RSC Advances

6,N^2-Diaryl-1,3,5-triazine-2,4-diamines: Synthesis, Antiproliferative Activity and 3D-QSAR Modeling

(Electronic Supplementary Information)

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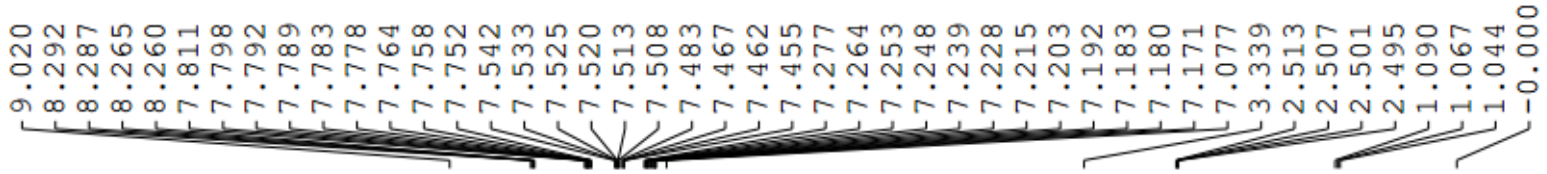
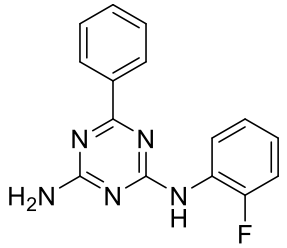
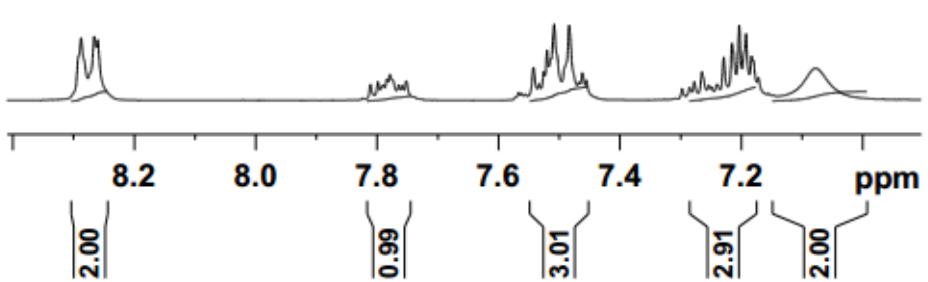
Copies of ^{1}H and ^{13}C NMR spectra for the prepared new 6,*N*^{2}-diaryl-1,3,5-triazine-2,4-diamines (**2**, **3**, **4**, **30**, **34**, **53**, **57**, **59**, **65**, **71**, **84**, **91**, **111**, **116**, **122**, and **123**)

N²-(2-fluorophenyl)-6-phenyl-1,3,5-triazine-2,4-diamine (2)



8.28 (dd, J=1.59, 8.13 Hz, 2 H)





Current Data Parameters
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EXPNO 2
PROCNO 1

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Date_ 20180326
Time 14.38
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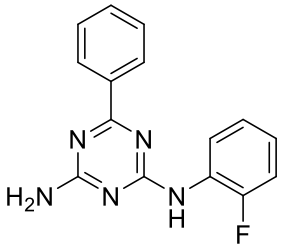
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 53.5092
DW 81.920 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1

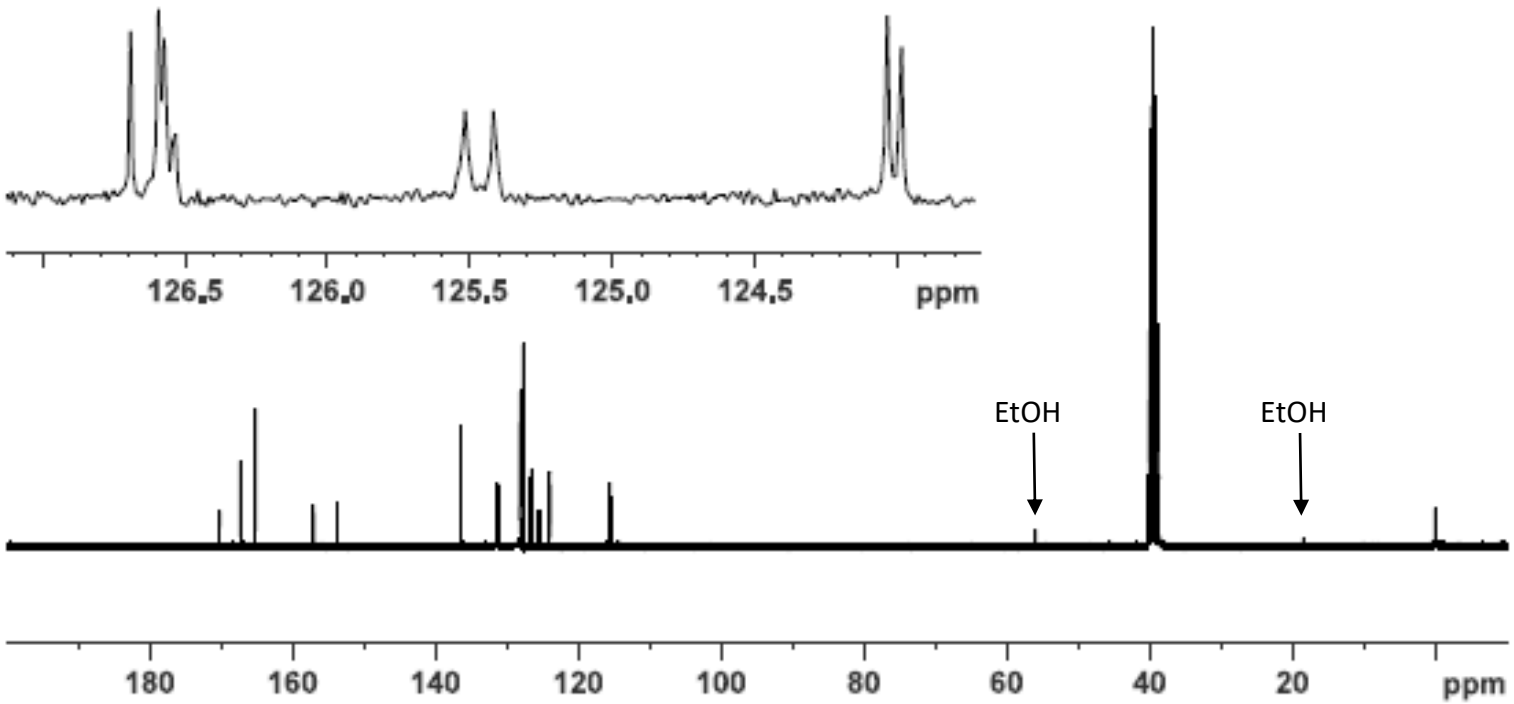
======== CHANNEL f1 ========
SFO1 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

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

N²-(2-fluorophenyl)-6-phenyl-1,3,5-triazine-2,4-diamine (2)

115.49 (d, J=19.37 Hz, 1 C)
124.02 (d, J=3.73 Hz, 1 C)
125.47 (d, J=7.45 Hz, 1 C)
126.59 (d, J=1.52 Hz, 1 C)
126.62 (d, J=11.96 Hz, 1 C)
155.44 (d, J=245.87 Hz, 1 C)





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EXPNO                  3
PROCNO                 1

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PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  3072
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                300.3 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                    3

======== 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        0 Hz
GB        0
PC                  1.40
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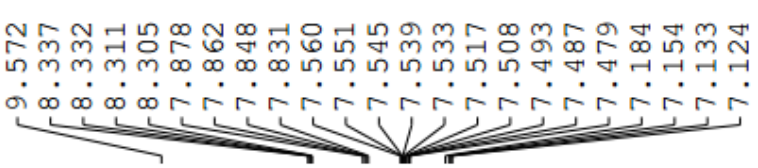
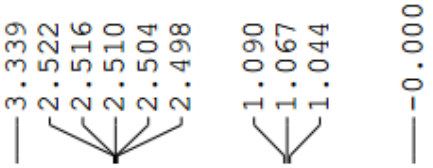
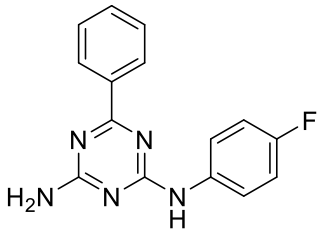
N²-(4-fluorophenyl)-6-phenyl-1,3,5-triazine-2,4-diamine (3)





7.15 (dd, J=8.84, 9.17 Hz, 2 H)
7.85 (dd, J=5.01, 9.15 Hz, 2 H)
8.32 (dd, J=1.71, 8.07 Hz, 2 H)

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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                   68.2444
DW                    81.920 usec
DE                     6.50 usec
TE                    300.1 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             300.1599981 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
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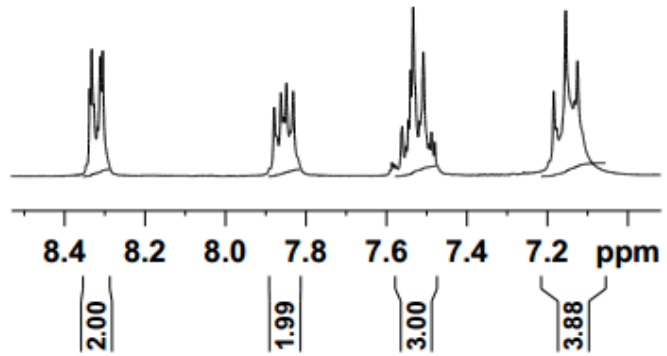
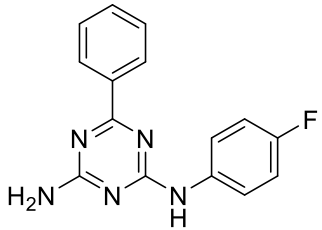
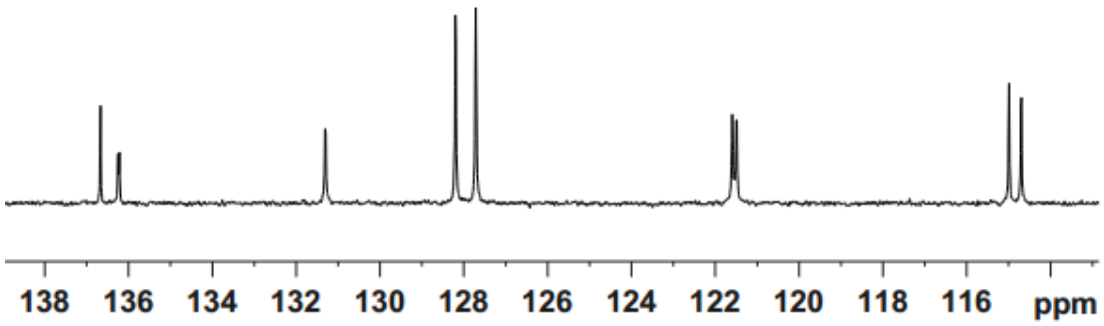


N²-(4-fluorophenyl)-6-phenyl-1,3,5-triazine-2,4-diamine (3)

114.85 (d, J=22.03 Hz, 2 C)
121.55 (d, J=8.20 Hz, 2 C)
136.24 (d, J=2.24 Hz, 1 C)
157.42 (d, J=238.62 Hz, 1 C)



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Current Data Parameters
NAME                  JA0027
EXPNO                      3
PROCNO                     1

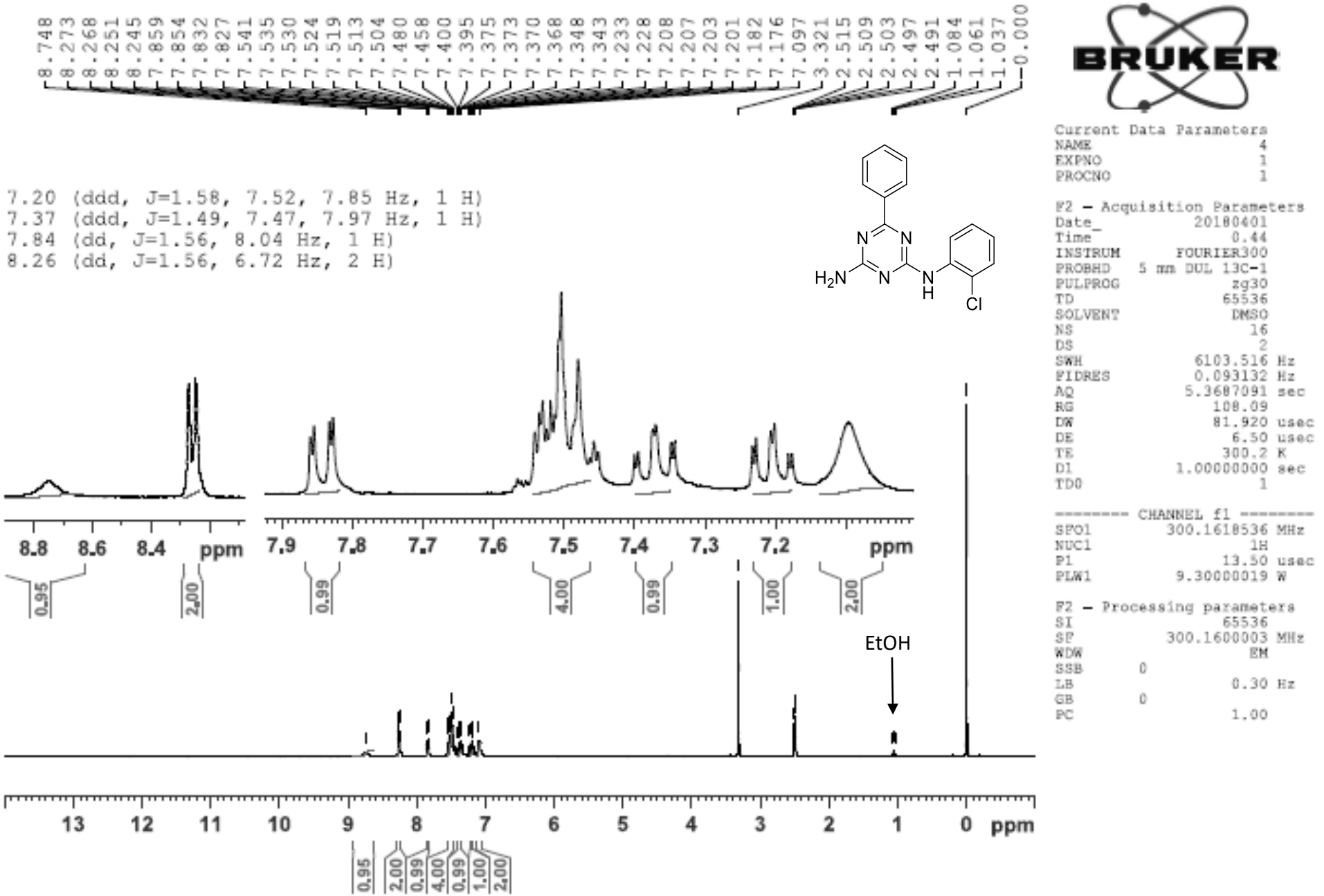
F2 - Acquisition Parameters
Date_              20180327
Time                 17.58
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                   65536
SOLVENT               DMSO
NS                    3072
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.4 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                      3

======== 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
```

N²-(2-chlorophenyl)-6-phenyl-1,3,5-triazine-2,4-diamine (4)

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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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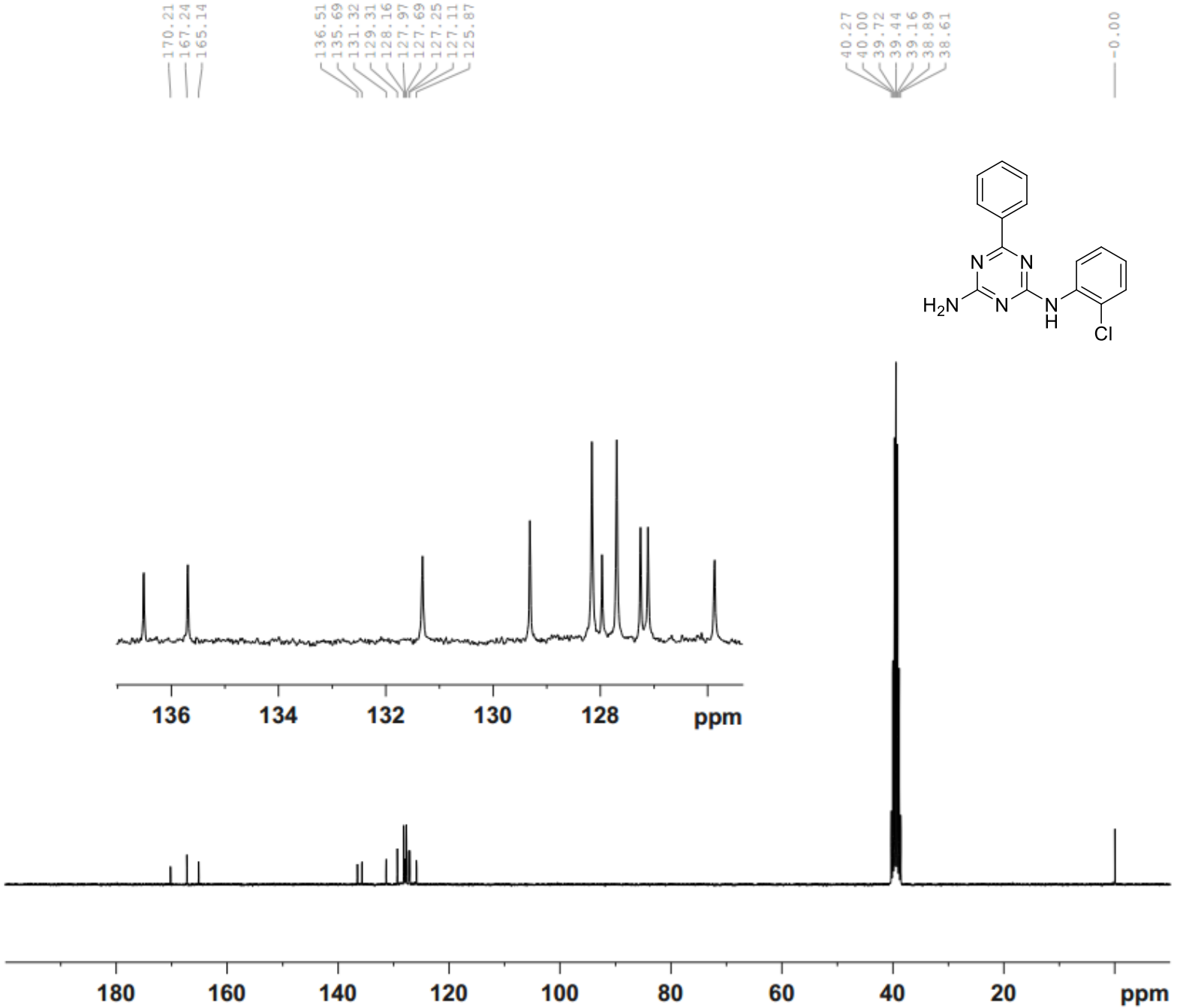
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             6103.516 Hz
FIDRES          0.093132 Hz
AQ              5.3687091 sec
RG                108.09
DW                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           300.1600003 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

N²-(2-chlorophenyl)-6-phenyl-1,3,5-triazine-2,4-diamine (4)



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Current Data Parameters
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EXPNO                      2
PROCNO                     1

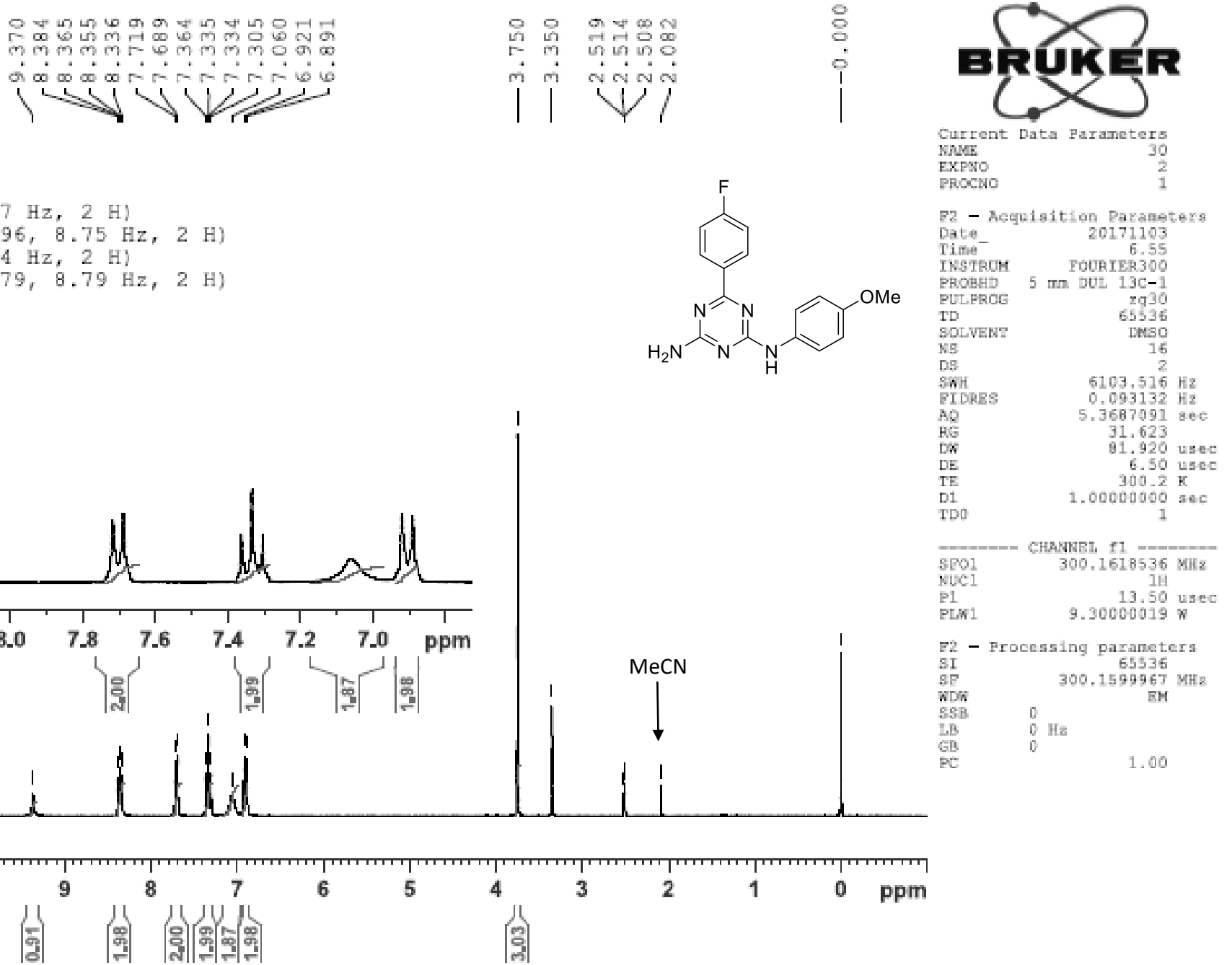
F2 - Acquisition Parameters
Date_              20180402
Time                   9.30
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     5120
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.3 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                        5

======== 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
```

6-(4-fluorophenyl)-N²-(4-methoxyphenyl)-1,3,5-triazine-2,4-diamine (30)



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EXPNO 2
PROCNO 1

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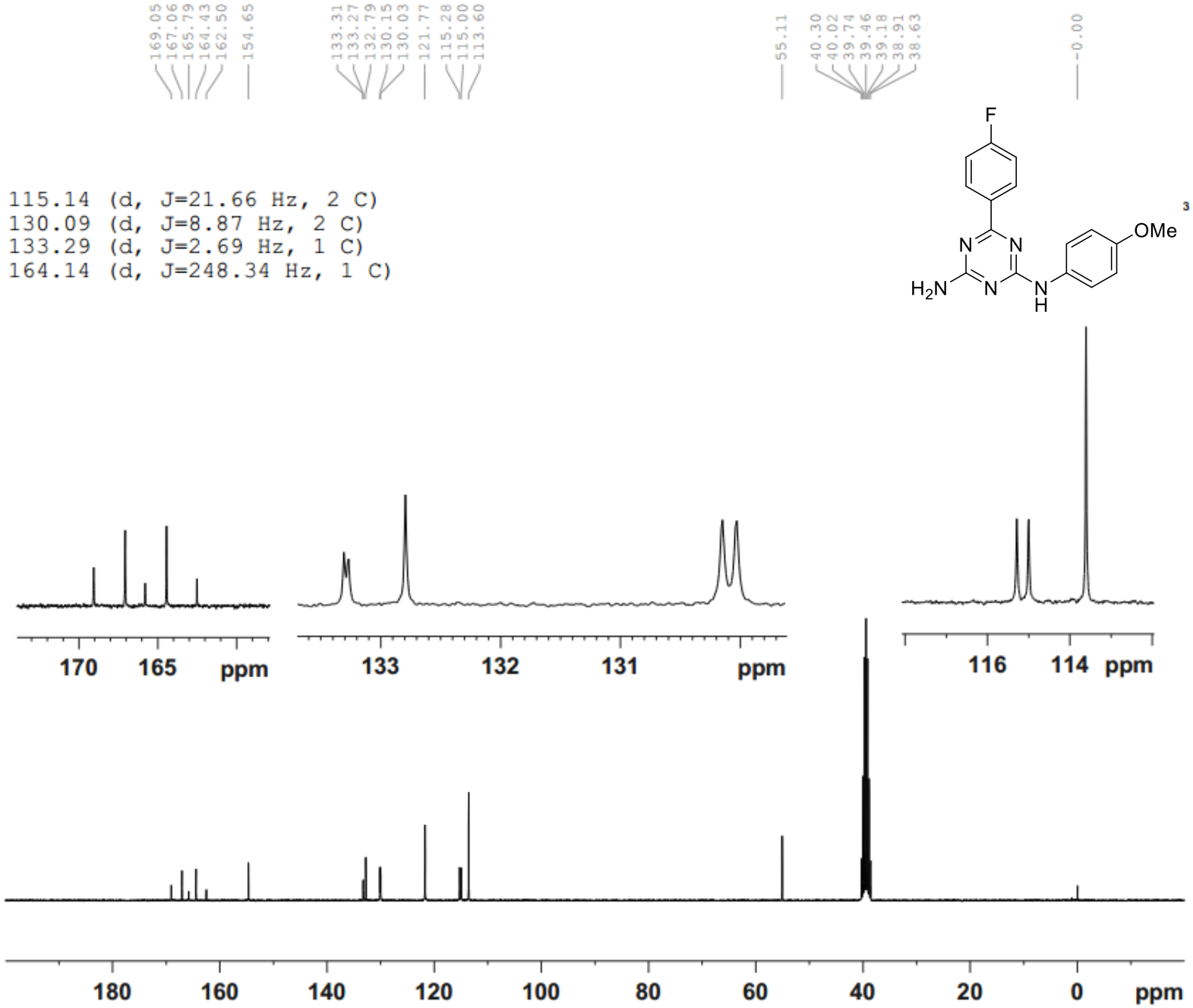
Time_ 6.55
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 31.623
DW 81.920 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 300.1599967 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

6-(4-fluorophenyl)-N²-(4-methoxyphenyl)-1,3,5-triazine-2,4-diamine (30)



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Current Data Parameters
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EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171104
Time                   2.49
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     3072
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                  300.3 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                       3

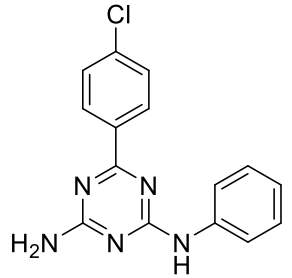
======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                  15.00 usec
PLW1          22.00000000 W

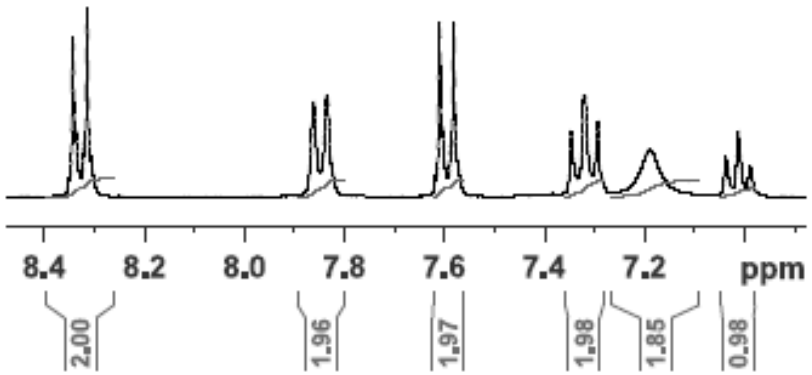
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

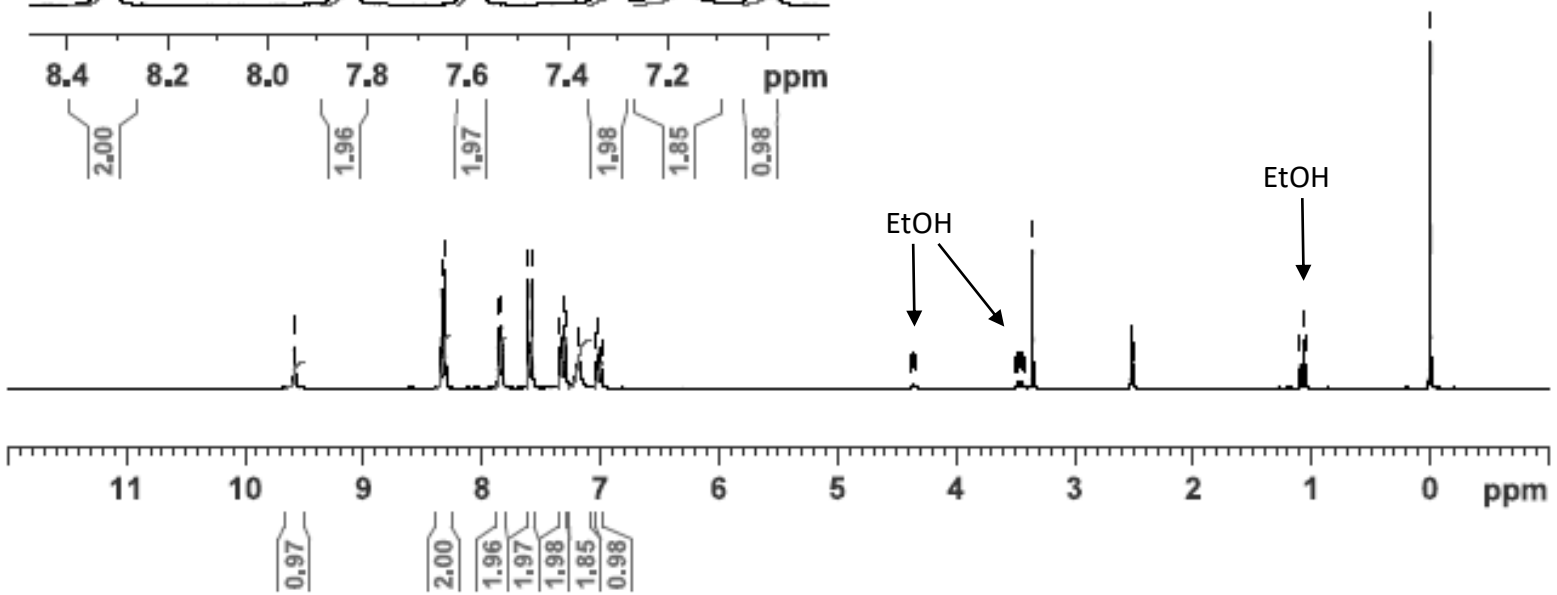
F2 - Processing parameters
SI                    32768
SF              75.4753322 MHz
WDW                      EM
SSB         0
LB                  1.00 Hz
GB          0
PC                  1.40
```

6-(4-chlorophenyl)-N²-phenyl-1,3,5-triazine-2,4-diamine (34)

7.01 (t, J=7.91 Hz, 1 H)
7.32 (t, J=7.94 Hz, 2 H)
7.60 (d, J=8.64 Hz, 2 H)
7.85 (d, J=7.89 Hz, 2 H)
8.33 (d, J=8.70 Hz, 2 H)





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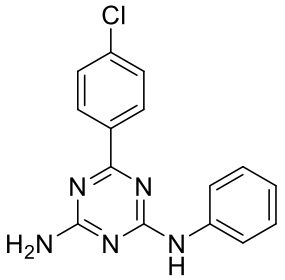
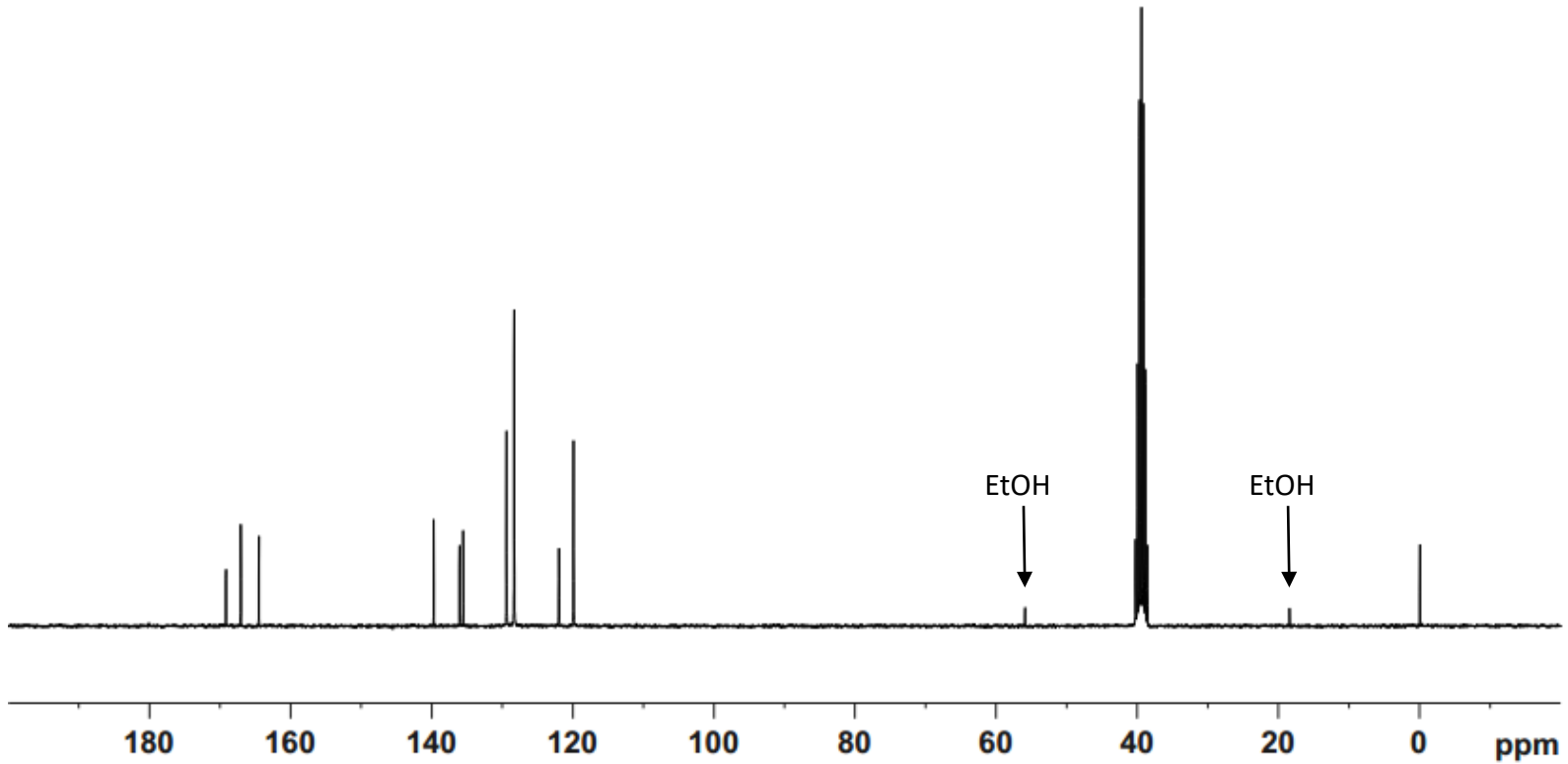
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES             0.093132 Hz
AQ                 5.3687091 sec
RG                    31.623
DW                    81.920 usec
DE                     6.50 usec
TE                    300.1 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             300.1599964 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

6-(4-chlorophenyl)-N²-phenyl-1,3,5-triazine-2,4-diamine (34)



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EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
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Time                  23.57
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PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     3072
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                  300.3 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                       3

======== 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
```

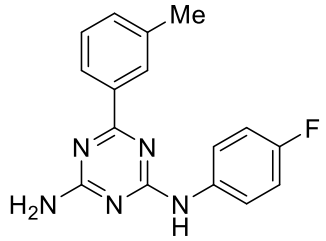
N^2-(4-fluorophenyl)-6-(m-tolyl)-1,3,5-triazine-2,4-diamine (53)

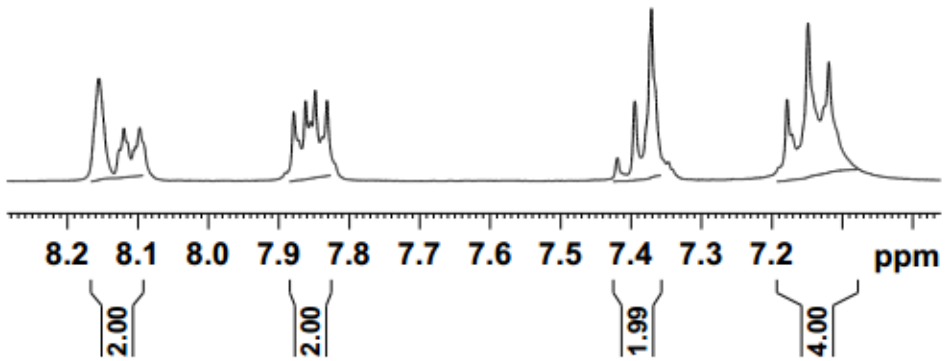
9.563 8.156 8.154 8.126 8.119 8.115 8.106 8.103 8.097 7.878 7.862 7.848 7.831 7.419 7.394 7.371 7.178 7.148 7.126 7.119

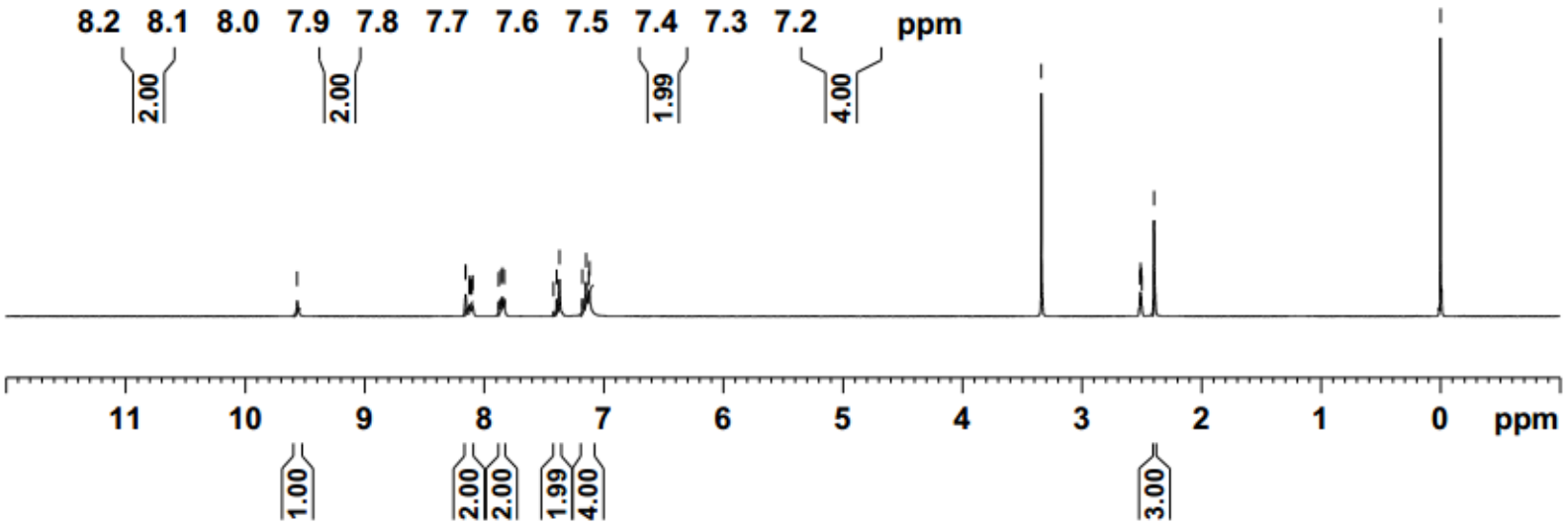
3.338 2.515 2.509 2.503 2.497 2.395

-0.000

7.15 (dd, J=8.90, 8.90 Hz, 2 H)
7.85 (dd, J=5.04, 9.12 Hz, 2 H)







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PROCNO 1

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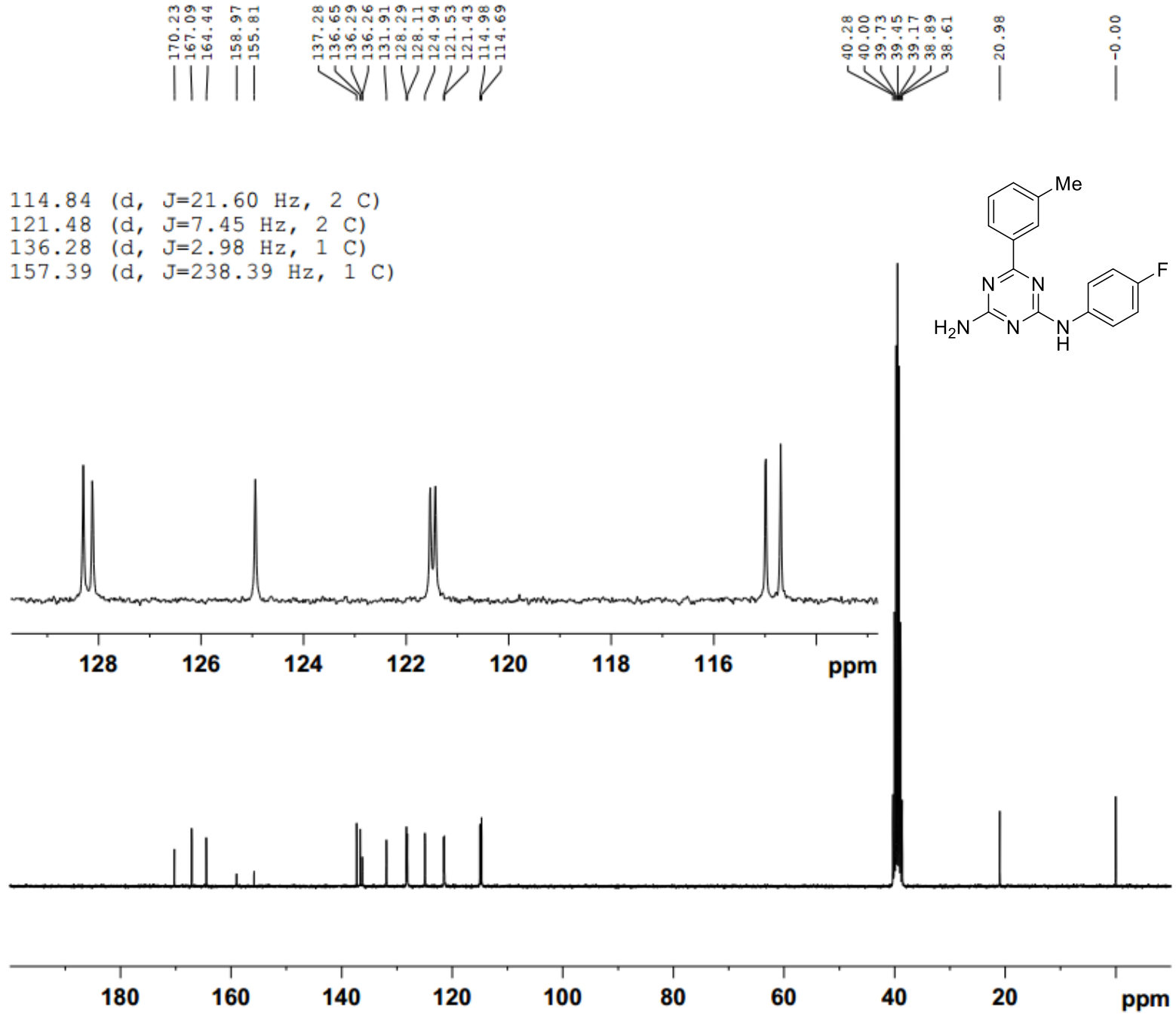
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6103.516 Hz
FIDRES 0.093132 Hz
AQ 5.3687091 sec
RG 67.1476
DW 81.920 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 300.1599984 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N^2-(4-fluorophenyl)-6-(m-tolyl)-1,3,5-triazine-2,4-diamine (53)



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Current Data Parameters
NAME                  JA0503
EXPNO                      4
PROCNO                     1

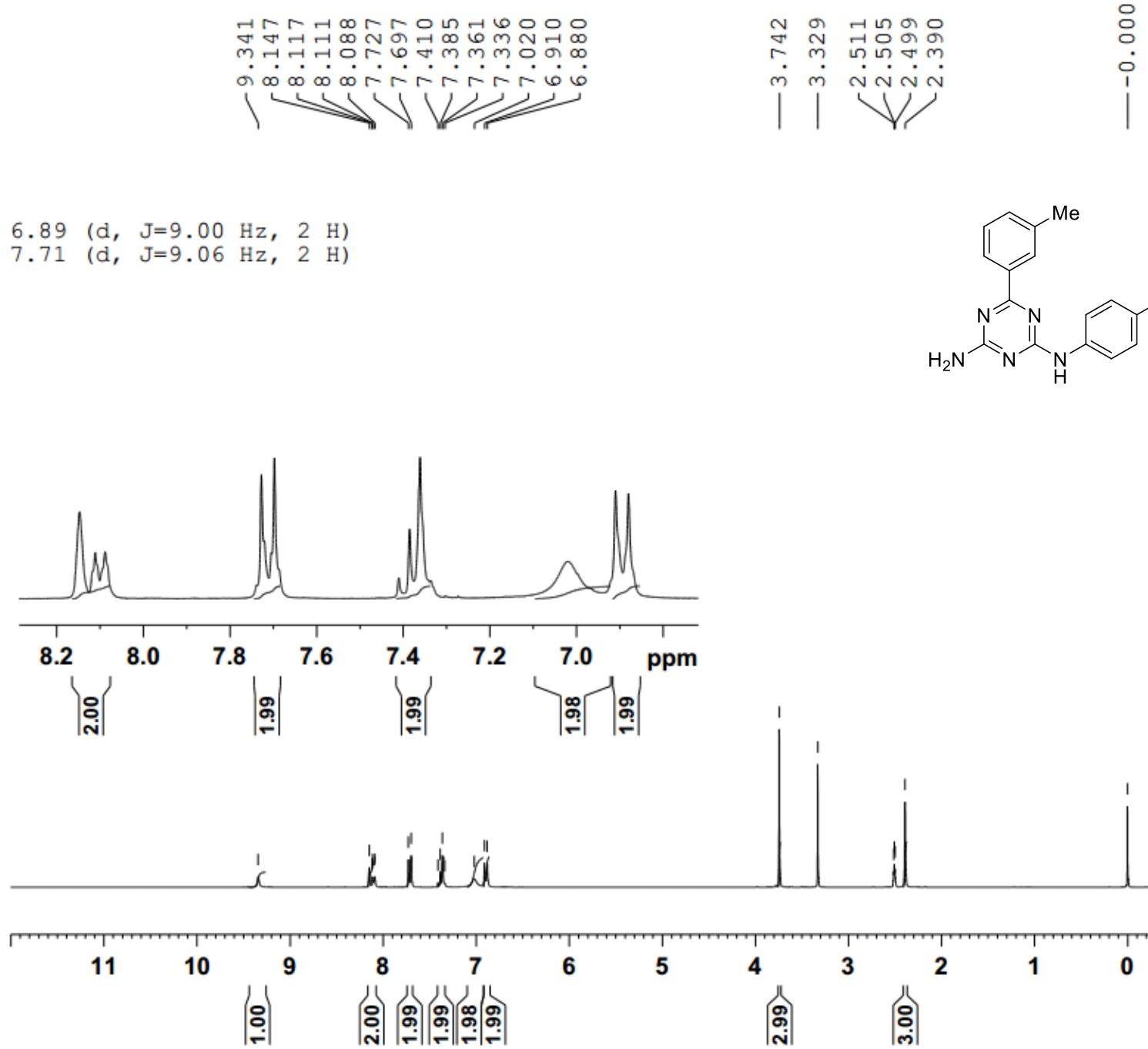
F2 - Acquisition Parameters
Date_              20180913
Time                  22.43
INSTRUM           FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     4096
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.3 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                        4

======== 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
```

N^2-(4-methoxyphenyl)-6-(m-tolyl)-1,3,5-triazine-2,4-diamine (57)



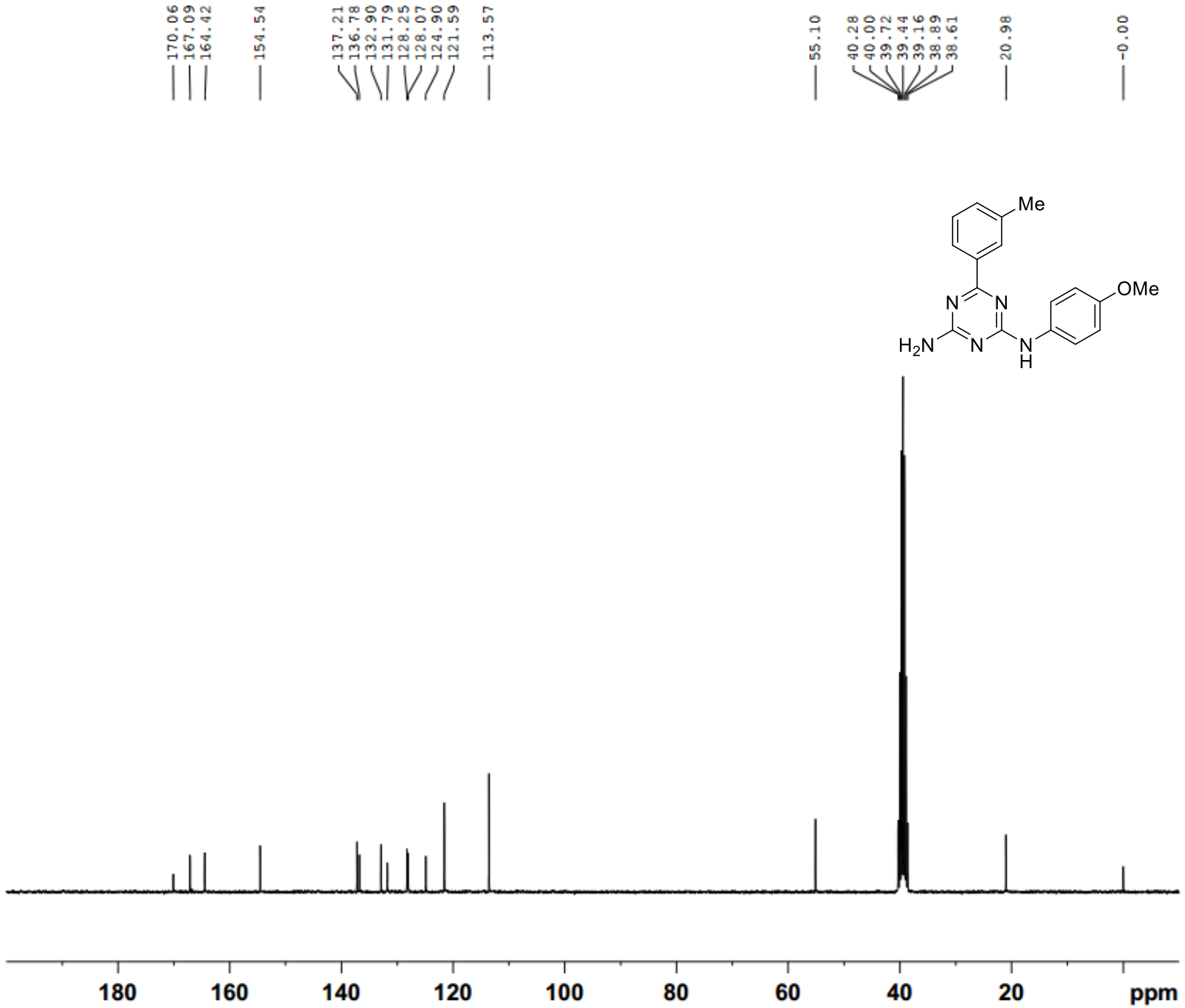

```
Current Data Parameters
NAME                  JA0504
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180903
Time                  18.36
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                    69.6761
DW                    81.920 usec
DE                     6.50 usec
TE                    300.1 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              300.1599995 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N²-(4-methoxyphenyl)-6-(m-tolyl)-1,3,5-triazine-2,4-diamine (57)



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```
Current Data Parameters
NAME                  JA0504
EXPNO                      3
PROCNO                     1

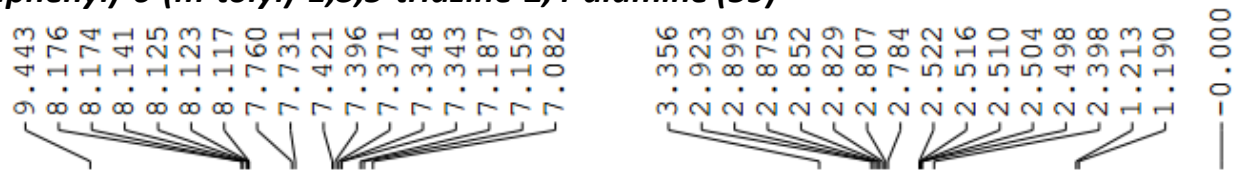
F2 - Acquisition Parameters
Date_              20180905
Time                   19.11
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH              24414.063 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                       3

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

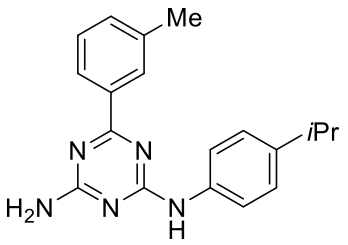
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2              98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

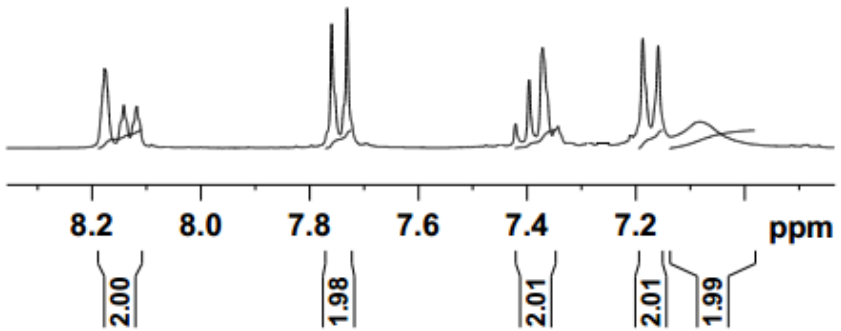
F2 - Processing parameters
SI                     32768
SF              75.4753342 MHz
WDW                       EM
SSB          0
LB                  1.00 Hz
GB           0
PC                  1.40
```

N^2-(4-isopropylphenyl)-6-(m-tolyl)-1,3,5-triazine-2,4-diamine (59)



1.20 (d, J=6.90 Hz, 6 H)
2.85 (m, J=6.96 Hz, 1 H)
7.17 (d, J=8.52 Hz, 2 H)
7.75 (d, J=8.57 Hz, 2 H)





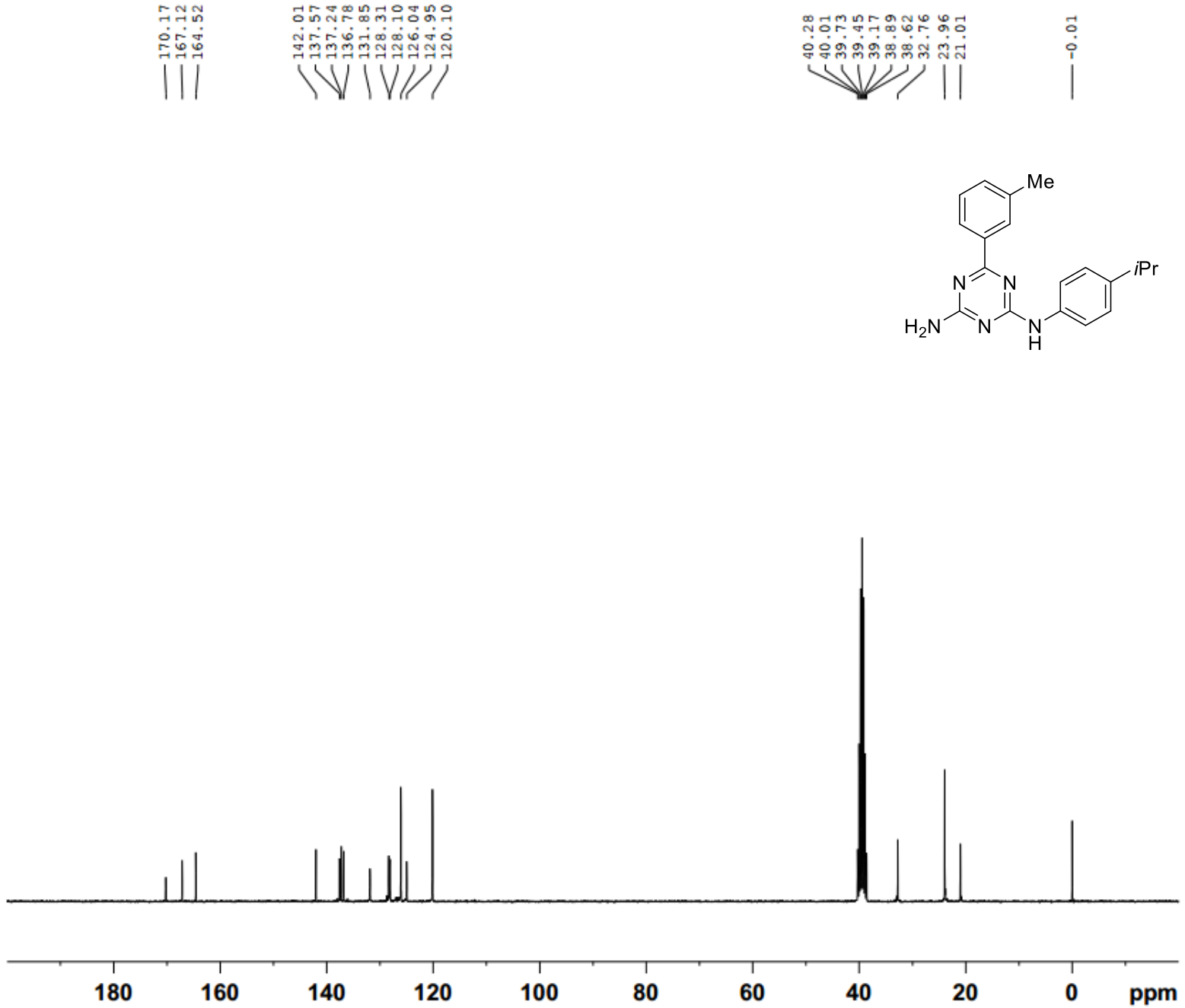

```
Current Data Parameters
NAME                  JA0513
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190410
Time                 14.56
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                   31.623
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              300.1599980 MHz
WDW                       EM
SSB         0
LB                     0.30 Hz
GB          0
PC                     1.00
```

N^2-(4-isopropylphenyl)-6-(m-tolyl)-1,3,5-triazine-2,4-diamine (59)



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```
Current Data Parameters
NAME                  JA0513
EXPNO                      6
PROCNO                     1

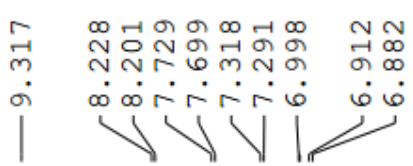
F2 - Acquisition Parameters
Date_              20190410
Time                   19.30
INSTRUM           FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zgpg30
TD                     65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    298.3 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                       3

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

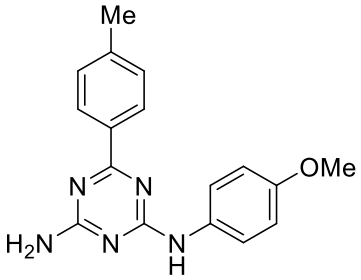
======== CHANNEL f2 ========
SFO2              300.1612006 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                 98.00 usec
PLW2               9.30000019 W
PLW12              0.29359001 W
PLW13              0.20359001 W

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

N^2-(4-methoxyphenyl)-6-(p-tolyl)-1,3,5-triazine-2,4-diamine (65)



6.90 (d, J=8.97 Hz, 2 H)
7.30 (d, J=8.16 Hz, 2 H)
7.71 (d, J=9.00 Hz, 2 H)
8.21 (d, J=8.13 Hz, 2 H)

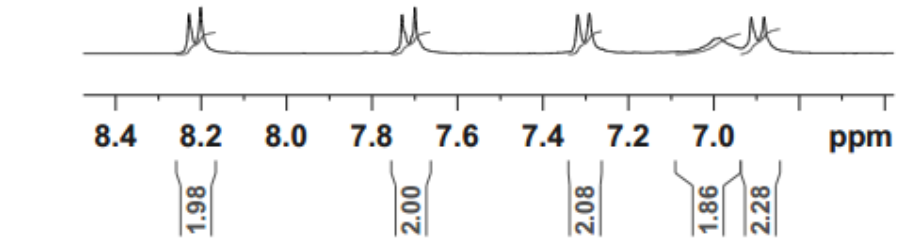


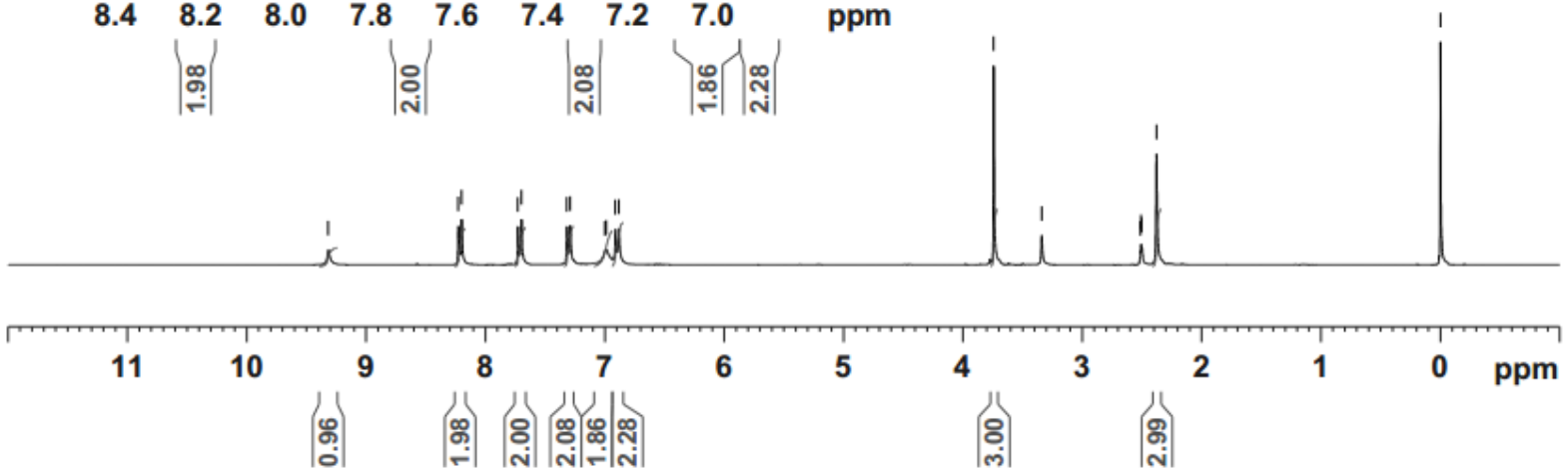

```
Current Data Parameters
NAME                  JA0007
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171030
Time                  14.39
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                    31.623
DW                    81.920 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                        1

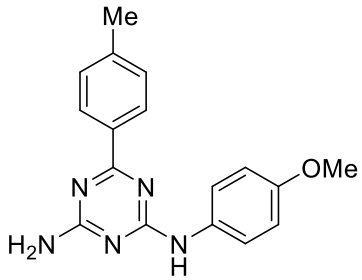
======== CHANNEL f1 ========
SFO1             300.1618536 MHz
NUC1                       1H
P1                    13.50 usec
PLW1              9.30000019 W

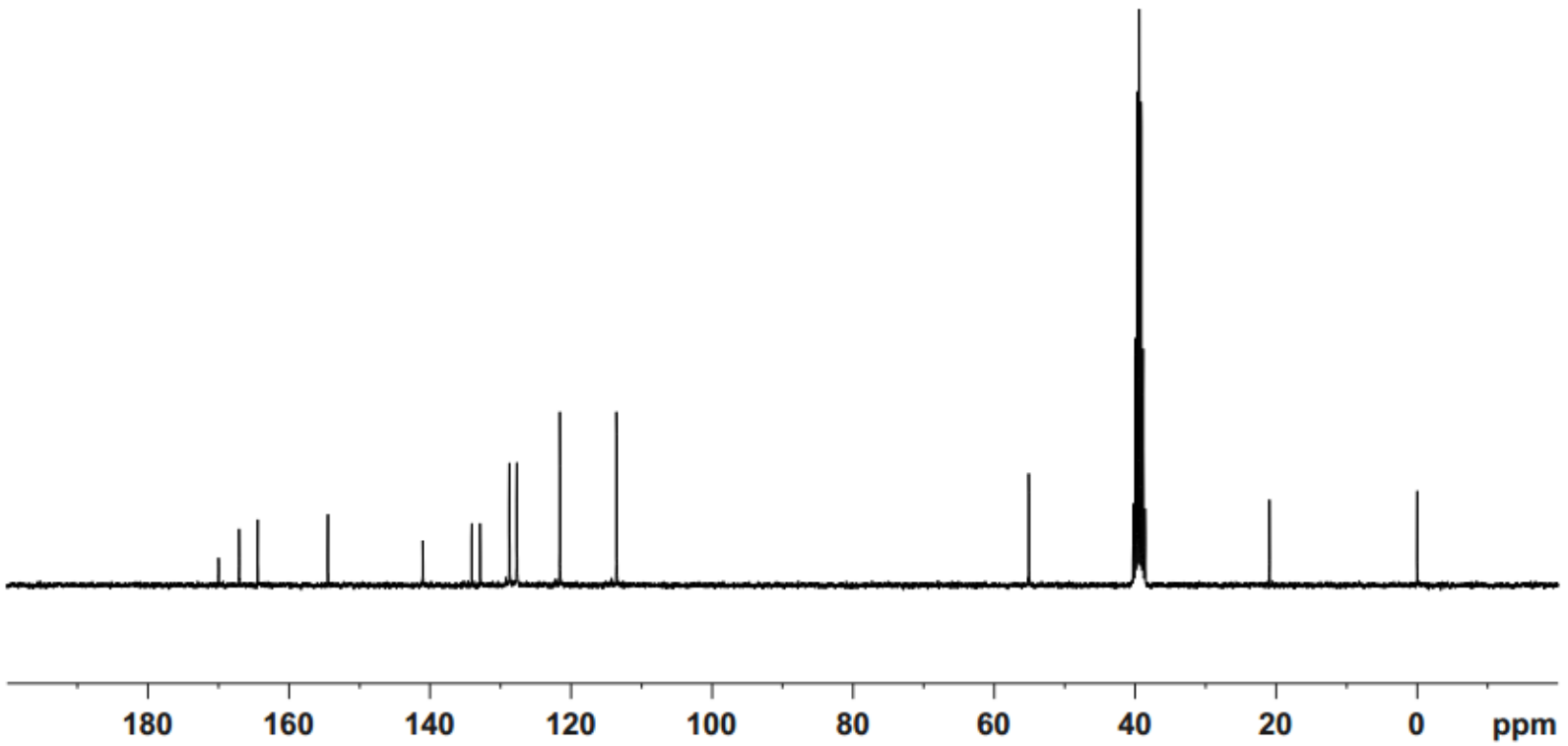
F2 - Processing parameters
SI                    65536
SF               300.1599989 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```





N²-(4-methoxyphenyl)-6-(p-tolyl)-1,3,5-triazine-2,4-diamine (65)





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```
Current Data Parameters
NAME                  JA0007
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171031
Time                   5.08
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     1024
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                        1

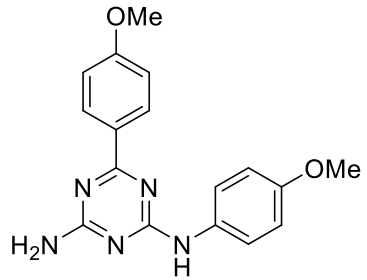
======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                    15.00 usec
PLW1           22.00000000 W

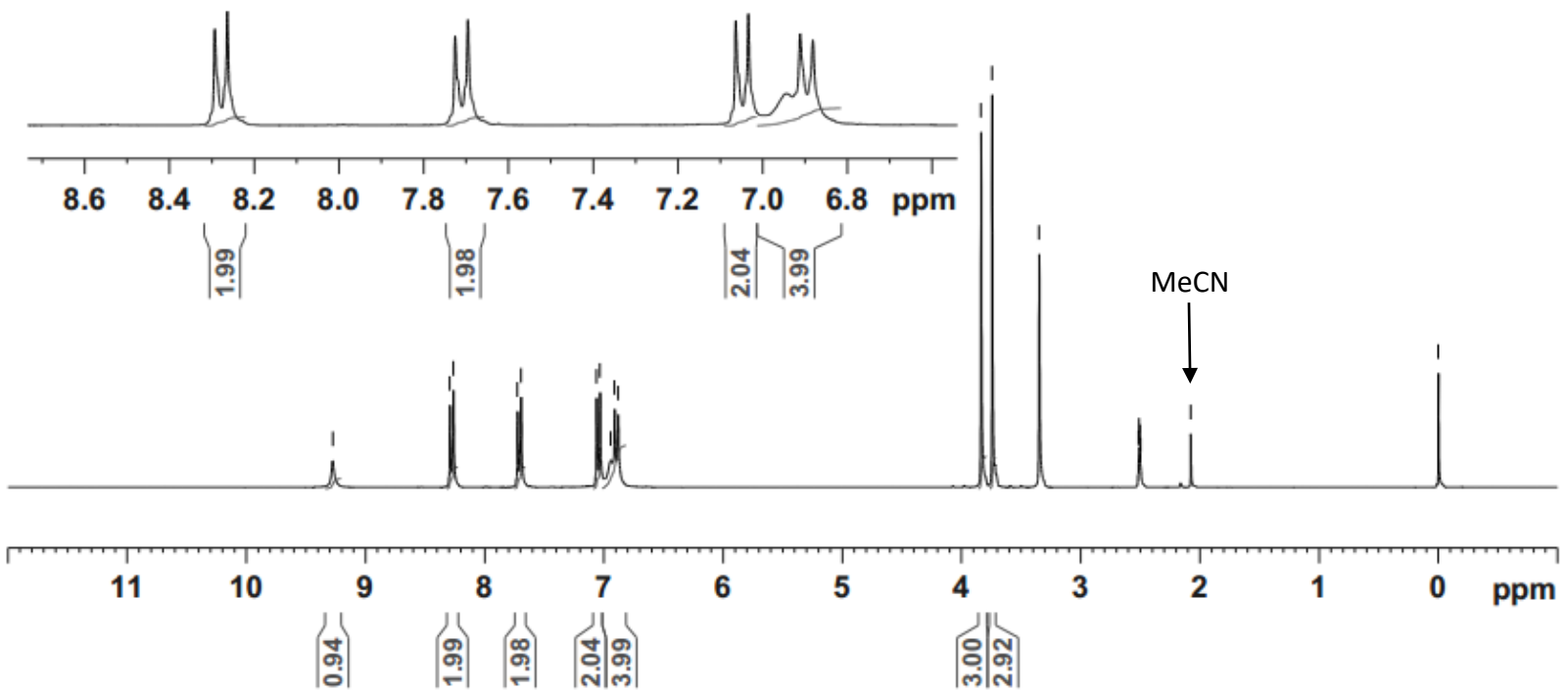
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

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

N²,6-bis(4-methoxyphenyl)-1,3,5-triazine-2,4-diamine (71)

6.90 (d, J=9.00 Hz, 2 H)
7.05 (d, J=8.94 Hz, 2 H)
7.71 (d, J=9.00 Hz, 2 H)
8.28 (d, J=8.88 Hz, 2 H)





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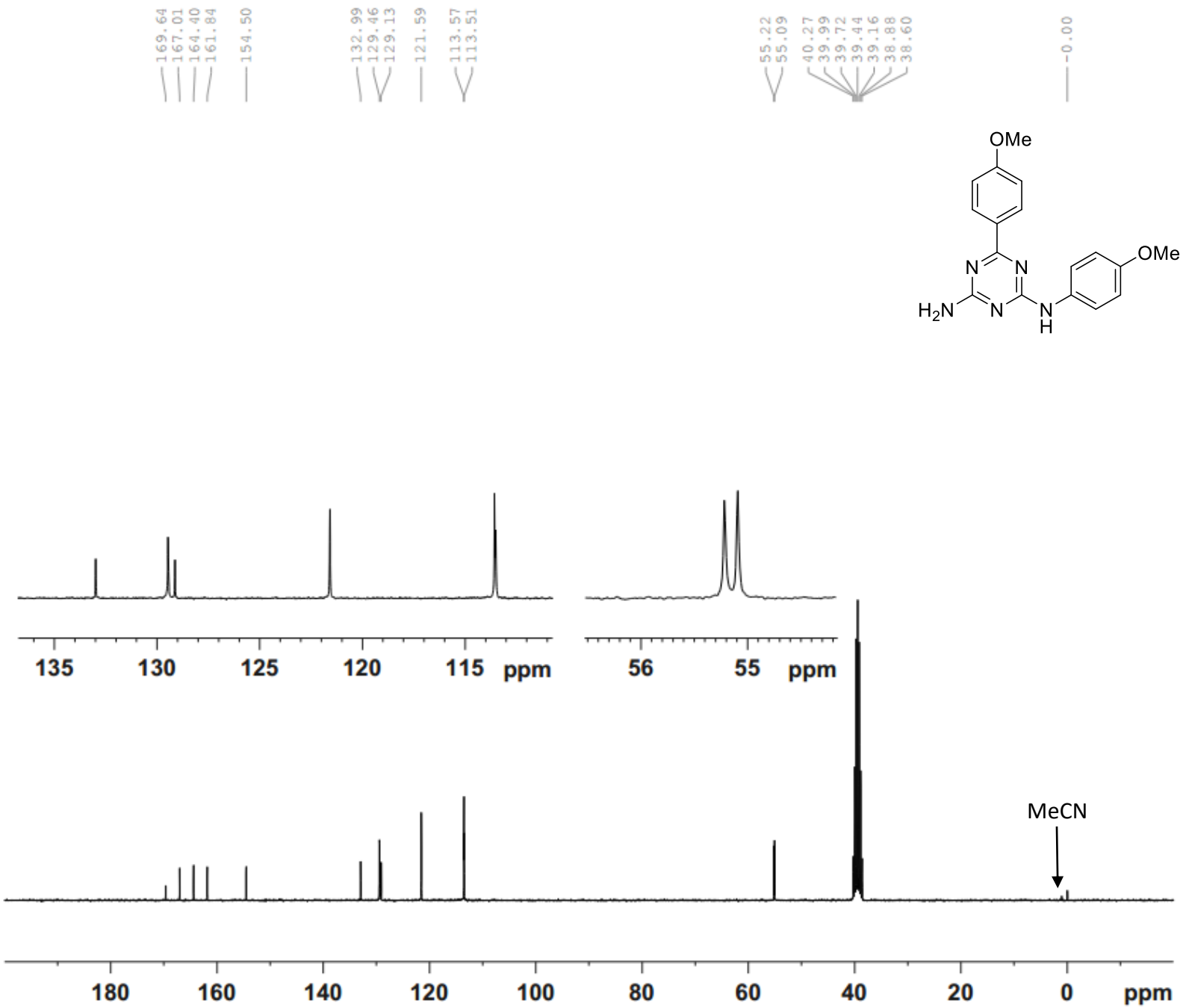
```
Current Data Parameters
NAME                  JA0004
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171029
Time                  15.31
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                    31.623
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             300.1599984 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

N²,6-bis(4-methoxyphenyl)-1,3,5-triazine-2,4-diamine (71)




```
Current Data Parameters
NAME                  JA0004
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171102
Time                   22.52
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                     65536
SOLVENT                DMSO
NS                      3072
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                    300.3 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                        3

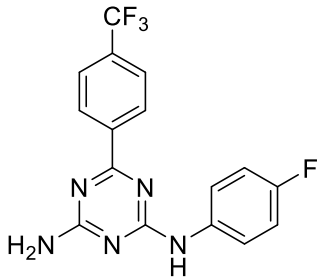
======== CHANNEL f1 ========
SFO1               75.4828392 MHz
NUC1                      13C
P1                    15.00 usec
PLW1              22.00000000 W

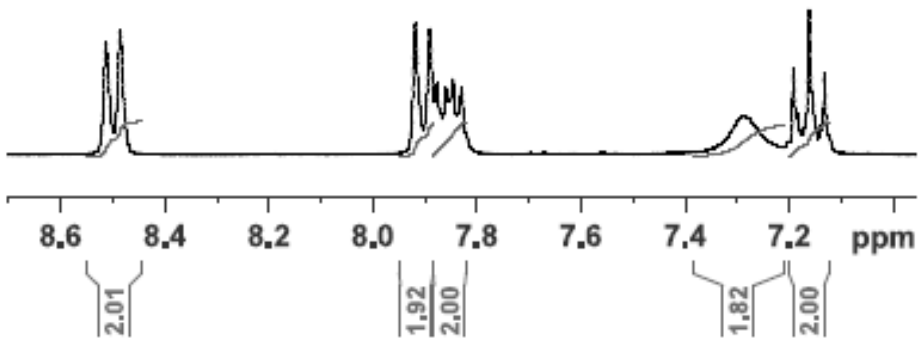
======== CHANNEL f2 ========
SFO2              300.1612006 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 98.00 usec
PLW2               9.30000019 W
PLW12              0.29359001 W
PLW13              0.20359001 W

F2 - Processing parameters
SI                        32768
SF                 75.4753334 MHz
WDW                       EM
SSB           0
LB                     1.00 Hz
GB            0
PC                     1.40
```

N^2-(4-fluorophenyl)-6-(4-(trifluoromethyl)phenyl)-1,3,5-triazine-2,4-diamine (84)

7.16 (dd, J=8.91, 8.91 Hz, 2 H)
7.85 (dd, J=5.12, 9.08 Hz, 2 H)
7.90 (d, J=8.64 Hz, 2 H)
8.50 (d, J=8.64 Hz, 2 H)





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```
Current Data Parameters
NAME                  84
EXPNO                  1
PROCNO                 1

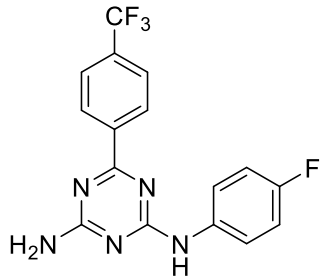
F2 - Acquisition Parameters
Date_           20180216
Time               10.05
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            6103.516 Hz
FIDRES         0.093132 Hz
AQ             5.3687091 sec
RG               67.6857
DW               81.920 usec
DE                6.50 usec
TE                300.2 K
D1           1.00000000 sec
TD0                    1

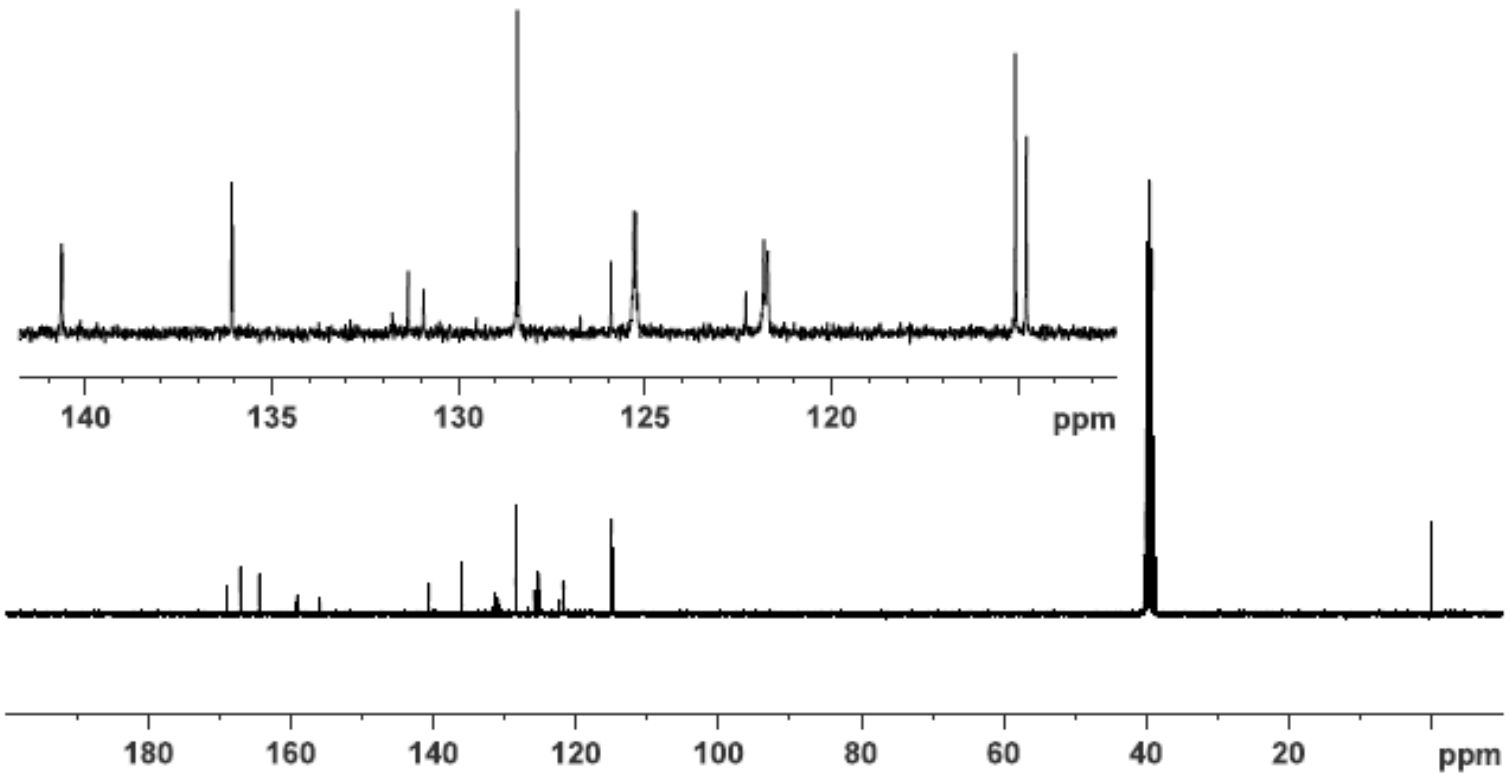
======== CHANNEL f1 ========
SFO1         300.1618536 MHz
NUC1                   1H
P1                 13.50 usec
PLW1          9.30000019 W

F2 - Processing parameters
SI                 65536
SF           300.1599959 MHz
WDW                   EM
SSB       0
LB                 0.01 Hz
GB        0
PC                 1.00
```

N²-(4-fluorophenyl)-6-(4-(trifluoromethyl)phenyl)-1,3,5-triazine-2,4-diamine (84)

114.92 (d, J=22.47 Hz, 2 C)
121.77 (d, J=7.46 Hz, 2 C)
124.13 (q, J=271.45 Hz, 1 C)
125.27 (q, J=3.73 Hz, 2 C)
131.14 (q, J=31.61 Hz, 1 C)
136.07 (d, J=2.23 Hz, 1 C)
140.64 (q, J=1.49 Hz, 2 C)
157.57 (d, J=238.84 Hz, 1 C)





BRUKER

```
Current Data Parameters
NAME                  84
EXPNO                  2
PROCNO                 1

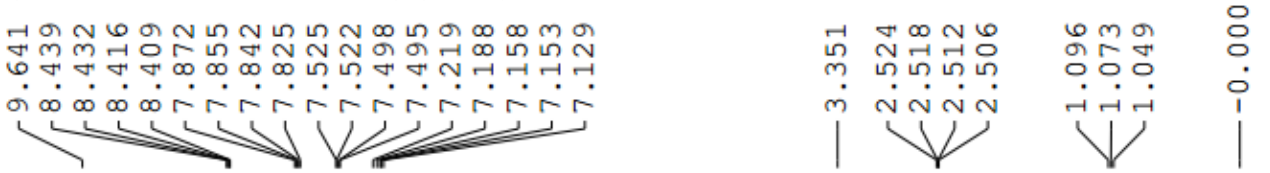
F2 - Acquisition Parameters
Date_           20180216
Time_              10.11
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                65536
SOLVENT            DMSO
NS                 3072
DS                    4
SWH           24414.063 Hz
FIDRES         0.372529 Hz
AQ             1.3421773 sec
RG               501.187
DW                20.480 usec
DE                 6.50 usec
TE                300.3 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                   3

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

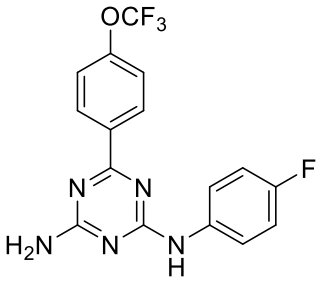
======== CHANNEL f2 ========
SFO2        300.1612006 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             98.00 usec
PLW2         9.30000019 W
PLW12        0.29359001 W
PLW13        0.20359001 W

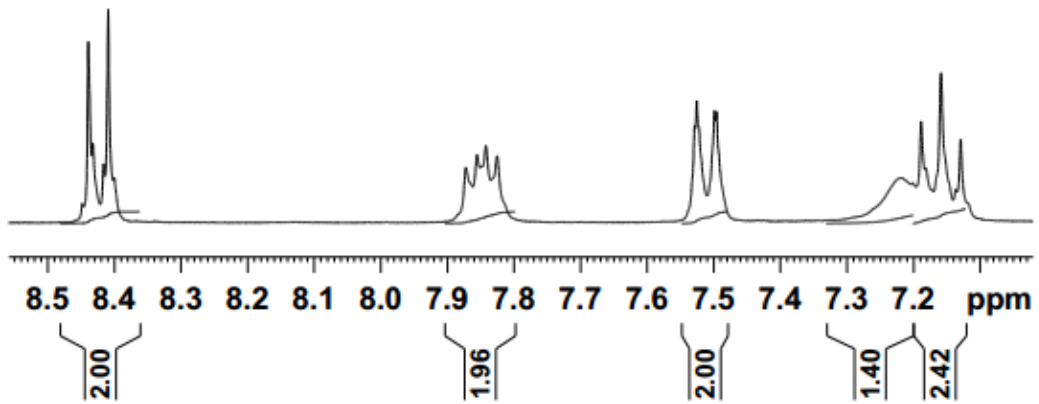
F2 - Processing parameters
SI                32768
SF           75.4753305 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                1.40
```

N^2-(4-fluorophenyl)-6-(4-(trifluoromethoxy)phenyl)-1,3,5-triazine-2,4-diamine (91)



7.16 (dd, J=8.90, 8.90 Hz, 2 H)
7.51 (d, J=8.04 Hz, 2 H)
7.85 (dd, J=5.01, 9.03 Hz, 2 H)
8.42 (d, J=8.94 Hz, 2 H)





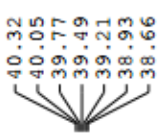

```
Current Data Parameters
NAME                  JA0205
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180218
Time                  17.50
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                   60.6025
DW                   81.920 usec
DE                    6.50 usec
TE                   300.1 K
D1                 1.00000000 sec
TD0                        1

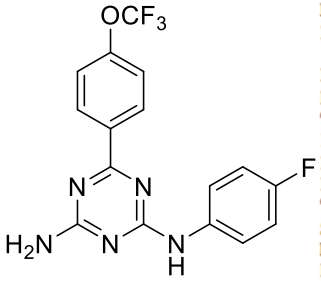
======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1            9.30000019 W

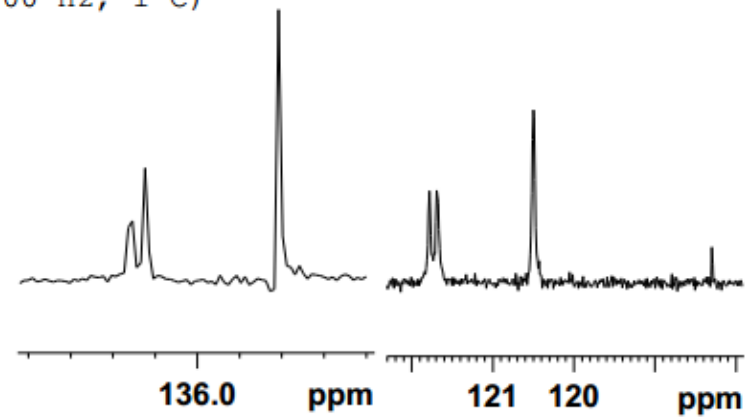
F2 - Processing parameters
SI                    65536
SF             300.1599958 MHz
WDW                       EM
SSB       0
LB                    0.10 Hz
GB        0
PC                    1.00
```

N²-(4-fluorophenyl)-6-(4-(trifluoromethoxy)phenyl)-1,3,5-triazine-2,4-diamine (91)



114.91 (d, J=22.13 Hz, 2 C)
116.73 (q, J=248.60 Hz, 1 C)
121.74 (d, J=7.40 Hz, 2 C)
136.14 (d, J=2.23 Hz, 1 C)
150.56 (q, J=1.49 Hz, 1 C)
157.54 (d, J=239.00 Hz, 1 C)






```
Current Data Parameters
NAME                  JA0205
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180219
Time                   2.54
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     3072
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                    300.3 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                        3

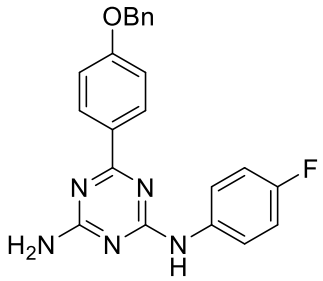
======== CHANNEL f1 ========
SFO1               75.4828392 MHz
NUC1                      13C
P1                    15.00 usec
PLW1              22.00000000 W

======== 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

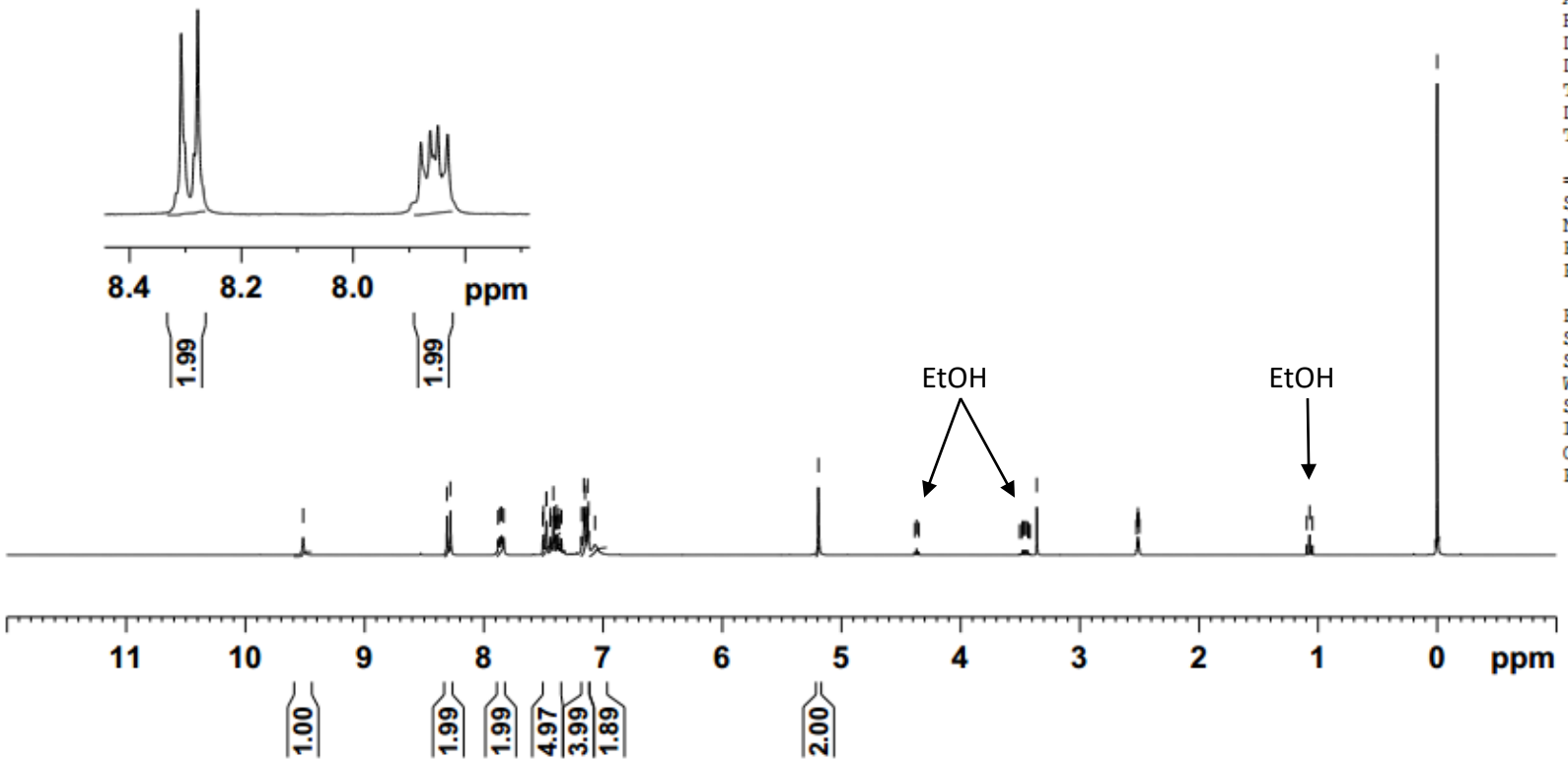
F2 - Processing parameters
SI                        32768
SF                 75.4753298 MHz
WDW                       EM
SSB           0
LB            0 Hz
GB            0
PC                     1.40
```

6-(4-(benzyloxy)phenyl)-N²-(4-fluorophenyl)-1,3,5-triazine-2,4-diamine (111)

9.515 8.307 8.278 8.879 7.862 7.848 7.832 7.503 7.498 7.475 7.471 7.441 7.437 7.414 7.409 7.394 7.389 7.376 7.370 7.365 7.347 7.178 7.158 7.149 7.135 7.128 7.119 7.065 5.191 4.383 4.366 4.349 3.478 3.461 3.455 3.438 3.432 3.358 2.522 2.516 2.510 2.504 2.498 1.093 1.070 1.047 -0.000



7.86 (dd, J=5.03, 9.14 Hz, 2 H)
8.29 (d, J=8.94 Hz, 2 H)



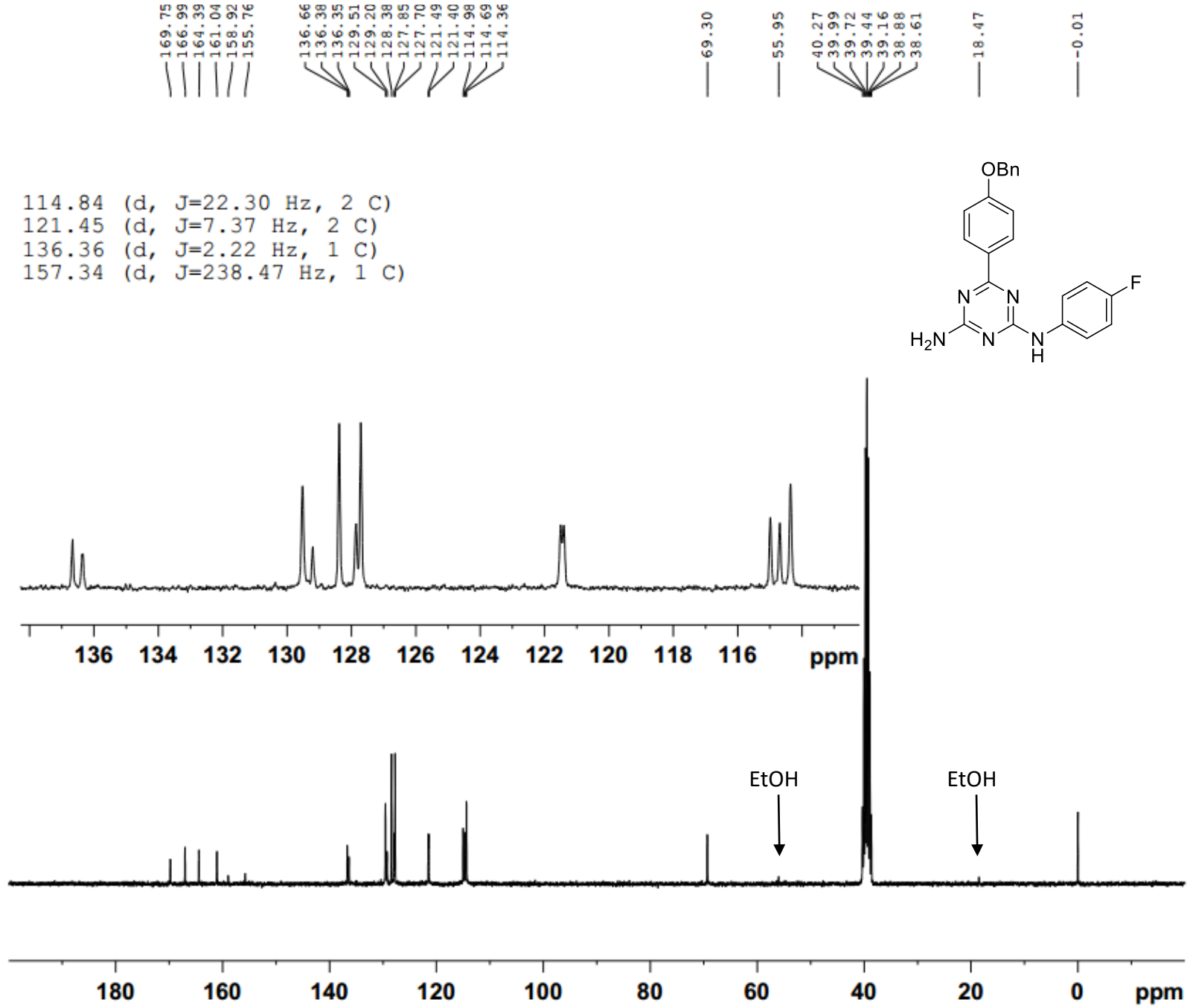
Current Data Parameters
NAME JA0253
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190410
Time 14.51
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 31.623
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 300.1599978 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

6-(4-(benzyloxy)phenyl)-N²-(4-fluorophenyl)-1,3,5-triazine-2,4-diamine (111)



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```
Current Data Parameters
NAME                  JA0253
EXPNO                      6
PROCNO                     1

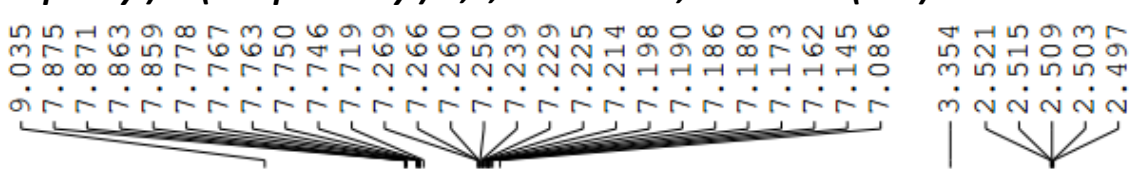
F2 - Acquisition Parameters
Date_              20190410
Time                  16.32
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    298.3 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                        3

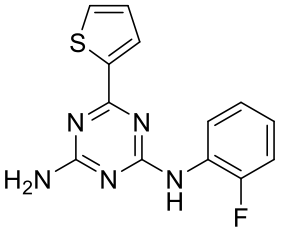
======== CHANNEL f1 ========
SFO1               75.4828392 MHz
NUC1                      13C
P1                    15.00 usec
PLW1              22.00000000 W

======== 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

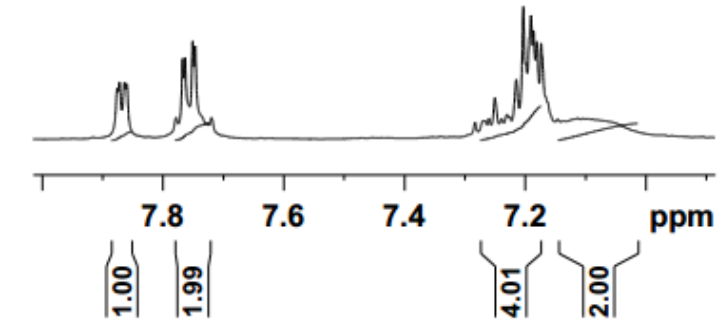
F2 - Processing parameters
SI                        32768
SF                 75.4753335 MHz
WDW                          EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

N^2-(2-fluorophenyl)-6-(thiophen-2-yl)-1,3,5-triazine-2,4-diamine (116)





7.87 (dd, J=1.14, 3.63 Hz, 1 H)



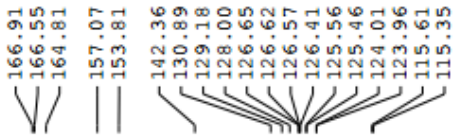

```
Current Data Parameters
NAME                  JA0283
EXPNO                      5
PROCNO                     1

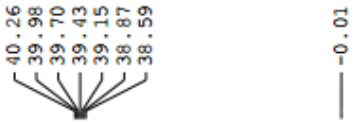
F2 - Acquisition Parameters
Date_              20190410
Time                 14.47
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                    50.413
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

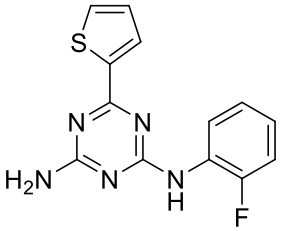
F2 - Processing parameters
SI                    65536
SF             300.1599980 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

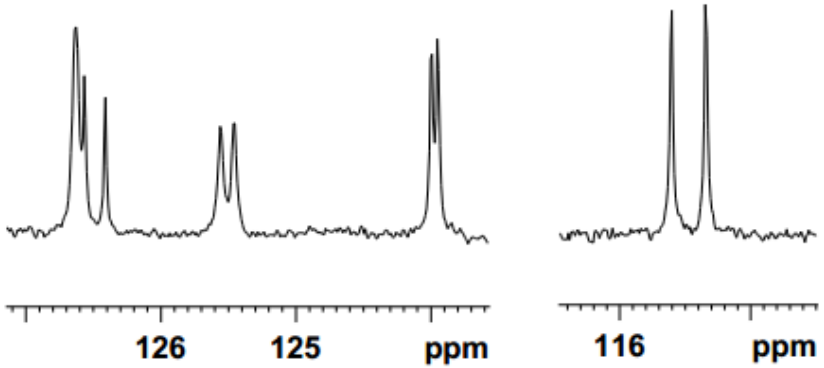
N²-(2-fluorophenyl)-6-(thiophen-2-yl)-1,3,5-triazine-2,4-diamine (116)





115.48 (d, J=19.37 Hz, 1 C)
123.98 (d, J=3.70 Hz, 1 C)
125.51 (d, J=7.56 Hz, 1 C)
126.49 (d, J=11.93 Hz, 1 C)
126.64 (d, J=2.24 Hz, 1 C)
155.44 (d, J=246.25 Hz, 1 C)






```
Current Data Parameters
NAME                  JA0283
EXPNO                      6
PROCNO                     1

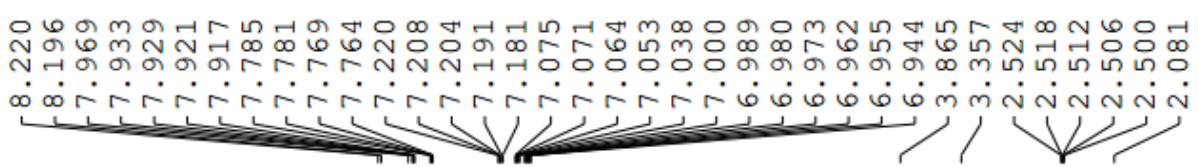
F2 - Acquisition Parameters
Date_              20190410
Time                  22.28
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   298.3 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                        3

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

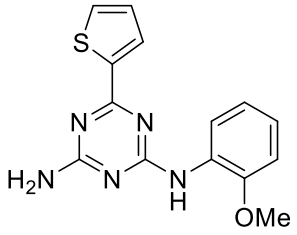
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 98.00 usec
PLW2             9.30000019 W
PLW12            0.29359001 W
PLW13            0.20359001 W

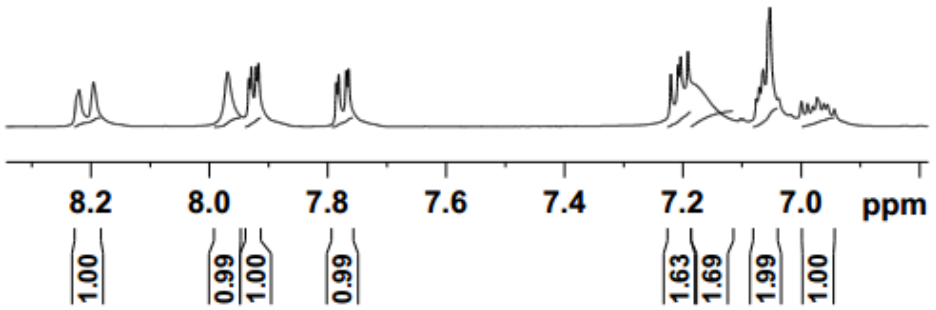
F2 - Processing parameters
SI                     32768
SF              75.4753342 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

N^2-(2-methoxyphenyl)-6-(thiophen-2-yl)-1,3,5-triazine-2,4-diamine (122)



7.21 (dd, J=3.69, 4.98 Hz, 1 H)
7.77 (dd, J=1.23, 4.98 Hz, 1 H)
7.92 (dd, J=1.26, 3.66 Hz, 1 H)
8.21 (d, J=7.32 Hz, 1 H)





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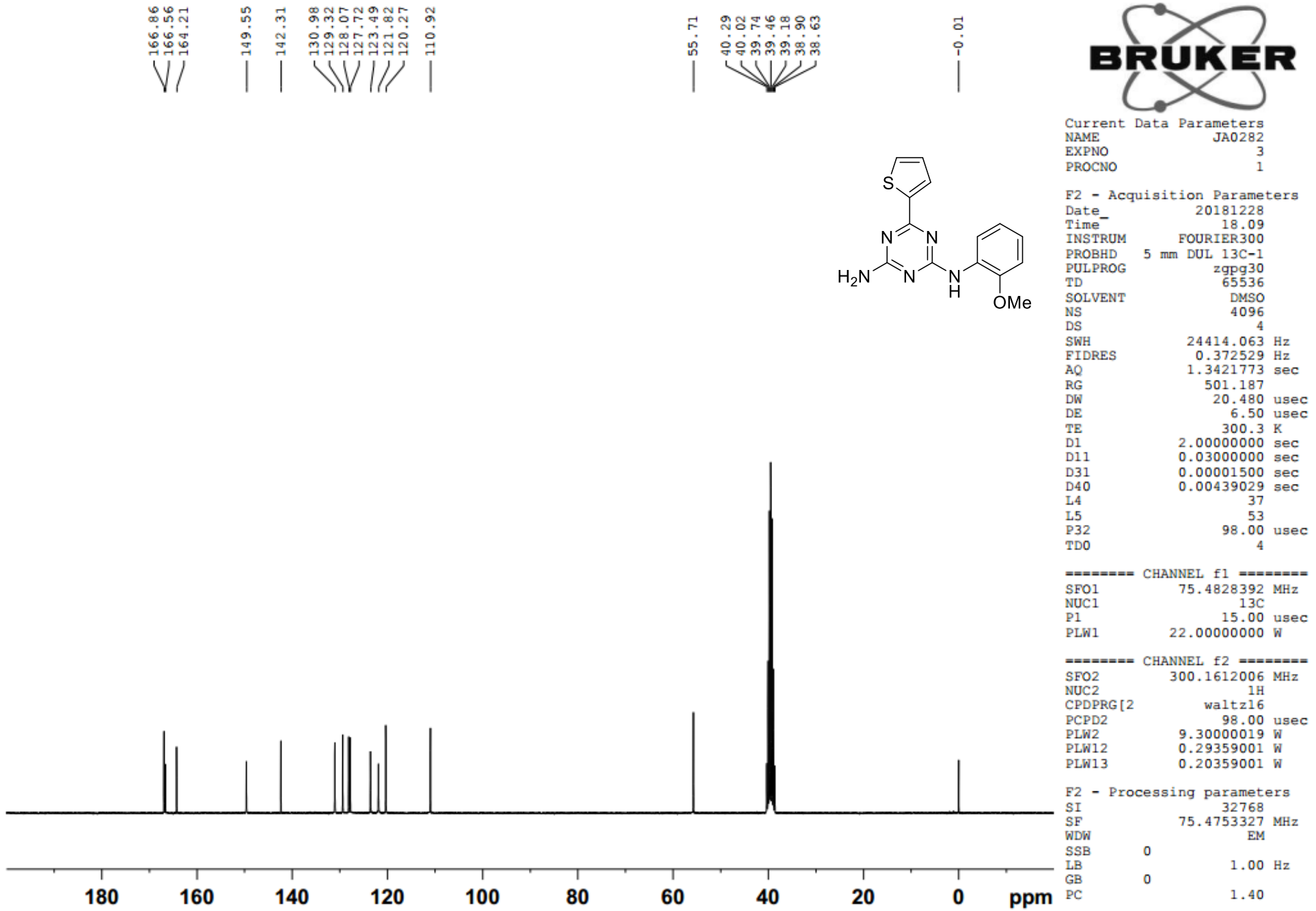
```
Current Data Parameters
NAME                  JA0282
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20181227
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                    31.623
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              300.1599976 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N²-(2-methoxyphenyl)-6-(thiophen-2-yl)-1,3,5-triazine-2,4-diamine (122)



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```
Current Data Parameters
NAME                  JA0282
EXPNO                      3
PROCNO                     1

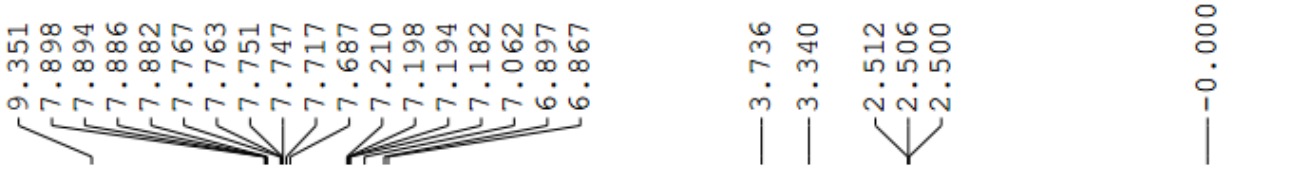
F2 - Acquisition Parameters
Date_              20181228
Time                  18.09
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     4096
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.3 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                       4

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

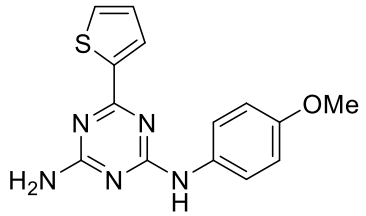
======== CHANNEL f2 ========
SFO2            300.1612006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 98.00 usec
PLW2              9.30000019 W
PLW12             0.29359001 W
PLW13             0.20359001 W

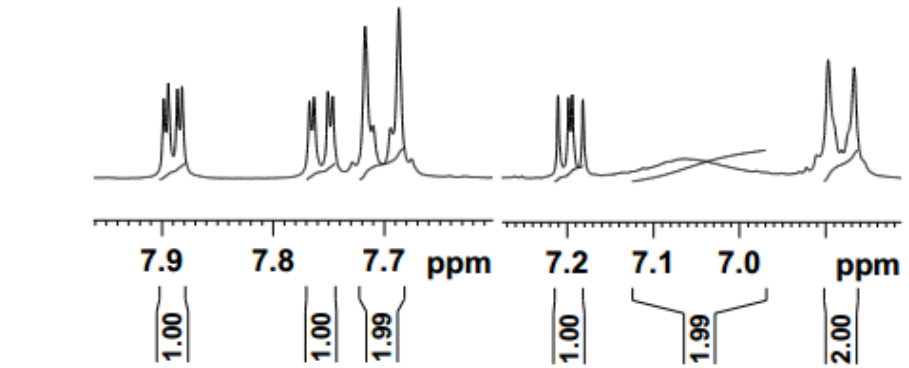
F2 - Processing parameters
SI                    32768
SF               75.4753327 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

N²-(4-methoxyphenyl)-6-(thiophen-2-yl)-1,3,5-triazine-2,4-diamine (123)



6.88 (d, J=9.03 Hz, 2 H)
7.20 (dd, J=3.69, 4.98 Hz, 1 H)
7.70 (d, J=9.09 Hz, 2 H)
7.76 (dd, J=1.25, 5.00 Hz, 1 H)
7.89 (dd, J=1.28, 3.68 Hz, 1 H)





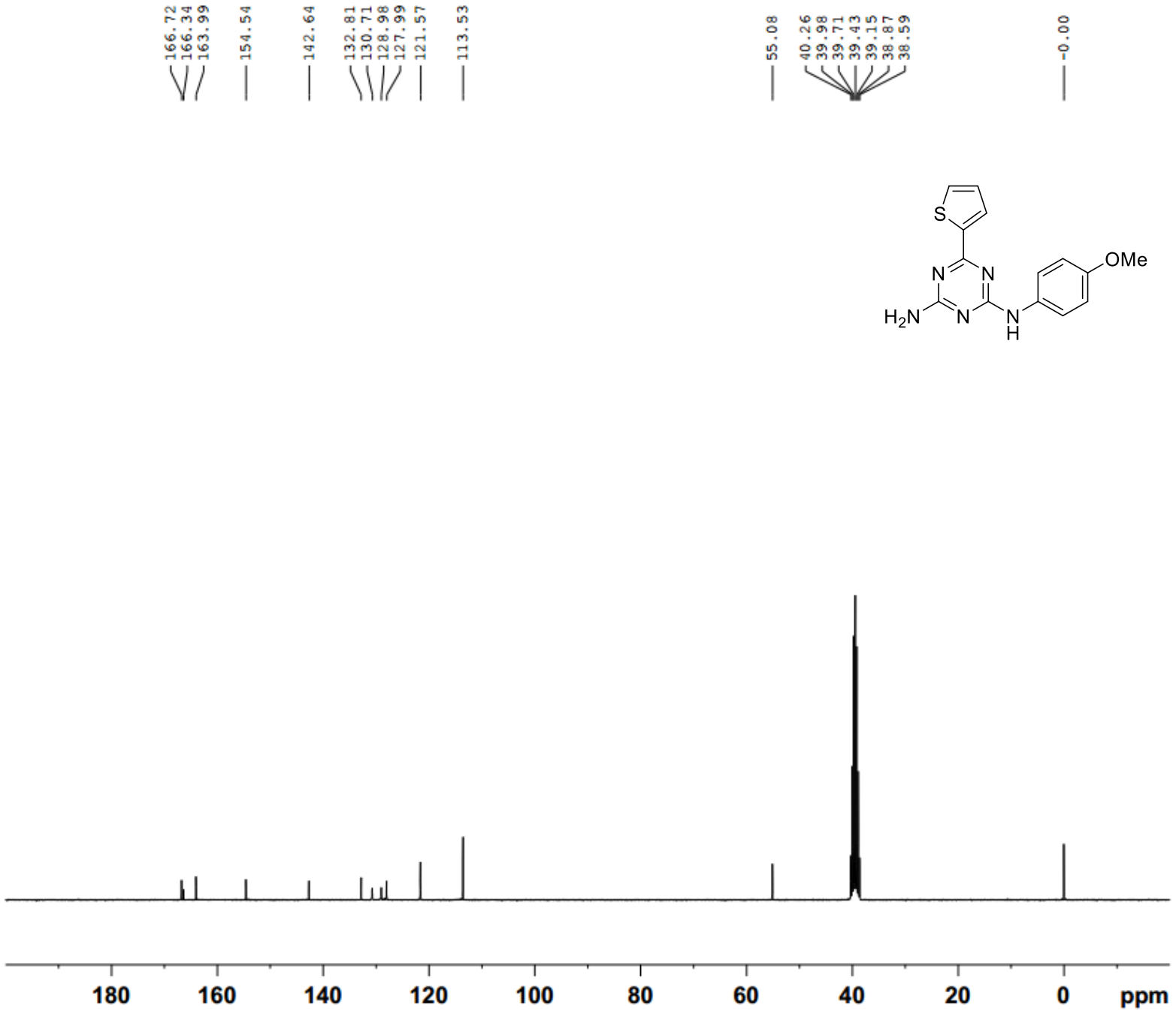

```
Current Data Parameters
NAME                  JA0276
EXPNO                      6
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190410
Time               14.42
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                 66.0182
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                 300.1599989 MHz
WDW                EM
SSB        0
LB                 0.30 Hz
GB         0
PC                 1.00
```

N²-(4-methoxyphenyl)-6-(thiophen-2-yl)-1,3,5-triazine-2,4-diamine (123)



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```
Current Data Parameters
NAME                  JA0276
EXPNO                      7
PROCNO                     1

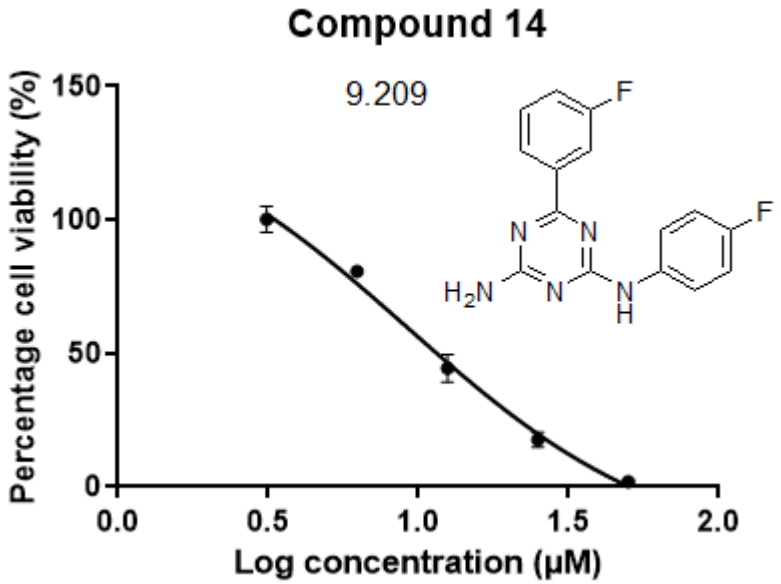
F2 - Acquisition Parameters
Date_              20190411
Time                   1.26
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     5120
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   298.3 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                        5

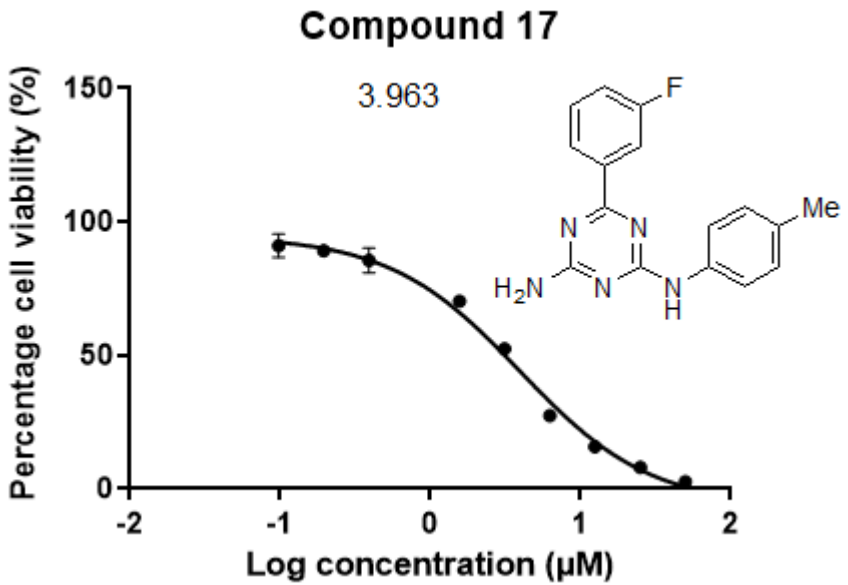
======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                    15.00 usec
PLW1          22.00000000 W

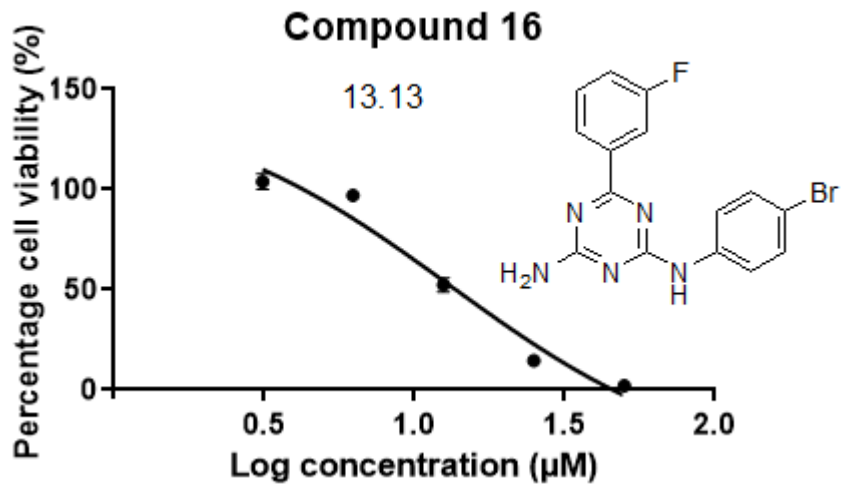
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

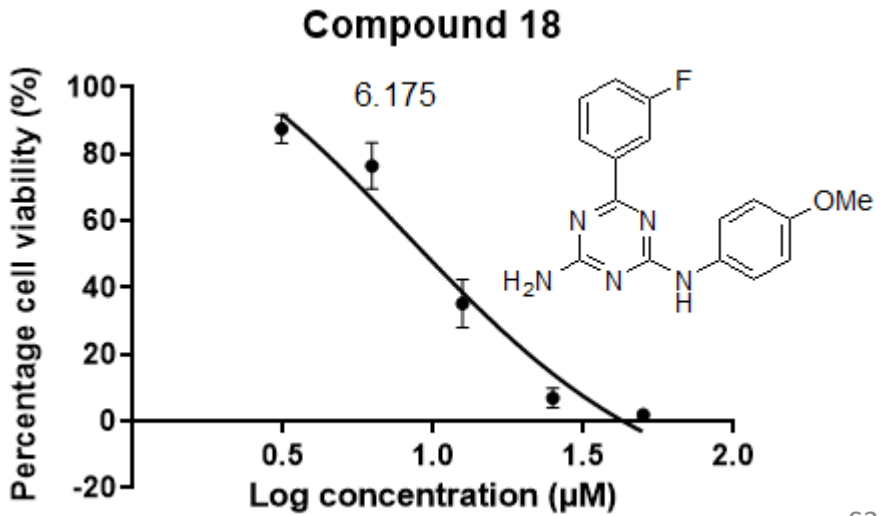
F2 - Processing parameters
SI                    32768
SF              75.4753342 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

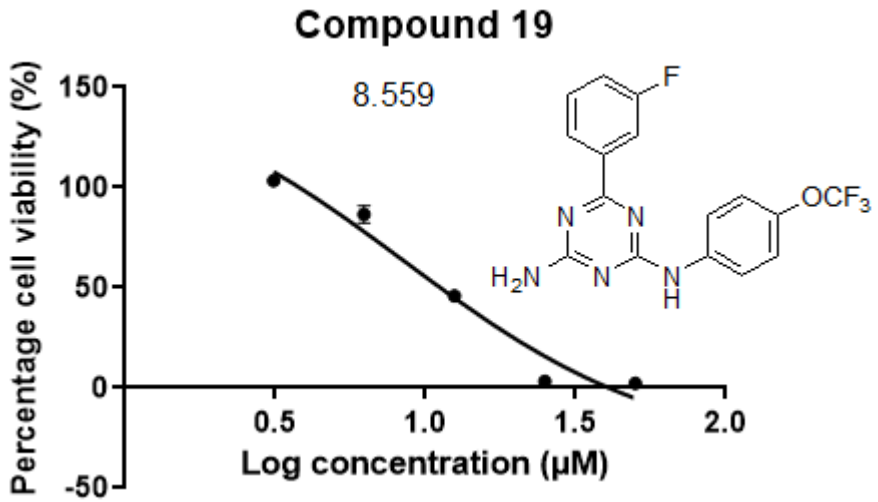
Concentration-response curves for the most active compounds
(**14**, **16-19**, **36**, **56**, **58**, **61**, **62**, **70**, **73**, **74**, **77**, **78**, **81**, **95**, **99**, **100-103**, **110**, **120**, and **121**)
tested against MDA-MB231 breast cancer cells

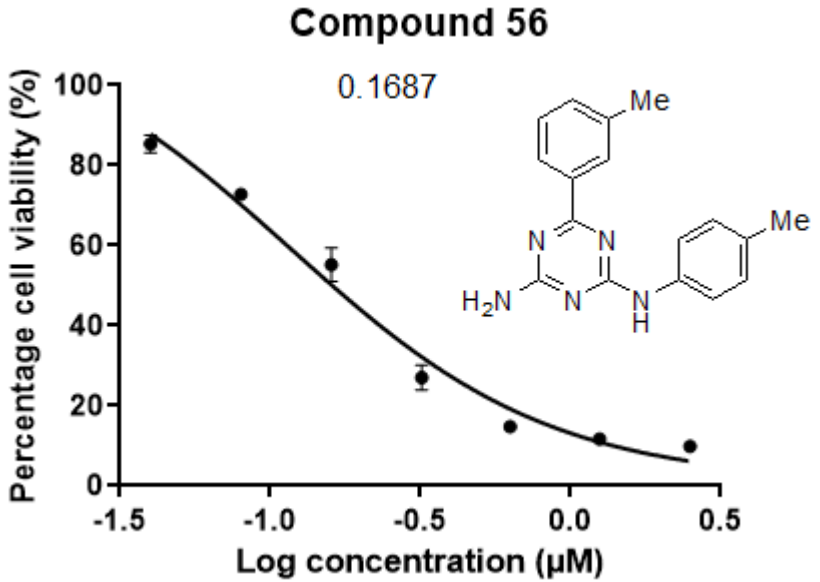

Compound 14
9.209
Percentage cell viability (%)
150
100
50
0
0.0
0.5
1.0
1.5
2.0
Log concentration (μM)
F
F
N
N
N
N
H
H2N

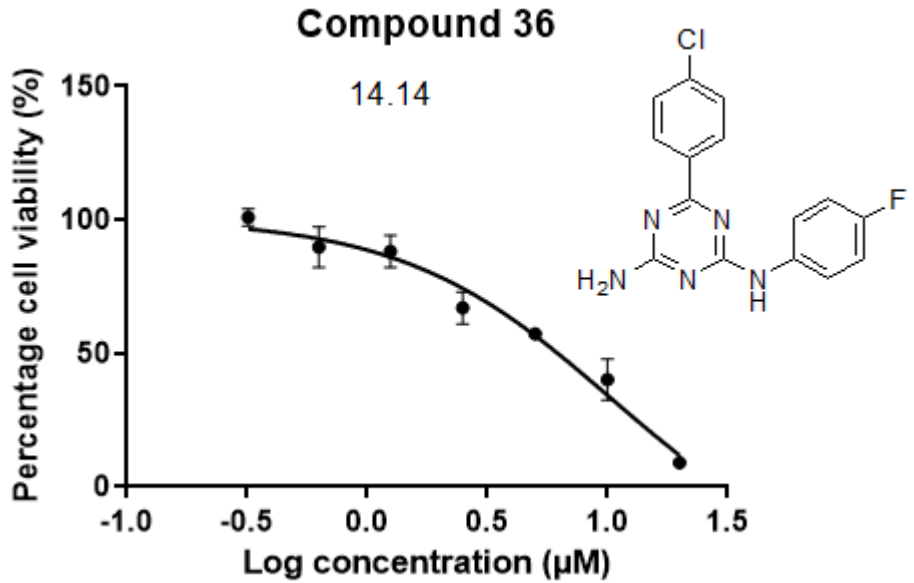

Compound 17
3.963
Percentage cell viability (%)
150
100
50
0
-2
-1
0
1
2
Log concentration (μM)
F
Me
N
N
N
N
H
H2N

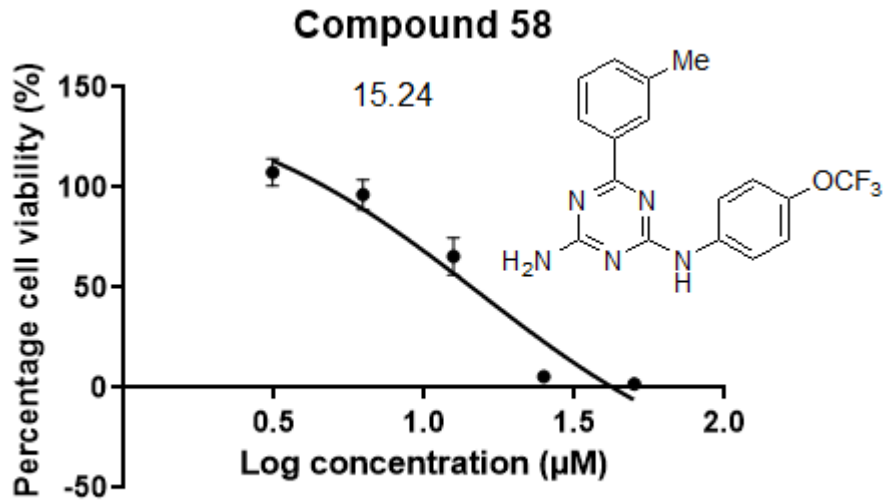

Compound 16
13.13
Percentage cell viability (%)
150
100
50
0
0.5
1.0
1.5
2.0
Log concentration (μM)
F
Br
N
N
N
N
H
H2N

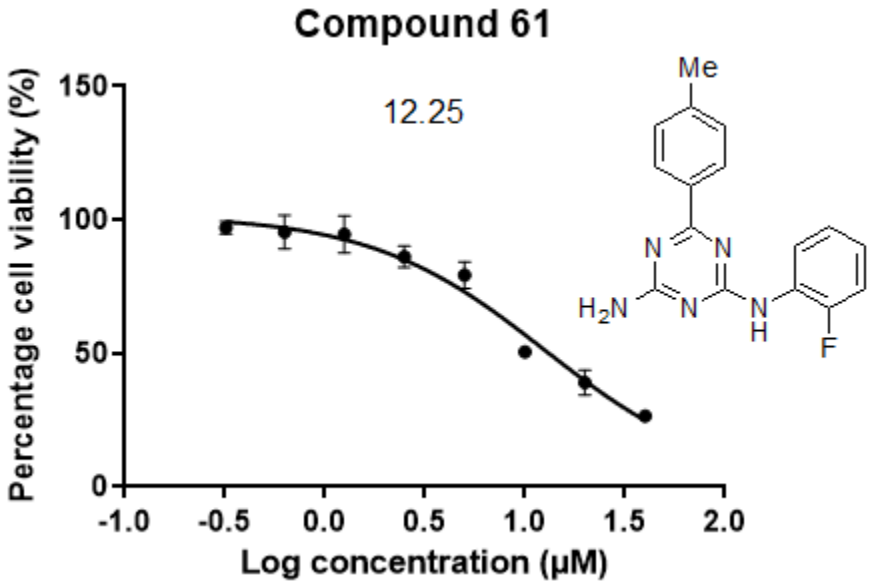

Compound 18
6.175
Percentage cell viability (%)
100
80
60
40
20
0
-20
0.5
1.0
1.5
2.0
Log concentration (μM)
F
OMe
N
N
N
N
H
H2N

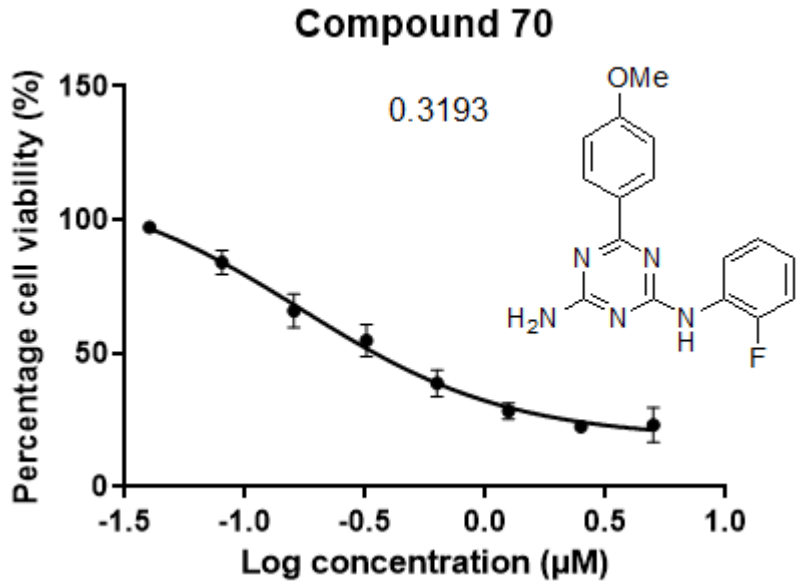

Compound 19
8.559
Percentage cell viability (%)
Log concentration (μM)
F
OCF3
H2N

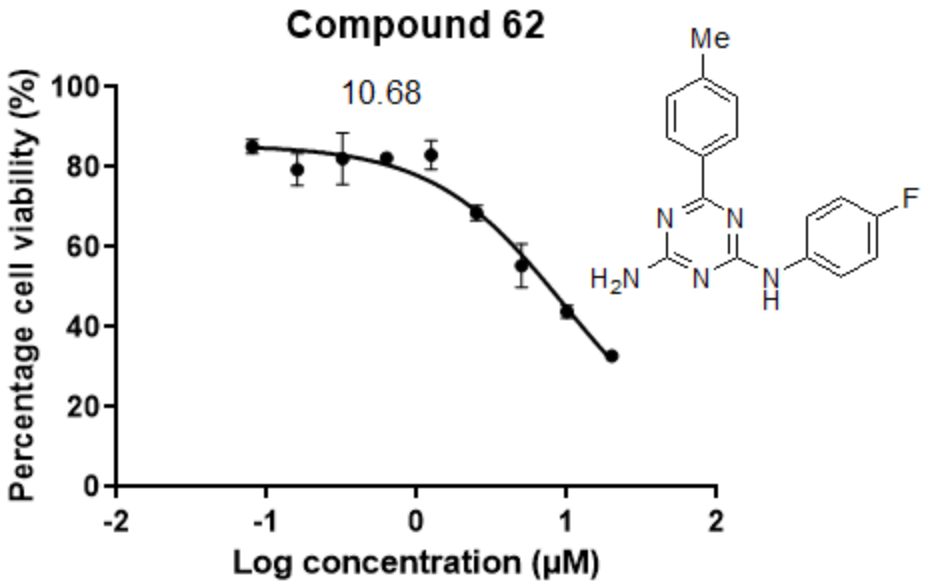

Compound 56
0.1687
Percentage cell viability (%)
Log concentration (μM)
Me
Me
H2N

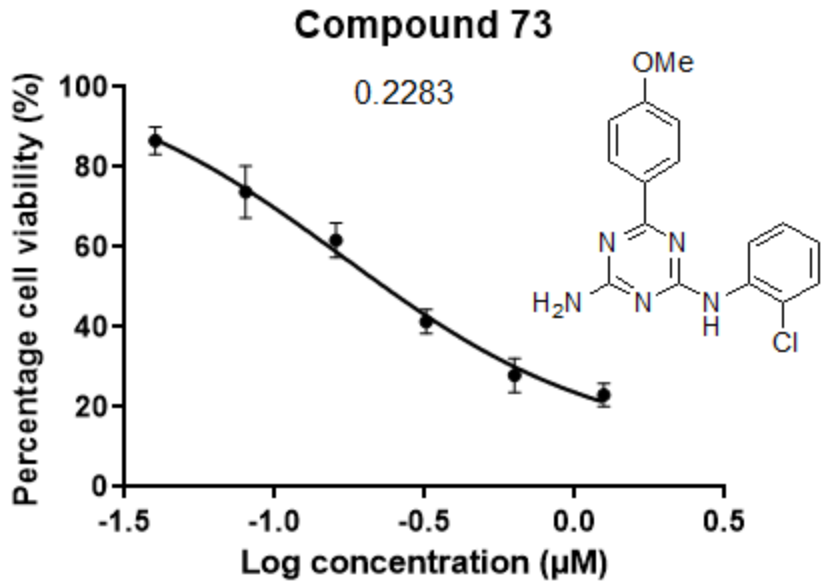

Compound 36
14.14
Percentage cell viability (%)
Log concentration (μM)
Cl
F
H2N

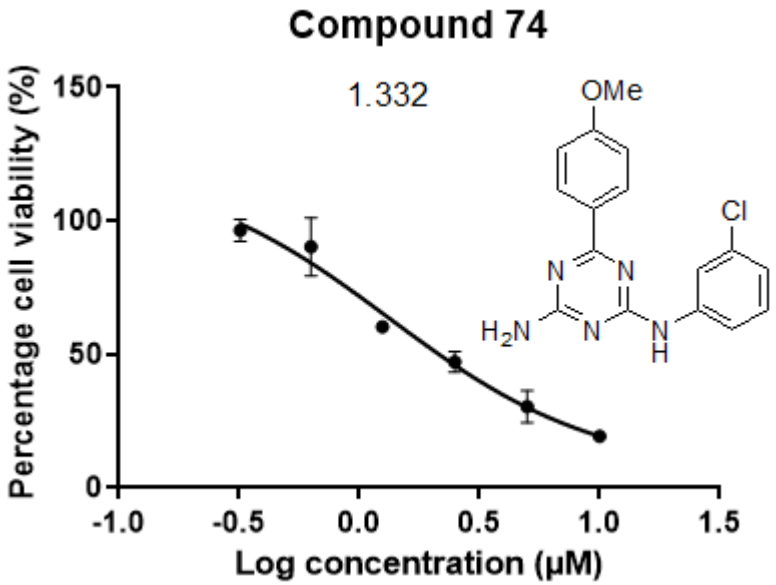

Compound 58
15.24
Percentage cell viability (%)
Log concentration (μM)
Me
OCF3
H2N

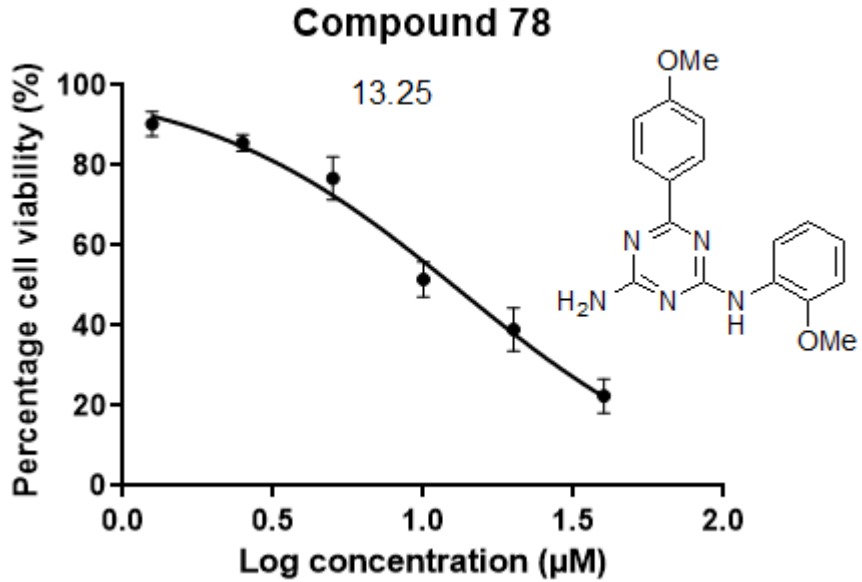

Compound 61
12.25
Me
N
N
H2N
N
N
H
F
Percentage cell viability (%)
150
100
50
0
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
Log concentration (μM)

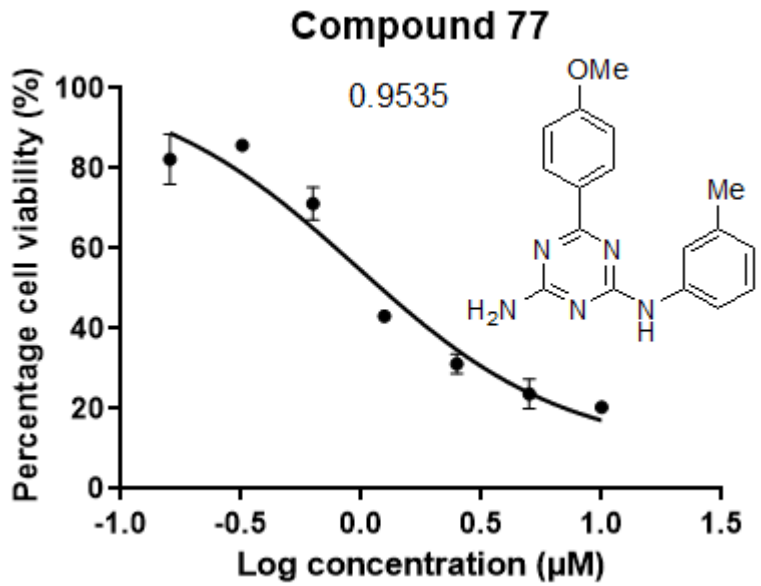

Compound 70
0.3193
OMe
N
N
H2N
N
N
H
F
Percentage cell viability (%)
150
100
50
0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Log concentration (μM)

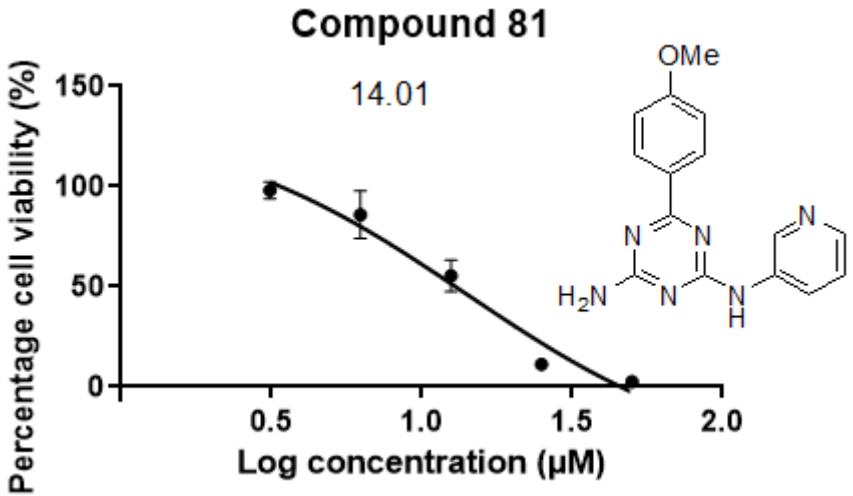

Compound 62
10.68
Me
N
N
H2N
N
N
H
F
Percentage cell viability (%)
100
80
60
40
20
0
-2
-1
0
1
2
Log concentration (μM)

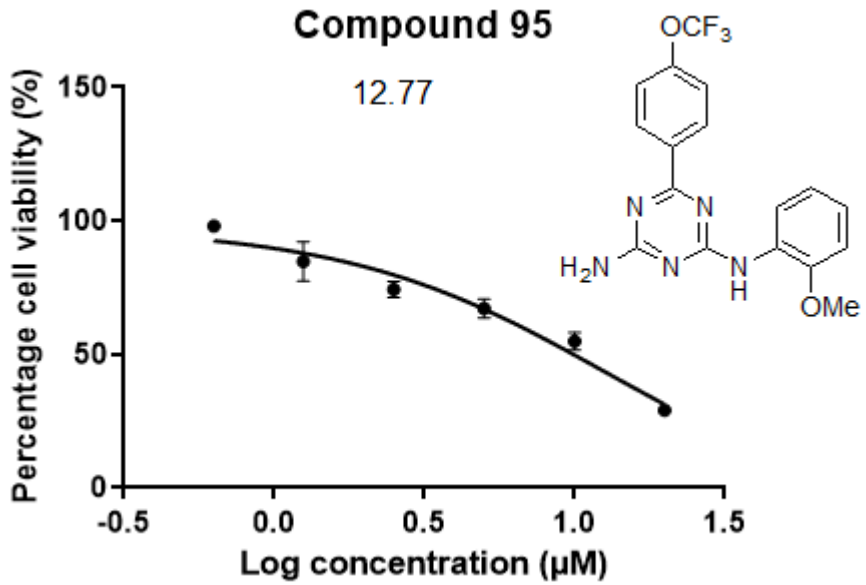

Compound 73
0.2283
OMe
N
N
H2N
N
N
H
Cl
Percentage cell viability (%)
100
80
60
40
20
0
-1.5
-1.0
-0.5
0.0
0.5
Log concentration (μM)

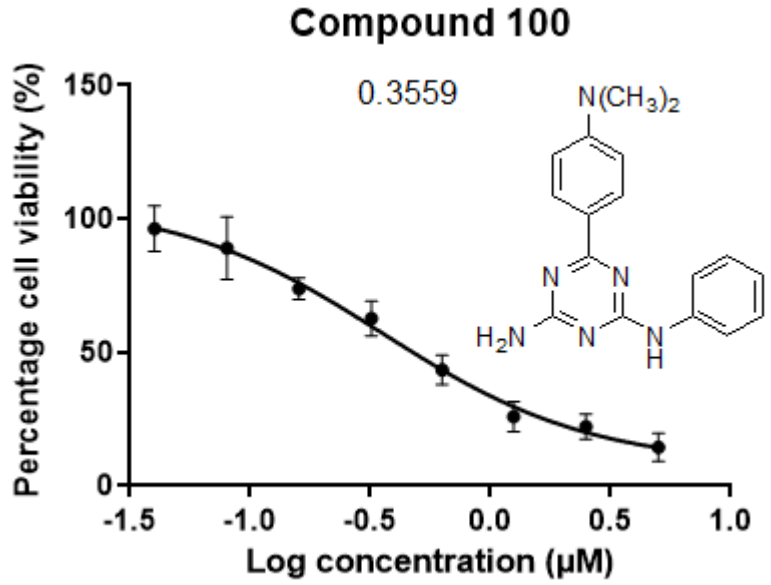

Compound 74
1.332
OMe
Cl
Percentage cell viability (%)
Log concentration (μM)

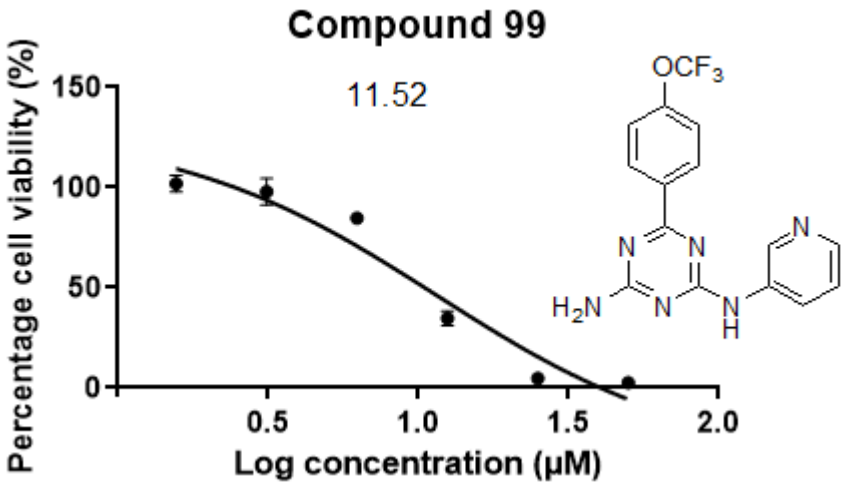

Compound 78
13.25
OMe
OMe
Percentage cell viability (%)
Log concentration (μM)

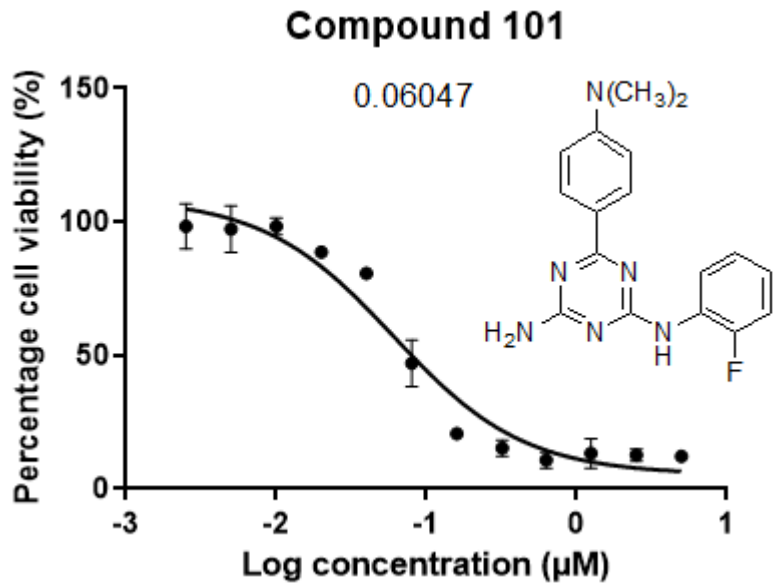

Compound 77
0.9535
OMe
Me
Percentage cell viability (%)
Log concentration (μM)

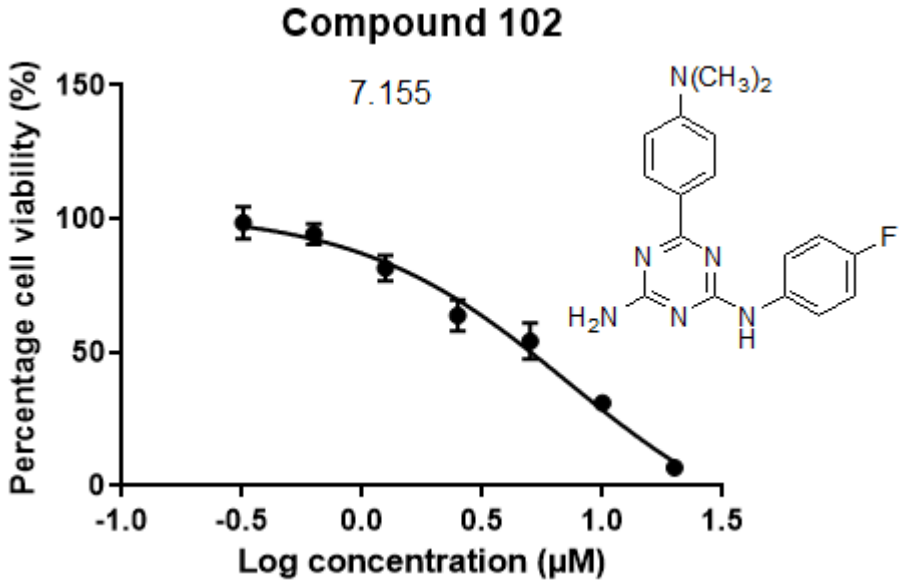

Compound 81
14.01
OMe
Percentage cell viability (%)
Log concentration (μM)

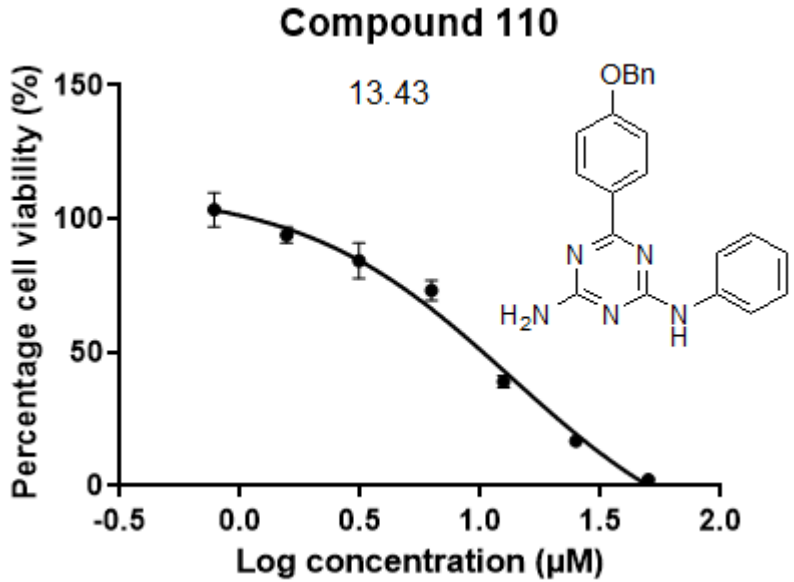

Compound 95
12.77
OCF3
N
N
H2N
N
N
H
OMe
Percentage cell viability (%)
150
100
50
0
-0.5
0.0
0.5
1.0
1.5
Log concentration (μM)

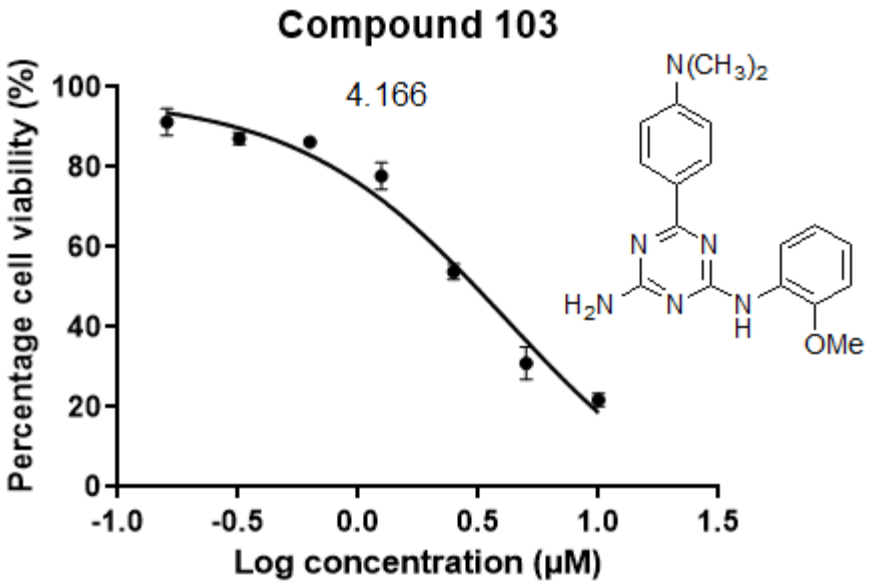

Compound 100
0.3559
N(CH3)2
N
N
H2N
N
N
H
Percentage cell viability (%)
150
100
50
0
-1.5
-1.0
-0.5
0.0
0.5
1.0
Log concentration (μM)

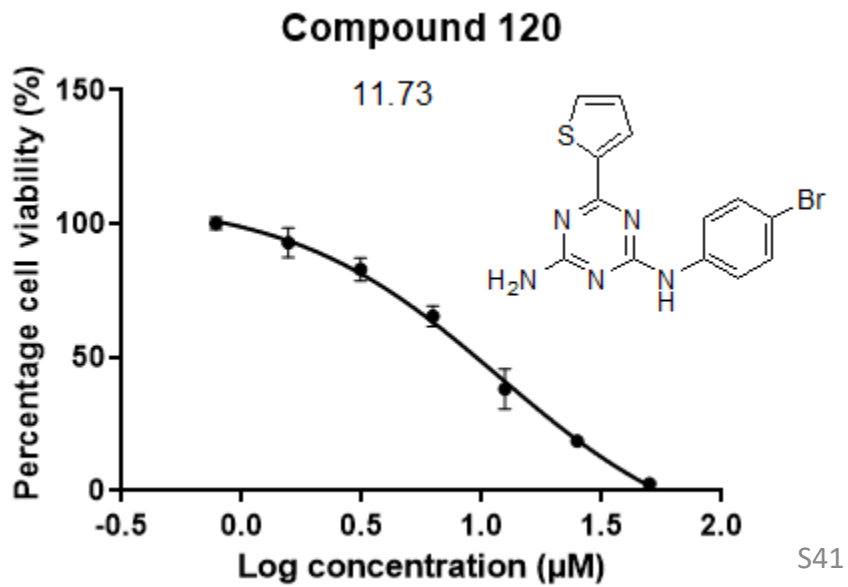

Compound 99
11.52
OCF3
N
N
H2N
N
N
H
N
Percentage cell viability (%)
150
100
50
0
0.5
1.0
1.5
2.0
Log concentration (μM)

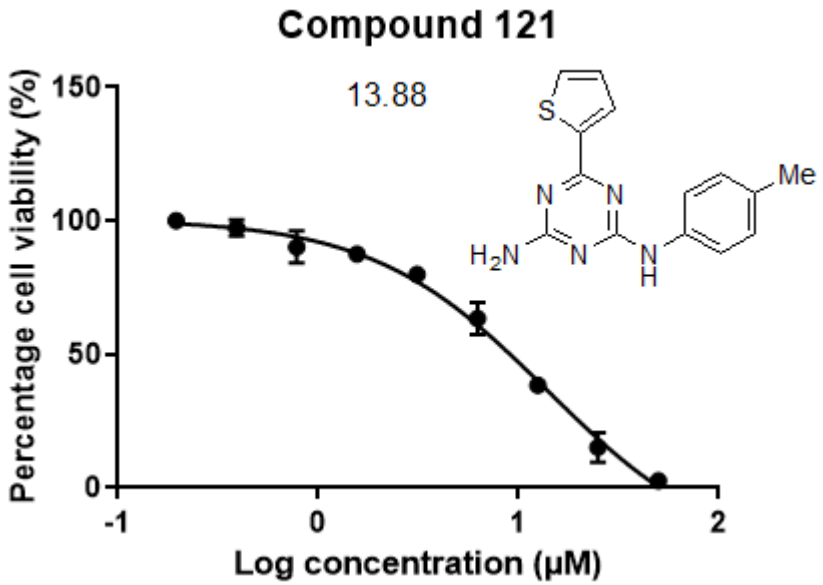

Compound 101
0.06047
N(CH3)2
N
N
H2N
N
N
H
F
Percentage cell viability (%)
150
100
50
0
-3
-2
-1
0
1
Log concentration (μM)

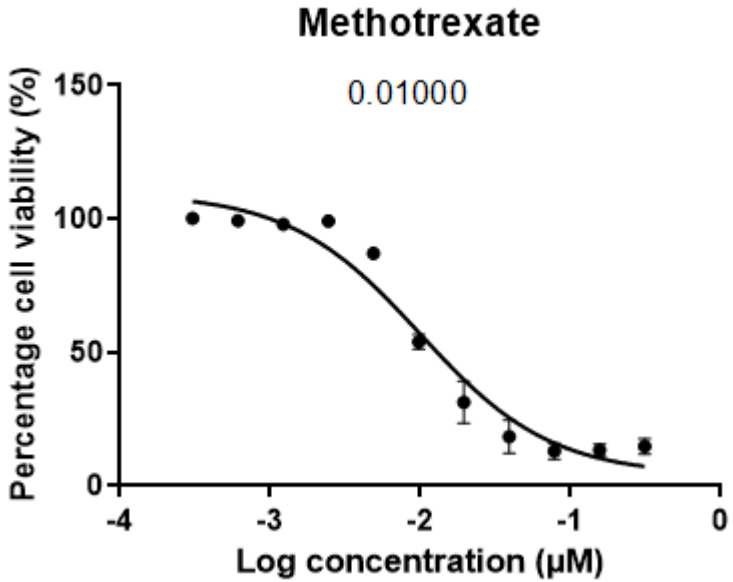

Compound 102
7.155
Percentage cell viability (%)
Log concentration (μM)
N(CH3)2
F
H2N
N
H

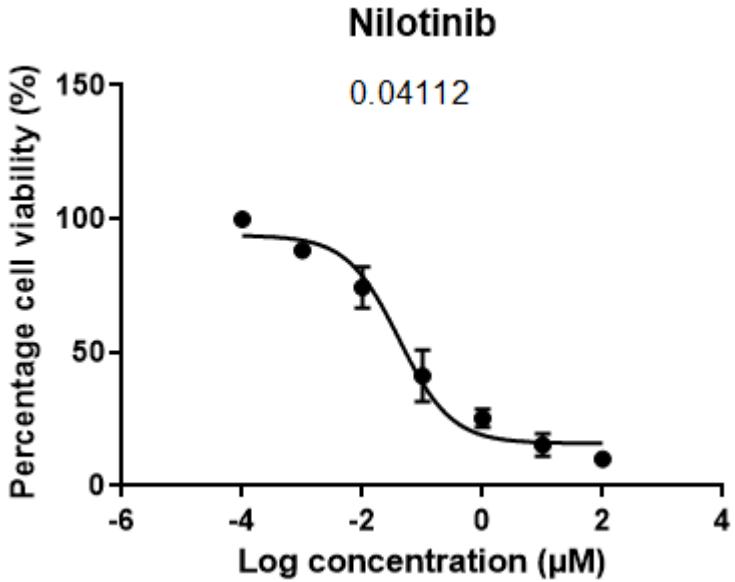

Compound 110
13.43
Percentage cell viability (%)
Log concentration (μM)
OBn
H2N
N
H


Compound 103
4.166
Percentage cell viability (%)
Log concentration (μM)
N(CH3)2
H2N
N
H
OMe

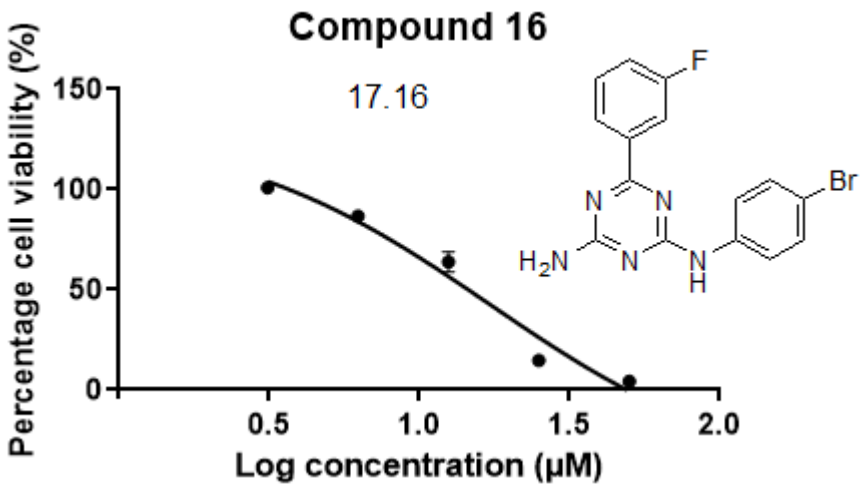

Compound 120
11.73
Percentage cell viability (%)
Log concentration (μM)
S
Br
H2N
N
H

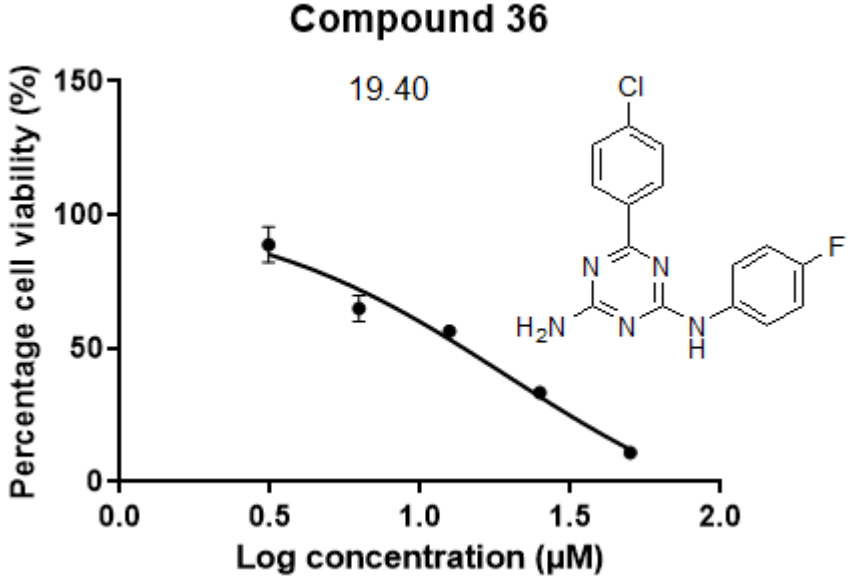

Compound 121
13.88
Percentage cell viability (%)
150
100
50
0
-1
0
1
2
Log concentration (μM)
S
N
N
H_2N
N
N
H
Me

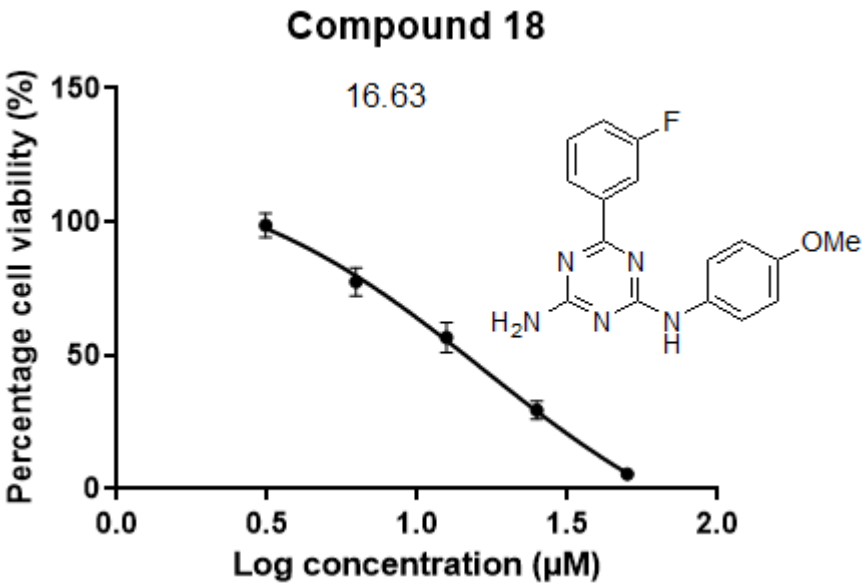

Methotrexate
0.01000
Percentage cell viability (%)
150
100
50
0
-4
-3
-2
-1
0
Log concentration (μM)

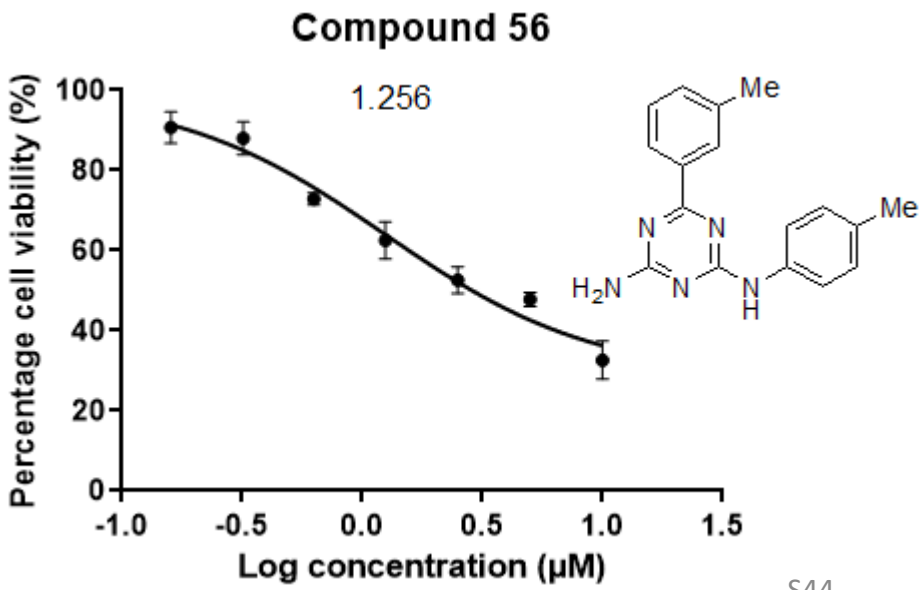

Nilotinib
0.04112
Percentage cell viability (%)
150
100
50
0
-6
-4
-2
0
2
4
Log concentration (μM)

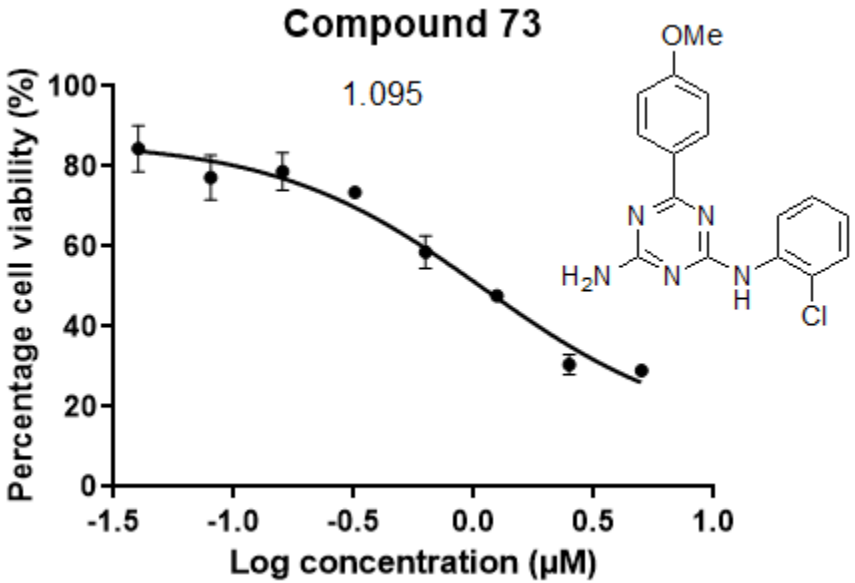
Concentration-response curves for the most active compounds
(**16**, **18**, **36**, **56**, **73**, **74**, **77**, **78**, **81**, **100**, **101**, and **103**)
tested against SKBR-3 breast cancer cells

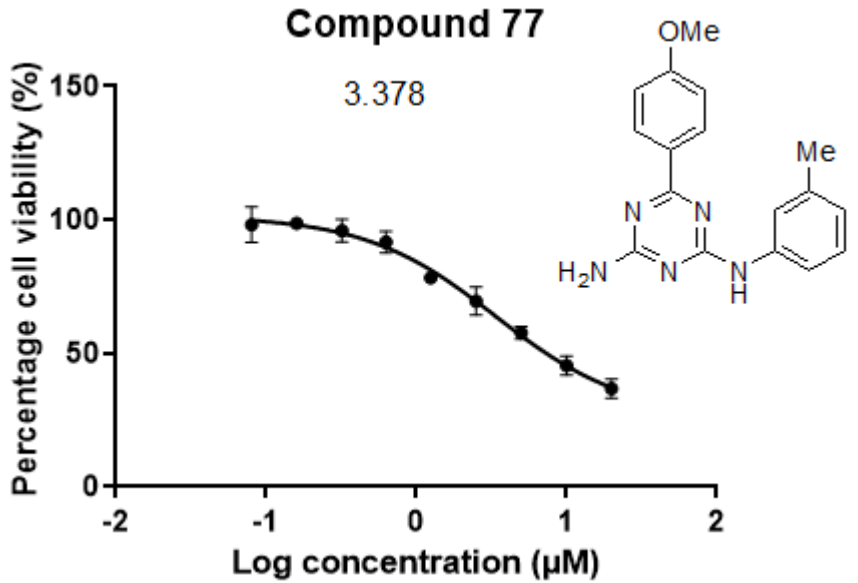

Compound 16
17.16
Percentage cell viability (%)
150
100
50
0
0.5
1.0
1.5
2.0
Log concentration (μM)
F
Br
N
N
H_2N
N
N
H

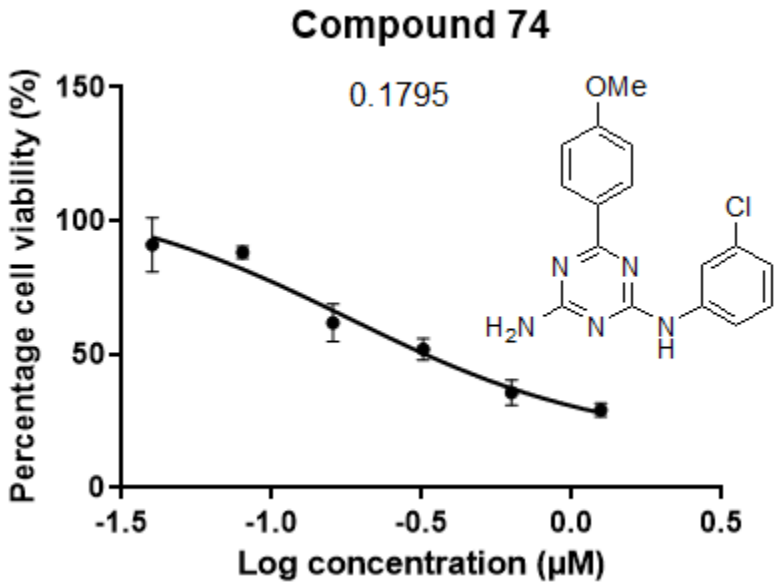

Compound 36
19.40
Percentage cell viability (%)
150
100
50
0
0.0
0.5
1.0
1.5
2.0
Log concentration (μM)
Cl
F
N
N
H_2N
N
N
H

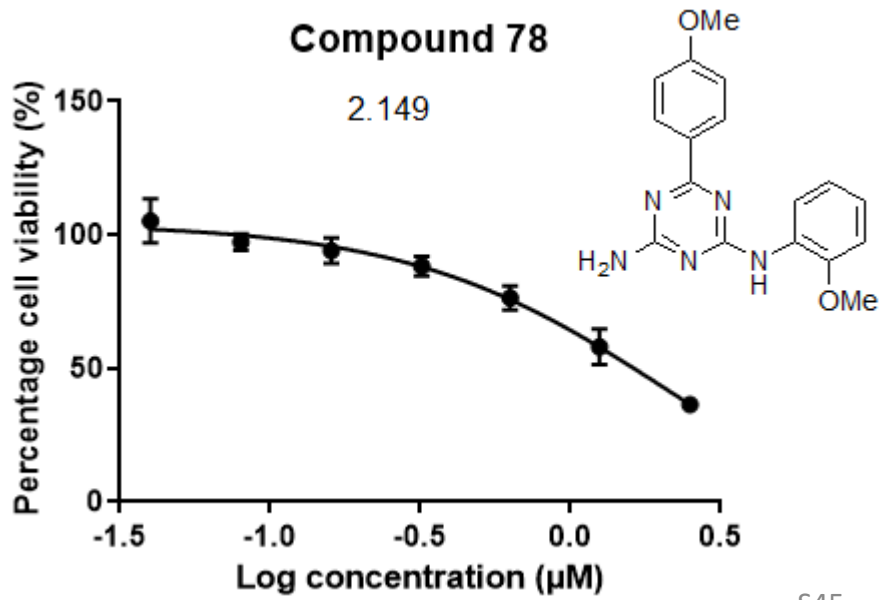

Compound 18
16.63
Percentage cell viability (%)
150
100
50
0
0.0
0.5
1.0
1.5
2.0
Log concentration (μM)
F
OMe
N
N
H_2N
N
N
H

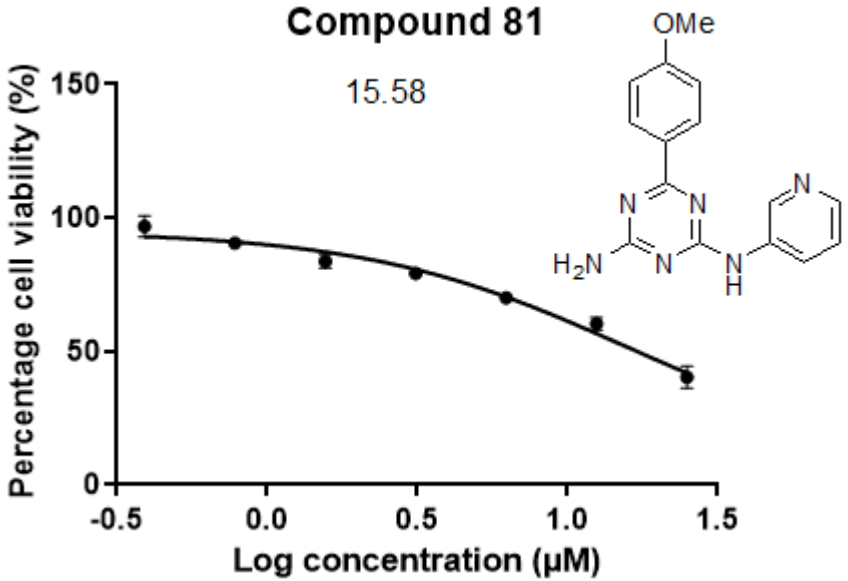

Compound 56
1.256
Percentage cell viability (%)
100
80
60
40
20
0
-1.0
-0.5
0.0
0.5
1.0
1.5
Log concentration (μM)
Me
Me
N
N
H_2N
N
N
H

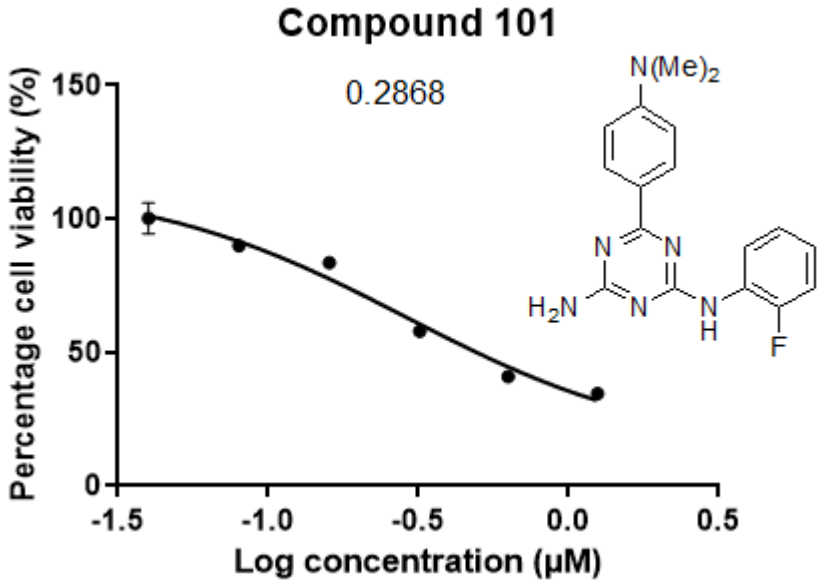

Compound 73
1.095
Percentage cell viability (%)
Log concentration (μM)
OMe
Cl

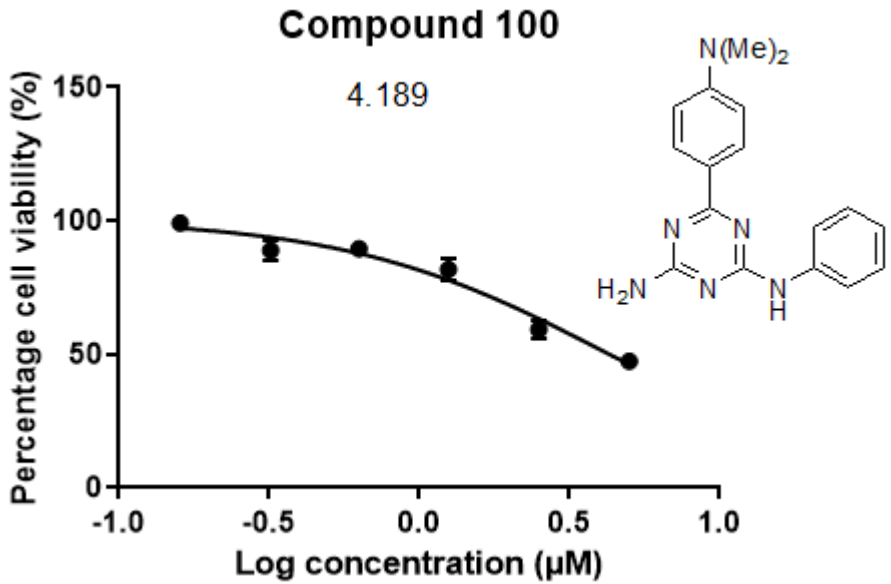

Compound 77
3.378
Percentage cell viability (%)
Log concentration (μM)
OMe
Me

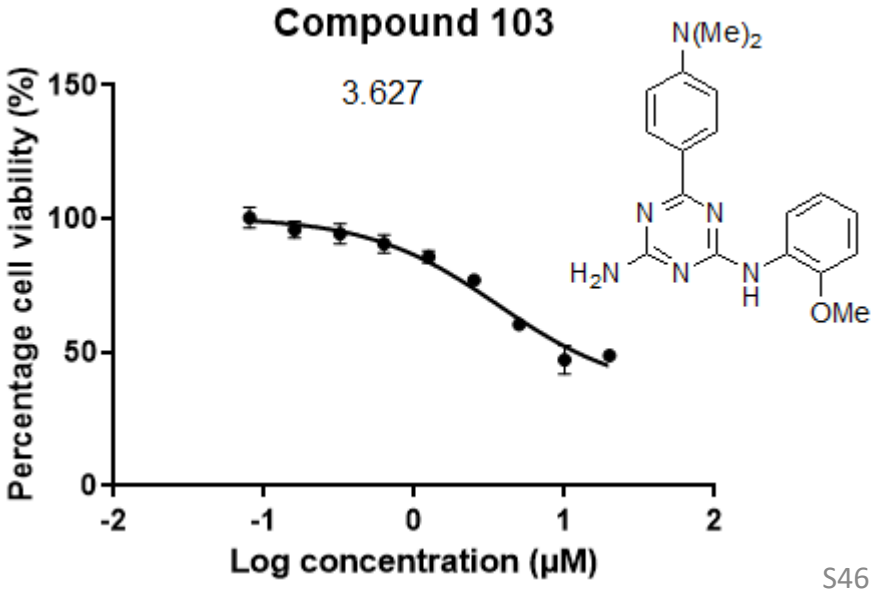

Compound 74
0.1795
Percentage cell viability (%)
Log concentration (μM)
OMe
Cl

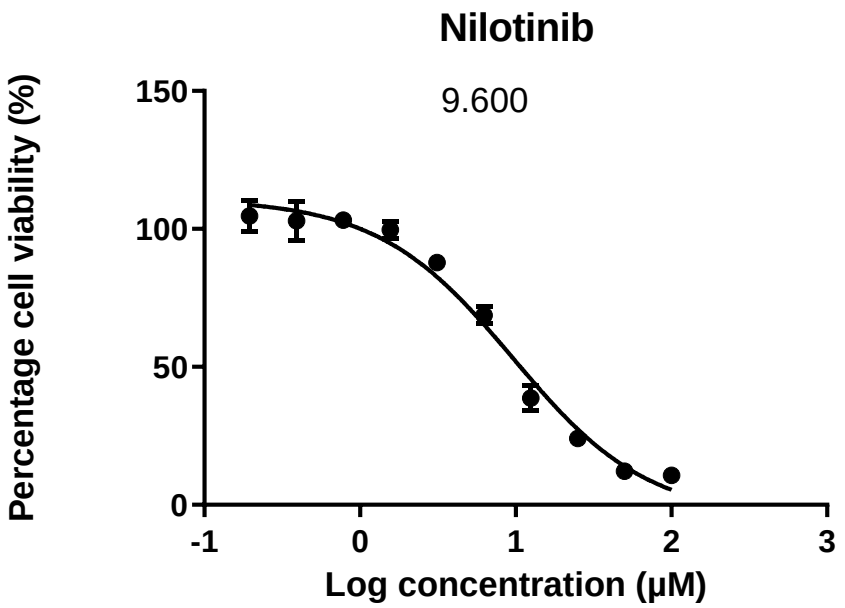

Compound 78
2.149
Percentage cell viability (%)
Log concentration (μM)
OMe
OMe


Compound 81
15.58
OMe
N
N
N
H_2N
N
N
H
Percentage cell viability (%)
150
100
50
0
-0.5
0.0
0.5
1.0
1.5
Log concentration (μM)


Compound 101
0.2868
$N(Me)_2$
N
N
H_2N
N
N
H
F
Percentage cell viability (%)
150
100
50
0
-1.5
-1.0
-0.5
0.0
0.5
Log concentration (μM)


Compound 100
4.189
$N(Me)_2$
N
N
H_2N
N
N
H
Percentage cell viability (%)
150
100
50
0
-1.0
-0.5
0.0
0.5
1.0
Log concentration (μM)


Compound 103
3.627
$N(Me)_2$
N
N
H_2N
N
N
H
OMe
Percentage cell viability (%)
150
100
50
0
-2
-1
0
1
2
Log concentration (μM)


Nilotinib
9.600
Percentage cell viability (%)
150
100
50
0
-1
0
1
2
3
Log concentration (μM)