

## 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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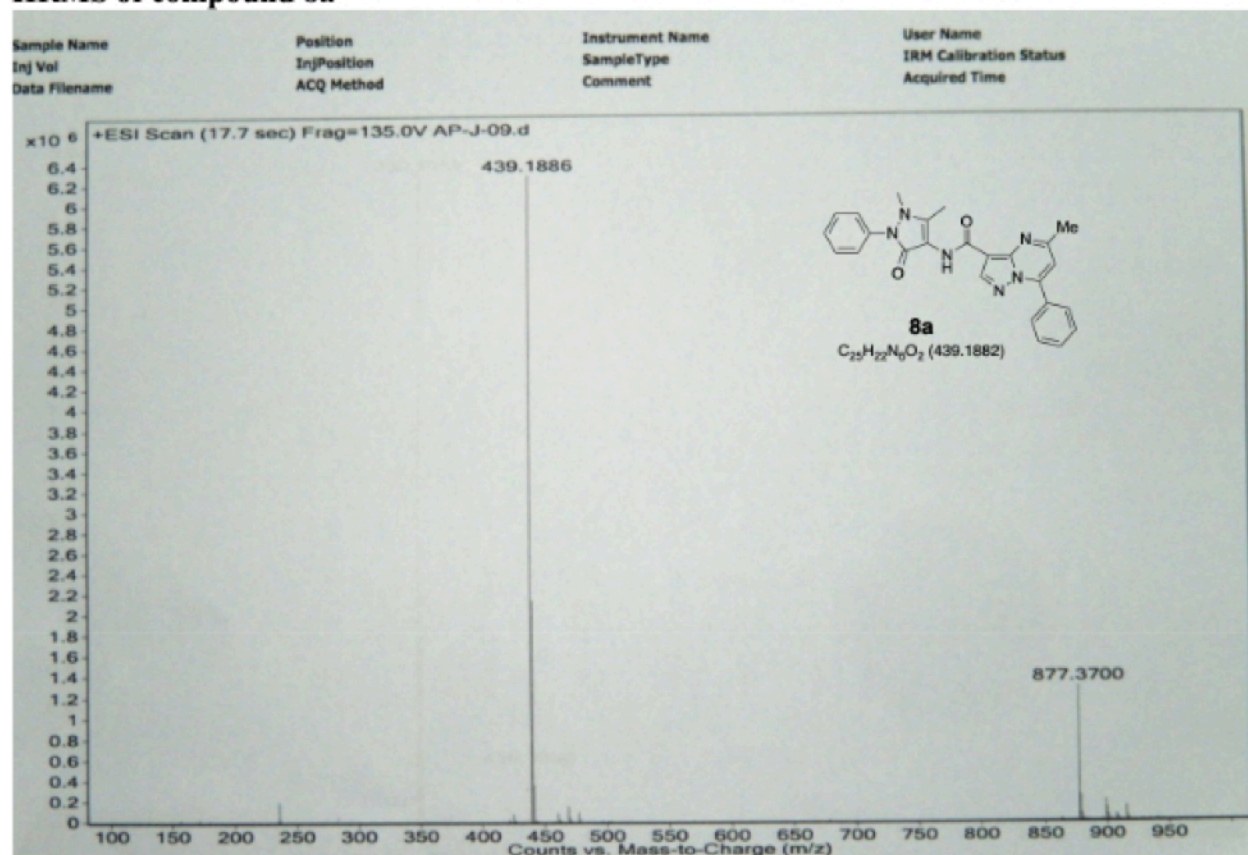
<sup>a</sup>*Organic Research Lab., Department of Chemistry, Assam Don Bosco University, Tapesia Gardens, Sonapur, 782402, Assam India*

<sup>b</sup>*Department of Bio-Sciences, Assam Don Bosco University, Tapesia Gardens, Sonapur, 782402, Assam, India*

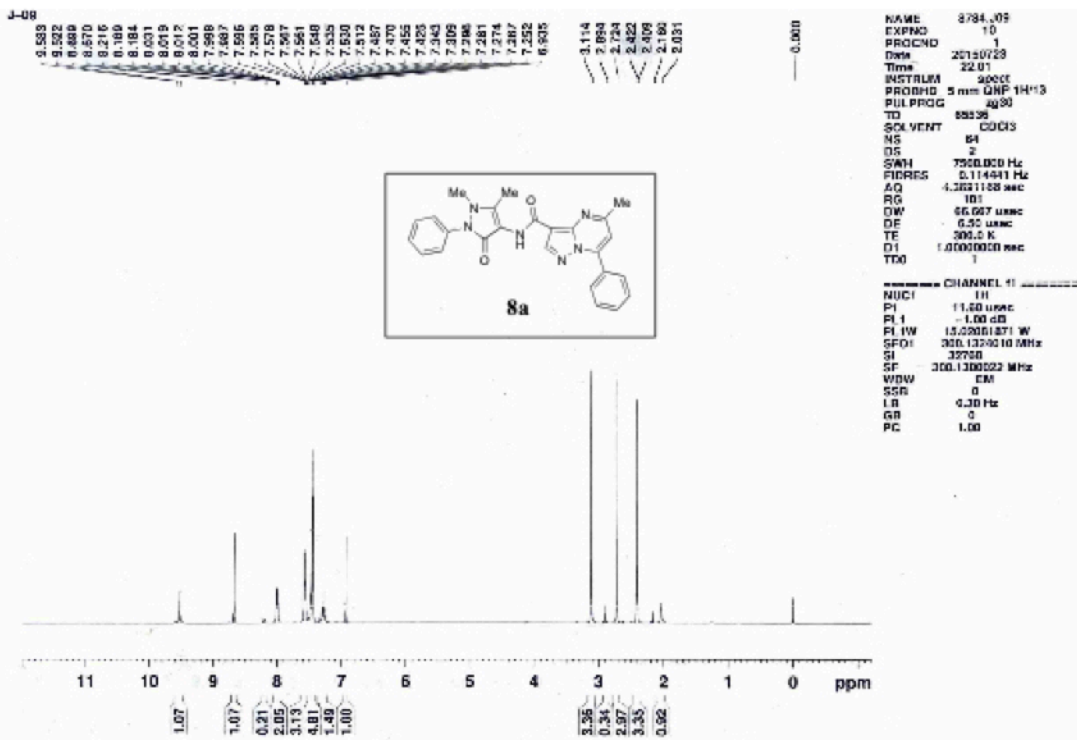
*e-mail: [jnvishwakarma@rediffmail.com](mailto:jnvishwakarma@rediffmail.com)*

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

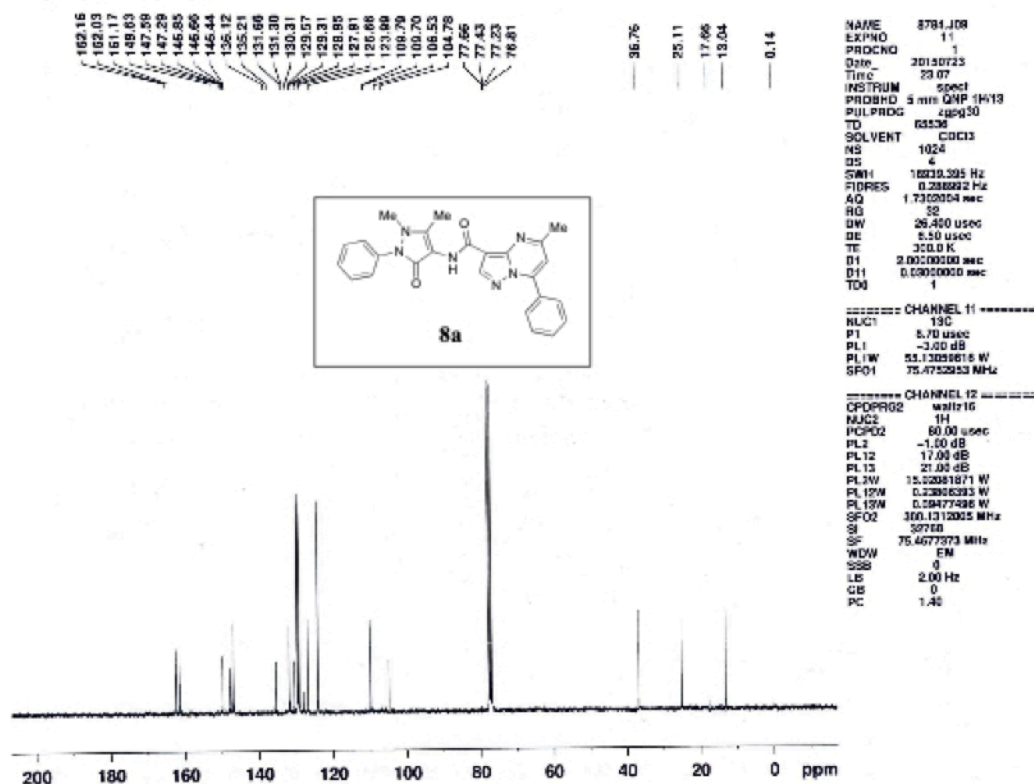
#### HRMS of compound **8a**



#### <sup>1</sup>H NMR of **8a**



**<sup>13</sup>C NMR of 8a**



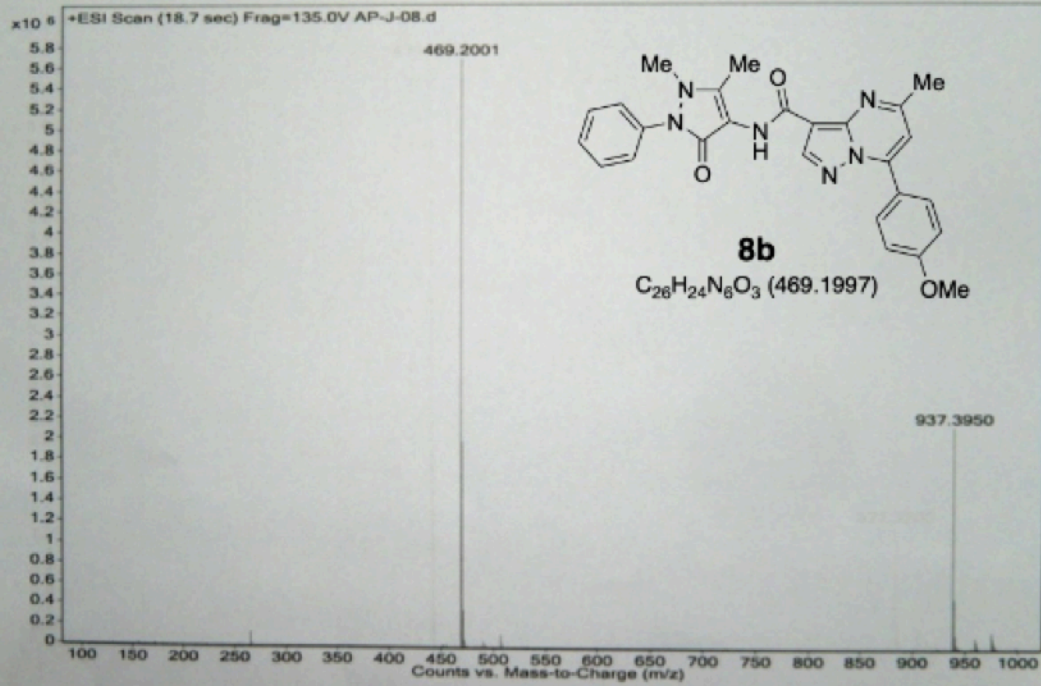
***N*-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)-7-(4-methoxyphenyl)-5-methylpyrazolo [1,5-*a*]pyrimidine-3-carboxamide (**8b**)**  
**HRMS of compound 8b**

Sample Name  
Inj Vol  
Data Filename

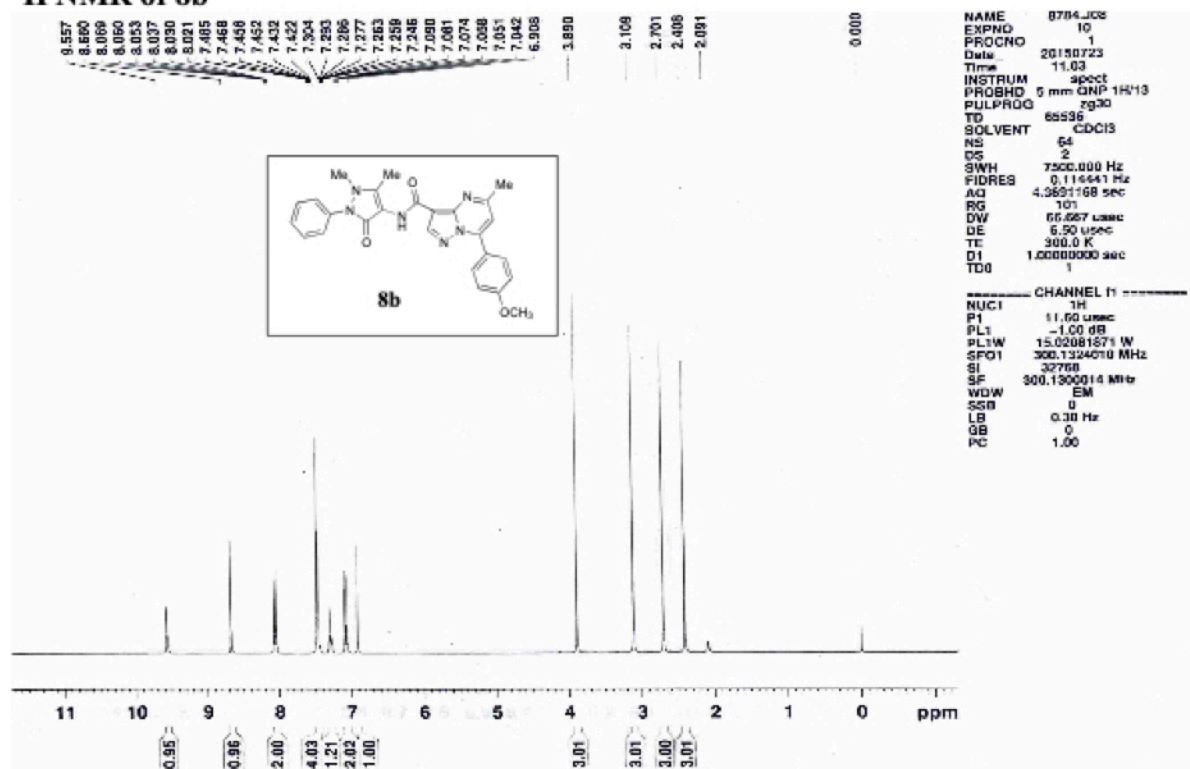
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

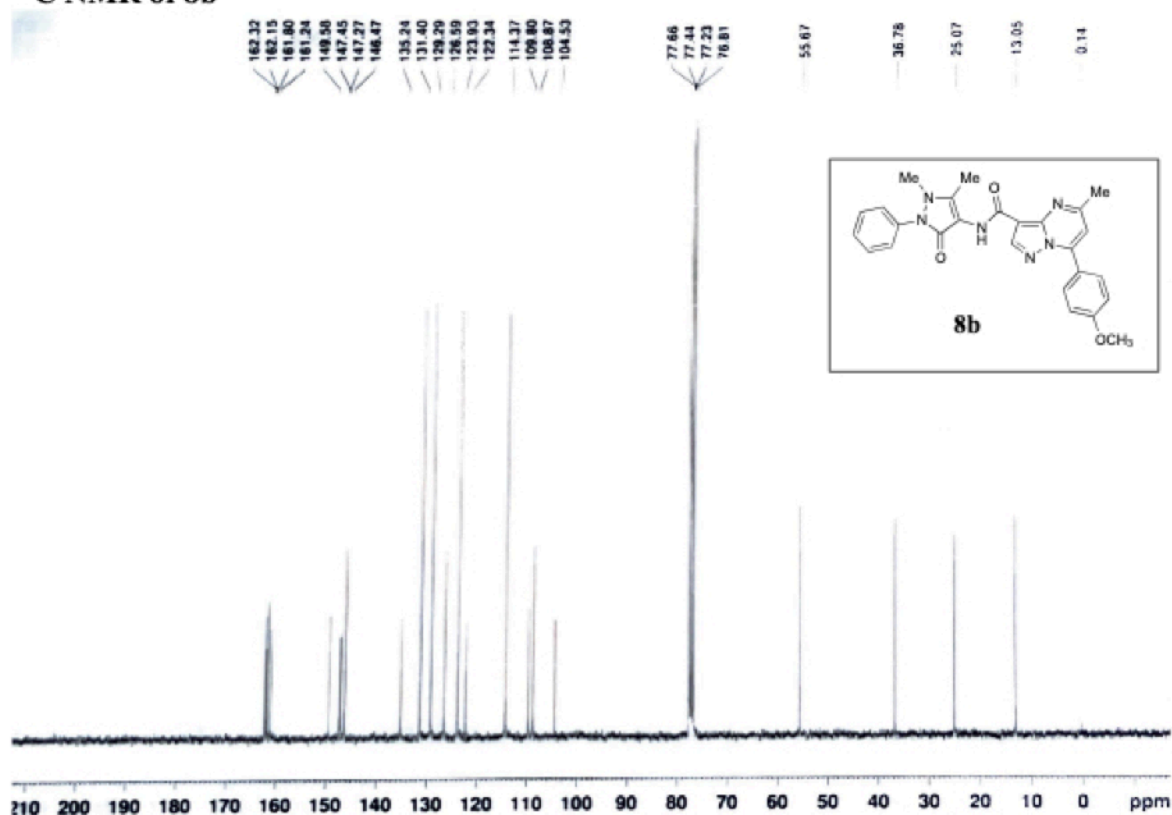
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Acquired Time



### <sup>1</sup>H NMR of 8b

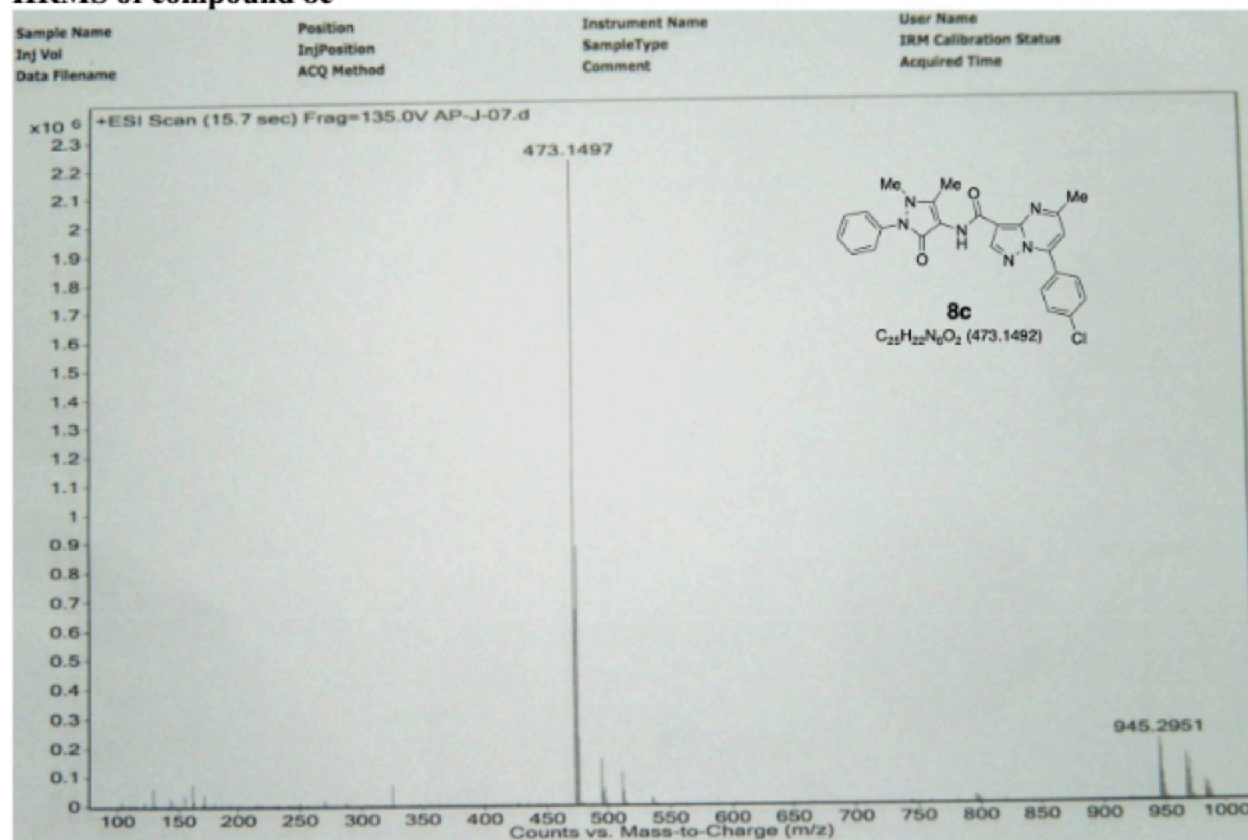


### <sup>13</sup>C NMR of 8b

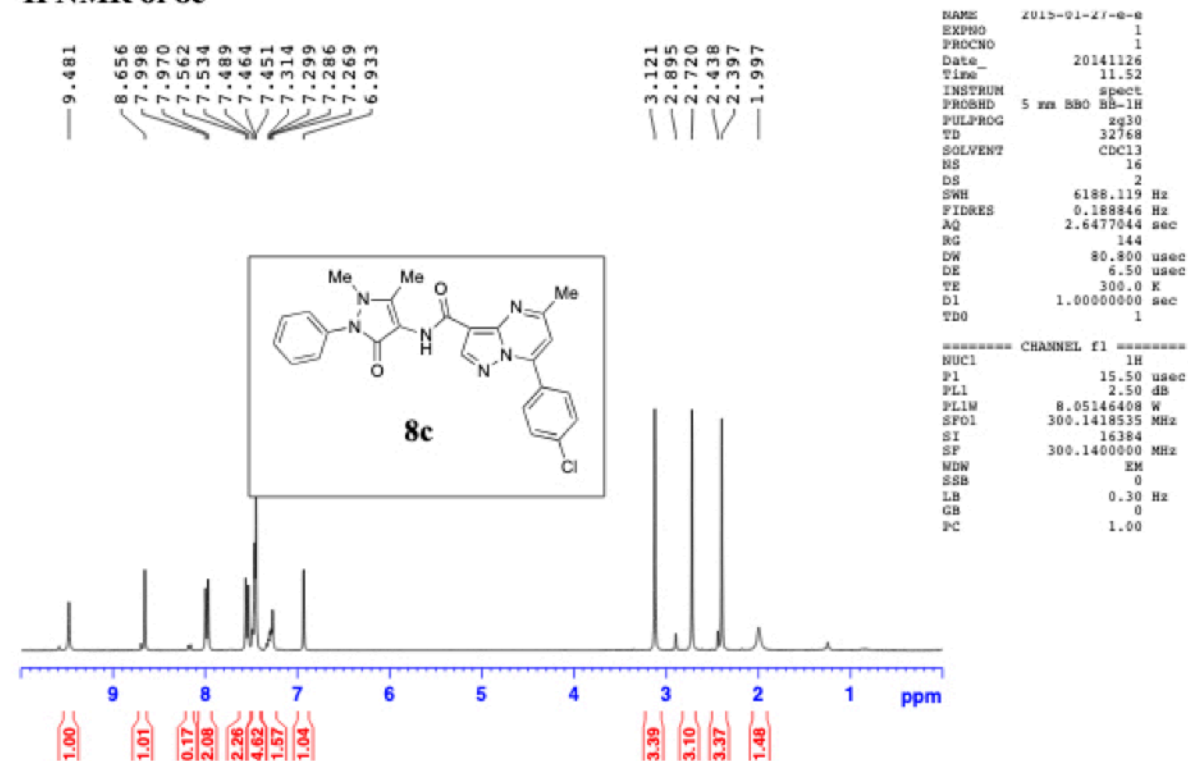


7-(4-Chlorophenyl)-N-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)-5-methylpyrazolo[1,5-a]pyrimidine-3-carboxamide (8c)

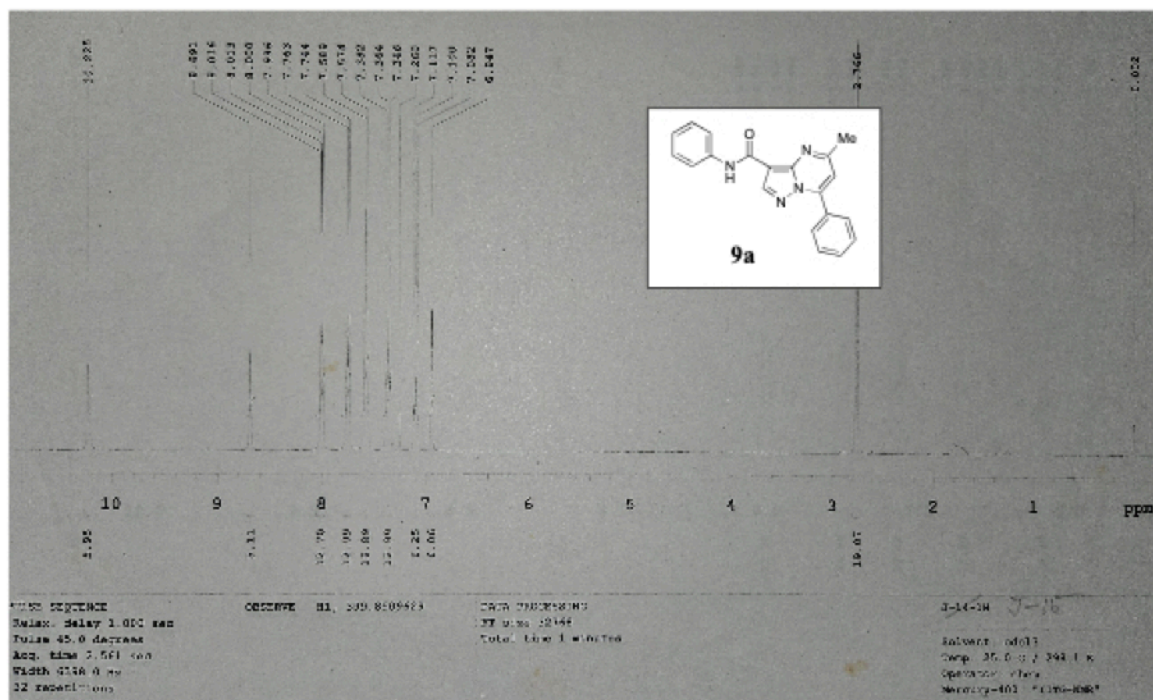
## HRMS of compound 8c



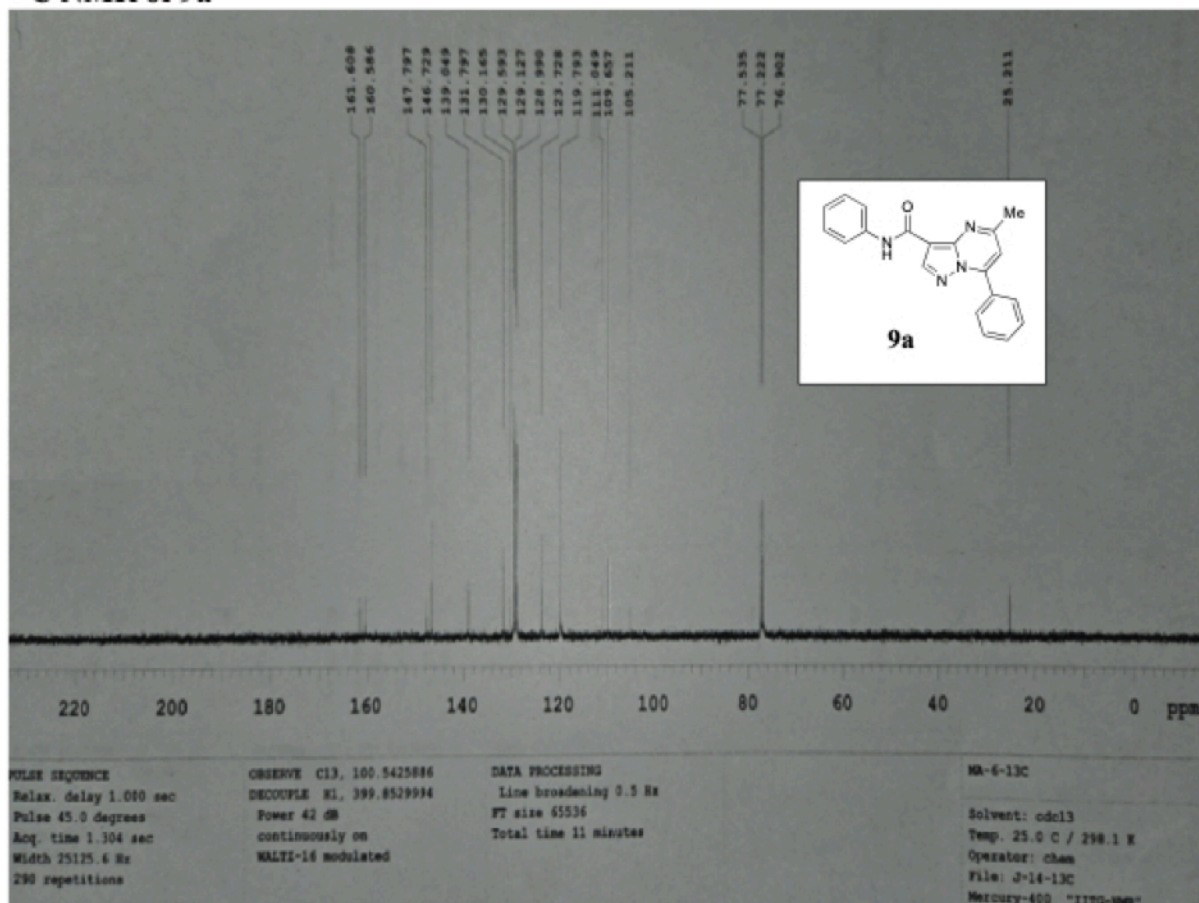
## <sup>1</sup>H NMR of 8c







**<sup>13</sup>C NMR of 9a**



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

## HRMS of 9b

### Single Mass Analysis

Tolerance = 100.0 mDa / Obs. m/z = 1.5, max = 500

Elemental prediction: C<sub>21</sub>H<sub>18</sub>N<sub>4</sub>O<sub>2</sub>

16 values of isotopic peaks used for FWHM = 3

Normalized Mass, Scale 0-1000000

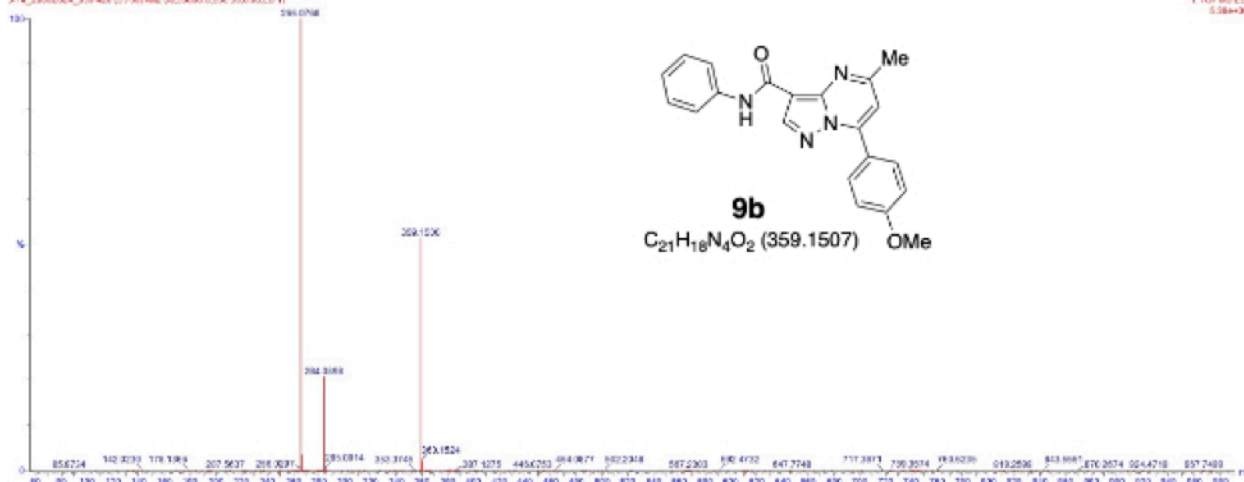
321 Data points evaluated after 134 results within 10 mDa difference (up to 1000 for each mass)

Chemical Link

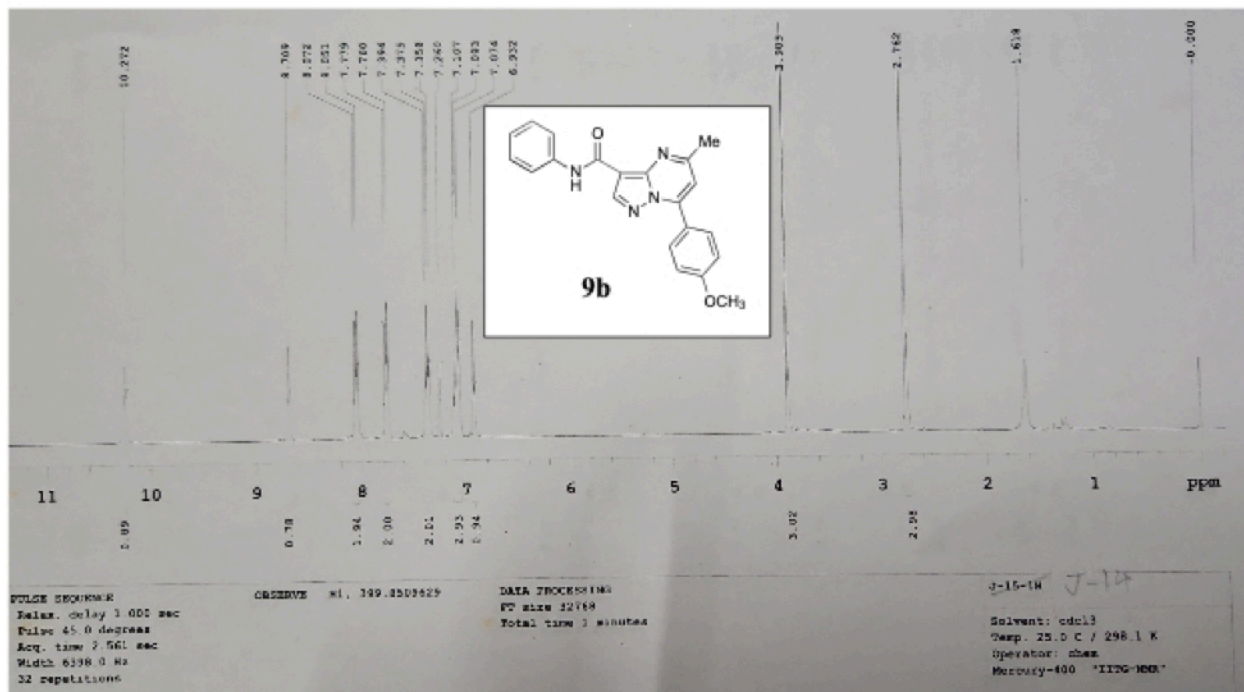
Mass	Cl. Mass	rdn	ISM	DBE	Formula	FWT	FWT Minors	Fit Conf%	C	H	N	O
359.1507	359.1508	52	10.5	10.5	C <sub>21</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	359.1507	0.00	100	21	18	4	2
359.1508	359.1508	36	12.7	12.5	C <sub>21</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	359.1507	0.00	100	21	18	4	2
359.1509	359.1509	12	15.1	15.0	C <sub>21</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	359.1507	0.00	100	21	18	4	2
359.1510	359.1510	10	16.9	16.5	C <sub>21</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	359.1507	0.00	100	21	18	4	2
359.1511	359.1511	10	18.7	18.0	C <sub>21</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	359.1507	0.00	100	21	18	4	2

2003204\_27\_47591

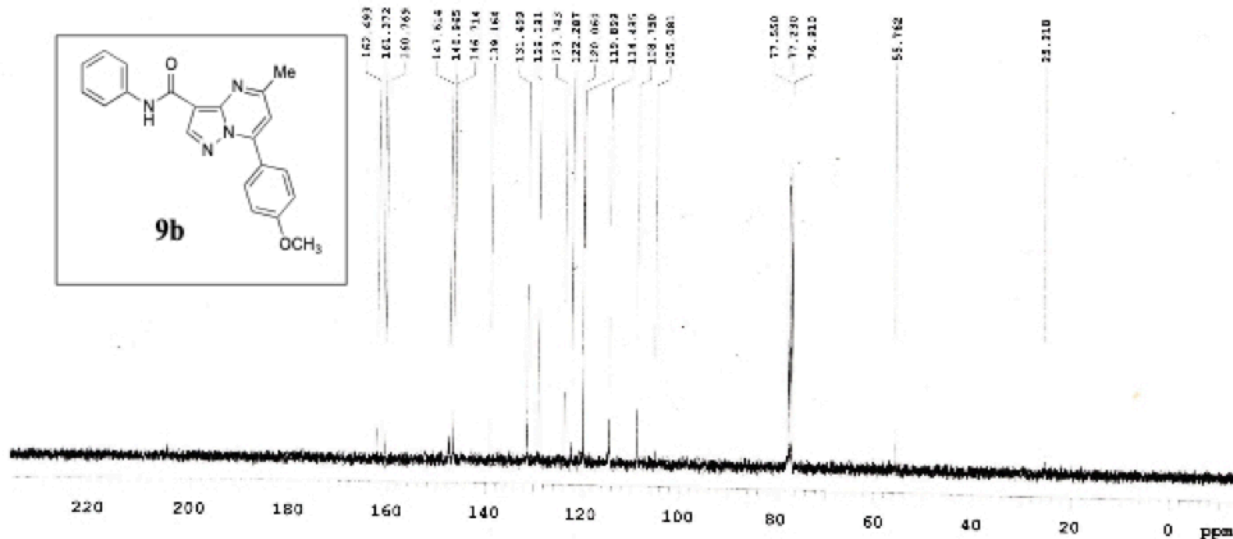
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## <sup>1</sup>H NMR of 9b



## <sup>13</sup>C NMR of 9b



POLAR ARGUMENT  
 Relax delay 1.000 sec  
 Pulse 45.0 degree  
 Acq. time 1.324 sec  
 Width 25125.6 Hz  
 930 repetitions

SEQUENCE CLS\_100\_5475832  
 DECPHPRM H1\_399\_8524964  
 Power 42 dB  
 continuously on  
 WAITS-15 modulated

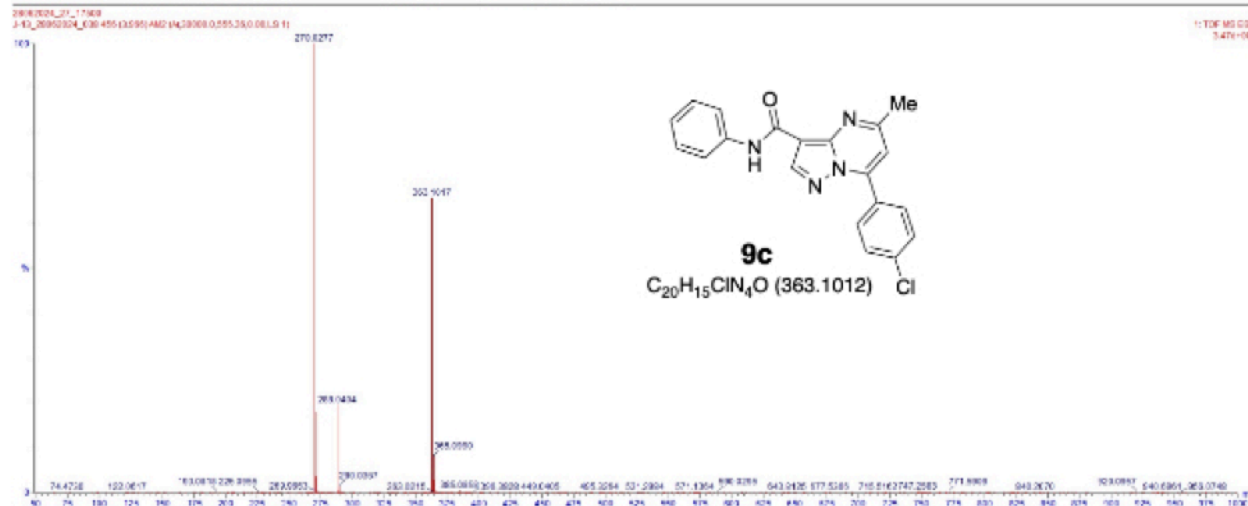
DATA ACQUISITION  
 Size expanding 0.5 Hz  
 FT size 65536  
 Total time 05 minutes

J-15-130

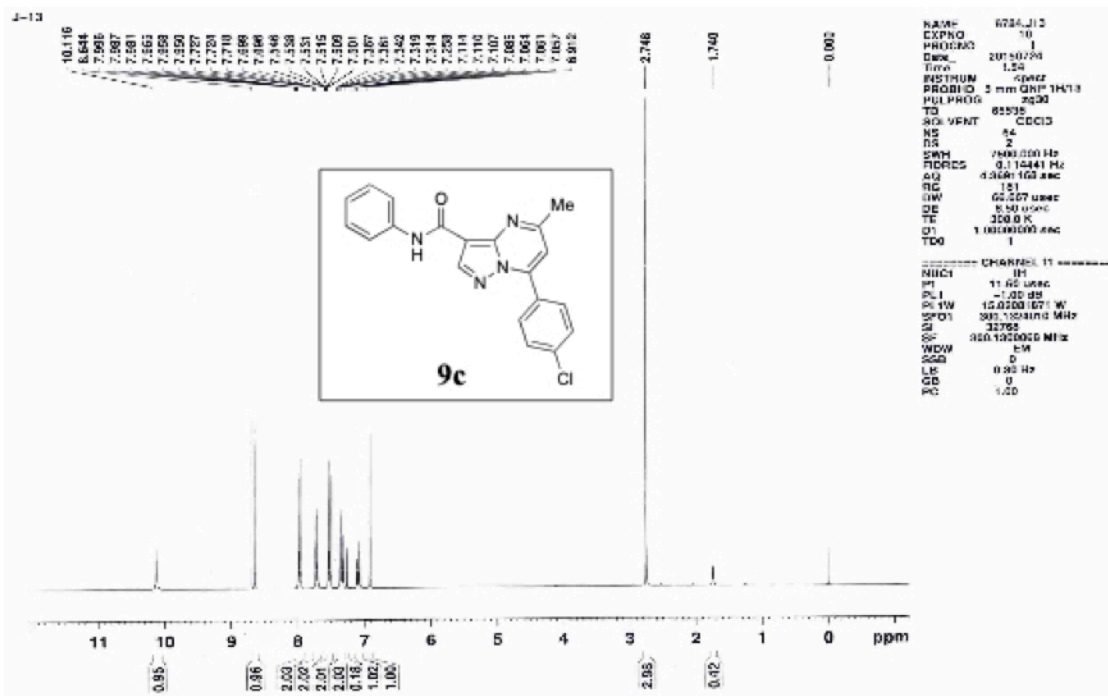
Solvent: cdcl3  
 Temp: 25.0 C / 298.1 K  
 Operator: chm  
 File: J-15-130  
 Mercury-400 \*H10-000\*

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

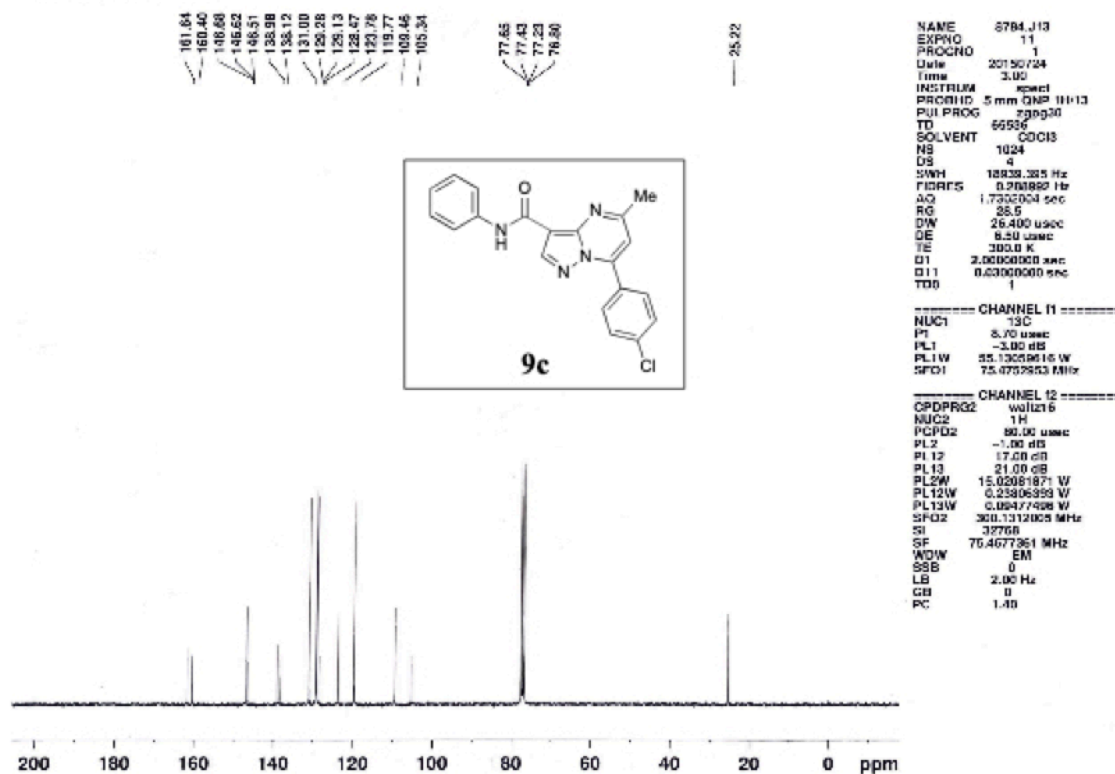
Mass	Calc. Mass	rel. I	PPM	DB	Formula	-101	+101	Mass	El. Conf.	C	H	N	O	Cl
363.021	363.021	100	0.0	0	C <sub>20</sub> H <sub>15</sub> ClN <sub>4</sub> O	0.0	0.0	27	15	4	1	0	0	0
363.021	363.021	100	0.0	0	C <sub>20</sub> H <sub>15</sub> ClN <sub>4</sub> O	0.0	0.0	27	15	4	1	0	0	0
363.021	363.021	100	0.0	0	C <sub>20</sub> H <sub>15</sub> ClN <sub>4</sub> O	0.0	0.0	27	15	4	1	0	0	0
363.021	363.021	100	0.0	0	C <sub>20</sub> H <sub>15</sub> ClN <sub>4</sub> O	0.0	0.0	27	15	4	1	0	0	0
363.021	363.021	100	0.0	0	C <sub>20</sub> H <sub>15</sub> ClN <sub>4</sub> O	0.0	0.0	27	15	4	1	0	0	0



### <sup>1</sup>H NMR of 9c



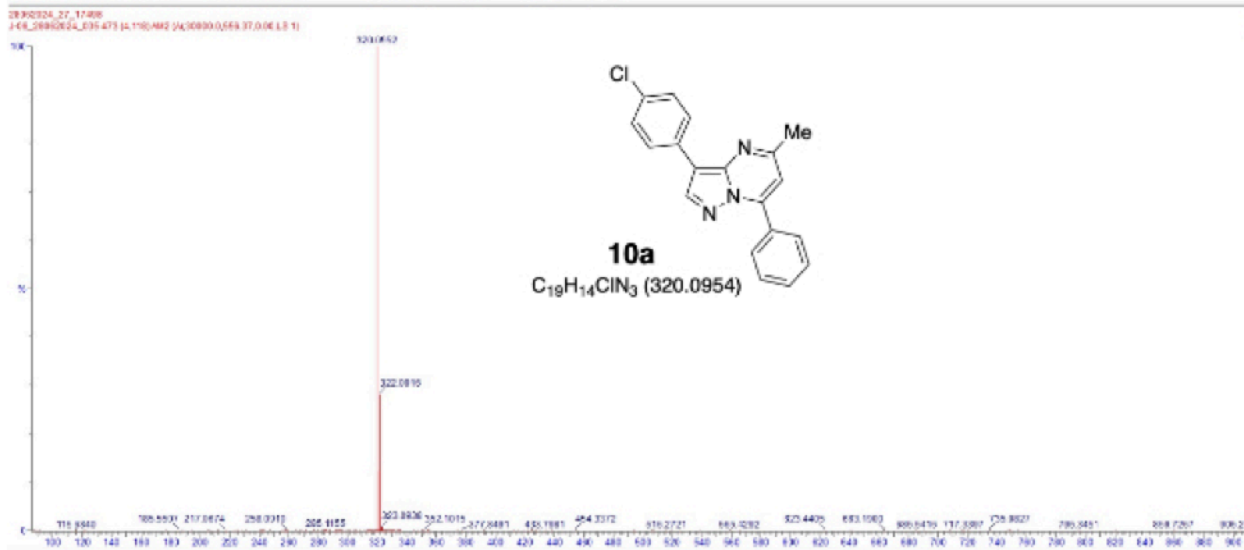
**<sup>13</sup>C NMR of 9c**



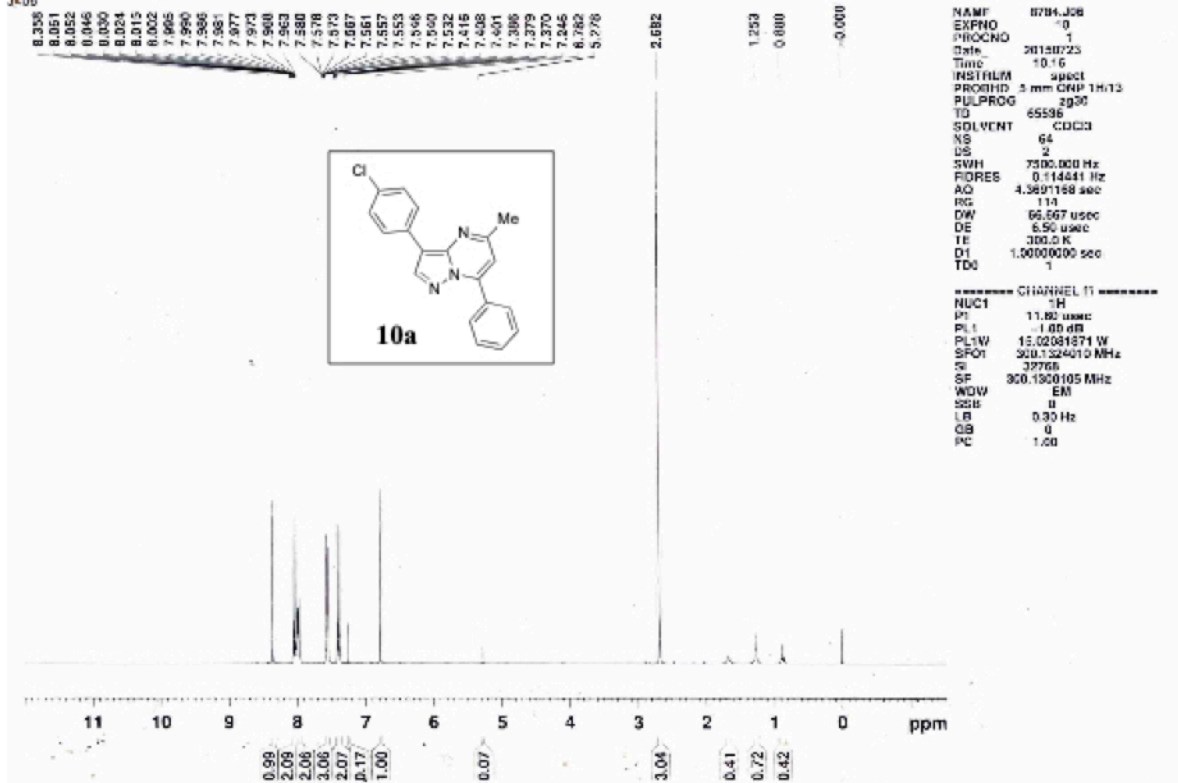
**3-(4-Chlorophenyl)-5-methyl-7-phenylpyrazolo[1,5-a]pyrimidine (10a)**

**HRMS of 10a**

Elem	Calc Mass	Found	Diff	Formula	-T	-T/T	Th Cont %	C	H	N	Cl
C <sub>19</sub> H <sub>14</sub> N <sub>3</sub>	320.0954	320.0954	0.0000	C <sub>19</sub> H <sub>14</sub> N <sub>3</sub>	320.2	95.98	0.00	79	13	3	1
	280.086	280.086	0.0000	C <sub>18</sub> H <sub>13</sub> N <sub>3</sub>	482.2	18.152	0.00	30	20	5	
	280.072	280.072	0.0000	C <sub>18</sub> H <sub>13</sub> N <sub>3</sub>	490.5	11.808	0.00	18	20	1	2
	280.078	280.078	0.0000	C <sub>18</sub> H <sub>13</sub> N <sub>3</sub>	540.0	13.048	0.00	8	21	1	4



**<sup>1</sup>H NMR of 10a**



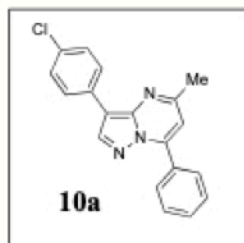
**<sup>13</sup>C NMR of 10a**

159.51  
146.50  
143.96  
142.47  
131.89  
131.25  
131.16  
129.40  
128.97  
128.89  
127.60  
113.00  
109.02  
108.58

77.06  
77.23  
76.81

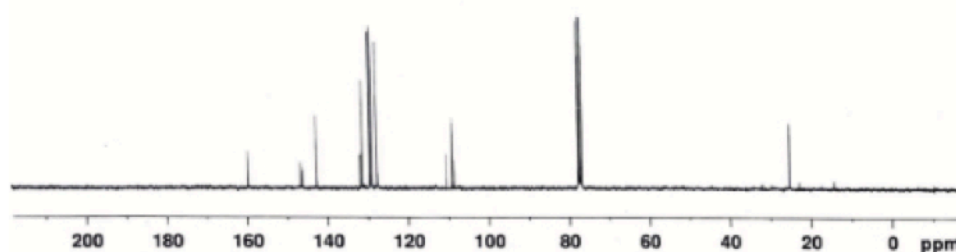
31.76  
25.23  
22.84  
14.31

NAME 8784\_206  
EXPNO 11  
PROCNO 1  
Date\_ 20150723  
Time 10.20  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 524  
DS 4  
SWH 16978.295 Hz  
FIDRES 0.268992 Hz  
AQ 1.732004 sec  
RG 28.5  
DW 26.400 usec  
DE 6.50 usec  
TE 300.6 K  
D1 2.0000000 sec  
D11 0.0200000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 13C  
P1 8.70 usec  
PL1 -3.00 dB  
PL1W 55.12059616 W  
SFO1 75.4752953 MHz

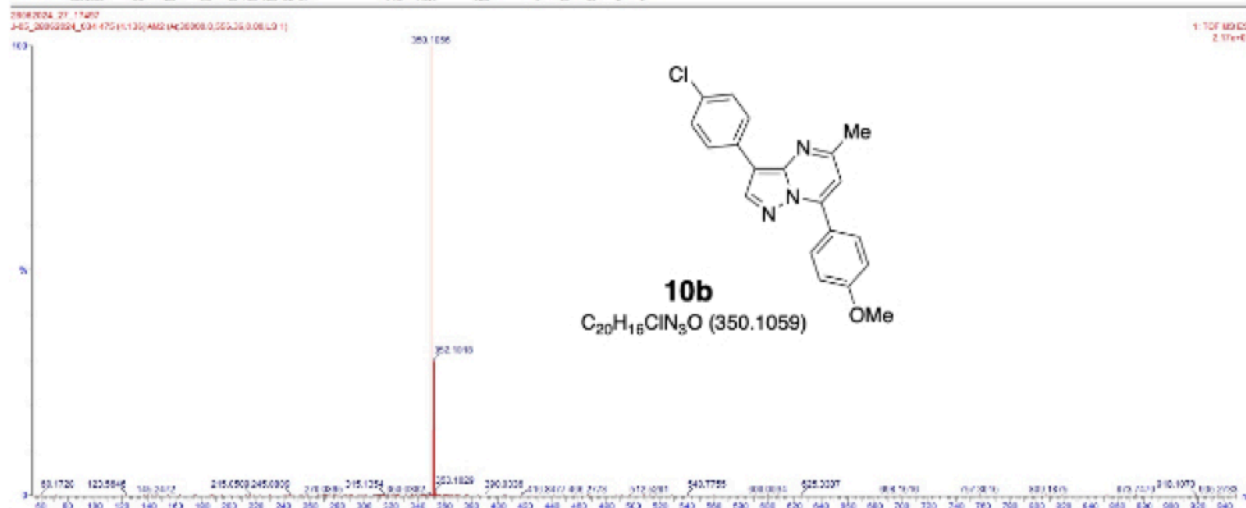
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 17.00 dB  
PL13 21.00 dB  
PL2W 15.02081871 W  
PL12W 0.23806393 W  
PL13W 0.09477496 W  
SFO2 399.1312005 MHz  
SI 32758  
SF 75.4677350 MHz  
WOW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.40



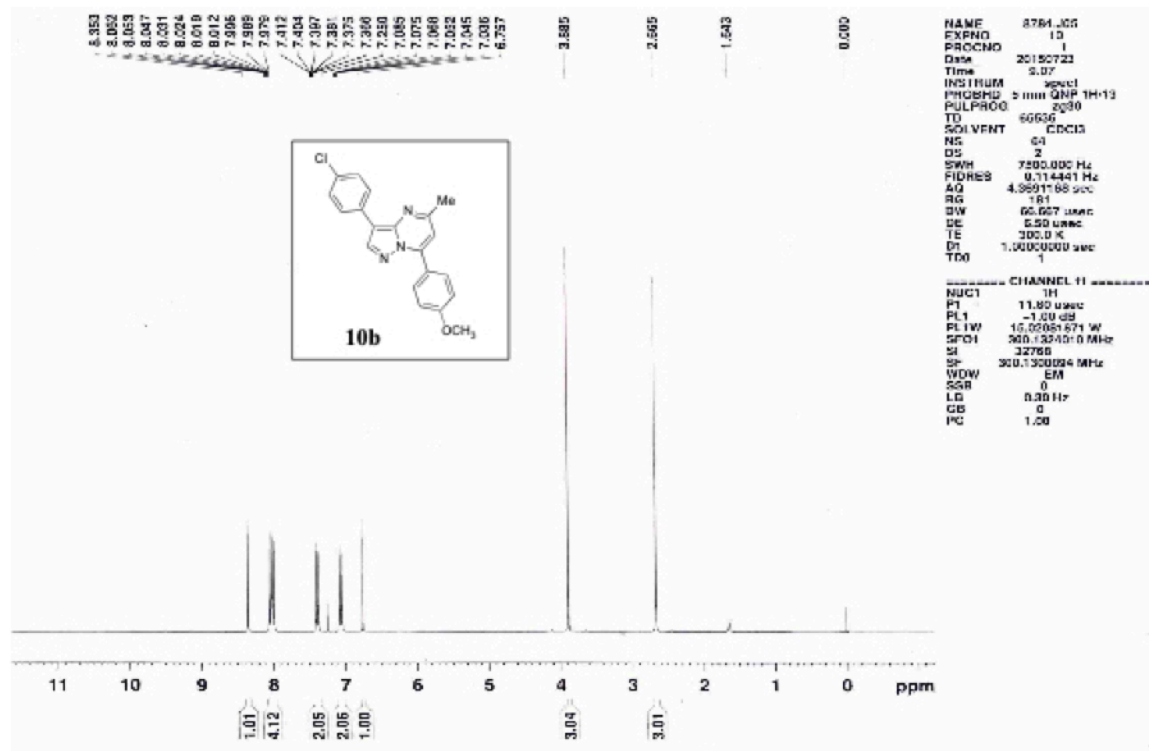
**3-(4-Chlorophenyl)-7-(4-methoxyphenyl)-5-methylpyrazolo[1,5-a]pyrimidine (10b)**

**HRMS of 10b**

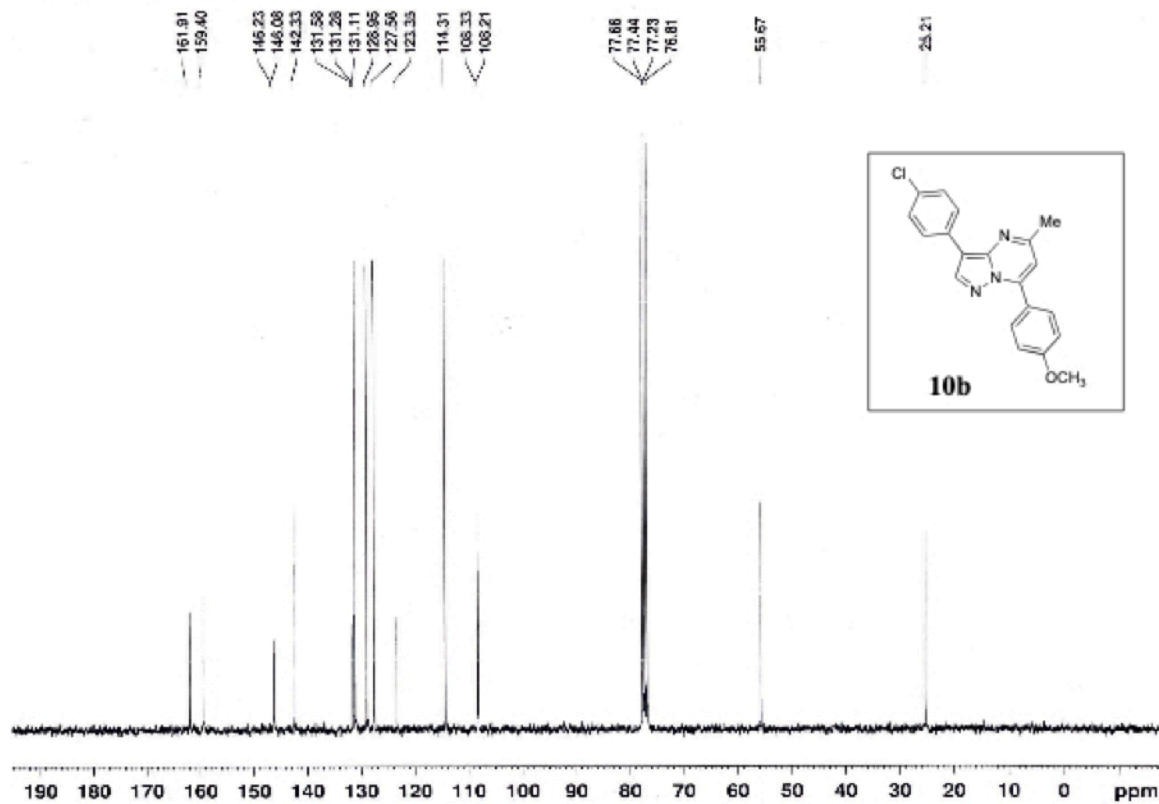
Mass	Calc	Obs	diff	Formula	LR1	LR1 Name	HR Calc %	C	H	M	O	N
350.058	350.105	350.105	-0.1	C <sub>20</sub> H <sub>16</sub> ClN <sub>3</sub> O	483.7	14129	100	20	16	1	1	3
350.105	350.105	350.105	0.0	C <sub>20</sub> H <sub>16</sub> ClN <sub>3</sub> O	170.0	9215	100	4	13	2	0	1
350.105	350.105	350.105	0.0	C <sub>20</sub> H <sub>16</sub> ClN <sub>3</sub> O	362.2	18514	100	8	16	1	0	1
350.105	350.105	350.105	0.0	C <sub>20</sub> H <sub>16</sub> ClN <sub>3</sub> O	470.0	9215	100	20	17	1	1	1
350.105	350.105	350.105	0.0	C <sub>20</sub> H <sub>16</sub> ClN <sub>3</sub> O	472.2	7485	100	5	13	2	2	1



**<sup>1</sup>H NMR of 10b**



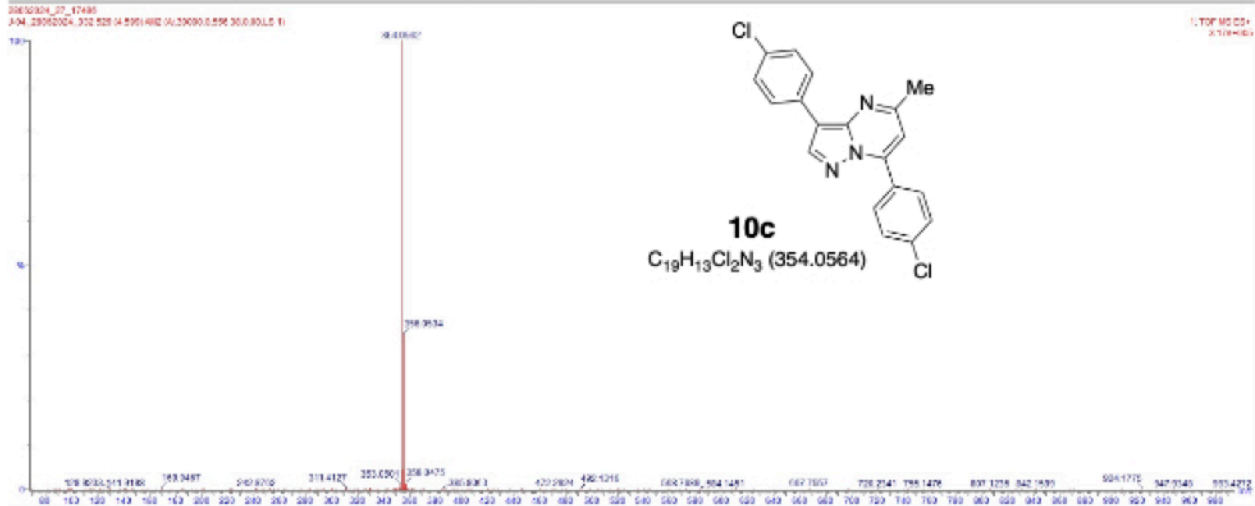
**<sup>13</sup>C NMR of 10b**



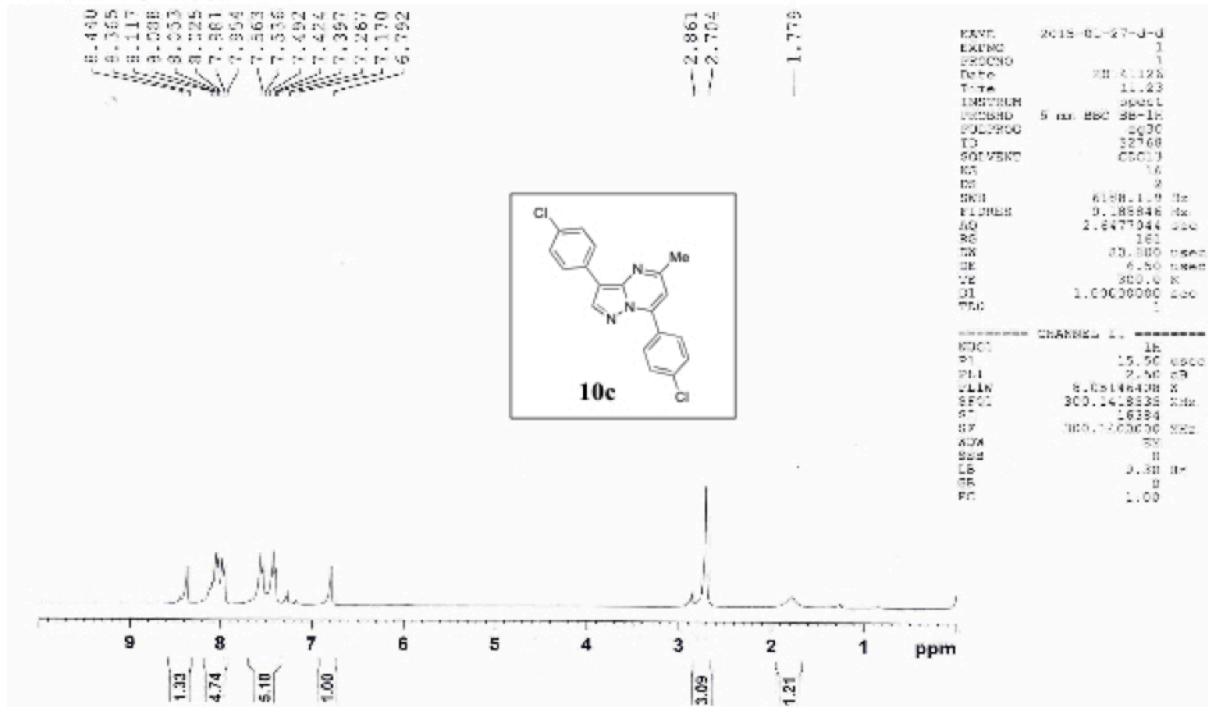
**3,7-Bis(4-chlorophenyl)-5-methylpyrazolo[1,5-*a*]pyrimidine (10c)**

**HRMS of 10c**

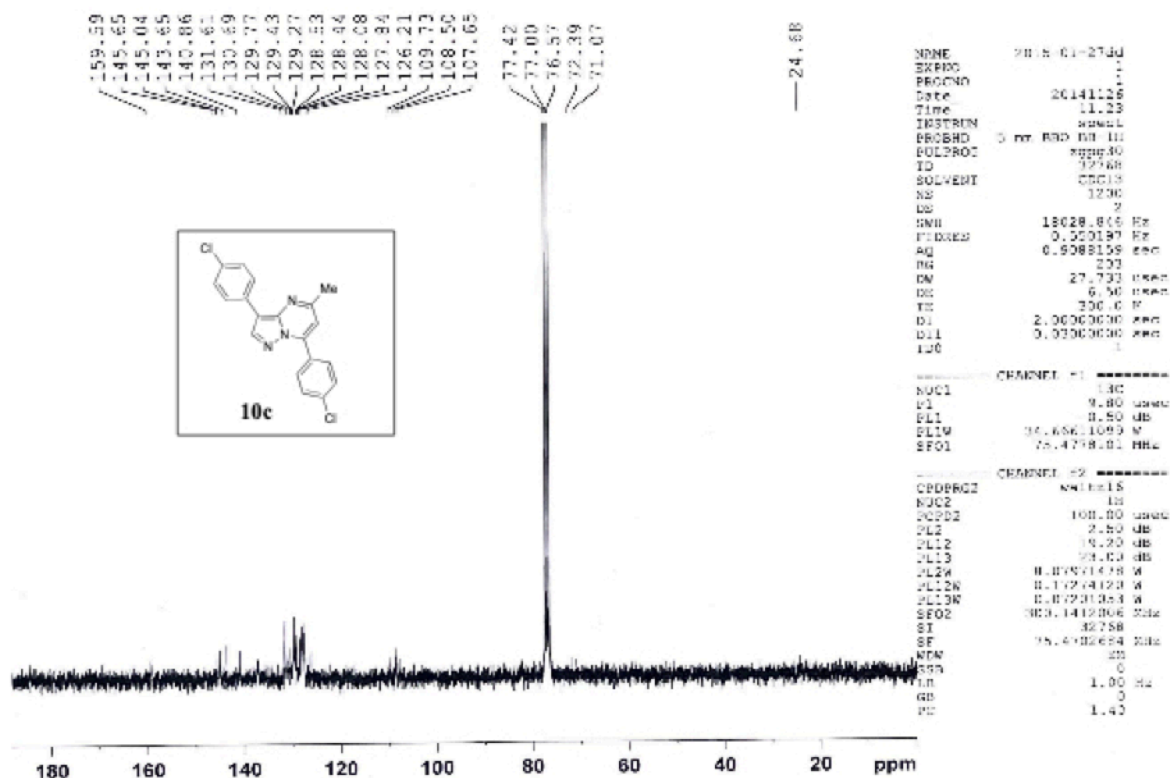
Mass	Calc. Mass	m/z	PPM	CCC	Formula	HTF	HTF Name	Th. Cont. %	C	H	N	Cl
354.056	354.056	354	0.0	100	C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub>	132.1	6.350	3.82	20	6	5	4
354.056	354.056	354	0.0	100	C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub>	132.1	6.350	3.82	20	6	5	4
354.056	354.056	354	0.0	100	C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub>	132.1	6.350	3.82	20	6	5	4
354.056	354.056	354	0.0	100	C <sub>19</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub>	132.1	6.350	3.82	20	6	5	4



### <sup>1</sup>H NMR of 10c

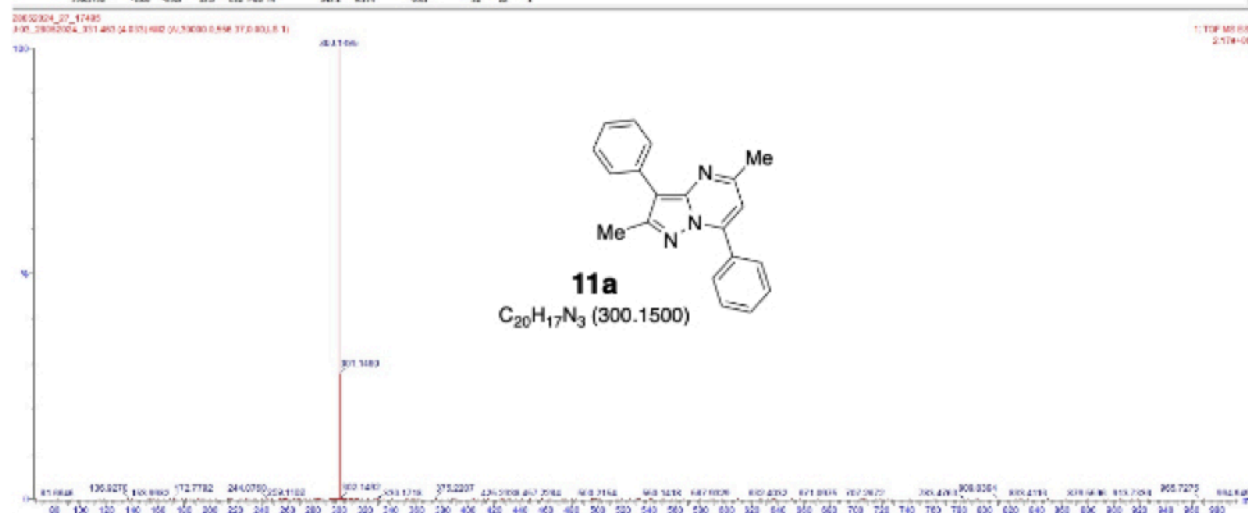


### <sup>13</sup>C NMR of 10c

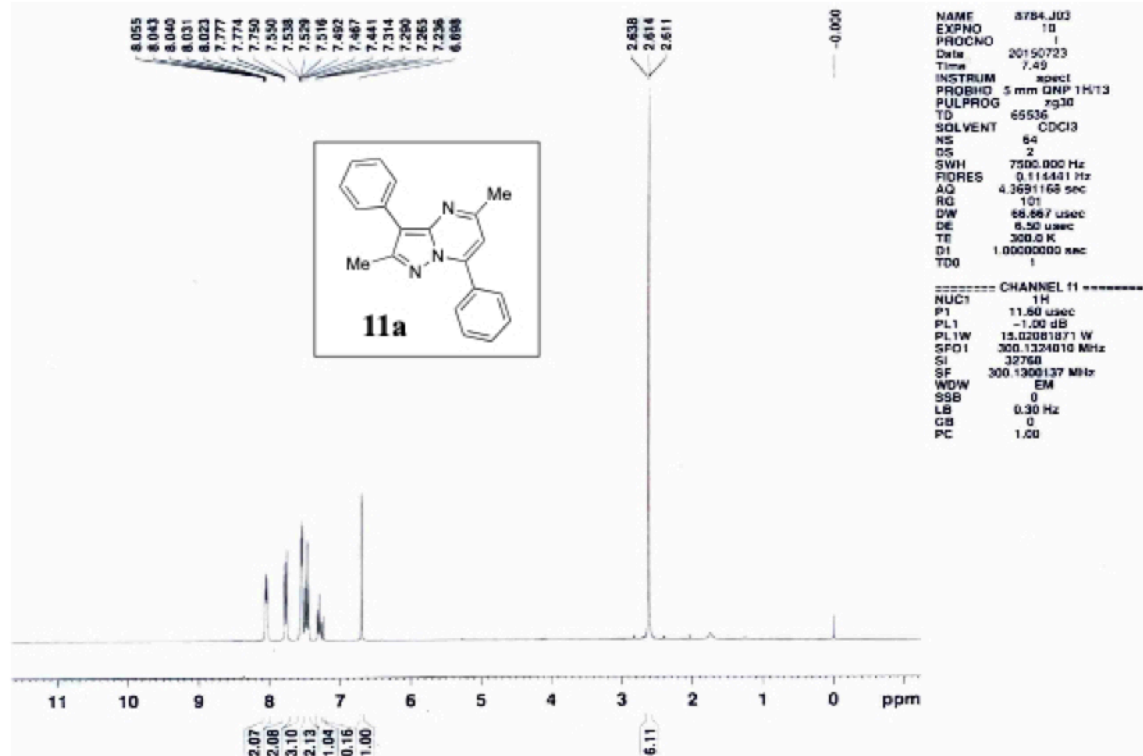


## 2,5-Dimethyl-3,7-diphenylpyrazolo[1,5-a]pyrimidine (11a) HRMS of 11a

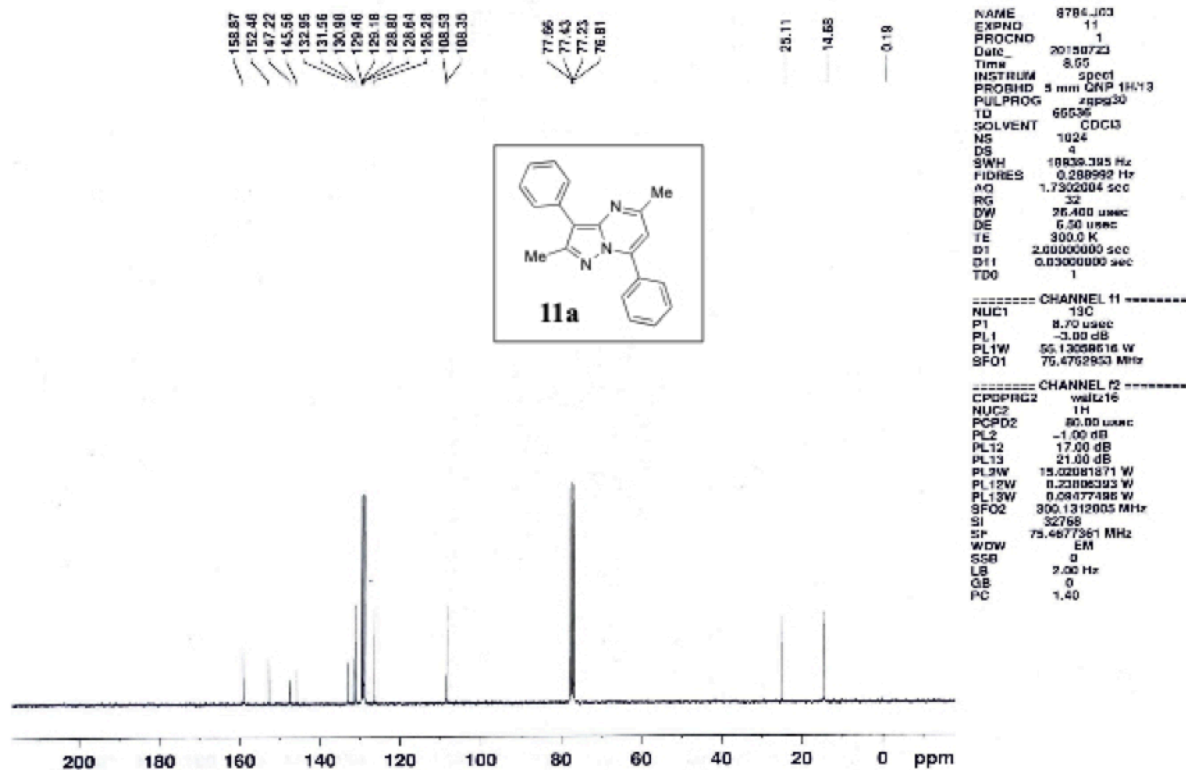
Mass	Calc. Mass	m/z	ppm	CCF	Formula	HT	HTT	HTT	HTT	C	H	N
300.150	300.150	300	0.0	100	C <sub>20</sub> H <sub>17</sub> N <sub>3</sub>	100	100	100	100	20	17	3
300.150	300.150	300	0.0	100	C <sub>20</sub> H <sub>17</sub> N <sub>3</sub>	100	100	100	100	20	17	3
300.150	300.150	300	0.0	100	C <sub>20</sub> H <sub>17</sub> N <sub>3</sub>	100	100	100	100	20	17	3



## <sup>1</sup>H NMR of 11a

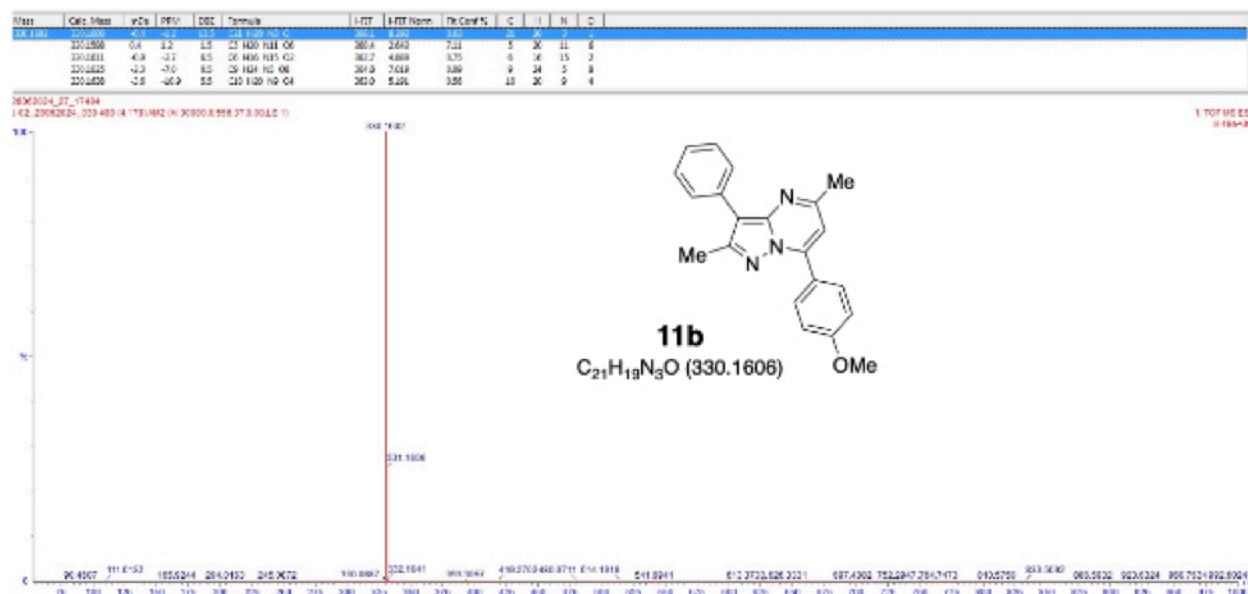


<sup>13</sup>C NMR of 11a

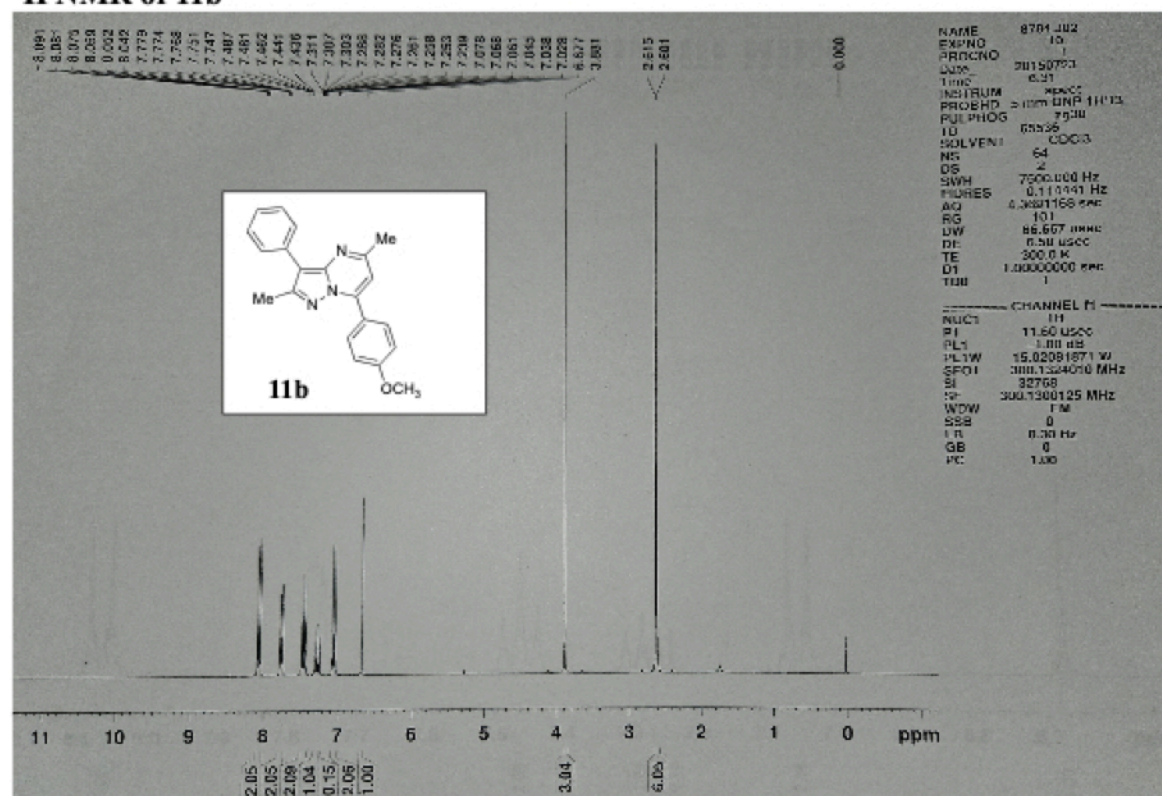


7-(4-Methoxyphenyl)-2,5-dimethyl-3-phenylpyrazolo[1,5-a]pyrimidine (11b)

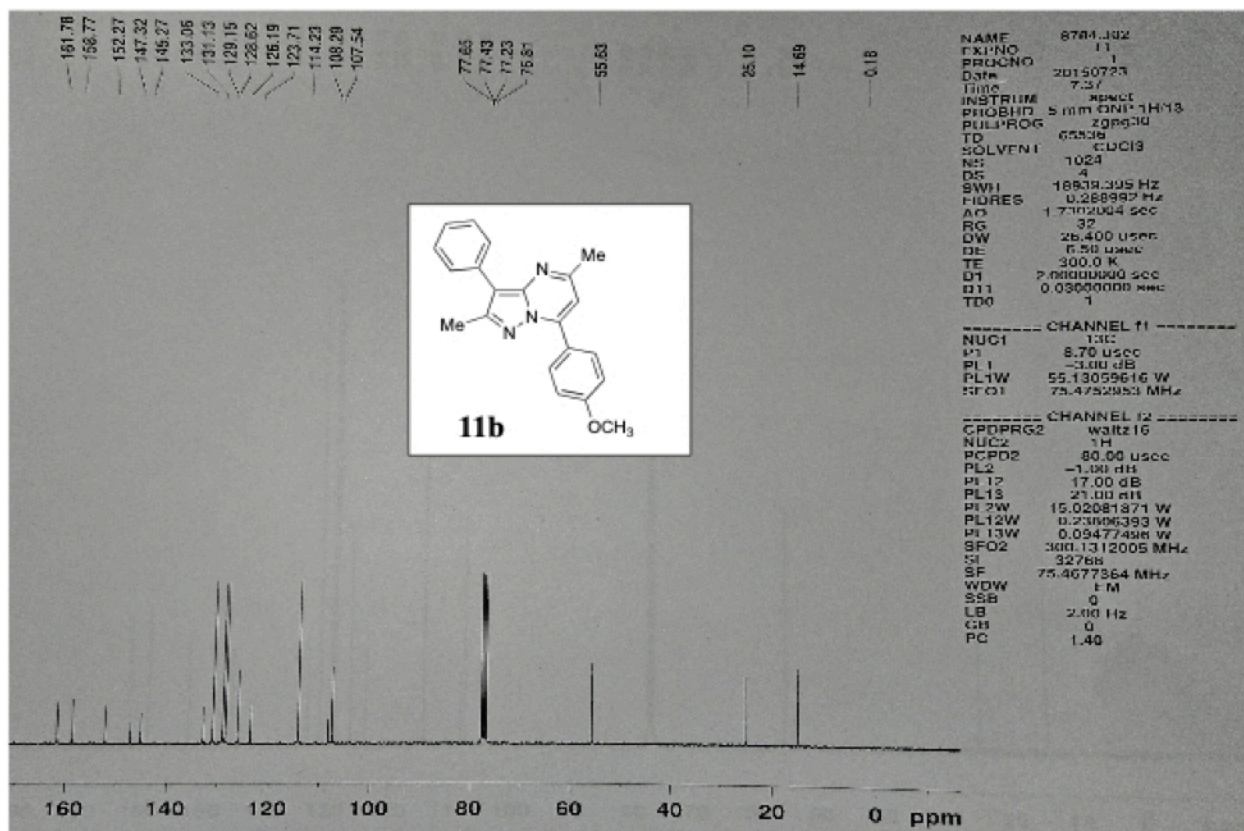
HRMS of 11b



### <sup>1</sup>H NMR of 11b



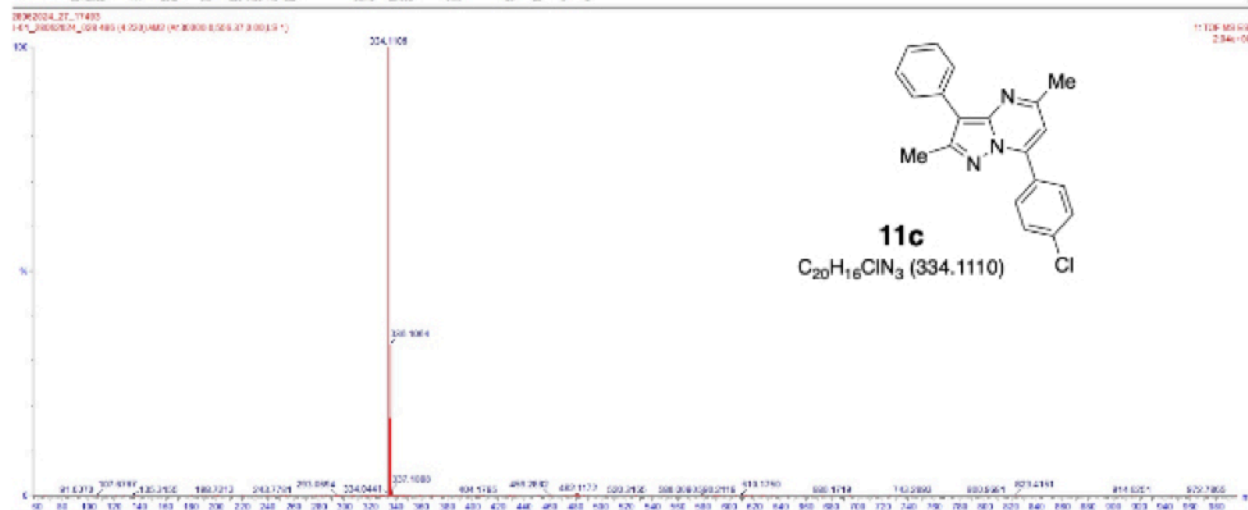
### <sup>13</sup>C NMR of 11b



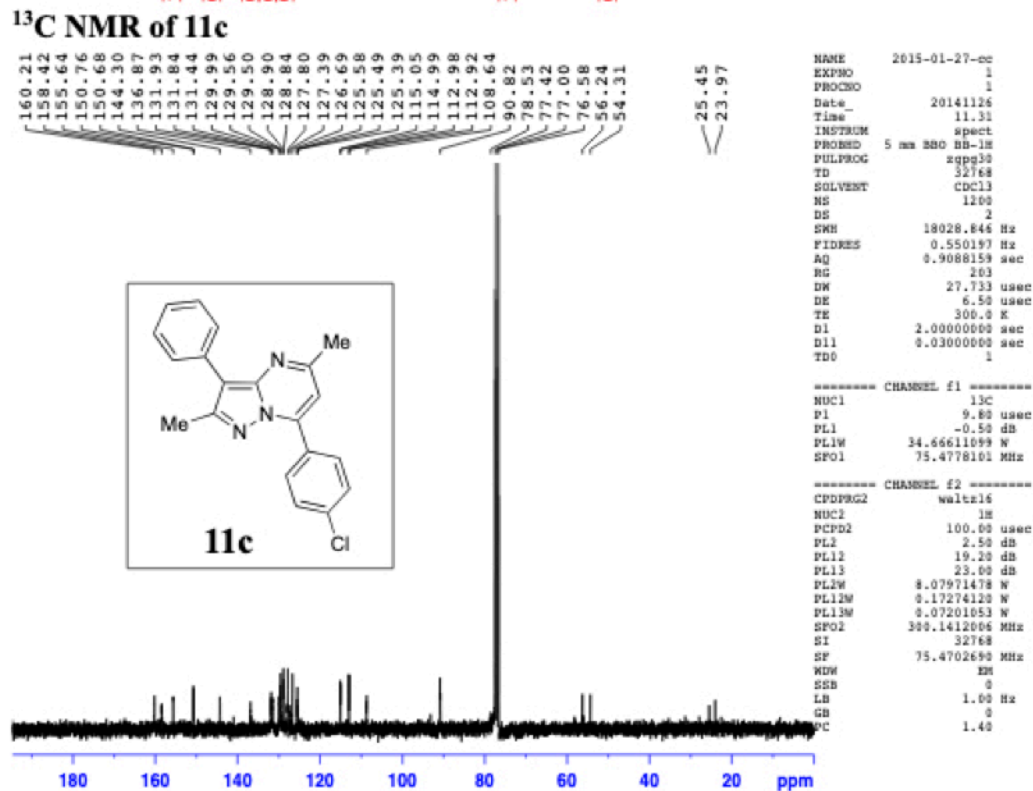
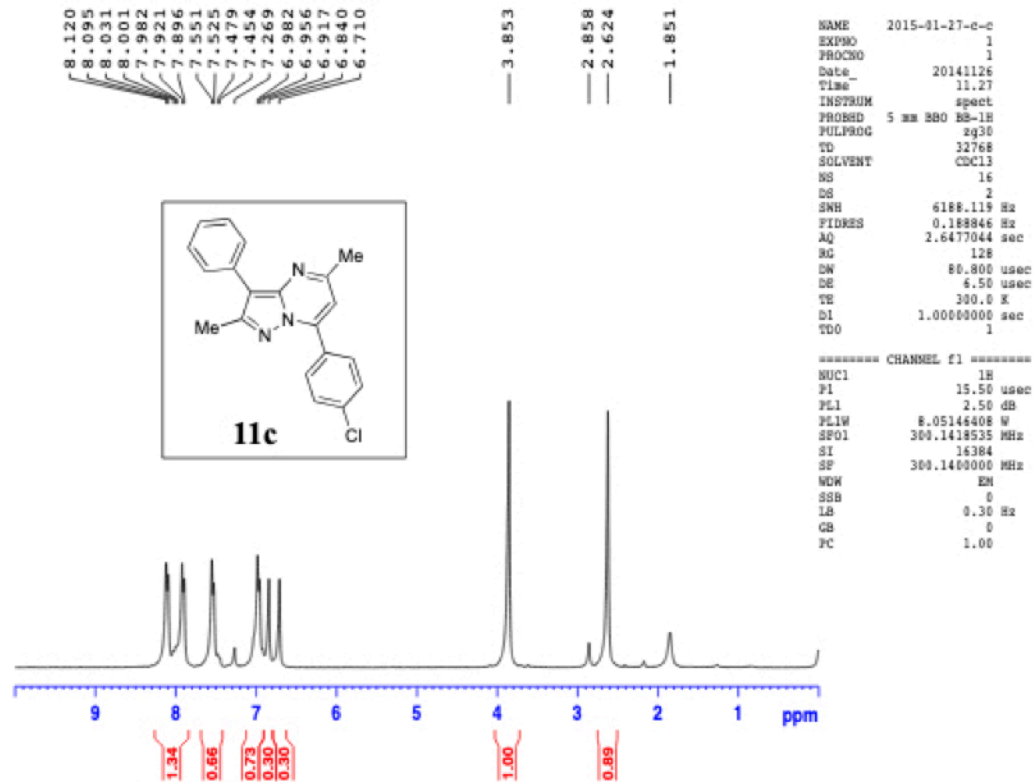
## 7-(4-Chlorophenyl)-2,5-dimethyl-3-phenylpyrazolo[1,5-a]pyrimidine (11c)

Mass of 11c

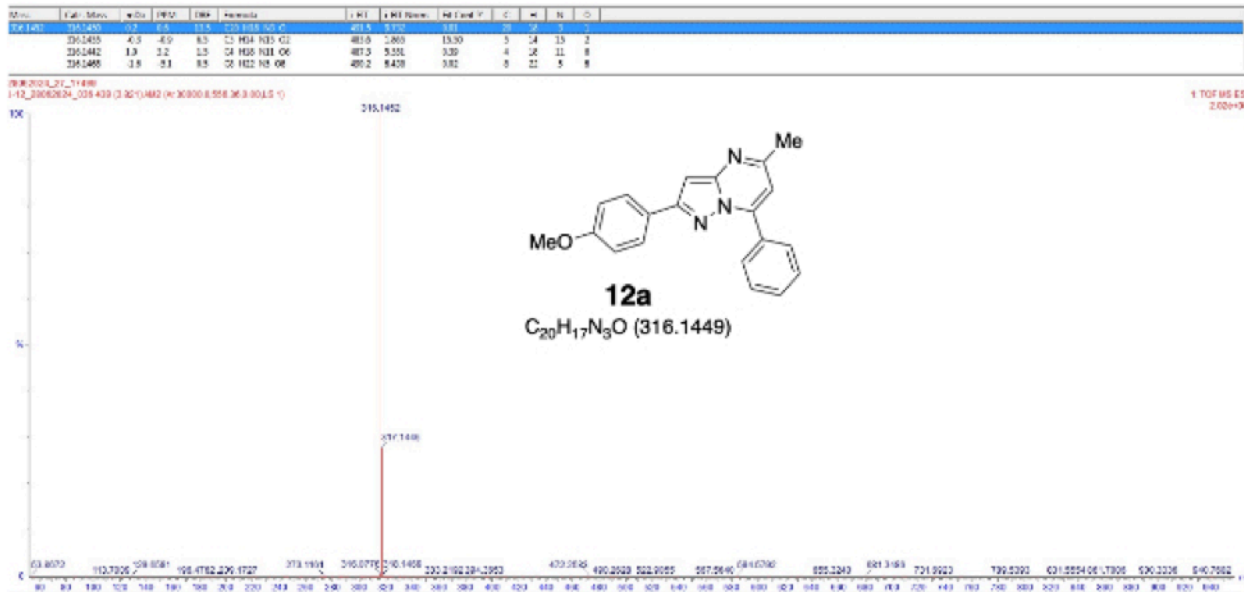
Mz	Lab. Mass	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%	Wt%
334.1110	334.1110	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00



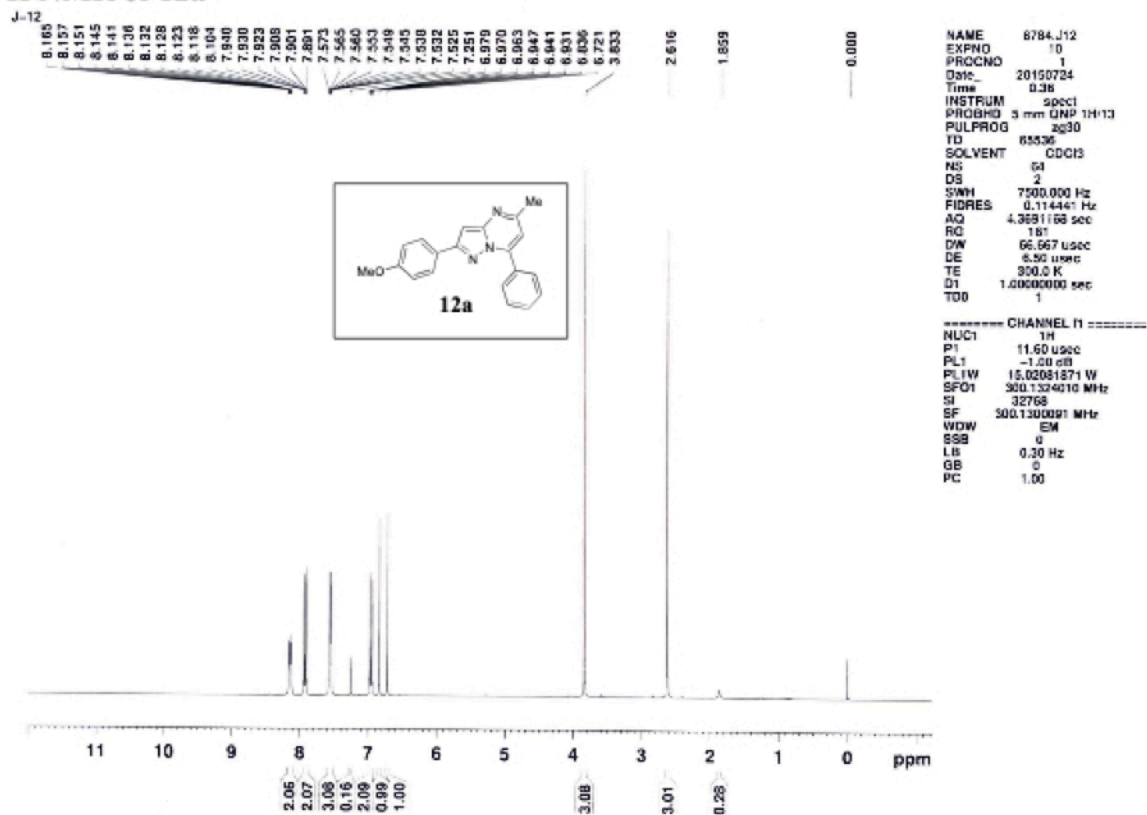
## <sup>1</sup>H NMR of 11c



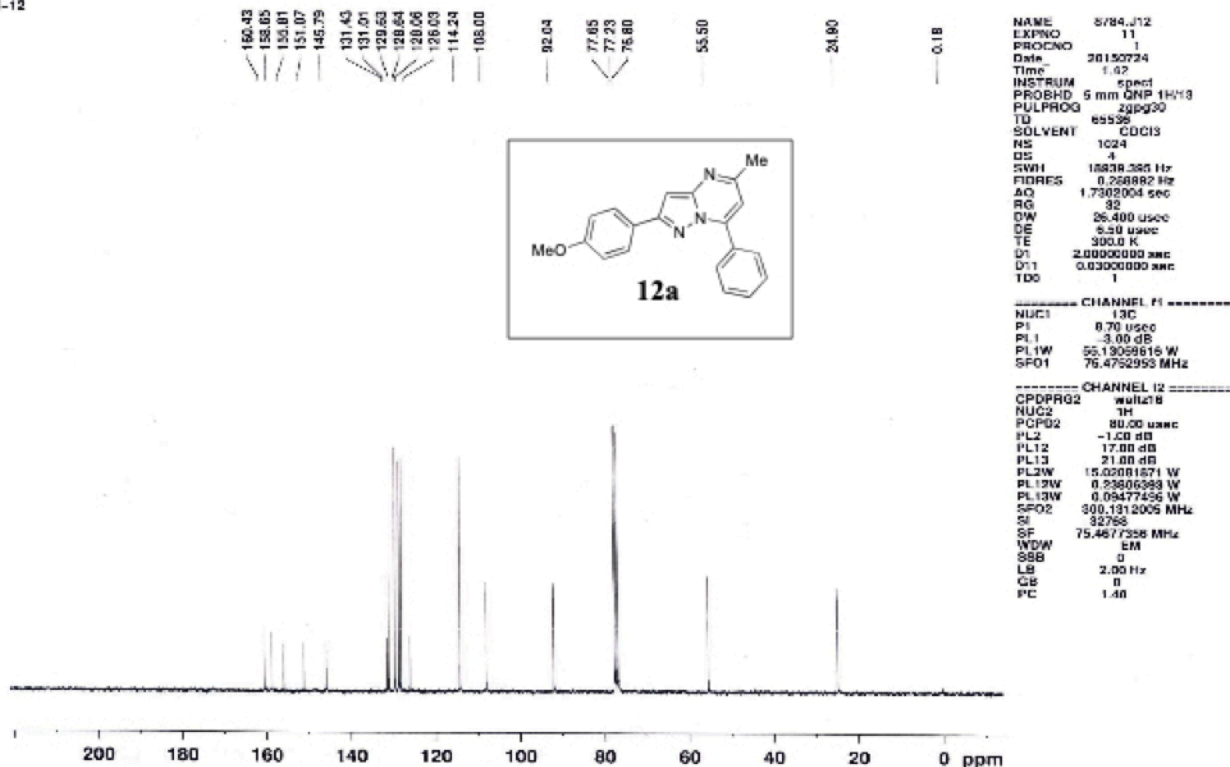
**2-(4-Methoxyphenyl)-5-methyl-7-phenylpyrazolo[1,5-*a*]pyrimidine (12a)**  
**Mass Spectrum of 12a**



### <sup>1</sup>H NMR of 12a

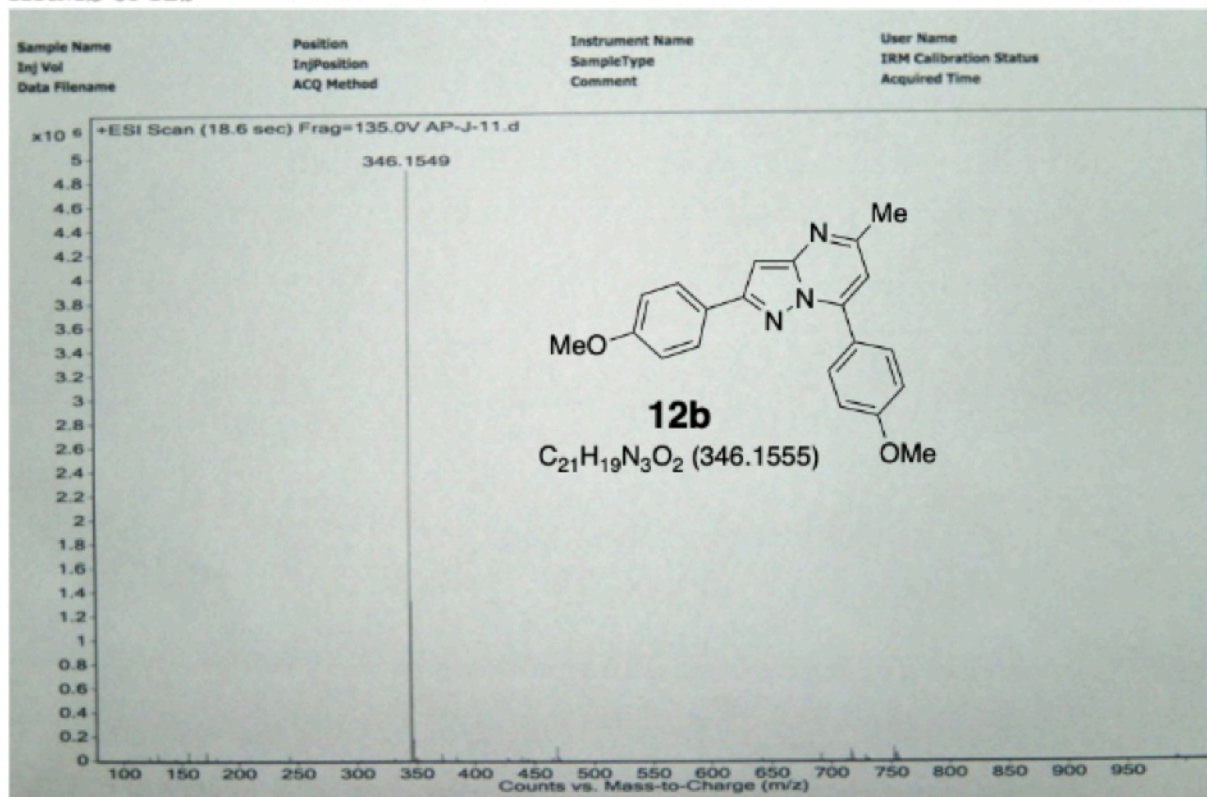


### <sup>13</sup>C NMR of 12a

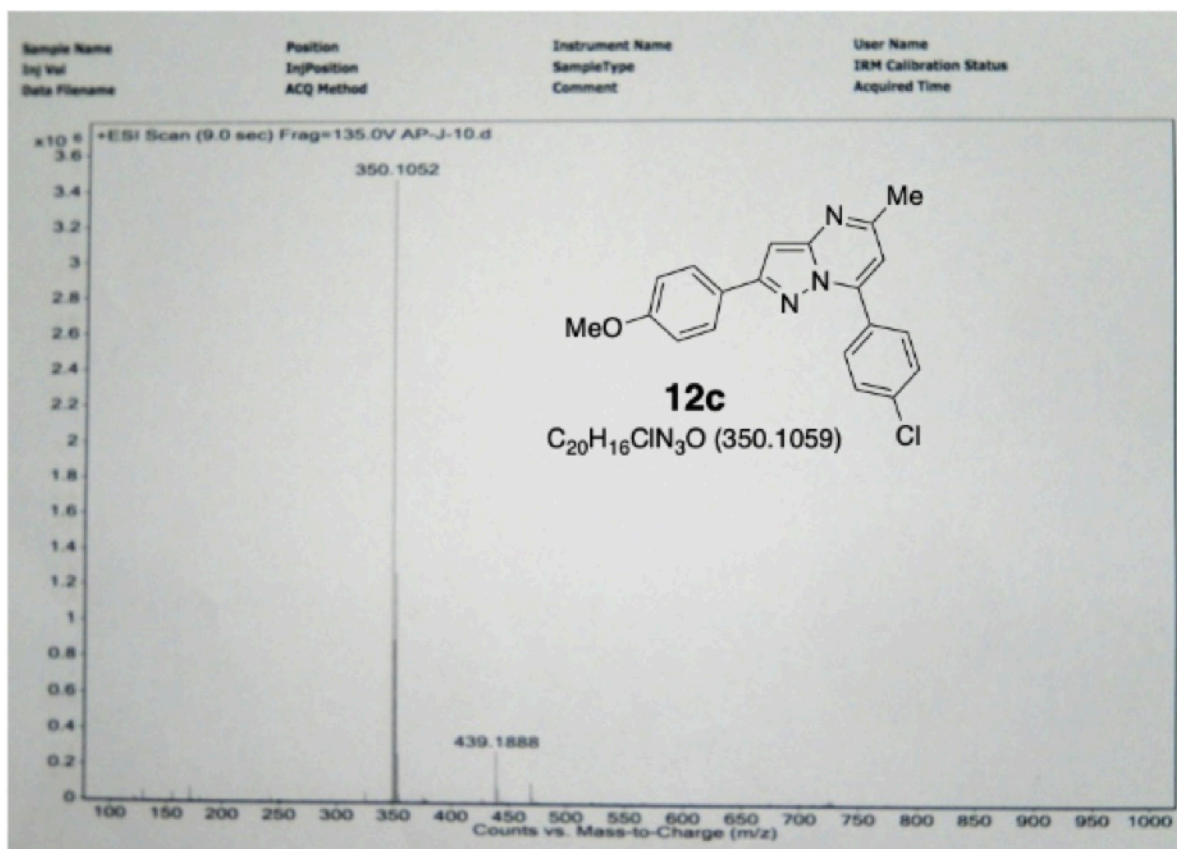


2,7-Bis(4-methoxyphenyl)-5-methylpyrazolo[1,5-a]pyrimidine (12b)

HRMS of 12b







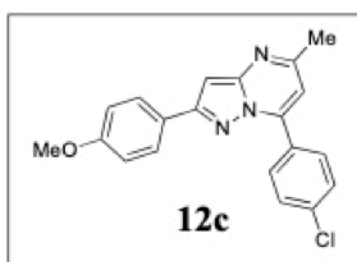
**$^1H$  NMR of 12c**

8.440  
8.365  
8.117  
8.088  
8.053  
8.025  
7.981  
7.954  
7.563  
7.536  
7.492  
7.424  
7.397  
7.267  
7.170  
6.792

2.861  
2.704  
1.779

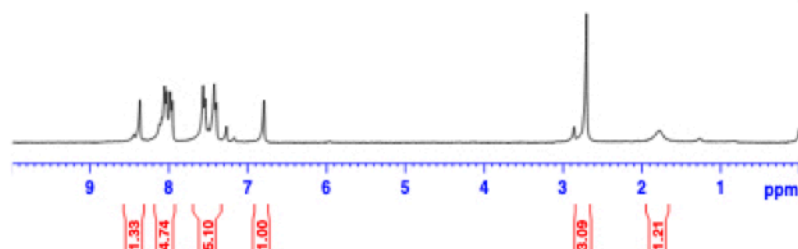
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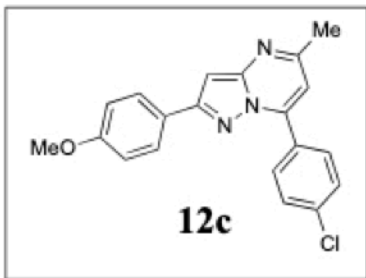
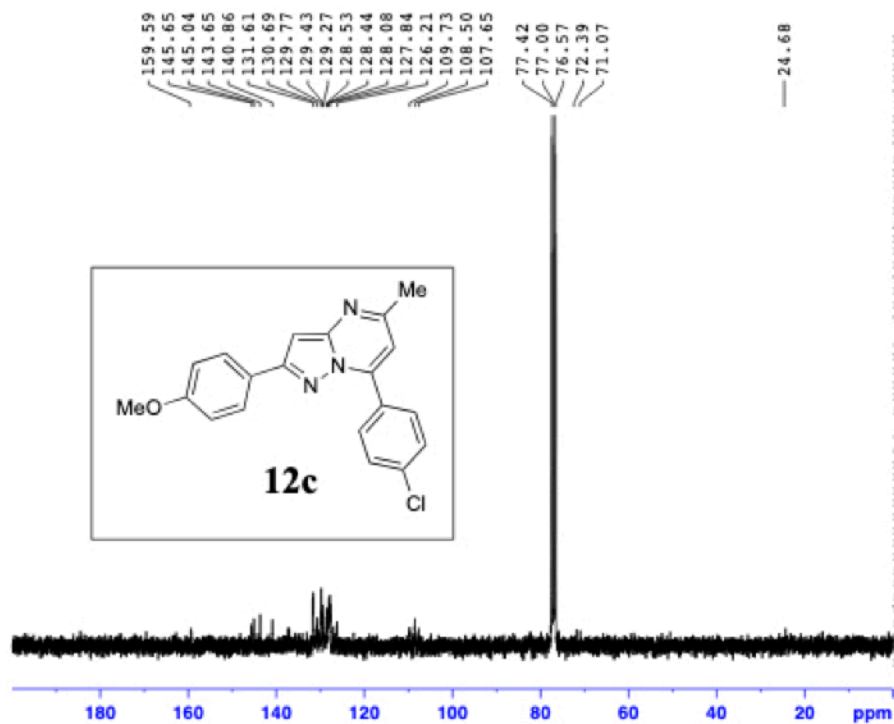
NAME      2015-01-27-d-3
EXPNO     1
PROCNO    1
Date_     20141126
Time      11.23
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SMH        6188.119 Hz
FIDRES     0.188846 Hz
AQ         2.6477044 sec
RG         161
SWH        86.800 usec
DE         4.56 usec
TE         300.0 K
D1         1.6000000 sec
TD0        1
  
```



```

----- CHANNEL f1 -----
NUC1       1H
P1         15.50 usec
PL1        2.50 dB
PL1W       8.05148408 W
SFO1       300.1418535 MHz
SI         16384
SF         300.1400000 MHz
VCN        EN
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```





```

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
PL1M       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
PL2M       8.07971478 W
PL12M      0.17274120 W
PL13M      0.07201053 W
SFO2       300.1412006 MHz
SI         32768
SF         75.4702684 MHz
WDW        EM
SSB        0
CB         1.00 Hz
GB         0
PC         1.40

```