Supplementary information

Synthesis of diversely substituted 5-methylpyrazolo[1,5-*a*]pyrimidines assisted by ultrasound in aqueous media: Molecular docking for potential antiviral, anticancer activities

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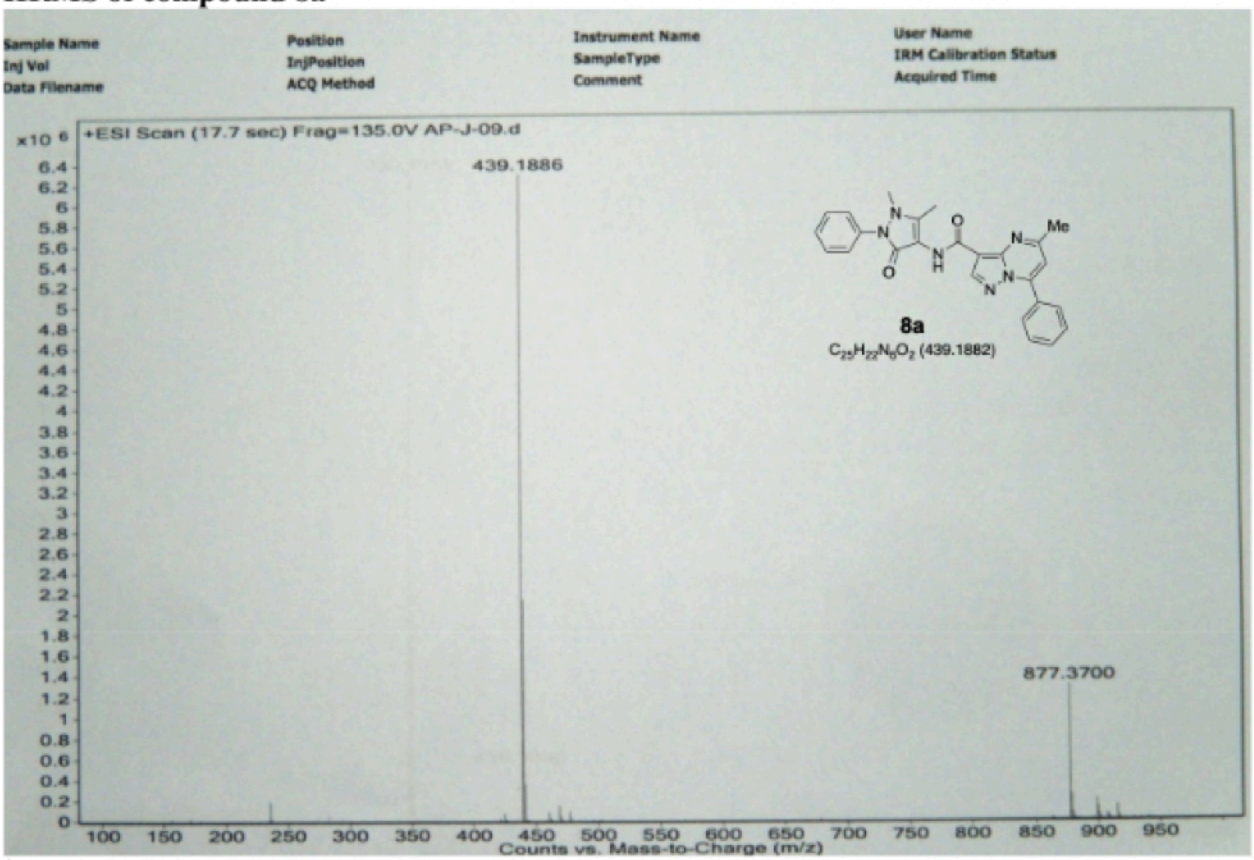
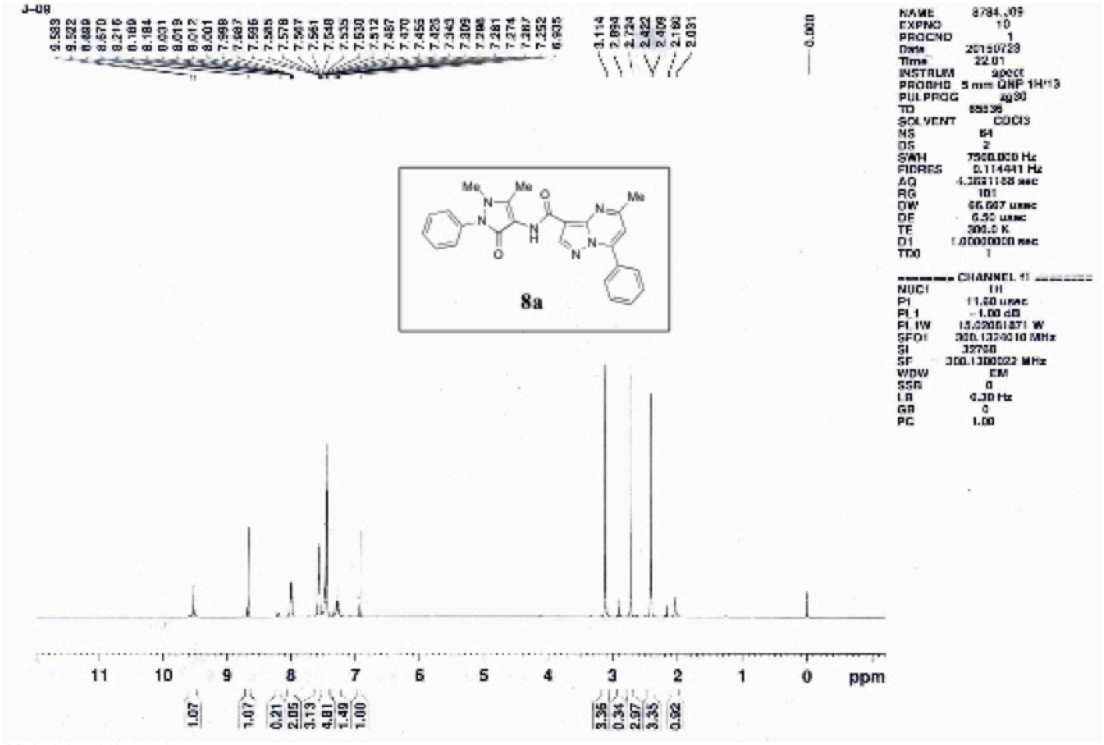
N-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-*1H*-pyrazol-4-yl)-5-methyl-7-phenylpyrazolo [1,5-*a*] pyrimidine-3-carboxamide (8a)

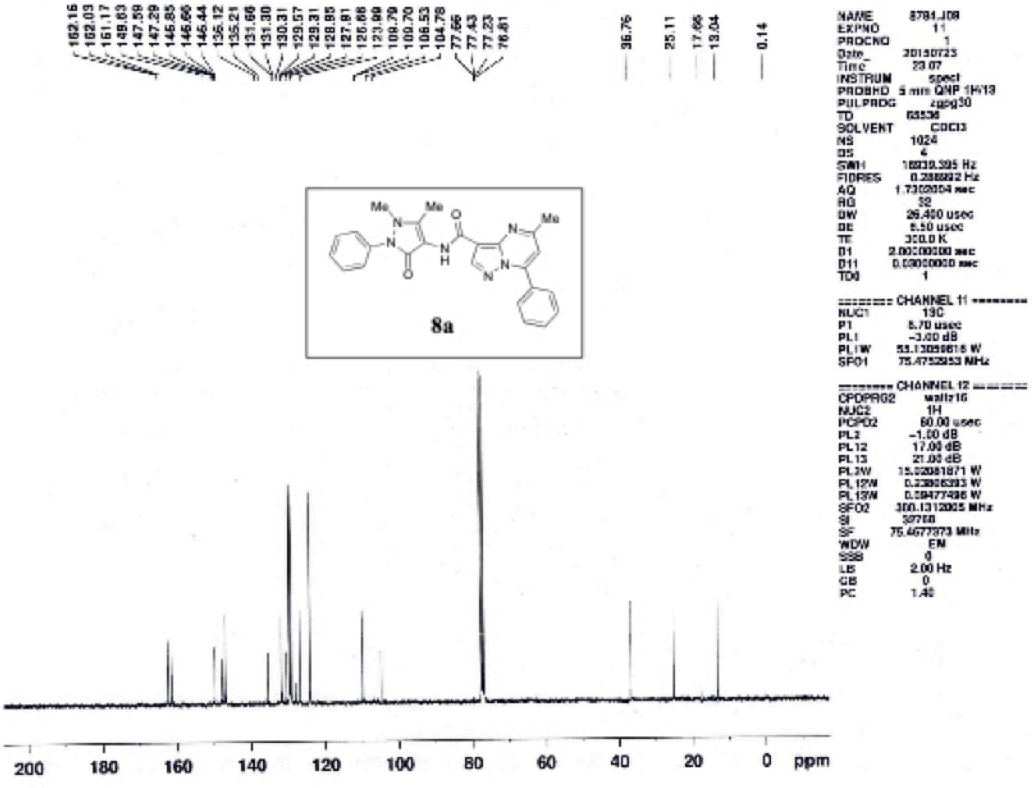
HRMS of compound 8a



^{1}H NMR of 8a

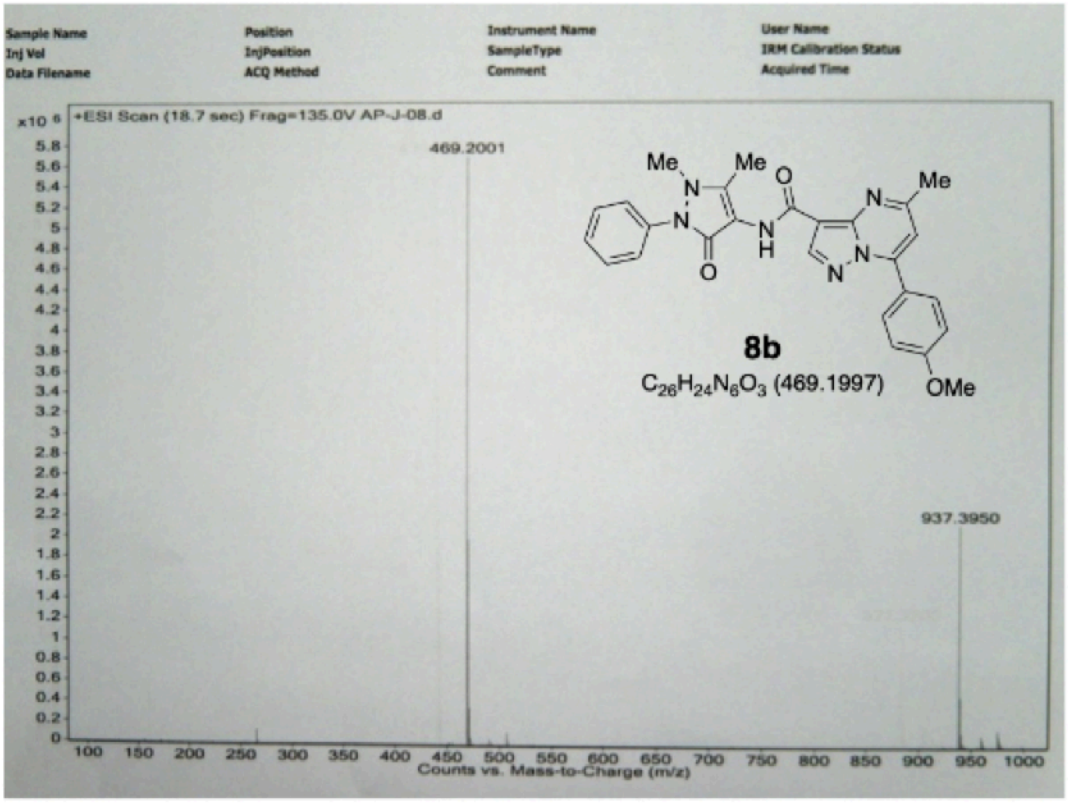


^{13}C NMR of 8a



***N*-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-*1H*-pyrazol-4-yl)-7-(4-methoxyphenyl)-5-methylpyrazolo [1,5-*a*]pyrimidine-3-carboxam- ide (8b)**

HRMS of compound 8b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Data Filename
Position
InjPosition
ACQ Method
Instrument Name
SampleType
Comment
User Name
IRM Calibration Status
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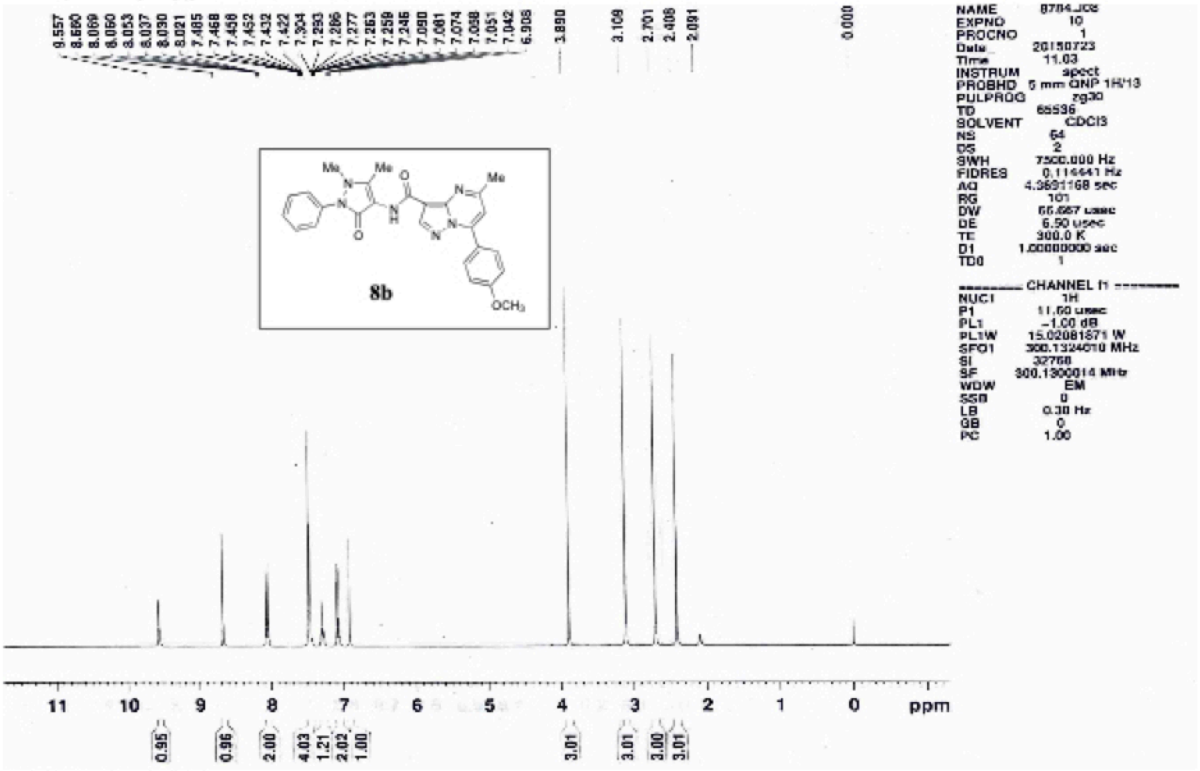
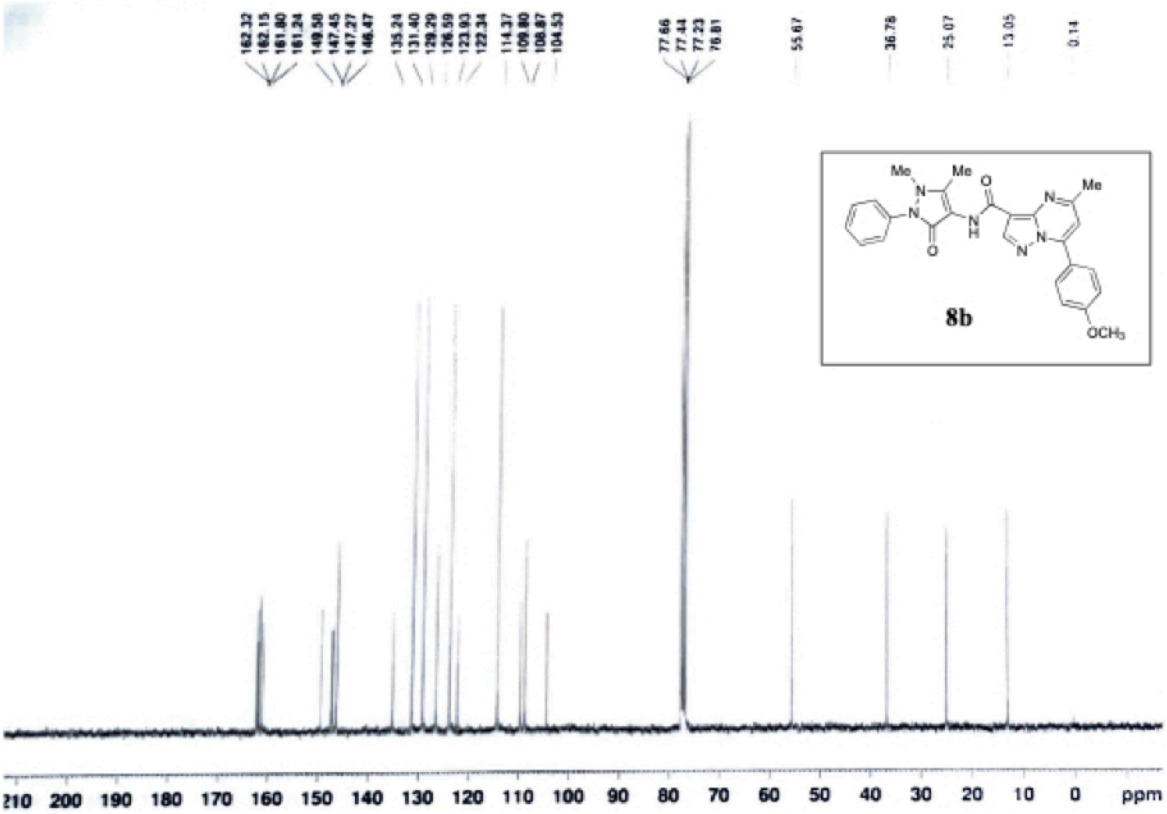
x10 6
469.2001
937.3950
Counts vs. Mass-to-Charge (m/z)
8b
C26H24N6O3 (469.1997)
OMe

^{1}H NMR of 8b

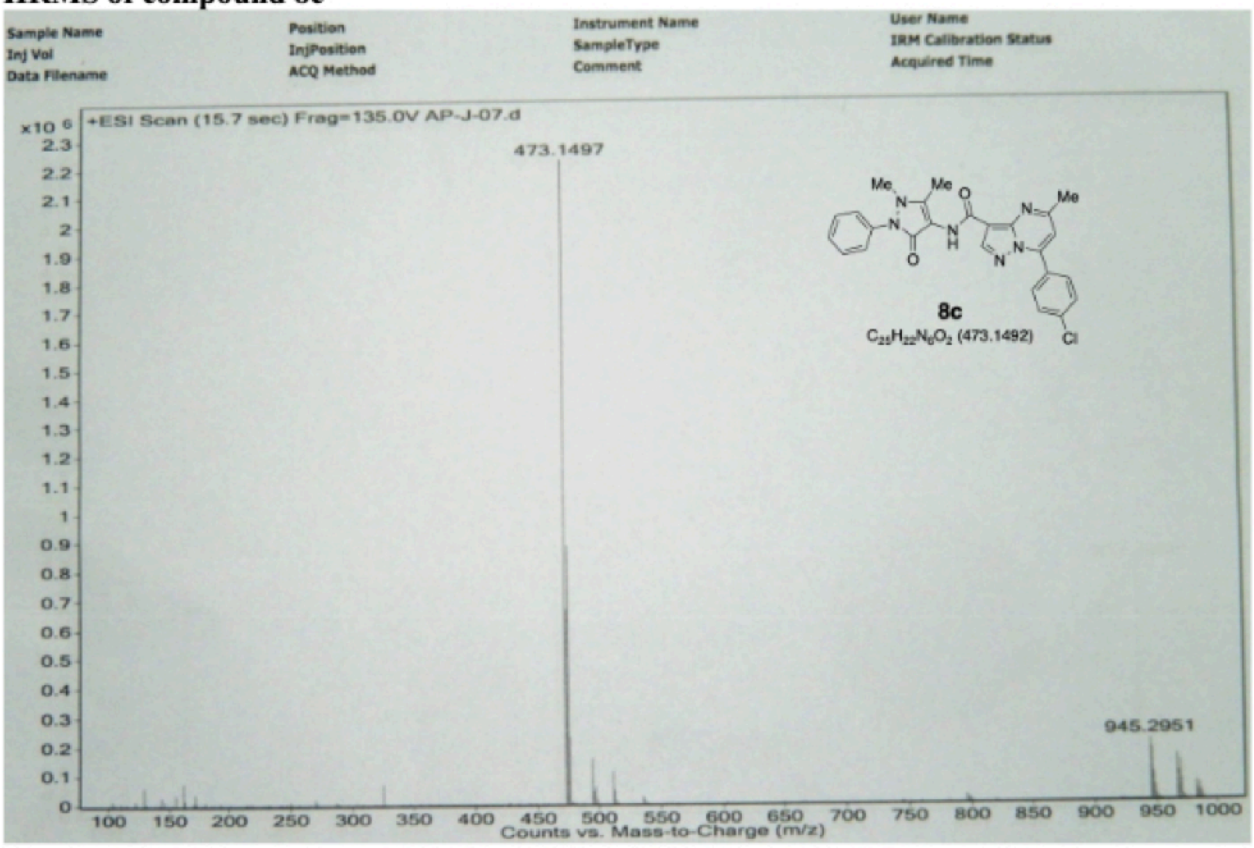


^{13}C NMR of 8b

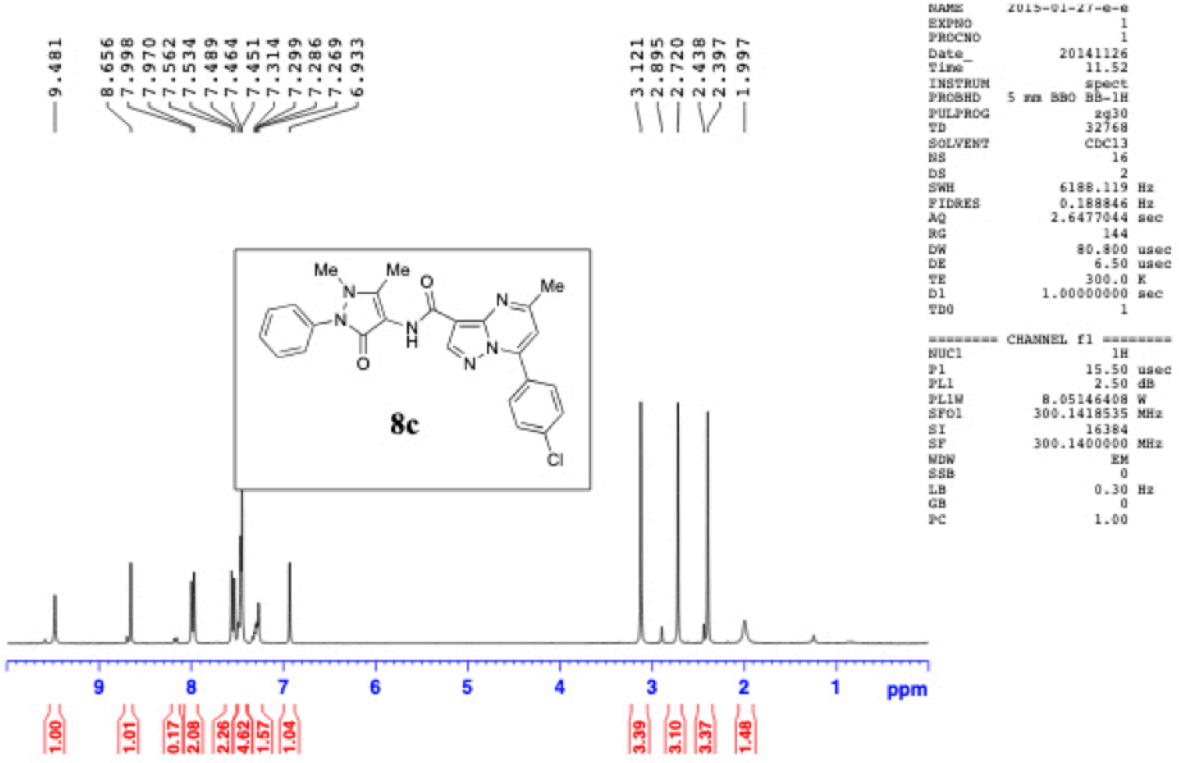


7-(4-Chlorophenyl)-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-*1H*-pyrazol-4-yl)-5-methylpyrazolo[1,5-*a*]pyrimidine-3-carboxamide (8c)

HRMS of compound 8c



^{1}H NMR of 8c



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TD	32768
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FIDRES	0.188846 Hz
AQ	2.6477044 sec
RG	144
DW	80.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
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PL1	2.50 dB
PL1W	8.05146408 W
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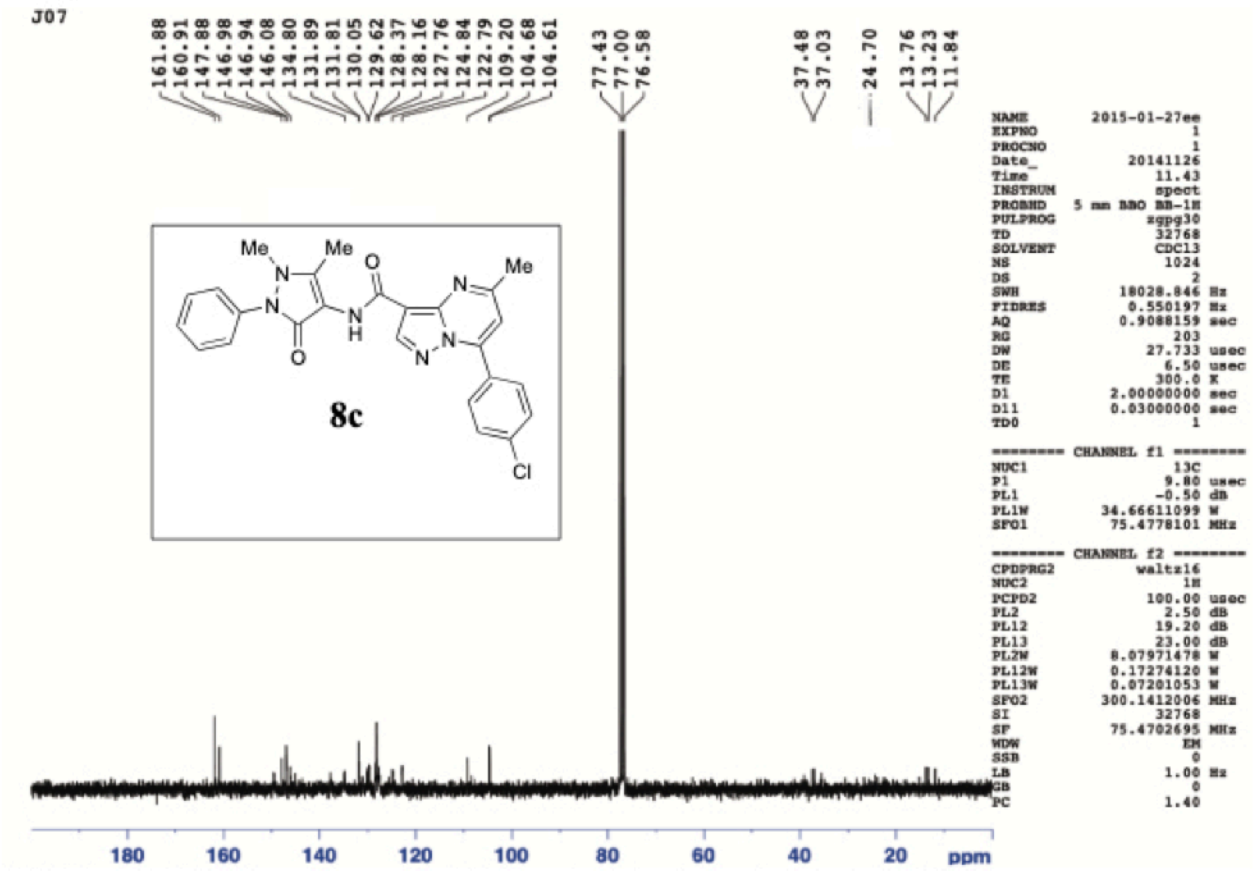
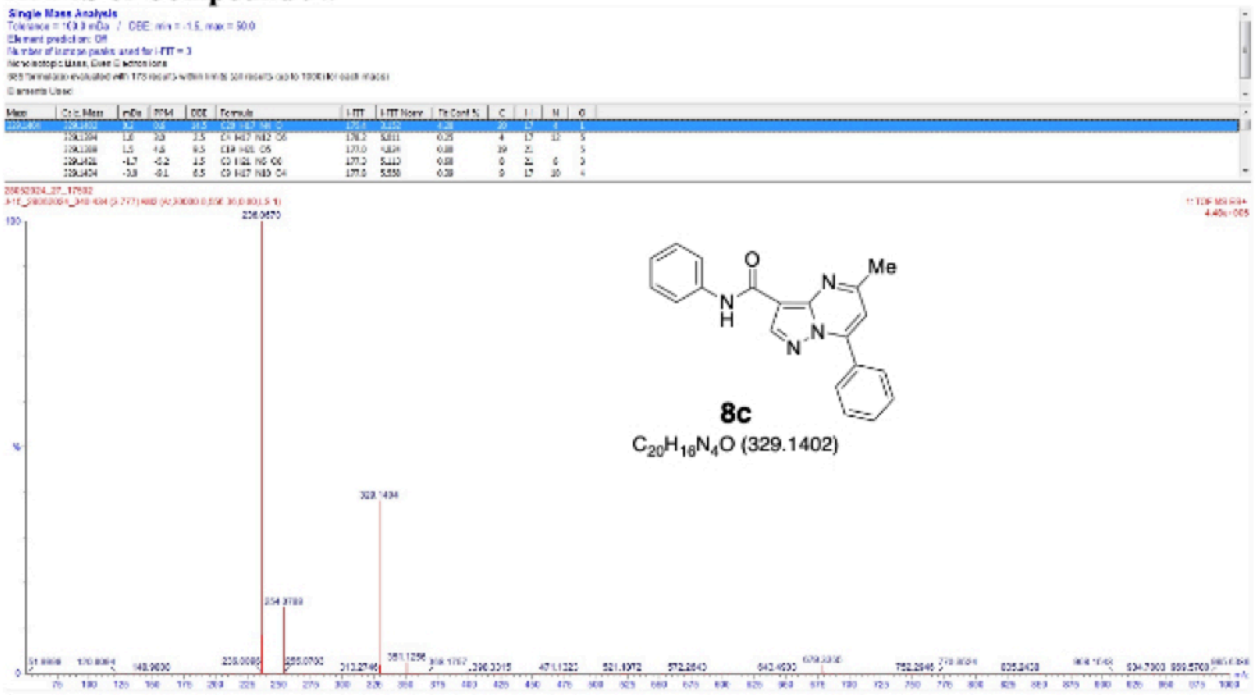
^{13}C NMR of 8c

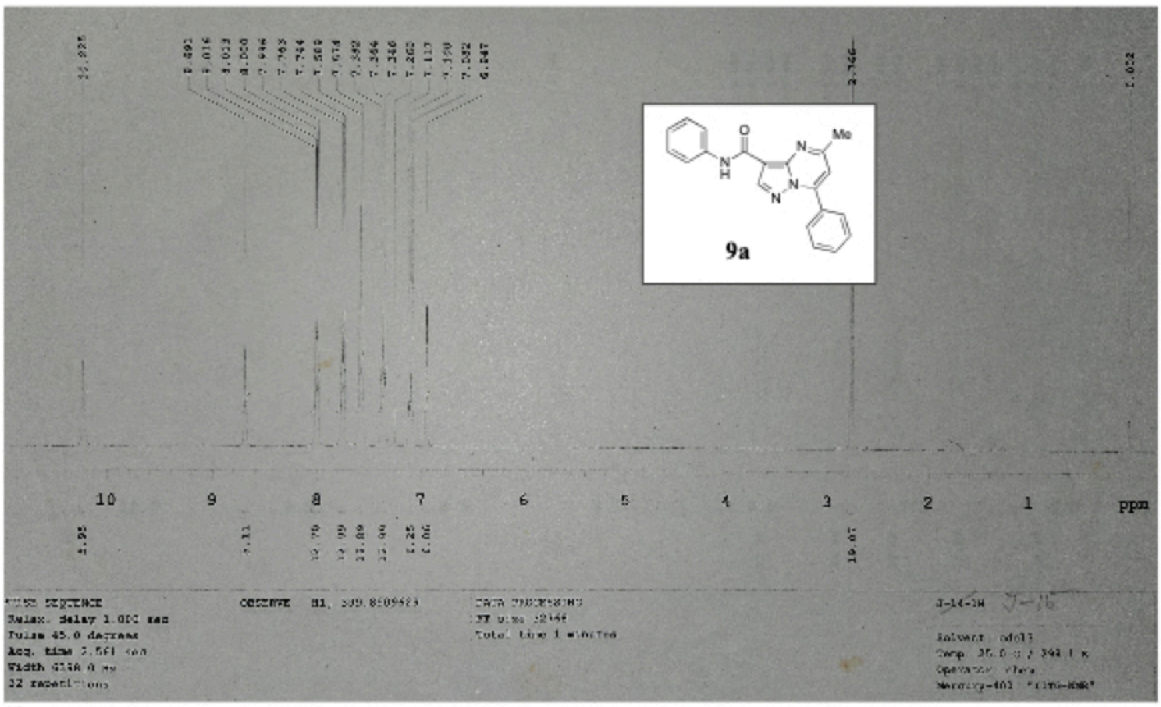


5-Methyl-*N*,7-diphenylpyrazolo[1,5-*a*]pyrimidine-3-carboxamide (9a)

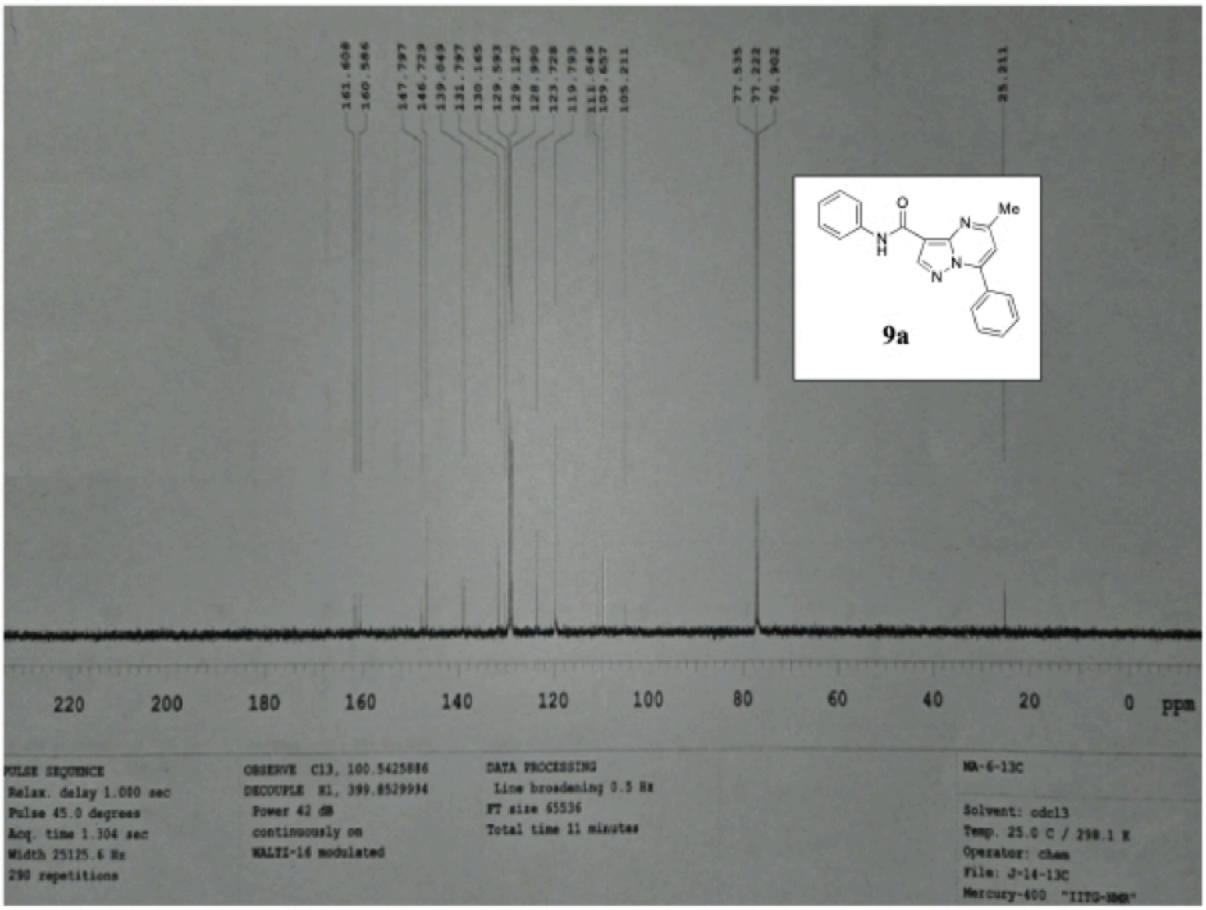
HRMS of Compound 9a



^{1}H NMR of 9a

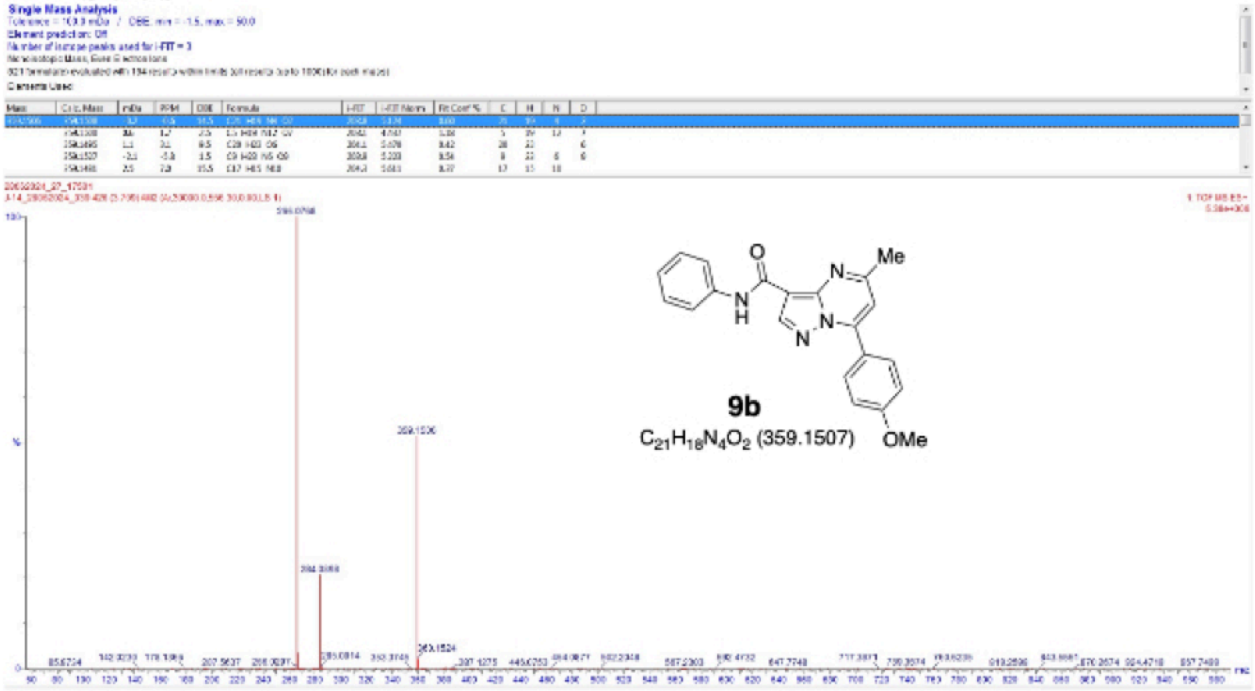


^{13}C NMR of 9a

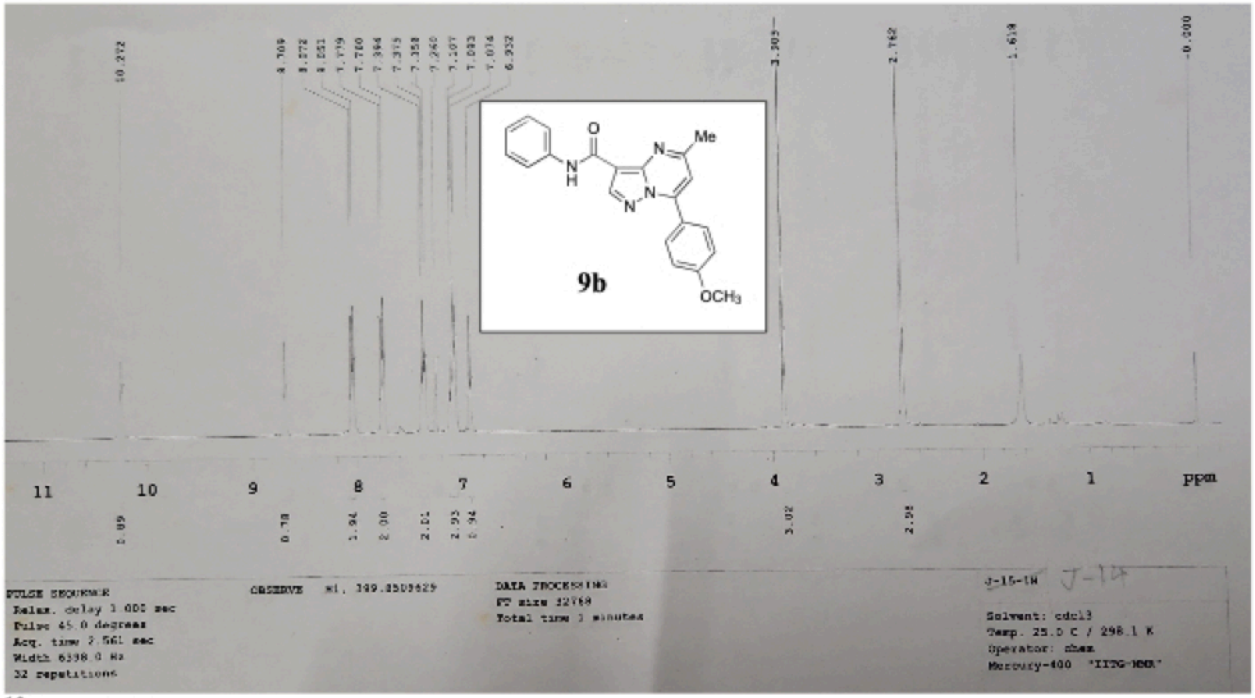


7-(4-Methoxyphenyl)-5-methyl-*N*-phenylpyrazolo[1,5-*a*]pyrimidine-3-carboxamide (9b)

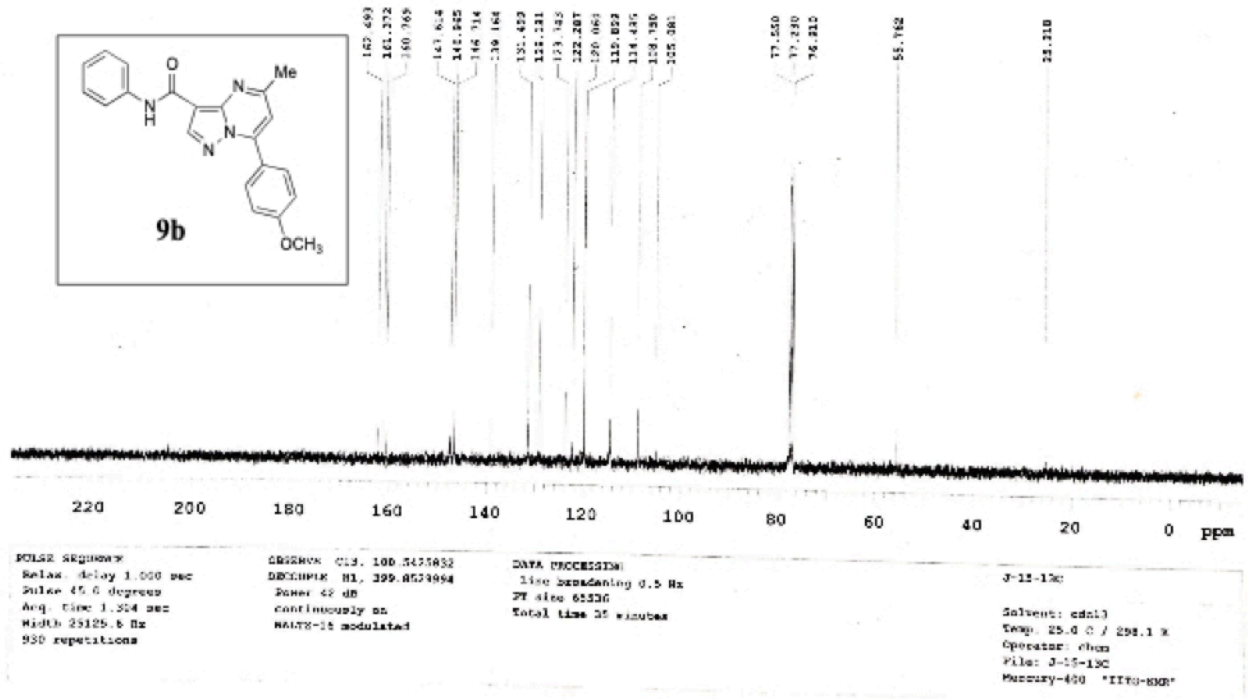
HRMS of 9b



^{1}H NMR of 9b

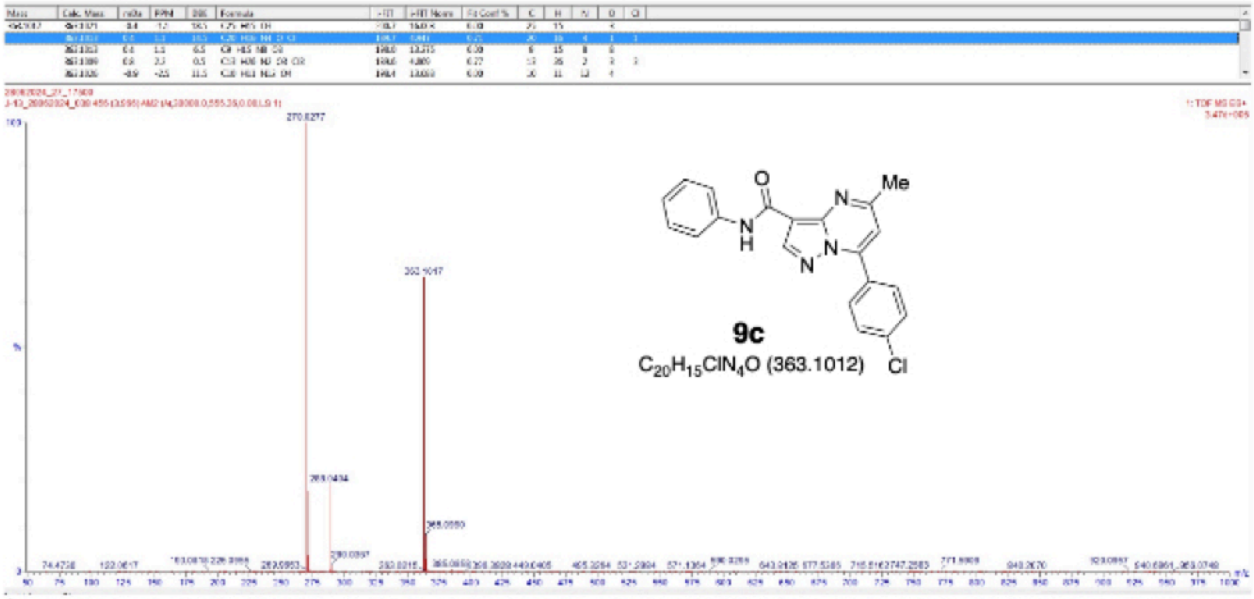


^{13}C NMR of 9b



7-(4-Chlorophenyl)-5-methyl-*N*-phenylpyrazolo[1,5-*a*]pyrimidine-3-carboxamide (9c)

HRMS of 9c



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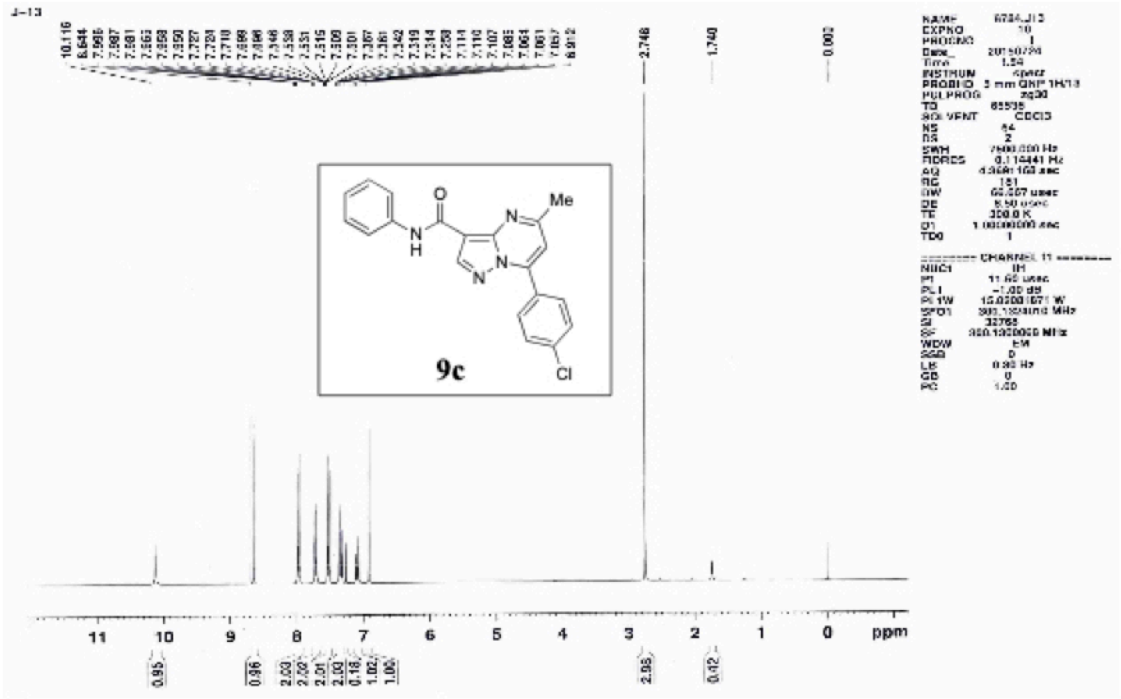

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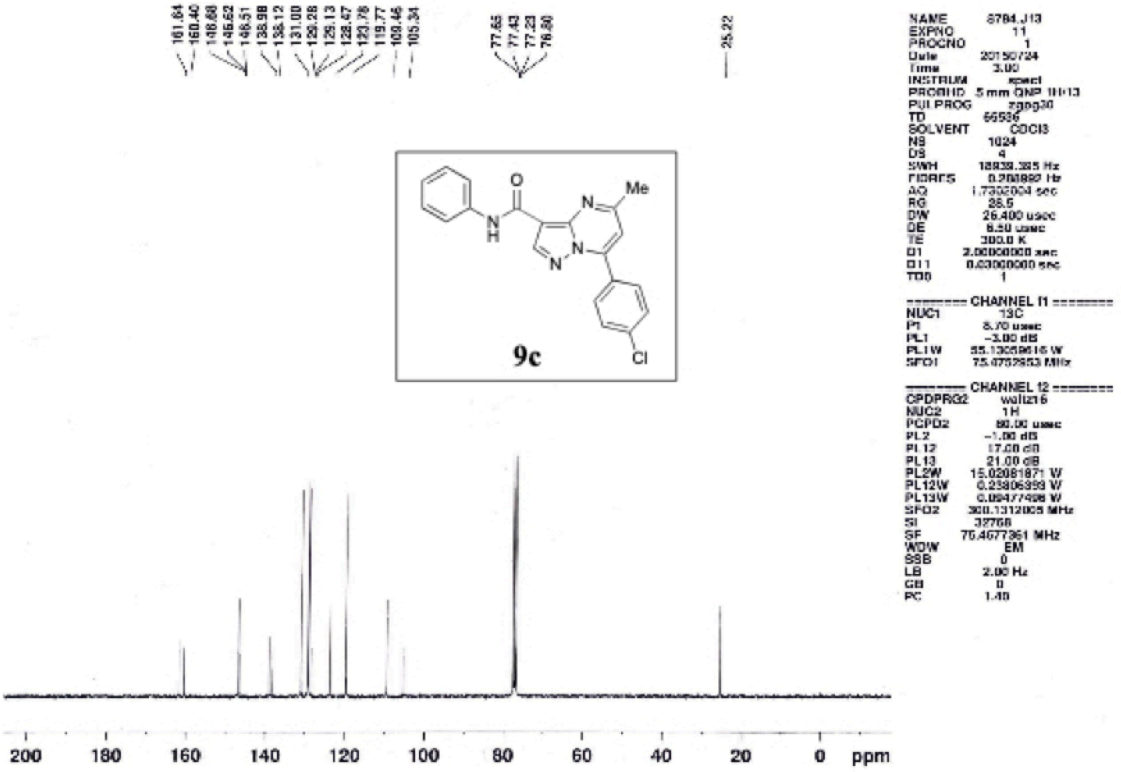
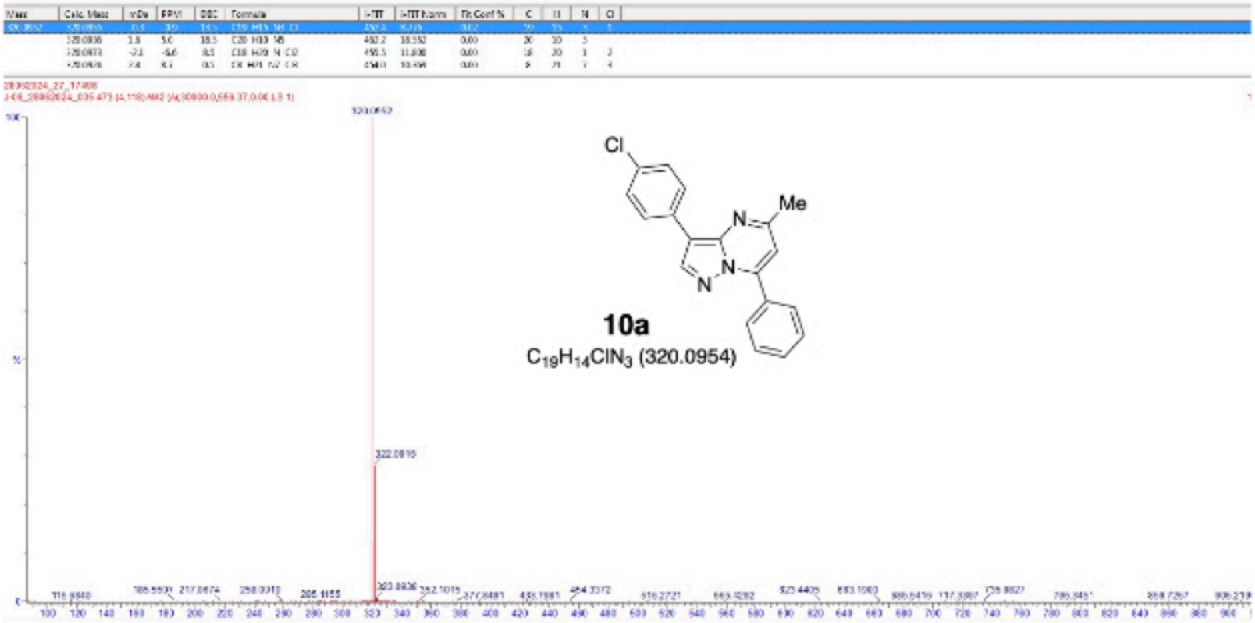
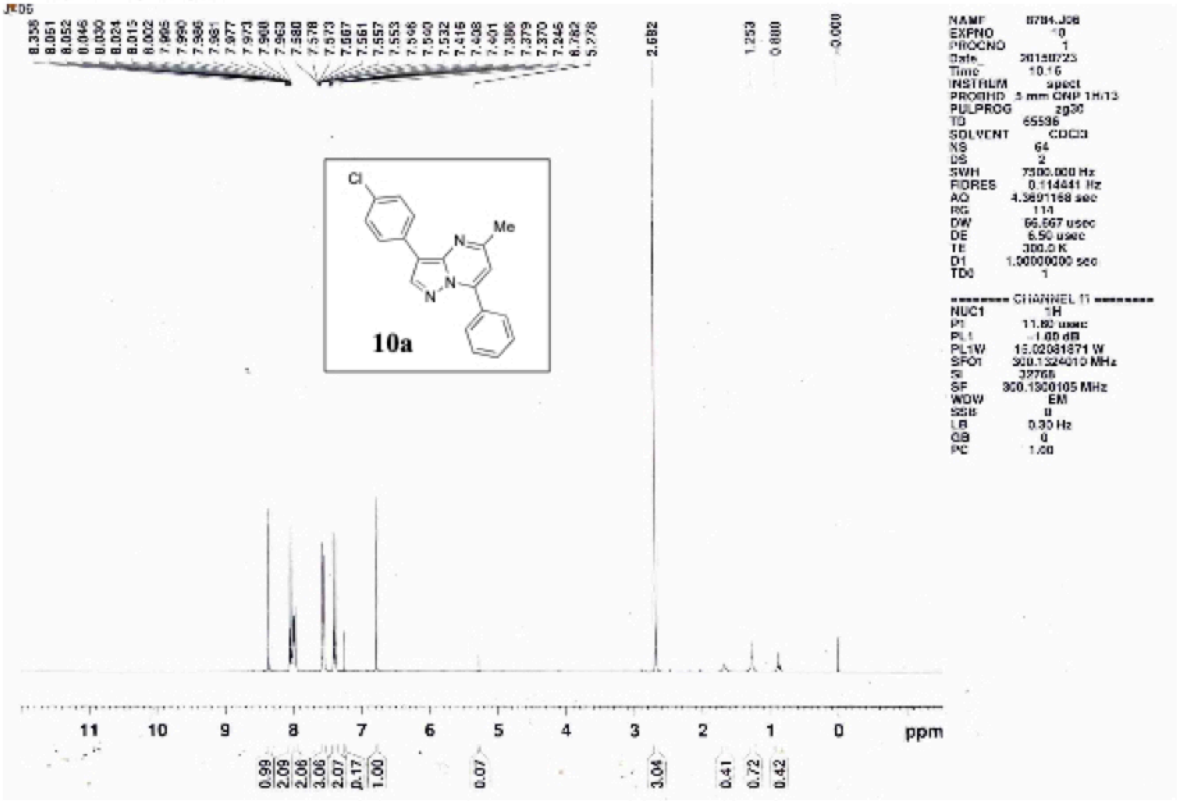


3-(4-Chlorophenyl)-5-methyl-7-phenylpyrazolo[1,5-*a*]pyrimidine (10a)

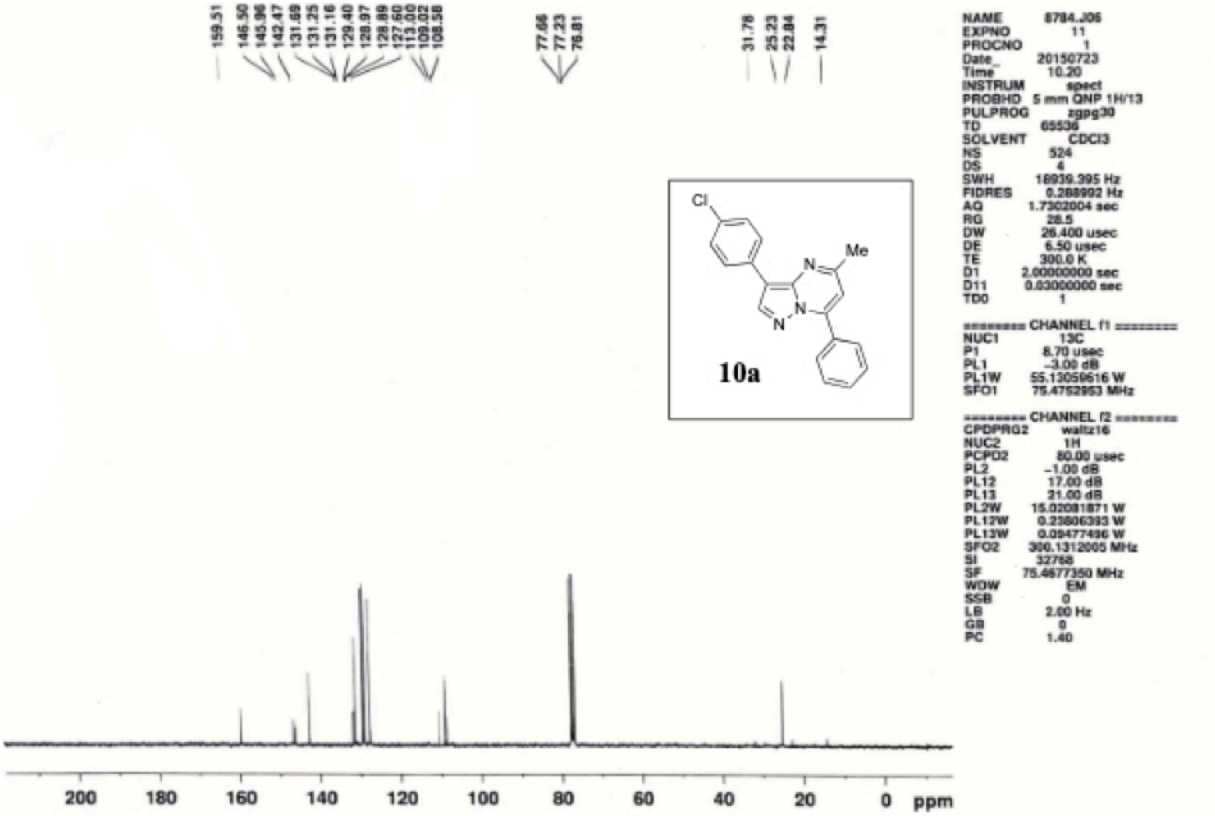
HRMS of 10a



^{1}H NMR of 10a



^{13}C NMR of 10a



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FIDRES 0.288992 Hz
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DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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PL1 -3.00 dB
PL1W 55.13059616 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
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PCPD2 80.00 usec
PL2 -1.00 dB
PL12 17.00 dB
PL13 21.00 dB
PL2W 15.02081871 W
PL12W 0.23806393 W
PL13W 0.09477496 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677350 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
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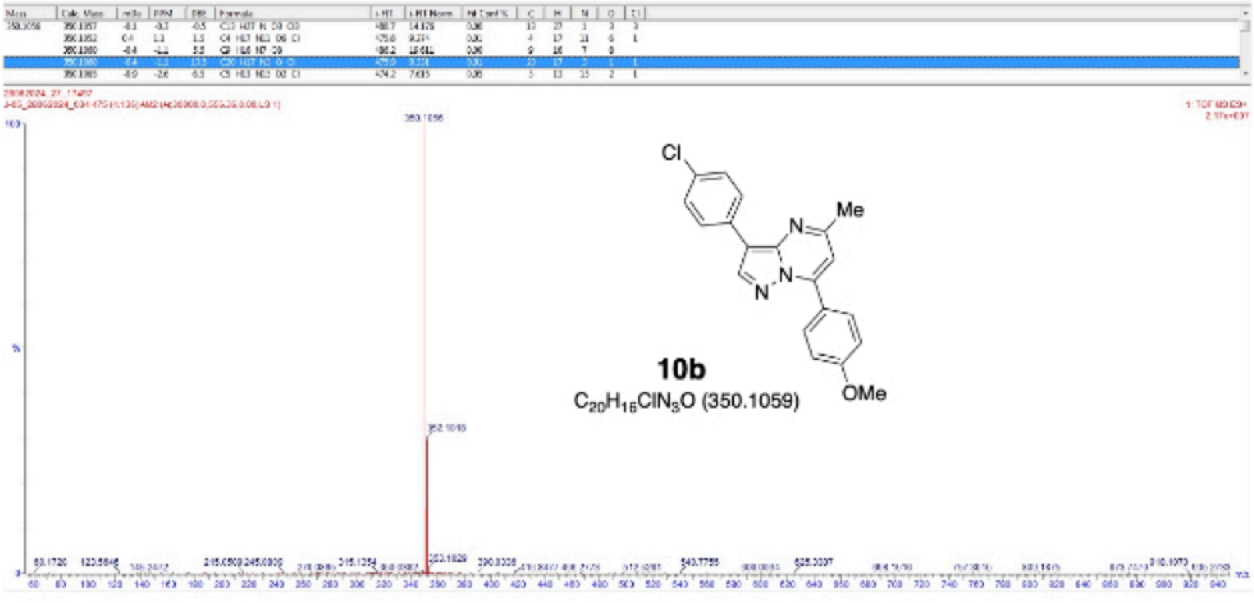
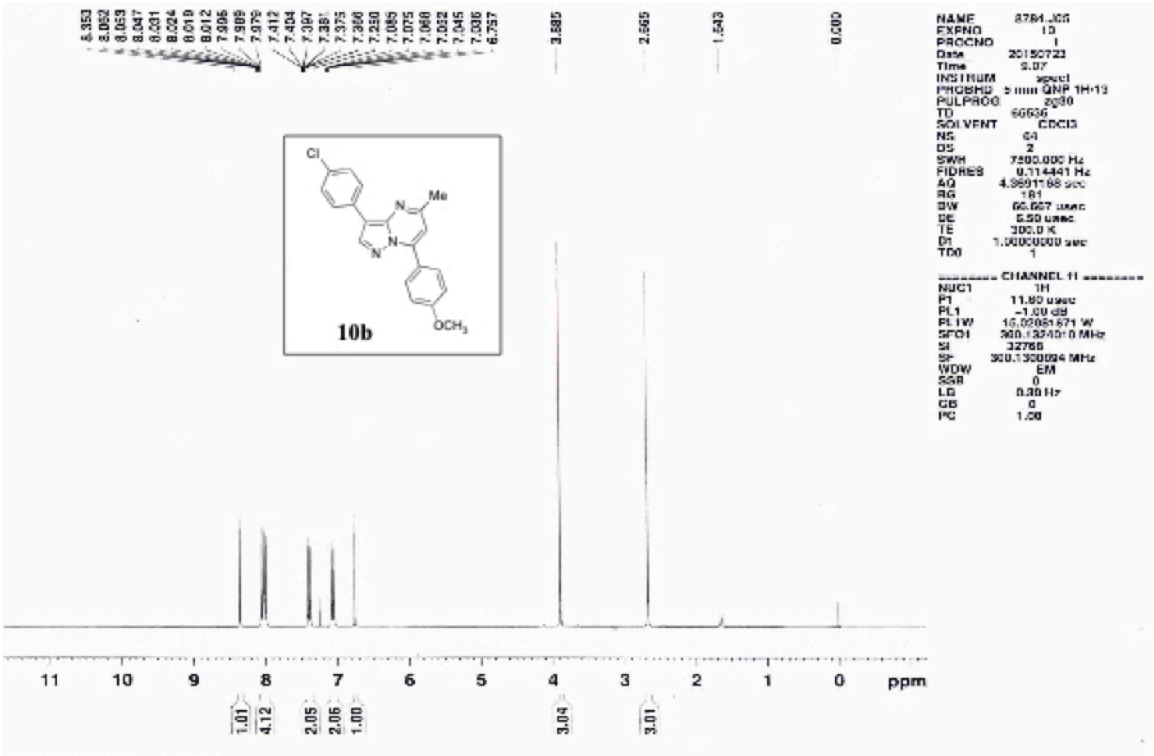
3-(4-Chlorophenyl)-7-(4-methoxyphenyl)-5-methylpyrazolo[1,5-*a*]pyrimidine (10b)

HRMS of 10b



^{1}H NMR of 10b



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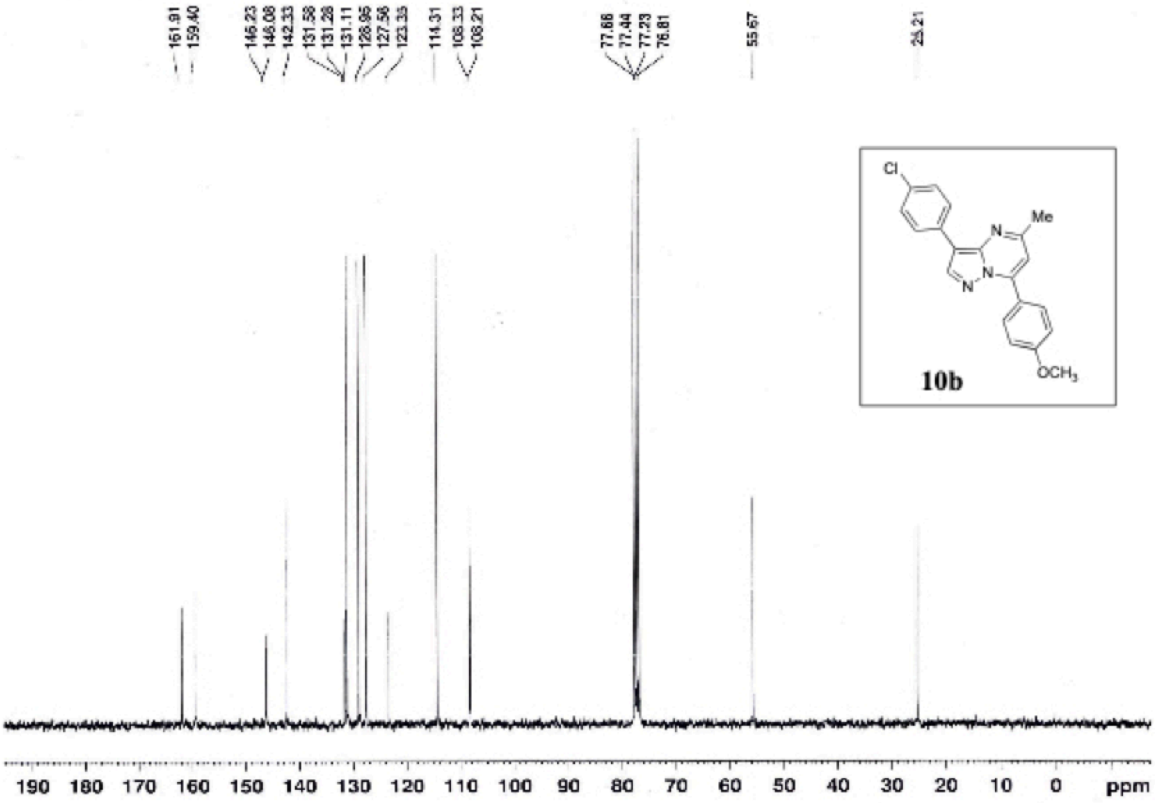
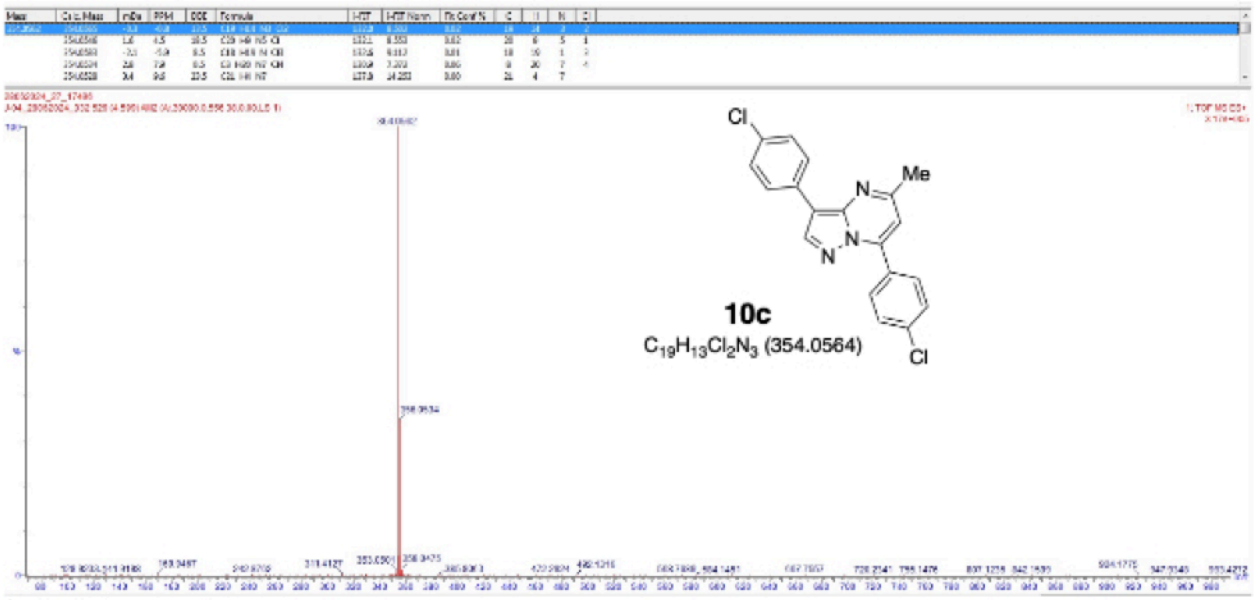
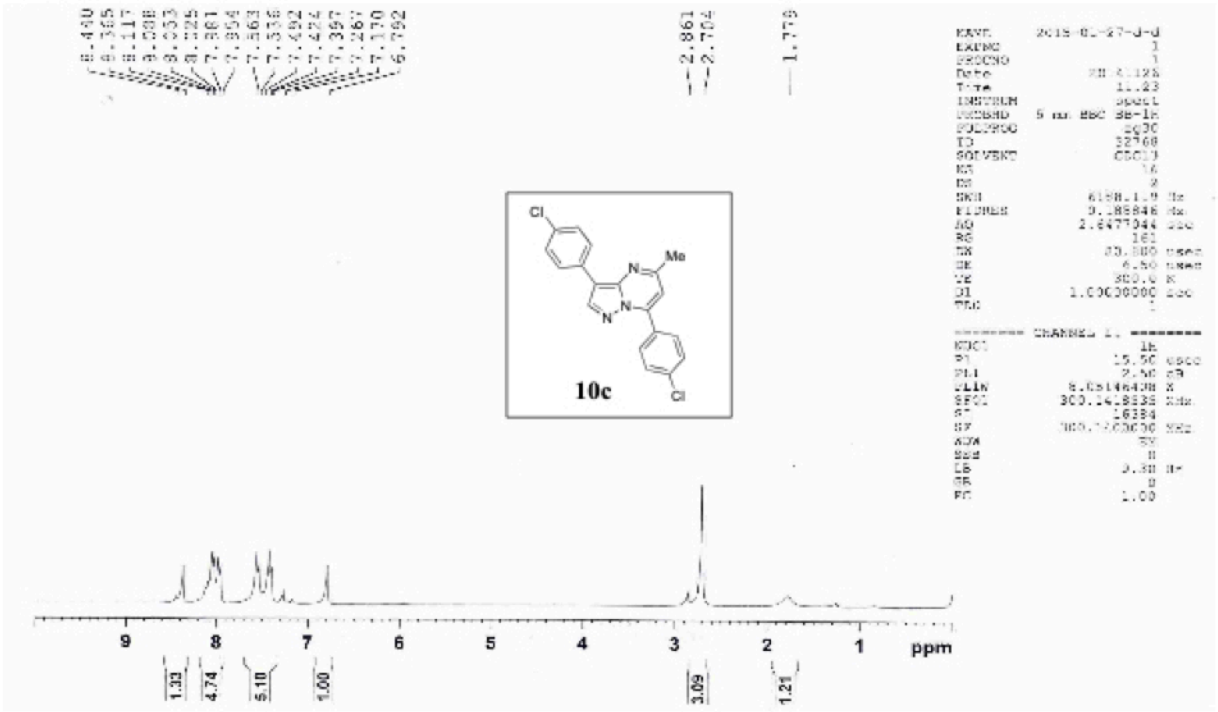


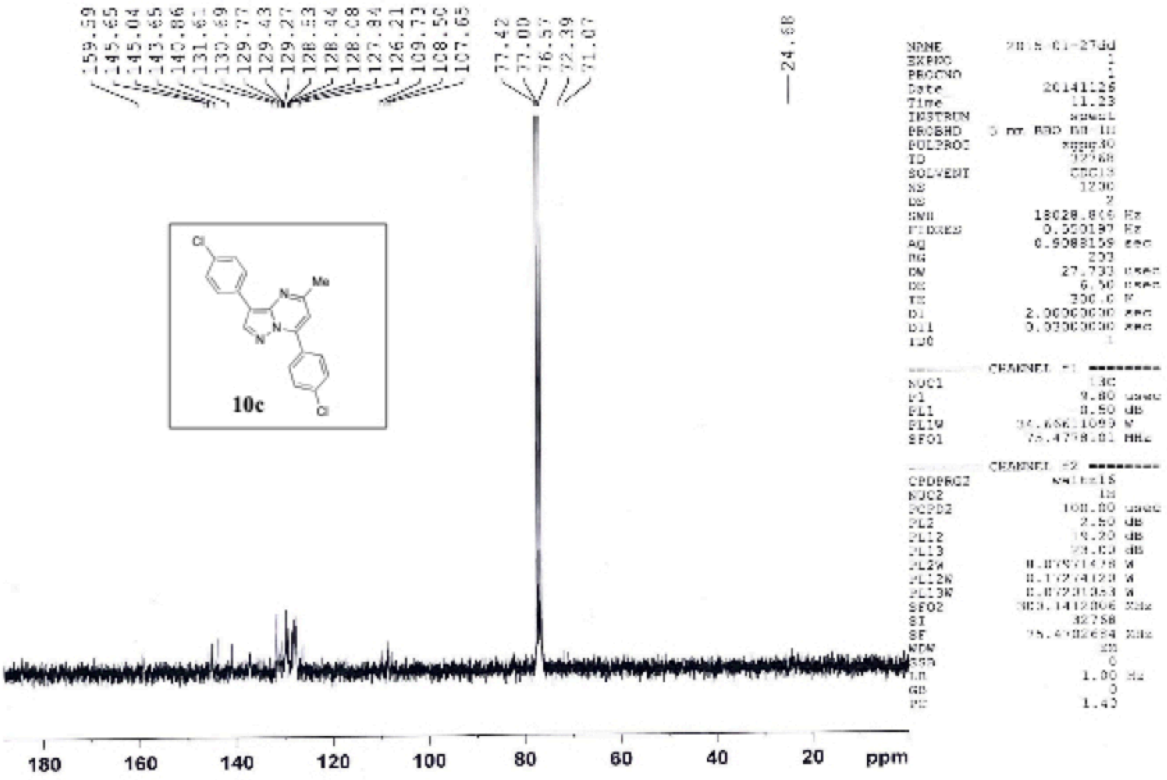
3,7-Bis(4-chlorophenyl)-5-methylpyrazolo[1,5-*a*]pyrimidine (10c)
HRMS of 10c



^{1}H NMR of 10c

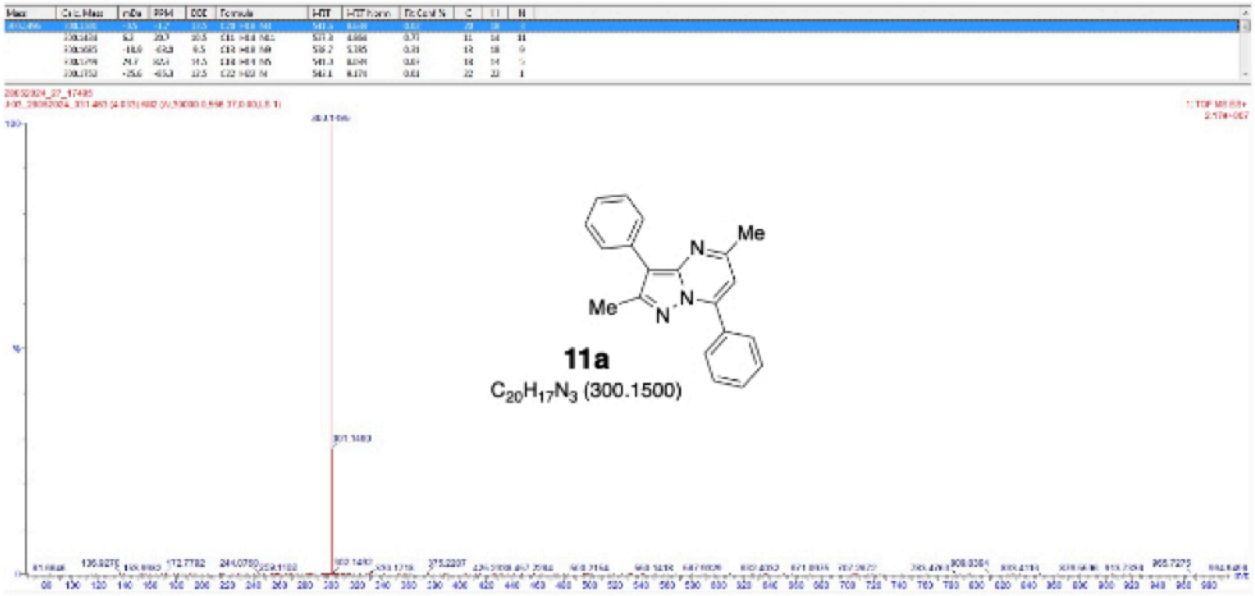


^{13}C NMR of 10c

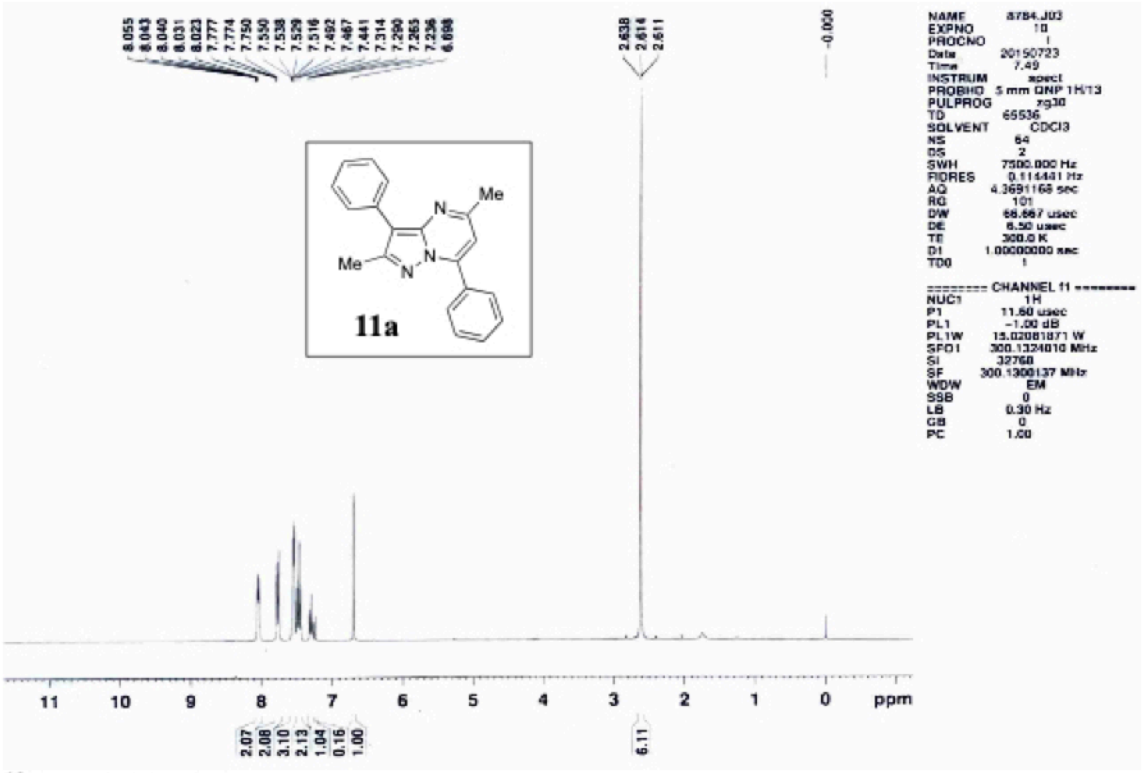


2,5-Dimethyl-3,7-diphenylpyrazolo[1,5-*a*]pyrimidine (11a)

HRMS of 11a



^{1}H NMR of 11a



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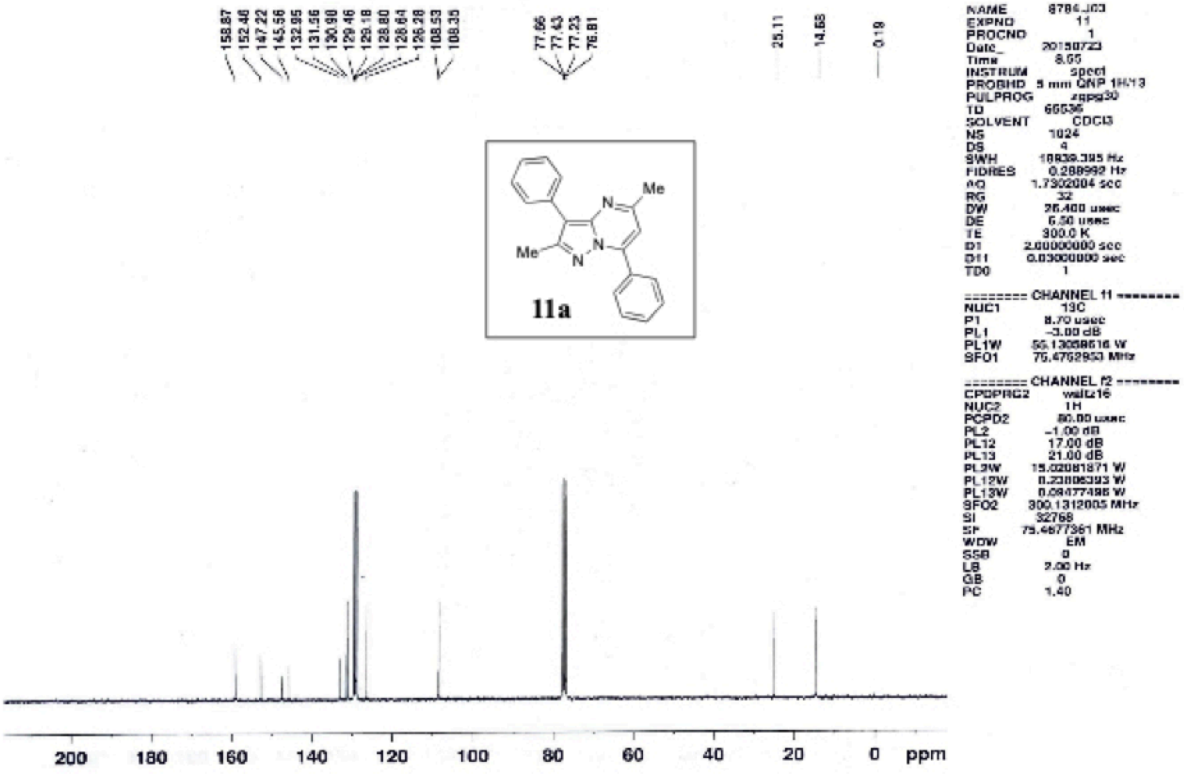
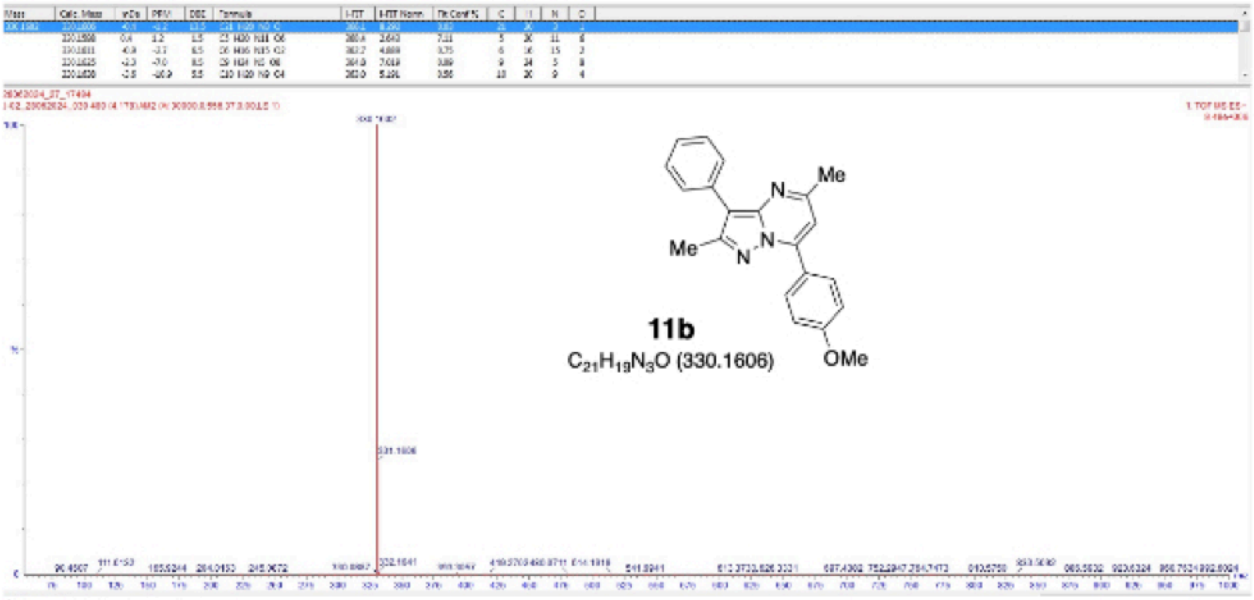
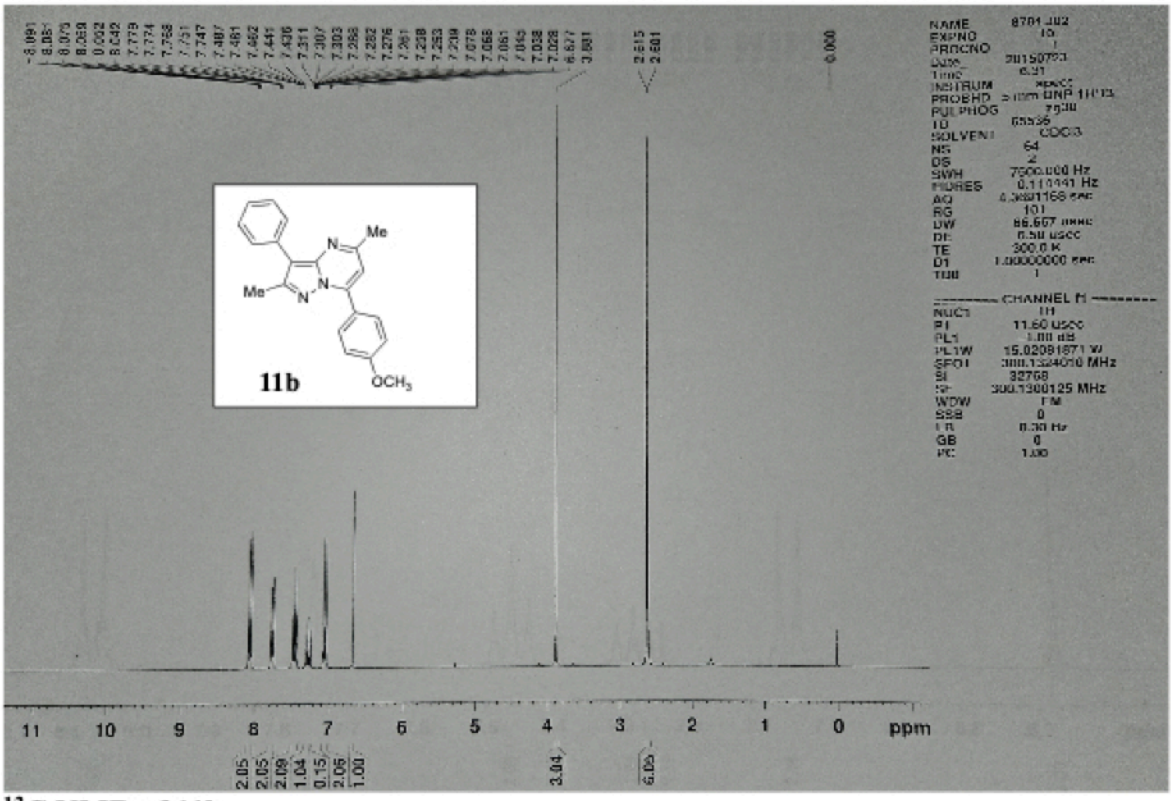


7-(4-Methoxyphenyl)-2,5-dimethyl-3-phenylpyrazolo[1,5-*a*]pyrimidine (11b)

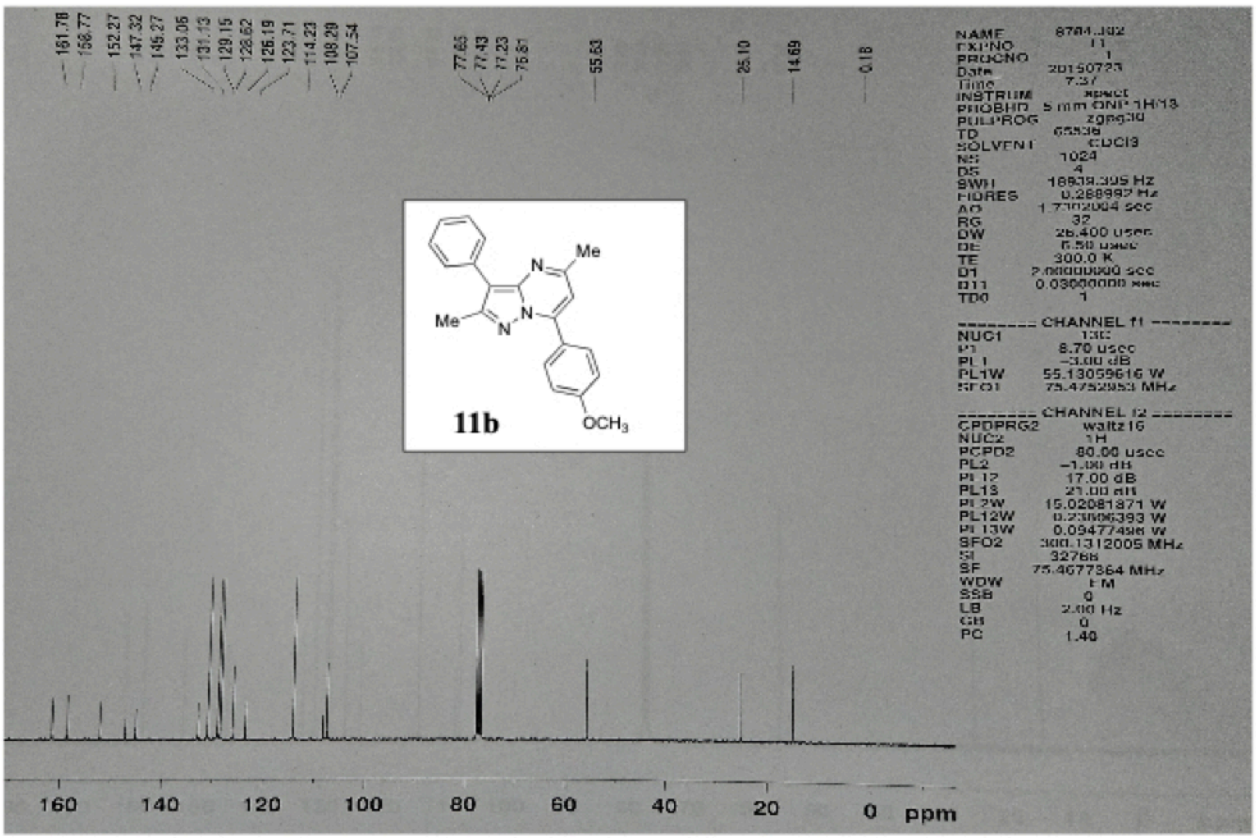
HRMS of 11b



^{1}H NMR of 11b

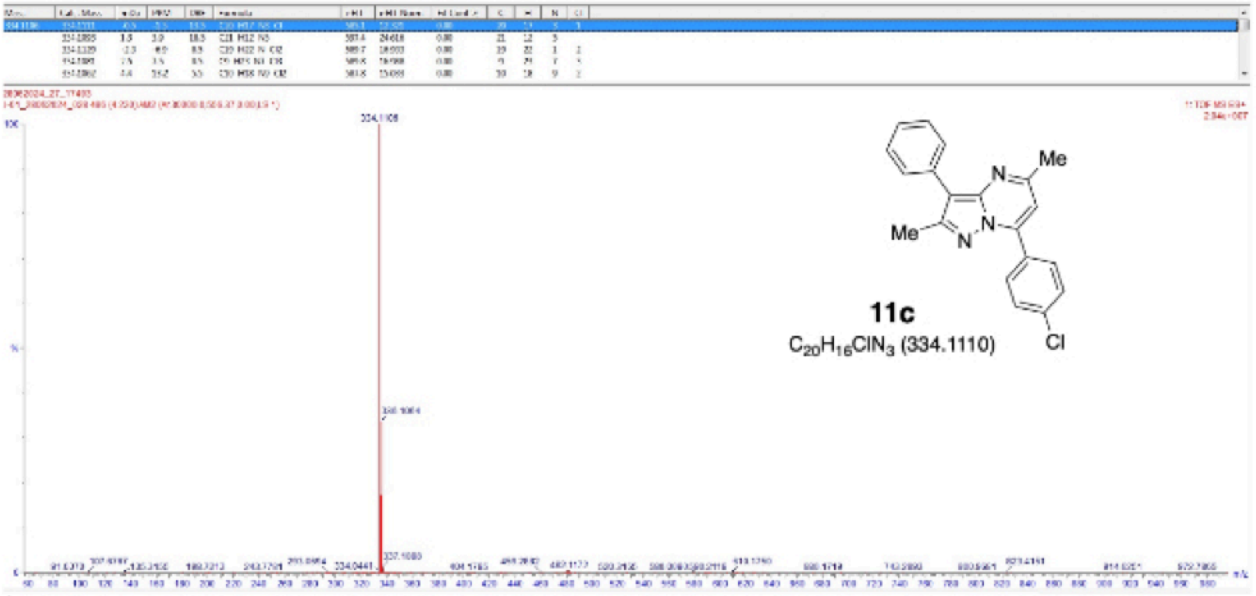


^{13}C NMR of 11b

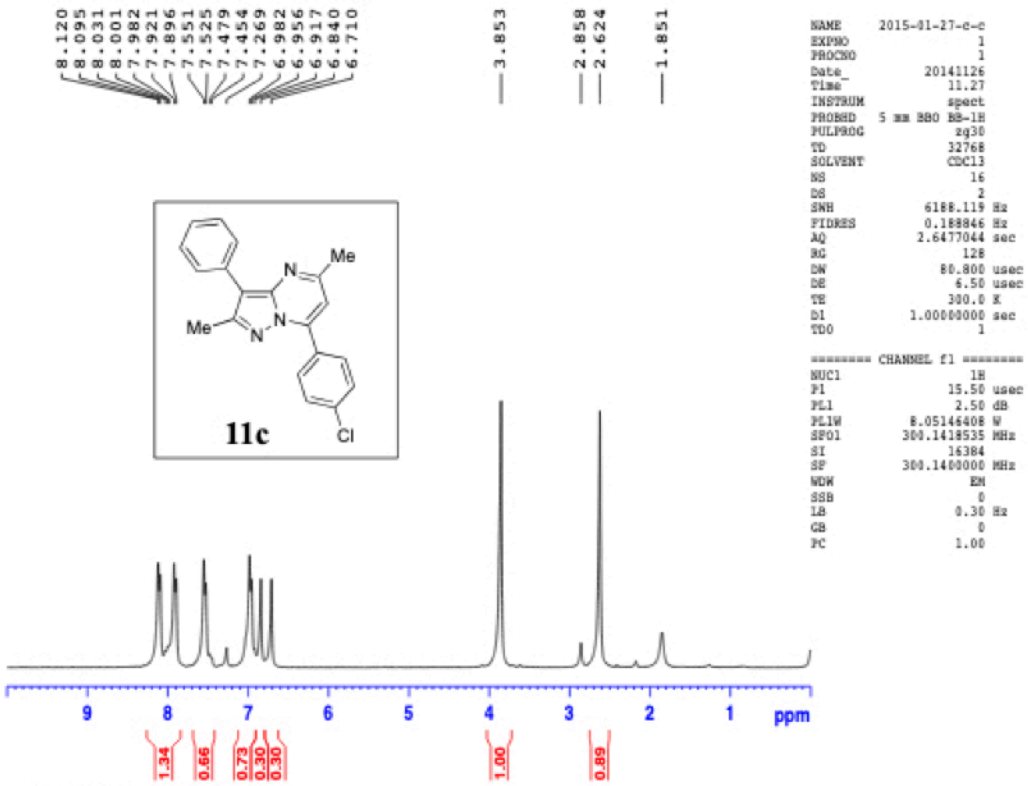


7-(4-Chlorophenyl)-2,5-dimethyl-3-phenylpyrazolo[1,5-*a*]pyrimidine (11c)

Mass of 11c



^{1}H NMR of 11c

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FIDRES             0.188846 Hz
AQ                 2.6477044 sec
RG                       128
DW                    80.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                    15.50 usec
PL1                    2.50 dB
PL1W               8.05146408 W
SFO1              300.1418535 MHz
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WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00
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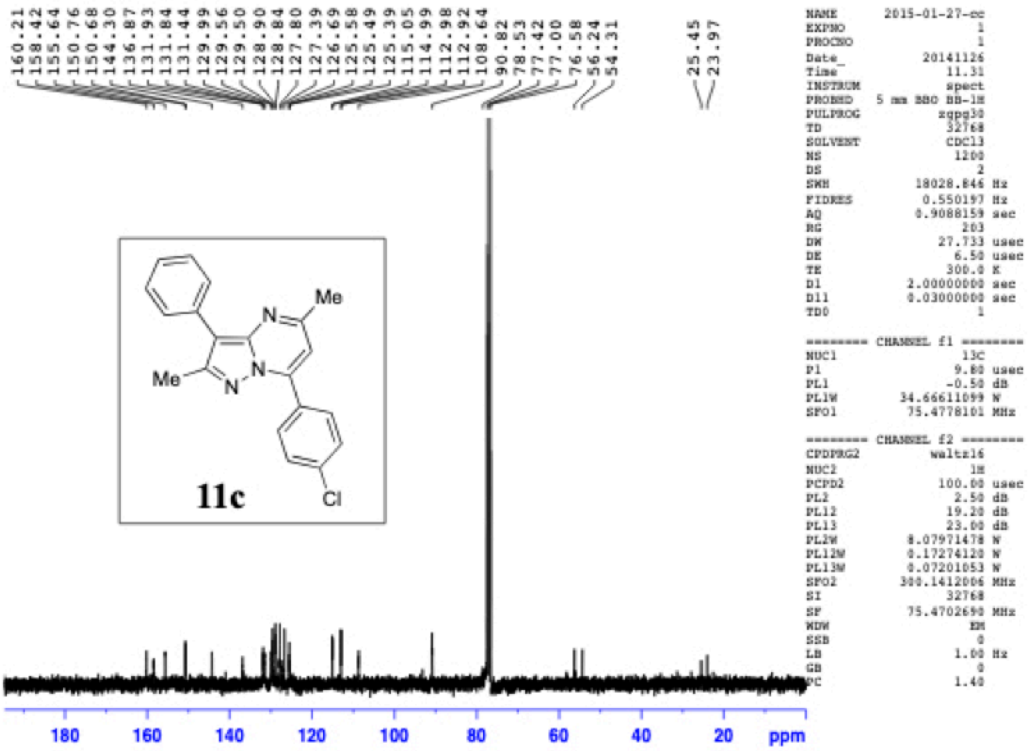
^{13}C NMR of 11c

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RG                       203
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DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

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NUC1                      13C
P1                     9.80 usec
PL1                   -0.50 dB
PL1W              34.66611099 W
SFO1              75.4778101 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                100.00 usec
PL2                    2.50 dB
PL12                  19.20 dB
PL13                  23.00 dB
PL2W               8.07971478 W
PL12W              0.17274120 W
PL13W              0.07201053 W
SFO2              300.1412006 MHz
SI                        32768
SF                75.4702690 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                      1.40
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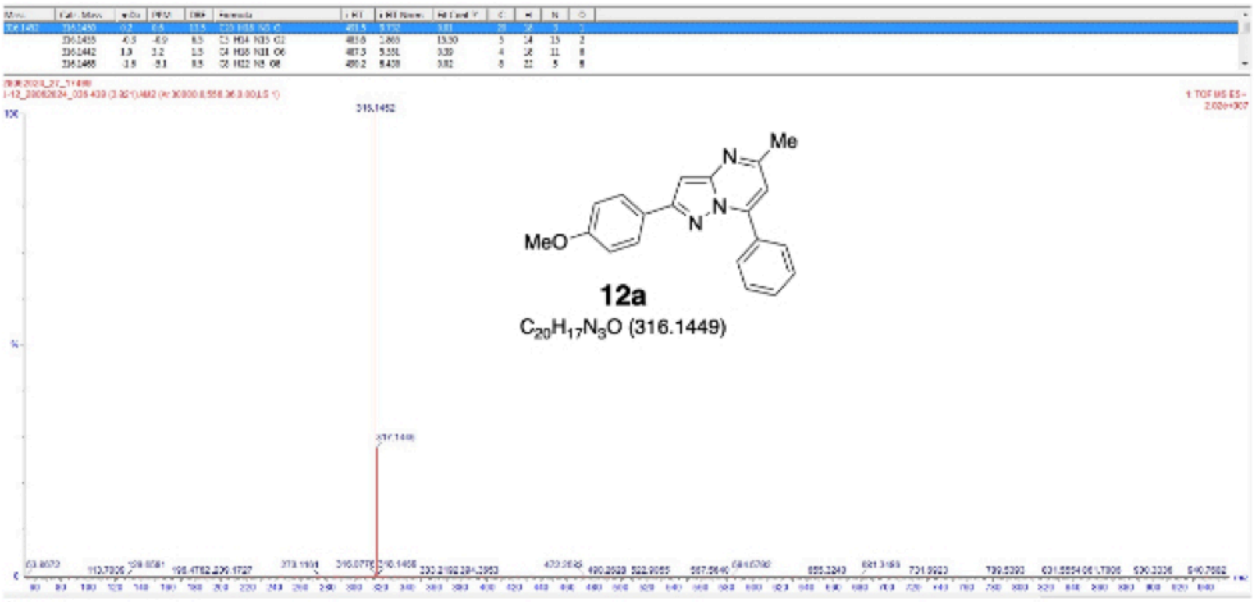
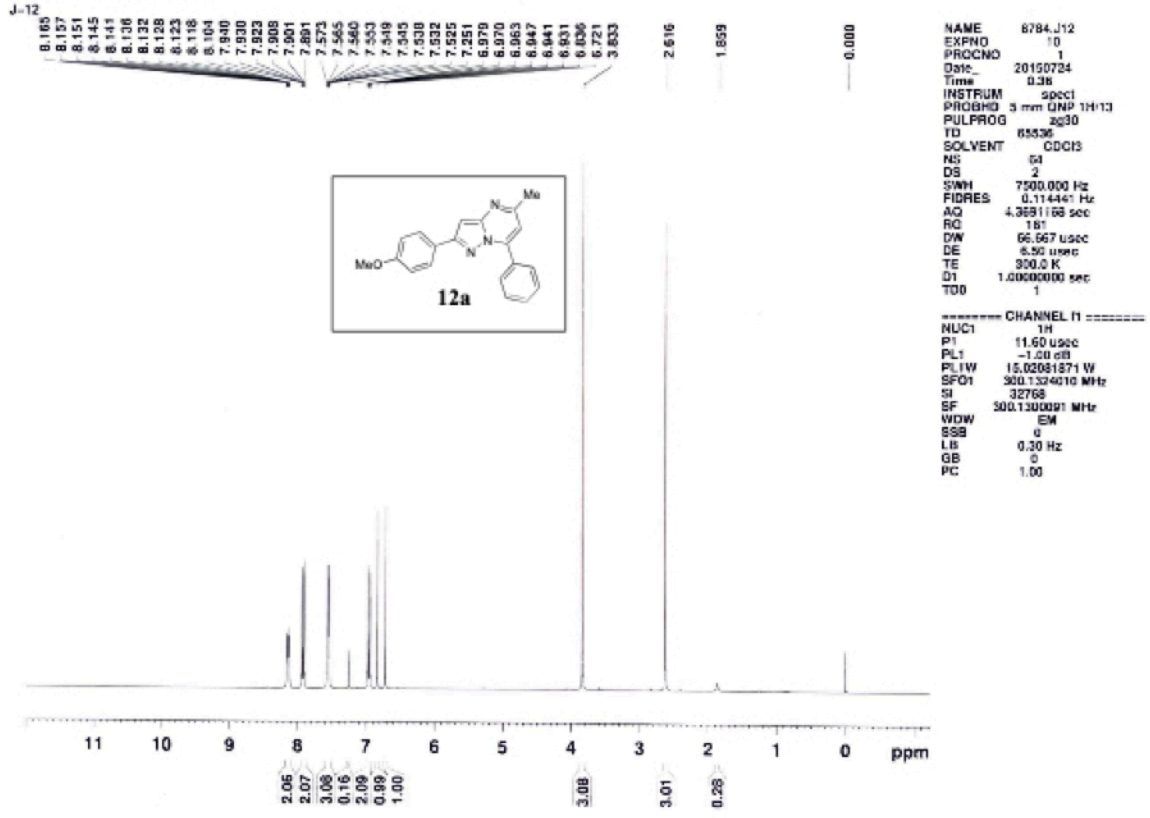
2-(4-Methoxyphenyl)-5-methyl-7-phenylpyrazolo[1,5-*a*]pyrimidine (12a)

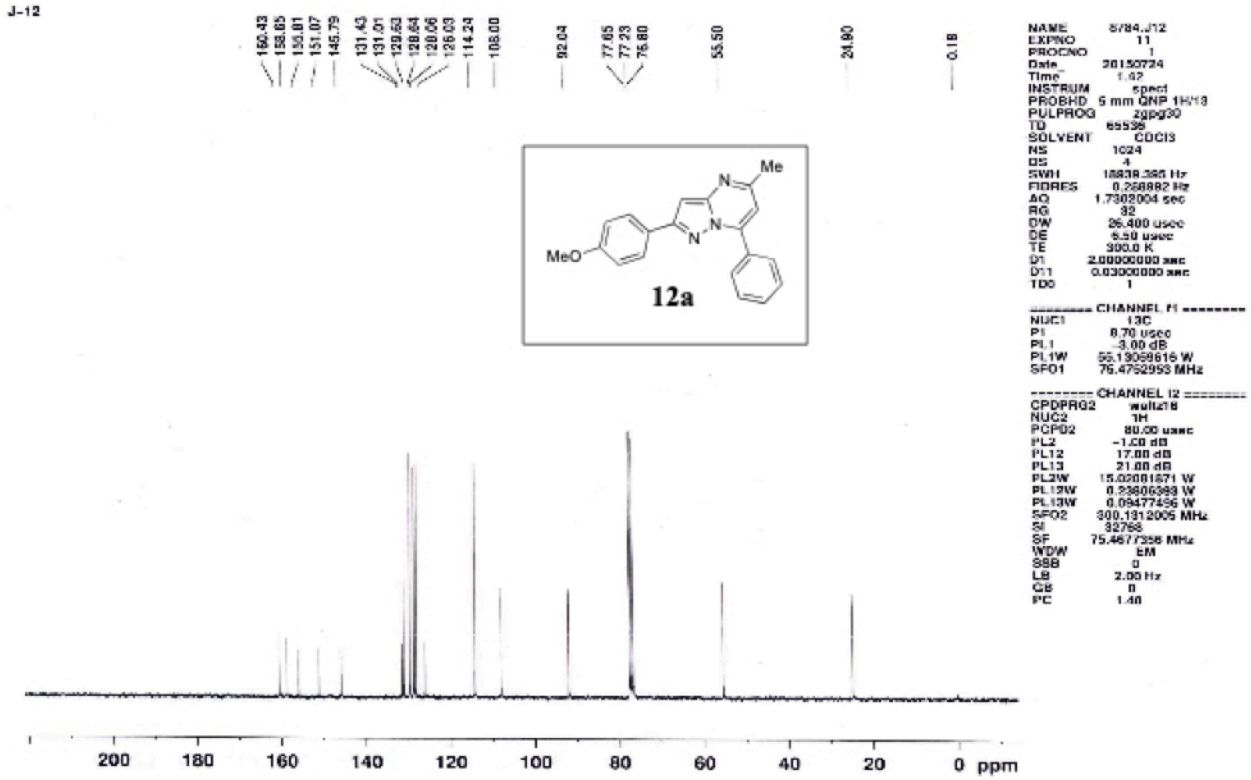
Mass Spectrum of 12a



^{1}H NMR of 12a

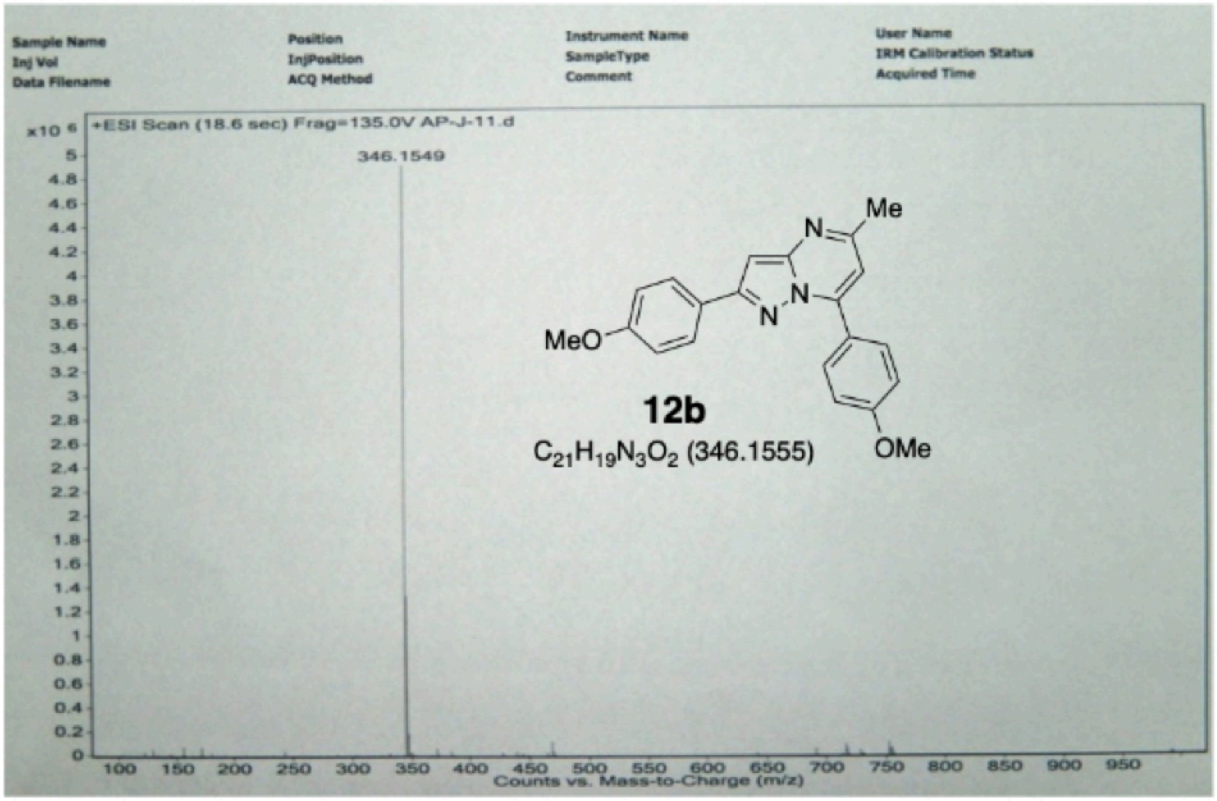


^{13}C NMR of 12a

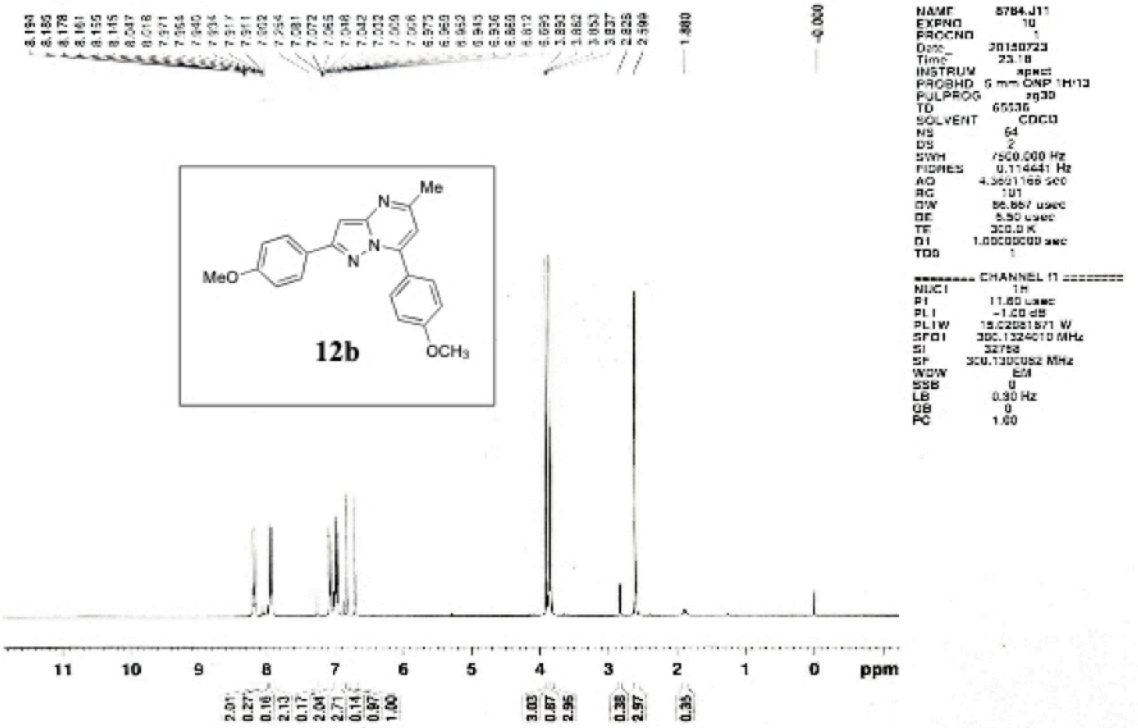


2,7-Bis(4-methoxyphenyl)-5-methylpyrazolo[1,5-*a*]pyrimidine (12b)

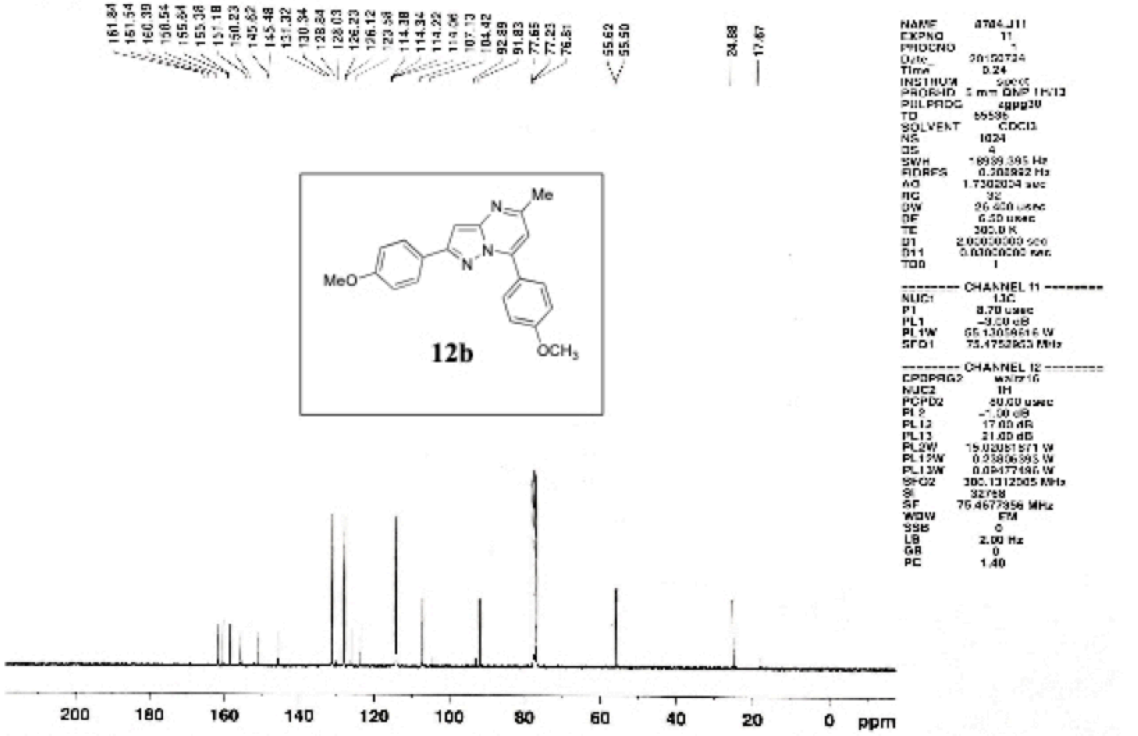
HRMS of 12b



^{1}H NMR of 12b

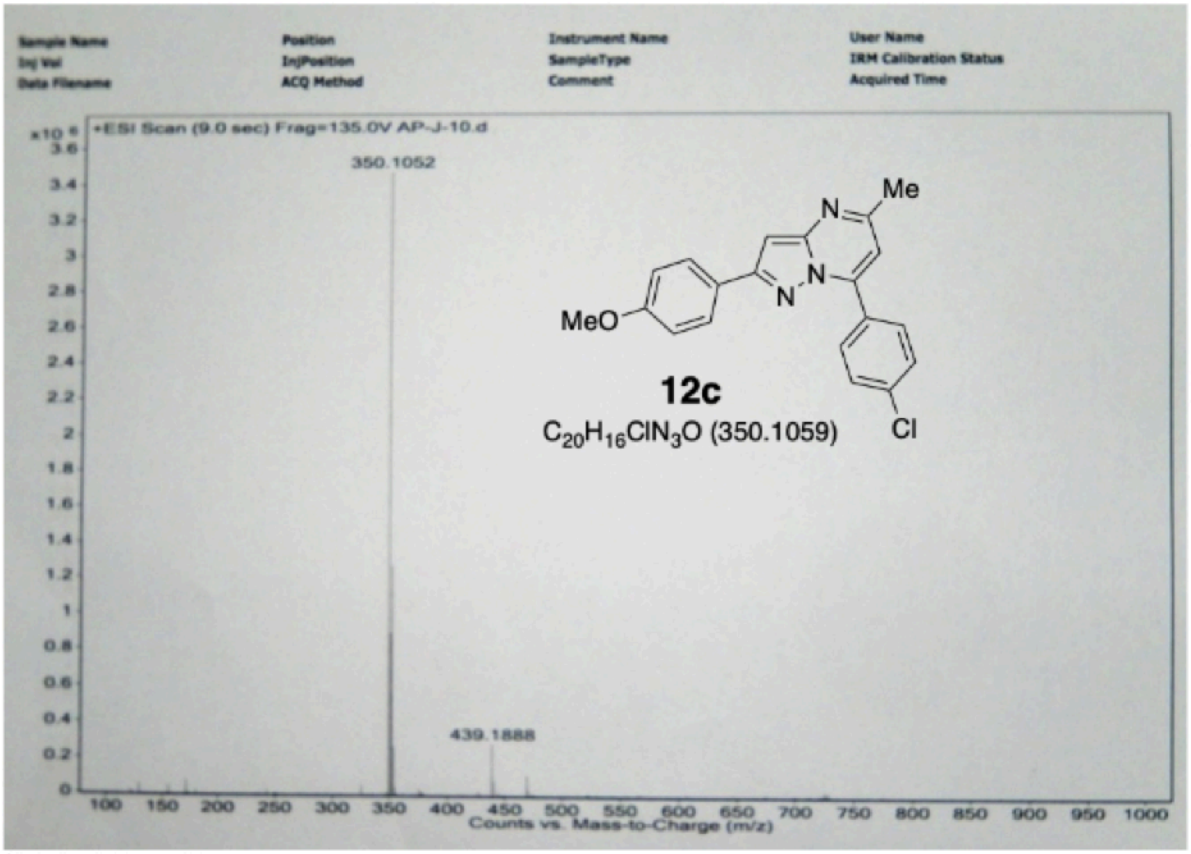


^{13}C NMR of 12b

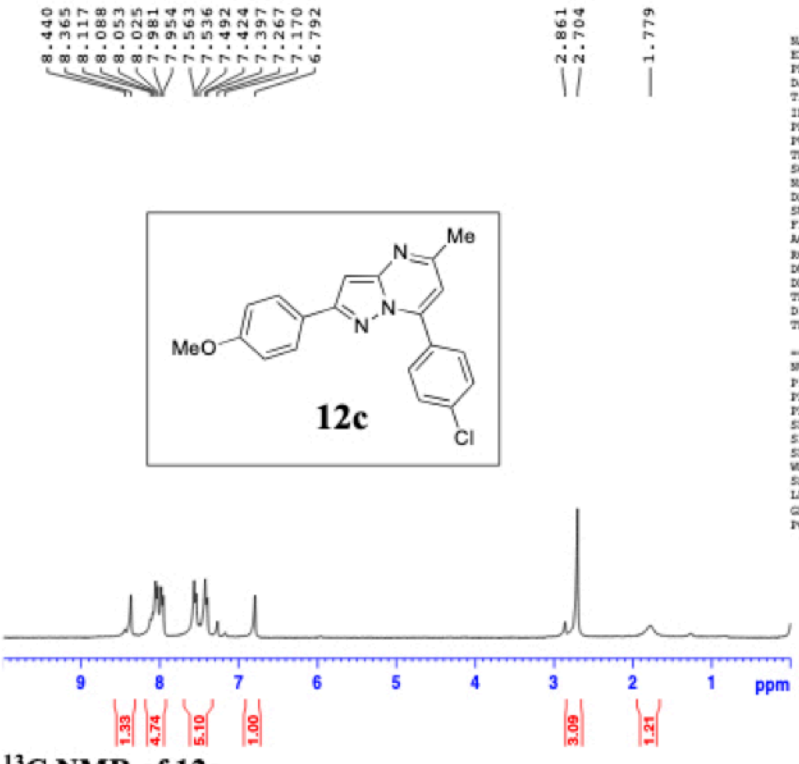


7-(4-Chlorophenyl)-2-(4-methoxyphenyl)-5-methylpyrazolo[1,5-*a*]pyrimidine (12c)

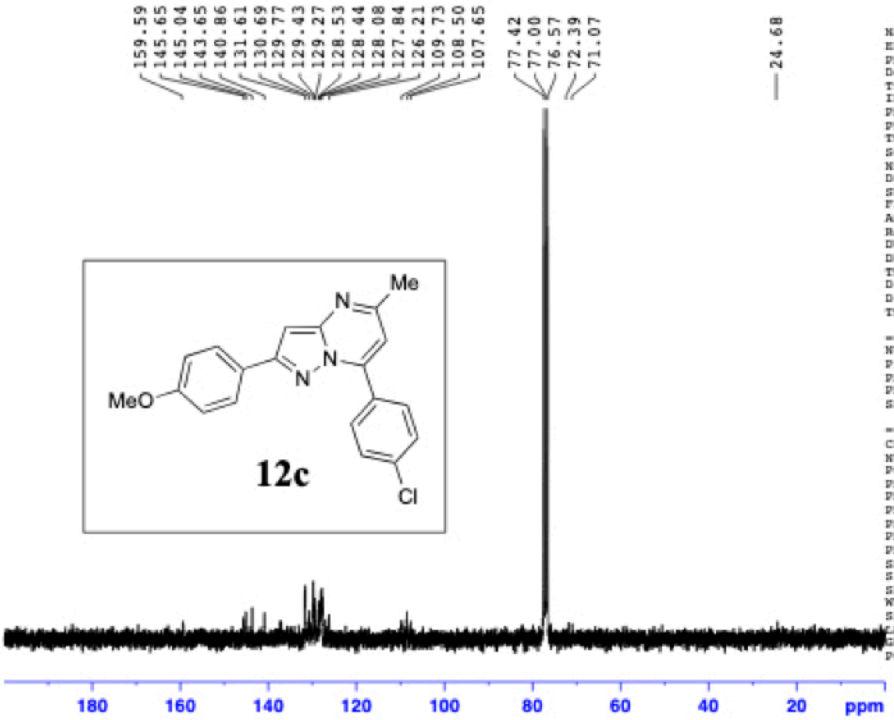
HRMS of 12c



^{1}H NMR of 12c



^{13}C NMR of 12c

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NAME          2015-01-27dd
EXPNO                    1
PROCNO                   1
Date_             20141126
Time                 11.23
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    1200
DS                       2
SWH              18028.846 Hz
FIDRES           0.550197 Hz
AQ               0.9088159 sec
RG                     203
DW                27.733 usec
DE                 6.50 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.80 usec
PL1                  -0.50 dB
PL1W         34.66611099 W
SFO1          75.4778101 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               100.00 usec
PL2                   2.50 dB
PL12                 19.20 dB
PL13                 23.00 dB
PL2W          8.07971478 W
PL12W         0.17274120 W
PL13W         0.07201053 W
SFO2         300.1412006 MHz
SI                   32768
SF            75.4702684 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```