supplementary Information

Metal-Free C-H Functionalization of Diazines and Related Heteroarenes with Organo boron Species and its Application in the Synthesis of CDK Inhibitor, Meriolin 1

Thanusha Thatikonda, Umed Singh, Srinivas Ambala, Ram A. Vishwakarm, and Parvinder Pal Singh*

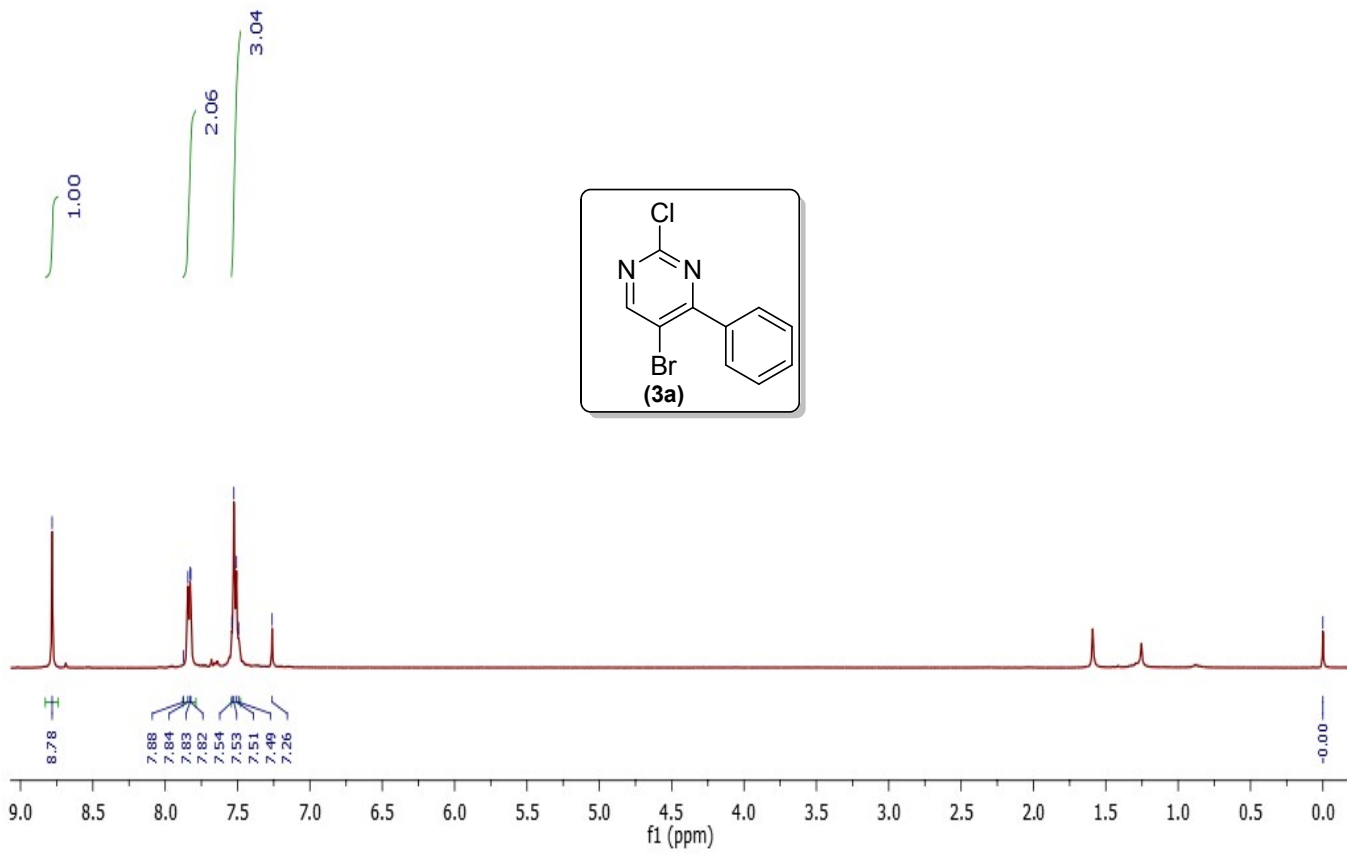
Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine and Academy of Scientific and Innovative Research, Canal Road, Jammu-180001, India.

Tel.: +91-191-2585006-13/15/18 (ext. 292), Fax: +91-191-2586333,

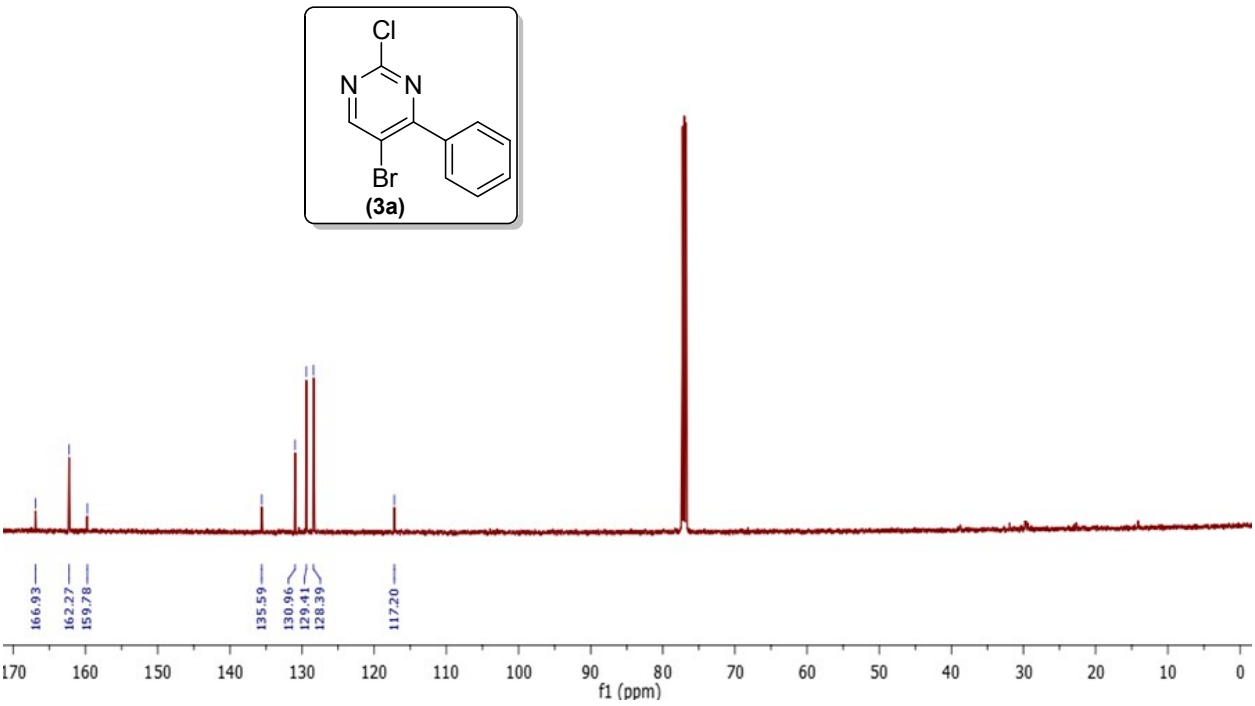
E-mail: ppsingh@iiim.ac.in

^{1}H NMR, ^{13}C NMR, DEPT, Mass spectra of compounds

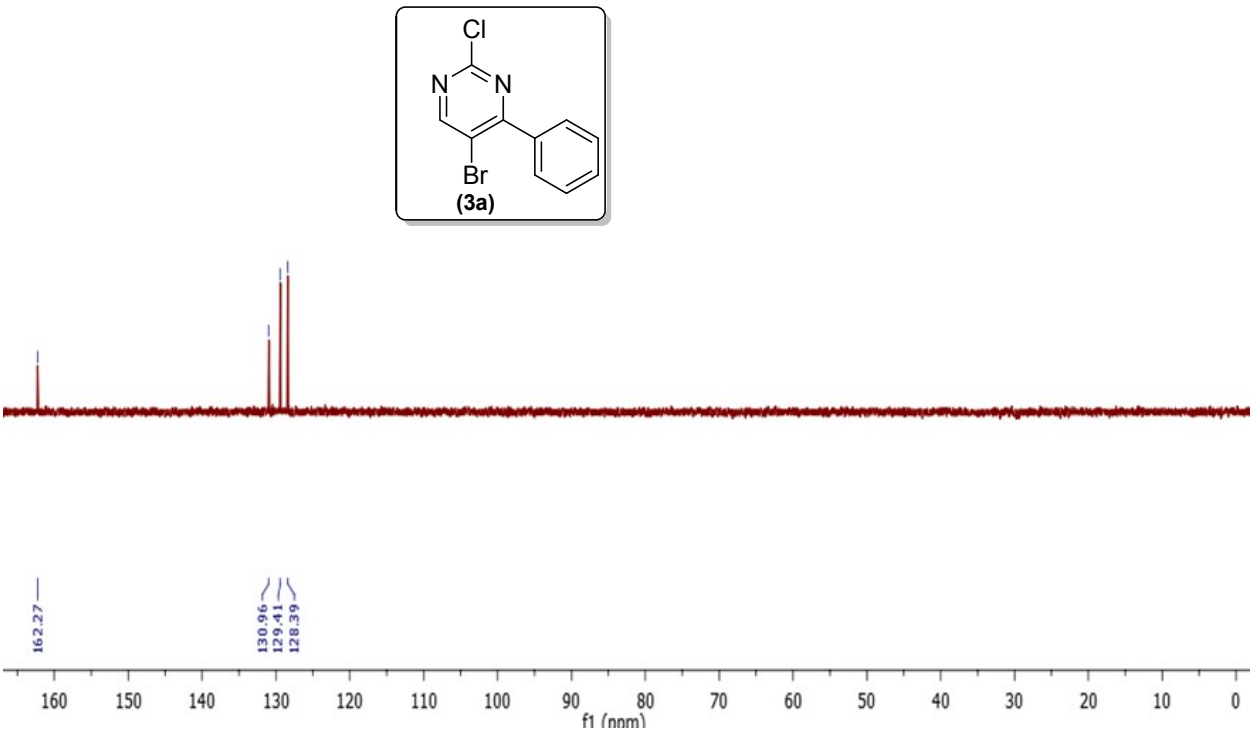
^{1}H NMR of 5-Bromo-2-chloro-4-phenylpyrimidine (3a)



^{13}C NMR of 5-Bromo-2-chloro-4-phenylpyrimidine (3a)



DEPT NMR of 5-Bromo-2-chloro-4-phenylpyrimidine (3a)

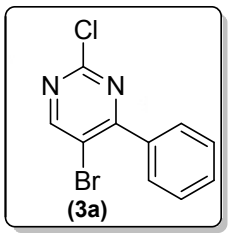


HRMS of 5-Bromo-2-chloro-4-phenylpyrimidine (3a)

Qualitative Compound Report

Data File	2Cl5Br-BA.d	**Sample Name**	2Cl5Br-BA
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	12-05-2015 PM 3:09:55
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



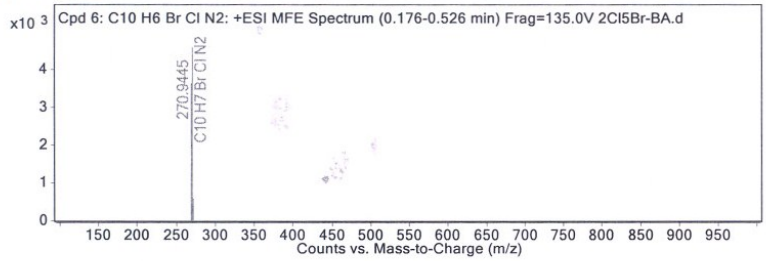
(3a)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C10 H6 Br Cl N2	0.274	267.9392	C10 H6 Br Cl N2	C10 H6 Br Cl N2	4.09	C10 H6 Br Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C10 H6 Br Cl N2	268.9467	0.274	Find by Molecular Feature	267.9392

MFE MS Spectrum



MS Spectrum Peak List

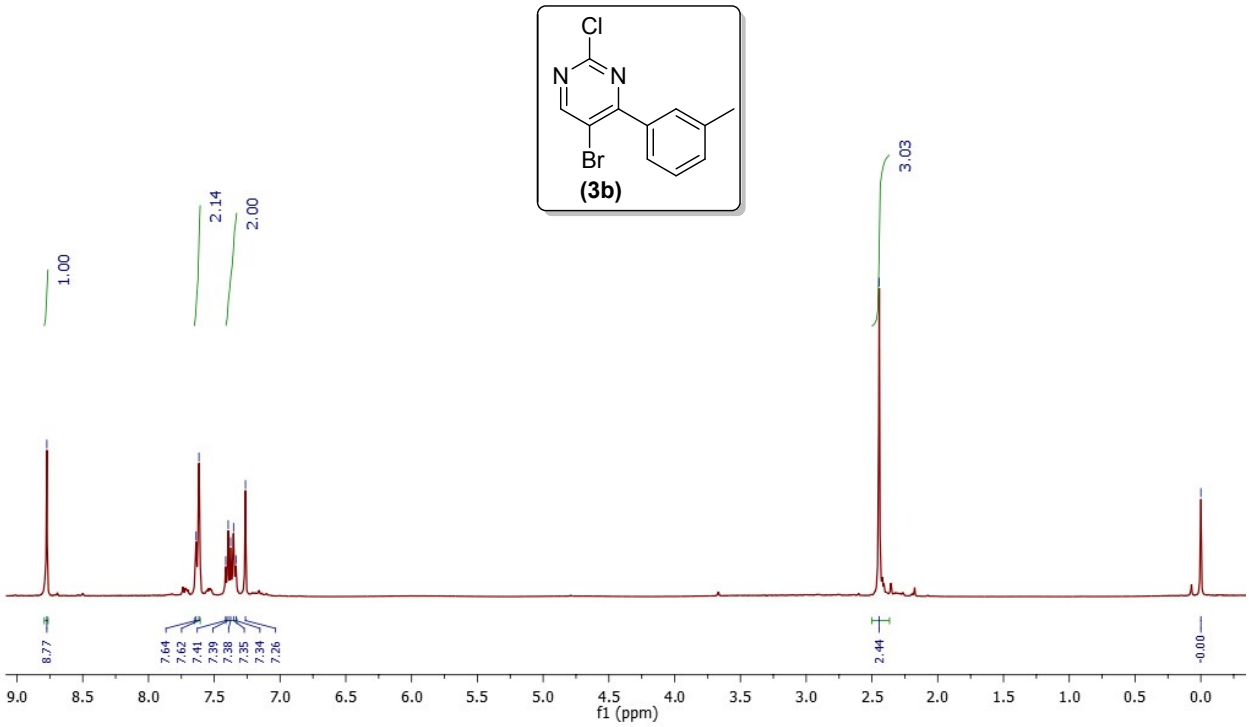
m/z	z	Abund	Formula	Ion
268.9467	1	3659.31	C10 H7 Br Cl N2	(M+H)+
269.9484	1	746.95	C10 H7 Br Cl N2	(M+H)+
270.9445	1	4592.01	C10 H7 Br Cl N2	(M+H)+
271.9454	1	598.97	C10 H7 Br Cl N2	(M+H)+

Predicted Isotope Match Table

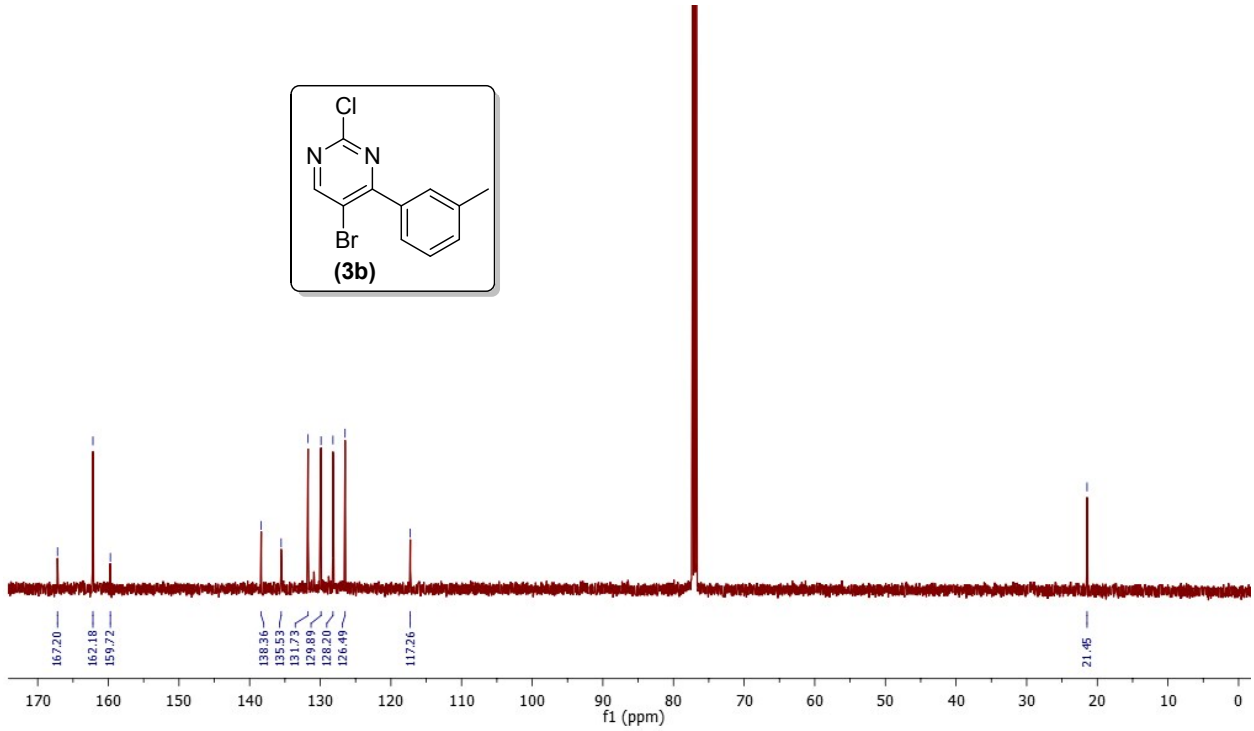
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	268.9467	268.9476	3.38	79.69	76.99	38.13	38.98
2	269.9484	269.9505	7.92	16.27	8.95	7.78	4.53
3	270.9445	270.9453	3.09	100	100	47.85	50.63
4	271.9454	271.9483	10.7	13.04	11.59	6.24	5.87

--- End Of Report ---

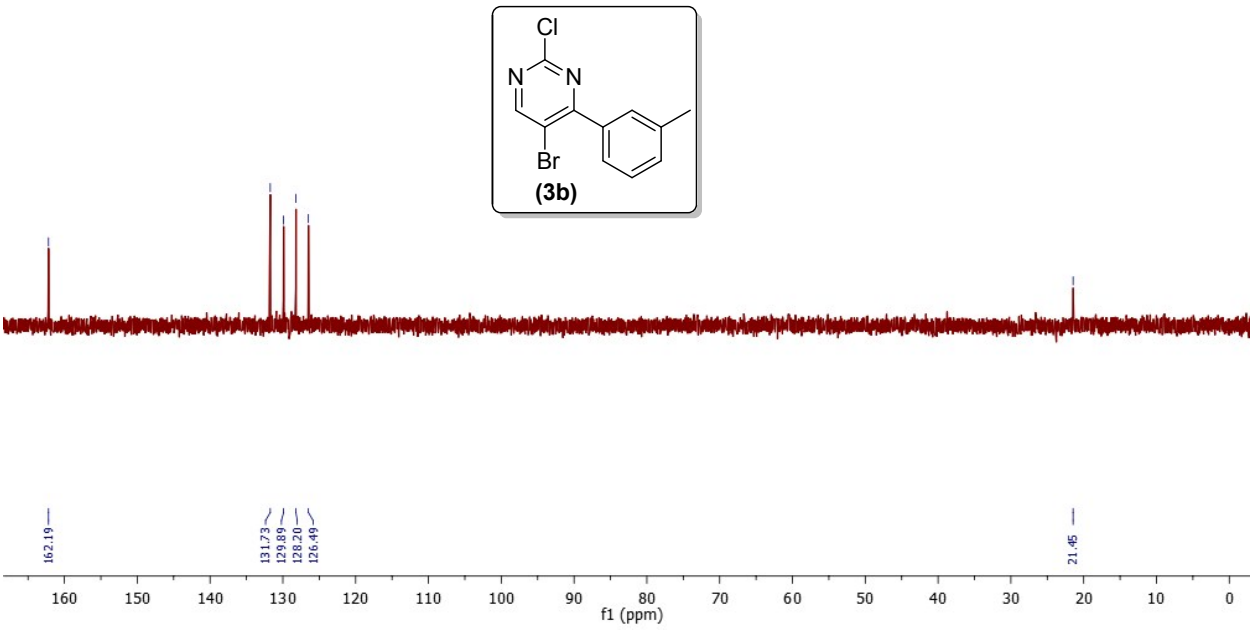
^{1}H NMR of 5-Bromo-2-chloro-4-(*m*-tolyl)pyrimidine (3b)



^{13}C NMR of 5-Bromo-2-chloro-4-(*m*-tolyl)pyrimidine (3b)



DEPT NMR of 5-Bromo-2-chloro-4-(*m*-tolyl)pyrimidine (3b)

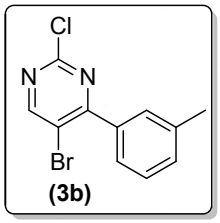


HRMS of 5-Bromo-2-chloro-4-(*m*-tolyl)pyrimidine (3b)

Qualitative Compound Report

Data File	2Cl5Br-3Me.d	**Sample Name**	2Cl5Br-3Me
Sample Type	Sample	**Position**	Vial 7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	12-05-2015 PM 3:18:41
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



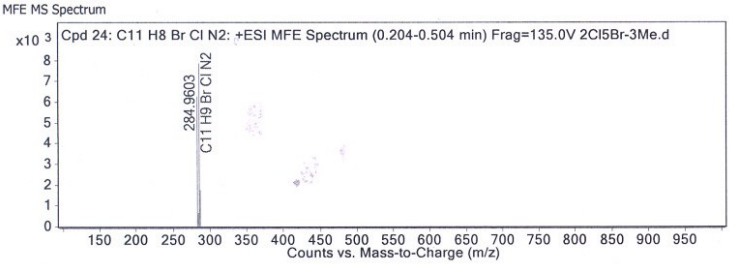
(3b)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 24: C11 H8 Br Cl N2	0.269	281.9554	C11 H8 Br Cl N2	C11 H8 Br Cl N2	2.05	C11 H8 Br Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 24: C11 H8 Br Cl N2	282.9629	0.269	Find by Molecular Feature	281.9554

MFE MS Spectrum



MS Spectrum Peak List

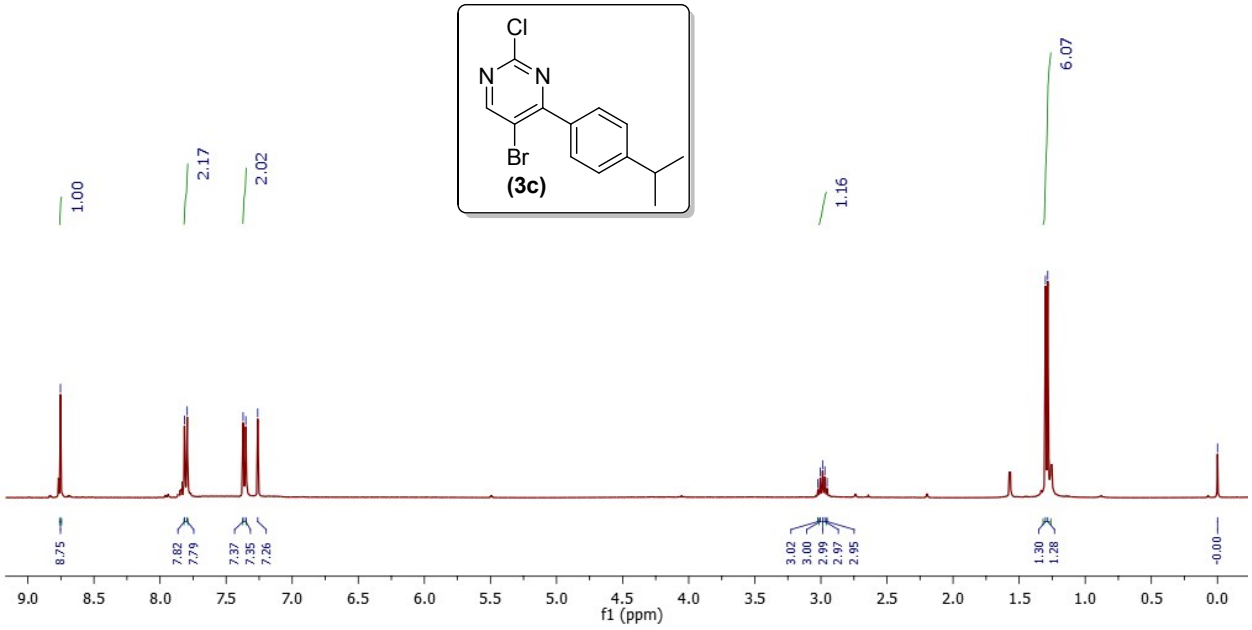
m/z	z	Abund	Formula	Ion
282.9629	1	6288.45	C11 H9 Br Cl N2	(M+H)+
283.9654	1	672.55	C11 H9 Br Cl N2	(M+H)+
284.9603	1	7862.28	C11 H9 Br Cl N2	(M+H)+
285.9635	1	1260.76	C11 H9 Br Cl N2	(M+H)+
286.9578	1	1747.49	C11 H9 Br Cl N2	(M+H)+

Predicted Isotope Match Table

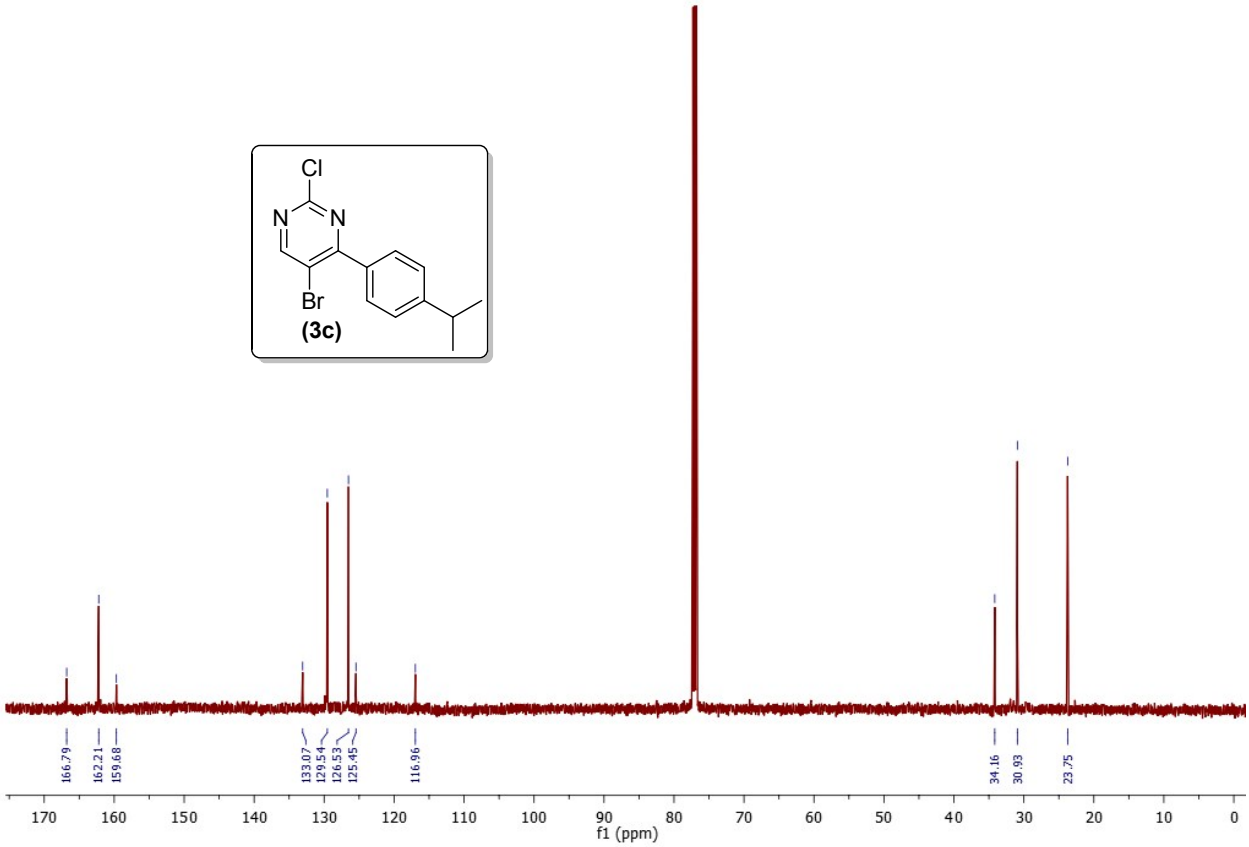
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	282.9629	282.9632	1.26	79.98	76.91	35.27	34.33
2	283.9654	283.9662	3.03	8.55	9.79	3.77	4.37
3	284.9603	284.961	2.58	100	100	44.09	44.63
4	285.9635	285.964	1.49	16.04	12.68	7.07	5.66
5	286.9578	286.9585	2.31	22.23	24.68	9.8	11.01

--- End Of Report ---

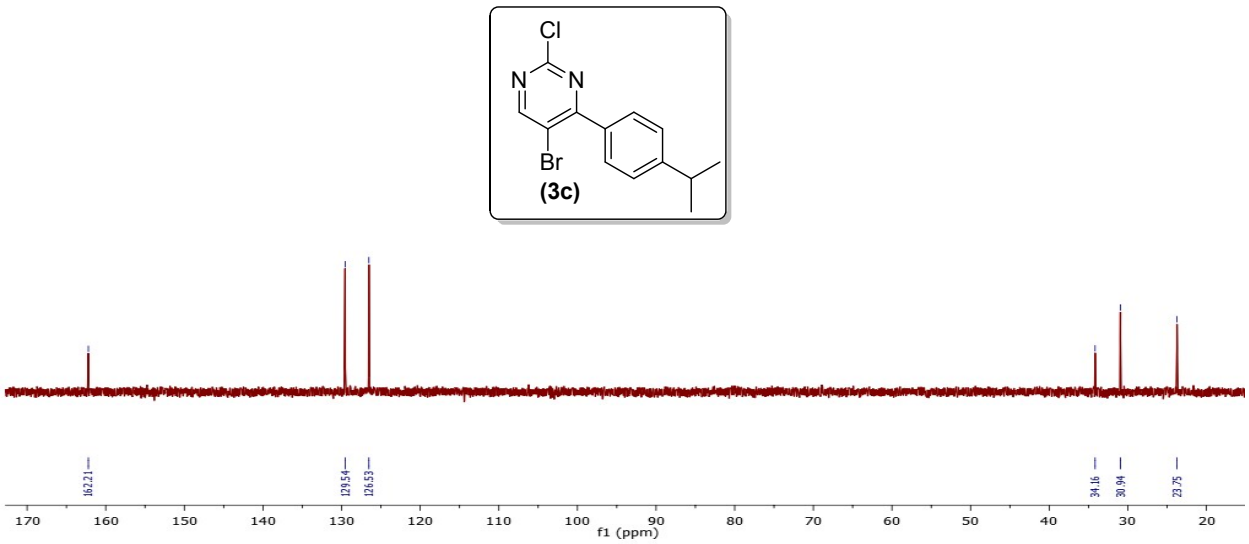
^{1}H NMR of 5-Bromo-2-chloro-4-(4-*iso*-propylphenyl)pyrimidine (3c)



^{13}C NMR of 5-Bromo-2-chloro-4-(4-*iso*-propylphenyl)pyrimidine (3c)



DEPT NMR of 5-Bromo-2-chloro-4-(4-*iso*-propylphenyl)pyrimidine (3c)

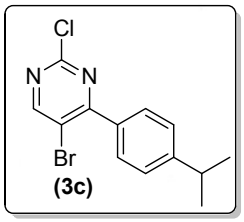


HRMS of 5-Bromo-2-chloro-4-(4-*iso*-propylphenyl)pyrimidine (3c)

Qualitative Compound Report

Data File	2Cl 5Br-4ISP.d	**Sample Name**	2Cl 5Br-4ISP
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	11-05-2015 PM 2:36:57
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

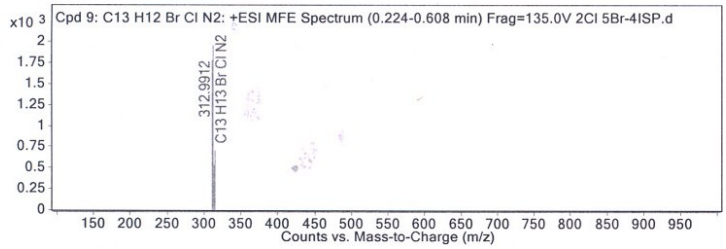


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C13 H12 Br Cl N2	0.351	309.9854	C13 H12 Br Cl N2	C13 H12 Br Cl N2	5.86	C13 H12 Br Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C13 H12 Br Cl N2	310.9927	0.351	Find by Molecular Feature	309.9854

MFE MS Spectrum



MS Spectrum Peak List

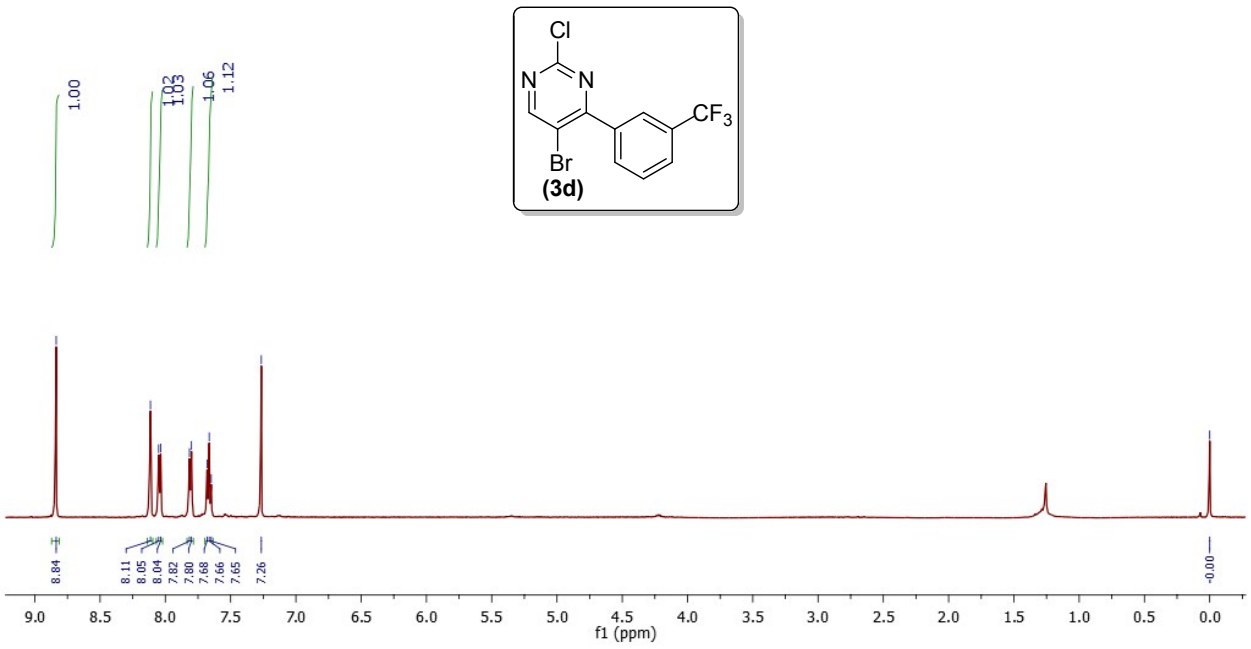
m/z	z	Abund	Formula	Ion
310.9927	1	1780.42	C13 H13 Br Cl N2	(M+H)+
311.9984	1	385.23	C13 H13 Br Cl N2	(M+H)+
312.9912	1	1958.67	C13 H13 Br Cl N2	(M+H)+
313.9912	1	538.24	C13 H13 Br Cl N2	(M+H)+
314.9866	1	715.12	C13 H13 Br Cl N2	(M+H)+

Predicted Isotope Match Table

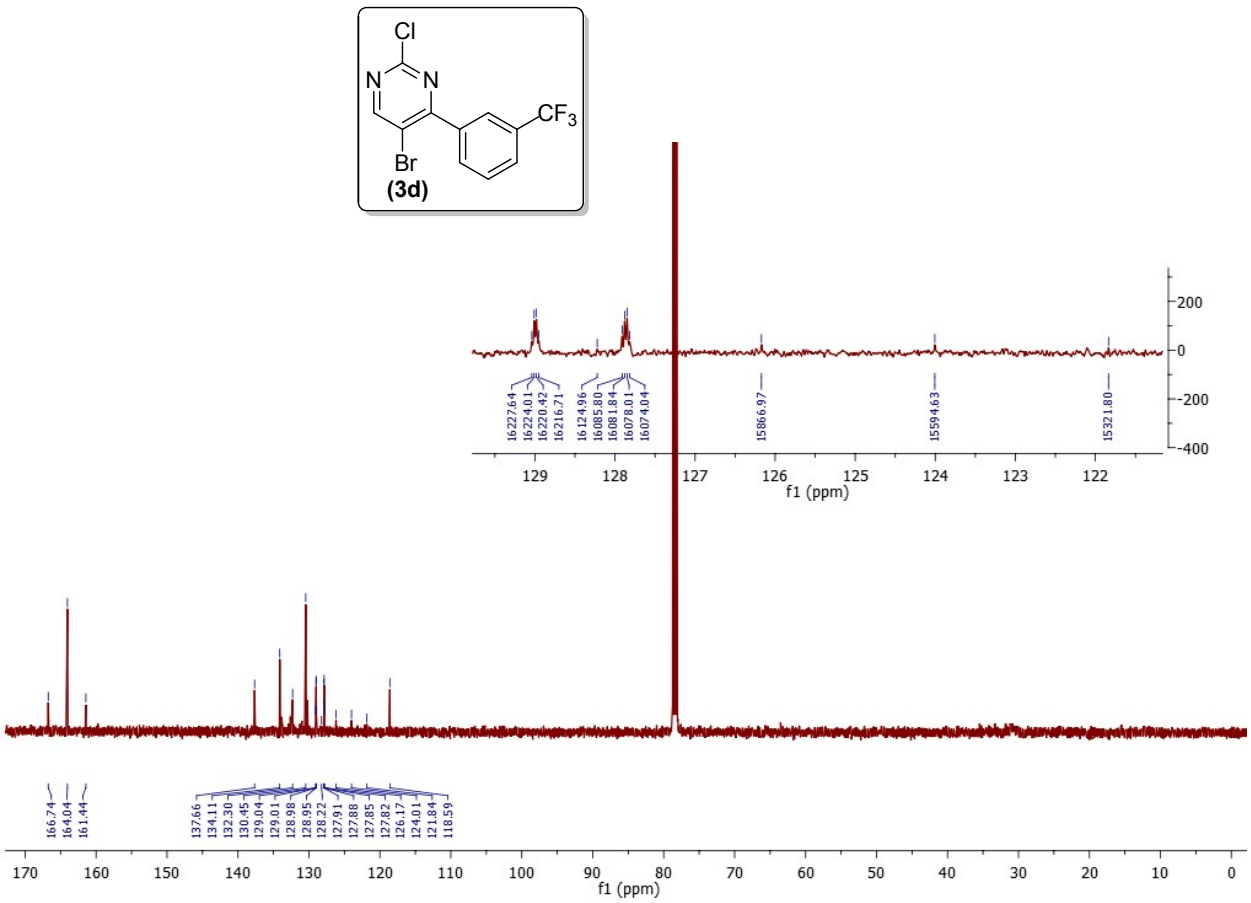
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	310.9927	310.9945	5.83	90.9	76.74	33.11	33.66
2	311.9984	311.9976	-2.44	19.67	11.47	7.16	5.03
3	312.9912	312.9923	3.71	100	100	36.42	43.86
4	313.9912	313.9953	13.19	27.48	14.86	10.01	6.52
5	314.9866	314.9899	10.38	36.51	24.92	13.3	10.93

--- End Of Report ---

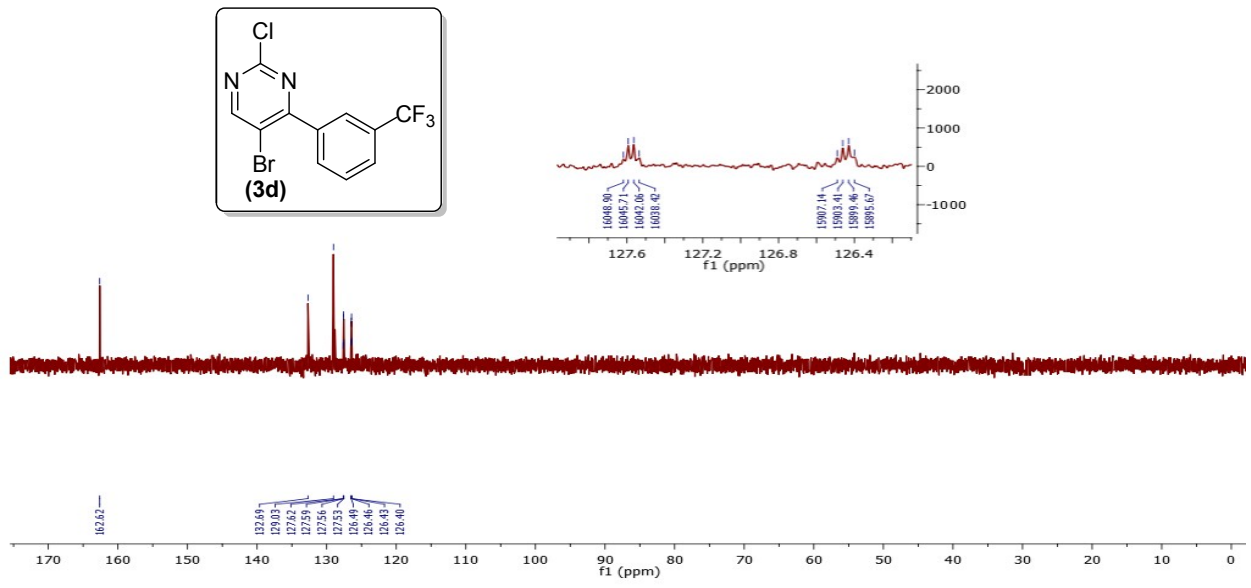
^{1}H NMR of 5-Bromo-2-chloro-4-(3-(trifluoromethyl)phenyl)pyrimidine (3d)



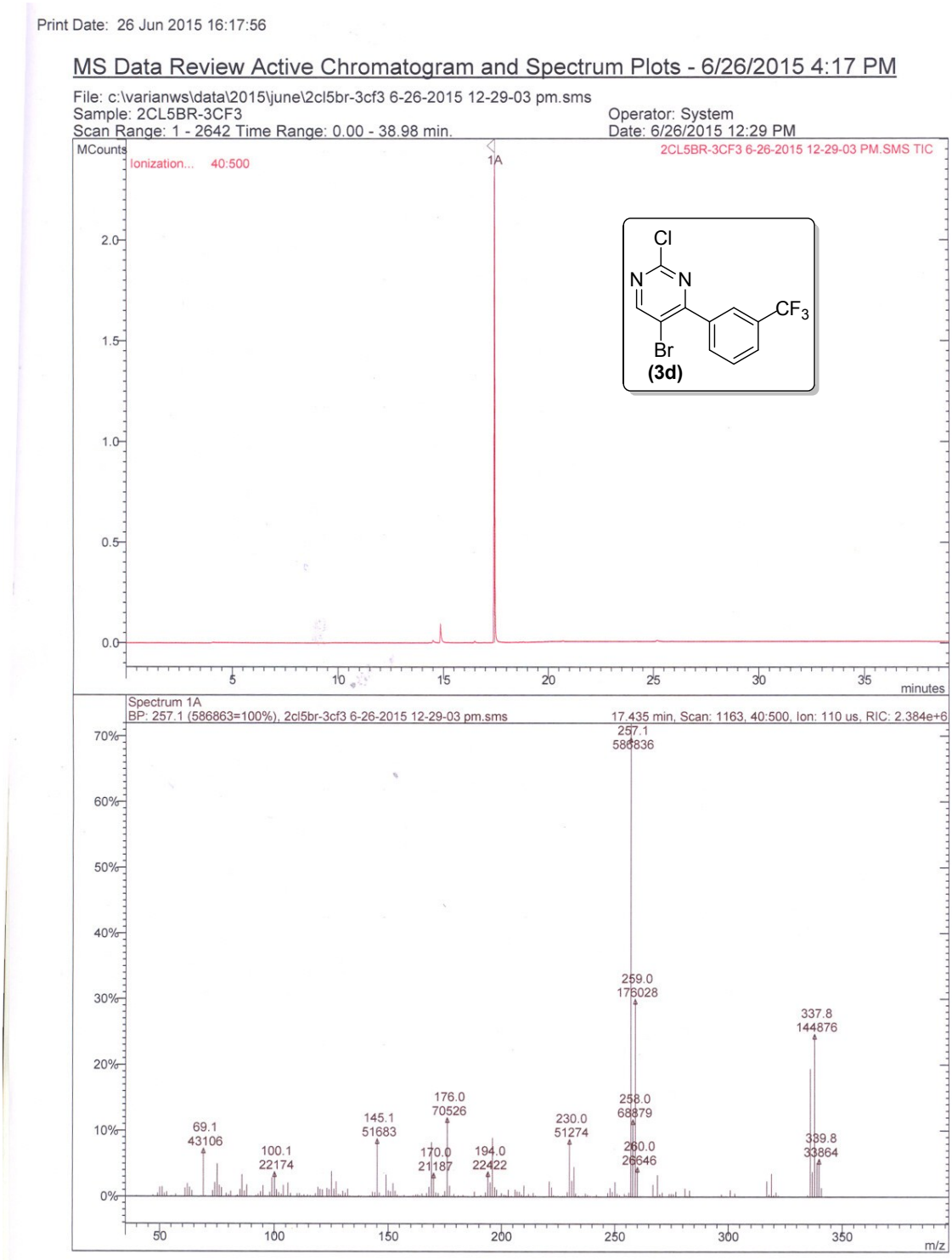
^{13}C NMR of 5-Bromo-2-chloro-4-(3-(trifluoromethyl)phenyl)pyrimidine (3d)



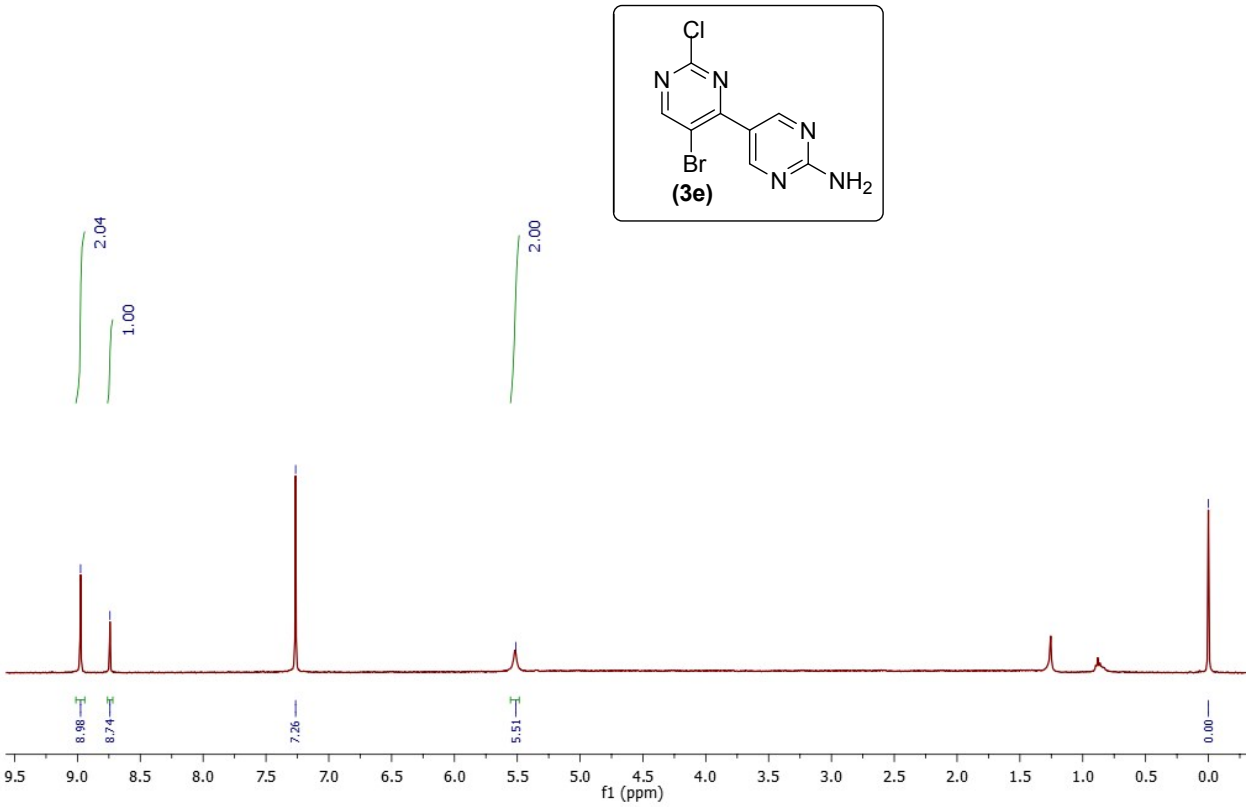
DEPT NMR of 5-Bromo-2-chloro-4-(3-(trifluoromethyl)phenyl)pyrimidine (3d)



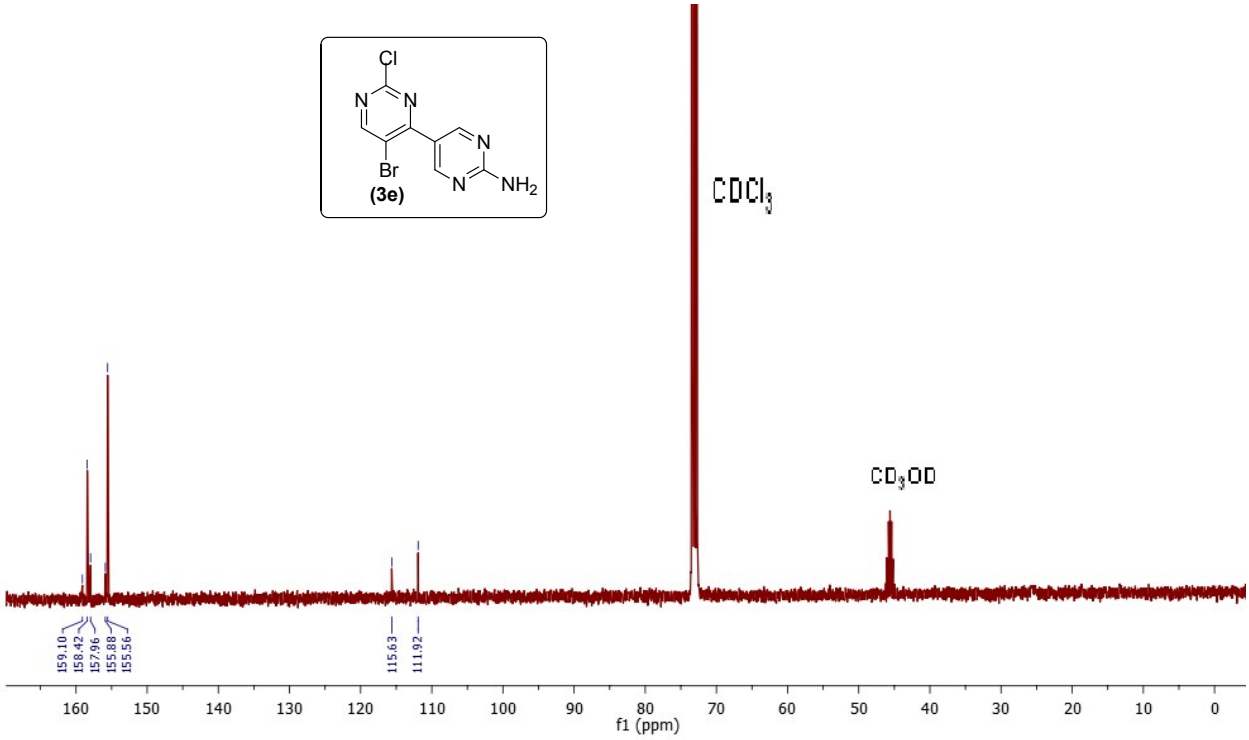
GCMS of 5-Bromo-2-chloro-4-(3-(trifluoromethyl) phenyl)pyrimidine (3d)



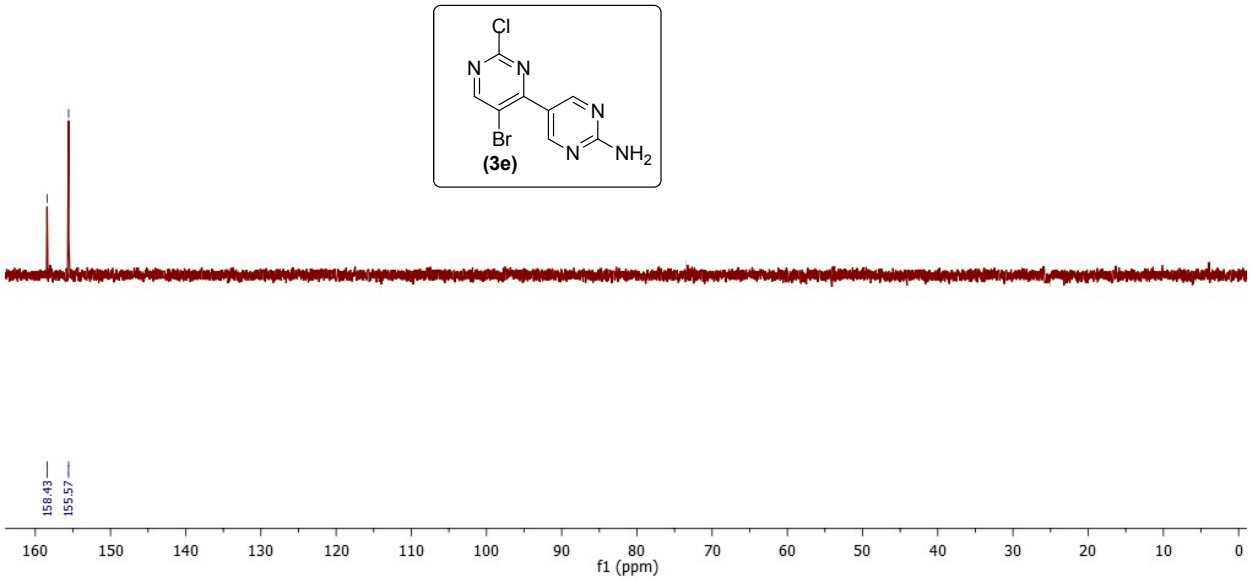
^{1}H NMR of 5-bromo-2-chloro-[4,5'-bipyrimidin]-2'-amine (3e)



^{13}C NMR of 5-bromo-2-chloro-[4,5'-bipyrimidin]-2'-amine (3e)



DEPT NMR of 5-bromo-2-chloro-[4,5'-bipyrimidin]-2'-amine (3e)

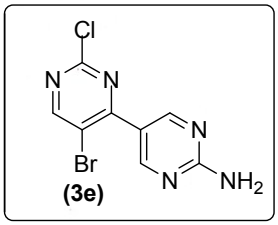


HRMS of 5-bromo-2-chloro-[4,5'-bipyrimidin]-2'-amine (3e)

Qualitative Compound Report

Data File	2APy5BA.d	**Sample Name**	2APy5BA
Sample Type	Sample	**Position**	Vial 18
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	28-10-2015 PM 2:32:29
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

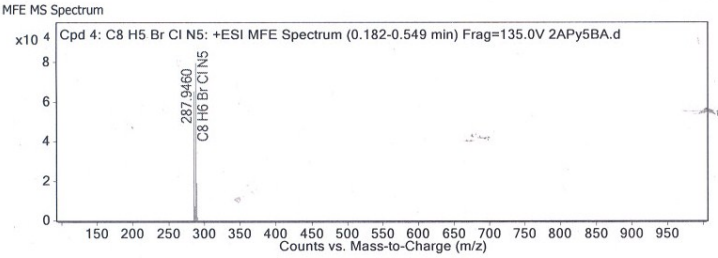


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C8 H5 Br Cl N5	0.343	284.9409	C8 H5 Br Cl N5	C8 H5 Br Cl N5	2.67	C8 H5 Br Cl N5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C8 H5 Br Cl N5	285.9481	0.343	Find by Molecular Feature	284.9409

MFE MS Spectrum



MS Spectrum Peak List

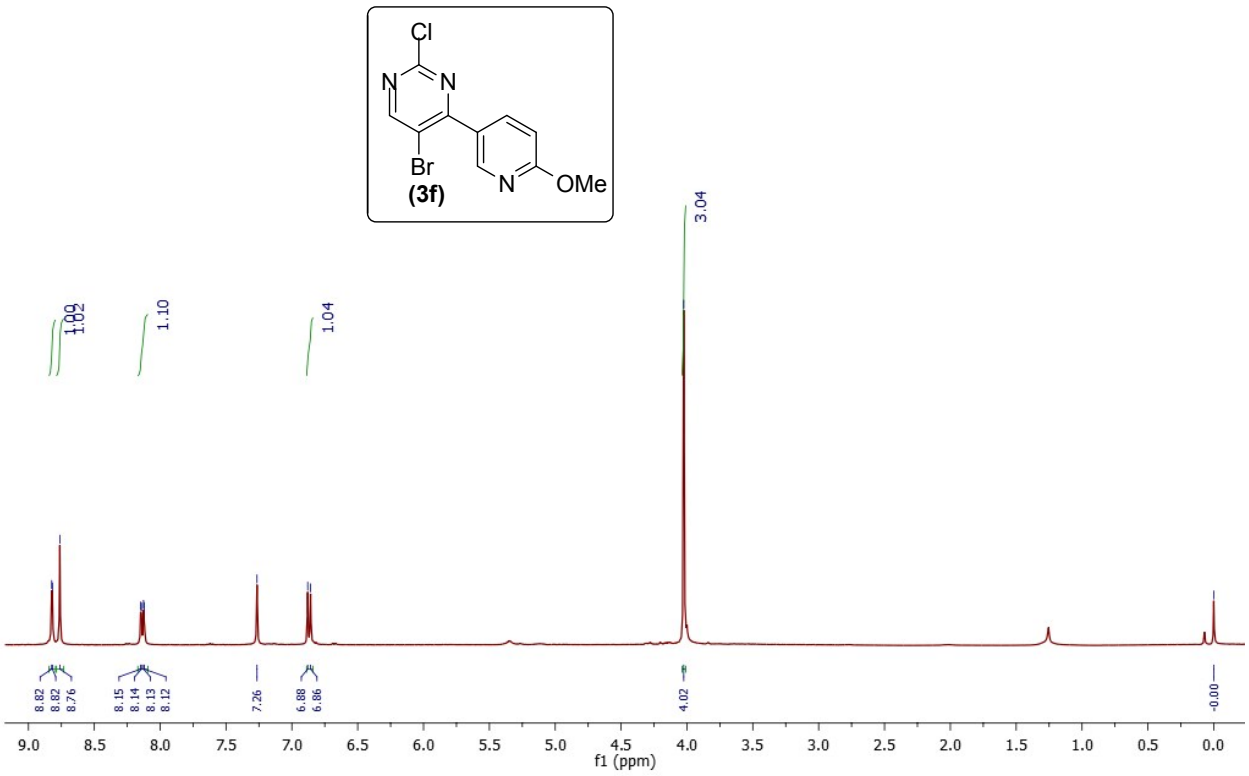
m/z	z	Abund	Formula	Ion
285.9481	1	65260.2	C8 H6 Br Cl N5	(M+H)+
286.9509	1	7068.98	C8 H6 Br Cl N5	(M+H)+
287.946	1	79643.21	C8 H6 Br Cl N5	(M+H)+
288.9484	1	8741.15	C8 H6 Br Cl N5	(M+H)+
289.9433	1	18736.69	C8 H6 Br Cl N5	(M+H)+

Predicted Isotope Match Table

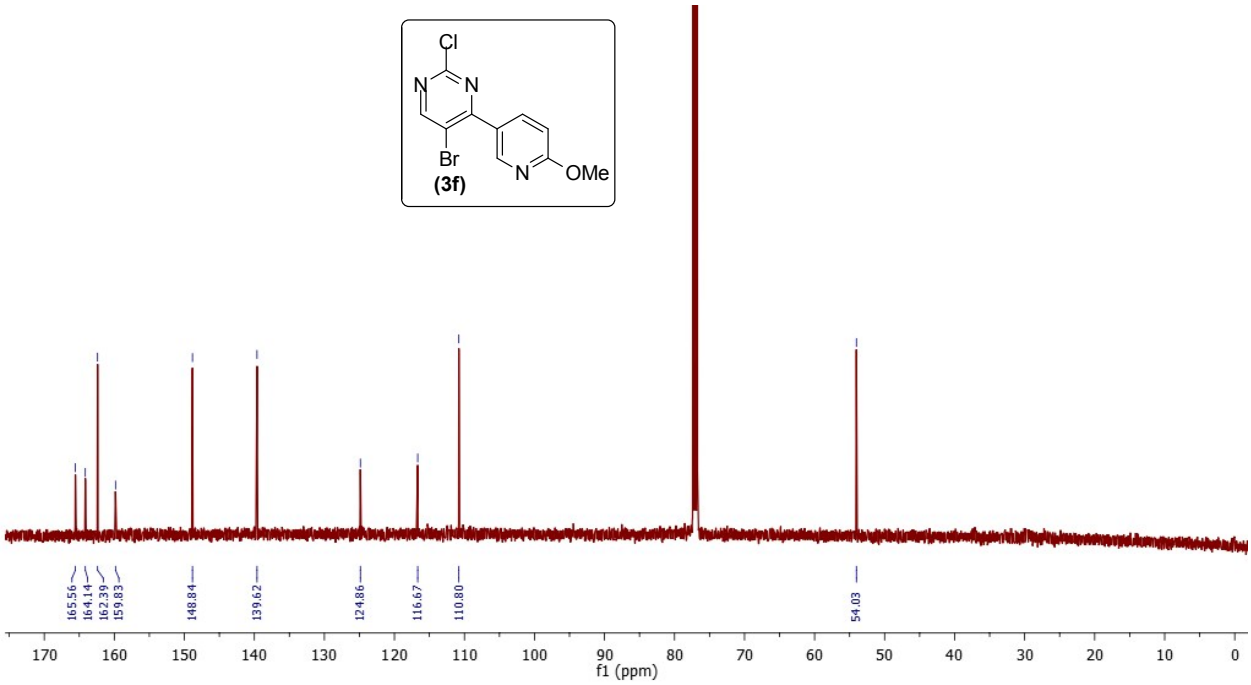
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	285.9481	285.949	2.98	81.94	77.05	35.99	34.59
2	286.9509	286.9512	1.14	8.88	8.13	3.9	3.65
3	287.946	287.9467	2.51	100	100	43.92	44.9
4	288.9484	288.949	1.85	10.98	10.52	4.82	4.72
5	289.9433	289.9441	2.8	23.53	24.49	10.33	10.99
6	290.9449	290.9463	4.87	2.35	2.54	1.03	1.14

--- End Of Report ---

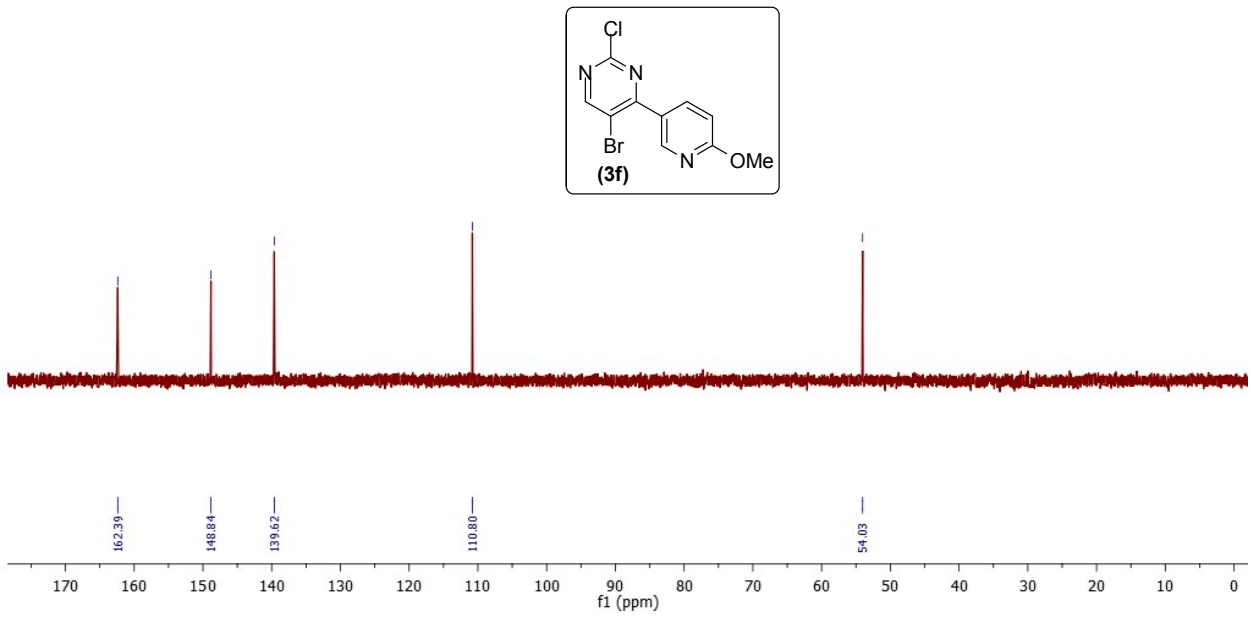
^{1}H NMR of 5-bromo-2-chloro-4-(6-methoxypyridin-3-yl)pyrimidine (3f)



^{13}C NMR of 5-bromo-2-chloro-4-(6-methoxypyridin-3-yl)pyrimidine (3f)

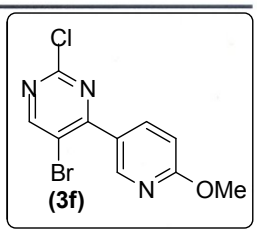


DEPT NMR of 5-bromo-2-chloro-4-(6-methoxypyridin-3-yl)pyrimidine (3f)



5-bromo-2-chloro-4-(6-methoxypyridin-3-yl)pyrimidine (3f)

Qualitative Compound Report



Data File	2OMe5BA.d	**Sample Name**	2OMe5BA
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	28-10-2015 PM 2:28:09
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

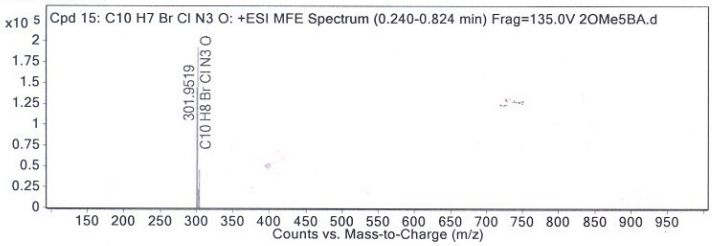
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C10 H7 Br Cl N3 O	0.346	298.9468	C10 H7 Br Cl N3 O	C10 H7 Br Cl N3 O	-2.49	C10 H7 Br Cl N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C10 H7 Br Cl N3 O	299.9541	0.346	Find by Molecular Feature	298.9468

MFE MS Spectrum



MS Spectrum Peak List

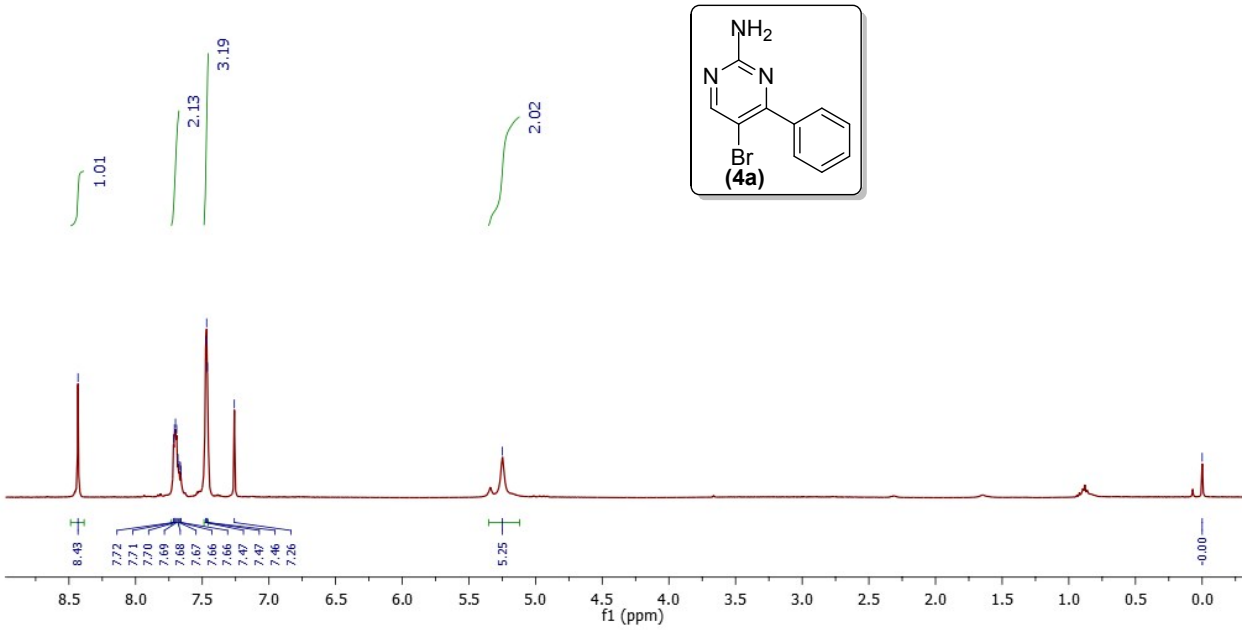
m/z	z	Abund	Formula	Ion
299.9541	1	144107.06	C10 H8 Br Cl N3 O	(M+H)+
300.9569	1	20130.49	C10 H8 Br Cl N3 O	(M+H)+
301.9519	1	192308.97	C10 H8 Br Cl N3 O	(M+H)+
302.9547	1	22834.04	C10 H8 Br Cl N3 O	(M+H)+
303.9493	1	45832.7	C10 H8 Br Cl N3 O	(M+H)+

Predicted Isotope Match Table

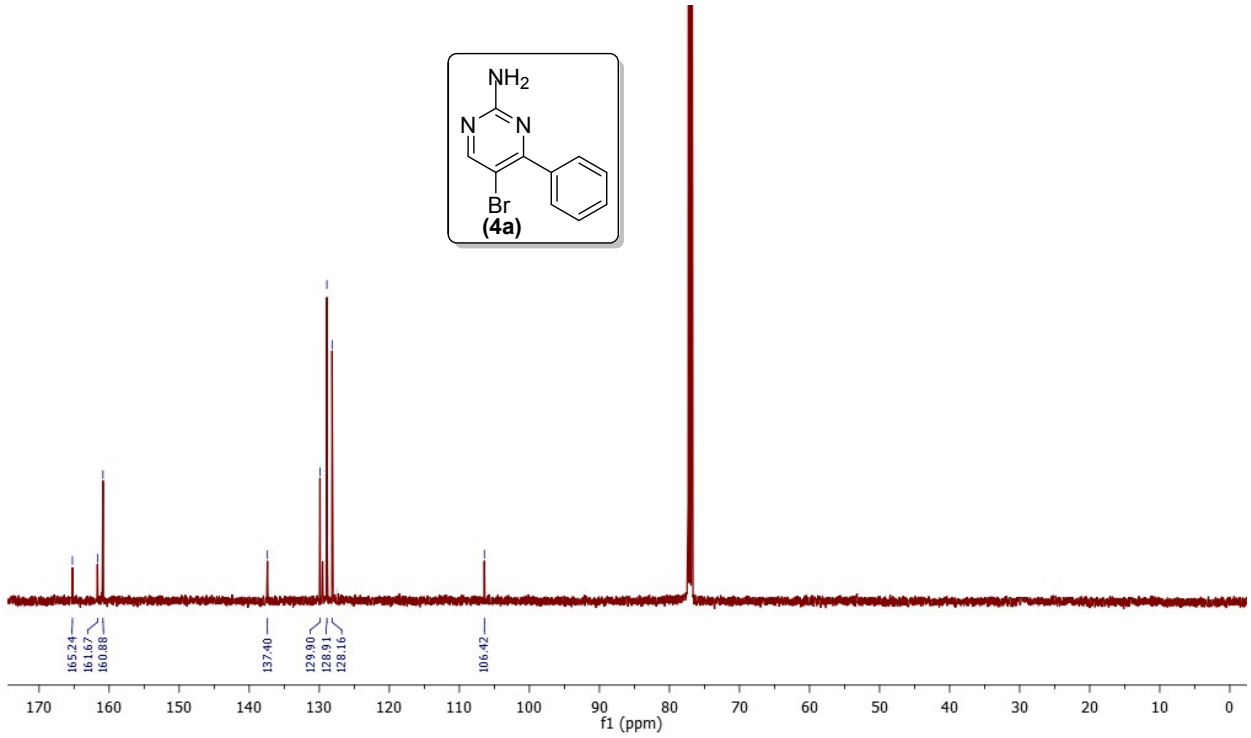
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	299.9541	299.9534	-2.43	74.94	76.84	33.39	34
2	300.9569	300.9562	-2.49	10.47	9.25	4.66	4.09
3	301.9519	301.9512	-2.49	100	100	44.56	44.25
4	302.9547	302.9539	-2.65	11.87	12	5.29	5.31
5	303.9493	303.9487	-2.22	23.83	24.78	10.62	10.96
6	304.9528	304.9513	-4.92	2.94	2.93	1.31	1.29
7	305.9527	305.9537	3.28	0.38	0.21	0.17	0.09

--- End Of Report ---

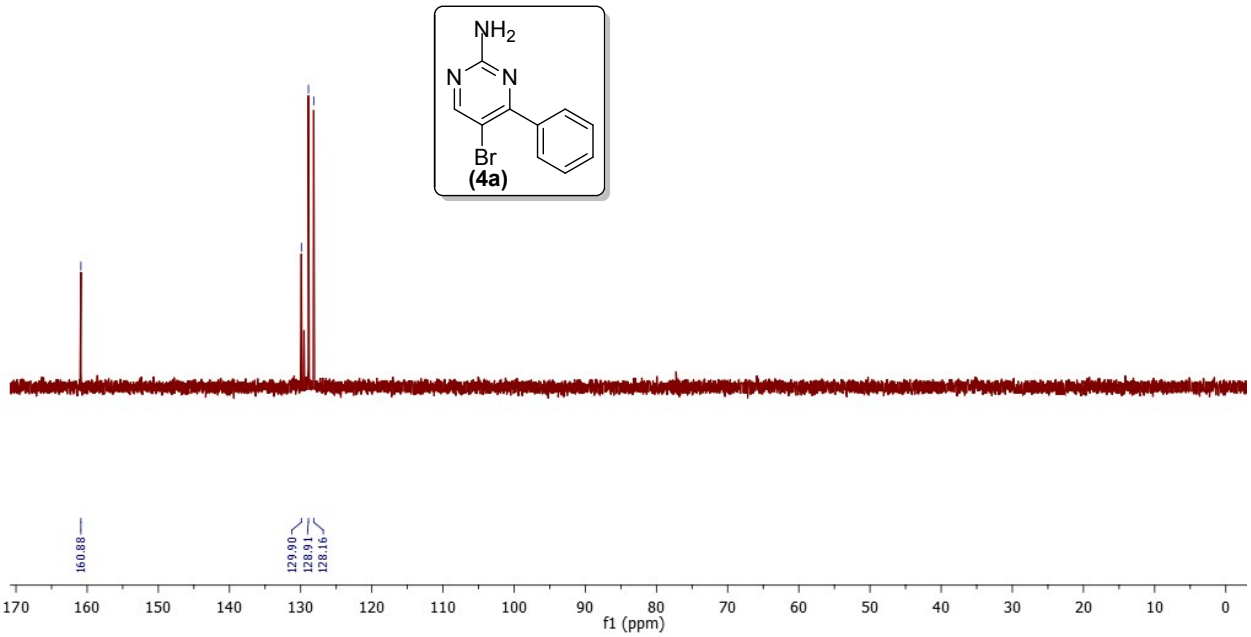
^{1}H NMR of 5-Bromo-4-phenylpyrimidin-2-amine (4a)



^{13}C NMR of 5-Bromo-4-phenylpyrimidin-2-amine (4a)



DEPT NMR of 5-Bromo-4-phenylpyrimidin-2-amine (4a)

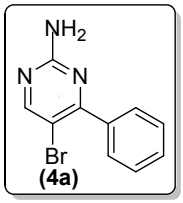


HRMS of 5-Bromo-4-phenylpyrimidin-2-amine (4a)

Qualitative Compound Report

Data File	2A5Br-BA.d	**Sample Name**	2A5Br-BA
Sample Type	Sample	**Position**	Vial 6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	06-05-2015 PM 1:39:38
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

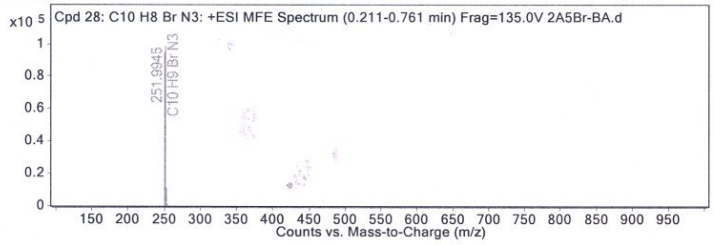


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C10 H8 Br N3	0.361	248.9894	C10 H8 Br N3	C10 H8 Br N3	3.21	C10 H8 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 28: C10 H8 Br N3	249.9965	0.361	Find by Molecular Feature	248.9894

MFE MS Spectrum



MS Spectrum Peak List

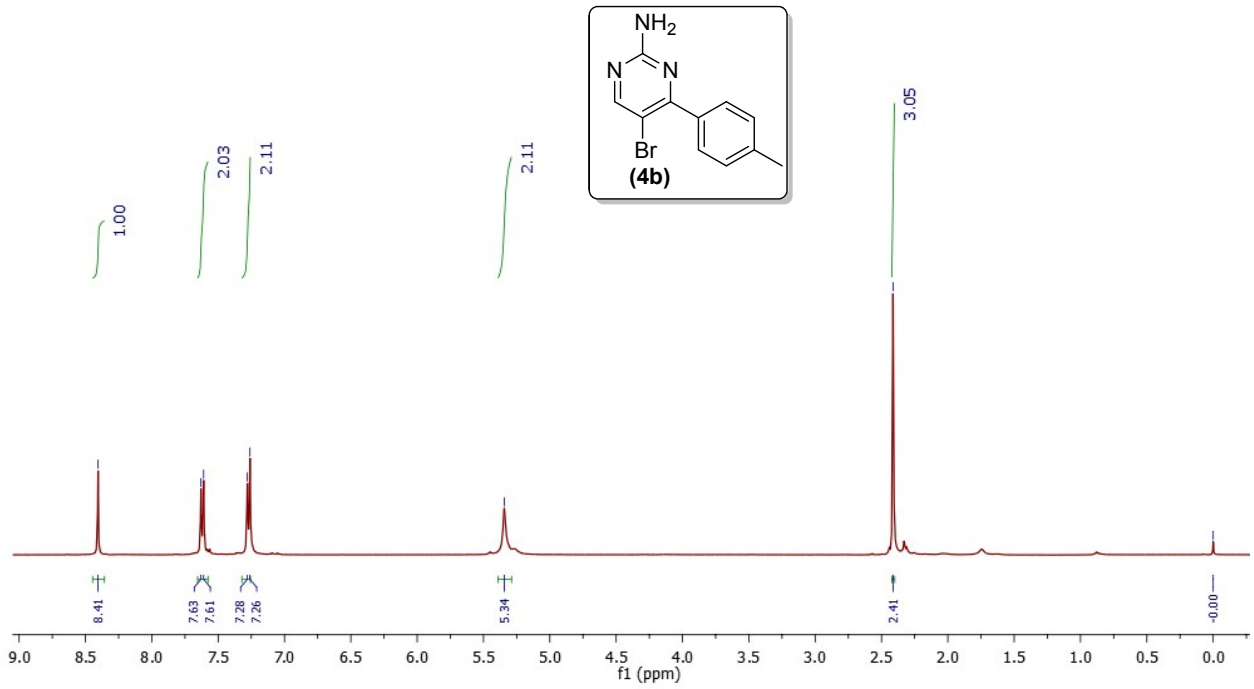
m/z	z	Abund	Formula	Ion
249.9965	1	94924.04	C10 H9 Br N3	(M+H)+
250.9996	1	10682.91	C10 H9 Br N3	(M+H)+
251.9945	1	98610.69	C10 H9 Br N3	(M+H)+
252.999	1	10906.32	C10 H9 Br N3	(M+H)+
254.0052	1	893.03	C10 H9 Br N3	(M+H)+

Predicted Isotope Match Table

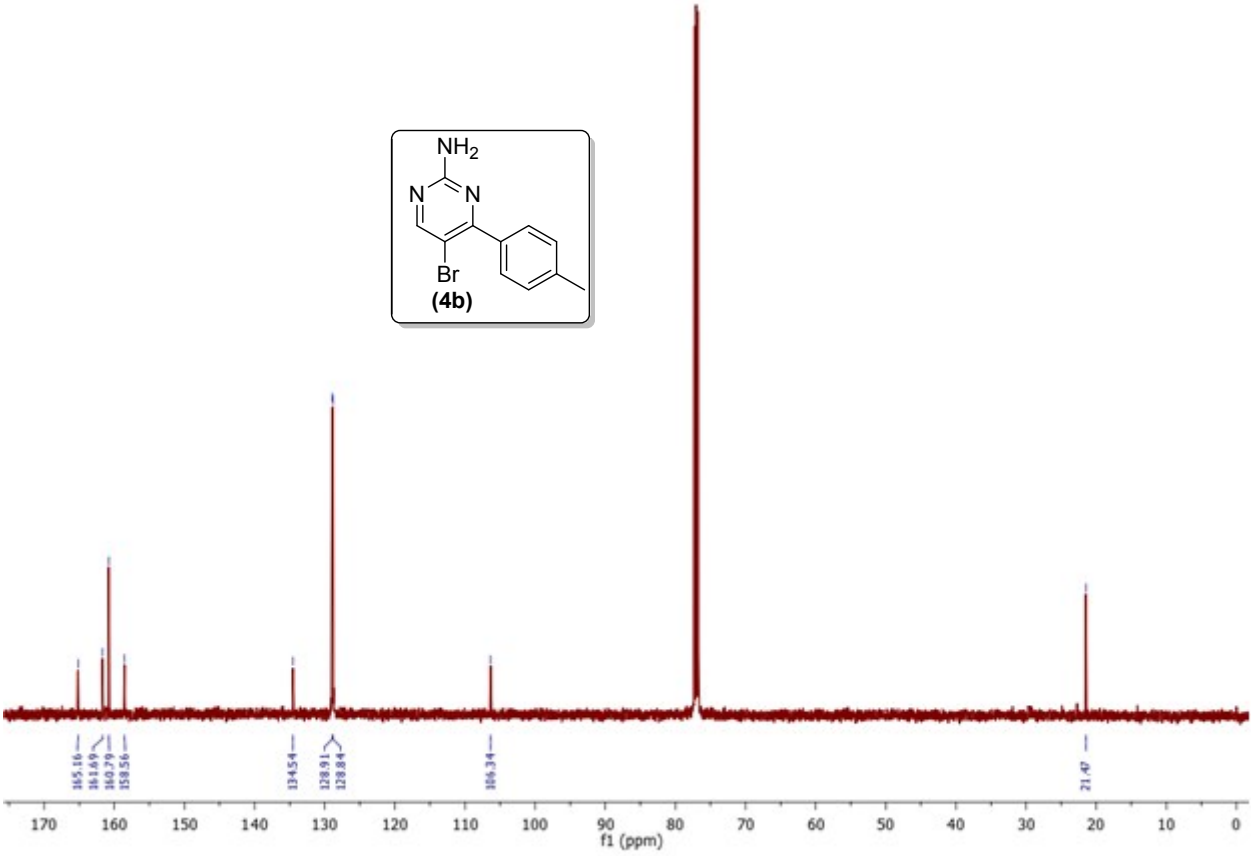
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	249.9965	249.9974	3.68	96.26	100	43.94	44.98
2	250.9996	251.0002	2.61	10.83	12.02	4.95	5.4
3	251.9945	251.9954	3.66	100	97.94	45.65	44.06
4	252.999	252.9982	-3.12	11.06	11.71	5.05	5.27
5	254.0052	254.0009	-16.71	0.91	0.64	0.41	0.29

--- End Of Report ---

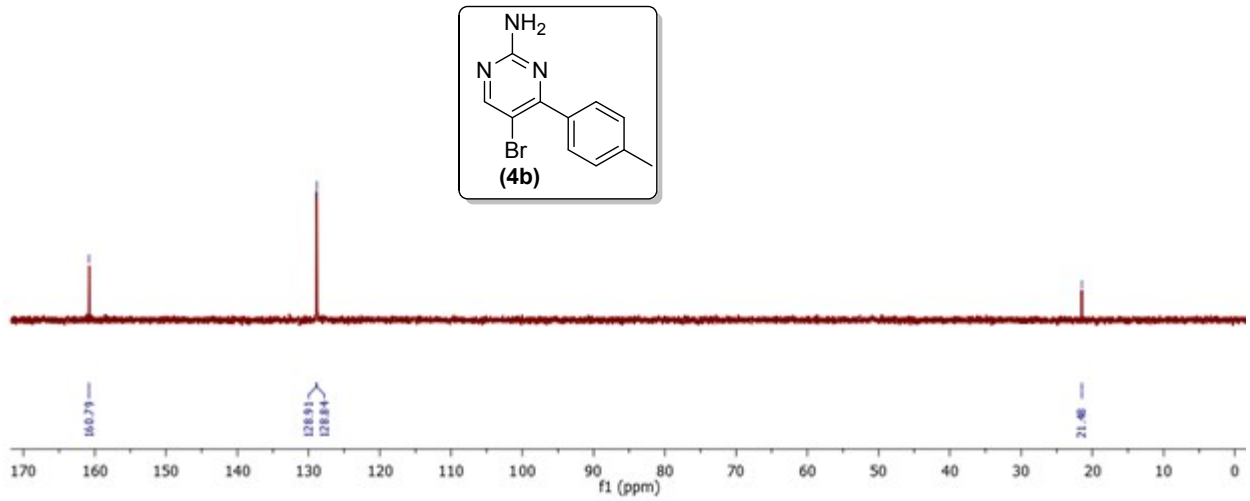
^{1}H NMR of 5-Bromo-4-(*p*-tolyl)pyrimidin-2-amine (4b)



^{13}C NMR of 5-Bromo-4-(*p*-tolyl)pyrimidin-2-amine (4b)



DEPT NMR of 5-Bromo-4-(*p*-tolyl)pyrimidin-2-amine (4b)

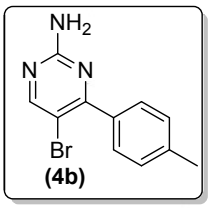


HRMS of 5-Bromo-4-(*p*-tolyl)pyrimidin-2-amine (4b)

Qualitative Compound Report

Data File	2A5Br-PTBA.d	**Sample Name**	2A5Br-PTBA
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	12-05-2015 PM 3:05:36
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



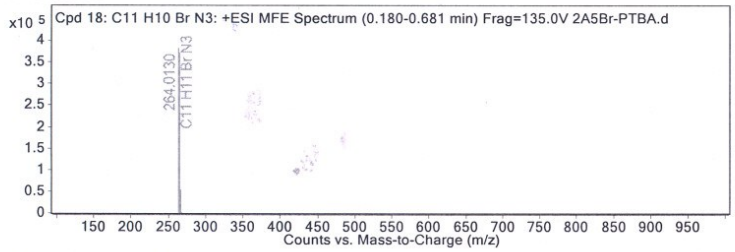
(4b)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C11 H10 Br N3	0.272	263.0057	C11 H10 Br N3	C11 H10 Br N3	0.46	C11 H10 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C11 H10 Br N3	264.013	0.272	Find by Molecular Feature	263.0057

MFE MS Spectrum



MS Spectrum Peak List

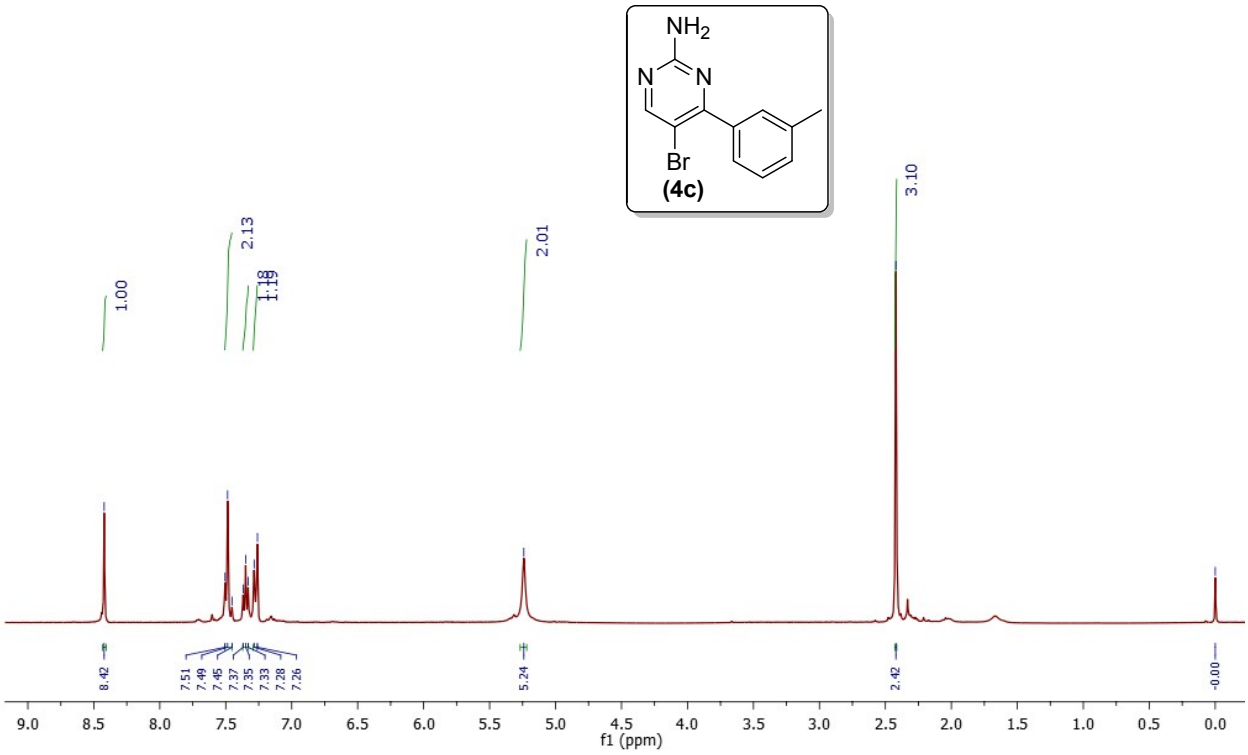
m/z	z	Abund	Formula	Ion
264.013	1	382743.53	C11 H11 Br N3	(M+H)+
265.0155	1	48332.71	C11 H11 Br N3	(M+H)+
266.011	1	372716.06	C11 H11 Br N3	(M+H)+
267.0137	1	54492.43	C11 H11 Br N3	(M+H)+
268.0162	1	3112.61	C11 H11 Br N3	(M+H)+

Predicted Isotope Match Table

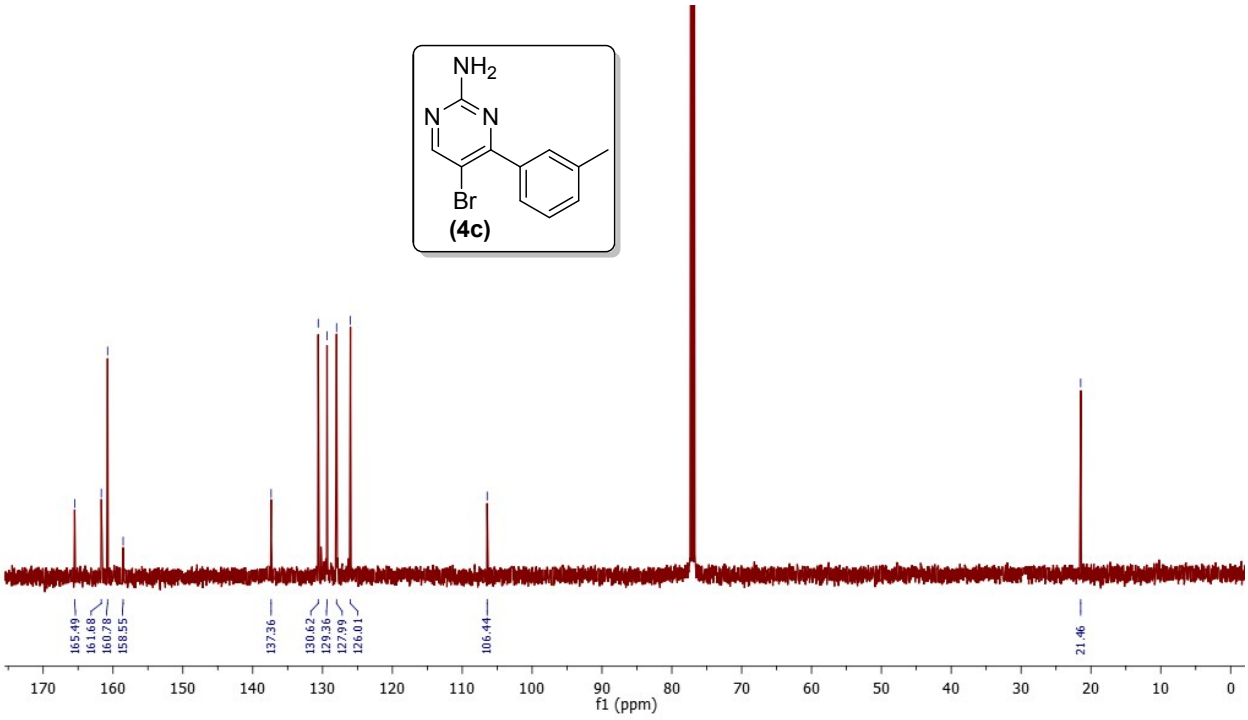
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	264.013	264.0131	0.41	100	100	44.43	44.49
2	265.0155	265.0159	1.75	12.63	13.12	5.61	5.84
3	266.011	266.0111	0.29	97.38	98.07	43.27	43.63
4	267.0137	267.0139	0.72	14.24	12.79	6.33	5.69
5	268.0162	268.0167	2.04	0.81	0.77	0.36	0.34

--- End Of Report ---

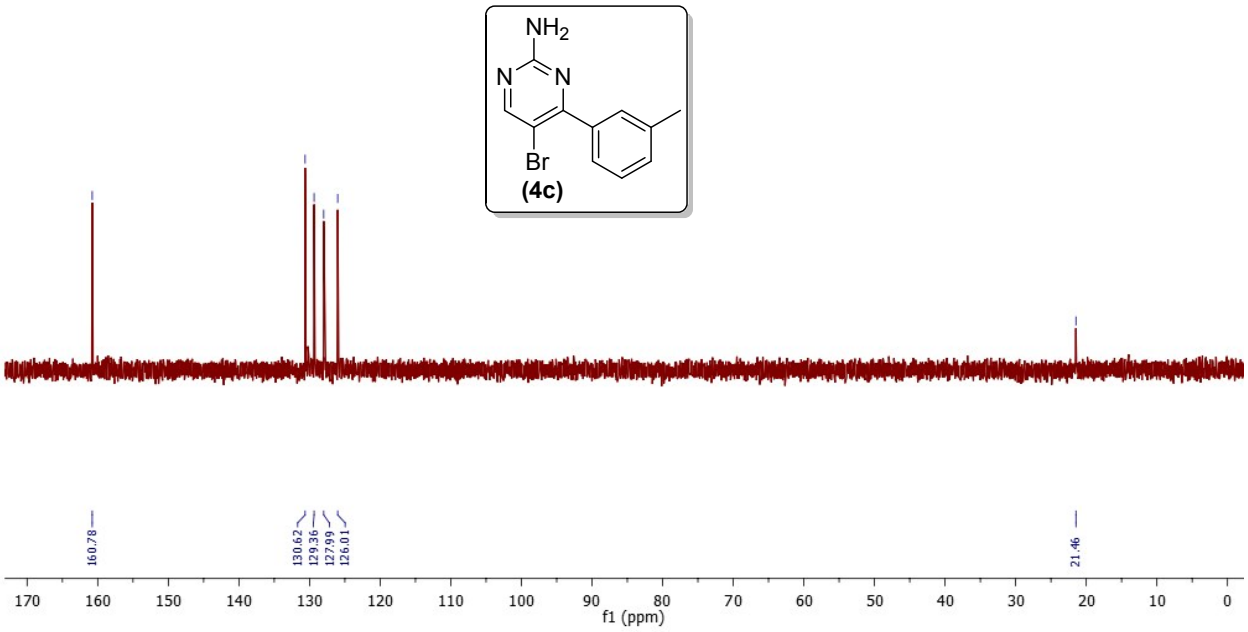
^{1}H NMR of 5-Bromo-4-(*m*-tolyl)pyrimidin-2-amine (4c)



^{13}C NMR of 5-Bromo-4-(*m*-tolyl)pyrimidin-2-amine (4c)



DEPT NMR of 5-Bromo-4-(*m*-tolyl)pyrimidin-2-amine (4c)

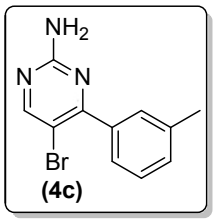


HRMS of 5-Bromo-4-(*m*-tolyl)pyrimidin-2-amine (4c)

Qualitative Compound Report

Data File	2A5Br-3Me.d	**Sample Name**	2A5Br-3Me
Sample Type	Sample	**Position**	Vial 7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	06-05-2015 PM 1:48:28
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



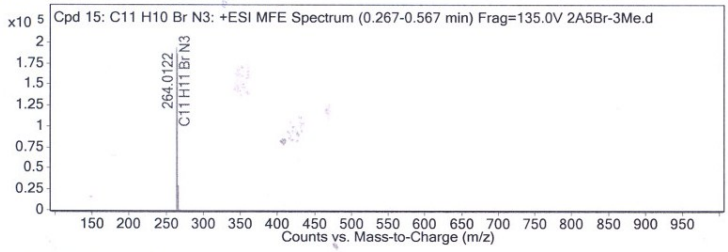
(4c)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C11 H10 Br N3	0.362	263.005	C11 H10 Br N3	C11 H10 Br N3	3.26	C11 H10 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C11 H10 Br N3	264.0122	0.362	Find by Molecular Feature	263.005

MFE MS Spectrum



MS Spectrum Peak List

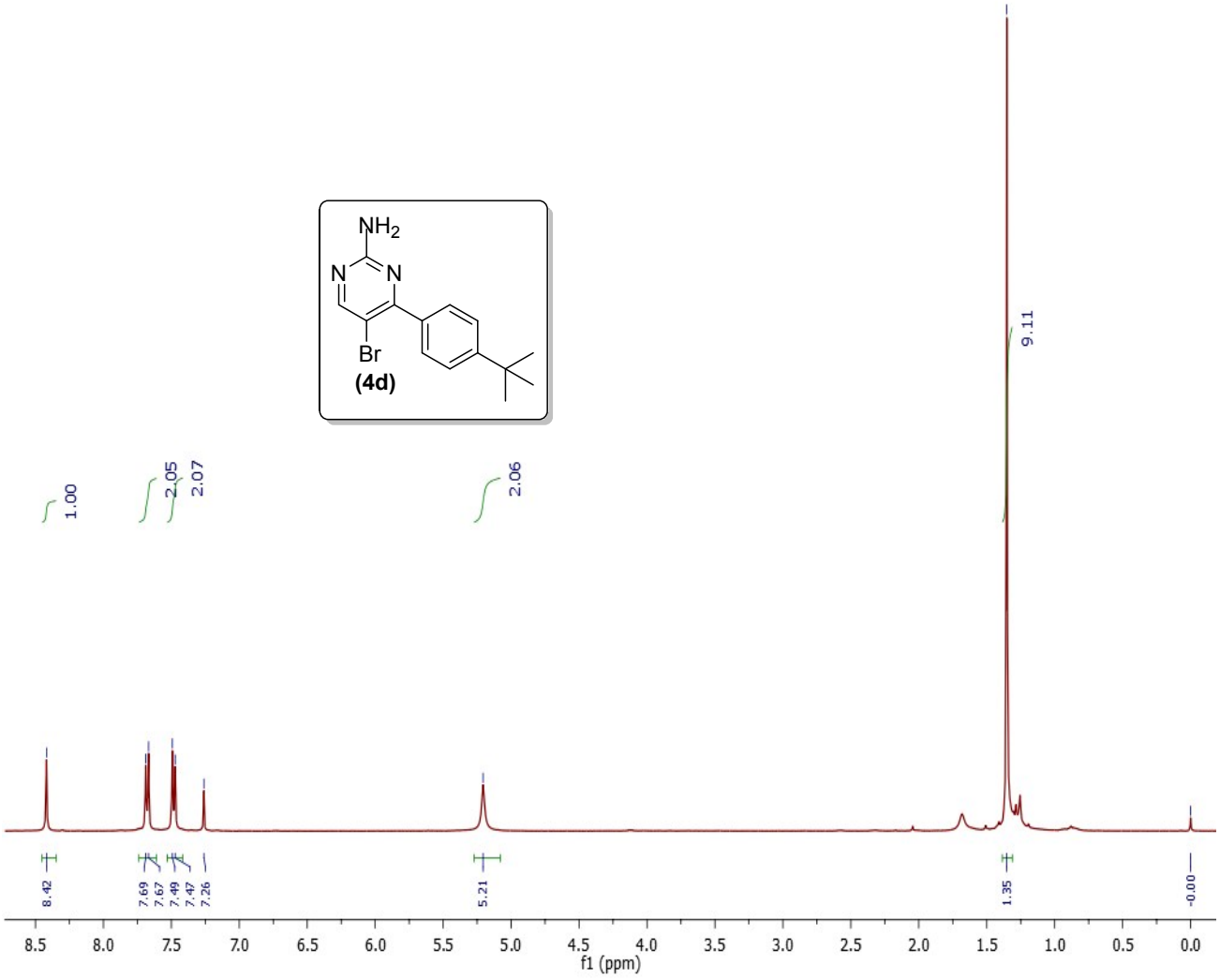
m/z	z	Abund	Formula	Ion
264.0122	1	194308.3	C11 H11 Br N3	(M+H)+
265.0155	1	25564.17	C11 H11 Br N3	(M+H)+
266.0102	1	186462.56	C11 H11 Br N3	(M+H)+
267.0129	1	29649.59	C11 H11 Br N3	(M+H)+
268.0164	1	1565.18	C11 H11 Br N3	(M+H)+

Predicted Isotope Match Table

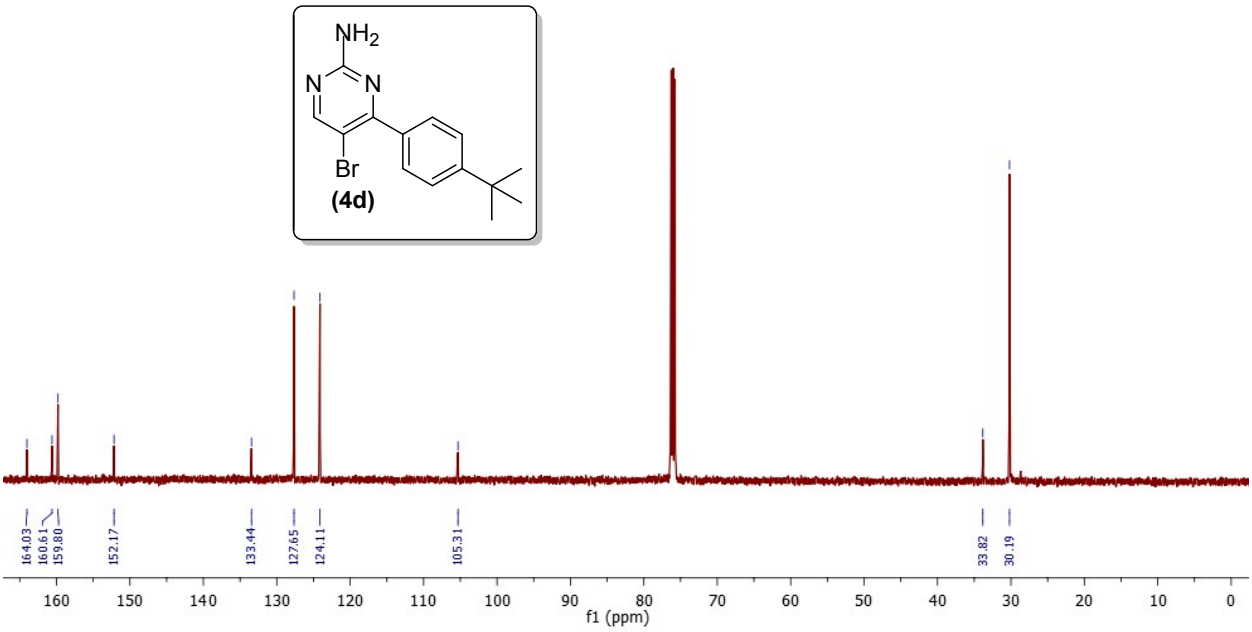
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	264.0122	264.0131	3.35	100	100	44.41	44.49
2	265.0155	265.0159	1.59	13.16	13.12	5.84	5.84
3	266.0102	266.0111	3.27	95.96	98.07	42.62	43.63
4	267.0129	267.0139	3.78	15.26	12.79	6.78	5.69
5	268.0164	268.0167	1.13	0.81	0.77	0.36	0.34

--- End Of Report ---

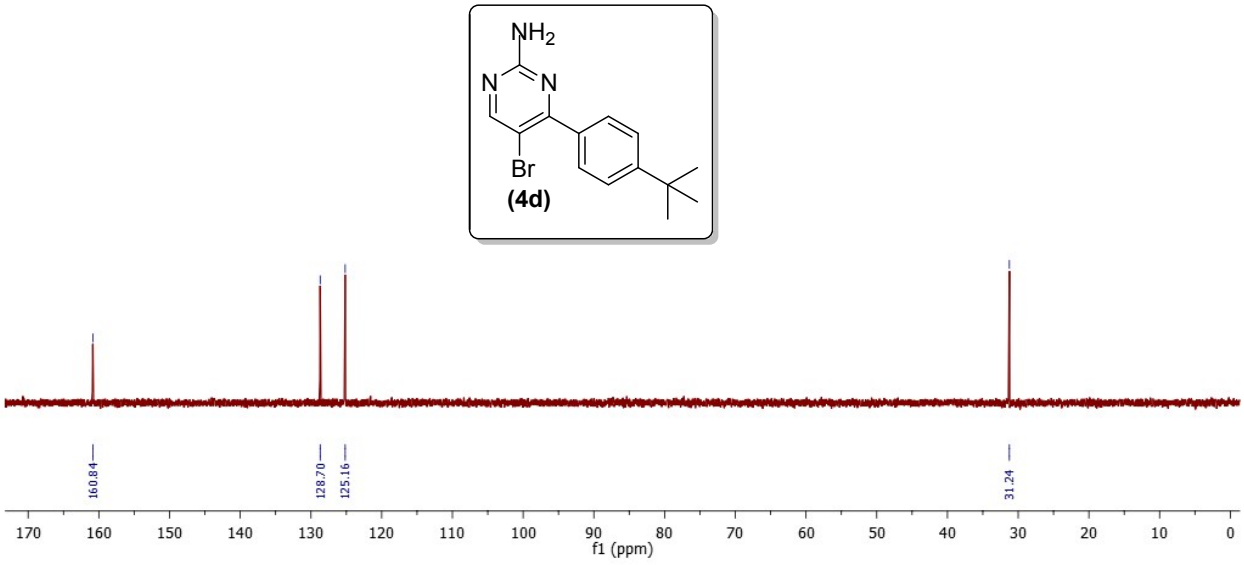
^{1}H NMR of 5-Bromo-4-(4-(*tert*-butyl)phenyl)pyrimidin-2-amine (4d)



^{13}C NMR of 5-Bromo-4-(4-(*tert*-butyl)phenyl)pyrimidin-2-amine (4d)



DEPT NMR of 5-Bromo-4-(4-(*tert*-butyl)phenyl)pyrimidin-2-amine (4d)

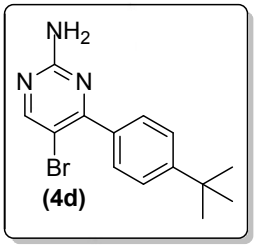


HRMS of 5-Bromo-4-(4-(*tert*-butyl)phenyl)pyrimidin-2-amine (4d)

Qualitative Compound Report

Data File	2A5Br-4TBU.d	**Sample Name**	2A5Br-4TBU
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	25-06-2015 PM 2:29:33
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

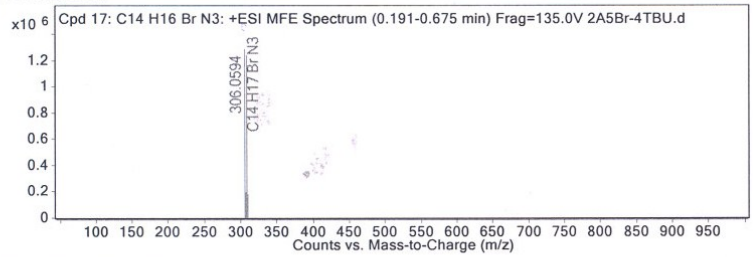


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 17: C14 H16 Br N3	0.264	305.0522	C14 H16 Br N3	C14 H16 Br N3	1.84	C14 H16 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 17: C14 H16 Br N3	306.0594	0.264	Find by Molecular Feature	305.0522

MFE MS Spectrum



MS Spectrum Peak List

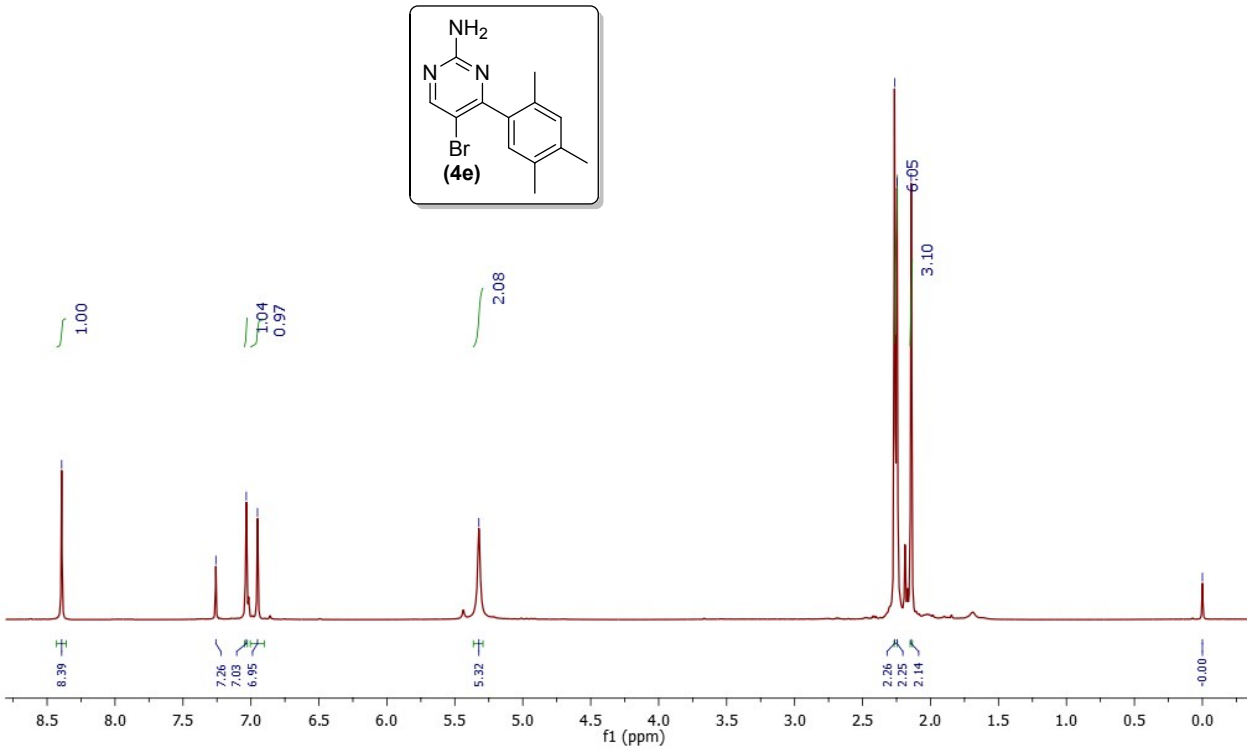
m/z	z	Abund	Formula	Ion
306.0594	1	1283835.13	C14 H17 Br N3	(M+H)+
307.0626	1	195634.39	C14 H17 Br N3	(M+H)+
308.0575	1	1242780	C14 H17 Br N3	(M+H)+
309.0606	1	184923.03	C14 H17 Br N3	(M+H)+
310.0636	1	14031.12	C14 H17 Br N3	(M+H)+
311.065	1	678.45	C14 H17 Br N3	(M+H)+

Predicted Isotope Match Table

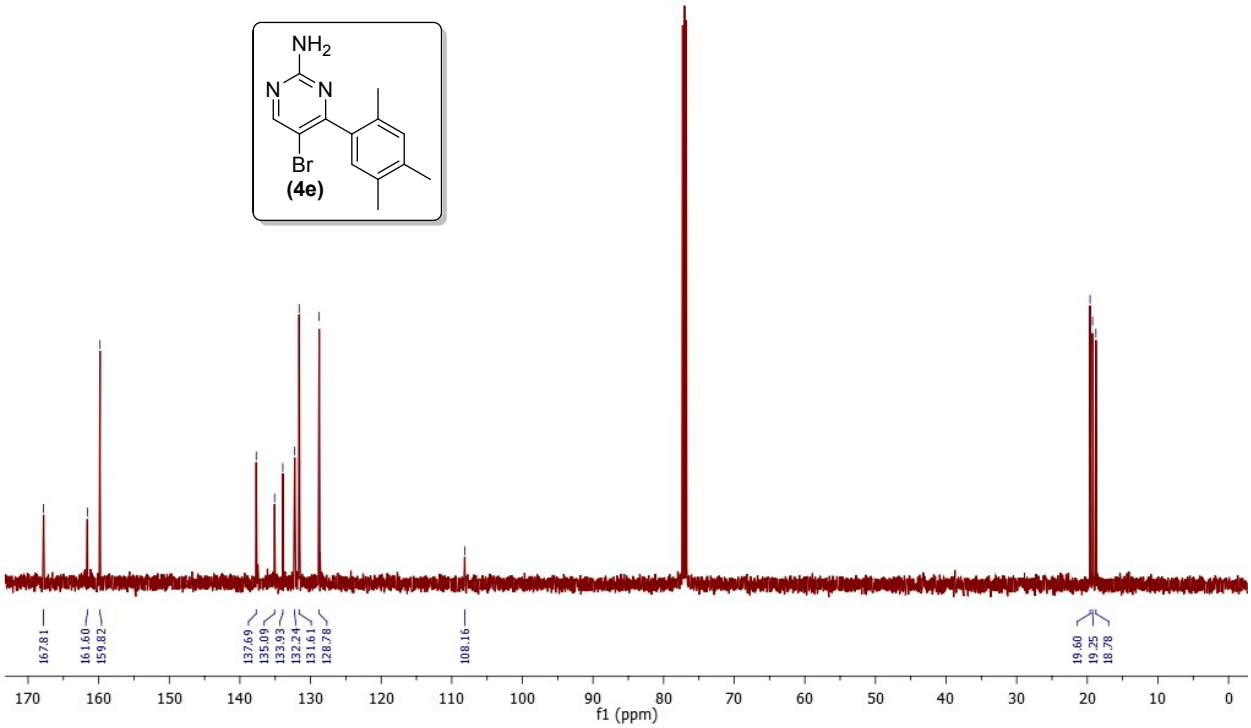
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	306.0594	306.06	2	100	100	43.94	43.04
2	307.0626	307.063	1.18	15.24	16.43	6.7	7.07
3	308.0575	308.0581	1.87	96.8	98.54	42.53	42.42
4	309.0606	309.061	1.15	14.4	16.05	6.33	6.91
5	310.0636	310.0639	0.84	1.09	1.23	0.48	0.53
6	311.065	311.0668	5.71	0.05	0.06	0.02	0.03

--- End Of Report ---

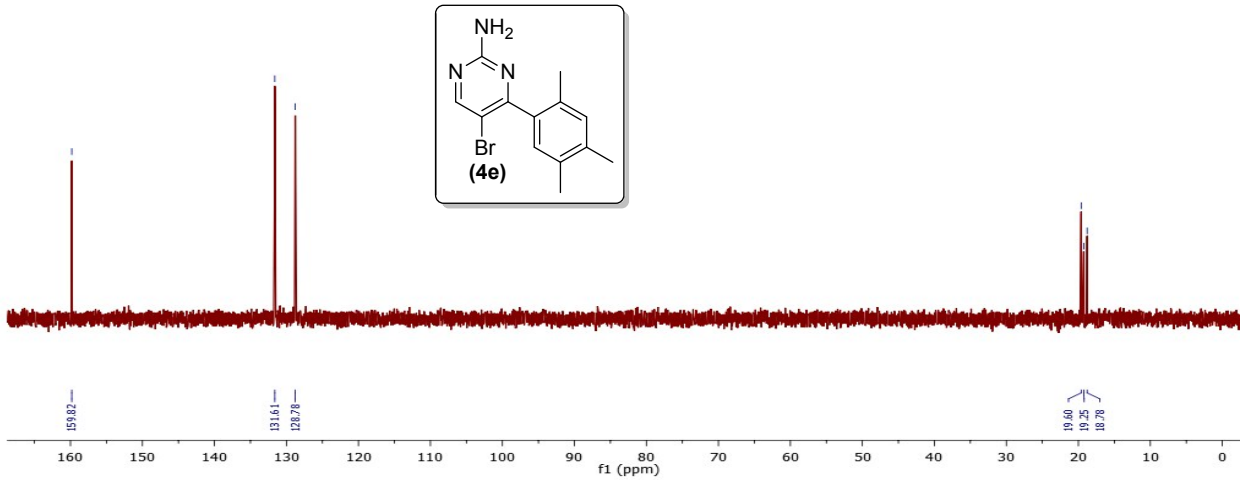
^{1}H NMR of 5-Bromo-4-(2,4,5-trimethylphenyl)pyrimidin-2-amine (4e)



^{13}C NMR of 5-Bromo-4-(2,4,5-trimethylphenyl)pyrimidin-2-amine (4e)



DEPT NMR of 5-Bromo-4-(2,4,5-trimethylphenyl)pyrimidin-2-amine (4e)

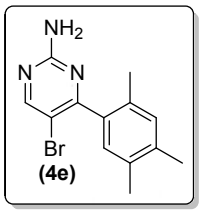


HRMS of 5-Bromo-4-(2,4,5-trimethylphenyl)pyrimidin-2-amine (4e)

Qualitative Compound Report

Data File	2A 5Br-245TM.d	**Sample Name**	2A 5Br-245TM
Sample Type	Sample	**Position**	Vial 19
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	11-05-2015 PM 2:45:36
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

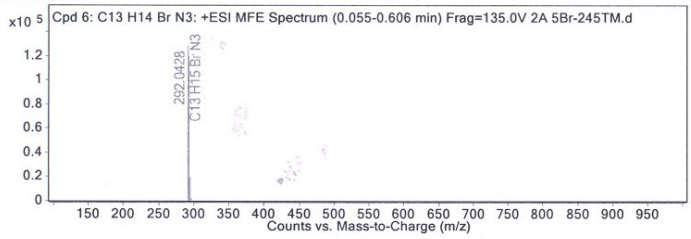


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C13 H14 Br N3	0.365	291.0356	C13 H14 Br N3	C13 H14 Br N3	5.36	C13 H14 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C13 H14 Br N3	292.0428	0.365	Find by Molecular Feature	291.0356

MFE MS Spectrum



MS Spectrum Peak List

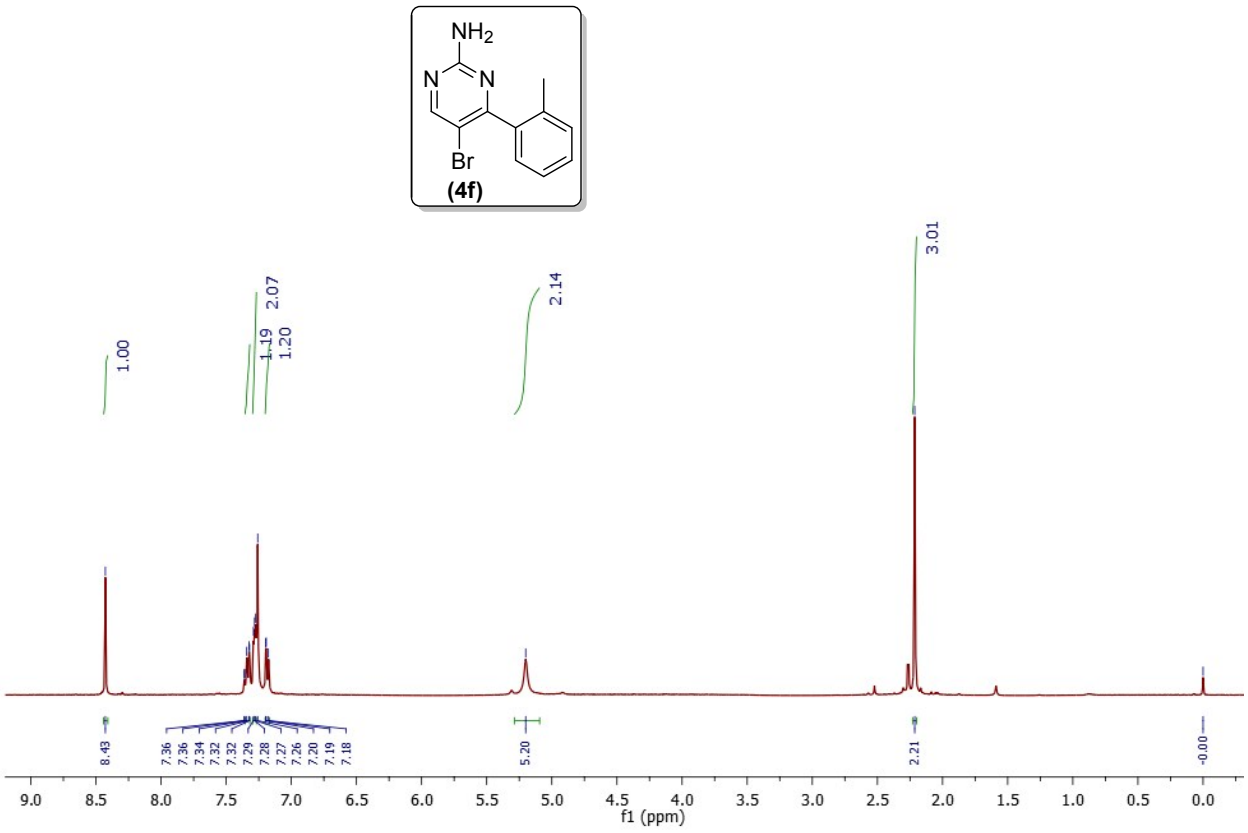
m/z	z	Abund	Formula	Ion
292.0428	1	128522.09	C13 H15 Br N3	(M+H)+
293.0458	1	19487.85	C13 H15 Br N3	(M+H)+
294.041	1	120221.61	C13 H15 Br N3	(M+H)+
295.0436	1	19753.19	C13 H15 Br N3	(M+H)+
296.0471	1	2383.28	C13 H15 Br N3	(M+H)+
297.0452	1	158.21	C13 H15 Br N3	(M+H)+

Predicted Isotope Match Table

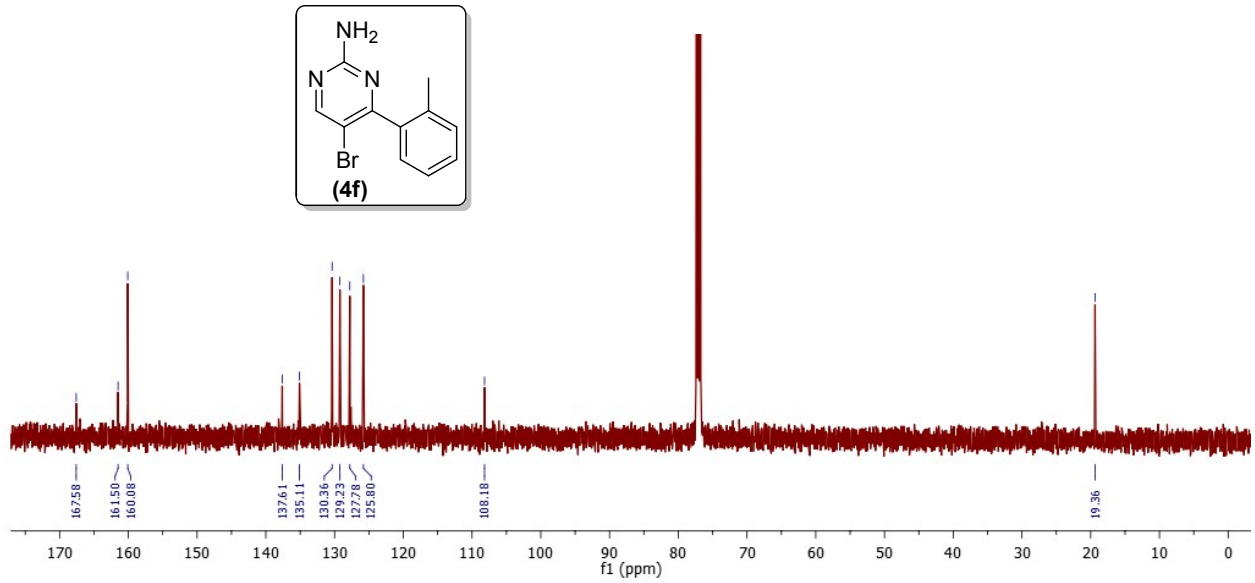
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	292.0428	292.0444	5.57	100	100	44.24	43.52
2	293.0458	293.0473	5.17	15.16	15.33	6.71	6.67
3	294.041	294.0424	4.99	93.54	98.37	41.38	42.81
4	295.0436	295.0453	5.9	15.37	14.96	6.8	6.51
5	296.0471	296.0482	3.76	1.85	1.07	0.82	0.46
6	297.0452	297.051	19.59	0.12	0.05	0.05	0.02

--- End Of Report ---

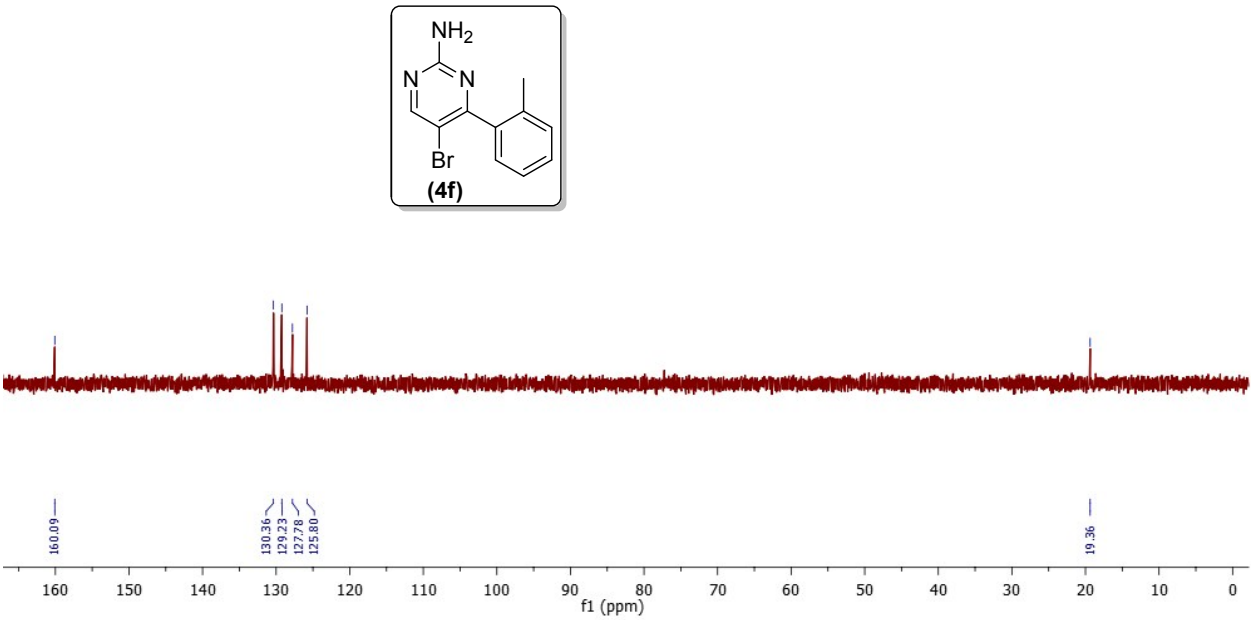
^{1}H NMR of 5-Bromo-4-(*o*-tolyl)pyrimidin-2-amine (4f)



^{13}C NMR of 5-Bromo-4-(*o*-tolyl)pyrimidin-2-amine (4f)



DEPT NMR of 5-Bromo-4-(*o*-tolyl)pyrimidin-2-amine (4f)

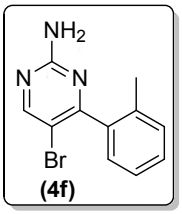


HRMS of 5-Bromo-4-(*o*-tolyl)pyrimidin-2-amine (4f)

Qualitative Compound Report

Data File	2A5Br-2Me.d	**Sample Name**	2A5Br-2Me
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	12-05-2015 PM 2:52:35
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



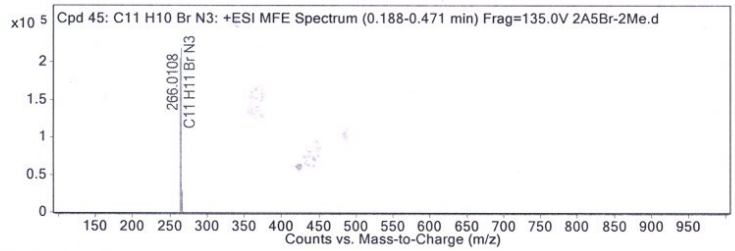
(4f)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 45: C11 H10 Br N3	0.272	263.0055	C11 H10 Br N3	C11 H10 Br N3	1.09	C11 H10 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 45: C11 H10 Br N3	264.0128	0.272	Find by Molecular Feature	263.0055

MFE MS Spectrum



MS Spectrum Peak List

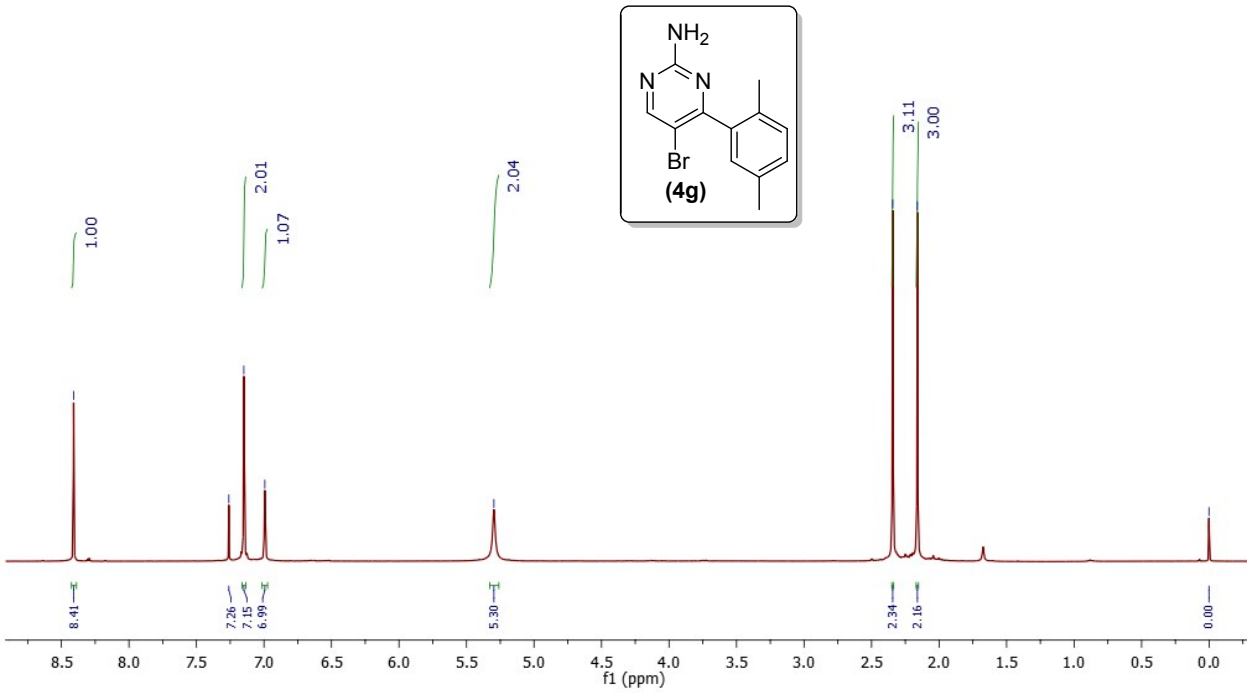
m/z	z	Abund	Formula	Ion
264.0128	1	205366.38	C11 H11 Br N3	(M+H)+
265.0159	1	26755.08	C11 H11 Br N3	(M+H)+
266.0108	1	218515.36	C11 H11 Br N3	(M+H)+
267.0136	1	29240.22	C11 H11 Br N3	(M+H)+
268.0176	1	1839.07	C11 H11 Br N3	(M+H)+

Predicted Isotope Match Table

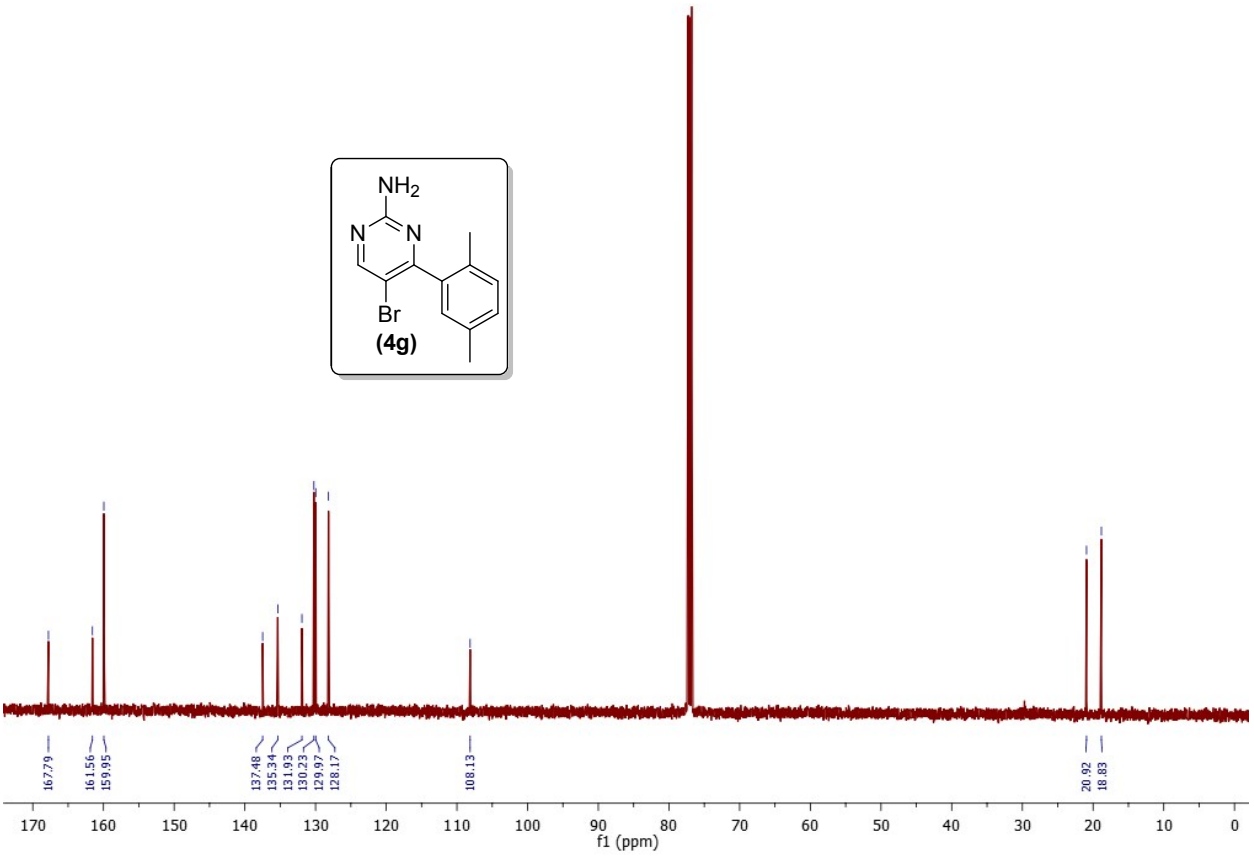
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	264.0128	264.0131	1.1	93.98	100	42.63	44.49
2	265.0159	265.0159	0.12	12.24	13.12	5.55	5.84
3	266.0108	266.0111	1.21	100	98.07	45.36	43.63
4	267.0136	267.0139	1.12	13.38	12.79	6.07	5.69
5	268.0176	268.0167	-3.17	0.84	0.77	0.38	0.34

--- End Of Report ---

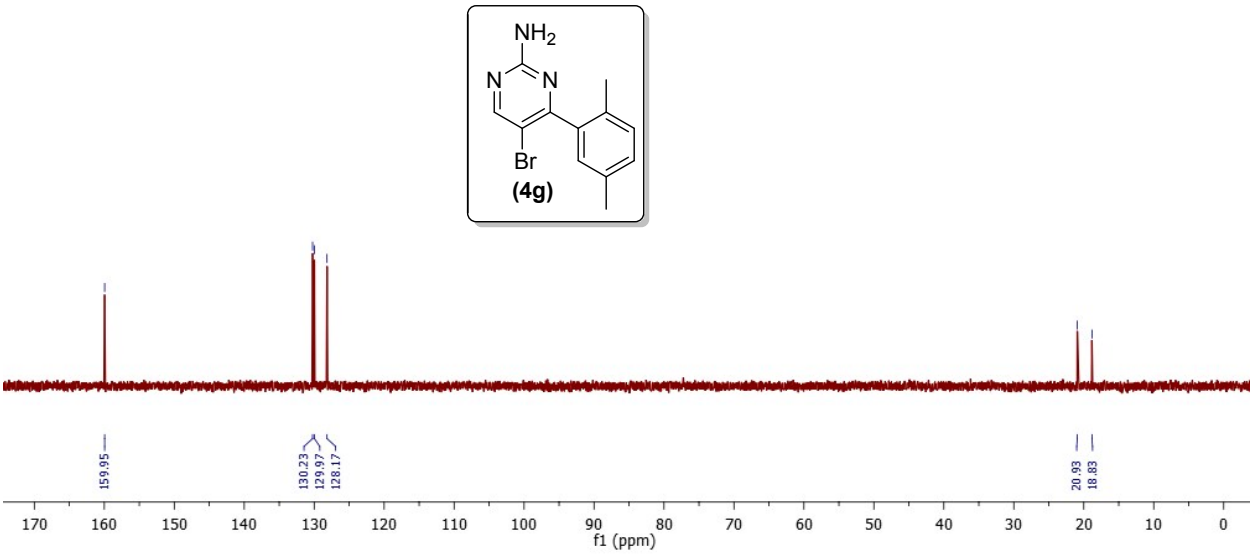
^{1}H NMR of 5-Bromo-4-(2,5-dimethylphenyl)pyrimidin-2-amine (4g)



^{13}C NMR of 5-Bromo-4-(2,5-dimethylphenyl)pyrimidin-2-amine (4g)



DEPT NMR of 5-Bromo-4-(2,5-dimethylphenyl)pyrimidin-2-amine (4g)

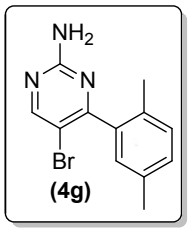


HRMS of 5-Bromo-4-(2,5-dimethylphenyl)pyrimidin-2-amine (4g)

Qualitative Compound Report

Data File	2A5Br-25DM.d	**Sample Name**	2A5Br-25DM
Sample Type	Sample	**Position**	Vial 7
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-05-2015 PM 1:46:03
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

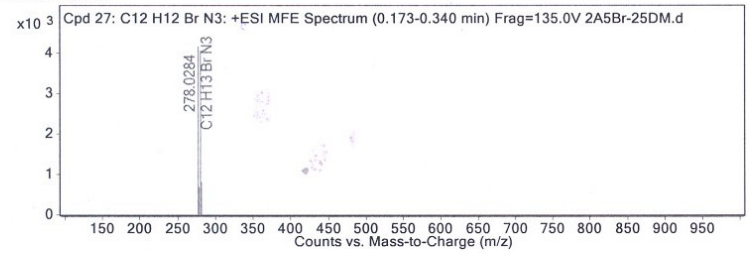


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 27: C12 H12 Br N3	0.265	277.0219	C12 H12 Br N3	C12 H12 Br N3	-1.43	C12 H12 Br N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 27: C12 H12 Br N3	278.0284	0.265	Find by Molecular Feature	277.0219

MFE MS Spectrum



MS Spectrum Peak List

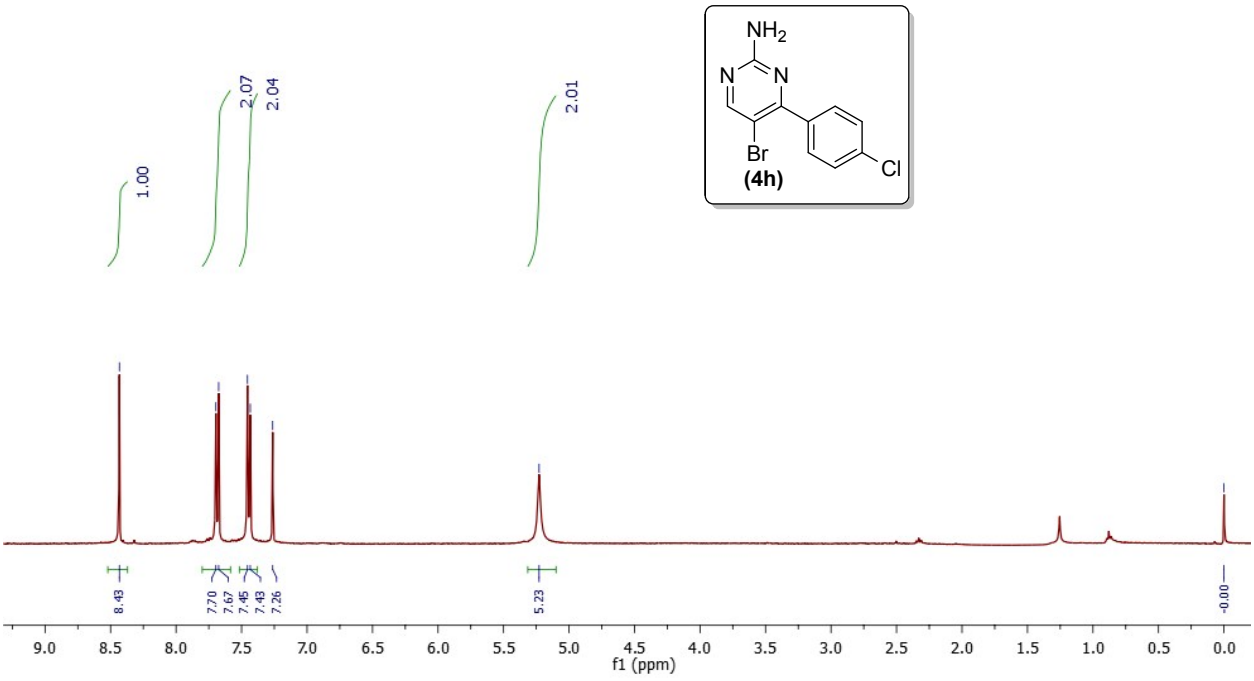
m/z	z	Abund	Formula	Ion
278.0284	1	4160.22	C12 H13 Br N3	(M+H)+
279.0317	1	688.85	C12 H13 Br N3	(M+H)+
280.0275	1	4066.46	C12 H13 Br N3	(M+H)+
281.0324	1	819.2	C12 H13 Br N3	(M+H)+

Predicted Isotope Match Table

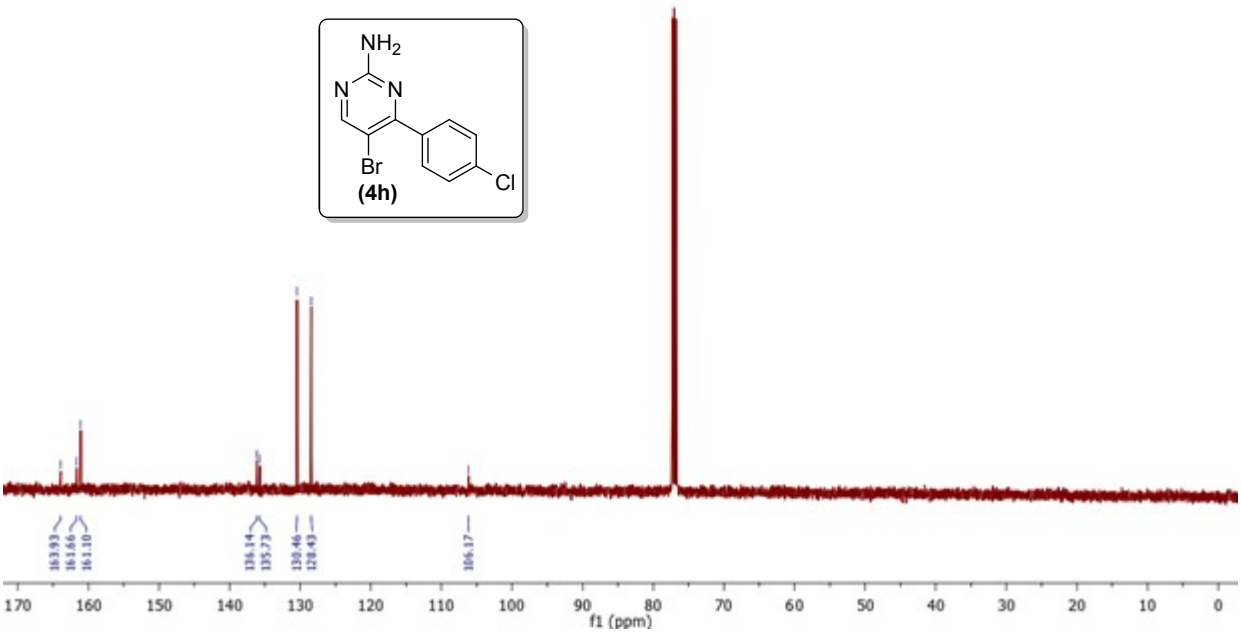
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	278.0284	278.0287	1.34	100	100	42.74	44.19
2	279.0317	279.0316	-0.3	16.56	14.22	7.08	6.29
3	280.0275	280.0268	-2.71	97.75	98.22	41.77	43.4
4	281.0324	281.0296	-9.79	19.69	13.88	8.42	6.13

--- End Of Report ---

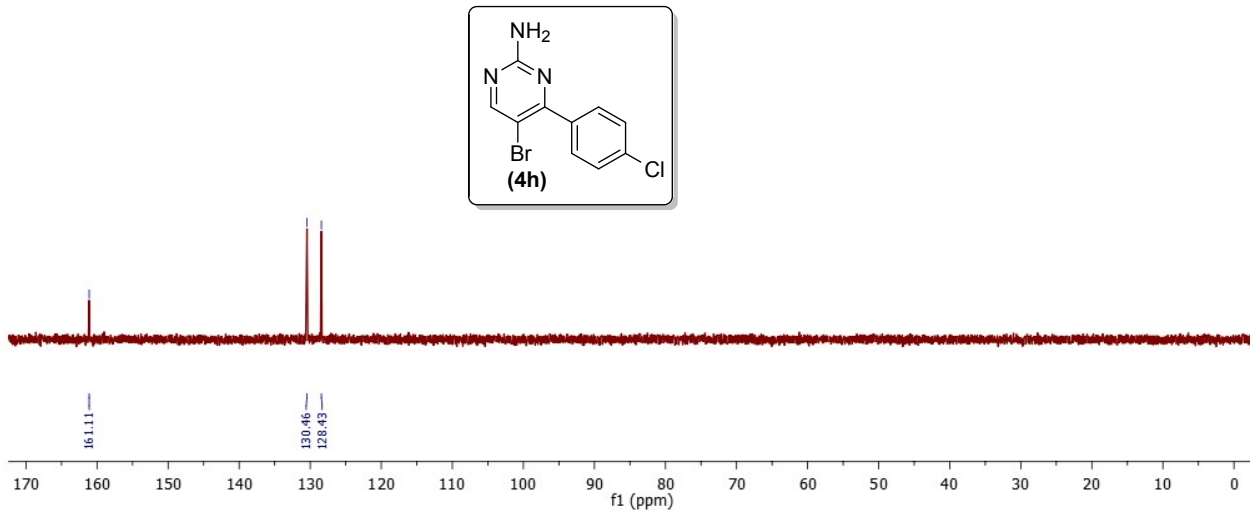
^{1}H NMR of 5-Bromo-4-(4-chlorophenyl)pyrimidin-2-amine (4h)



^{13}C NMR of 5-Bromo-4-(4-chlorophenyl)pyrimidin-2-amine (4h)



DEPT NMR of 5-Bromo-4-(4-chlorophenyl)pyrimidin-2-amine (4h)

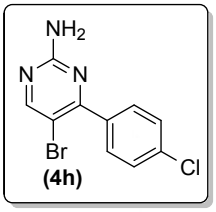


HRMS of 5-Bromo-4-(4-chlorophenyl)pyrimidin-2-amine (4h)

Qualitative Compound Report

Data File	2A5Br-4Cl. d.d	**Sample Name**	2A5Br-4Cl
Sample Type	Sample	**Position**	Vial 9
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-05-2015 PM 4:30:25
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



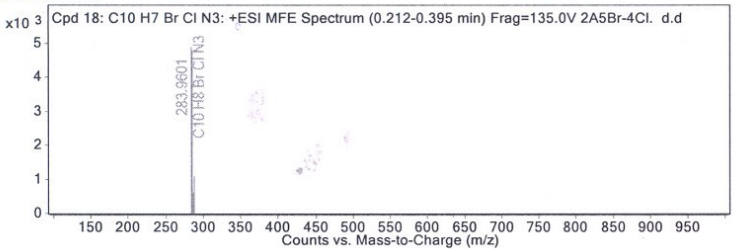
(4h)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C10 H7 Br Cl N3	0.264	282.9527	C10 H7 Br Cl N3	C10 H7 Br Cl N3	-5.43	C10 H7 Br Cl N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C10 H7 Br Cl N3	283.9601	0.264	Find by Molecular Feature	282.9527

MFE MS Spectrum



MS Spectrum Peak List

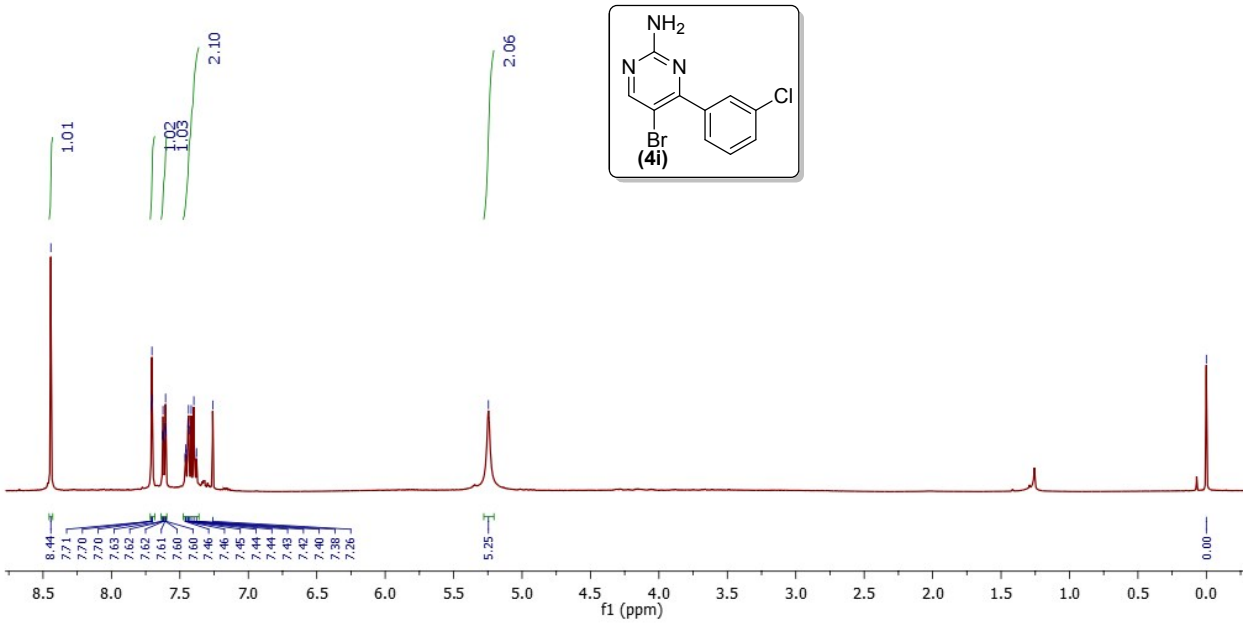
m/z	z	Abund	Formula	Ion
283.9601	1	4890.92	C10 H8 Br Cl N3	(M+H)+
284.9636	1	518.17	C10 H8 Br Cl N3	(M+H)+
285.9578	1	4757.68	C10 H8 Br Cl N3	(M+H)+
286.9605	1	594.89	C10 H8 Br Cl N3	(M+H)+
287.9542	1	1088.76	C10 H8 Br Cl N3	(M+H)+

Predicted Isotope Match Table

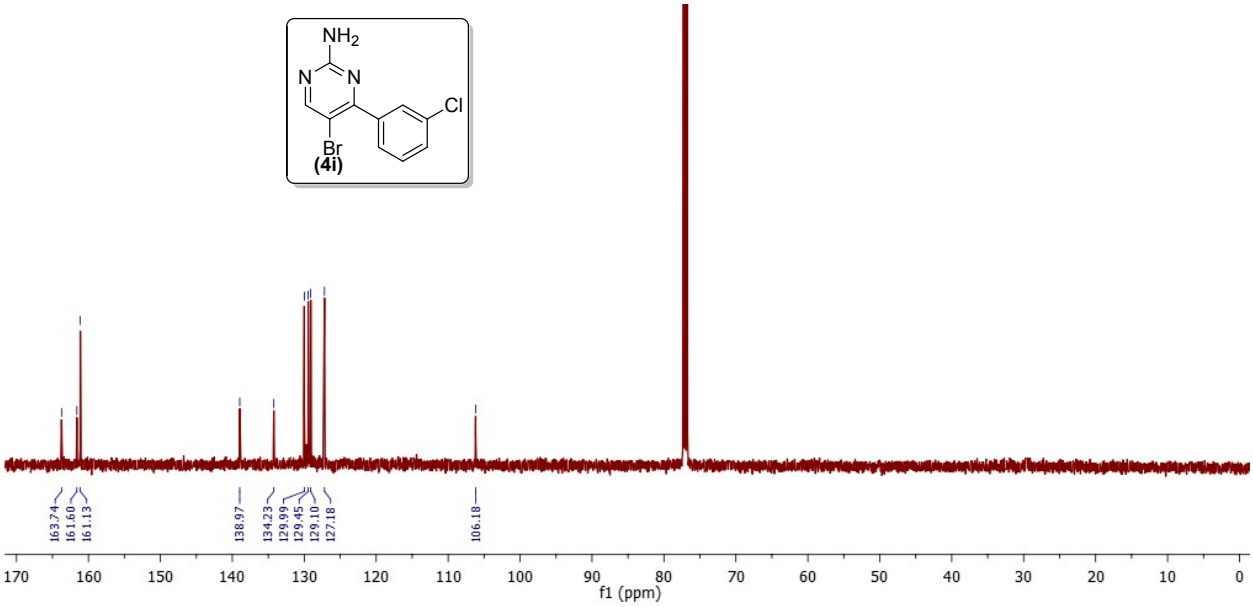
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	283.9601	283.9585	-5.75	100	76.96	41.27	34.55
2	284.9636	284.9613	-8.19	10.59	9.24	4.37	4.15
3	285.9578	285.9562	-5.54	97.28	100	40.15	44.89
4	286.9605	286.959	-5.33	12.16	11.96	5.02	5.37
5	287.9542	287.9537	-1.76	22.26	24.61	9.19	11.05

--- End Of Report ---

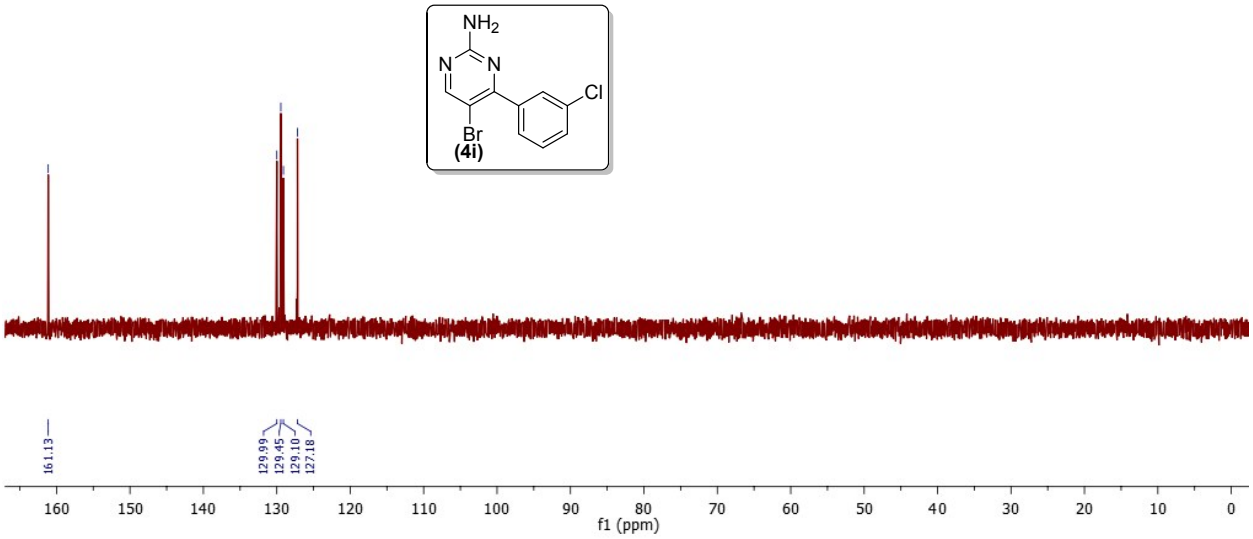
^{1}HNMR of 5-Bromo-4-(3-chlorophenyl)pyrimidin-2-amine (4i)



^{13}C NMR of 5-Bromo-4-(3-chlorophenyl)pyrimidin-2-amine (4i)



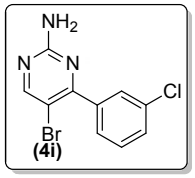
DEPT NMR of 5-Bromo-4-(3-chlorophenyl)pyrimidin-2-amine (4i)



HRMS of 5-Bromo-4-(3-chlorophenyl)pyrimidin-2-amine (4i)

Qualitative Compound Report

Data File	2A5Br-3Cl.d	**Sample Name**	2A5Br-3Cl
Sample Type	Sample	**Position**	Vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	29-05-2015 PM 1:24:07
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



(4i)

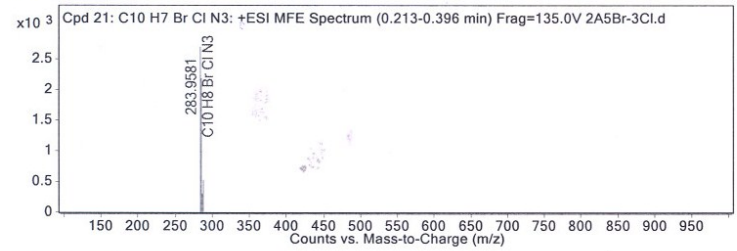
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C10 H7 Br Cl N3	0.271	282.9508	C10 H7 Br Cl N3	C10 H7 Br Cl N3	1.48	C10 H7 Br Cl N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C10 H7 Br Cl N3	283.9581	0.271	Find by Molecular Feature	282.9508

MFE MS Spectrum



MS Spectrum Peak List

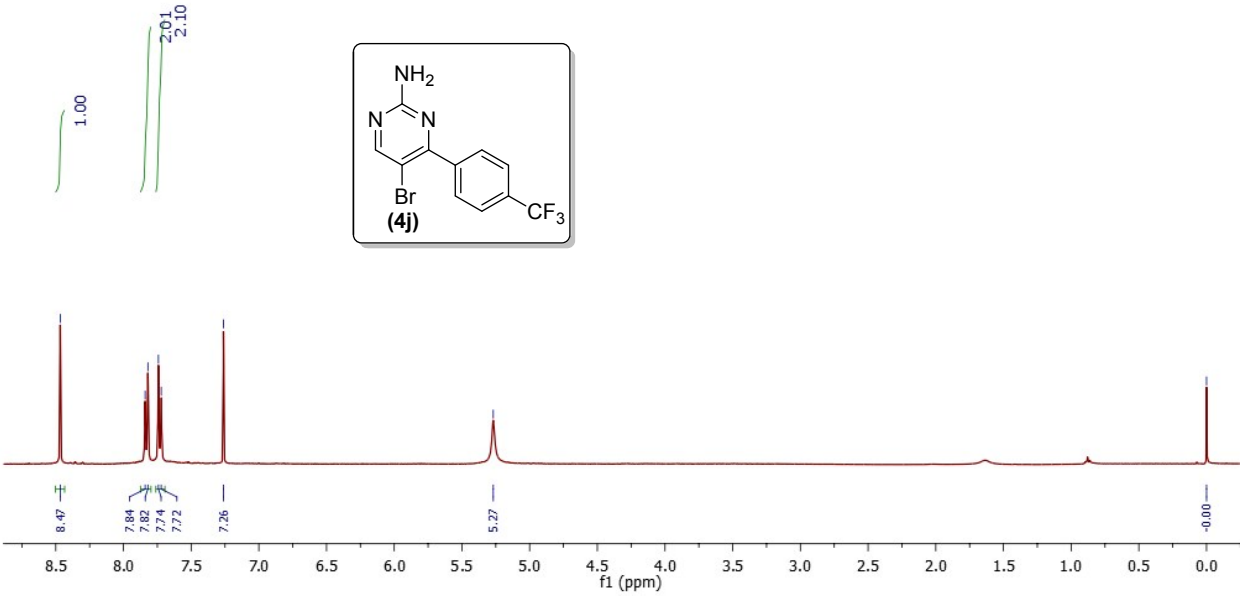
m/z	z	Abund	Formula	Ion
283.9581	1	2706.22	C10 H8 Br Cl N3	(M+H)+
284.9558	1	361.02	C10 H8 Br Cl N3	(M+H)+
285.956	1	2184.86	C10 H8 Br Cl N3	(M+H)+
286.9623	1	300.96	C10 H8 Br Cl N3	(M+H)+
287.9539	1	531.61	C10 H8 Br Cl N3	(M+H)+

Predicted Isotope Match Table

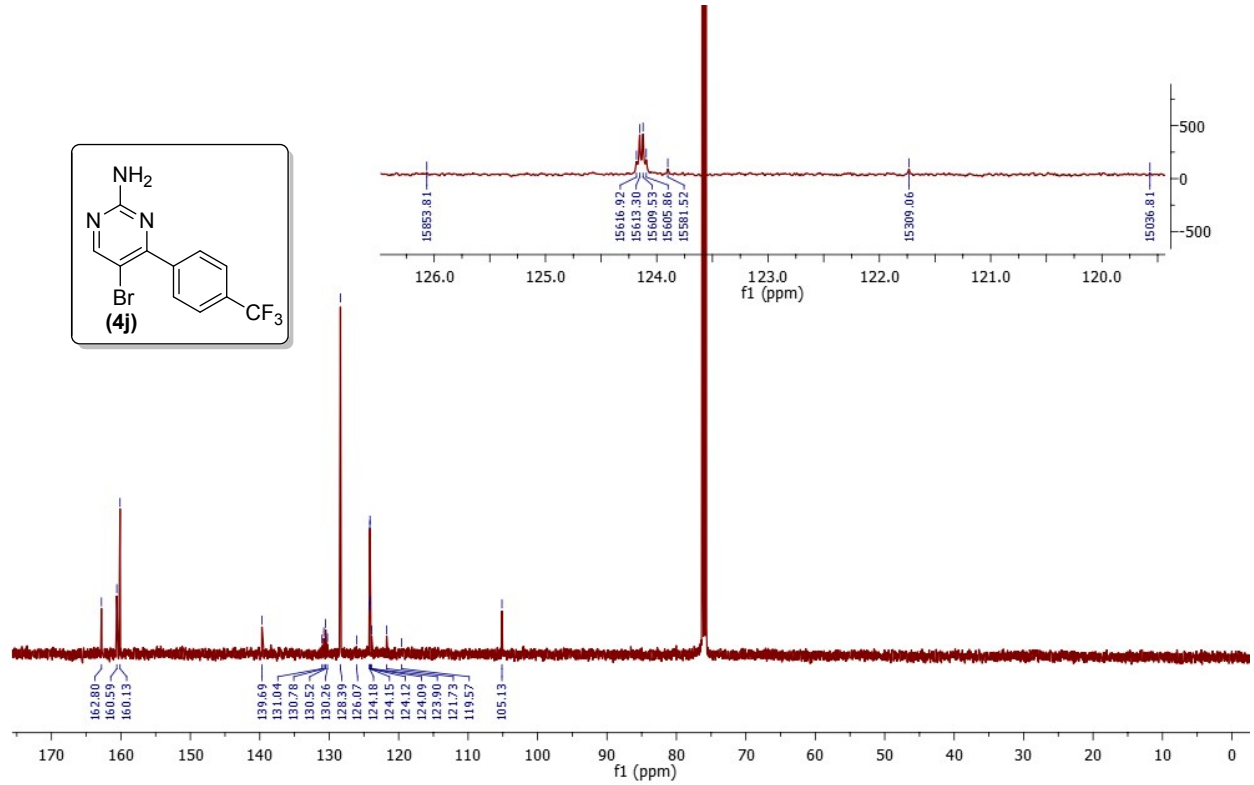
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	283.9581	283.9585	1.39	100	76.96	44.48	34.55
2	284.9558	284.9613	19.11	13.34	9.24	5.93	4.15
3	285.956	285.9562	0.99	80.73	100	35.91	44.89
4	286.9623	286.959	-11.45	11.12	11.96	4.95	5.37
5	287.9539	287.9537	-0.73	19.64	24.61	8.74	11.05

--- End Of Report ---

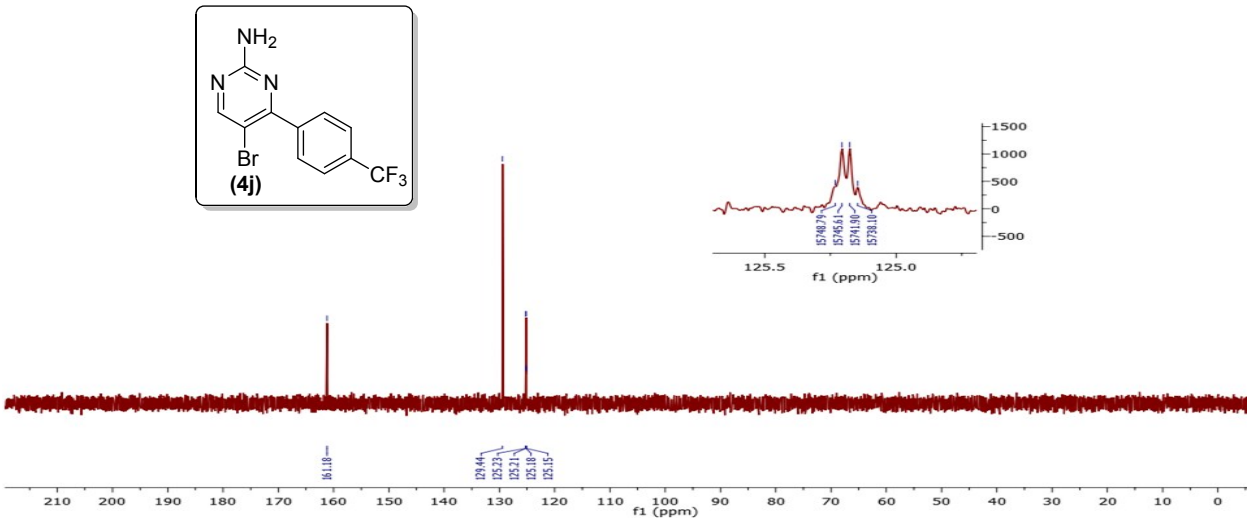
^{1}H NMR of 5-Bromo-4-(4-(trifluoromethyl)phenyl)pyrimidin-2-amine (4j)



^{13}C NMR of 5-Bromo-4-(4-(trifluoromethyl)phenyl)pyrimidin-2-amine (4j)



DEPT NMR of 5-Bromo-4-(4-(trifluoromethyl)phenyl)pyrimidin-2-amine (4j)

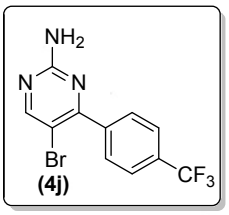


HRMS of 5-Bromo-4-(4-(trifluoromethyl)phenyl)pyrimidin-2-amine (4j)

Qualitative Compound Report

Data File	2A5Br-4CF3.d	**Sample Name**	2A5Br-4CF3
Sample Type	Sample	**Position**	Vial 8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	12-05-2015 PM 3:23:00
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



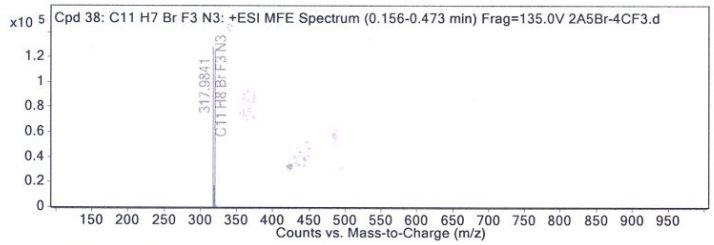
(4j)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 38: C11 H7 Br F3 N3	0.27	316.9768	C11 H7 Br F3 N3	C11 H7 Br F3 N3	2.22	C11 H7 Br F3 N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 38: C11 H7 Br F3 N3	317.9841	0.27	Find by Molecular Feature	316.9768

MFE MS Spectrum



MS Spectrum Peak List

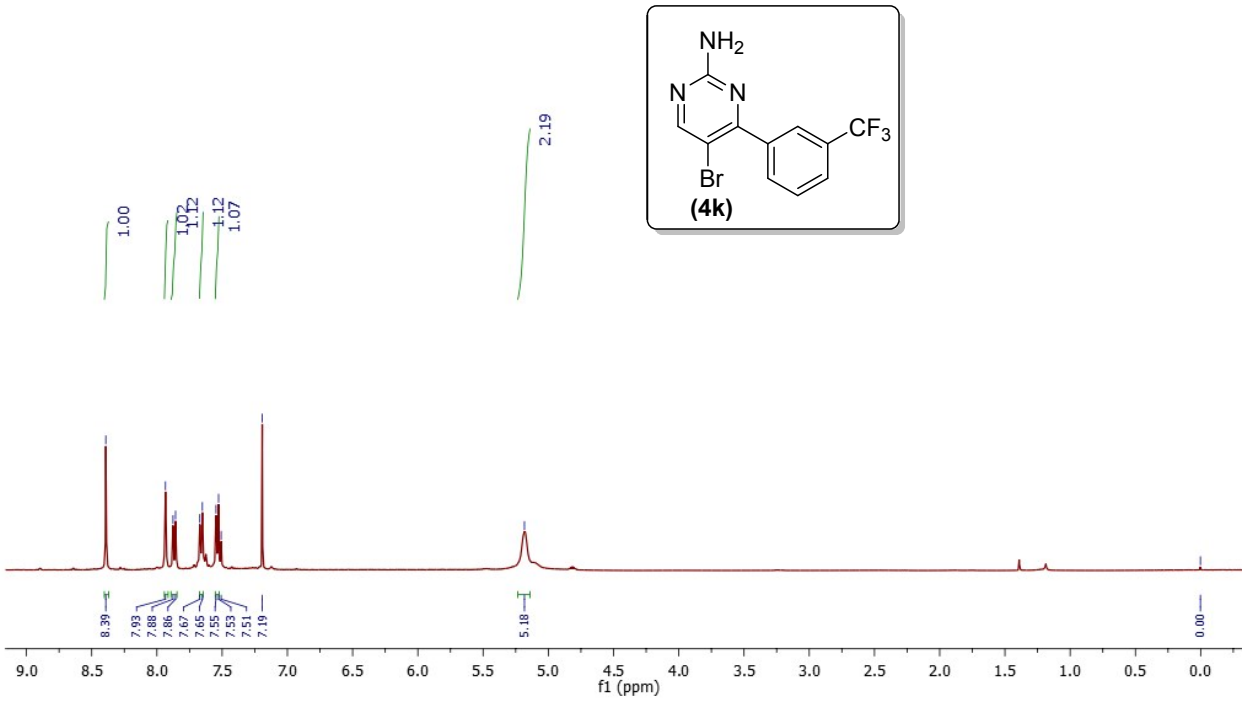
m/z	z	Abund	Formula	Ion
317.9841	1	128084.8	C11 H8 Br F3 N3	(M+H)+
318.9874	1	17606.21	C11 H8 Br F3 N3	(M+H)+
319.982	1	125440.72	C11 H8 Br F3 N3	(M+H)+
320.9853	1	17696.49	C11 H8 Br F3 N3	(M+H)+
321.9883	1	1294.89	C11 H8 Br F3 N3	(M+H)+

Predicted Isotope Match Table

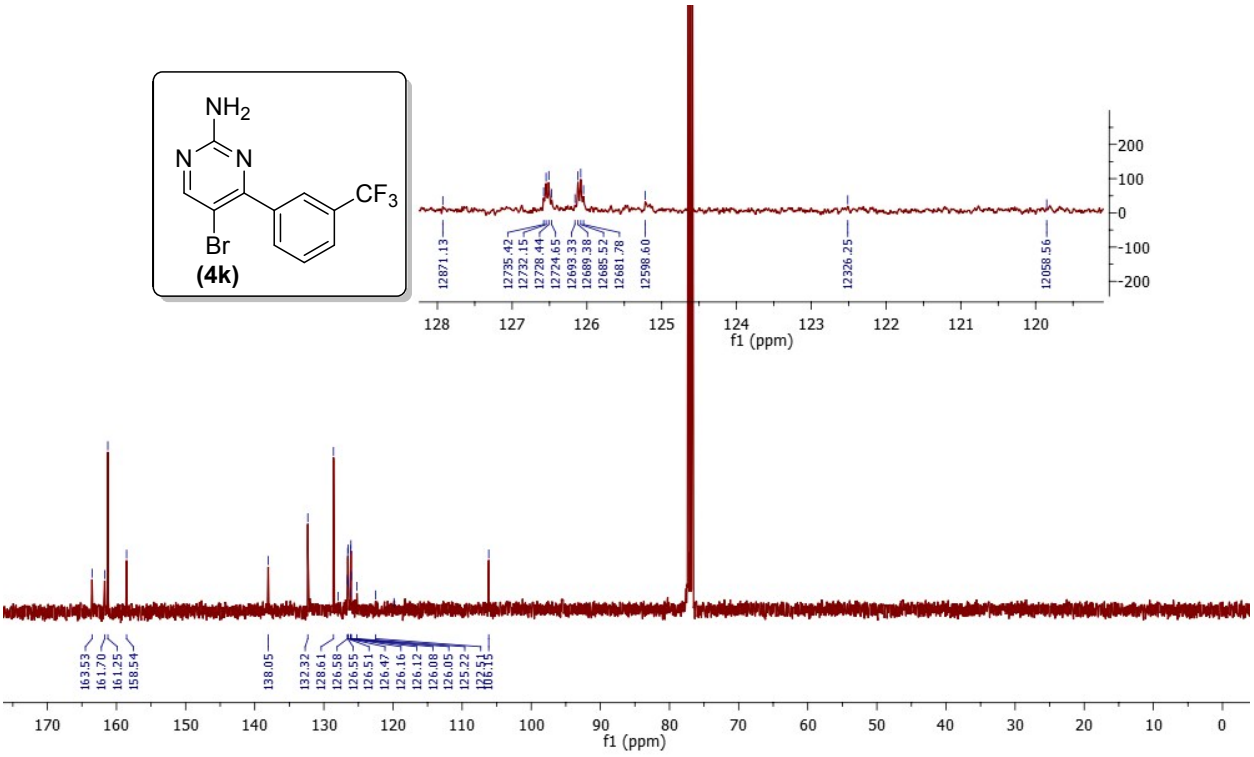
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.9841	317.9848	2.26	100	100	44.15	44.51
2	318.9874	318.9877	0.98	13.75	13.09	6.07	5.82
3	319.982	319.9828	2.49	97.94	98.07	43.24	43.65
4	320.9853	320.9856	1.2	13.82	12.76	6.1	5.68
5	321.9883	321.9884	0.4	1.01	0.77	0.45	0.34

--- End Of Report ---

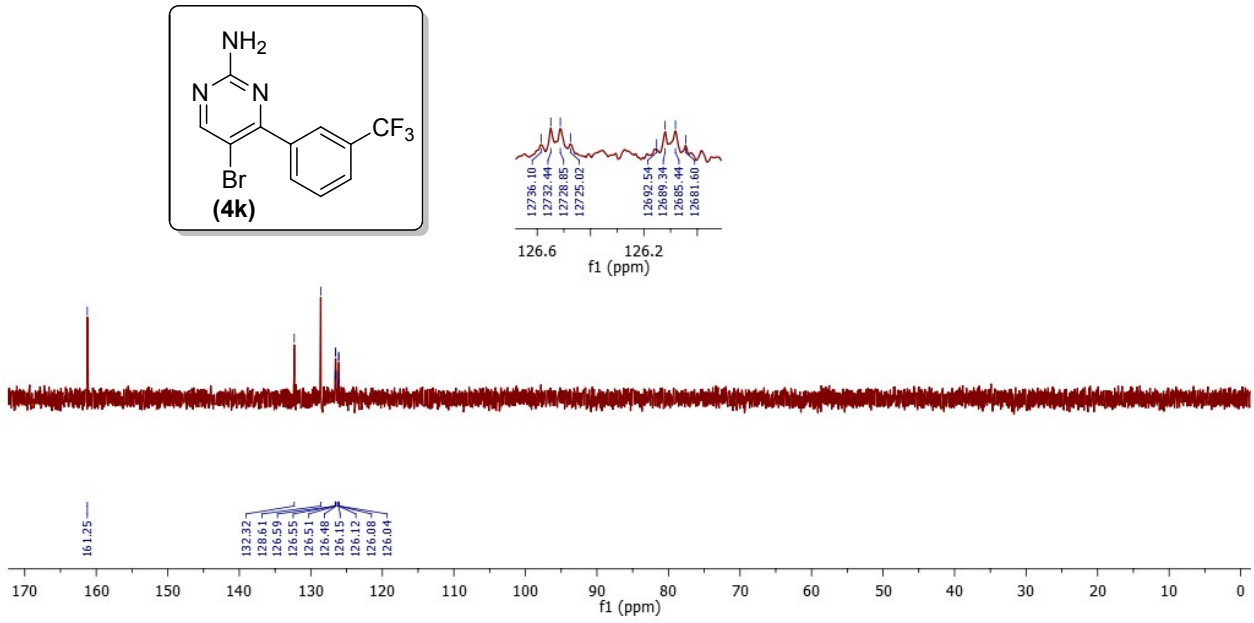
^{1}H NMR of 5-Bromo-4-(3-(trifluoromethyl)phenyl)pyrimidin-2-amine (4k)



^{13}C NMR of 5-Bromo-4-(3-(trifluoromethyl)phenyl)pyrimidin-2-amine (4k)



DEPT NMR of 5-Bromo-4-(3-(trifluoromethyl)phenyl)pyrimidin-2-amine (4k)

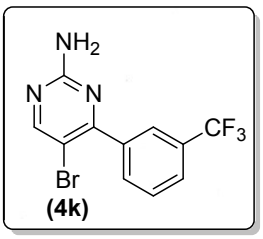


HRMS of 5-Bromo-4-(3-(trifluoromethyl)phenyl)pyrimidin-2-amine (4k)

Qualitative Compound Report

Data File	2A 5Br-3CF3.d	**Sample Name**	2A 5Br-3CF3
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	11-05-2015 PM 2:54:19
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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



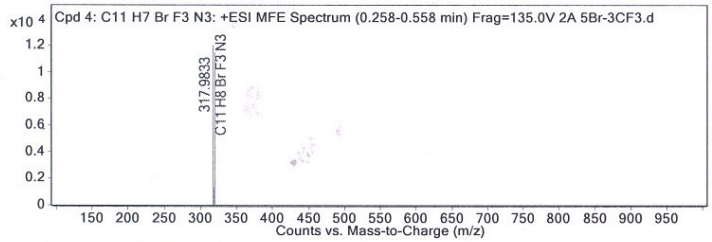
(4k)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C11 H7 Br F3 N3	0.366	316.9756	C11 H7 Br F3 N3	C11 H7 Br F3 N3	6.04	C11 H7 Br F3 N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C11 H7 Br F3 N3	317.9833	0.366	Find by Molecular Feature	316.9756

MFE MS Spectrum



MS Spectrum Peak List

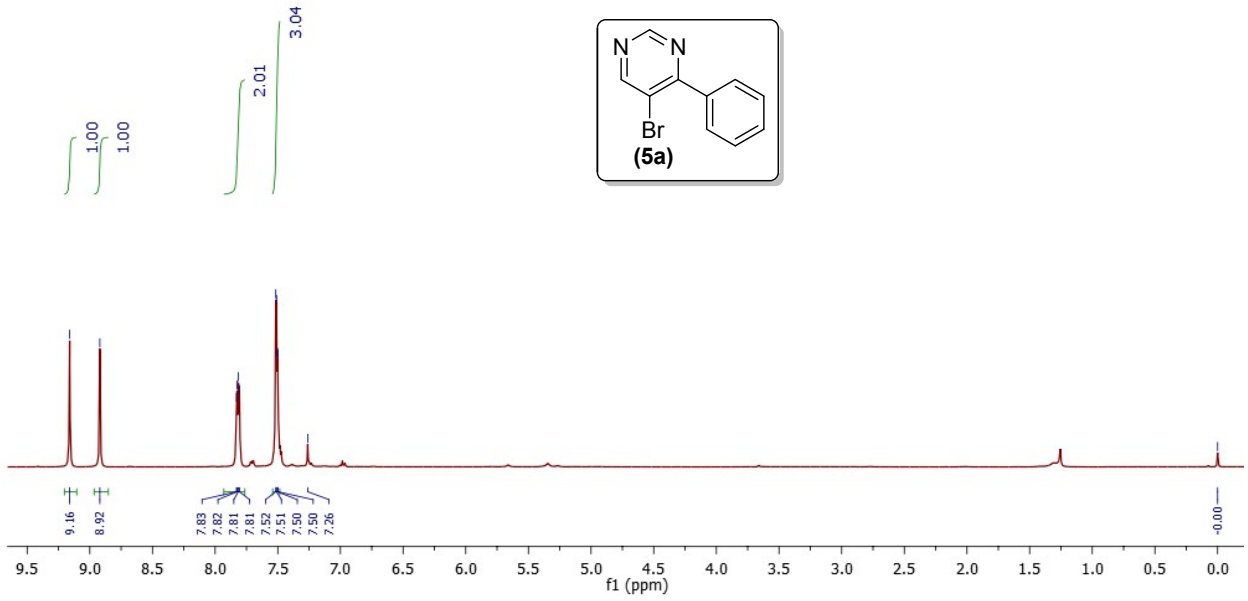
m/z	z	Abund	Formula	Ion
317.9833	1	12018.33	C11 H8 Br F3 N3	(M+H)+
318.9848	1	1321.51	C11 H8 Br F3 N3	(M+H)+
319.9809	1	11460.47	C11 H8 Br F3 N3	(M+H)+
320.9817	1	1543.94	C11 H8 Br F3 N3	(M+H)+

Predicted Isotope Match Table

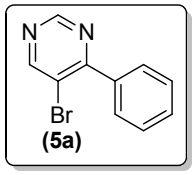
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.9833	317.9848	4.82	100	100	45.62	44.66
2	318.9848	318.9877	8.86	11	13.09	5.02	5.84
3	319.9809	319.9828	6.05	95.36	98.07	43.5	43.8
4	320.9817	320.9856	12.18	12.85	12.76	5.86	5.7

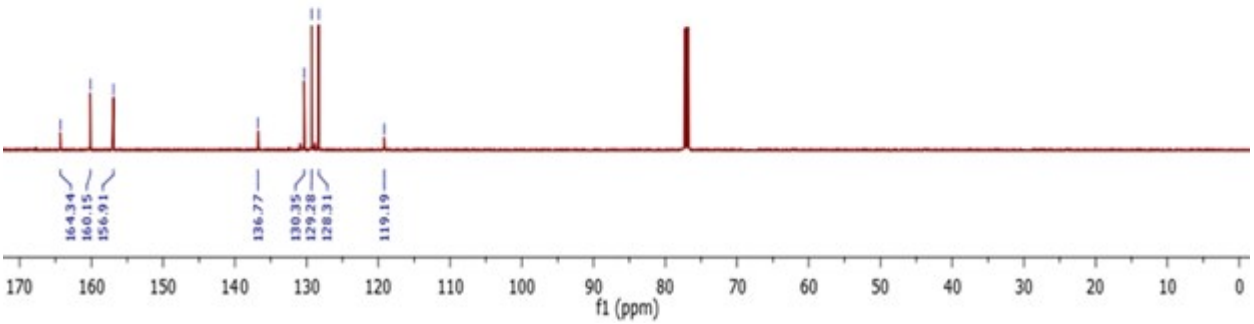
--- End Of Report ---

[1]H NMR of 5-Bromo-4-phenylpyrimidine (5a)

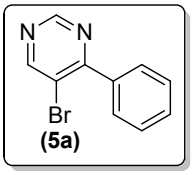


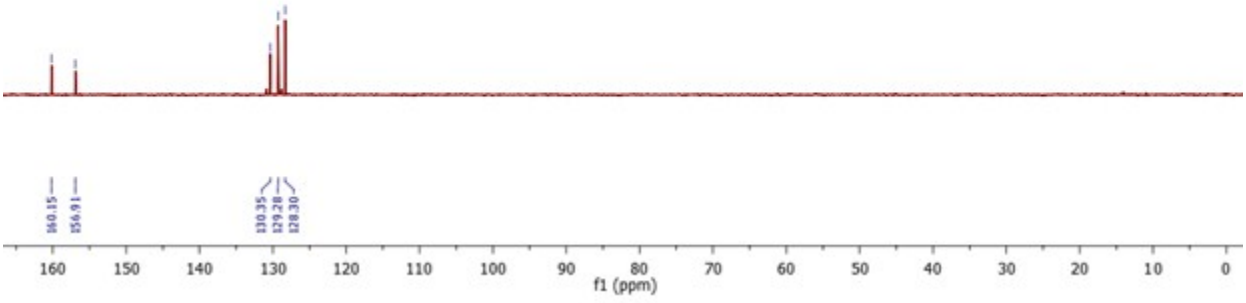
^{13}C NMR of 5-Bromo-4-phenylpyrimidine (5a)





DEPT NMR of 5-Bromo-4-phenylpyrimidine (5a)

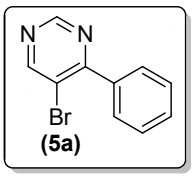




HRMS of 5-Bromo-4-phenylpyrimidine (5a)

Qualitative Compound Report

Data File	5BrPY-BA.d	**Sample Name**	5BrPY-BA
Sample Type	Sample	**Position**	Vial 5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	06-05-2015 PM 1:35:19
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



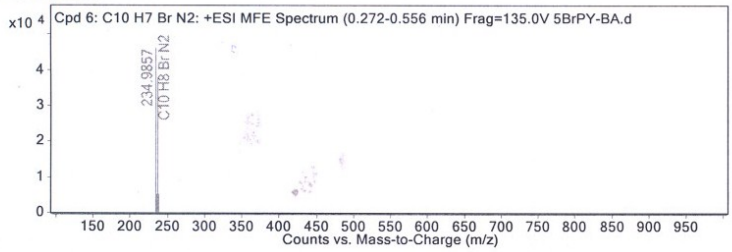
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C10 H7 Br N2	0.364	233.9785	C10 H7 Br N2	C10 H7 Br N2	3.34	C10 H7 Br N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C10 H7 Br N2	234.9857	0.364	Find by Molecular Feature	233.9785

MFE MS Spectrum



MS Spectrum Peak List

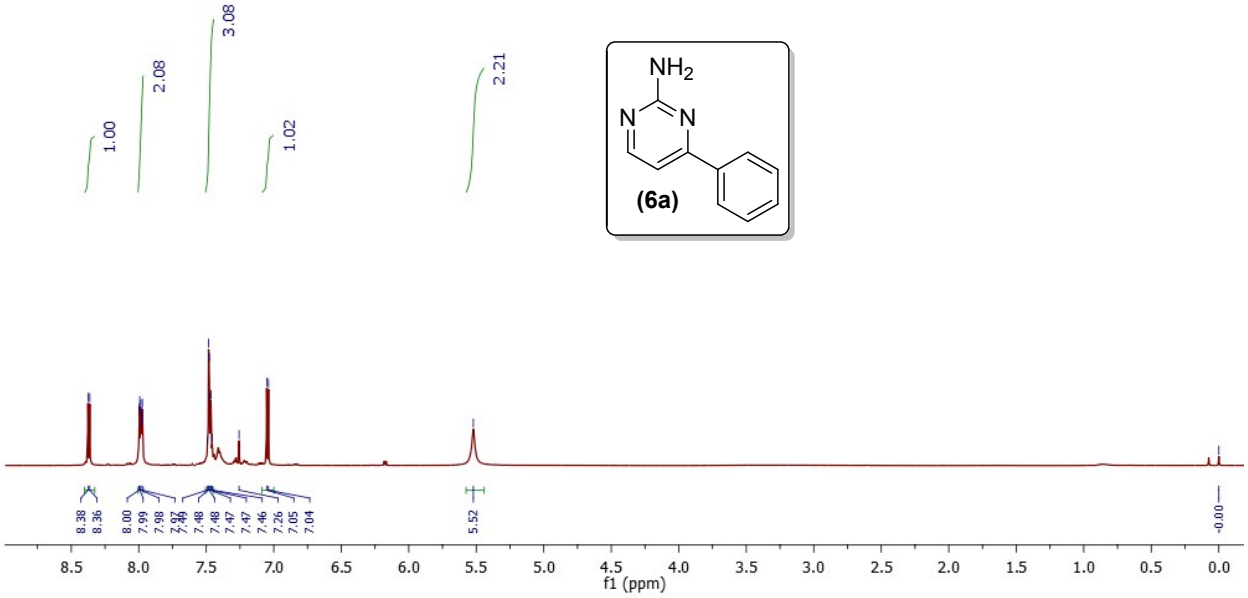
m/z	z	Abund	Formula	Ion
234.9857	1	46115.86	C10 H8 Br N2	(M+H)+
235.9889	1	5305.34	C10 H8 Br N2	(M+H)+
236.9838	1	37620.57	C10 H8 Br N2	(M+H)+
237.9874	1	5165.84	C10 H8 Br N2	(M+H)+
238.9812	1	311.66	C10 H8 Br N2	(M+H)+

Predicted Isotope Match Table

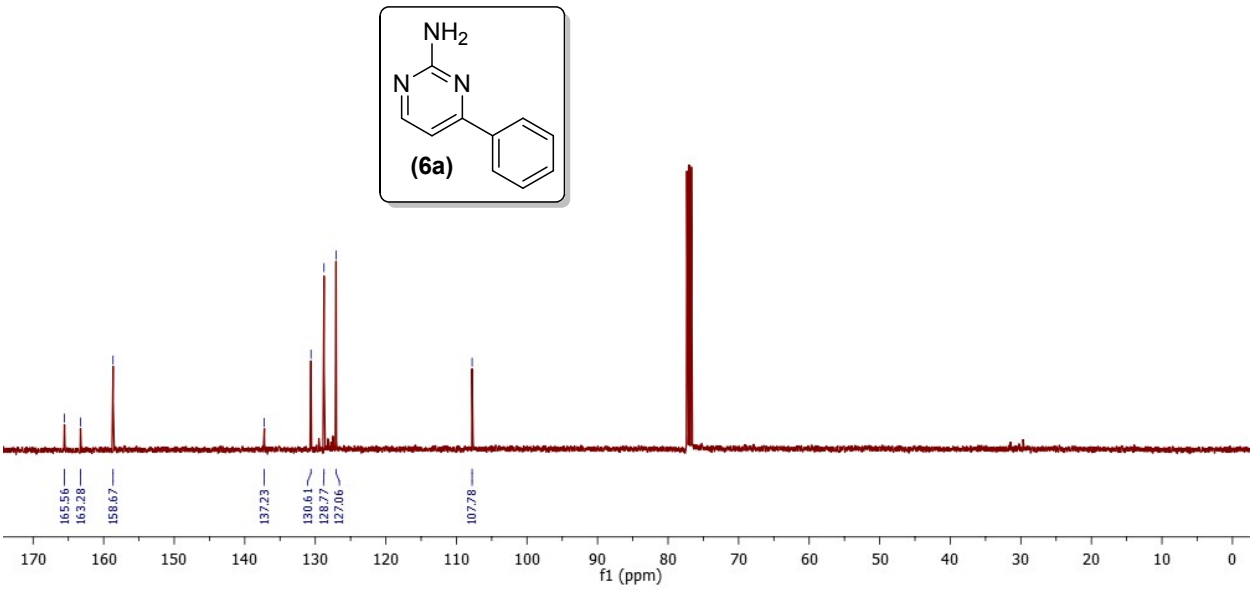
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	234.9857	234.9865	3.61	100	100	48.79	45.15
2	235.9889	235.9895	2.69	11.5	11.64	5.61	5.25
3	236.9838	236.9845	3.12	81.58	97.9	39.8	44.2
4	237.9874	237.9875	0.52	11.2	11.34	5.47	5.12
5	238.9812	238.9904	38.46	0.68	0.6	0.33	0.27

--- End Of Report ---

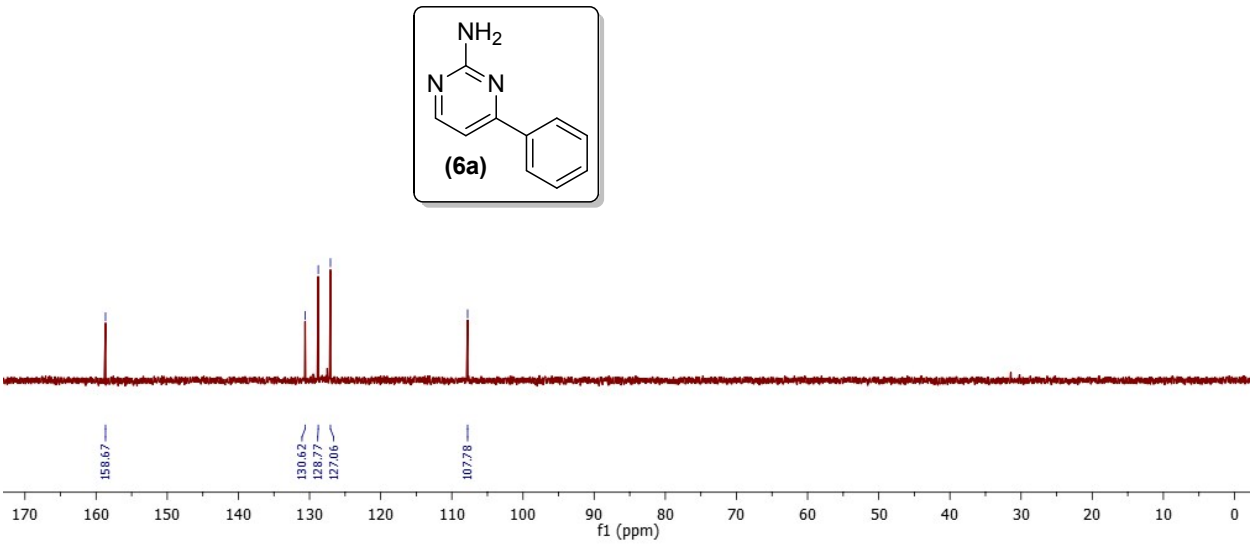
^{1}H NMR of 4-Phenylpyrimidin-2-amine (6a)



^{13}C NMR of 4-Phenylpyrimidin-2-amine (6a)



DEPT NMR of 4-Phenylpyrimidin-2-amine (6a)

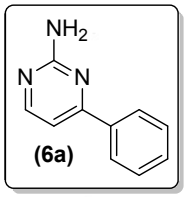


HRMS of 4-Phenylpyrimidin-2-amine (6a)

Qualitative Compound Report

Data File	2APY-BA.d	**Sample Name**	2APY-BA
Sample Type	Sample	**Position**	Vial 12
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	10-06-2015 PM 2:34:44
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

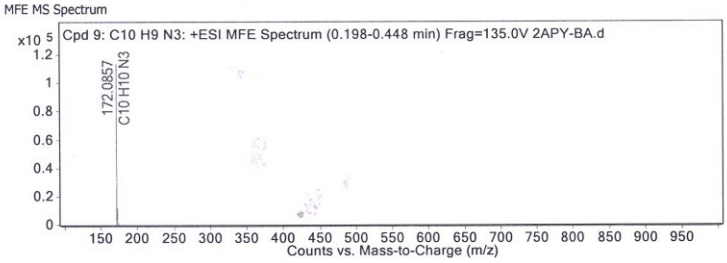


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C10 H9 N3	0.273	171.0785	C10 H9 N3	C10 H9 N3	6.77	C10 H9 N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C10 H9 N3	172.0857	0.273	Find by Molecular Feature	171.0785

MFE MS Spectrum



MS Spectrum Peak List

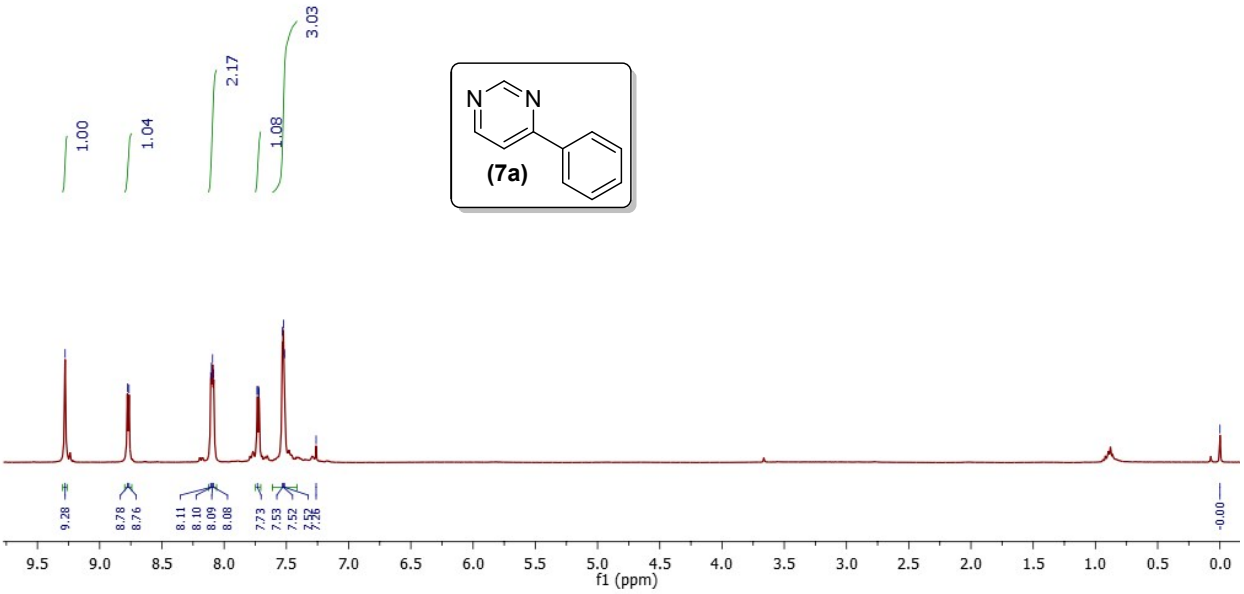
m/z	z	Abund	Formula	Ion
172.0857	1	113634.98	C10 H10 N3	(M+H)+
173.0887	1	12065.85	C10 H10 N3	(M+H)+
174.0929	1	1004.12	C10 H10 N3	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	172.0857	172.0869	6.88	100	100	89.68	88.74
2	173.0887	173.0897	6.01	10.62	12.03	9.52	10.67
3	174.0929	174.0925	-2.47	0.88	0.66	0.79	0.59

--- End Of Report ---

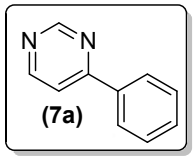
^{1}H NMR of 4-Phenylpyrimidine (7a) [1]



HRMS of 4-Phenylpyrimidine (7a)

Qualitative Compound Report

Data File	PY-BA.d	**Sample Name**	PY-BA
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	10-06-2015 PM 3:00:42
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



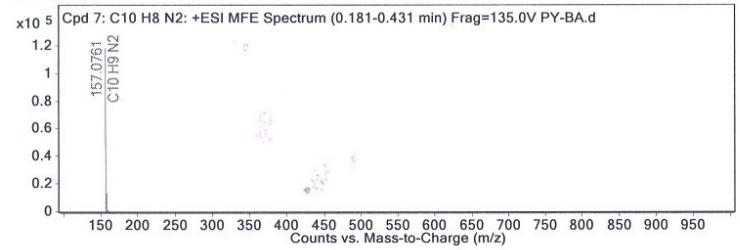
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C10 H8 N2	0.266	156.0689	C10 H8 N2	C10 H8 N2	-0.79	C10 H8 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C10 H8 N2	157.0761	0.266	Find by Molecular Feature	156.0689

MFE MS Spectrum



MS Spectrum Peak List

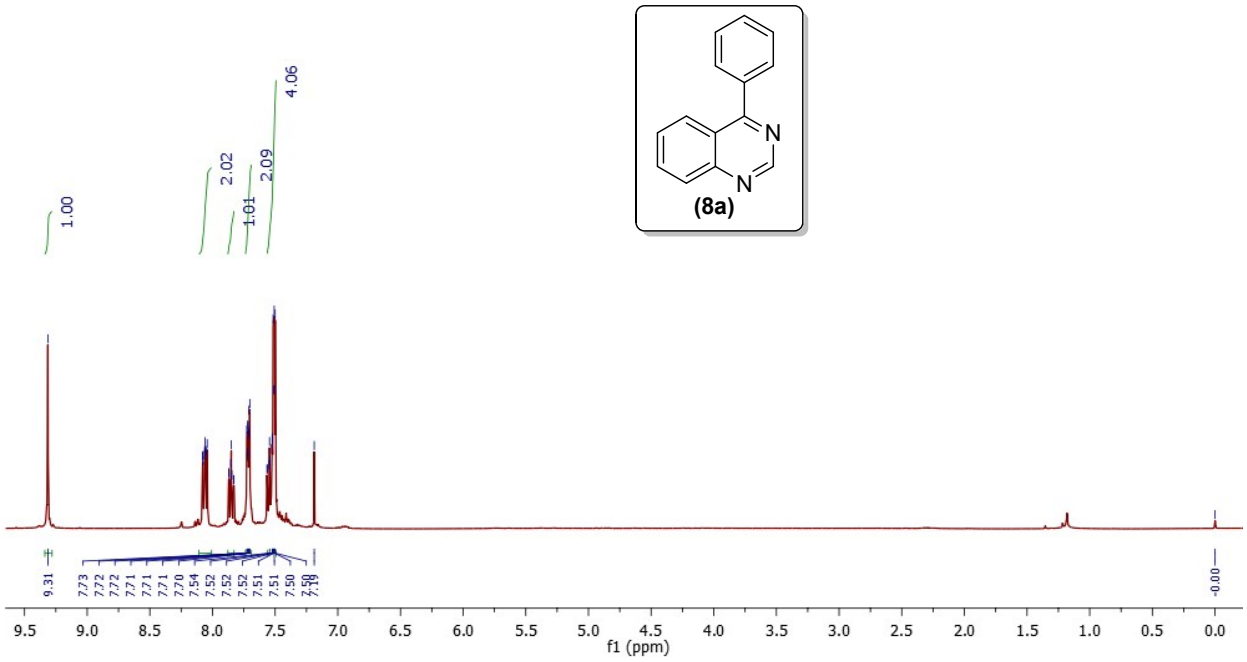
m/z	z	Abund	Formula	Ion
157.0761	1	118539.23	C10 H9 N2	(M+H)+
158.0791	1	13674.22	C10 H9 N2	(M+H)+
159.083	1	1631.47	C10 H9 N2	(M+H)+

Predicted Isotope Match Table

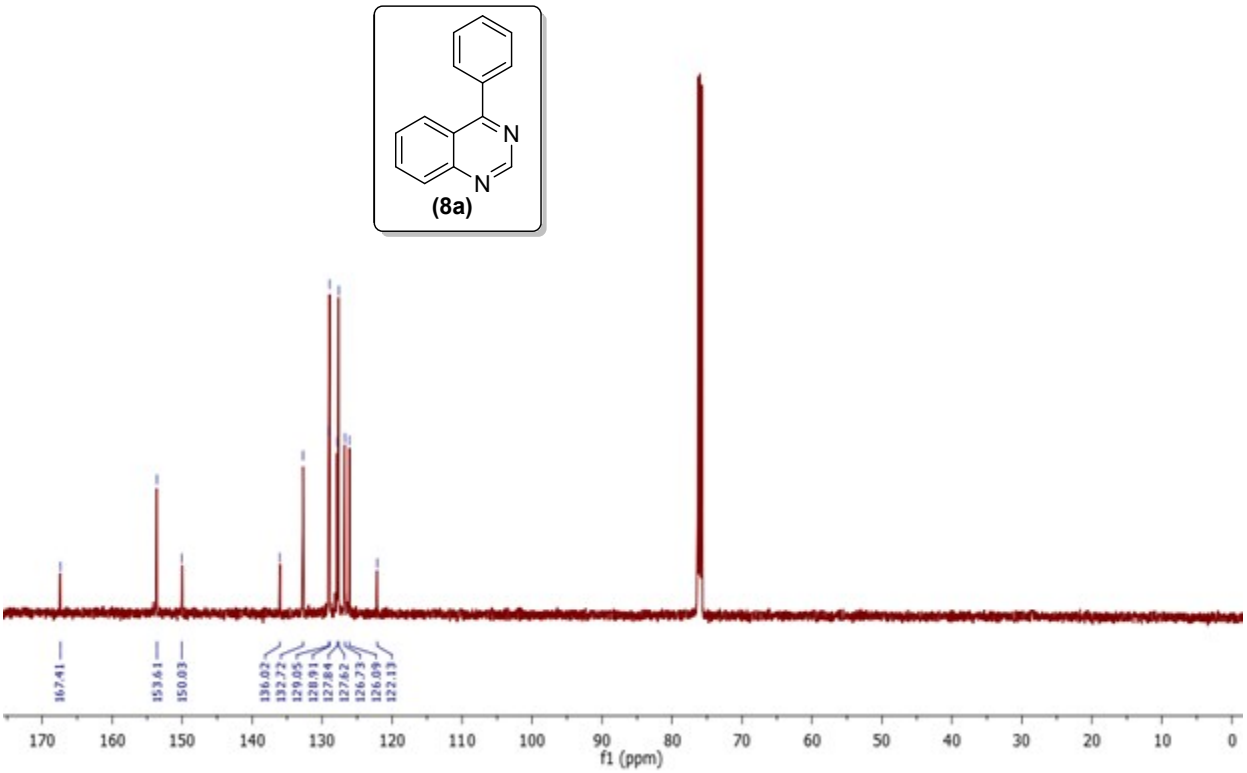
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	157.0761	157.076	-0.71	100	100	88.56	89.07
2	158.0791	158.079	-0.7	11.54	11.65	10.22	10.38
3	159.083	159.0819	-6.7	1.38	0.62	1.22	0.55

--- End Of Report ---

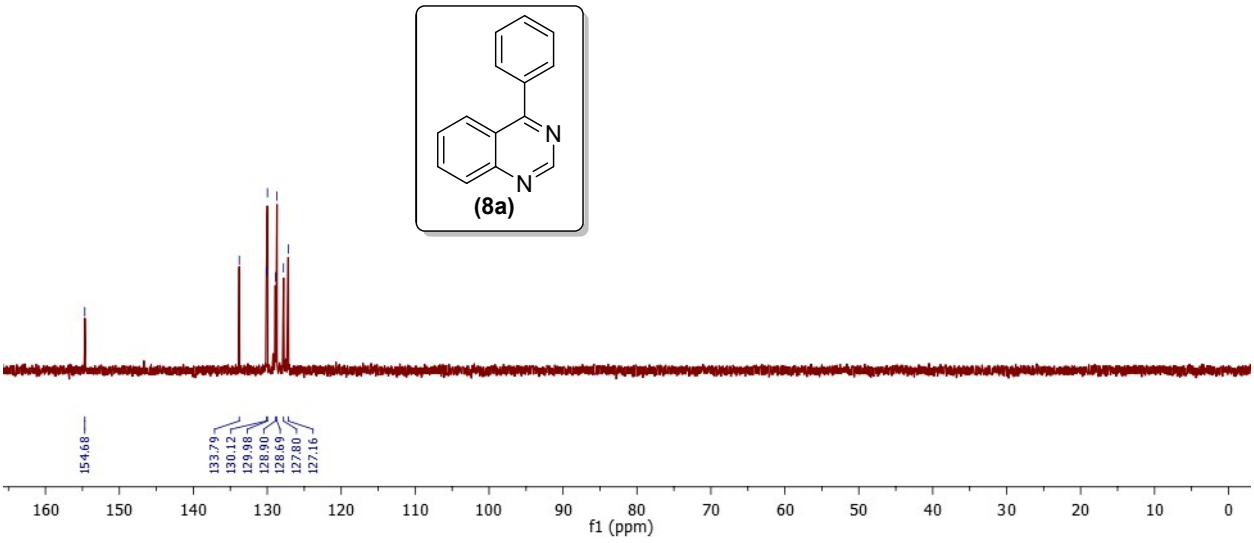
^{1}H NMR of 4-Phenylquinazoline (8a)



^{13}C NMR of 4-Phenylquinazoline (8a)



DEPT NMR of 4-Phenylquinazoline (8a)

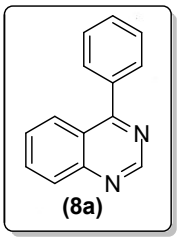


HRMS of 4-Phenylquinazoline (8a)

Qualitative Compound Report

Data File	BPY-BA.d	**Sample Name**	BPY-BA
Sample Type	Sample	**Position**	Vial 15
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	11-05-2015 PM 2:23:46
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

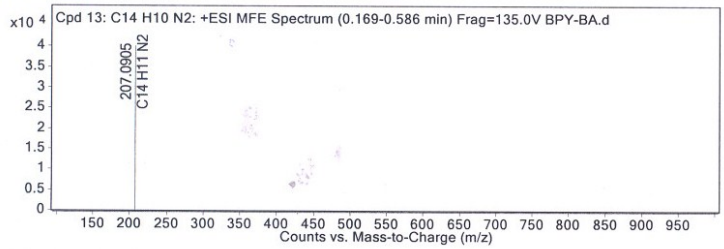


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C14 H10 N2	0.362	206.0833	C14 H10 N2	C14 H10 N2	5.3	C14 H10 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C14 H10 N2	207.0905	0.362	Find by Molecular Feature	206.0833

MFE MS Spectrum



MS Spectrum Peak List

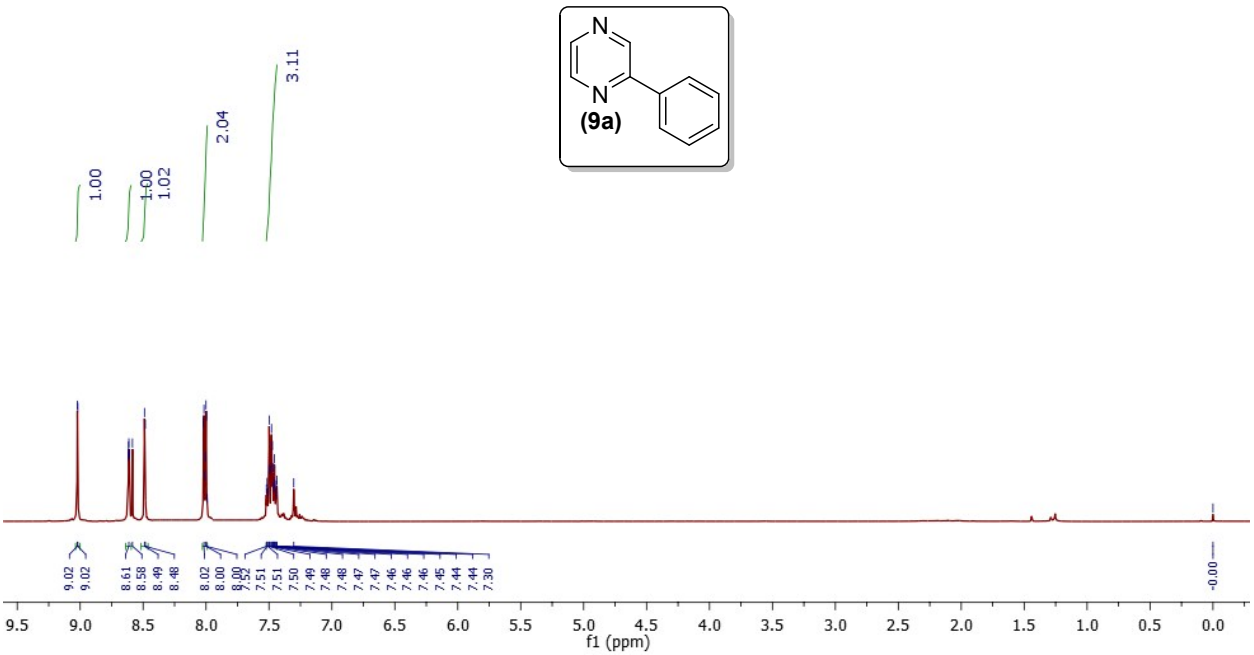
m/z	z	Abund	Formula	Ion
207.0905	1	40014.82	C14 H11 N2	(M+H)+
208.0945	1	6202.19	C14 H11 N2	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	207.0905	207.0917	5.87	100	100	86.58	86.21
2	208.0945	208.0948	1.47	15.5	16	13.42	13.79

--- End Of Report ---

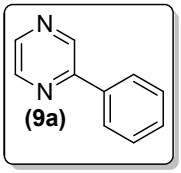
^{1}H NMR of 2-Phenylpyrazine (9a) [3]



HRMS of 2-Phenylpyrazine (9a)

Qualitative Compound Report

Data File	PYZ-BA.d	**Sample Name**	PYZ-BA
Sample Type	Sample	**Position**	Vial 27
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	08-06-2015 PM 3:32:06
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



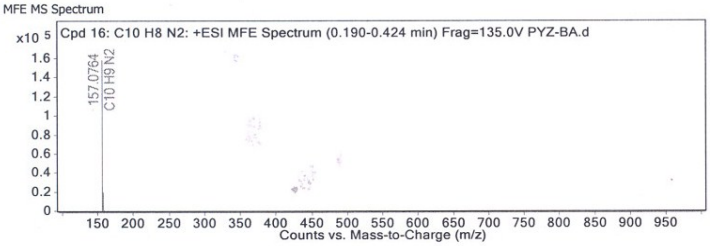
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C10 H8 N2	0.269	156.0691	C10 H8 N2	C10 H8 N2	-2.39	C10 H8 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C10 H8 N2	157.0764	0.269	Find by Molecular Feature	156.0691

MFE MS Spectrum



MS Spectrum Peak List

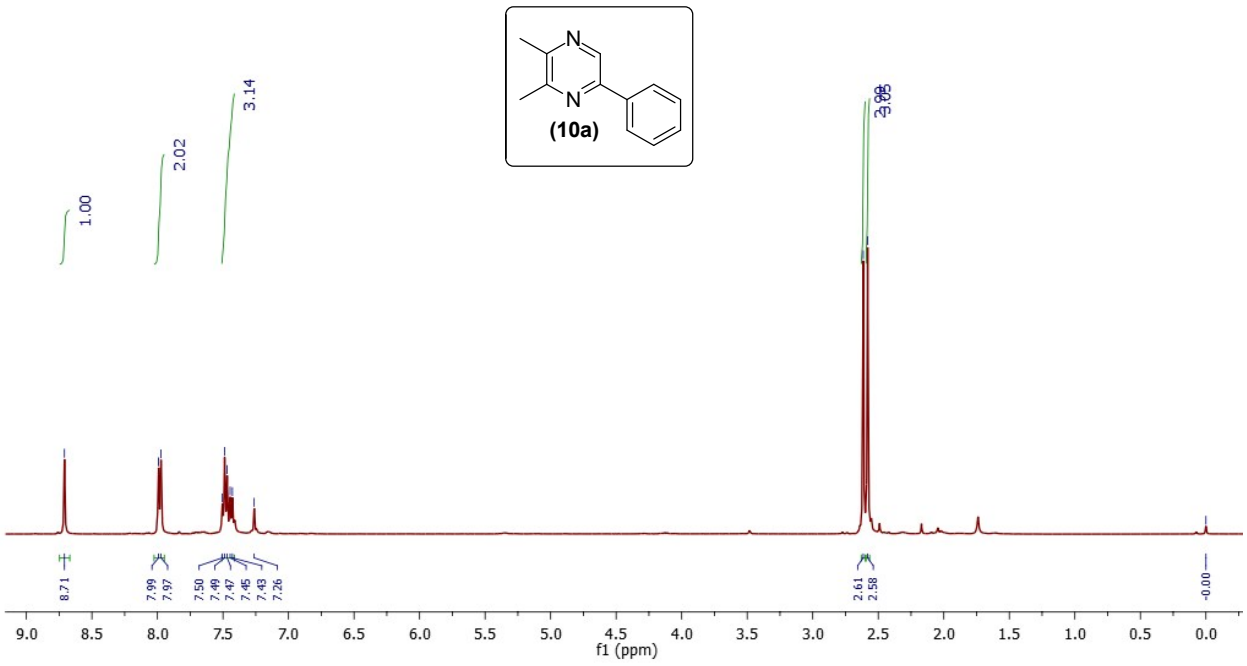
m/z	z	Abund	Formula	Ion
157.0764	1	158245.72	C10 H9 N2	(M+H)+
158.0795	1	19684.8	C10 H9 N2	(M+H)+
159.0823	1	1159.64	C10 H9 N2	(M+H)+

Predicted Isotope Match Table

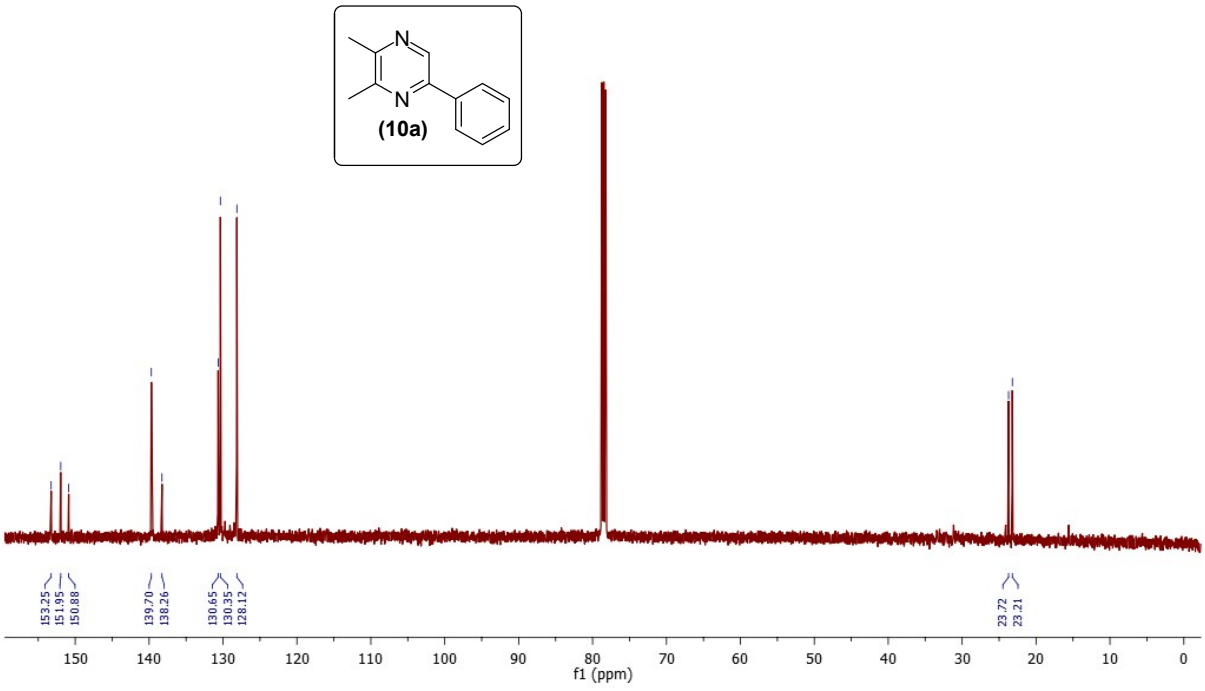
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	157.0764	157.076	-2.29	100	100	88.36	89.07
2	158.0795	158.079	-3.03	12.44	11.65	10.99	10.38
3	159.0823	159.0819	-2.39	0.73	0.62	0.65	0.55

--- End Of Report ---

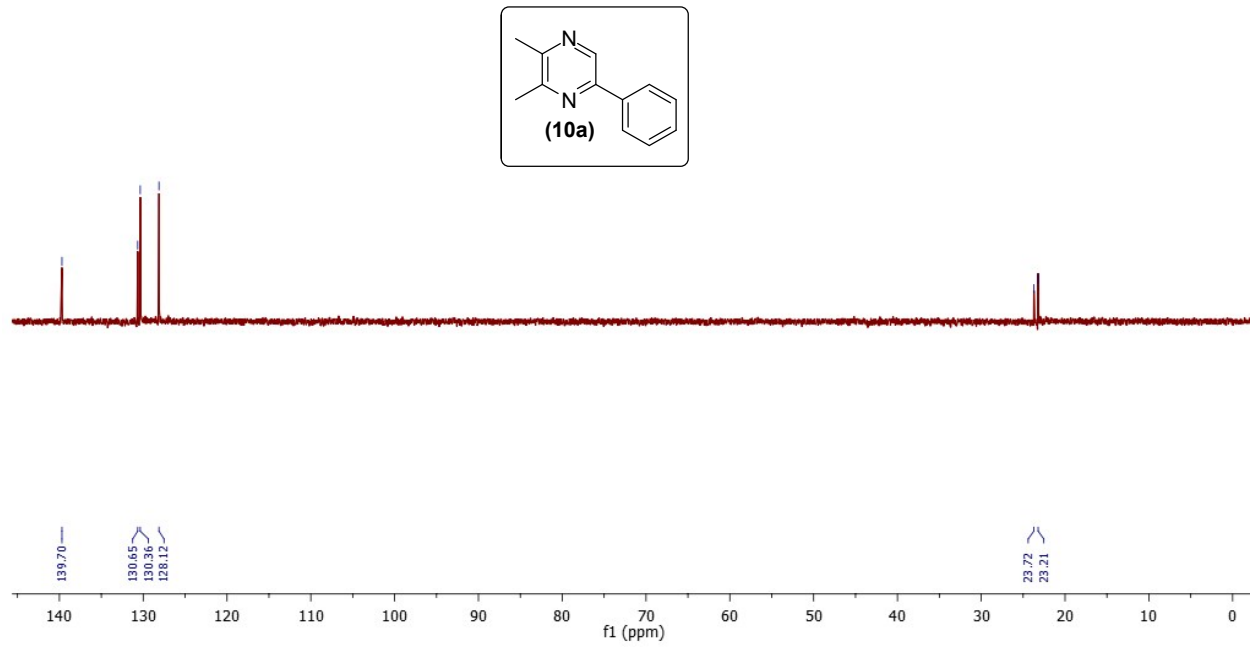
^{1}H NMR of 2,3-Dimethyl-5-phenylpyrazine (10a)



^{13}C NMR of 2,3-Dimethyl-5-phenylpyrazine (10a)



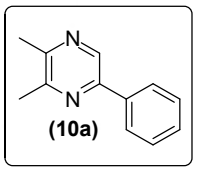
DEPT NMR of 2,3-Dimethyl-5-phenylpyrazine (10a)



HRMS of 2,3-Dimethyl-5-phenylpyrazine (10a)

Qualitative Compound Report

Data File	2,3DIMEPY.d	**Sample Name**	2,3DIMEPY
Sample Type	Sample	**Position**	Vial 11
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	30-10-2015 PM 1:53:14
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

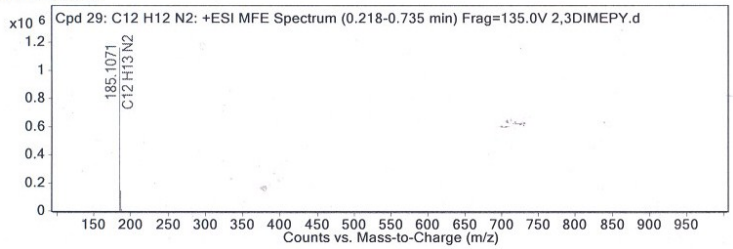


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C12 H12 N2	0.35	184.0999	C12 H12 N2	C12 H12 N2	0.79	C12 H12 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 29: C12 H12 N2	185.1071	0.35	Find by Molecular Feature	184.0999

MFE MS Spectrum



MS Spectrum Peak List

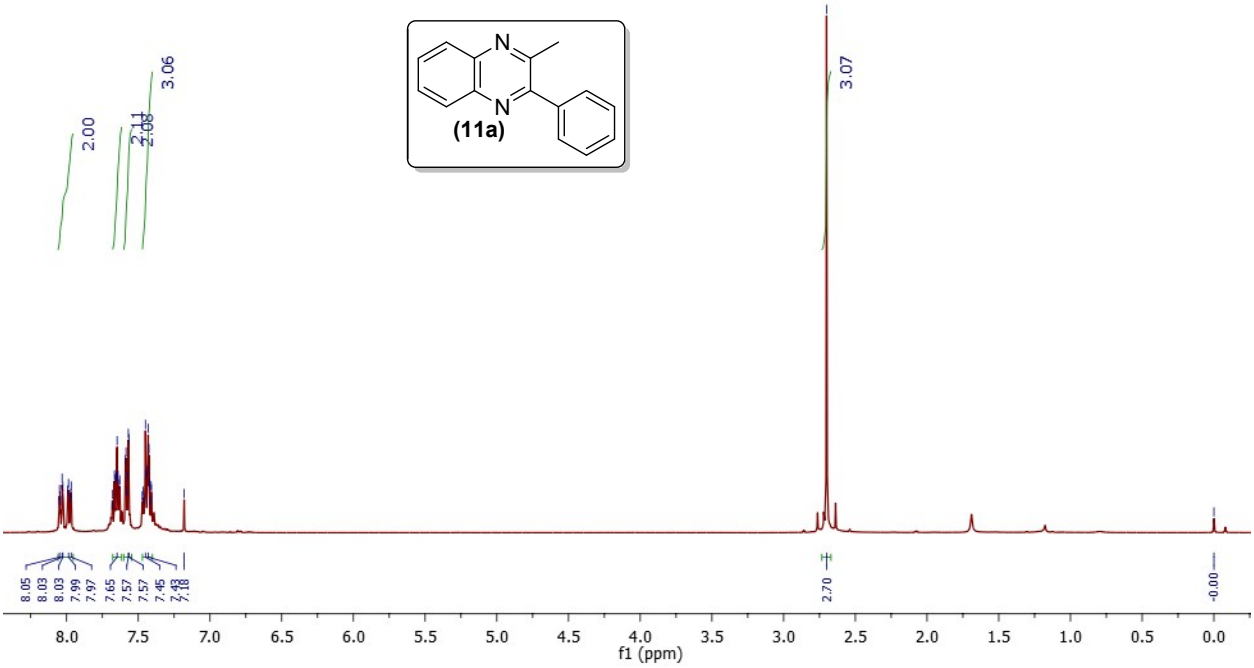
m/z	z	Abund	Formula	Ion
185.1071	1	1160536.5	C12 H13 N2	(M+H)+
186.1106	1	147295.13	C12 H13 N2	(M+H)+
187.1138	1	10663.52	C12 H13 N2	(M+H)+
188.1143	1	630.69	C12 H13 N2	(M+H)+

Predicted Isotope Match Table

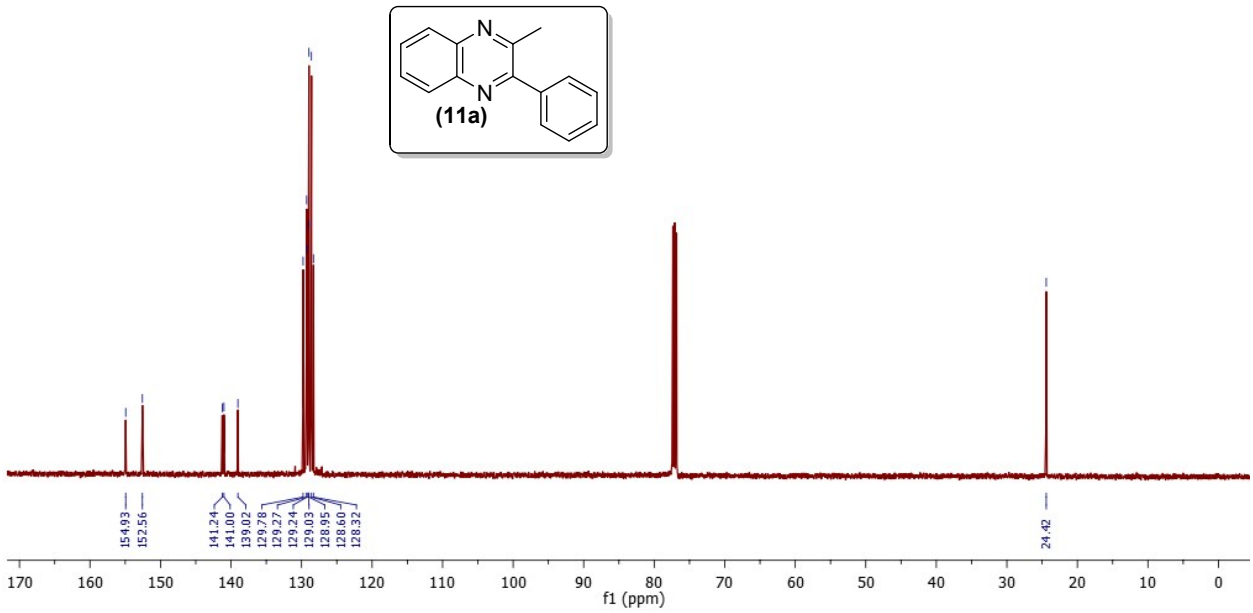
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	185.1071	185.1073	1.06	100	100	87.98	87.12
2	186.1106	186.1104	-1.19	12.69	13.86	11.17	12.07
3	187.1138	187.1134	-2.21	0.92	0.89	0.81	0.77
4	188.1143	188.1164	11.02	0.05	0.03	0.05	0.03

--- End Of Report ---

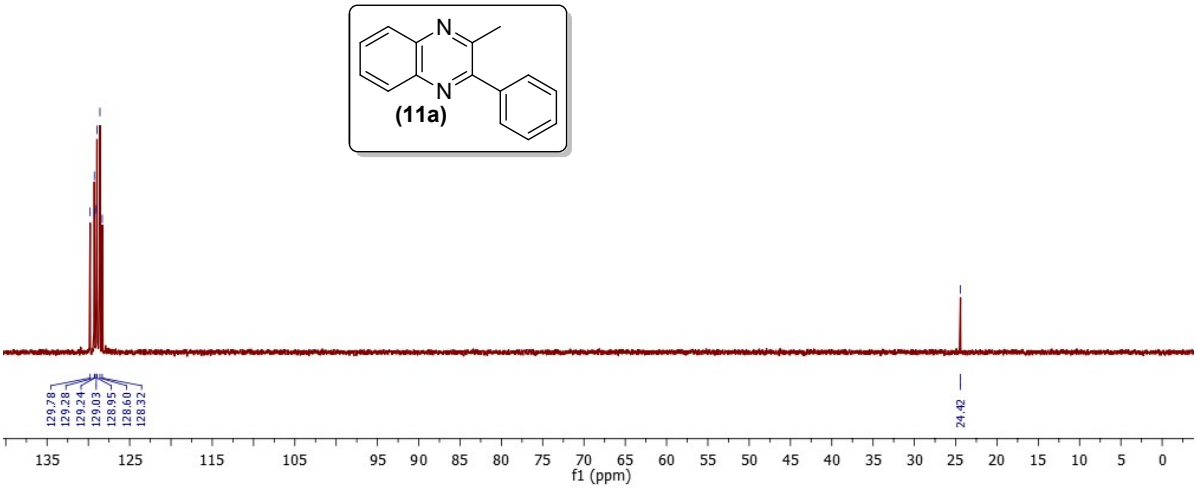
^{1}H NMR of 2-Methyl-3-phenylquinoxaline (11a)



^{13}C NMR of 2-Methyl-3-phenylquinoxaline (11a)



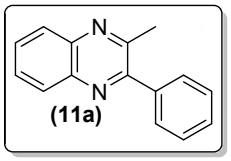
DEPT NMR of 2-Methyl-3-phenylquinoxaline (11a)



HRMS of 2-Methyl-3-phenylquinoxaline (11a)

Qualitative Compound Report

Data File	2MEQX-BA.d	**Sample Name**	2MEQX-BA
Sample Type	Sample	**Position**	Vial 26
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	08-06-2015 PM 3:27:47
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



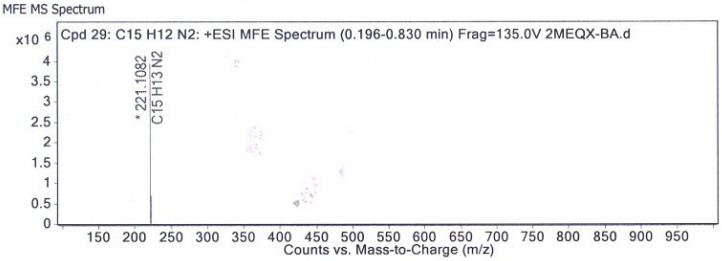
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 29: C15 H12 N2	0.266	220.1013	C15 H12 N2	C15 H12 N2	-5.69	C15 H12 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 29: C15 H12 N2	221.1082	0.266	Find by Molecular Feature	220.1013

MFE MS Spectrum



MS Spectrum Peak List

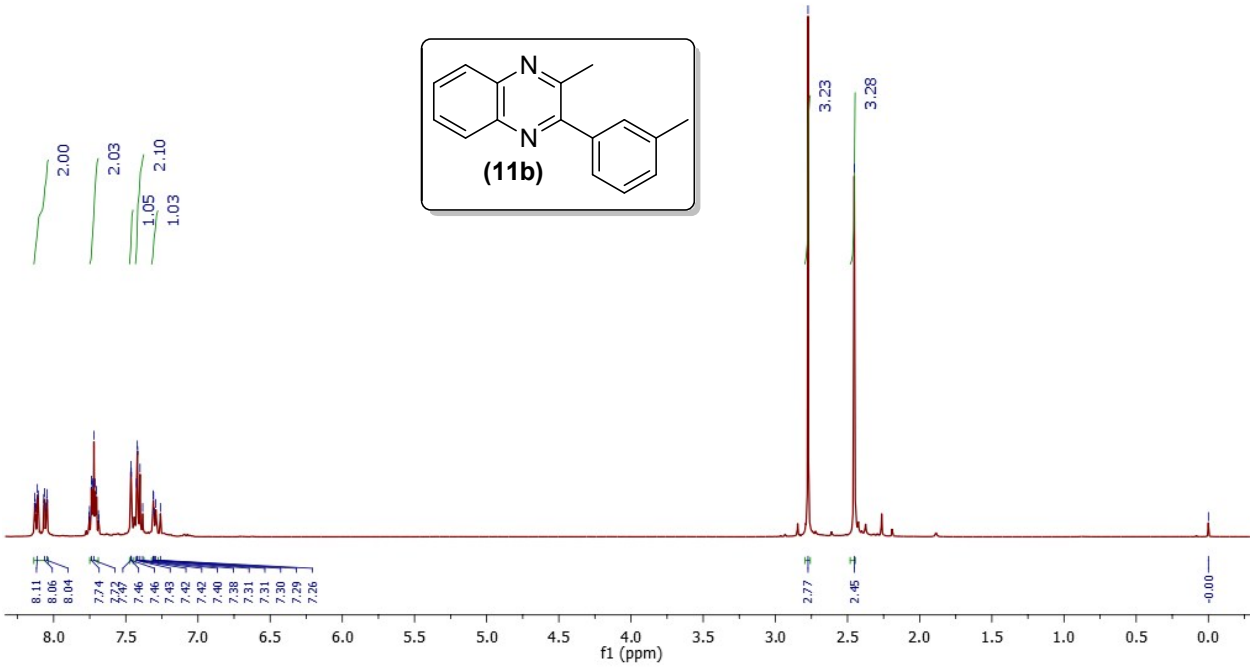
m/z	z	Abund	Formula	Ion
221.1082	1	3943351.25	C15 H13 N2	(M+H)+
222.1138	1	700514.56	C15 H13 N2	(M+H)+
223.1176	1	51740.73	C15 H13 N2	(M+H)+
224.1216	1	1943.22	C15 H13 N2	(M+H)+

Predicted Isotope Match Table

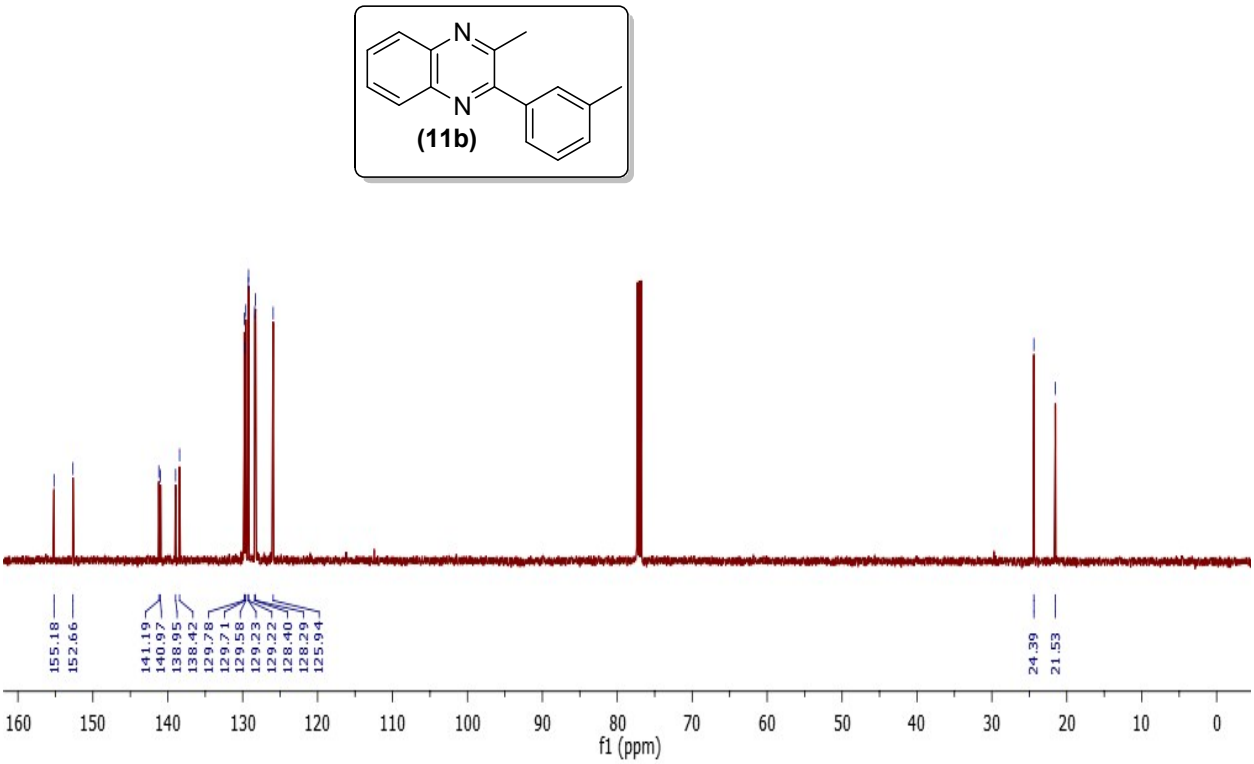
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	221.1082	221.1073	-3.8	100	100	83.94	84.36
2	222.1138	222.1104	-15.12	17.76	17.1	14.91	14.43
3	223.1176	223.1135	-18.07	1.31	1.37	1.1	1.16
4	224.1216	224.1166	-22.45	0.05	0.07	0.04	0.06

--- End Of Report ---

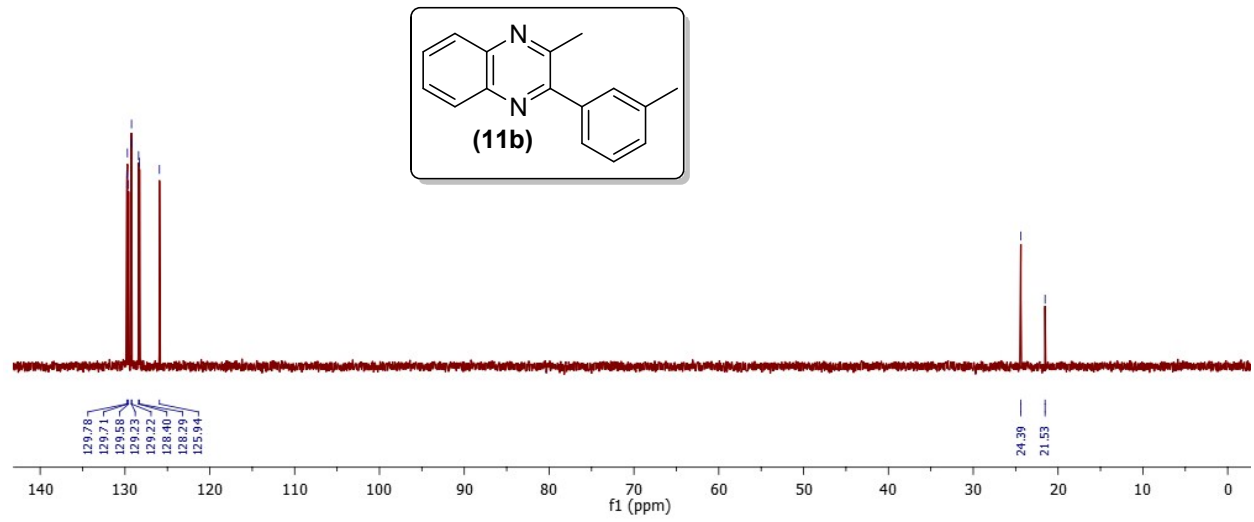
^{1}H NMR of 2-Methyl-3-(*m*-tolyl)quinoxaline (11b)



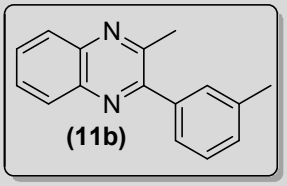
^{13}C NMR of 2-methyl-3-(*m*-tolyl)quinoxaline (11b)



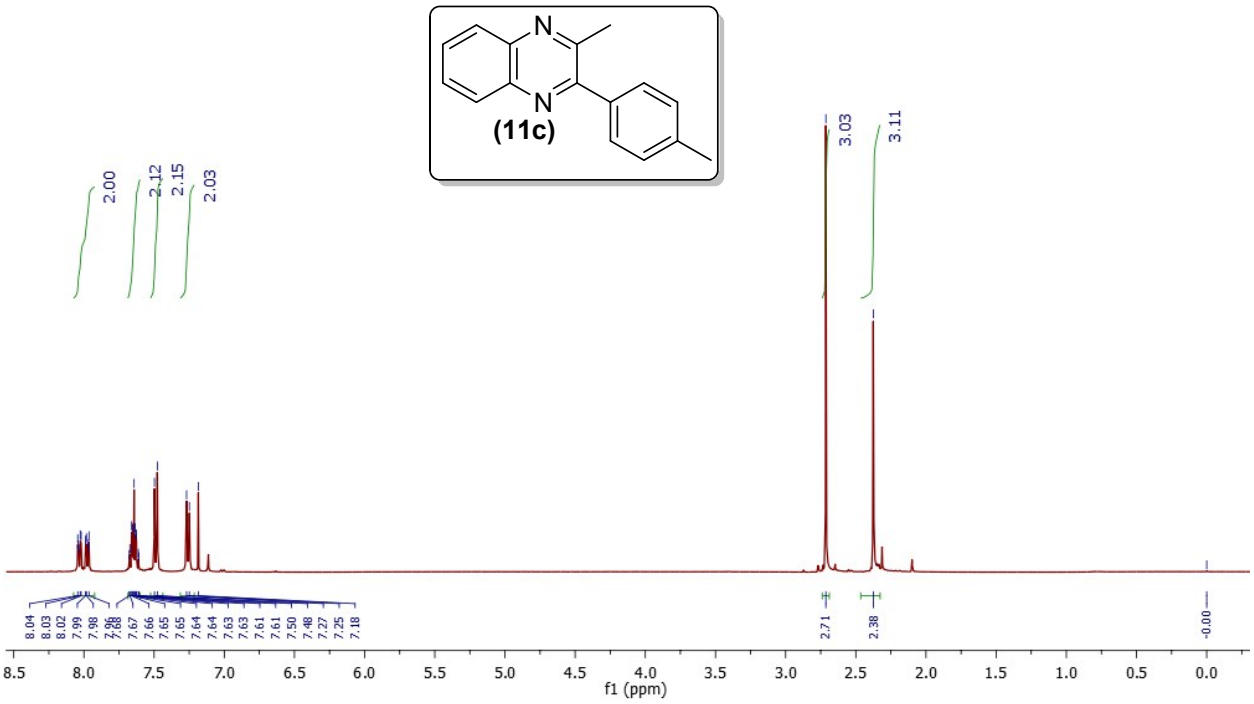
DEPT NMR of 2-methyl-3-(*m*-tolyl)quinoxaline (11b)



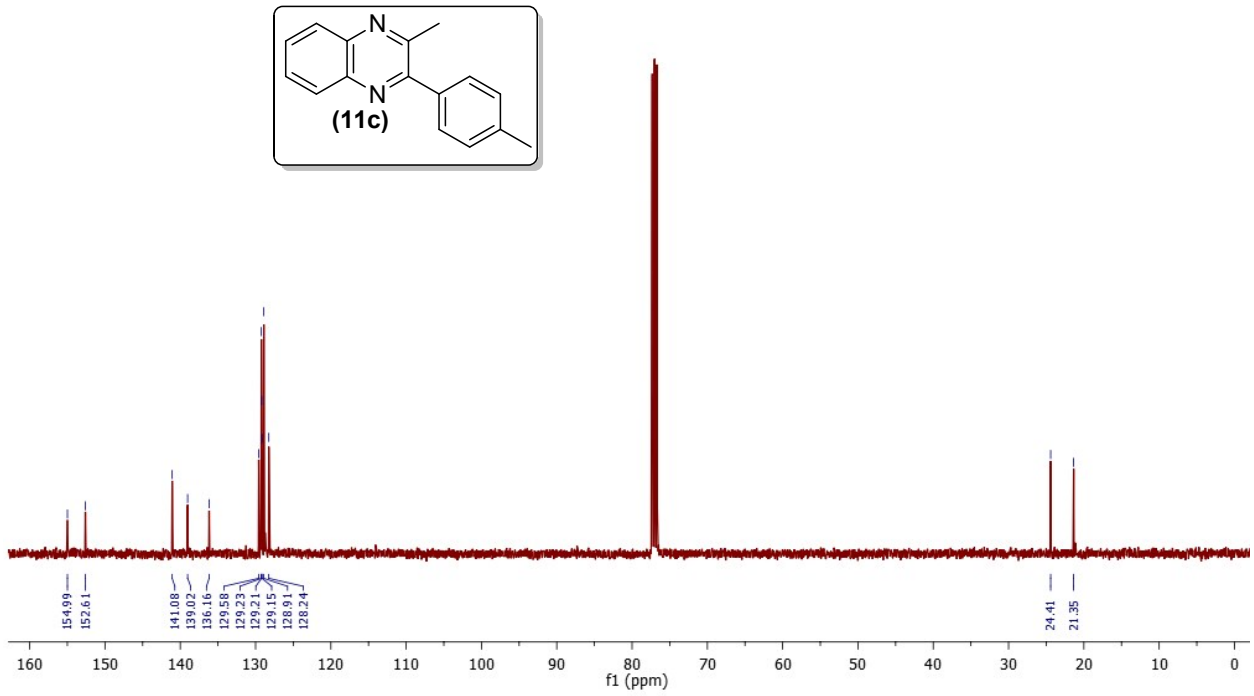
HRMS of 2-methyl-3-(*m*-tolyl)quinoxaline (11b)



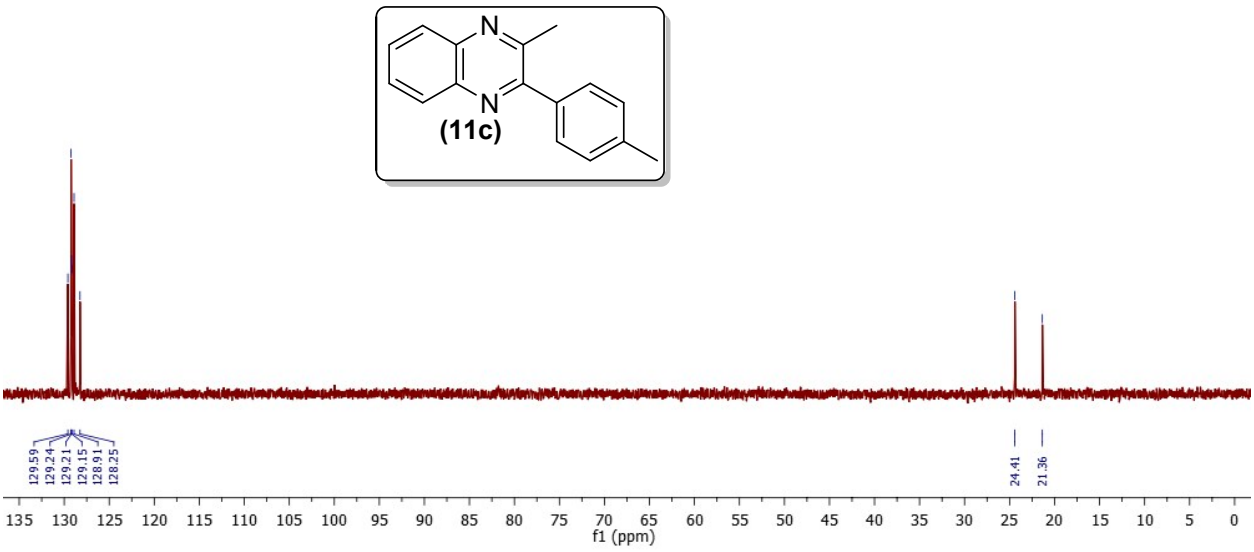
^{1}H NMR of 2-Methyl-3-(*p*-tolyl)quinoxaline (11c)



^{13}C NMR of 2-Methyl-3-(*p*-tolyl)quinoxaline (11c)



DEPT NMR of 2-Methyl-3-(*p*-tolyl)quinoxaline (11c)

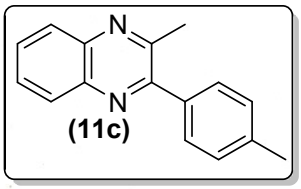


HRMS of 2-Methyl-3-(*p*-tolyl)quinoxaline (11c)

Qualitative Compound Report

Data File	2MCQX-4CH3.d	**Sample Name**	2MCQX-4CH3
Sample Type	Sample	**Position**	Vial 27
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	15-06-2015 PM 6:13:44
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

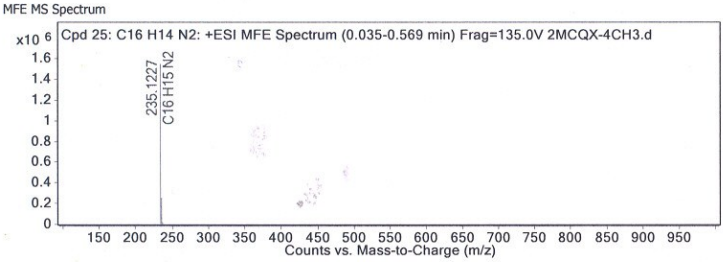


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 25: C16 H14 N2	0.268	234.1155	C16 H14 N2	C16 H14 N2	0.85	C16 H14 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 25: C16 H14 N2	235.1227	0.268	Find by Molecular Feature	234.1155

MFE MS Spectrum



MS Spectrum Peak List

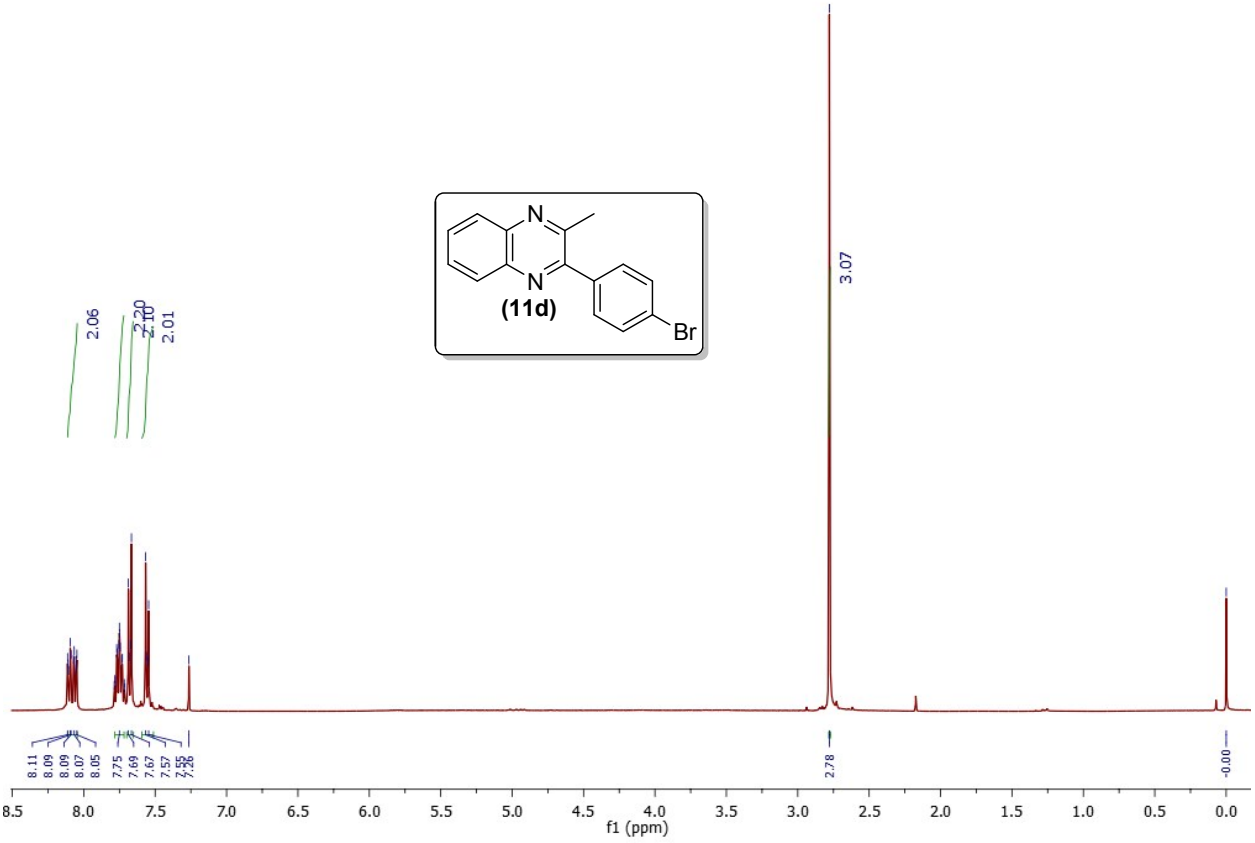
m/z	z	Abund	Formula	Ion
235.1227	1	1546248.38	C16 H15 N2	(M+H)+
236.1264	1	249880.92	C16 H15 N2	(M+H)+
237.1293	1	20919.47	C16 H15 N2	(M+H)+
238.1337	1	1352.89	C16 H15 N2	(M+H)+

Predicted Isotope Match Table

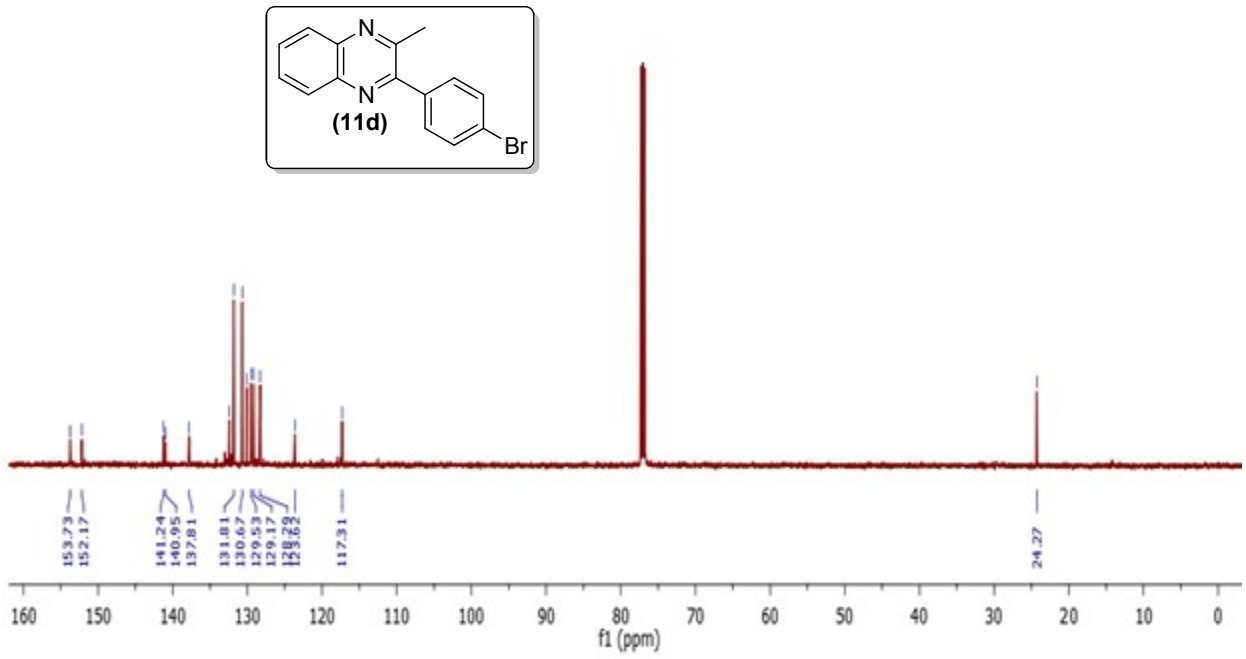
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	235.1227	235.123	1.22	100	100	85.03	83.43
2	236.1264	236.1261	-1.38	16.16	18.21	13.74	15.19
3	237.1293	237.1292	-0.24	1.35	1.56	1.15	1.3
4	238.1337	238.1323	-5.9	0.09	0.08	0.07	0.07

--- End Of Report ---

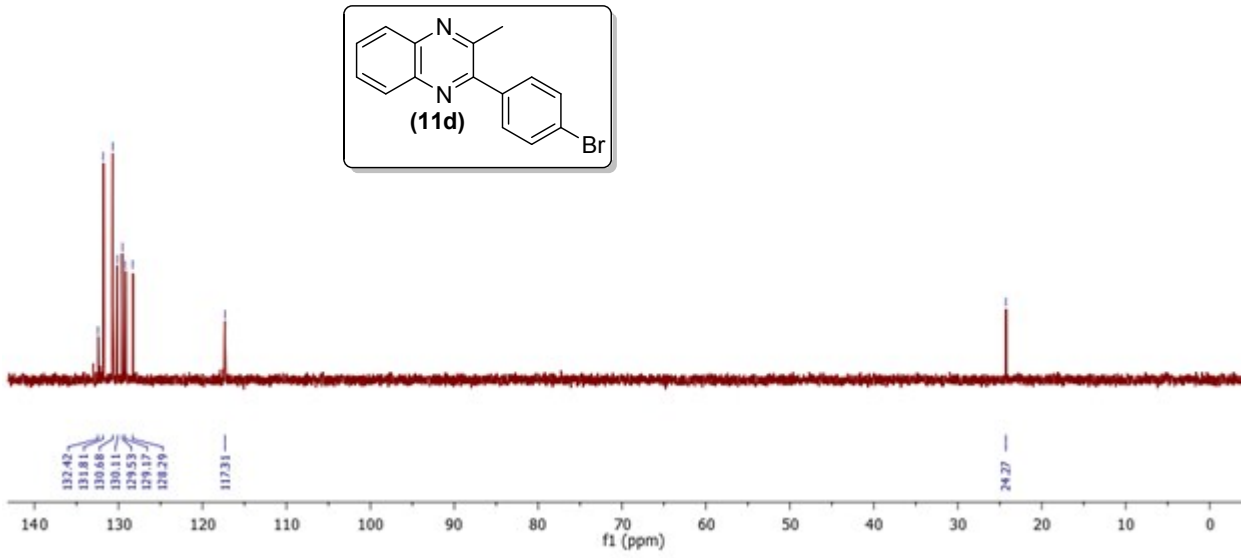
^{1}H NMR of 2-(4-Bromophenyl)-3-methylquinoxaline (11d):



^{13}C NMR of 2-(4-Bromophenyl)-3-methylquinoxaline (11d)



DEPT NMR of 2-(4-Bromophenyl)-3-methylquinoxaline (11d)

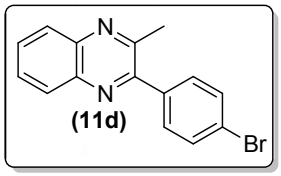


HRMS of 2-(4-Bromophenyl)-3-methylquinoxaline (11d)

Qualitative Compound Report

Data File	3MCQX-4Br.d	**Sample Name**	3MCQX-4Br
Sample Type	Sample	**Position**	Vial 28
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	15-06-2015 PM 6:18:04
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

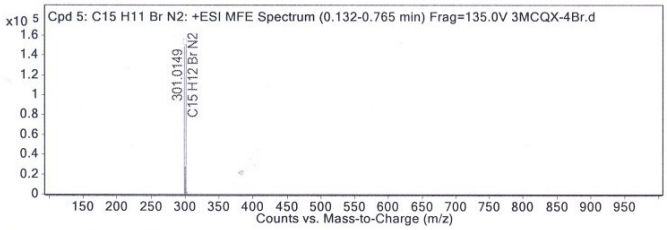


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C15 H11 Br N2	0.268	298.0095	C15 H11 Br N2	C15 H11 Br N2	3.53	C15 H11 Br N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C15 H11 Br N2	299.0168	0.268	Find by Molecular Feature	298.0095

MFE MS Spectrum



MS Spectrum Peak List

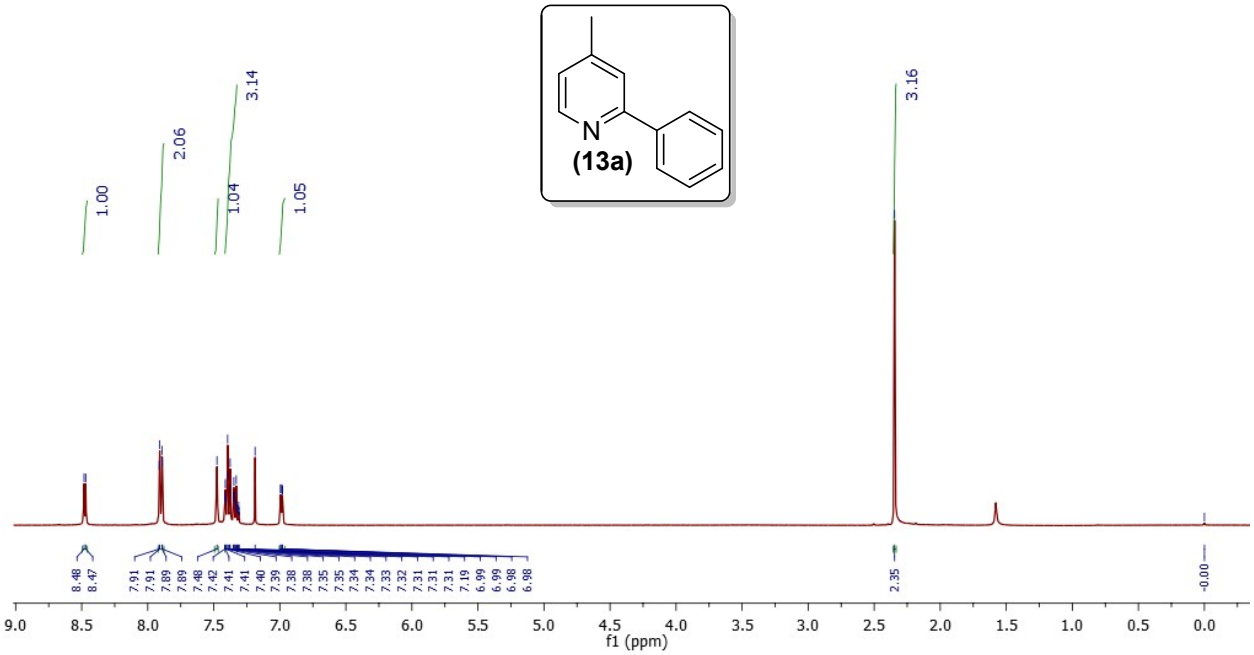
m/z	z	Abund	Formula	Ion
299.0168	1	148714.17	C15 H12 Br N2	(M+H)+
300.0197	1	27395.5	C15 H12 Br N2	(M+H)+
301.0149	1	151261.89	C15 H12 Br N2	(M+H)+
302.0179	1	25167.54	C15 H12 Br N2	(M+H)+
303.0212	1	2439.92	C15 H12 Br N2	(M+H)+
304.026	1	235.05	C15 H12 Br N2	(M+H)+

Predicted Isotope Match Table

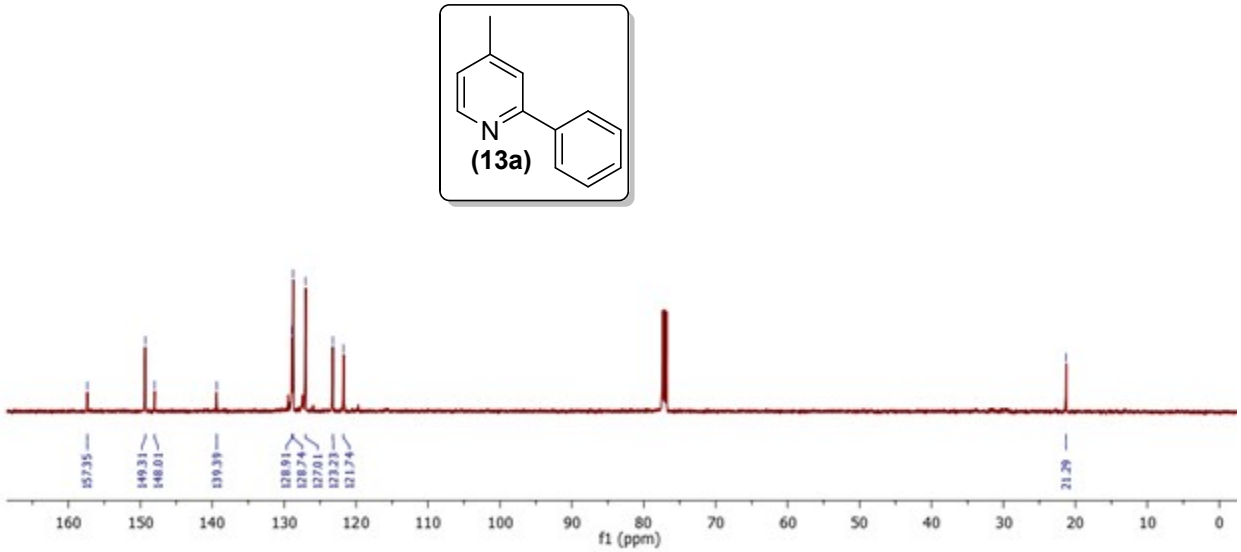
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	299.0168	299.0178	3.49	98.32	100	41.87	42.76
2	300.0197	300.0209	4.2	18.11	17.09	7.71	7.31
3	301.0149	301.0159	3.43	100	98.65	42.58	42.19
4	302.0179	302.0189	3.38	16.64	16.7	7.09	7.14
5	303.0212	303.022	2.76	1.61	1.34	0.69	0.57
6	304.026	304.0251	-3.02	0.16	0.07	0.07	0.03

--- End Of Report ---

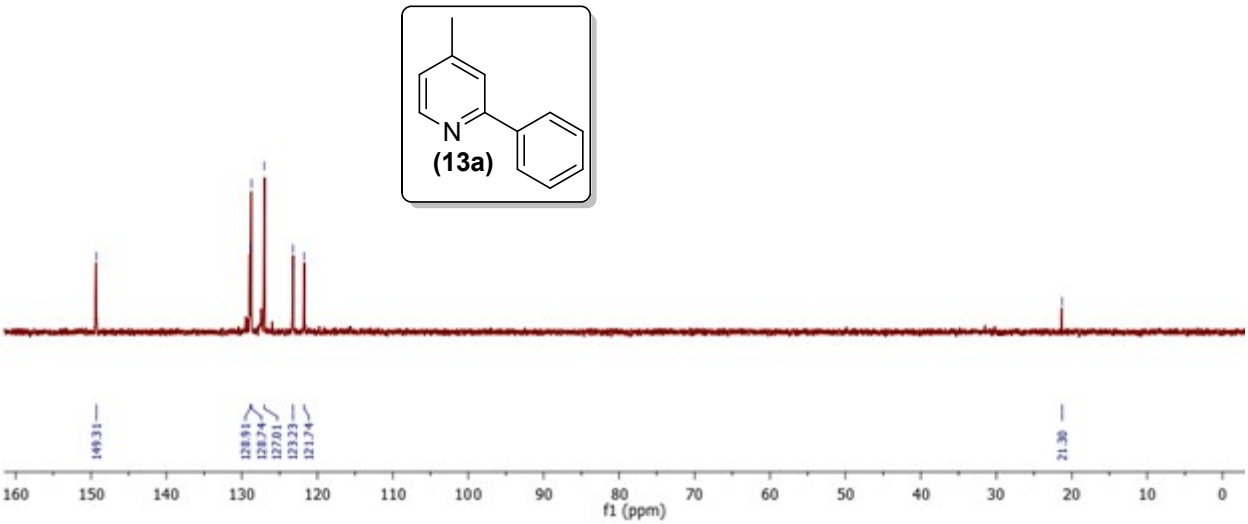
^{1}H NMR of 4-Methyl-2-phenylpyridine (13a)



^{13}C NMR of 4-Methyl-2-phenylpyridine (13a)



DEPT NMR of 4-Methyl-2-phenylpyridine (13a)

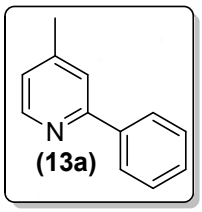


HRMS of 4-Methyl-2-phenylpyridine (13a)

Qualitative Compound Report

Data File	2Cl5Br-3CF3.d	**Sample Name**	2Cl5Br-3CF3
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	26-06-2015 PM 3:05:55
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

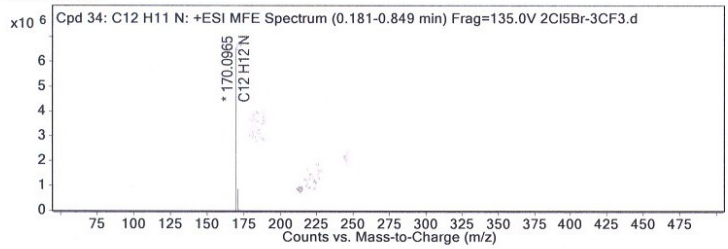


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 34: C12 H11 N	0.27	169.0893	C12 H11 N	C12 H11 N	-1.14	C12 H11 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 34: C12 H11 N	170.0965	0.27	Find by Molecular Feature	169.0893

MFE MS Spectrum



MS Spectrum Peak List

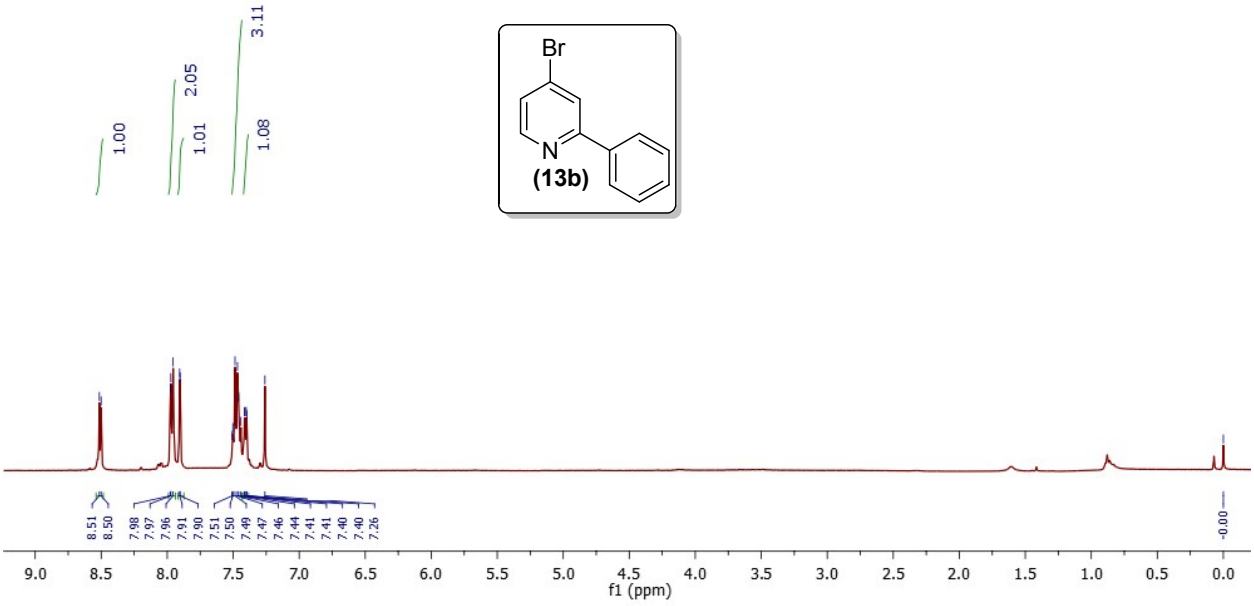
m/z	z	Abund	Formula	Ion
170.0965	1	6533840	C12 H12 N	(M+H)+
171.1009	1	861323.69	C12 H12 N	(M+H)+
172.1044	1	48148.21	C12 H12 N	(M+H)+
173.108	1	1036.15	C12 H12 N	(M+H)+

Predicted Isotope Match Table

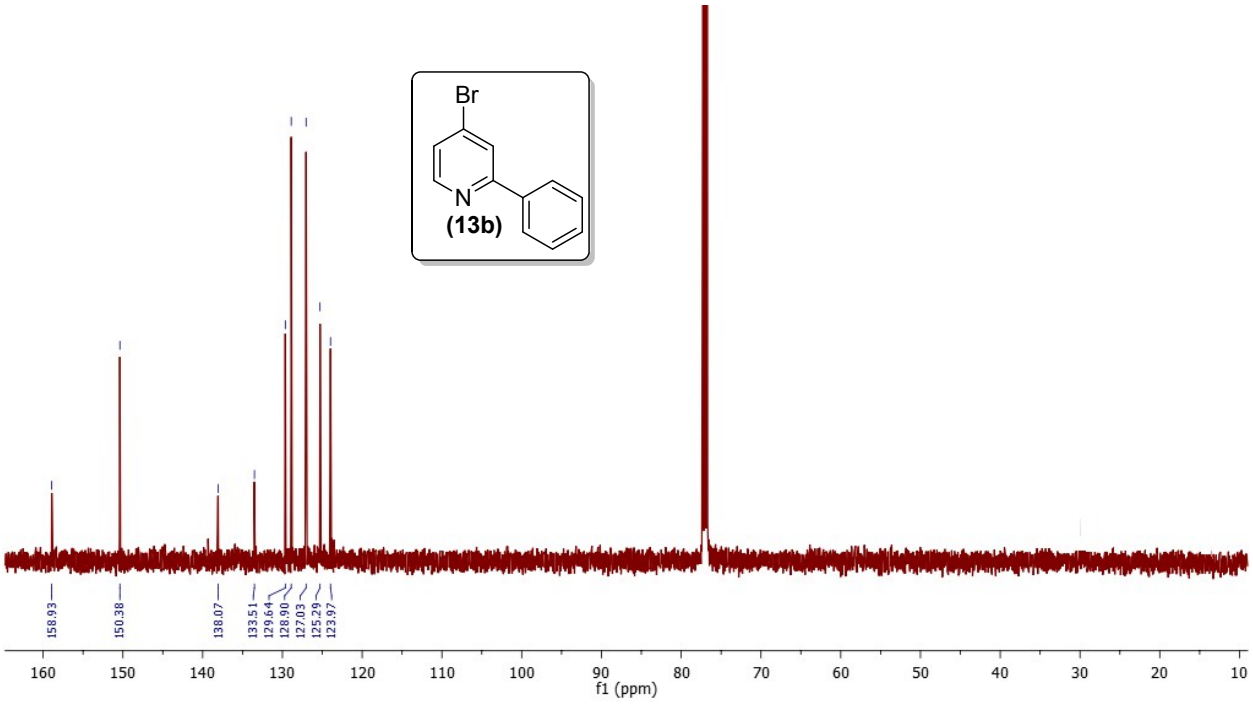
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	170.0965	170.0964	-0.22	100	100	87.77	87.45
2	171.1009	171.0996	-7.55	13.18	13.48	11.57	11.79
3	172.1044	172.1028	-9.02	0.74	0.84	0.65	0.73
4	173.108	173.106	-11.47	0.02	0.03	0.01	0.03

--- End Of Report ---

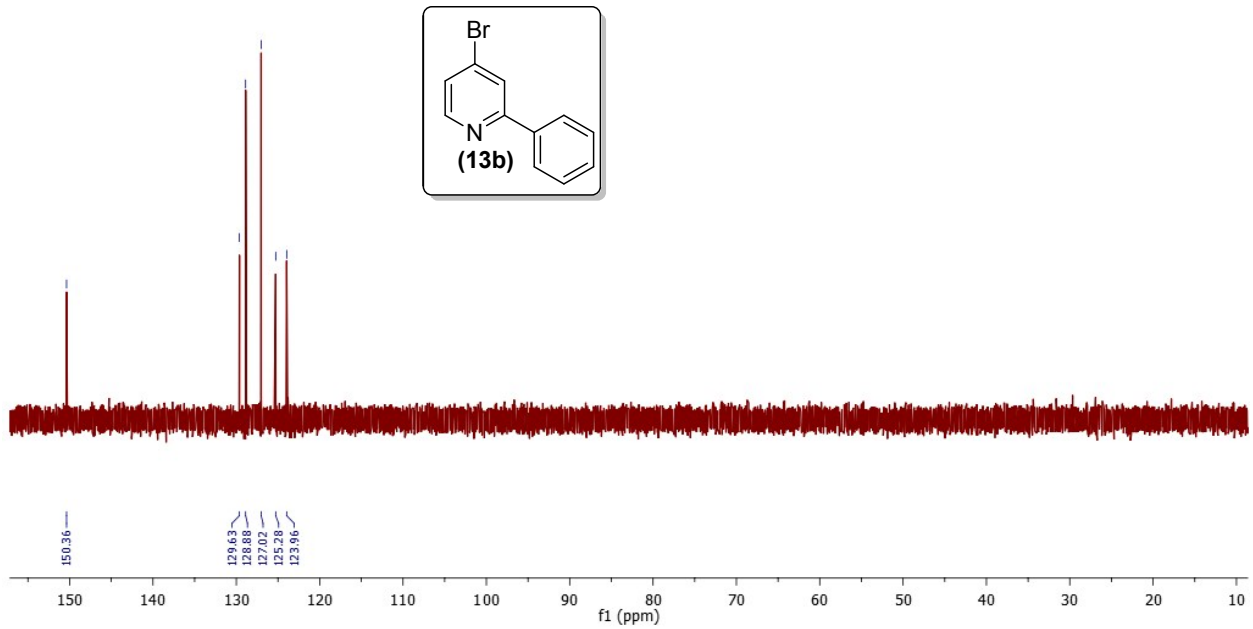
^{1}H NMR of 4-Bromo-2-phenylpyridine (13b)



^{13}C NMR 4-Bromo-2-phenylpyridine (13b)



DEPT NMR of 4-Bromo-2-phenylpyridine (13b)

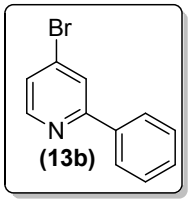


HRMS of 4-Bromo-2-phenylpyridine (13b)

Qualitative Compound Report

Data File	4BrPY-BA.d	**Sample Name**	4BrPY-BA
Sample Type	Sample	**Position**	Vial 17
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	25-06-2015 PM 2:38:11
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

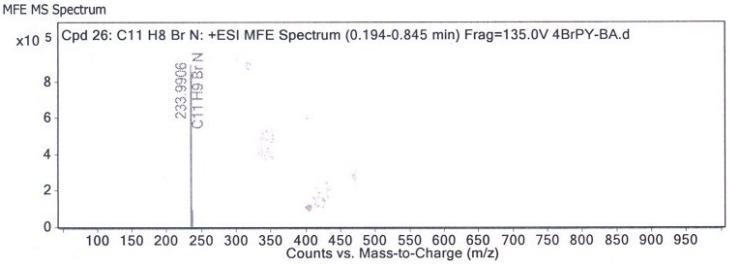


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 26: C11 H8 Br N	0.265	232.9834	C11 H8 Br N	C11 H8 Br N	2.59	C11 H8 Br N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 26: C11 H8 Br N	233.9906	0.265	Find by Molecular Feature	232.9834

MFE MS Spectrum



MS Spectrum Peak List

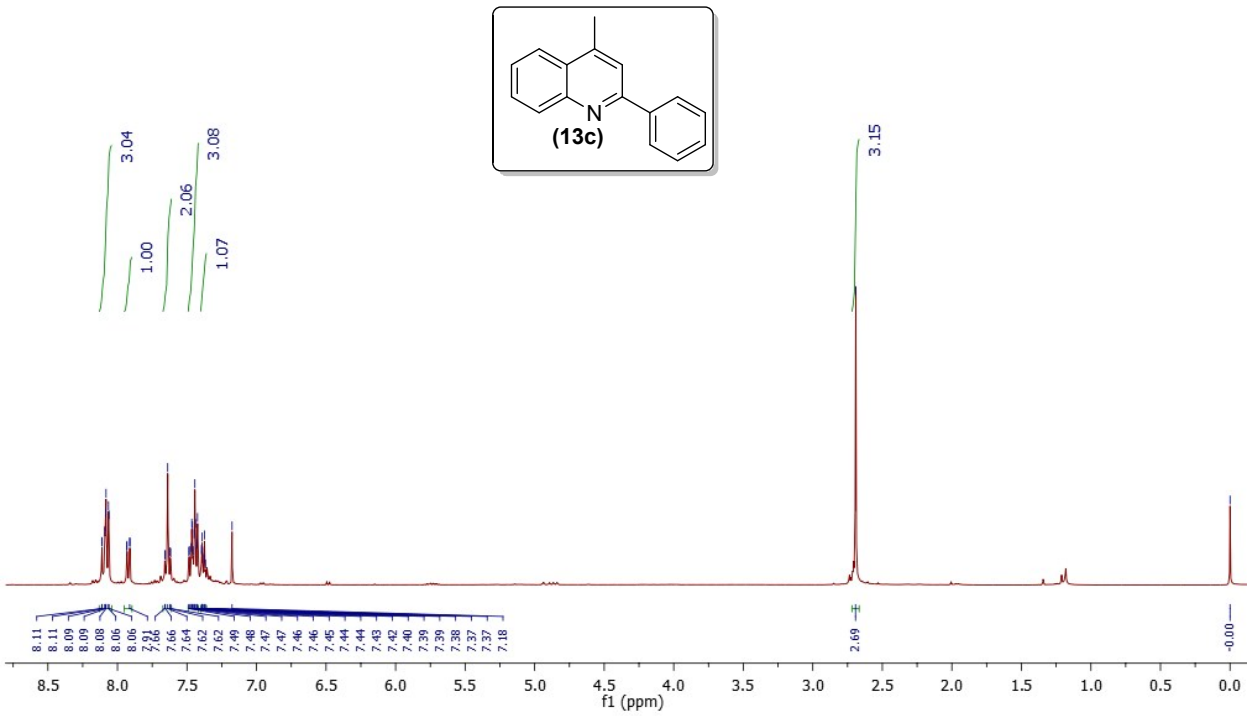
m/z	z	Abund	Formula	Ion
233.9906	1	894817.56	C11 H9 Br N	(M+H)+
234.994	1	98024.2	C11 H9 Br N	(M+H)+
235.9888	1	854566.94	C11 H9 Br N	(M+H)+
236.9921	1	94634.07	C11 H9 Br N	(M+H)+
237.9956	1	6283.51	C11 H9 Br N	(M+H)+
238.9974	1	316.59	C11 H9 Br N	(M+H)+

Predicted Isotope Match Table

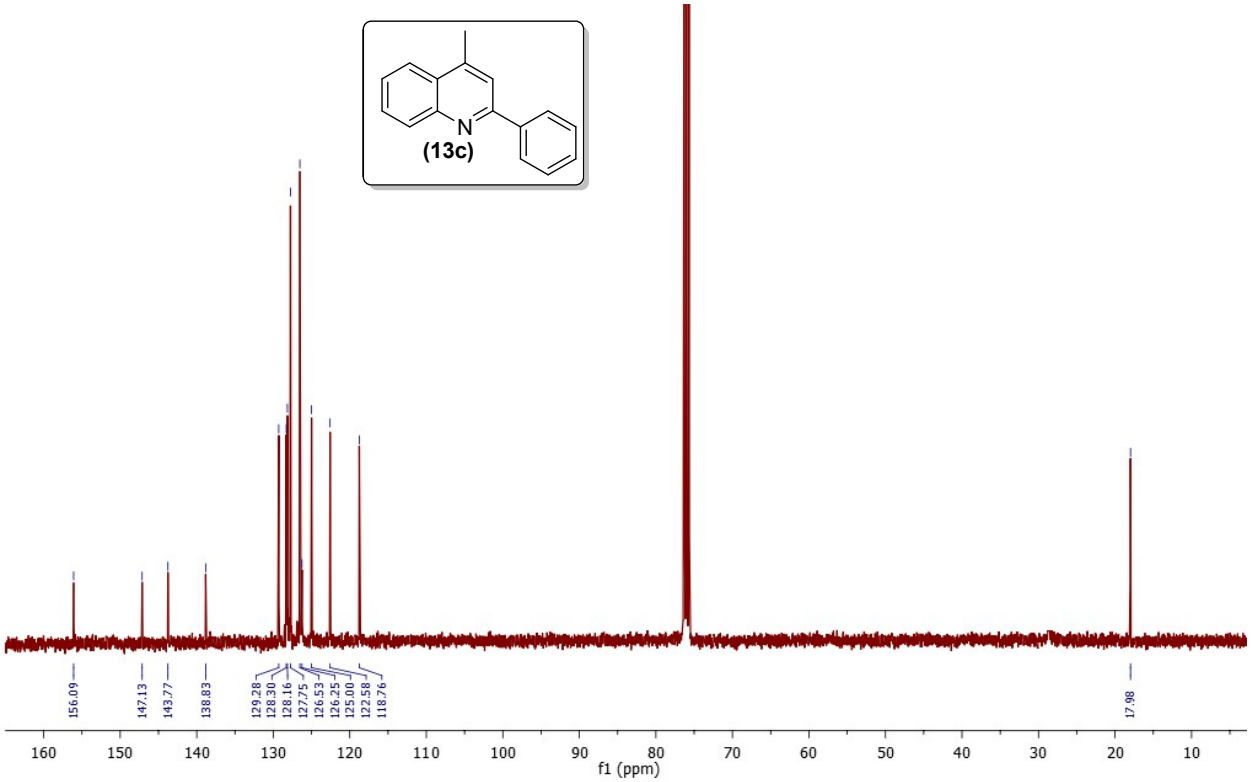
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	233.9906	233.9913	2.99	100	100	45.92	44.82
2	234.994	234.9945	2.12	10.95	12.37	5.03	5.54
3	235.9888	235.9893	2.31	95.5	97.98	43.85	43.92
4	236.9921	236.9925	1.65	10.58	12.05	4.86	5.4
5	237.9956	237.9956	-0.01	0.7	0.68	0.32	0.31
6	238.9974	238.9988	5.84	0.04	0.02	0.02	0.01

--- End Of Report ---

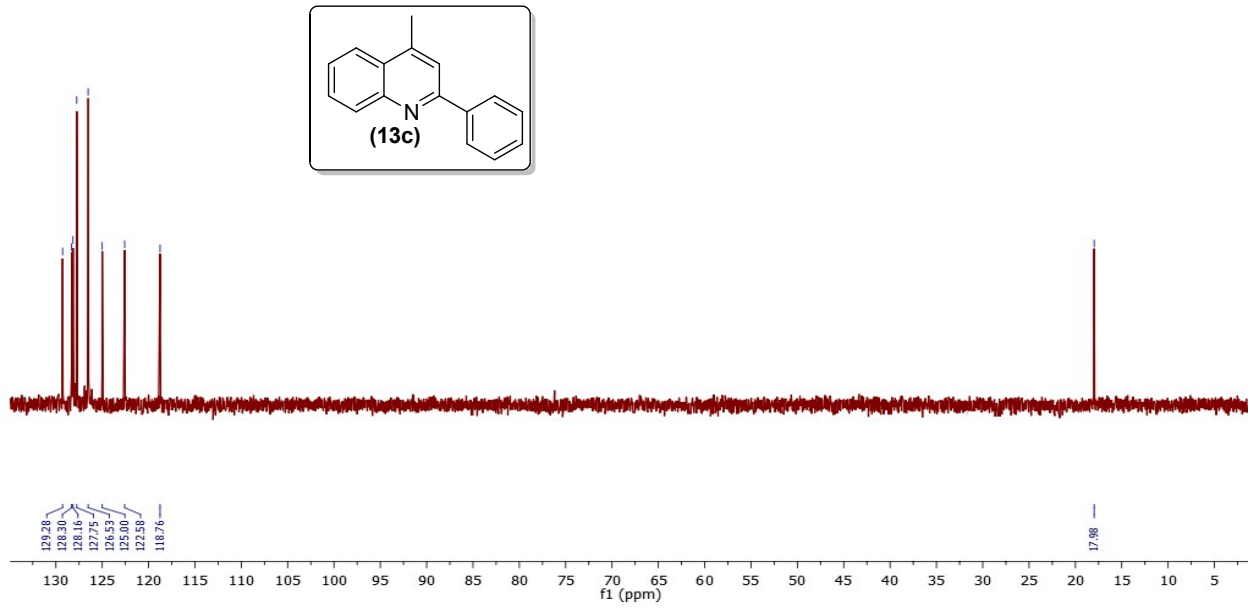
^{1}H NMR of 4-Methyl-2-phenylquinoline (13c)



^{13}C NMR of 4-Methyl-2-phenylquinoline (13c)



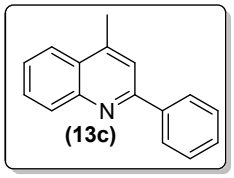
DEPT NMR of 4-Methyl-2-phenylquinoline (13c)



HRMS of 4-Methyl-2-phenylquinoline (13c)

Qualitative Compound Report

Data File	LEP-BA.d	**Sample Name**	LEP-BA
Sample Type	Sample	**Position**	Vial 21
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	08-06-2015 PM 3:01:45
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			



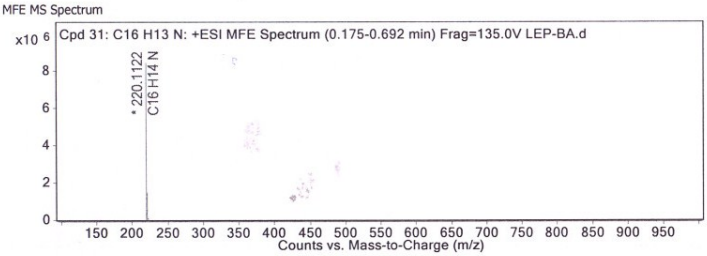
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 31: C16 H13 N	0.271	219.1056	C16 H13 N	C16 H13 N	-3.82	C16 H13 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 31: C16 H13 N	220.1122	0.271	Find by Molecular Feature	219.1056

MFE MS Spectrum



MS Spectrum Peak List

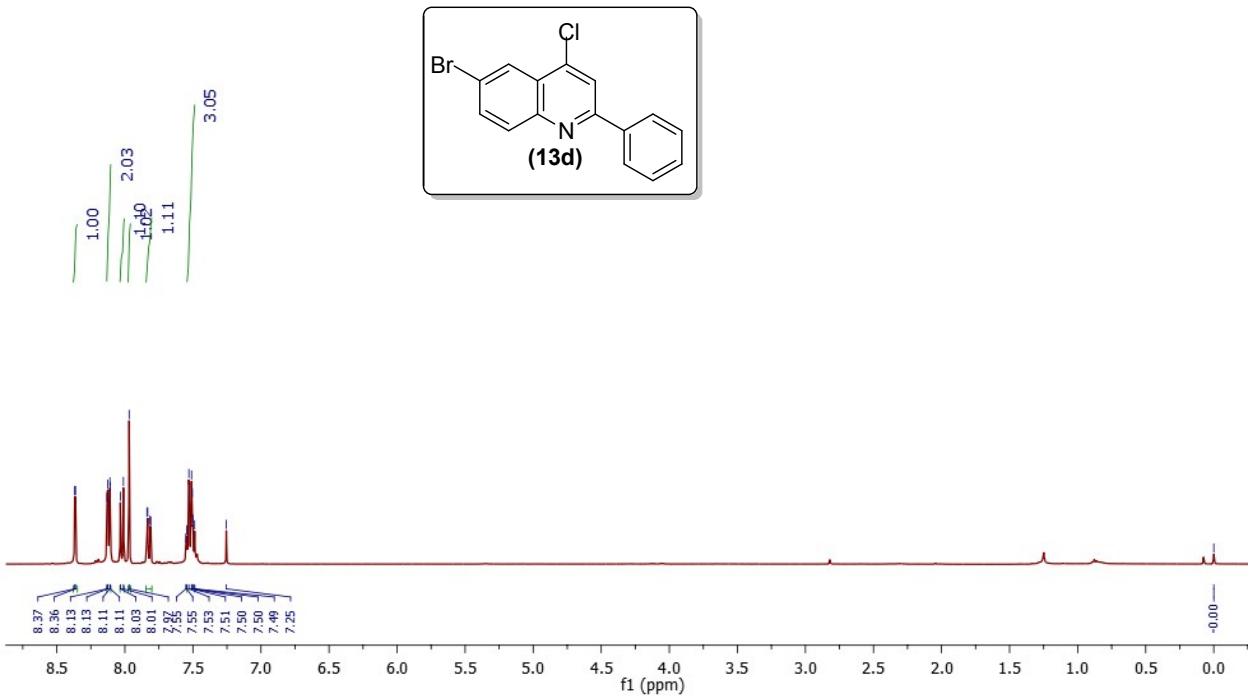
m/z	z	Abund	Formula	Ion
220.1122	1	8395797	C16 H14 N	(M+H)+
221.1199	1	1454878.5	C16 H14 N	(M+H)+
222.1232	1	107626.35	C16 H14 N	(M+H)+
223.1273	1	5853.88	C16 H14 N	(M+H)+

Predicted Isotope Match Table

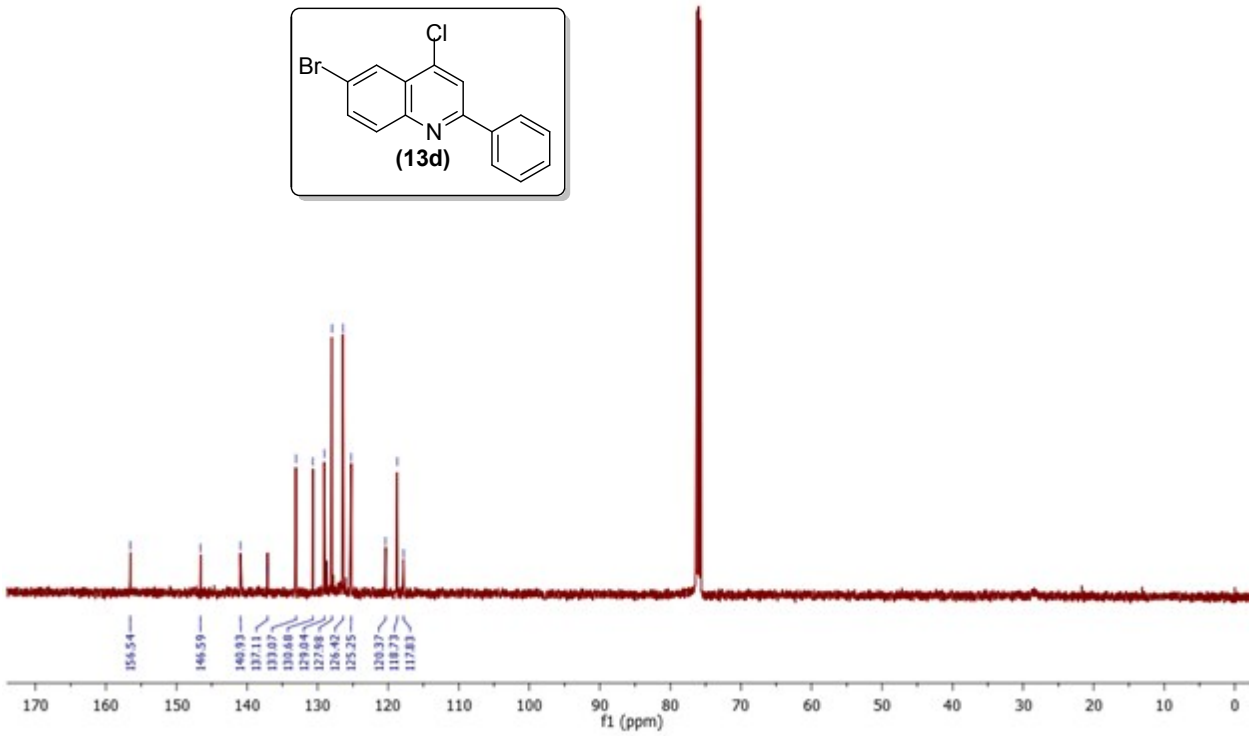
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	220.1122	220.1121	-0.62	100	100	84.26	83.75
2	221.1199	221.1153	-20.74	17.33	17.83	14.6	14.93
3	222.1232	222.1186	-20.71	1.28	1.5	1.08	1.25
4	223.1273	223.1218	-24.72	0.07	0.08	0.06	0.07

--- End Of Report ---

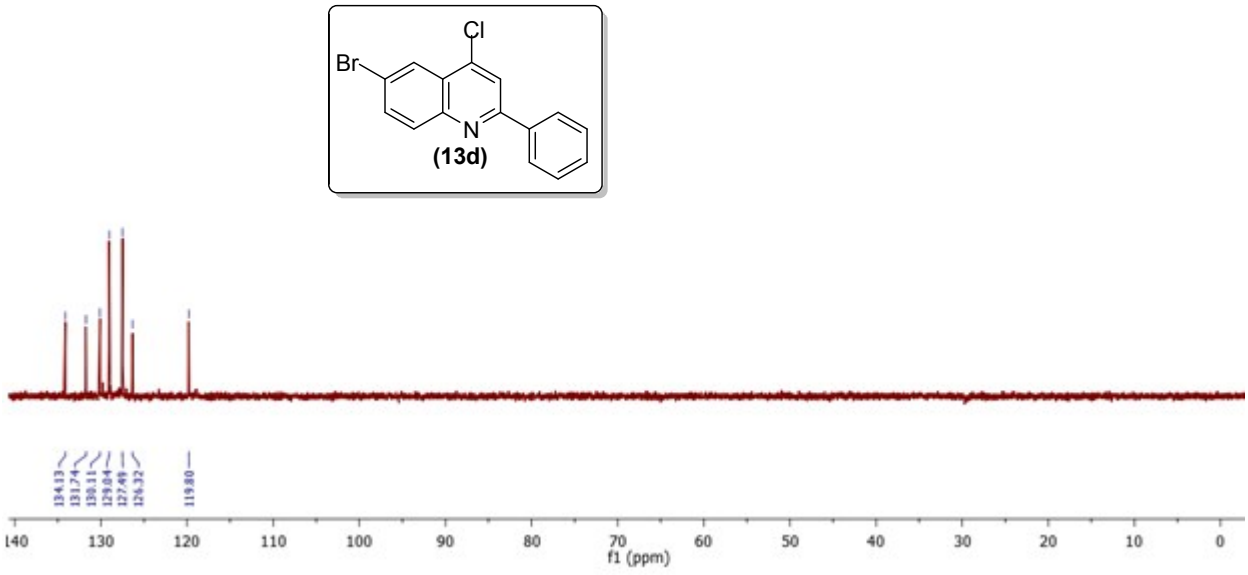
^{1}H NMR of 6-Bromo-4-chloro-2-phenylquinoline (13d)



^{13}C NMR of 6-Bromo-4-chloro-2-phenylquinoline (13d)



DEPT NMR of 6-Bromo-4-chloro-2-phenylquinoline (13d)

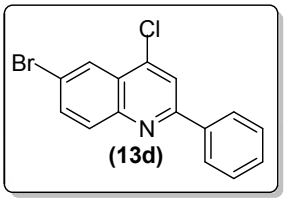


HRMS of 6-Bromo-4-chloro-2-phenylquinoline (13d)

Qualitative Compound Report

Data File	4Cl6BrQU-BA.d	**Sample Name**	4Cl6BrQU-BA
Sample Type	Sample	**Position**	Vial 29
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	15-06-2015 PM 6:22:21
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

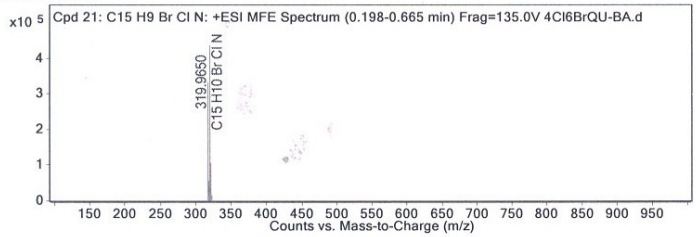


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 21: C15 H9 Br Cl N	0.273	316.9598	C15 H9 Br Cl N	C15 H9 Br Cl N	2.79	C15 H9 Br Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 21: C15 H9 Br Cl N	317.9672	0.273	Find by Molecular Feature	316.9598

MFE MS Spectrum



MS Spectrum Peak List

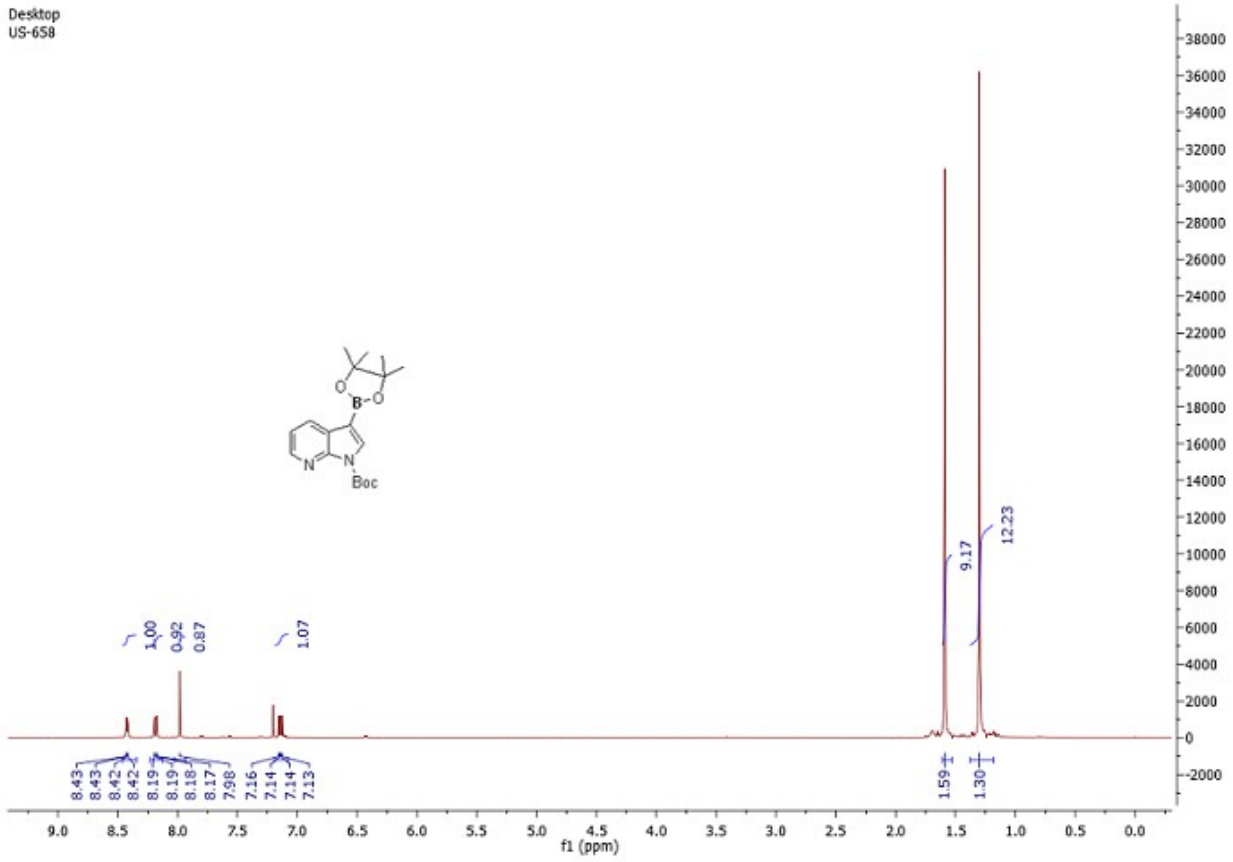
m/z	z	Abund	Formula	Ion
317.9672	1	331821.53	C15 H10 Br Cl N	(M+H)+
318.9698	1	55930.92	C15 H10 Br Cl N	(M+H)+
319.965	1	435874.91	C15 H10 Br Cl N	(M+H)+
320.9679	1	73124.92	C15 H10 Br Cl N	(M+H)+
321.9623	1	105597.23	C15 H10 Br Cl N	(M+H)+
322.9653	1	15203.95	C15 H10 Br Cl N	(M+H)+
323.9683	1	1160.71	C15 H10 Br Cl N	(M+H)+

Predicted Isotope Match Table

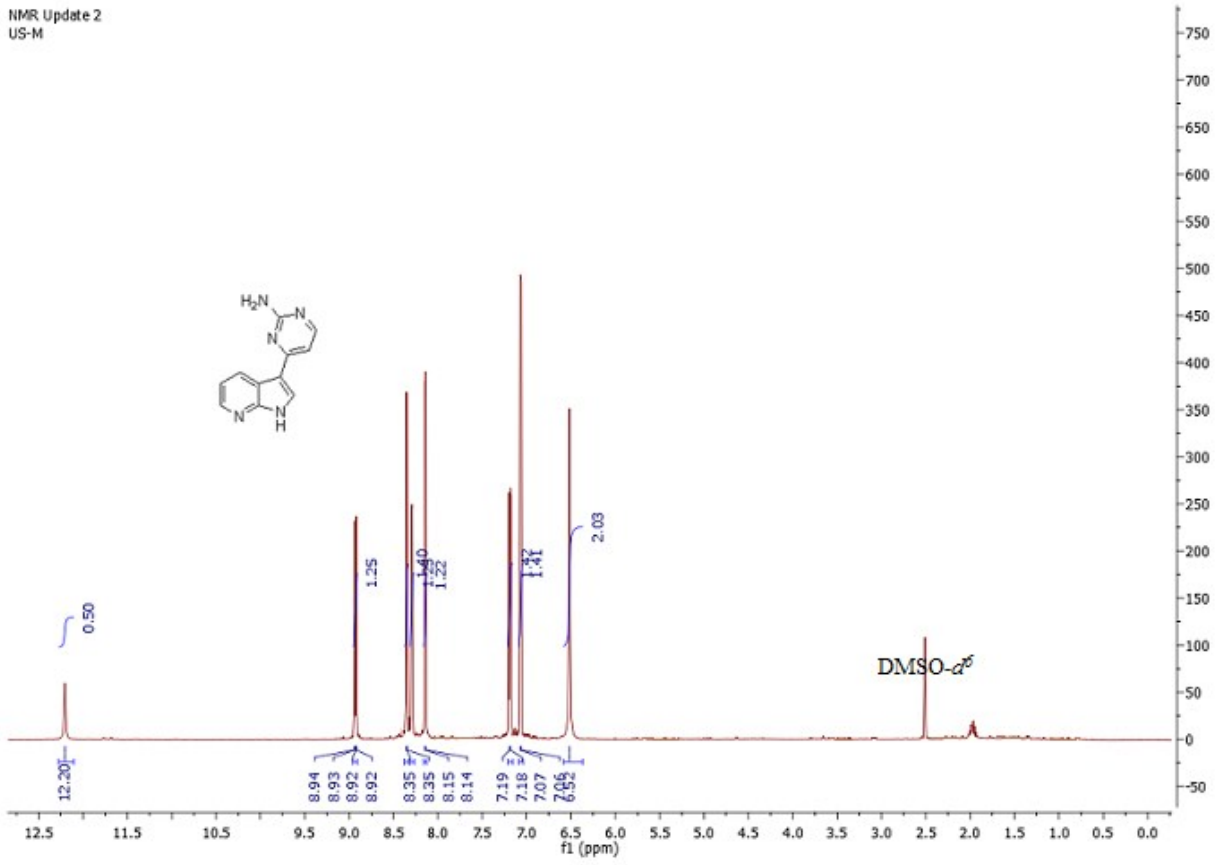
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.9672	317.968	2.45	76.13	76.58	32.57	32.53
2	318.9698	318.9712	4.36	12.83	12.79	5.49	5.43
3	319.965	319.9658	2.44	100	100	42.79	42.47
4	320.9679	320.969	3.42	16.78	16.59	7.18	7.04
5	321.9623	321.9634	3.66	24.23	25.13	10.37	10.67
6	322.9653	322.9663	3.4	3.49	4.04	1.49	1.72
7	323.9683	323.9695	3.63	0.27	0.31	0.11	0.13

--- End Of Report ---

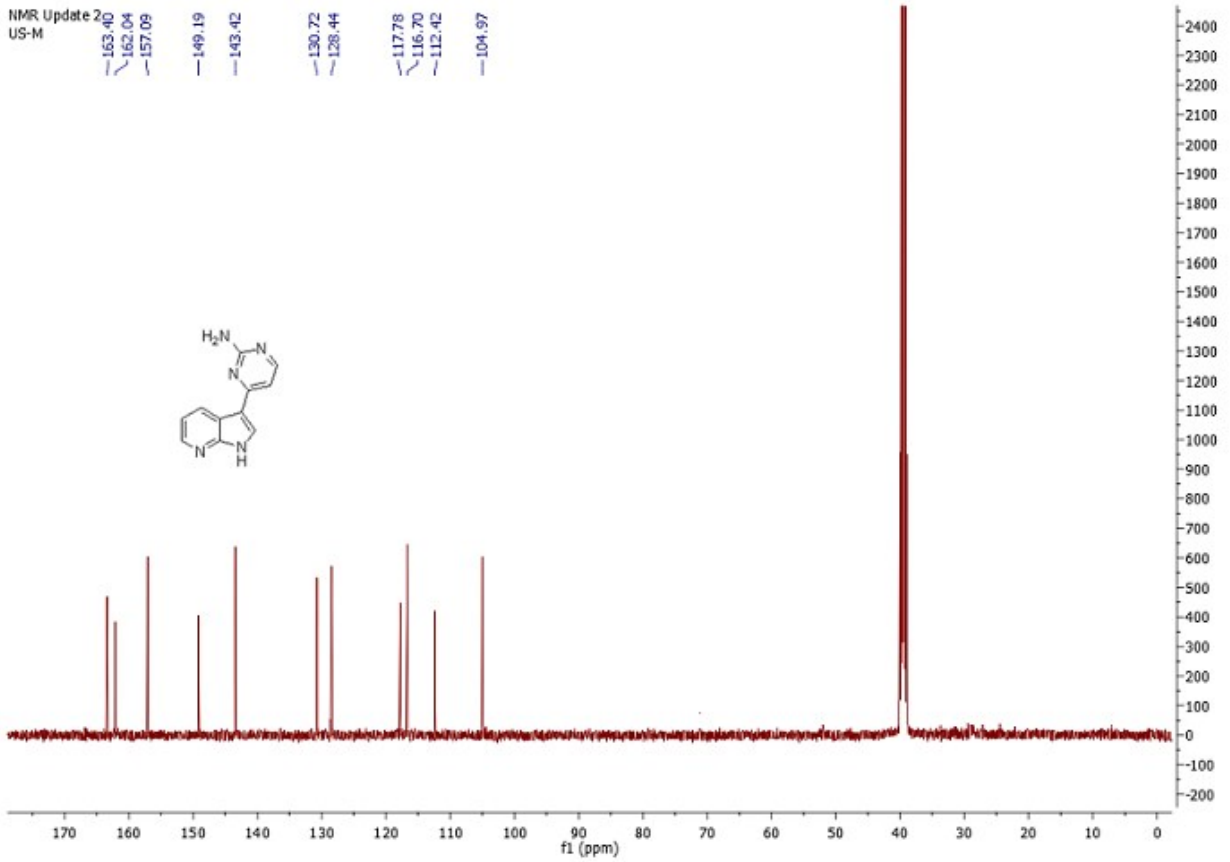
^{1}H NMR of *tert*-butyl 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1*H*-pyrrolo[2,3-*b*]pyridine-1-carboxylate (21)



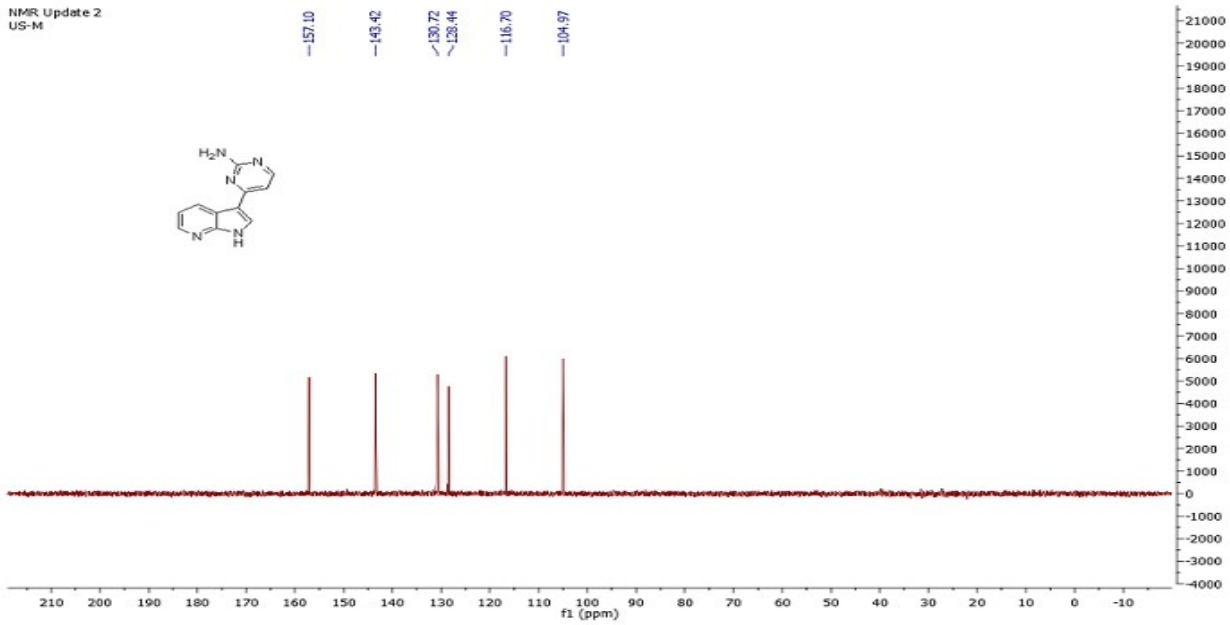
^{1}H NMR of 4-(1*H*-pyrrolo [2, 3-*b*] pyridin-3-yl) pyrimidin-2-amine (Meriolin1)



^{13}C NMR of 4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)pyrimidin-2-amine (Meriolin1)



DEPT NMR of 4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)pyrimidin-2-amine (Meriolin1)

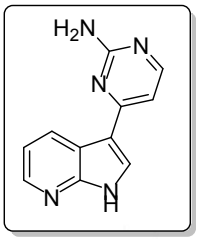


HRMS of 4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)pyrimidin-2-amine (Meriolin1)

Qualitative Compound Report

Data File	US-M.d	**Sample Name**	US-M
Sample Type	Sample	**Position**	Vial 23
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vikram-may'15.m	**Acquired Time**	11-05-2015 PM 3:07:26
IRM Calibration Status	Success	**DA Method**	daily_report.m
Comment			

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

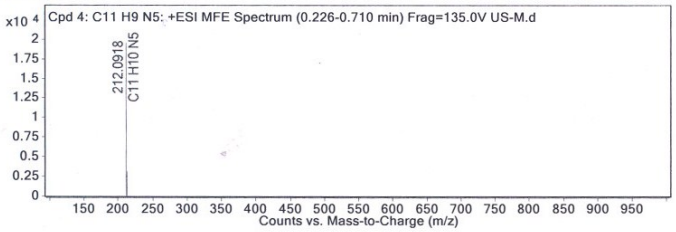


Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C11 H9 N5	0.368	211.0848	C11 H9 N5	C11 H9 N5	4.7	C11 H9 N5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C11 H9 N5	212.0918	0.368	Find by Molecular Feature	211.0848

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
212.0918	1	19514.51	C11 H10 N5	(M+H)+
213.0966	1	3156.12	C11 H10 N5	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	212.0918	212.0931	6.18	100	100	86.08	87.84
2	213.0966	213.0956	-4.59	16.17	13.84	13.92	12.16

--- End Of Report ---