Supporting information

Iron catalyzed cross coupling of electron-deficient heterocycles and quinone with organoboron species *via* innate C-H functionalization: Application in total synthesis of pyrazine alkaloid Botryllazine A

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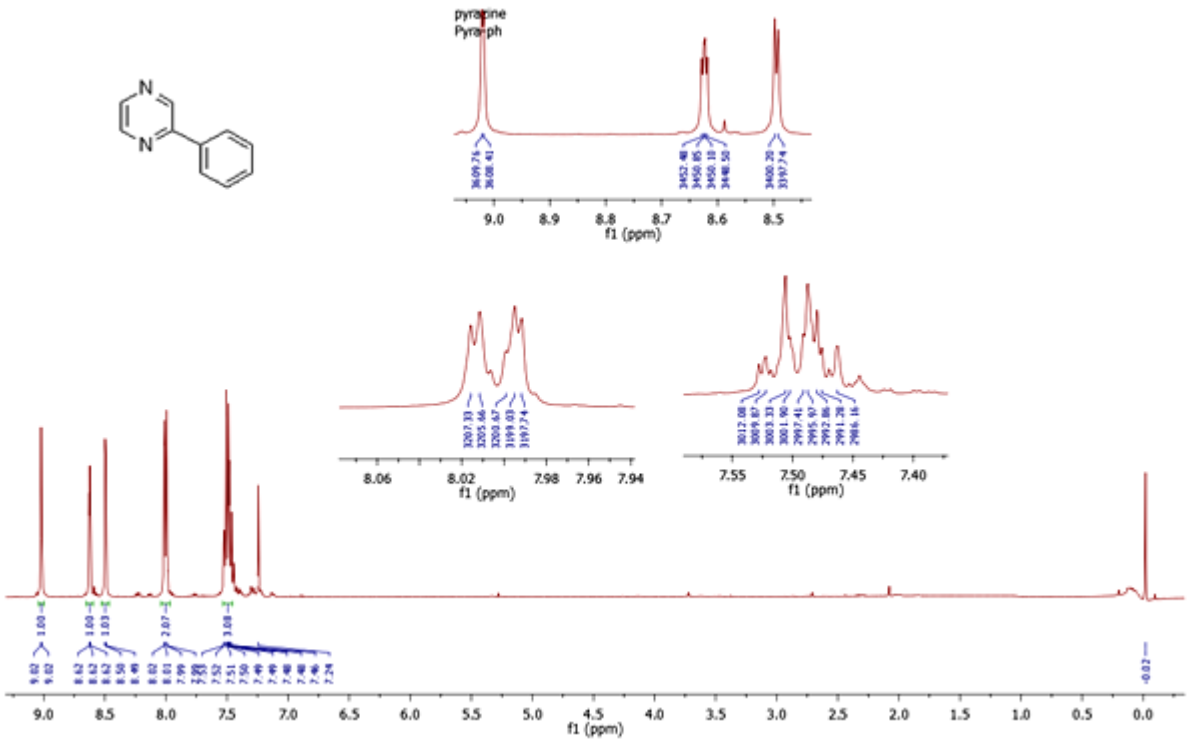
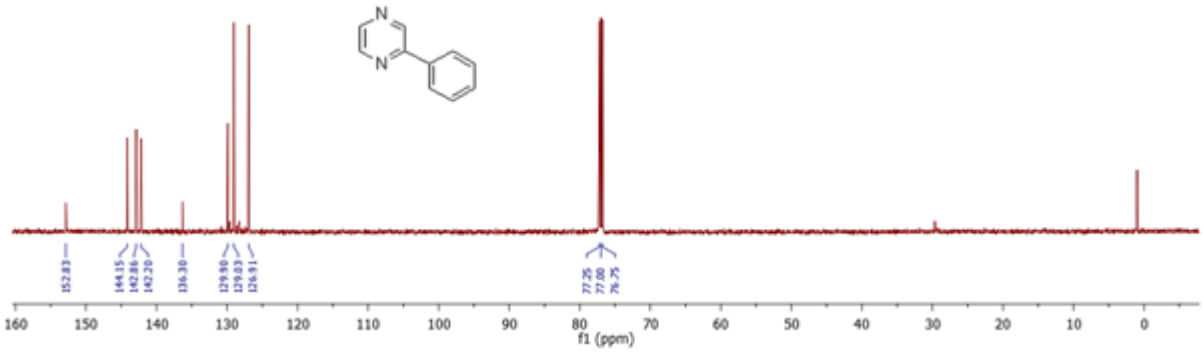
1. Spectral copies of ^{1}H, ^{13}C NMR, DEPT and HRMS data obtained in this Study:

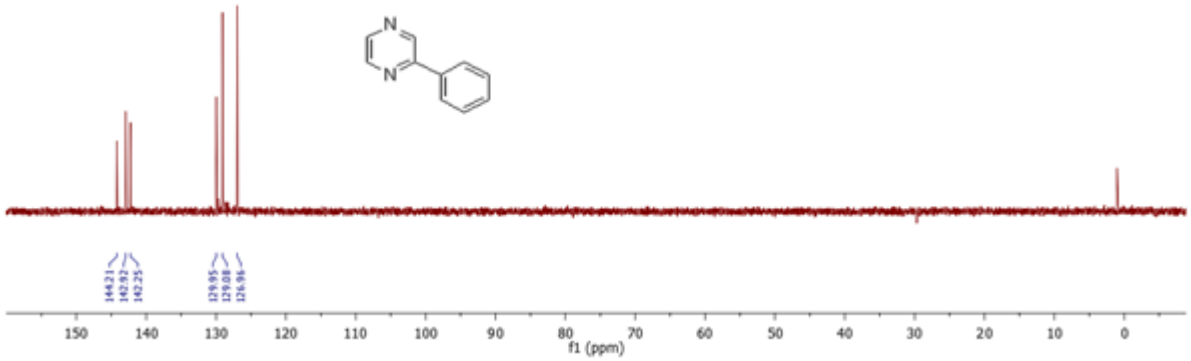
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3a**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3a**:



DEPT (125 MHz, $CDCl_3$) of compound **3a**:



HRMS (ESI-TOF) of compound **3a**:

Qualitative Compound Report

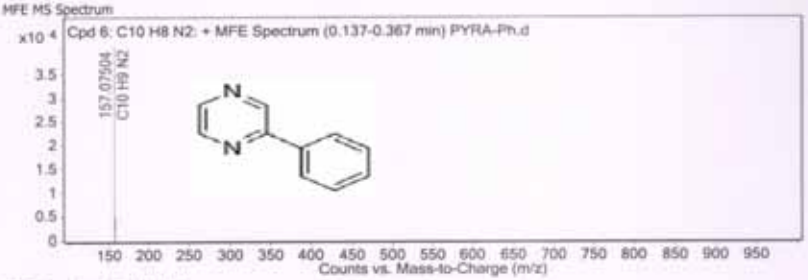
Data File	PYRA-Ph.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	as.m
Comment	Sample information is unavailable		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C10 H8 N2	0.178	156.06777	C10 H8 N2	C10 H8 N2	6.28	C10 H8 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C10 H8 N2	157.07504	0.178	Find by Molecular Feature	156.06777

MFE MS Spectrum



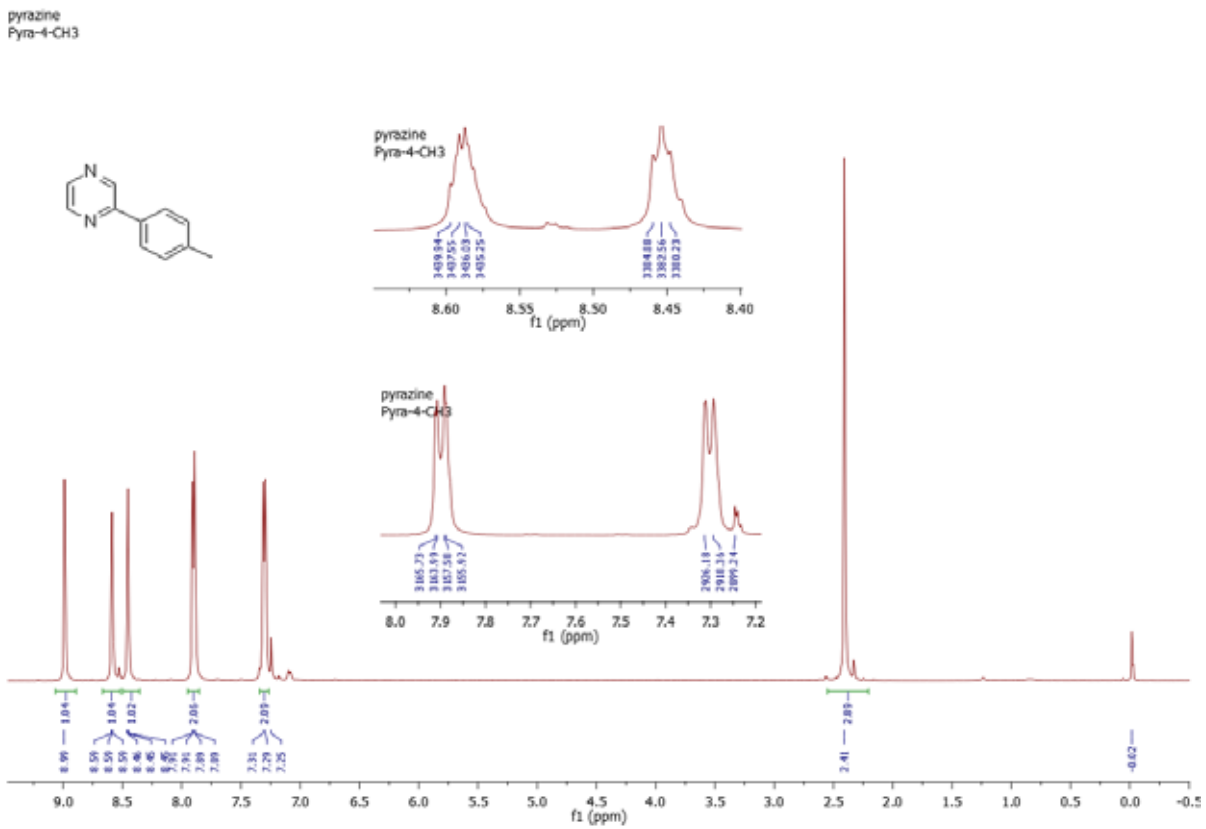
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
157.07504	1	40877.1	C10 H9 N2	(M+H)+
158.0788	1	5223.1	C10 H9 N2	(M+H)+

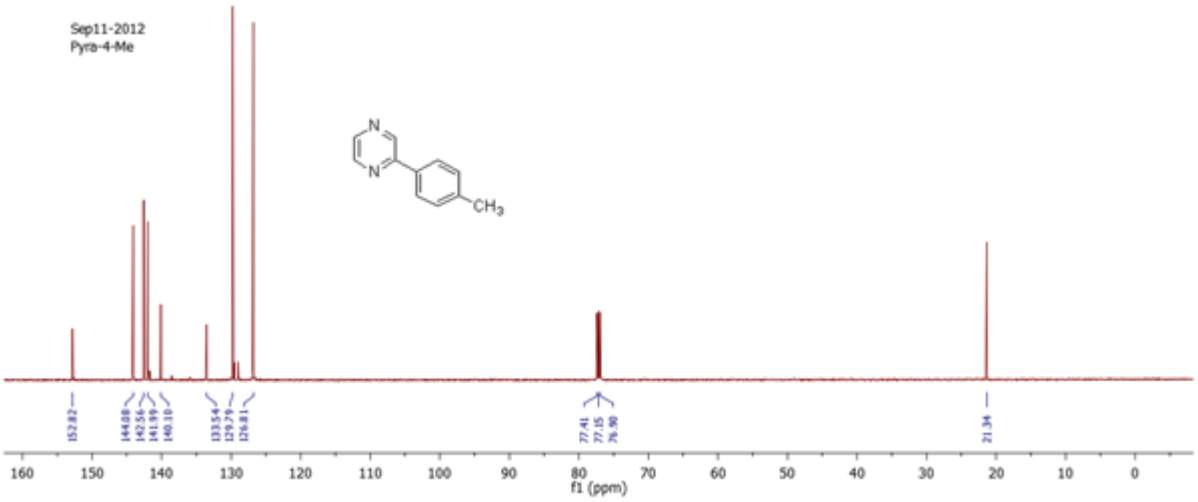
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	157.07504	157.07602	6.25	100	100	88.67	89.57
2	158.0788	158.07901	1.35	12.78	11.65	11.33	10.43

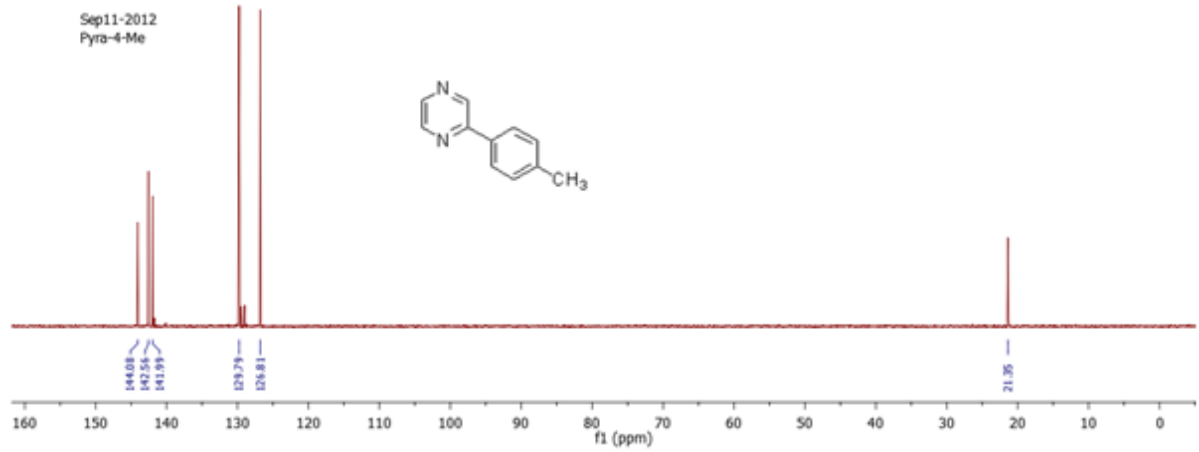
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3b**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3b**:



DEPT (125 MHz, $CDCl_3$) of compound **3b**:



HRMS (ESI-TOF) of compound **3b**:

Qualitative Compound Report

Data File	PYRA-4-Me.d	**Sample Name**	PYRA-4-Me
Sample Type	Sample	**Position**	Vial 43
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 5:19:32 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

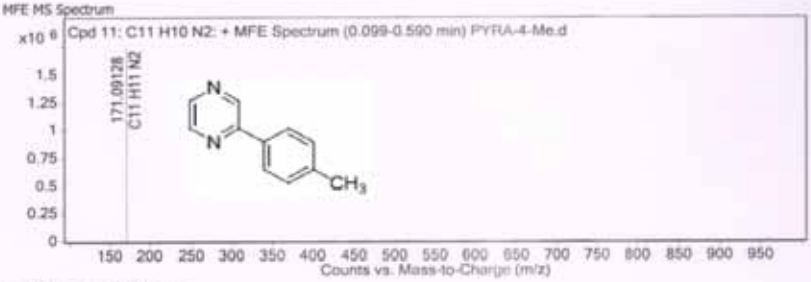
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C11 H10 N2	0.177	170.08401	C11 H10 N2	C11 H10 N2	2.3	C11 H10 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C11 H10 N2	171.09128	0.177	Find by Molecular Feature	170.08401

MFE MS Spectrum



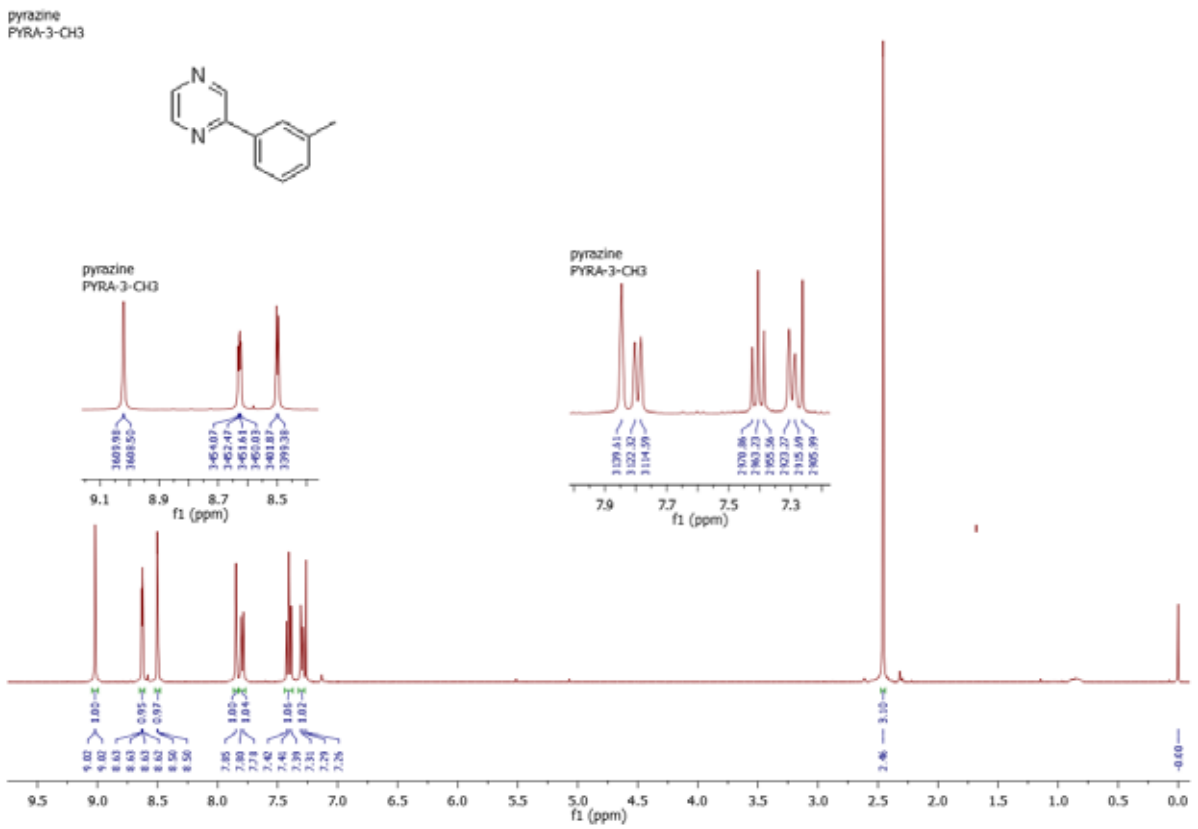
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
171.09128	1	1753125.6	C11 H11 N2	(M+H)+
172.0941	1	198443	C11 H11 N2	(M+H)+
173.09664	1	11160.7	C11 H11 N2	(M+H)+

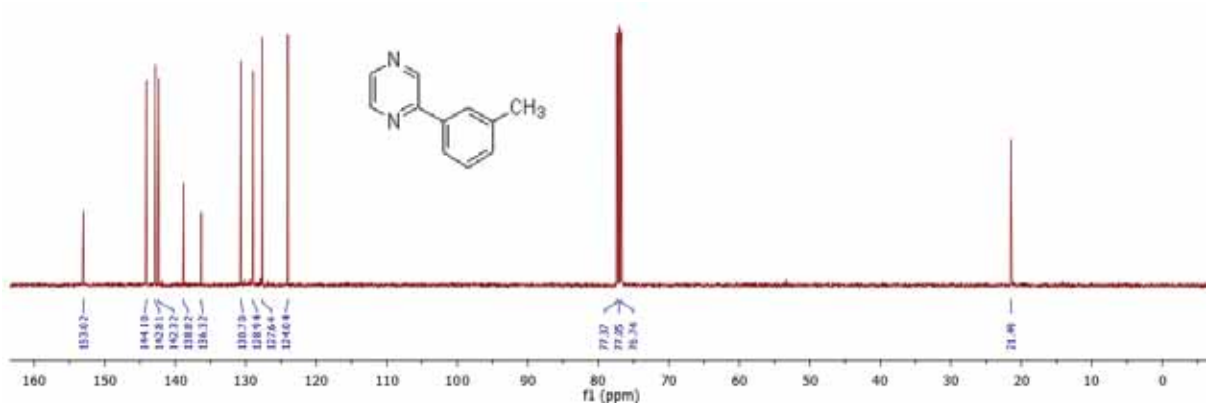
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	171.09128	171.09167	2.28	100	100	89.32	88.1
2	172.0941	172.0947	3.48	11.32	12.75	10.11	11.24
3	173.09664	173.09768	6.01	0.64	0.75	0.57	0.66

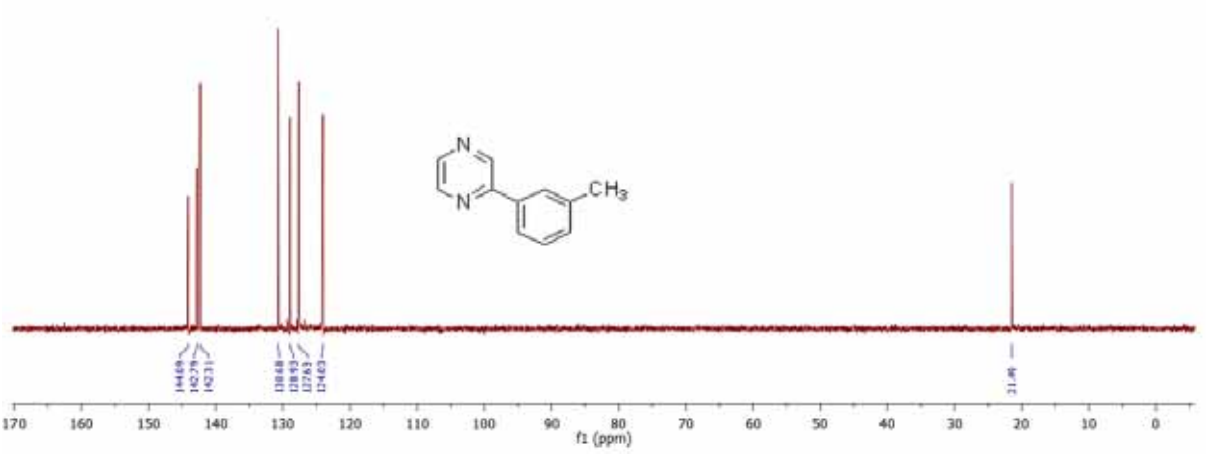
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3c**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **3c**:



DEPT (125 MHz, $CDCl_3$) of compound **3c**:



HRMS (ESI-TOF) of compound **3c**:

Qualitative Compound Report

Data File	PYRA-3-Me.d	Sample Name	PYRA-3-Me
Sample Type	Sample	Position	Vial 44
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_MS_25072012.m	Acquired Time	9/12/2012 4:24:11 PM
IRM Calibration Status	Success	DA Method	as.m
Comment			

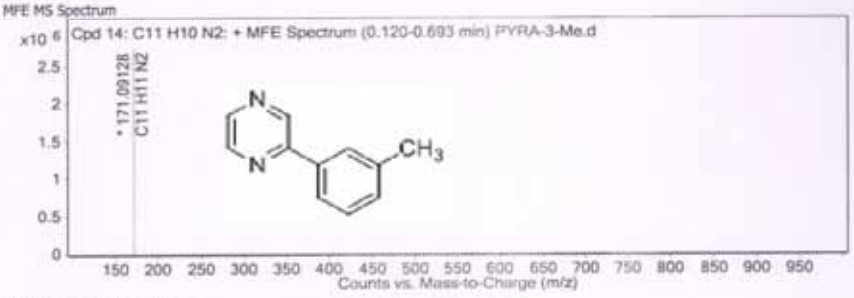
Sample Group Info.

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C11 H10 N2	0.177	170.084	C11 H10 N2	C11 H10 N2	2.35	C11 H10 N2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 14: C11 H10 N2	171.09128	0.177	Find by Molecular Feature	170.084

MFE MS Spectrum



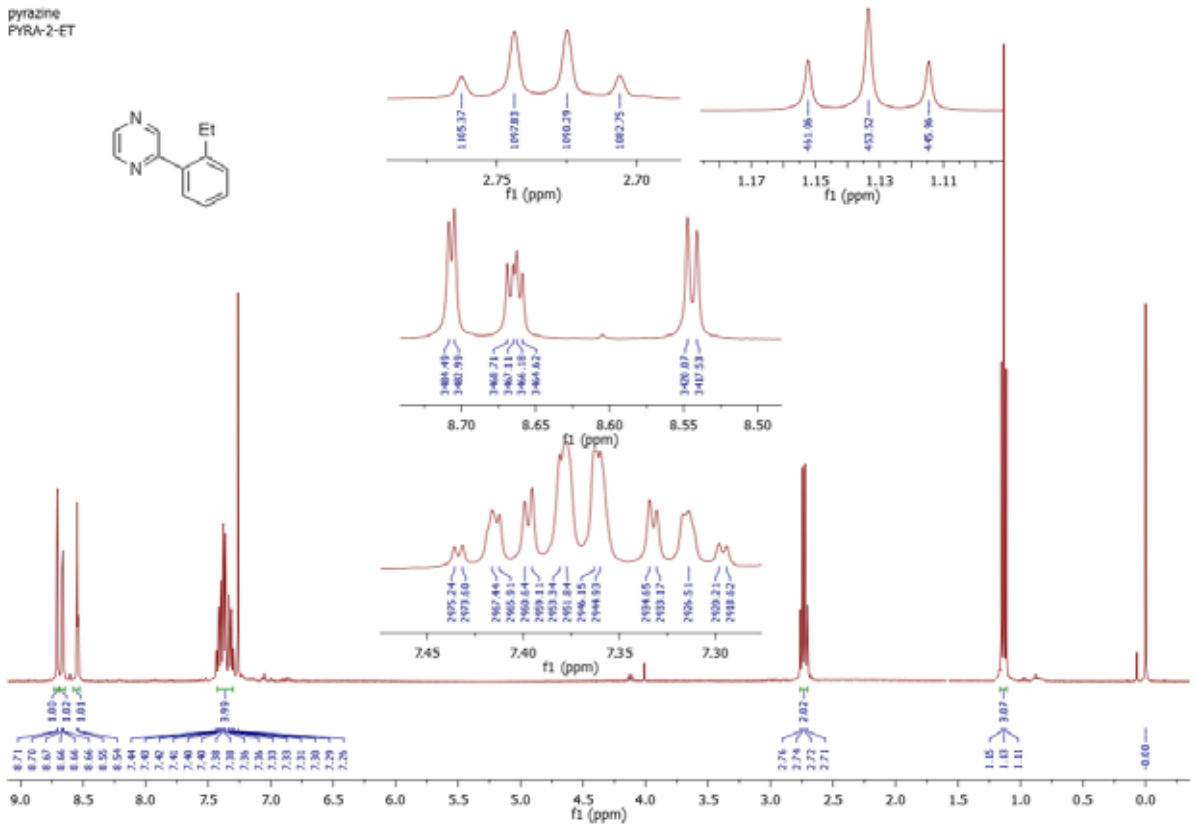
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
171.09128	1	2739250.5	C11 H11 N2	(M+H)+
172.09419	1	325642.7	C11 H11 N2	(M+H)+
173.097	1	20394	C11 H11 N2	(M+H)+
174.09737	1	299.3	C11 H11 N2	(M+H)+

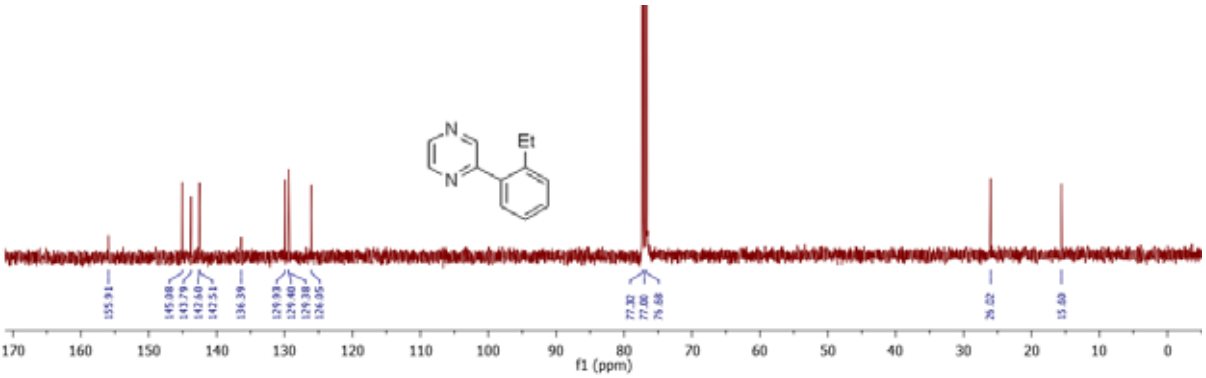
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	171.09128	171.09167	2.34	100	100	88.78	88.08
2	172.09419	172.0947	2.96	11.89	12.75	10.55	11.23
3	173.097	173.09768	3.93	0.74	0.75	0.66	0.66
4	174.09737	174.10063	18.68	0.01	0.03	0.01	0.02

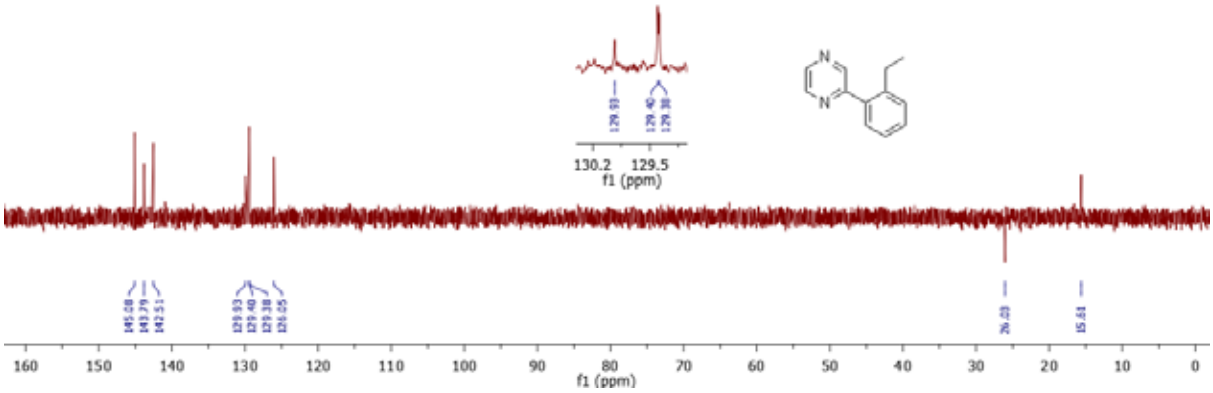
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3d**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **3d**:



DEPT (100 MHz, $CDCl_3$) of compound **3d**:



HRMS (ESI-TOF) of compound **3d**:

Qualitative Compound Report

Data File	PYRA-2ET.d	**Sample Name**	PYRA-2ET
Sample Type	Sample	**Position**	Vial 83
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/24/2012 5:58:09 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

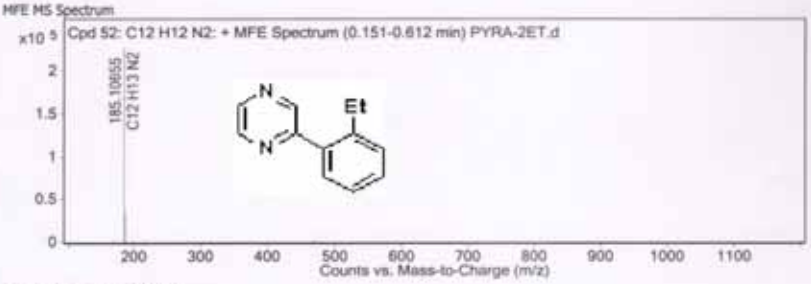
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 52: C12 H12 N2	0.218	184.09927	C12 H12 N2	C12 H12 N2	4.23	C12 H12 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 52: C12 H12 N2	185.10655	0.218	Find by Molecular Feature	184.09927

MFE MS Spectrum



MS Spectrum Peak List

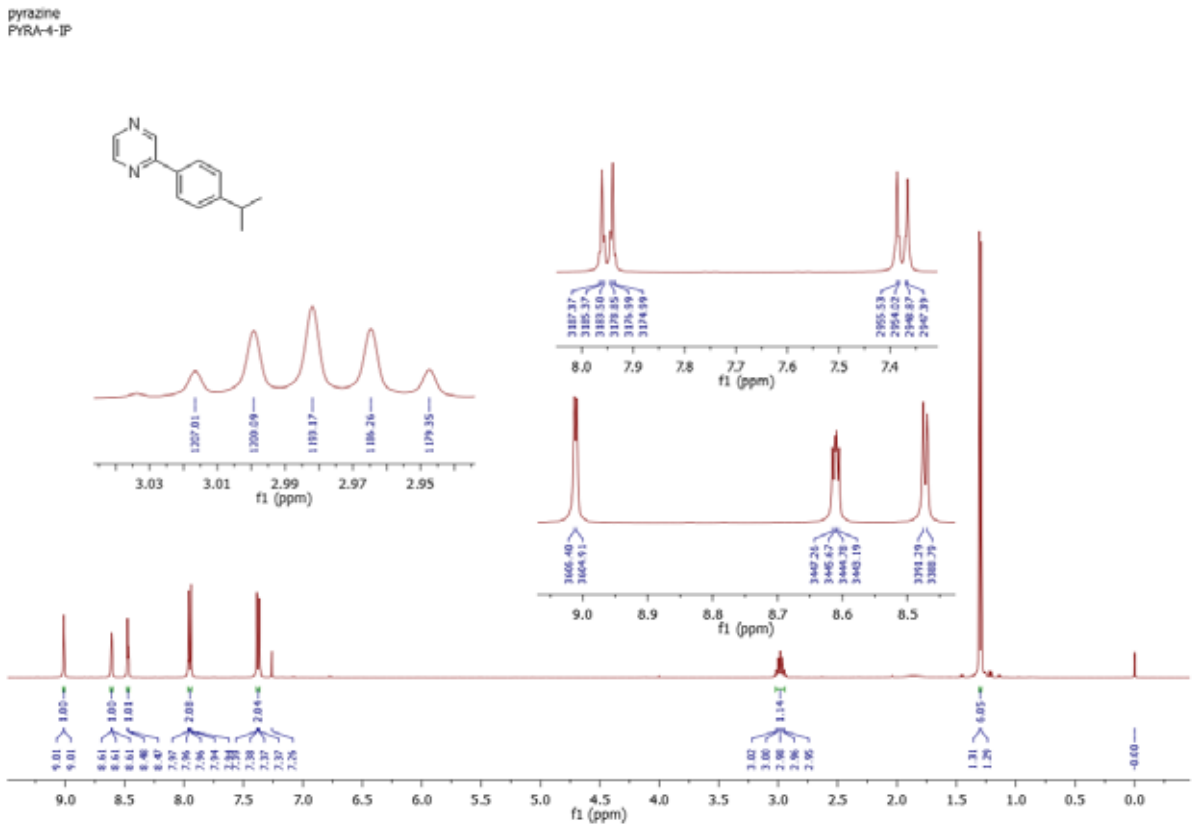
m/z	z	Abund	Formula	Ion
185.10655	1	227066.7	C12 H13 N2	(M+H)+
186.10958	1	37073.5	C12 H13 N2	(M+H)+
187.11069	1	2878.6	C12 H13 N2	(M+H)+

Predicted Isotope Match Table

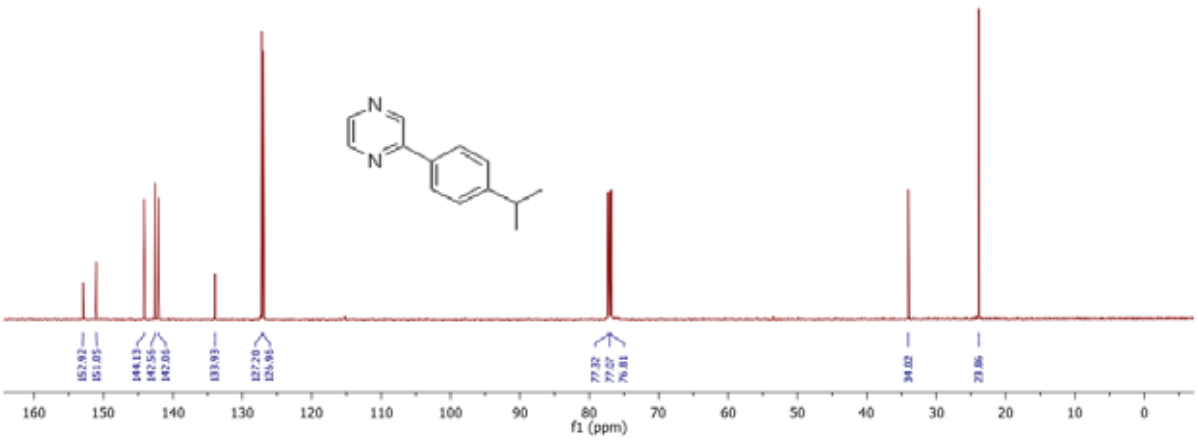
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	185.10655	185.10732	4.21	100	100	85.04	87.15
2	186.10958	186.11038	4.27	16.33	13.86	13.88	12.08
3	187.11069	187.1134	14.49	1.27	0.89	1.08	0.77

--- End Of Report ---

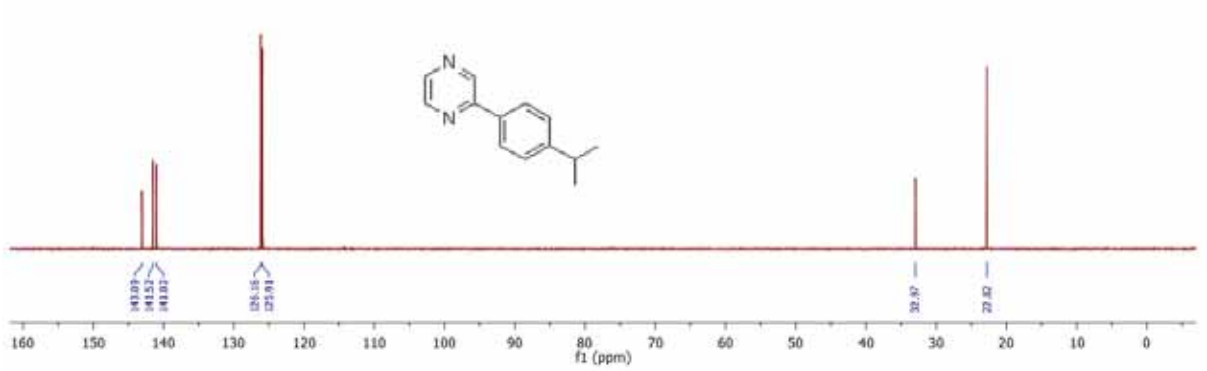
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3e**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3e**:



DEPT (125 MHz, $CDCl_3$) of compound **3e**:



HRMS (ESI-TOF) of compound **3e**:

Qualitative Compound Report

Data File	PY-RA4-IP.d	**Sample Name**	PY-RA4-IP
Sample Type	Sample	**Position**	Vial 71
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/24/2012 7:17:26 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

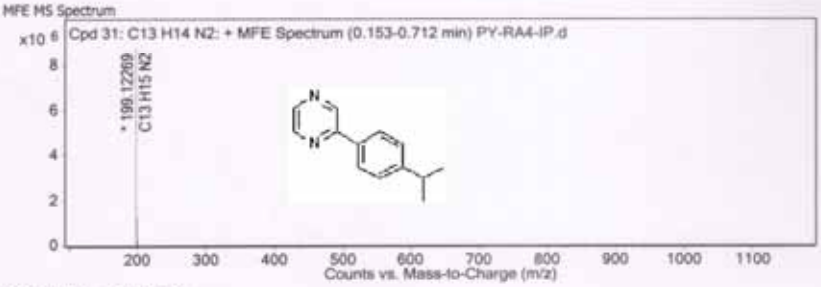
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 31: C13 H14 N2	0.221	198.11541	C13 H14 N2	C13 H14 N2	1.45	C13 H14 N2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 31: C13 H14 N2	199.12269	0.221	Find by Molecular Feature	198.11541

MFE MS Spectrum



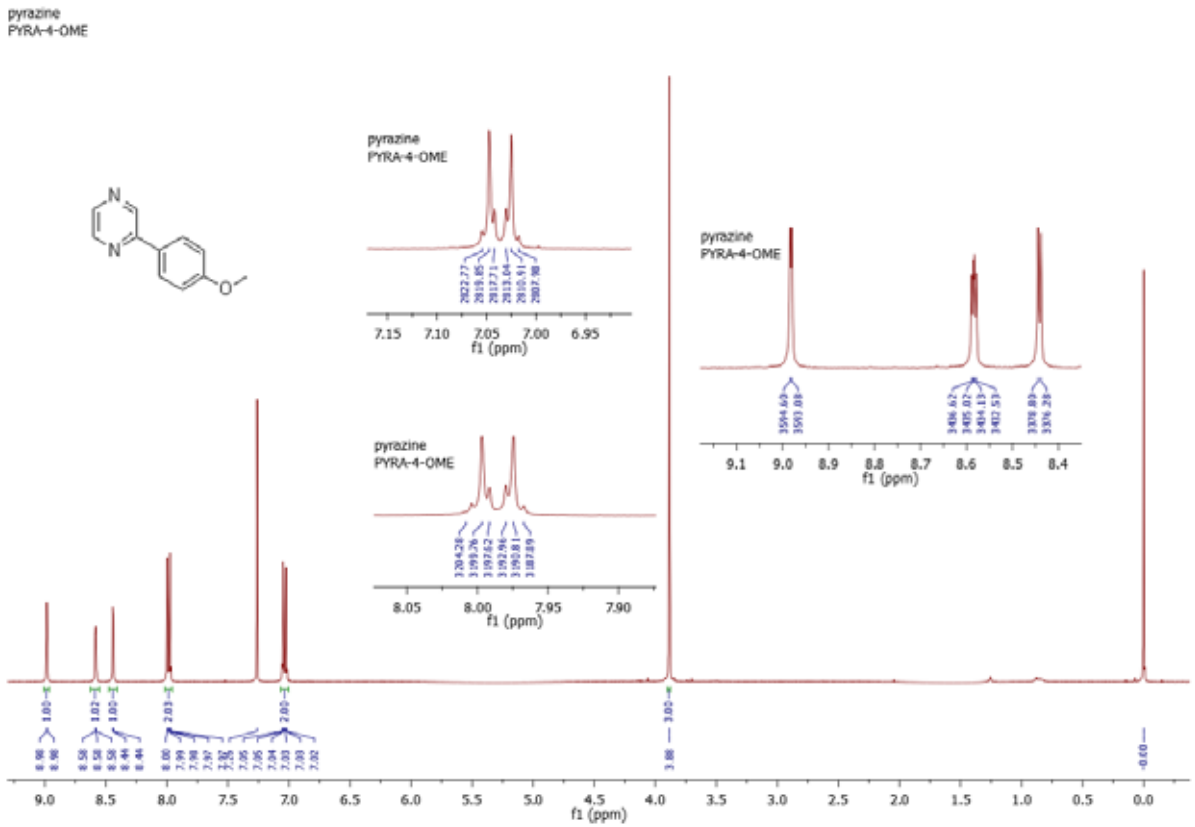
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
199.12269	1	8731708	C13 H15 N2	(M+H)+
200.12606	1	1230524.4	C13 H15 N2	(M+H)+
201.12874	1	86817.3	C13 H15 N2	(M+H)+
202.13094	1	5794	C13 H15 N2	(M+H)+
221.10668	1	15915.9	C13 H14 N2 Na	(M+Na)+
222.11028	1	3082.2	C13 H14 N2 Na	(M+Na)+

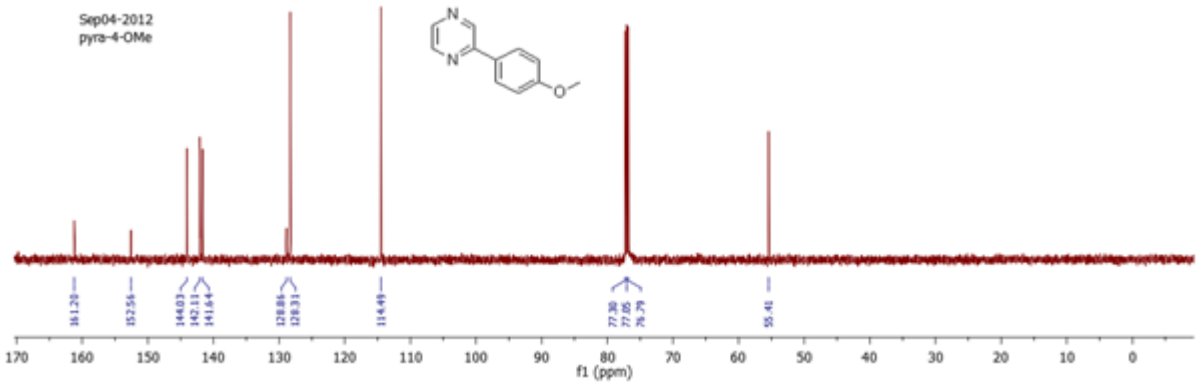
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	199.12269	199.12297	1.45	100	100	86.84	86.17
2	200.12606	200.12605	-0.03	14.09	14.96	12.24	12.89
3	201.12874	201.12911	1.85	0.99	1.04	0.86	0.9
4	202.13094	202.13214	5.92	0.07	0.04	0.06	0.04

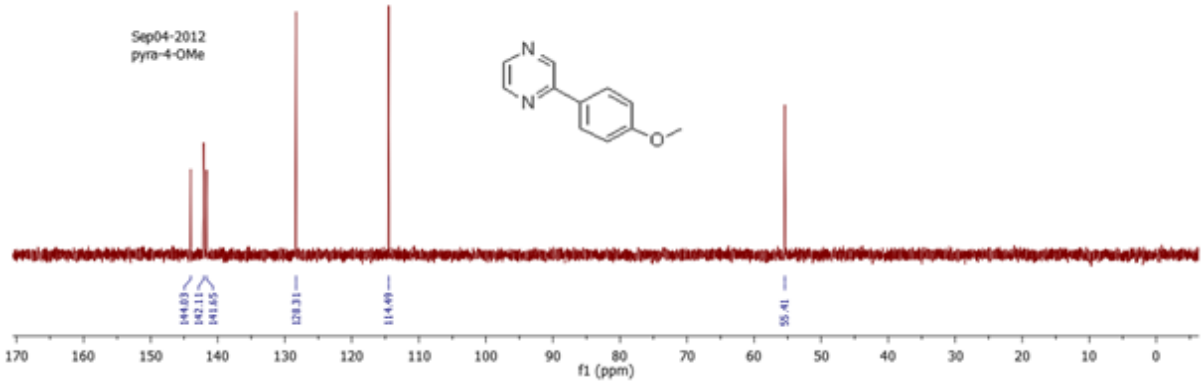
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3f**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3f**:



DEPT (125 MHz, $CDCl_3$) of compound **3f**:



HRMS (ESI-TOF) of compound **3f**:

Qualitative Compound Report

Data File	PYRA-4-OMe.d	Sample Name	PYRA-4-OMe
Sample Type	Sample	Position	Vial 53
Instrument Name	Instrument 1	User Name	
Acq Method	vishal_MS_25072012.m	Acquired Time	9/12/2012 4:44:44 PM
IRM Calibration Status	Success	DA Method	as.m
Comment			

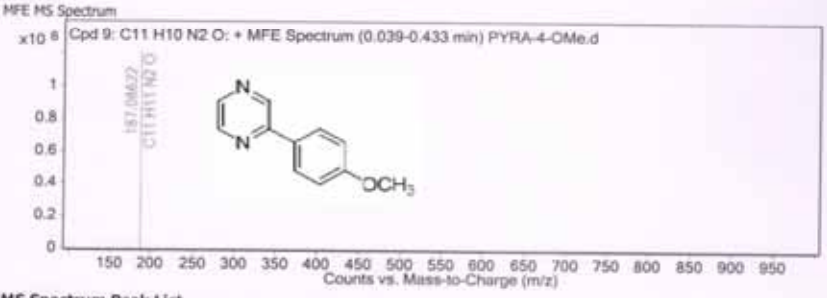
Sample Group Info.

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C11 H10 N2 O	0.175	186.07895	C11 H10 N2 O	C11 H10 N2 O	1.97	C11 H10 N2 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 9: C11 H10 N2 O	187.08622	0.175	Find by Molecular Feature	186.07895

MFE MS Spectrum



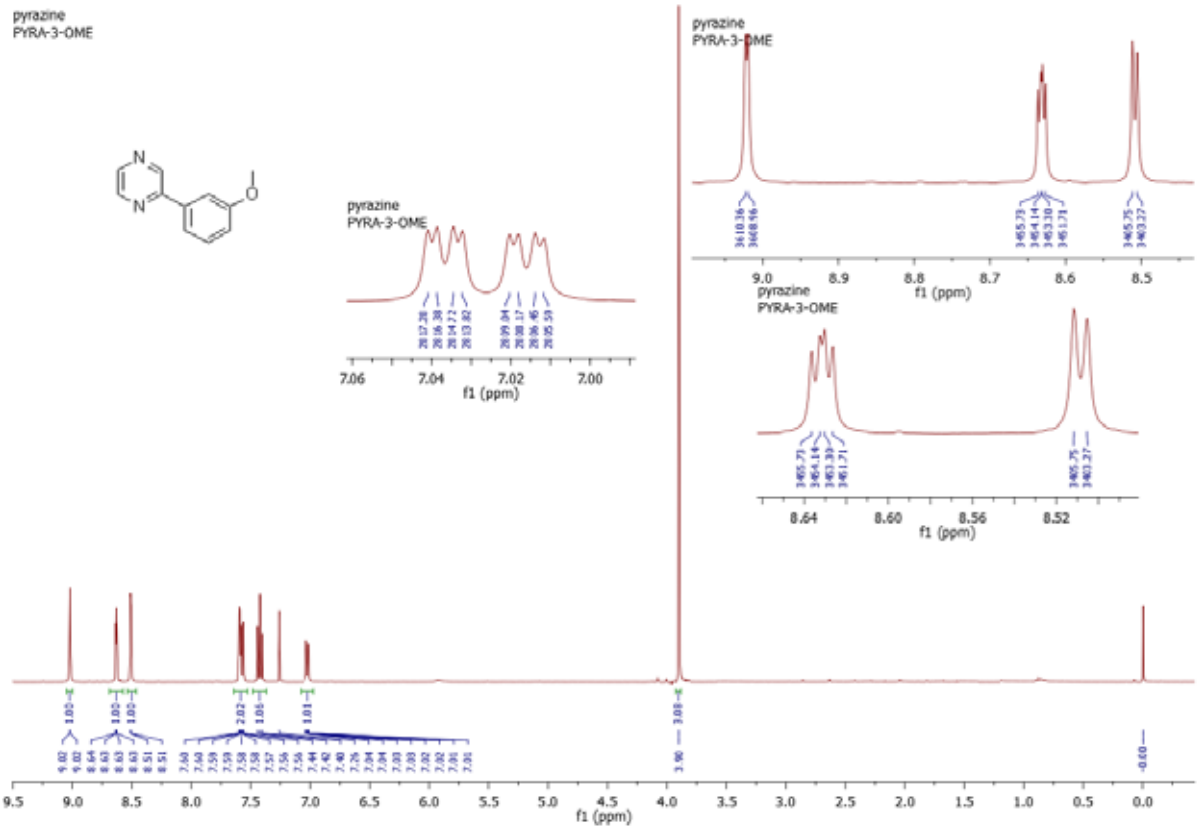
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
187.08622	1	1219713.5	C11 H11 N2 O	(M+H)+
188.08893	1	132899.1	C11 H11 N2 O	(M+H)+
189.09111	1	8643.8	C11 H11 N2 O	(M+H)+
190.09487	1	877.4	C11 H11 N2 O	(M+H)+

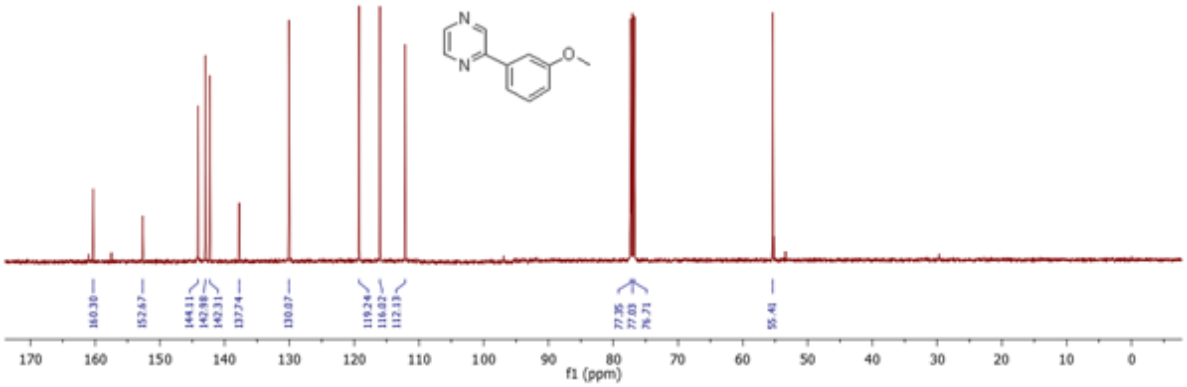
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	187.08622	187.08659	1.96	100	100	89.54	87.87
2	188.08893	188.08961	3.66	10.9	12.79	9.76	11.24
3	189.09111	189.09223	5.91	0.71	0.96	0.63	0.84
4	190.09487	190.09472	-0.8	0.07	0.05	0.06	0.05

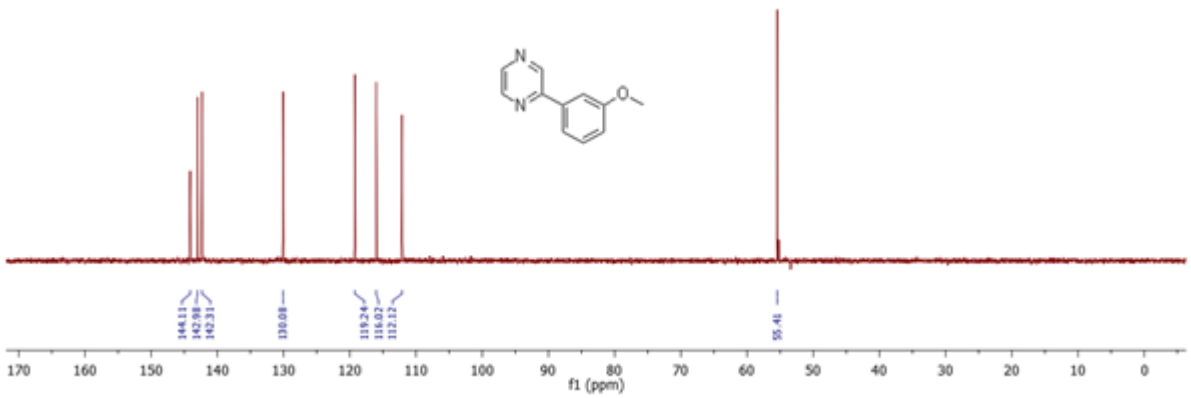
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3g**:



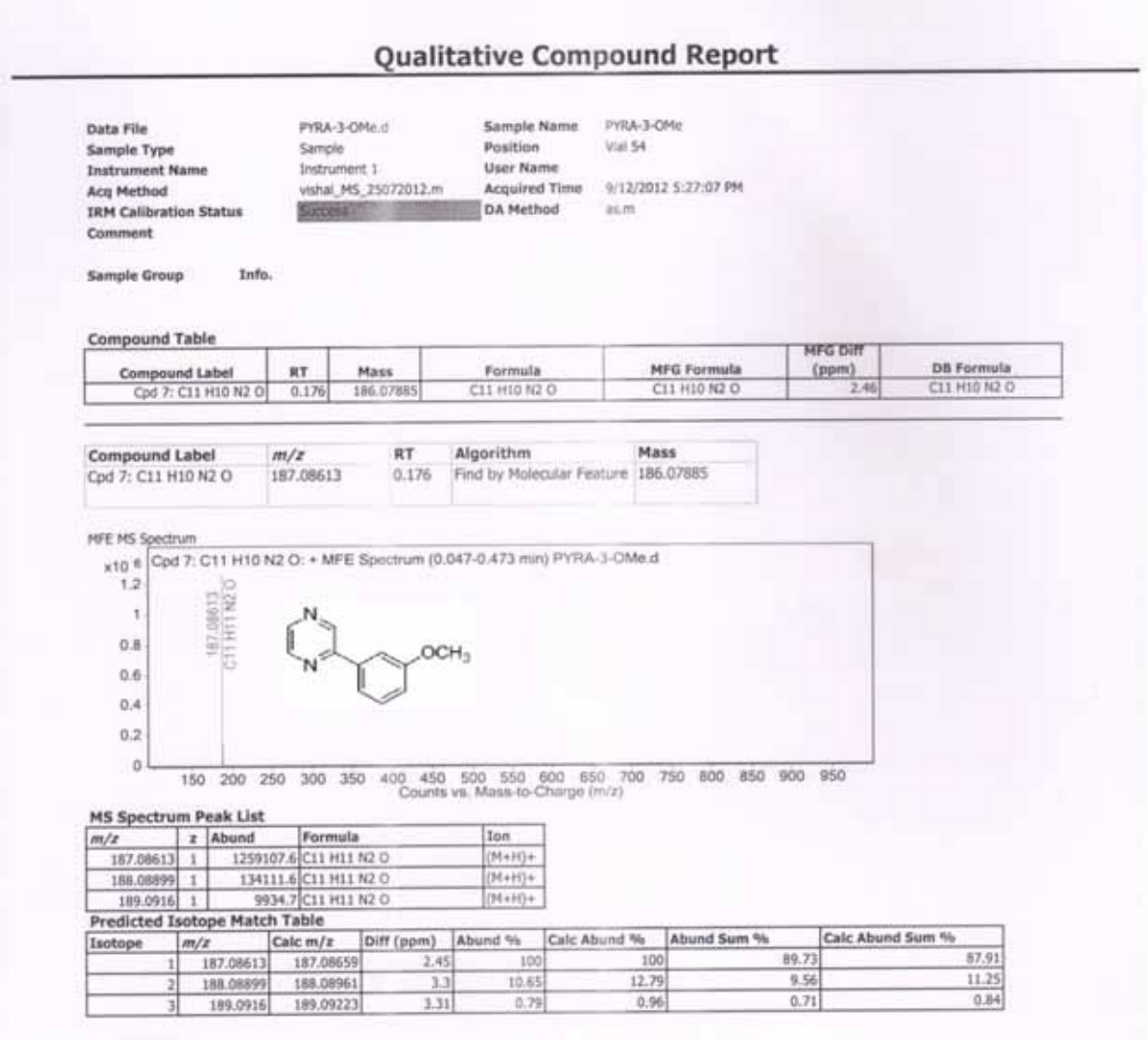
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3g**:



DEPT (100 MHz, $CDCl_3$) of compound **3g**:



HRMS (ESI-TOF) of compound **3g**:



Qualitative Compound Report

Data File	PYRA-3-OMe.d	**Sample Name**	PYRA-3-OMe
Sample Type	Sample	**Position**	Vial 54
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 5:27:07 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C11 H10 N2 O	0.176	186.07885	C11 H10 N2 O	C11 H10 N2 O	2.46	C11 H10 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C11 H10 N2 O	187.08613	0.176	Find by Molecular Feature	186.07885

MFE MS Spectrum

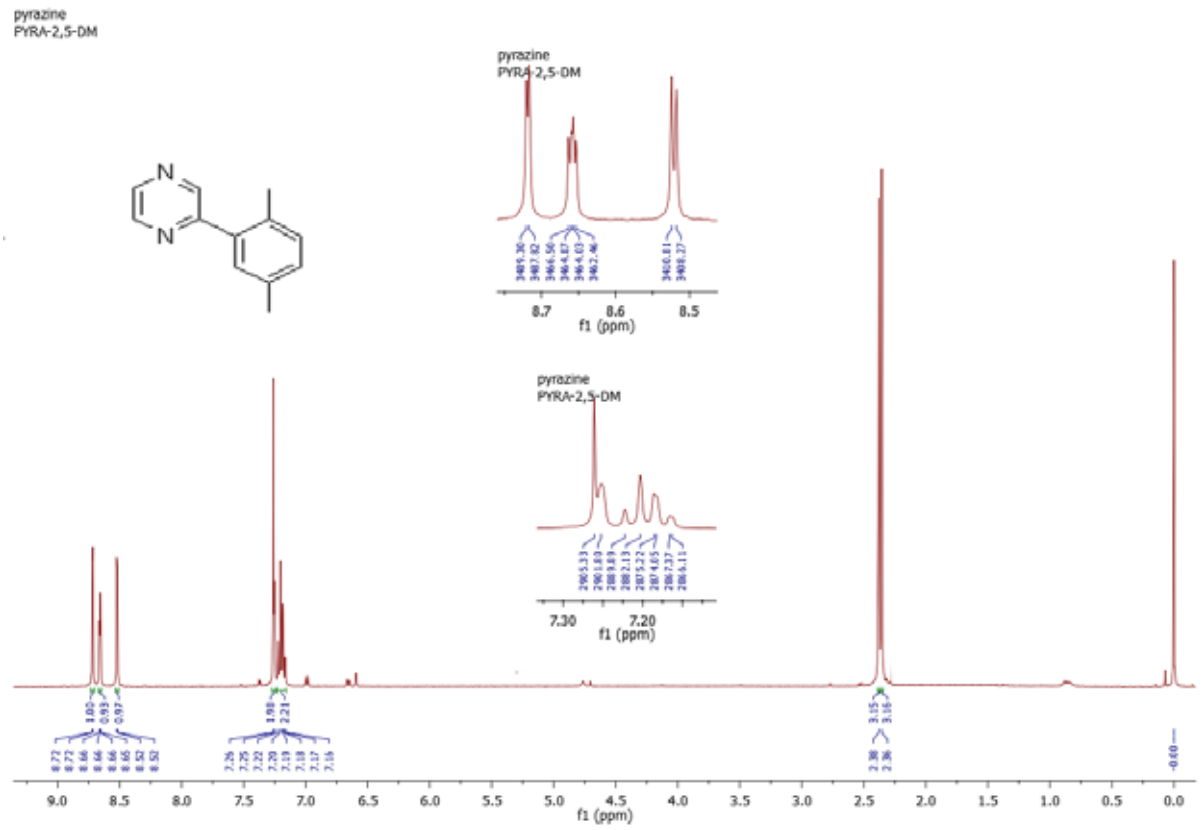
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
187.08613	1	1259107.6	C11 H11 N2 O	(M+H)+
188.08899	1	134111.6	C11 H11 N2 O	(M+H)+
189.0916	1	9934.7	C11 H11 N2 O	(M+H)+

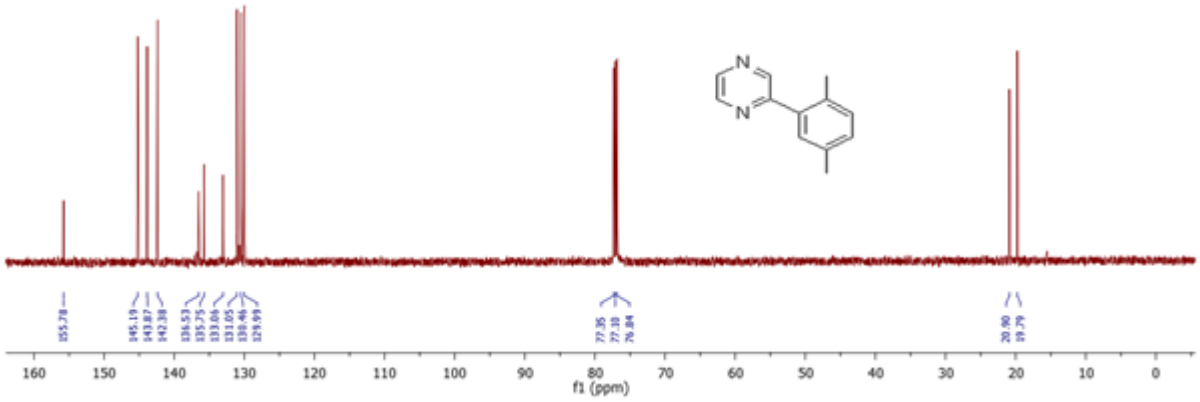
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	187.08613	187.08659	2.45	100	100	89.73	87.91
2	188.08899	188.08961	3.3	10.65	12.79	9.56	11.25
3	189.0916	189.09223	3.31	0.79	0.96	0.71	0.84

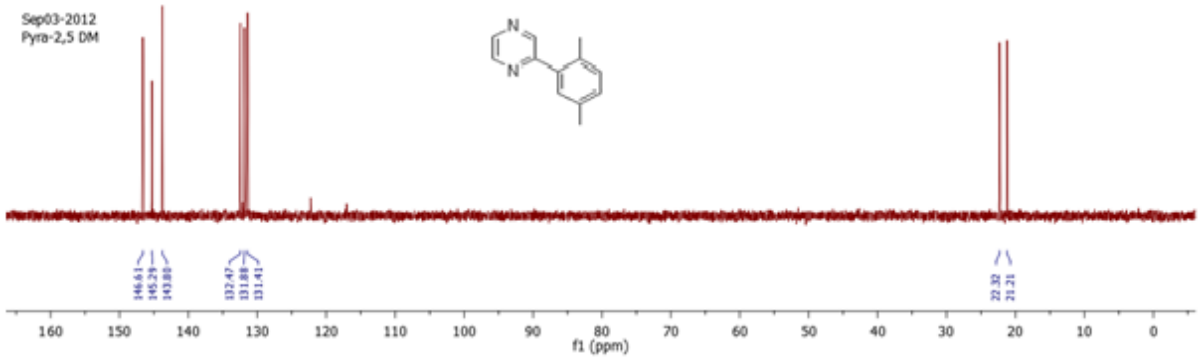
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3h**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3h**:



DEPT (125 MHz, $CDCl_3$) of compound **3h**:



HRMS (ESI-TOF) of compound **3h**:

Qualitative Compound Report

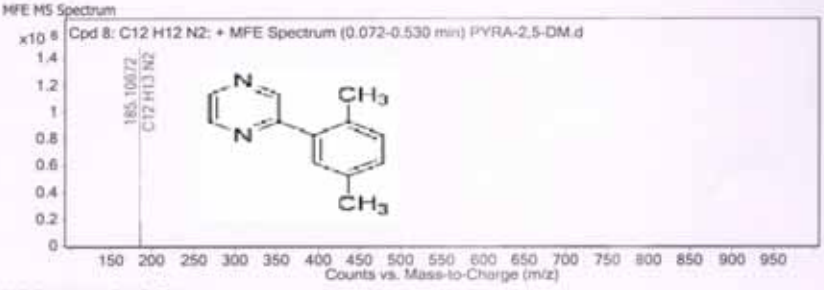
Data File	PYRA-2,5-DM.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	as.m
Comment	Sample Information is unavailable		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C12 H12 N2	0.176	184.09944	C12 H12 N2	C12 H12 N2	3.29	C12 H12 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C12 H12 N2	185.10672	0.176	Find by Molecular Feature	184.09944

MFE MS Spectrum



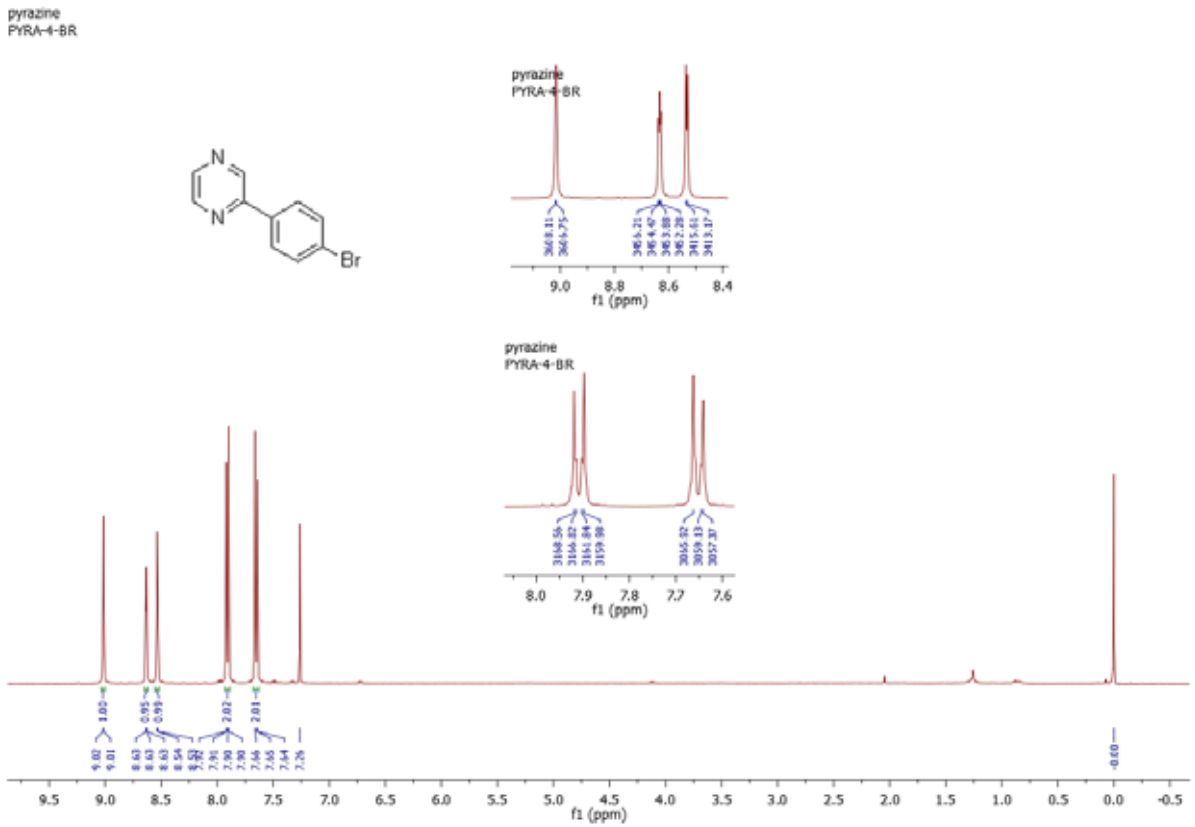
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
185.10672	1	1479957	C12 H13 N2	(M+H)+
186.10941	1	178870.6	C12 H13 N2	(M+H)+
187.11268	1	12025.2	C12 H13 N2	(M+H)+
188.11451	1	641.7	C12 H13 N2	(M+H)+

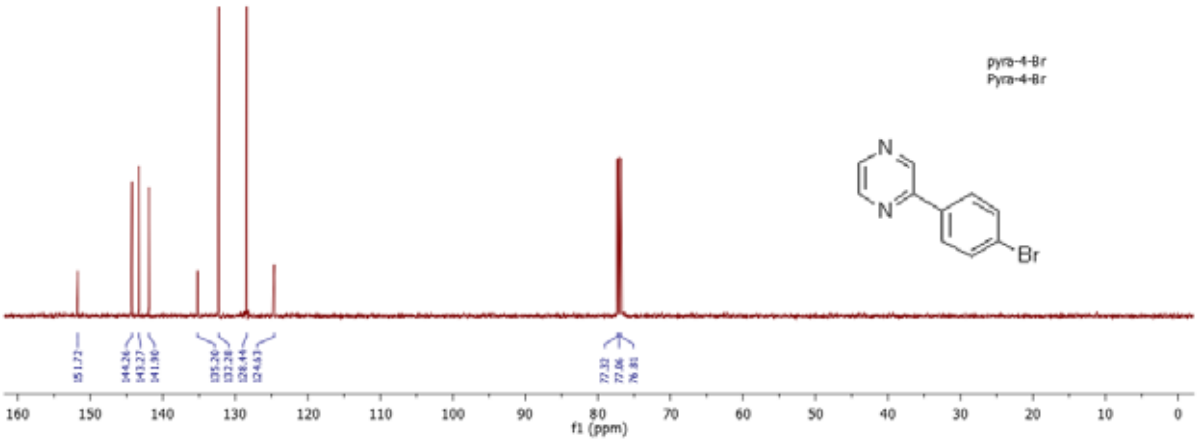
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	185.10672	185.10732	3.27	100	100	88.54	87.12
2	186.10941	186.11038	5.2	12.09	13.86	10.7	12.07
3	187.11268	187.1134	3.88	0.81	0.89	0.72	0.77
4	188.11451	188.11639	9.98	0.04	0.03	0.04	0.03

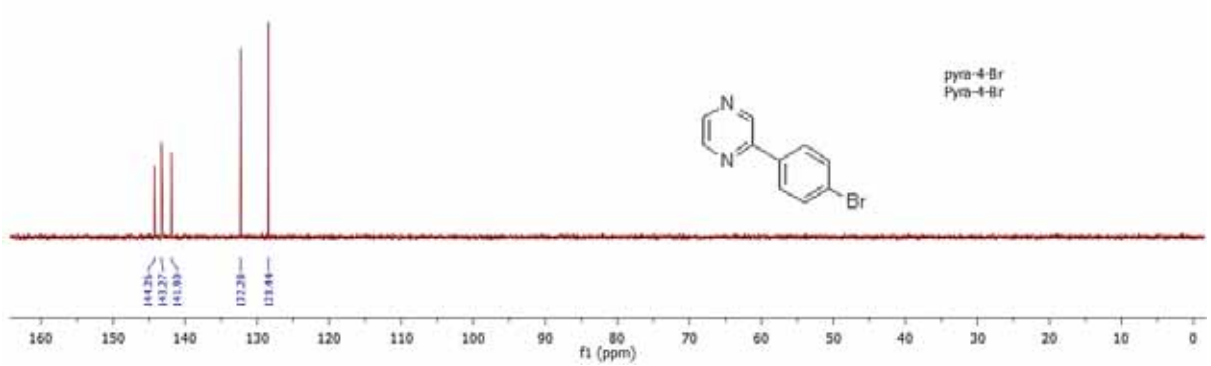
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3i**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3i**:



DEPT (125 MHz, $CDCl_3$) of compound **3i**:



HRMS (ESI-TOF) of compound **3i**:

Qualitative Compound Report

Data File	PYRA-4-Br.d	**Sample Name**	PYRA-4-Br
Sample Type	Sample	**Position**	Vial 52
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:42:09 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

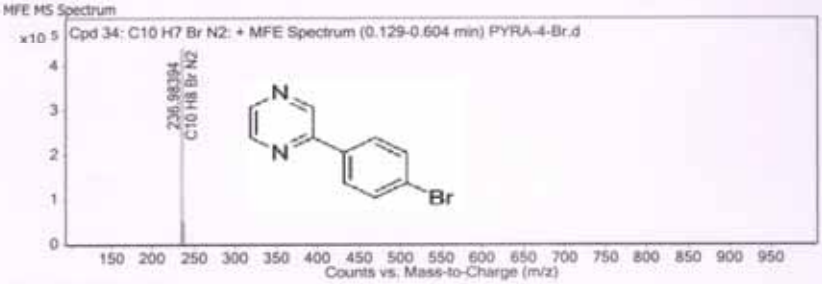
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 34: C10 H7 Br N2	0.176	233.97863	C10 H7 Br N2	C10 H7 Br N2	2.72	C10 H7 Br N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 34: C10 H7 Br N2	234.98587	0.176	Find by Molecular Feature	233.97863

MFE MS Spectrum



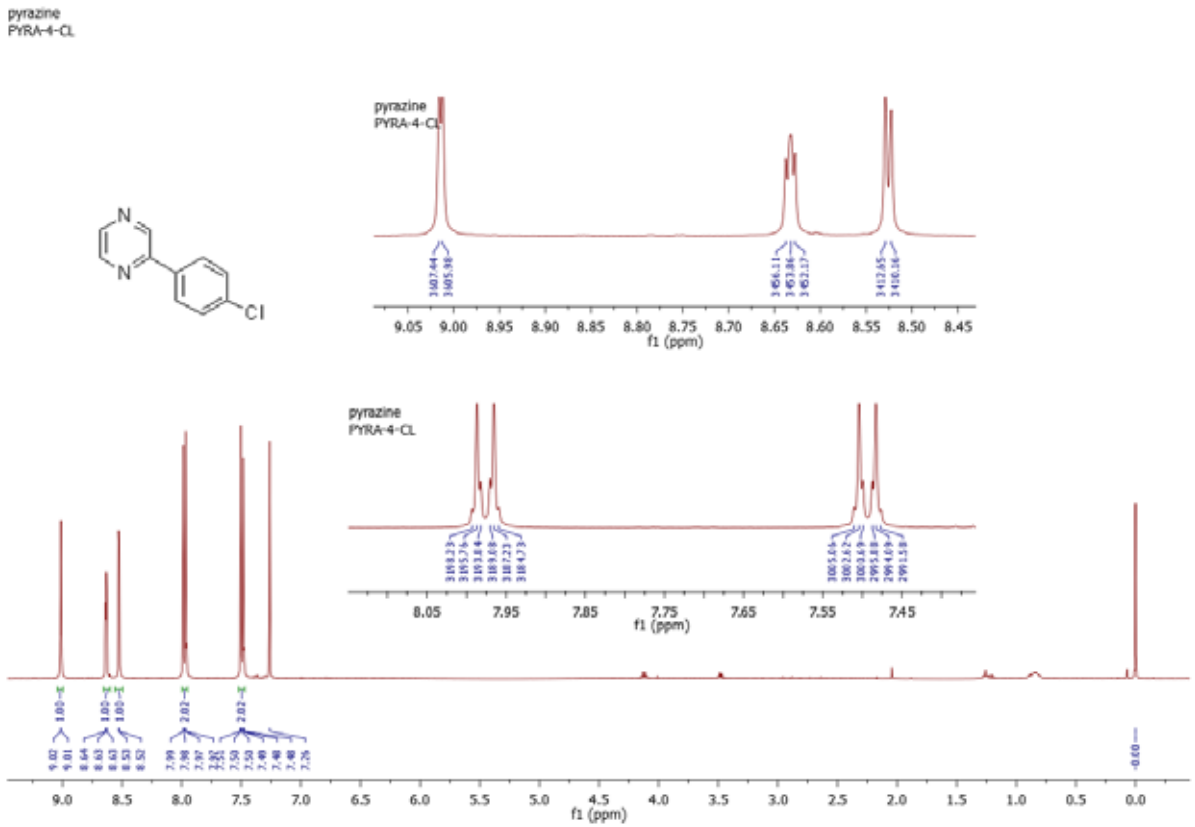
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
234.98587	1	436566.3	C10 H8 Br N2	(M+H)+
235.98881	1	53905.9	C10 H8 Br N2	(M+H)+
236.98394	1	441896.6	C10 H8 Br N2	(M+H)+
237.98648	1	51050.2	C10 H8 Br N2	(M+H)+
238.98991	1	3142.2	C10 H8 Br N2	(M+H)+

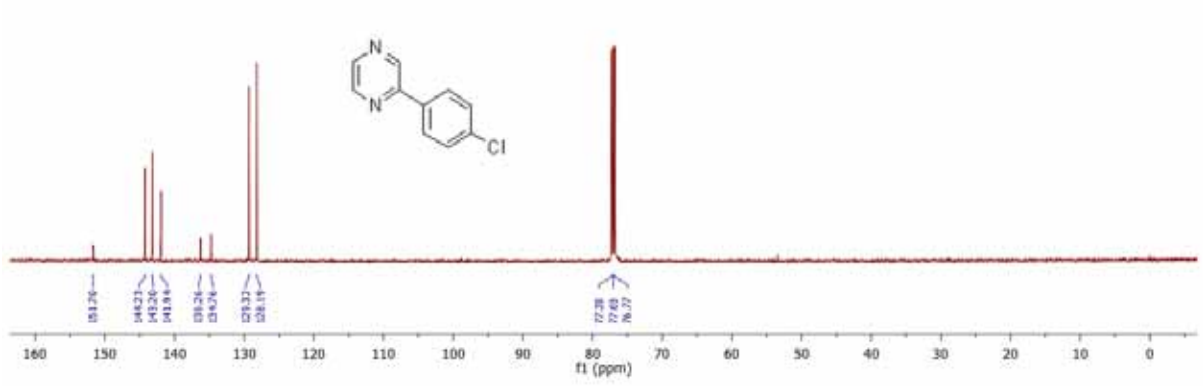
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	234.98587	234.98654	2.84	98.79	100	44.25	45.15
2	235.98881	235.98952	3.01	12.2	11.64	5.46	5.25
3	236.98394	236.98454	2.55	100	97.9	44.79	44.2
4	237.98648	237.98749	4.23	11.55	11.34	5.17	5.12
5	238.98991	238.99041	2.11	0.71	0.6	0.32	0.27

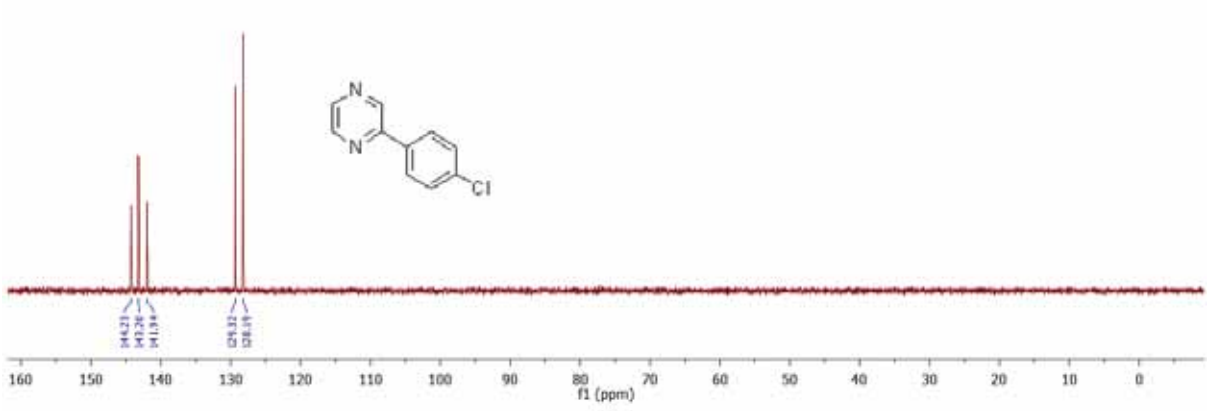
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3j**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3j**:



DEPT (125 MHz, $CDCl_3$) of compound **3j**:



HRMS (ESI-TOF) of compound **3j**:

Qualitative Compound Report

Data File	PYRA-4-Cl.d	**Sample Name**	PYRA-4-Cl
Sample Type	Sample	**Position**	Vial 45
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:26:45 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

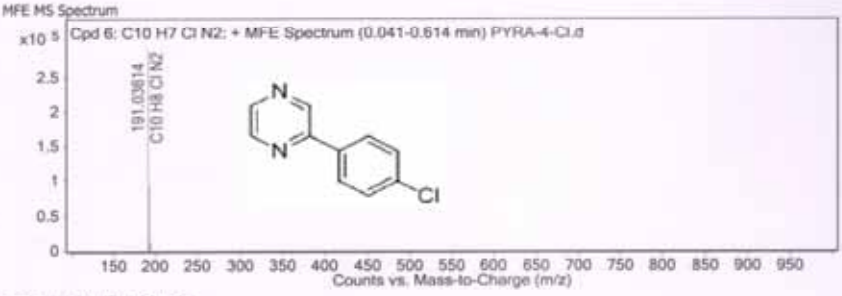
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C10 H7 Cl N2	0.177	190.02886	C10 H7 Cl N2	C10 H7 Cl N2	4.84	C10 H7 Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C10 H7 Cl N2	191.03614	0.177	Find by Molecular Feature	190.02886

MFE MS Spectrum



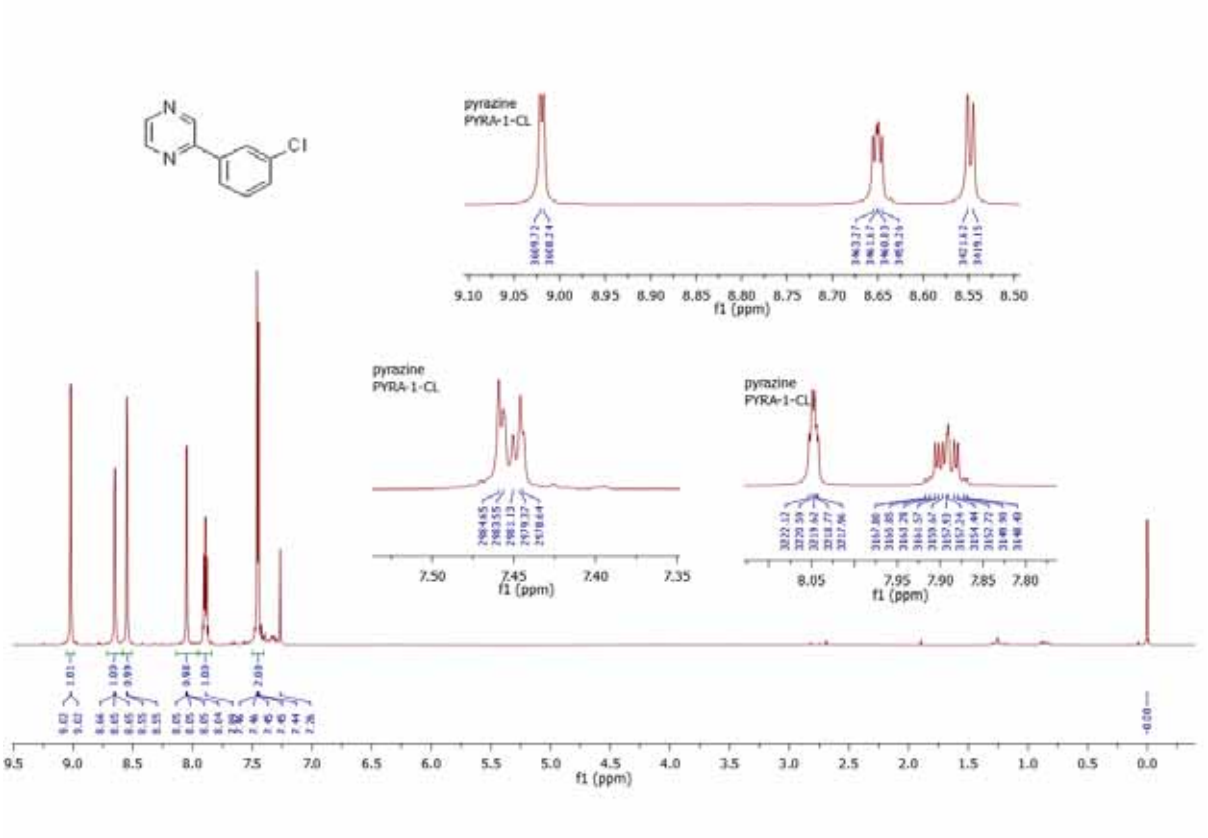
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
191.03614	1	291689.1	C10 H8 Cl N2	(M+H)+
192.03897	1	33108.5	C10 H8 Cl N2	(M+H)+
193.03307	1	92154.3	C10 H8 Cl N2	(M+H)+
194.03601	1	11883.4	C10 H8 Cl N2	(M+H)+

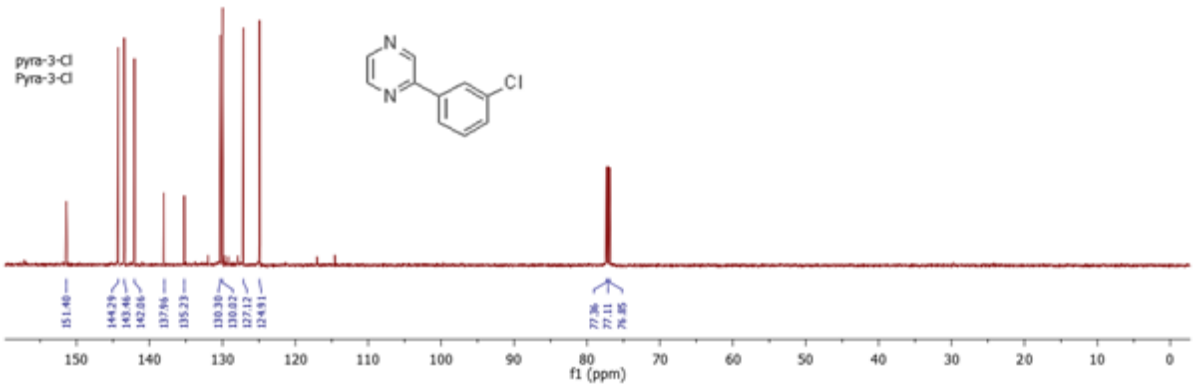
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	191.03614	191.03705	4.77	100	100	68.02	67.57
2	192.03897	192.04003	5.51	11.35	11.64	7.72	7.86
3	193.03307	193.03427	6.21	31.59	32.61	21.49	22.04
4	194.03601	194.03713	5.79	4.07	3.74	2.77	2.53

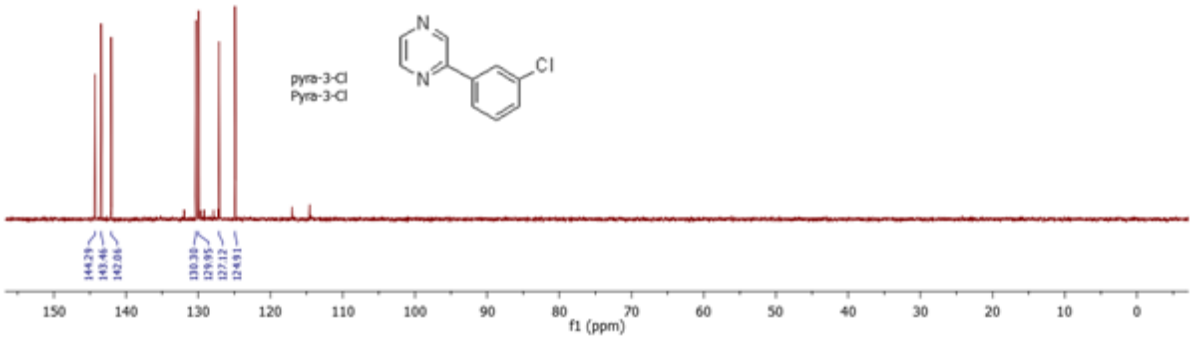
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3k**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3k**:



DEPT (125 MHz, $CDCl_3$) of compound **3k**:



HRMS (ESI-TOF) of compound **3k**:

Qualitative Compound Report

Data File	PYRA-3-Cl.d	**Sample Name**	PYRA-3-Cl
Sample Type	Sample	**Position**	Vial 47
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:29:15 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

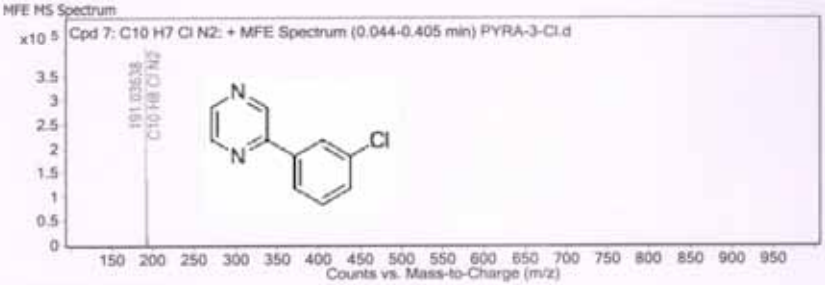
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C10 H7 Cl N2	0.178	190.02908	C10 H7 Cl N2	C10 H7 Cl N2	3.65	C10 H7 Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C10 H7 Cl N2	191.03638	0.178	Find by Molecular Feature	190.02908

MFE MS Spectrum



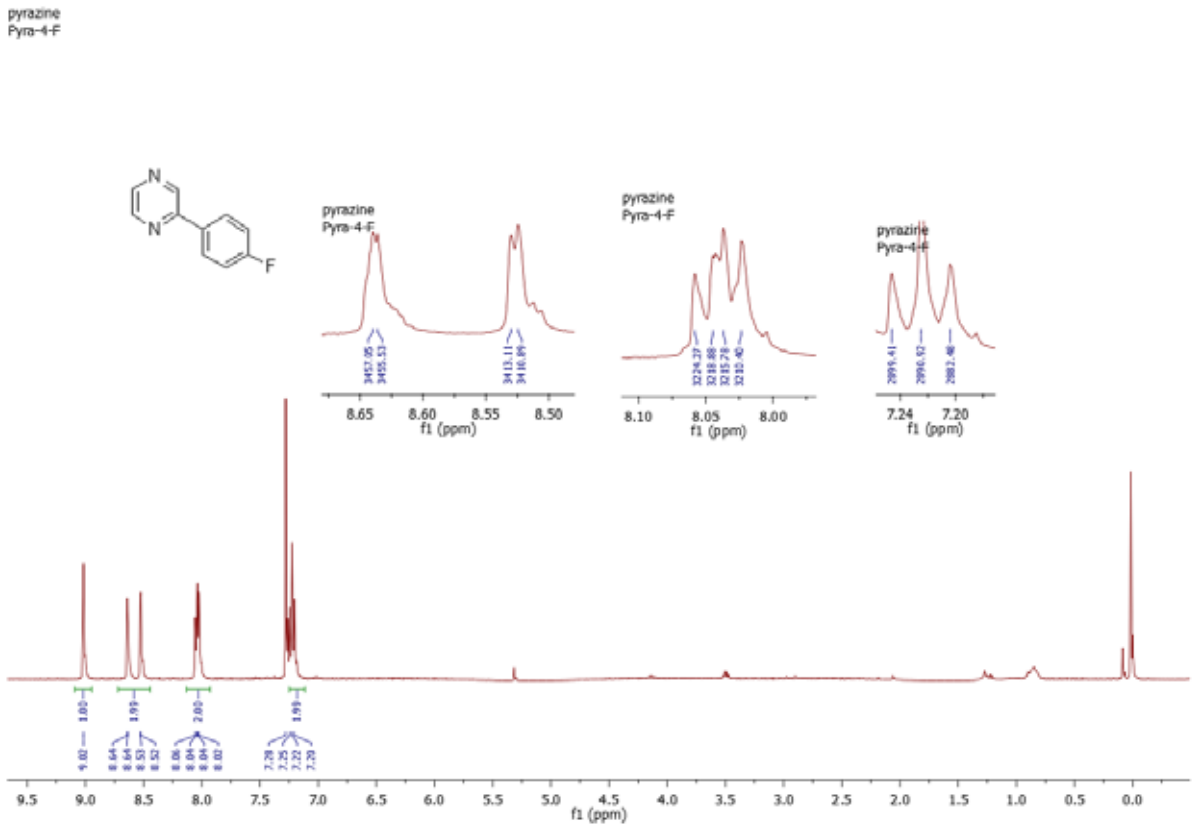
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
191.03638	1	411060.3	C10 H8 Cl N2	(M+H)+
192.03954	1	53858.5	C10 H8 Cl N2	(M+H)+
193.03311	1	138550	C10 H8 Cl N2	(M+H)+
194.03638	1	19766	C10 H8 Cl N2	(M+H)+
195.03783	1	802	C10 H8 Cl N2	(M+H)+

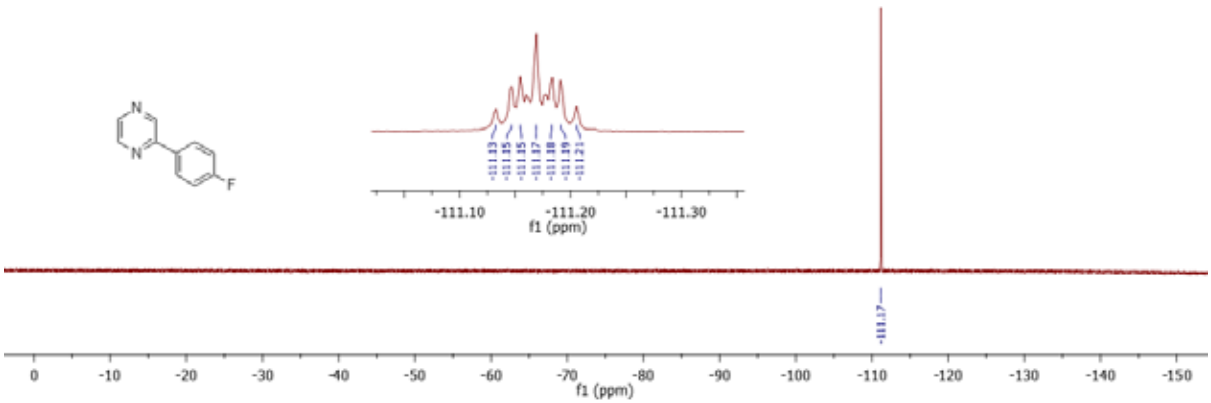
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	191.03638	191.03705	3.54	100	100	65.87	67.48
2	192.03954	192.04003	2.55	13.1	11.64	8.63	7.85
3	193.03311	193.03427	6.01	33.71	32.61	22.2	22.01
4	194.03638	194.03713	3.85	4.81	3.74	3.17	2.53
5	195.03783	195.04004	11.31	0.2	0.2	0.13	0.13

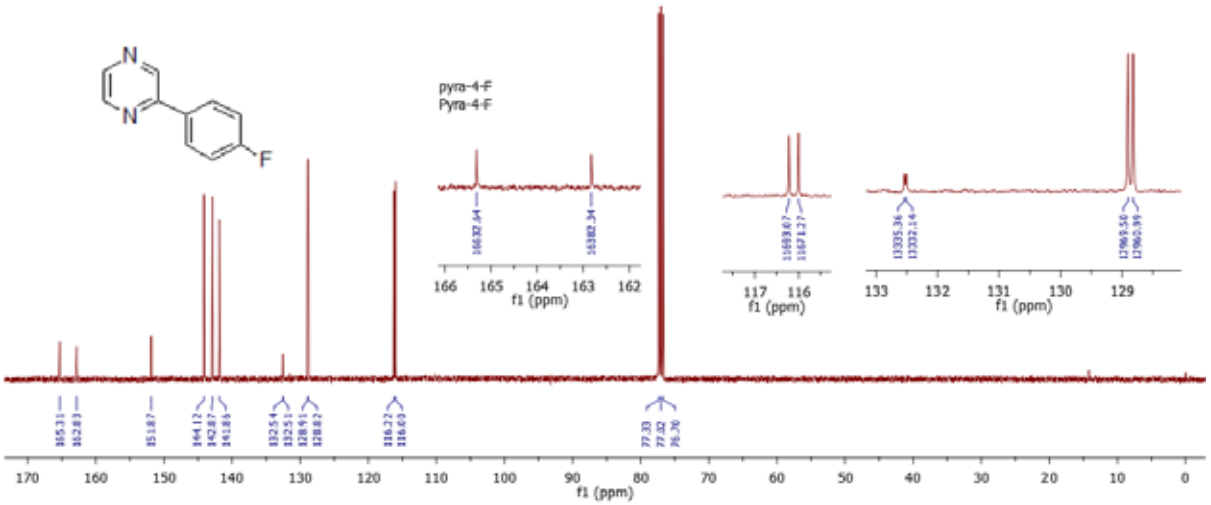
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3l**:



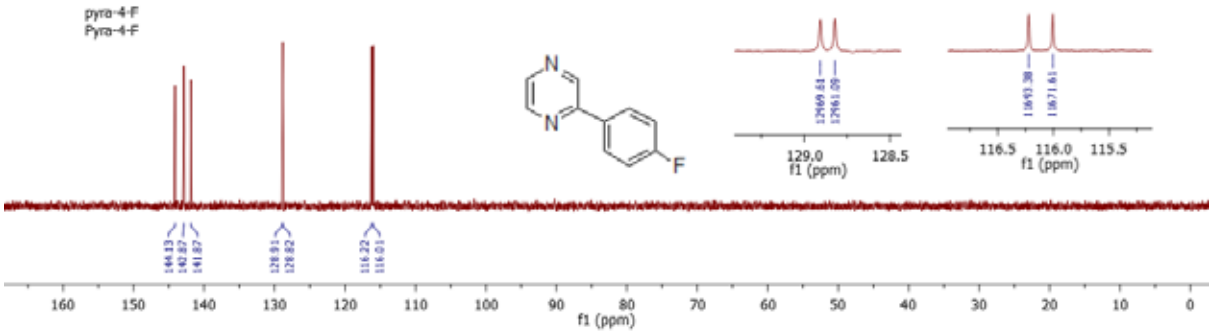
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3l:**



^{13}C NMR (100 MHz, $CDCl_3$) of compound **3l**:



DEPT (100 MHz, $CDCl_3$) of compound **3l**:



HRMS (ESI-TOF) of compound **3l**:

Qualitative Compound Report

Data File	PYRA-4-F.d	**Sample Name**	PYRA-4-F
Sample Type	Sample	**Position**	Vial 48
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:31:47 PM
IRM Calibration Status	[redacted]	**DA Method**	as.m
Comment			

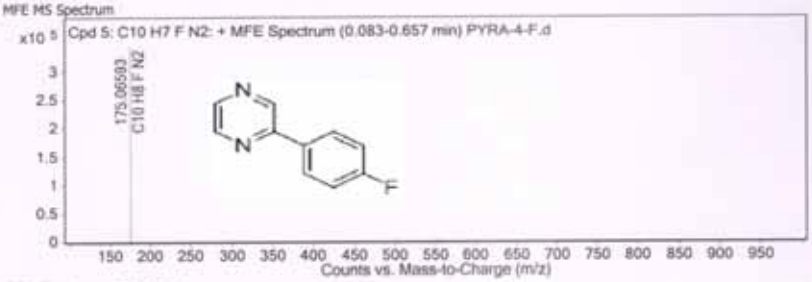
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C10 H7 F N2	0.178	174.05866	C10 H7 F N2	C10 H7 F N2	3.86	C10 H7 F N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C10 H7 F N2	175.06593	0.178	Find by Molecular Feature	174.05866

MFE MS Spectrum



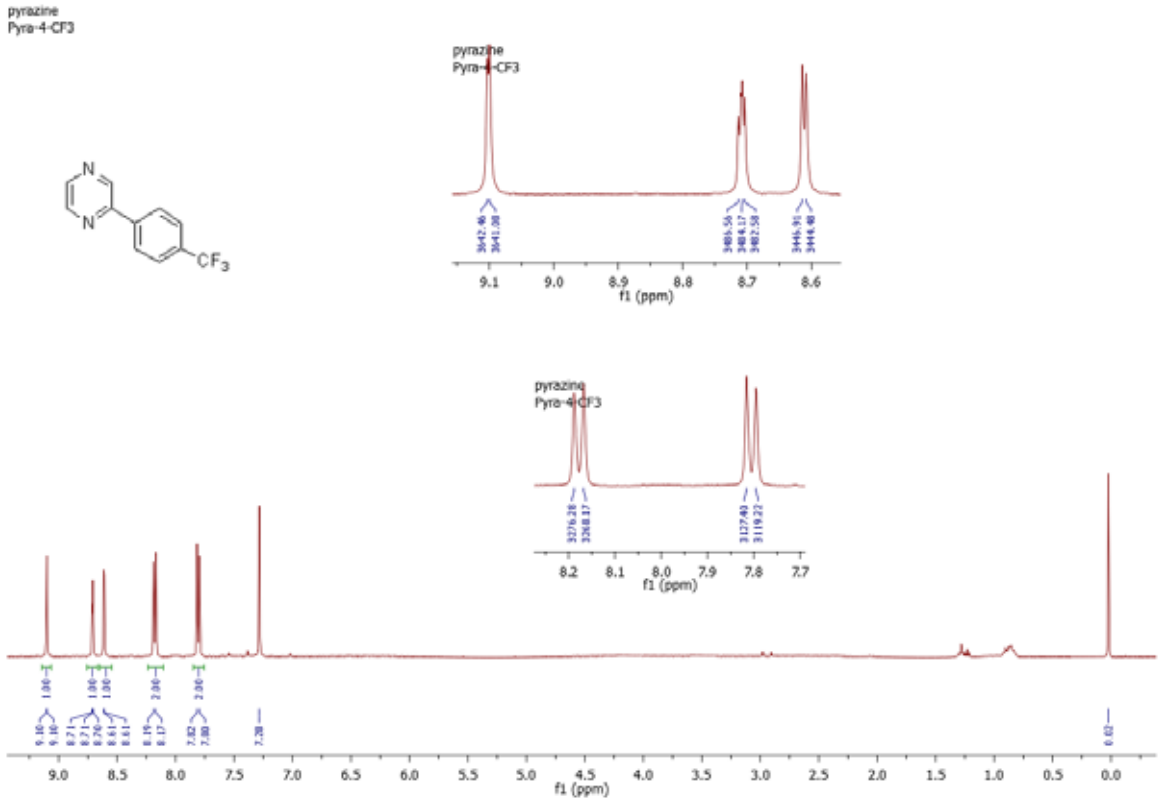
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
175.06593	1	344539.9	C10 H8 F N2	(M+H)+
176.0686	1	47231.5	C10 H8 F N2	(M+H)+
177.07051	1	3116.4	C10 H8 F N2	(M+H)+

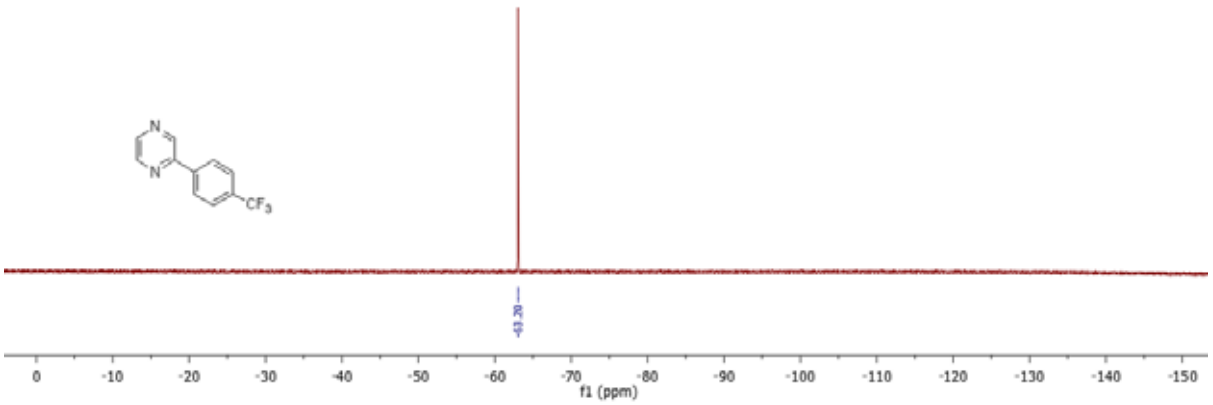
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	175.06593	175.0666	3.83	100	100	87.25	89.08
2	176.0686	176.06958	5.58	13.71	11.64	11.96	10.37
3	177.07051	177.07252	11.35	0.9	0.62	0.79	0.55

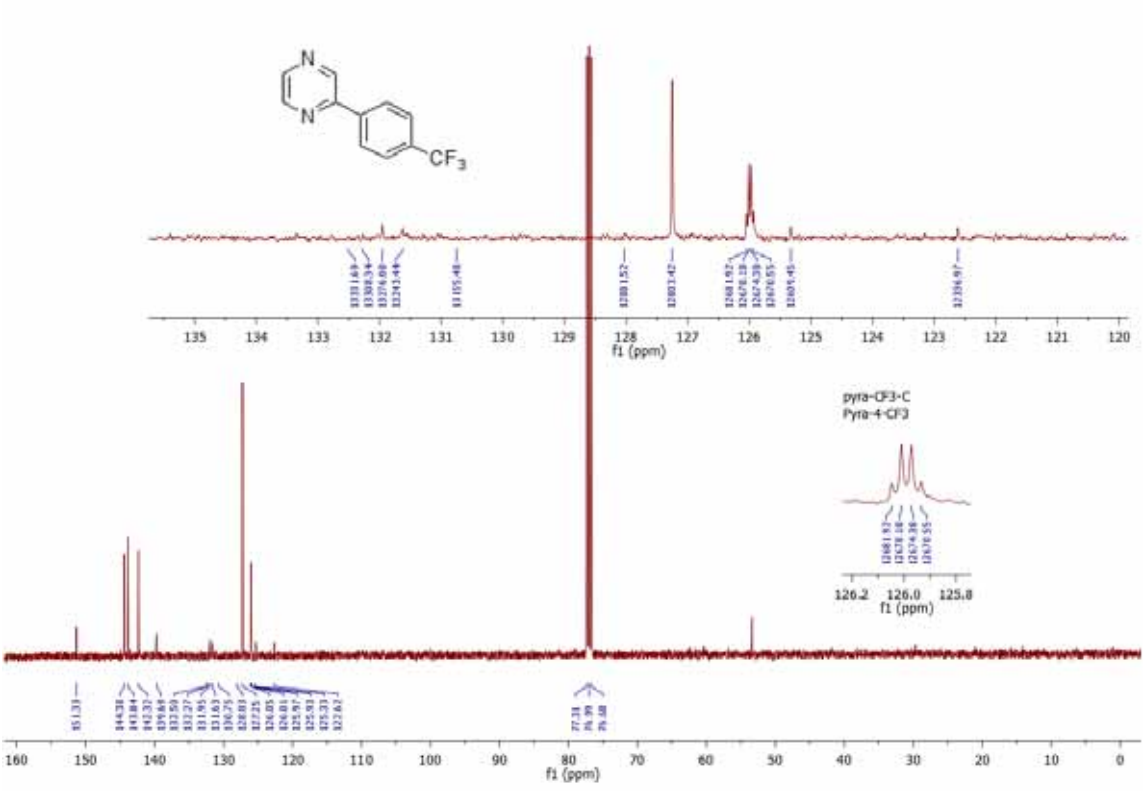
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3m**:



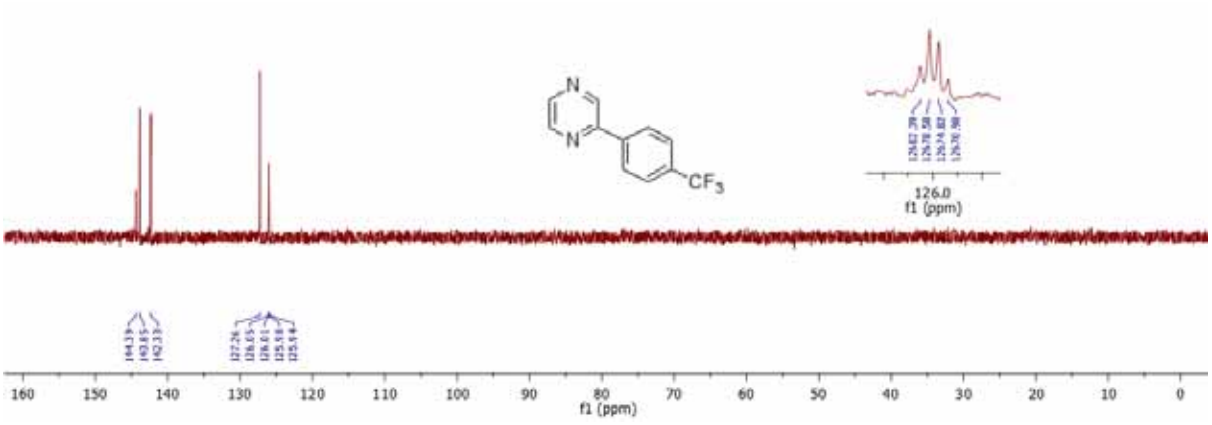
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3m:**



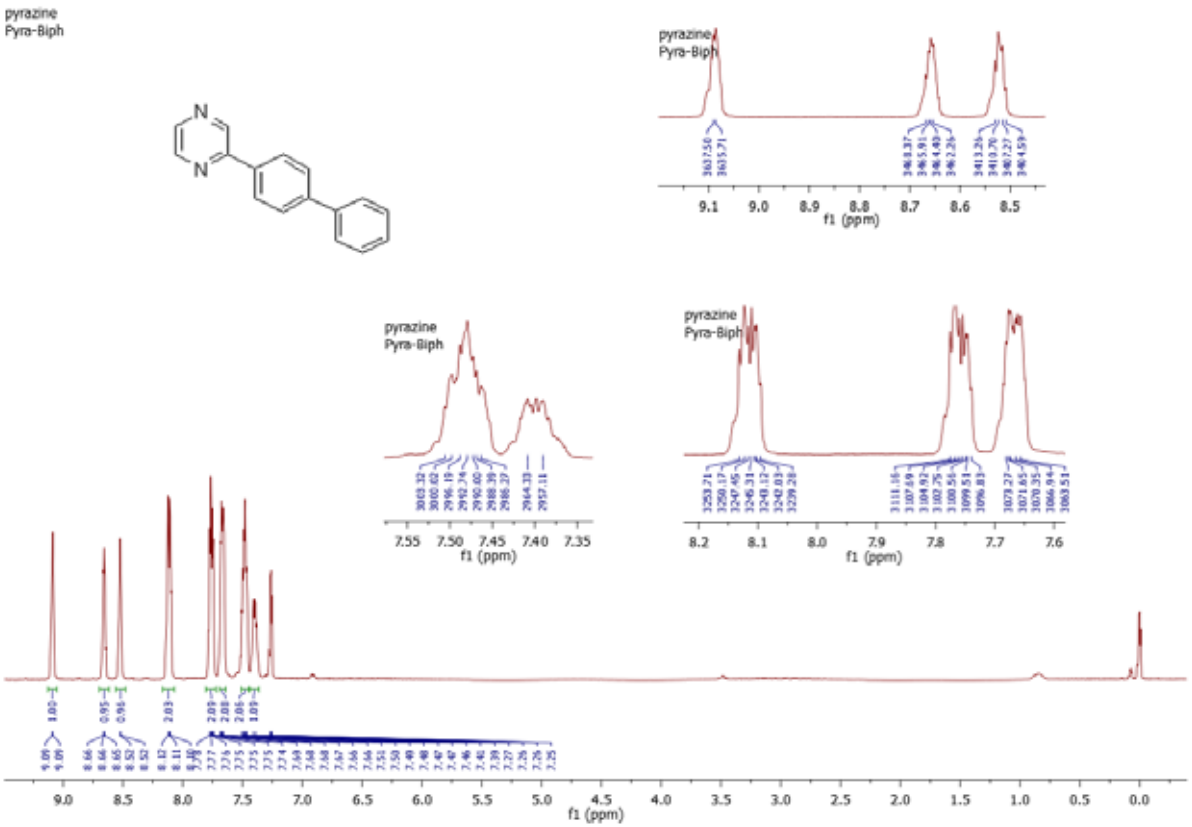
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3m**:



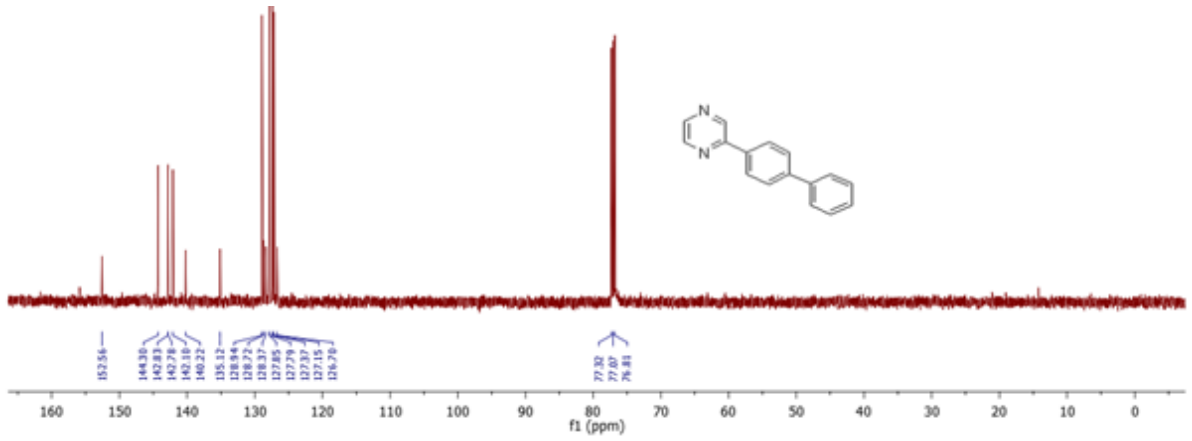
DEPT (100 MHz, $CDCl_3$) of compound **3m**:



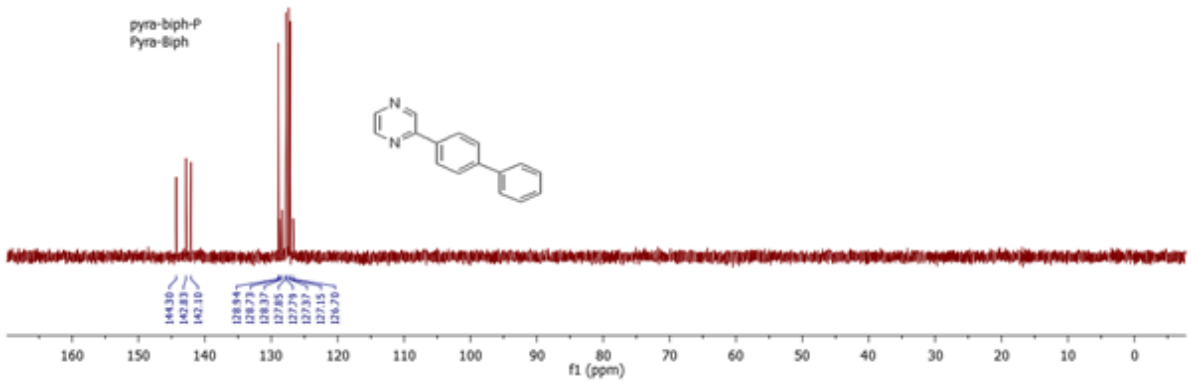
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3n**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3n**:



DEPT (125 MHz, $CDCl_3$) of compound **3n**:



HRMS (ESI-TOF) of compound **3n**:

Qualitative Compound Report

Data File	PYRA-BiPh.d	**Sample Name**	PYRA-BiPh
Sample Type	Sample	**Position**	Vial 51
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:39:24 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

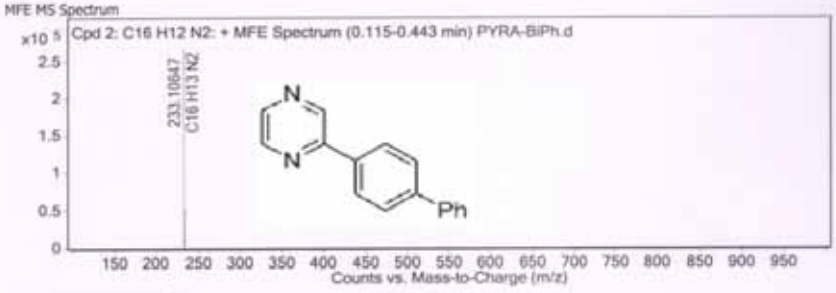
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C16 H12 N2	0.176	232.0992	C16 H12 N2	C16 H12 N2	3.67	C16 H12 N2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C16 H12 N2	233.10647	0.176	Find by Molecular Feature	232.0992

MFE MS Spectrum



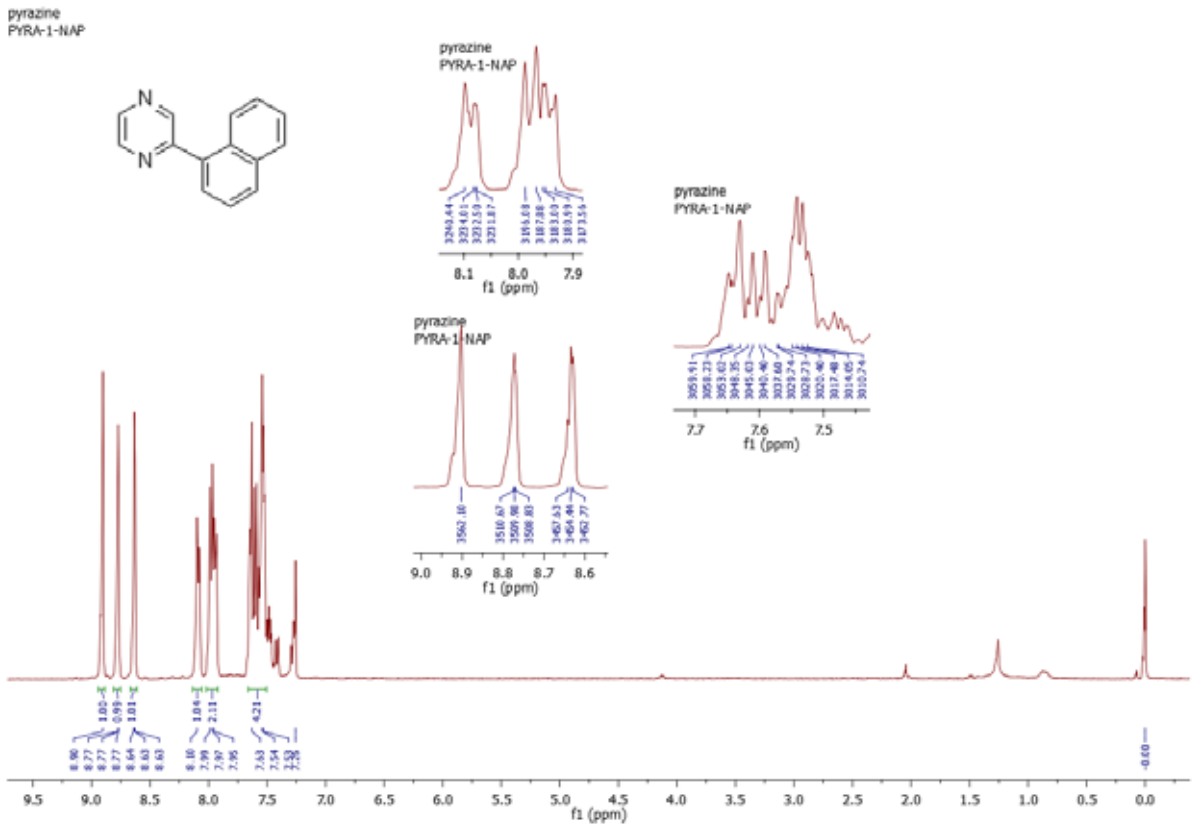
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
233.10647	1	267274.2	C16 H13 N2	(M+H)+
234.1096	1	50602.9	C16 H13 N2	(M+H)+
235.11261	1	4067	C16 H13 N2	(M+H)+

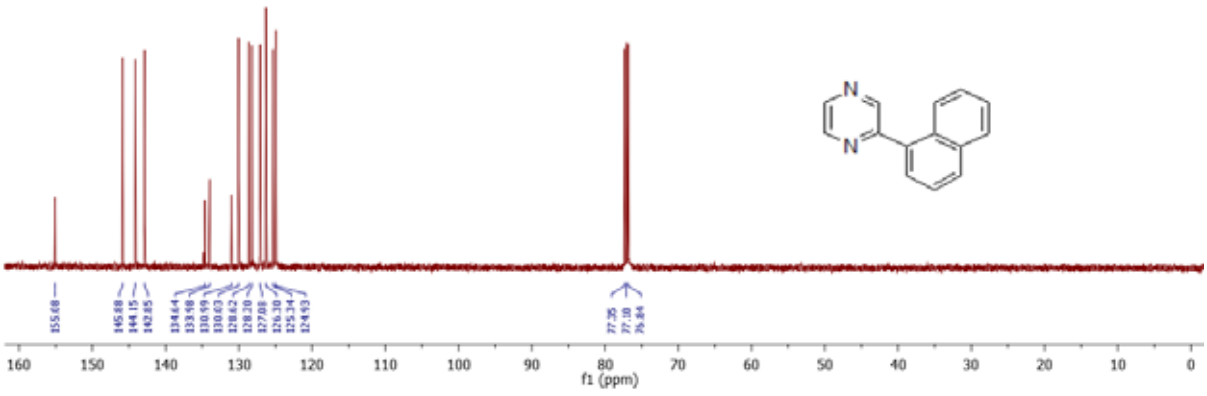
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	233.10647	233.10732	3.65	100	100	83.02	83.51
2	234.1096	234.11045	3.64	18.93	18.19	15.72	15.19
3	235.11261	235.11356	4.05	1.52	1.56	1.26	1.3

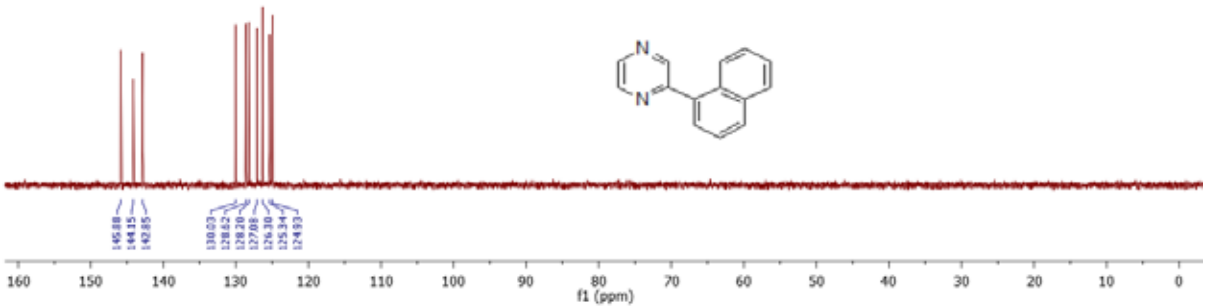
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3o**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3o**:



DEPT (125 MHz, $CDCl_3$) of compound **3o**:



HRMS (ESI-TOF) of compound **3o**:

Qualitative Compound Report

Data File	PYRA-1-NAP.d	**Sample Name**	PYRA-1-NAP
Sample Type	Sample	**Position**	Vial 50
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:36:54 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

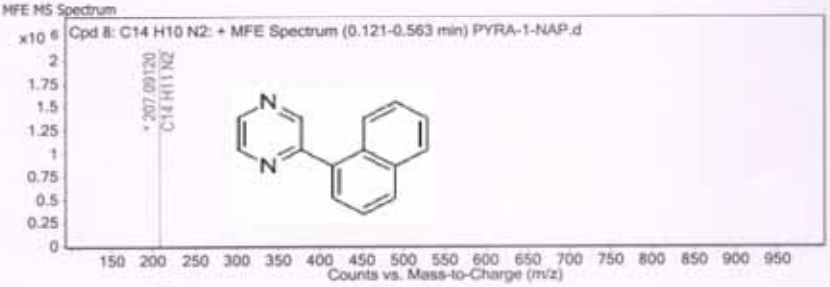
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C14 H10 N2	0.175	206.08392	C14 H10 N2	C14 H10 N2	2.31	C14 H10 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C14 H10 N2	207.0912	0.175	Find by Molecular Feature	206.08392

MFE MS Spectrum



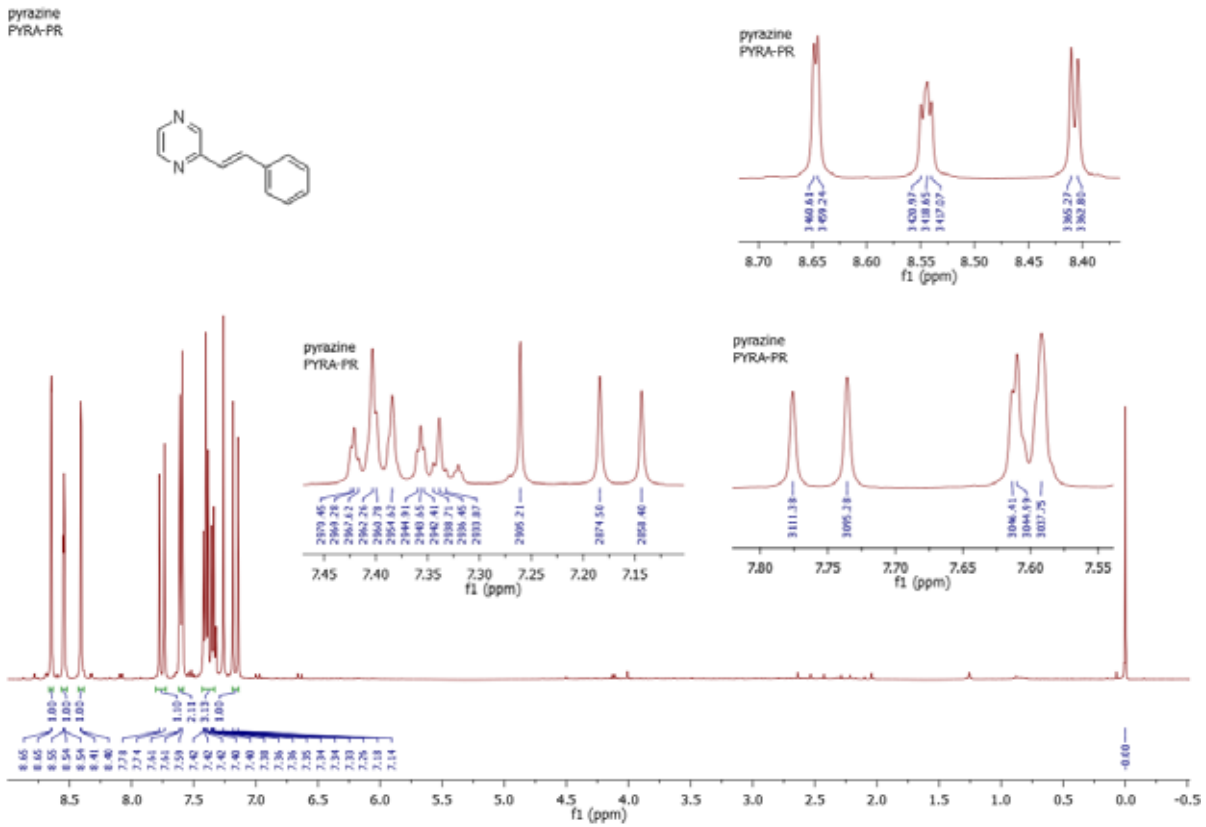
MS Spectrum Peak List

m/z	*z*	Abund	Formula	Ion
207.0912	1	2146200.3	C14 H11 N2	(M+H)+
208.09411	1	318334.9	C14 H11 N2	(M+H)+
209.09685	1	24313.3	C14 H11 N2	(M+H)+
210.10005	1	1355.2	C14 H11 N2	(M+H)+

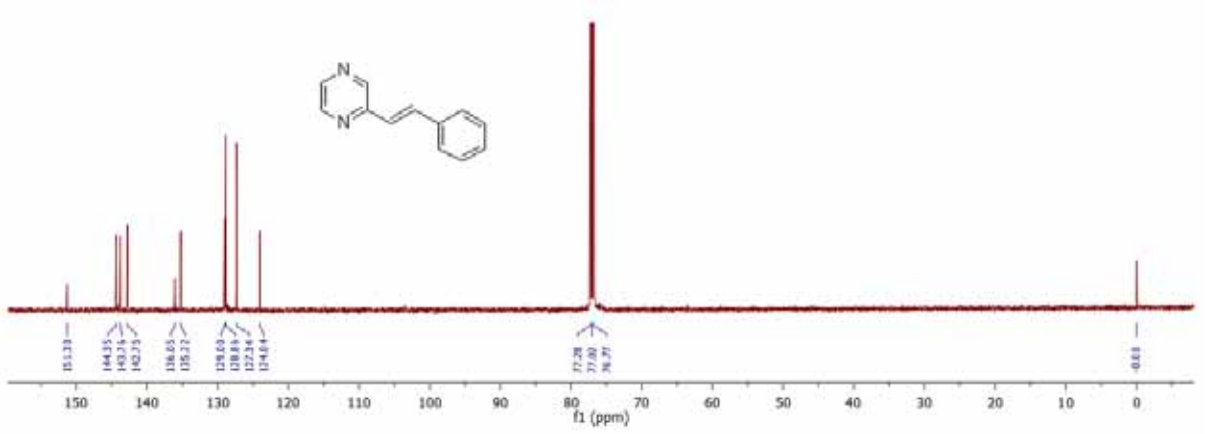
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	207.0912	207.09167	2.3	100	100	86.19	85.29
2	208.09411	208.09476	3.15	14.83	16	12.78	13.65
3	209.09685	209.09783	4.68	1.13	1.2	0.98	1.02
4	210.10005	210.10087	3.92	0.06	0.06	0.05	0.05

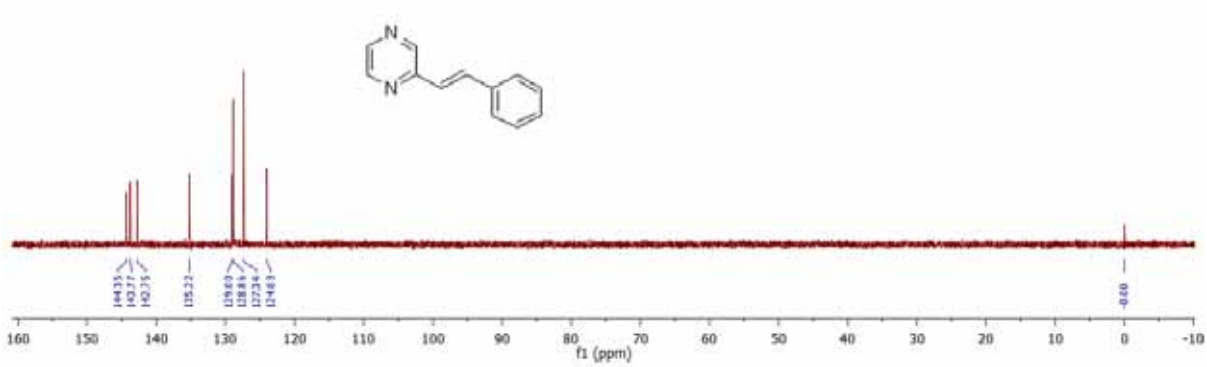
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3p**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3p**:



DEPT (125 MHz, $CDCl_3$) of compound **3p**:



HRMS (ESI-TOF) of compound **3p**:

Qualitative Compound Report

Data File	PYRA-PV.d	**Sample Name**	PYRA-PV
Sample Type	Sample	**Position**	Vial 76
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/24/2012 5:38:53 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

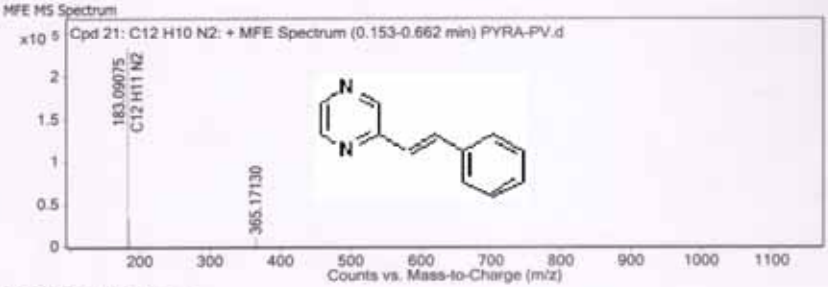
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C12 H10 N2	0.217	182.08347	C12 H10 N2	C12 H10 N2	5.1	C12 H10 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C12 H10 N2	183.09075	0.217	Find by Molecular Feature	182.08347

MFE MS Spectrum



MS Spectrum Peak List

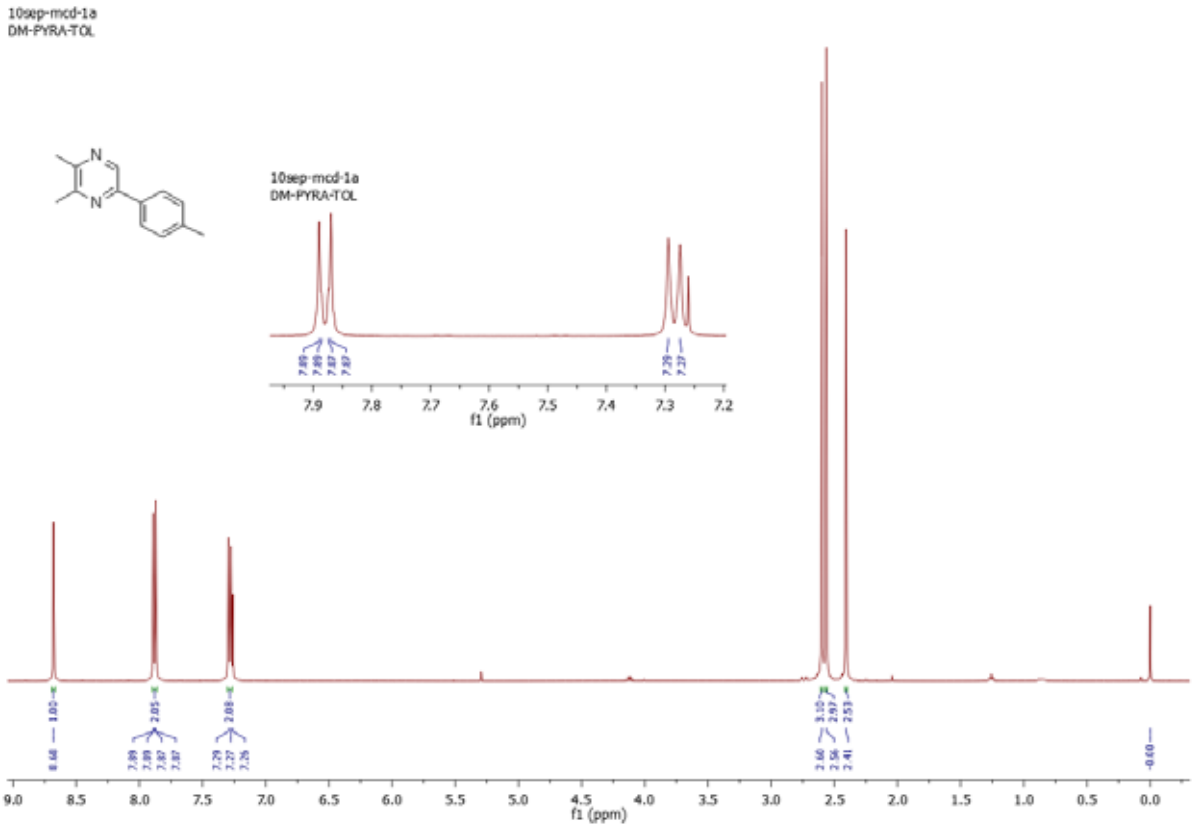
m/z	z	Abund	Formula	Ion
183.09075	1	233781.8	C12 H11 N2	(M+H)+
184.09392	1	33656.6	C12 H11 N2	(M+H)+
185.09783	1	4125.2	C12 H11 N2	(M+H)+
365.1713	1	9049.7		(2M+H)+
366.17567	1	2963.9		(2M+H)+

Predicted Isotope Match Table

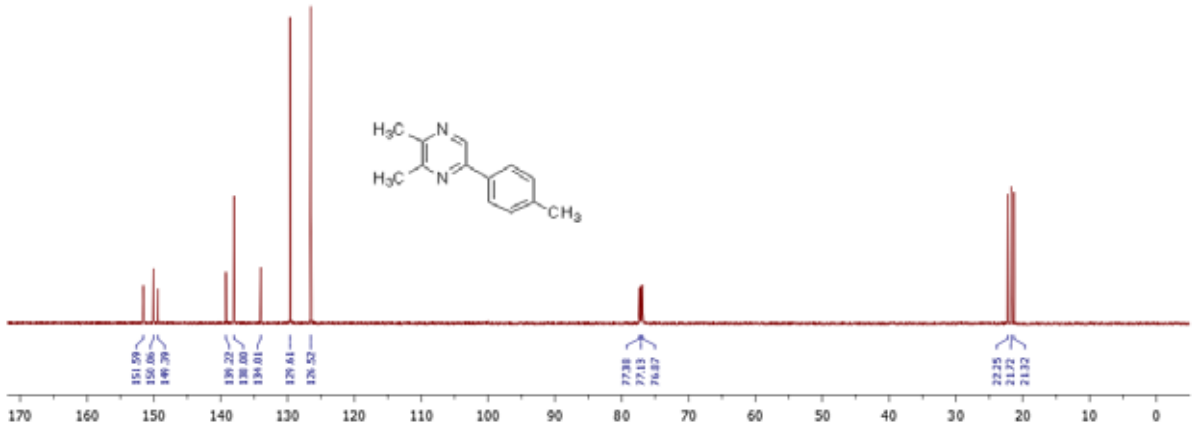
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	183.09075	183.09167	5.07	100	100	86.09	87.17
2	184.09392	184.09472	4.36	14.4	13.84	12.39	12.06
3	185.09783	185.09774	-0.48	1.76	0.89	1.52	0.77

--- End Of Report ---

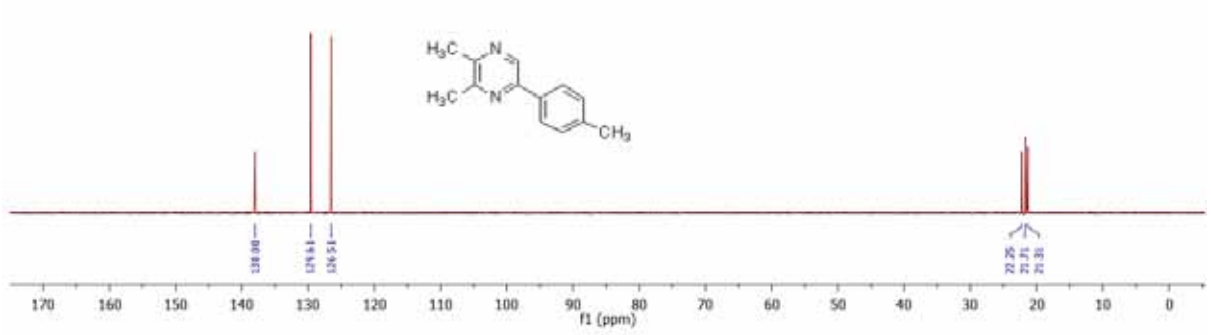
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3q**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3q**:



DEPT (125 MHz, $CDCl_3$) of compound **3q**:



HRMS (ESI-TOF) of compound **3q**:

Qualitative Compound Report

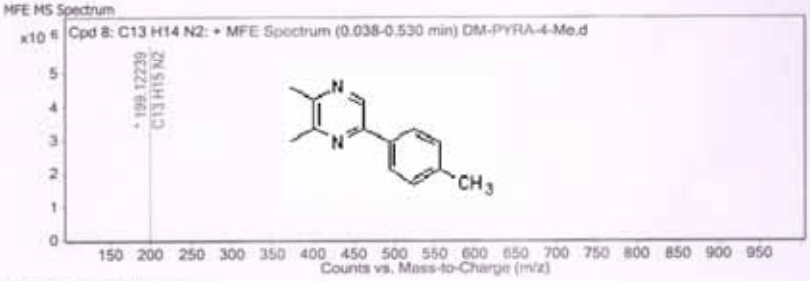
Data File	DM-PYRA-4-Me.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	as.m
Comment	Sample information is unavailable		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C13 H14 N2	0.178	198.11512	C13 H14 N2	C13 H14 N2	2.94	C13 H14 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C13 H14 N2	199.12239	0.178	Find by Molecular Feature	198.11512

MFE MS Spectrum



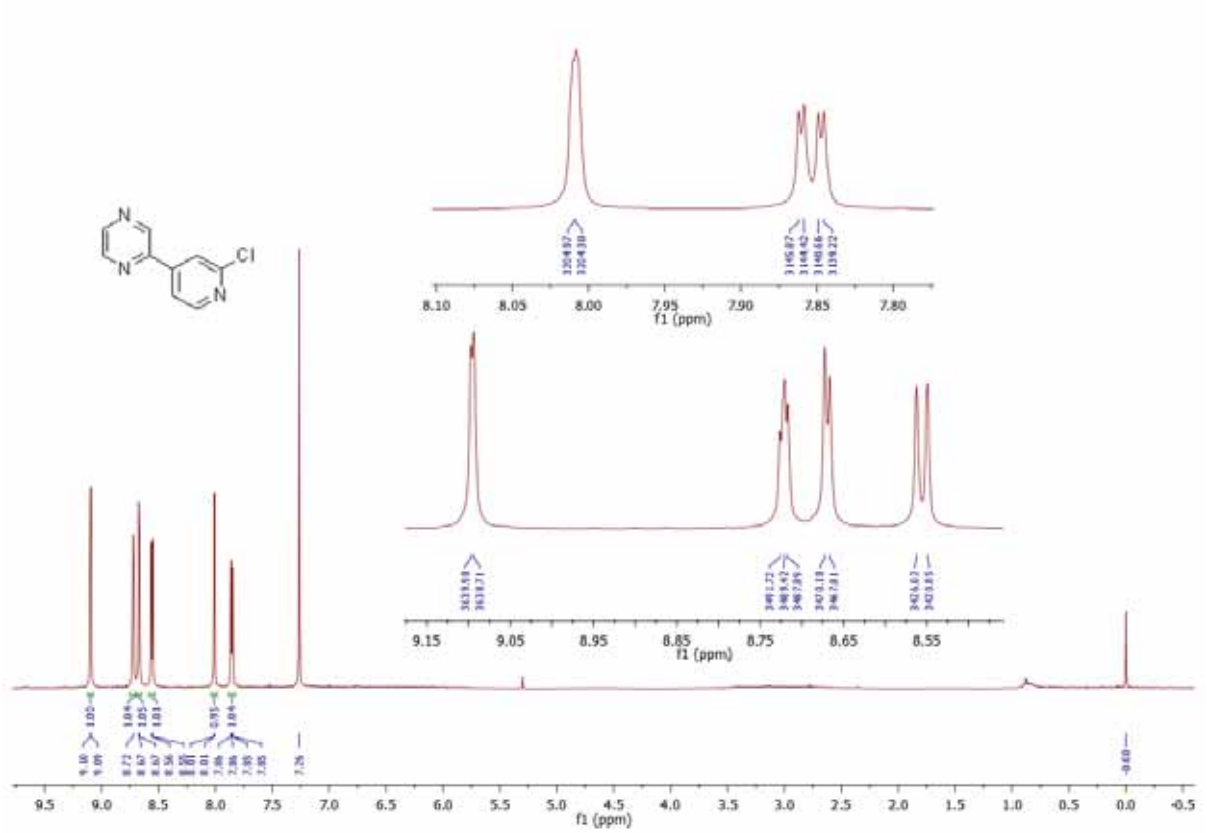
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
199.12239	1	5820319.5	C13 H15 N2	(M+H)+
200.12575	1	865348.4	C13 H15 N2	(M+H)+
201.12836	1	44181.6	C13 H15 N2	(M+H)+
202.1313	1	823.7	C13 H15 N2	(M+H)+

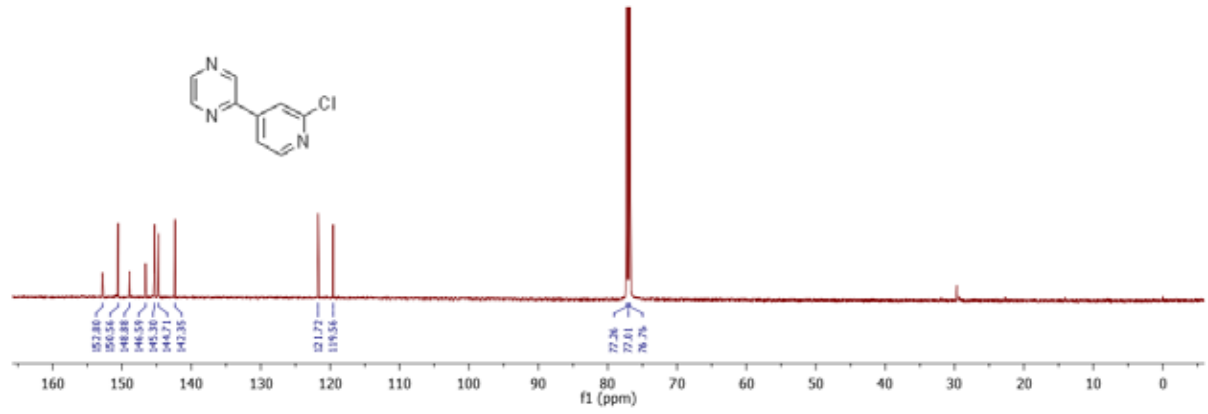
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	199.12239	199.12297	2.93	100	100	86.47	86.17
2	200.12575	200.12605	1.52	14.87	14.96	12.86	12.89
3	201.12836	201.12911	3.73	0.76	1.04	0.66	0.9
4	202.1313	202.13214	4.12	0.01	0.04	0.01	0.04

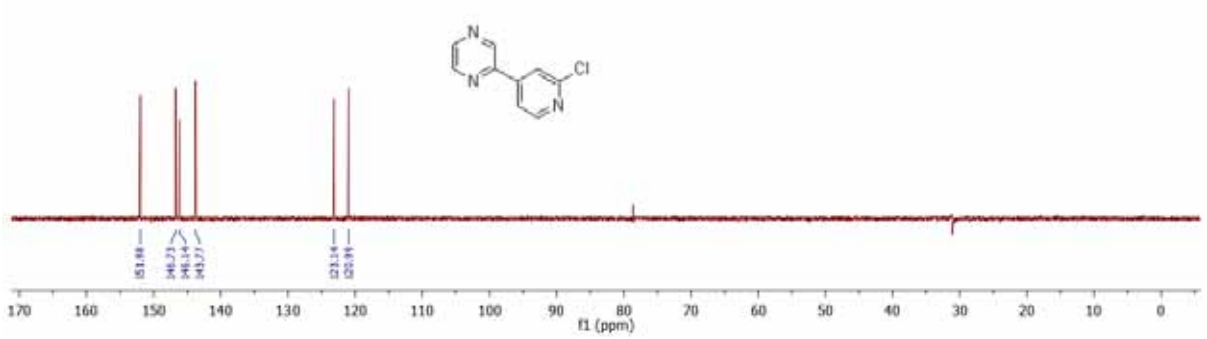
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3r**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **3r**:



DEPT (125 MHz, $CDCl_3$) of compound **3r**:



HRMS (ESI-TOF) of compound **3r**:

Qualitative Compound Report

Data File	PYRA-2Cl-Py.d	**Sample Name**	PYRA-2Cl-Py
Sample Type	Sample	**Position**	Vial 42
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/7/2012 1:59:07 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

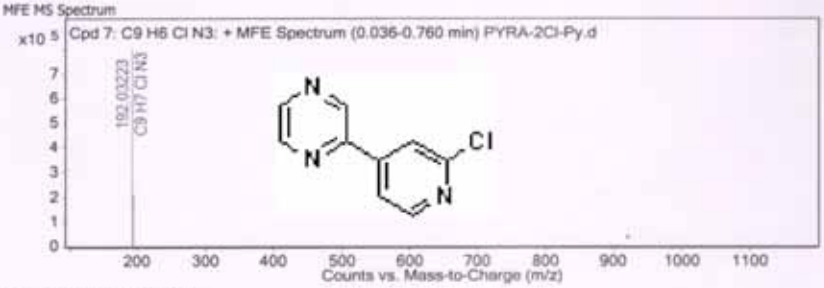
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C9 H6 Cl N3	0.286	191.02495	C9 H6 Cl N3	C9 H6 Cl N3	0.4	C9 H6 Cl N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C9 H6 Cl N3	192.03223	0.286	Find by Molecular Feature	191.02495

MFE MS Spectrum



MS Spectrum Peak List

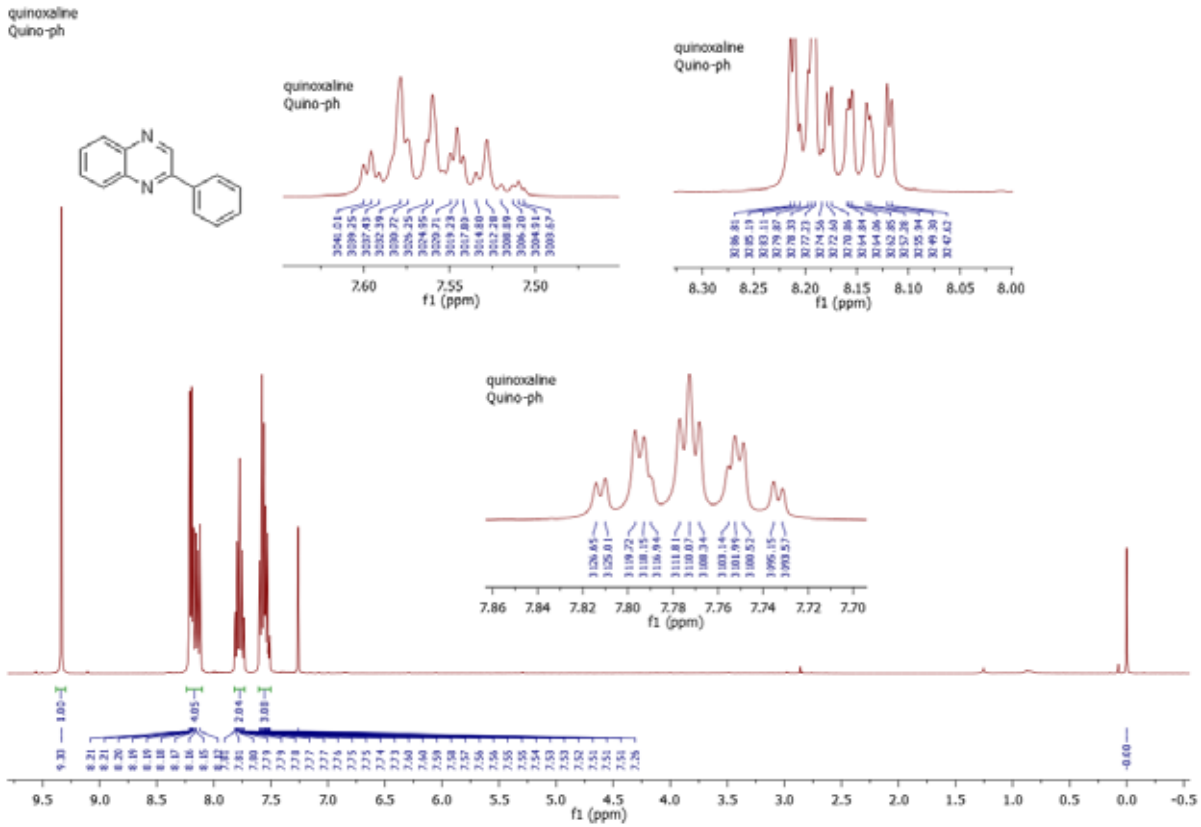
m/z	z	Abund	Formula	Ion
192.03223	1	802706.4	C9 H7 Cl N3	(M+H)+
193.03511	1	77497.2	C9 H7 Cl N3	(M+H)+
194.02923	1	215686.5	C9 H7 Cl N3	(M+H)+
195.03209	1	22655.2	C9 H7 Cl N3	(M+H)+
196.03629	1	871.4	C9 H7 Cl N3	(M+H)+

Predicted Isotope Match Table

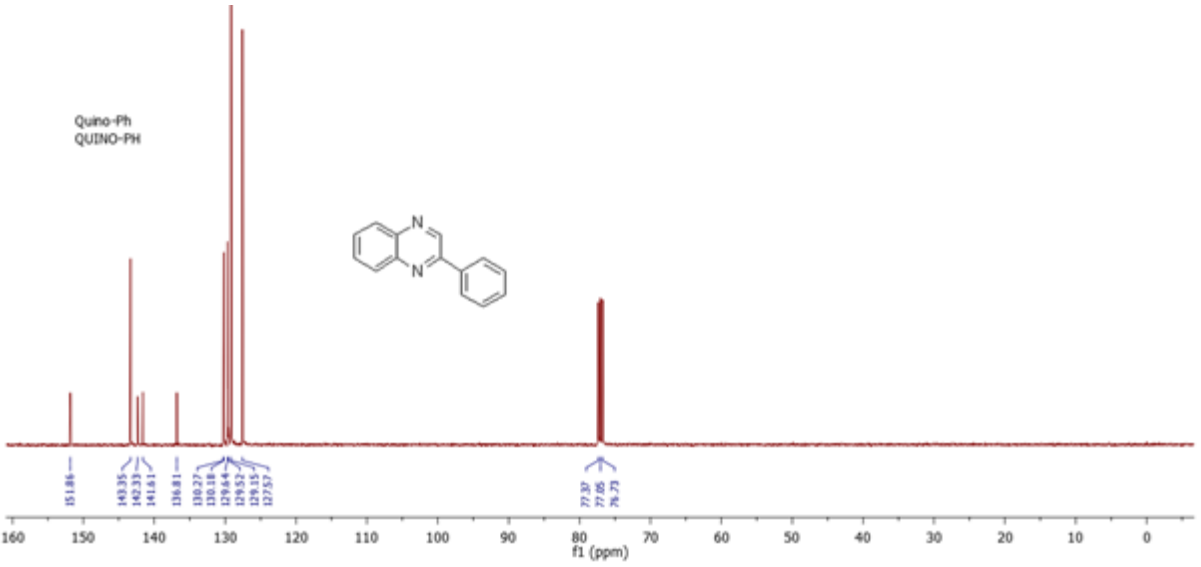
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	192.03223	192.0323	0.38	100	100	71.71	67.97
2	193.03511	193.03504	-0.33	9.65	10.91	6.92	7.42
3	194.02923	194.02949	1.35	26.87	32.54	19.27	22.11
4	195.03209	195.03213	0.21	2.82	3.51	2.02	2.38
5	196.03629	196.03477	-7.75	0.11	0.17	0.08	0.12

--- End Of Report ---

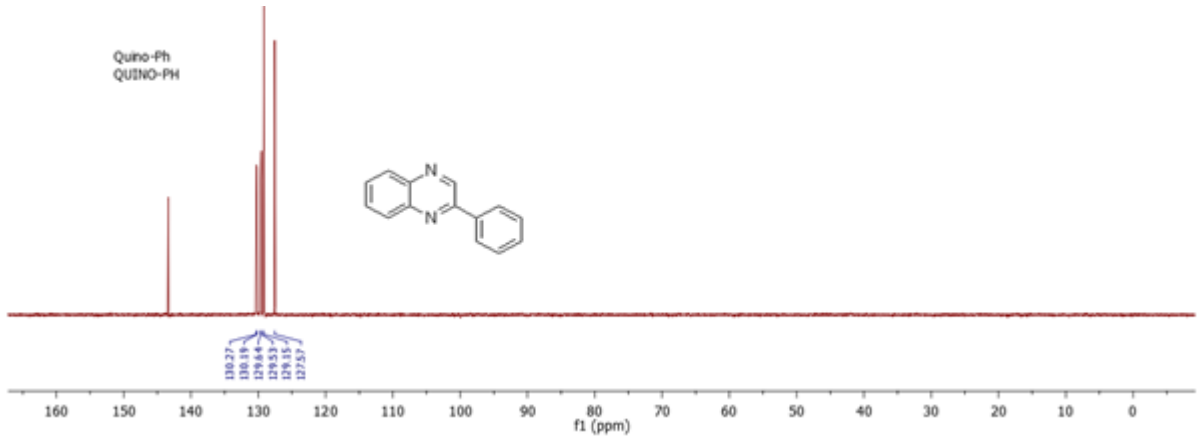
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6a**:



^{13}C NMR (100MHz, $CDCl_3$) of compound **6a**:



DEPT (100 MHz, $CDCl_3$) of compound **6a**:



HRMS (ESI-TOF) of compound **6a**:

Qualitative Compound Report

Data File	QUINO-Ph.d	**Sample Name**	QUINO-Ph
Sample Type	Sample	**Position**	Vial 56
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:52:23 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

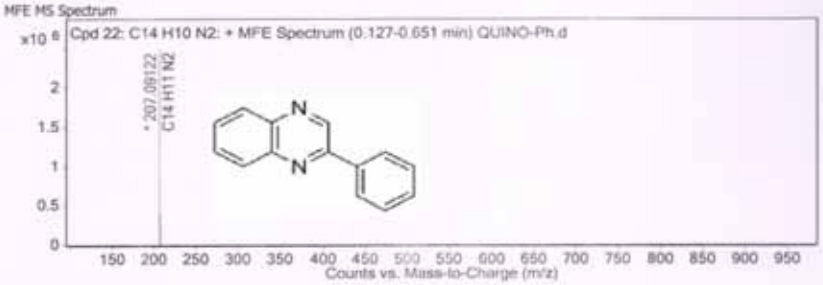
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C14 H10 N2	0.176	206.08394	C14 H10 N2	C14 H10 N2	2.23	C14 H10 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C14 H10 N2	207.09122	0.176	Find by Molecular Feature	206.08394

MFE MS Spectrum



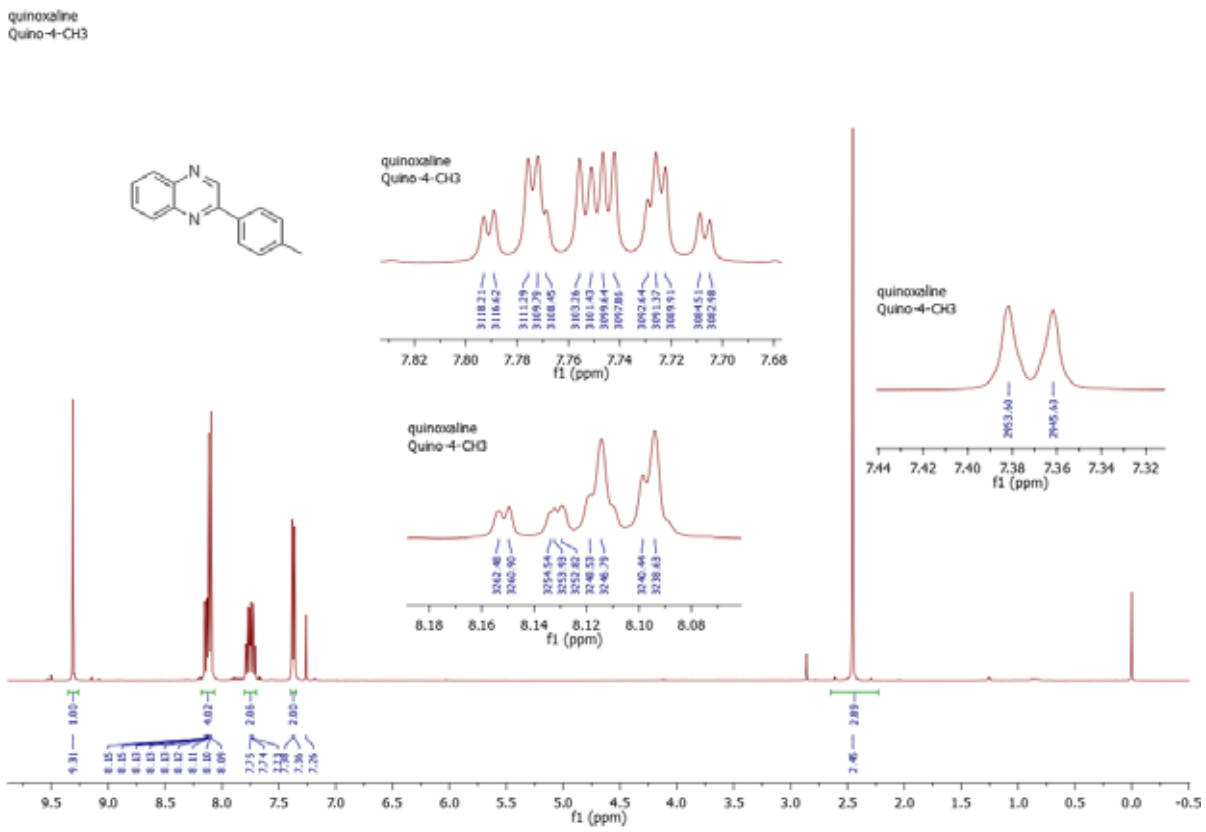
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
207.09122	1	2506758.5	C14 H11 N2	(M+H)+
208.09407	1	392421.3	C14 H11 N2	(M+H)+
209.09683	1	29461.2	C14 H11 N2	(M+H)+
210.10316	1	1389	C14 H11 N2	(M+H)+

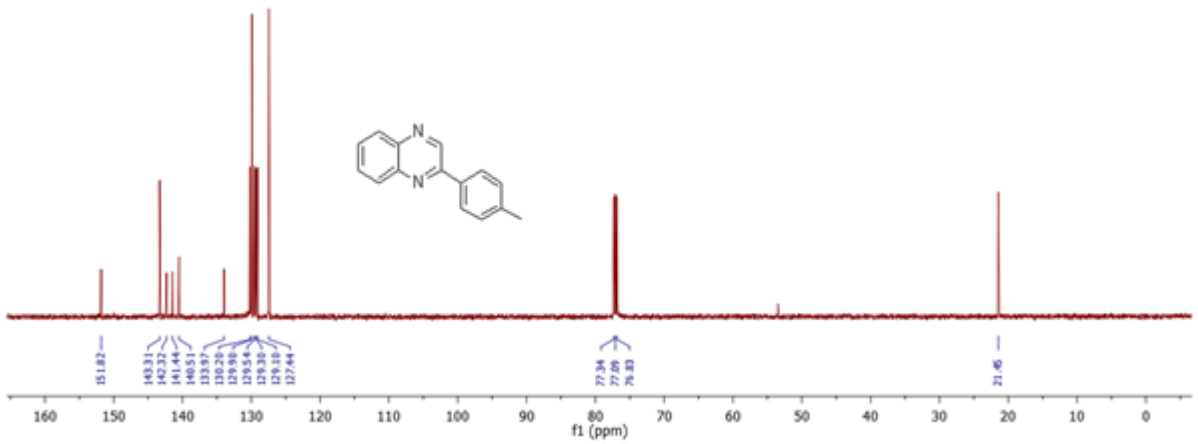
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	207.09122	207.09167	2.22	100	100	85.55	85.29
2	208.09407	208.09476	3.34	15.55	16	13.39	13.65
3	209.09683	209.09783	4.81	1.18	1.2	1.01	1.02
4	210.10316	210.10087	-10.9	0.06	0.06	0.05	0.05

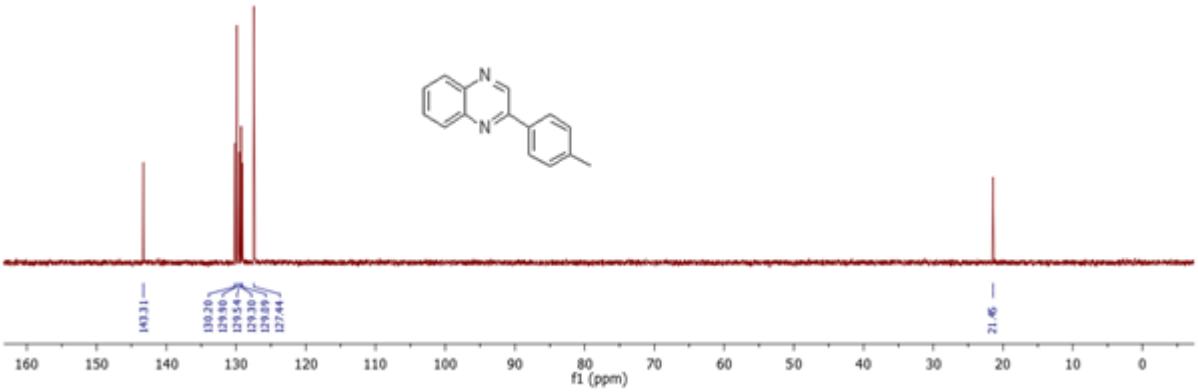
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6b**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **6b**:



DEPT (125 MHz, $CDCl_3$) of compound **6b**:



HRMS (ESI-TOF) of compound **6b**:

Qualitative Compound Report

Data File	QUINO-4-Me.d	**Sample Name**	QUINO-4-Me
Sample Type	Sample	**Position**	Vial 57
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:54:56 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

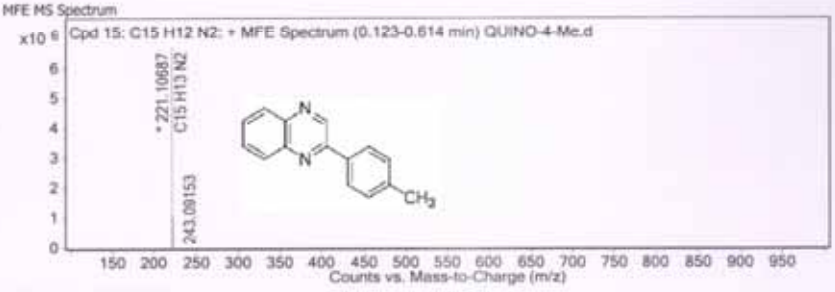
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C15 H12 N2	0.176	220.0996	C15 H12 N2	C15 H12 N2	2.05	C15 H12 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C15 H12 N2	221.10687	0.176	Find by Molecular Feature	220.0996

MFE MS Spectrum



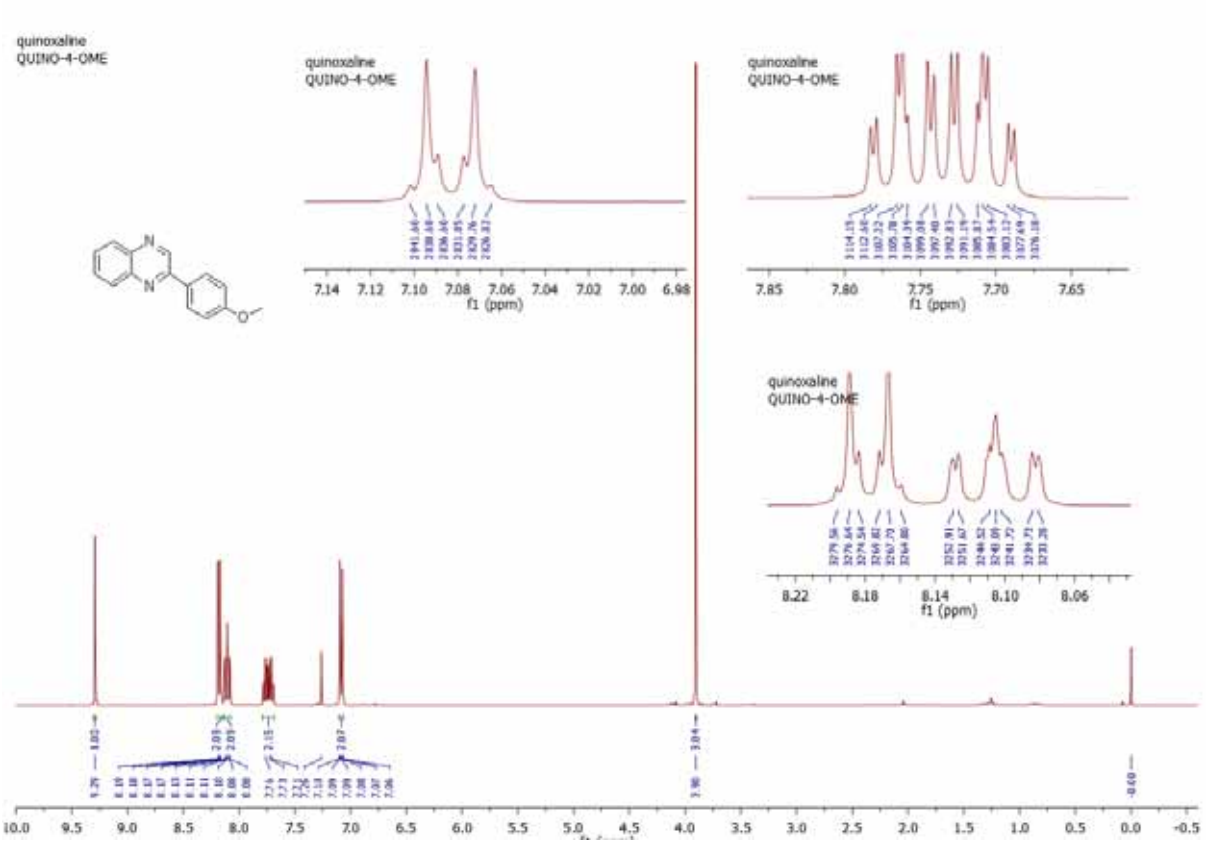
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
221.10687	1	6689054.5	C15 H13 N2	(M+H)+
222.10999	1	1052115.5	C15 H13 N2	(M+H)+
223.11278	1	82308.7	C15 H13 N2	(M+H)+
224.11543	1	1954.8	C15 H13 N2	(M+H)+
243.09153	1	1073		(M+Na)+

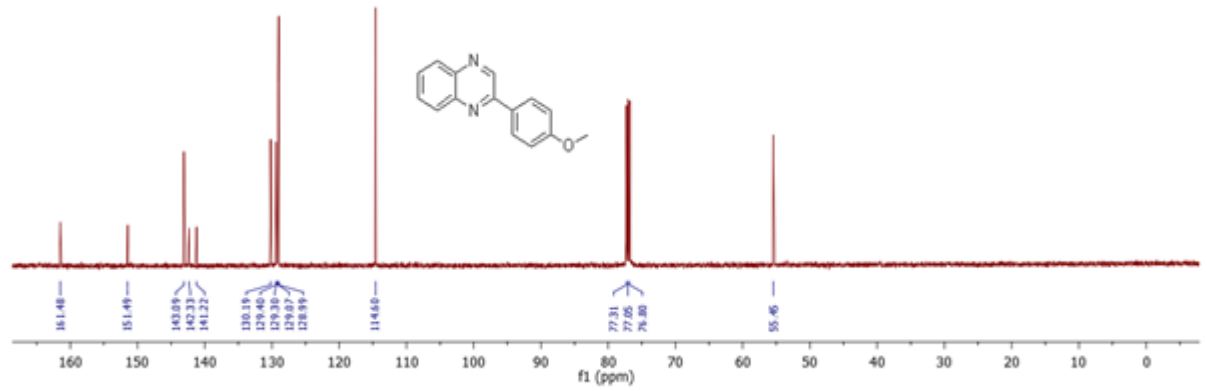
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	221.10687	221.10732	2.04	100	100	85.48	84.36
2	222.10999	222.11044	2	15.73	17.1	13.44	14.43
3	223.11278	223.11353	3.37	1.23	1.37	1.05	1.16
4	224.11543	224.1166	5.21	0.03	0.07	0.02	0.06

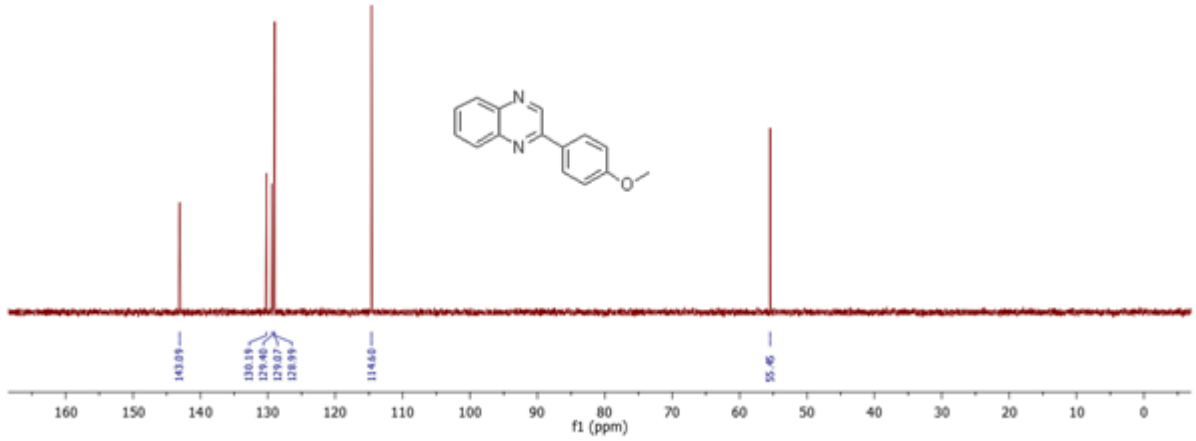
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6c**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **6c**:



DEPT (125 MHz, $CDCl_3$) of compound **6c**:



HRMS (ESI-TOF) of compound **6c**:

Qualitative Compound Report

Data File	QUINO-4-OMe.d	**Sample Name**	QUINO-4-OMe
Sample Type	Sample	**Position**	Vial 61
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 5:05:01 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

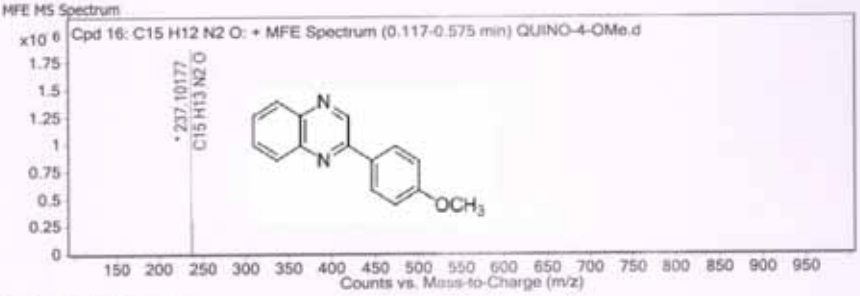
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C15 H12 N2 O	0.176	236.0945	C15 H12 N2 O	C15 H12 N2 O	1.98	C15 H12 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C15 H12 N2 O	237.10177	0.176	Find by Molecular Feature	236.0945

MFE MS Spectrum



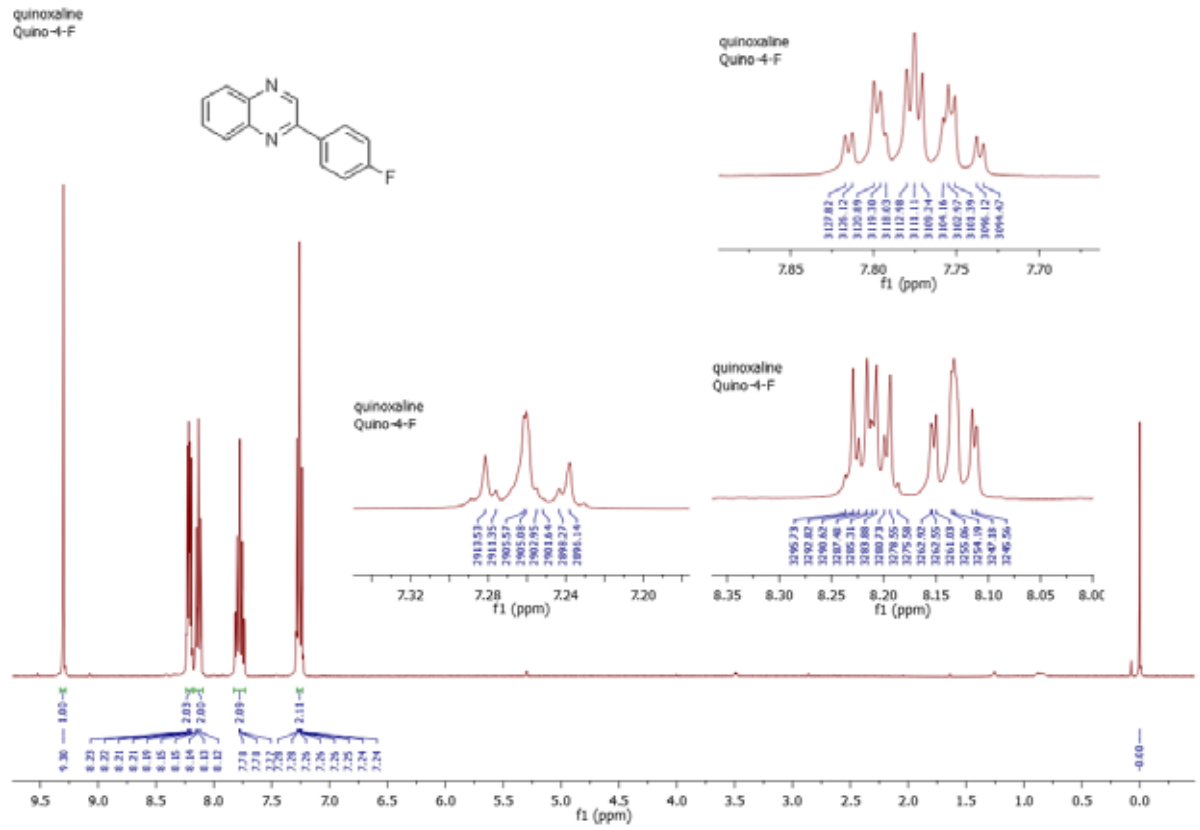
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
237.10177	1	1889205.1	C15 H13 N2 O	(M+H)+
238.1045	1	299427.8	C15 H13 N2 O	(M+H)+
239.10742	1	27798.2	C15 H13 N2 O	(M+H)+
240.10948	1	2370.6	C15 H13 N2 O	(M+H)+
241.11111	1	182.4	C15 H13 N2 O	(M+H)+

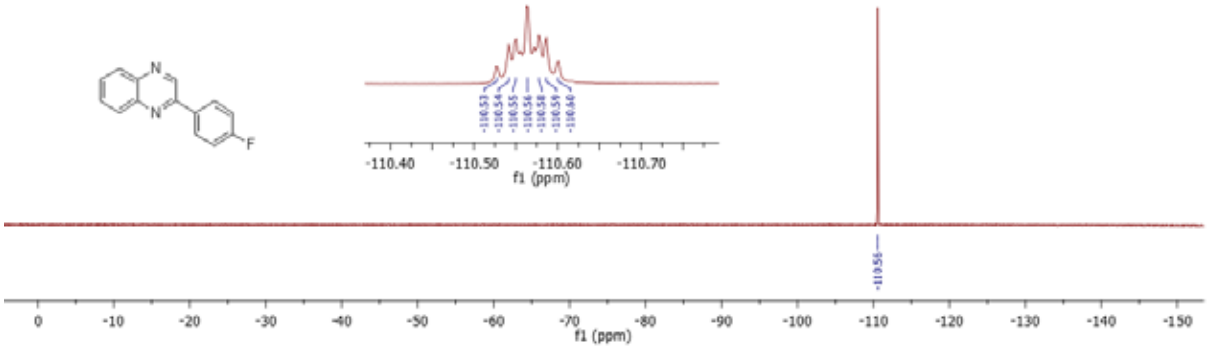
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	237.10177	237.10224	1.96	100	100	85.14	84.15
2	238.1045	238.10535	3.59	15.85	17.14	13.49	14.42
3	239.10742	239.10819	3.23	1.47	1.59	1.25	1.33
4	240.10948	240.11087	5.78	0.13	0.1	0.11	0.09
5	241.11111	241.11356	10.16	0.01	0.01	0.01	0

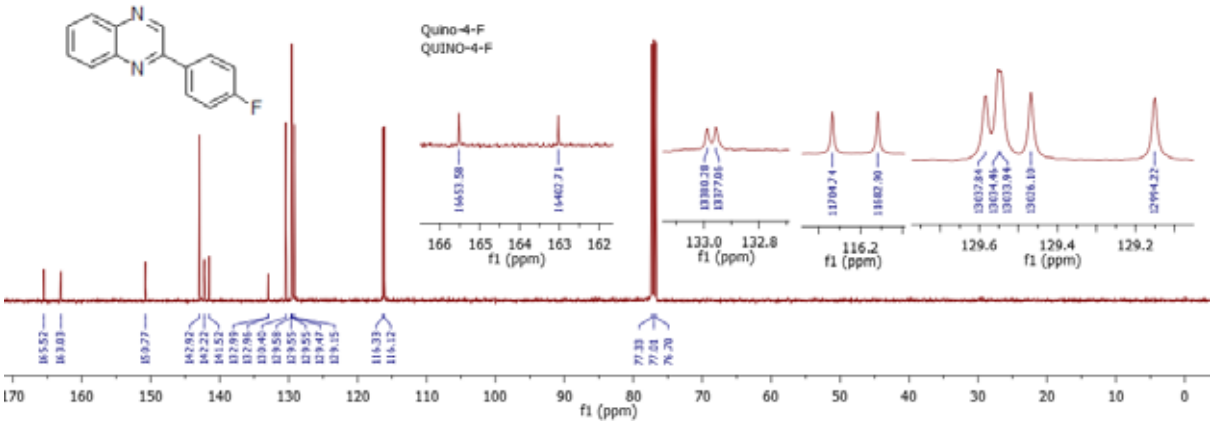
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6d**:



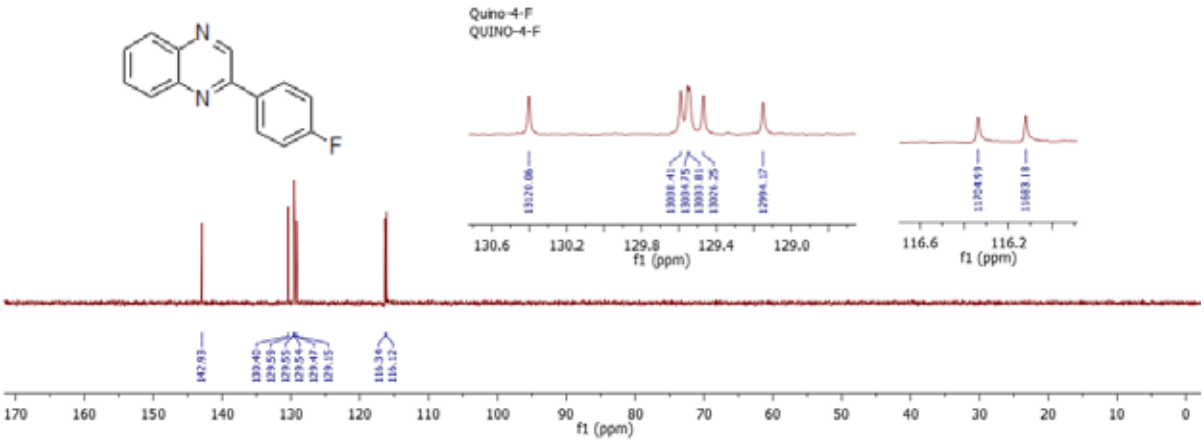
^{19}F NMR (376 MHz, $CDCl_3$) of compound **6d**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **6d**:



DEPT (100 MHz, $CDCl_3$) of compound **6d**:



HRMS (ESI-TOF) of compound **6d**:

Qualitative Compound Report

Data File	QUINO-4-F.d	**Sample Name**	QUINO-4-F
Sample Type	Sample	**Position**	Vial 58
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:57:26 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

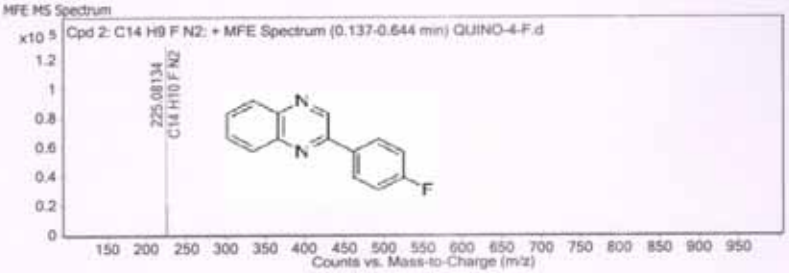
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C14 H9 F N2	0.176	224.07406	C14 H9 F N2	C14 H9 F N2	4.07	C14 H9 F N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C14 H9 F N2	225.08134	0.176	Find by Molecular Feature	224.07406

MFE MS Spectrum



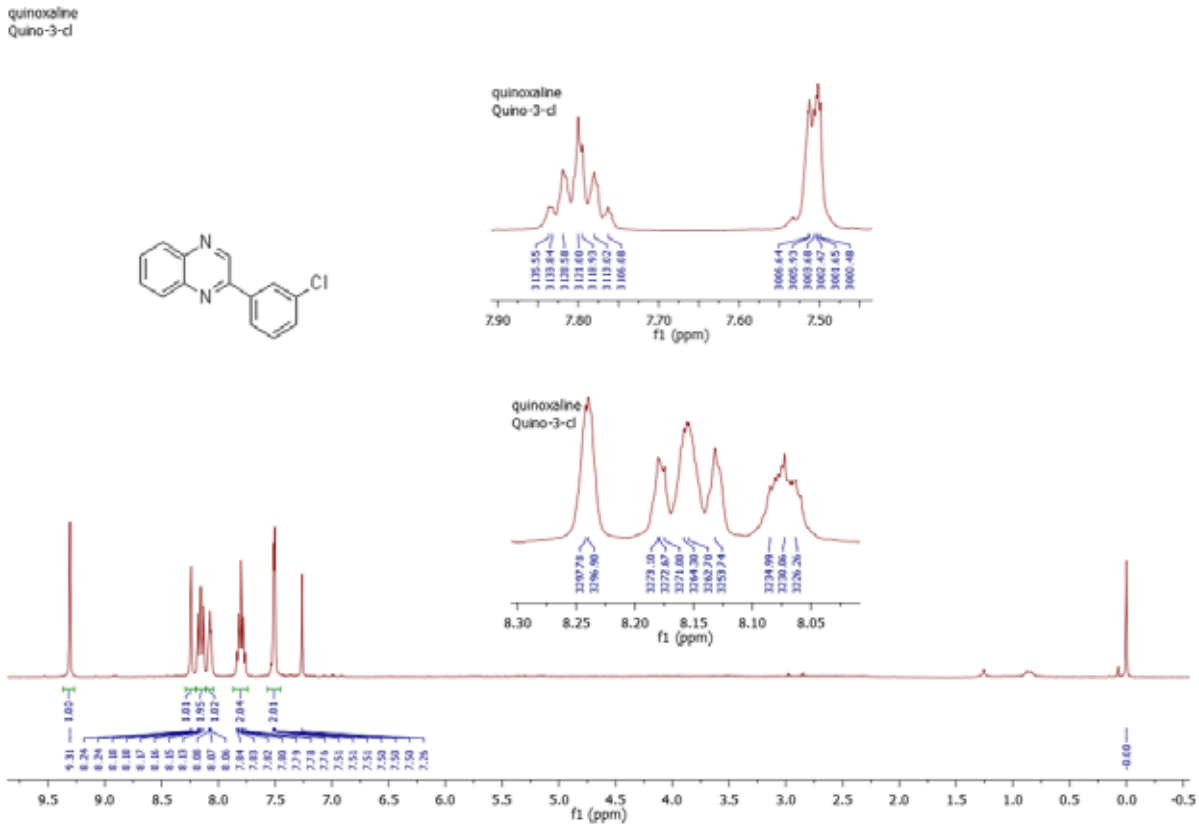
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
225.08134	1	129324.2	C14 H10 F N2	(M+H)+
226.08487	1	20614.3	C14 H10 F N2	(M+H)+
227.08665	1	2524.3	C14 H10 F N2	(M+H)+

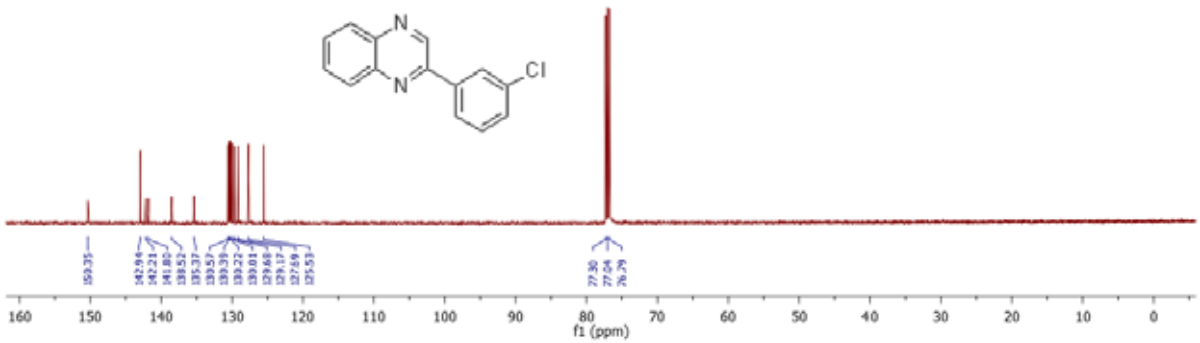
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	225.08134	225.08225	4.06	100	100	84.82	85.34
2	226.08487	226.08534	2.06	15.94	15.99	13.52	13.64
3	227.08665	227.0884	7.7	1.95	1.19	1.66	1.02

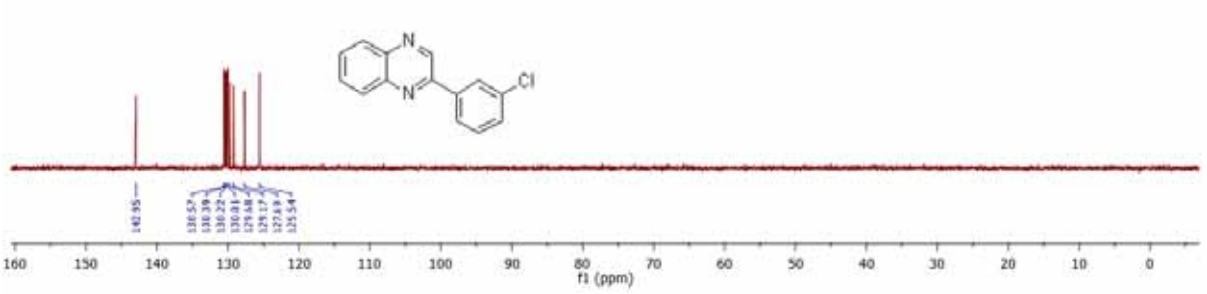
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6e**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **6e**:



DEPT (125 MHz, $CDCl_3$) of compound **6e**:



HRMS (ESI-TOF) of compound **6e**:

Qualitative Compound Report

Data File	QUINO-3-Cl.d	**Sample Name**	QUINO-3-Cl
Sample Type	Sample	**Position**	Vial 59
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/12/2012 4:59:59 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

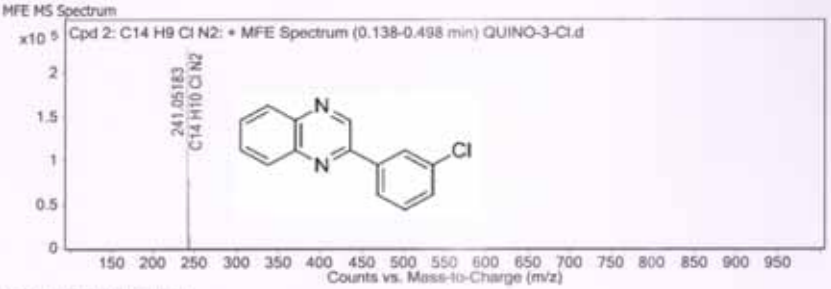
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C14 H9 Cl N2	0.176	240.04455	C14 H9 Cl N2	C14 H9 Cl N2	3.66	C14 H9 Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C14 H9 Cl N2	241.05183	0.176	Find by Molecular Feature	240.04455

MFE MS Spectrum



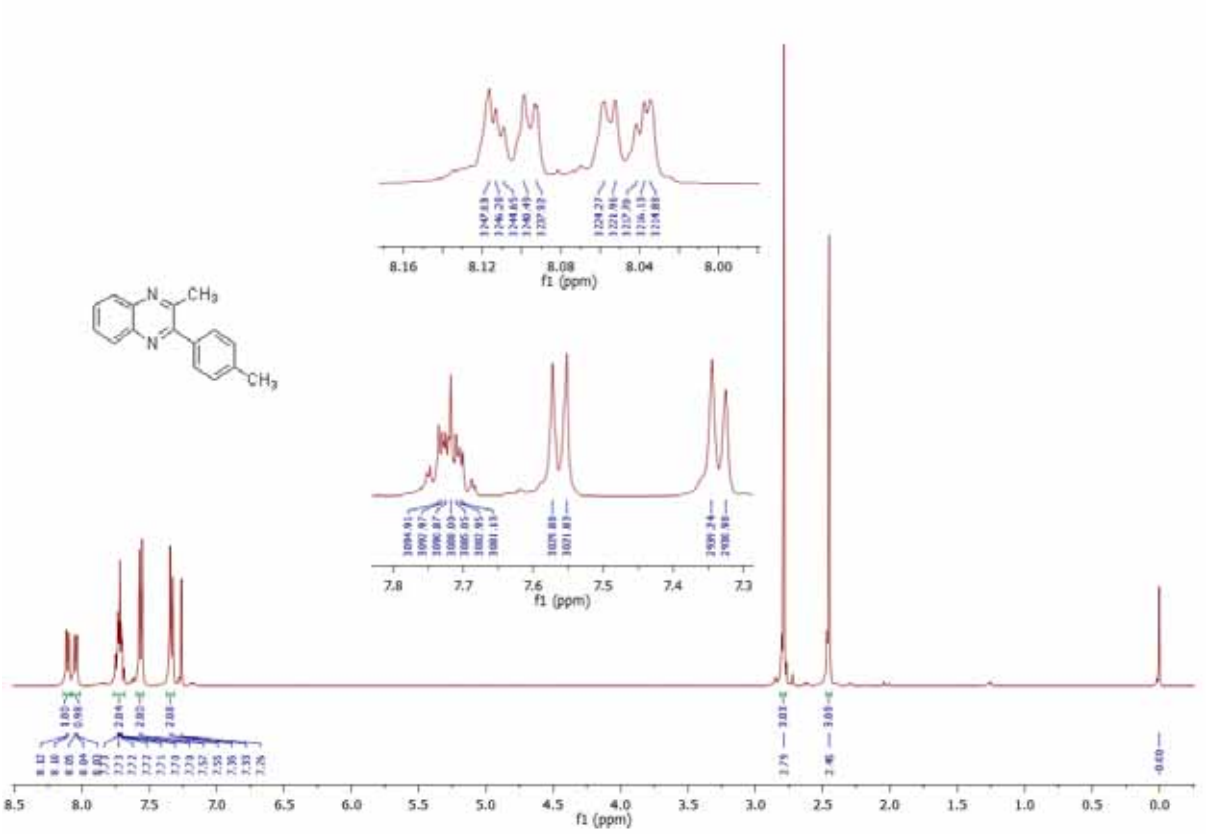
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
241.05183	1	228734.5	C14 H10 Cl N2	(M+H)+
242.05513	1	35537.1	C14 H10 Cl N2	(M+H)+
243.04903	1	78249.6	C14 H10 Cl N2	(M+H)+
244.05198	1	13492.4	C14 H10 Cl N2	(M+H)+

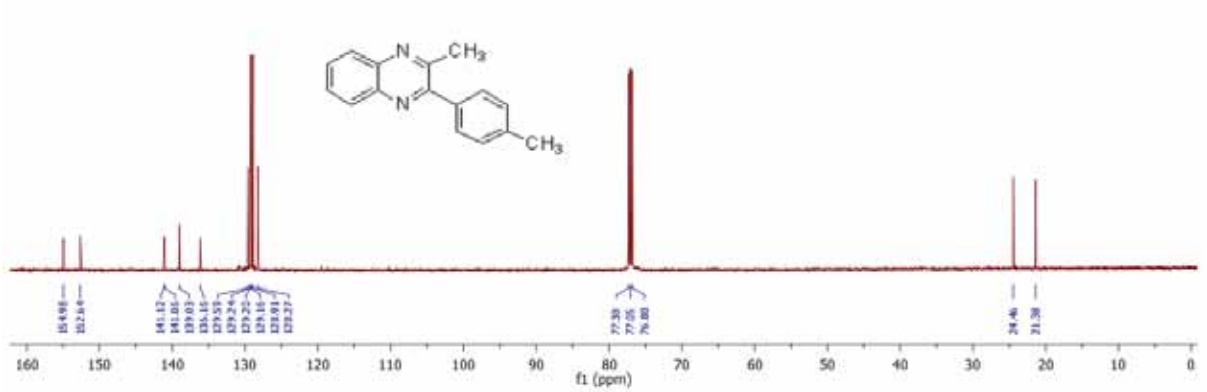
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	241.05183	241.0527	3.62	100	100	64.25	64.79
2	242.05513	242.05579	2.72	15.54	15.99	9.98	10.36
3	243.04903	243.05008	4.3	34.21	33.19	21.98	21.5
4	244.05198	244.05294	3.91	5.9	5.17	3.79	3.35

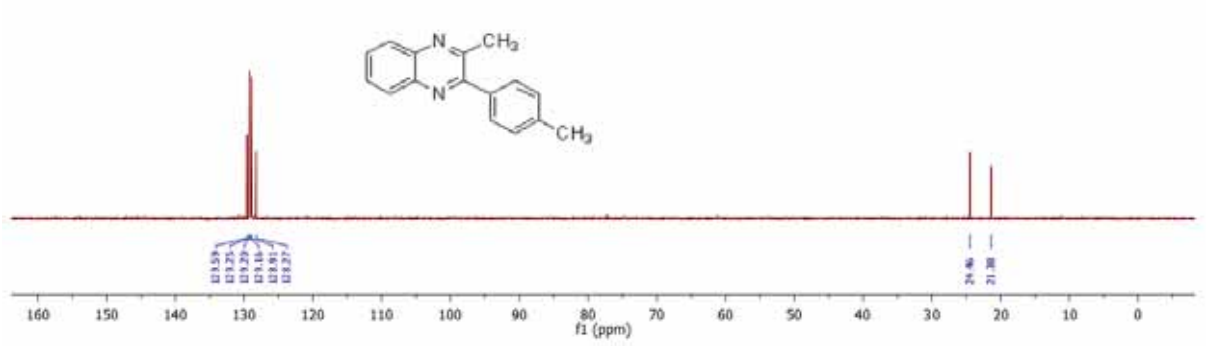
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6f**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **6f**:



DEPT (125 MHz, $CDCl_3$) of compound **6f**:



HRMS (ESI-TOF) of compound **6f**:

Qualitative Compound Report

Data File	3ME-Q-4-ME.d	**Sample Name**	3ME-Q-4-ME
Sample Type	Sample	**Position**	Vial 73
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/24/2012 5:30:39 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

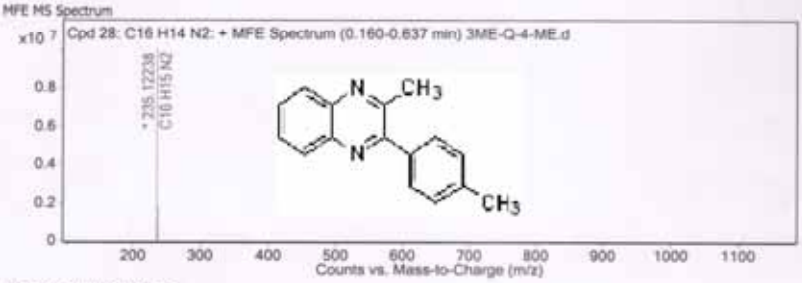
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C16 H14 N2	0.217	234.11511	C16 H14 N2	C16 H14 N2	2.52	C16 H14 N2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 28: C16 H14 N2	235.12238	0.217	Find by Molecular Feature	234.11511

MFE MS Spectrum



MS Spectrum Peak List

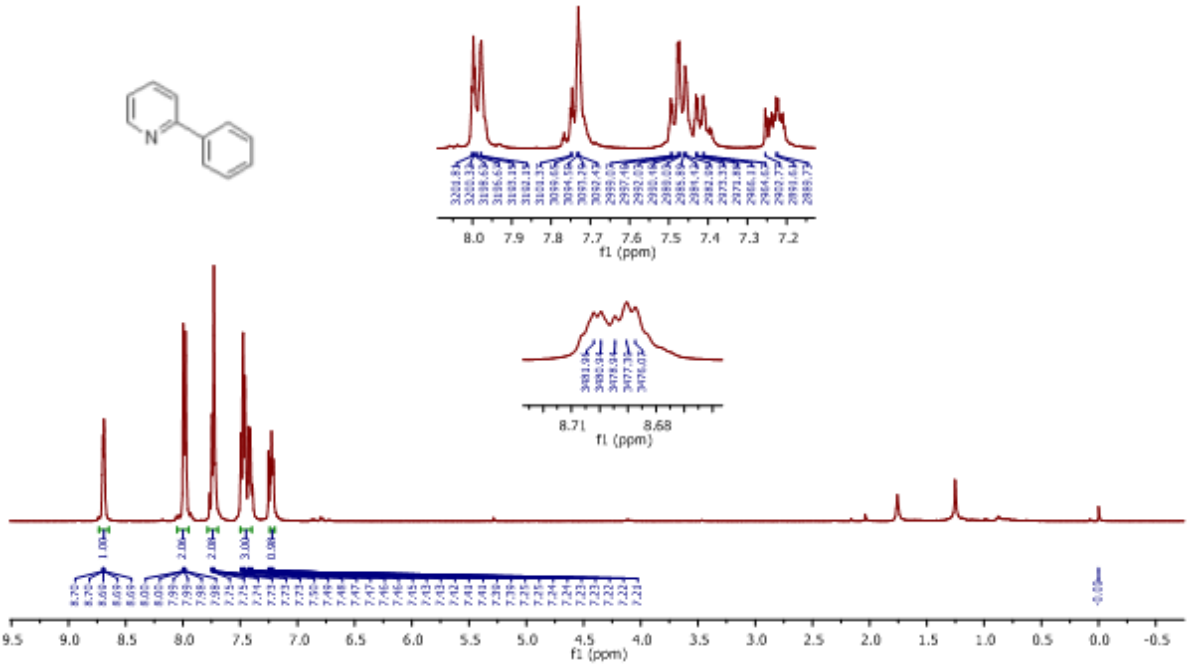
m/z	z	Abund	Formula	Ion
235.12238	1	10104805	C16 H15 N2	(M+H)+
236.12571	1	1752780.4	C16 H15 N2	(M+H)+
237.12835	1	141383.7	C16 H15 N2	(M+H)+
238.1315	1	12026.4	C16 H15 N2	(M+H)+

Predicted Isotope Match Table

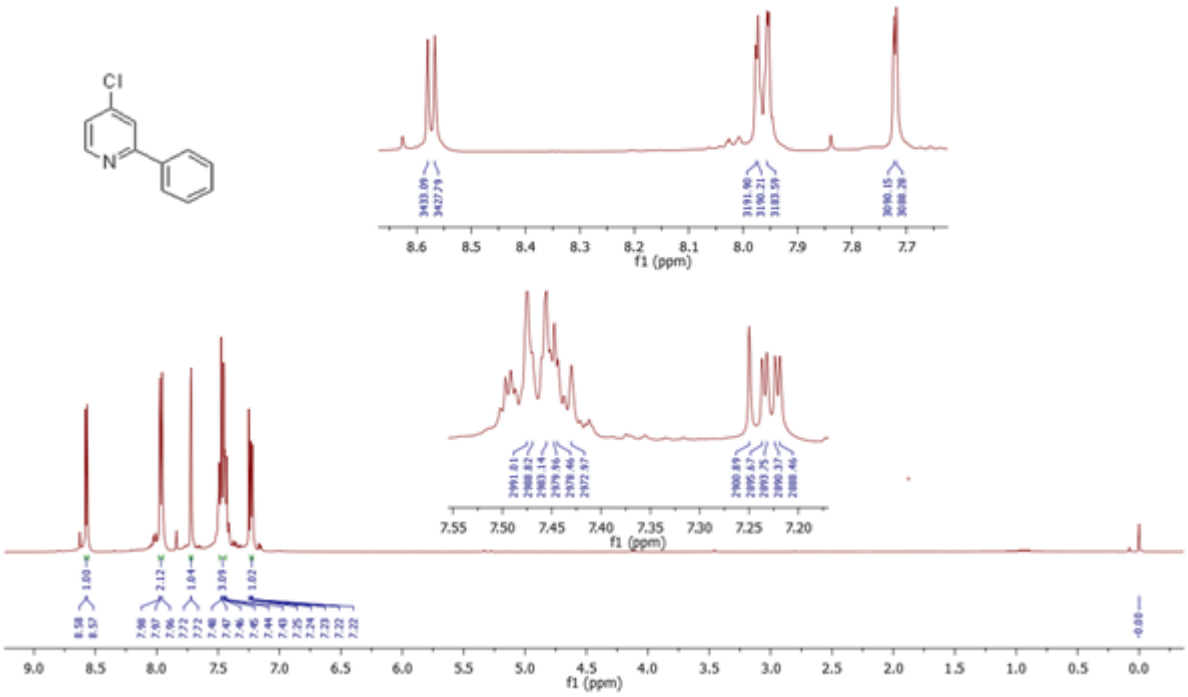
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	235.12238	235.12297	2.51	100	100	84.13	83.43
2	236.12571	236.1261	1.65	17.35	18.21	14.59	15.19
3	237.12835	237.12922	3.63	1.4	1.56	1.18	1.3
4	238.1315	238.13231	3.42	0.12	0.08	0.1	0.07

--- End Of Report ---

^{1}H NMR (400 MHz, $CDCl_3$) of compound **8a**:



^{1}H NMR (400 MHz, $CDCl_3$) of compound **8b**:



HRMS (ESI-TOF) of compound **8b**:

Qualitative Compound Report

Data File	Cl-PY-PH.d	**Sample Name**	Cl-PY-PH
Sample Type	Sample	**Position**	Vial 62
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:31:59 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

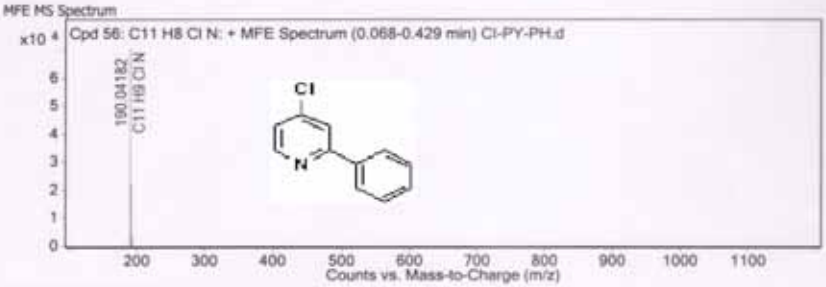
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 56: C11 H8 Cl N	0.179	189.03454	C11 H8 Cl N	C11 H8 Cl N	-0.05	C11 H8 Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 56: C11 H8 Cl N	190.04182	0.179	Find by Molecular Feature	189.03454

MFE MS Spectrum



MS Spectrum Peak List

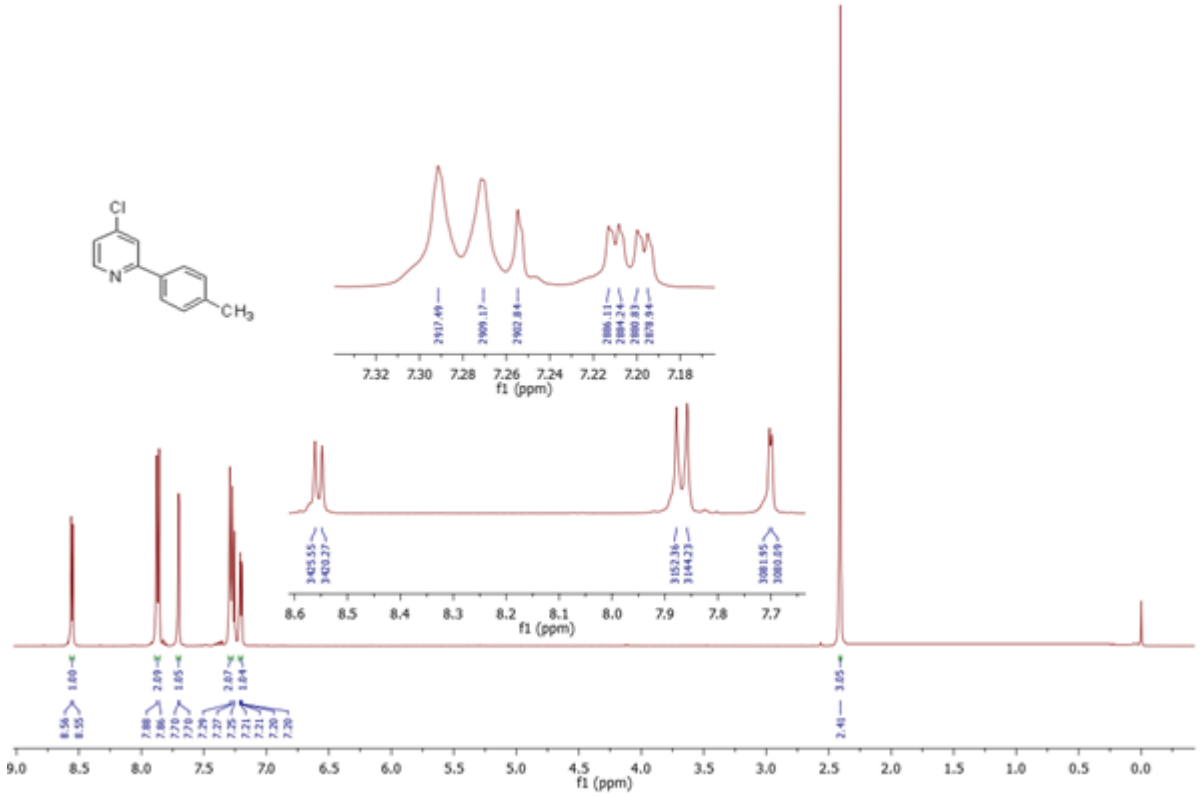
m/z	z	Abund	Formula	Ion
190.04182	1	70442.8	C11 H9 Cl N	(M+H)+
191.04447	1	10674.6	C11 H9 Cl N	(M+H)+
192.03874	1	22209.8	C11 H9 Cl N	(M+H)+
193.04209	1	3263.1	C11 H9 Cl N	(M+H)+

Predicted Isotope Match Table

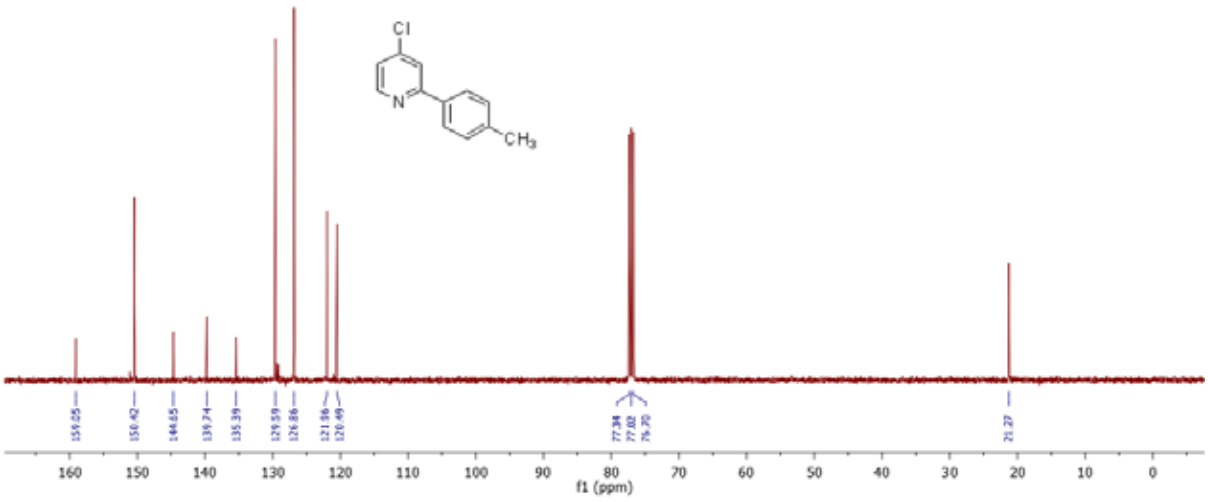
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	190.04182	190.0418	-0.11	100	100	66.09	67.1
2	191.04447	191.045	2.76	15.15	12.37	10.01	8.3
3	192.03874	192.03905	1.65	31.53	32.7	20.84	21.94
4	193.04209	193.0421	0.04	4.63	3.98	3.06	2.67

--- End Of Report ---

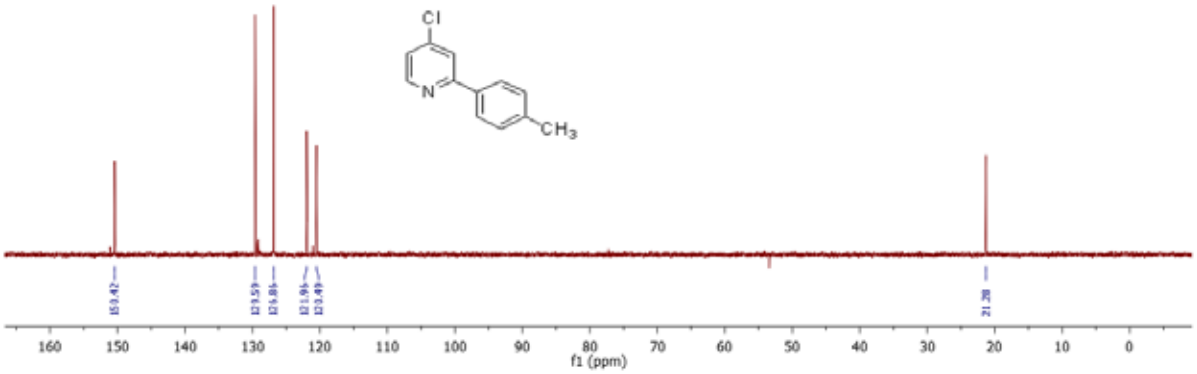
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8c**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **8c**:



DEPT (100 MHz, $CDCl_3$) of compound **8c**:



HRMS (ESI-TOF) of compound **8c**:

Qualitative Compound Report

Data File	CL-PY-4ME.d	**Sample Name**	CL-PY-4ME
Sample Type	Sample	**Position**	Vial 60
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 3:15:57 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

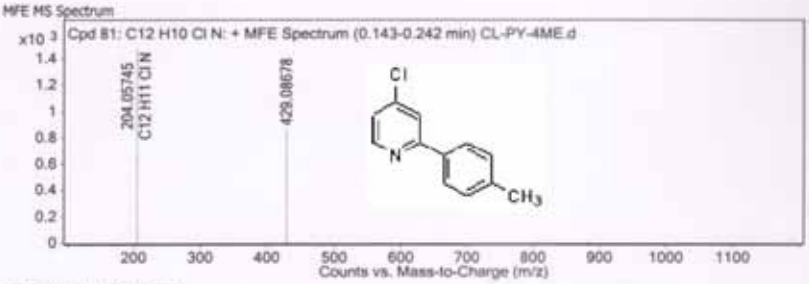
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 81: C12 H10 Cl N	0.184	203.05018	C12 H10 Cl N	C12 H10 Cl N	0	C12 H10 Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 81: C12 H10 Cl N	204.05745	0.184	Find by Molecular Feature	203.05018

MFE MS Spectrum



MS Spectrum Peak List

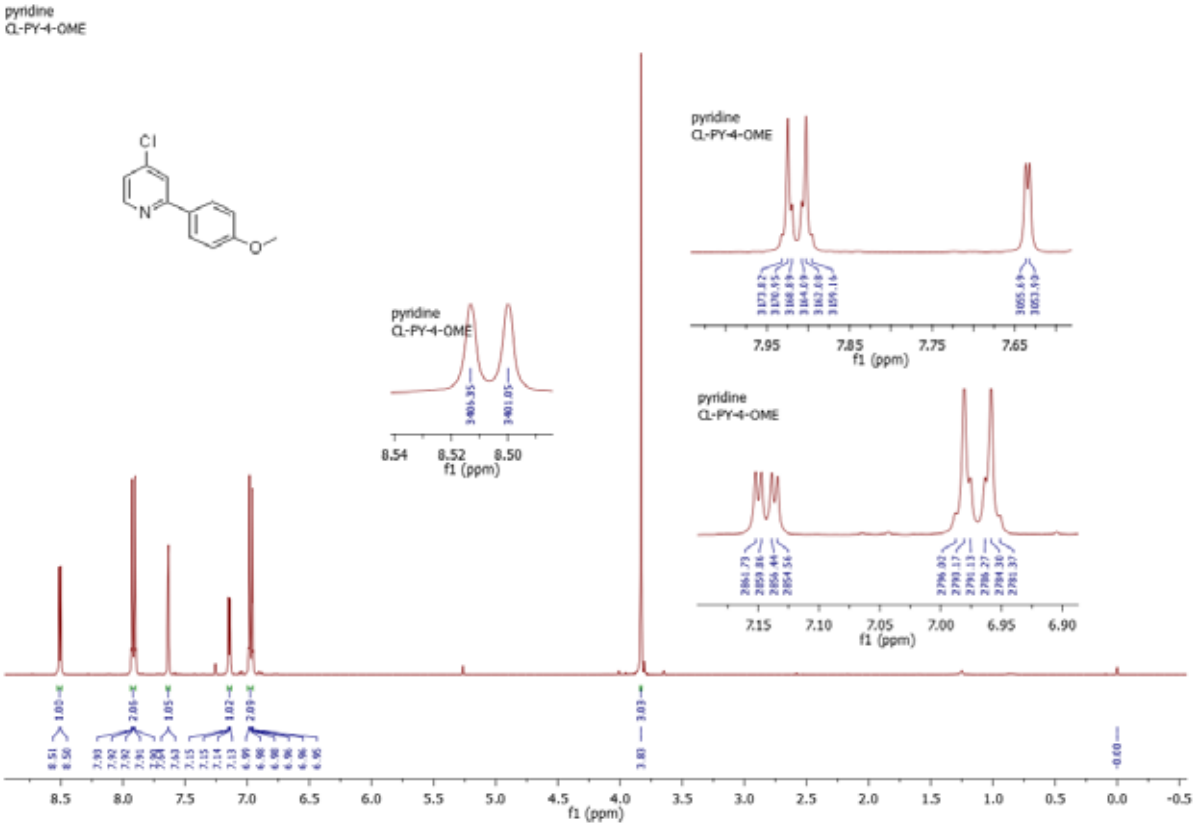
m/z	z	Abund	Formula	Ion
204.05745	1	1476.5	C12 H11 Cl N	(M+H)+
429.08678	1	865.2		(2M+Na)+

Predicted Isotope Match Table

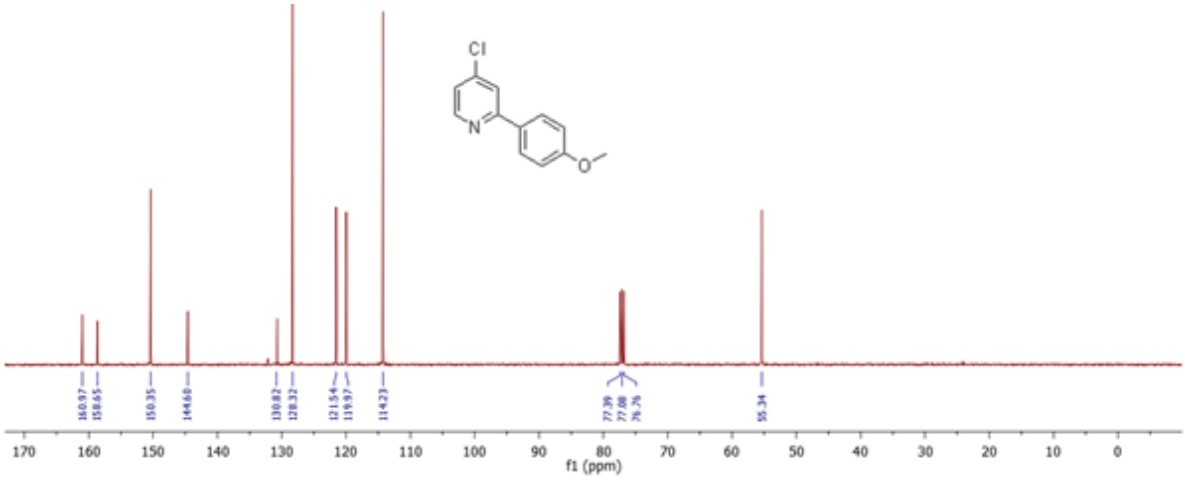
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	204.05745	204.05745	0	100	100	100	100

--- End Of Report ---

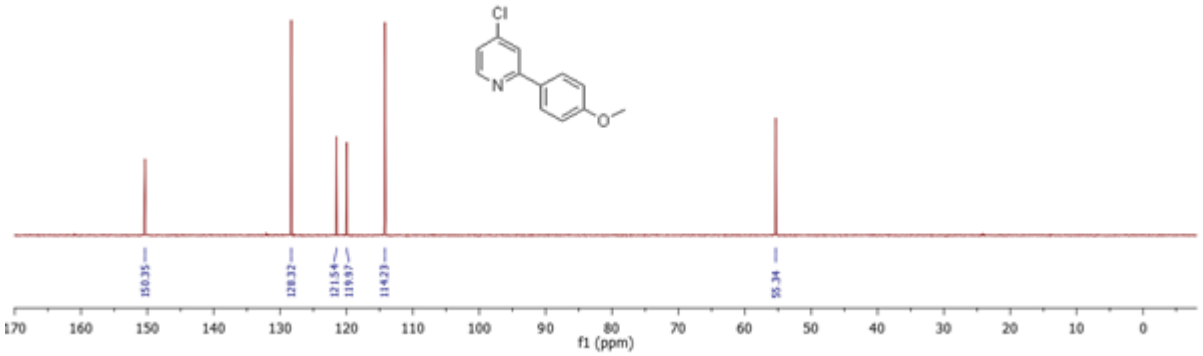
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8d**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **8d**:



DEPT (100 MHz, $CDCl_3$) of compound **8d**:



HRMS (ESI-TOF) of compound **8d**:

Qualitative Compound Report

Data File	Cl-PY-4-OME.d	**Sample Name**	Cl-PY-4-OME
Sample Type	Sample	**Position**	Vial 60
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:26:35 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

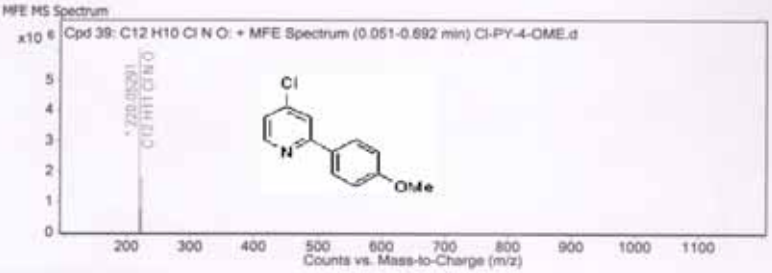
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 39: C12 H10 Cl N O	0.177	219.04563	C12 H10 Cl N O	C12 H10 Cl N O	-2.44	C12 H10 Cl N O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 39: C12 H10 Cl N O	220.05291	0.177	Find by Molecular Feature	219.04563

MFE MS Spectrum



MS Spectrum Peak List

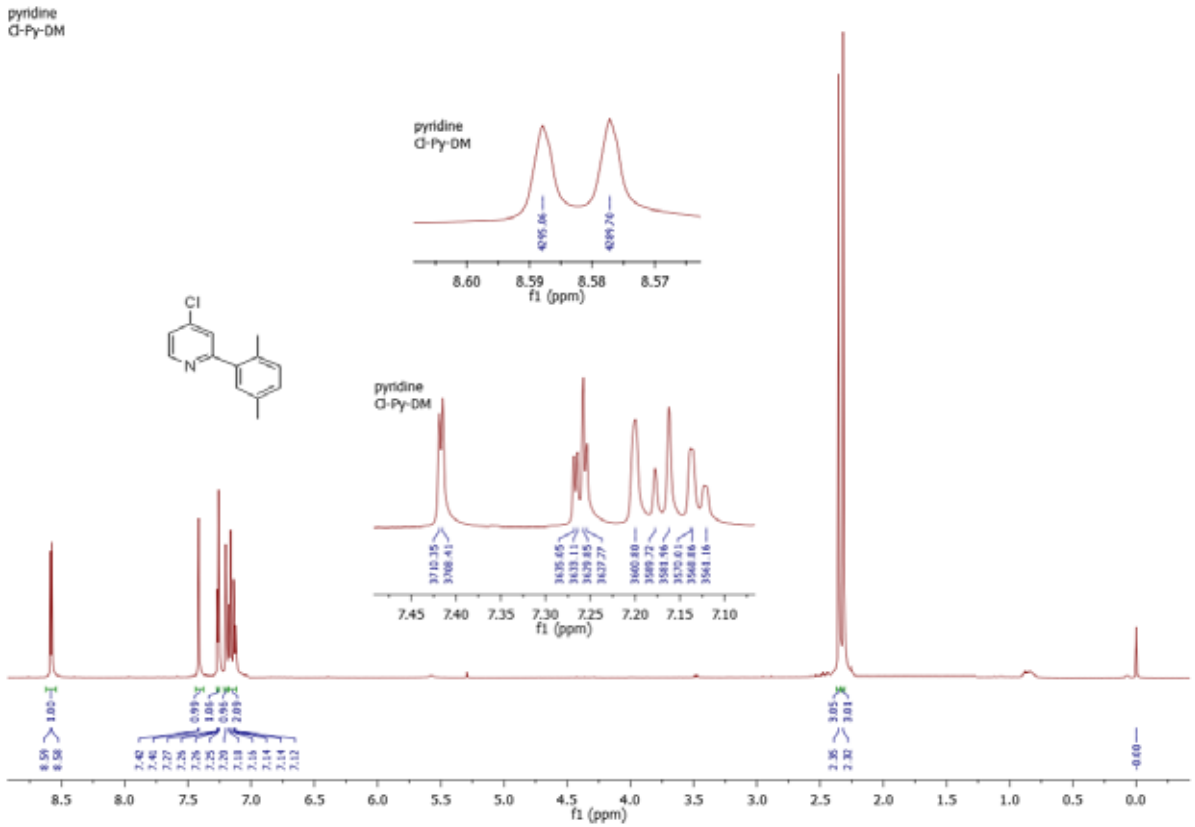
m/z	z	Abund	Formula	Ion
220.05291	1	6083666	C12 H11 Cl N O	(M+H)+
221.05602	1	798322.7	C12 H11 Cl N O	(M+H)+
222.0501	1	1814864.9	C12 H11 Cl N O	(M+H)+
223.05305	1	215926.4	C12 H11 Cl N O	(M+H)+
224.05579	1	20481.6	C12 H11 Cl N O	(M+H)+
225.05996	1	965.1	C12 H11 Cl N O	(M+H)+

Predicted Isotope Match Table

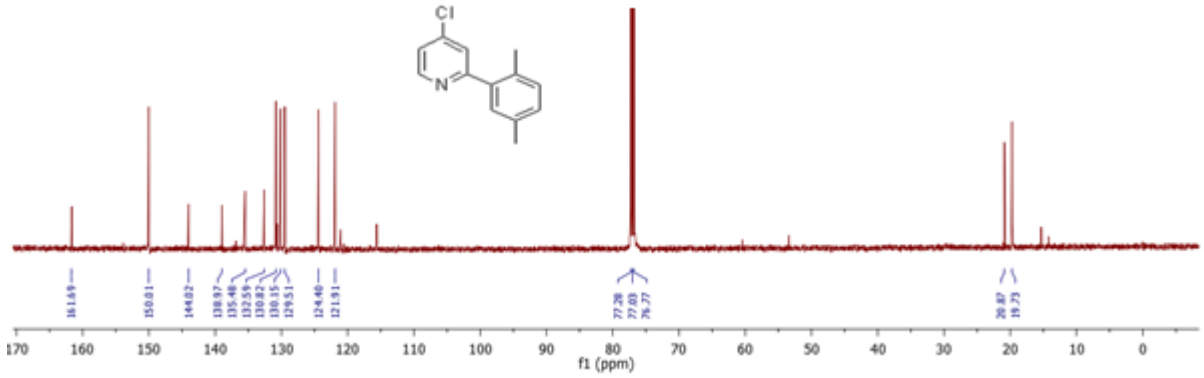
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	220.05291	220.05237	-2.44	100	100	68.09	66.1
2	221.05602	221.05558	-1.99	13.12	13.51	8.94	8.93
3	222.0501	222.0497	-1.8	29.83	33.04	20.31	21.84
4	223.05305	223.05275	-1.37	3.55	4.38	2.42	2.9
5	224.05579	224.05547	-1.44	0.34	0.34	0.23	0.22
6	225.05996	225.05806	-8.43	0.02	0.02	0.01	0.01

--- End Of Report ---

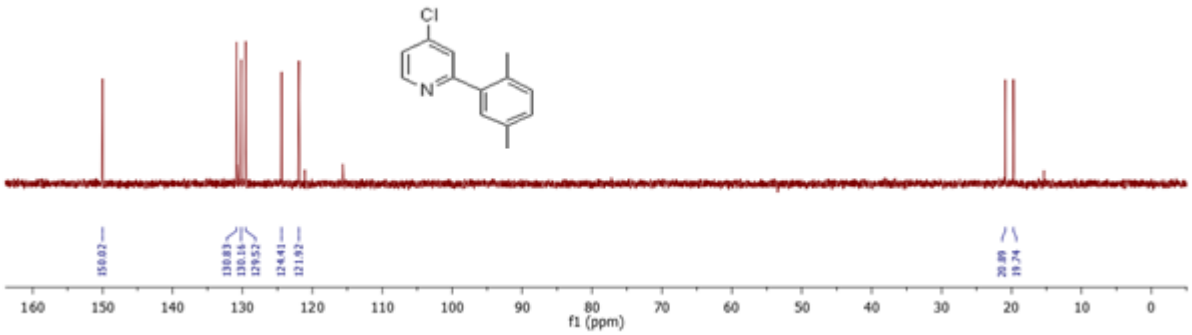
^{1}H NMR (500 MHz, $CDCl_3$) of compound **8e**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **8e**:



DEPT (125 MHz, $CDCl_3$) of compound **8e**:



HRMS (ESI-TOF) of compound **8e**:

Qualitative Compound Report

Data File	CL-PY-DM.d	**Sample Name**	CL-PY-DM
Sample Type	Sample	**Position**	Vial 63
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:34:41 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

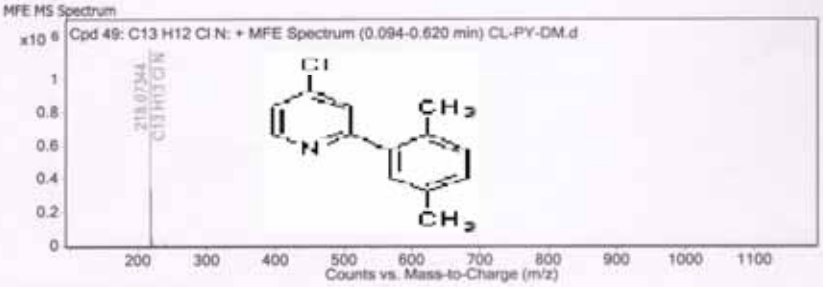
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 49: C13 H12 Cl N	0.176	217.06616	C13 H12 Cl N	C13 H12 Cl N	-1.54	C13 H12 Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 49: C13 H12 Cl N	218.07344	0.176	Find by Molecular Feature	217.06616

MFE MS Spectrum



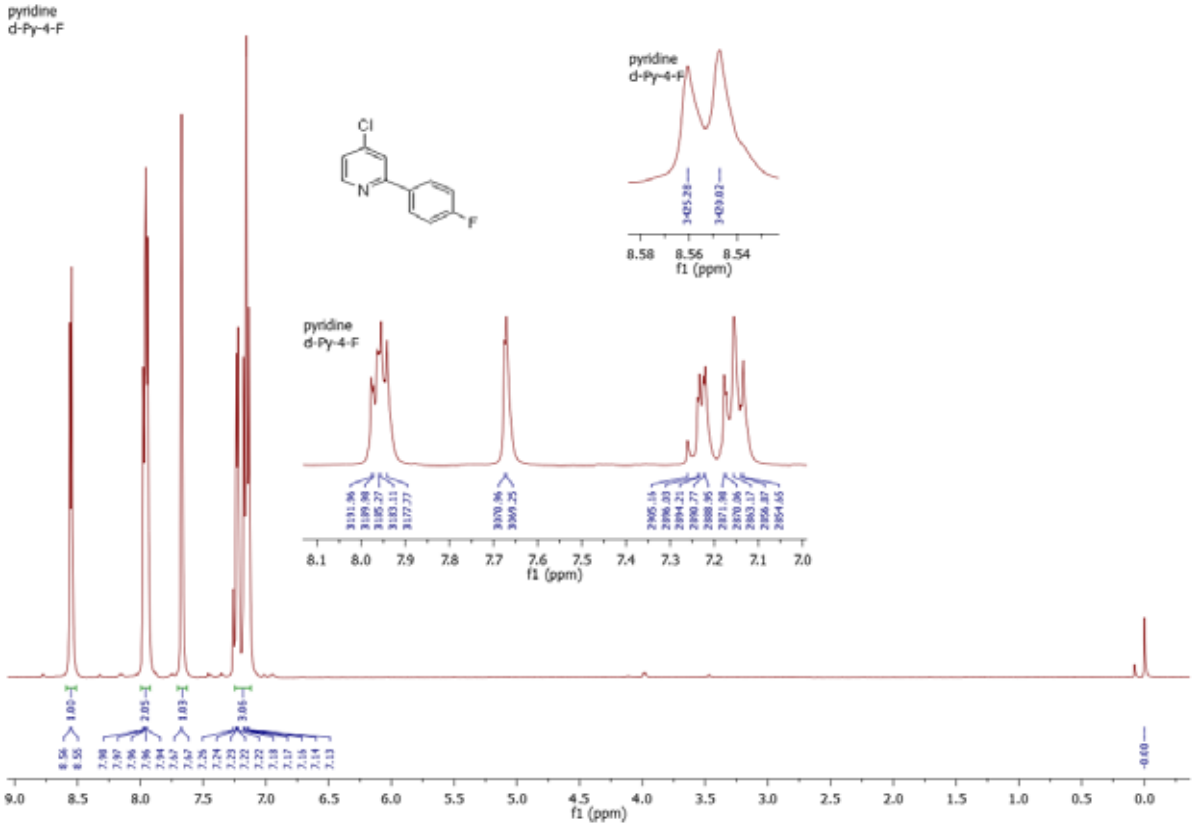
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
218.07344	1	1182044.6	C13 H13 Cl N	(M+H)+
219.07634	1	153521.4	C13 H13 Cl N	(M+H)+
220.07062	1	343494.6	C13 H13 Cl N	(M+H)+
221.07345	1	50231.3	C13 H13 Cl N	(M+H)+
222.07625	1	3874.1	C13 H13 Cl N	(M+H)+
240.05766	1	15836.9	C13 H12 Cl N Na	(M+Na)+
241.06531	1	3032.4	C13 H12 Cl N Na	(M+Na)+
242.0545	1	6644.6	C13 H12 Cl N Na	(M+Na)+

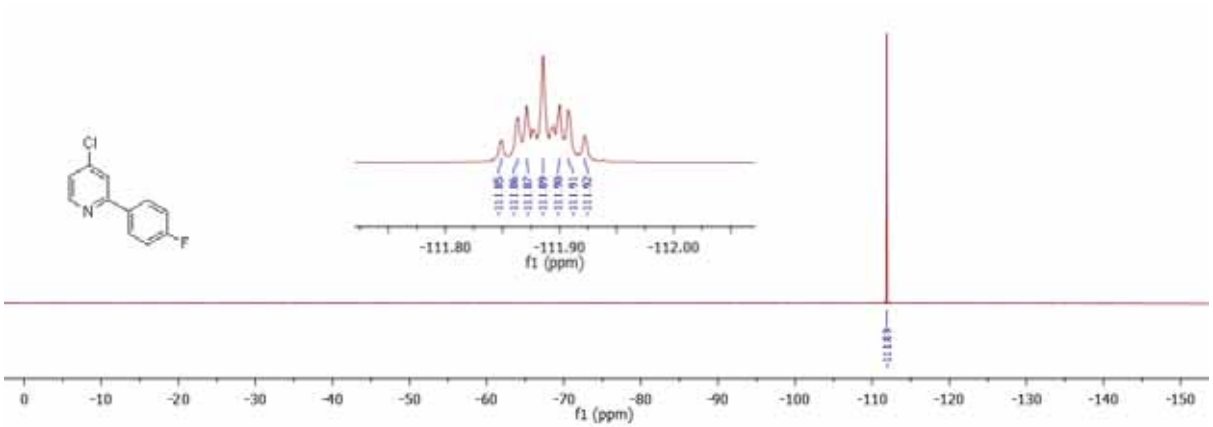
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	218.07344	218.0731	-1.55	100	100	68.2	65.54
2	219.07634	219.07633	-0.05	12.99	14.58	8.86	9.55
3	220.07062	220.07043	-0.84	29.06	32.98	19.82	21.62
4	221.07345	221.07346	0.07	4.25	4.7	2.9	3.08
5	222.07625	222.07663	1.69	0.33	0.32	0.22	0.21

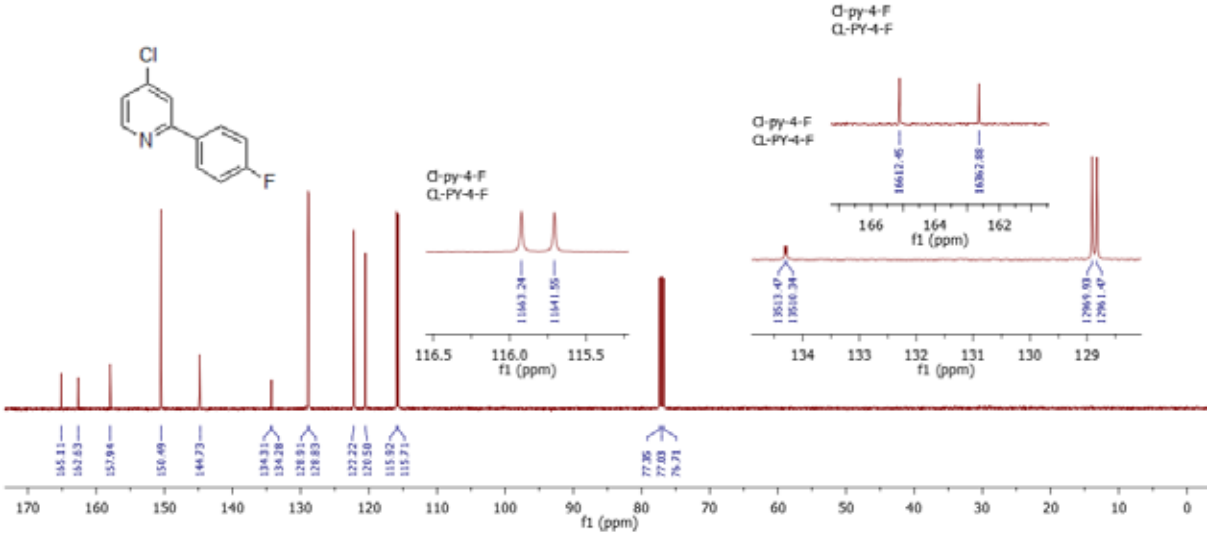
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8f**:



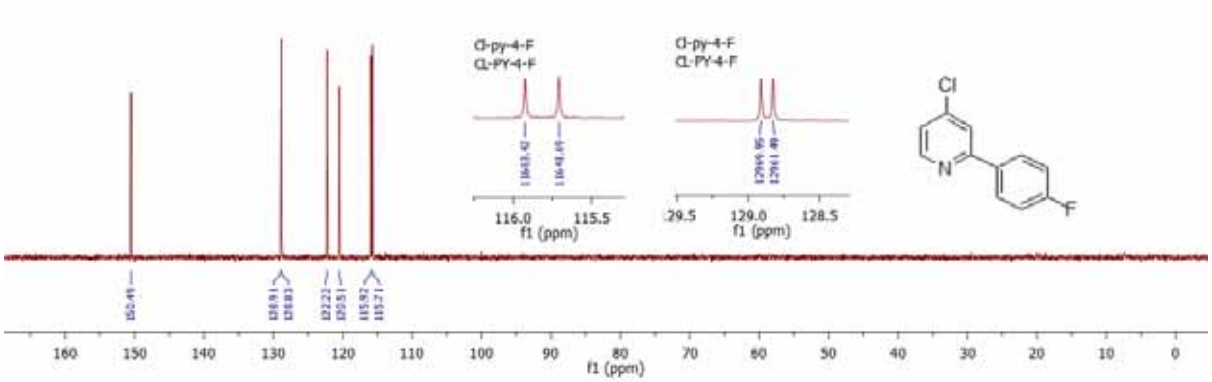
^{19}F NMR (376 MHz, $CDCl_3$) of compound **8f**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **8f**:



DEPT (100 MHz, $CDCl_3$) of compound **8f**:



HRMS (ESI-TOF) of compound **8f**:

Qualitative Compound Report

Data File	CL-PY-4F.d	**Sample Name**	CL-PY-4F
Sample Type	Sample	**Position**	Vial 64
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:37:23 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

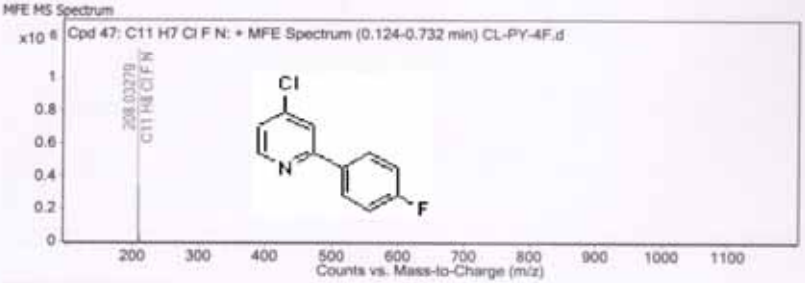
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 47: C11 H7 Cl F N	0.178	207.02551	C11 H7 Cl F N	C11 H7 Cl F N	-1.97	C11 H7 Cl F N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 47: C11 H7 Cl F N	208.03279	0.178	Find by Molecular Feature	207.02551

MFE MS Spectrum



MS Spectrum Peak List

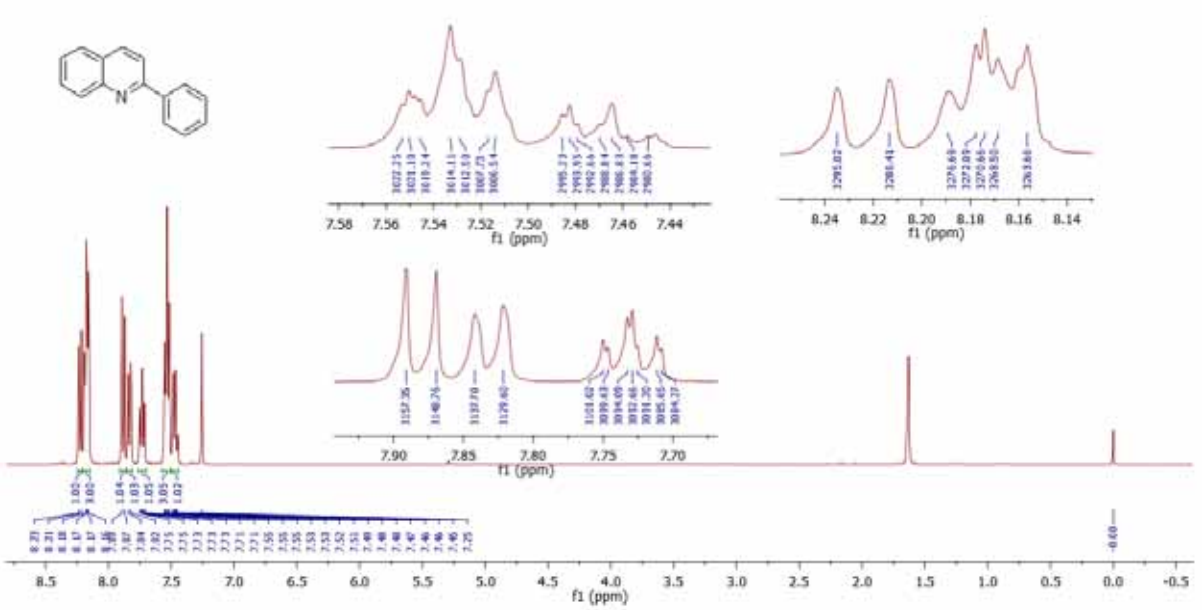
m/z	z	Abund	Formula	Ion
208.03279	1	1186238.6	C11 H8 Cl F N	(M+H)+
209.03566	1	123484.4	C11 H8 Cl F N	(M+H)+
210.02983	1	339801.4	C11 H8 Cl F N	(M+H)+
211.03273	1	41636.9	C11 H8 Cl F N	(M+H)+
212.03579	1	2083.3	C11 H8 Cl F N	(M+H)+

Predicted Isotope Match Table

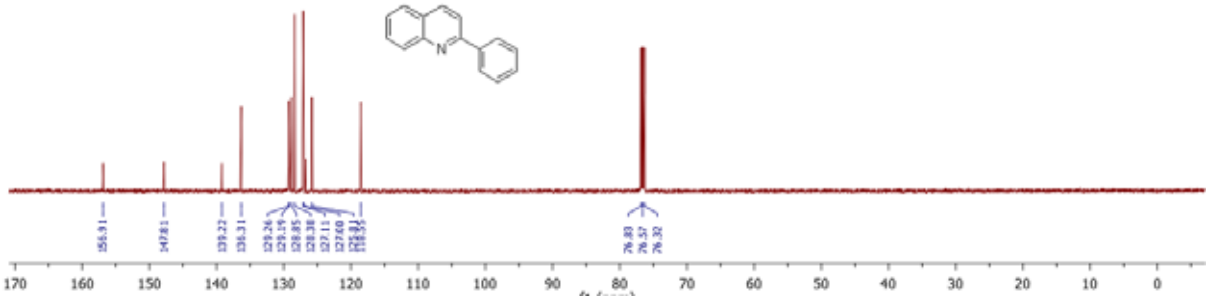
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	208.03279	208.03238	-1.99	100	100	70.06	67
2	209.03566	209.03557	-0.43	10.41	12.35	7.29	8.28
3	210.02983	210.02963	-0.97	28.65	32.69	20.07	21.91
4	211.03273	211.03268	-0.27	3.51	3.98	2.46	2.66
5	212.03579	212.03581	0.1	0.18	0.22	0.12	0.15

--- End Of Report ---

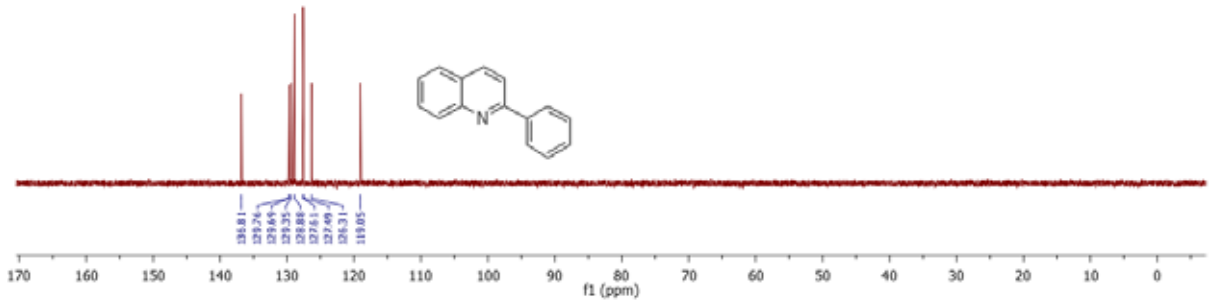
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8g**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **8g**:



DEPT (125 MHz, $CDCl_3$) of compound **8g**:



HRMS (ESI-TOF) of compound **8g**:

Qualitative Compound Report

Data File	2PQ.d	**Sample Name**	2PQ
Sample Type	Sample	**Position**	Vial 76
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 7:10:09 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

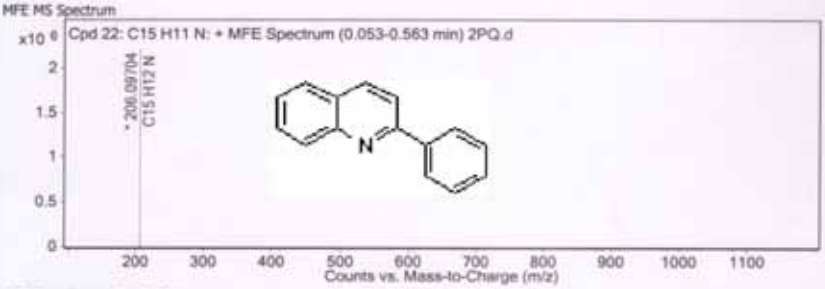
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C15 H11 N	0.175	205.08976	C15 H11 N	C15 H11 N	-2.97	C15 H11 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C15 H11 N	206.09704	0.175	Find by Molecular Feature	205.08976

MFE MS Spectrum



MS Spectrum Peak List

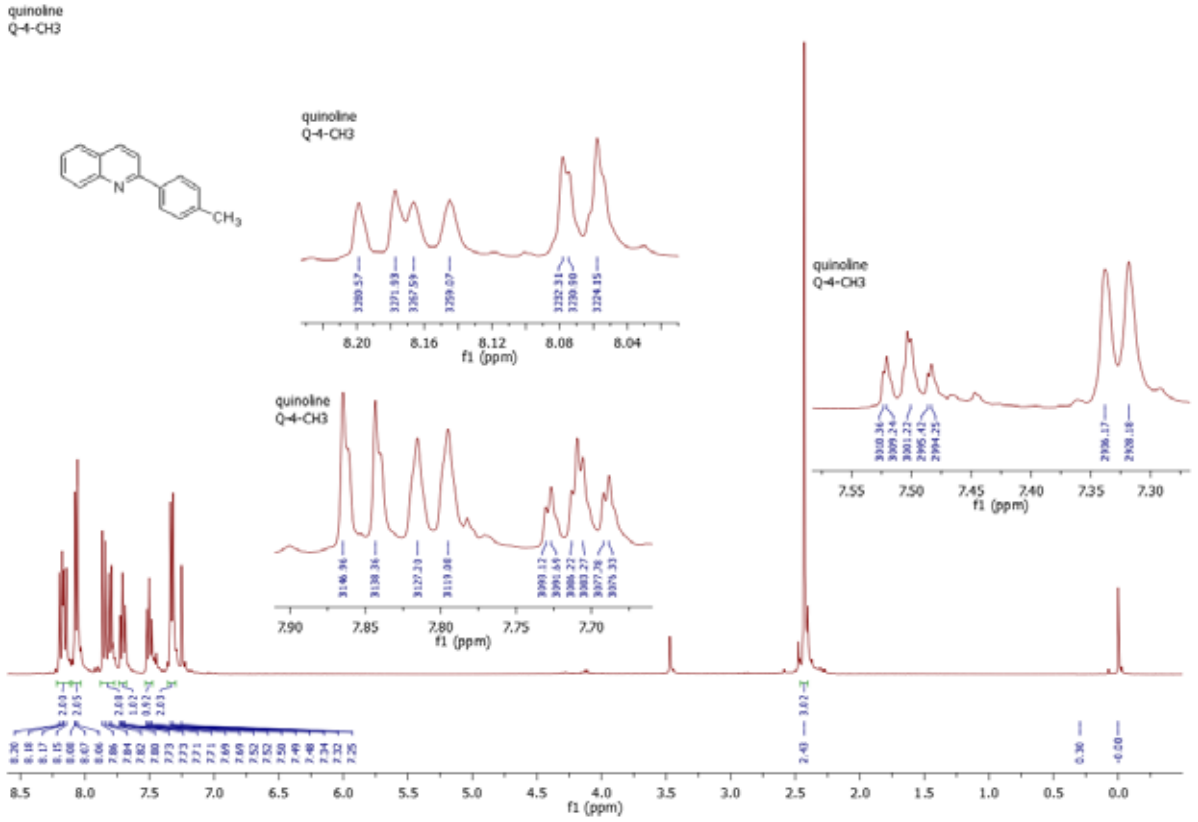
m/z	z	Abund	Formula	Ion
206.09704	1	2214556.5	C15 H12 N	(M+H)+
207.09987	1	343492.3	C15 H12 N	(M+H)+
208.10322	1	31740.8	C15 H12 N	(M+H)+
209.10658	1	2454.9	C15 H12 N	(M+H)+

Predicted Isotope Match Table

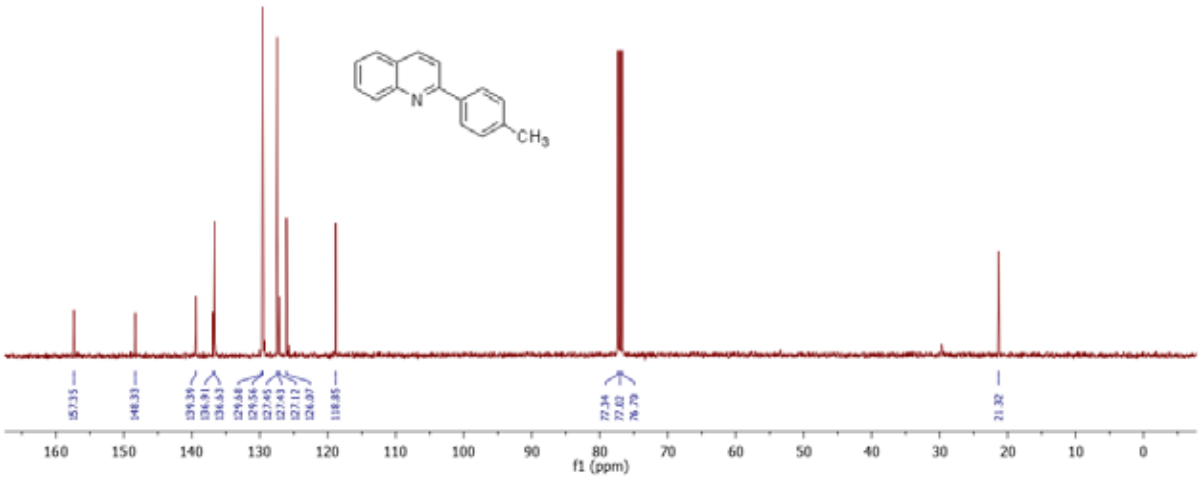
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	206.09704	206.09643	-2.96	100	100	85.43	84.67
2	207.09987	207.09967	-0.99	15.51	16.73	13.25	14.16
3	208.10322	208.1029	-1.57	1.43	1.31	1.22	1.11
4	209.10658	209.10612	-2.22	0.11	0.06	0.09	0.05

— End Of Report —

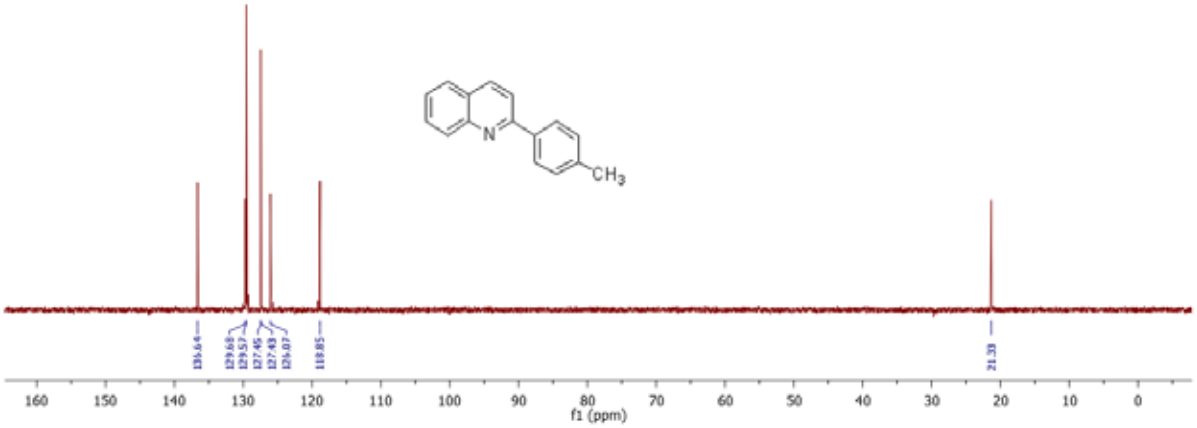
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8h**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **8h**:



DEPT (100 MHz, $CDCl_3$) of compound **8h**:



HRMS (ESI-TOF) of compound **8h**:

Qualitative Compound Report

Data File	Q4-ME.d	**Sample Name**	Q4-ME
Sample Type	Sample	**Position**	Vial 65
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:40:04 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

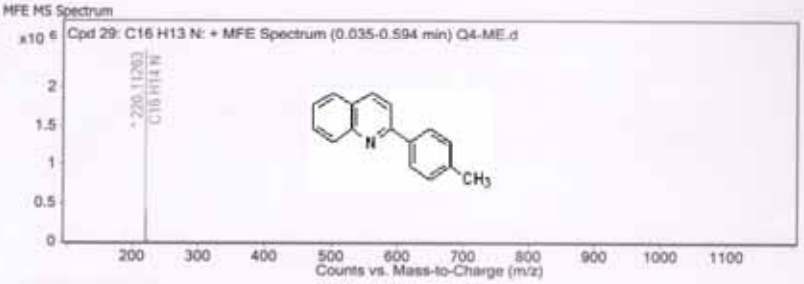
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C16 H13 N	0.175	219.10535	C16 H13 N	C16 H13 N	-2.53	C16 H13 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 29: C16 H13 N	220.11263	0.175	Find by Molecular Feature	219.10535

MFE MS Spectrum



MS Spectrum Peak List

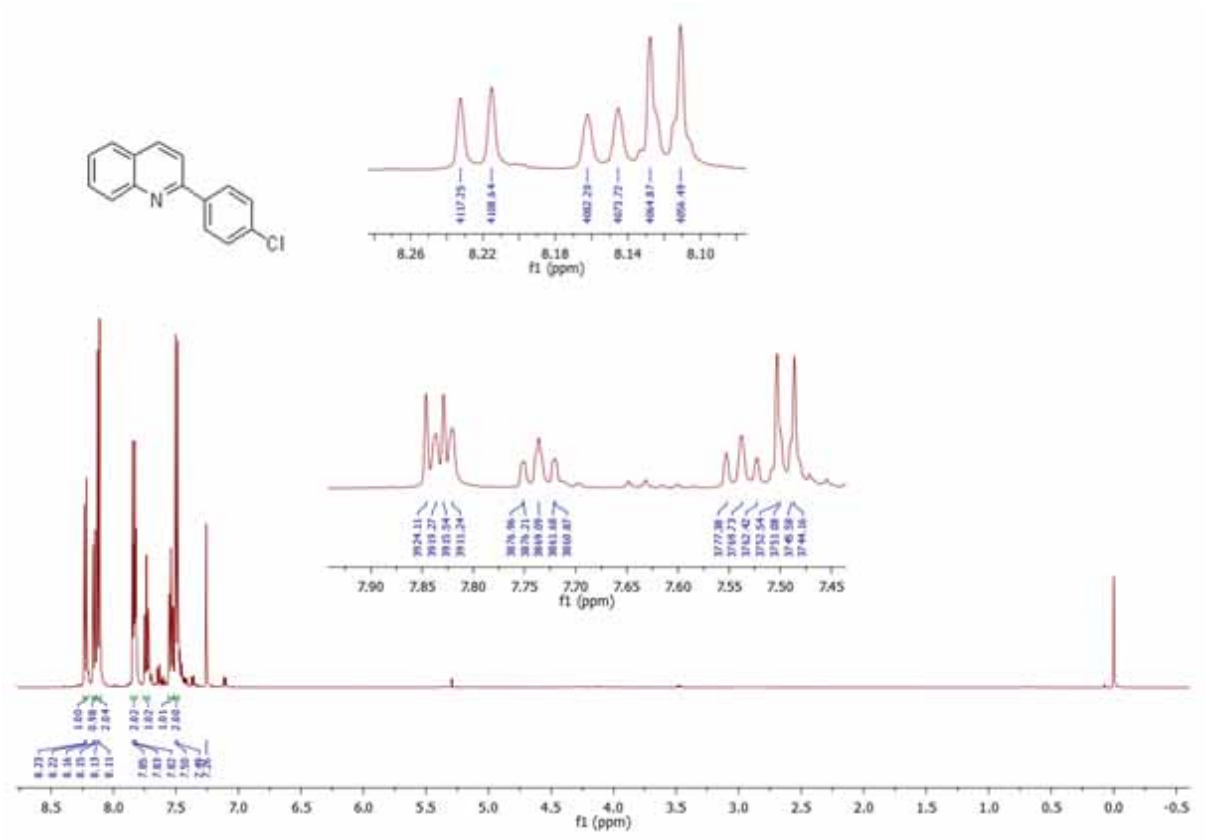
m/z	z	Abund	Formula	Ion
220.11263	1	2499558.3	C16 H14 N	(M+H)+
221.11571	1	410686	C16 H14 N	(M+H)+
222.1181	1	39815.3	C16 H14 N	(M+H)+
223.12217	1	3675	C16 H14 N	(M+H)+

Predicted Isotope Match Table

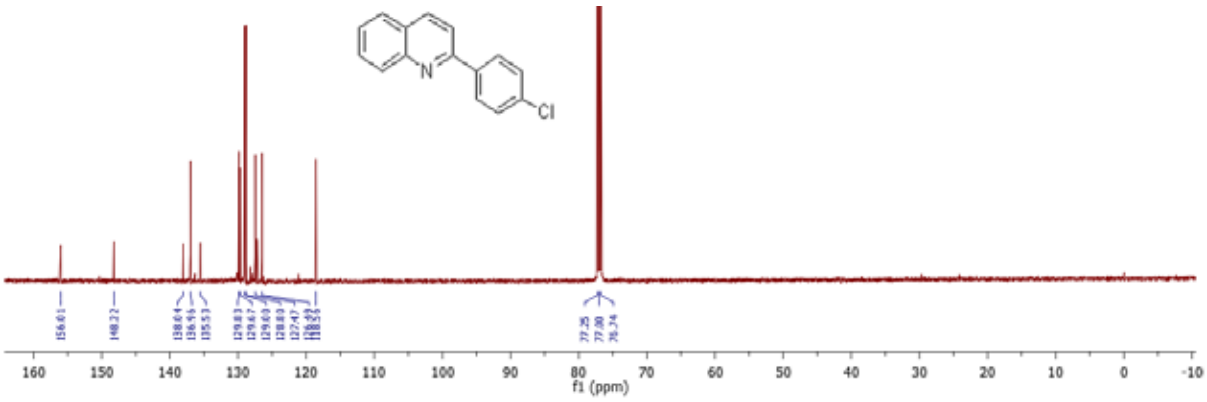
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	220.11263	220.11208	-2.52	100	100	84.62	83.75
2	221.11571	221.11533	-1.75	16.43	17.83	13.9	14.93
3	222.1181	222.11857	2.11	1.59	1.5	1.35	1.25
4	223.12217	223.12181	-1.64	0.15	0.08	0.12	0.07

--- End Of Report ---

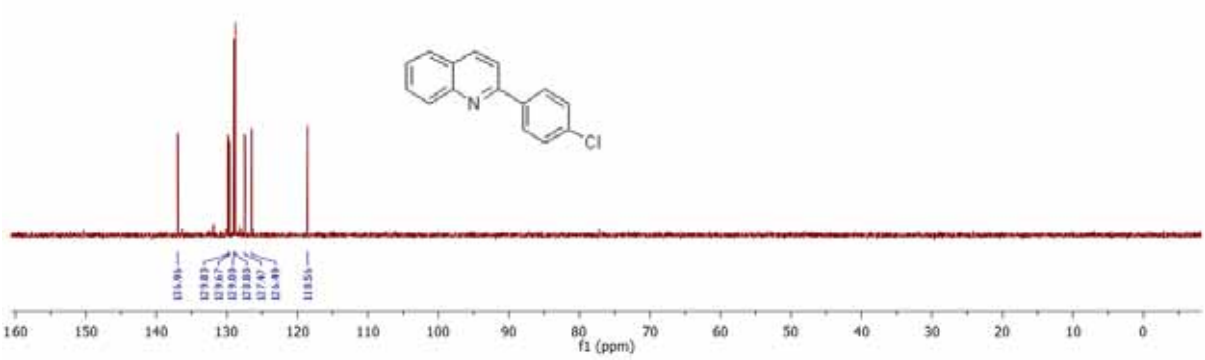
^{1}H NMR (500 MHz, $CDCl_3$) of compound **8i**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **8i**:



DEPT (125 MHz, $CDCl_3$) of compound **8i**:



HRMS (ESI-TOF) of compound **8i**:

Qualitative Compound Report

Data File	Q4-CL.d	**Sample Name**	Q4-CL
Sample Type	Sample	**Position**	Vial 67
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:45:32 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

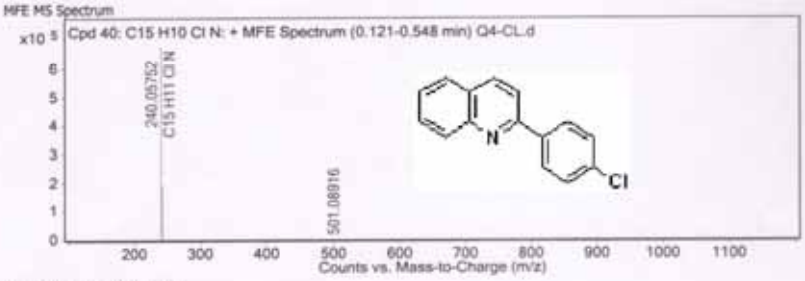
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 40: C15 H10 Cl N	0.177	239.05025	C15 H10 Cl N	C15 H10 Cl N	-0.31	C15 H10 Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 40: C15 H10 Cl N	240.05752	0.177	Find by Molecular Feature	239.05025

MFE MS Spectrum



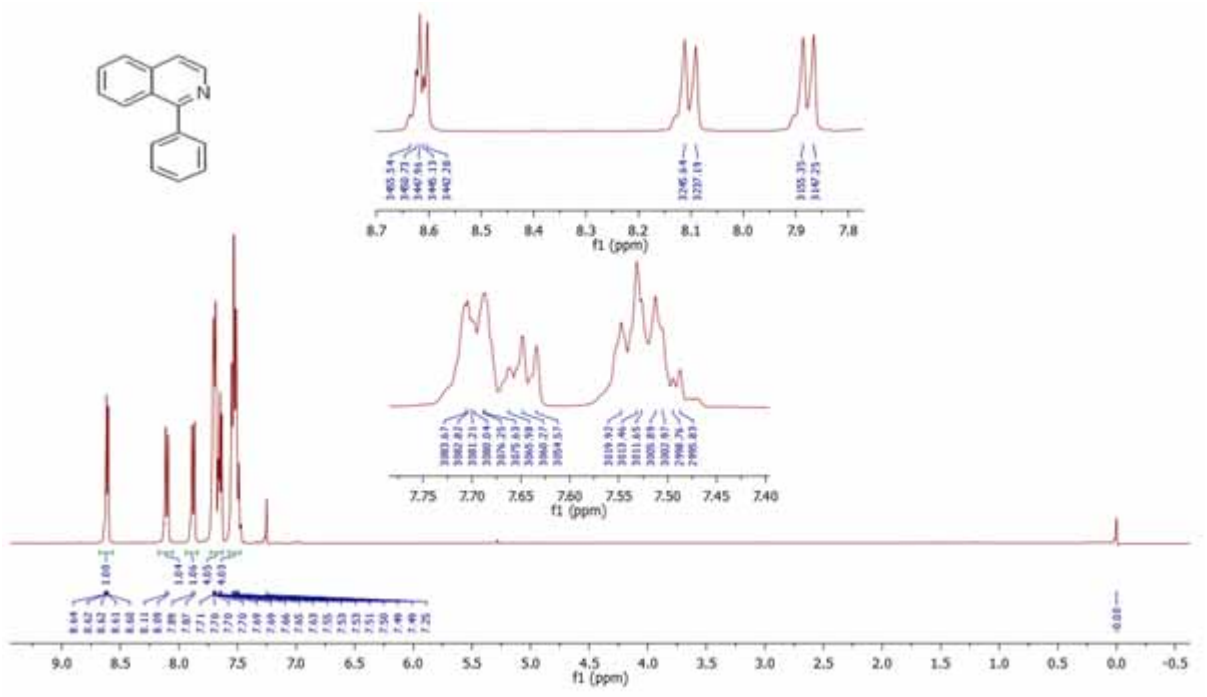
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
240.05752	1	677321.9	C15 H11 Cl N	(M+H)+
241.06103	1	107964.7	C15 H11 Cl N	(M+H)+
242.05509	1	191361.9	C15 H11 Cl N	(M+H)+
243.05808	1	36106.1	C15 H11 Cl N	(M+H)+
244.06077	1	2605.5	C15 H11 Cl N	(M+H)+
501.08916	1	1546.9		(2M+Na)+
502.09345	1	800.6		(2M+Na)+

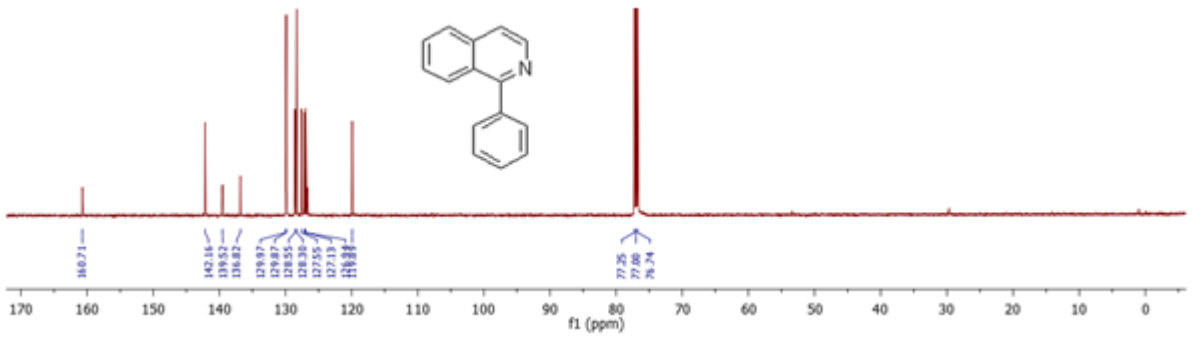
Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	240.05752	240.05745	-0.29	100	100	66.71	64.16
2	241.06103	241.06069	-1.39	15.94	16.72	10.63	10.73
3	242.05509	242.05487	-0.88	28.25	33.3	18.85	21.37
4	243.05808	243.05785	-0.92	5.33	5.41	3.56	3.47
5	244.06077	244.06102	1.03	0.38	0.42	0.26	0.27

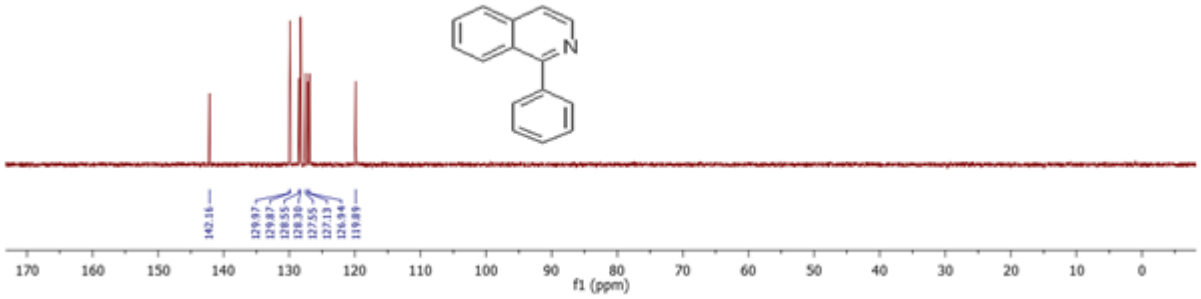
^{1}H NMR (400 MHz, $CDCl_3$) of compound **8j**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **8j**:



DEPT (125 MHz, $CDCl_3$) of compound **8j**:



HRMS (ESI-TOF) of compound **8j**:

Qualitative Compound Report

Data File	ISO-Q-PH.d	**Sample Name**	ISO-Q-PH
Sample Type	Sample	**Position**	Vial 61
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	9/26/2012 6:29:18 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

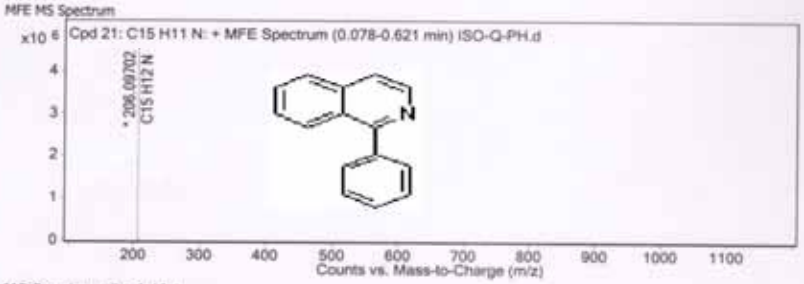
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C15 H11 N	0.174	205.08974	C15 H11 N	C15 H11 N	-2.9	C15 H11 N

Compound Label	m/z	RT	Algorithm	Mass
Cpd 21: C15 H11 N	206.09702	0.174	Find by Molecular Feature	205.08974

MFE MS Spectrum



MS Spectrum Peak List

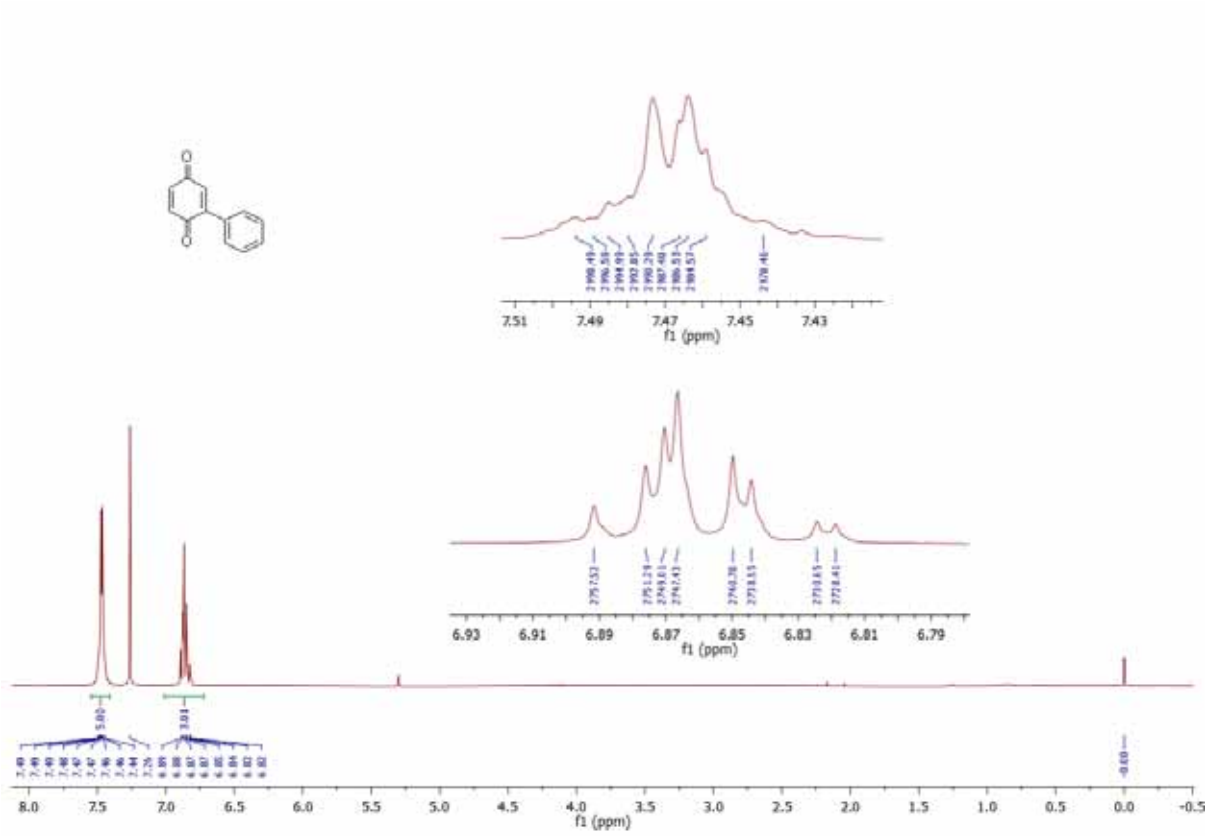
m/z	z	Abund	Formula	Ion
206.09702	1	4532293.5	C15 H12 N	(M+H)+
207.09985	1	690794.3	C15 H12 N	(M+H)+
208.10318	1	56023.5	C15 H12 N	(M+H)+
209.10622	1	2427.3	C15 H12 N	(M+H)+

Predicted Isotope Match Table

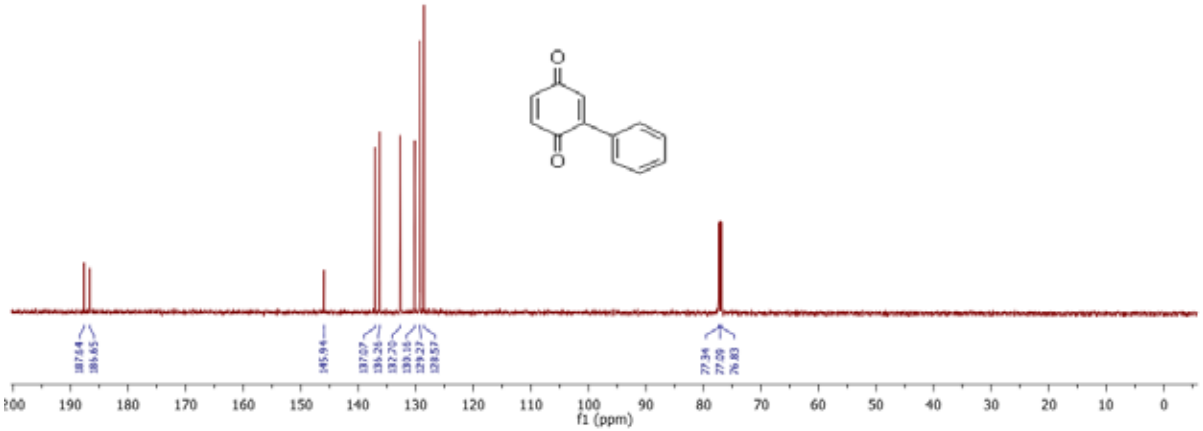
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	206.09702	206.09643	-2.89	100	100	85.81	84.67
2	207.09985	207.09967	-0.89	15.24	16.73	13.08	14.16
3	208.10318	208.1029	-1.33	1.24	1.31	1.06	1.11
4	209.10622	209.10612	-0.48	0.05	0.06	0.05	0.05

--- End Of Report ---

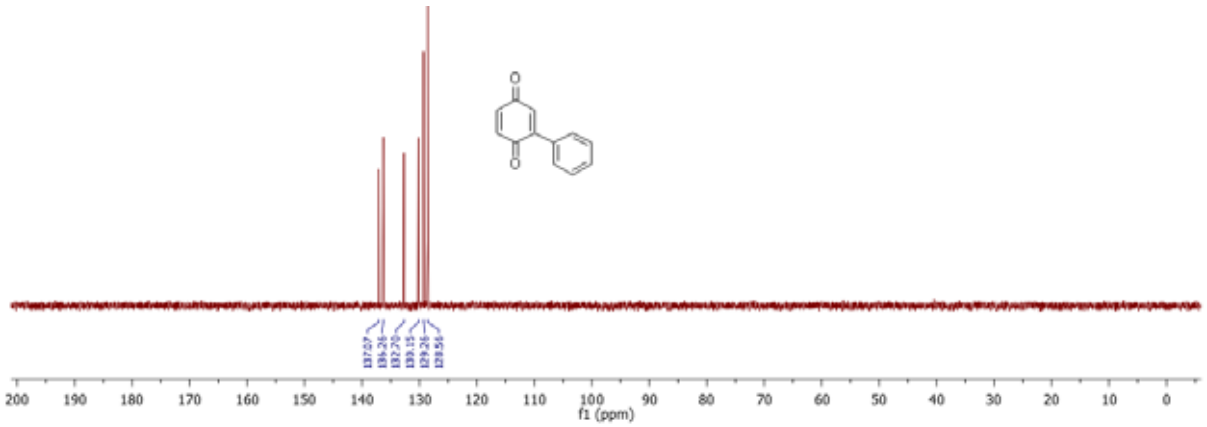
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10a**:



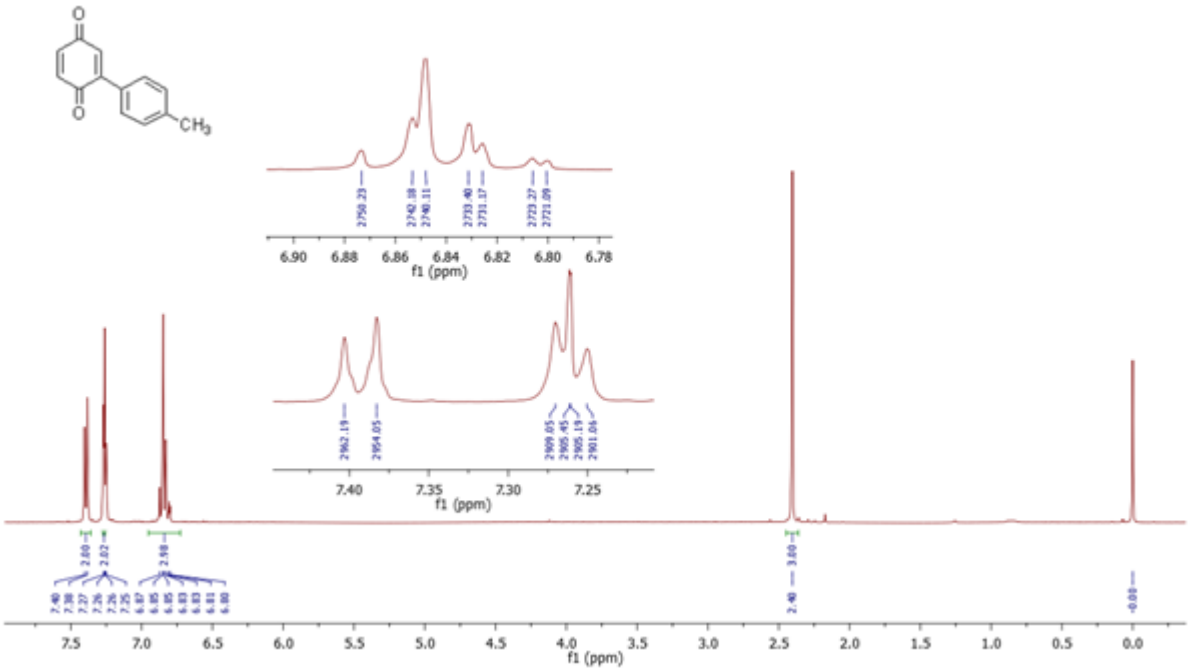
^{13}C NMR (125 MHz, $CDCl_3$) of compound **10a**:



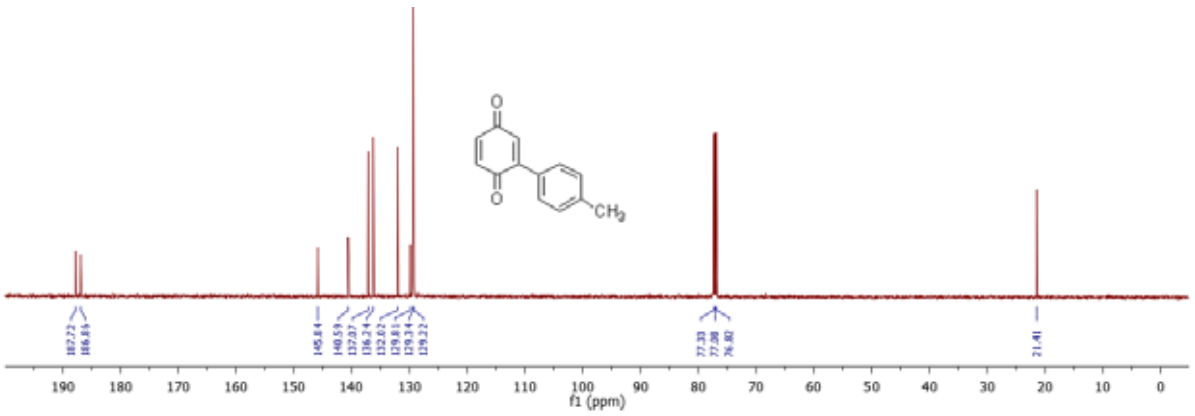
DEPT (125 MHz, $CDCl_3$) of compound **10a**:



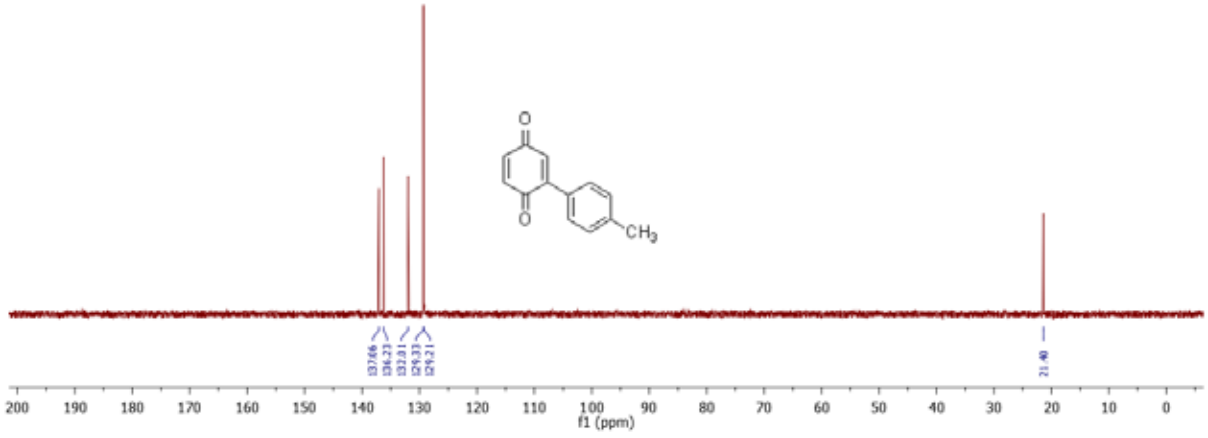
^1H NMR (400 MHz, $CDCl_3$) of compound **10b**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **10b**:



DEPT (125 MHz, $CDCl_3$) of compound **10b**:



HRMS (ESI-TOF) of compound **10b**:

Qualitative Compound Report

Data File	BQ-4-Me.d	**Sample Name**	BQ-4-Me
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	10/18/2012 1:38:44 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

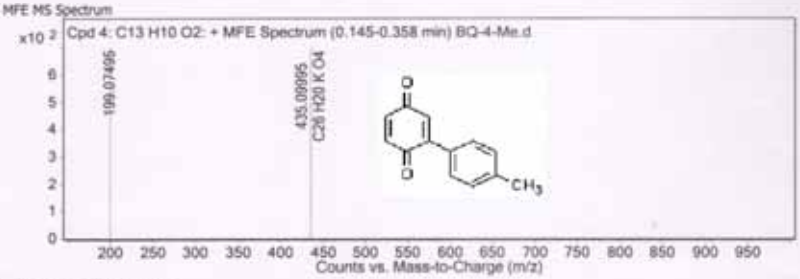
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C13 H10 O2	0.173	198.06872	C13 H10 O2	C13 H10 O2	-3.21	C13 H10 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C13 H10 O2	199.07495	0.173	Find by Molecular Feature	198.06872

MFE MS Spectrum



MS Spectrum Peak List

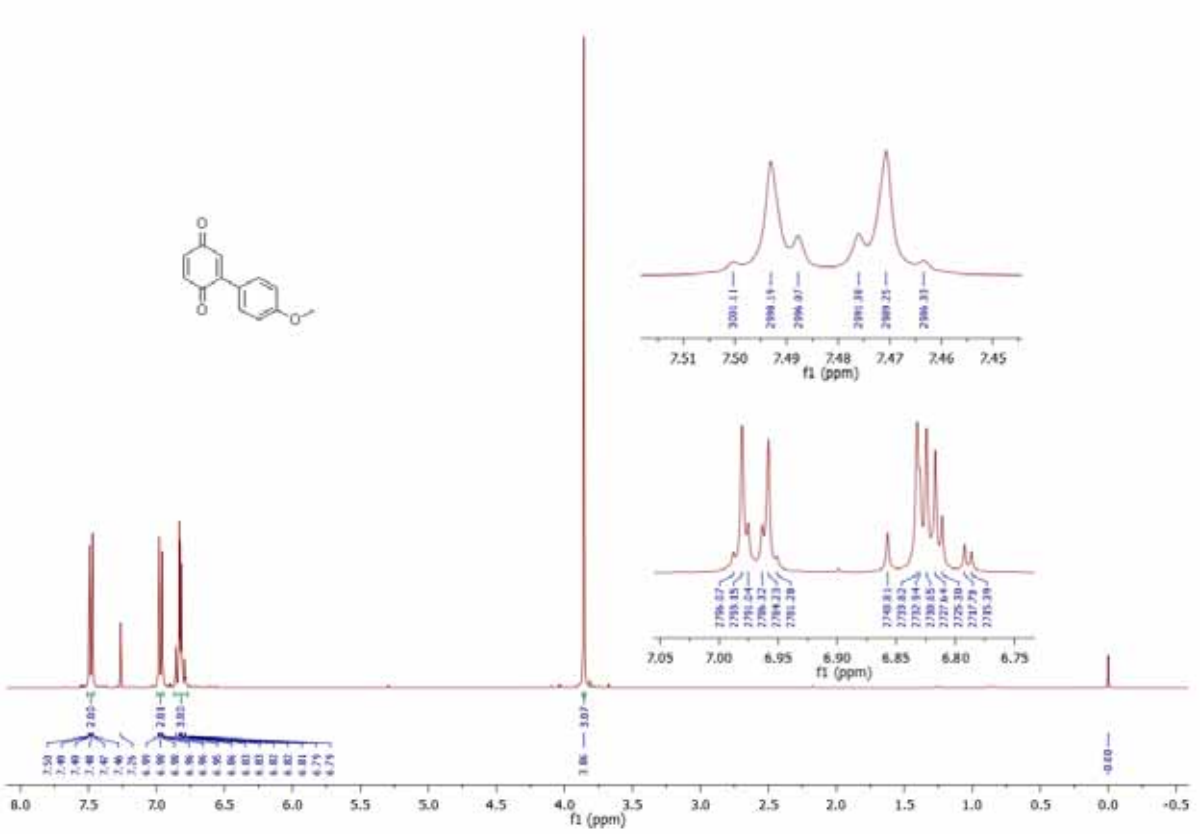
m/z	z	Abund	Formula	Ion
199.07495	1	7429.5		(M+H)+
200.08163	1	2395		(M+H)+
435.09995	1	701	C26 H20 K O4	(2M+K)+

Predicted Isotope Match Table

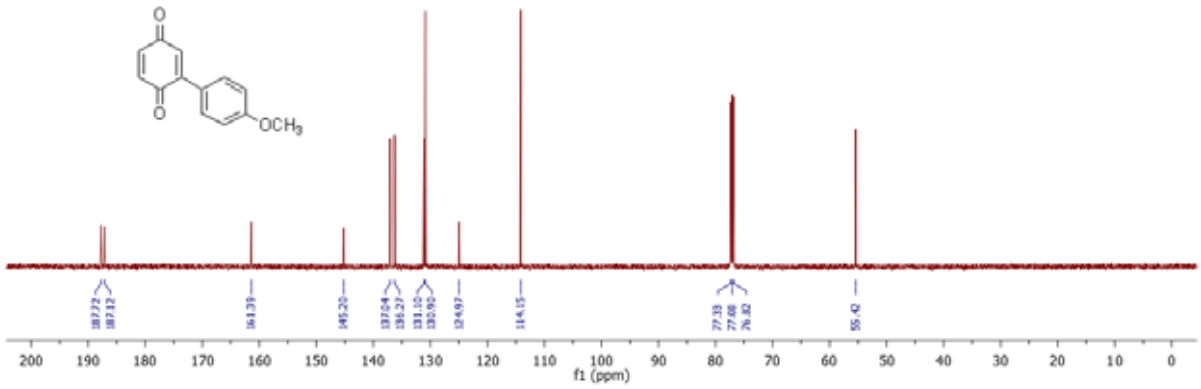
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	435.09995	435.09932	-1.46	100	100	100	100

--- End Of Report ---

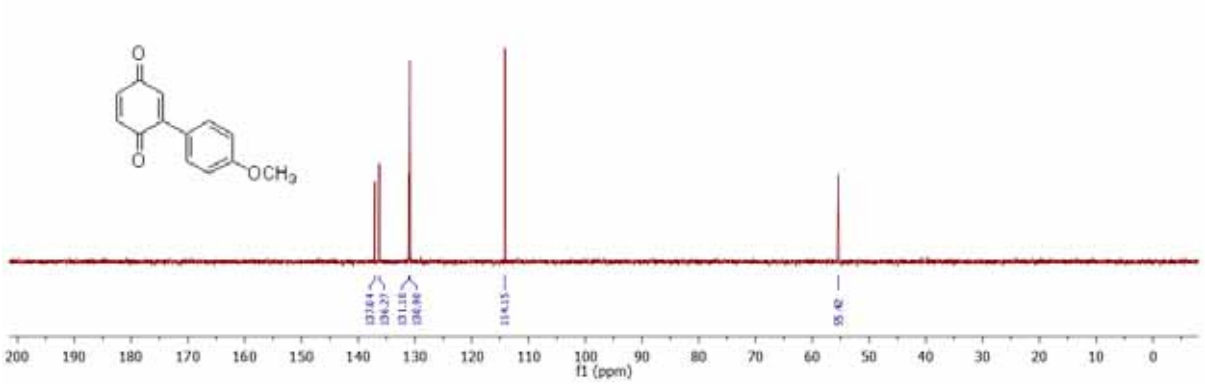
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10c**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **10c**:



DEPT (125 MHz, $CDCl_3$) of compound **10c**:



HRMS (ESI-TOF) of compound **10c**:

Qualitative Compound Report

Data File	BQ-4-OMe.d	**Sample Name**	BQ-4-OMe
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	10/18/2012 2:00:59 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

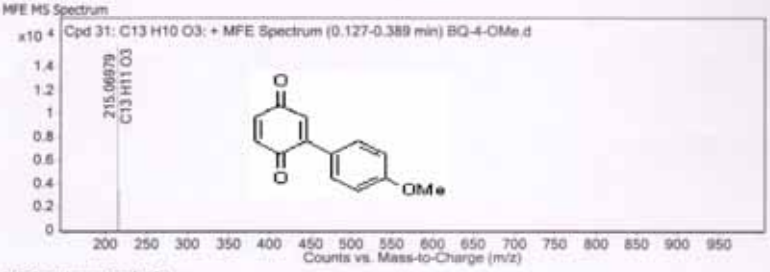
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 31: C13 H10 O3	0.175	214.06254	C13 H10 O3	C13 H10 O3	2.1	C13 H10 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 31: C13 H10 O3	215.06979	0.175	Find by Molecular Feature	214.06254

MFE MS Spectrum



MS Spectrum Peak List

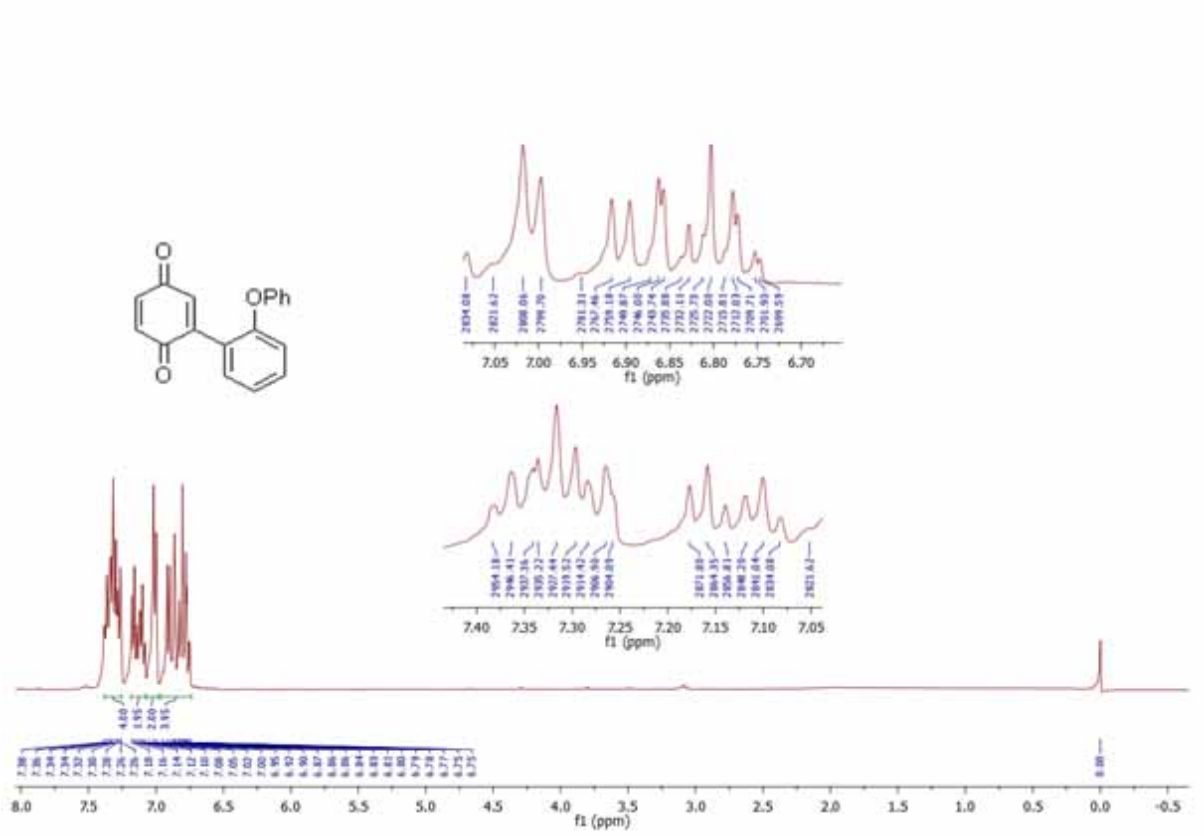
m/z	z	Abund	Formula	Ion
215.06979	1	15799.8	C13 H11 O3	(M+H)+
216.07568	1	3475.8	C13 H11 O3	(M+H)+

Predicted Isotope Match Table

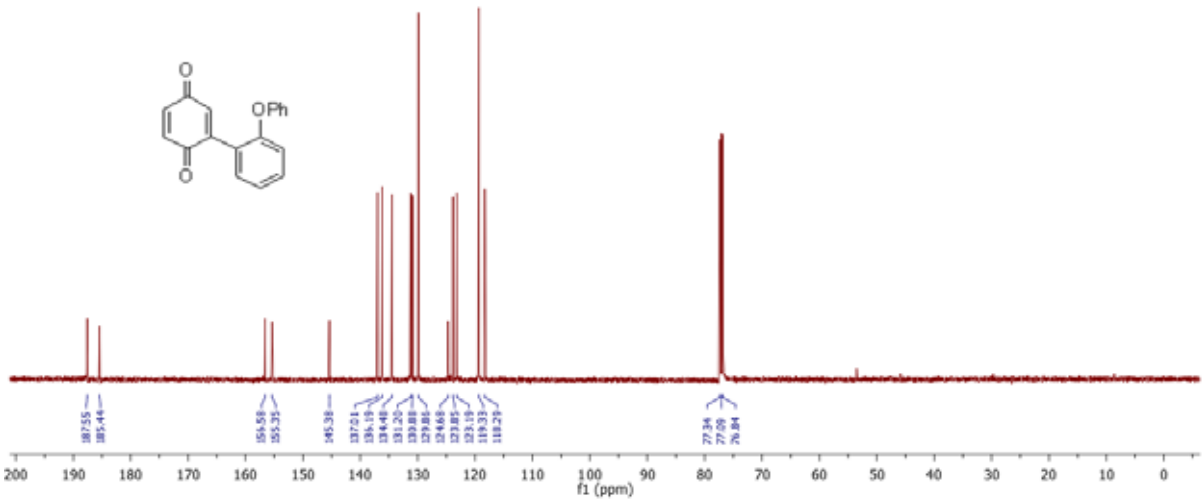
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	215.06979	215.07027	2.22	100	100	81.97	87.49
2	216.07568	216.07366	-9.37	22	14.3	18.03	12.51

--- End Of Report ---

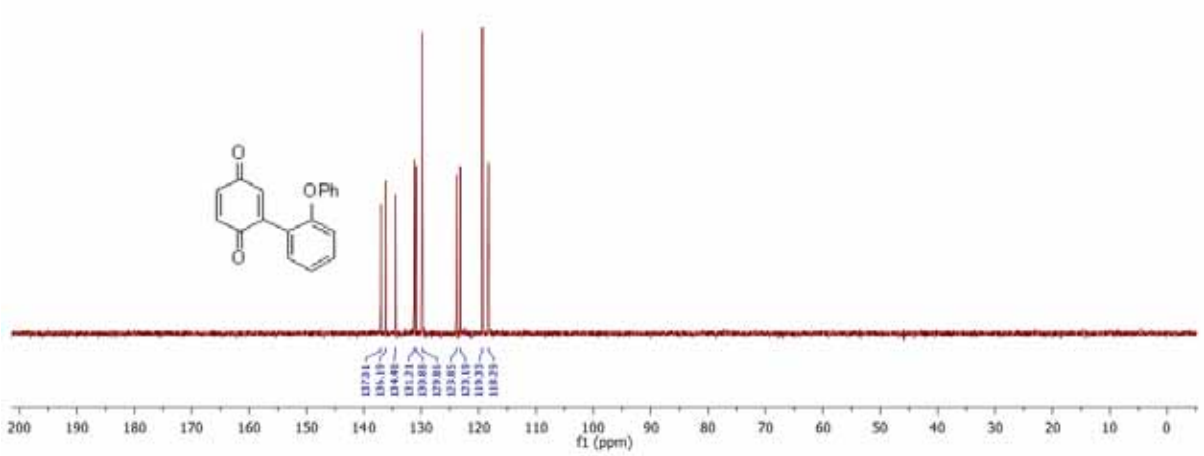
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10d**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **10d**:



DEPT (125 MHz, $CDCl_3$) of compound **10d**:



HRMS (ESI-TOF) of compound **10d**:

Qualitative Compound Report

Data File	BQ-2-OPh.d	**Sample Name**	BQ-2-OPh
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	10/18/2012 12:23:01 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

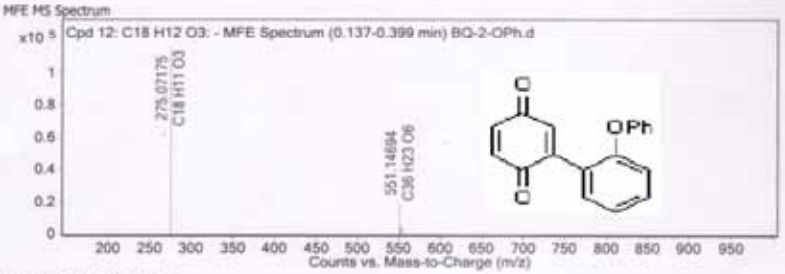
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C18 H12 O3	0.175	276.07902	C18 H12 O3	C18 H12 O3	-1.37	C18 H12 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 12: C18 H12 O3	275.07175	0.175	Find by Molecular Feature	276.07902

MFE MS Spectrum



MS Spectrum Peak List

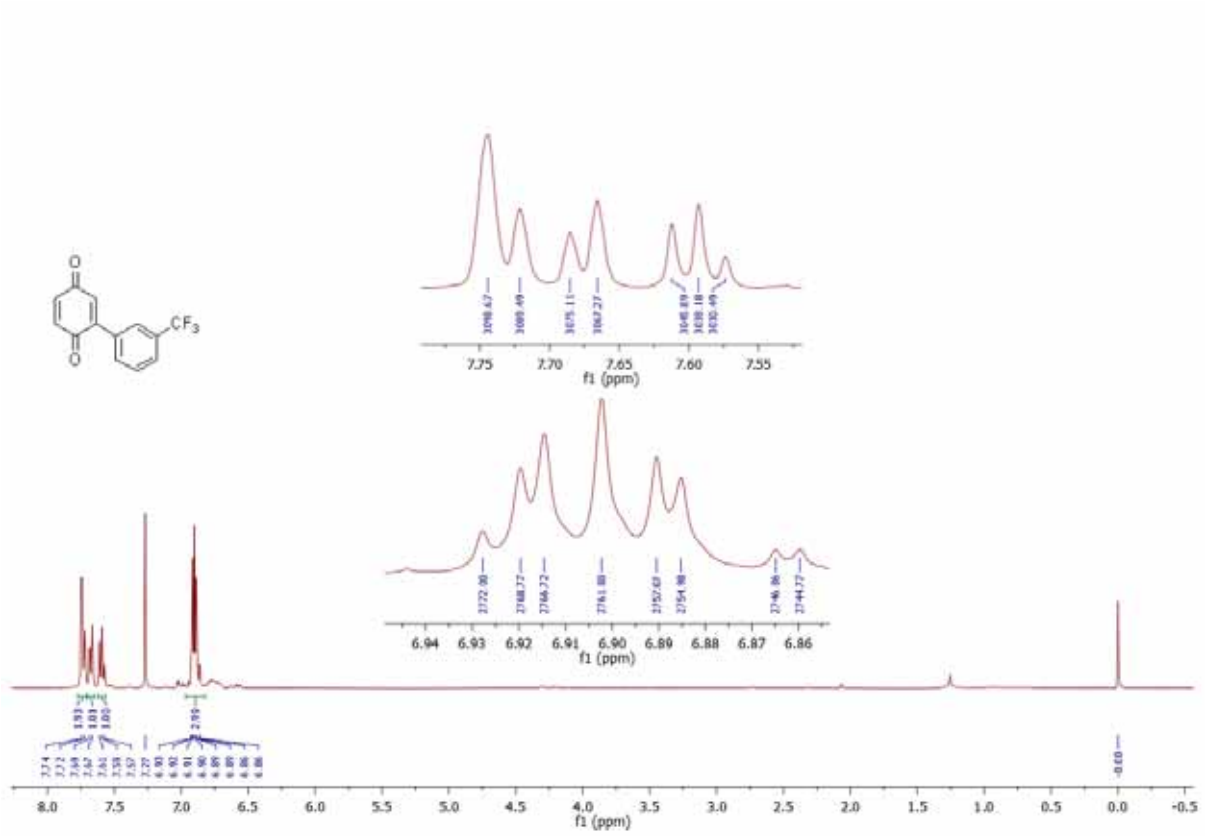
m/z	z	Abund	Formula	Ion
275.07175	-1	116093.5	C18 H11 O3	(M-H)-
551.14694	-1	18332.2	C36 H23 O6	(2M-H)-
552.15183	-1	5783.6	C36 H23 O6	(2M-H)-
553.157	-1	3112.1	C36 H23 O6	(2M-H)-

Predicted Isotope Match Table

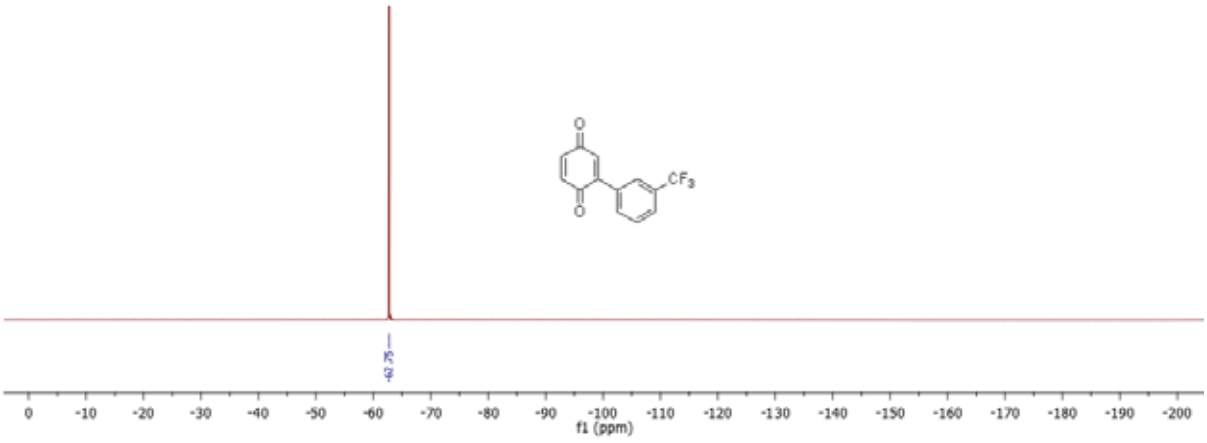
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	275.07175	275.07137	-1.37	100	100	100	100

— End Of Report —

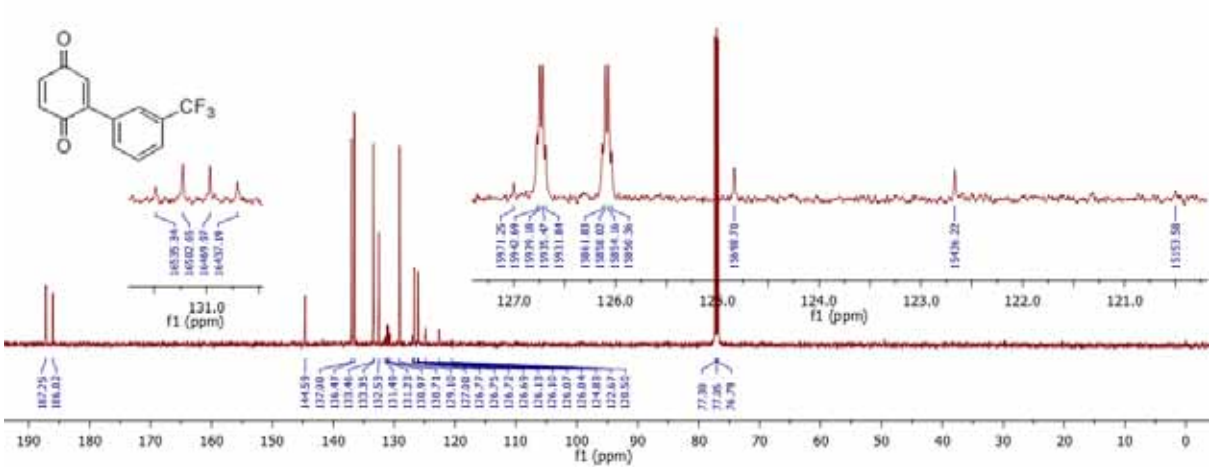
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10e**:



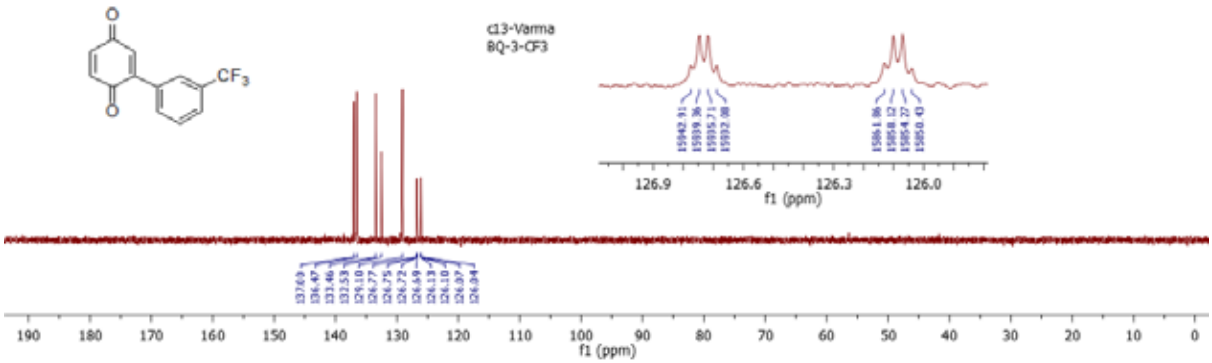
^{19}F NMR (376 MHz, $CDCl_3$) of compound **10e**:



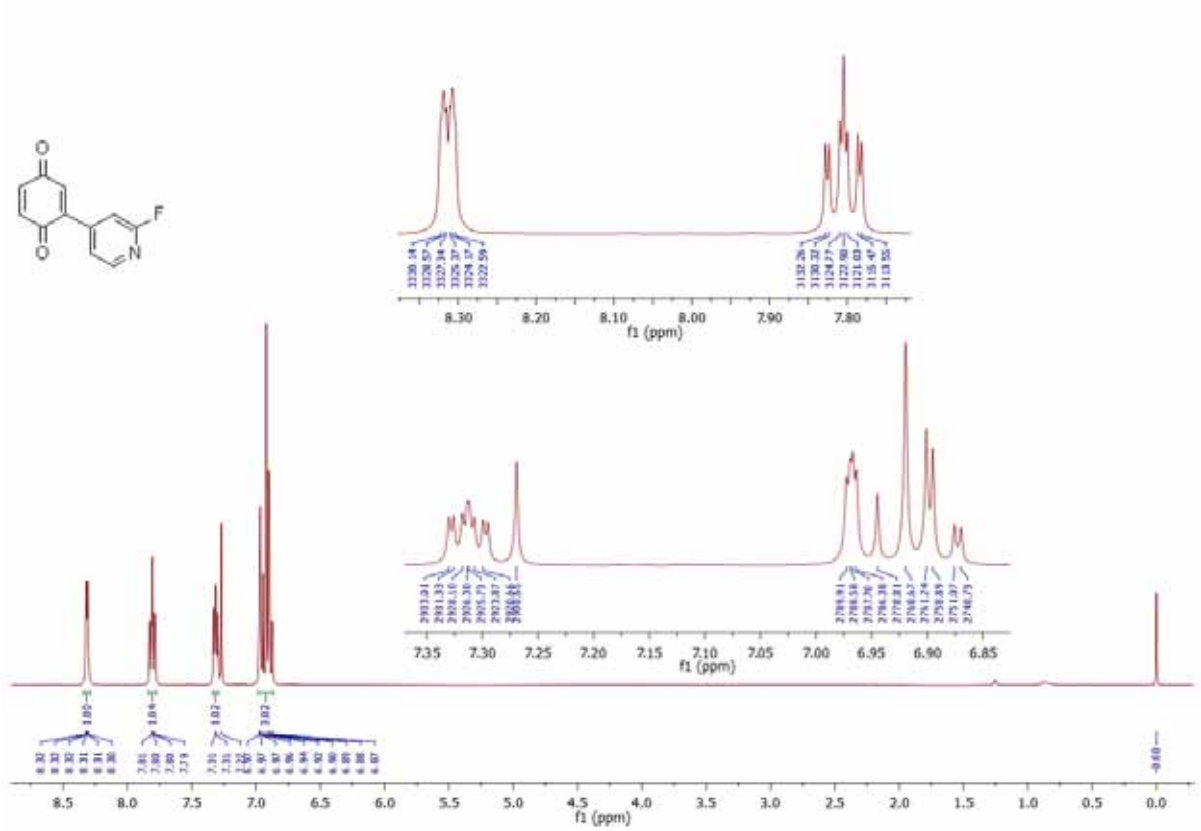
^{13}C NMR (125 MHz, $CDCl_3$) of compound **10e**:



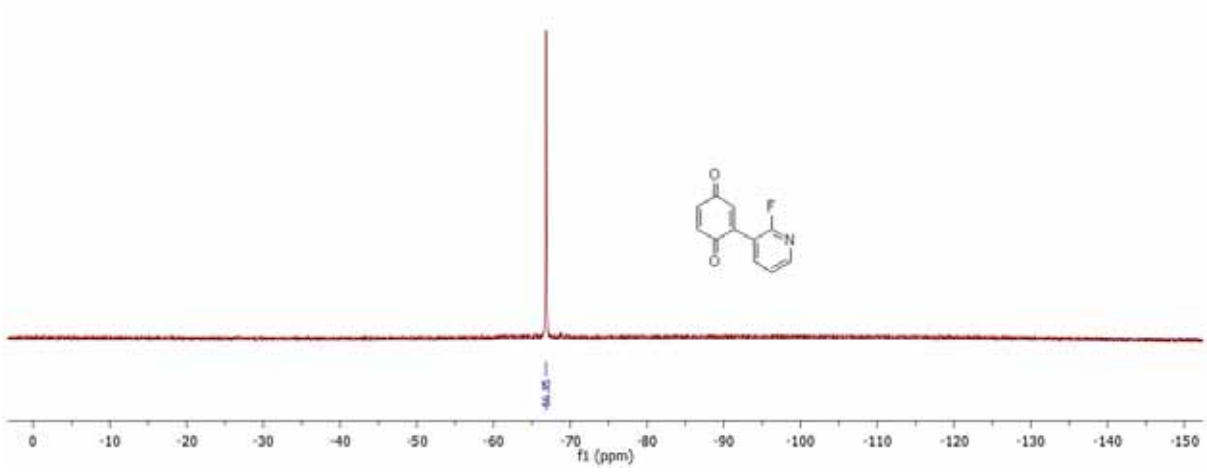
DEPT (125 MHz, $CDCl_3$) of compound **10e**:



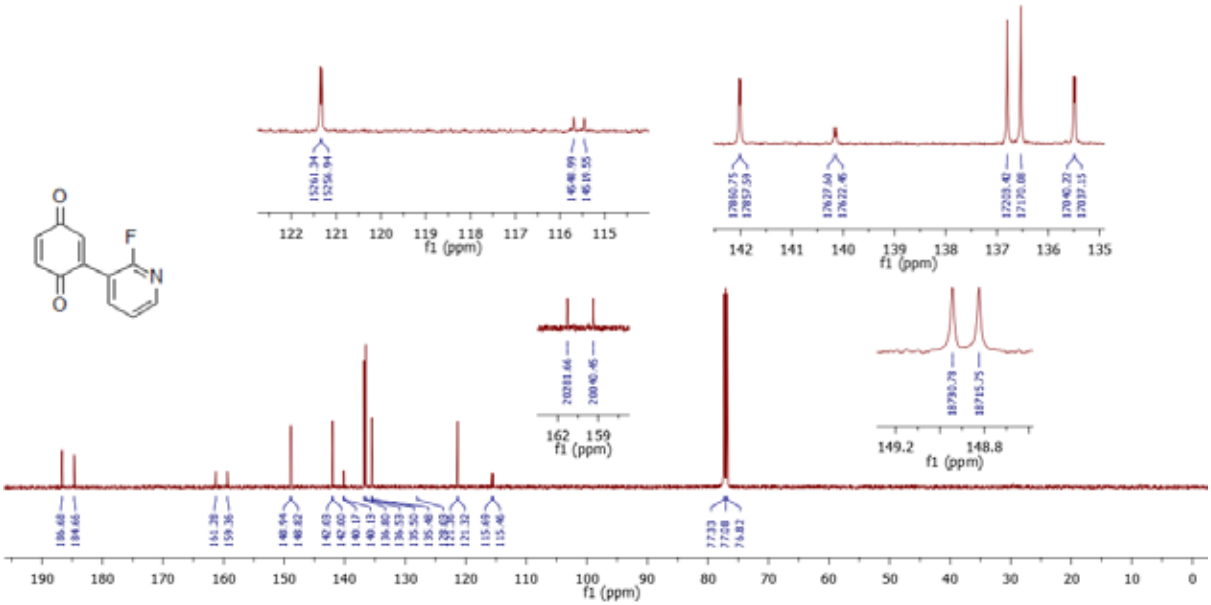
^{1}H NMR (400 MHz, $CDCl_3$) of compound **10f**:



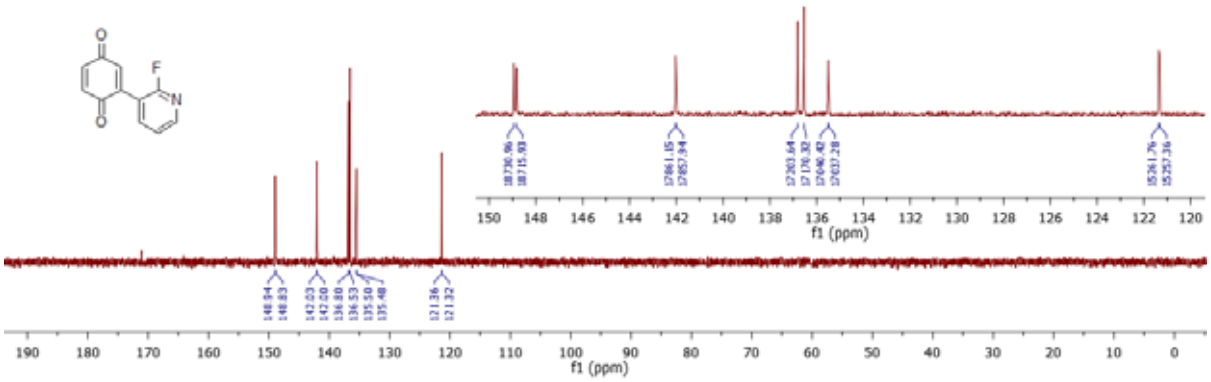
^{19}F NMR (376 MHz, $CDCl_3$) of compound **10f**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **10f**:



DEPT (125 MHz, $CDCl_3$) of compound **10f**:



HRMS (ESI-TOF) of compound **10f**:

Qualitative Compound Report

Data File	BQ-2-F-PY.d	**Sample Name**	BQ-2-F-PY
Sample Type	Sample	**Position**	Vial 4
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	10/18/2012 12:38:15 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

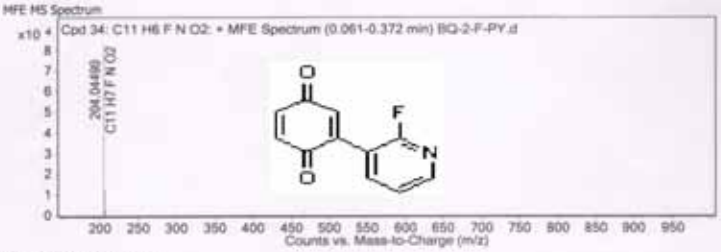
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 34: C11 H6 F N O2	0.176	203.03767	C11 H6 F N O2	C11 H6 F N O2	2.89	C11 H6 F N O2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 34: C11 H6 F N O2	204.0449	0.176	Find by Molecular Feature	203.03767

MFE MS Spectrum



MS Spectrum Peak List

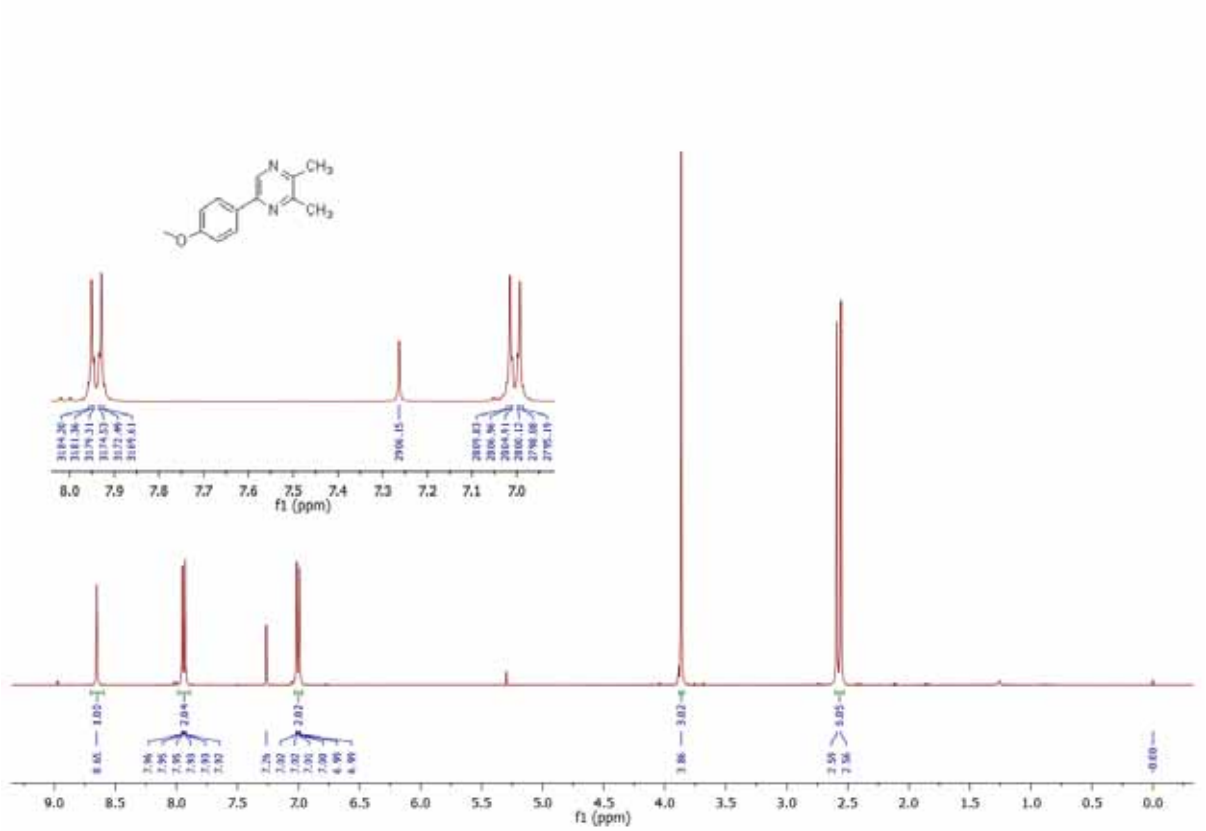
m/z	z	Abund	Formula	Ion
204.0449	1	83903.4	C11 H7 F N O2	(M+H)+
205.04965	1	14138.8	C11 H7 F N O2	(M+H)+
206.06045	1	12709.9	C11 H7 F N O2	(M+H)+
207.06328	1	1959.6	C11 H7 F N O2	(M+H)+

Predicted Isotope Match Table

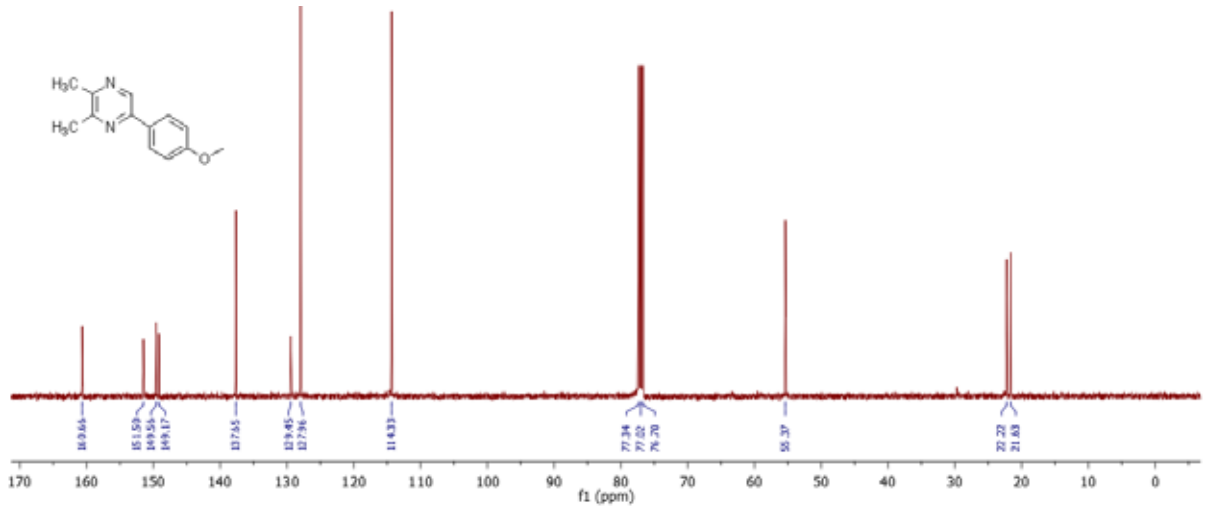
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	204.0449	204.04553	3.09	100	100	74.44	88.02
2	205.04965	205.04873	-4.5	16.85	12.42	12.54	10.93
3	206.06045	206.05112	-45.26	15.15	1.12	11.28	0.98
4	207.06328	207.05364	-46.53	2.34	0.08	1.74	0.07

— End Of Report —

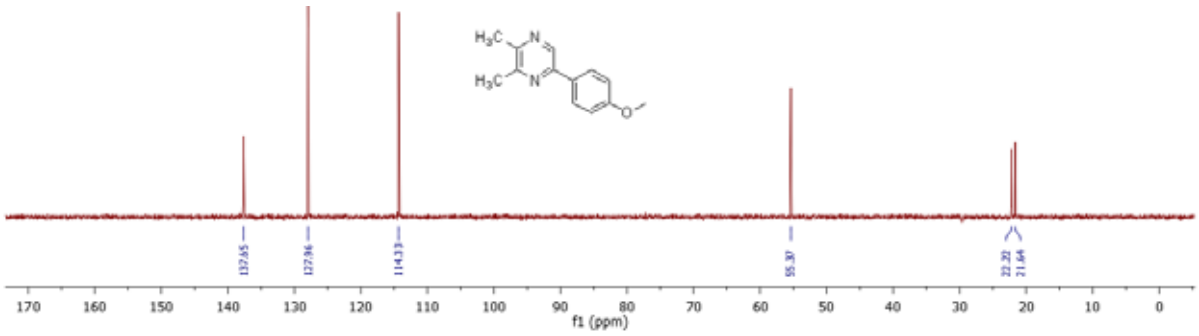
^{1}H NMR (400 MHz, $CDCl_3$) of compound **19**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **19**:



DEPT (100 MHz, $CDCl_3$) of compound **19**:



HRMS (ESI-TOF) of compound **19**:

Qualitative Compound Report

Data File	DM-PYRA-4-OME.d	**Sample Name**	DM-PYRA-4-OME
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/12/2012 11:31:03 AM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

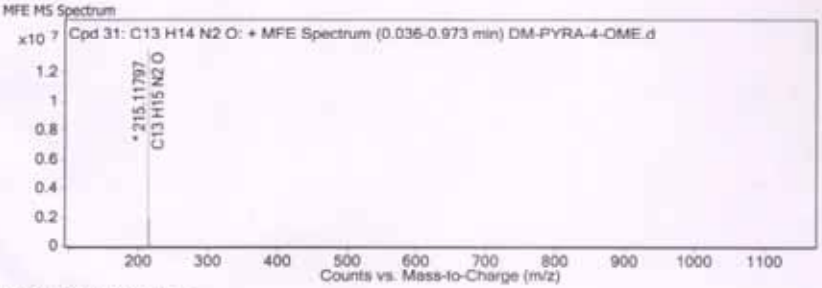
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 31: C13 H14 N2 O	0.292	214.1107	C13 H14 N2 O	C13 H14 N2 O	-0.38	C13 H14 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 31: C13 H14 N2 O	215.11797	0.292	Find by Molecular Feature	214.1107

MFE MS Spectrum



MS Spectrum Peak List

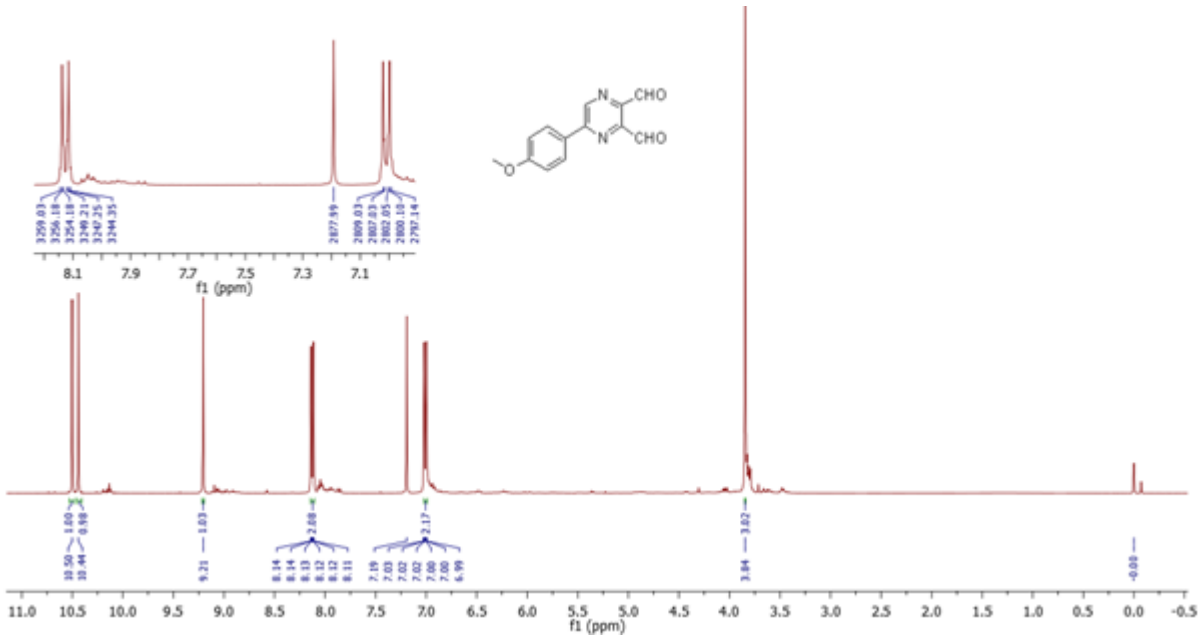
m/z	z	Abund	Formula	Ion
215.11797	1	13638252	C13 H15 N2 O	(M+H)+
216.12124	1	1943522.9	C13 H15 N2 O	(M+H)+
217.12378	1	154034.8	C13 H15 N2 O	(M+H)+
218.12601	1	2606.5	C13 H15 N2 O	(M+H)+

Predicted Isotope Match Table

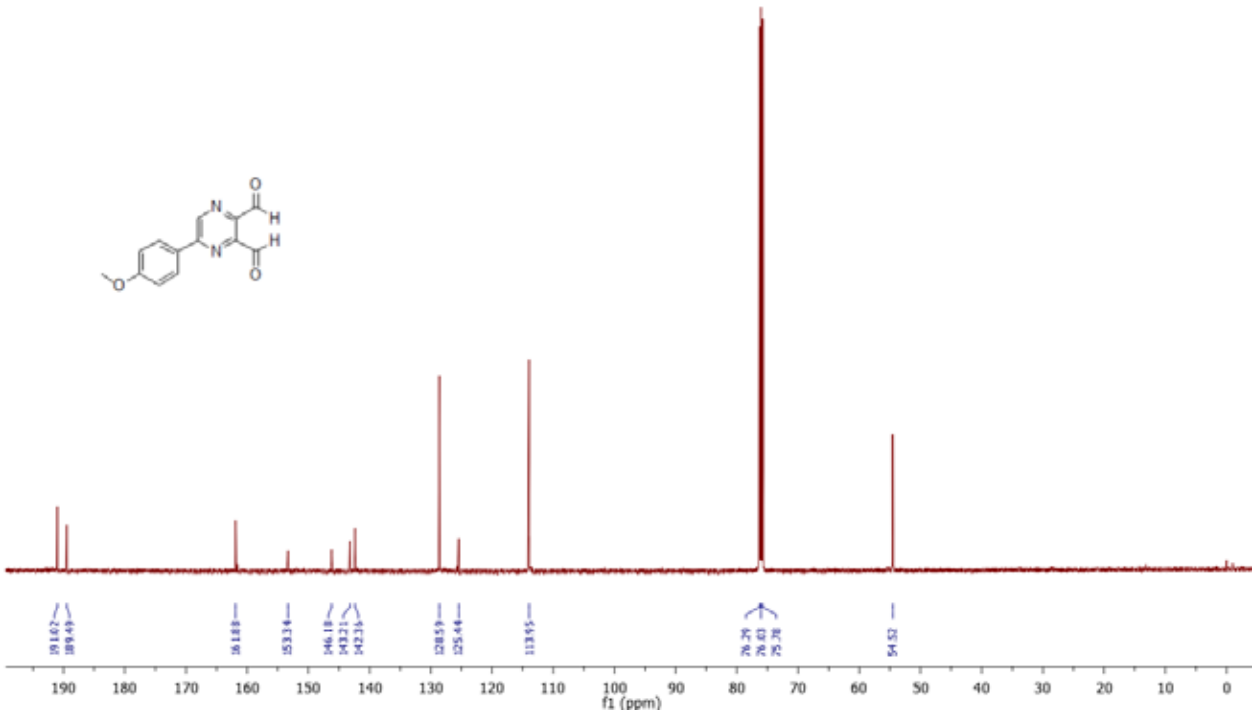
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	215.11797	215.11789	-0.38	100	100	86.66	85.96
2	216.12124	216.12097	-1.22	14.25	15	12.35	12.9
3	217.12378	217.12372	-0.26	1.13	1.25	0.98	1.08
4	218.12601	218.12631	1.4	0.02	0.08	0.02	0.07

--- End Of Report ---

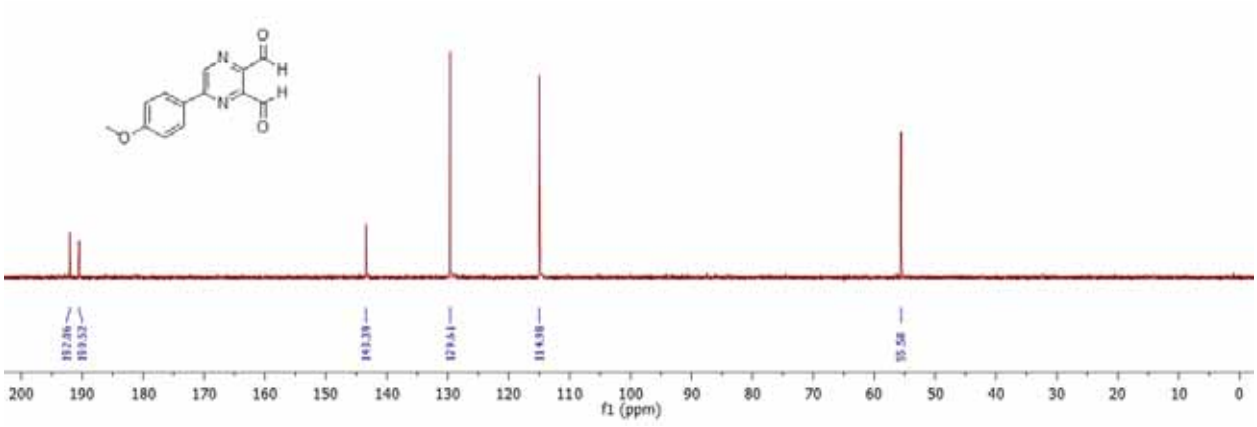
^{1}H NMR (400 MHz, $CDCl_3$) of compound **20**:



^{13}C NMR (125 MHz, $CDCl_3$) of compound **20**:



DEPT (125 MHz, $CDCl_3$) of compound **20**:



HRMS (ESI-TOF) of compound **20**:

Qualitative Compound Report

Data File	DIAL.d	**Sample Name**	DIAL
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/12/2012 11:27:33 AM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

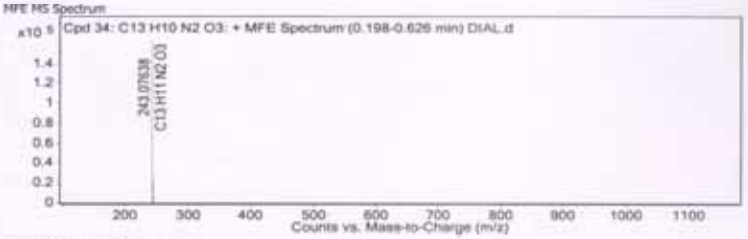
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 34: C13 H10 N2 O3	0.286	242.0691	C13 H10 N2 O3	C13 H10 N2 O3	0.16	C13 H10 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 34: C13 H10 N2 O3	243.07638	0.286	Find by Molecular Feature	242.0691

MFE MS Spectrum



MS Spectrum Peak List

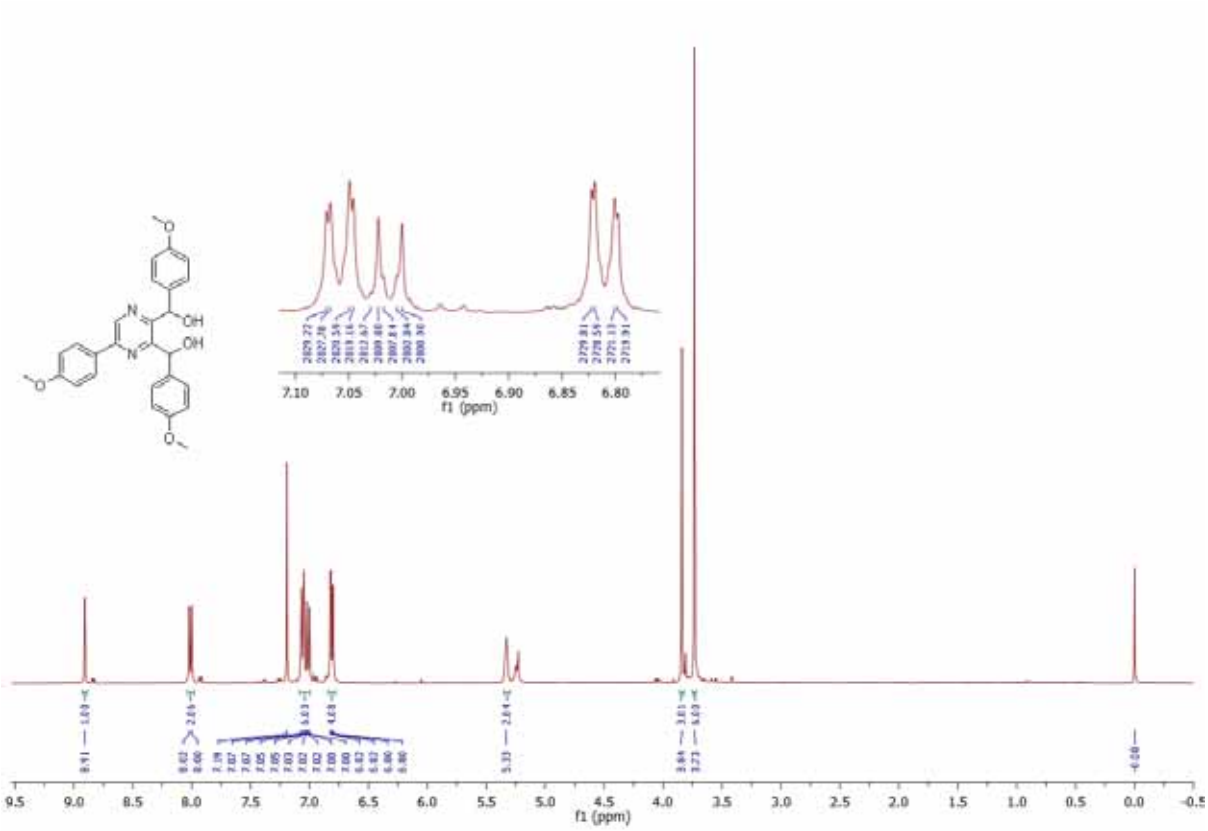
m/z	*z*	Abund	Formula	Ion
243.07638	1	163357.7	C13 H11 N2 O3	(M+H)+
244.07931	1	25676	C13 H11 N2 O3	(M+H)+
245.08142	1	3498.5	C13 H11 N2 O3	(M+H)+

Predicted Isotope Match Table

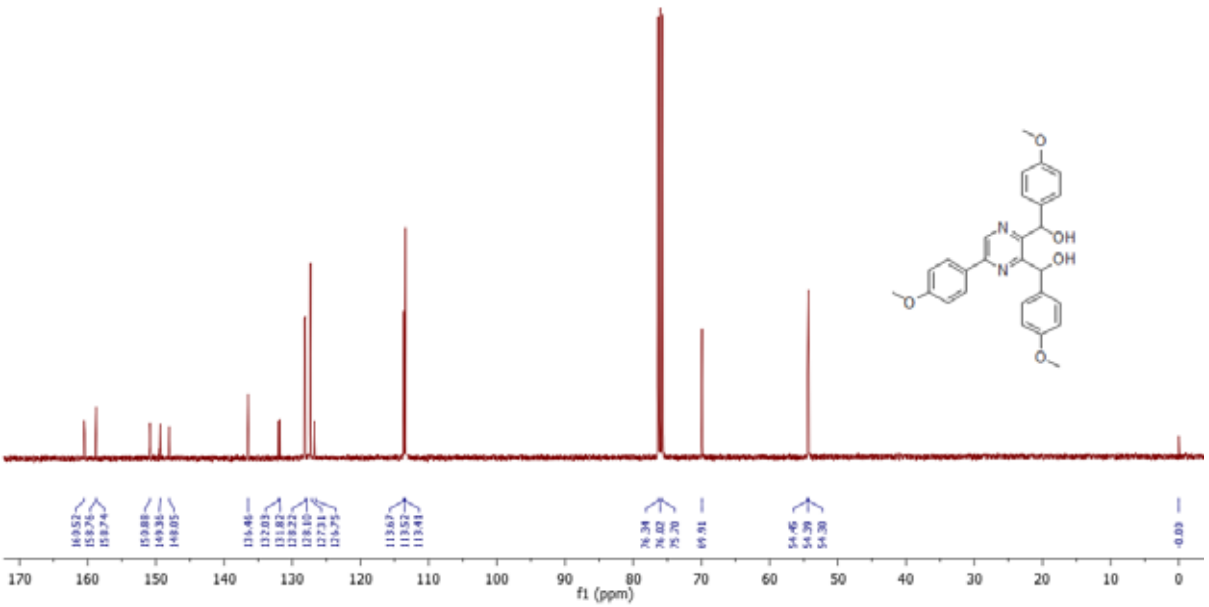
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	243.07638	243.07642	0.16	100	100	84.85	85.69
2	244.07931	244.0795	0.78	15.72	15.03	13.34	12.88
3	245.08142	245.08185	1.76	2.14	1.67	1.82	1.43

--- End Of Report ---

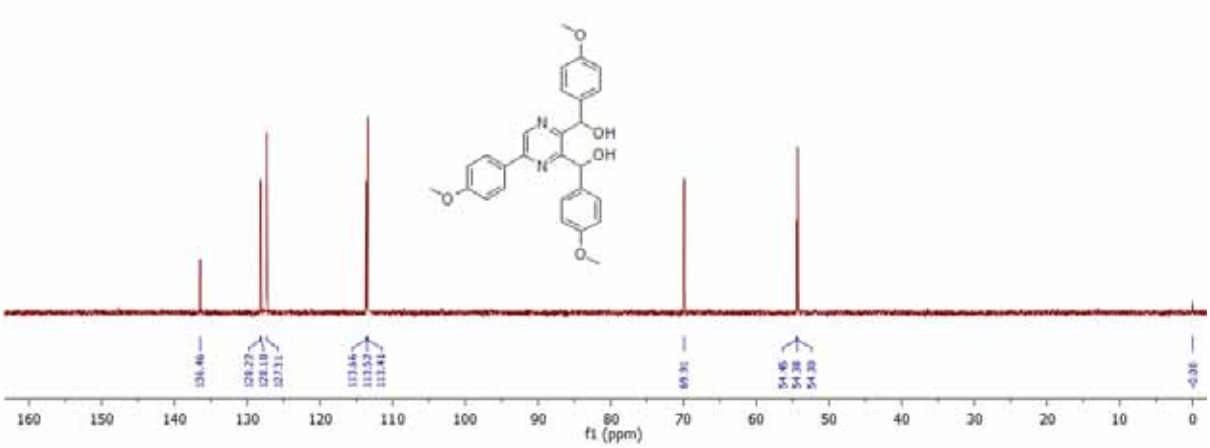
^{1}H NMR (400 MHz, $CDCl_3$) of compound **21**:



^{13}C NMR (100 MHz, $CDCl_3$) of compound **21**:



DEPT (100 MHz, $CDCl_3$) of compound **21**:



HRMS (ESI-TOF) of compound **21**:

Qualitative Compound Report

Data File	DIOL.d	**Sample Name**	DIOL
Sample Type	Sample	**Position**	Vial 13
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 12:50:55 PM
IRM Calibration Status	Success	**DA Method**	as.m
Comment			

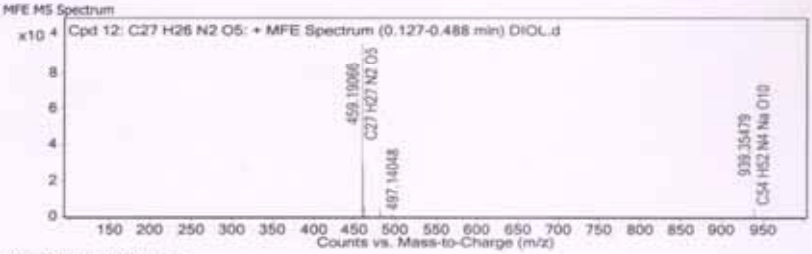
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C27 H26 N2 O5	0.172	458.18339	C27 H26 N2 O5	C27 H26 N2 O5	1.7	C27 H26 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 12: C27 H26 N2 O5	459.19066	0.172	Find by Molecular Feature	458.18339

MFE MS Spectrum



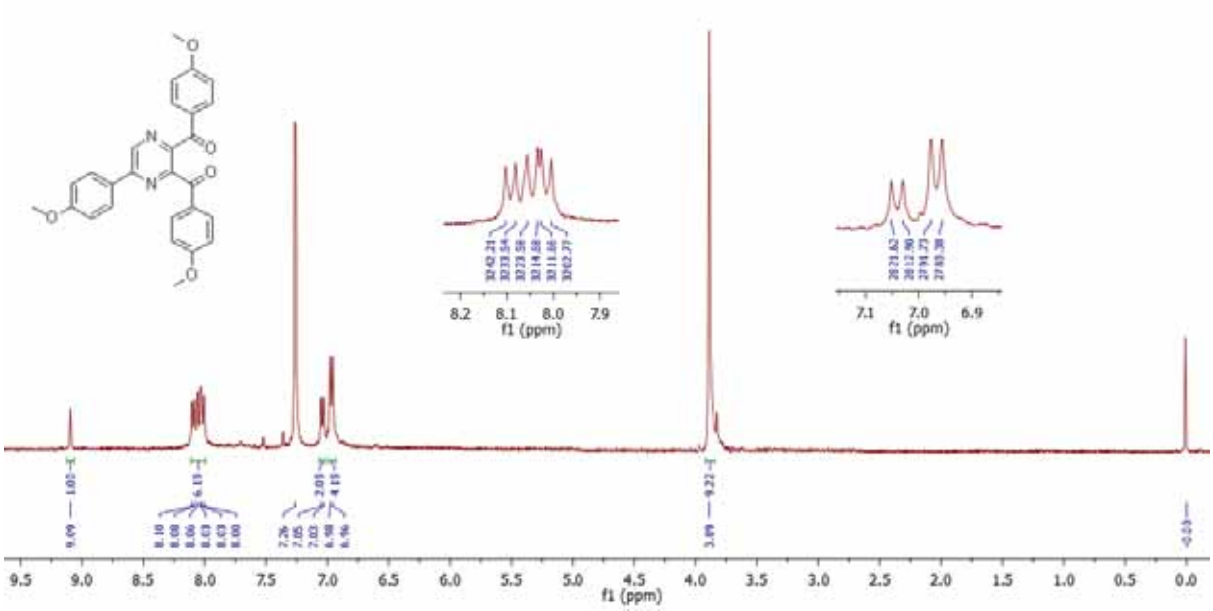
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
459.19066	1	96207.7	C27 H27 N2 O5	(M+H)+
460.19402	1	30187.7	C27 H27 N2 O5	(M+H)+
461.19565	1	5737.8	C27 H27 N2 O5	(M+H)+
462.20204	1	788.3	C27 H27 N2 O5	(M+H)+
481.17149	1	5157.8	C27 H26 N2 Na O5	(M+Na)+
482.17673	1	1702.1	C27 H26 N2 Na O5	(M+Na)+
483.18347	1	641	C27 H26 N2 Na O5	(M+Na)+
497.14048	1	1359.8		(M+K)+
939.35479	1	3891.7	C54 H52 N4 Na O10	(2M+Na)+
940.35856	1	2446.5	C54 H52 N4 Na O10	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	459.19066	459.19145	1.71	100	100	72.38	73.17
2	460.19402	460.19469	1.44	31.38	30.43	22.71	22.27
3	461.19565	461.1975	4.03	5.96	5.5	4.32	4.02
4	462.20204	462.20021	-3.98	0.82	0.73	0.59	0.54

^{1}H NMR (400 MHz, $CDCl_3$) of compound **17**:



HRMS (ESI-TOF) of compound **17**:

Qualitative Compound Report

Data File	BOT.d	**Sample Name**	BOT
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_MS_25072012.m	**Acquired Time**	11/18/2012 12:47:25 PM
IRM Calibration Status	Success	**DA Method**	es.m
Comment			

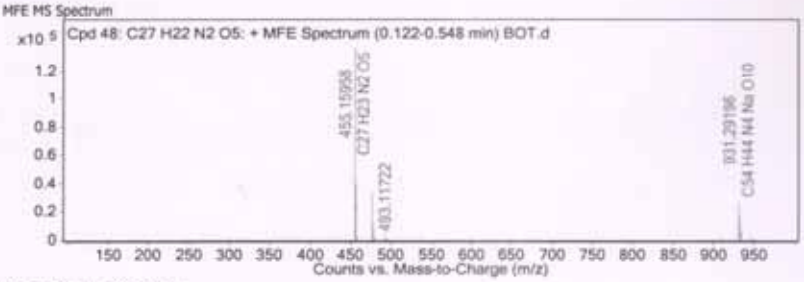
Sample Group **Info.**

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 48: C27 H22 N2 O5	0.175	454.15229	C27 H22 N2 O5	C27 H22 N2 O5	1.28	C27 H22 N2 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 48: C27 H22 N2 O5	455.15958	0.175	Find by Molecular Feature	454.15229

MFE MS Spectrum



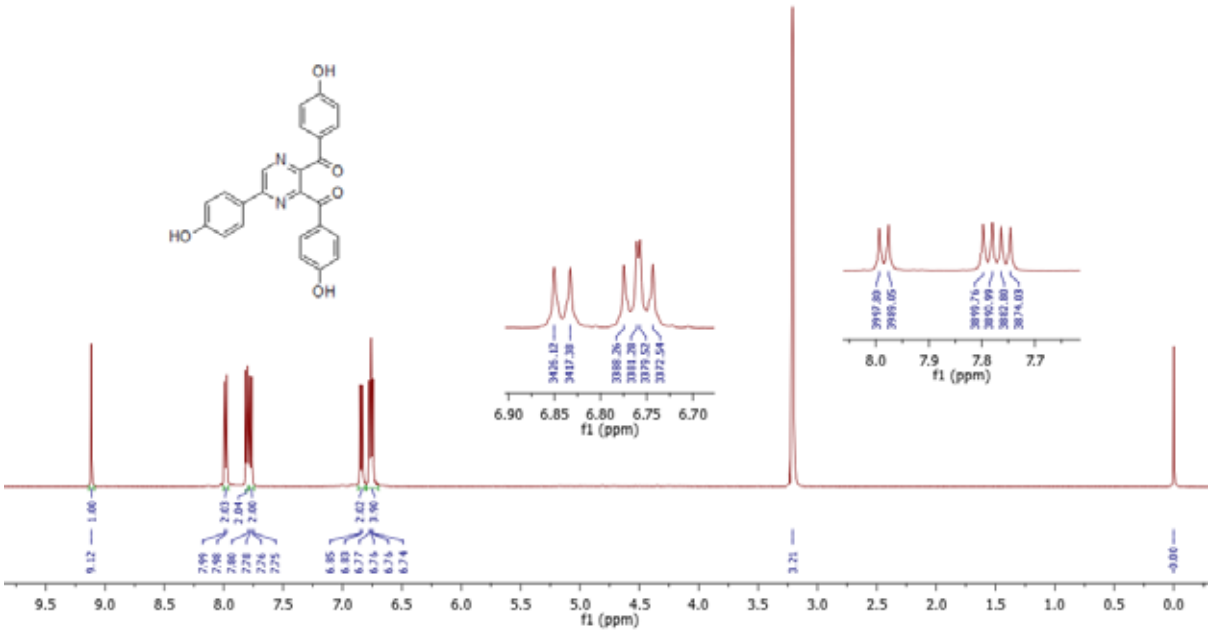
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
455.15958	1	135926.3	C27 H23 N2 O5	(M+H)+
456.16242	1	40364.7	C27 H23 N2 O5	(M+H)+
457.1661	1	7903.7	C27 H23 N2 O5	(M+H)+
477.14112	1	32958.4	C27 H22 N2 Na O5	(M+Na)+
478.14471	1	10336.1	C27 H22 N2 Na O5	(M+Na)+
479.14585	1	2569.3	C27 H22 N2 Na O5	(M+Na)+
493.11722	1	3099.4		(M+K)+
931.29196	1	26934.2	C54 H44 N4 Na O10	(2M+Na)+
932.29631	1	16340	C54 H44 N4 Na O10	(2M+Na)+
933.29957	1	5468.5	C54 H44 N4 Na O10	(2M+Na)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	455.15958	455.16015	1.26	100	100	73	73.2
2	456.16242	456.16338	2.1	29.7	30.39	21.68	22.25
3	457.1661	457.1662	0.22	5.81	5.49	4.24	4.02
4	458.16739	458.16889	3.28	1.48	0.73	1.08	0.54

^{1}H NMR (500 MHz, CD_3OD) of Botryllazine A **22**:

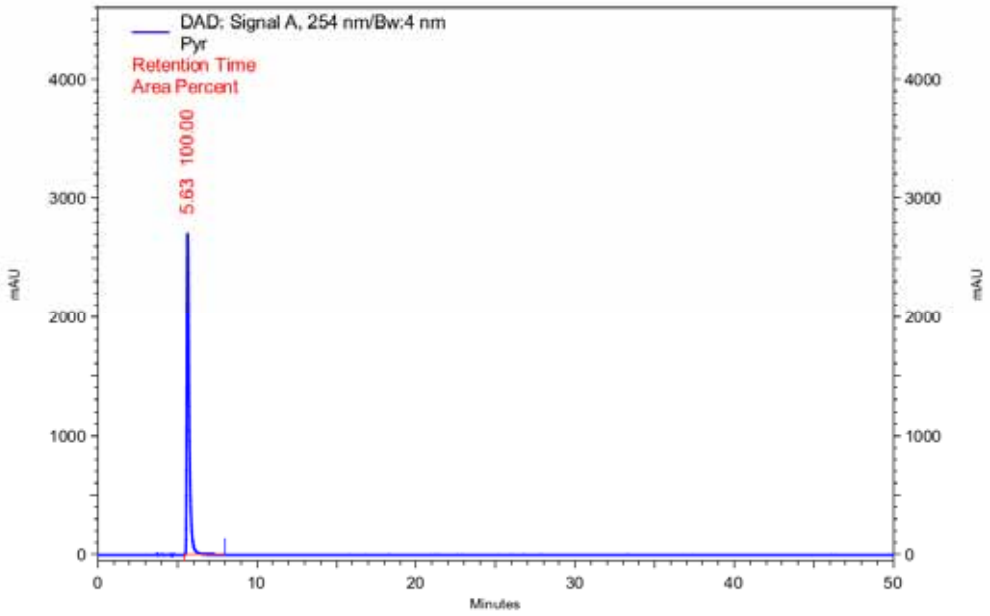


2. HPLC analysis of crude product of reaction of pyrazine with phenylboronic acid (Table 2, entry i):

a. HPLC graph of Pyrazine (as standard):

Area % Report

Data File: D:\Agilent Technologies\Result\Varun\01.09.2012 S.rslt\23
Method: D:\Agilent Technologies\Method\varun\ACN- water 10-90 S.met
Acquired: 9/2/2012 2:26:05 PM (GMT +05:30)
Printed: 9/7/2012 12:24:35 AM (GMT +05:30)



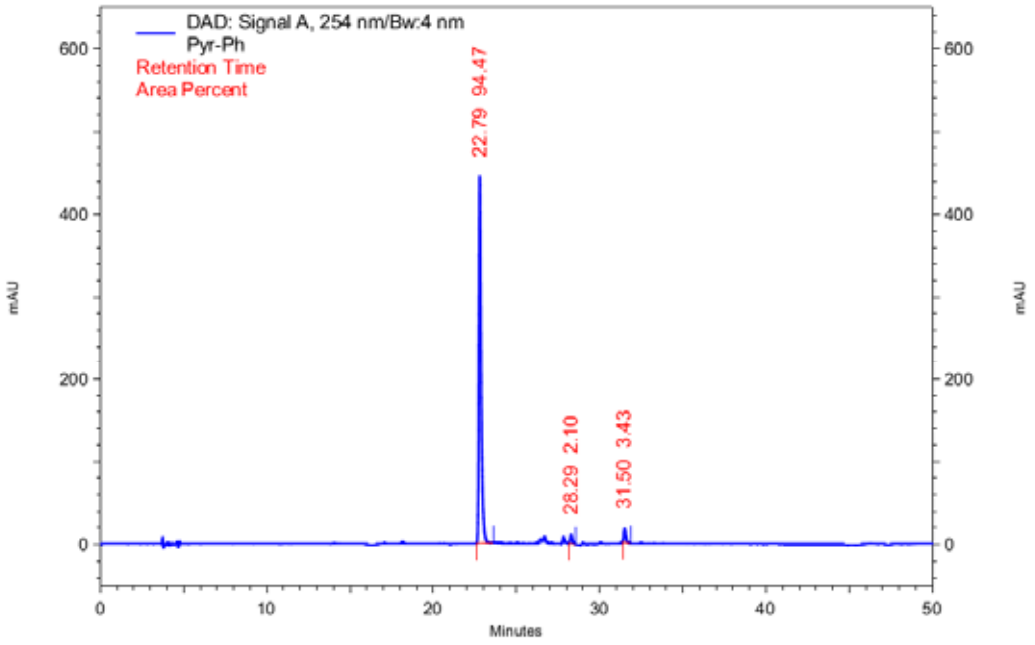
DAD: Signal A, 254 nm/Bw:4 nm Results

Retention Time	Area	Height	Area %
5.63	63368453	5668417	100.00
Totals	63368453	5668417	100.00

b. HPLC graph of 2-phenyl pyrazine (as standard):

Area % Report

Data File: D:\Agilent Technologies\Result\Varun\01.09.2012 S.rslt\12
Method: D:\Agilent Technologies\Method\varun\ACN- water 10-90 S.met
Acquired: 9/2/2012 9:15:25 AM (GMT +05:30)
Printed: 9/7/2012 12:51:32 AM (GMT +05:30)



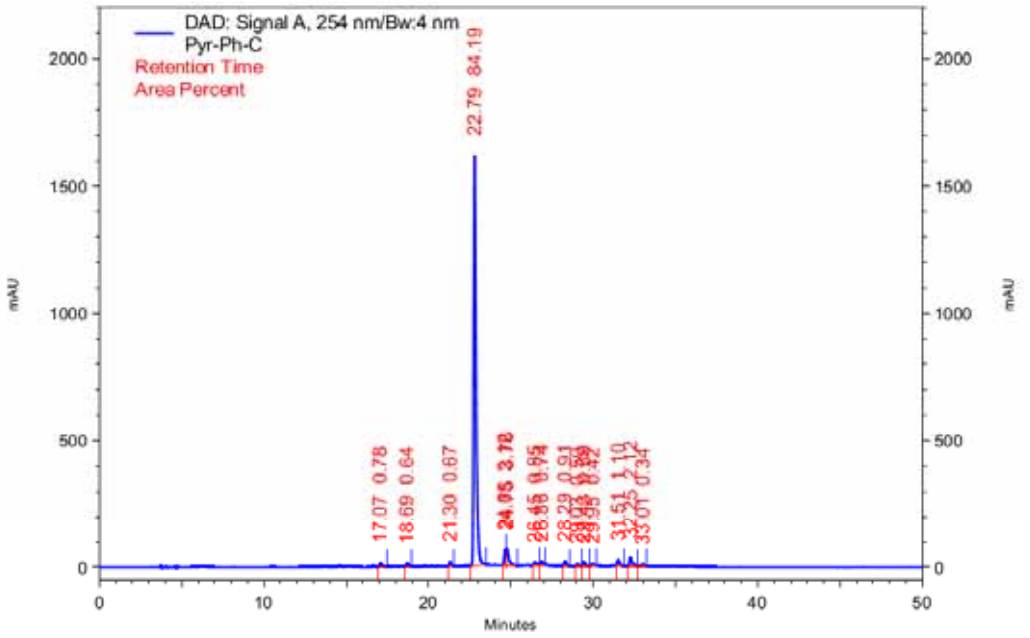
DAD: Signal A, 254 nm/Bw:4 nm Results

Retention Time	Area	Height	Area %
22.79	8858300	930677	94.47
28.29	197247	22399	2.10
31.50	321276	34965	3.43
Totals	9376823	988041	100.00

c. HPLC graph of reaction mixture:

Area % Report

Data File: D:\Agilent Technologies\Result\Varun\01.09.2012 S.rslt\13
Method: D:\Agilent Technologies\Method\varun\ACN- water 10-90 S.met
Acquired: 9/2/2012 10:07:09 AM (GMT +05:30)
Printed: 9/7/2012 12:55:53 AM (GMT +05:30)



DAD: Signal A, 254 nm/Bw:4 nm Results

Retention Time	Area	Height	Area %
17.07	306435	31478	0.78
18.69	251397	27613	0.64
21.30	263847	35623	0.67
22.79	33236827	3378055	84.19
24.65	835093	126767	2.12
24.75	1483273	133753	3.76
26.45	334303	24164	0.85
26.86	292185	32920	0.74
28.29	357934	39333	0.91
29.03	195797	15531	0.50
29.43	353055	33907	0.89
29.95	167182	15553	0.42
31.51	432826	47194	1.10
32.25	835182	70184	2.12
33.01	133579	13211	0.34
Totals	39478915	4025286	100.00