Supporting Information

Regioselective 6-*endo*-*dig* Iodocyclization: An accessible approach for Iodo-benzo[*a*]phenazines

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X-ray crystallographic studies

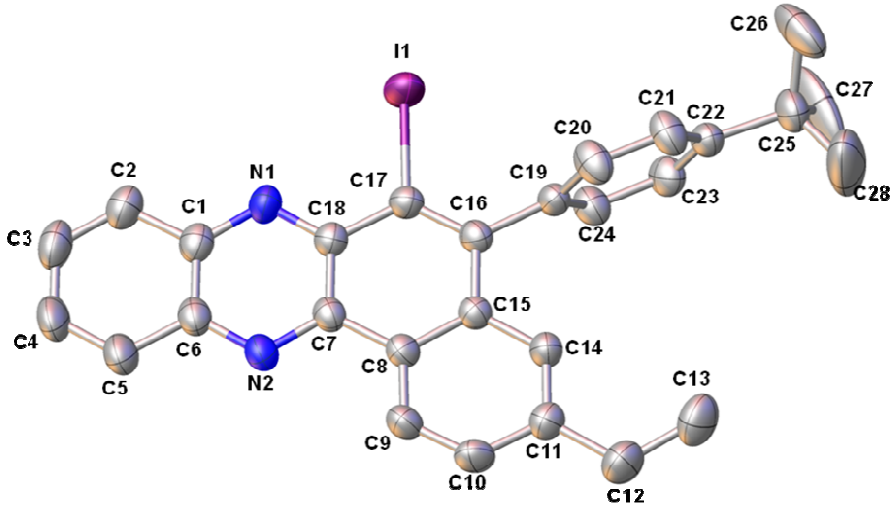


Figure S1. ORTEP drawing of compound **5e** drawn at 50% probability level

The structure of **5e** was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97.[2] The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package.[3]

CCDC numbers of **5e** is 1518194.

Table 1. Crystal data and structure refinement for **5**e

Empirical formula	$C_{28}H_{25}I\ N_2$	
Formula weight	516.40	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 9.6023(3) Å	α = 118.262(4)°
	b = 11.8204(4) Å	β = 99.616(3)°
	c = 12.0014(6) Å	γ = 94.267(3)°
Volume	1164.32(9) $Å^3$	
Z	2	
Density (calculated)	1.473 Mg/m^3	
Absorption coefficient	1.393 mm^{-1}	
F(000)	520	
Crystal size	0.230 x 0.220 x 0.180 mm^3	
Theta range for data collection	3.204 to 24.998°.	
Index ranges	$-11 \le h \le 11$, $-14 \le k \le 14$, $-14 \le l \le 14$	
Reflections collected	13986	
Independent reflections	4098 [R(int) = 0.0298]	
Completeness to theta = 24.998°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.776 and 0.735	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4098 / 0 / 284	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2σ (I)][a,b]	R_1 = 0.0314, wR_2 = 0.0697	
R indices (all data)	R_1 = 0.0391, wR_2 = 0.0728	
Largest diff. peak and hole	0.678 and -0.303 e.$Å^{-3}$	

[a] $R = \sum(\| Fo | - | Fc \|) / \sum | Fo |$; [b] $wR = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$

References

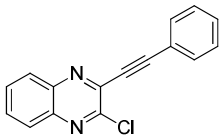
1. a) *SMART: Bruker Molecular Analysis Research Tool*, version 5.618. Bruker Analytical X-ray System, **2000**. b) *SAINT-NT*, version 6.45, Bruker Analytical X-Ray System, **2003**. c) *SHELXTL-NT*, version 6.10, Bruker Analytical X-ray System, **2000**.

2. G. M. Sheldrick, Acta Cryst., **2008**, A64, 112-122.

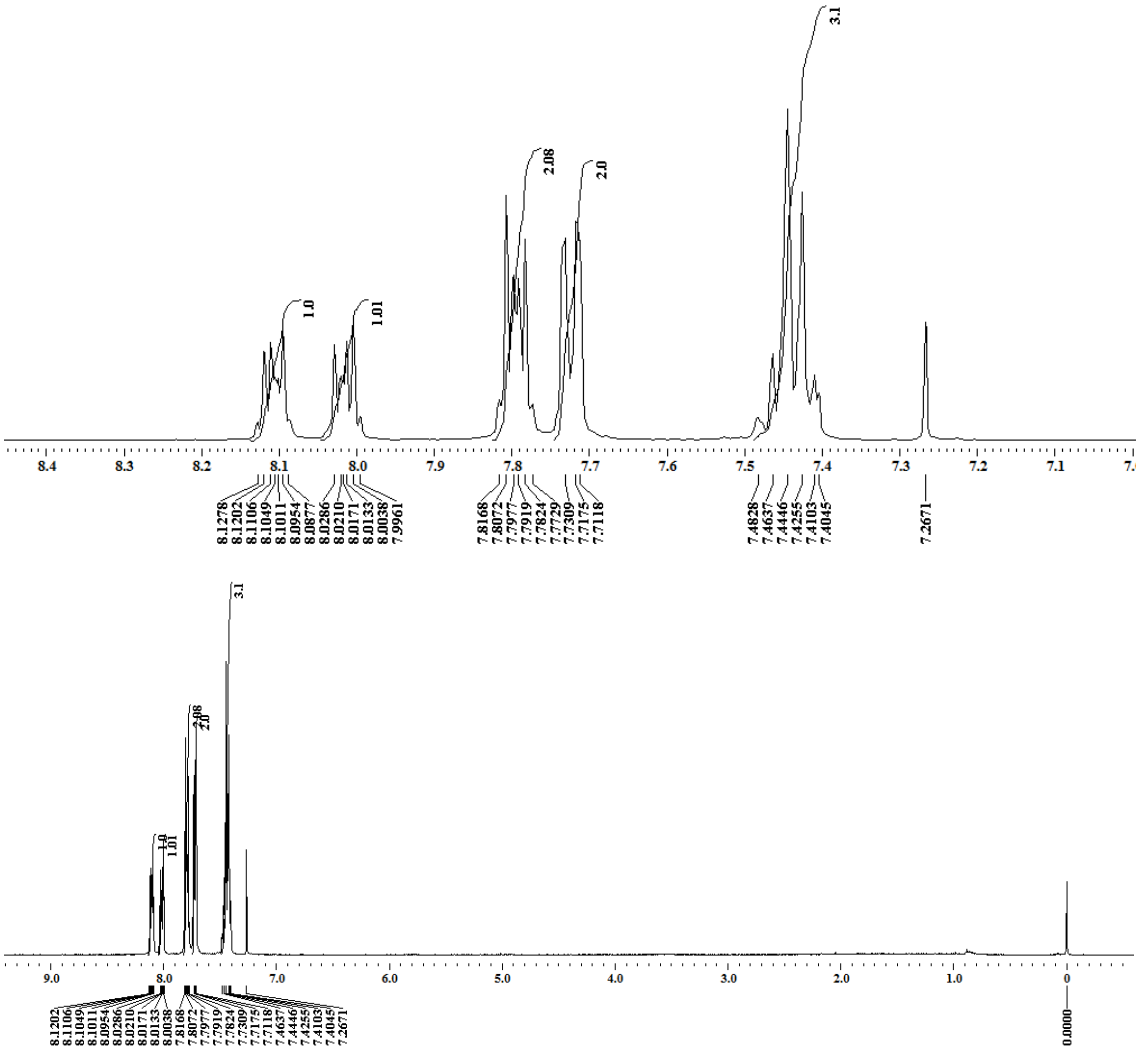
3. L. J. Farrugia, WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data;* Department of Chemistry, University of Glasgow (**1997-2009**).

Copies of ^{1}H and ^{13}C NMR

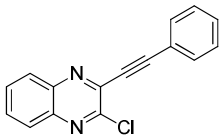
^{1}H NMR



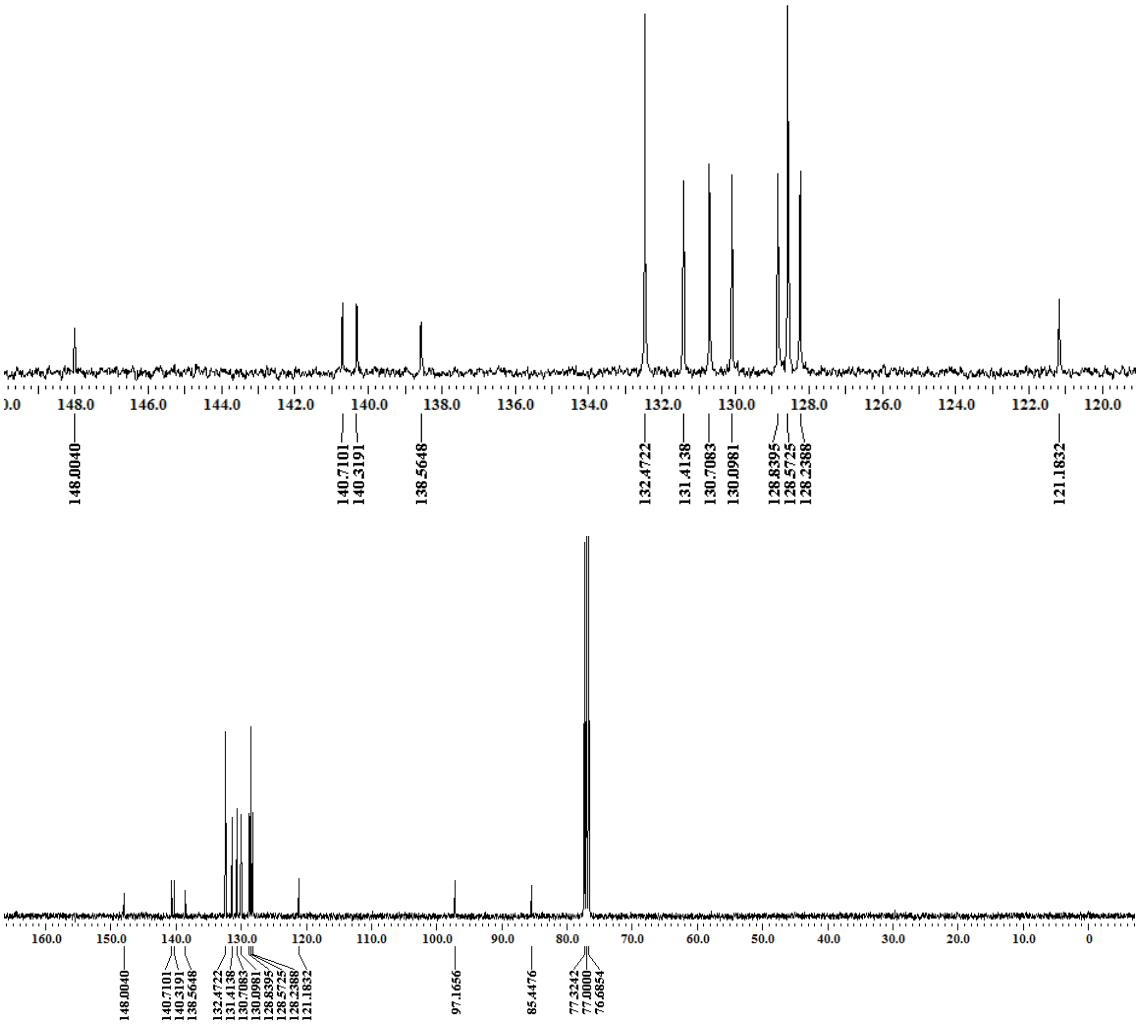
2-Chloro-3-(phenylethynyl)quinoxaline (1aa)



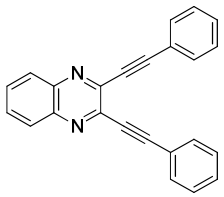
$^{13}C\{^{1}H\}$ NMR



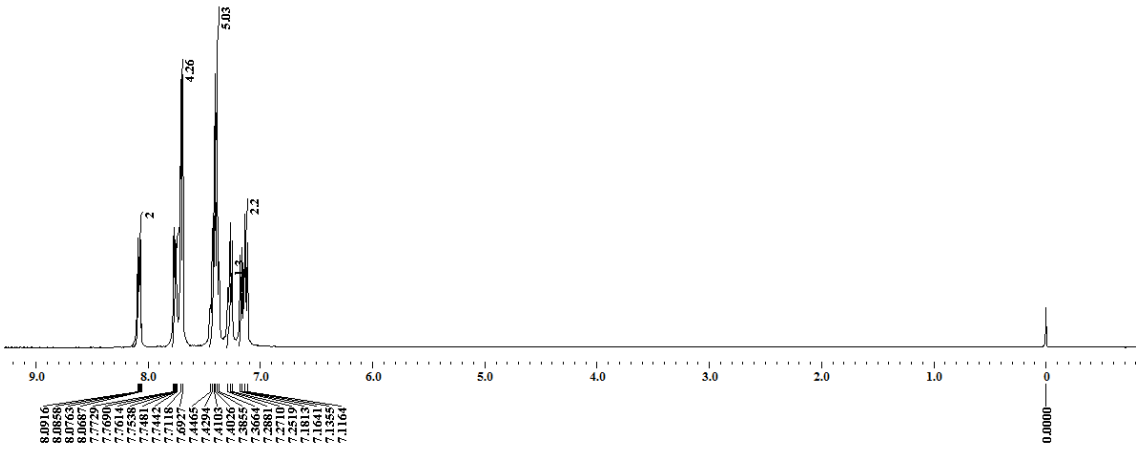
2-Chloro-3-(phenylethynyl)quinoxaline (1aa)



^{1}H NMR



2,3-bis(Phenylethynyl)quinoxaline (1ab)



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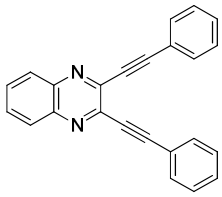

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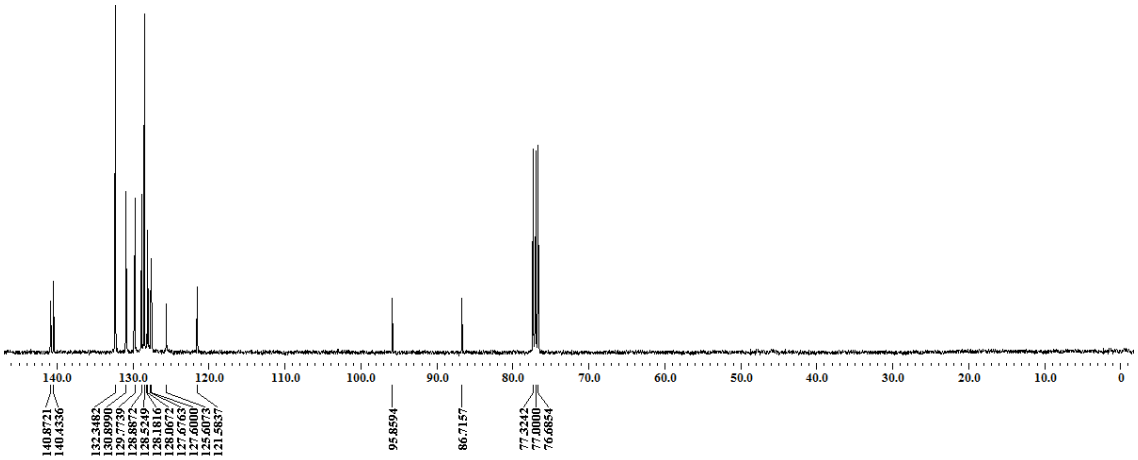

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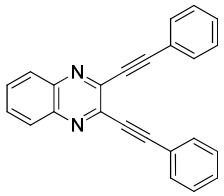

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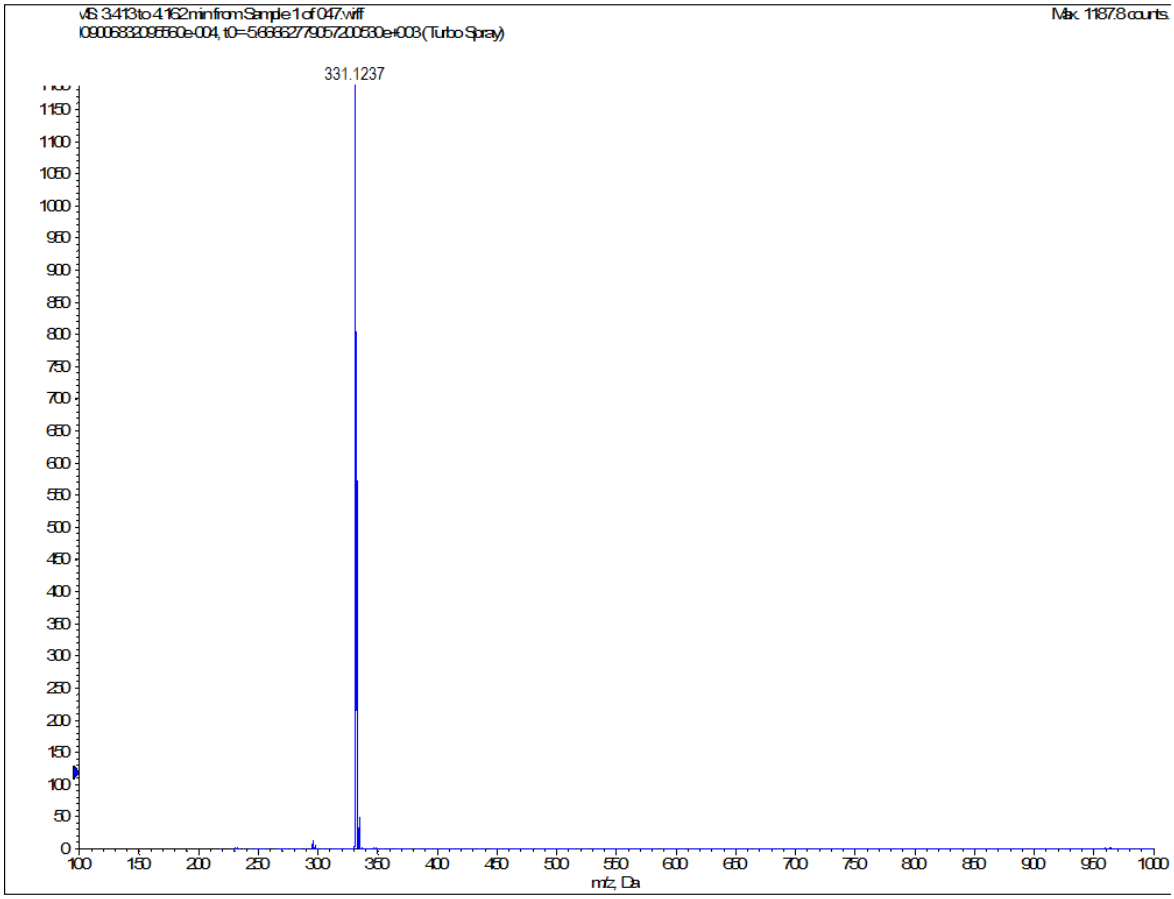
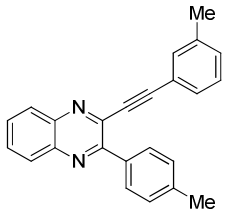


^{1}H NMR



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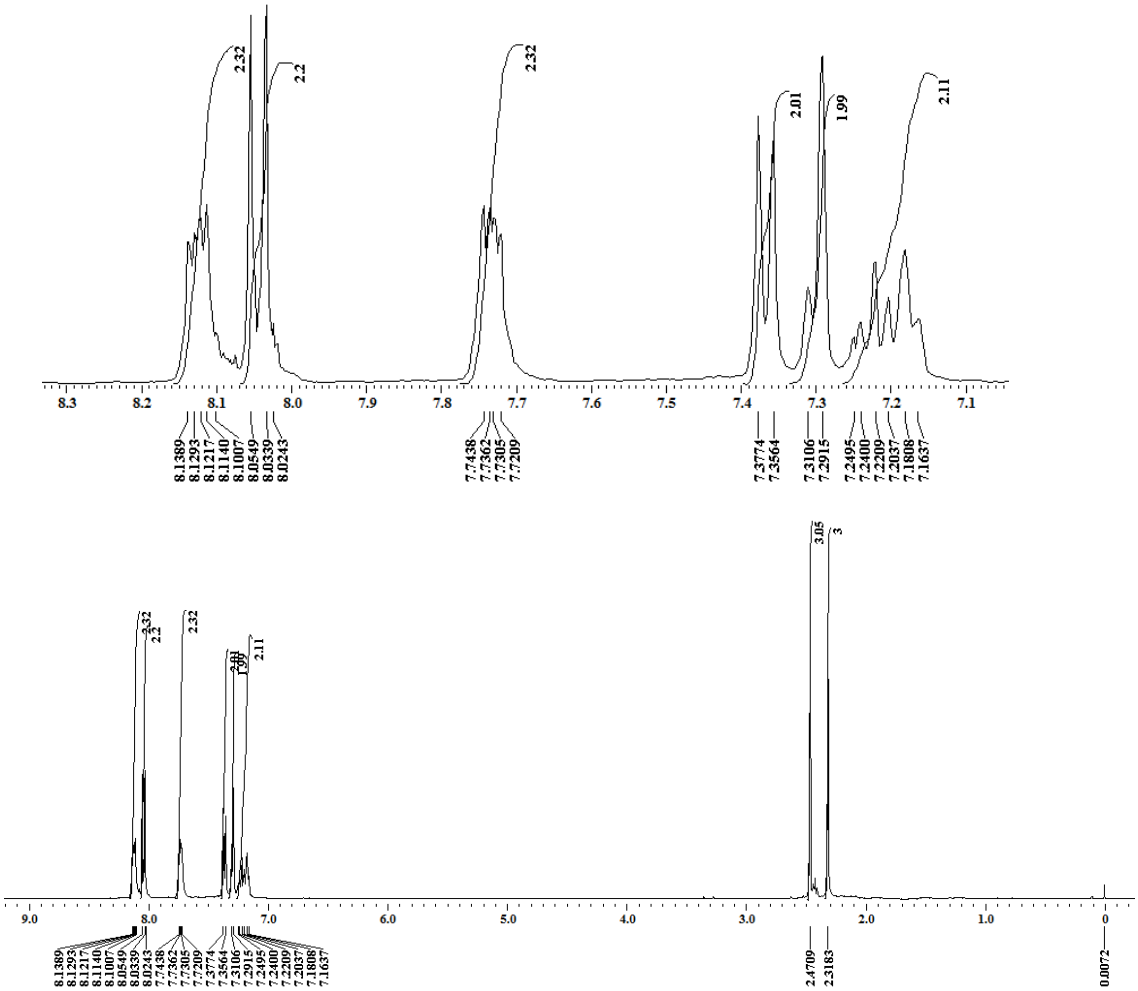
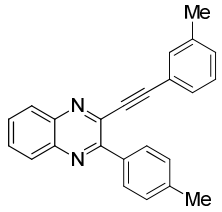


$^{13}C\{^{1}H\}$ NMR



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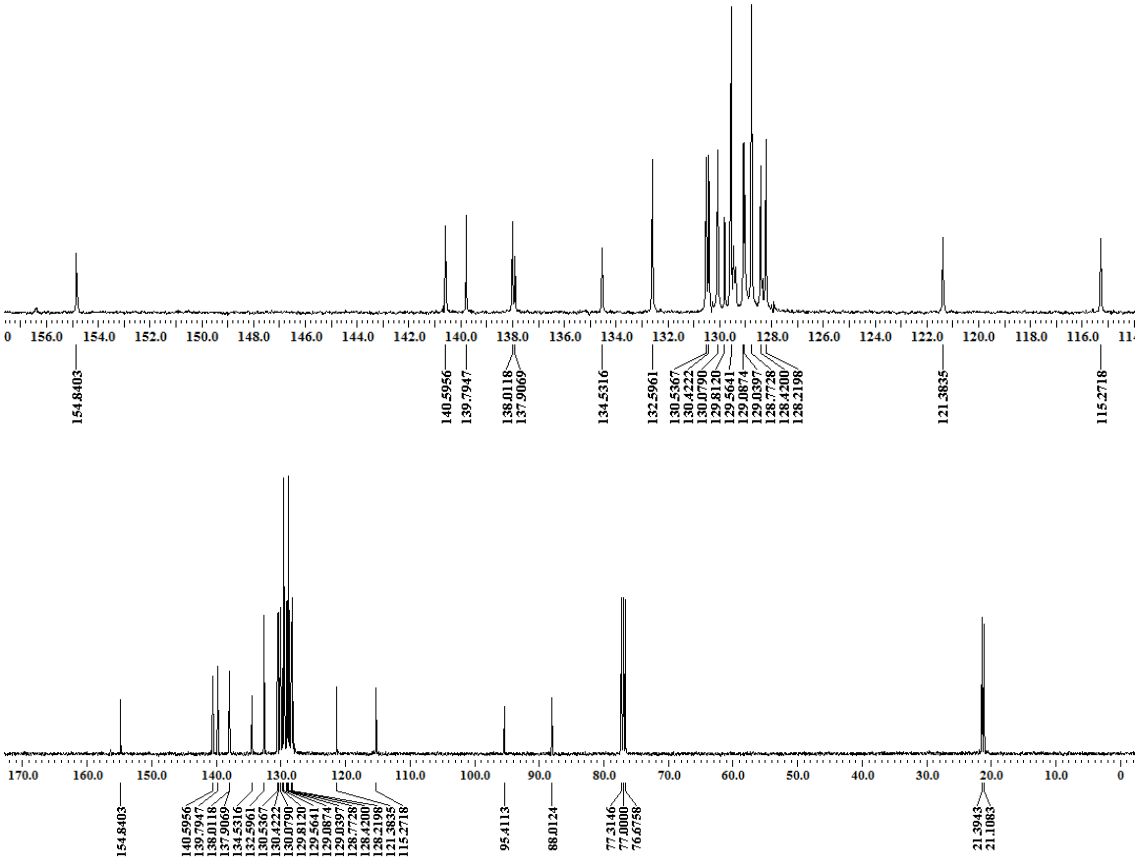

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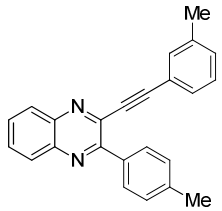

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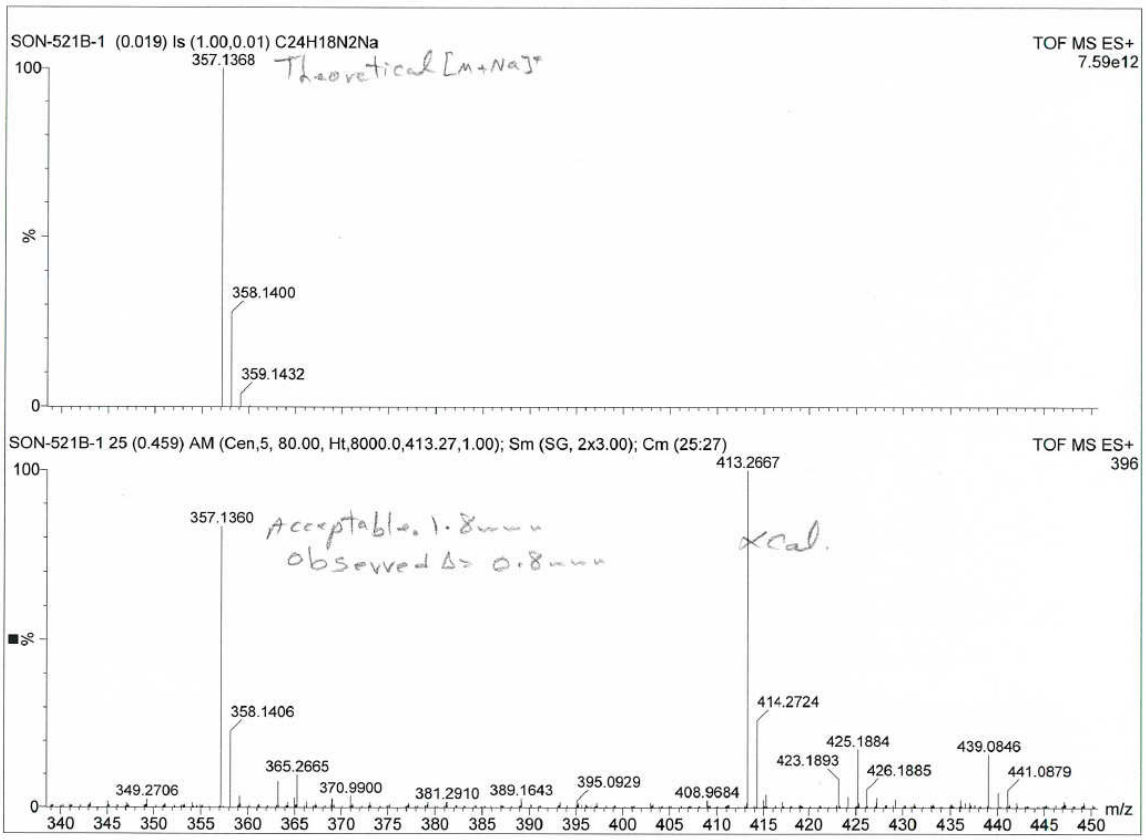

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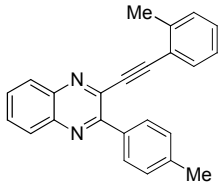

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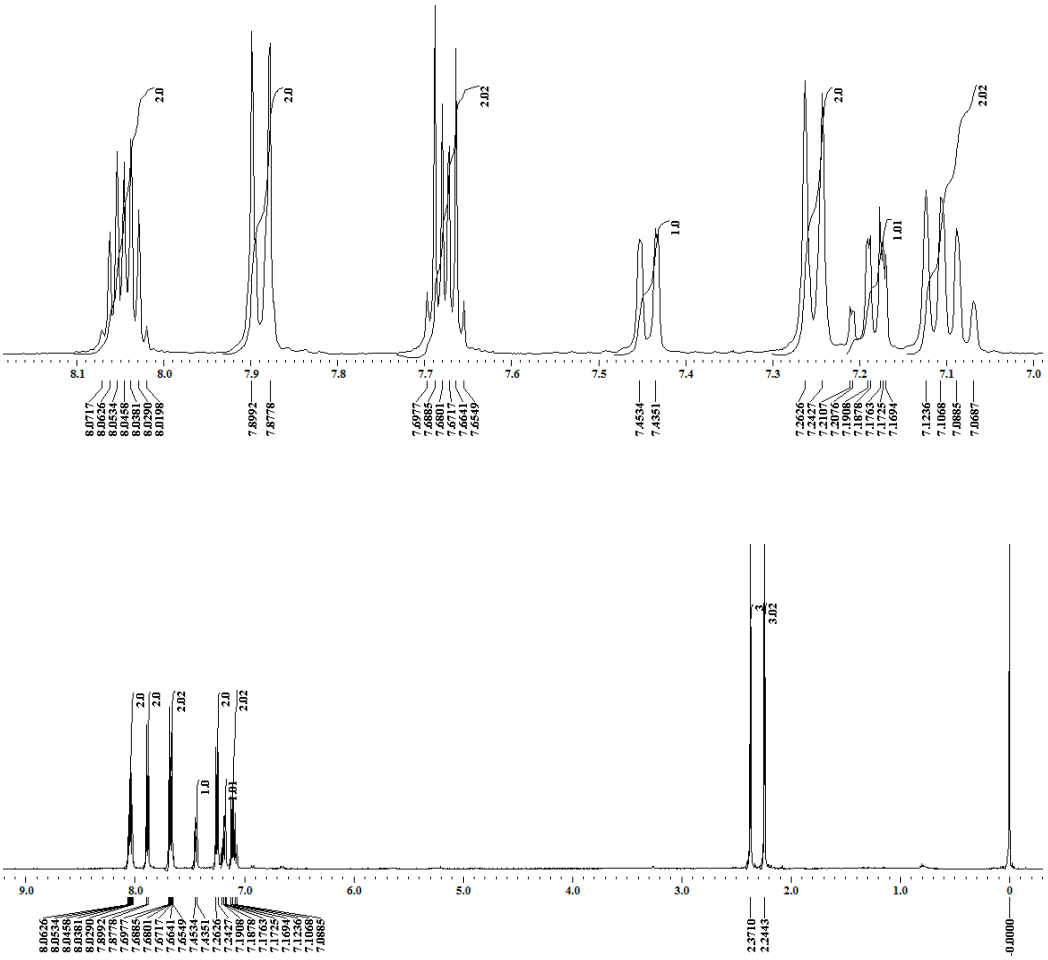
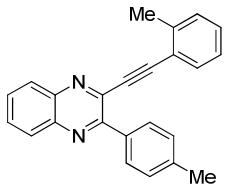


$^{13}C\{^{1}H\}$ NMR



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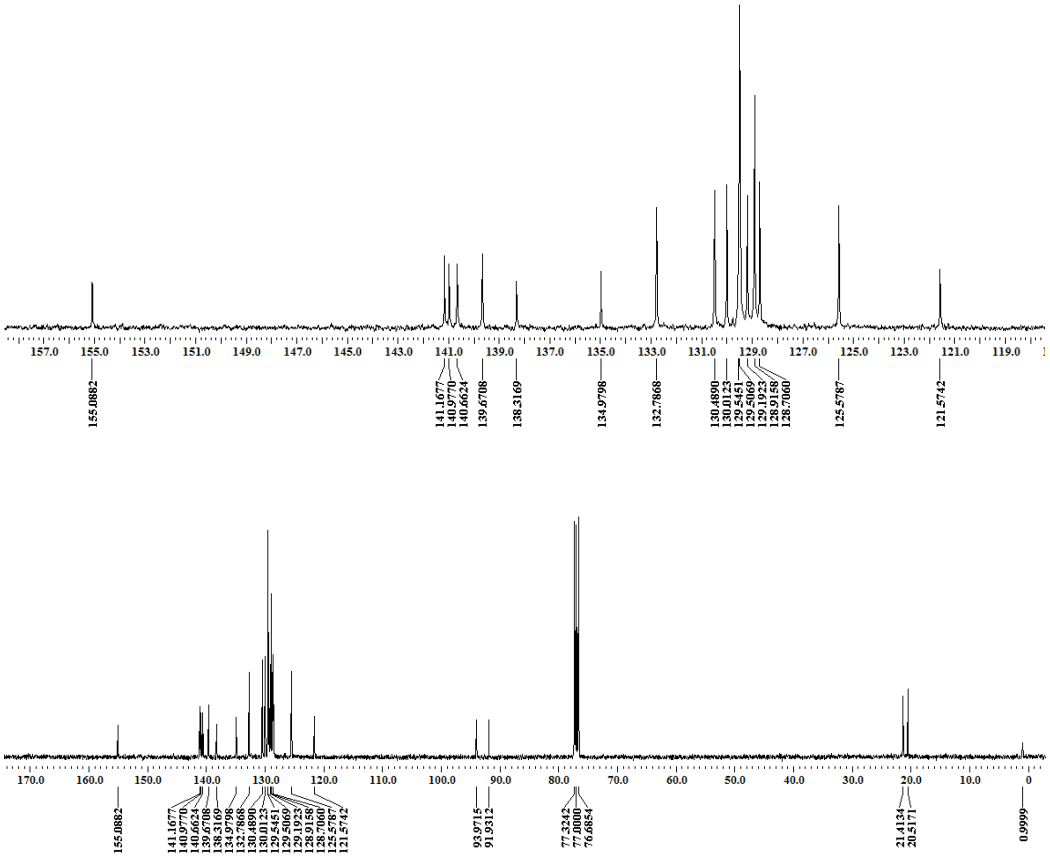

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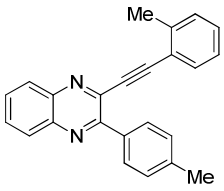
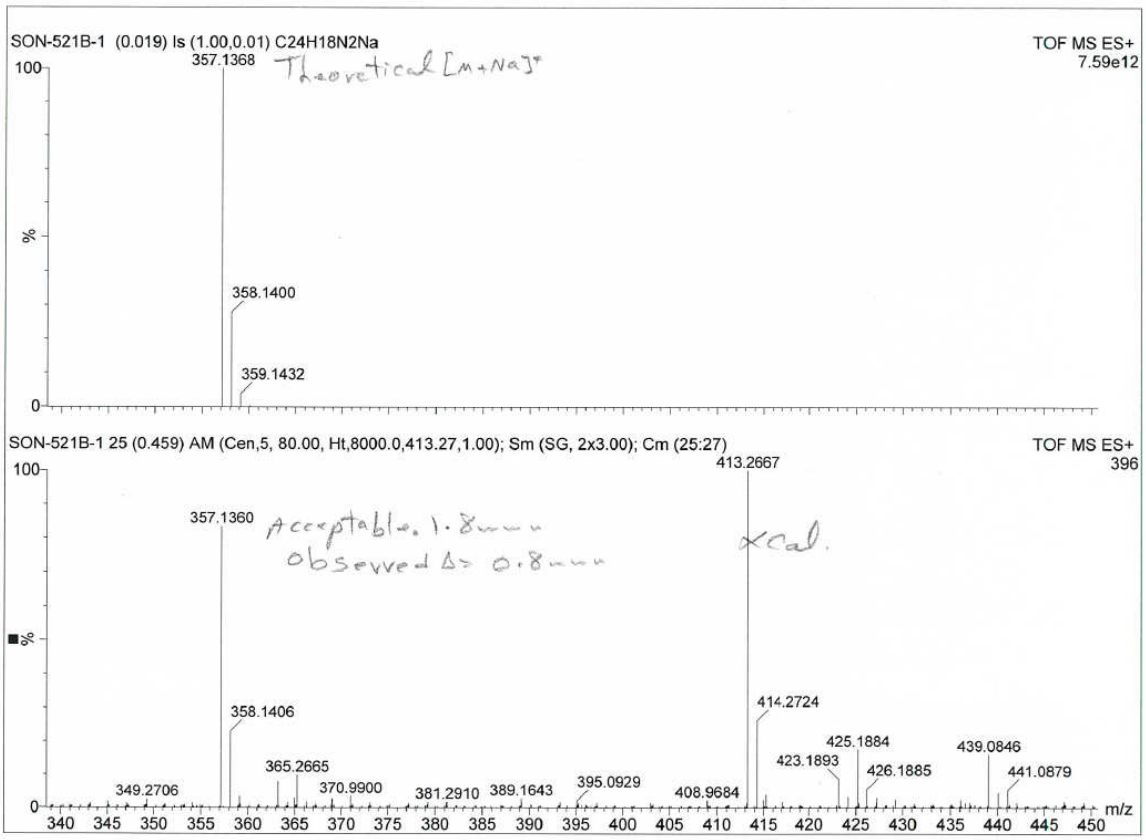
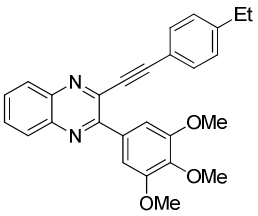


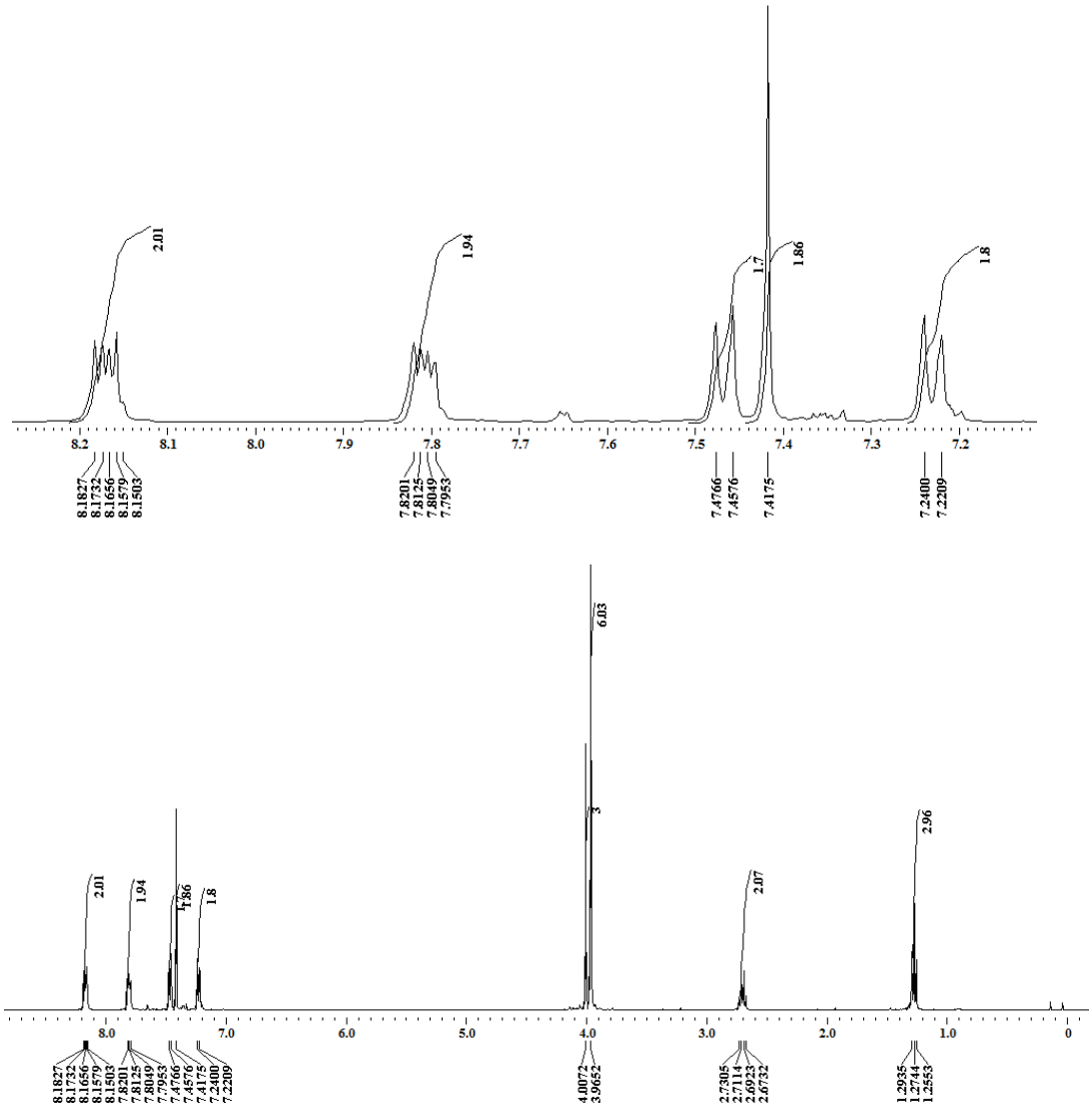
2-(*p*-Tolyl)-3-(*o*-tolylethynyl)quinoxaline (4c)



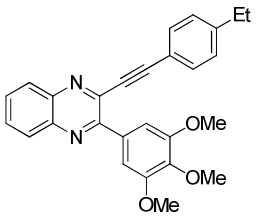
^{1}H NMR



2-((4-Ethylphenyl)ethynyl)-3-(3,4,5-trimethoxyphenyl)quinoxaline (4k)



$^{13}C\{^{1}H\}$ NMR



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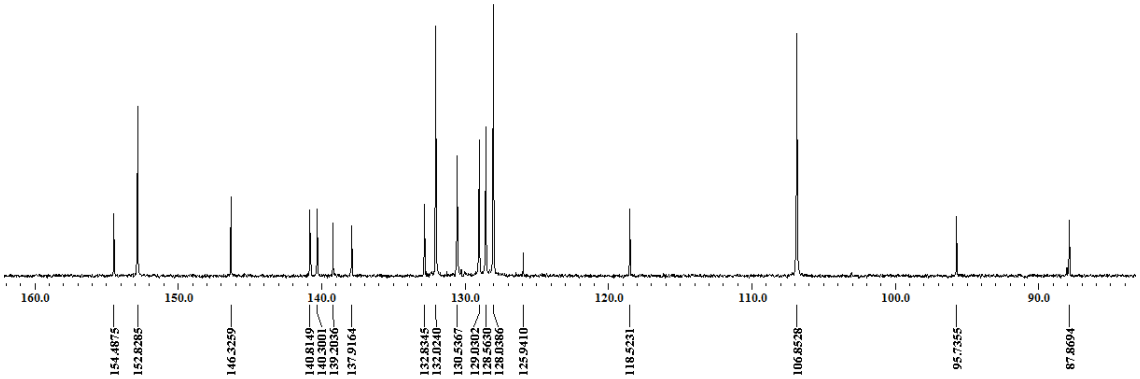

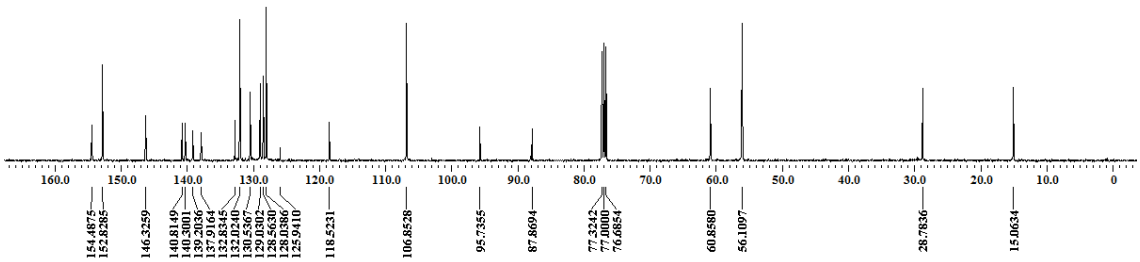

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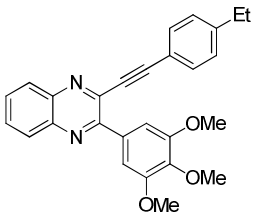

2-((4-Ethylphenyl)ethynyl)-3-(3,4,5-trimethoxyphenyl)quinoxaline (4k)

Qualitative Compound Report

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Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	22-12-2015 14:46:10
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

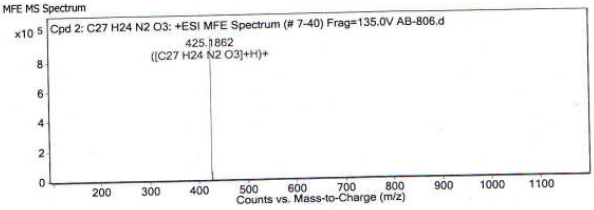
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

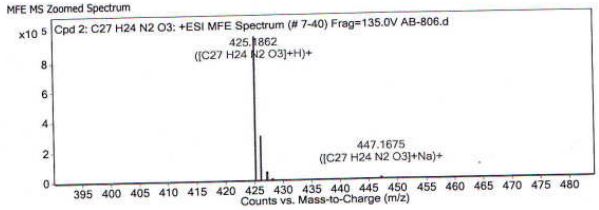
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C27 H24 N2 O3	11	424.1789	C27 H24 N2 O3	C27 H24 N2 O3	-0.6	C27 H24 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C27 H24 N2 O3	425.1862	11	Find by Molecular Feature	424.1789

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
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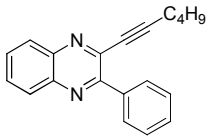
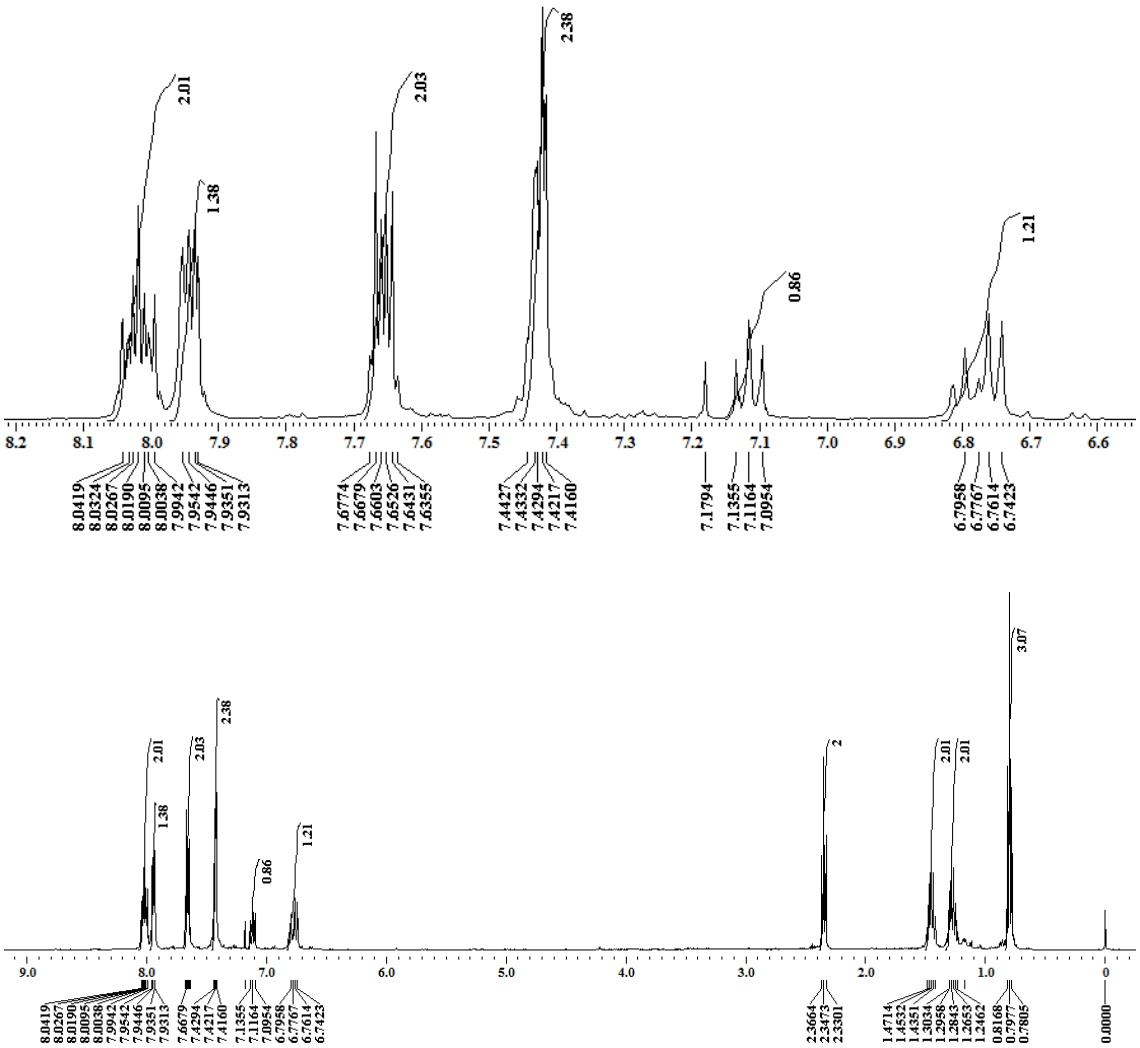
426.1893	1	282890.66	C27 H24 N2 O3	(M+H)+
427.1935	1	52579.08	C27 H24 N2 O3	(M+H)+
428.1981	1	7854.3	C27 H24 N2 O3	(M+H)+
429.2045	1	968.76	C27 H24 N2 O3	(M+H)+
447.1675	1	6535.51	C27 H24 N2 O3	(M+Na)+
448.1708	1	1949.64	C27 H24 N2 O3	(M+Na)+
449.171	1	518.09	C27 H24 N2 O3	(M+Na)+

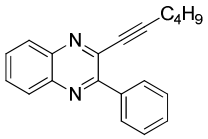
^{1}H NMR



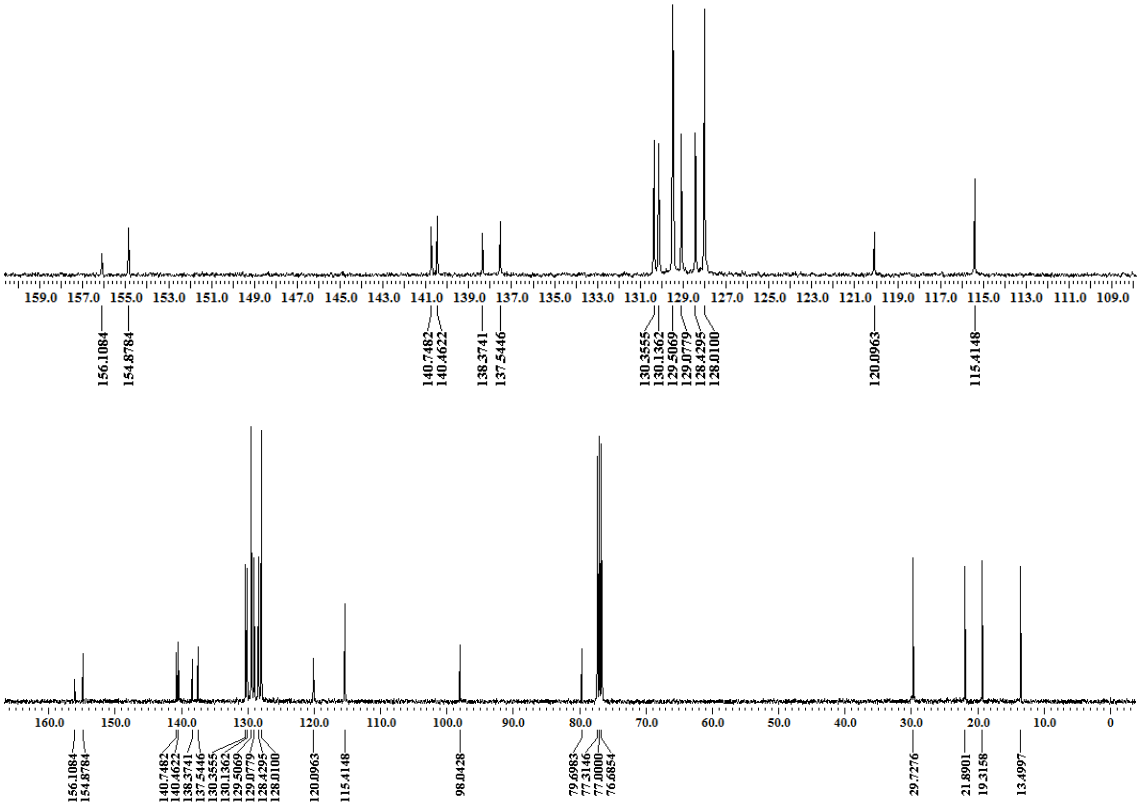
2-(Hex-1-yn-1-yl)-3-phenylquinoxaline (4s)



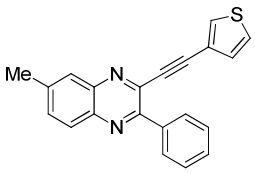
$^{13}C\{^{1}H\}$ NMR



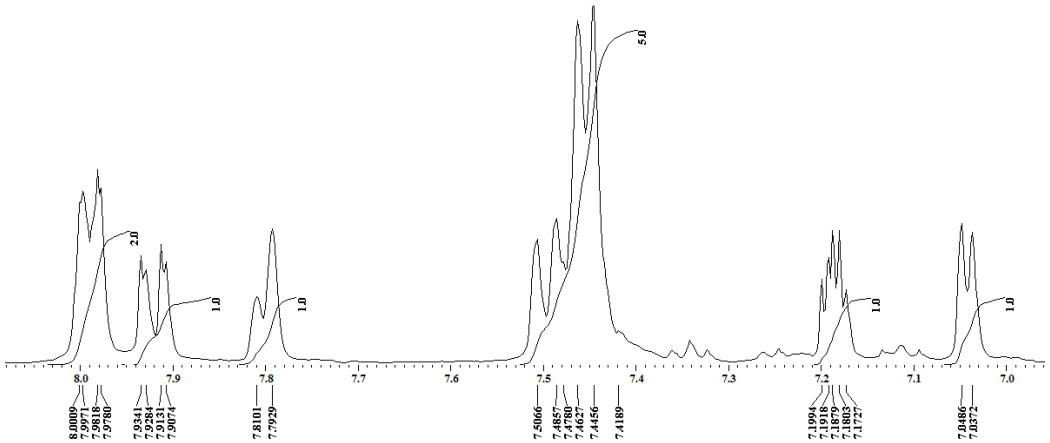
2-(Hex-1-yn-1-yl)-3-phenylquinoxaline (4s)

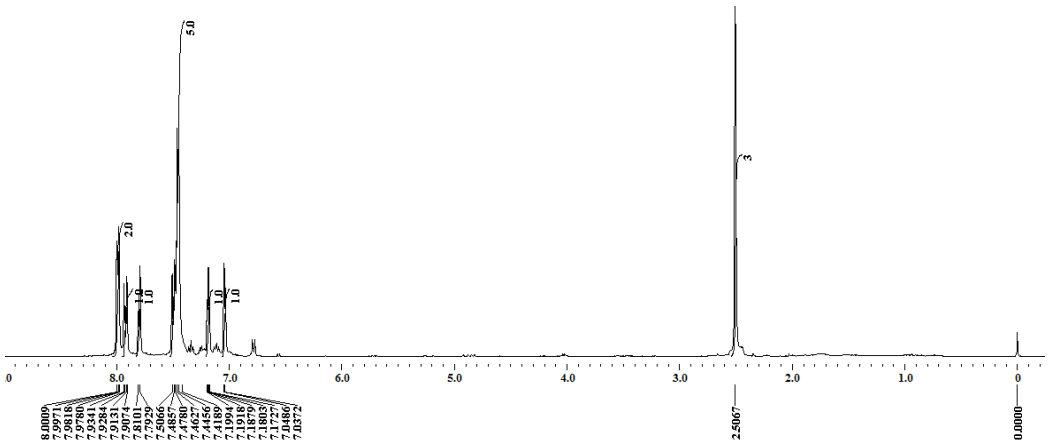


^{1}H NMR

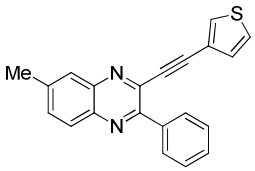


6-methyl-2-phenyl-3-(thiophen-3-ylethynyl)quinoxaline (6a)

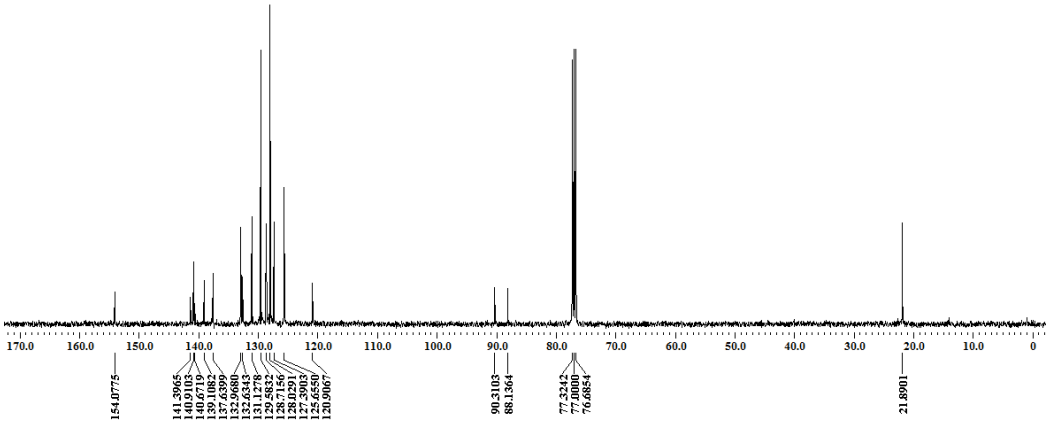




$^{13}C\{^{1}H\}$ NMR



6-methyl-2-phenyl-3-(thiophen-3-ylethynyl)quinoxaline (6a)



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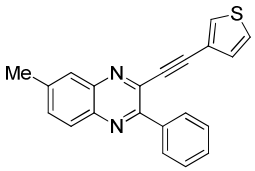
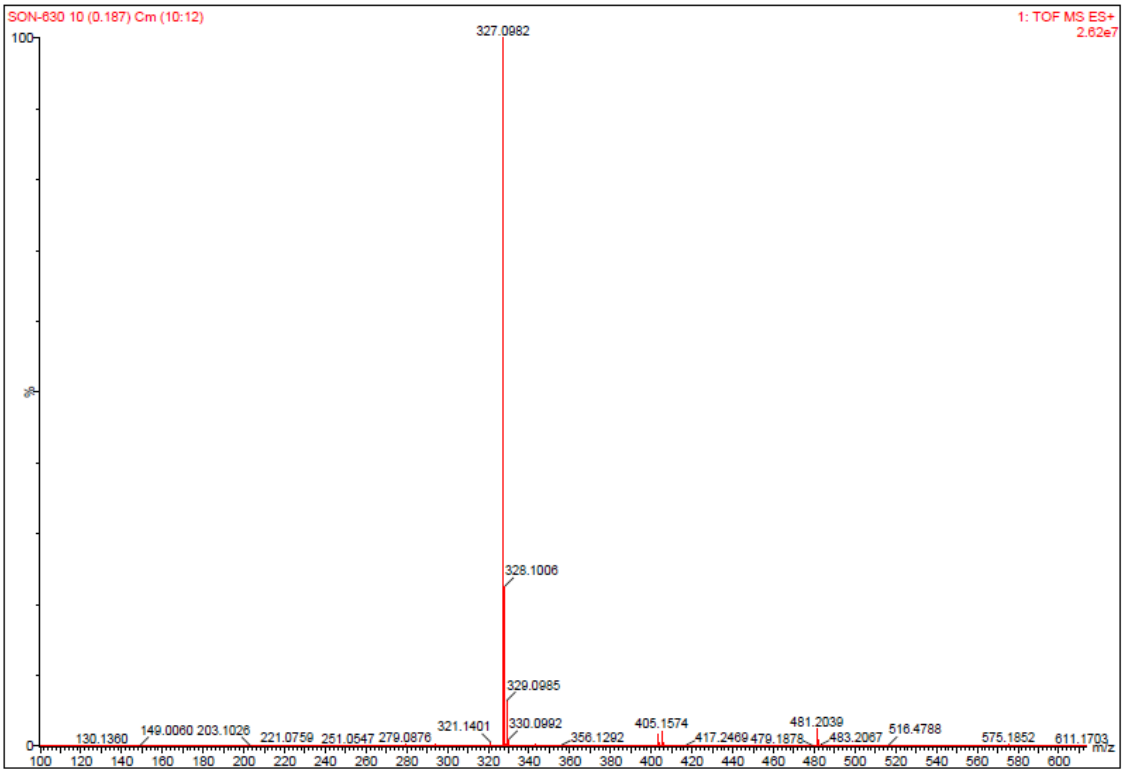
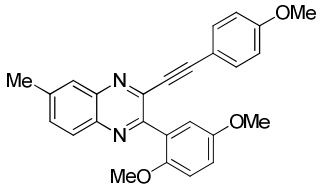


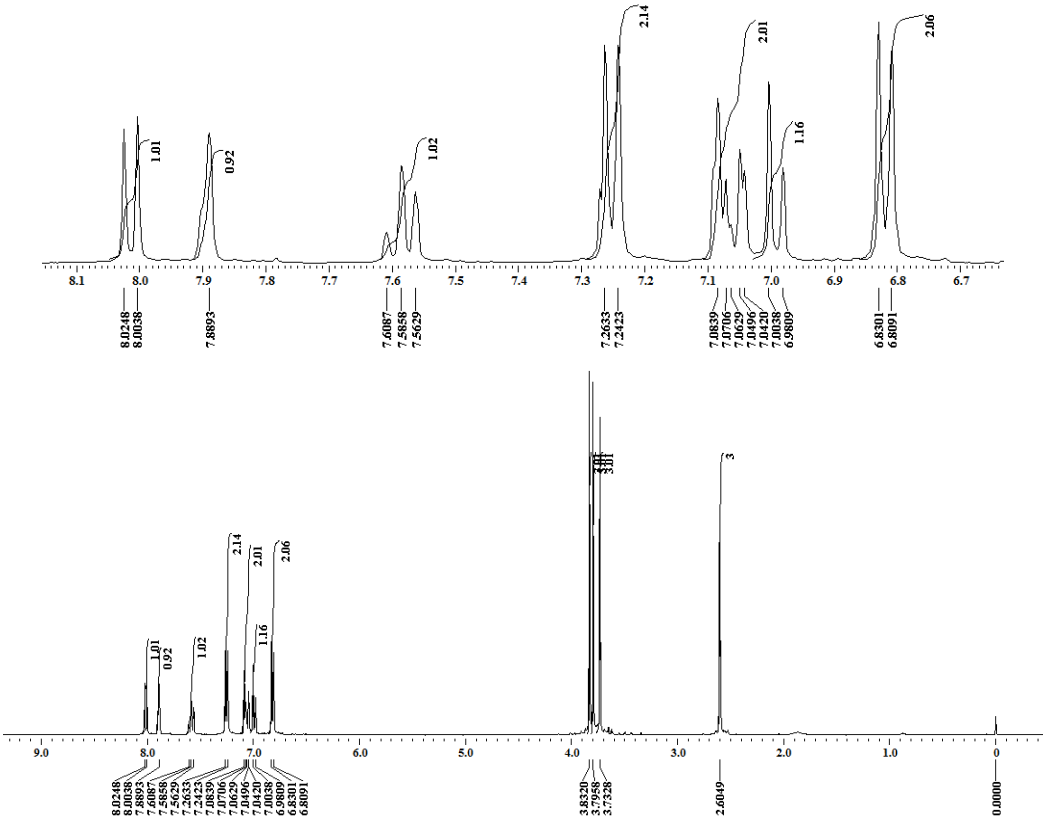
6-methyl-2-phenyl-3-(thiophen-3-ylethynyl)quinoxaline (6a)



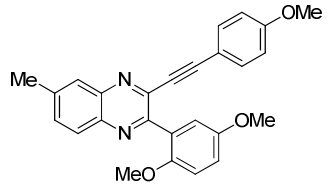
^{1}H NMR



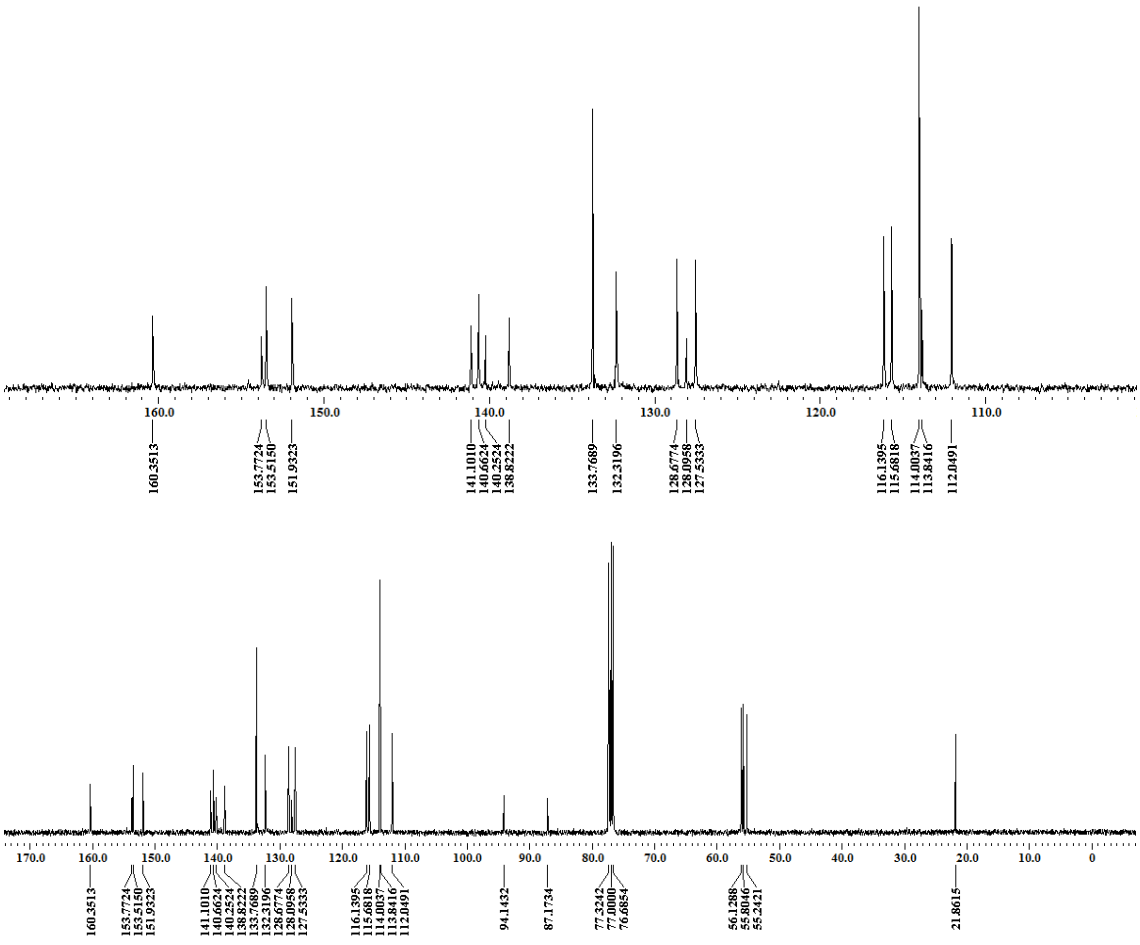
2-(2,5-Dimethoxyphenyl)-3-((4-methoxyphenyl)ethynyl)-6-methylquinoxaline (6c)



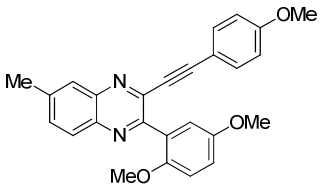
$^{13}C\{^{1}H\}$ NMR



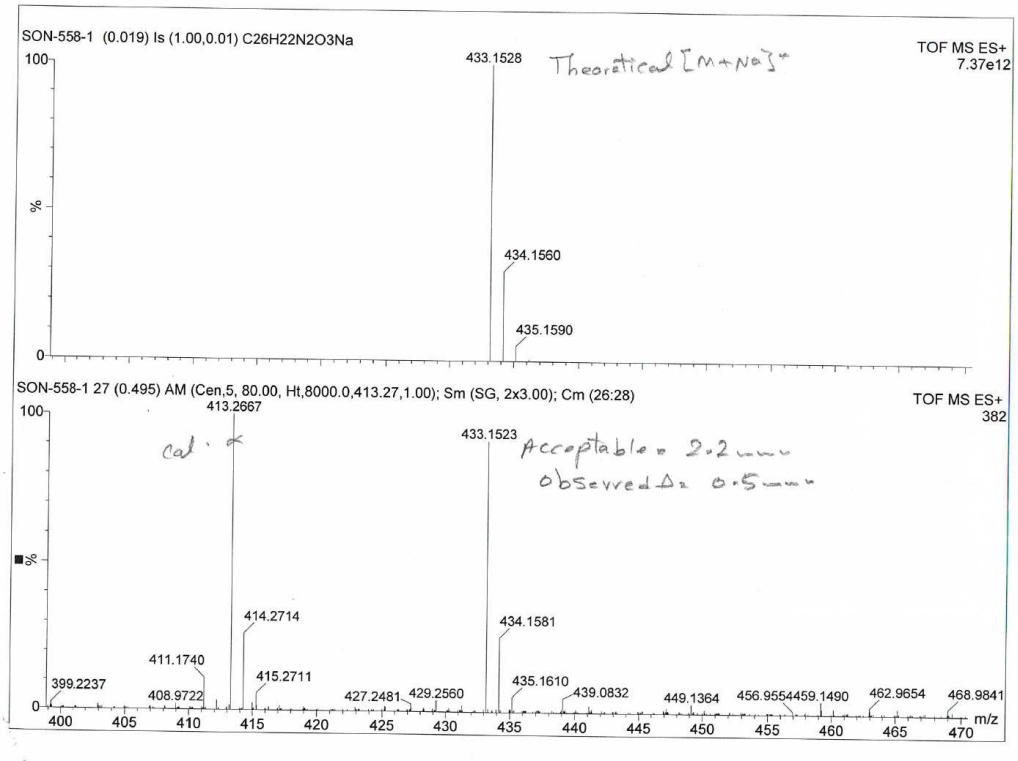
2-(2,5-Dimethoxyphenyl)-3-((4-methoxyphenyl)ethynyl)-6-methylquinoxaline (6c)



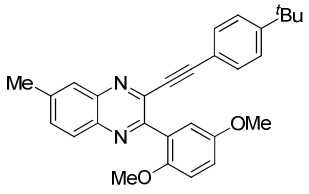
HRMS



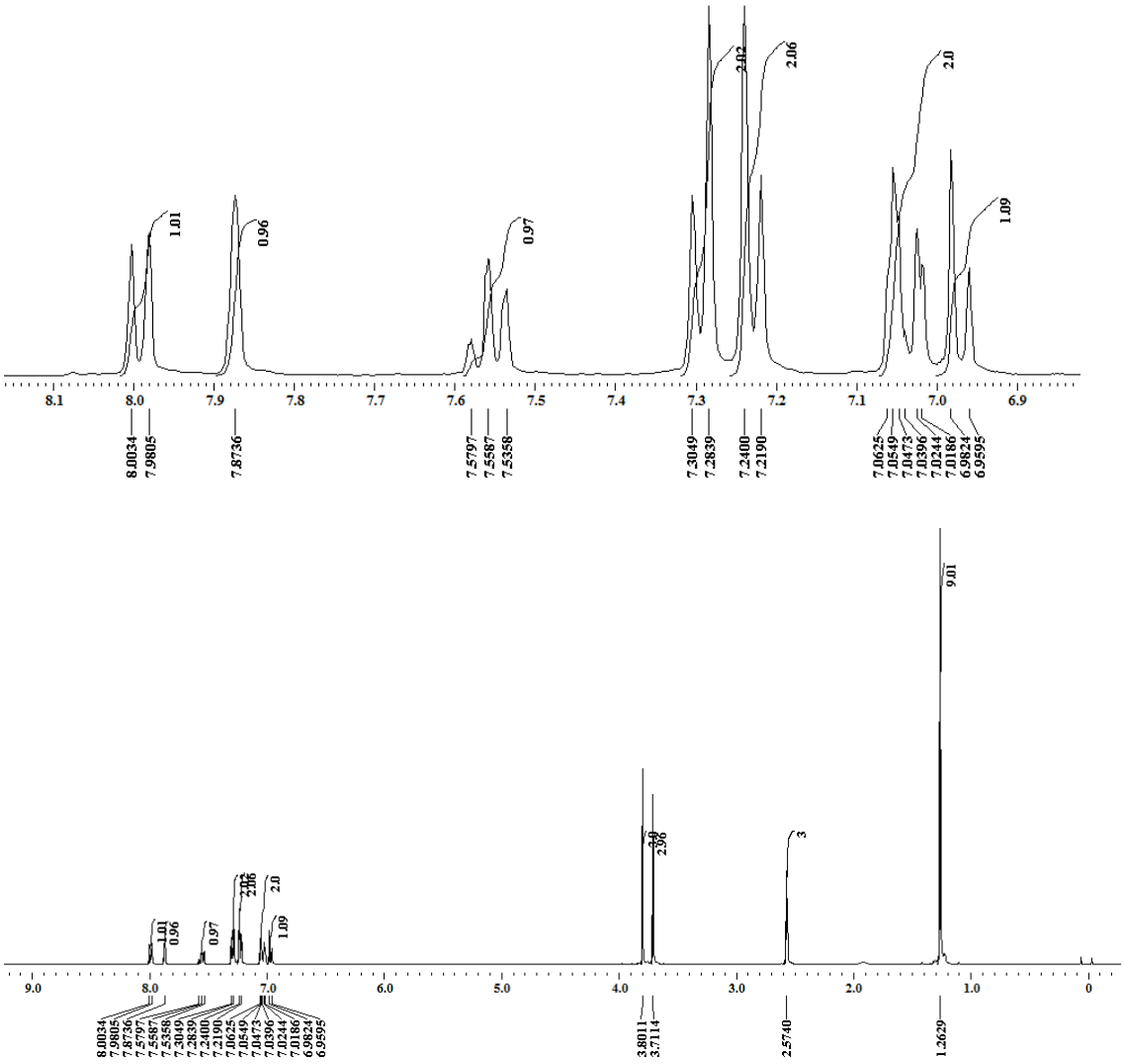
2-(2,5-Dimethoxyphenyl)-3-((4-methoxyphenyl)ethynyl)-6-methylquinoxaline (6c)



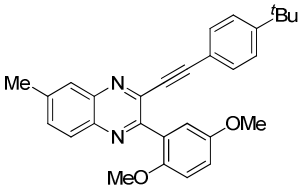
^{1}H NMR



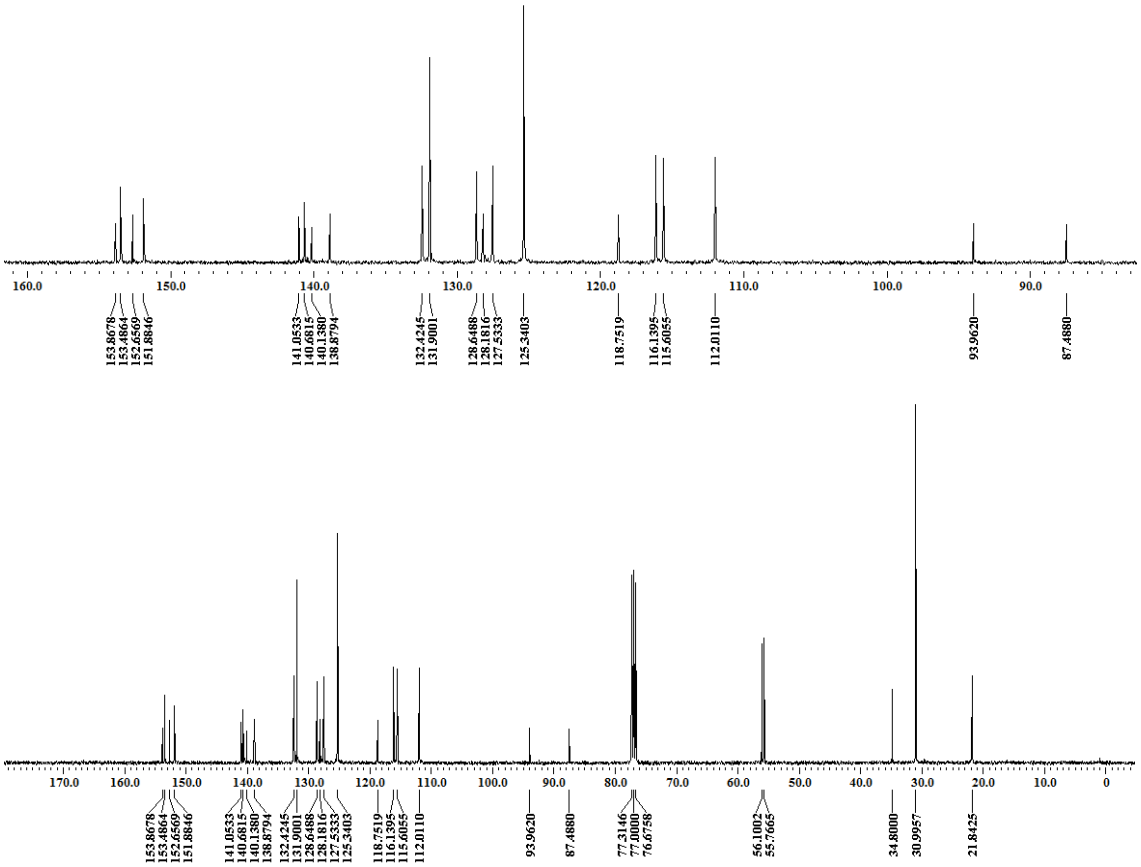
3-((4-(tert-Butyl)phenyl)ethynyl)-2-(2,5-dimethoxyphenyl)-6-methylquinoxaline (6d)



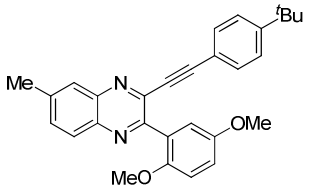
$^{13}C\{^{1}H\}$ NMR



3-((4-(tert-Butyl)phenyl)ethynyl)-2-(2,5-dimethoxyphenyl)-6-methylquinoxaline (6d)



HRMS



3-((4-(tert-Butyl)phenyl)ethynyl)-2-(2,5-dimethoxyphenyl)-6-methylquinoxaline (6d)

Qualitative Compound Report

Data File	SON-919.d	**Sample Name**	SON-919
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	12-07-2016 15:35:03
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

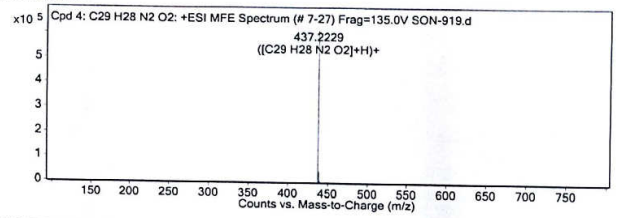
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

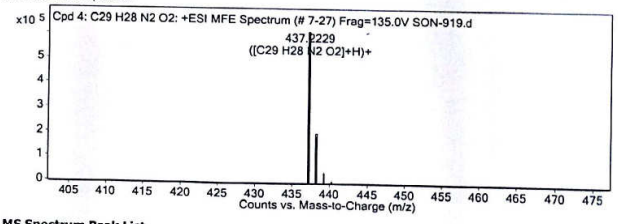
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C29 H28 N2 O2	11	436.2158	C29 H28 N2 O2	C29 H28 N2 O2	-1.55	C29 H28 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C29 H28 N2 O2	437.2229	11	Find by Molecular Feature	436.2158

MFE MS Spectrum



MFE MS Zoomed Spectrum

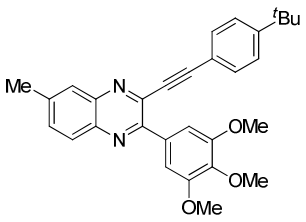


MS Spectrum Peak List

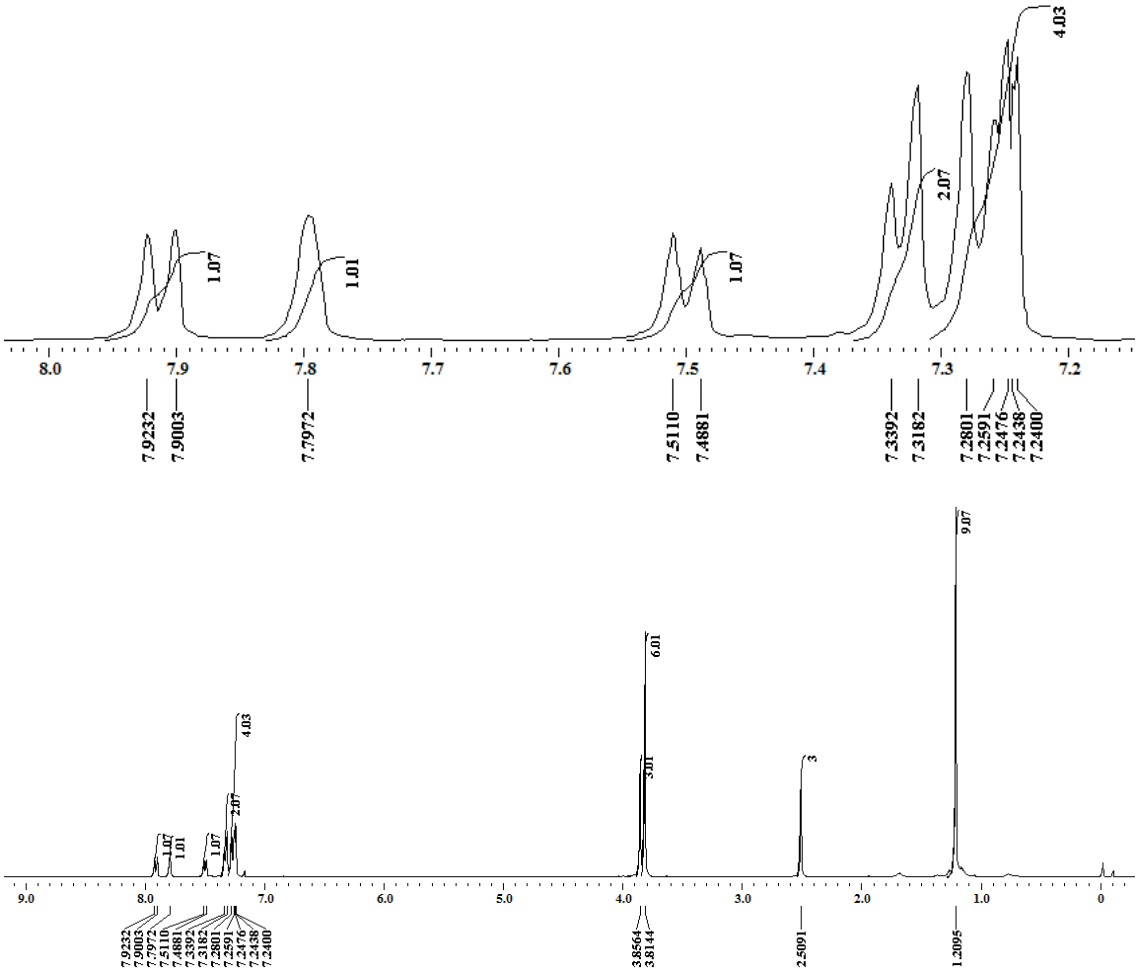
m/z	z	Abund	Formula	Ion
437.2229	1	612949.44	C29 H28 N2 O2	(M+H)+
438.2259	1	189387	C29 H28 N2 O2	(M+H)+
439.2322	1	43319.19	C29 H28 N2 O2	(M+H)+
440.2372	1	7966.13	C29 H28 N2 O2	(M+H)+
441.2402	1	1143.29	C29 H28 N2 O2	(M+H)+
442.2444	1	173.04	C29 H28 N2 O2	(M+H)+

--- End Of Report ---

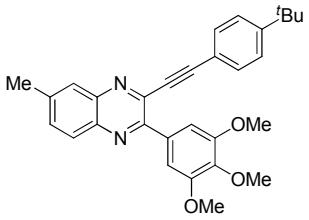
^{1}H NMR



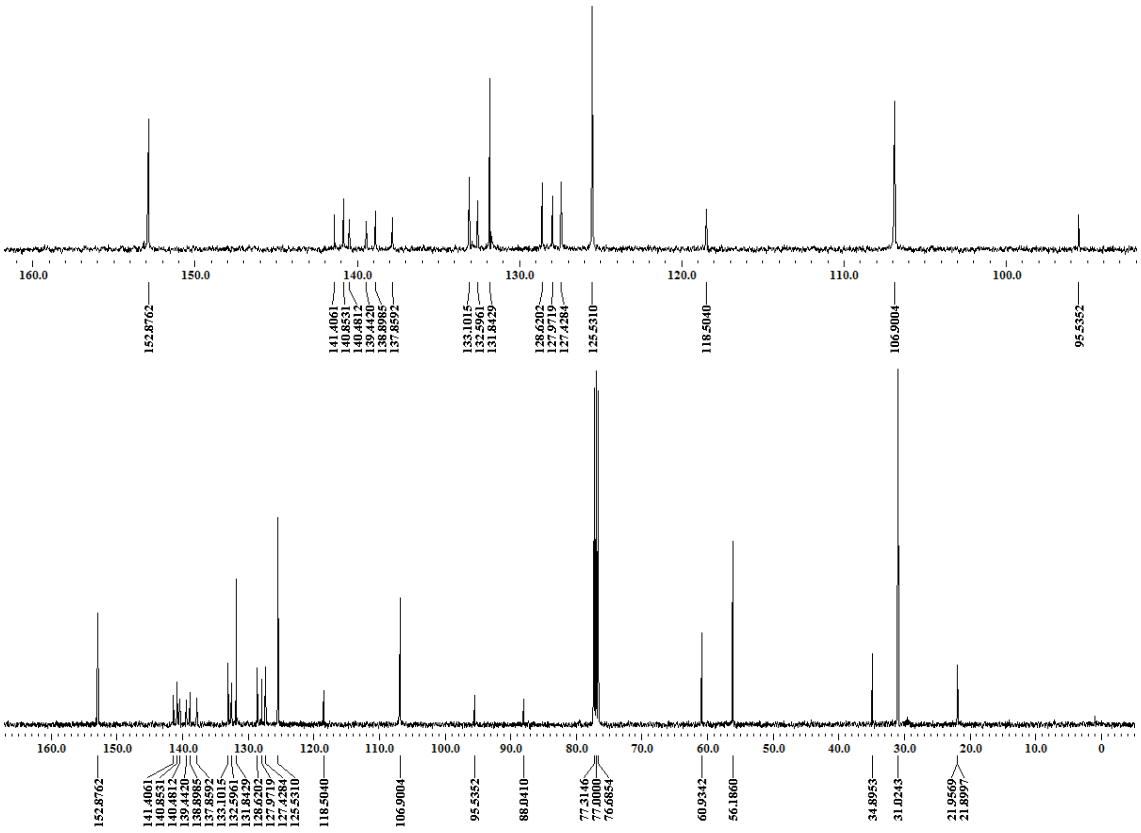
3-((4-(*tert*-Butyl)phenyl)ethynyl)-6-methyl-2-(3,4,5-trimethoxyphenyl)quinoxalin e (6e)



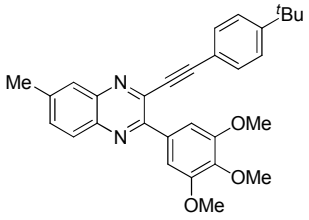
$^{13}C\{^{1}H\}$ NMR



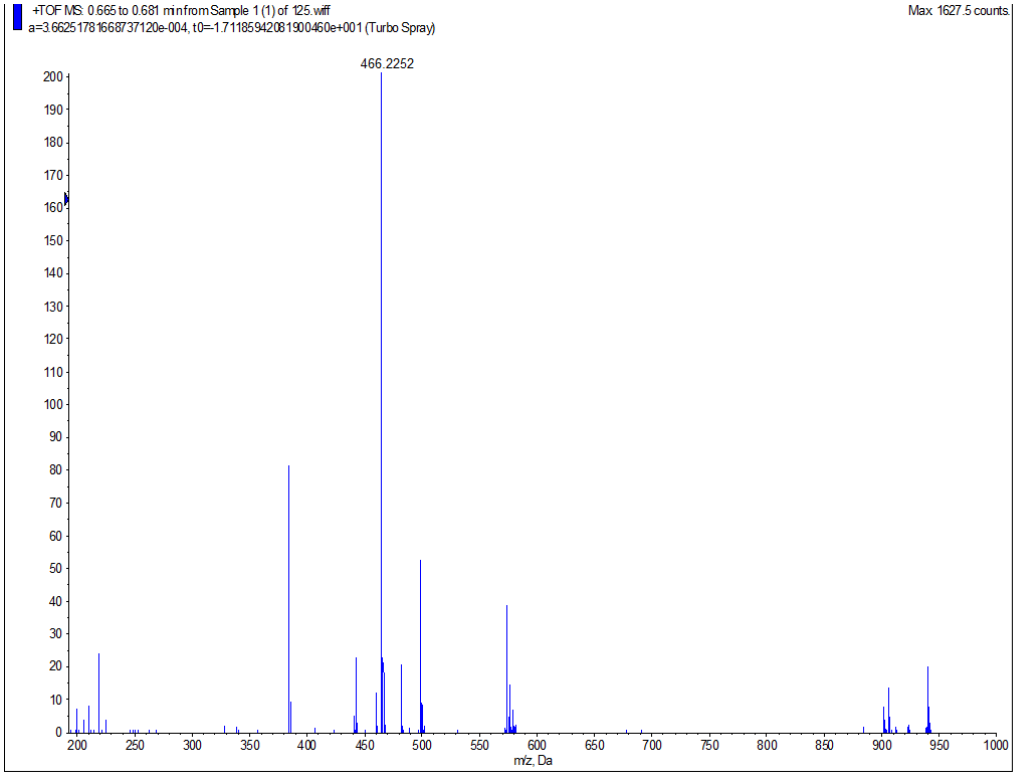
3-((4-(*tert*-Butyl)phenyl)ethynyl)-6-methyl-2-(3,4,5-trimethoxyphenyl)quinoxalin e (6e)



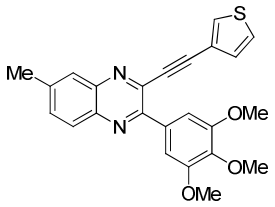
HRMS



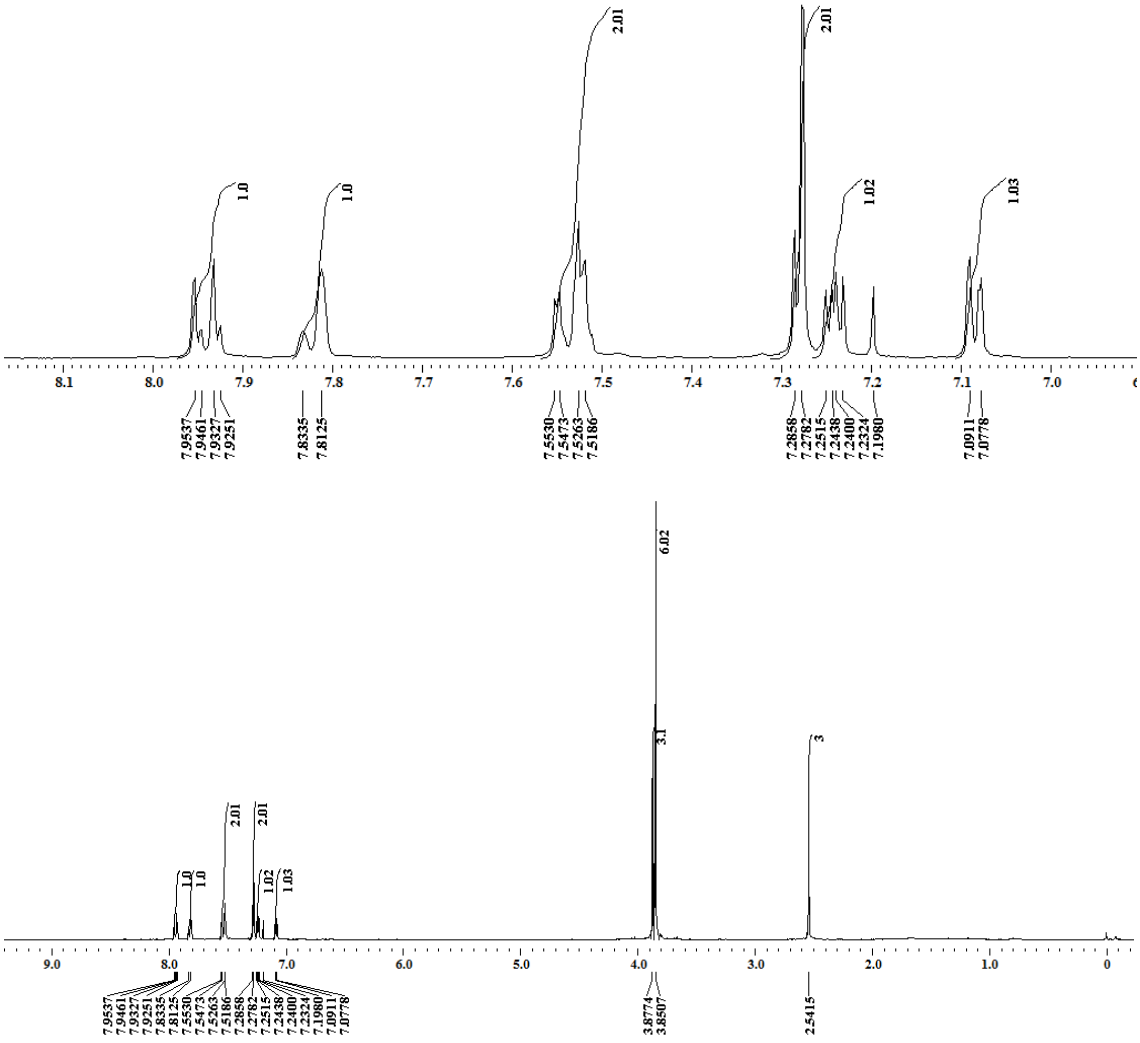
3-((4-(*tert*-Butyl)phenyl)ethynyl)-6-methyl-2-(3,4,5-trimethoxyphenyl)quinoxaline (6e)



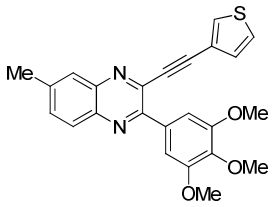
^{1}H NMR



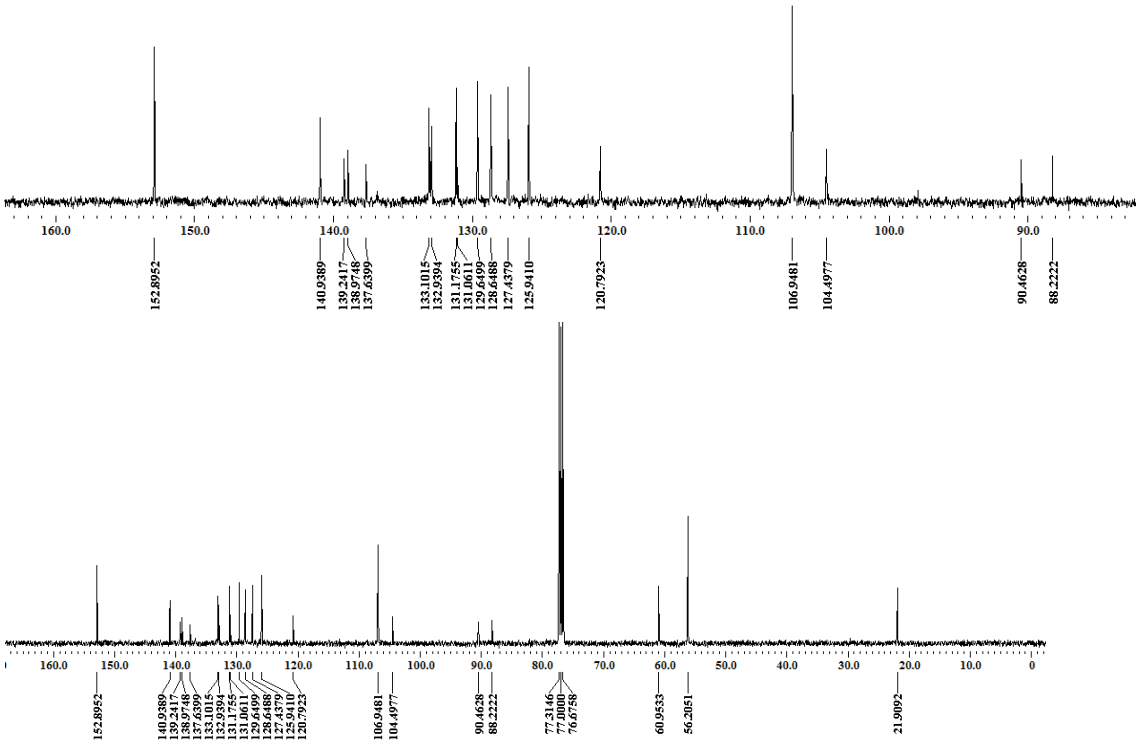
6-Methyl-3-(thiophen-3-ylethynyl)-2-(3,4,5-trimethoxyphenyl)quinoxaline (6f)



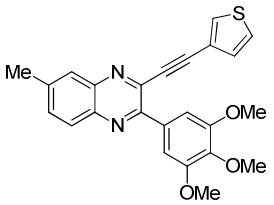
$^{13}C\{^{1}H\}$ NMR



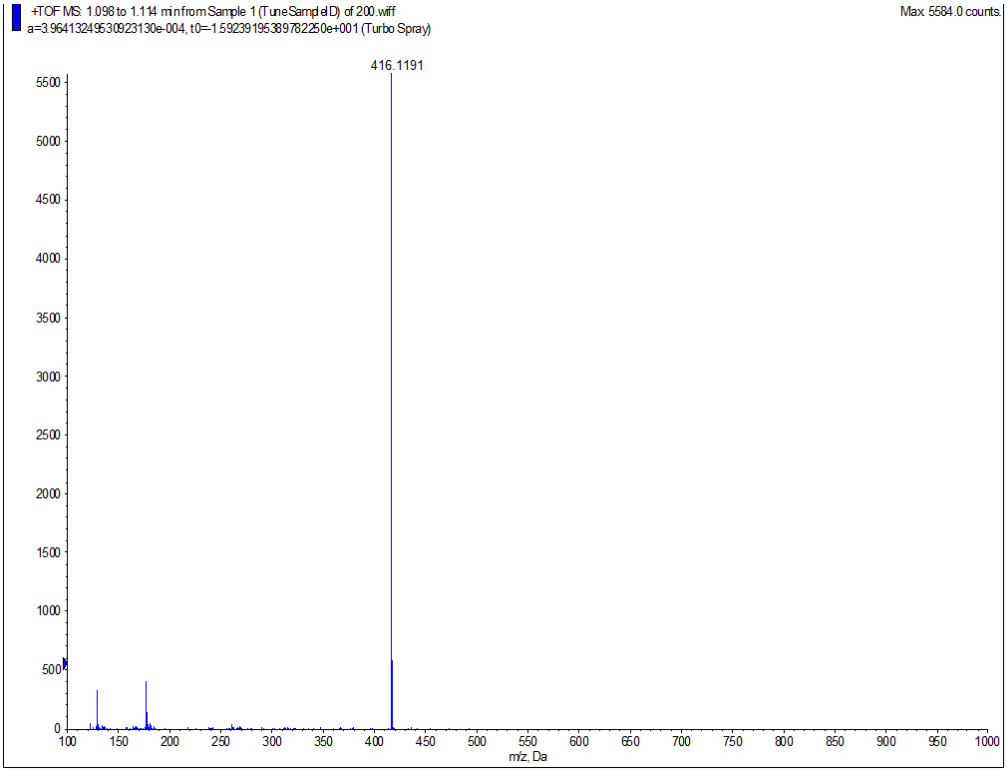
6-Methyl-3-(thiophen-3-ylethynyl)-2-(3,4,5-trimethoxyphenyl)quinoxaline (6f)



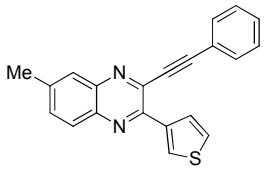
HRMS



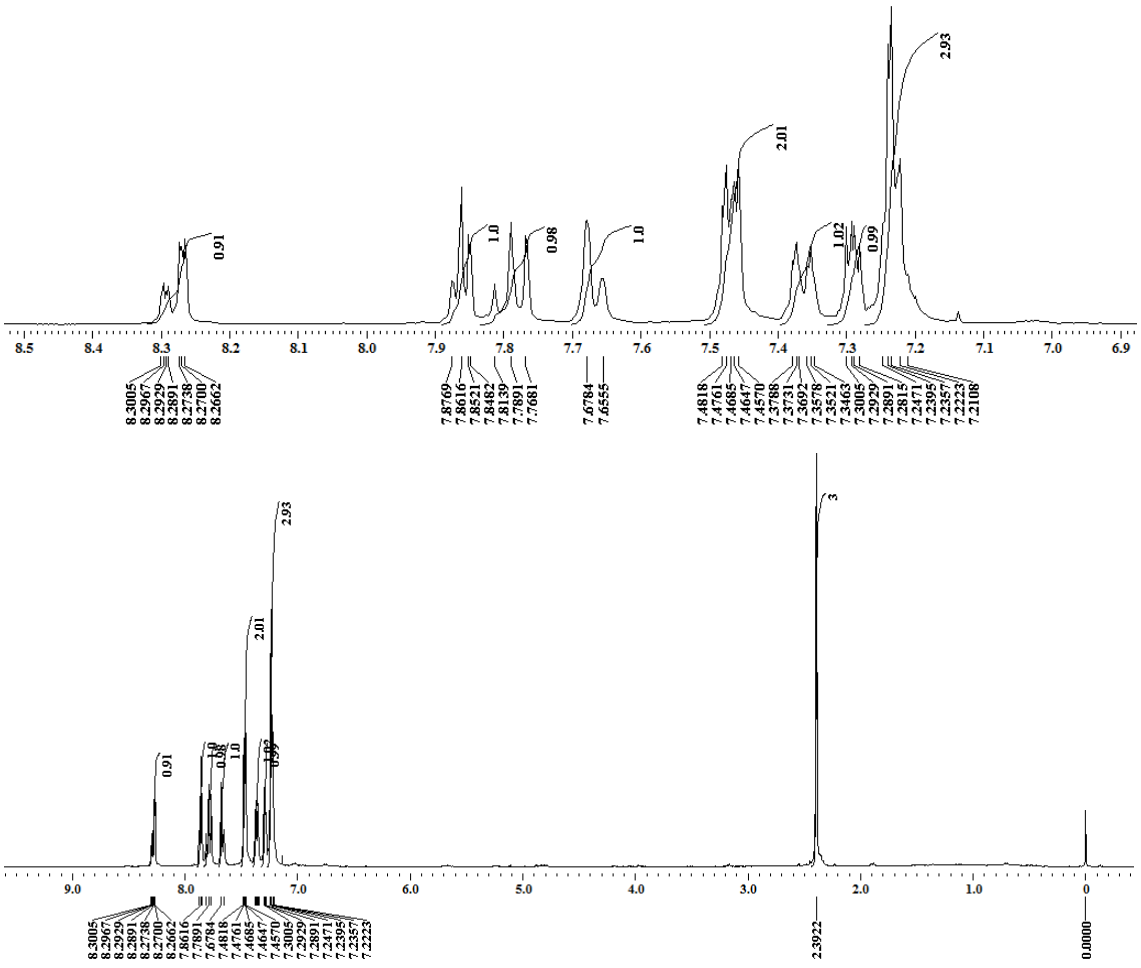
6-Methyl-3-(thiophen-3-ylethynyl)-2-(3,4,5-trimethoxyphenyl)quinoxaline (6f)



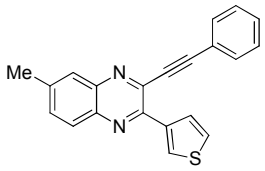
^{1}H NMR



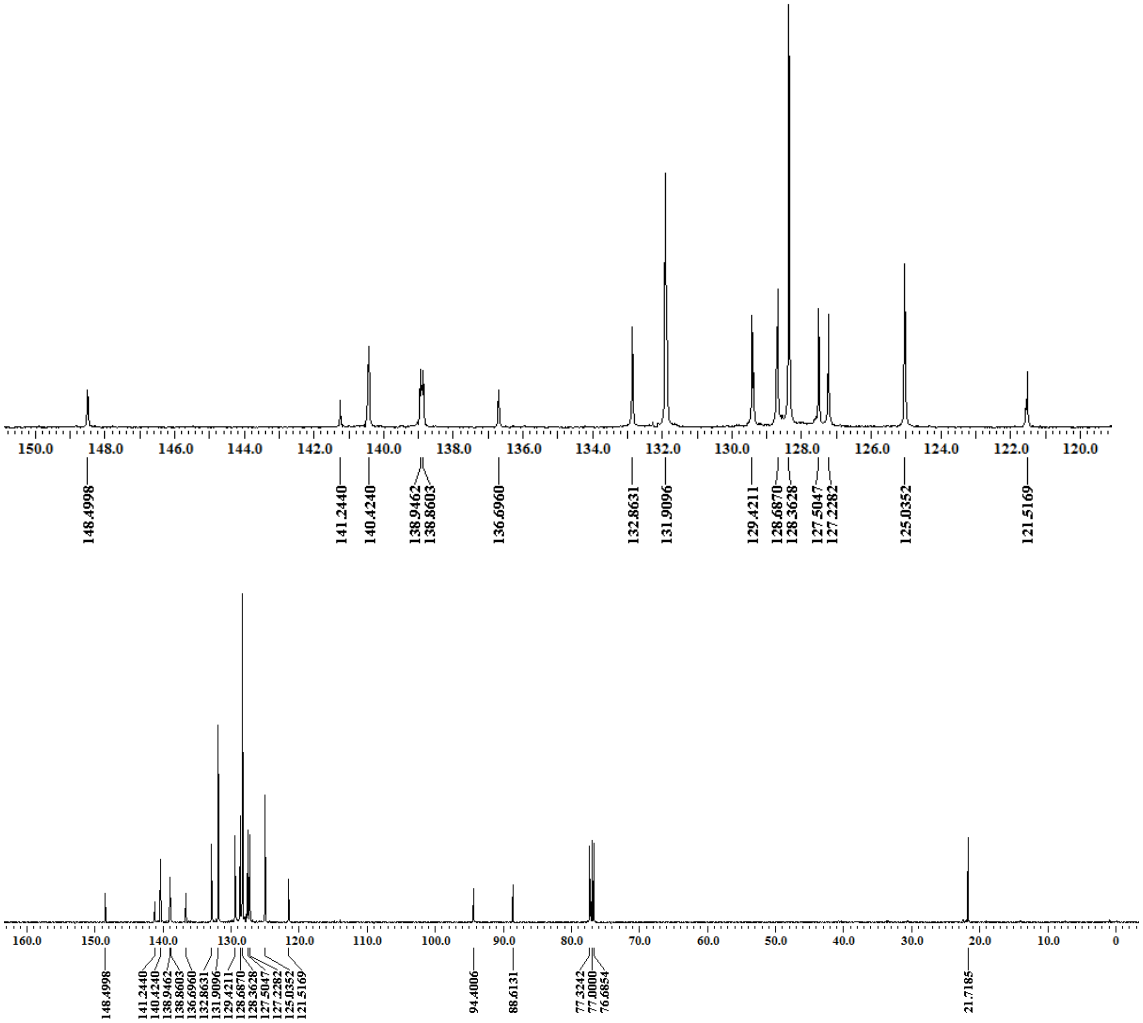
6-Methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoxaline
(6g)



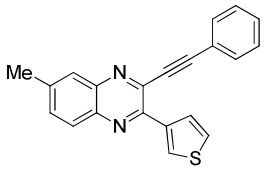
$^{13}C\{^{1}H\}$ NMR



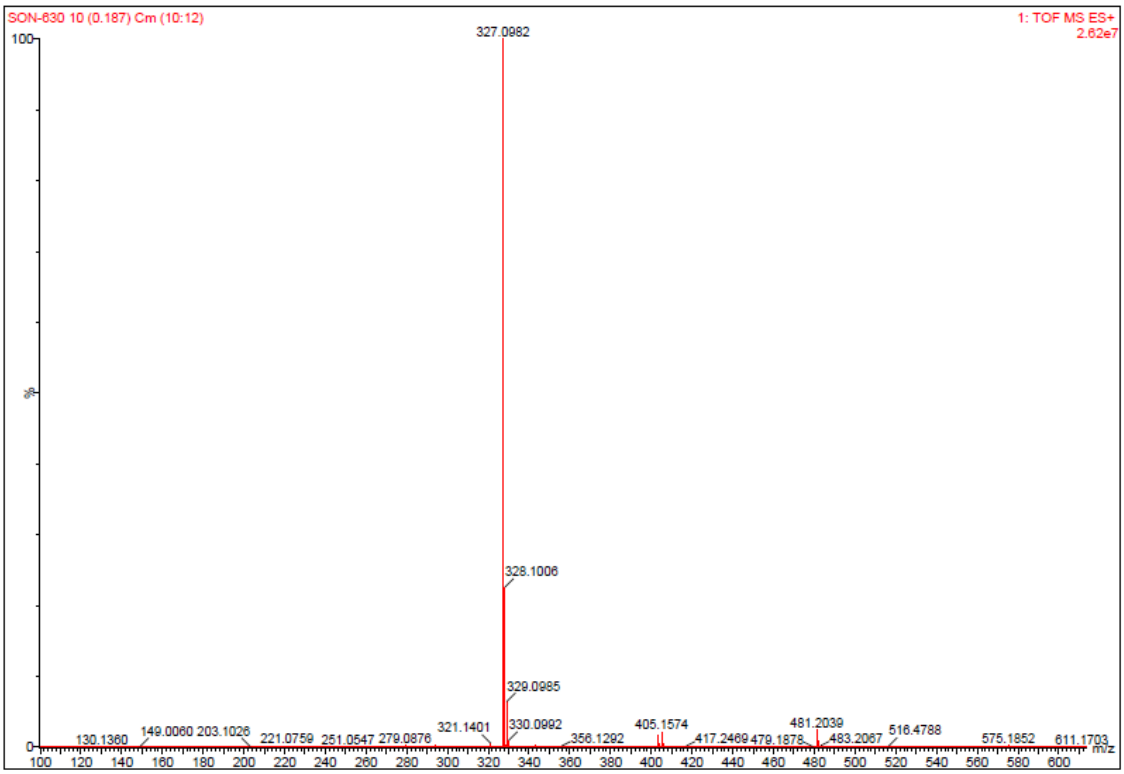
6-Methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoxaline
(6g)



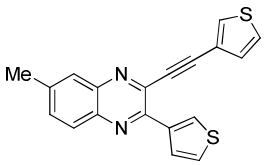
HRMS



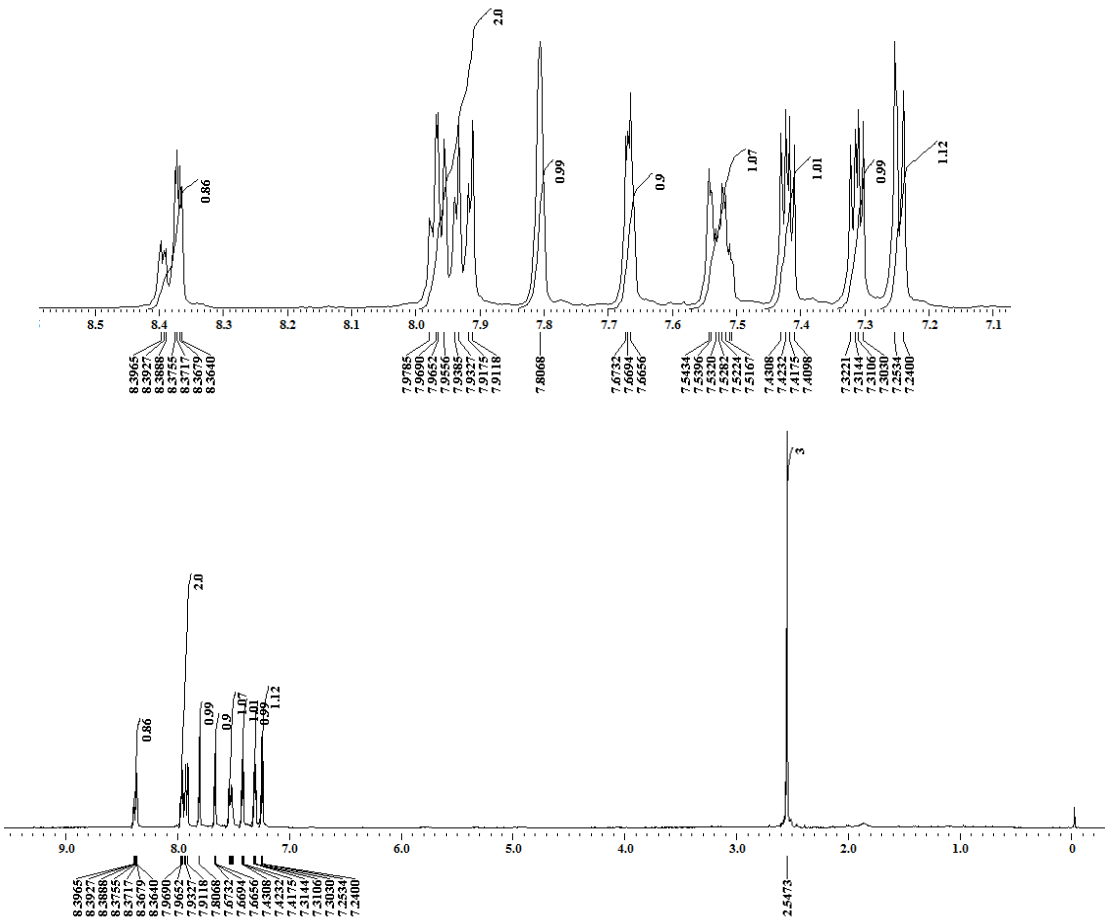
6-Methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoxaline
(6g)



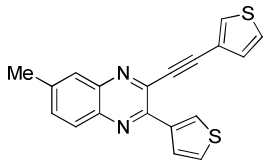
^{1}H NMR



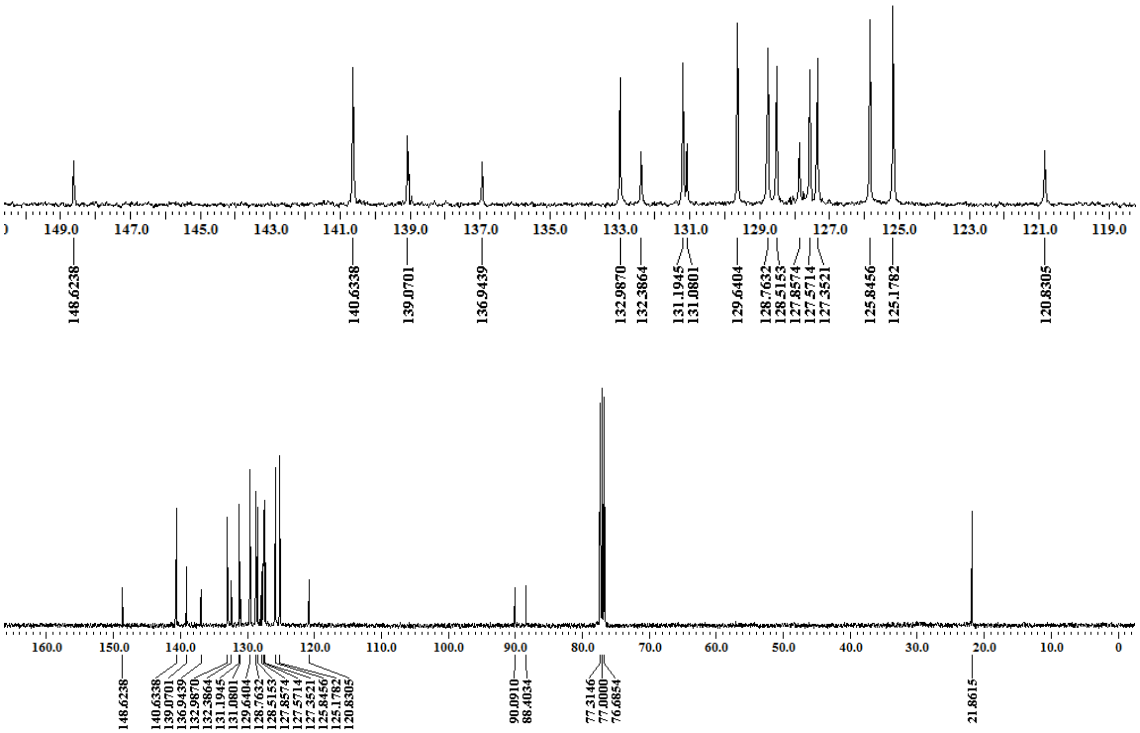
6-Methyl-2-(thiophen-3-yl)-3-(thiophen-3-ylethynyl)quinoxaline (6i)



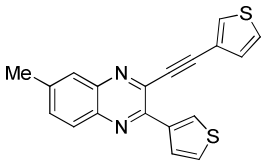
$^{13}C\{^{1}H\}$ NMR



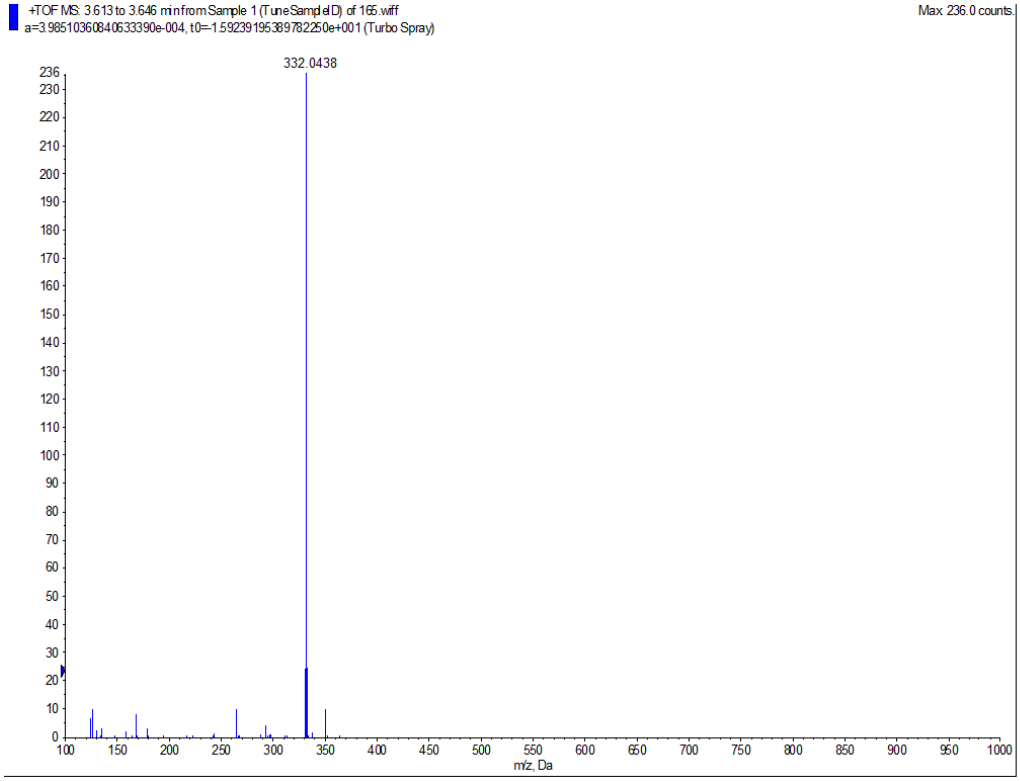
6-Methyl-2-(thiophen-3-yl)-3-(thiophen-3-ylethynyl)quinoxaline (6i)



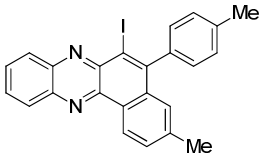
HRMS



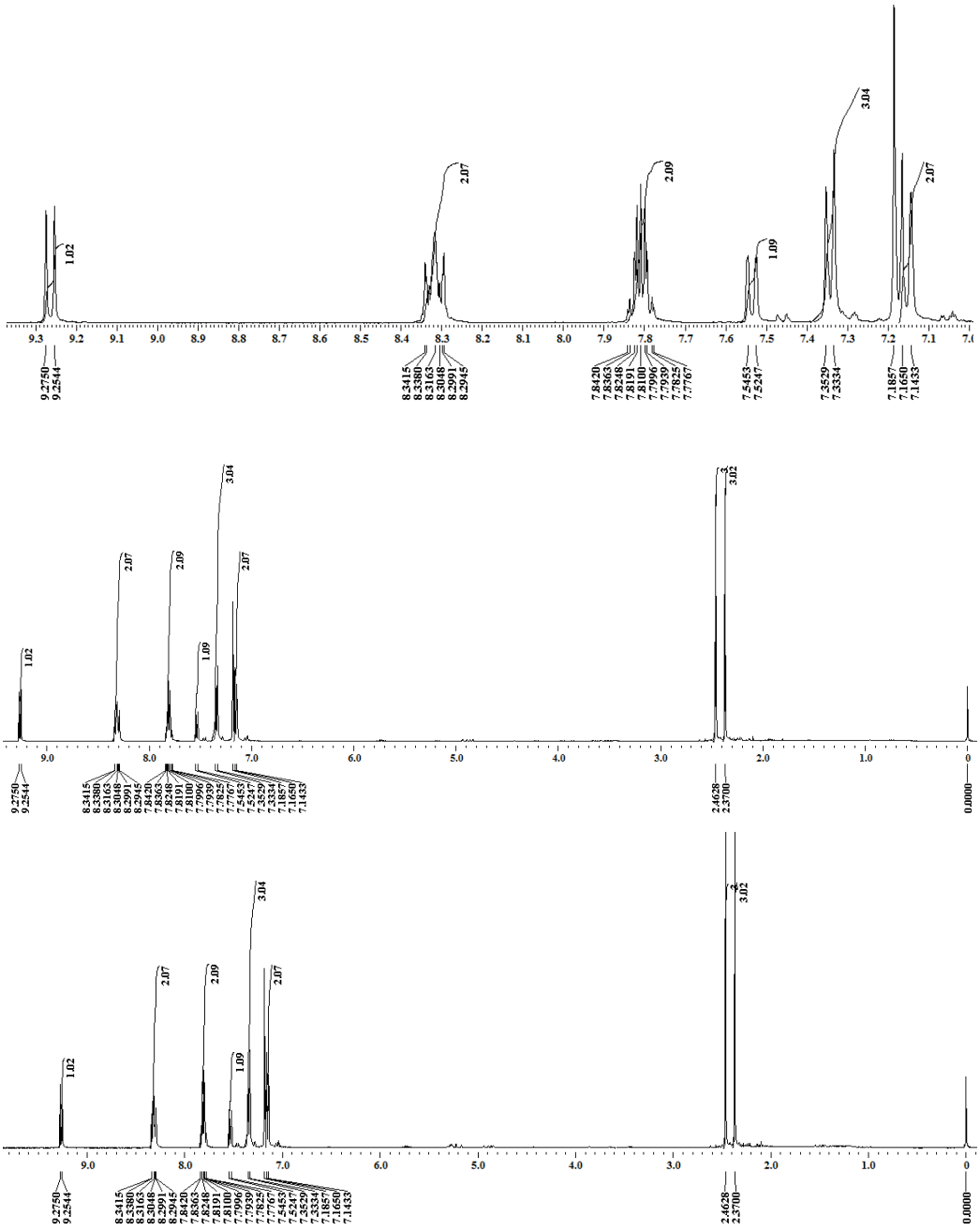
6-Methyl-2-(thiophen-3-yl)-3-(thiophen-3-ylethynyl)quinoxaline (6i)



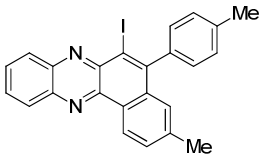
^{1}H NMR



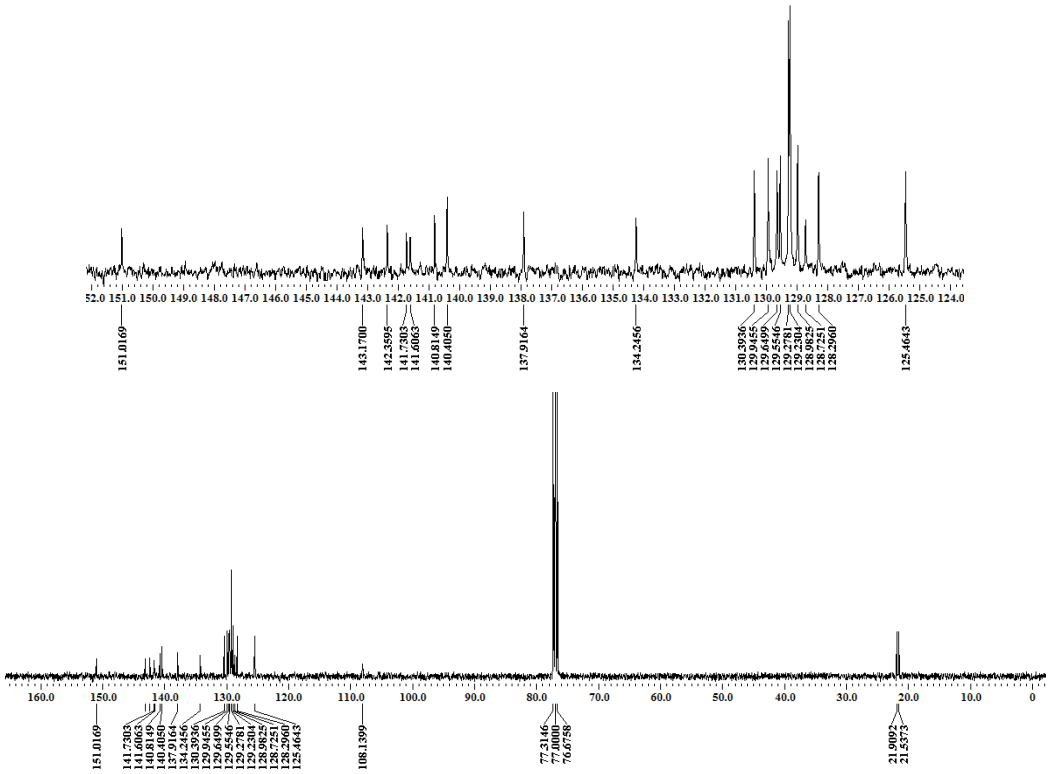
6-Iodo-3-methyl-5-(*p*-tolyl)benzo[*a*]phenazine (5a)



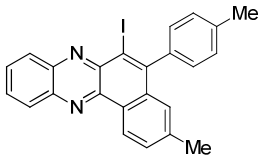
$^{13}C\{^{1}H\}$ NMR



6-Iodo-3-methyl-5-(*p*-tolyl)benzo[*a*]phenazine (5a)

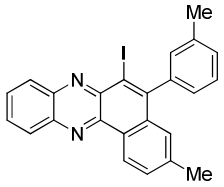


HRMS

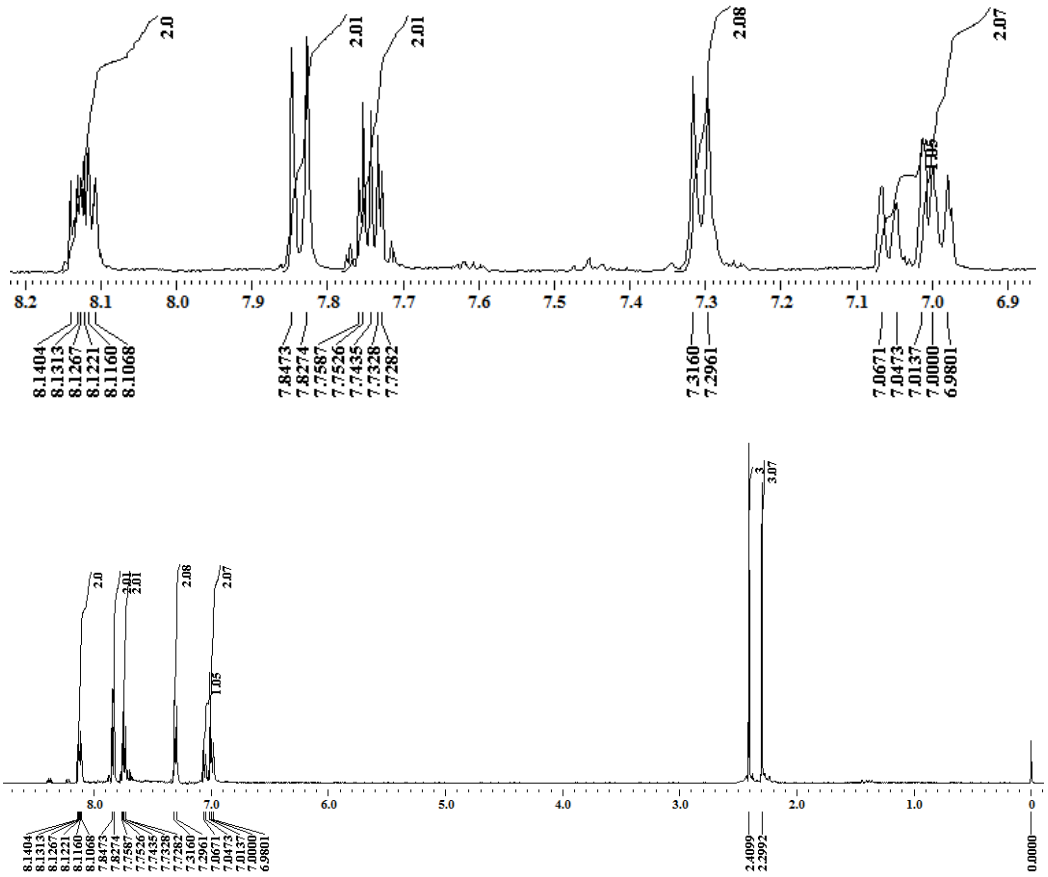


6-Iodo-3-methyl-5-(*p*-tolyl)benzo[*a*]phenazine (5a)

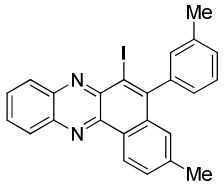
^{1}H NMR



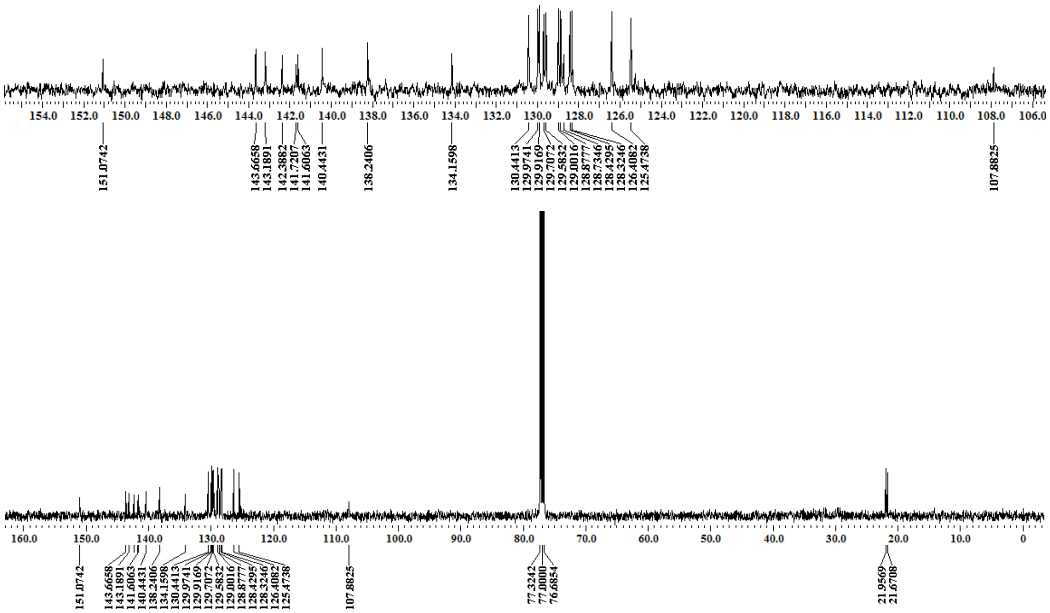
6-Iodo-3-methyl-5-(*m*-tolyl)benzo[*a*]phenazine (5b)



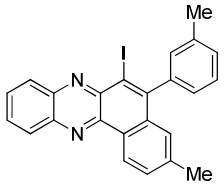
$^{13}C\{^{1}H\}$ NMR



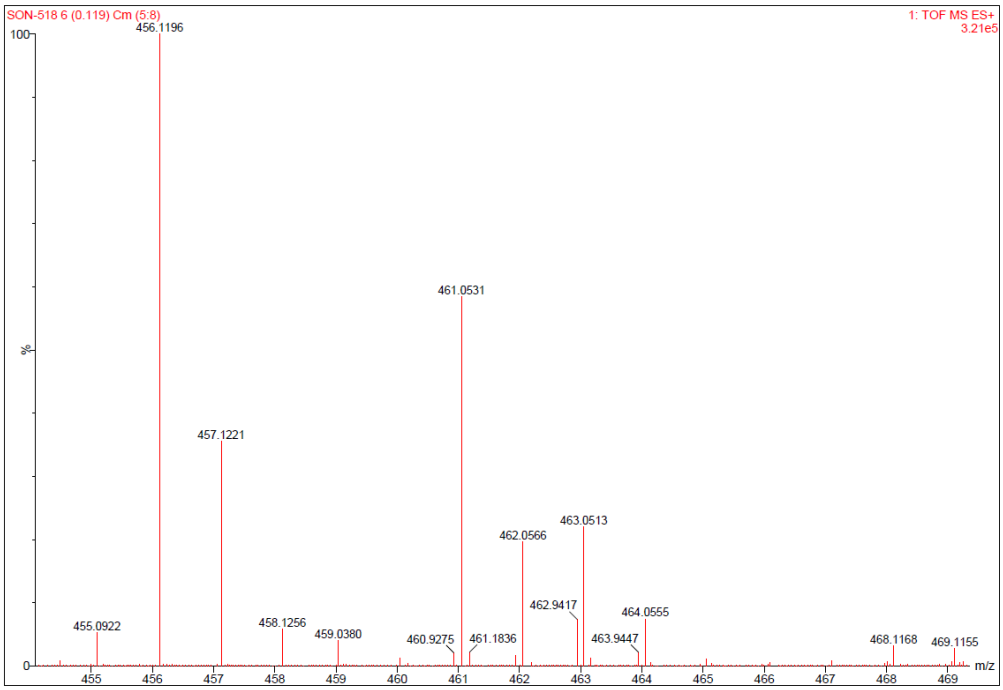
6-Iodo-3-methyl-5-(*m*-tolyl)benzo[*a*]phenazine (5b)



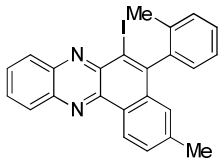
HRMS



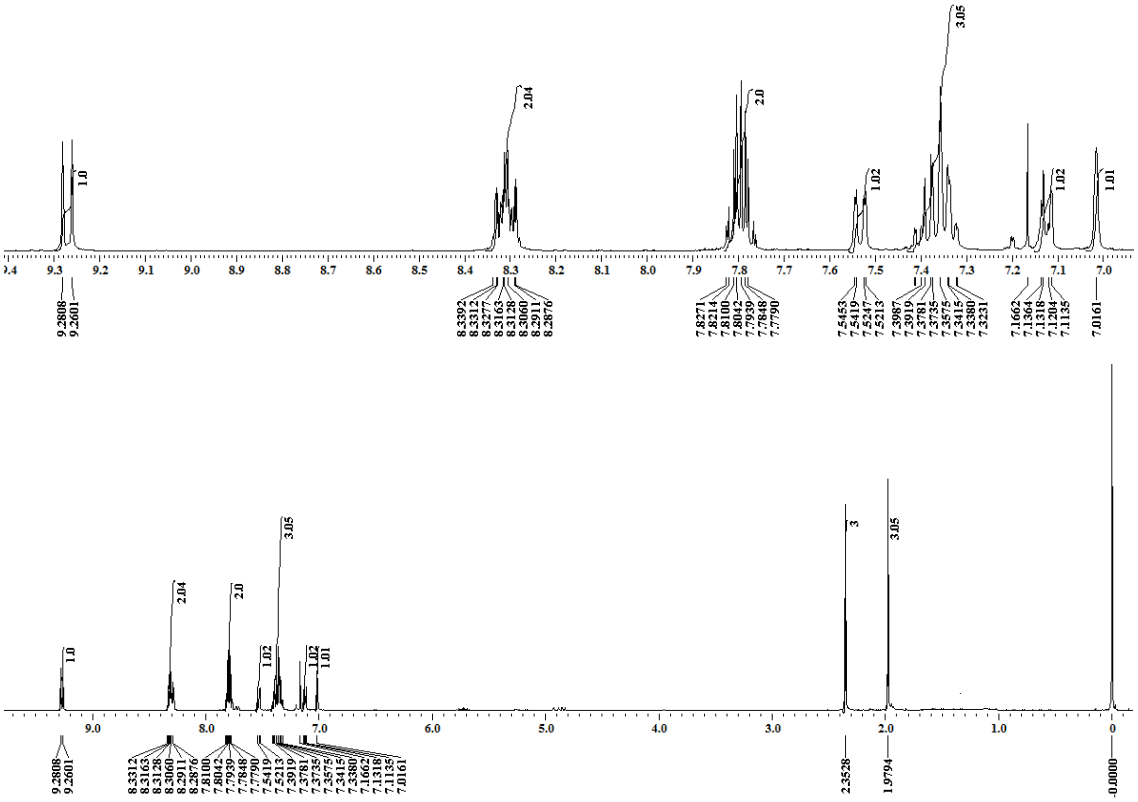
6-Iodo-3-methyl-5-(*m*-tolyl)benzo[*a*]phenazine (5b)



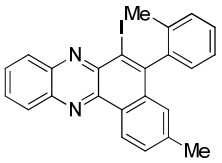
^{1}H NMR



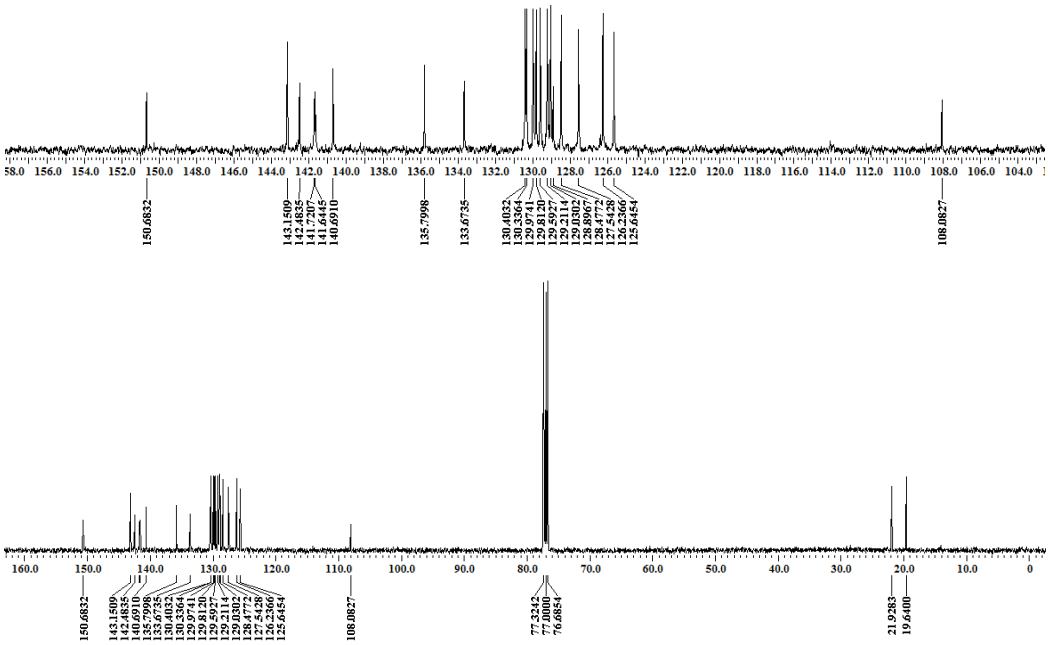
6-Iodo-3-methyl-5-(*o*-tolyl)benzo[*a*]phenazine (5c)



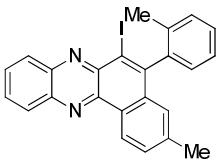
$^{13}C\{^{1}H\}$ NMR



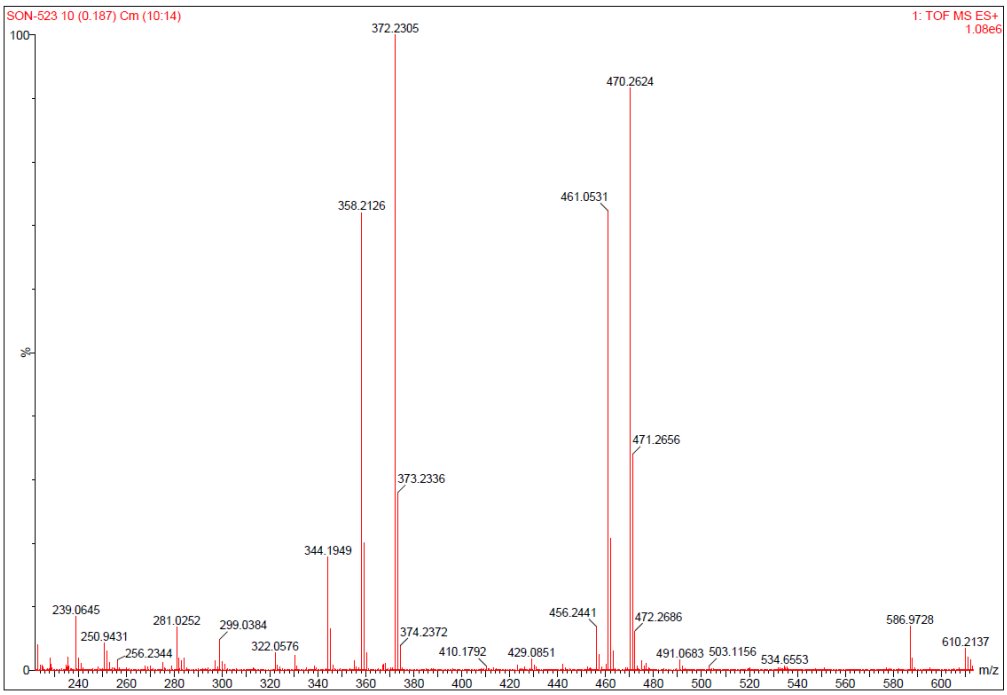
6-Iodo-3-methyl-5-(*o*-tolyl)benzo[*a*]phenazine (5c)



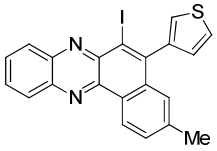
HRMS



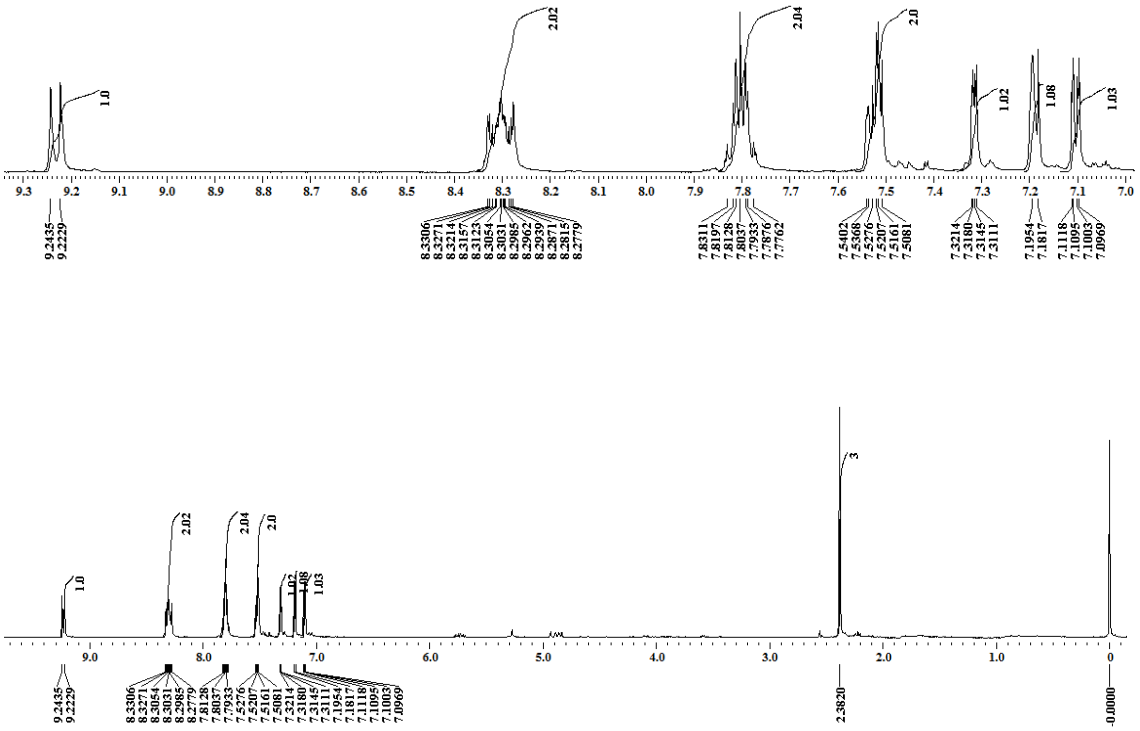
6-Iodo-3-methyl-5-(*o*-tolyl)benzo[*a*]phenazine (5c)



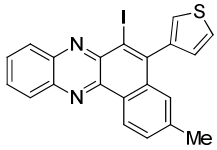
^{1}H NMR



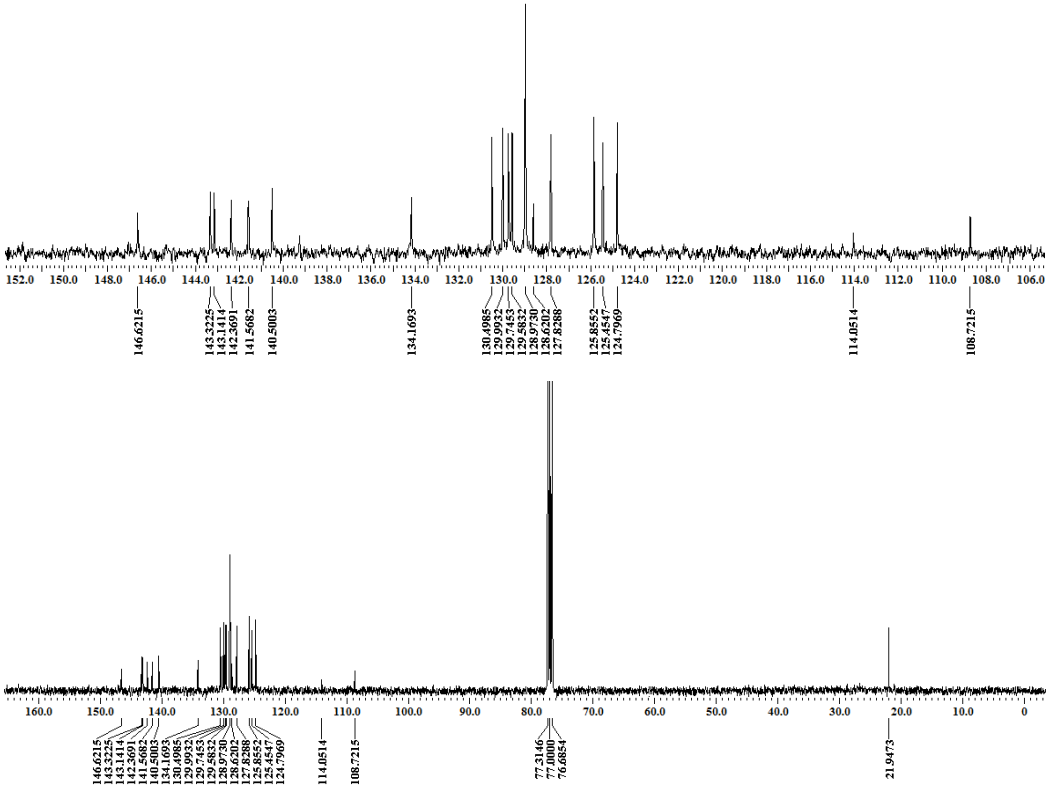
6-Iodo-3-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (5d)



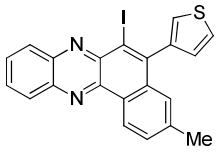
$^{13}C\{^{1}H\}$ NMR



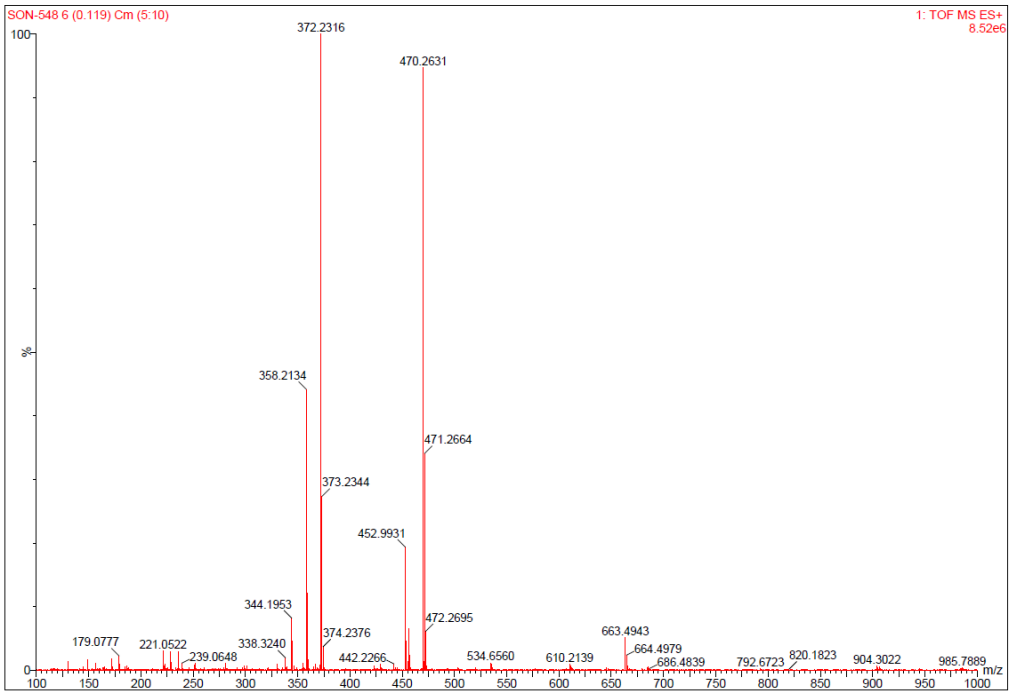
6-Iodo-3-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (5d)



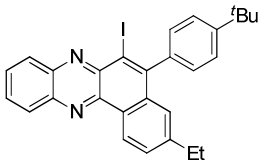
HRMS



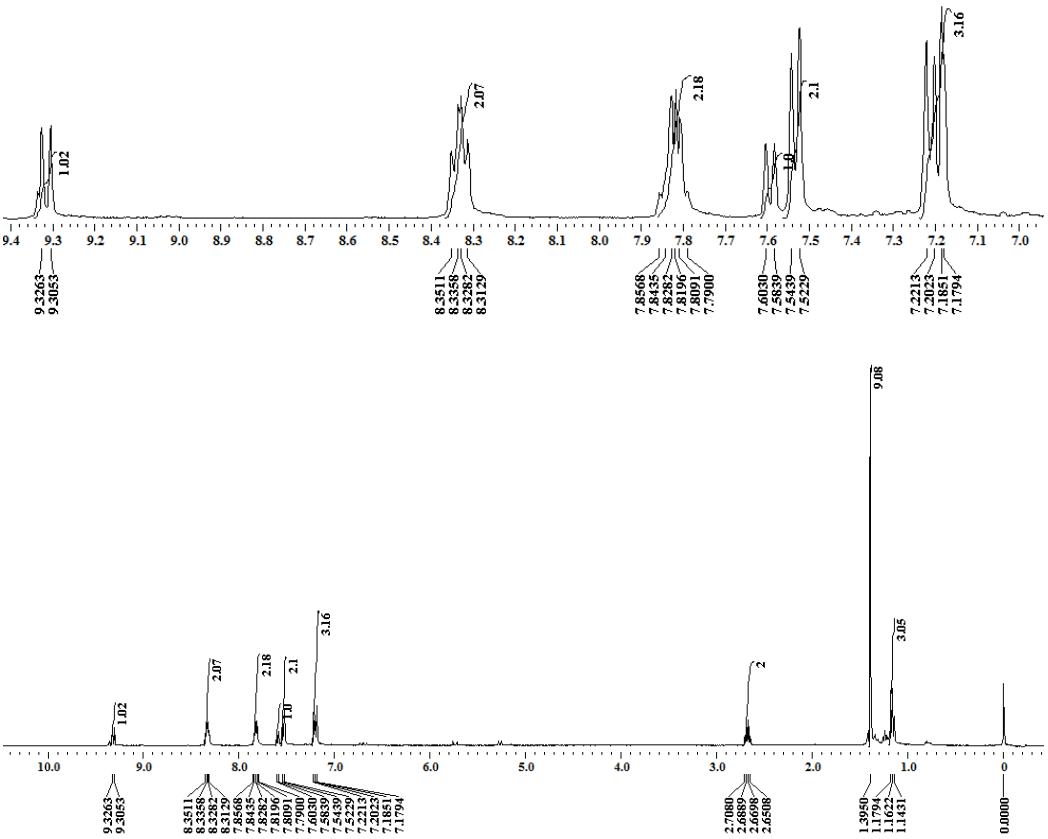
6-Iodo-3-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (5d)



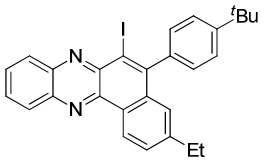
^{1}H NMR



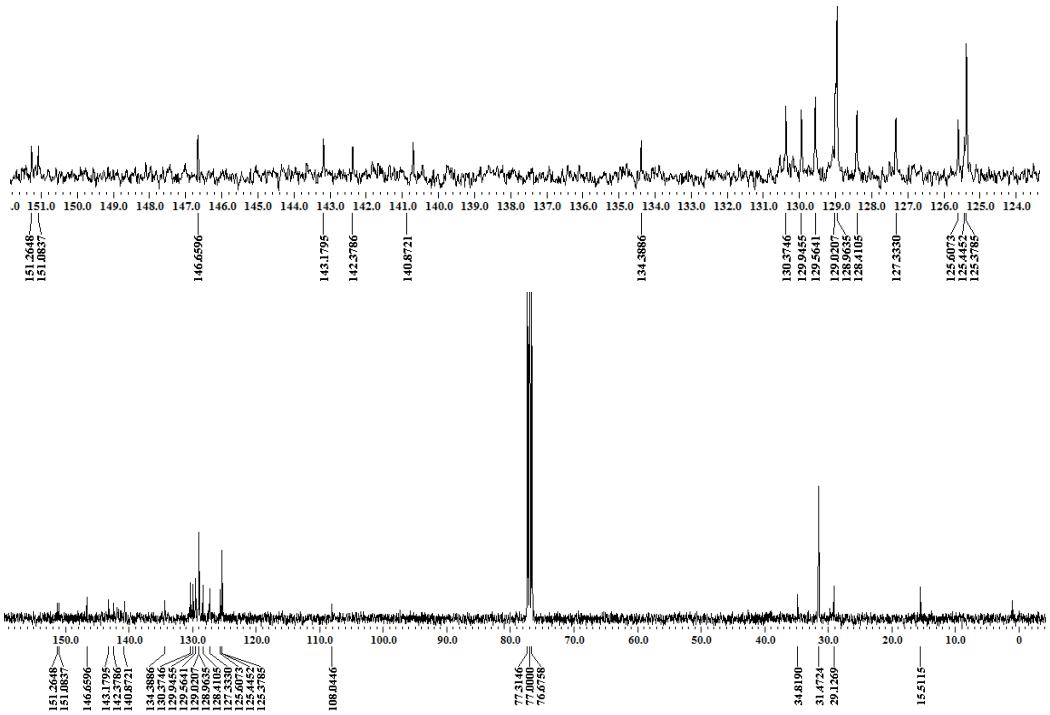
5-(4-(*tert*-Butyl)phenyl)-3-ethyl-6-iodobenzo[*a*]phenazine (5e)



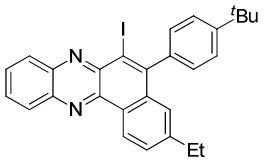
$^{13}C\{^{1}H\}$ NMR



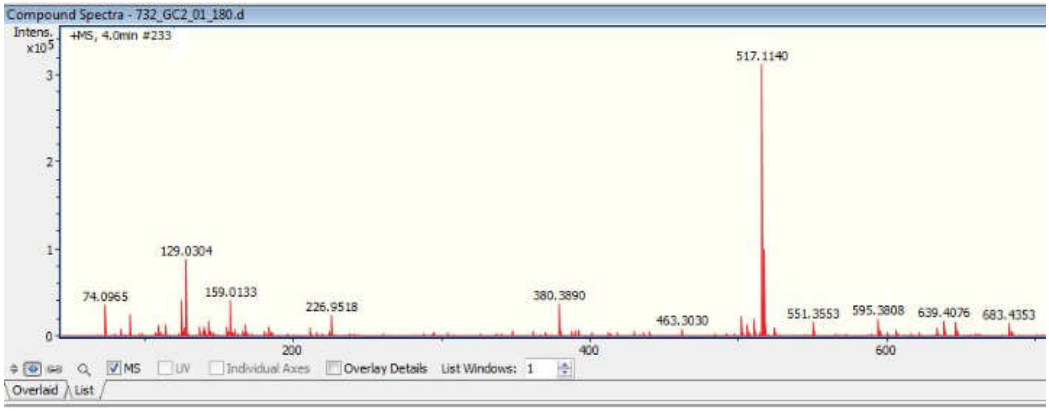
5-(4-(*tert*-Butyl)phenyl)-3-ethyl-6-iodobenzo[*a*]phenazine (5e)



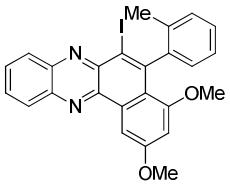
HRMS



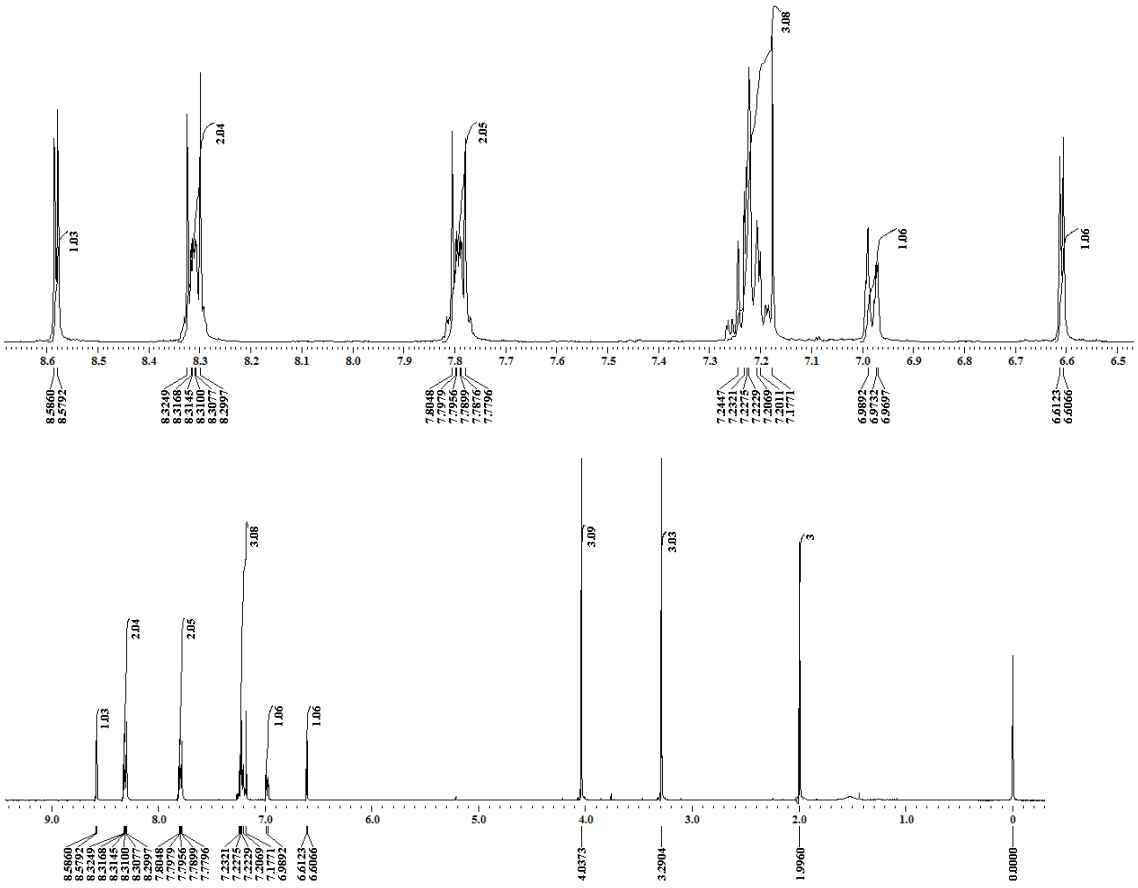
5-(4-(*tert*-Butyl)phenyl)-3-ethyl-6-iodobenzo[*a*]phenazine (5e)



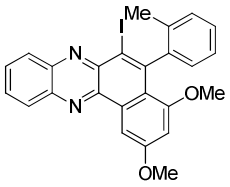
^{1}H NMR



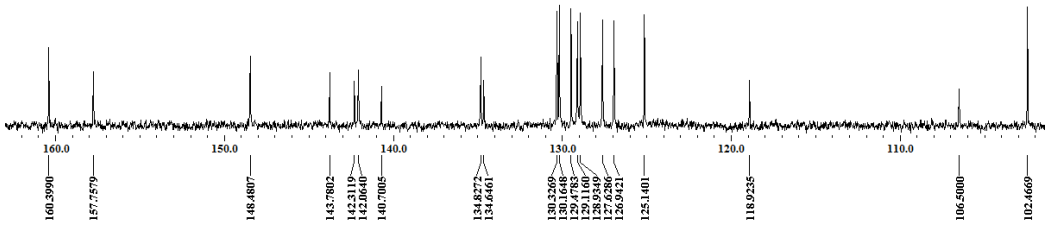
6-Iodo-2,4-dimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5f)

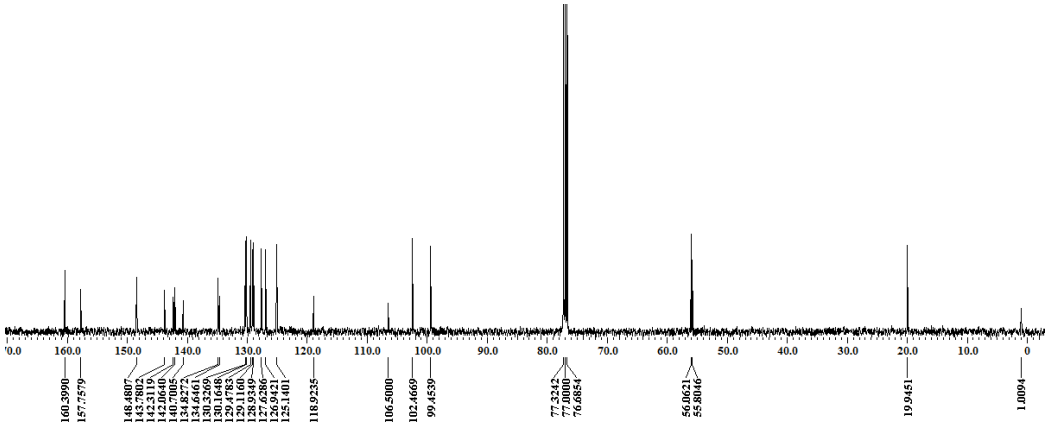


$^{13}C\{^{1}H\}$ NMR

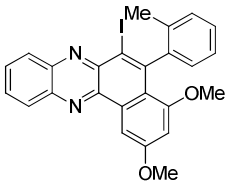


6-Iodo-2,4-dimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5f)

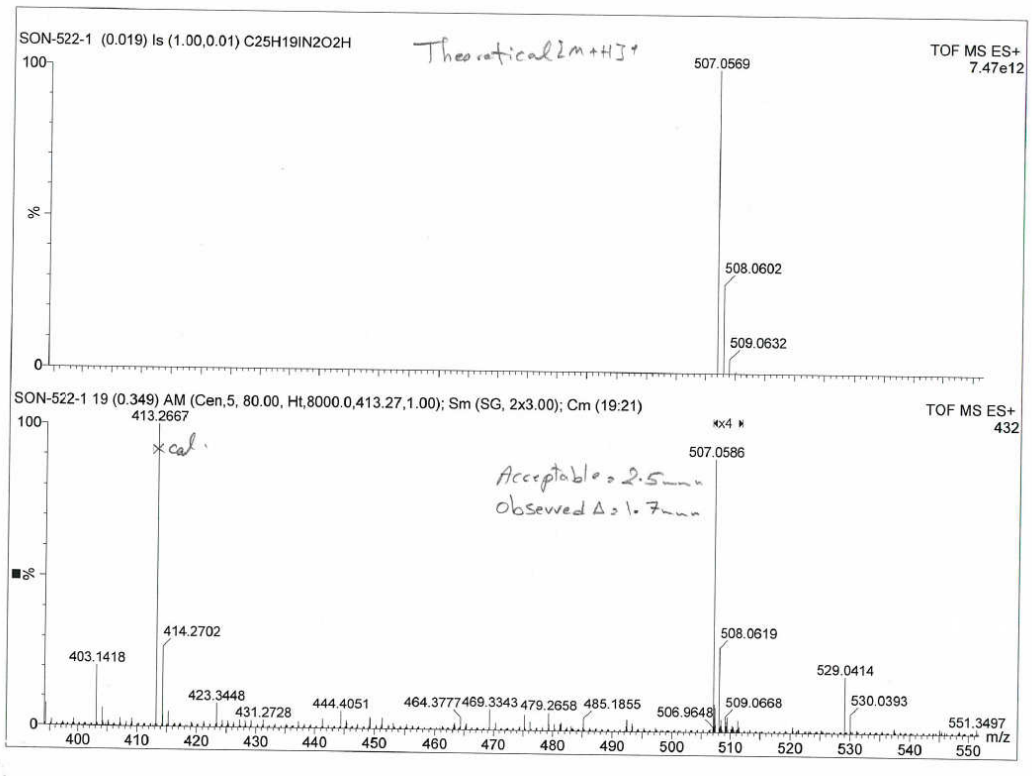




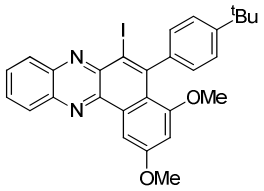
HRMS



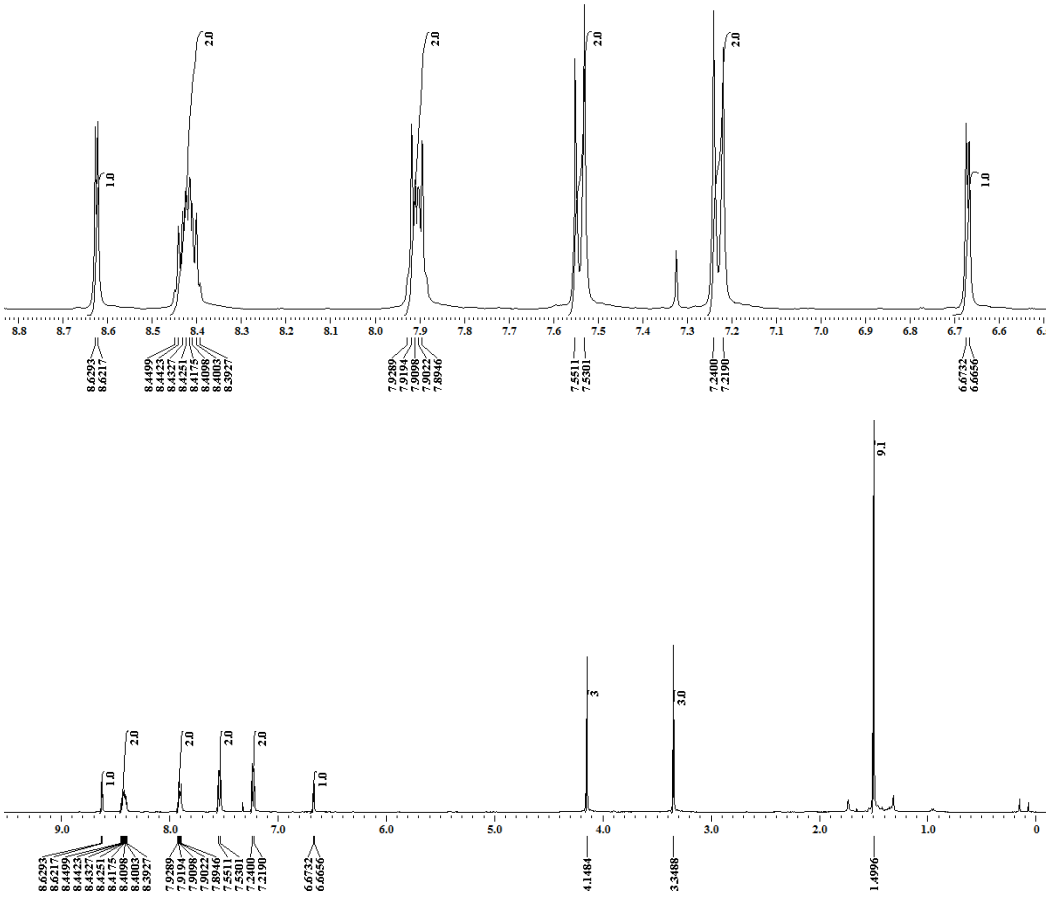
6-Iodo-2,4-dimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5f)



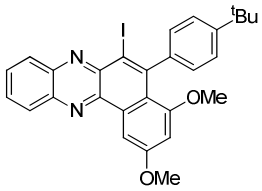
^{1}H NMR



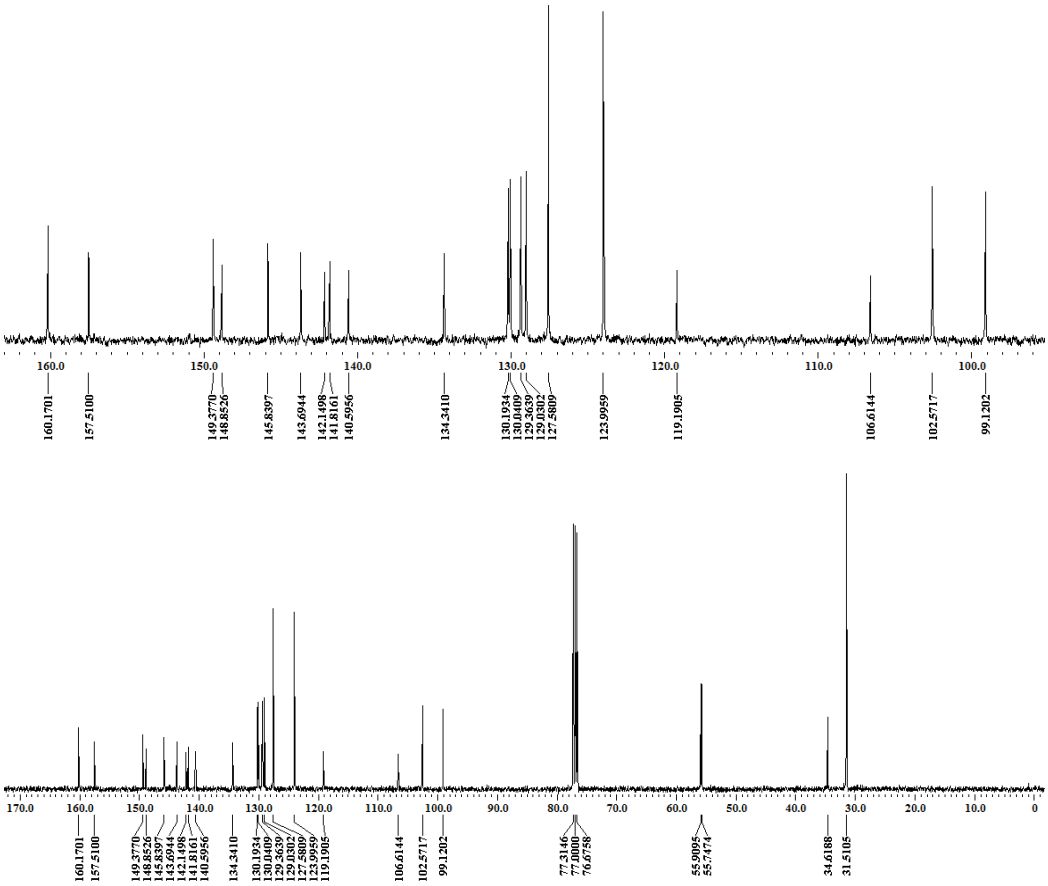
5-(4-(*tert*-Butyl)phenyl)-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5g)



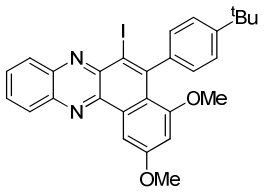
$^{13}C\{^{1}H\}$ NMR



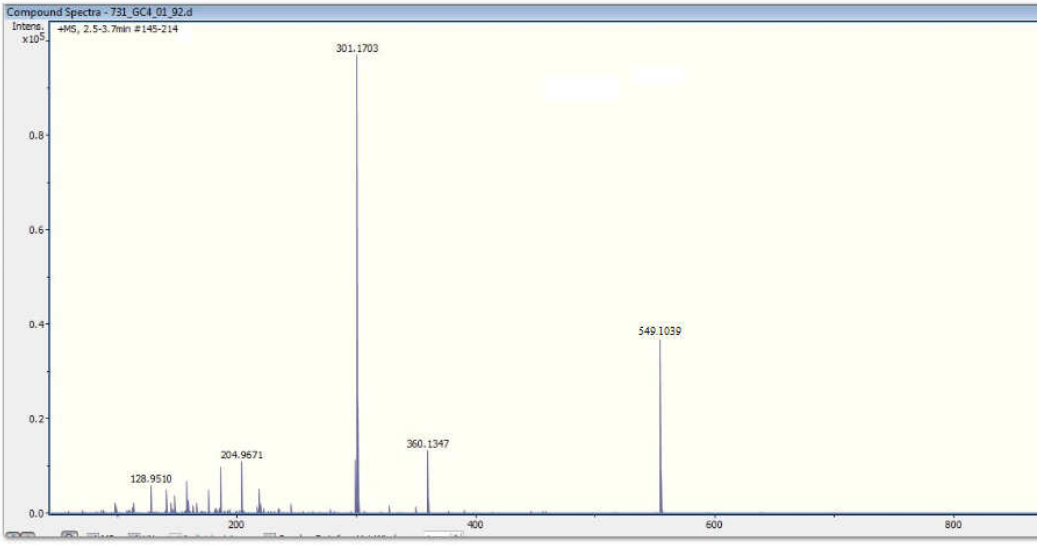
5-(4-(*tert*-Butyl)phenyl)-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5g)



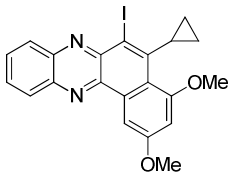
HRMS



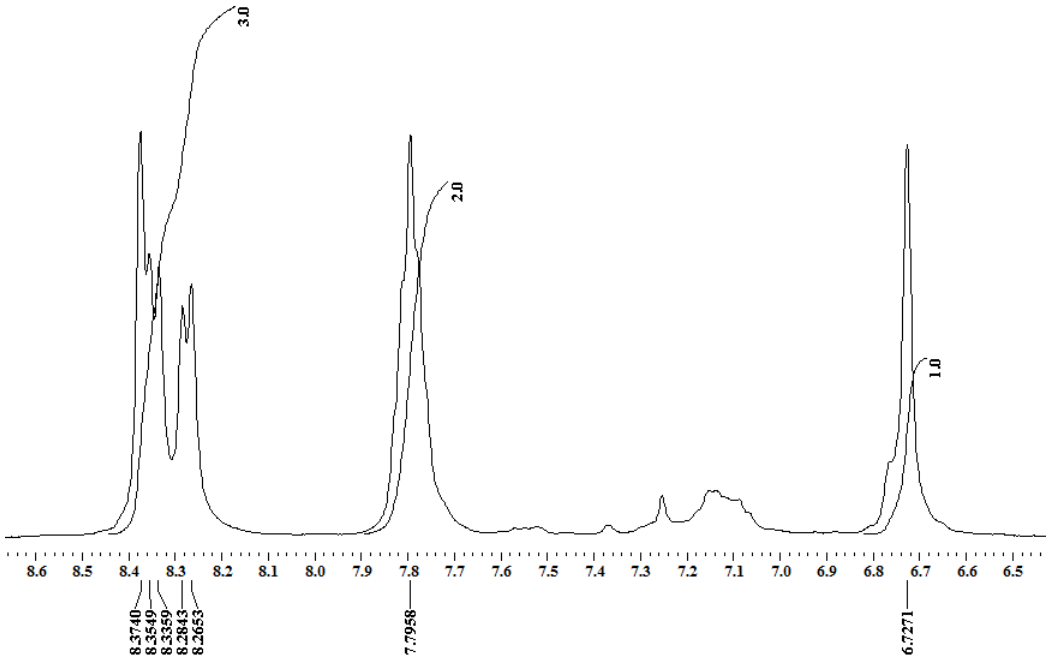
5-(4-(*tert*-Butyl)phenyl)-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5g)

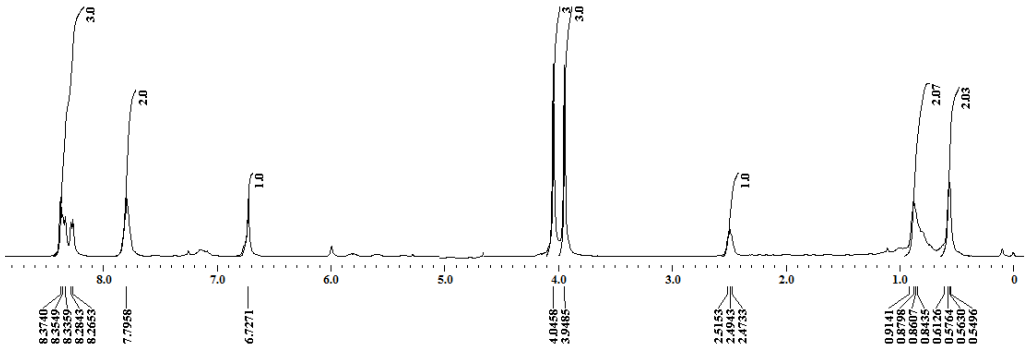


^{1}H NMR

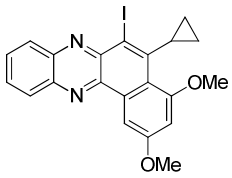


5-Cyclopropyl-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5h)

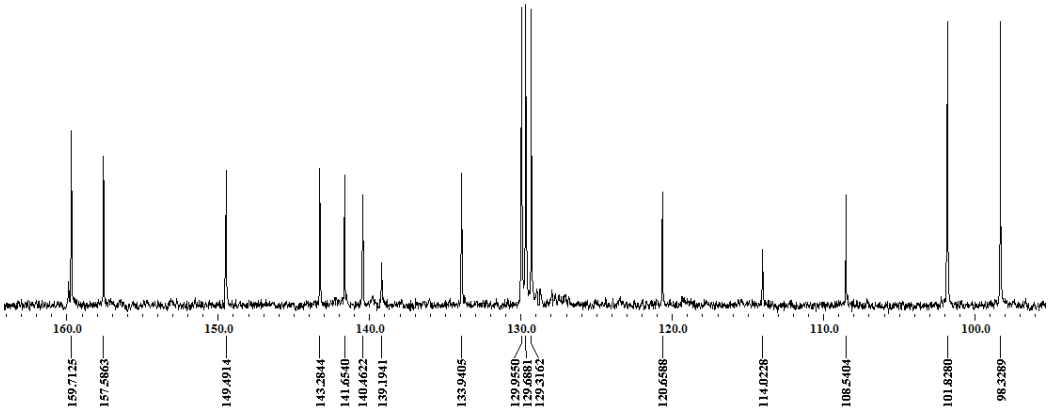


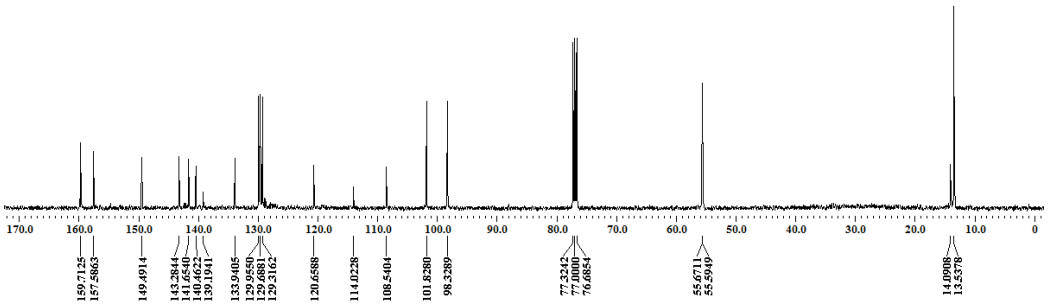


$^{13}C\{^{1}H\}$ NMR

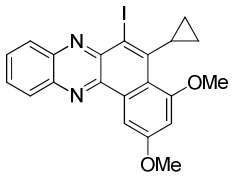


5-Cyclopropyl-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5h)

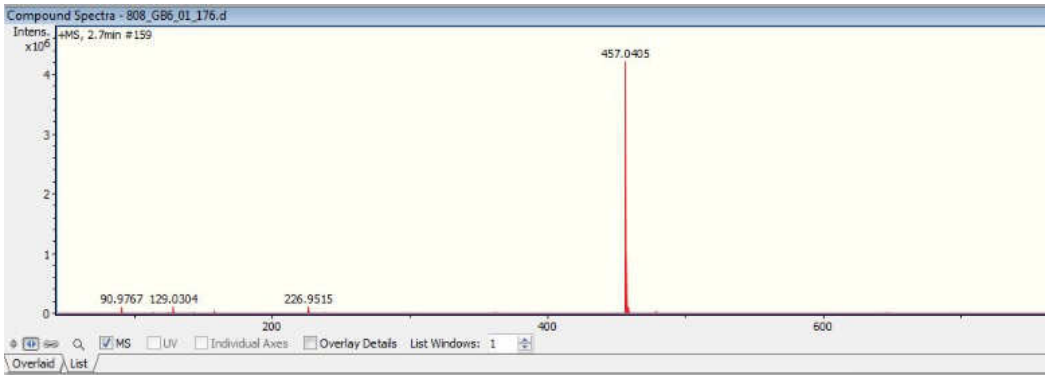




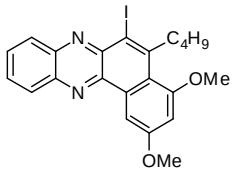
HRMS



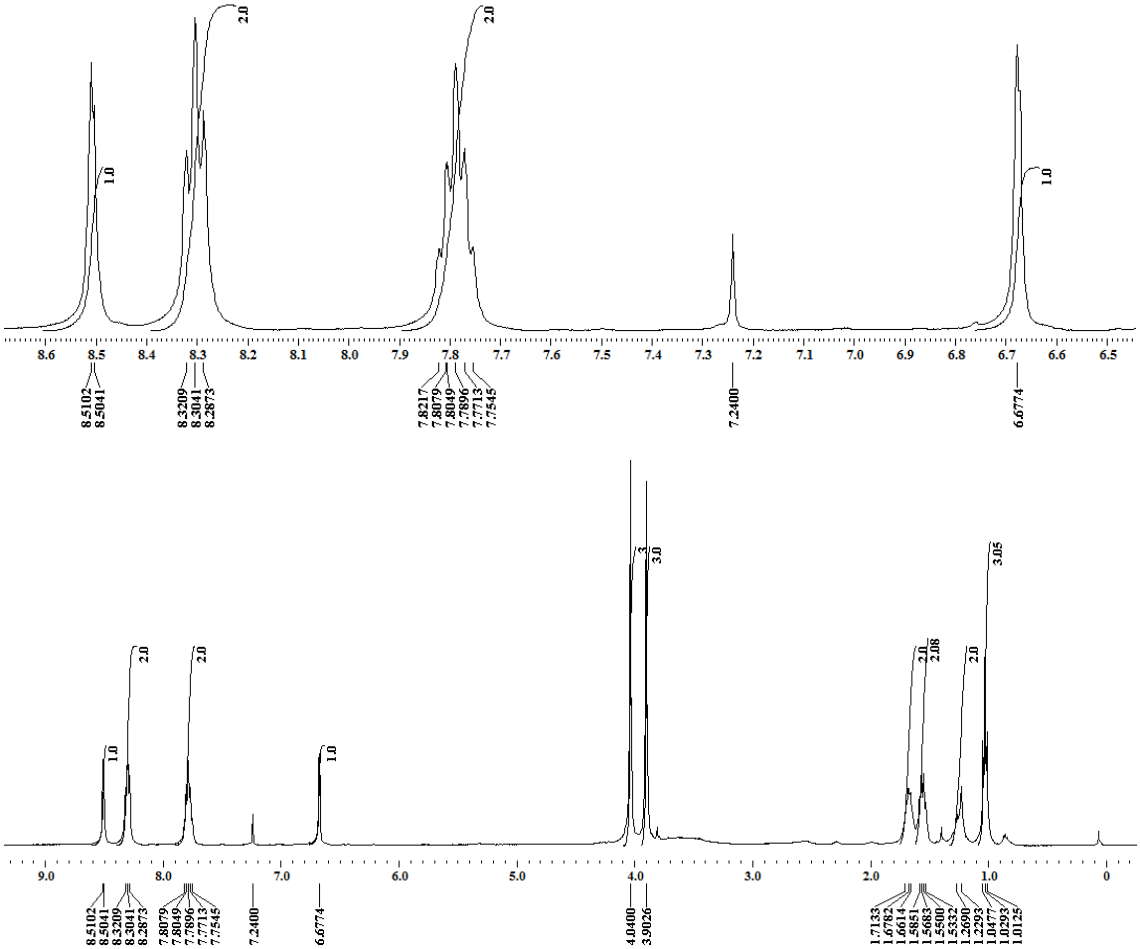
5-Cyclopropyl-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5h)



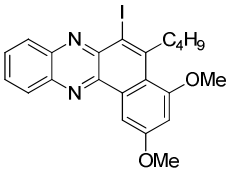
^{1}H NMR



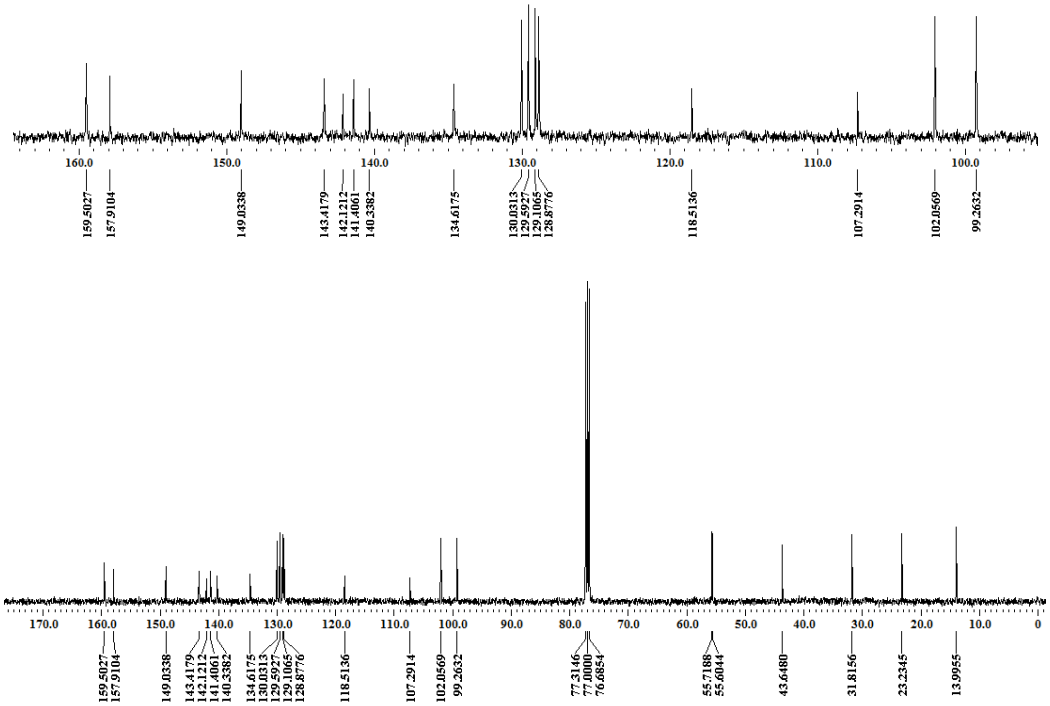
5-Butyl-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5i)



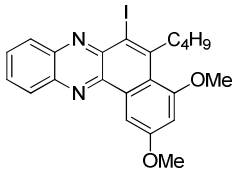
$^{13}C\{^{1}H\}$ NMR



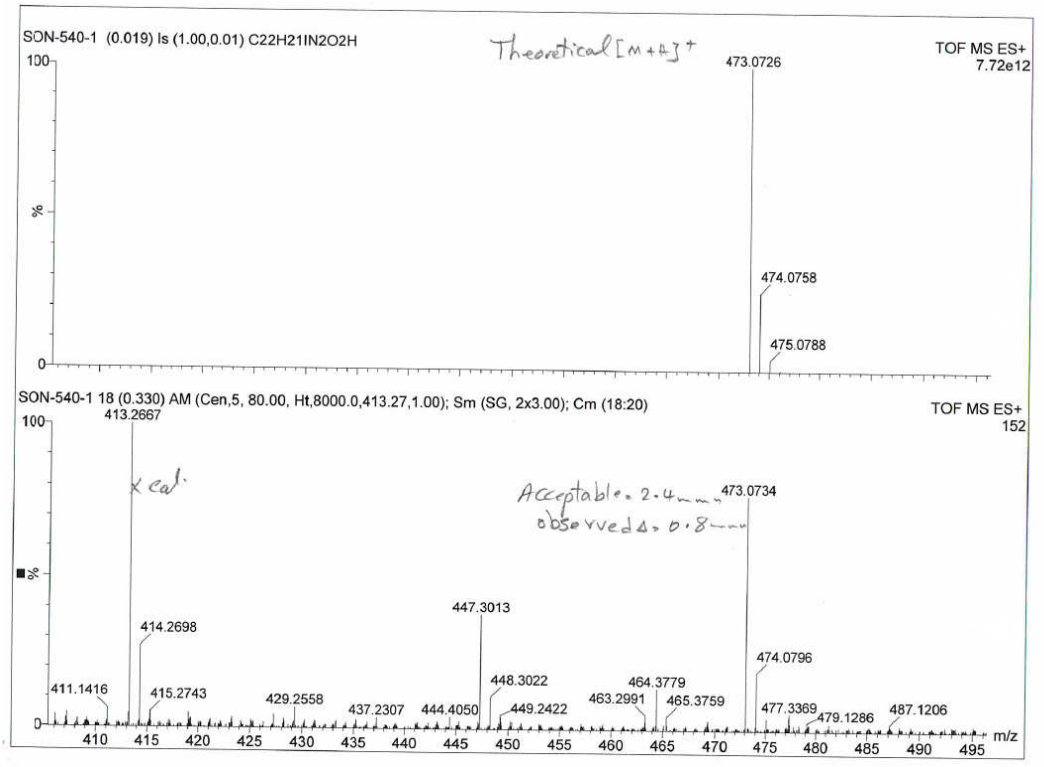
5-Butyl-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5i)



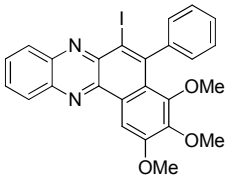
HRMS



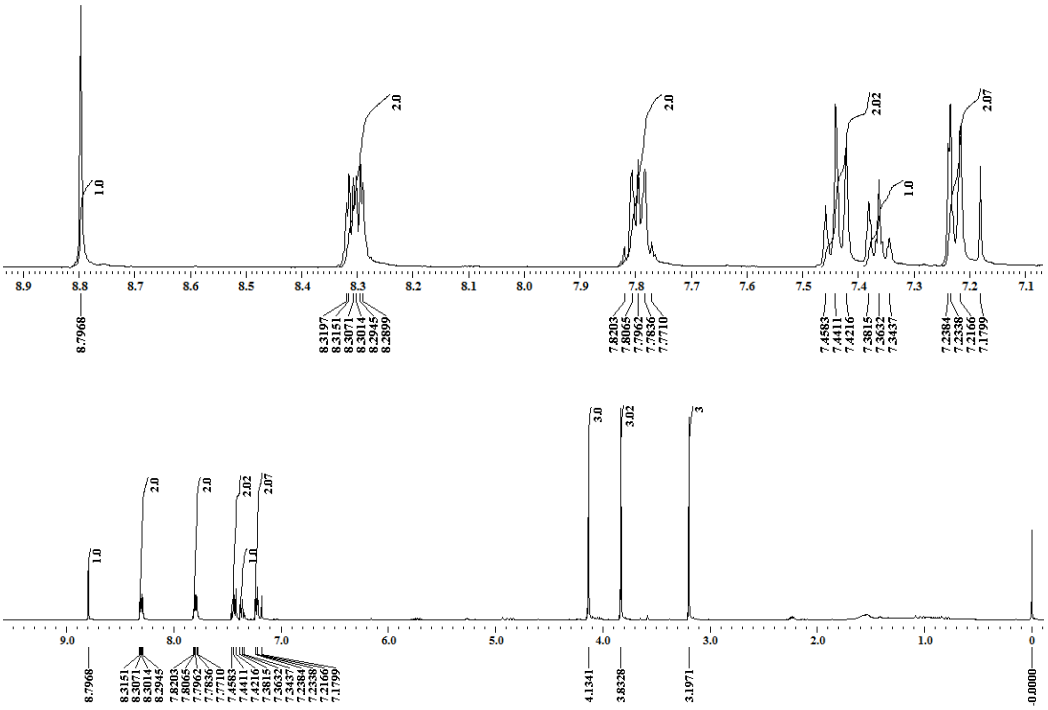
5-Butyl-6-iodo-2,4-dimethoxybenzo[*a*]phenazine (5i)



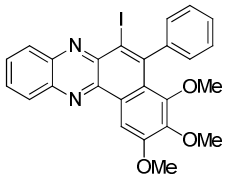
^{1}H NMR



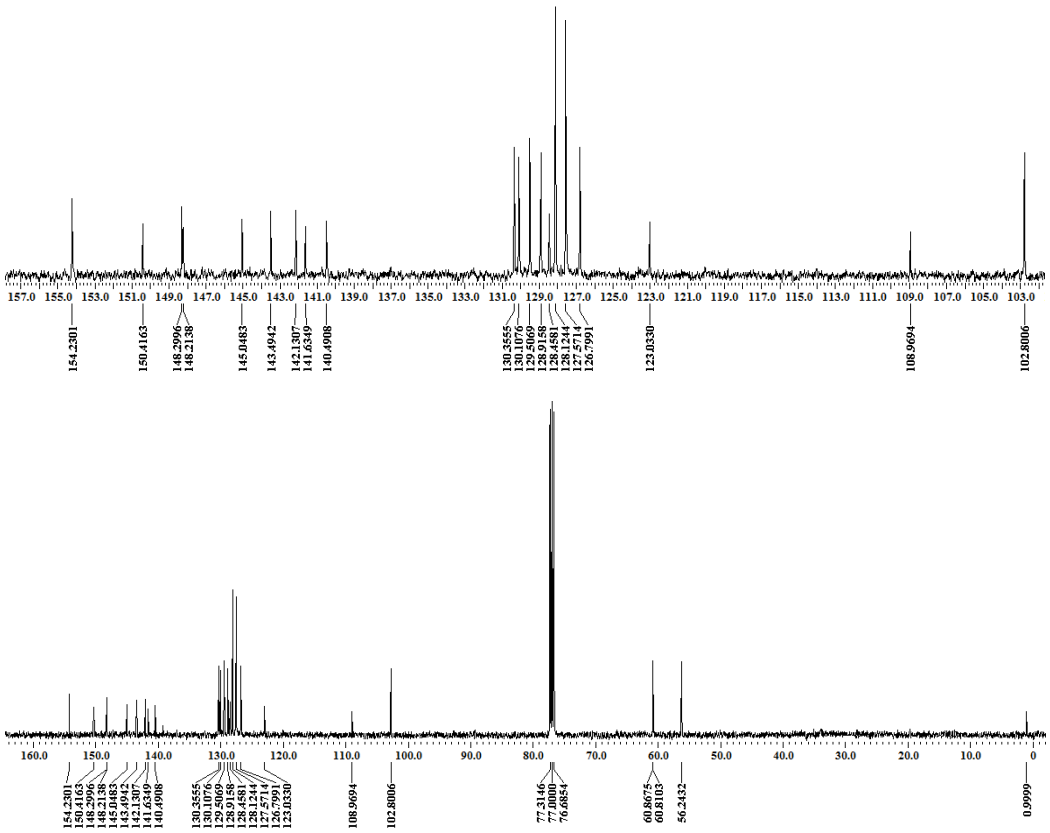
6-Iodo-2,3,4-trimethoxy-5-phenylbenzo[*a*]phenazine (5j)



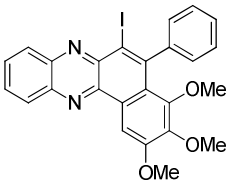
$^{13}C\{^{1}H\}$ NMR



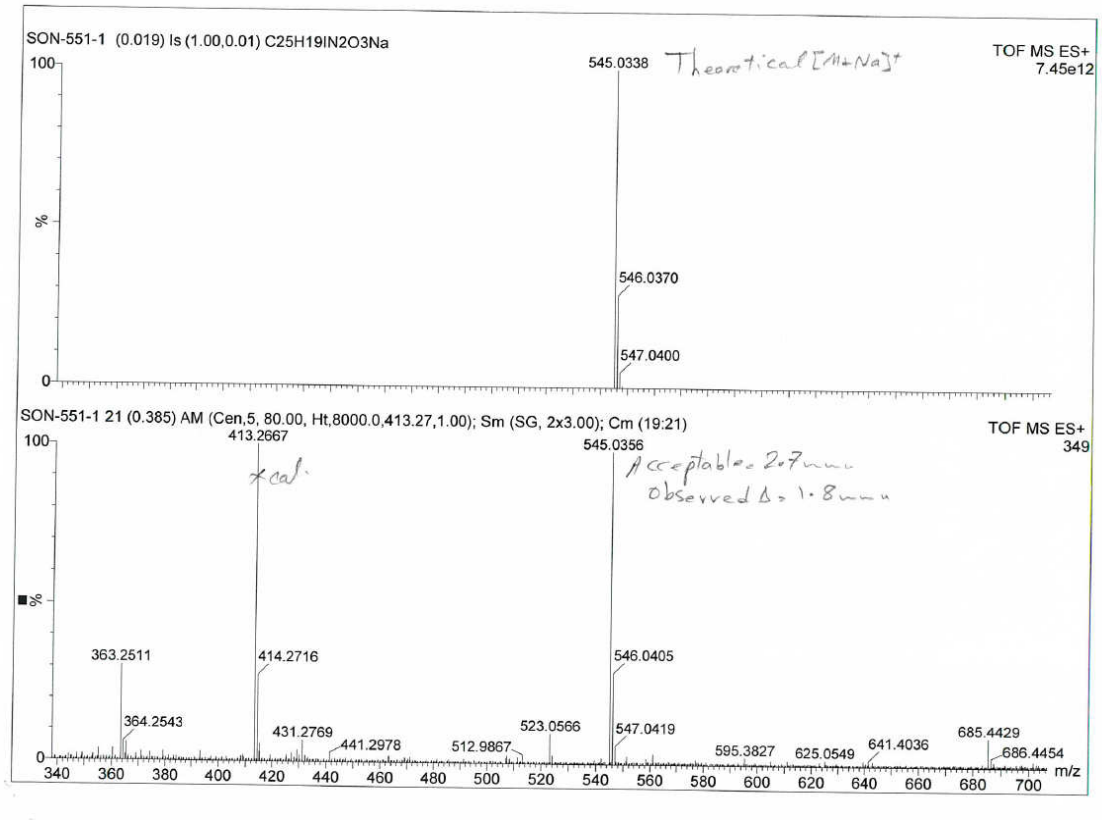
6-Iodo-2,3,4-trimethoxy-5-phenylbenzo[*a*]phenazine (5j)



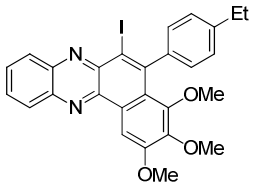
HRMS



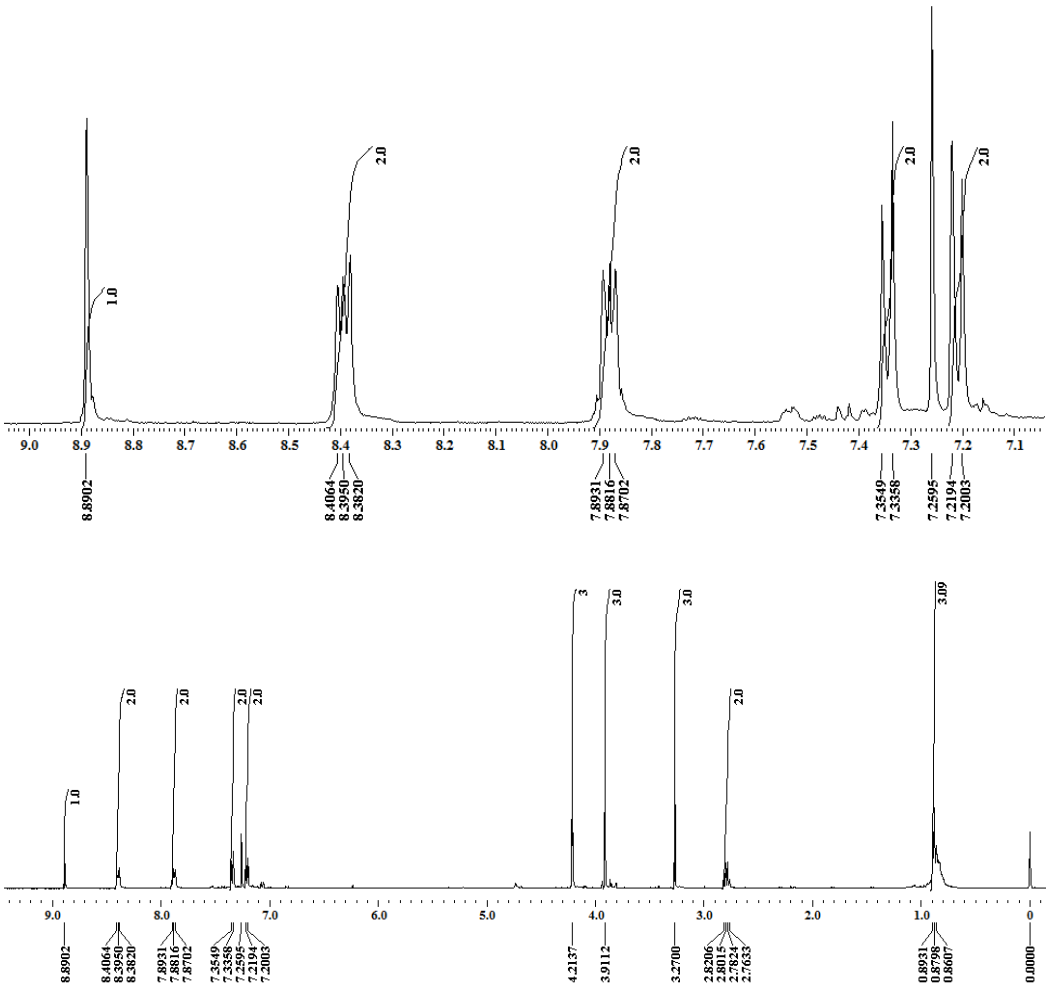
6-Iodo-2,3,4-trimethoxy-5-phenylbenzo[*a*]phenazine (5j)



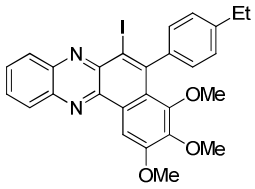
^{1}H NMR



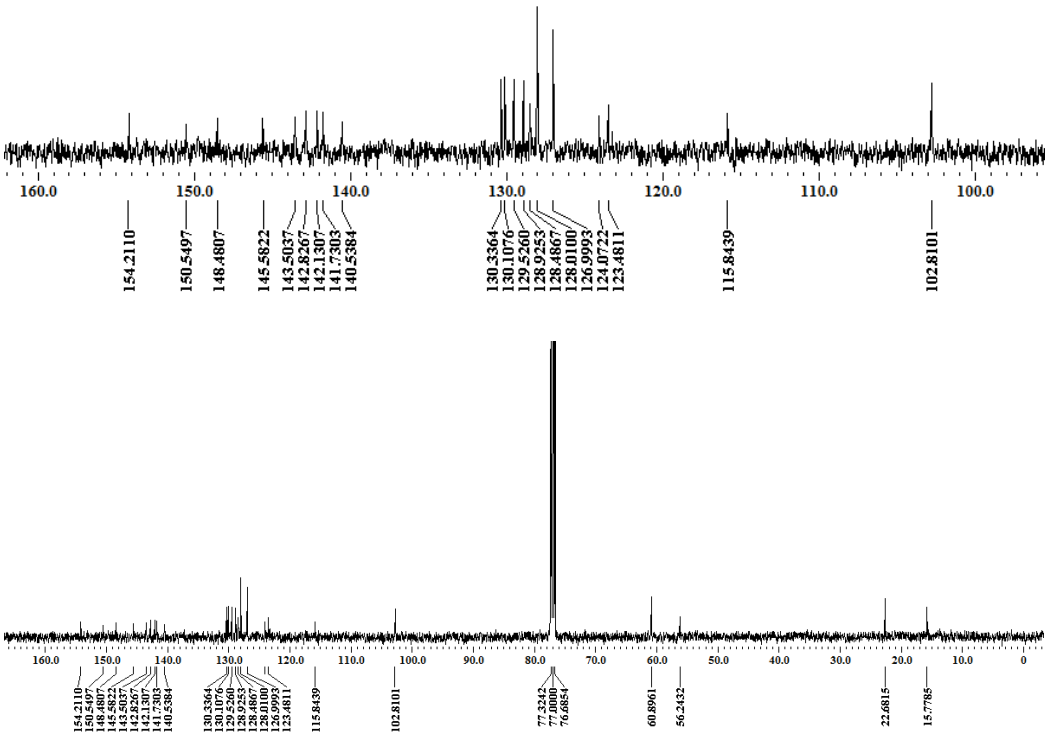
5-(4-Ethylphenyl)-6-iodo-2,3,4-trimethoxybenzo[*a*]phenazine (5k)



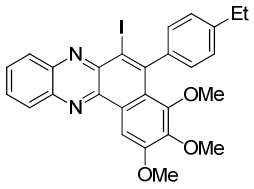
$^{13}C\{^{1}H\}$ NMR



5-(4-Ethylphenyl)-6-iodo-2,3,4-trimethoxybenzo[*a*]phenazine (5k)



HRMS



5-(4-Ethylphenyl)-6-iodo-2,3,4-trimethoxybenzo[*a*]phenazine (5k)

Qualitative Compound Report

Data File	SON 820.d	**Sample Name**	SON 820
Sample Type	Sample	**Position**	P2-A5
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	17-12-2015 14:34:08
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

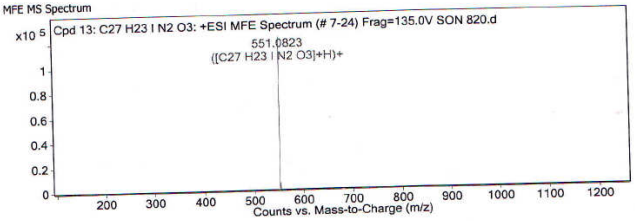
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

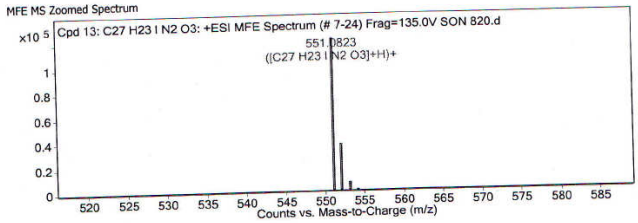
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C27 H23 I N2 O3	11	550.075	C27 H23 I N2 O3	C27 H23 I N2 O3	0.67	C27 H23 I N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C27 H23 I N2 O3	551.0823	11	Find by Molecular Feature	550.075

MFE MS Spectrum



MFE MS Zoomed Spectrum

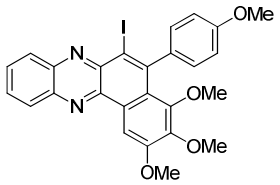


MS Spectrum Peak List

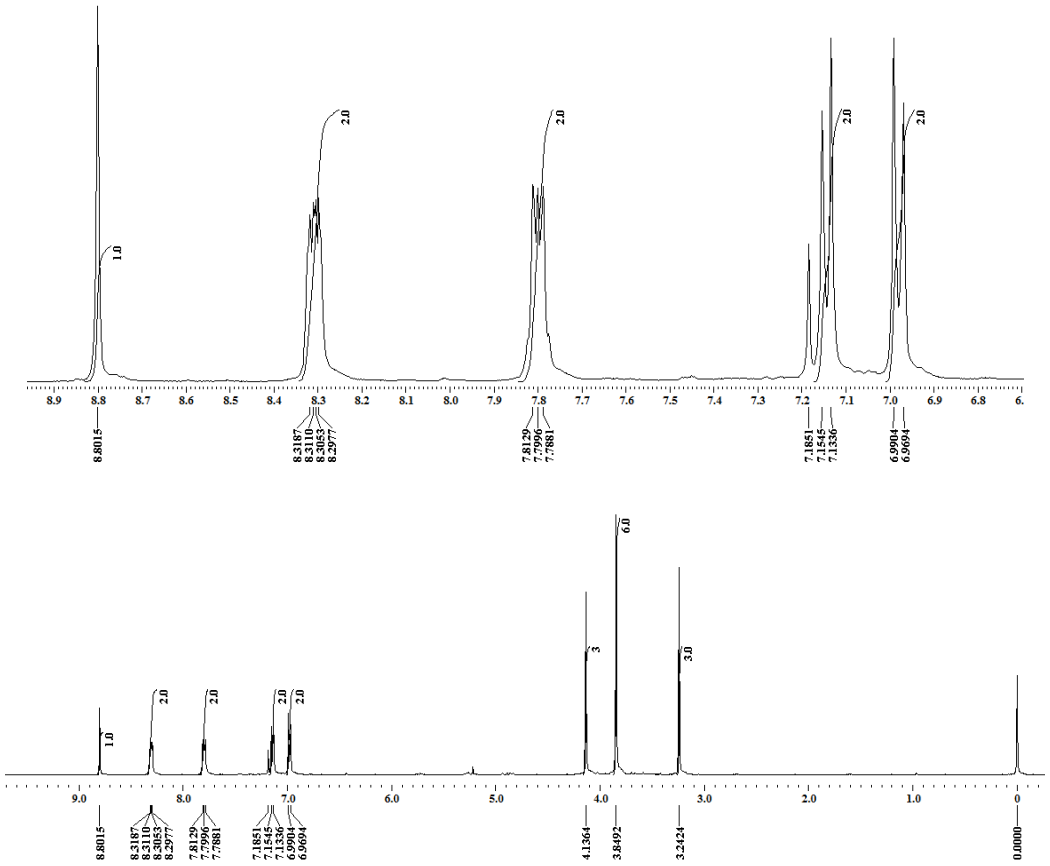
m/z	z	Abund	Formula	Ion
551.0823	1	123185.05	C27 H23 I N2 O3	(M+H)+
552.0854	1	36037.03	C27 H23 I N2 O3	(M+H)+
553.0884	1	5930.81	C27 H23 I N2 O3	(M+H)+
554.0917	1	663.33	C27 H23 I N2 O3	(M+H)+

--- End Of Report ---

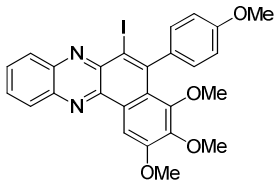
^{1}H NMR



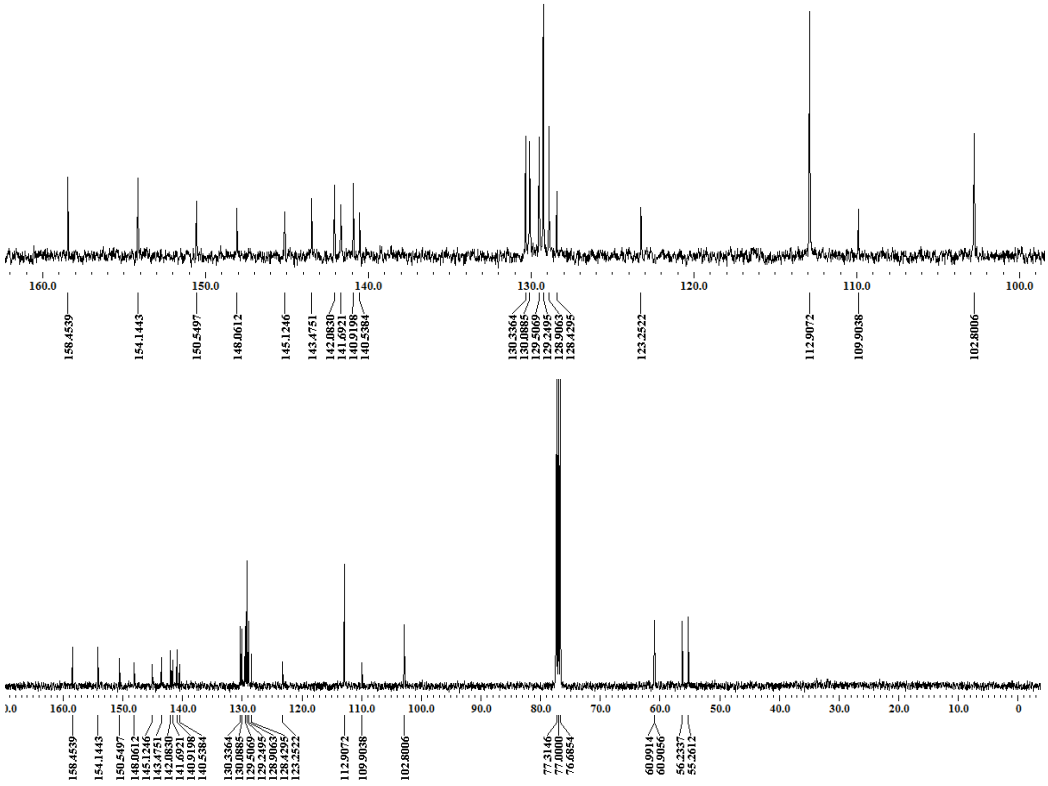
6-Iodo-2,3,4-trimethoxy-5-(4-methoxyphenyl)benzo[*a*]phenazine (5l)



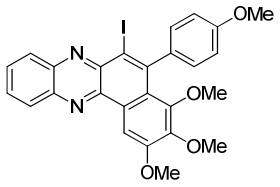
$^{13}C\{^{1}H\}$ NMR



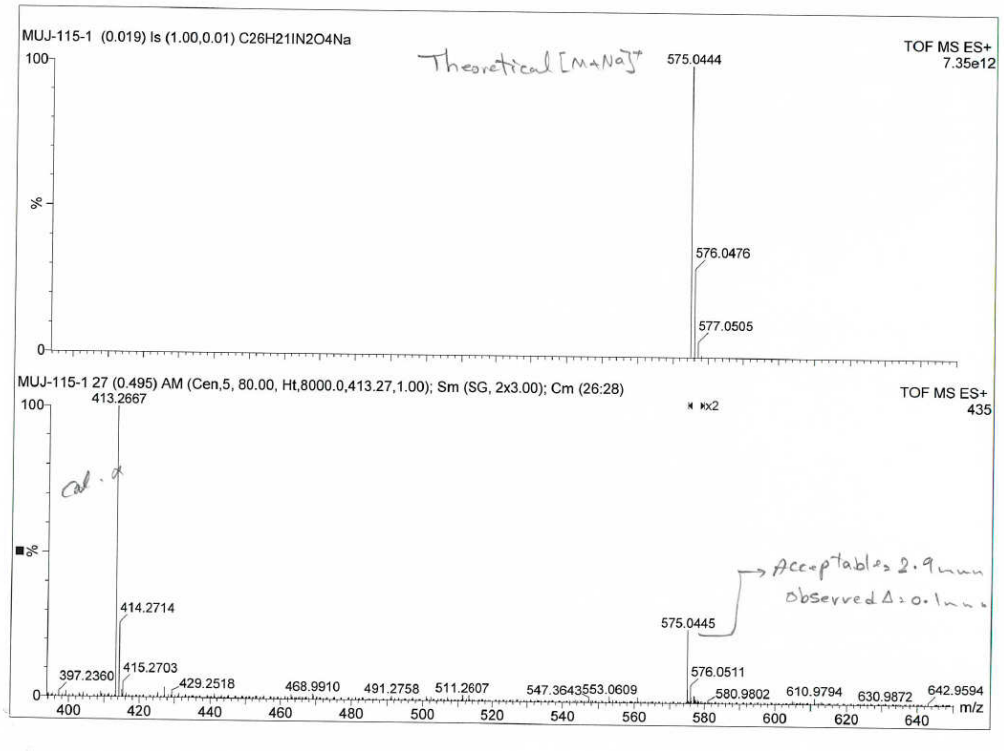
6-Iodo-2,3,4-trimethoxy-5-(4-methoxyphenyl)benzo[*a*]phenazine (5l)



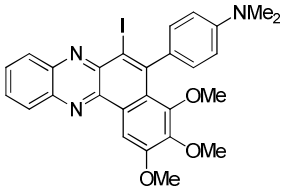
HRMS



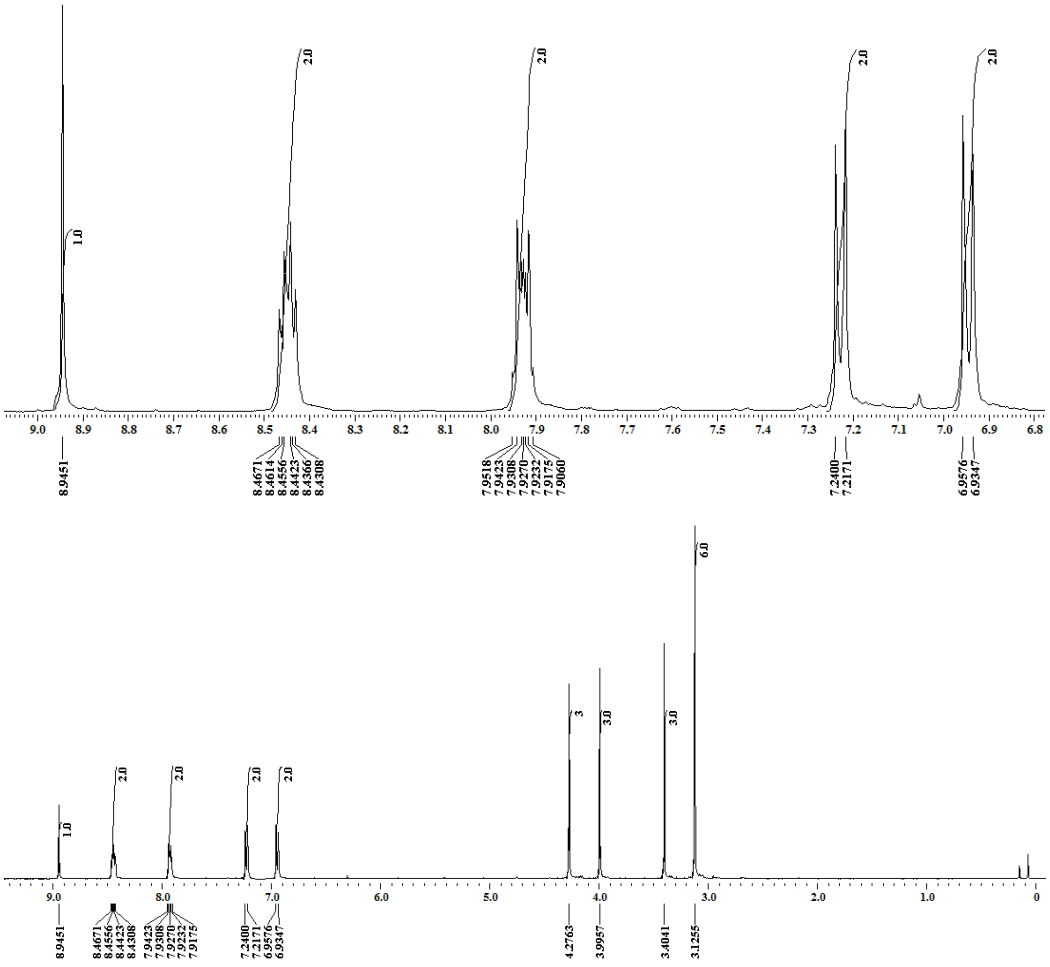
6-Iodo-2,3,4-trimethoxy-5-(4-methoxyphenyl)benzo[*a*]phenazine (5l)



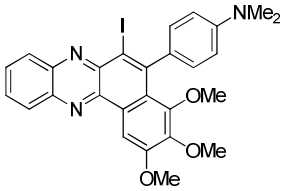
^{1}H NMR



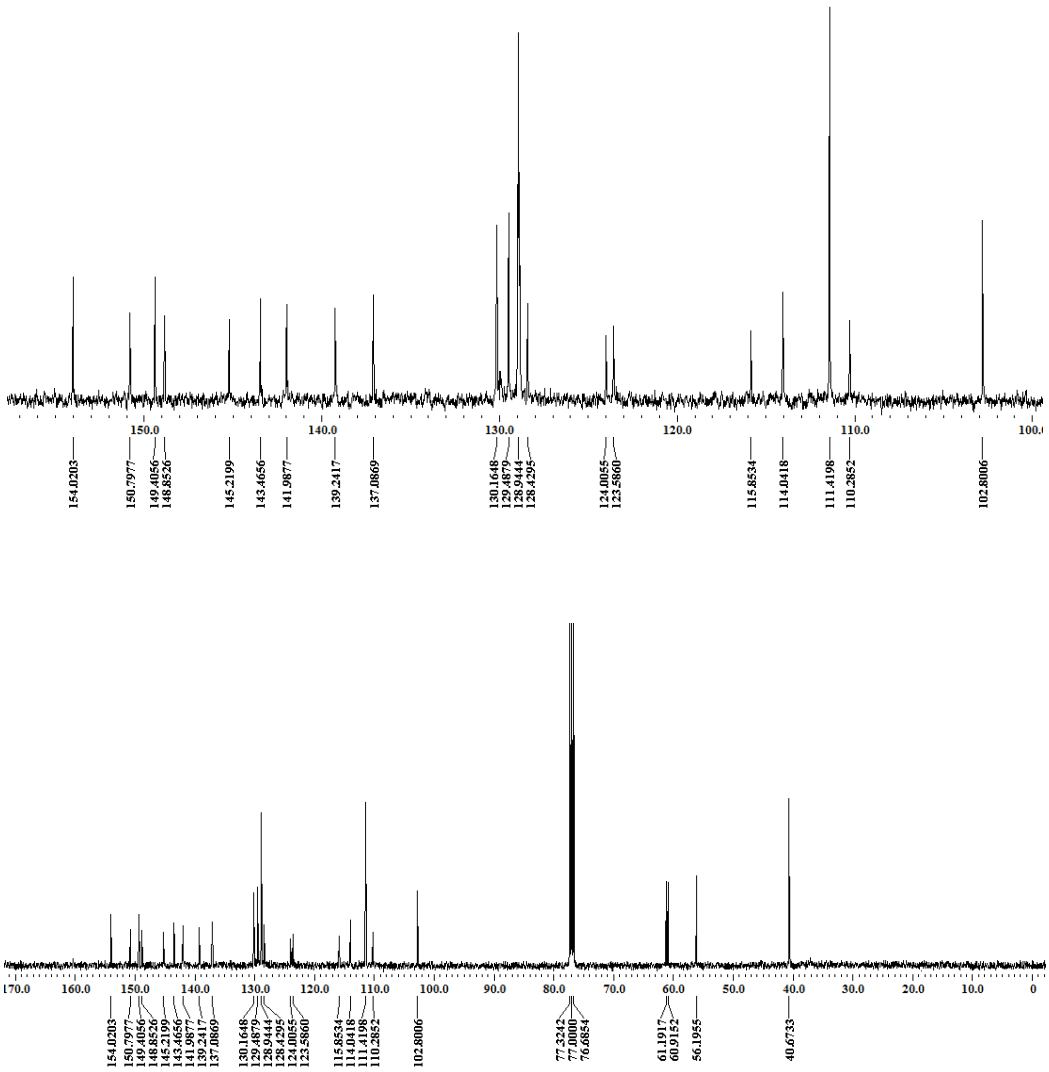
4-(6-Iodo-2,3,4-trimethoxybenzo[*a*]phenazin-5-yl)-*N*,*N*-dimethylaniline (5m)



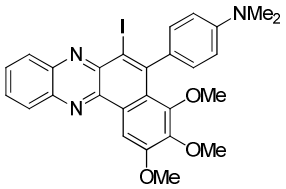
$^{13}C\{^{1}H\}$ NMR



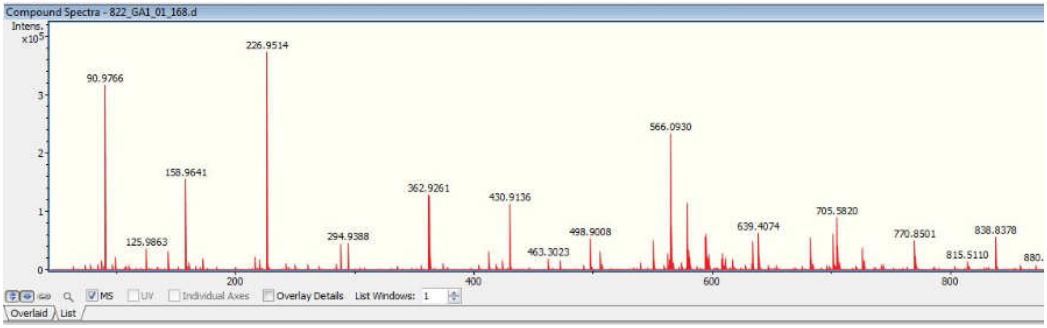
4-(6-Iodo-2,3,4-trimethoxybenzo[*a*]phenazin-5-yl)-*N*,*N*-dimethylaniline (5m)



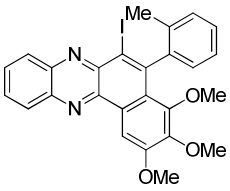
HRMS



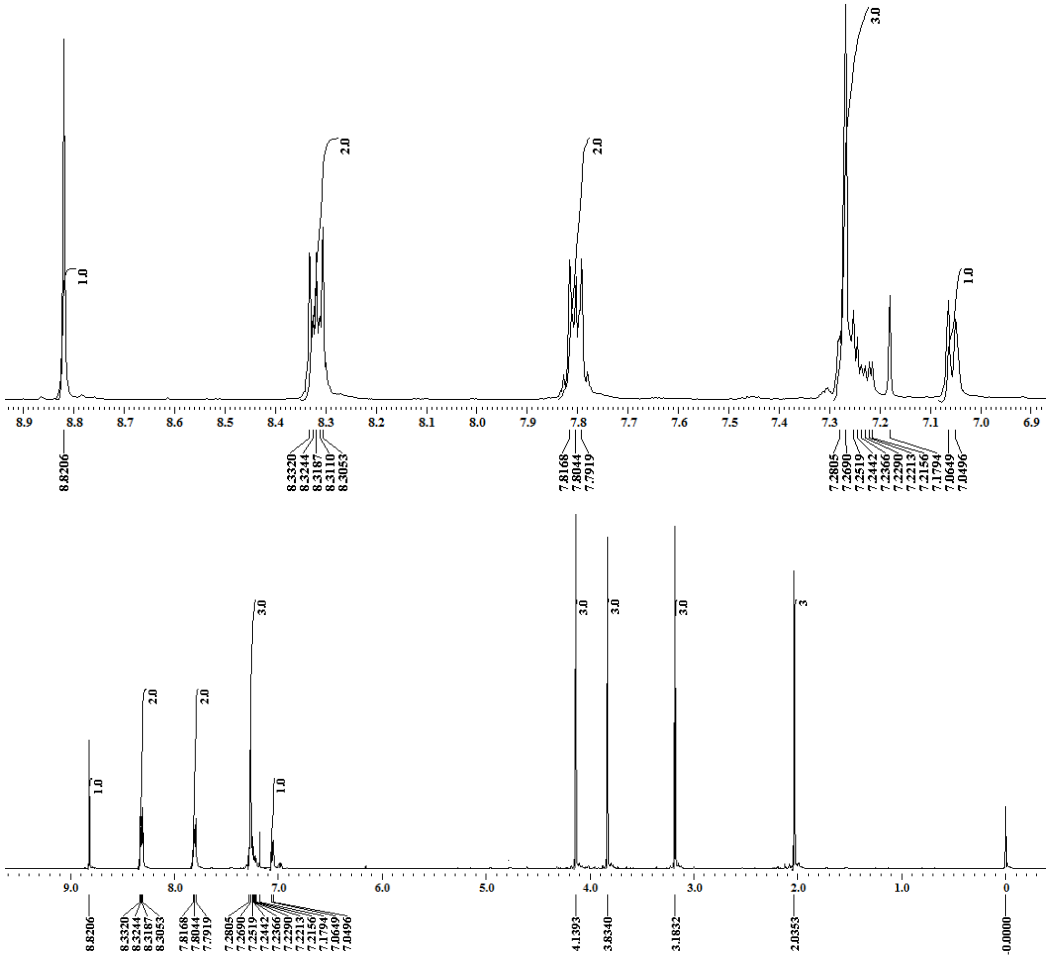
4-(6-Iodo-2,3,4-trimethoxybenzo[*a*]phenazin-5-yl)-*N*,*N*-dimethylaniline (5m)



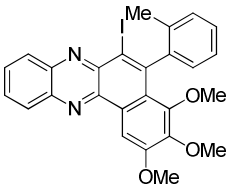
^{1}H NMR



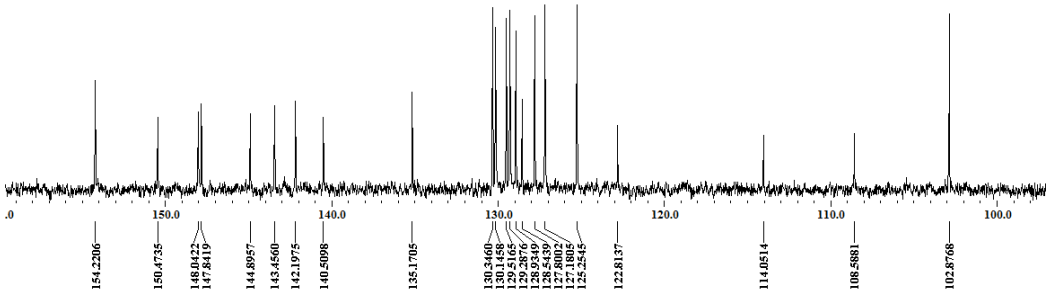
6-Iodo-2,3,4-trimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5n)

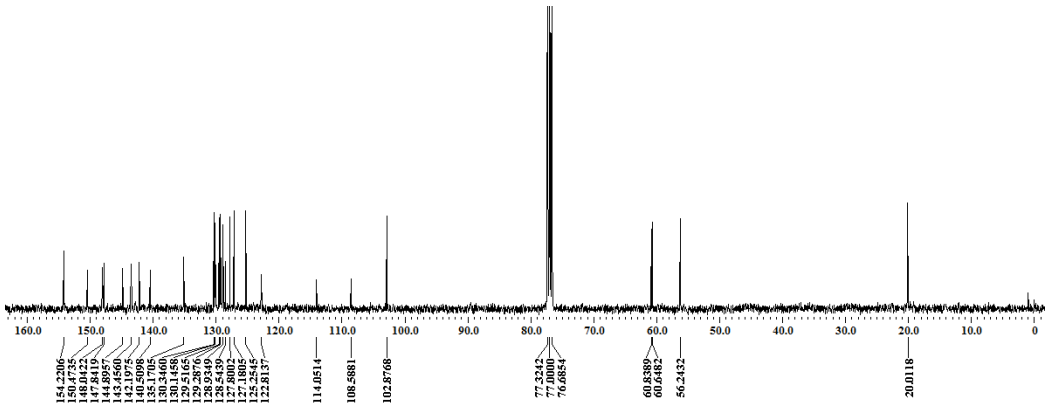


$^{13}C\{^{1}H\}$ NMR

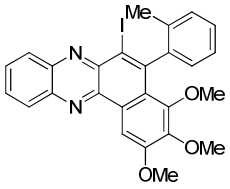


6-Iodo-2,3,4-trimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5n)





HRMS



6-Iodo-2,3,4-trimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5n)

Qualitative Compound Report

Data File	AB 821.d	**Sample Name**	AB 821
Sample Type	Sample	**Position**	P2-B5
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	17-12-2015 14:33:16
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

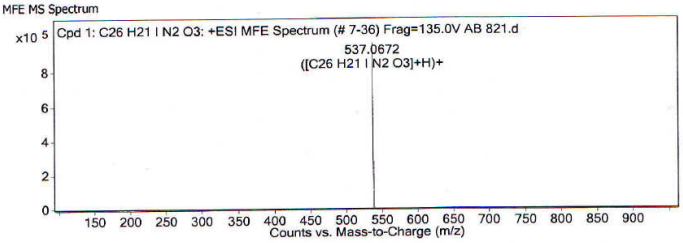
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

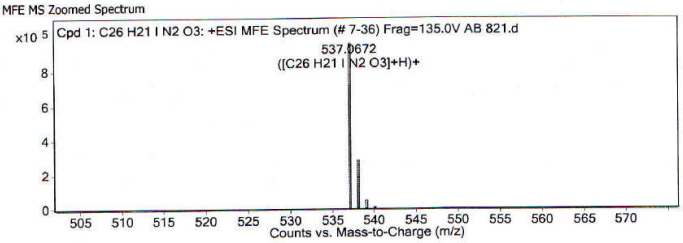
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C26 H21 I N2 O3	11	536.0598	C26 H21 I N2 O3	C26 H21 I N2 O3	-0.2	C26 H21 I N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C26 H21 I N2 O3	537.0672	11	Find by Molecular Feature	536.0598

MFE MS Spectrum



MFE MS Zoomed Spectrum

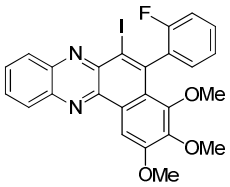


MS Spectrum Peak List

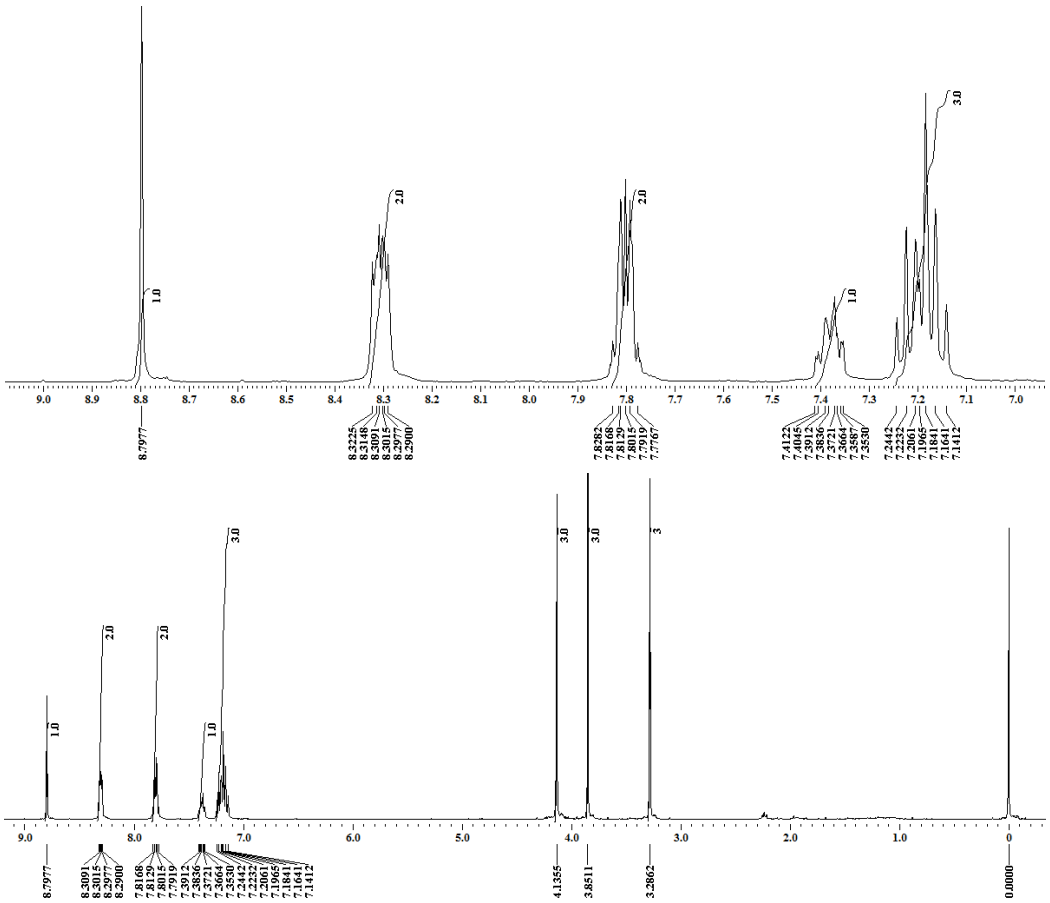
m/z	z	Abund	Formula	Ion
537.0672	1	966871.94	C26 H21 I N2 O3	(M+H)+
538.0699	1	276025.55	C26 H21 I N2 O3	(M+H)+
539.0726	1	41984.22	C26 H21 I N2 O3	(M+H)+
540.0755	1	5186.54	C26 H21 I N2 O3	(M+H)+
541.0787	1	394.95	C26 H21 I N2 O3	(M+H)+

--- End Of Report ---

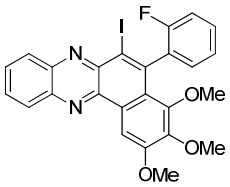
^{1}H NMR



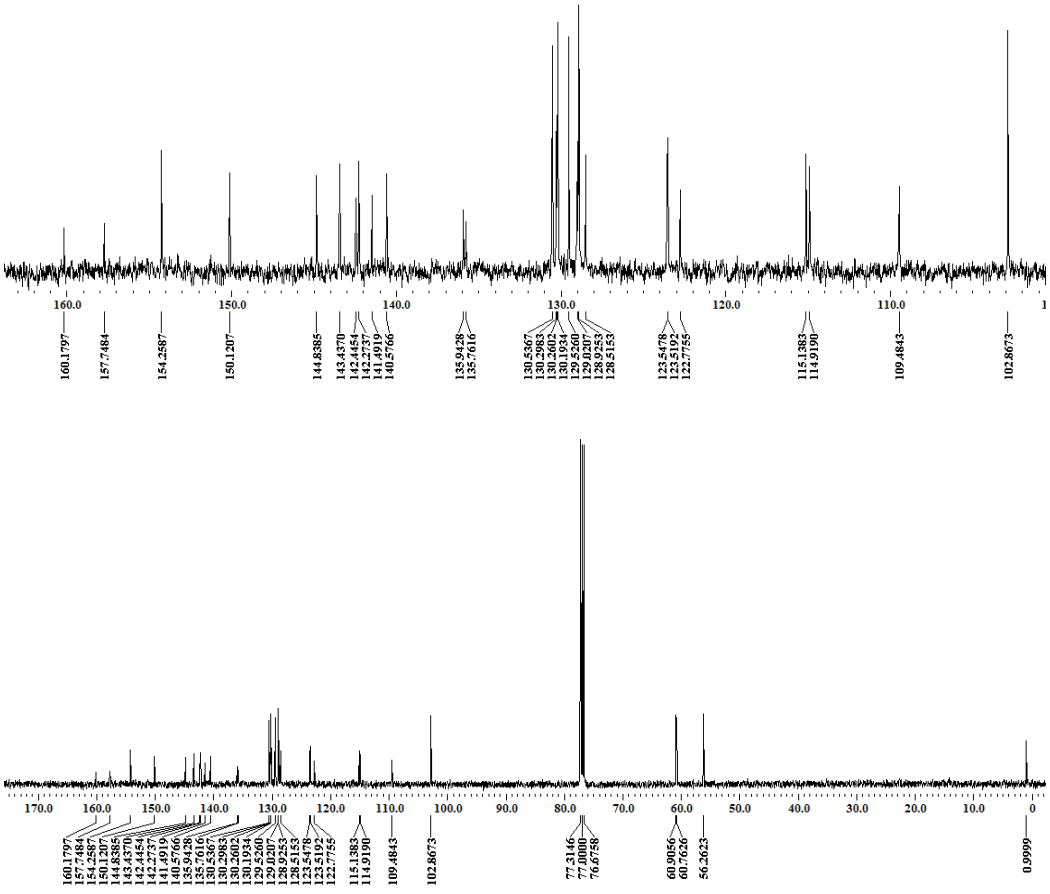
5-(2-Fluorophenyl)-6-iodo-2,3,4-trimethoxybenzo[*a*]phenazine (5o)



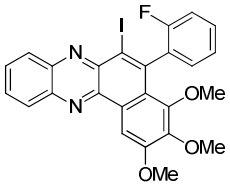
$^{13}C\{^{1}H\}$ NMR



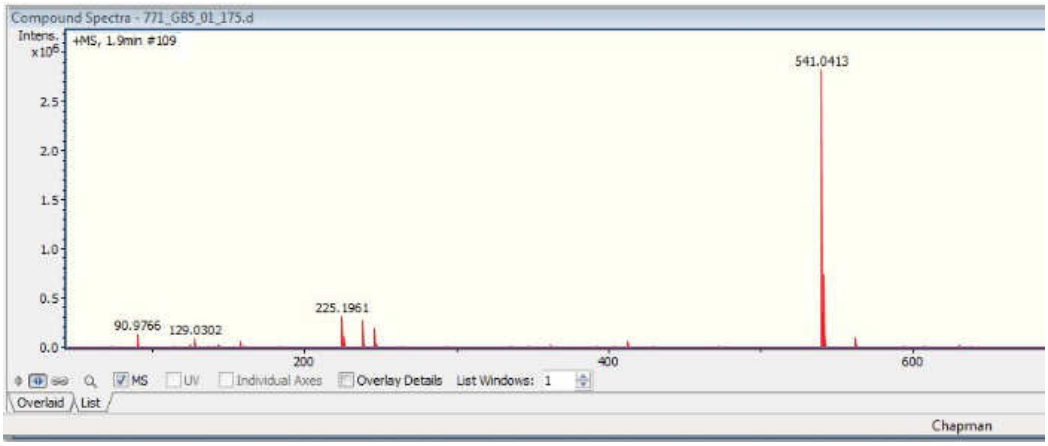
5-(2-Fluorophenyl)-6-iodo-2,3,4-trimethoxybenzo[*a*]phenazine (5o)



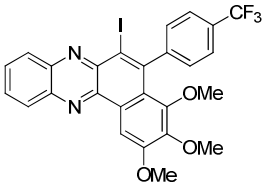
HRMS



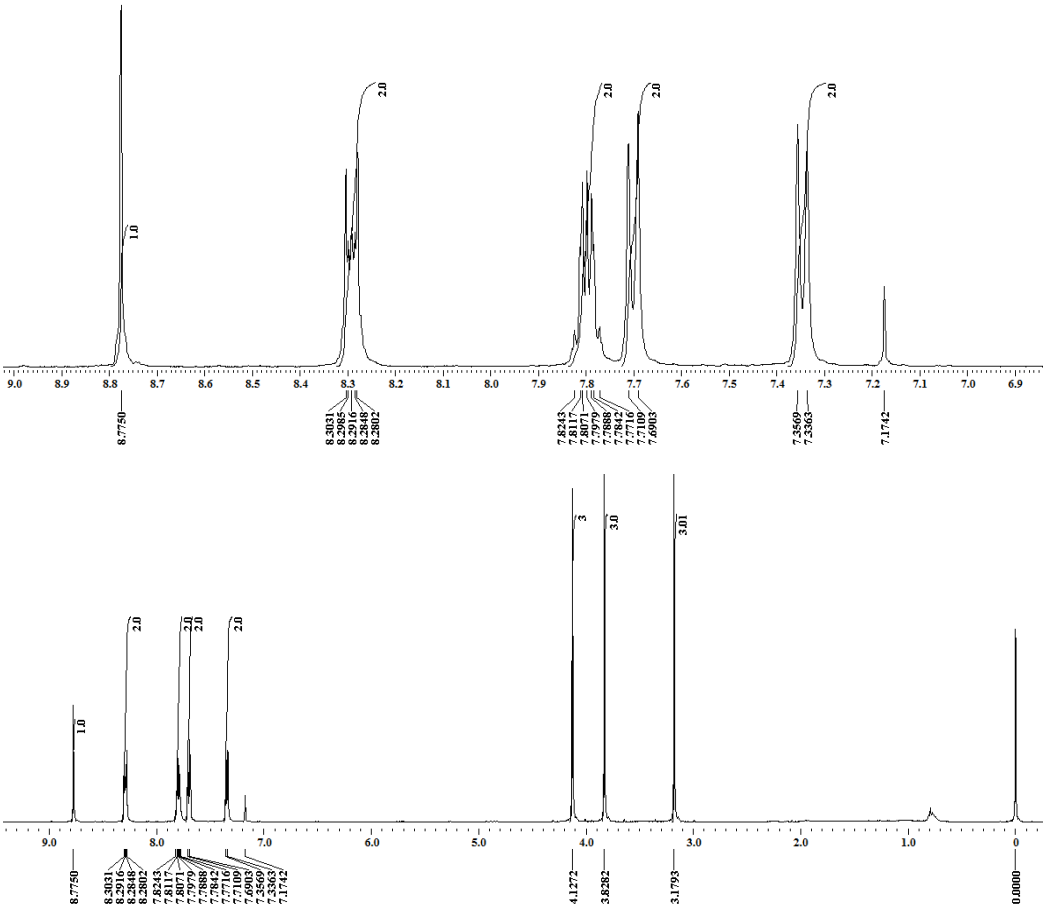
5-(2-Fluorophenyl)-6-iodo-2,3,4-trimethoxybenzo[*a*]phenazine (5o)



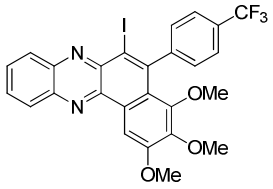
^{1}H NMR



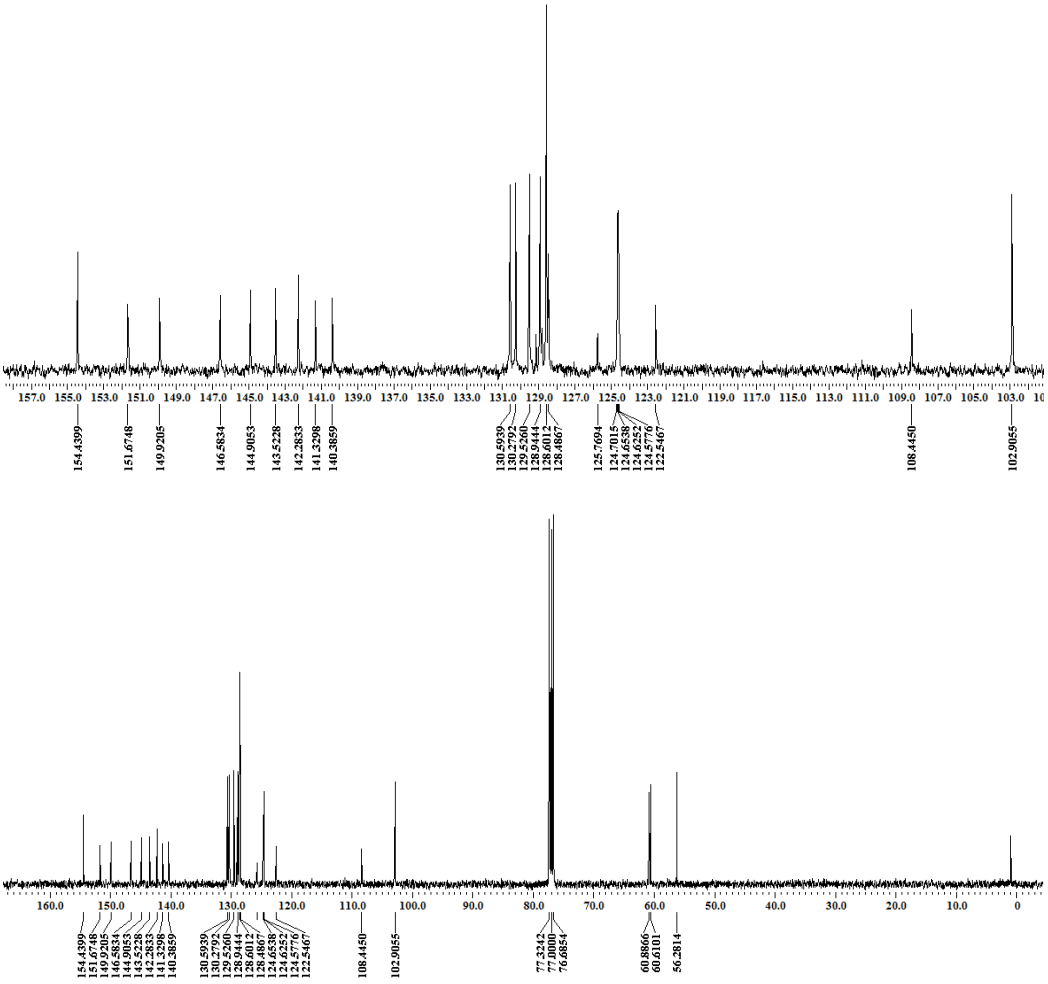
6-Iodo-2,3,4-trimethoxy-5-(4-(trifluoromethyl)phenyl)benzo[*a*]phenazine (5p)



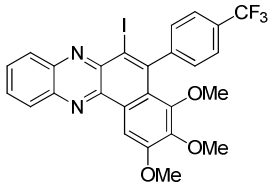
$^{13}C\{^{1}H\}$ NMR



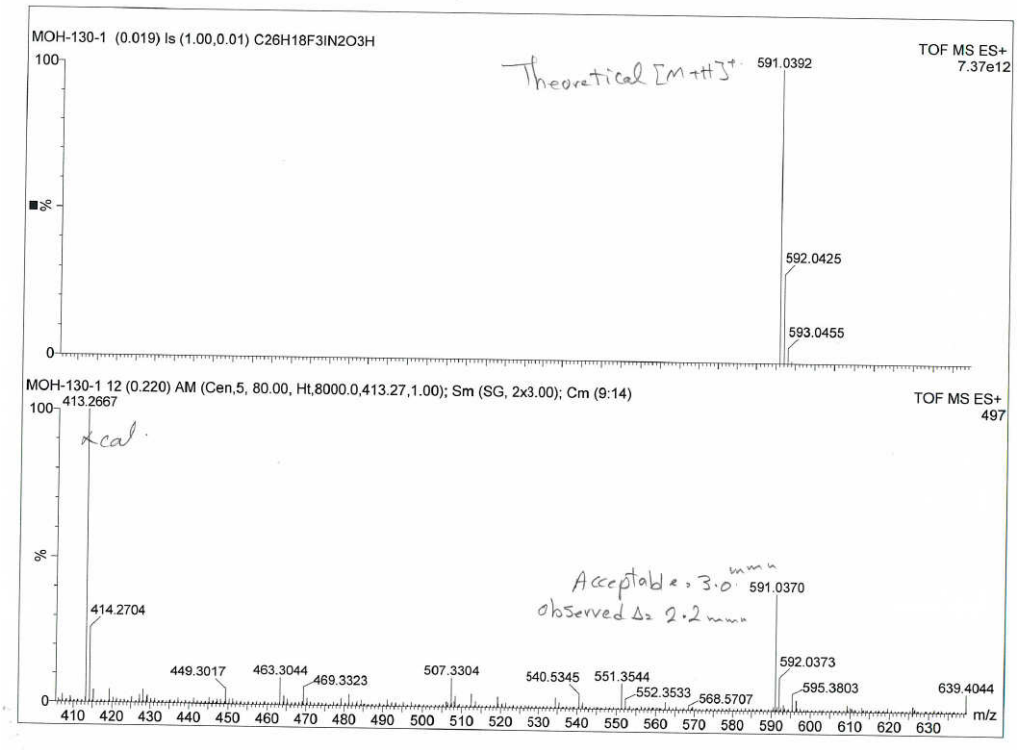
6-Iodo-2,3,4-trimethoxy-5-(4-(trifluoromethyl)phenyl)benzo[*a*]phenazine (5p)



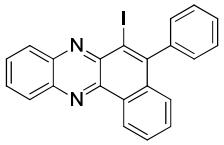
HRMS



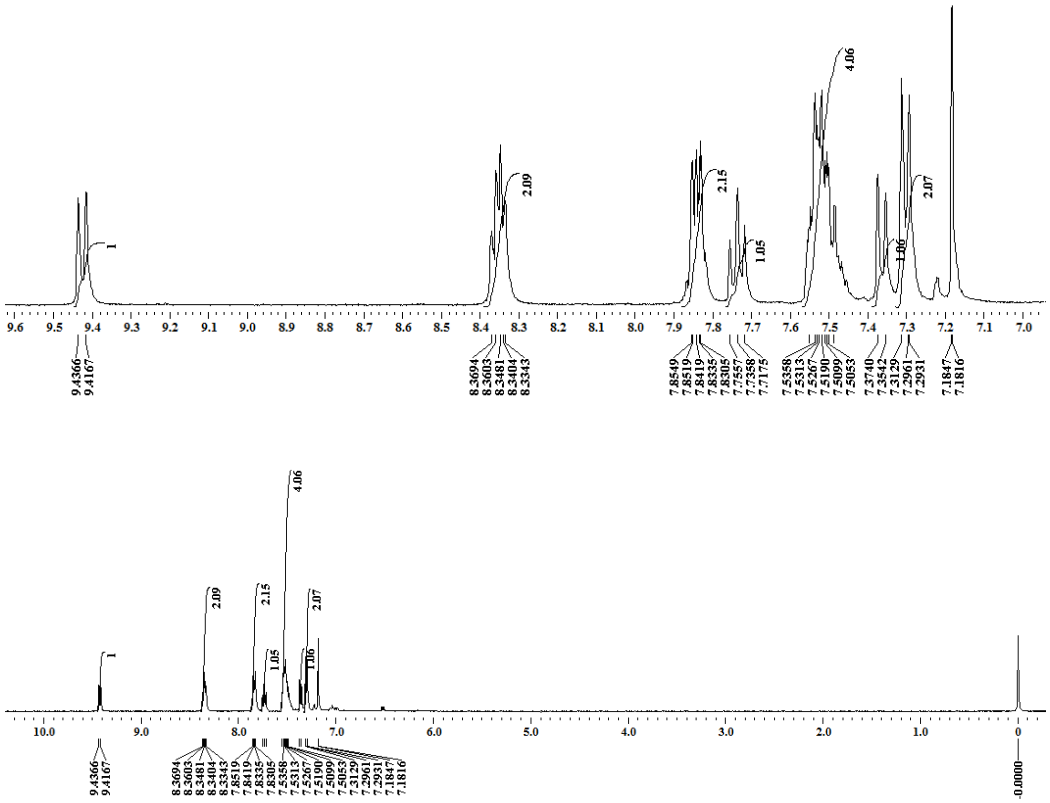
6-Iodo-2,3,4-trimethoxy-5-(4-(trifluoromethyl)phenyl)benzo[*a*]phenazine (5p)



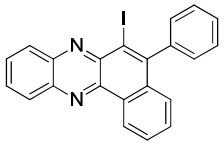
^{1}H NMR



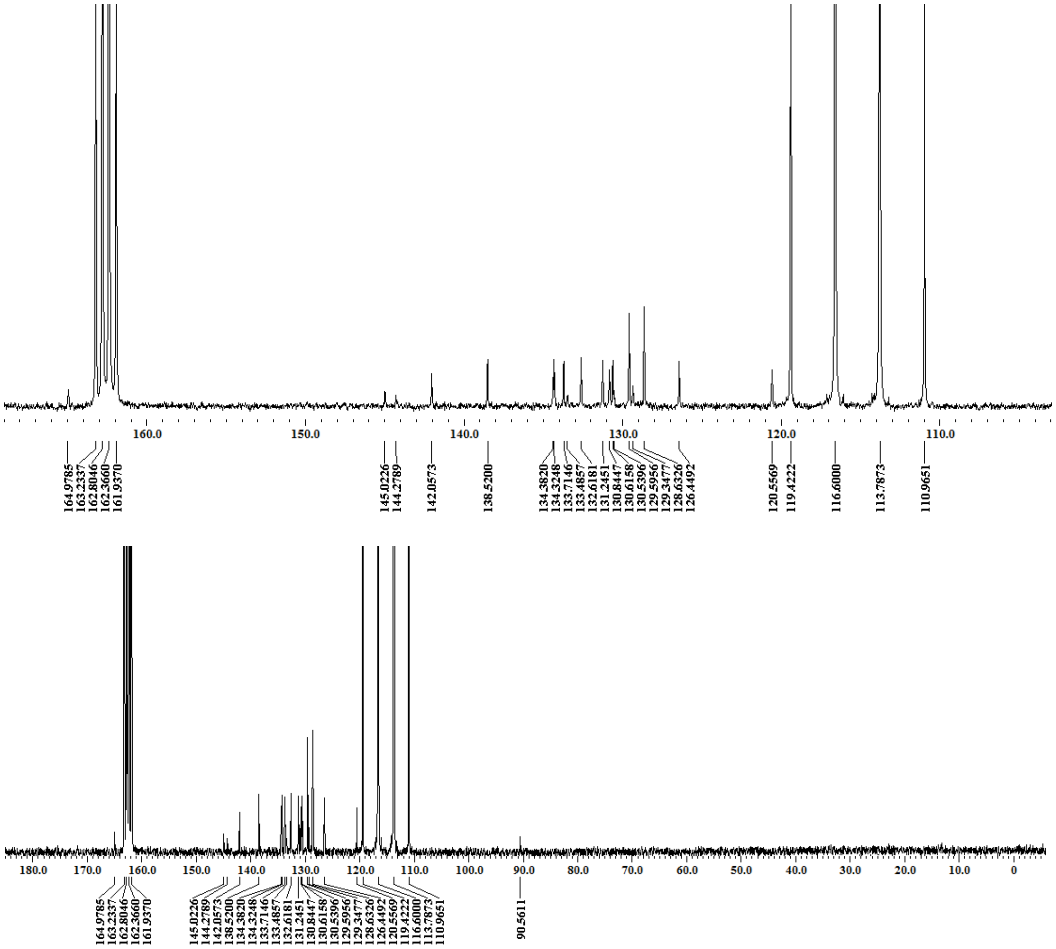
6-Iodo-5-phenylbenzo[*a*]phenazine (5q)



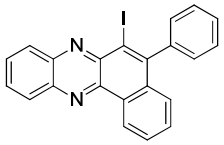
$^{13}C\{^{1}H\}$ NMR



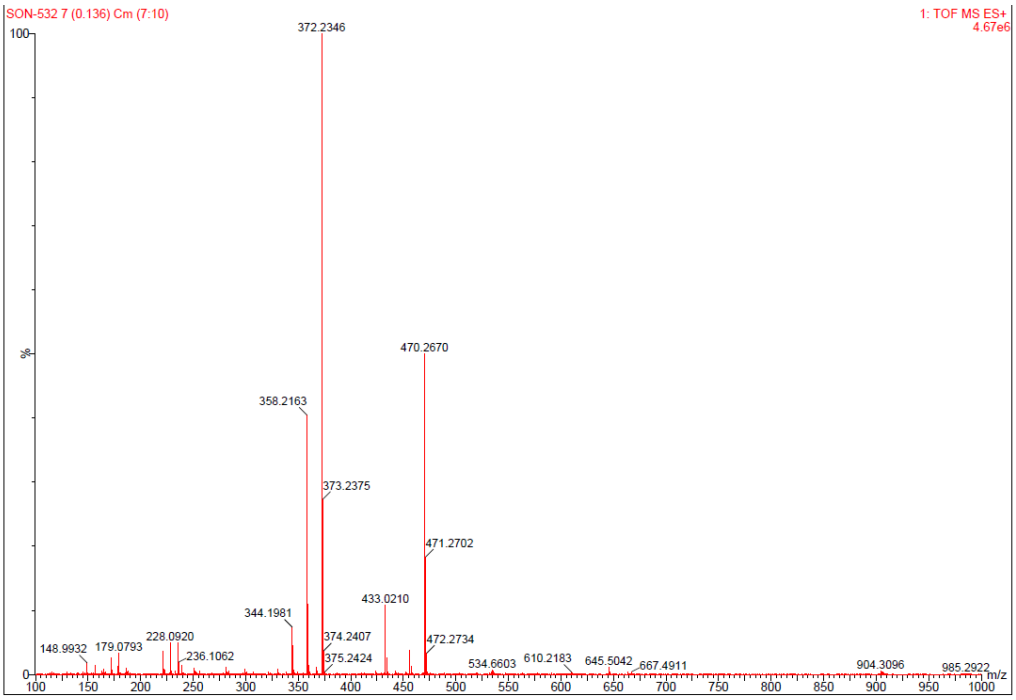
6-Iodo-5-phenylbenzo[*a*]phenazine (5q)



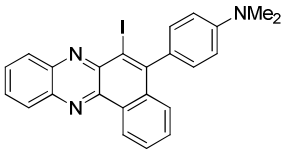
HRMS



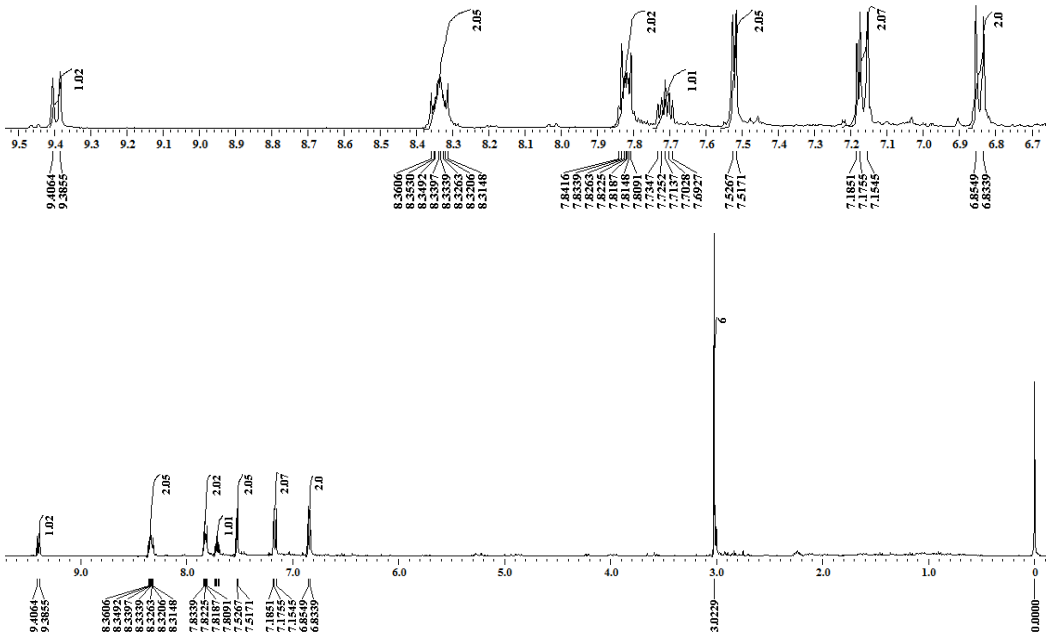
6-Iodo-5-phenylbenzo[*a*]phenazine (5q)



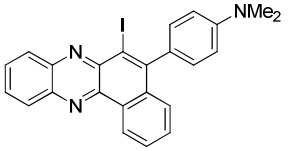
^{1}HNMR



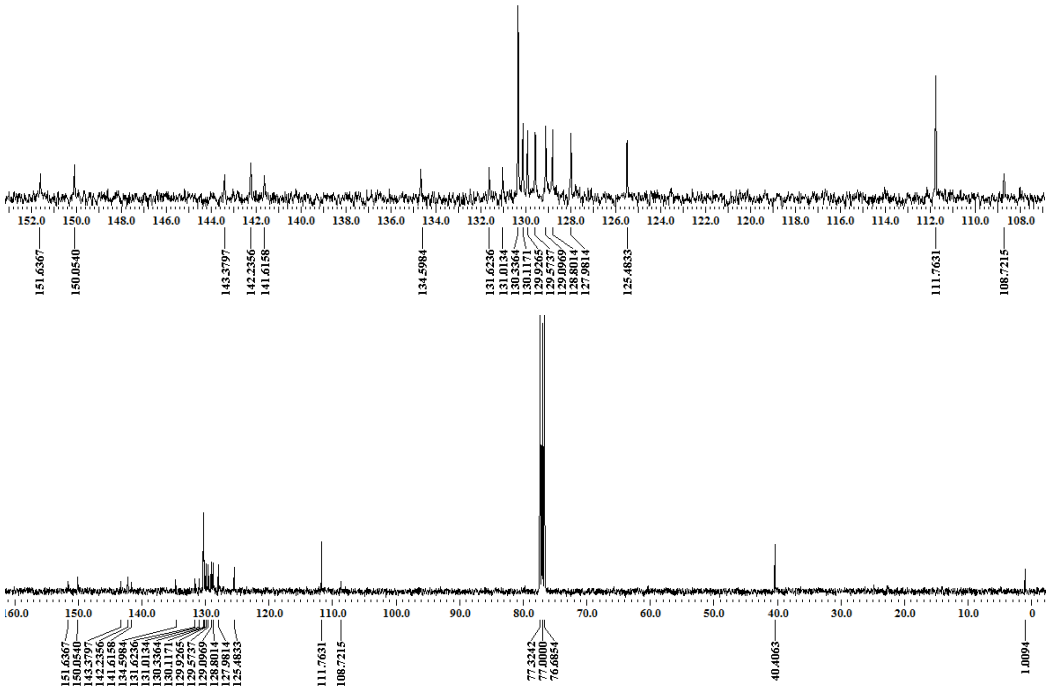
4-(6-Iodobenzo[*a*]phenazin-5-yl)-N,N-dimethylaniline (5r)



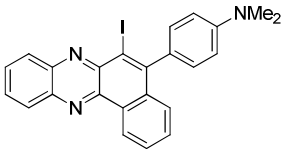
$^{13}C\{^{1}H\}$ NMR



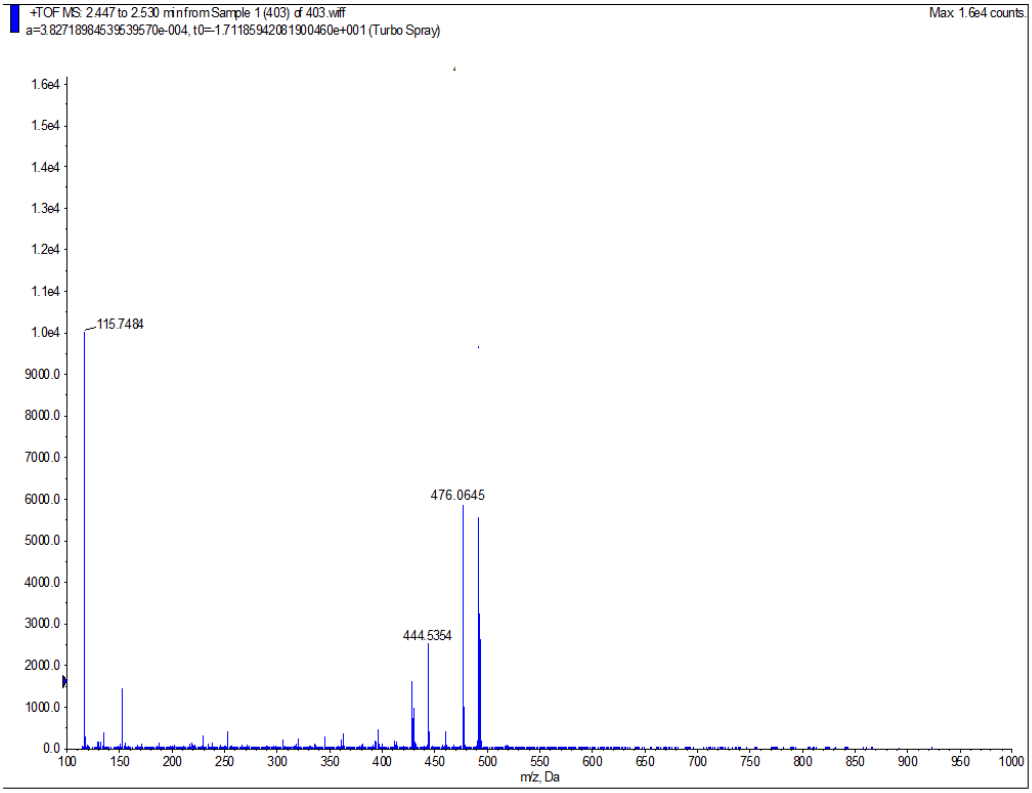
4-(6-Iodobenzo[*a*]phenazin-5-yl)-N,N-dimethylaniline (5r)



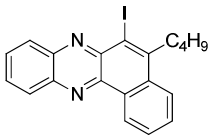
HRMS



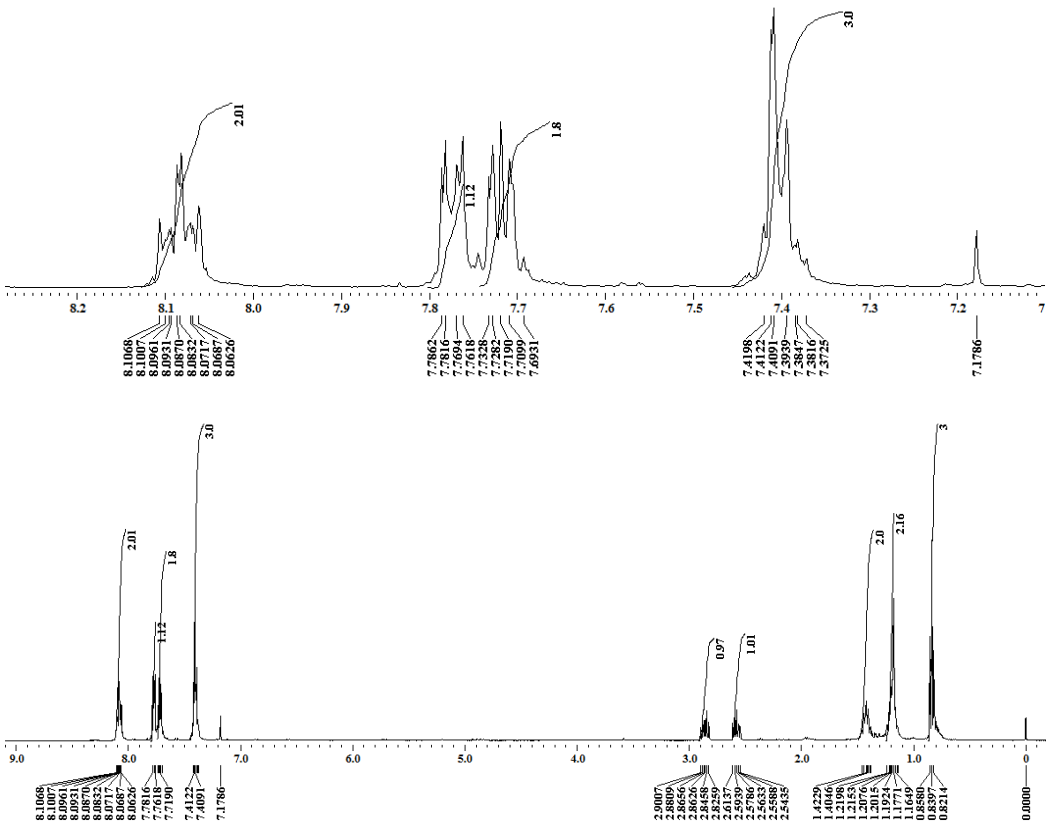
4-(6-Iodobenzo[*a*]phenazin-5-yl)-N,N-dimethylaniline (5r)



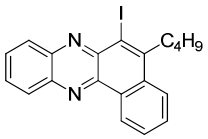
^{1}H NMR



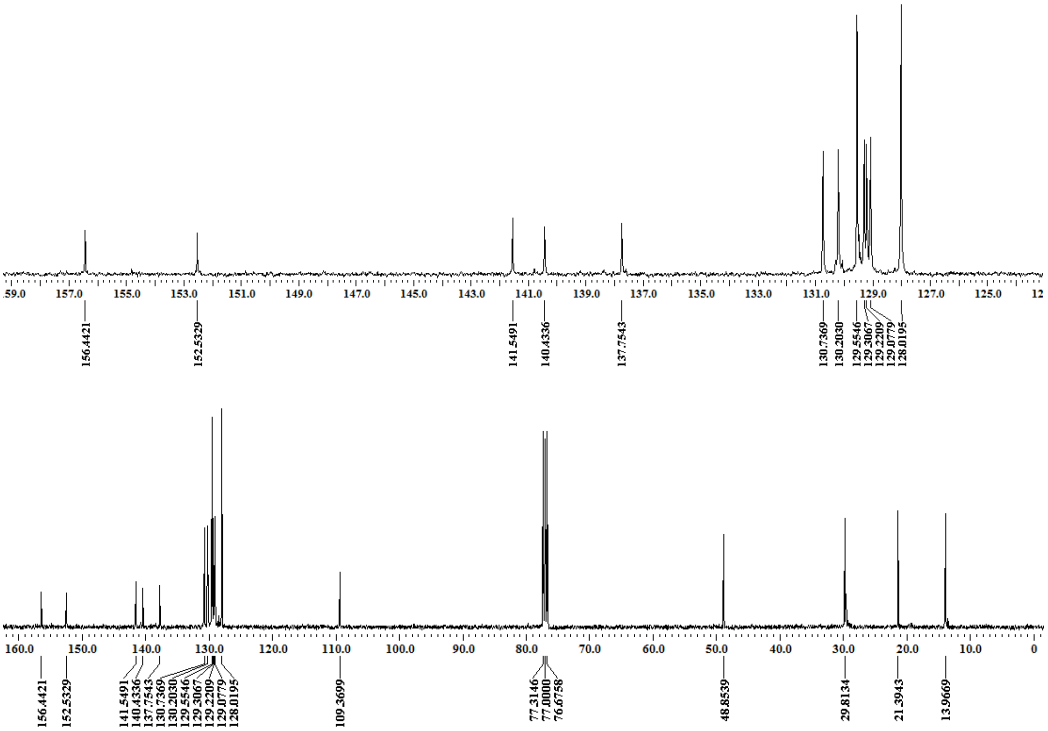
5-Butyl-6-iodobenzo[*a*]phenazine (5s)



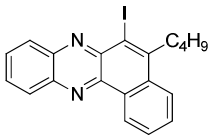
$^{13}C\{^{1}H\}$ NMR



5-Butyl-6-iodobenzo[*a*]phenazine (5s)



HRMS



5-Butyl-6-iodobenzo[*a*]phenazine (5s)

Qualitative Compound Report

Data File	SON-536.d	**Sample Name**	SON-536
Sample Type	Sample	**Position**	P1-E4
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	08-11-2016 12:24:42
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

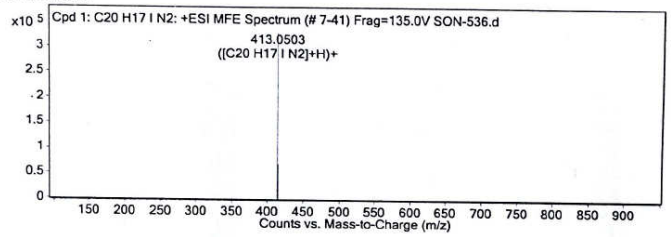
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

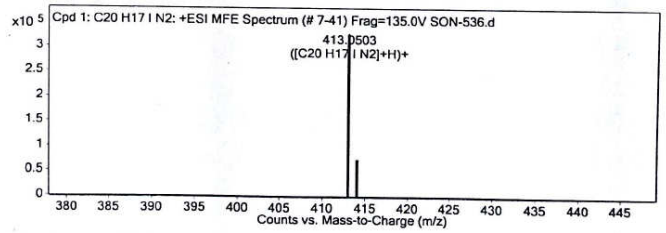
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C20 H17 I N2	11	412.043	C20 H17 I N2	C20 H17 I N2	1.55	C20 H17 I N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C20 H17 I N2	413.0503	11	Find by Molecular Feature	412.043

MFE MS Spectrum



MFE MS Zoomed Spectrum

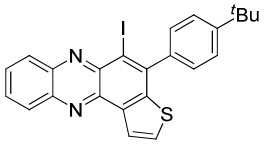


MS Spectrum Peak List

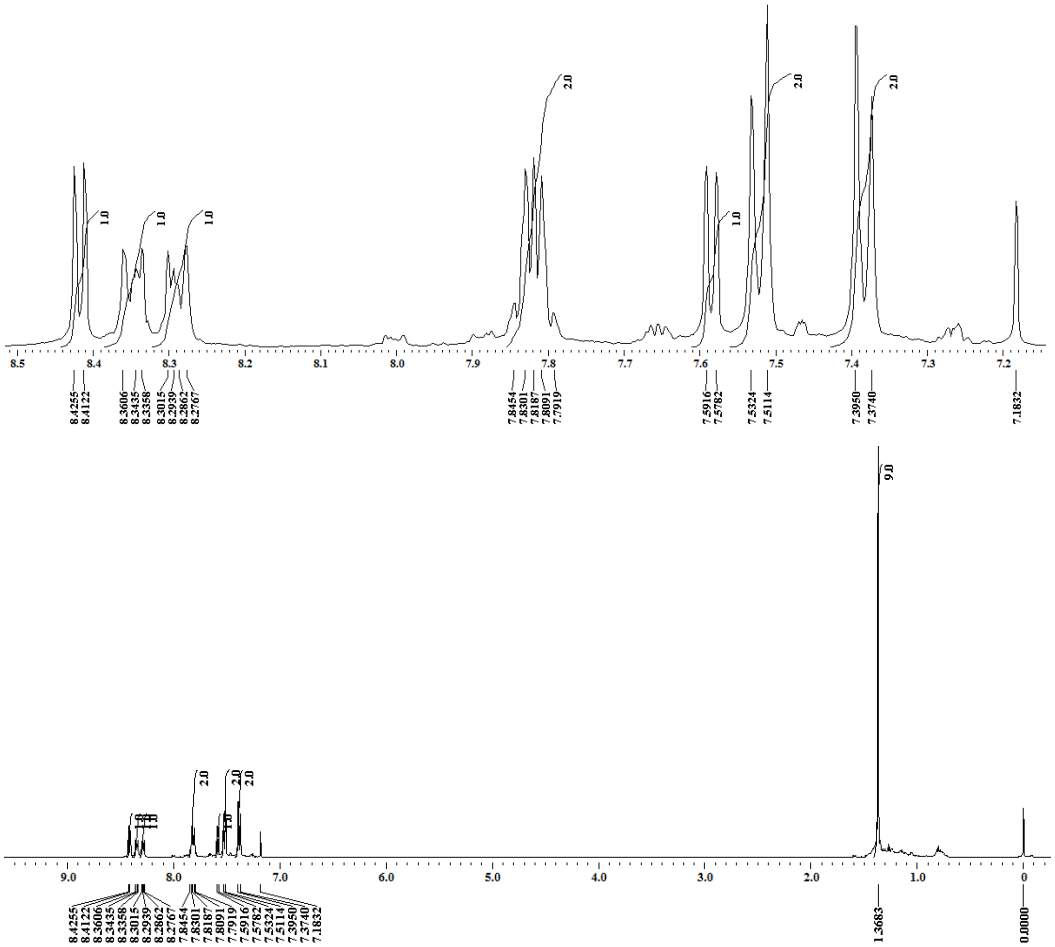
m/z	z	Abund	Formula	Ion
413.0503	1	327969.75	C20 H17 I N2	(M+H)+
414.0533	1	69269.71	C20 H17 I N2	(M+H)+

--- End Of Report ---

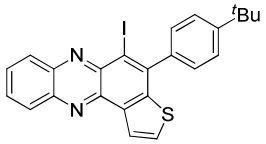
^{1}H NMR



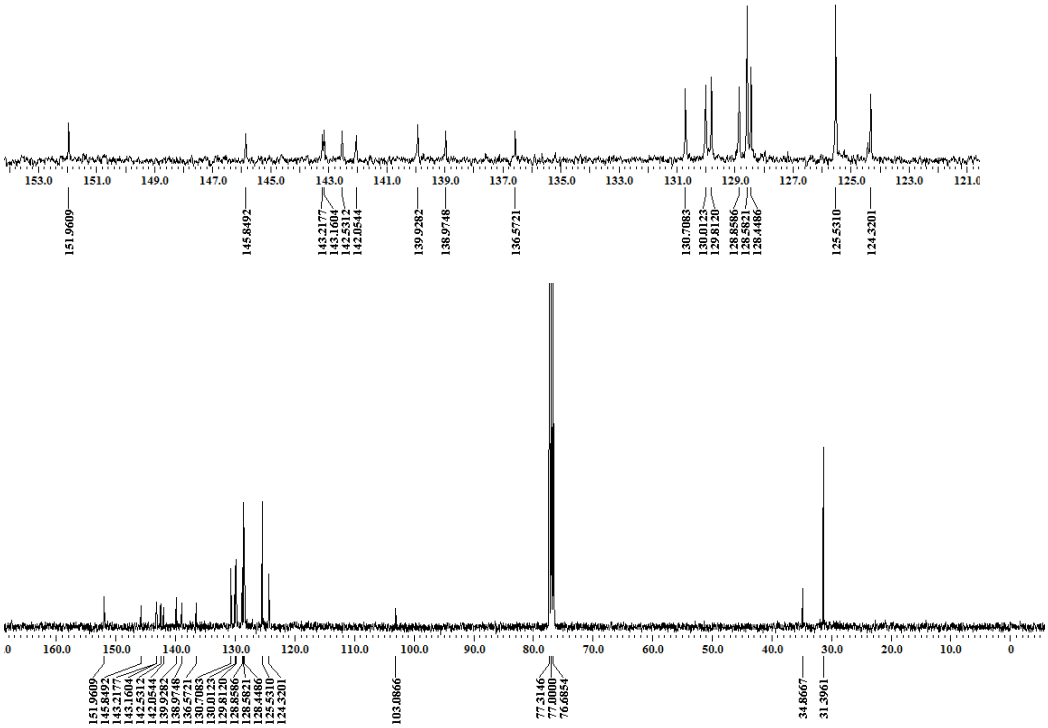
4-(4-(*tert*-Butyl)phenyl)-5-iodothieno[3,2-*a*]phenazine (5t)



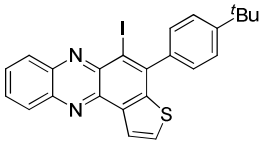
$^{13}C\{^{1}H\}$ NMR



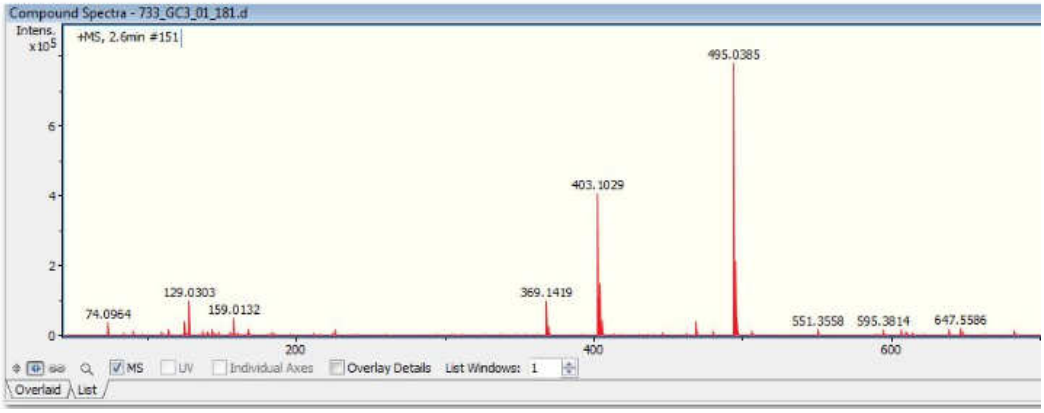
4-(4-(*tert*-Butyl)phenyl)-5-iodothieno[3,2-*a*]phenazine (5t)



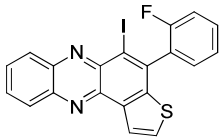
HRMS



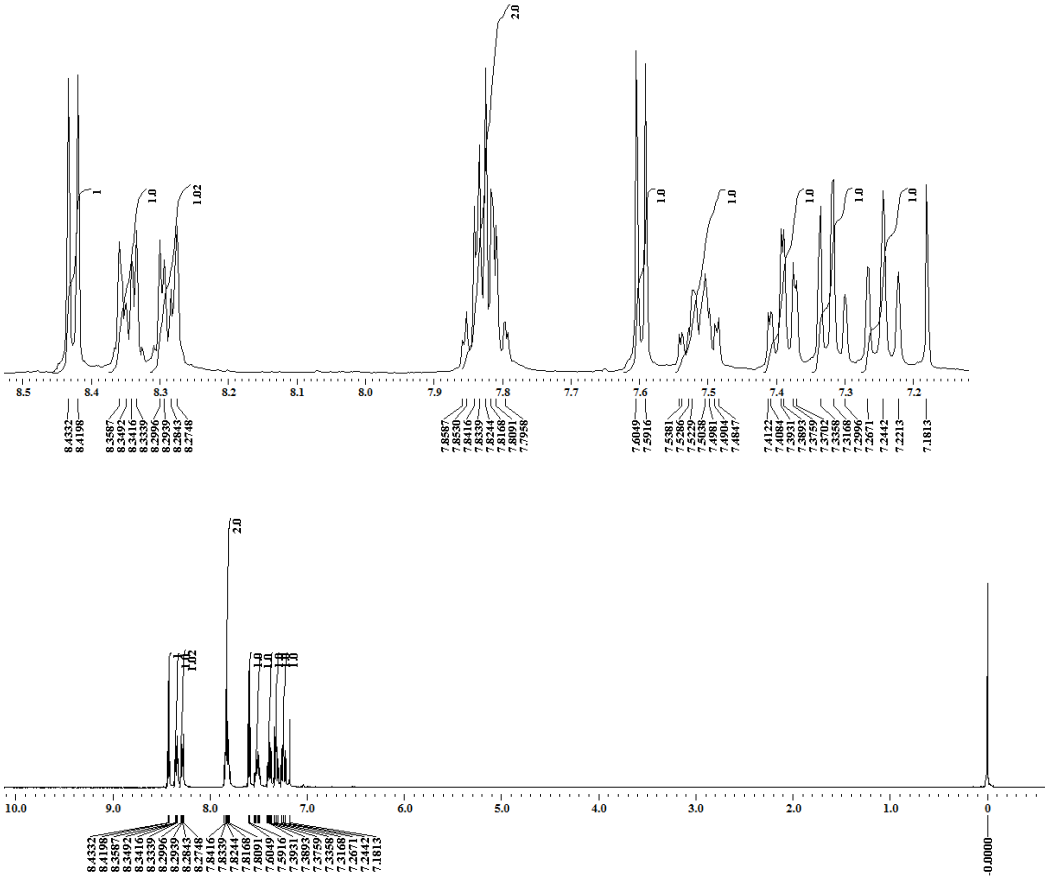
4-(4-(*tert*-Butyl)phenyl)-5-iodothieno[3,2-*a*]phenazine (5t)



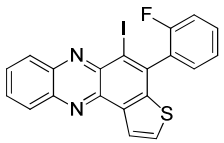
^{1}H NMR



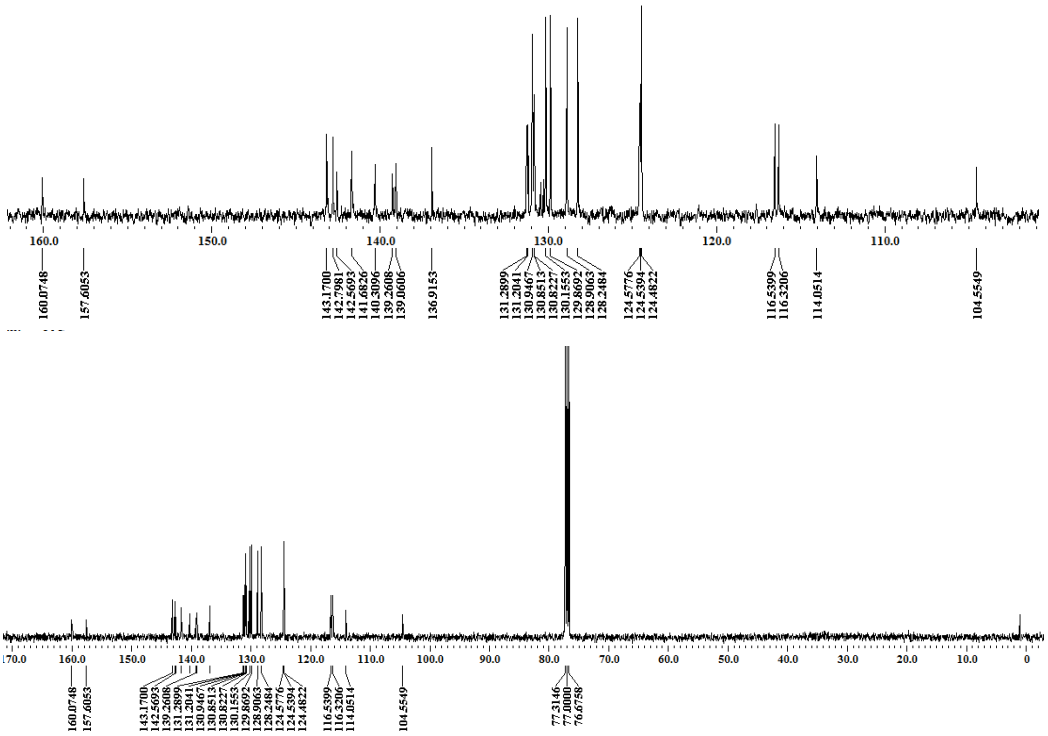
4-(2-Fluorophenyl)-5-iodothieno[3,2-*a*]phenazine (5u)



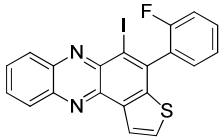
$^{13}C\{^{1}H\}$ NMR



4-(2-Fluorophenyl)-5-iodothieno[3,2-*a*]phenazine (5u)



HRMS



4-(2-Fluorophenyl)-5-iodothieno[3,2-*a*]phenazine (5u)

Qualitative Compound Report

Data File	SON 772.d	**Sample Name**	SON 772
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	28-09-2015 12:35:47
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

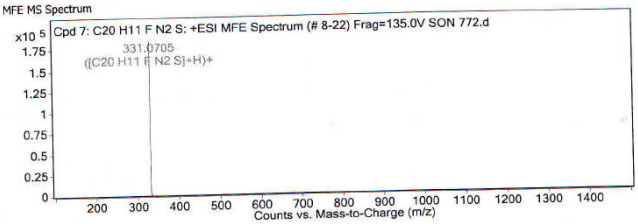
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

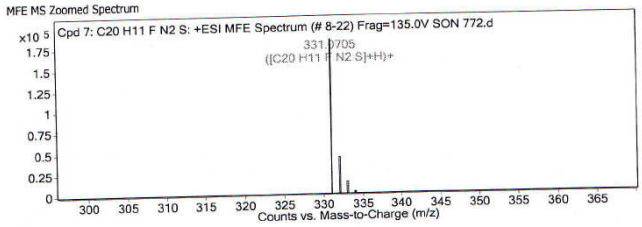
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C20 H11 F N2 S	11	330.0633	C20 H11 F N2 S	C20 H11 F N2 S	-1.83	C20 H11 F N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C20 H11 F N2 S	331.0705	11	Find by Molecular Feature	330.0633

MFE MS Spectrum



MFE MS Zoomed Spectrum

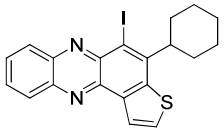


MS Spectrum Peak List

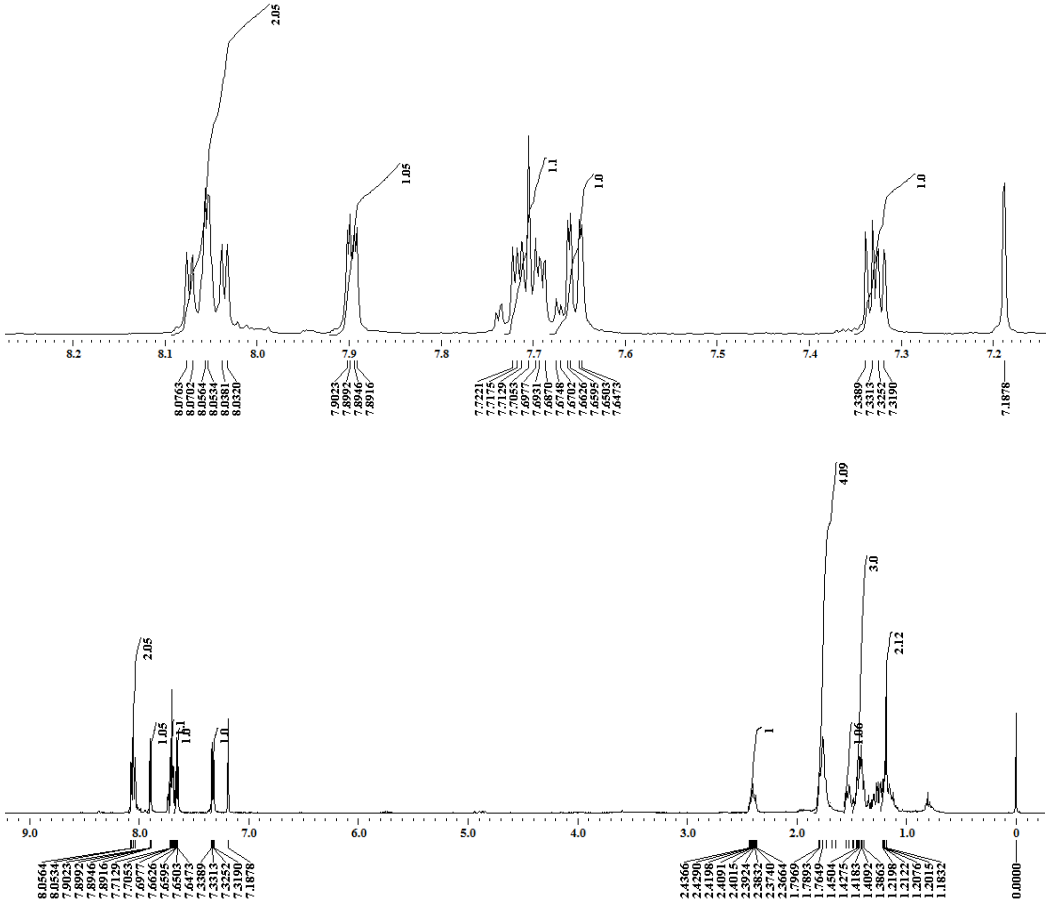
m/z	z	Abund	Formula	Ion
331.0705	1	184856.3	C20 H11 F N2 S	(M+H)+
332.0734	1	42994.79	C20 H11 F N2 S	(M+H)+
333.0711	1	11522.01	C20 H11 F N2 S	(M+H)+
334.0727	1	2266.18	C20 H11 F N2 S	(M+H)+
335.0731	1	262.54	C20 H11 F N2 S	(M+H)+

--- End Of Report ---

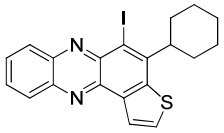
^{1}HNMR



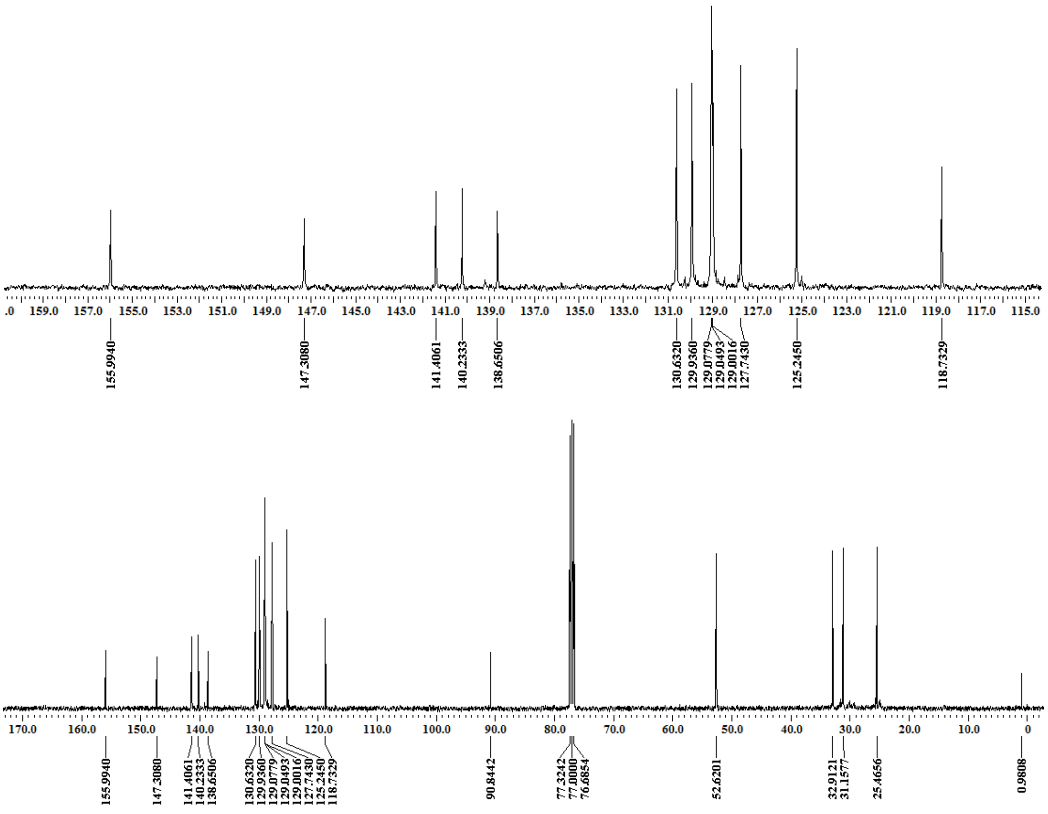
4-Cyclohexyl-5-iodothieno[3,2-*a*]phenazine (5v)



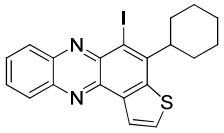
$^{13}C\{^{1}H\}$ NMR



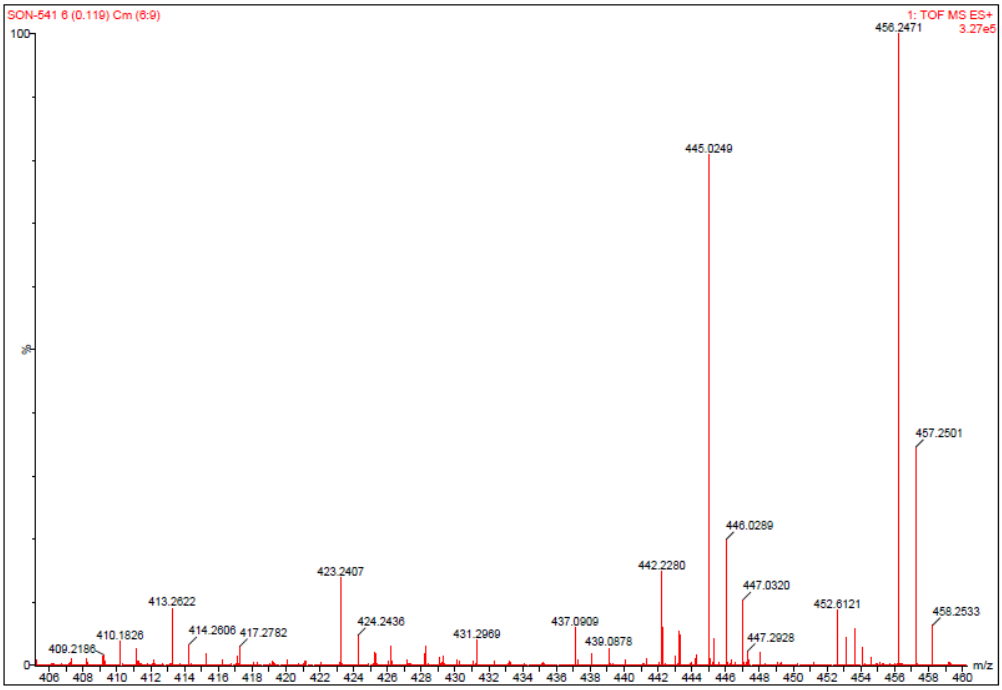
4-Cyclohexyl-5-iodothieno[3,2-*a*]phenazine (5v)



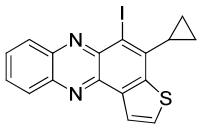
HRMS



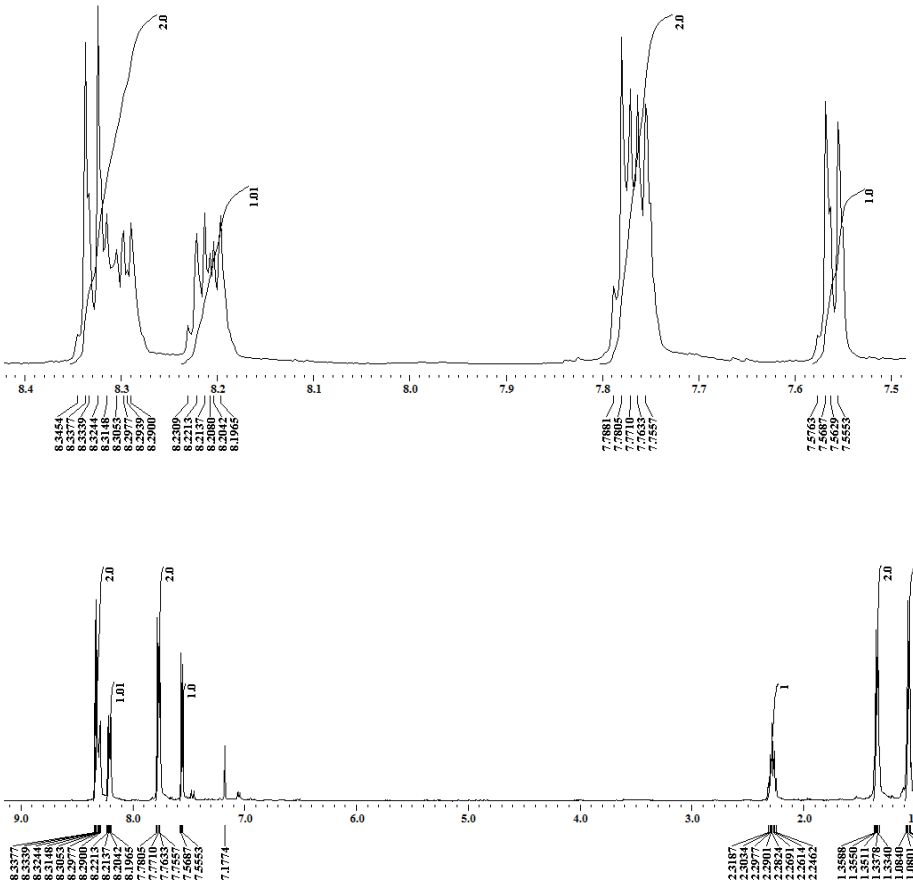
4-Cyclohexyl-5-iodothieno[3,2-*a*]phenazine (5v)



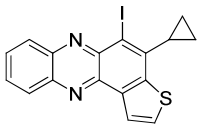
^{1}H NMR



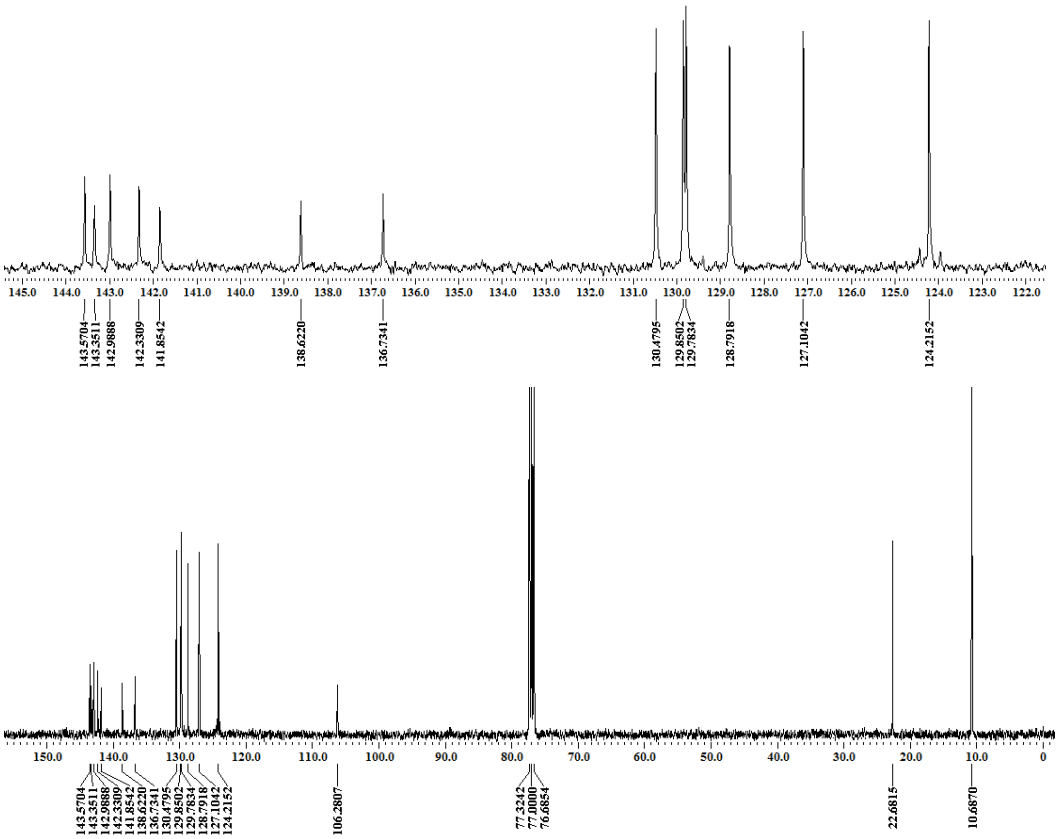
4-Cyclopropyl-5-iodothieno[3,2-*a*]phenazine (5w)



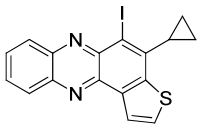
$^{13}C\{^{1}H\}$ NMR



4-Cyclopropyl-5-iodothieno[3,2-*a*]phenazine (5w)



HRMS



4-Cyclopropyl-5-iodothieno[3,2-*a*]phenazine (5w)

Qualitative Compound Report

Data File	SON 807A.d	**Sample Name**	SON 807A
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	05-11-2015 14:32:44
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

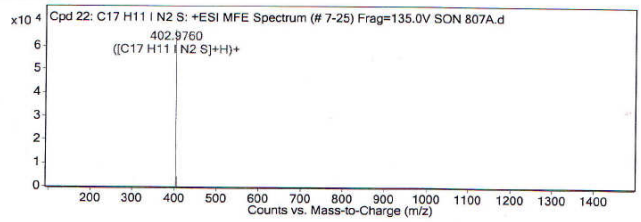
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

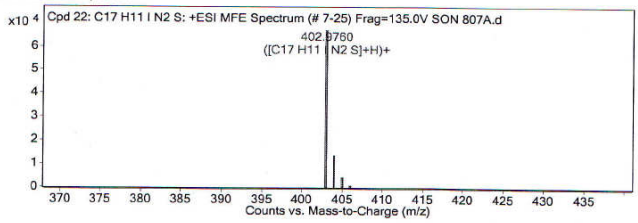
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C17 H11 I N2 S	12	401.9688	C17 H11 I N2 S	C17 H11 I N2 S	-0.1	C17 H11 I N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C17 H11 I N2 S	402.976	12	Find by Molecular Feature	401.9688

MFE MS Spectrum



MFE MS Zoomed Spectrum

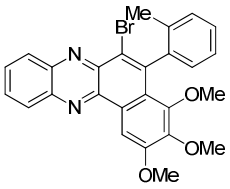


MS Spectrum Peak List

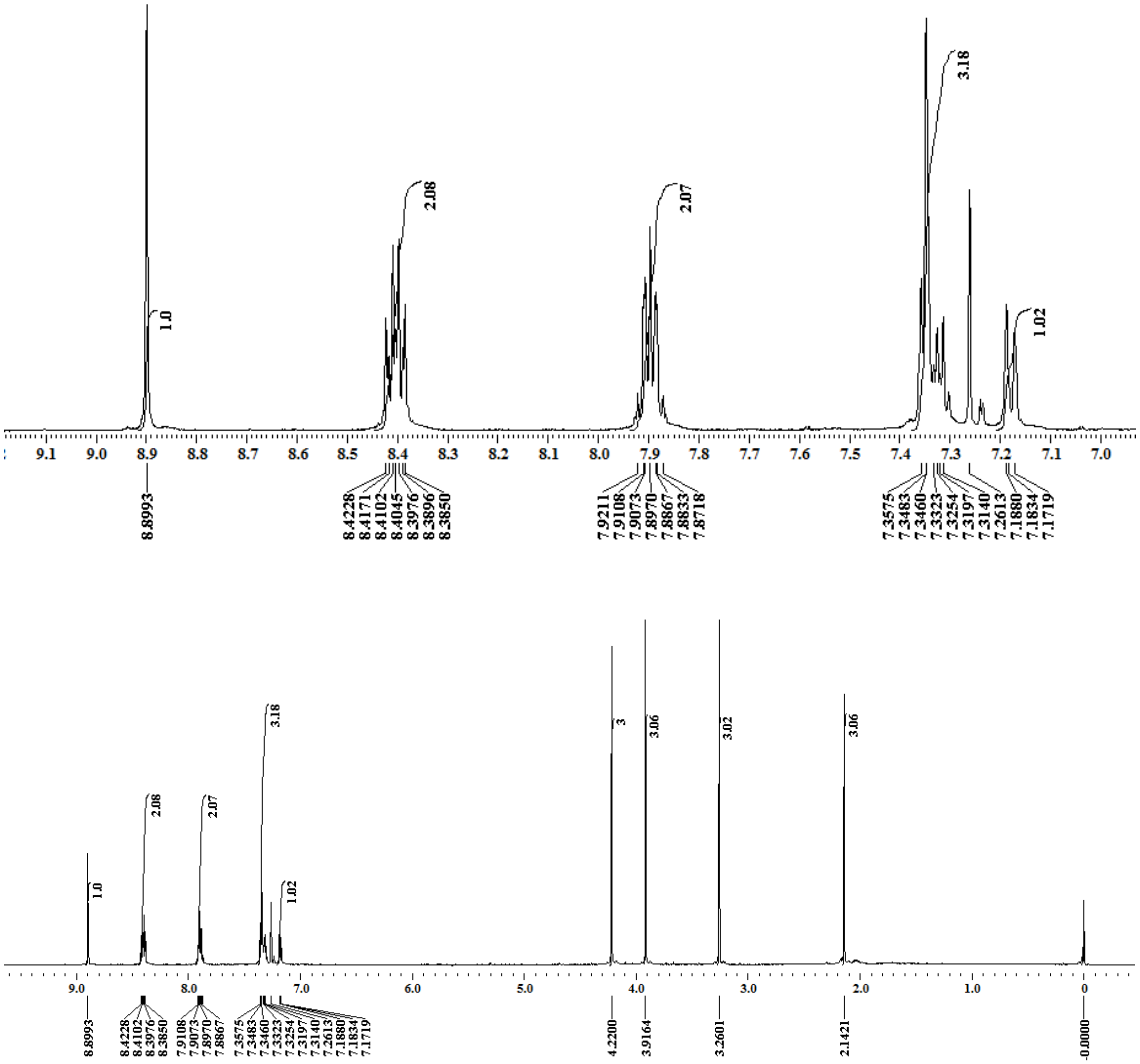
m/z	z	Abund	Formula	Ion
402.976	1	67112.62	C17 H11 I N2 S	(M+H)+
403.9791	1	13464.91	C17 H11 I N2 S	(M+H)+
404.9758	1	4244.01	C17 H11 I N2 S	(M+H)+
405.9746	1	752.08	C17 H11 I N2 S	(M+H)+

--- End Of Report ---

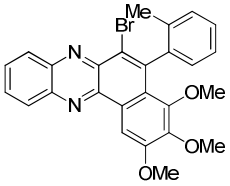
^{1}H NMR



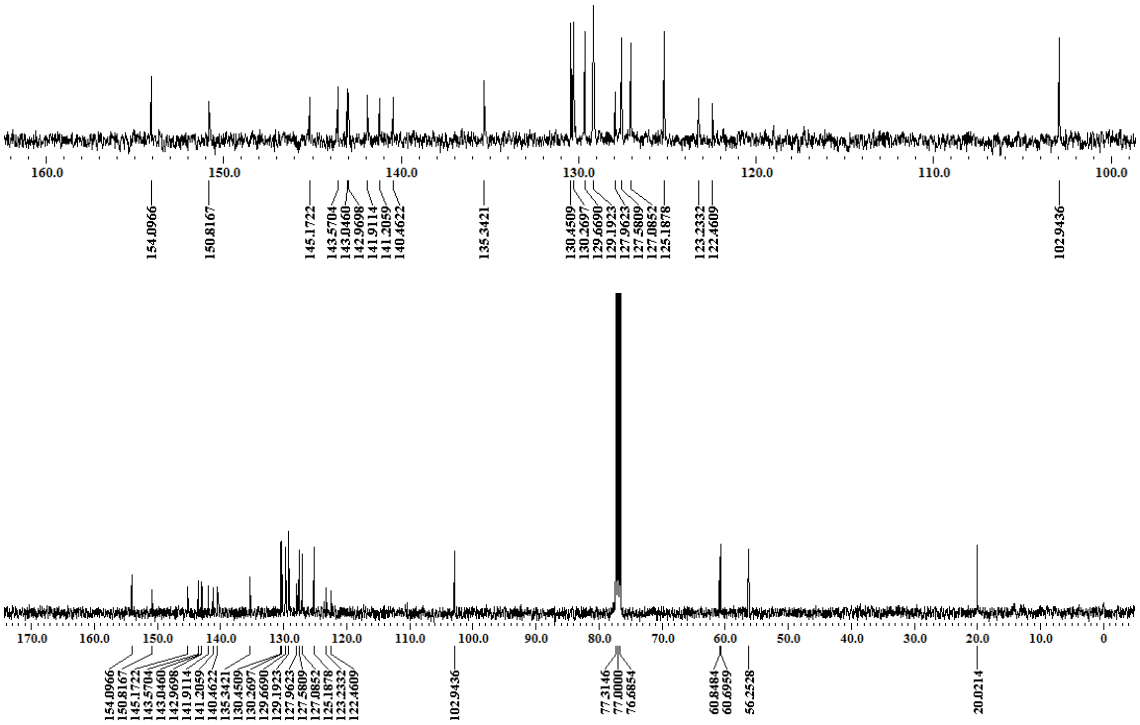
6-Bromo-2,3,4-trimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5x)



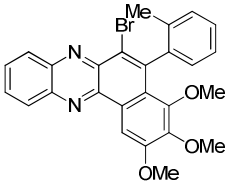
$^{13}C\{^{1}H\}$ NMR



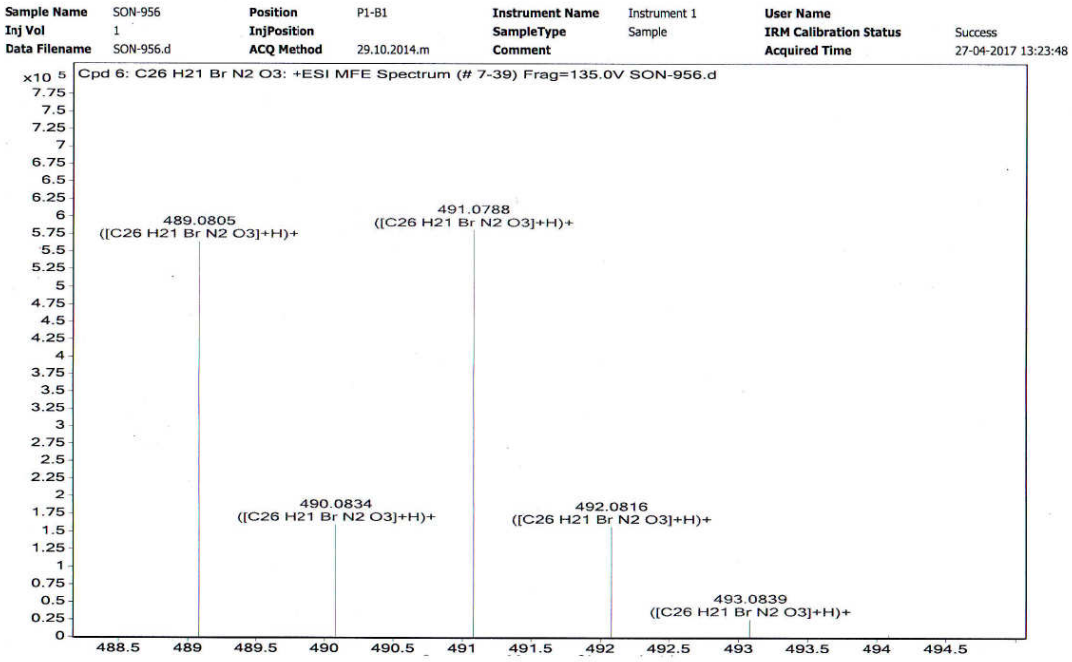
6-Bromo-2,3,4-trimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5x)



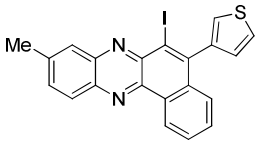
HRMS



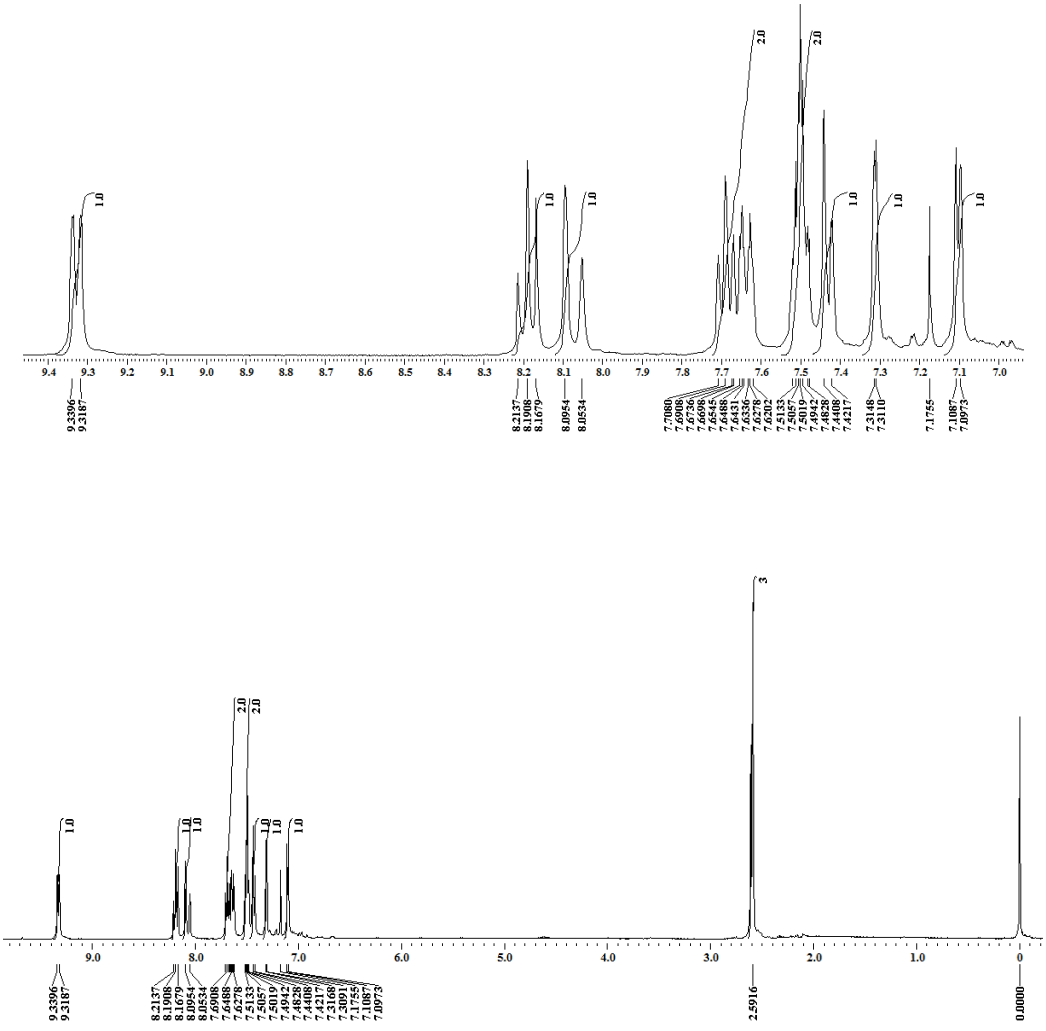
6-Bromo-2,3,4-trimethoxy-5-(*o*-tolyl)benzo[*a*]phenazine (5x)



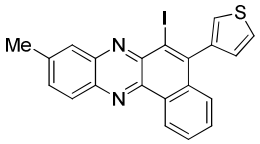
^{1}H NMR



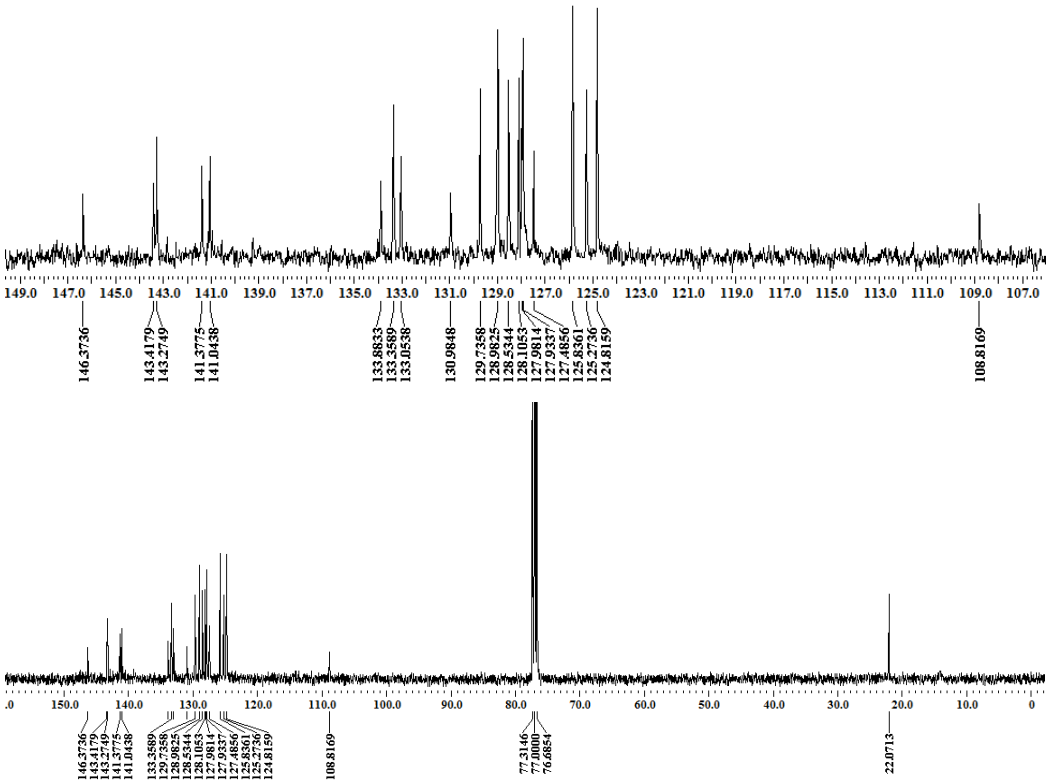
6-Iodo-9-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (7a)



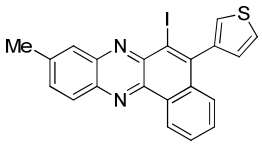
$^{13}C\{^{1}H\}$ NMR



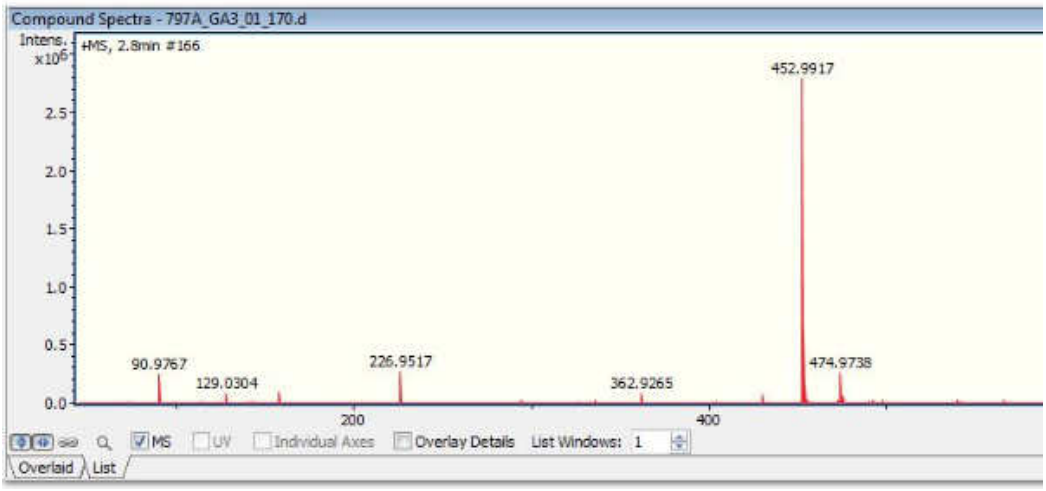
6-Iodo-9-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (7a)



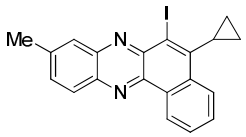
HRMS



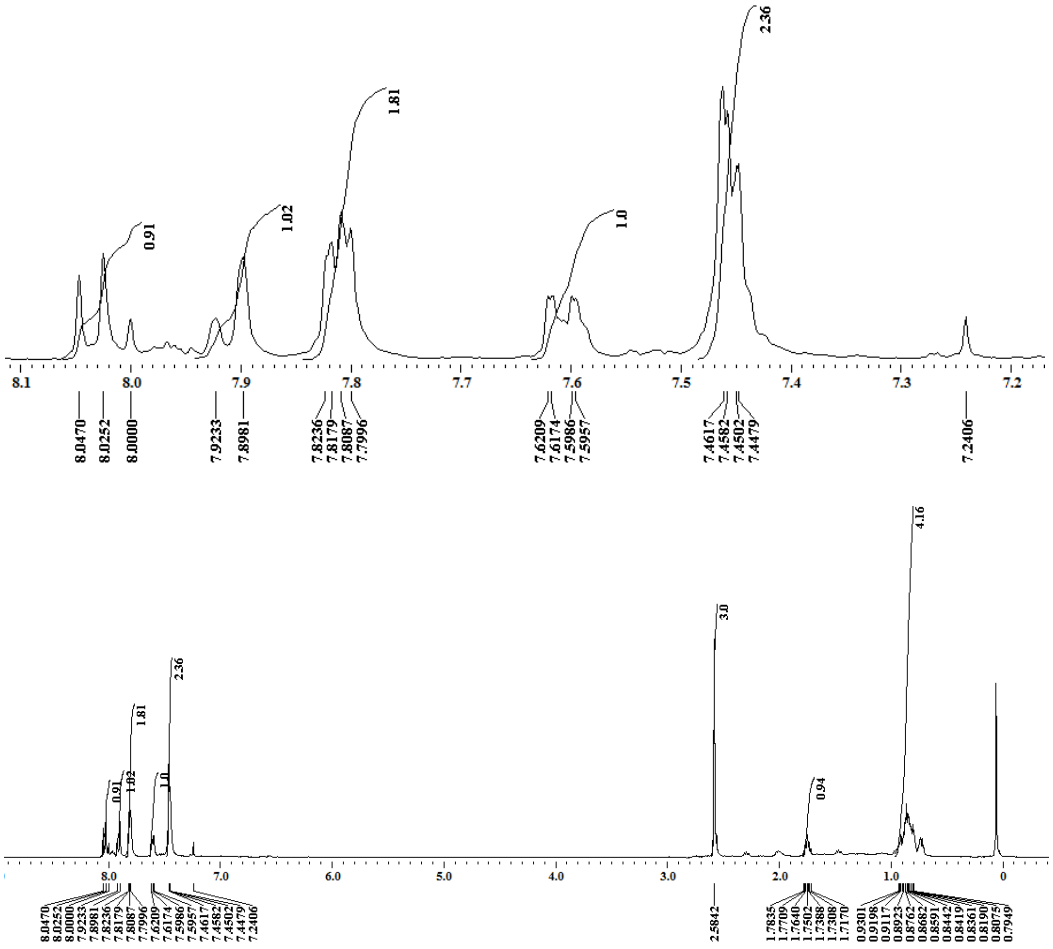
6-Iodo-9-methyl-5-(thiophen-3-yl)benzo[a]phenazine (7a)



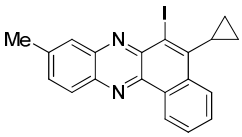
^{1}H NMR



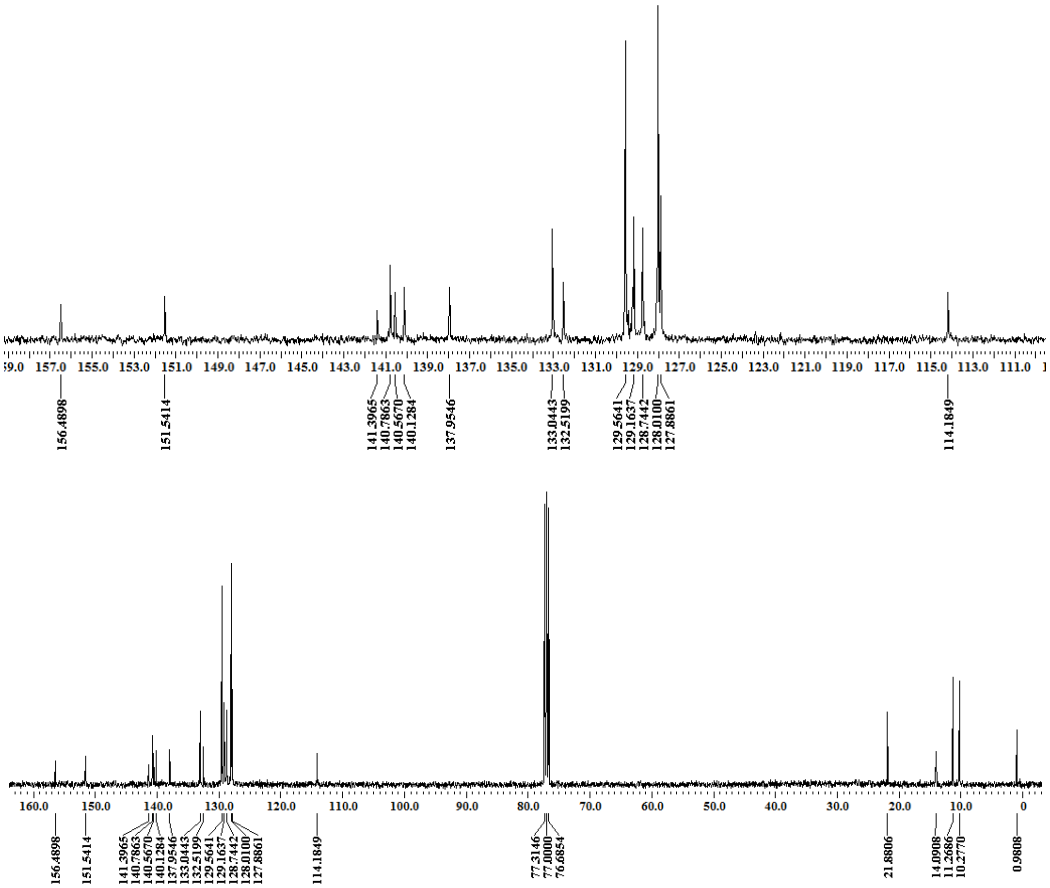
5-Cyclopropyl-6-iodo-9-methylbenzo[*a*]phenazine (7b)



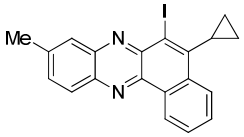
$^{13}C\{^{1}H\}$ NMR



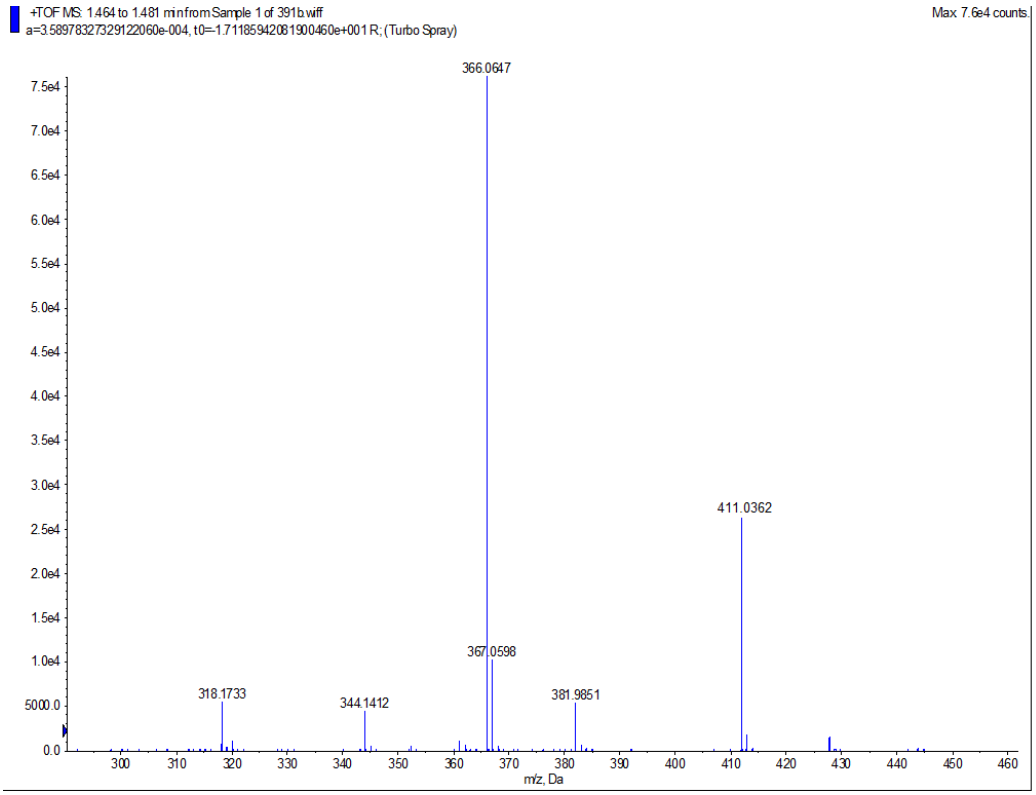
5-Cyclopropyl-6-iodo-9-methylbenzo[*a*]phenazine (7b)



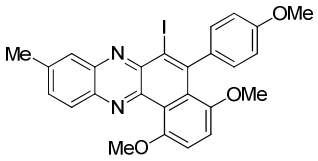
HRMS



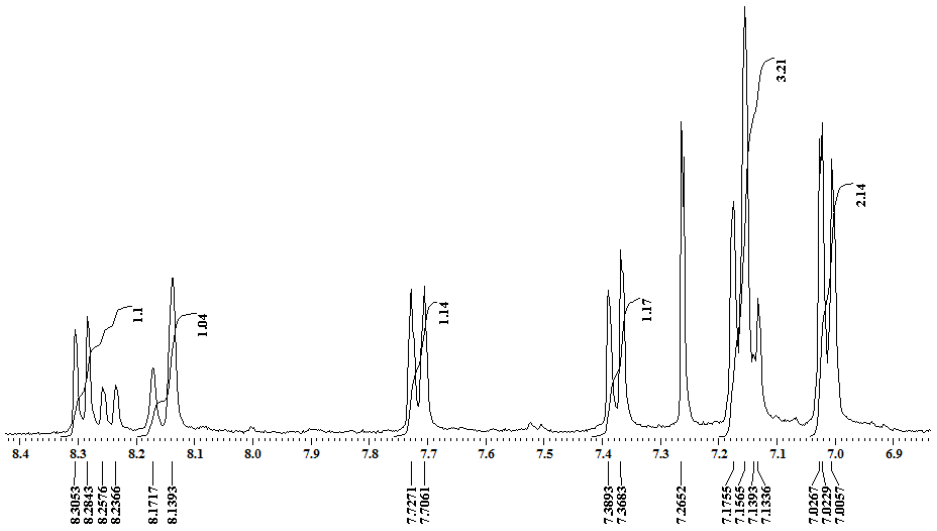
5-Cyclopropyl-6-iodo-9-methylbenzo[*a*]phenazine (7b)

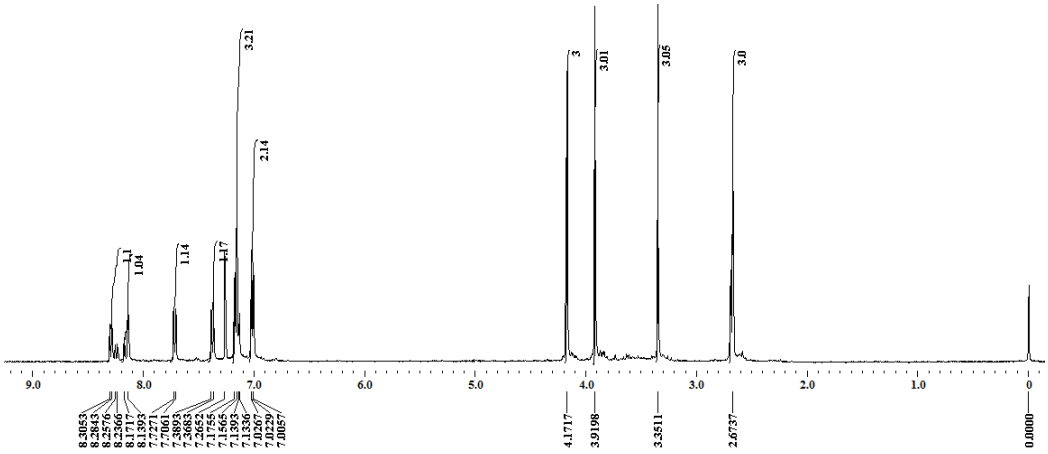


^{1}H NMR

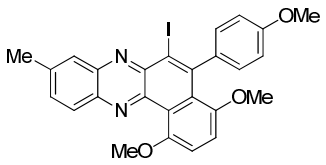


6-iodo-1,4-dimethoxy-5-(4-methoxyphenyl)-9-methylbenzo[*a*]phenazine (7c)

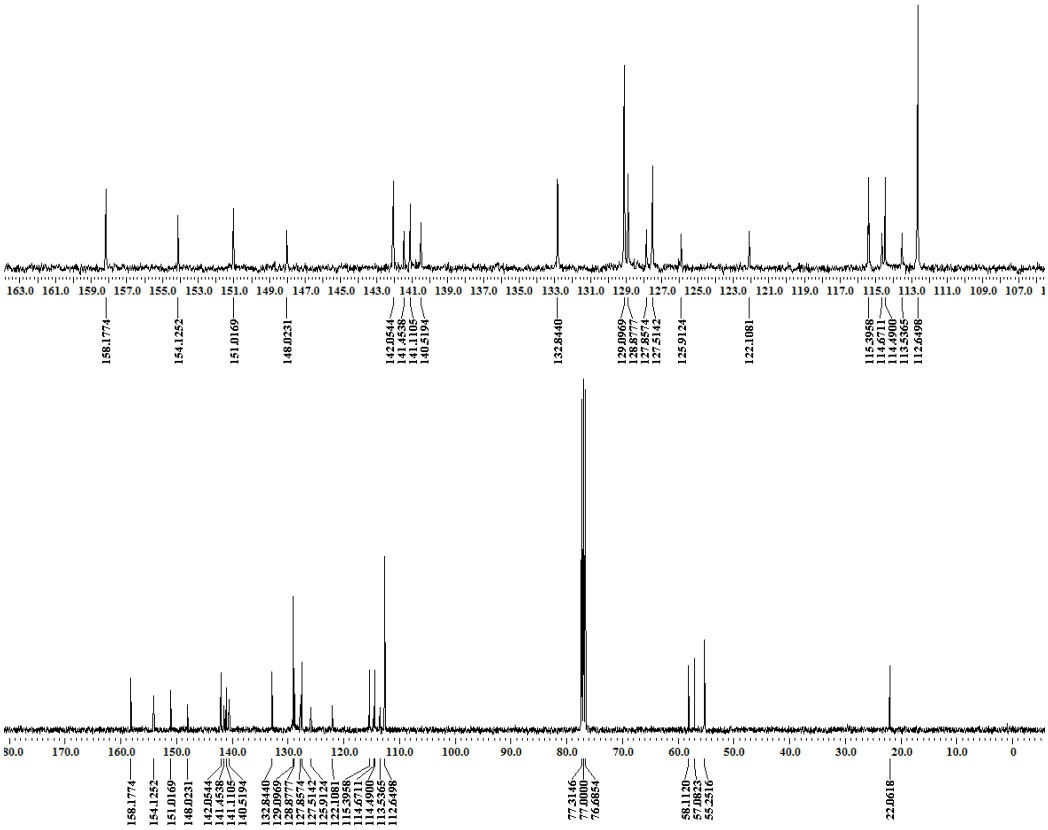




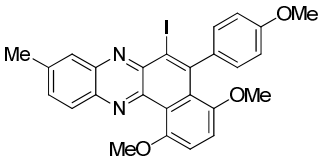
$^{13}C\{^{1}H\}$ NMR



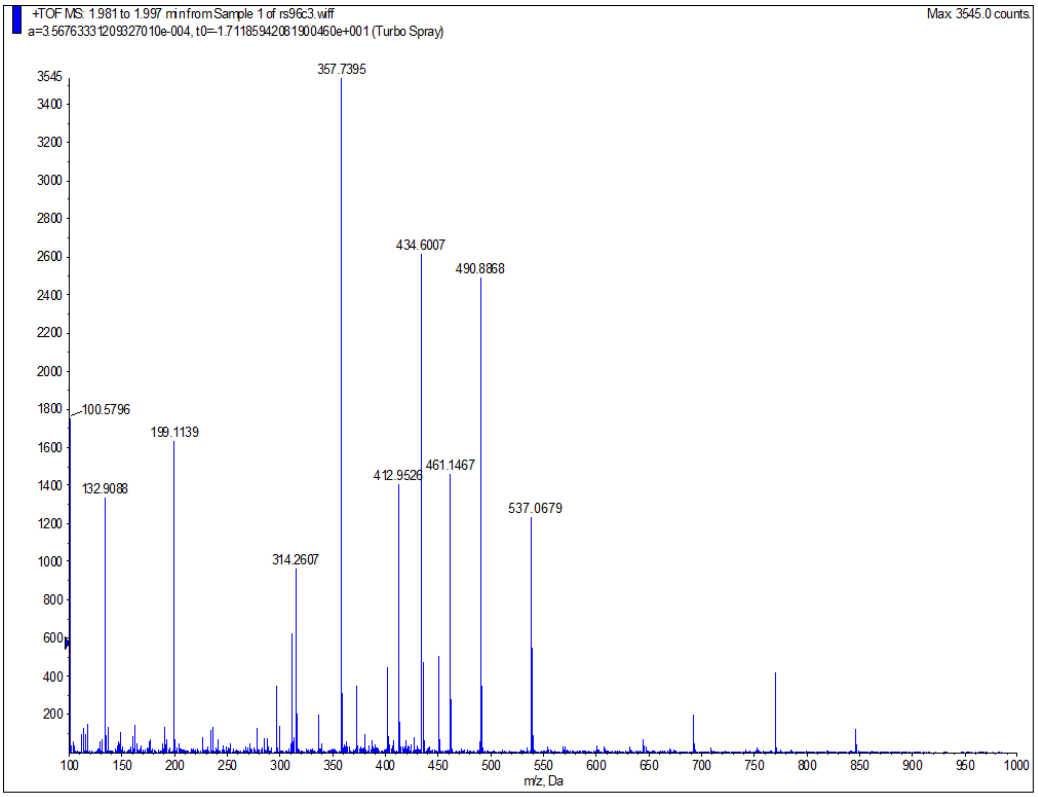
6-iodo-1,4-dimethoxy-5-(4-methoxyphenyl)-9-methylbenzo[a]phenazine (7c)



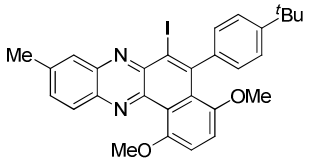
HRMS



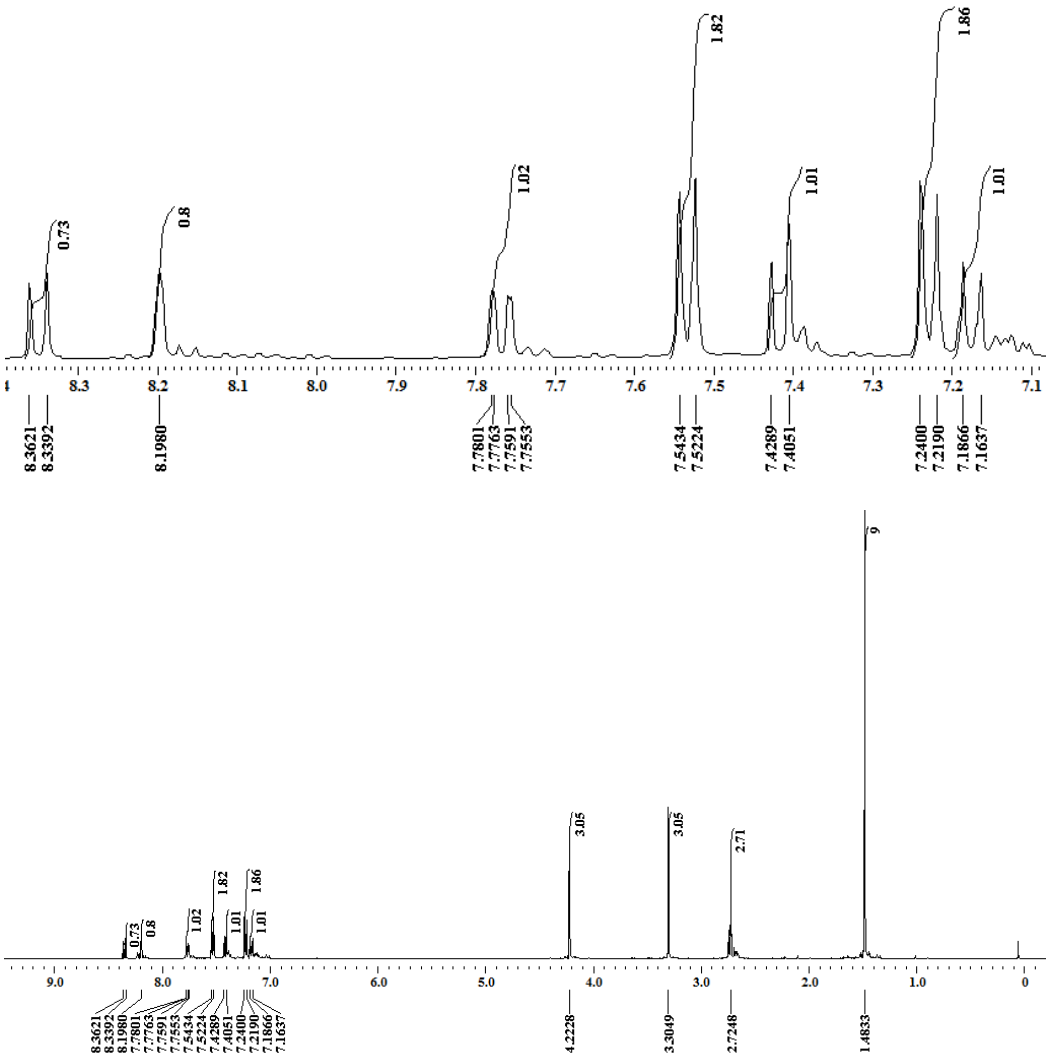
6-iodo-1,4-dimethoxy-5-(4-methoxyphenyl)-9-methylbenzo[a]phenazine (7c)



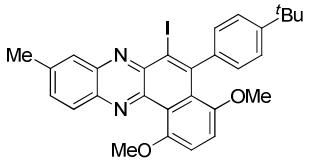
^{1}H NMR



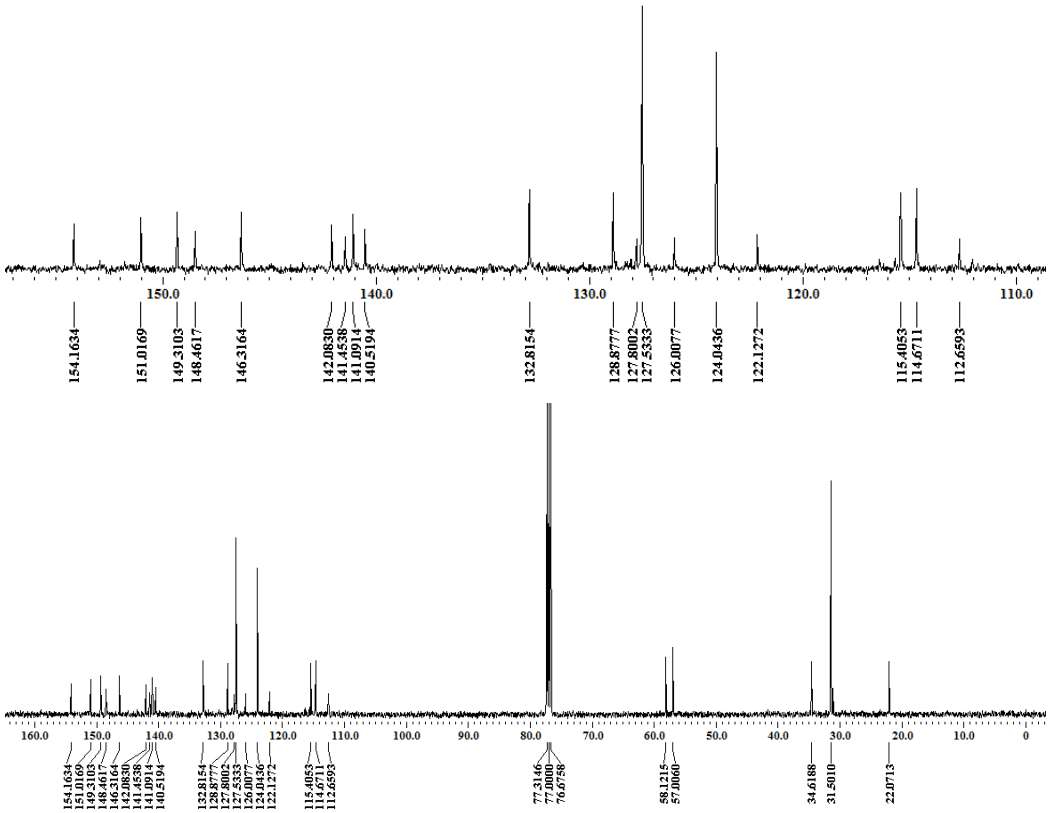
5-(4-(*tert*-Butyl)phenyl)-6-iodo-1,4-dimethoxy-9-methylbenzo[*a*]phenazine (7d)



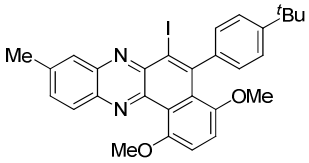
$^{13}C\{^{1}H\}$ NMR



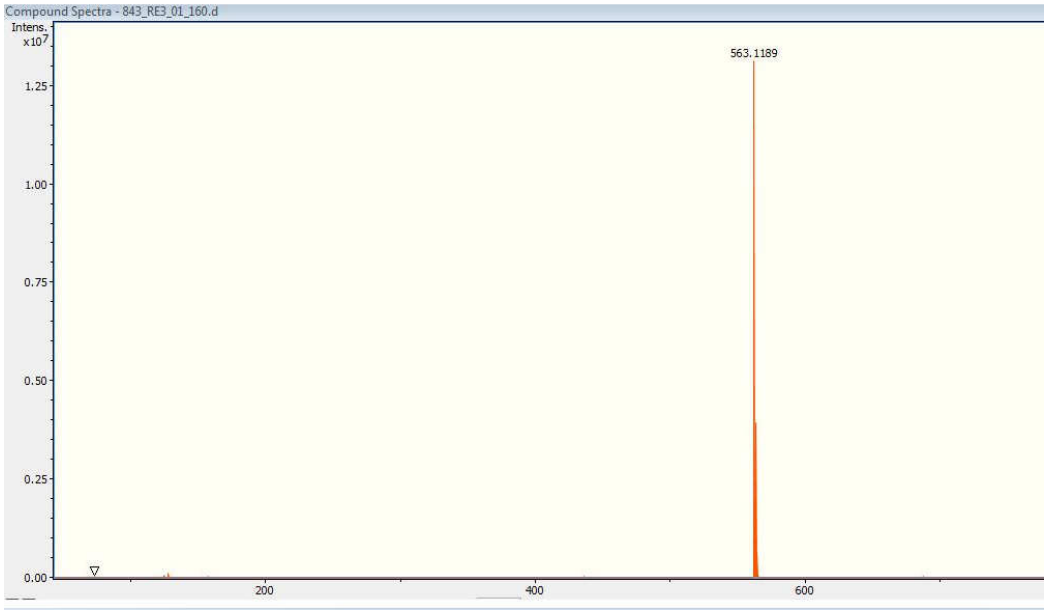
5-(4-(*tert*-Butyl)phenyl)-6-iodo-1,4-dimethoxy-9-methylbenzo[*a*]phenazine (7d)



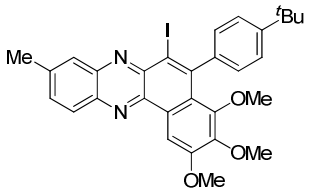
HRMS



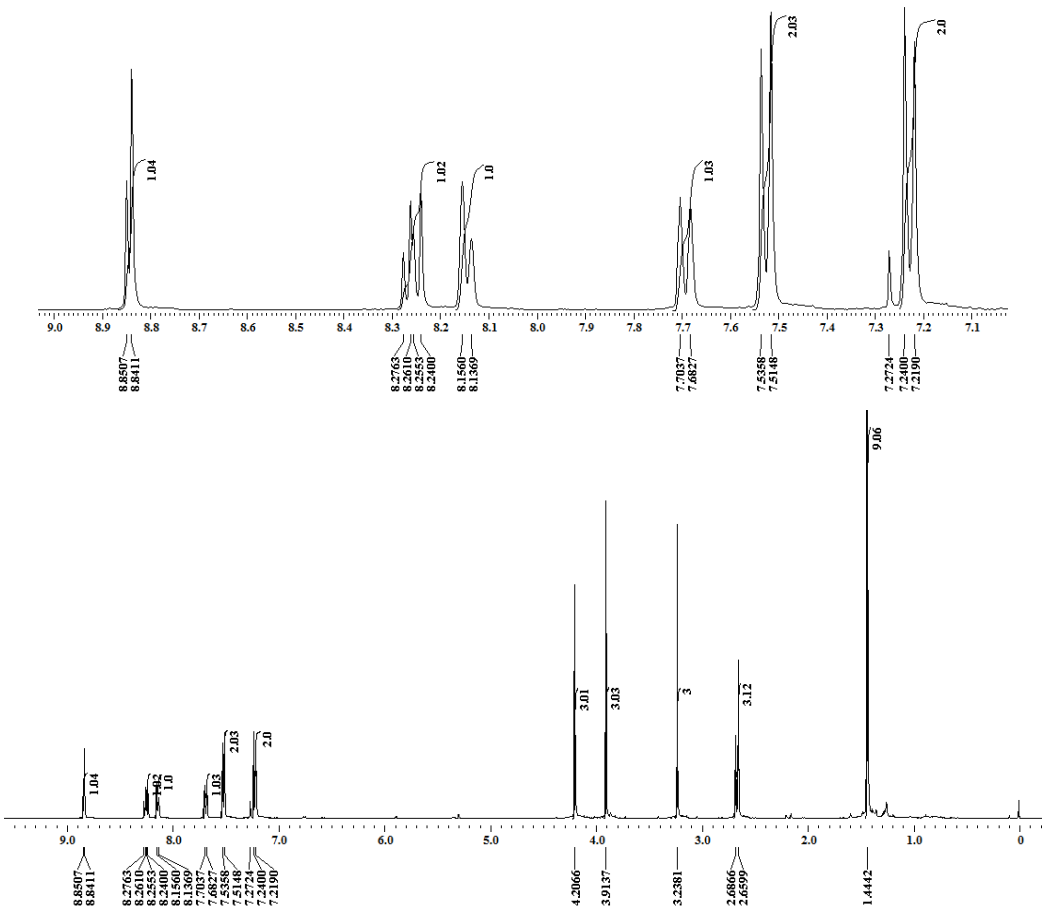
5-(4-(*tert*-Butyl)phenyl)-6-iodo-1,4-dimethoxy-9-methylbenzo[*a*]phenazine (7d)



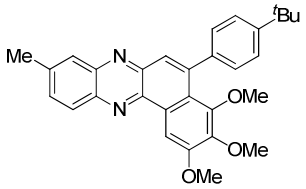
^{1}H NMR



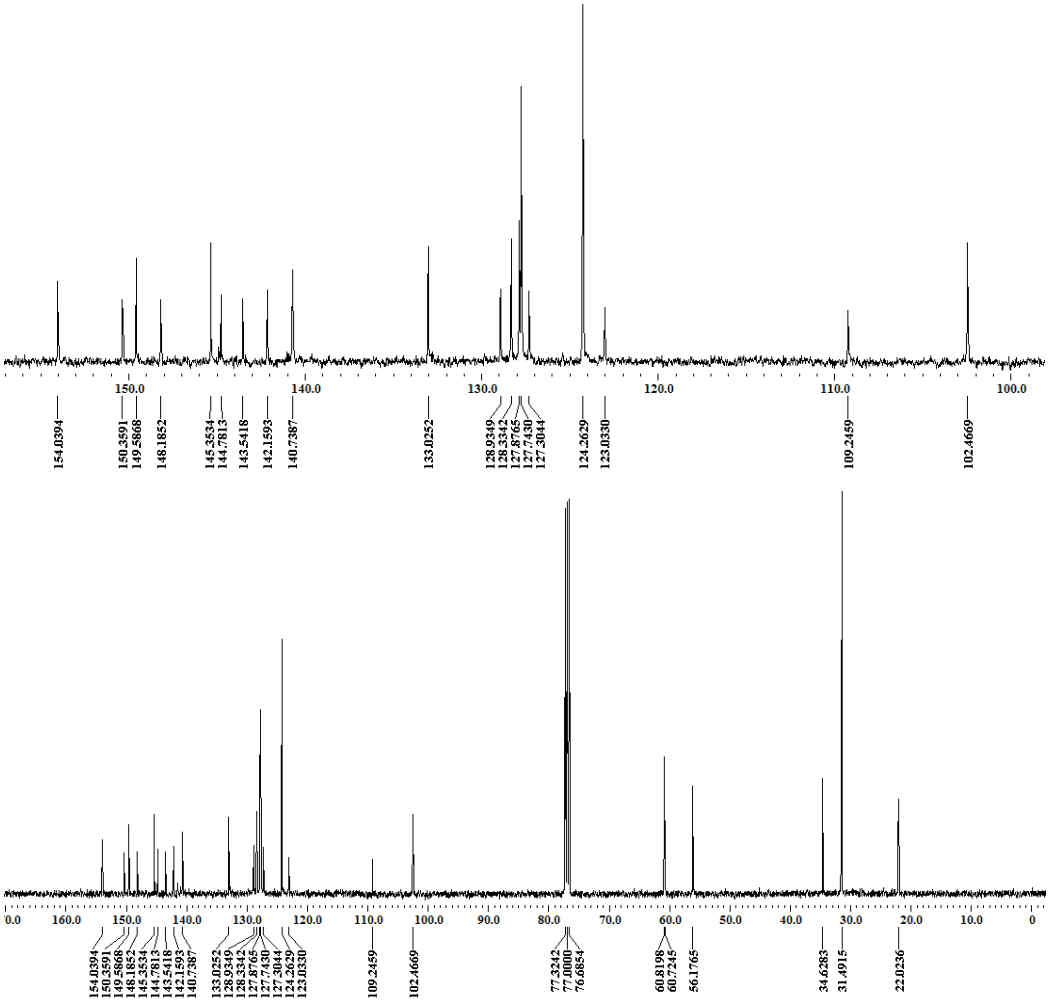
5-(4-(*tert*-Butyl)phenyl)-6-iodo-2,3,4-trimethoxy-9-methylbenzo[*a*]phenazine (7e)



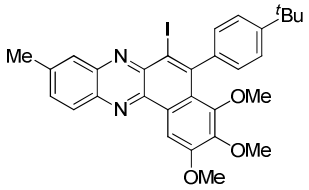
$^{13}C\{^{1}H\}$ NMR



5-(4-(*tert*-Butyl)phenyl)-6-iodo-2,3,4-trimethoxy-9-methylbenzo[*a*]phenazine (7e)



HRMS



5-(4-(*tert*-Butyl)phenyl)-6-iodo-2,3,4-trimethoxy-9-methylbenzo[*a*]phenazine (7e)

Qualitative Compound Report

Data File	SON-845.d	**Sample Name**	SON-845
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	02-11-2016 13:33:02
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

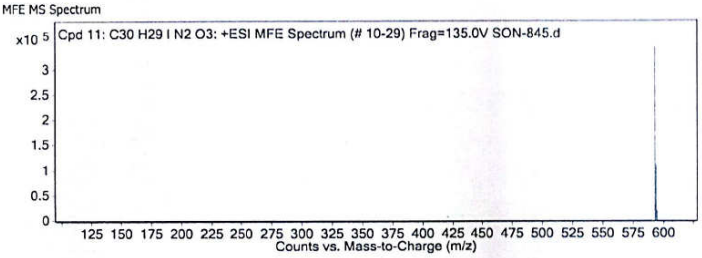
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

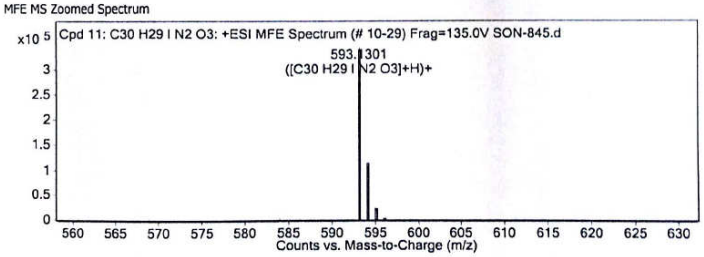
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C30 H29 I N2 O3	15	592.1227	C30 H29 I N2 O3	C30 H29 I N2 O3	-0.68	C30 H29 I N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C30 H29 I N2 O3	593.1301	15	Find by Molecular Feature	592.1227

MFE MS Spectrum



MFE MS Zoomed Spectrum

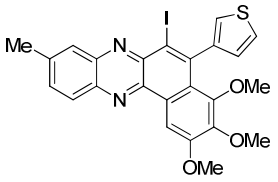


MS Spectrum Peak List

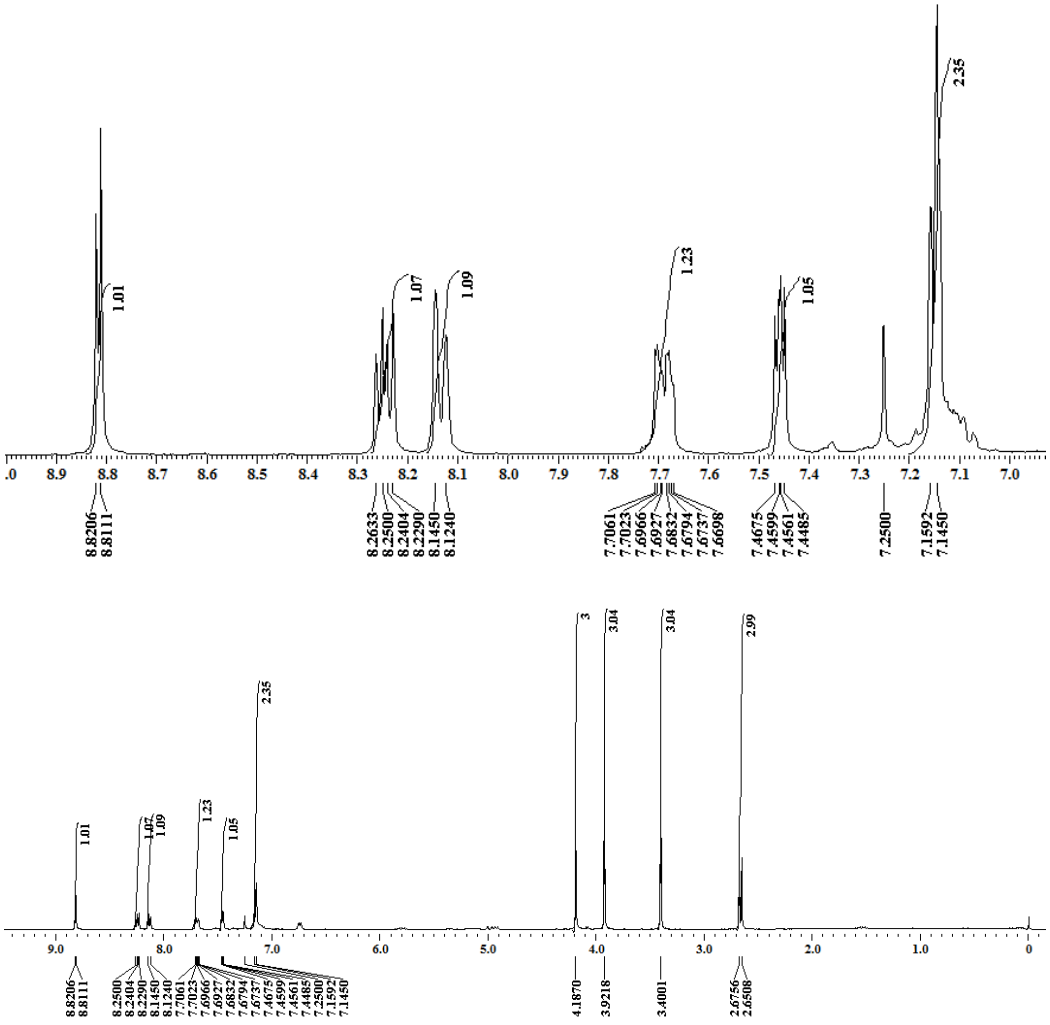
m/z	z	Abund	Formula	Ion
593.1301	1	344171.44	C30 H29 I N2 O3	(M+H)+
594.133	1	110022.57	C30 H29 I N2 O3	(M+H)+
595.1355	1	19191.32	C30 H29 I N2 O3	(M+H)+
596.1398	1	2618.55	C30 H29 I N2 O3	(M+H)+
597.1407	1	266.96	C30 H29 I N2 O3	(M+H)+

--- End Of Report ---

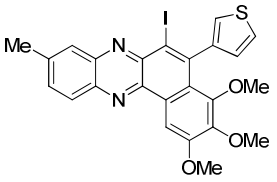
^{1}H NMR



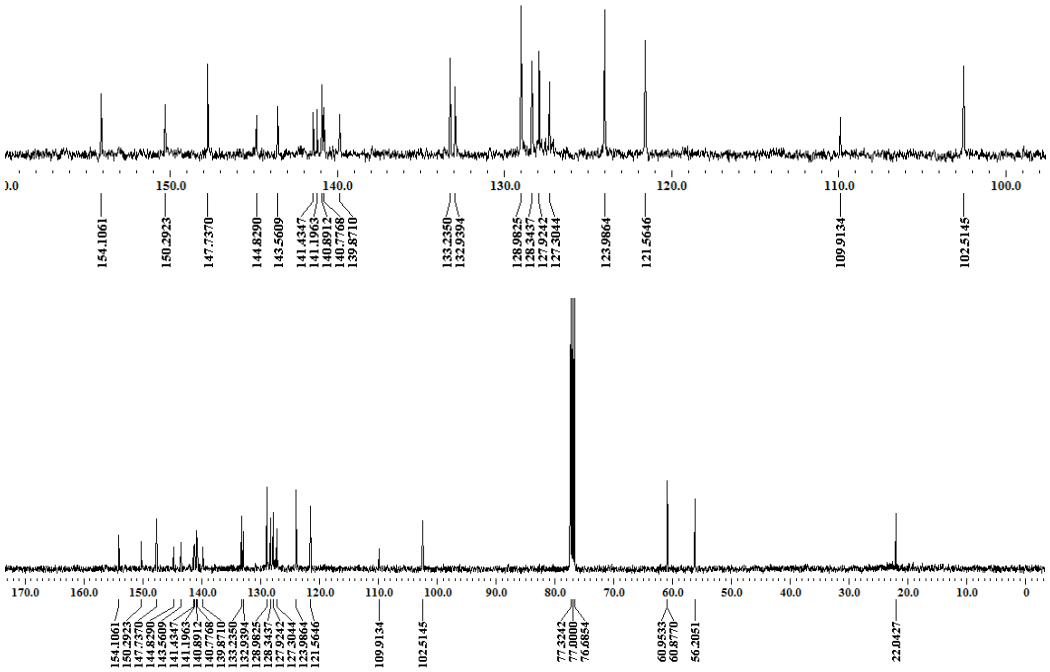
6-Iodo-2,3,4-trimethoxy-9-methyl-5-(thiophen-3-yl)benzo[a]phenazine (7f)



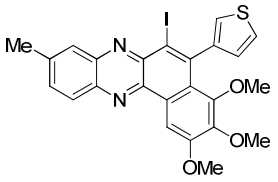
$^{13}C\{^{1}H\}$ NMR



6-Iodo-2,3,4-trimethoxy-9-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (7f)



HRMS



6-Iodo-2,3,4-trimethoxy-9-methyl-5-(thiophen-3-yl)benzo[*a*]phenazine (7f)

Qualitative Compound Report

Data File	SON-841.d	Sample Name	SON-841
Sample Type	Sample	Position	P1-E6
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	02-11-2016 14:09:46
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Info.

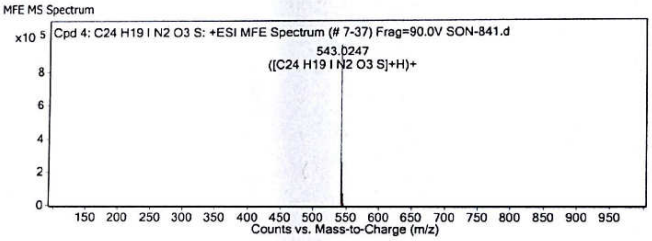
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

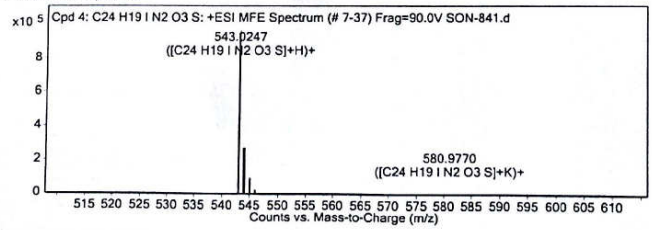
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C24 H19 I N2 O3 S	11	542.0173	C24 H19 I N2 O3 S	C24 H19 I N2 O3 S	-2.19	C24 H19 I N2 O3 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C24 H19 I N2 O3 S	543.0247	11	Find by Molecular Feature	542.0173

MFE MS Spectrum



MFE MS Zoomed Spectrum

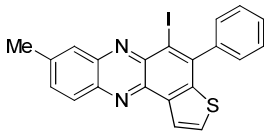


MS Spectrum Peak List

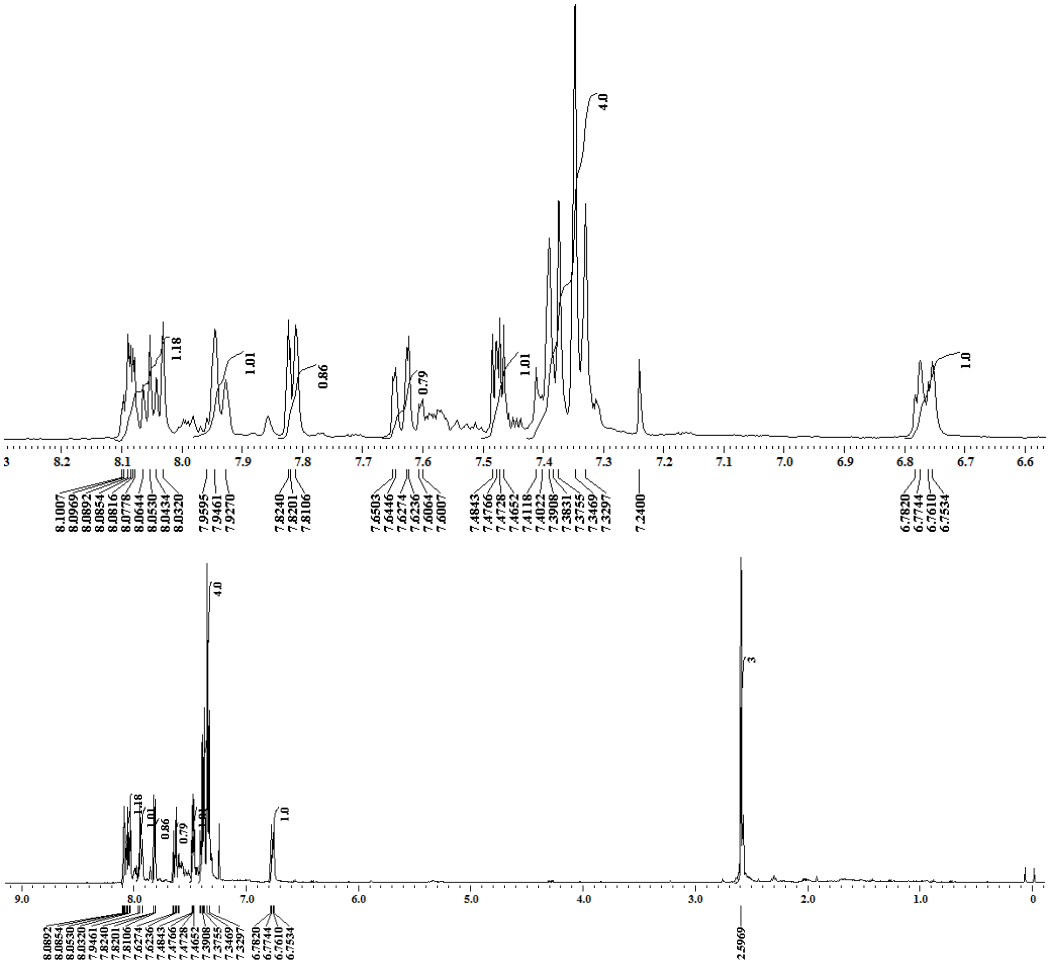
m/z	z	Abund	Formula	Ion
543.0247	1	964477.56	C24 H19 I N2 O3 S	(M+H)+
544.0274	1	257485.45	C24 H19 I N2 O3 S	(M+H)+
545.025	1	73423.08	C24 H19 I N2 O3 S	(M+H)+
546.0257	1	13653.27	C24 H19 I N2 O3 S	(M+H)+
547.0269	1	1971.22	C24 H19 I N2 O3 S	(M+H)+
548.023	1	208.47	C24 H19 I N2 O3 S	(M+H)+
580.977	1	316.52	C24 H19 I N2 O3 S	(M+K)+

--- End Of Report ---

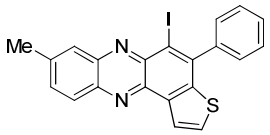
^{1}H NMR



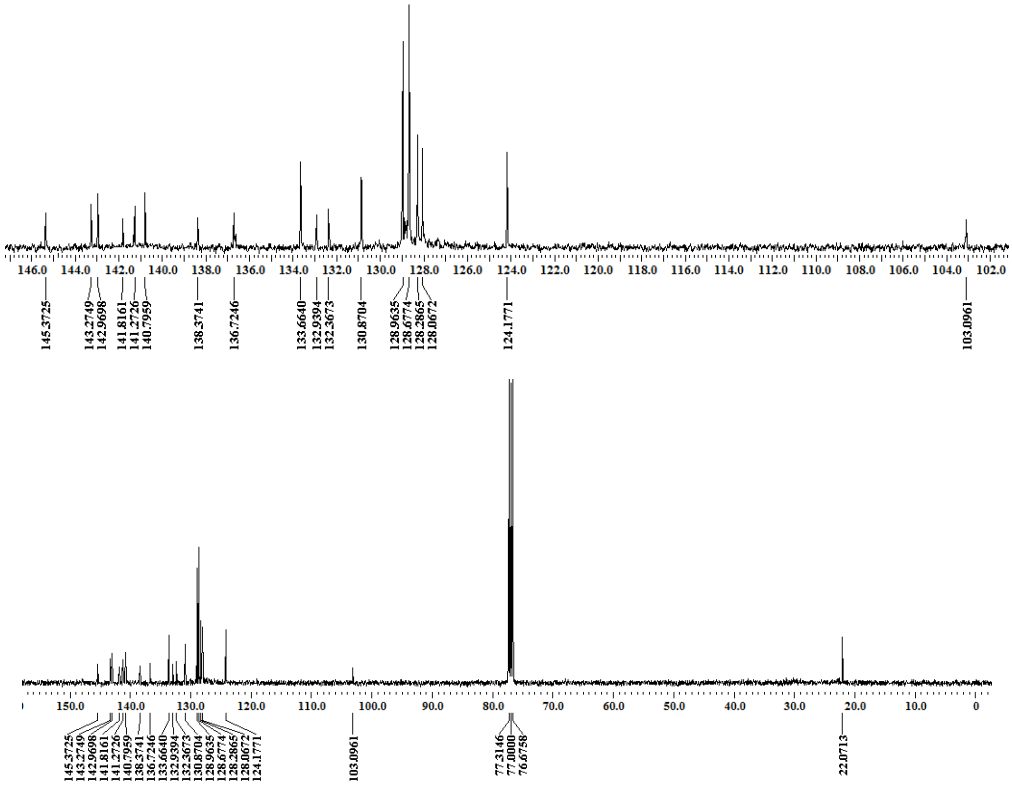
5-Iodo-8-methyl-4-phenylthieno[3,2-*a*]phenazine (7g)



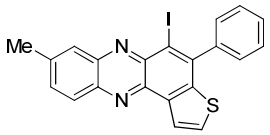
$^{13}C\{^{1}H\}$ NMR



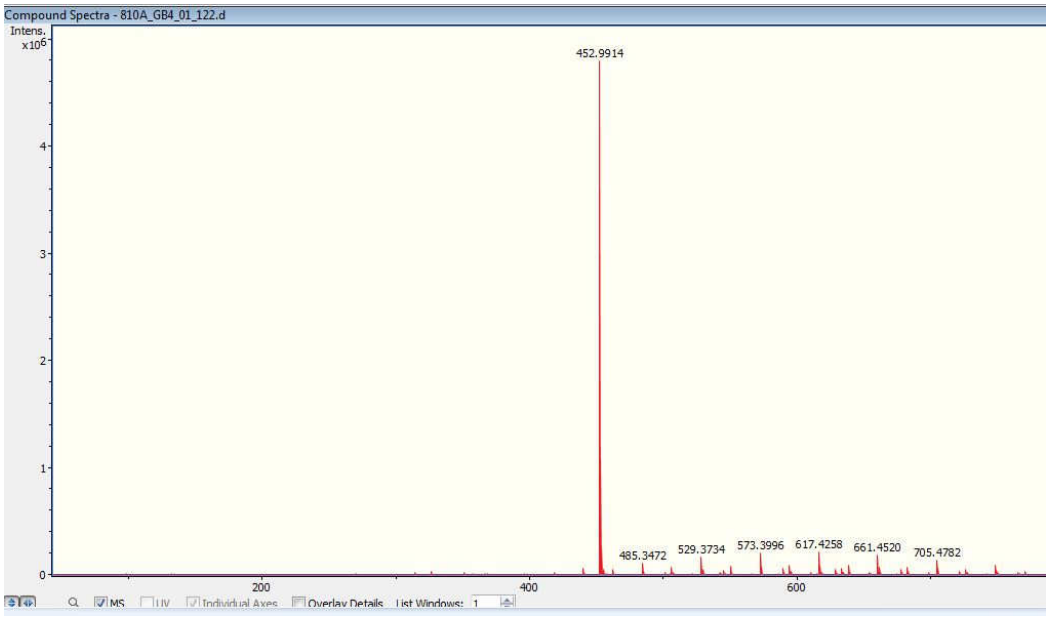
5-Iodo-8-methyl-4-phenylthieno[3,2-*a*]phenazine (7g)



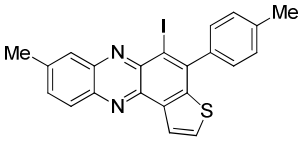
HRMS



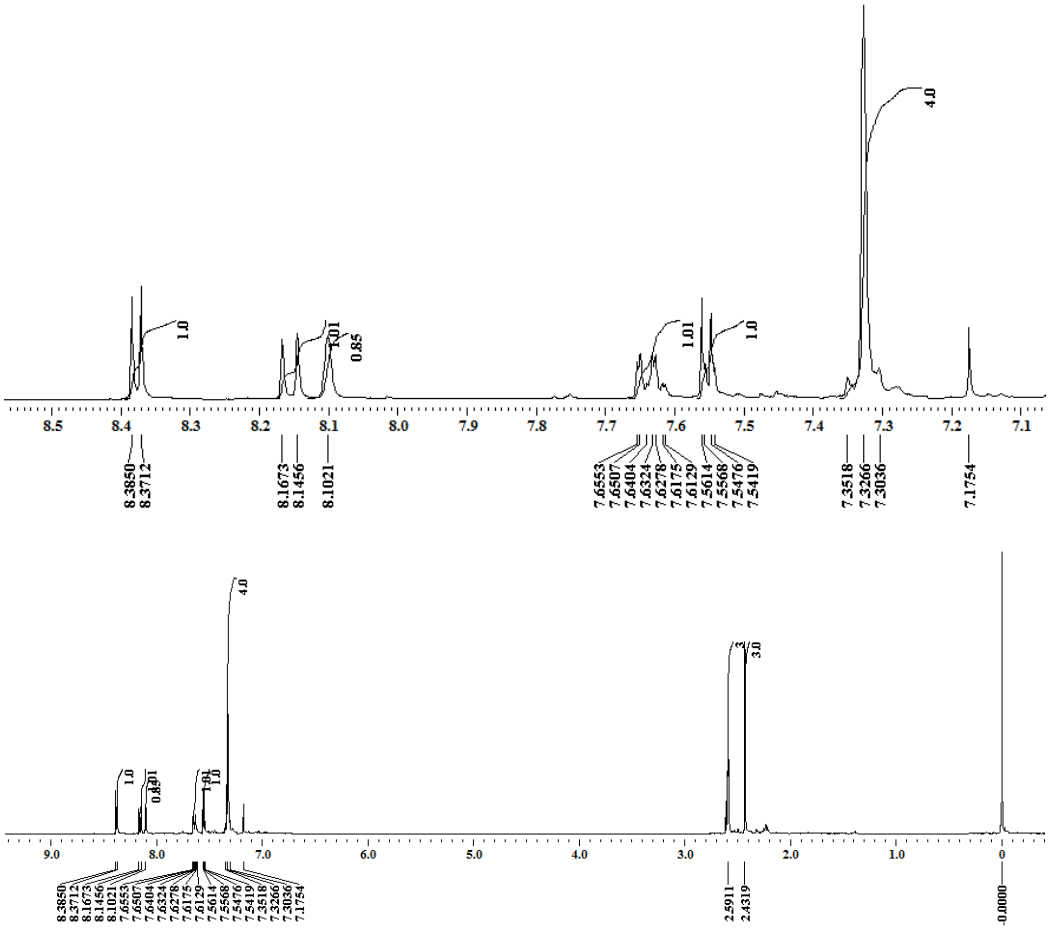
5-Iodo-8-methyl-4-phenylthieno[3,2-*a*]phenazine (7g)



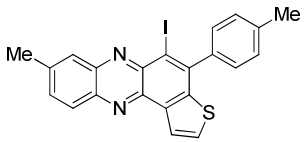
^{1}H NMR



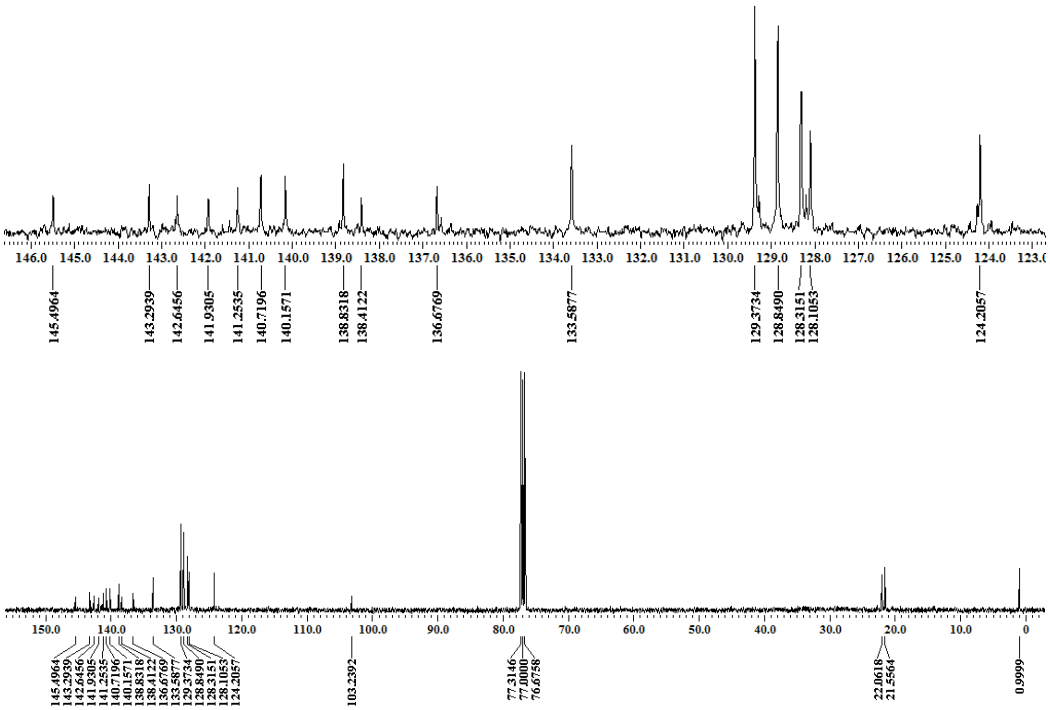
5-Iodo-8-methyl-4-(*p*-tolyl)thieno[3,2-*a*]phenazine (7h)



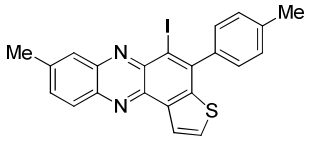
$^{13}C\{^{1}H\}$ NMR



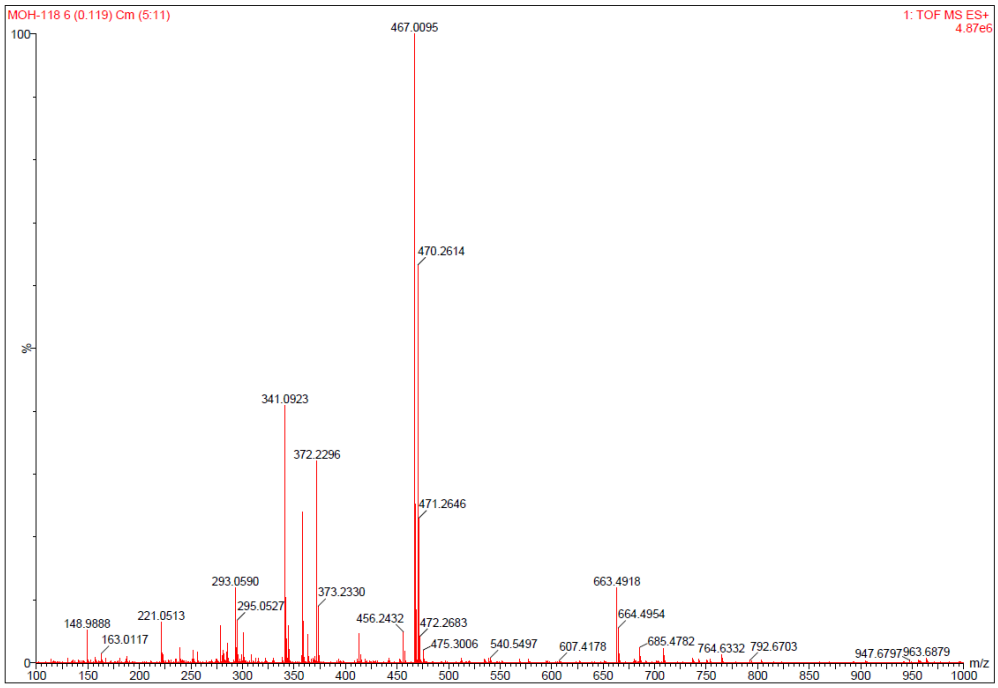
5-Iodo-8-methyl-4-(*p*-tolyl)thieno[3,2-*a*]phenazine (7h)



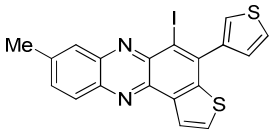
HRMS



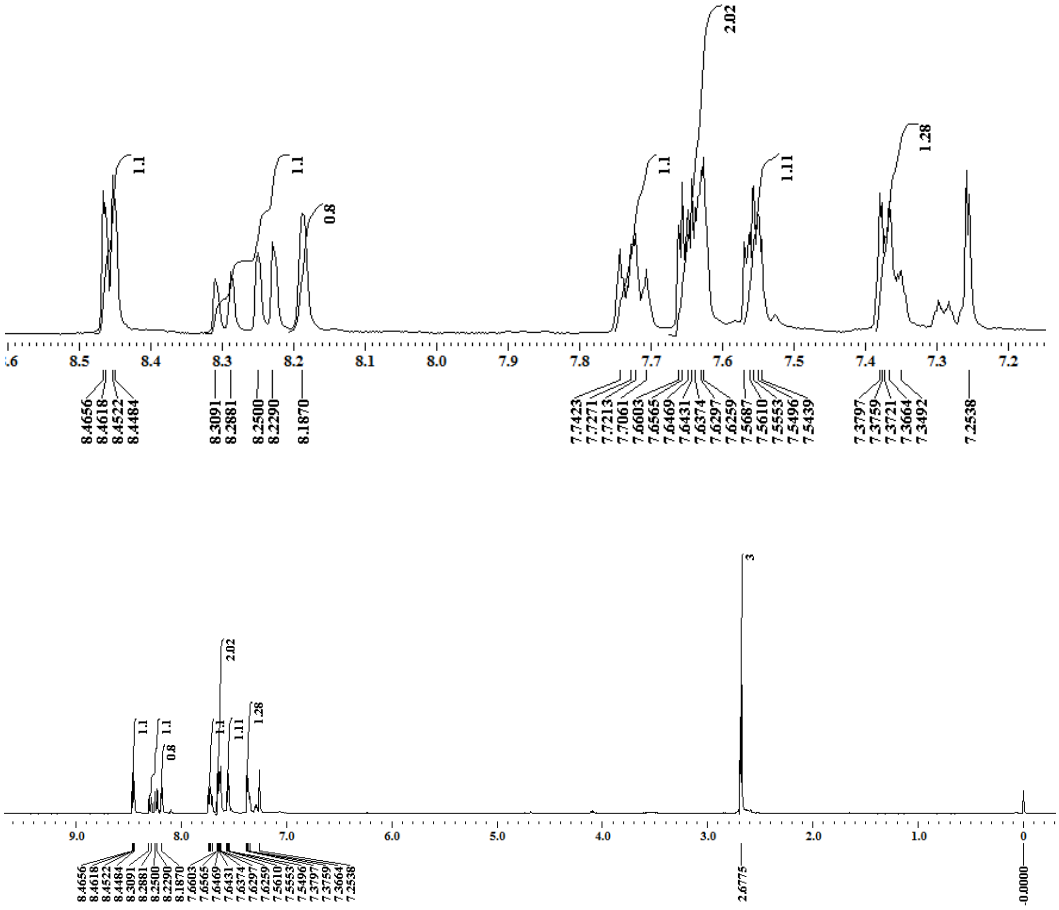
5-Iodo-8-methyl-4-(*p*-tolyl)thieno[3,2-*a*]phenazine (7h)



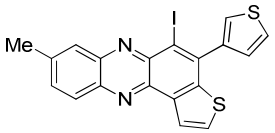
^{1}H NMR



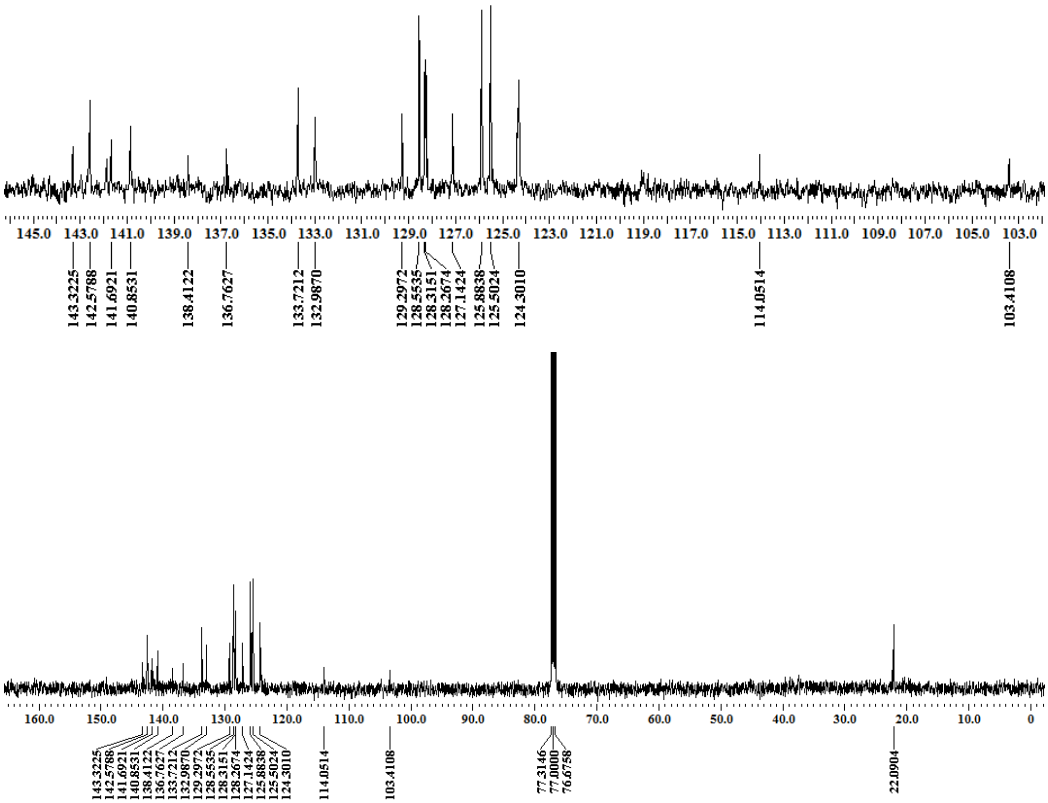
5-Iodo-8-methyl-4-(thiophen-3-yl)thieno[3,2-*a*]phenazine (7i)



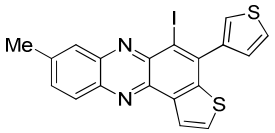
$^{13}C\{^{1}H\}$ NMR



5-Iodo-8-methyl-4-(thiophen-3-yl)thieno[3,2-*a*]phenazine (7i)



HRMS



5-Iodo-8-methyl-4-(thiophen-3-yl)thieno[3,2-*a*]phenazine (7i)

Qualitative Compound Report

Data File	SON-846.d	**Sample Name**	SON-846
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	03-11-2016 12:26:35
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

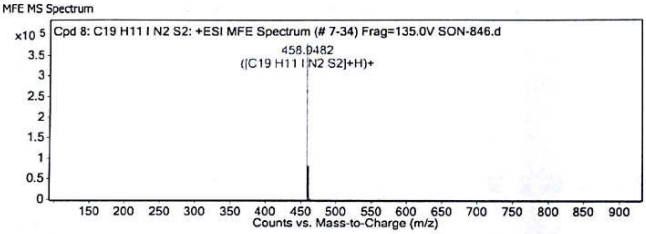
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

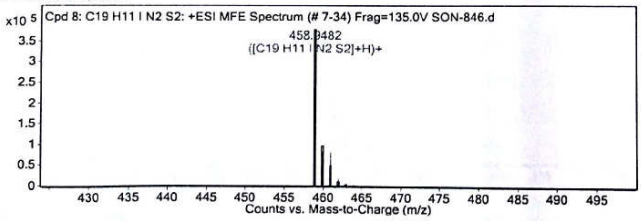
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C19 H11 I N2 S2	11	457.943	C19 H11 I N2 S2	C19 H11 I N2 S2	-4.84	C19 H11 I N2 S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C19 H11 I N2 S2	458.9482	11	Find by Molecular Feature	457.943

MFE MS Spectrum



MFE MS Zoomed Spectrum

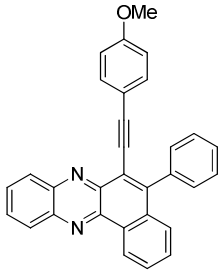


MS Spectrum Peak List

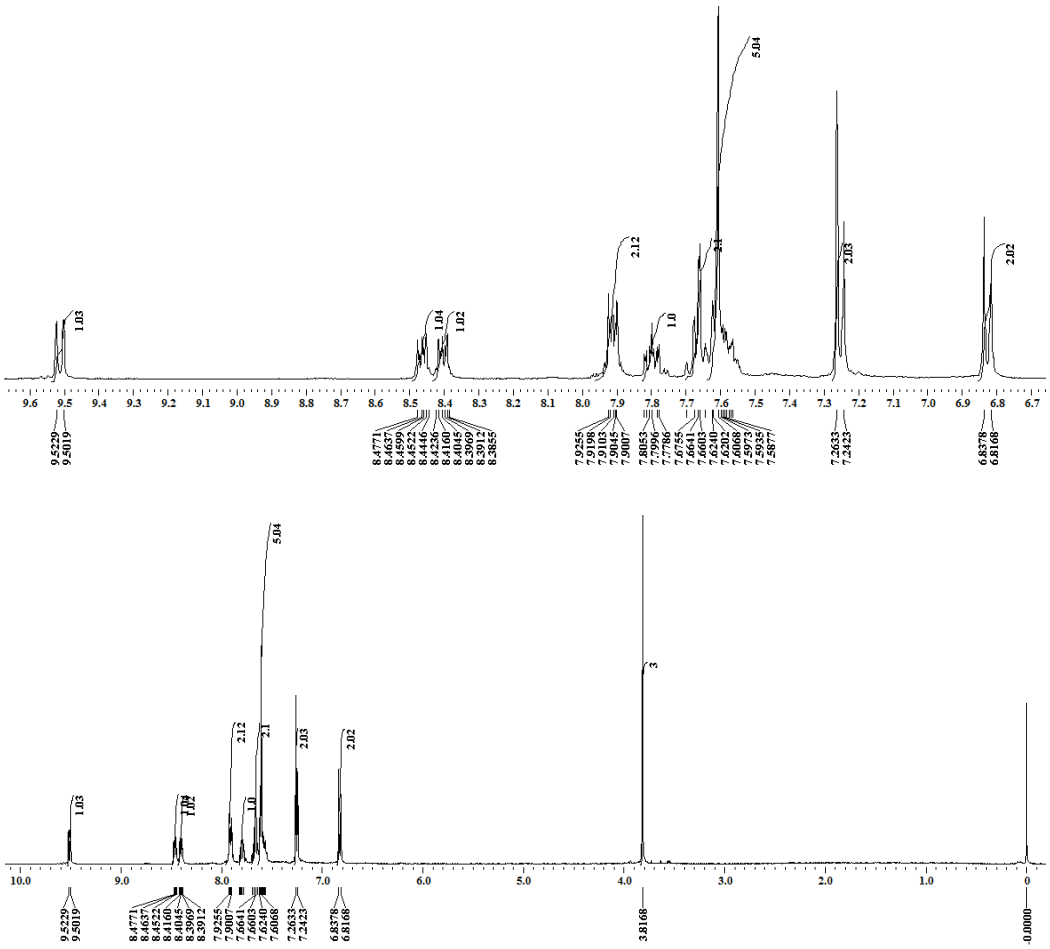
m/z	z	Abund	Formula	Ion
458.9482	1	378854.38	C19 H11 I N2 S2	(M+H)+
459.9508	1	82025.02	C19 H11 I N2 S2	(M+H)+
460.9574	1	81069.12	C19 H11 I N2 S2	(M+H)+
461.961	1	16956.36	C19 H11 I N2 S2	(M+H)+
462.9585	1	6599.04	C19 H11 I N2 S2	(M+H)+
463.9646	1	1302.4	C19 H11 I N2 S2	(M+H)+
464.956	1	201.26	C19 H11 I N2 S2	(M+H)+

--- End Of Report ---

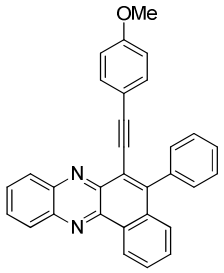
^{1}HNMR



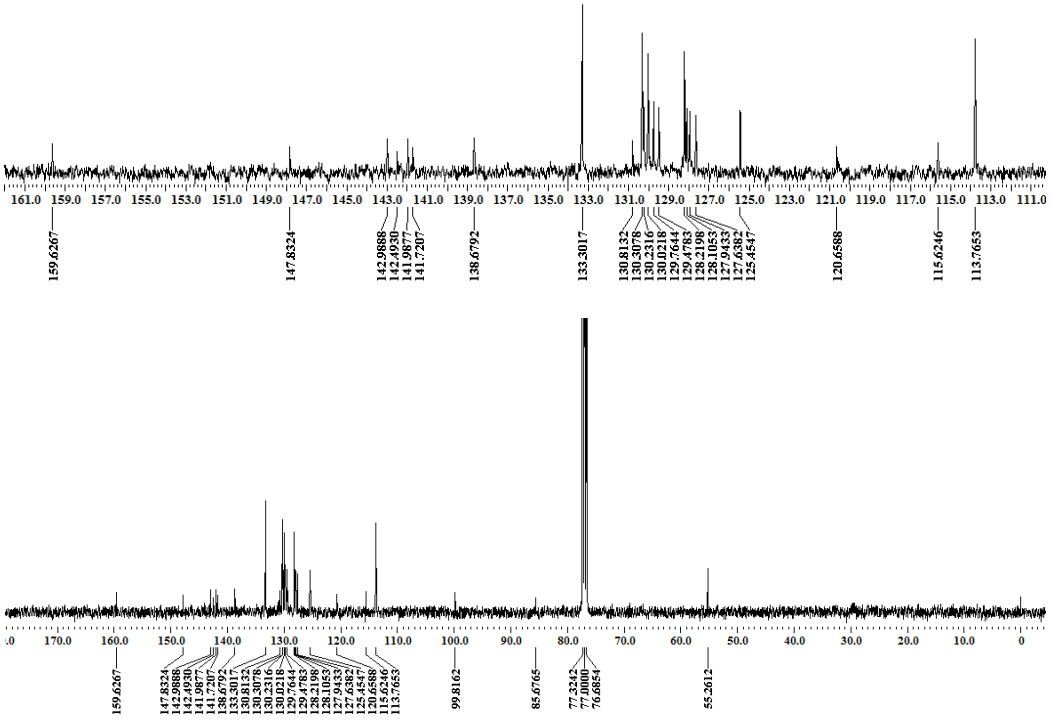
6-((4-Methoxyphenyl)ethynyl)-5-phenylbenzo[*a*]phenazine (10)



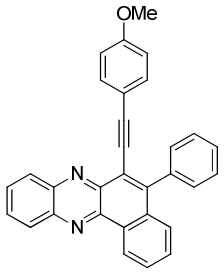
$^{13}C\{^{1}H\}$ NMR



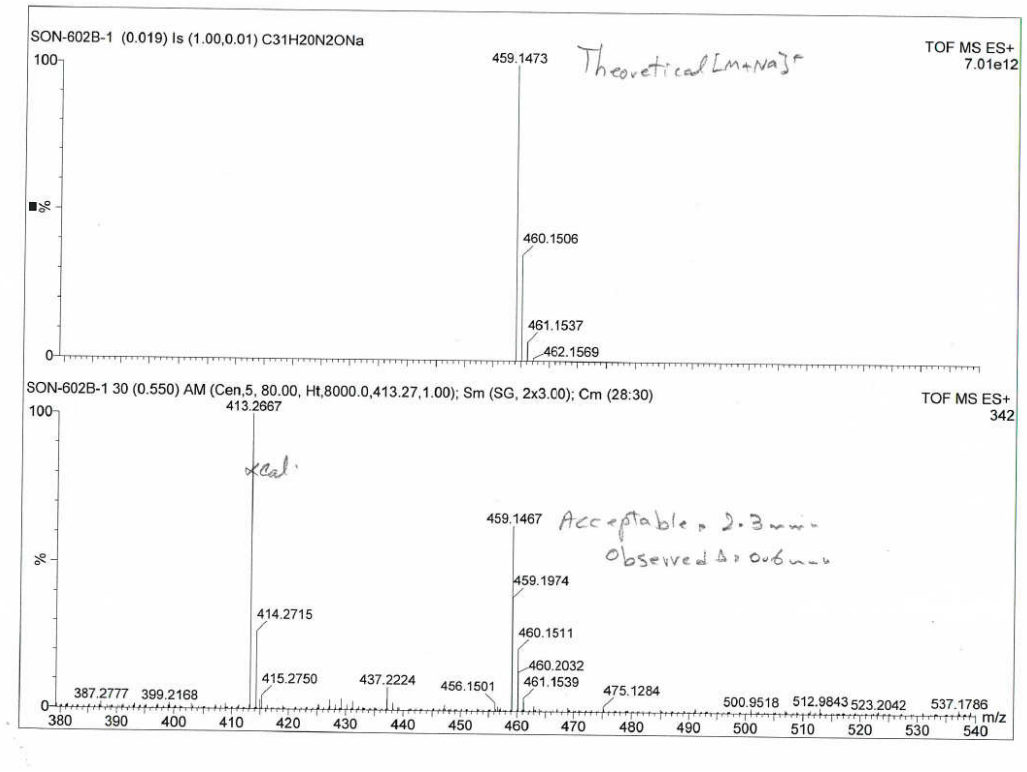
6-((4-Methoxyphenyl)ethynyl)-5-phenylbenzo[*a*]phenazine (10)



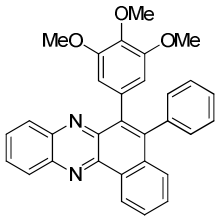
HRMS



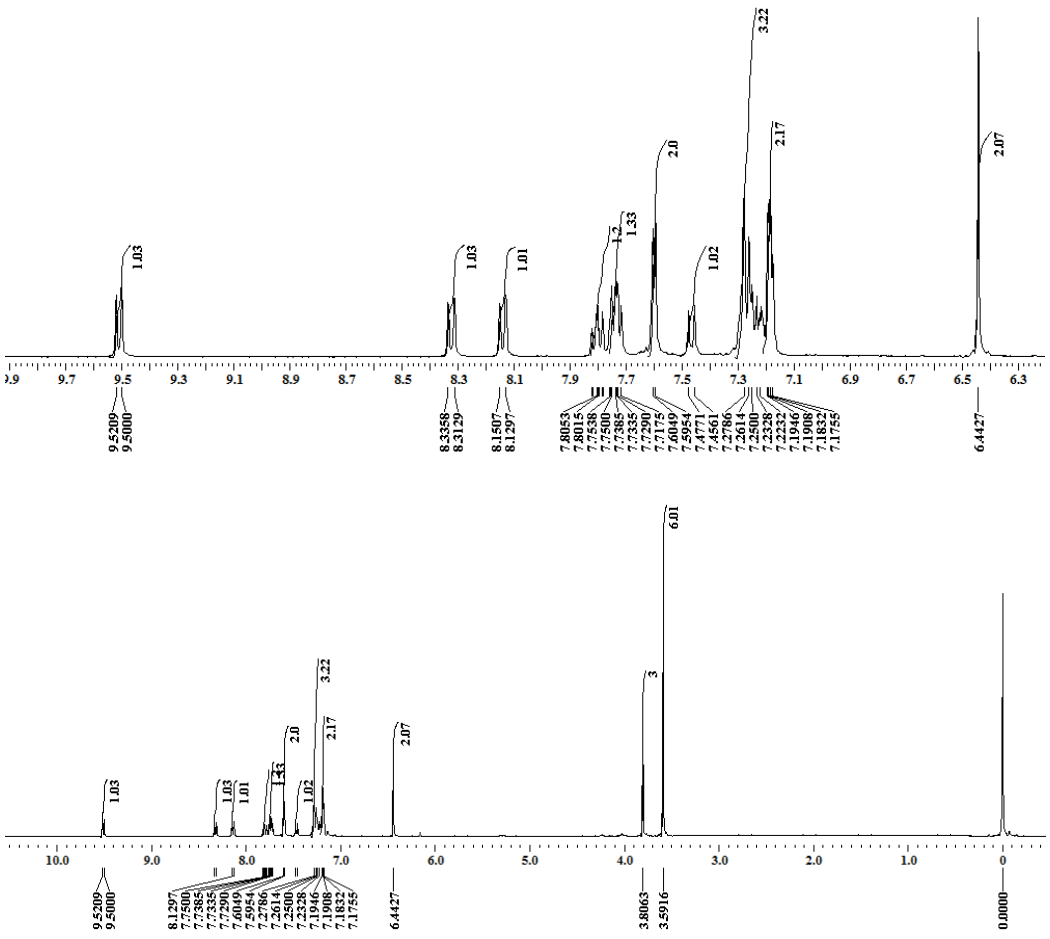
6-((4-Methoxyphenyl)ethynyl)-5-phenylbenzo[*a*]phenazine (10)



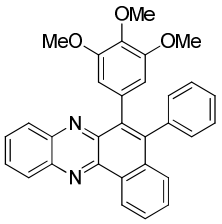
^{1}H NMR



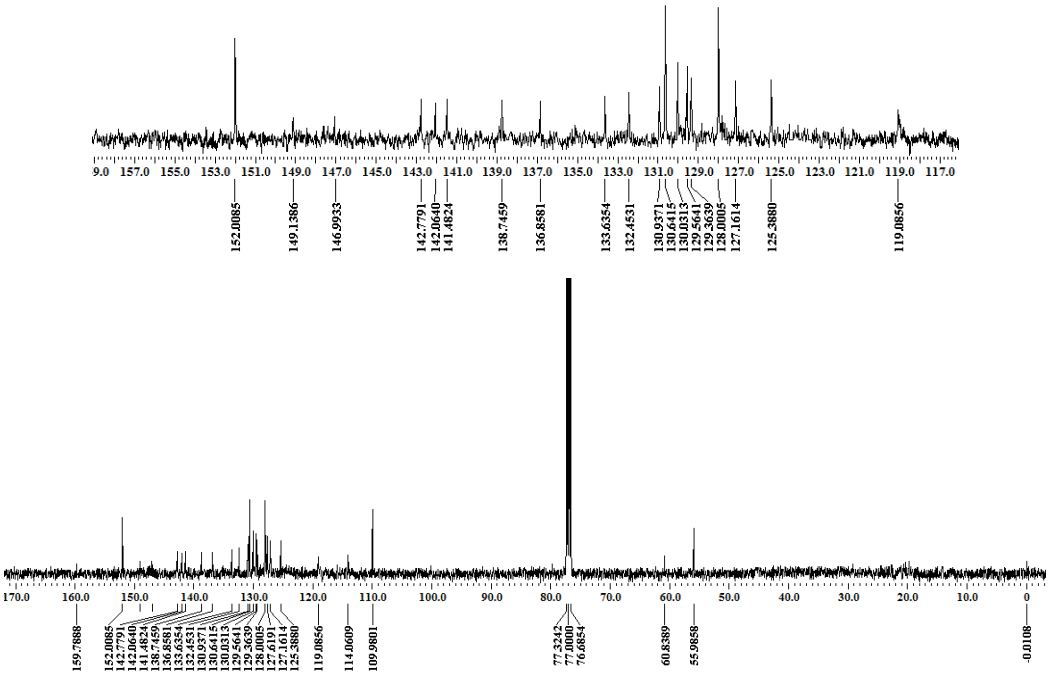
5-Phenyl-6-(3,4,5-trimethoxyphenyl)benzo[*a*]phenazine (11)



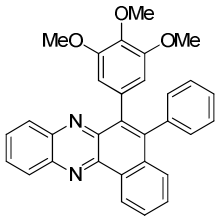
$^{13}C\{^{1}H\}$ NMR



5-Phenyl-6-(3,4,5-trimethoxyphenyl)benzo[*a*]phenazine (11)



HRMS



5-Phenyl-6-(3,4,5-trimethoxyphenyl)benzo[*a*]phenazine (11)