

Supplementary Information

Synthesis of 3,6 Diaryl-1*H*-Pyrazolo[3,4-*b*]Pyridines via One-pot Sequential Suzuki-Miyaura Coupling

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1. X-ray crystal data (3g and 4f)

The single crystal X-ray data were collected on an Oxford Xcalibur CCD diffractometer using graphite monochromated MoK α -radiation ($\lambda = 0.71073 \text{ \AA}$) at 293(2) K. The multi-scan correction was applied. The structure was solved by the direct method using SIR-92 and refined by fullmatrix least-square refinement technique on F^2 using SHELXL 97.² The hydrogen atoms were placed into the calculated position and included in the last cycle of the refinement. All calculations were done using Win GX software package.³ The main crystallographic data and structural refinement details are given in Table 1. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compound **3g** and **4f** have been deposited at the Cambridge Crystallographic Data Centre (CCDC, deposit no. 1828970 and 1817412 respectively).

Figure. 1s. Hydrogen bonding in the crystal lattice of (3g).

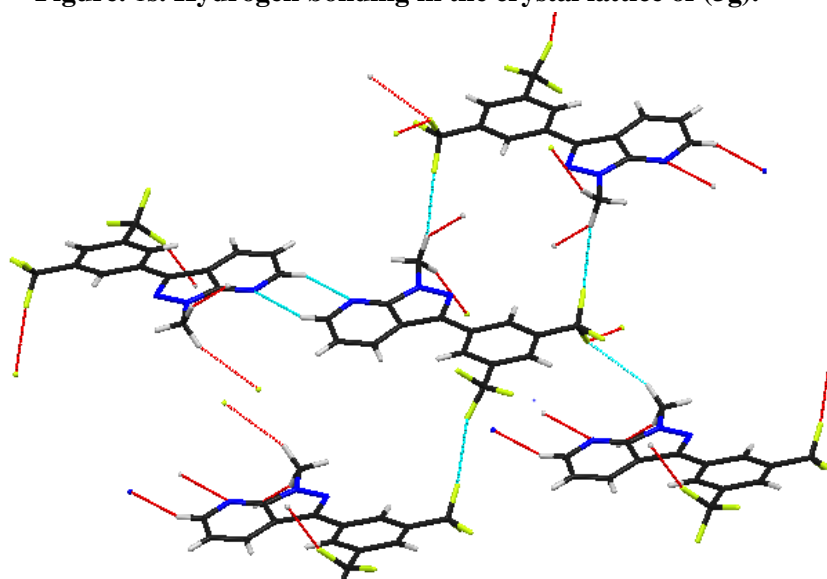


Figure. 2s. X-ray crystallographic ORTEP diagram of compound 3g.

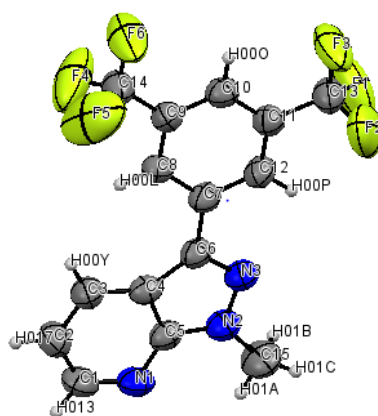


Table S1. Crystal data and structure refinement for 3g.

Empirical Formula	C ₁₅ H ₉ F ₆ N ₃
Formula Weight	345.25
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	<i>P</i> -1
a [Å]	9.9699(8)
b [Å]	11.2846(10)
c [Å]	13.4112(11)
α [°]	87.684(7)
β [°]	88.220(7)
λ [°]	75.359(8)
Volume [Å ³]	1458.3(2)
Z	4
Density (calculated) [Mg/m ³]	1.573
Absorption coefficient [mm ⁻¹]	0.150
F(000)	696
Crystal size [mm ³]	0.28 x 0.19 x 0.12 mm ³
Theta range for data collection [°]	3.152 to 25.00
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 12, -15 ≤ l ≤ 15
Reflections collected / independent reflection	16198 / 5119
R(int)	0.0433
Completeness of Theta at 25 °C (%)	99.8
Refinement method	Full-matrix least square on F ²
Data/ restraints/ parameters	5119/ 0/ 433
Goodness-of-fit on F ²	1.064

Final R indices $[I > 2\sigma(I)]^{a,b}$	R1 = 0.1064, wR2 = 0.2881
R indices (all data)	R1 = 0.1665, wR2 = 0.3417
Largest diff. peak and hole $[\text{\AA}^{-3}]$	0.717 and -0.528 $e.\text{\AA}^{-3}$
Extinction coefficient	n/a

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

Figure. 3s. X-ray crystallographic ORTEP diagram of compound 4f.

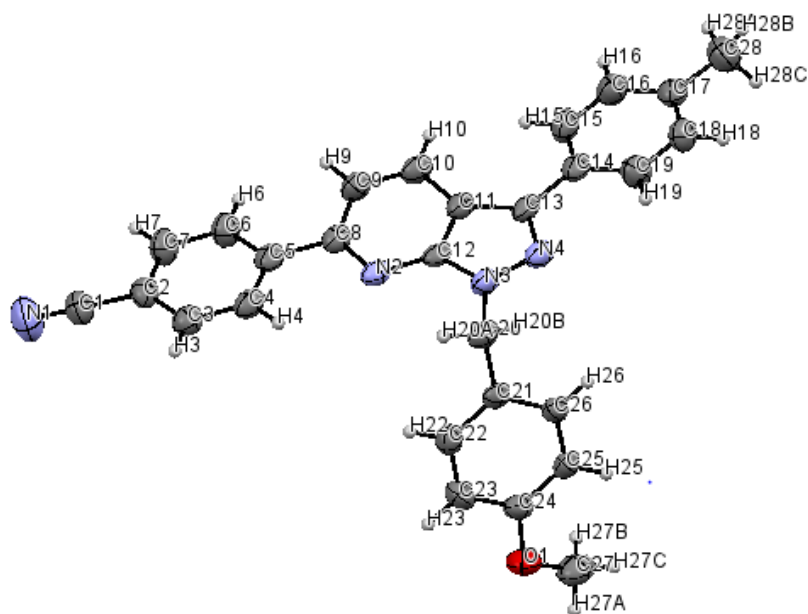


Figure. 4s. Hydrogen bonding in the crystal lattice of (4f).

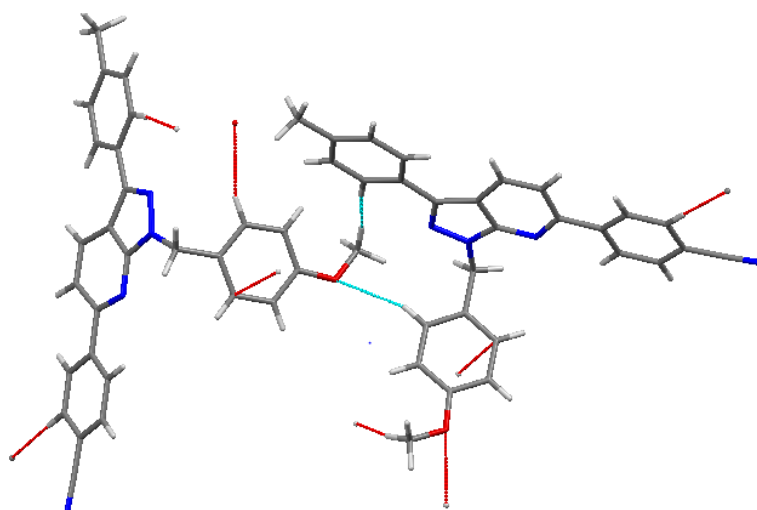


Table S2. Crystal data and structure refinement for 4f.

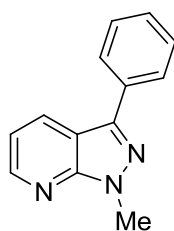
Empirical Formula	C ₂₈ H ₂₂ N ₄ O ₁
Formula Weight	430.49
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	<i>P</i> -21/ <i>c</i>
a [Å]	7.9835(2)
b [Å]	12.3524(3)
c [Å]	22.3908(5)
α [°]	90
β [°]	96.078(2)
λ [°]	90
Volume [Å ³]	2195.66(9)
Z	31
Density (calculated) [Mg/m ³]	1.840
Absorption coefficient [mm ⁻¹]	1.048
F(000)	1209
Crystal size [mm ³]	0.12 x 0.14 x 0.16 mm ³
Theta range for data collection [°]	3.415 to 29.550
Index ranges	-11 ≤ h ≤ 10, -16 ≤ k ≤ 17, -30 ≤ l ≤ 30
Reflections collected / independent reflection	33036 / 5591
R(int)	0.0322
Completeness of Theta at 25 °C (%)	99.7
Refinement method	Full-matrix least square on F ²
Data/ restraints/ parameters	5591/ 0/ 298
Goodness-of-fit on F ²	1.274

Final R indices [$I > 2\sigma(I)$] ^{a,b}	R1 = 0.0776, wR2 = 0.3004
R indices (all data)	R1 = 0.0956, wR2 = 0.3165
Largest diff. peak and hole [\AA^{-3}]	0.706 and -0.295 e. \AA^{-3}
Extinction coefficient	n/a

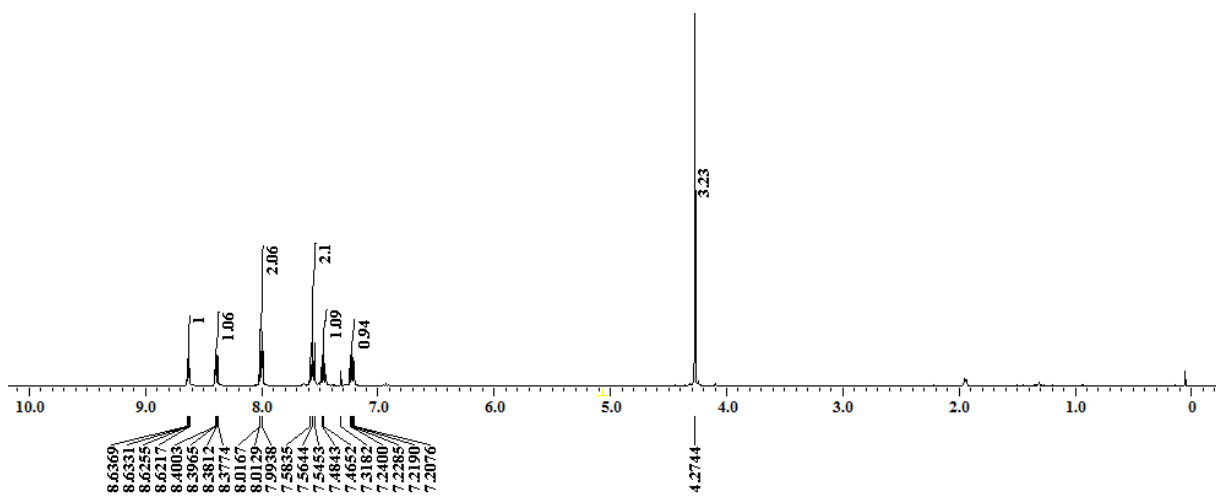
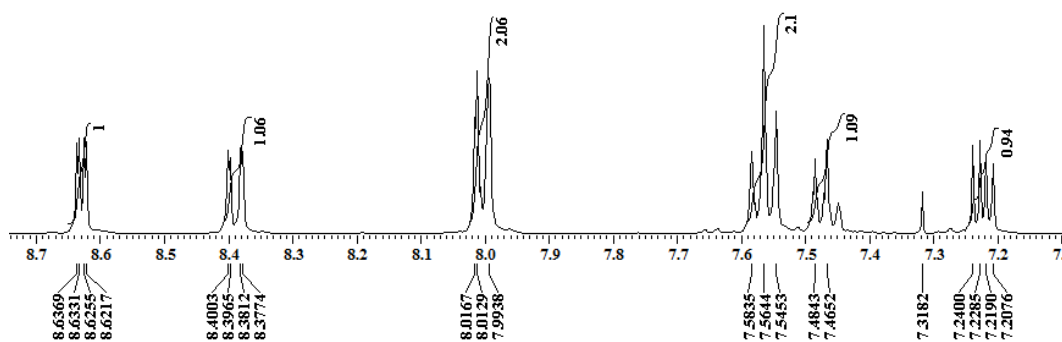
$${}^aR = \sum(|F_o| - |F_c|) / \sum |F_o|; {}^bR_w = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)]\}^{1/2}$$

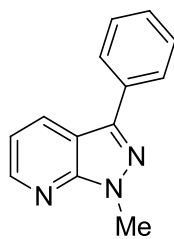
References:

1. G. M. Sheldrick, *Acta Crystallogr., Sect. A*, **1990**, 46, 467.
2. G. M. Sheldrick, *SHELXL-97, Computer program for crystal structure refinement*, University of Göttingen, Germany. **1997**, 1456.
3. L. J. Farrugia, WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data*; Department of Chemistry, University of Glasgow. **1997-2009**, 32, 837 – 838.

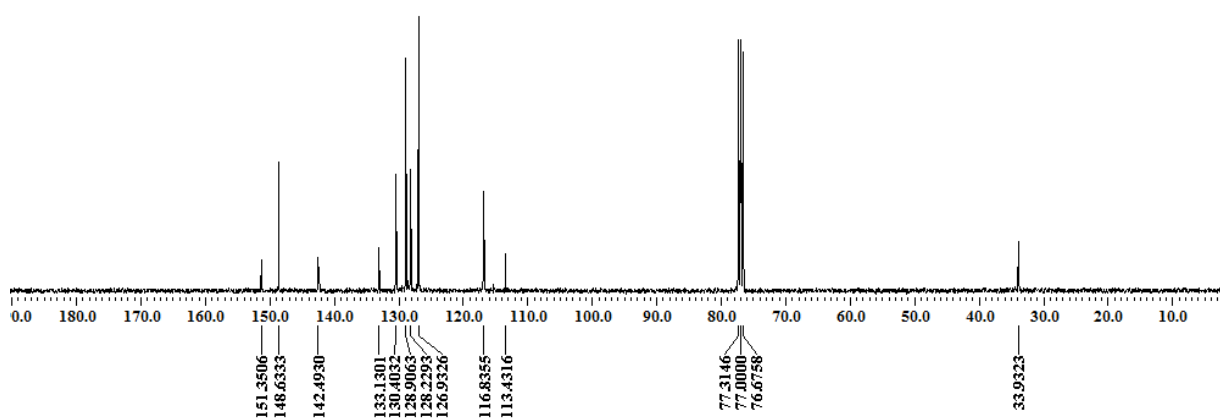
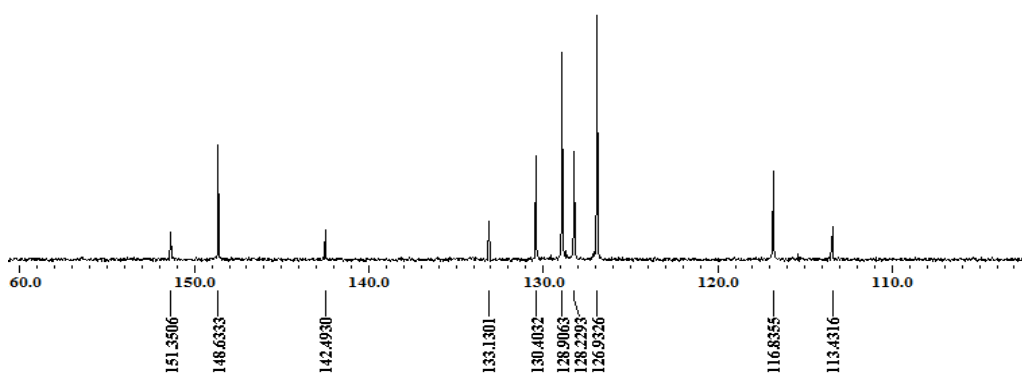


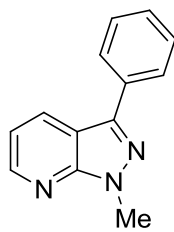
1-methyl-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**3a**)



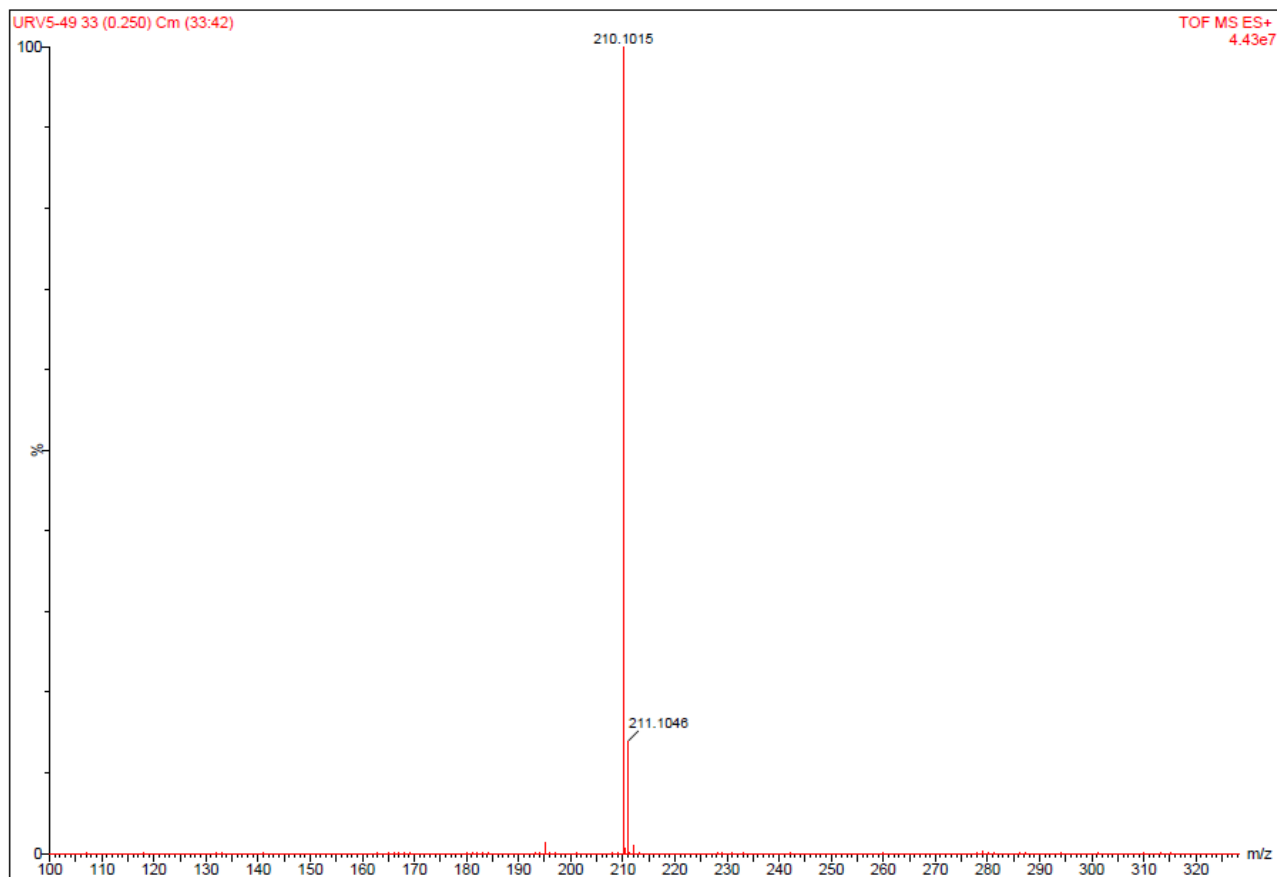


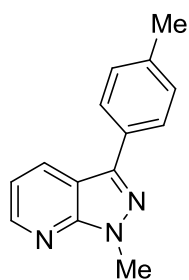
1-methyl-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**3a**)



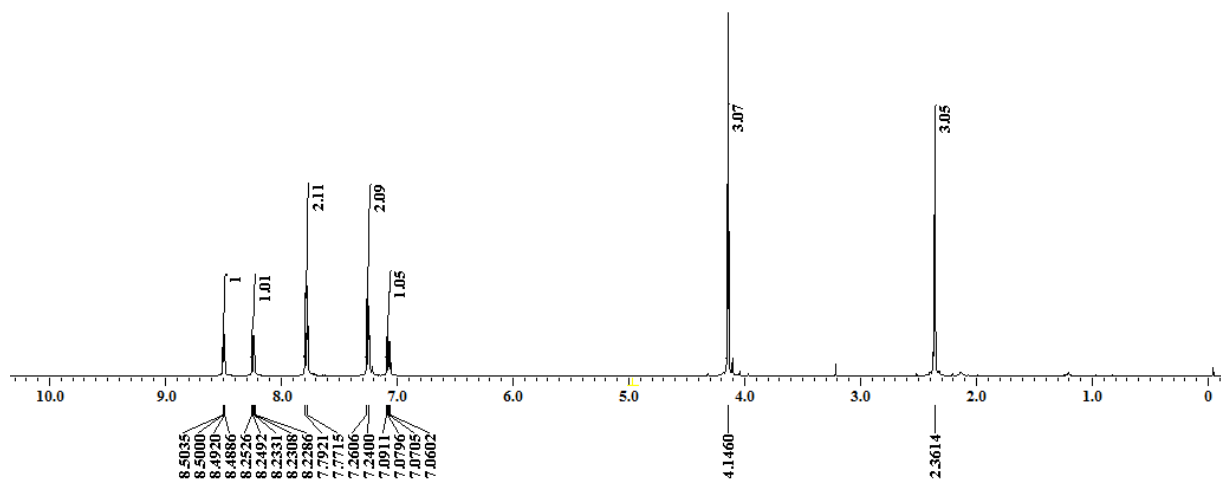
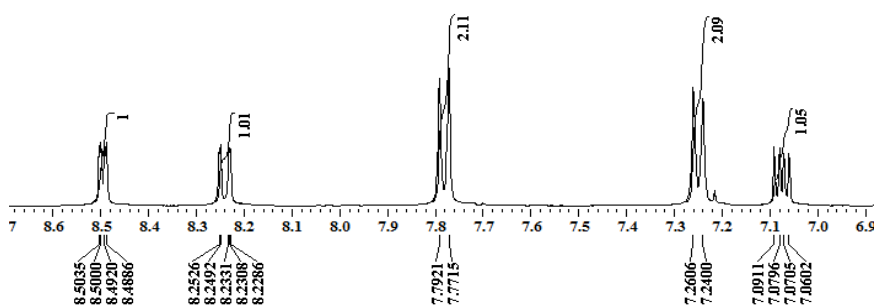


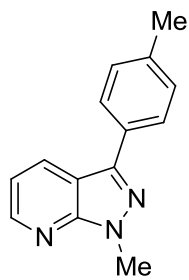
1-methyl-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**3a**)



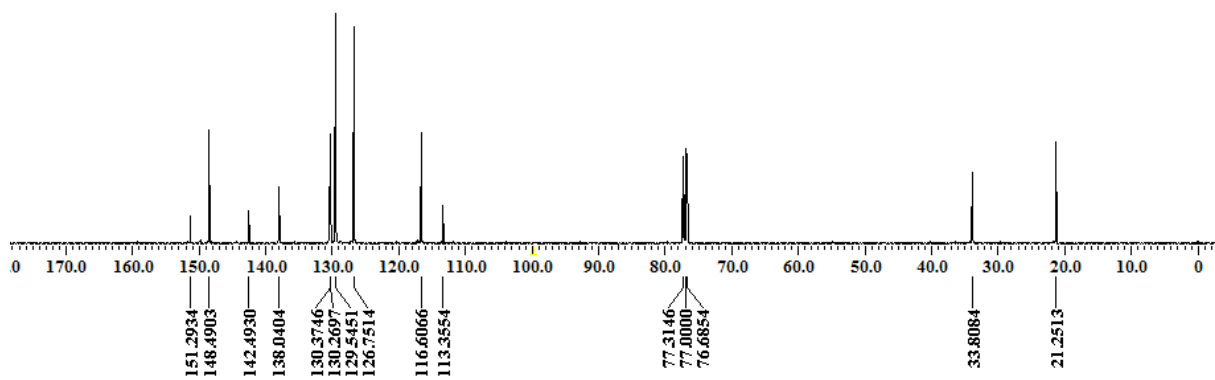
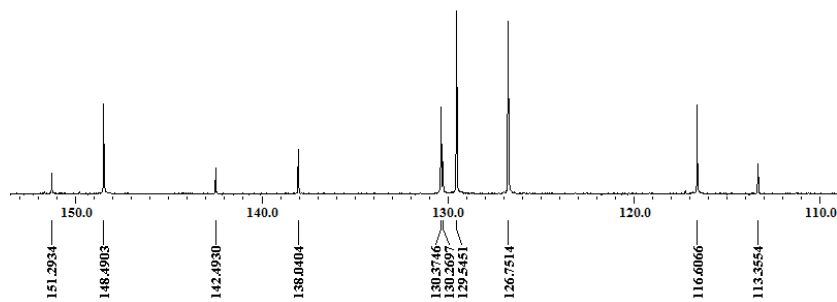


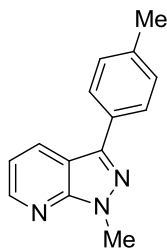
1-methyl-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridine (**3b**)





1-methyl-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (3b)





1-methyl-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3b**)

Qualitative Compound Report

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Comment			

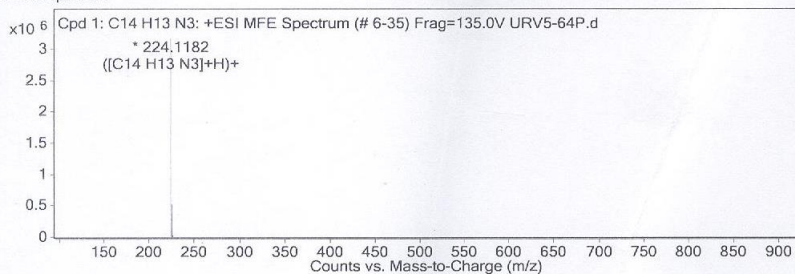
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Version	Q-TOF B.05.01 (B5125)	

Compound Table

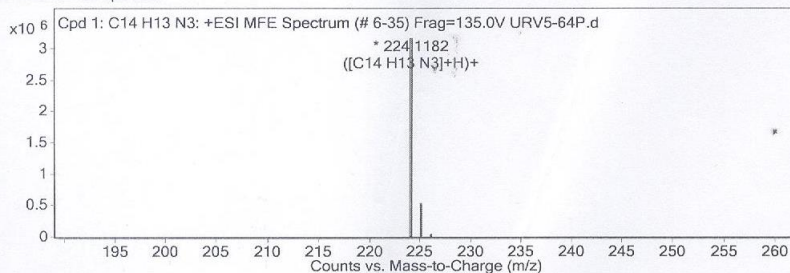
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Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C14 H13 N3	224.1182	11	Find by Molecular Feature	223.1109

MFE MS Spectrum



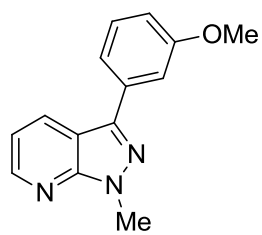
MFE MS Zoomed Spectrum



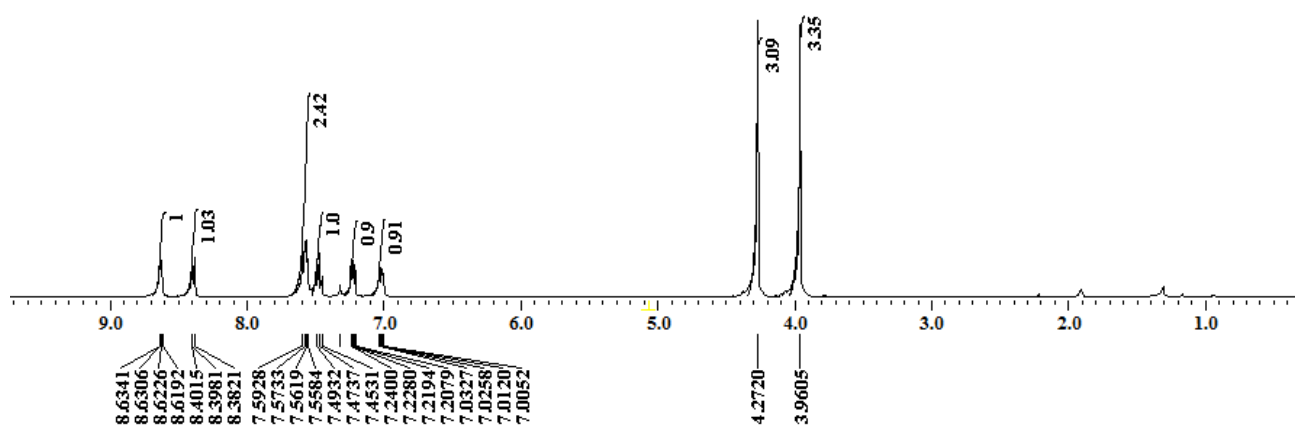
MS Spectrum Peak List

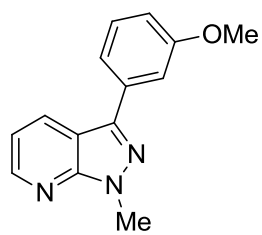
m/z	z	Abund	Formula	Ion
224.1182	1	3167287	C14 H13 N3	(M+H)+
225.1212	1	520245.9	C14 H13 N3	(M+H)+
226.124	1	38124.61	C14 H13 N3	(M+H)+
227.126	1	3075.84	C14 H13 N3	(M+H)+

--- End Of Report ---

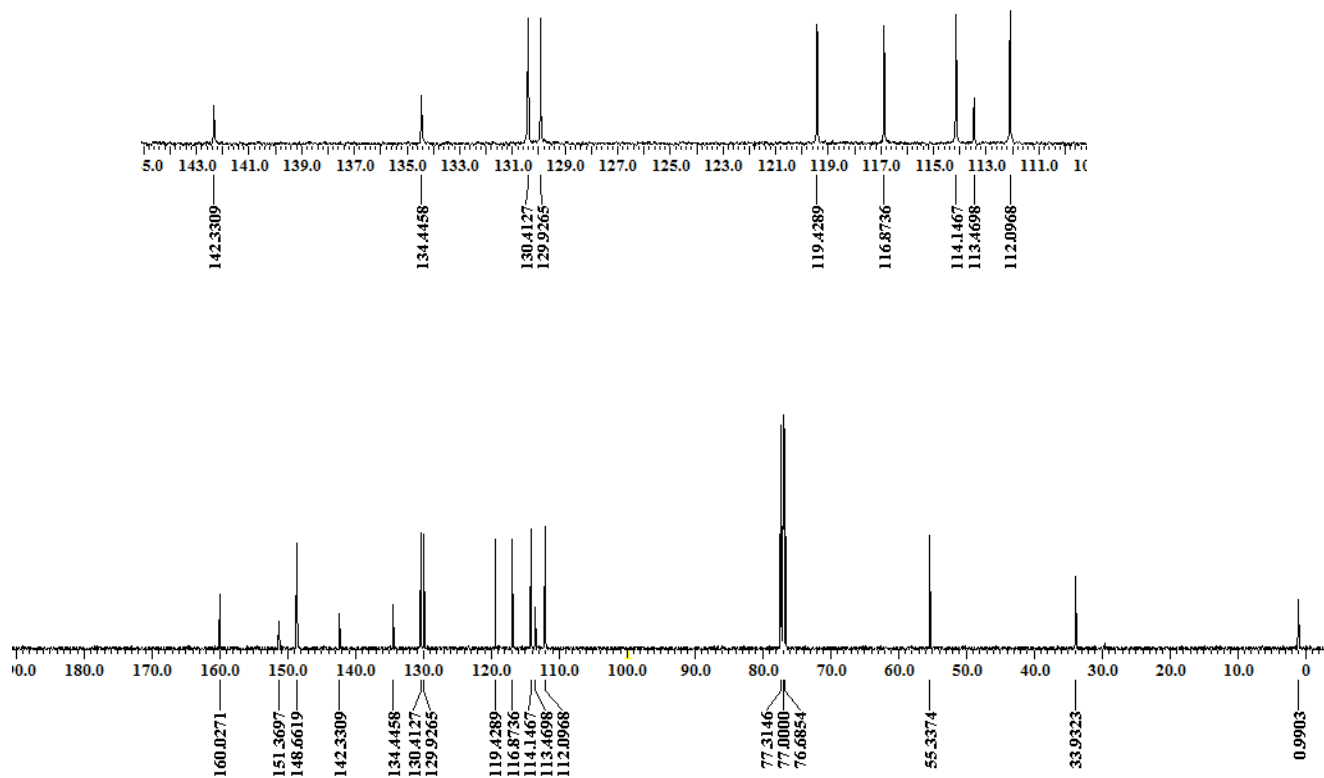


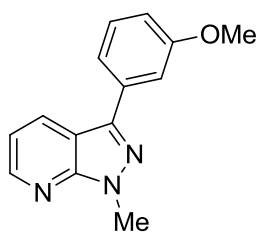
3-(3-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3c**)





3-(3-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (3c)





3-(3-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3c**)

Qualitative Compound Report

Data File	URV5-81.d	Sample Name	URV5-81
Sample Type	Sample	Position	P1-C9
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IRM Calibration Status	Success	DA Method	Default.m
Comment			

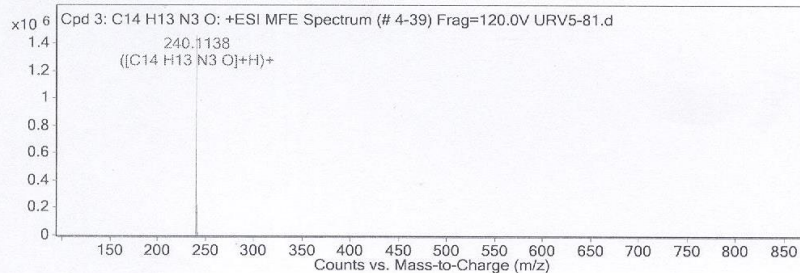
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Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

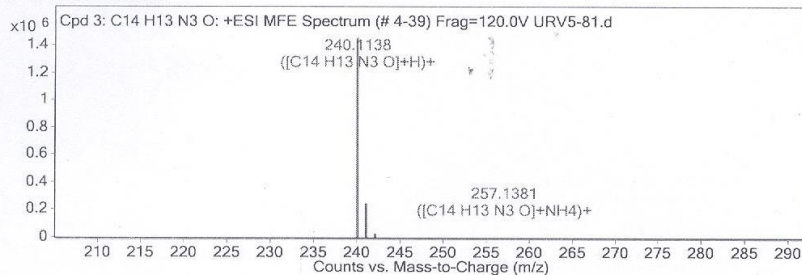
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Cpd 3: C14 H13 N3 O	10	239.1066	C14 H13 N3 O	C14 H13 N3 O	-2.88	C14 H13 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C14 H13 N3 O	240.1138	10	Find by Molecular Feature	239.1066

MFE MS Spectrum



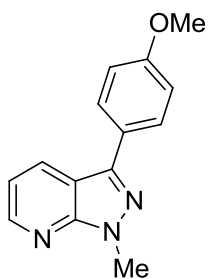
MFE MS Zoomed Spectrum



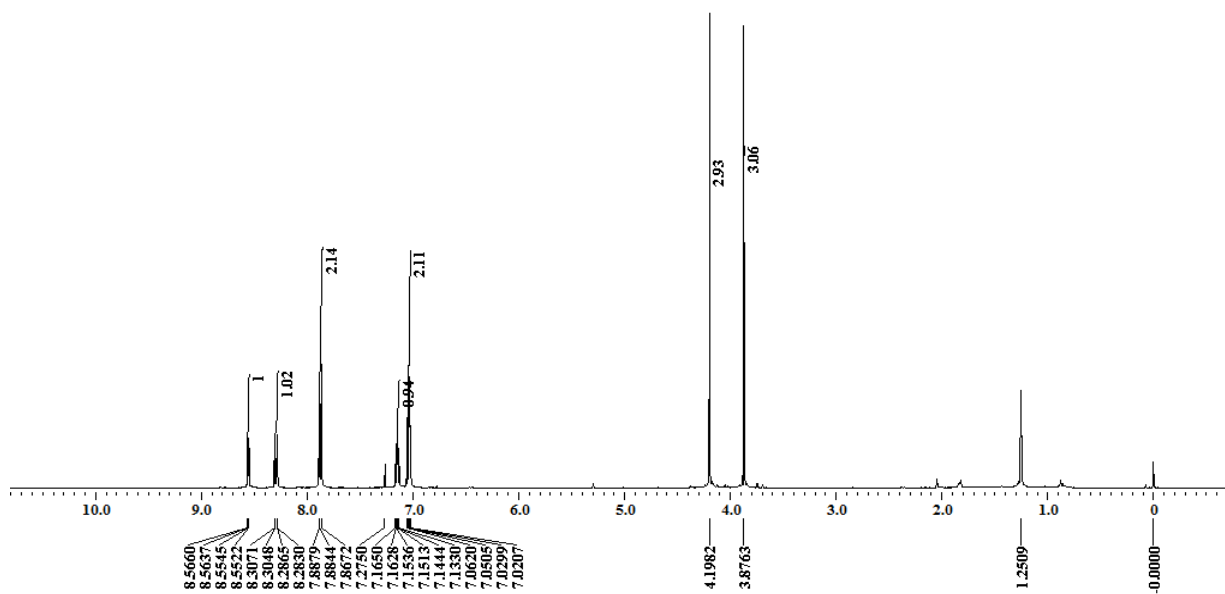
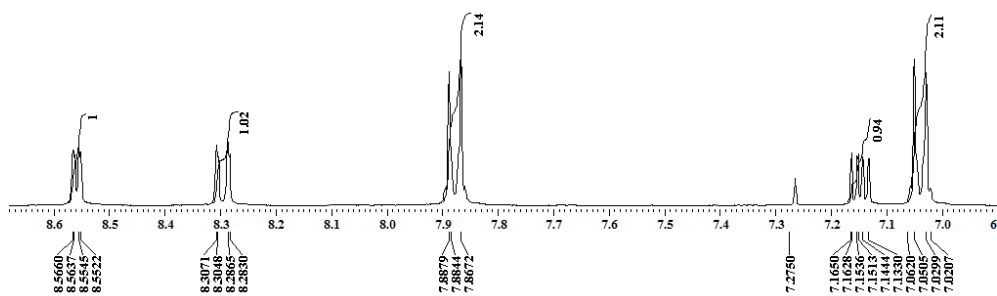
MS Spectrum Peak List

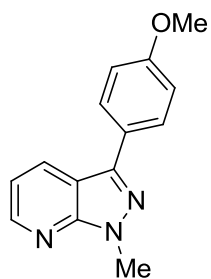
m/z	z	Abund	Formula	Ion
240.1138	1	1462283.75	C14 H13 N3 O	(M+H)+
241.1167	1	226490.51	C14 H13 N3 O	(M+H)+
242.1195	1	20024.68	C14 H13 N3 O	(M+H)+
243.1228	1	1880.09	C14 H13 N3 O	(M+H)+
244.1296	1	239.53	C14 H13 N3 O	(M+H)+
257.1381	1	1279.99	C14 H13 N3 O	(M+NH4)+

--- End Of Report ---

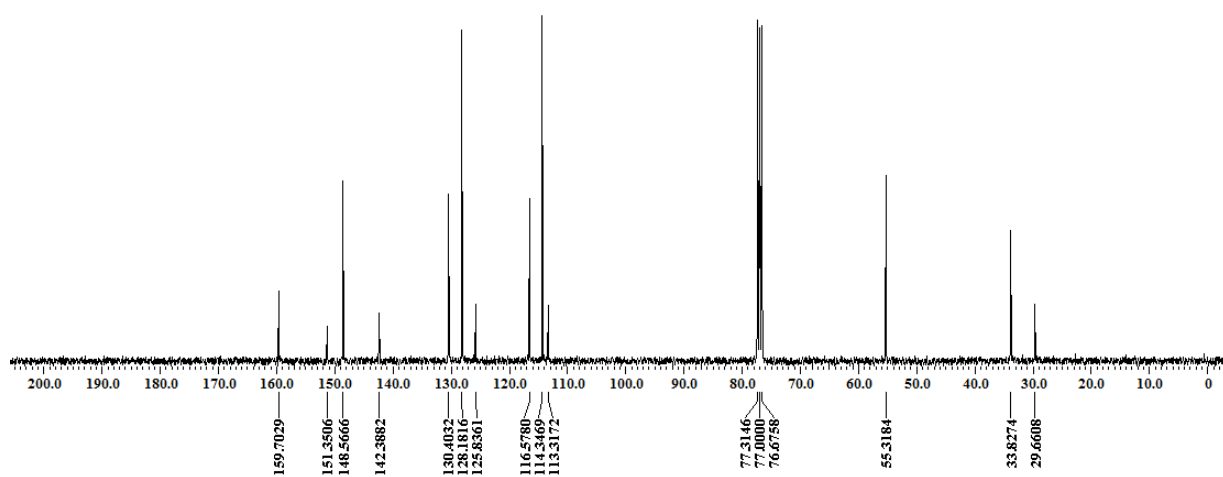
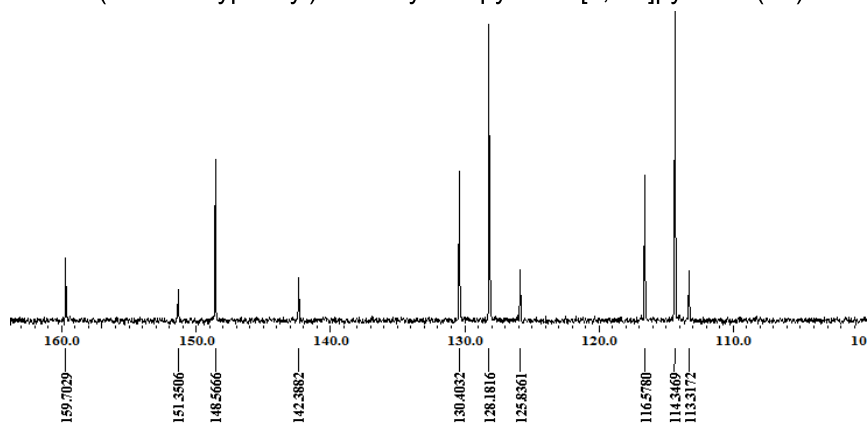


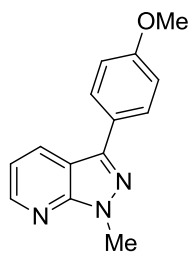
3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3d**)





3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (3d)





3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (3d)

Qualitative Compound Report

Data File	URV5-84.d	Sample Name	URV5-84
Sample Type	Sample	Position	P1-A9
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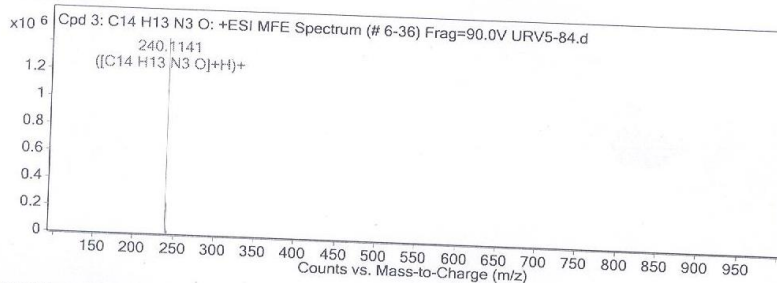
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Version	Q-TOF B.05.01 (B5125)	

Compound Table

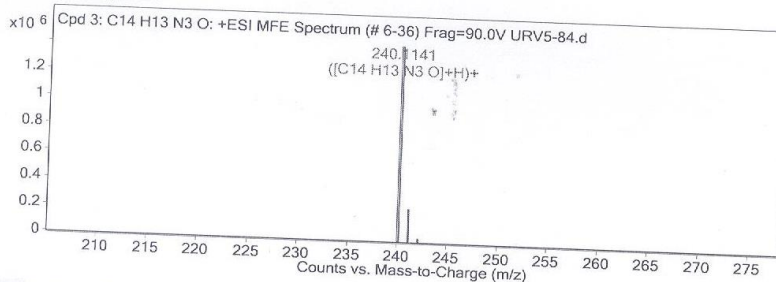
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C14 H13 N3 O	11	239.1068	C14 H13 N3 O	C14 H13 N3 O	-3.78	C14 H13 N3 O

Compound Label	m/z	RT	Algorithm	Mass
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MFE MS Spectrum



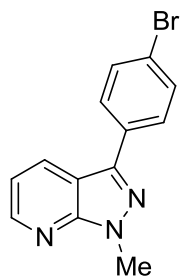
MFE MS Zoomed Spectrum



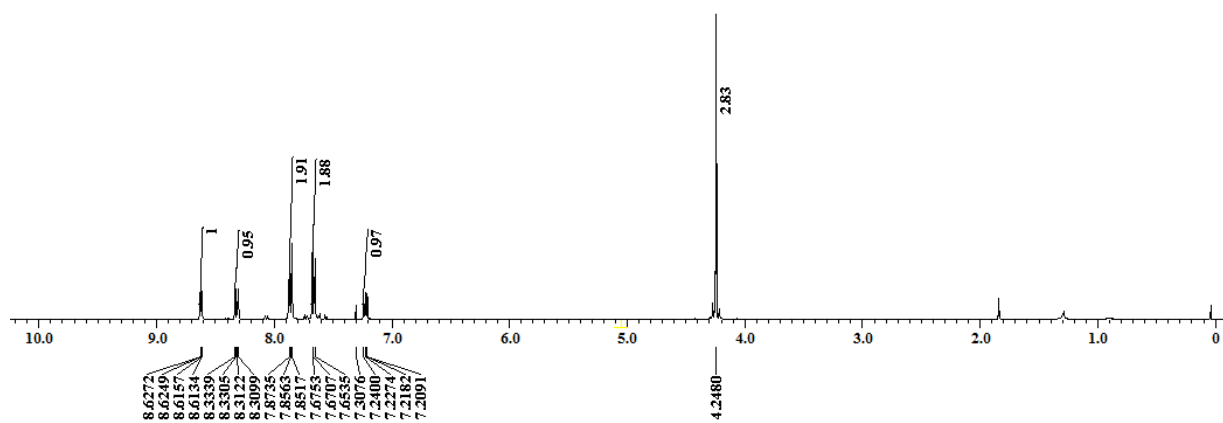
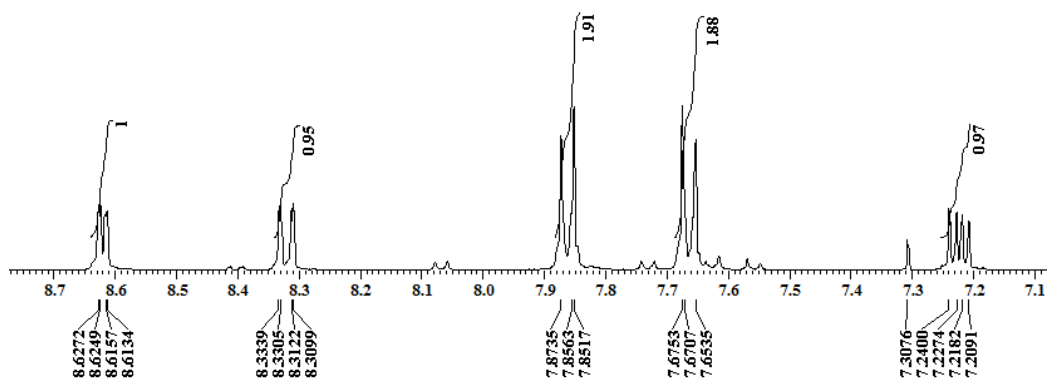
MS Spectrum Peak List

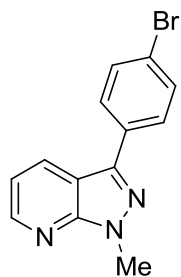
m/z	z	Abund	Formula	Ion
240.1141	1	1435305.88	C14 H13 N3 O	(M+H)+
241.1168	1	228163.1	C14 H13 N3 O	(M+H)+
242.1198	1	19562.13	C14 H13 N3 O	(M+H)+
243.1213	1	1715.49	C14 H13 N3 O	(M+H)+

--- End Of Report ---

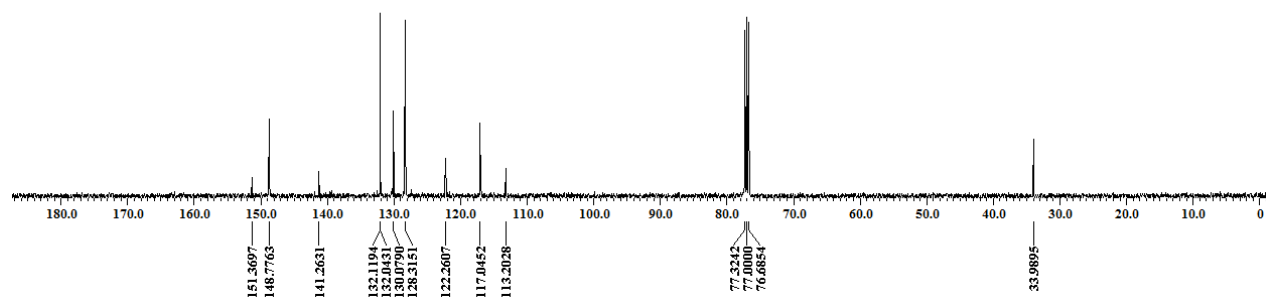
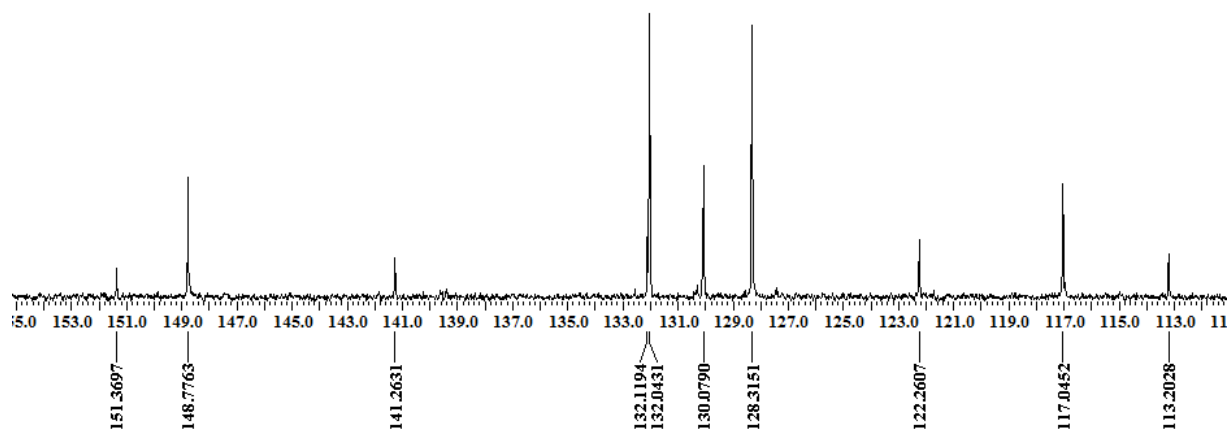


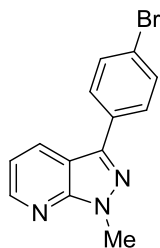
3-(4-bromophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (3e)





3-(4-bromophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (3e)





3-(4-bromophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3e**)

Qualitative Compound Report

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Comment			

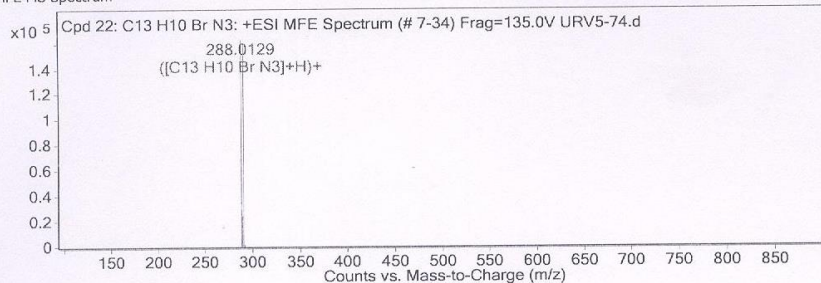
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Version	Q-TOF B.05.01 (B5125)	

Compound Table

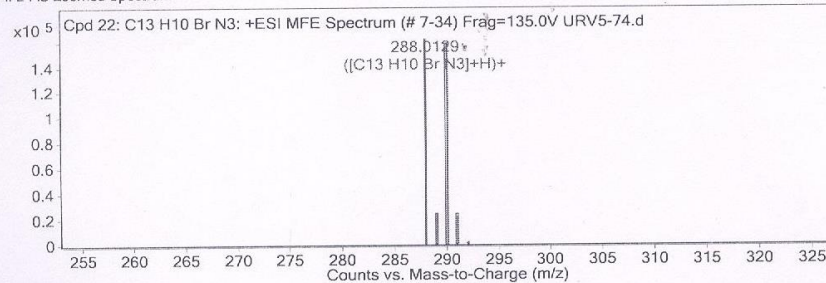
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Cpd 22: C13 H10 Br N3	10	287.0055	C13 H10 Br N3	C13 H10 Br N3	1.05	C13 H10 Br N3

Compound Label	m/z	RT	Algorithm	Mass
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MFE MS Spectrum



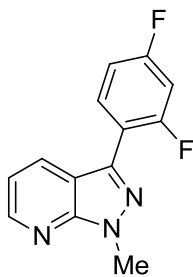
MFE MS Zoomed Spectrum



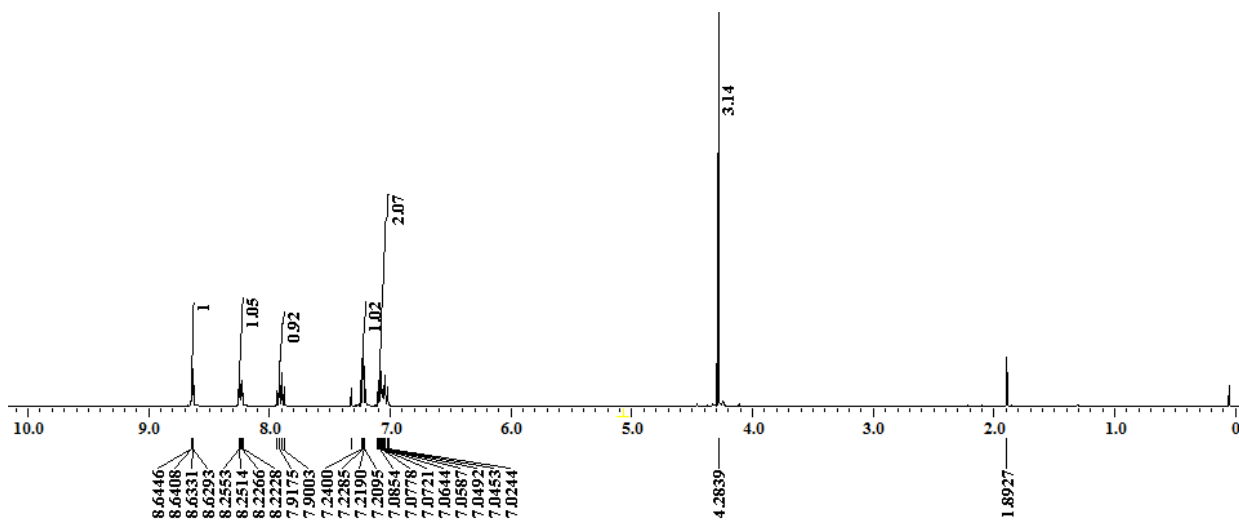
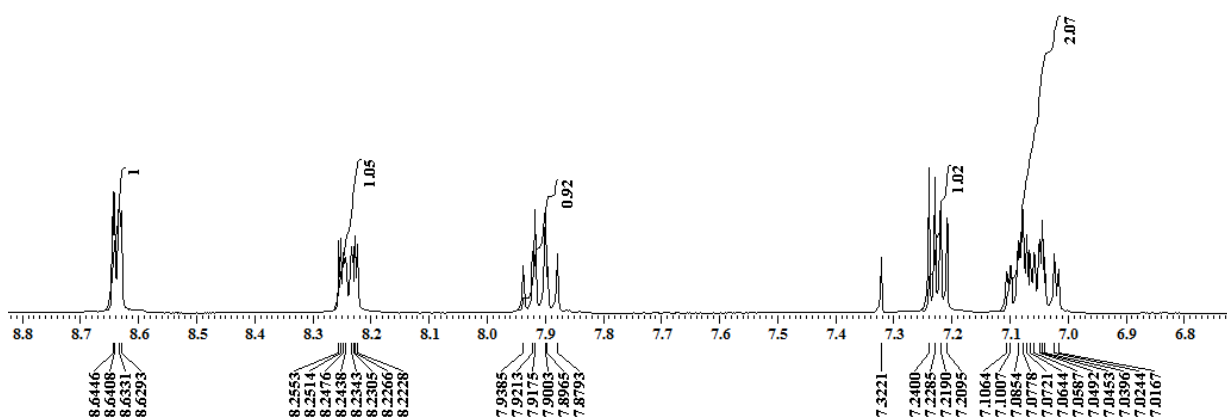
MS Spectrum Peak List

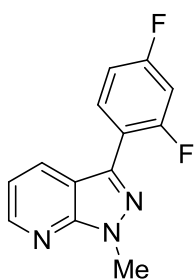
m/z	z	Abund	Formula	Ion
288.0129	1	162205.59	C13 H10 Br N3	(M+H)+
289.0158	1	24480.41	C13 H10 Br N3	(M+H)+
290.0108	1	158587.51	C13 H10 Br N3	(M+H)+
291.0136	1	22745.08	C13 H10 Br N3	(M+H)+
292.0171	1	1718.36	C13 H10 Br N3	(M+H)+

--- End Of Report ---

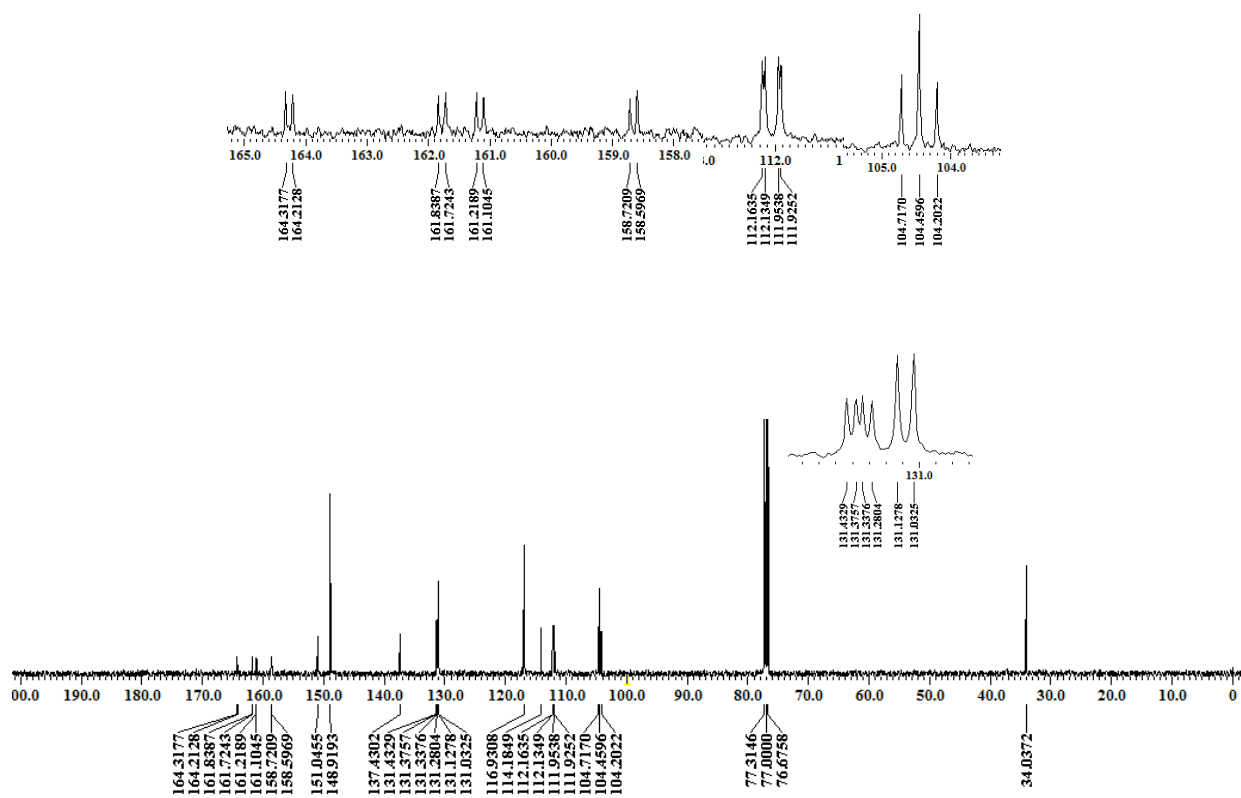


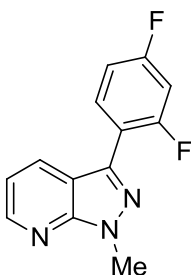
3-(2,4-difluorophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3f**)





3-(2,4-difluorophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3f**)





3-(2,4-difluorophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3f**)

Qualitative Compound Report

Data File	URV5-51.d	Sample Name	URV5-51
Sample Type	Sample	Position	P1-B5
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	15-03-2017 13:47:03
IRM Calibration Status	Success	DA Method	Default.m
Comment			

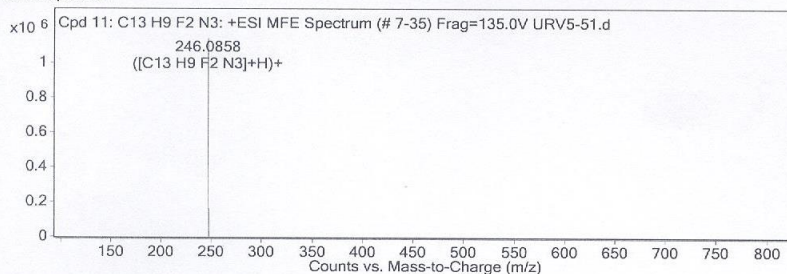
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

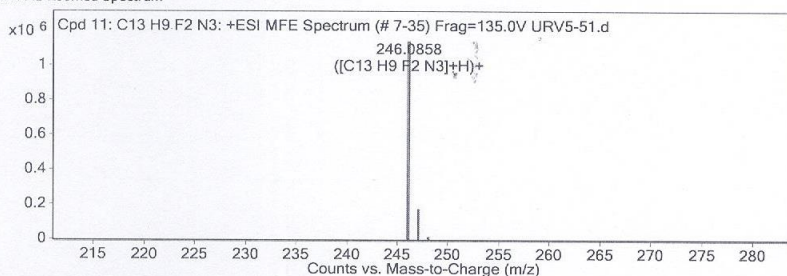
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C13 H9 F2 N3	12	245.0785	C13 H9 F2 N3	C13 H9 F2 N3	-8.29	C13 H9 F2 N3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 11: C13 H9 F2 N3	246.0858	12	Find by Molecular Feature	245.0785

MFE MS Spectrum



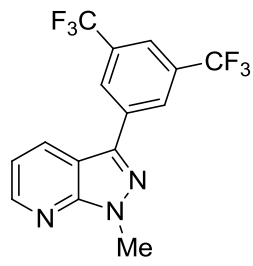
MFE MS Zoomed Spectrum



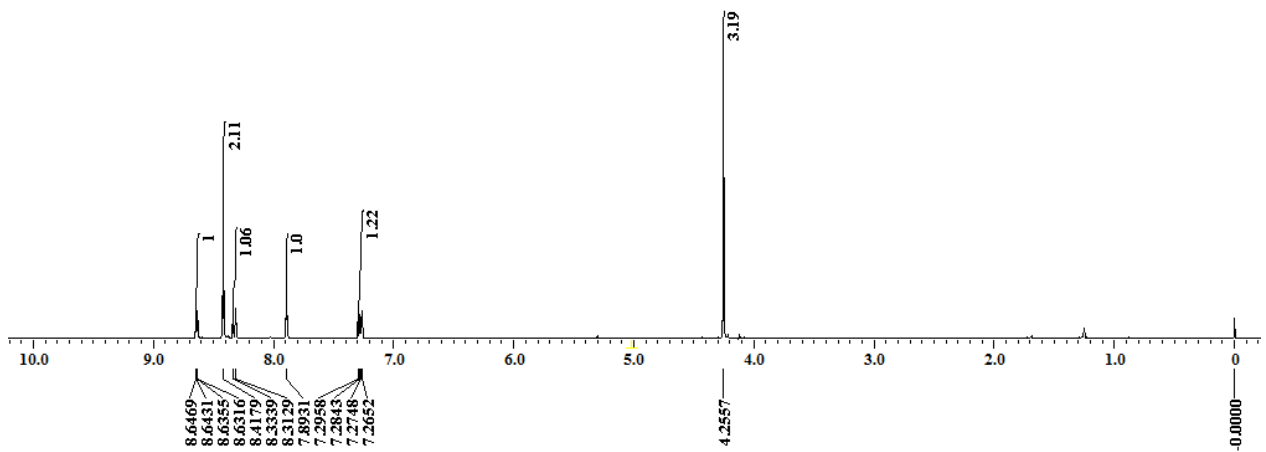
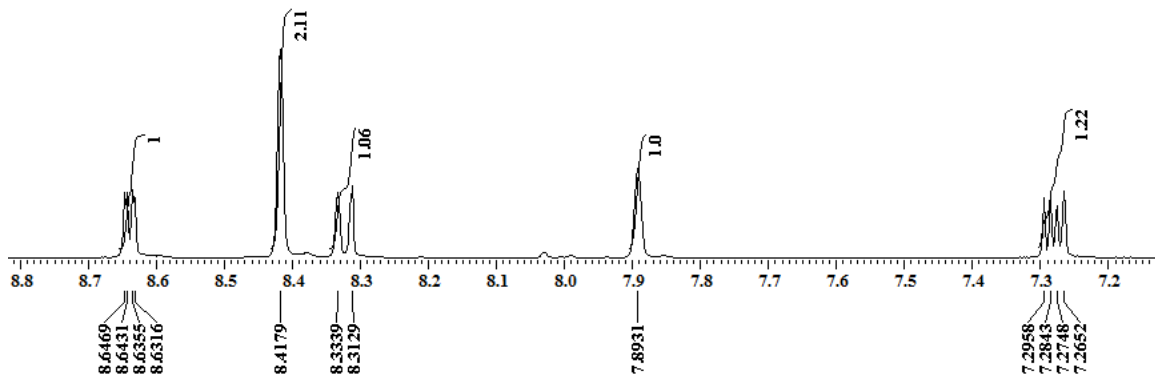
MS Spectrum Peak List

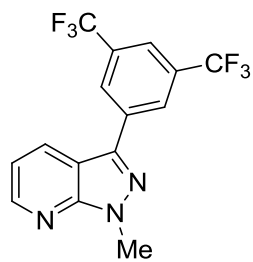
m/z	z	Abund	Formula	Ion
246.0858	1	1141598	C13 H9 F2 N3	(M+H)+
247.0886	1	165492	C13 H9 F2 N3	(M+H)+
248.0918	1	11599.09	C13 H9 F2 N3	(M+H)+
249.085	1	268.56	C13 H9 F2 N3	(M+H)+

--- End Of Report ---

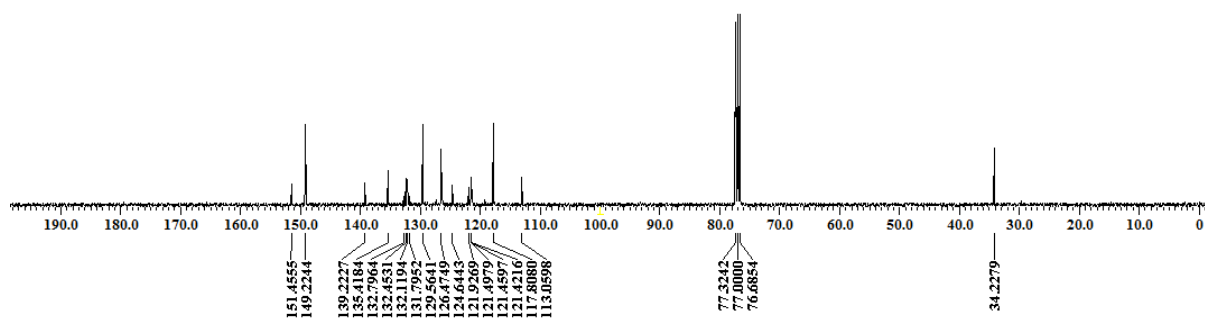
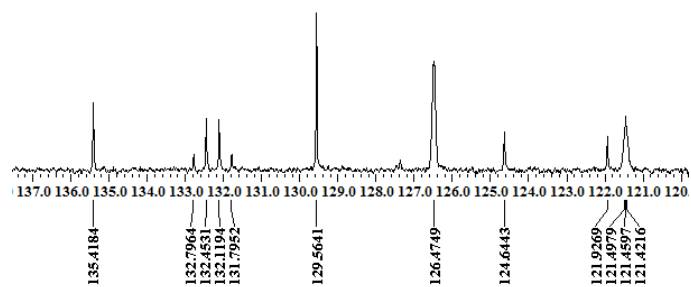


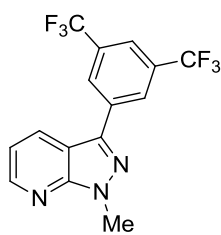
3-(3,5-bis(trifluoromethyl)phenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3g**)





3-(3,5-bis(trifluoromethyl)phenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3g**)





3-(3,5-bis(trifluoromethyl)phenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3g**)

Qualitative Compound Report

Data File	URV5-50FI.d	Sample Name	URV5-50FI
Sample Type	Sample	Position	P1-B9
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	27-04-2017 13:41:02
IRM Calibration Status	Success	DA Method	Default.m
Comment			

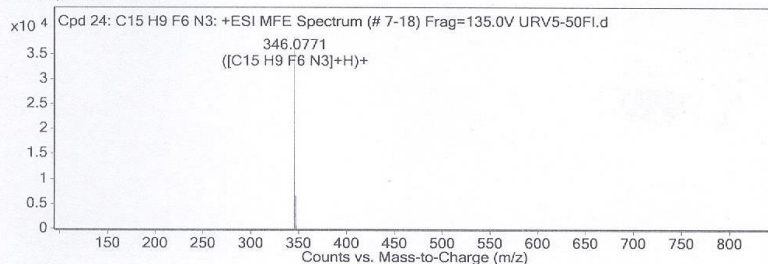
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

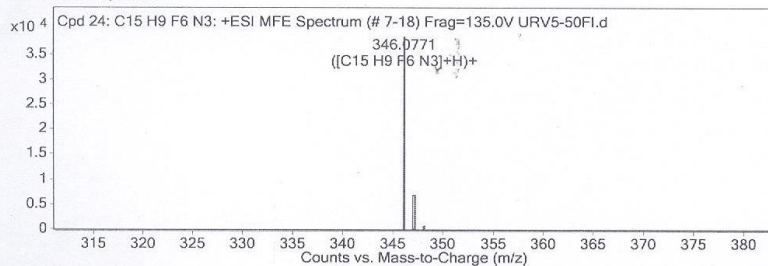
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 24: C15 H9 F6 N3	10	345.0699	C15 H9 F6 N3	C15 H9 F6 N3	0.39	C15 H9 F6 N3

Compound Label	m/z	RT	Algorithm	Mass
Cpd 24: C15 H9 F6 N3	346.0771	10	Find by Molecular Feature	345.0699

MFE MS Spectrum



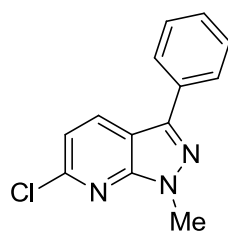
MFE MS Zoomed Spectrum



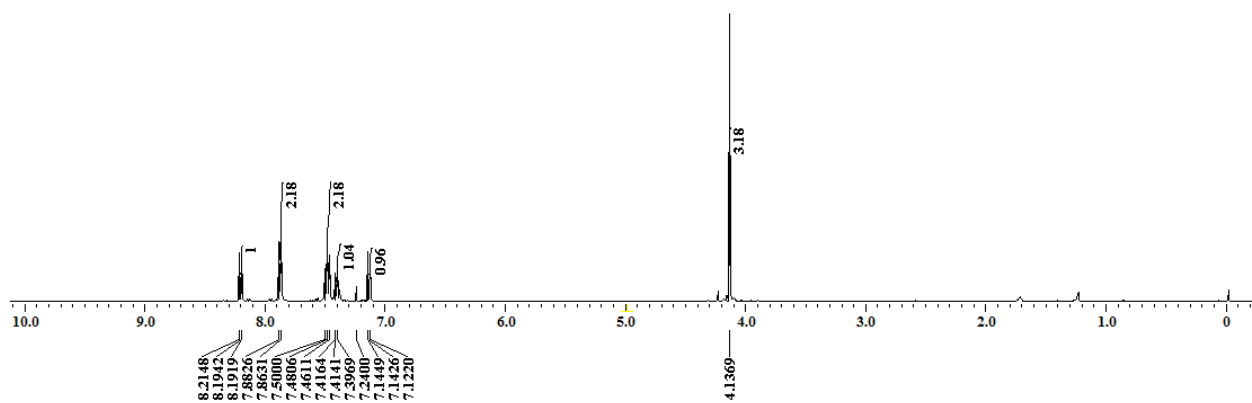
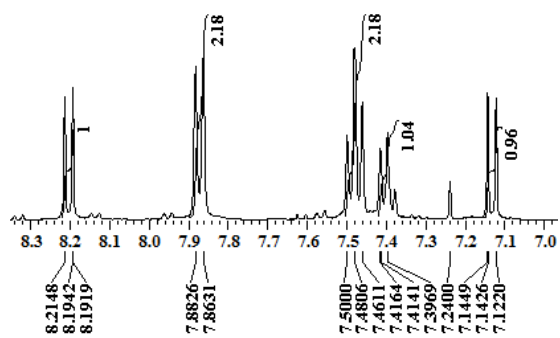
MS Spectrum Peak List

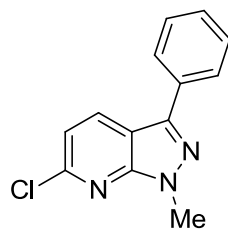
m/z	z	Abund	Formula	Ion
346.0771	1	38484.7	C15 H9 F6 N3	(M+H)+
347.0801	1	6687.71	C15 H9 F6 N3	(M+H)+
348.0873	1	705.14	C15 H9 F6 N3	(M+H)+

--- End Of Report ---

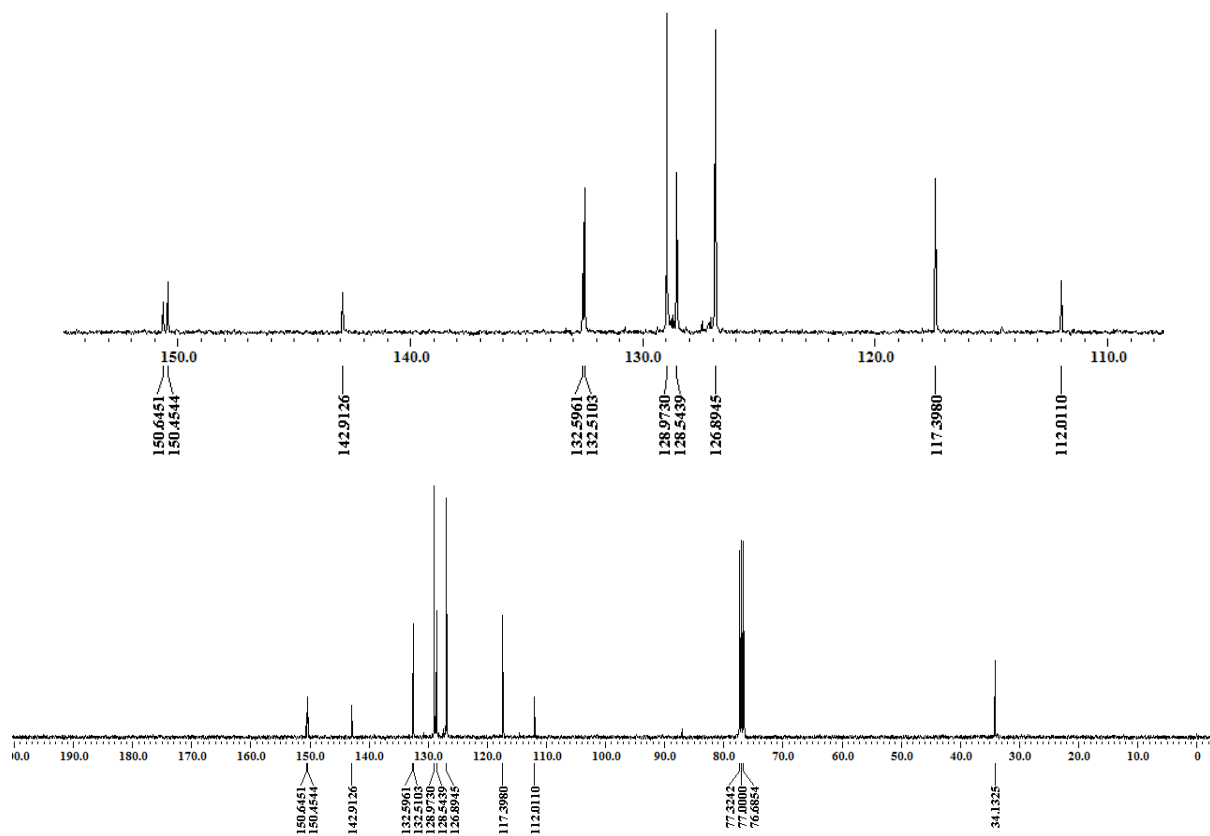


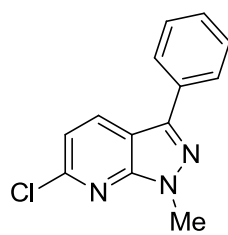
6-chloro-1-methyl-3-phenyl-1H-pyrazolo[3,4-b]pyridine (3h)



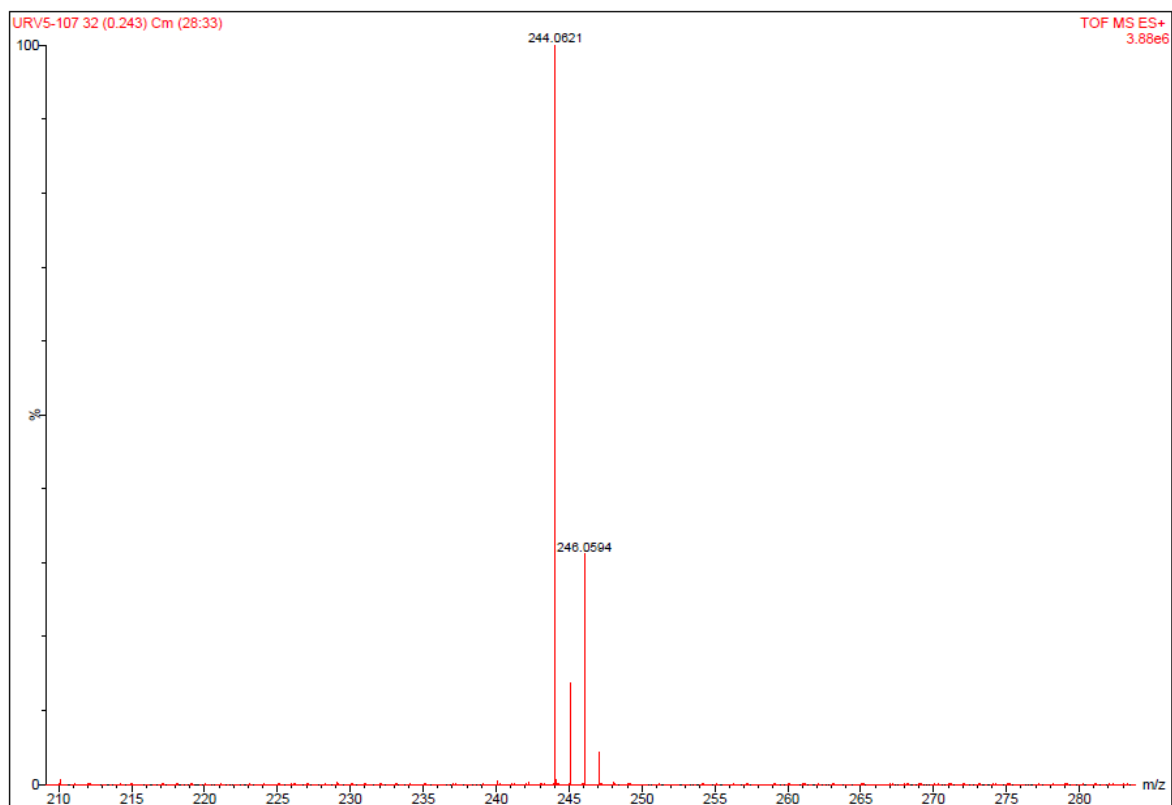


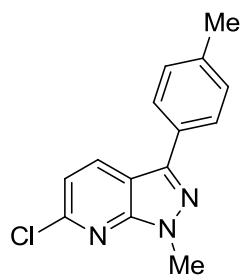
6-chloro-1-methyl-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (3h)



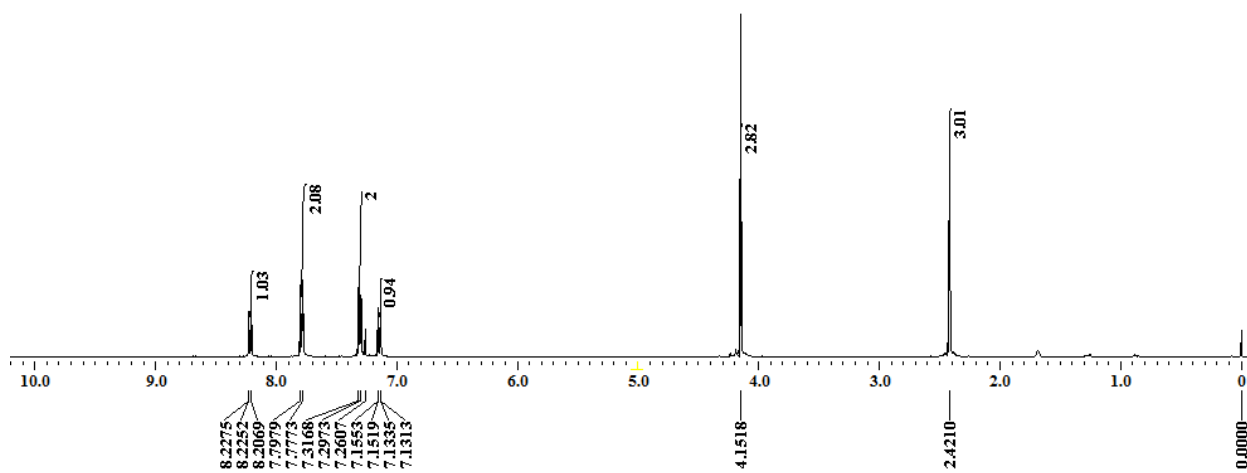
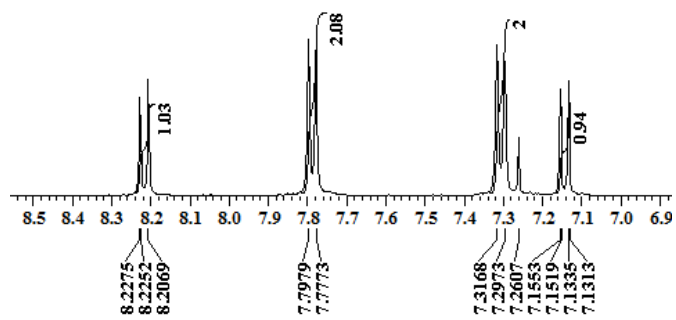


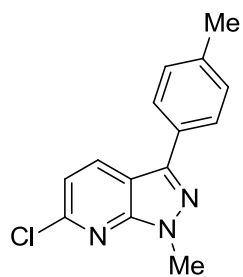
6-chloro-1-methyl-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**3h**)



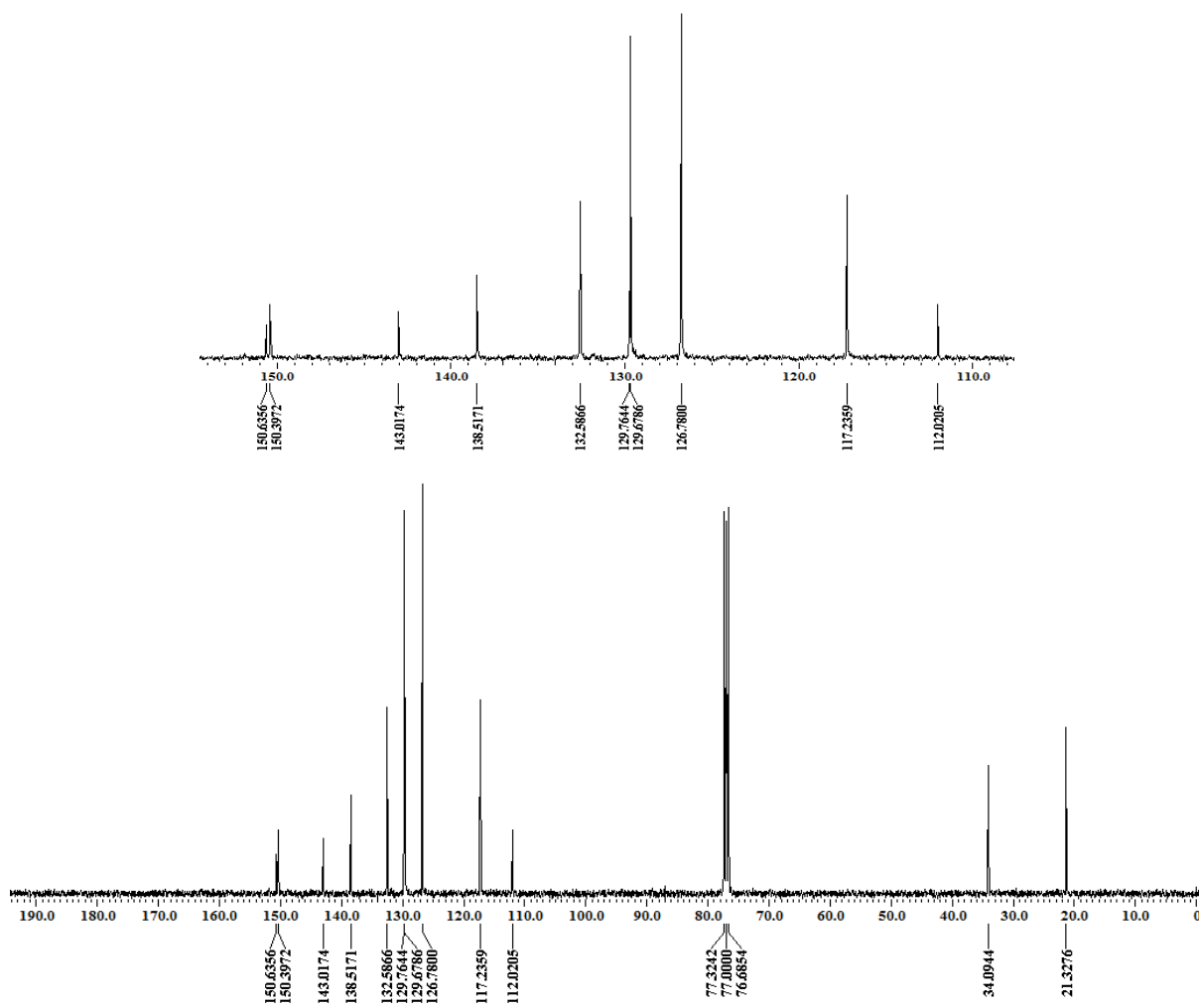


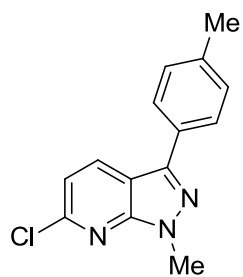
6-chloro-1-methyl-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3i**)



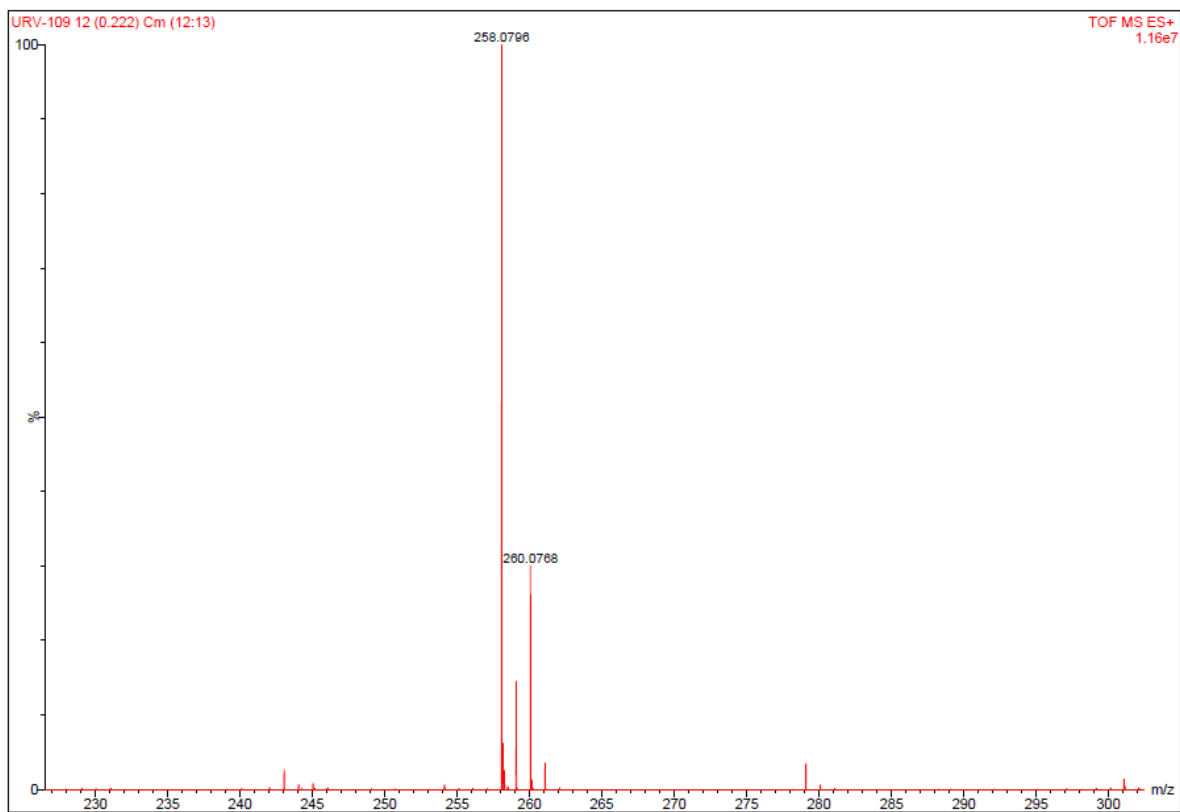


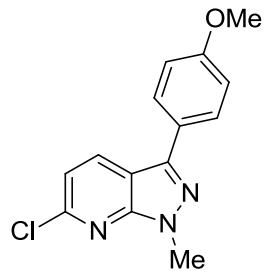
6-chloro-1-methyl-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridine (3i)



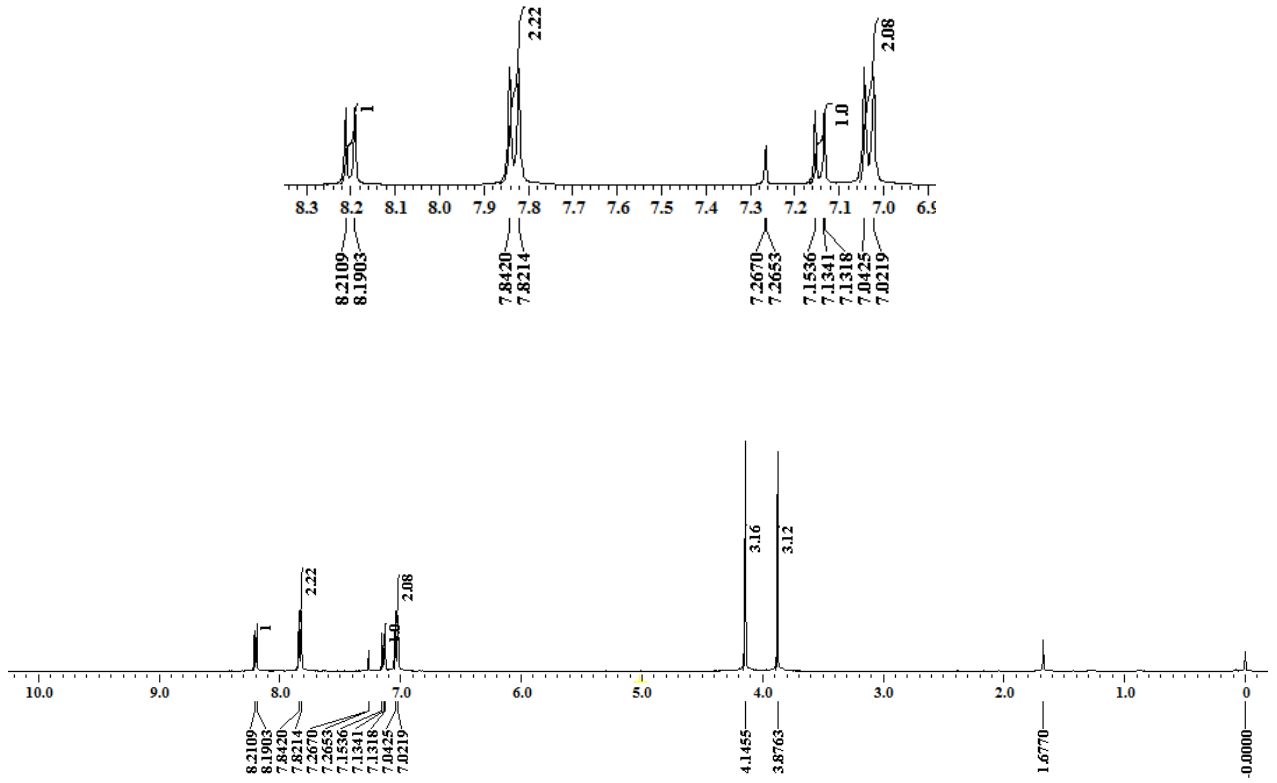


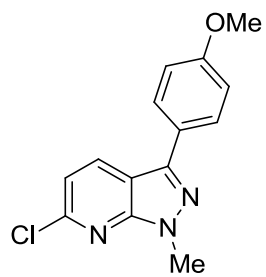
6-chloro-1-methyl-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3i**)



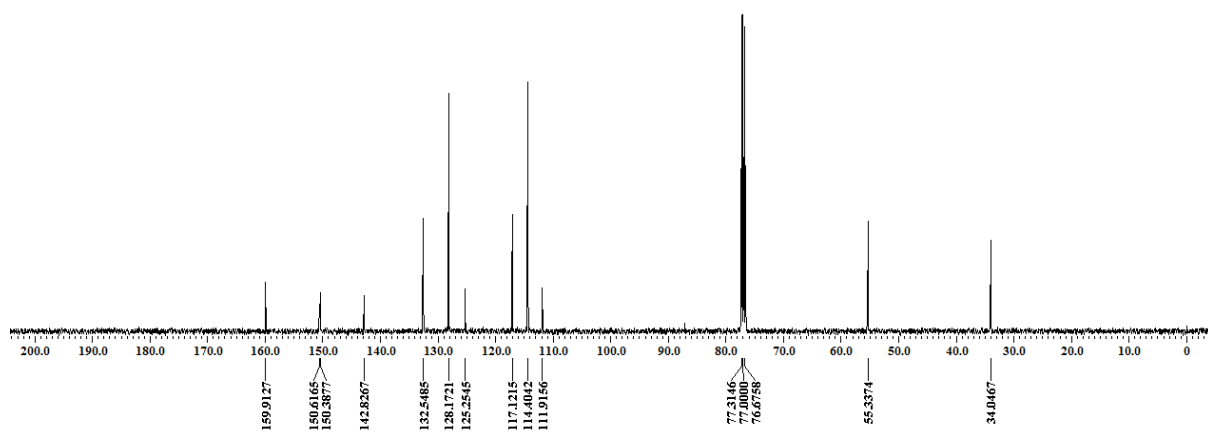
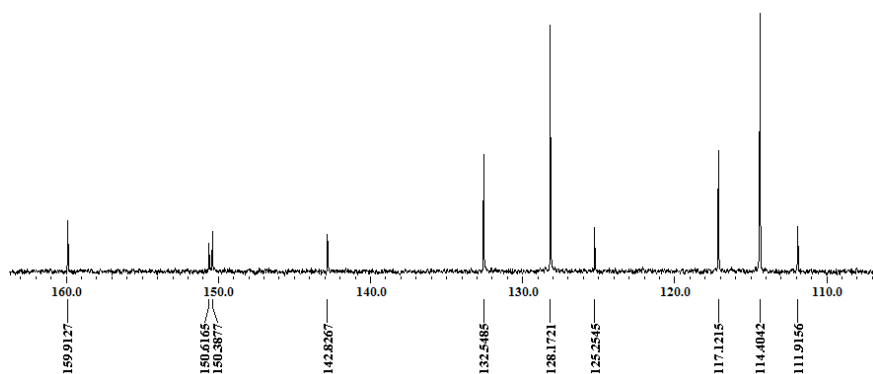


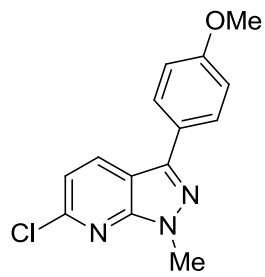
6-chloro-3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3j**)



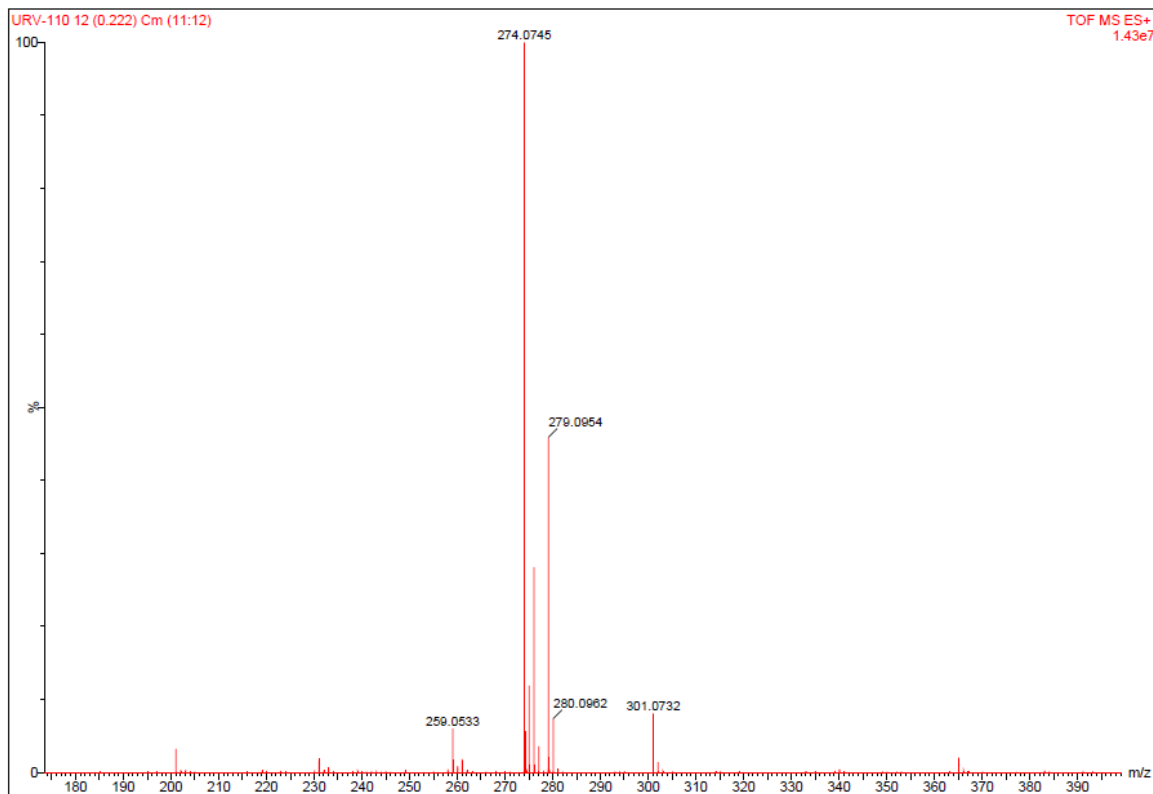


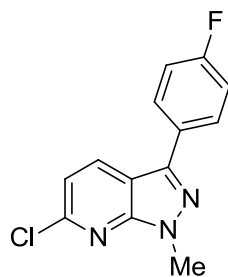
6-chloro-3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3j**)



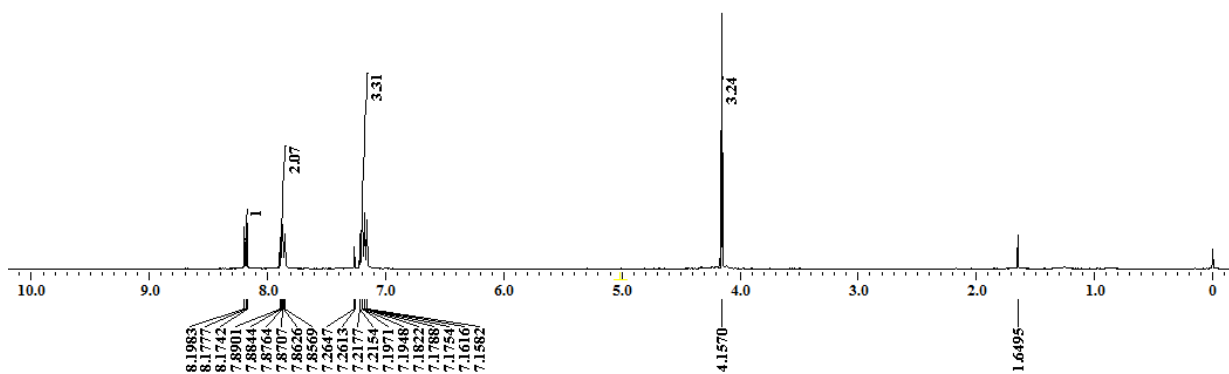
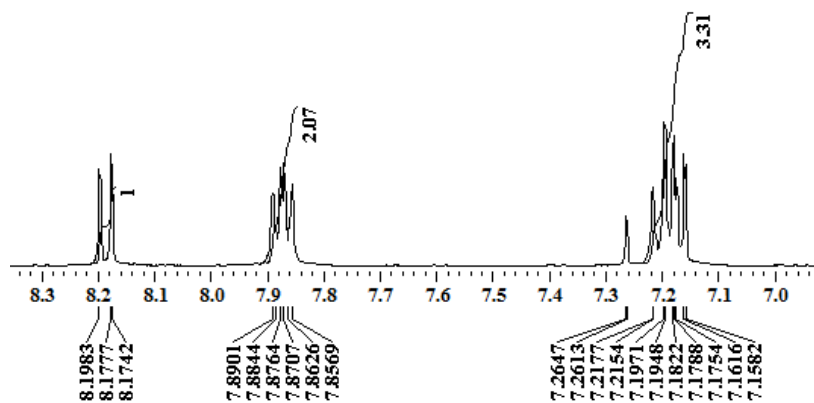


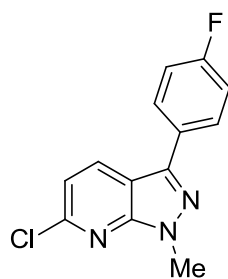
6-chloro-3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3j**)



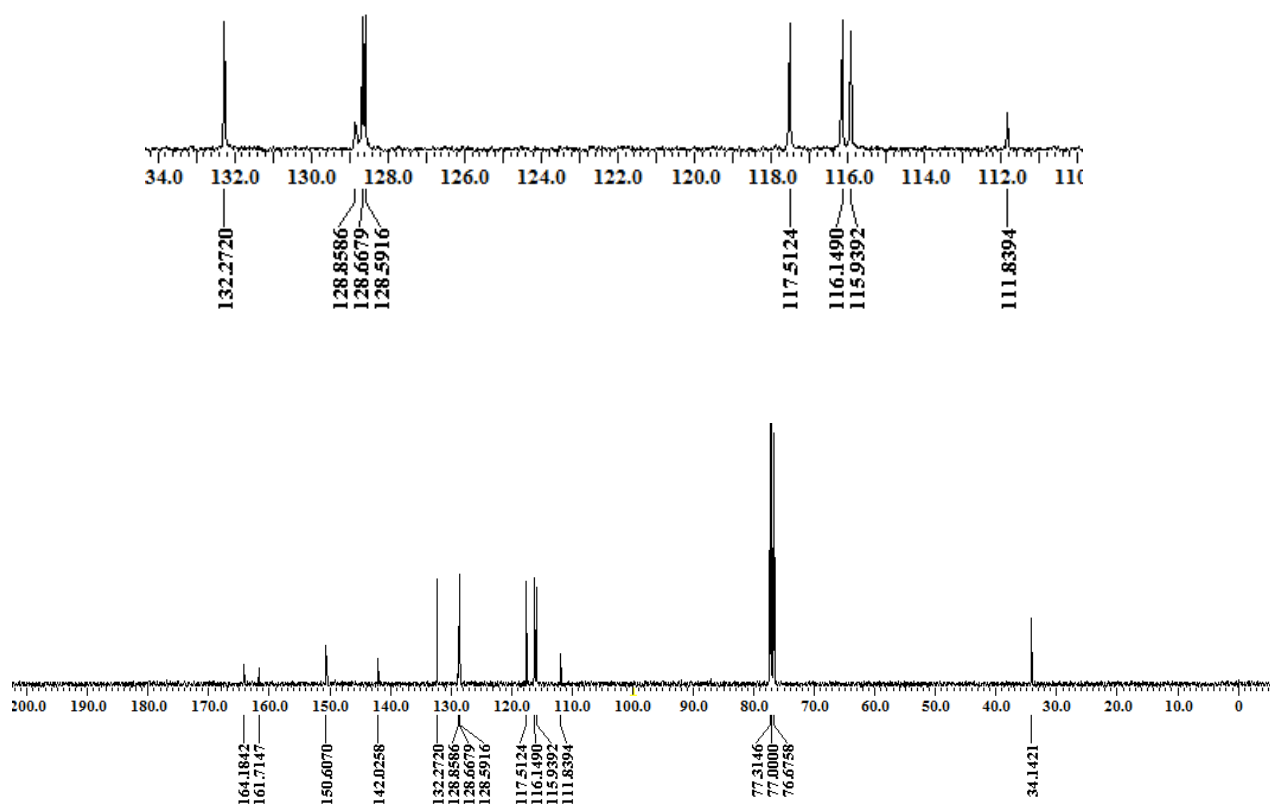


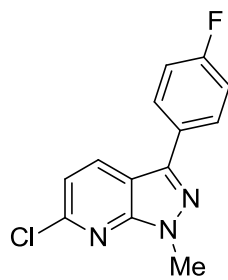
6-chloro-3-(4-fluorophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3k**)



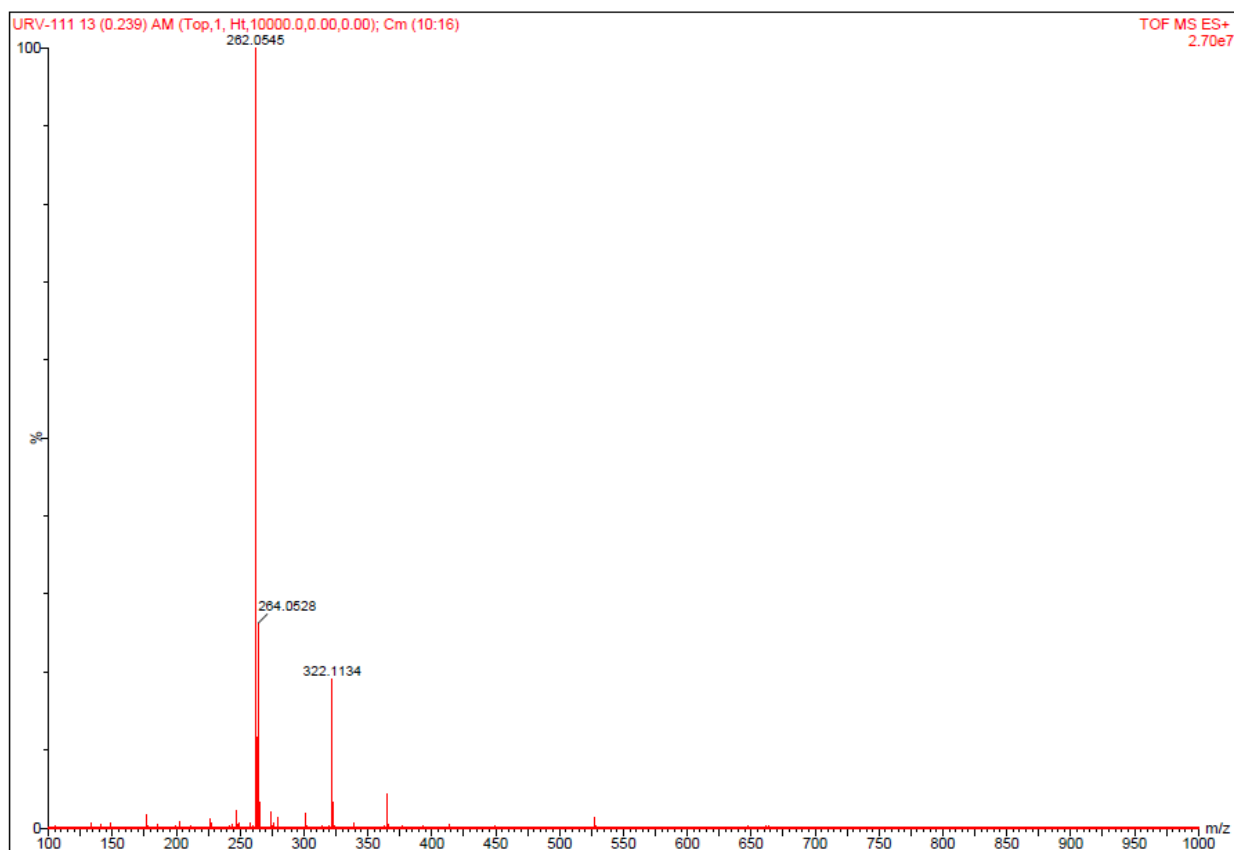


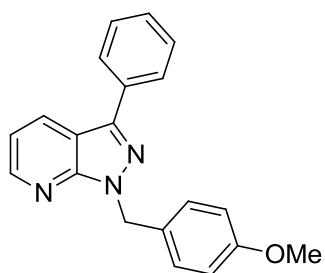
6-chloro-3-(4-fluorophenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridine (**3k**)



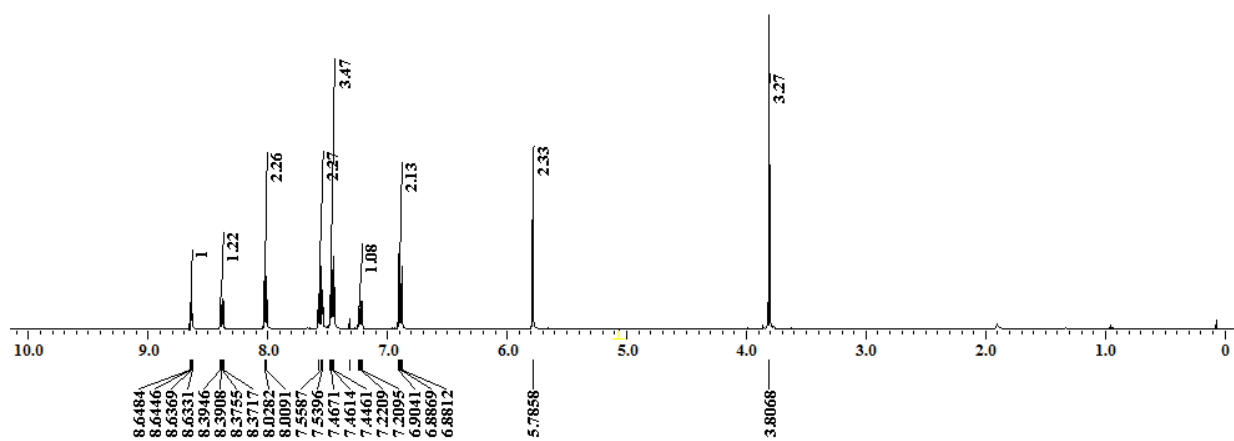
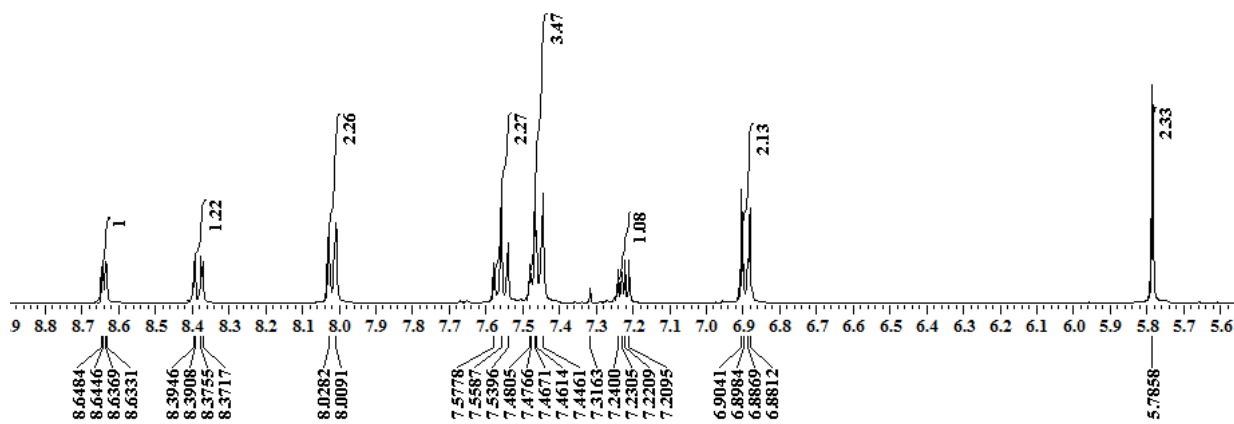


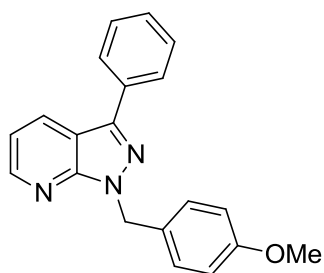
6-chloro-3-(4-fluorophenyl)-1-methyl-1*H*-pyrazolo[3,4-*b*]pyridine (**3k**)



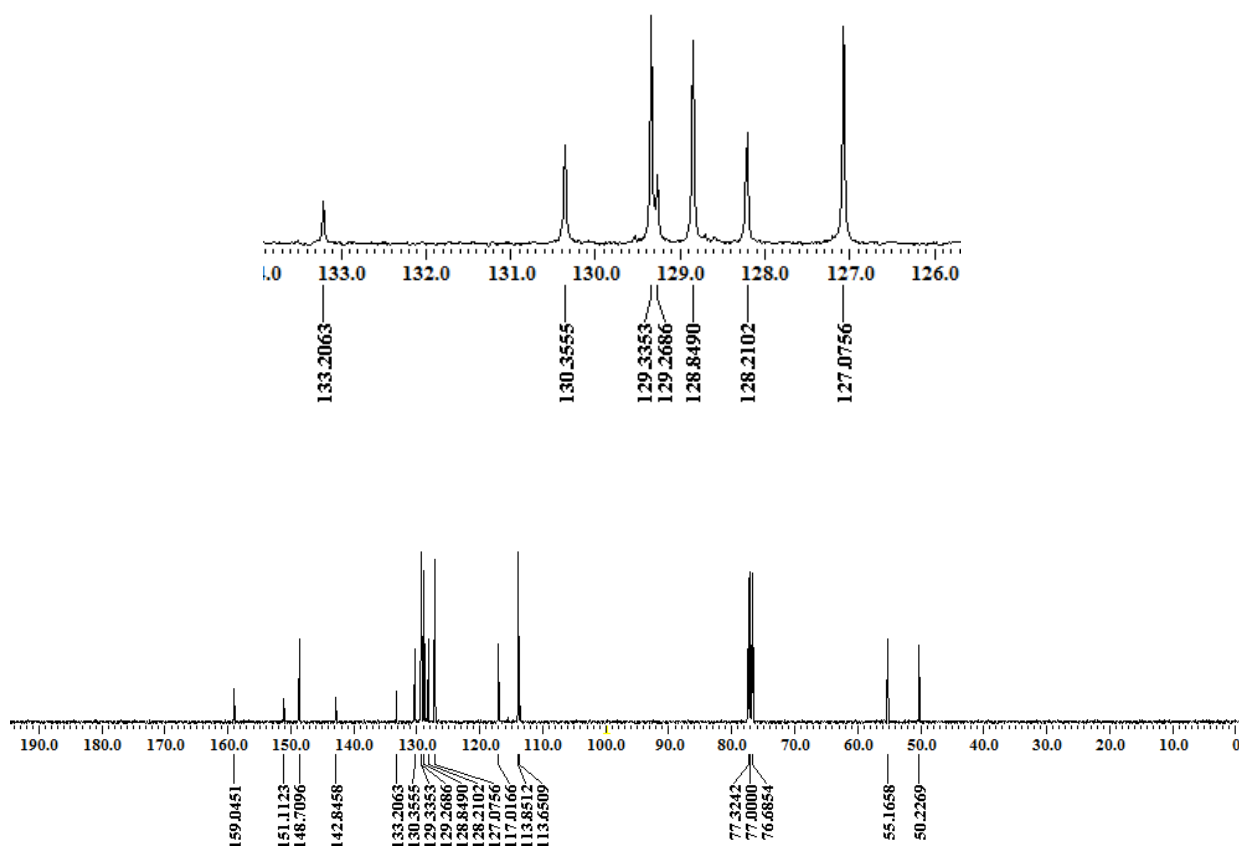


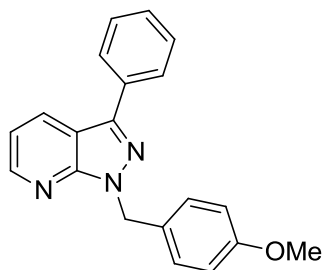
1-(4-methoxybenzyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**31**)





1-(4-methoxybenzyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**3I**)





1-(4-methoxybenzyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**3I**)

Qualitative Compound Report

Data File	URV5-52.d	Sample Name	URV5-52
Sample Type	Sample	Position	P1-B6
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	15-03-2017 13:48:56
IRM Calibration Status	Success	DA Method	Default.m
Comment			

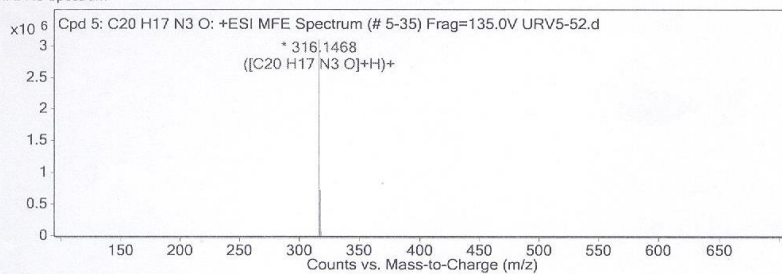
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

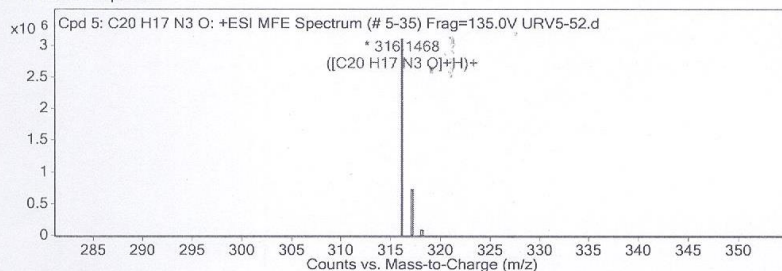
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C20 H17 N3 O	11	315.1396	C20 H17 N3 O	C20 H17 N3 O	-7.63	C20 H17 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 5: C20 H17 N3 O	316.1468	11	Find by Molecular Feature	315.1396

MFE MS Spectrum



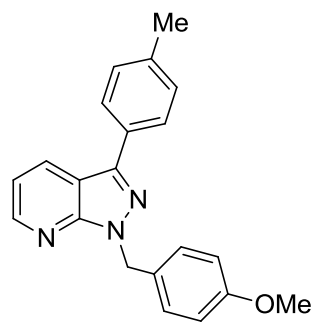
MFE MS Zoomed Spectrum



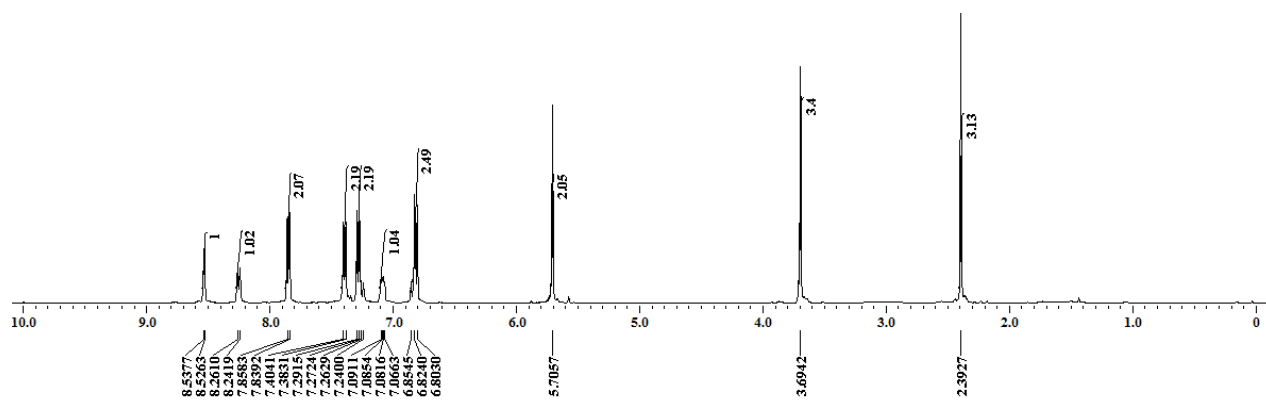
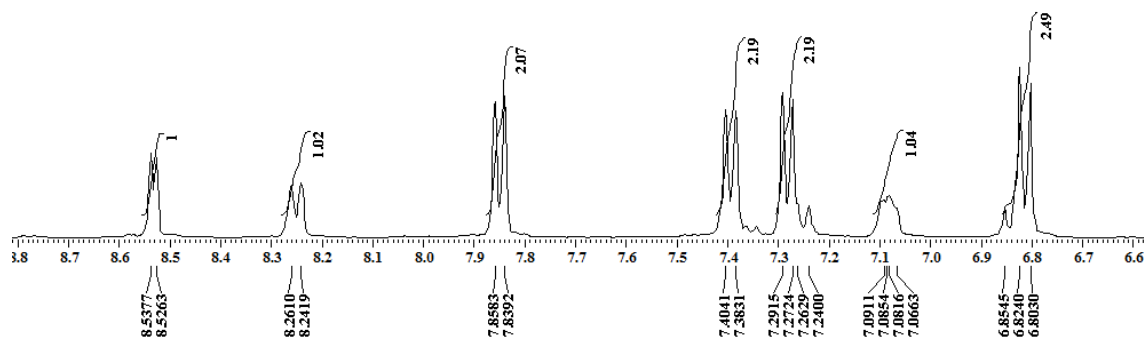
MS Spectrum Peak List

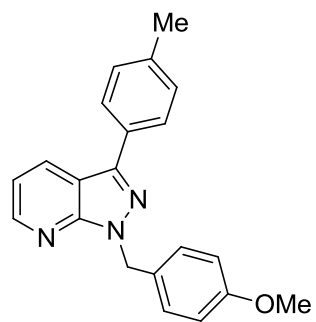
m/z	z	Abund	Formula	Ion
316.1468	1	3106500	C20 H17 N3 O	(M+H)+
317.15	1	713660.16	C20 H17 N3 O	(M+H)+
318.1526	1	78632.41	C20 H17 N3 O	(M+H)+
319.1585	1	7594.01	C20 H17 N3 O	(M+H)+
320.1535	1	478.53	C20 H17 N3 O	(M+H)+

--- End Of Report ---

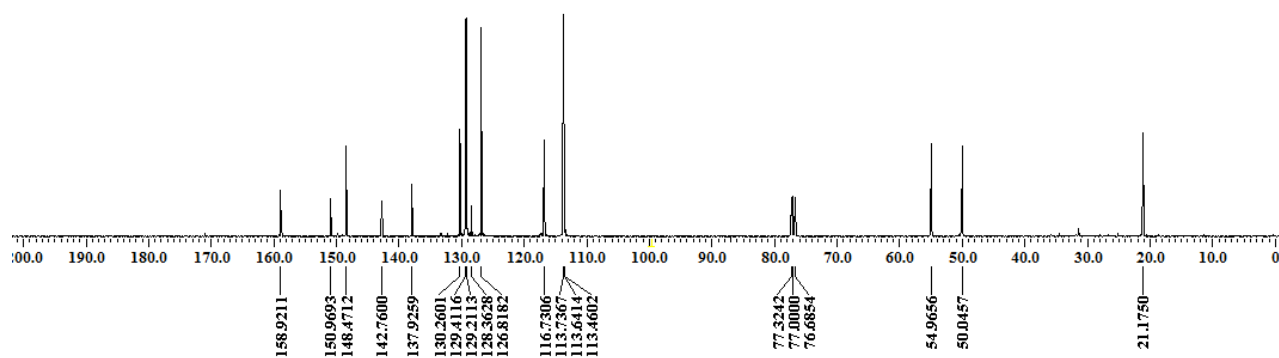


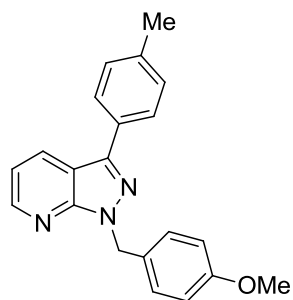
1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3m**)





1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3m**)





1-(4-methoxybenzyl)-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridine (3m)

Qualitative Compound Report

Data File	URV5-67.d	Sample Name	URV5-67
Sample Type	Sample	Position	P1-A8
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	24-04-2017 13:10:01
IRM Calibration Status	Success	DA Method	Default.m
Comment			

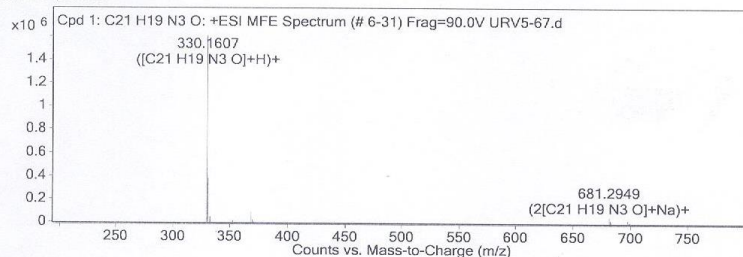
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

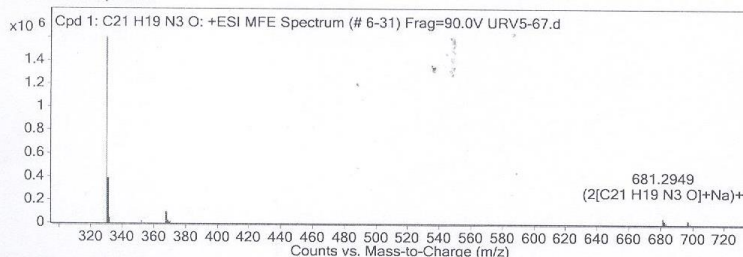
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H19 N3 O	11	329.1528	C21 H19 N3 O	C21 H19 N3 O	0.04	C21 H19 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C21 H19 N3 O	330.1607	11	Find by Molecular Feature	329.1528

MFE MS Spectrum



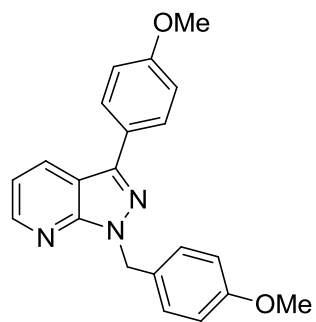
MFE MS Zoomed Spectrum



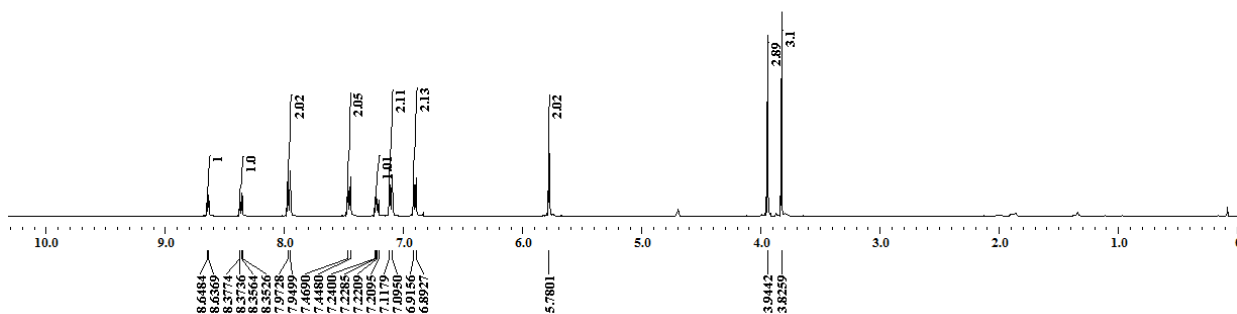
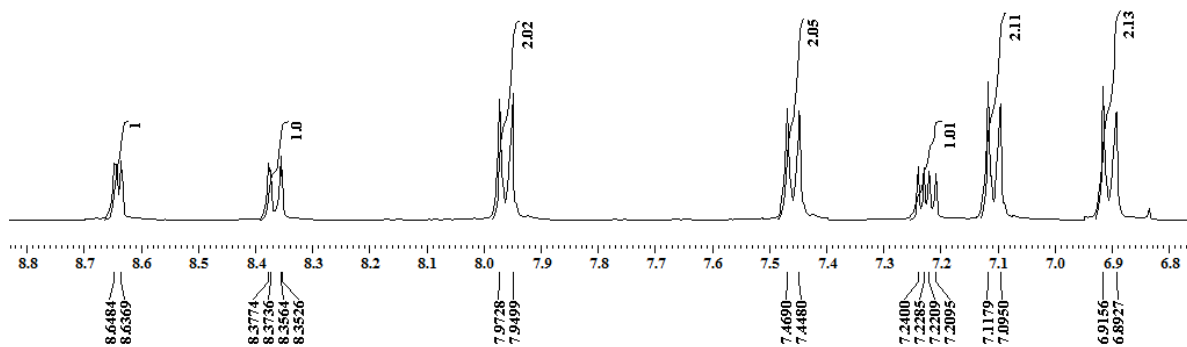
MS Spectrum Peak List

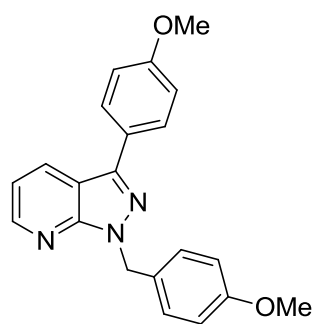
m/z	z	Abund	Formula	Ion
330.1607	1	1605653	C21 H19 N3 O	(M+H)+
331.1636	1	378299.55	C21 H19 N3 O	(M+H)+
332.1664	1	45619.94	C21 H19 N3 O	(M+H)+
352.1424	1	14614.36	C21 H19 N3 O	(M+Na)+
368.116	1	93162.54	C21 H19 N3 O	(M+K)+
369.1193	1	22353.53	C21 H19 N3 O	(M+K)+
681.2949	1	48981.82	C21 H19 N3 O	(2M+Na)+
682.2982	1	24242.31	C21 H19 N3 O	(2M+Na)+
697.2691	1	24685.19	C21 H19 N3 O	(2M+K)+
698.2711	1	11940.49	C21 H19 N3 O	(2M+K)+

--- End Of Report ---

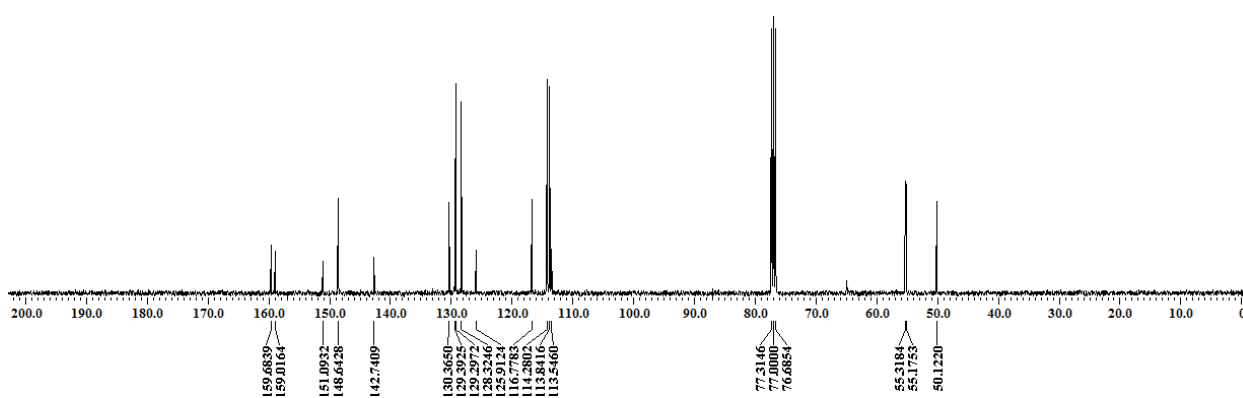
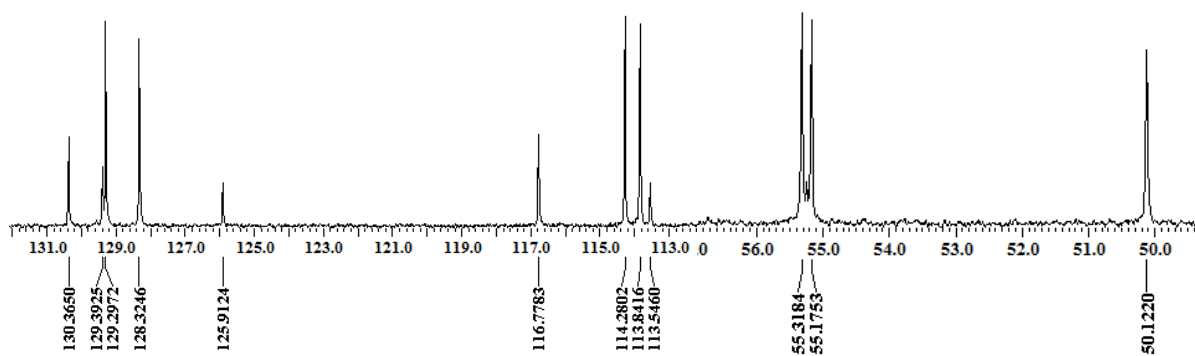


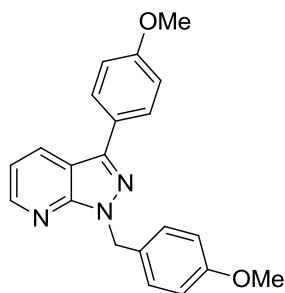
1-(4-methoxybenzyl)-3-(4-methoxyphenyl)-1H-pyrazolo[3,4-b]pyridine (**3n**)





1-(4-methoxybenzyl)-3-(4-methoxyphenyl)-1H-pyrazolo[3,4-b]pyridine (3n)





1-(4-methoxybenzyl)-3-(4-methoxyphenyl)-1H-pyrazolo[3,4-b]pyridine (**3n**)

Qualitative Compound Report

Data File	URV5-68.d	Sample Name	URV5-68
Sample Type	Sample	Position	P1-A2
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	21-04-2017 13:58:02
IRM Calibration Status	Success	DA Method	Default.m
Comment			

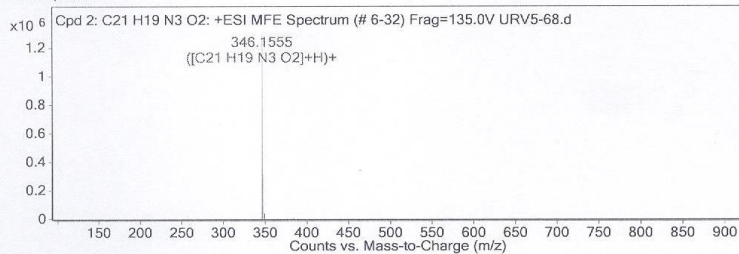
Sample Group Info.
 Acquisition SW 6200 series TOF/6500 series
 Version Q-TOF B.05.01 (B5125)

Compound Table

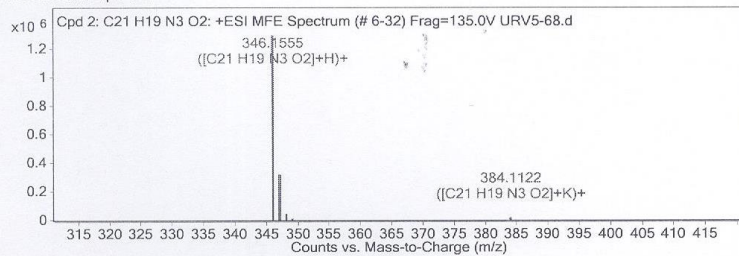
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C21 H19 N3 O2	10	345.1482	C21 H19 N3 O2	C21 H19 N3 O2	-1.32	C21 H19 N3 O2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C21 H19 N3 O2	346.1555	10	Find by Molecular Feature	345.1482

MFE MS Spectrum



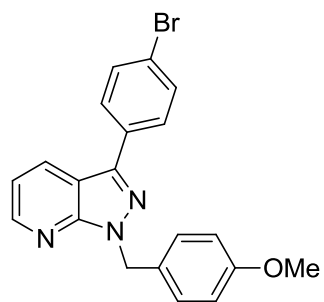
MFE MS Zoomed Spectrum



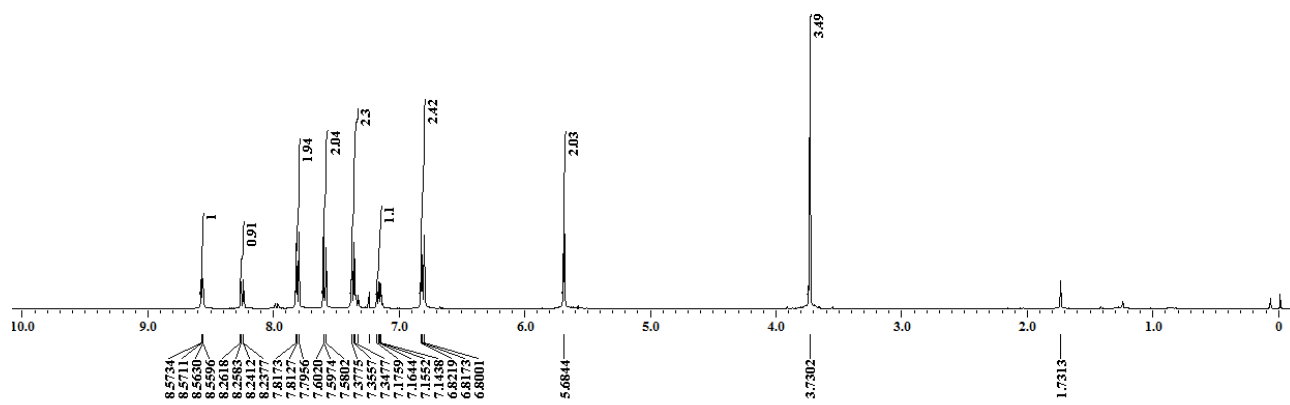
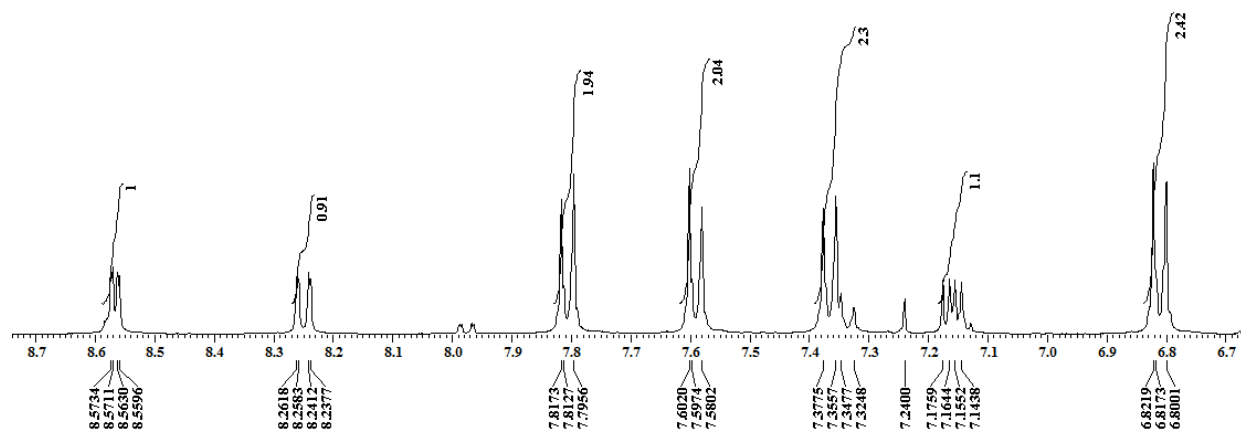
MS Spectrum Peak List

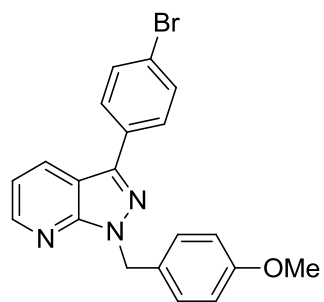
m/z	z	Abund	Formula	Ion
346.1555	1	1289776.63	C21 H19 N3 O2	(M+H)+
347.1584	1	309043.58	C21 H19 N3 O2	(M+H)+
348.1613	1	39045.37	C21 H19 N3 O2	(M+H)+
349.1696	1	4343.15	C21 H19 N3 O2	(M+H)+
350.1849	1	618.34	C21 H19 N3 O2	(M+H)+
384.1122	1	9947.79	C21 H19 N3 O2	(M+K)+
385.118	1	2495.26	C21 H19 N3 O2	(M+K)+
386.1115	1	1173.98	C21 H19 N3 O2	(M+K)+

--- End Of Report ---

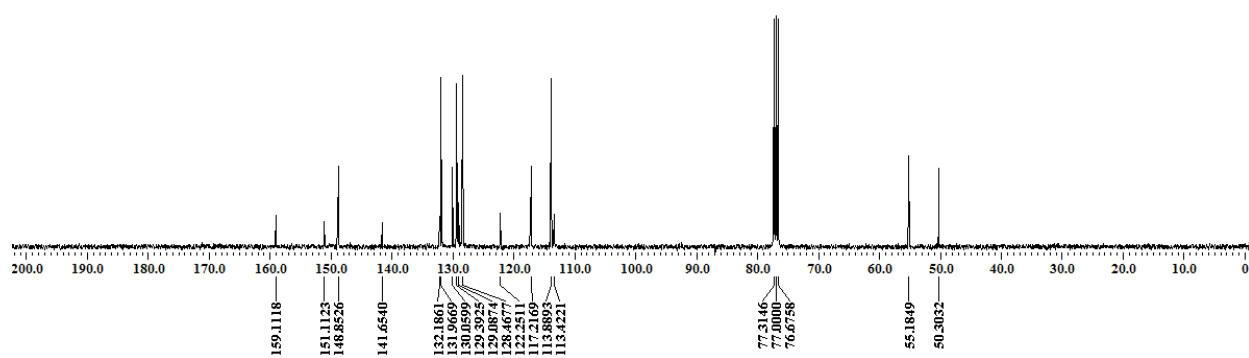
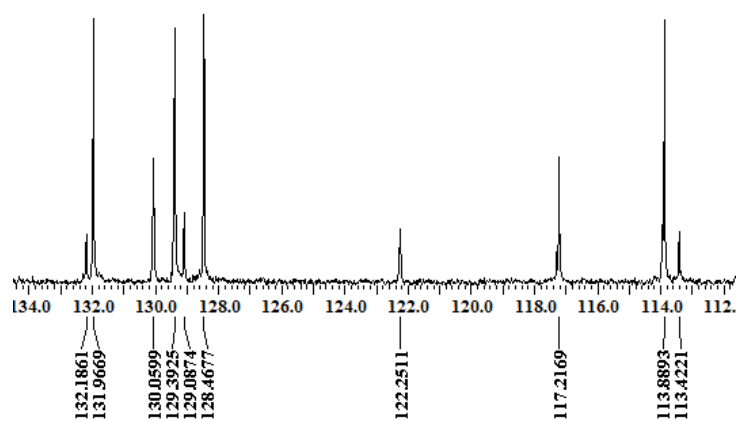


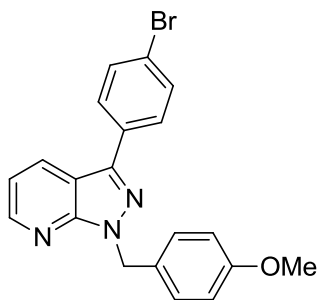
3-(4-bromophenyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3o**)





3-(4-bromophenyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3o**)





3-(4-bromophenyl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3o**)

Qualitative Compound Report

Data File	URV5-78.d	Sample Name	URV5-78
Sample Type	Sample	Position	P1-B8
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	04-05-2017 13:39:23
IRM Calibration Status	Success	DA Method	Default.m
Comment			

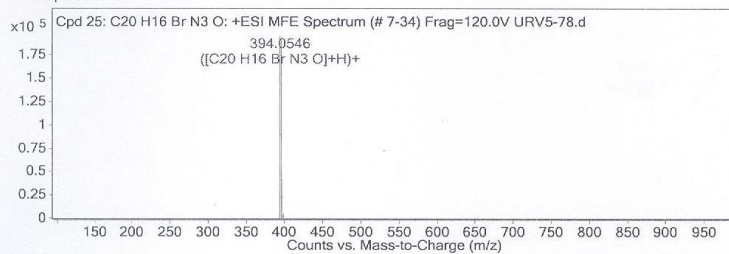
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

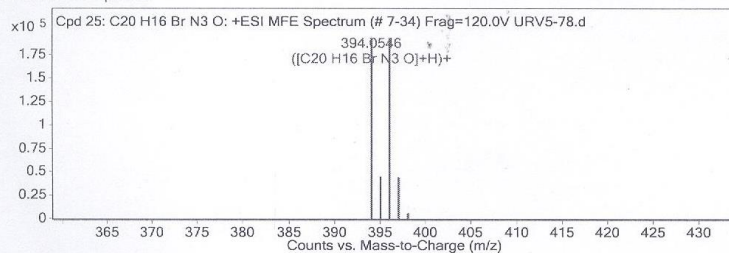
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 25: C20 H16 Br N3 O	11	393.0473	C20 H16 Br N3 O	C20 H16 Br N3 O	0.9	C20 H16 Br N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 25: C20 H16 Br N3 O	394.0546	11	Find by Molecular Feature	393.0473

MFE MS Spectrum



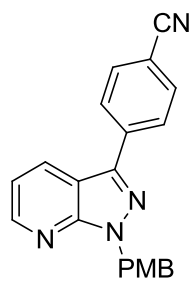
MFE MS Zoomed Spectrum



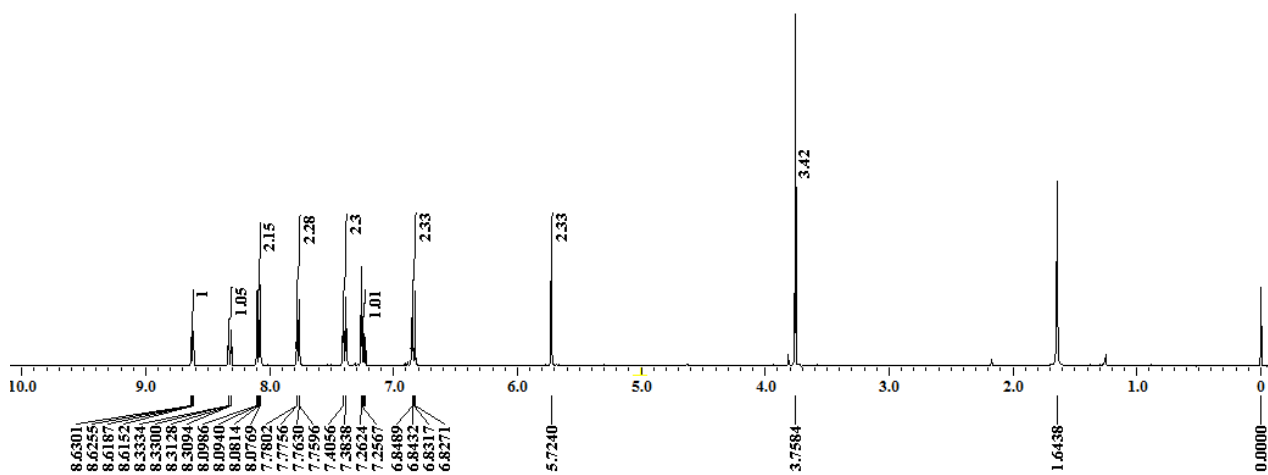
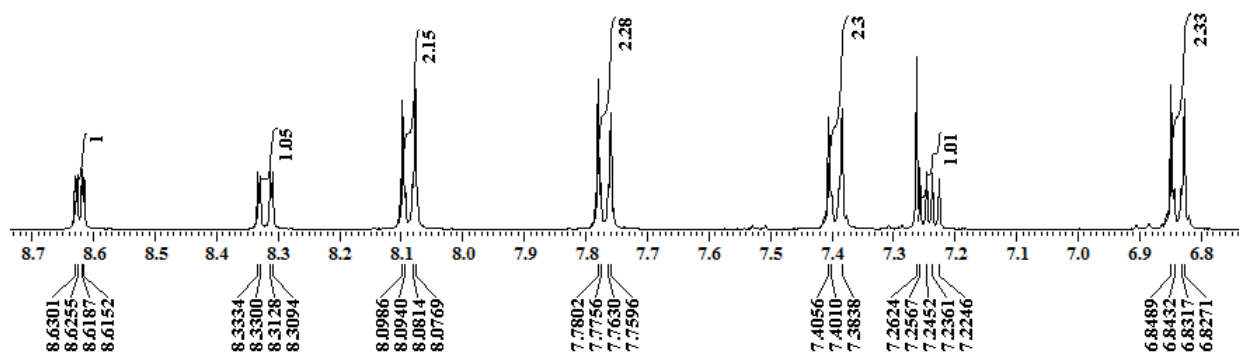
MS Spectrum Peak List

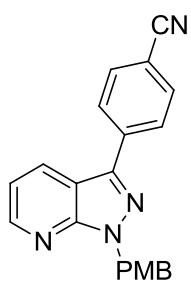
m/z	z	Abund	Formula	Ion
394.0546	1	195572.84	C20 H16 Br N3 O	(M+H)+
395.0576	1	42915.55	C20 H16 Br N3 O	(M+H)+
396.0528	1	193829.16	C20 H16 Br N3 O	(M+H)+
397.0555	1	41997.89	C20 H16 Br N3 O	(M+H)+
398.0588	1	5082.82	C20 H16 Br N3 O	(M+H)+
399.0584	1	141.5	C20 H16 Br N3 O	(M+H)+

--- End Of Report ---

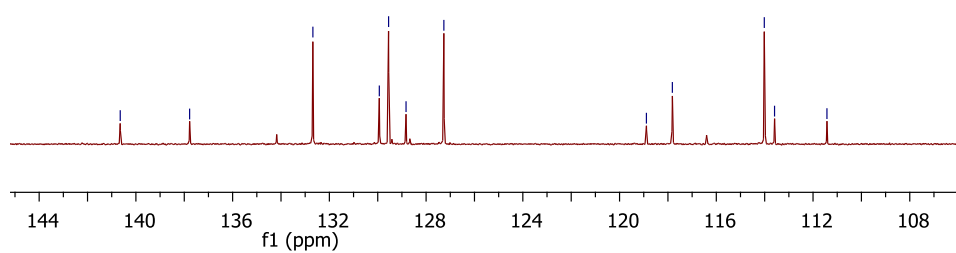


4-(1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridin-3-yl)benzonitrile (**3p**)

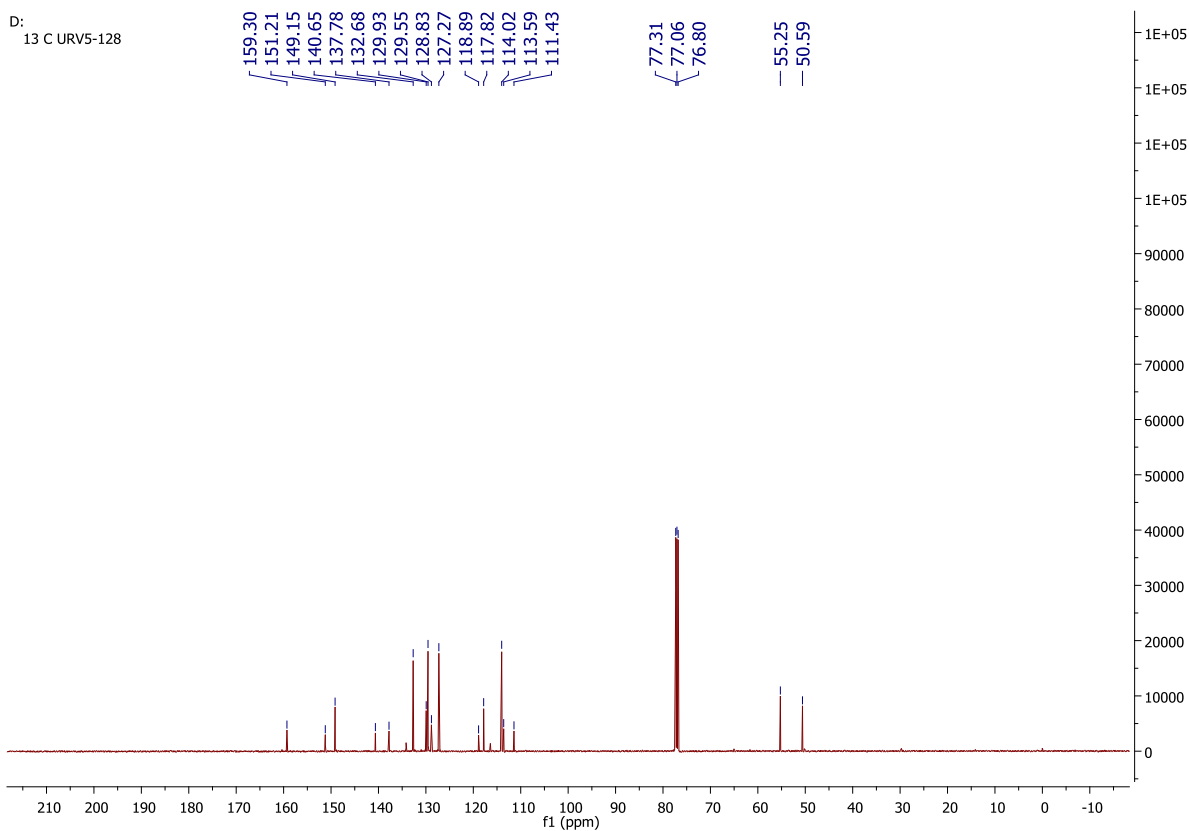


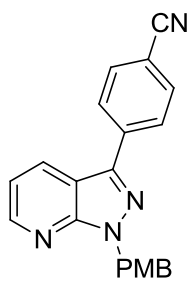


4-(1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl)benzonitrile (**3p**)

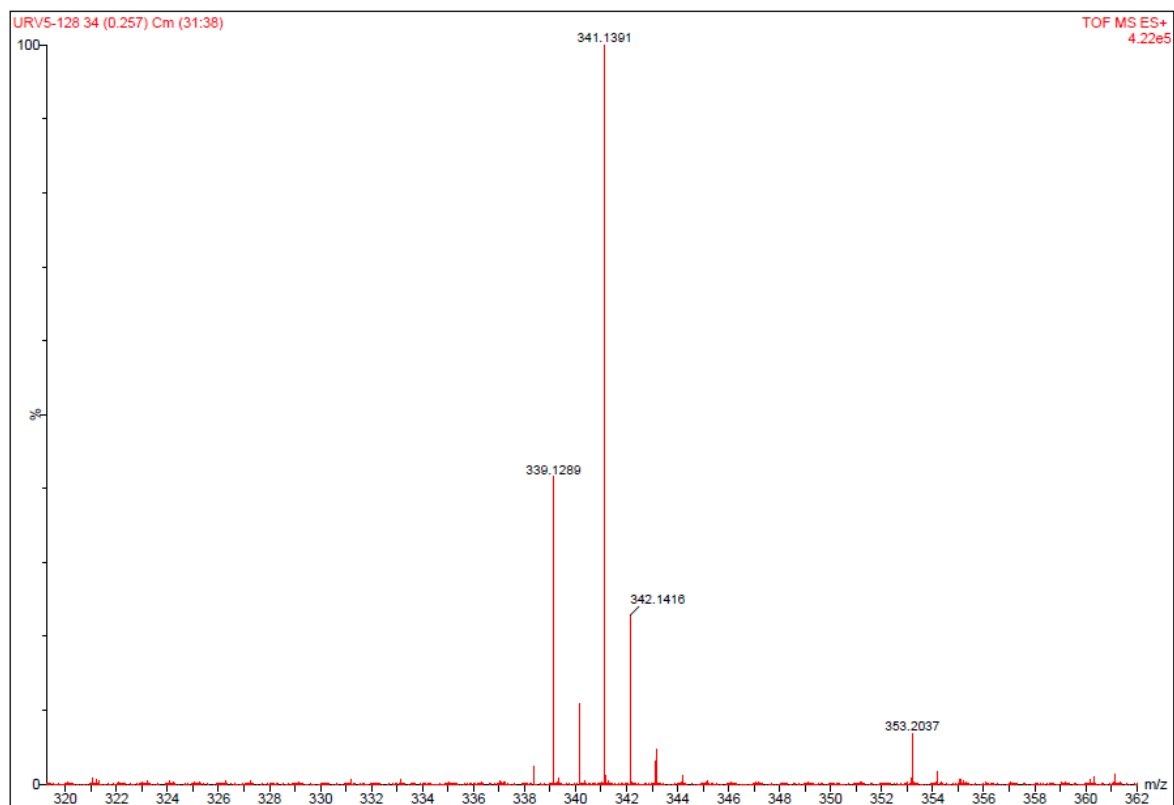


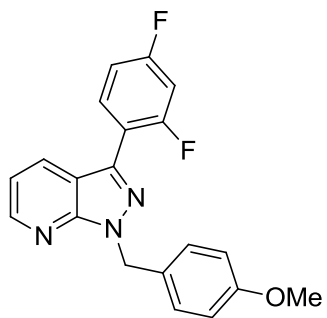
D:
13 C URV5-128



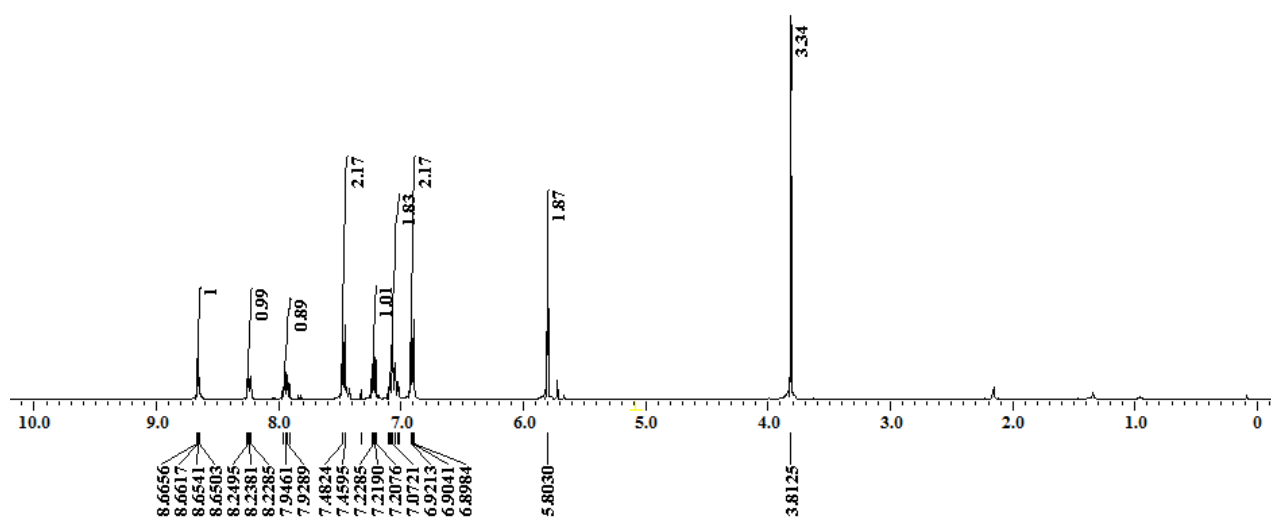
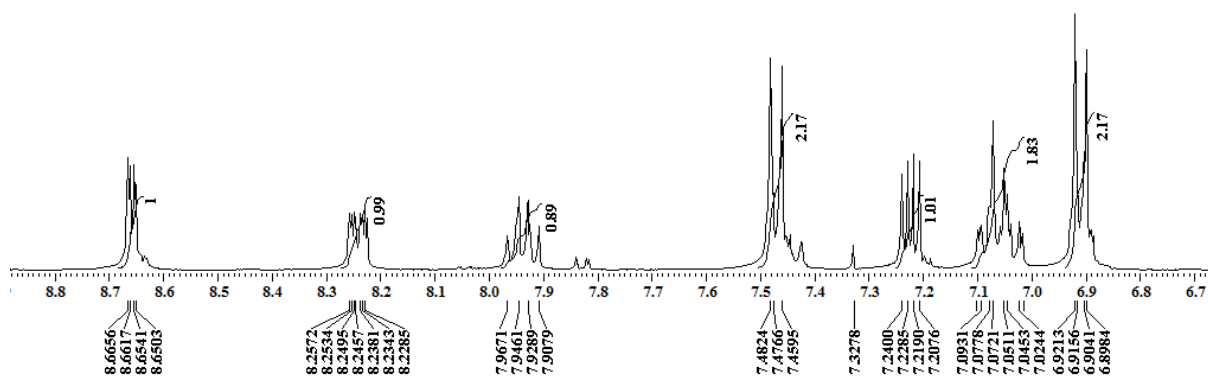


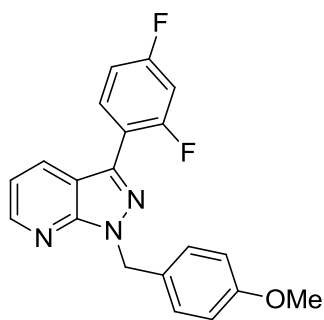
4-(1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl)benzonitrile (**3p**)



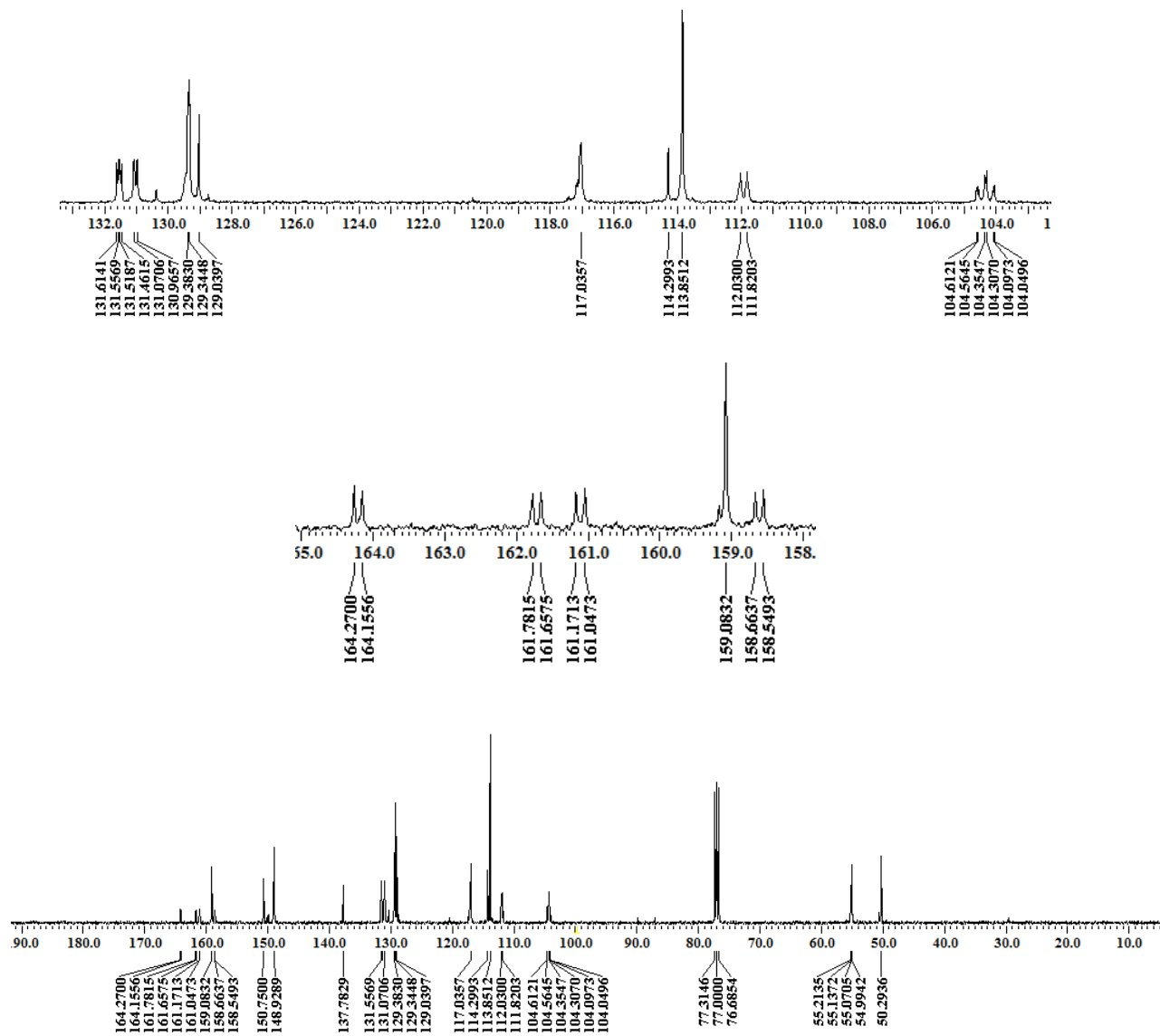


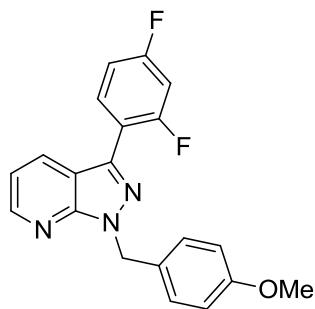
3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3q**)





3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3q**)





3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3q**)

Qualitative Compound Report

Data File	URV-57.d	Sample Name	URV-57
Sample Type	Sample	Position	P1-A3
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	28-03-2017 12:25:33
IRM Calibration Status	Success	DA Method	Default.m
Comment			

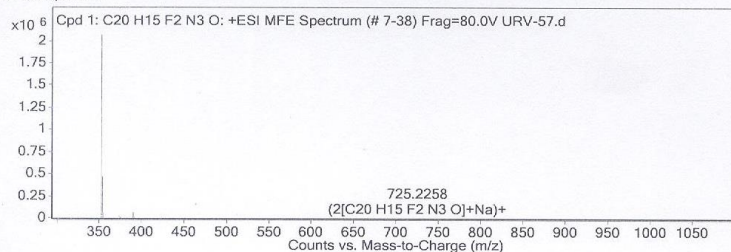
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

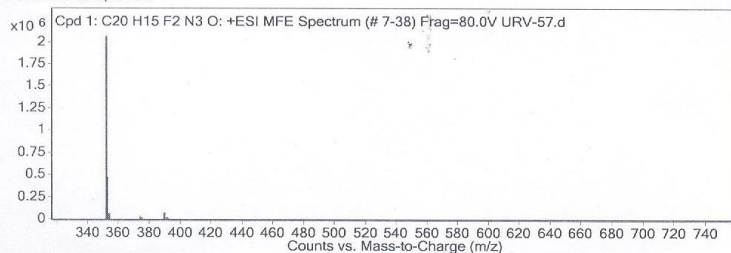
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C20 H15 F2 N3 O	11	351.1187	C20 H15 F2 N3 O	C20 H15 F2 N3 O	-1.01	C20 H15 F2 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C20 H15 F2 N3 O	352.1265	11	Find by Molecular Feature	351.1187

MFE MS Spectrum



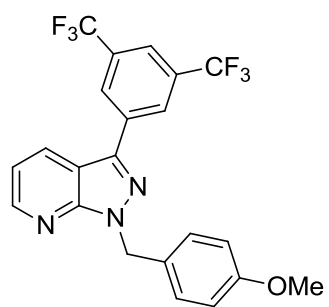
MFE MS Zoomed Spectrum



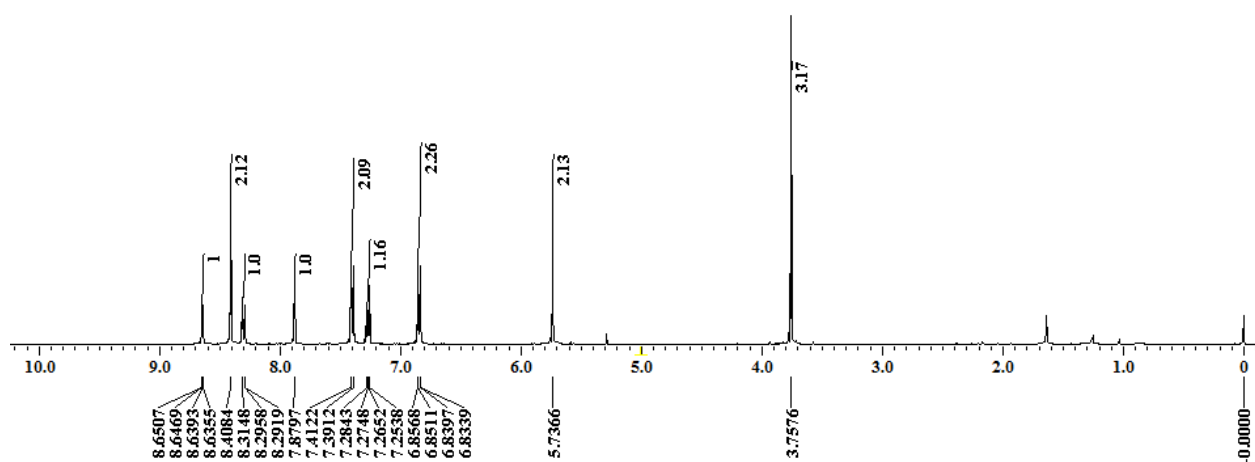
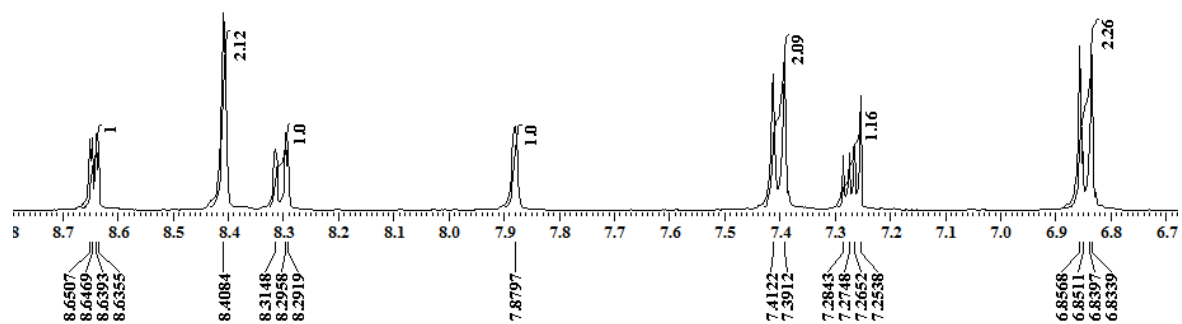
MS Spectrum Peak List

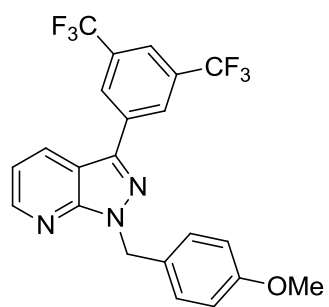
m/z	z	Abund	Formula	Ion
352.1265	1	2070263.5	C20 H15 F2 N3 O	(M+H)+
353.1295	1	468027.3	C20 H15 F2 N3 O	(M+H)+
354.1322	1	52484.76	C20 H15 F2 N3 O	(M+H)+
355.1353	1	4457.63	C20 H15 F2 N3 O	(M+H)+
374.108	1	26806.63	C20 H15 F2 N3 O	(M+Na)+
375.1109	1	6365.49	C20 H15 F2 N3 O	(M+Na)+
390.0823	1	65581.3	C20 H15 F2 N3 O	(M+K)+
391.0856	1	15535.42	C20 H15 F2 N3 O	(M+K)+
392.0841	1	5974.42	C20 H15 F2 N3 O	(M+K)+
725.2258	1	2441.97	C20 H15 F2 N3 O	(2M+Na)+

--- End Of Report ---

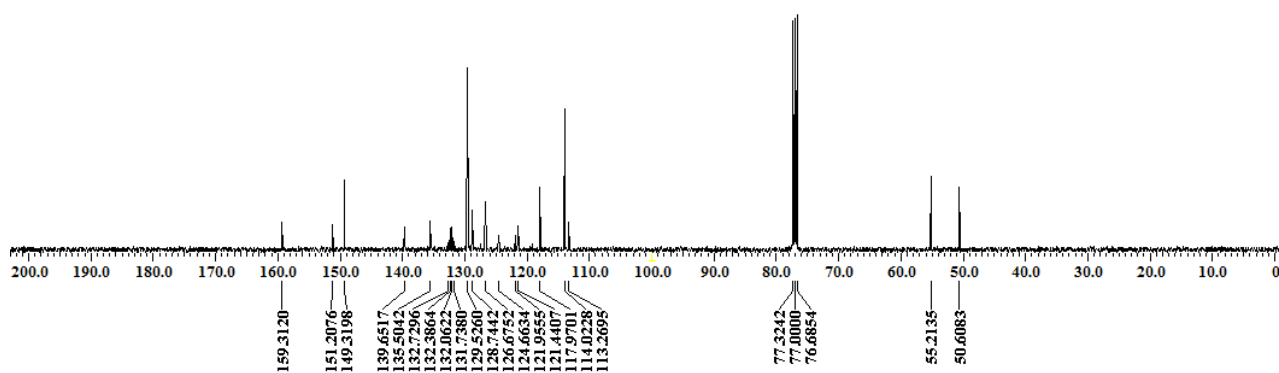
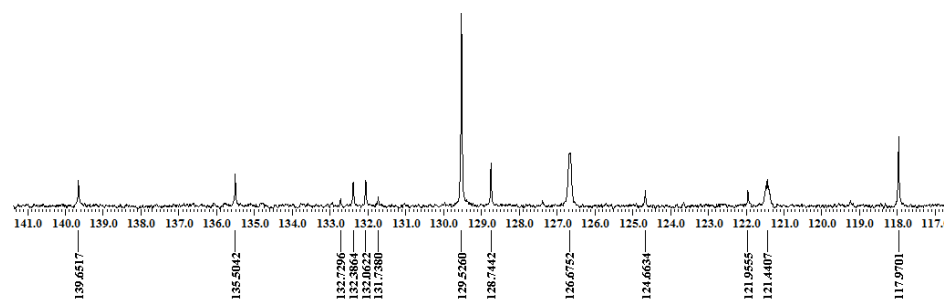


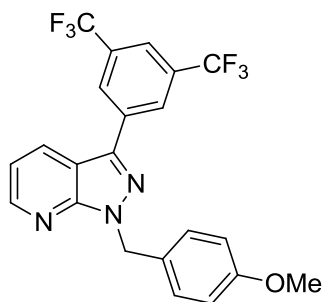
3-(3,5-bis(trifluoromethyl)phenyl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3r**)





3-(3,5-bis(trifluoromethyl)phenyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3r**)





3-(3,5-bis(trifluoromethyl)phenyl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3r**)

Qualitative Compound Report

Data File	URV5-53FI.d	Sample Name	URV5-53FI
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	24-04-2017 13:07:06
IRM Calibration Status	Success	DA Method	Default.m
Comment			

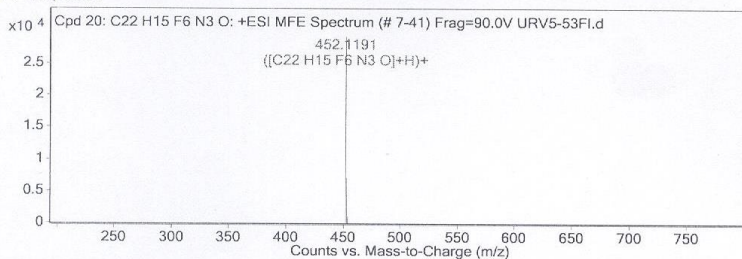
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

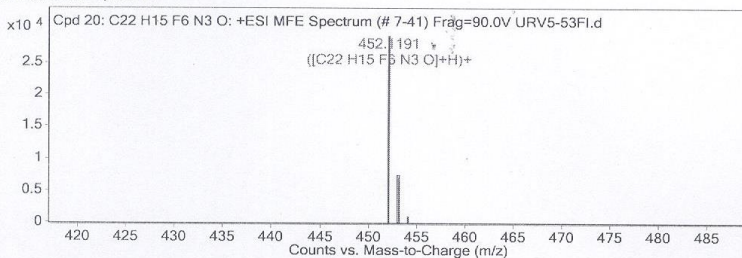
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 20: C22 H15 F6 N3 O	12	451.1122	C22 H15 F6 N3 O	C22 H15 F6 N3 O	-0.56	C22 H15 F6 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 20: C22 H15 F6 N3 O	452.1191	12	Find by Molecular Feature	451.1122

MFE MS Spectrum



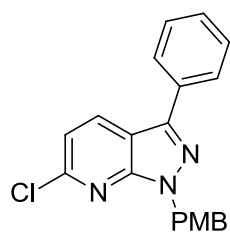
MFE MS Zoomed Spectrum



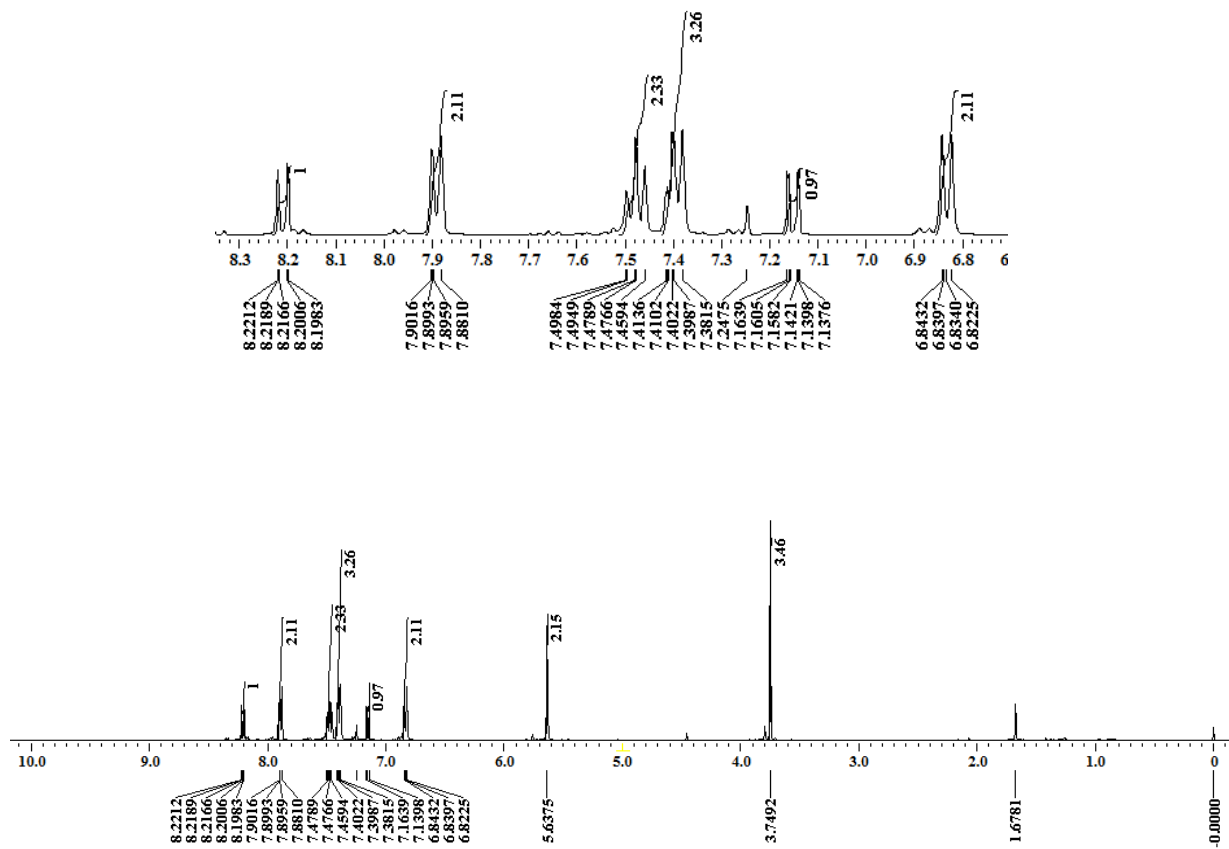
MS Spectrum Peak List

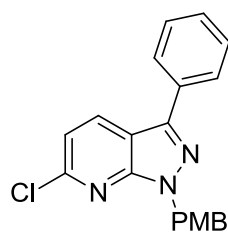
m/z	z	Abund	Formula	Ion
452.1191	1	29204.81	C22 H15 F6 N3 O	(M+H)+
453.1236	1	7108.65	C22 H15 F6 N3 O	(M+H)+
454.1289	1	1073.09	C22 H15 F6 N3 O	(M+H)+

--- End Of Report ---

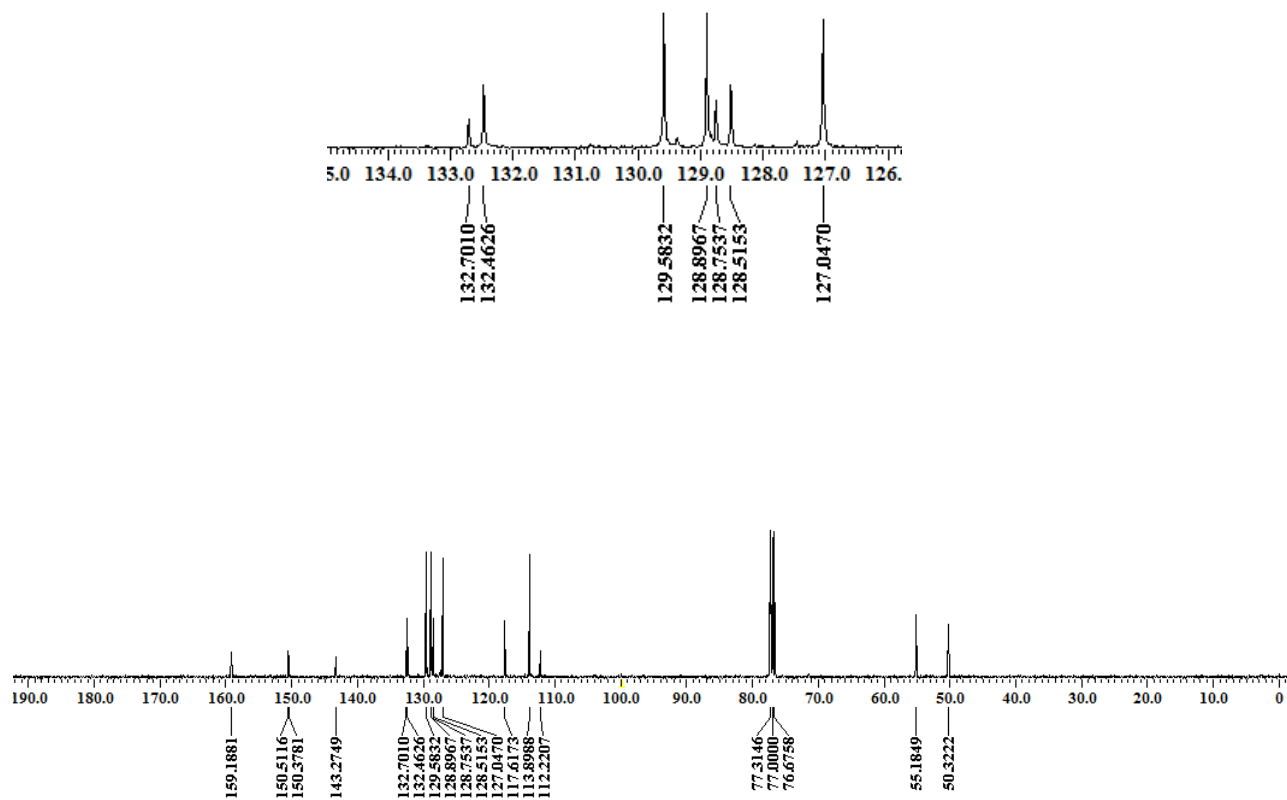


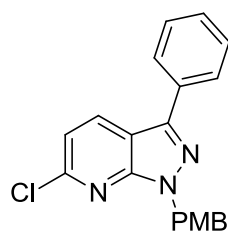
6-chloro-1-(4-methoxybenzyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**3s**)



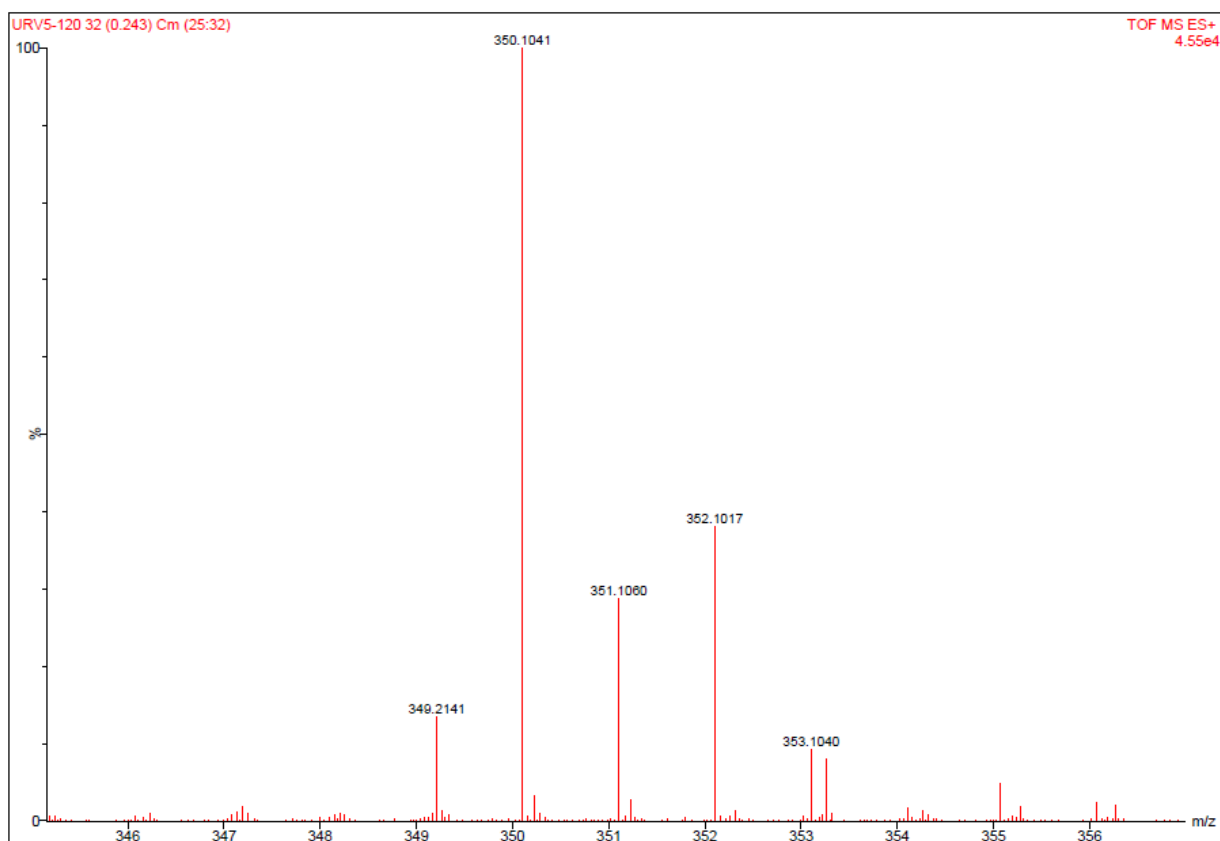


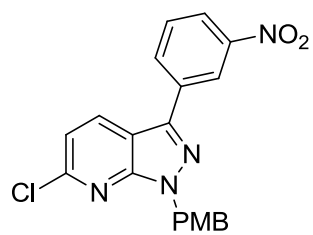
6-chloro-1-(4-methoxybenzyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (3s)



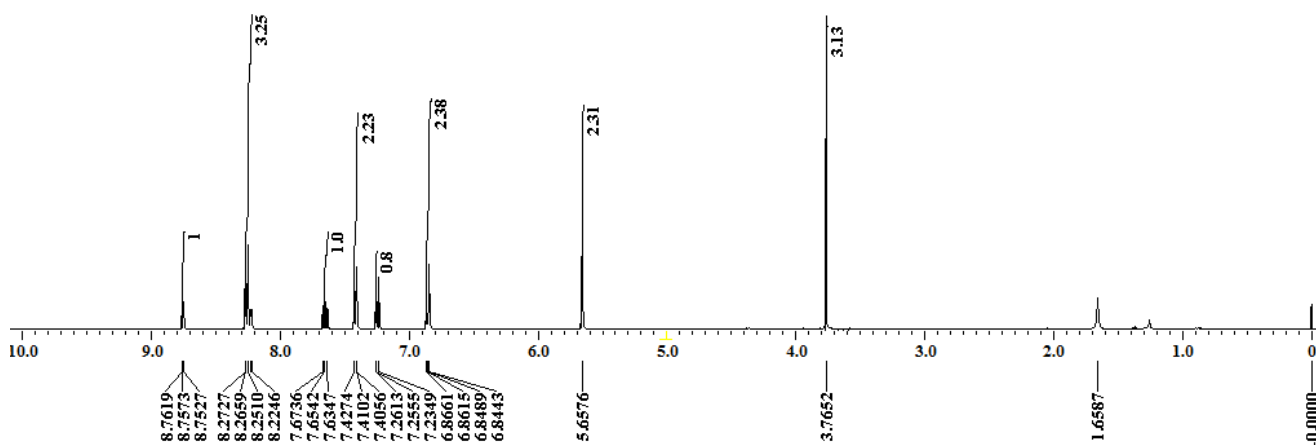
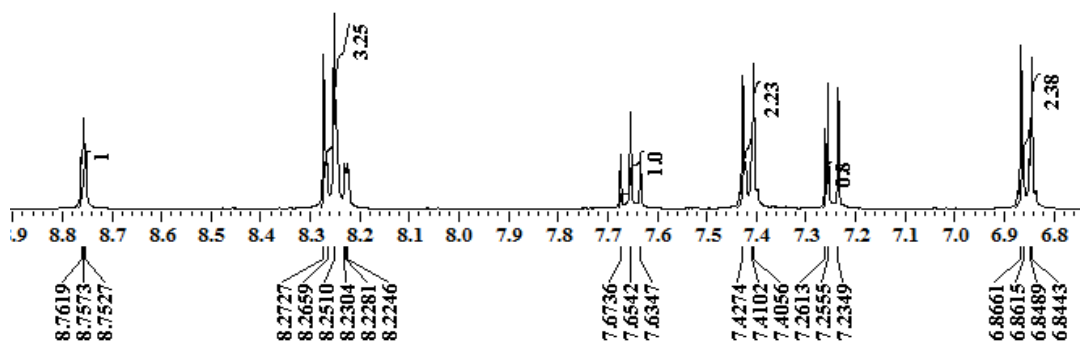


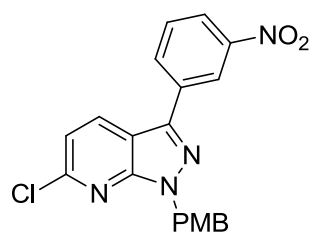
6-chloro-1-(4-methoxybenzyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**3s**)



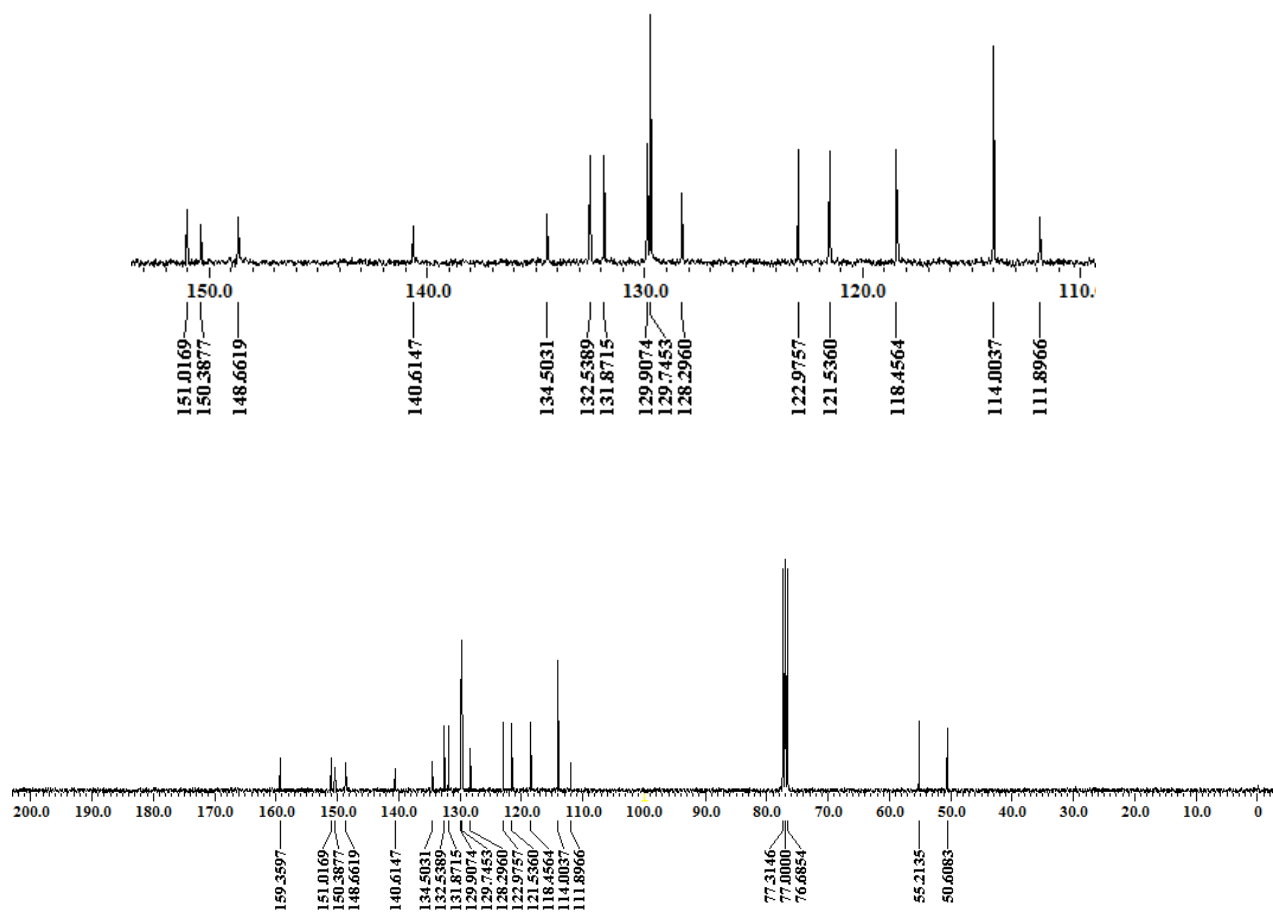


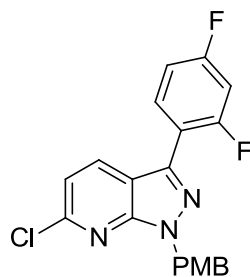
6-chloro-1-(4-methoxybenzyl)-3-(3-nitrophenyl)-1H-pyrazolo[3,4-b]pyridine (**3t**)



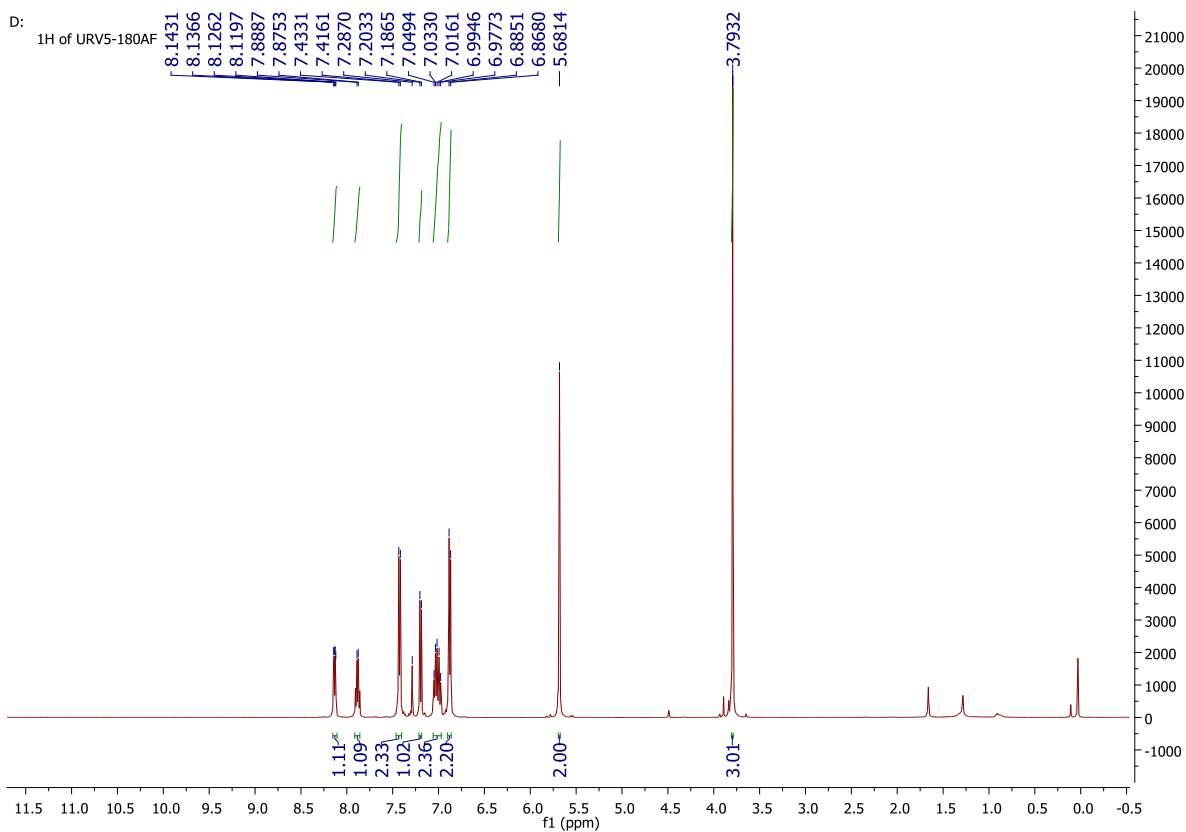
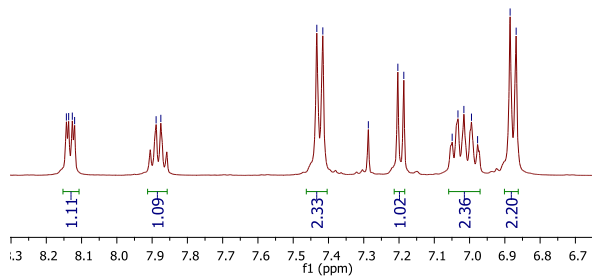


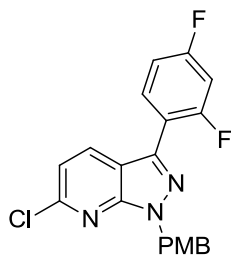
6-chloro-1-(4-methoxybenzyl)-3-(3-nitrophenyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3t**)



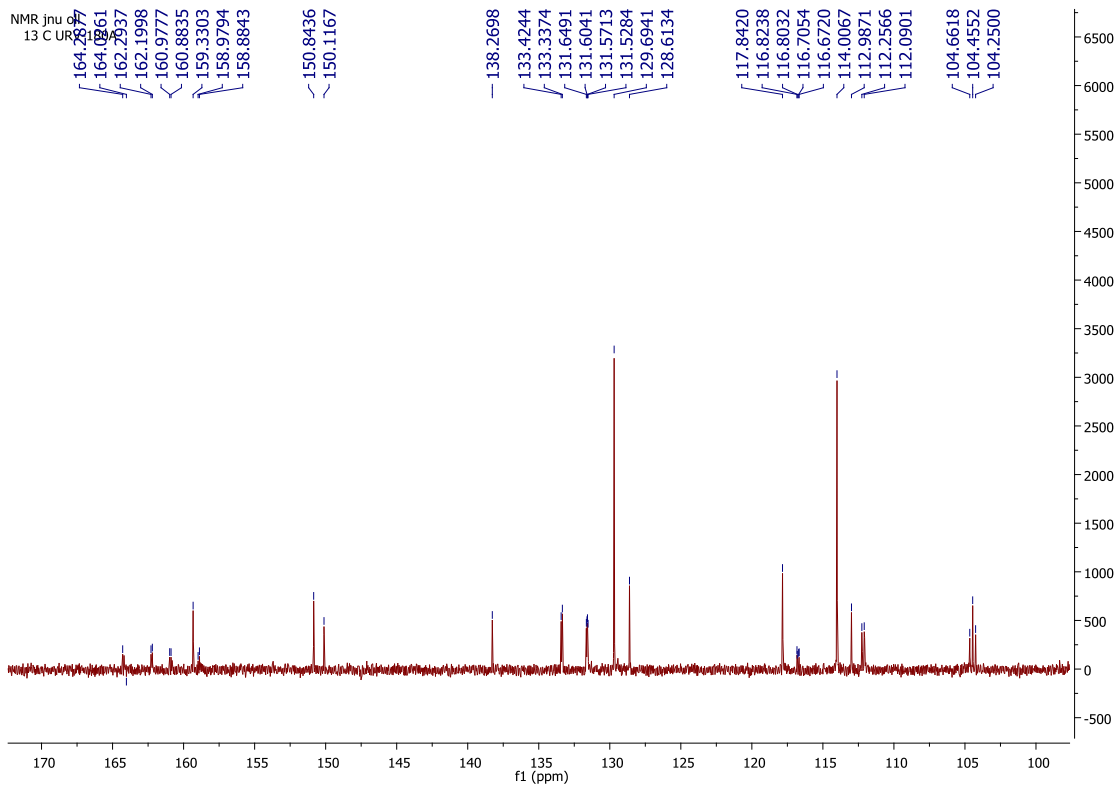
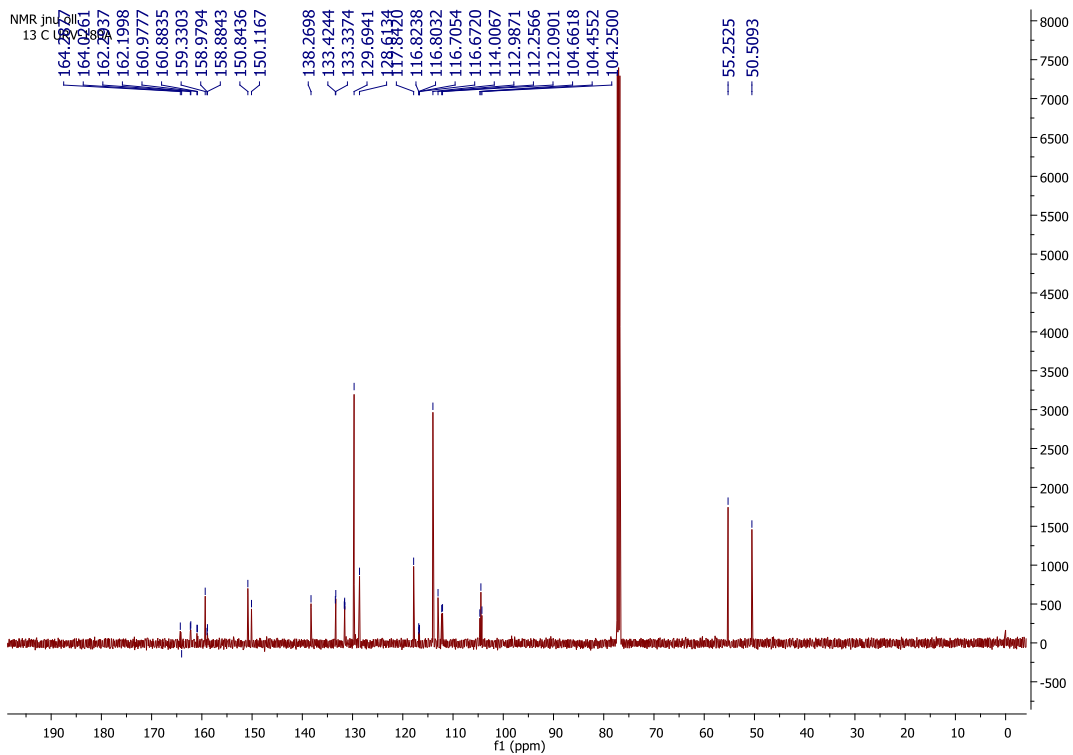


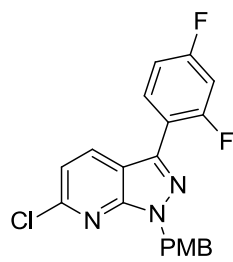
6-chloro-3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3u**)



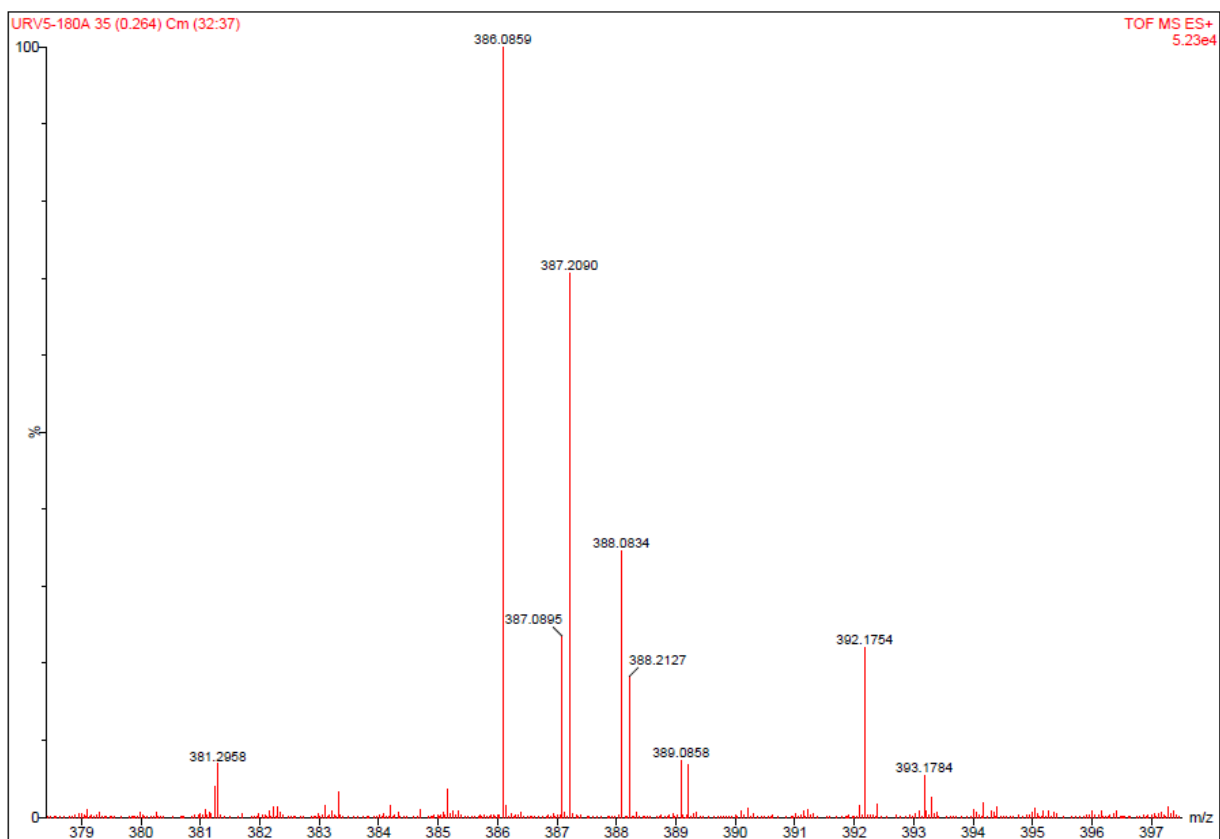


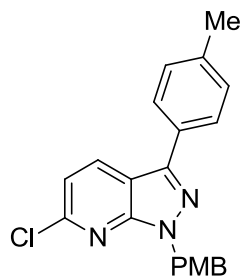
6-chloro-3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3u**)



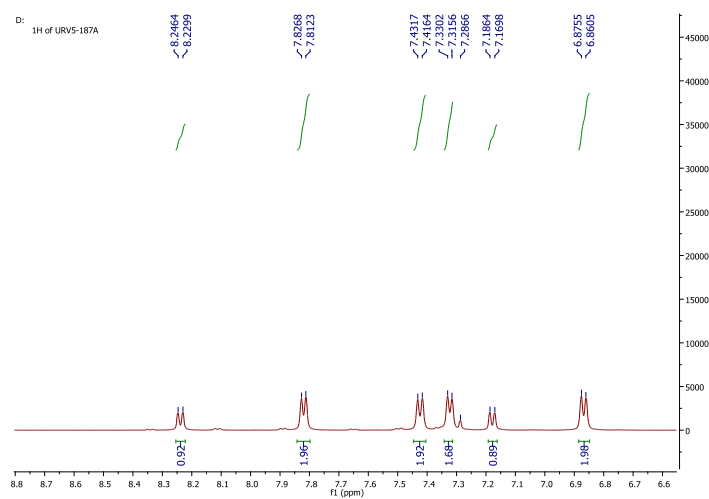
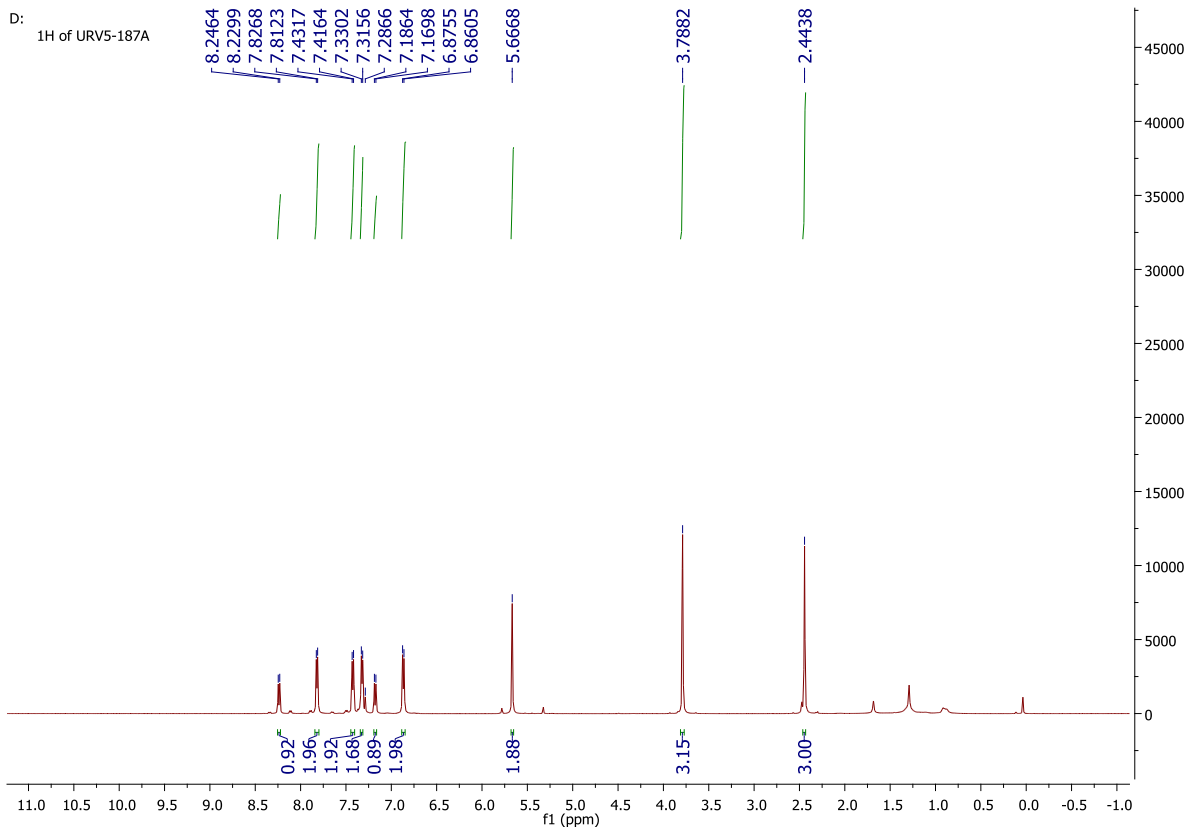


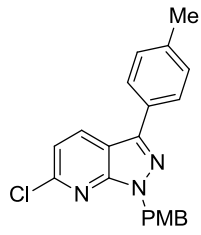
6-chloro-3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3u**)





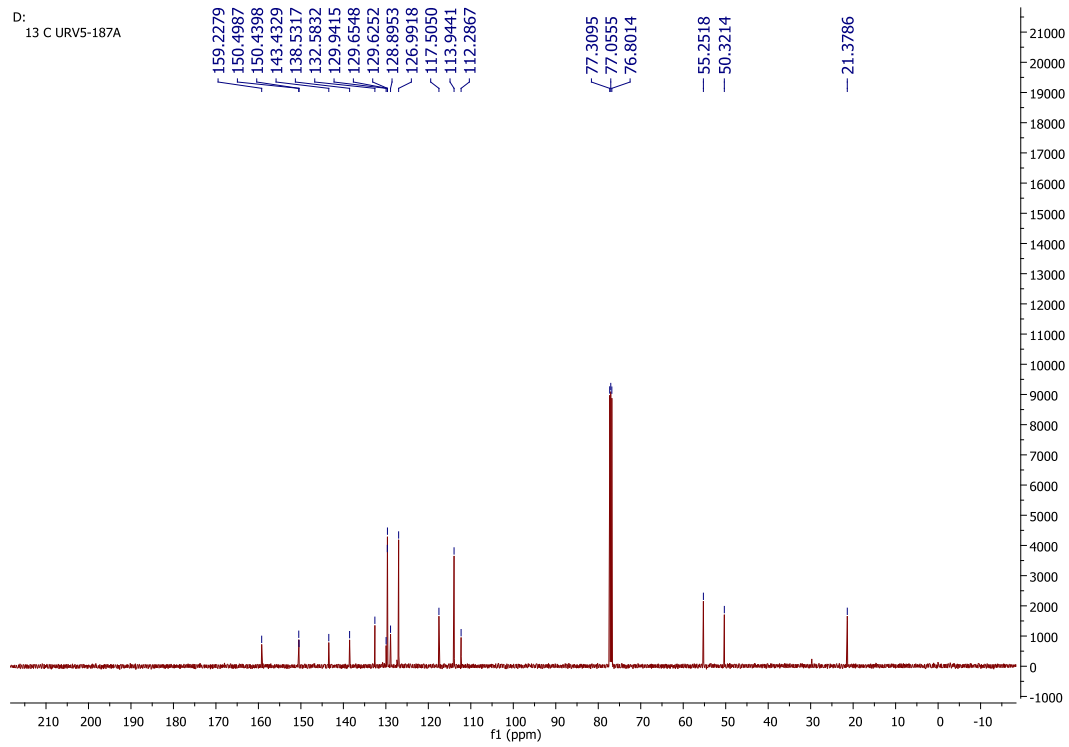
6-chloro-1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3v**)



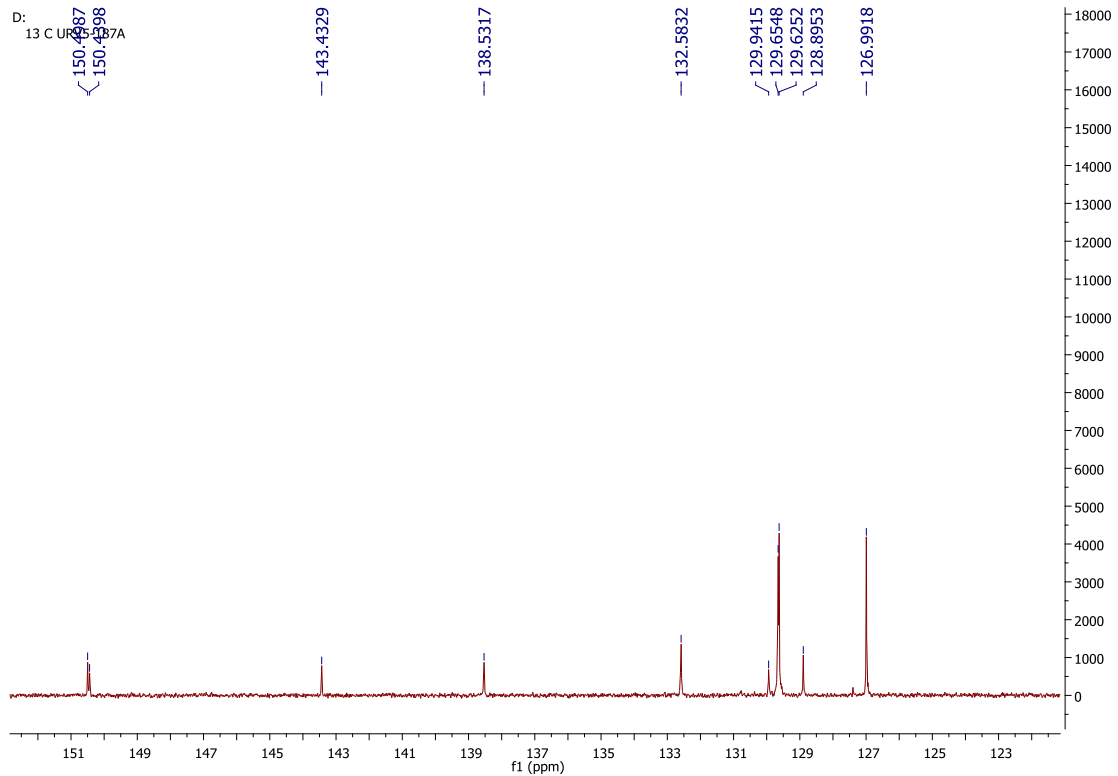


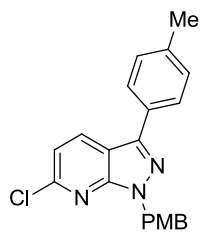
6-chloro-1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3v**)

D:
13 C URV5-187A

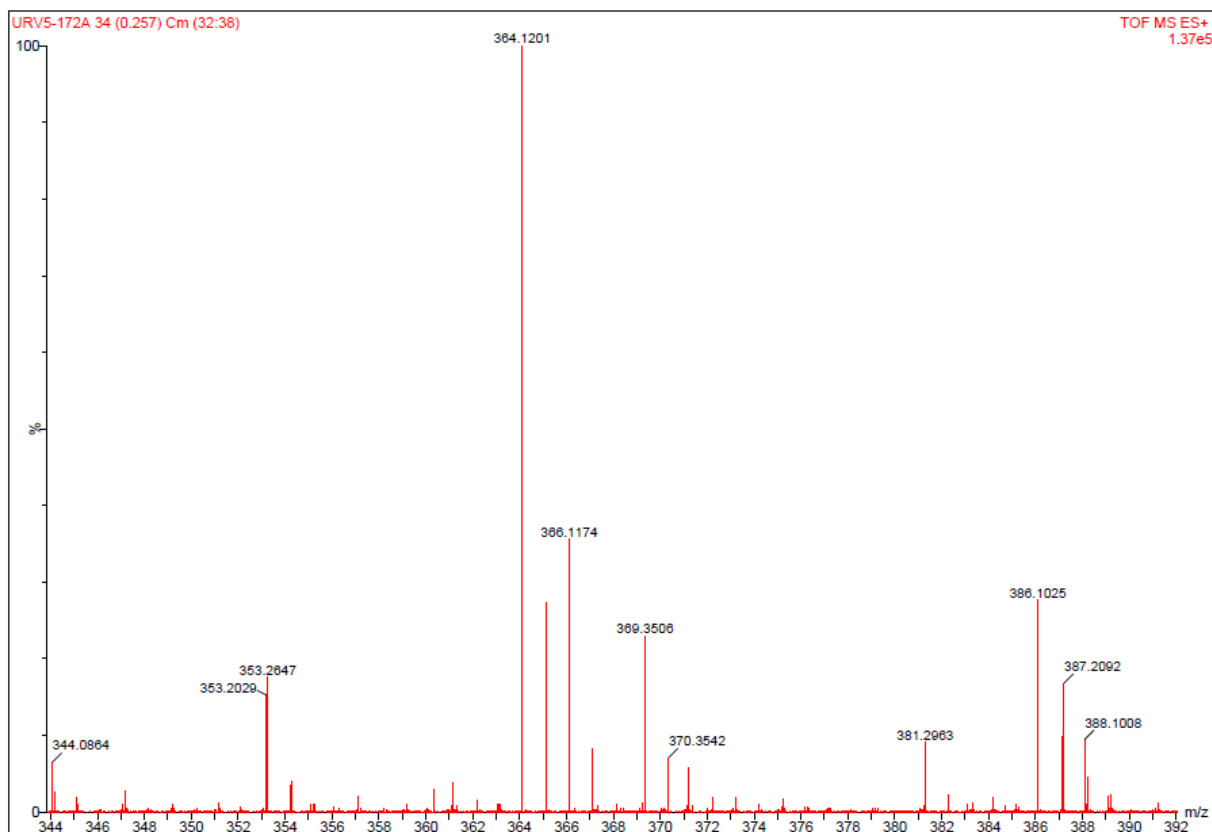


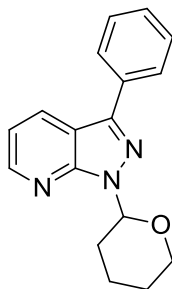
D:
13 C URV5-187A



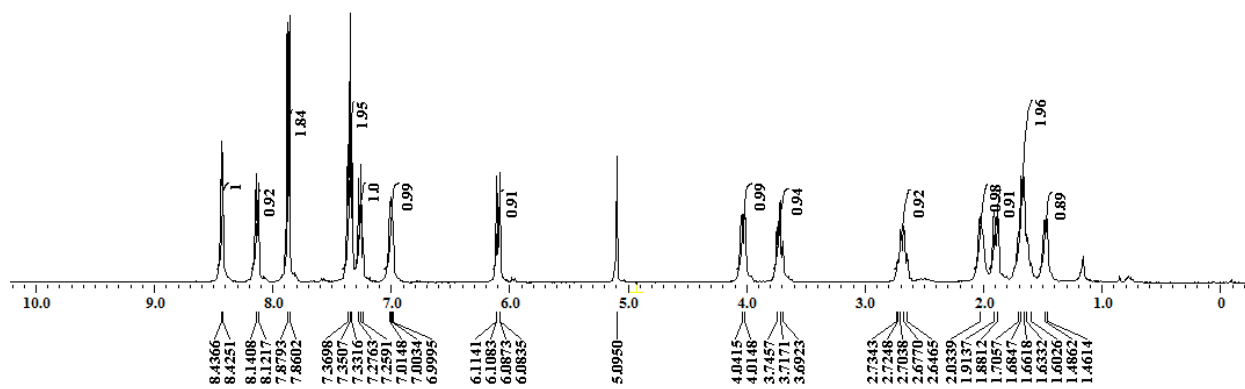
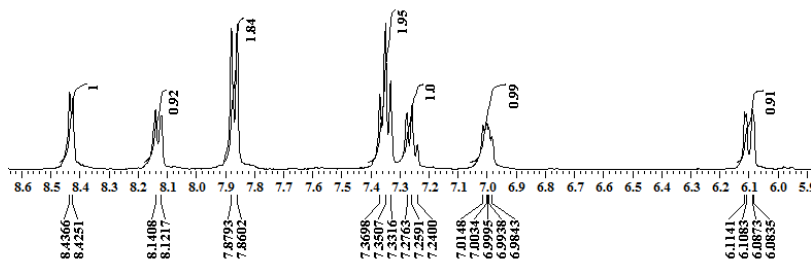


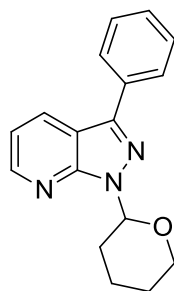
6-chloro-1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3v**)



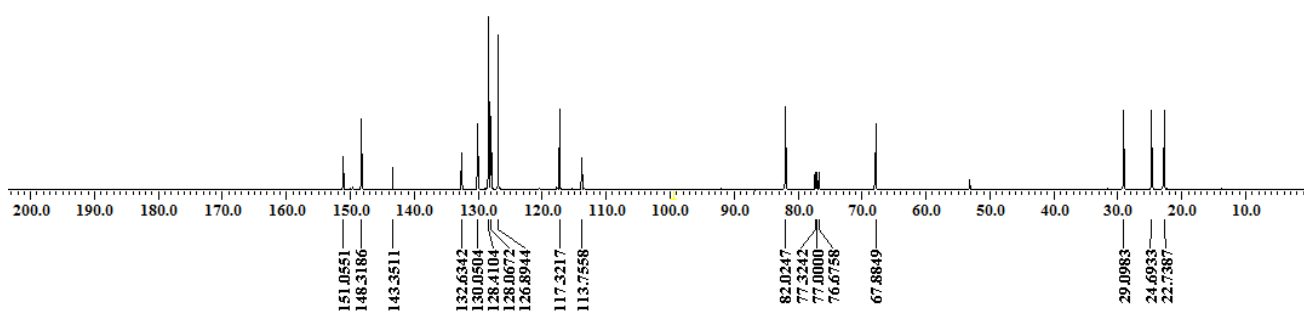
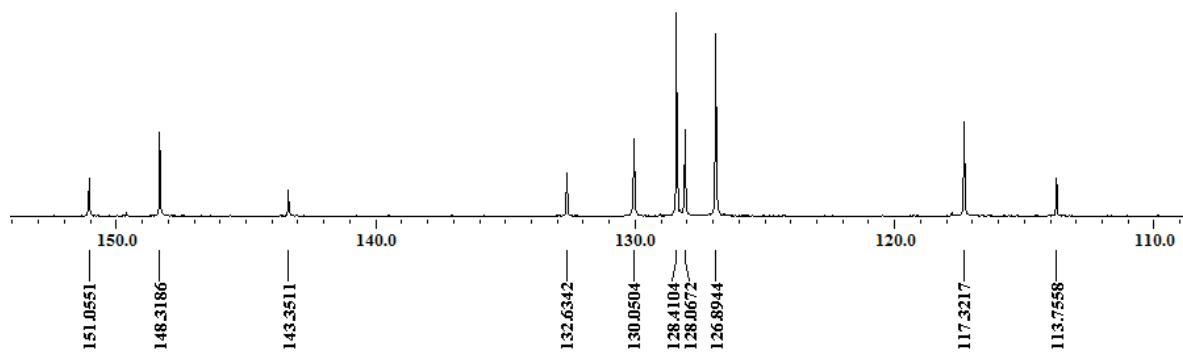


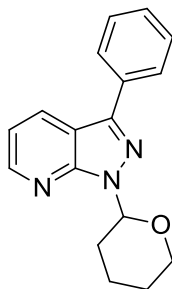
3-phenyl-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3w**)





3-phenyl-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3w**)





3-phenyl-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3w**)

Qualitative Compound Report

Data File: URV5-61F.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: 29.10.2014.m
 IRM Calibration Status: Success
 Comment:

Sample Name: URV5-61F
 Position: P1-F5
 User Name:
 Acquired Time: 02-05-2017 14:42:08
 DA Method: Default.m

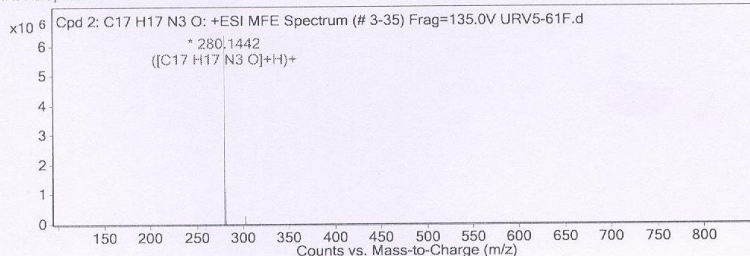
Sample Group: Info.
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF B.05.01 (B5125)

Compound Table

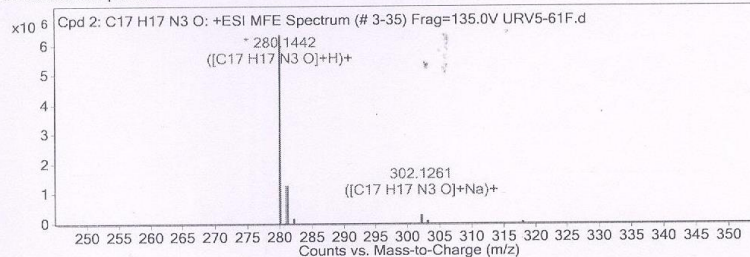
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H17 N3 O	11	279.1369	C17 H17 N3 O	C17 H17 N3 O	0.9	C17 H17 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C17 H17 N3 O	280.1442	11	Find by Molecular Feature	279.1369

MFE MS Spectrum



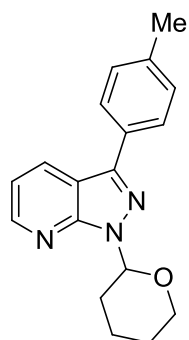
MFE MS Zoomed Spectrum



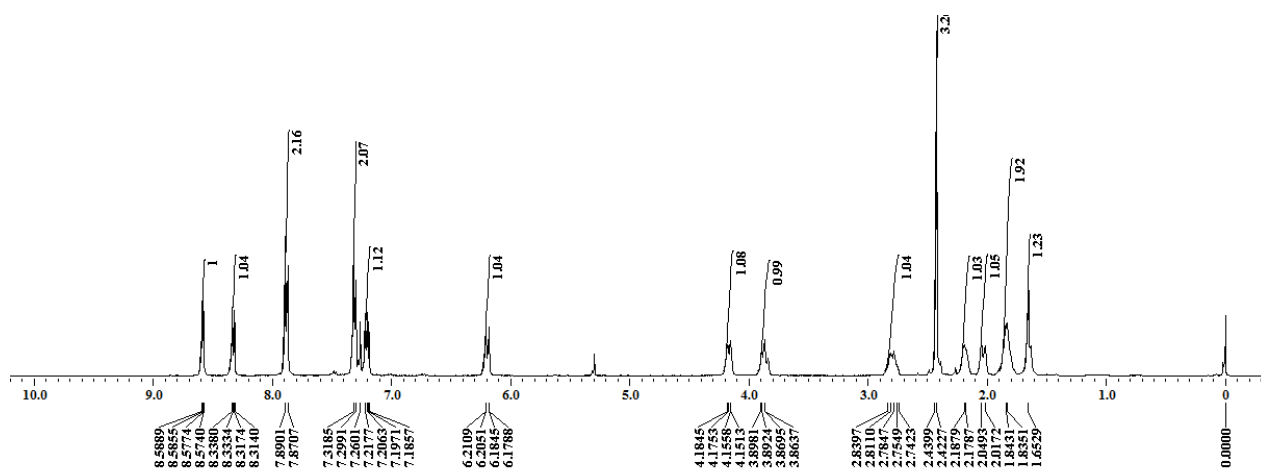
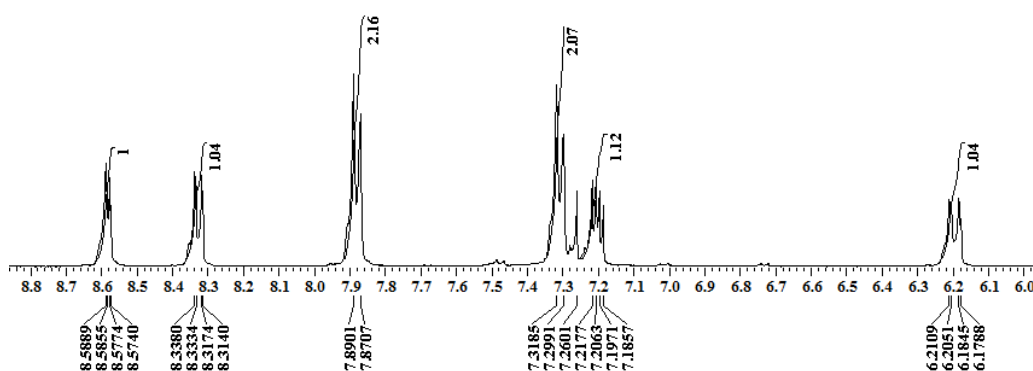
MS Spectrum Peak List

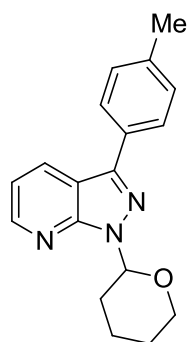
m/z	z	Abund	Formula	Ion
280.1442	1	6344692.5	C17 H17 N3 O	(M+H)+
281.1476	1	1251173.85	C17 H17 N3 O	(M+H)+
282.1502	1	126032.01	C17 H17 N3 O	(M+H)+
283.1536	1	8815.85	C17 H17 N3 O	(M+H)+
302.1261	1	269895.91	C17 H17 N3 O	(M+Na)+
303.1293	1	52023.5	C17 H17 N3 O	(M+Na)+
304.1318	1	5678.95	C17 H17 N3 O	(M+Na)+
318.1001	1	37866.95	C17 H17 N3 O	(M+K)+
319.1042	1	7731.97	C17 H17 N3 O	(M+K)+
320.1009	1	3597.92	C17 H17 N3 O	(M+K)+

--- End Of Report ---

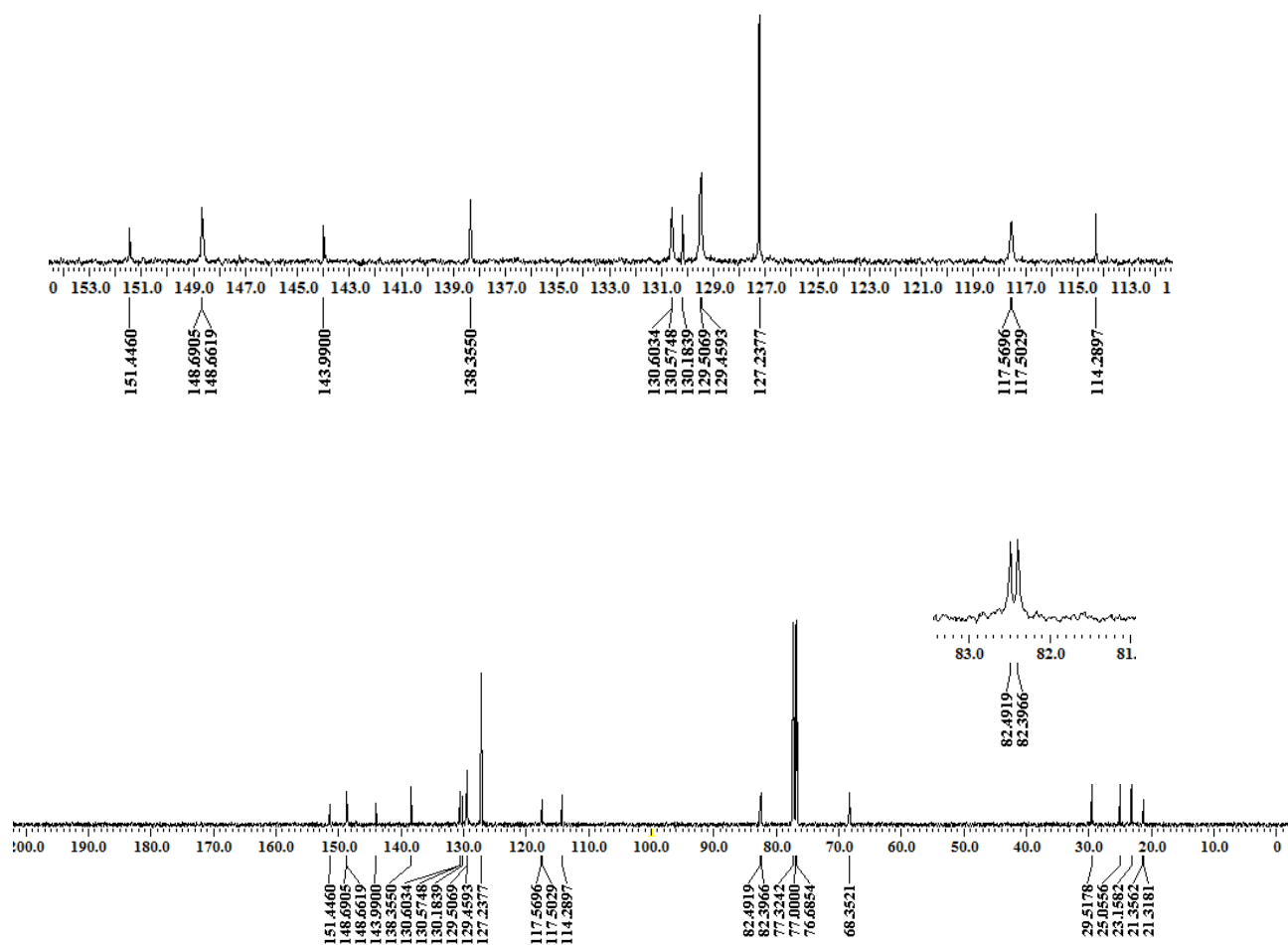


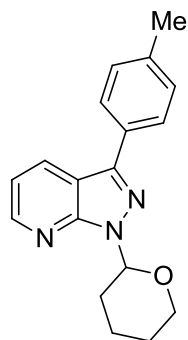
1-(tetrahydro-2H-pyran-2-yl)-3-(*p*-tolyl)-1H-pyrazolo[3,4-*b*]pyridine (**3x**)





1-(tetrahydro-2H-pyran-2-yl)-3-(*p*-tolyl)-1H-pyrazolo[3,4-*b*]pyridine (**3x**)





1-(tetrahydro-2H-pyran-2-yl)-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridine (3x)

Qualitative Compound Report

Data File	URV5-80F.d	Sample Name	URV5-80F
Sample Type	Sample	Position	P1-C4
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	03-05-2017 13:52:42
IRM Calibration Status	Success	DA Method	Default.m
Comment			

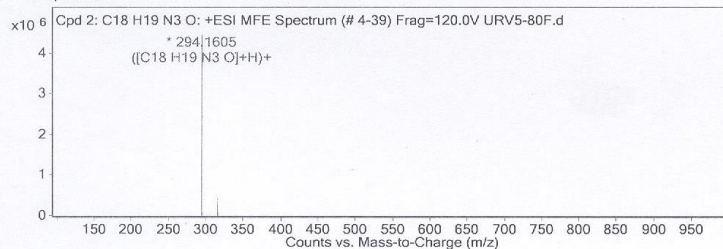
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

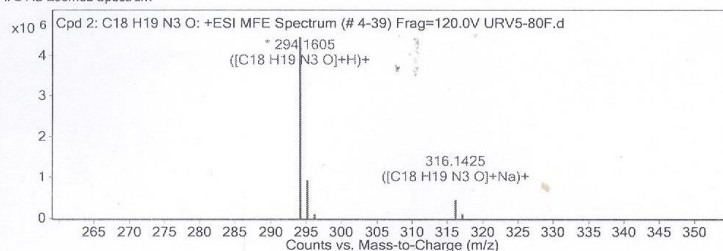
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C18 H19 N3 O	11	293.1533	C18 H19 N3 O	C18 H19 N3 O	-1.61	C18 H19 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C18 H19 N3 O	294.1605	11	Find by Molecular Feature	293.1533

MFE MS Spectrum



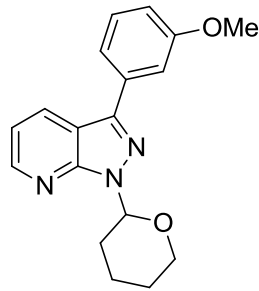
MFE MS Zoomed Spectrum



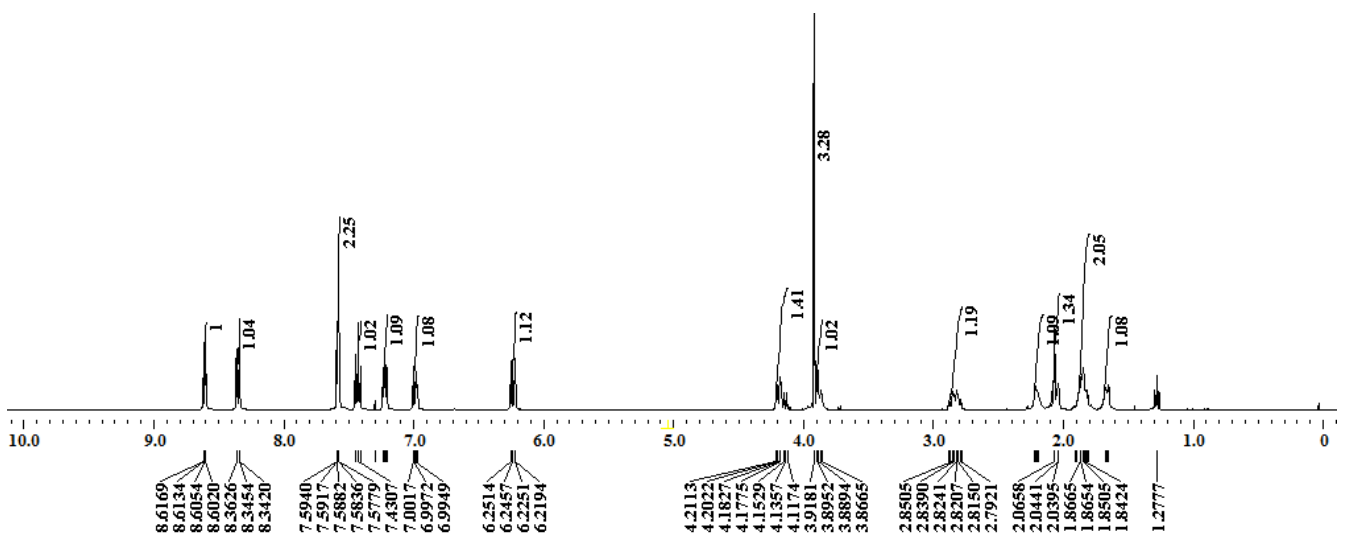
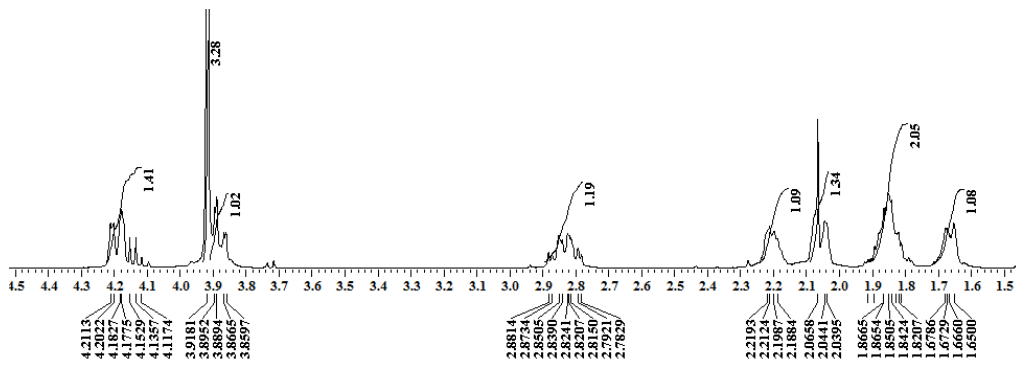
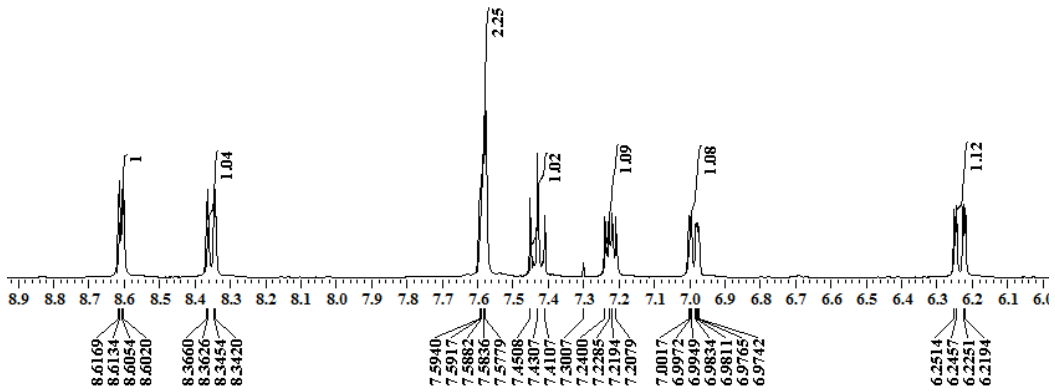
MS Spectrum Peak List

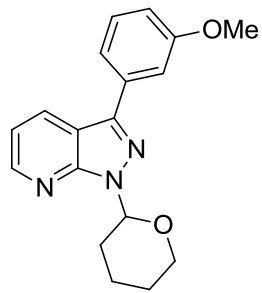
m/z	z	Abund	Formula	Ion
294.1605	1	4459341	C18 H19 N3 O	(M+H)+
295.1638	1	928137.47	C18 H19 N3 O	(M+H)+
296.1665	1	95351.72	C18 H19 N3 O	(M+H)+
297.1691	1	7475.5	C18 H19 N3 O	(M+H)+
298.1651	1	613.77	C18 H19 N3 O	(M+H)+
316.1425	1	437508.53	C18 H19 N3 O	(M+Na)+
317.1454	1	89284.05	C18 H19 N3 O	(M+Na)+
318.1481	1	9720.9	C18 H19 N3 O	(M+Na)+
319.1619	1	2338.55	C18 H19 N3 O	(M+Na)+
320.1748	1	184.26	C18 H19 N3 O	(M+Na)+

--- End Of Report ---

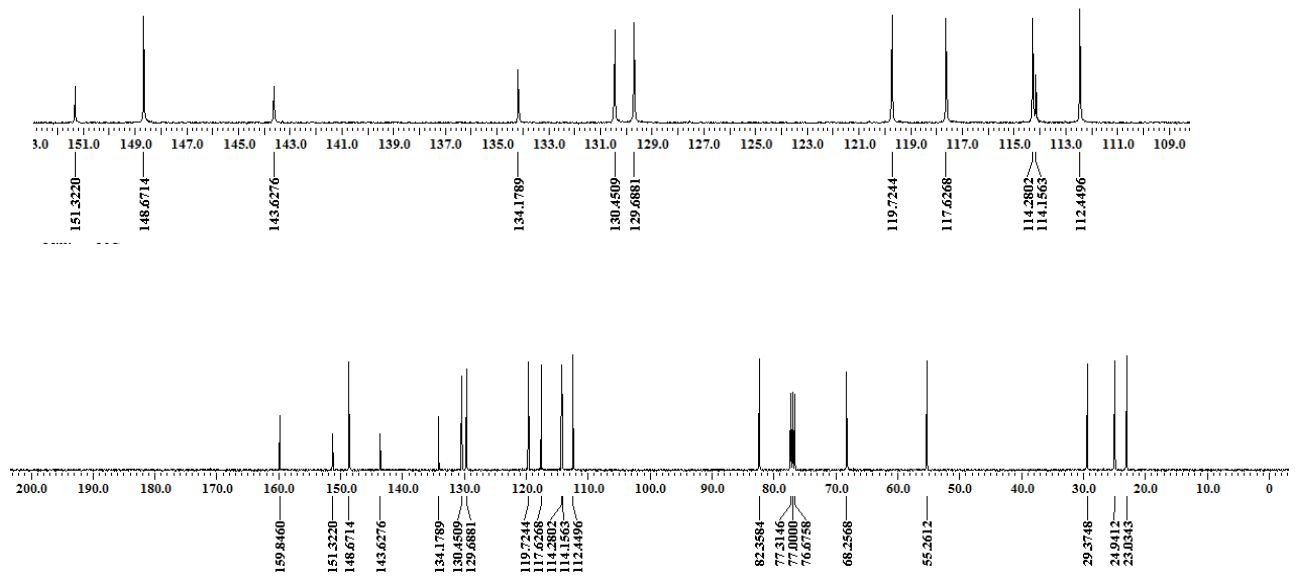


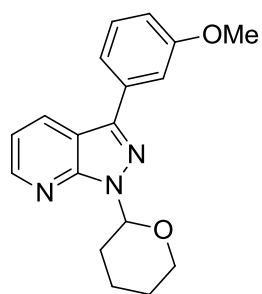
3-(3-methoxyphenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3y**)



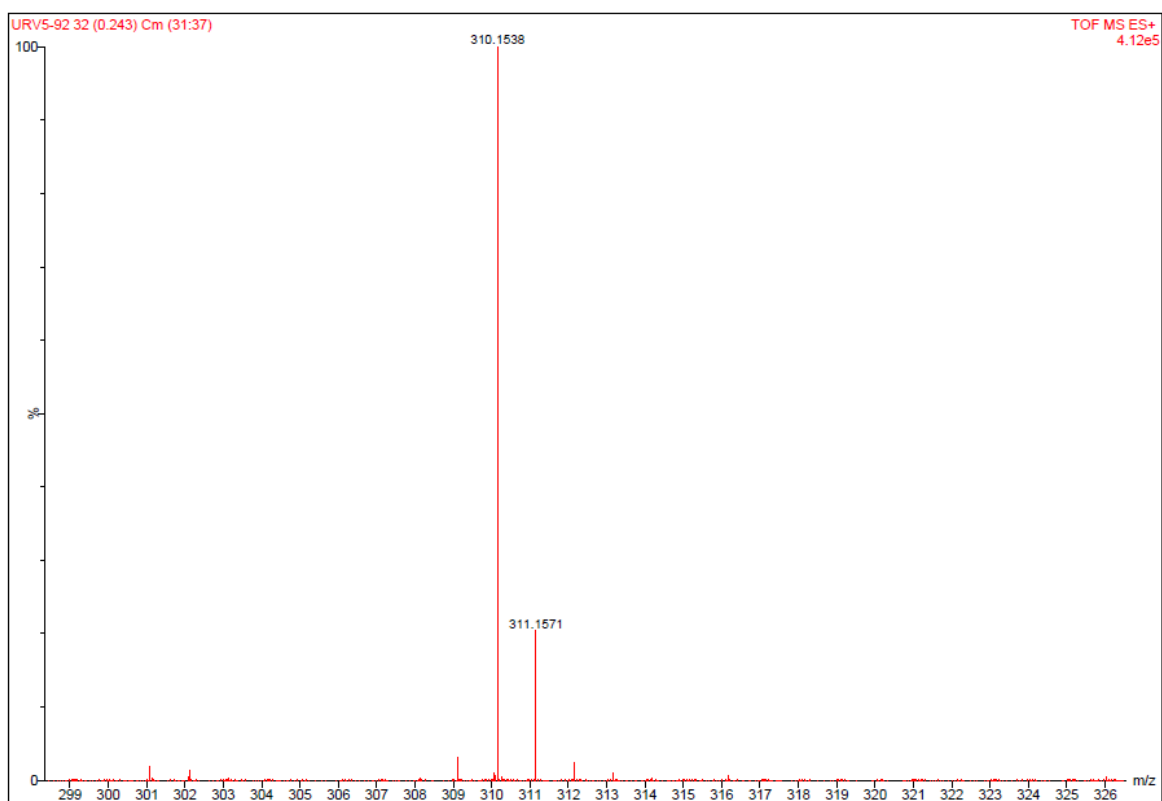


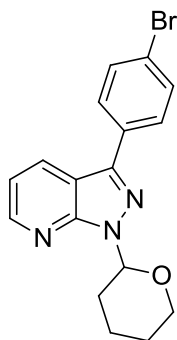
3-(3-methoxyphenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3y**)



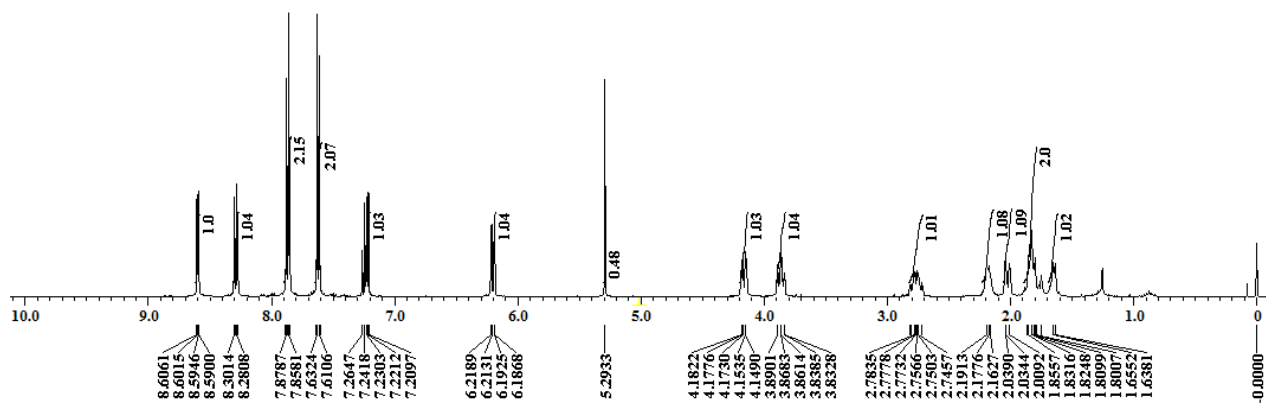
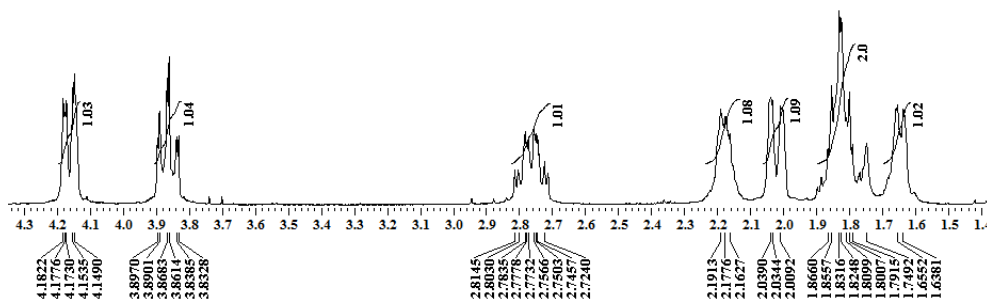
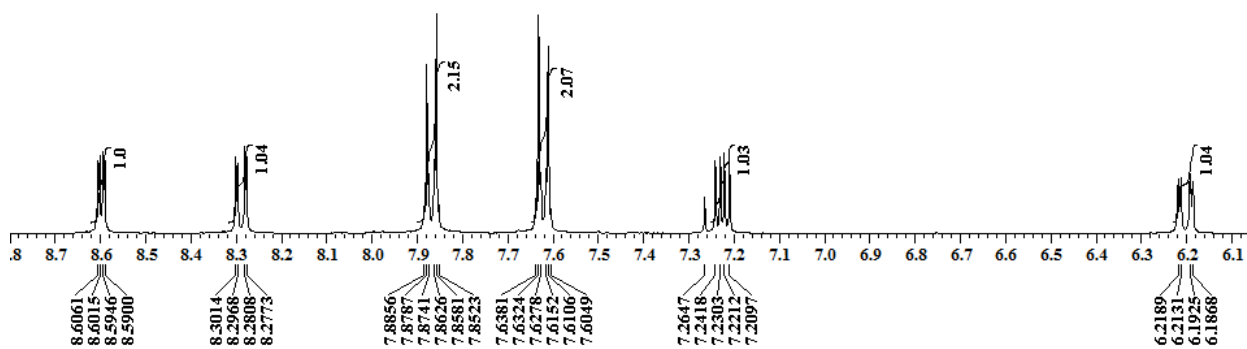


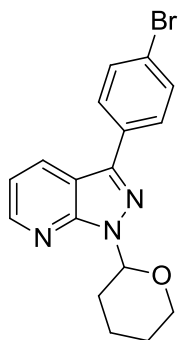
3-(3-methoxyphenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3y**)



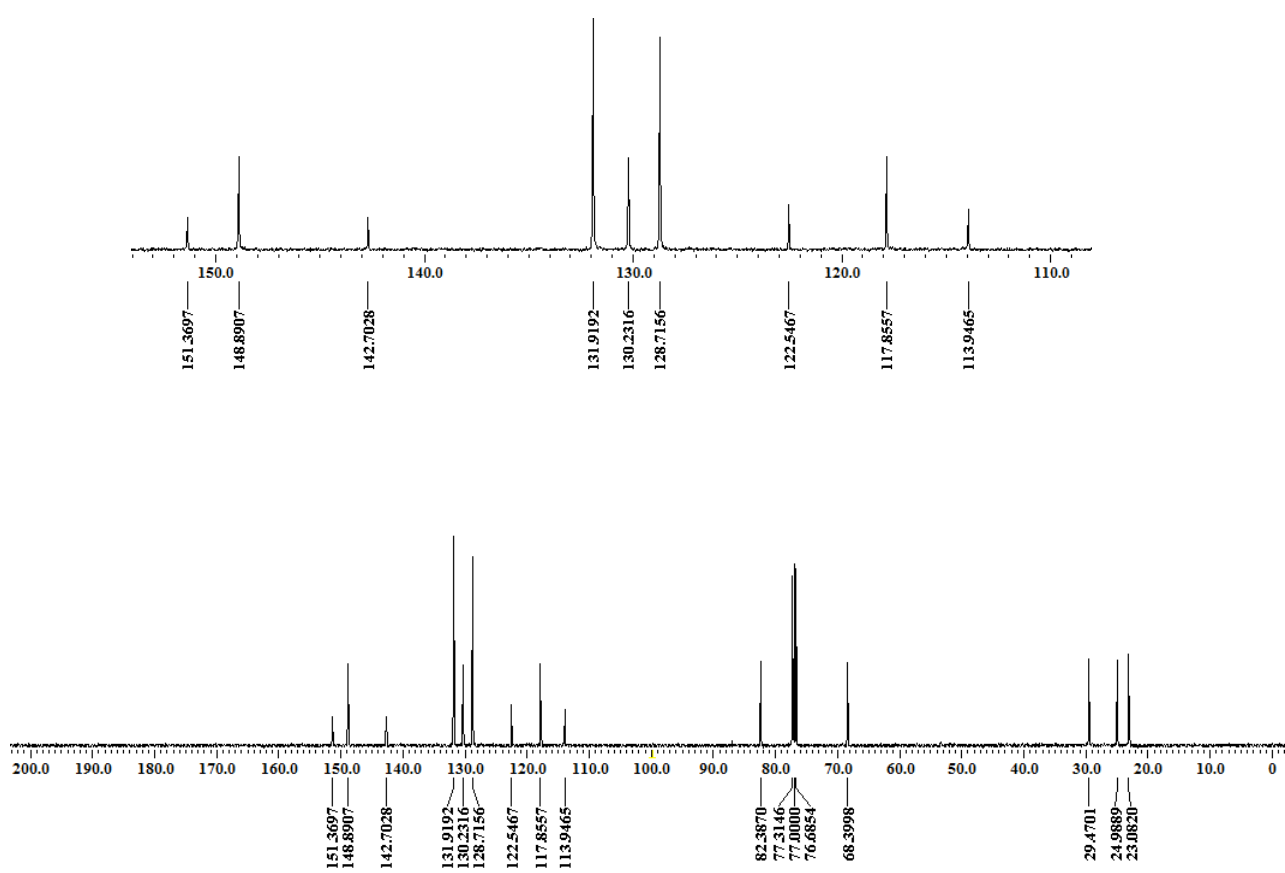


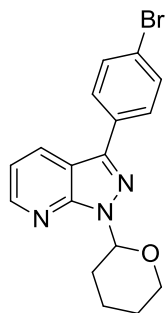
3-(4-bromophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3z**)





3-(4-bromophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3z**)





3-(4-bromophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (3z)

Qualitative Compound Report

Data File	URV5-79.d	Sample Name	URV5-79
Sample Type	Sample	Position	P1-C5
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	04-05-2017 13:36:30
IRM Calibration Status	Success	DA Method	Default.m
Comment			

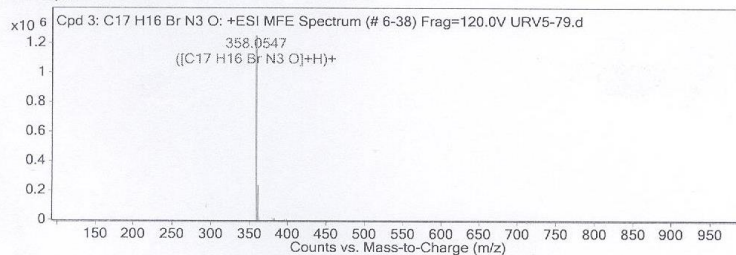
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

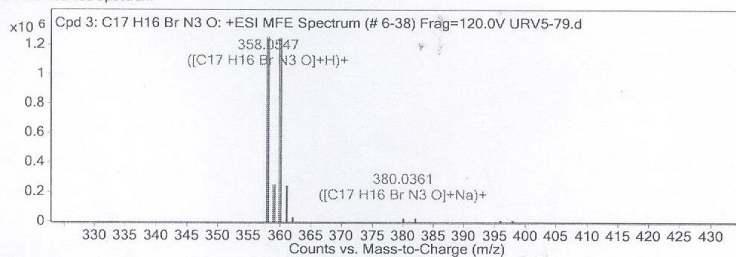
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C17 H16 Br N3 O	10	357.0474	C17 H16 Br N3 O	C17 H16 Br N3 O	0.71	C17 H16 Br N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 3: C17 H16 Br N3 O	358.0547	10	Find by Molecular Feature	357.0474

MFE MS Spectrum



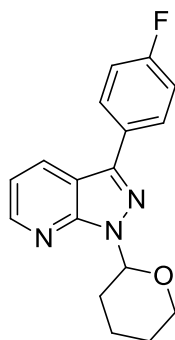
MFE MS Zoomed Spectrum



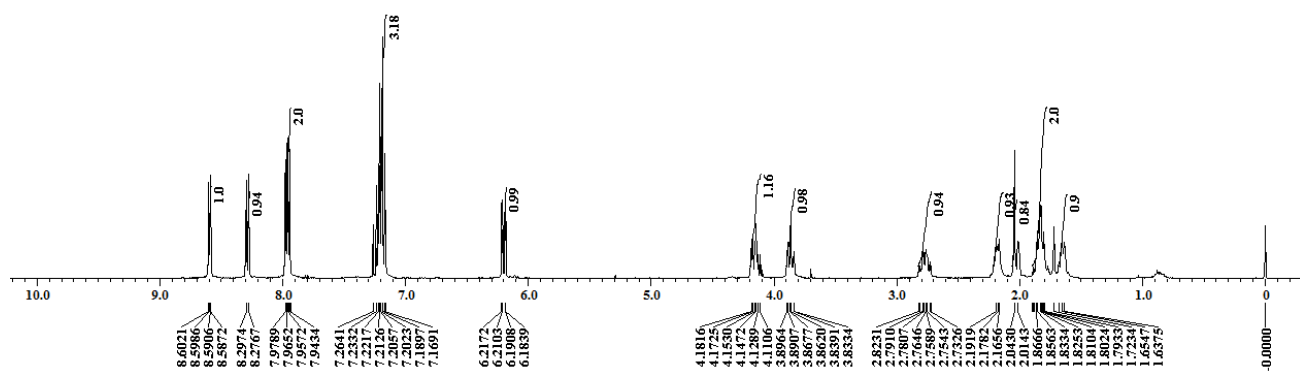
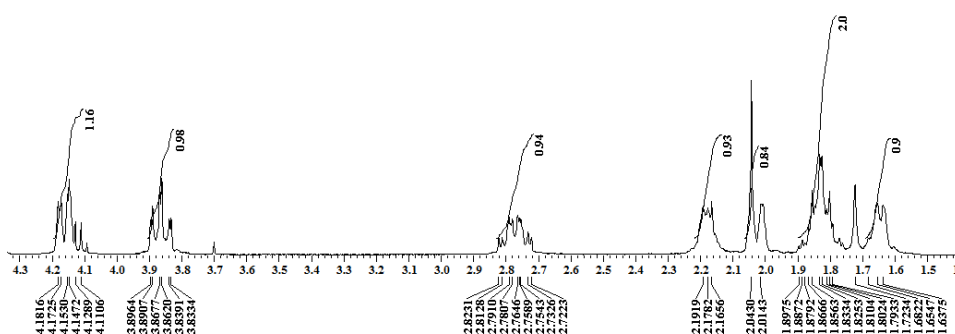
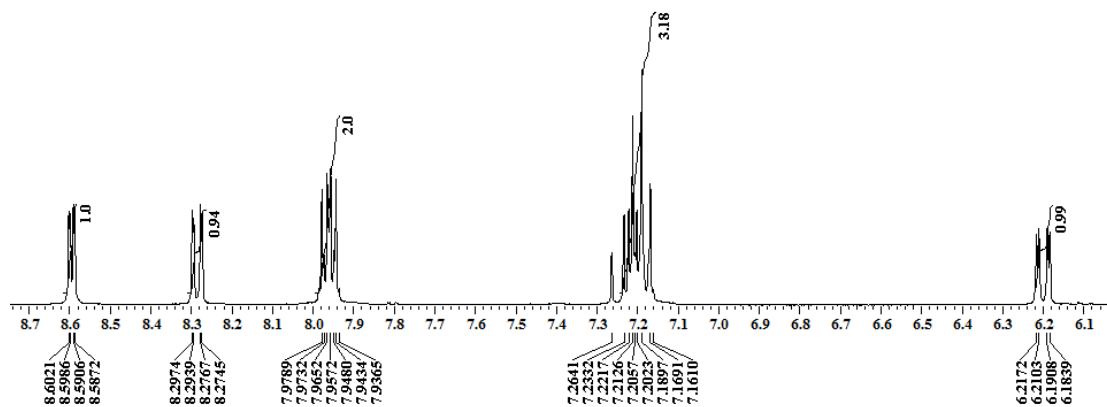
MS Spectrum Peak List

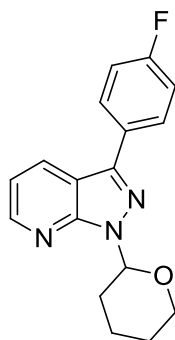
m/z	z	Abund	Formula	Ion
358.0547	1	1249394.75	C17 H16 Br N3 O	(M+H)+
359.0575	1	237703.25	C17 H16 Br N3 O	(M+H)+
360.0529	1	1249030.34	C17 H16 Br N3 O	(M+H)+
361.0555	1	238231.74	C17 H16 Br N3 O	(M+H)+
362.0582	1	24301.57	C17 H16 Br N3 O	(M+H)+
380.0361	1	16483.84	C17 H16 Br N3 O	(M+Na)+
381.0385	1	3412.34	C17 H16 Br N3 O	(M+Na)+
382.0344	1	15942.2	C17 H16 Br N3 O	(M+Na)+
396.0096	1	5955.04	C17 H16 Br N3 O	(M+K)+
398.009	1	6378.76	C17 H16 Br N3 O	(M+K)+

--- End Of Report ---

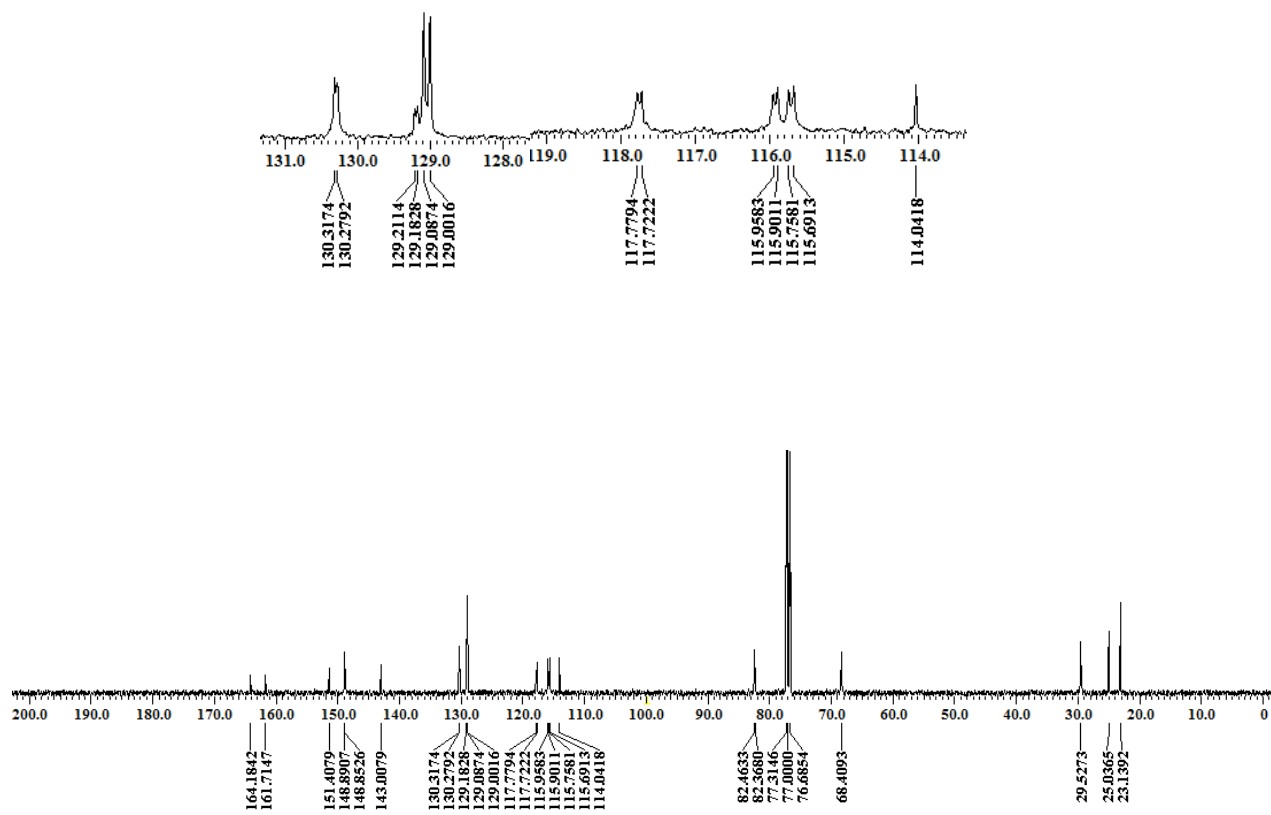


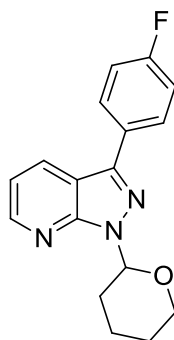
3-(4-fluorophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3aa**)





3-(4-fluorophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3aa**)





3-(4-fluorophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (3aa)

Qualitative Compound Report

Data File: URV5-98.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: 29.10.2014.m
 IRM Calibration Status: Success
 Comment:

Sample Name: URV5-98
 Position: P1-F6
 User Name:
 Acquired Time: 18-05-2017 13:44:38
 DA Method: Default.m

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

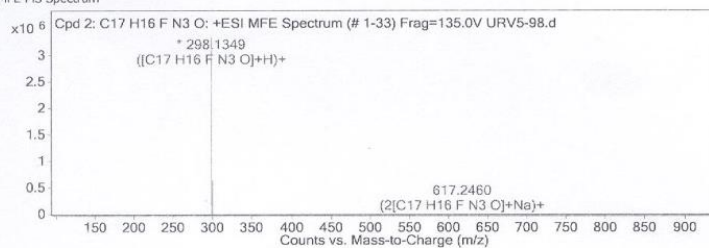


Compound Table

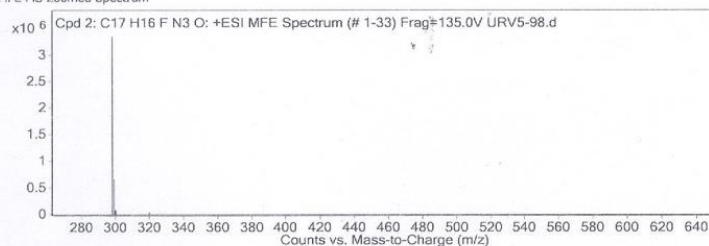
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H16 F N3 O	10	297.1276	C17 H16 F N3 O	C17 H16 F N3 O	0.5	C17 H16 F N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C17 H16 F N3 O	298.1349	10	Find by Molecular Feature	297.1276

MFE MS Spectrum



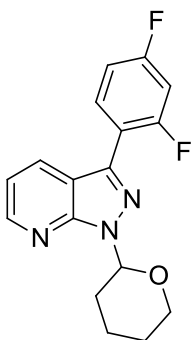
MFE MS Zoomed Spectrum



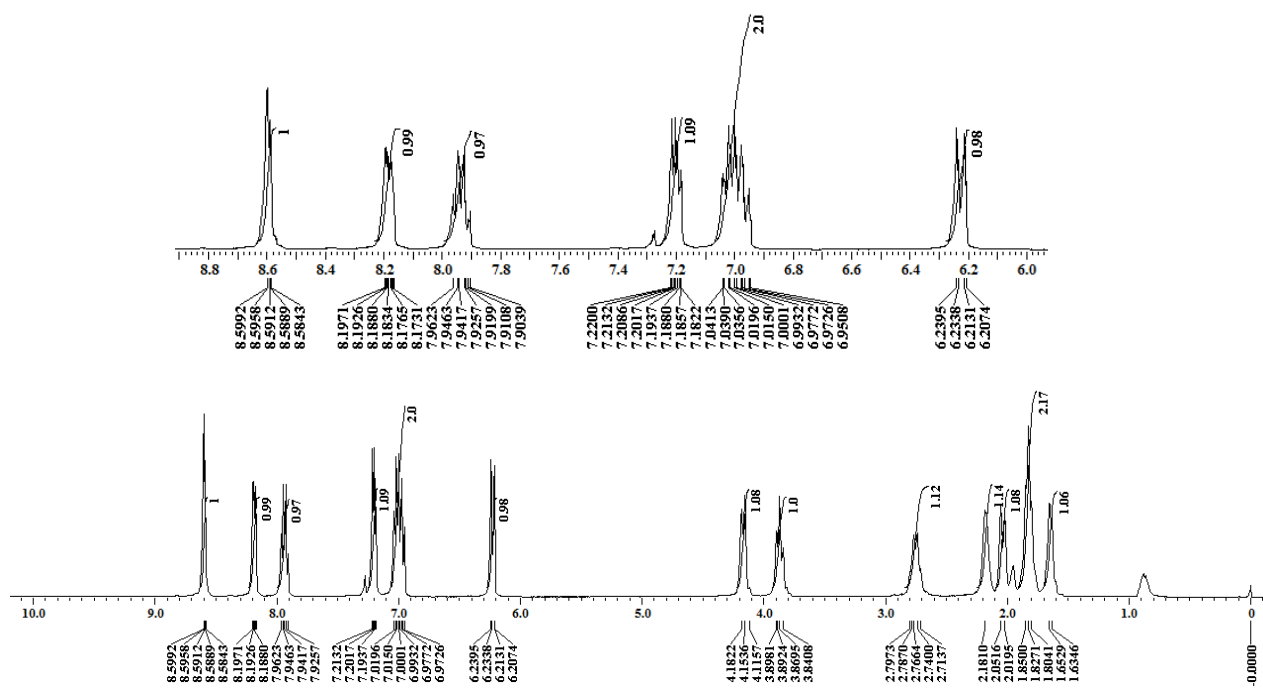
MS Spectrum Peak List

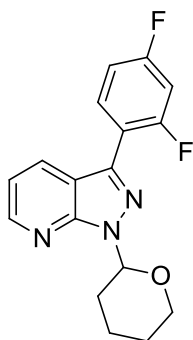
m/z	z	Abund	Formula	Ion
298.1349	1	3336459	C17 H16 F N3 O	(M+H)+
299.138	1	641066.42	C17 H16 F N3 O	(M+H)+
300.1406	1	65379.57	C17 H16 F N3 O	(M+H)+
301.1433	1	8028.83	C17 H16 F N3 O	(M+H)+
320.1163	1	26685.55	C17 H16 F N3 O	(M+Na)+
321.1197	1	5501.2	C17 H16 F N3 O	(M+Na)+
322.1272	1	756.22	C17 H16 F N3 O	(M+Na)+
336.0911	1	5170.53	C17 H16 F N3 O	(M+K)+
337.0946	1	1157.52	C17 H16 F N3 O	(M+K)+
338.0907	1	579.47	C17 H16 F N3 O	(M+K)+

--- End Of Report ---

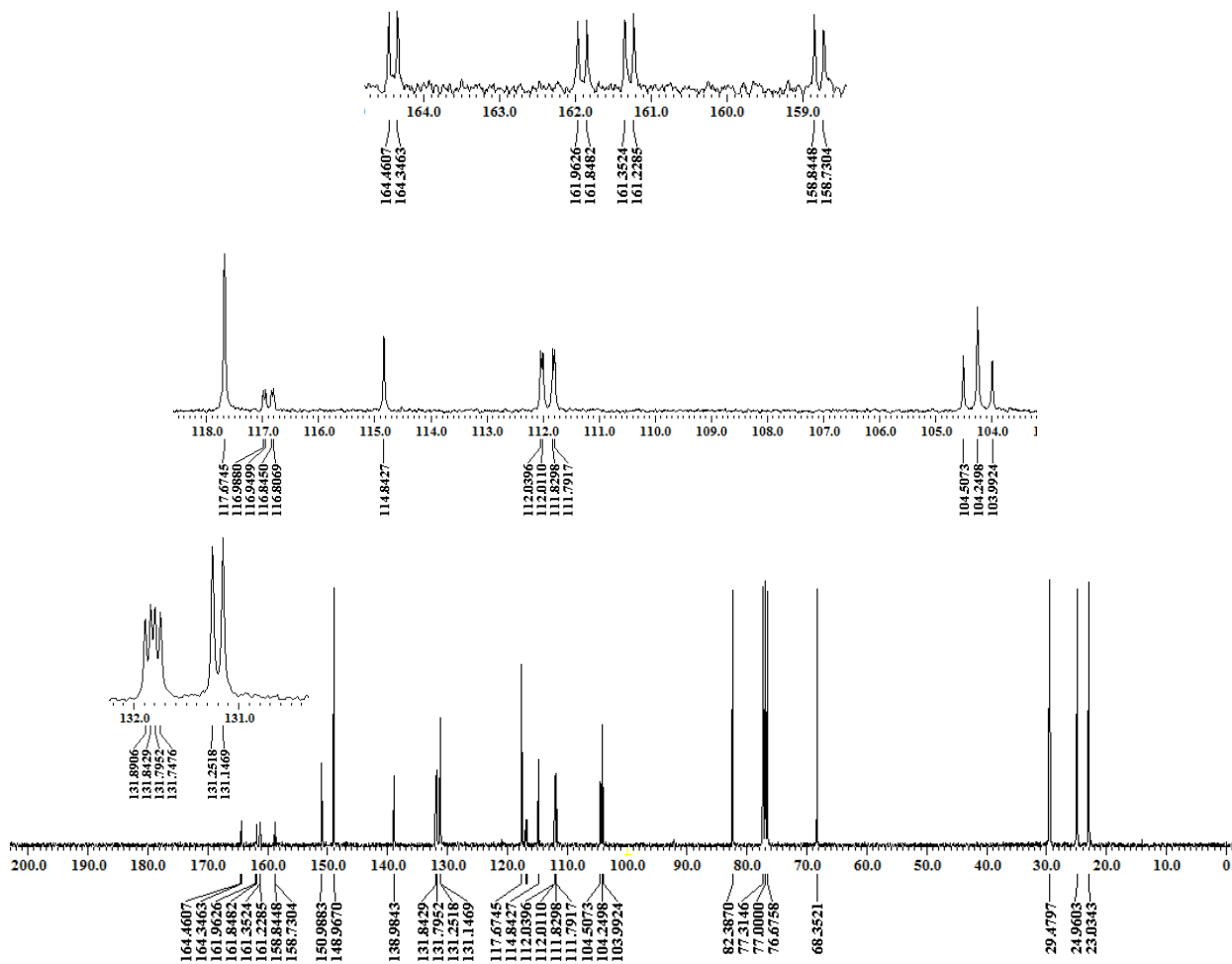


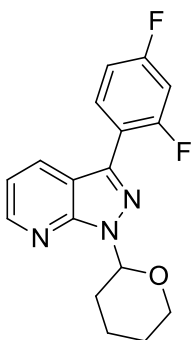
3-(2,4-difluorophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ab**)





3-(2,4-difluorophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ab**)



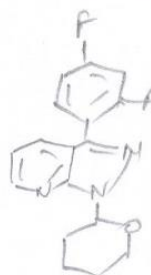


3-(2,4-difluorophenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ab**)

Qualitative Compound Report

Data File	URV5-91.d	Sample Name	URV5-91
Sample Type	Sample	Position	P1-D8
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	16-05-2017 13:29:11
IRM Calibration Status	Success	DA Method	Default.m
Comment			

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

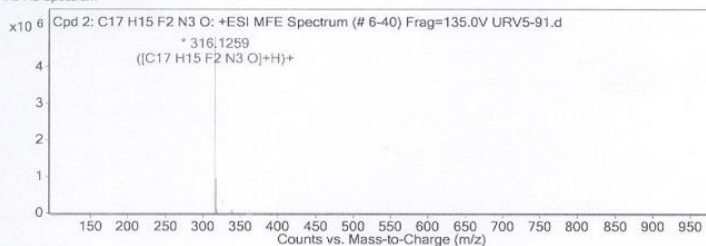


Compound Table

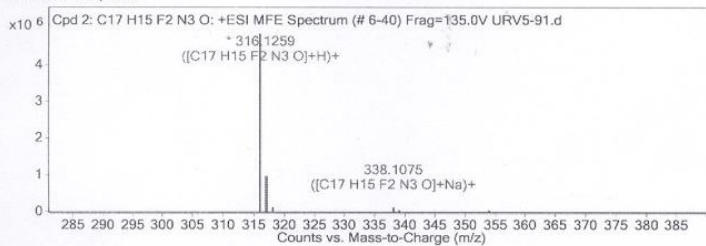
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H15 F2 N3 O	10	315.1186	C17 H15 F2 N3 O	C17 H15 F2 N3 O	-0.98	C17 H15 F2 N3 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C17 H15 F2 N3 O	316.1259	10	Find by Molecular Feature	315.1186

MFE MS Spectrum



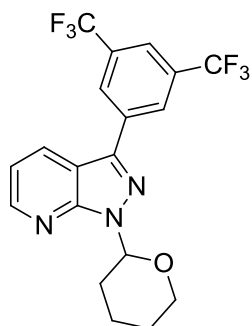
MFE MS Zoomed Spectrum



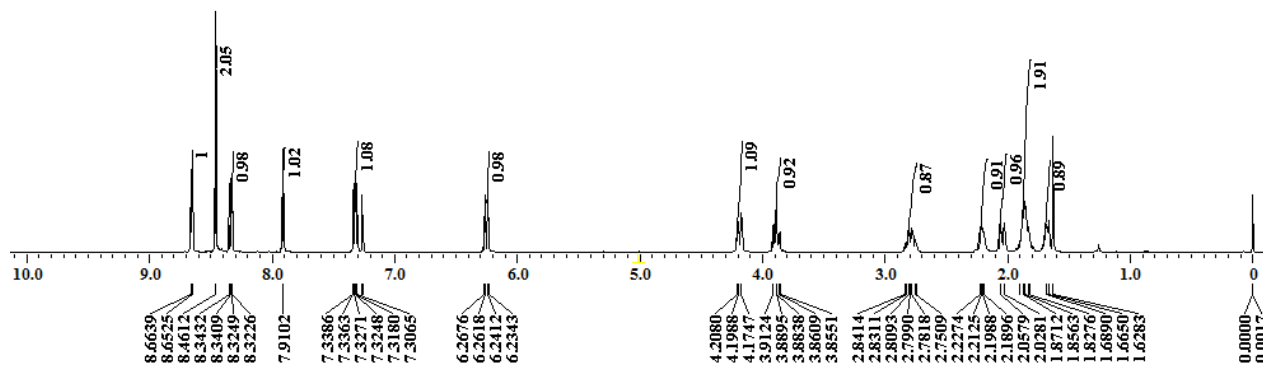
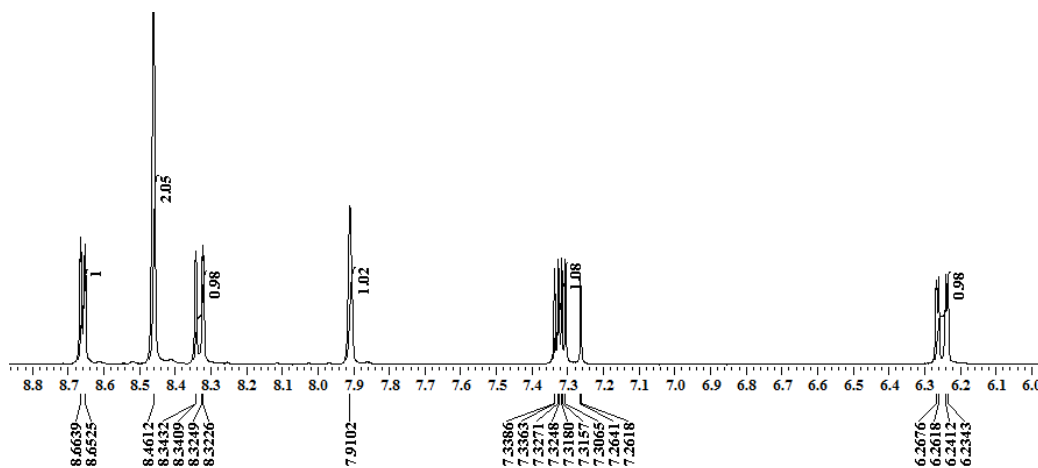
MS Spectrum Peak List

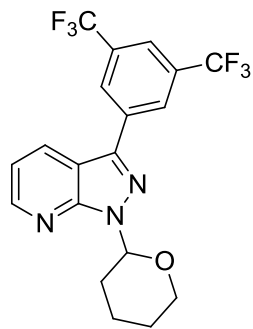
m/z	z	Abund	Formula	Ion
316.1259	1	4863810.5	C17 H15 F2 N3 O	(M+H)+
317.1292	1	953143.87	C17 H15 F2 N3 O	(M+H)+
318.1316	1	98928.36	C17 H15 F2 N3 O	(M+H)+
319.1351	1	6556.25	C17 H15 F2 N3 O	(M+H)+
320.1357	1	650.77	C17 H15 F2 N3 O	(M+H)+
338.1075	1	95669.2	C17 H15 F2 N3 O	(M+Na)+
339.1105	1	18298.4	C17 H15 F2 N3 O	(M+Na)+
354.0817	1	19328.12	C17 H15 F2 N3 O	(M+K)+
355.0825	1	4451.46	C17 H15 F2 N3 O	(M+K)+
356.0837	1	2037.3	C17 H15 F2 N3 O	(M+K)+

--- End Of Report ---

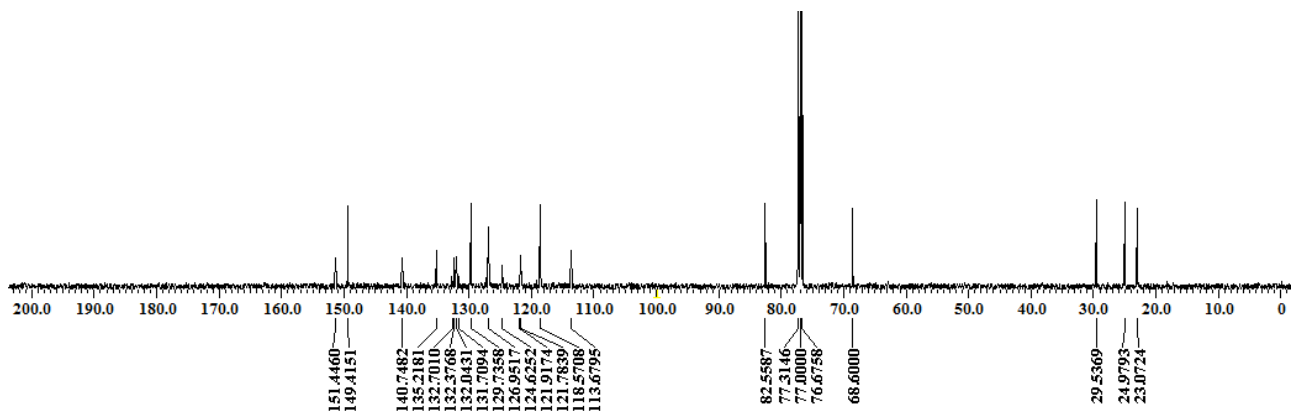
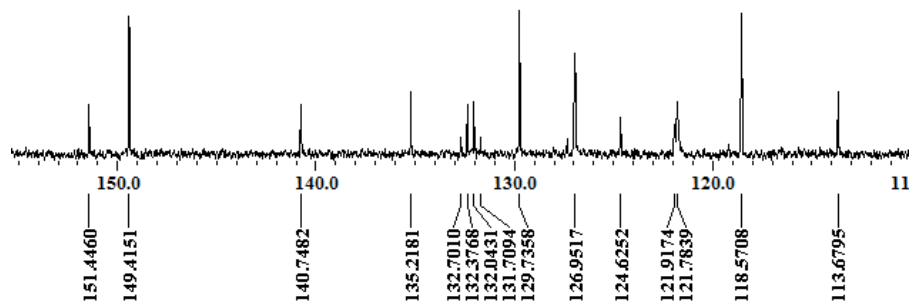


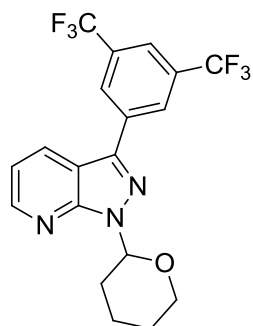
3-(3,5-bis(trifluoromethyl)phenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ac**)



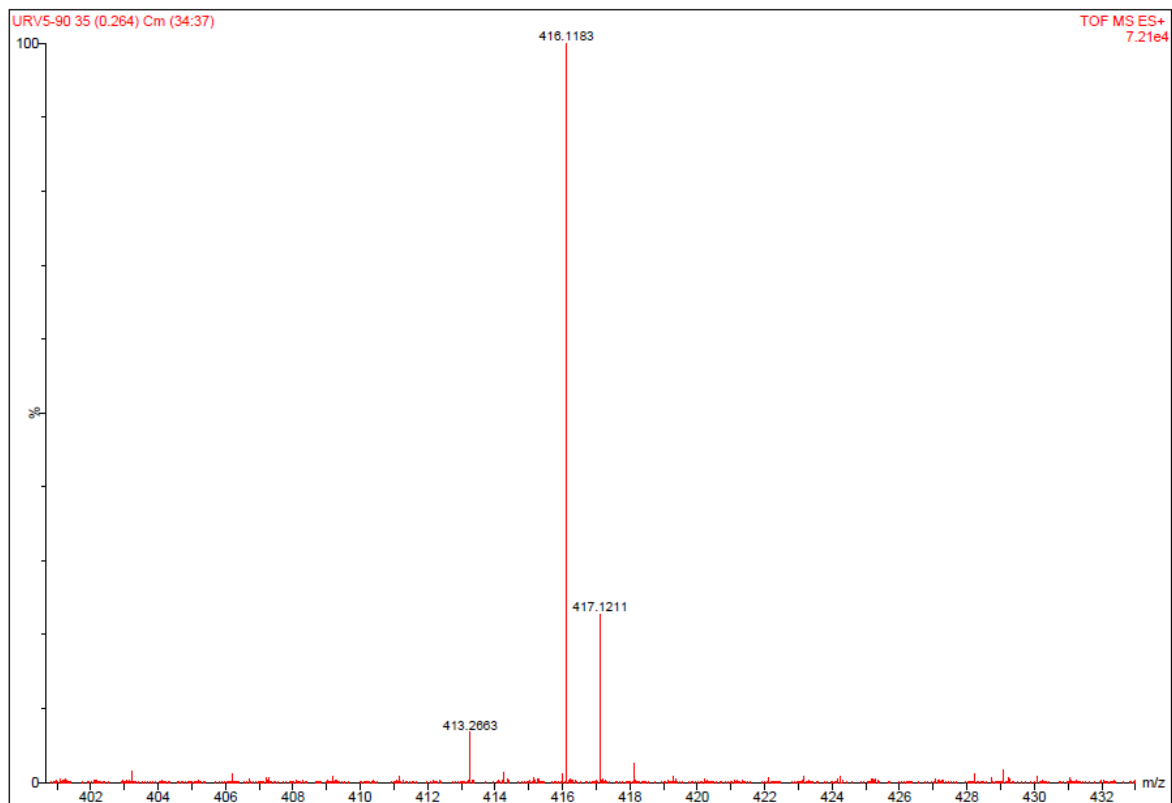


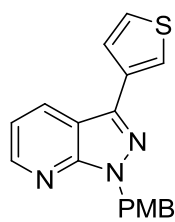
3-(3,5-bis(trifluoromethyl)phenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ac**)



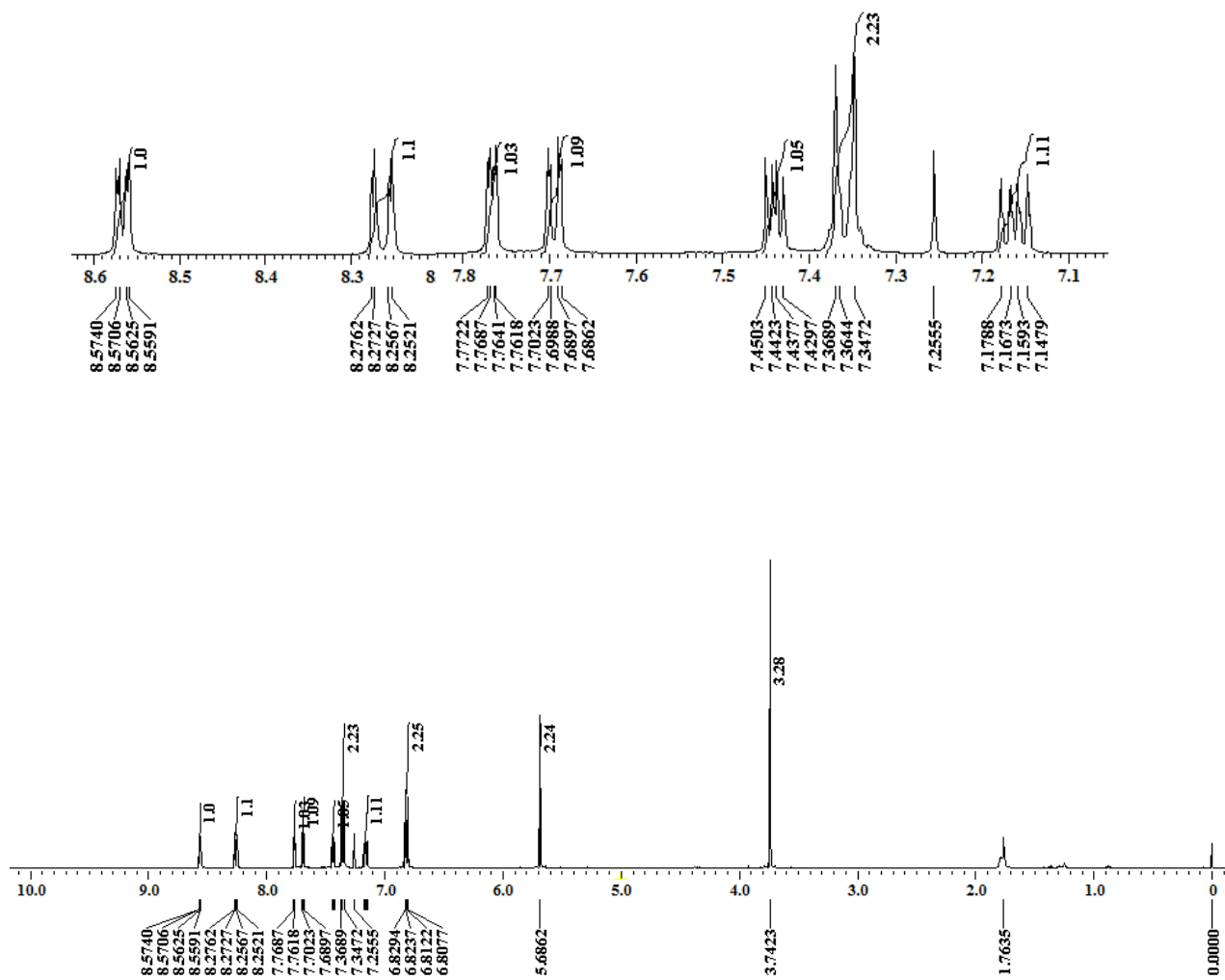


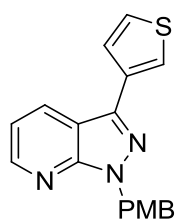
3-(3,5-bis(trifluoromethyl)phenyl)-1-(tetrahydro-2H-pyran-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ac**)



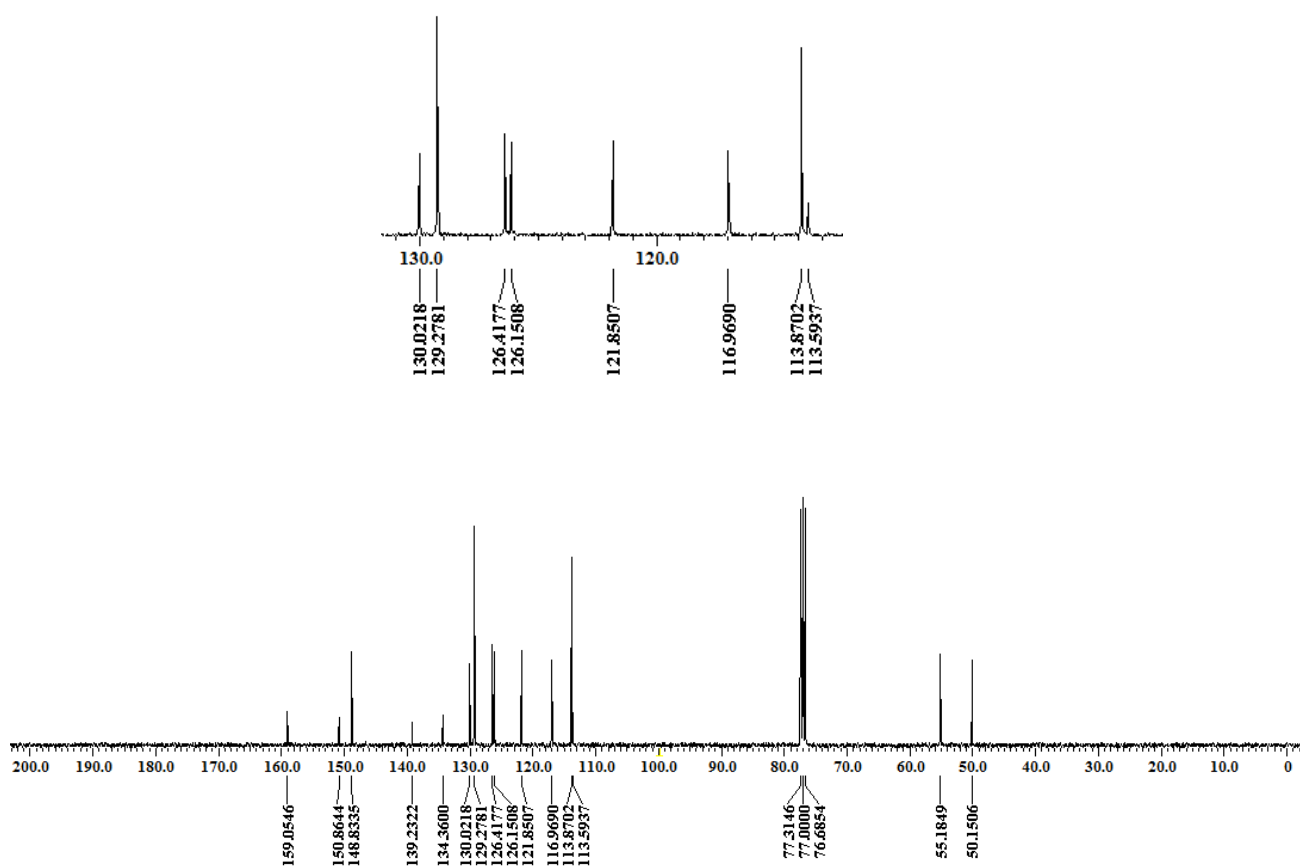


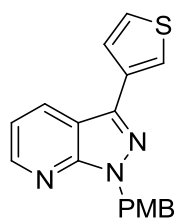
1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ad**)



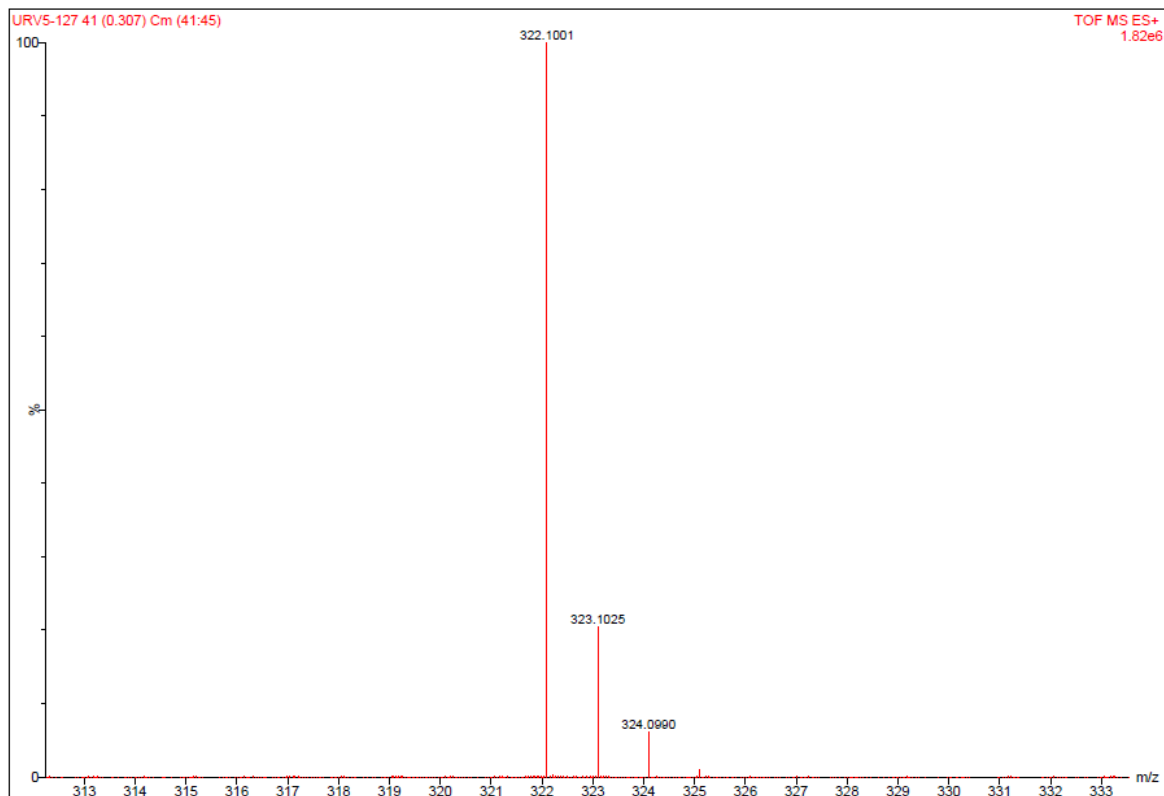


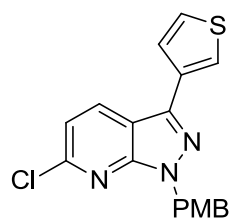
1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1H-pyrazolo[3,4-b]pyridine (3ad)



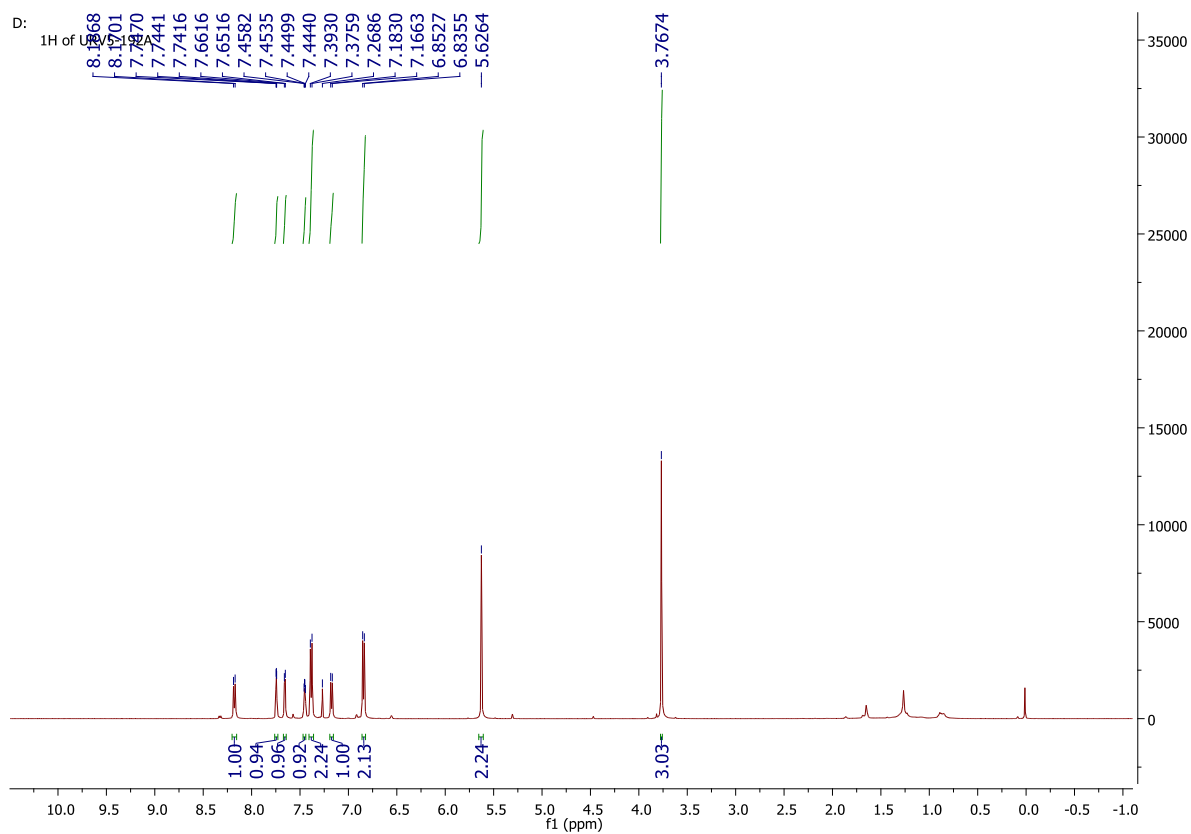
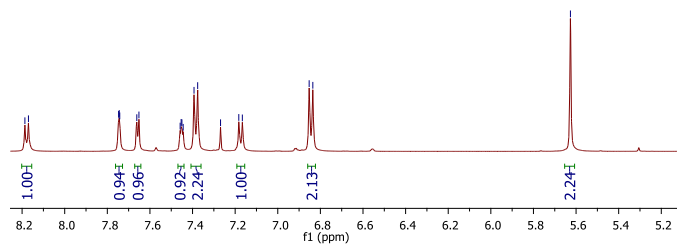


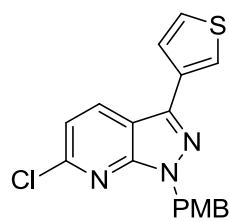
1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1H-pyrazolo[3,4-b]pyridine (**3ad**)



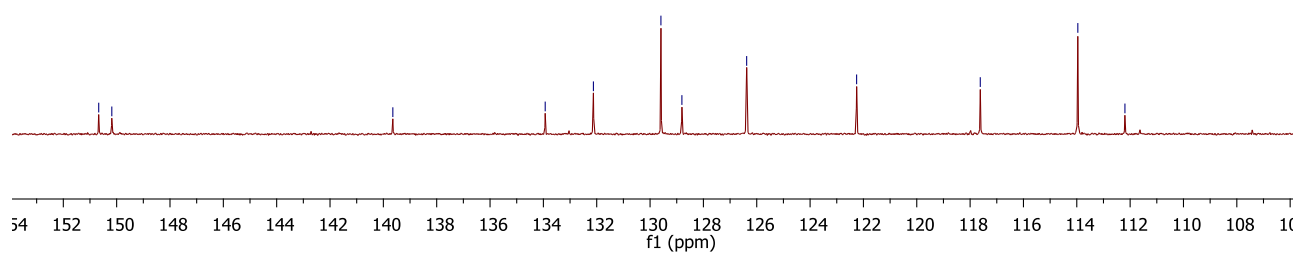


6-chloro-1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ae**)





6-chloro-1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1H-pyrazolo[3,4-b]pyridine (**3ae**)

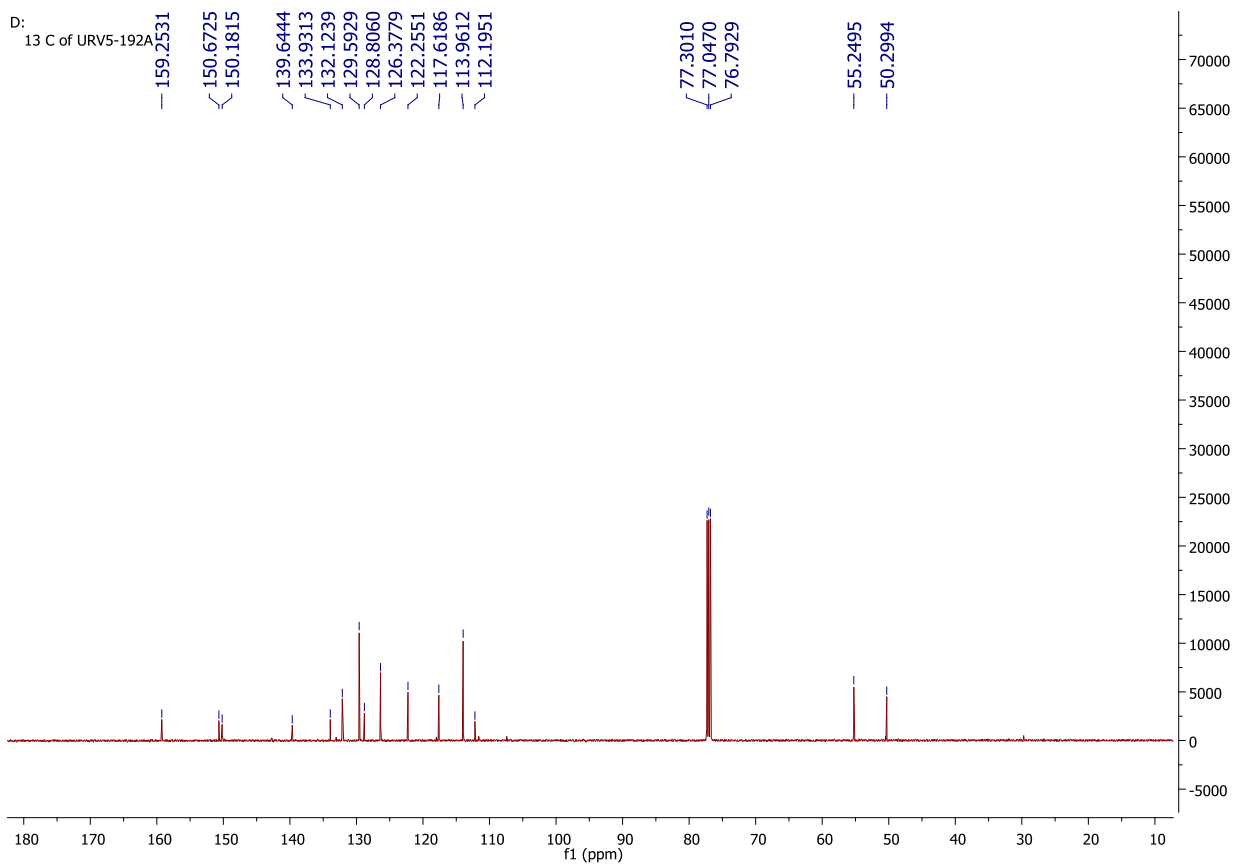


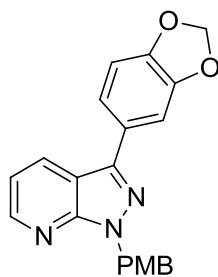
D:
13 C of URV5-192A

159.2531
150.6725
150.1815
139.6444
133.9313
132.1239
129.5929
128.8060
126.3779
122.2551
117.6186
113.9612
112.1951

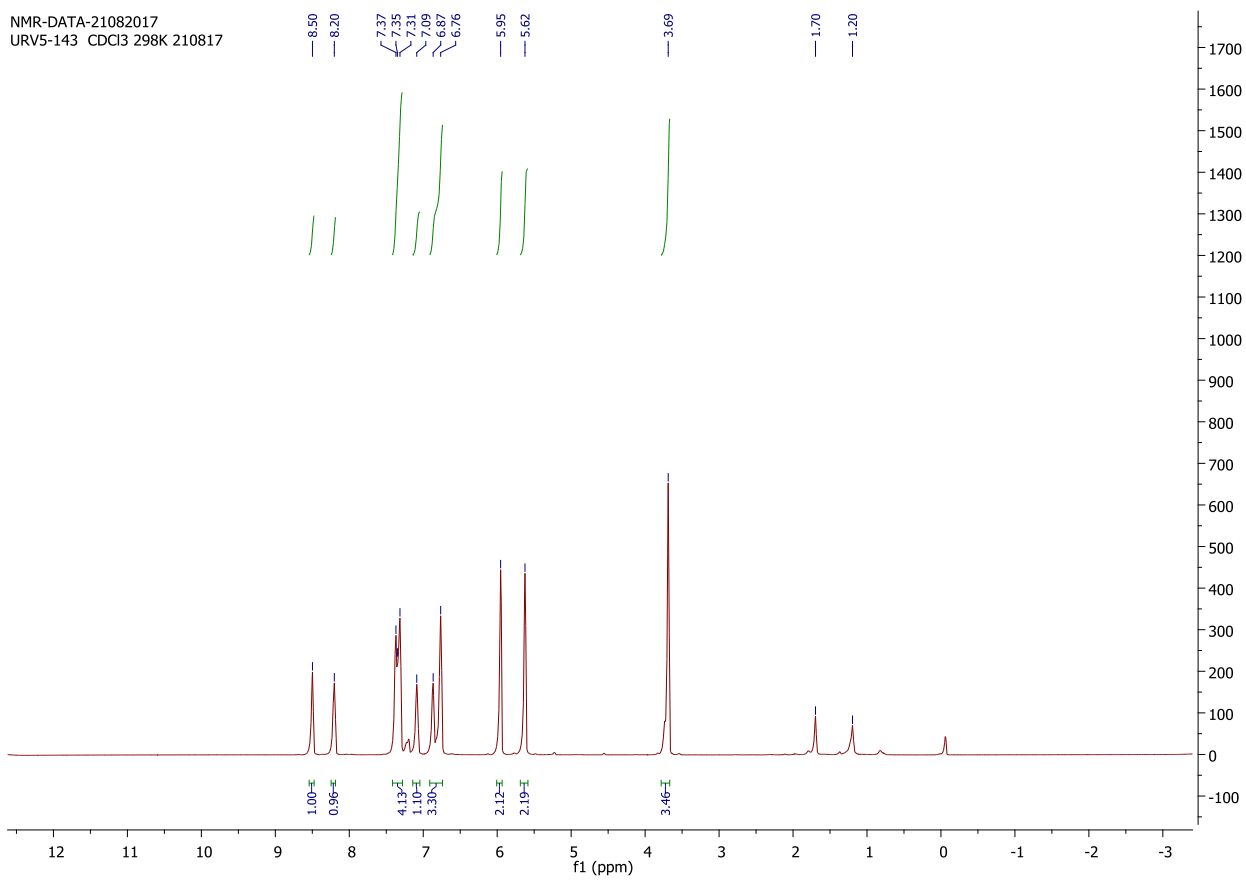
77.3010
77.0470
76.7929

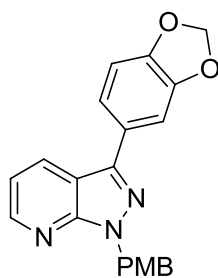
55.2495
50.2994



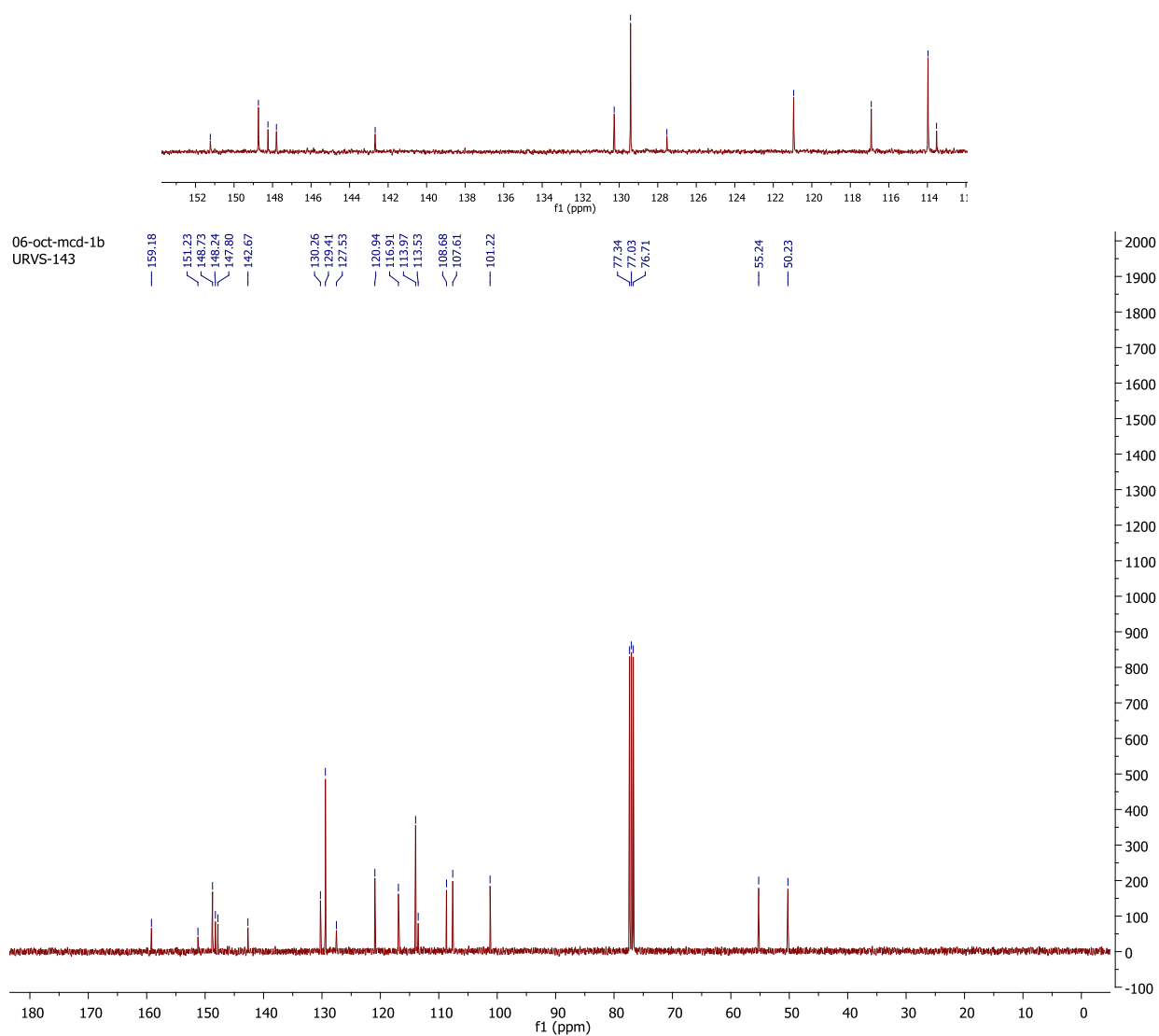


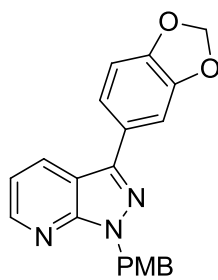
3-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3af**)



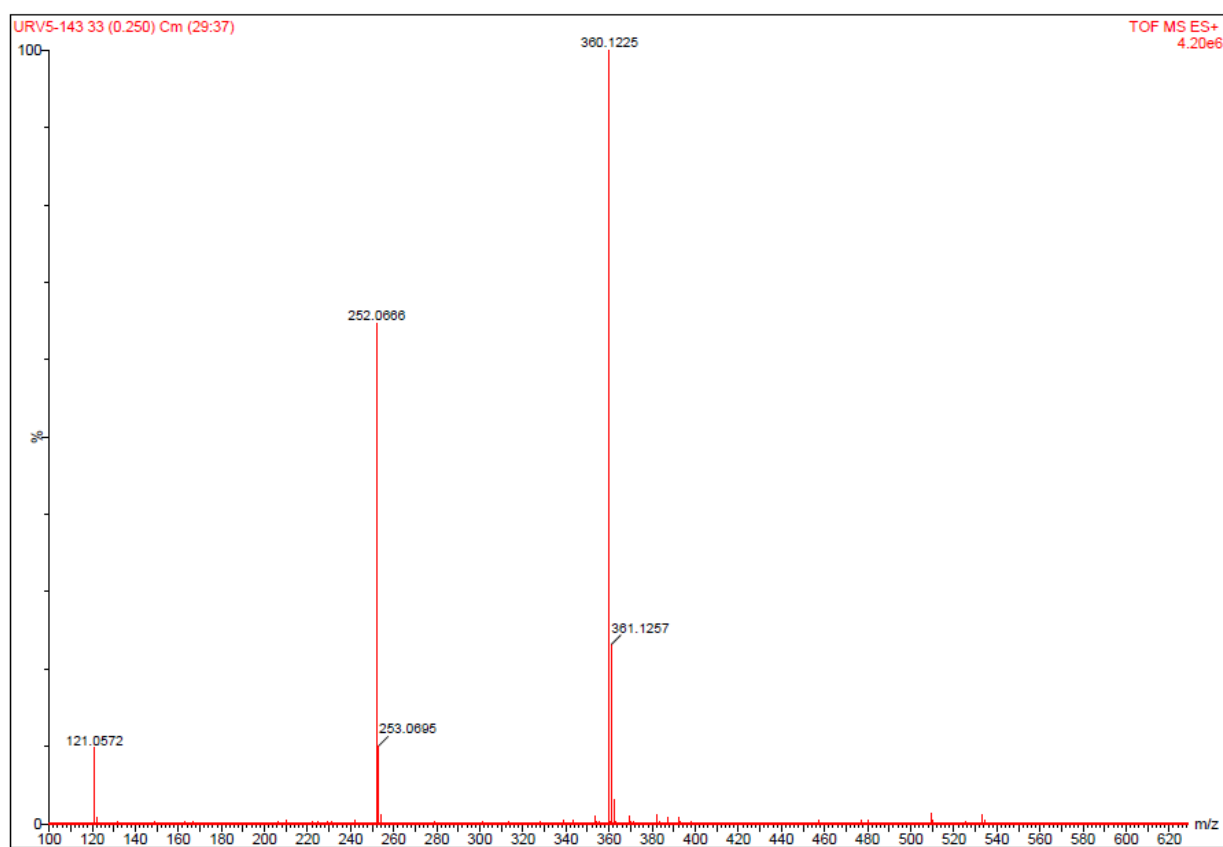


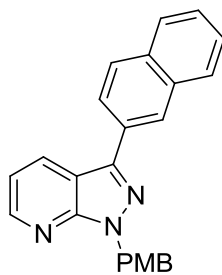
3-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridine (**3af**)



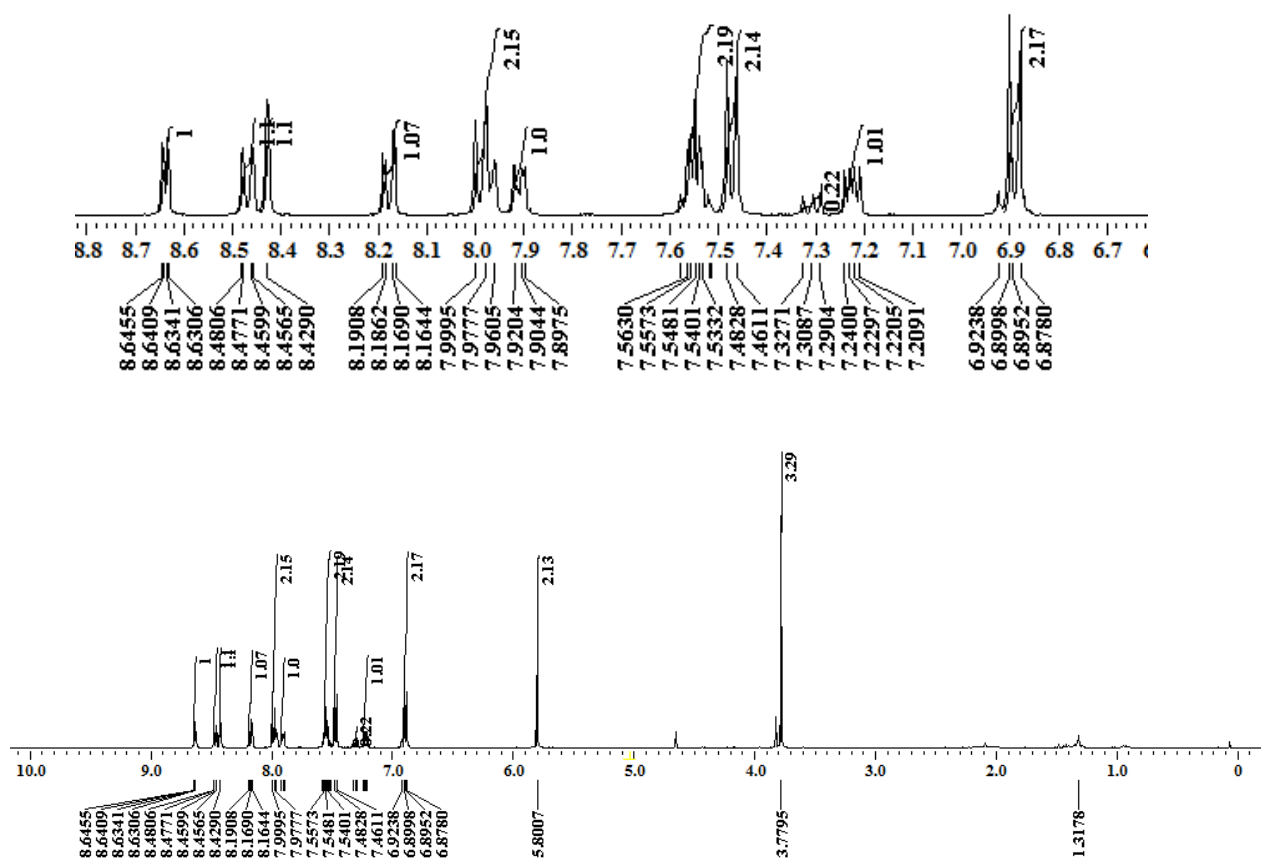


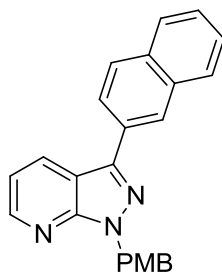
3-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxybenzyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3af**)



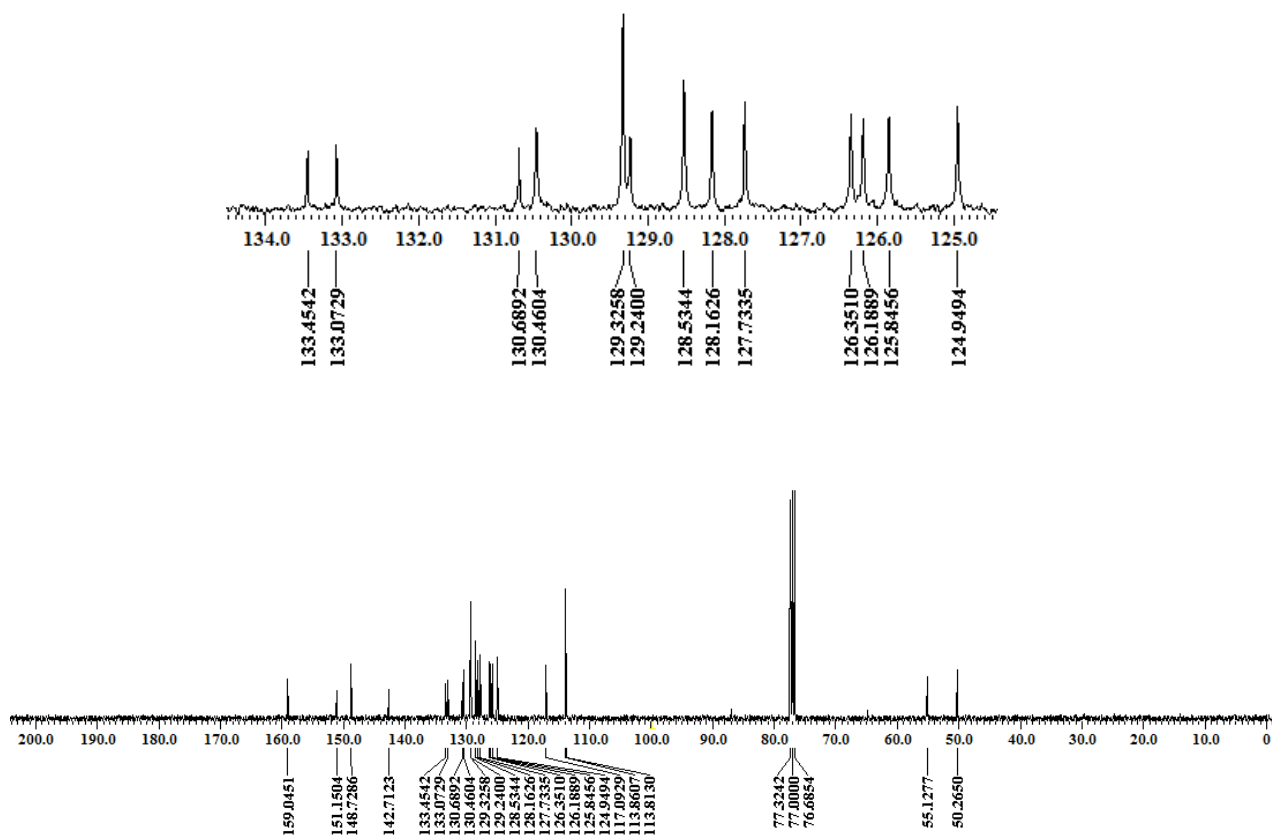


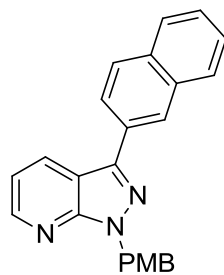
1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ag**)



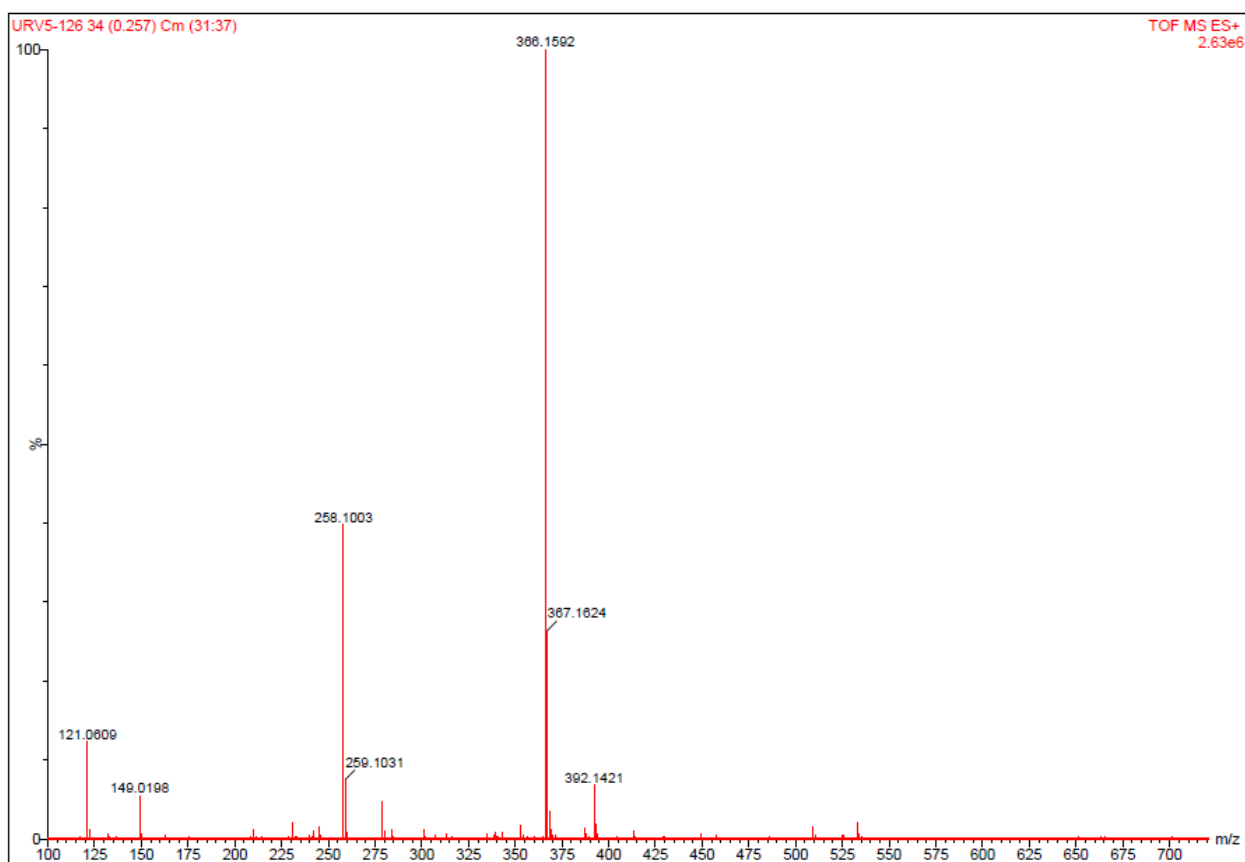


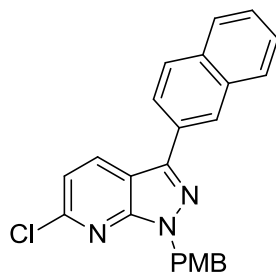
1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ag**)



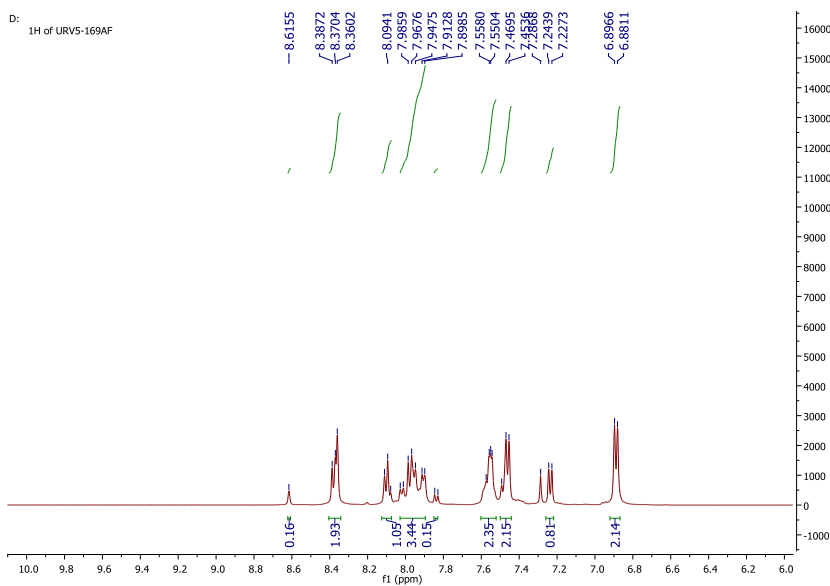
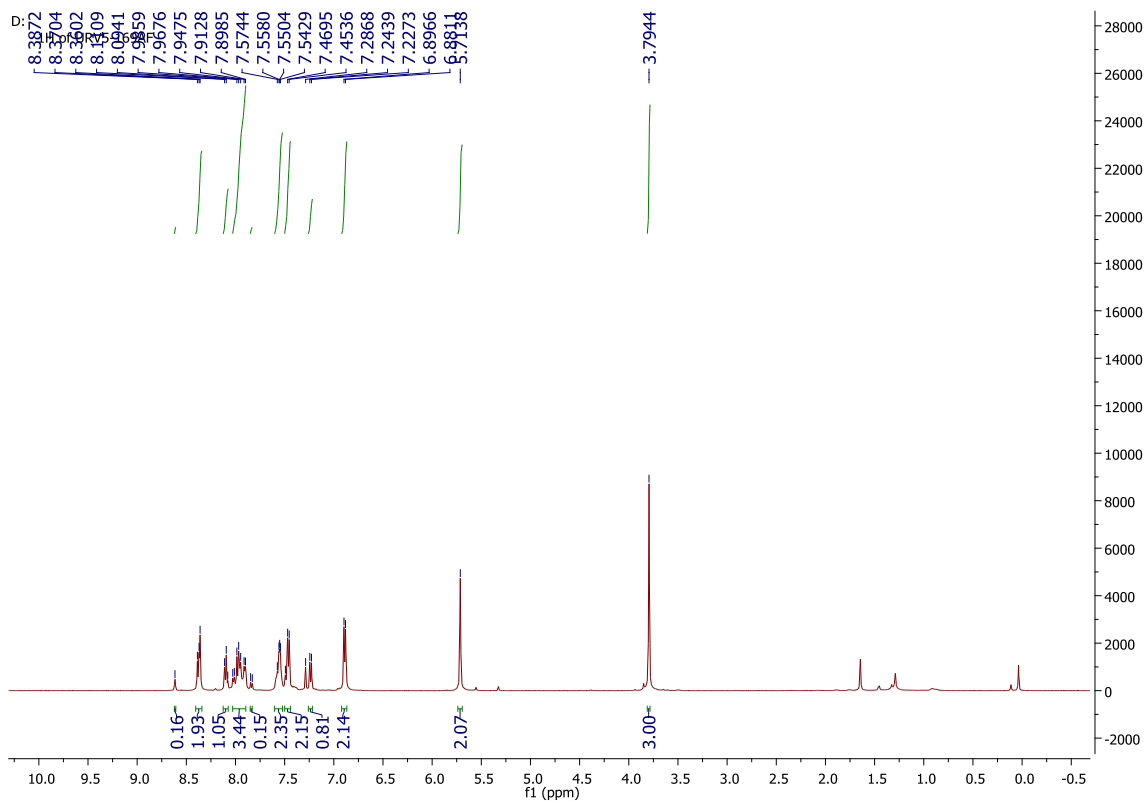


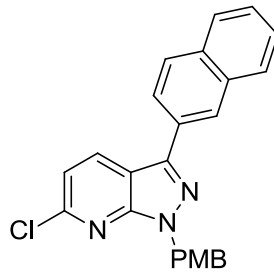
1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ag**)



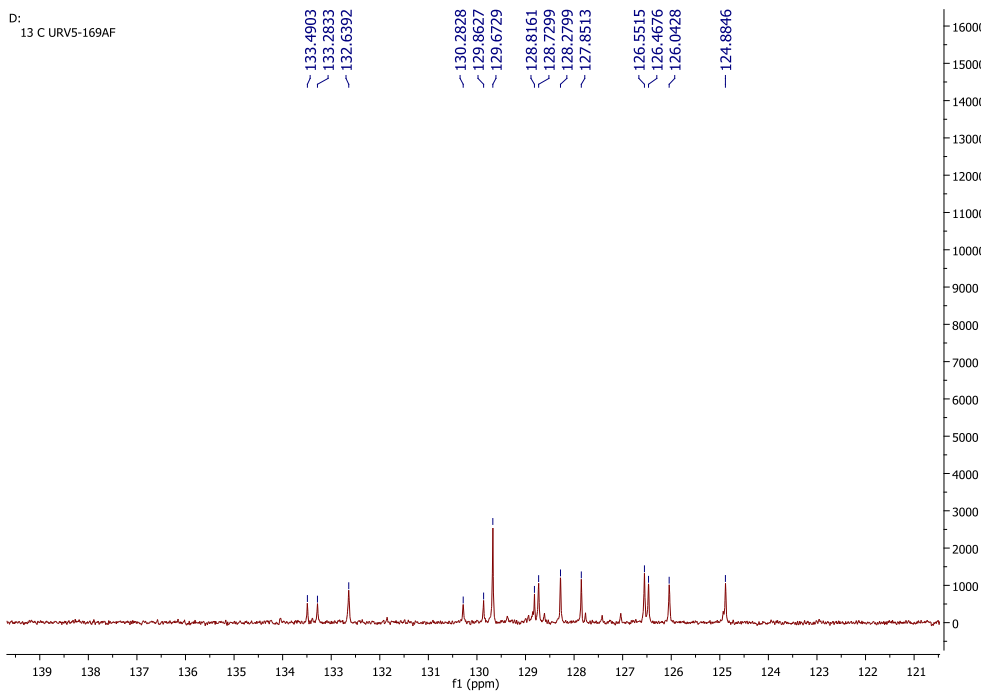
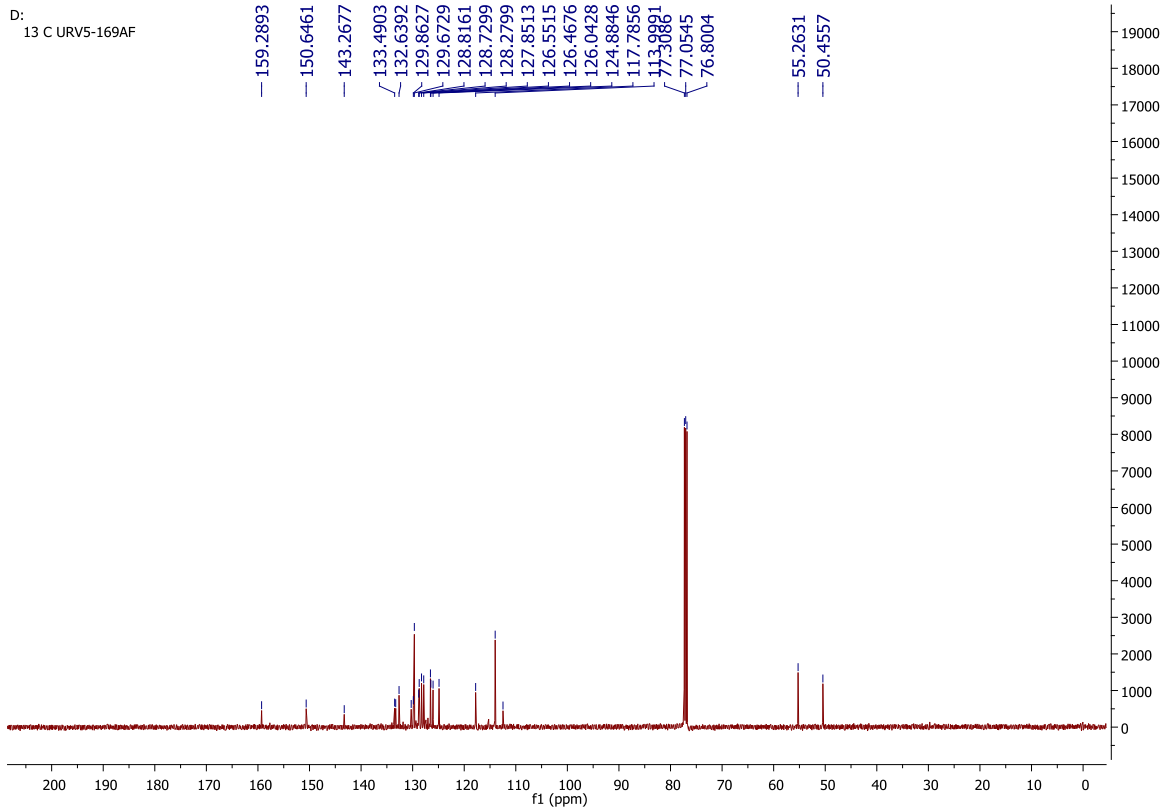


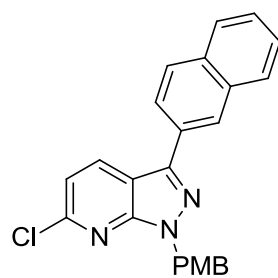
6-chloro-1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ah**)



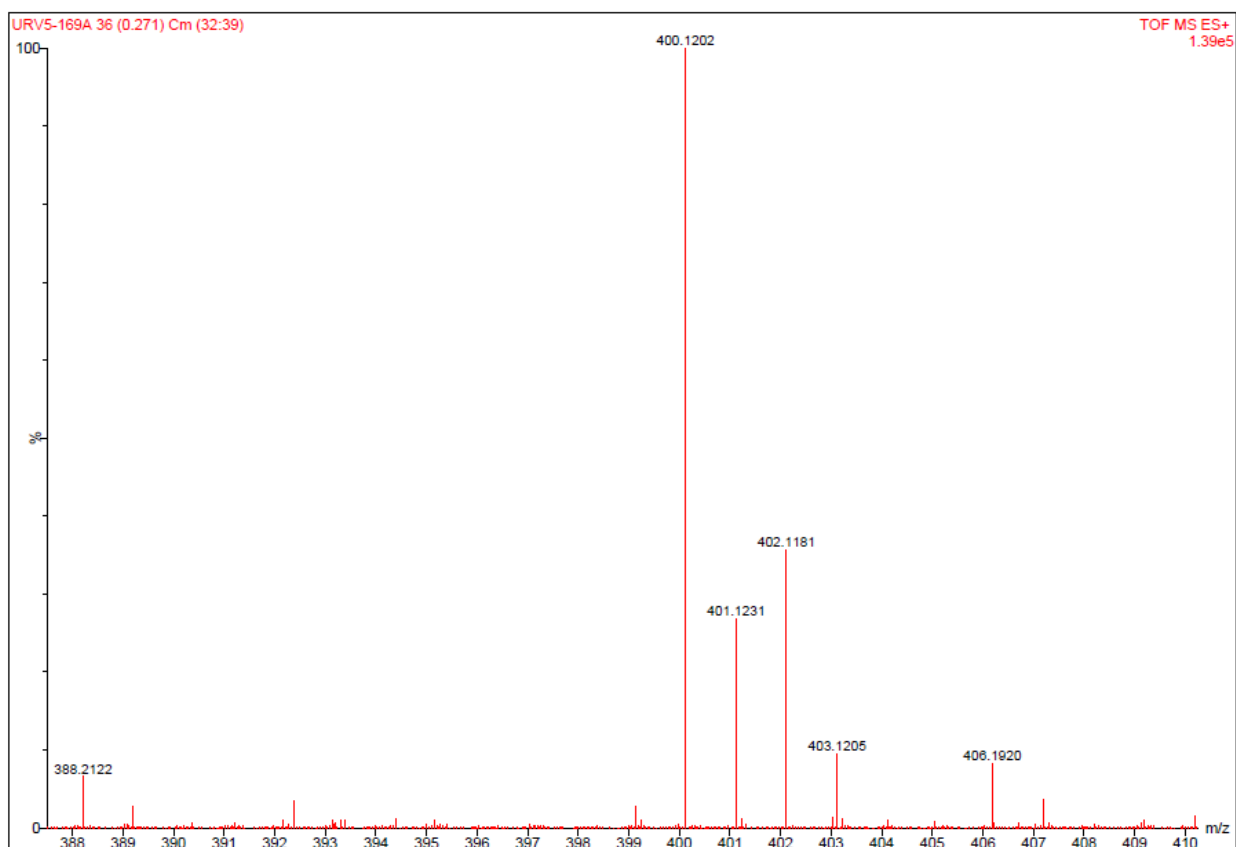


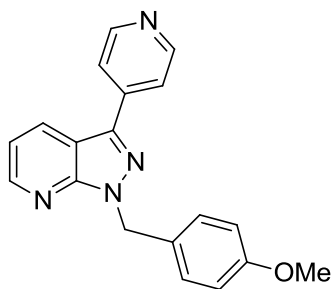
6-chloro-1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ah**)



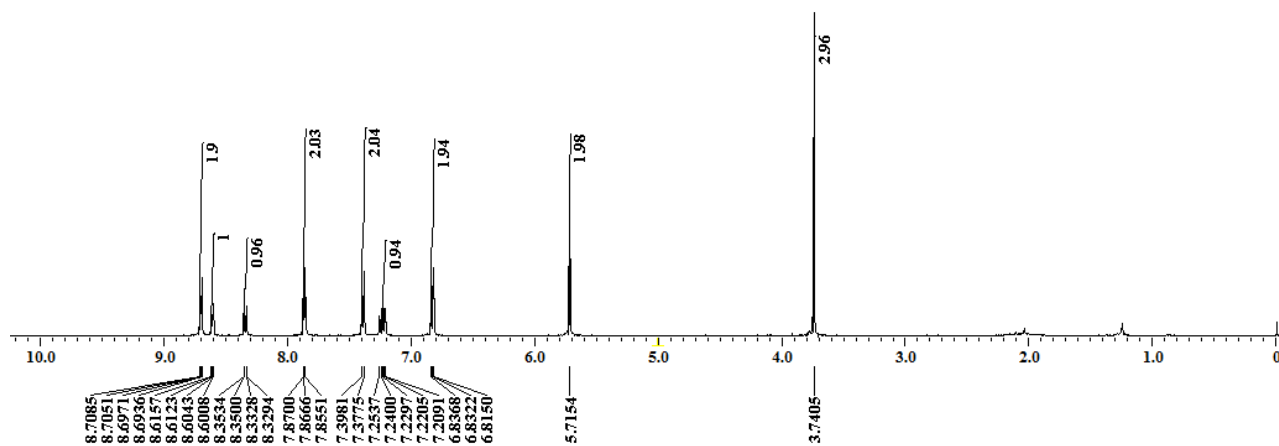
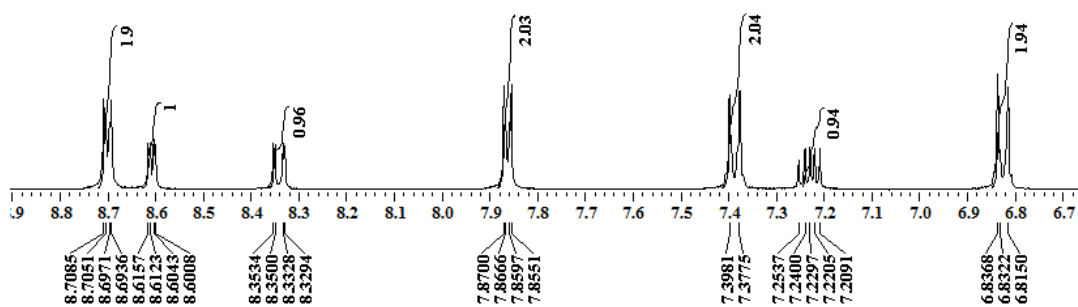


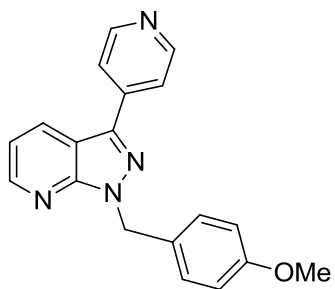
6-chloro-1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1H-pyrazolo[3,4-b]pyridine (**3ah**)



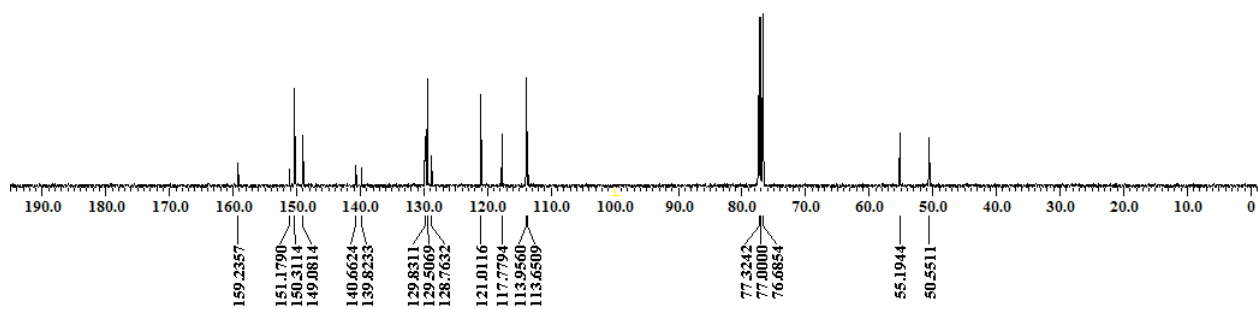
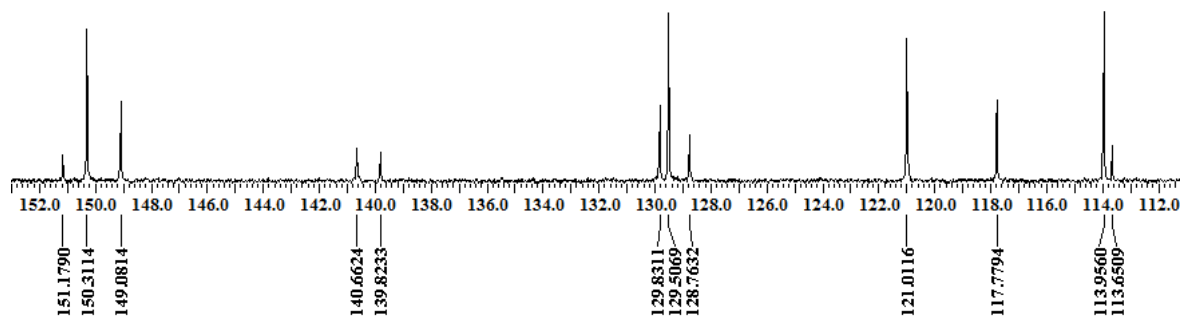


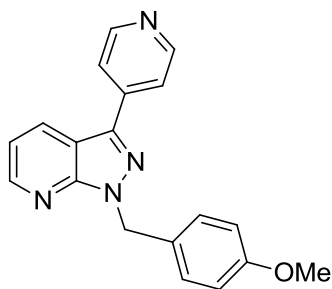
1-(4-methoxybenzyl)-3-(pyridin-4-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ai**)





1-(4-methoxybenzyl)-3-(pyridin-4-yl)-1H-pyrazolo[3,4-b]pyridine (**3ai**)





1-(4-methoxybenzyl)-3-(pyridin-4-yl)-1H-pyrazolo[3,4-b]pyridine (**3ai**)

Qualitative Compound Report

Data File	URV5-89.d	Sample Name	URV5-89
Sample Type	Sample	Position	P1-C3
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	25-05-2017 13:02:05
IRM Calibration Status	Success	DA Method	Default.m
Comment			

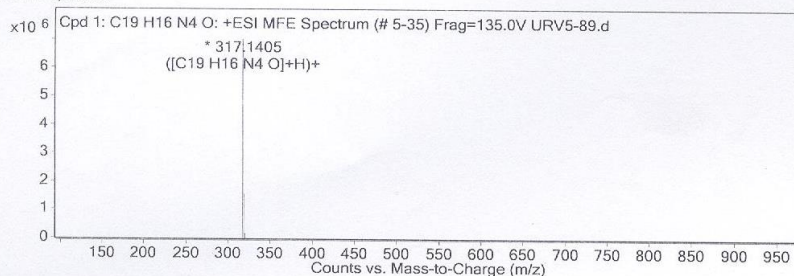
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

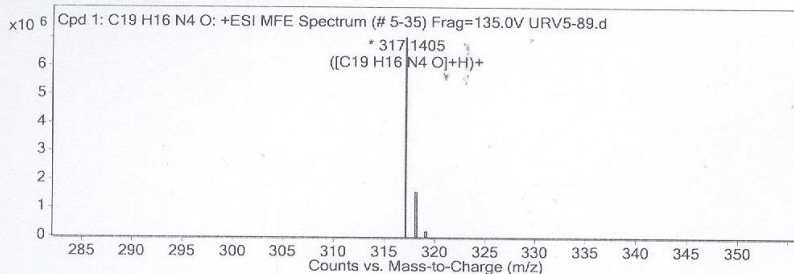
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C19 H16 N4 O	11	316.1332	C19 H16 N4 O	C19 H16 N4 O	-2.6	C19 H16 N4 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H16 N4 O	317.1405	11	Find by Molecular Feature	316.1332

MFE MS Spectrum



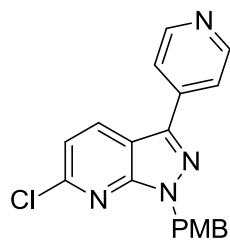
MFE MS Zoomed Spectrum



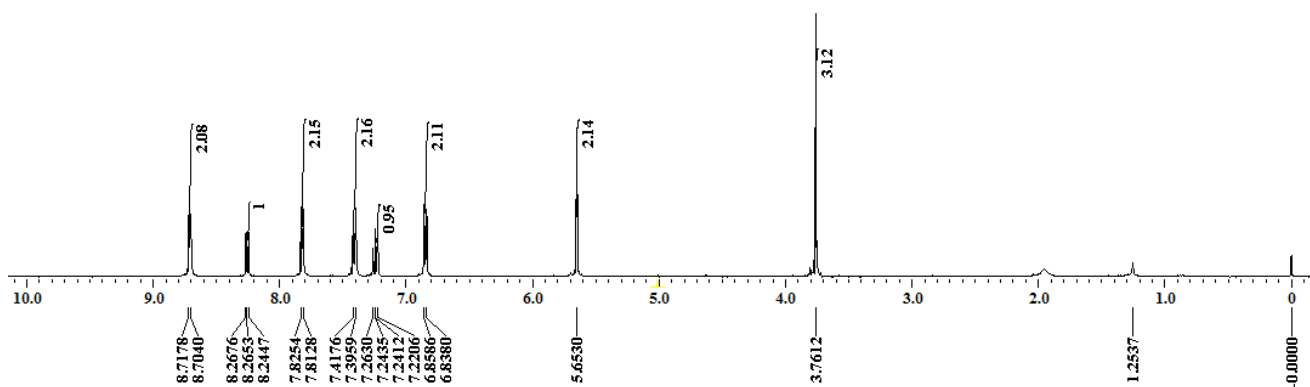
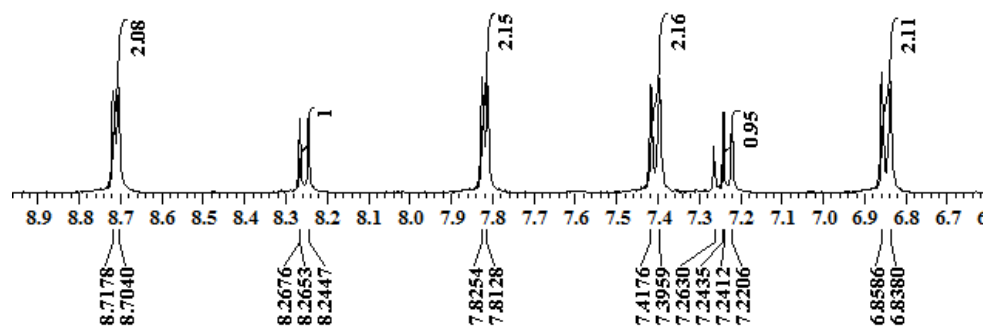
MS Spectrum Peak List

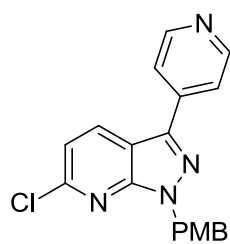
m/z	z	Abund	Formula	Ion
317.1405	1	7024204.5	C19 H16 N4 O	(M+H)+
318.1436	1	1563277.56	C19 H16 N4 O	(M+H)+
319.1469	1	167976.24	C19 H16 N4 O	(M+H)+
320.15	1	13228.89	C19 H16 N4 O	(M+H)+
321.1483	1	1212.23	C19 H16 N4 O	(M+H)+

--- End Of Report ---

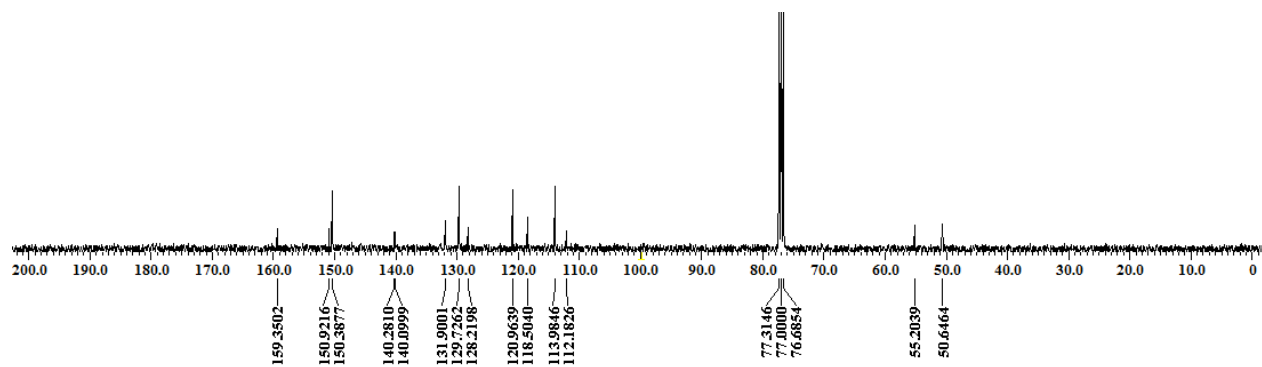
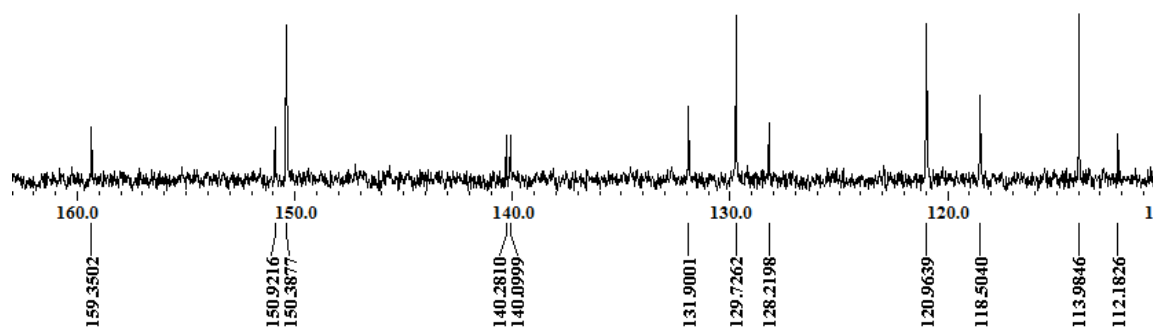


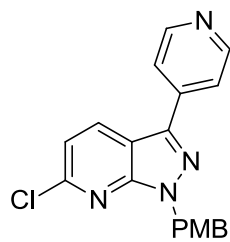
6-chloro-1-(4-methoxybenzyl)-3-(pyridin-4-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3aj**)



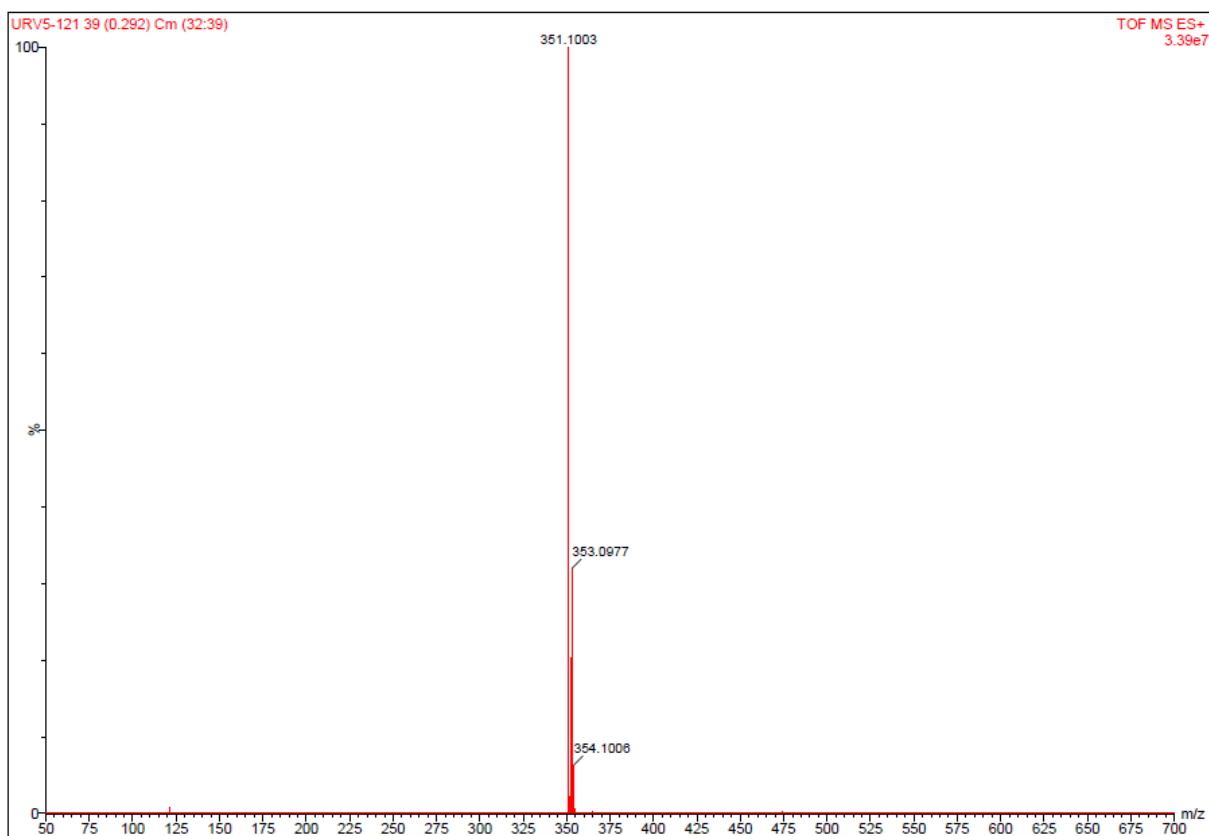


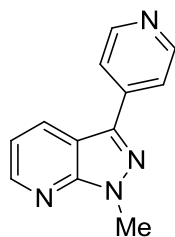
6-chloro-1-(4-methoxybenzyl)-3-(pyridin-4-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3aj**)



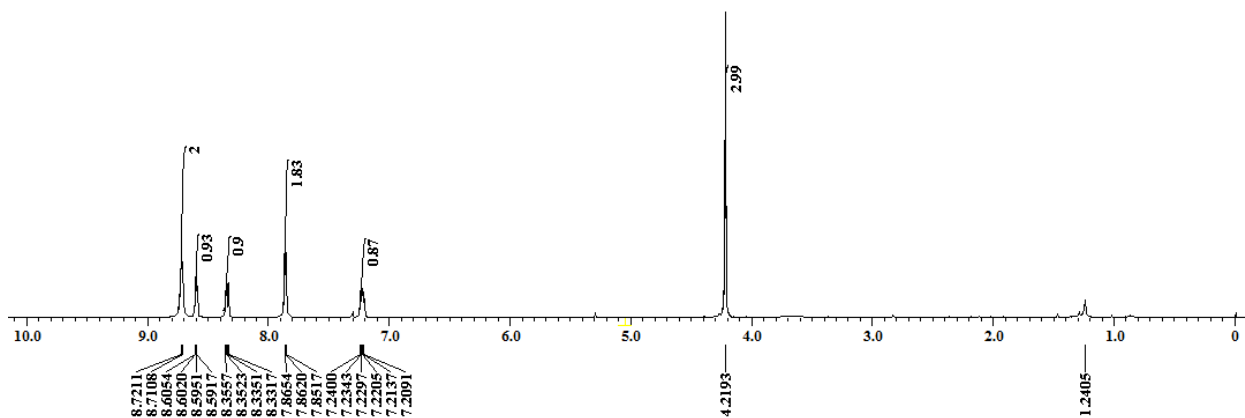
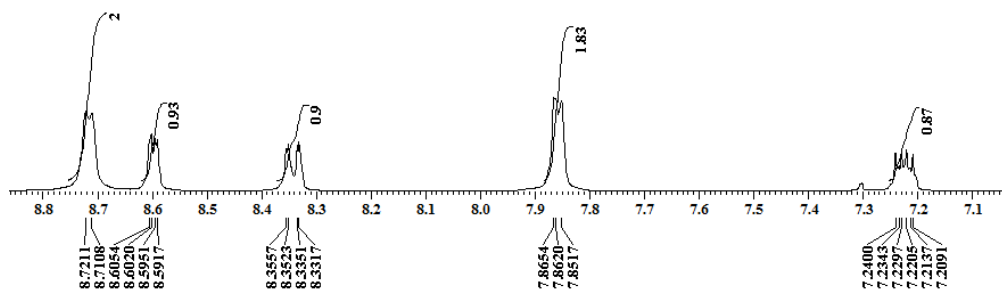


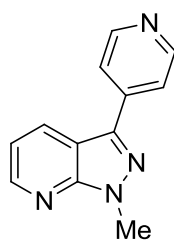
6-chloro-1-(4-methoxybenzyl)-3-(pyridin-4-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3aj**)



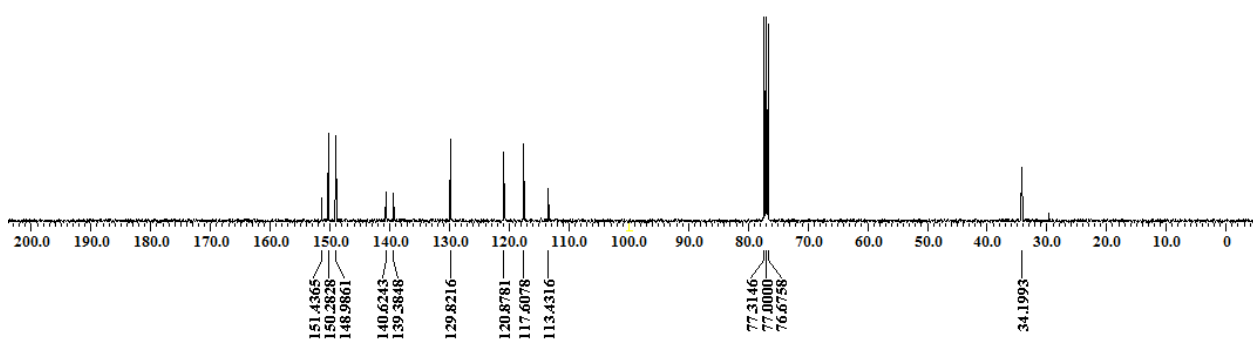
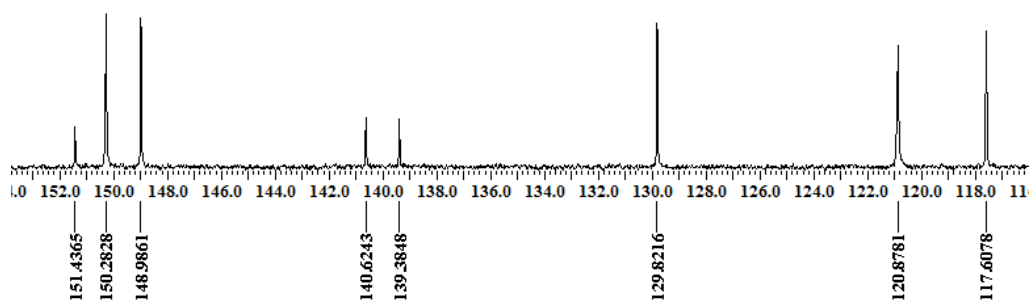


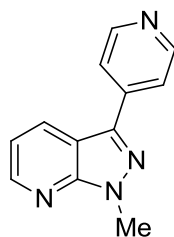
1-methyl-3-(pyridin-4-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**3ak**)





1-methyl-3-(pyridin-4-yl)-1H-pyrazolo[3,4-b]pyridine (**3ak**)





1-methyl-3-(pyridin-4-yl)-1H-pyrazolo[3,4-b]pyridine (**3ak**)

Qualitative Compound Report

Data File	URV5-85.d	Sample Name	URV5-85
Sample Type	Sample	Position	P1-A8
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	08-05-2017 13:53:42
IRM Calibration Status	Success	DA Method	Default.m
Comment			

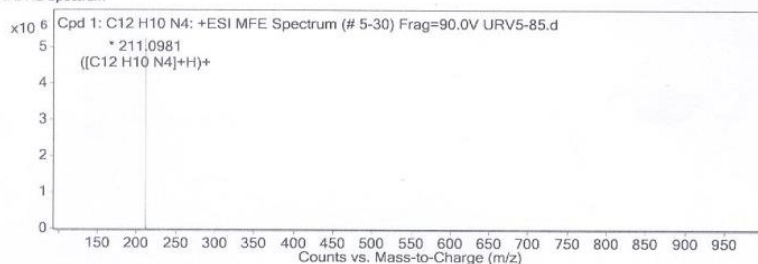
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

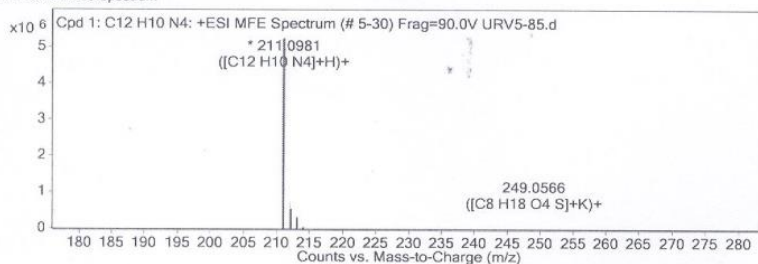
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C12 H10 N4	11	210.0909	C12 H10 N4	C12 H10 N4	-1.64	C12 H10 N4

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C12 H10 N4	211.0981	11	Find by Molecular Feature	210.0909

MFE MS Spectrum



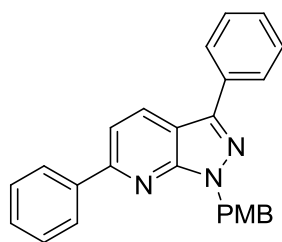
MFE MS Zoomed Spectrum



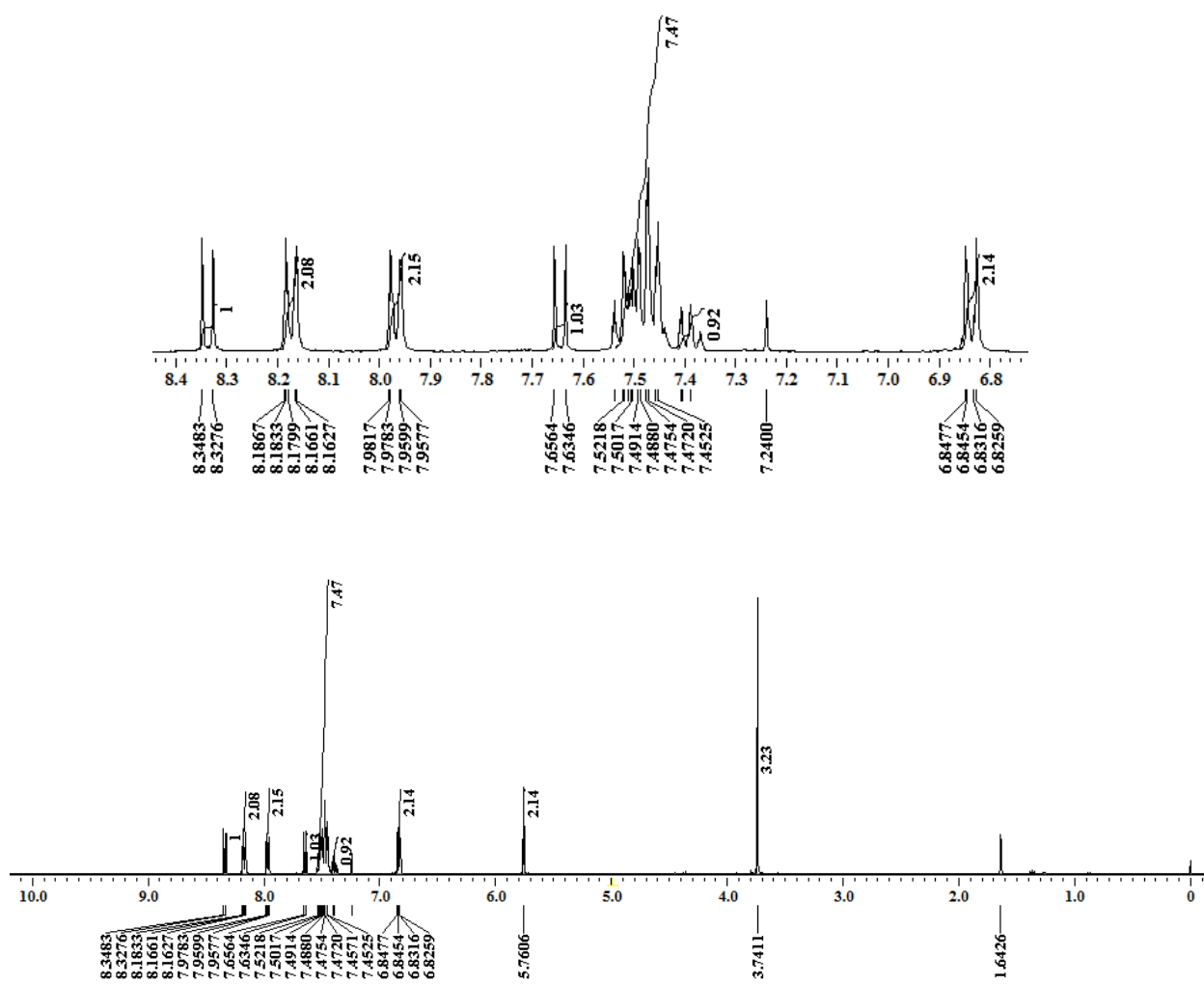
MS Spectrum Peak List

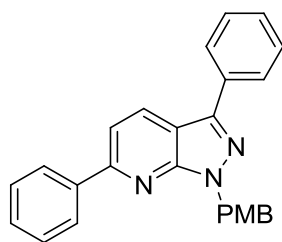
m/z	z	Abund	Formula	Ion
211.0981	1	5253705.5	C12 H10 N4	(M+H)+
212.1011	1	749166.59	C12 H10 N4	(M+H)+
213.1041	1	46007.94	C12 H10 N4	(M+H)+
214.1067	1	1751.98	C12 H10 N4	(M+H)+
249.0566	1	886.49	C8 H18 O4 S	(M+K)+

--- End Of Report ---

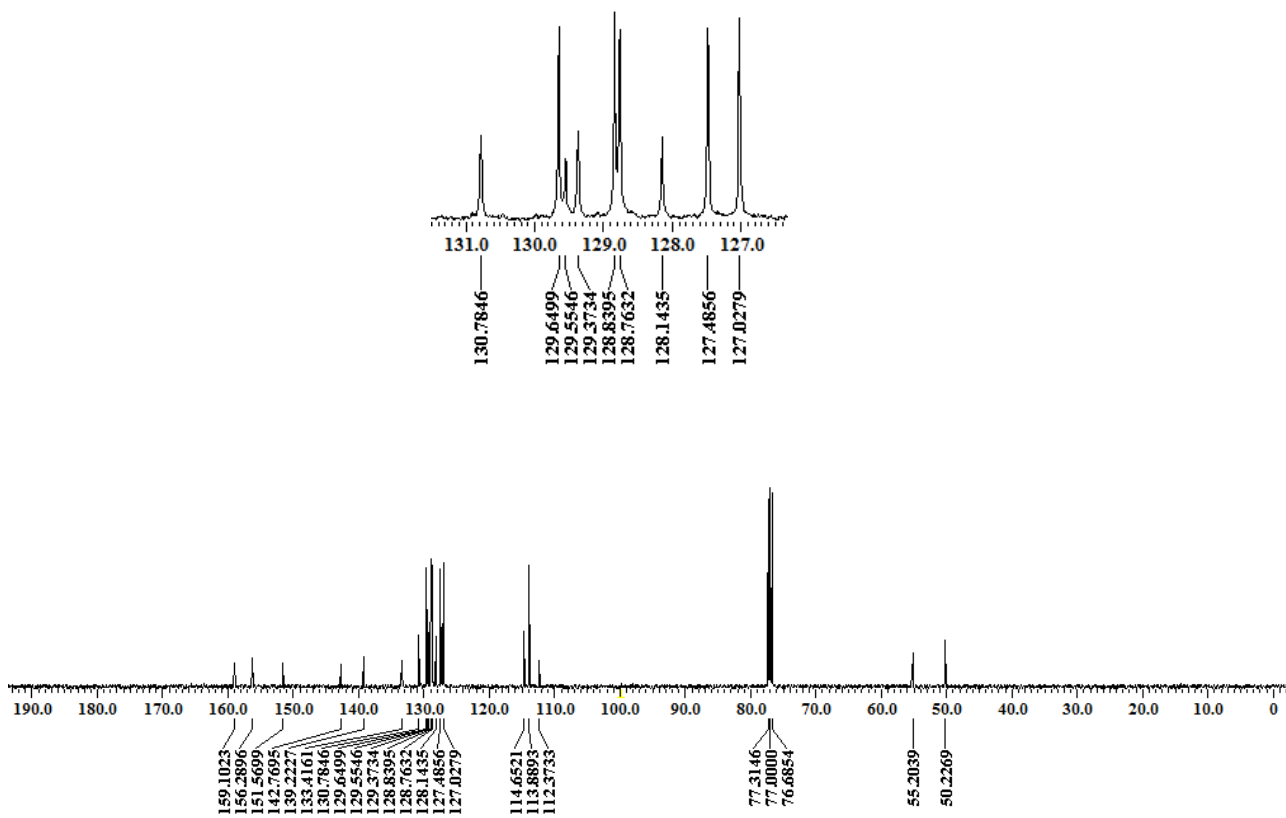


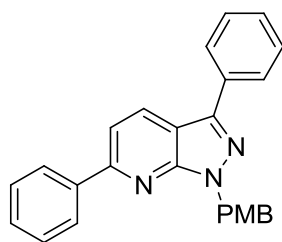
1-(4-methoxybenzyl)-3,6-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**4a**)



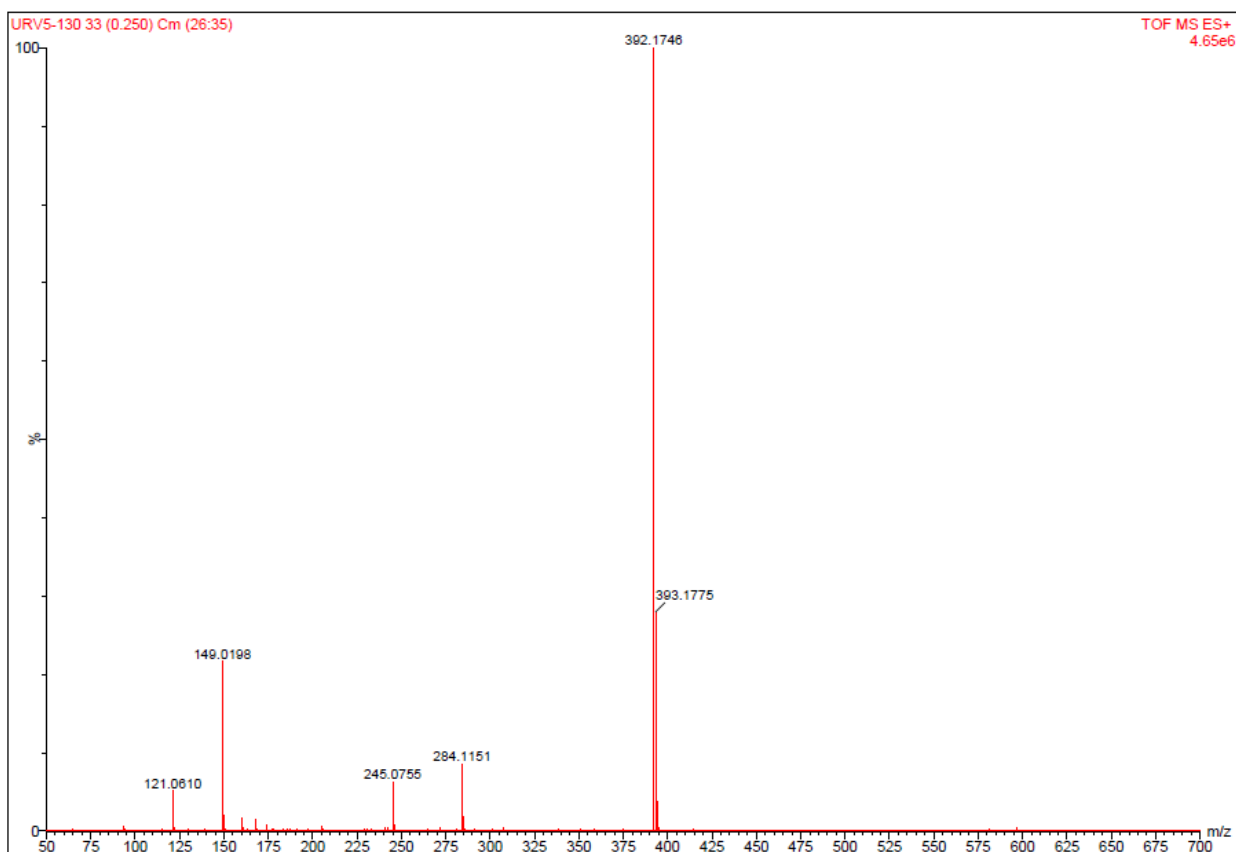


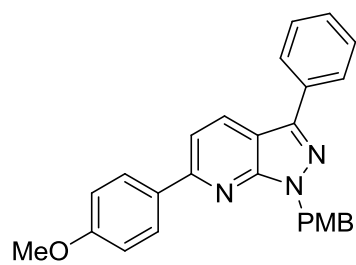
1-(4-methoxybenzyl)-3,6-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**4a**)



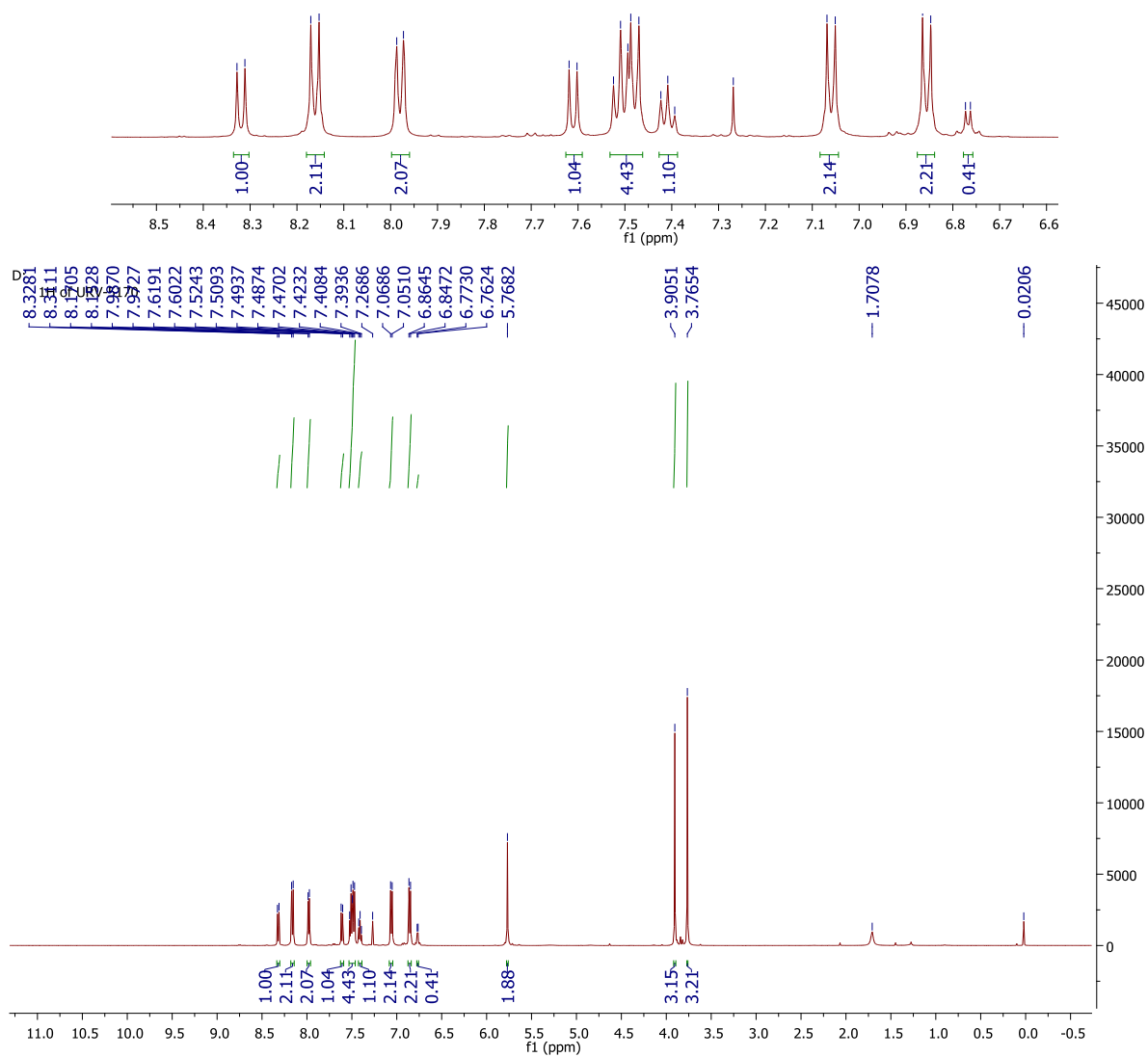


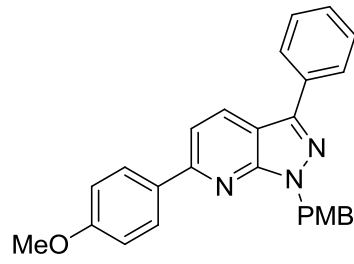
1-(4-methoxybenzyl)-3,6-diphenyl-1H-pyrazolo[3,4-b]pyridine (**4a**)



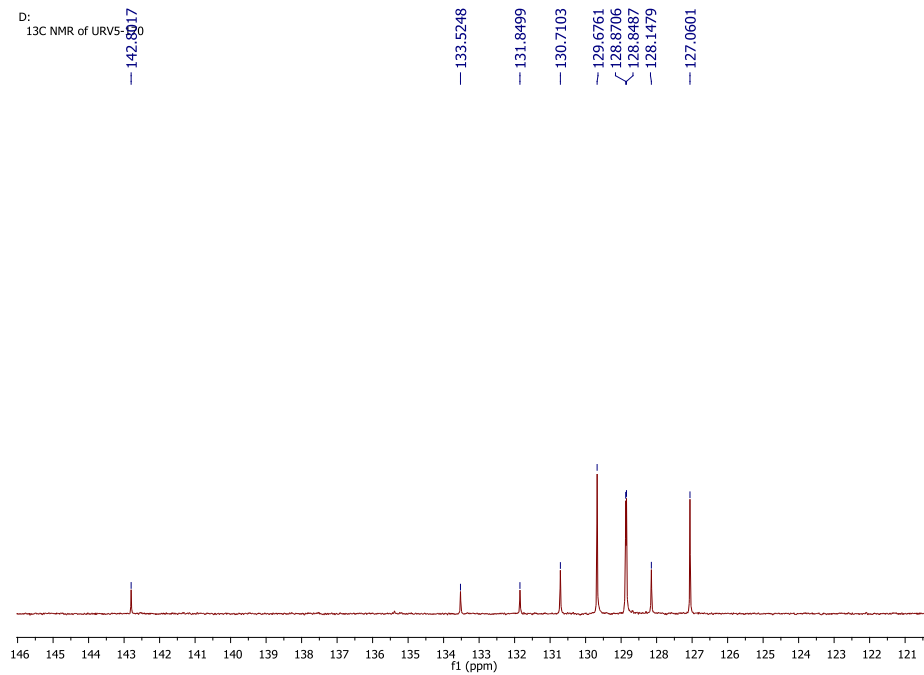
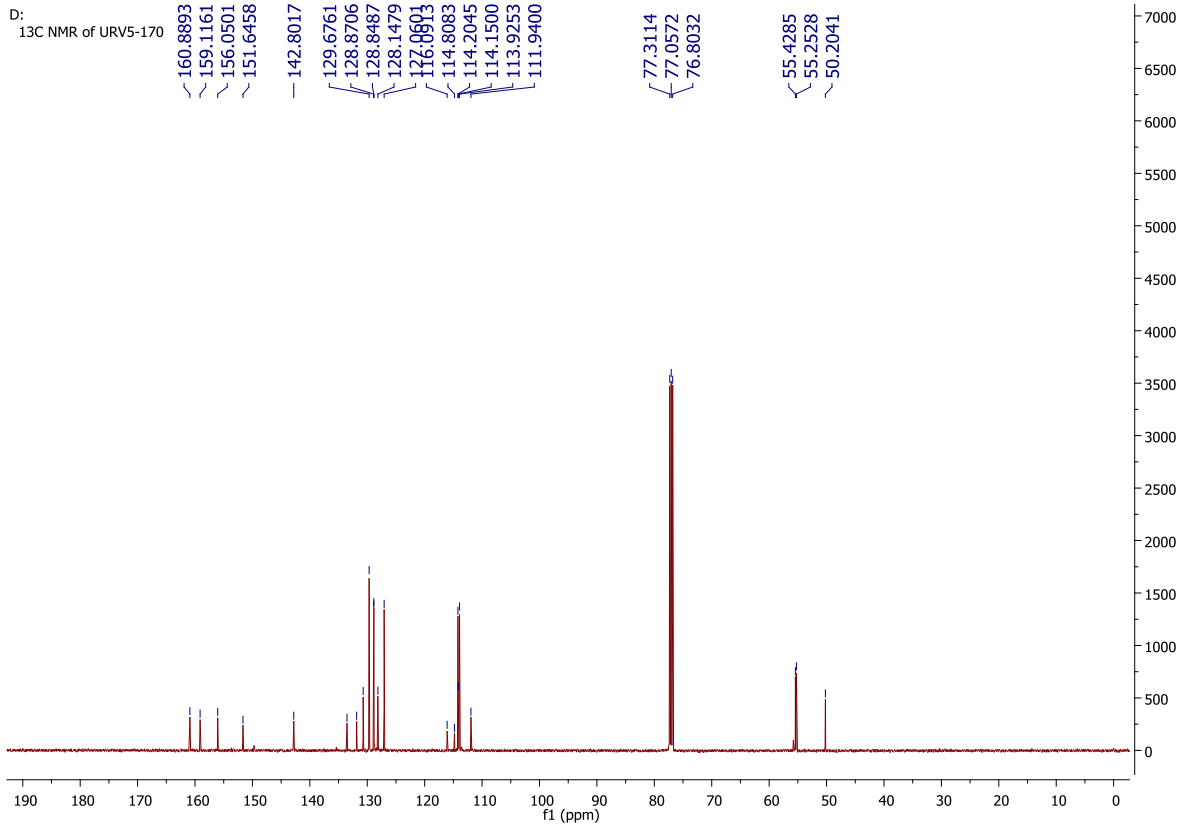


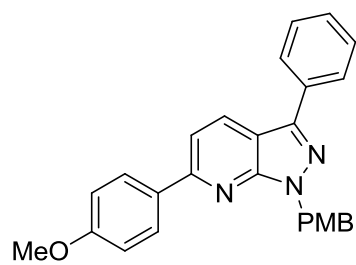
1-(4-methoxybenzyl)-6-(4-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**4b**)



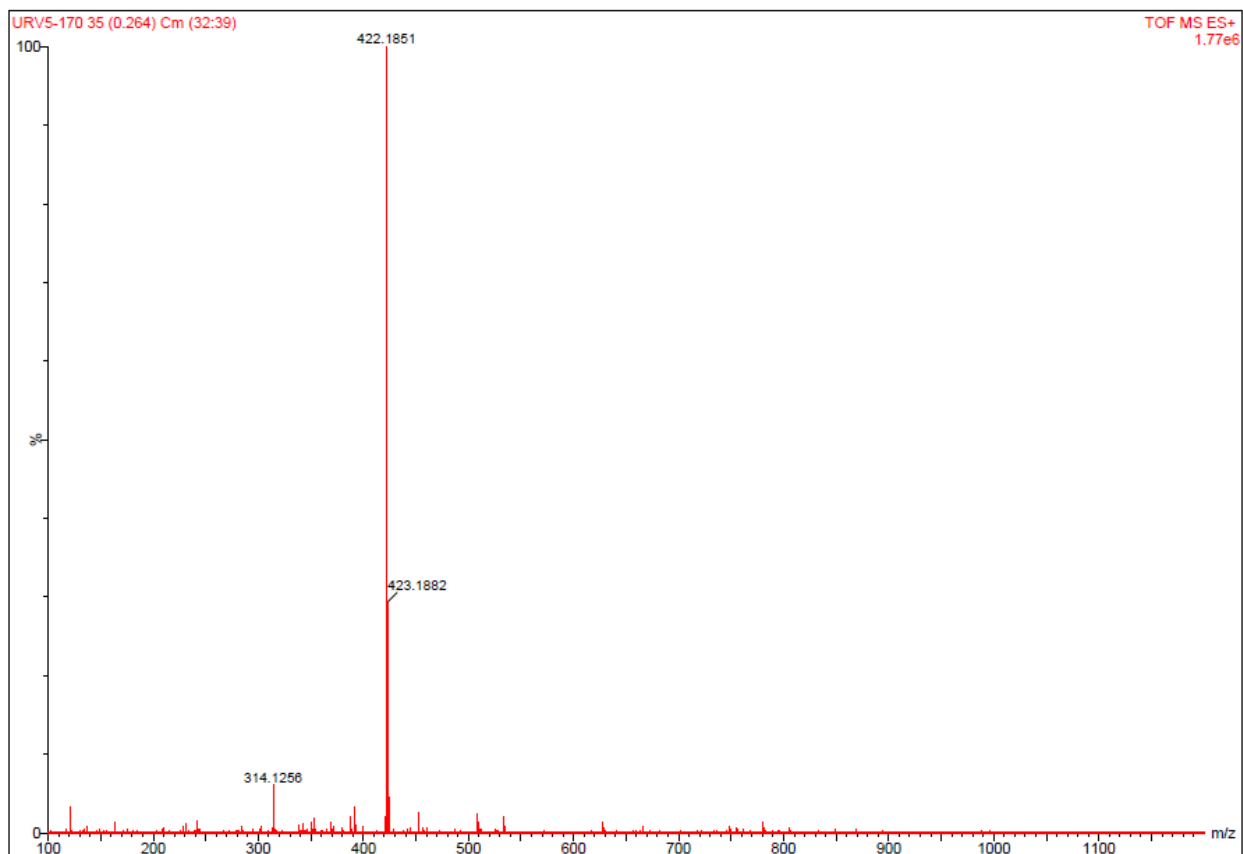


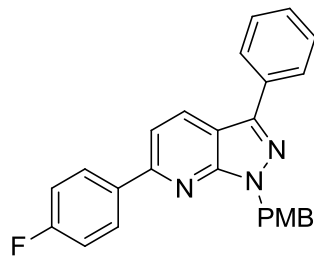
1-(4-methoxybenzyl)-6-(4-methoxyphenyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**4b**)



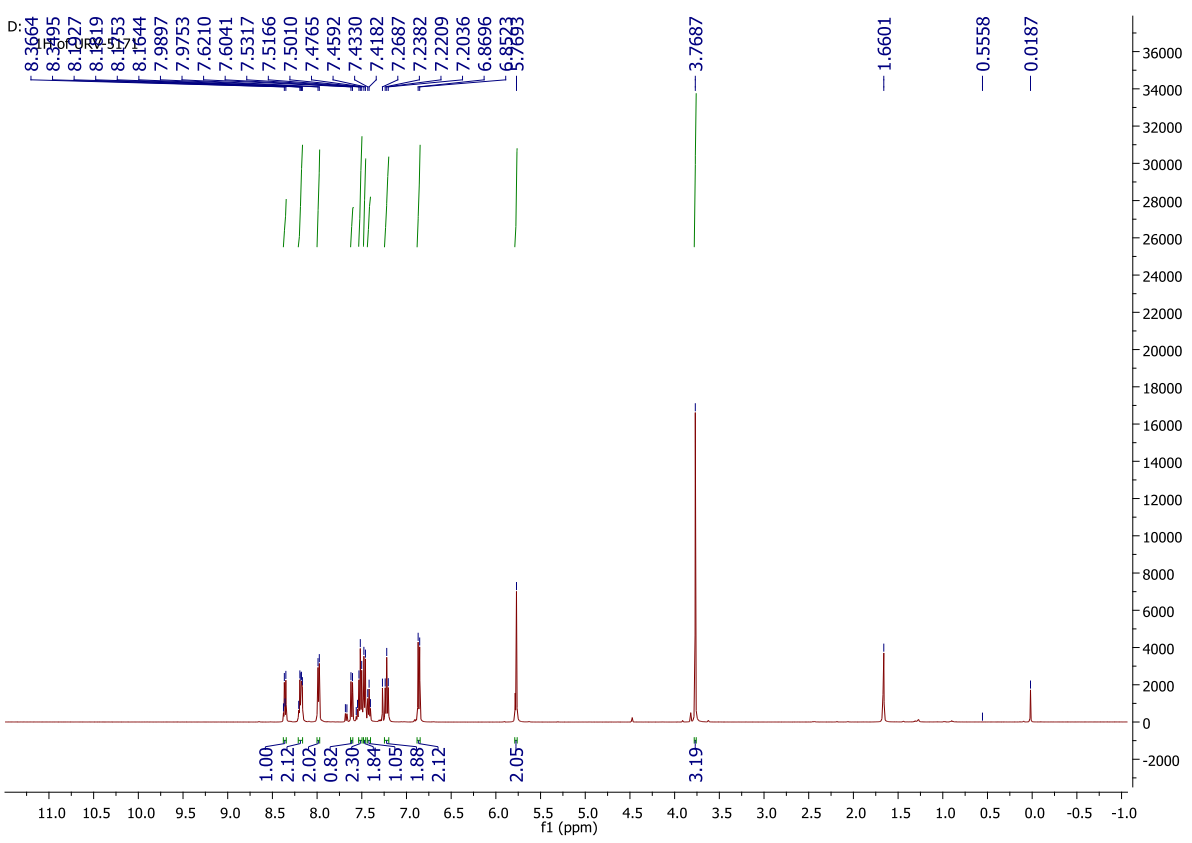
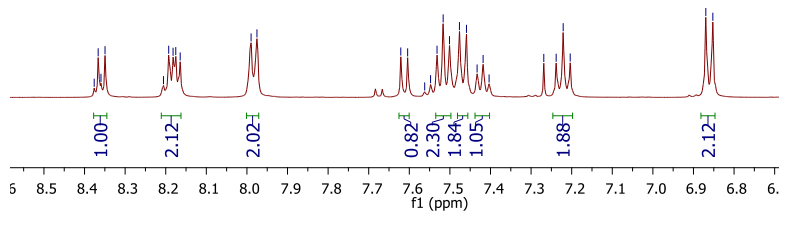


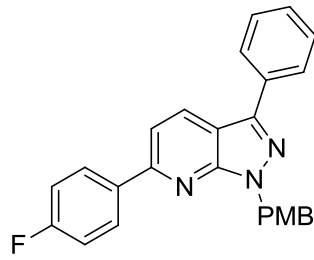
1-(4-methoxybenzyl)-6-(4-methoxyphenyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**4b**)



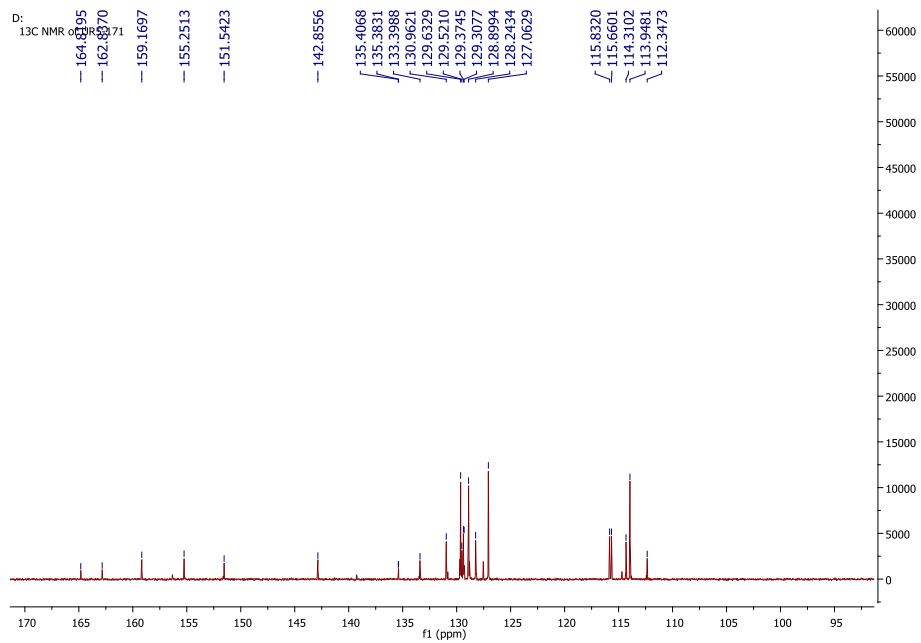
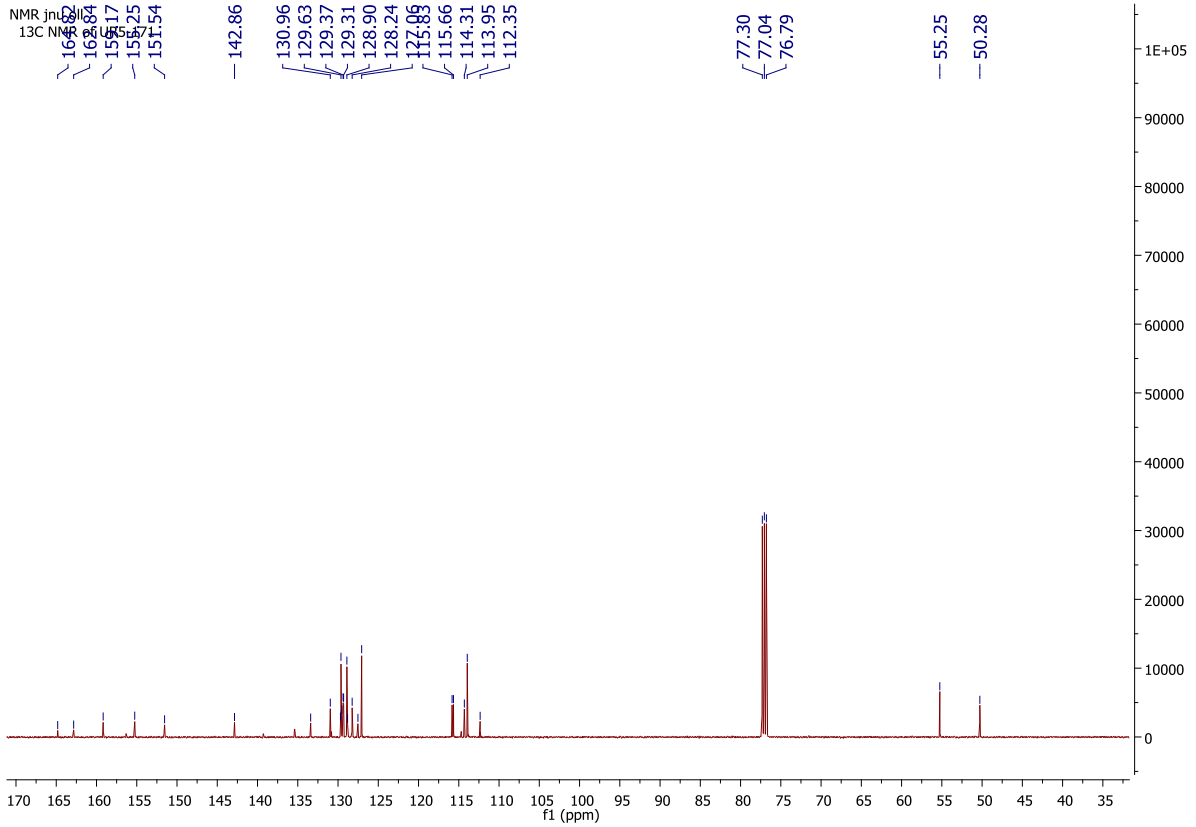


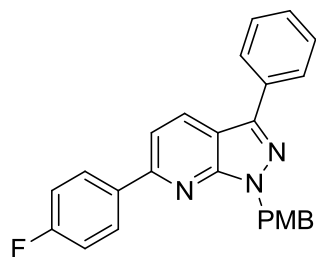
6-(4-fluorophenyl)-1-(4-methoxybenzyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**4c**)



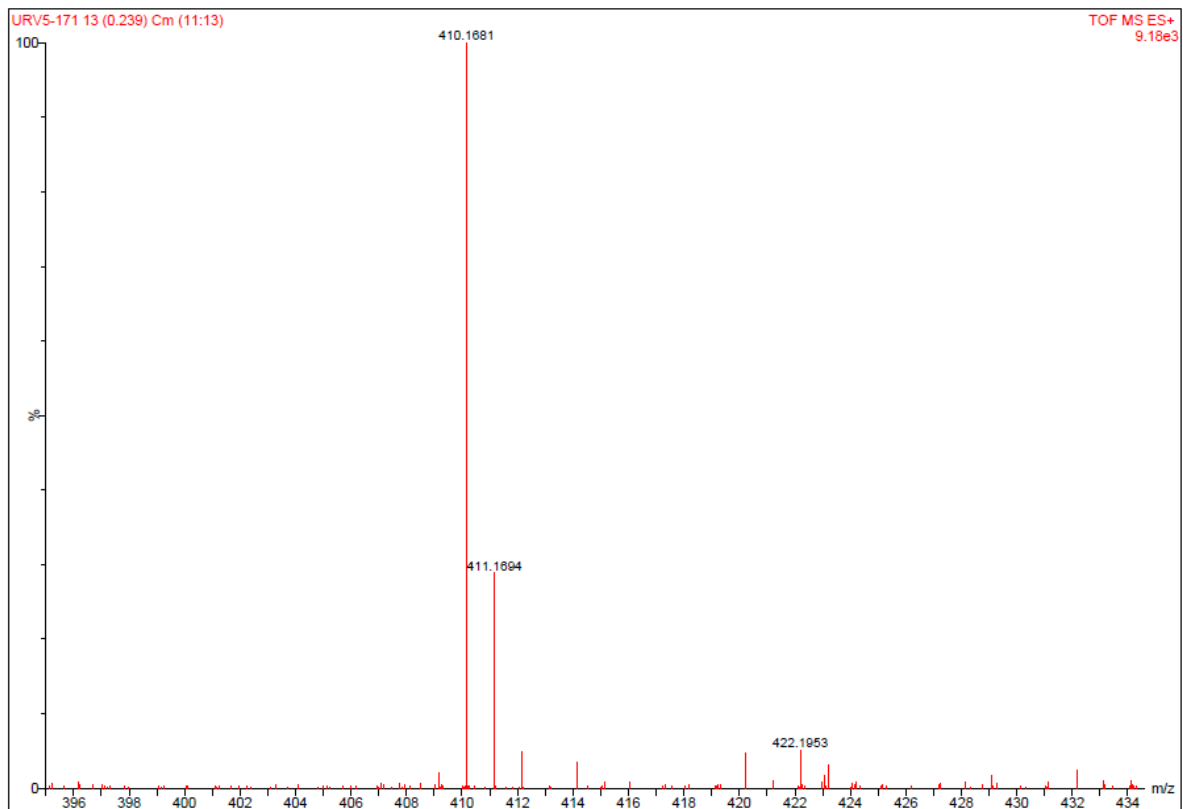


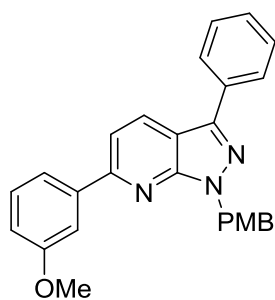
6-(4-fluorophenyl)-1-(4-methoxybenzyl)-3-phenyl-1H-pyrazolo[3,4-*b*]pyridine (**4c**)



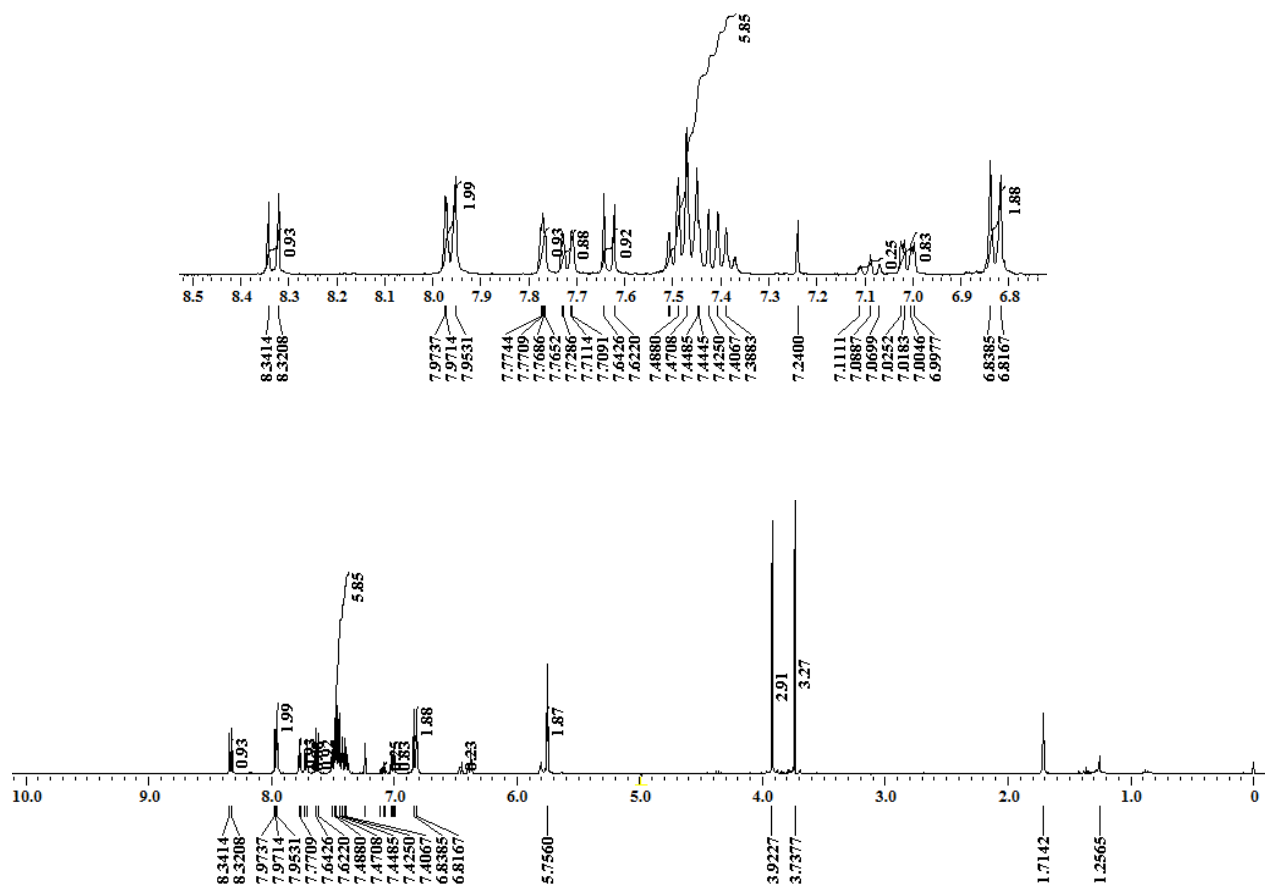


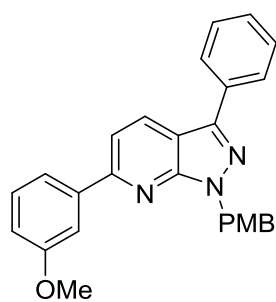
6-(4-fluorophenyl)-1-(4-methoxybenzyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**4c**)



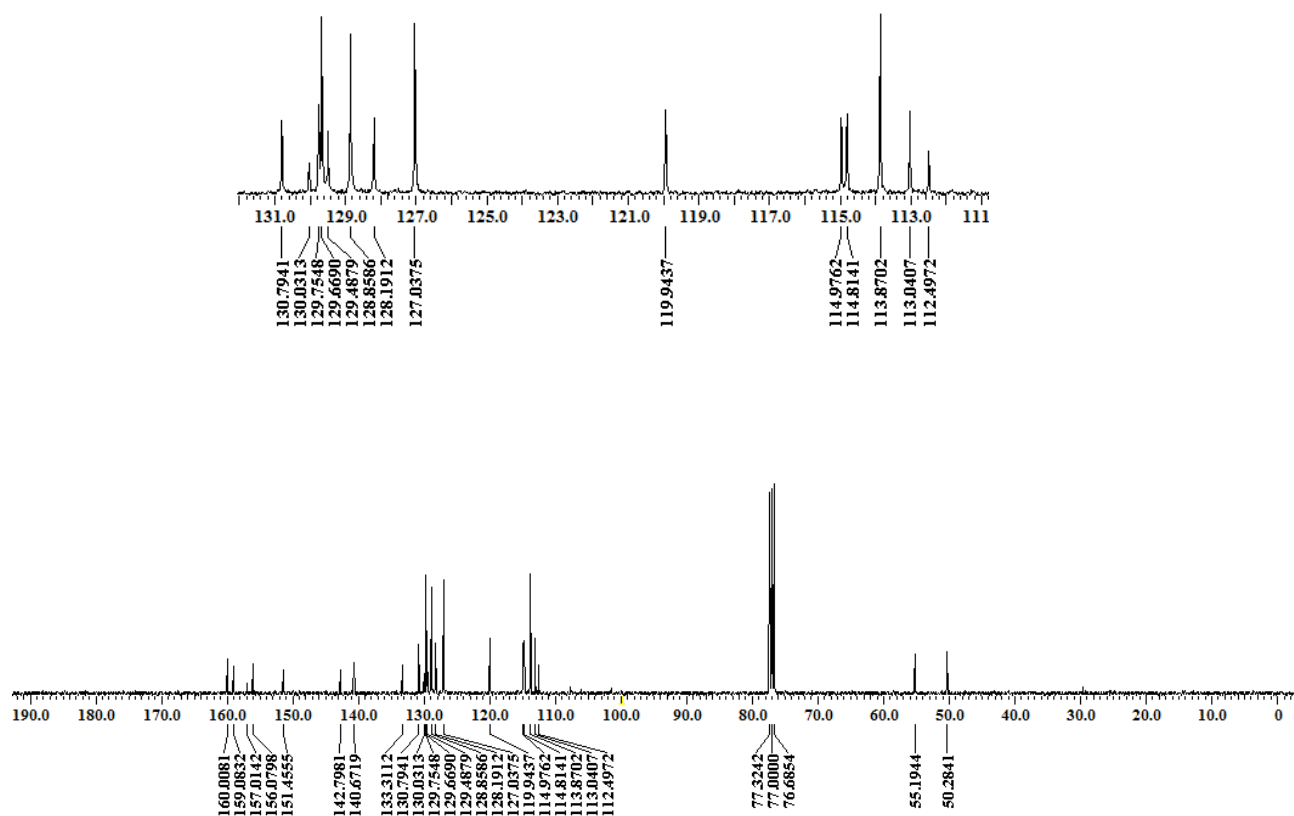


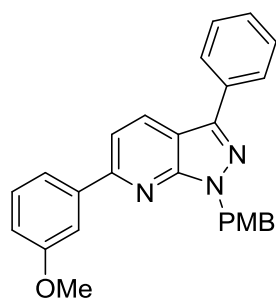
1-(4-methoxybenzyl)-6-(3-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**4d**)



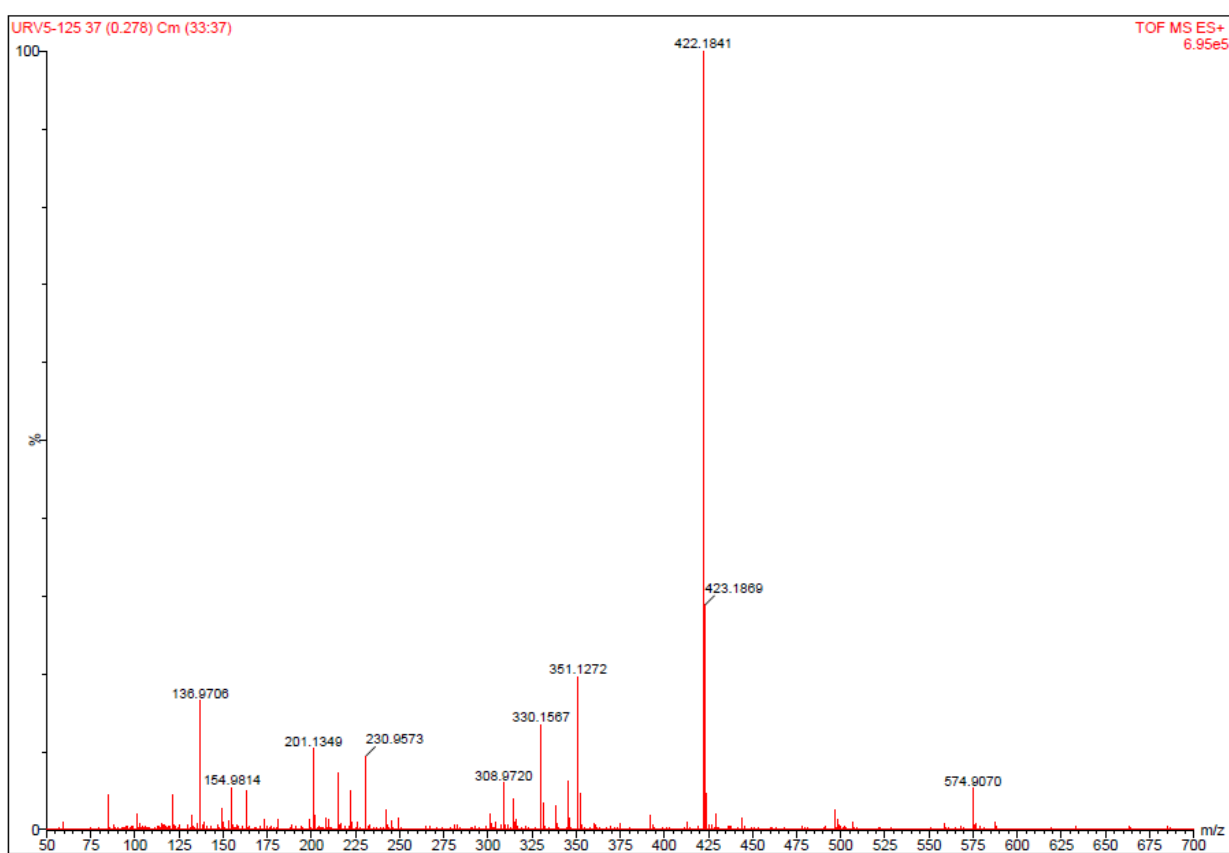


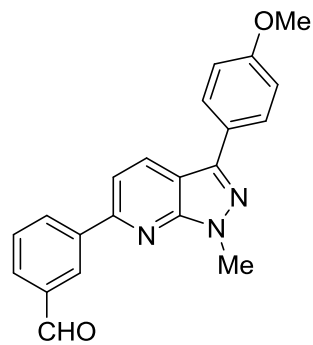
1-(4-methoxybenzyl)-6-(3-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**4d**)



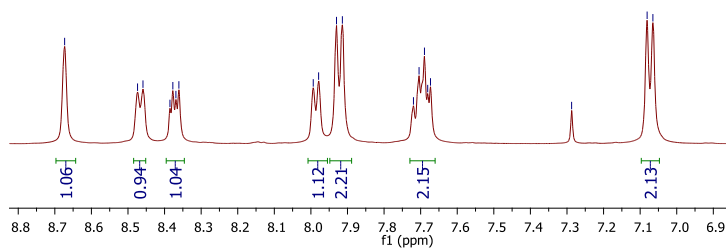


1-(4-methoxybenzyl)-6-(3-methoxyphenyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**4d**)

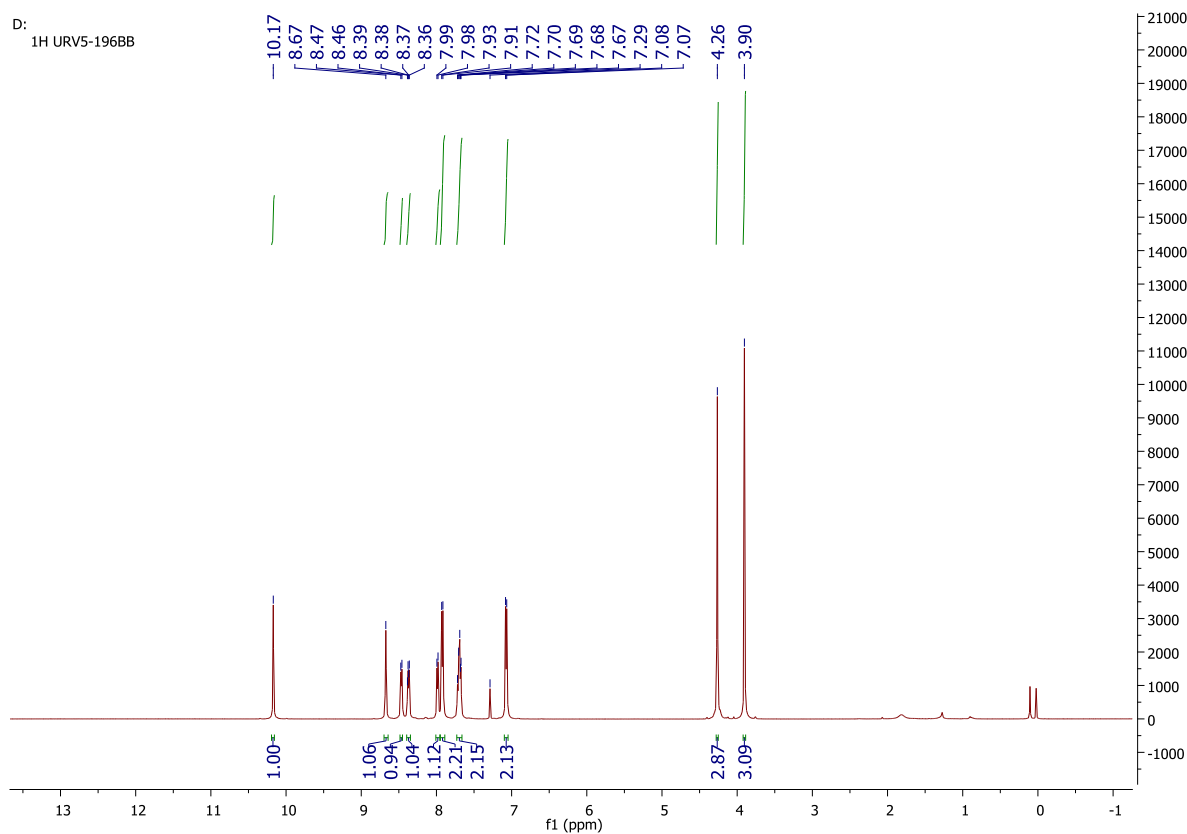


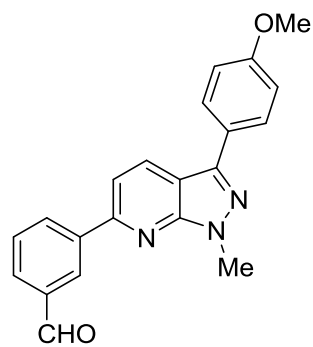


3-(3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridin-6-yl)benzaldehyde (**4e**)

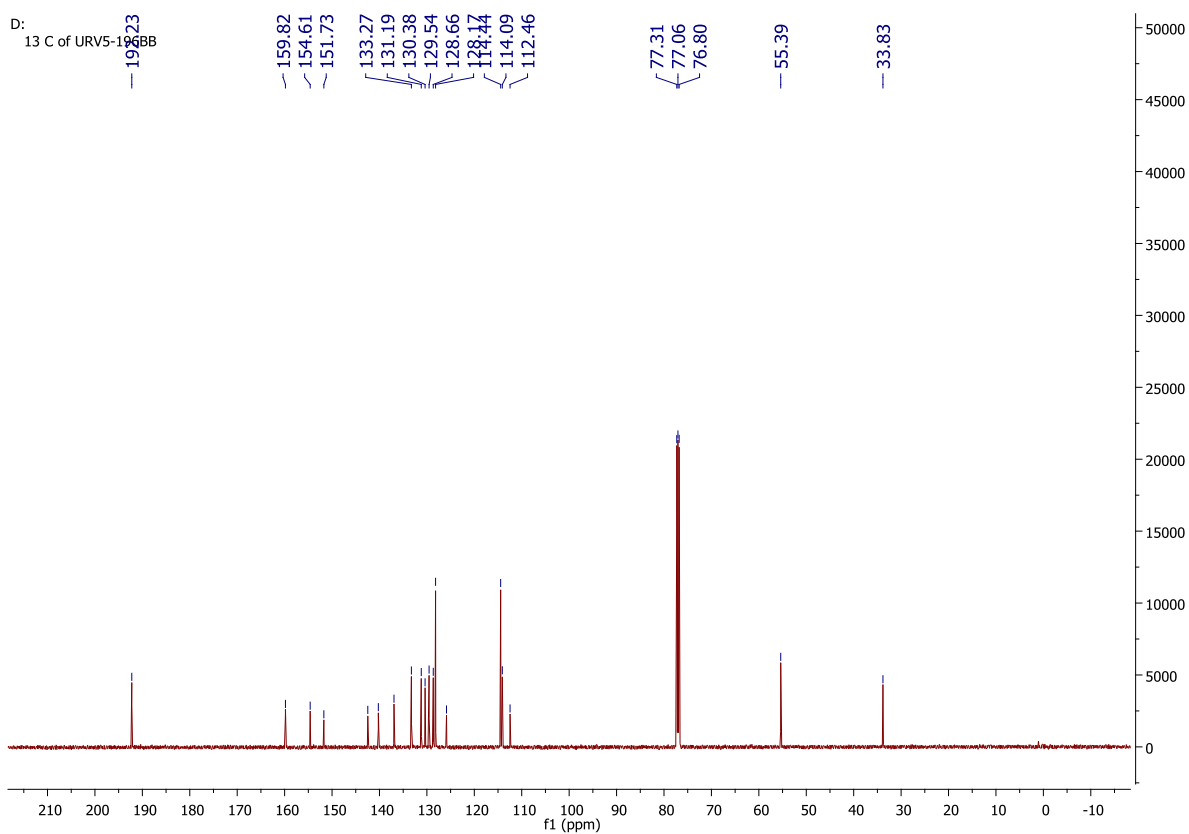
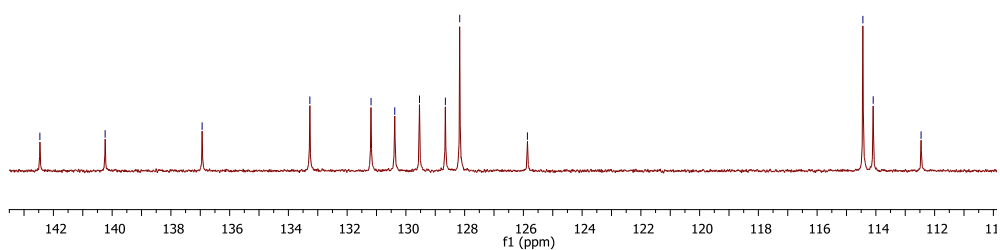


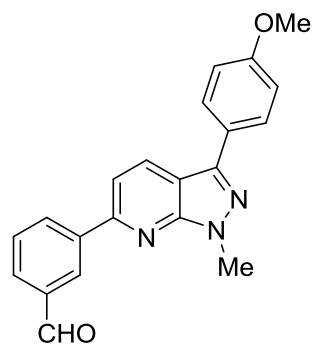
D:
1H URV5-196BB



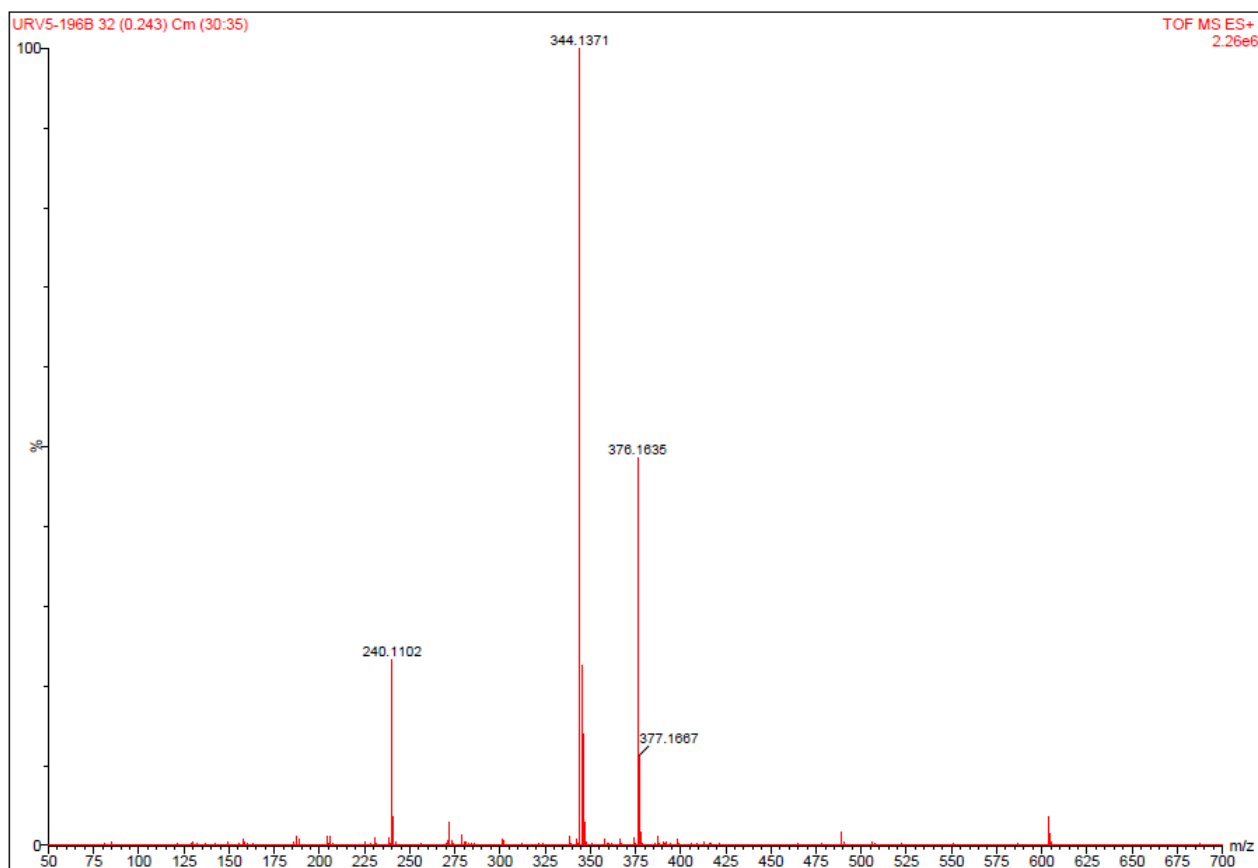


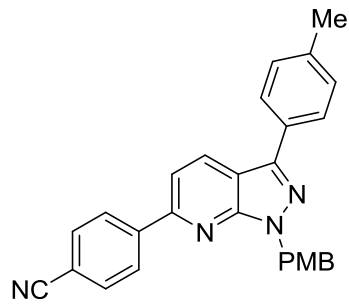
3-(3-(4-methoxyphenyl)-1-methyl-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzaldehyde(**4e**)



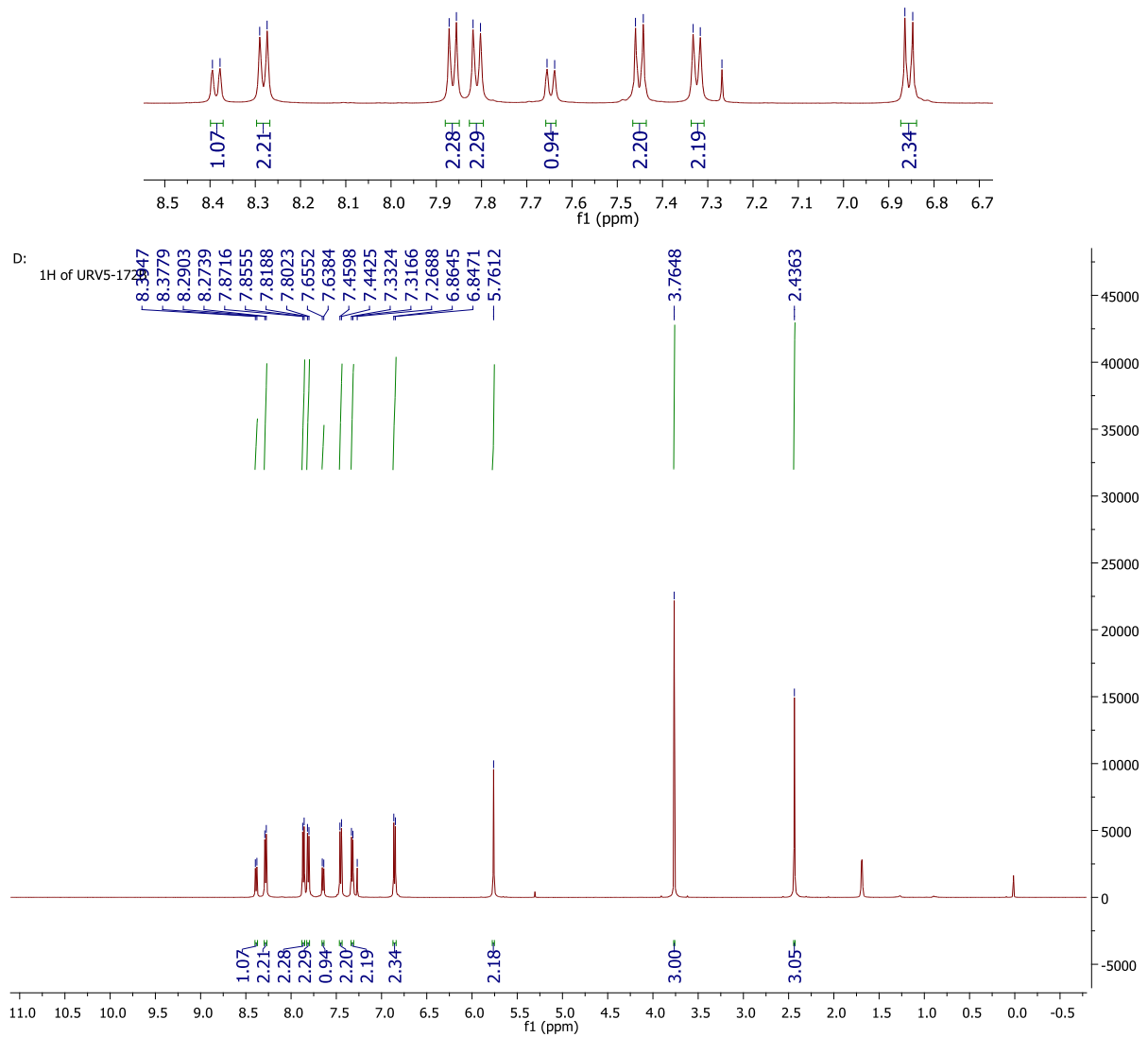


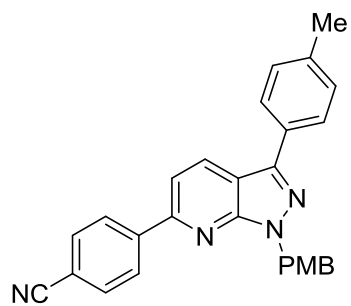
3-(3-(4-methoxyphenyl)-1-methyl-1H-pyrazolo[3,4-b]pyridin-6-yl)benzaldehyde(4e)



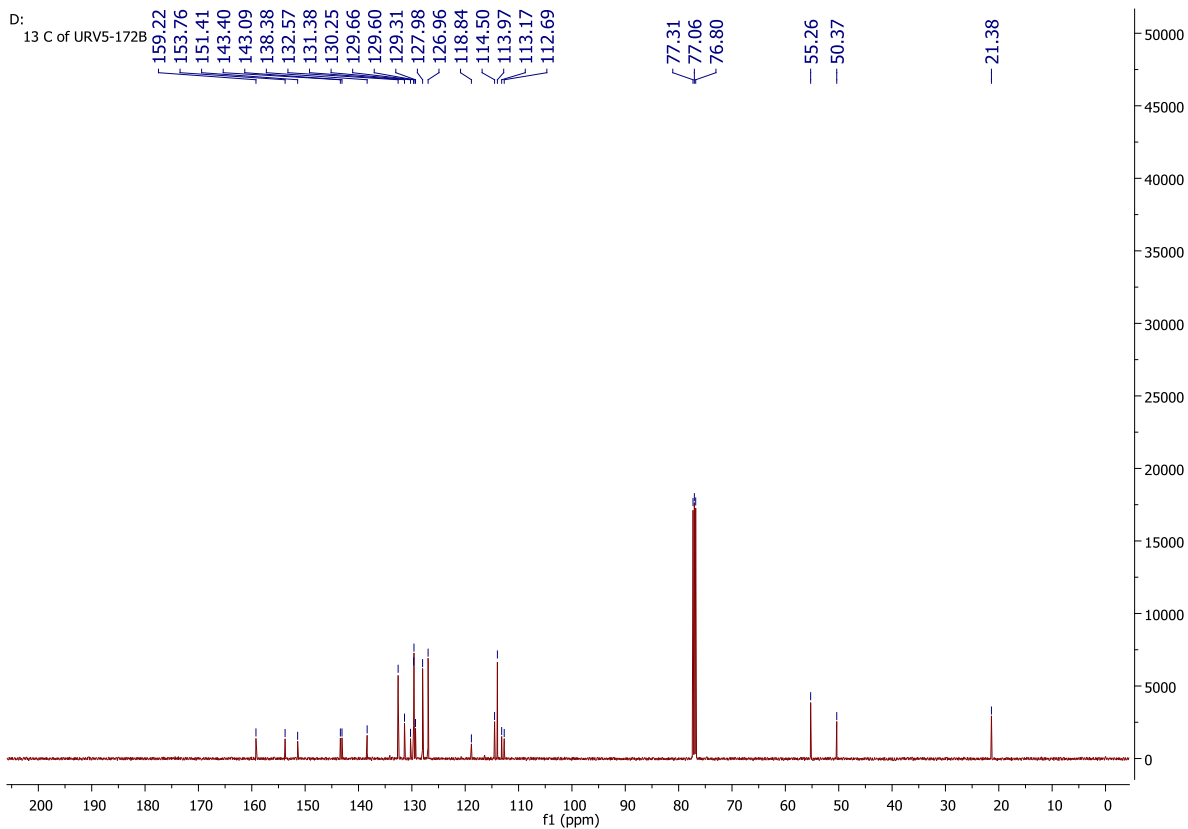
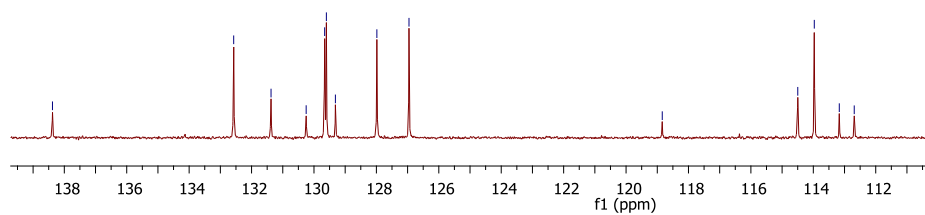


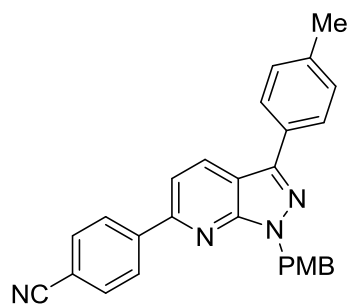
4-(1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzonitrile (**4f**)



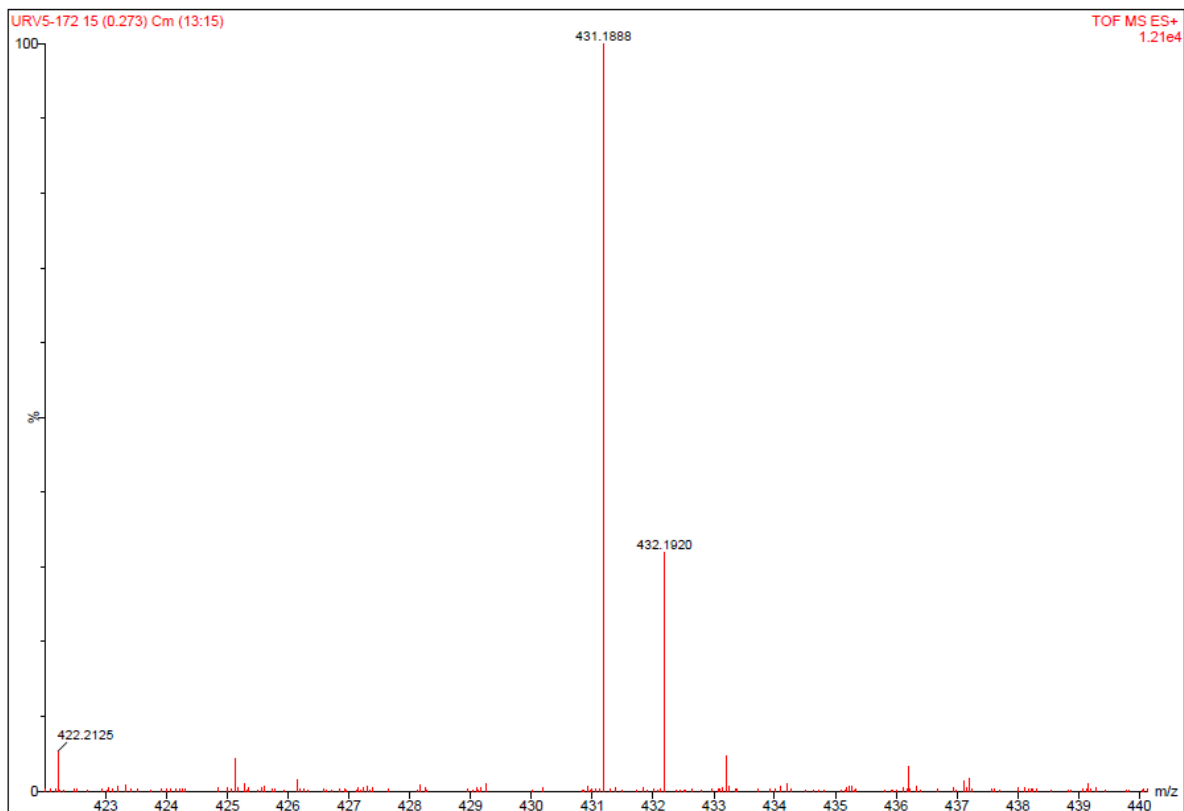


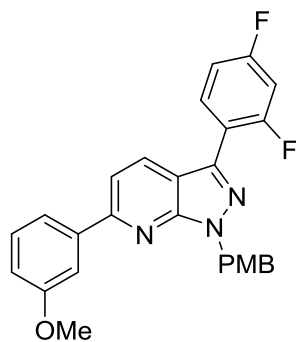
4-(1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzonitrile (**4f**)



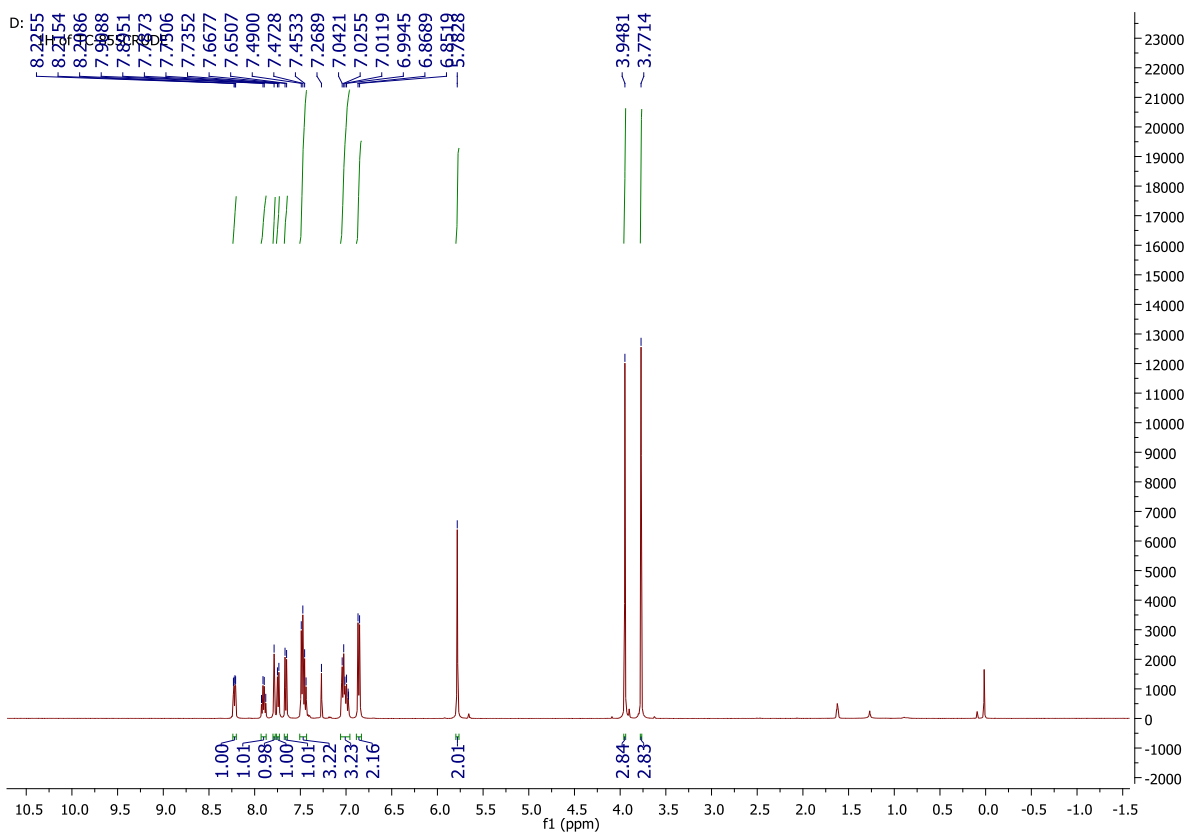
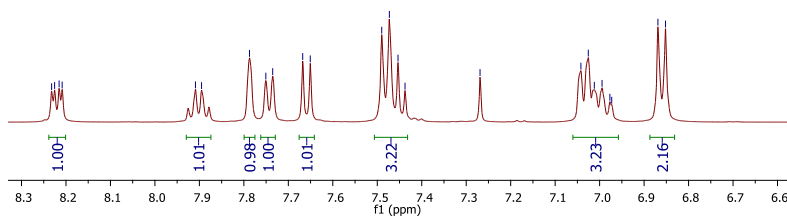


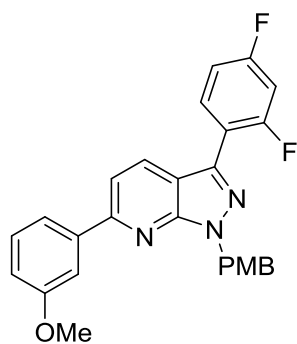
4-(1-(4-methoxybenzyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)benzonitrile (**4f**)



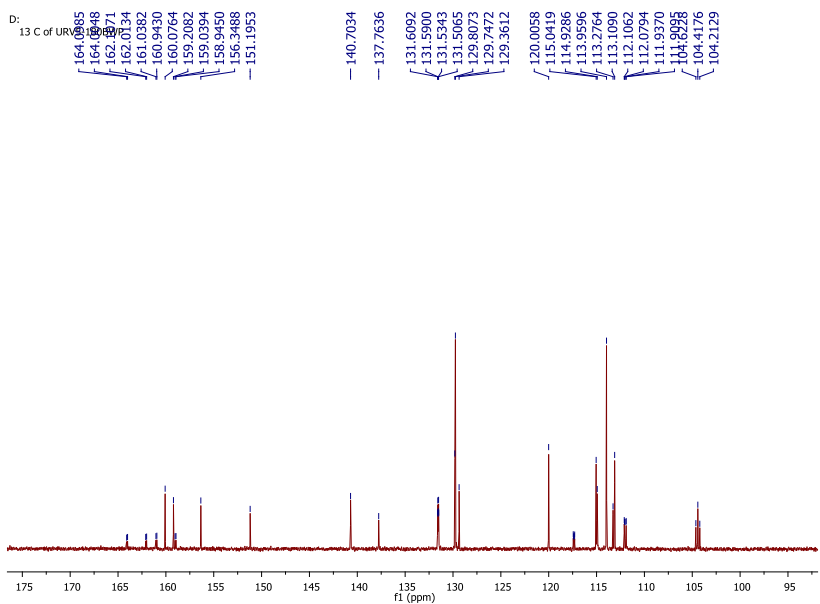
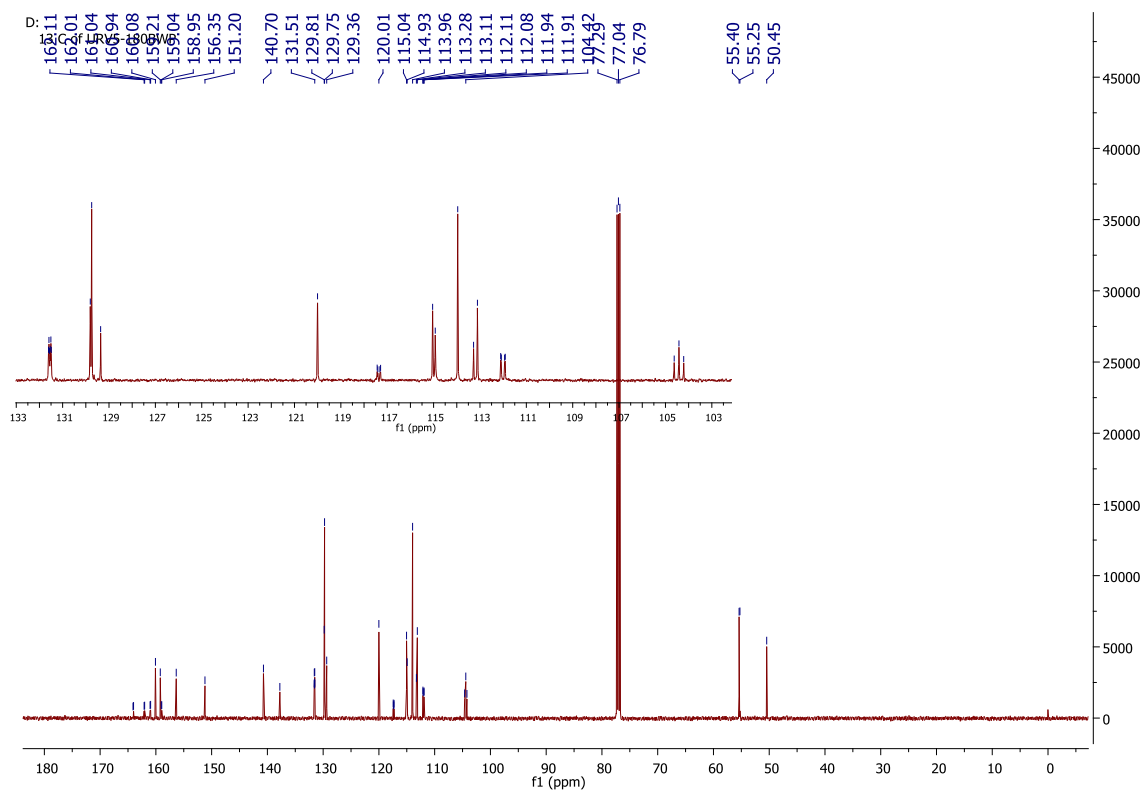


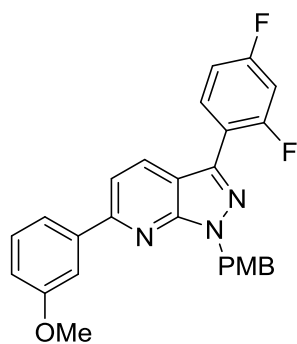
3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-6-(3-methoxyphenyl)-1H-pyrazolo[3,4-b]pyridine (**4g**)



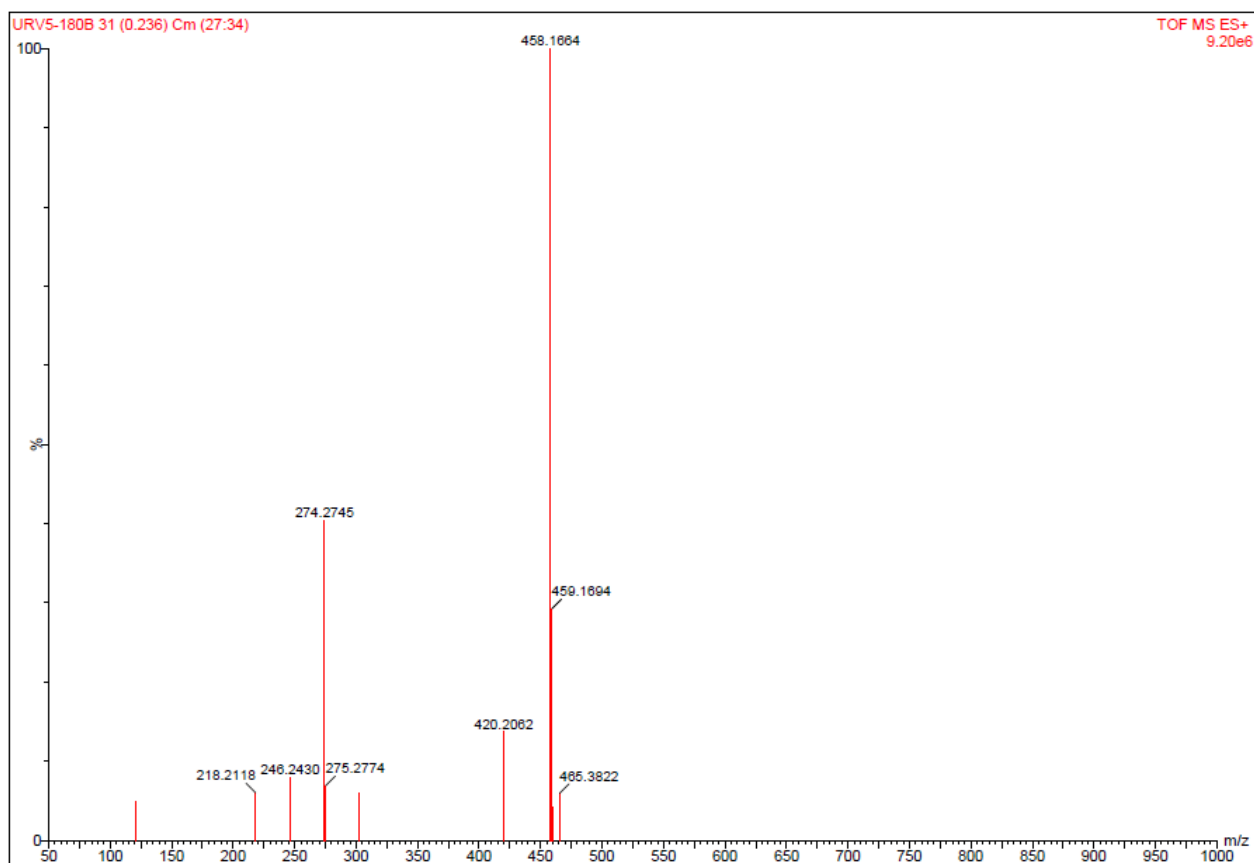


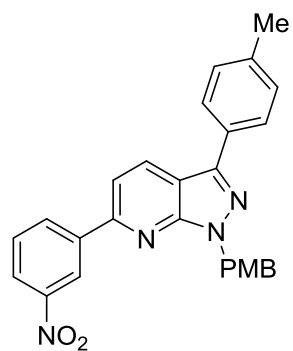
3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-6-(3-methoxyphenyl)-1H-pyrazolo[3,4-b]pyridine (**4g**)



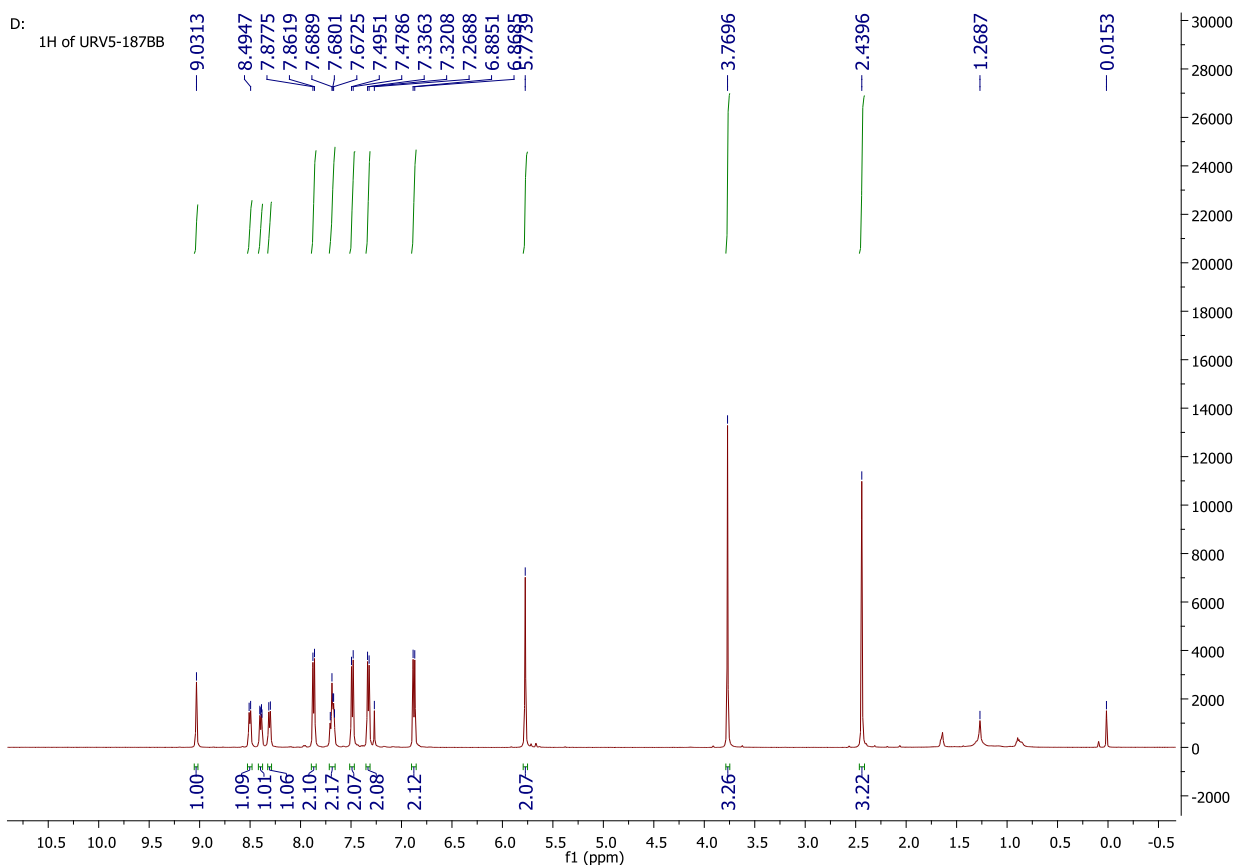
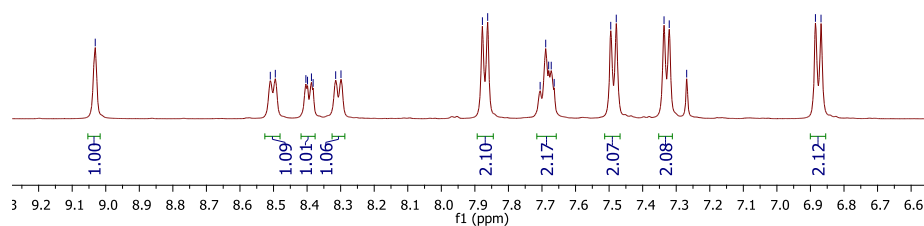


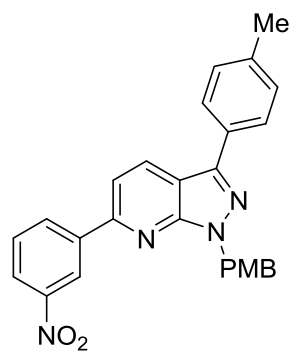
3-(2,4-difluorophenyl)-1-(4-methoxybenzyl)-6-(3-methoxyphenyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4g**)



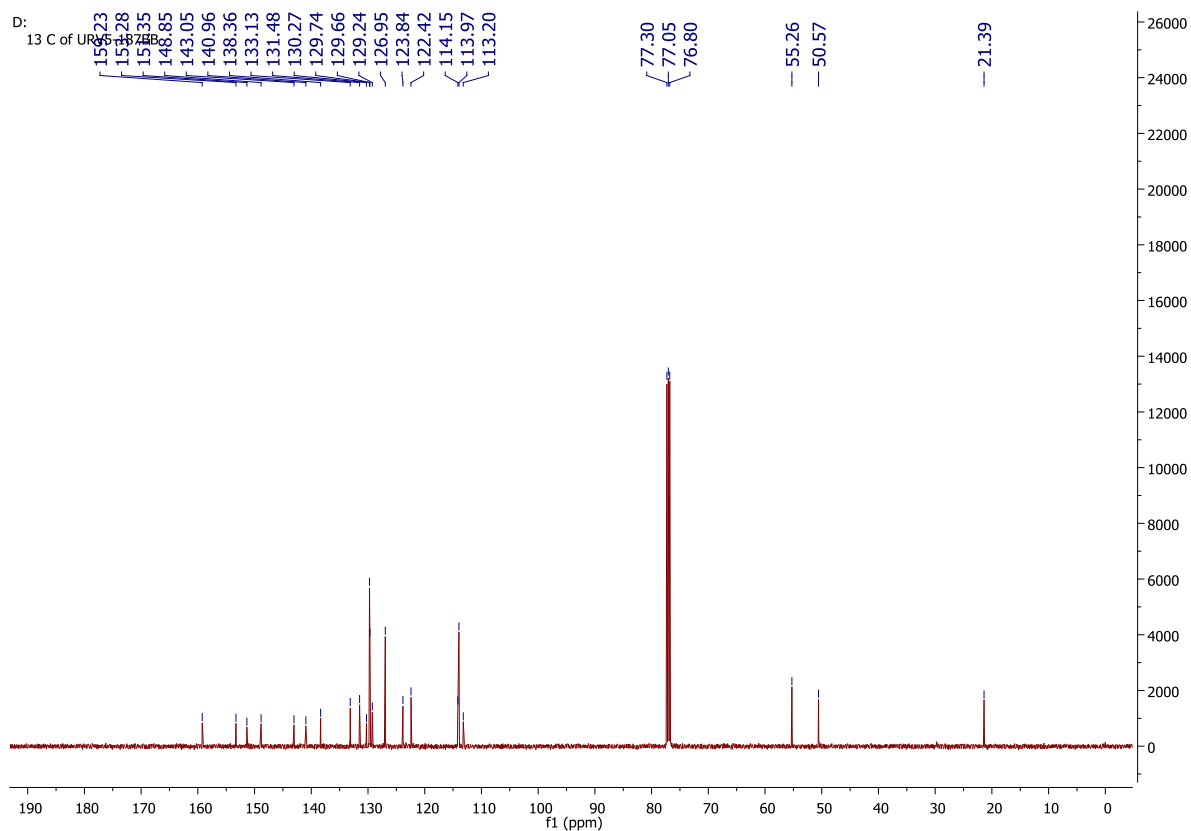
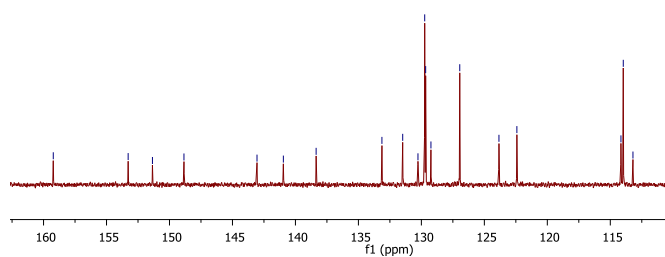


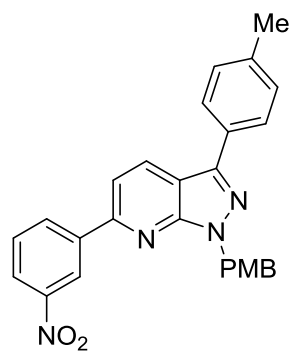
1-(4-methoxybenzyl)-6-(3-nitrophenyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4h**)



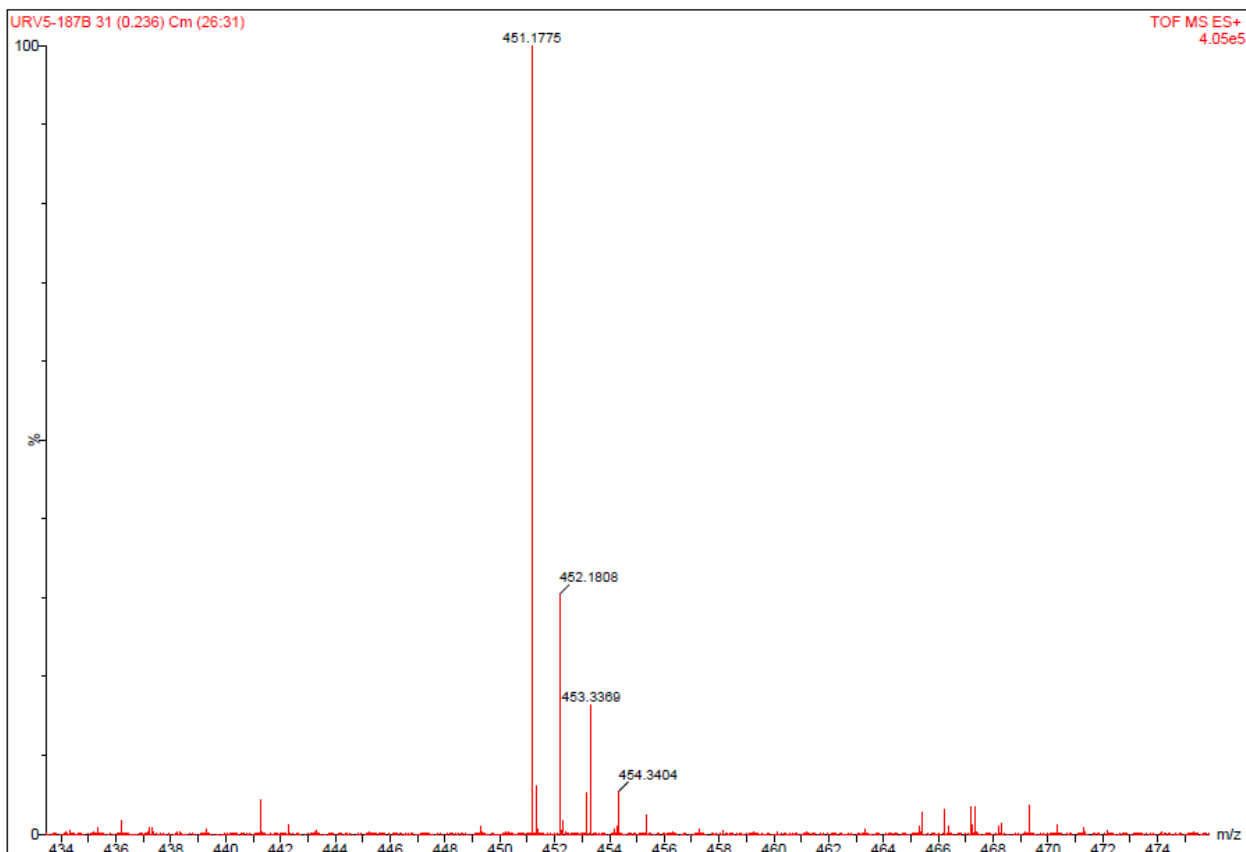


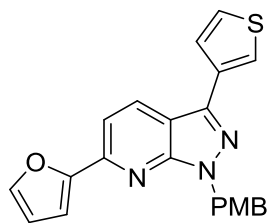
1-(4-methoxybenzyl)-6-(3-nitrophenyl)-3-(*p*-tolyl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4h**)



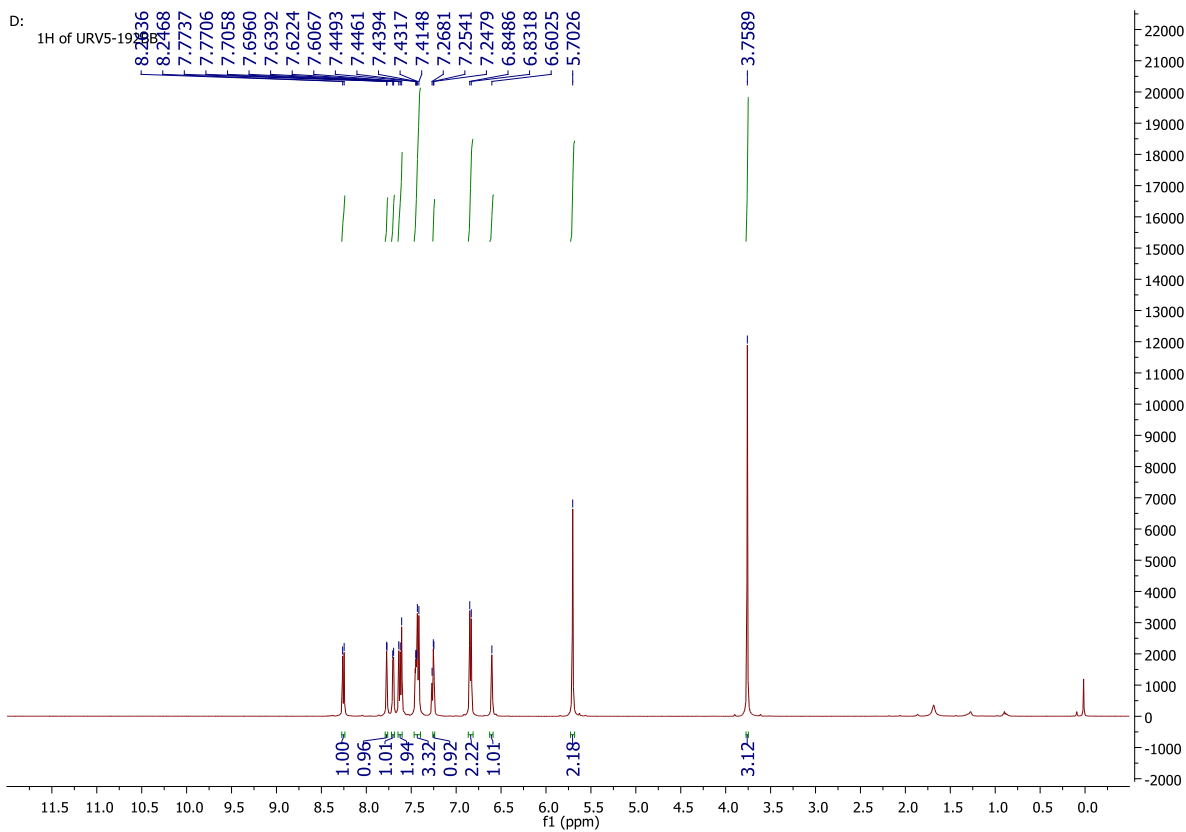
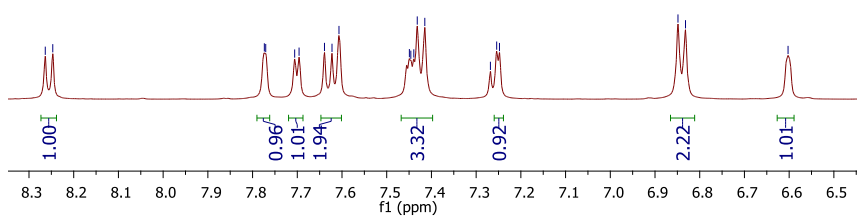


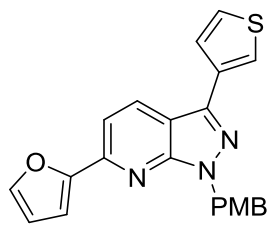
1-(4-methoxybenzyl)-6-(3-nitrophenyl)-3-(p-tolyl)-1H-pyrazolo[3,4-b]pyridine (**4h**)



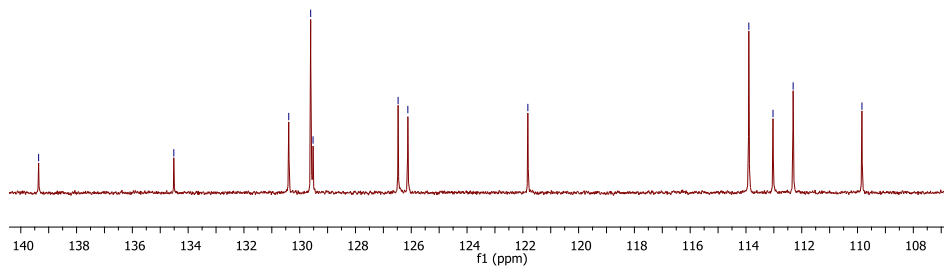


6-(furan-2-yl)-1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1H-pyrazolo[3,4-b]pyridine (**4i**)

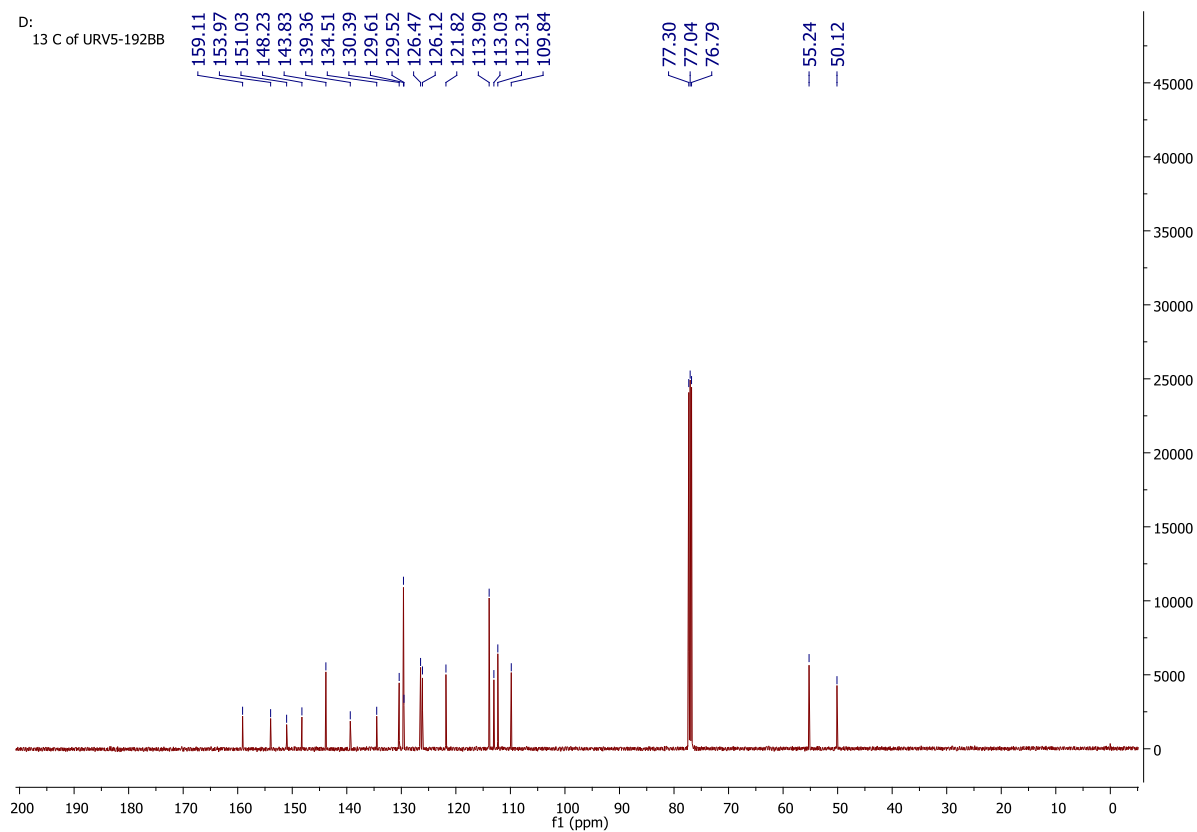


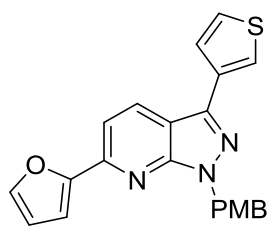


6-(furan-2-yl)-1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4i**)



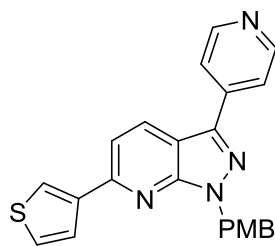
D:
13 C of URV5-192BB



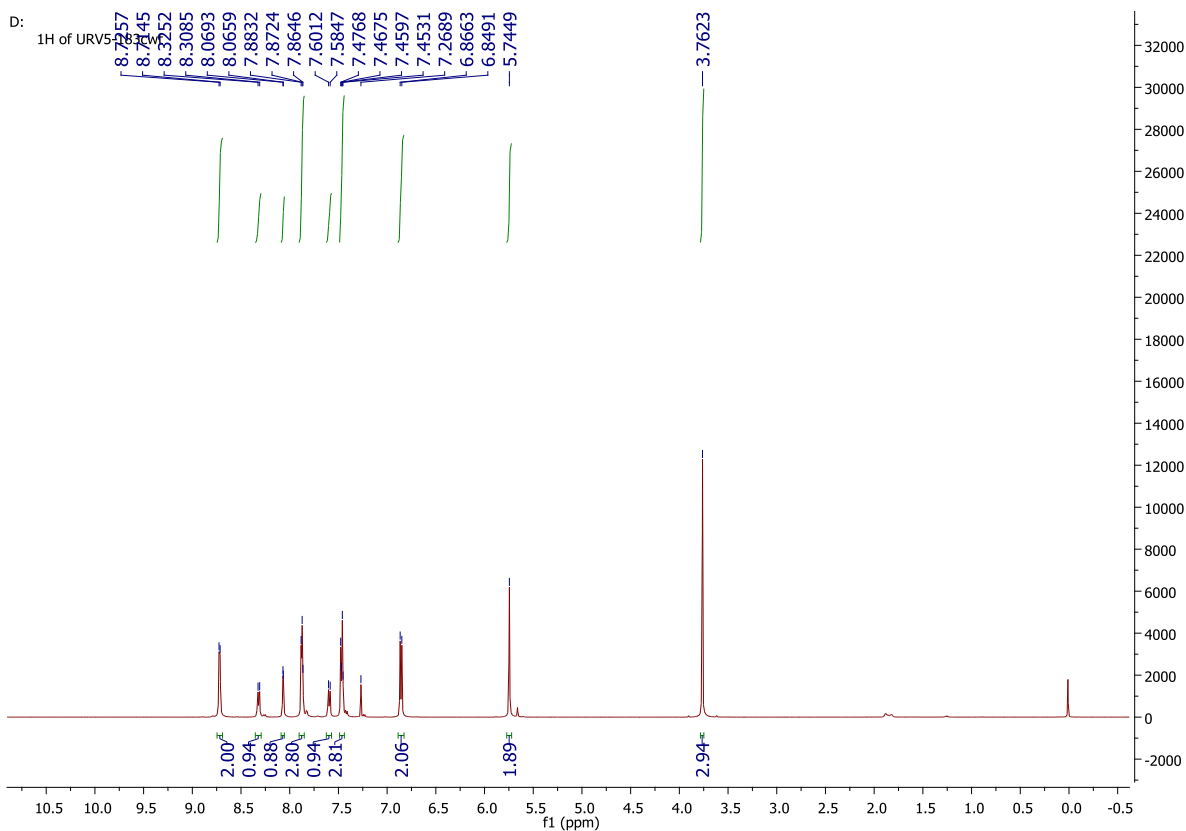
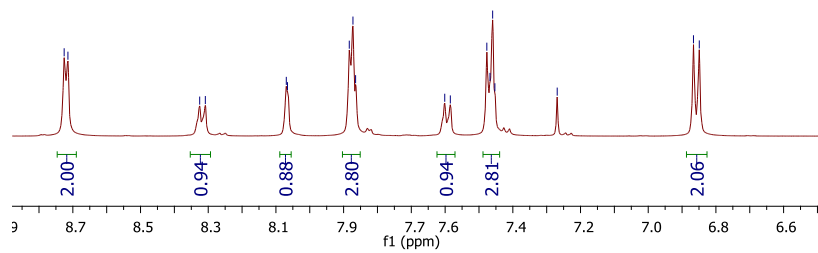


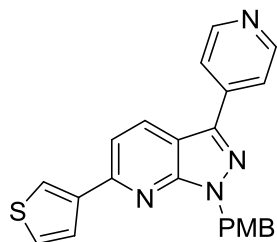
6-(furan-2-yl)-1-(4-methoxybenzyl)-3-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4i**)



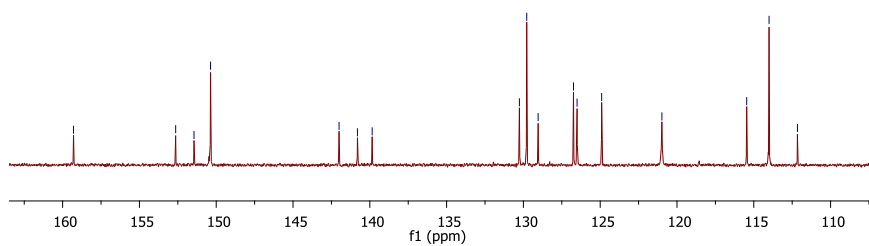


1-(4-methoxybenzyl)-3-(pyridin-4-yl)-6-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4j**)

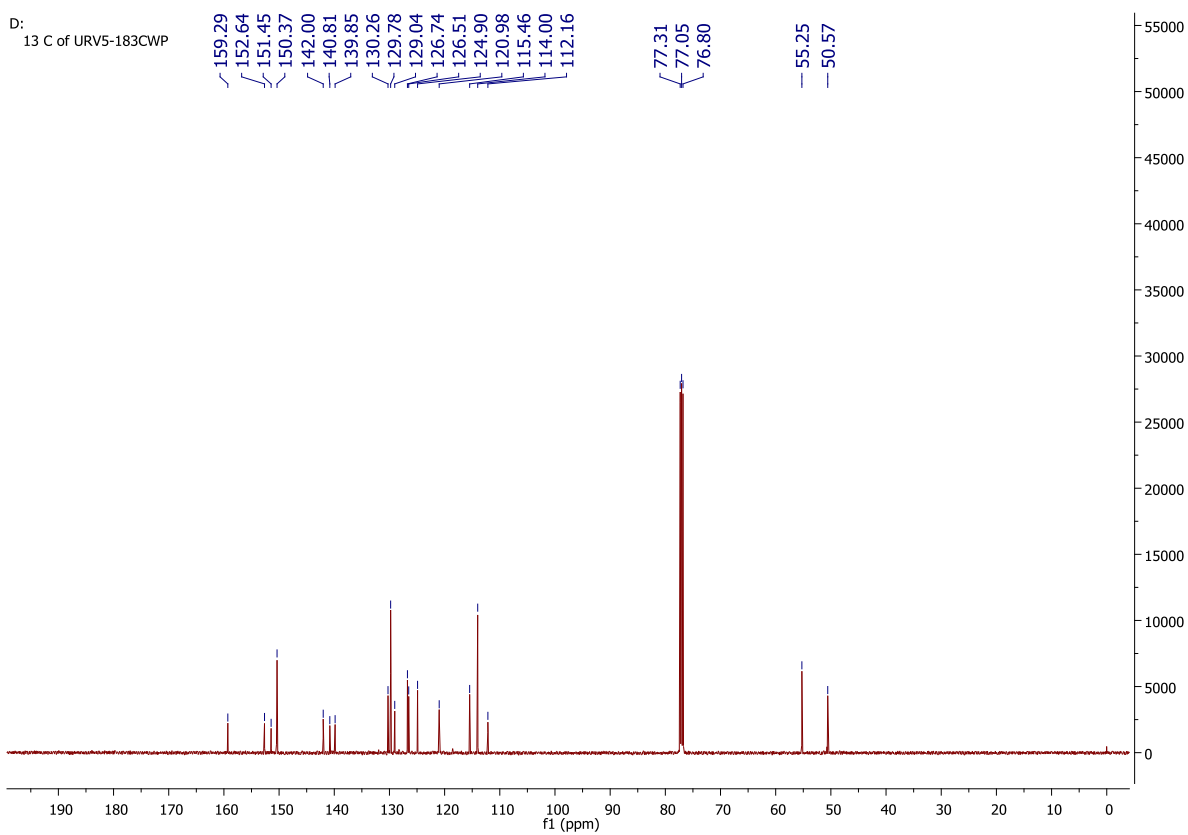


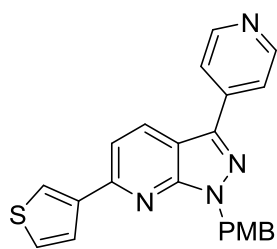


1-(4-methoxybenzyl)-3-(pyridin-4-yl)-6-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4j**)

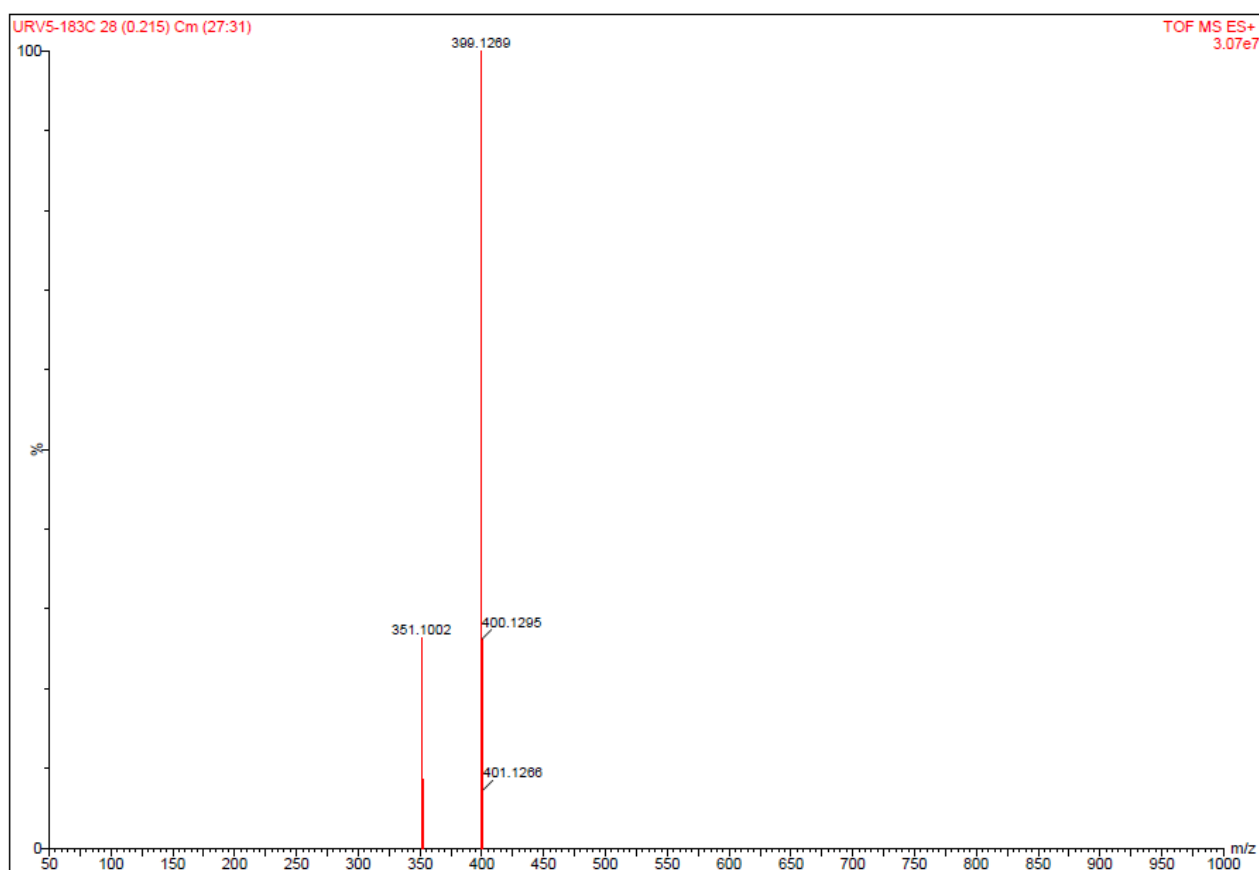


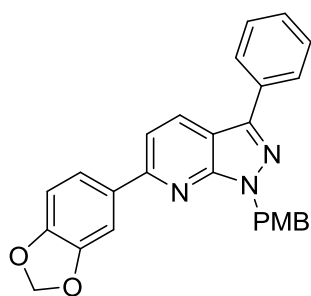
D:
13 C of URV5-183CWP



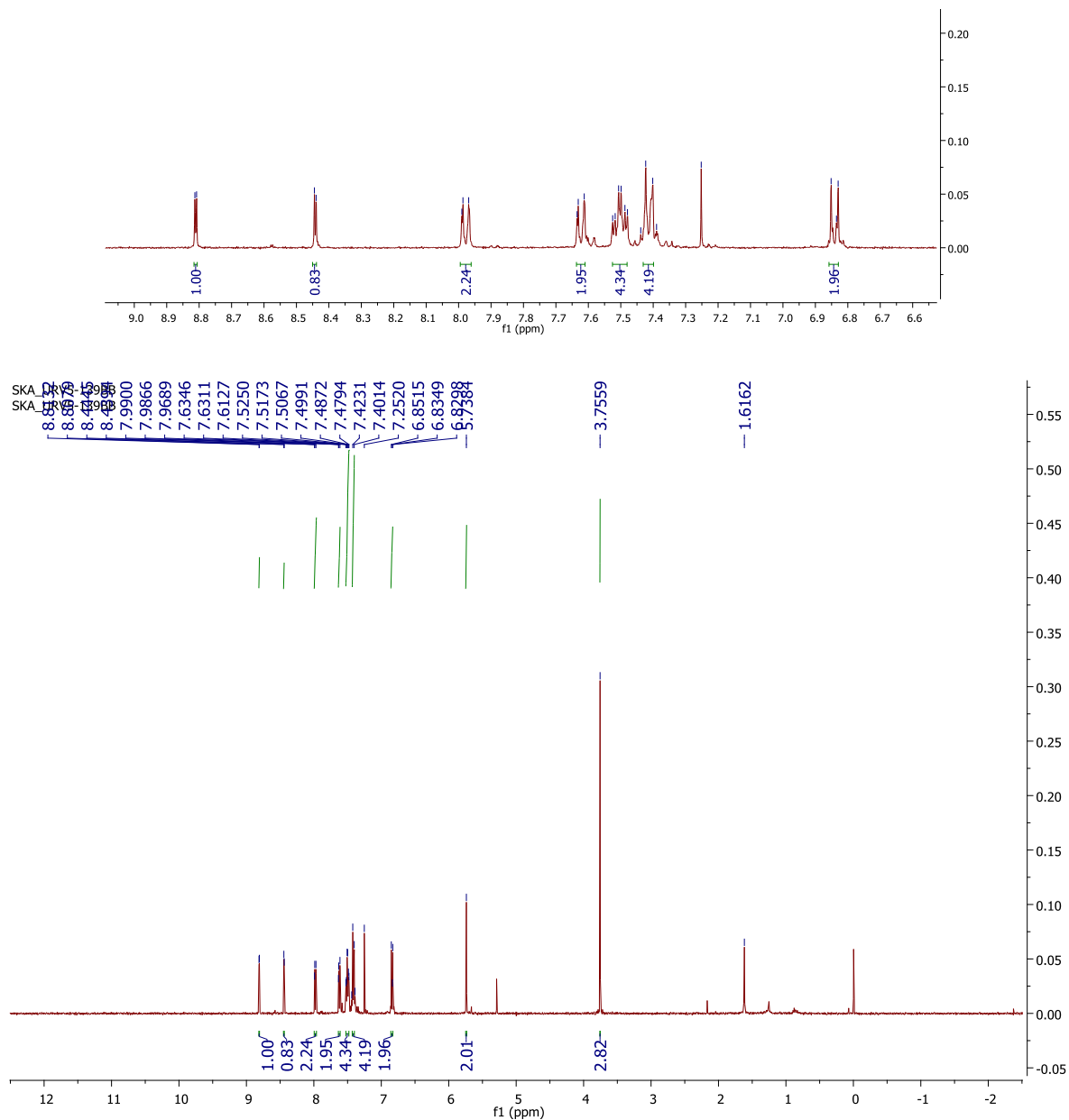


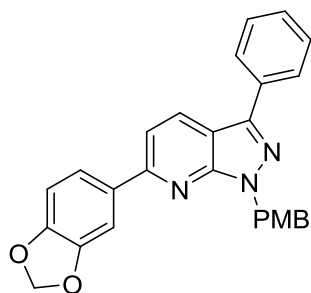
1-(4-methoxybenzyl)-3-(pyridin-4-yl)-6-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**4j**)



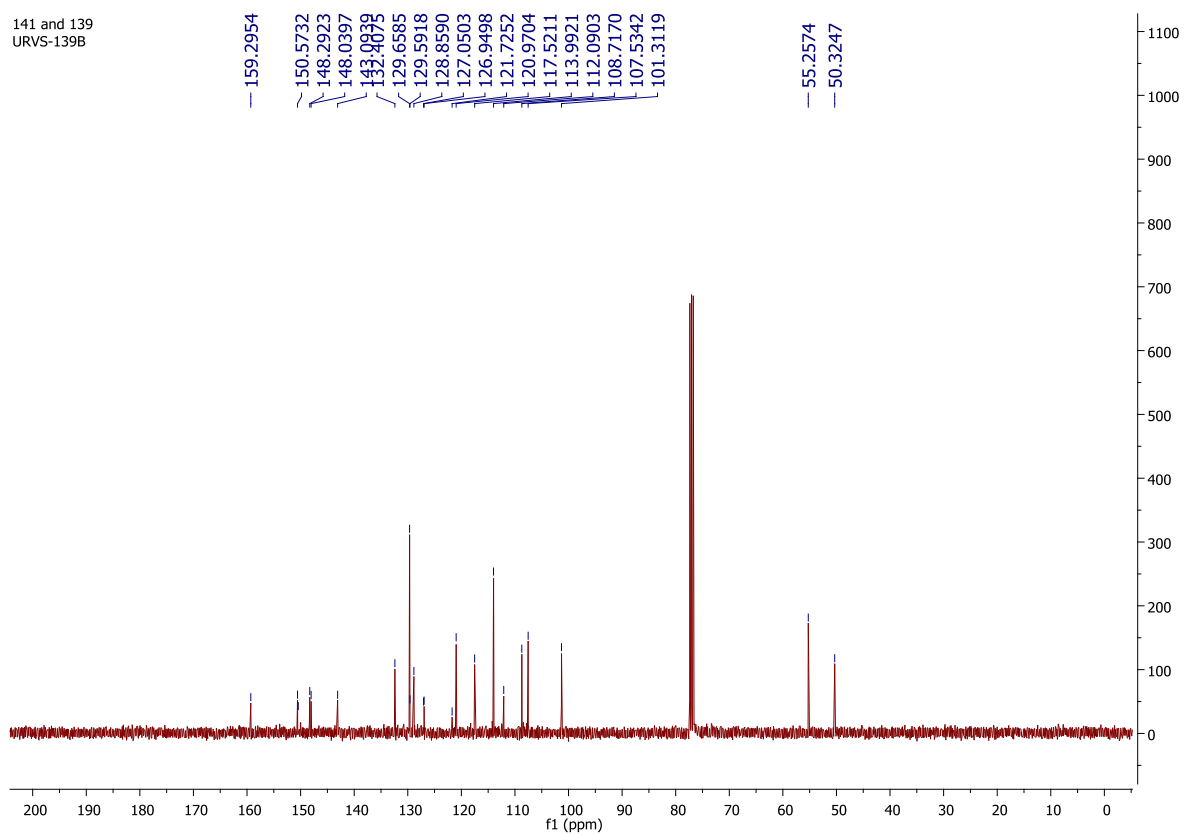


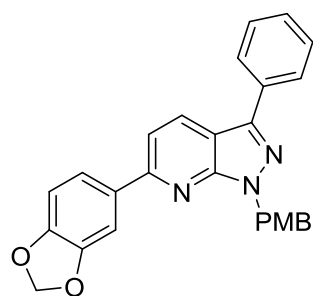
6-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxybenzyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine
(4k)



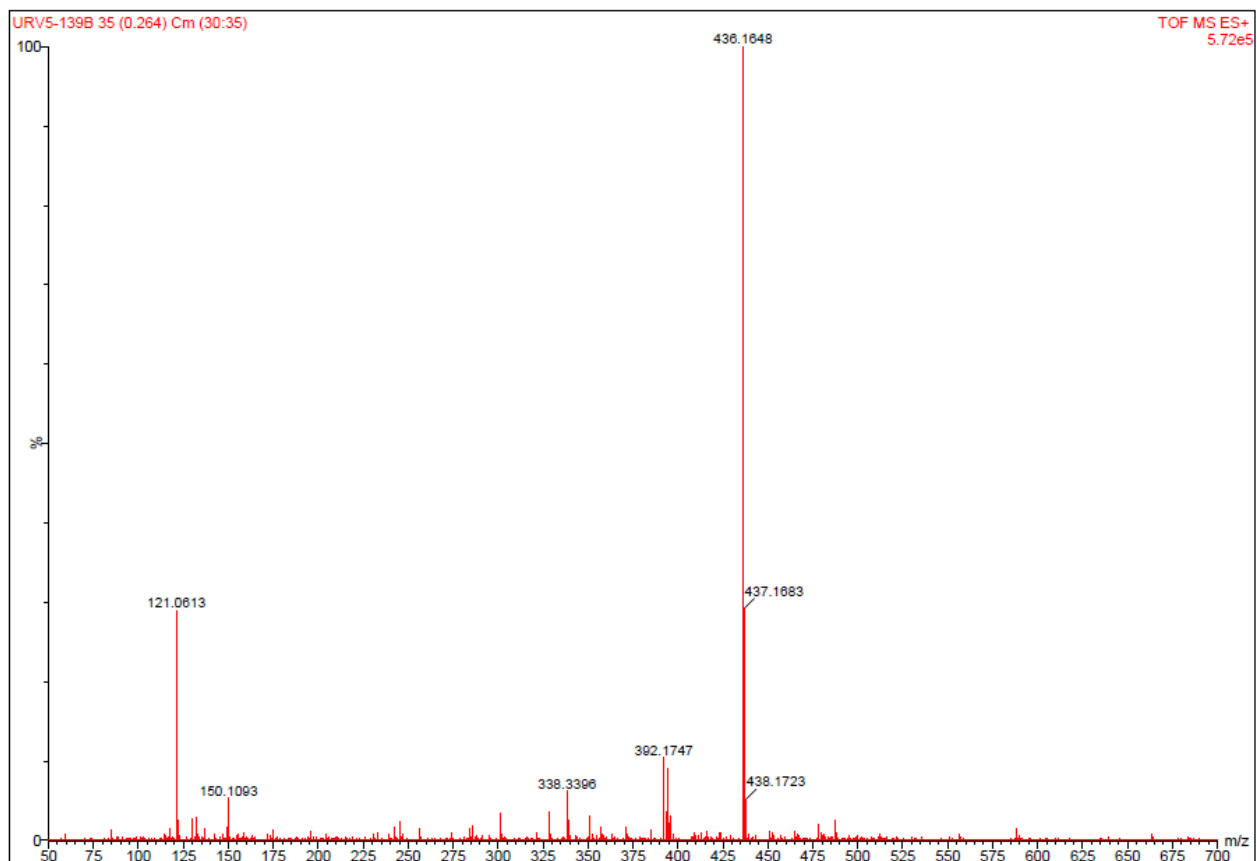


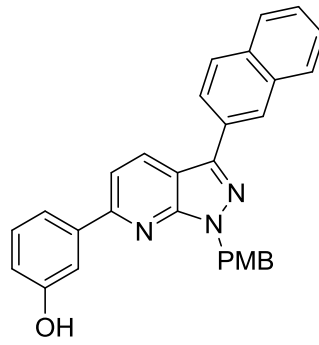
6-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxybenzyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine
(4k)



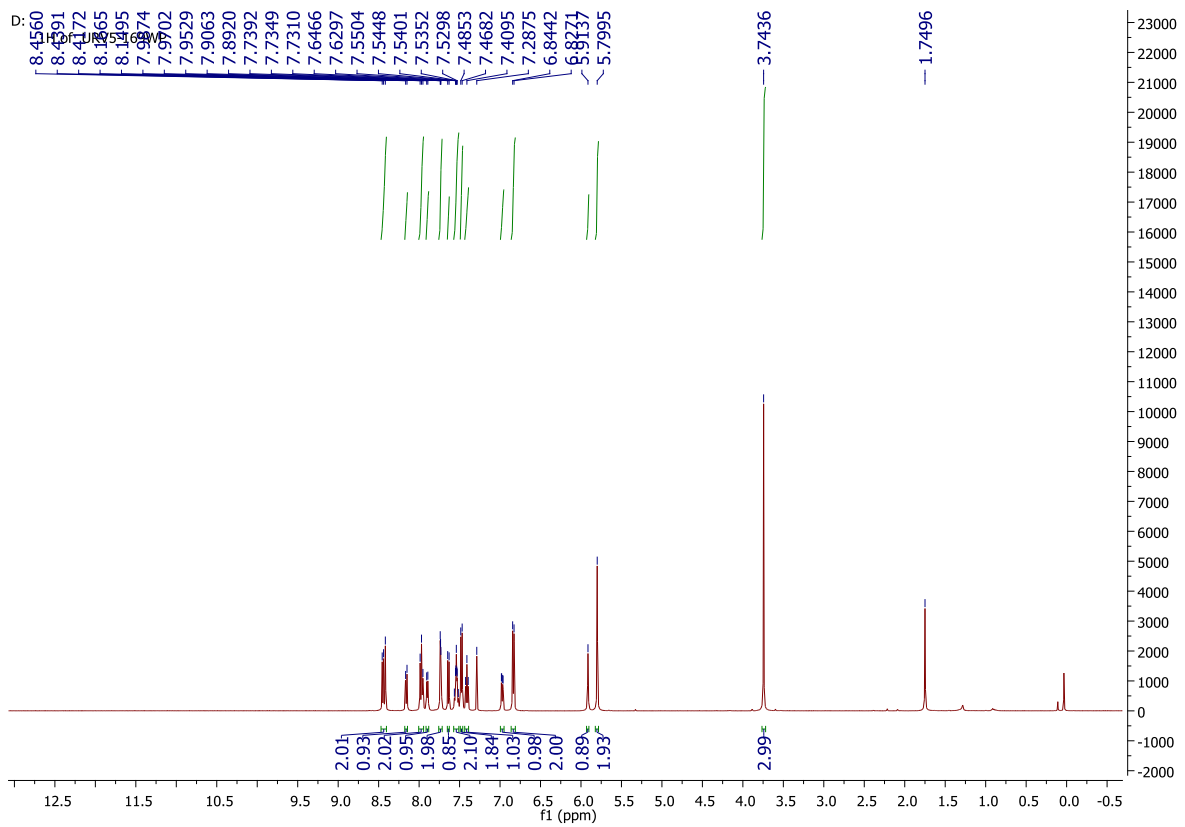
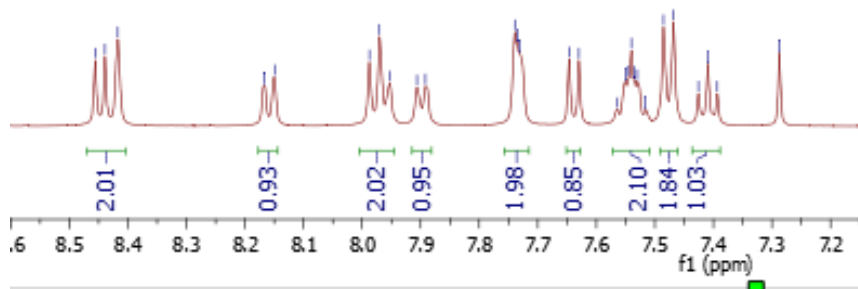


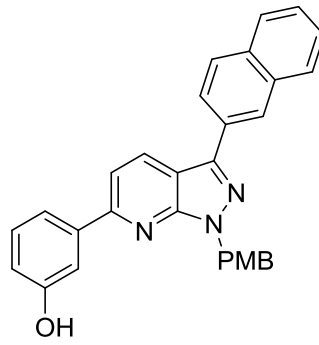
6-(benzo[d][1,3]dioxol-5-yl)-1-(4-methoxybenzyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine
(**4k**)



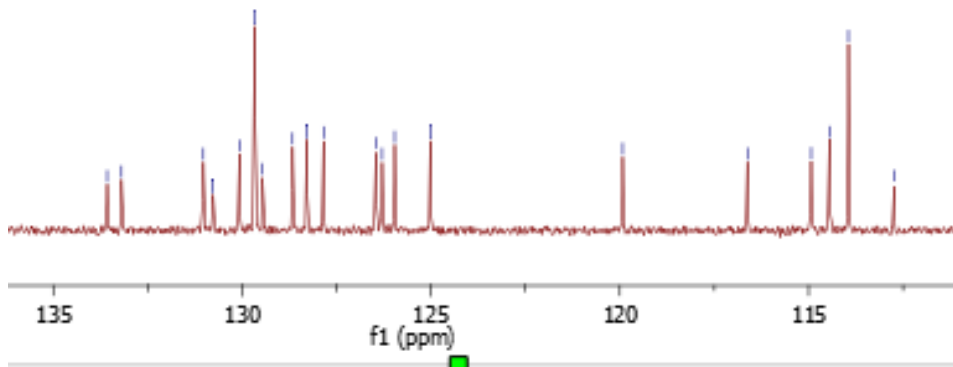


3-(1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1H-pyrazolo[3,4-b]pyridin-6-yl)phenol (**41**)

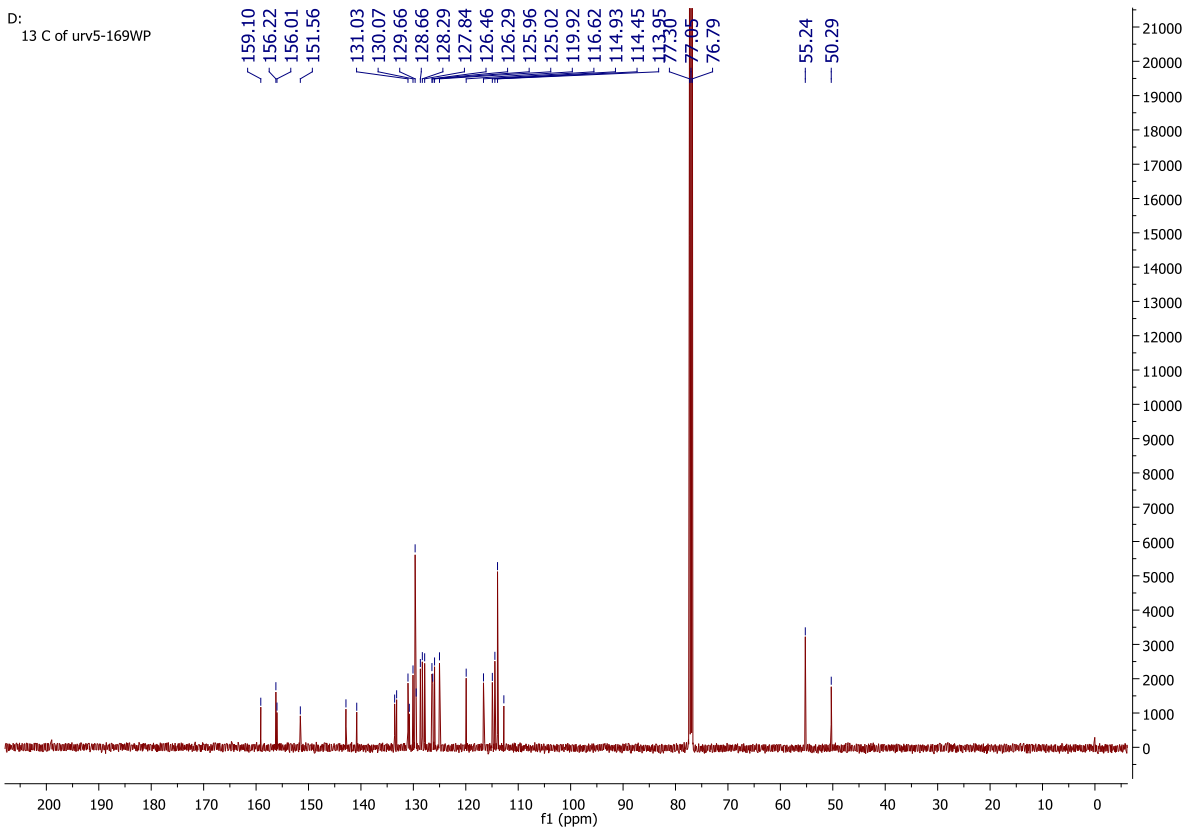


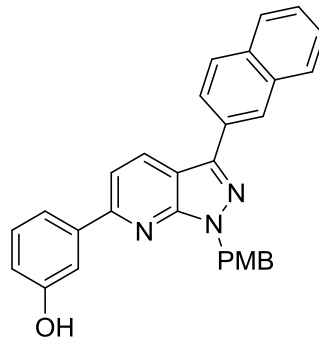


3-(1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)phenol (**41**)

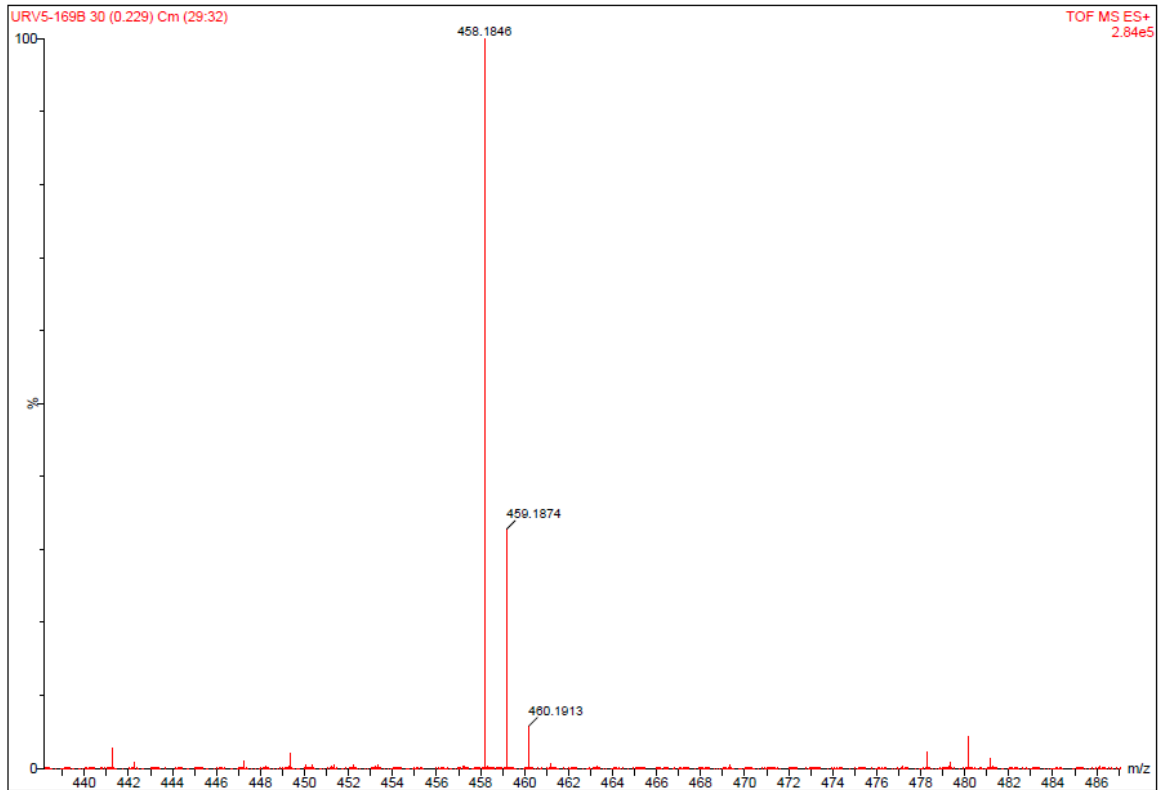


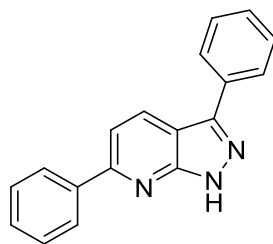
D:
13 C of urv5-169WP



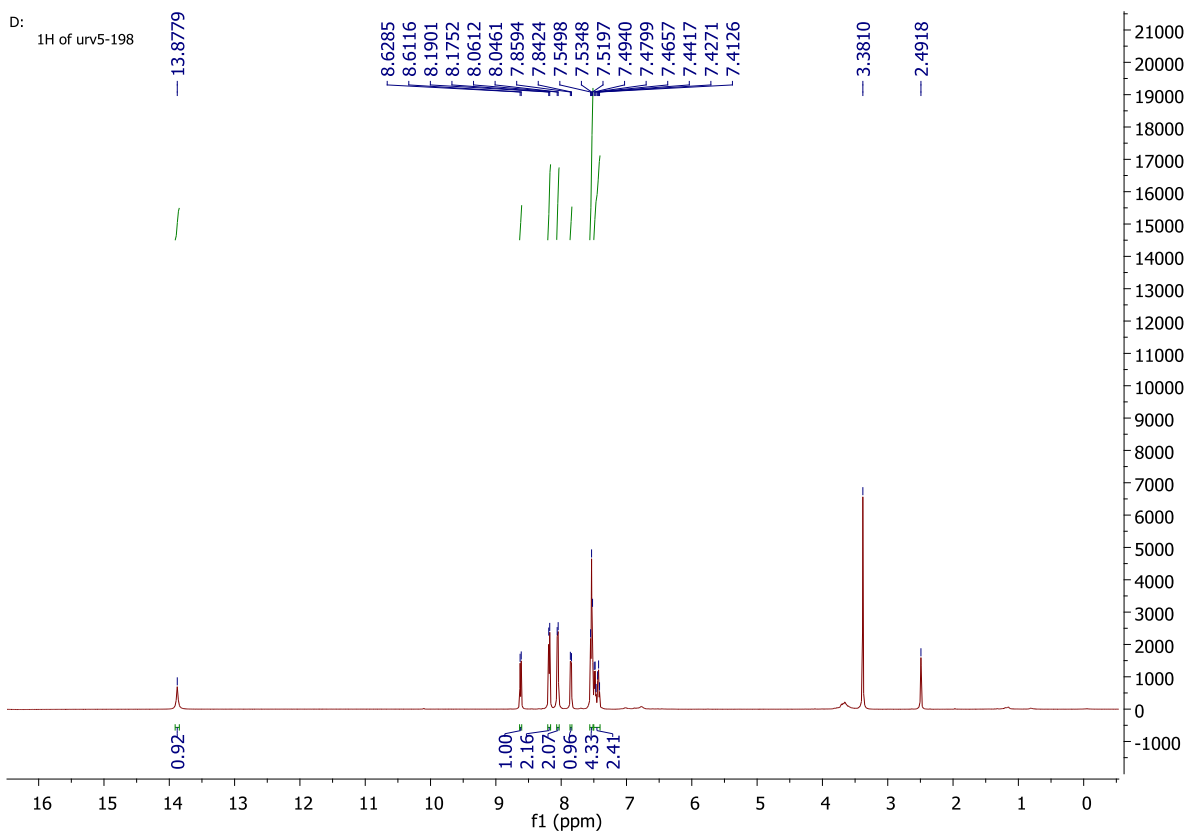
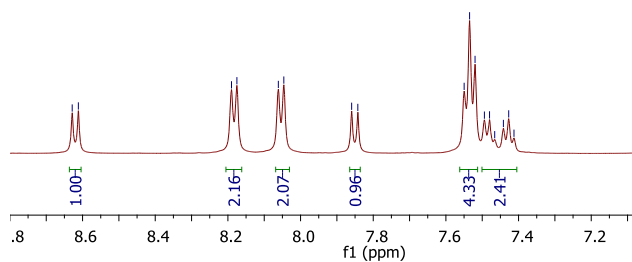


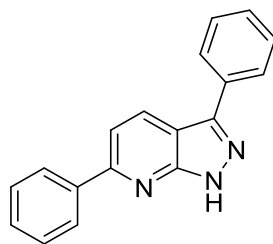
3-(1-(4-methoxybenzyl)-3-(naphthalen-2-yl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl)phenol (**4**)



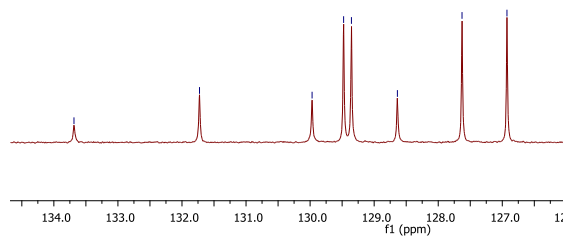


3,6-diphenyl-1H-pyrazolo[3,4-b]pyridine (**5a**)

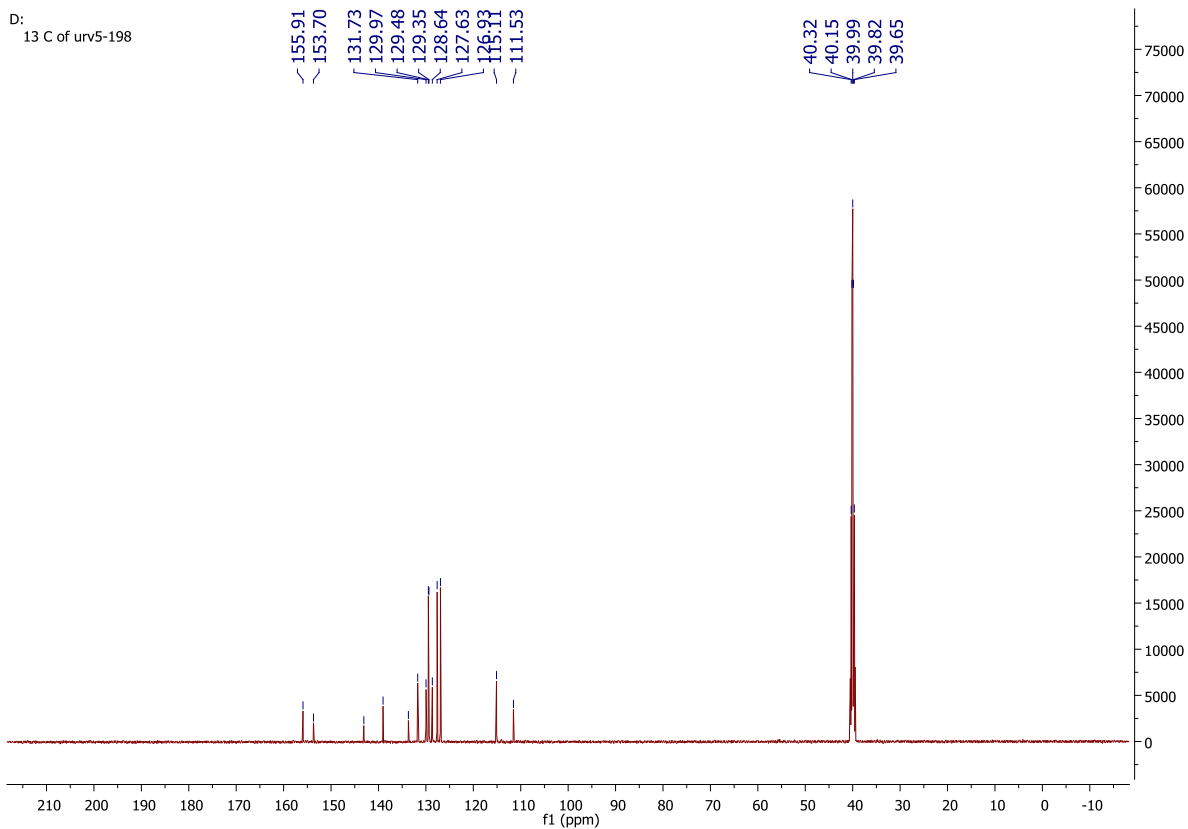


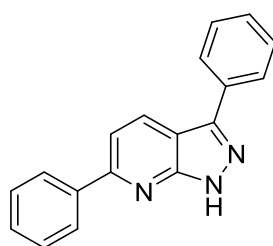


3,6-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5a**)



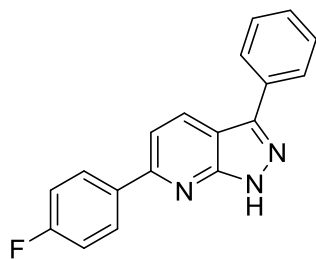
D:
13 C of urv5-198



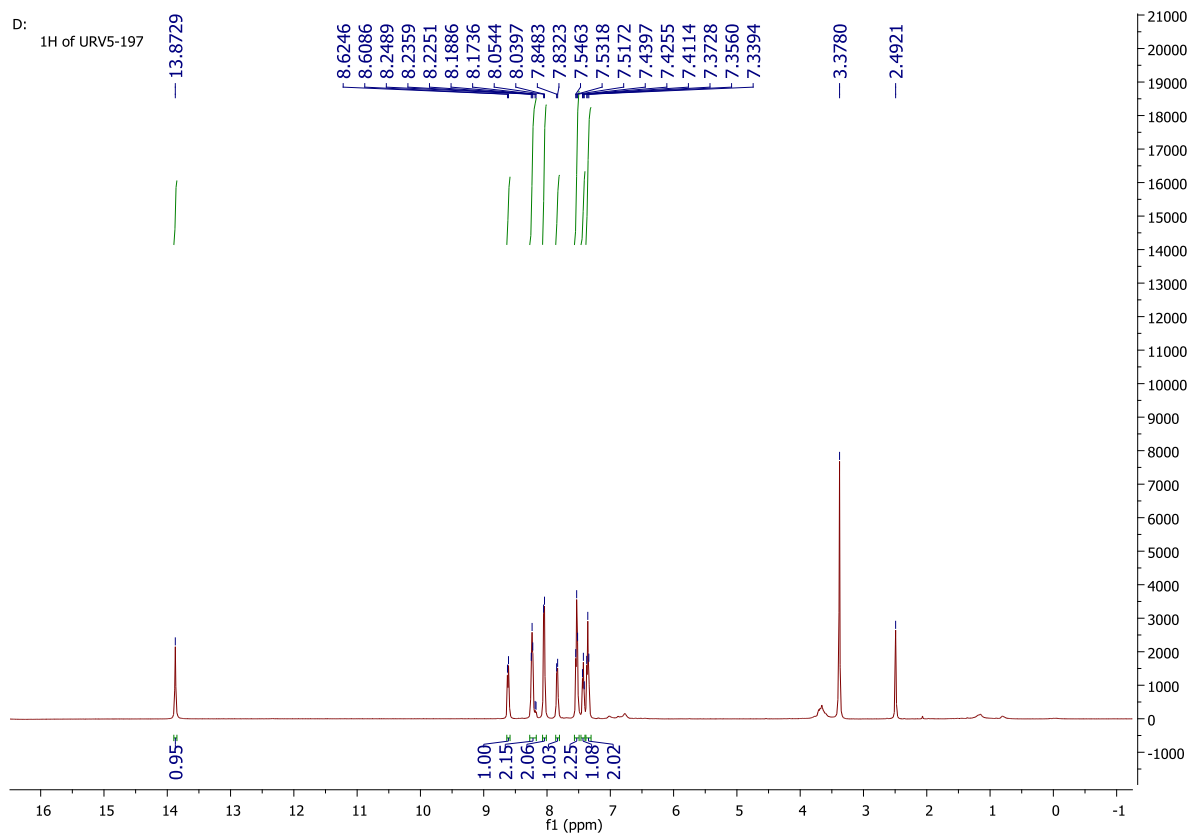
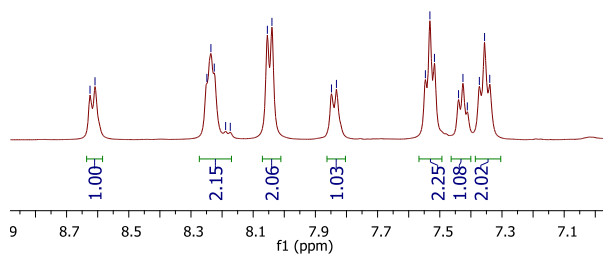


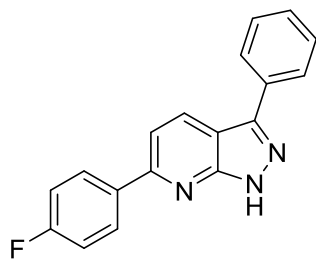
3,6-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5a**)



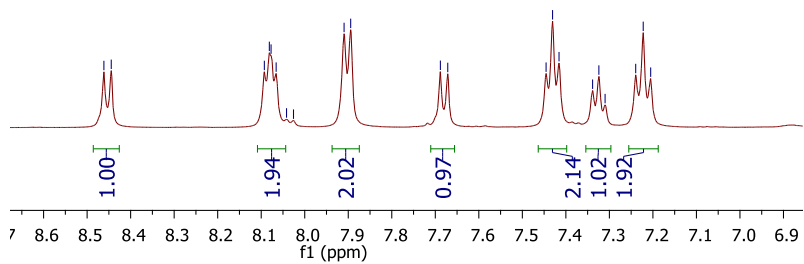


6-(4-fluorophenyl)-3-phenyl-1H-pyrazolo[3,4-*b*]pyridine (**5b**)

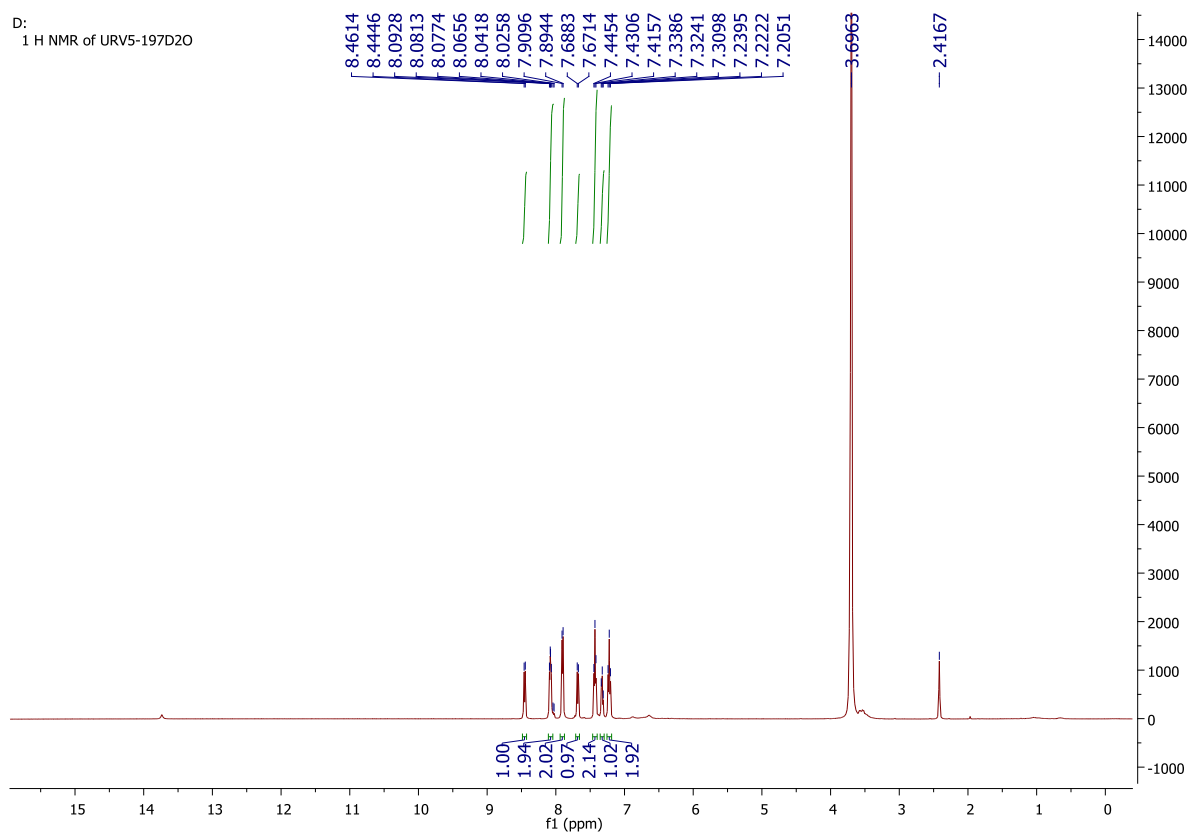


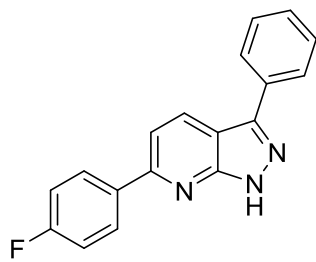


6-(4-fluorophenyl)-3-phenyl-1H-pyrazolo[3,4-b]pyridine (**5b**)

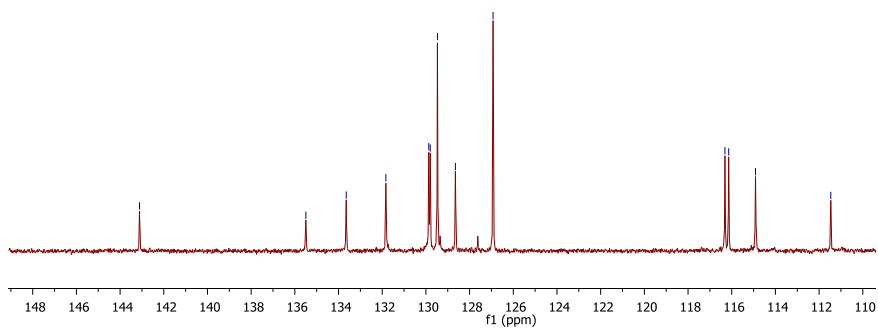


D:
1 H NMR of URV5-197D2O

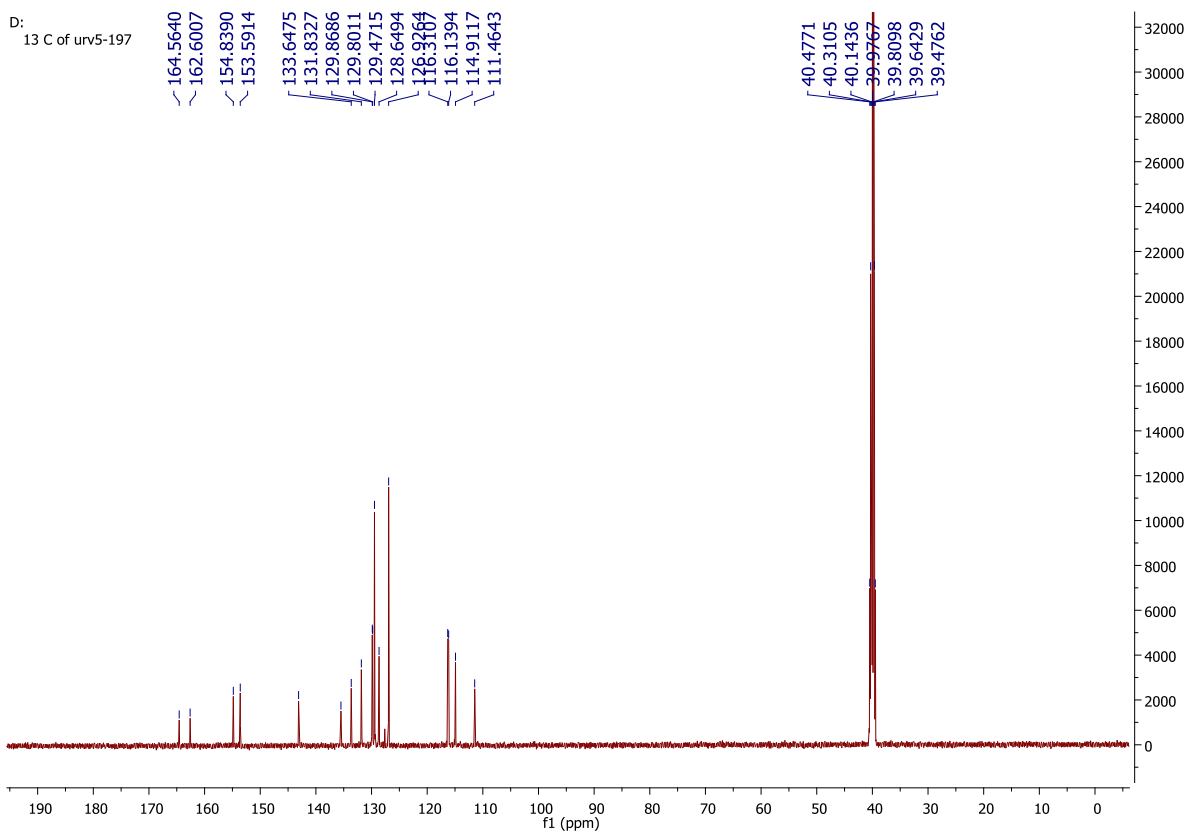


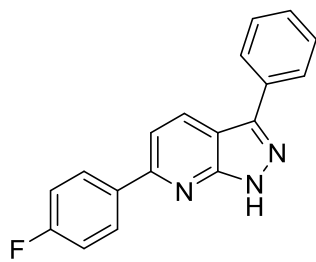


6-(4-fluorophenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5b**)



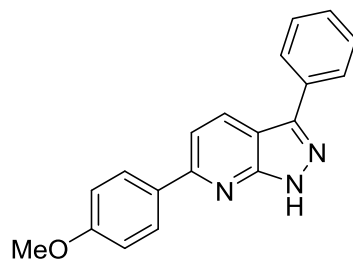
D:
13 C of urv5-197



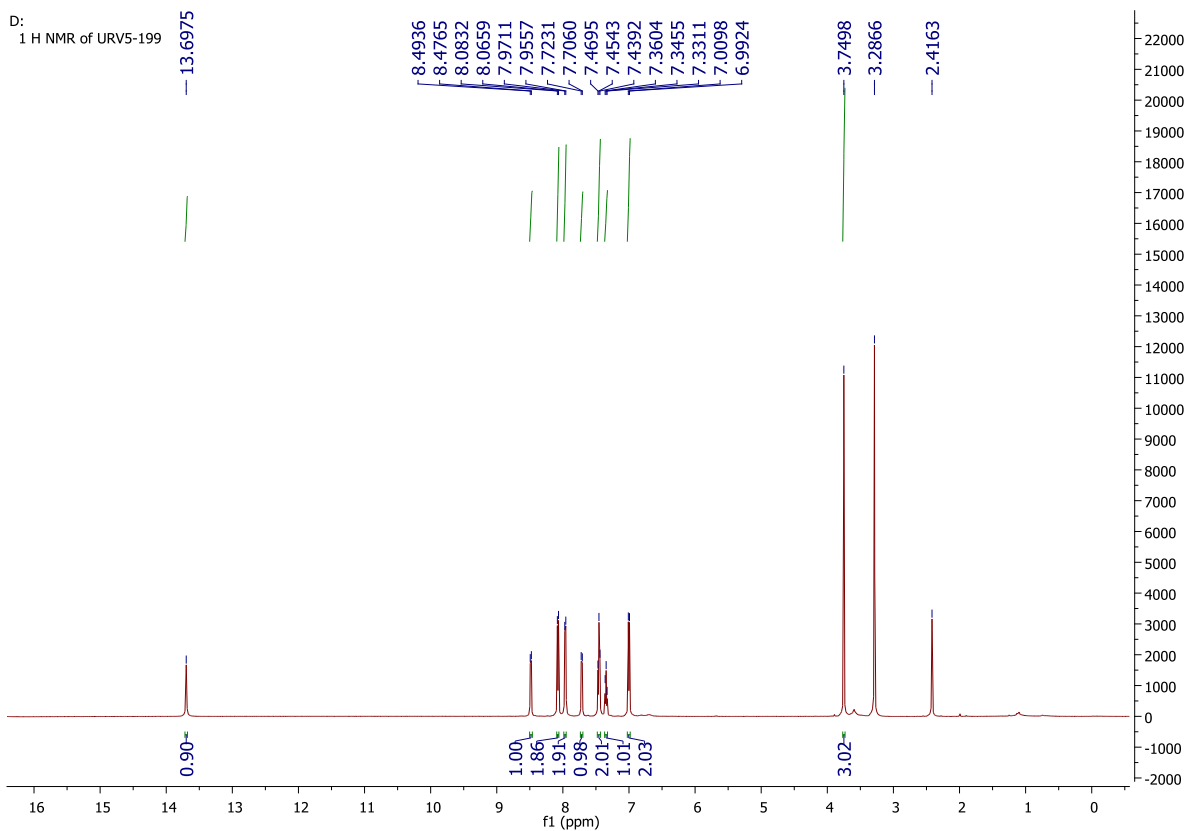
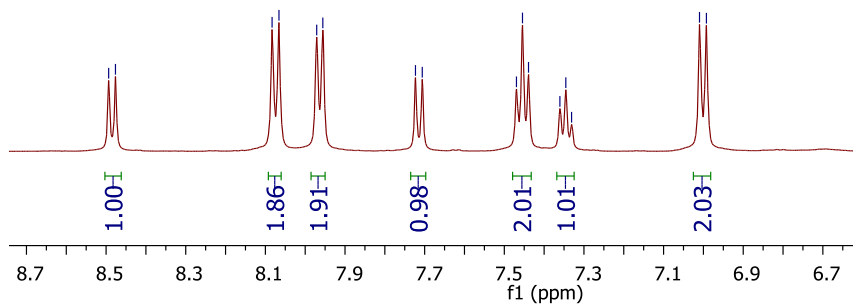


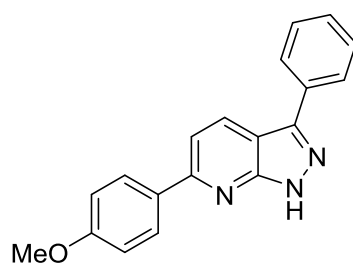
6-(4-fluorophenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5b**)



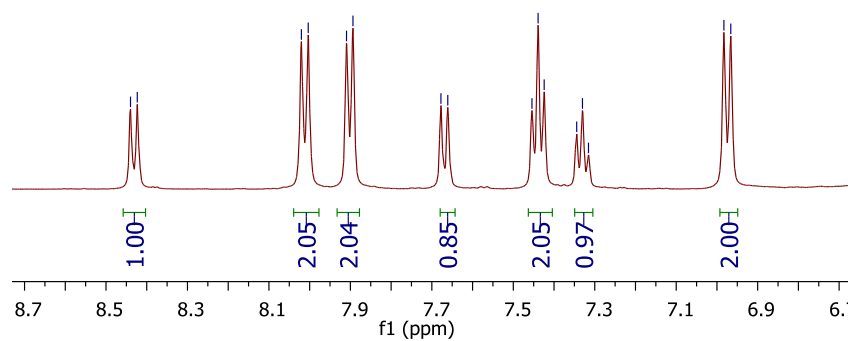


6-(4-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5c**)

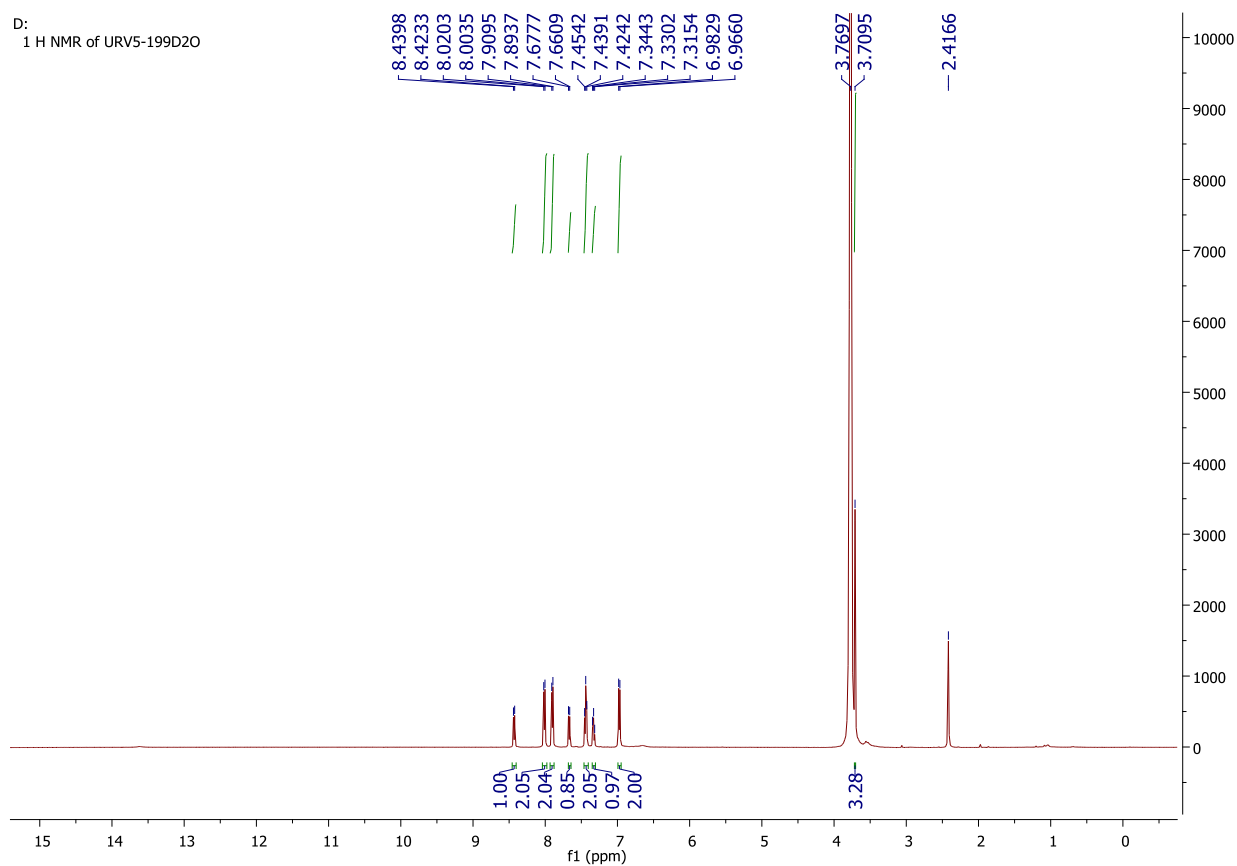


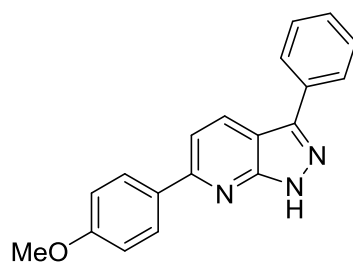


6-(4-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5c**)

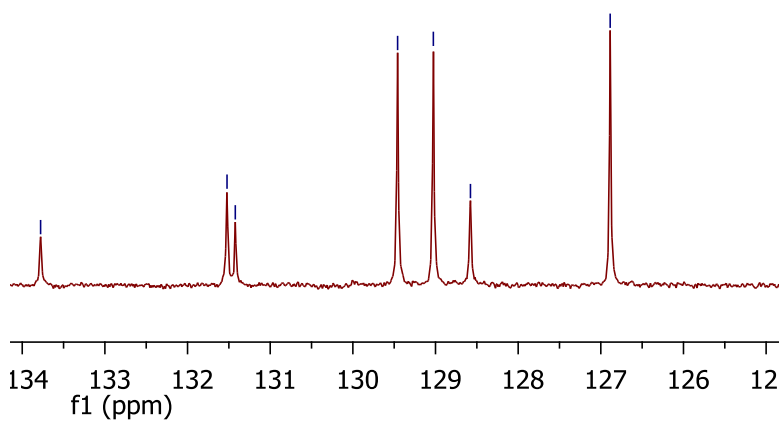


D:
1 H NMR of URV5-199D20

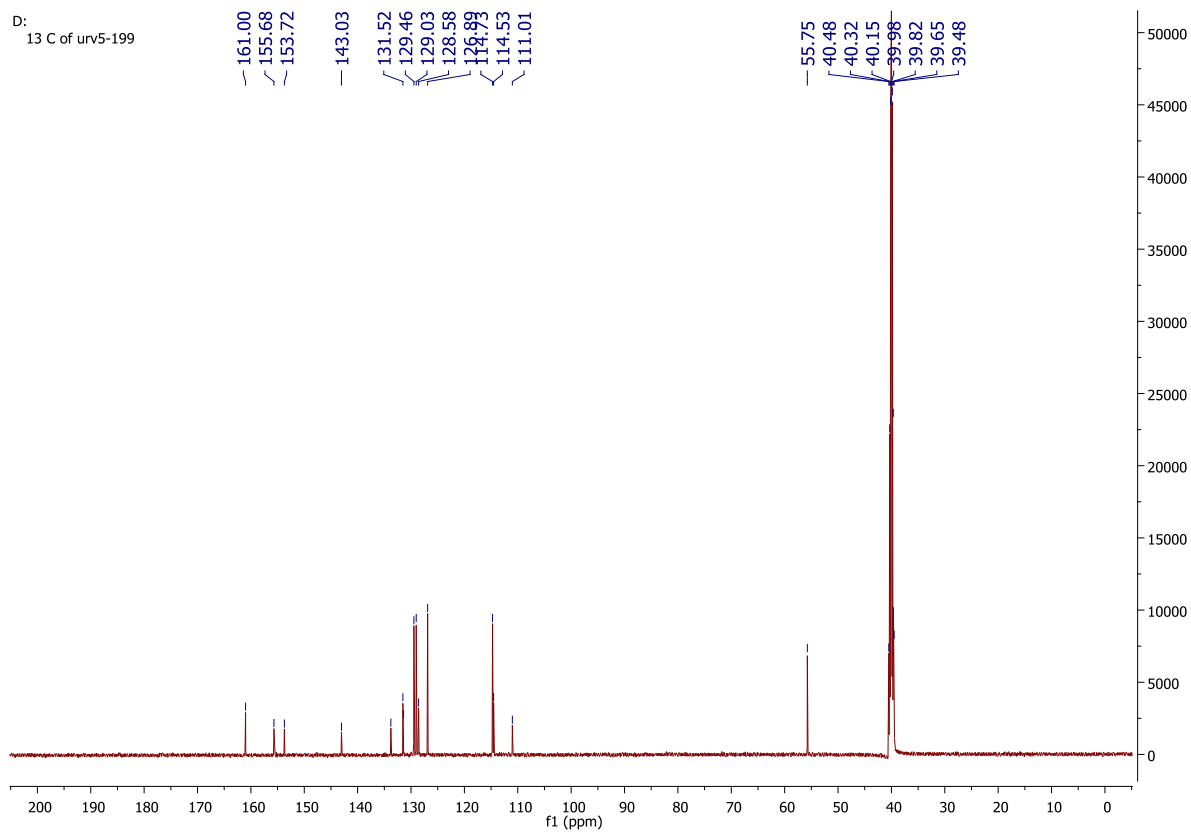


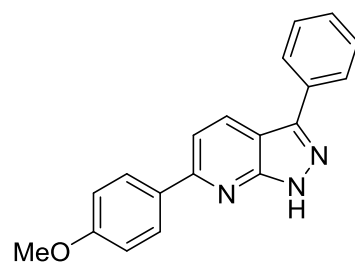


6-(4-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5c**)



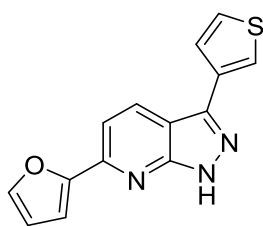
D:
13 C of urv5-199



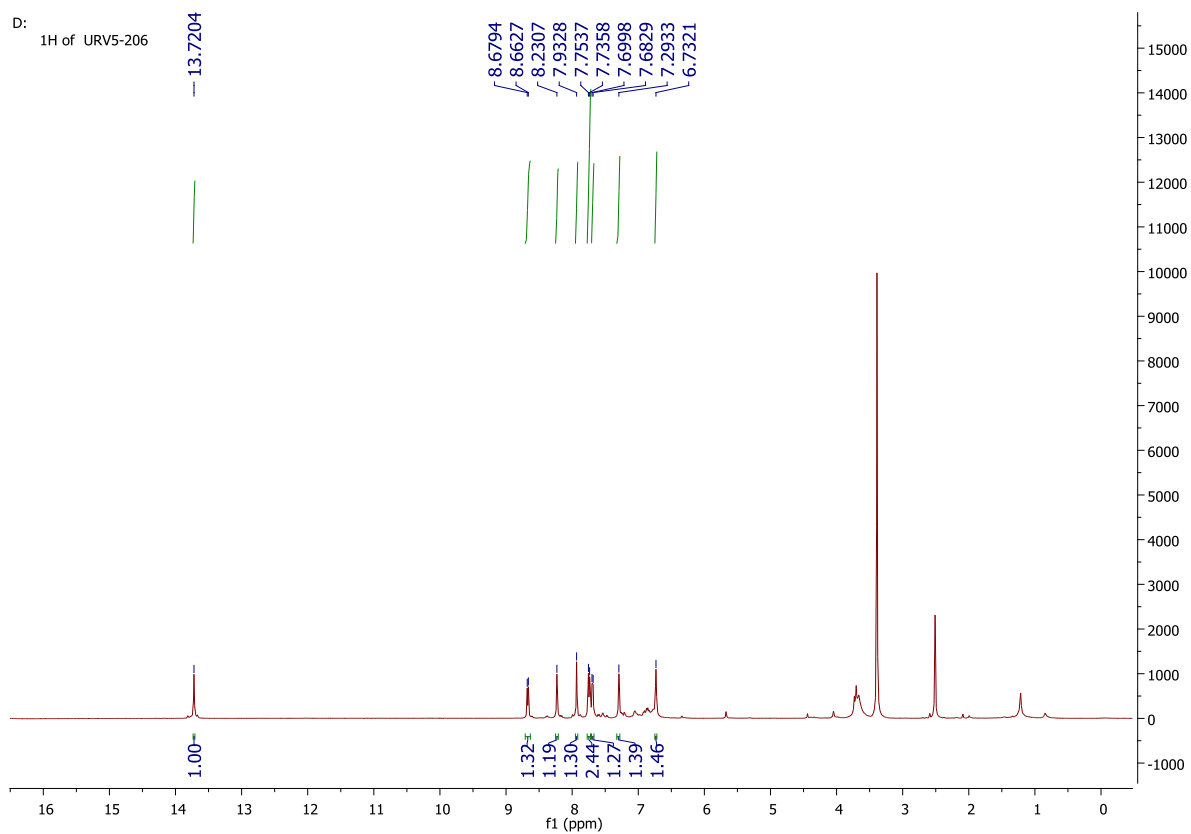
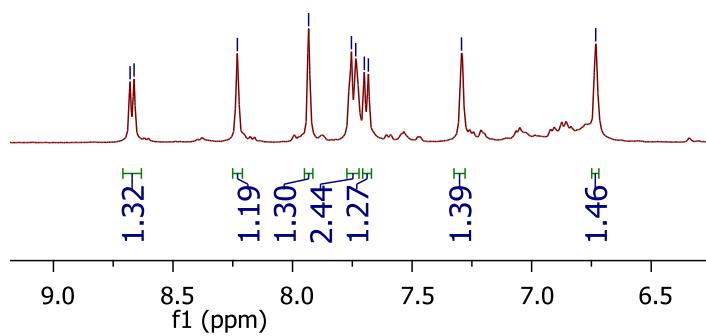


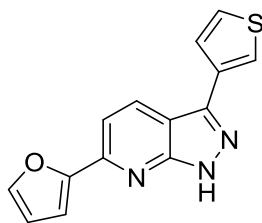
6-(4-methoxyphenyl)-3-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine (**5c**)





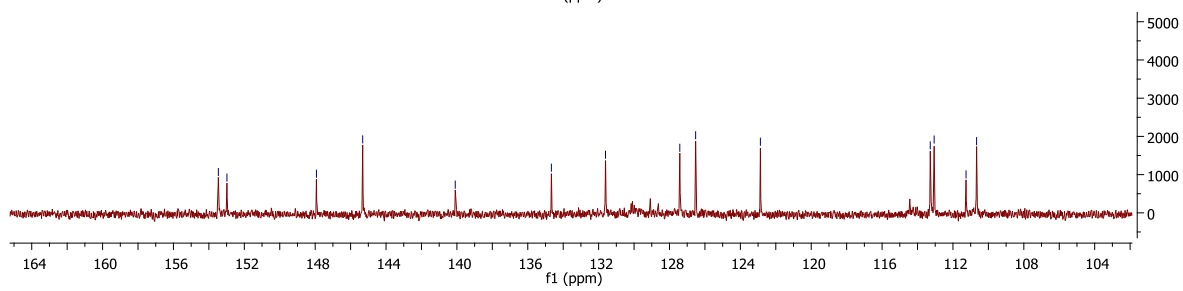
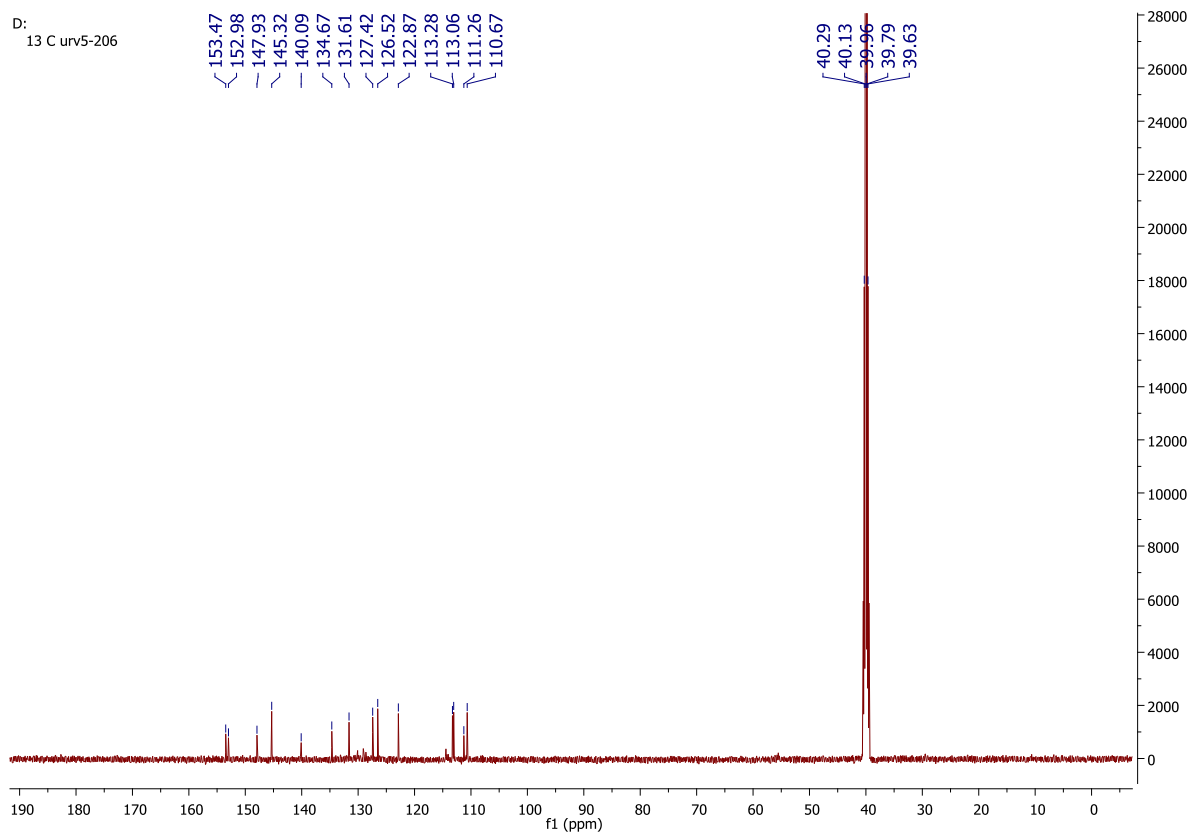
6-(furan-2-yl)-3-(thiophen-3-yl)-1H-pyrazolo[3,4-b]pyridine (**5d**)

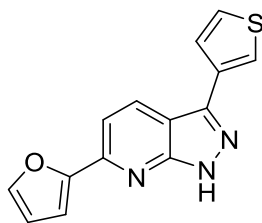




6-(furan-2-yl)-3-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**5d**)

D:
13 C urv5-206





6-(furan-2-yl)-3-(thiophen-3-yl)-1*H*-pyrazolo[3,4-*b*]pyridine (**5d**)

