

*RSC Advances*

**A one-pot, multicomponent reaction for the synthesis of novel 2-alkyl substituted  
4-aminoimidazo[1,2-*a*][1,3,5]triazines**

(Electronic Supplementary Information)

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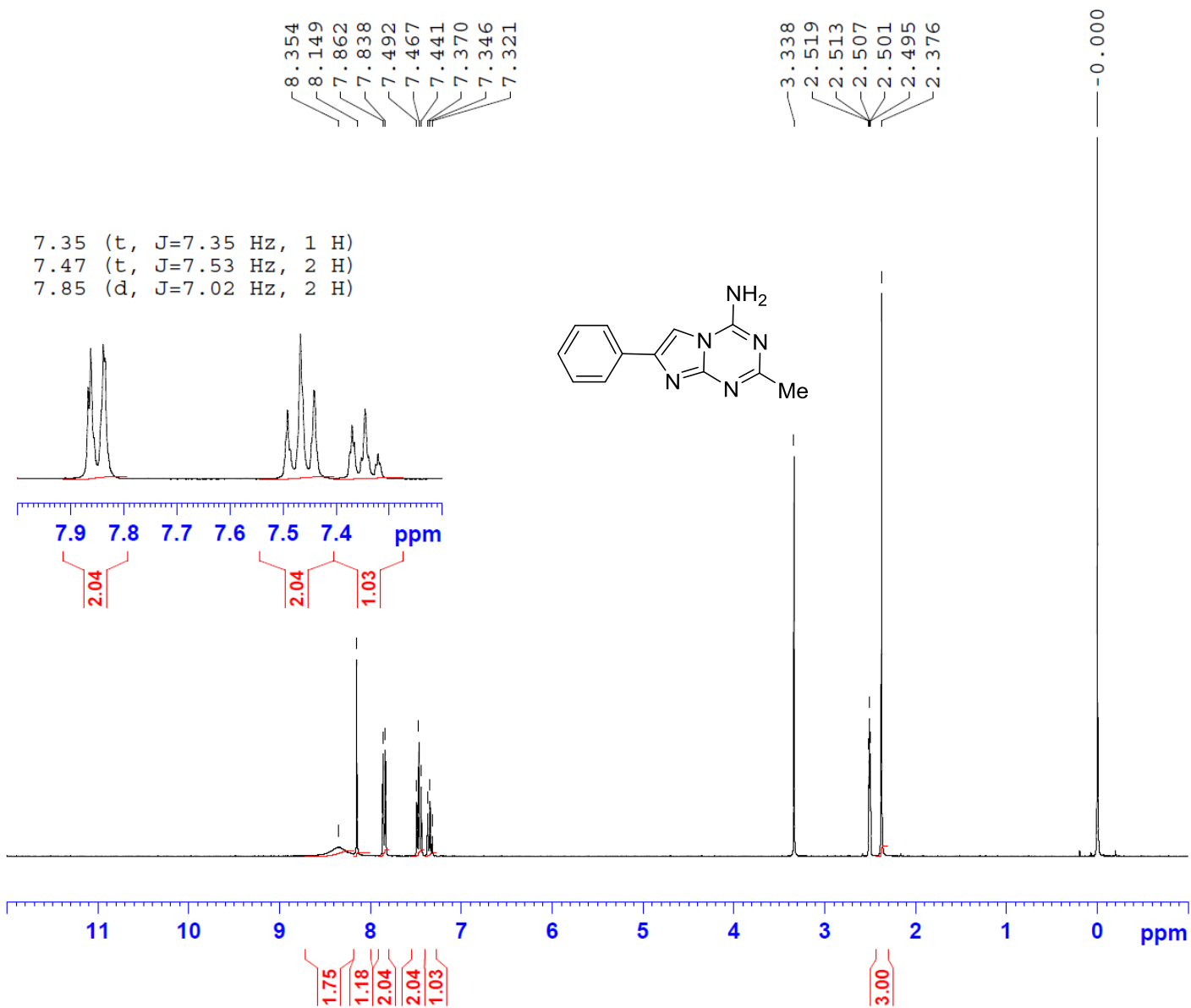
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## *Table of Contents*

$^1\text{H}$ and $^{13}\text{C}$ NMR spectra for compounds <b>5a-x</b> and <b>6</b>	S3
X-Ray crystallographic data for <b>5g</b> and <b>5p</b>	S57

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for compounds  
**5a-x** and **6**

4-Amino-2-methyl-7-phenylimidazo[1,2-a][1,3,5]triazine (5a)



Current Data Parameters  
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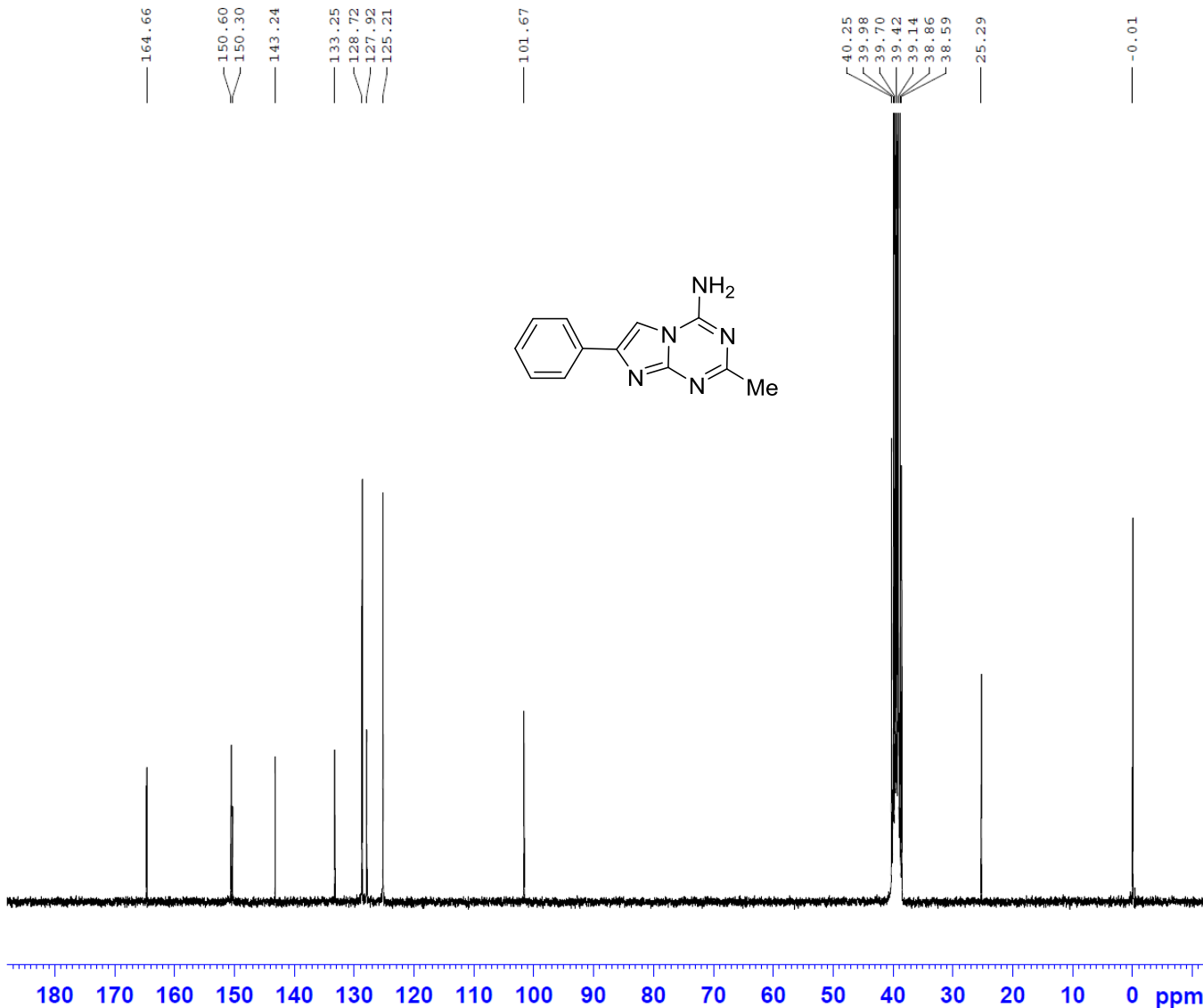
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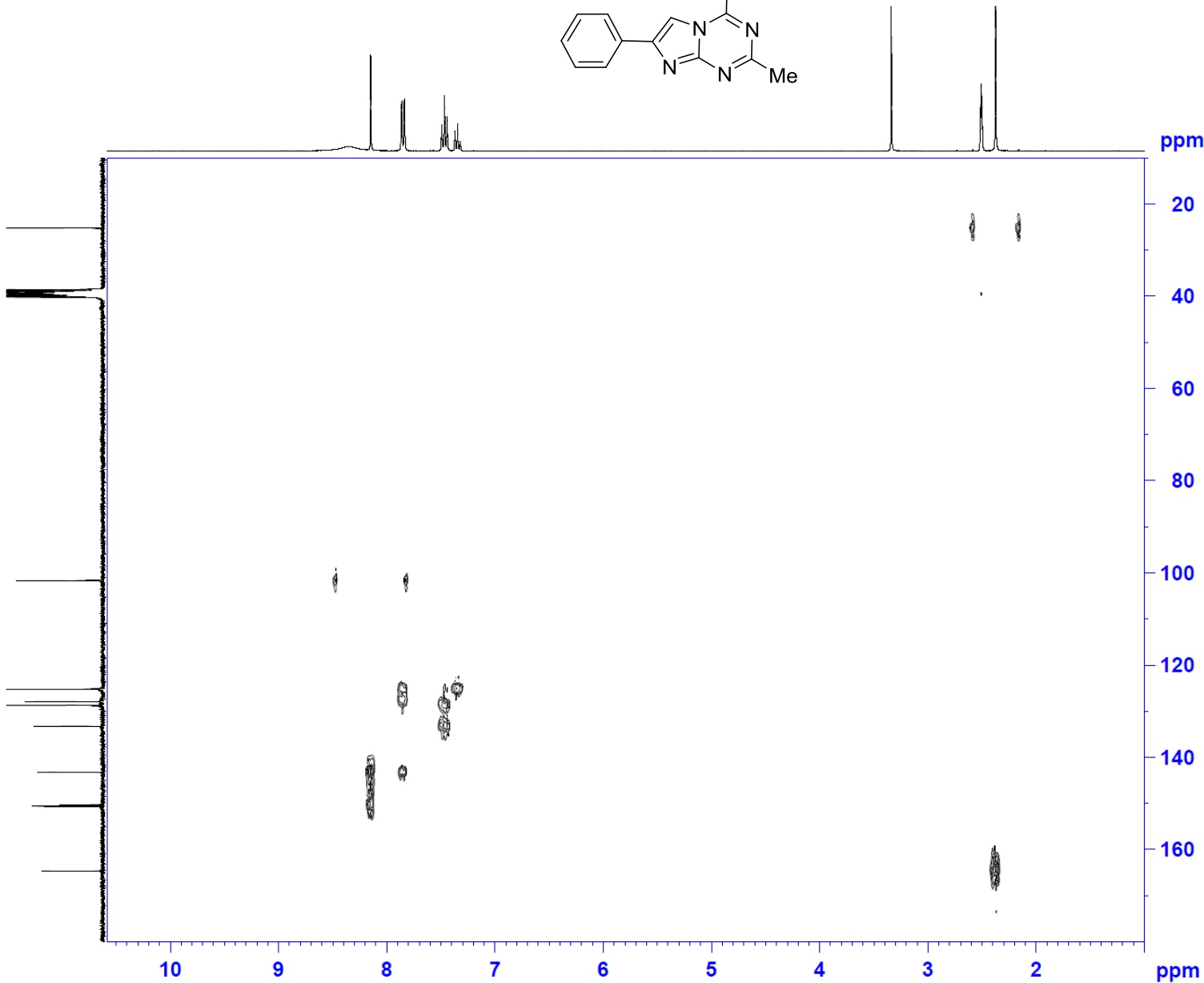
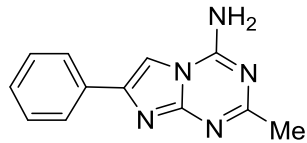
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SOLVENT      DMSO
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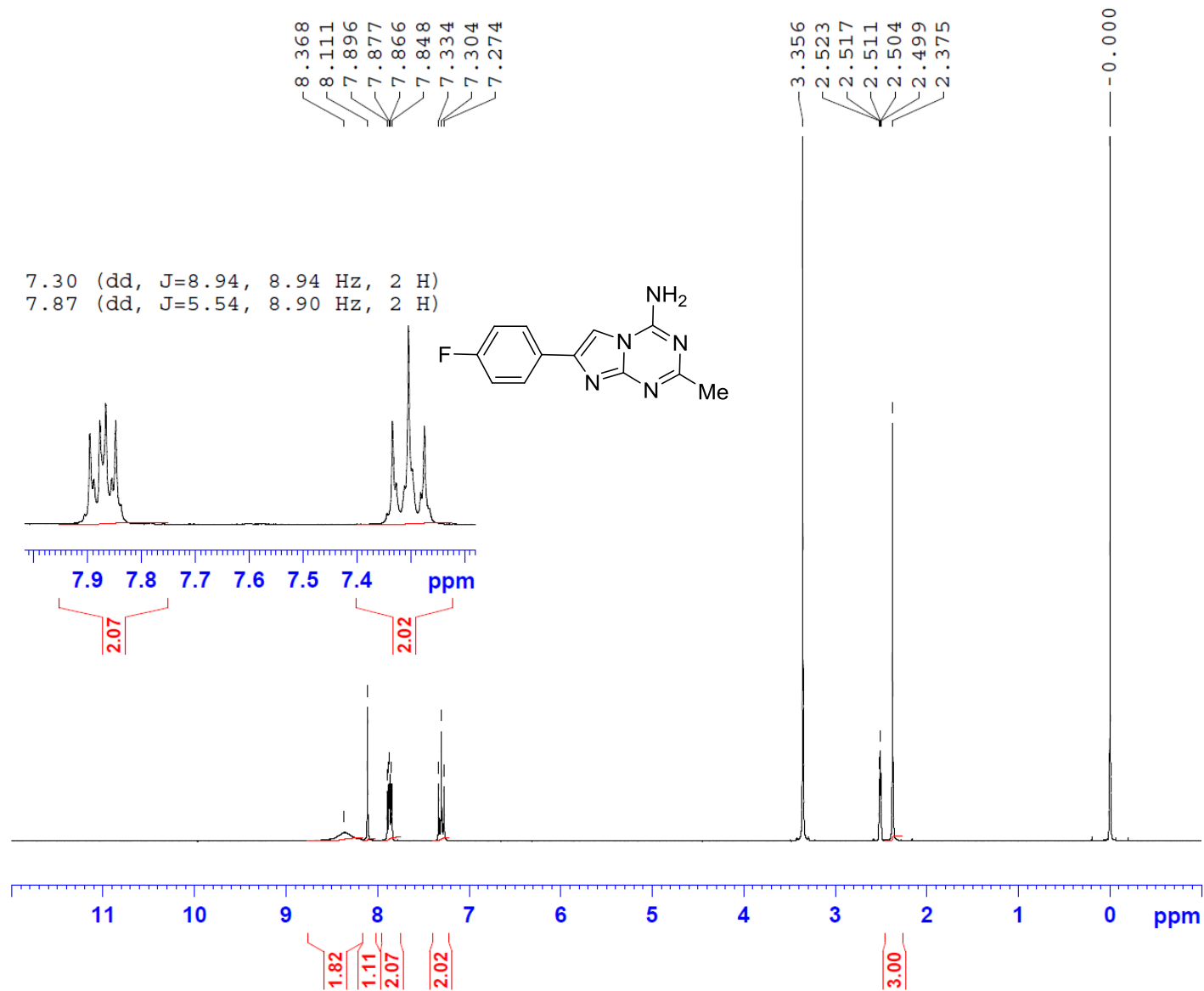
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**4-Amino-2-methyl-7-(4-fluorophenyl)imidazo[1,2-a][1,3,5]triazine (5b)**



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 FIDRES 0.093132 Hz  
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 PROCNO 1

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 TD 65536  
 SOLVENT DMSO  
 NS 14336  
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 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 298.2 K  
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 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 14

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 PLW13 0.20359001 W

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150.61  
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142.33

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 127.14

115.81  
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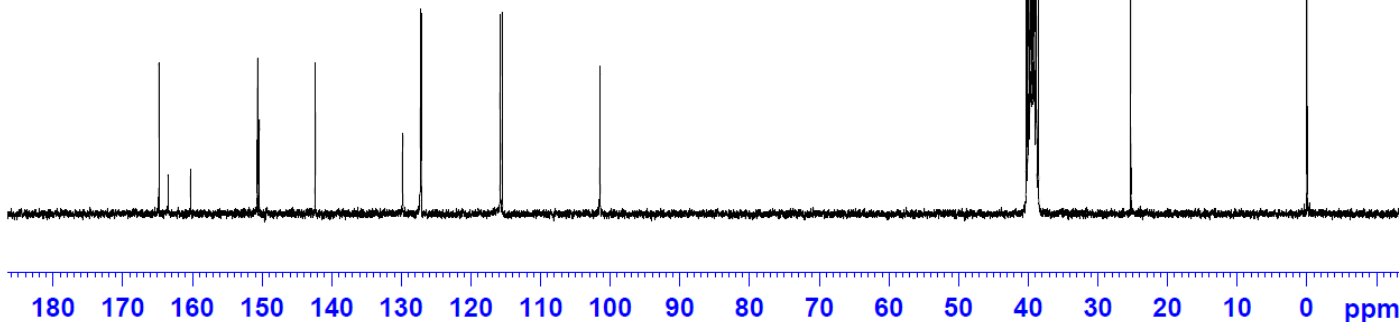
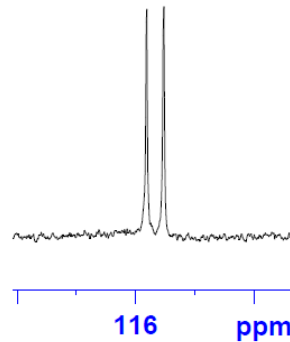
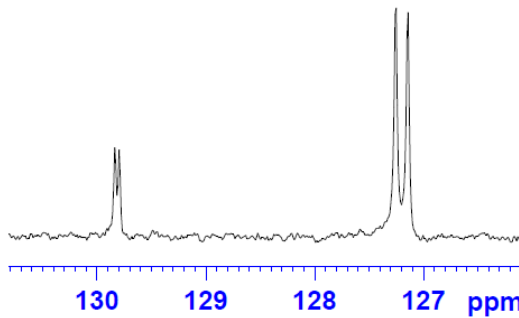
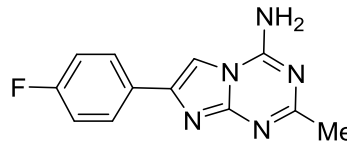
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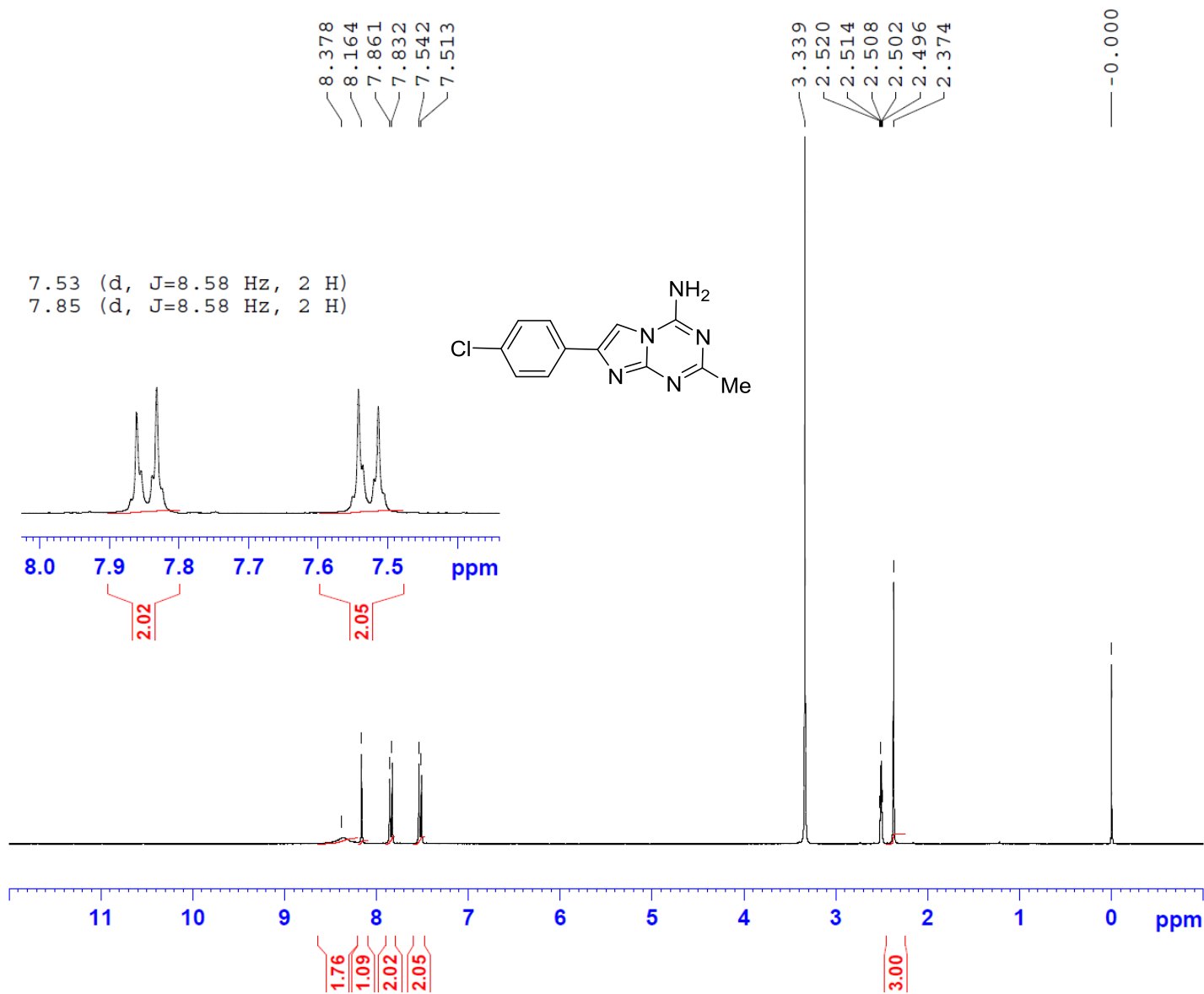
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4-Amino-2-methyl-7-(4-chlorophenyl)imidazo[1,2-a][1,3,5]triazine (5c)



Current Data Parameters  
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 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 113.521  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.1 K  
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 TD0 1

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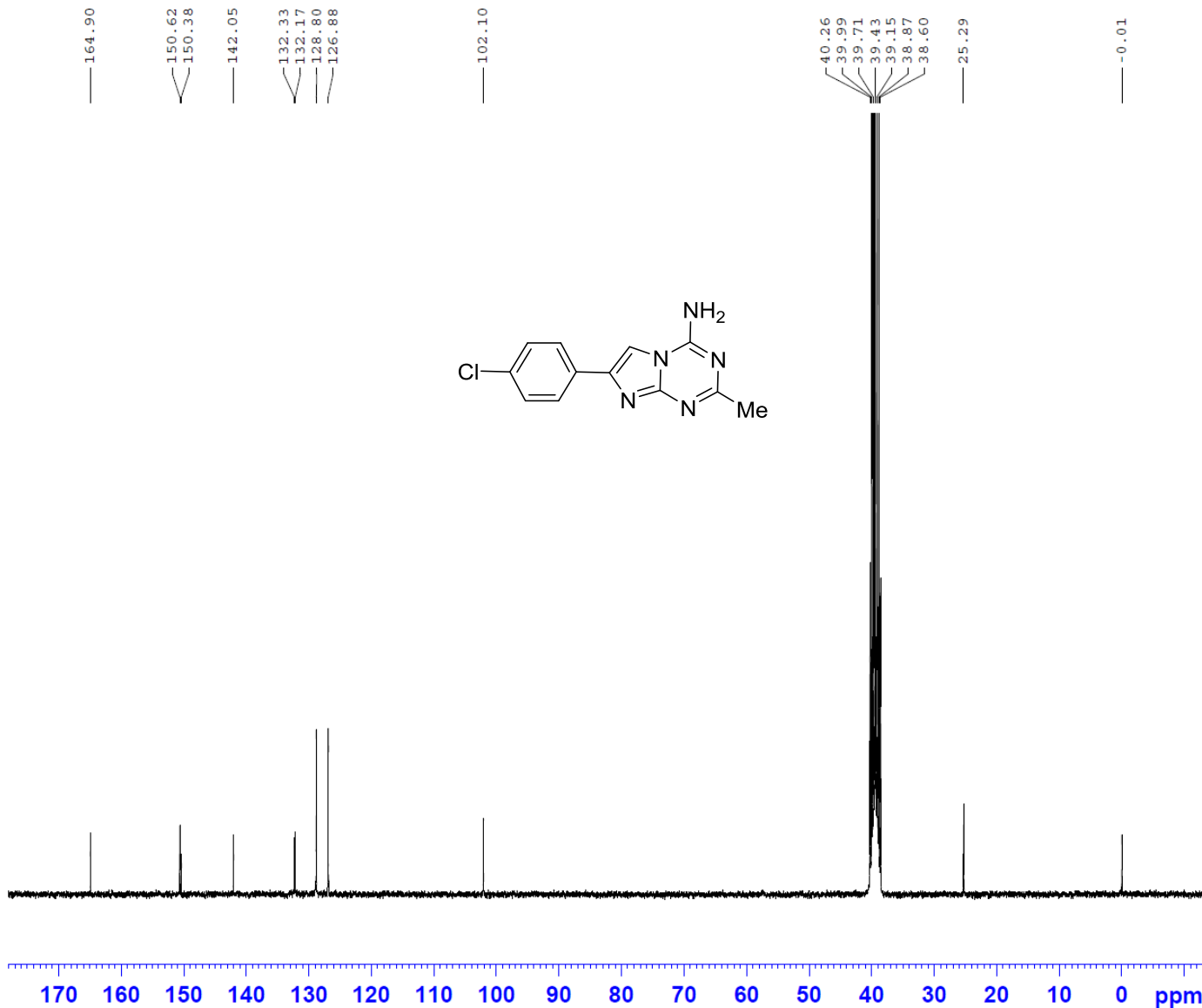
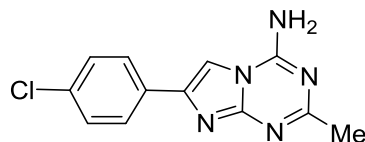
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NS 14336  
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FIDRES 0.372529 Hz  
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RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.2 K  
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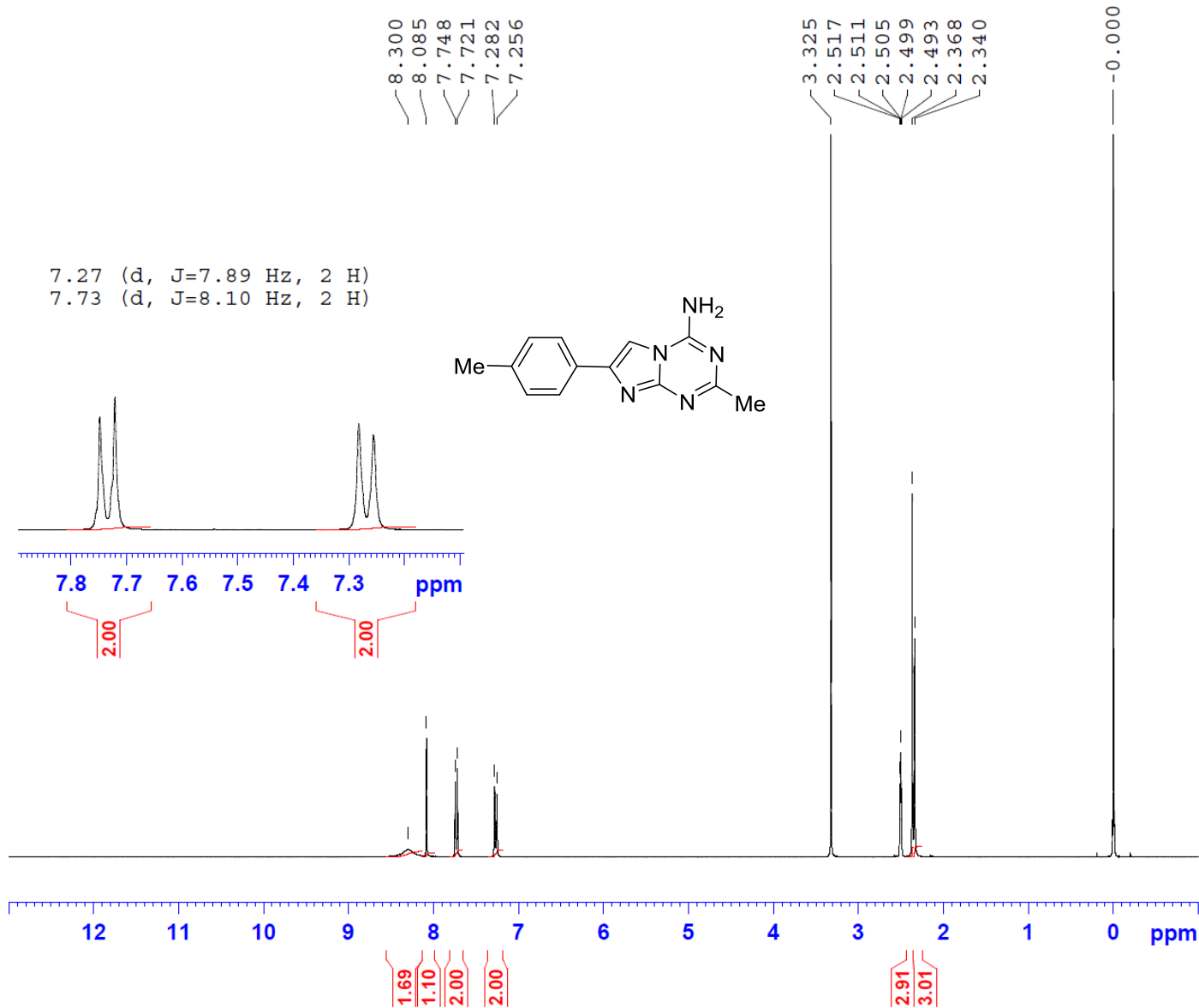
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PLW12 0.29359001 W  
PLW13 0.20359001 W

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**4-Amino-2-methyl-7-(4-methylphenyl)imidazo[1,2-a][1,3,5]triazine (5d)**



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 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 107.611  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 299.9 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
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 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

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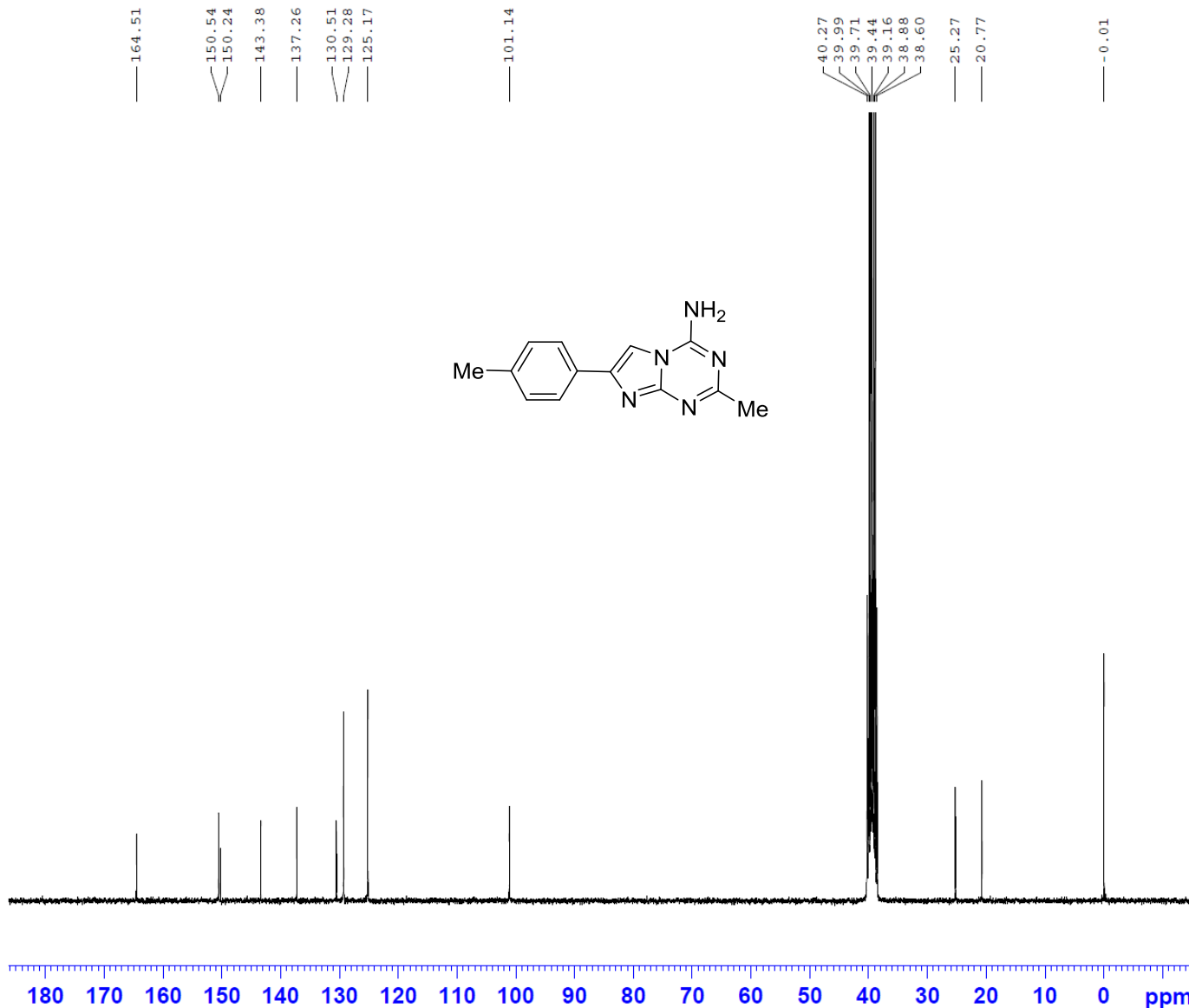
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TD 65536  
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NS 15360  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
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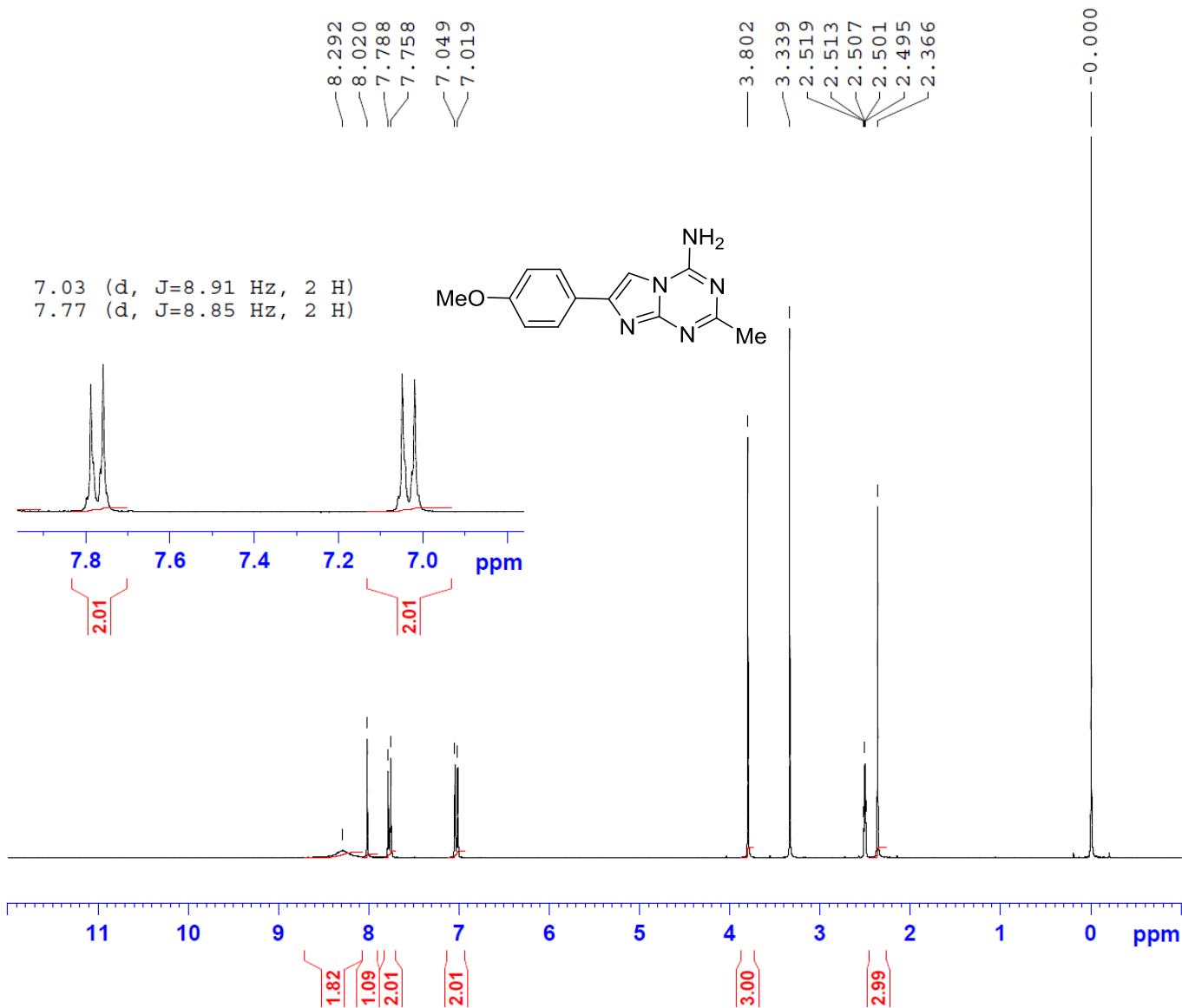
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PLW12 0.29359001 W  
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PC 1.40



# 4-Amino-2-methyl-7-(4-methoxyphenyl)imidazo[1,2-a][1,3,5]triazine (5e)



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 FIDRES 0.093132 Hz  
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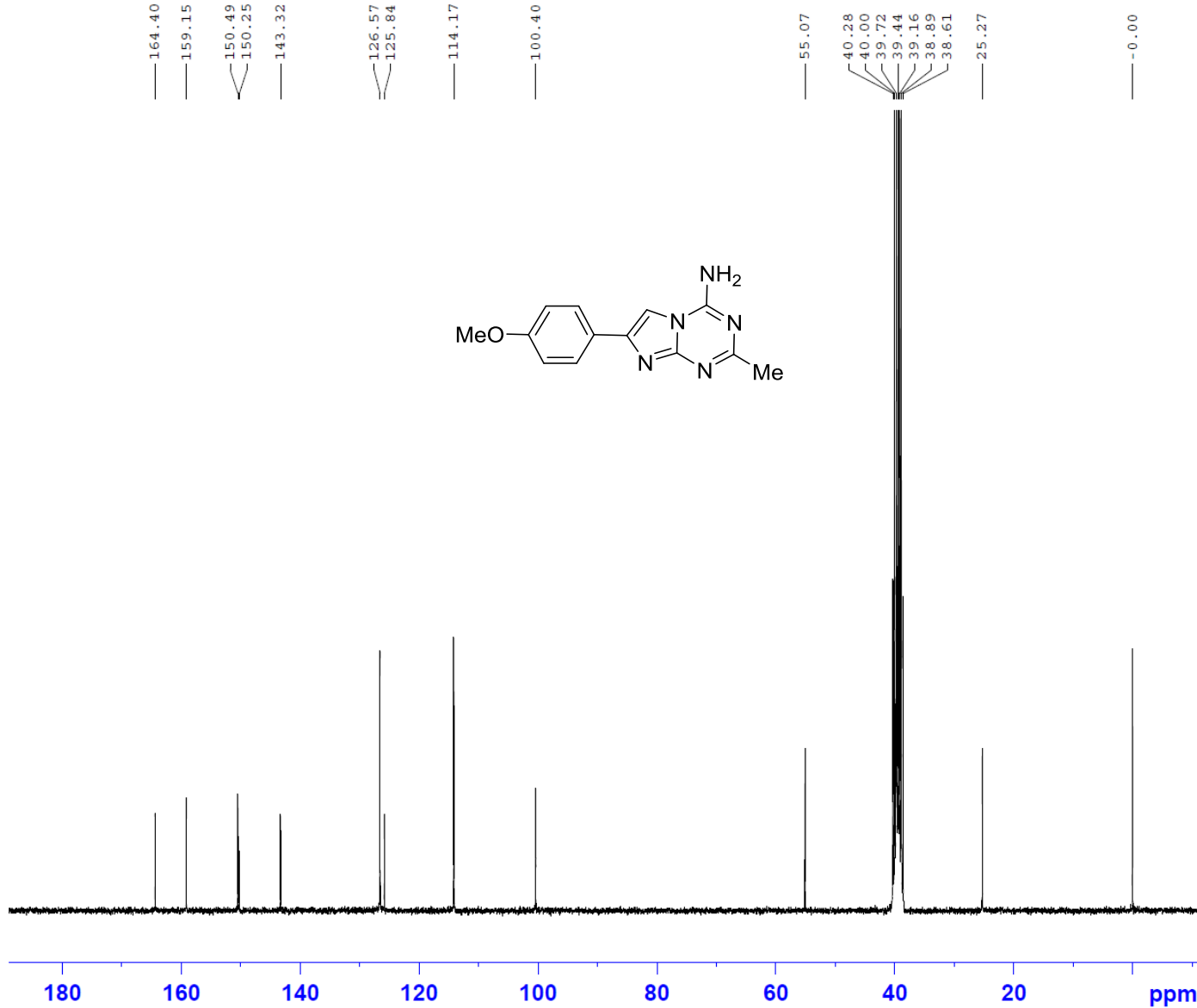
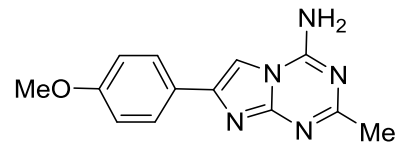
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FIDRES 0.372529 Hz  
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RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TDO 15

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P1 15.00 usec  
PLW1 22.00000000 W

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PLW13 0.20359001 W

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4-Amino-2-methyl-7-(4-biphenyl)imidazo[1,2-a][1,3,5]triazine (5f)

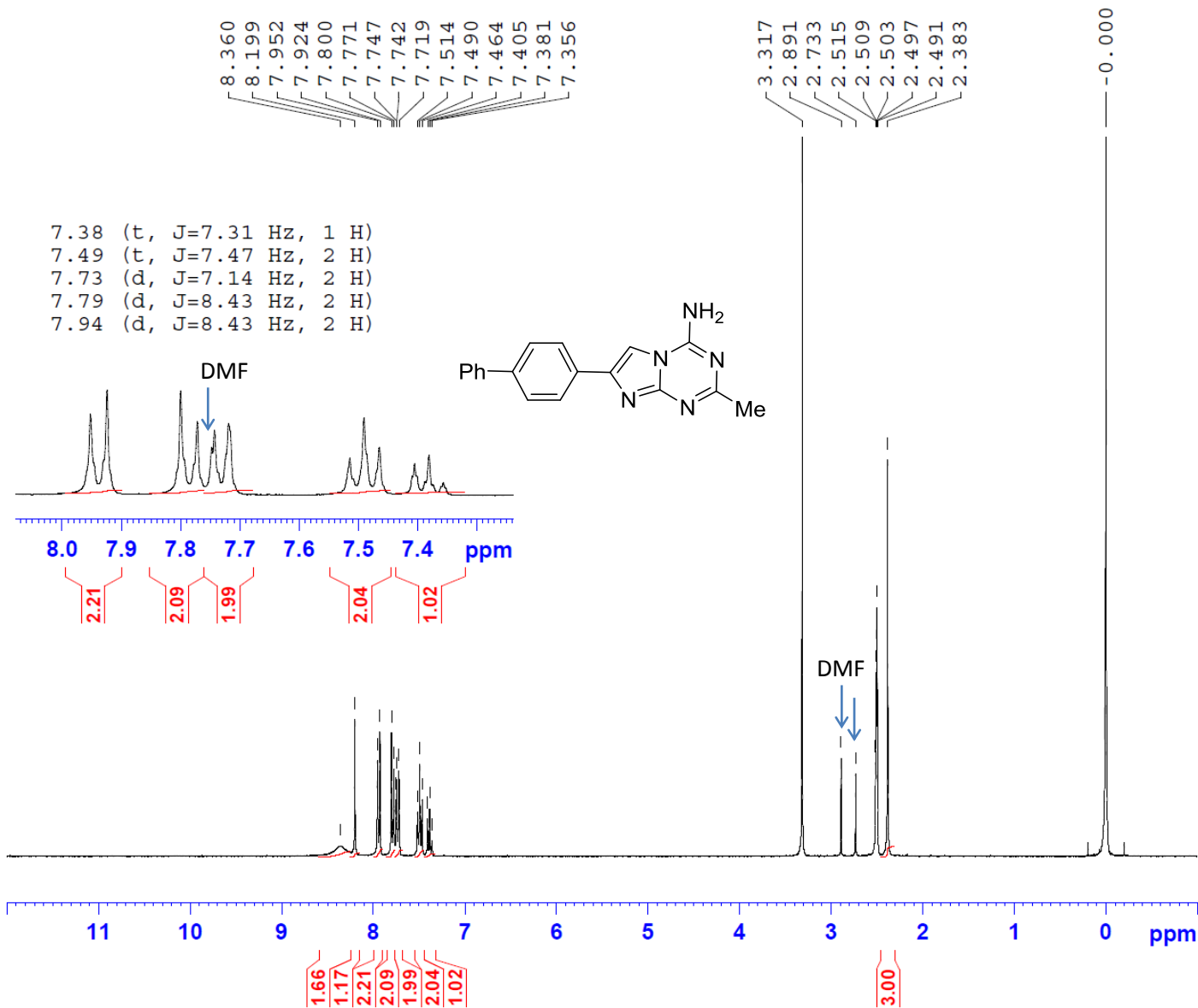


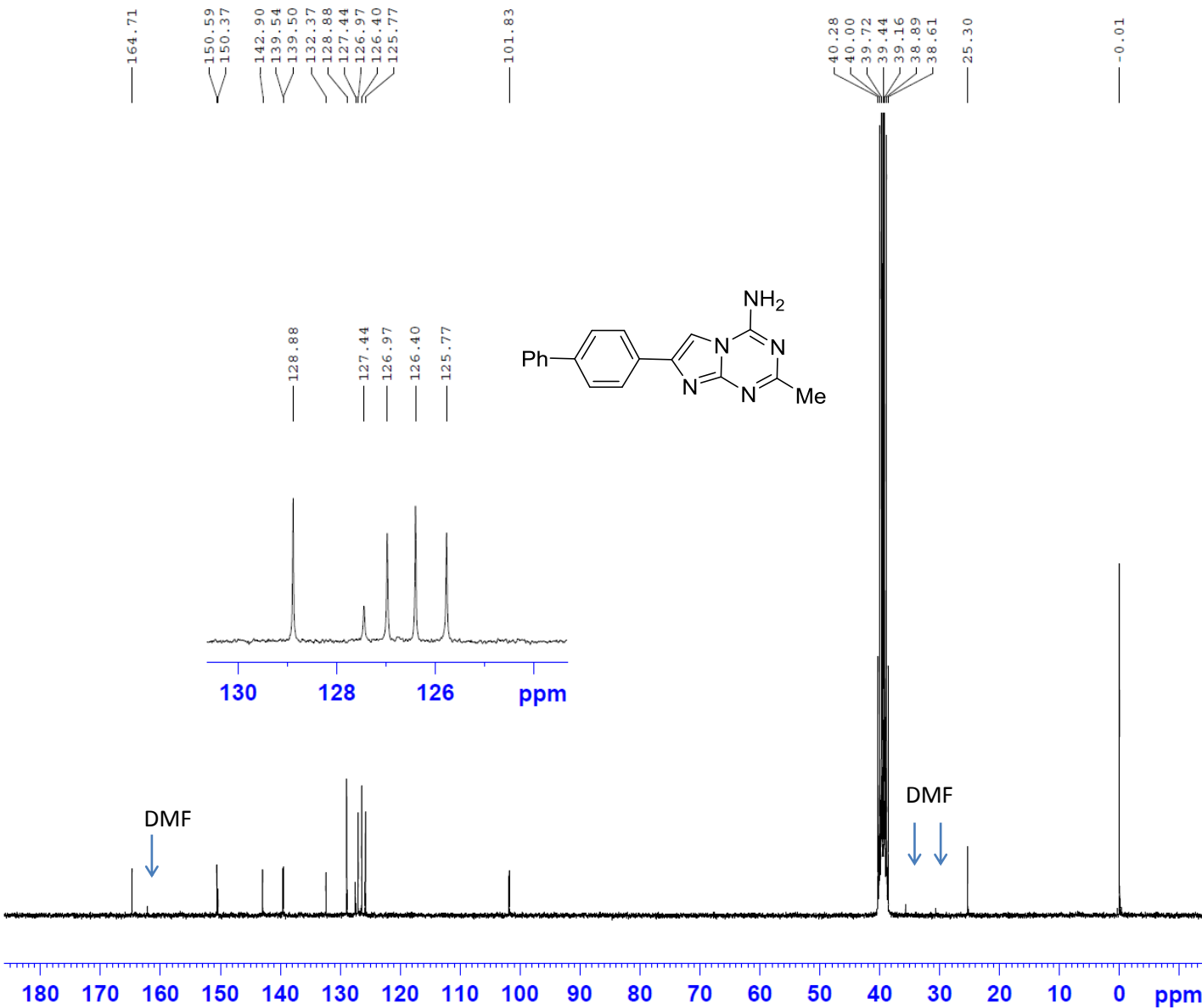
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 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 118.833  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

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Current Data Parameters  
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PROCNO 1

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Time\_ 18.06  
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TD 65536  
SOLVENT DMSO  
NS 15360  
DS 4  
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FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
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L5 53  
P32 98.00 usec  
TD0 15

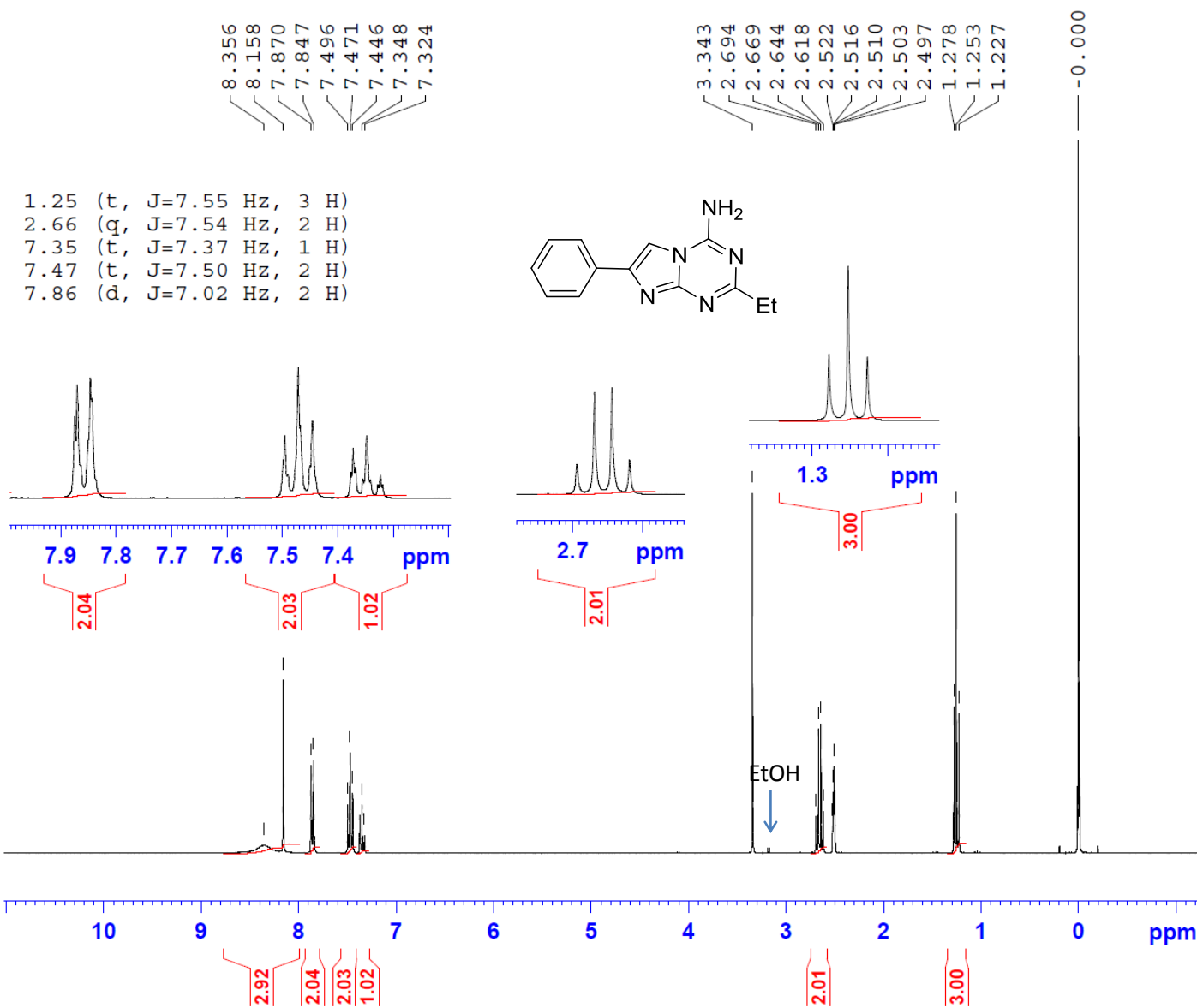
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PLW13 0.20359001 W

F2 - Processing parameters  
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# 4-Amino-2-ethyl-7-phenylimidazo[1,2-a][1,3,5]triazine (5g)

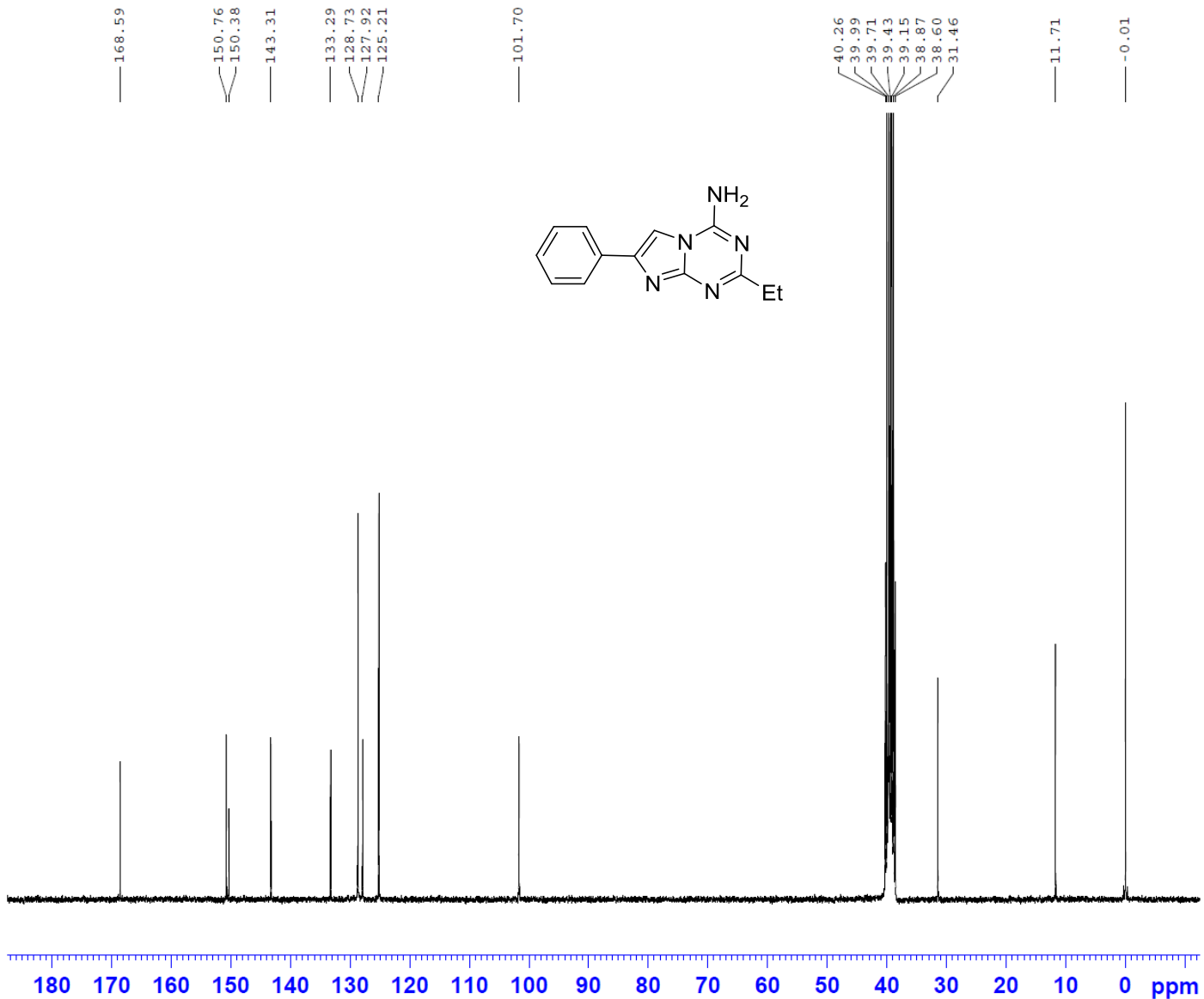


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 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
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 DW 81.920 usec  
 DE 6.50 usec  
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 TD0 1

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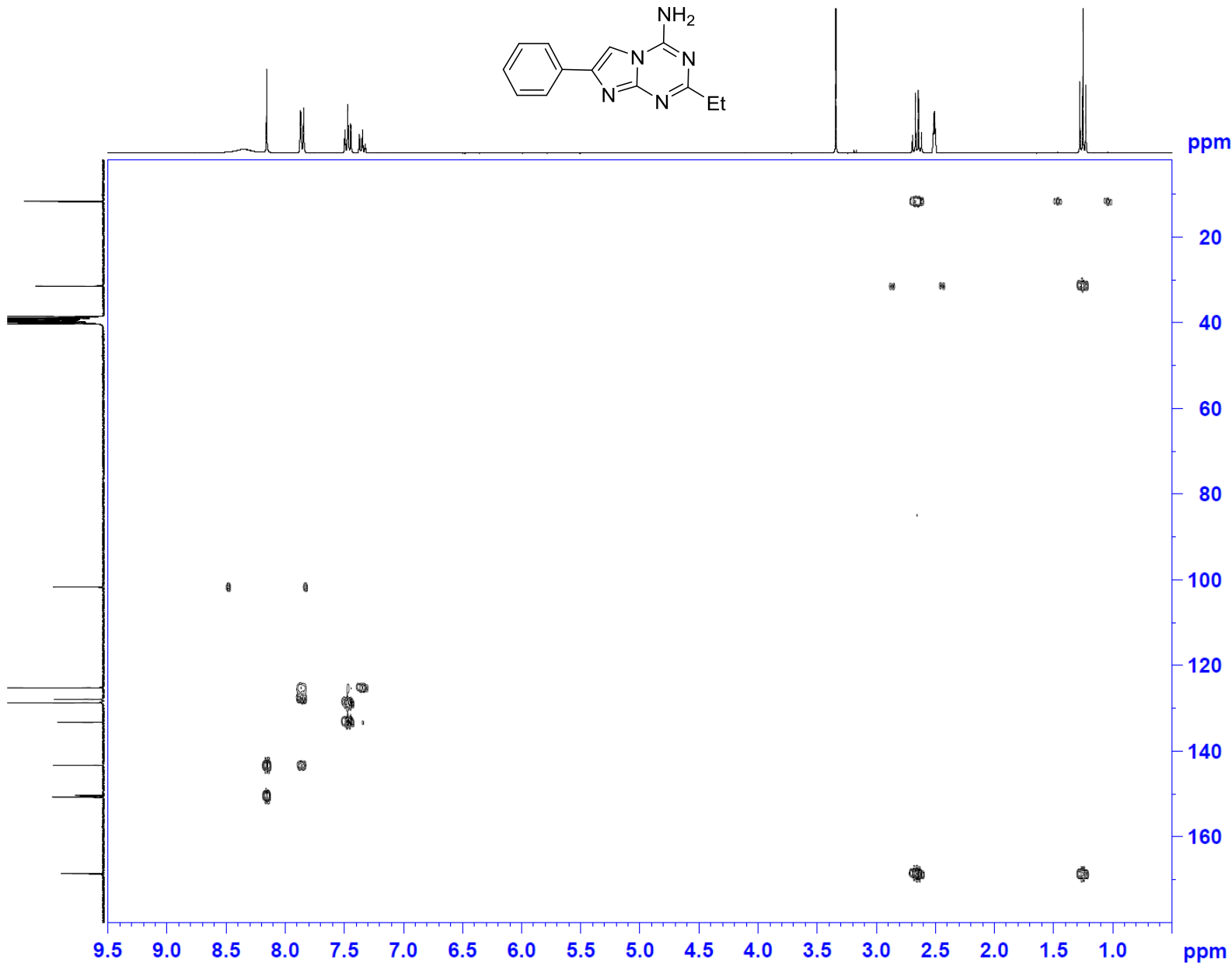
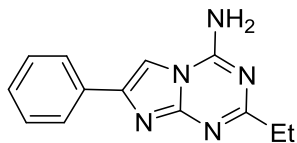
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 Date\_ 20170530  
 Time 19.05  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 14336  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 14

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753342 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



```

Current Data Parameters
NAME      FL328
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20170607
Time     18.02
INSTRUM  FOURIER300
PROBHD   5 mm DUL 13C-1
FULPROG  hmbogp1pndqf
TD       2048
SOLVENT  DMSO
NS       250
DS       16
SWH      3051.758 Hz
FIDRES   1.490116 Hz
AQ       0.3355443 sec
RG       501.187
DW       163.840 usec
DE       6.50 usec
TE       300.0 K
CNST2    145.0000000
DO       10.0000000
D0       0.00000300 sec
D1       1.26226795 sec
D2       0.00344828 sec
D6       0.05000000 sec
D16      0.00020000 sec
D31      0.00001350 sec
D32      0.00002700 sec
D33      0.00001200 sec
D36      0.00100000 sec
D38      0.00002980 sec
INO      0.0002980 sec

===== CHANNEL f1 =====
SFO1     300.1614875 MHz
NUC1     1H
P1       13.50 usec
P2       27.00 usec
PLW1     9.30000019 W

===== CHANNEL f2 =====
SFO2     75.4828272 MHz
NUC2     13C
P3       12.00 usec
PLW2     22.00000000 W

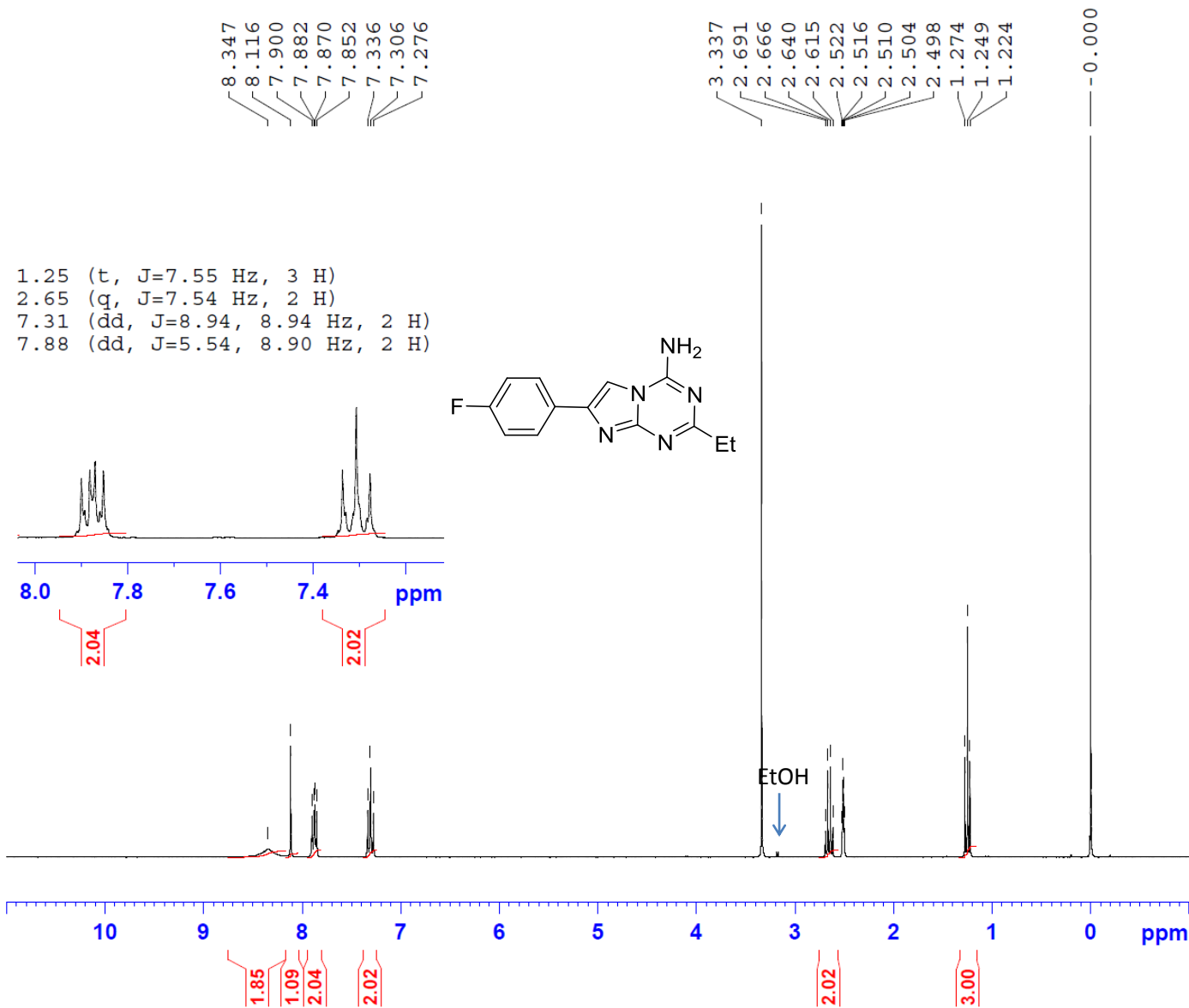
===== GRADIENT CHANNEL =====
GPNAM[1] RECT.1
GPNAM[2] RECT.1
GPNAM[3] RECT.1
GPZ1     50.00 %
GPZ2     30.00 %
GPZ3     40.10 %
P16      1000.00 usec

F1 - Acquisition parameters
TD       128
SFO1     75.48283 MHz
FIDRES   131.082214 Hz
SW       222.283 ppm
FtMODE   QF

F2 - Processing parameters
SI       2048
SF       300.1599991 MHz
WDW      SINE
SGB      0
LB       0 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       75.4753250 MHz
WDW      SINE
SGB      0
LB       0 Hz
GB       0
  
```

# 4-Amino-2-ethyl-7-(4-fluorophenyl)imidazo[1,2-a][1,3,5]triazine (5h)



Current Data Parameters  
 NAME FL352  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170816  
 Time\_ 17.31  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 98.8762  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 299.9 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599979 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



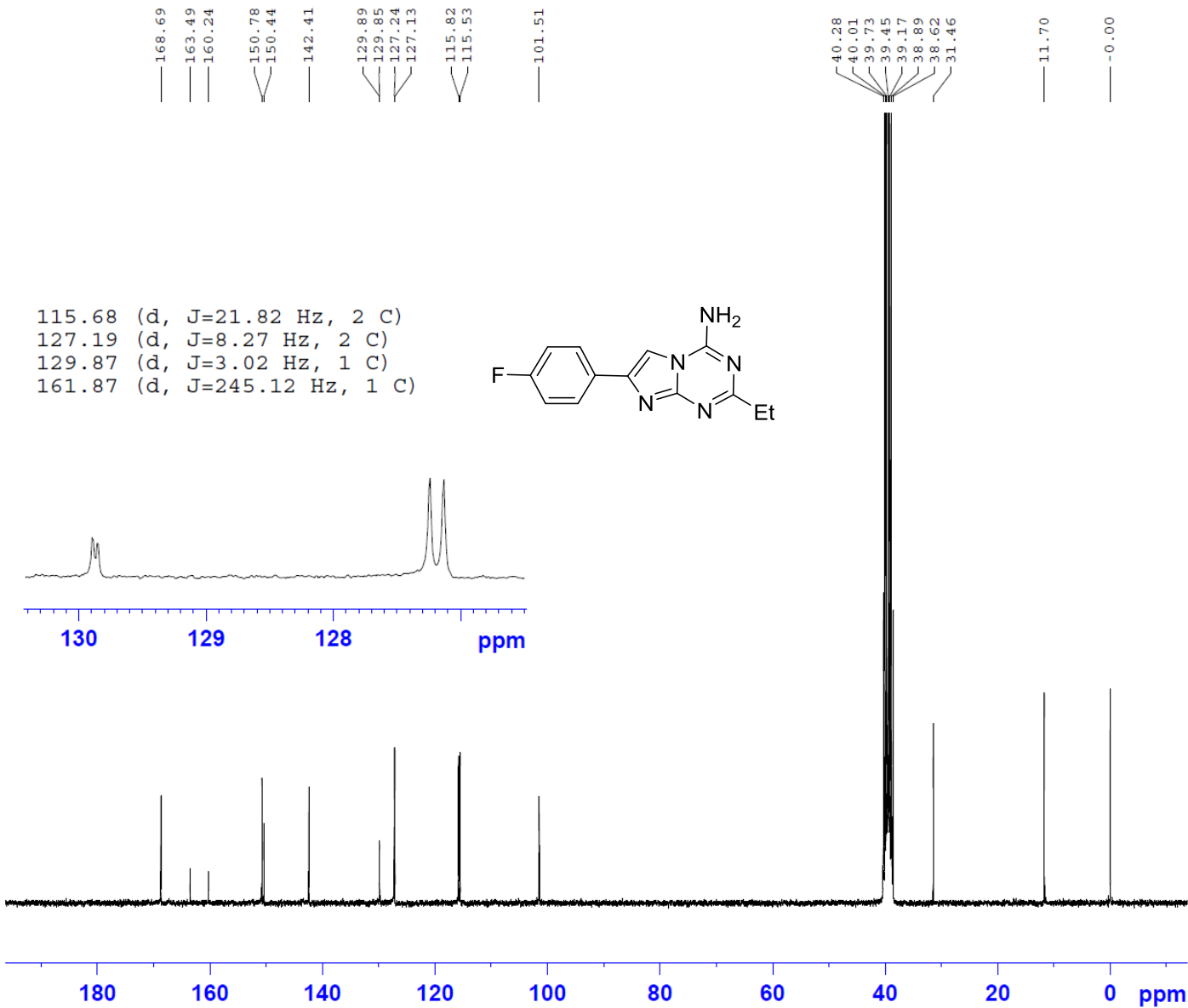
Current Data Parameters  
NAME FL352  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time\_ 18.05  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 14336  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 14

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753335 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



4-Amino-2-ethyl-7-(4-chlorophenyl)imidazo[1,2-a][1,3,5]triazine (5i)

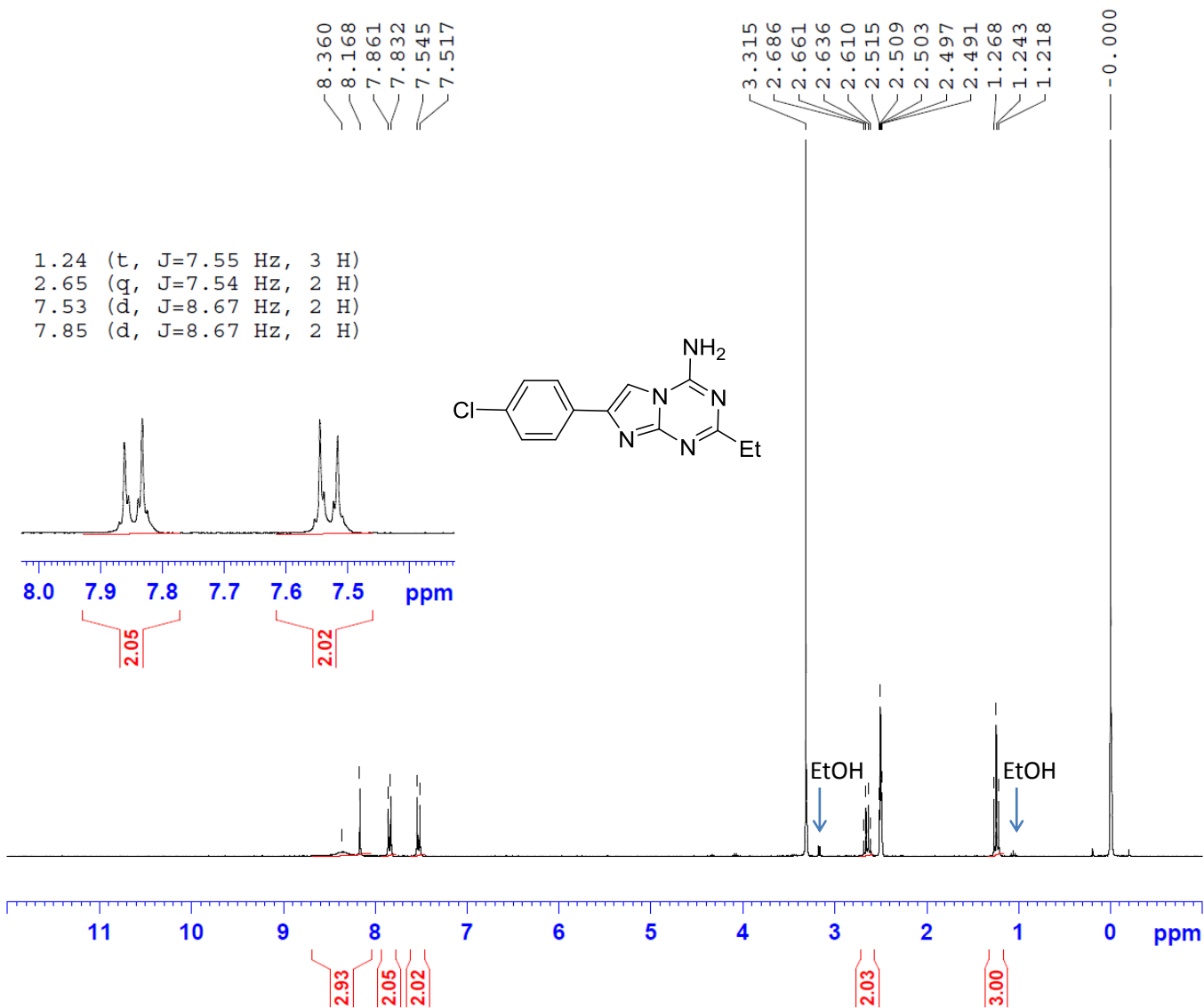


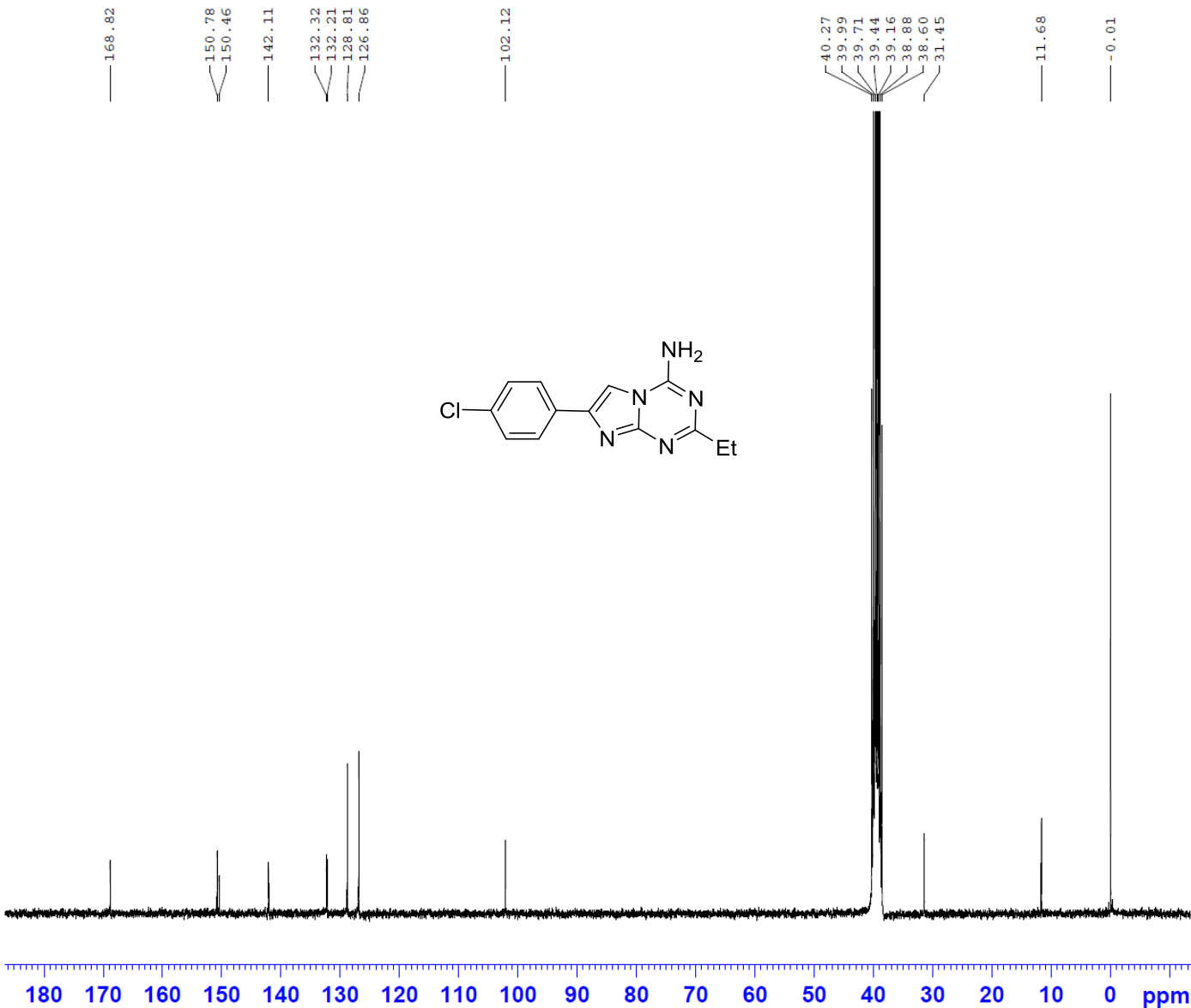
Current Data Parameters  
 NAME FL357  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170818  
 Time\_ 14.10  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 133.856  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1600001 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME FL357  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170820  
 Time 14.26  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20480  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 20

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753350 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4-Amino-2-ethyl-7-(4-methylphenyl)imidazo[1,2-a][1,3,5]triazine (5j)

8.310  
8.098  
7.759  
7.732  
7.285  
7.259

3.339  
2.690  
2.665  
2.640  
2.615  
2.523  
2.517  
2.511  
2.505  
2.499  
2.342  
1.276  
1.251  
1.226

— 0.000



Current Data Parameters  
NAME FL366  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

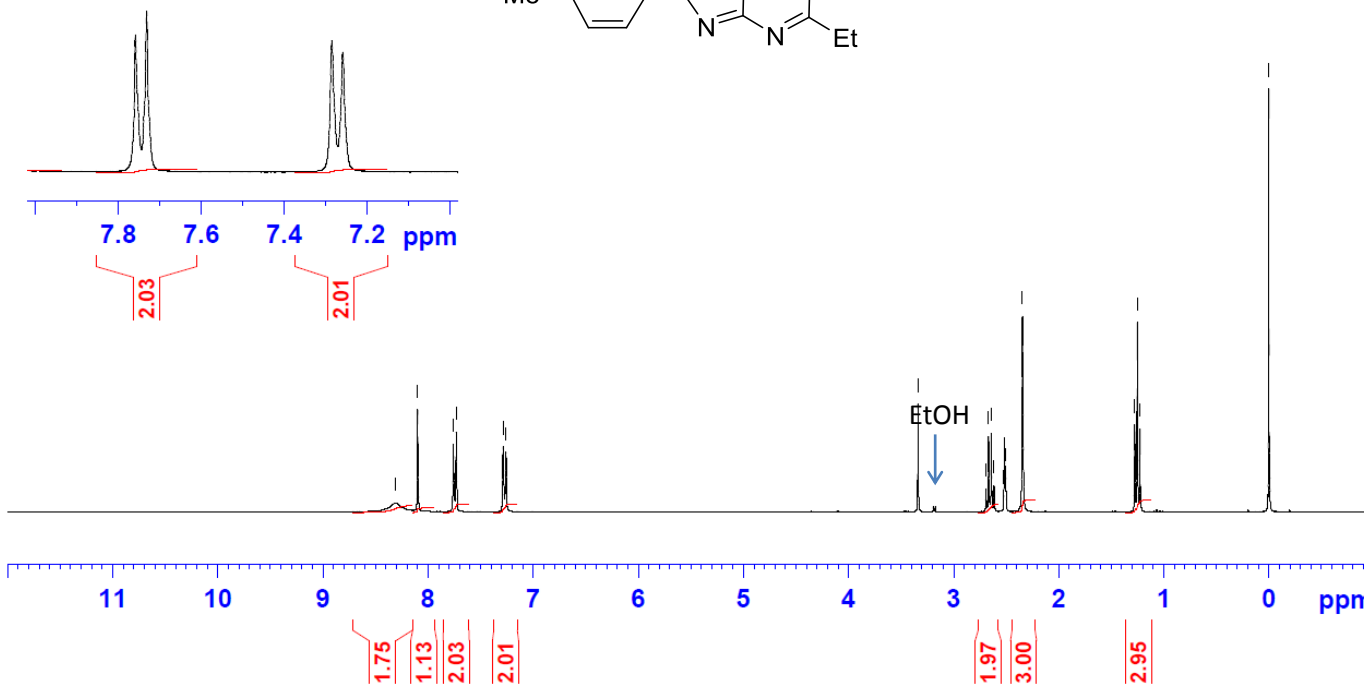
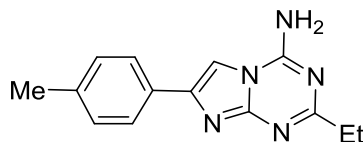
Date\_ 20170924  
Time 15.48  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 63.4837  
DW 81.920 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
SFO1 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

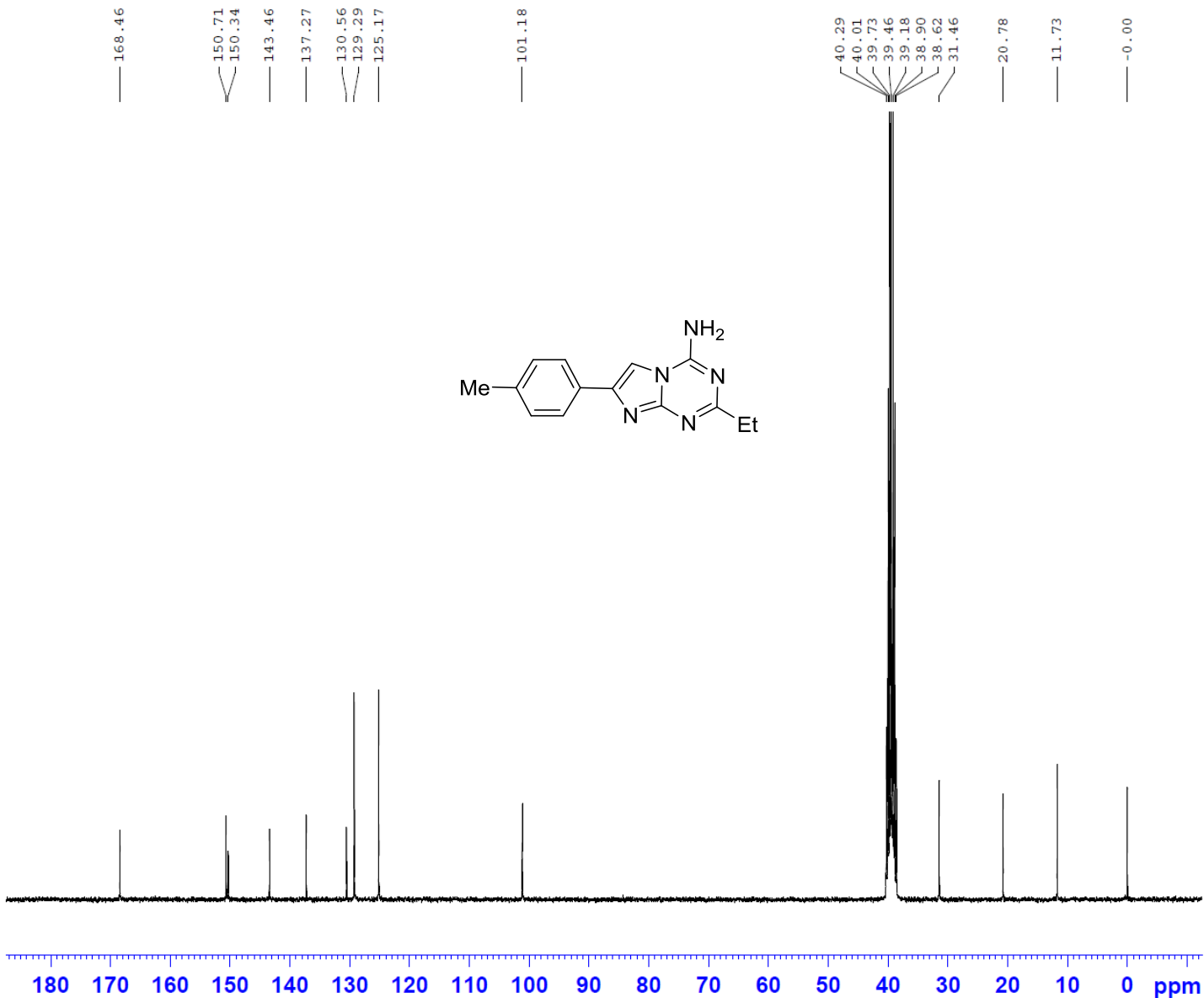
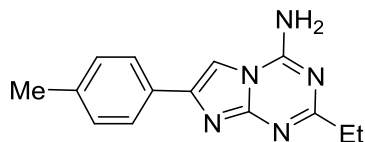
F2 - Processing parameters

SI 65536  
SF 300.1599976 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1.25 (t, J=7.55 Hz, 3 H)  
2.65 (q, J=7.54 Hz, 2 H)  
7.27 (d, J=7.95 Hz, 2 H)  
7.75 (d, J=8.10 Hz, 2 H)







Current Data Parameters  
 NAME FL366  
 EXPNO 2  
 PROCNO 1

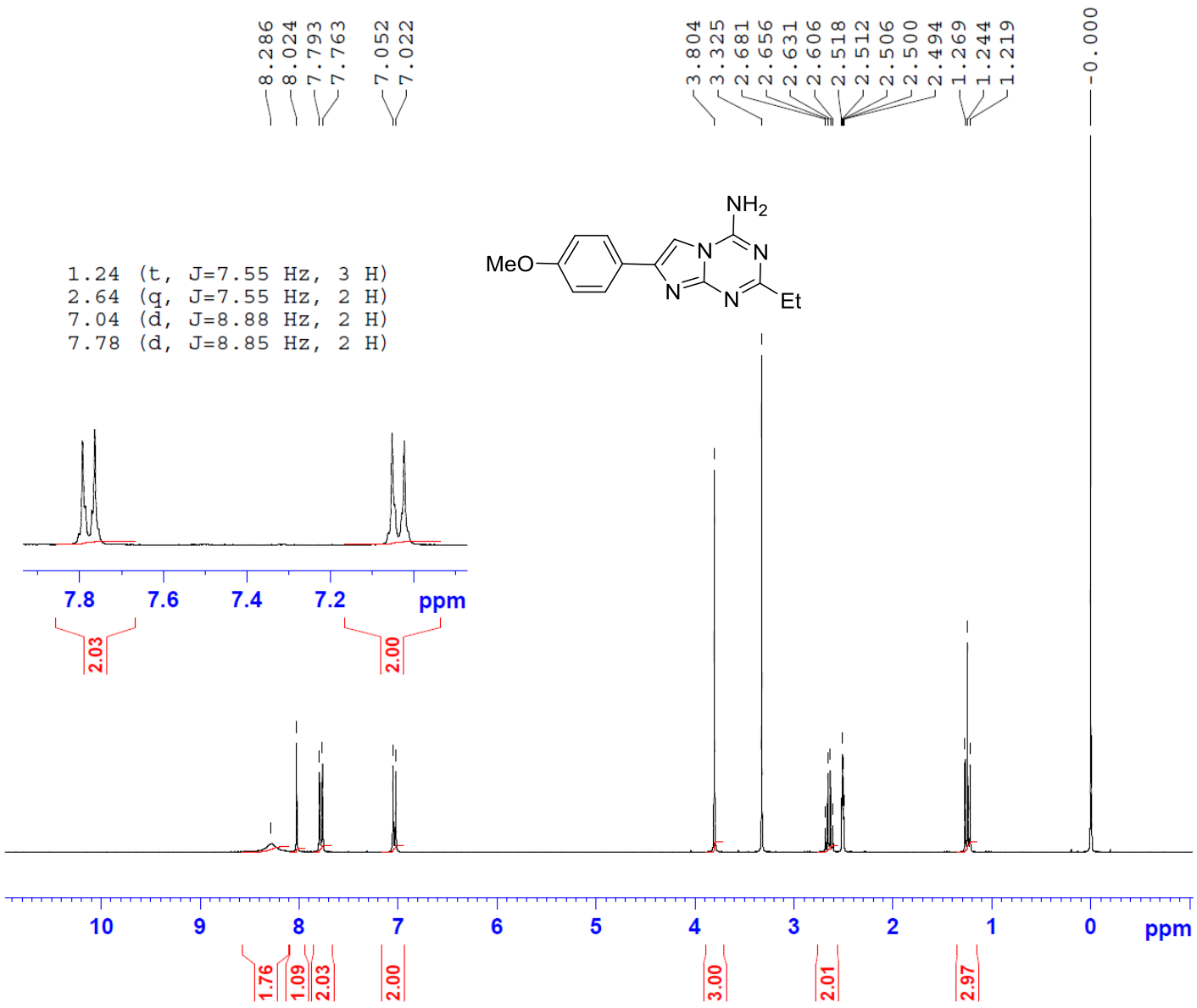
F2 - Acquisition Parameters  
 Date\_ 20170924  
 Time\_ 16.10  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 9216  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 9

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753335 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4-Amino-2-ethyl-7-(4-methoxyphenyl)imidazo[1,2-a][1,3,5]triazine (5k)



Current Data Parameters  
 NAME FL347  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170804  
 Time 16.36  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 113.921  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599991 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



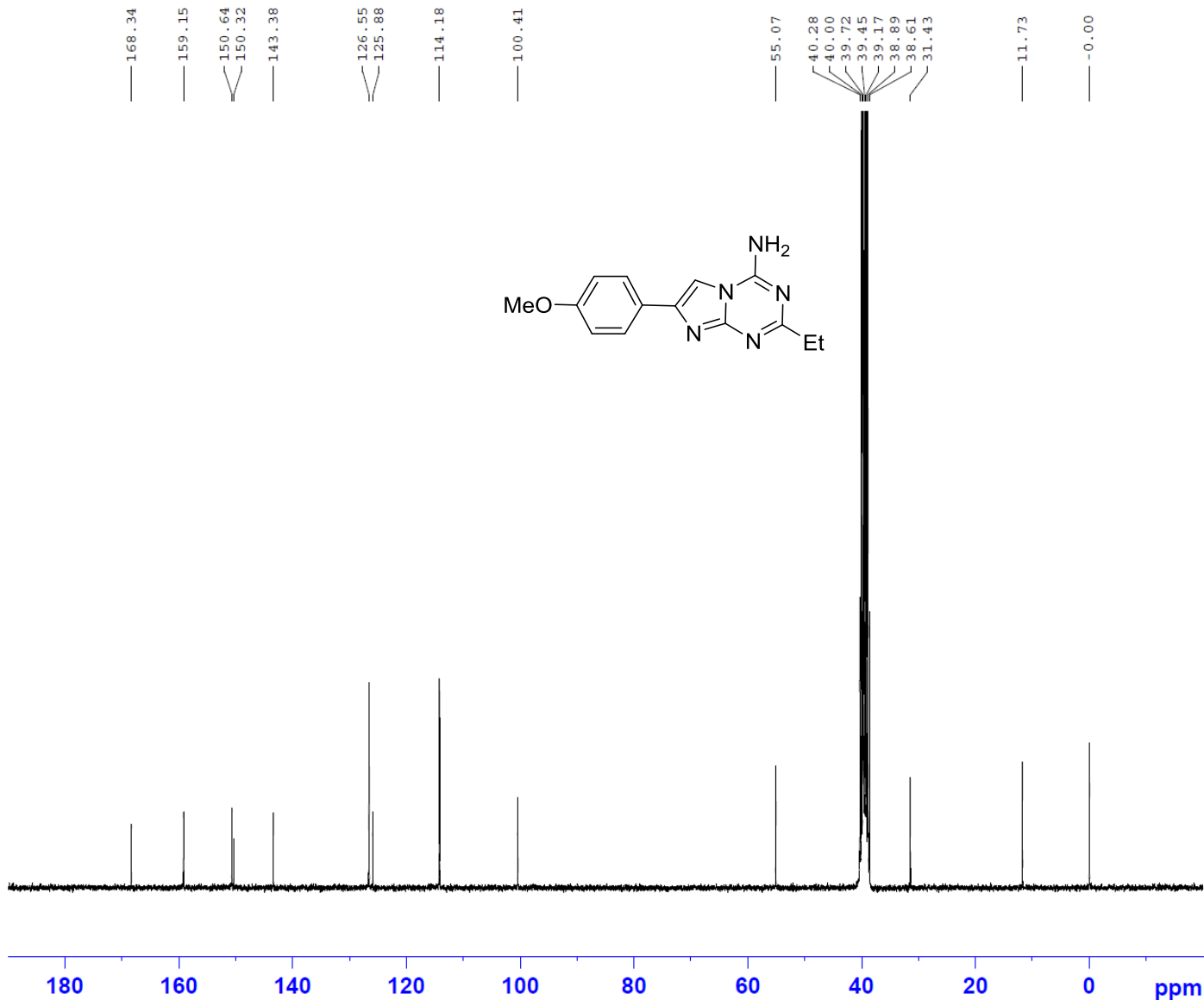
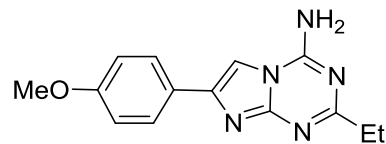
Current Data Parameters  
NAME FL347  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170804  
Time\_ 18.05  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 14336  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TDO 14

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753343 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



**4-Amino-2-ethyl-7-(4-biphenyl)imidazo[1,2-a][1,3,5]triazine (5I)**

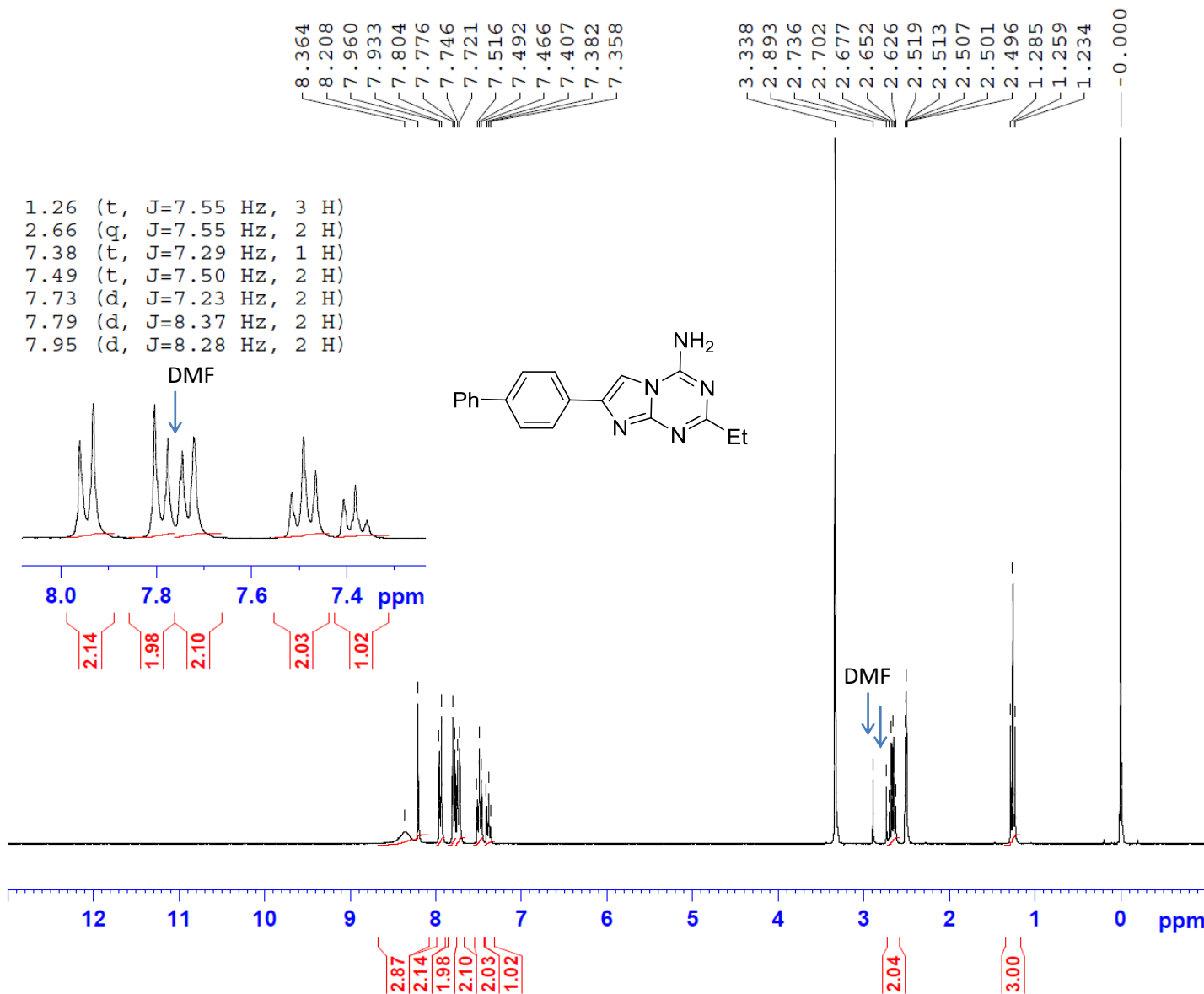


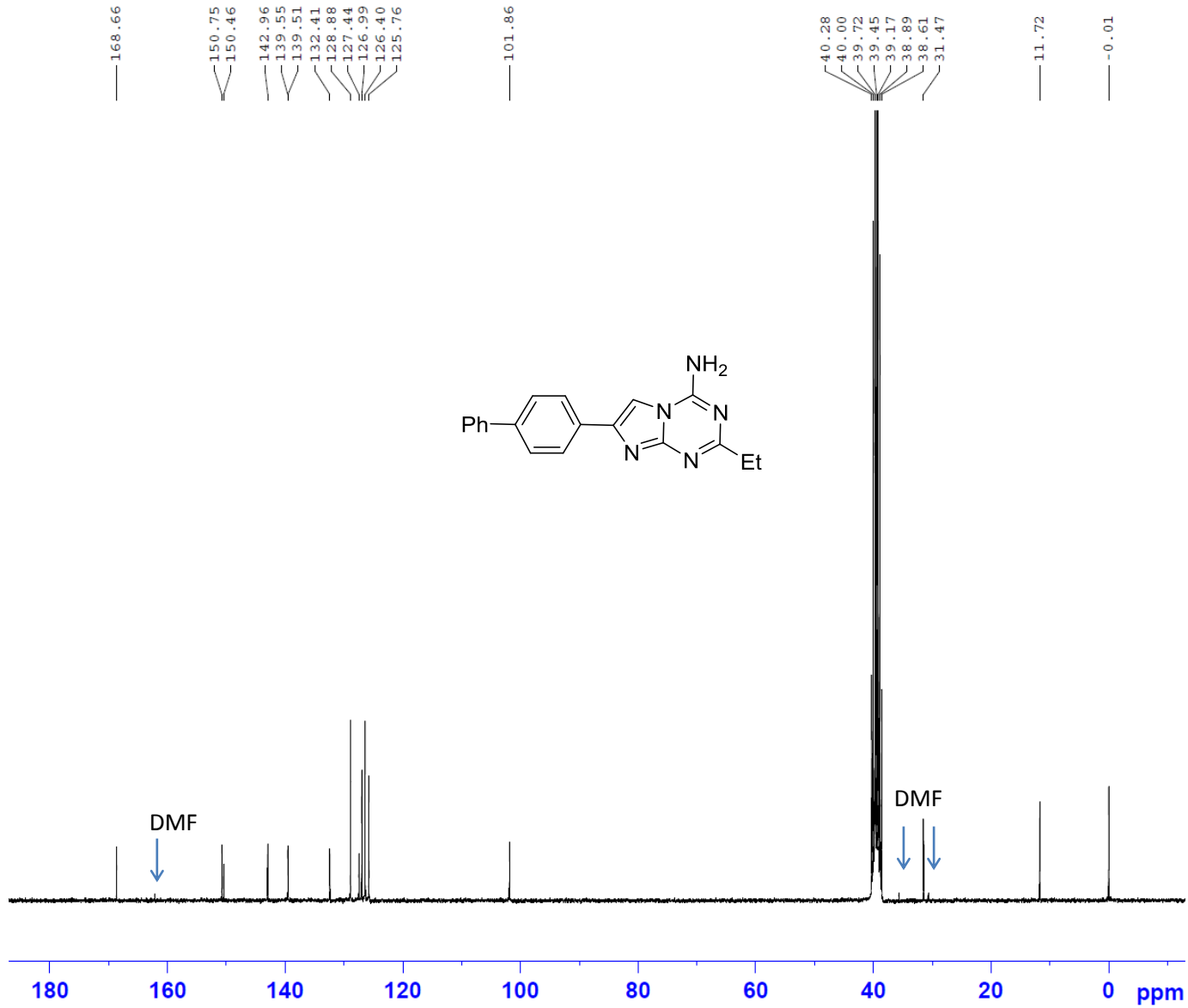
Current Data Parameters  
 NAME FL373  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171023  
 Time\_ 16.56  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 111.726  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599988 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME FL373  
 EXPNO 2  
 PROCNO 1

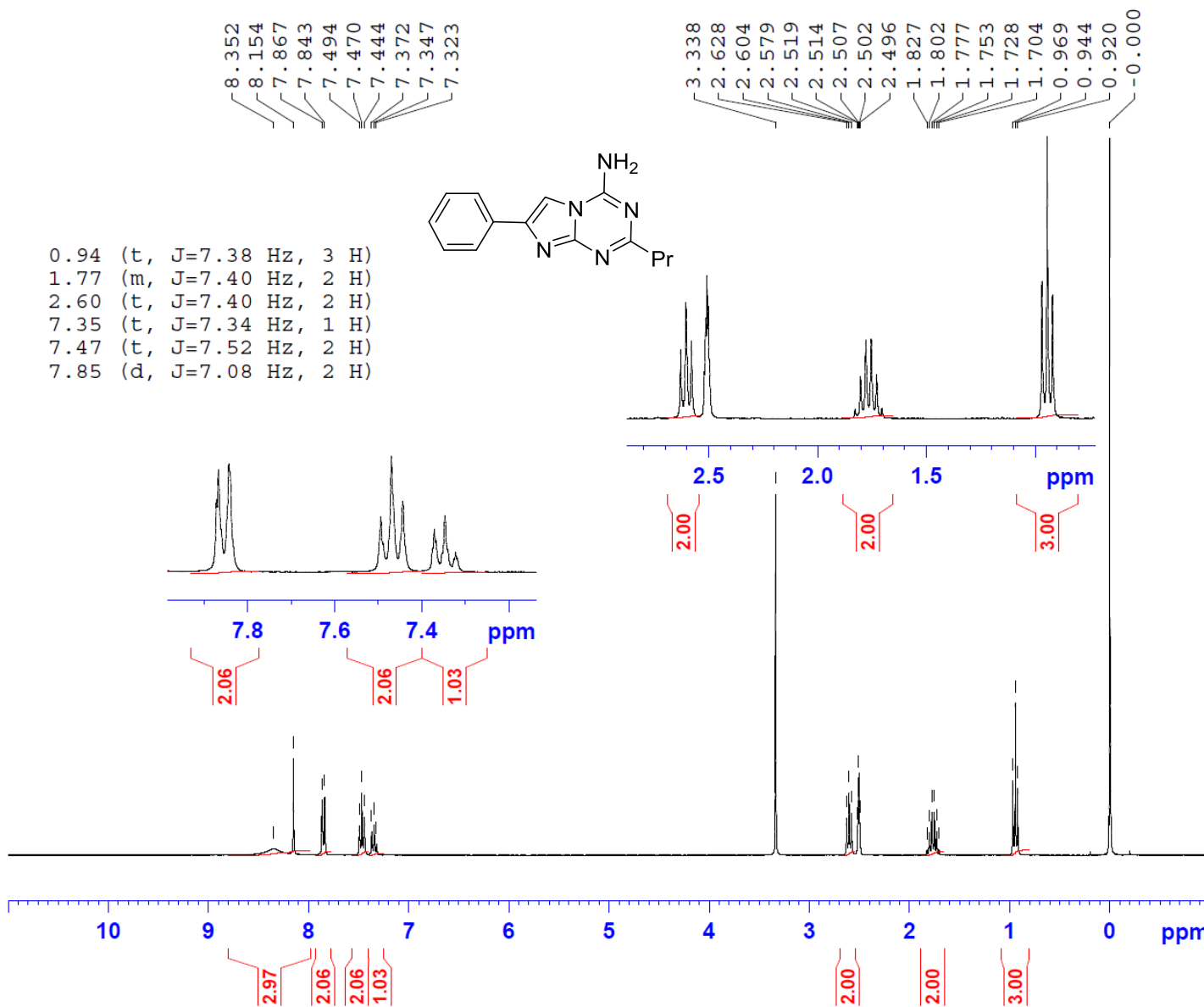
F2 - Acquisition Parameters  
 Date\_ 20171020  
 Time 18.05  
 INSTRUM FOURIER300  
 PROBHID 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 17408  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 17

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753346 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

**4-Amino-2-propyl-7-phenylimidazo[1,2-a][1,3,5]triazine (5m)**



Current Data Parameters  
 NAME FL334  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170601  
 Time\_ 14.09  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 88.2542  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599986 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



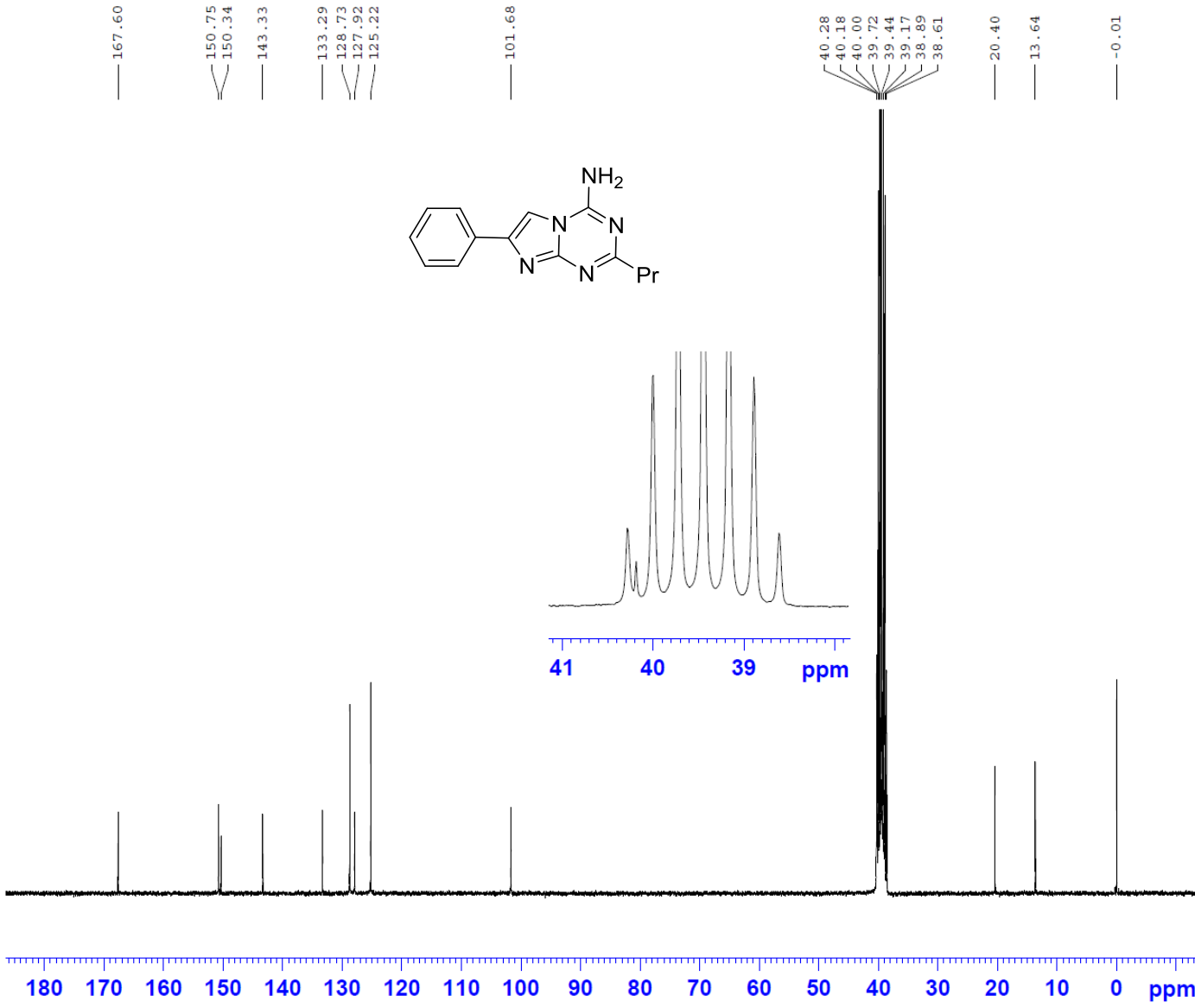
Current Data Parameters  
NAME FL334  
EXPNO 2  
PROCNO 1

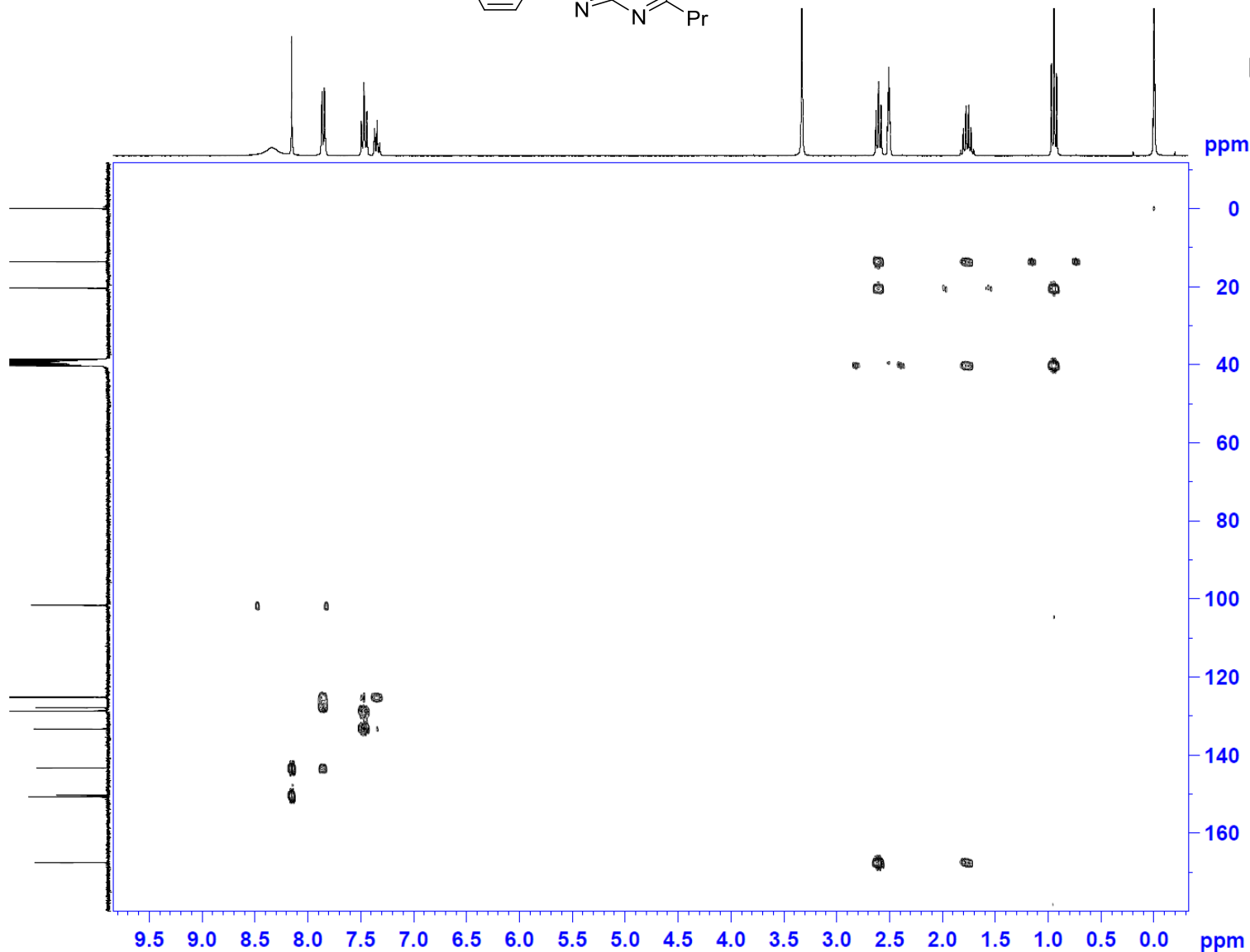
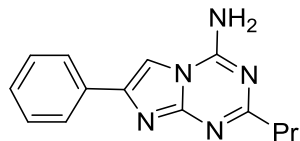
F2 - Acquisition Parameters  
Date\_ 20170610  
Time\_ 18.06  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 15360  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 15

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753342 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
 NAME FL334  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170611  
 Time 18.02  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG hmbcgp1pndqf  
 TD 2048  
 SOLVENT DMSO  
 NS 250  
 DS 16  
 SWH 3051.758 Hz  
 FIDRES 1.490116 Hz  
 AQ 0.3355443 sec  
 RG 501.187  
 DW 163.840 usec  
 DE 6.50 usec  
 TE 300.0 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.00000300 sec  
 D1 1.27660406 sec  
 D2 0.00344828 sec  
 D5 0.05000000 sec  
 D16 0.00020000 sec  
 D31 0.00001350 sec  
 D32 0.00002700 sec  
 D33 0.00001200 sec  
 D36 0.00100000 sec  
 D38 0.00002980 sec  
 IN0 0.00002980 sec

==== CHANNEL f1 =====  
 SFO1 300.1614277 MHz  
 NUC1 1H  
 P1 13.50 usec  
 P2 27.00 usec  
 PLW1 9.30000019 W

==== CHANNEL f2 =====  
 SFO2 75.4828272 MHz  
 NUC2 13C  
 P3 12.00 usec  
 PLW2 22.00000000 W

==== GRADIENT CHANNEL =====  
 GPNAM[1] RECT.1  
 GPNAM[2] RECT.1  
 GPNAM[3] RECT.1  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.10 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 TD 128  
 SFO1 75.48283 MHz  
 FIDRES 131.082214 Hz  
 SW 222.283 ppm  
 FhMODE QF

F2 - Processing parameters  
 SI 2048  
 SF 300.1599993 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40

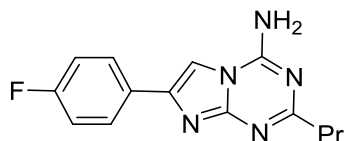
F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 75.4753250 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0



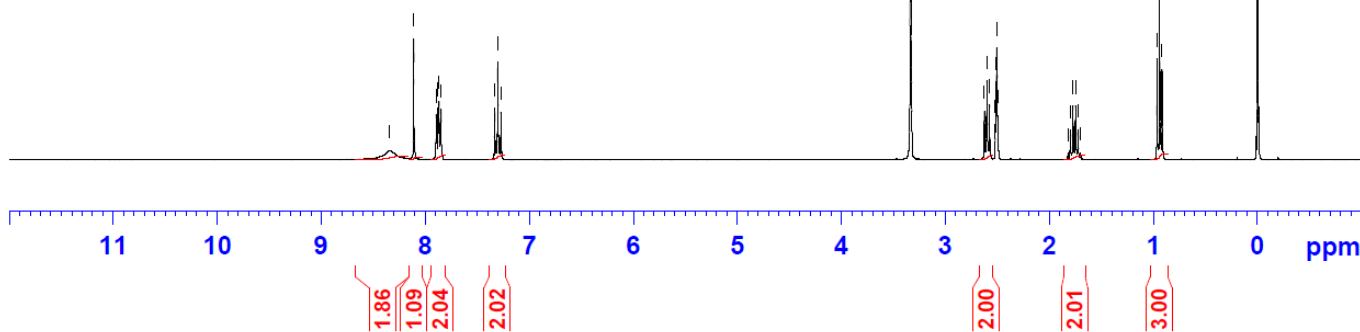
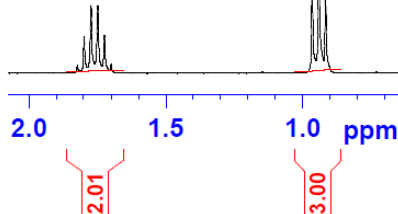
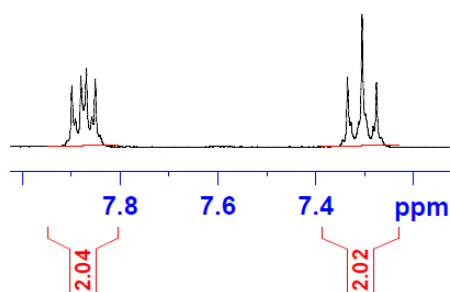
4-Amino-2-propyl-7-(4-fluorophenyl)imidazo[1,2-a][1,3,5]triazine (5n)

8.343  
8.114  
7.899  
7.880  
7.869  
7.851  
7.335  
7.305  
7.276

3.338  
2.626  
2.602  
2.577  
2.521  
2.515  
2.509  
2.502  
2.496  
1.824  
1.799  
1.774  
1.749  
1.725  
1.701  
0.966  
0.942  
0.917  
-0.000



0.94 (t, J=7.38 Hz, 3 H)  
1.76 (m, J=7.40 Hz, 2 H)  
2.60 (t, J=7.41 Hz, 2 H)  
7.31 (dd, J=8.94, 8.94 Hz, 2 H)  
7.87 (dd, J=5.54, 8.90 Hz, 2 H)



Current Data Parameters  
NAME FL353  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time 12.56  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 87.6175  
DW 81.920 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
SFO1 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

F2 - Processing parameters  
SI 65536  
SF 300.1599983 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



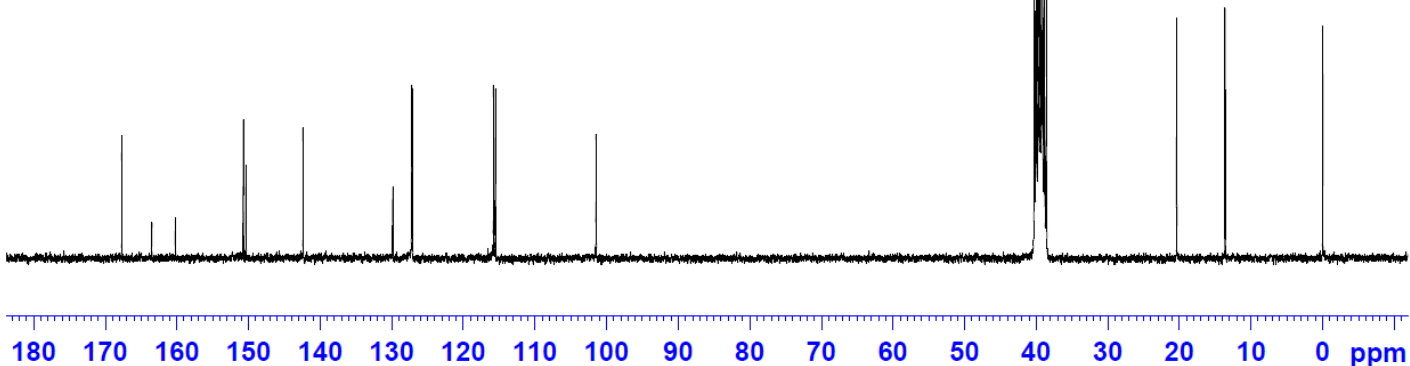
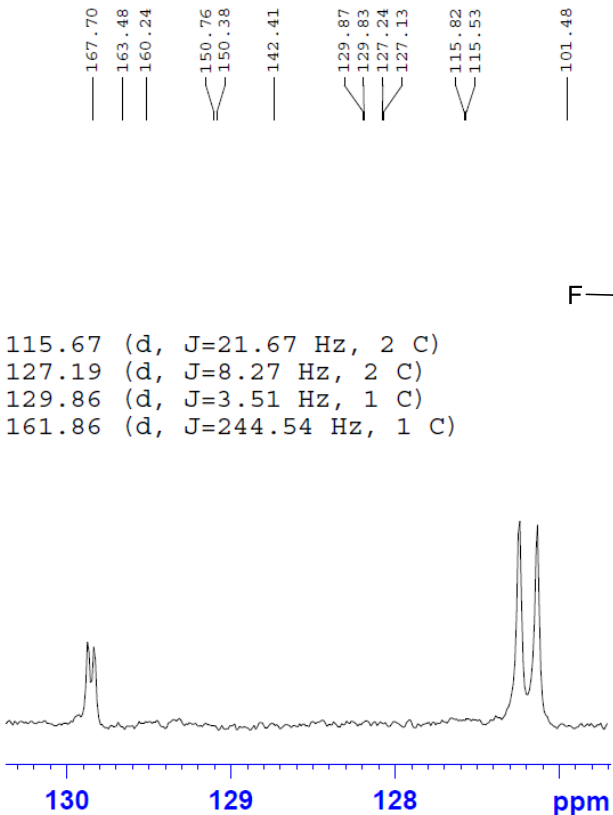
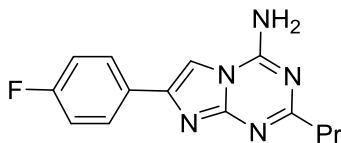
Current Data Parameters  
NAME FL353  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time\_ 18.05  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 15360  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 15

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

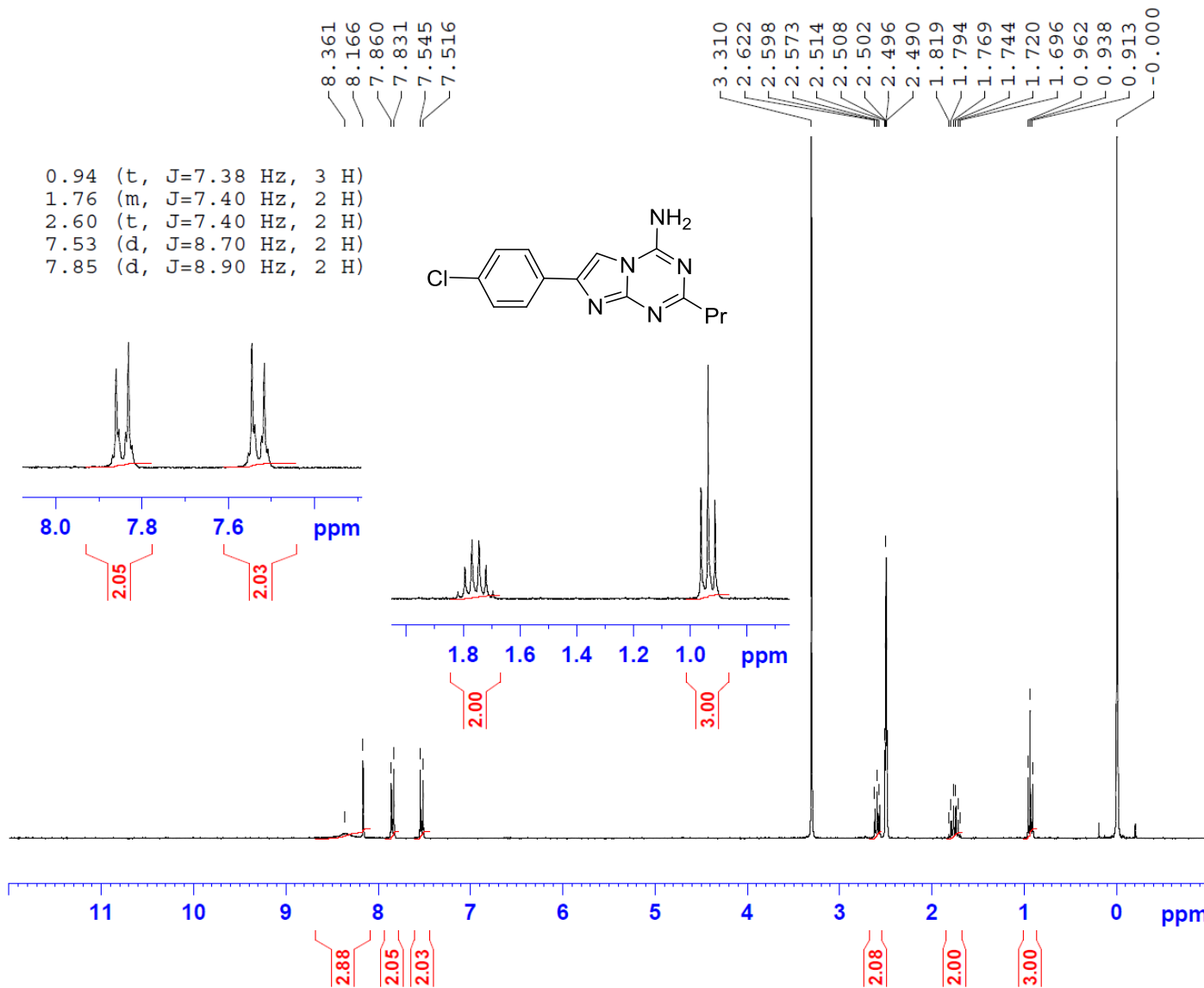
----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753342 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



40.27  
40.17  
39.99  
39.71  
39.43  
39.16  
38.88  
38.60  
20.39  
13.63  
-0.01

4-Amino-2-propyl-7-(4-chlorophenyl)imidazo[1,2-a][1,3,5]triazine (5o)



Current Data Parameters  
 NAME FL363  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170918  
 Time 12.33  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 145.81  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1600004 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

167.82  
 150.77  
 150.41  
 142.11  
 132.33  
 132.21  
 128.82  
 126.87

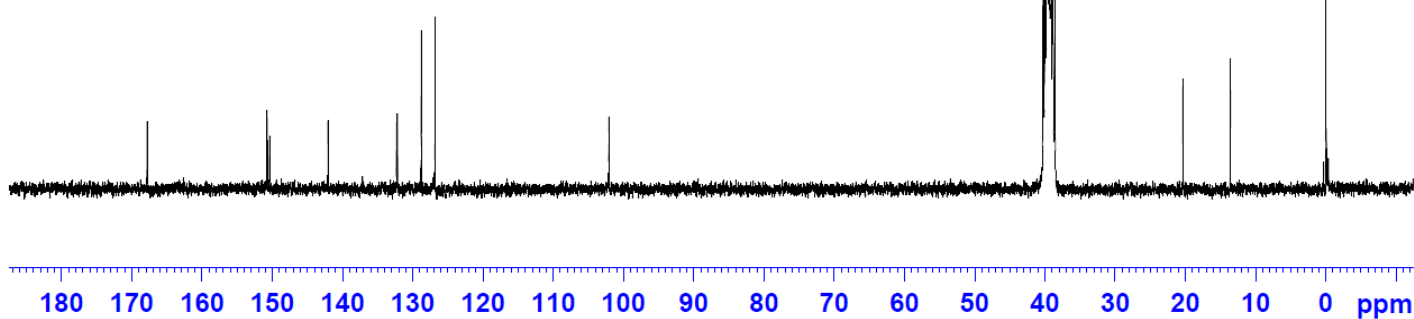
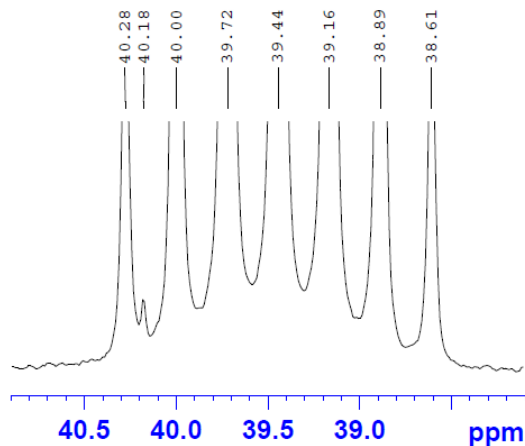
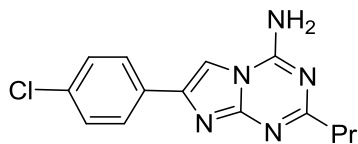
102.10

40.28  
 40.18  
 40.00  
 39.72  
 39.44  
 39.16  
 38.89  
 38.61

20.38

13.62

-0.00



Current Data Parameters  
 NAME FL363  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170918  
 Time 17.05  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16384  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 16

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

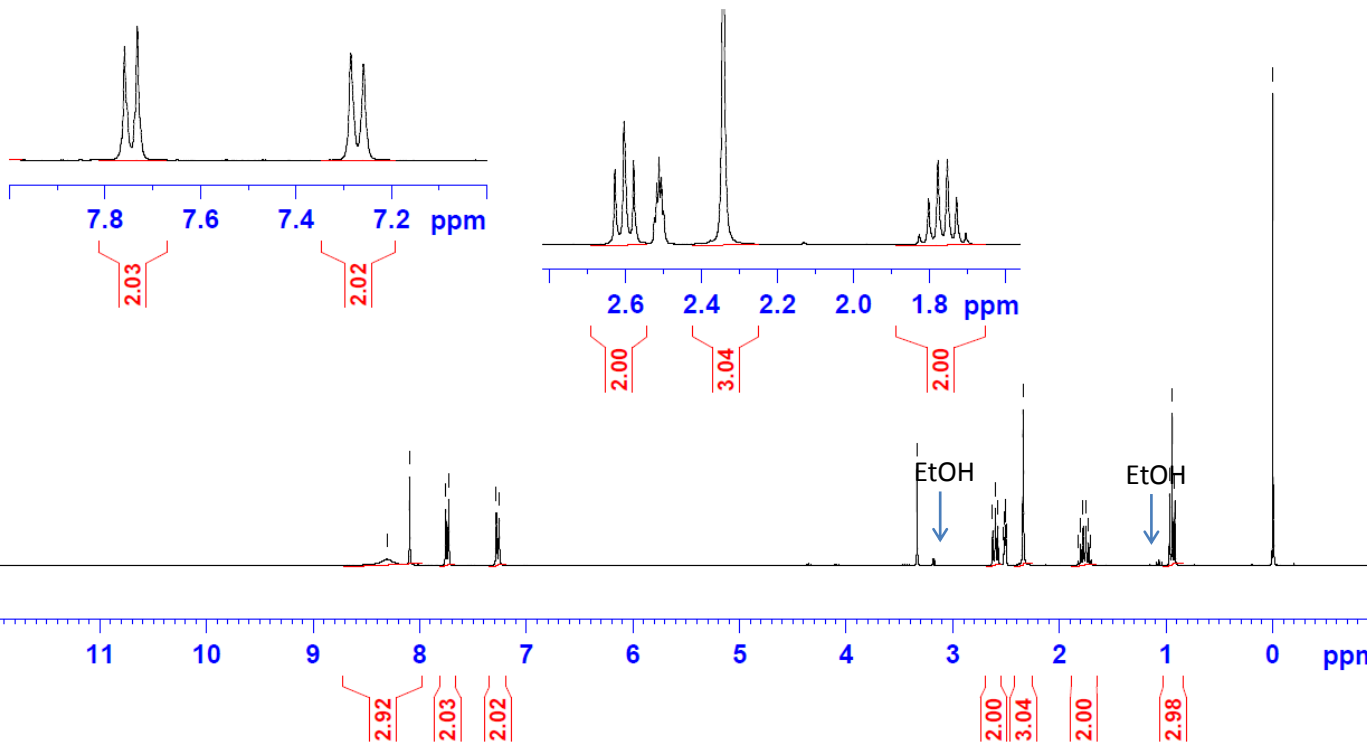
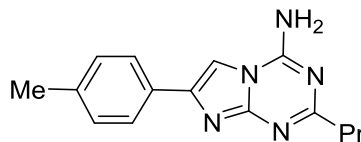
F2 - Processing parameters  
 SI 32768  
 SF 75.4753350 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

# 4-Amino-2-propyl-7-(4-methylphenyl)imidazo[1,2-a][1,3,5]triazine (5p)

8.304  
8.098  
7.759  
7.732  
7.285  
7.259

3.338  
2.628  
2.604  
2.578  
2.524  
2.518  
2.511  
2.505  
2.499  
2.343  
1.828  
1.803  
1.778  
1.753  
1.729  
1.704  
0.969  
0.944  
0.919  
-0.000

0.94 (t, J=7.40 Hz, 3 H)  
1.77 (m, J=7.40 Hz, 2 H)  
2.60 (t, J=7.40 Hz, 2 H)  
7.27 (d, J=7.89 Hz, 2 H)  
7.75 (d, J=8.07 Hz, 2 H)

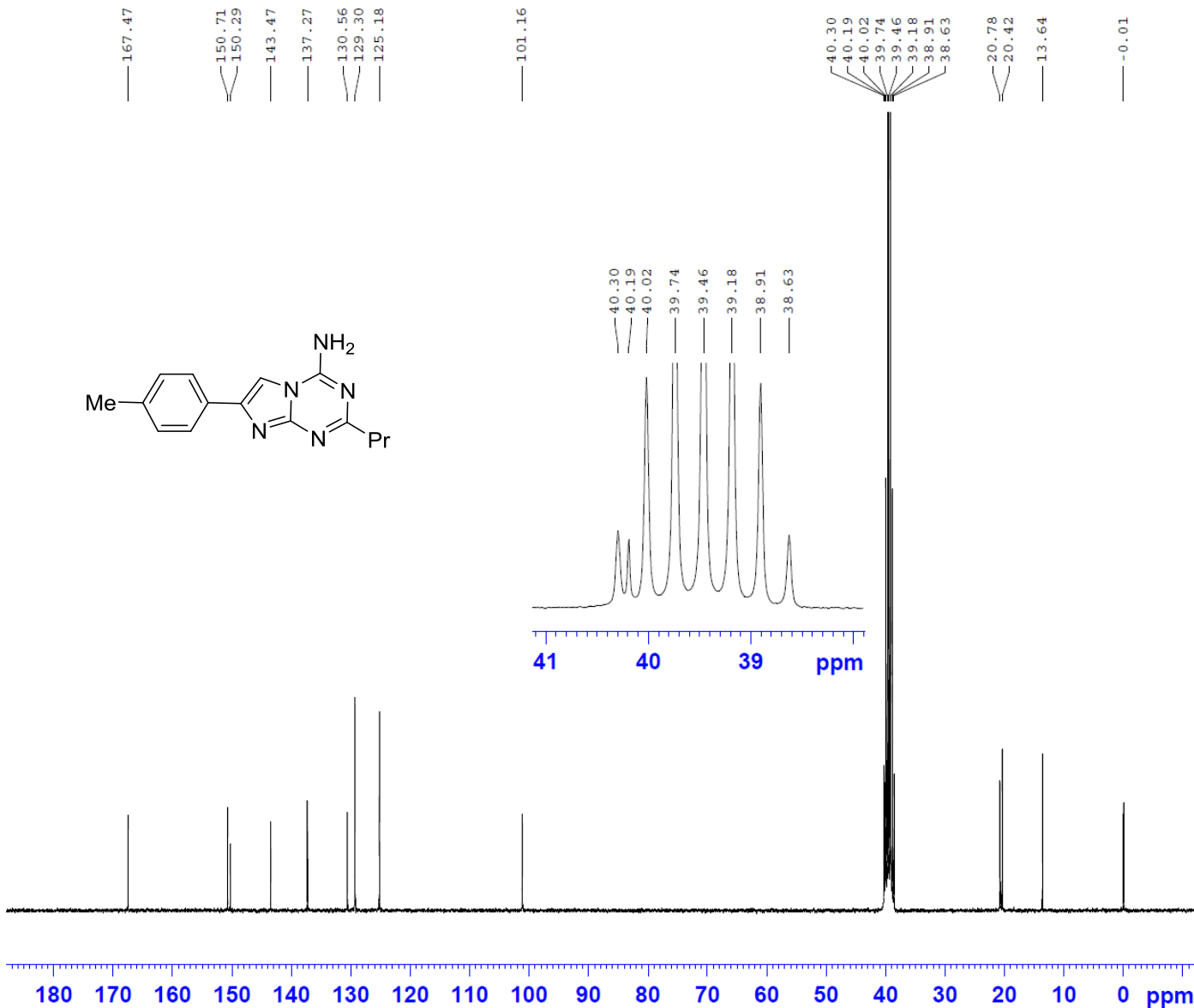
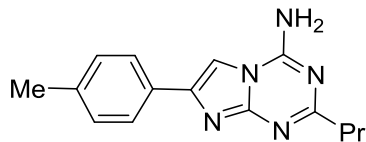


Current Data Parameters  
NAME FL367  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170924  
Time 15.53  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 59.2172  
DW 81.920 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

F2 - Processing parameters  
SI 65536  
SF 300.1599975 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME FL367  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170925  
 Time 0.55  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 9216  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 9

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

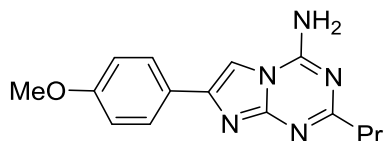
----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753331 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

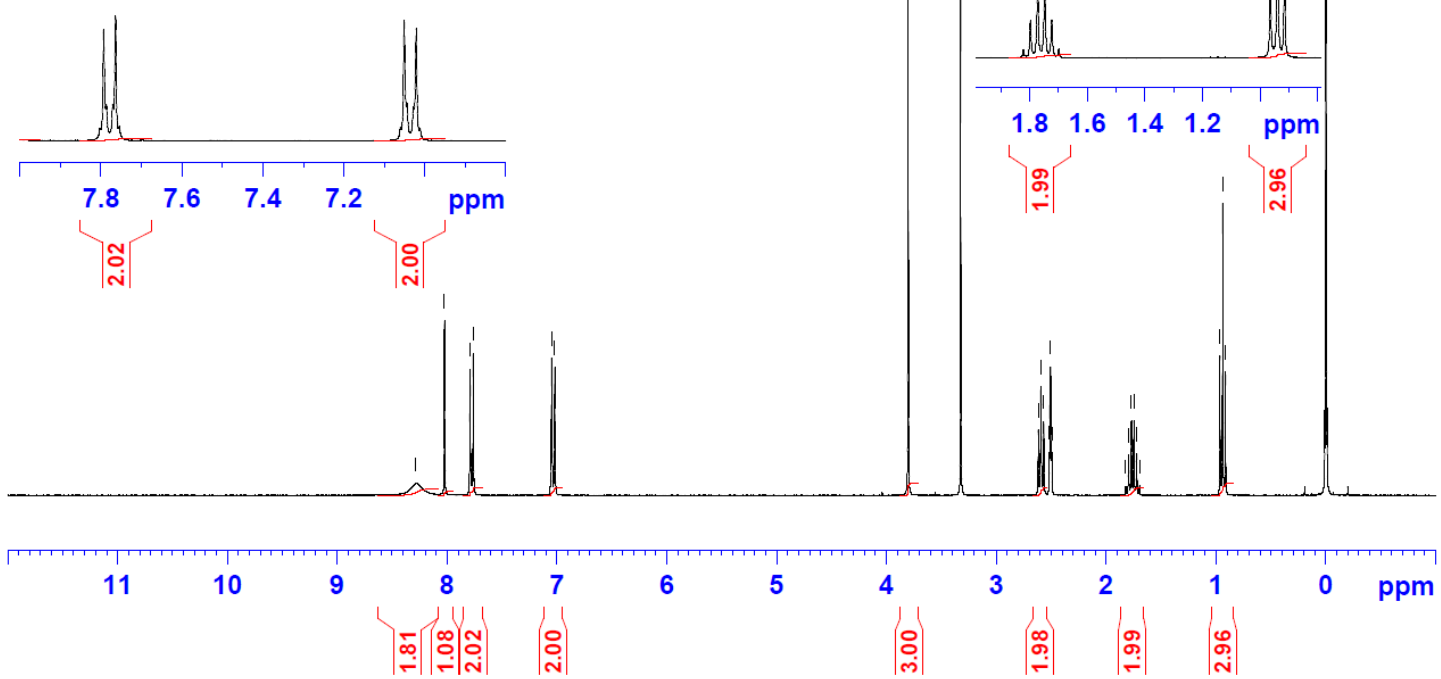
4-Amino-2-propyl-7-(4-methoxyphenyl)imidazo[1,2-a][1,3,5]triazine (5q)

8.288  
8.025  
7.793  
7.764  
7.051  
7.021

3.804  
3.325  
2.619  
2.595  
2.570  
2.519  
2.513  
2.507  
2.501  
2.494  
1.821  
1.797  
1.772  
1.747  
1.723  
1.698  
0.965  
0.940  
0.915  
-0.000



0.94 (t, J=7.38 Hz, 3 H)  
1.76 (m, J=7.39 Hz, 2 H)  
2.59 (t, J=7.41 Hz, 2 H)  
7.04 (d, J=8.88 Hz, 2 H)  
7.78 (d, J=8.85 Hz, 2 H)



Current Data Parameters  
NAME FL348  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170808  
Time\_ 14.04  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 87.3614  
DW 81.920 usec  
DE 6.50 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SF01 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

F2 - Processing parameters  
SI 65536  
SF 300.1599988 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME FL348  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170808  
Time 18.05  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 14336  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 14

===== CHANNEL f1 =====  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

===== CHANNEL f2 =====  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753342 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

167.34  
159.15  
150.63  
150.27  
143.38

126.55  
125.87

114.17

100.39

55.07

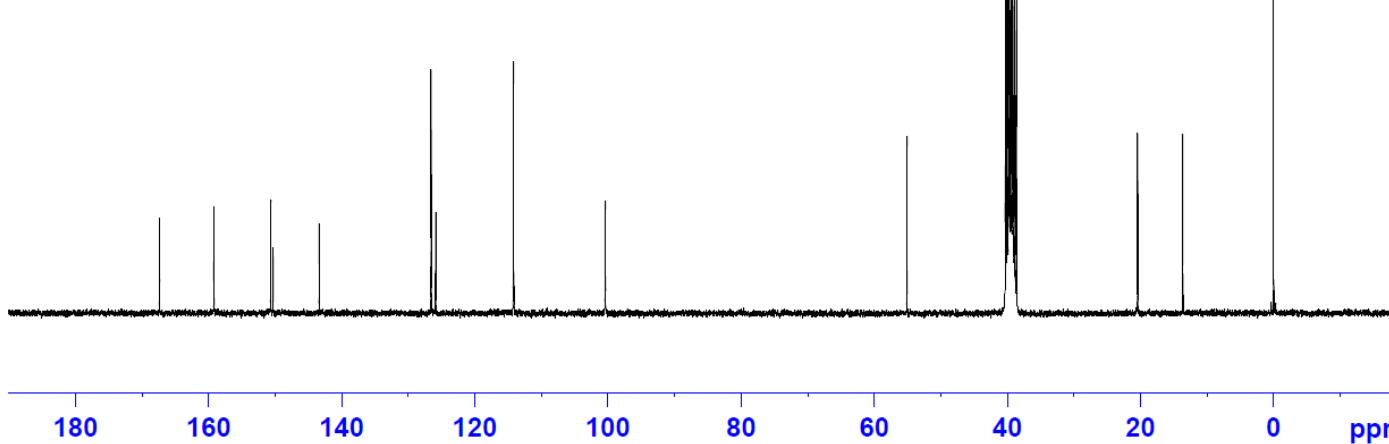
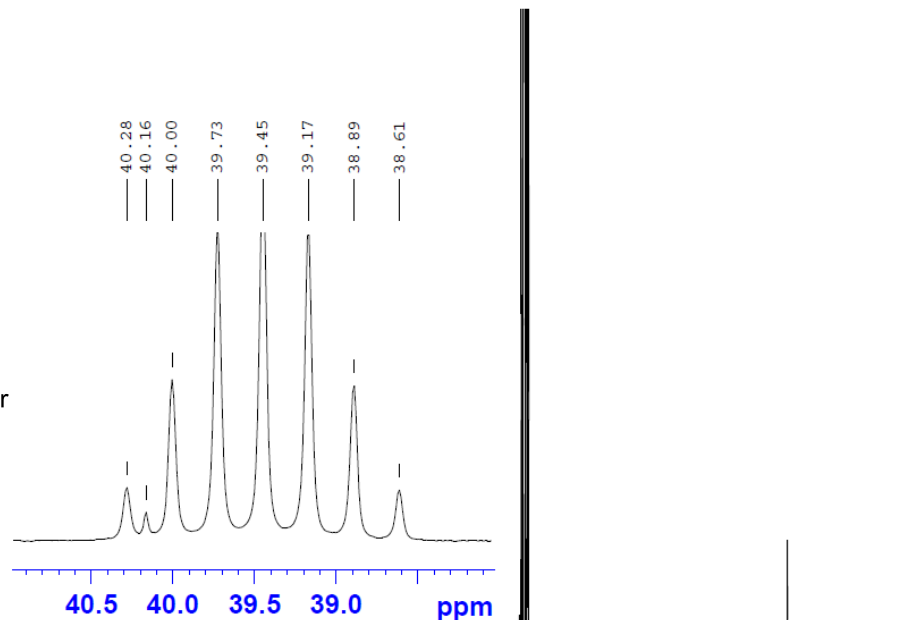
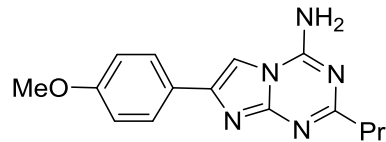
40.28  
40.16  
40.00  
39.73  
39.45  
39.17  
38.89  
38.61

20.41

13.63

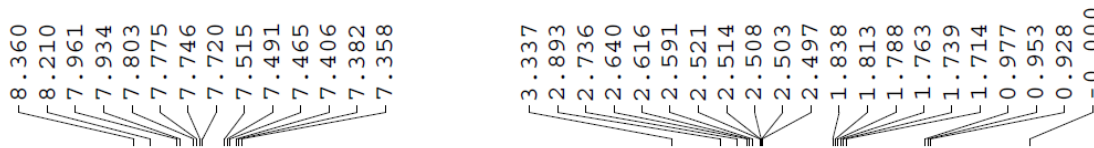
-0.01

40.28  
40.16  
40.00  
39.73  
39.45  
39.17  
38.89  
38.61

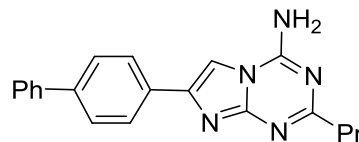




# 4-Amino-2-propyl-7-(4-biphenyl)imidazo[1,2-a][1,3,5]triazine (5r)



0.95 (t, J=7.37 Hz, 3 H)  
 1.78 (m, J=7.39 Hz, 2 H)  
 2.62 (t, J=7.40 Hz, 2 H)  
 7.38 (t, J=7.28 Hz, 1 H)  
 7.49 (t, J=7.52 Hz, 2 H)  
 7.73 (d, J=7.65 Hz, 2 H)  
 7.79 (d, J=8.37 Hz, 2 H)  
 7.95 (d, J=8.28 Hz, 2 H)

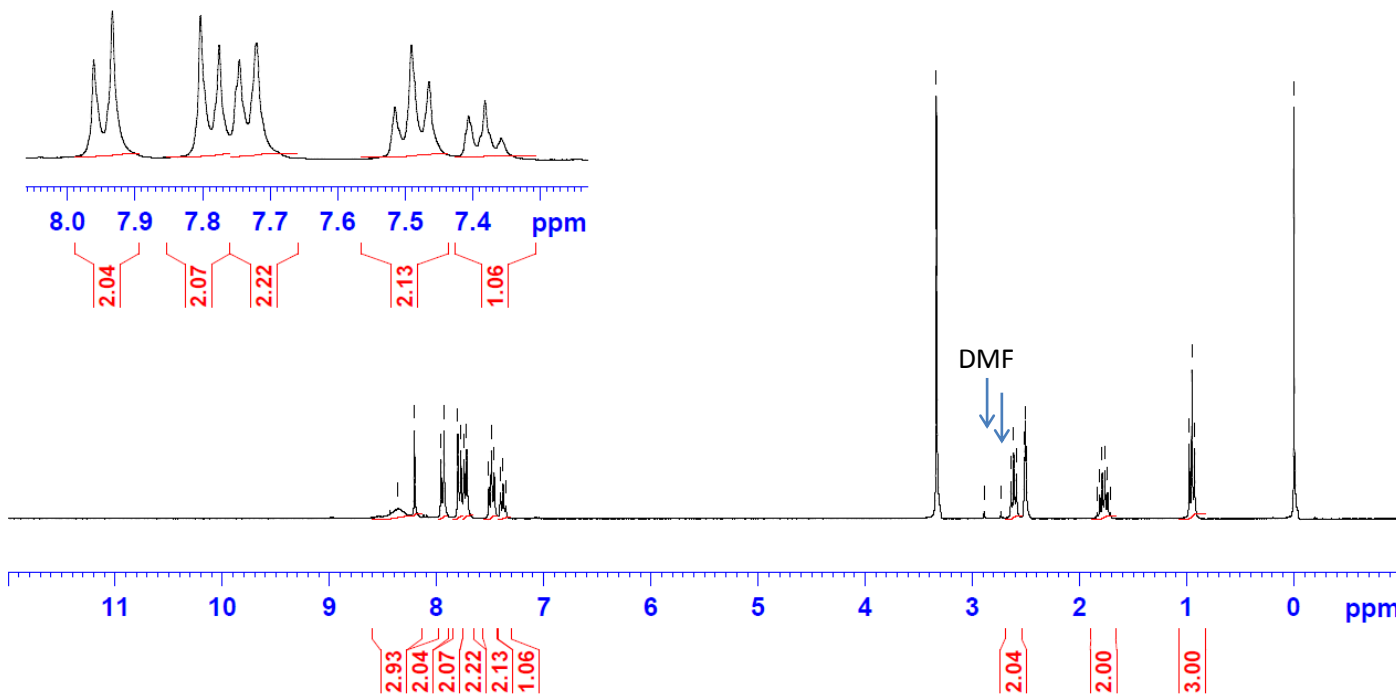


Current Data Parameters  
 NAME FL374  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171023  
 Time 17.01  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 86.1986  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599986 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



167.66

150.75  
150.41  
142.97  
139.55  
139.51  
132.41  
128.88  
127.44  
126.98  
126.41  
125.77

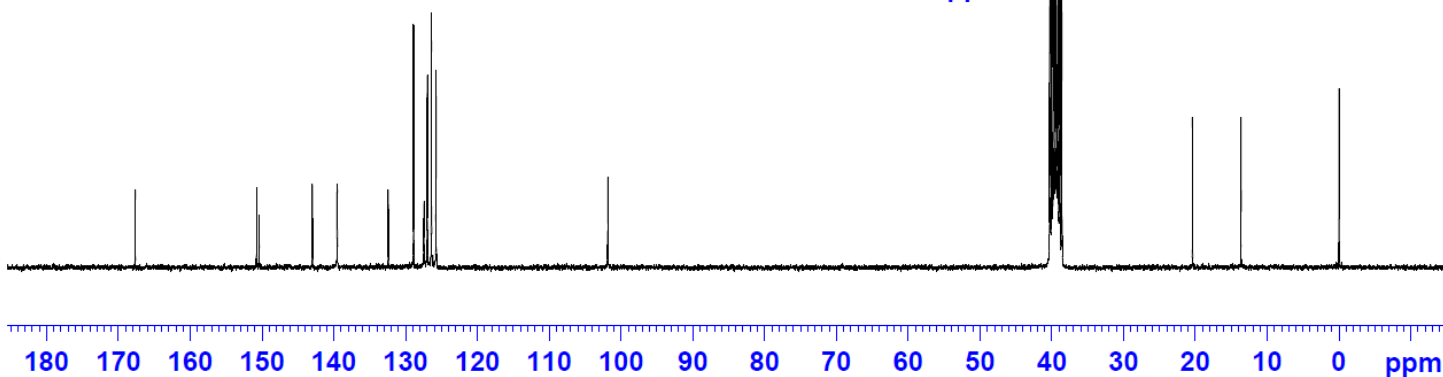
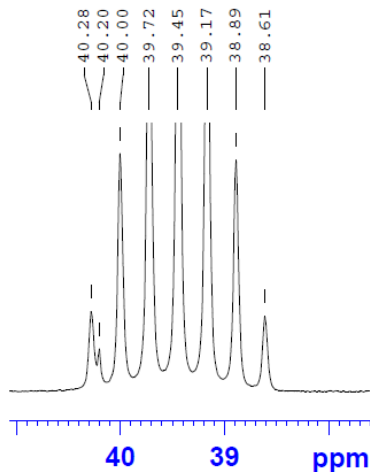
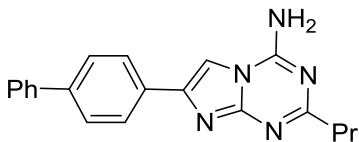
101.85

40.28  
40.20  
40.00  
39.72  
39.45  
39.17  
38.89  
38.61

20.41

13.65

-0.01



Current Data Parameters  
 NAME FL374  
 EXPNO 3  
 PROCNO 1

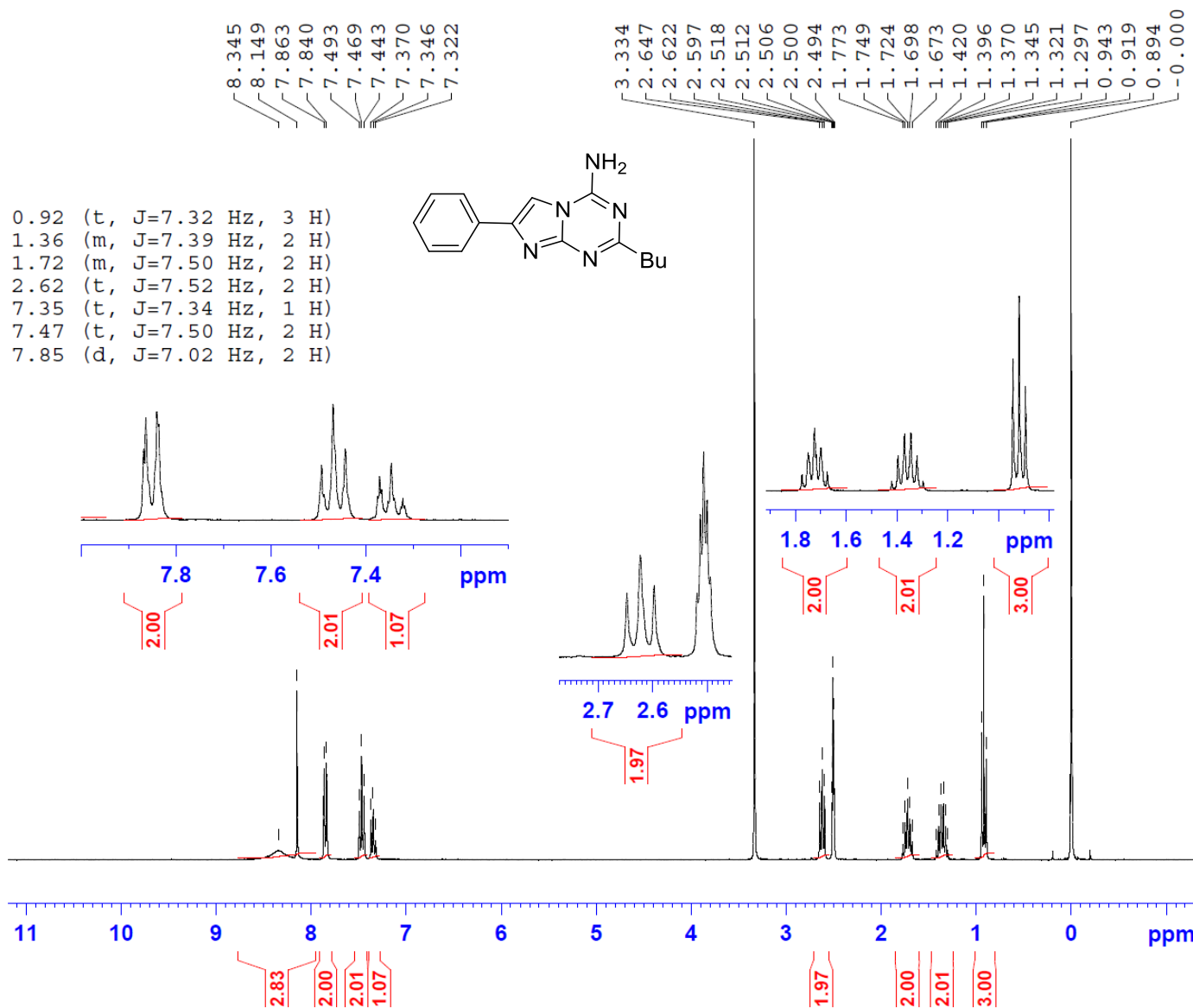
F2 - Acquisition Parameters  
 Date\_ 20171021  
 Time 18.05  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 17408  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 17

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753342 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4-amino-2-butyl-7-phenylimidazo[1,2-a][1,3,5]triazine (5s)



0.92 (t, J=7.32 Hz, 3 H)  
 1.36 (m, J=7.39 Hz, 2 H)  
 1.72 (m, J=7.50 Hz, 2 H)  
 2.62 (t, J=7.52 Hz, 2 H)  
 7.35 (t, J=7.34 Hz, 1 H)  
 7.47 (t, J=7.50 Hz, 2 H)  
 7.85 (d, J=7.02 Hz, 2 H)

Current Data Parameters  
 NAME FL335  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170601  
 Time 14.14  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 107.76  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599990 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



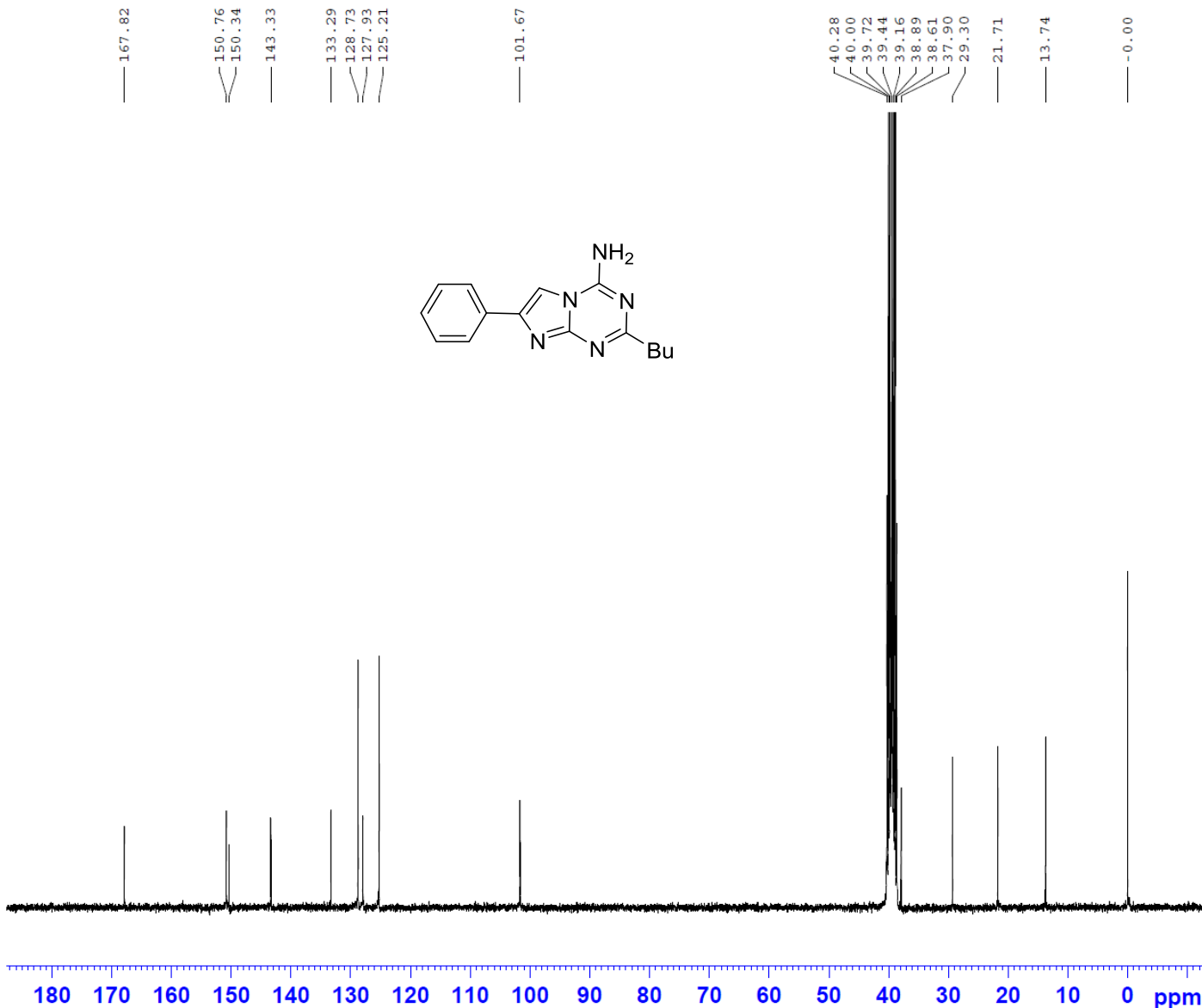
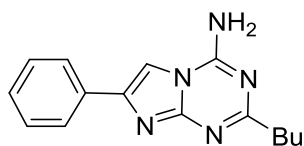
Current Data Parameters  
NAME FL335  
EXPNO 2  
PROCNO 1

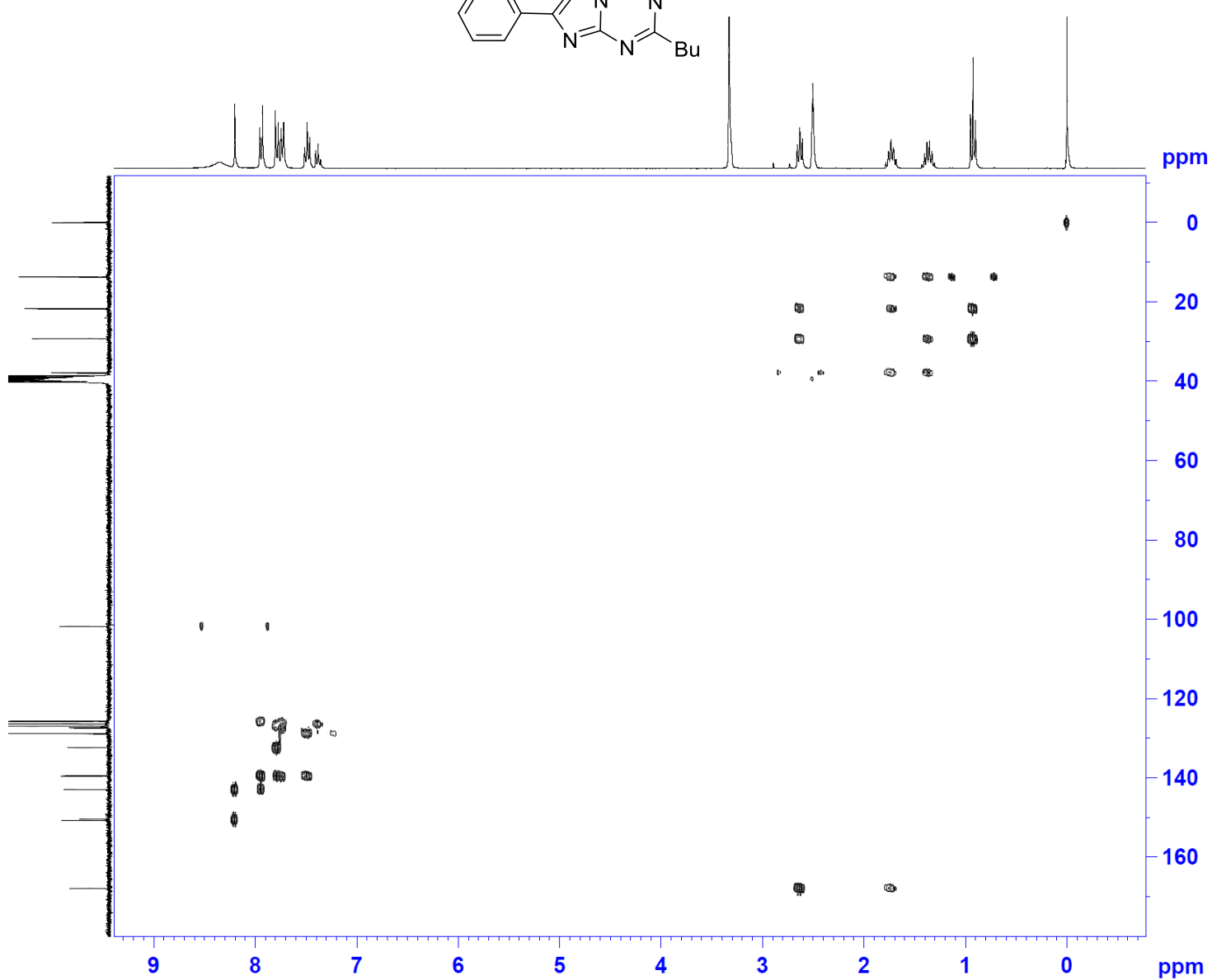
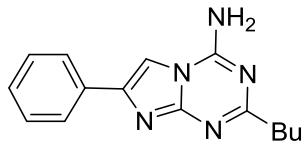
F2 - Acquisition Parameters  
Date\_ 20170608  
Time 18.10  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 15360  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TDO 15

===== CHANNEL f1 =====  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

===== CHANNEL f2 =====  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753343 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





Current Data Parameters  
 NAME FL375  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171123  
 Time\_ 19.03  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG hmbcgg1pndqf  
 TD 2048  
 SOLVENT DMSO  
 NS 250  
 DS 16  
 SWH 3051.758 Hz  
 FIDRES 1.490116 Hz  
 AQ 0.3355443 sec  
 RG 501.187  
 DW 163.840 usec  
 DE 6.50 usec  
 TE 300.0 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 D0 0.00000300 sec  
 D1 1.32780397 sec  
 D2 0.00344828 sec  
 D6 0.05000000 sec  
 D16 0.00020000 sec  
 D31 0.00001350 sec  
 D32 0.00002700 sec  
 D33 0.00001200 sec  
 D36 0.00100000 sec  
 D38 0.00002980 sec  
 INO 0.00002980 sec

==== CHANNEL f1 =====  
 SFO1 300.1612919 MHz  
 NUC1 1H  
 P1 13.50 usec  
 P2 27.00 usec  
 PLW1 9.30000019 W

==== CHANNEL f2 =====  
 SFO2 75.4828272 MHz  
 NUC2 13C  
 P3 12.00 usec  
 PLW2 22.00000000 W

==== GRADIENT CHANNEL =====  
 GPNAM[1] RECT.1  
 GPNAM[2] RECT.1  
 GPNAM[3] RECT.1  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.10 %  
 F16 1000.00 usec

F1 - Acquisition parameters  
 TD 128  
 SFO1 75.48383 MHz  
 FIDRES 131.082214 Hz  
 SW 222.283 ppm  
 FhMODE QF

F2 - Processing parameters  
 SI 2048  
 SF 300.1599992 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 1.40

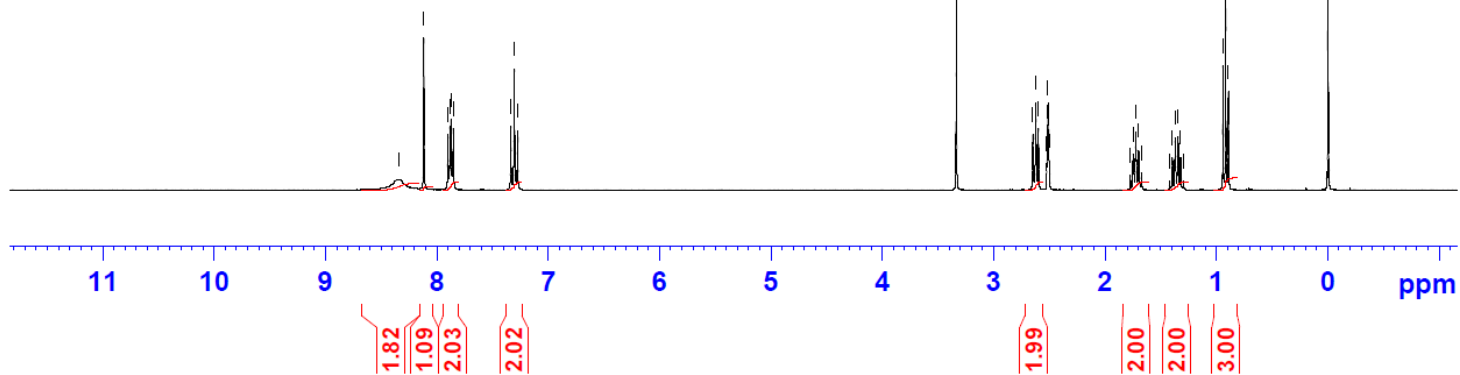
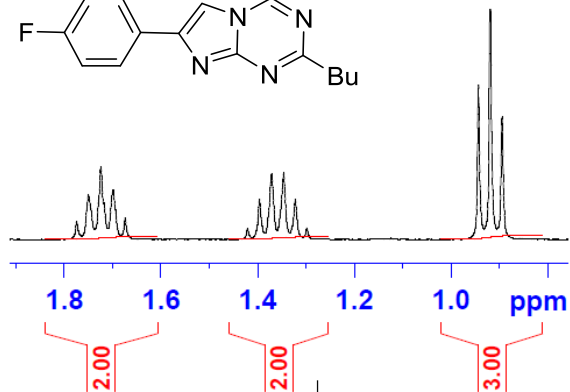
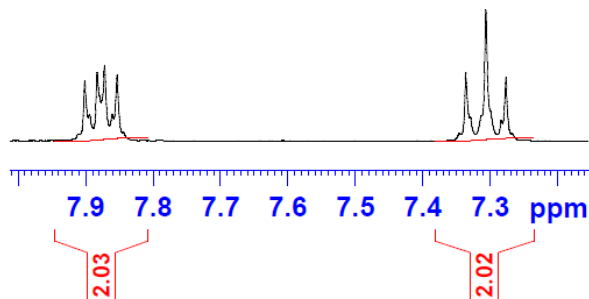
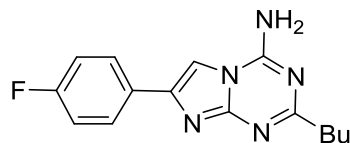
F1 - Processing parameters  
 SI 1024  
 MC2 QF  
 SF 75.4753292 MHz  
 WDW SINE  
 SSB 0  
 LB 0 Hz  
 GB 0

4-Amino-2-butyl-7-(4-fluorophenyl)imidazo[1,2-a][1,3,5]triazine (5t)

8.344  
8.117  
7.901  
7.883  
7.872  
7.853  
7.336  
7.306  
7.277

3.339  
2.649  
2.625  
2.599  
2.525  
2.519  
2.513  
2.507  
2.501  
1.774  
1.750  
1.725  
1.700  
1.675  
1.421  
1.396  
1.371  
1.346  
1.322  
1.298  
0.943  
0.919

0.92 (t, J=7.34 Hz, 3 H)  
1.36 (m, J=7.38 Hz, 2 H)  
1.72 (m, J=7.49 Hz, 2 H)  
2.62 (t, J=7.52 Hz, 2 H)  
7.31 (dd, J=8.93, 8.93 Hz, 2 H)  
7.88 (dd, J=5.55, 8.88 Hz, 2 H)



Current Data Parameters  
NAME FL354  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time 13.00  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 71.026  
DW 81.920 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

F2 - Processing parameters  
SI 65536  
SF 300.1599969 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



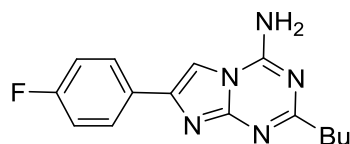
Current Data Parameters  
NAME FL354  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170818  
Time 18.05  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 15360  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 15

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

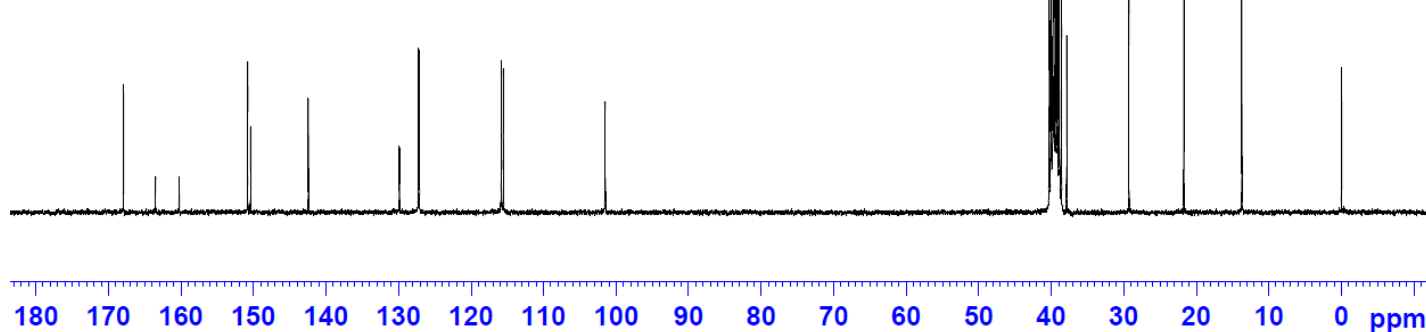
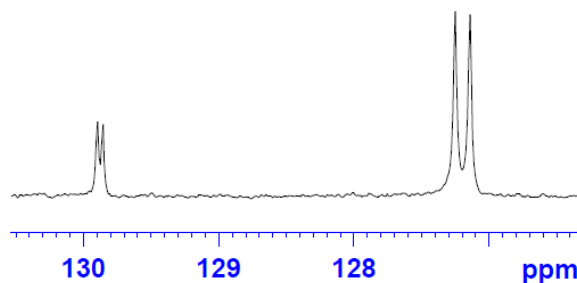
F2 - Processing parameters  
SI 32768  
SF 75.4753327 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



167.92  
163.50  
160.25  
150.78  
150.40  
142.43  
129.90  
129.86  
127.25  
127.14  
115.82  
115.54  
101.50

40.30  
40.02  
39.74  
39.46  
39.19  
38.91  
38.63  
37.91  
29.31  
21.73  
13.75  
-0.00

115.68 (d, J=21.74 Hz, 2 C)  
127.20 (d, J=8.25 Hz, 2 C)  
129.88 (d, J=2.97 Hz, 1 C)  
161.87 (d, J=244.80 Hz, 1 C)

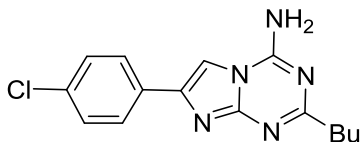


4-Amino-2-butyl-7-(4-chlorophenyl)imidazo[1,2-a][1,3,5]triazine (5u)

8.359  
8.163  
7.859  
7.830  
7.545  
7.516

3.318  
2.642  
2.618  
2.592  
2.514  
2.508  
2.502  
2.496  
2.490  
1.766  
1.742  
1.717  
1.692  
1.667  
1.416  
1.391  
1.365  
1.341  
1.316  
1.293  
0.938  
0.914

0.91 (t, J=7.32 Hz, 3 H)  
1.35 (m, J=7.38 Hz, 2 H)  
1.72 (m, J=7.49 Hz, 2 H)  
2.62 (t, J=7.52 Hz, 2 H)  
7.53 (d, J=8.61 Hz, 2 H)  
7.84 (d, J=8.58 Hz, 2 H)

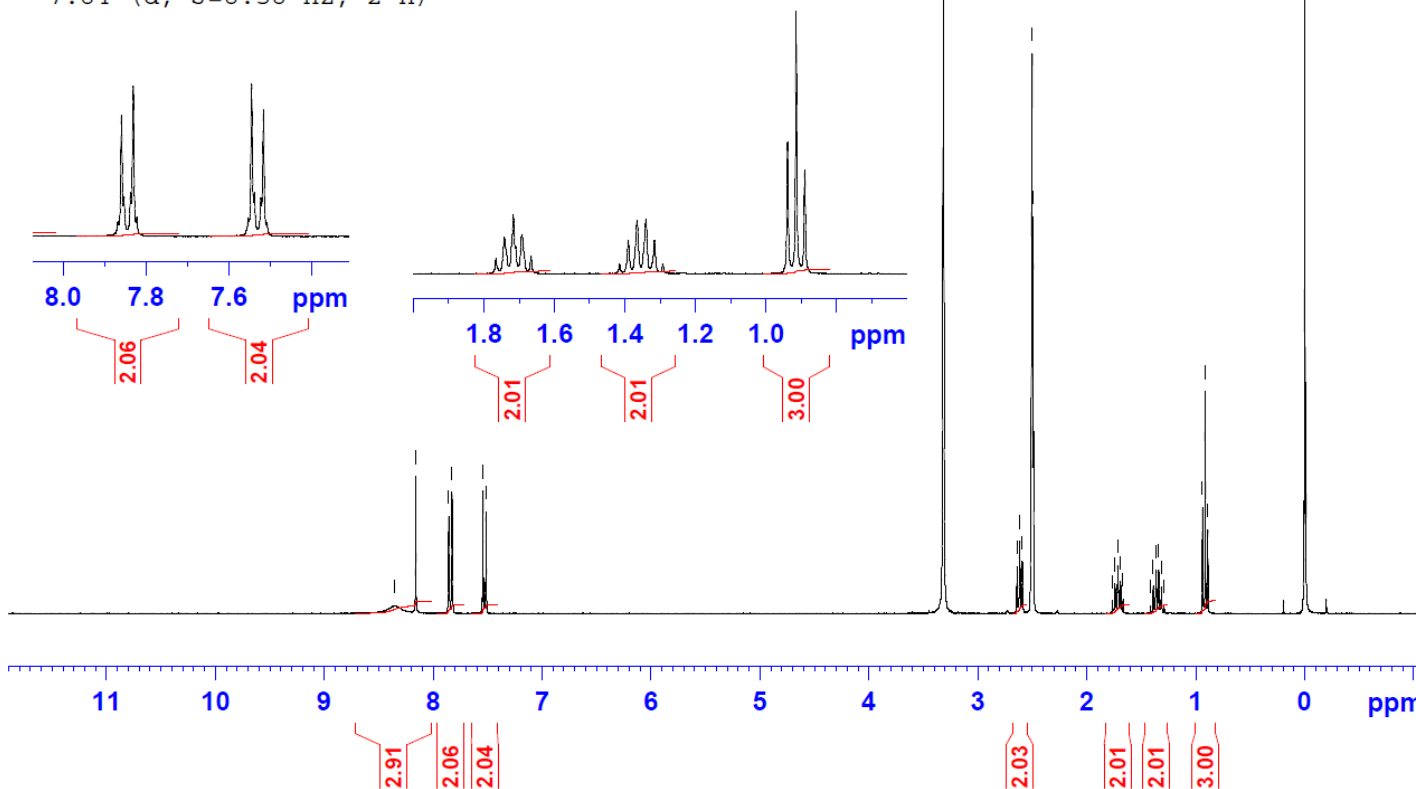


Current Data Parameters  
NAME FL362  
EXPNO 4  
PROCNO 1

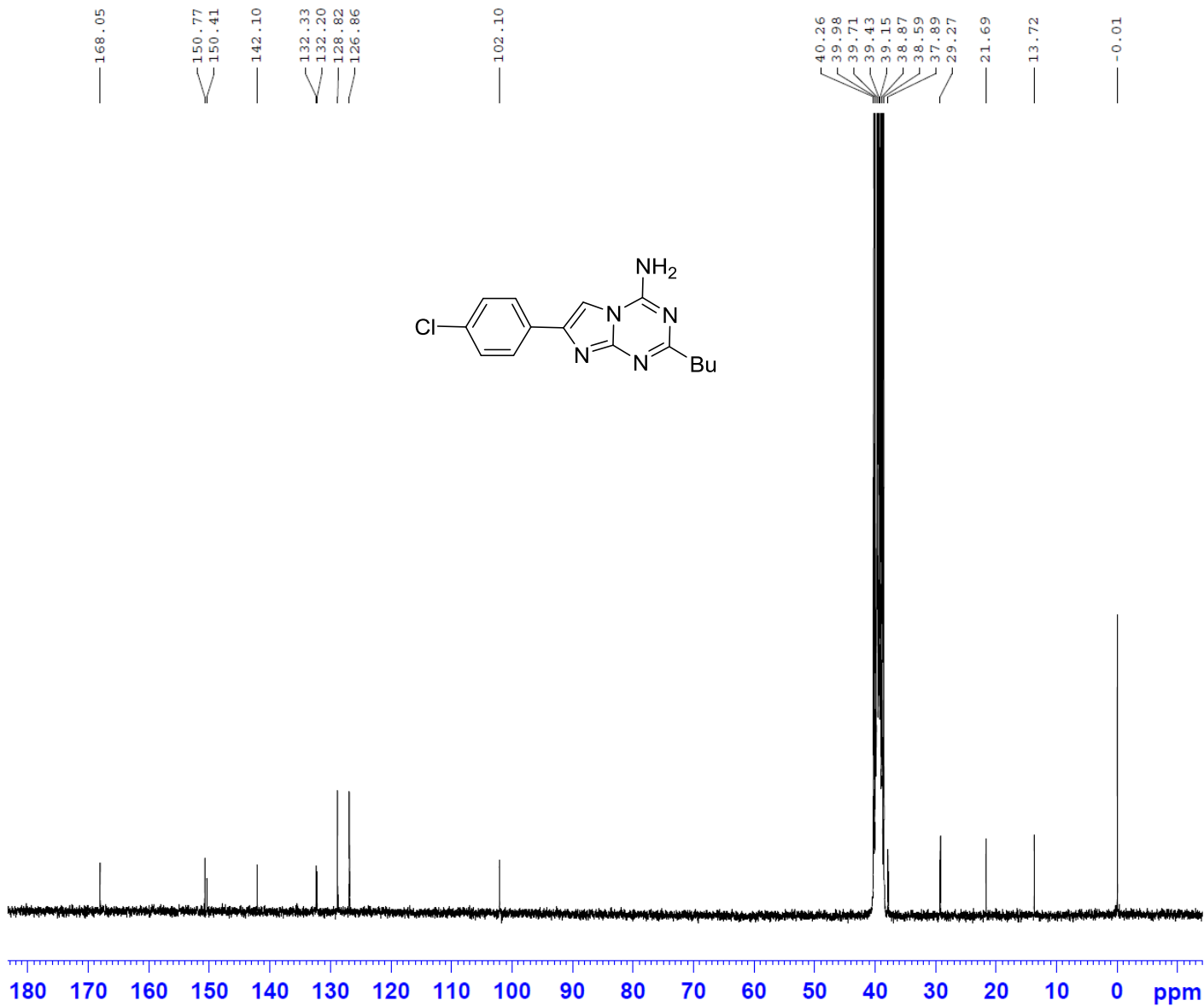
F2 - Acquisition Parameters  
Date\_ 20170915  
Time 13.16  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 144.508  
DW 81.920 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

F2 - Processing parameters  
SI 65536  
SF 300.1600001 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







Current Data Parameters  
 NAME FL362  
 EXPNO 5  
 PROCNO 1

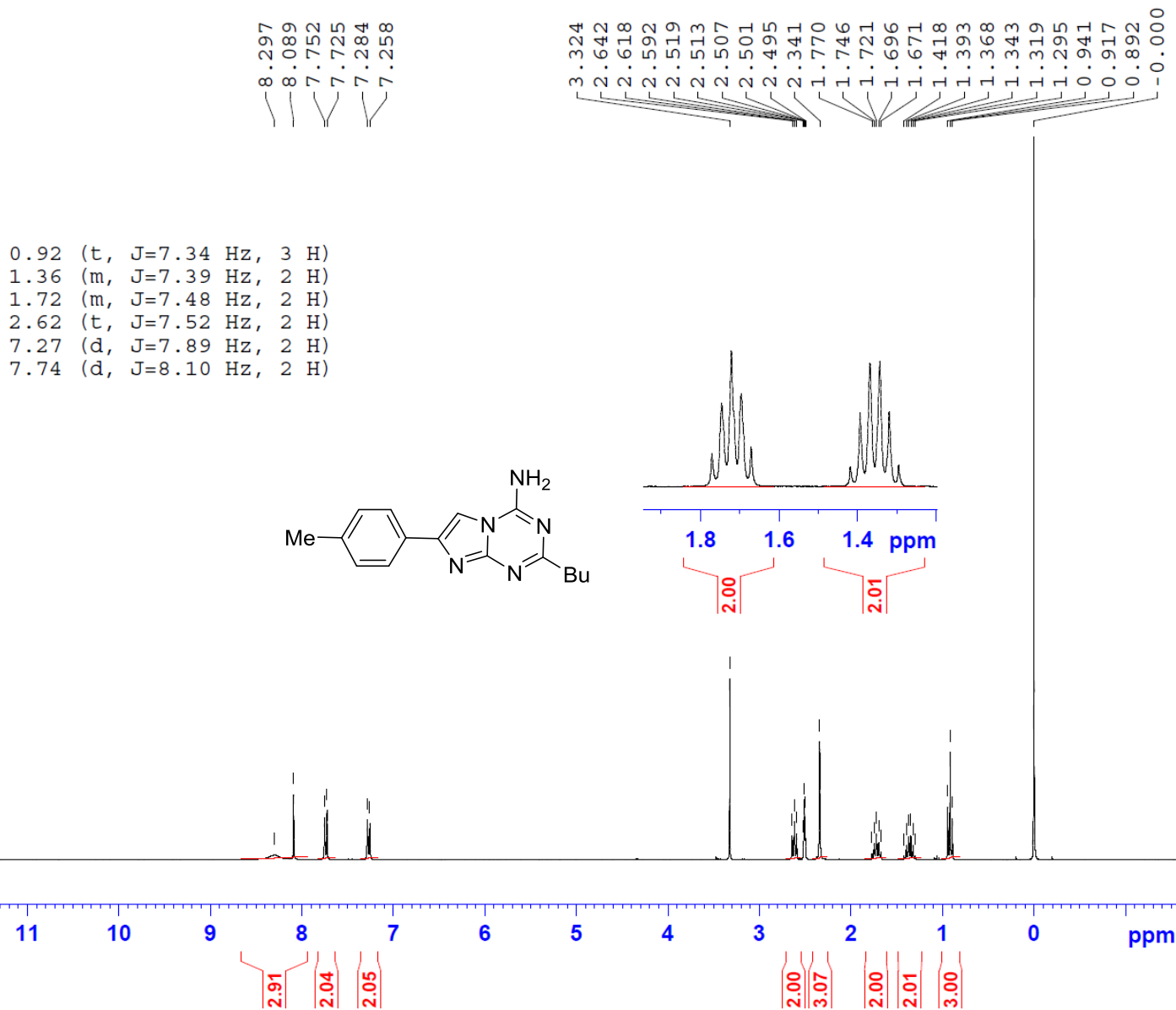
F2 - Acquisition Parameters  
 Date\_ 20170915  
 Time\_ 18.10  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 40960  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 40

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4754001 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

4-Amino-2-butyl-7-(4-methylphenyl)imidazo[1,2-a][1,3,5]triazine (5v)



Current Data Parameters  
 NAME FL368  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170924  
 Time 16.04  
 INSTRUM FOURIER300  
 PROBHND 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 82.2225  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599989 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



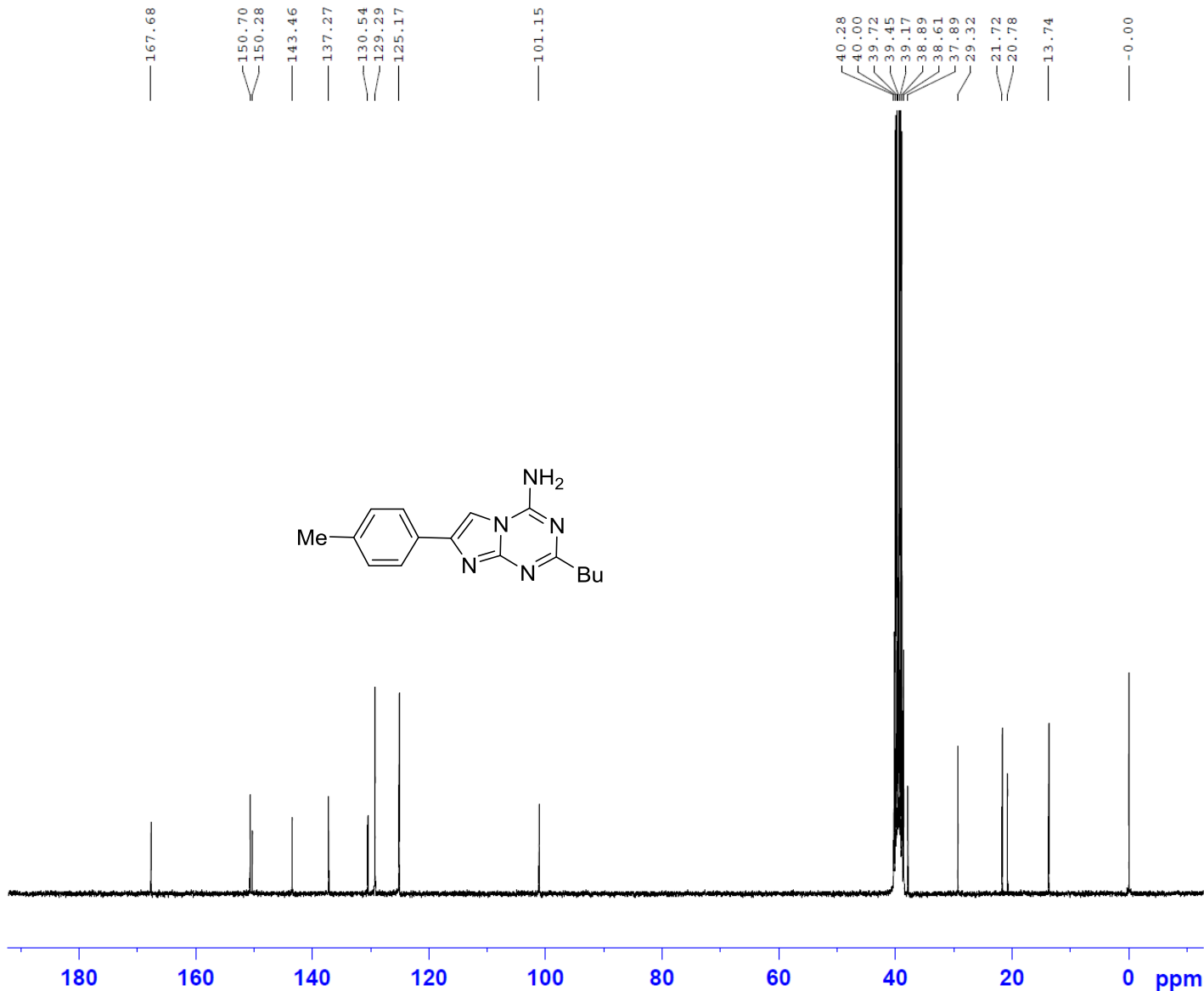
Current Data Parameters  
NAME FL368  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170925  
Time 18.09  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 13312  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 13

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753339 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

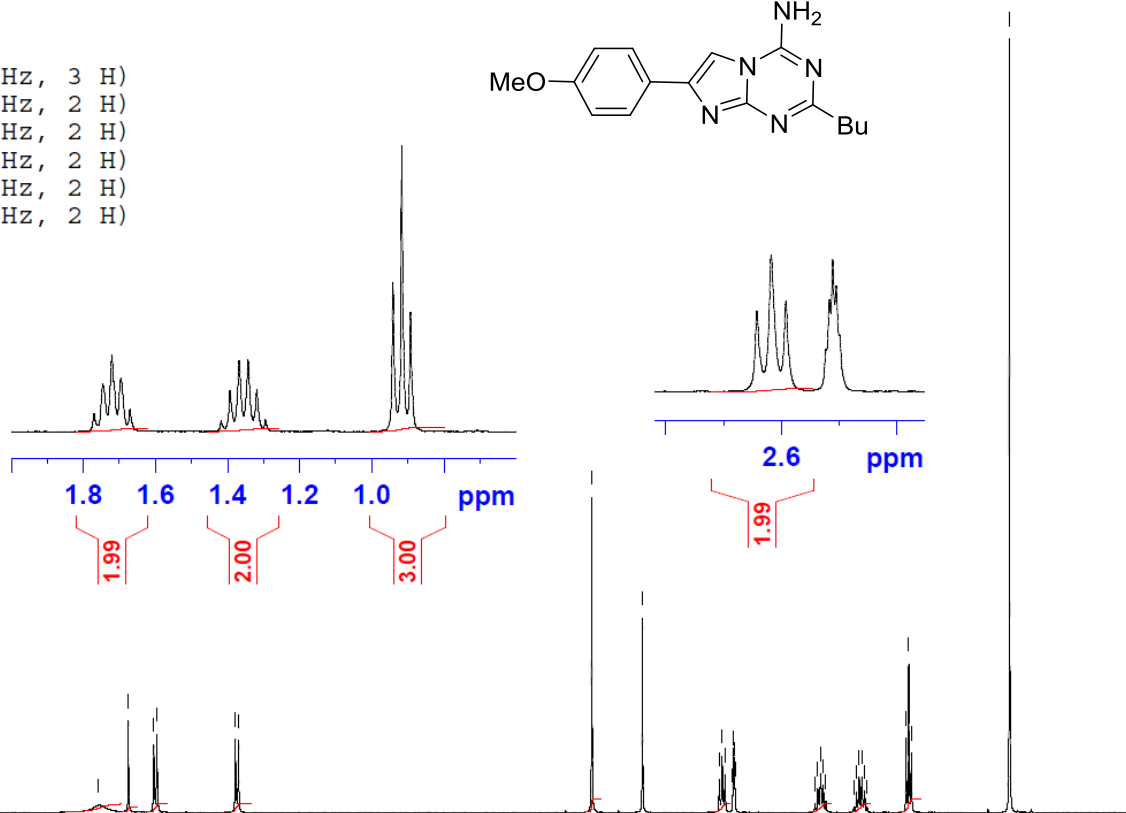
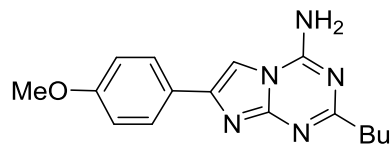


4-Amino-2-butyl-7-(4-methoxyphenyl)imidazo[1,2-a][1,3,5]triazine (5w)

8.300  
8.028  
7.796  
7.766  
7.053  
7.024

3.805  
3.344  
2.642  
2.617  
2.592  
2.523  
2.517  
2.511  
2.505  
2.499  
1.771  
1.746  
1.721  
1.696  
1.671  
1.418  
1.393  
1.368  
1.343  
1.319  
1.295  
0.941  
0.917

0.92 (t, J=7.34 Hz, 3 H)  
1.36 (m, J=7.39 Hz, 2 H)  
1.72 (m, J=7.49 Hz, 2 H)  
2.62 (t, J=7.50 Hz, 2 H)  
7.04 (d, J=8.85 Hz, 2 H)  
7.78 (d, J=8.79 Hz, 2 H)



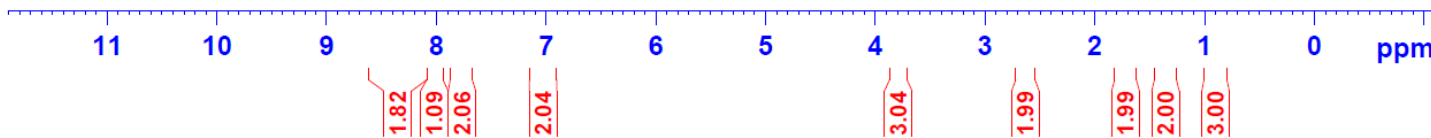
Current Data Parameters  
NAME FL349  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170809  
Time 18.41  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6103.516 Hz  
FIDRES 0.093132 Hz  
AQ 5.3687091 sec  
RG 63.9644  
DW 81.920 usec  
DE 6.50 usec  
TE 298.2 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 300.1618536 MHz  
NUC1 1H  
P1 13.50 usec  
PLW1 9.30000019 W

F2 - Processing parameters  
SI 65536  
SF 300.1599977 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





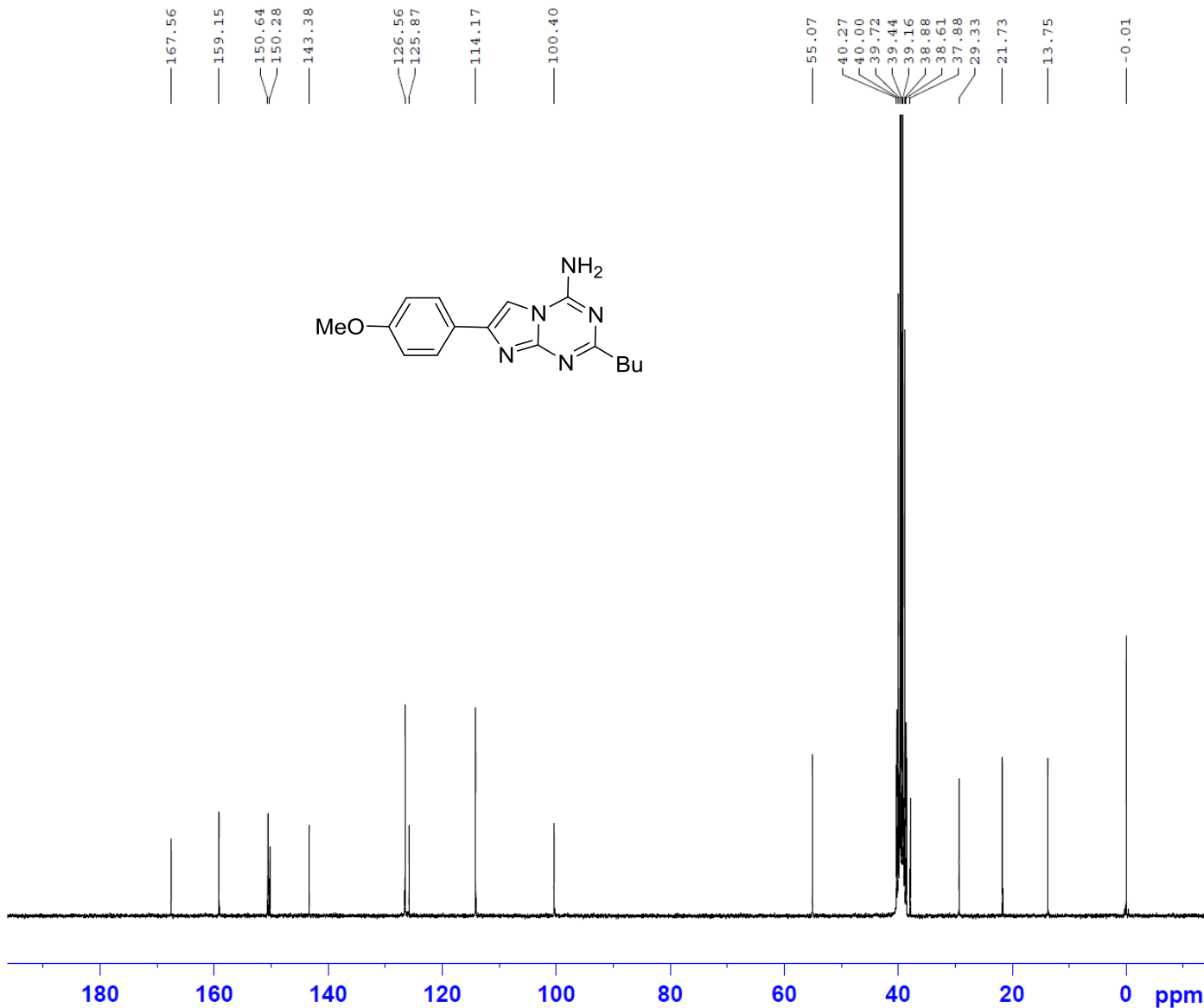
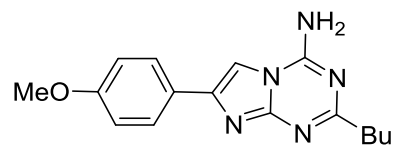
Current Data Parameters  
NAME FL349  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170809  
Time\_ 18.59  
INSTRUM FOURIER300  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 14336  
DS 4  
SWH 24414.063 Hz  
FIDRES 0.372529 Hz  
AQ 1.3421773 sec  
RG 501.187  
DW 20.480 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
D31 0.00001500 sec  
D40 0.00439029 sec  
L4 37  
L5 53  
P32 98.00 usec  
TD0 14

----- CHANNEL f1 -----  
SFO1 75.4828392 MHz  
NUC1 13C  
P1 15.00 usec  
PLW1 22.00000000 W

----- CHANNEL f2 -----  
SFO2 300.1612006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 98.00 usec  
PLW2 9.30000019 W  
PLW12 0.29359001 W  
PLW13 0.20359001 W

F2 - Processing parameters  
SI 32768  
SF 75.4753335 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



# 4-Amino-2-butyl-7-(4-biphenyl)imidazo[1,2-a][1,3,5]triazine (5x)

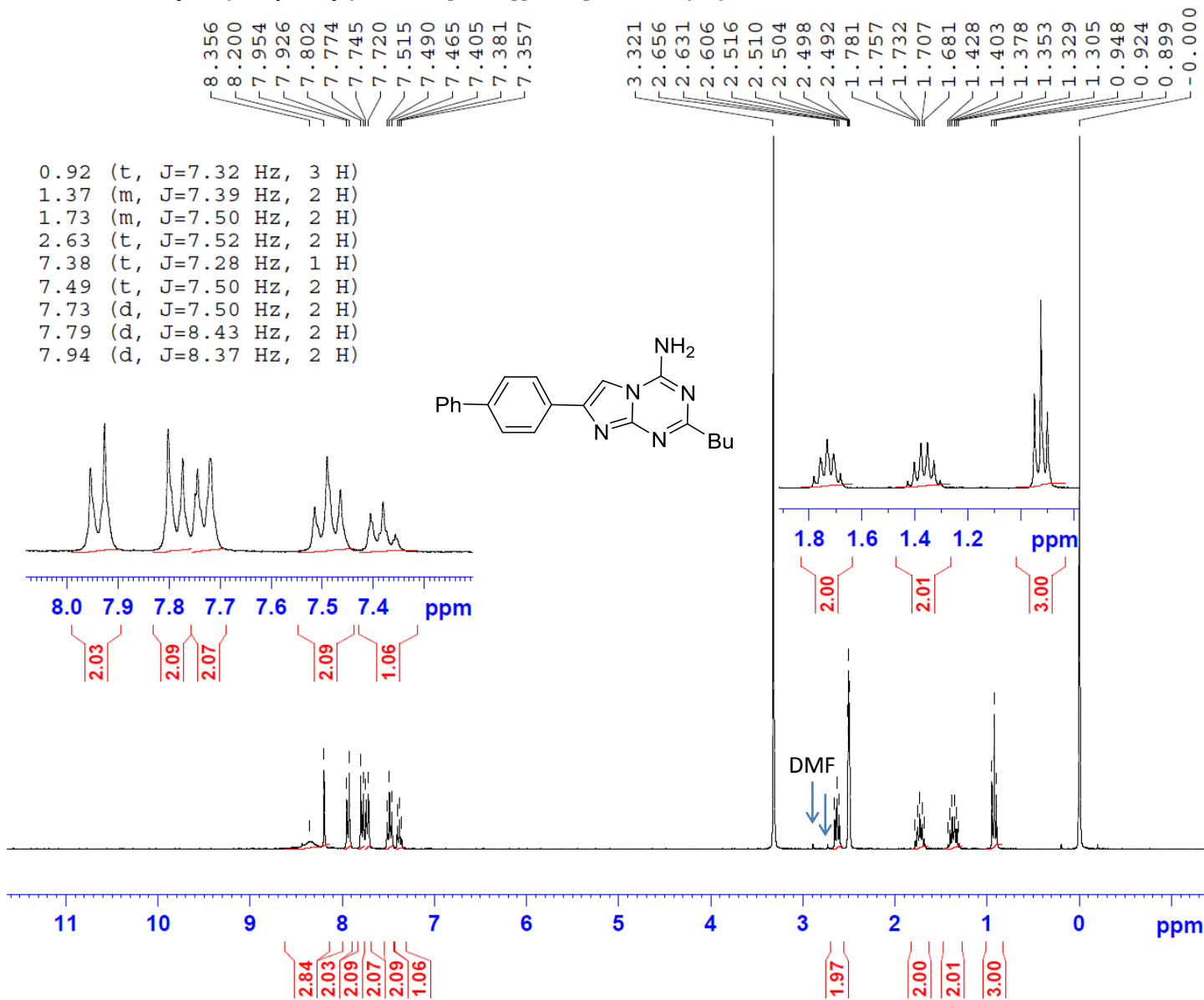
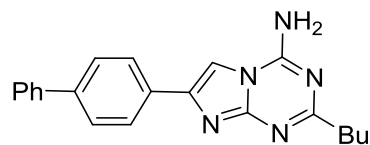


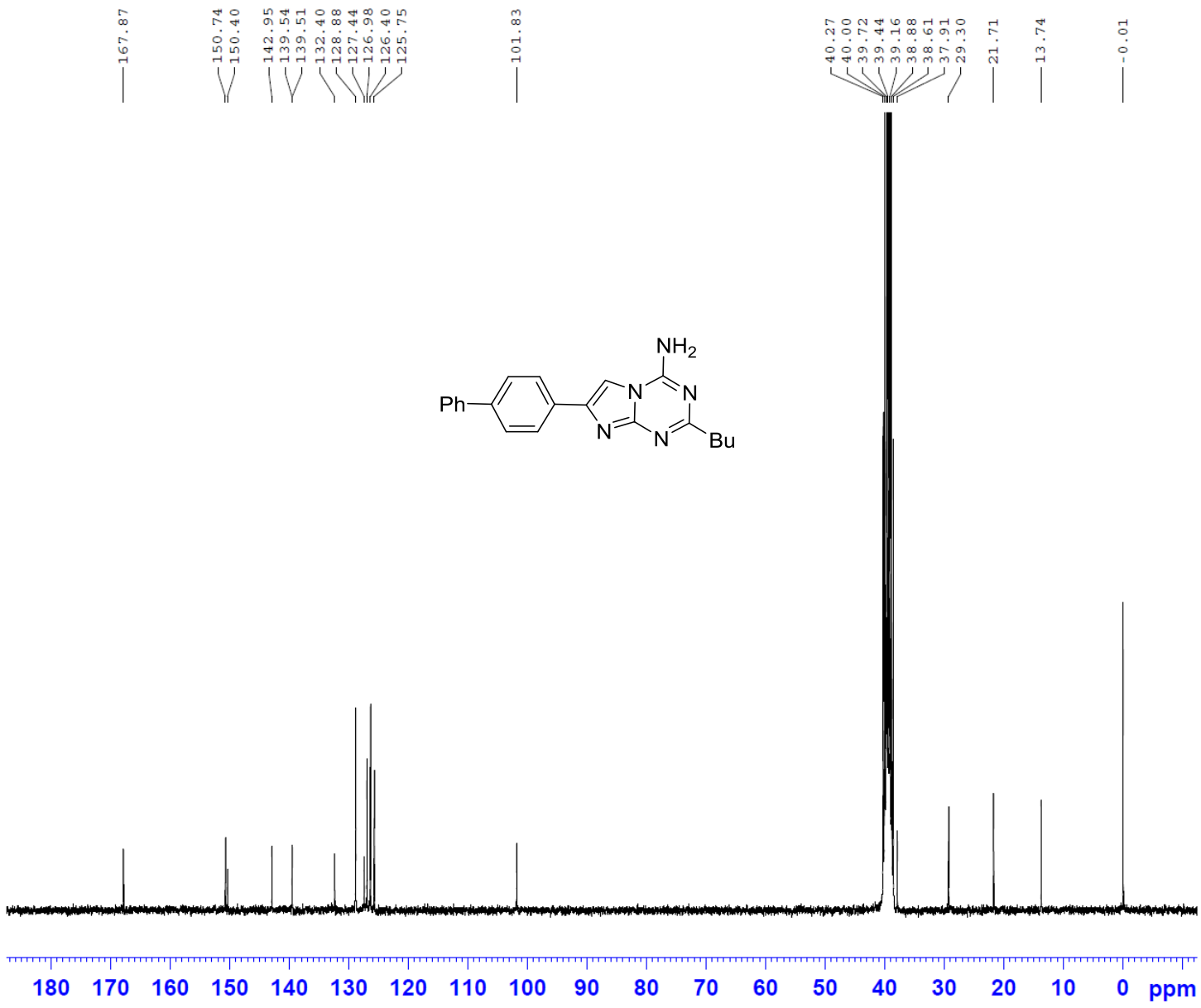
Current Data Parameters  
 NAME FL375  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171023  
 Time 17.05  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 147.582  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1599999 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME FL375  
 EXPNO 2  
 PROCNO 1

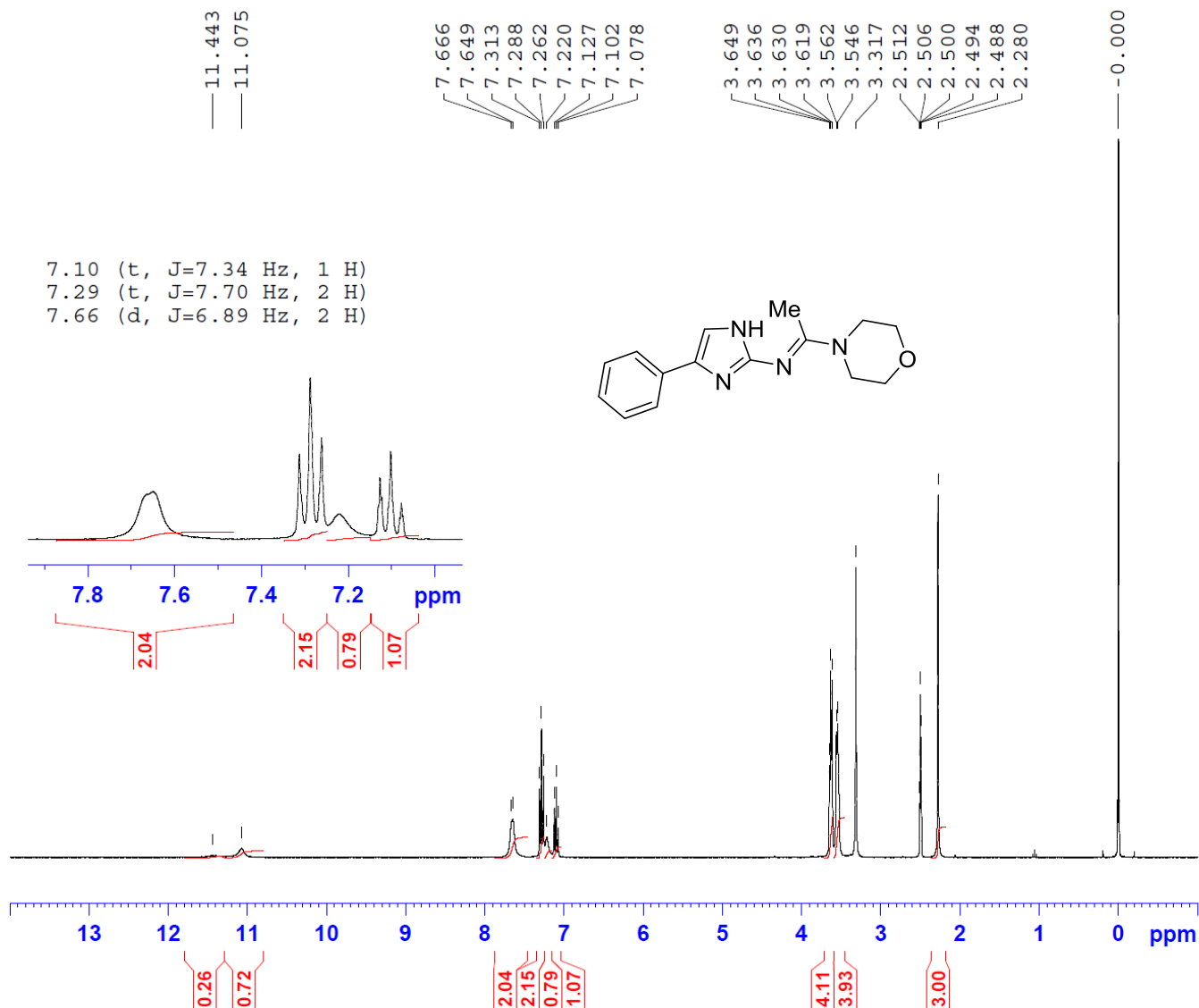
F2 - Acquisition Parameters  
 Date\_ 20171022  
 Time 14.10  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20480  
 DS 4  
 SWH 24414.063 Hz  
 FIDRES 0.372529 Hz  
 AQ 1.3421773 sec  
 RG 501.187  
 DW 20.480 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 D31 0.00001500 sec  
 D40 0.00439029 sec  
 L4 37  
 L5 53  
 P32 98.00 usec  
 TD0 20

----- CHANNEL f1 -----  
 SFO1 75.4828392 MHz  
 NUC1 13C  
 P1 15.00 usec  
 PLW1 22.00000000 W

----- CHANNEL f2 -----  
 SFO2 300.1612006 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 98.00 usec  
 PLW2 9.30000019 W  
 PLW12 0.29359001 W  
 PLW13 0.20359001 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4753350 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

*N,N'*-morpholino-*N*-[3(5)-phenylimidazo-5(3)yl] acetamide (**6**)



Current Data Parameters  
 NAME FL371  
 EXPNO 9  
 PROCNO 1

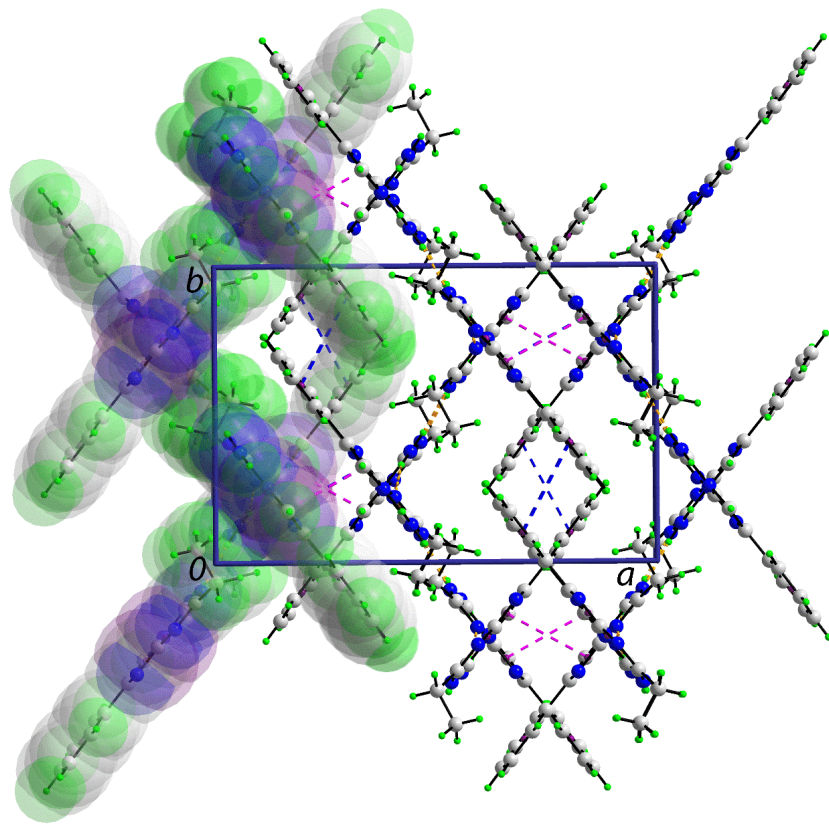
F2 - Acquisition Parameters  
 Date\_ 20180416  
 Time\_ 16.18  
 INSTRUM FOURIER300  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6103.516 Hz  
 FIDRES 0.093132 Hz  
 AQ 5.3687091 sec  
 RG 79.824  
 DW 81.920 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 300.1618536 MHz  
 NUC1 1H  
 P1 13.50 usec  
 PLW1 9.30000019 W

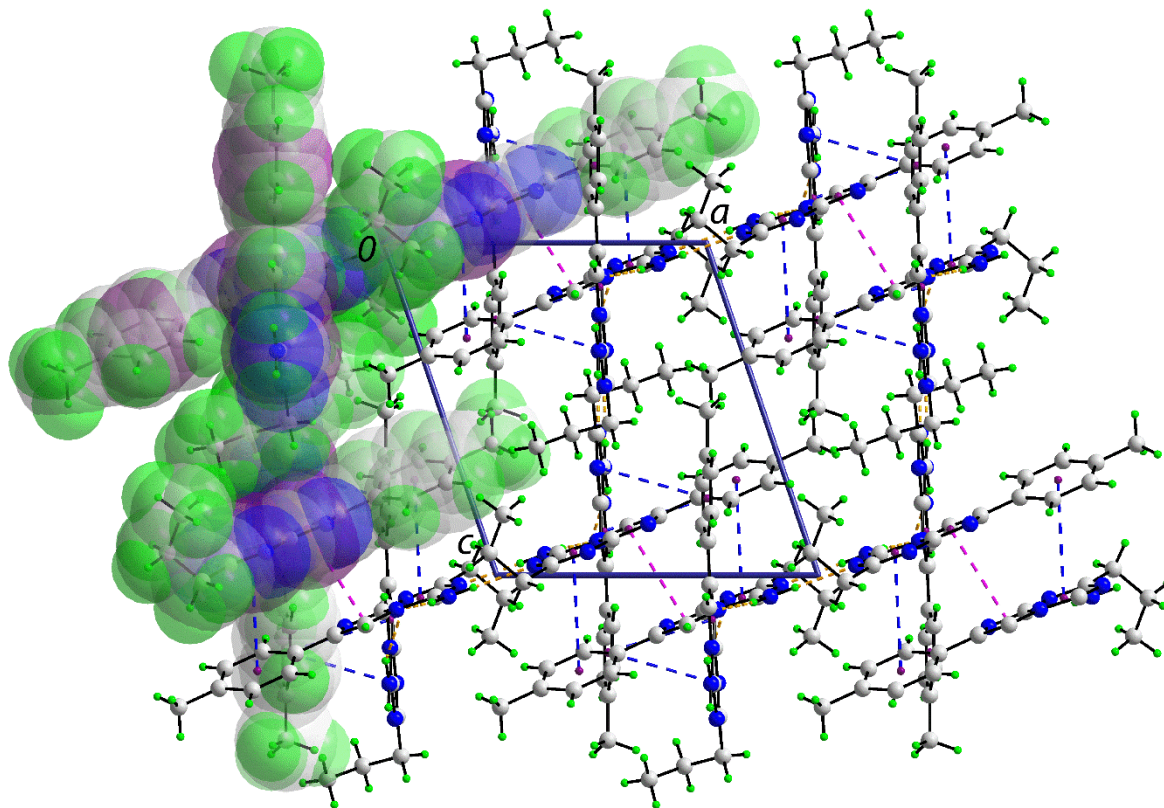
F2 - Processing parameters  
 SI 65536  
 SF 300.1600009 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



# X-Ray crystallographic data for **5g** and **5p**



**ESI Figure S1.** A view in projection down the *c*-axis of the unit cell contents for **5g**. One supramolecular layer is highlighted in space-filling mode. The N–H···N,  $\pi$ (imidazo)··· $\pi$ (imidazo) and  $\pi$ (phenyl)··· $\pi$ (phenyl) interactions are shown as orange, pink and blue dashed lines, respectively. Geometric parameters characterising the identified intermolecular interactions. N–H···N: N41–H4n1···N3<sup>i</sup> = 2.088(11) Å, N41···N3<sup>i</sup> = 2.9669(13) Å and angle at H4n1 = 174.5(11)°; N41–H4n2···N1<sup>ii</sup> = 2.064(12) Å, N41···N1<sup>ii</sup> = 2.9277(12) Å and angle at H4n2 = 163.9(11)°.  $\pi$ (imidazo)··· $\pi$ (imidazo): Cg(N5,C6,C7,N8,C9)···Cg(N5,C6,C7,N8,C9)<sup>iii</sup> = 3.4699(6) Å and angle of inclination = 5.41(6)°.  $\pi$ (phenyl)··· $\pi$ (phenyl): Cg(C71-C76)···Cg(C71-C76)<sup>iv</sup> = 3.8142(7) Å and angle of inclination = 6.53(5)°. Symmetry operations: (i) 1-*x*, 1-*y*, 1-*z*; (ii) *x*, ½-*y*, ½+*z*; (iii) ½-*x*, ½-*y*, *z*; (iv) ½-*x*, -½-*y*, *z*.



**ESI Figure S2.** A view in projection down the *b*-axis of the unit cell contents for **5p**. One supramolecular layer is highlighted in space-filling mode. The N–H⋯N, p(imidazo)⋯p(imidazo) and p(triazine)⋯p(phenyl) interactions are shown as orange, pink and blue dashed lines, respectively. Geometric parameters characterising the identified intermolecular interactions. N–H⋯N: N41–H4n1⋯N3<sup>i</sup> = 2.171(12) Å, N41⋯N3<sup>i</sup> = 3.0501(16) Å and angle at H4n1 = 179.9(18)°; N41–H4n2⋯N8a<sup>ii</sup> = 2.192(13) Å, N41⋯N8a<sup>ii</sup> = 3.0636(15) Å and angle at H4n2 = 173.5(13)°; N41a–H4n3⋯N3a<sup>iii</sup> = 2.081(12) Å, N41a⋯N3a<sup>iii</sup> = 2.9561(14) Å and angle at H4n3 = 176.6(13)°; N41a–H4n4⋯N1<sup>iii</sup> = 2.501(12) Å, N41a⋯N1<sup>iii</sup> = 3.3320(15) Å and angle at H4n4 = 156.8(15)°. p(imidazo)⋯p(imidazo): Cg(N5,C6,C7,N8,C9)⋯Cg(N5,C6,C7,N8,C9)<sup>iv</sup> = 3.5695(7) Å and angle of inclination = 0°. p(triazine)⋯p(phenyl): Cg(N1,N3,N5,C2,C4,C9)⋯Cg(C71-C76)<sup>iv</sup> = 3.8946(7) Å and angle of inclination = 18.43(6)°; Cg(N1a,N3a,N5a,C2a,C4a,C9a)⋯Cg(C71a-C76a)<sup>v</sup> = 3.9224(7) Å and angle of inclination = 10.30(6)°. Symmetry operations: (i)  $-x, -y, 2-z$ ; (ii)  $1-x, -y, 1-z$ ; (iii)  $1-x, 1-y, 1-z$ ; (iv)  $1-x, -y, 2-z$ ; (v)  $1-x, 1-y, -z$ .