d1	1.000	gf	0.084
nt	16	gfs	not used
2D ACQUISITION		fn	2048
sw1	5629.0	F1 PROCESSING	
ni	400	gf1	0.033
TRANSMITTER		gfs1	not used
tn	H1	proc1	lp
sfrq	499.626	fn1	2048
tof	-182.5	DISPLAY	
tpwr	58	sp	-104.4
pw	6.450	wp	4590.1
NOESY		sp1	-66.0
mix	0.600	wp1	4562.6
PRESATURATION		rf1	511.2
satmode	nnnn	rfp	0
satpwr	0	rfl1	511.2
satdly	0	rfp1	0
satfrq	0	PLOT	
DECOUPLER		wc	138.9
dn	C13	sc	10.0
dm	nnn	wc2	138.9
		sc2	0
		vs	493
		th	2
		ai cdc ph	

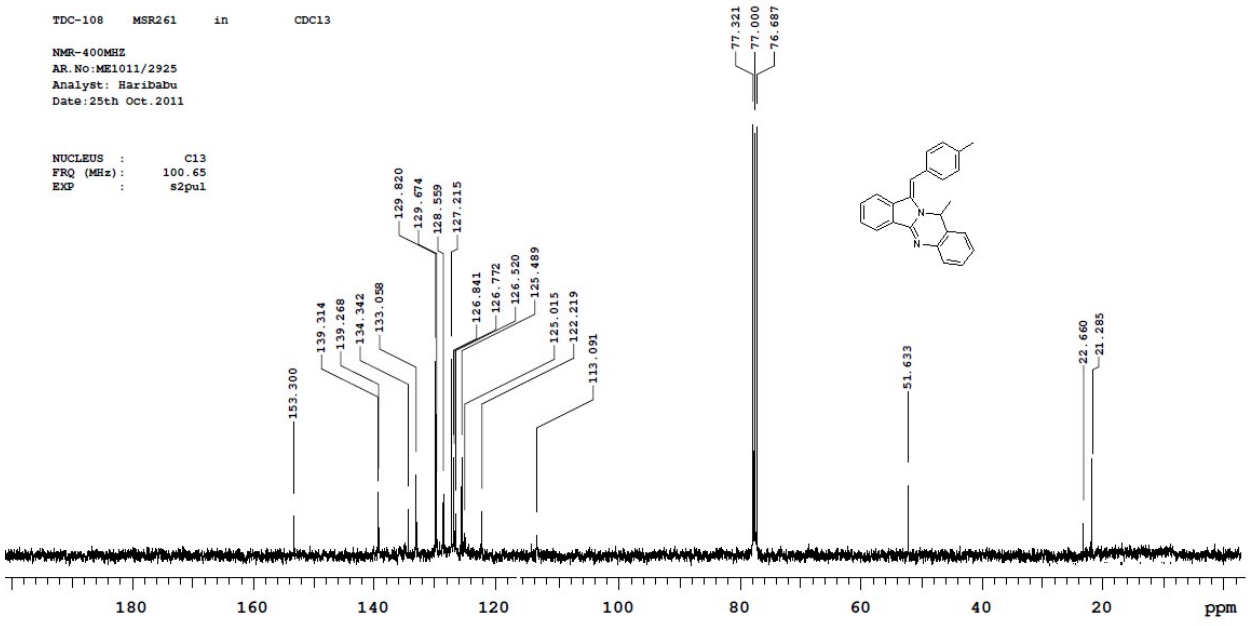




4. **(*Z*)-10-methyl-12-(4-methylbenzylidene)-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11d):**




TDC-108 MSR-261 in CDCl3
NMR-400MHZ
AR.No:ME1011/2184
Analyst: Ganesh
Date:20th Oct.2011
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul
11d
9
8
7
6
5
4
3
2
1
ppm
1.00
3.85
3.02
3.18
2.31
1.08
1.06
3.59
3.92

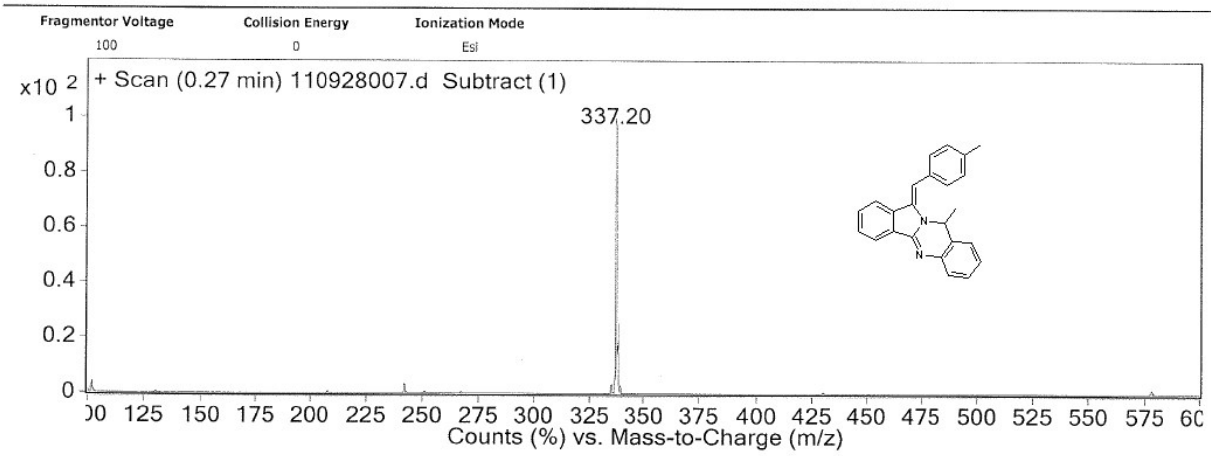

TDC-108 MSR261 in CDCl3
NMR-400MHZ
AR.No:ME1011/2925
Analyst: Haribabu
Date:25th Oct.2011
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul
77.321
77.000
76.687
129.820
129.674
128.559
127.215
126.841
126.772
126.520
125.489
125.015
122.219
113.091
153.300
139.314
139.268
134.342
133.058
51.633
22.660
21.285
180
160
140
120
100
80
60
40
20
ppm

CPS,MIYAPUR

Mass Analysis Report

Data Filename	110928007.d	**Sample Name**	MSR261
Sample Type	Sample	**Position**	Vial 77
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	EDC-5.m	**Comment**	

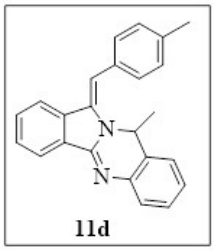
User Spectra



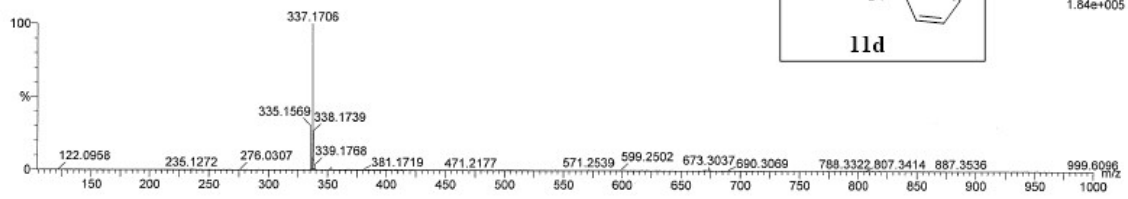
Elemental Composition Report

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: 0-30 N: 0-2 O: 0-5
C117/284
150922003 9 (0.177) Cm (9:10)

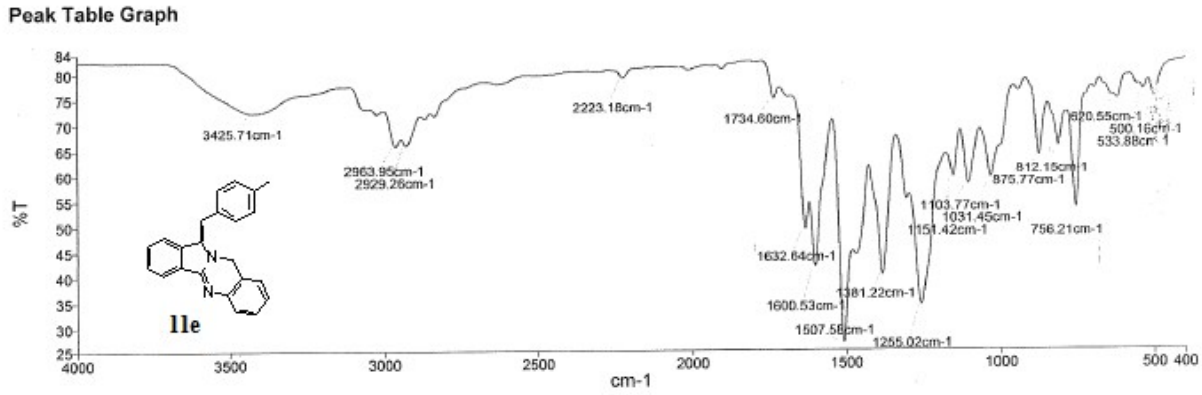


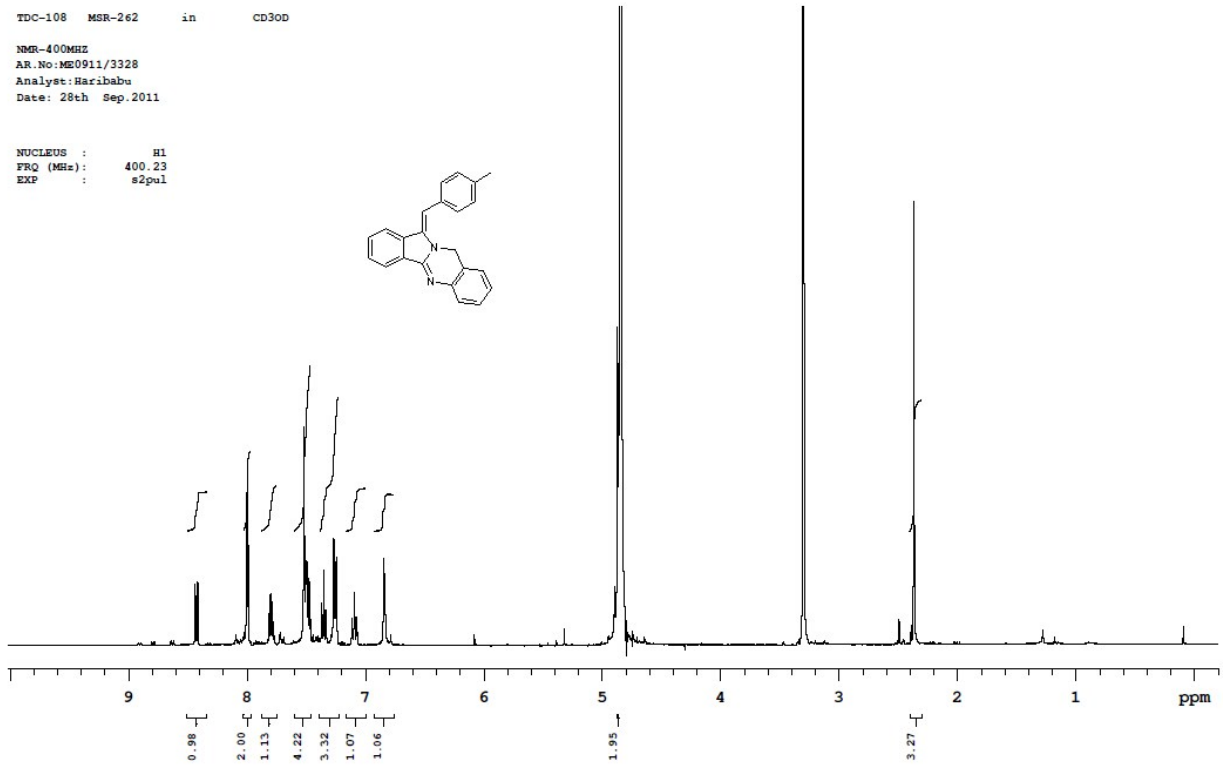
1: TOF MS ES+
1.84e+005



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
337.1706	337.1705	0.1	0.3	15.5	26.1	C24 H21 N2

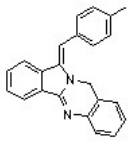
5. **(Z)-12-(4-methylbenzylidene)-10,12-dihydroisoindolo[1,2-b]quinazoline (11e):**

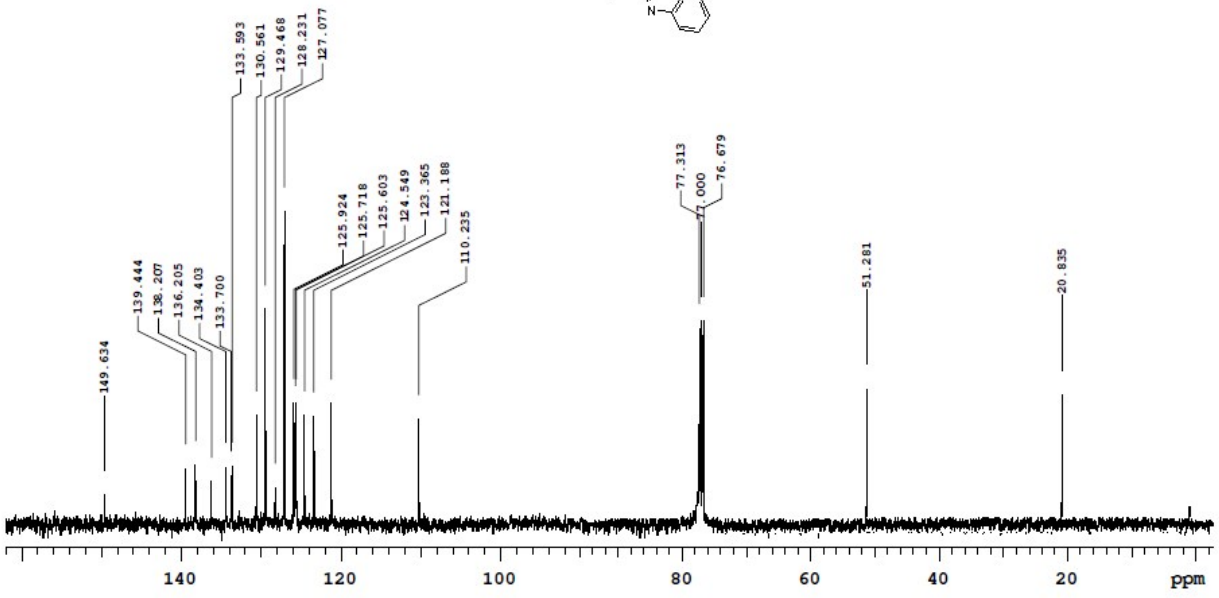




TDC-108 MSR/285 in CDCl3
NMR-400MHz
AR.No:ME0312/1713
Analyst: Haribabu
Date: 12th March.2012

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





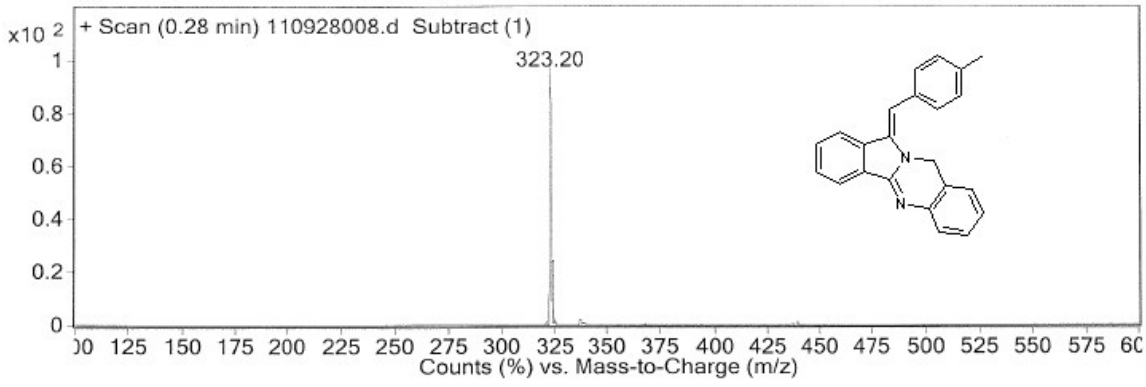
CPS,MIYAPUR

Mass Analysis Report

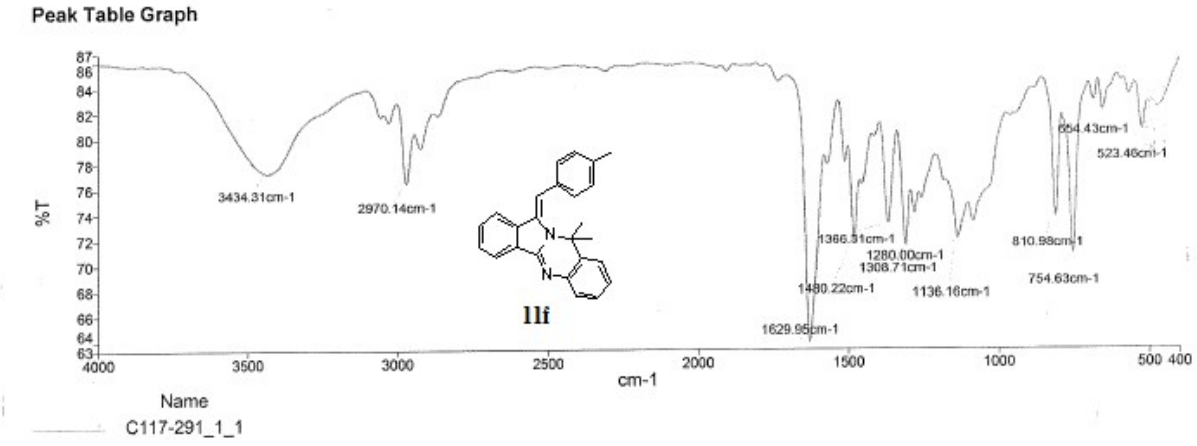
Data Filename	110928008.d	**Sample Name**	MSR262
Sample Type	Sample	**Position**	Vial 78
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	EDC-5.m	**Comment**	

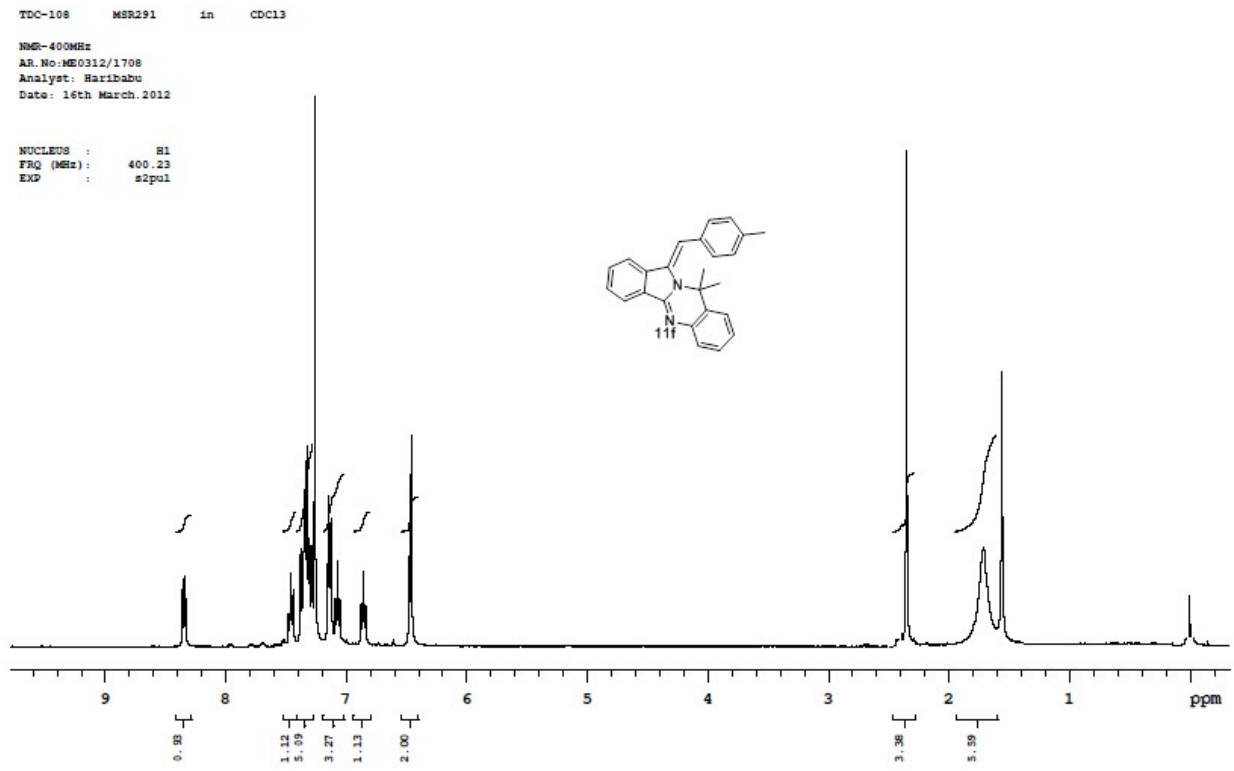
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi



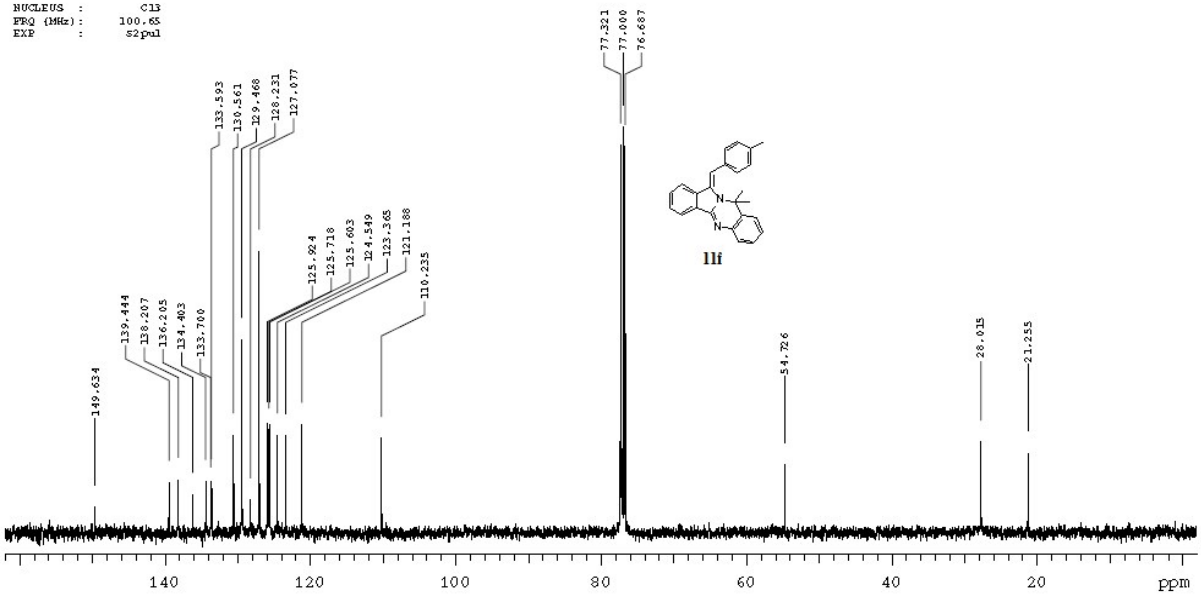
6. **(Z)-10,10-dimethyl-12-(4-methylbenzylidene)-10,12-dihydroisoindolo[1,2-b]quinazoline (11f):**





NMR-400MHz
AR.No:ME0312/1713
Analyst: Haribabu
Date: 16th March.2012

NUCLEUS : C13
FRQ (MHz): 100.65
EXP : S2pul



1li

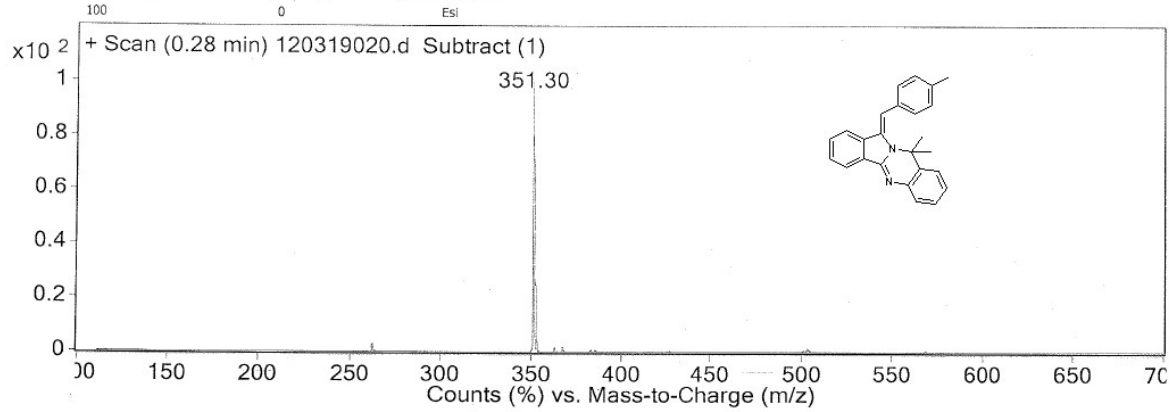
CPS,MIYAPUR

Mass Analysis Report

Data Filename	120319020.d	**Sample Name**	MSR291
Sample Type	Sample	**Position**	Vial 68
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.m	**IRM Calibration Status**	Success
DA Method	EDC-5.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
100	0	Esi

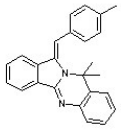


Elemental Composition Report

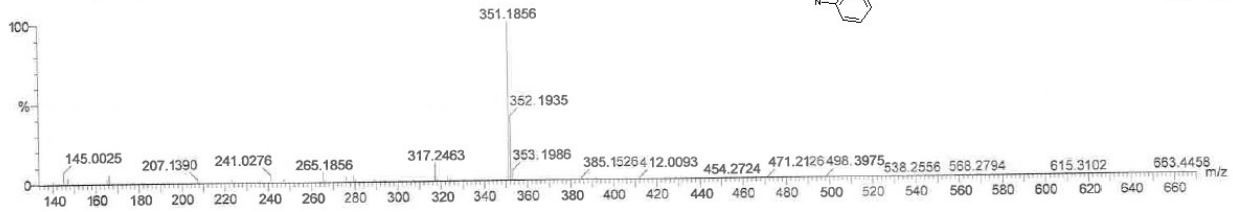
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
7 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

MSR291
140618006 21 (0.579) Cm (21:22)

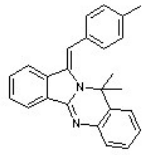


1: TOF MS ES+
1.26e+004

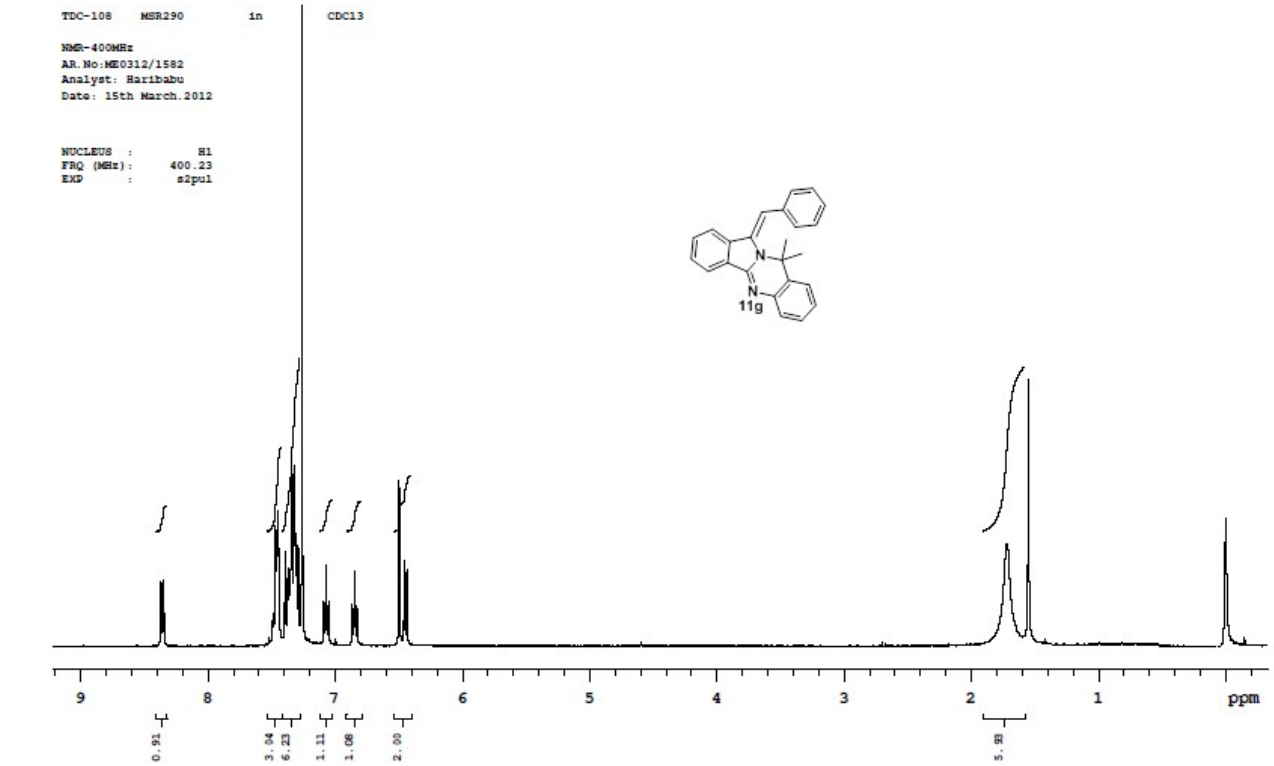


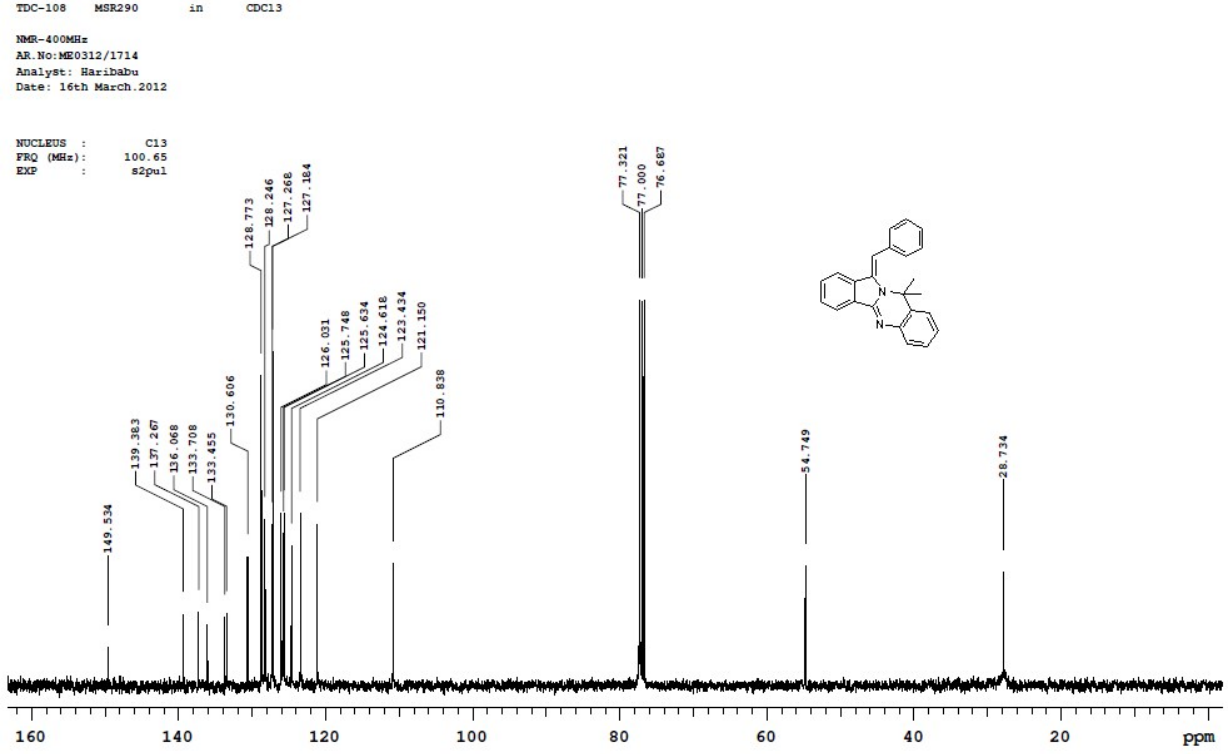
Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
351.1856	351.1861	-0.5	-1.4	15.5	235.1	C25 H23 N2

MSR291
140618006 21 (0.579) Cm (21:22)
1: TOF MS ES+
1.26e4



7. **(Z)-12-benzylidene-10,10-dimethyl-10,12-dihydroisoindolo[1,2-b]quinazoline (11g):**





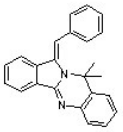
Elemental Composition Report

Single Mass Analysis

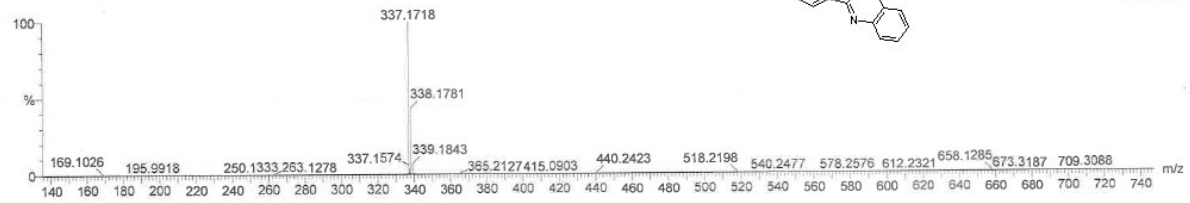
Tolerance = 5.0 PPM / DBE: min = -5.0, max = 80.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
36 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-2 O: 0-2

MSR290
140618003 8 (0.212) Cm (6:9-1:5)



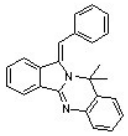
1: TOF MS ES+
3.67e+005



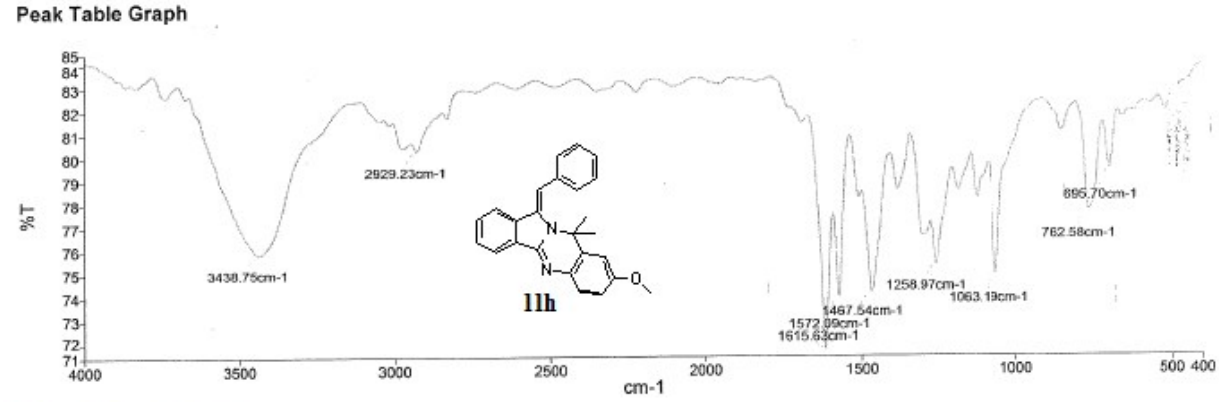
Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
337.1718	337.1705	1.3	3.9	15.5	10770.0	C24 H21 N2

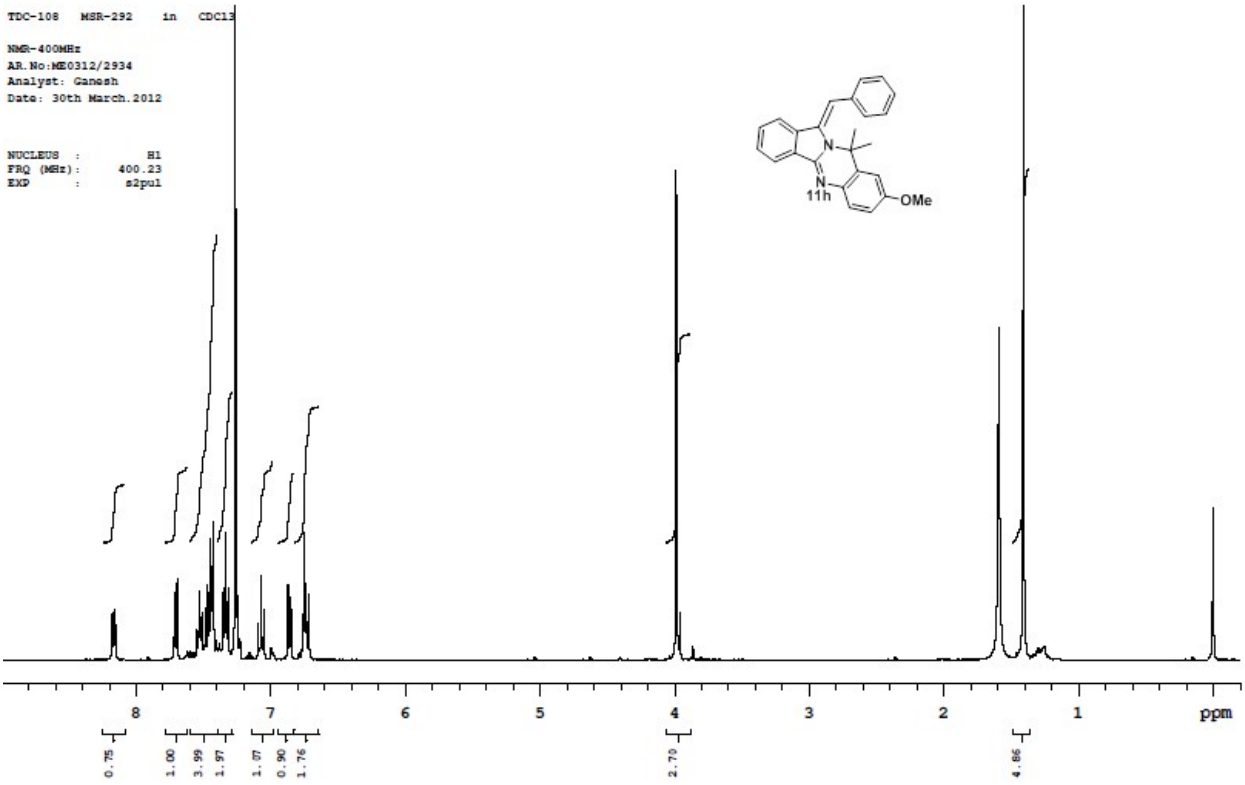
MSR290
140618003 8 (0.212) Cm (6:9-1:5)

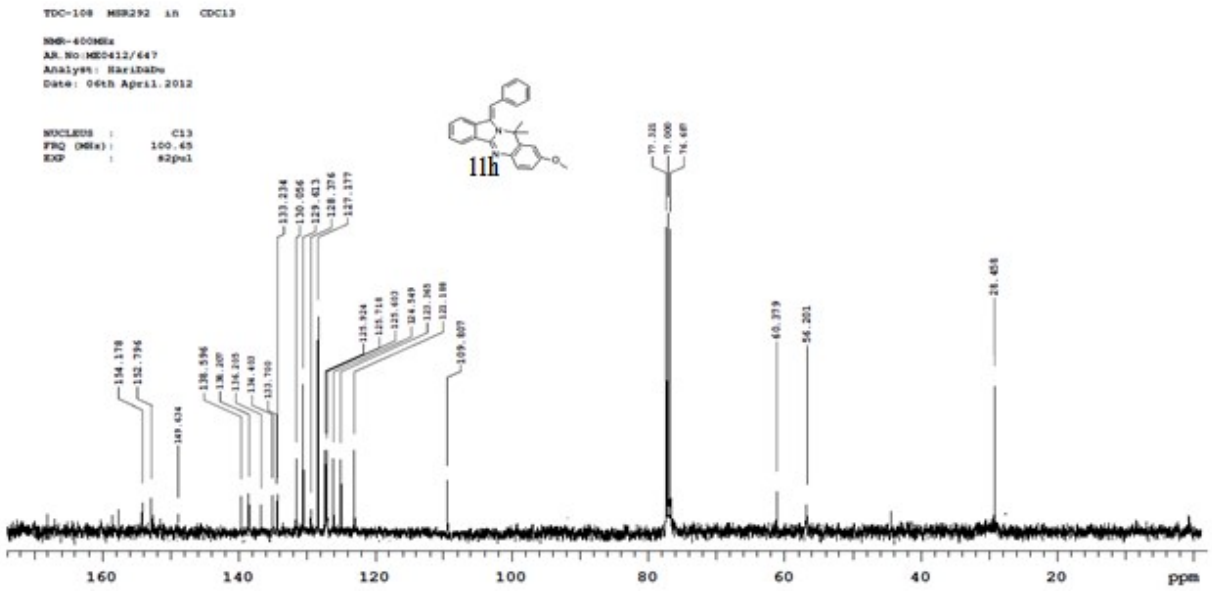
1: TOF MS ES+
3.67e5



8. **(Z)-12-benzylidene-8-methoxy-10,10-dimethyl-10,12-dihydroisoindolo[1,2-b]quinazoline (11h):**





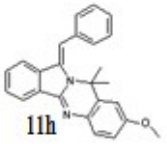


Elemental Composition Report

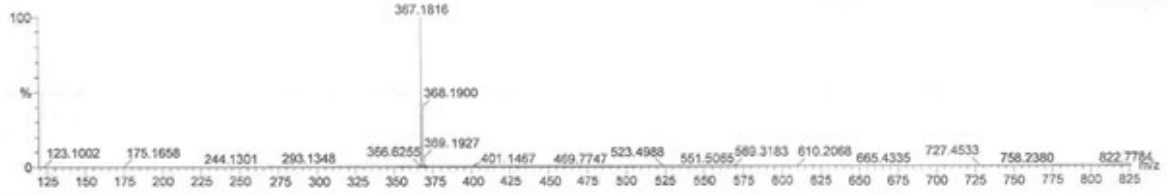
Single Mass Analysis

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

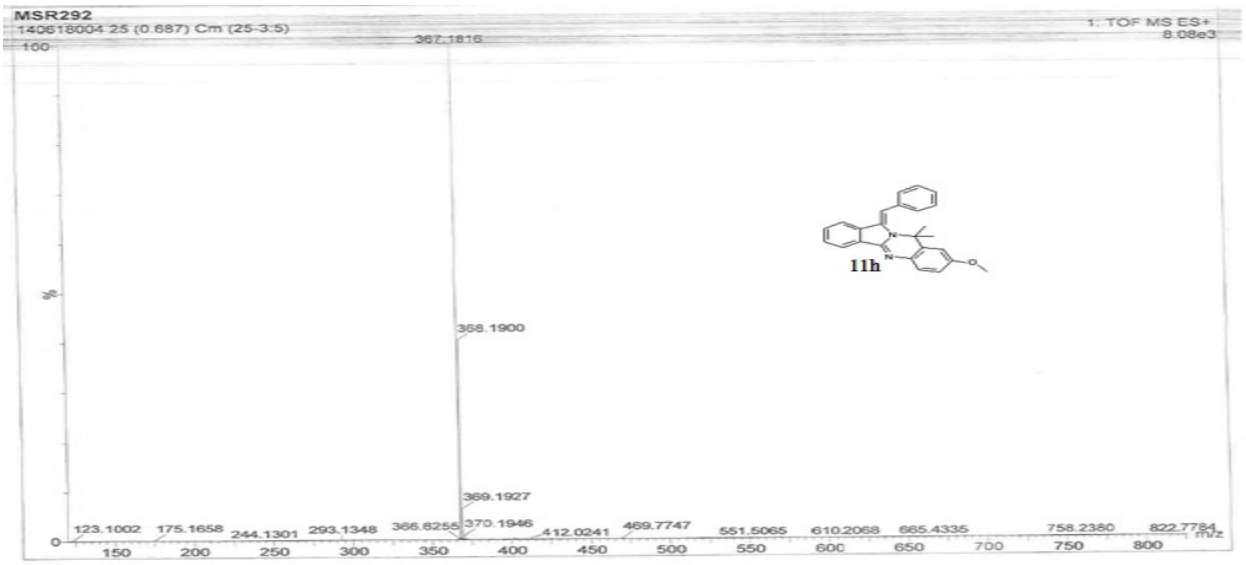
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-25 N: 0-2 O: 0-1
MSR292
140618004 25 (0.687) Cm (25-35)



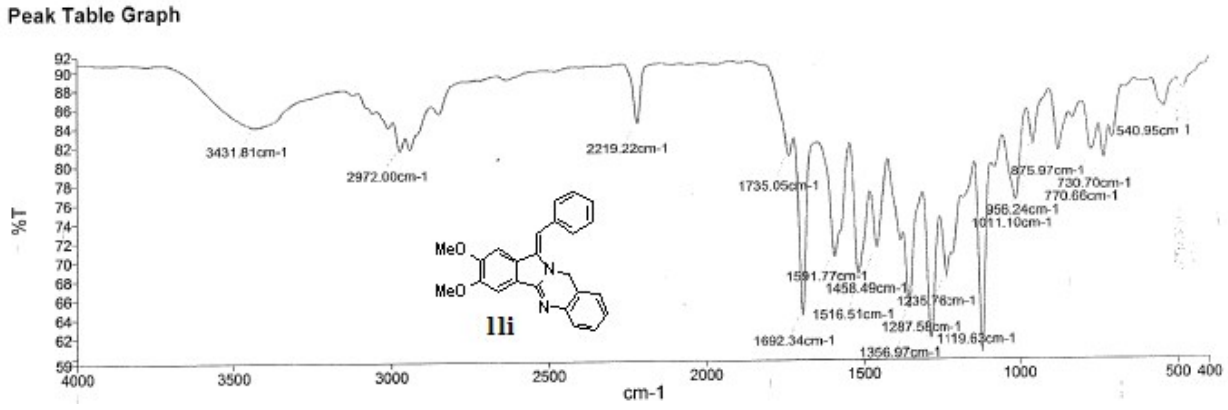
1: TOF MS ES+
8.06e+003

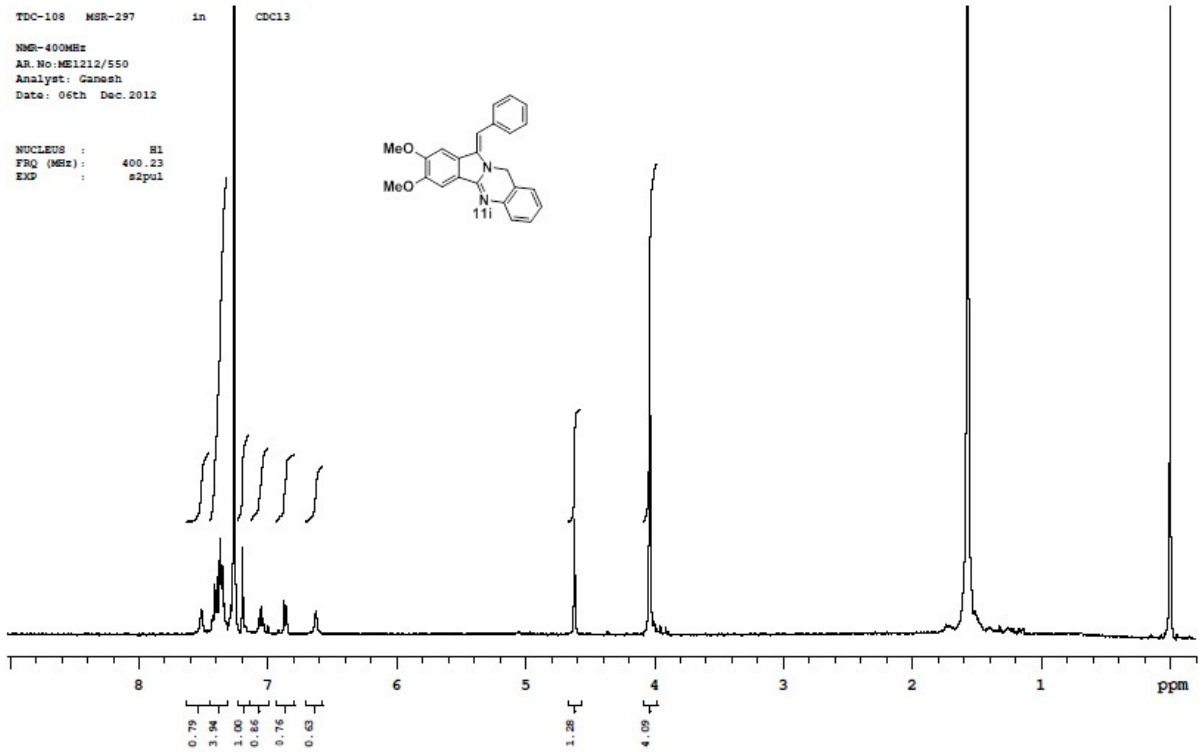


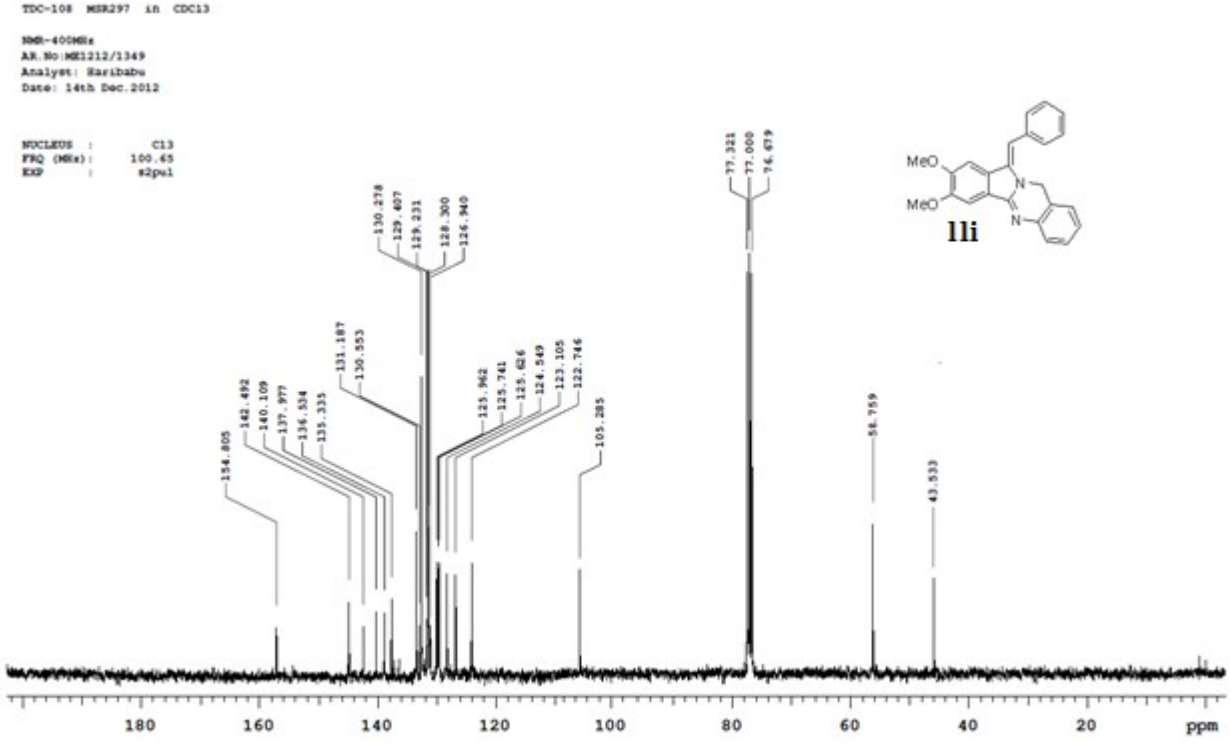
Minimum:				-5.0		
Maximum:		5.0	5.0	80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
367.1816	367.1810	0.6	1.6	15.5	134.5	C25 H23 N2 O



9. **(Z)-12-benzylidene-2,3-dimethoxy-10,12-dihydroisoindolo[1,2-b]quinazoline (11i):**



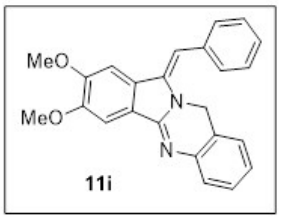

TDC-108 MSR-297 in CDCl3
NMR-400MHz
AR.No:ME1212/550
Analyst: Ganesh
Date: 06th Dec.2012
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul
MeO
MeO
N
N
11i
8
7
6
5
4
3
2
1
ppm
0.79
3.94
1.00
0.86
0.76
0.63
1.28
4.09


TDC-108 MSR297 in CDCl3
NMR-400MHz
AR.No:ME1212/1349
Analyst: Haribabu
Date: 14th Dec.2012
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul
MeO
MeO
N
N
1li
77.321
77.000
76.679
130.278
129.407
129.231
128.300
126.940
154.805
142.492
140.109
137.977
136.534
135.335
131.187
130.553
125.962
125.741
125.626
124.549
123.105
122.746
105.285
58.759
43.533
180
160
140
120
100
80
60
40
20
ppm

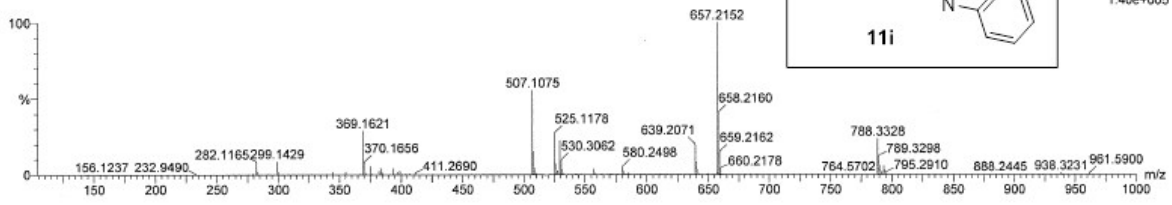
Elemental Composition Report **Page 1**

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: 0-30 N: 0-2 O: 0-5
C117/297
150922002 21 (0.399) Cm (21:24)

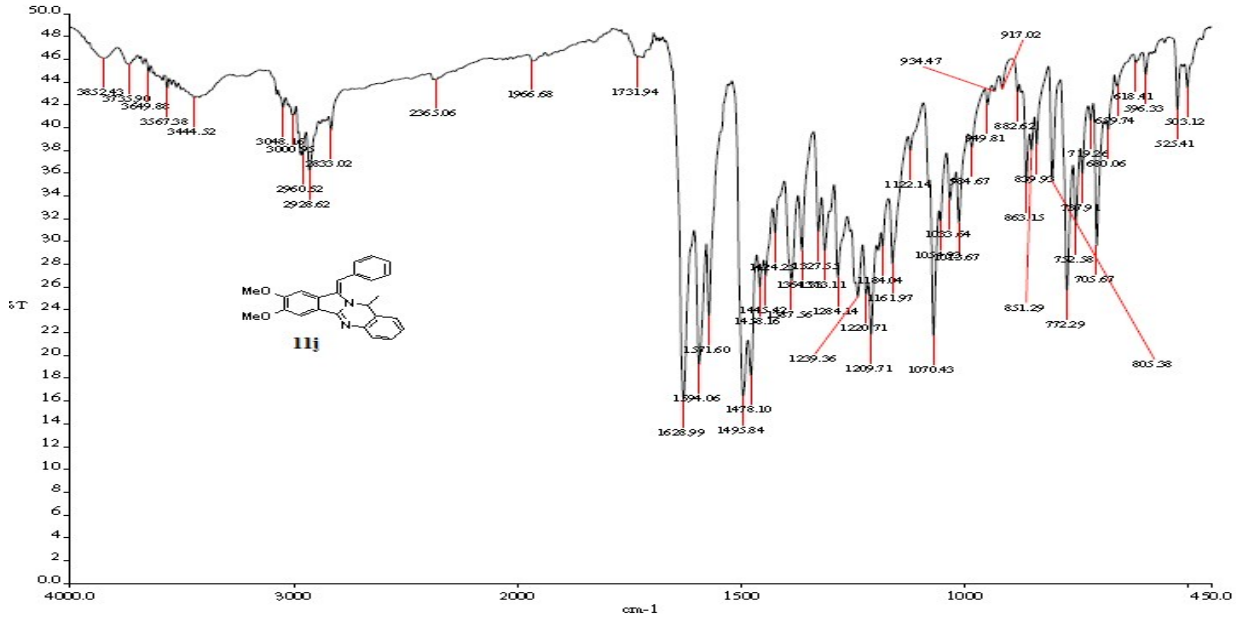


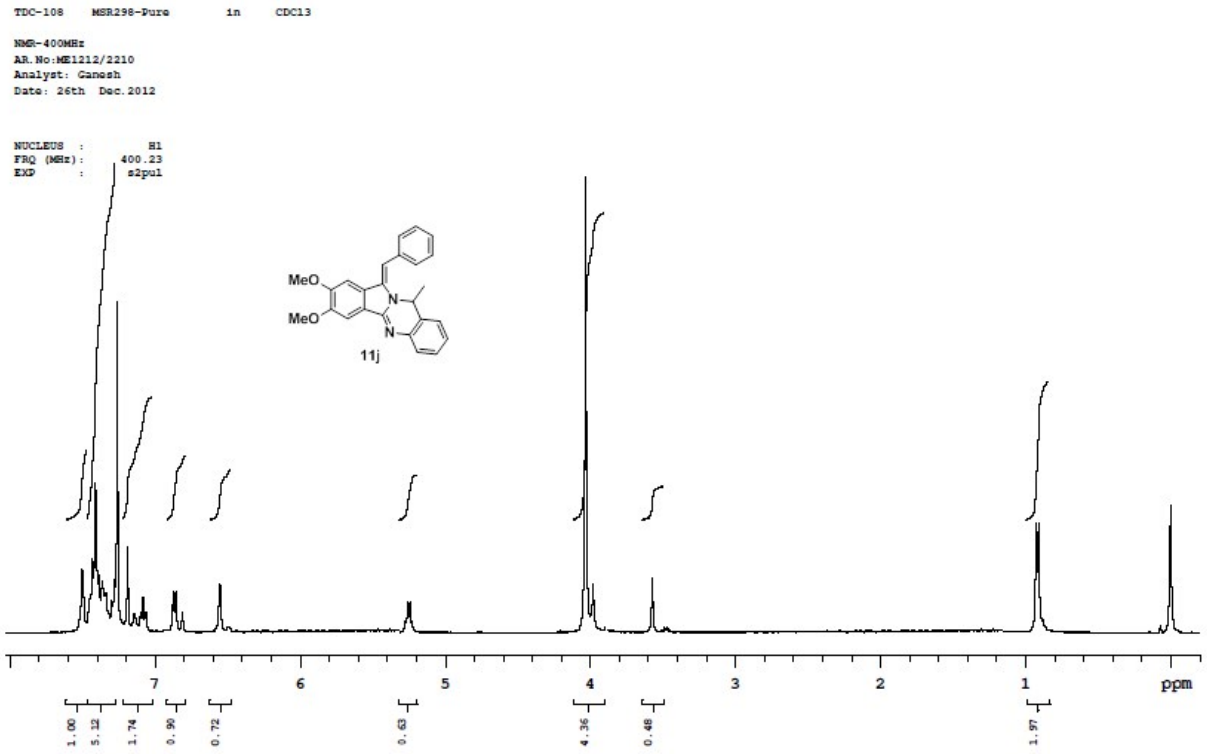
1: TOF MS ES+
1.40e+005

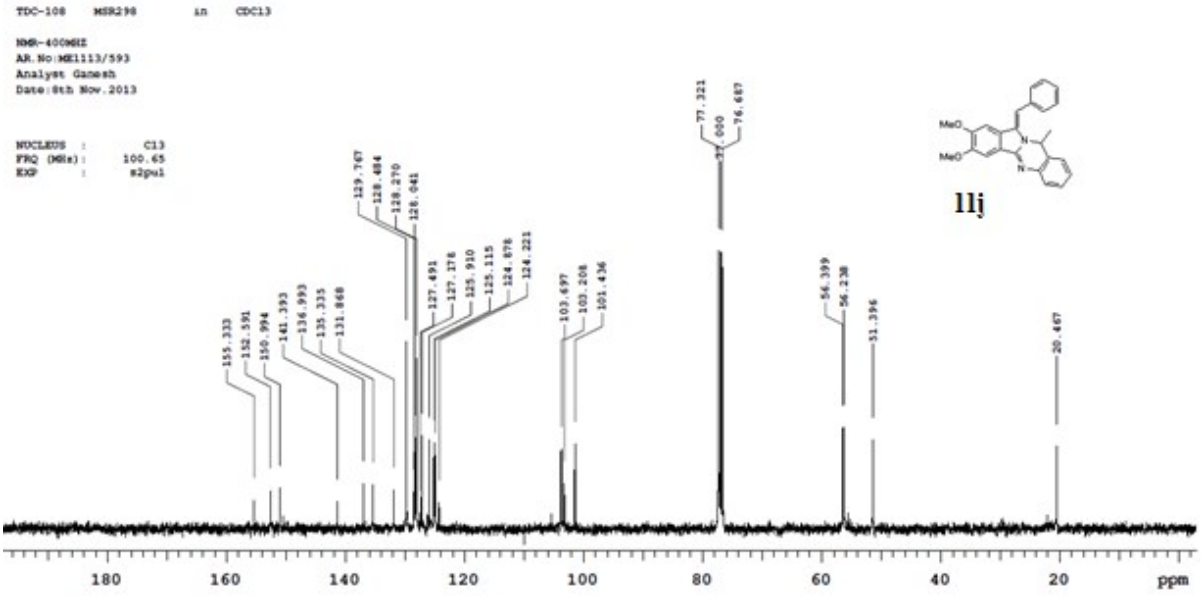


Minimum:			-1.5			
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
369.1621	369.1603	1.8	4.9	15.5	3.6	C24 H21 N2 O2

10. **(*Z*)-12-benzylidene-2,3-dimethoxy-10-methyl-10,12-dihydroisoindolo[1,2-*b*]quinazoline (11j):**




TDC-108 MSR298-Pure in CDCl3
NMR-400MHz
AR.No:ME1212/2210
Analyst: Ganesh
Date: 26th Dec.2012
NUCLEUS : H1
FRQ (MHz): 400.23
EXP : s2pul
MeO
MeO
N
N
11j
7
6
5
4
3
2
1
ppm
1.00
5.12
1.74
0.90
0.72
0.63
4.36
0.48
1.97

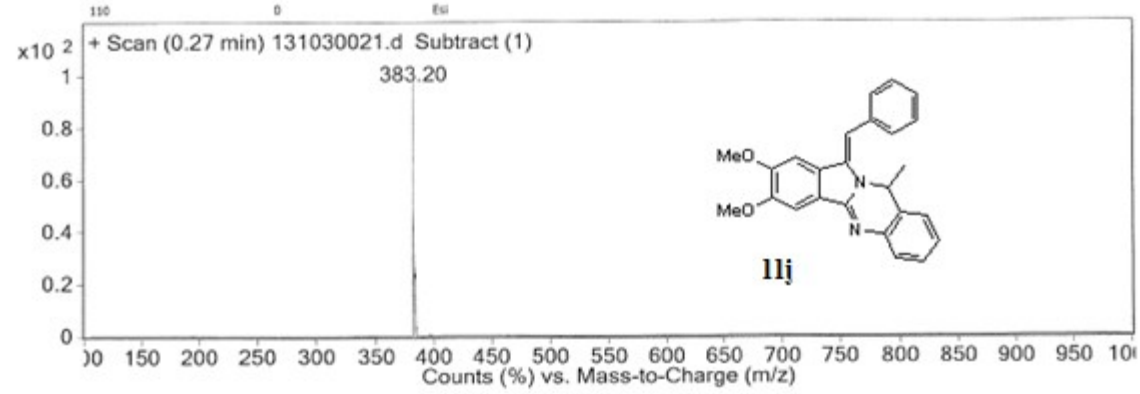

TDC-108 MSR298 in CDCl3
NMR-400MHZ
AR.No:ME1113/593
Analyst Ganesh
Date:8th Nov.2013
NUCLEUS : C13
FRQ (MHz): 100.65
EXP : s2pul
155.333
152.591
150.994
141.393
136.993
135.335
131.868
129.767
128.484
128.270
128.041
127.491
127.178
125.910
125.115
124.878
124.221
103.697
103.204
101.436
77.321
77.000
76.687
56.399
56.238
51.396
20.467
MeO
MeO
N
N
11j
180
160
140
120
100
80
60
40
20
ppm

Mass Analysis Report

Data Filename	131030021.d	**Sample Name**	MSR298
Sample Type	Sample	**Position**	Vial 60
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI.M	**IRM Calibration Status**	Success
DA Method	CAO4B.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
110	0	Esi



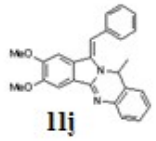
1lj

Elemental Composition Report

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

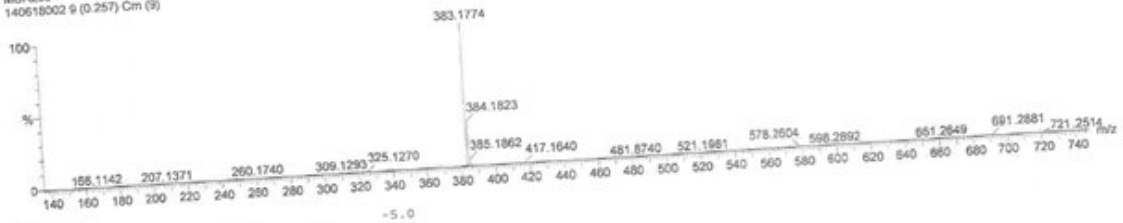
Monoisotopic Mass, Even Electron Ions
34 formula(e) evaluated with 1 results within limits (up to 4 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-45 N: 0-2 O: 0-2

MSR298
140618002 9 (0.257) Cm (9)

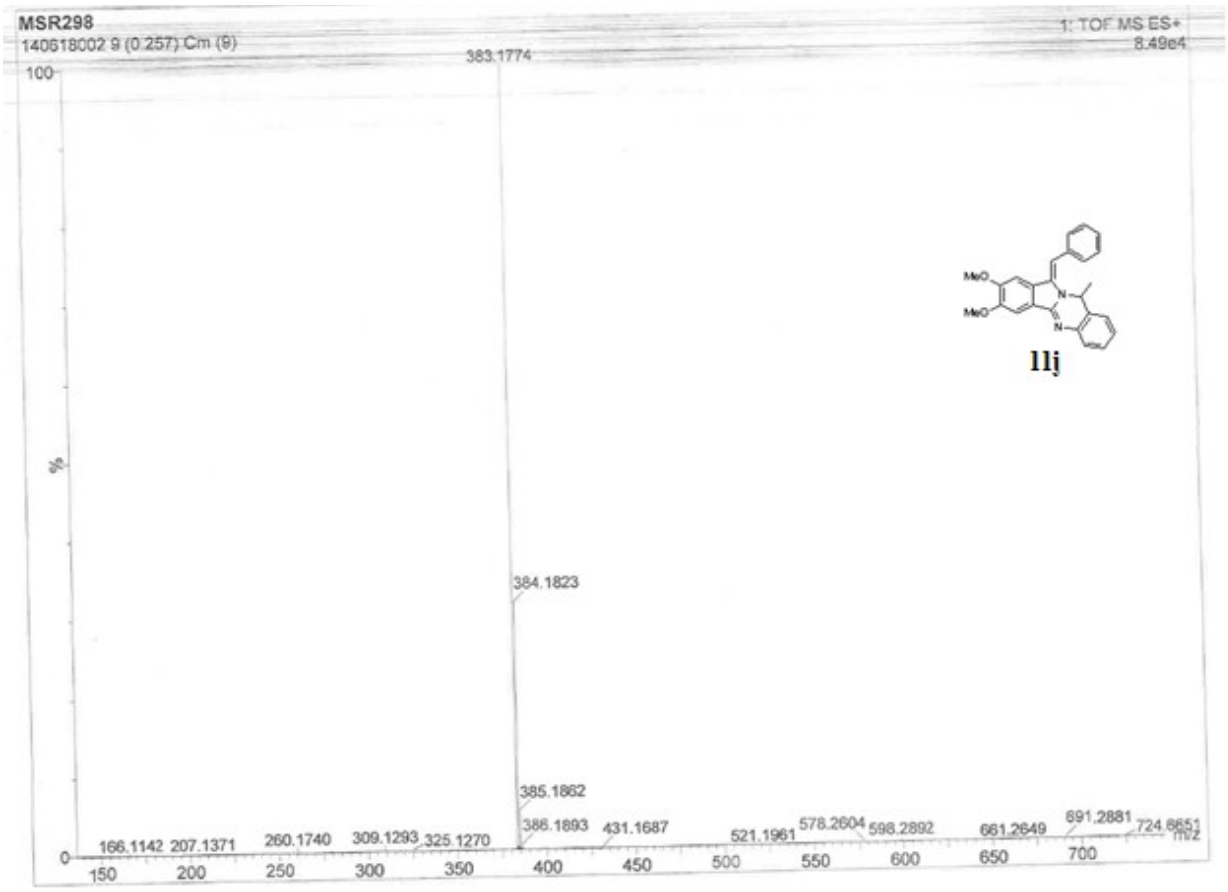


1lj

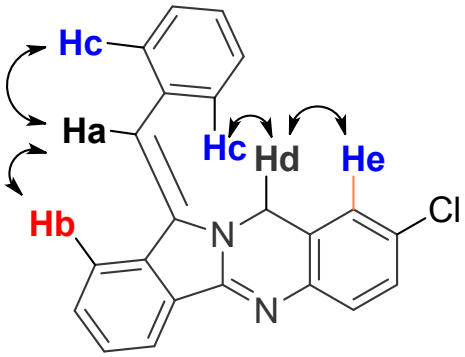
1: TOF MS ES+
8.49e+004



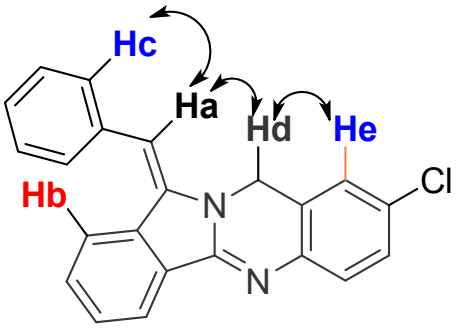
Minimum:		5.0	5.0	-5.0		
Maximum:				80.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.1774	383.1760	1.4	3.7	15.5	97.9	C25 H23 N2 O2


MSR298
140618002 9 (0.257) Cm (9)
1: TOF MS ES+
8.49e4
383.1774
100
%
0
384.1823
385.1862
386.1893
166.1142
207.1371
260.1740
309.1293
325.1270
431.1687
521.1961
578.2604
598.2892
661.2649
691.2881
724.8651
m/z
150
200
250
300
350
400
450
500
550
600
650
700
MeO
MeO
N
N

11j



11c



16

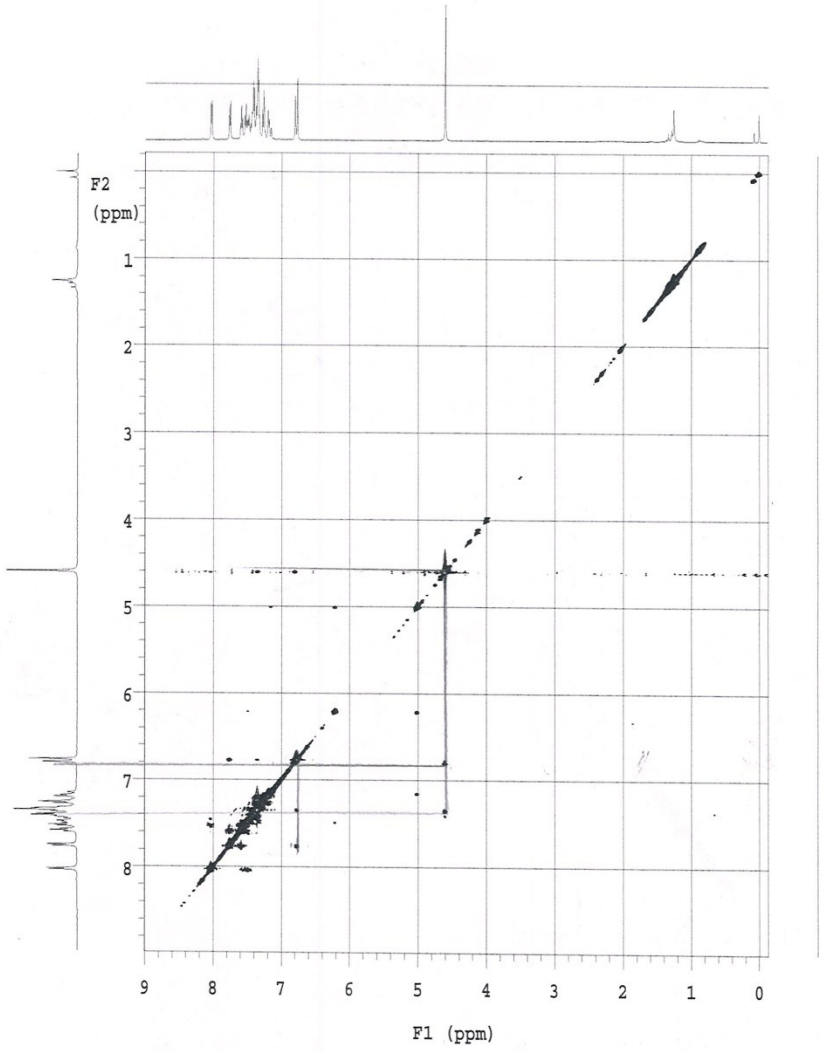
Compound **16** was ruled out by 2D NMR study and NOE study. NOE study clearly indicated that 2-bond interaction was observed, **Hd** with **Hc** and **He** (4.60 with 6.82 and 7.35) and **Ha** with **Hb** and **Hc (**6.76 with 7.76 and 7.35) and we are not observed any interaction between **Hd** with **Ha,** Moreover, literature survey revealed that, similar compounds have been characterized earlier they are clearly written olefinic CH of E compounds appeared singlet at δ 7.58 and olefinic CH of Z is coming singlet at δ 6.79, all these compounds olefinic CH appeared singlet at δ 6.76, Thus, **11c** appeared to be the chemical structure of the isolated product. NOE data was attached below.

MSR283 in CDCl3
TDC-108

AR.No:IN0514/129
Date:22nd May.2014
Analyst: Haribabu.R

exp2 NOESY

SAMPLE		FLAGS	
date	May 22 2014	hs	n
solvent	CDCl3	sspul	y
sample		PFGflg	y
ACQUISITION		hsglvl	4255
sw	5629.0	SPECIAL	
at	0.182	temp	25.0
np	2048	gain	38
fb	not used	spin	not used
ss	32	F2 PROCESSING	
d1	1.000	gf	0.084
nt	16	gfs	not used
2D ACQUISITION		fn	2048
sw1	5629.0	F1 PROCESSING	
ni	400	gf1	0.033
TRANSMITTER		gfs1	not used
tn	H1	proc1	lp
sfrq	499.626	fn1	2048
tof	-182.5	DISPLAY	
tpwr	58	sp	-104.4
pw	6.450	wp	4590.1
NOESY		sp1	-66.0
mix	0.600	wp1	4562.6
PRESATURATION		rf1	511.2
satmode	nnnn	rfp	0
satpwr	0	rfl1	511.2
satdly	0	rfp1	0
satfrq	0	PLOT	
DECOUPLER		wc	138.9
dn	C13	sc	10.0
dm	nnn	wc2	138.9
		sc2	0
		vs	493
		th	2
		ai cdc ph	



MSR283 in CDCl3
TDC-108

AR.No:IN0514/129
Date:22nd May.2014
Analyst: Haribabu.R

NUCLEUS : H1
FRQ (MHz): 499.63
EXP : NOESY