

Supporting Information

Title: Synthesis of 4-Aryl and Unsymmetrical 4,6-Diarylpyrimidines by the Suzuki-Miyaura Cross-Coupling Reaction

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General information

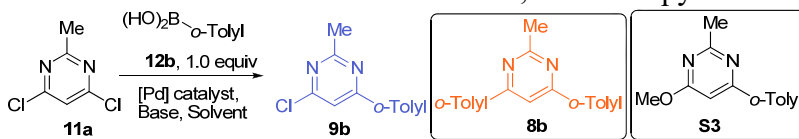
Melting points were obtained on a Electrothermal IA9100 Melting Point Apparatus and are uncorrected. ^1H and ^{13}C spectra were recorded on Bruker Avance-400 MHz spectrometer. The chemical shifts of ^1H and ^{13}C NMR signals are quoted relative to internal CHCl_3 ($\delta = 7.26$) and CDCl_3 ($\delta = 77.0$) or tetramethylsilane ($\delta = 0.0$). Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), doublet of triplets (dt), triplet (t), quartet (q), multiplet (m) and broad singlet (brs). The GC-MS analyses were performed on an Agilent 6890 GC coupled with an Agilent 5973 inert MS under EI conditions. High resolution mass spectra were obtained on a GCT Mass Spectrometer (Waters, Micromass) and a QSTAR XL hybrid mass Spectrometer (Applied Biosystems/MDS Sciex). IR spectra were recorded on a Bruker Alpha FT-IR spectrometer. Column chromatography was performed using silica gel (230-400 mesh) as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All reagents and solvents were purchased from commercial sources and used without purification. *N*-Benzyl-6-chloropyrimidin-4-amine was prepared by a reported procedure.¹

Synthesis of 4-chloro-6-methoxy-2-methylpyrimidine (**S1**)



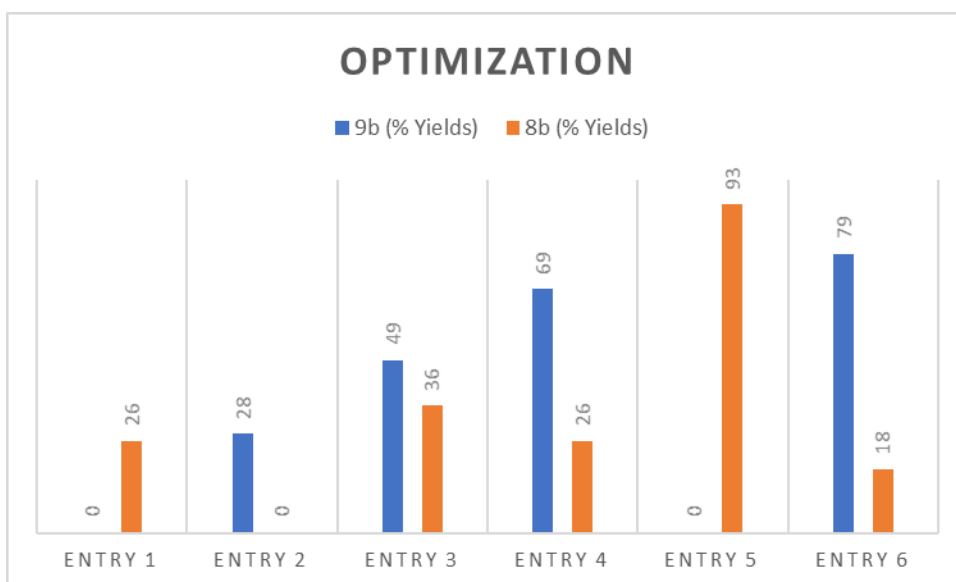
To a stirred solution of 4,6-dichloro-2-methylpyrimidine (2 g, 1.0 equiv) in MeOH (20 mL) was added dropwise a solution of NaOMe (25 wt% in MeOH, 1.0 equiv) and stirred for 20 min at rt. The reaction mixture was diluted with H₂O and extracted with EtOAc (3 X 30 mL). The combined organic extracts were washed with brine, dried (Na₂SO₄), and evaporated under reduced pressure. The resulting crude material was purified by flash column chromatography using EtOAc/hexane as eluent to afford compound **S1** (1.5 g, 77%) as a colorless oil, FT-IR (neat) ν_{max} 3031-2994, 2955-2858, 1553-1402, 1382, 1116 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 6.58 (s, 1H), 3.97 (s, 3H), 2.60 (s, 3H); ¹³C NMR (50 MHz, CDCl₃): δ 170.5, 168.7, 160.2, 104.3, 54.3, 25.8 ppm; HRMS (EI) calcd for C₆H₇ClN₂O [M] 158.0247, found 158.0242.

Table S1: Optimization table for Suzuki reaction of 4,6-dichloropyrimidine **11a**



entry	conditions	9b/8b, % yield ^a
1	Pd(PPh ₃) ₄ (3 mol%), K ₂ CO ₃ (3.0 equiv), Toluene/MeOH (4:1), 90 °C, 18 h, RBF	--/26 ^b
2	Pd(PPh ₃) ₄ (3 mol%), K ₂ CO ₃ (3.0 equiv), Toluene, 90 °C, 20 h, RBF	28/-- ^c
3	Pd(OAc) ₂ (5 mol%), PPh ₃ (10 mol%), Na ₂ CO ₃ (3.1 equiv, dissolved in min amt of H ₂ O), DME, reflux, 18 h, RBF	49/36
4	Pd(PPh₃)₄ (5 mol%), Na₂CO₃ (2 M, 2.5 equiv), <i>i</i>PrOH, reflux, 18 h, microwave vial	69/26
5	Same as entry 4 except 2.3 equiv of <i>o</i> -tolyl boronic acid was used	--/93
6	Same as entry 4 except 0.8 equiv of <i>o</i> -tolyl boronic acid was used	79/18 ^d

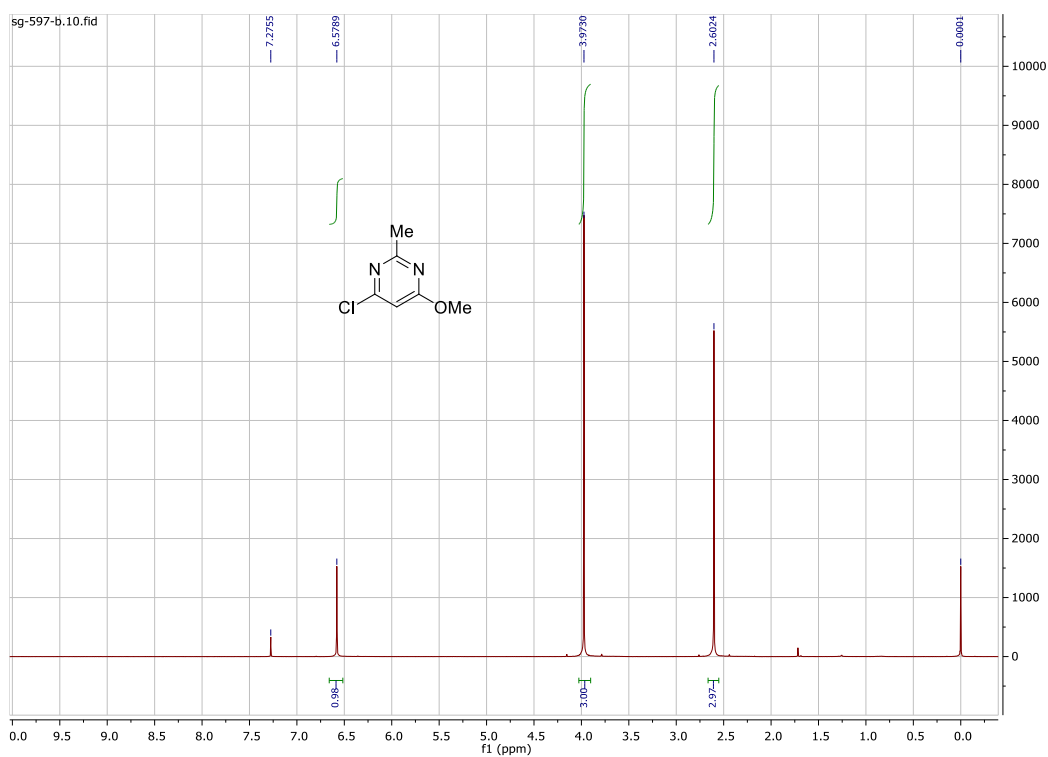
^aYield of isolated product. ^b**S3** was also isolated in 72% yield. ^c**1a** was recovered in 50% yield. ^dYield was calculated considering boronic acid as the limiting reagent.



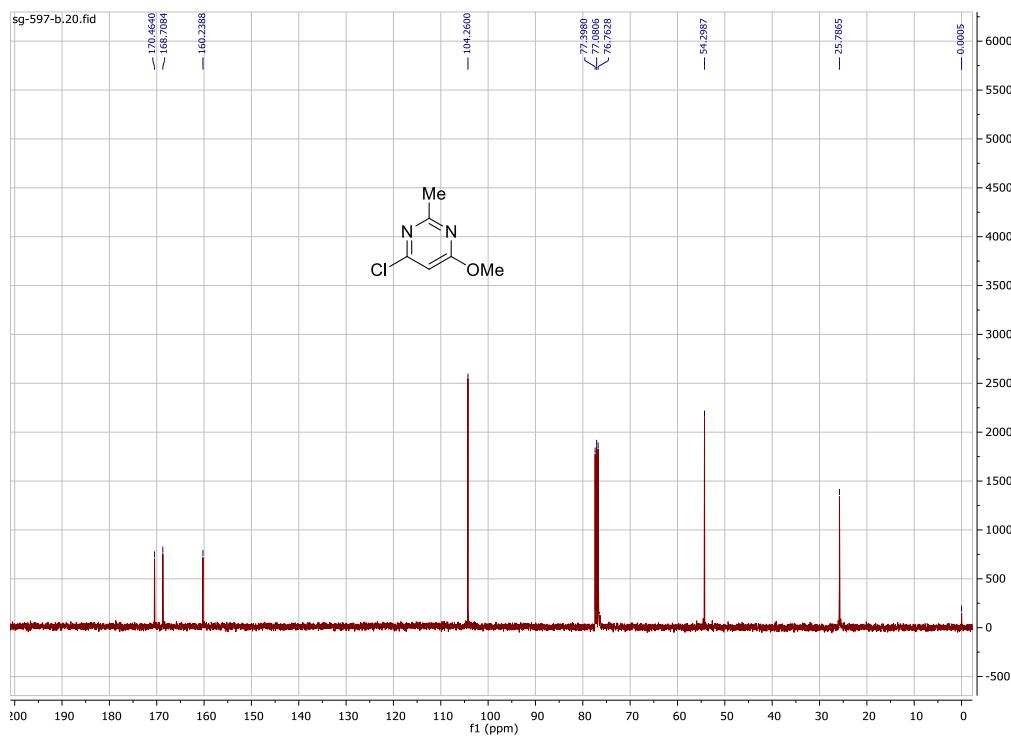
References:

¹ C. W. van der Westhuyzen, A. L. Rousseau, and C. J. Parkinson, *Tetrahedron*, 2007, **63**, 5394.

^1H , ^{13}C and HRMS Spectra



^1H NMR spectrum of S1 (in CDCl_3)

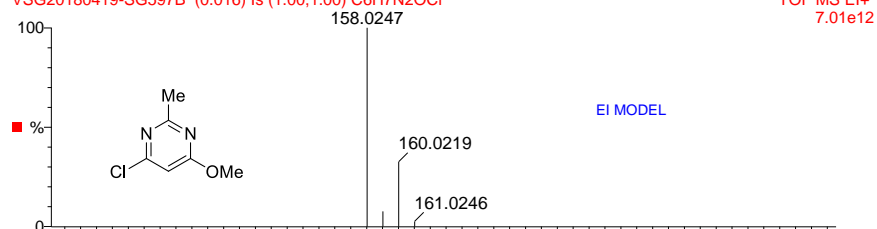


^{13}C NMR spectrum of S1 (in CDCl_3)

VSG20180419-SG597B

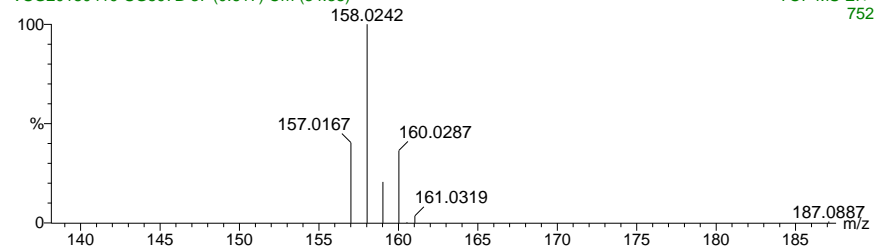
VSG20180419-SG597B (0.016) Is (1.00,1.00) C6H7N2OCl

TOF MS EI+
7.01e12



VSG20180419-SG597B 37 (0.617) Cm (34:38)

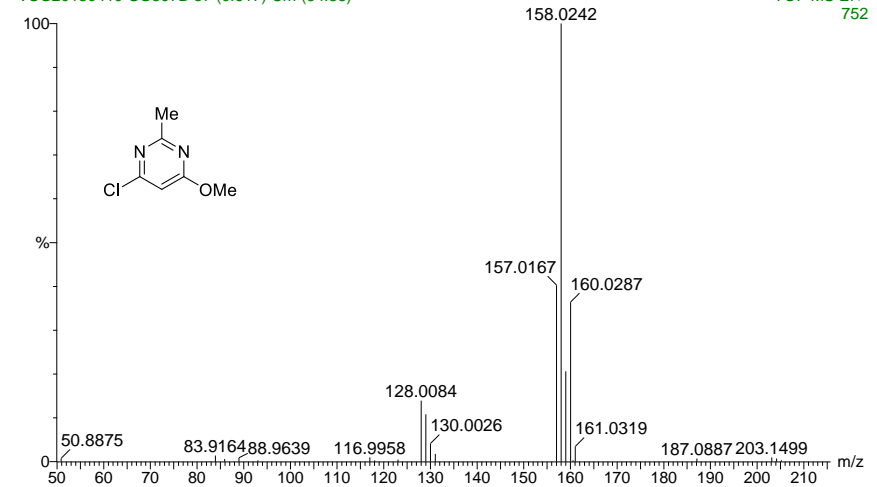
TOF MS EI+
752



VSG20180419-SG597B

VSG20180419-SG597B 37 (0.617) Cm (34:38)

TOF MS EI+
752

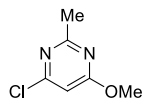


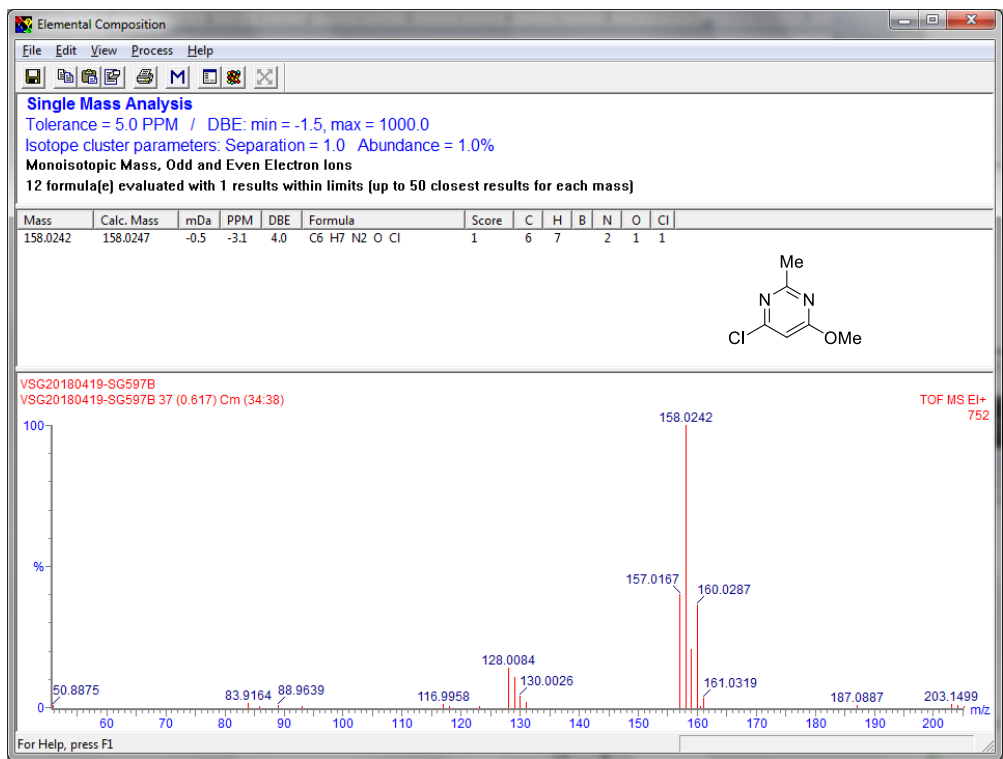
VSG20180419-SG597B

VSG20180419-SG597B 37 (0.617) Cm (34:38)

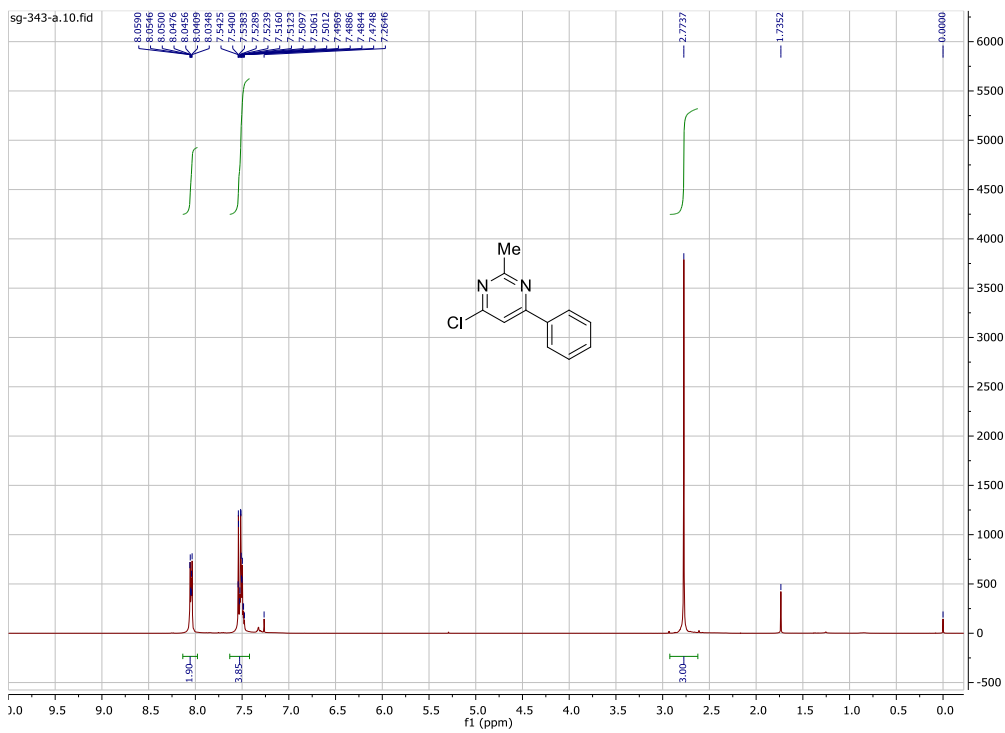
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	50.8875	5.06e0	0.67	0.26										
2:	83.9164	1.01e1	1.35	0.51										
3:	85.9168	4.05e0	0.54	0.21										
4:	88.9639	6.08e0	0.81	0.31										
5:	93.0209	2.03e0	0.27	0.10										
6:	116.9958	7.09e0	0.94	0.36										
7:	118.0484	2.03e0	0.27	0.10										
8:	123.0384	3.04e0	0.40	0.15										
9:	128.0084	1.04e2	13.87	5.28										
10:	129.0185	8.10e1	10.77	4.10										
11:	130.0026	3.04e1	4.04	1.54										
12:	131.0180	1.32e1	1.75	0.67										
13:	157.0167	3.03e2	40.26	15.33										
14:	158.0242	7.52e2	100.05	38.10										
15:	159.0182	1.55e2	20.60	7.85										
16:	160.0287	2.73e2	36.36	13.85										
17:	160.5374	2.03e0	0.27	0.10										
18:	161.0319	2.53e1	3.37	1.28										
19:	187.0887	5.06e0	0.67	0.26										
20:	203.1499	7.09e0	0.94	0.36										
21:	204.1623	5.06e0	0.67	0.26										
22:	205.1923	2.03e0	0.27	0.10										

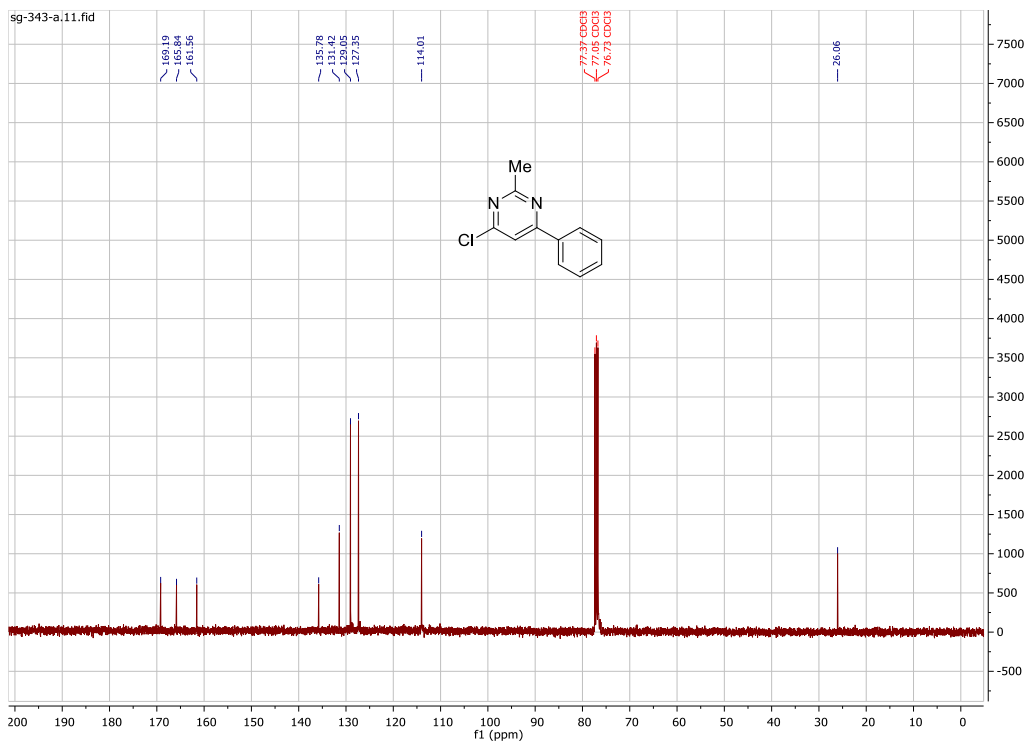




HRMS spectra of S1



^1H NMR spectrum of **9a** (in CDCl_3)

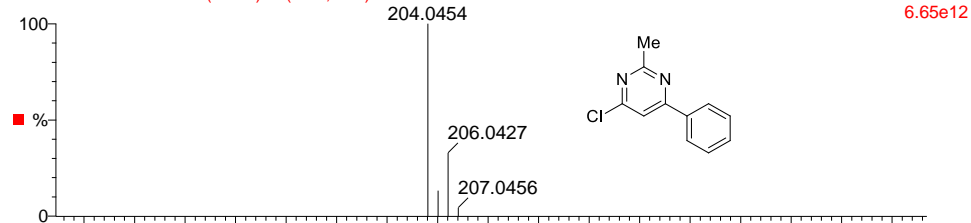


¹³C NMR spectrum of **9a** (in CDCl₃)

VSG20180129-SG-354

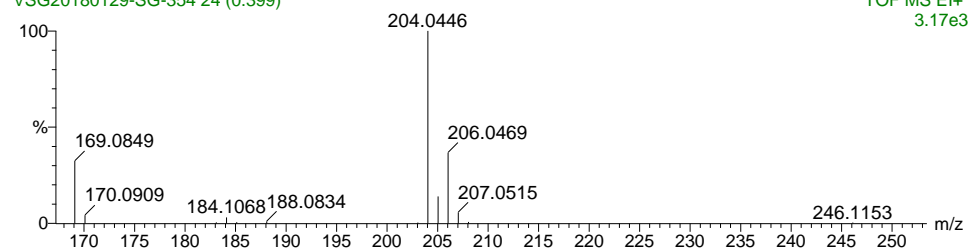
VSG20180129-SG-354 (0.399) Is (1.00,1.00) C₁₁H₉ClN₂

TOF MS EI+
6.65e12



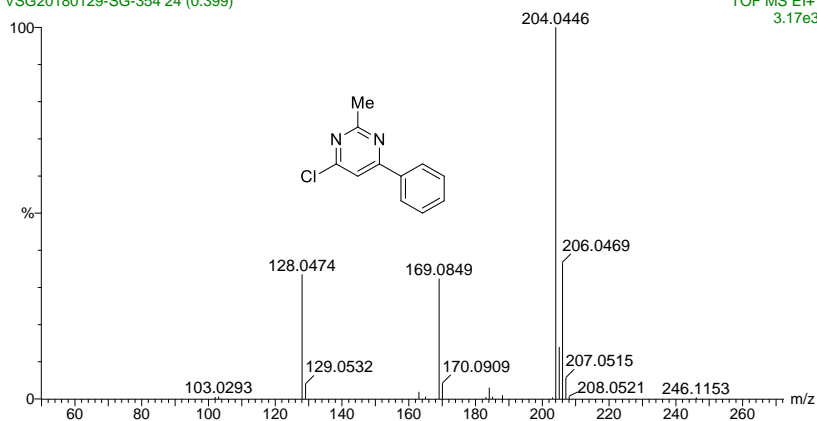
VSG20180129-SG-354 24 (0.399)

TOF MS EI+
3.17e3



VSG20180129-SG-354
 VSG20180129-SG-354 24 (0.399)

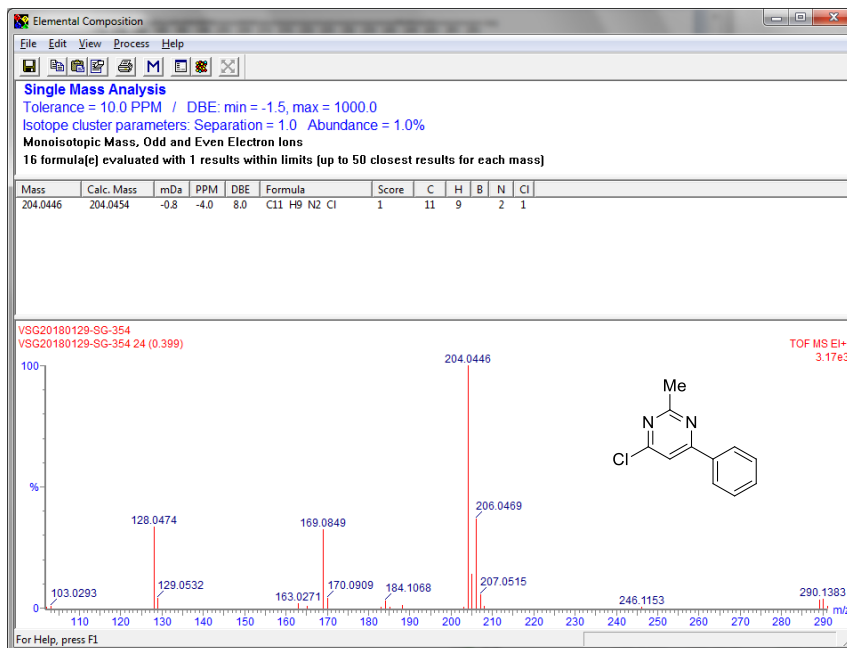
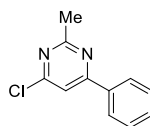
TOF MS EI+
 3.17e3



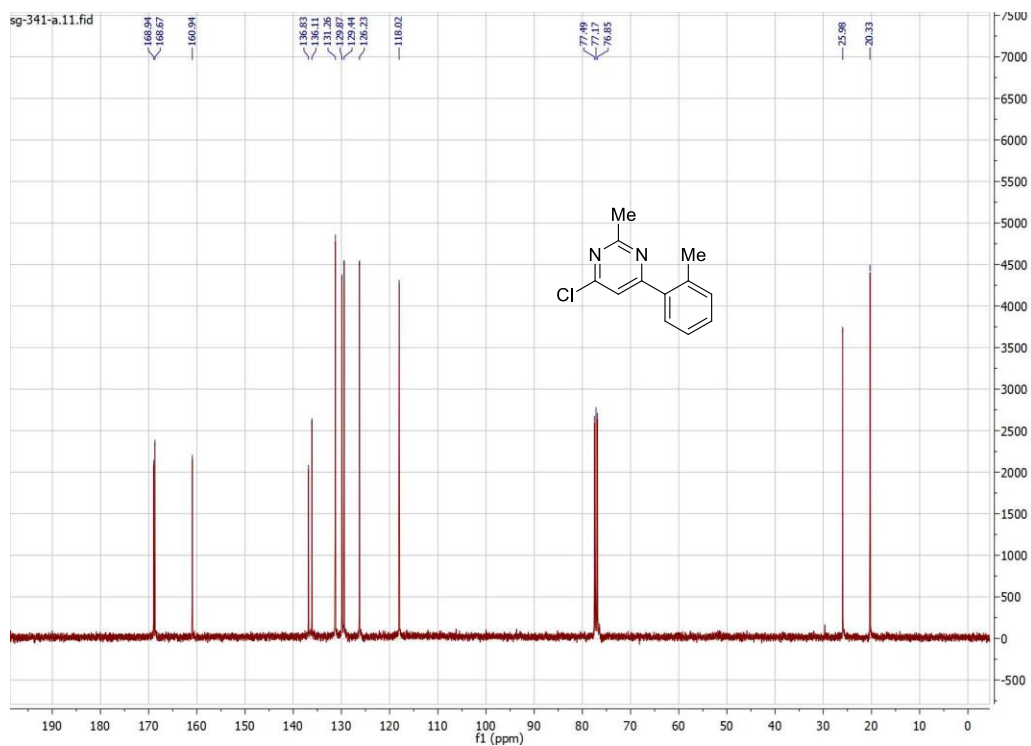
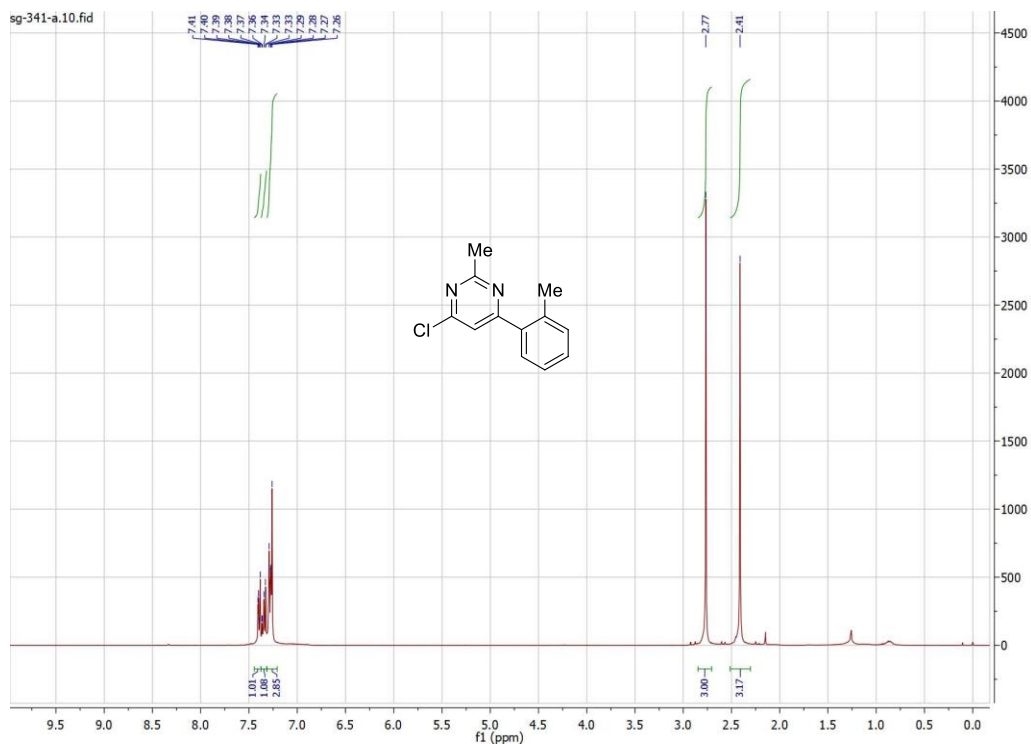
VSG20180129-SG-354
 VSG20180129-SG-354 24 (0.399)

TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	102.0290	1.52e1	0.48	0.19										
2:	103.0293	1.92e1	0.61	0.24										
3:	128.0474	1.06e3	33.52	13.23										
4:	129.0532	1.26e2	3.96	1.56										
5:	163.0271	5.87e1	1.85	0.73										
6:	165.0343	1.82e1	0.58	0.23										
7:	169.0849	1.02e3	32.32	12.76										
8:	170.0909	1.32e2	4.15	1.64										
9:	183.1017	1.42e1	0.45	0.18										
10:	184.1068	9.52e1	3.00	1.19										
11:	185.1035	1.72e1	0.54	0.21										
12:	188.0834	3.14e1	0.99	0.39										
13:	203.0409	1.11e1	0.35	0.14										
14:	204.0446	3.17e3	99.99	39.48										
15:	205.0567	4.41e2	13.93	5.50										
16:	206.0469	1.16e3	36.71	14.50										
17:	207.0515	1.79e2	5.66	2.23										
18:	208.0521	2.03e1	0.64	0.25										
19:	246.1153	1.11e1	0.35	0.14										



HRMS spectra of 9a

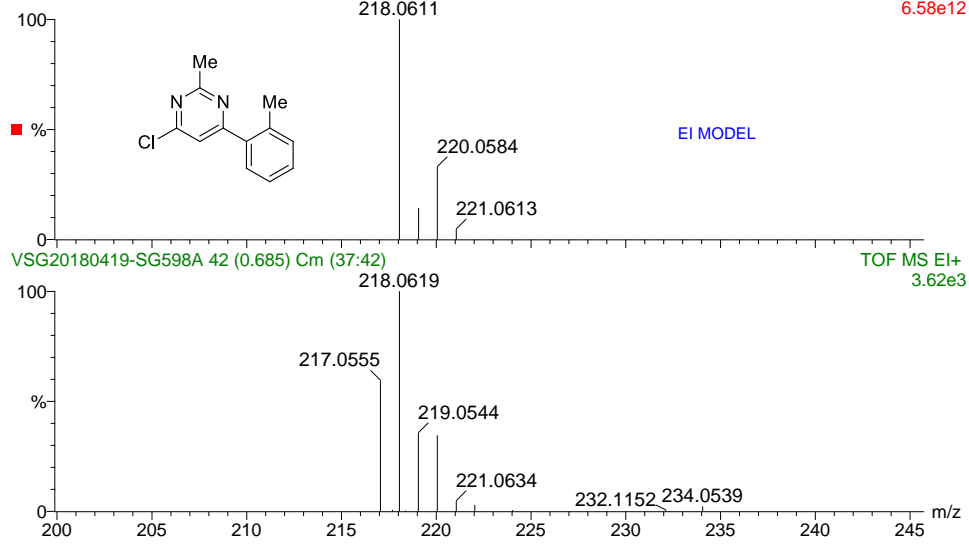


¹³C NMR spectrum of **9b** (in CDCl₃)

VSG20180419-SG598A

VSG20180419-SG598A (0.002) Is (1.00,1.00) C₁₂H₁₁ClN₂

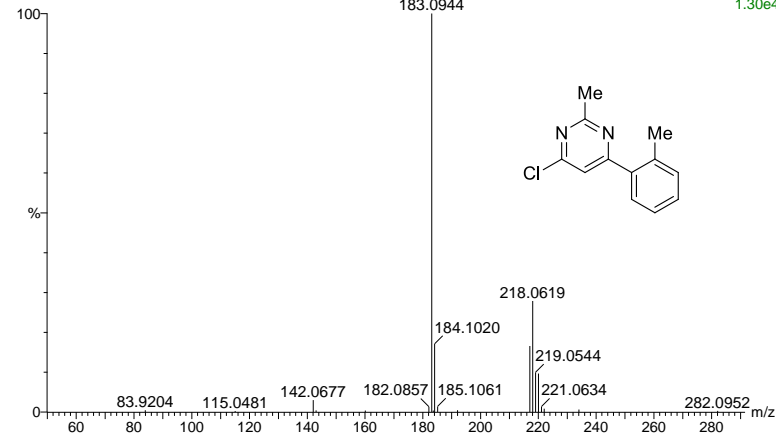
TOF MS EI+
6.58e12



VSG20180419-SG598A

VSG20180419-SG598A 42 (0.685) Cm (37:42)

TOF MS EI+
1.30e4

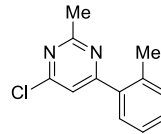


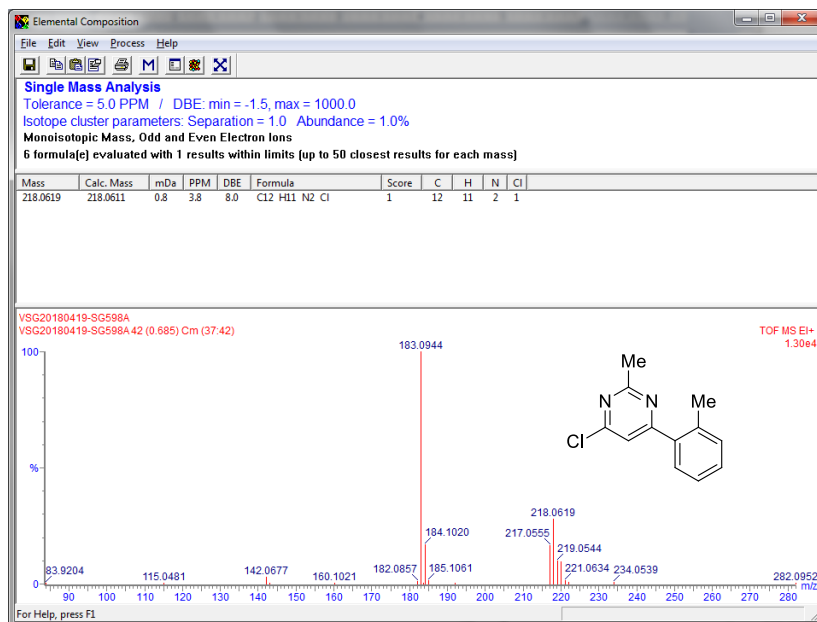
VSG20180419-SG598A

VSG20180419-SG598A 42 (0.685) Cm (37:42)

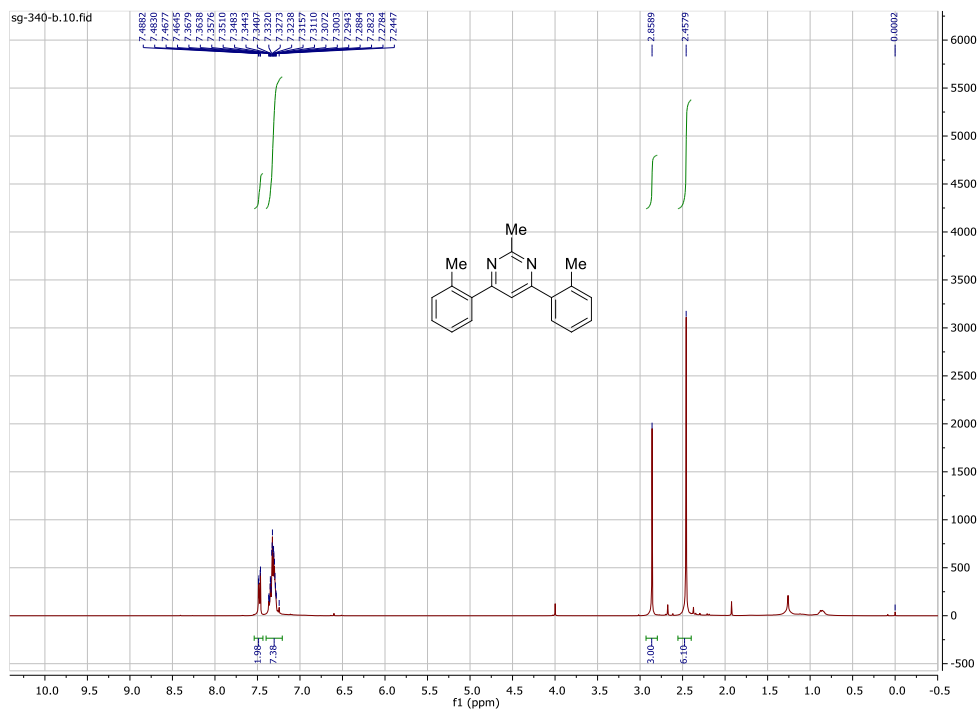
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	83.9204	5.47e1	0.42	0.22										
2:	115.0481	2.73e1	0.21	0.11										
3:	142.0677	3.85e2	2.96	1.52										
4:	143.0714	4.76e1	0.37	0.19										
5:	160.1021	4.25e1	0.33	0.17										
6:	182.0857	1.66e2	1.28	0.66										
7:	183.0944	1.30e4	100.00	51.31										
8:	183.6367	4.66e1	0.36	0.18										
9:	184.1020	2.21e3	17.02	8.73										
10:	185.1061	1.75e2	1.35	0.69										
11:	192.0241	5.47e1	0.42	0.22										
12:	217.0555	2.15e3	16.54	8.49										
13:	218.0619	3.62e3	27.84	14.28										
14:	219.0544	1.29e3	9.91	5.09										
15:	220.0605	1.25e3	9.62	4.93										
16:	221.0634	1.71e2	1.32	0.68										
17:	222.0400	1.04e2	0.80	0.41										
18:	234.0539	7.90e1	0.61	0.31										
19:	282.0952	3.34e1	0.26	0.13										

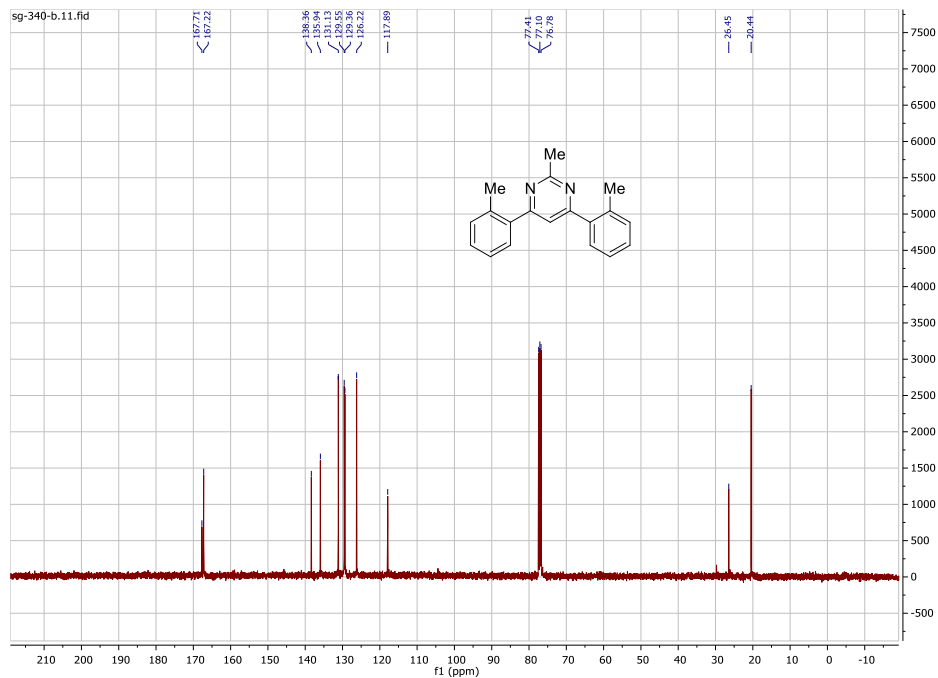




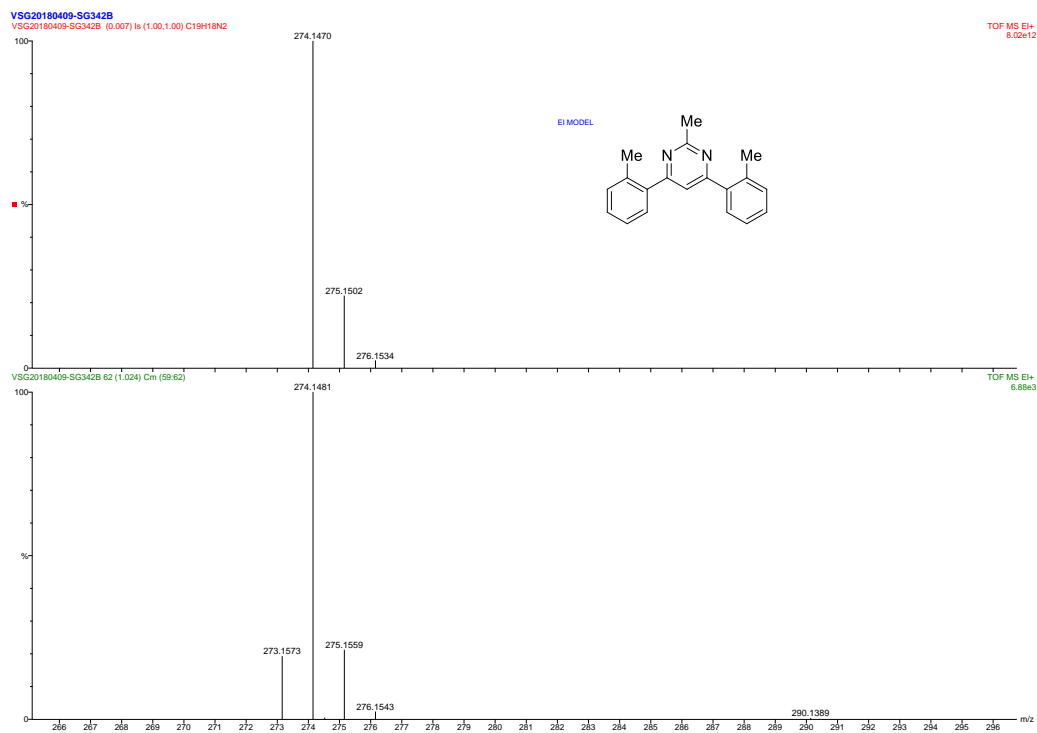
HRMS spectra of **9b**



^1H NMR spectrum of **8b** (in CDCl_3)



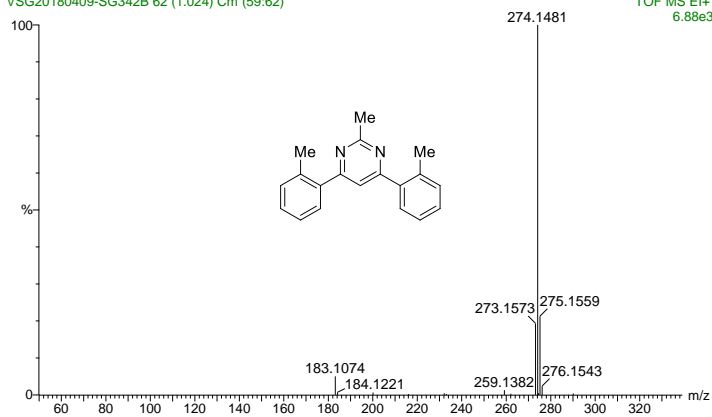
^{13}C NMR spectrum of **8b** (in CDCl_3)



VSG20180409-SG342B

VSG20180409-SG342B 62 (1.024) Cm (59:62)

TOF MS EI+
6.88e3

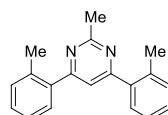


VSG20180409-SG342B

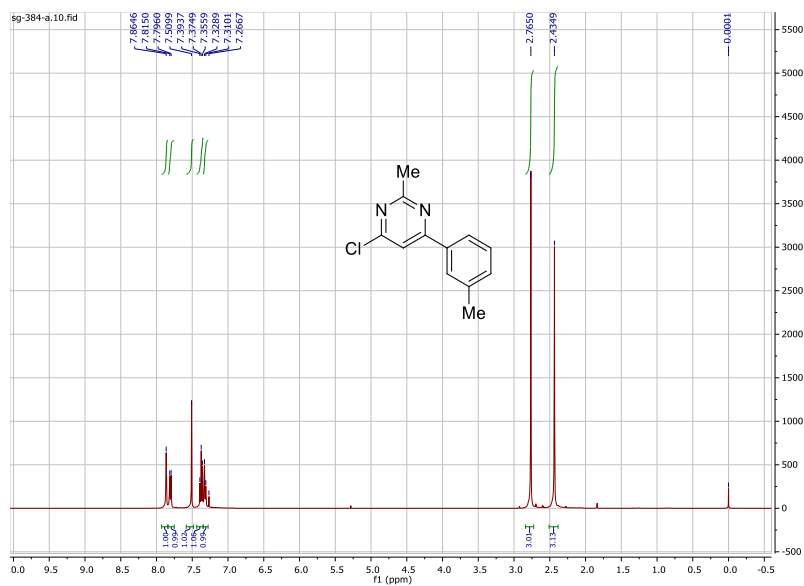
VSG20180409-SG342B 62 (1.024) Cm (59:62)

TOF MS EI+

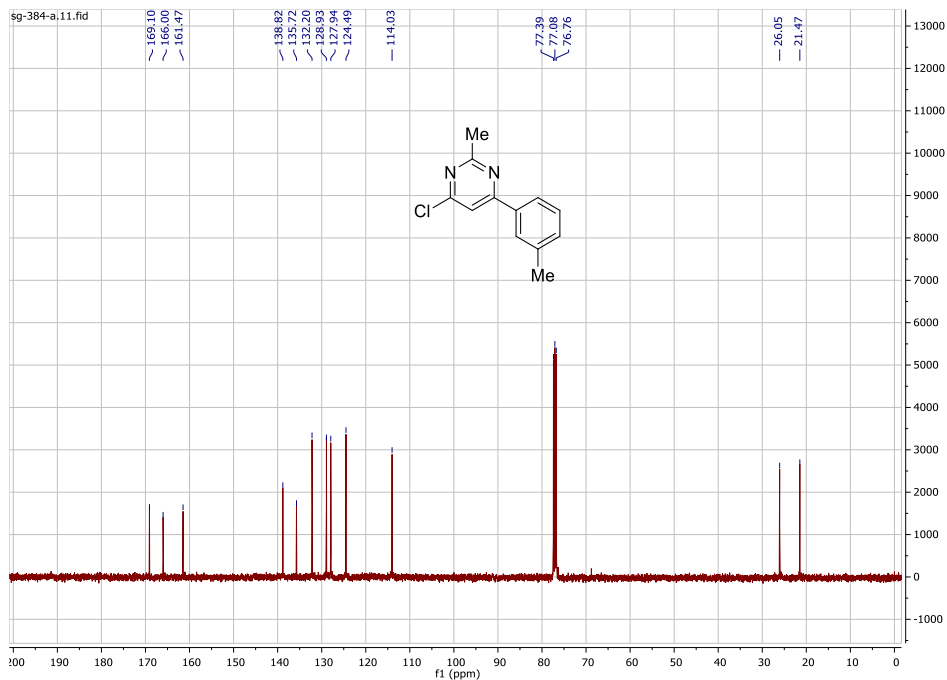
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	183.1074	3.42e2	4.98	3.22					
2:	184.1221	4.25e1	0.62	0.40					
3:	200.1021	4.15e1	0.60	0.39					
4:	216.1223	1.42e1	0.21	0.13					
5:	232.1290	2.94e1	0.43	0.28					
6:	233.1284	1.52e1	0.22	0.14					
7:	259.1382	8.71e1	1.27	0.82					
8:	262.0932	1.92e1	0.28	0.18					
9:	273.1573	1.32e3	19.26	12.45					
10:	274.1481	6.88e3	100.00	64.67					
11:	274.5247	3.14e1	0.46	0.30					
12:	275.1559	1.46e3	21.22	13.73					
13:	276.1543	1.59e2	2.31	1.49					
14:	290.1389	2.33e1	0.34	0.22					



HRMS spectra of 8b



¹H NMR spectrum of 9c (in CDCl₃)

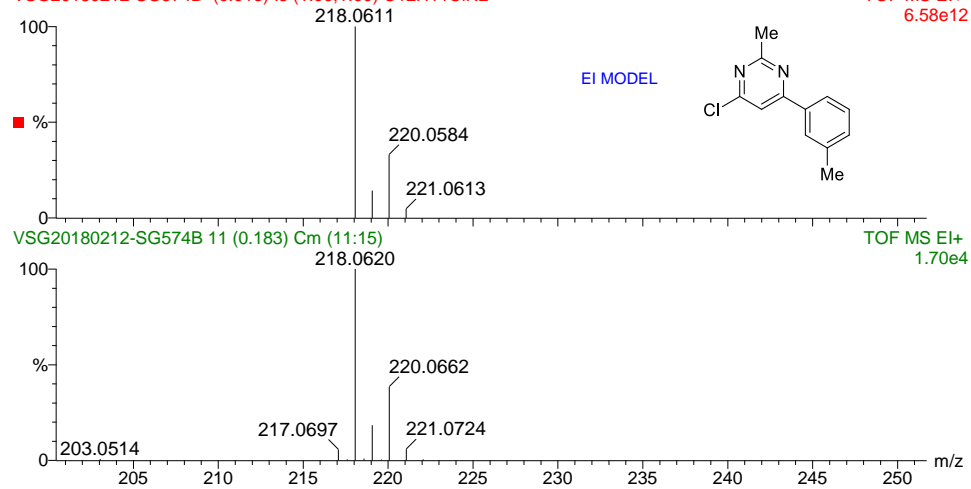


^{13}C NMR spectrum of **9c** (in CDCl_3)

VSG20180212-SG574B

VSG20180212-SG574B (0.016) Is (1.00,1.00) C₁₂H₁₁ClN₂

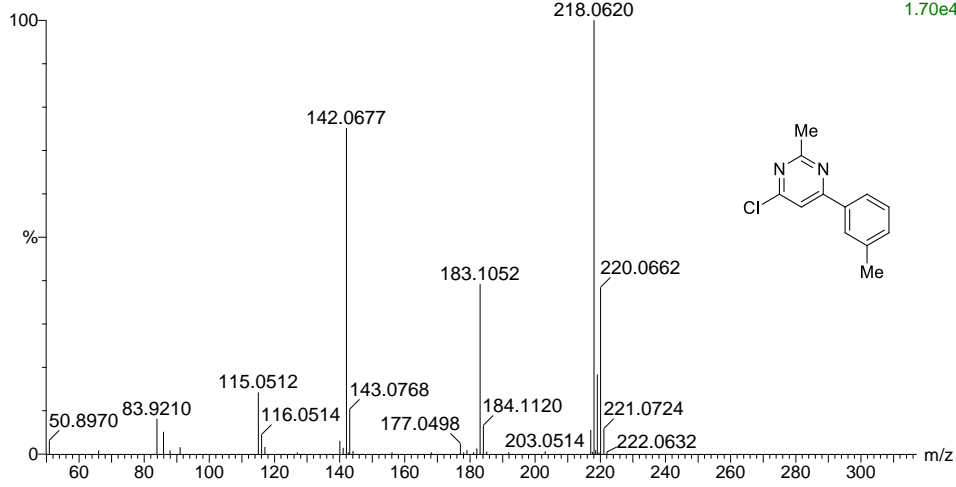
TOF MS EI+
6.58e12



VSG20180212-SG574B

VSG20180212-SG574B 11 (0.183) Cm (11:15)

TOF MS EI+
1.70e4

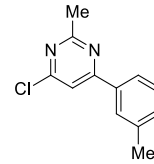


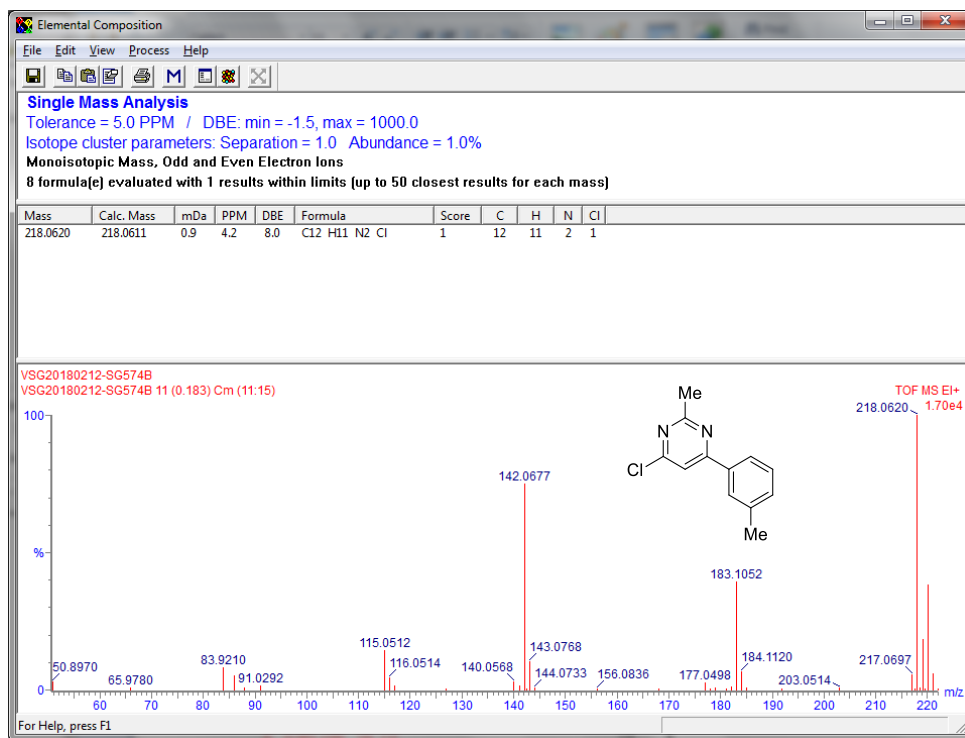
VSG20180212-SG574B

VSG20180212-SG574B 11 (0.183) Cm (11:15)

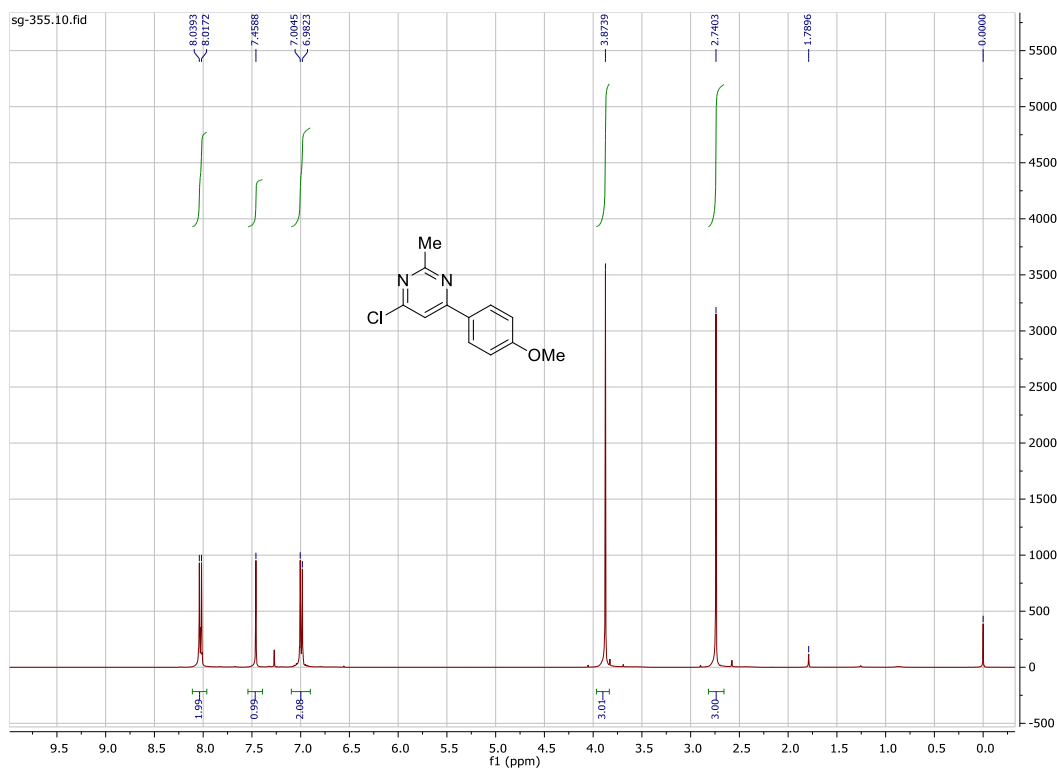
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	50.8970	5.31e2	3.11	0.86	28:	203.0514	1.08e2	0.64	0.18					
2:	65.9780	1.35e2	0.79	0.22	29:	217.0697	9.44e2	5.54	1.53					
3:	83.9210	1.39e3	8.13	2.25	30:	217.5902	7.39e1	0.43	0.12					
4:	85.9201	8.72e2	5.12	1.41	31:	218.0620	1.70e4	100.00	27.61					
5:	87.9211	1.33e2	0.78	0.21	32:	218.5768	1.42e2	0.83	0.23					
6:	91.0292	2.62e2	1.54	0.42	33:	219.0721	3.12e3	18.31	5.06					
7:	115.0512	2.42e3	14.19	3.92	34:	219.6147	5.37e1	0.31	0.09					
8:	116.0514	7.59e2	4.46	1.23	35:	220.0662	6.54e3	38.38	10.60					
9:	117.0534	2.69e2	1.58	0.44	36:	221.0724	9.90e2	5.81	1.60					
10:	127.0237	5.37e1	0.31	0.09	37:	222.0632	7.59e1	0.45	0.12					
11:	140.0568	5.16e2	3.03	0.84										
12:	141.0694	2.42e2	1.42	0.39										
13:	142.0677	1.28e4	75.14	20.75										
14:	142.6166	6.68e1	0.39	0.11										
15:	143.0768	1.76e3	10.30	2.84										
16:	144.0733	1.11e2	0.65	0.18										
17:	156.0836	6.58e1	0.39	0.11										
18:	168.0796	6.48e1	0.38	0.10										
19:	177.0498	4.09e2	2.40	0.66										
20:	178.0544	6.38e1	0.37	0.10										
21:	179.0503	1.56e2	0.91	0.25										
22:	181.0876	6.08e1	0.36	0.10										
23:	182.1062	2.14e2	1.25	0.35										
24:	183.1052	6.67e3	39.15	10.81										
25:	184.1120	1.12e3	6.55	1.81										
26:	185.0996	9.92e1	0.58	0.16										
27:	191.9334	7.49e1	0.44	0.12										

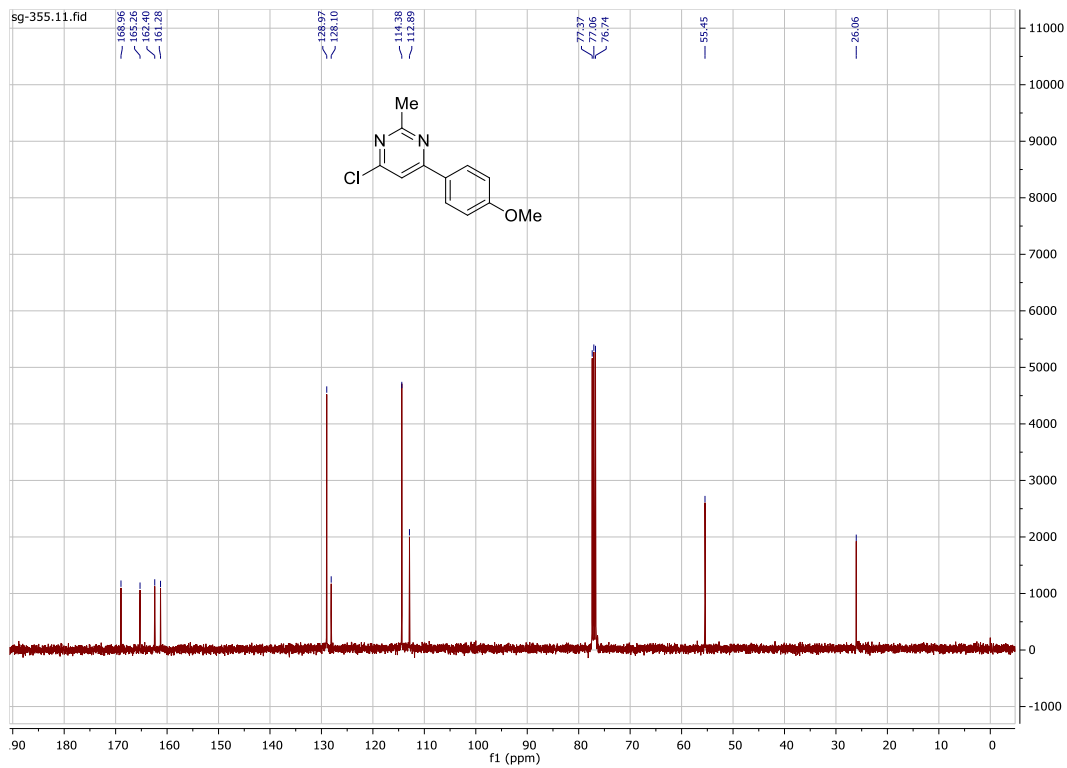




HRMS spectrum of **9c**



^1H NMR spectrum of **9d** (in CDCl_3)

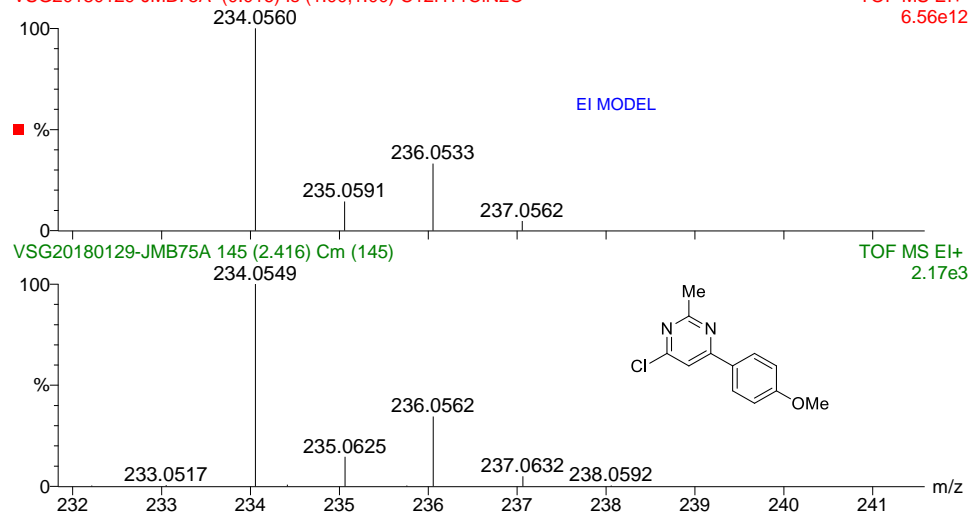


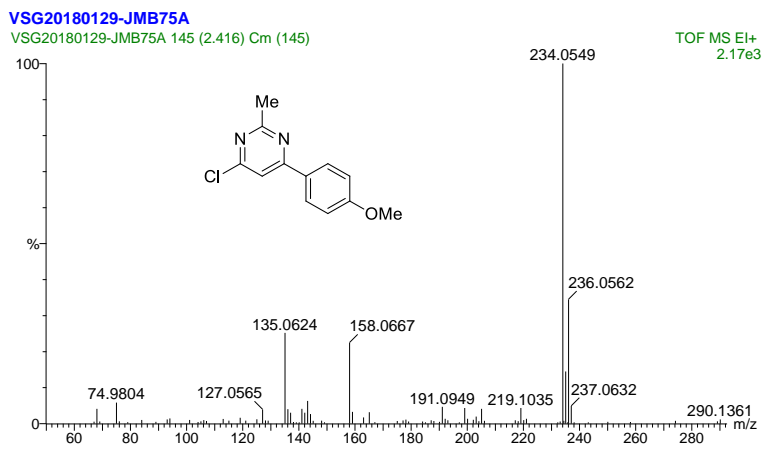
^{13}C NMR spectrum of **9d** (in CDCl_3)

VSG20180129-JMB75A

VSG20180129-JMB75A (0.016) Is (1.00,1.00) C₁₂H₁₁ClN₂O

TOF MS EI+
6.56e12



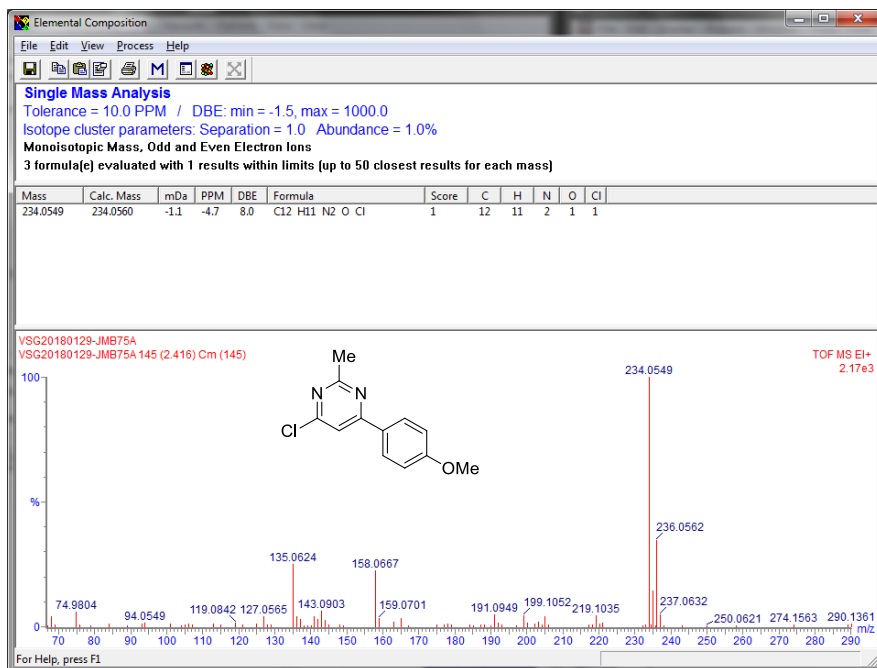


VSG20180129-JMB75A

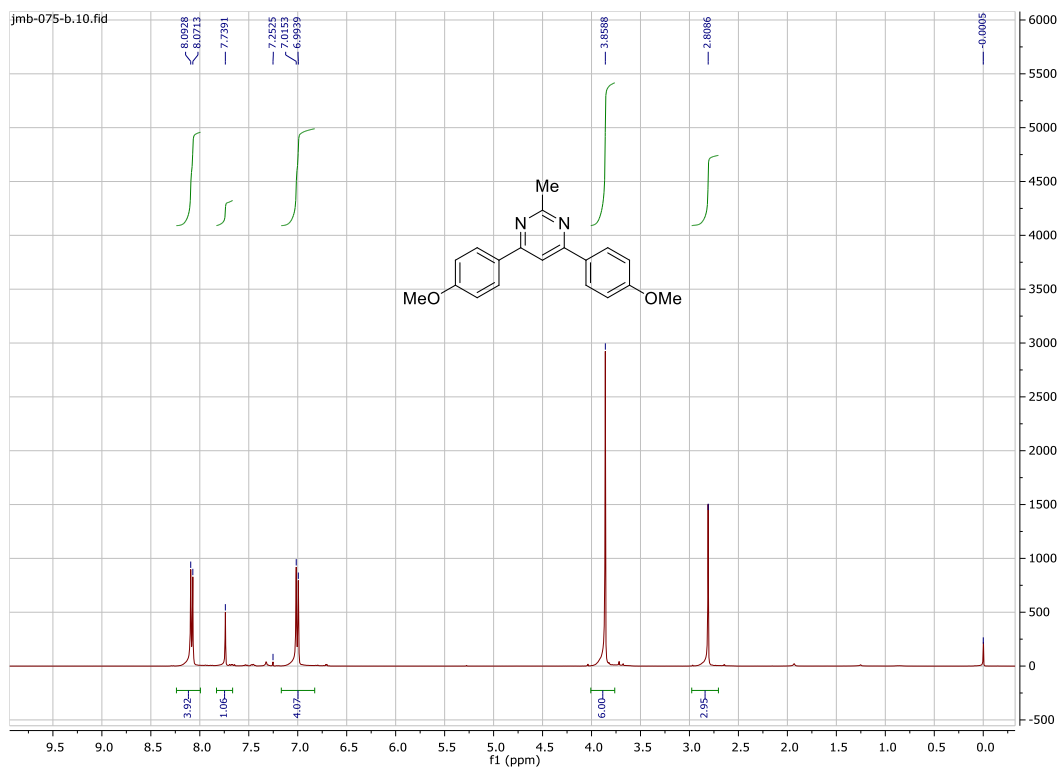
m/z	Abundance	Label
74.9804	0.01	
94.0549	0.01	
119.0842	0.01	
127.0565	0.01	
135.0624	0.01	
143.0903	0.01	
158.0667	0.01	
159.0701	0.01	
191.0949	0.01	
199.1052	0.01	
219.1035	0.01	
234.0549	1.00	
236.0562	0.01	
237.0632	0.01	
250.0621	0.01	
274.1563	0.01	
290.1361	0.01	

TOF MS EI+

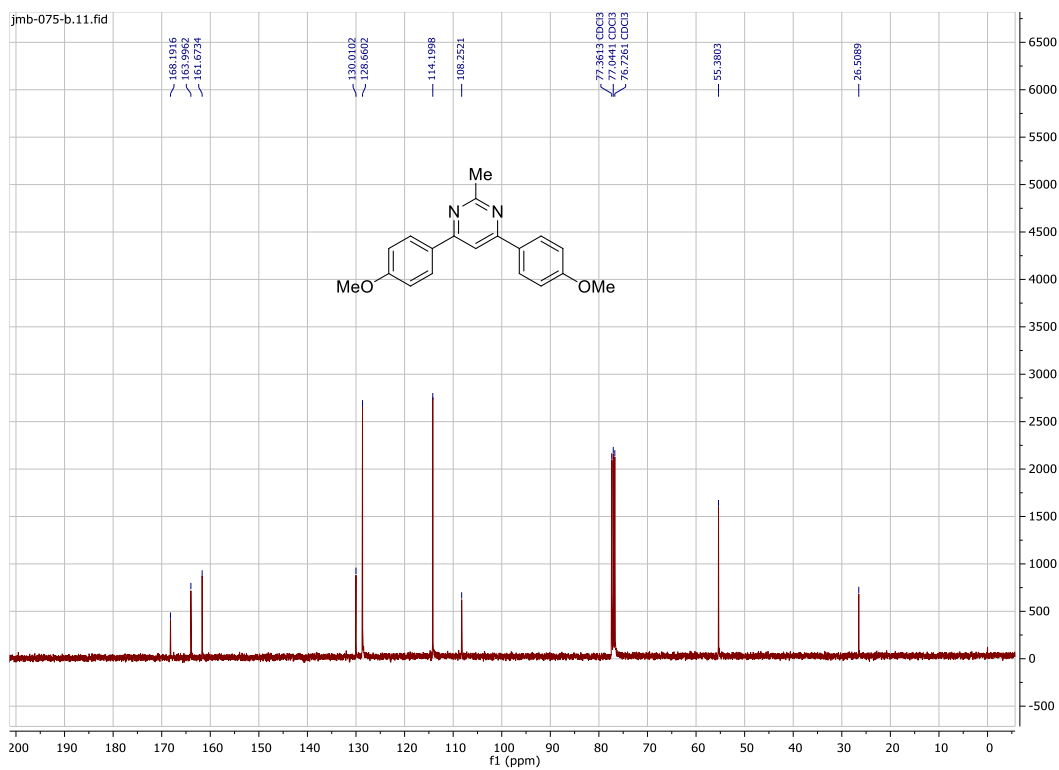
Chemical structure of 9d: Cc1nc(Cl)c(Cc2ccc(OC)cc2)n1



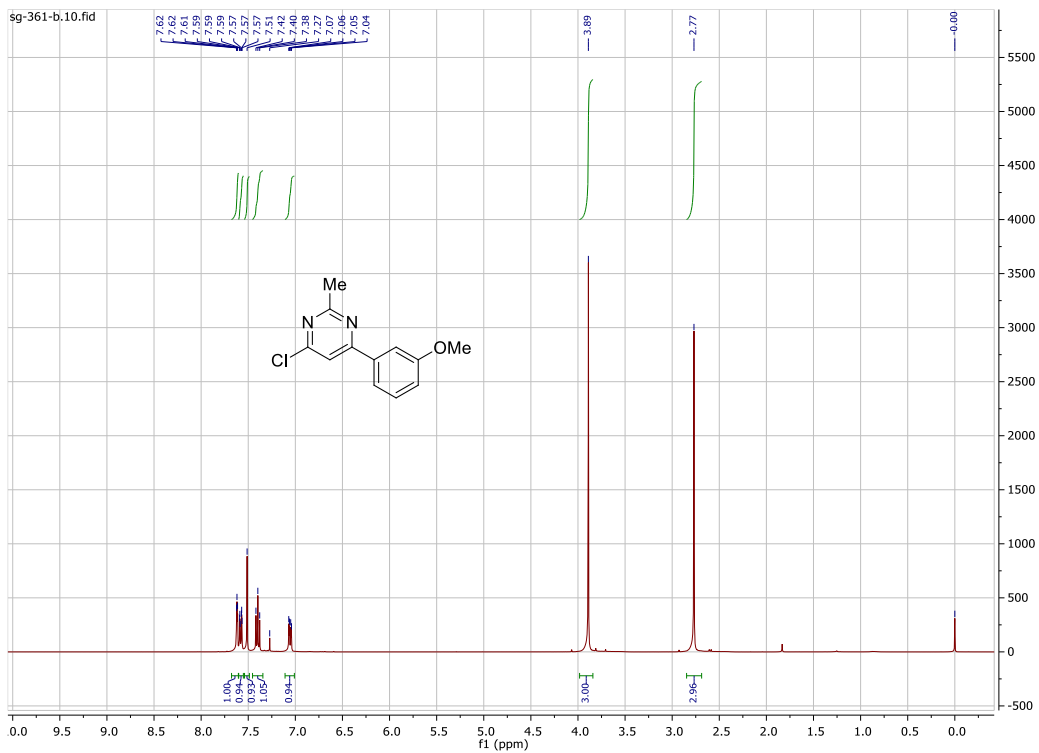
HRMS spectra of 9d



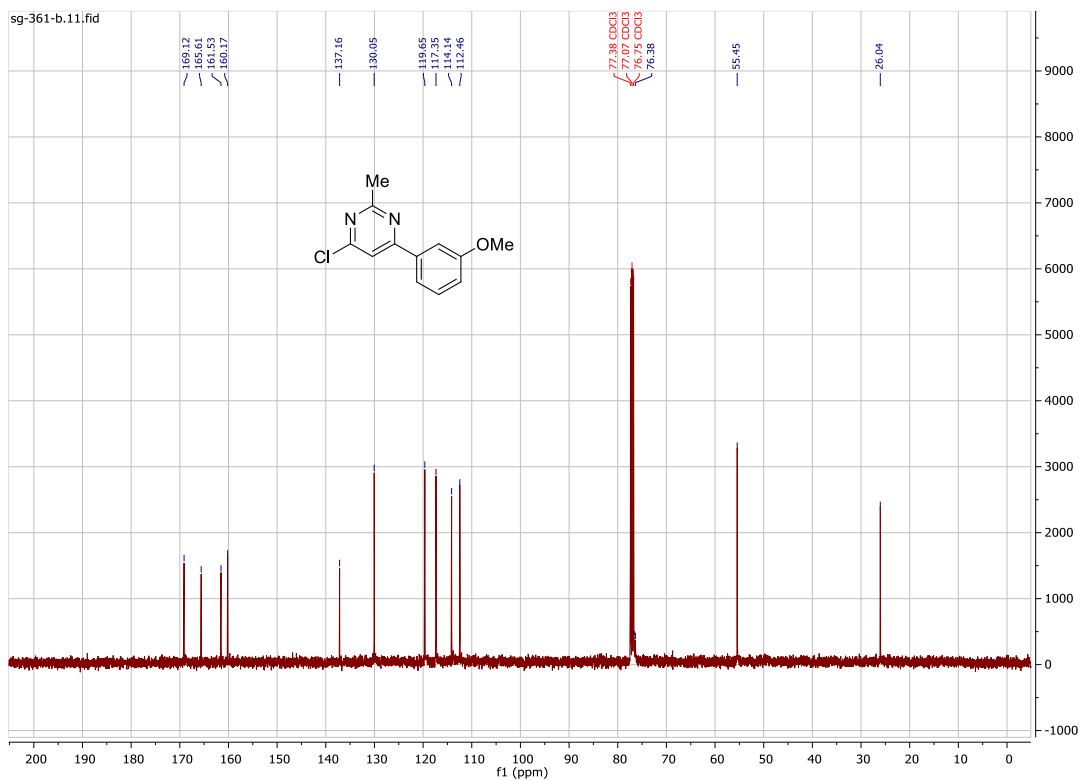
¹H NMR spectrum of **8d** (in CDCl₃)



¹³C NMR spectrum of **8d** (in CDCl₃)



^1H NMR spectrum of **9e** (in CDCl_3)

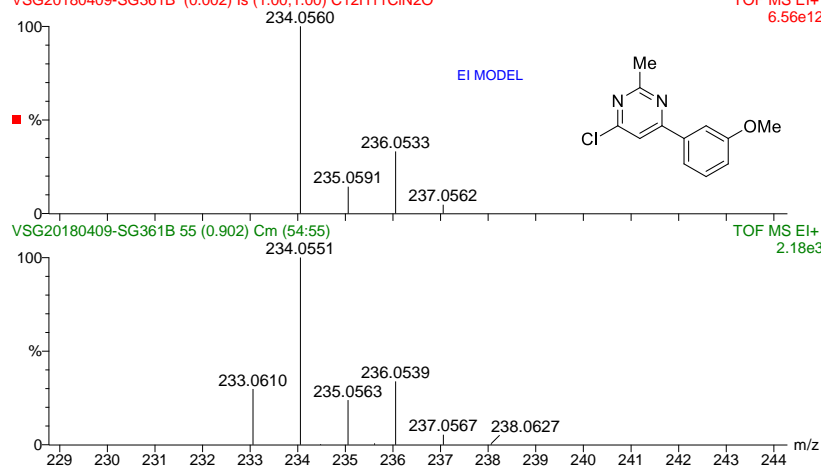


^{13}C NMR spectrum of **9e** (in CDCl_3)

VSG20180409-SG361B

VSG20180409-SG361B (0.002) Is (1.00,1.00) C12H11ClN2O

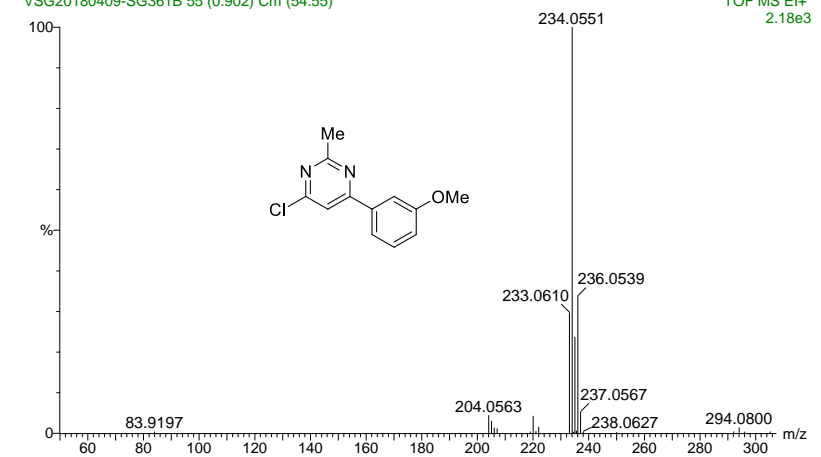
TOF MS EI+
6.56e12



VSG20180409-SG361B

VSG20180409-SG361B 55 (0.902) Cm (54:55)

TOF MS EI+
2.18e3

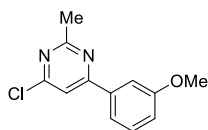


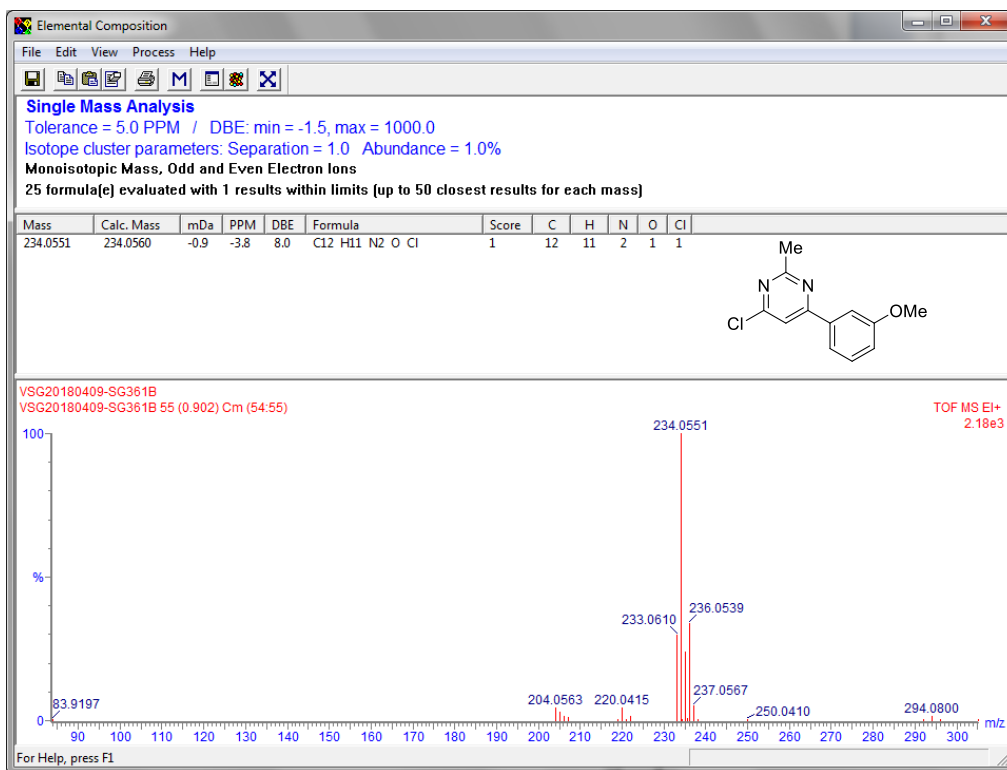
VSG20180409-SG361B

VSG20180409-SG361B 55 (0.902) Cm (54:55)

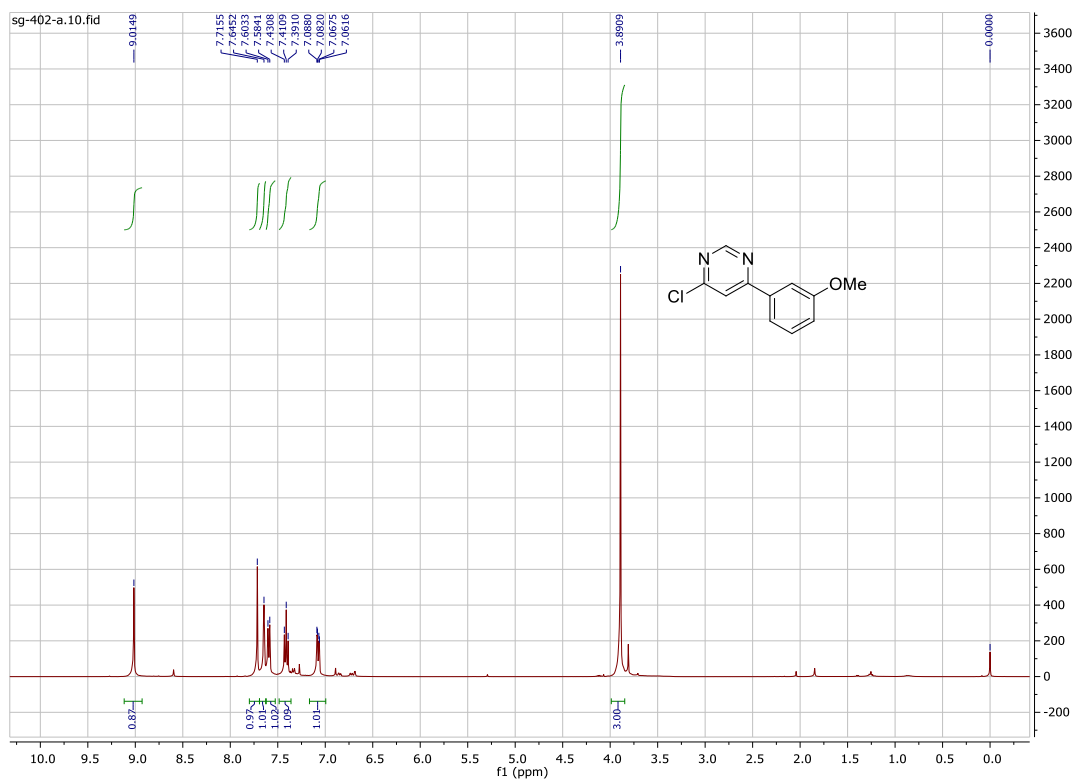
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	83.9197	8.10e0	0.37	0.17										
2:	204.0563	9.62e1	4.41	2.05										
3:	205.0578	6.58e1	3.02	1.40										
4:	206.0604	2.94e1	1.35	0.62										
5:	207.0617	2.53e1	1.16	0.54										
6:	219.0164	8.10e0	0.37	0.17										
7:	220.0415	9.32e1	4.28	1.98										
8:	221.0526	1.11e1	0.51	0.24										
9:	222.0379	3.44e1	1.58	0.73										
10:	233.0610	6.48e2	29.74	13.78										
11:	234.0551	2.18e3	100.00	46.35										
12:	234.4794	7.09e0	0.33	0.15										
13:	235.0563	5.17e2	23.75	11.01										
14:	235.6126	1.42e1	0.65	0.30										
15:	236.0539	7.36e2	33.79	15.66										
16:	237.0567	1.14e2	5.25	2.43										
17:	238.0627	9.11e0	0.42	0.19										
18:	250.0410	5.06e0	0.23	0.11										
19:	292.1000	9.11e0	0.42	0.19										
20:	294.0800	3.04e1	1.39	0.65										
21:	296.0500	8.10e0	0.37	0.17										
22:	305.1631	9.11e0	0.42	0.19										

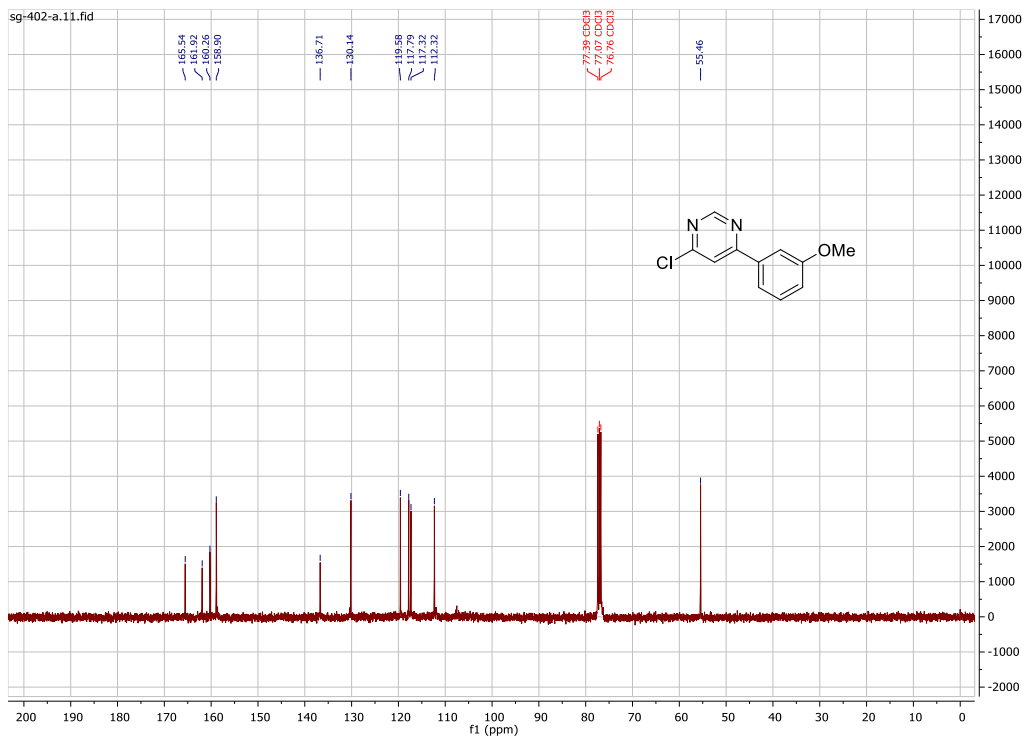




HRMS spectra of **9e**



^1H NMR spectrum of **9f** (in CDCl_3)

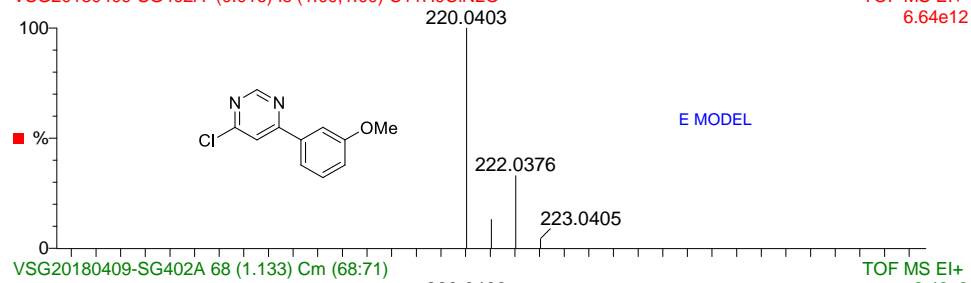


^{13}C NMR spectrum of **9f** (in CDCl_3)

VSG20180409-SG402A

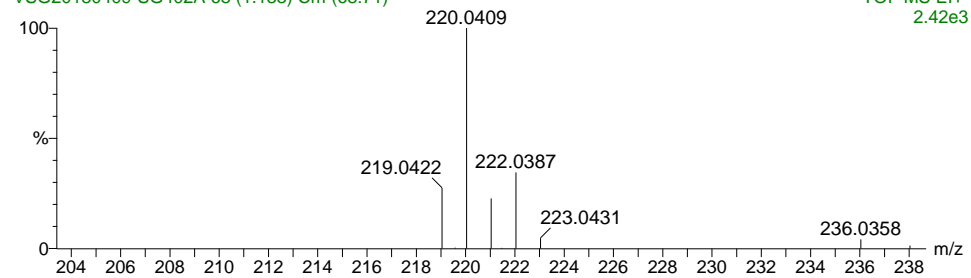
VSG20180409-SG402A (0.016) Is (1.00,1.00) C11H9ClN2O

TOF MS EI+
6.64e12



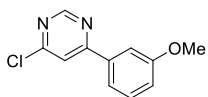
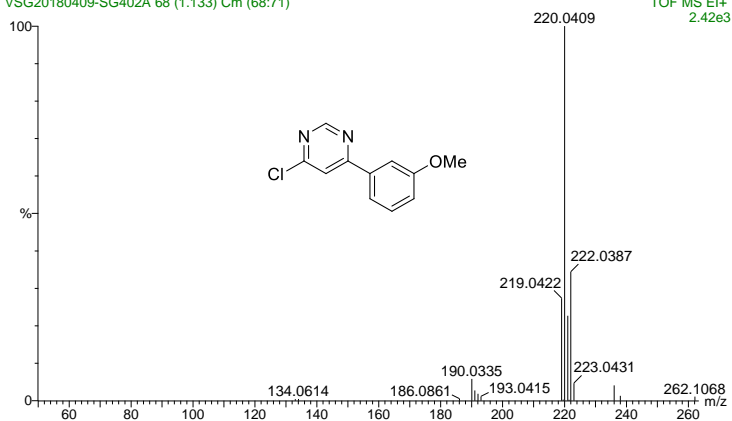
VSG20180409-SG402A 68 (1.133) Cm (68:71)

TOF MS EI+
2.42e3



VSG20180409-SG402A

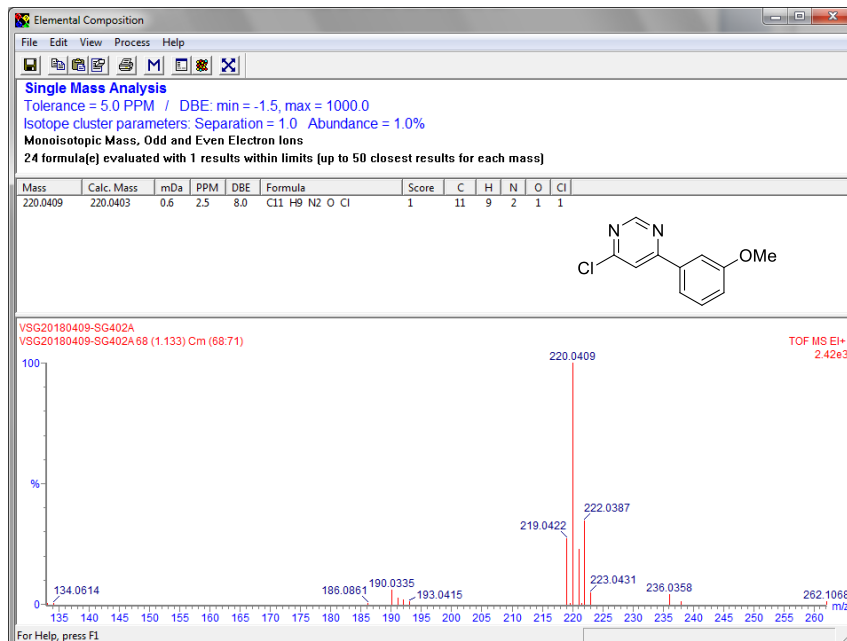
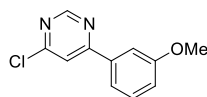
VSG20180409-SG402A 68 (1.133) Cm (68:71)



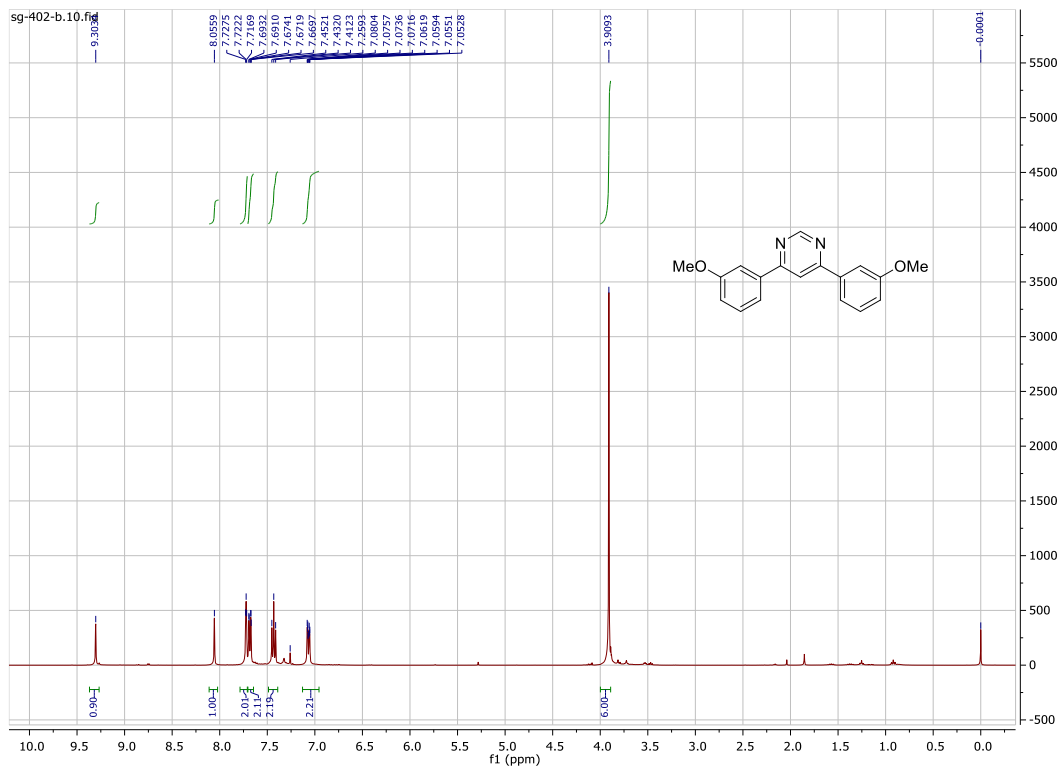
VSG20180409-SG402A

VSG20180409-SG402A 68 (1.133) Cm (68:71)

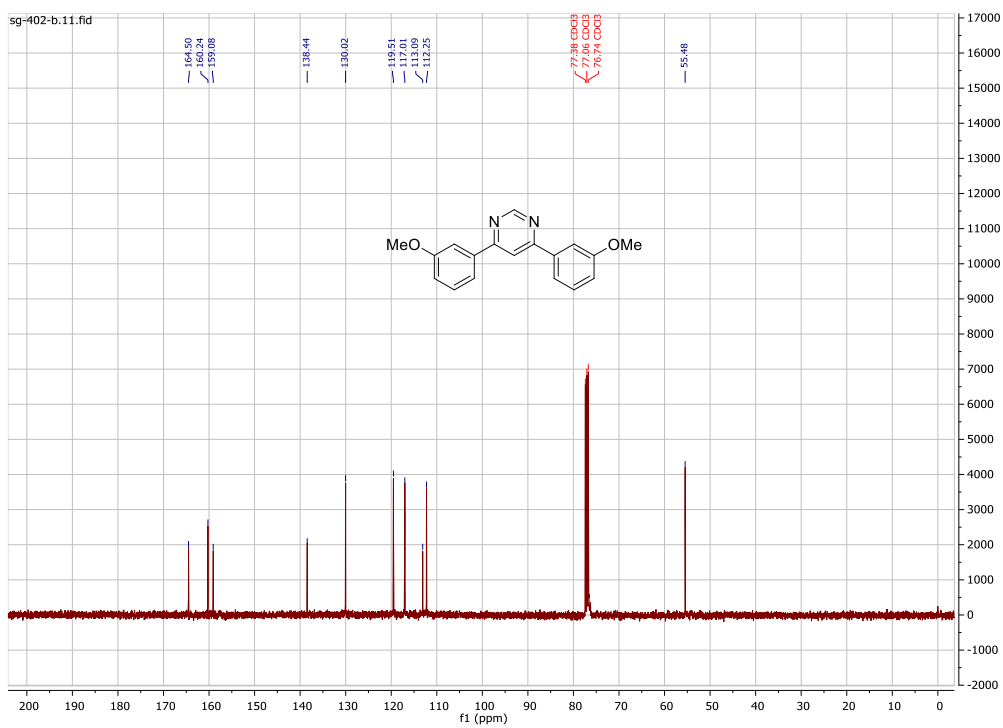
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	133.0504	9.11e0	0.38	0.17										
2:	134.0614	1.01e1	0.42	0.19										
3:	186.0861	1.11e1	0.46	0.21										
4:	190.0335	1.40e2	5.78	2.65										
5:	191.0454	6.48e1	2.68	1.23										
6:	192.0366	4.35e1	1.80	0.82										
7:	193.0415	2.63e1	1.09	0.50										
8:	219.0422	6.60e2	27.32	12.51										
9:	219.5709	6.08e0	0.25	0.12										
10:	220.0409	2.42e3	100.02	45.79										
11:	221.0402	5.48e2	22.67	10.38										
12:	221.4659	5.06e0	0.21	0.10										
13:	222.0387	8.31e2	34.40	15.75										
14:	223.0431	1.12e2	4.65	2.13										
15:	236.0358	9.82e1	4.06	1.86										
16:	238.0321	3.04e1	1.26	0.58										
17:	262.1068	2.53e1	1.05	0.48										



HRMS spectra of 9f



^1H NMR spectrum of **8f** (in CDCl_3)

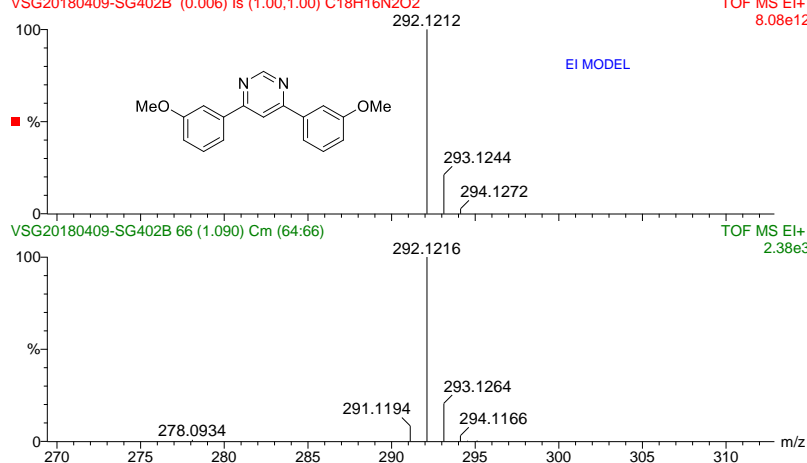


^{13}C NMR spectrum of **8f** (in CDCl_3)

VSG20180409-SG402B

VSG20180409-SG402B (0.006) Is (1.00,1.00) C18H16N2O2

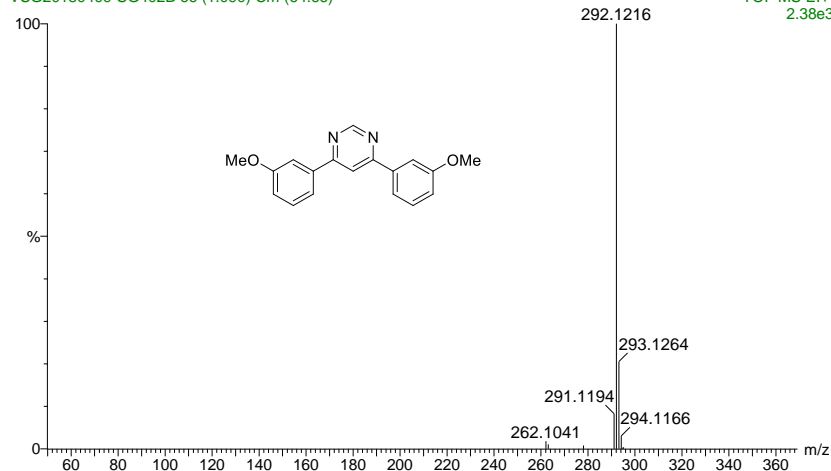
TOF MS EI+
8.08e12



VSG20180409-SG402B

VSG20180409-SG402B 66 (1.090) Cm (64:66)

TOF MS EI+
2.38e3

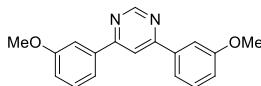


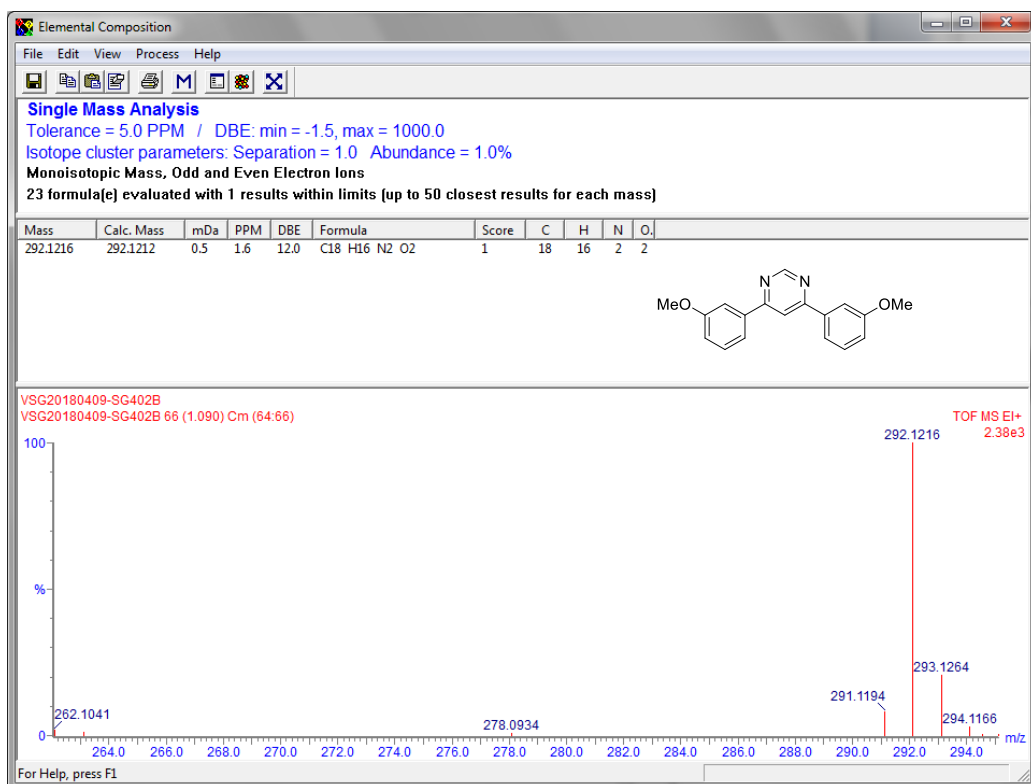
VSG20180409-SG402B

VSG20180409-SG402B 66 (1.090) Cm (64:66)

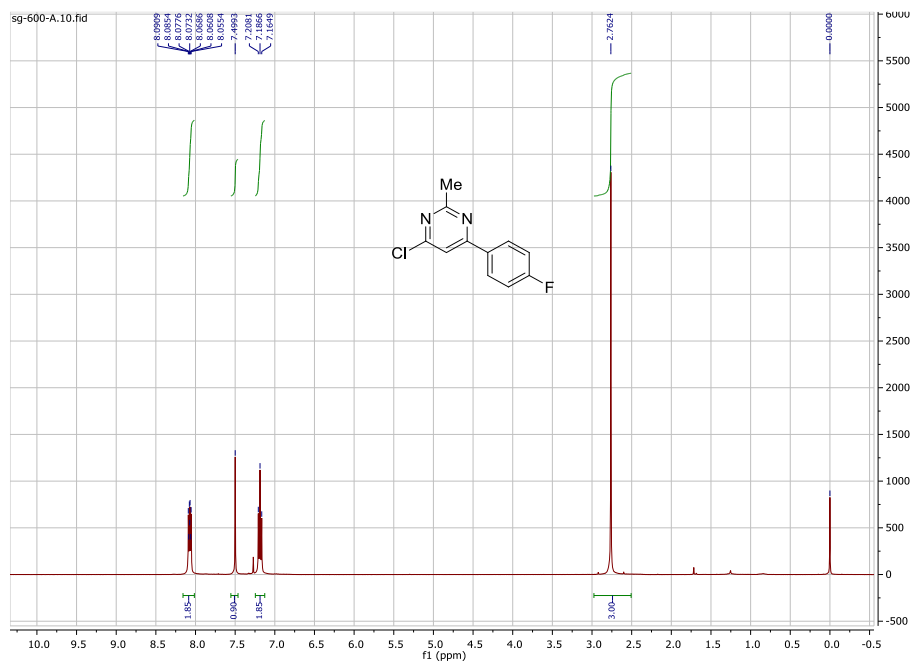
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	262.1041	4.25e1	1.79	1.30										
2:	263.1137	2.43e1	1.02	0.74										
3:	278.0934	1.82e1	0.77	0.56										
4:	291.1194	1.94e2	8.17	5.94										
5:	292.1216	2.38e3	100.00	72.77										
6:	293.1264	4.87e2	20.46	14.89										
7:	294.1166	6.99e1	2.93	2.14										
8:	294.5481	6.08e0	0.26	0.19										
9:	295.1140	8.10e0	0.34	0.25										





HRMS spectra of **8f**



¹H NMR spectrum of **9g** (in CDCl₃)

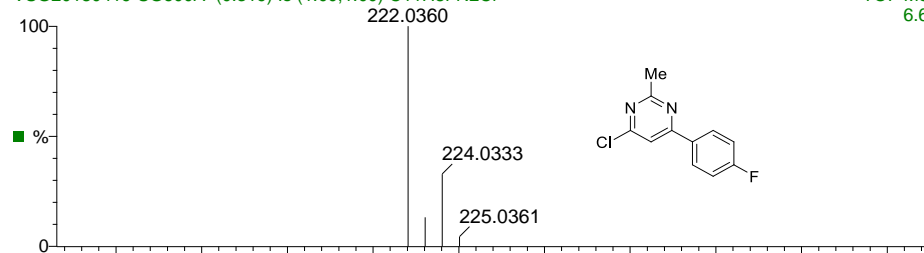


¹³C NMR spectrum of **9g** (in CDCl₃)

VSG20180419-SG600A

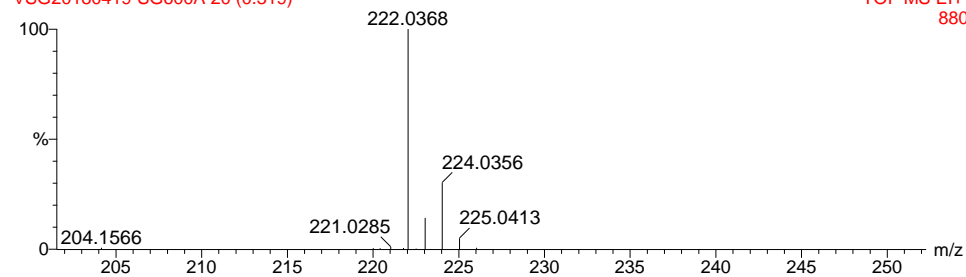
VSG20180419-SG600A (0.319) Is (1.00,1.00) C₁₁H₈FN₂Cl

TOF MS EI+
6.65e12



VSG20180419-SG600A 20 (0.319)

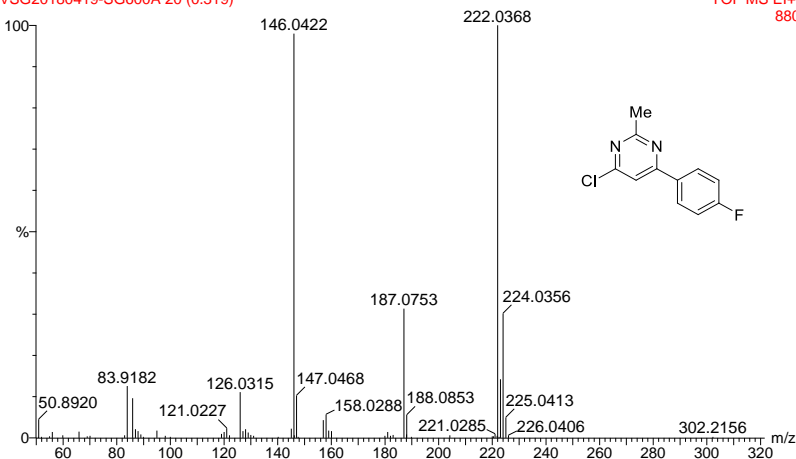
TOF MS EI+
880



VSG20180419-SG600A

VSG20180419-SG600A 20 (0.319)

TOF MS EI+
880

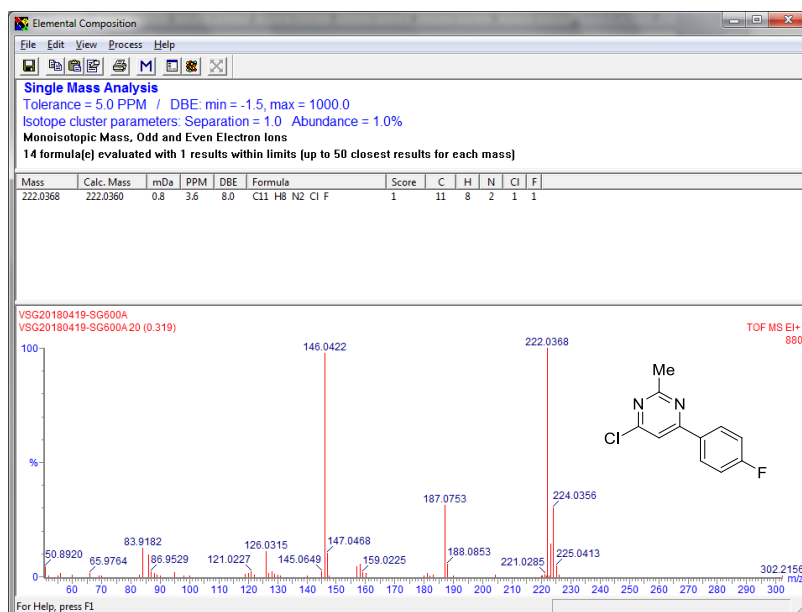
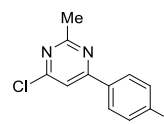


VSG20180419-SG600A

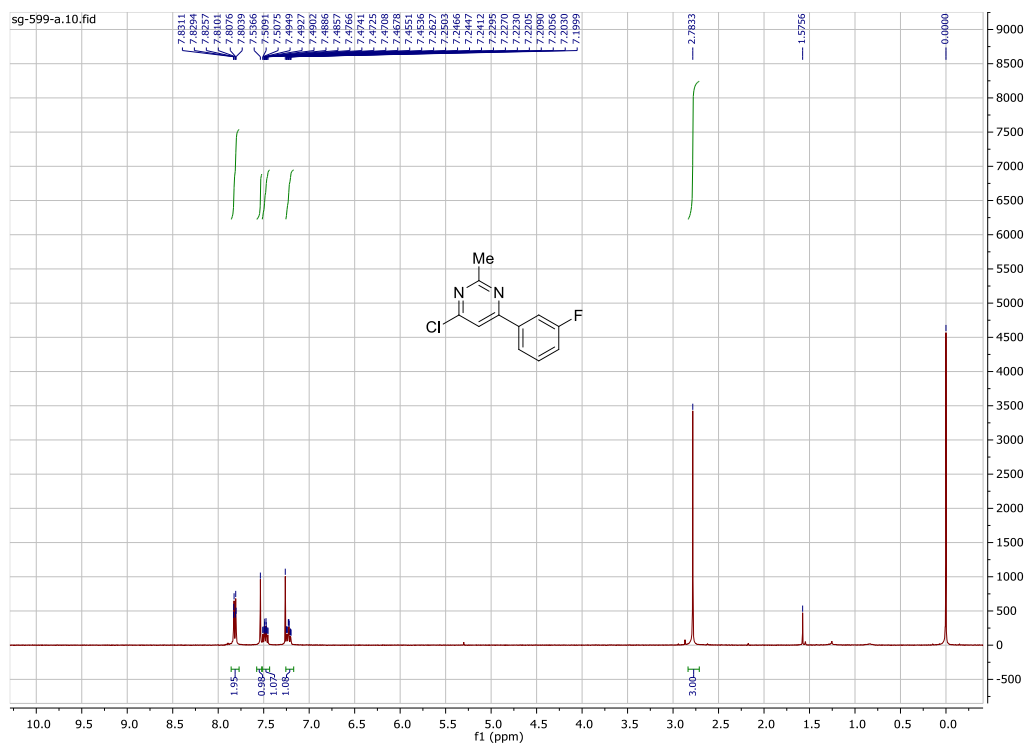
VSG20180419-SG600A 20 (0.319)

TOF MS EI+

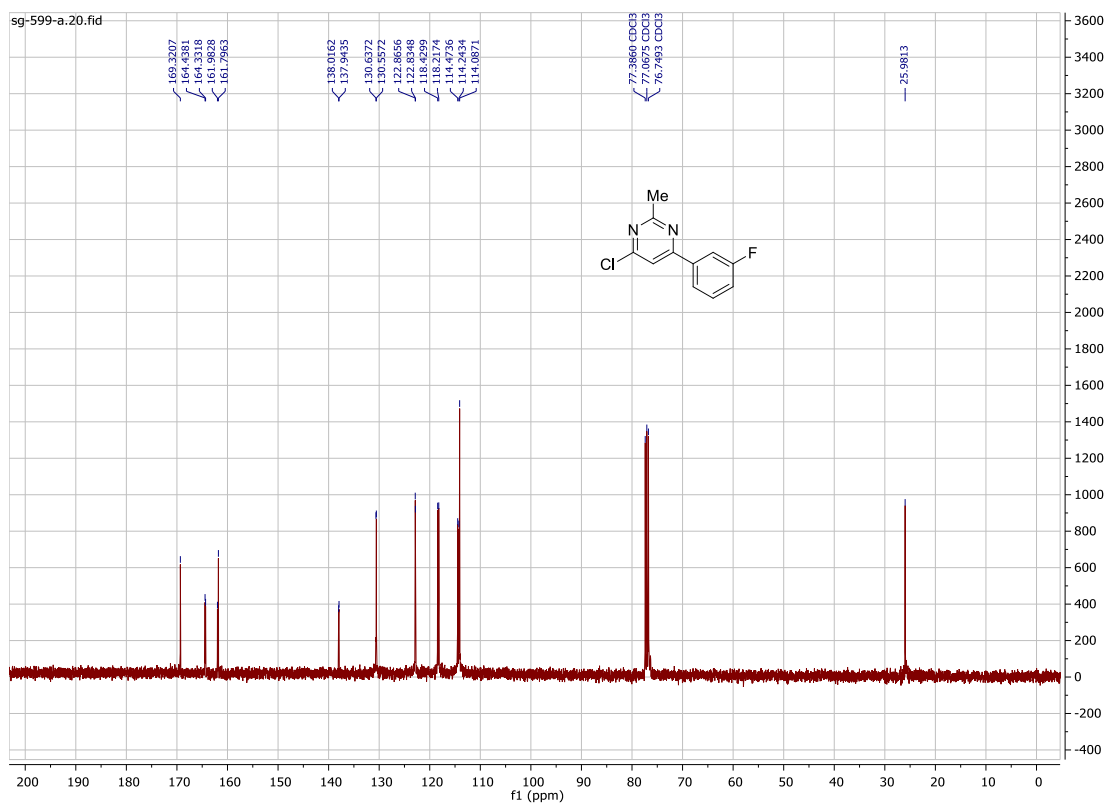
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	50.7776	2.03e0	0.23	0.06	31:	145.0649	1.92e1	2.19	0.58					
2:	50.8920	3.95e1	4.49	1.18	32:	146.0422	8.62e2	97.93	25.77					
3:	51.9301	2.03e0	0.23	0.06	33:	146.2049	5.06e0	0.58	0.15					
4:	54.9778	3.04e0	0.35	0.09	34:	147.0468	9.01e1	10.24	2.69					
5:	55.9771	1.22e1	1.38	0.36	35:	147.6183	2.03e0	0.23	0.06					
6:	59.9043	5.06e0	0.58	0.15	36:	157.0202	3.75e1	4.26	1.12					
7:	65.9764	1.32e1	1.50	0.39	37:	158.0288	4.96e1	5.64	1.48					
8:	69.0241	3.04e0	0.35	0.09	38:	159.0225	1.52e1	1.73	0.45					
9:	70.0268	4.05e0	0.46	0.12	39:	160.0337	1.42e1	1.61	0.42					
10:	82.9091	5.06e0	0.58	0.15	40:	179.9894	4.05e0	0.46	0.12					
11:	83.9182	1.10e2	12.54	3.30	41:	181.0199	1.22e1	1.38	0.36					
12:	85.9150	8.41e1	9.55	2.51	42:	182.0165	4.05e0	0.46	0.12					
13:	86.9529	1.82e1	2.07	0.55	43:	183.0107	6.08e0	0.69	0.18					
14:	87.9144	1.42e1	1.61	0.42	44:	187.0753	2.75e2	31.30	8.24					
15:	88.9593	7.09e0	0.81	0.21	45:	188.0384	7.09e0	0.81	0.21					
16:	89.9727	2.03e0	0.23	0.06	46:	188.0853	4.86e1	5.52	1.45					
17:	95.0018	1.52e1	1.73	0.45	47:	189.8407	2.03e0	0.23	0.06					
18:	98.0870	4.05e0	0.46	0.12	48:	204.1566	5.06e0	0.58	0.15					
19:	100.0072	2.03e0	0.23	0.06	49:	220.0063	3.04e0	0.35	0.09					
20:	119.0172	8.10e0	0.92	0.24	50:	220.4177	3.04e0	0.35	0.09					
21:	120.0330	1.22e1	1.38	0.36	51:	221.0285	8.10e0	0.92	0.24					
22:	121.0227	2.03e1	2.30	0.61	52:	221.7785	4.05e0	0.46	0.12					
23:	122.0347	5.06e0	0.58	0.15	53:	222.0368	8.80e2	99.97	26.30					
24:	126.0315	9.72e1	11.05	2.91	54:	222.5115	2.03e0	0.23	0.06					
25:	127.0402	1.42e1	1.61	0.42	55:	223.0389	1.25e2	14.15	3.72					
26:	128.0148	1.82e1	2.07	0.55	56:	224.0356	2.65e2	30.15	7.93					
27:	129.0273	1.11e1	1.27	0.33	57:	225.0413	4.35e1	4.95	1.30					
28:	130.0000	6.08e0	0.69	0.18	58:	226.0406	5.06e0	0.58	0.15					
29:	131.0252	4.05e0	0.46	0.12	59:	302.2156	2.03e0	0.23	0.06					
30:	140.1742	2.03e0	0.23	0.06										



HRMS spectra of 9g



¹H NMR spectrum of **9h** (in CDCl₃)

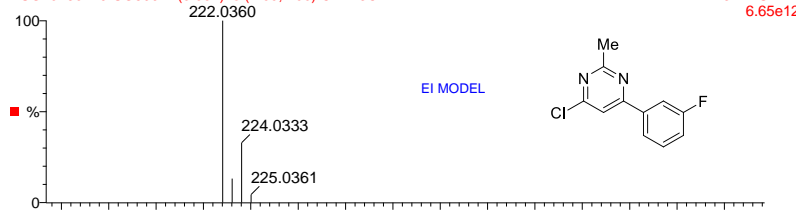


¹³C NMR spectrum of **9h** (in CDCl₃)

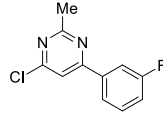
VSG20180419-SG599A

VSG20180419-SG599A (0.001) Is (1.00,1.00) C11H8ClFN2

TOF MS EI+
6.65e12

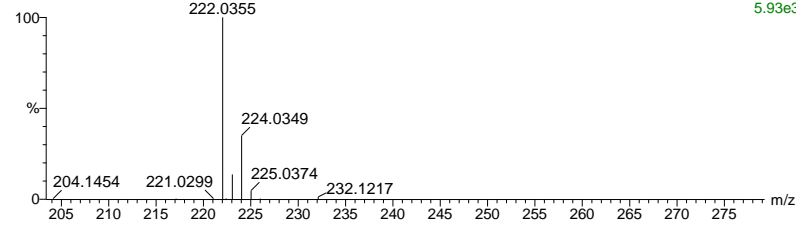


EI MODEL



VSG20180419-SG599A 8 (0.116) Cm (8:12)

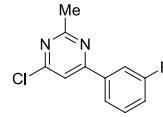
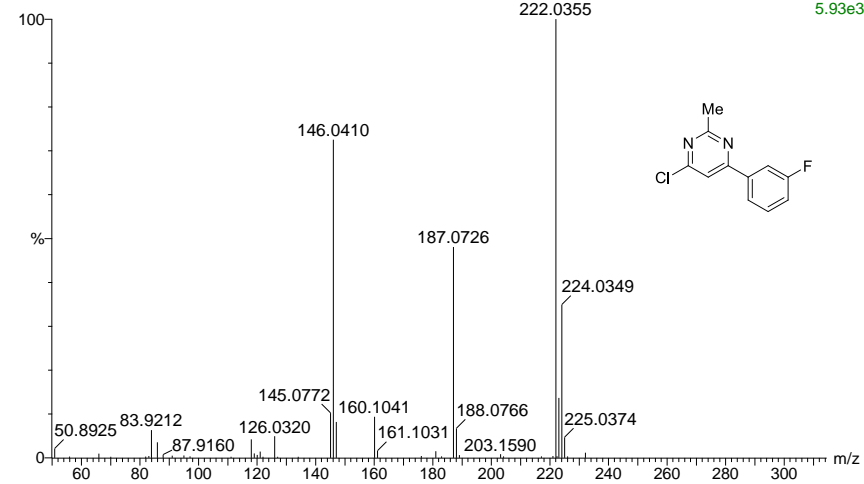
TOF MS EI+
5.93e3



VSG20180419-SG599A

VSG20180419-SG599A 8 (0.116) Cm (8:12)

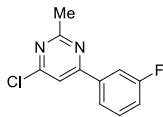
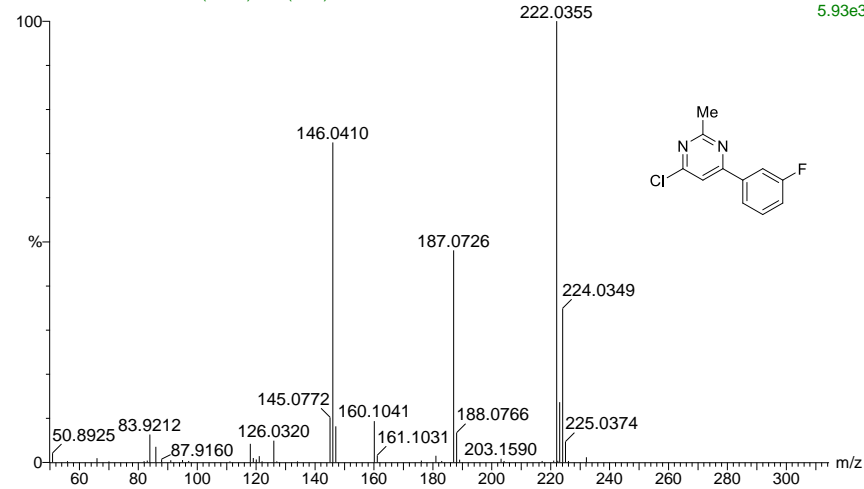
TOF MS EI+
5.93e3



VSG20180419-SG599A

VSG20180419-SG599A 8 (0.116) Cm (8:12)

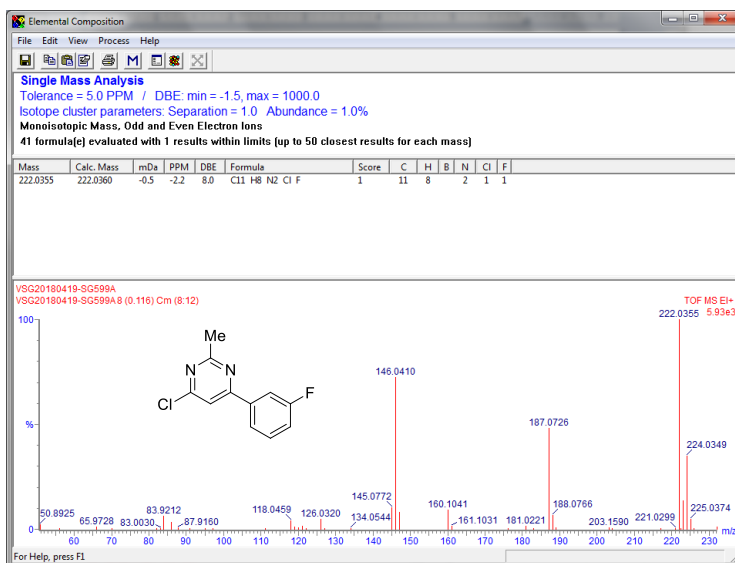
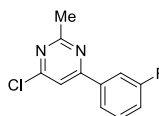
TOF MS EI+
5.93e3



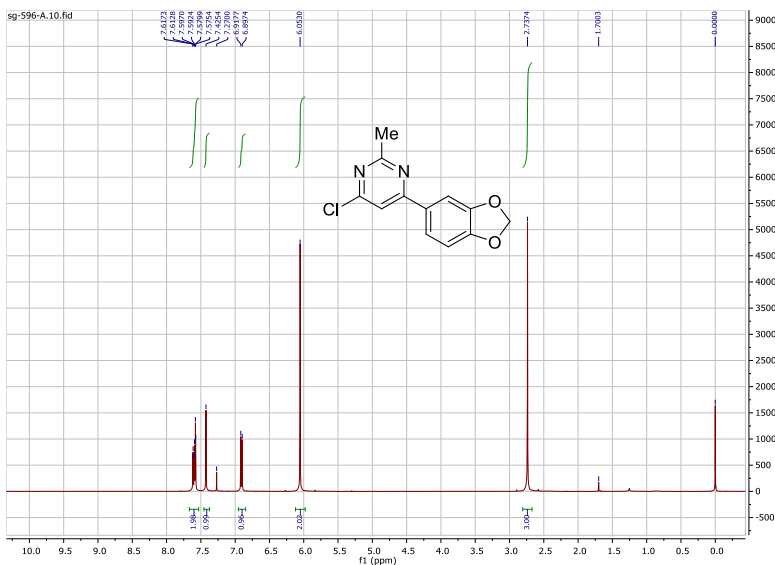
VSG20180419-SG599A

VSG20180419-SG599A 8 (0.116) Cm (8:12)

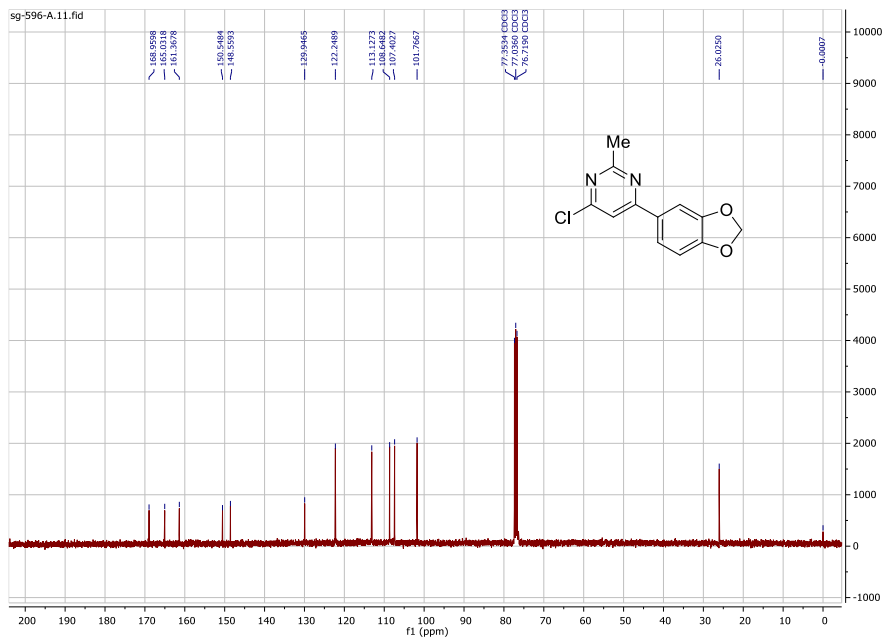
				TOF MS EI+					
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	50.8925	1.24e2	2.08	0.60	31:	188.0766	3.95e2	6.66	1.90
2:	55.9825	1.52e1	0.26	0.07	32:	189.0773	3.44e1	0.58	0.17
3:	65.9728	5.57e1	0.94	0.27	33:	203.1590	4.86e1	0.82	0.23
4:	70.0285	1.22e1	0.20	0.06	34:	204.1454	1.72e1	0.29	0.08
5:	81.9576	1.62e1	0.27	0.08	35:	217.1083	1.72e1	0.29	0.08
6:	83.0030	2.33e1	0.39	0.11	36:	221.0299	2.33e1	0.39	0.11
7:	83.9212	3.73e2	6.29	1.80	37:	222.0355	5.93e3	100.00	28.59
8:	85.9157	2.07e2	3.48	1.00	38:	222.4023	2.03e1	0.34	0.10
9:	87.9160	4.05e1	0.68	0.20	39:	223.0418	8.08e2	13.63	3.90
10:	91.0150	2.84e1	0.48	0.14	40:	224.0349	2.07e3	34.89	9.97
11:	95.0002	3.04e1	0.51	0.15	41:	225.0374	2.75e2	4.85	1.33
12:	97.0027	1.82e1	0.31	0.09	42:	226.0016	1.82e1	0.31	0.09
13:	111.1039	1.22e1	0.20	0.06	43:	232.1217	6.68e1	1.13	0.32
14:	118.0459	2.47e2	4.17	1.19					
15:	119.0438	5.67e1	0.96	0.27					
16:	120.0291	3.85e1	0.65	0.19					
17:	121.0279	8.30e1	1.40	0.40					
18:	122.0271	1.22e1	0.20	0.06					
19:	126.0320	2.91e2	4.90	1.40					
20:	127.0440	1.32e1	0.22	0.06					
21:	134.0544	1.32e1	0.22	0.06					
22:	145.0772	6.02e2	10.15	2.90					
23:	146.0410	4.30e3	72.49	20.72					
24:	147.0449	4.83e2	8.15	2.33					
25:	160.1041	5.52e2	9.31	2.66					
26:	161.1031	9.22e1	1.55	0.44					
27:	176.0930	2.23e1	0.38	0.11					
28:	181.0221	8.71e1	1.47	0.42					
29:	183.0206	1.72e1	0.29	0.08					
30:	187.0726	2.85e3	48.04	13.73					



HRMS spectra of 9h



¹H NMR spectrum of 9i (in CDCl₃)

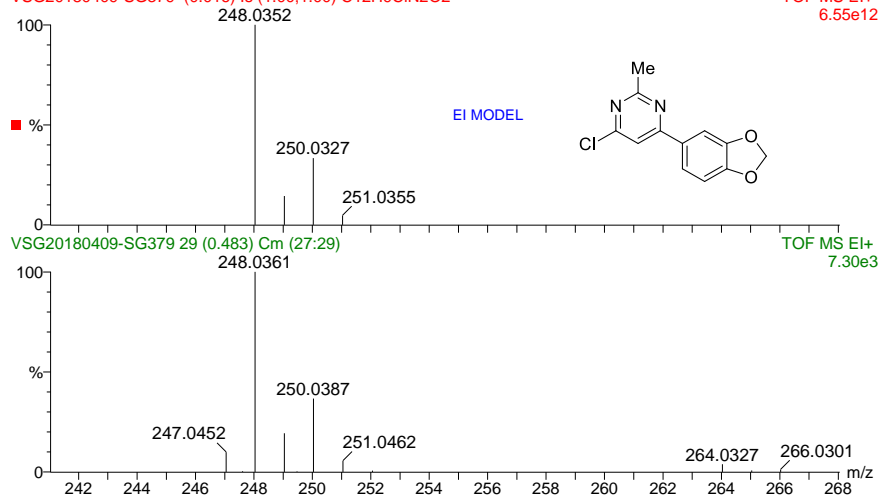


^{13}C NMR spectrum of **9i** (in CDCl_3)

VSG20180409-SG379

VSG20180409-SG379 (0.016) Is (1.00,1.00) C12H9ClN2O2

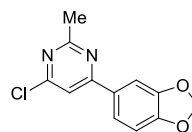
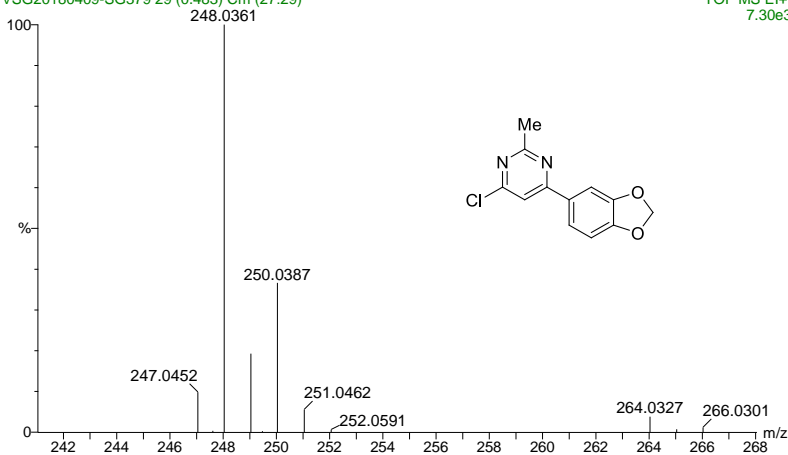
TOF MS EI+
6.55e12



VSG20180409-SG379

VSG20180409-SG379 29 (0.483) Cm (27:29)

TOF MS EI+
7.30e3

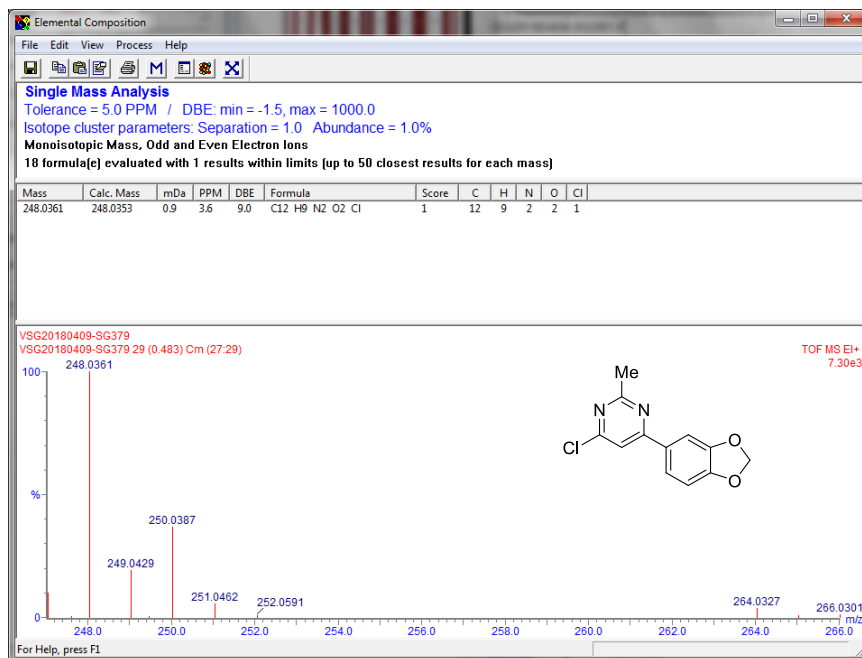
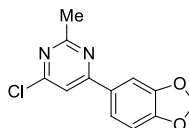


VSG20180409-SG379

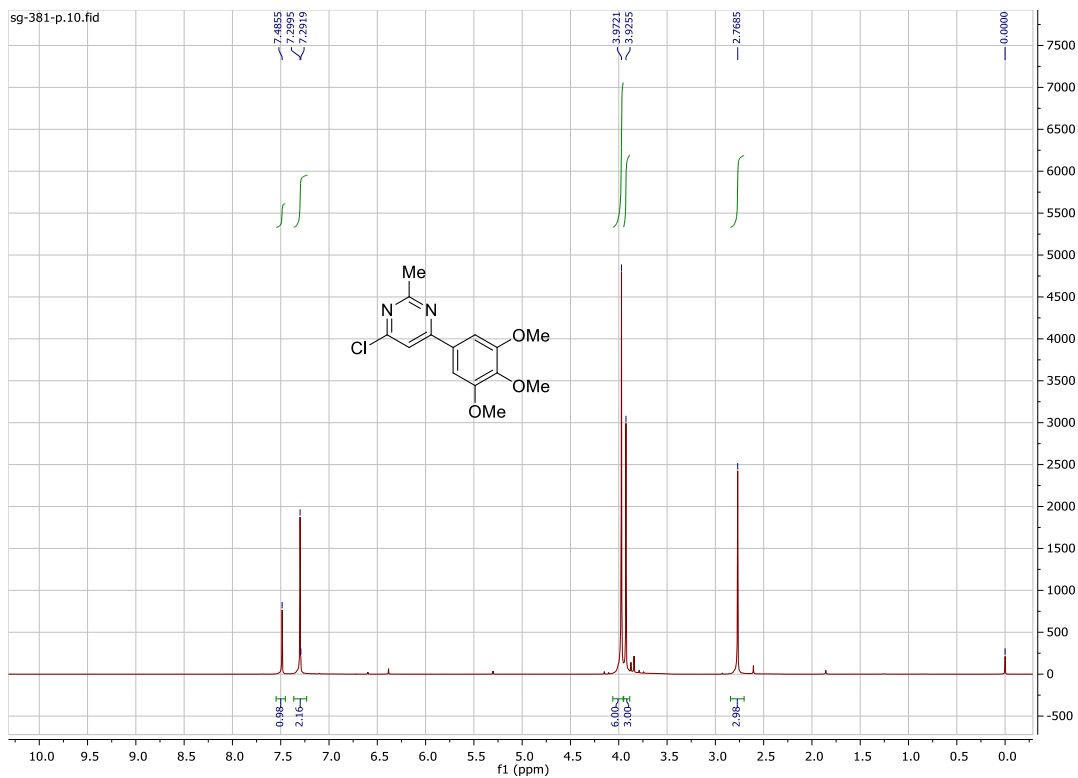
VSG20180409-SG379 29 (0.483) Cm (27:29)

TOF MS EI+

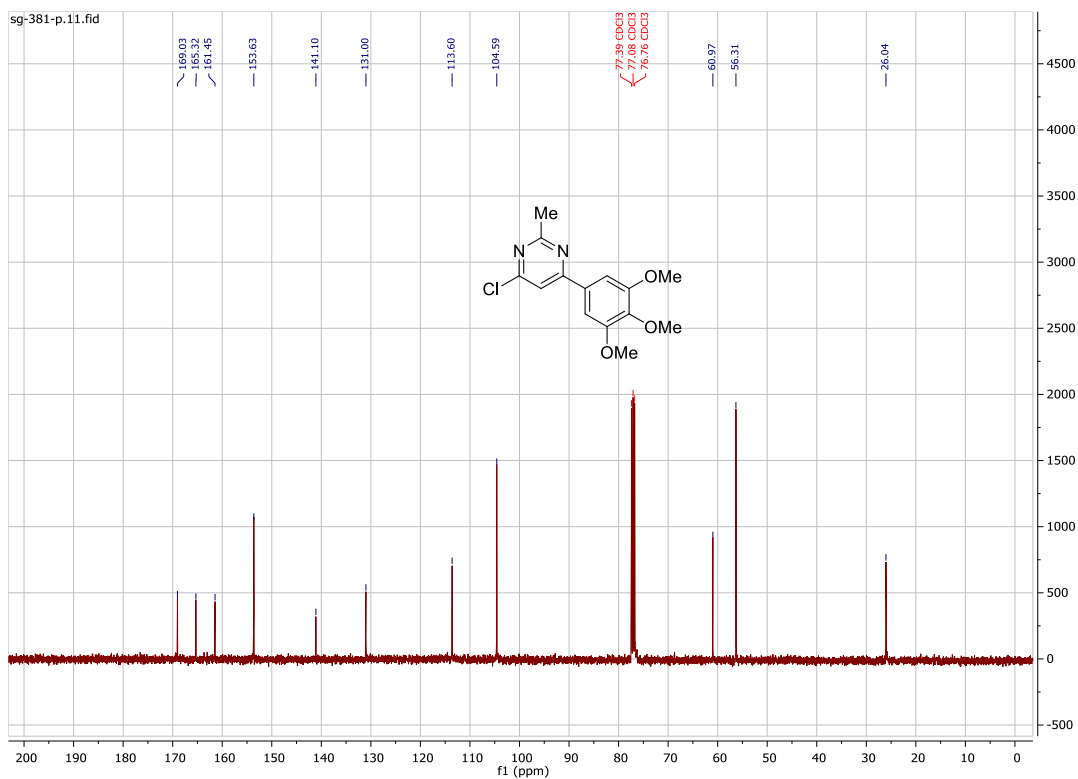
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	247.0452	7.15e2	9.79	4.64										
2:	247.6120	2.03e1	0.28	0.13										
3:	248.0361	7.30e3	100.00	47.41										
4:	249.0429	1.40e3	19.22	9.11										
5:	249.4759	1.62e1	0.22	0.11										
6:	250.0387	2.67e3	36.60	17.35										
7:	251.0462	4.03e2	5.52	2.62										
8:	252.0591	4.35e1	0.60	0.28										
9:	264.0327	2.74e2	3.76	1.78										
10:	265.0410	5.06e1	0.69	0.33										
11:	266.0301	8.20e1	1.12	0.53										



HRMS spectra of **9i**



^1H NMR spectrum of **9j** (in CDCl_3)

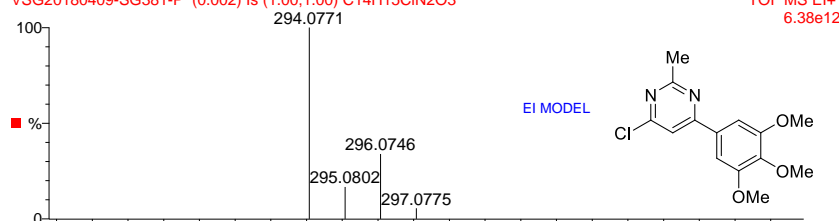


^{13}C NMR spectrum of **9j** (in CDCl_3)

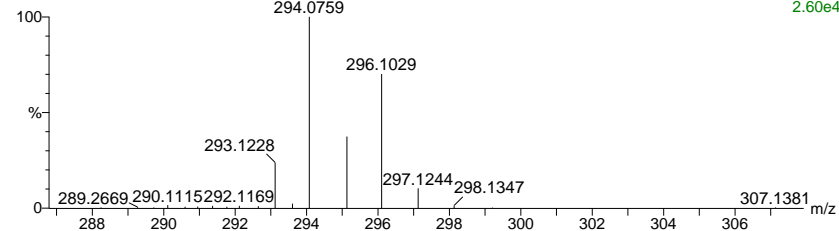
VSG20180409-SG381-P

VSG20180409-SG381-P (0.002) Is (1.00,1.00) C14H15ClN2O3

TOF MS EI+
6.38e12



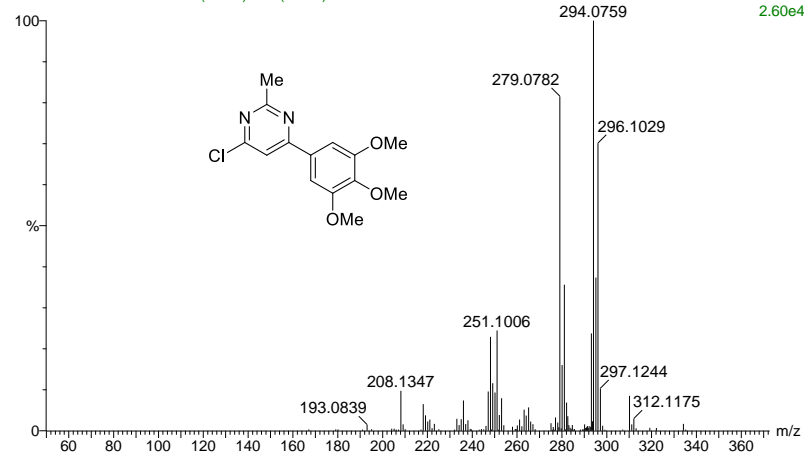
VSG20180409-SG381-P 69 (1.135) Cm (67:70) TOF MS EI+
2.60e4



VSG20180409-SG381-P

VSG20180409-SG381-P 69 (1.135) Cm (67:70)

TOF MS EI+
2.60e4

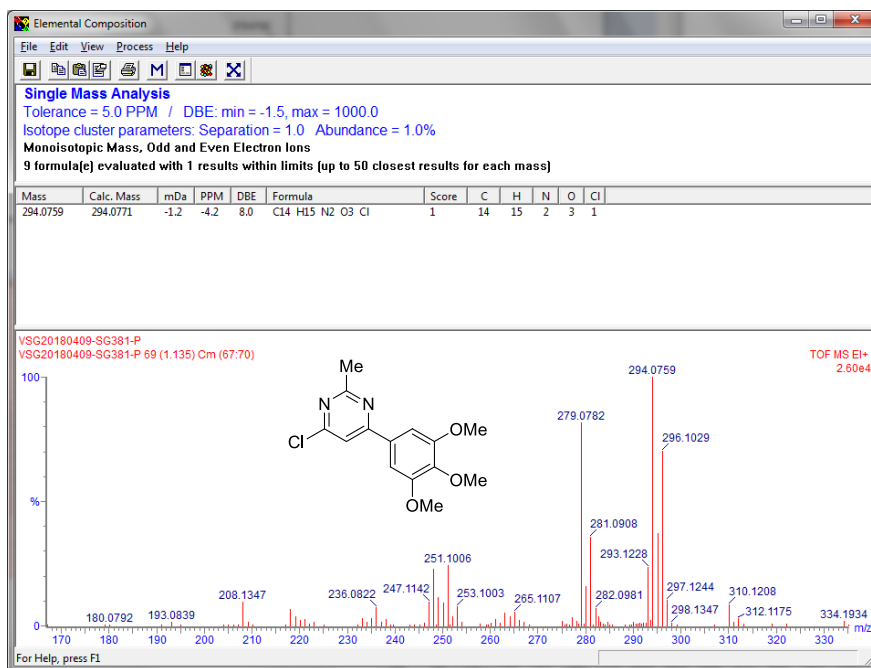


VSG20180409-SG381-P
VSG20180409-SG381-P 69 (1.135) Cm (67:70)

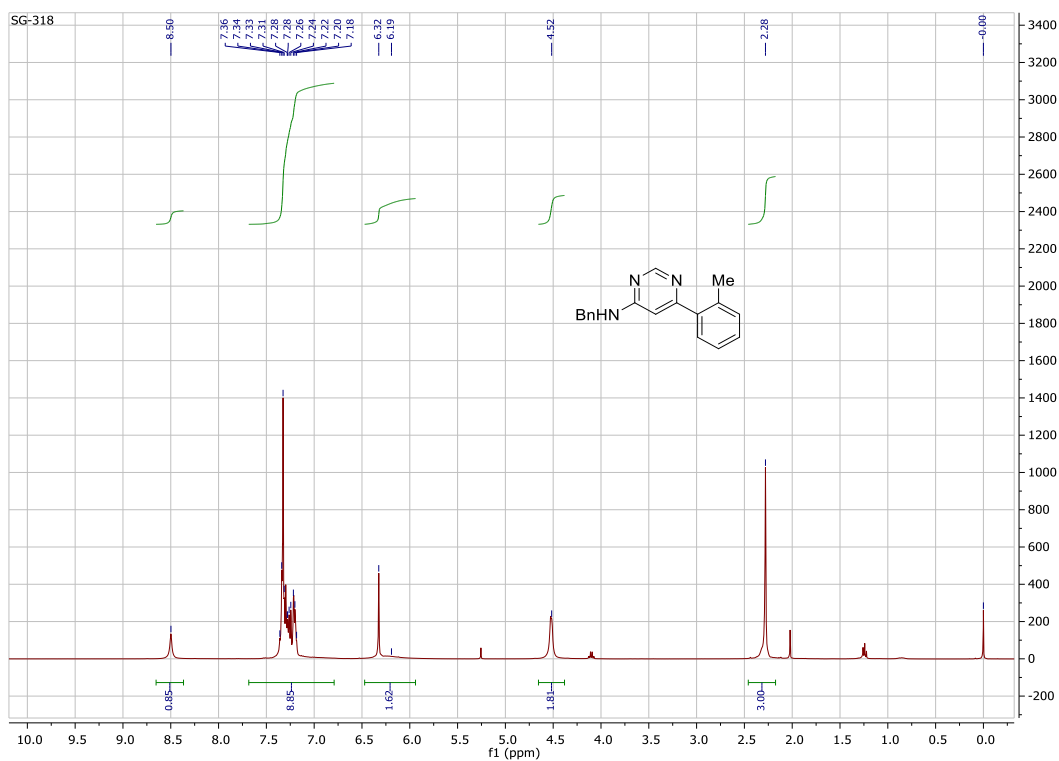
m/z	Abundance	Label
193.0839	0.05	
208.1347	0.15	
251.1006	0.35	
279.0782	0.85	
294.0759	1.00	
296.1029	0.95	
297.1244	0.15	
312.1175	0.05	

TOF MS EI+

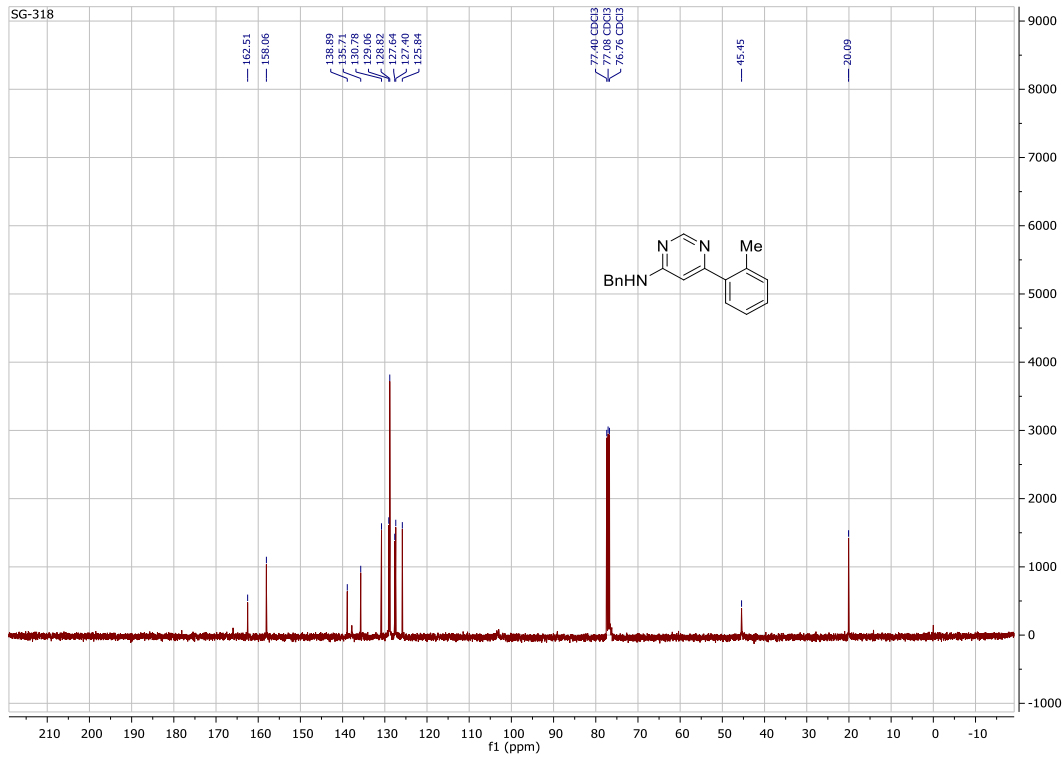
Cc1nc(Cl)cc(c1)-c2cc(OC)c(OC)c2



HRMS spectra of **9j**



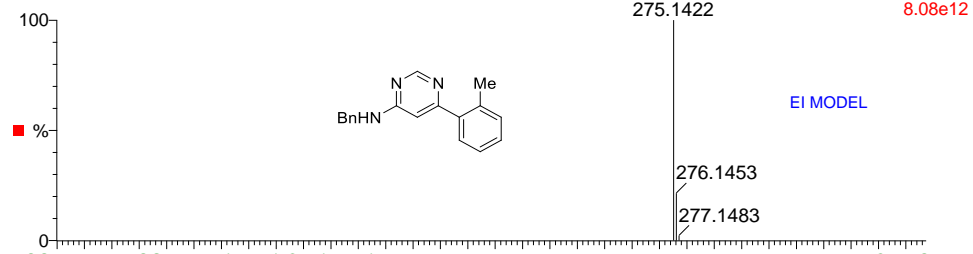
^1H NMR spectrum of **15a** (in CDCl_3)



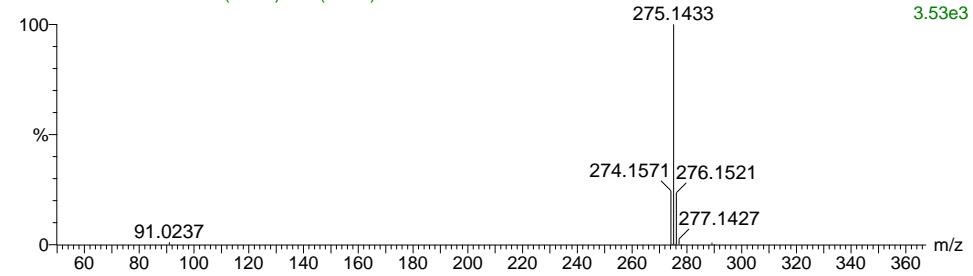
¹³C NMR spectrum of **15a** (in CDCl₃)

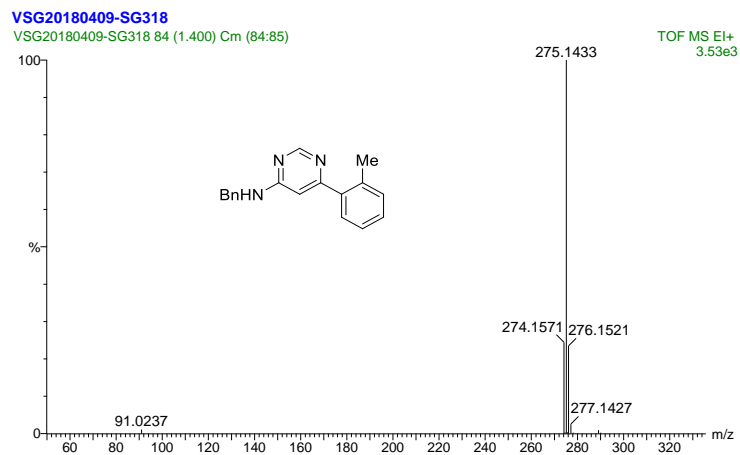
VSG20180409-SG318

VSG20180409-SG318 (0.017) Is (1.00,1.00) C18H17N3



VSG20180409-SG318 84 (1.40) Cm (84:85)



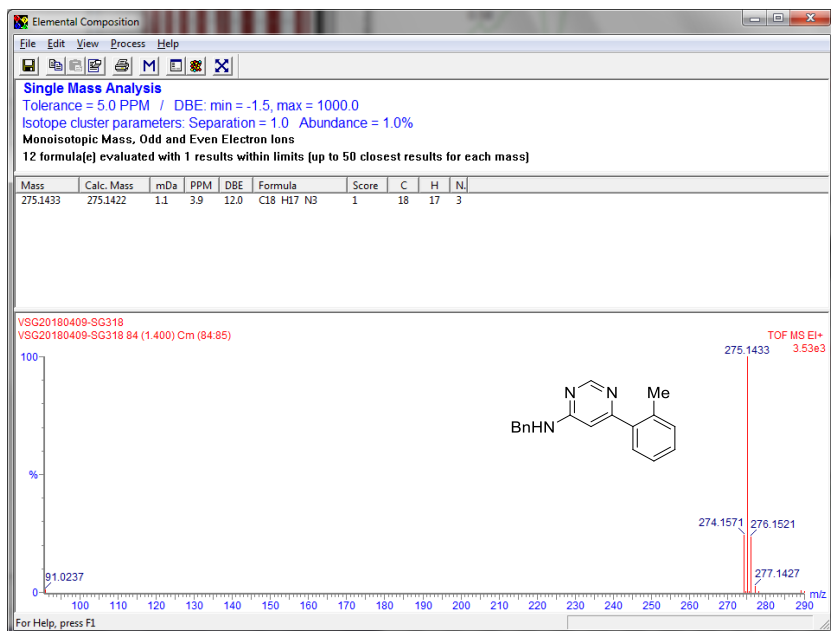


VSG20180409-SG318
VSG20180409-SG318 84 (1.400) Cm (84:85)

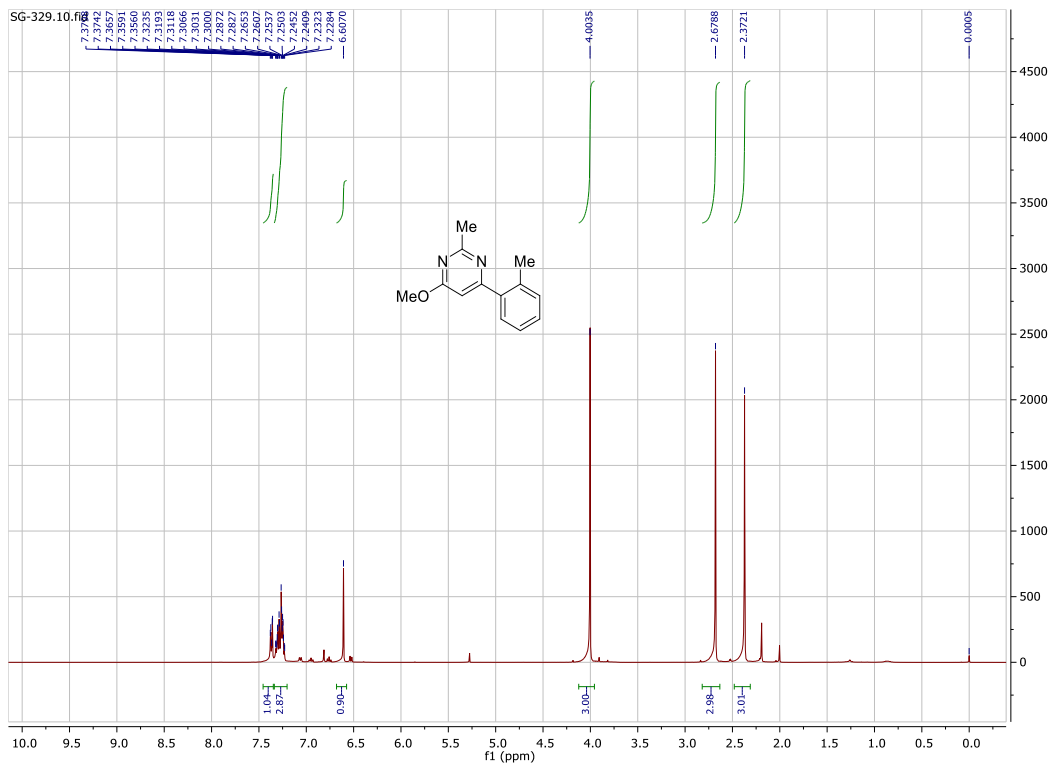
TOF MS EI+
3.53e3

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	91.0237	3.75e1	1.06	0.69										
2:	274.1571	8.59e2	24.36	15.71										
3:	274.6103	1.01e1	0.29	0.19										
4:	275.1433	3.53e3	99.99	64.51										
5:	275.6656	1.11e1	0.32	0.20										
6:	276.1521	8.26e2	23.42	15.11										
7:	277.1427	8.71e1	2.47	1.59										
8:	278.1600	7.09e0	0.20	0.13										
9:	289.1291	8.14e1	0.89	0.57										
10:	290.1085	7.09e0	0.20	0.13										

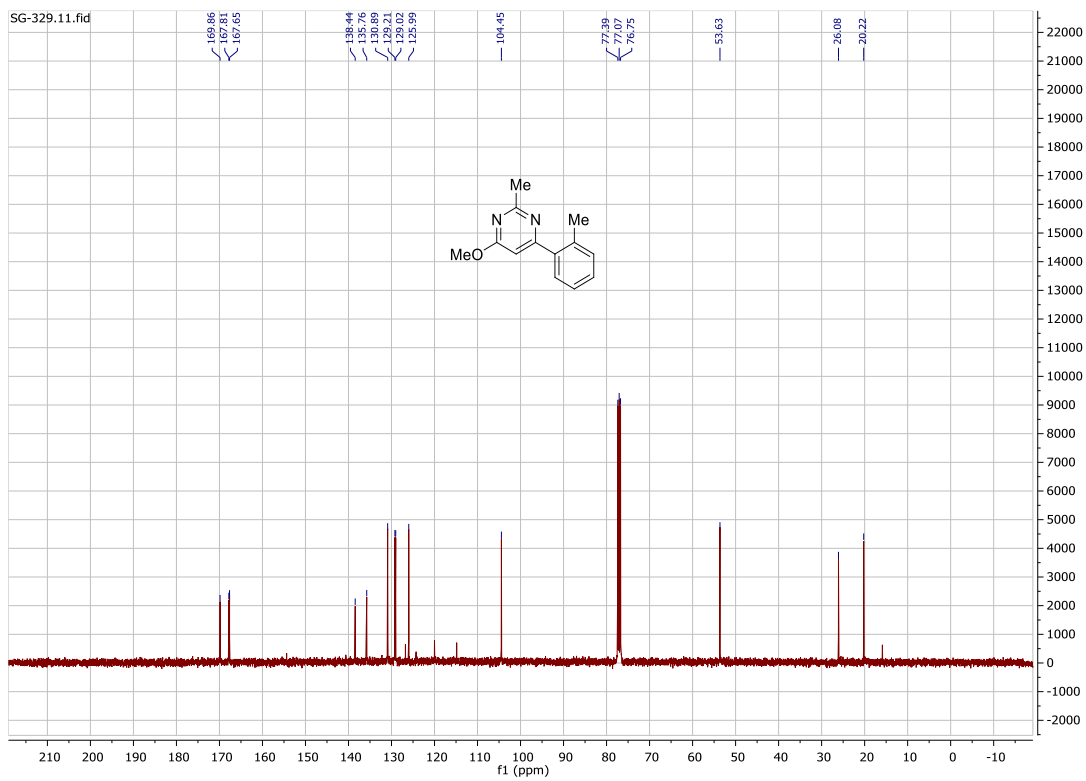
Chemical structure of 15a: Cc1ccc(cc1)C2=CN=CN2Nc3ccccc3



HRMS spectra of 15a



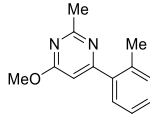
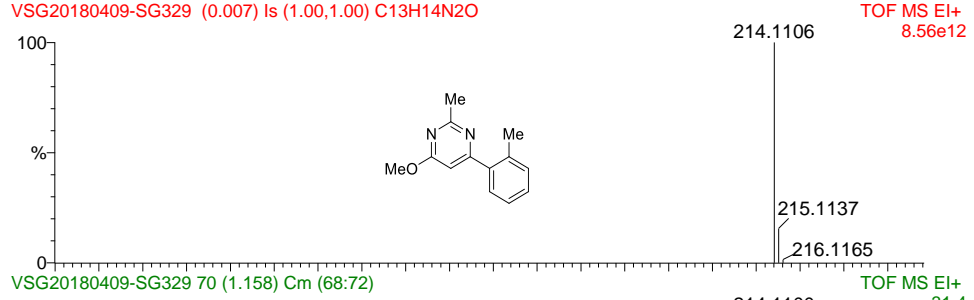
¹H NMR spectrum of **15b** (in CDCl₃)



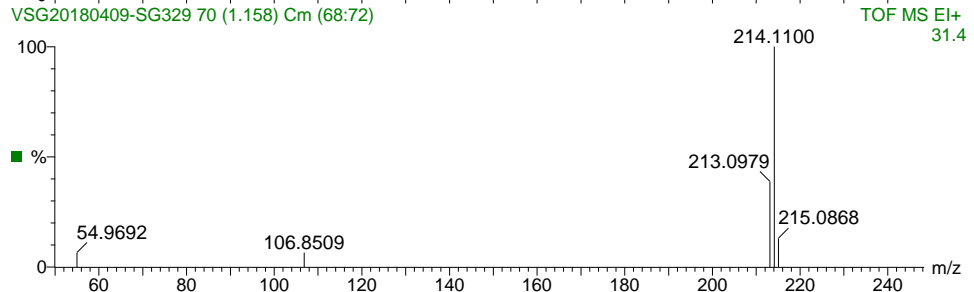
¹³C NMR spectrum of **15b** (in CDCl₃)

VSG20180409-SG329

VSG20180409-SG329 (0.007) Is (1.00,1.00) C₁₃H₁₄N₂O

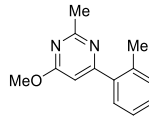
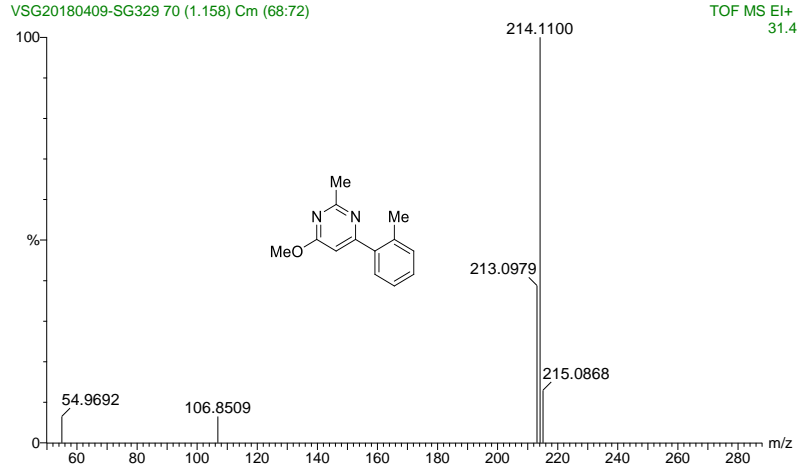


VSG20180409-SG329 70 (1.158) Cm (68:72)



VSG20180409-SG329

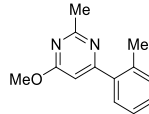
VSG20180409-SG329 70 (1.158) Cm (68:72)

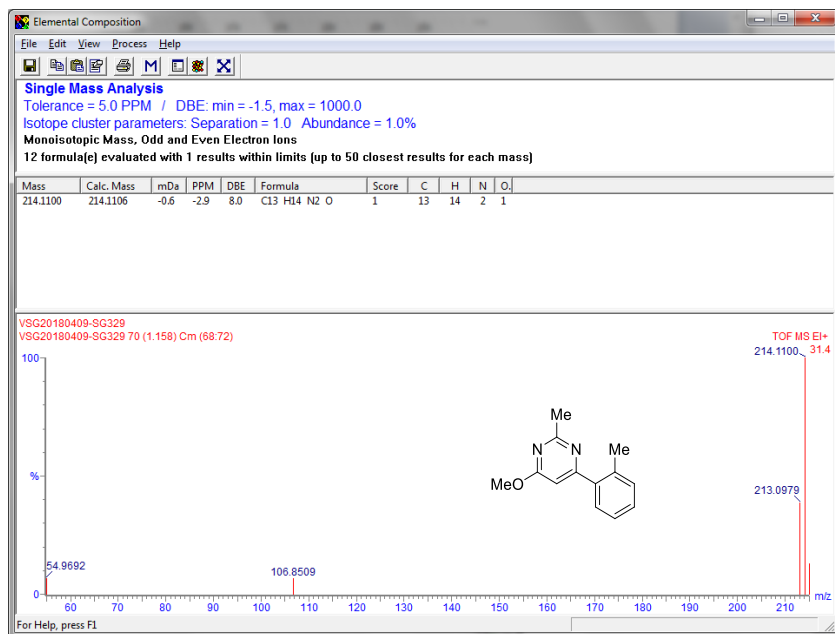


VSG20180409-SG329

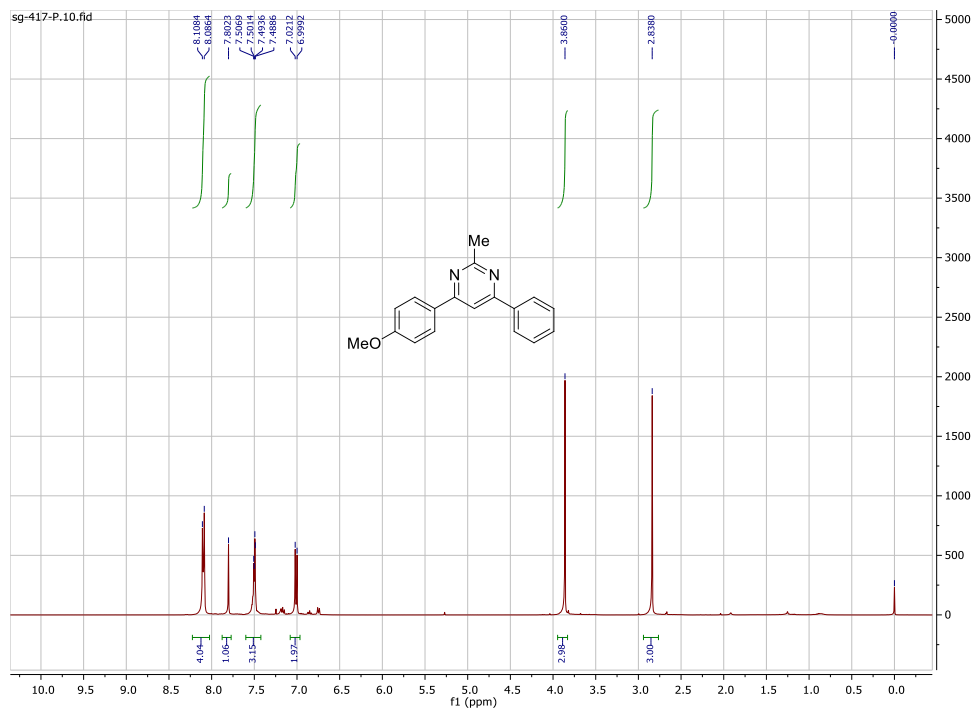
VSG20180409-SG329 70 (1.158) Cm (68:72)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	54.9692	2.03e0	6.53	3.51										
2:	106.8509	2.03e0	6.53	3.51										
3:	213.0979	1.22e1	39.20	21.05										
4:	214.1100	3.14e1	101.27	54.39										
5:	215.0868	4.05e0	13.07	7.02										

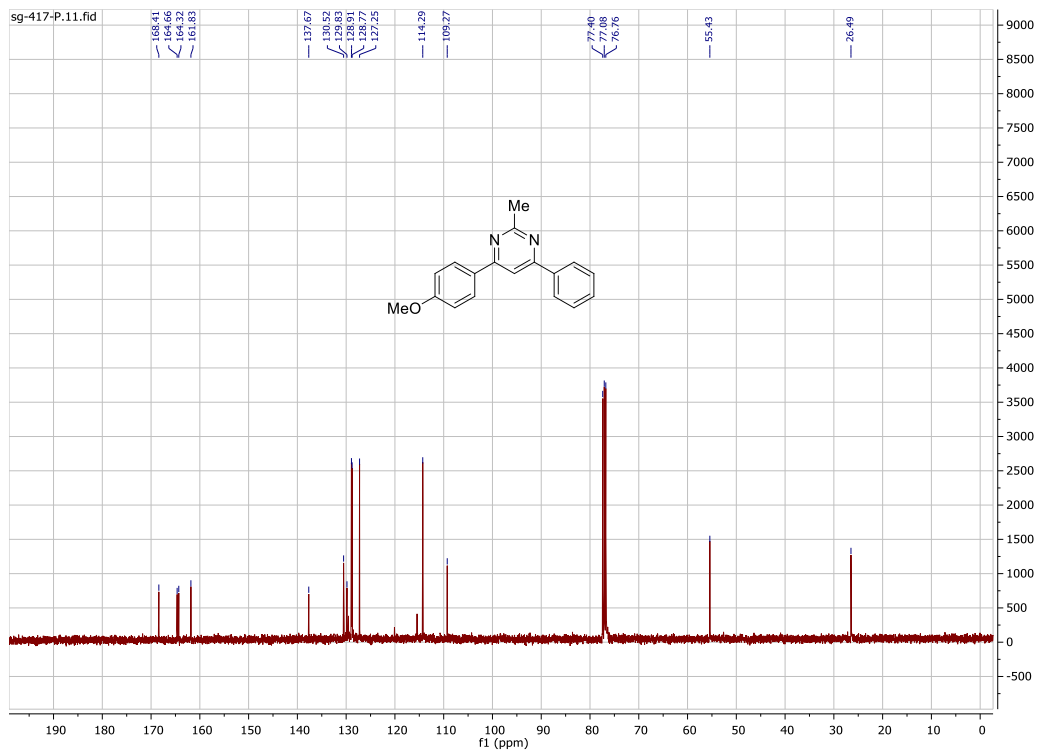




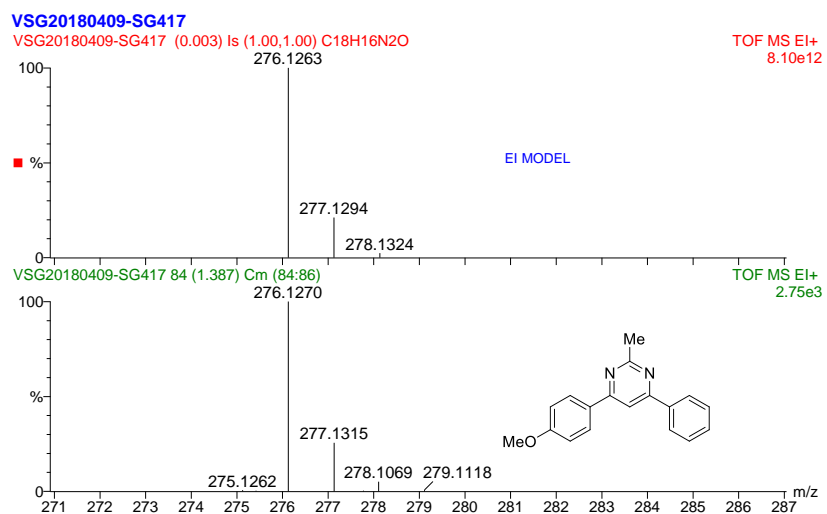
HRMS spectra of **15b**



¹H NMR spectrum of **15c** (in CDCl₃)

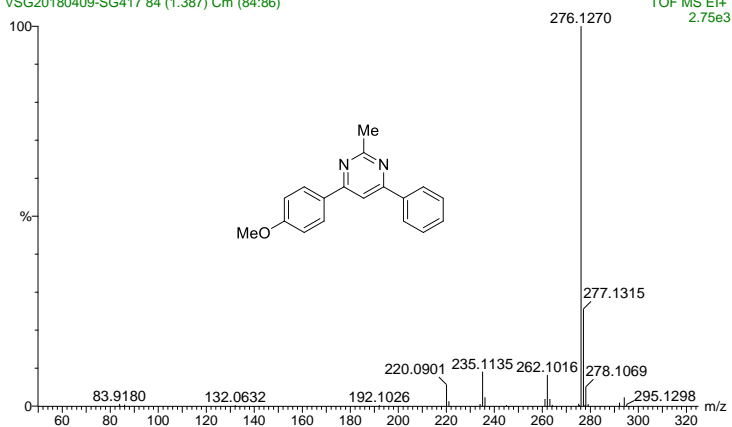


¹³C NMR spectrum of **15c** (in CDCl₃)



VSG20180409-SG417

VSG20180409-SG417 84 (1.387) Cm (84:86)

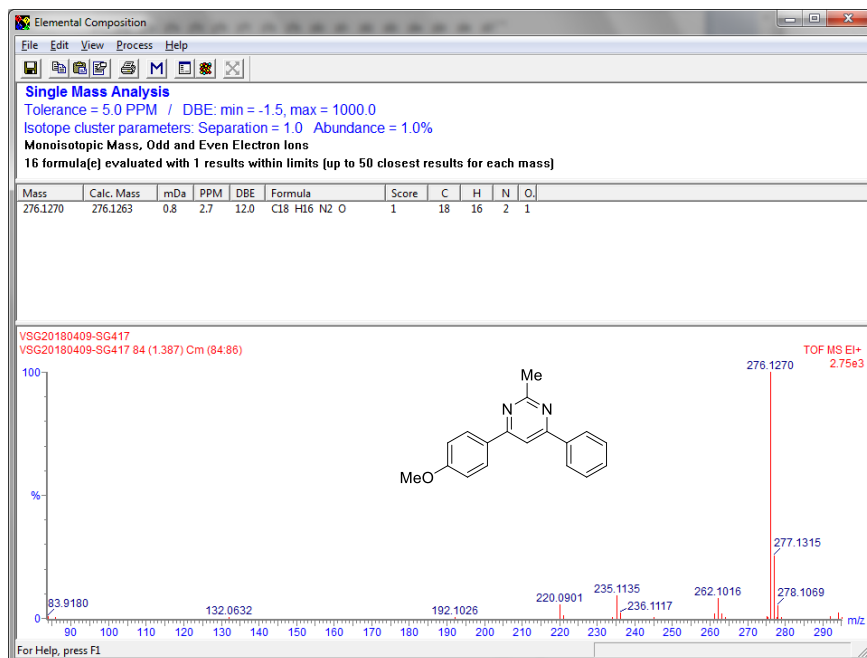


VSG20180409-SG417

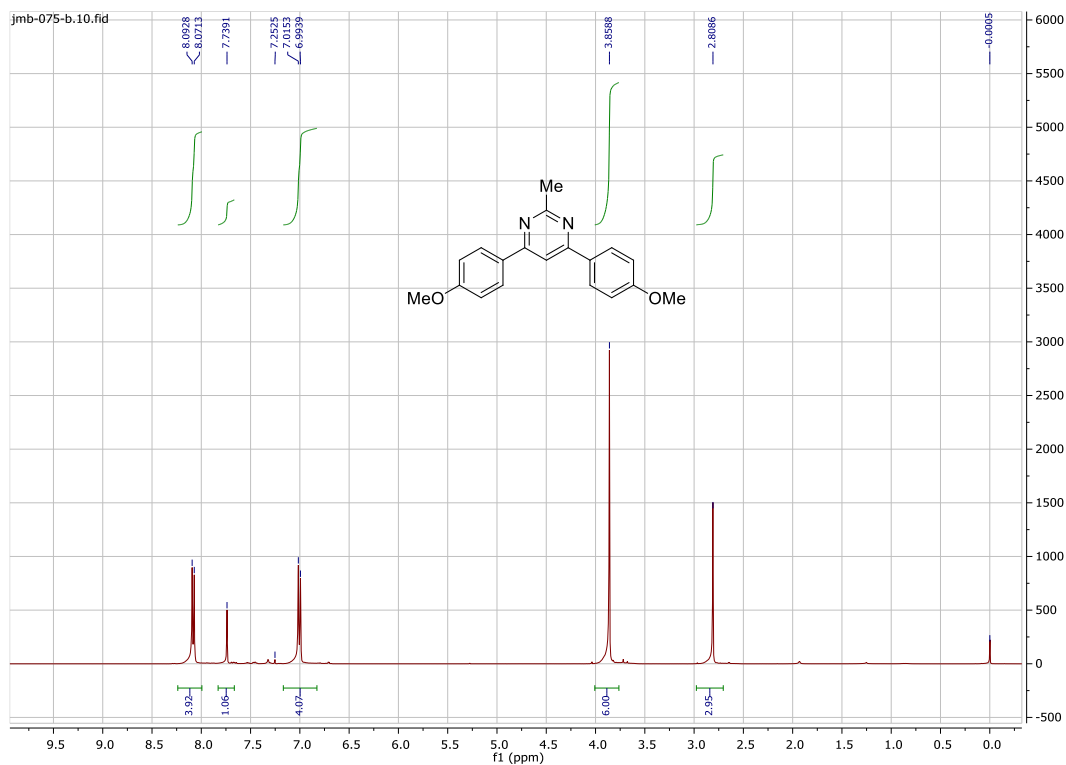
VSG20180409-SG417 84 (1.387) Cm (84:86)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	83.9180	1.52e1	0.55	0.32										
2:	85.9177	9.11e0	0.33	0.19										
3:	132.0632	6.08e0	0.22	0.13										
4:	192.1026	6.08e0	0.22	0.13										
5:	220.0901	1.53e2	5.56	3.25										
6:	221.1007	3.44e1	1.25	0.73										
7:	234.0852	1.32e1	0.48	0.28										
8:	235.1135	2.48e2	9.02	5.27										
9:	236.1117	6.28e1	2.28	1.33										
10:	245.1022	6.08e0	0.22	0.13										
11:	261.1039	5.06e1	1.84	1.07										
12:	262.1016	2.25e2	8.17	4.77										
13:	263.1070	5.06e1	1.84	1.07										
14:	264.1388	8.10e0	0.29	0.17										
15:	275.1262	1.62e1	0.59	0.34										
16:	275.4206	7.09e0	0.26	0.15										
17:	276.1270	2.75e3	99.99	58.39										
18:	277.1315	7.02e2	25.51	14.90										
19:	277.7746	8.10e0	0.29	0.17										
20:	278.1069	1.38e2	5.01	2.92										
21:	279.1118	1.42e1	0.52	0.30										
22:	292.1193	2.43e1	0.88	0.52										
23:	294.1255	6.28e1	2.28	1.33										
24:	295.1298	1.01e1	0.37	0.21										

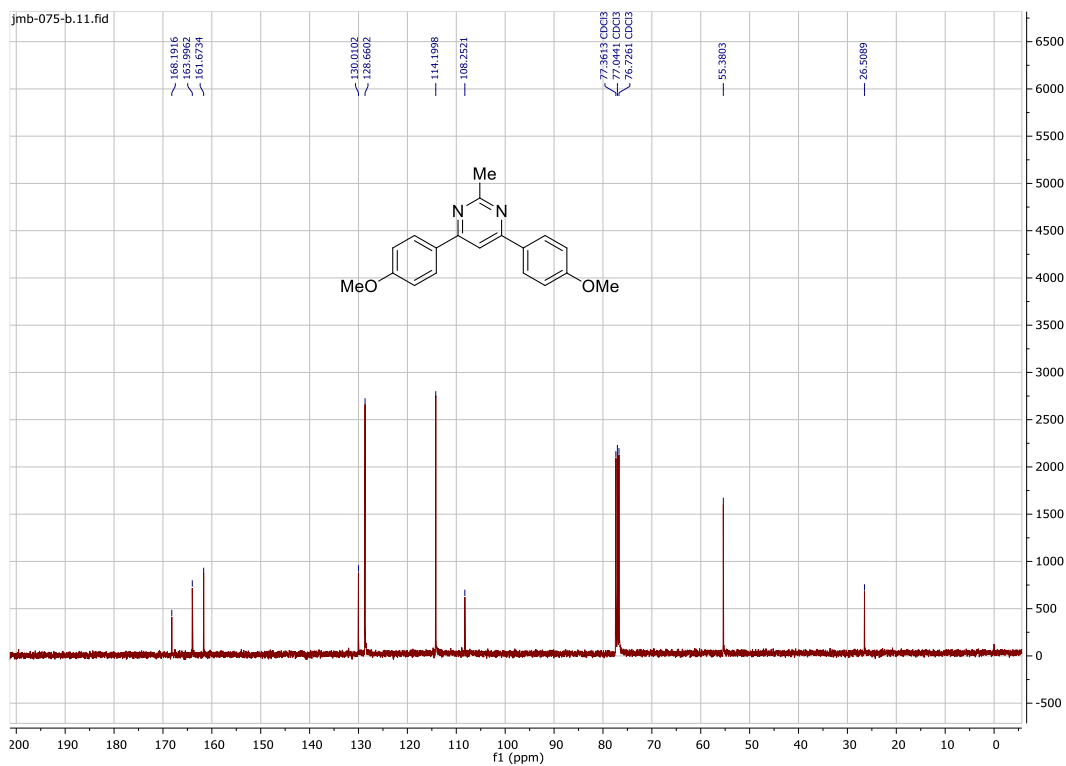
TOF MS EI+
2.75e3



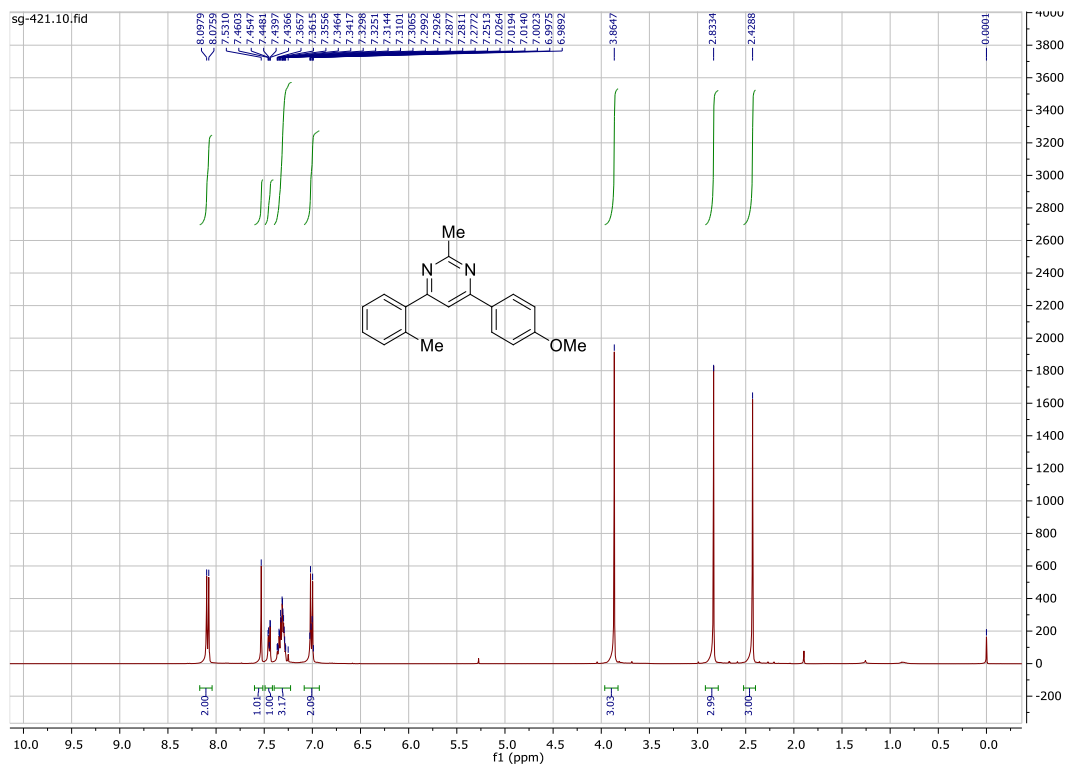
HRMS spectra of 15c



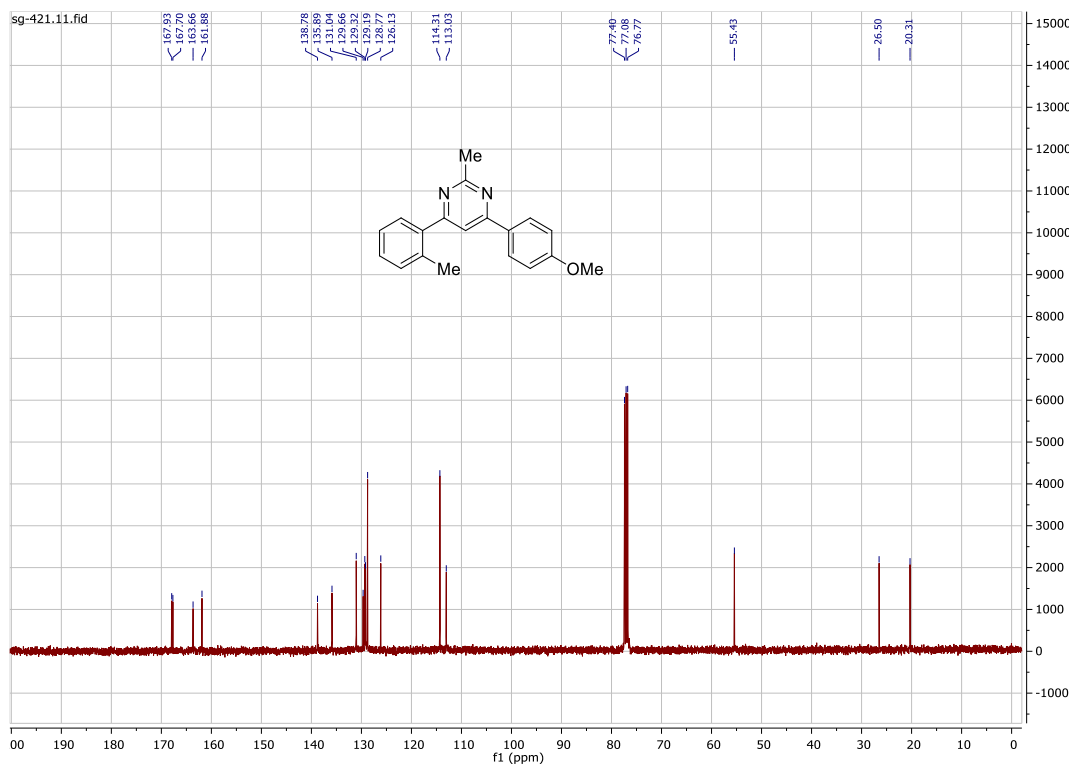
^1H NMR spectrum of **15d** (in CDCl_3)



^{13}C NMR spectrum of **15d** (in CDCl_3)



^1H NMR spectrum of **15e** (in CDCl_3)

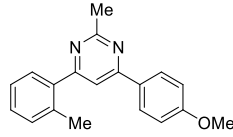
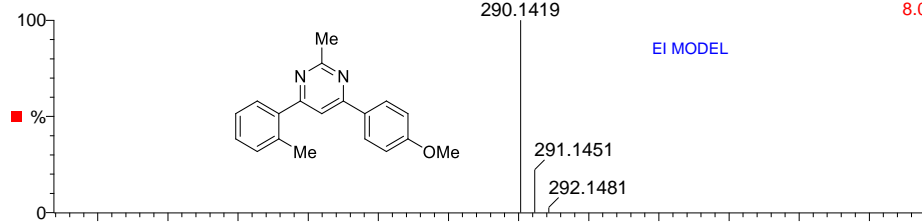


^{13}C NMR spectrum of **15e** (in CDCl_3)

VSG20180129-SG-421

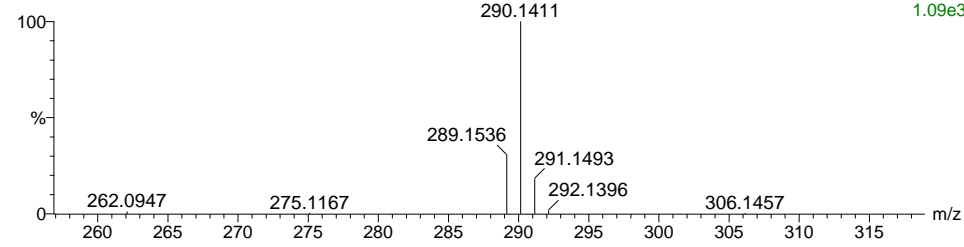
VSG20180129-SG-421 (0.002) Is (1.00,1.00) C₁₉H₁₈N₂O

TOF MS EI+
8.00e12



VSG20180129-SG-421 79 (1.302) Cm (77:79)

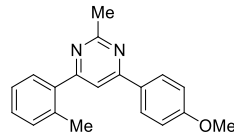
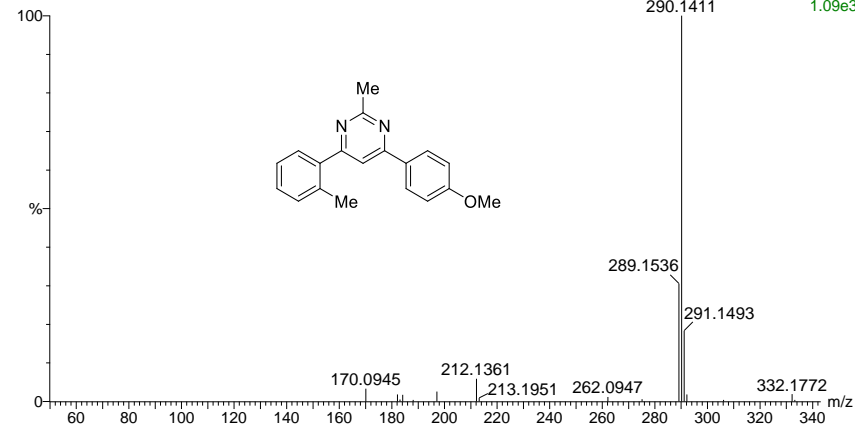
TOF MS EI+
1.09e3



VSG20180129-SG-421

VSG20180129-SG-421 79 (1.302) Cm (77:79)

TOF MS EI+
1.09e3

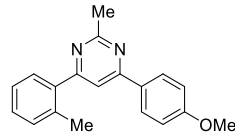


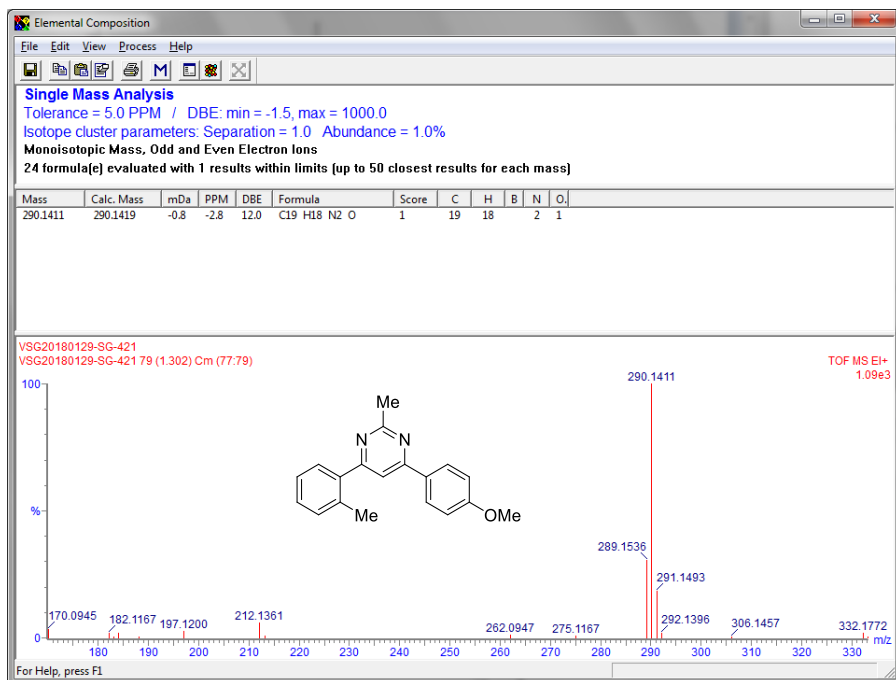
VSG20180129-SG-421

VSG20180129-SG-421 79 (1.302) Cm (77:79)

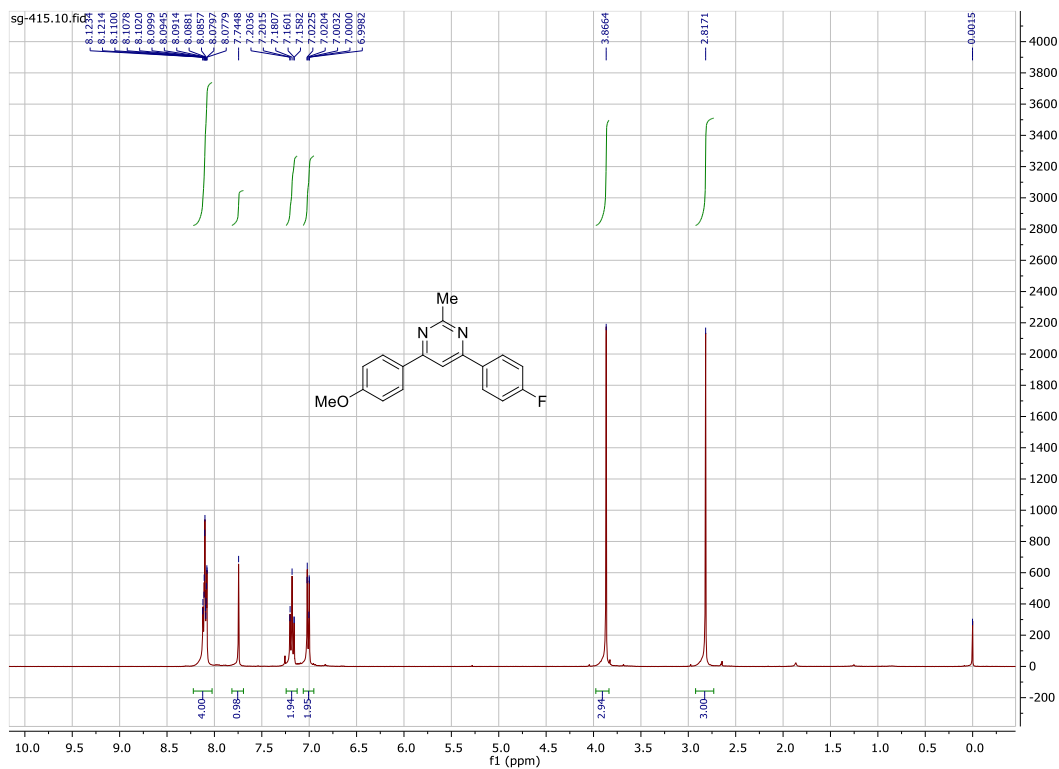
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	170.0945	3.54e1	3.25	1.88										
2:	182.1167	1.92e1	1.77	1.02										
3:	183.1052	5.06e0	0.46	0.27										
4:	184.1129	1.82e1	1.67	0.96										
5:	188.0887	4.05e0	0.37	0.21										
6:	197.1200	2.73e1	2.51	1.45										
7:	212.1361	6.39e1	5.86	3.38										
8:	213.1951	9.11e0	0.84	0.48										
9:	262.0947	1.22e1	1.12	0.64										
10:	275.1167	6.08e0	0.56	0.32										
11:	289.1536	3.32e2	30.50	17.57										
12:	290.1411	1.09e3	100.01	57.62										
13:	291.1493	1.99e2	18.32	10.55										
14:	292.1396	1.92e1	1.77	1.02										
15:	306.1457	4.05e0	0.37	0.21										
16:	332.1772	2.03e1	1.86	1.07										
17:	333.1929	4.05e0	0.37	0.21										

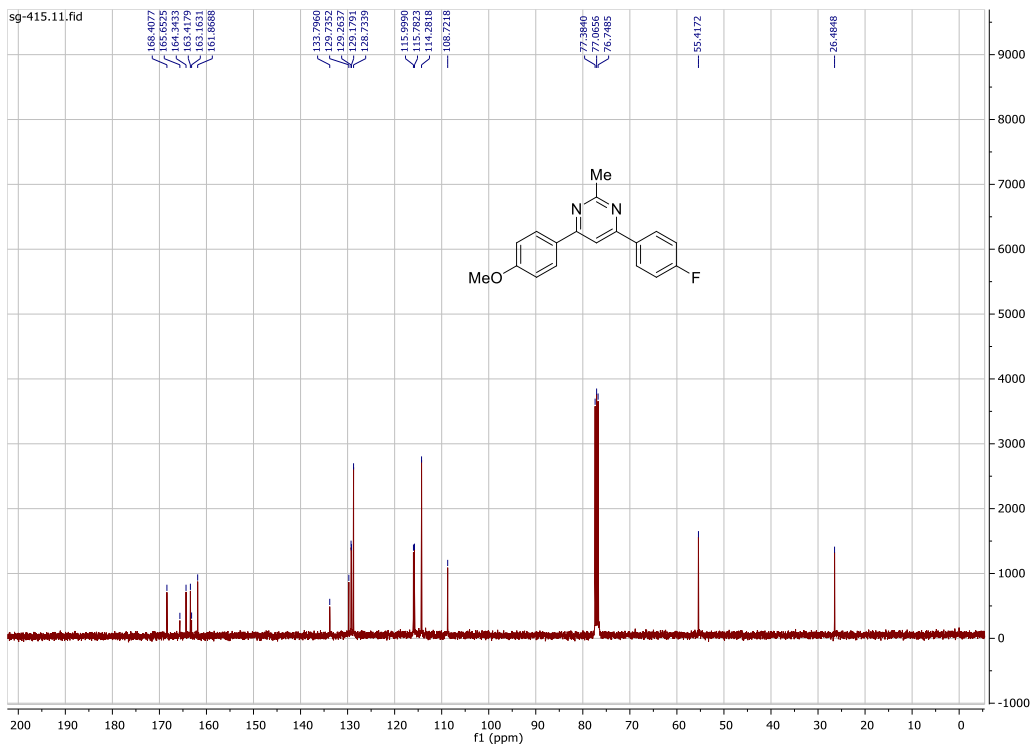




HRMS spectra of **15e**



¹H NMR spectrum of **15f** (in CDCl₃)

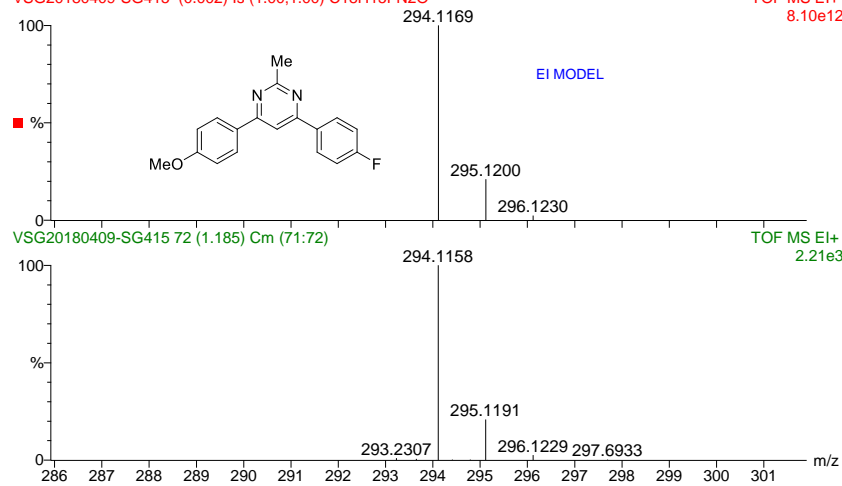


^{13}C NMR spectrum of **15f** (in CDCl_3)

VSG20180409-SG415

VSG20180409-SG415 (0.002) Is (1.00,1.00) C18H15FN2O

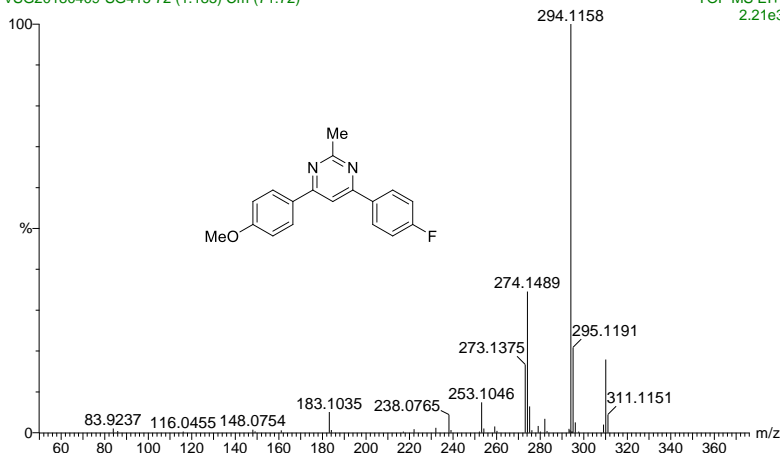
TOF MS EI+
8.10e12



VSG20180409-SG415

VSG20180409-SG415 72 (1.185) Cm (71:72)

TOF MS EI+
2.21e3

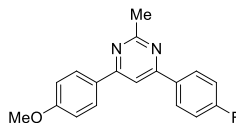


VSG20180409-SG415

VSG20180409-SG415 72 (1.185) Cm (71:72)

TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	83.9237	2.23e1	1.01	0.41	32:	295.1191	4.60e2	20.83	8.56					
2:	85.9268	8.10e0	0.37	0.15	33:	296.1229	5.47e1	2.48	1.02					
3:	116.0455	5.06e0	0.23	0.09	34:	297.6933	5.06e0	0.23	0.09					
4:	148.0754	1.52e1	0.69	0.28	35:	309.1200	4.35e1	1.97	0.81					
5:	149.0625	6.09e0	0.28	0.11	36:	310.1160	3.95e2	17.89	7.36					
6:	161.0742	1.22e1	0.55	0.23	37:	311.1151	9.72e1	4.40	1.81					
7:	183.1035	1.11e2	5.05	2.07										
8:	184.0992	1.42e1	0.64	0.26										
9:	217.1171	5.06e0	0.23	0.09										
10:	222.0899	1.82e1	0.83	0.34										
11:	232.1190	2.53e1	1.15	0.47										
12:	238.0765	9.62e1	4.36	1.79										
13:	239.0734	1.42e1	0.64	0.26										
14:	252.0804	5.06e0	0.23	0.09										
15:	253.1046	1.63e2	7.39	3.04										
16:	254.0962	2.23e1	1.01	0.41										
17:	259.1248	3.34e1	1.51	0.62										
18:	260.1161	9.11e0	0.41	0.17										
19:	273.1375	9.69e2	16.66	6.85										
20:	274.1489	7.62e2	34.53	14.19										
21:	275.1540	1.42e2	6.42	2.64										
22:	276.1719	1.32e1	0.60	0.25										
23:	279.0982	3.54e1	1.61	0.66										
24:	280.1226	5.06e0	0.23	0.09										
25:	282.1255	7.39e1	3.35	1.38										
26:	283.1074	8.10e0	0.37	0.15										
27:	293.2307	2.03e1	0.92	0.38										
28:	293.6493	1.32e1	0.60	0.25										
29:	294.1158	2.21e3	99.98	41.09										
30:	294.4128	5.06e0	0.23	0.09										
31:	294.7921	5.06e0	0.23	0.09										



Elemental Composition

File Edit View Process Help

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 1000.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
43 formula[e] evaluated with 1 results within limits (up to 50 closest results for each mass)

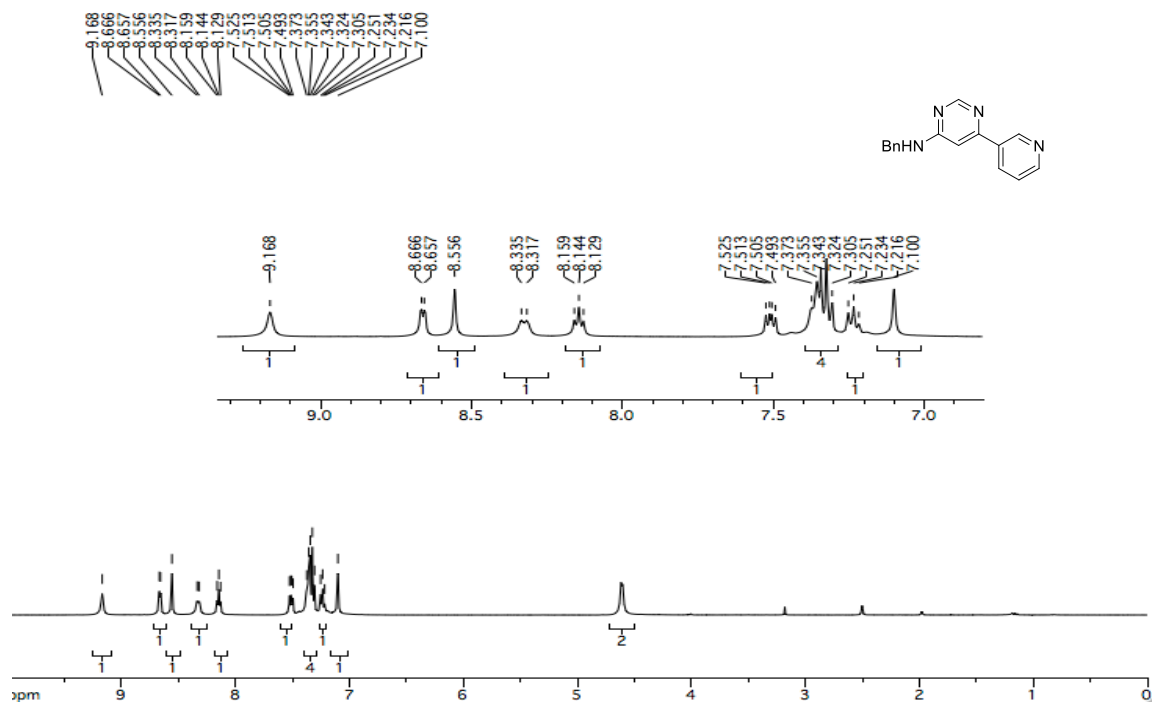
Mass	Calc. Mass	mDa	PPM	DBE	Formula	Score	C	H	N	O	F
294.1158	294.1168	-1.0	-3.5	12.0	C18 H15 N2 O F	1	18	15	2	1	1

VSG20180409-SG415
VSG20180409-SG415 72 (1.185) Cm (71:72)

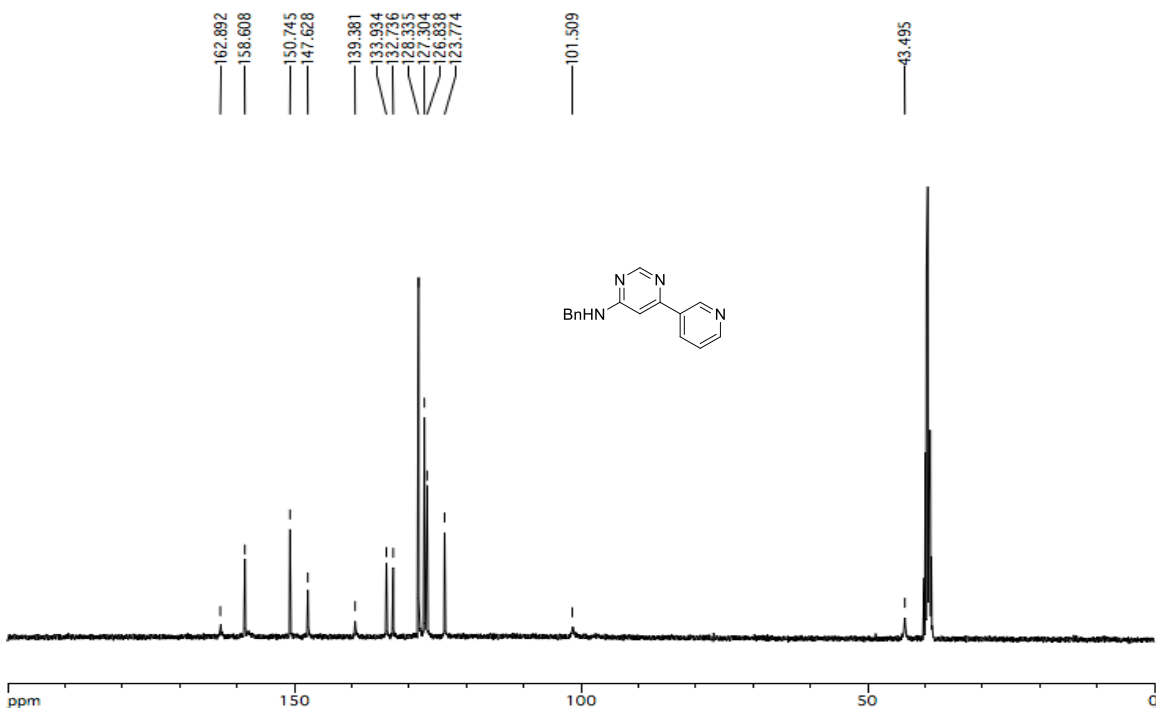
Chemical structure: Cc1nc2cc(OC)ccc2n1-c1ccc(F)cc1

For Help, press F1

HRMS spectra of 15f



¹H NMR spectrum of 16a (DMSO-*d*₆)

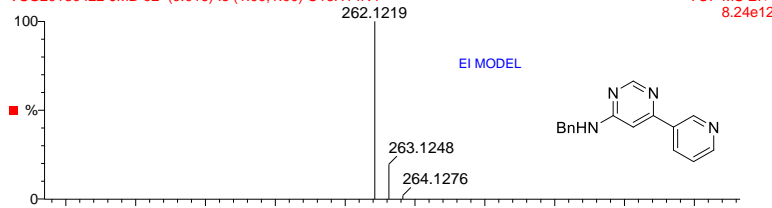


¹³C NMR spectrum of 16a (in DMSO-*d*₆)

VSG20180422-JMB-92

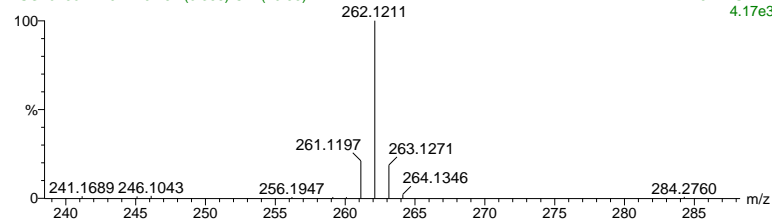
VSG20180422-JMB-92 (0.016) Is (1.00,1.00) C16H14N4

TOF MS EI+
8.24e12



VSG20180422-JMB-92 52 (0.866) Cm (49:53)

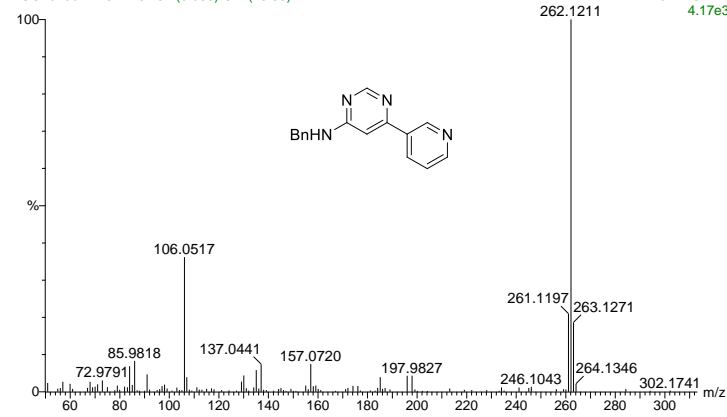
TOF MS EI+
4.17e3



VSG20180422-JMB-92

VSG20180422-JMB-92 52 (0.866) Cm (49:53)

TOF MS EI+
4.17e3

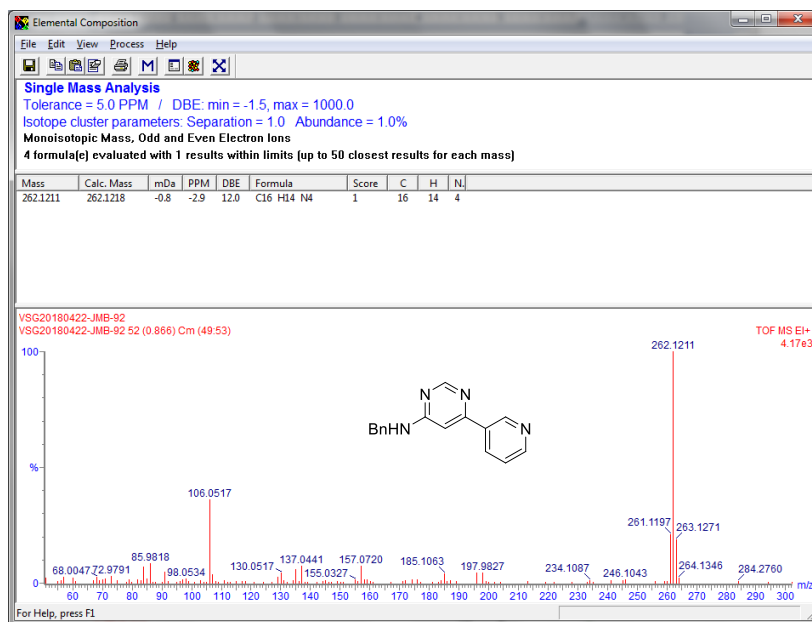


VSG20180422-JMB-92
VSG20180422-JMB-92 52 (0.866) Cm (49:53)

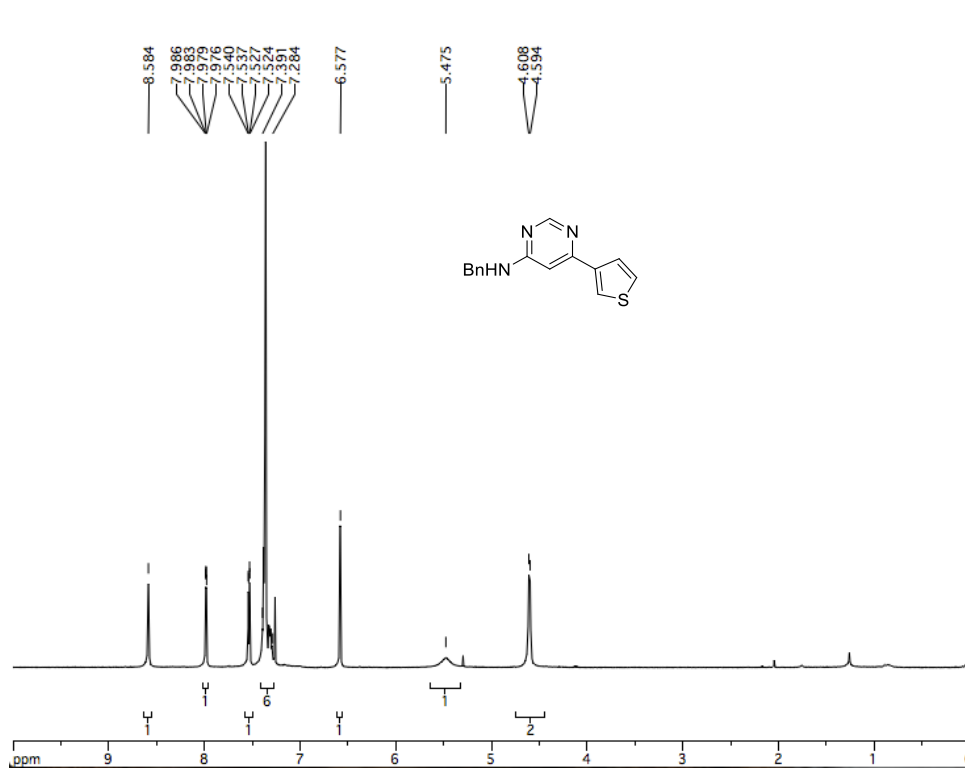
m/z	Abundance	Label
72.9791	Low	
85.9818	Low	
106.0517	High	
137.0441	Low	
157.0720	Low	
197.9827	Low	
246.1043	Low	
261.1197	High	
262.1211	100	Base Peak
263.1271	High	
264.1346	Low	
302.1741	Low	

TOF MS EI+

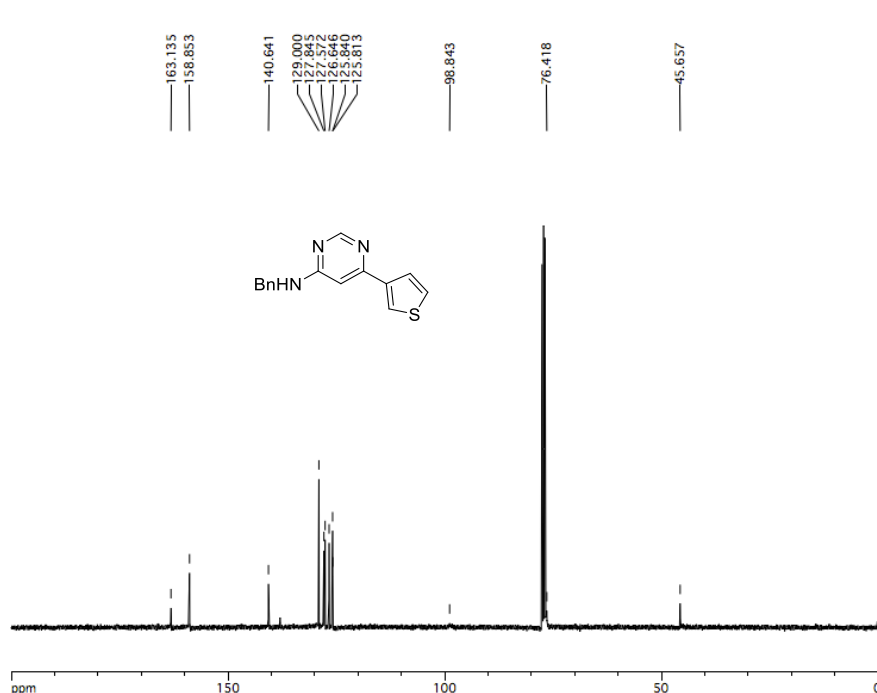
Chemical structure of the compound: N-benzyl-1H-imidazo[4,5-b]pyridine.



HRMS spectra of **16a**



¹H NMR spectrum of **16b** (in CDCl₃)

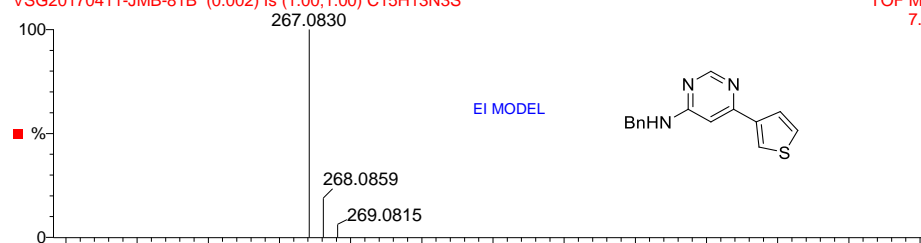


¹³C NMR spectrum of **16b** (in CDCl₃)

VSG20170411-JMB-81B

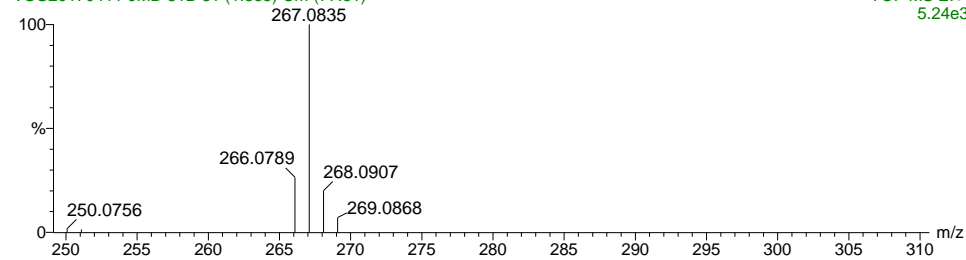
VSG20170411-JMB-81B (0.002) Is (1.00,1.00) C₁₅H₁₃N₃S

TOF MS EI+
7.95e12



VSG20170411-JMB-81B 81 (1.335) Cm (77:81)

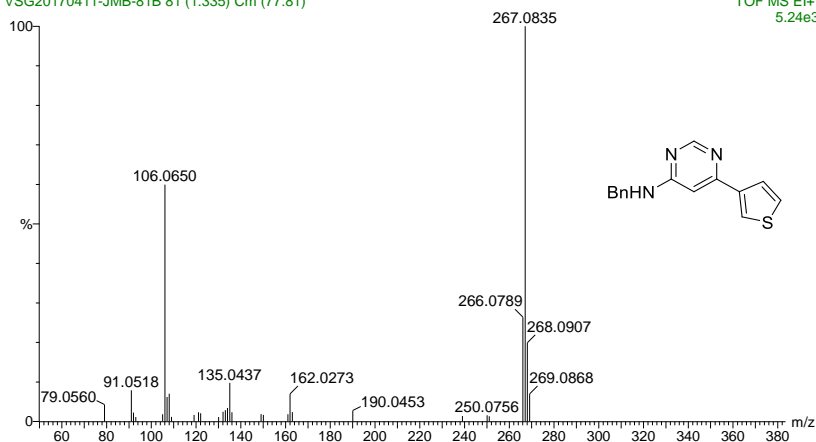
TOF MS EI+
5.24e3



VSG20170411-JMB-81B

VSG20170411-JMB-81B 81 (1.335) Cm (77:81)

TOF MS EI+
5.24e3

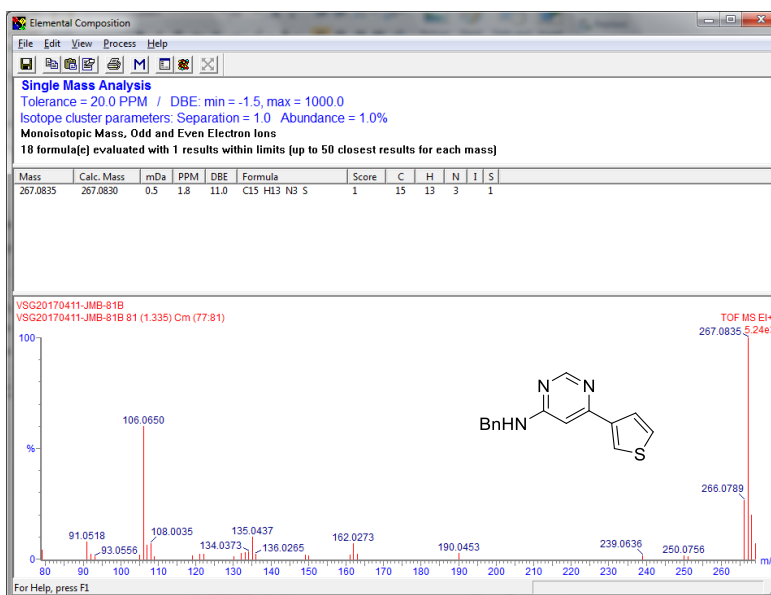


VSG20170411-JMB-81B

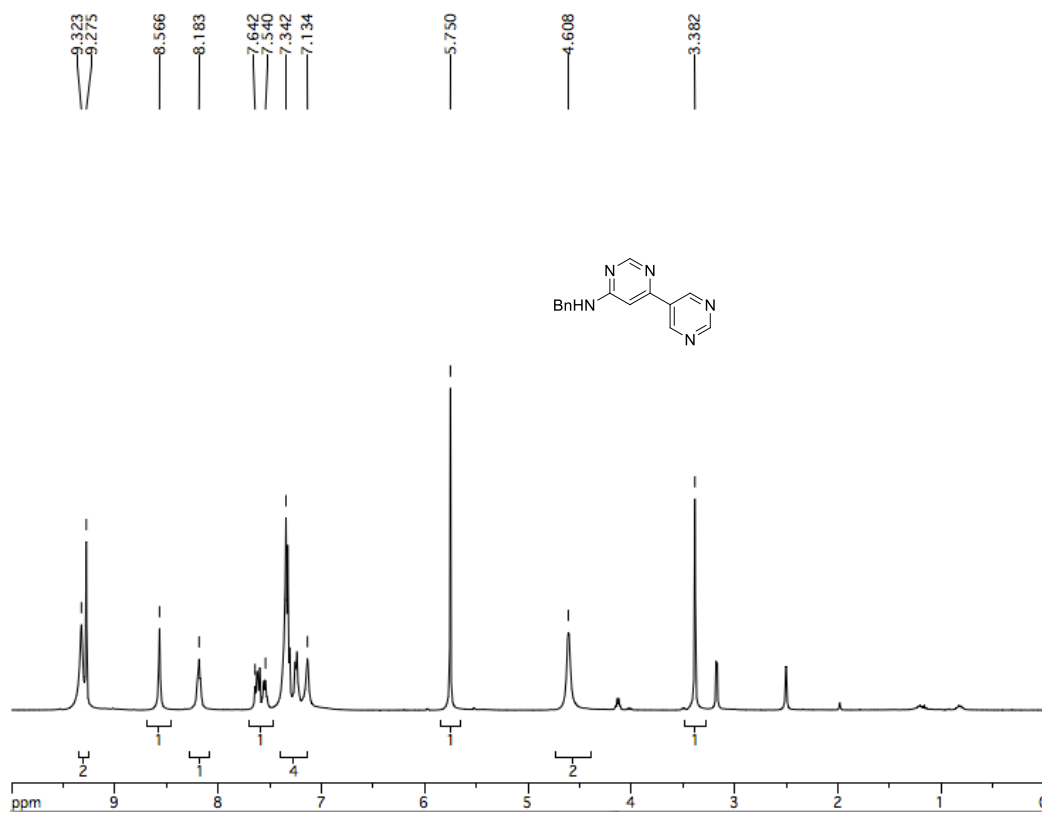
VSG20170411-JMB-81B 81 (1.335) Cm (77:81)

TOF MS EI+

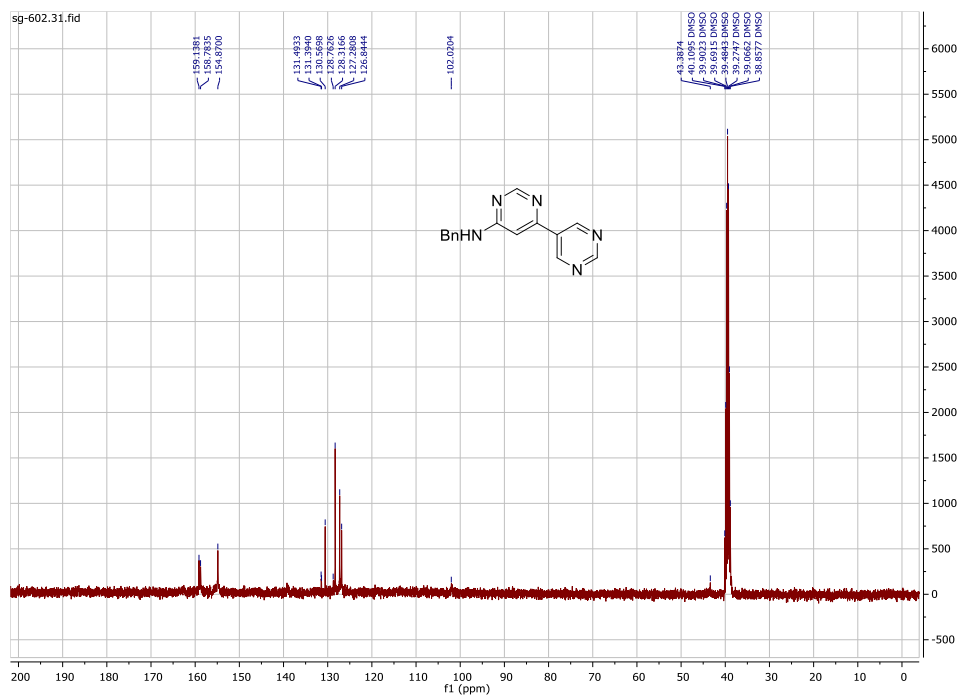
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No
1:	79.0560	2.21e2	4.22	1.29											
2:	91.0518	4.12e2	7.87	2.42											
3:	92.0562	1.14e2	2.19	0.67											
4:	93.0556	5.67e1	1.08	0.33											
5:	105.0609	9.42e1	1.80	0.55											
6:	106.0650	3.14e3	59.90	18.38											
7:	107.0629	3.22e2	6.15	1.89											
8:	108.0035	3.66e2	6.98	2.14											
9:	109.0128	5.97e1	1.14	0.35											
10:	119.0815	8.51e1	1.62	0.50											
11:	121.0649	1.19e2	2.28	0.70											
12:	122.0493	1.07e2	2.05	0.63											
13:	130.0856	5.71e1	1.10	0.34											
14:	132.0829	1.27e2	2.42	0.74											
15:	133.0913	1.49e2	2.84	0.87											
16:	134.0373	1.76e2	3.36	1.03											
17:	135.0437	5.10e2	9.75	2.99											
18:	136.0265	1.19e2	2.28	0.70											
19:	149.0779	9.52e1	1.82	0.56											
20:	150.0934	8.41e1	1.60	0.49											
21:	161.0266	9.42e1	1.80	0.55											
22:	162.0273	3.62e2	6.90	2.12											
23:	163.0328	1.23e2	2.34	0.72											
24:	190.0453	1.41e2	2.69	0.82											
25:	239.0636	6.99e1	1.33	0.41											
26:	250.0756	8.11e1	1.55	0.47											
27:	251.0811	6.68e1	1.28	0.39											
28:	266.0789	1.38e3	26.34	8.08											
29:	267.0835	5.24e3	100.00	30.69											
30:	268.0907	1.04e3	19.84	6.09											
31:	269.0868	3.63e2	6.92	2.12											



HRMS spectra of **16b**



¹H NMR spectrum of **16c** (in DMSO-*d*₆)

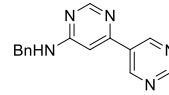
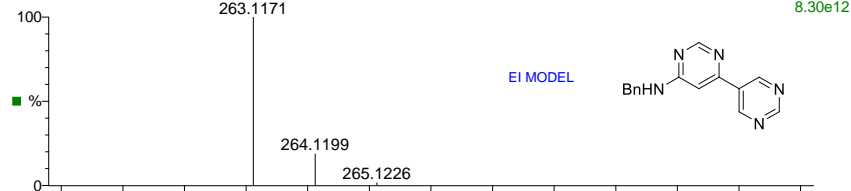


¹³C NMR spectrum of **16c** (in CDCl₃)

VSG20180105-JMB88

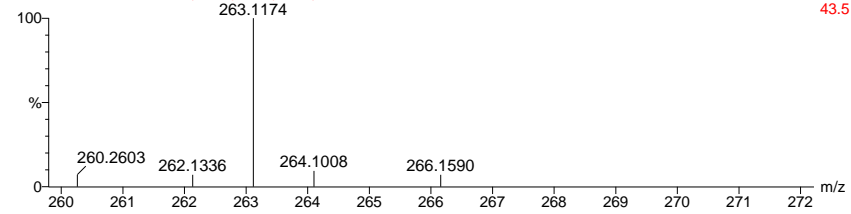
VSG20180105-JMB88 (0.004) Is (1.00,1.00) C15H13N5

TOF MS EI+
8.30e12



VSG20180105-JMB88 79 (1.304) Cm (75:79)

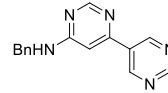
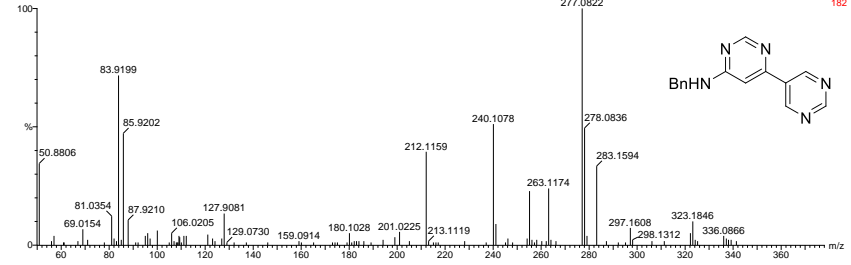
TOF MS EI+
43.5



VSG20180105-JMB88

VSG20180105-JMB88 79 (1.304) Cm (75:79)

TOF MS EI+
182

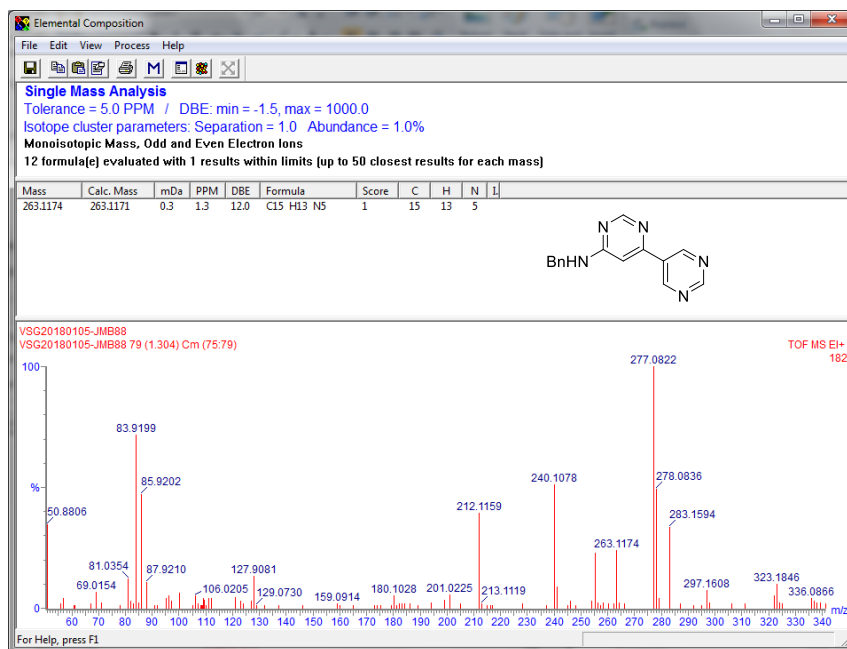


VSG20180105-JMB88

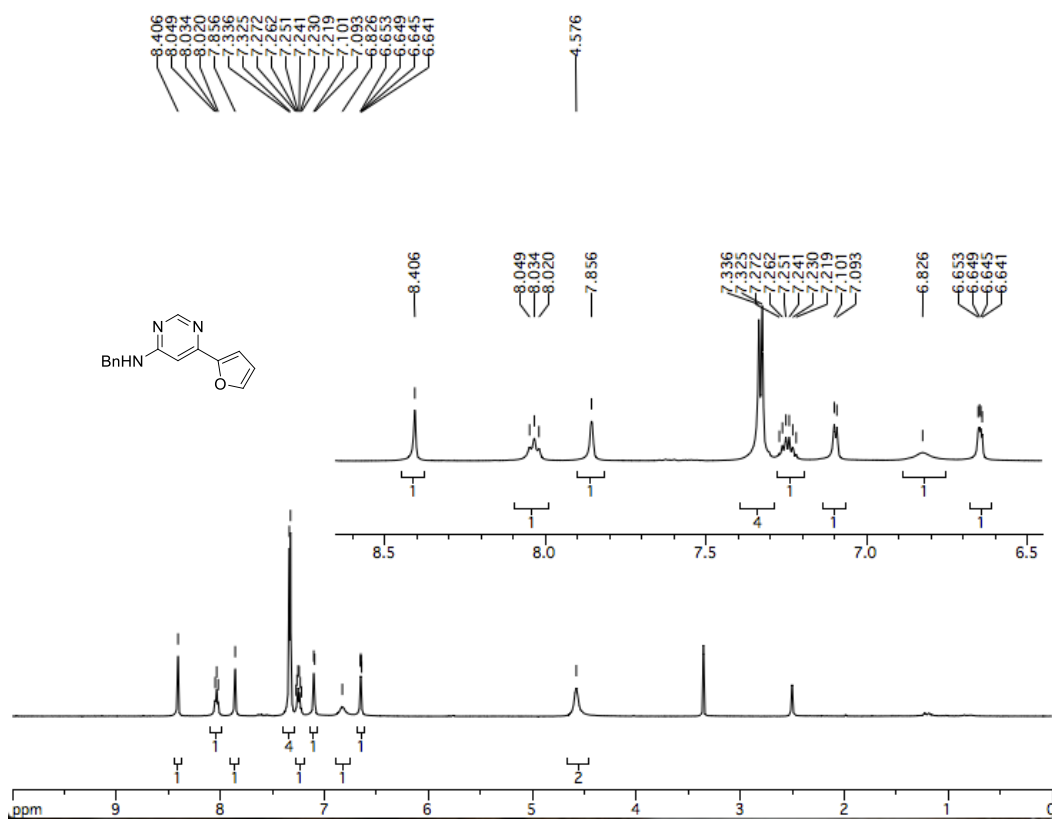
VSG20180105-JMB88 79 (1.304) Cm (75:79)

TOF MS EI+

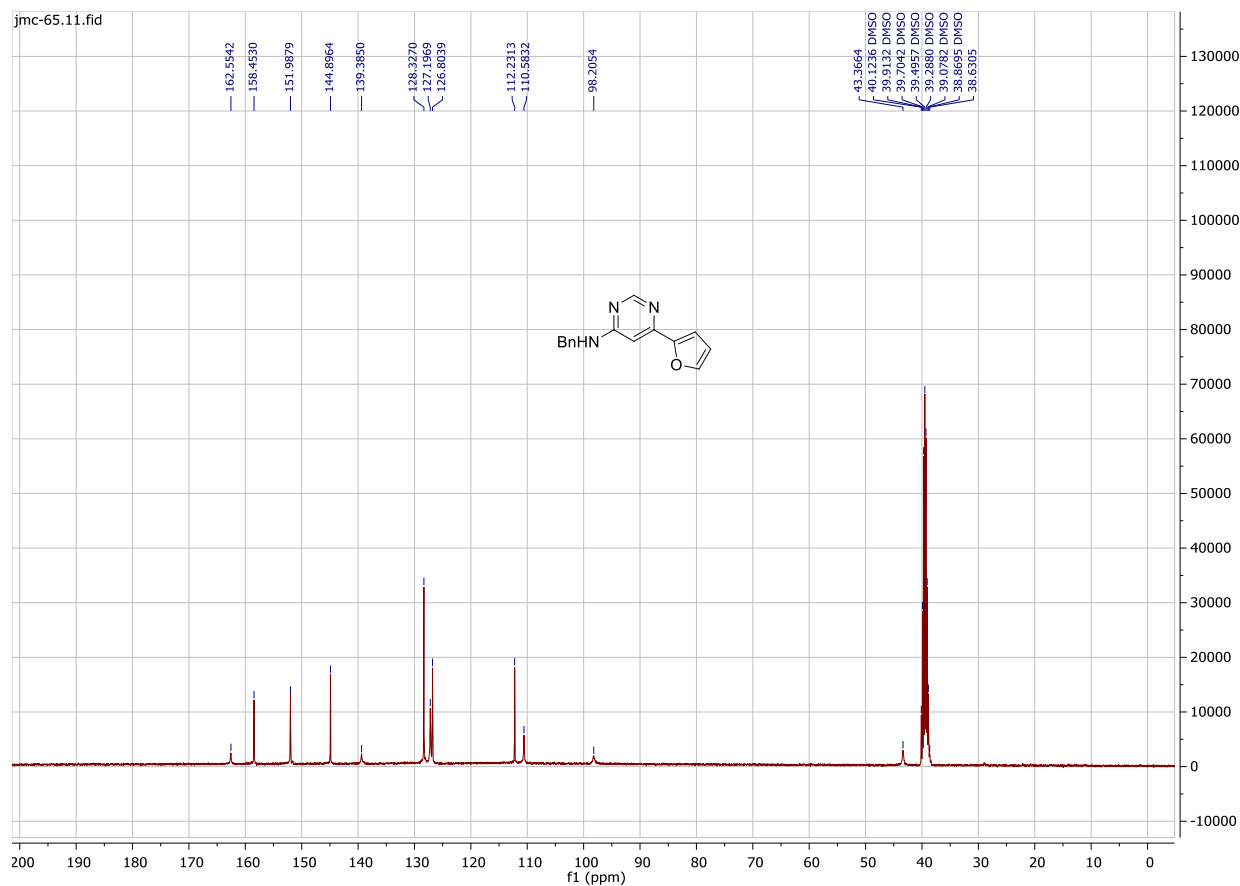
No	Mass	Inten	Ratio	Label	No	Mass	Inten	Ratio	Label	No	Mass	Inten	Ratio	Label	No	Mass	Inten	Ratio	Label
1	50.8806	0.0001	0.0001		82	263.1174	1.0000	1.0000		164	336.0866	0.0001	0.0001		246	508.8806	0.0001	0.0001	
2	55.0319	0.0001	0.0001		83	264.1199	0.0001	0.0001		165	337.0981	0.0001	0.0001		247	509.8921	0.0001	0.0001	
3	69.0154	0.0001	0.0001		84	265.1226	0.0001	0.0001		166	338.1096	0.0001	0.0001		248	510.9036	0.0001	0.0001	
4	81.0354	0.0001	0.0001		85	266.1590	0.0001	0.0001		167	339.1211	0.0001	0.0001		249	511.9151	0.0001	0.0001	
5	81.0354	0.0001	0.0001		86	267.1805	0.0001	0.0001		168	340.1326	0.0001	0.0001		250	512.9266	0.0001	0.0001	
6	83.9199	0.0001	0.0001		87	268.2020	0.0001	0.0001		169	341.1441	0.0001	0.0001		251	513.9376	0.0001	0.0001	
7	85.9202	0.0001	0.0001		88	269.2235	0.0001	0.0001		170	342.1556	0.0001	0.0001		252	514.9486	0.0001	0.0001	
8	87.9210	0.0001	0.0001		89	270.2450	0.0001	0.0001		171	343.1671	0.0001	0.0001		253	515.9596	0.0001	0.0001	
9	89.9218	0.0001	0.0001		90	271.2665	0.0001	0.0001		172	344.1786	0.0001	0.0001		254	516.9706	0.0001	0.0001	
10	89.9218	0.0001	0.0001		91	272.2880	0.0001	0.0001		173	345.1901	0.0001	0.0001		255	517.9816	0.0001	0.0001	
11	91.9226	0.0001	0.0001		92	273.3095	0.0001	0.0001		174	346.2016	0.0001	0.0001		256	518.9926	0.0001	0.0001	
12	91.9226	0.0001	0.0001		93	274.3310	0.0001	0.0001		175	347.2131	0.0001	0.0001		257	519.0036	0.0001	0.0001	
13	93.9234	0.0001	0.0001		94	275.3525	0.0001	0.0001		176	348.2246	0.0001	0.0001		258	520.0146	0.0001	0.0001	
14	93.9234	0.0001	0.0001		95	276.3740	0.0001	0.0001		177	349.2361	0.0001	0.0001		259	521.0256	0.0001	0.0001	
15	95.9242	0.0001	0.0001		96	277.3955	0.0001	0.0001		178	350.2476	0.0001	0.0001		260	522.0366	0.0001	0.0001	
16	95.9242	0.0001	0.0001		97	278.4170	0.0001	0.0001		179	351.2591	0.0001	0.0001		261	523.0476	0.0001	0.0001	
17	97.9250	0.0001	0.0001		98	279.4385	0.0001	0.0001		180	352.2706	0.0001	0.0001		262	524.0586	0.0001	0.0001	
18	97.9250	0.0001	0.0001		99	280.4600	0.0001	0.0001		181	353.2821	0.0001	0.0001		263	525.0696	0.0001	0.0001	
19	99.9258	0.0001	0.0001		100	281.4815	0.0001	0.0001		182	354.2936	0.0001	0.0001		264	526.0806	0.0001	0.0001	
20	99.9258	0.0001	0.0001		101	282.5030	0.0001	0.0001		183	355.3051	0.0001	0.0001		265	527.0916	0.0001	0.0001	
21	101.9266	0.0001	0.0001		102	283.5245	0.0001	0.0001		184	356.3166	0.0001	0.0001		266	528.1026	0.0001	0.0001	
22	101.9266	0.0001	0.0001		103	284.5460	0.0001	0.0001		185	357.3281	0.0001	0.0001		267	529.1136	0.0001	0.0001	
23	103.9274	0.0001	0.0001		104	285.5675	0.0001	0.0001		186	358.3396	0.0001	0.0001		268	530.1246	0.0001	0.0001	
24	103.9274	0.0001	0.0001		105	286.5890	0.0001	0.0001		187	359.3511	0.0001	0.0001		269	531.1356	0.0001	0.0001	
25	105.9282	0.0001	0.0001		106	287.6105	0.0001	0.0001		188	360.3626	0.0001	0.0001		270	532.1466	0.0001	0.0001	
26	105.9282	0.0001	0.0001		107	288.6320	0.0001	0.0001		189	361.3741	0.0001	0.0001		271	533.1576	0.0001	0.0001	
27	105.9282	0.0001	0.0001		108	289.6535	0.0001	0.0001		190	362.3856	0.0001	0.0001		272	534.1686	0.0001	0.0001	
28	107.9290	0.0001	0.0001		109	290.6750	0.0001	0.0001		191	363.3971	0.0001	0.0001		273	535.1796	0.0001	0.0001	
29	107.9290	0.0001	0.0001		110	291.6965	0.0001	0.0001		192	364.4086	0.0001	0.0001		274	536.1906	0.0001	0.0001	
30	109.9304	0.0001	0.0001		111	292.7180	0.0001	0.0001		193	365.4201	0.0001	0.0001		275	537.2016	0.0001	0.0001	
31	109.9304	0.0001	0.0001		112	293.7395	0.0001	0.0001		194	366.4316	0.0001	0.0001		276	538.2126	0.0001	0.0001	
32	111.9312	0.0001	0.0001		113	294.7610	0.0001	0.0001		195	367.4431	0.0001	0.0001		277	539.2236	0.0001	0.0001	
33	111.9312	0.0001	0.0001		114	295.7825	0.0001	0.0001		196	368.4546	0.0001	0.0001		278	540.2346	0.0001	0.0001	
34	113.9320	0.0001	0.0001		115	296.8040	0.0001	0.0001		197	369.4661	0.0001	0.0001		279	541.2456	0.0001	0.0001	
35	113.9320	0.0001	0.0001		116	297.8255	0.0001	0.0001		198	370.4776	0.0001	0.0001		280	542.2566	0.0001	0.0001	
36	115.9328	0.0001	0.0001		117	298.8470	0.0001	0.0001		199	371.4891	0.0001	0.0001		281	543.2676	0.0001	0.0001	
37	115.9328	0.0001	0.0001		118	299.8685	0.0001	0.0001		200	372.5006	0.0001	0.0001		282	544.2786	0.0001	0.0001	
38	117.9336	0.0001	0.0001		119	300.8900	0.0001	0.0001		201	373.5121	0.0001	0.0001		283	545.2896	0.0001	0.0001	
39	117.9336	0.0001	0.0001		120	301.9115	0.0001	0.0001		202	374.5236	0.0001	0.0001		284	546.3006	0.0001	0.0001	
40	119.9344	0.0001	0.0001		121	302.9330	0.0001	0.0001		203	375.5351	0.0001	0.0001		285	547.3116	0.0001	0.0001	
41	119.9344	0.0001	0.0001		122	303.9545	0.0001	0.0001		204	376.5466	0.0001	0.0001		286	548.3226	0.0001	0.0001	
42	121.9352	0.0001	0.0001		123	304.9760	0.0001	0.0001		205	377.5581	0.0001	0.0001		287	549.3336	0.0001	0.0001	
43	121.9352	0.0001	0.0001		124	305.9975	0.0001	0.0001		206	378.5696	0.0001	0.0001		288	550.3446	0.0001	0.0001	
44	123.9360	0.0001	0.0001		125	307.0190	0.0001	0.0001		207	379.5811	0.0001	0.0001		289	551.3556	0.0001	0.0001	
45	123.9360	0.0001	0.0001		126	308.0405	0.0001	0.0001		208	380.5926	0.0001	0.0001		290	552.3666	0.0001	0.0001	
46	125.9368	0.0001	0.0001		127	309.0620	0.0001	0.0001		209	381.6041	0.0001	0.0001		291	553.3776	0.0001	0.0001	
47	125.9368	0.0001	0.0001		128	310.0835	0.0001	0.0001		210	382.6156	0.0001	0.0001		292	554.3886	0.0001	0.0001	
48	127.9376	0.0001	0.0001		129	311.1050	0.0001	0.0001		211	383.6271	0.0001	0.0001		293	555.3996	0.0001	0.0001	
49	127.9376	0.0001	0.0001		130	312.1265	0.0001	0.0001		212	384.6386	0.0001	0.0001		294	556.4106	0.0001	0.0001	
50	129.9384	0.0001	0.0001		131	313.1480	0.0001	0.0001		213	385.6501	0.0001	0.0001		295	557.4216	0.0001	0.0001	
51	129.9384	0.0001	0.0001		132	314.1695	0.0001	0.0001		214	386.6616	0.0001	0.0001		296	558.4326	0.0001	0.0001	
52	131.9392	0.0001	0.0001		133	315.1910	0.0001	0.0001		215	387.6731	0.0001	0.0001		297	559.4436	0.0001	0.0001	
53	131.9392	0.0001	0.0001		134	316.2125	0.0001	0.0001		216	388.6846	0.0001	0.0001		298	560.4546	0.0001	0.0001	
54	133.9400	0.0001	0.0001		135	317.2340	0.0001	0.0001		217	389.6961	0.0001	0.0001		299	561.4656	0.0001	0.0001	
55	133.9400	0.0001	0.0001		136	318.2555	0.0001	0.0001		218	390.7076	0.0001	0.0001		300	562.4766	0.0001	0.0001	
56	135.9408	0.0001	0.0001		137	319.2770	0.0001	0.0001		219	391.7191	0.0001	0.0001		301	563.4876	0.0001	0.0001	
57	135.9408	0.0001	0.0																



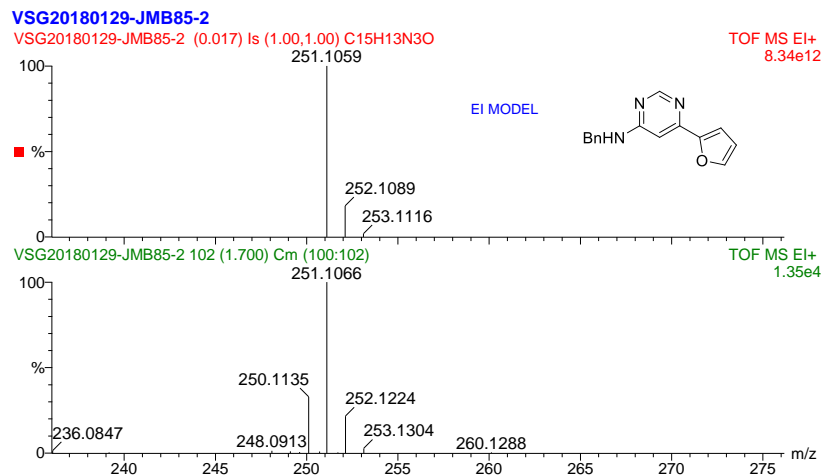
HRMS spectra of **16c**



¹H NMR spectrum of **16d** (in DMSO-*d*₆)



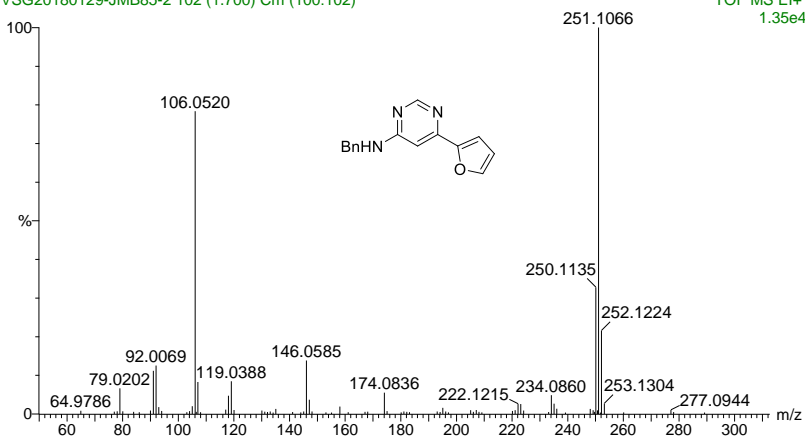
¹³C NMR spectrum of **16d** (in DMSO-d₆)



VSG20180129-JMB85-2

VSG20180129-JMB85-2 102 (1.700) Cm (100:102)

TOF MS EI+
1.35e4

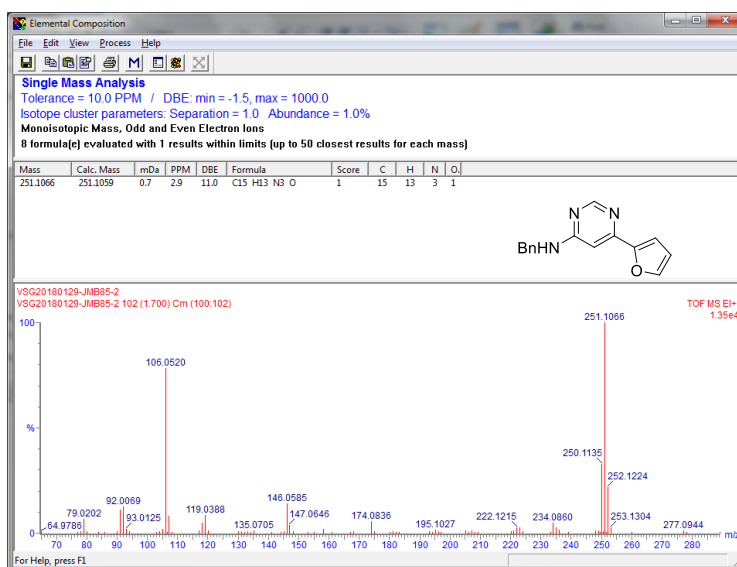
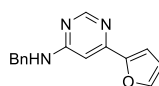


VSG20180129-JMB85-2

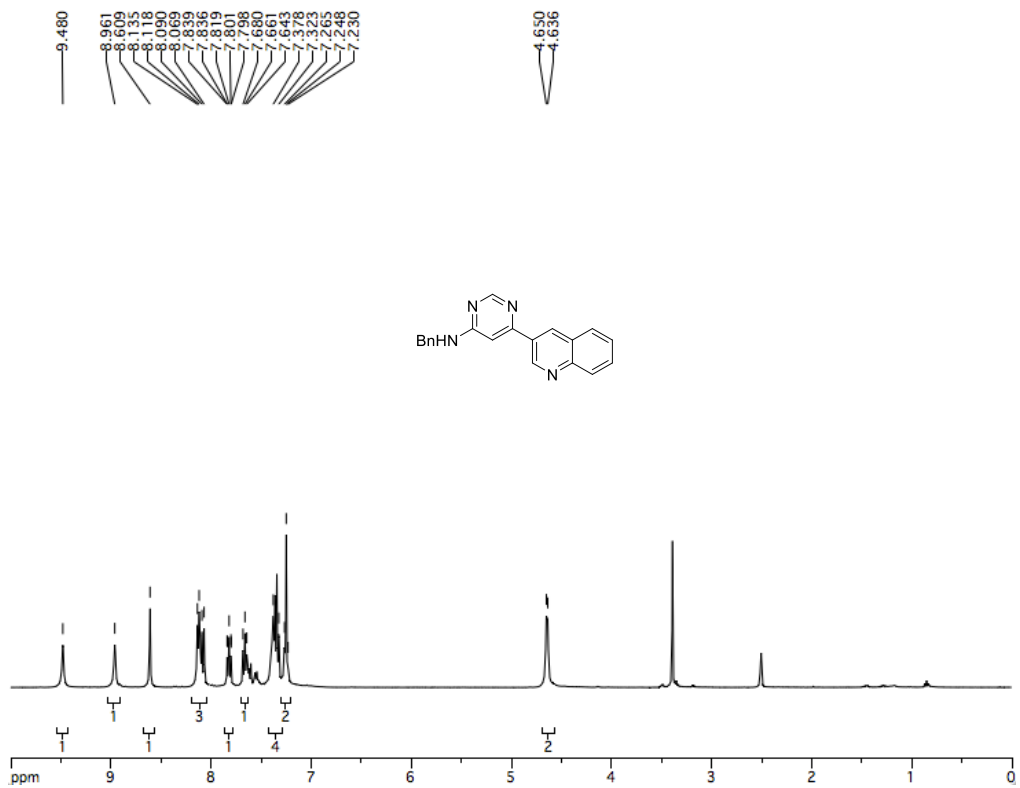
VSG20180129-JMB85-2 102 (1.700) Cm (100:102)

TOF MS EI+

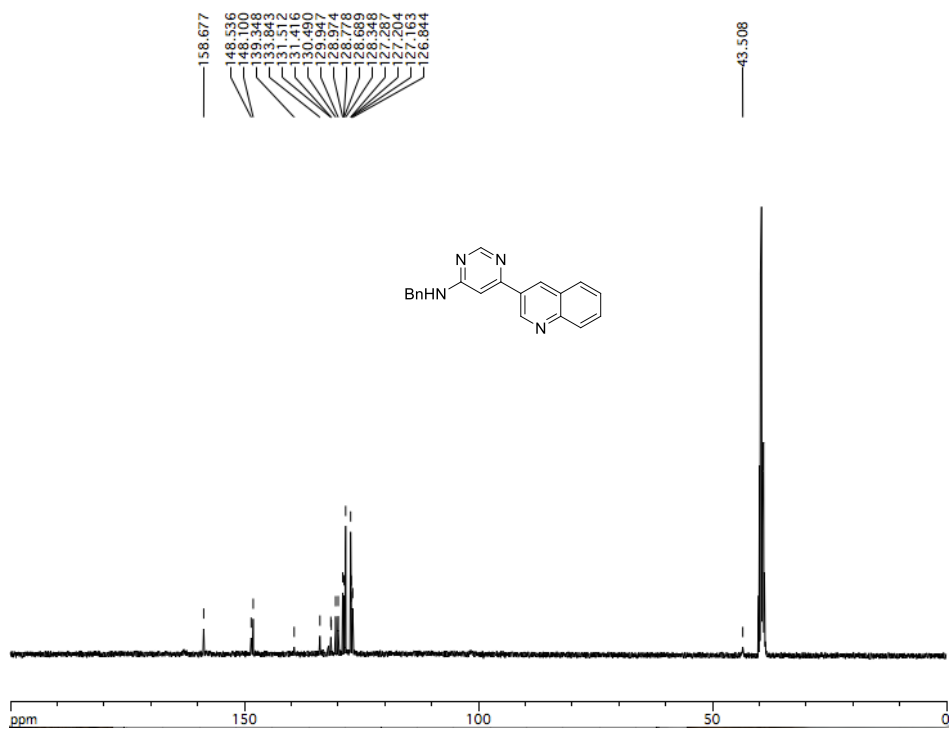
No.	Mass	Abun.	No.	Mass	Abun.	No.	Mass	Abun.	No.	Mass	Abun.	No.	Mass	Abun.
1	64.9786	0.01	17	164.0714	0.01	33	264.0742	0.01	49	364.0770	0.01	65	464.0798	0.01
2	79.0202	0.01	18	165.0936	0.01	34	265.0962	0.01	50	365.0998	0.01	66	465.1014	0.01
3	79.0202	0.01	19	166.1158	0.01	35	266.1184	0.01	51	366.1214	0.01	67	466.1230	0.01
4	80.0424	0.01	20	167.1380	0.01	36	267.1406	0.01	52	367.1436	0.01	68	467.1452	0.01
5	80.0424	0.01	21	168.1602	0.01	37	268.1628	0.01	53	368.1658	0.01	69	468.1674	0.01
6	80.0424	0.01	22	169.1824	0.01	38	269.1850	0.01	54	369.1878	0.01	70	469.1890	0.01
7	80.0424	0.01	23	170.2046	0.01	39	270.2072	0.01	55	370.2102	0.01	71	470.2114	0.01
8	80.0424	0.01	24	171.2268	0.01	40	271.2294	0.01	56	371.2322	0.01	72	471.2334	0.01
9	80.0424	0.01	25	172.2490	0.01	41	272.2516	0.01	57	372.2546	0.01	73	472.2558	0.01
10	80.0424	0.01	26	173.2712	0.01	42	273.2738	0.01	58	373.2766	0.01	74	473.2778	0.01
11	80.0424	0.01	27	174.2934	0.01	43	274.2960	0.01	59	374.2988	0.01	75	474.2994	0.01
12	80.0424	0.01	28	175.3156	0.01	44	275.3182	0.01	60	375.3210	0.01	76	475.3216	0.01
13	80.0424	0.01	29	176.3378	0.01	45	276.3404	0.01	61	376.3432	0.01	77	476.3438	0.01
14	80.0424	0.01	30	177.3600	0.01	46	277.3626	0.01	62	377.3654	0.01	78	477.3660	0.01
15	80.0424	0.01	31	178.3822	0.01	47	278.3848	0.01	63	378.3876	0.01	79	478.3882	0.01
16	80.0424	0.01	32	179.4044	0.01	48	279.4070	0.01	64	379.4100	0.01	80	479.4106	0.01
17	80.0424	0.01	33	180.4266	0.01	49	280.4292	0.01	65	380.4320	0.01			
18	80.0424	0.01	34	181.4488	0.01	50	281.4514	0.01	66	381.4542	0.01			
19	80.0424	0.01	35	182.4710	0.01	51	282.4736	0.01	67	382.4764	0.01			
20	80.0424	0.01	36	183.4932	0.01	52	283.4958	0.01	68	383.4986	0.01			
21	80.0424	0.01	37	184.5154	0.01	53	284.5180	0.01	69	384.5208	0.01			
22	80.0424	0.01	38	185.5376	0.01	54	285.5402	0.01	70	385.5430	0.01			
23	80.0424	0.01	39	186.5598	0.01	55	286.5624	0.01	71	386.5652	0.01			
24	80.0424	0.01	40	187.5820	0.01	56	287.5846	0.01	72	387.5874	0.01			
25	80.0424	0.01	41	188.6042	0.01	57	288.6068	0.01	73	388.6096	0.01			
26	80.0424	0.01	42	189.6264	0.01	58	289.6290	0.01	74	389.6318	0.01			
27	80.0424	0.01	43	190.6486	0.01	59	290.6512	0.01	75	390.6540	0.01			
28	80.0424	0.01	44	191.6708	0.01	60	291.6734	0.01	76	391.6762	0.01			
29	80.0424	0.01	45	192.6930	0.01	61	292.6956	0.01	77	392.6984	0.01			
30	80.0424	0.01	46	193.7152	0.01	62	293.7178	0.01	78	393.7206	0.01			
31	80.0424	0.01	47	194.7374	0.01	63	294.7400	0.01	79	394.7428	0.01			
32	80.0424	0.01	48	195.7596	0.01	64	295.7622	0.01	80	395.7650	0.01			
33	80.0424	0.01	49	196.7818	0.01	65	296.7844	0.01						
34	80.0424	0.01	50	197.8040	0.01	66	297.8066	0.01						
35	80.0424	0.01	51	198.8262	0.01	67	298.8288	0.01						
36	80.0424	0.01	52	199.8484	0.01	68	299.8510	0.01						
37	80.0424	0.01	53	200.8706	0.01	69	300.8732	0.01						
38	80.0424	0.01	54	201.8928	0.01	70	301.8954	0.01						
39	80.0424	0.01	55	202.9150	0.01	71	302.9176	0.01						
40	80.0424	0.01	56	203.9372	0.01	72	303.9398	0.01						
41	80.0424	0.01	57	204.9594	0.01	73	304.9620	0.01						
42	80.0424	0.01	58	205.9816	0.01	74	305.9842	0.01						
43	80.0424	0.01	59	207.0038	0.01	75	307.0064	0.01						
44	80.0424	0.01	60	208.0260	0.01	76	308.0286	0.01						
45	80.0424	0.01	61	209.0482	0.01	77	309.0508	0.01						
46	80.0424	0.01	62	210.0704	0.01	78	310.0730	0.01						
47	80.0424	0.01	63	211.0926	0.01	79	311.0952	0.01						
48	80.0424	0.01	64	212.1148	0.01	80	312.1174	0.01						
49	80.0424	0.01	65	213.1370	0.01									
50	80.0424	0.01	66	214.1592	0.01									
51	80.0424	0.01	67	215.1814	0.01									
52	80.0424	0.01	68	216.2036	0.01									
53	80.0424	0.01	69	217.2258	0.01									
54	80.0424	0.01	70	218.2480	0.01									
55	80.0424	0.01	71	219.2702	0.01									
56	80.0424	0.01	72	220.2924	0.01									
57	80.0424	0.01	73	221.3146	0.01									
58	80.0424	0.01	74	222.3368	0.01									
59	80.0424	0.01	75	223.3590	0.01									
60	80.0424	0.01	76	224.3812	0.01									
61	80.0424	0.01	77	225.4034	0.01									
62	80.0424	0.01	78	226.4256	0.01									
63	80.0424	0.01	79	227.4478	0.01									
64	80.0424	0.01	80	228.4700	0.01									
65	80.0424	0.01												
66	80.0424	0.01												
67	80.0424	0.01												
68	80.0424	0.01												
69	80.0424	0.01												
70	80.0424	0.01												
71	80.0424	0.01												
72	80.0424	0.01												
73	80.0424	0.01												
74	80.0424	0.01												
75	80.0424	0.01												
76	80.0424	0.01												
77	80.0424	0.01												
78	80.0424	0.01												
79	80.0424	0.01												
80	80.0424	0.01												



HRMS spectra of 16d



^1H NMR spectrum of **16e** (in $\text{DMSO-}d_6$)

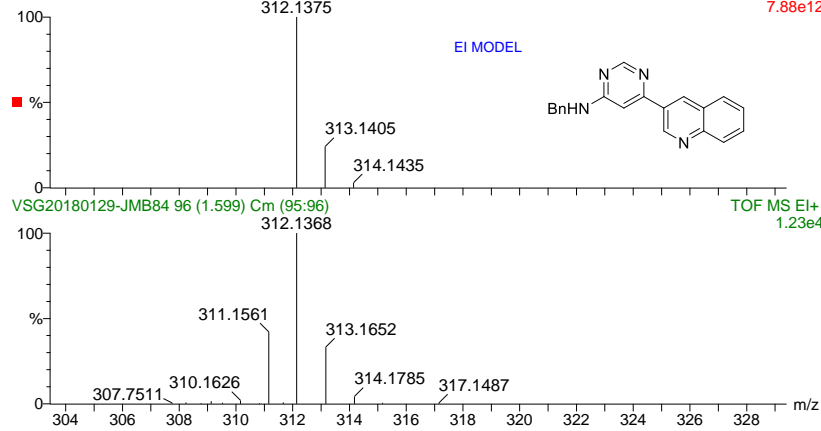


^{13}C NMR spectrum of **16e** (in $\text{DMSO-}d_6$)

VSG20180129-JMB84

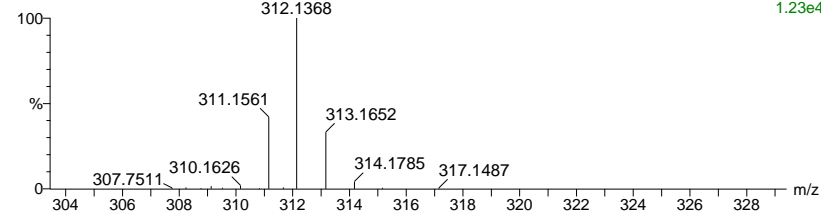
VSG20180129-JMB84 (0.016) Is (1.00,1.00) C20H16N4

TOF MS EI+
7.88e12



VSG20180129-JMB84 96 (1.599) Cm (95:96)

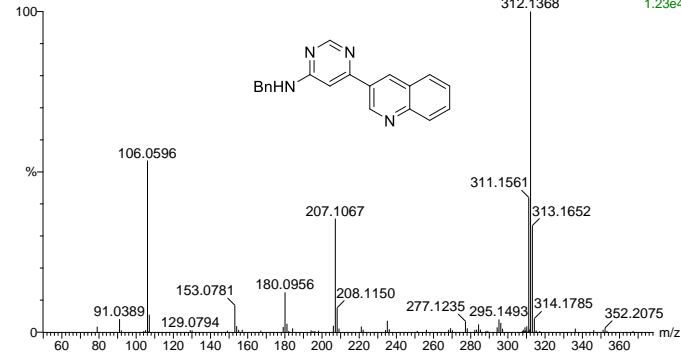
TOF MS EI+
1.23e4



VSG20180129-JMB84

VSG20180129-JMB84 96 (1.599) Cm (95:96)

TOF MS EI+
1.23e4

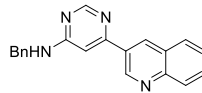


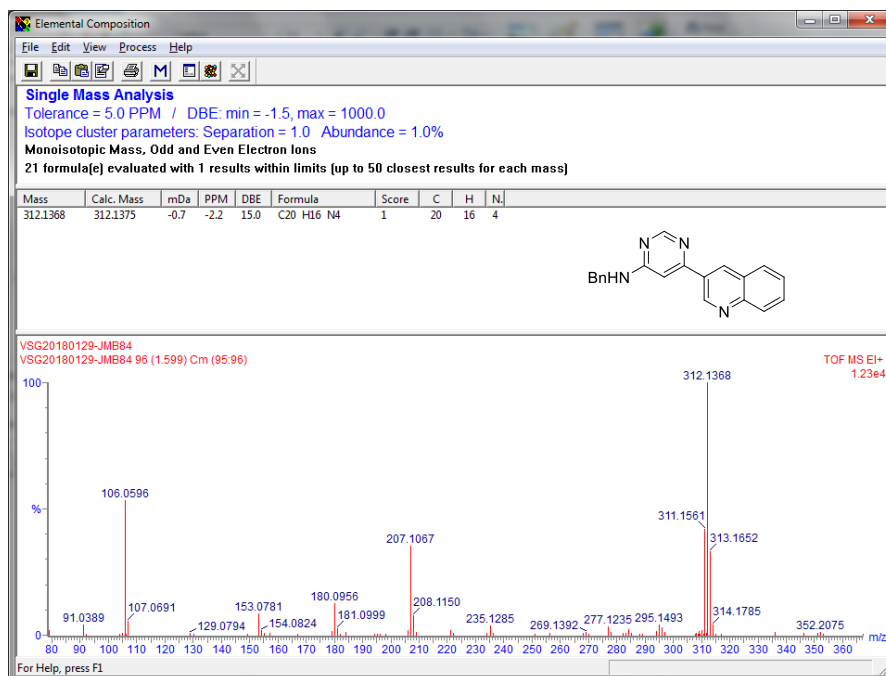
VSG20180129-JMB84

VSG20180129-JMB84 96 (1.599) Cm (95:96)

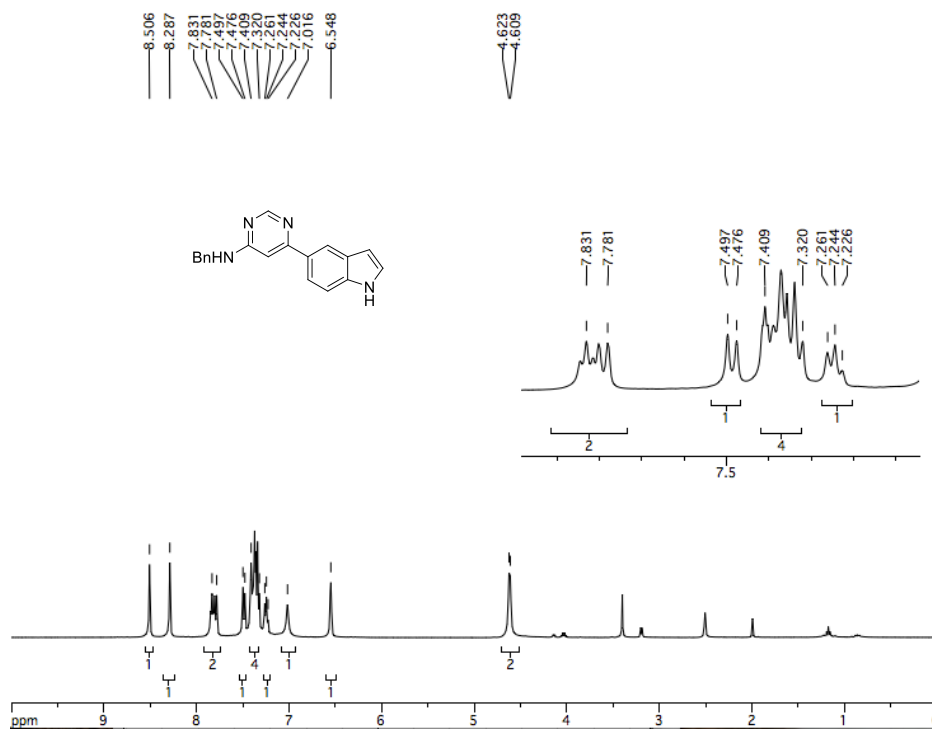
TOF MS EI+

m/z	Relative Intensity (%)	Label
91.0389	~5	
106.0596	~40	
129.0794	~5	
153.0781	~10	
180.0956	~15	
207.1067	~30	
208.1150	~10	
277.1235	~5	
295.1493	~5	
311.1561	~40	
312.1368	100	
313.1652	~30	
314.1785	~10	
352.2075	~5	

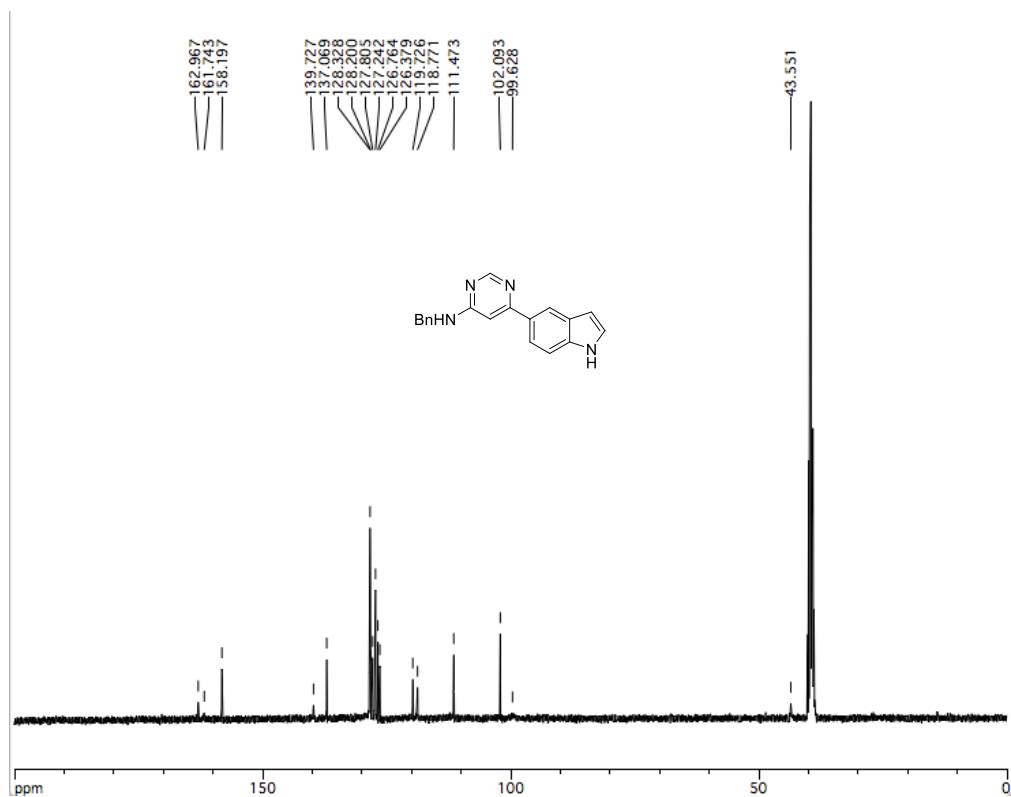




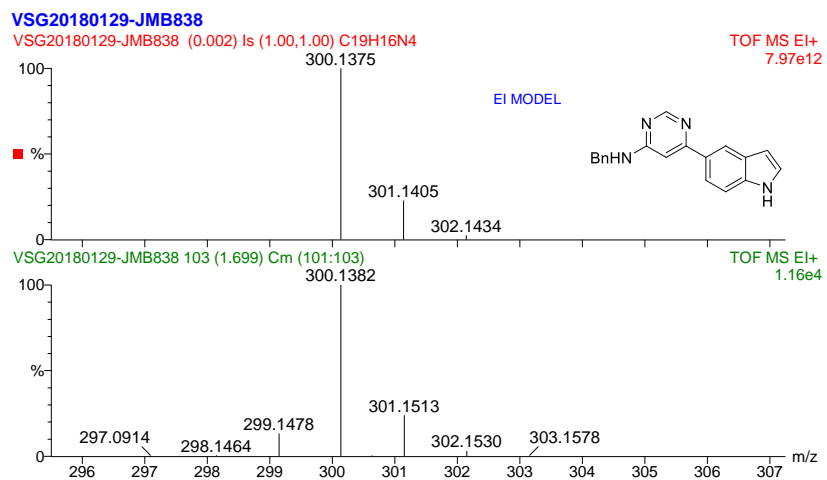
HRMS spectra of **16e**



¹H NMR spectrum of **16f** (in DMSO-*d*₆)

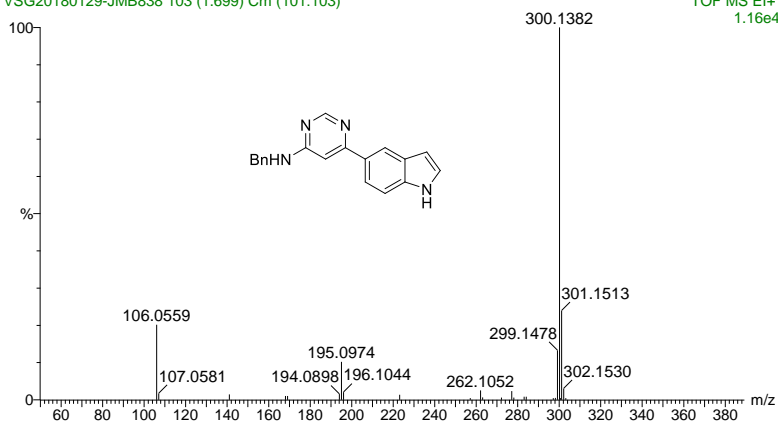


¹³C NMR spectrum of **16f** (in DMSO-*d*₆)



VSG20180129-JMB838

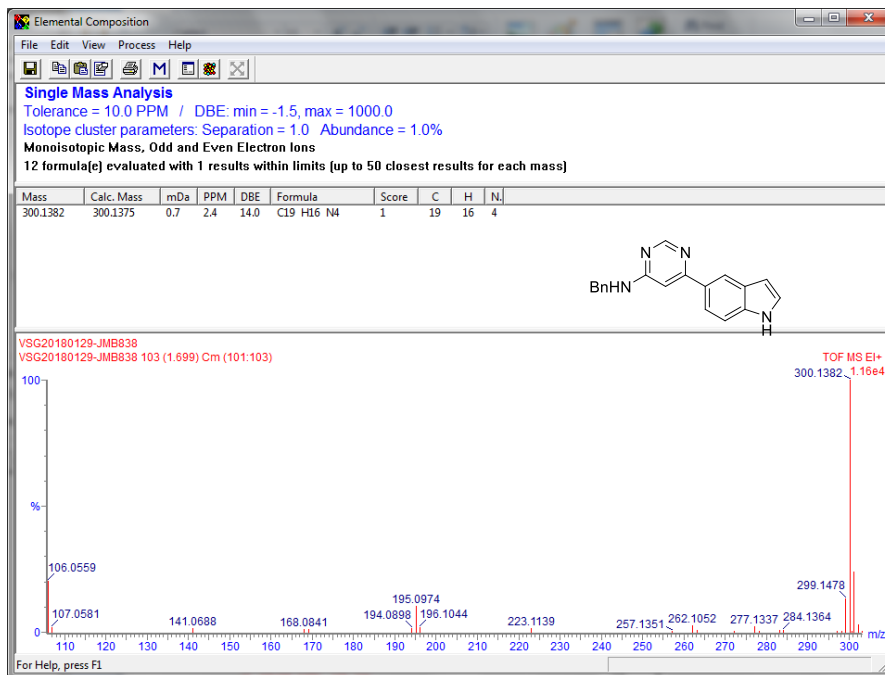
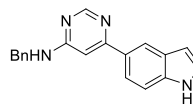
VSG20180129-JMB838 103 (1.699) Cm (101:103)



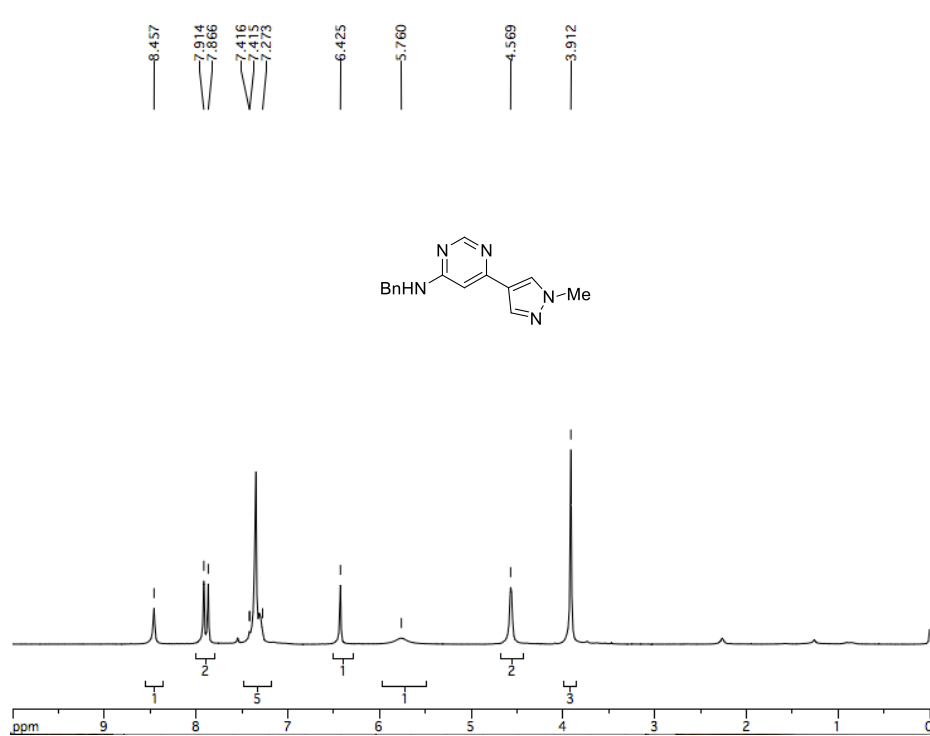
VSG20180129-JMB838

VSG20180129-JMB838 103 (1.699) Cm (101:103)

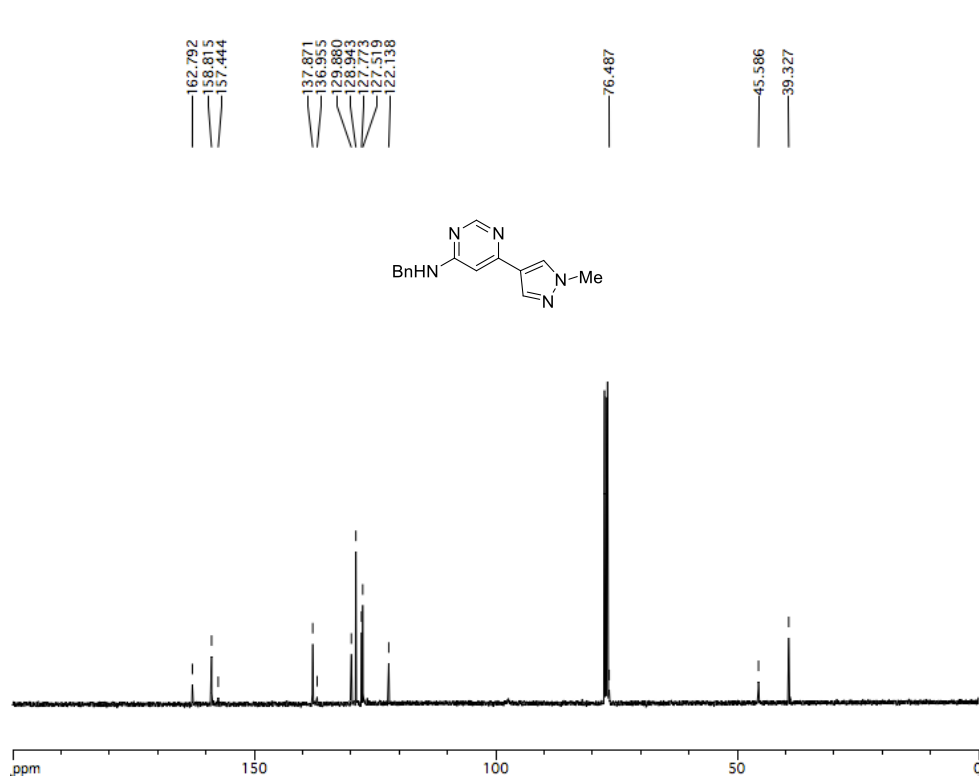
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	106.0559	2.33e3	20.12	10.01										
2:	107.0581	1.96e2	1.70	0.84										
3:	141.0688	1.62e2	1.40	0.70										
4:	168.0841	1.16e2	1.01	0.50										
5:	169.0962	1.13e2	0.98	0.49										
6:	194.0898	1.73e2	1.50	0.74										
7:	195.0974	1.17e3	10.14	5.04										
8:	196.1044	2.32e2	2.00	1.00										
9:	223.1139	1.52e2	1.31	0.65										
10:	257.1351	4.66e1	0.40	0.20										
11:	262.1052	2.89e2	2.49	1.24										
12:	263.1082	7.29e1	0.63	0.31										
13:	272.1359	6.38e1	0.55	0.27										
14:	277.1337	2.65e2	2.29	1.14										
15:	278.1324	6.28e1	0.54	0.27										
16:	283.1200	9.11e1	0.79	0.39										
17:	284.1364	9.22e1	0.80	0.40										
18:	297.0914	4.76e1	0.41	0.20										
19:	298.1464	5.57e1	0.48	0.24										
20:	299.1478	1.53e3	13.24	6.59										
21:	300.1382	1.16e4	100.00	49.73										
22:	300.6387	4.66e1	0.40	0.20										
23:	301.1513	2.77e3	23.89	11.88										
24:	302.1530	3.45e2	2.98	1.48										
25:	303.1578	4.86e1	0.42	0.21										



HRMS spectra of 16f



¹H NMR spectrum of **16g** (in CDCl₃)

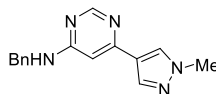
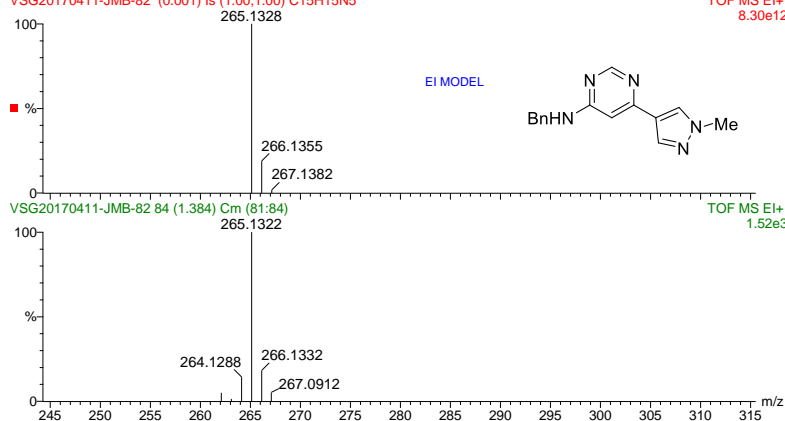


¹³C NMR spectrum of **16g** (in CDCl₃)

VSG20170411-JMB-82

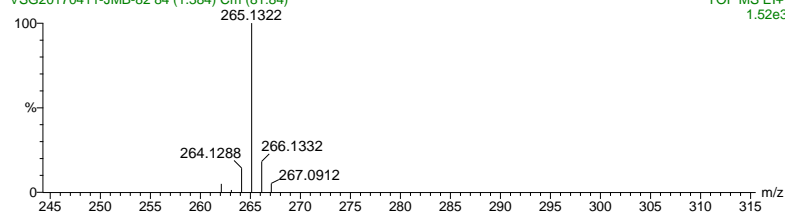
VSG20170411-JMB-82 (0.001) Is (1.00,1.00) C15H15N5

TOF MS EI+
8.30e12



VSG20170411-JMB-82 84 (1.384) Cm (81:84)

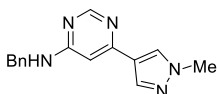
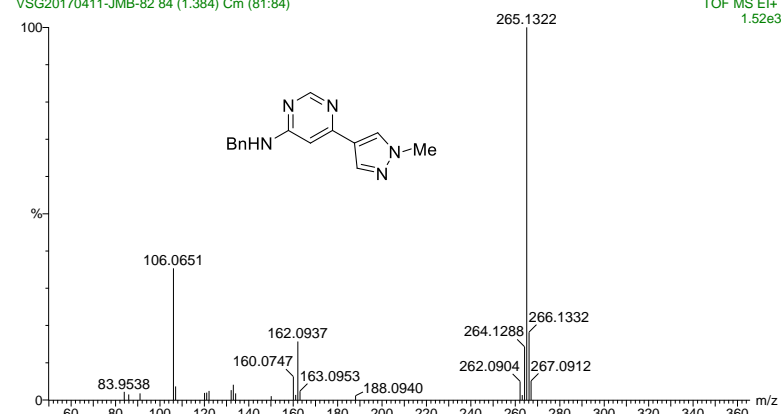
TOF MS EI+
1.52e3



VSG20170411-JMB-82

VSG20170411-JMB-82 84 (1.384) Cm (81:84)

TOF MS EI+
1.52e3

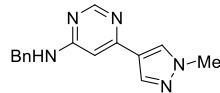


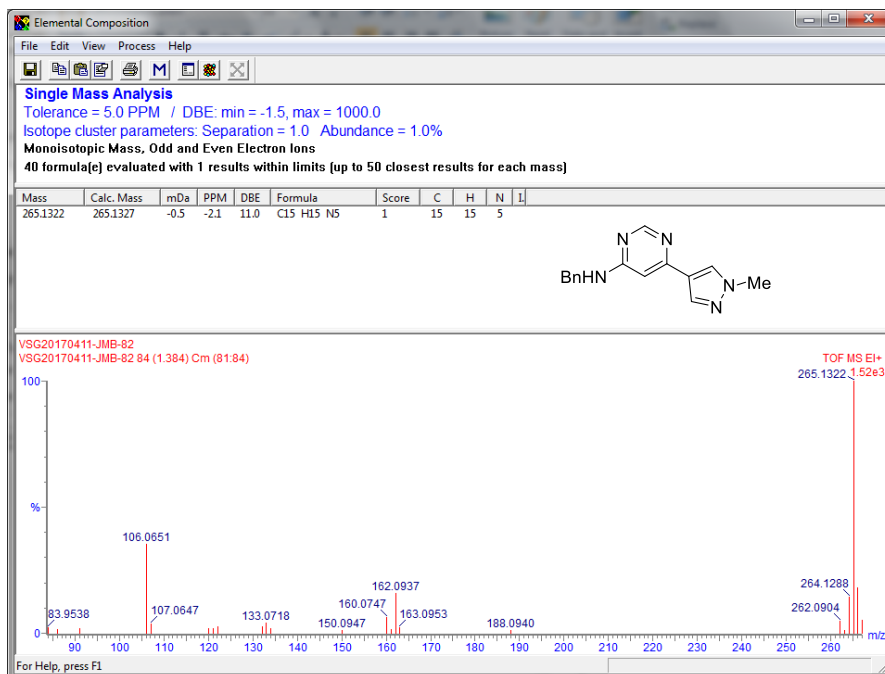
VSG20170411-JMB-82

VSG20170411-JMB-82 84 (1.384) Cm (81:84)

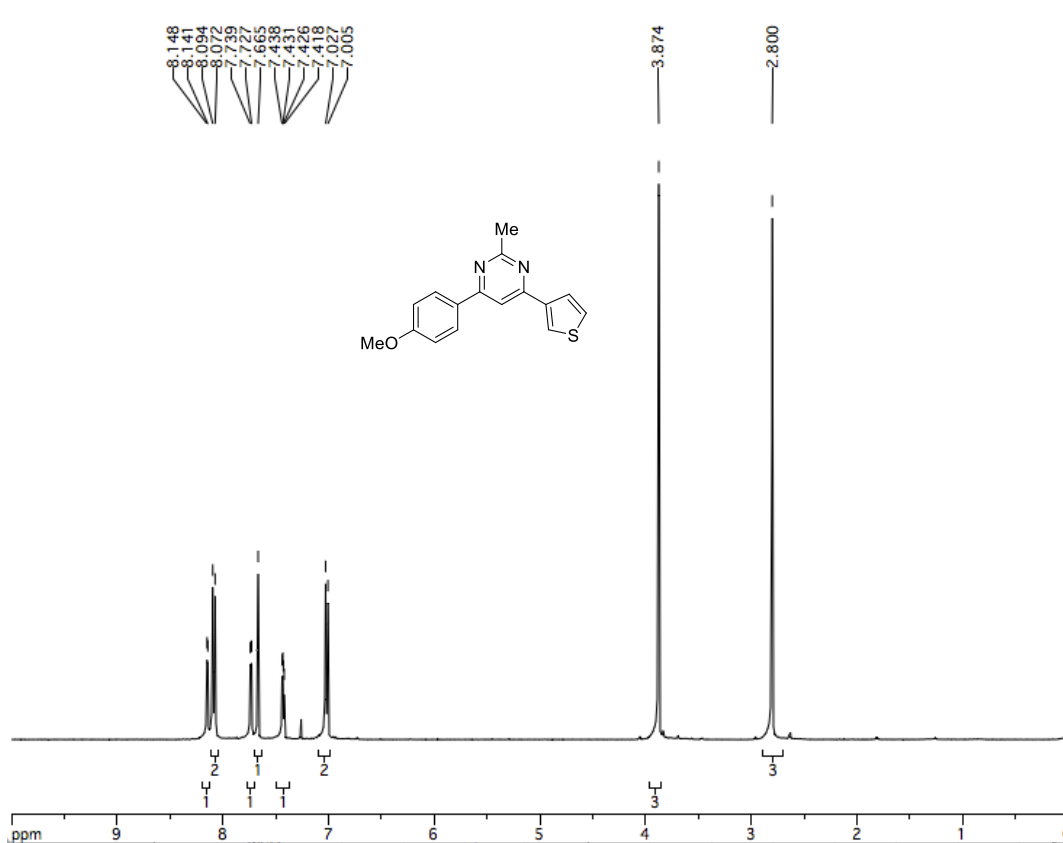
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No
1:	83.9538	3.24e1	2.13	0.86											
2:	85.9536	2.23e1	1.47	0.59											
3:	91.0549	2.63e1	1.73	0.70											
4:	106.0651	5.36e2	35.29	14.25											
5:	107.0647	5.47e1	3.60	1.45											
6:	120.0563	2.94e1	1.87	0.75											
7:	121.0646	2.94e1	1.93	0.78											
8:	122.0715	3.65e1	2.40	0.97											
9:	132.0795	3.95e1	2.60	1.05											
10:	133.0719	6.19e1	4.07	1.64											
11:	134.0781	2.63e1	1.73	0.70											
12:	150.0947	1.52e1	1.00	0.40											
13:	160.0747	9.42e1	6.20	2.51											
14:	161.0815	2.03e1	1.33	0.54											
15:	162.0937	2.38e2	15.68	6.33											
16:	163.0953	3.54e1	2.33	0.94											
17:	168.0940	1.62e1	1.07	0.43											
18:	262.0904	7.49e1	4.94	1.99											
19:	263.1039	1.92e1	1.27	0.51											
20:	264.1288	2.16e2	14.21	5.74											
21:	265.1322	1.52e3	99.99	40.38											
22:	266.1332	2.75e2	18.15	7.33											
23:	267.0912	7.70e1	5.07	2.05											

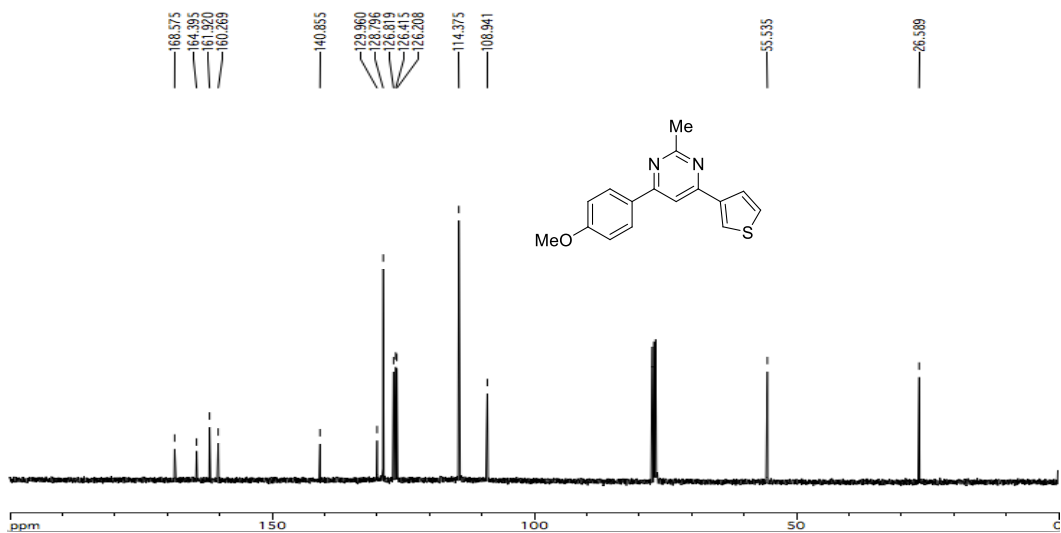




HRMS spectra of **16g**



¹H NMR spectrum of **16h** (in CDCl₃)

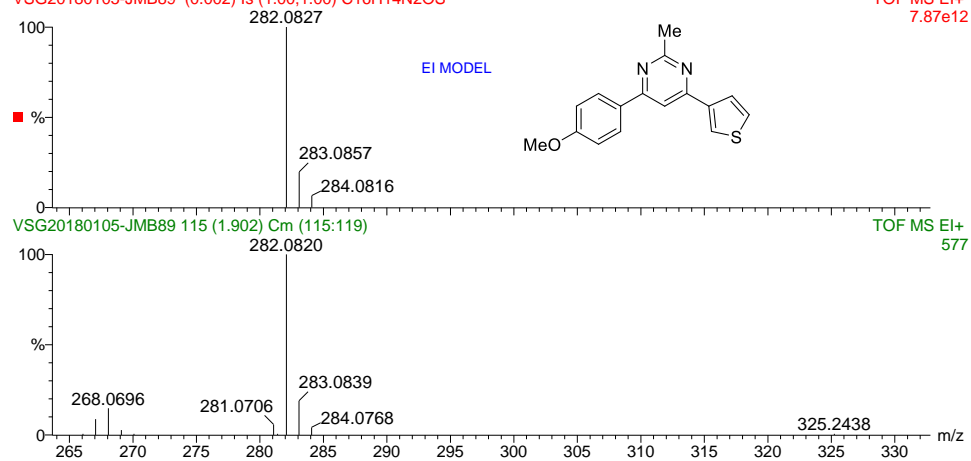


¹³C NMR spectrum of **16h** (in CDCl₃)

VSG20180105-JMB89

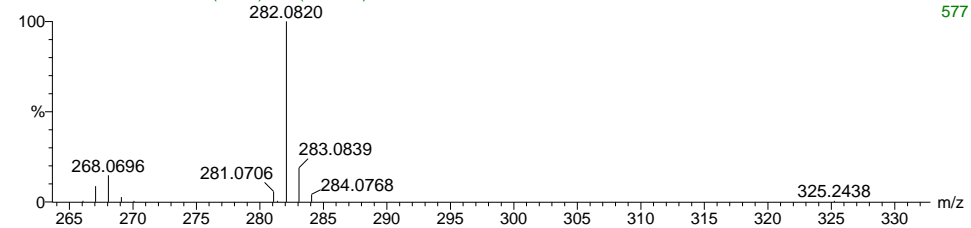
VSG20180105-JMB89 (0.002) Is (1.00,1.00) C₁₆H₁₄N₂O₂S

TOF MS EI+
7.87e12



VSG20180105-JMB89 115 (1.902) Cm (115:119)

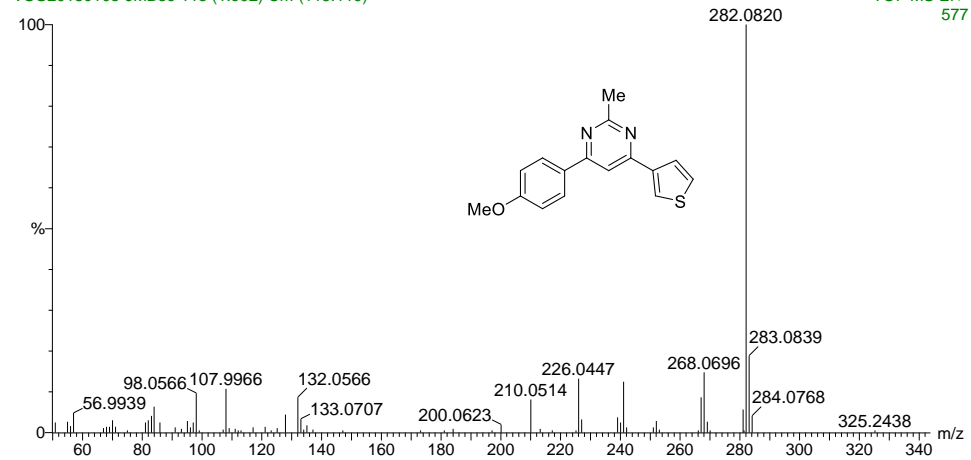
TOF MS EI+
577



VSG20180105-JMB89

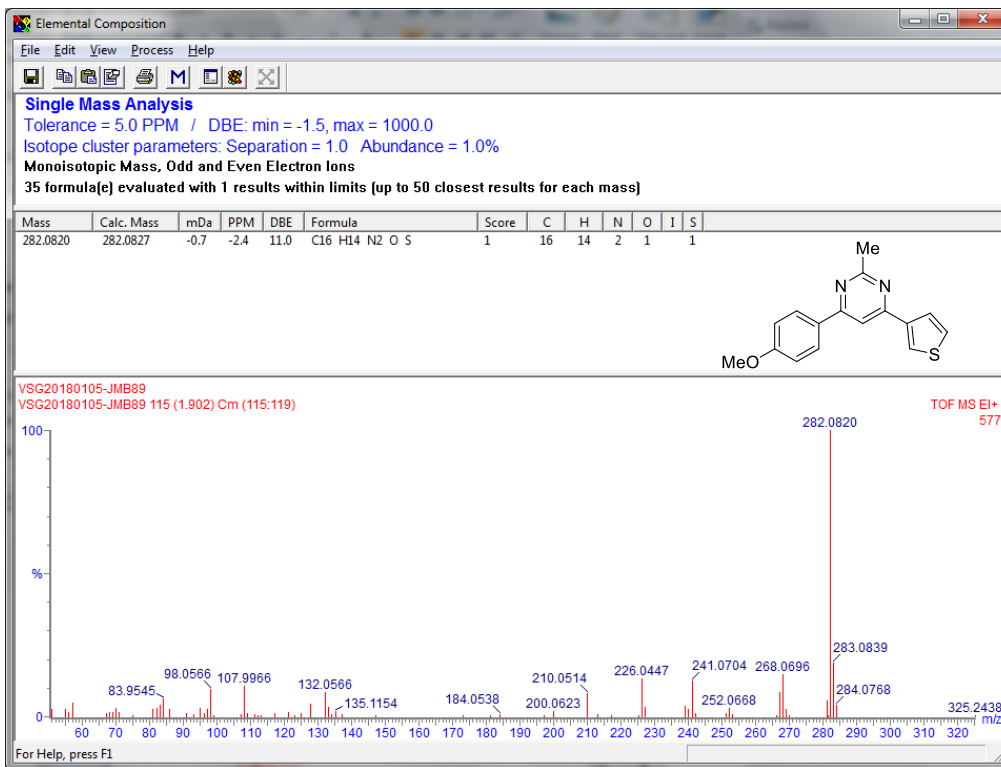
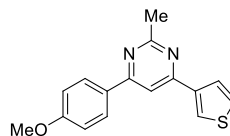
VSG20180105-JMB89 115 (1.902) Cm (115:119)

TOF MS EI+
577

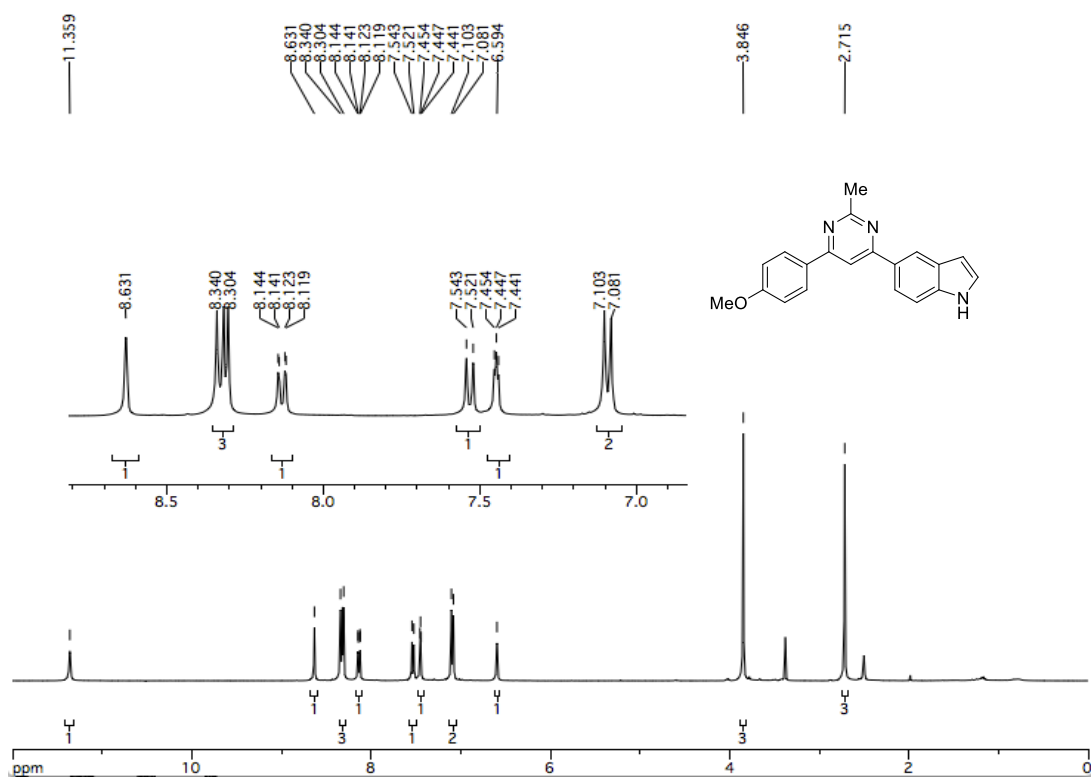


VSG20180105-JMB89 (1.902) Cm (115:119) TOF MS E+

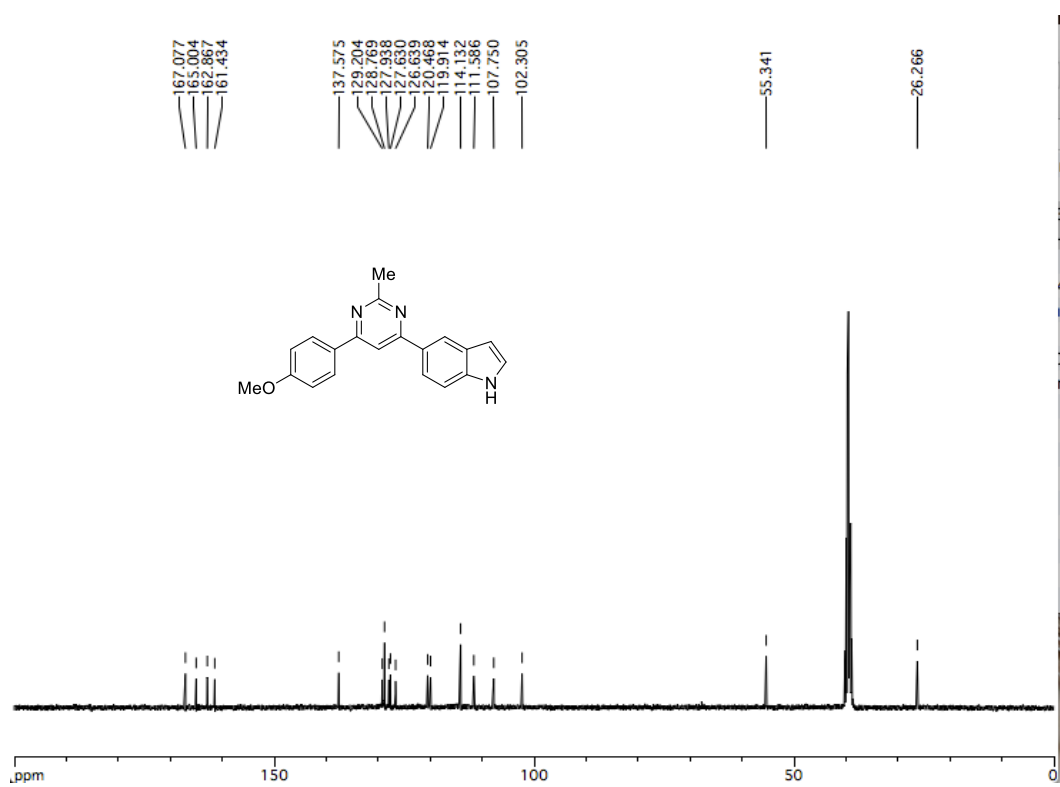
No.	Mass	Inten	%BPI	%TIC	No.	Mass	Inten	%BPI	%TIC	No.	Mass	Inten	%BPI	%TIC	No.	Mass	Inten	%BPI	%TIC
2	54.9740	1.52e1	2.63	0.82	17	93.0557	5.05e0	0.88	0.27										
3	55.9811	9.11e0	1.58	0.49	18	95.0665	1.52e1	2.81	0.88										
4	56.9939	2.73e1	4.74	1.48	19	96.0788	7.05e0	1.23	0.38										
5	68.9936	6.08e0	1.06	0.33	20	97.0481	1.52e1	2.46	0.77										
6	68.0076	8.10e0	1.40	0.44	21	98.0588	5.17e1	8.94	3.02										
7	69.0178	8.10e0	1.40	0.44	22	99.0584	3.04e0	0.53	0.16										
8	70.0178	1.72e1	2.98	0.95	23	101.0593	4.55e0	0.79	0.25										
9	71.0292	8.10e0	1.40	0.44	24	107.9968	8.18e1	10.71	3.34										
10	74.9988	3.04e0	0.53	0.16	25	109.1033	6.08e0	1.06	0.33										
11	81.0344	1.42e1	2.46	0.77	26	111.0687	5.05e0	0.88	0.27										
12	83.0354	1.72e1	2.98	0.95	27	112.0713	3.04e0	0.53	0.16										
13	83.0344	2.33e1	4.04	1.26	28	113.0486	3.04e0	0.53	0.16										
14	83.9545	3.05e1	5.32	1.67	29	117.0452	7.09e0	1.23	0.38										
15	85.9173	1.42e1	2.46	0.77	30	121.1050	8.10e0	1.40	0.44										
16	87.0162	7.09e0	1.23	0.38	31	123.1110	3.04e0	0.53	0.16										
17	93.0557	5.05e0	0.88	0.27	32	125.1090	8.08e0	1.39	0.43										
18	95.0665	1.52e1	2.81	0.88	33	127.9120	2.52e1	4.39	1.37										
19	96.0788	7.05e0	1.23	0.38	34	131.0288	4.09e1	6.94	2.09										
20	97.0481	1.52e1	2.46	0.77	35	133.0707	1.92e1	3.33	1.04										
21	98.0588	5.17e1	8.94	3.02	36	134.0320	4.55e0	0.79	0.25										
22	99.0584	3.04e0	0.53	0.16	37	135.1154	1.01e1	1.76	0.55										
23	101.0593	4.55e0	0.79	0.25	38	137.1144	4.05e0	0.70	0.22										
24	107.9968	8.18e1	10.71	3.34	39	147.1167	3.04e0	0.53	0.16										
25	109.1033	6.08e0	1.06	0.33	40	147.1527	3.04e0	0.53	0.16										
26	111.0687	5.05e0	0.88	0.27	41	161.0210	3.04e0	0.53	0.16										
27	112.0713	3.04e0	0.53	0.16	42	184.0538	5.05e0	0.88	0.27										
28	113.0486	3.04e0	0.53	0.16	43	197.0553	3.04e0	0.53	0.16										
29	117.0452	7.09e0	1.23	0.38	44	209.0521	1.17e1	1.93	0.60										
30	121.1050	8.10e0	1.40	0.44	45	210.0514	4.05e1	6.97	2.12										
31	123.1110	3.04e0	0.53	0.16	46	213.1229	5.05e0	0.88	0.27										
32	125.1090	8.08e0	1.39	0.43	47	217.2821	3.04e0	0.53	0.16										
33	127.9120	2.52e1	4.39	1.37	48	225.1388	3.04e0	0.53	0.16										
34	131.0288	4.09e1	6.94	2.09	49	226.0447	5.17e1	8.94	3.02										
35	133.0707	1.92e1	3.33	1.04	50	227.0612	1.82e1	3.16	0.99										
36	134.0320	4.55e0	0.79	0.25	51	239.0785	2.13e1	3.68	1.15										
37	135.1154	1.01e1	1.76	0.55	52	240.0504	1.42e1	2.46	0.77										
38	137.1144	4.05e0	0.70	0.22	53	245.0704	7.19e1	12.46	3.88										
39	147.1167	3.04e0	0.53	0.16	54	242.0648	7.09e0	1.23	0.38										
40	147.1527	3.04e0	0.53	0.16	55	251.0628	7.09e0	1.23	0.38										
41	161.0210	3.04e0	0.53	0.16	56	252.0948	1.62e1	2.81	0.88										
42	184.0538	5.05e0	0.88	0.27	57	253.0788	4.05e0	0.70	0.22										
43	197.0553	3.04e0	0.53	0.16	58	260.0714	3.04e0	0.53	0.16										
44	209.0521	1.17e1	1.93	0.60	59	267.0624	6.08e1	8.92	2.69										
45	210.0514	4.05e1	6.97	2.12	60	268.0888	8.18e1	10.74	3.34										
46	213.1229	5.05e0	0.88	0.27	61	269.0826	1.52e1	2.46	0.77										
47	217.2821	3.04e0	0.53	0.16	62	270.0808	3.04e0	0.53	0.16										
48	225.1388	3.04e0	0.53	0.16	63	281.0788	3.24e1	5.62	1.75										
49	226.0447	5.17e1	8.94	3.02	64	281.9823	3.04e0	0.53	0.16										
50	227.0612	1.82e1	3.16	0.99	65	282.0820	5.77e2	100.04	31.25										
51	239.0785	2.13e1	3.68	1.15	66	283.0820	1.92e0	0.33	0.10										
52	240.0504	1.42e1	2.46	0.77	67	284.0788	2.33e1	4.04	1.26										
53	245.0704	7.19e1	12.46	3.88	68	325.2438	3.04e0	0.53	0.16										
54	242.0648	7.09e0	1.23	0.38															
55	251.0628	7.09e0	1.23	0.38															
56	252.0948	1.62e1	2.81	0.88															
57	253.0788	4.05e0	0.70	0.22															
58	260.0714	3.04e0	0.53	0.16															
59	267.0624	6.08e1	8.92	2.69															
60	268.0888	8.18e1	10.74	3.34															
61	269.0826	1.52e1	2.46	0.77															
62	270.0808	3.04e0	0.53	0.16															
63	281.0788	3.24e1	5.62	1.75															
64	281.9823	3.04e0	0.53	0.16															
65	282.0820	5.77e2	100.04	31.25															
66	283.0820	1.92e0	0.33	0.10															
67	284.0788	2.33e1	4.04	1.26															
68	325.2438	3.04e0	0.53	0.16															



HRMS spectra of 16h



¹H NMR spectrum of **16i (in DMSO-*d*₆)**

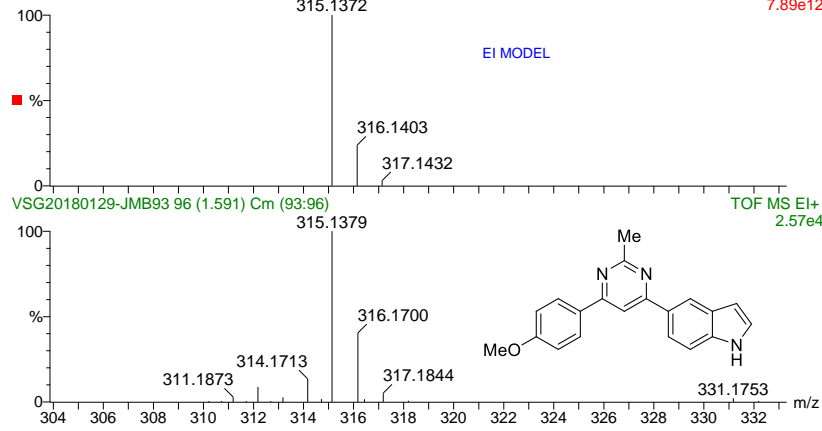


¹³C NMR spectrum of **16i (in DMSO-*d*₆)**

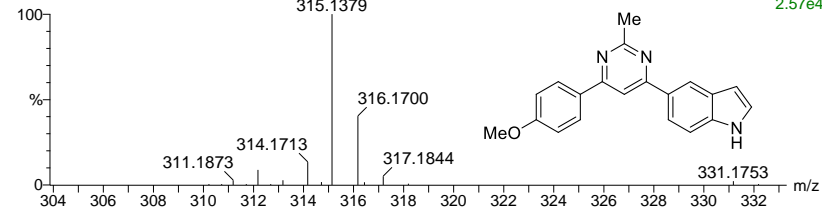
VSG20180129-JMB93

VSG20180129-JMB93 (0.007) Is (1.00,1.00) C20H17N3O

TOF MS EI+
7.89e12



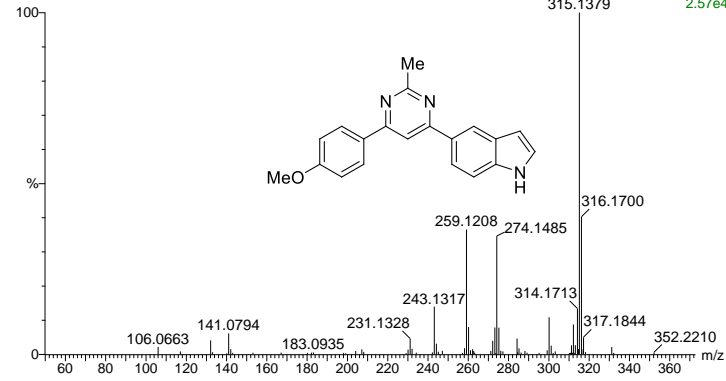
VSG20180129-JMB93 96 (1.591) Cm (93:96) TOF MS EI+ 2.57e4



VSG20180129-JMB93

VSG20180129-JMB93 96 (1.591) Cm (93:96)

TOF MS EI+
2.57e4

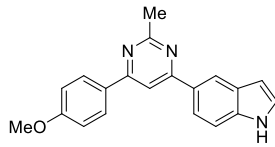


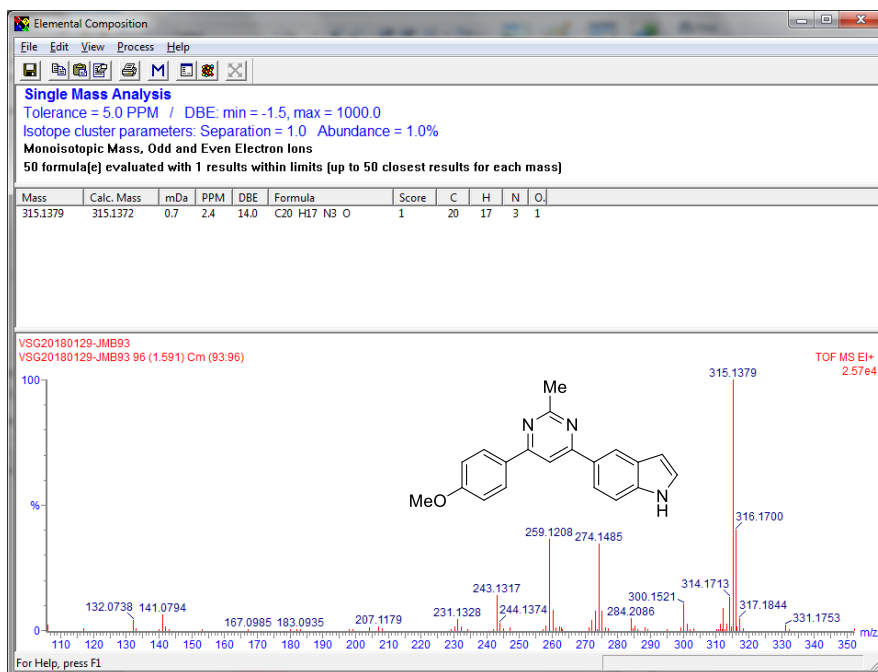
VSG20180129-JMB93

VSG20180129-JMB93 96 (1.591) Cm (93:96)

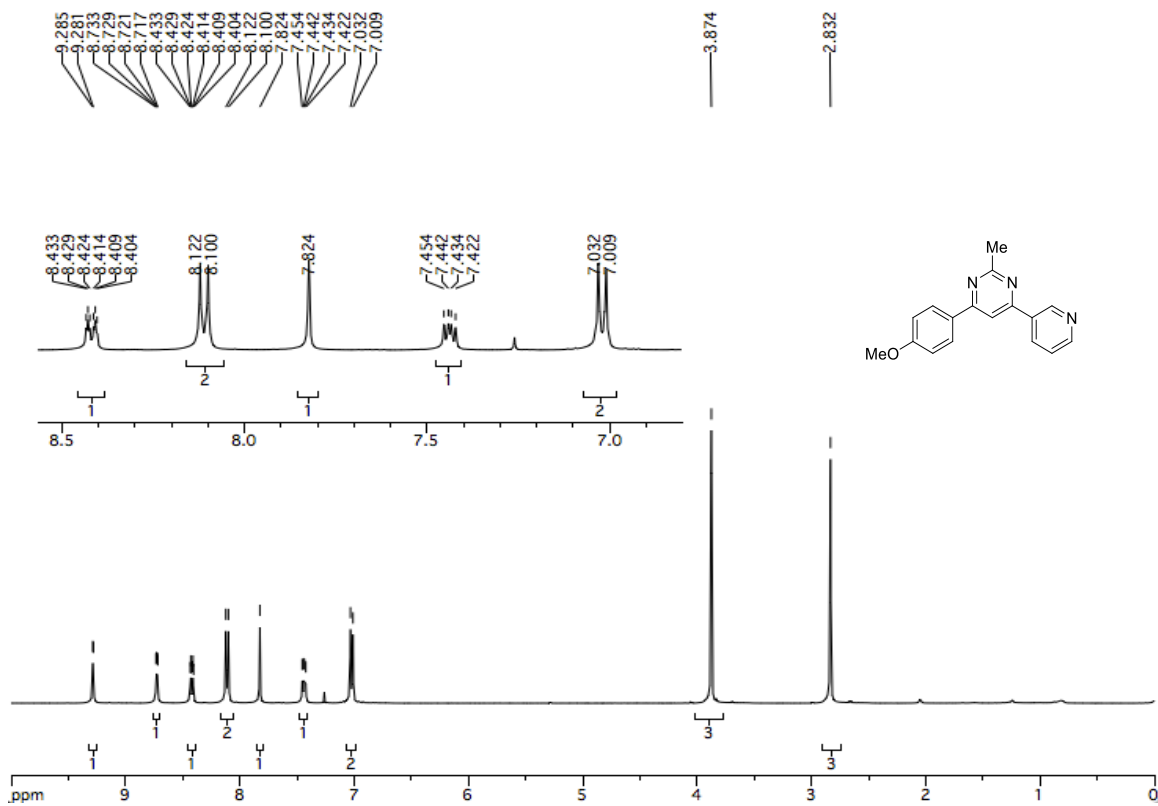
TOF MS EI+

m/z	Intensity	Label
106.0663	Low	106.0663
141.0794	Low	141.0794
183.0935	Low	183.0935
231.1328	Low	231.1328
243.1317	Low	243.1317
259.1208	Medium	259.1208
274.1485	Medium	274.1485
314.1713	Low	314.1713
315.1379	High	315.1379
316.1700	Medium	316.1700
317.1844	Low	317.1844
352.2210	Low	352.2210

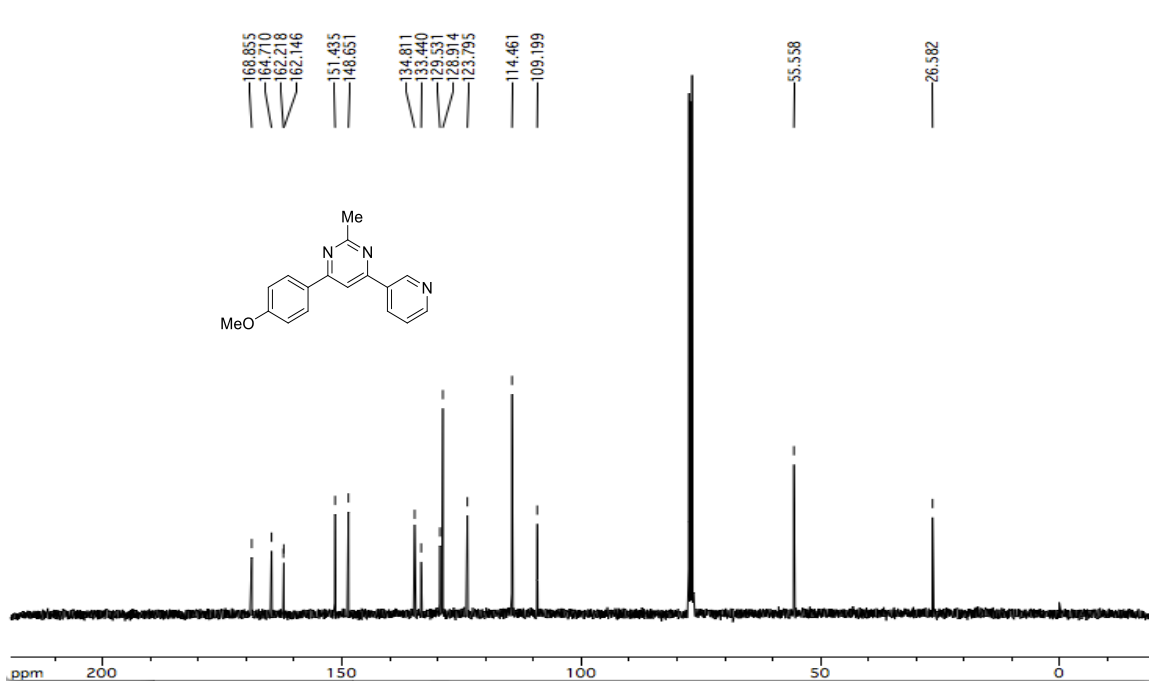




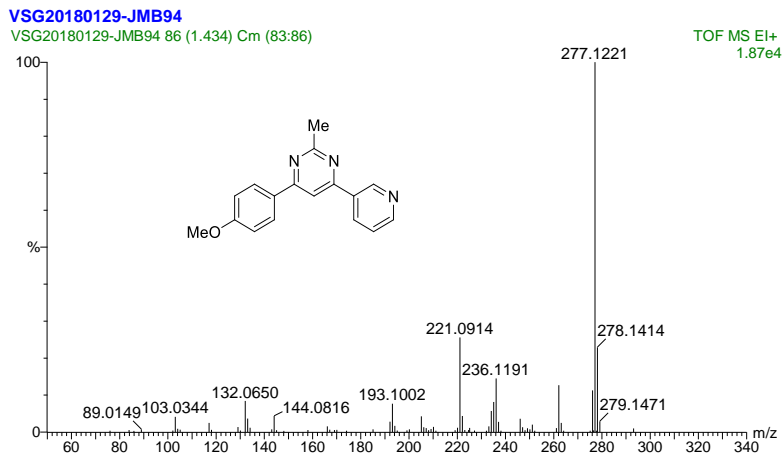
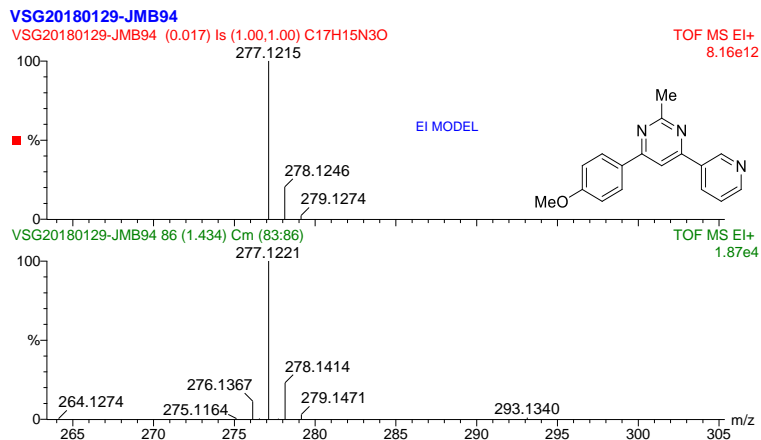
HRMS spectra of **16i**



¹H NMR spectrum of **16j** (in CDCl₃)

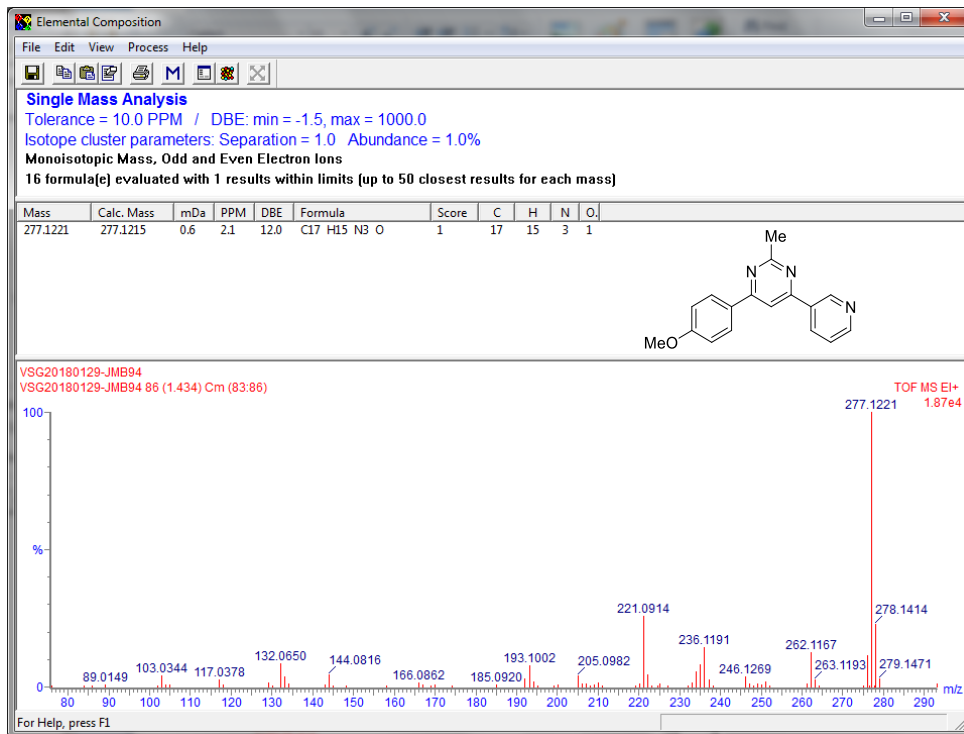
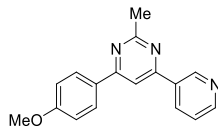


^{13}C NMR spectrum of **16j** (in CDCl_3)

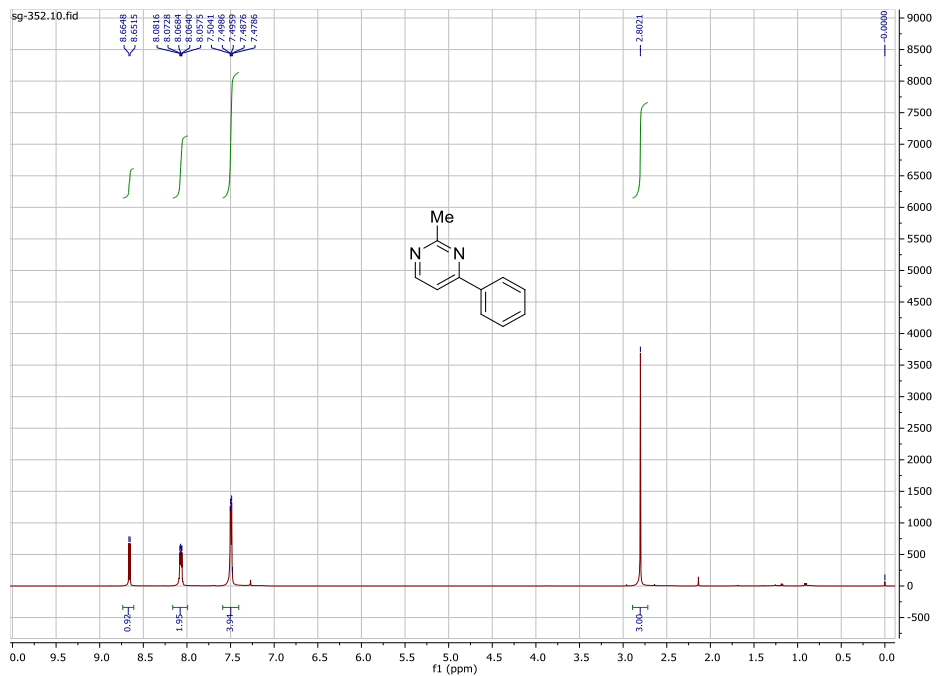


VSG20180129-JMB94
VSG20180129-JMB94 86 (1.434) Cm (83.86)

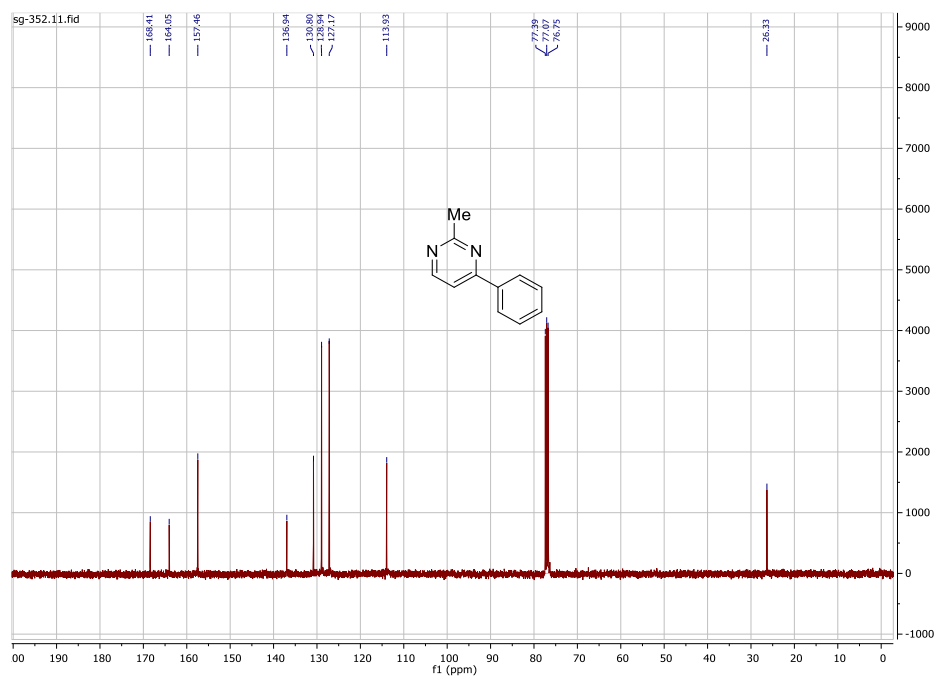
No.	Mass	Score	DBE	Formula	No.	Mass	Score	DBE	Formula	No.	Mass	Score	DBE	Formula	No.	Mass	Score	DBE	Formula
1	83.0200	0.26	0.11	C5H5	21	180.0802	0.87	1.26	C10H9	41	220.0805	0.70	1.10	C17H15					
2	85.0226	0.87	0.30	C5H7	22	182.0774	0.26	0.33	C10H7	42	222.0769	0.56	1.17	C17H13					
3	85.0226	0.87	0.30	C5H7	23	184.0800	0.26	0.33	C10H9	43	222.0769	0.56	1.17	C17H13					
4	89.0140	0.14	0.10	C6H5	24	184.0774	0.26	0.33	C10H7	44	224.0800	0.26	0.33	C17H13					
5	102.0373	7.19	0.38	C7H7	25	186.0800	0.26	0.33	C10H9	45	224.0774	0.26	0.33	C17H13					
6	103.0344	1.86	0.21	C7H9	26	186.0774	0.26	0.33	C10H7	46	224.0774	0.26	0.33	C17H13					
7	104.0381	1.86	0.21	C7H9	27	188.0800	0.26	0.33	C10H9	47	226.0800	0.26	0.33	C17H13					
8	117.0378	0.86	0.24	C8H7	28	190.0800	0.26	0.33	C10H9	48	226.0774	0.26	0.33	C17H13					
9	117.0378	0.86	0.24	C8H7	29	190.0774	0.26	0.33	C10H7	49	228.0800	0.26	0.33	C17H13					
10	118.0419	1.86	0.28	C8H9	30	192.0800	0.26	0.33	C10H9	50	230.0800	0.26	0.33	C17H13					
11	119.0416	0.43	0.10	C8H7	31	192.0774	0.26	0.33	C10H7	51	230.0774	0.26	0.33	C17H13					
12	130.0650	7.19	0.38	C9H7	32	194.0800	0.26	0.33	C10H9	52	232.0800	0.26	0.33	C17H13					
13	130.0650	7.19	0.38	C9H7	33	194.0774	0.26	0.33	C10H7	53	232.0774	0.26	0.33	C17H13					
14	133.0645	0.76	0.22	C9H9	34	196.0800	0.26	0.33	C10H9	54	234.0800	0.26	0.33	C17H13					
15	134.0716	2.13	0.14	C9H7	35	196.0774	0.26	0.33	C10H7	55	234.0774	0.26	0.33	C17H13					
16	144.0816	0.26	0.10	C10H9	36	198.0800	0.26	0.33	C10H9	56	236.0800	0.26	0.33	C17H13					
17	144.0816	0.26	0.10	C10H9	37	198.0774	0.26	0.33	C10H7	57	236.0774	0.26	0.33	C17H13					
18	145.0855	0.14	0.09	C10H7	38	200.0800	0.26	0.33	C10H9	58	238.0800	0.26	0.33	C17H13					
19	145.0855	0.14	0.09	C10H7	39	200.0774	0.26	0.33	C10H7	59	238.0774	0.26	0.33	C17H13					
20	146.0894	0.26	0.10	C10H9	40	202.0800	0.26	0.33	C10H9	60	240.0800	0.26	0.33	C17H13					
21	146.0894	0.26	0.10	C10H9	41	202.0774	0.26	0.33	C10H7	61	240.0774	0.26	0.33	C17H13					
22	167.0927	1.32	0.21	C11H9	42	204.0800	0.26	0.33	C10H9	62	242.0800	0.26	0.33	C17H13					
23	167.0927	1.32	0.21	C11H9	43	204.0774	0.26	0.33	C10H7	63	242.0774	0.26	0.33	C17H13					
24	170.0978	1.26	0.21	C11H7	44	206.0800	0.26	0.33	C10H9	64	244.0800	0.26	0.33	C17H13					
25	174.1141	0.26	0.10	C12H9	45	206.0774	0.26	0.33	C10H7	65	244.0774	0.26	0.33	C17H13					
26	180.0900	1.32	0.21	C11H9	46	208.0800	0.26	0.33	C10H9	66	246.0800	0.26	0.33	C17H13					
27	180.0899	0.26	0.10	C11H7	47	208.0774	0.26	0.33	C10H7	67	246.0774	0.26	0.33	C17H13					
28	191.1002	1.42	0.21	C12H9	48	210.0800	0.26	0.33	C10H9	68	248.0800	0.26	0.33	C17H13					
29	191.1017	0.14	0.10	C12H7	49	210.0774	0.26	0.33	C10H7	69	248.0774	0.26	0.33	C17H13					
30	192.0945	0.43	0.10	C12H9	50	212.0800	0.26	0.33	C10H9	70	250.0800	0.26	0.33	C17H13					
31	199.1122	7.49	0.40	C13H9	51	212.0774	0.26	0.33	C10H7	71	250.0774	0.26	0.33	C17H13					
32	200.0982	0.86	0.18	C13H7	52	214.0800	0.26	0.33	C10H9	72	252.0800	0.26	0.33	C17H13					
33	200.0982	0.86	0.18	C13H7	53	214.0774	0.26	0.33	C10H7	73	252.0774	0.26	0.33	C17H13					
34	206.1026	1.32	0.21	C13H9	54	216.0800	0.26	0.33	C10H9										
35	206.1026	1.32	0.21	C13H9	55	216.0774	0.26	0.33	C10H7										
36	208.1097	0.43	0.10	C13H7	56	218.0800	0.26	0.33	C10H9										
37	209.1051	1.42	0.21	C13H9	57	218.0774	0.26	0.33	C10H7										
38	210.1122	2.50	0.24	C13H7	58	220.0800	0.26	0.33	C10H9										
39	211.1216	0.87	0.24	C13H9	59	220.0774	0.26	0.33	C10H7										
40	213.1300	0.87	0.24	C13H9	60	222.0800	0.26	0.33	C10H9										
41	220.0805	0.70	1.10	C17H15	61	222.0774	0.26	0.33	C10H7										
42	221.0814	0.76	0.22	C17H13	62	224.0800	0.26	0.33	C10H9										
43	222.0769	0.56	1.17	C17H13	63	224.0774	0.26	0.33	C10H7										
44	223.0774	0.26	0.10	C17H11	64	226.0800	0.26	0.33	C10H9										
45	224.0769	0.56	1.17	C17H13	65	226.0774	0.26	0.33	C10H7										
46	224.0769	0.56	1.17	C17H13	66	228.0800	0.26	0.33	C10H9										
47	227.0815	0.86	0.18	C17H11	67	228.0774	0.26	0.33	C10H7										
48	232.0817	0.87	0.24	C17H13	68	230.0800	0.26	0.33	C10H9										
49	232.0817	0.87	0.24	C17H13	69	230.0774	0.26	0.33	C10H7										
50	233.0800	0.26	0.10	C17H11	70	232.0800	0.26	0.33	C10H9										
51	234.1233	1.06	0.28	C17H13	71	234.0800	0.26	0.33	C10H9										
52	235.1131	0.26	0.10	C17H11	72	234.0774	0.26	0.33	C10H7										
53	235.1131	0.26	0.10	C17H11	73	236.0800	0.26	0.33	C10H9										
54	236.1191	0.26	0.10	C17H11	74	236.0774	0.26	0.33	C10H7										
55	238.1275	0.26	0.10	C17H11	75	238.0800	0.26	0.33	C10H9										
56	246.1269	0.26	0.10	C17H11	76	240.0800	0.26	0.33	C10H9										
57	246.1269	0.26	0.10	C17H11	77	240.0774	0.26	0.33	C10H7										
58	248.1449	0.43	0.10	C17H11	78	242.0800	0.26	0.33	C10H9										
59	248.1449	0.43	0.10	C17H11	79	242.0774	0.26	0.33	C10H7										
60	250.1529	0.26	0.10	C17H11	80	244.0800	0.26	0.33	C10H9										
61	251.1572	0.26	0.10	C17H11	81	244.0774	0.26	0.33	C10H7										
62	261.1158	1.86	0.28	C17H13	82	246.0800	0.26	0.33	C10H9										
63	262.1167	0.26	0.10	C17H11	83	246.0774	0.26	0.33	C10H7										
64	263.1193	0.26	0.10	C17H11	84	248.0800	0.26	0.33	C10H9										
65	276.1474	0.26	0.10	C17H11	85	248.0774	0.26	0.33	C10H7										
66	276.1474	0.26	0.10	C17H11	86	250.0800	0.26	0.33	C10H9										
67	276.1474	0.26	0.10	C17H11	87	250.0774	0.26	0.33	C10H7										
68	276.1474	0.26	0.10	C17H11	88	252.0800	0.26	0.33	C10H9										
69	277.1221	0.26	0.10	C17H11	89	252.0774	0.26	0.33	C10H7										
70	277.1221	0.26	0.10	C17H11	90	254.0800	0.26	0.33	C10H9										
71	278.1414	0.26	0.10	C17H11	91	254.0774	0.26	0.33	C10H7										
72	279.1471	0.26	0.10	C17H11	92	256.0800	0.26	0.33	C10H9										
73	283.1540	1.32	0.21	C17H13															



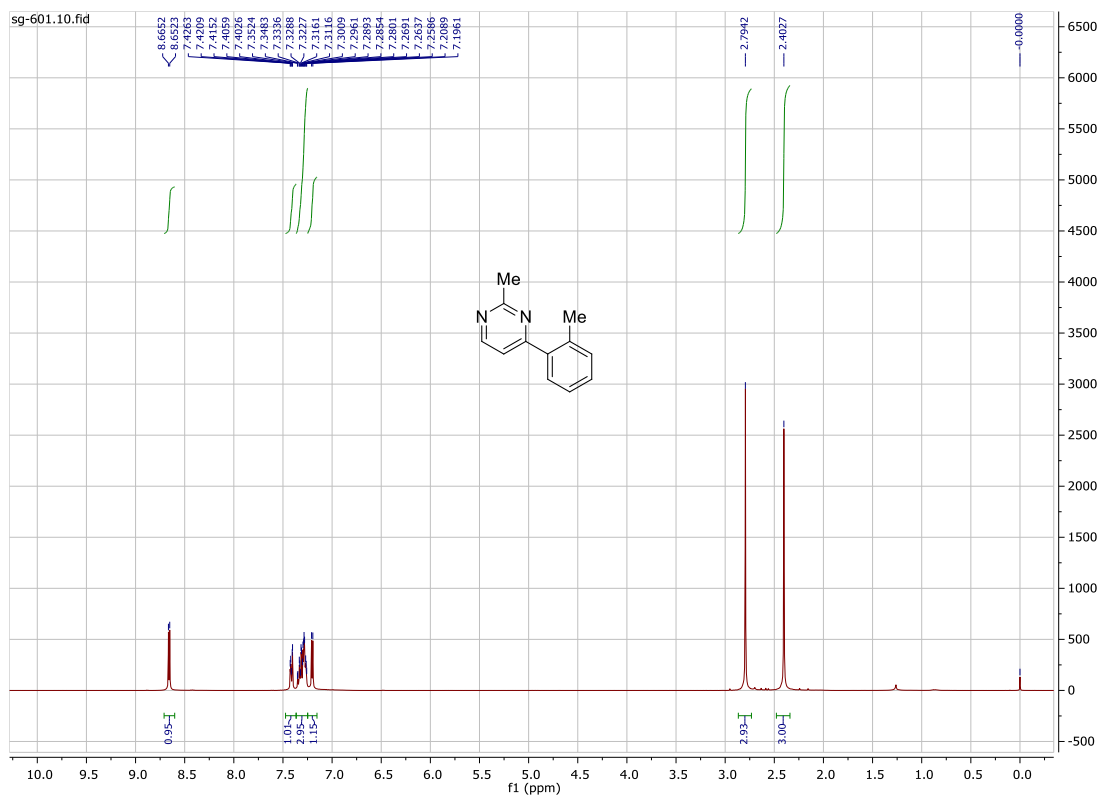
HRMS spectra of 16j



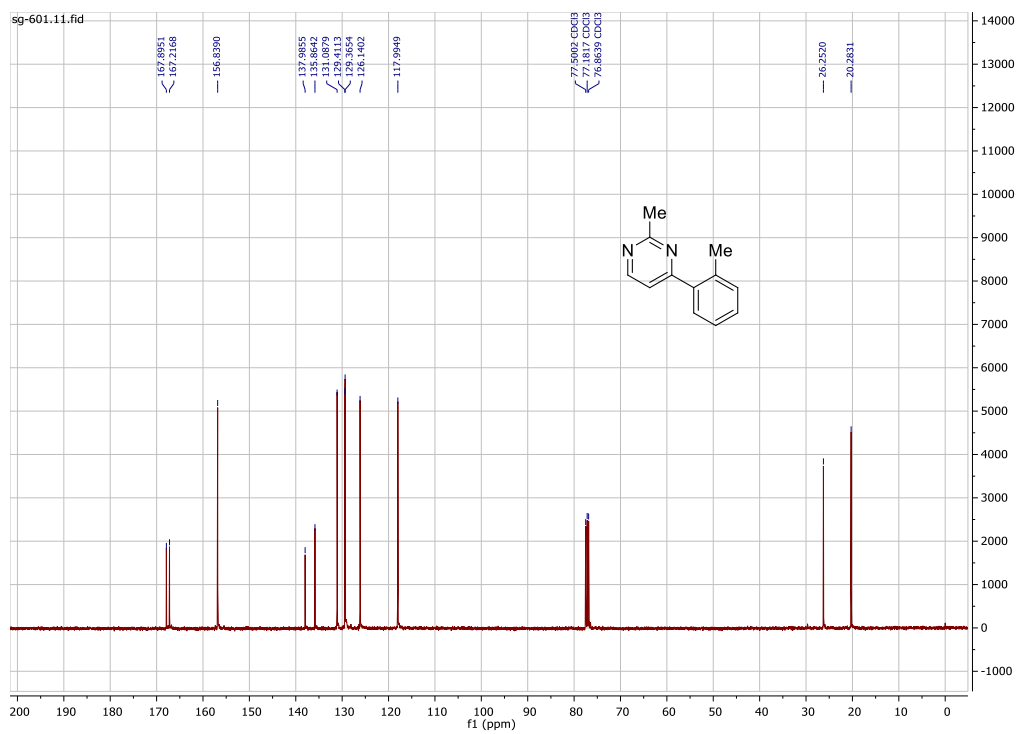
^1H NMR spectrum of **17a** (in CDCl_3)



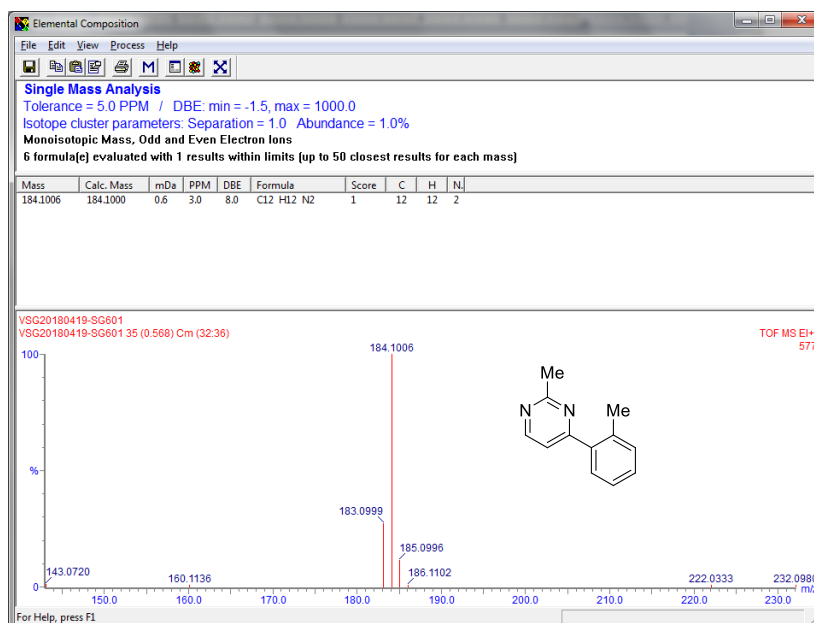
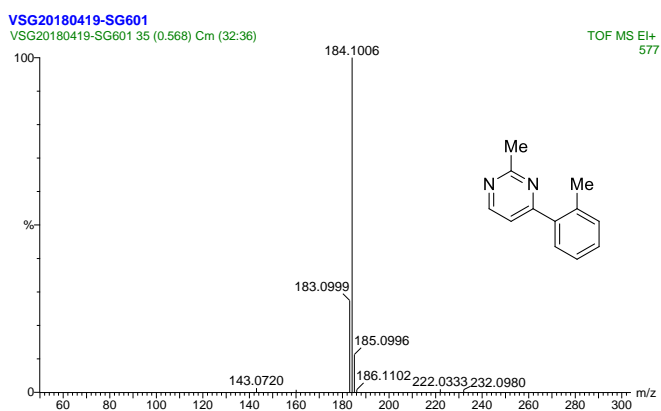
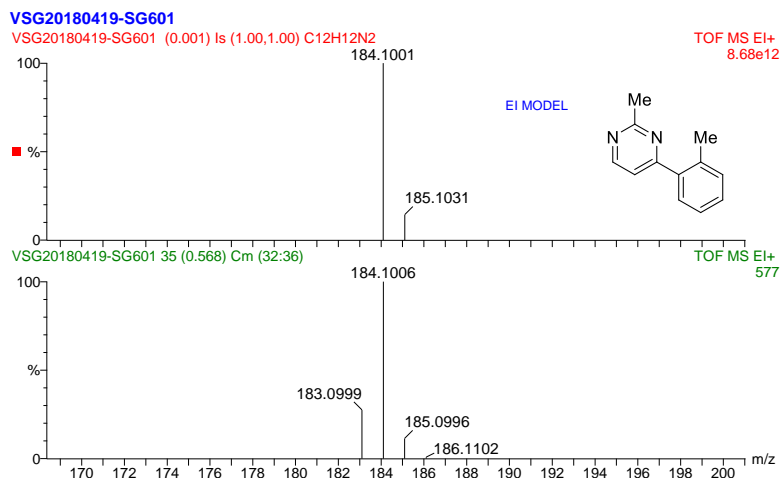
^{13}C NMR spectrum of **17a** (in CDCl_3)



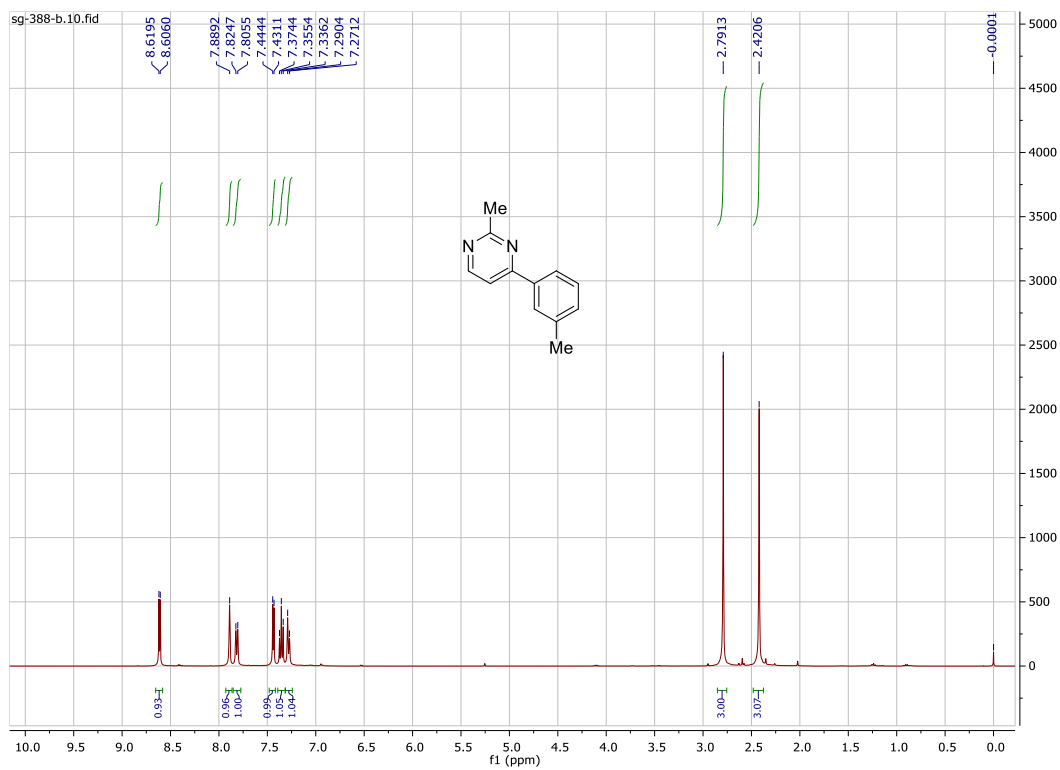
^1H NMR spectrum of **17b** (in CDCl_3)



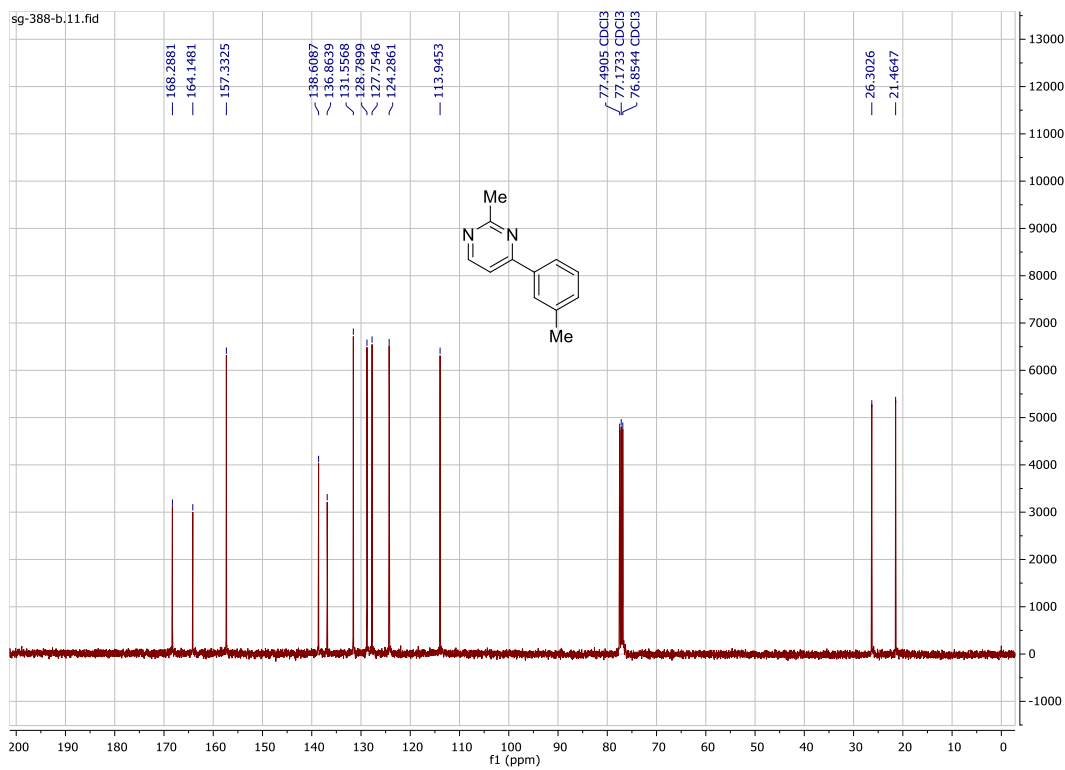
^{13}C NMR spectrum of **17b** (in CDCl_3)



HRMS spectra of 17b



¹H NMR spectrum of **17c** (in CDCl₃)

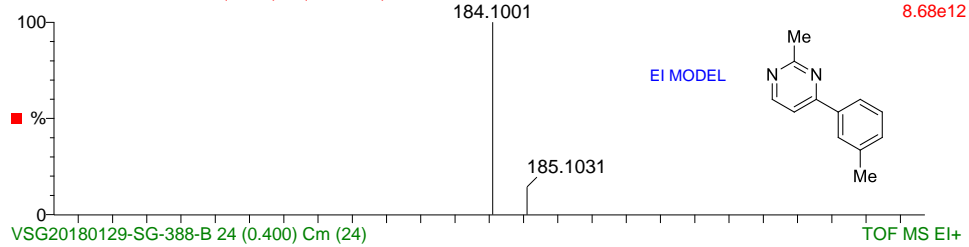


¹³C NMR spectrum of **17c** (in CDCl₃)

VSG20180129-SG-388-B

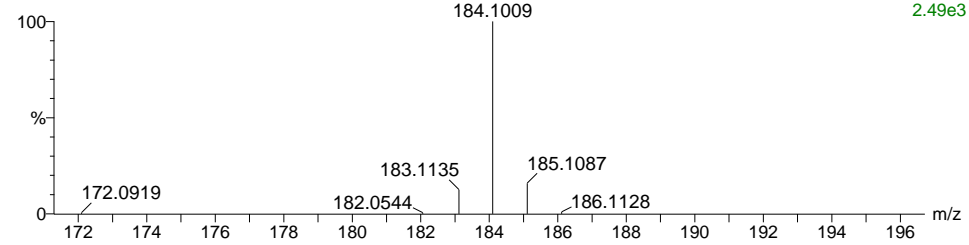
VSG20180129-SG-388-B (0.017) Is (1.00,1.00) C₁₂H₁₂N₂

TOF MS EI+
8.68e12



VSG20180129-SG-388-B 24 (0.400) Cm (24)

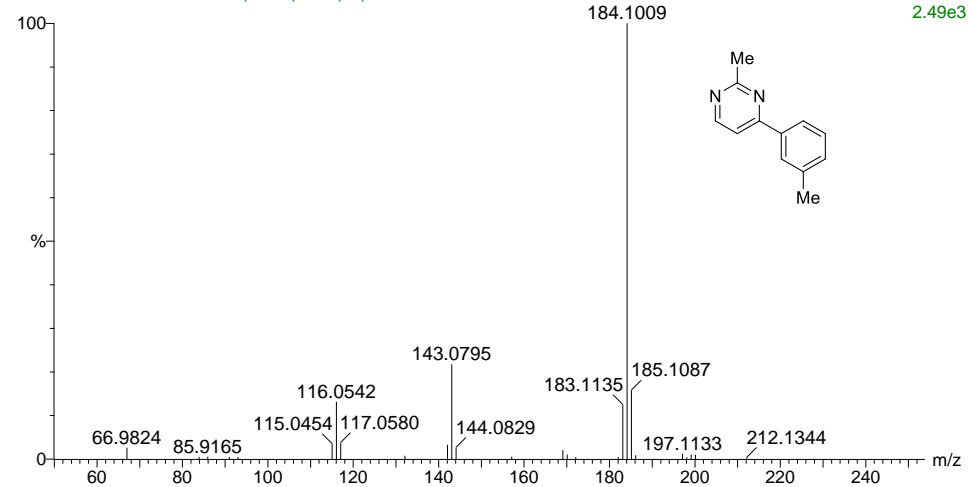
TOF MS EI+
2.49e3



VSG20180129-SG-388-B

VSG20180129-SG-388-B 24 (0.400) Cm (24)

TOF MS EI+
2.49e3

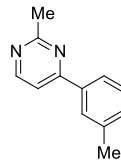


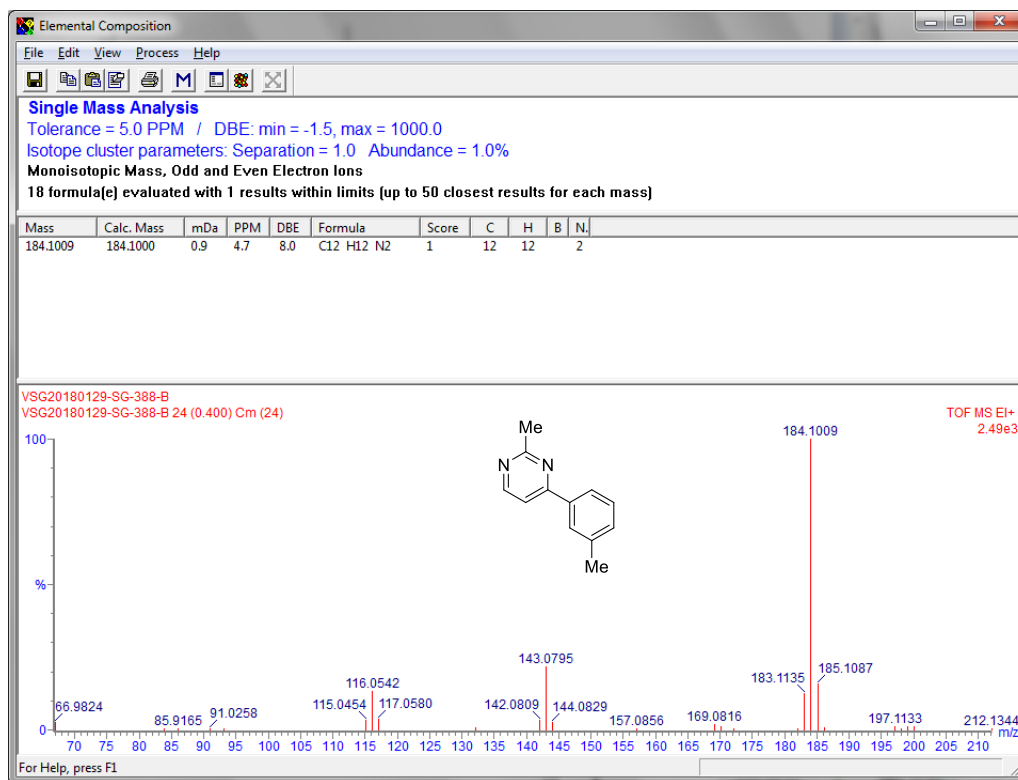
VSG20180129-SG-388-B

VSG20180129-SG-388-B 24 (0.400) Cm (24)

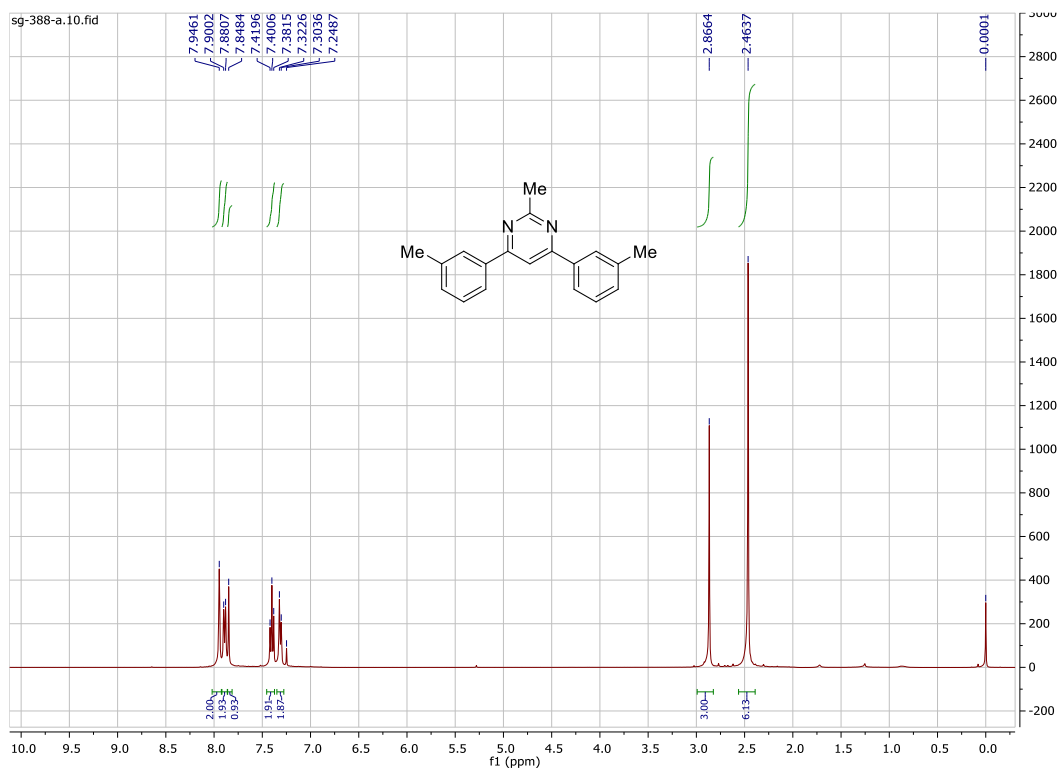
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	66.9824	6.38e1	2.56	1.32										
2:	83.9200	1.11e1	0.45	0.23										
3:	85.9165	1.32e1	0.53	0.27										
4:	91.0258	1.11e1	0.45	0.23										
5:	93.0230	1.01e1	0.41	0.21										
6:	115.0454	8.61e1	3.45	1.78										
7:	116.0542	3.27e2	13.13	6.77										
8:	117.0580	9.32e1	3.74	1.93										
9:	132.0802	1.92e1	0.77	0.40										
10:	142.0809	8.10e1	3.25	1.68										
11:	143.0795	5.41e2	21.70	11.19										
12:	144.0829	6.48e1	2.60	1.34										
13:	157.0856	1.32e1	0.53	0.27										
14:	169.0816	4.96e1	1.99	1.03										
15:	170.1016	2.53e1	1.02	0.52										
16:	172.0919	1.01e1	0.41	0.21										
17:	182.0544	1.01e1	0.41	0.21										
18:	183.1135	3.10e2	12.43	6.41										
19:	184.1009	2.49e3	100.01	51.58										
20:	185.1087	3.93e2	15.77	8.13										
21:	186.1128	2.13e1	0.85	0.44										
22:	197.1133	2.94e1	1.18	0.61										
23:	198.1176	9.11e0	0.37	0.19										
24:	199.0991	2.43e1	0.98	0.50										
25:	200.0995	2.33e1	0.93	0.48										
26:	212.1344	8.10e0	0.33	0.17										

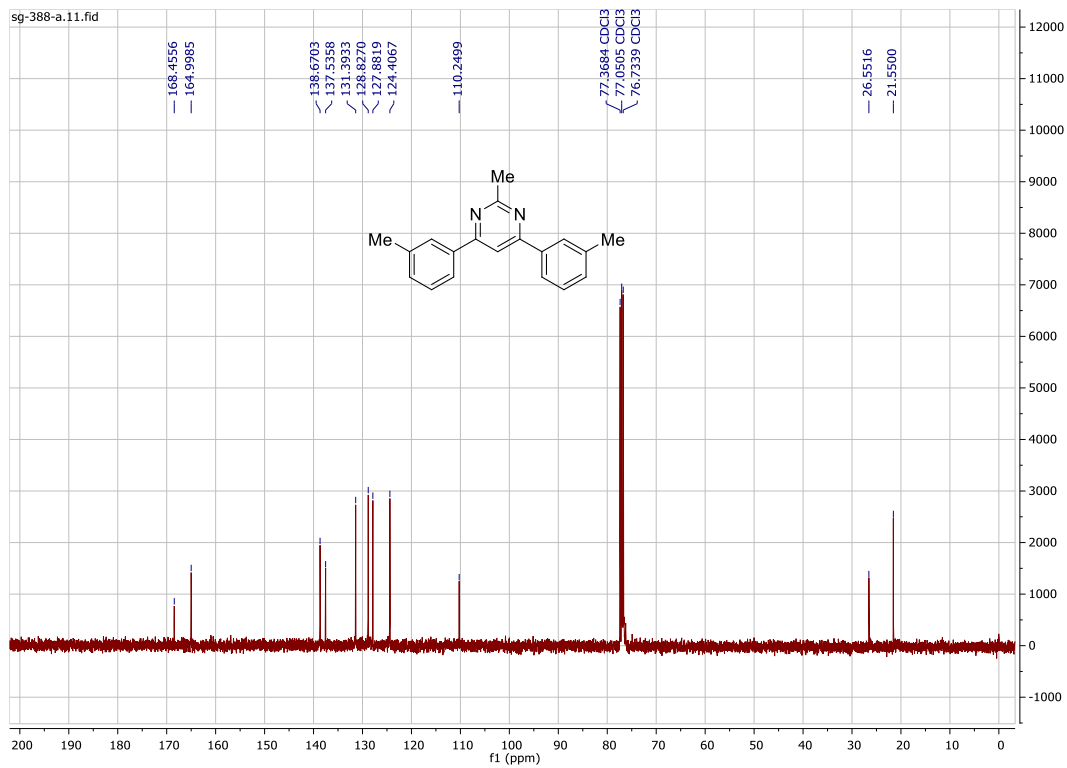




HRMS spectra of **17c**



¹H NMR spectrum of **8c** (in CDCl₃)

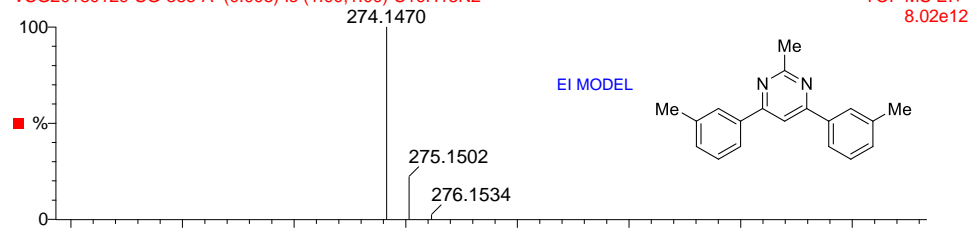


¹³C NMR spectrum of **8c** (in CDCl₃)

VSG20180129-SG-388-A

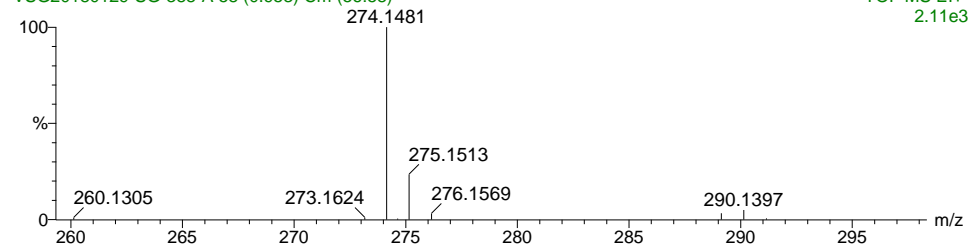
VSG20180129-SG-388-A (0.003) Is (1.00,1.00) C₁₉H₁₈N₂

TOF MS EI+
8.02e12



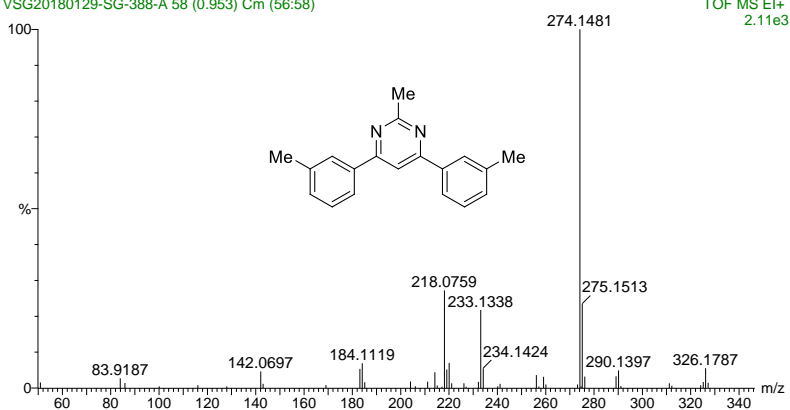
VSG20180129-SG-388-A 58 (0.953) Cm (56:58)

TOF MS EI+
2.11e3



VSG20180129-SG-388-A

VSG20180129-SG-388-A 58 (0.953) Cm (56:58)

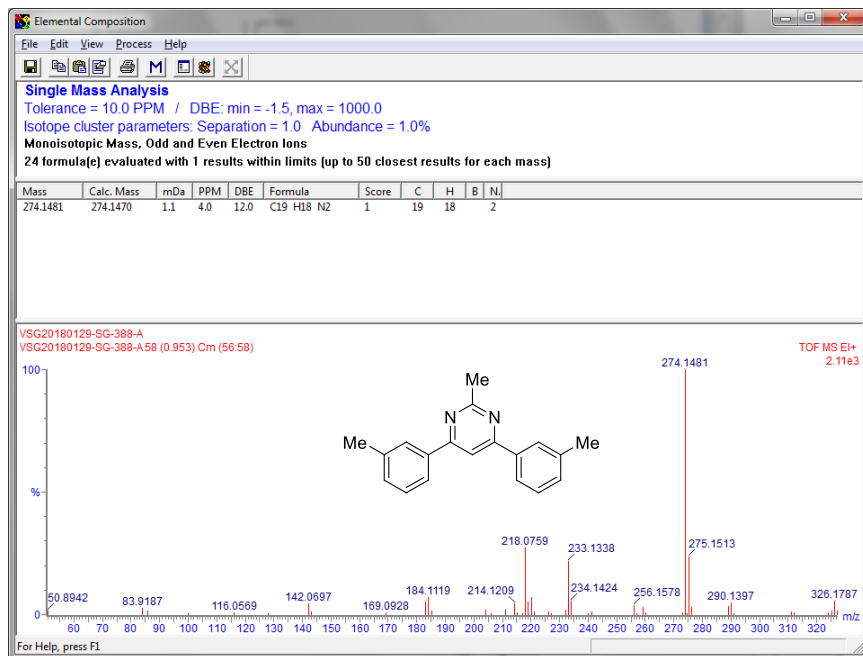


VSG20180129-SG-388-A

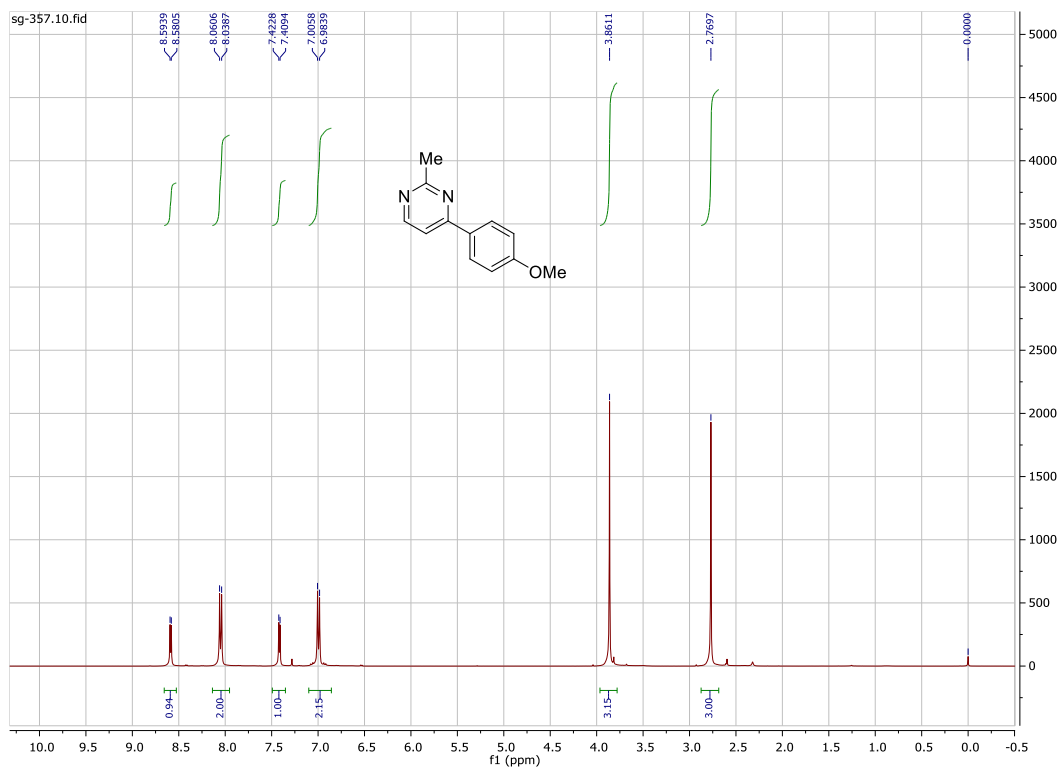
VSG20180129-SG-388-A 58 (0.953) Cm (56:58)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	50.8942	3.14e1	1.49	0.55	29:	241.1344	2.33e1	1.10	0.41					
2:	83.9187	5.67e1	2.69	0.99	30:	256.1578	7.49e1	3.55	1.31					
3:	85.9200	2.84e1	1.35	0.49	31:	257.1576	8.10e0	0.38	0.14					
4:	100.0628	9.11e0	0.43	0.16	32:	259.1265	6.48e1	3.07	1.13					
5:	116.0569	1.62e1	0.77	0.28	33:	260.1305	1.92e1	0.91	0.34					
6:	128.0537	9.11e0	0.43	0.16	34:	273.1624	1.92e1	0.91	0.34					
7:	142.0697	9.62e1	4.56	1.68	35:	274.1481	2.11e3	100.02	36.72					
8:	143.0728	2.33e1	1.10	0.41	36:	274.6392	9.11e0	0.43	0.16					
9:	169.0928	1.72e1	0.82	0.30	37:	275.1513	4.94e2	23.44	8.61					
10:	183.1054	1.11e2	5.28	1.94	38:	276.1569	6.58e1	3.12	1.15					
11:	184.1119	1.45e2	6.87	2.52	39:	289.1331	6.78e1	3.22	1.18					
12:	185.1078	3.24e1	1.54	0.56	40:	290.1397	1.02e2	4.85	1.78					
13:	204.0552	3.75e1	1.78	0.65	41:	291.1525	1.11e1	0.53	0.19					
14:	206.0605	9.11e0	0.43	0.16	42:	311.1555	2.63e1	1.25	0.46					
15:	211.1317	3.65e1	1.73	0.63	43:	312.1638	1.32e1	0.62	0.23					
16:	214.1209	9.22e1	4.37	1.60	44:	324.1587	1.62e1	0.77	0.28					
17:	215.1310	1.42e1	0.67	0.25	45:	325.1786	3.44e1	1.63	0.60					
18:	217.0601	7.09e0	0.34	0.12	46:	326.1787	1.15e2	5.48	2.01					
19:	218.0759	5.73e2	27.19	9.98	47:	327.1864	2.94e1	1.39	0.51					
20:	219.0853	1.07e2	5.09	1.87										
21:	220.0890	1.47e2	6.97	2.56										
22:	221.0946	2.63e1	1.25	0.46										
23:	226.1523	2.63e1	1.25	0.46										
24:	227.1018	7.09e0	0.34	0.12										
25:	232.1163	3.54e1	1.68	0.62										
26:	233.1338	4.58e2	21.71	7.97										
27:	234.1424	1.15e2	5.48	2.01										
28:	240.1563	9.11e0	0.43	0.16										

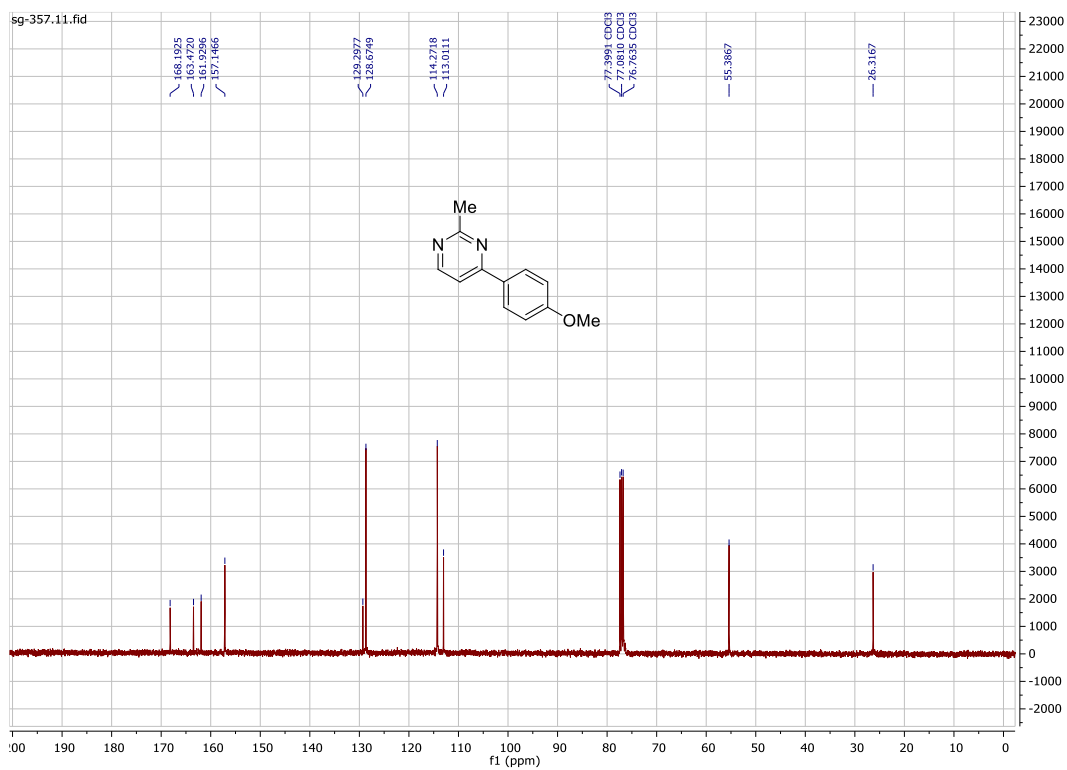
TOF MS EI+
2.11e3



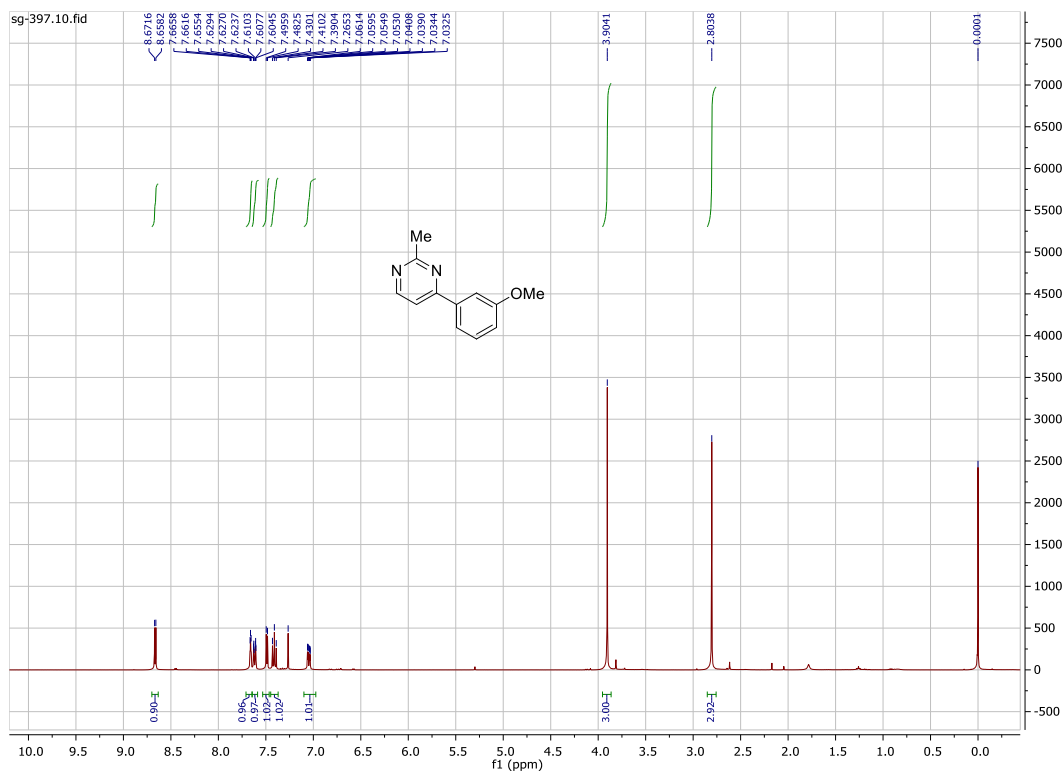
HRMS spectra of 8c



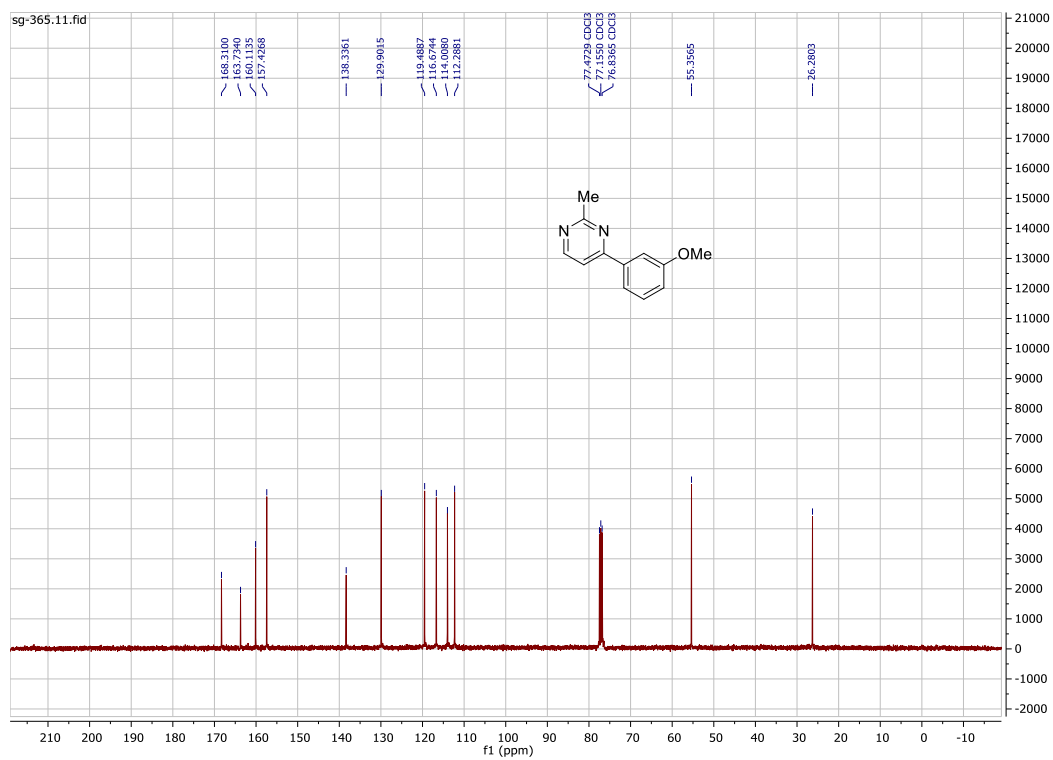
^1H NMR spectrum of **17d** (in CDCl_3)



^{13}C NMR spectrum of **17d** (in CDCl_3)



¹H NMR spectrum of **17e** (in CDCl₃)

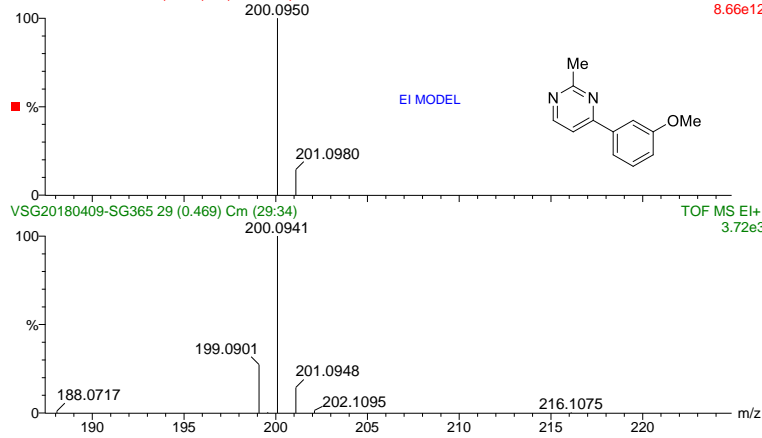


¹³C NMR spectrum of **17e** (in CDCl₃)

VSG20180409-SG365

VSG20180409-SG365 (0.002) Is (1.00,1.00) C12H12N2O

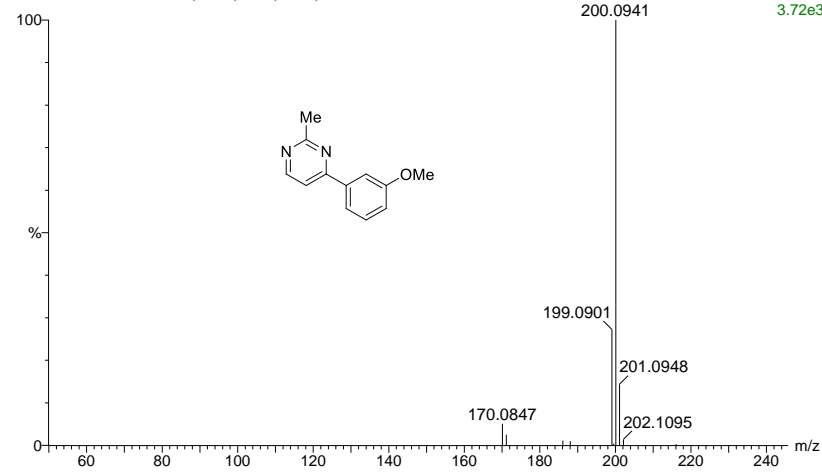
TOF MS EI+
8.66e12



VSG20180409-SG365

VSG20180409-SG365 29 (0.469) Cm (29:34)

TOF MS EI+
3.72e3

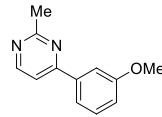


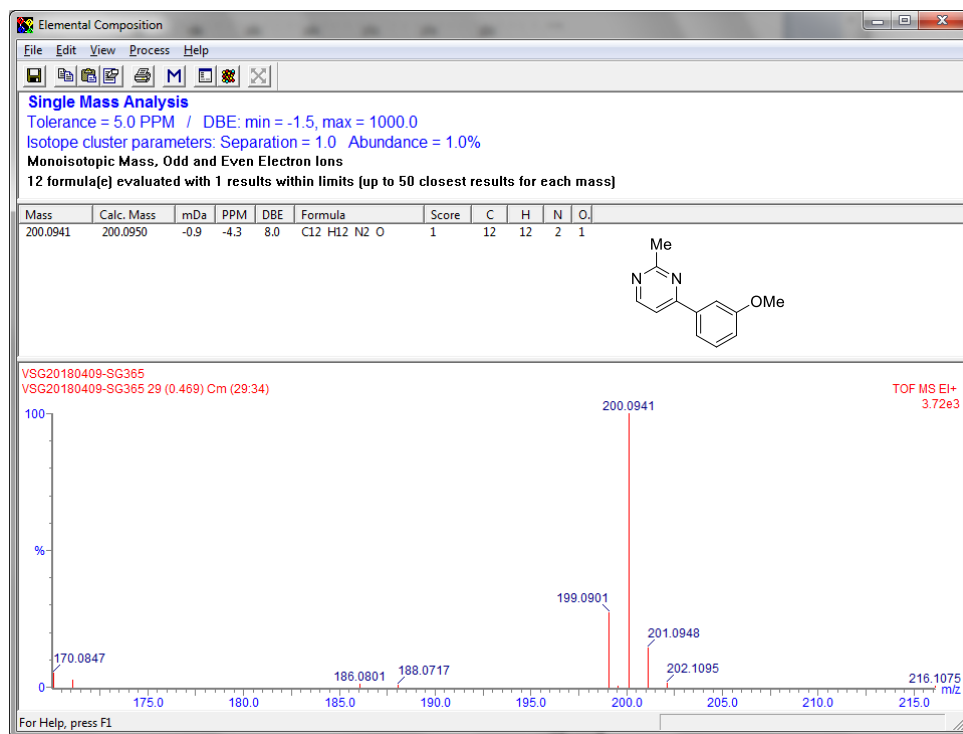
VSG20180409-SG365

VSG20180409-SG365 29 (0.469) Cm (29:34)

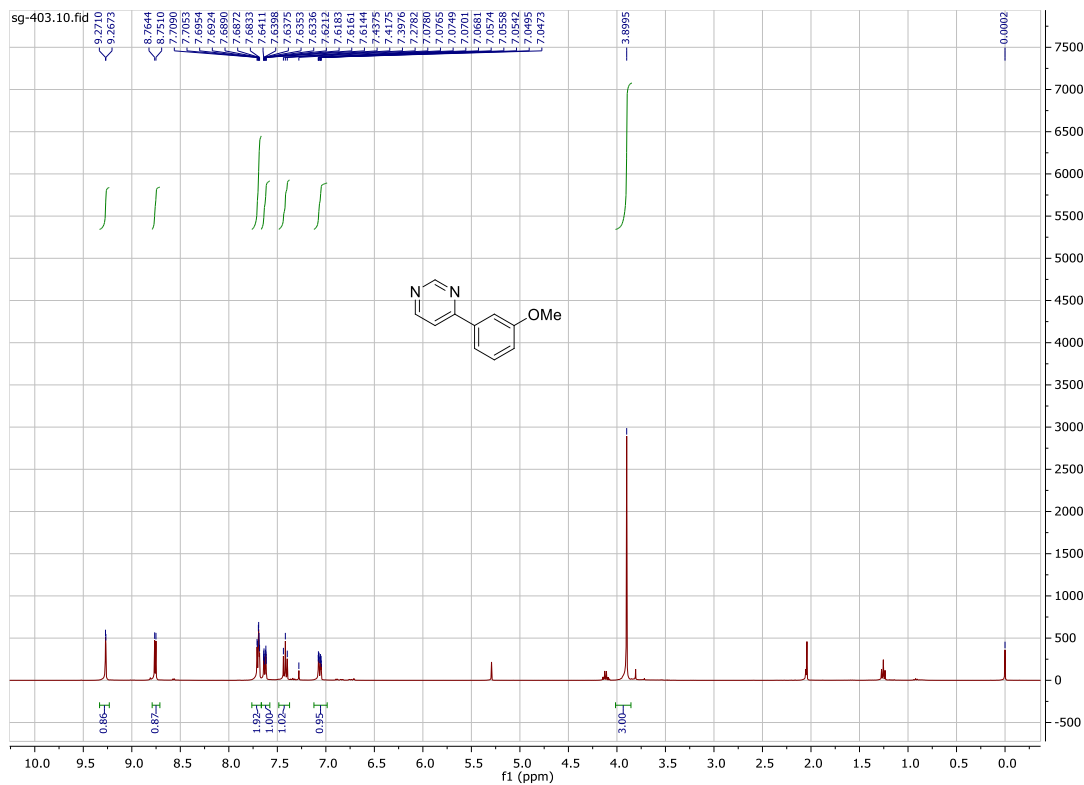
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	170.0847	1.87e2	5.04	3.20										
2:	171.0950	9.11e1	2.45	1.56										
3:	186.0801	3.95e1	1.06	0.68										
4:	188.0717	3.34e1	0.90	0.57										
5:	199.0901	1.01e3	27.17	17.28										
6:	199.5618	1.42e1	0.38	0.24										
7:	200.0941	3.72e3	100.01	63.60										
8:	201.0948	5.32e2	14.30	9.09										
9:	202.1095	4.96e1	1.33	0.85										
10:	216.1075	9.11e0	0.25	0.16										

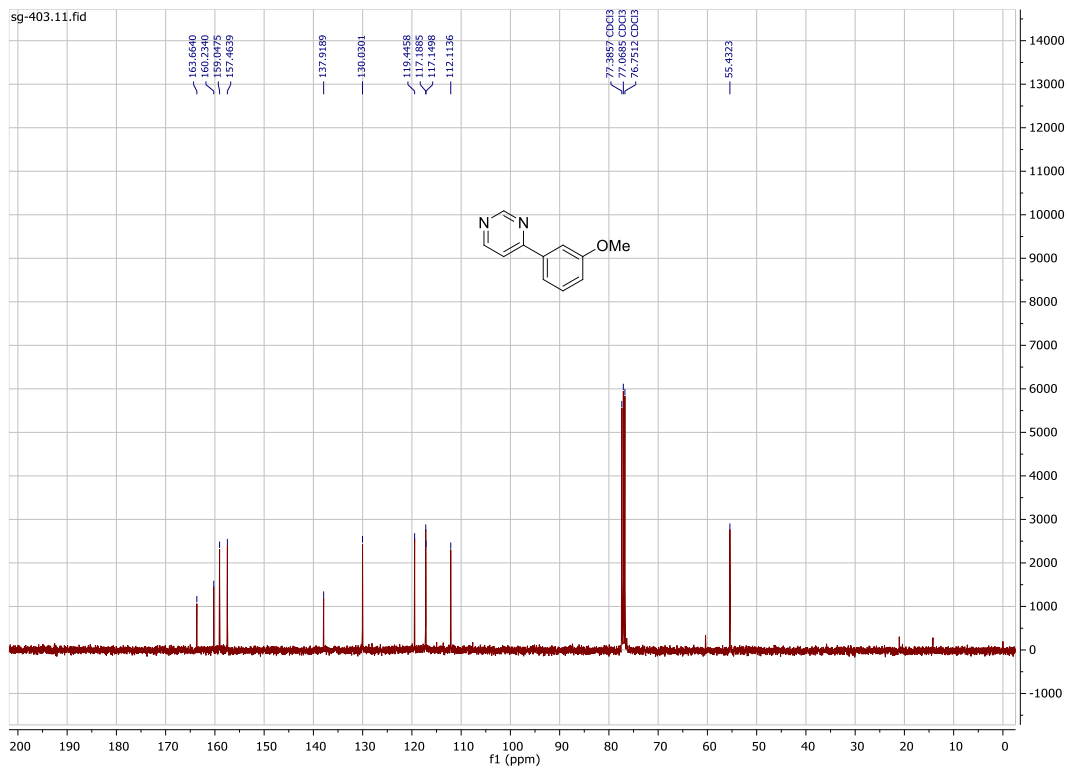




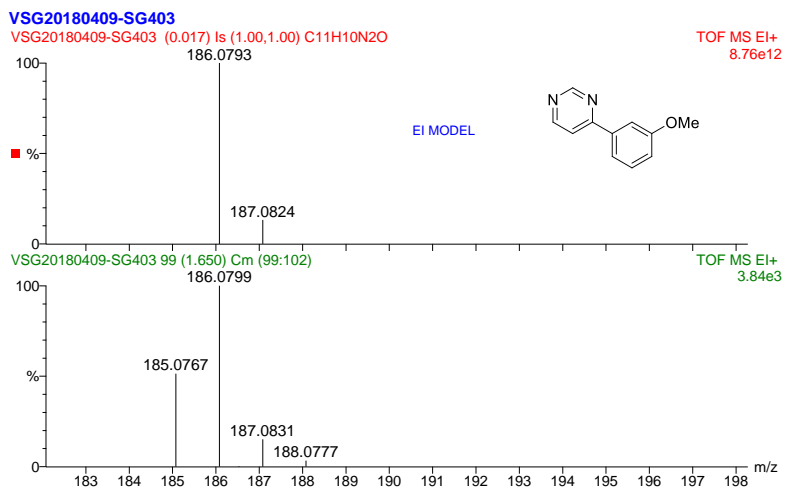
HRMS spectra of **17e**



^1H NMR spectrum of **17f** (in CDCl_3)



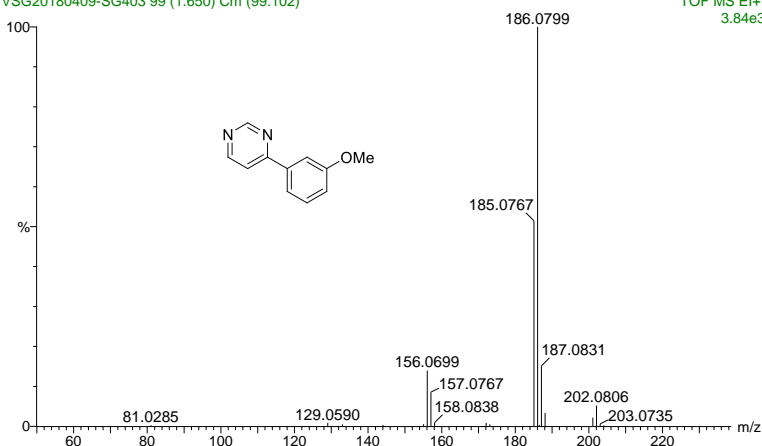
^{13}C NMR spectrum of **17f** (in CDCl_3)



VSG20180409-SG403

VSG20180409-SG403 99 (1.650) Cm (99:102)

TOF MS EI+
3.84e3

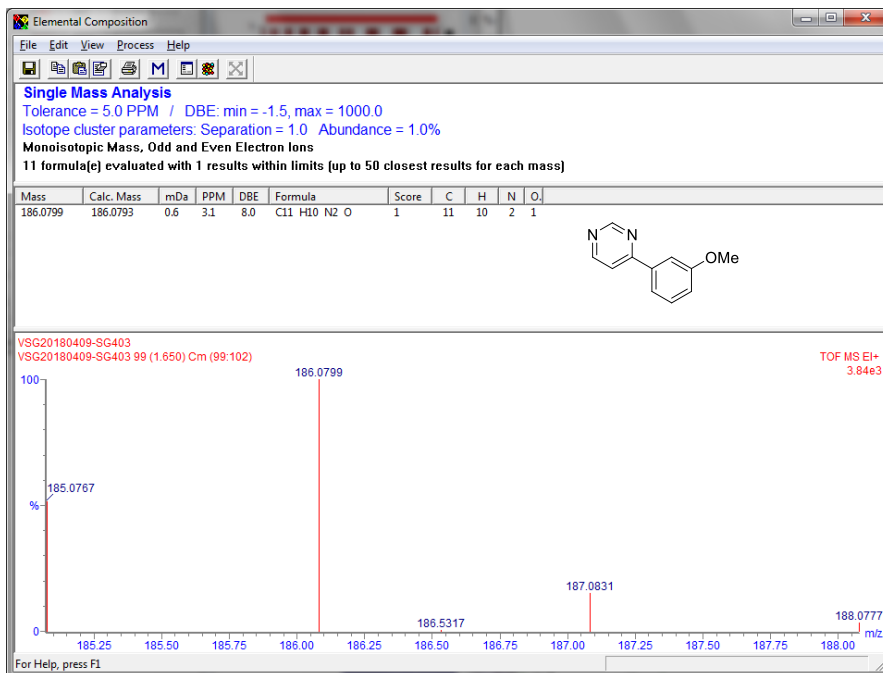
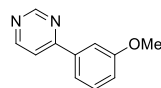


VSG20180409-SG403

VSG20180409-SG403 99 (1.650) Cm (99:102)

TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	81.0285	9.11e0	0.24	0.11					
2:	129.0590	3.24e1	0.84	0.41					
3:	133.0494	1.82e1	0.48	0.23					
4:	144.0746	1.11e1	0.29	0.14					
5:	155.0653	1.92e1	0.50	0.24					
6:	156.0699	5.35e2	13.93	6.69					
7:	157.0767	3.25e2	8.47	4.07					
8:	158.0838	3.24e1	0.84	0.41					
9:	172.0734	3.24e1	0.84	0.41					
10:	173.0748	1.72e1	0.45	0.22					
11:	185.0767	1.97e3	51.37	24.67					
12:	186.0799	3.84e3	100.00	48.03					
13:	186.5317	1.22e1	0.32	0.15					
14:	187.0831	5.78e2	15.07	7.24					
15:	188.0777	1.26e2	3.27	1.57					
16:	201.0667	8.20e1	2.14	1.03					
17:	202.0806	1.97e2	5.15	2.47					
18:	203.0735	2.13e1	0.55	0.27					
19:	204.0785	8.10e0	0.21	0.10					

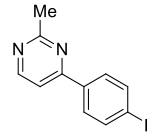
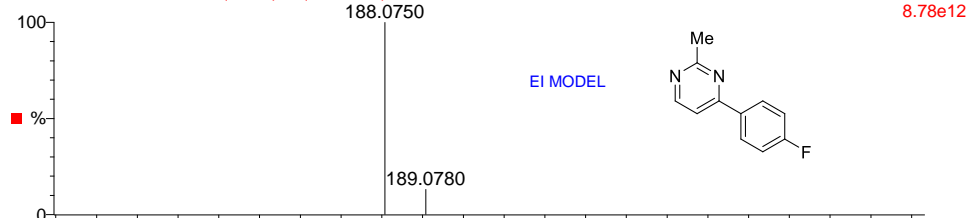


HRMS spectra of 17f

VSG20180129-SG-368-B

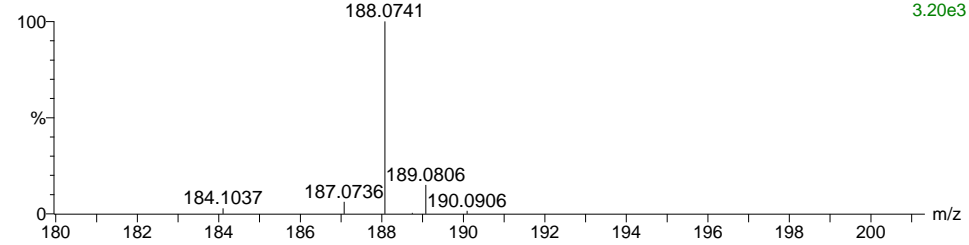
VSG20180129-SG-368-B (0.001) Is (1.00,1.00) C₁₁H₉FN₂

TOF MS EI+
8.78e12



VSG20180129-SG-368-B 15 (0.234) Cm (15)

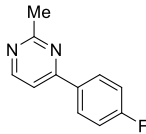
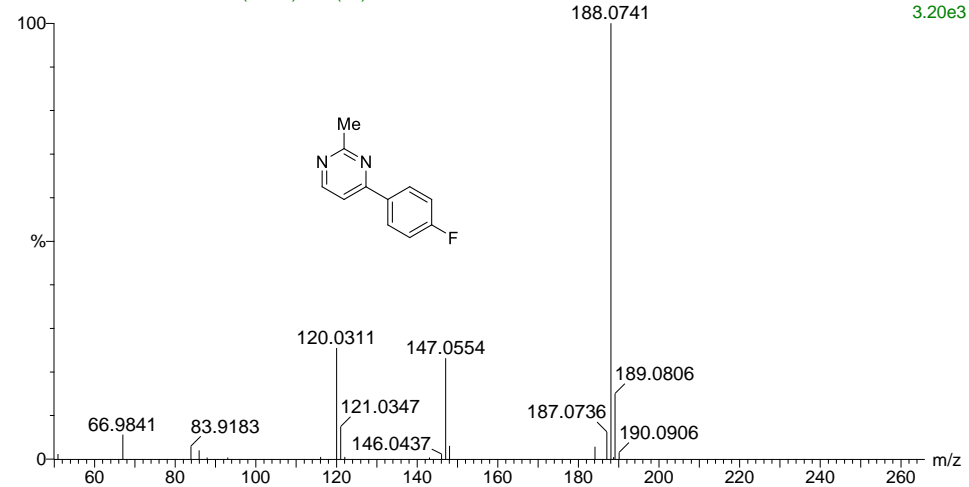
TOF MS EI+
3.20e3



VSG20180129-SG-368-B

VSG20180129-SG-368-B 15 (0.234) Cm (15)

TOF MS EI+
3.20e3

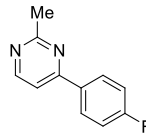


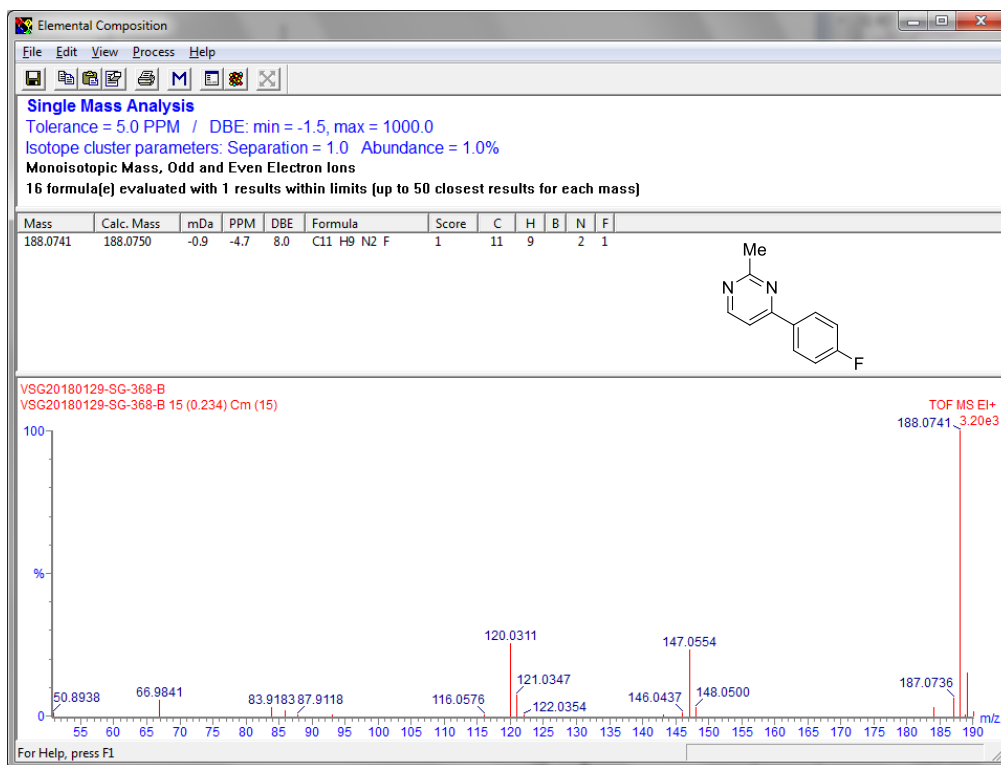
VSG20180129-SG-368-B

VSG20180129-SG-368-B 15 (0.234) Cm (15)

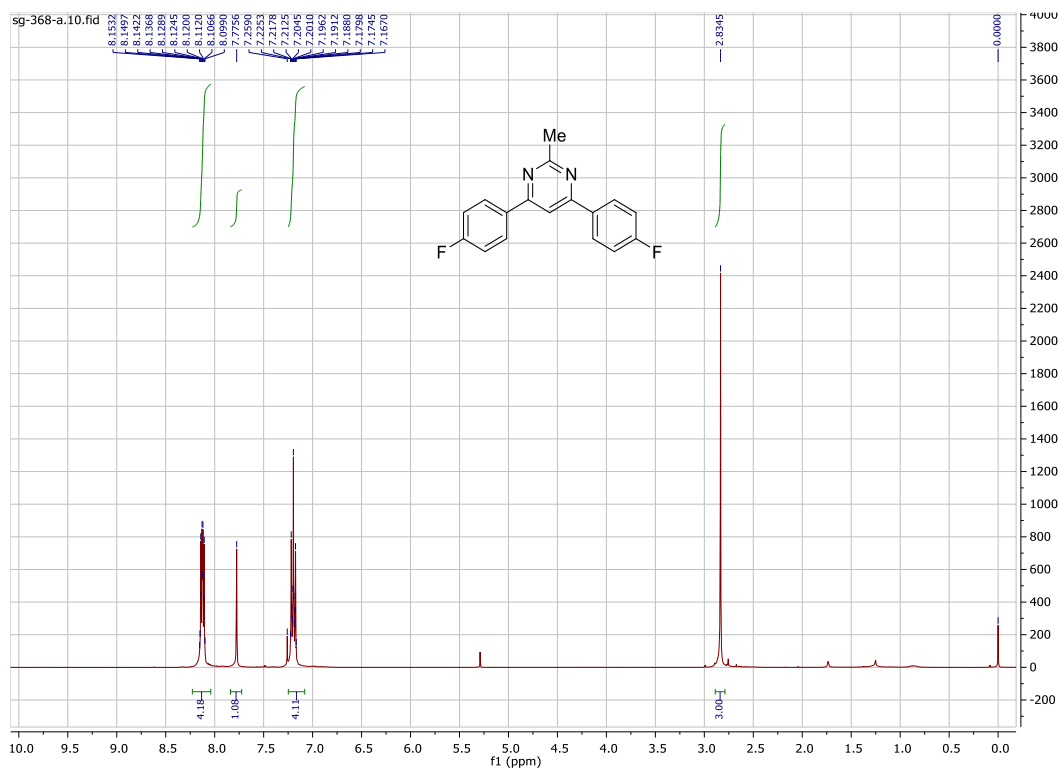
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	50.8938	3.65e1	1.14	0.56										
2:	66.9841	1.78e2	5.57	2.73										
3:	83.9183	9.32e1	2.91	1.43										
4:	85.9196	6.28e1	1.96	0.96										
5:	87.9118	1.11e1	0.35	0.17										
6:	93.0188	1.01e1	0.32	0.15										
7:	116.0576	1.52e1	0.47	0.23										
8:	120.0311	8.15e2	25.47	12.47										
9:	121.0347	2.36e2	7.37	3.61										
10:	122.0354	1.52e1	0.47	0.23										
11:	143.0844	1.01e1	0.32	0.15										
12:	146.0437	3.44e1	1.08	0.53										
13:	147.0554	7.39e2	23.10	11.31										
14:	148.0500	9.62e1	3.01	1.47										
15:	184.1037	8.91e1	2.78	1.36										
16:	187.0736	1.97e2	6.17	3.02										
17:	188.0741	3.20e3	100.00	48.96										
18:	188.7453	1.32e1	0.41	0.20										
19:	189.0806	4.79e2	14.96	7.32										
20:	190.0906	4.66e1	1.46	0.71										

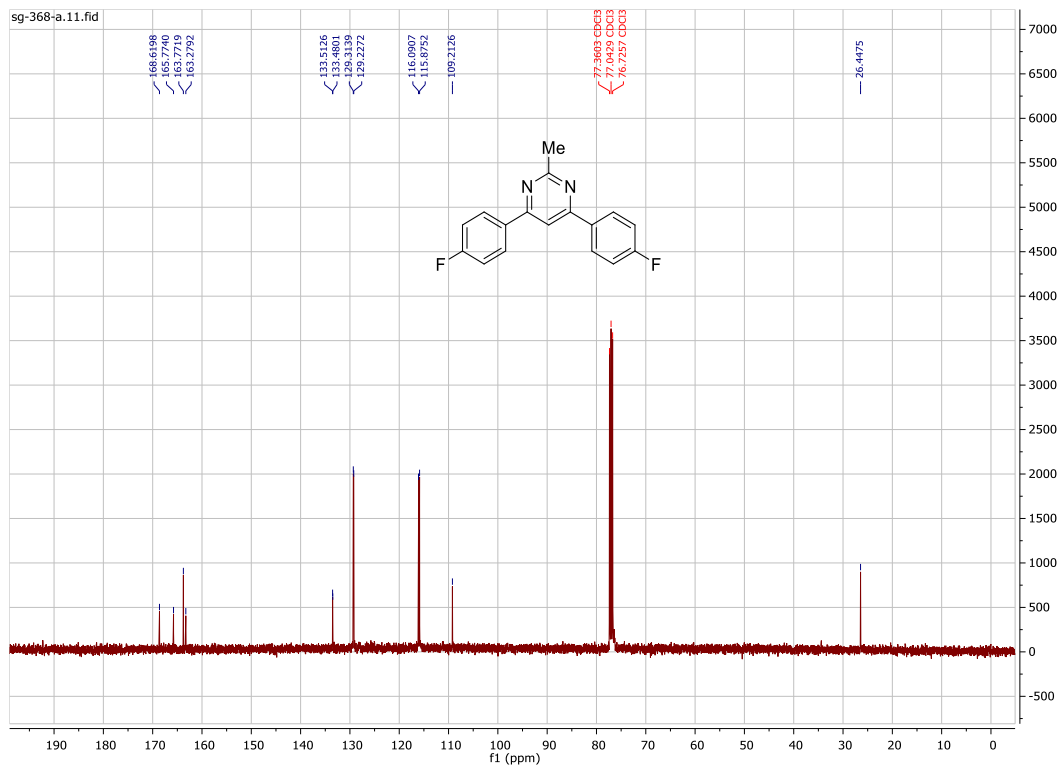




HRMS spectra of **17g**



¹H NMR spectrum of **8g** (in CDCl₃)

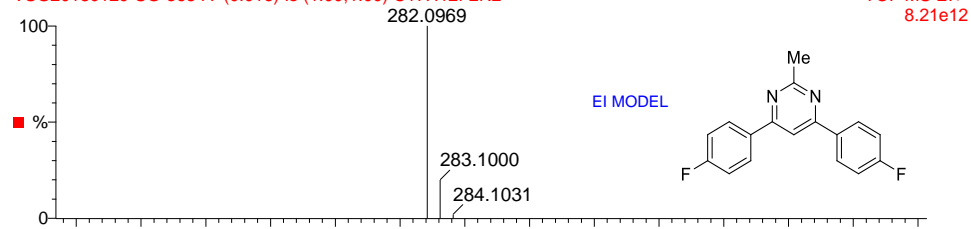


^{13}C NMR spectrum of **8g** (in CDCl_3)

VSG20180129-SG-368-A

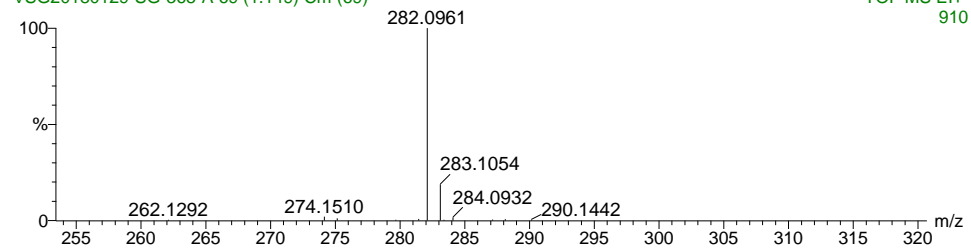
VSG20180129-SG-368-A (0.016) Is (1.00,1.00) $\text{C}_{17}\text{H}_{12}\text{F}_2\text{N}_2$

TOF MS EI+
8.21e12



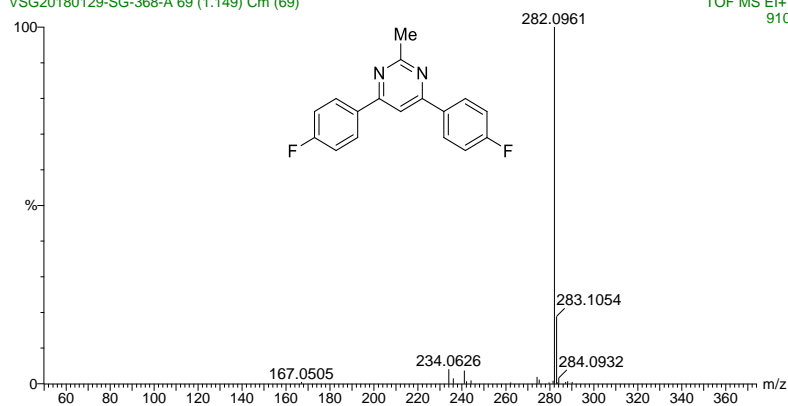
VSG20180129-SG-368-A 69 (1.149) Cm (69)

TOF MS EI+
910



VSG20180129-SG-368-A

VSG20180129-SG-368-A 69 (1.149) Cm (69)

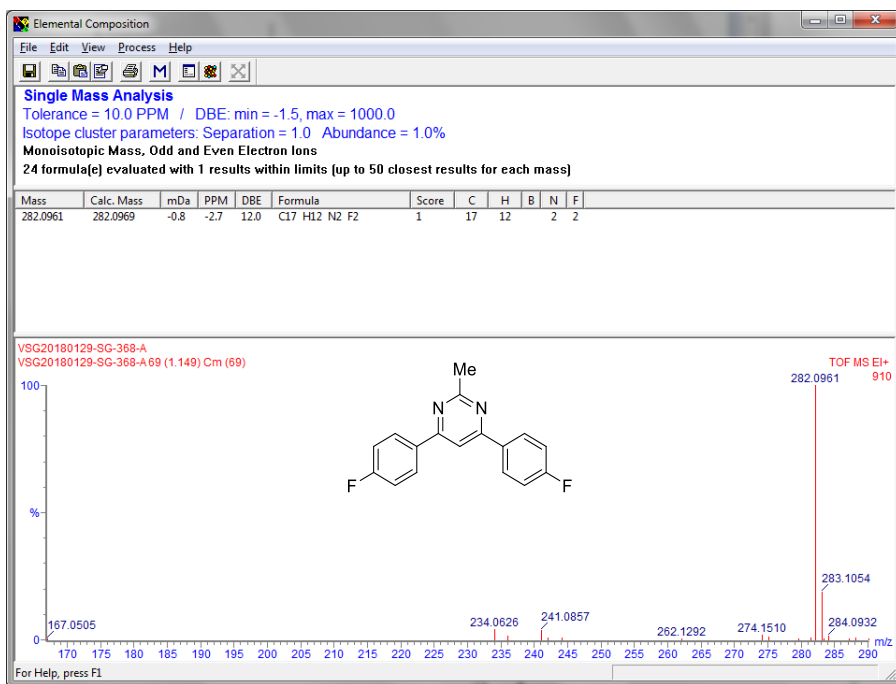


VSG20180129-SG-368-A

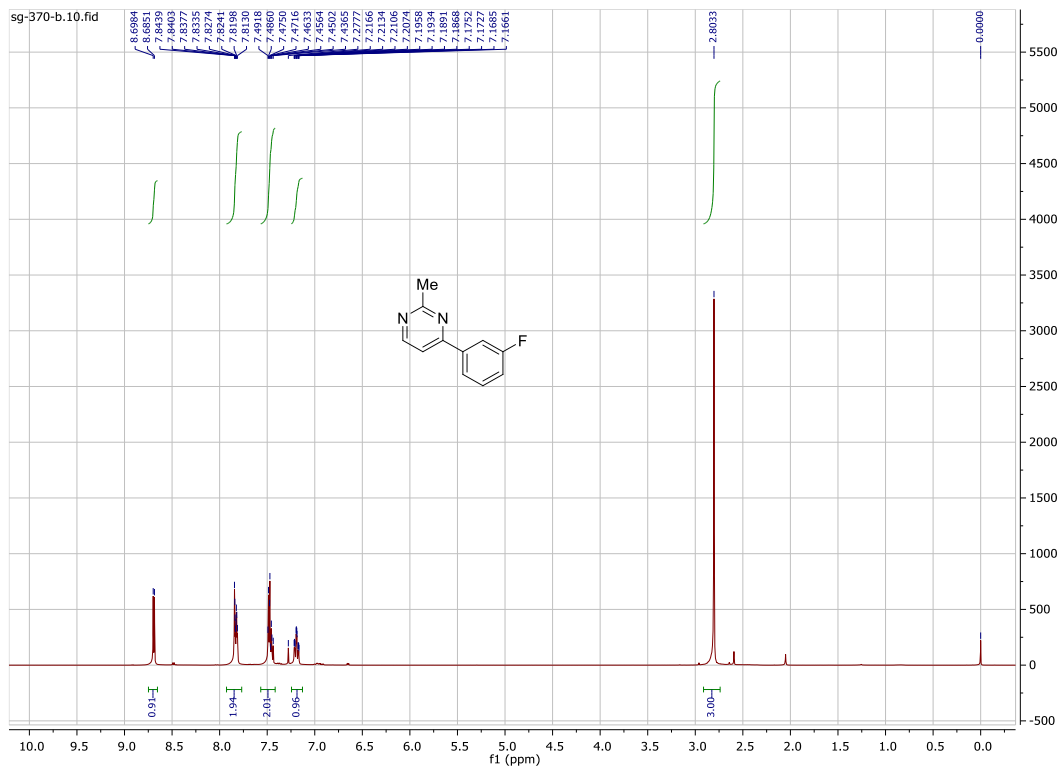
VSG20180129-SG-368-A 69 (1.149) Cm (69)

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	167.0505	4.05e0	0.45	0.32										
2:	234.0626	3.65e1	4.01	2.86										
3:	236.0622	1.32e1	1.45	1.03										
4:	241.0857	3.34e1	3.67	2.62										
5:	242.0919	6.08e0	0.67	0.48										
6:	244.1470	8.10e0	0.89	0.63										
7:	262.1292	3.04e0	0.33	0.24										
8:	274.1510	1.72e1	1.89	1.35										
9:	275.1436	1.01e1	1.11	0.79										
10:	279.6667	3.04e0	0.33	0.24										
11:	281.4350	7.09e0	0.78	0.56										
12:	282.0961	9.10e2	100.03	71.29										
13:	283.1054	1.71e2	18.81	13.40										
14:	283.3096	3.04e0	0.33	0.24										
15:	284.0932	1.42e1	1.56	1.11										
16:	287.1534	4.05e0	0.45	0.32										
17:	288.1237	6.08e0	0.67	0.48										
18:	290.1442	4.05e0	0.45	0.32										

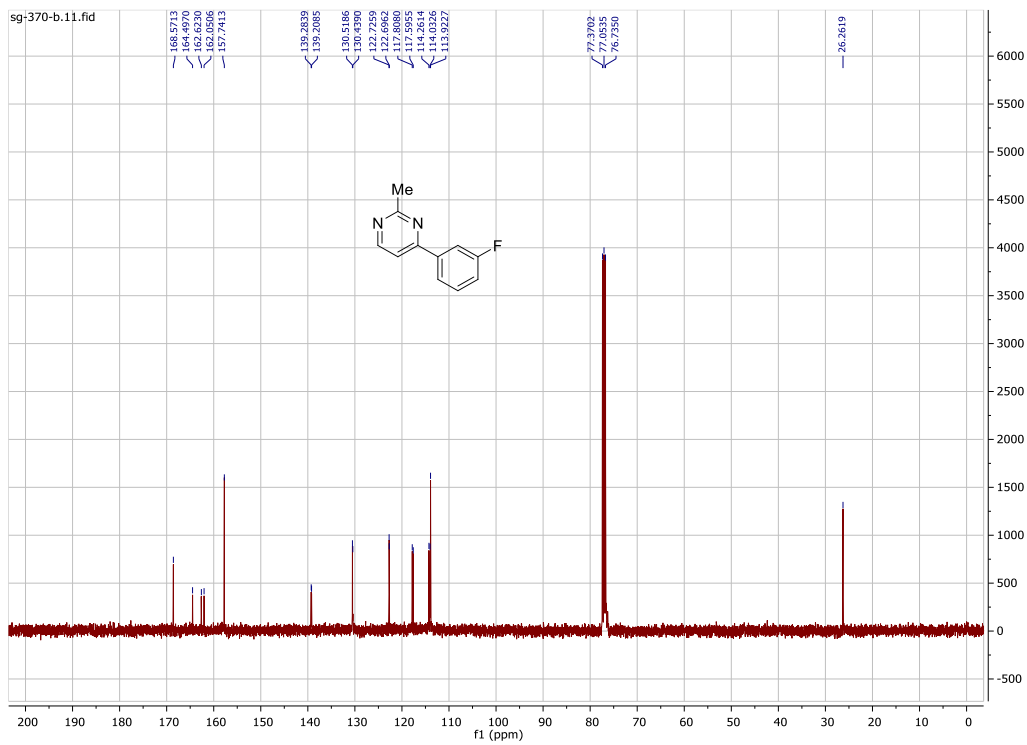
TOF MS EI+ 910



HRMS spectra of 8g



^1H NMR spectrum of **17h** (in CDCl_3)

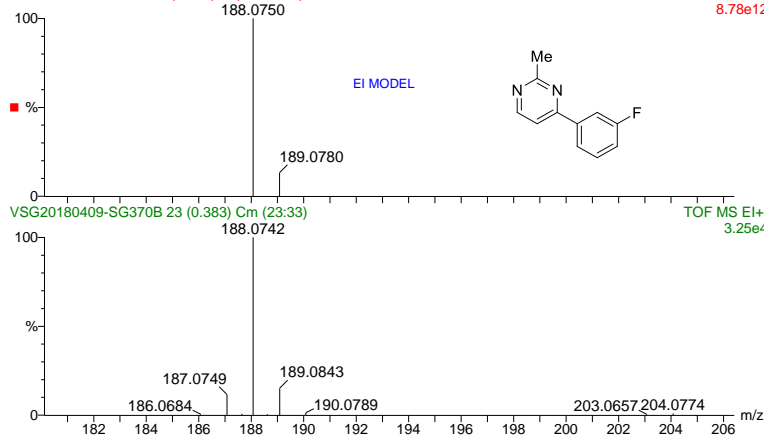


^{13}C NMR spectrum of **17h** (in CDCl_3)

VSG20180409-SG370B

VSG20180409-SG370B (0.016) Is (1.00,1.00) C11H9FN2

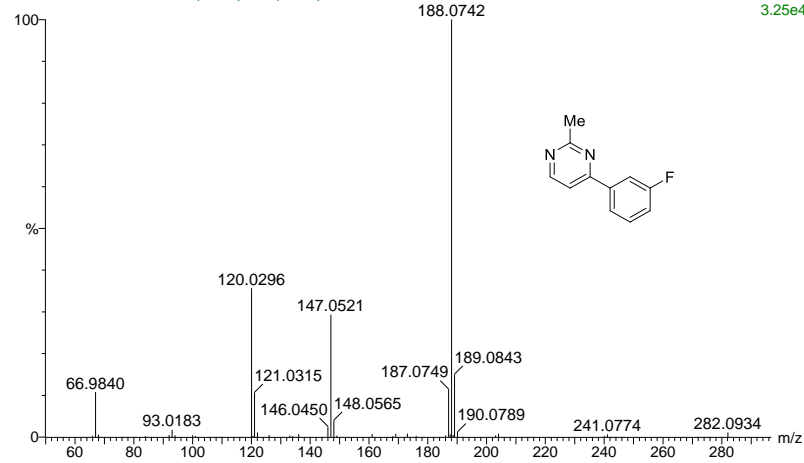
TOF MS EI+
8.78e12



VSG20180409-SG370B

VSG20180409-SG370B 23 (0.383) Cm (23:33)

TOF MS EI+
3.25e4

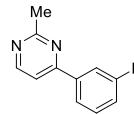


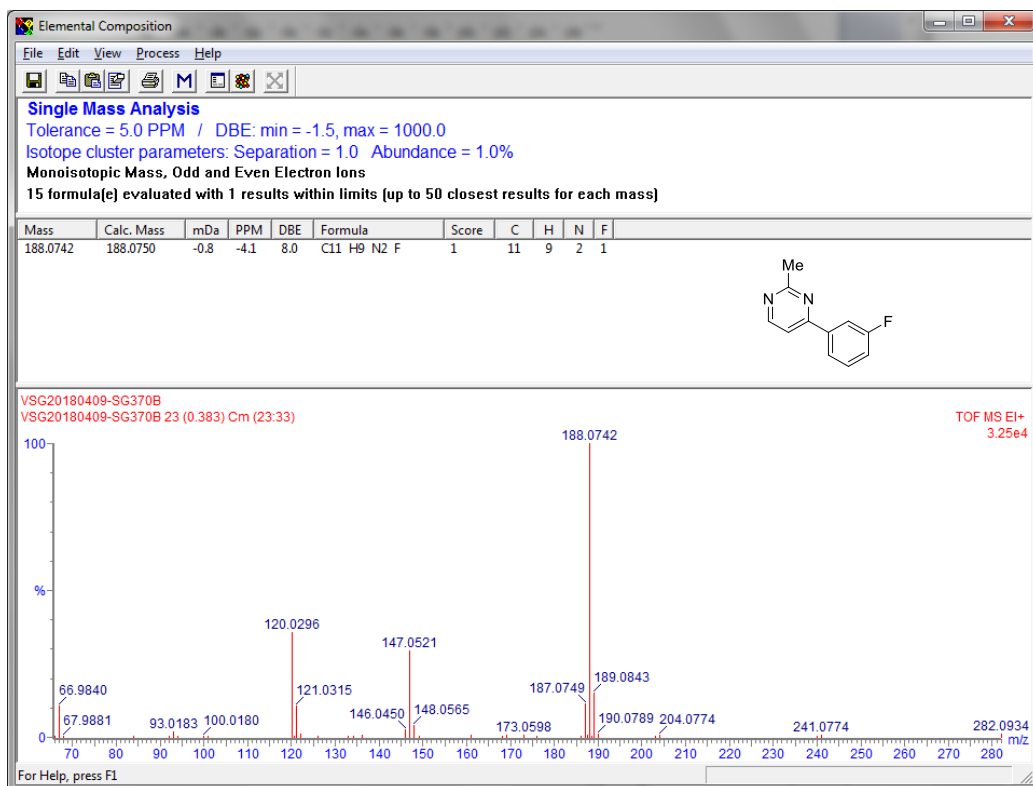
VSG20180409-SG370B

VSG20180409-SG370B 23 (0.383) Cm (23:33)

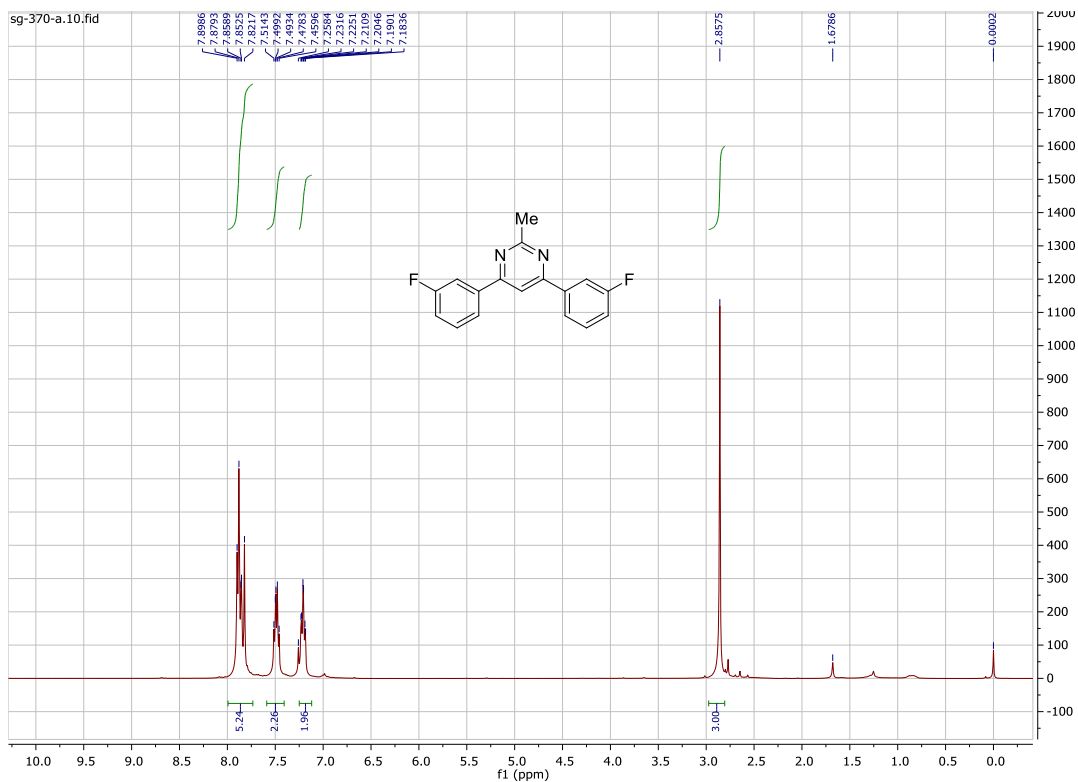
TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	65.9746	9.01e1	0.28	0.12	32:	189.0843	4.88e3	15.03	6.28					
2:	66.9840	3.50e3	10.78	4.50	33:	190.0789	3.80e2	1.17	0.49					
3:	67.9881	1.77e2	0.55	0.23	34:	203.0657	1.21e2	0.37	0.16					
4:	83.9205	6.68e1	0.21	0.09	35:	204.0774	2.61e2	0.80	0.34					
5:	92.0135	1.63e2	0.50	0.21	36:	240.0656	8.20e1	0.25	0.11					
6:	93.0183	5.55e2	1.71	0.71	37:	241.0774	1.97e2	0.61	0.25					
7:	94.0037	1.15e2	0.36	0.15	38:	282.0934	3.55e2	1.10	0.46					
8:	100.0180	1.36e2	0.42	0.17										
9:	101.0219	7.70e1	0.24	0.10										
10:	120.0296	1.16e4	35.64	14.89										
11:	120.4987	7.80e1	0.24	0.10										
12:	121.0315	3.46e3	10.67	4.46										
13:	122.0323	3.45e2	1.06	0.44										
14:	126.0330	1.55e2	0.48	0.20										
15:	133.0461	1.11e2	0.34	0.14										
16:	134.0489	7.59e1	0.23	0.10										
17:	136.0576	2.13e2	0.66	0.27										
18:	146.0450	8.10e2	2.50	1.04										
19:	147.0521	9.50e3	29.28	12.23										
20:	148.0565	1.30e3	4.01	1.67										
21:	149.0592	1.09e2	0.34	0.14										
22:	161.0698	2.36e2	0.73	0.30										
23:	168.0782	7.39e1	0.23	0.10										
24:	169.0830	2.37e2	0.73	0.31										
25:	173.0598	2.51e2	0.77	0.32										
26:	176.0752	8.61e1	0.27	0.11										
27:	186.0684	1.19e2	0.37	0.15										
28:	187.0749	3.72e3	11.46	4.79										
29:	187.6414	2.04e2	0.63	0.26										
30:	188.0742	3.25e4	100.00	41.78										
31:	188.6118	1.49e2	0.46	0.19										

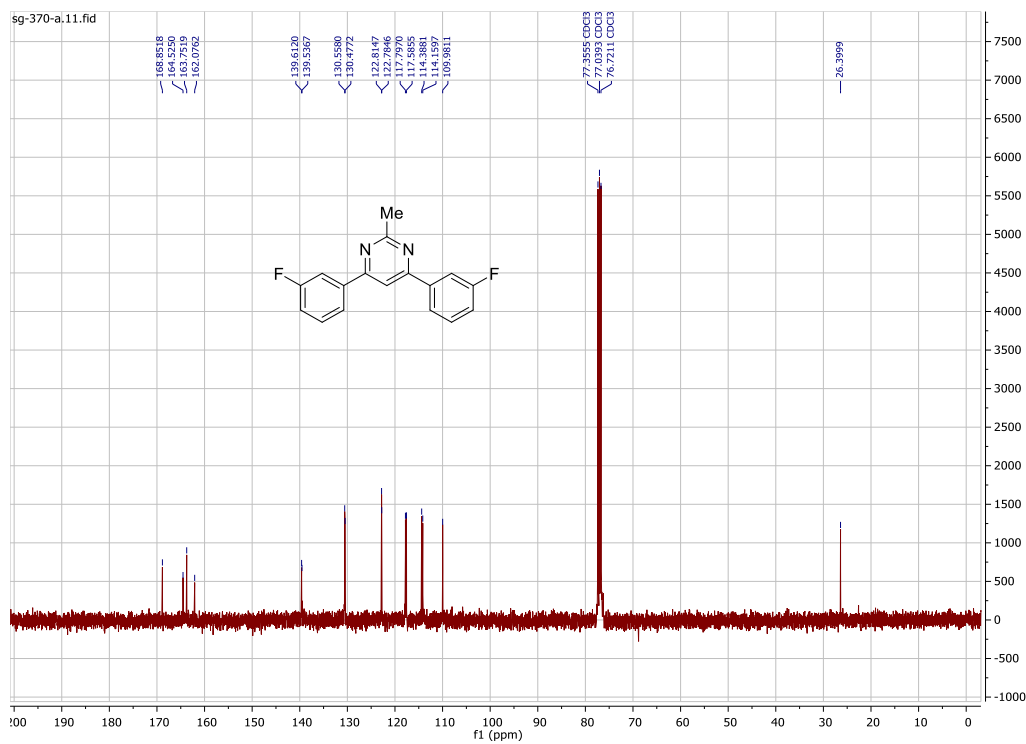




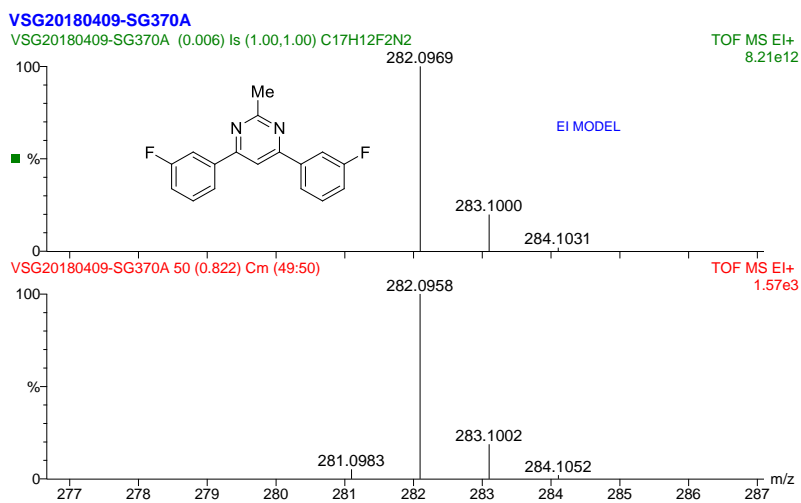
HRMS spectra of **17h**



^1H NMR spectrum of **8h** (in CDCl_3)



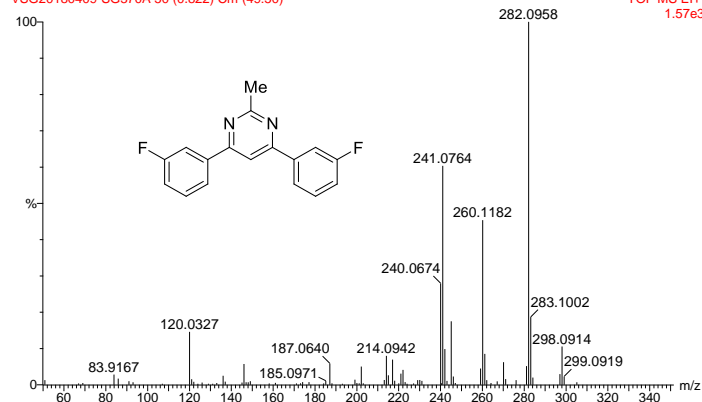
^{13}C NMR spectrum of **8h** (in CDCl₃)



VSG20180409-SG370A

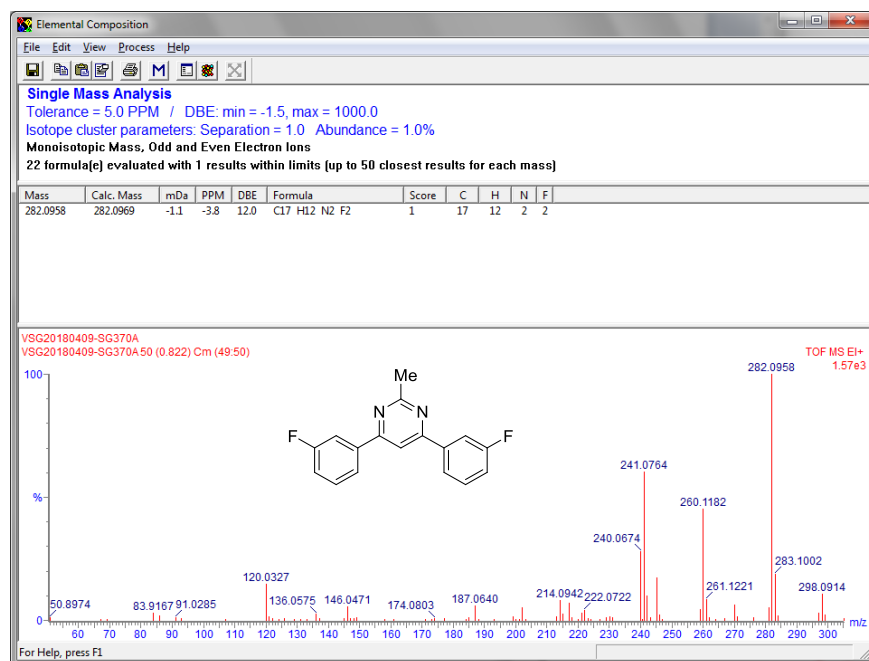
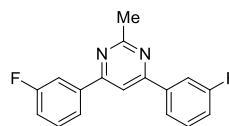
VSG20180409-SG370A 50 (0.822) Cm (49:50)

TOF MS EI+
1.57e3

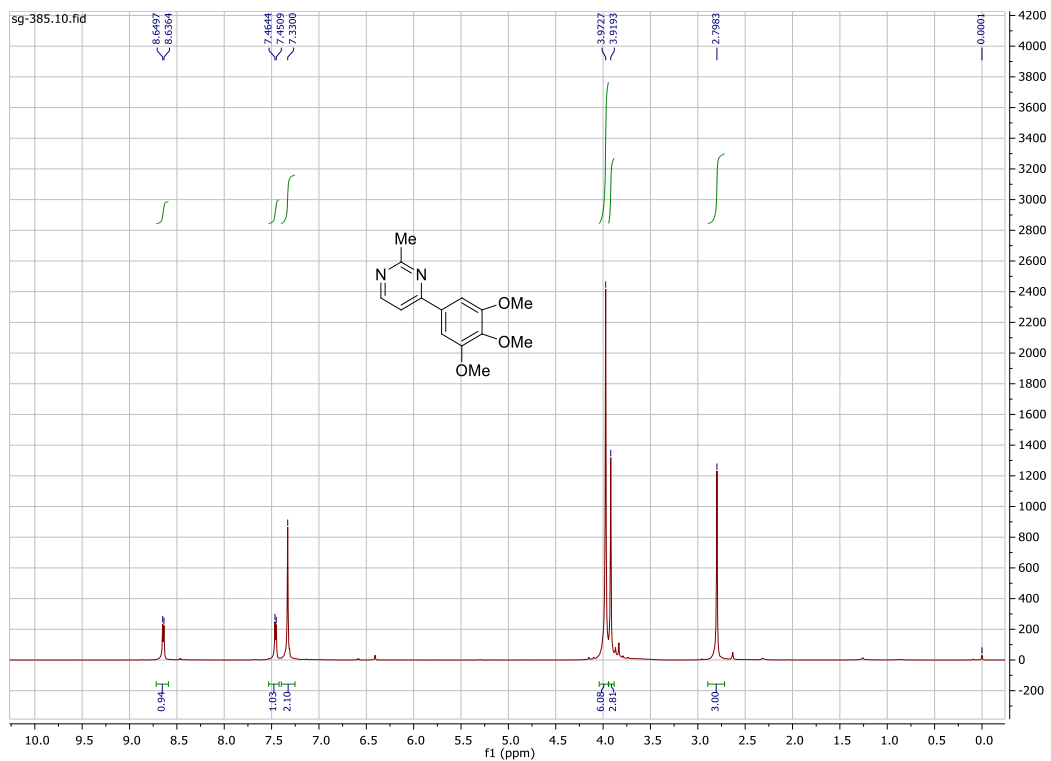


VSG20180409-SG370A

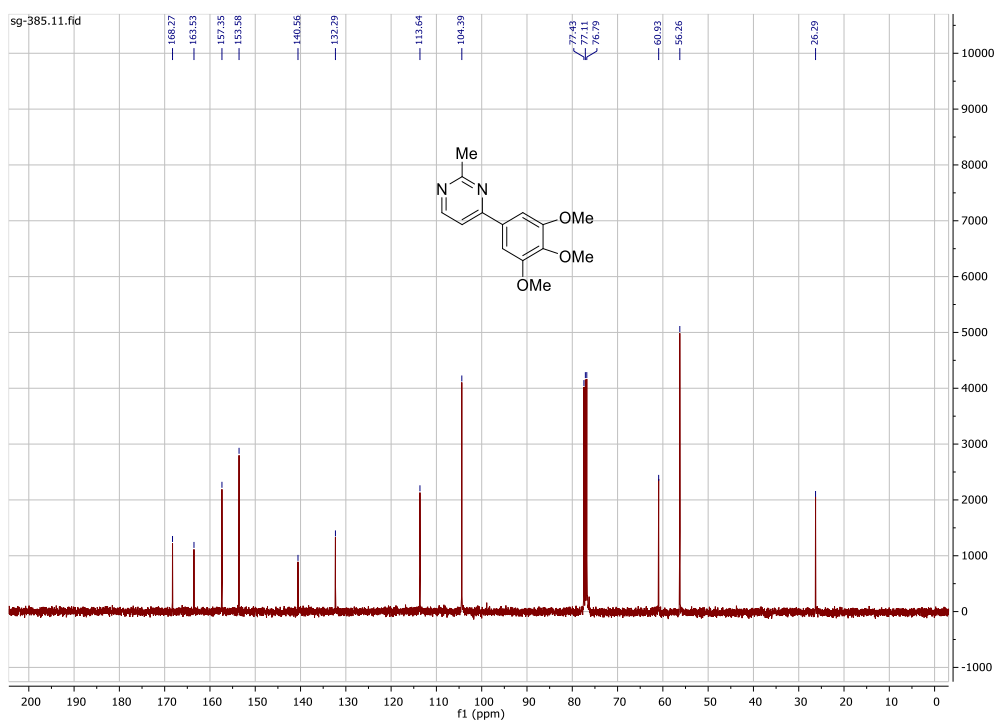
m/z	Abundance
83.9167	0.01
120.0327	0.05
136.0575	0.01
146.0471	0.01
174.0803	0.01
185.0971	0.02
187.0640	0.03
214.0942	0.04
240.0674	0.15
241.0764	0.25
260.1182	0.18
282.0958	1.00
283.1002	0.12
298.0914	0.08
299.0919	0.07



HRMS spectra of 8h



^1H NMR spectrum of **17j** (in CDCl_3)

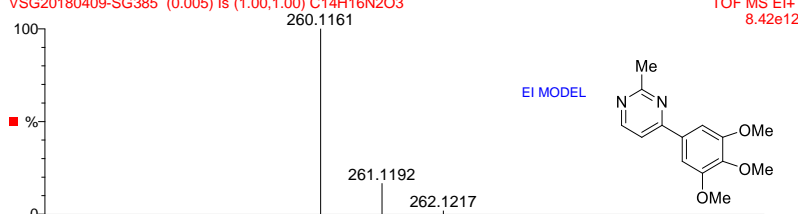


^{13}C NMR spectrum of **17j** (in CDCl_3)

VSG20180409-SG385

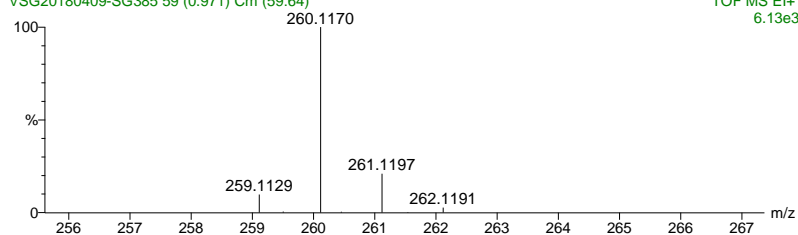
VSG20180409-SG385 (0.005) Is (1.00,1.00) C₁₄H₁₆N₂O₃

TOF MS EI+
8.42e12



VSG20180409-SG385 59 (0.971) Cm (59.64)

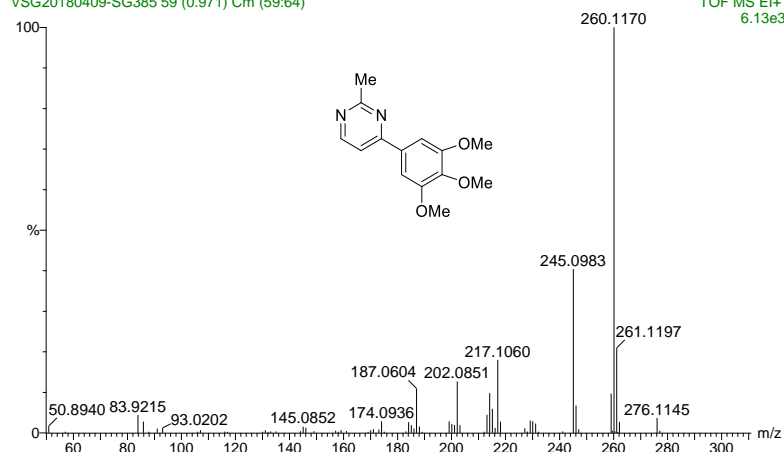
TOF MS EI+
6.13e3



VSG20180409-SG385

VSG20180409-SG385 59 (0.971) Cm (59.64)

TOF MS EI+
6.13e3



VSG20180409-SG385
VSG20180409-SG385 59 (0.971) Cm (59.64)

m/z	Relative Intensity (%)
50.8940	0.0001
52.0400	0.0001
54.0400	0.0001
56.0400	0.0001
58.0400	0.0001
60.0400	0.0001
62.0400	0.0001
64.0400	0.0001
66.0400	0.0001
68.0400	0.0001
70.0400	0.0001
72.0400	0.0001
74.0400	0.0001
76.0400	0.0001
78.0400	0.0001
80.0400	0.0001
82.0400	0.0001
84.0400	0.0001
86.0400	0.0001
88.0400	0.0001
90.0400	0.0001
92.0400	0.0001
94.0400	0.0001
96.0400	0.0001
98.0400	0.0001
100.0400	0.0001
102.0400	0.0001
104.0400	0.0001
106.0400	0.0001
108.0400	0.0001
110.0400	0.0001
112.0400	0.0001
114.0400	0.0001
116.0400	0.0001
118.0400	0.0001
120.0400	0.0001
122.0400	0.0001
124.0400	0.0001
126.0400	0.0001
128.0400	0.0001
130.0400	0.0001
132.0400	0.0001
134.0400	0.0001
136.0400	0.0001
138.0400	0.0001
140.0400	0.0001
142.0400	0.0001
144.0400	0.0001
146.0400	0.0001
148.0400	0.0001
150.0400	0.0001
152.0400	0.0001
154.0400	0.0001
156.0400	0.0001
158.0400	0.0001
160.0400	0.0001
162.0400	0.0001
164.0400	0.0001
166.0400	0.0001
168.0400	0.0001
170.0400	0.0001
172.0400	0.0001
174.0400	0.0001
176.0400	0.0001
178.0400	0.0001
180.0400	0.0001
182.0400	0.0001
184.0400	0.0001
186.0400	0.0001
188.0400	0.0001
190.0400	0.0001
192.0400	0.0001
194.0400	0.0001
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224.0400	0.0001
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228.0400	0.0001
230.0400	0.0001
232.0400	0.0001
234.0400	0.0001
236.0400	0.0001
238.0400	0.0001
240.0400	0.0001
242.0400	0.0001
244.0400	0.0001
246.0400	0.0001
248.0400	0.0001
250.0400	0.0001
252.0400	0.0001
254.0400	0.0001
256.0400	0.0001
258.0400	0.0001
260.0400	0.0001
262.0400	0.0001
264.0400	0.0001
266.0400	0.0001
268.0400	0.0001
270.0400	0.0001
272.0400	0.0001
274.0400	0.0001
276.0400	0.0001
278.0400	0.0001
280.0400	0.0001
282.0400	0.0001
284.0400	0.0001
286.0400	0.0001
288.0400	0.0001
290.0400	0.0001
292.0400	0.0001
294.0400	0.0001
296.0400	0.0001
298.0400	0.0001
300.0400	0.0001

HRMS spectra of 17j