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

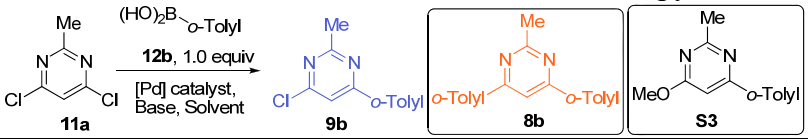
Melting points were obtained on a Electrothermal IA9100 Melting Point Apparatus and are uncorrected. ^{1}H and ^{13}C spectra were recorded on Bruker Avance-400 MHz spectrometer. The chemical shifts of ^{1}H and ^{13}C NMR signals are quoted relative to internal C*H*Cl3 (δ = 7.26) and *C*DCl3 (δ =77.0) or tetramethylsilane (δ = 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)

S1

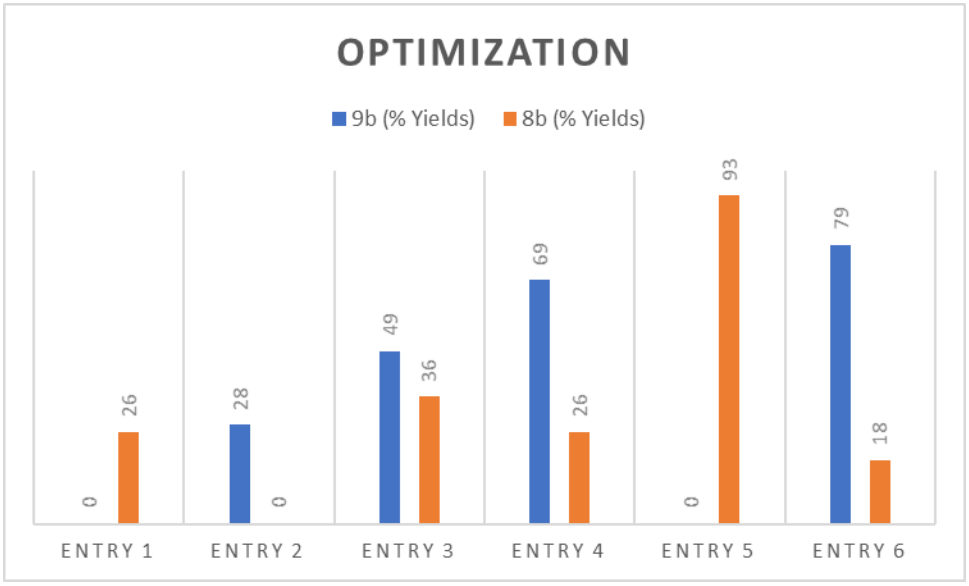
To a stirred solution of 4,6-dichloro-2-methylpyrimidine (2 g, 1.0 equiv) in MeOH (20 mL) was added dropwise a solution of NaOMe (25 wt% in MeOH, 1.0 equiv) and stirred for 20 min at rt. The reaction mixture was diluted with H_2O and extracted with EtOAc (3 X 30 mL). The combined organic extracts were washed with brine, dried (Na_2SO_4), 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, $CDCl_3$): δ 6.58 (s, 1H), 3.97 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 170.5, 168.7, 160.2, 104.3, 54.3, 25.8 ppm; HRMS (EI) calcd for $C_6H_7ClN_2O$ [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_2CO_3 (3.0 equiv), Toluene/MeOH (4:1), 90 °C, 18 h, RBF	--/26[b]
2	$Pd(PPh_3)_4$ (3 mol%), K_2CO_3 (3.0 equiv), Toluene, 90 °C, 20 h, RBF	28/--[c]
3	$Pd(OAc)_2$ (5 mol%), PPh_3 (10 mol%), Na_2CO_3 (3.1 equiv, dissolved in min amt of H_2O), DME, reflux, 18 h, RBF	49/36
4	**$Pd(PPh_3)_4$ (5 mol%), Na_2CO_3 (2 M, 2.5 equiv), *i*PrOH, reflux, 18 h, microwave vial**	**69/26**
5	Same as entry 4 except 2.3 equiv of o-tolyl boronic acid was used	--/93
6	Same as entry 4 except 0.8 equiv of o-tolyl boronic acid was used	79/18[d]

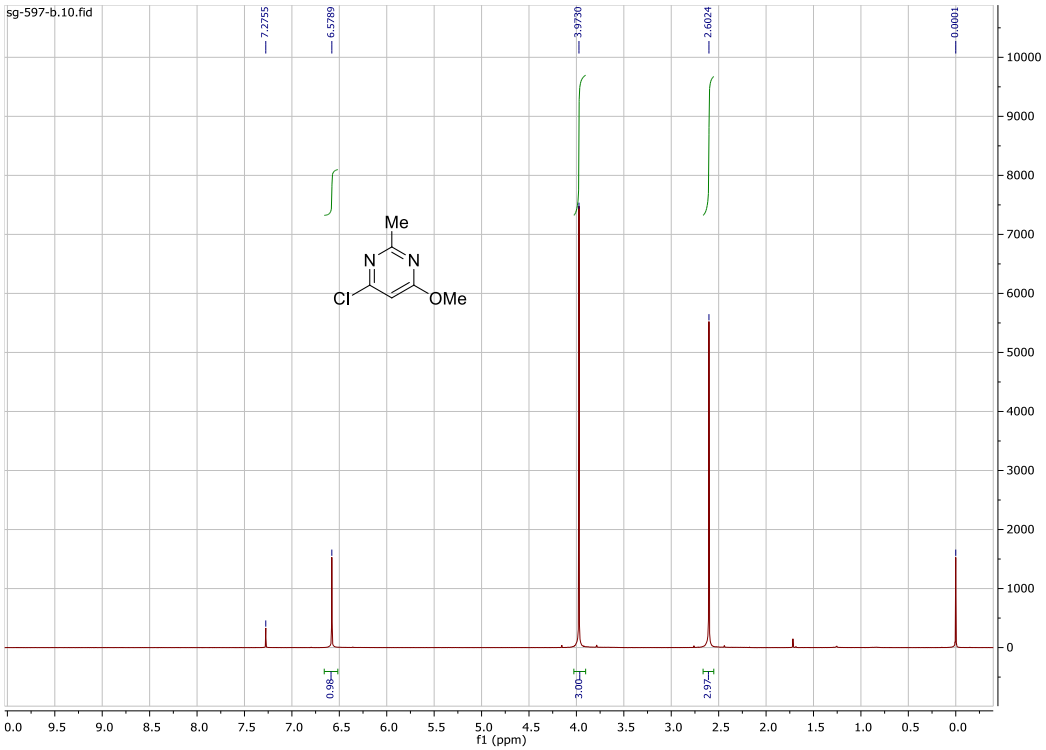
[a]Yield of isolated product. [b]**S3** was also isolated in 72% yield. [c]**1a** was recovered in 50% yield. [d]Yield was calculated considering boronic acid as the limiting reagent.



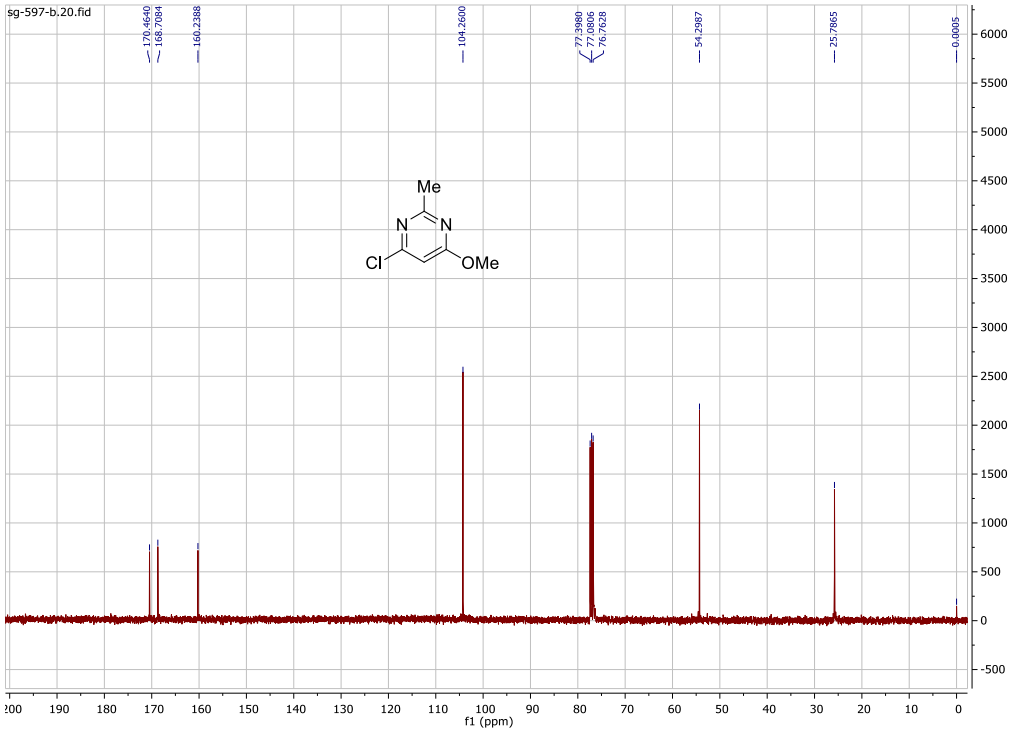
References:

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

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



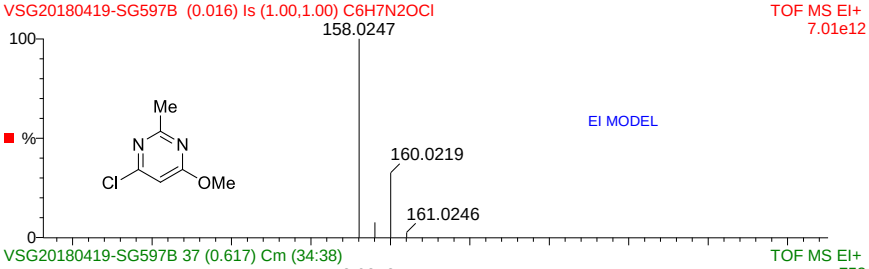
^{1}H NMR spectrum of **S1** (in $CDCl_3$)



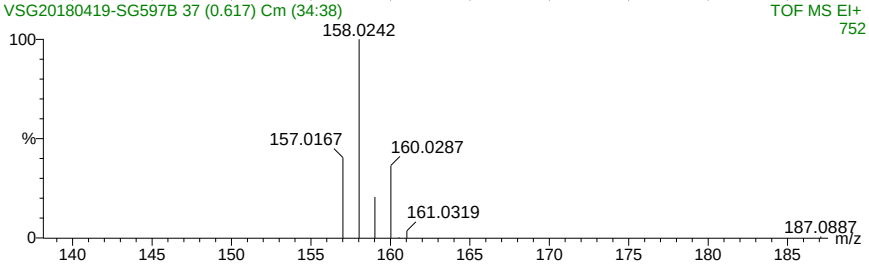
^{13}C NMR spectrum of **S1** (in $CDCl_3$)

VSG20180419-SG597B

VSG20180419-SG597B (0.016) Is (1.00,1.00) C6H7N2OCl — TOF MS EI+ 7.01e12

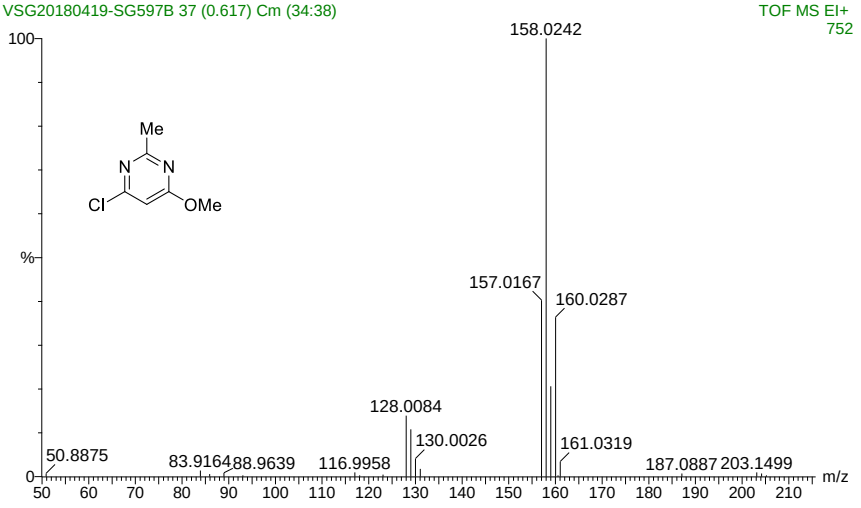


VSG20180419-SG597B 37 (0.617) Cm (34:38) — TOF MS EI+ 752



VSG20180419-SG597B

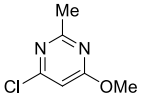
VSG20180419-SG597B 37 (0.617) Cm (34:38) — TOF MS EI+ 752

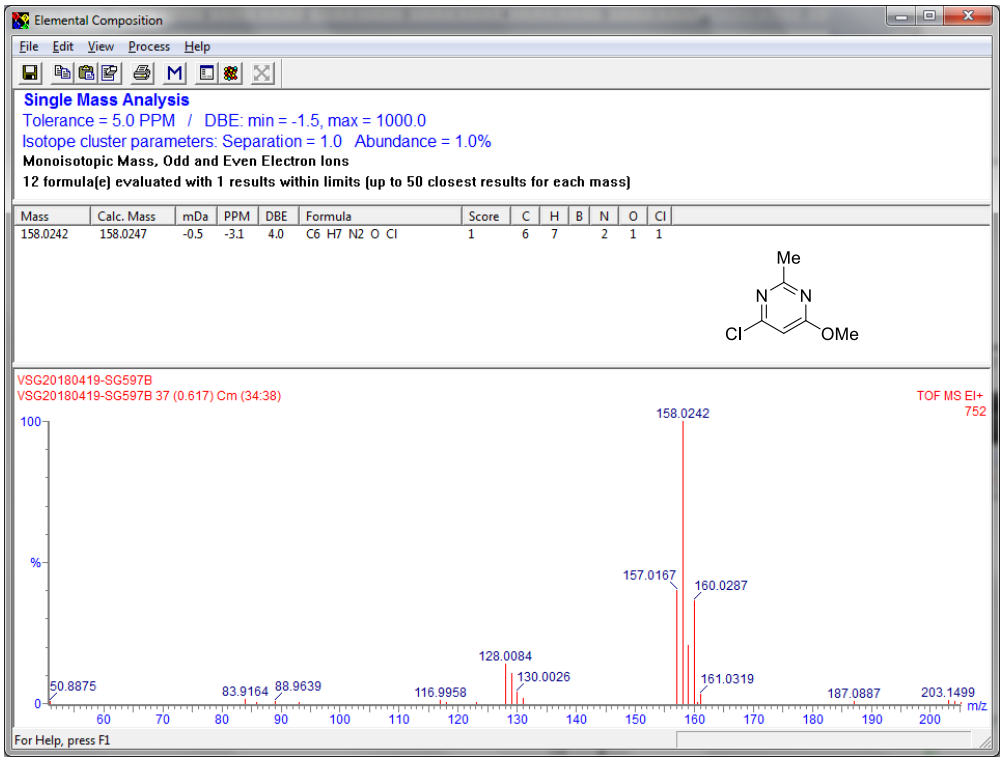


VSG20180419-SG597B

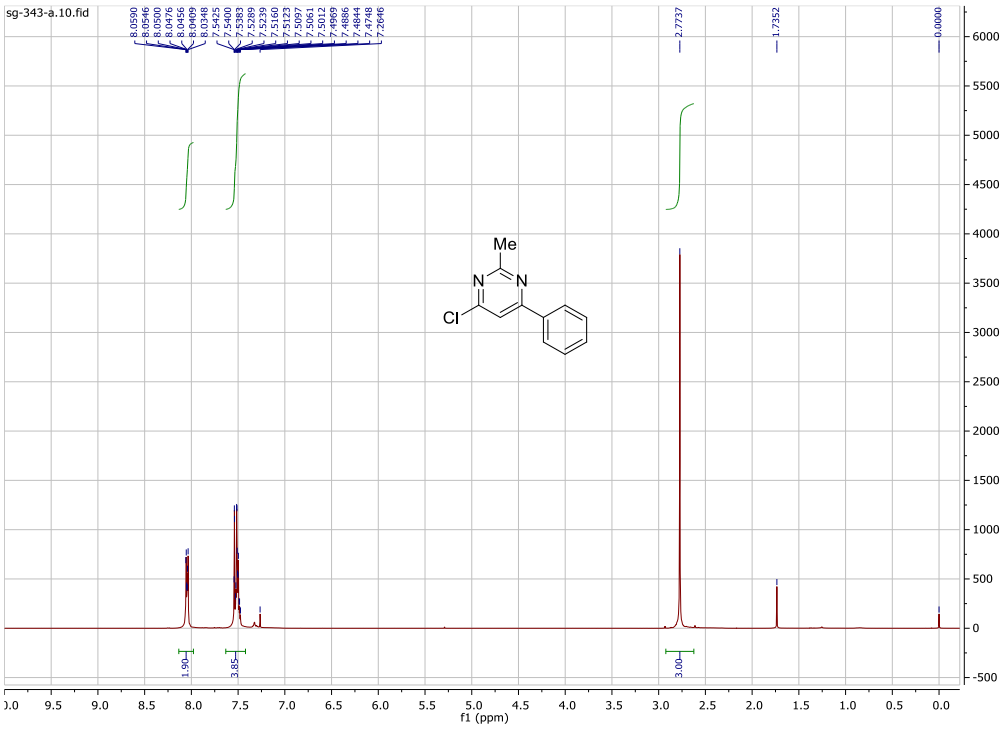
VSG20180419-SG597B 37 (0.617) Cm (34:38) — TOF MS EI+

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										

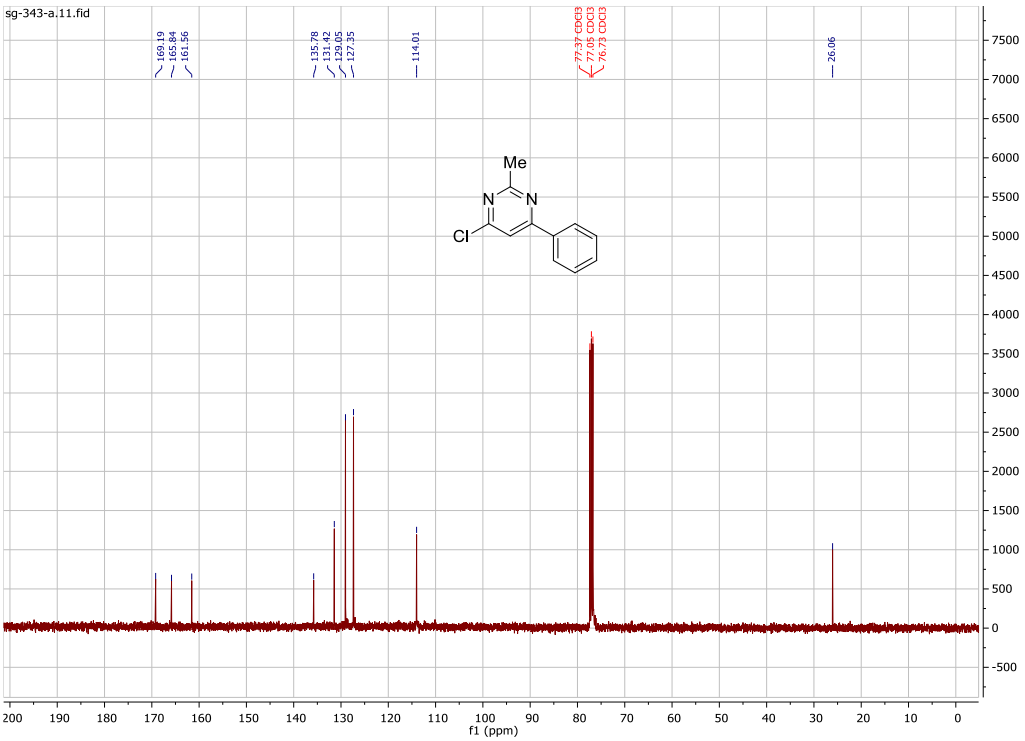




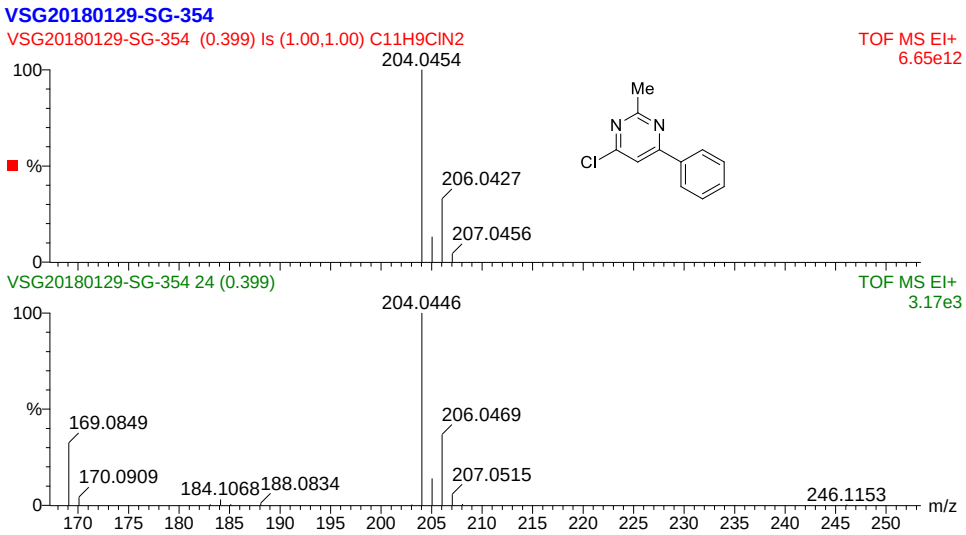
HRMS spectra of **S1**



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



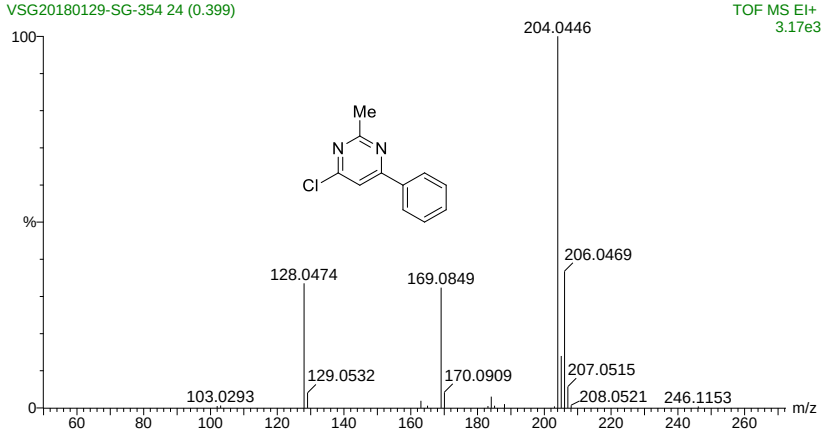
^{13}C NMR spectrum of **9a** (in $CDCl_3$)



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+

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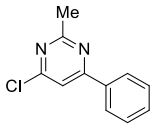
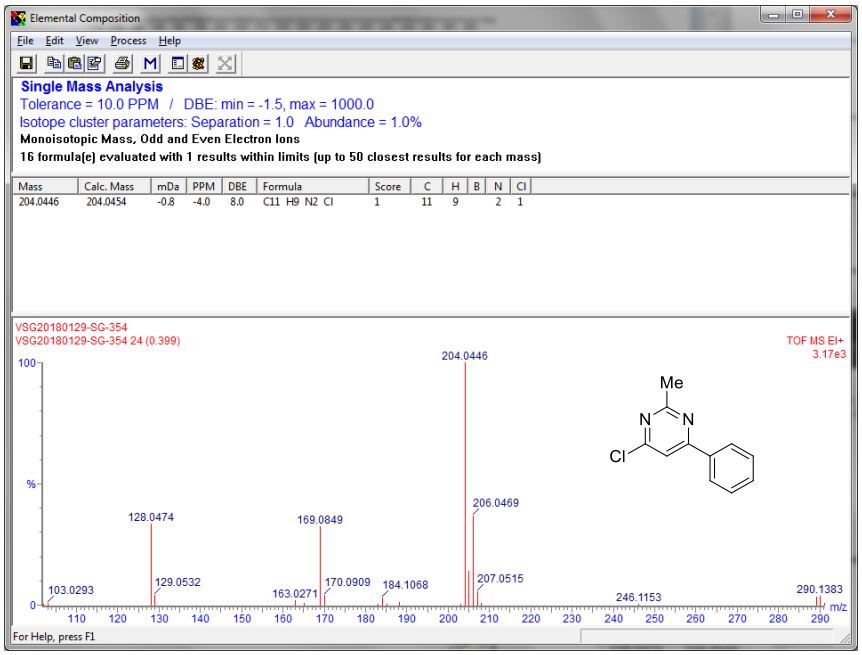
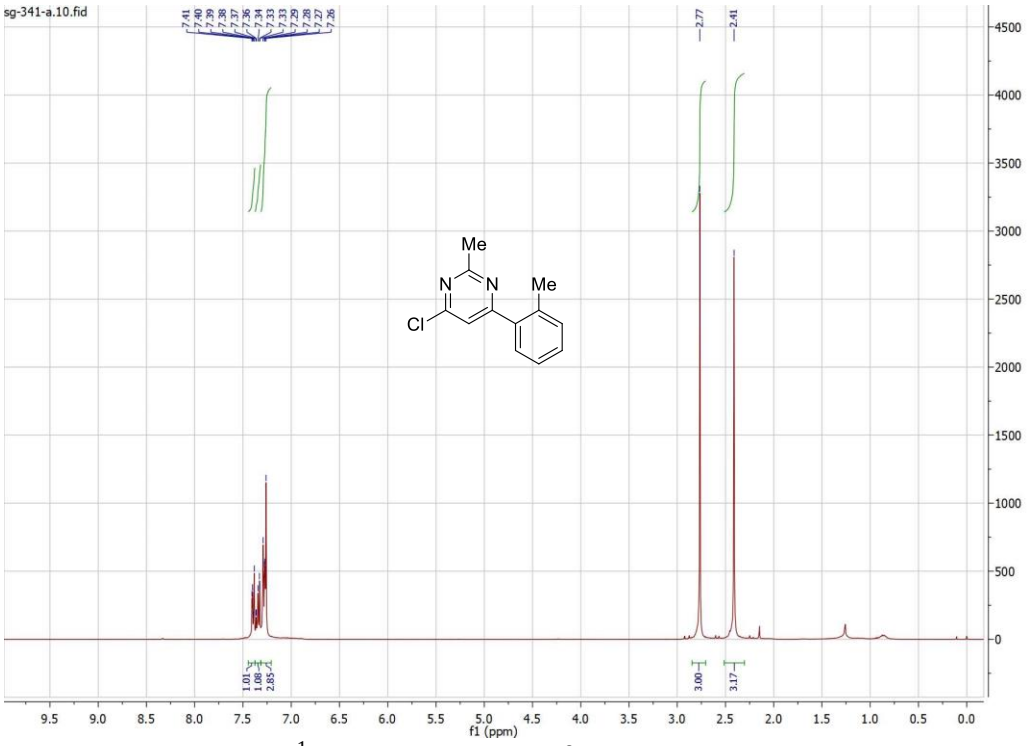
1:	102.0290	1.52e1	0.48	0.19										
2:	103.0293	1.92e1	0.61	0.24										
3:	128.0474	1.06e3	33.52	13.23										
4:	129.0532	1.26e2	3.96	1.56										
5:	163.0271	5.87e1	1.85	0.73										
6:	165.0343	1.82e1	0.58	0.23										
7:	169.0849	1.02e3	32.32	12.76										
8:	170.0909	1.32e2	4.15	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										

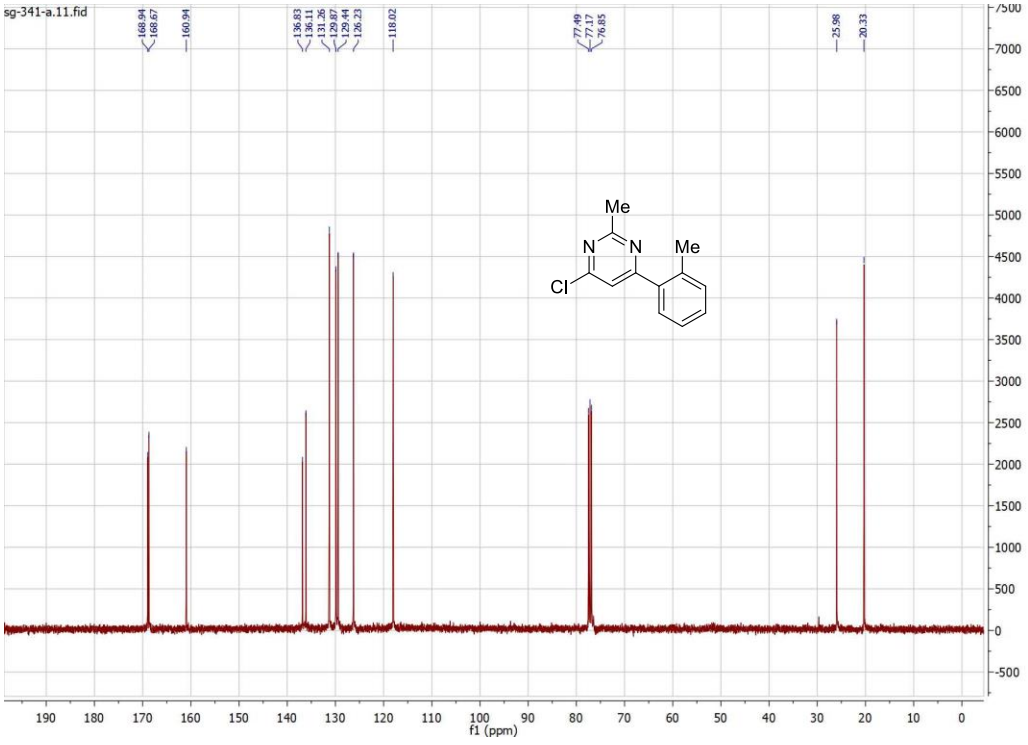




HRMS spectra of **9a**



^{1}H NMR spectrum of **9b** (in $CDCl_3$)

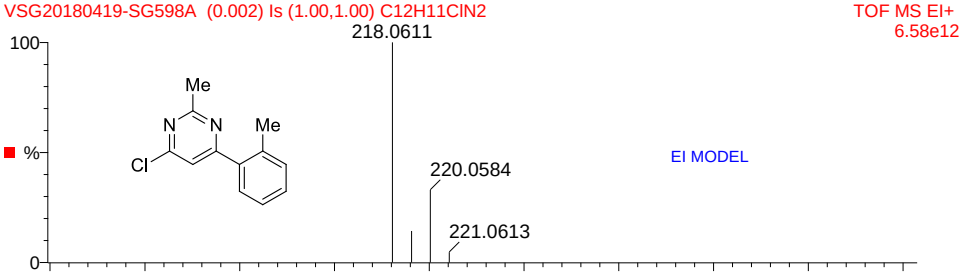


^{13}C NMR spectrum of **9b** (in $CDCl_3$)

VSG20180419-SG598A

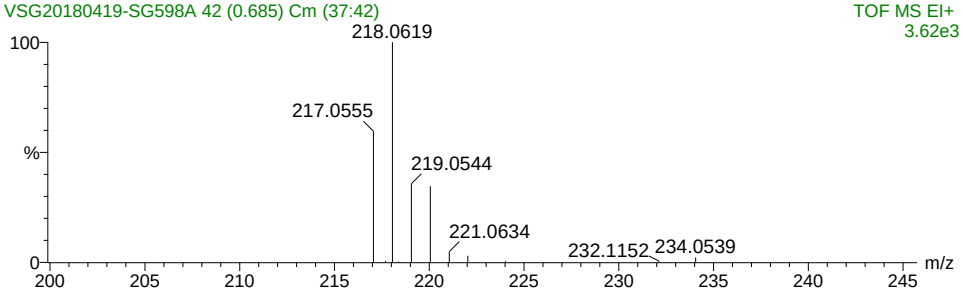
VSG20180419-SG598A (0.002) Is (1.00,1.00) C12H11ClN2

TOF MS EI+
6.58e12



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

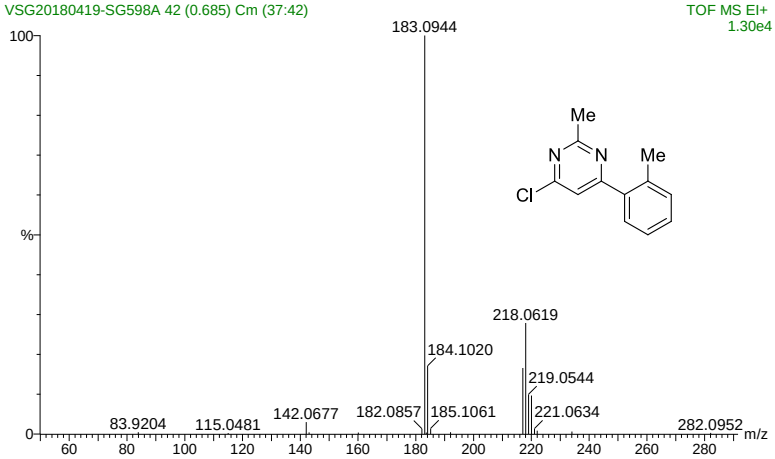
TOF MS EI+
3.62e3



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+

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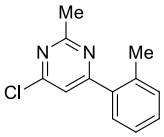
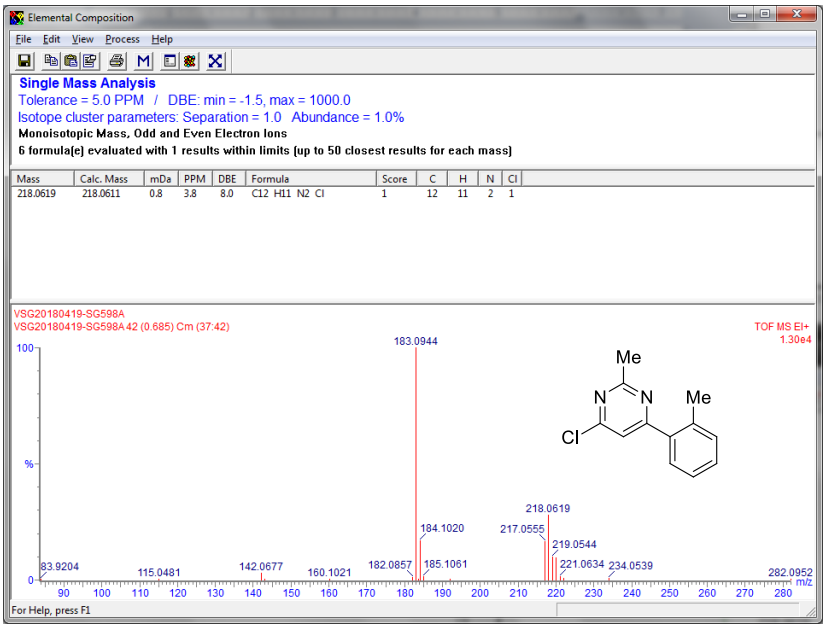
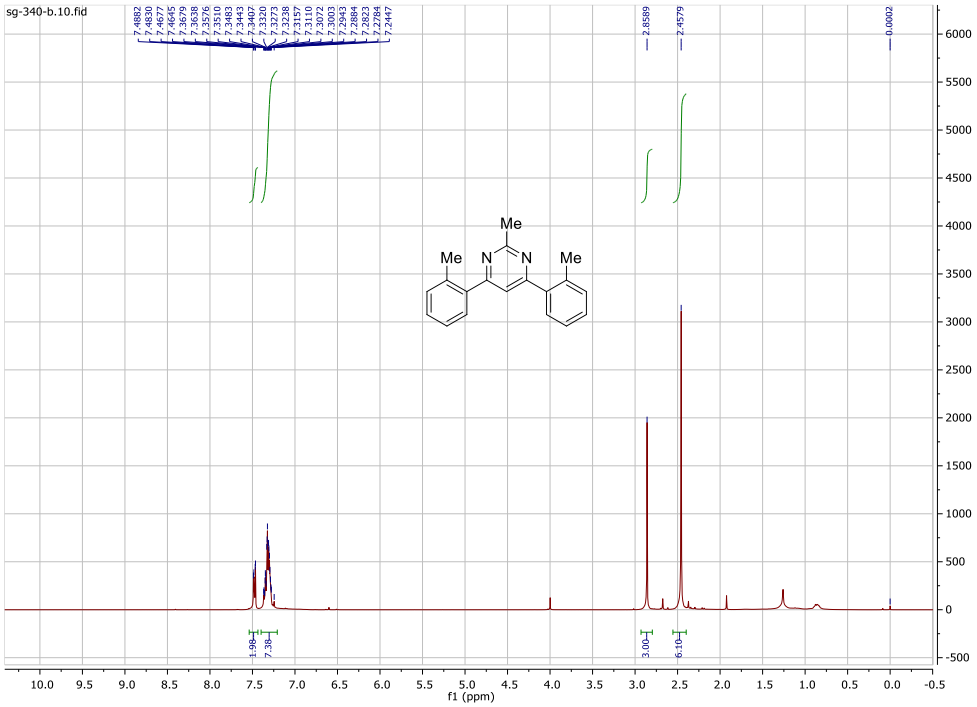
1:	83.9204	5.47e1	0.42	0.22										
2:	115.0481	2.73e1	0.21	0.11										
3:	142.0677	3.85e2	2.96	1.52										
4:	143.0714	4.76e1	0.37	0.19										
5:	160.1021	4.25e1	0.33	0.17										
6:	182.0857	1.66e2	1.28	0.66										
7:	183.0944	1.30e4	100.00	51.31										
8:	183.6367	4.66e1	0.36	0.18										
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										

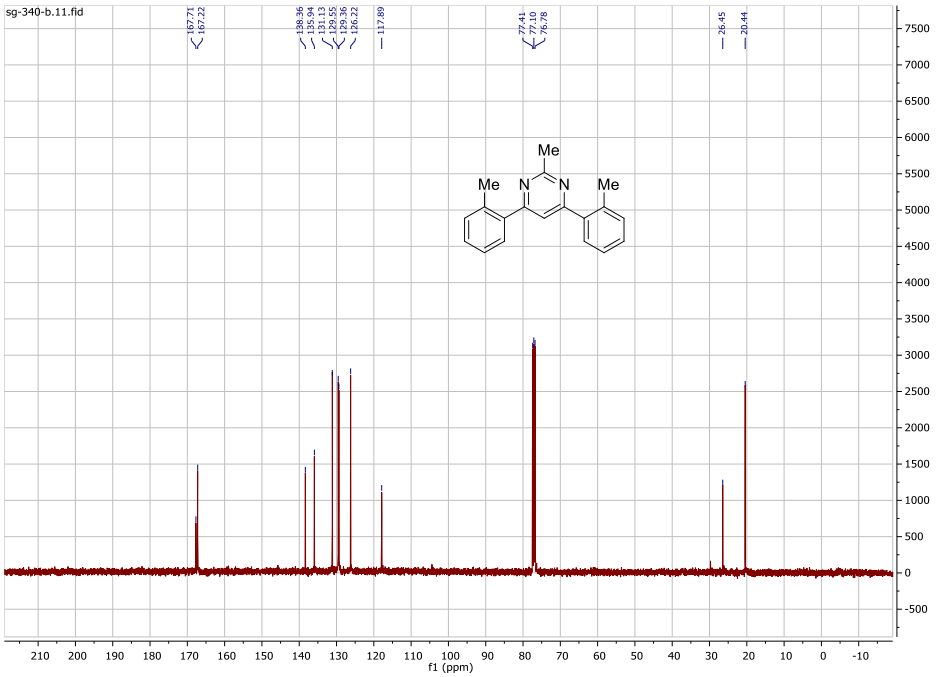




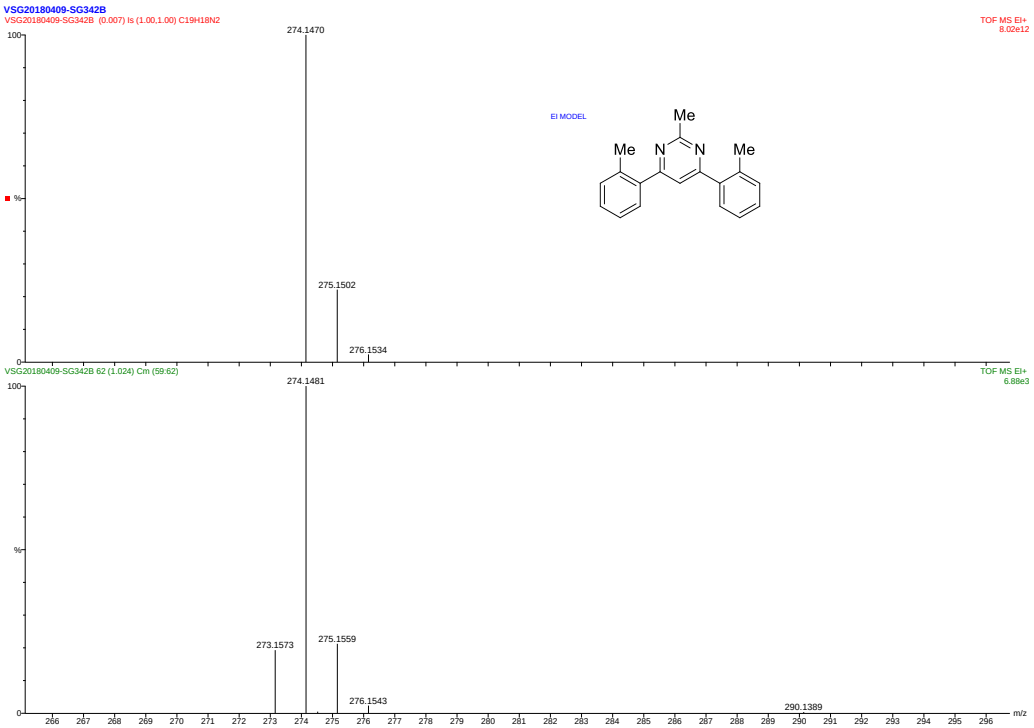
HRMS spectra of **9b**

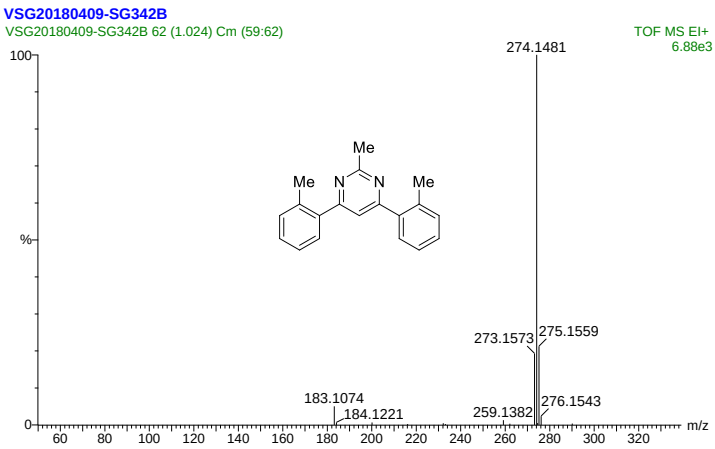


^{1}H NMR spectrum of **8b** (in $CDCl_3$)



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



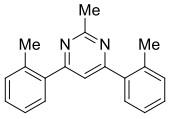


VSG20180409-SG342B

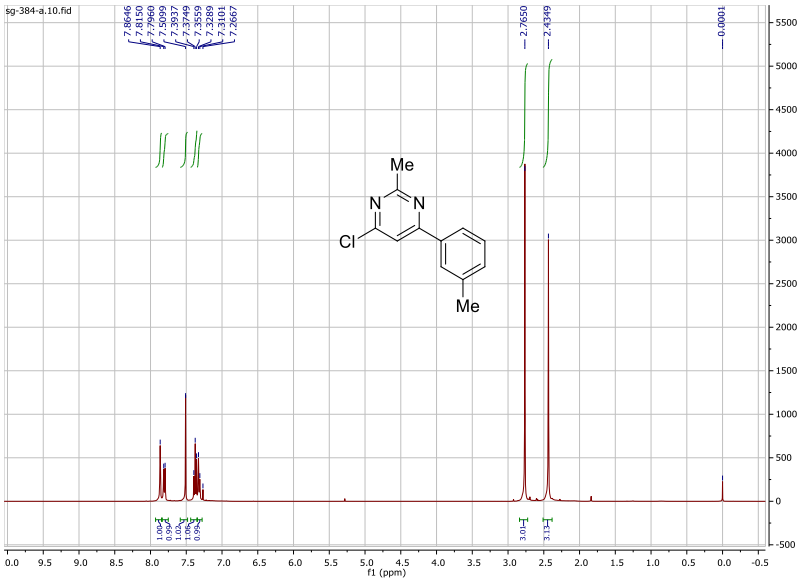
VSG20180409-SG342B 62 (1.024) Cm (59:62)

TOF MS EI+

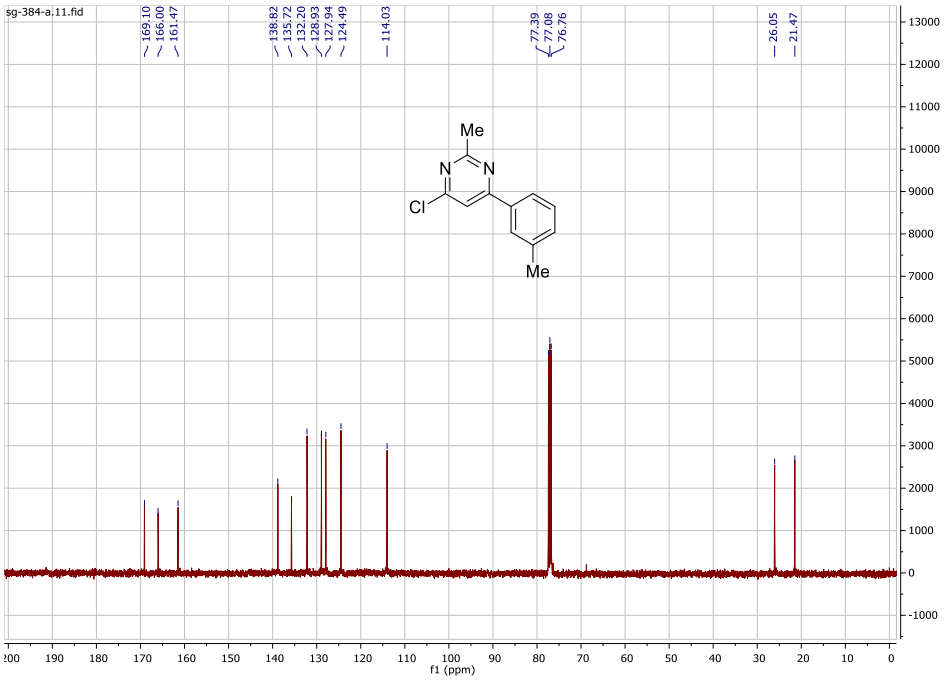
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	183.1074	3.42e2	4.98	3.22										
2:	184.1221	4.25e1	0.62	0.40										
3:	200.1021	4.15e1	0.60	0.39										
4:	216.1223	1.42e1	0.21	0.13										
5:	232.1290	2.94e1	0.43	0.28										
6:	233.1284	1.52e1	0.22	0.14										
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										



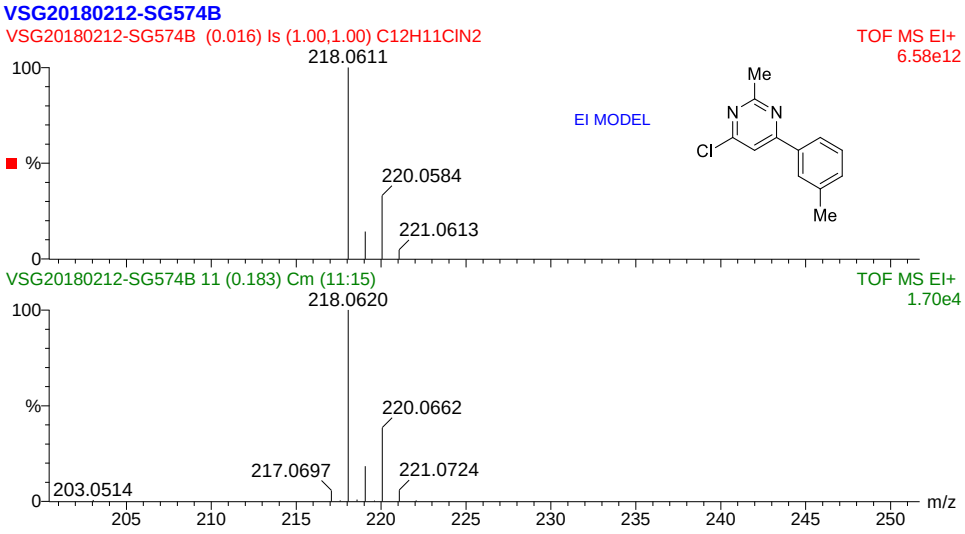
HRMS spectra of **8b**



^{1}H NMR spectrum of **9c** (in $CDCl_3$)



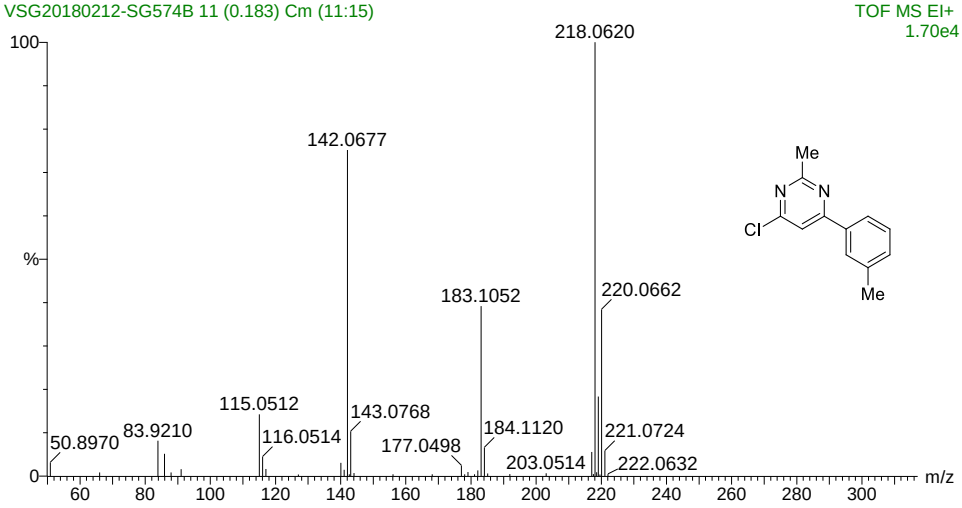
^{13}C NMR spectrum of **9c** (in $CDCl_3$)



VSG20180212-SG574B

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

TOF MS EI+
1.70e4

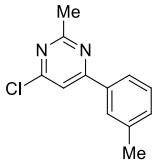


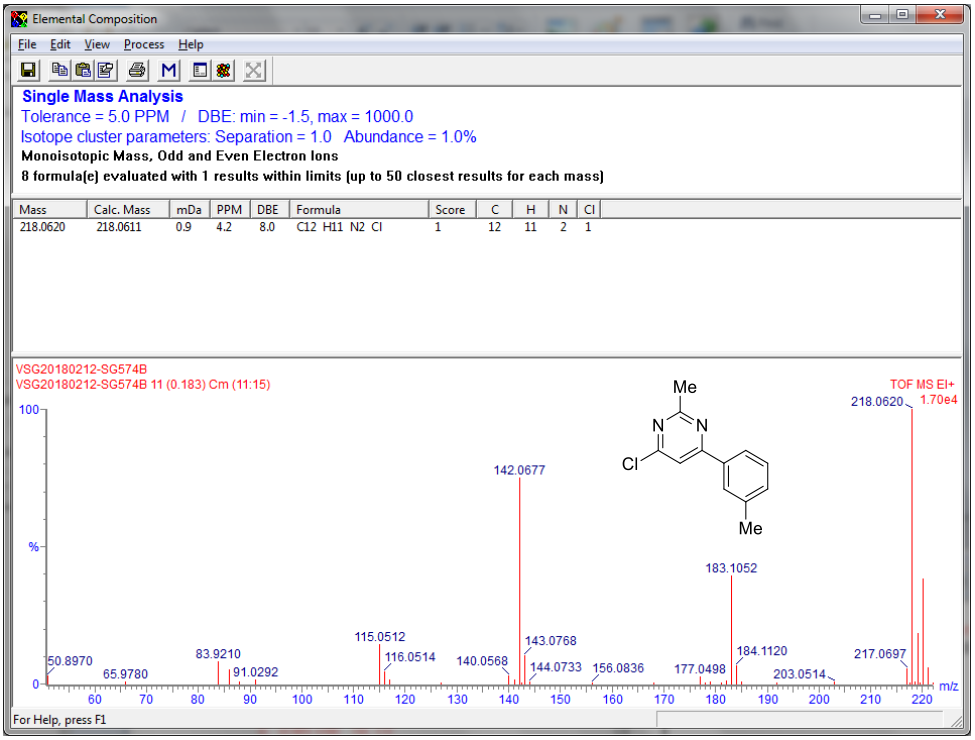
VSG20180212-SG574B

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

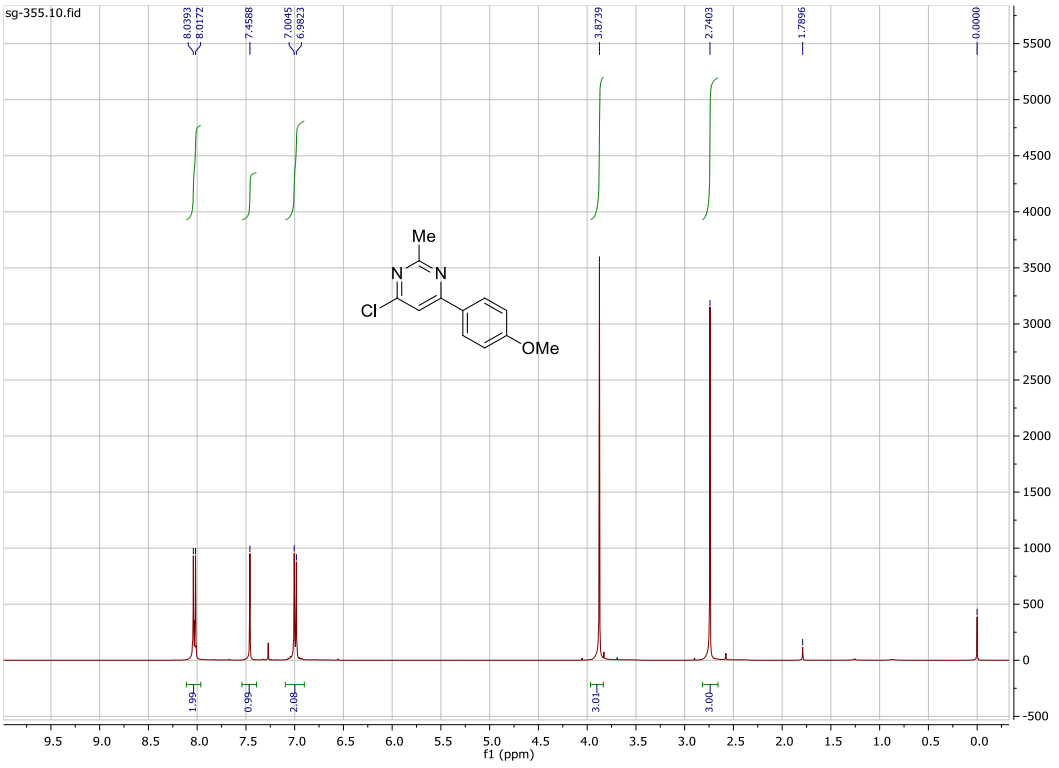
TOF MS EI+

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										

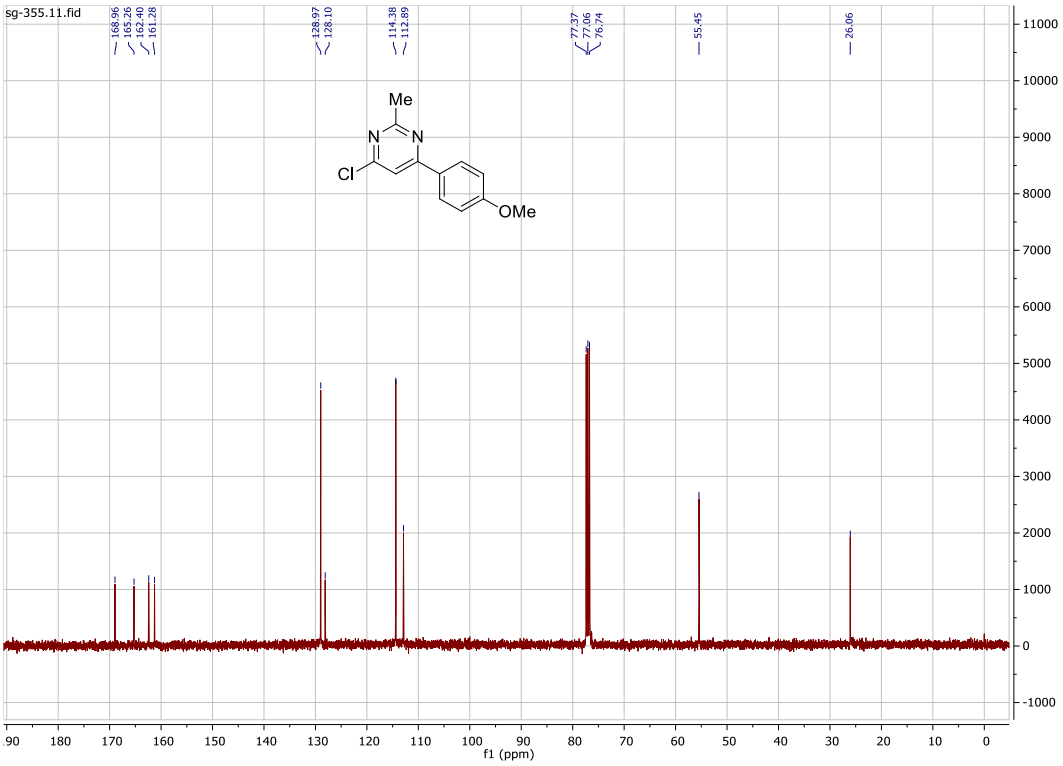




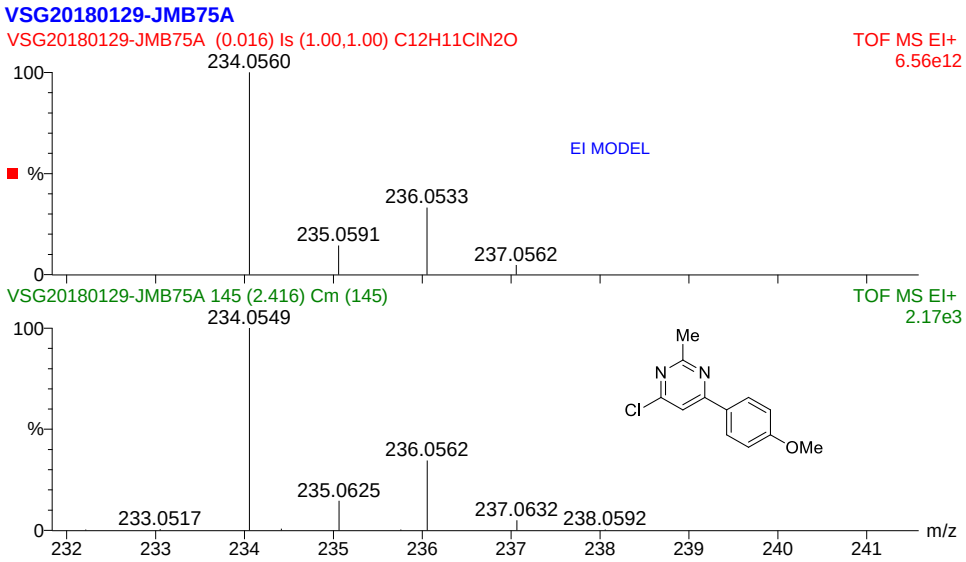
HRMS spectrum of **9c**

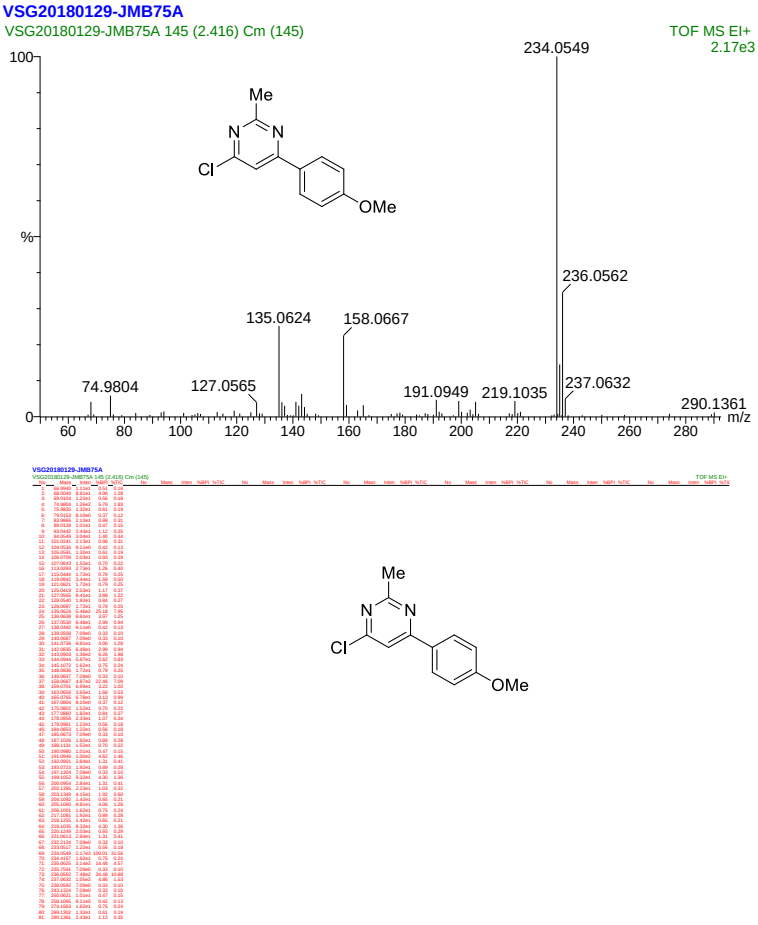


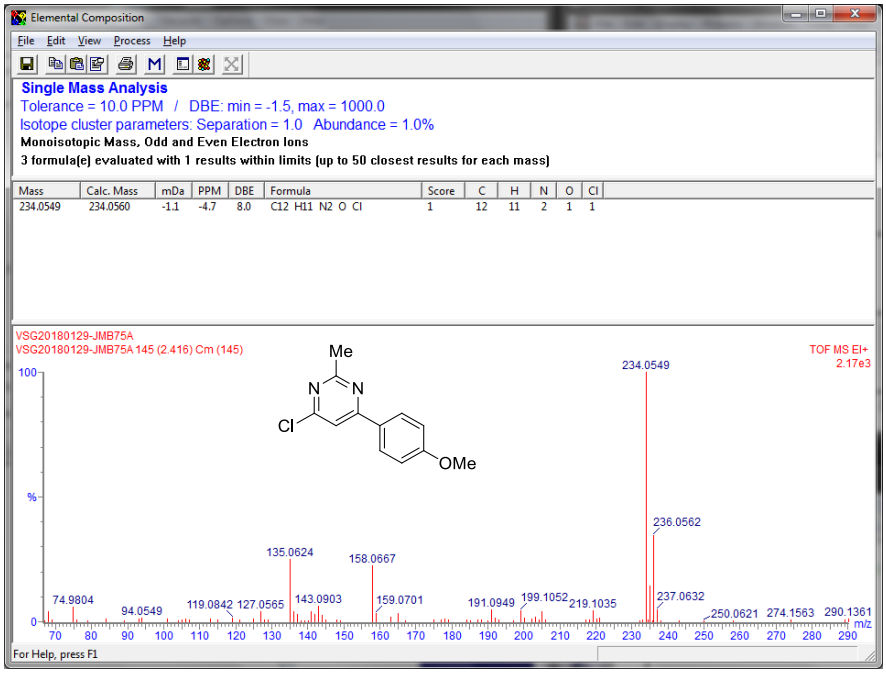
^{1}H NMR spectrum of **9d** (in $CDCl_3$)



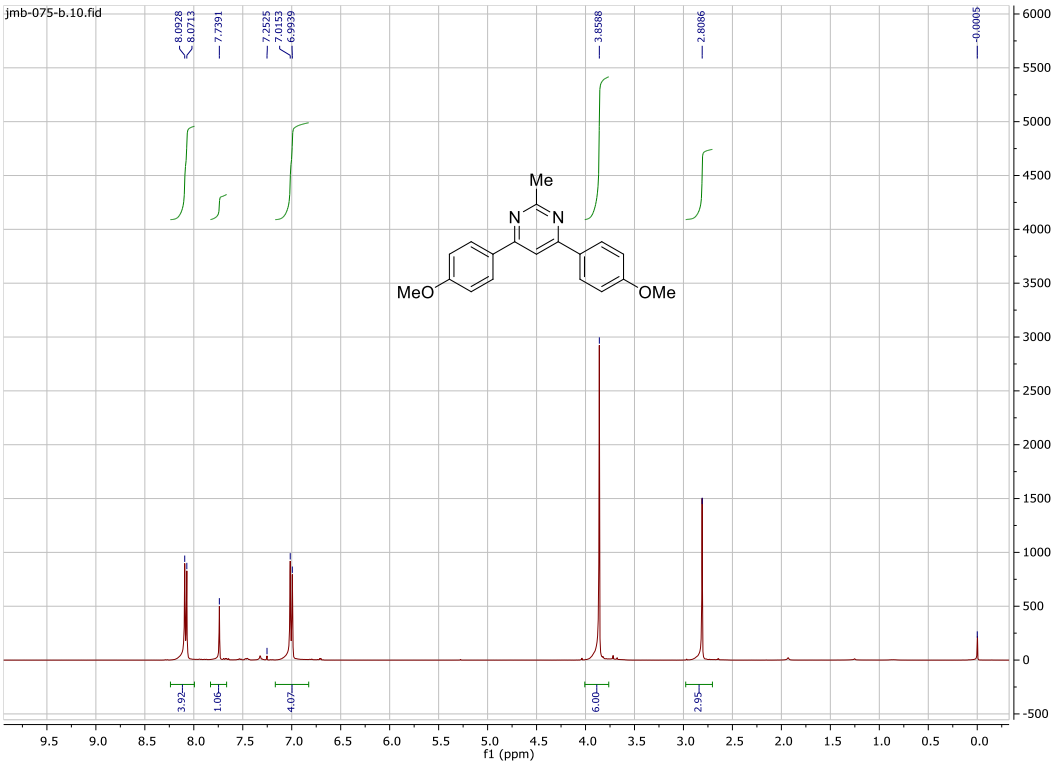
^{13}C NMR spectrum of **9d** (in $CDCl_3$)



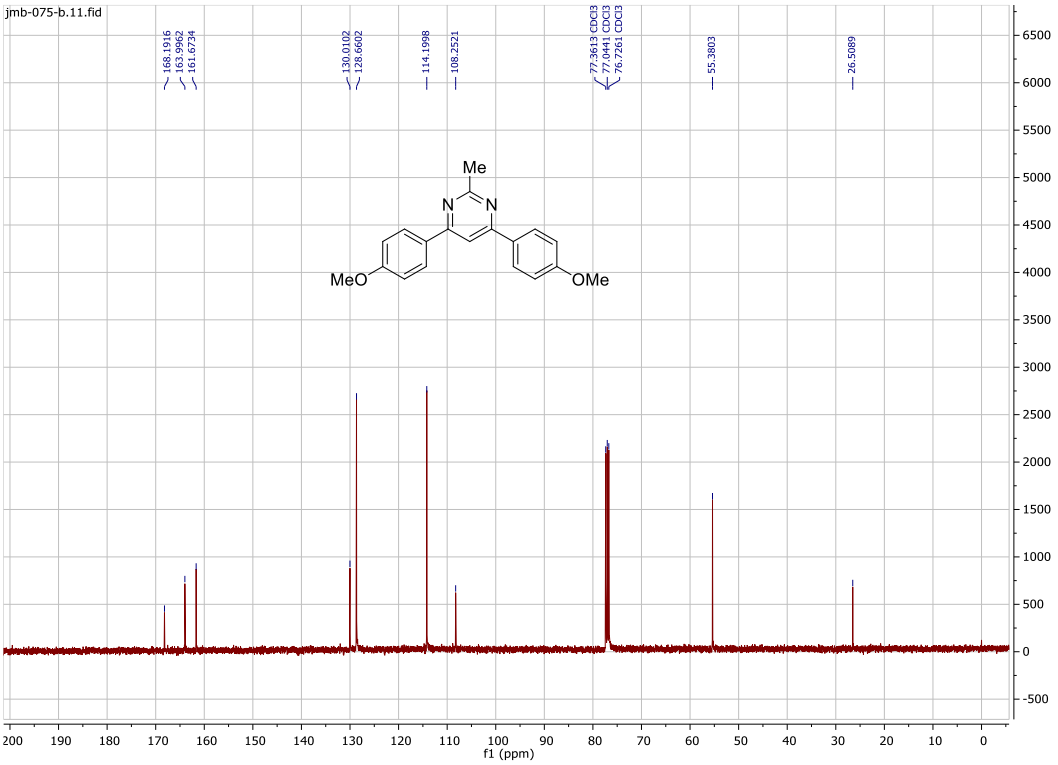




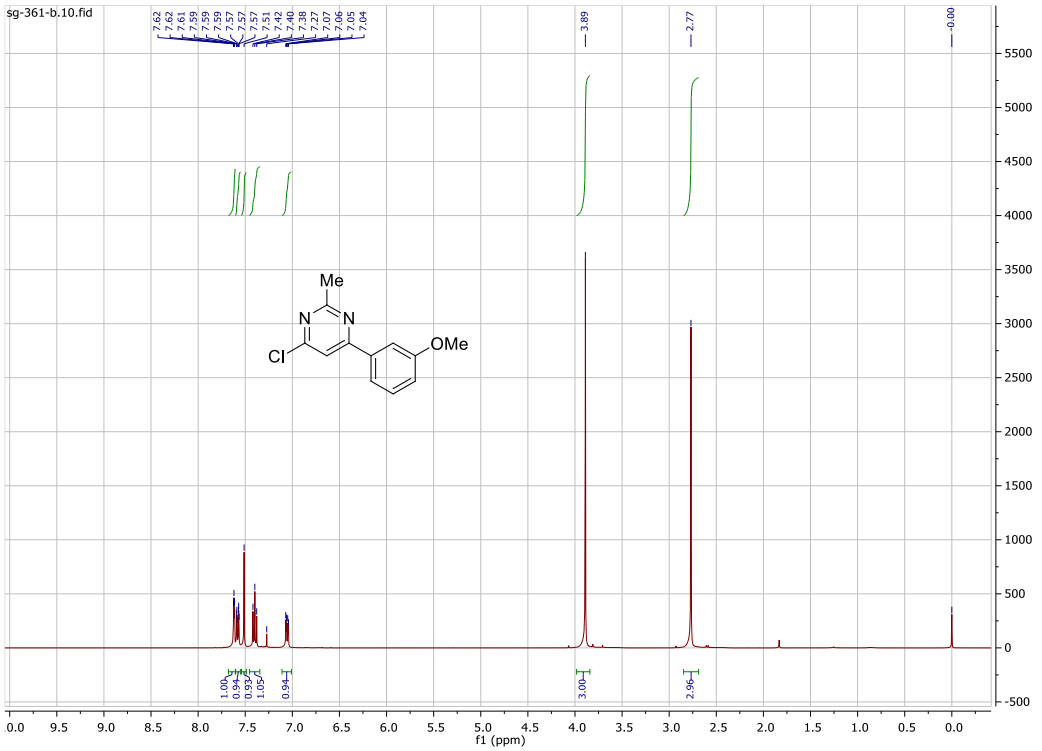
HRMS spectra of **9d**



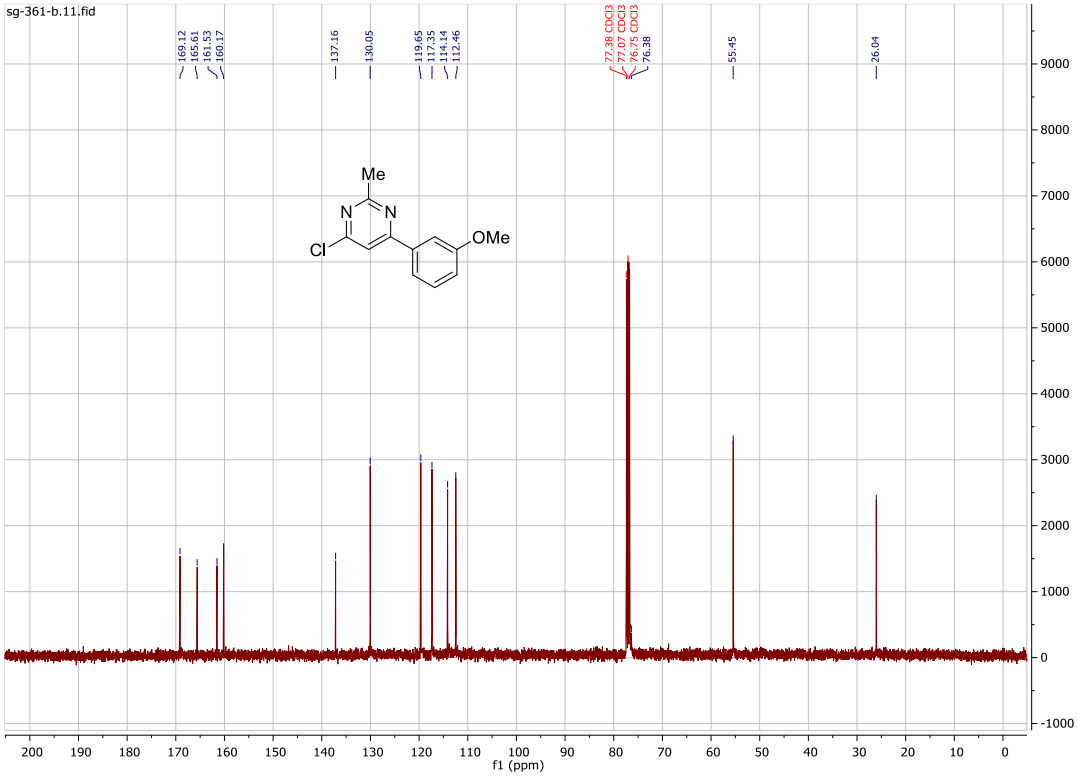
^{1}H NMR spectrum of **8d** (in $CDCl_3$)



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



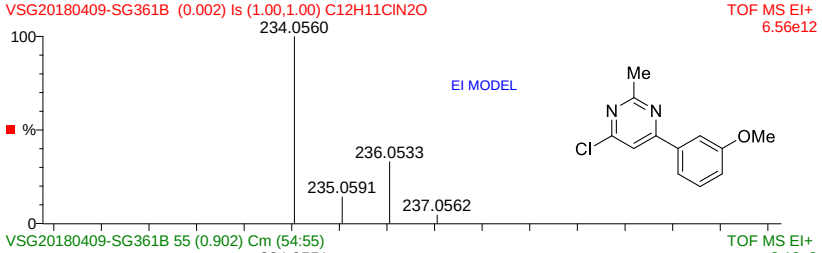
^{1}H NMR spectrum of **9e** (in $CDCl_3$)



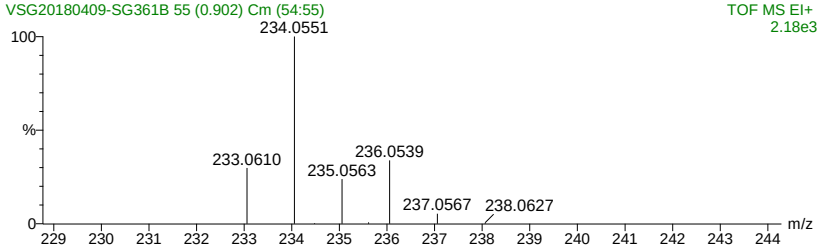
^{13}C NMR spectrum of **9e** (in $CDCl_3$)

VSG20180409-SG361B

VSG20180409-SG361B (0.002) Is (1.00,1.00) C12H11ClN2O — TOF MS EI+ 6.56e12

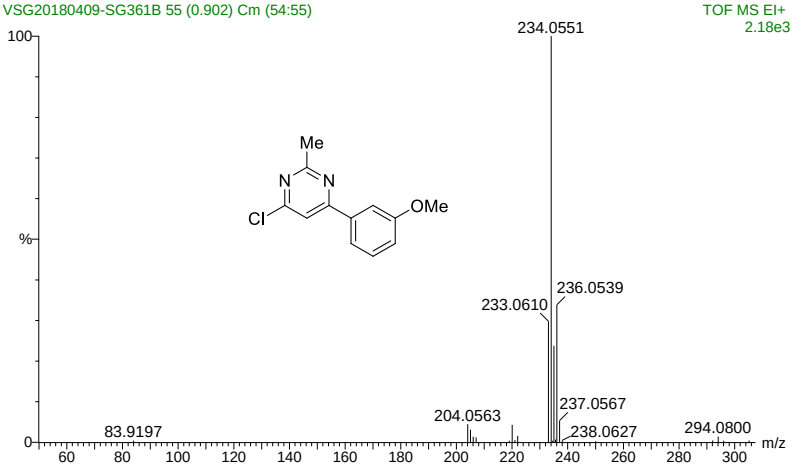


VSG20180409-SG361B 55 (0.902) Cm (54:55) — TOF MS EI+ 2.18e3



VSG20180409-SG361B

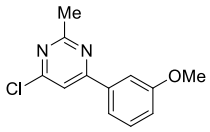
VSG20180409-SG361B 55 (0.902) Cm (54:55) — TOF MS EI+ 2.18e3

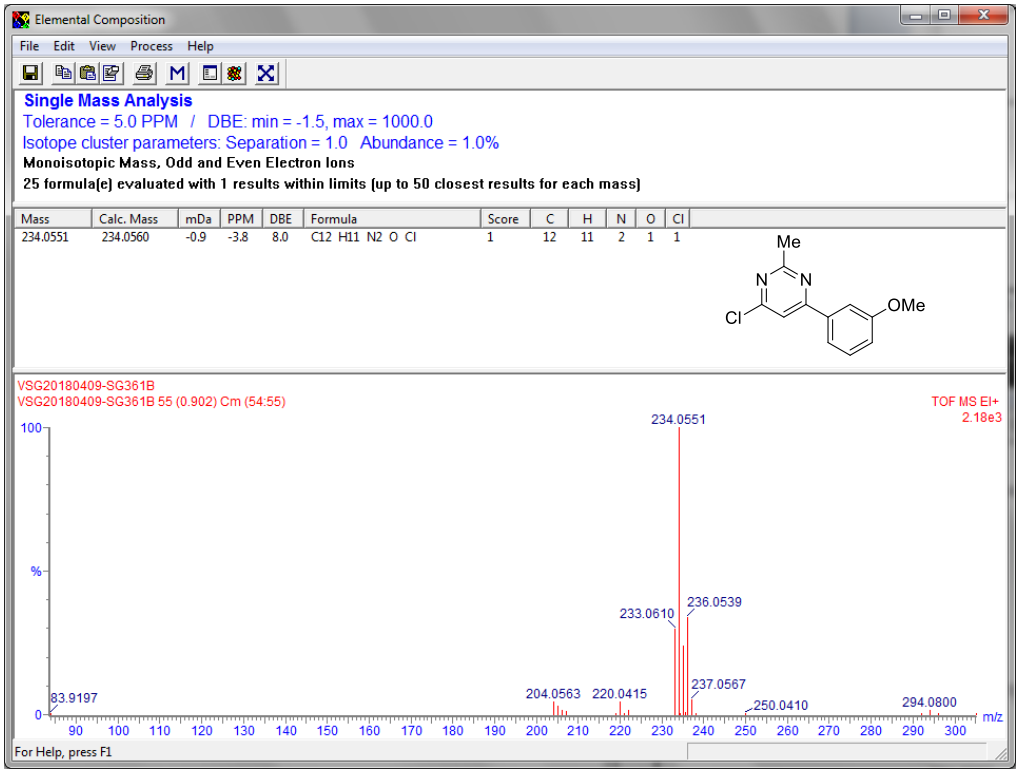


VSG20180409-SG361B

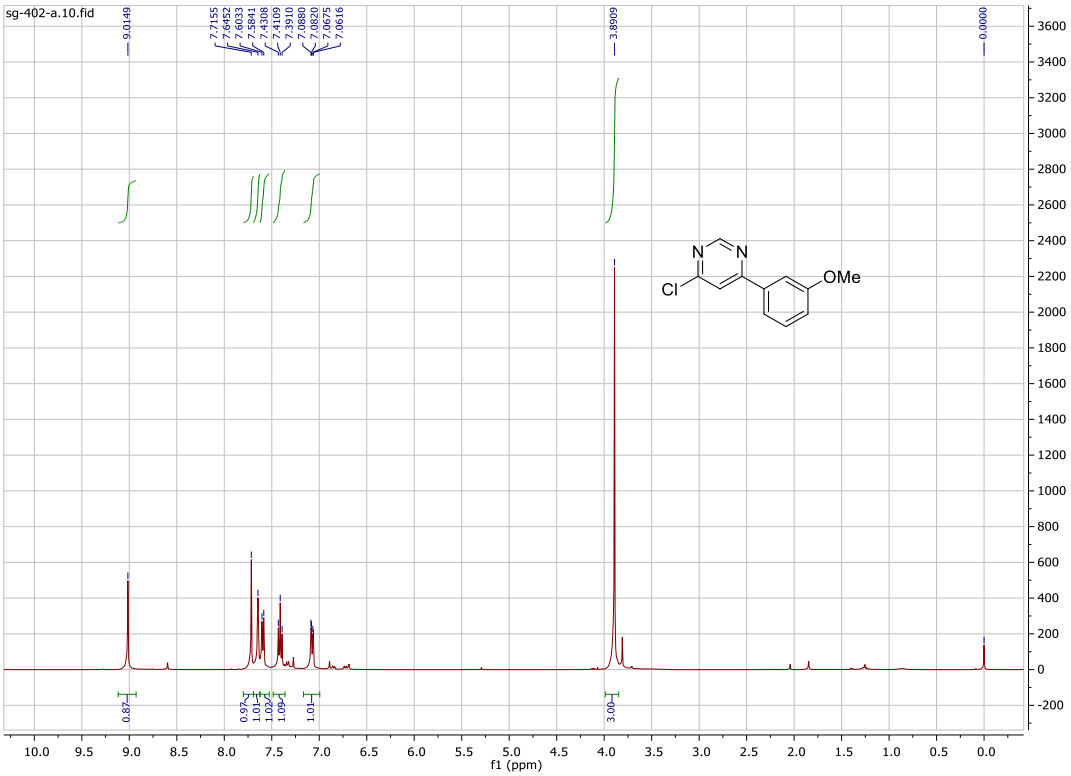
VSG20180409-SG361B 55 (0.902) Cm (54:55) — TOF MS EI+

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										

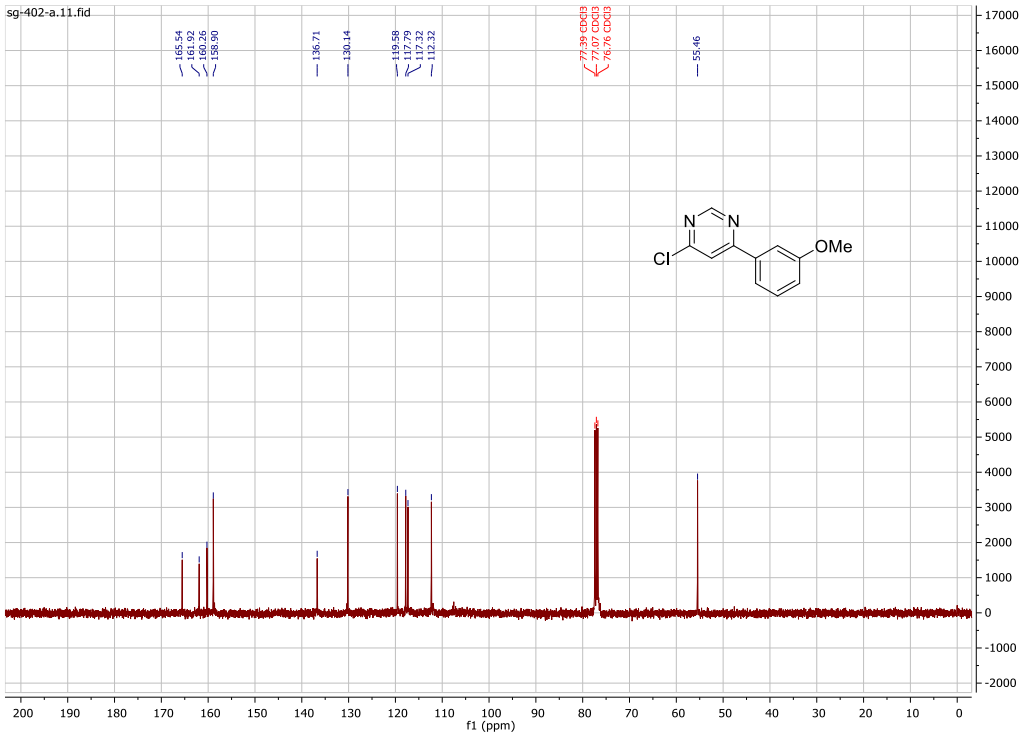




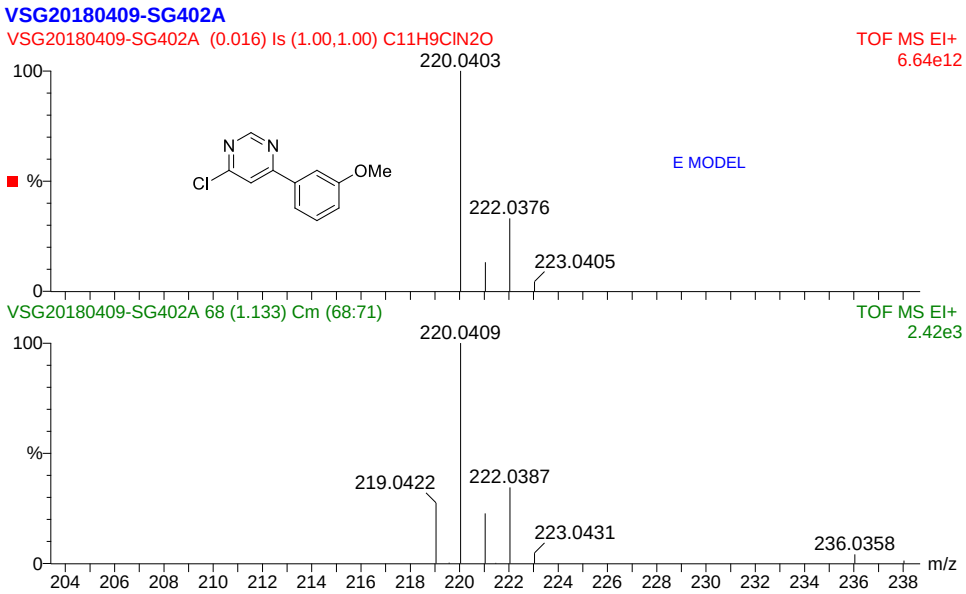
HRMS spectra of **9e**



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



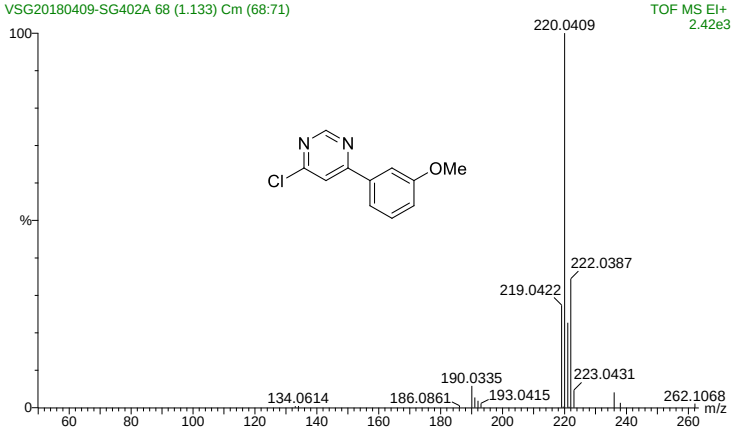
^{13}C NMR spectrum of **9f** (in $CDCl_3$)



VSG20180409-SG402A

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

TOF MS EI+
2.42e3

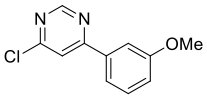


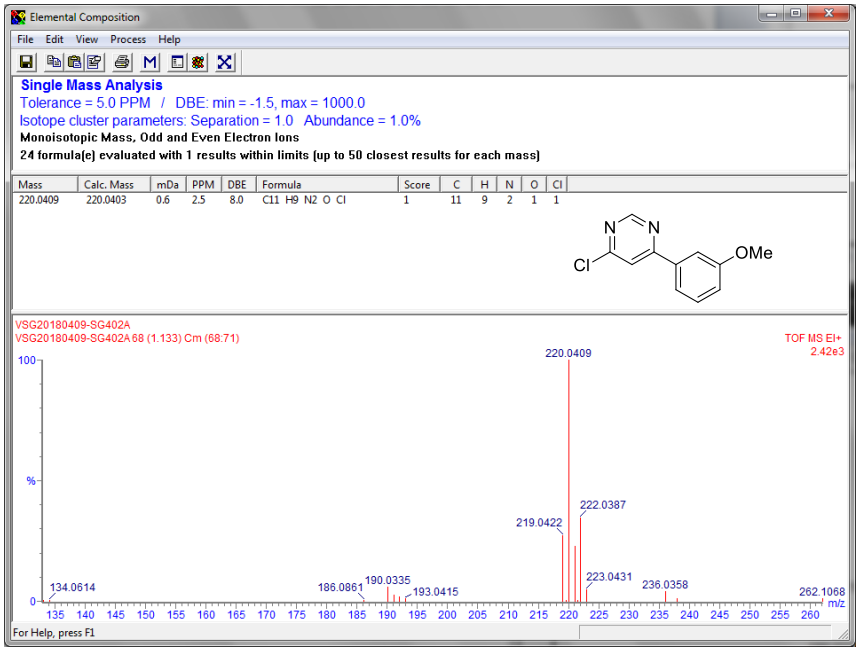
VSG20180409-SG402A

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

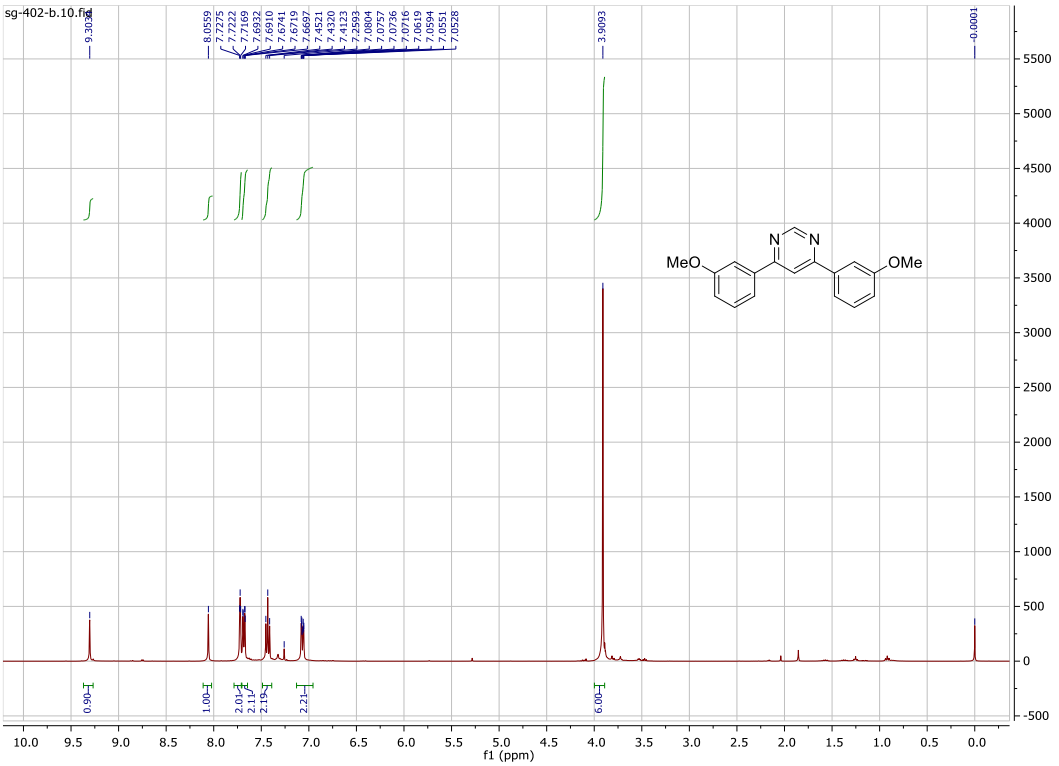
TOF MS EI+

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										

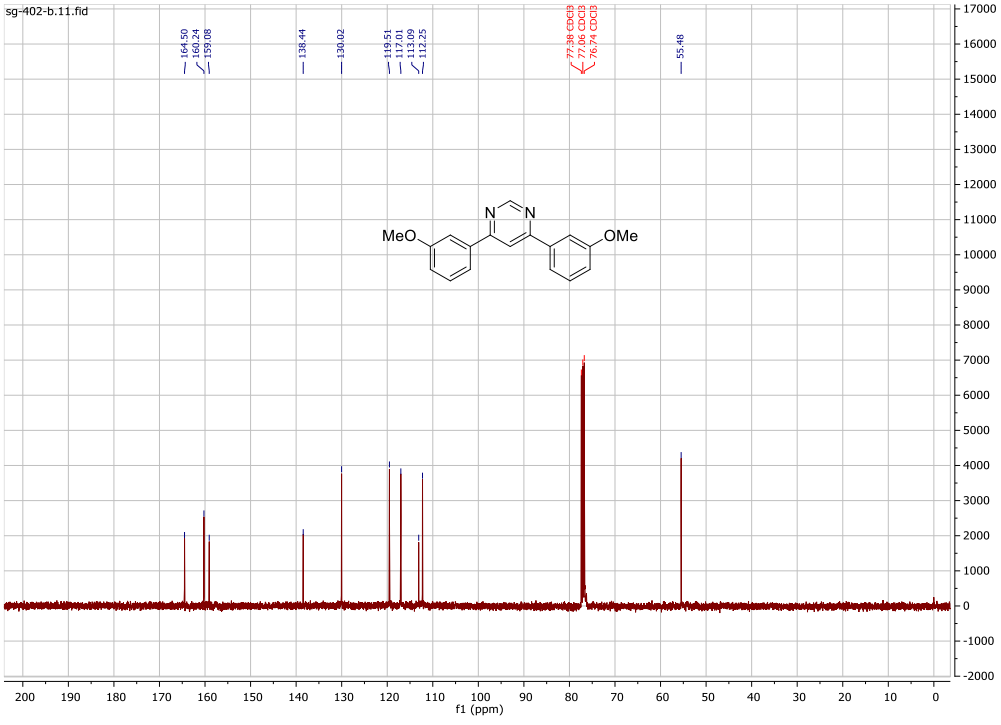




HRMS spectra of **9f**



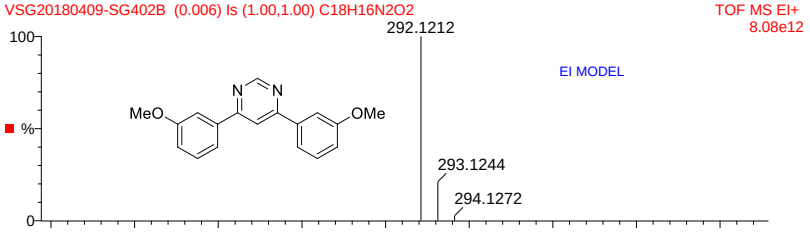
^{1}H NMR spectrum of **8f** (in $CDCl_3$)



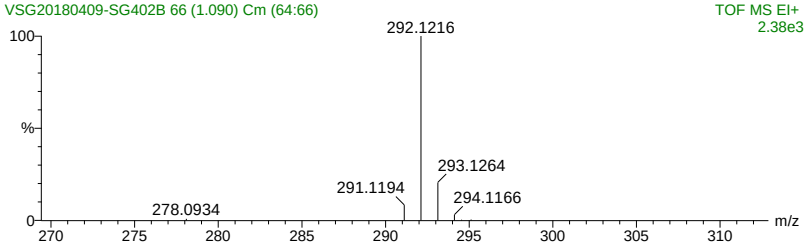
^{13}C NMR spectrum of **8f** (in $CDCl_3$)

VSG20180409-SG402B

VSG20180409-SG402B (0.006) Is (1.00,1.00) C18H16N2O2 — TOF MS EI+ 8.08e12

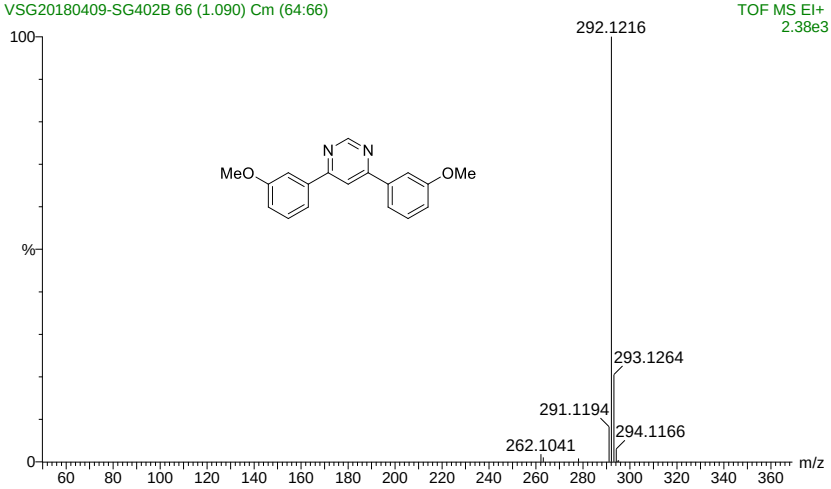


VSG20180409-SG402B 66 (1.090) Cm (64:66) — TOF MS EI+ 2.38e3



VSG20180409-SG402B

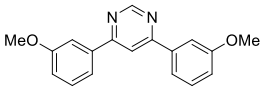
VSG20180409-SG402B 66 (1.090) Cm (64:66) — TOF MS EI+ 2.38e3

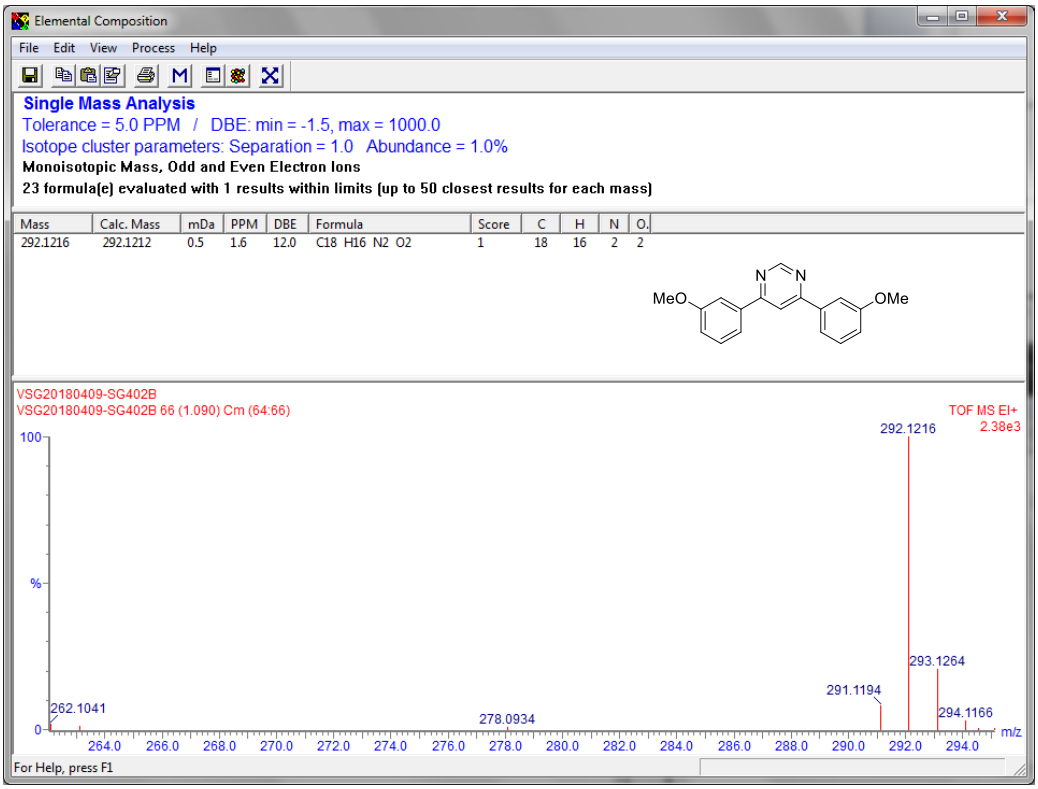


VSG20180409-SG402B

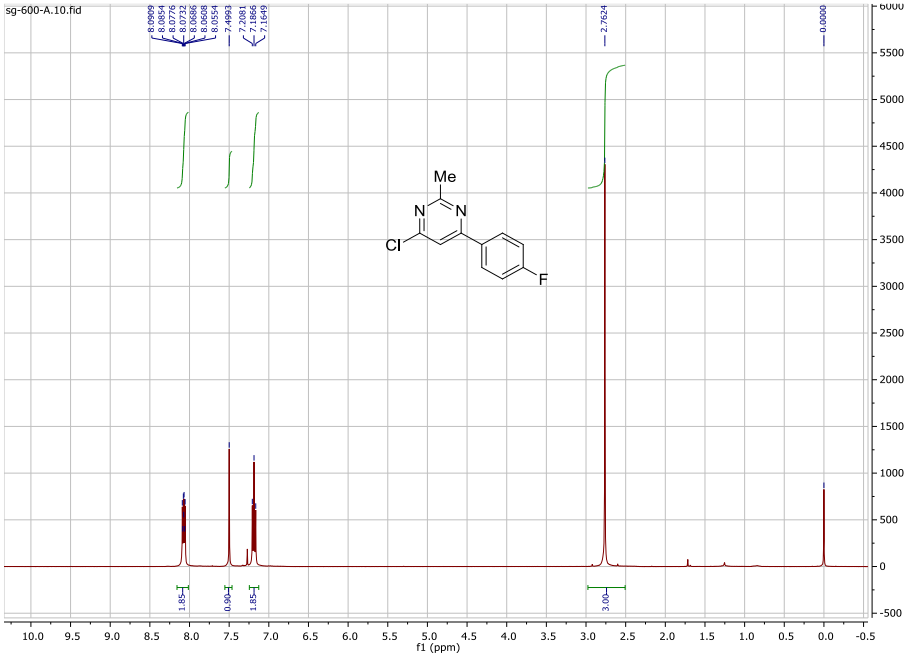
VSG20180409-SG402B 66 (1.090) Cm (64:66) — TOF MS EI+

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										

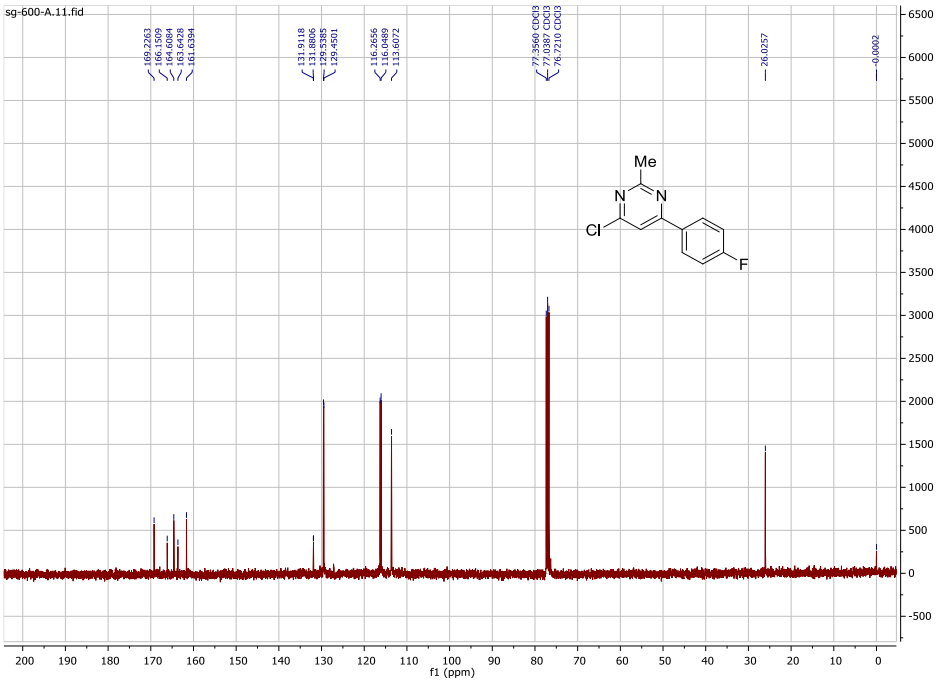




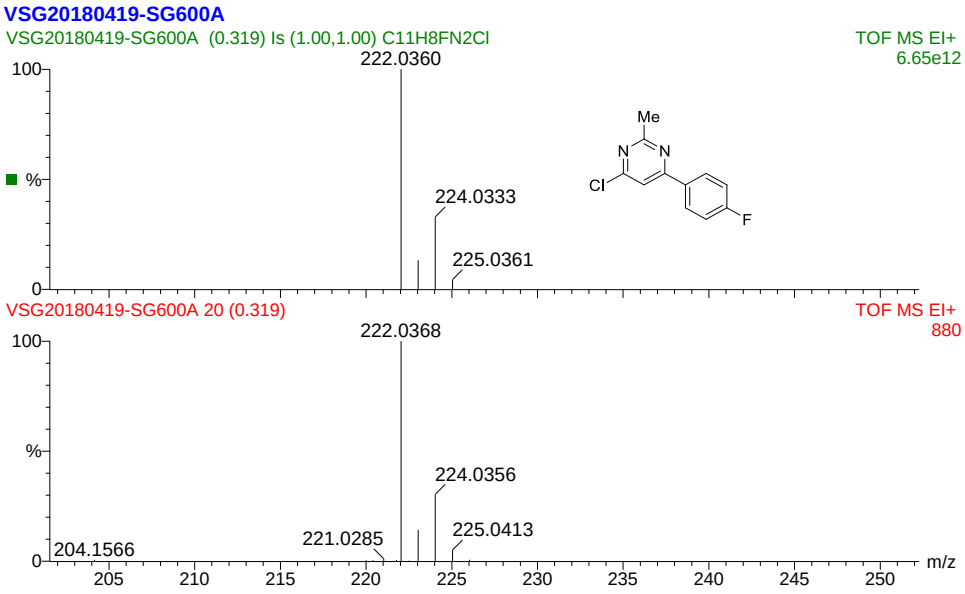
HRMS spectra of **8f**



^{1}H NMR spectrum of **9g** (in $CDCl_3$)



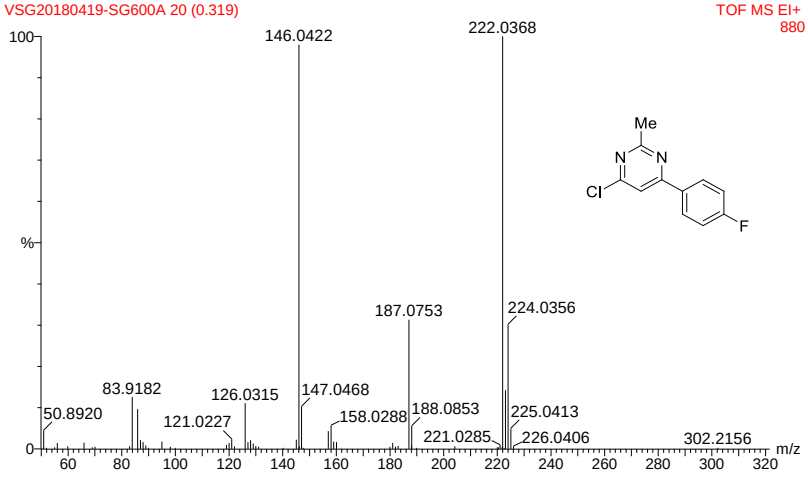
^{13}C NMR spectrum of **9g** (in $CDCl_3$)



VSG20180419-SG600A

VSG20180419-SG600A 20 (0.319)

TOF MS EI+
880

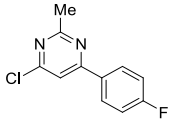


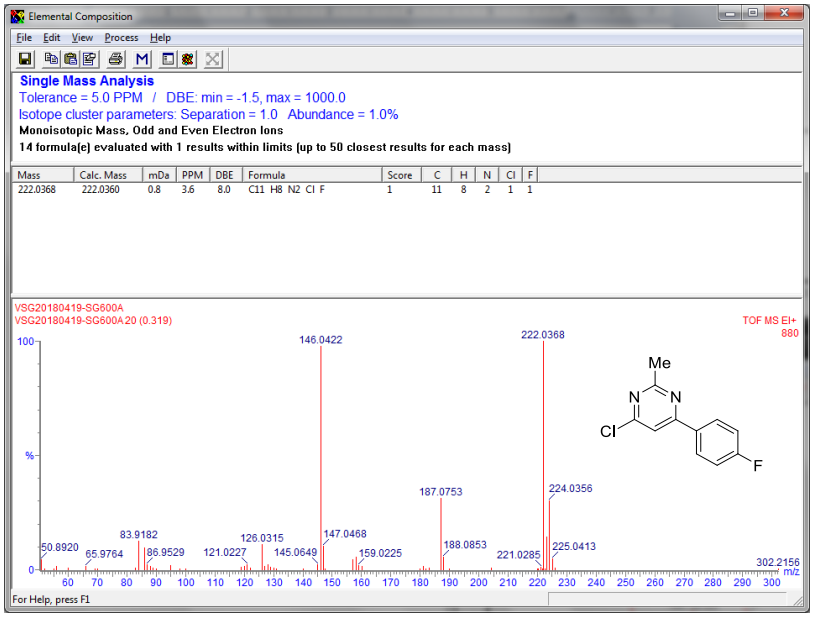
VSG20180419-SG600A

VSG20180419-SG600A 20 (0.319)

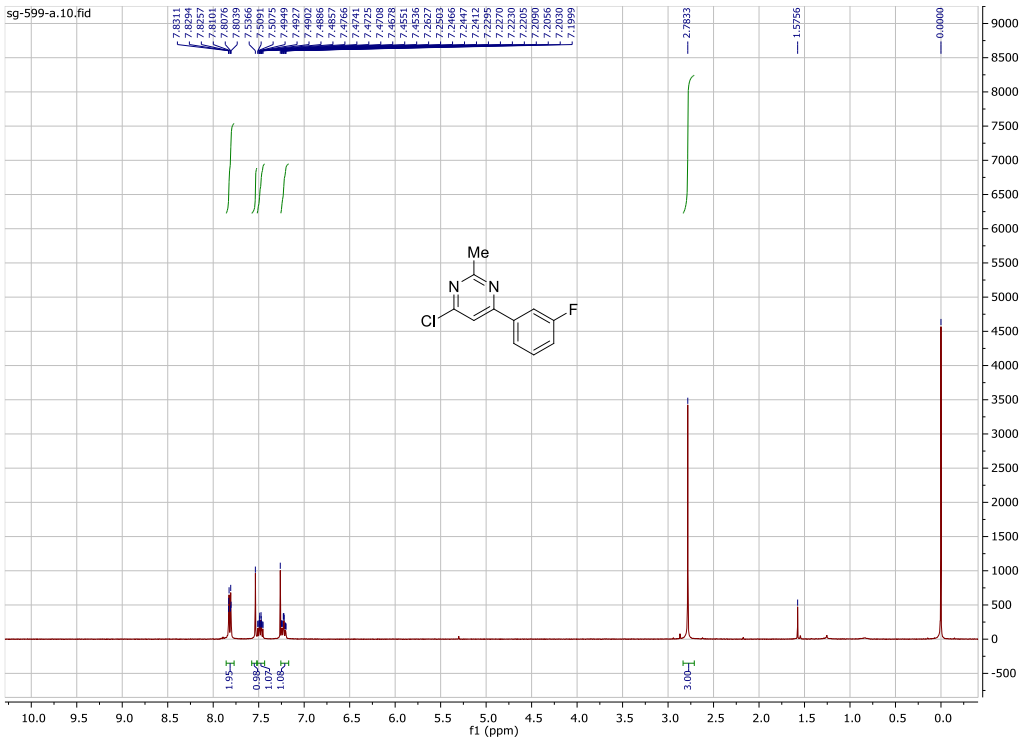
TOF MS EI+

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										

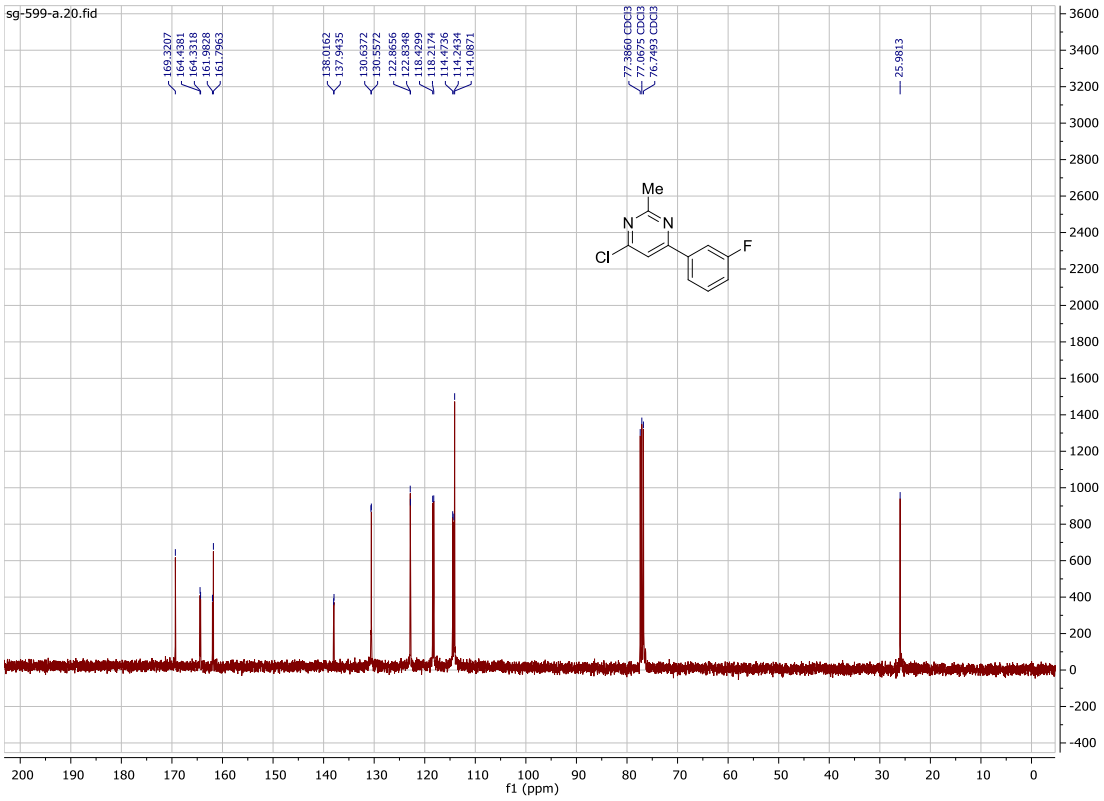




HRMS spectra of **9g**



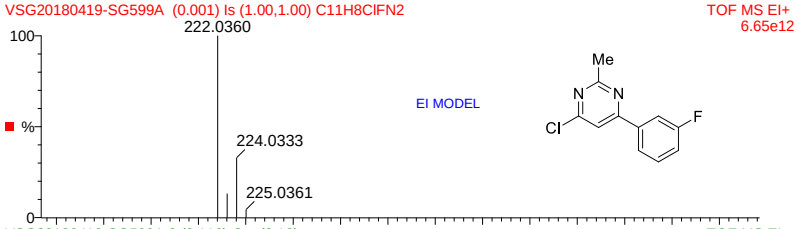
^{1}H NMR spectrum of **9h** (in $CDCl_3$)



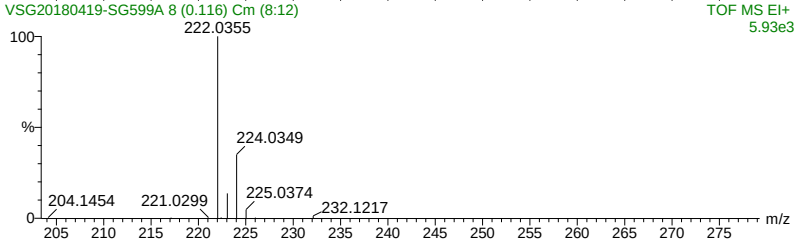
^{13}C NMR spectrum of **9h** (in $CDCl_3$)

VSG20180419-SG599A

VSG20180419-SG599A (0.001) Is (1.00,1.00) C11H8ClFN2 — TOF MS EI+ 6.65e12

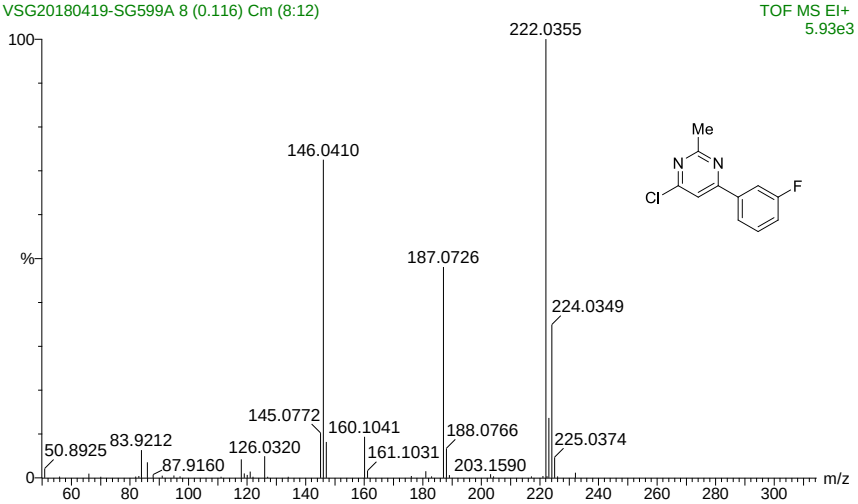


VSG20180419-SG599A 8 (0.116) Cm (8:12) — TOF MS EI+ 5.93e3



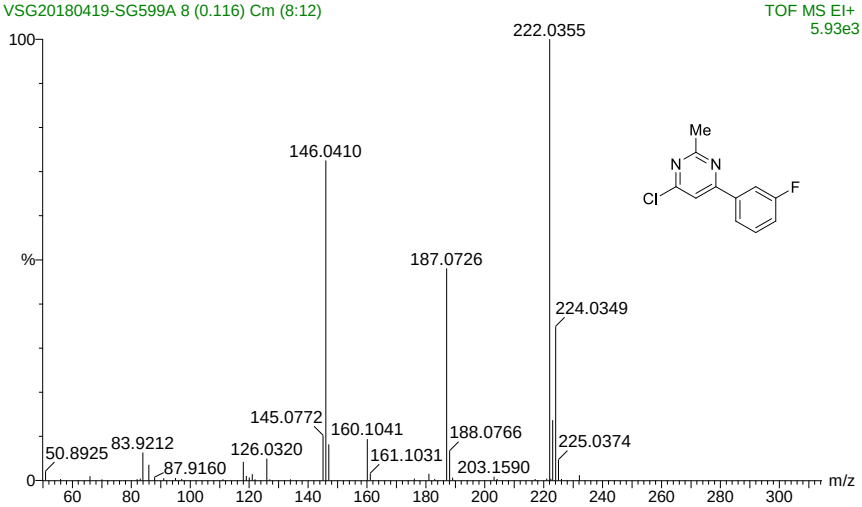
VSG20180419-SG599A

VSG20180419-SG599A 8 (0.116) Cm (8:12) — TOF MS EI+ 5.93e3



VSG20180419-SG599A

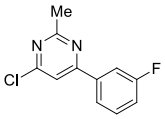
VSG20180419-SG599A 8 (0.116) Cm (8:12) — TOF MS EI+ 5.93e3

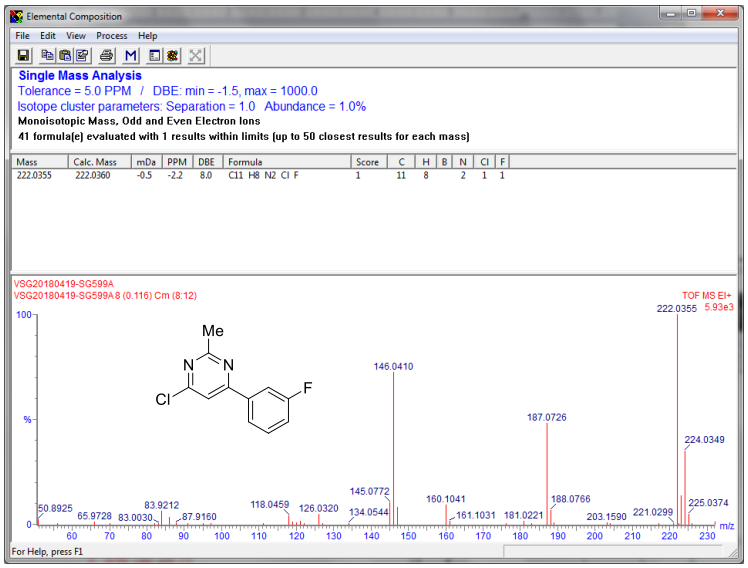


VSG20180419-SG599A

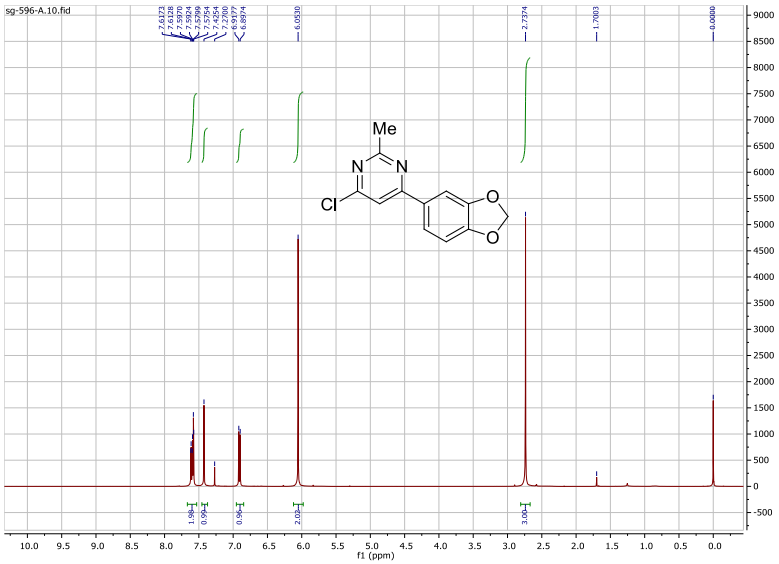
VSG20180419-SG599A 8 (0.116) Cm (8:12) TOF MS EI+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	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	4.65	1.33					
12:	97.0827	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										

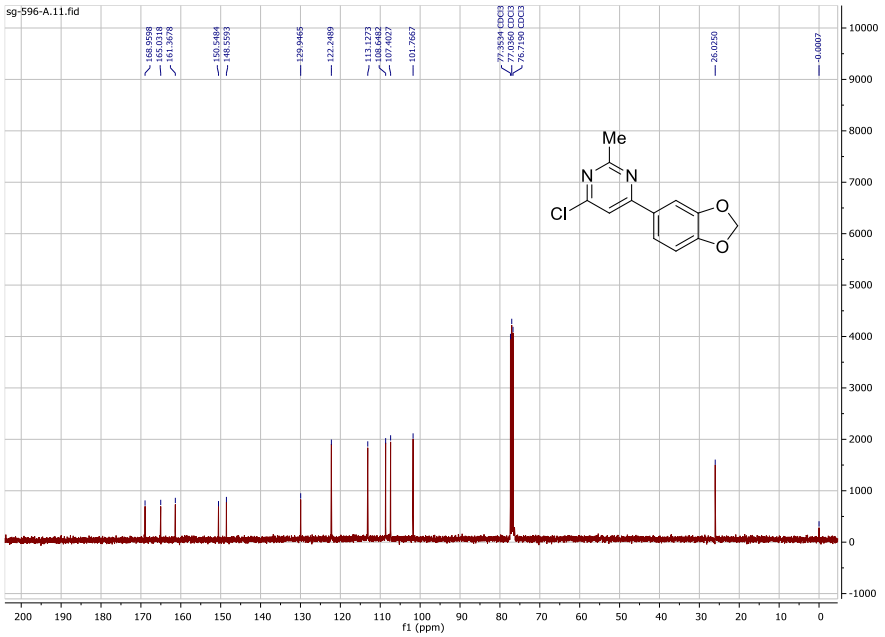




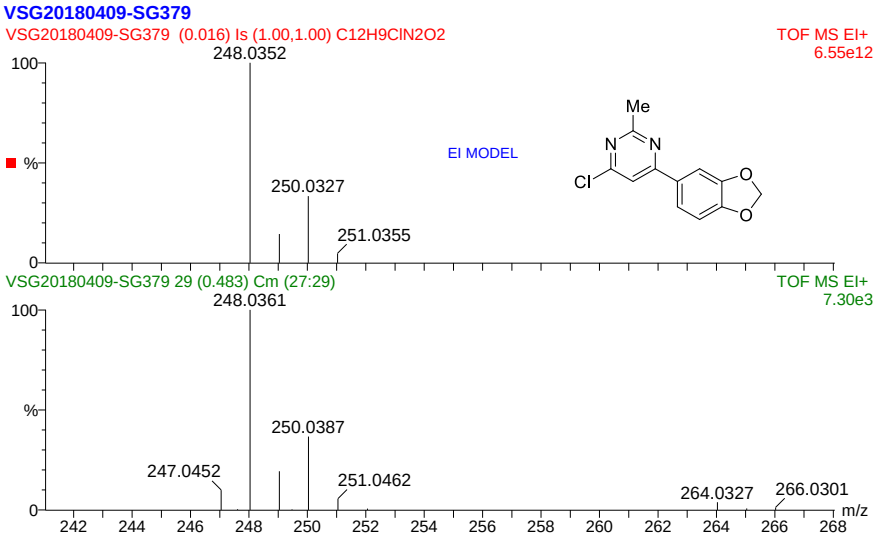
HRMS spectra of **9h**

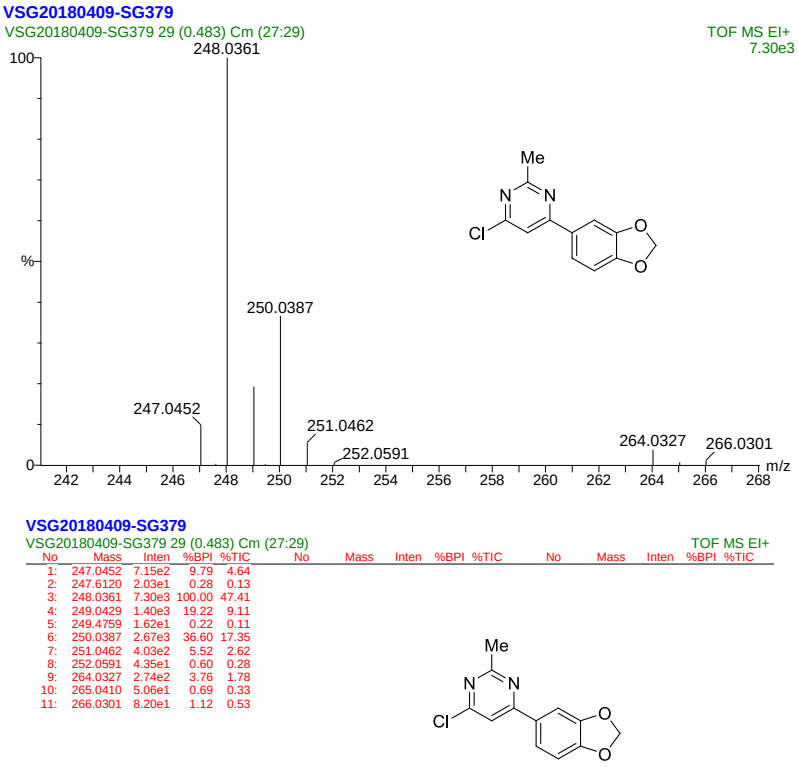


^{1}H NMR spectrum of **9i** (in $CDCl_3$)



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

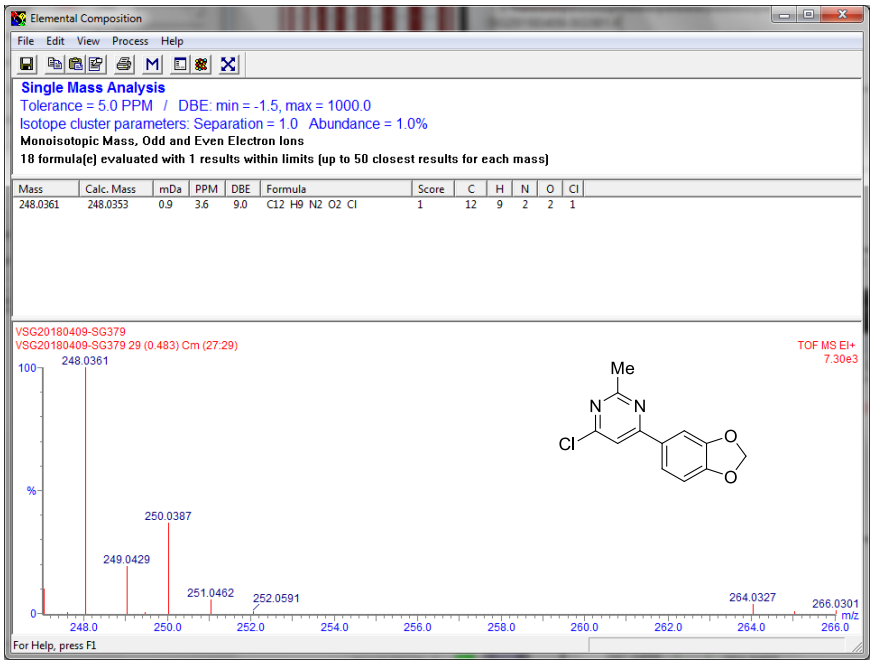




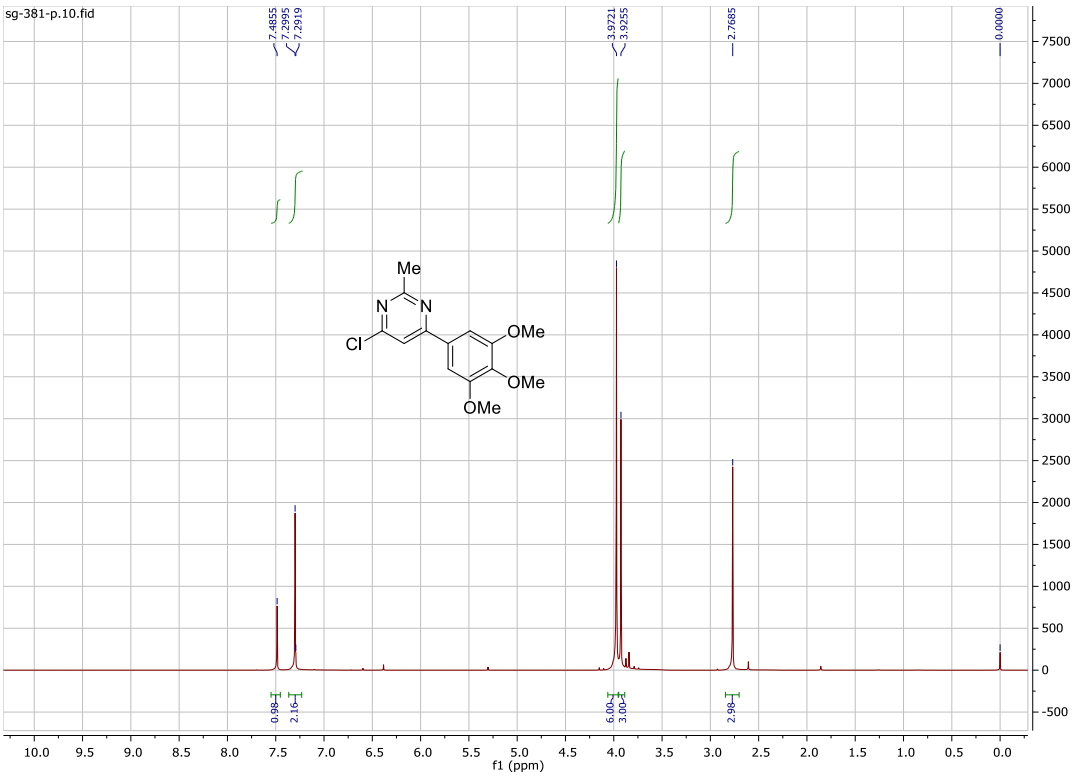
VSG20180409-SG379

VSG20180409-SG379 29 (0.483) Cm (27:29) TOF MS EI+

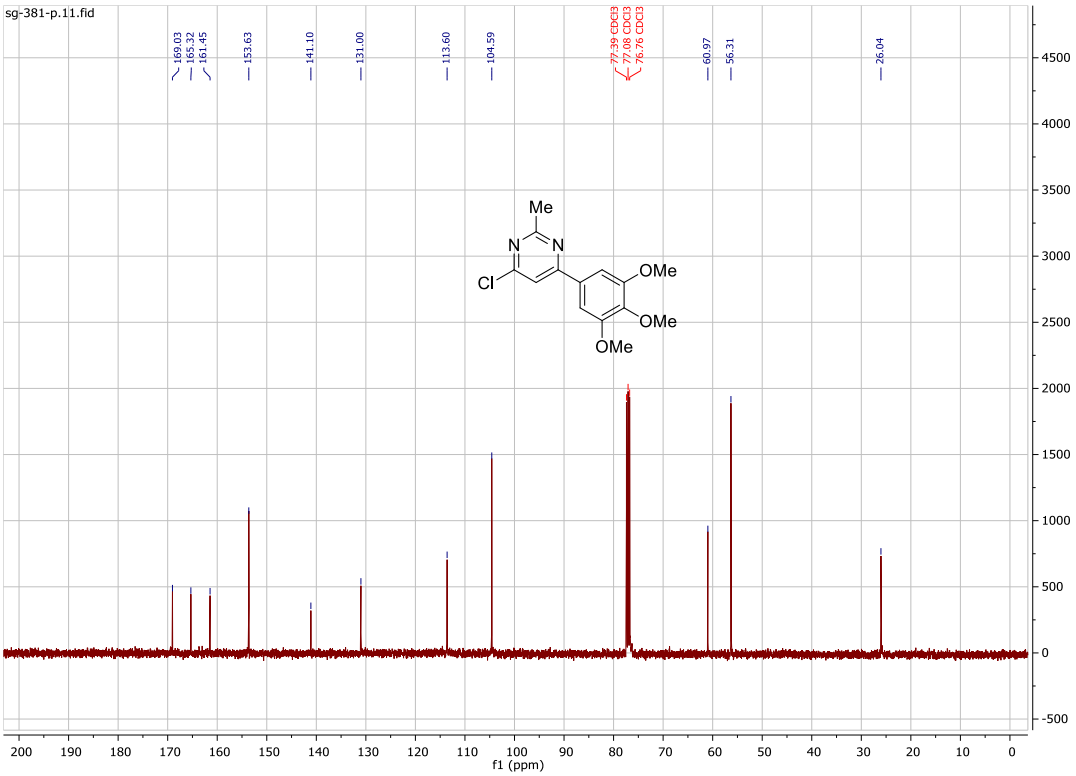
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	247.0452	7.15e2	9.79	4.64										
2:	247.6120	2.03e1	0.28	0.13										
3:	248.0361	7.30e3	100.00	47.41										
4:	249.0429	1.40e3	19.22	9.11										
5:	249.4759	1.62e1	0.22	0.11										
6:	250.0387	2.67e3	36.60	17.35										
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**



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

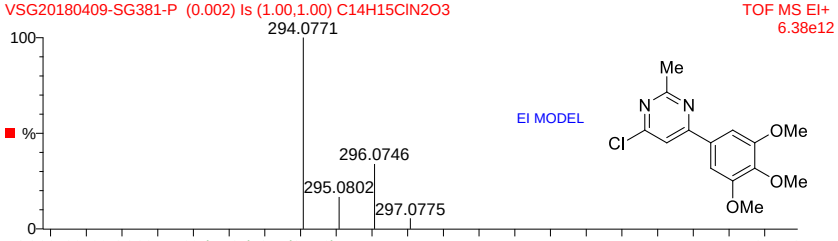


^{13}C NMR spectrum of **9j** (in $CDCl_3$)

VSG20180409-SG381-P

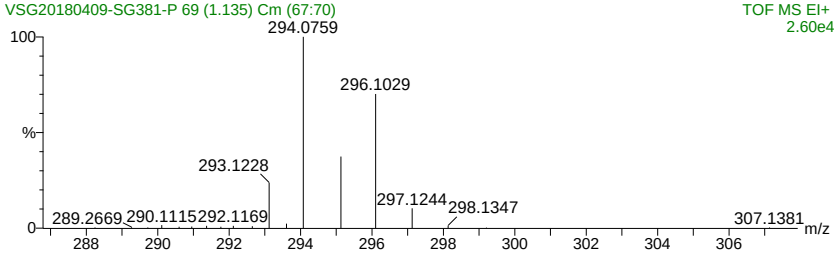
VSG20180409-SG381-P (0.002) Is (1.00,1.00) C14H15ClN2O3

TOF MS EI+
6.38e12



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

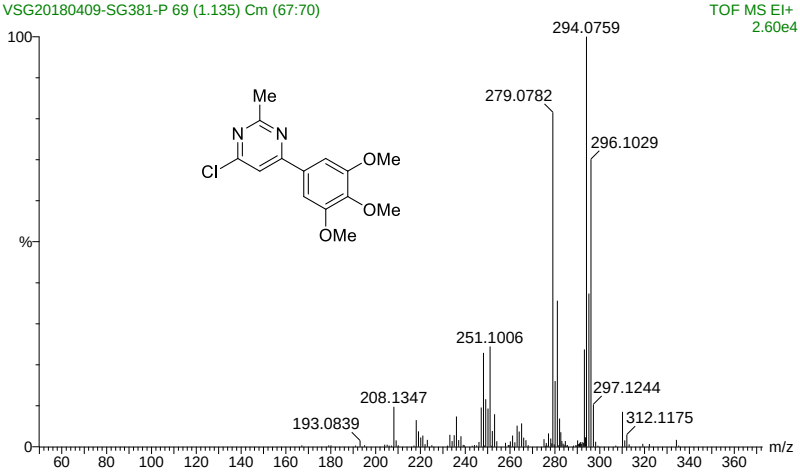
TOF MS EI+
2.60e4

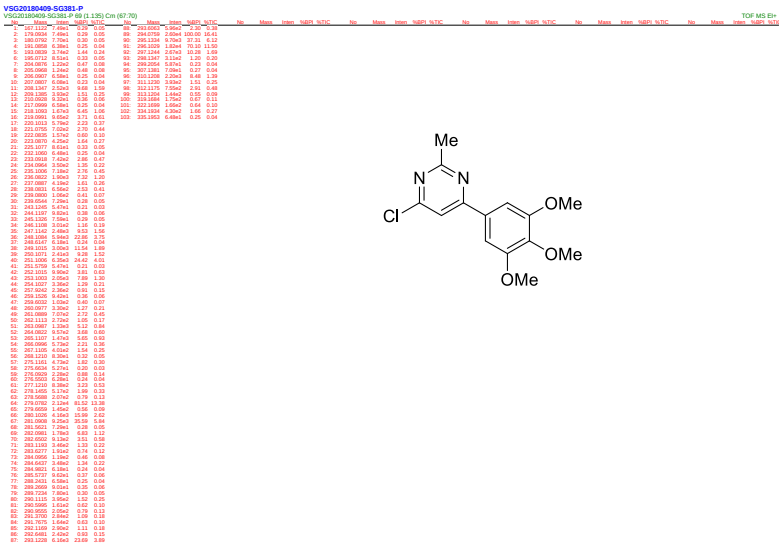


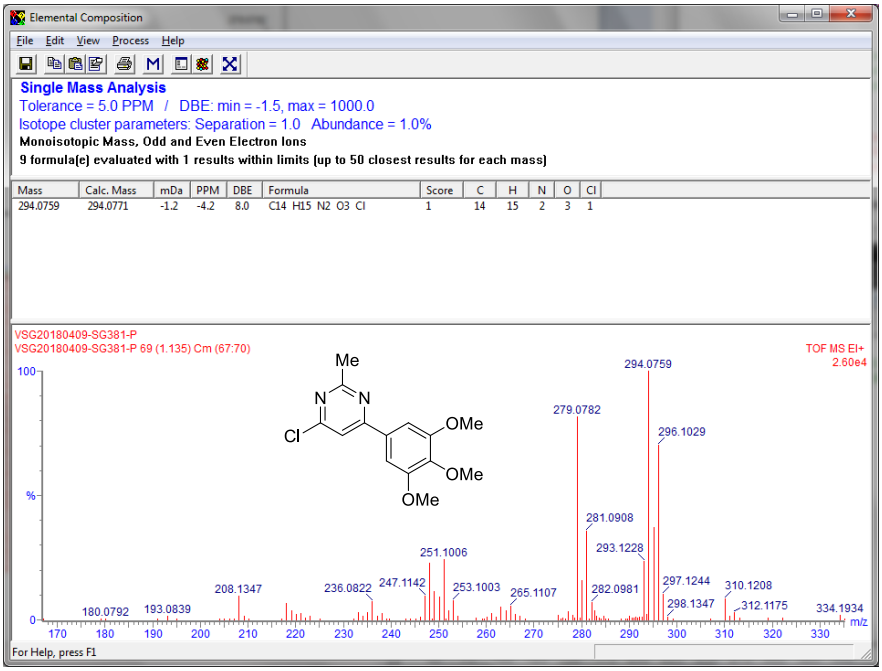
VSG20180409-SG381-P

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

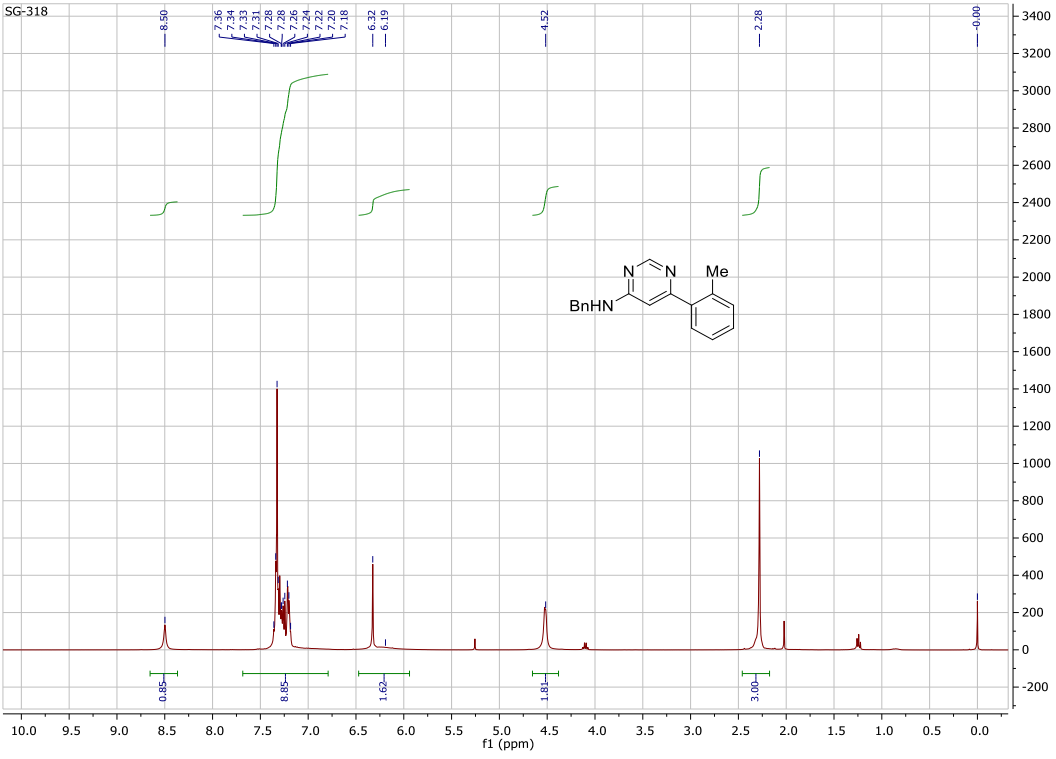
TOF MS EI+
2.60e4





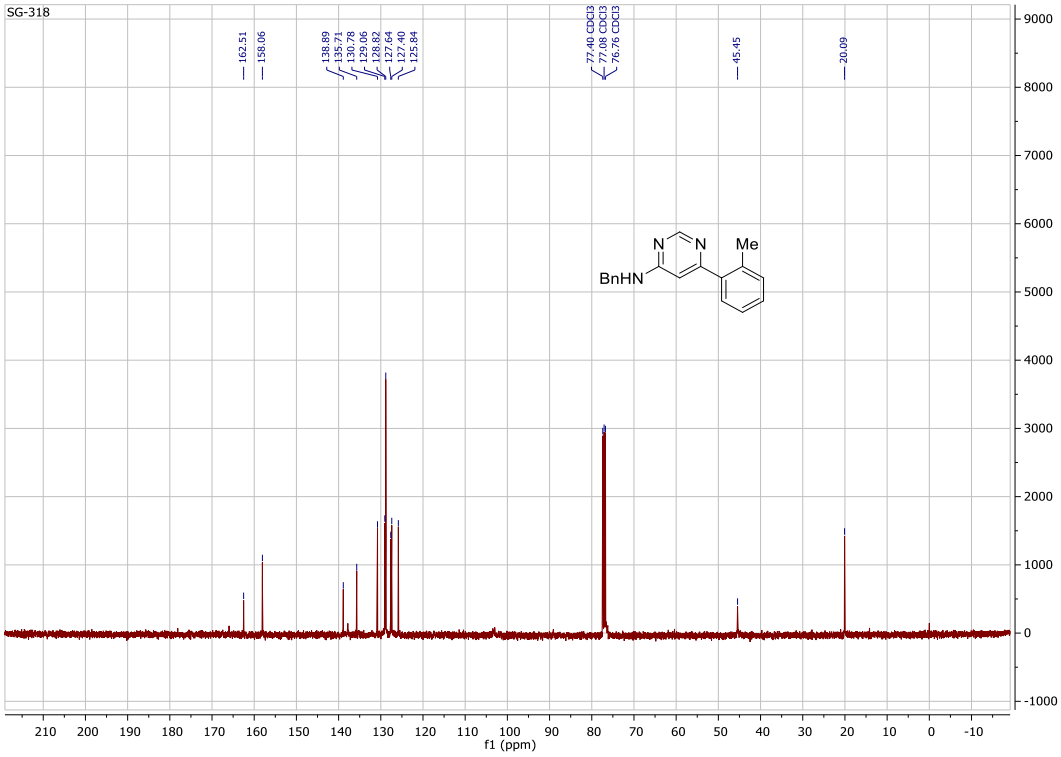


HRMS spectra of **9j**

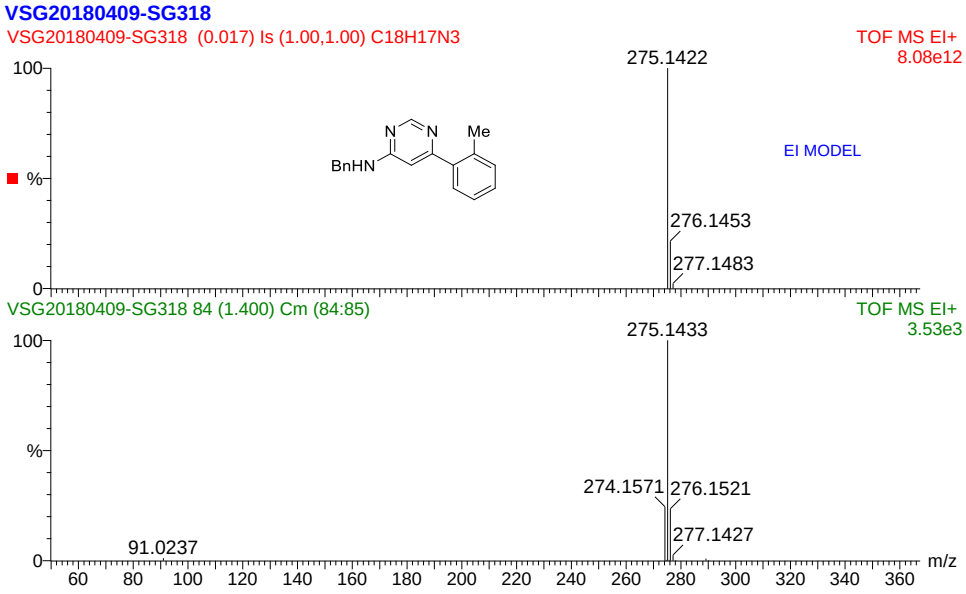


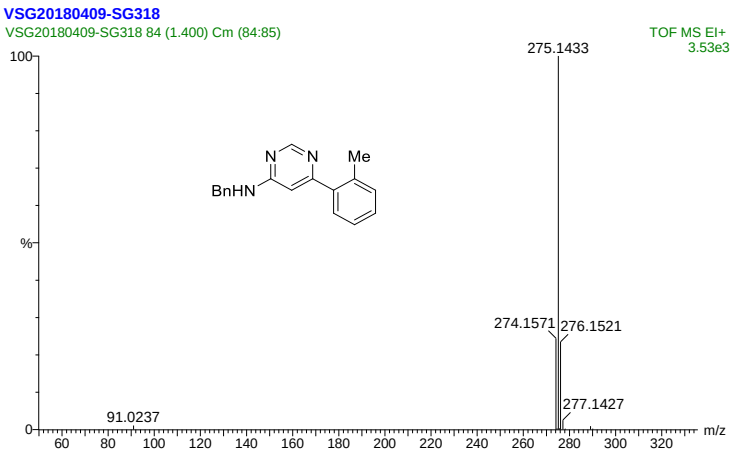
^{1}H NMR spectrum of **15a** (in $CDCl_3$)

OMe



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

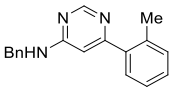


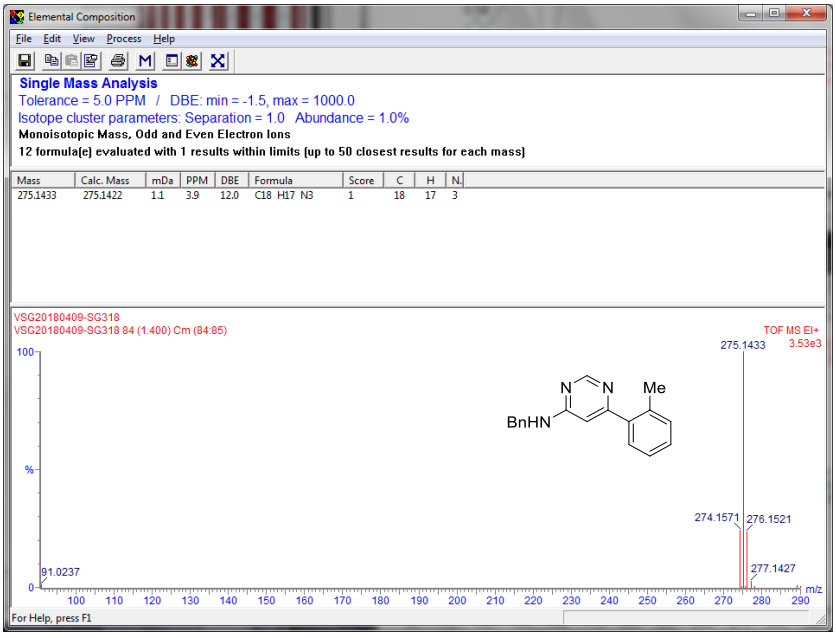


VSG20180409-SG318

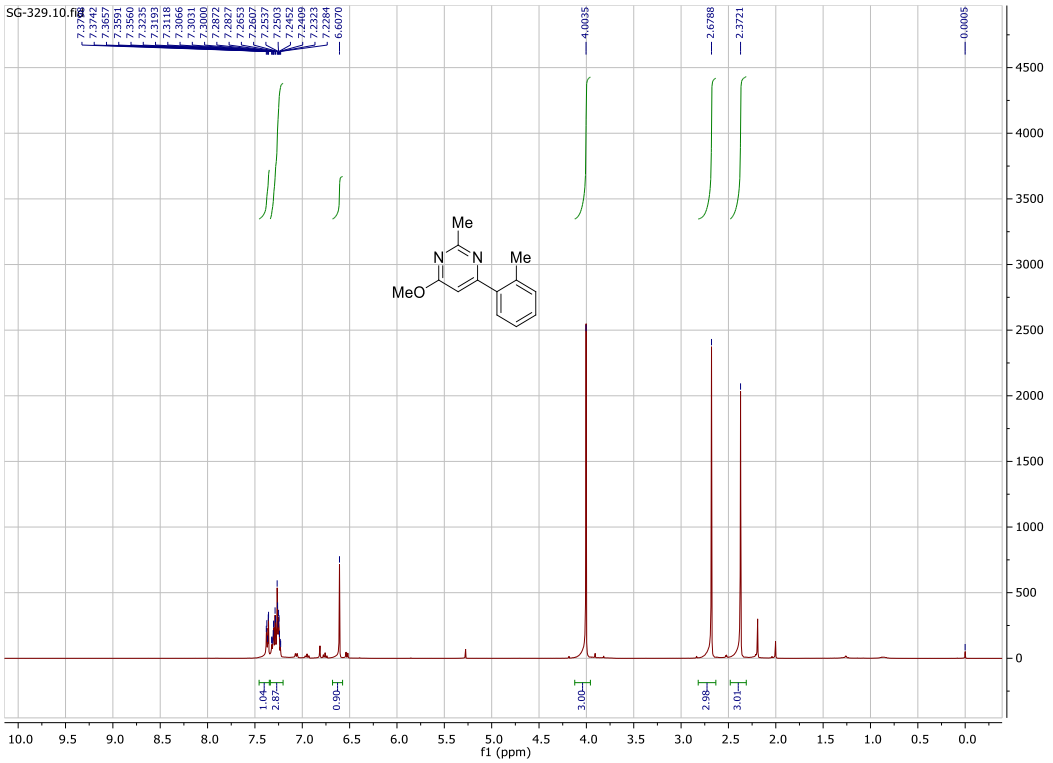
VSG20180409-SG318 84 (1.400) Cm (84:85) TOF MS EI+

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	3.14e1	0.89	0.57										
10:	290.1085	7.09e0	0.20	0.13										

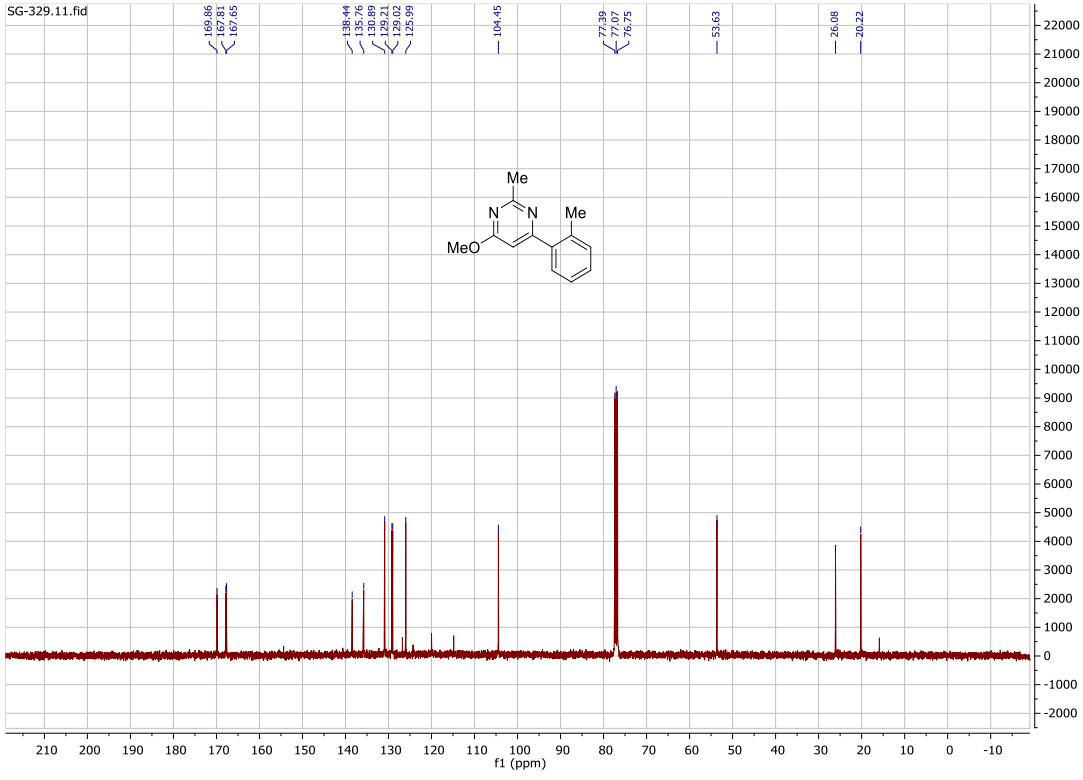




HRMS spectra of **15a**



^{1}H NMR spectrum of **15b** (in $CDCl_3$)

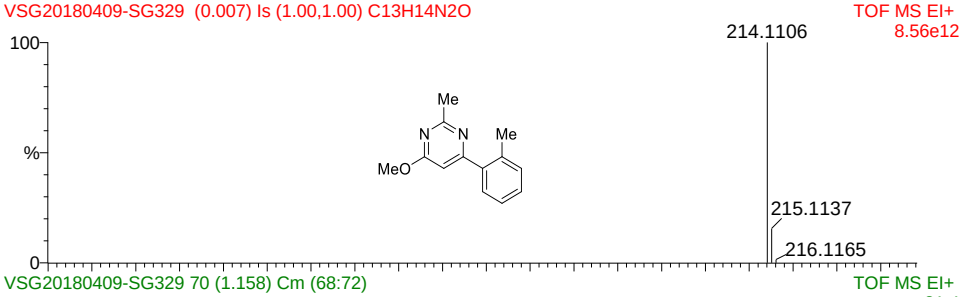


^{13}C NMR spectrum of **15b** (in $CDCl_3$)

VSG20180409-SG329

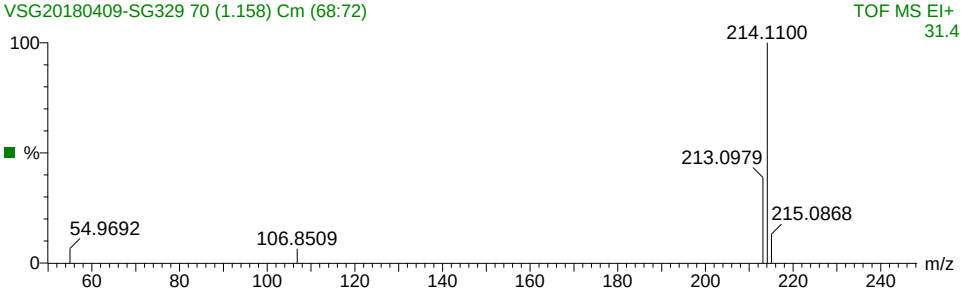
VSG20180409-SG329 (0.007) Is (1.00,1.00) C13H14N2O

TOF MS EI+
8.56e12



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

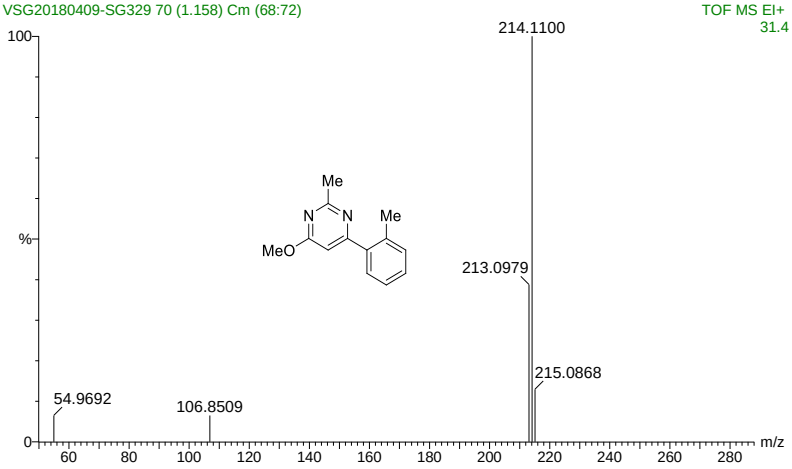
TOF MS EI+
31.4



VSG20180409-SG329

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

TOF MS EI+
31.4

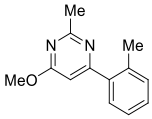


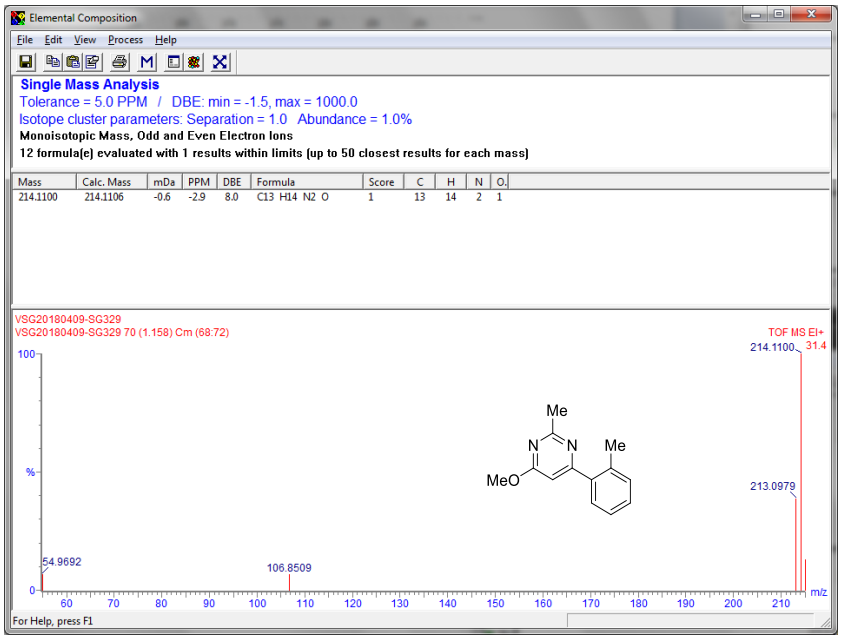
VSG20180409-SG329

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

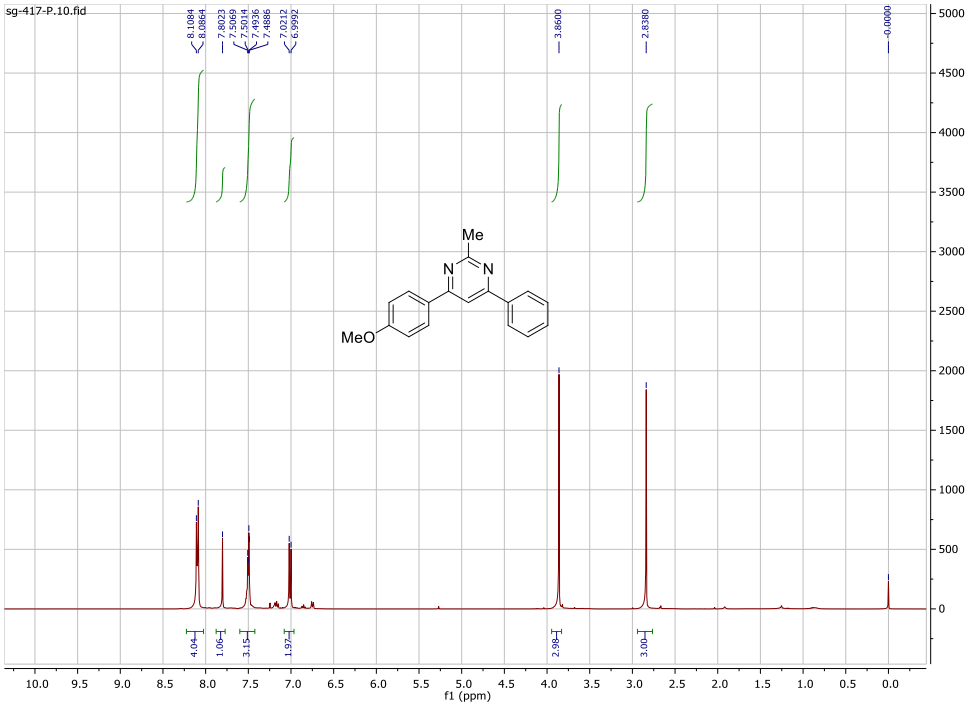
TOF MS EI+

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										

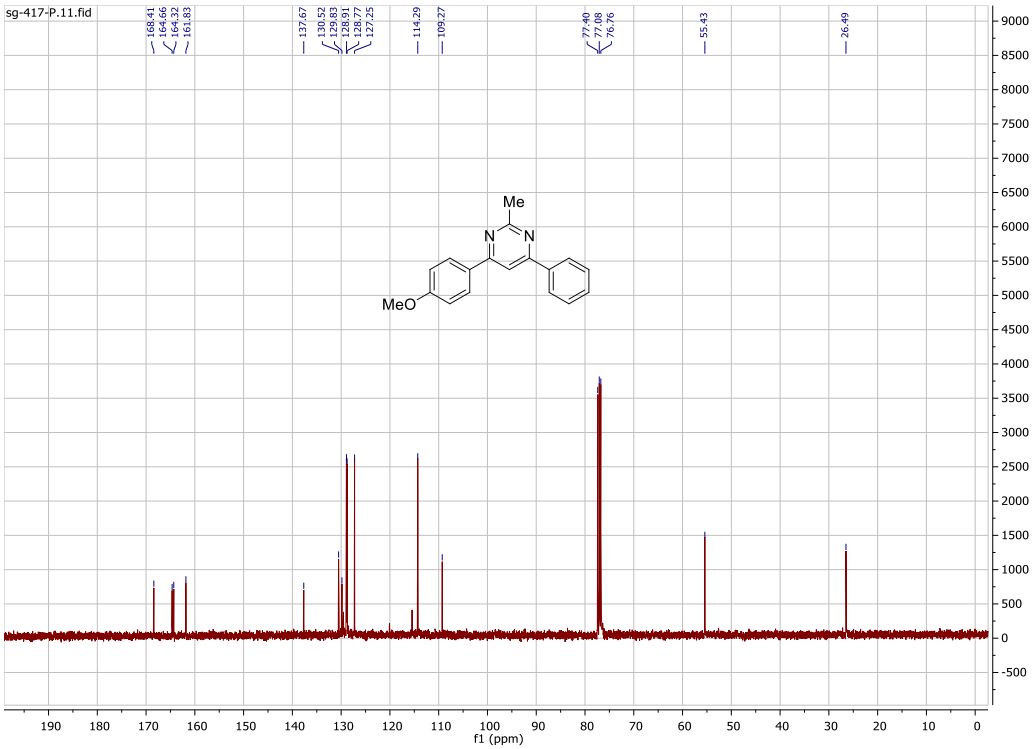




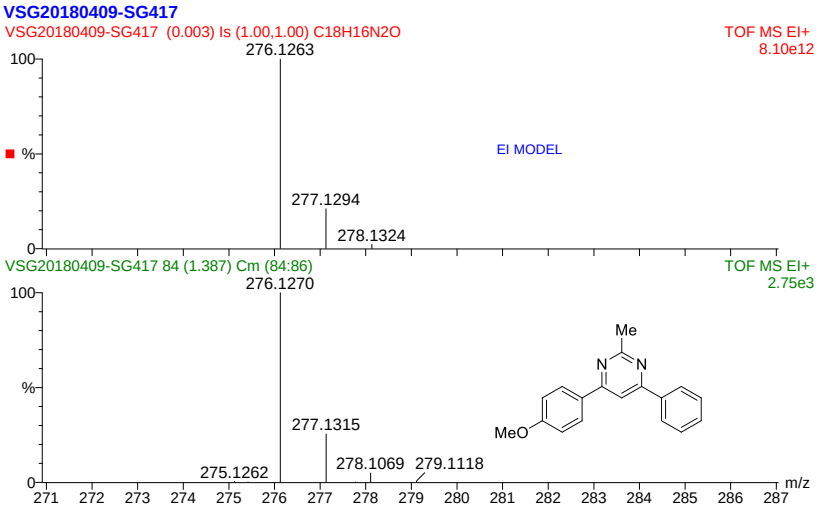
HRMS spectra of **15b**



^{1}H NMR spectrum of **15c** (in $CDCl_3$)



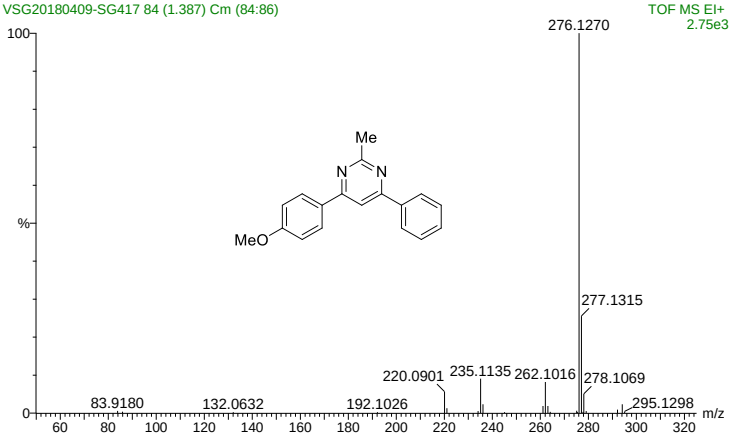
^{13}C NMR spectrum of **15c** (in $CDCl_3$)



VSG20180409-SG417

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

TOF MS EI+ 2.75e3

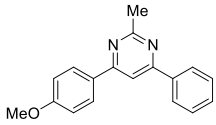


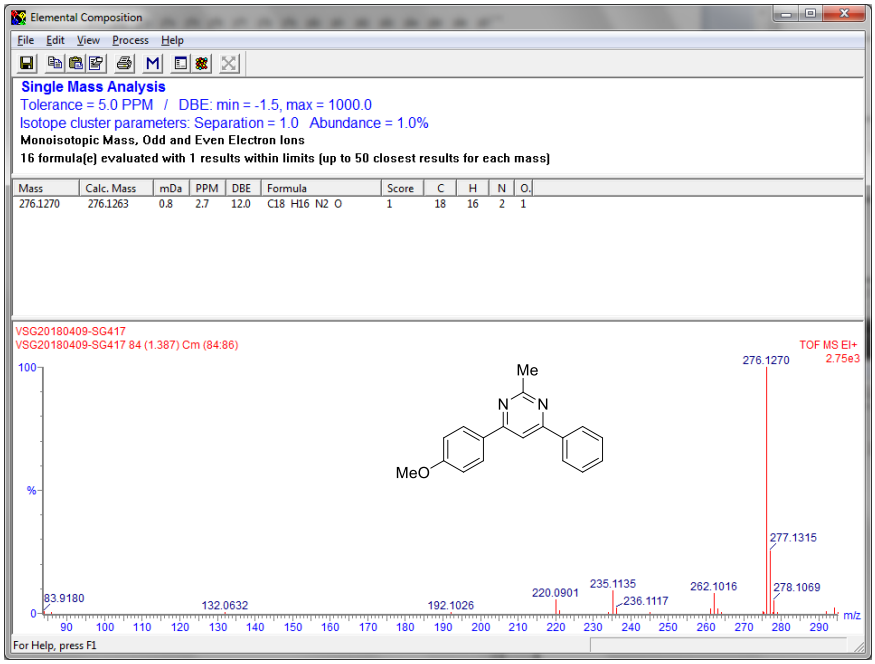
VSG20180409-SG417

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

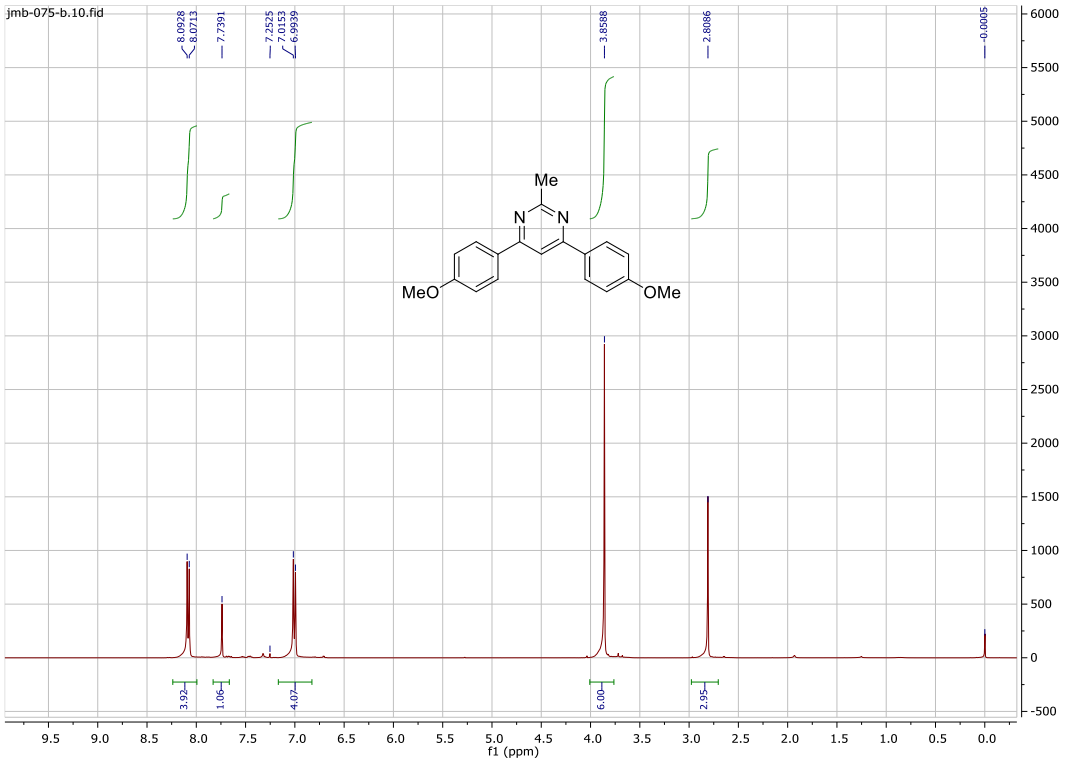
TOF MS EI+

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										

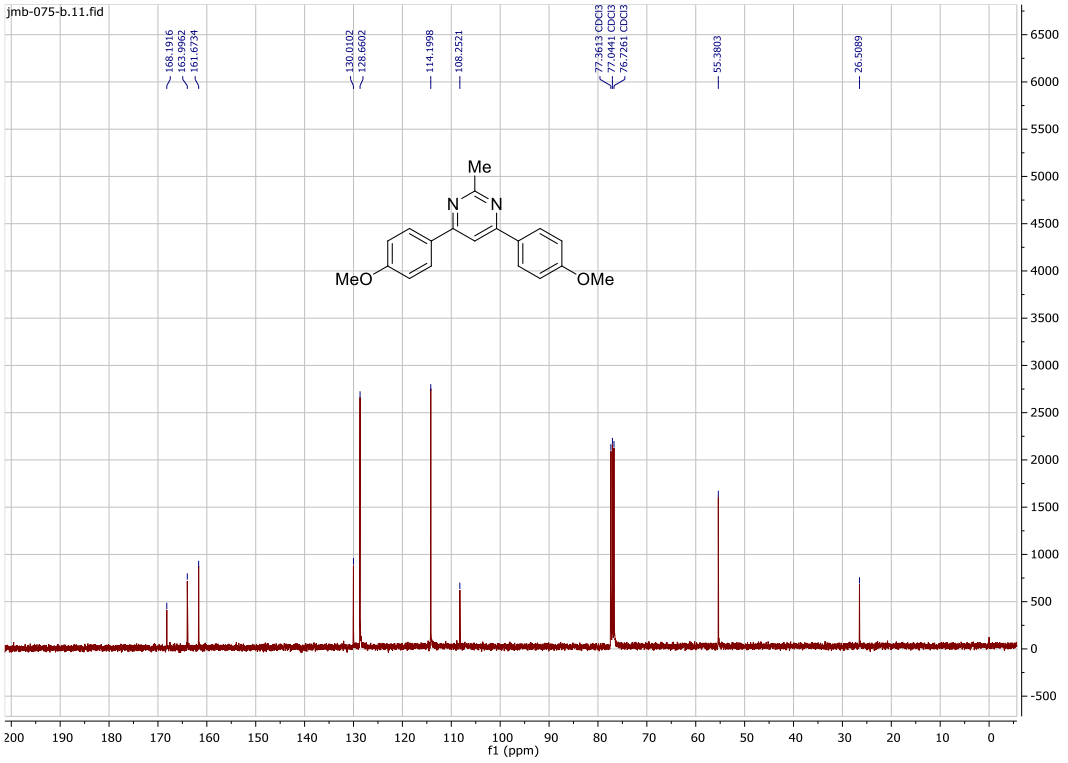




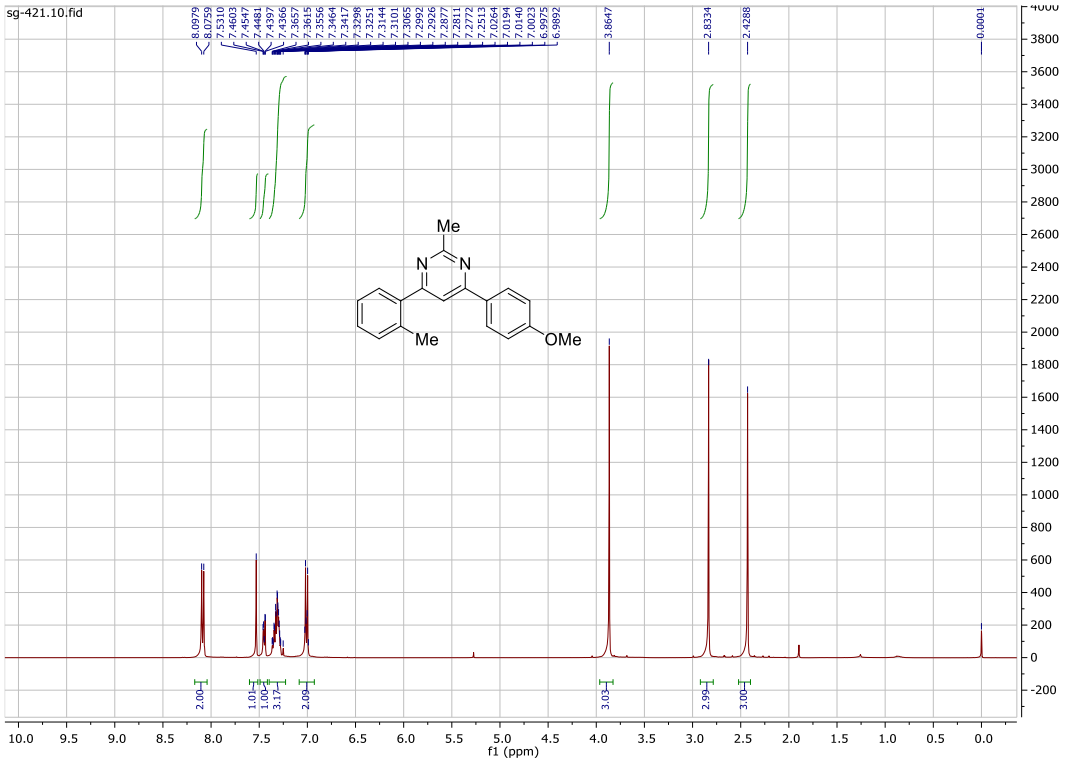
HRMS spectra of **15c**



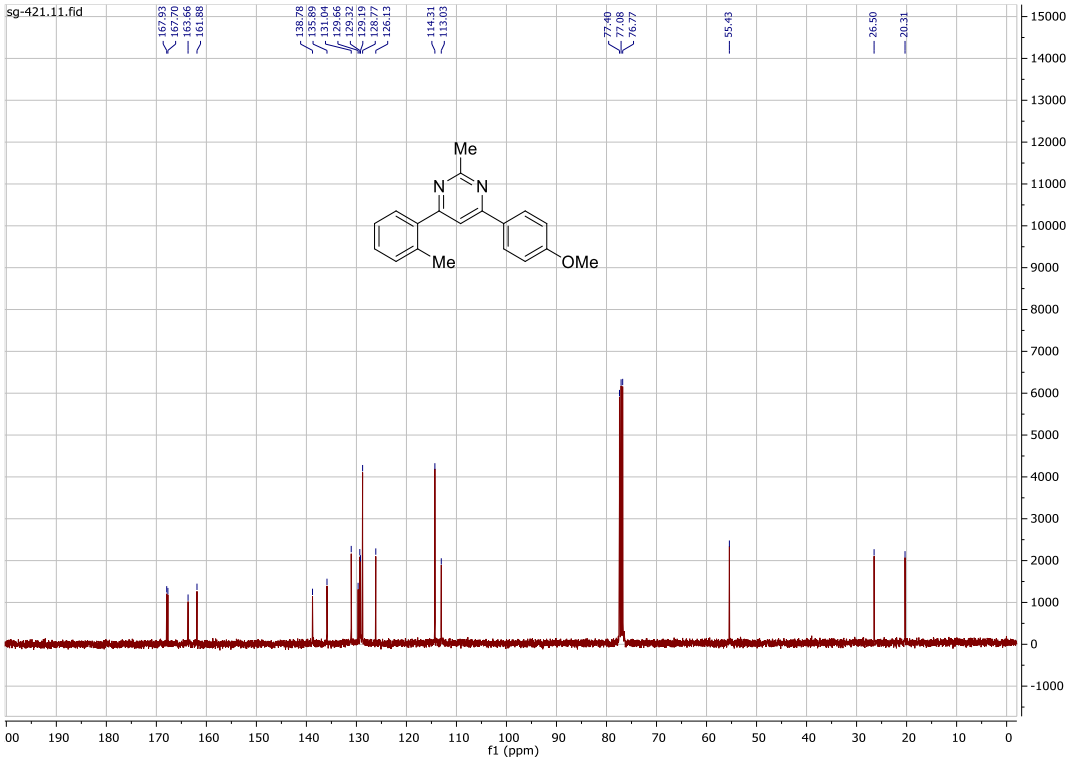
^{1}H NMR spectrum of **15d** (in $CDCl_3$)



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



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

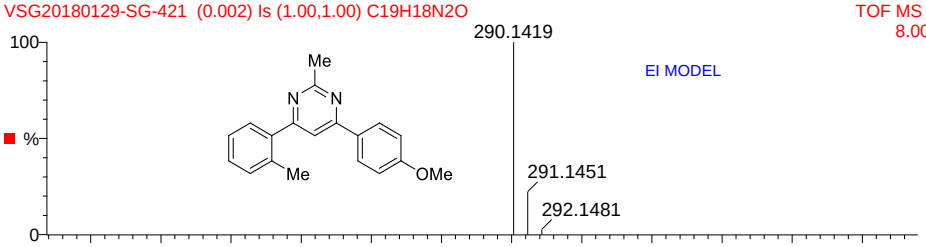


^{13}C NMR spectrum of **15e** (in $CDCl_3$)

VSG20180129-SG-421

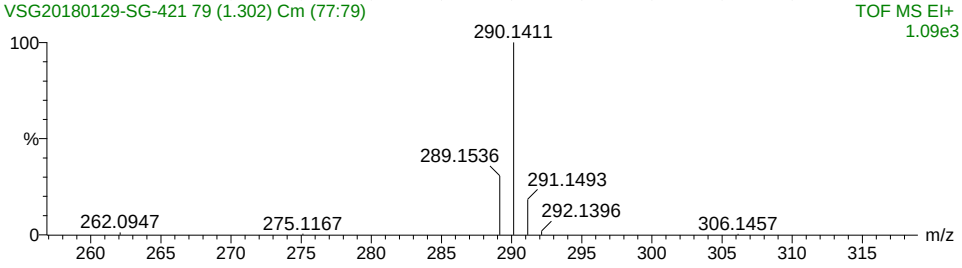
VSG20180129-SG-421 (0.002) Is (1.00,1.00) C19H18N2O

TOF MS EI+
8.00e12



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

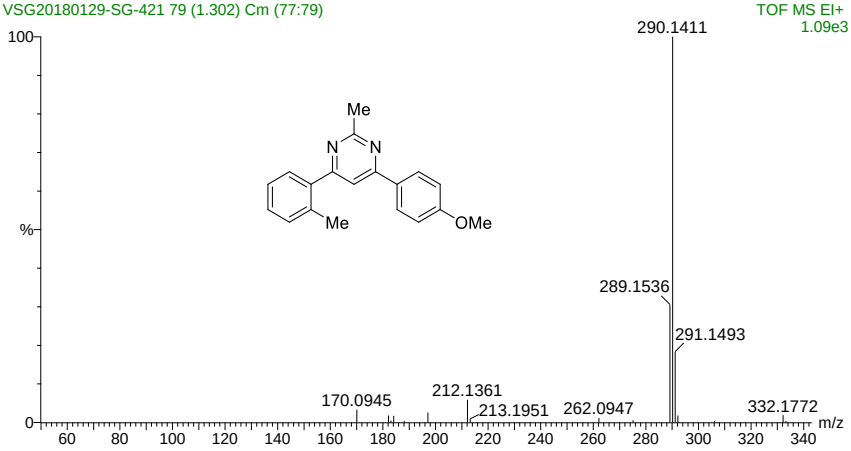
TOF MS EI+
1.09e3



VSG20180129-SG-421

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

TOF MS EI+
1.09e3

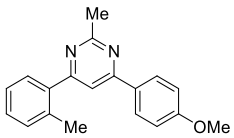


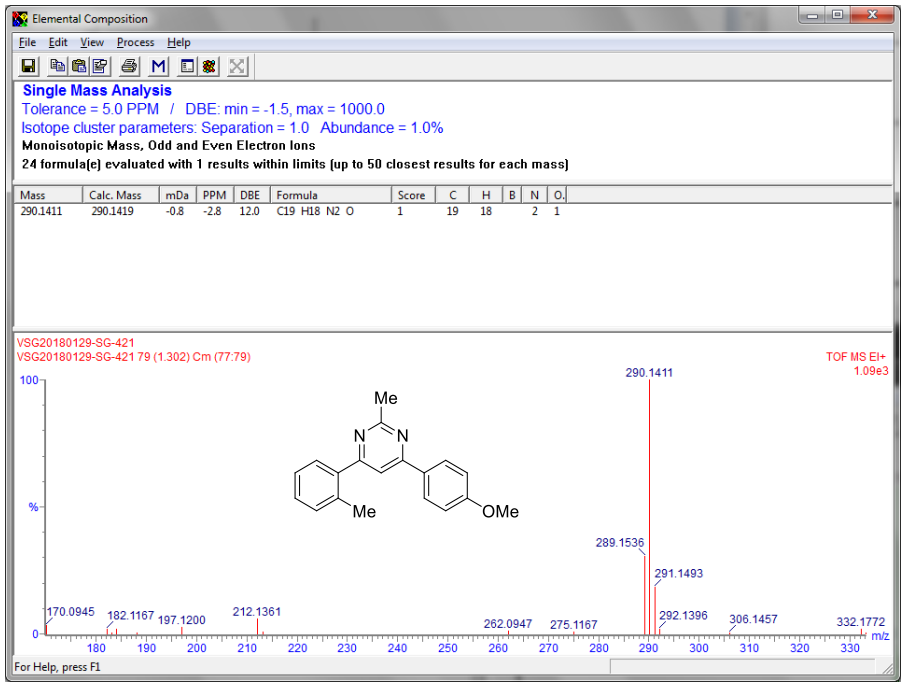
VSG20180129-SG-421

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

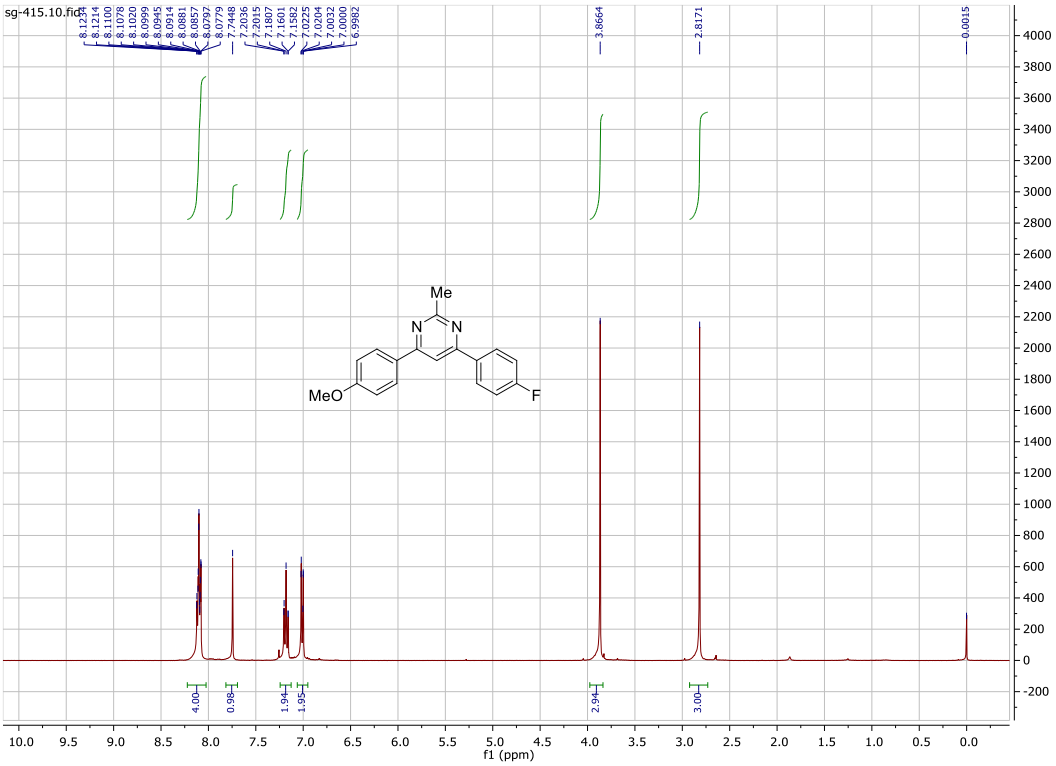
TOF MS EI+

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	6.38e1	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										

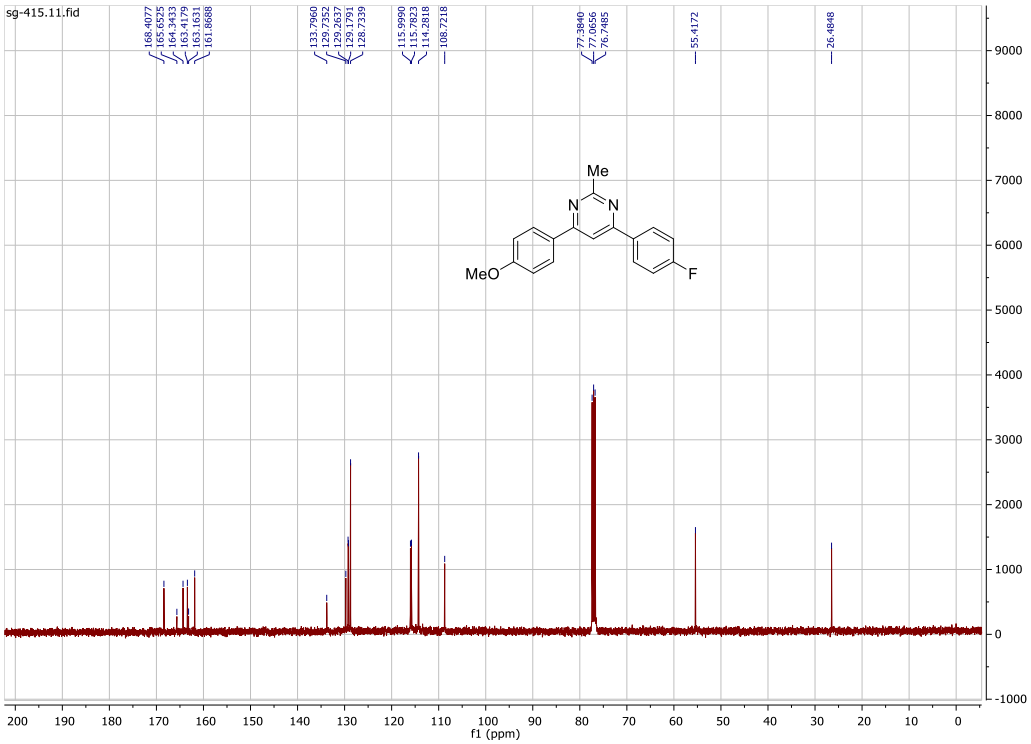




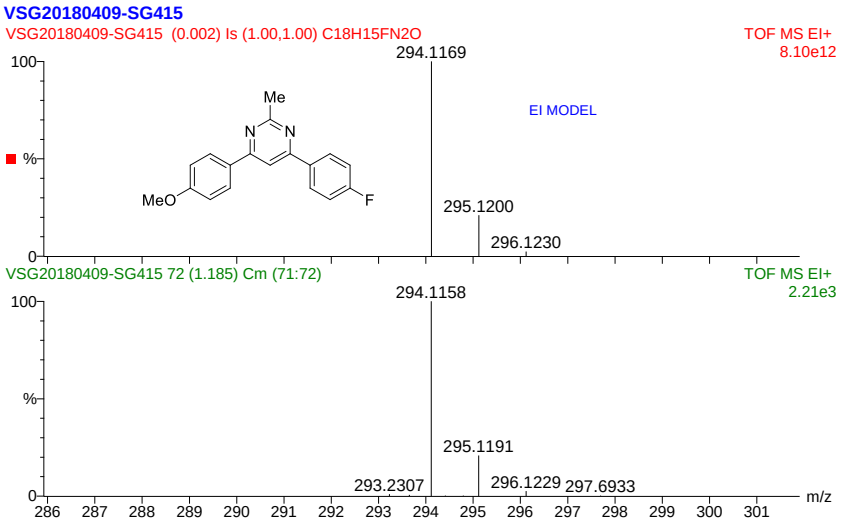
HRMS spectra of **15e**



^{1}H NMR spectrum of **15f** (in $CDCl_3$)



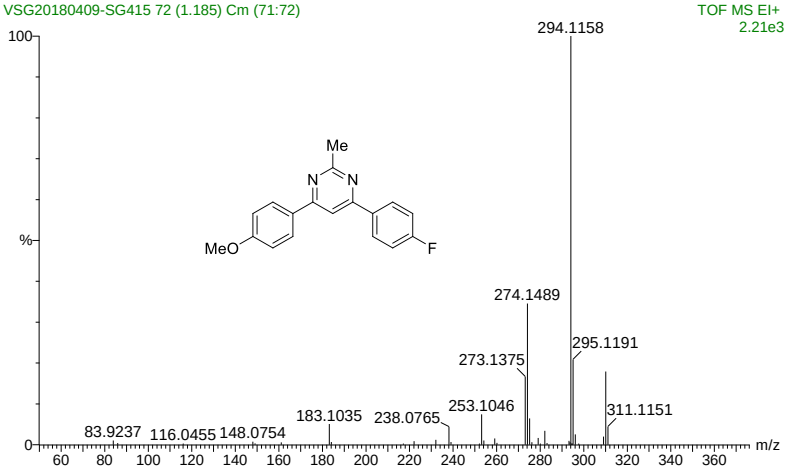
^{13}C NMR spectrum of **15f** (in $CDCl_3$)



VSG20180409-SG415

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

TOF MS EI+
2.21e3

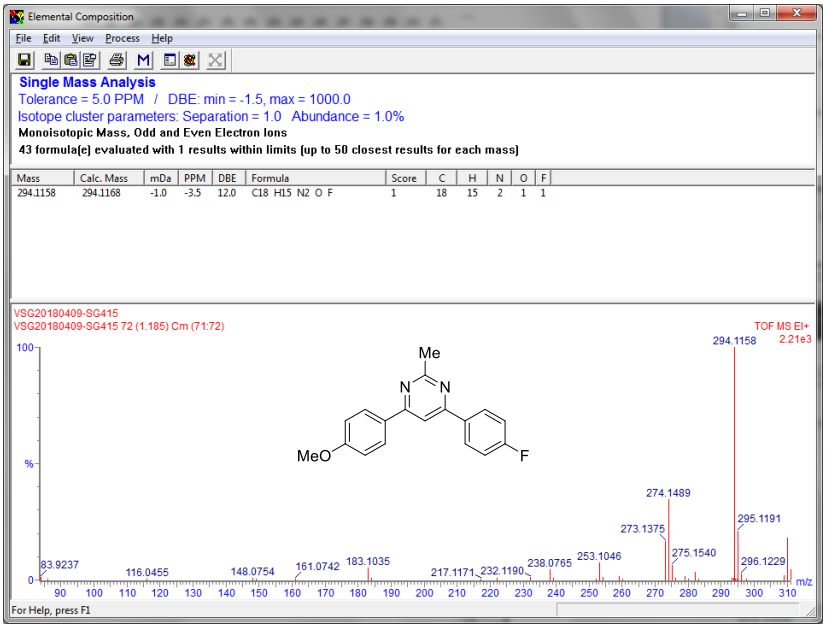


VSG20180409-SG415

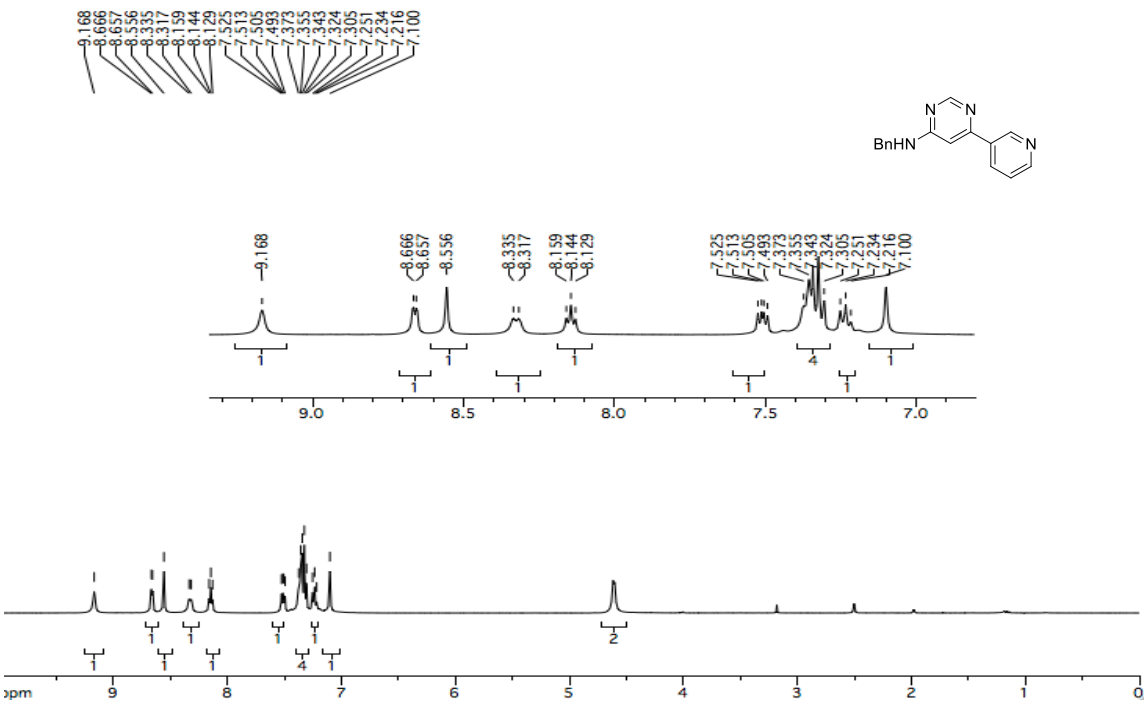
VSG20180409-SG415 72 (1.185) Cm (71:72)

TOF MS EI+

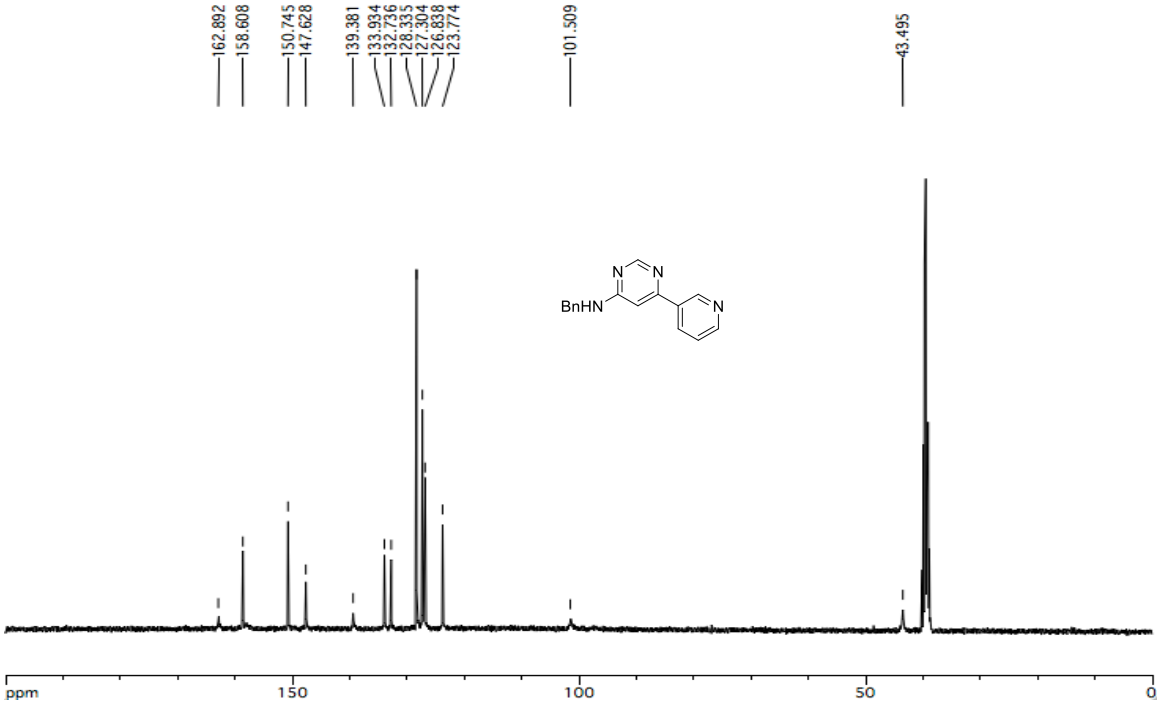
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	83.9237	2.23e1	1.01	0.41	32:	295.1191	4.60e2	20.83	8.56					
2:	85.9268	8.10e0	0.37	0.15	33:	296.1229	5.47e1	2.48	1.02					
3:	116.0455	5.06e0	0.23	0.09	34:	297.6933	5.06e0	0.23	0.09					
4:	148.0754	1.52e1	0.69	0.28	35:	309.1200	4.35e1	1.97	0.81					
5:	149.0625	6.08e0	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	3.68e2	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										



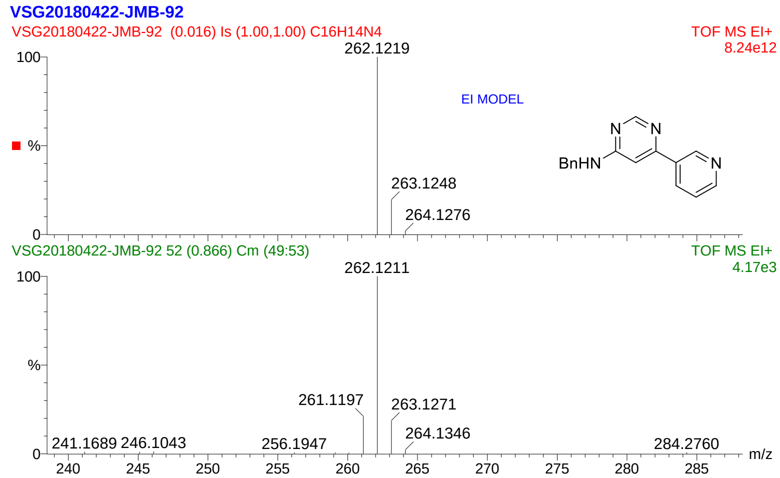
HRMS spectra of **15f**

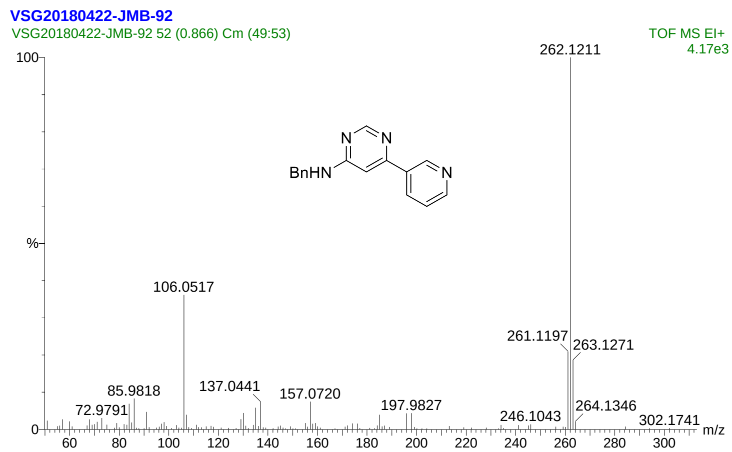


^{1}H NMR spectrum of **16a** (DMSO-d_6)



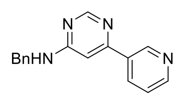
^{13}C NMR spectrum of **16a** (in DMSO-d_6)

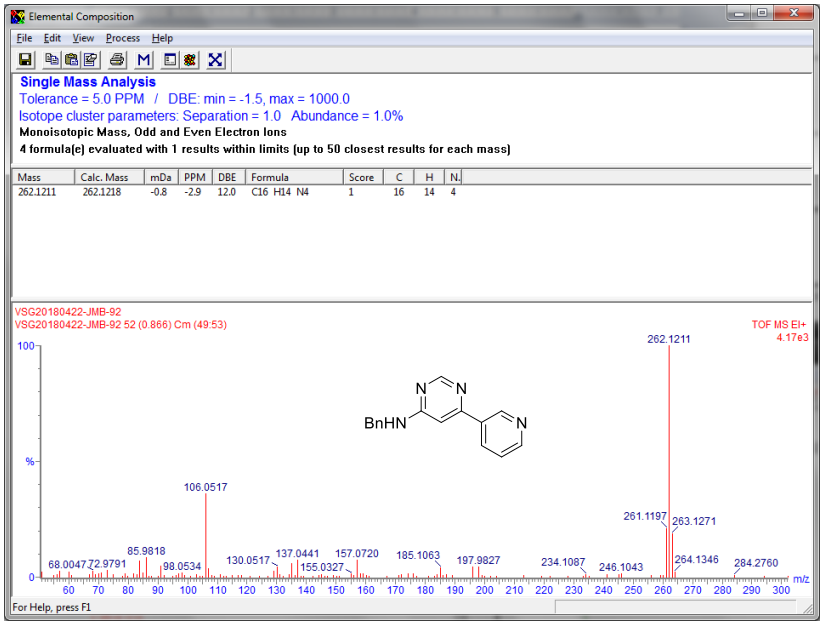




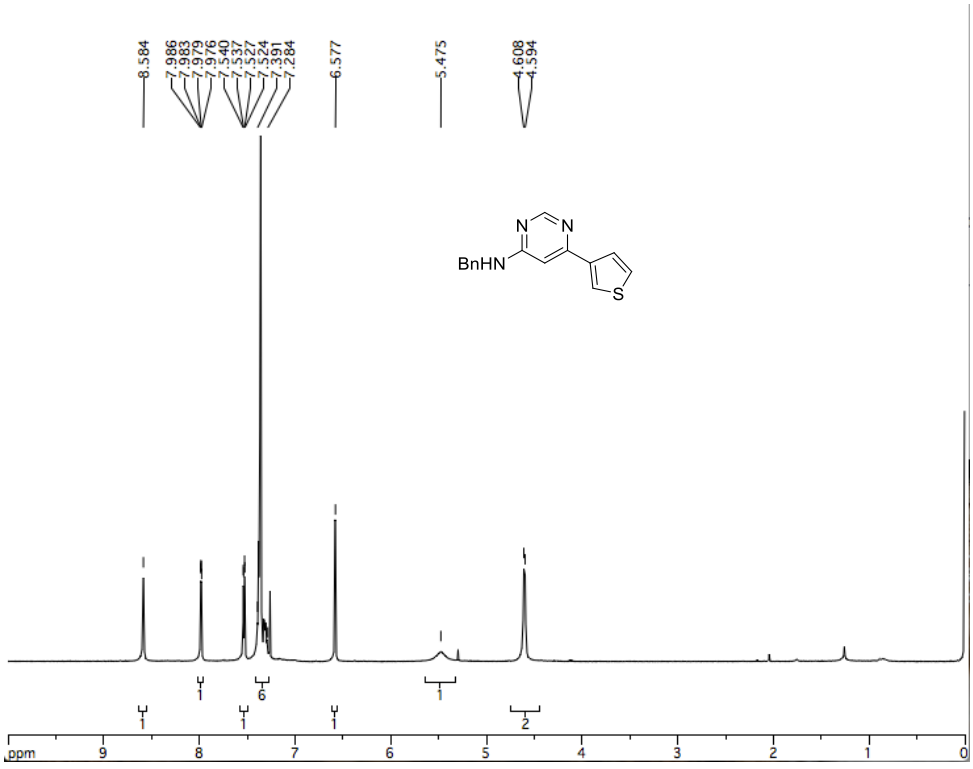
VSG20180422-JMB-92
VSG20180422-JMB-92 52 (0.866) Cm (49:53)
TOF MS EI+

No	Mass	Inten	%BPI	%TIC
1:	50.8944	9.62e1	2.31	0.70
2:	54.9759	3.34e1	0.80	0.24
3:	55.9829	4.05e1	0.97	0.29
4:	56.9955	1.10e2	2.65	0.80
5:	59.9509	8.71e1	2.09	0.63
6:	60.9583	3.14e1	0.75	0.23
7:	66.9994	4.15e1	1.00	0.30
8:	68.0047	1.11e2	2.67	0.81
9:	69.0127	4.96e1	1.19	0.36
10:	70.0221	5.67e1	1.36	0.41
11:	71.0336	8.20e1	1.97	0.59
12:	72.9791	1.25e2	2.99	0.90
13:	74.9816	5.16e1	1.24	0.37
14:	78.0071	1.52e1	0.36	0.11
15:	79.0138	6.89e1	1.65	0.50
16:	79.9342	2.13e1	0.51	0.15
17:	81.9435	5.57e1	1.34	0.40
18:	83.0430	4.96e1	1.19	0.36
19:	83.9292	2.86e2	6.85	2.07
20:	85.0554	7.59e1	1.82	0.55
21:	85.9818	3.45e2	8.28	2.50
22:	87.0120	1.62e1	0.39	0.12
23:	87.9196	1.01e1	0.24	0.07
24:	90.0096	1.11e1	0.27	0.08
25:	91.0279	1.93e2	4.64	1.40
26:	92.0339	2.33e1	0.56	0.17
27:	95.0602	1.82e1	0.44	0.13
28:	96.0740	2.73e1	0.66	0.20
29:	97.0737	6.18e1	1.48	0.45
30:	98.0534	8.00e1	1.92	0.58
31:	99.0781	3.44e1	0.83	0.25
32:	101.0431	1.22e1	0.29	0.09
33:	103.0253	4.56e1	1.09	0.33
34:	104.0245	1.72e1	0.41	0.12
35:	105.0383	1.62e1	0.39	0.12
36:	106.0517	1.51e3	36.15	10.92
37:	107.0569	1.61e2	3.86	1.17
38:	108.0553	2.33e1	0.56	0.17
39:	109.0506	1.32e1	0.32	0.10
40:	111.1075	4.86e1	1.17	0.35
41:	112.0821	2.23e1	0.53	0.16
42:	113.1235	2.13e1	0.51	0.15
43:	115.0632	3.24e1	0.78	0.23
44:	117.0453	3.75e1	0.90	0.27
45:	118.0393	2.63e1	0.63	0.19
46:	121.0655	1.72e1	0.41	0.12
47:	124.0724	1.42e1	0.34	0.10
48:	127.1078	1.22e1	0.29	0.09
49:	129.0832	1.12e2	2.69	0.81
50:	130.0517	1.81e2	4.35	1.31
51:	131.0609	3.85e1	0.92	0.28
52:	132.0555	1.32e1	0.32	0.10
53:	134.0464	4.76e1	1.14	0.34
54:	135.0631	2.41e2	5.78	1.75
55:	136.0649	3.54e1	0.85	0.26
56:	137.0441	3.07e2	7.36	2.22
57:	138.0511	2.03e1	0.49	0.15
58:	139.1263	1.82e1	0.44	0.13
59:	142.0876	1.11e1	0.27	0.08
60:	144.0905	2.94e1	0.70	0.21
61:	145.0748	4.05e1	0.97	0.29
62:	146.0644	1.72e1	0.41	0.12
63:	147.0914	9.11e0	0.22	0.07
64:	149.0497	3.14e1	0.75	0.23
65:	150.0920	9.11e0	0.22	0.07
66:	151.1286	9.11e0	0.22	0.07
67:	155.0327	6.78e1	1.63	0.49
68:	156.0574	2.84e1	0.68	0.21
69:	157.0720	3.09e2	7.40	2.24
70:	158.0751	6.08e1	1.46	0.44
71:	159.0879	6.78e1	1.63	0.49
72:	160.0933	3.24e1	0.78	0.23
73:	161.0550	1.72e1	0.41	0.12
74:	167.0856	9.11e0	0.22	0.07
75:	171.1030	2.73e1	0.66	0.20
76:	172.0871	4.15e1	1.00	0.30
77:	174.1064	6.48e1	1.55	0.47
78:	176.1024	6.38e1	1.53	0.46
79:	177.1125	1.32e1	0.32	0.10
80:	181.1170	1.42e1	0.34	0.10
81:	183.0688	1.11e1	0.27	0.08
82:	184.0791	4.15e1	1.00	0.30
83:	185.1063	1.62e2	3.88	1.17
84:	186.0898	3.14e1	0.75	0.23
85:	187.1115	4.05e1	0.97	0.29
86:	189.0609	2.53e1	0.61	0.18
87:	195.9674	1.78e2	4.27	1.29
88:	197.9827	1.80e2	4.32	1.31
89:	199.1186	2.53e1	0.61	0.18
90:	200.1080	9.11e0	0.22	0.07
91:	202.1346	9.11e0	0.22	0.07
92:	204.1056	9.11e0	0.22	0.07
93:	213.1473	3.44e1	0.83	0.25
94:	219.1002	2.03e1	0.49	0.15
95:	222.0591	1.82e1	0.44	0.13
96:	228.0973	1.72e1	0.41	0.12
97:	233.1198	9.11e0	0.22	0.07
98:	234.1087	4.76e1	1.14	0.34
99:	235.1145	1.22e1	0.29	0.09
100:	241.1689	4.66e1	1.12	0.34
101:	245.1031	4.25e1	1.02	0.31
102:	246.1043	5.47e1	1.31	0.40
103:	256.1947	2.73e1	0.66	0.20
104:	259.1134	2.73e1	0.66	0.20
105:	260.0842	2.43e1	0.58	0.18
106:	261.1197	8.72e2	20.90	6.32
107:	262.1211	4.17e3	100.01	30.22
108:	263.1271	7.76e2	18.60	5.62
109:	264.1346	8.71e1	2.09	0.63
110:	284.2760	3.04e1	0.73	0.22
111:	294.0818	1.11e1	0.27	0.08
112:	302.1741	1.22e1	0.29	0.09

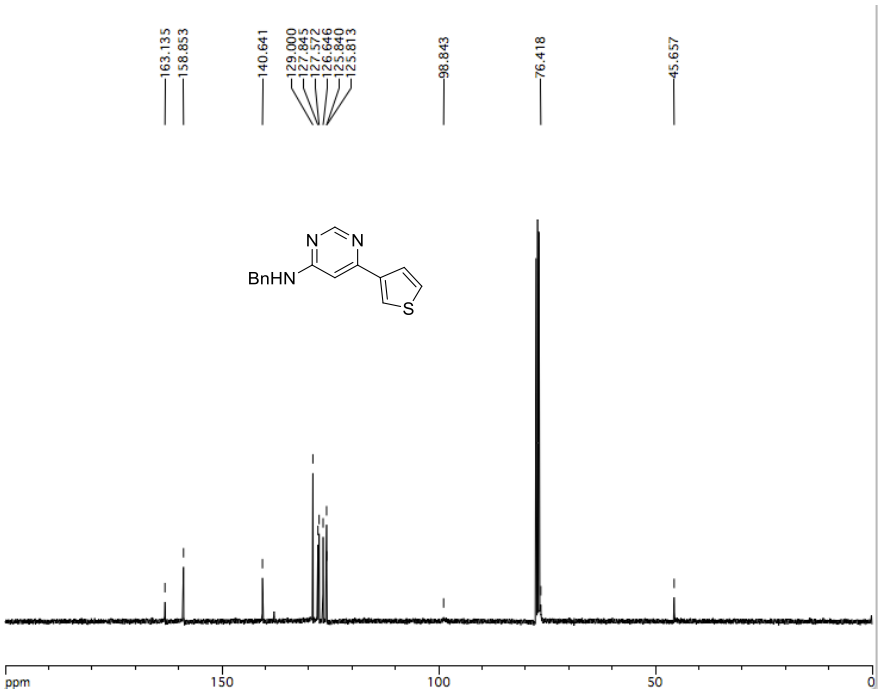




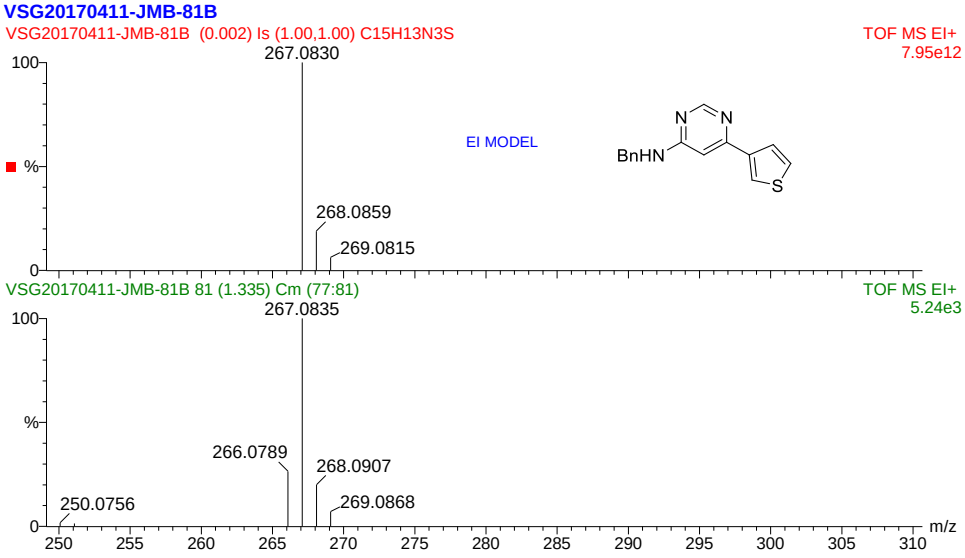
HRMS spectra of **16a**



^{1}H NMR spectrum of **16b** (in $CDCl_3$)



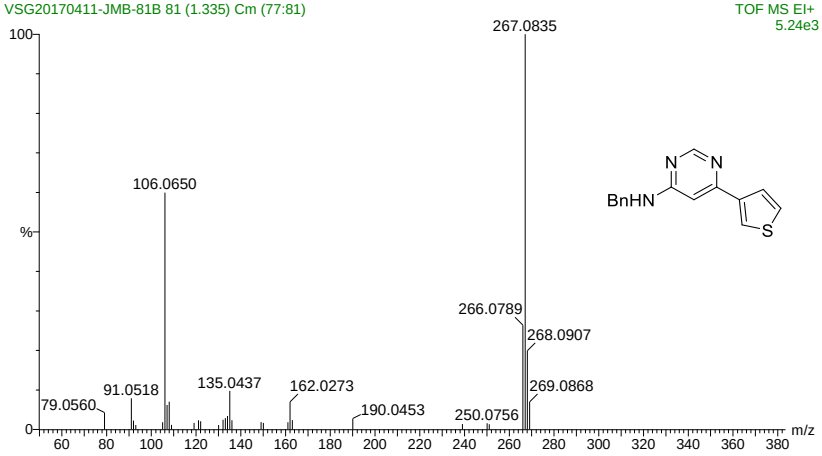
^{13}C NMR spectrum of **16b** (in $CDCl_3$)



VSG20170411-JMB-81B

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

TOF MS EI+
5.24e3

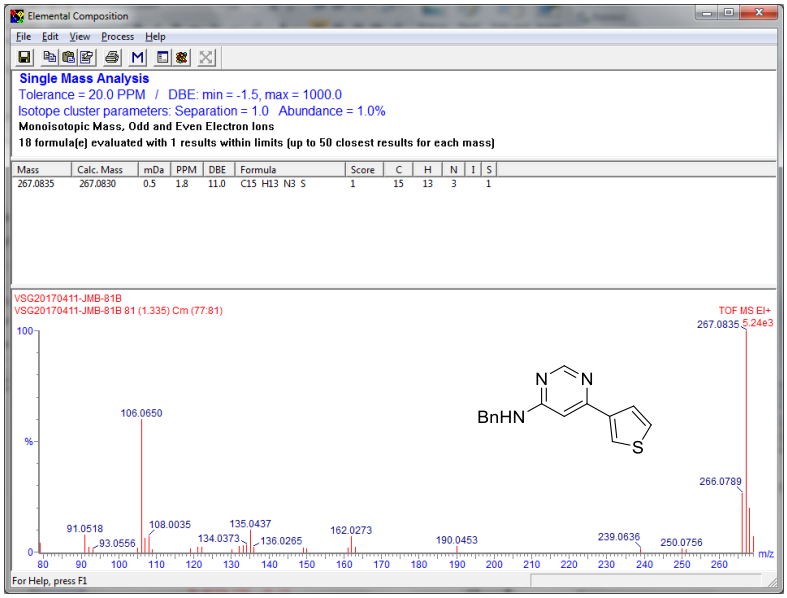


VSG20170411-JMB-81B

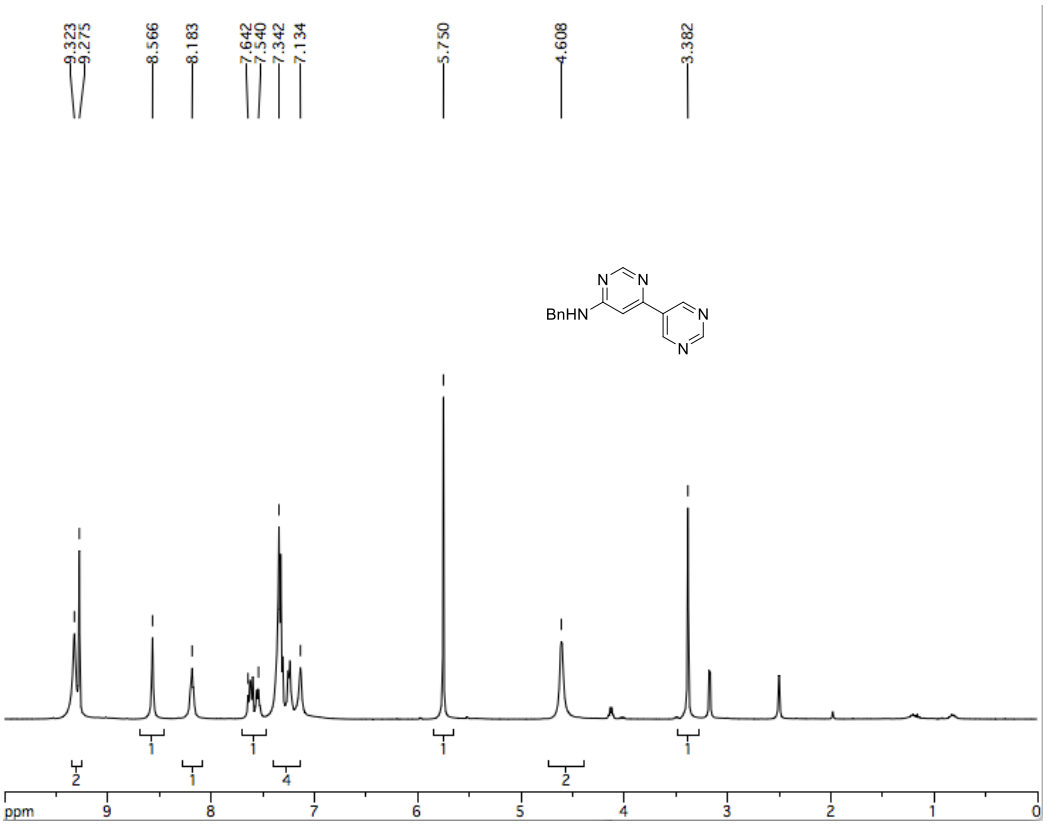
VSG20170411-JMB-81B 81 (1.335) Cm (77:81)

TOF MS EI+

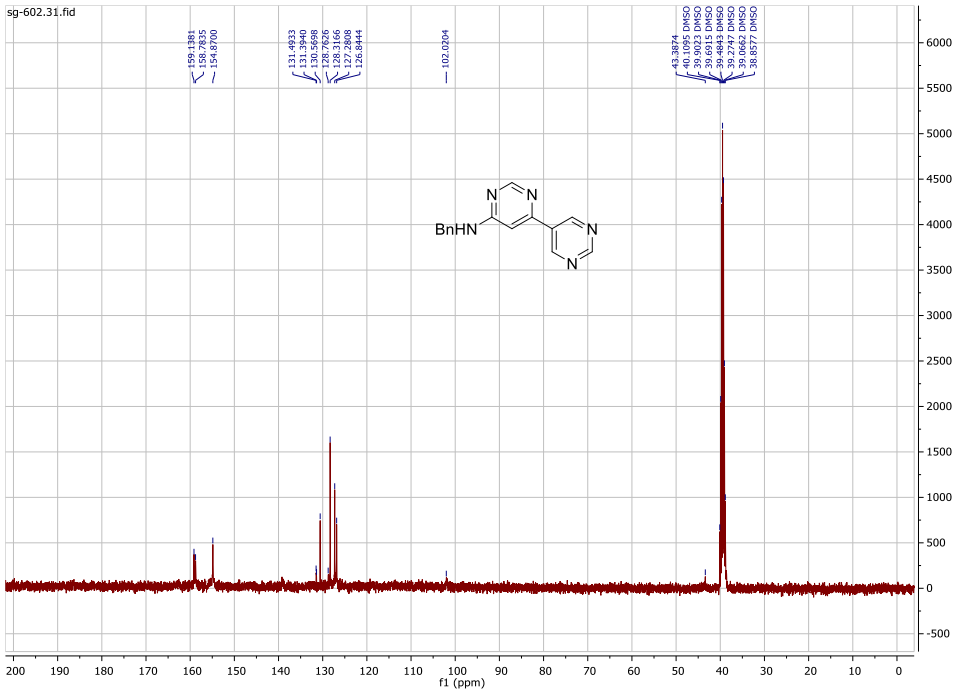
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No
1:	79.0560	2.21e2	4.22	1.29											
2:	91.0518	4.12e2	7.87	2.42											
3:	92.0562	1.14e2	2.19	0.67											
4:	93.0556	5.67e1	1.08	0.33											
5:	105.0609	9.42e1	1.80	0.55											
6:	106.0650	3.14e3	59.90	18.38											
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:	130.0656	5.77e1	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	8.10e1	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**



^{1}H NMR spectrum of **16c** (in DMSO-d_6)

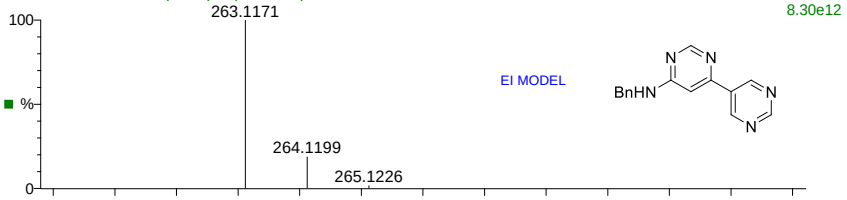


^{13}C NMR spectrum of **16c** (in $CDCl_3$)

VSG20180105-JMB88

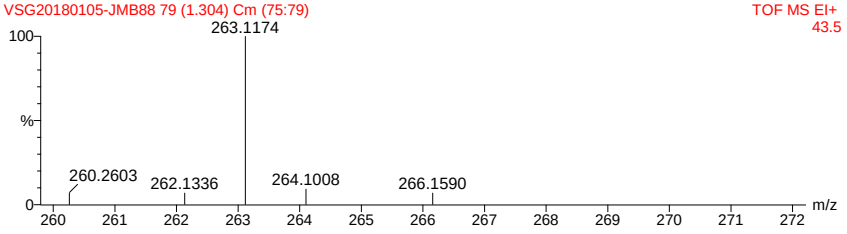
VSG20180105-JMB88 (0.004) Is (1.00,1.00) C15H13N5

TOF MS EI+
8.30e12



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

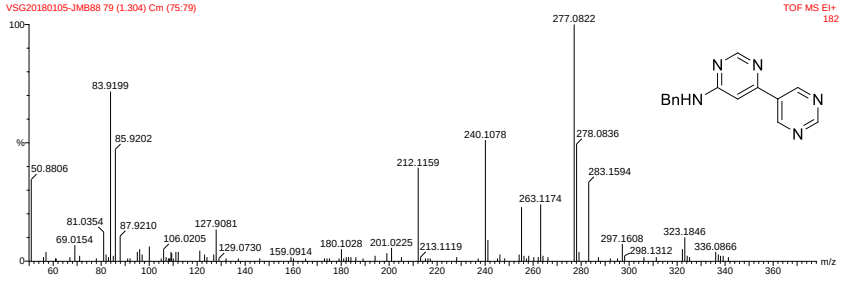
TOF MS EI+
43.5



VSG20180105-JMB88

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

TOF MS EI+
182

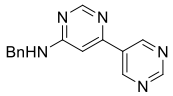


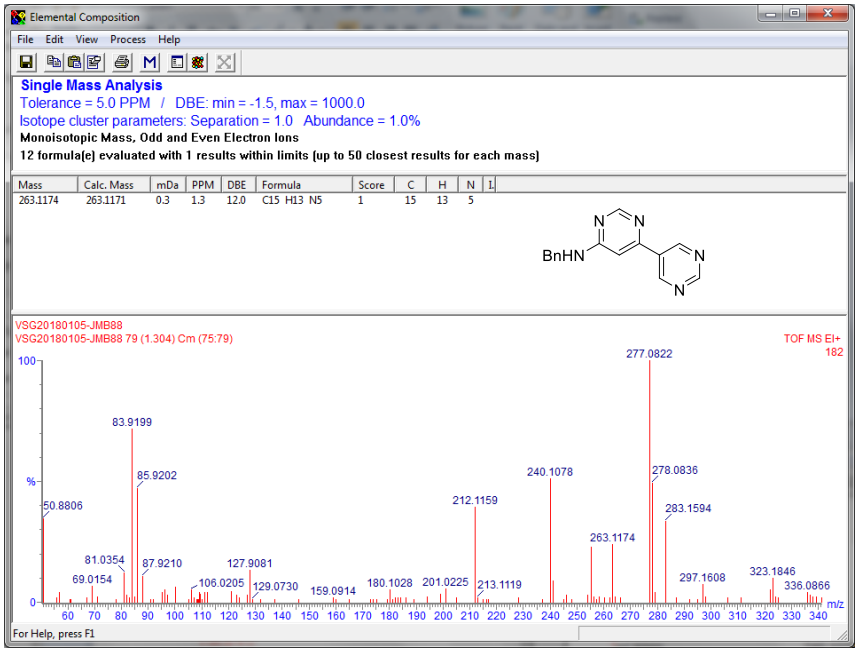
VSG20180105-JMB88

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

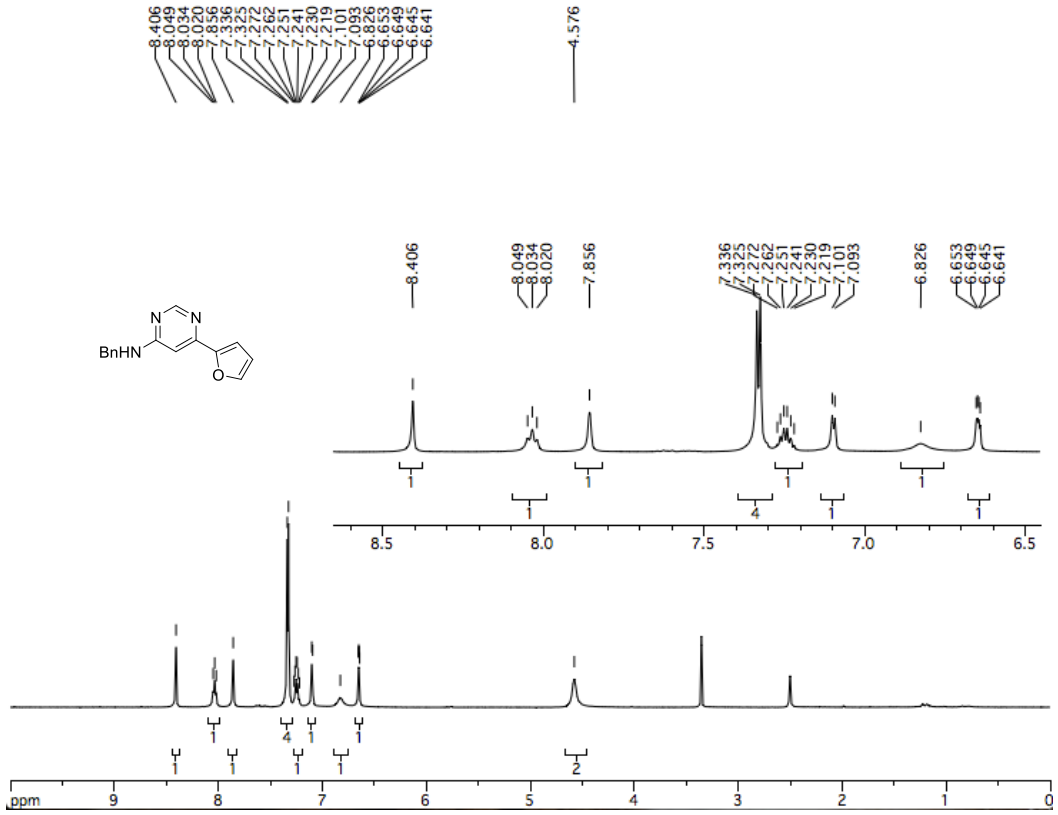
TOF MS EI+

No	Mass	Inten	%BPI	%TIC
1:	50.8806	6.28e1	24.44	4.58
2:	55.9819	3.04e0	1.67	0.22
3:	56.9905	7.09e0	3.89	0.52
4:	60.9635	2.03e0	1.11	0.15
5:	61.2630	2.03e0	1.11	0.15
6:	66.9965	3.04e0	1.67	0.22
7:	69.0154	1.22e1	6.67	0.89
8:	71.0421	4.05e0	2.22	0.30
9:	77.9960	2.03e0	1.11	0.15
10:	81.0354	2.23e1	12.22	1.62
11:	82.0338	5.06e0	2.78	0.37
12:	83.0515	3.04e0	1.67	0.22
13:	83.9199	1.31e2	71.67	9.55
14:	85.0284	4.05e0	2.22	0.30
15:	85.9202	8.62e1	47.22	6.28
16:	87.9210	1.92e1	10.56	1.40
17:	91.0504	2.03e0	1.11	0.15
18:	92.0373	2.03e0	1.11	0.15
19:	95.0690	7.09e0	3.89	0.52
20:	96.0710	9.11e0	5.00	0.66
21:	97.0671	5.06e0	2.78	0.37
22:	100.0561	1.11e1	6.11	0.81
23:	105.0322	2.03e0	1.11	0.15
24:	106.0205	9.11e0	5.00	0.66
25:	107.0316	3.04e0	1.67	0.22
26:	107.9746	2.03e0	1.11	0.15
27:	108.0781	2.03e0	1.11	0.15
28:	108.9738	2.03e0	1.11	0.15
29:	109.0687	7.09e0	3.89	0.52
30:	109.3844	6.08e0	3.33	0.44
31:	110.0686	2.03e0	1.11	0.15
32:	111.1058	7.09e0	3.89	0.52
33:	112.1163	7.09e0	3.89	0.52
34:	121.0946	8.10e0	4.44	0.59
35:	123.0851	5.06e0	2.78	0.37
36:	124.0736	3.04e0	1.67	0.22
37:	126.9008	5.06e0	2.78	0.37
38:	127.9081	2.43e1	13.33	1.77
39:	129.0730	2.03e0	1.11	0.15
40:	132.0738	2.03e0	1.11	0.15
41:	132.1027	2.03e0	1.11	0.15
42:	146.0922	2.03e0	1.11	0.15
43:	159.0914	3.04e0	1.67	0.22
44:	160.0997	2.03e0	1.11	0.15
45:	165.1730	2.03e0	1.11	0.15
46:	170.0734	2.03e0	1.11	0.15
47:	174.0919	2.03e0	1.11	0.15
48:	175.1022	2.03e0	1.11	0.15
49:	179.0975	2.03e0	1.11	0.15
50:	180.1028	9.11e0	5.00	0.66
51:	181.0808	2.03e0	1.11	0.15
52:	182.1035	3.04e0	1.67	0.22
53:	183.0547	3.04e0	1.67	0.22
54:	184.0628	3.04e0	1.67	0.22
55:	186.1038	3.04e0	1.67	0.22
56:	186.1330	2.03e0	1.11	0.15
57:	194.1134	4.05e0	2.22	0.30
58:	199.0413	6.08e0	3.33	0.44
59:	201.0225	1.01e1	5.56	0.74
60:	205.1155	3.04e0	1.67	0.22
61:	212.1159	7.19e1	39.44	5.24
62:	213.1119	3.04e0	1.67	0.22
63:	215.1070	2.03e0	1.11	0.15
64:	216.1475	2.03e0	1.11	0.15
65:	217.1011	2.03e0	1.11	0.15
66:	228.1179	3.04e0	1.67	0.22
67:	237.0858	2.03e0	1.11	0.15
68:	240.1078	9.32e1	51.11	6.78
69:	241.1109	3.04e0	1.67	0.22
70:	245.1588	2.03e0	1.11	0.15
71:	246.1512	5.06e0	2.78	0.37
72:	246.1161	2.03e0	1.11	0.15
73:	254.1491	5.06e0	2.78	0.37
74:	255.1591	4.15e1	22.78	3.03
75:	256.1636	4.05e0	2.22	0.30
76:	257.1923	2.03e0	1.11	0.15
77:	258.1782	4.05e0	2.22	0.30
78:	260.2603	3.04e0	1.67	0.22
79:	262.1336	3.04e0	1.67	0.22
80:	263.1174	4.35e1	23.89	3.18
81:	264.1008	4.05e0	2.22	0.30
82:	265.1226	3.04e0	1.67	0.22
83:	266.1590	1.82e1	10.00	1.33
84:	277.0822	1.82e2	100.00	13.29
85:	278.0836	7.09e1	38.89	5.17
86:	283.1594	9.08e1	49.44	6.63
87:	287.1757	3.04e0	1.67	0.22
88:	290.1728	2.03e0	1.11	0.15
89:	295.1685	2.03e0	1.11	0.15
90:	297.1608	1.32e1	7.22	0.96
91:	298.1312	4.05e0	2.22	0.30
92:	308.1799	3.04e0	1.67	0.22
93:	311.2985	3.04e0	1.67	0.22
94:	322.1859	9.11e0	5.00	0.66
95:	323.1846	1.82e1	10.00	1.33
96:	324.1966	4.05e0	2.22	0.30
97:	325.1948	3.04e0	1.67	0.22
98:	336.0866	7.09e0	3.89	0.52
99:	337.1850	5.06e0	2.78	0.37
100:	338.0636	4.05e0	2.22	0.30
101:	339.1809	4.05e0	2.22	0.30
102:	341.3325	3.04e0	1.67	0.22

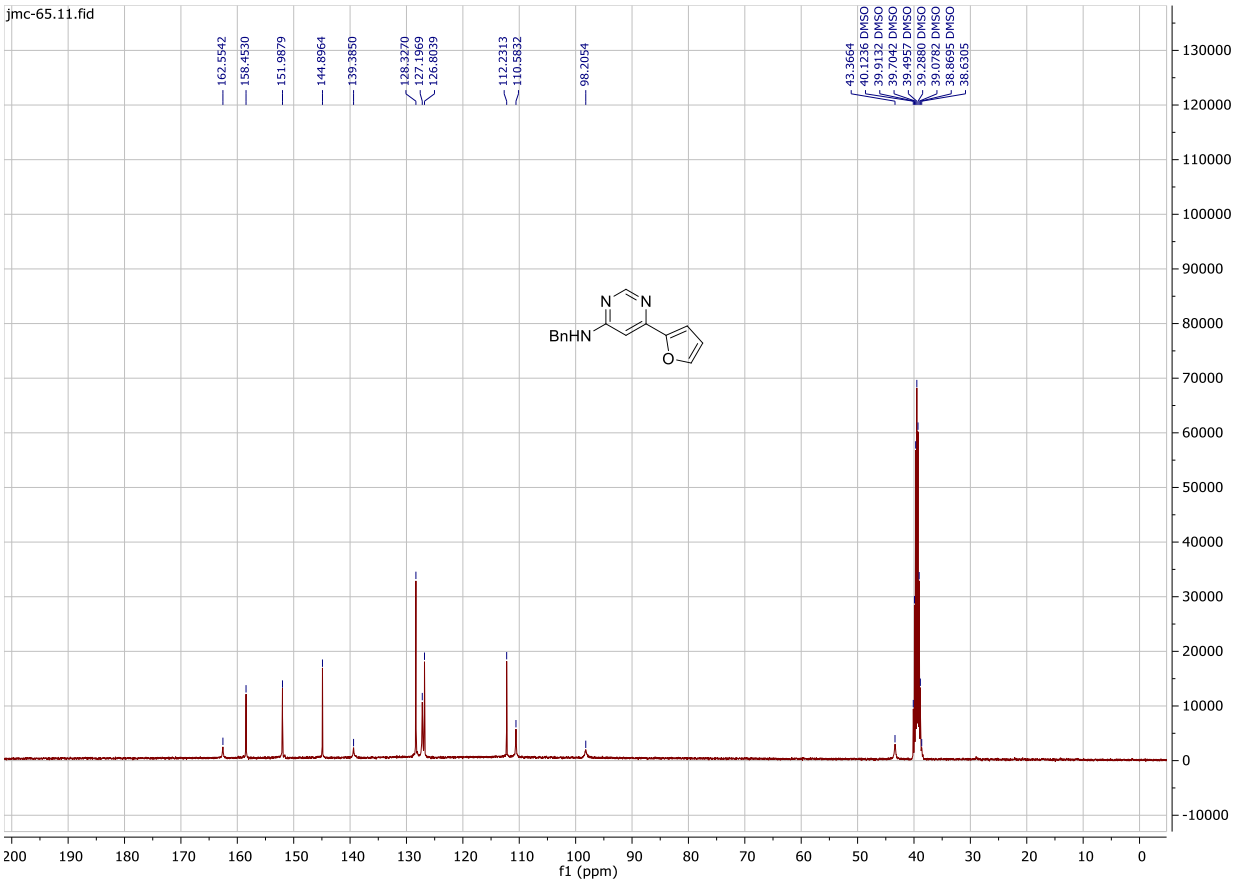




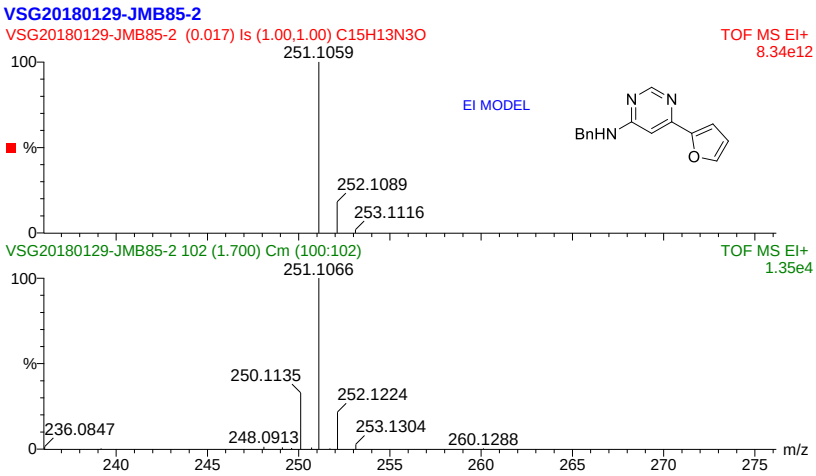
HRMS spectra of **16c**

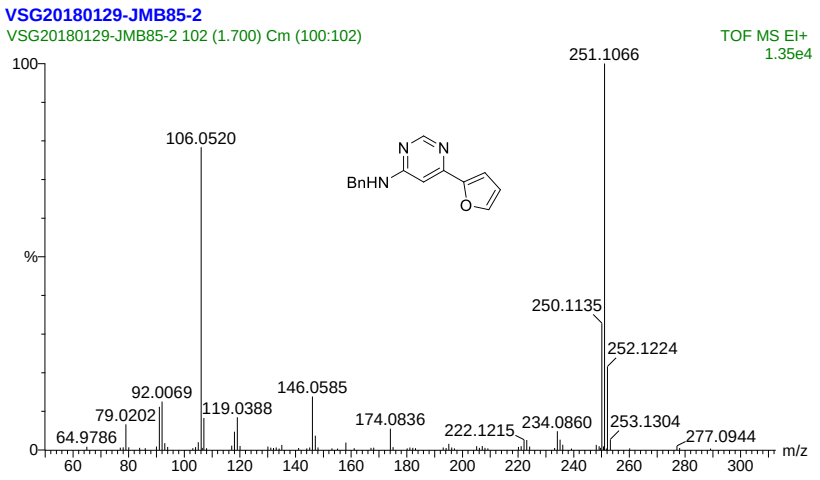


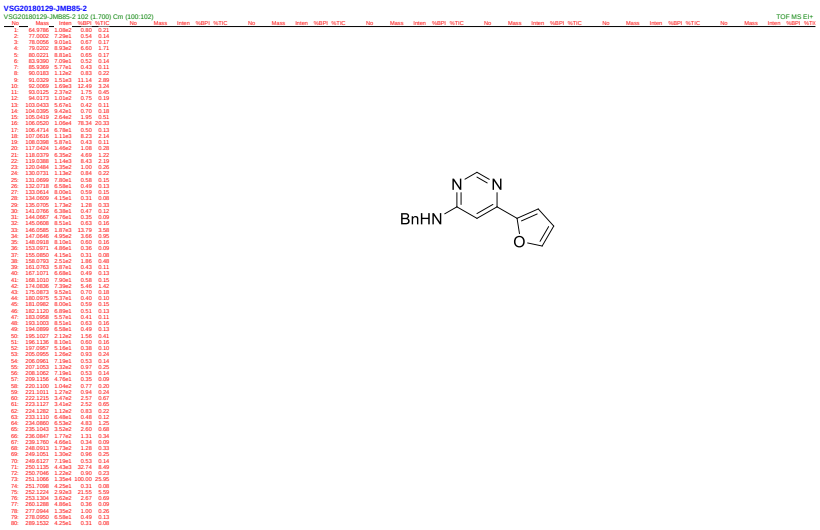
^{1}H NMR spectrum of **16d** (in DMSO-d_6)

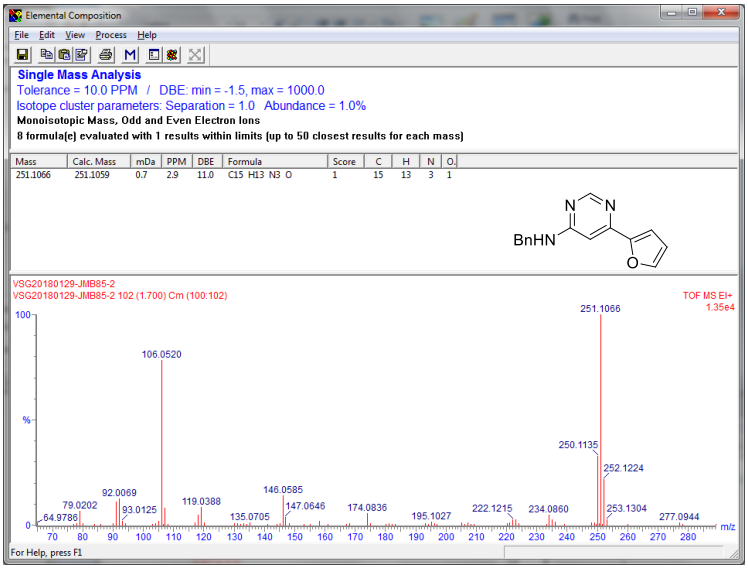


^{13}C NMR spectrum of **16d** (in DMSO-d_6)

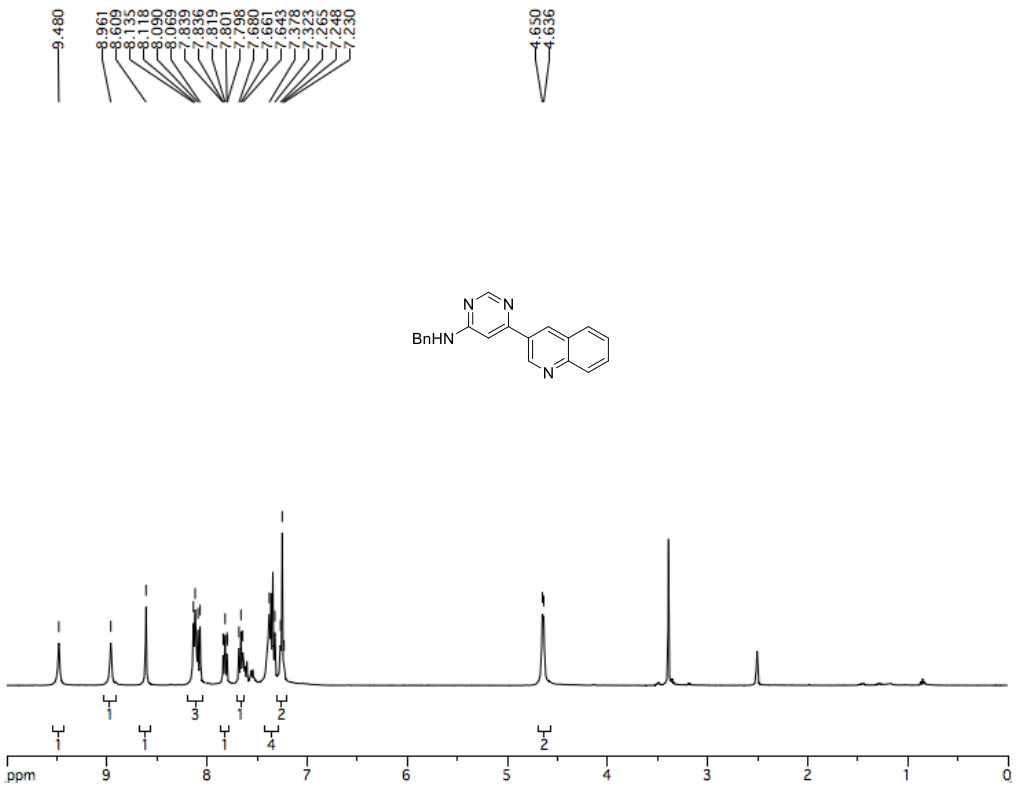




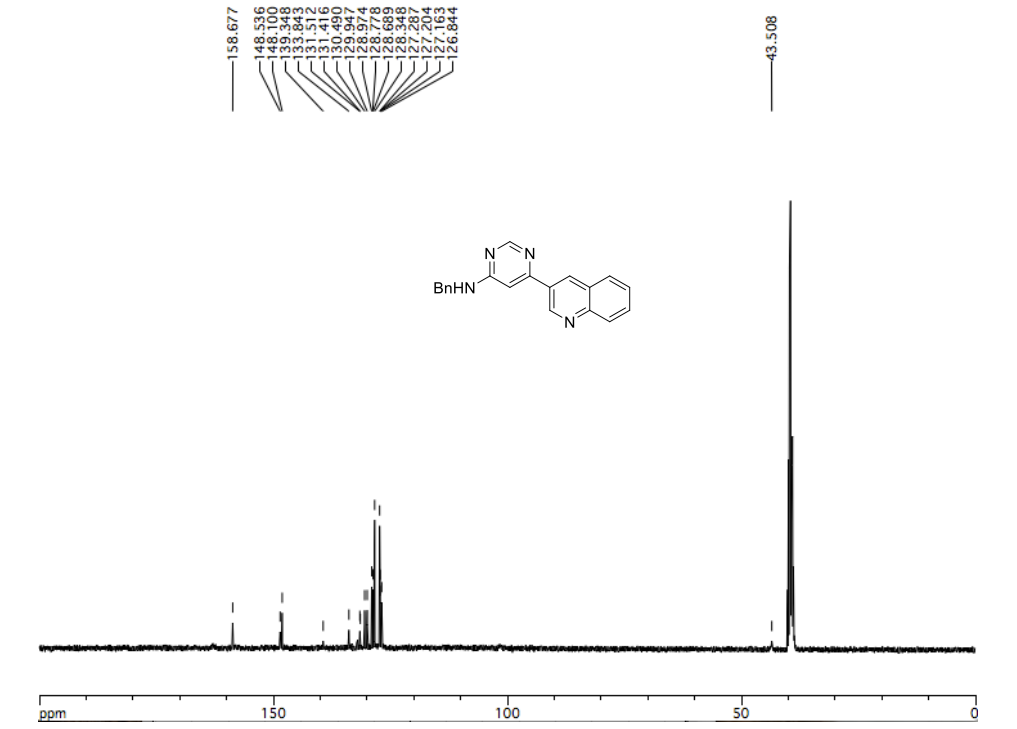




HRMS spectra of **16d**



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

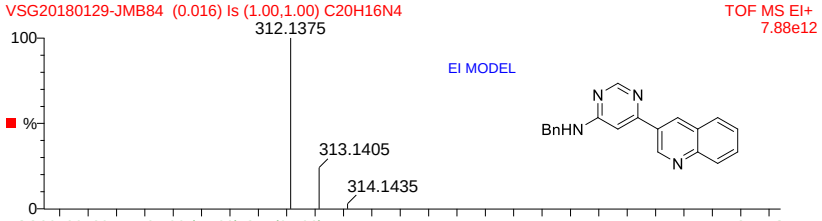


^{13}C NMR spectrum of **16e** (in DMSO-d_6)

VSG20180129-JMB84

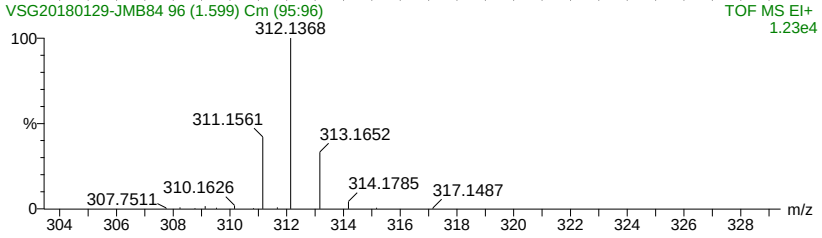
VSG20180129-JMB84 (0.016) Is (1.00,1.00) C20H16N4

TOF MS EI+
7.88e12



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

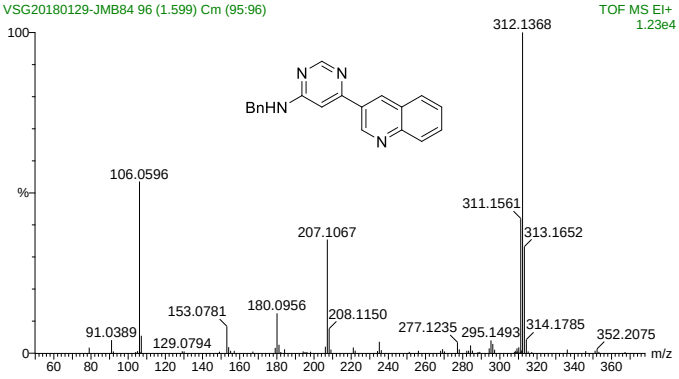
TOF MS EI+
1.23e4

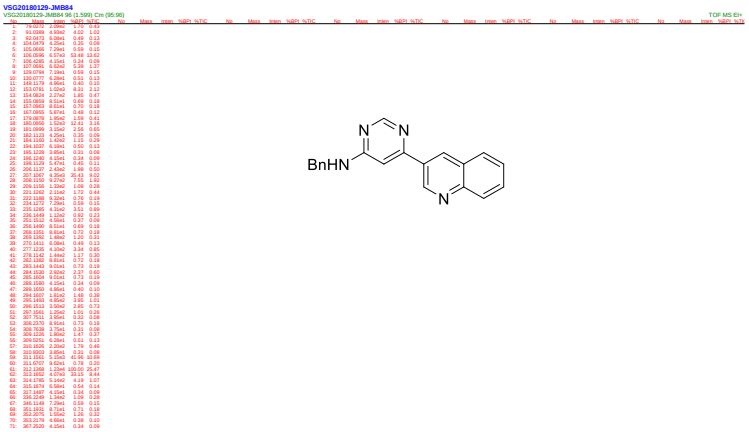


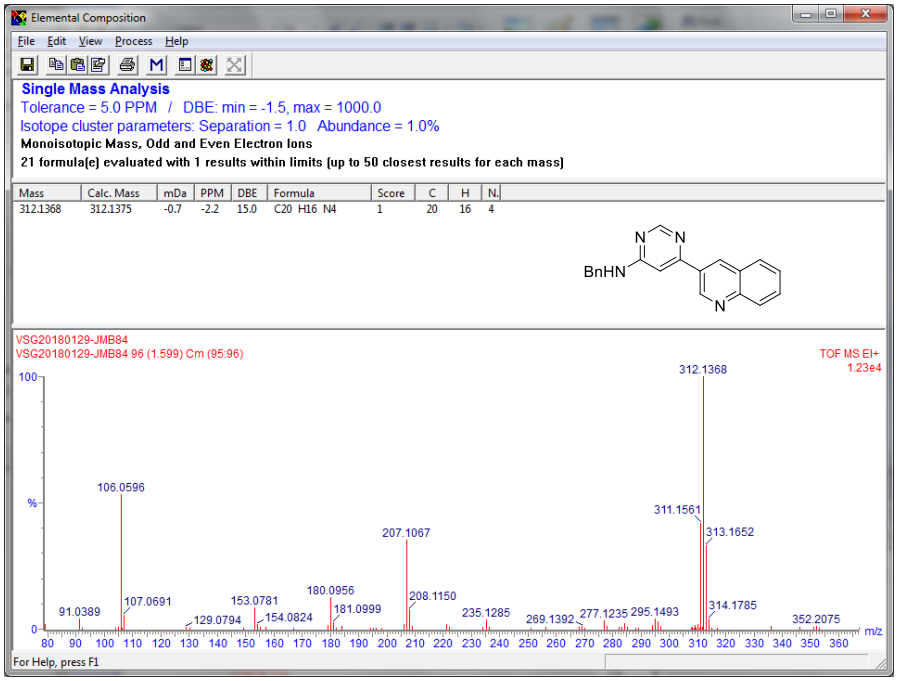
VSG20180129-JMB84

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

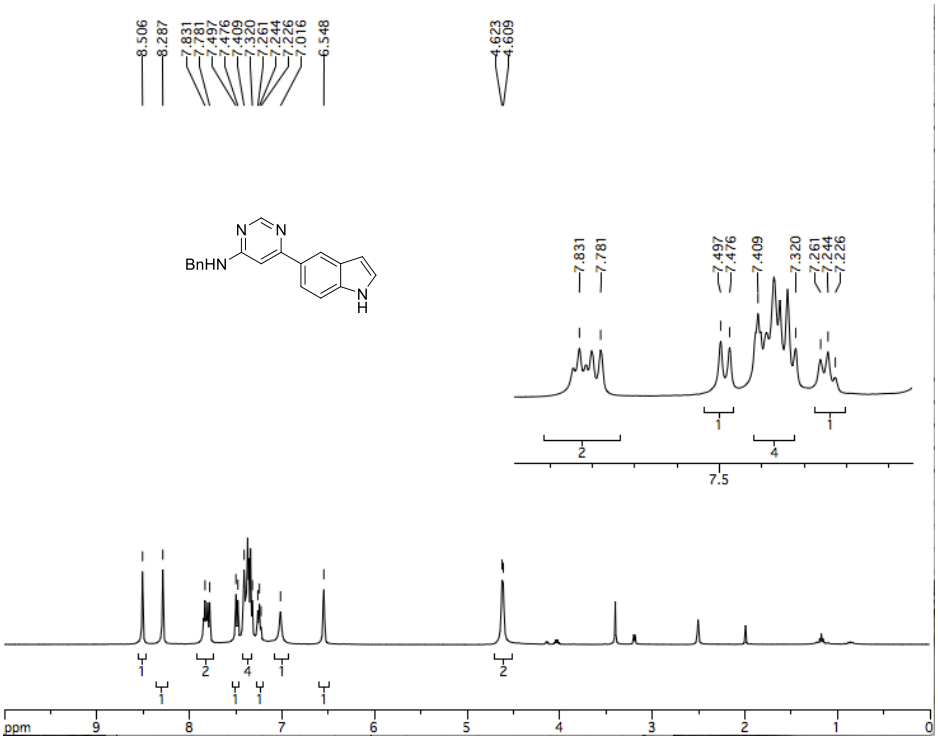
TOF MS EI+
1.23e4



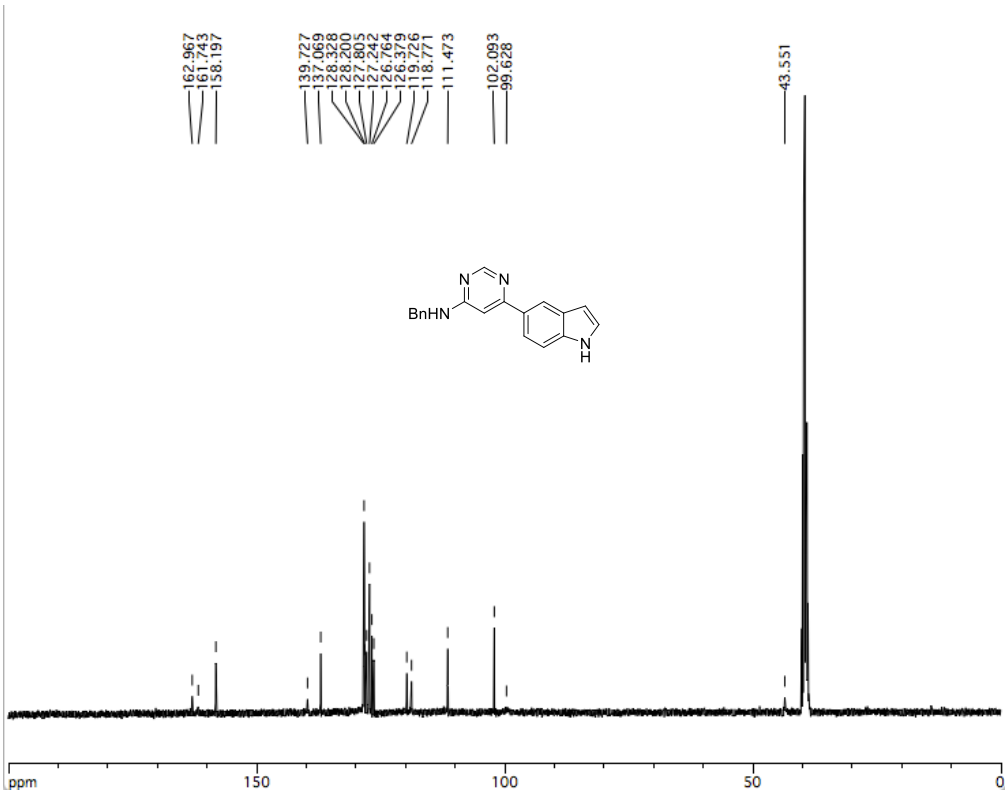




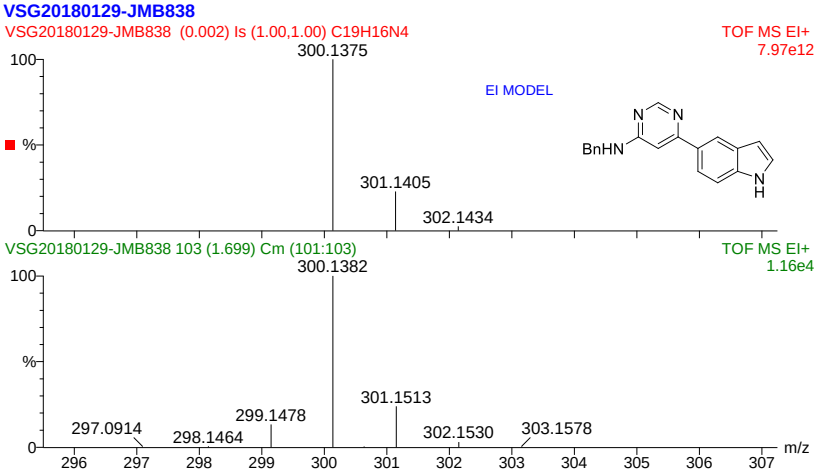
HRMS spectra of **16e**



^{1}H NMR spectrum of **16f** (in DMSO-d_6)

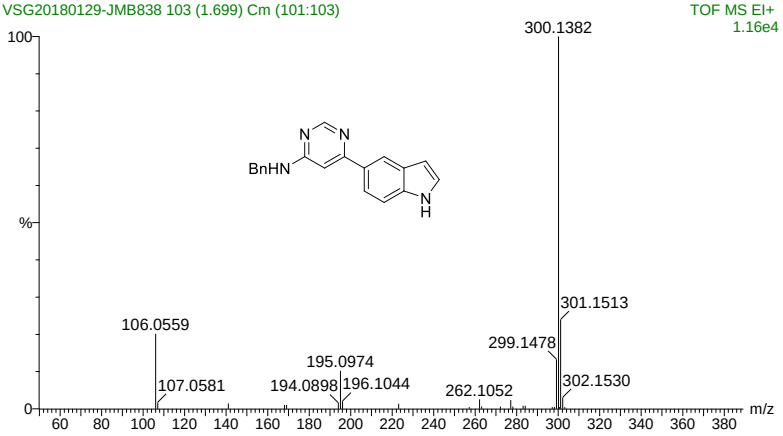


^{13}C NMR spectrum of **16f** (in DMSO-d_6)



VSG20180129-JMB838

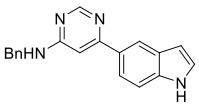
VSG20180129-JMB838 103 (1.699) Cm (101:103) TOF MS EI+ 1.16e4

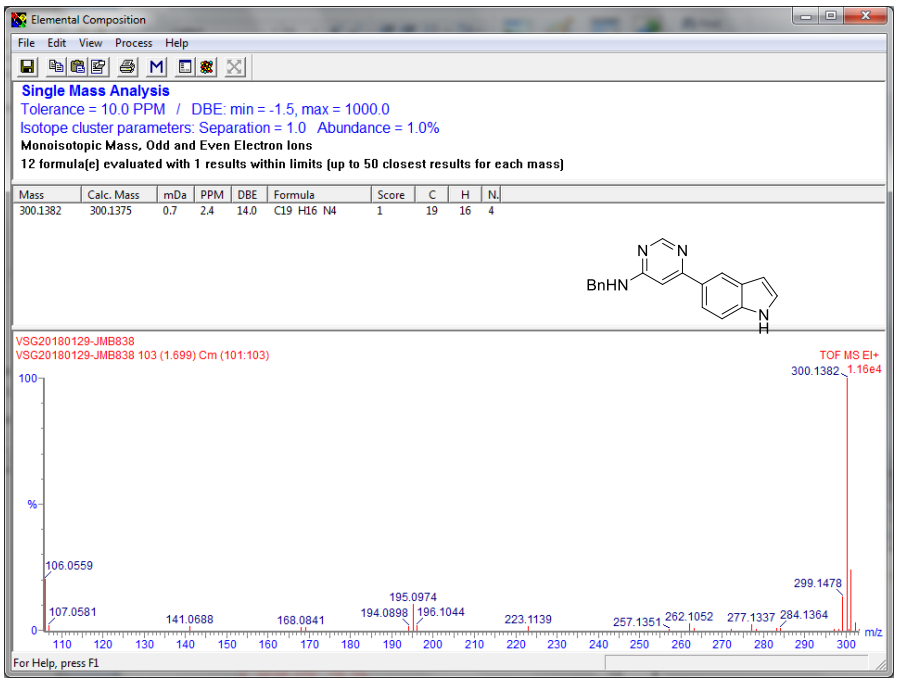


VSG20180129-JMB838

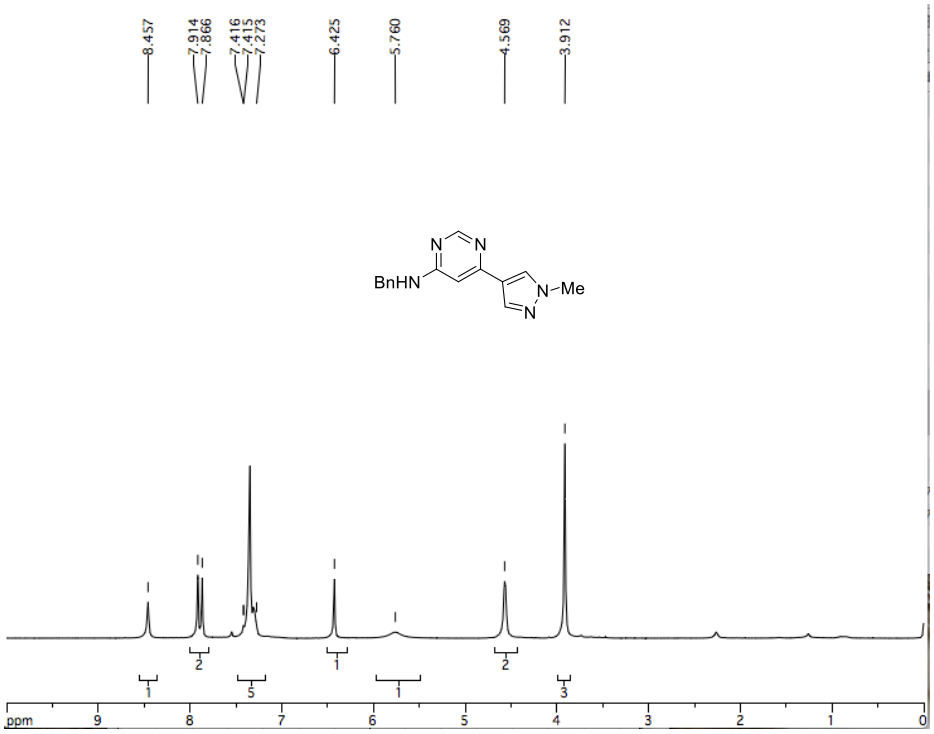
VSG20180129-JMB838 103 (1.699) Cm (101:103) TOF MS EI+

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										

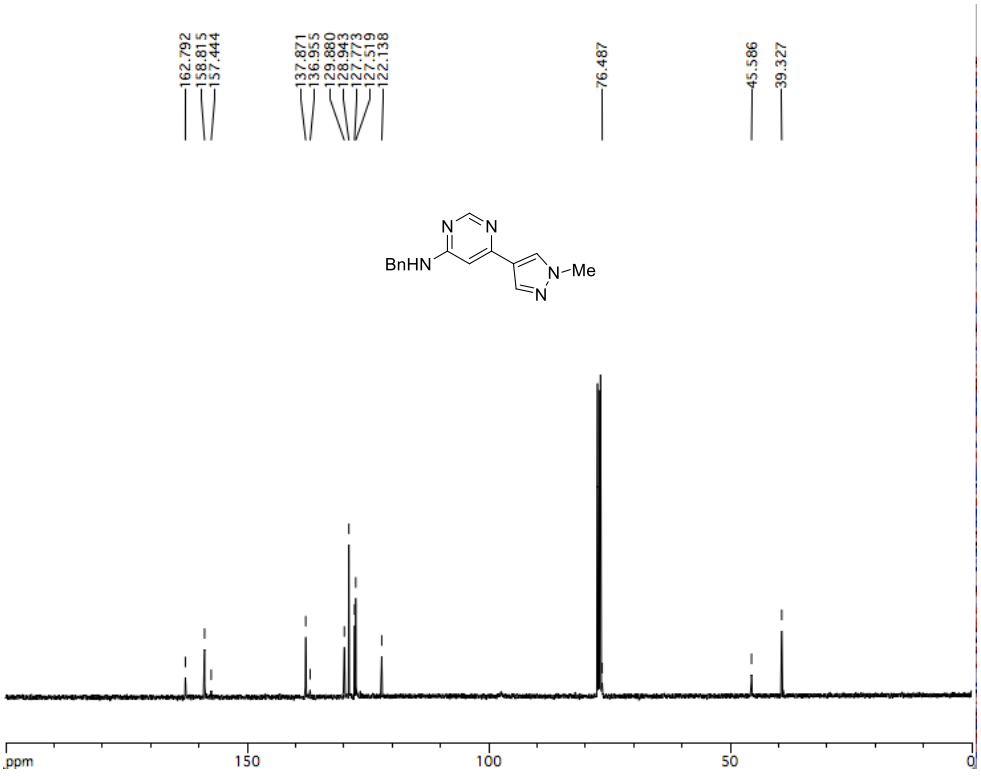




HRMS spectra of **16f**



^{1}H NMR spectrum of **16g** (in $CDCl_3$)

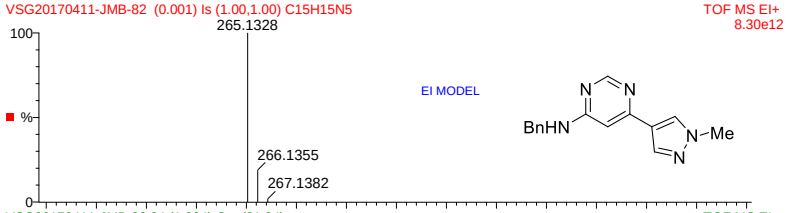


^{13}C NMR spectrum of **16g** (in $CDCl_3$)

VSG20170411-JMB-82

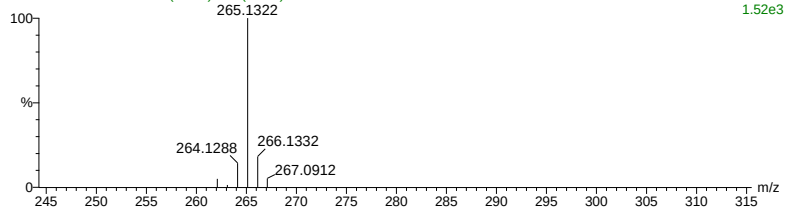
VSG20170411-JMB-82 (0.001) Is (1.00,1.00) C15H15N5

TOF MS EI+
8.30e12



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

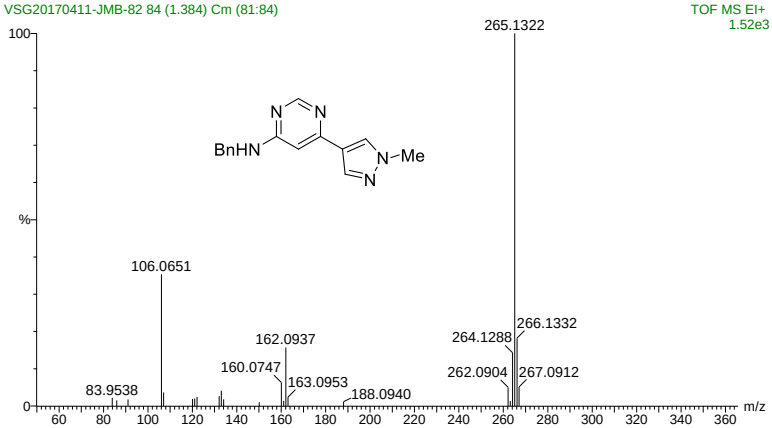
TOF MS EI+
1.52e3



VSG20170411-JMB-82

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

TOF MS EI+
1.52e3

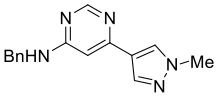


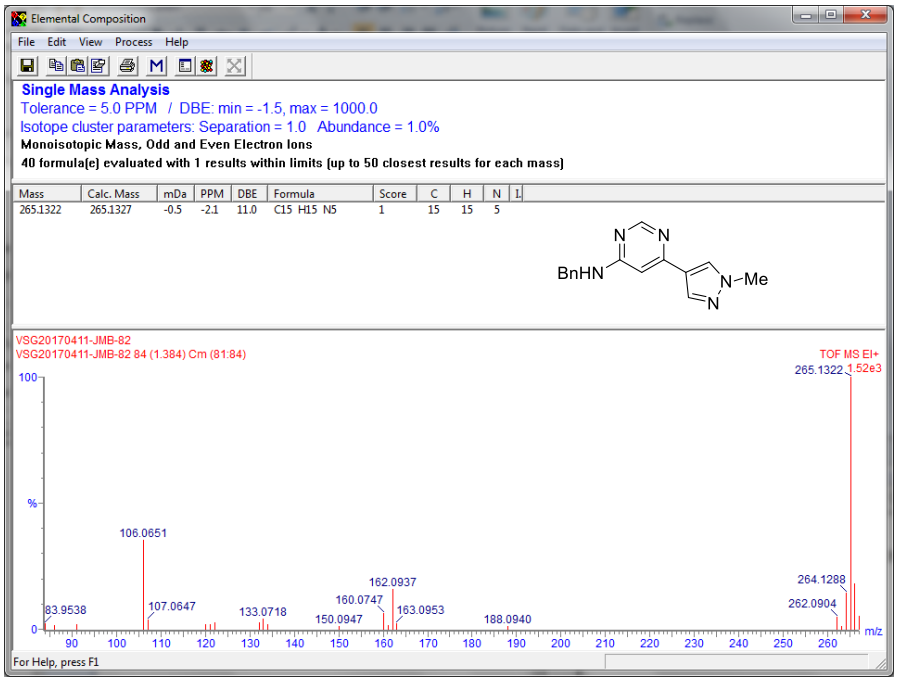
VSG20170411-JMB-82

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

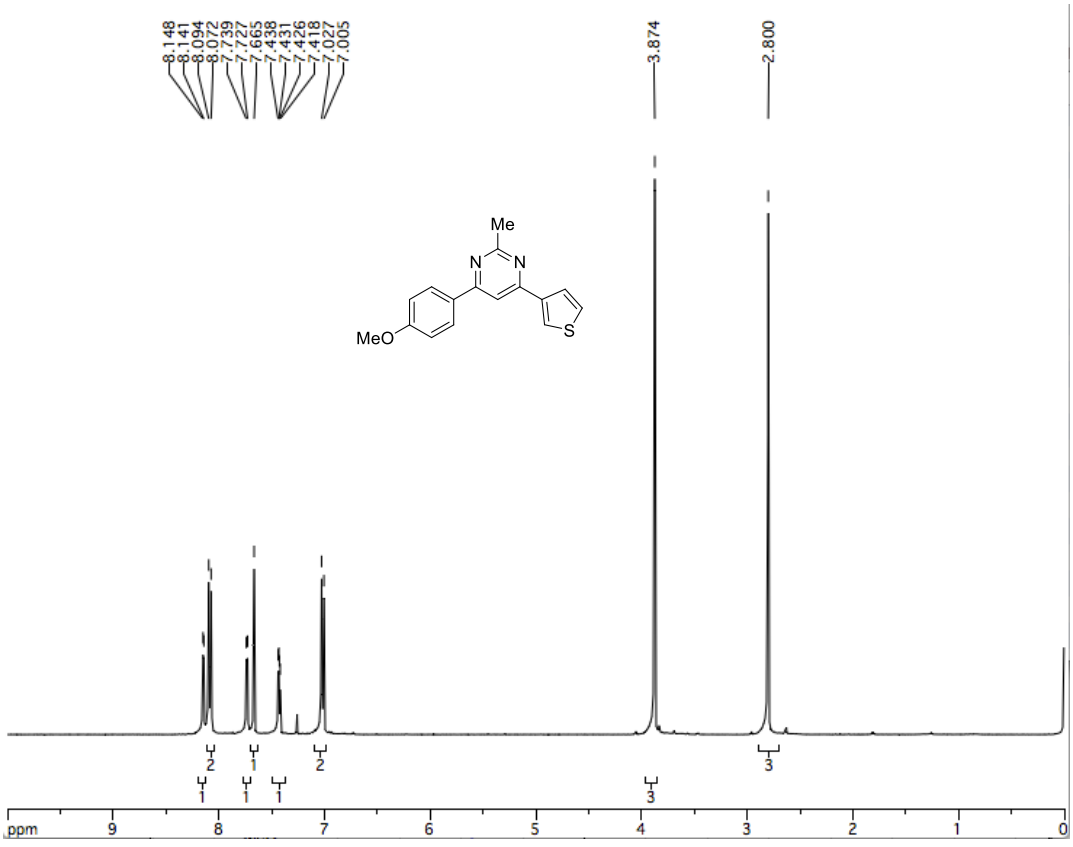
TOF MS EI+

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	2.84e1	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:	133.0718	6.18e1	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:	188.0940	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											

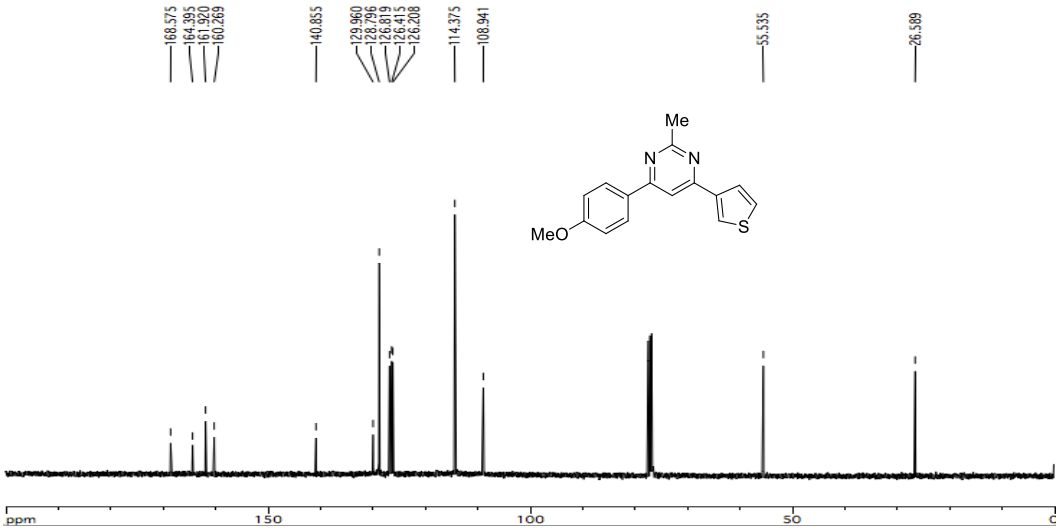




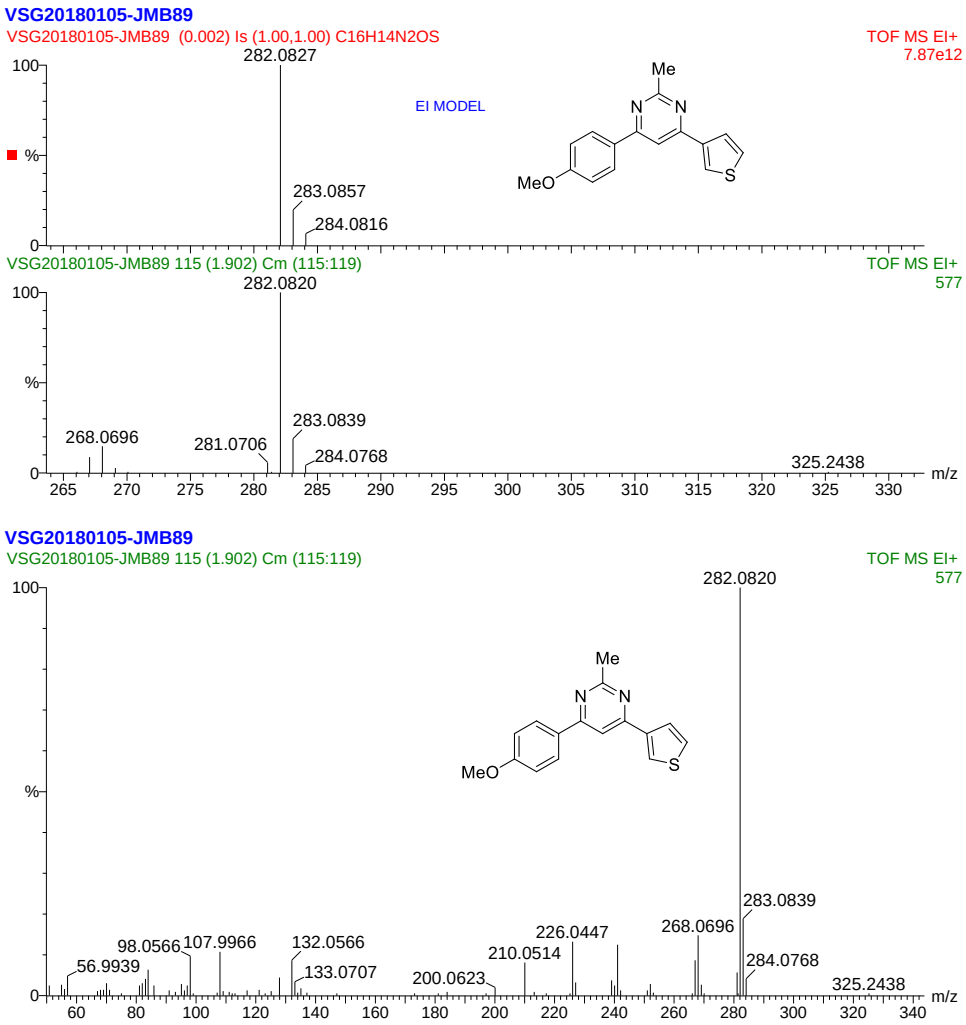
HRMS spectra of **16g**

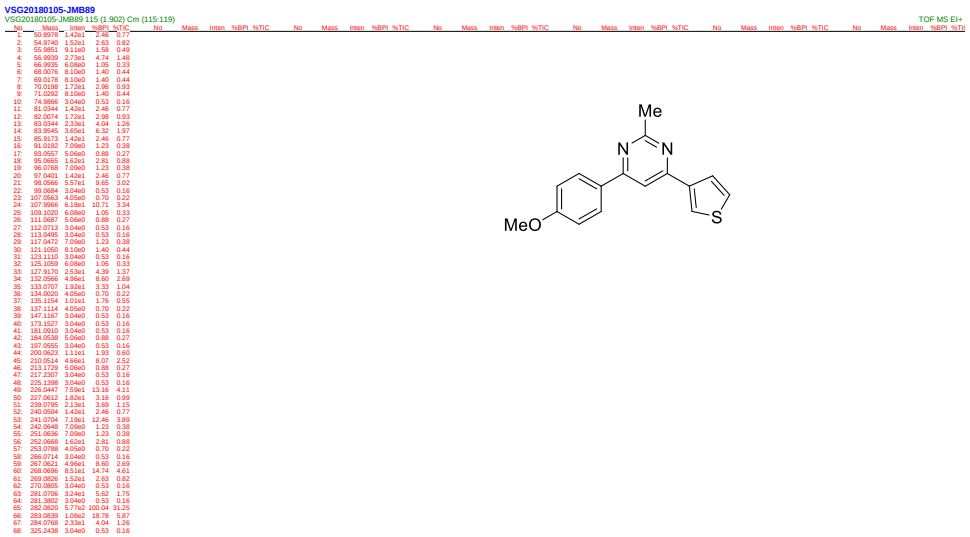


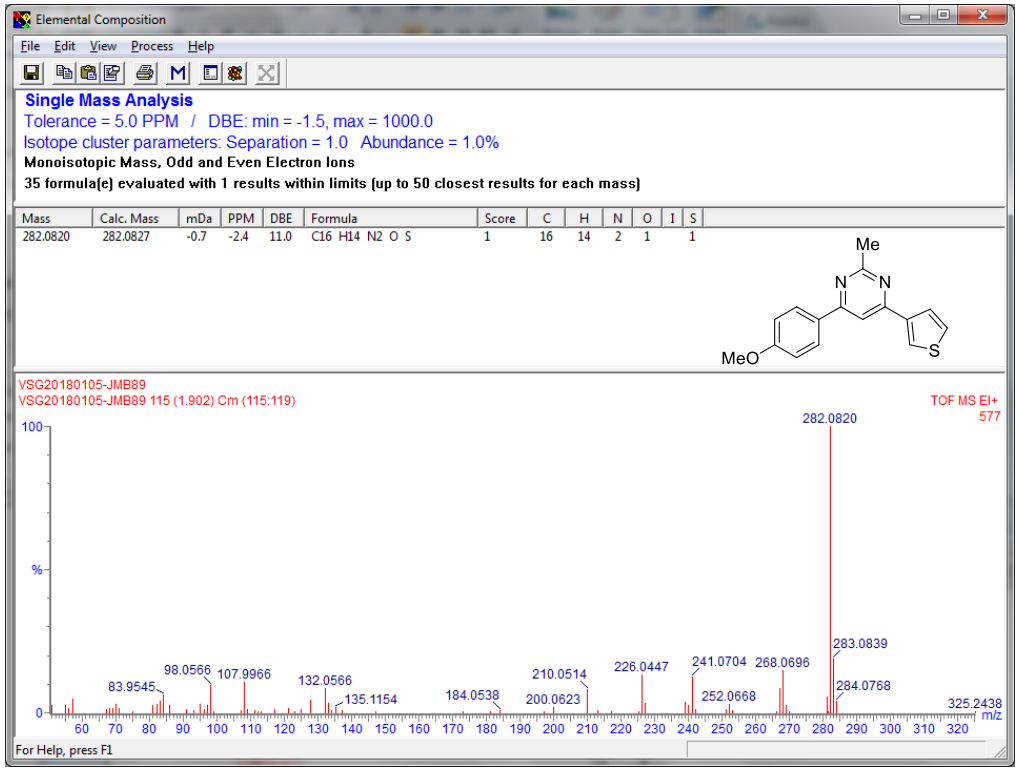
^{1}H NMR spectrum of **16h** (in $CDCl_3$)



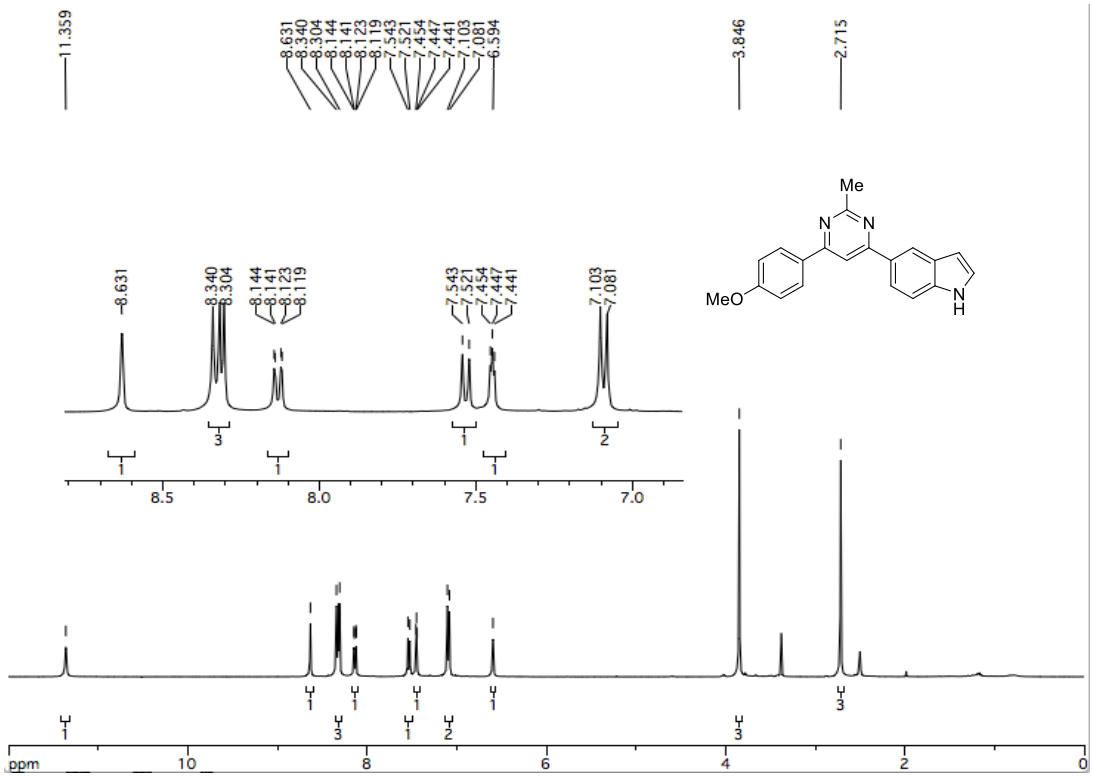
^{13}C NMR spectrum of **16h** (in $CDCl_3$)



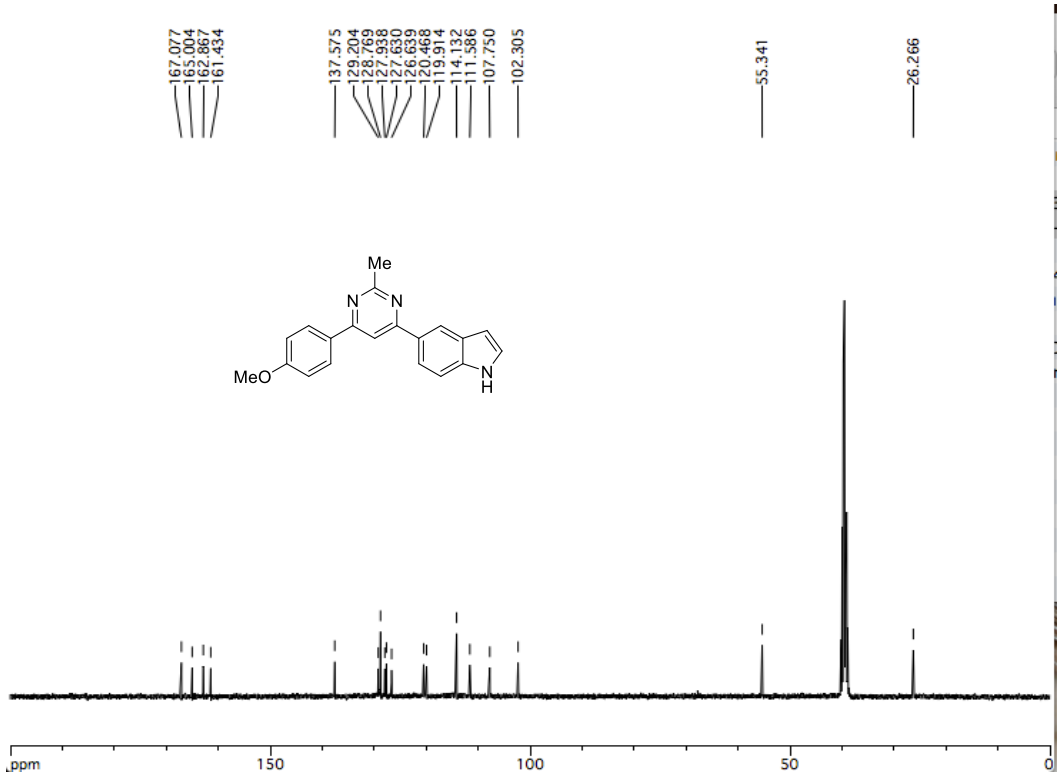




HRMS spectra of **16h**



^{1}H NMR spectrum of **16i** (in DMSO-d_6)

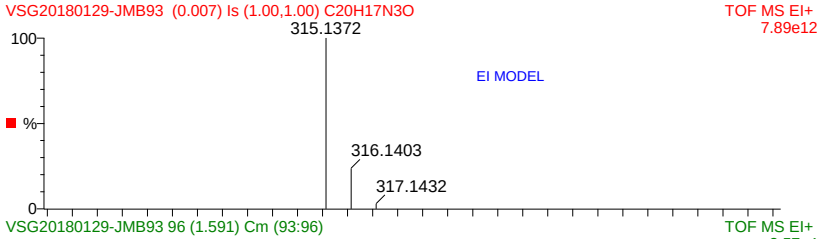


^{13}C NMR spectrum of **16i** (in DMSO-d_6)

VSG20180129-JMB93

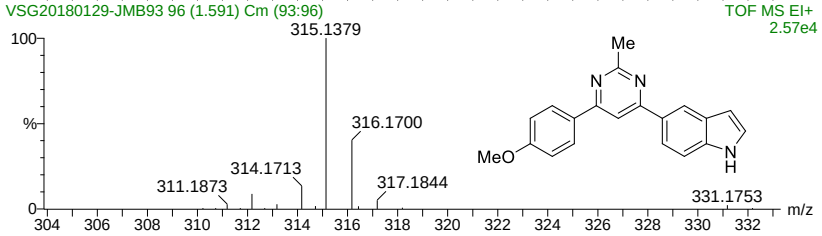
VSG20180129-JMB93 (0.007) Is (1.00,1.00) C20H17N3O

TOF MS EI+
7.89e12



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

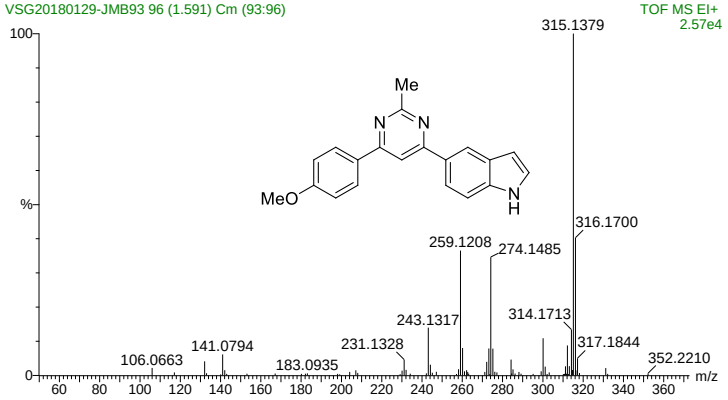
TOF MS EI+
2.57e4

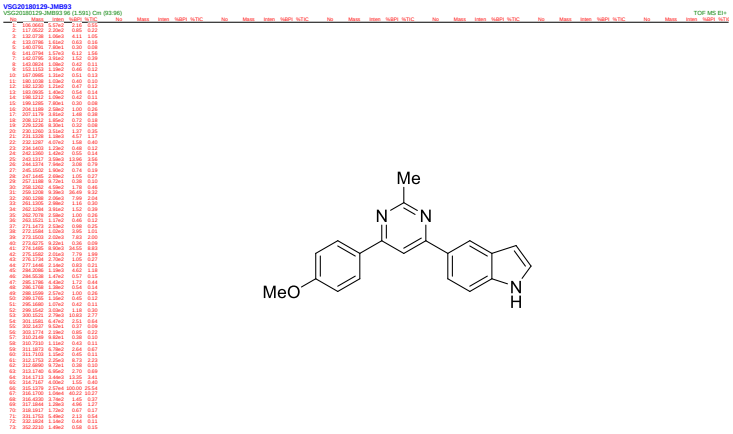


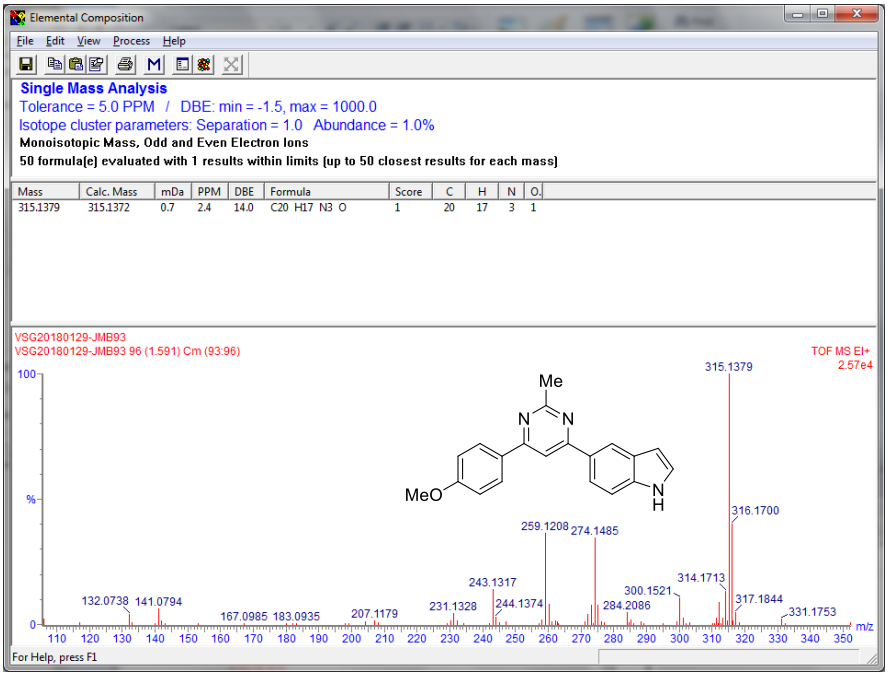
VSG20180129-JMB93

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

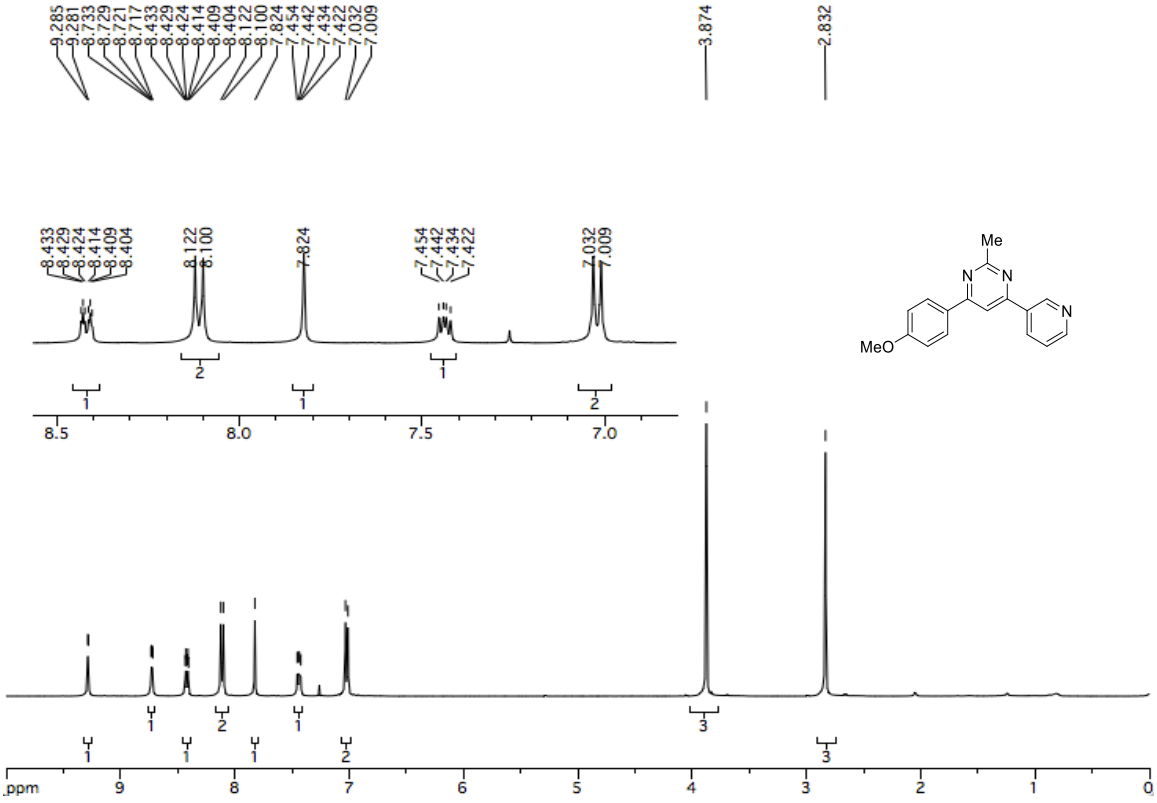
TOF MS EI+
2.57e4



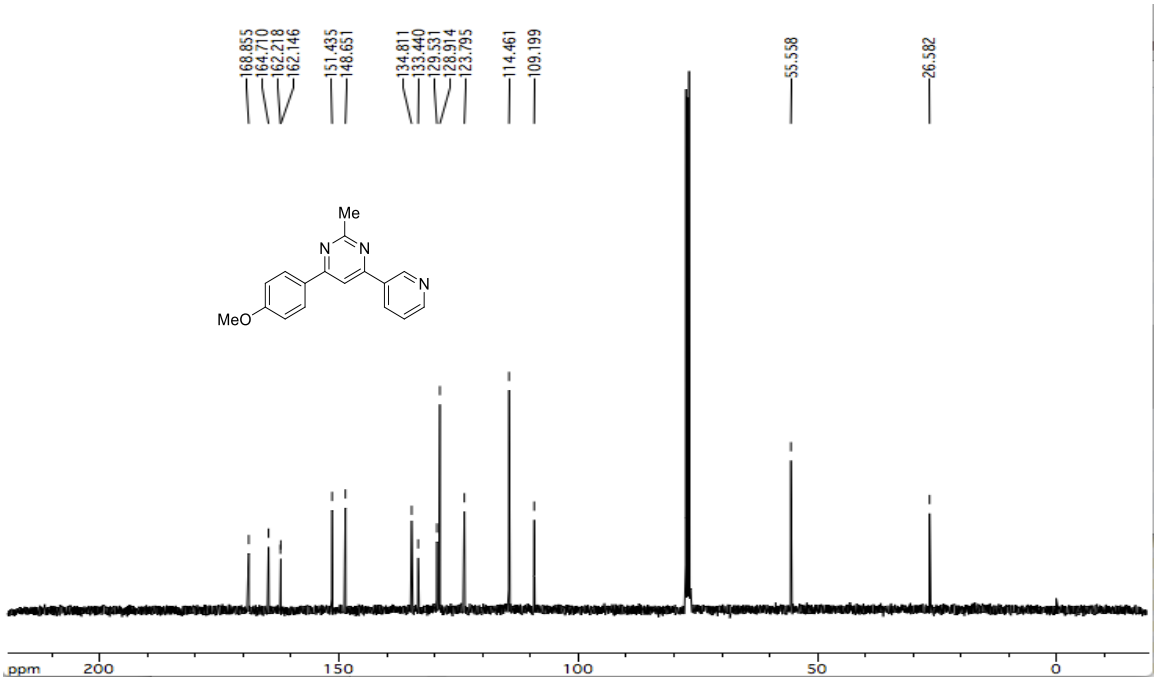




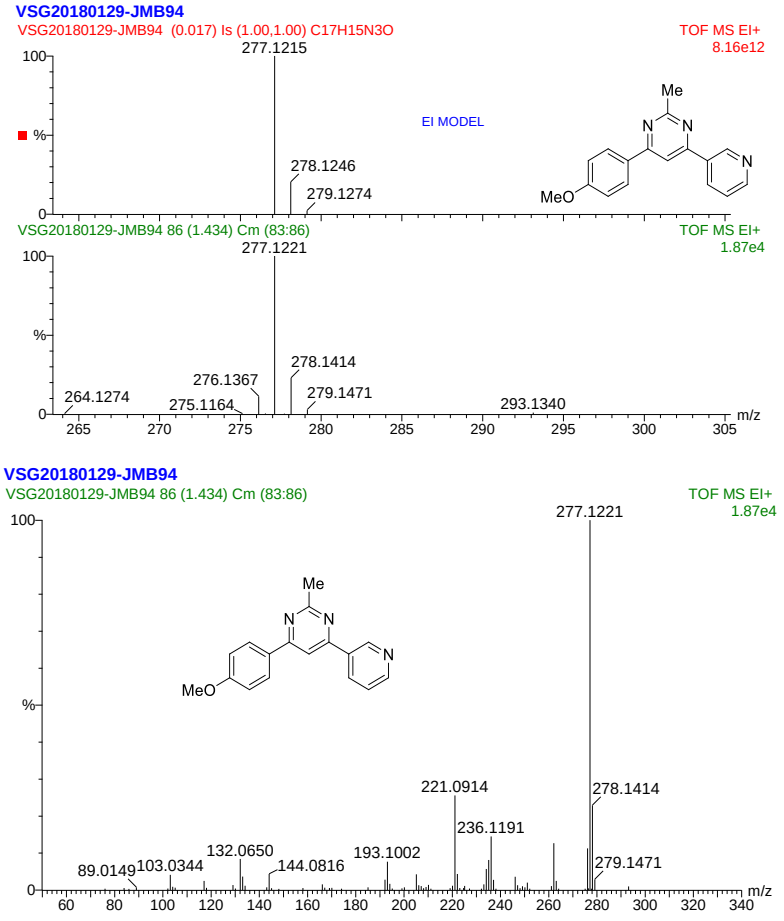
HRMS spectra of **16i**

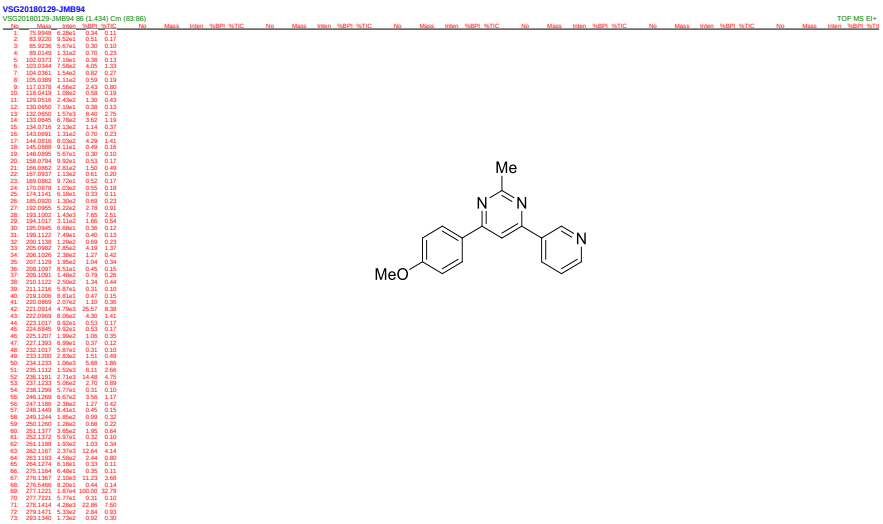


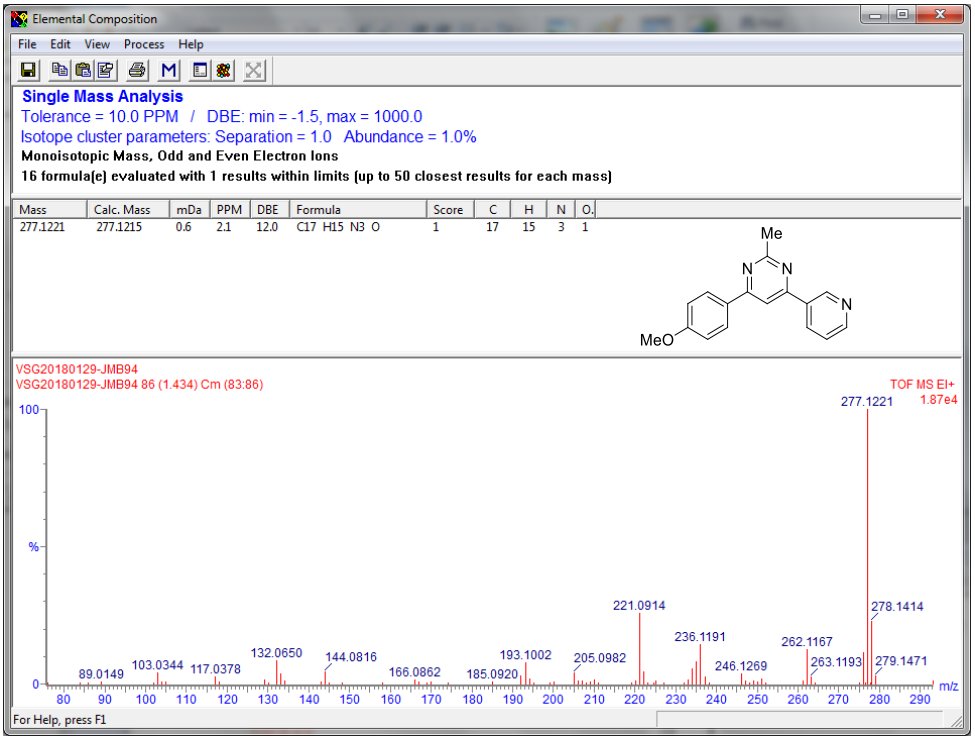
^{1}H NMR spectrum of **16j** (in $CDCl_3$)



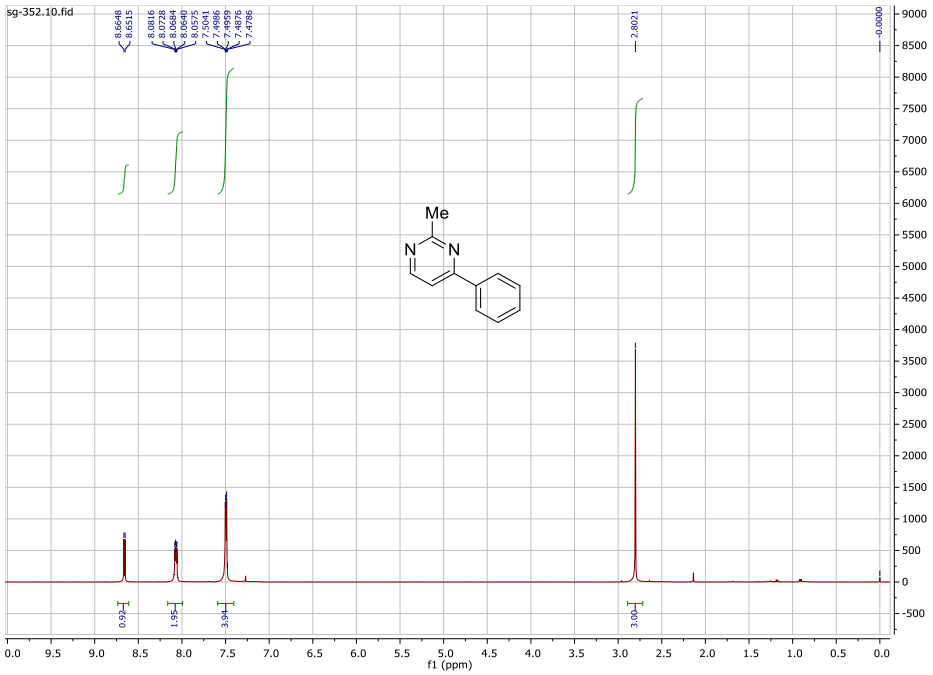
^{13}C NMR spectrum of **16j** (in $CDCl_3$)



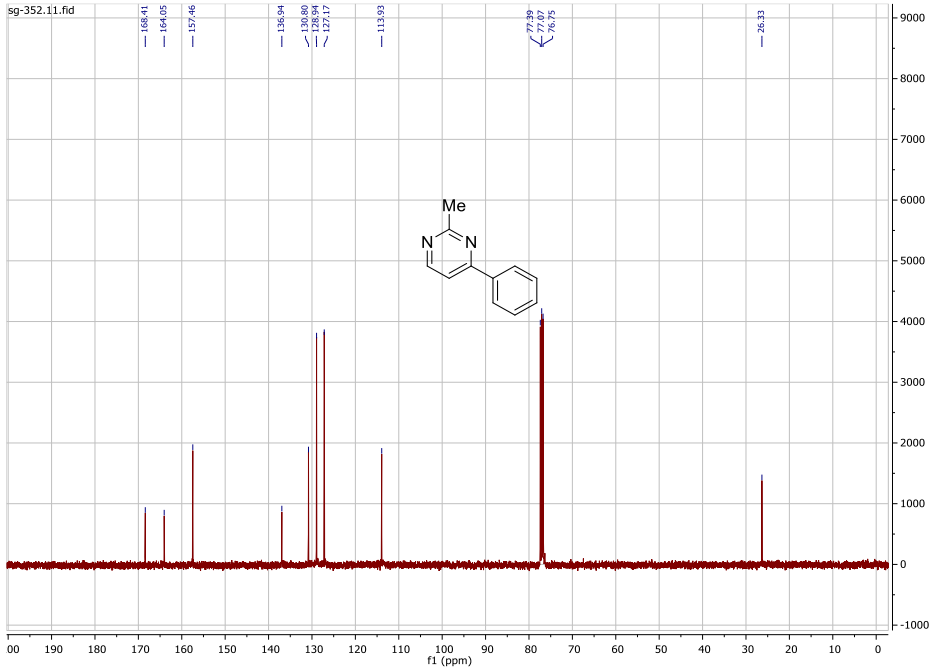




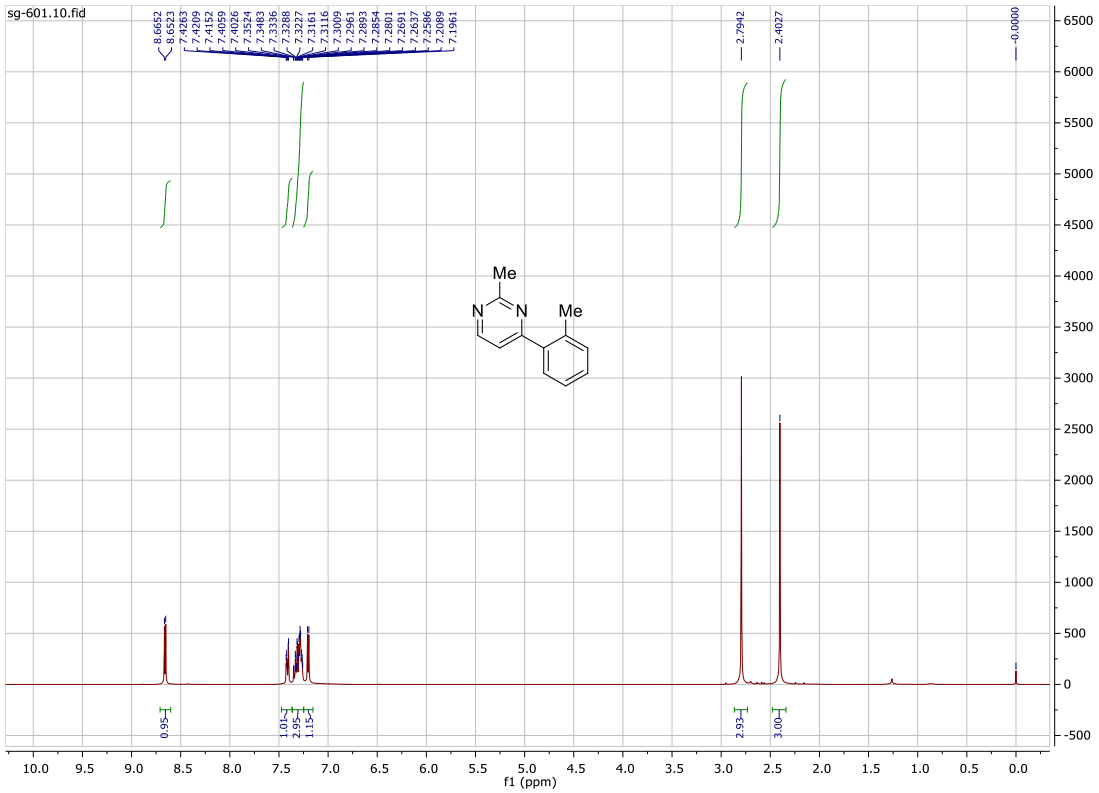
HRMS spectra of **16j**



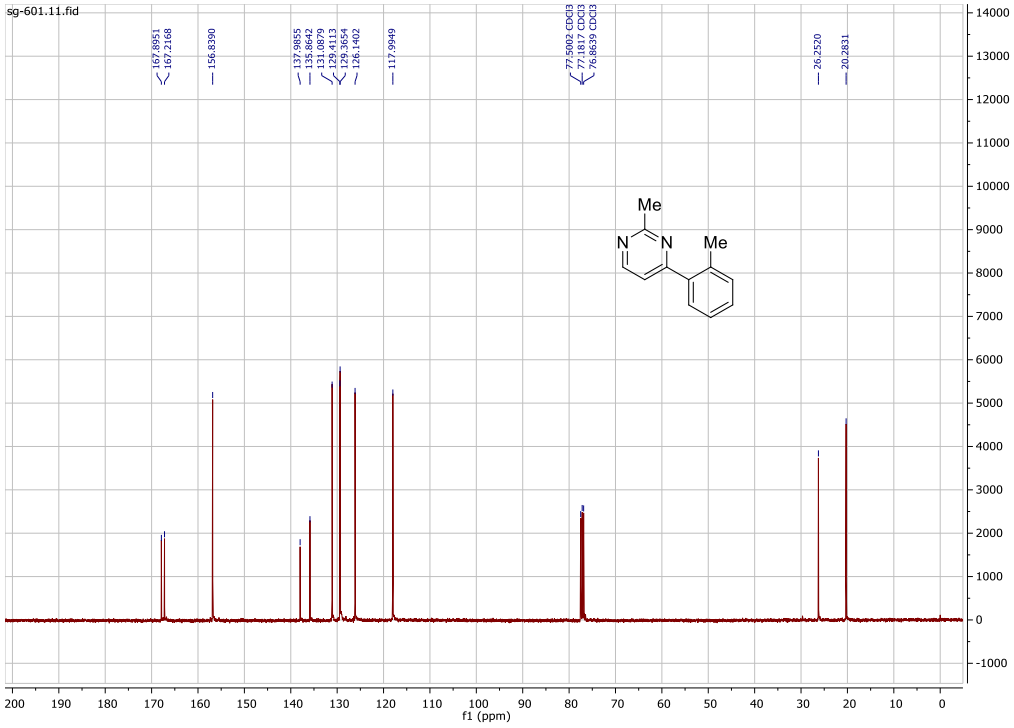
^{1}H NMR spectrum of **17a** (in $CDCl_3$)



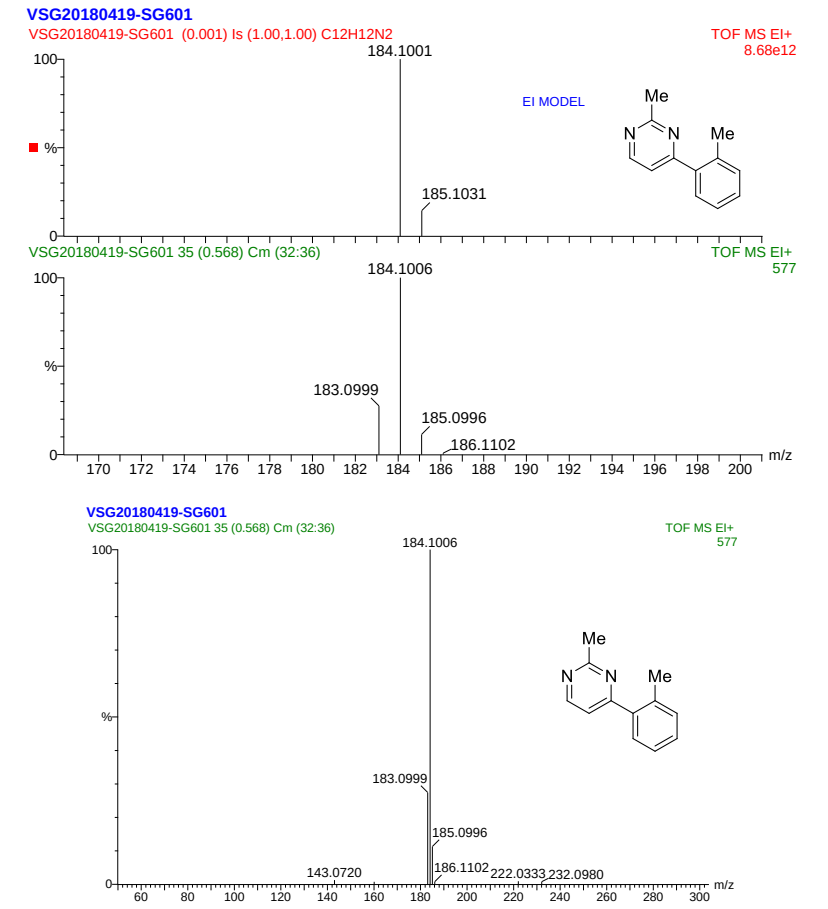
^{13}C NMR spectrum of **17a** (in $CDCl_3$)

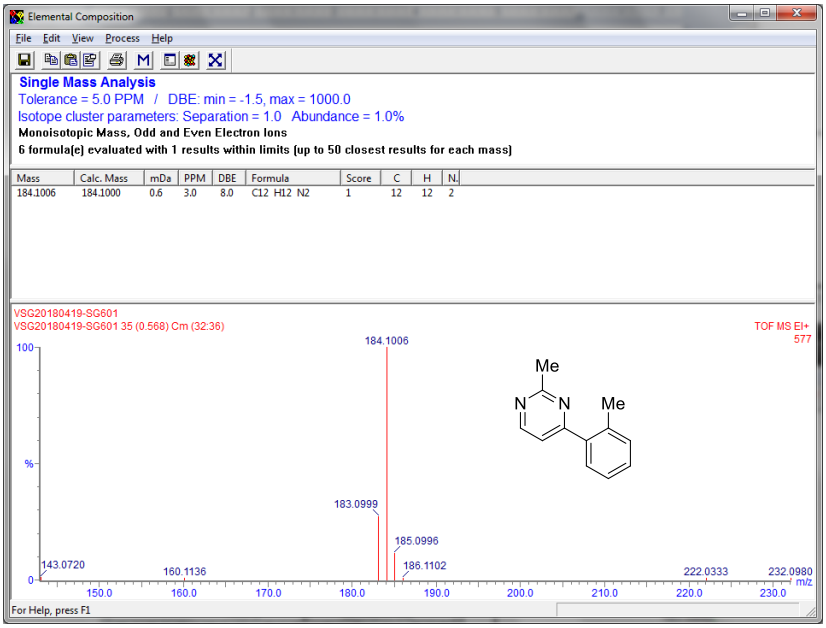


^{1}H NMR spectrum of **17b** (in $CDCl_3$)

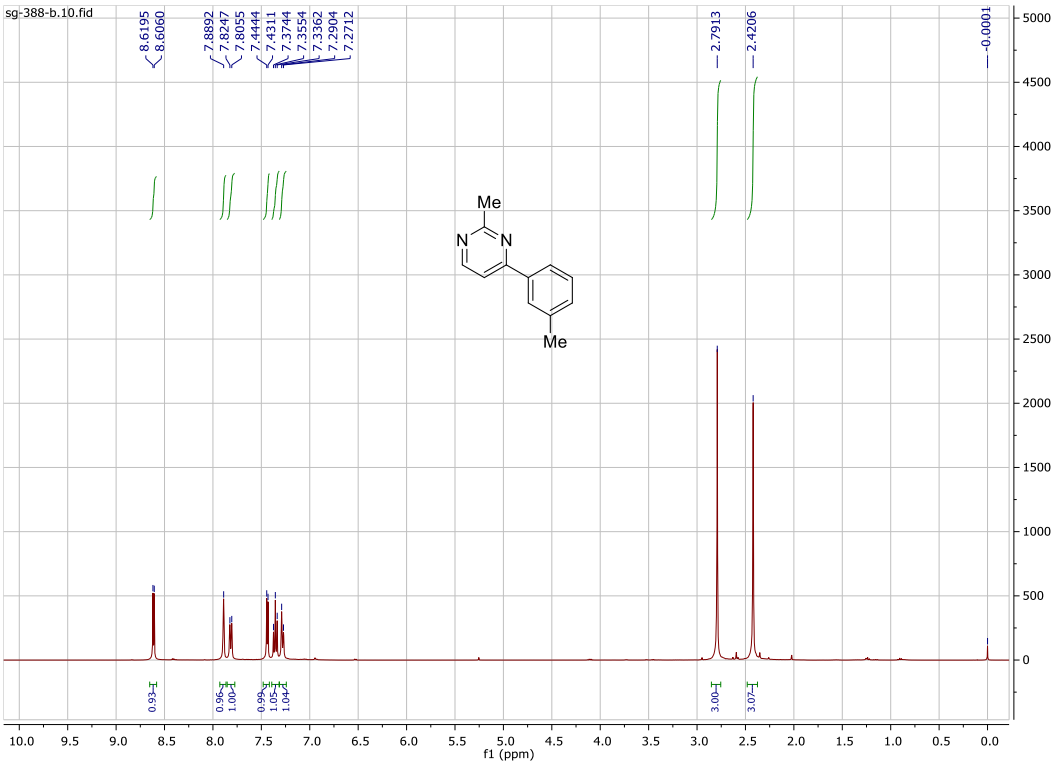


^{13}C NMR spectrum of **17b** (in $CDCl_3$)

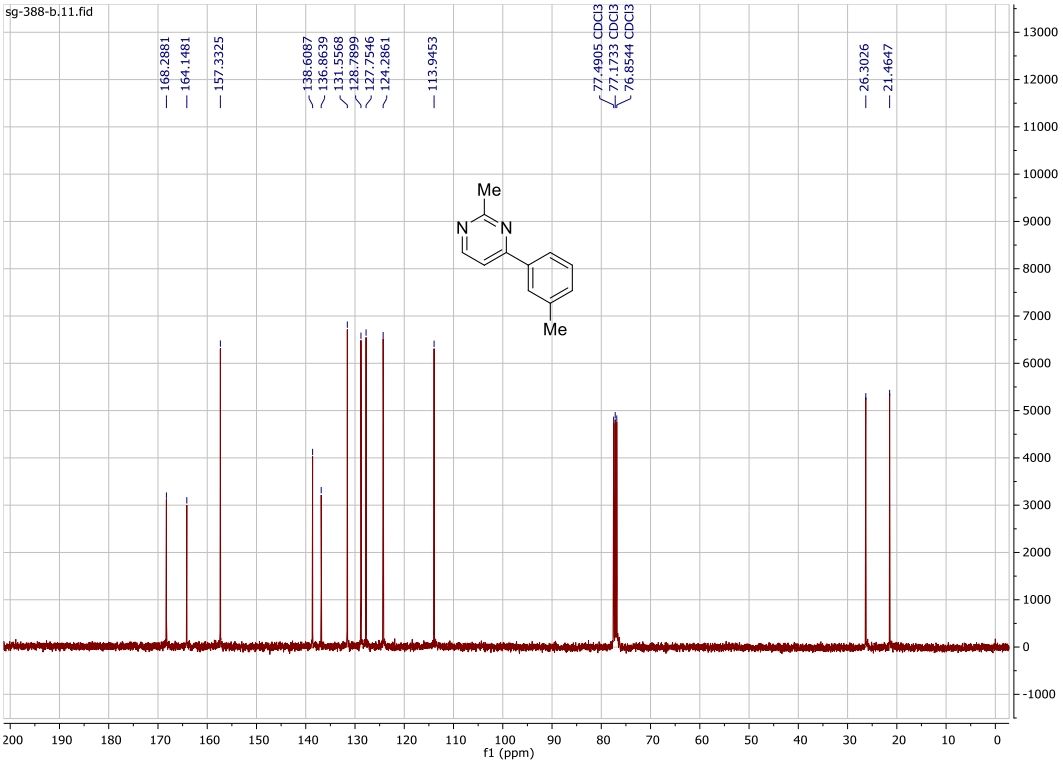




HRMS spectra of **17b**



^{1}H NMR spectrum of **17c** (in $CDCl_3$)

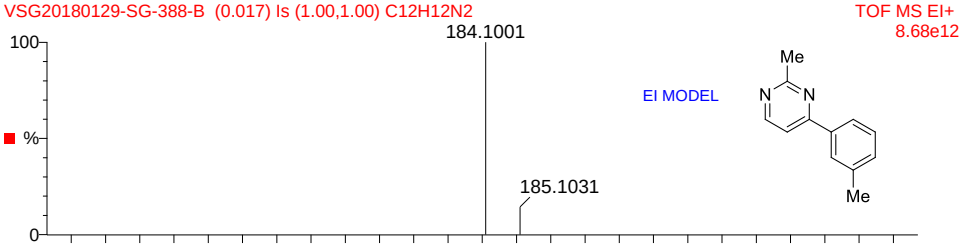


^{13}C NMR spectrum of **17c** (in $CDCl_3$)

VSG20180129-SG-388-B

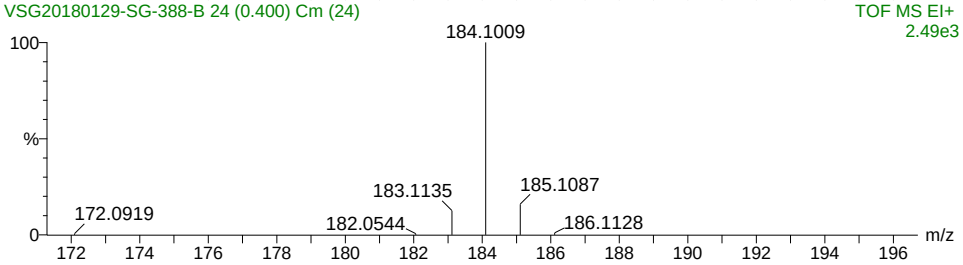
VSG20180129-SG-388-B (0.017) Is (1.00,1.00) C12H12N2

TOF MS EI+
8.68e12



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

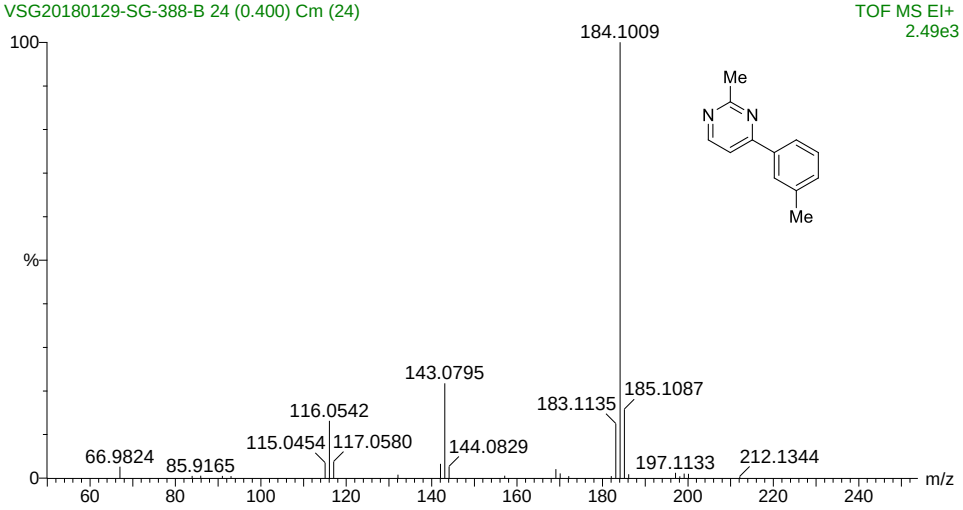
TOF MS EI+
2.49e3



VSG20180129-SG-388-B

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

TOF MS EI+
2.49e3

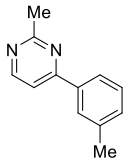


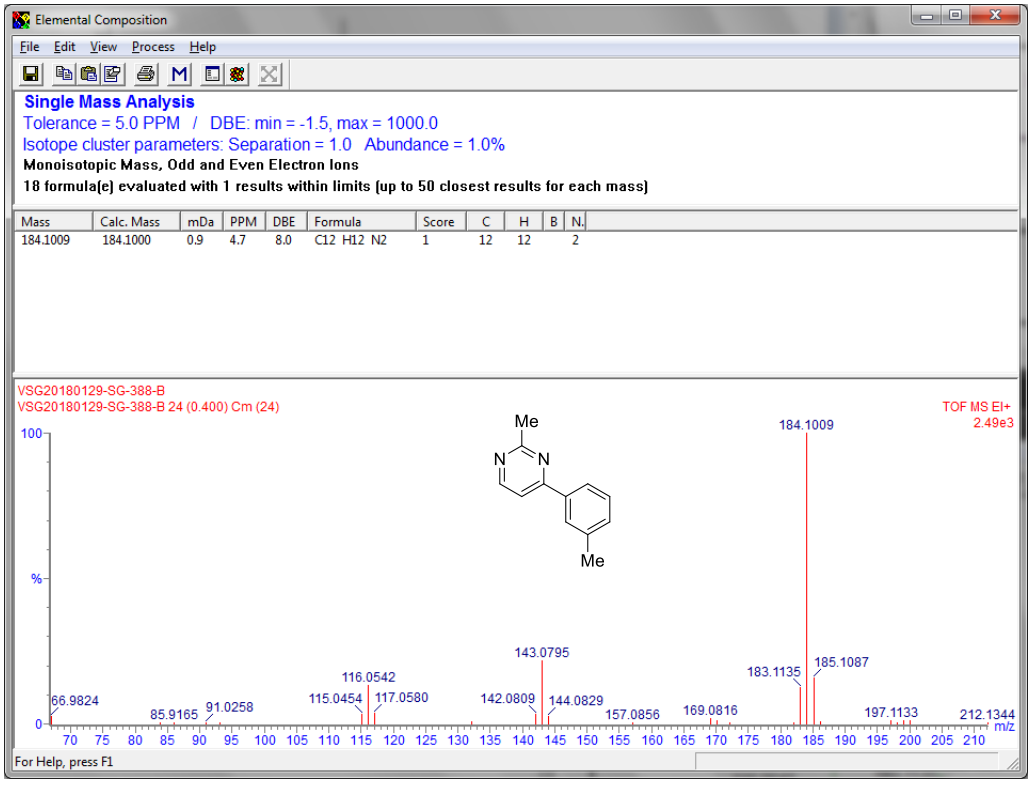
VSG20180129-SG-388-B

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

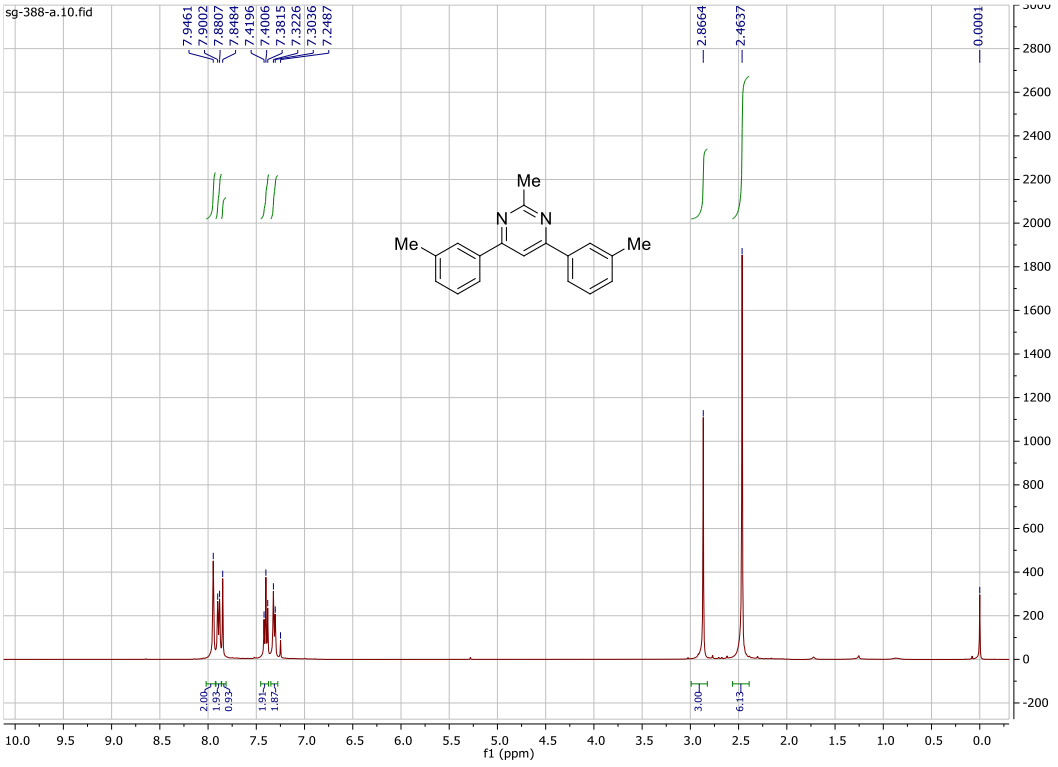
TOF MS EI+

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										

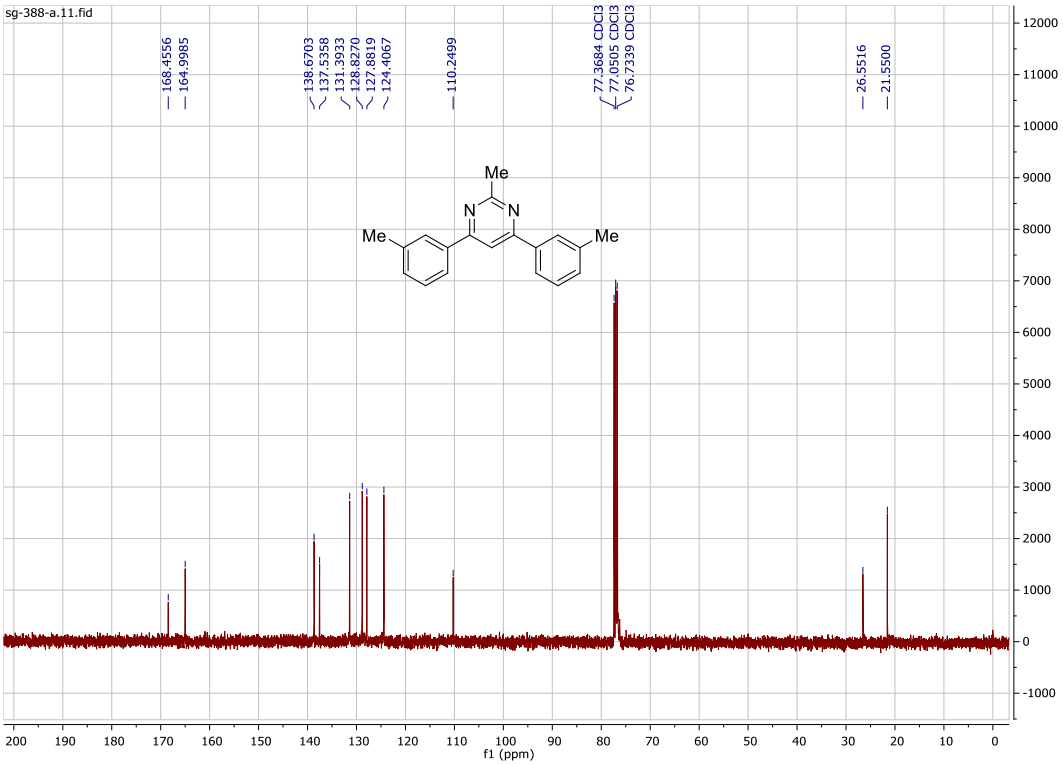




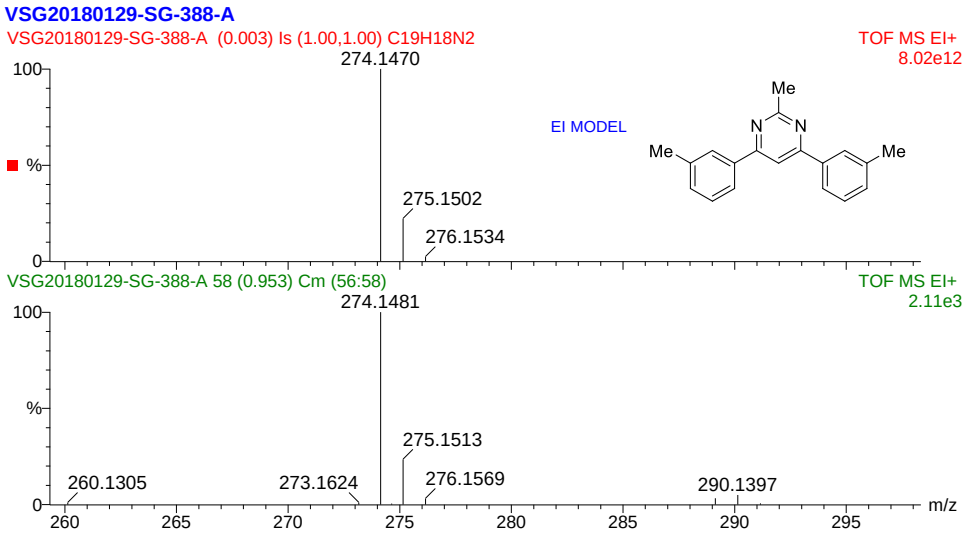
HRMS spectra of **17c**

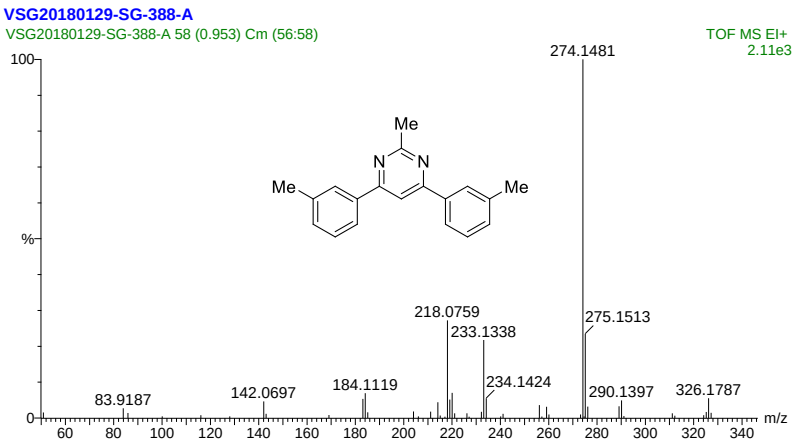


^{1}H NMR spectrum of **8c** (in $CDCl_3$)



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

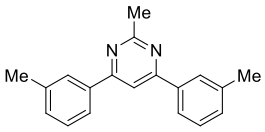


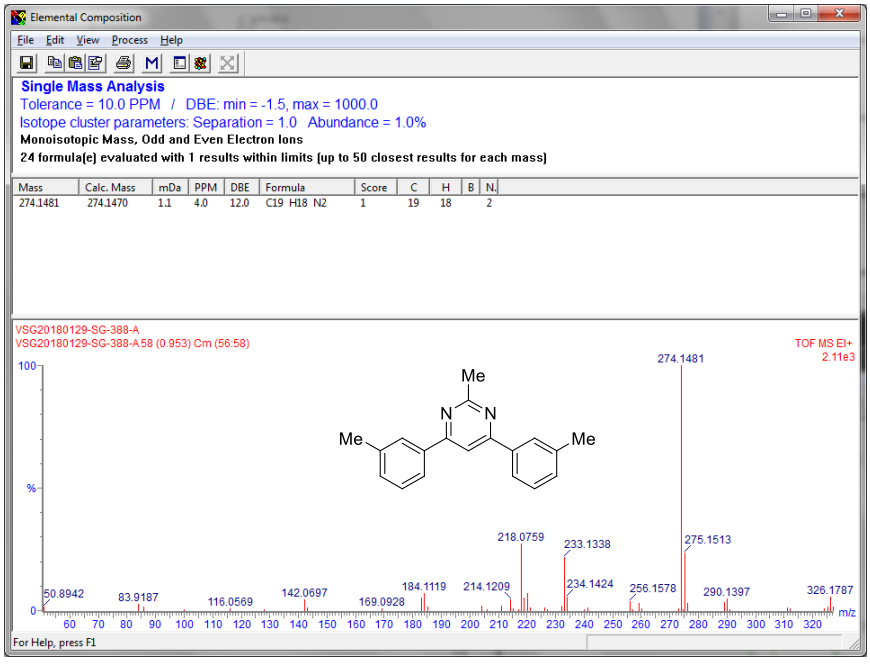


VSG20180129-SG-388-A

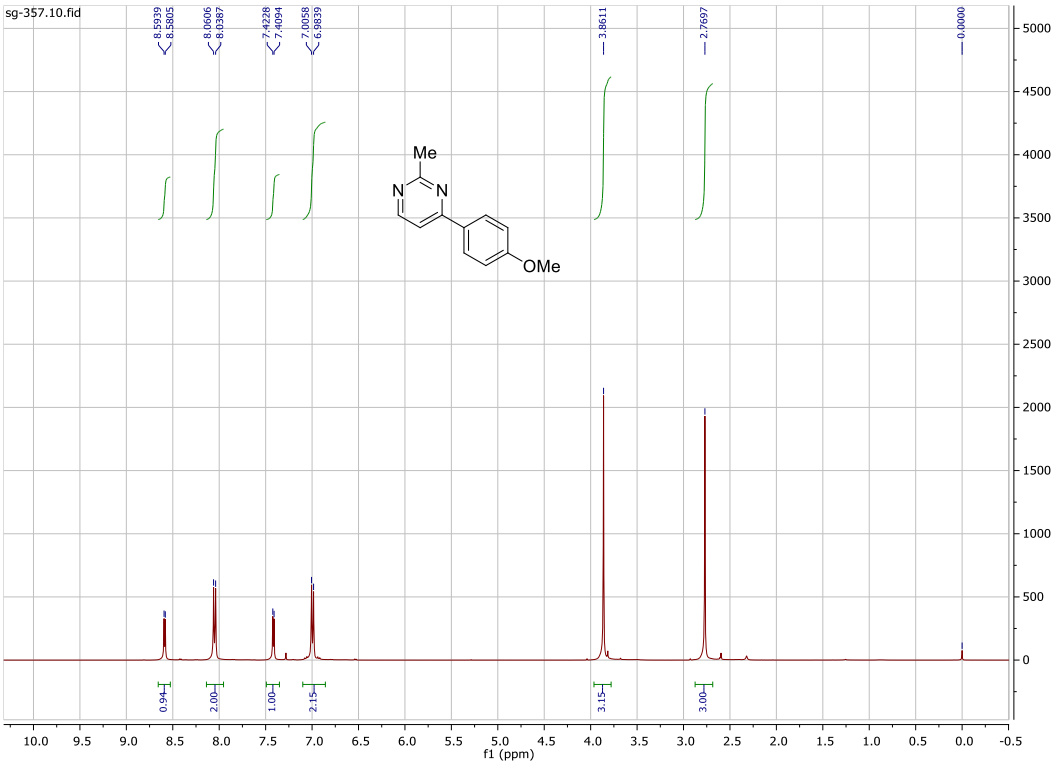
VSG20180129-SG-388-A 58 (0.953) Cm (56:58) TOF MS EI+

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:	220.0680	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										

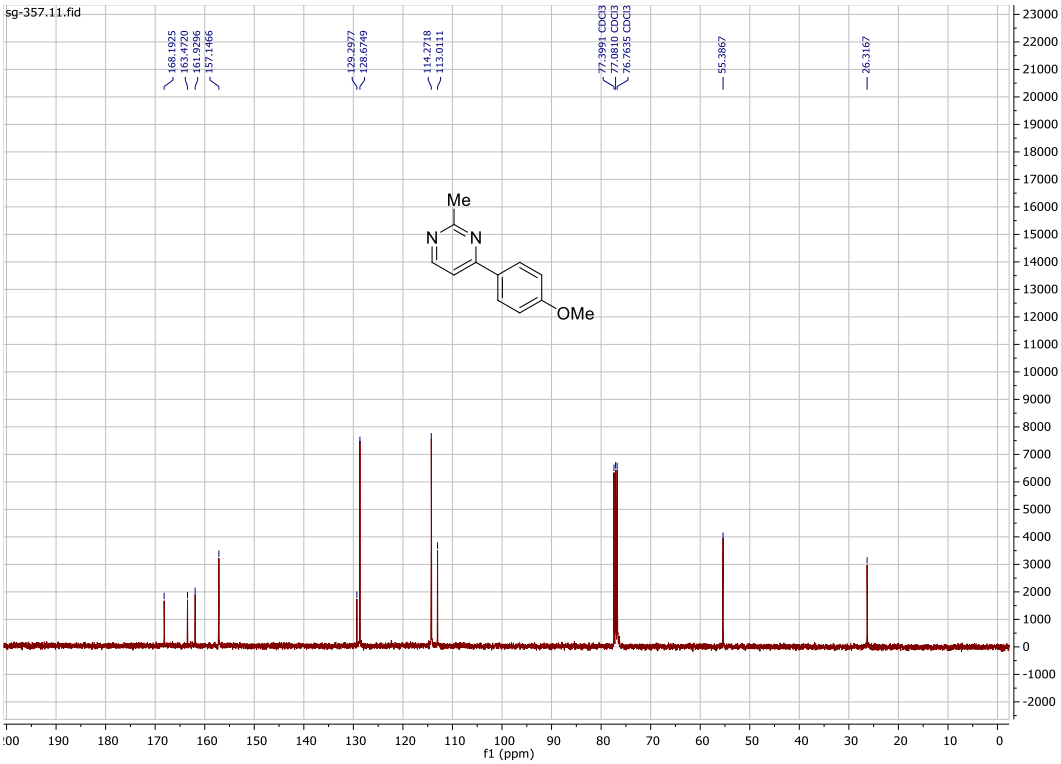




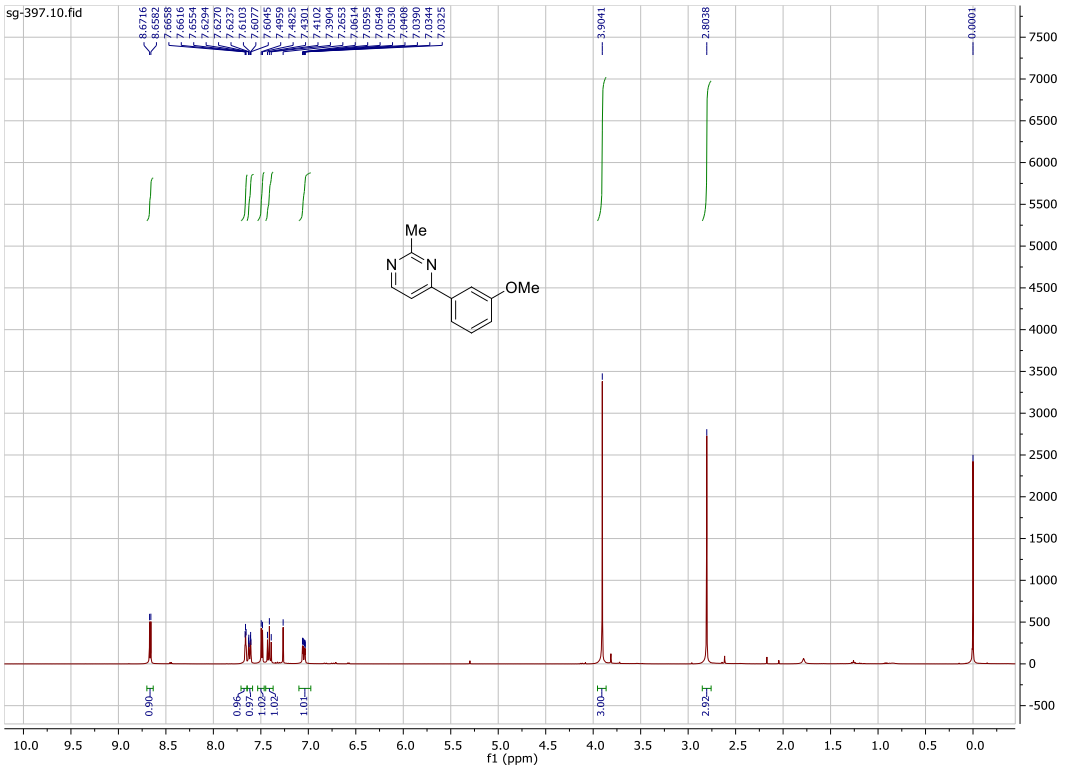
HRMS spectra of **8c**



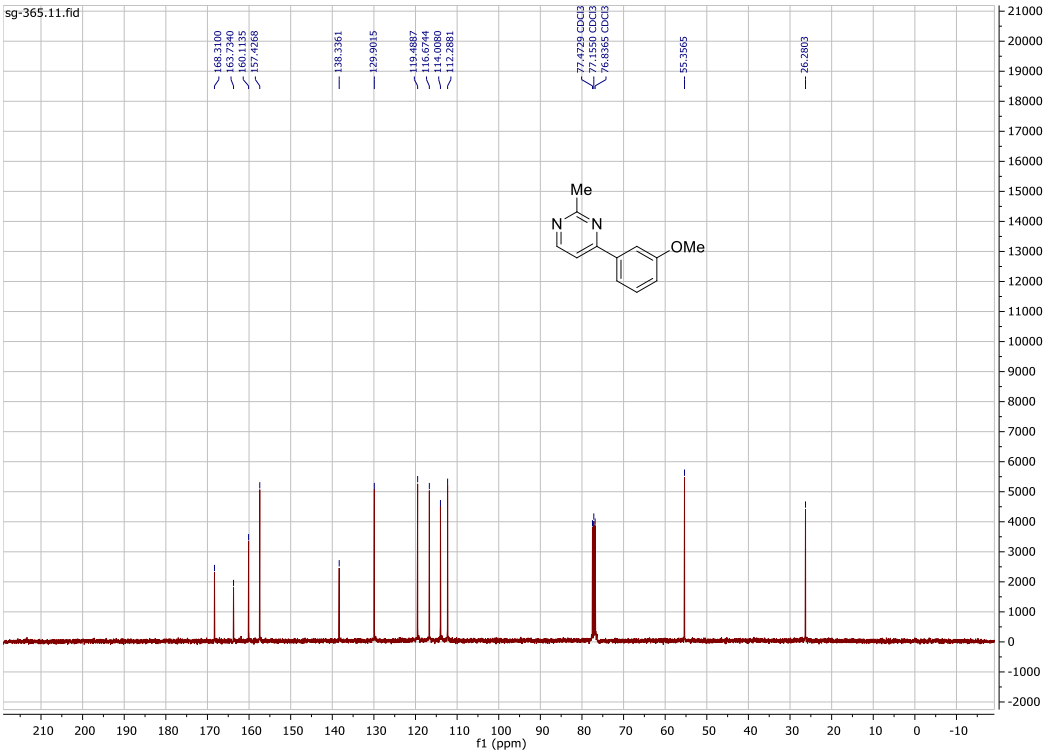
^{1}H NMR spectrum of **17d** (in $CDCl_3$)



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



^{1}H NMR spectrum of **17e** (in $CDCl_3$)

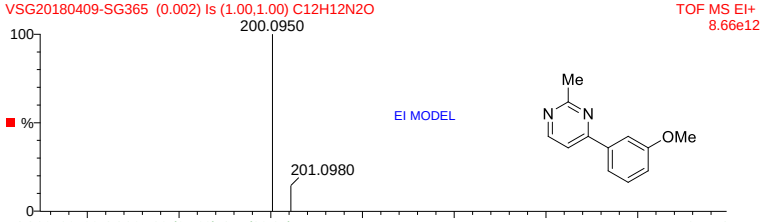


^{13}C NMR spectrum of **17e** (in $CDCl_3$)

VSG20180409-SG365

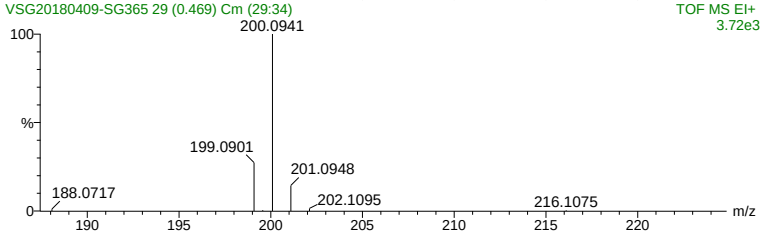
VSG20180409-SG365 (0.002) Is (1.00,1.00) C12H12N2O

TOF MS EI+
8.66e12



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

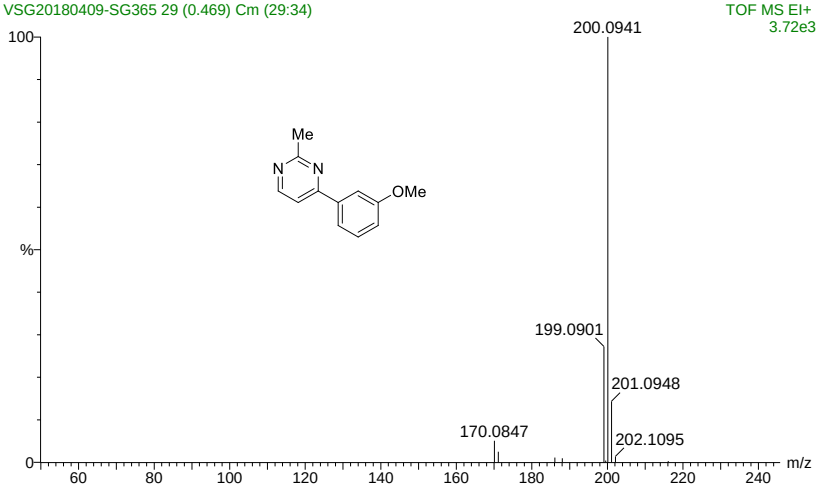
TOF MS EI+
3.72e3



VSG20180409-SG365

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

TOF MS EI+
3.72e3

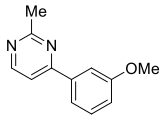


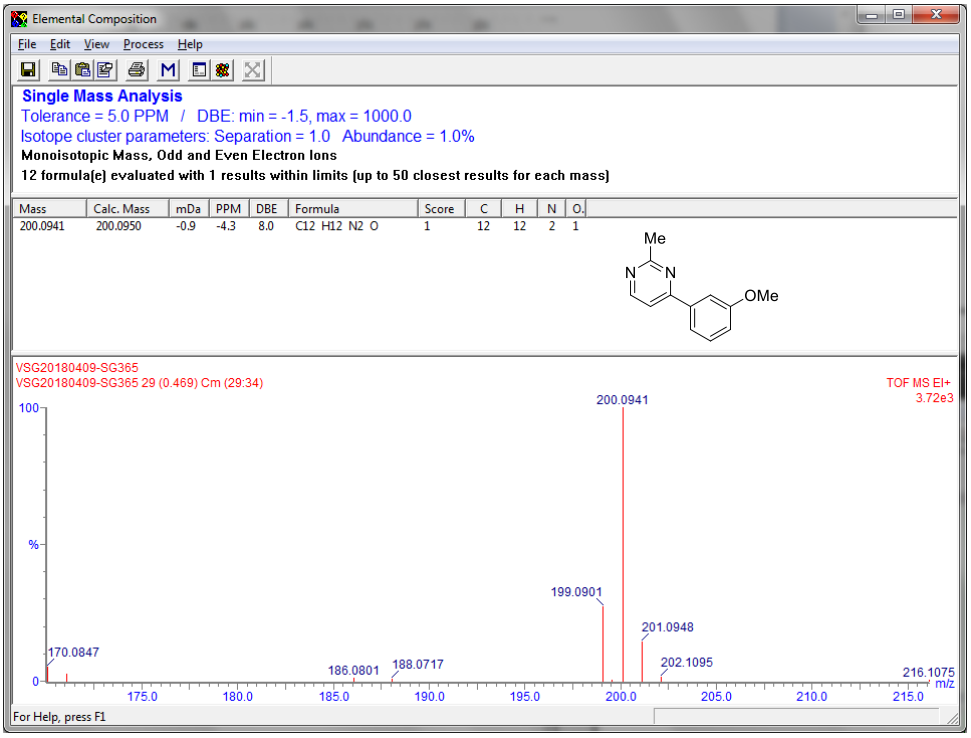
VSG20180409-SG365

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

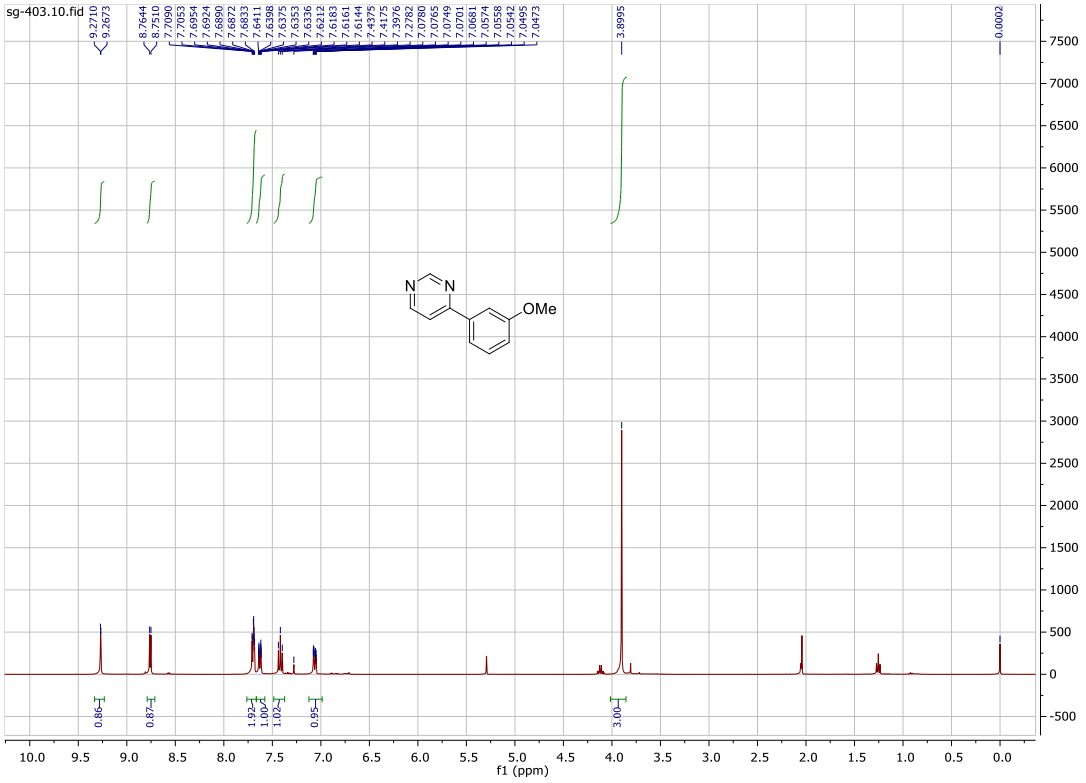
TOF MS EI+

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										

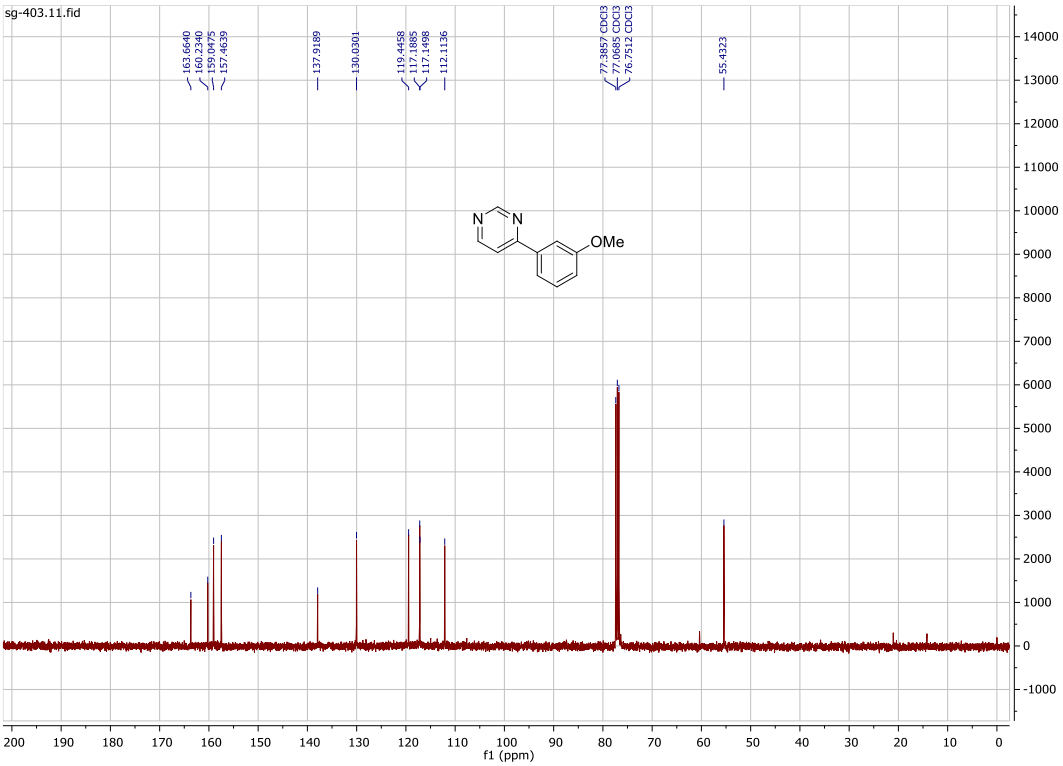




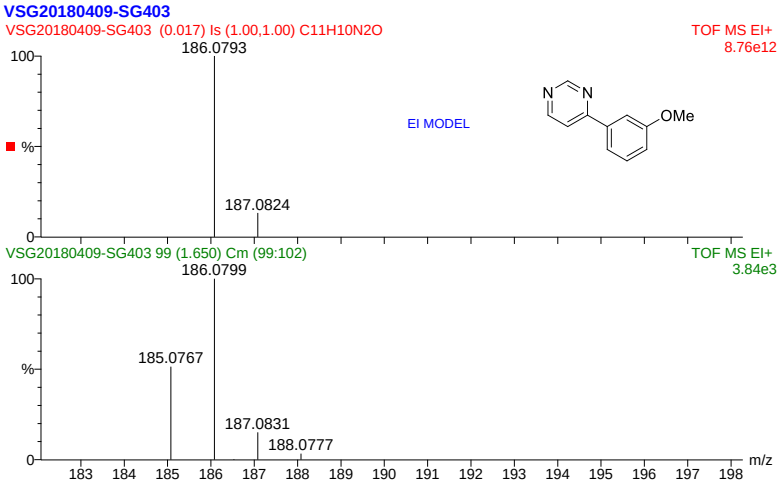
HRMS spectra of **17e**

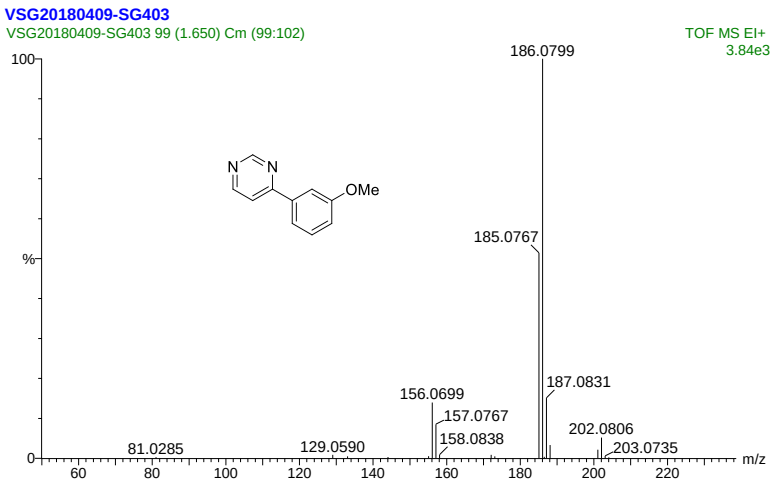


^{1}H NMR spectrum of **17f** (in $CDCl_3$)



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

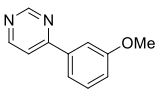


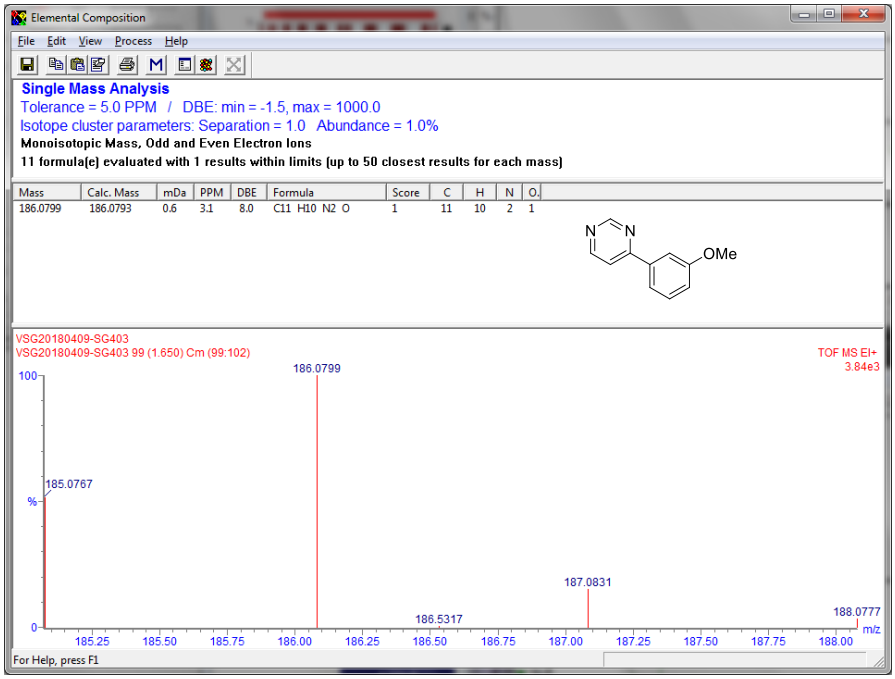


VSG20180409-SG403

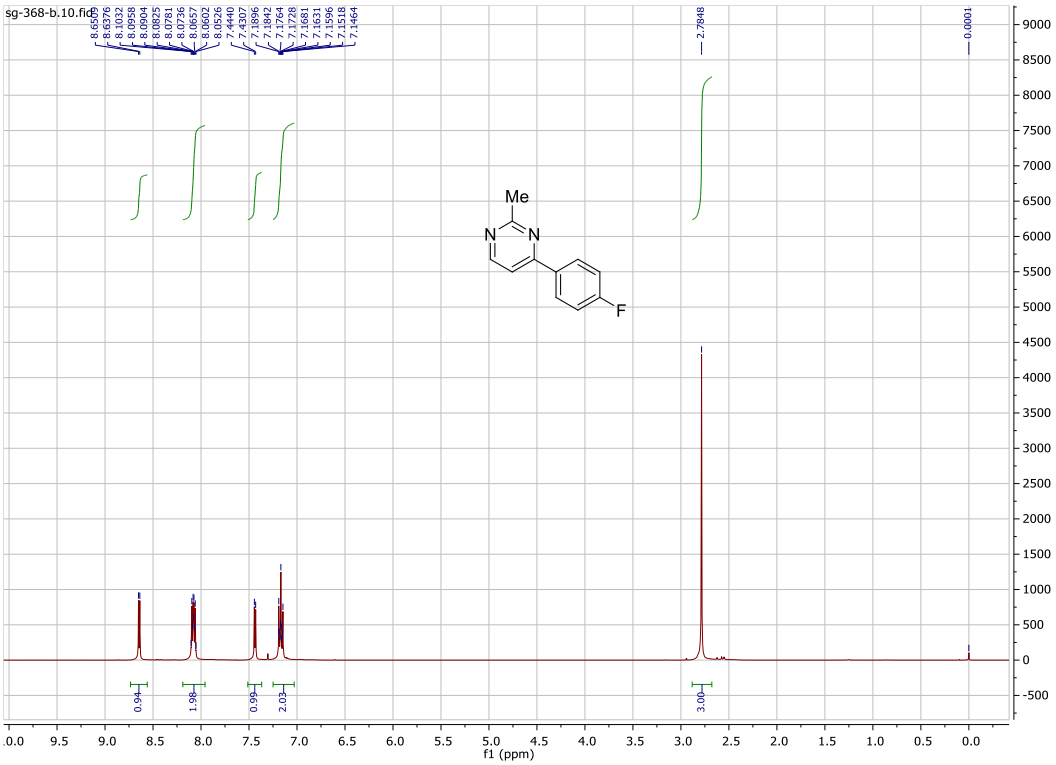
VSG20180409-SG403 99 (1.650) Cm (99:102) TOF MS EI+

No	Mass	Inten	%BPI	%TIC	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										

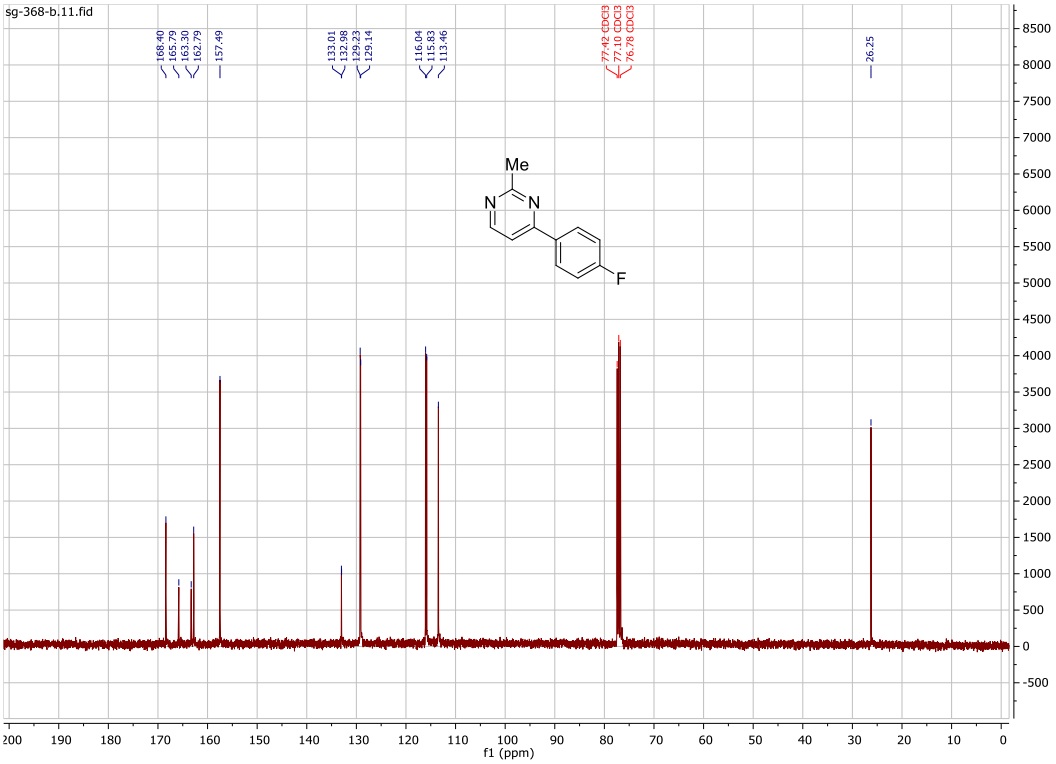




HRMS spectra of **17f**



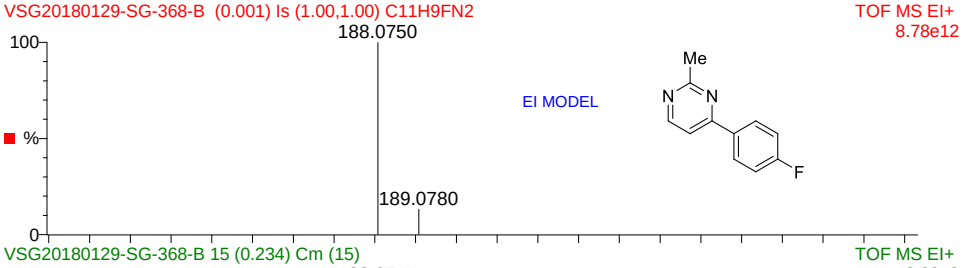
^{1}H NMR spectrum of **17g** (in $CDCl_3$)



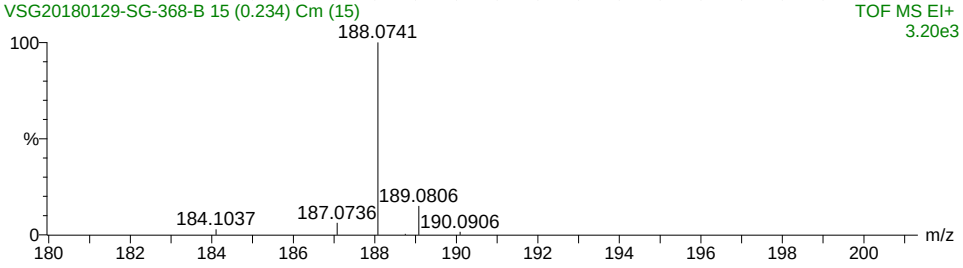
^{13}C NMR spectrum of **17g** (in $CDCl_3$)

VSG20180129-SG-368-B

VSG20180129-SG-368-B (0.001) Is (1.00,1.00) C11H9FN2 — TOF MS EI+ 8.78e12

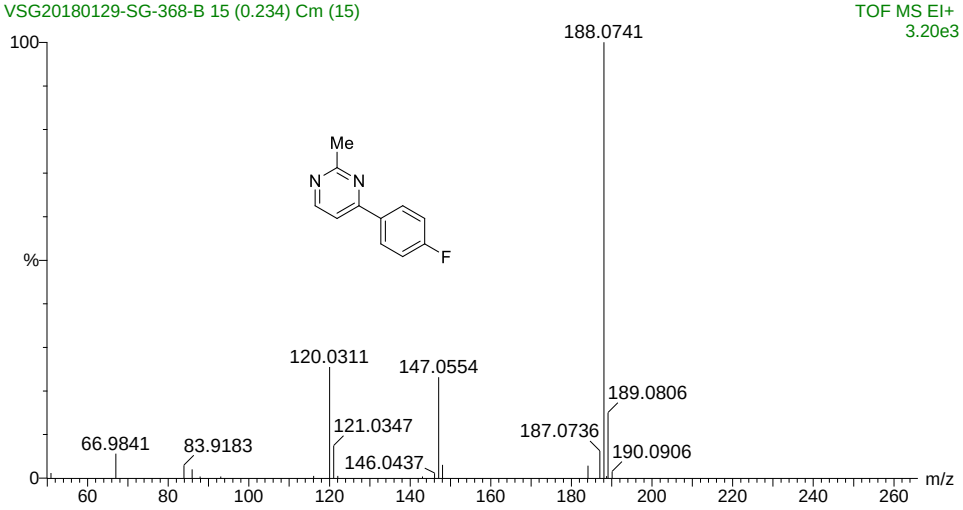


VSG20180129-SG-368-B 15 (0.234) Cm (15) — TOF MS EI+ 3.20e3



VSG20180129-SG-368-B

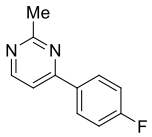
VSG20180129-SG-368-B 15 (0.234) Cm (15) — TOF MS EI+ 3.20e3

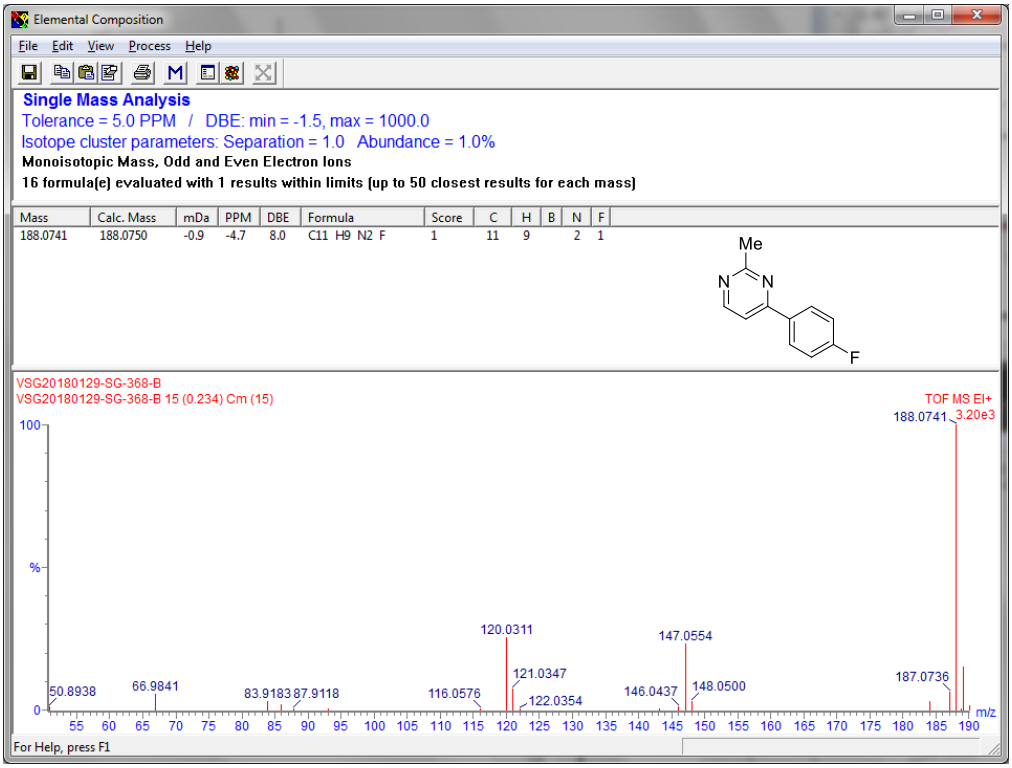


VSG20180129-SG-368-B

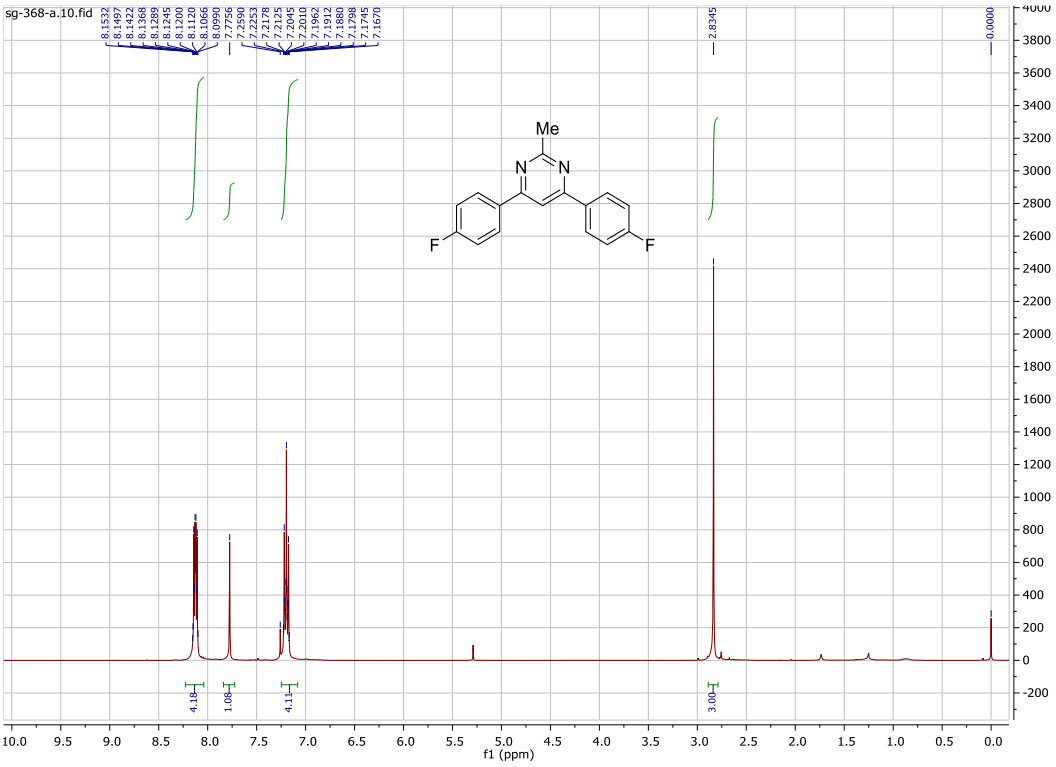
VSG20180129-SG-368-B 15 (0.234) Cm (15) — TOF MS EI+

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										

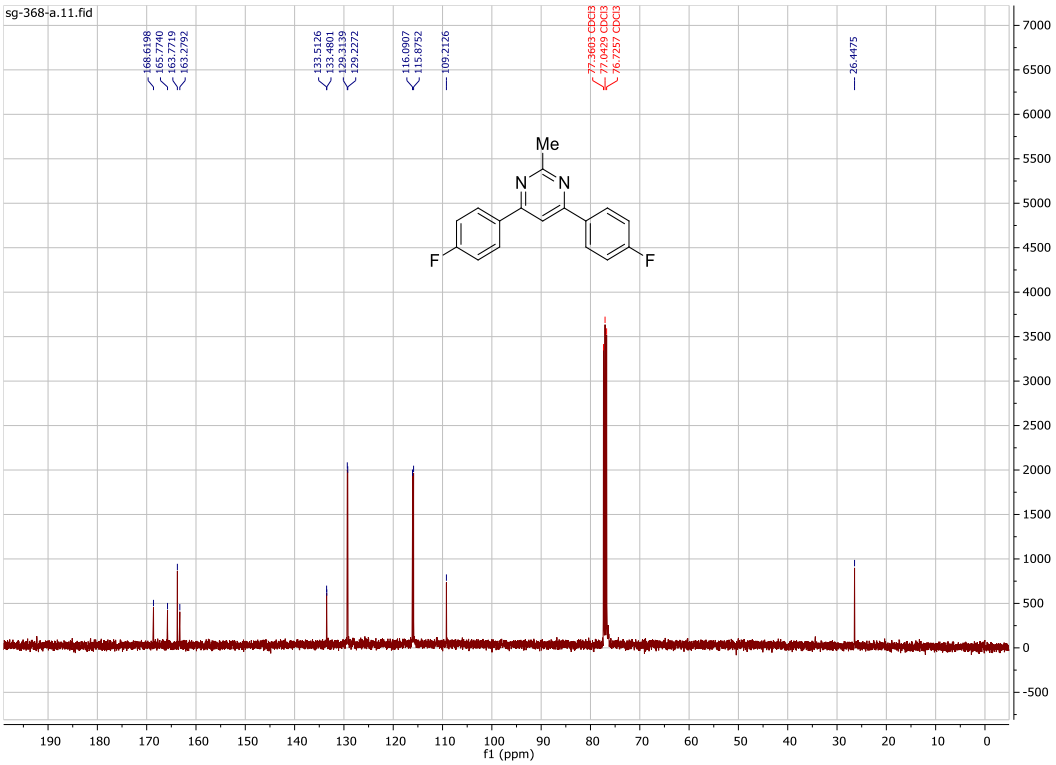




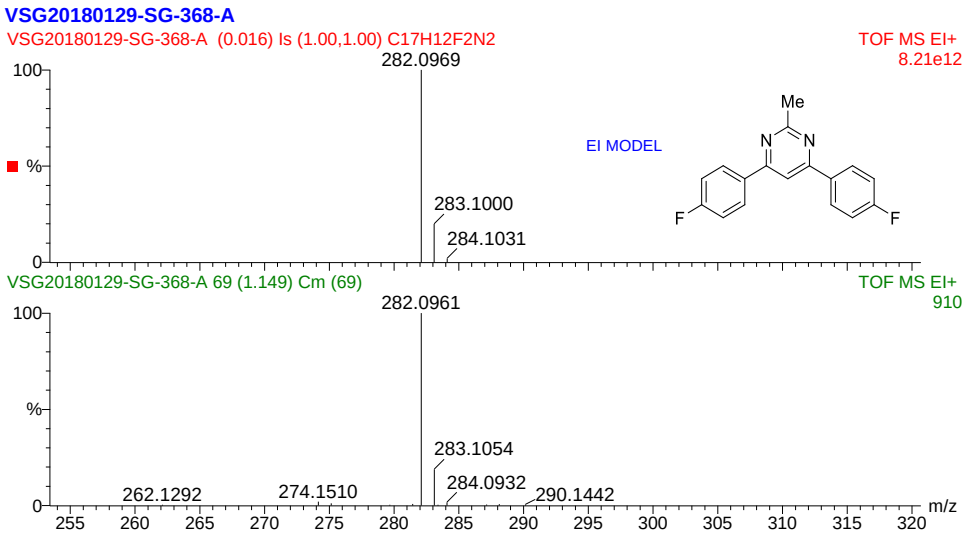
HRMS spectra of **17g**



^{1}H NMR spectrum of **8g** (in $CDCl_3$)



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

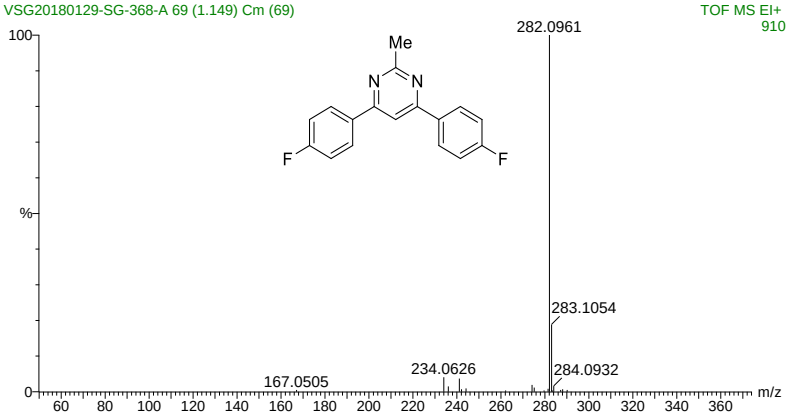


VSG20180129-SG-368-A

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

TOF MS EI+

910

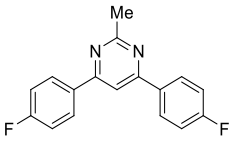


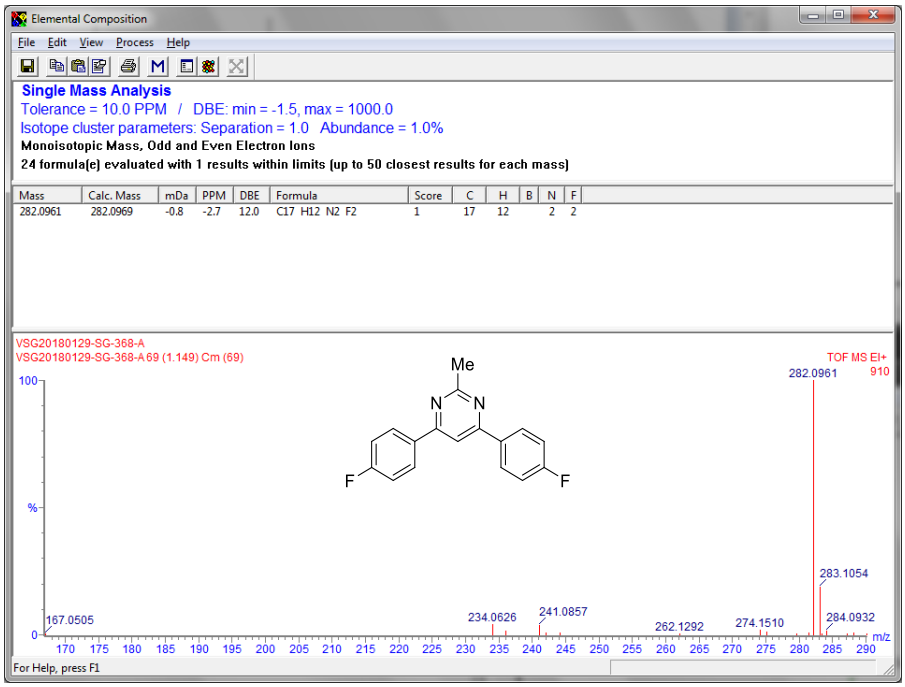
VSG20180129-SG-368-A

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

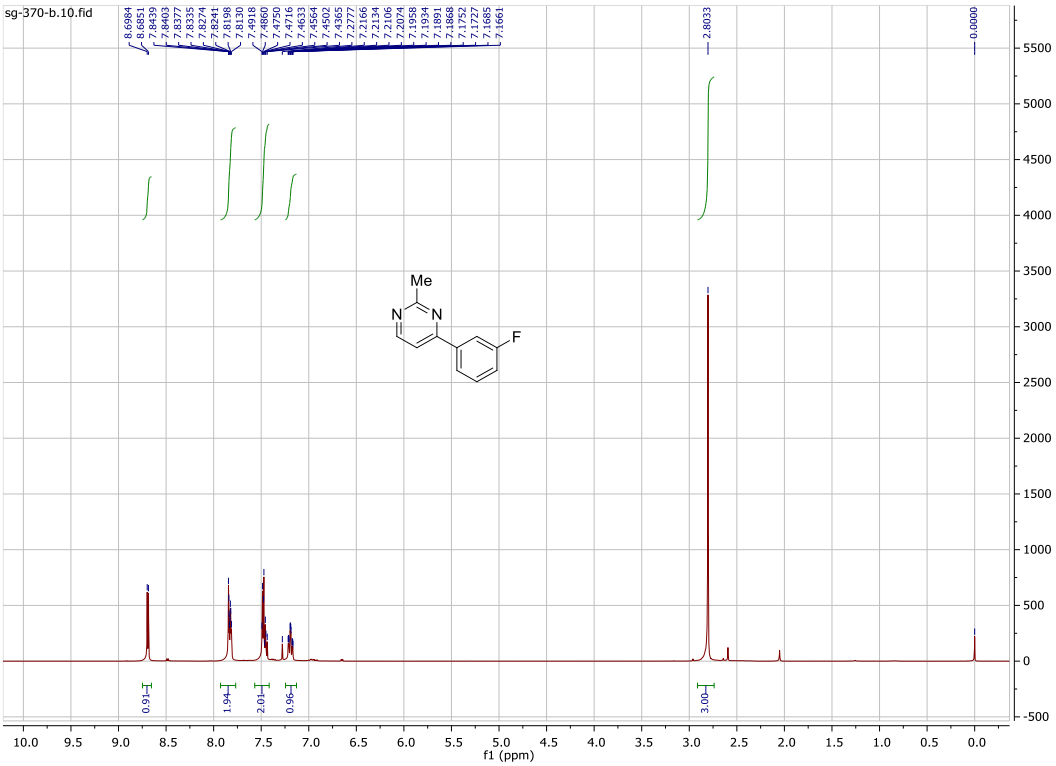
TOF MS EI+

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:	283.3896	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										

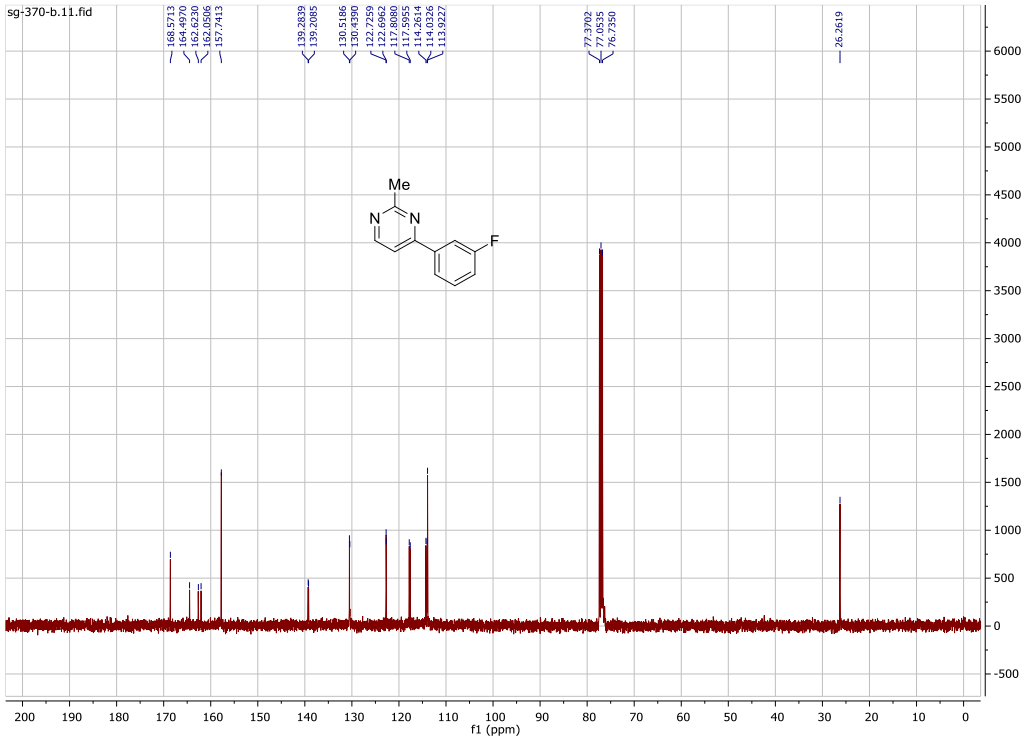




HRMS spectra of **8g**



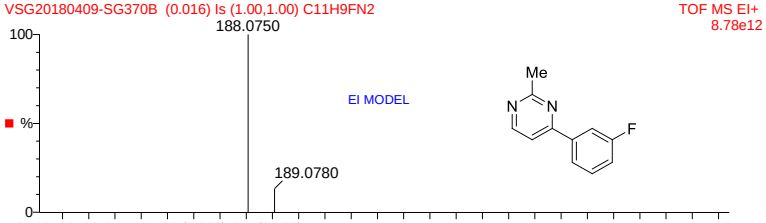
^{1}H NMR spectrum of **17h** (in $CDCl_3$)



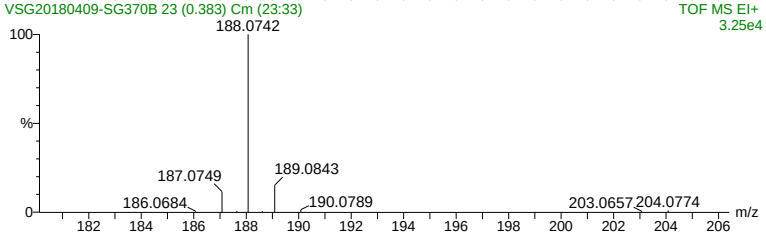
^{1}H NMR spectrum of **17h** (in $CDCl_3$)

VSG20180409-SG370B

VSG20180409-SG370B (0.016) Is (1.00,1.00) C11H9FN2 — TOF MS EI+ 8.78e12

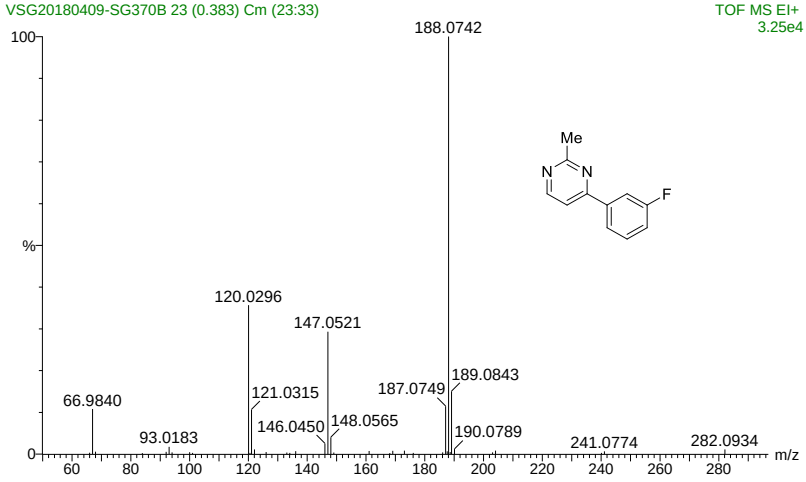


VSG20180409-SG370B 23 (0.383) Cm (23:33) — TOF MS EI+ 3.25e4



VSG20180409-SG370B

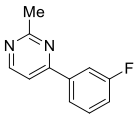
VSG20180409-SG370B 23 (0.383) Cm (23:33) — TOF MS EI+ 3.25e4

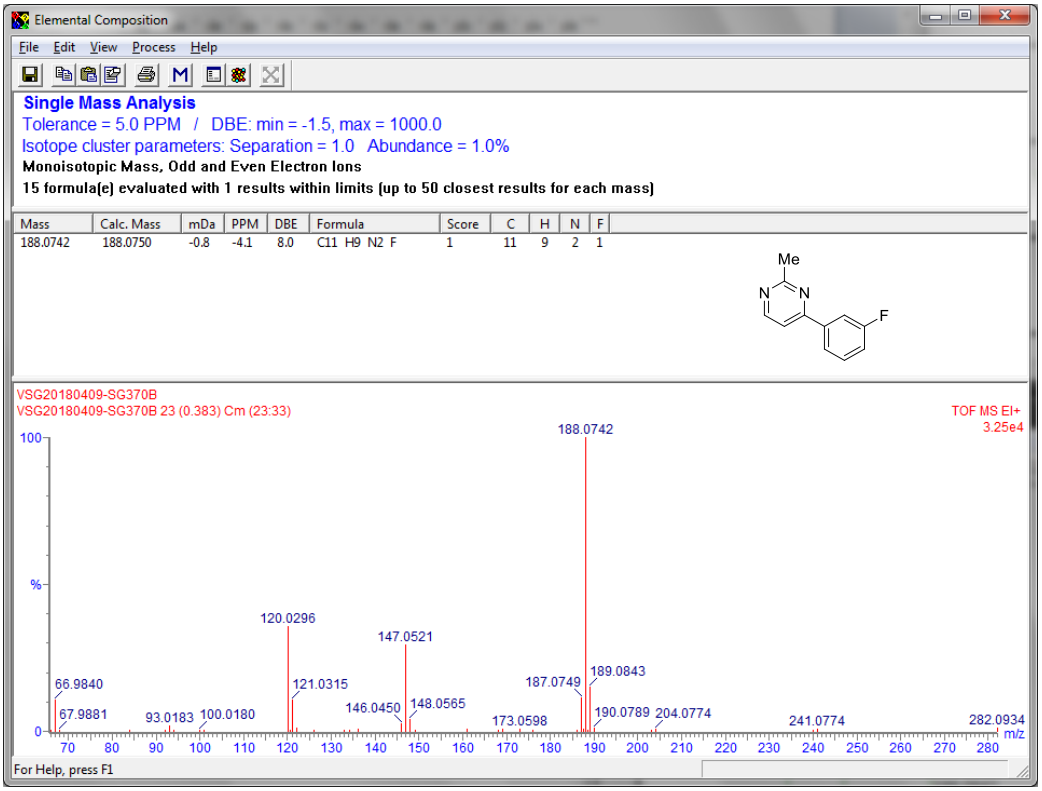


VSG20180409-SG370B

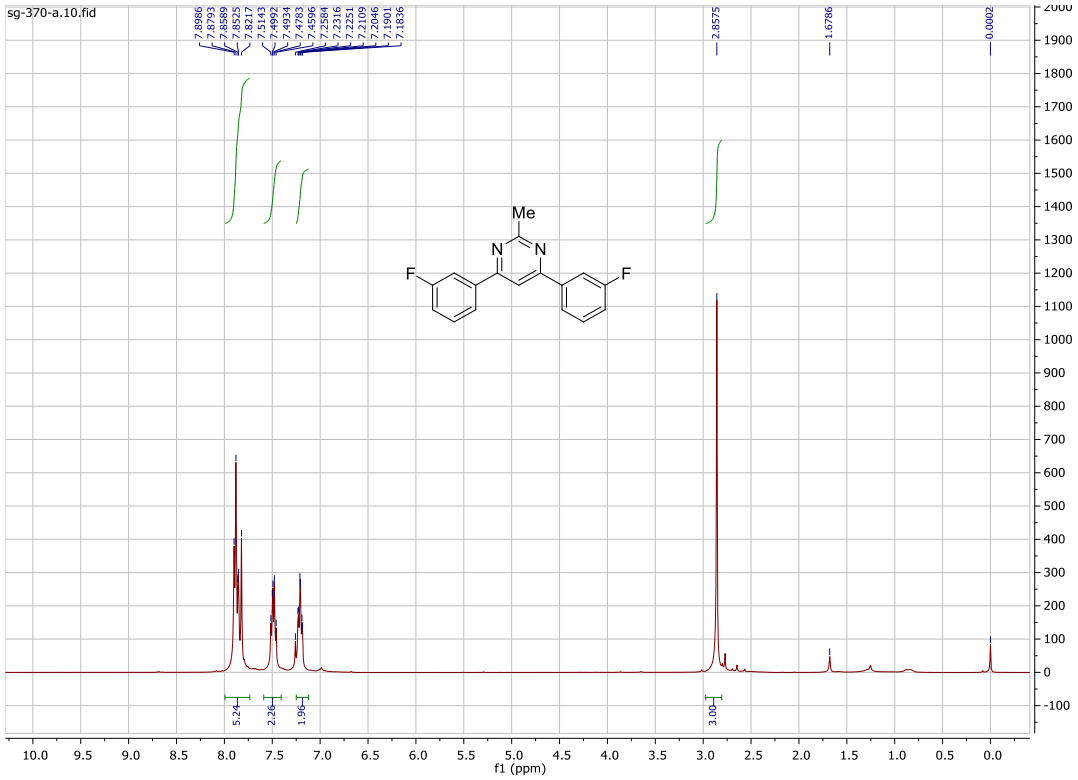
VSG20180409-SG370B 23 (0.383) Cm (23:33) — TOF MS EI+

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										

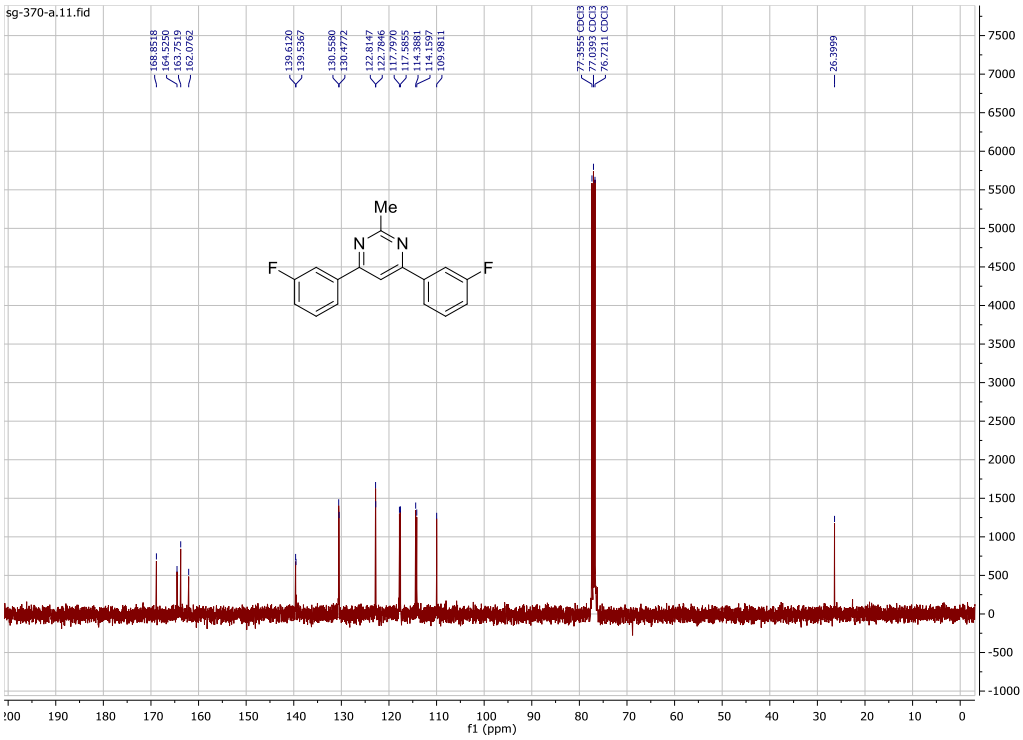




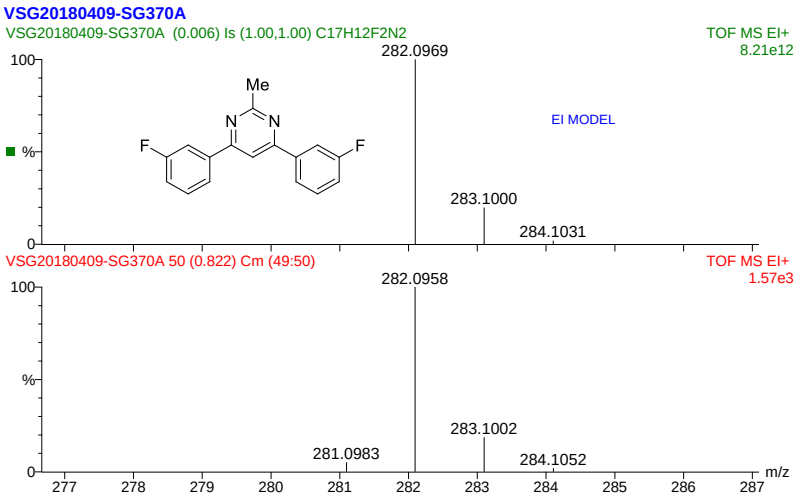
HRMS spectra of **17h**

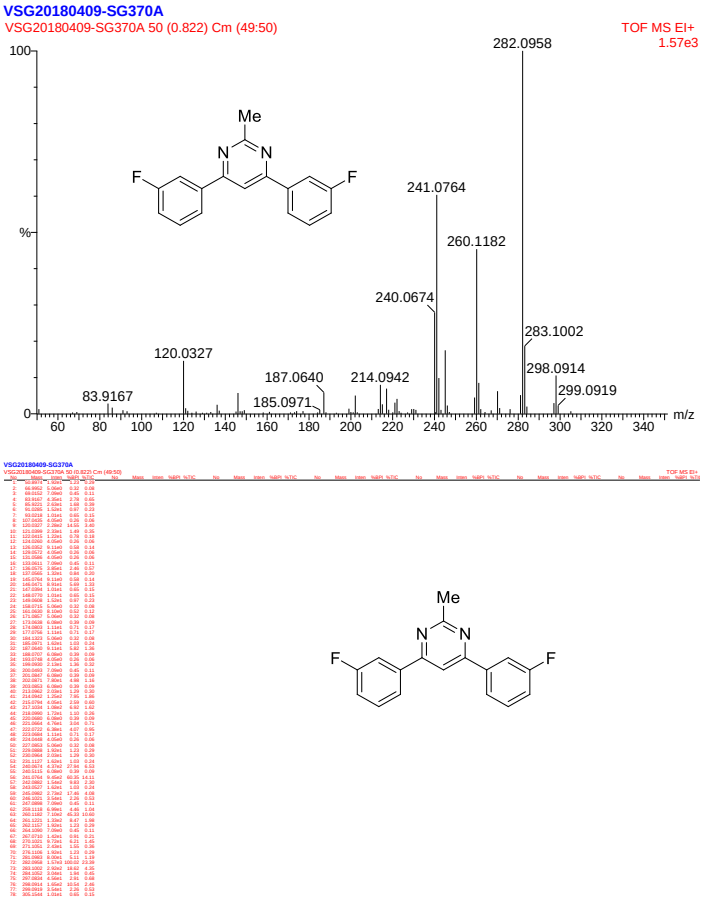


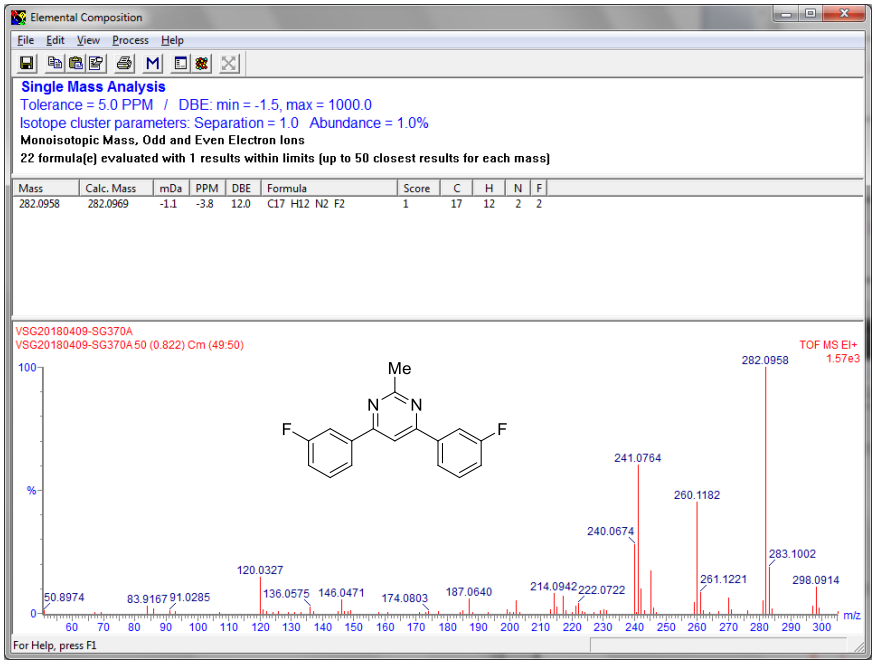
^{1}H NMR spectrum of **8h** (in $CDCl_3$)



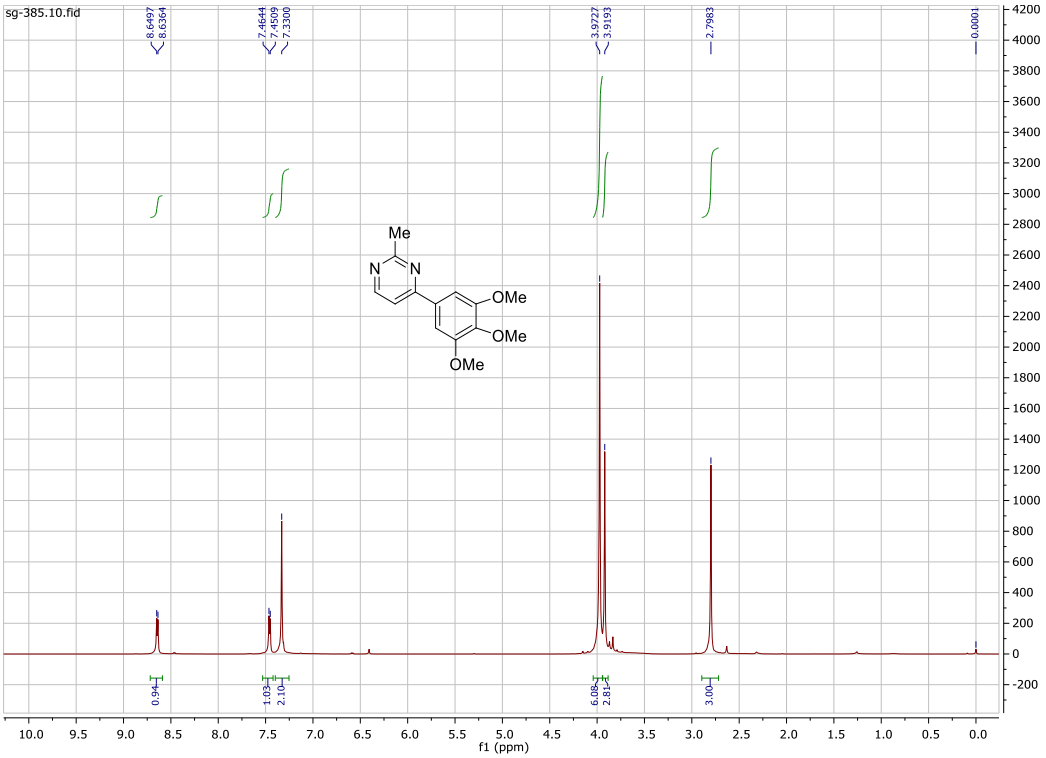
^{13}C NMR spectrum of **8h** (in $CDCl_3$)



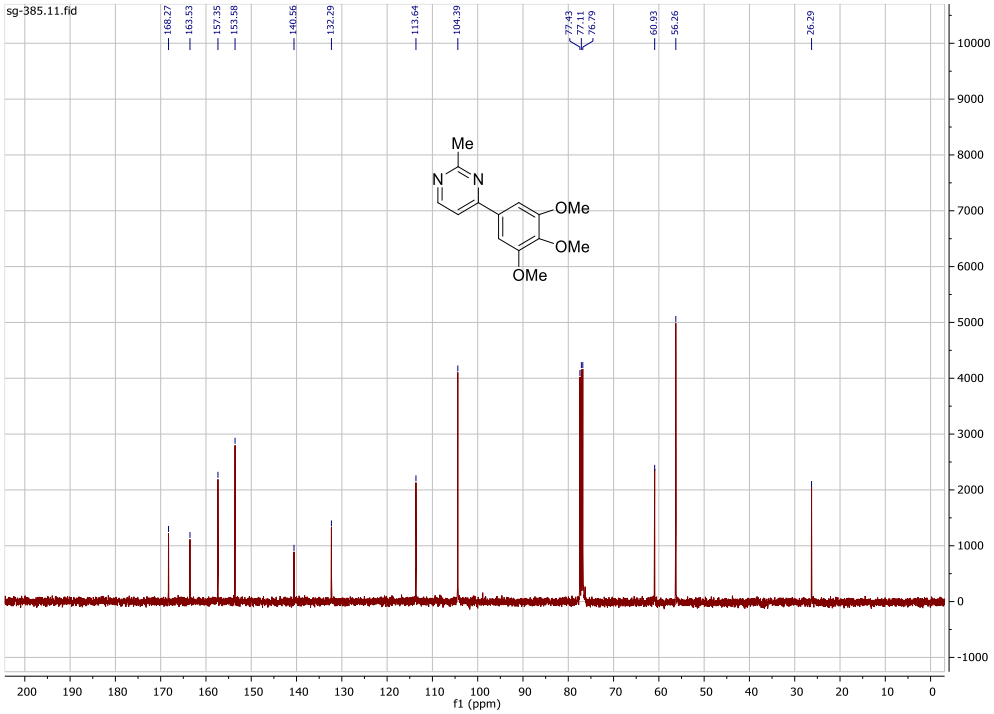




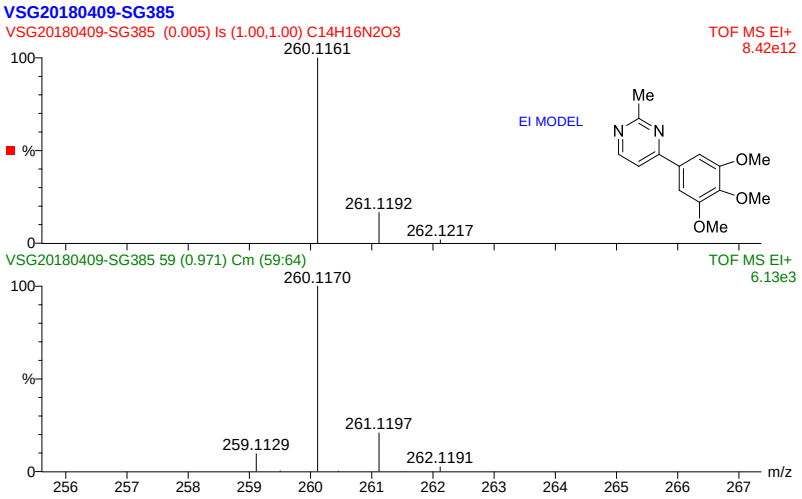
HRMS spectra of **8h**

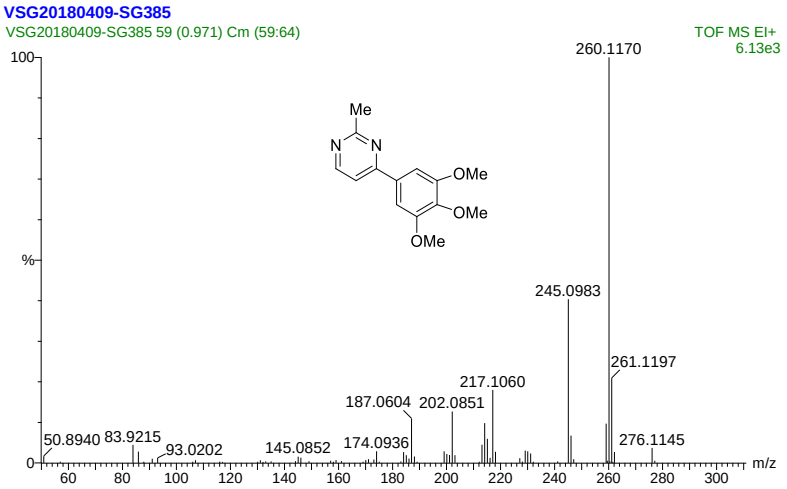


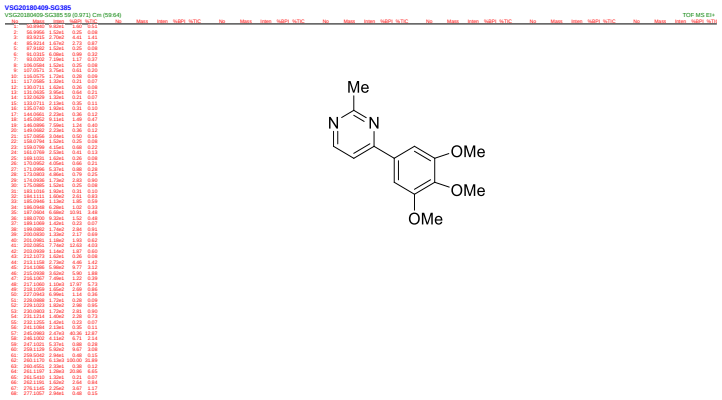
^{1}H NMR spectrum of **17j** (in $CDCl_3$)



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







HRMS spectra of **17j**