

Electronic Supplementary Information

6-Aryl-4-cycloamino-1,3,5-triazine-2-amines: Synthesis, antileukemic activity, and 3D-QSAR modeling

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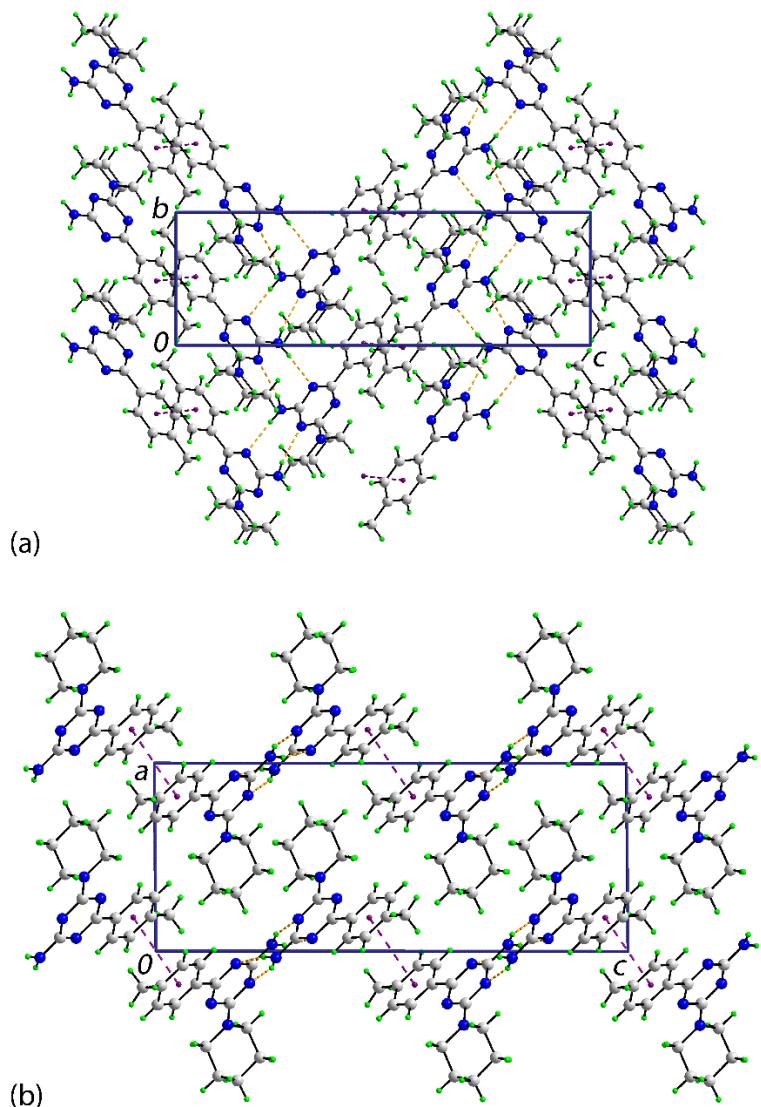
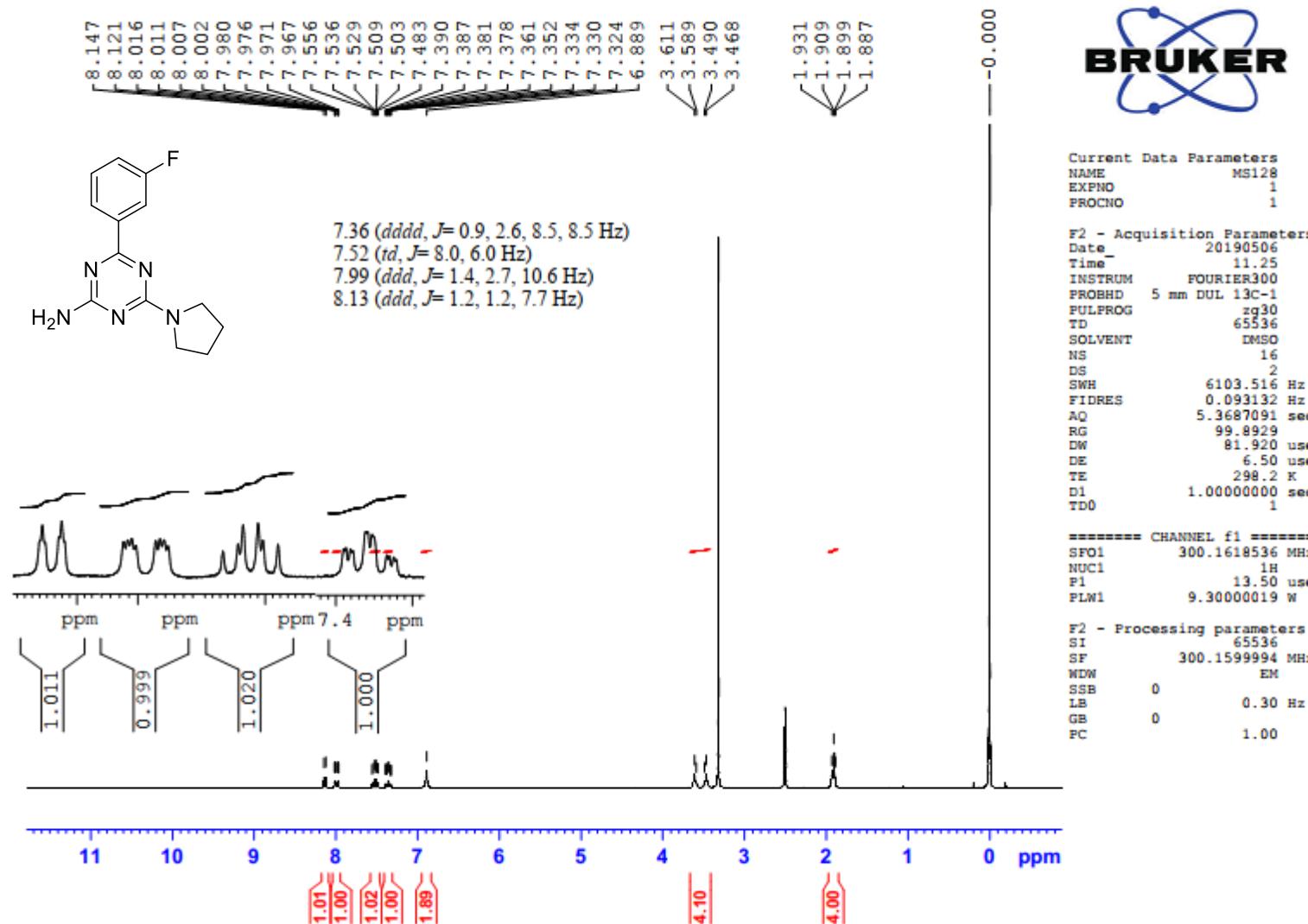
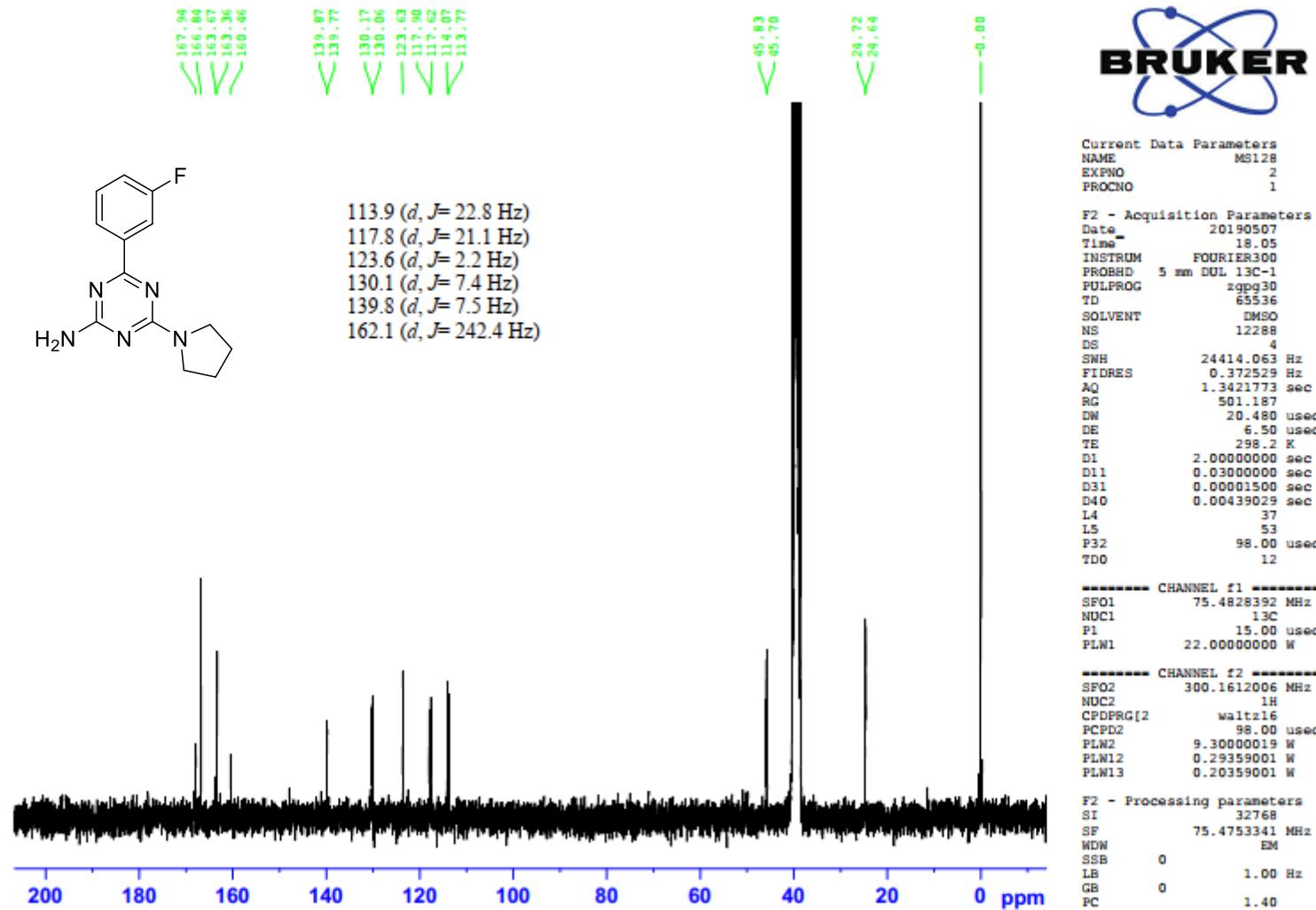


Figure S1. Molecular packing diagrams for **9{2,6}**: (a) a view of the supramolecular layer in the *bc*-plane and (b) a view of the unit-cell contents in projection down the *b*-axis. The amine-N–H \cdots N(triazine) hydrogen-bonding and π -stacking interactions are highlighted as orange and purple dashed lines, respectively. Intermolecular contacts: N21–H1n \cdots N3ⁱ: H1n \cdots N3ⁱ = 2.327(12) Å, N21 \cdots N3ⁱ = 3.1774(13) Å with angle at H1n = 161.7(12) $^\circ$; N21–H2n \cdots N1ⁱⁱ: N21–H2n \cdots N1ⁱⁱ = 2.166(12) Å, N21 \cdots N1ⁱⁱ = 3.0304(13) Å with angle at H2n = 167.3(13) $^\circ$; ring centroid(C61-C66) \cdots ring centroid(C61-C66)ⁱⁱⁱ = 3.8345(7) Å with an off-set = 1.642 Å for symmetry operations (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (iii) $-x, 2-y, 1-z$.

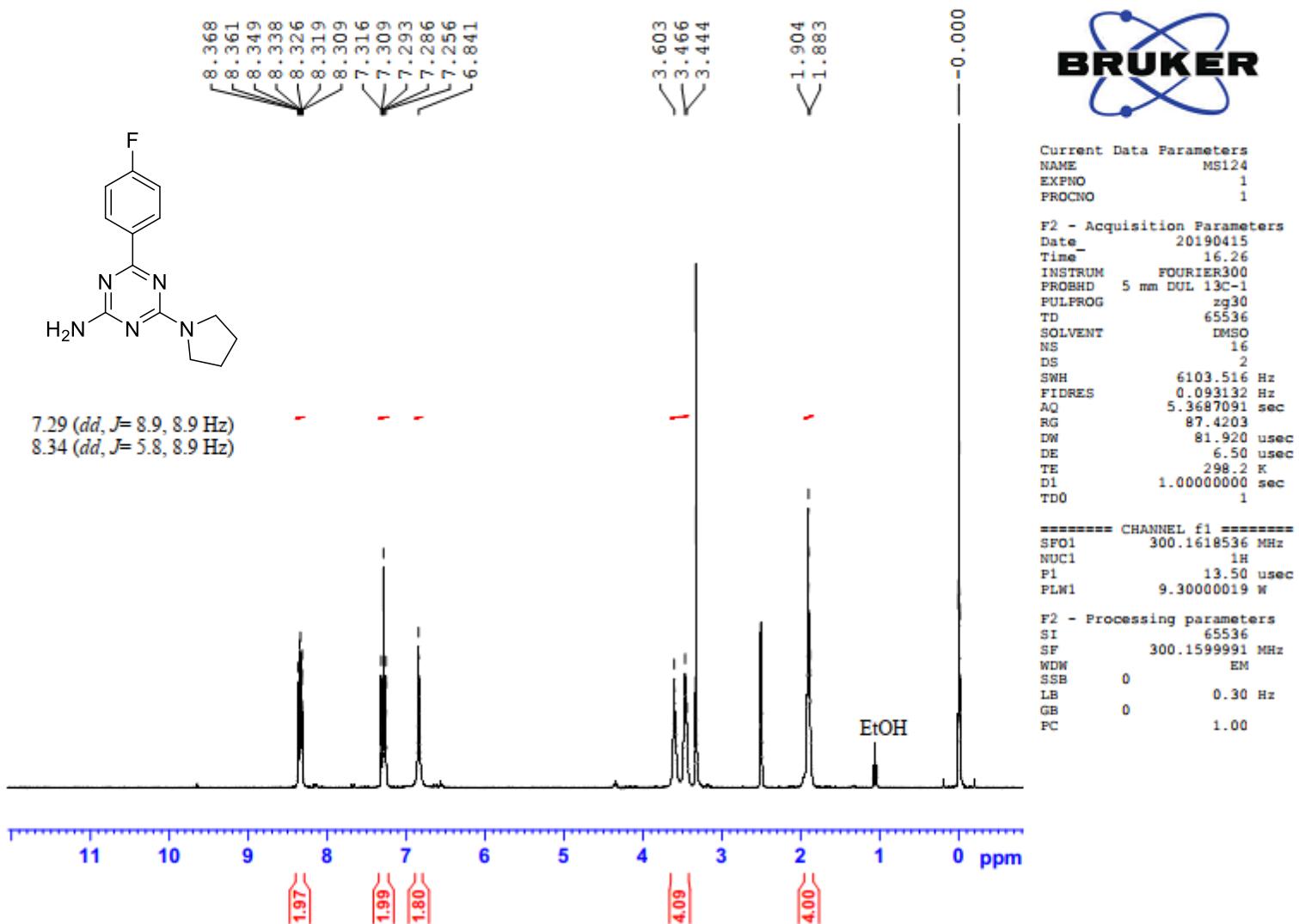
6-(3-Fluorophenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,2}**)



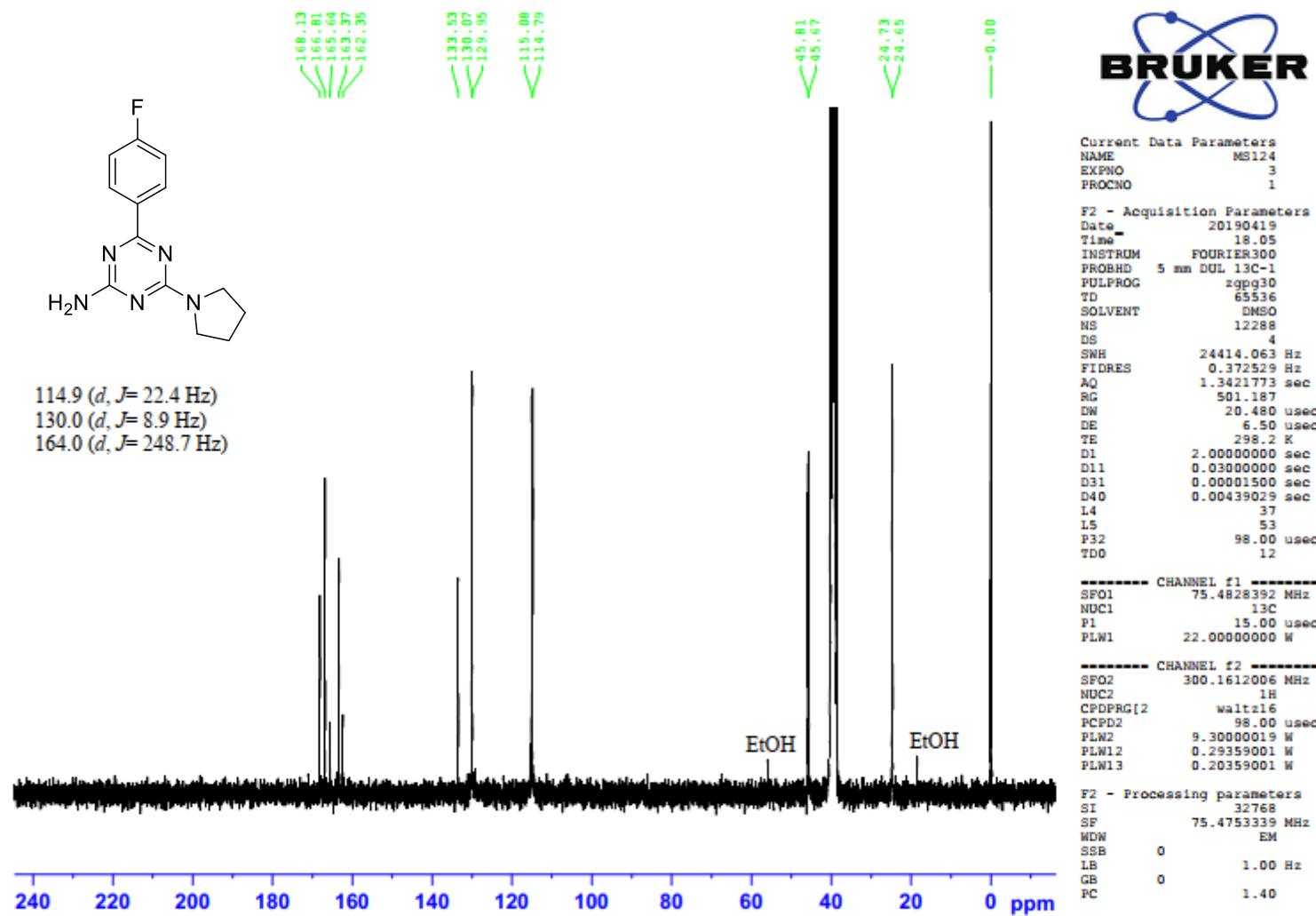
6-(3-Fluorophenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,2}**)



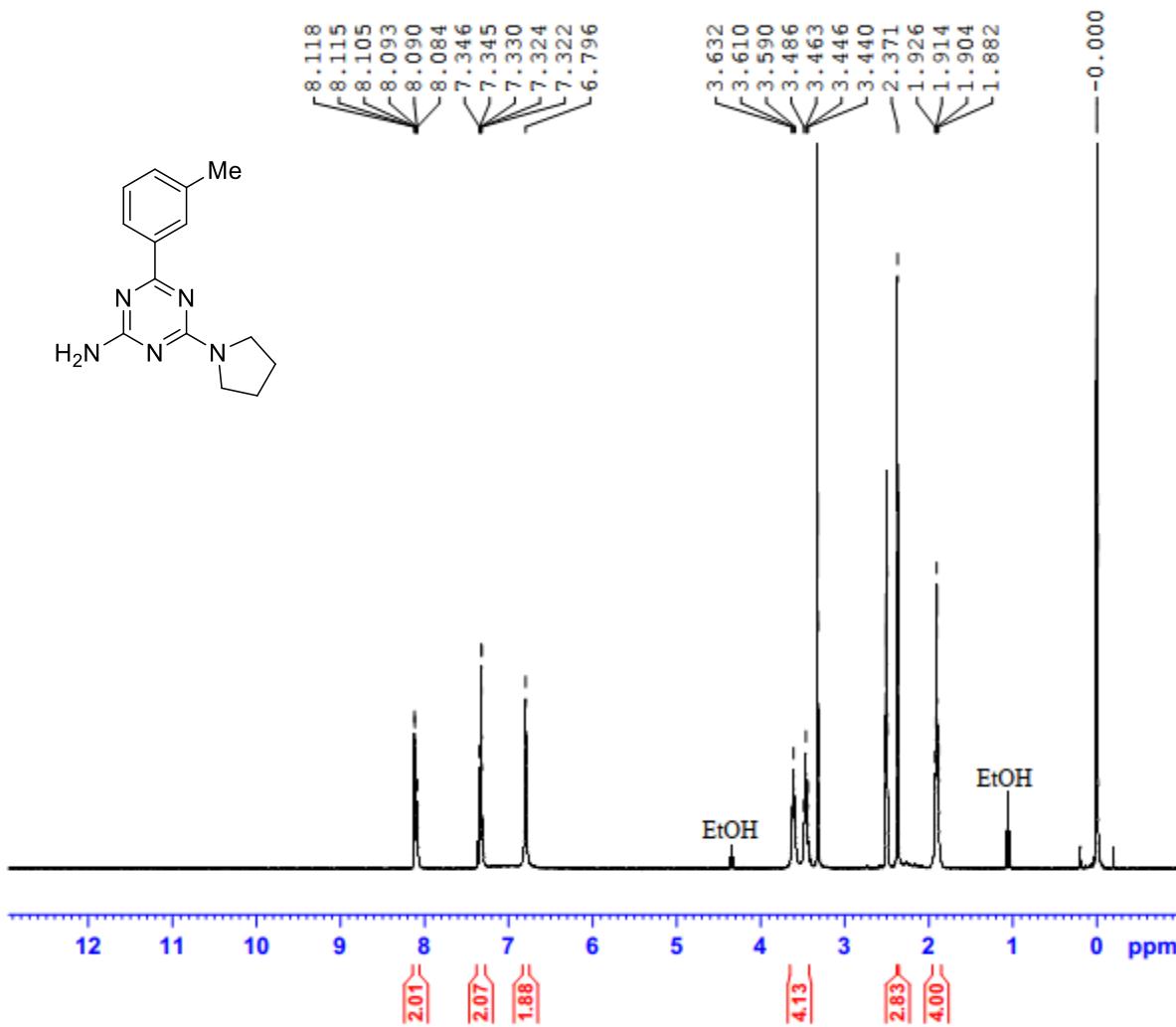
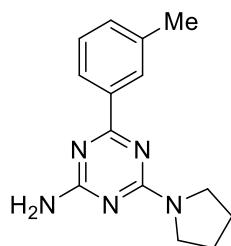
6-(4-Fluorophenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,3}**)



6-(4-Fluorophenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,3}**)



6-(3-Methylphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,5}**)



BRUKER

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EXPNO
PROCNO

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TD0           1

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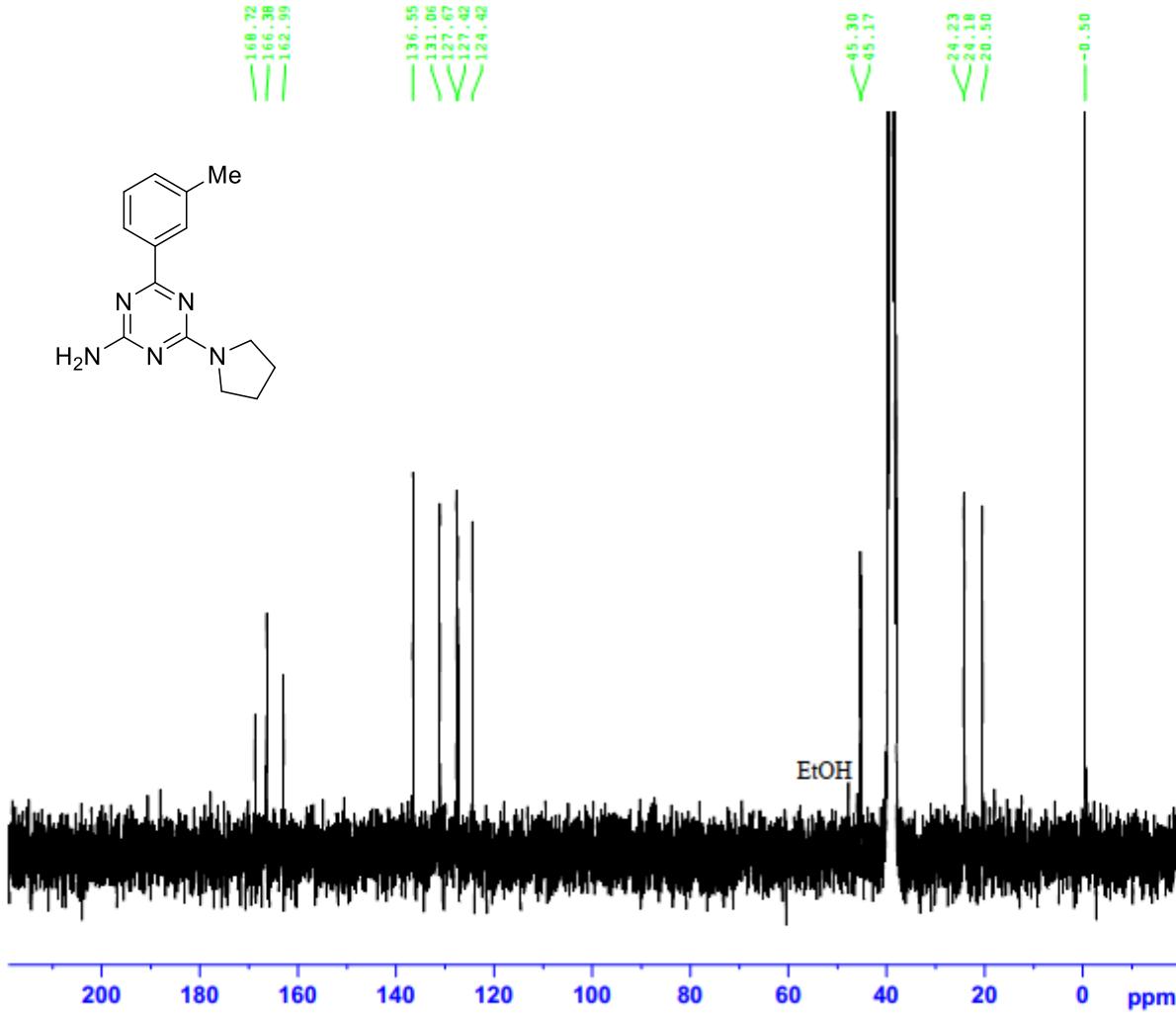
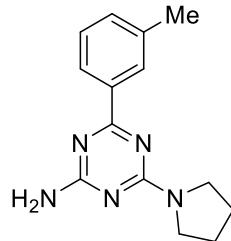
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6-(3-Methylphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,5}**)



BRUKER

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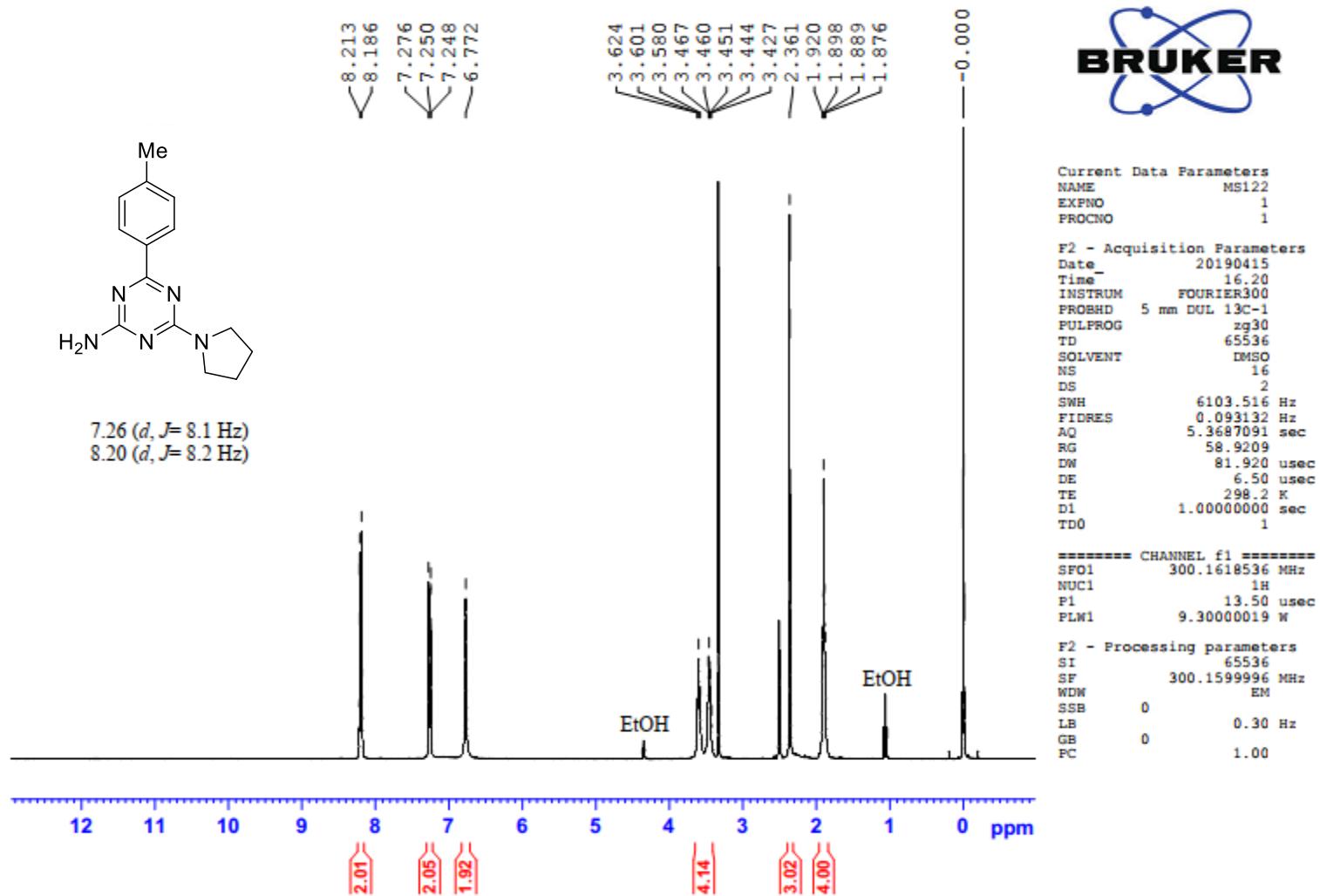
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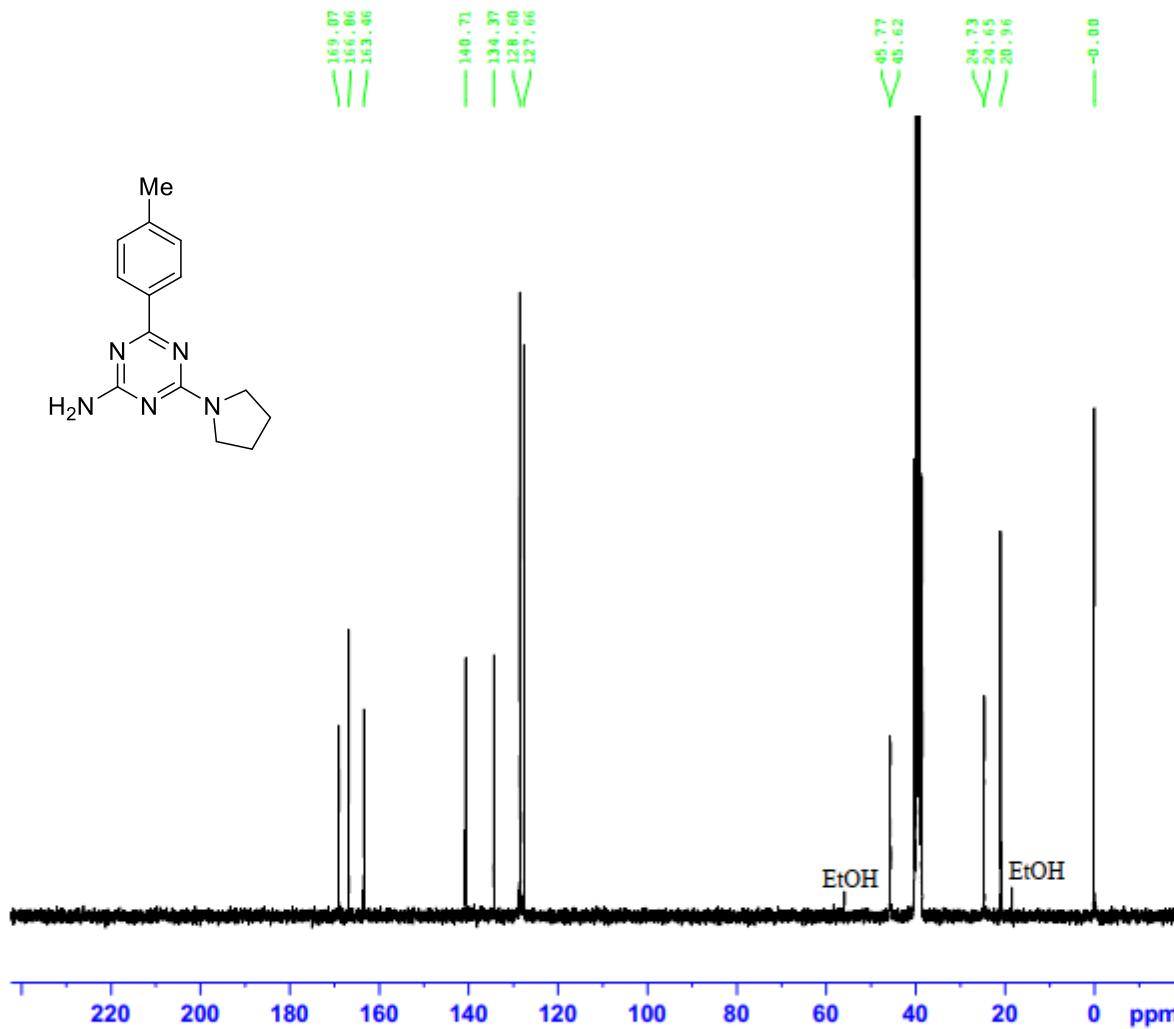
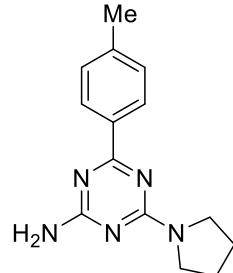
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PLW12 0.29359001 W
PLW13 0.20359001 W

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WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

6-(4-Methylphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,6}**)



6-(4-Methylphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,6}**)



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Current Data Parameter
NAME MS12
EXPNO
PROCNO

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NS        6144
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SWH       24414.063 Hz
FIDRES_  0.372529 Hz
AQ        1.3421773 sec
RG        501.187
DW        20.480 used
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TE        298.2 K
D1        2.00000000 sec
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L4        37
L5        53
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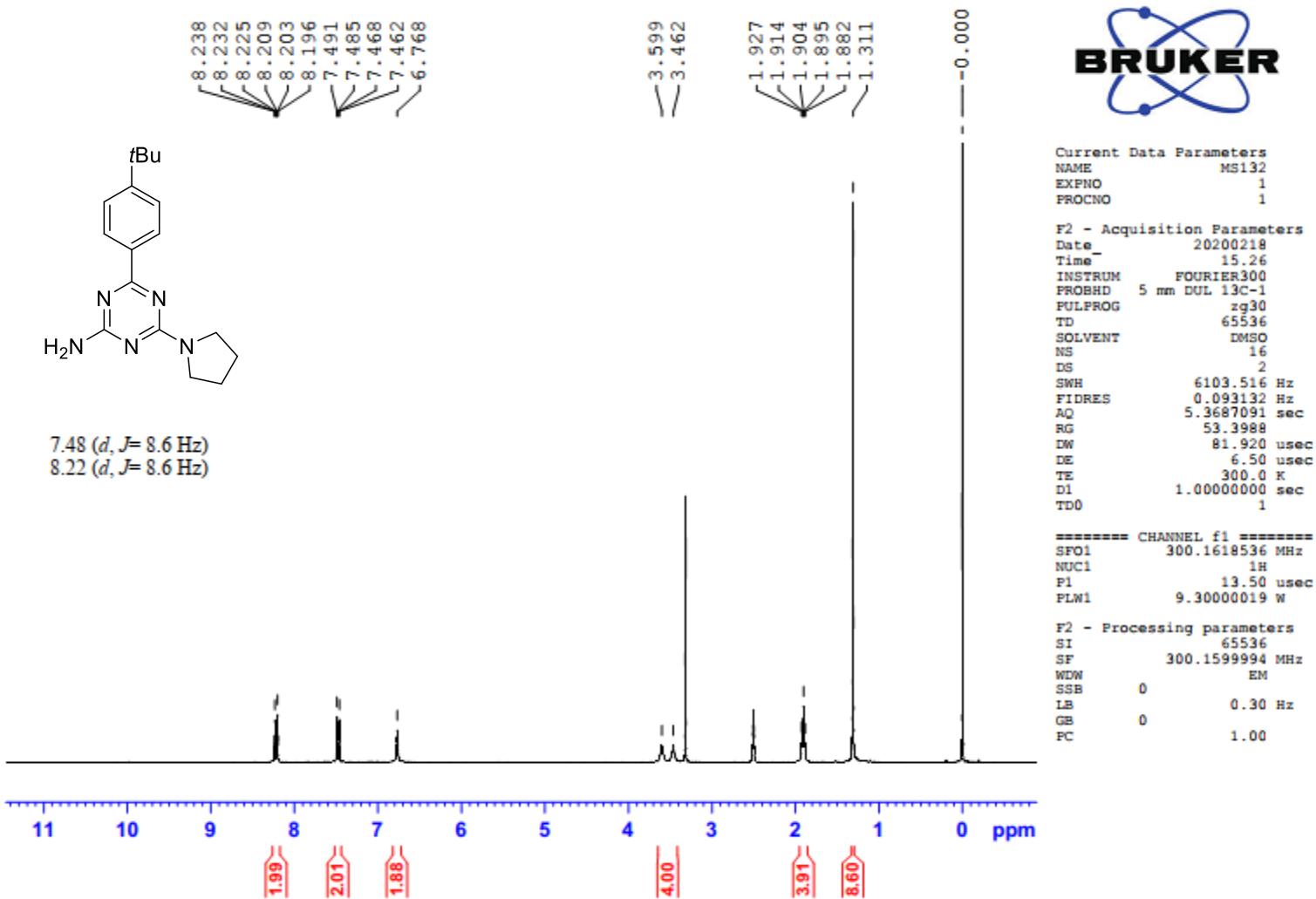
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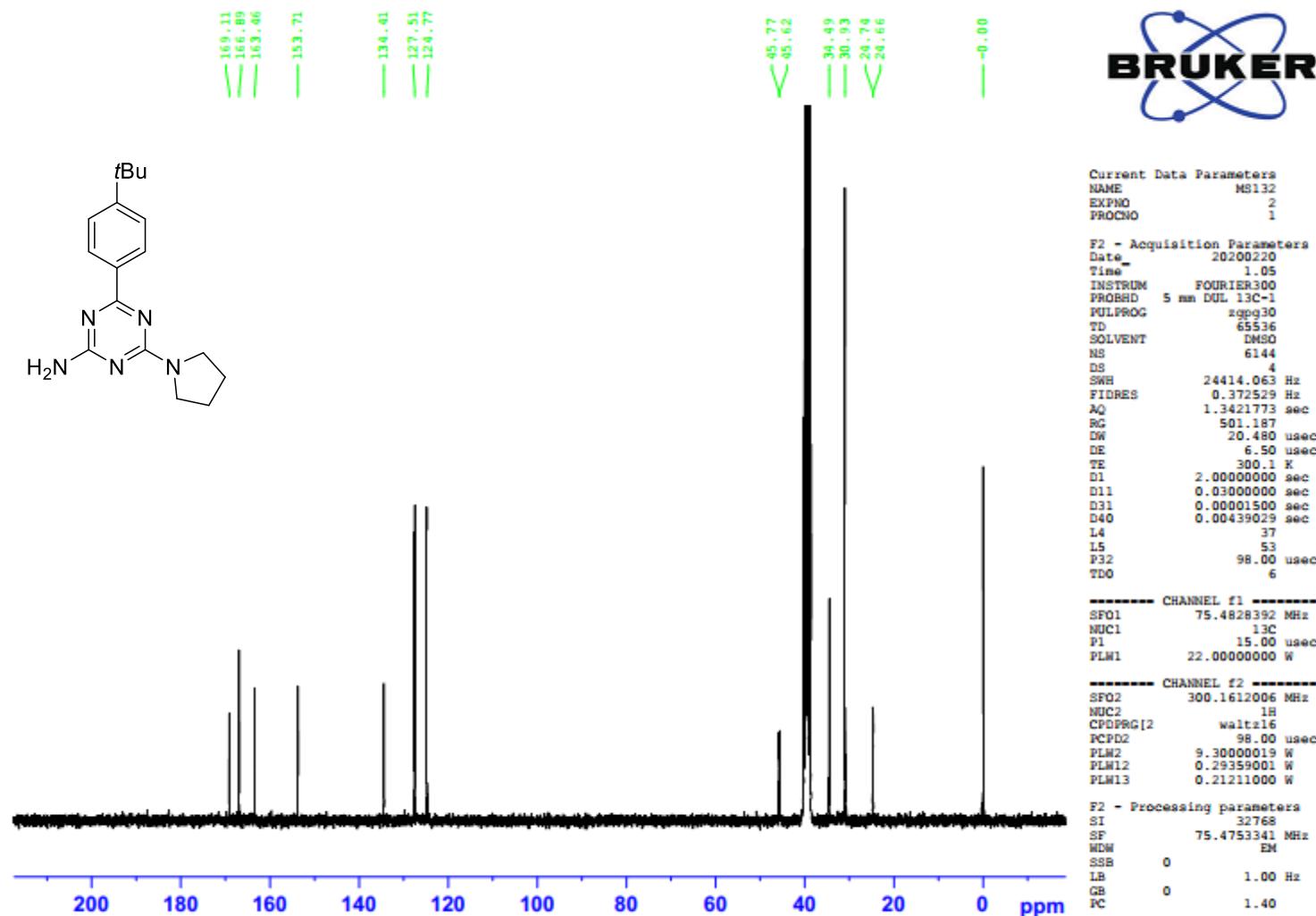
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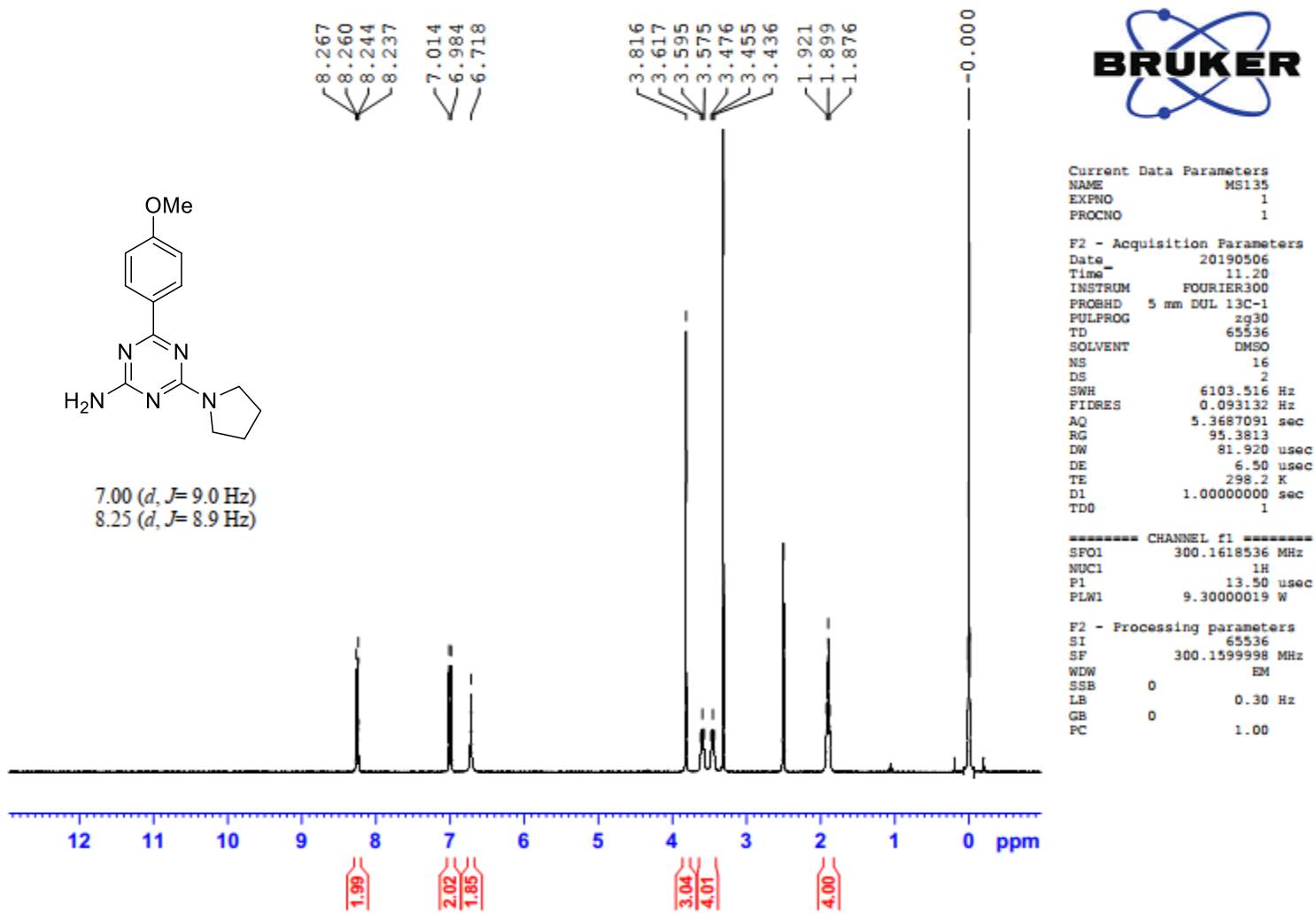
6-[4-(*tert*-Butyl)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,7}**)



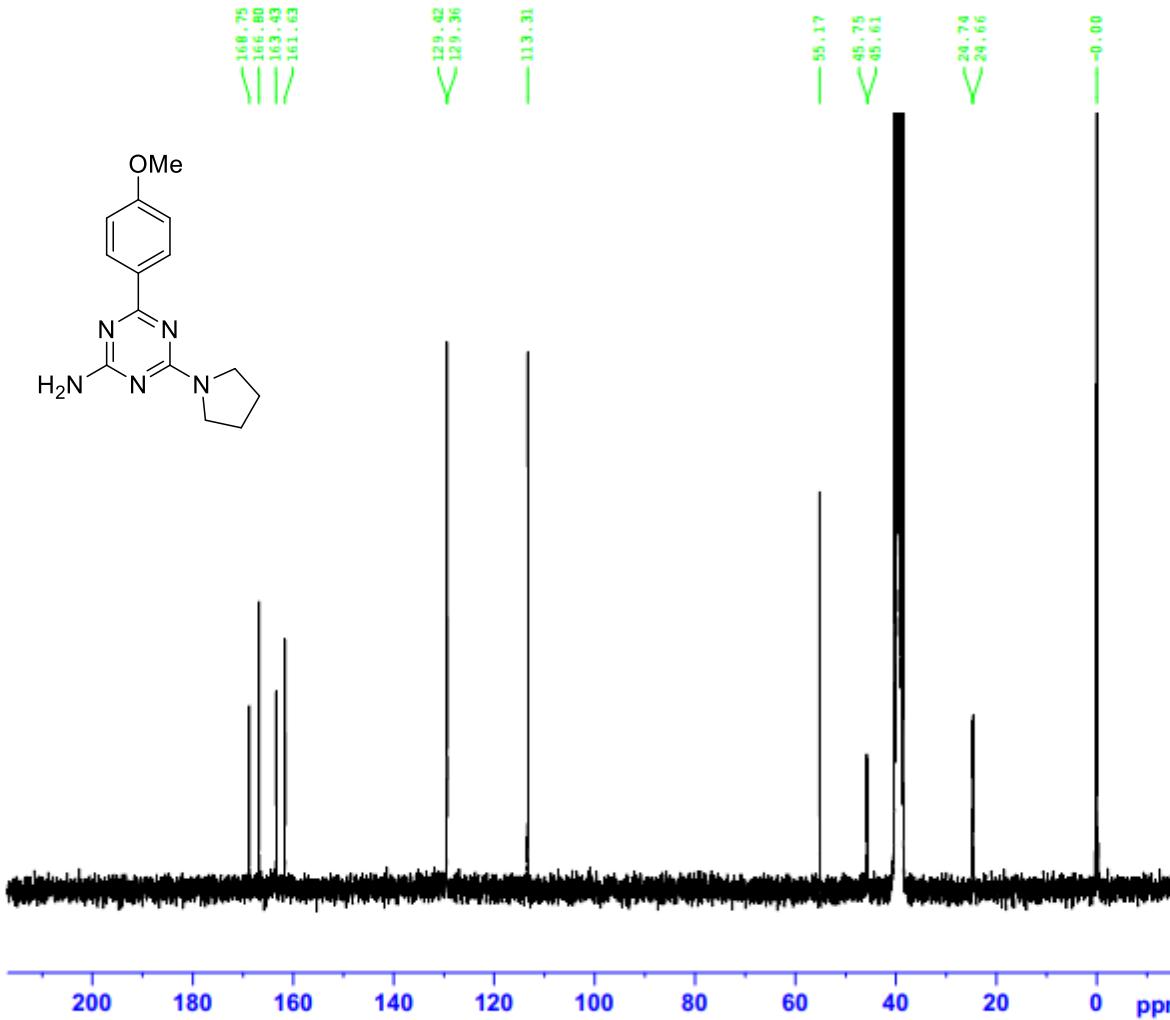
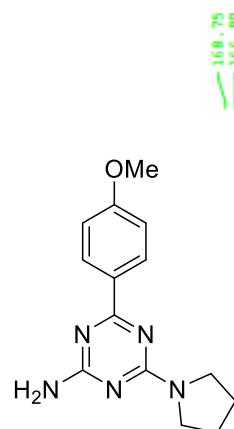
6-[4-(*tert*-Butyl)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,7}**)



6-(4-Methoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,9}**)



6-(4-Methoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,9}**)



BRUKER

Current Data Parameter
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EXPNO
PROCNO

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PULPROG  zgpg30
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FIDRES   0.372529 Hz
AQ        1.3421773 sec
RG        501.187
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DE        6.50  usec
TE        298.2 K
D1        2.0000000 sec
D11       0.03000000 sec
D31       0.00001500 sec
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L4        37
L5        53
P32       98.00 usec
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PLW1 22.00000000 W

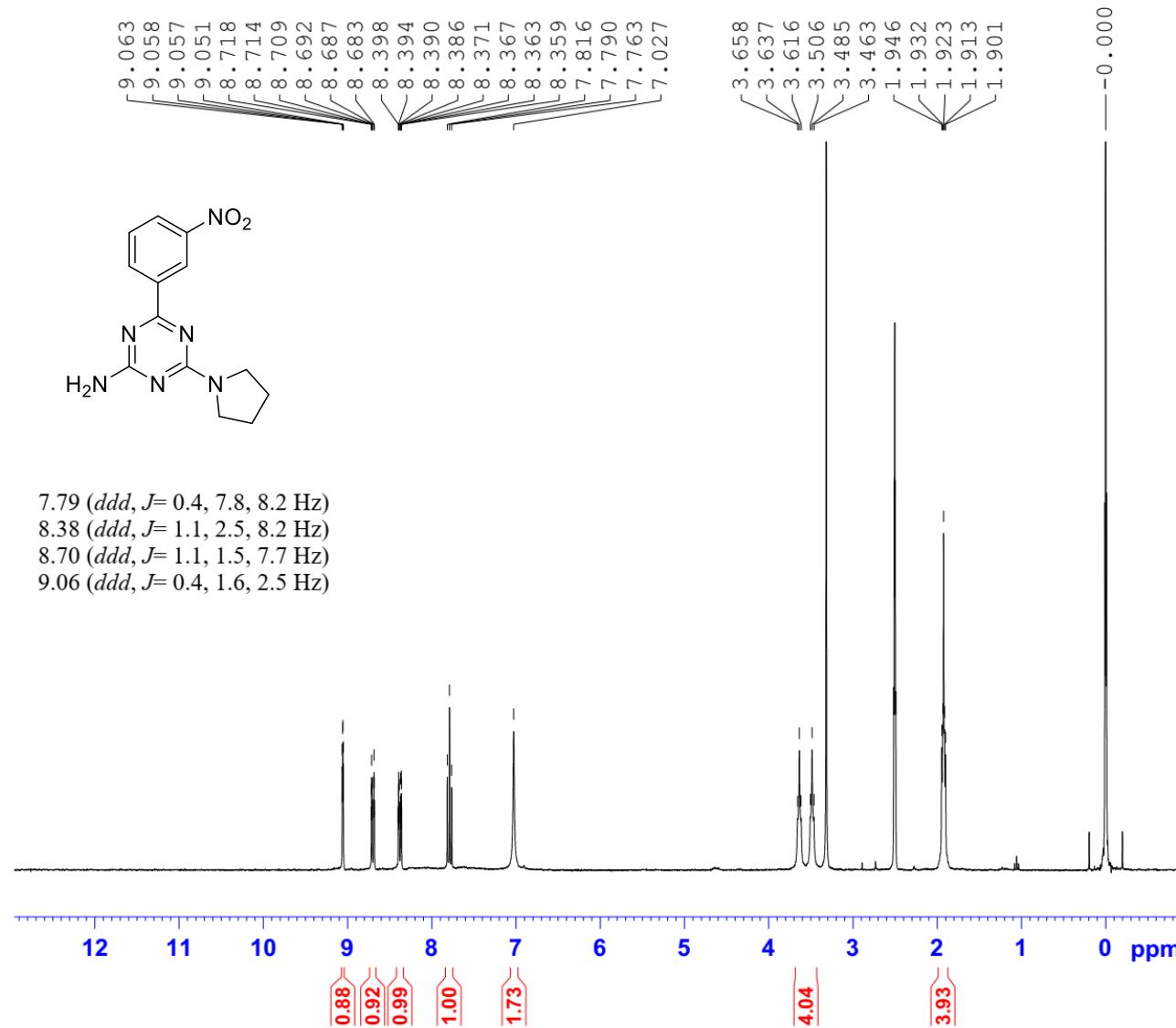
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PLW13	0.20359001	W

```

F2 - Processing parameters
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6-(3-Nitrophenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,10}**)



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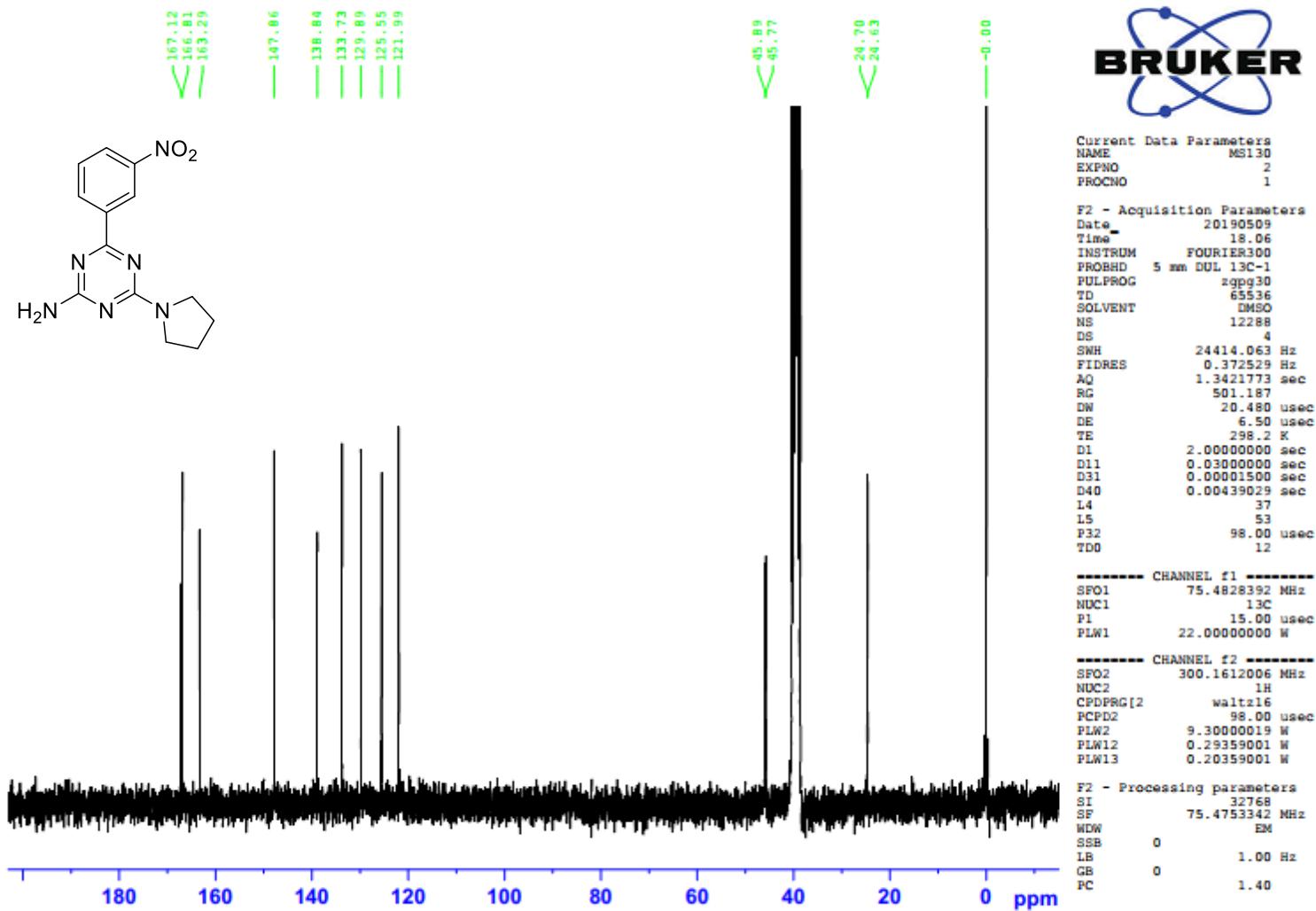
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PULPROG	zg30
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NS	16
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SWH	6103.516 Hz
FIDRES	0.093132 Hz
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RG	104.824
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DE	6.50 usec
TE	298.2 K
D1	1.0000000 sec
TD0	1

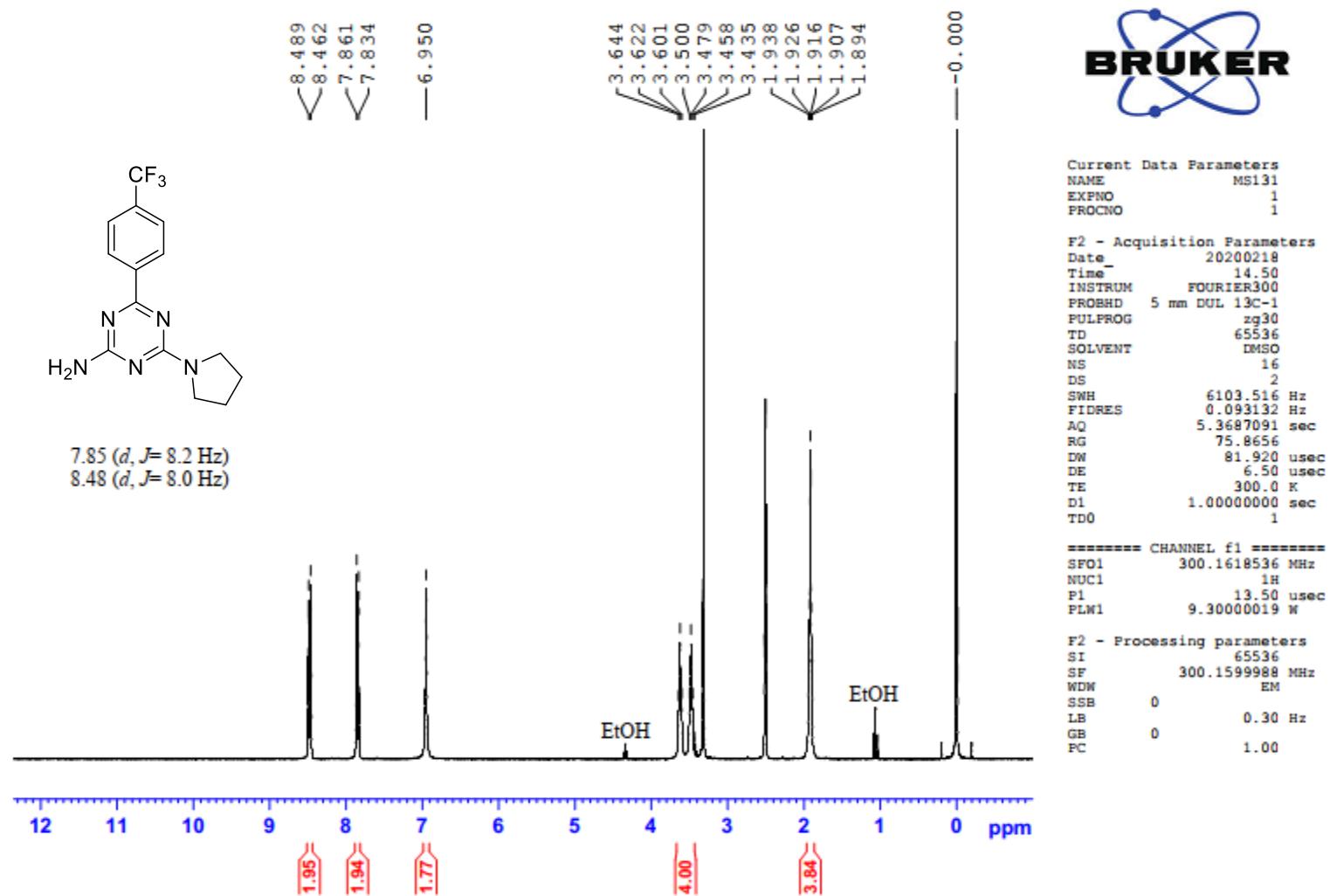
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 P1 13.50 usec
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F2 - Processing parameters
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 GB 0
 PC 1.00

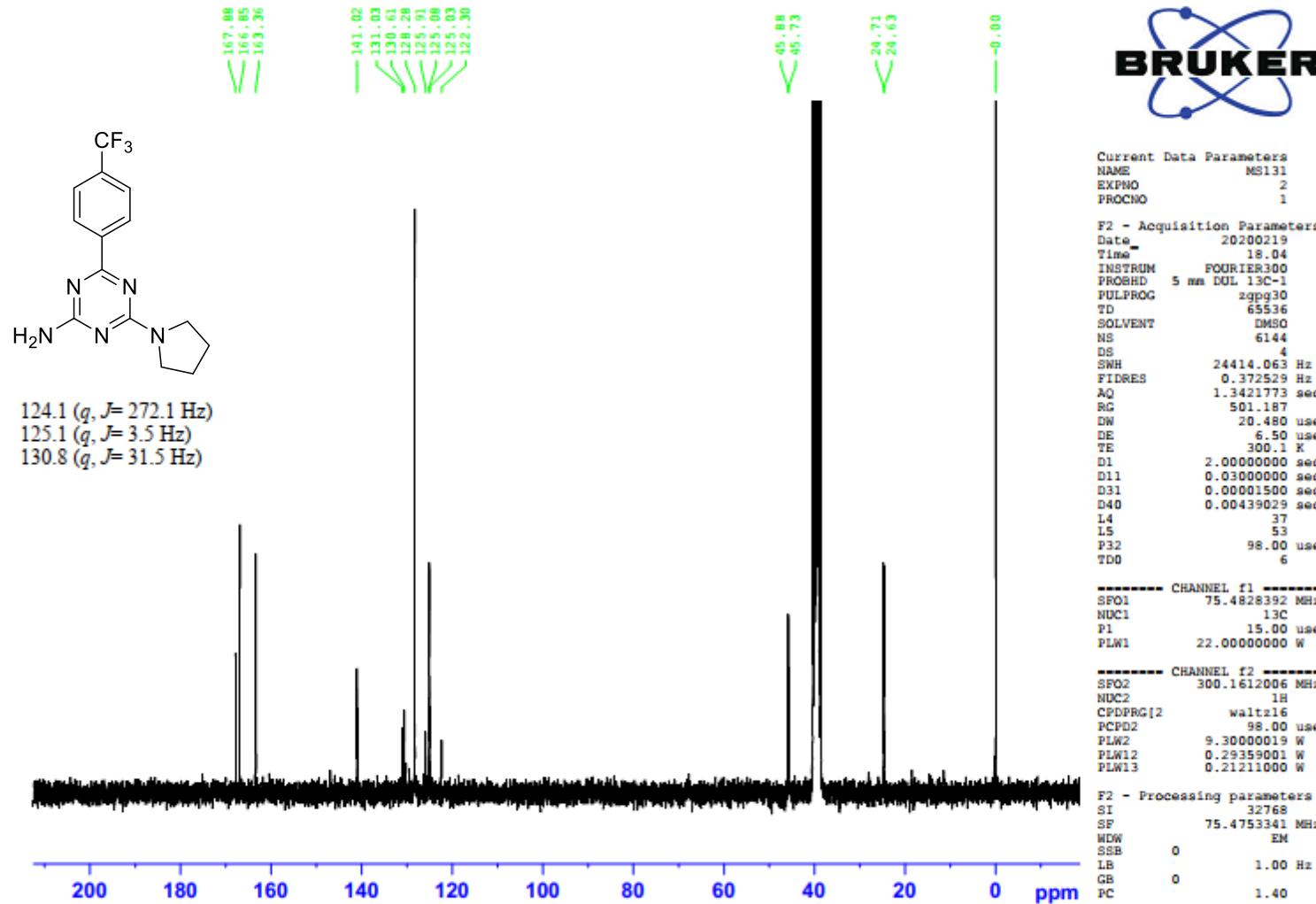
6-(3-Nitrophenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,10}**)



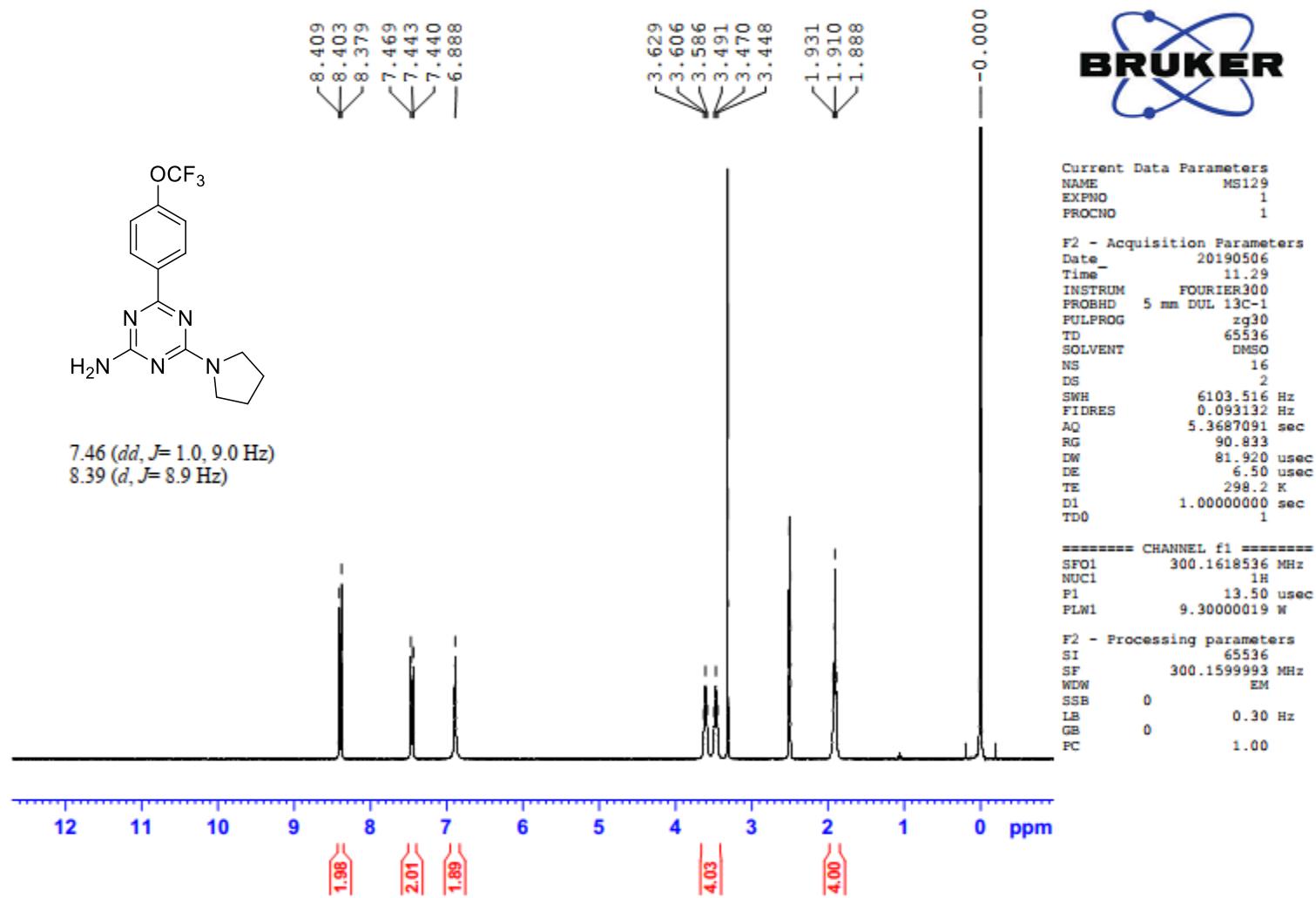
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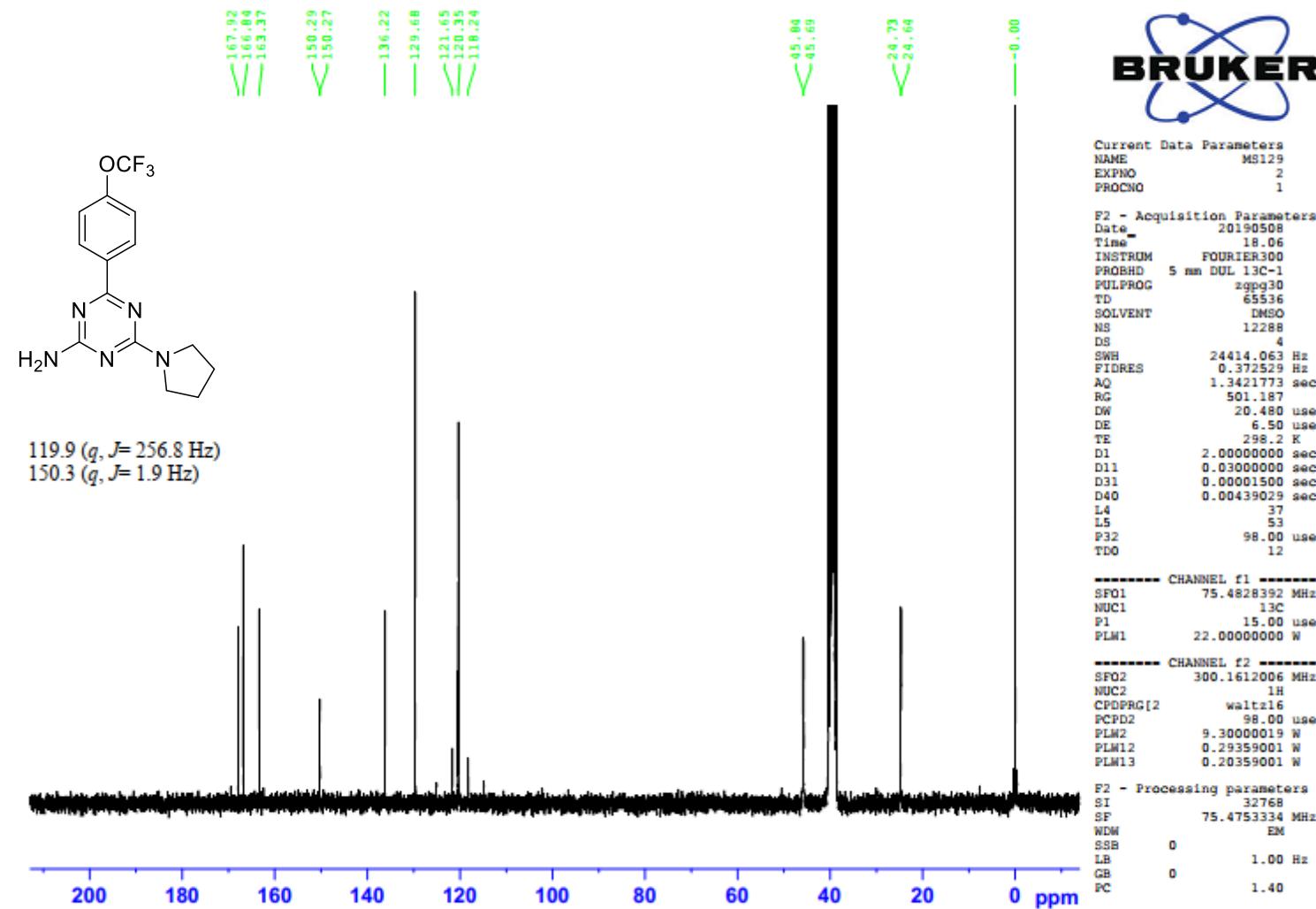
6-[4-(Trifluoromethyl)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,11}**)



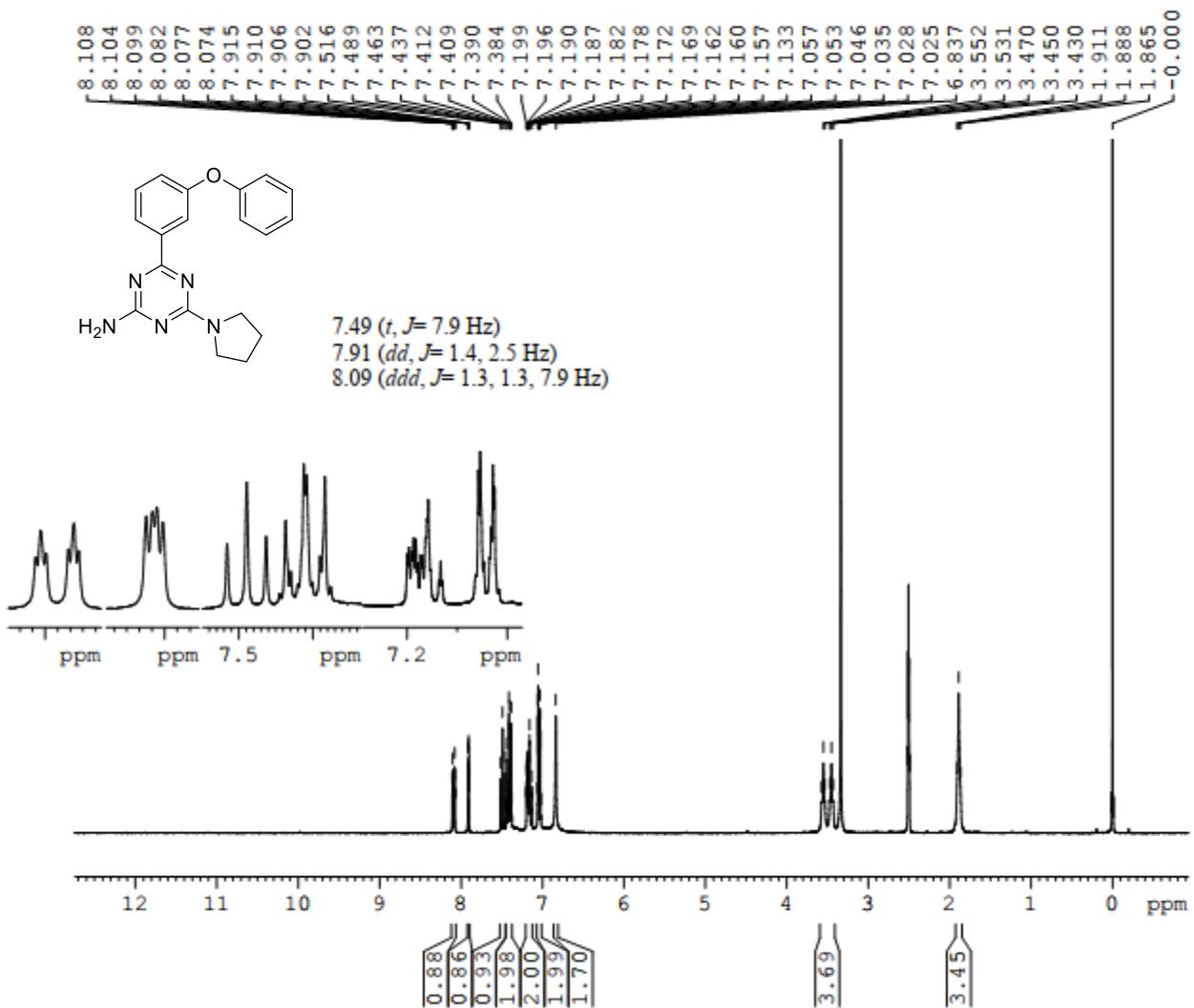
6-[4-(Trifluoromethoxy)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,12}**)



6-[4-(Trifluoromethoxy)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,12}**)



6-(3-Phenoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9**{1,13})



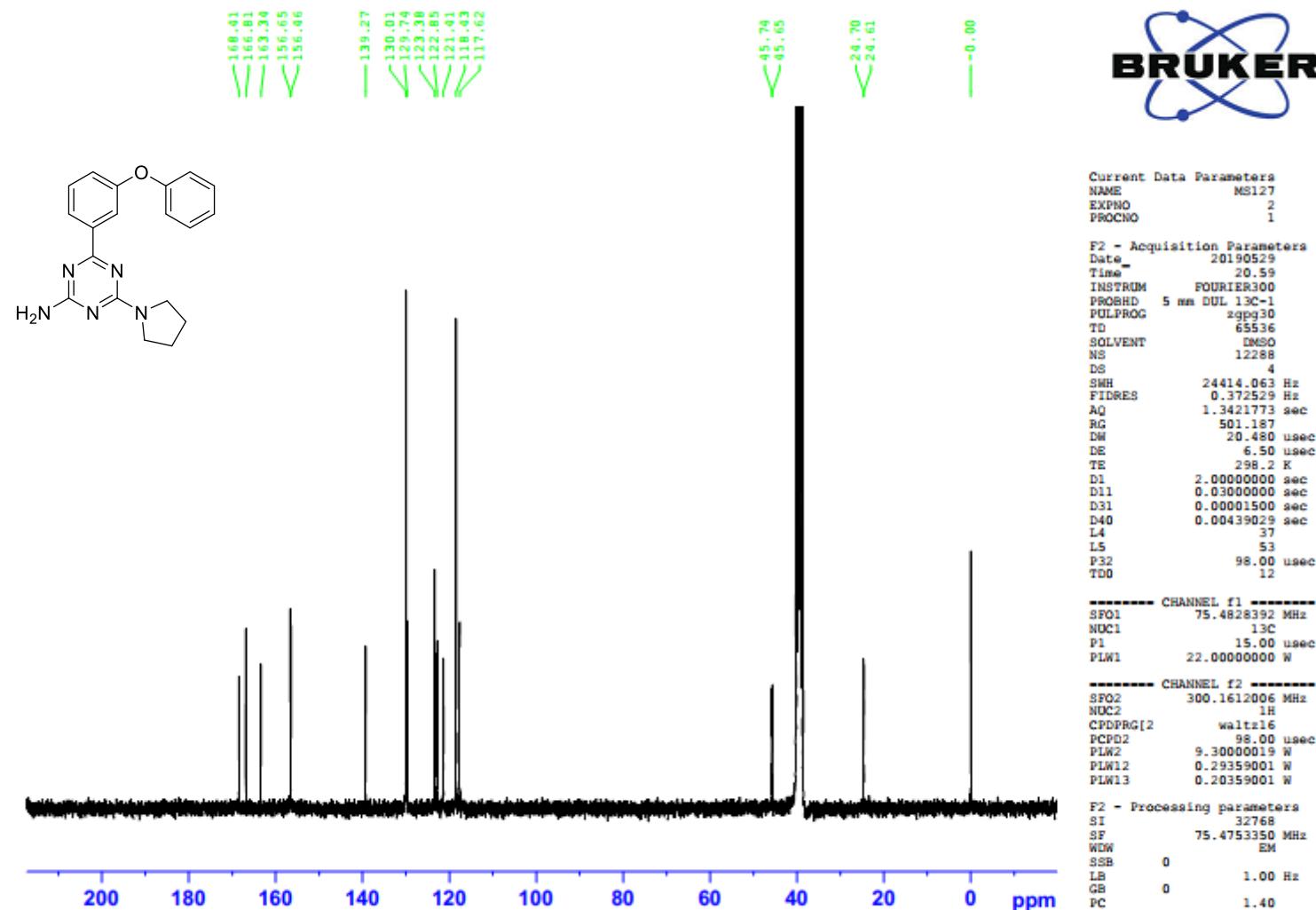
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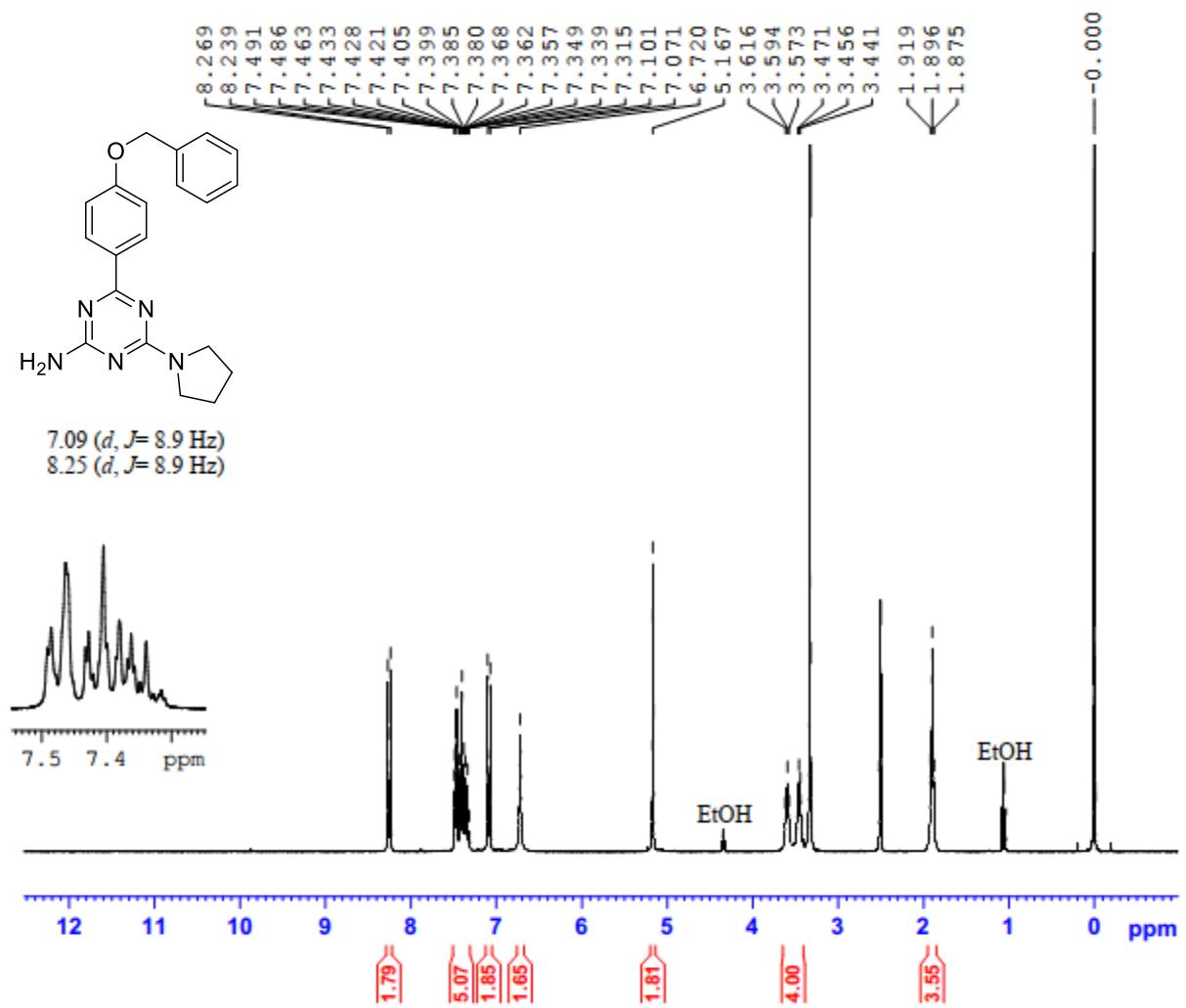
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GB 0
PC 1.00

6-(3-Phenoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,13}**)



6-[4-(Benzyl)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,15}**)



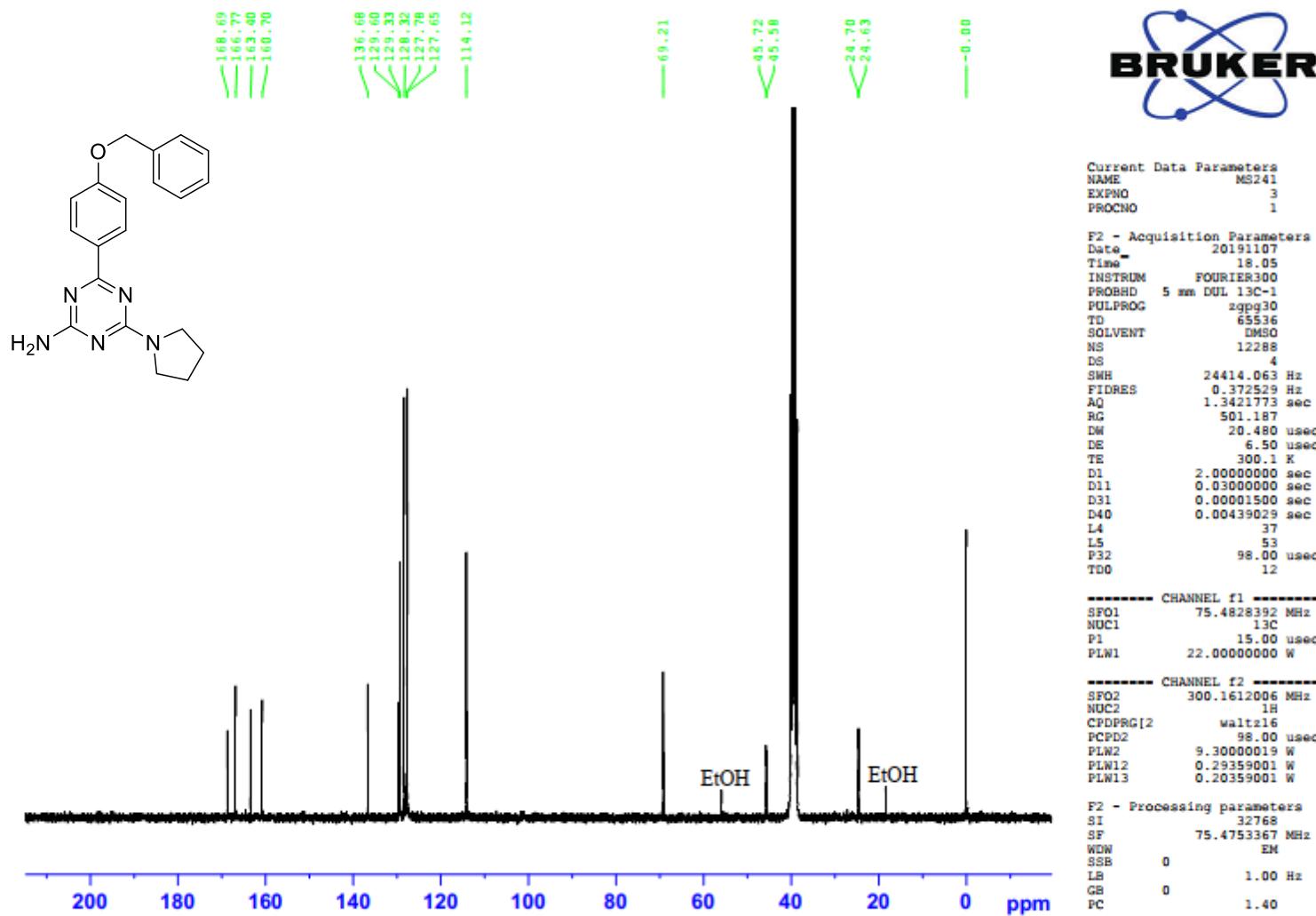
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D1 1.0000000 sec
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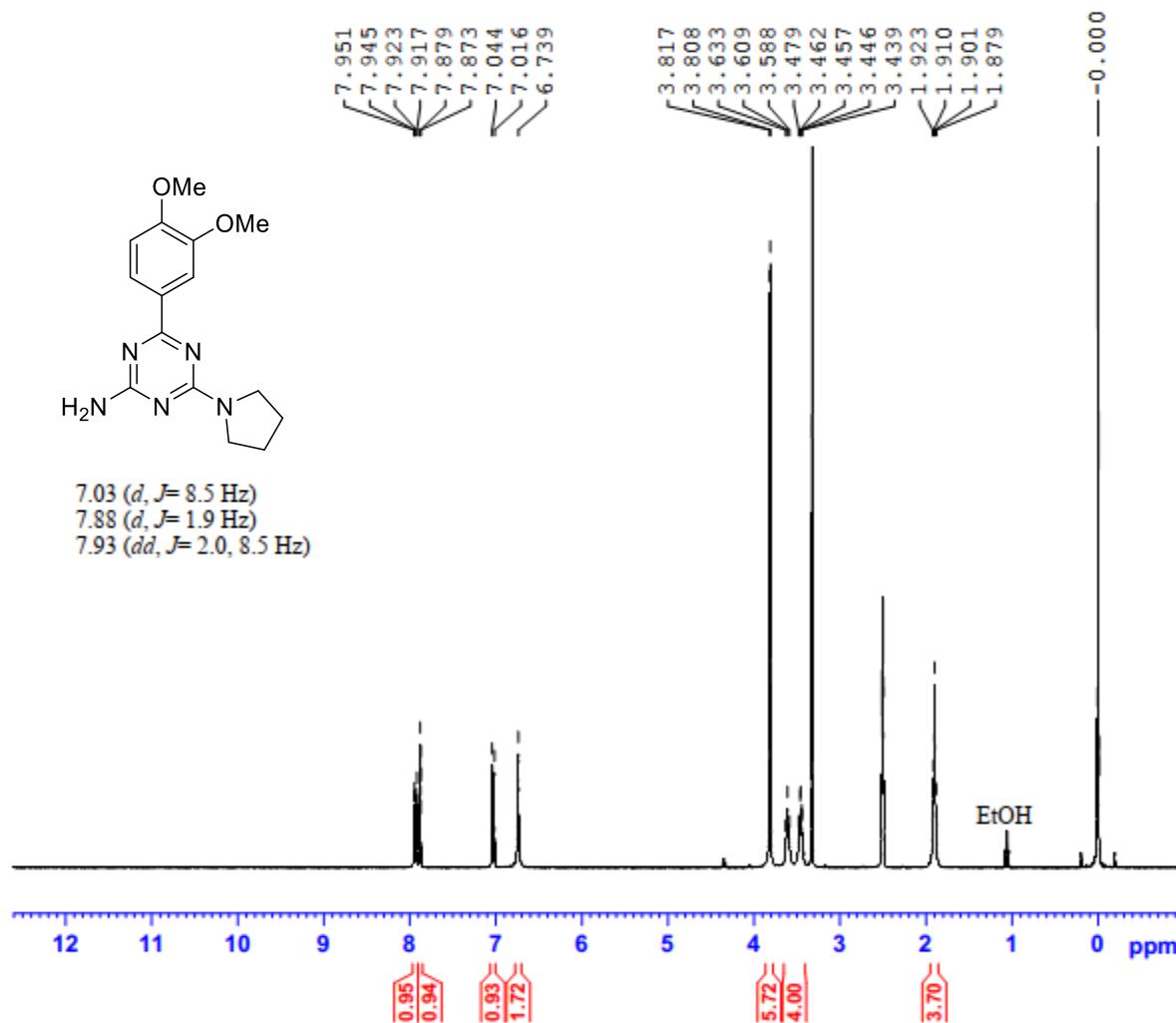
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6-[4-(Benzyl)phenyl]-4-pyrrolidino-1,3,5-triazine-2-amine (**9**{1,15})



6-(3,4-Dimethoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,16}**)



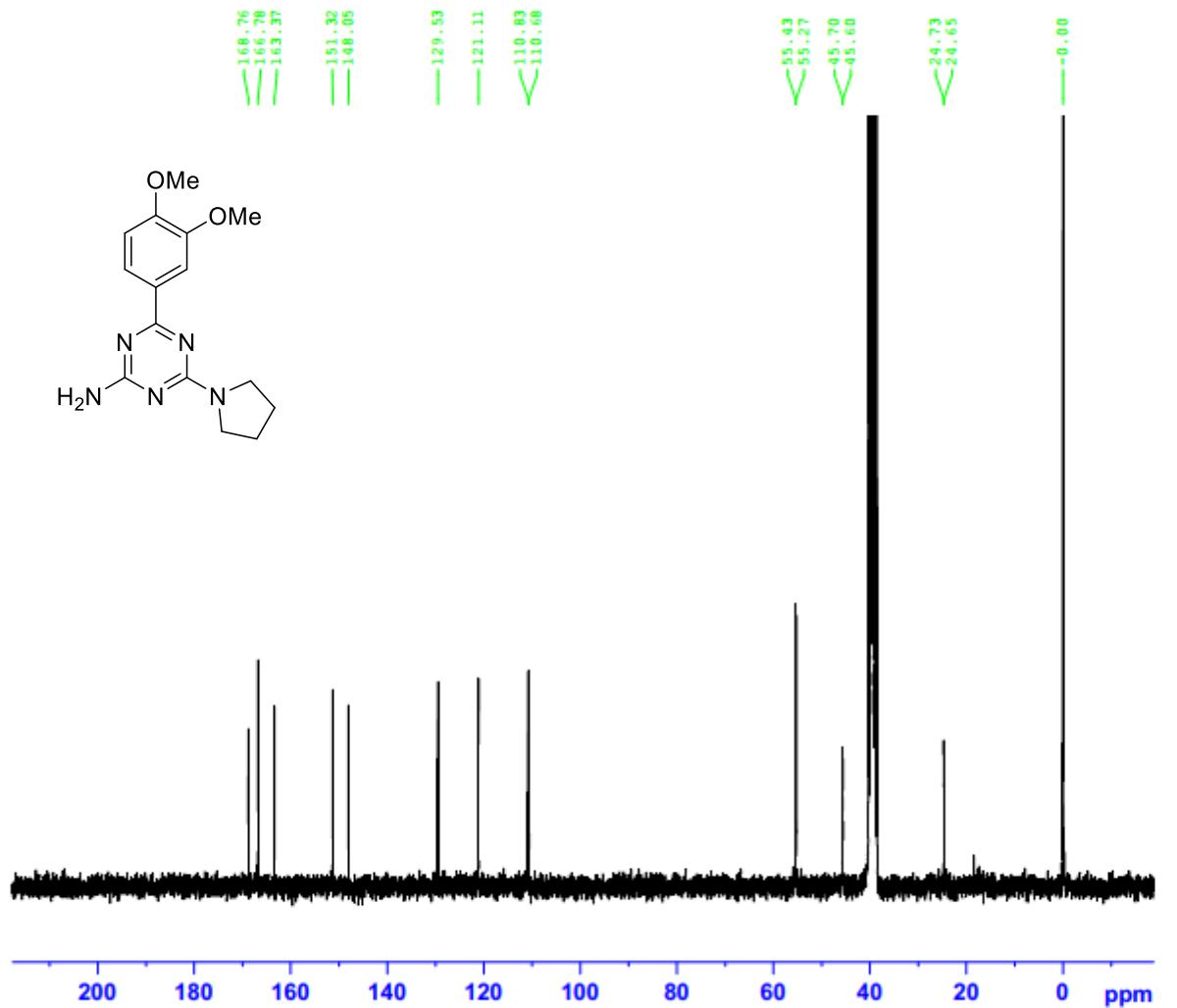
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 FIDRES 0.093132 Hz
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 RG 69.8765
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

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

F2 - Processing parameters
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6-(3,4-Dimethoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,16}**)



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PROCNO 1

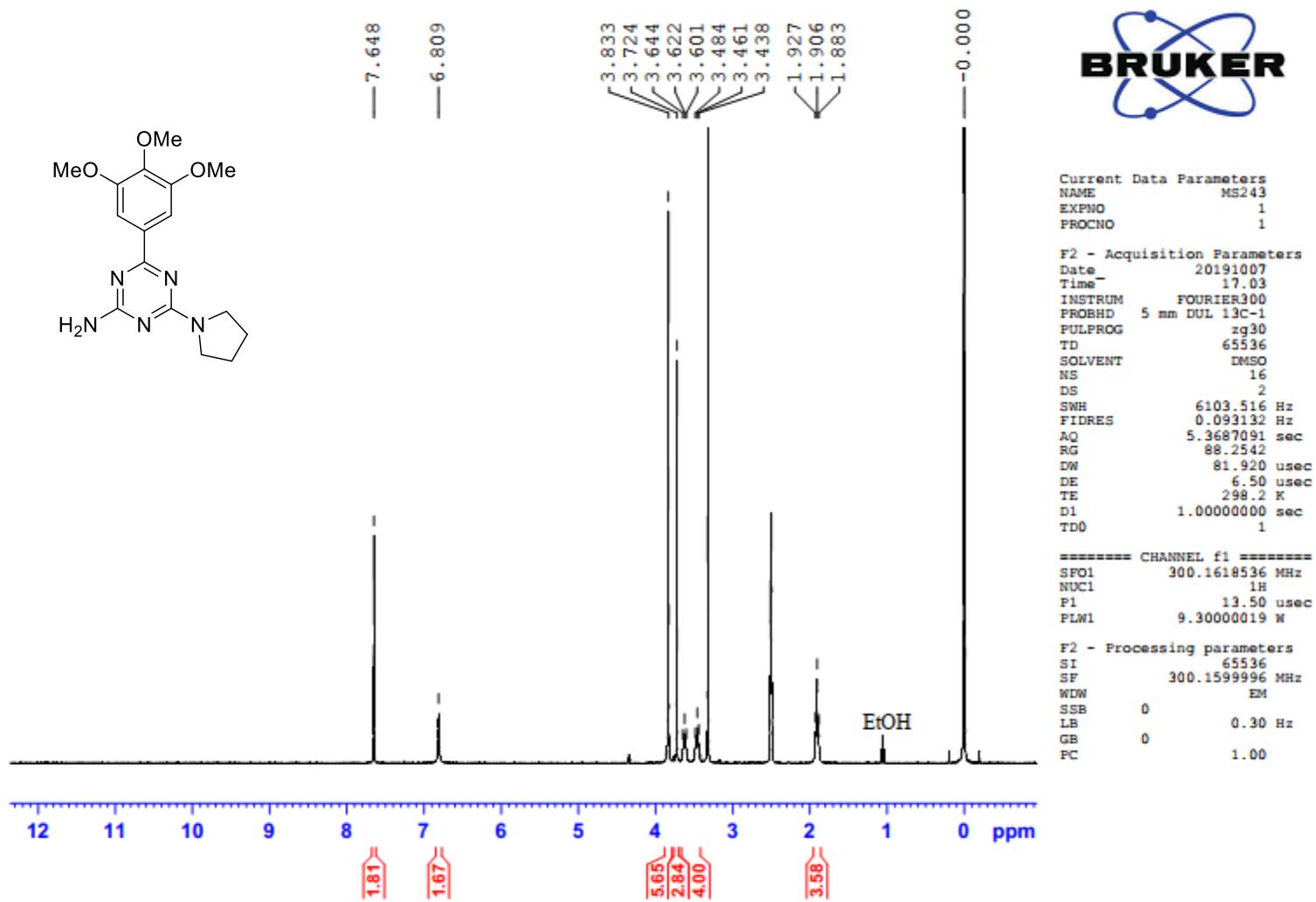
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NS 6144
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D40 0.00439029 sec
L1 37
L2 53
P32 98.00 usec
TDO 6

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NUC1 13C
PL 15.00 usec
PLW1 22.00000000 W

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NUC2 1H
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PLW2 9.30000019 W
PLW12 0.29359001 W
PLW13 0.20359001 W

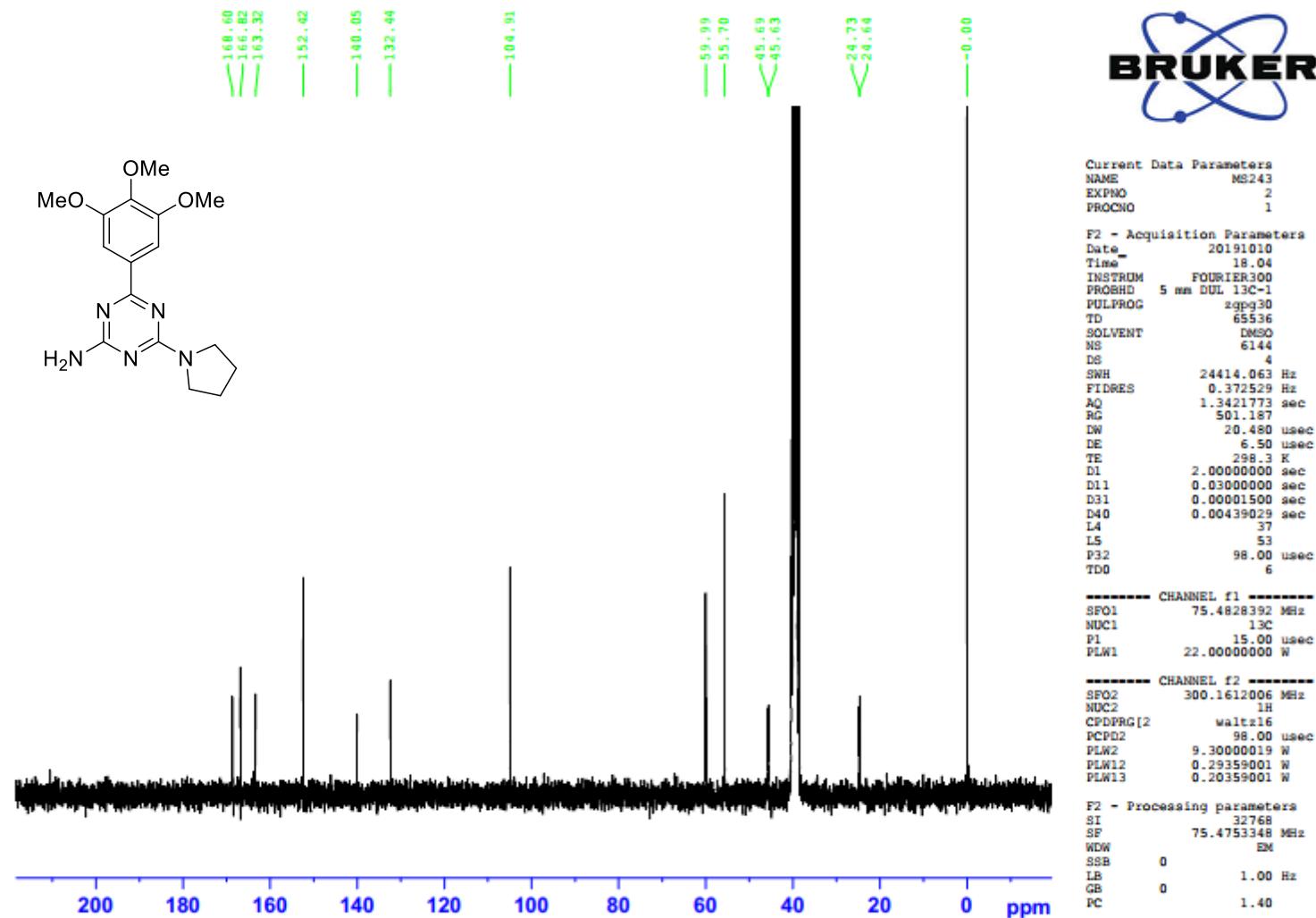
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6-(3,4,5-Trimethoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,17}**)

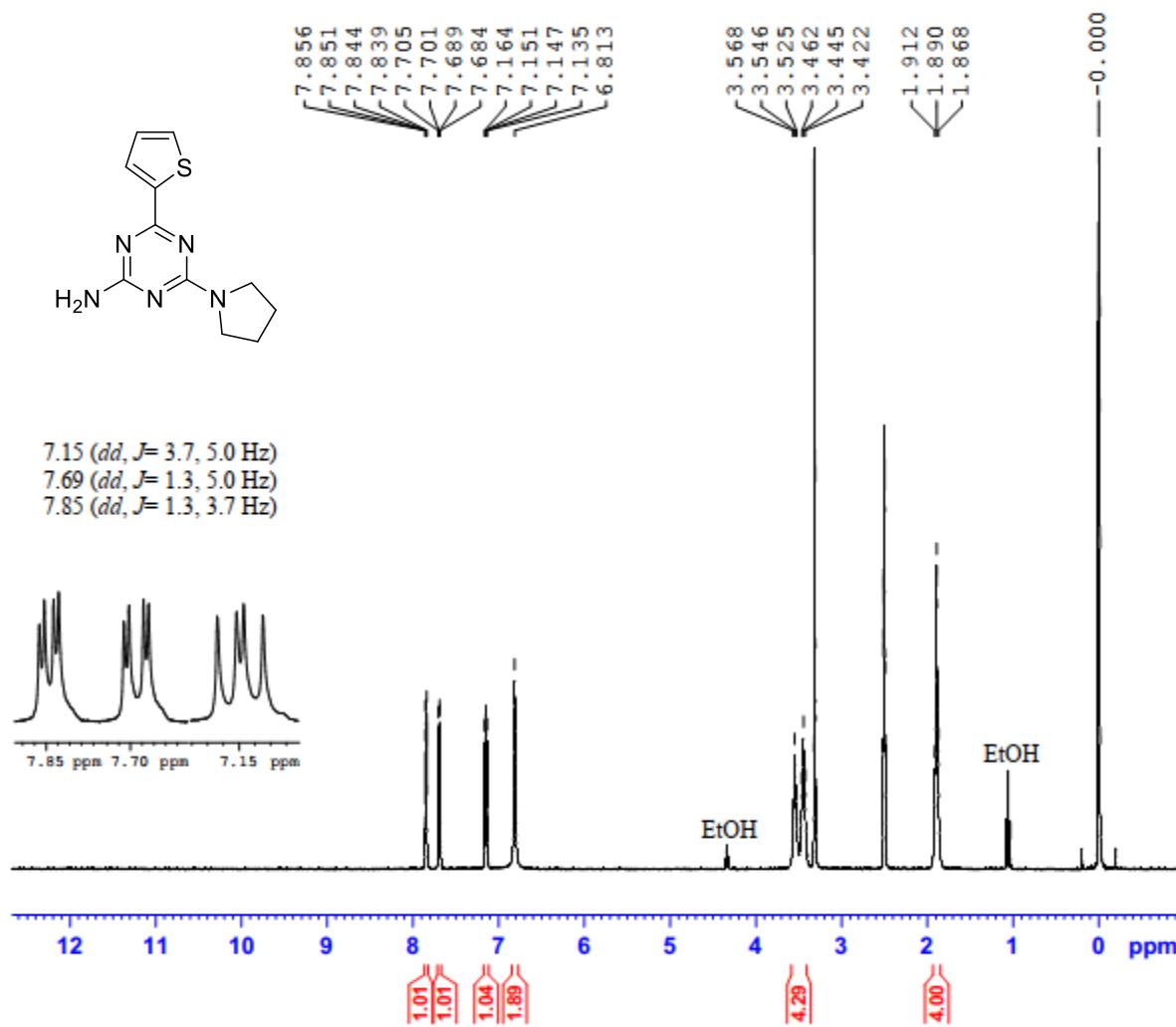


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6-(3,4,5-Trimethoxyphenyl)-4-pyrrolidino-1,3,5-triazine-2-amine (**9{1,17}**)



4-Pyrrolidino-6-(2-thienyl)-1,3,5-triazine-2-amine (**9{1,18}**)



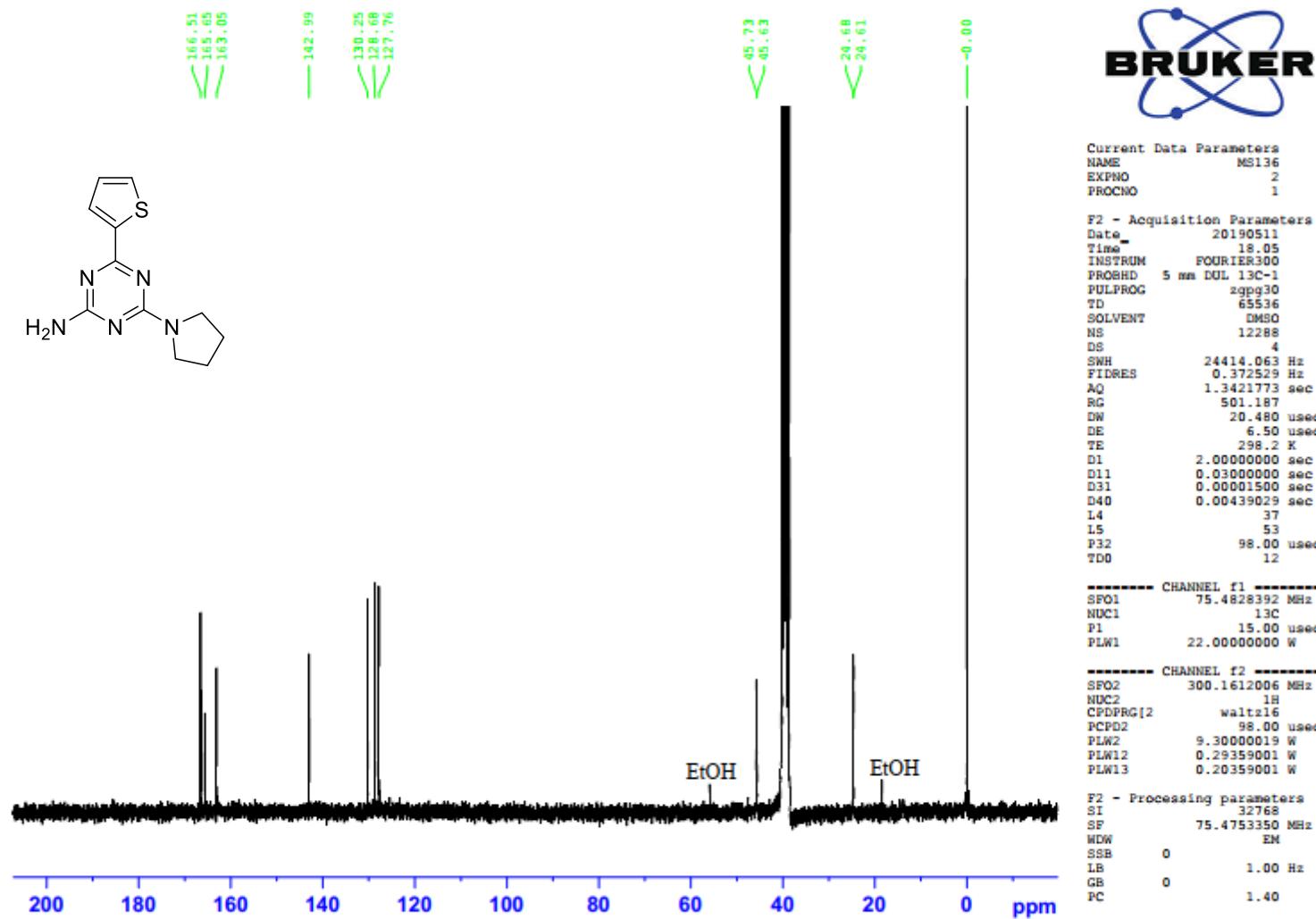
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 SOLVENT DMSO
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 DS 2
 SWH 6103.516 Hz
 FIDRES 0.093132 Hz
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 RG 99.2044
 DW 81.920 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.0000000 sec
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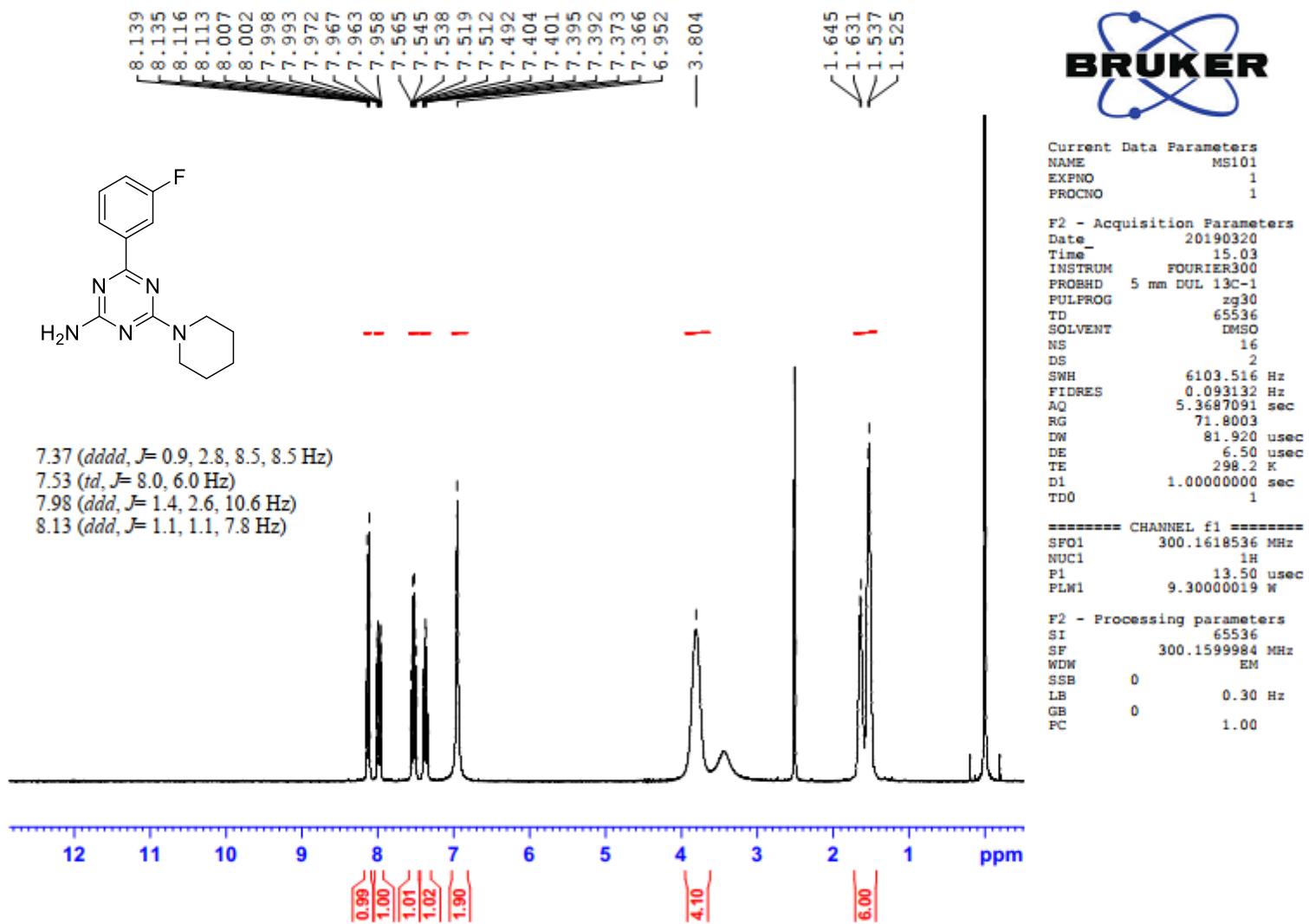
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 PC 1.00

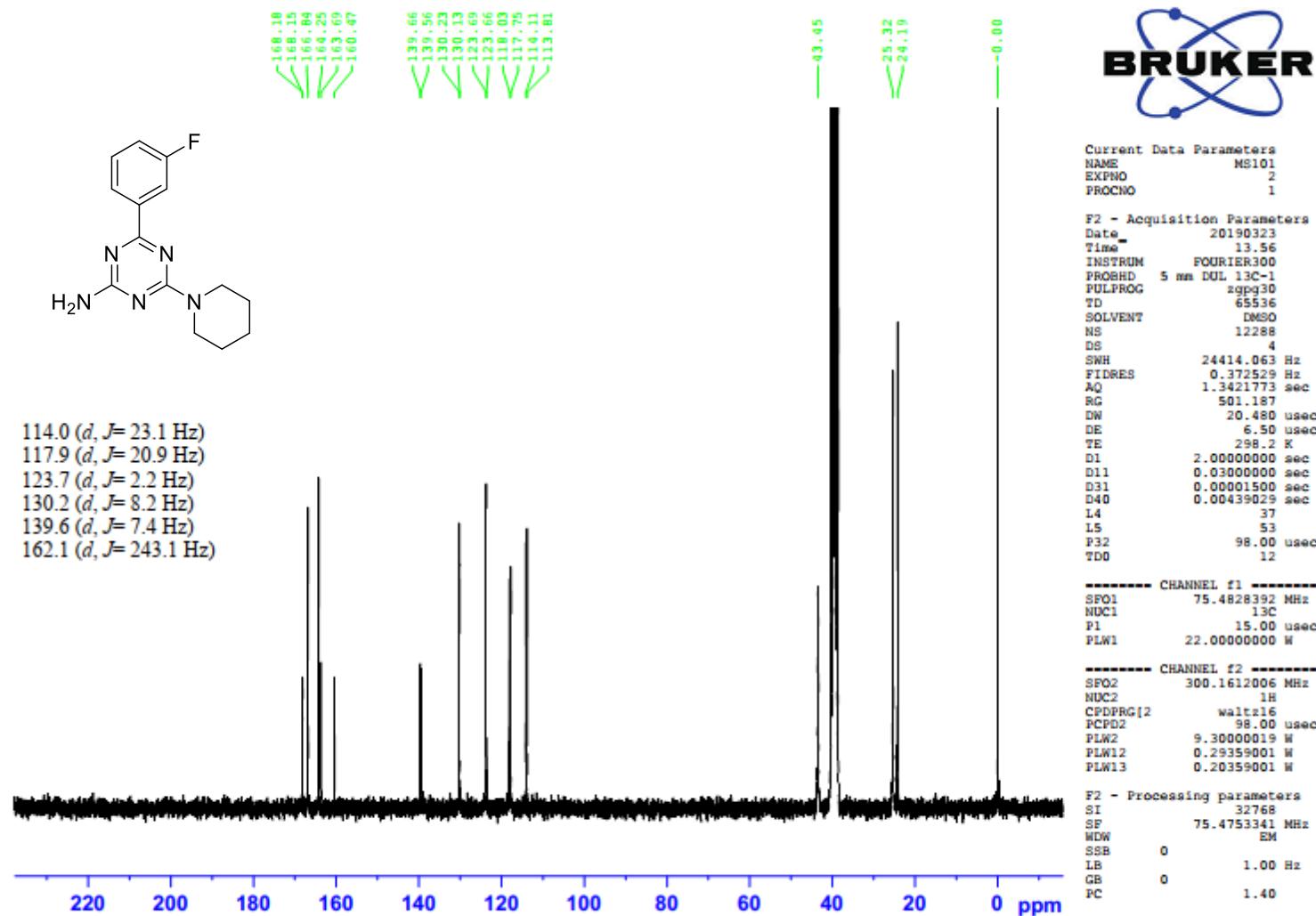
4-Pyrrolidino-6-(2-thienyl)-1,3,5-triazine-2-amine (**9{1,18}**)



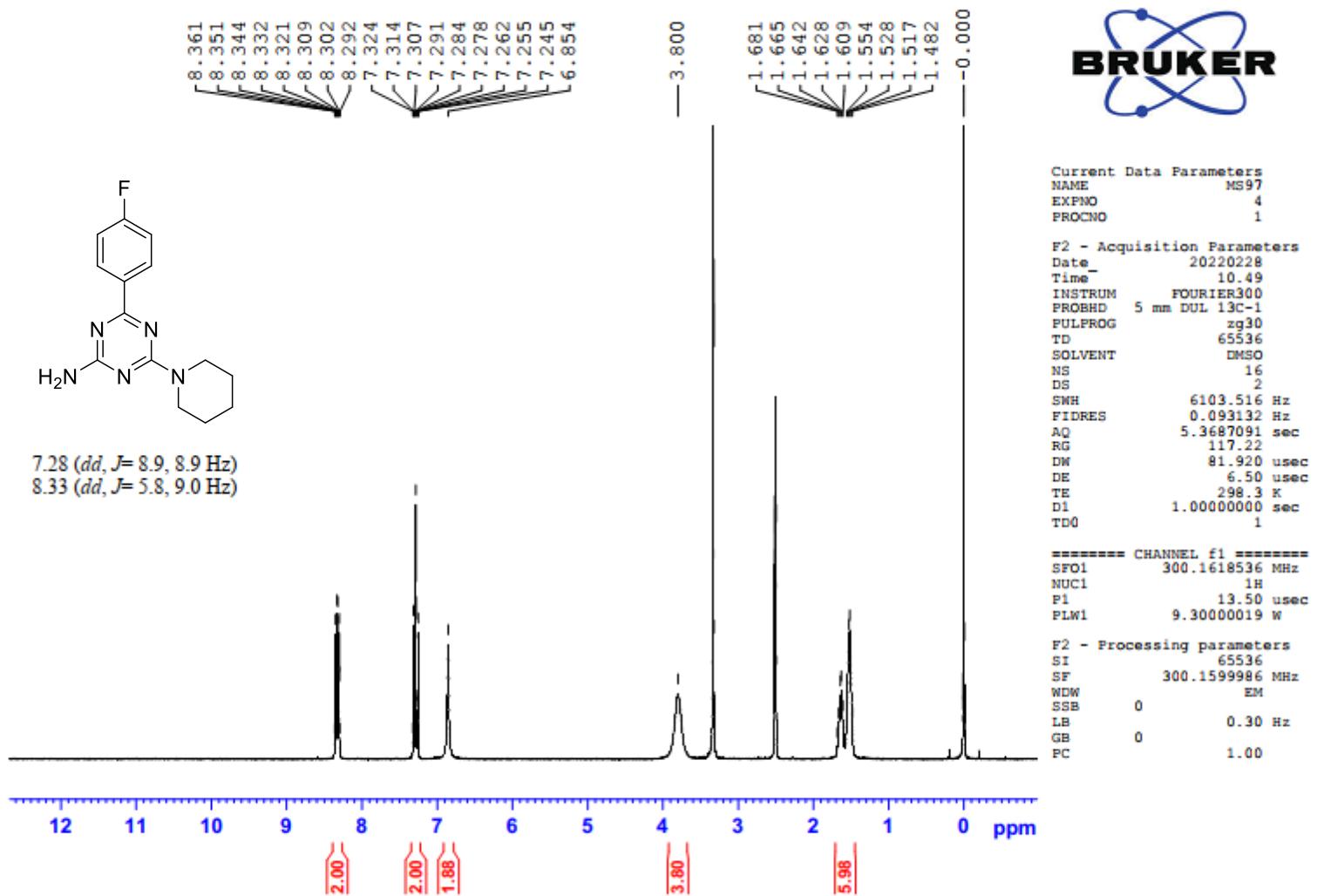
6-(3-Fluorophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,2}**)



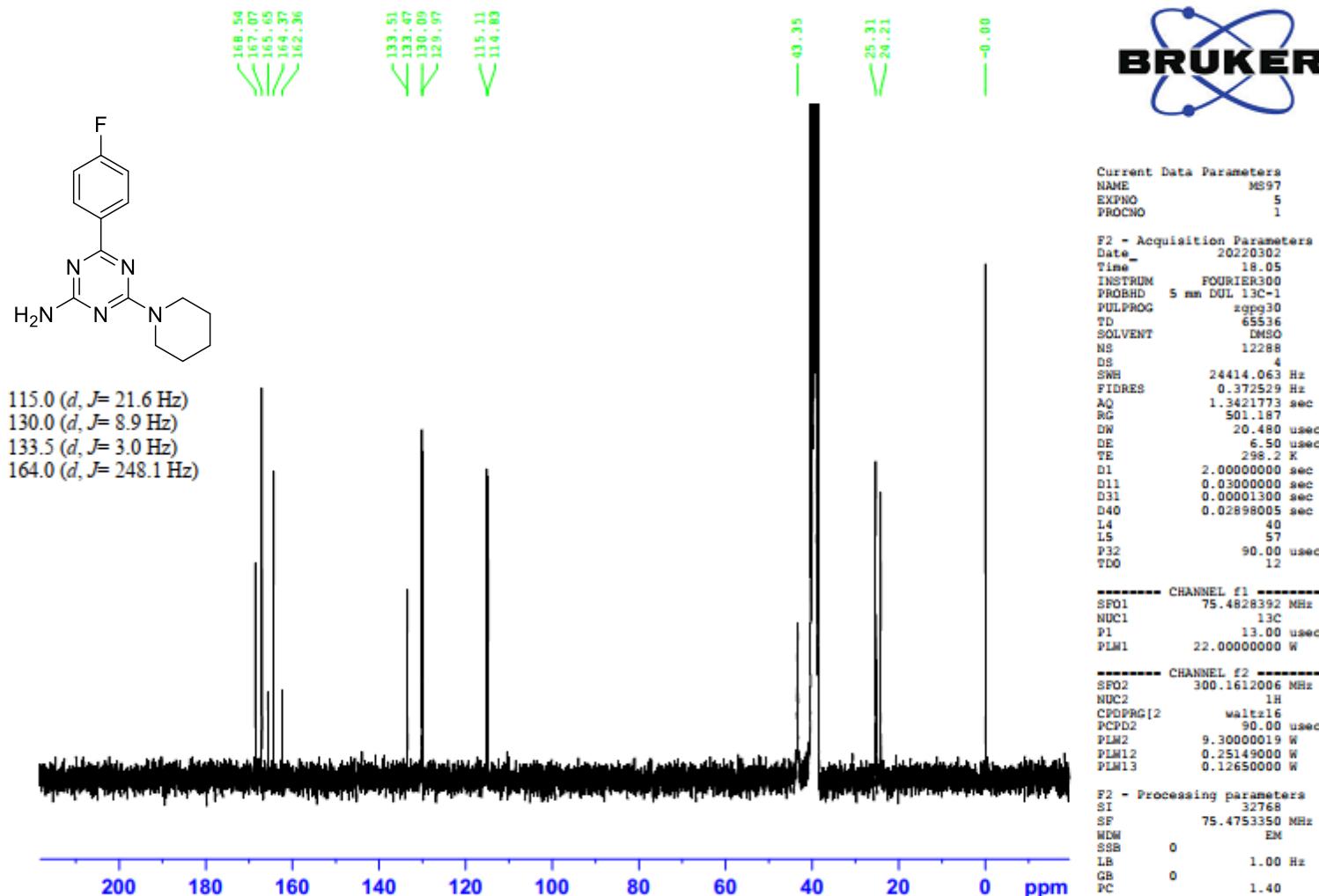
6-(3-Fluorophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,2}**)



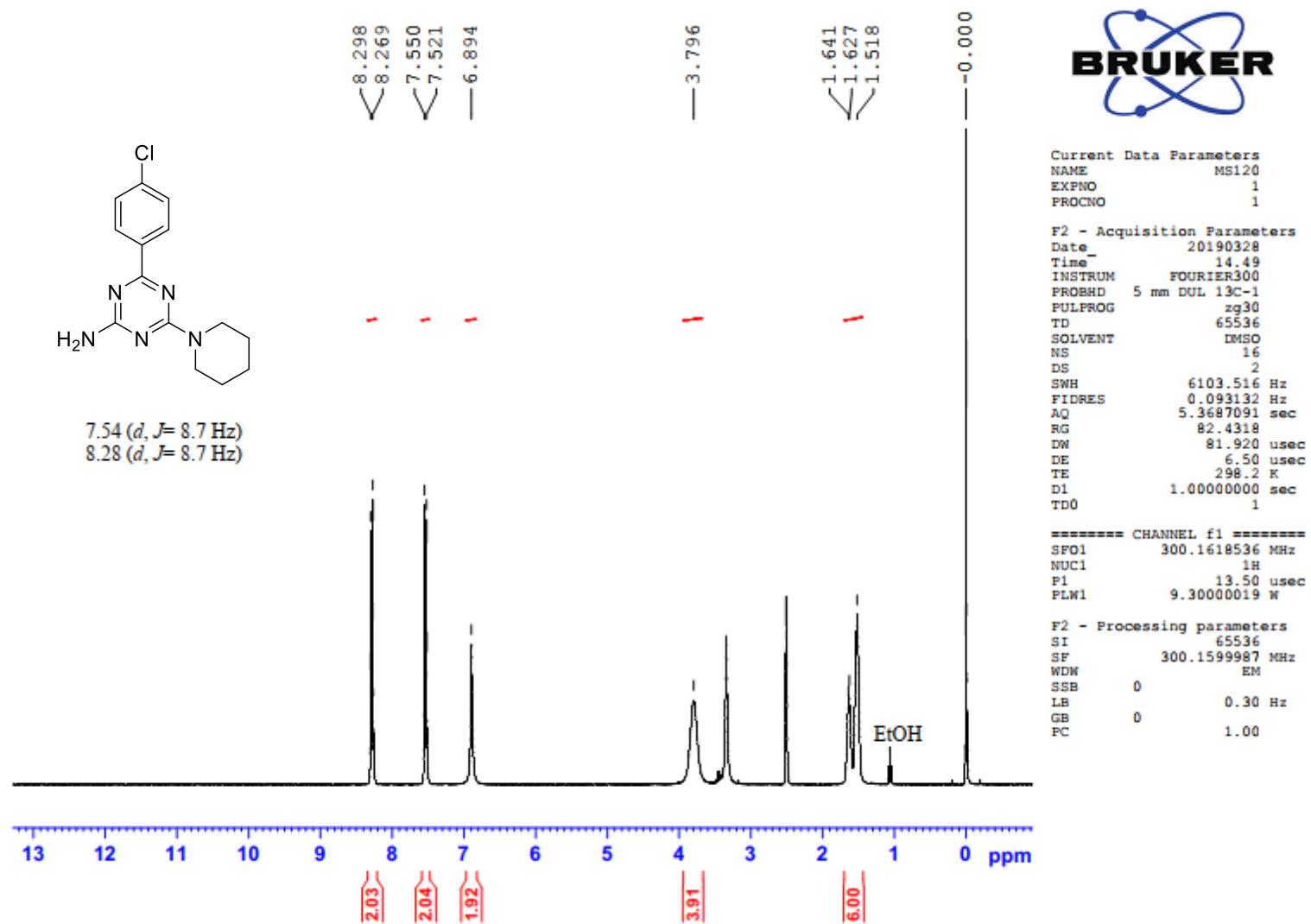
6-(4-Fluorophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,3}**)



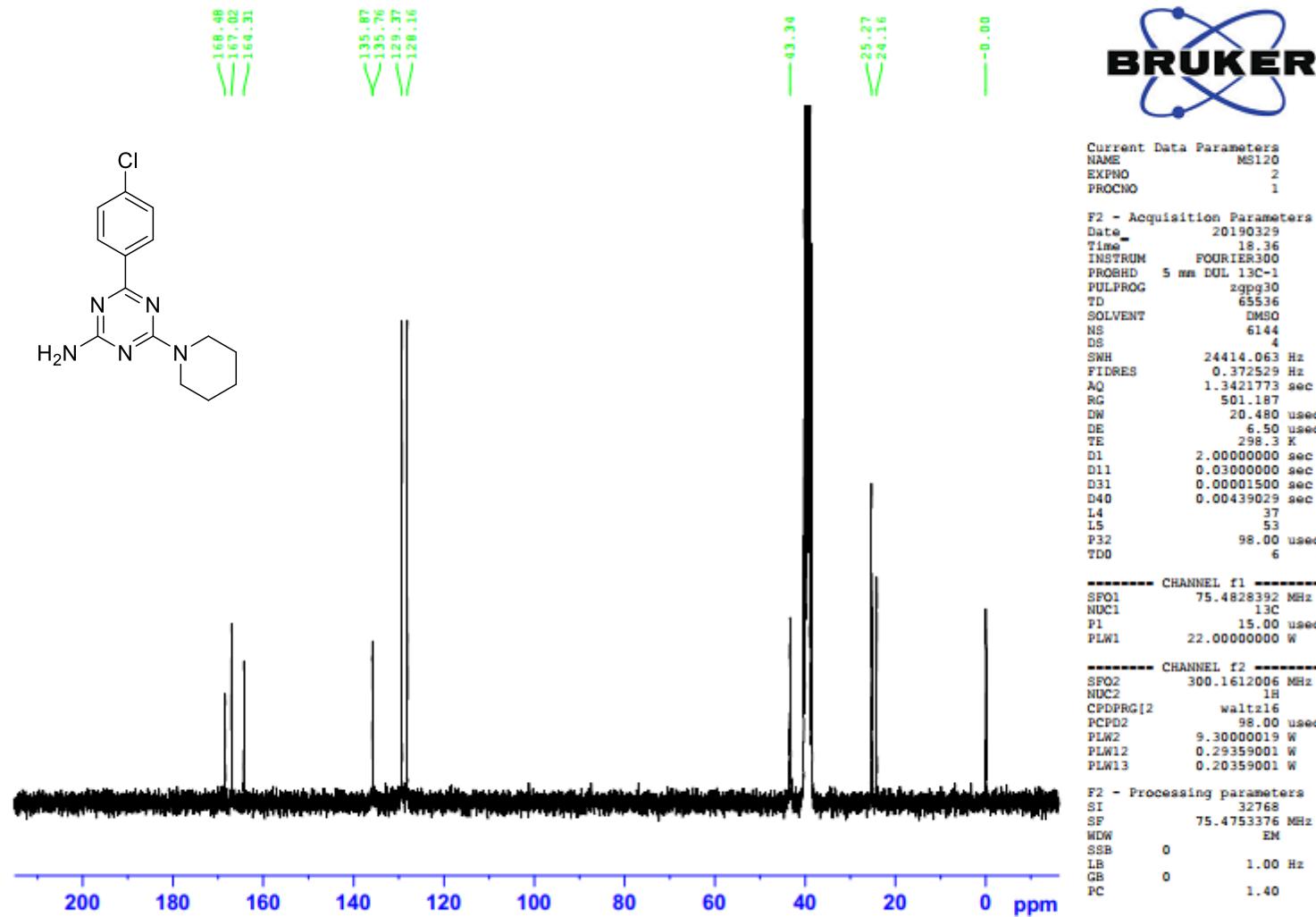
6-(4-Fluorophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,3}**)



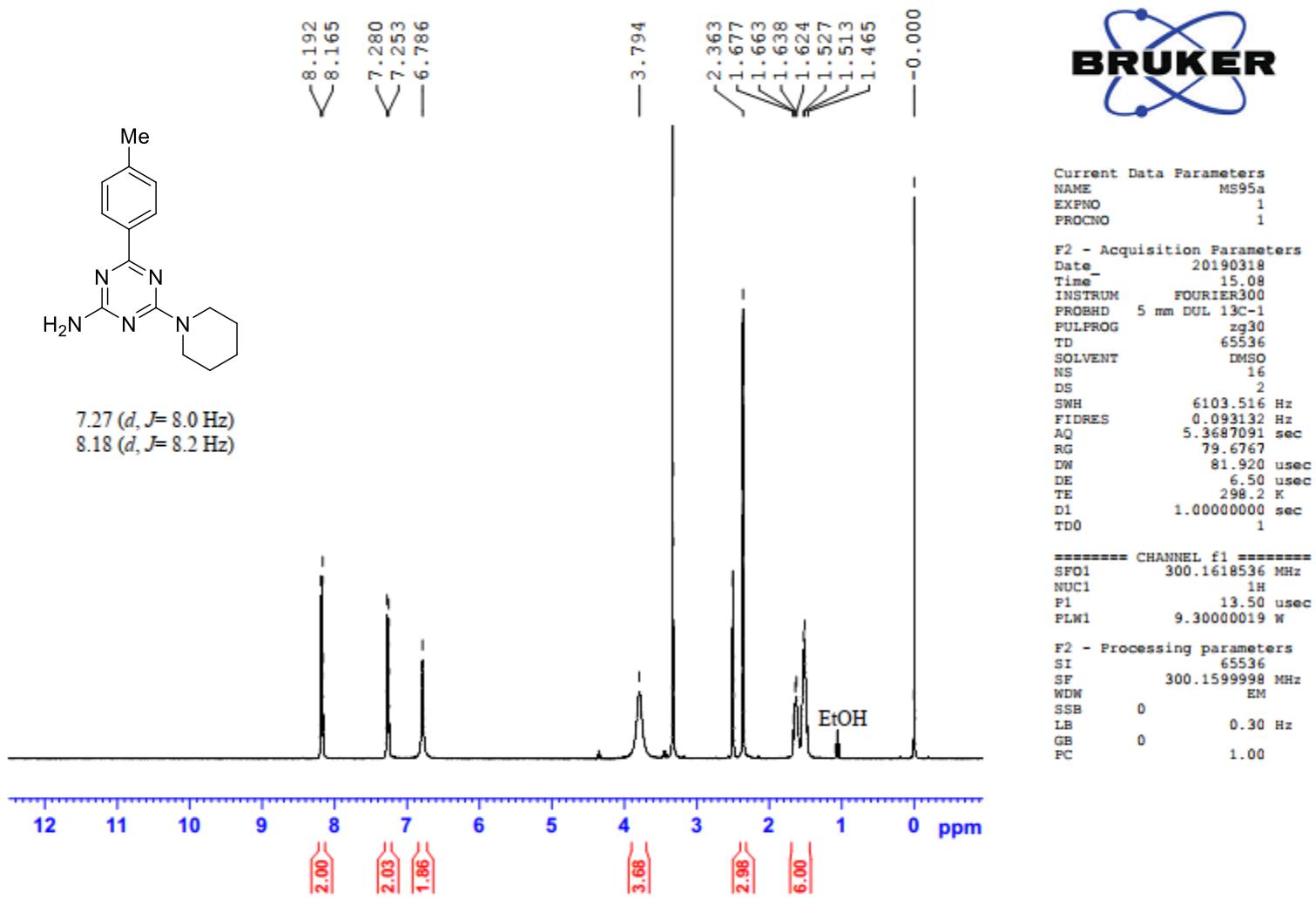
6-(4-Chlorophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,4}**)



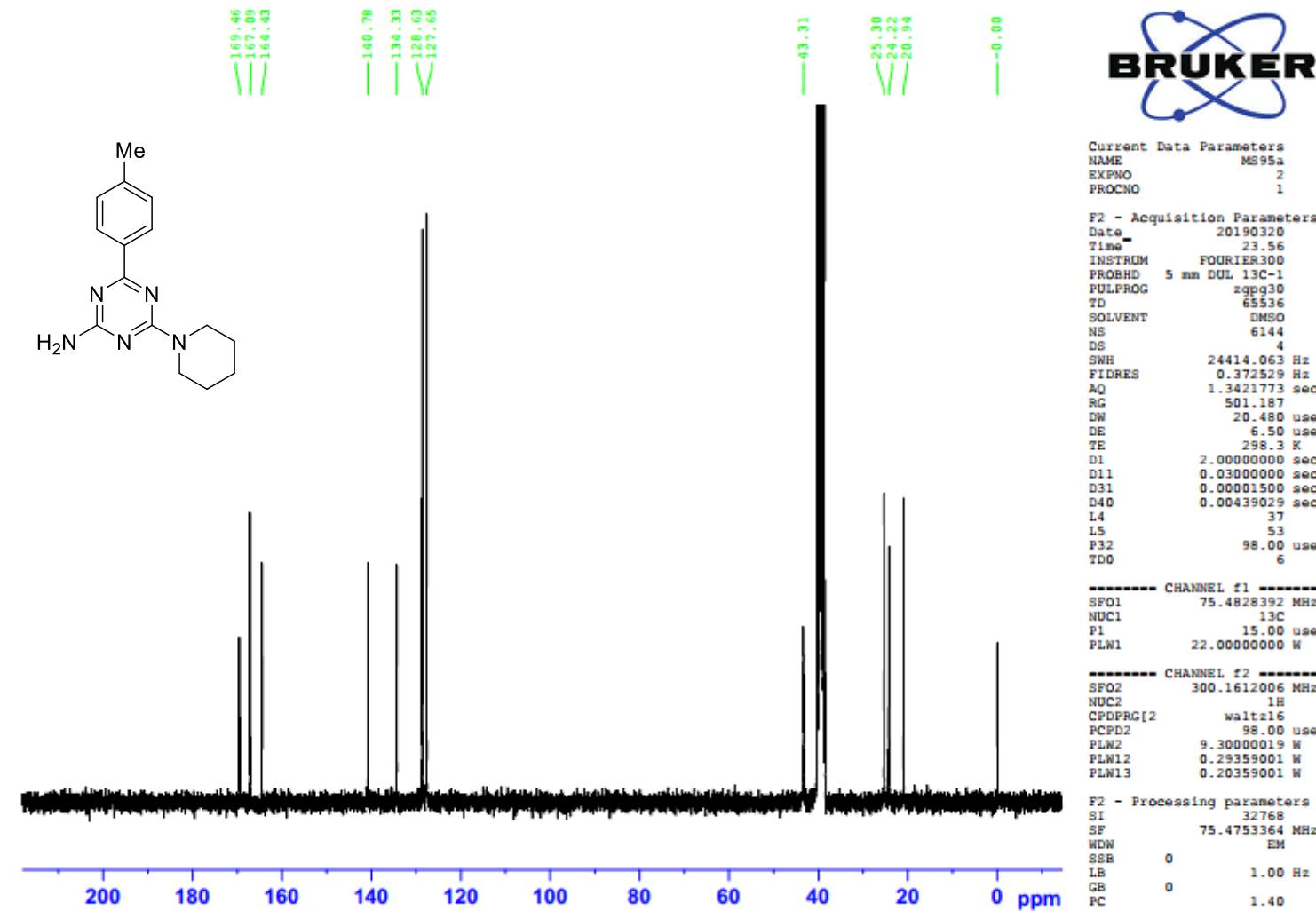
6-(4-Chlorophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,4}**)



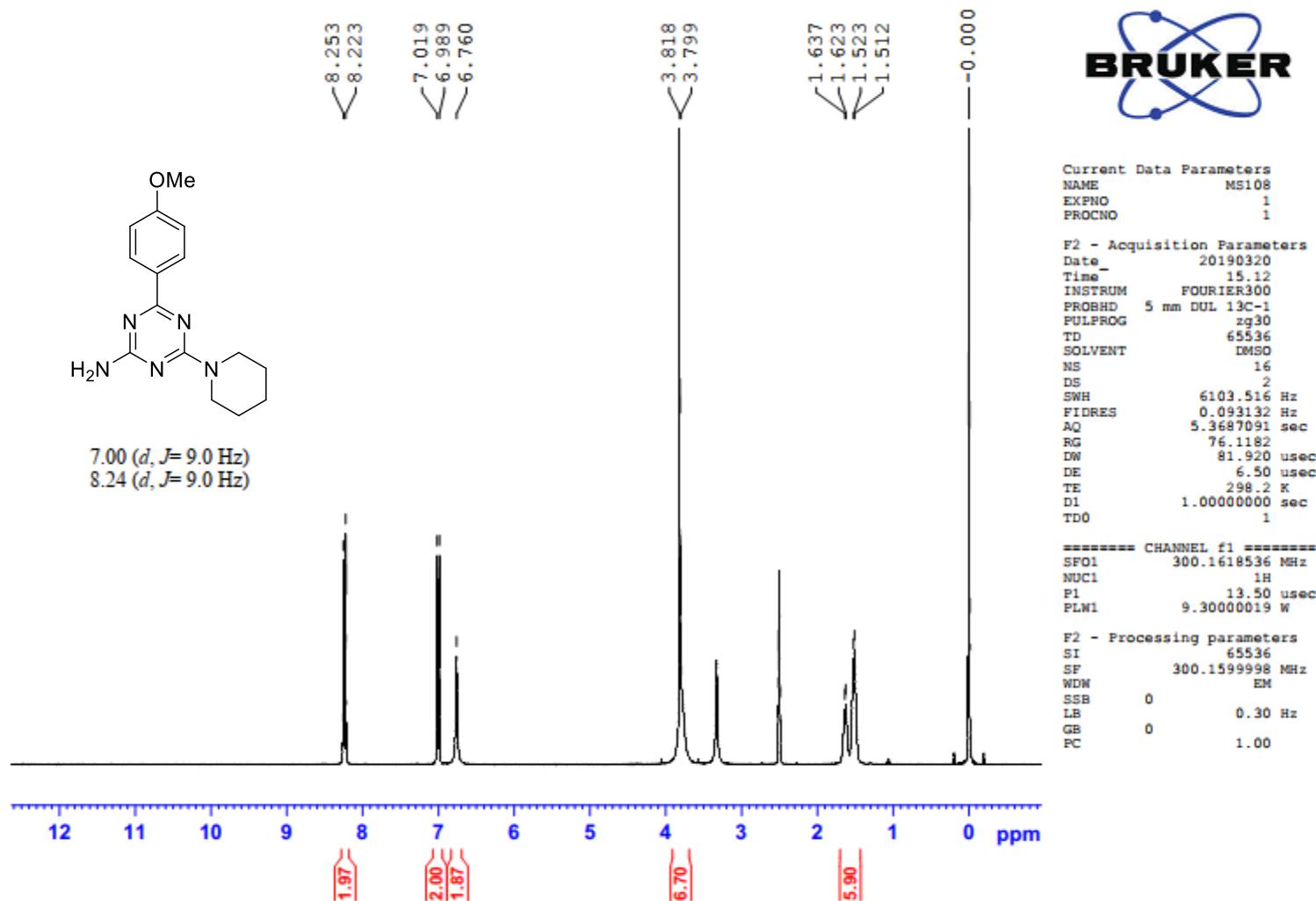
6-(4-Methylphenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,6}**)



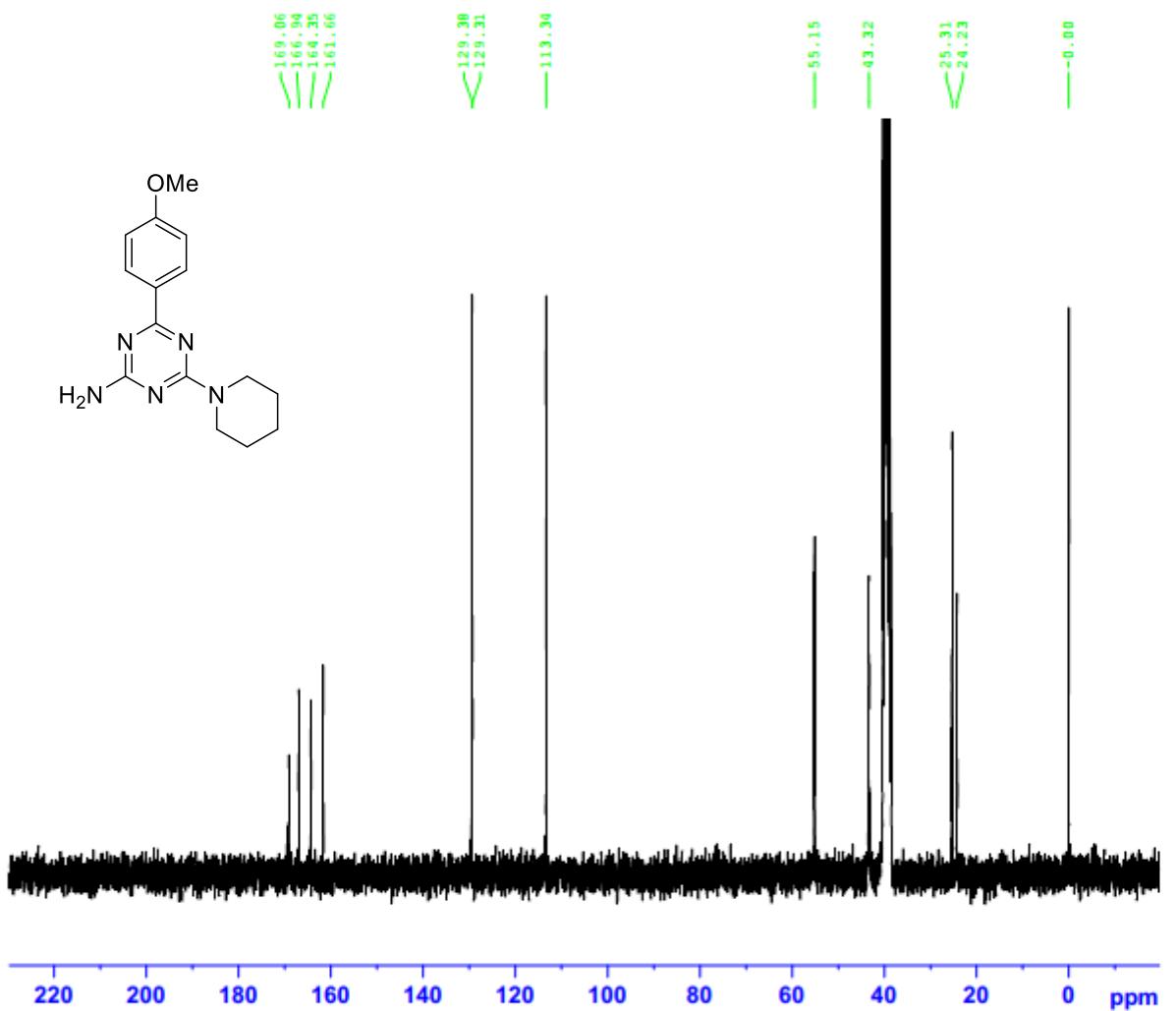
6-(4-Methylphenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,6}**)



6-(4-Methoxyphenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,9}**)



6-(4-Methoxyphenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,9}**)



Current Data Parameters
 NAME MS108
 EXPNO 2
 PROCN0 1

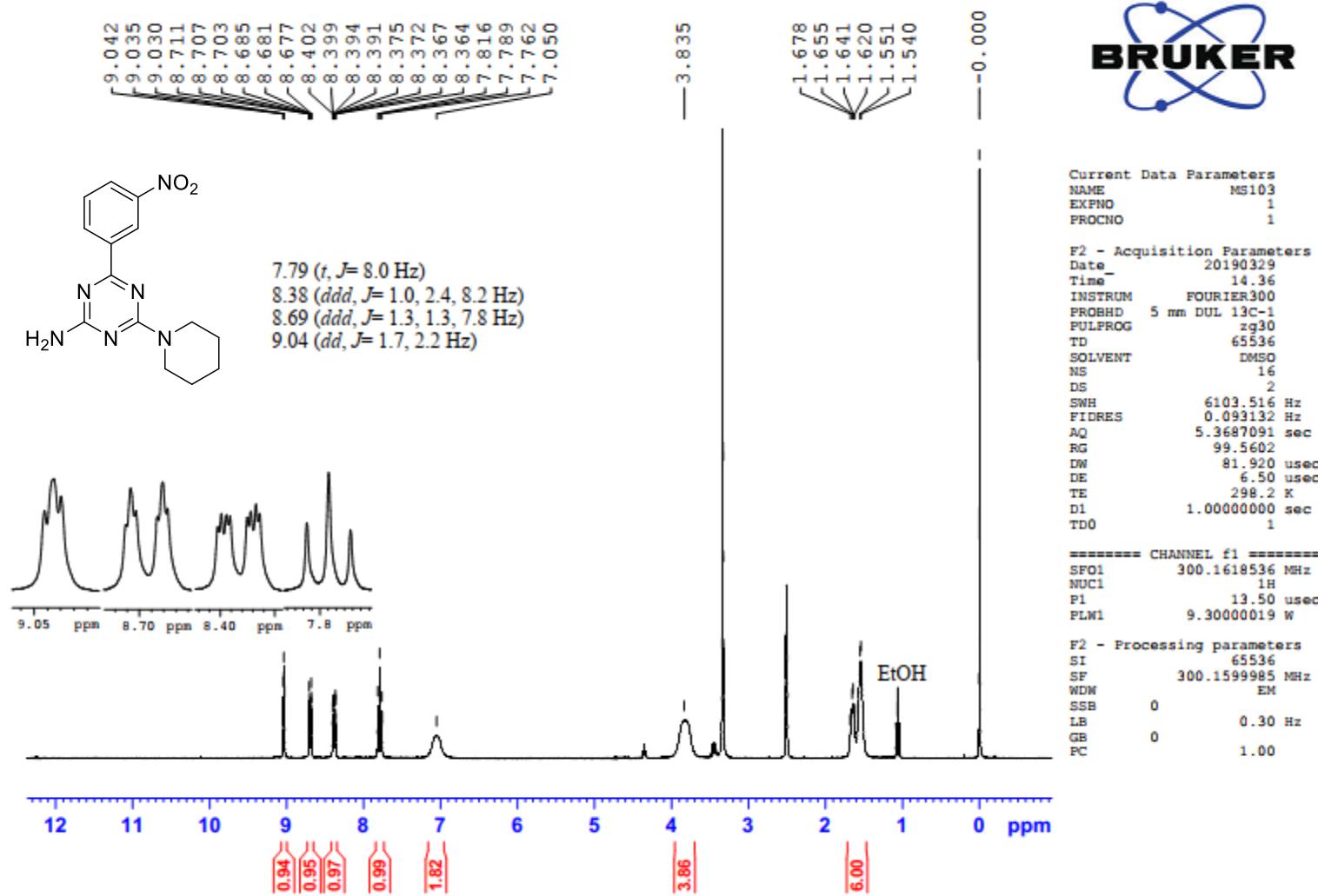
F2 - Acquisition Parameters
 Date 20190323
 Time 8.04
 INSTRUM FOURIER300
 PROBHD 5 mm DUL 13C-1
 PULPROG zpg30
 TD 65536
 SOLVENT DMSO
 NS 6144
 DS 4
 SWH 24414.063 Hz
 FIDRES 0.372529 Hz
 AQ 1.3421773 sec
 RG 501.187
 DW 20.480 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 D31 0.00001500 sec
 D40 0.00439029 sec
 L1 37
 L5 53
 P32 98.00 usec
 TDO 6

----- CHANNEL f1 -----
 SFO1 75.4828392 MHz
 NUC1 ¹³C
 P1 15.00 usec
 PLW1 22.0000000 W

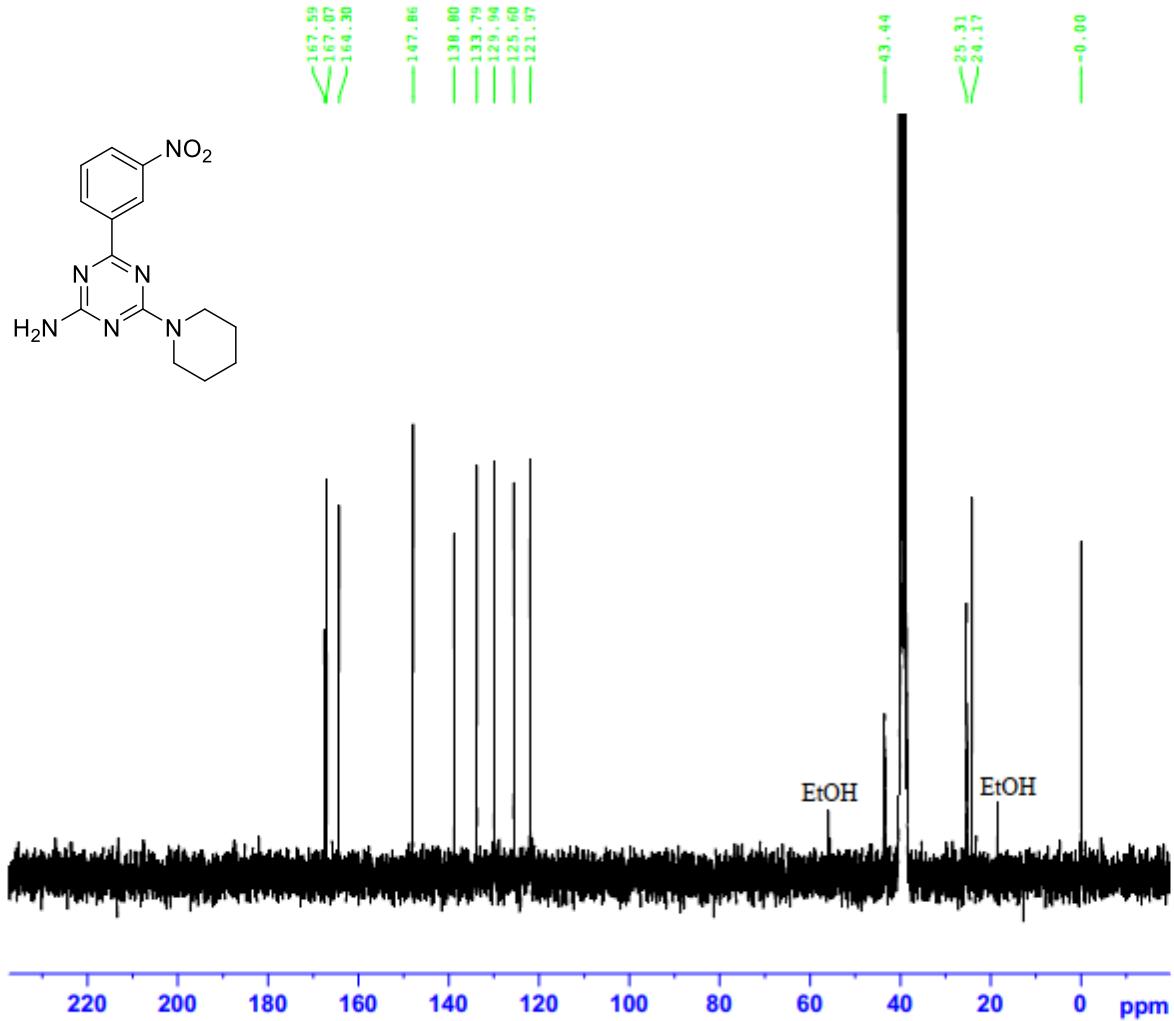
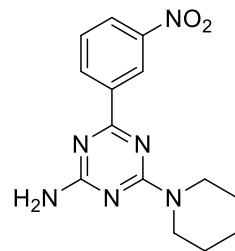
----- CHANNEL f2 -----
 SFO2 300.1612006 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 98.00 usec
 PLW2 9.30000019 W
 PLW12 0.29359001 W
 PLW13 0.20359001 W

F2 - Processing parameters
 SI 32768
 SF 75.4753363 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

6-(3-Nitrophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,10}**)



6-(3-Nitrophenyl)-4-piperidino-1,3,5-triazine-2-amine (**9{2,10}**)



BRUKER

Current	Data	Parameters
NAME		MS103
EXPNNO		2
PROCNO		1

```

P2 - Acquisition Parameters
Date_      20100411
Time_      6.19
INSTRUM_   FOURIER300
PROBHD_    5 mm DUL 13c-1
PROBTYPE_  PULPROG
TE_        30000
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
TDD_       3

```

----- CHANNEL f1 -----
SFO1 75.4828392 MHz
NUC1 13C
P1 15.00 usec
NUC2 00.00000000

```
----- CHANNEL f2 -----
SF02      300.1612006 MHz
NUC2      1H
CPDPRG[2]  waltr16
PCPD2     98.00 user
PUS2      9.300000019 m
```

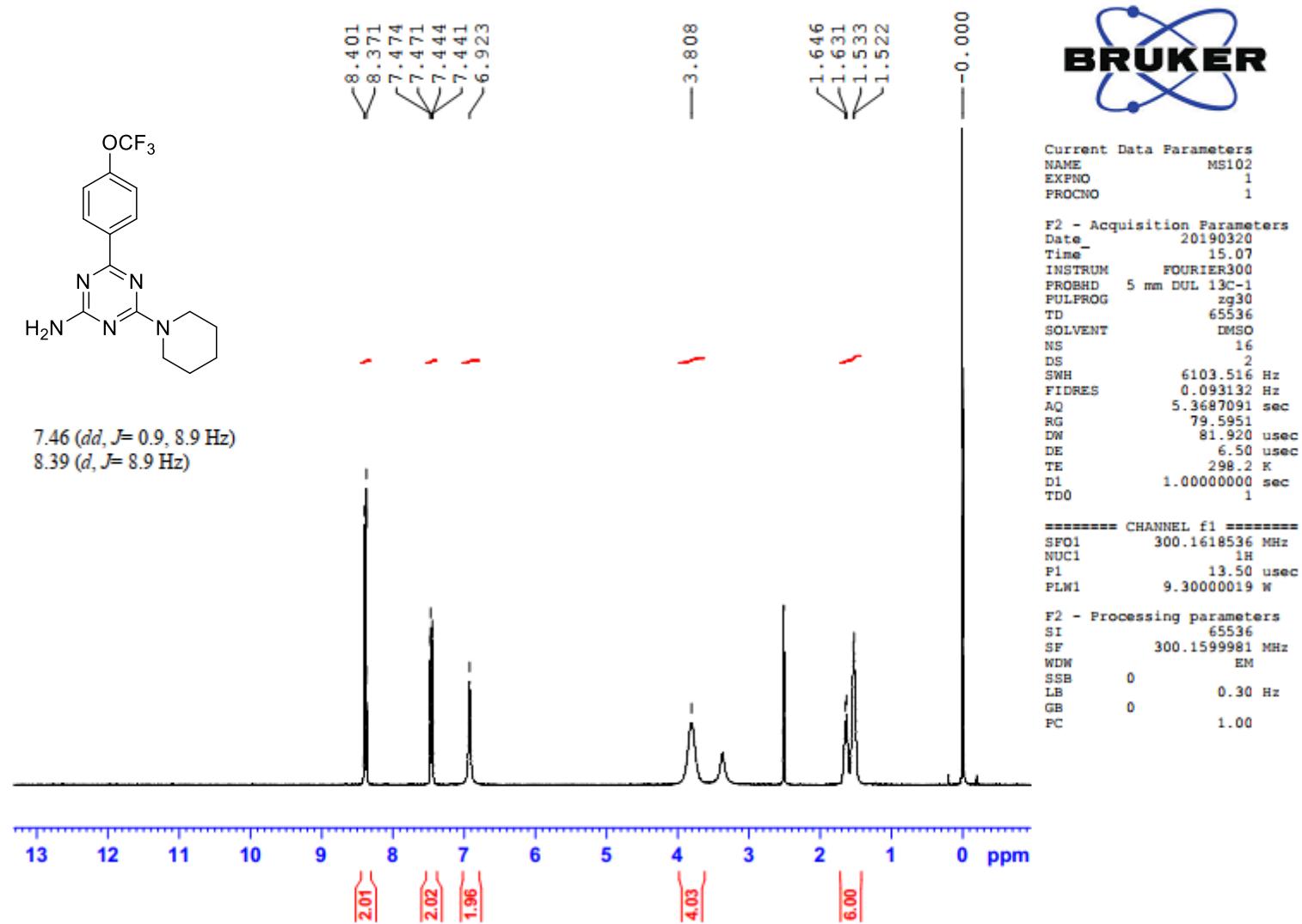
```

PLW13          0.20359001 W

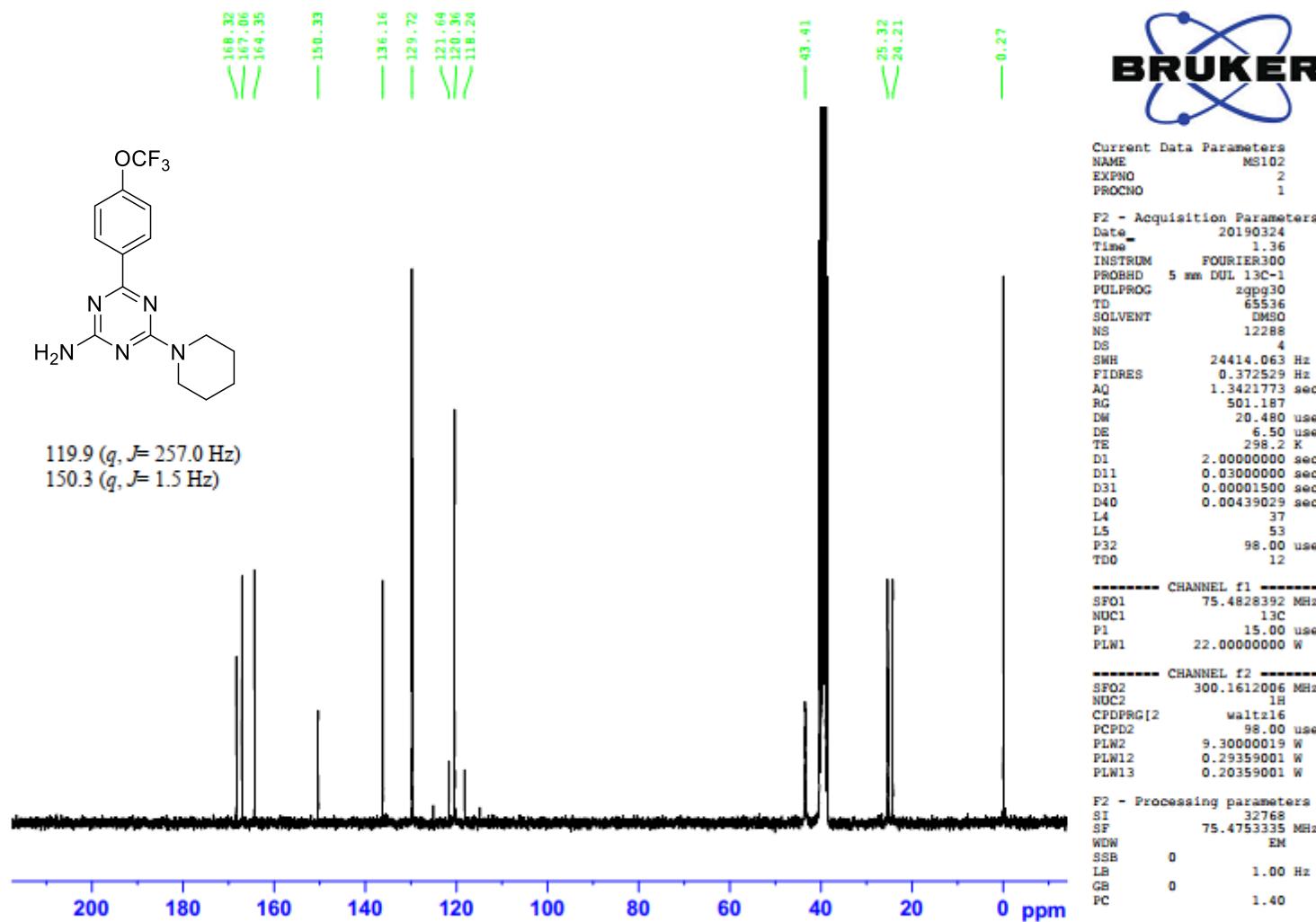
P2 = Processing parameters
SI           32768
SF      75.4753344 MHz
MDW          EM
SSB          0
LB           1.00 Hz
GB          0
PC          1.40

```

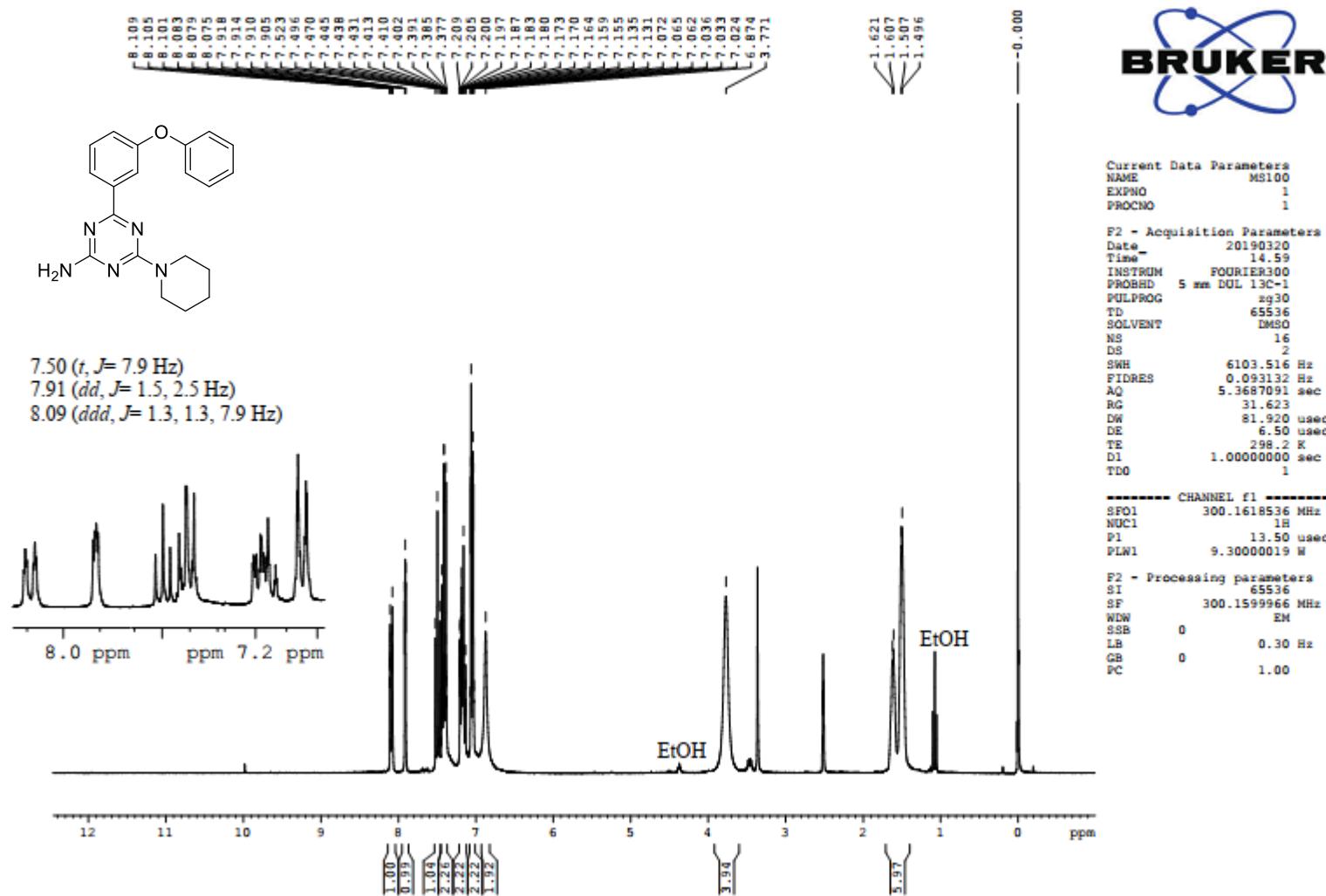
6-[4-(Trifluoromethoxy)phenyl]-4-piperidino-1,3,5-triazine-2-amine (**9{2,12}**)



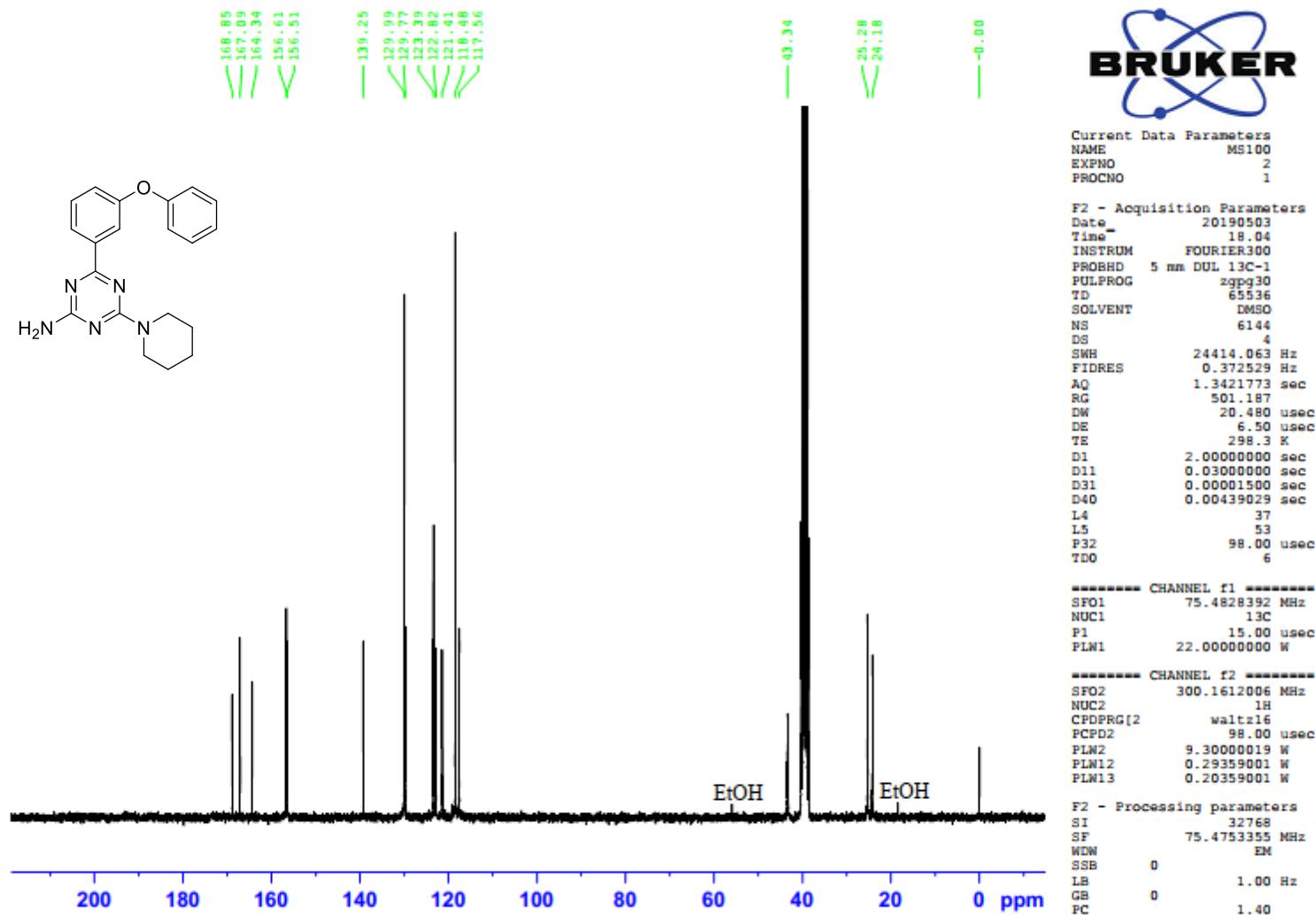
6-[4-(Trifluoromethoxy)phenyl]-4-piperidino-1,3,5-triazine-2-amine (**9{2,12}**)



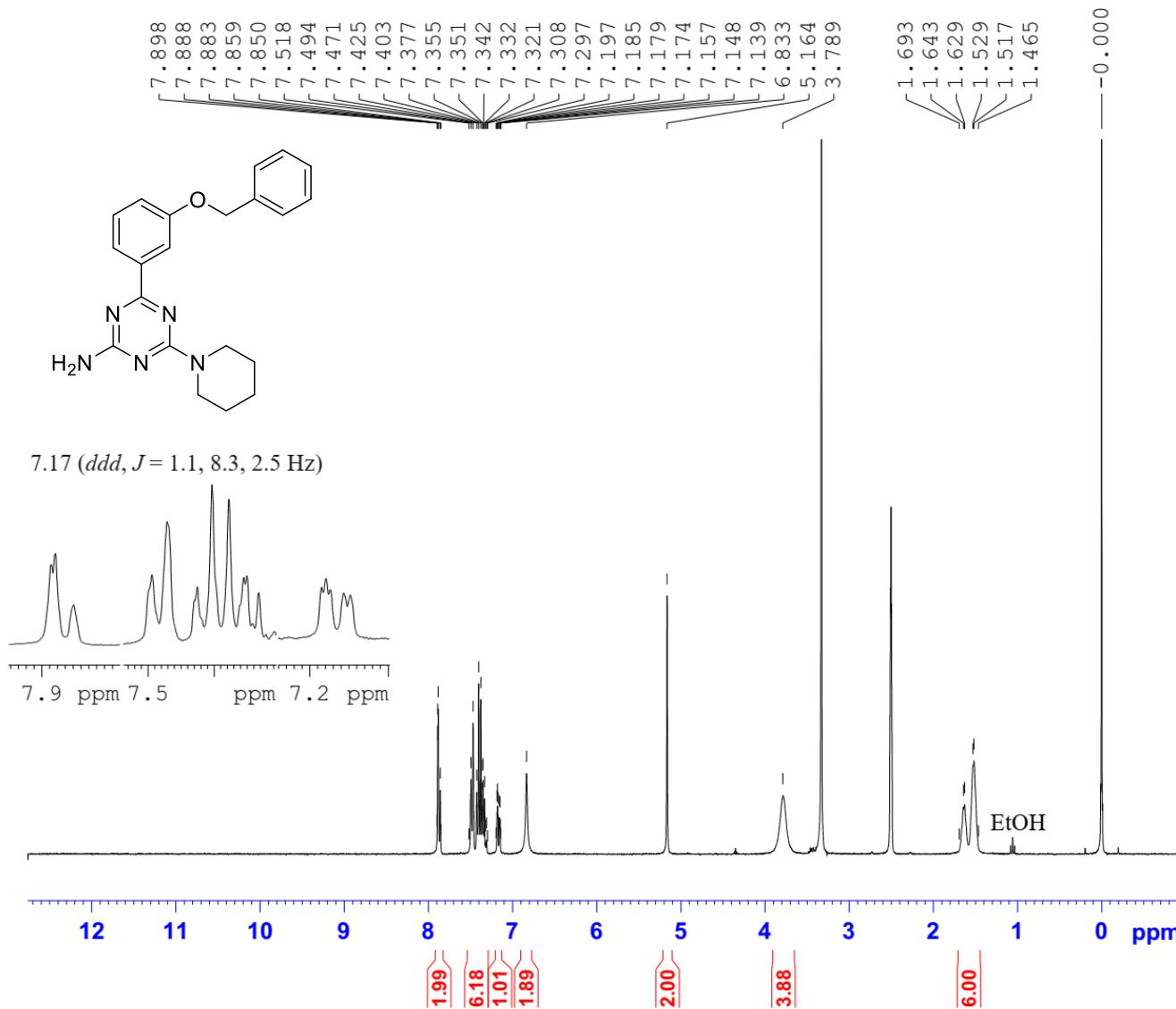
4-Piperidino-6-(3-phenoxyphenyl)-1,3,5-triazine-2-amine (**9{2,13}**)



4-Piperidino-6-(3-phenoxyphenyl)-1,3,5-triazine-2-amine (**9{2,13}**)



6-[3-(BenzylOxy)phenyl]-4-piperidino-1,3,5-triazine-2-amine (**9{2,14}**)



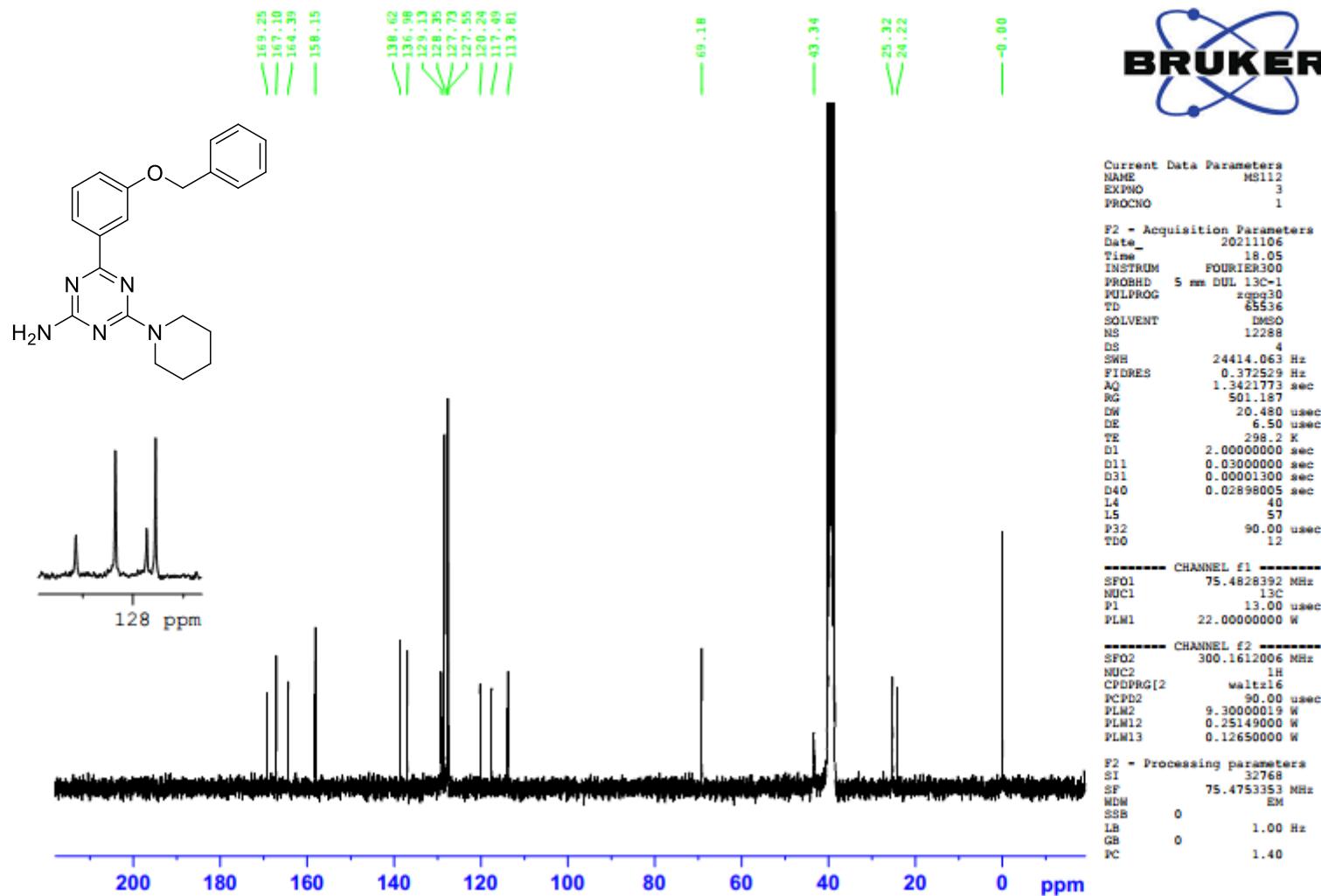
Current Data Parameters
NAME MS112
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20211105
Time 9.55
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 132.171
DW 81.920 usec
DE 6.50 usec
TE 298.1 K
D1 1.0000000 sec
TD0 1

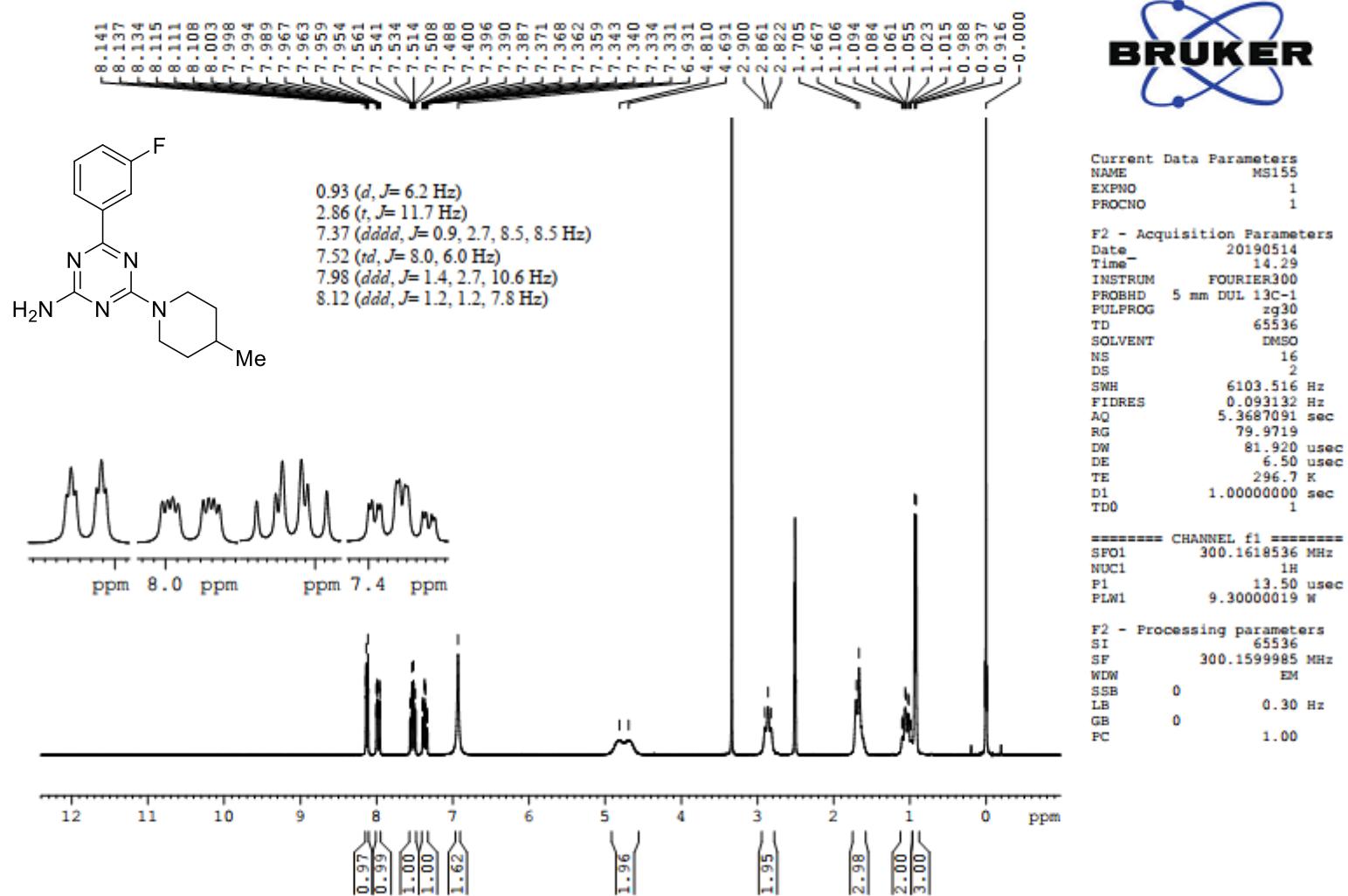
===== CHANNEL f1 =====
SFO1 300.1618536 MHz
NUC1 ¹H
P1 13.50 usec
PLW1 9.30000019 W

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

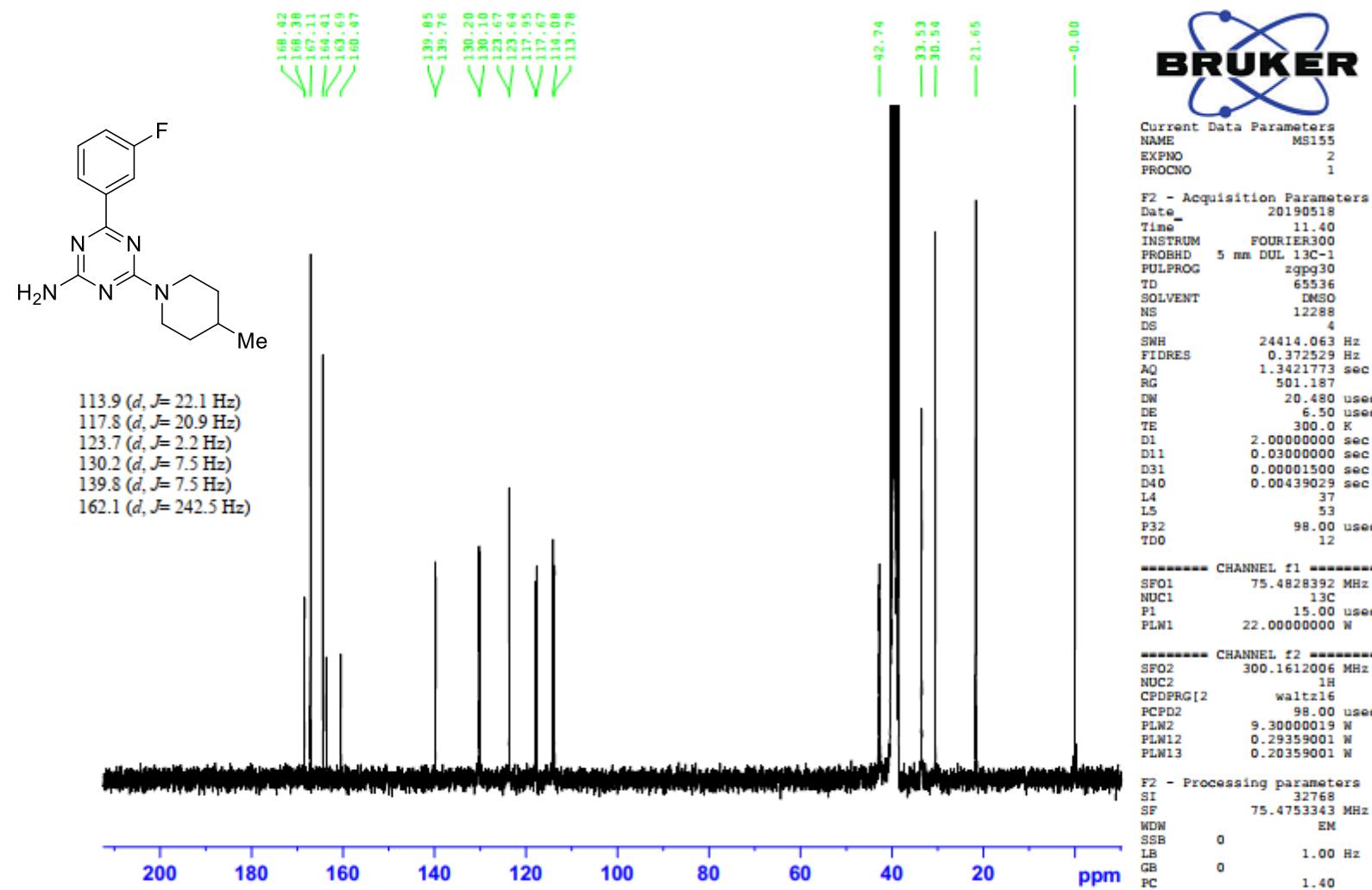
6-[3-(Benzylxy)phenyl]-4-piperidino-1,3,5-triazine-2-amine (**9**{2,14})



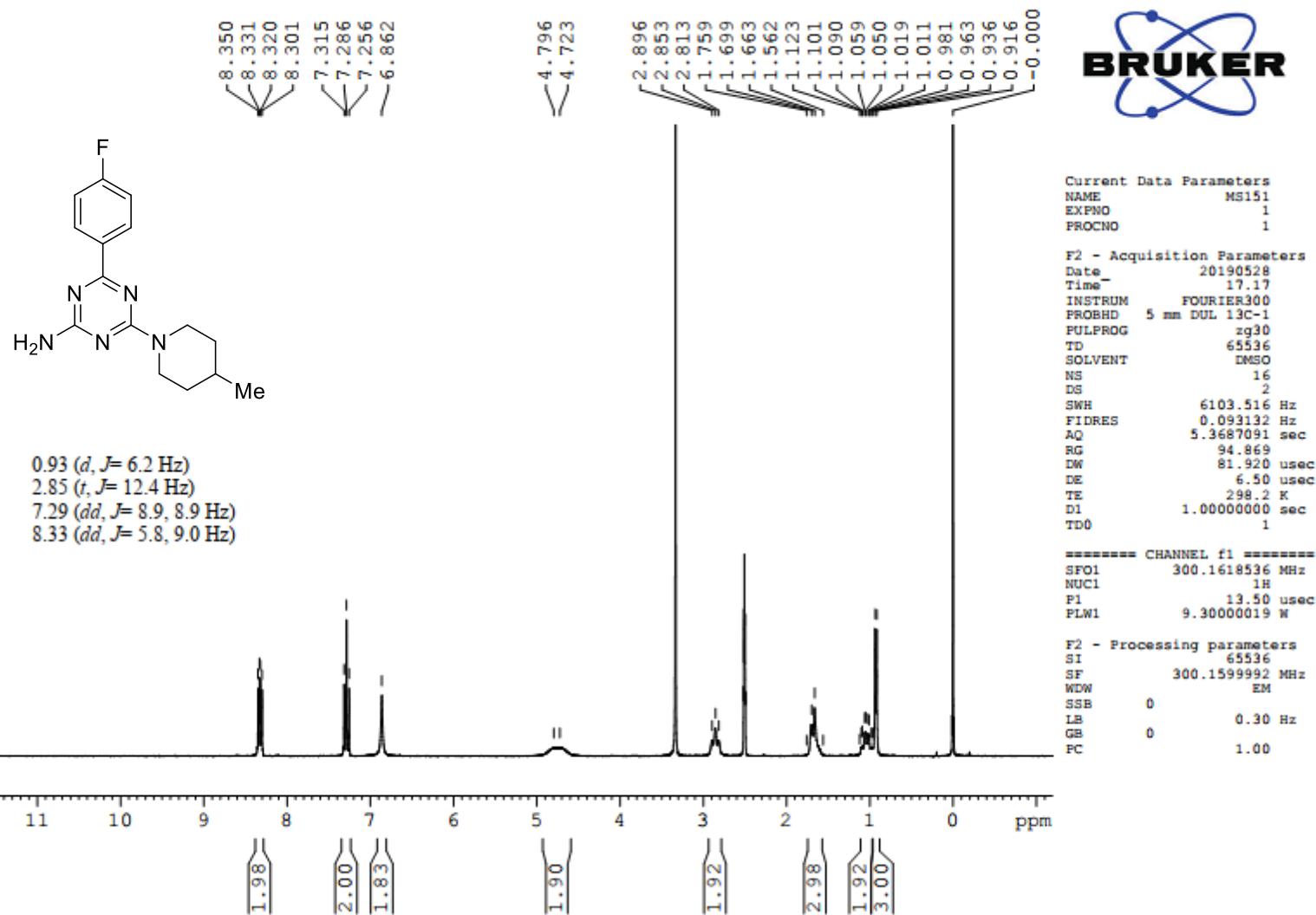
6-(3-Fluorophenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,2}**)



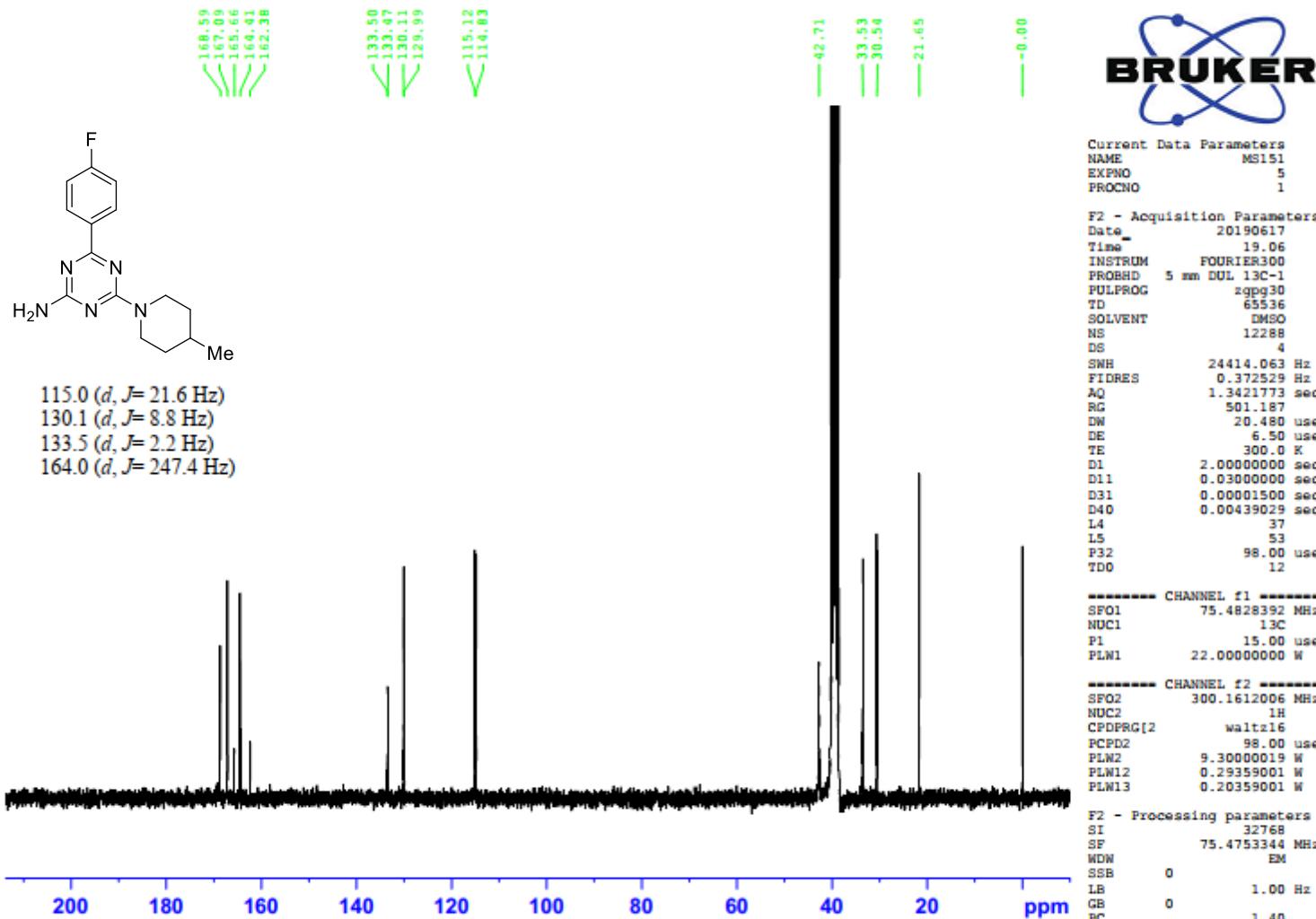
6-(3-Fluorophenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,2}**)



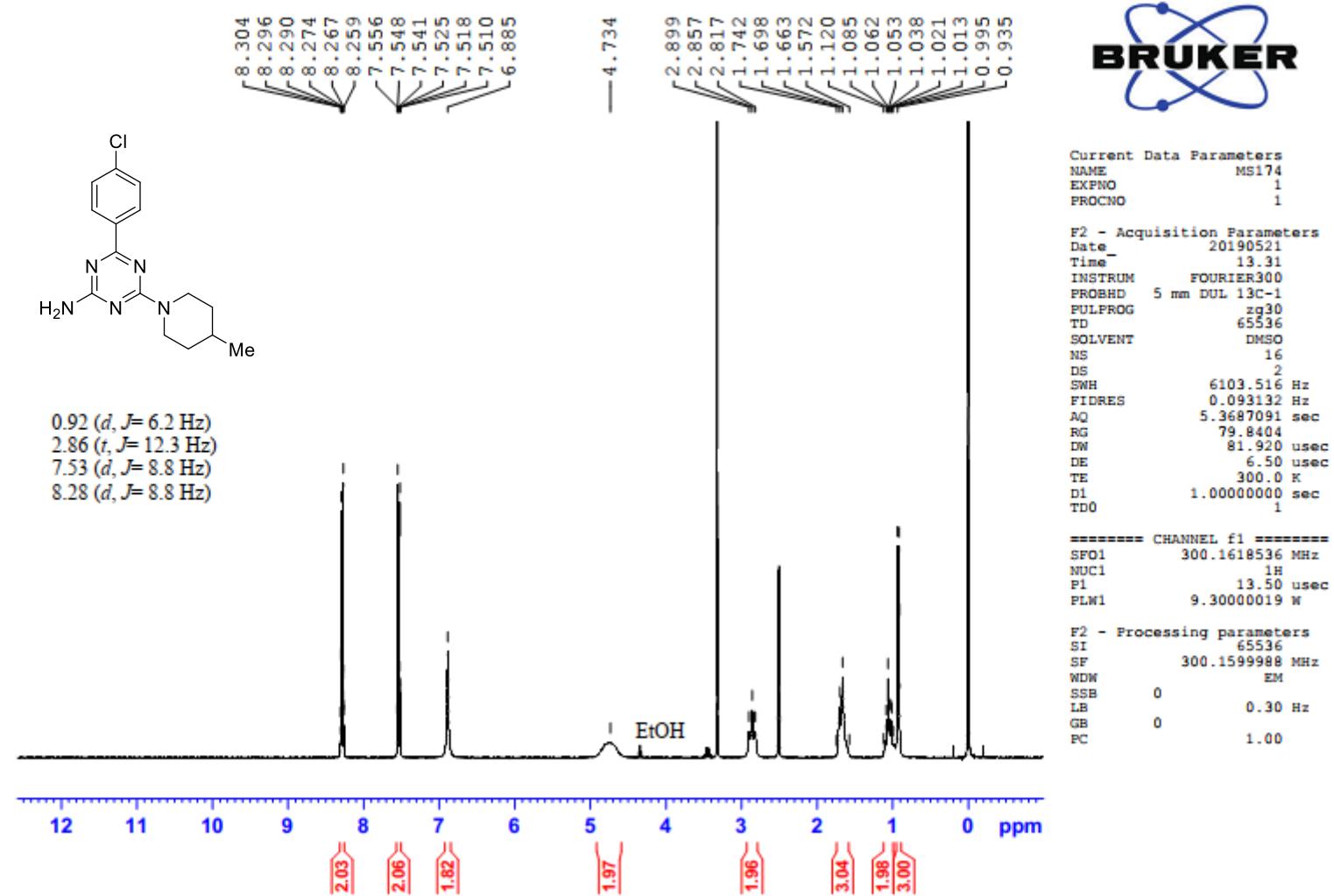
6-(4-Fluorophenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,3}**)



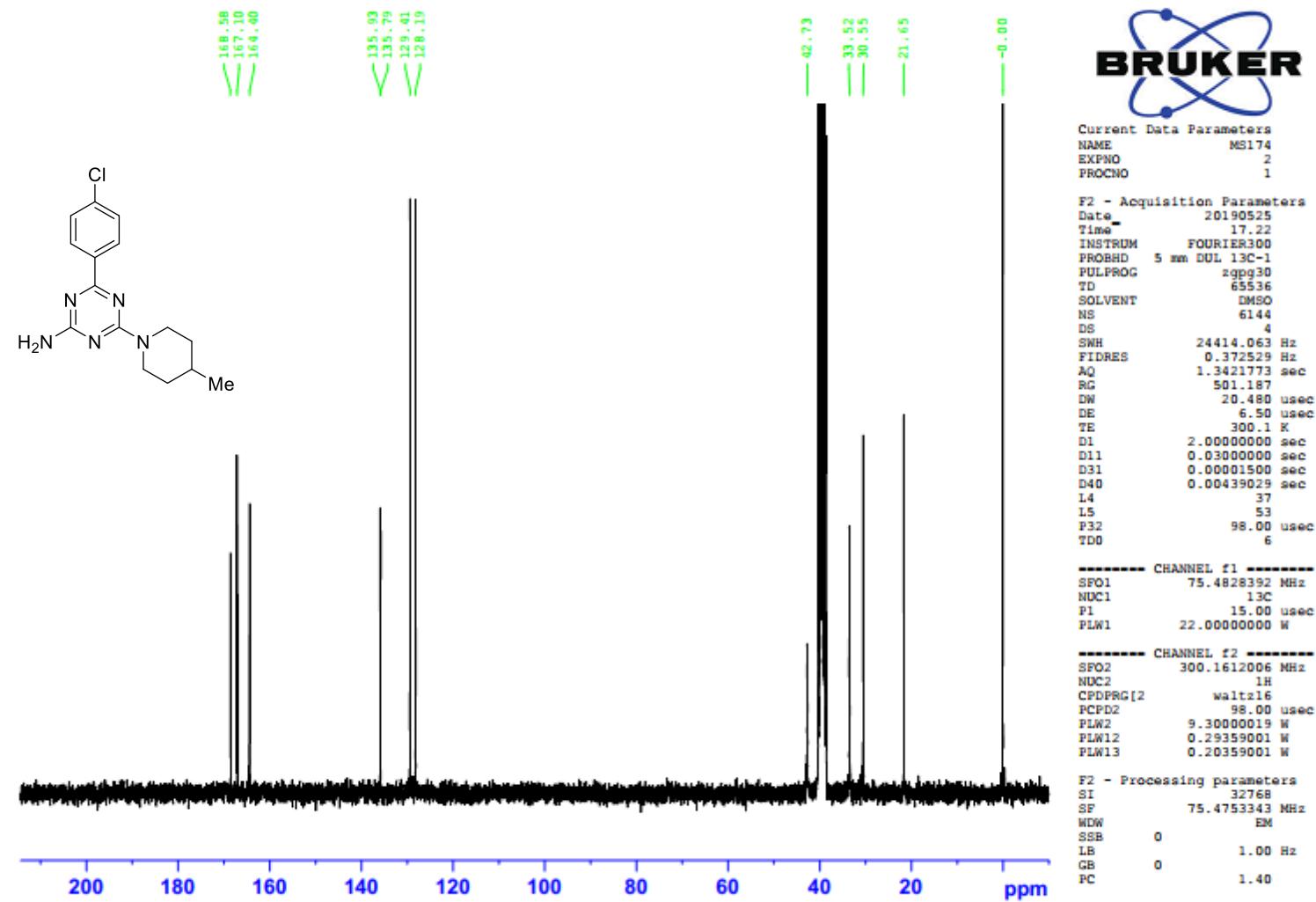
6-(4-Fluorophenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,3}**)



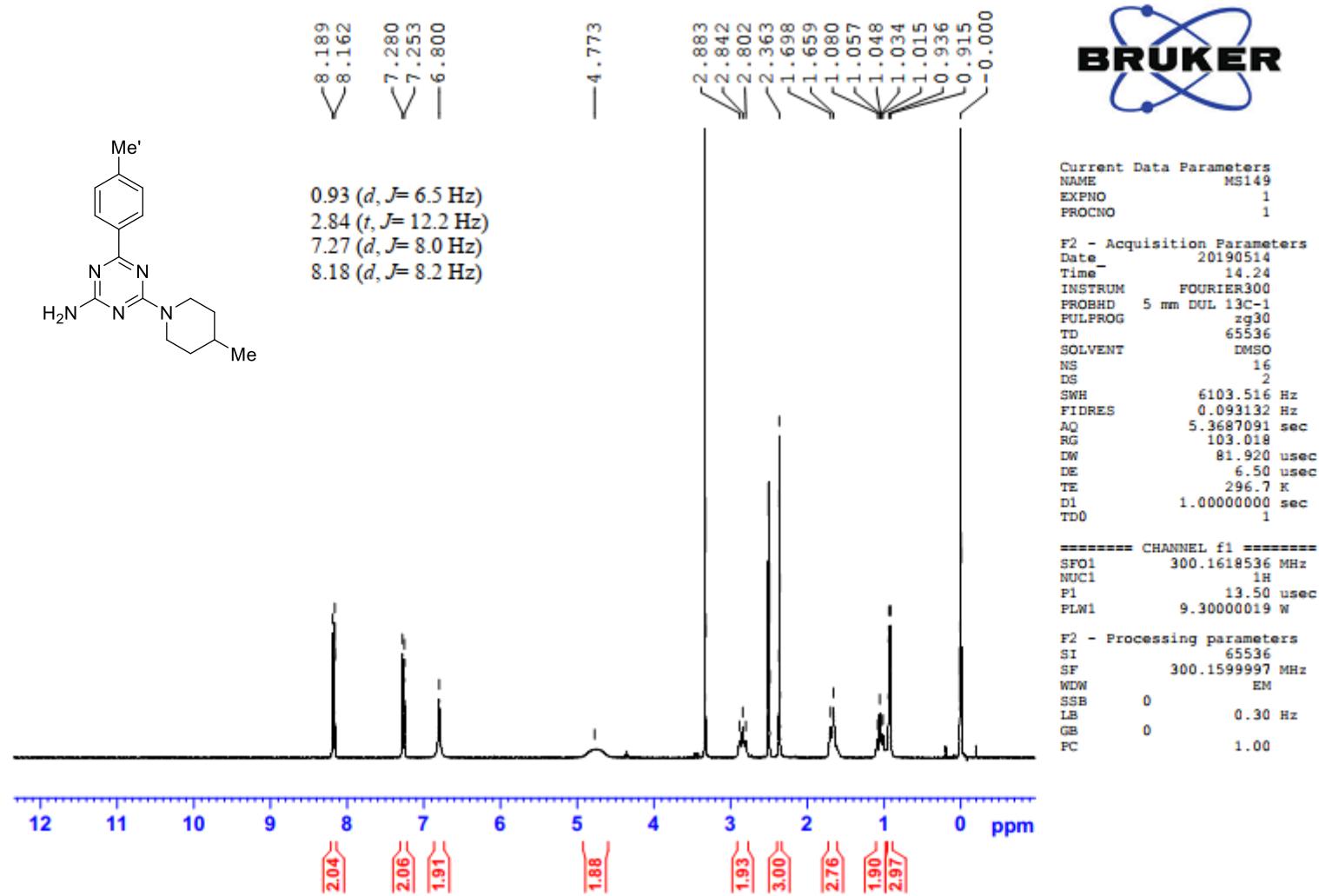
6-(4-Chlorophenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,4}**)



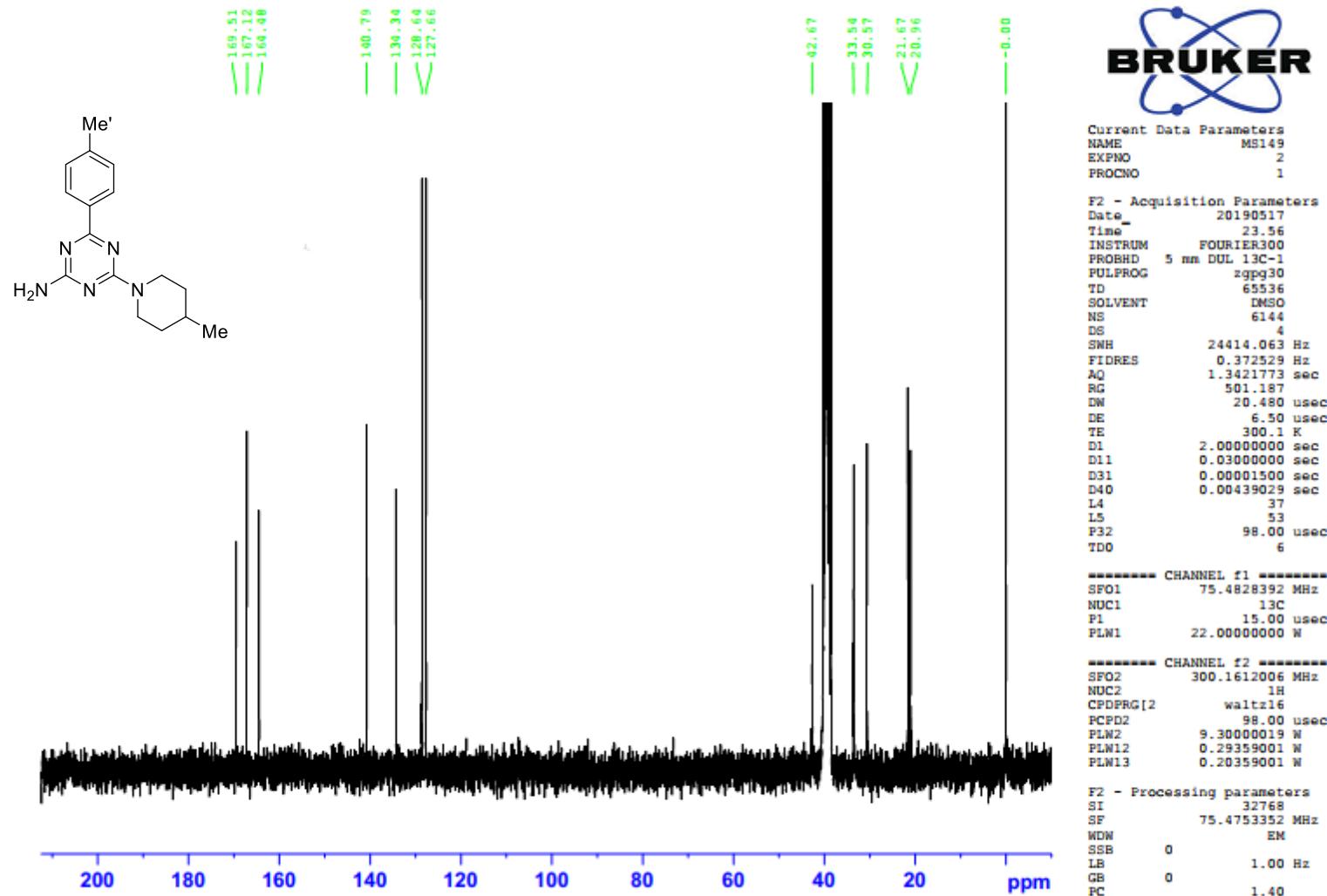
6-(4-Chlorophenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,4}**)



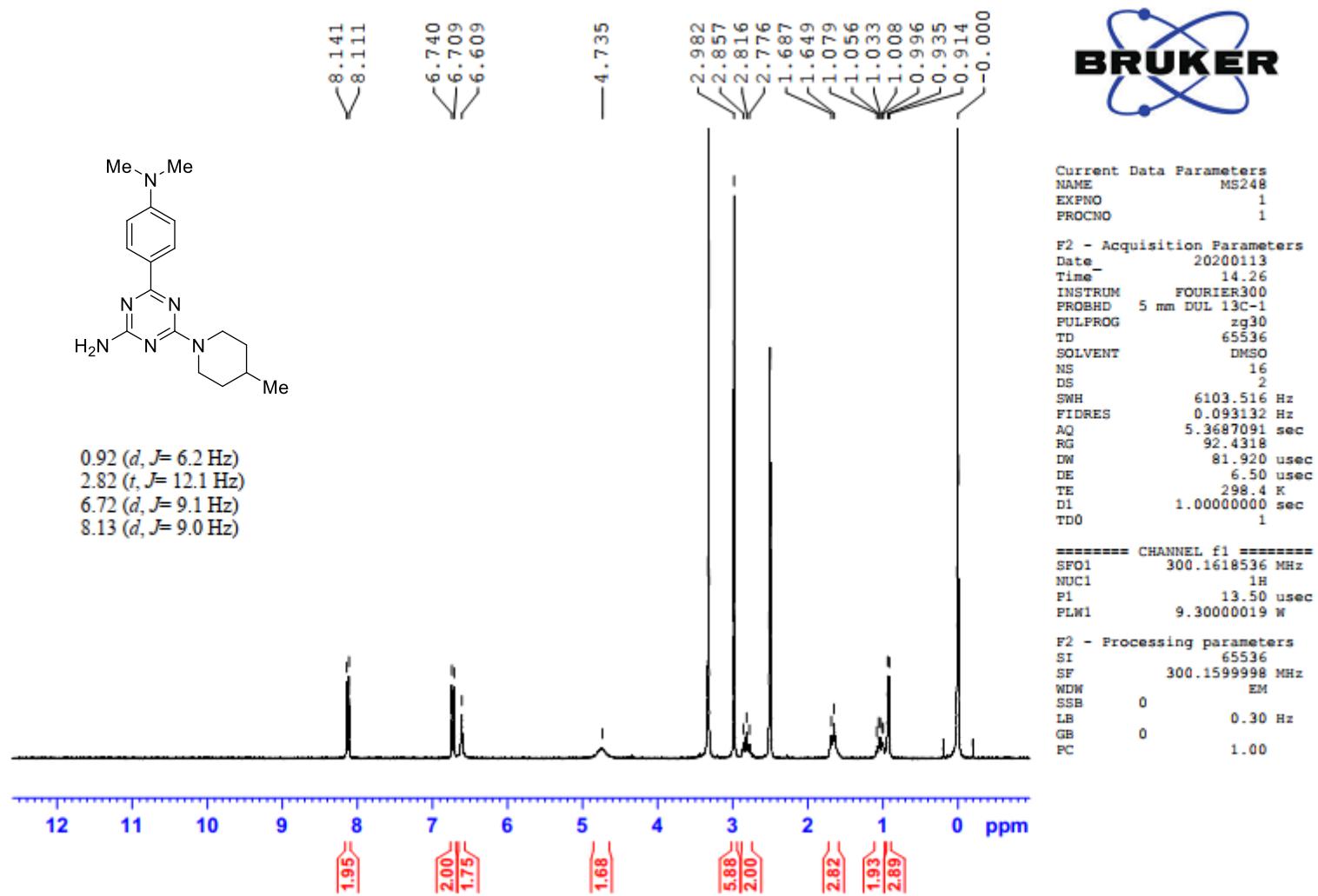
6-(4-Methylphenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,6}**)



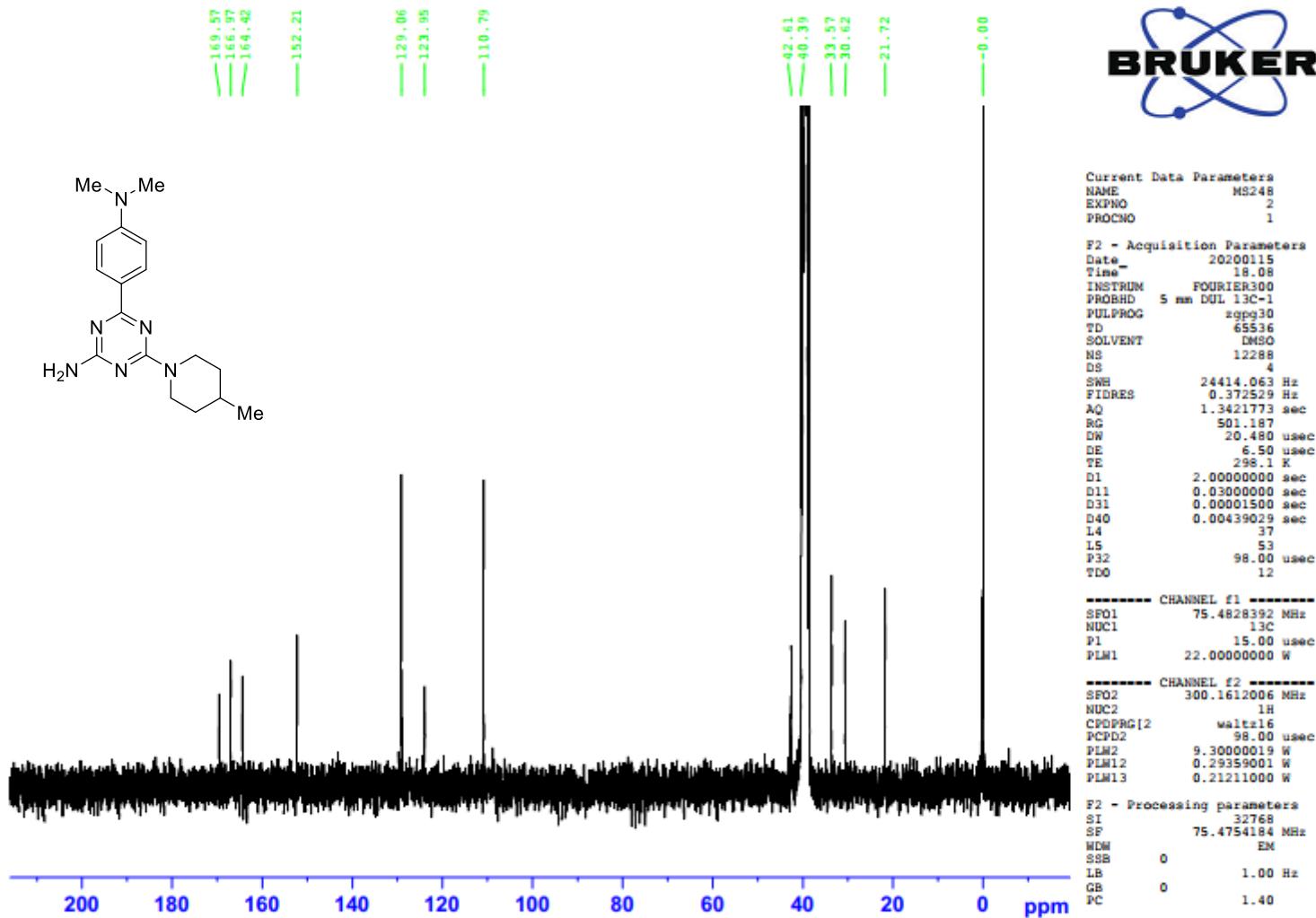
6-(4-Methylphenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,6}**)



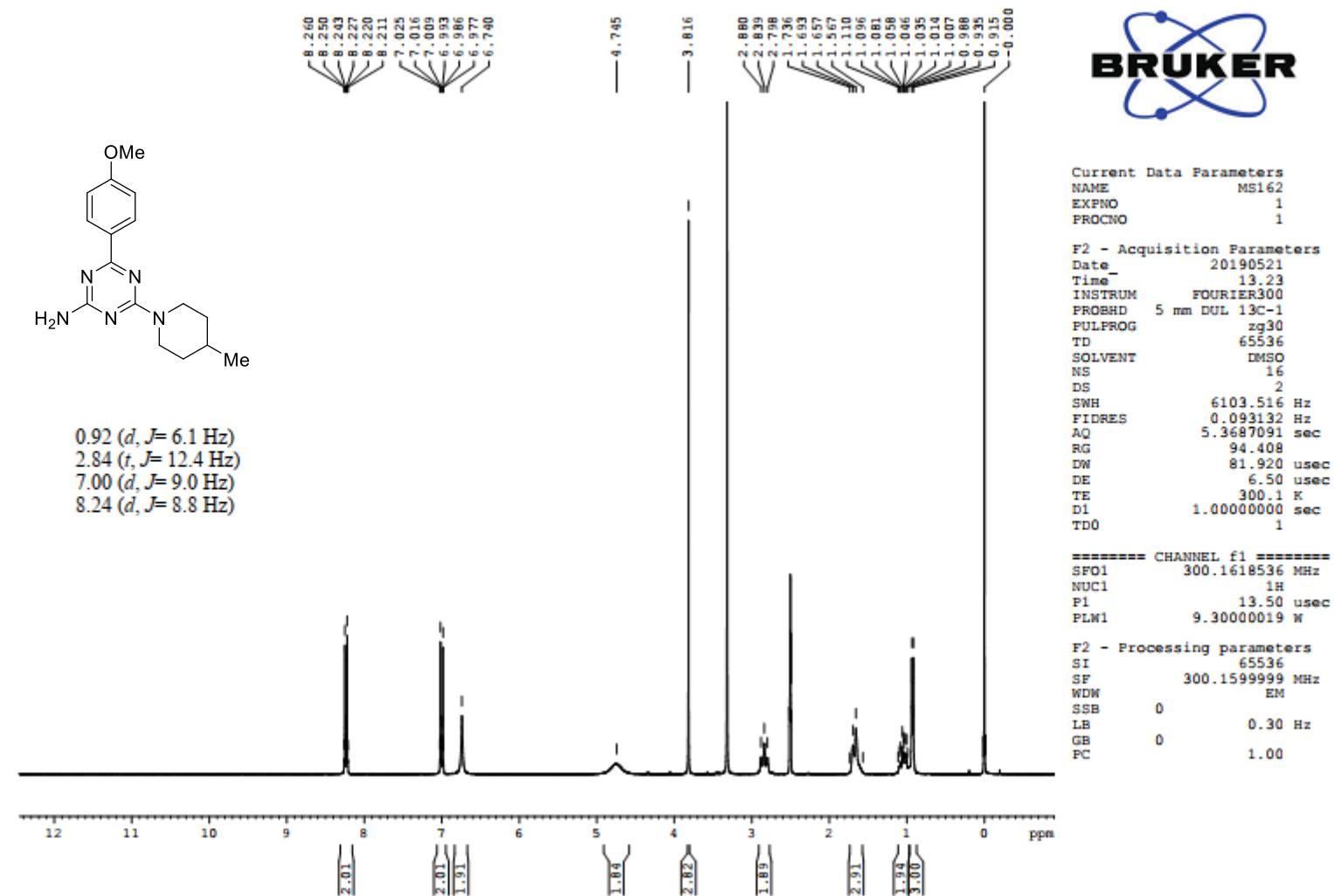
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,8}**)



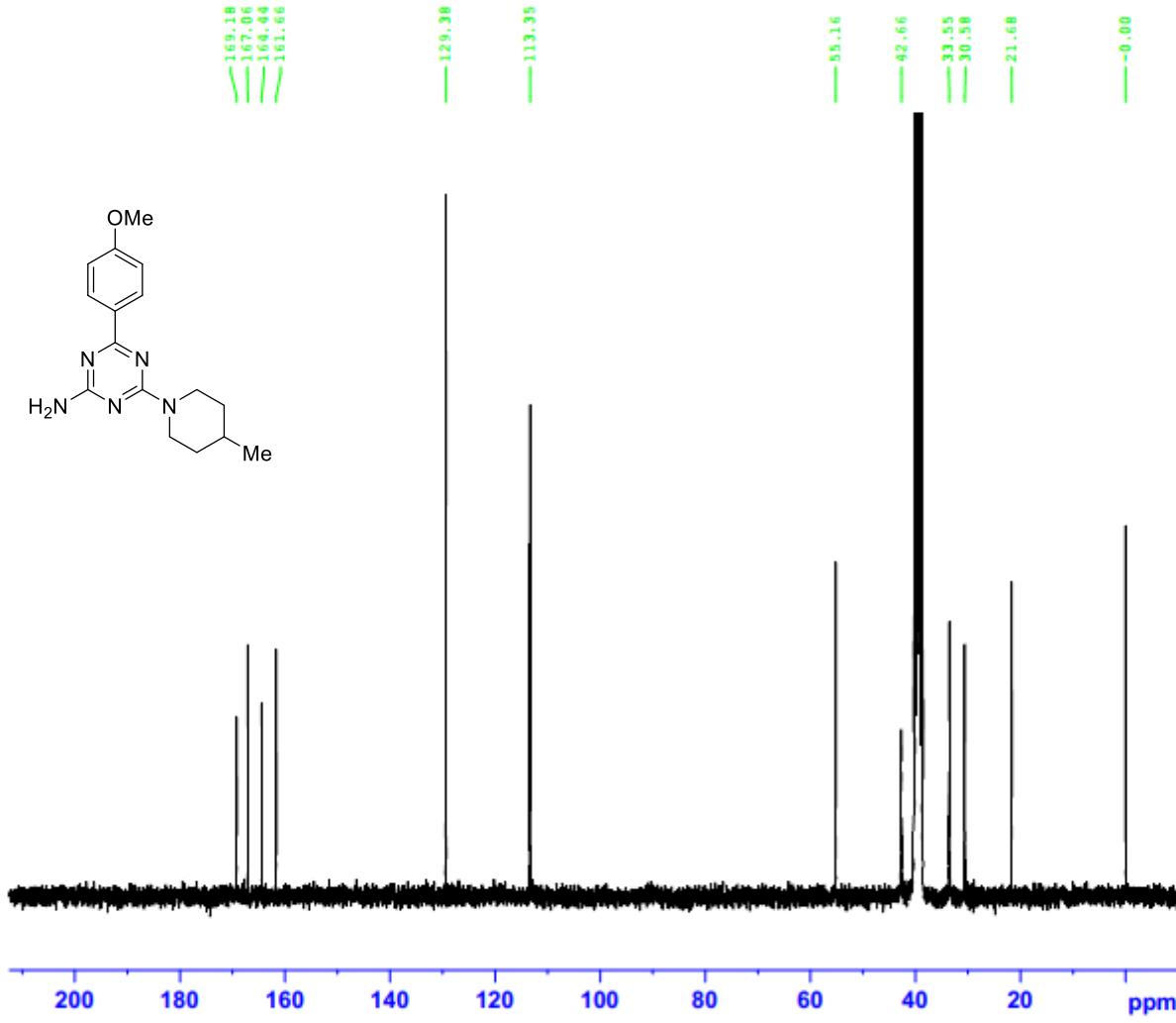
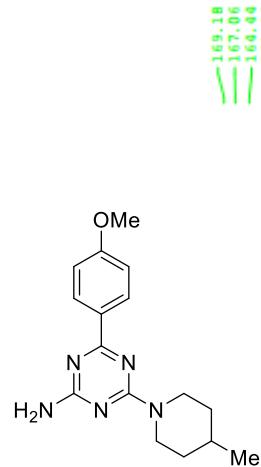
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,8}**)



6-(4-Methoxyphenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,9}**)



6-(4-Methoxyphenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,9}**)



 BRUKER

Current Data Parameters
NAME MS16
EXPNO :
PROCNO :
LAMPCOEF :

```

F2 - Acquisition Parameters
Date       20190524
Time       18.05
INSTRUM   FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG  zgpp30
TD        65536
SOLVENT   DMSO
NS        12288
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        2.0000000 sec
D11       0.03000000 sec
D31       0.00001500 sec
D40       0.00439029 sec
L4         37
L5         53
P32       98.00 usec
TDD       12

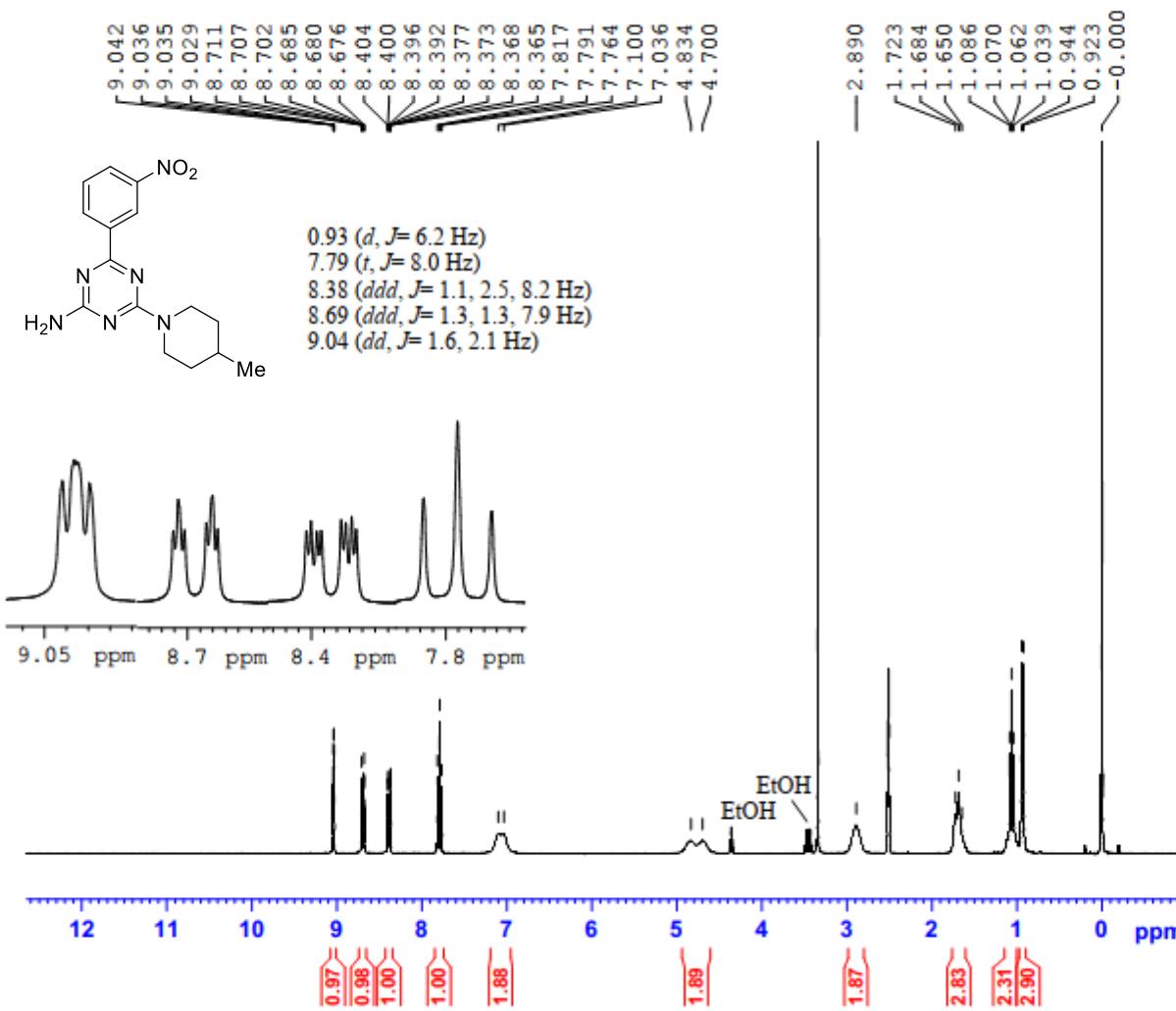
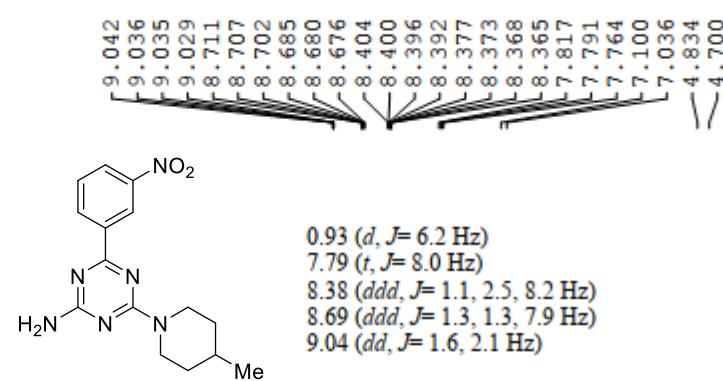
```

----- CHANNEL f1 -----
SFO1 75.4828392 MHz
NUC1 13C
P1 15.00 usec
PLN1 22.00000000 N

==== 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          75.4753352 MHz  
WDW          EM  
SSB           0  
LB           1.00 Hz  
GB           0  
PC           1.40
```

4-(4-Methylpiperidino)-6-(3-nitrophenyl)-1,3,5-triazine-2-amine (**9{3,10}**)



BRUKER

Current Data Parameters
NAME MS157
EXPNO 1
PROCNO 1

```

F2 - Acquisition Parameters
Date _           20190514
Time _          14.38
INSTRUM   FOURIER300
PROBOD   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        72.6053
DW        81.920 usec
DE        6.50 usec
TE        296.5 K
D1        1.0000000 sec
TD0          1

```

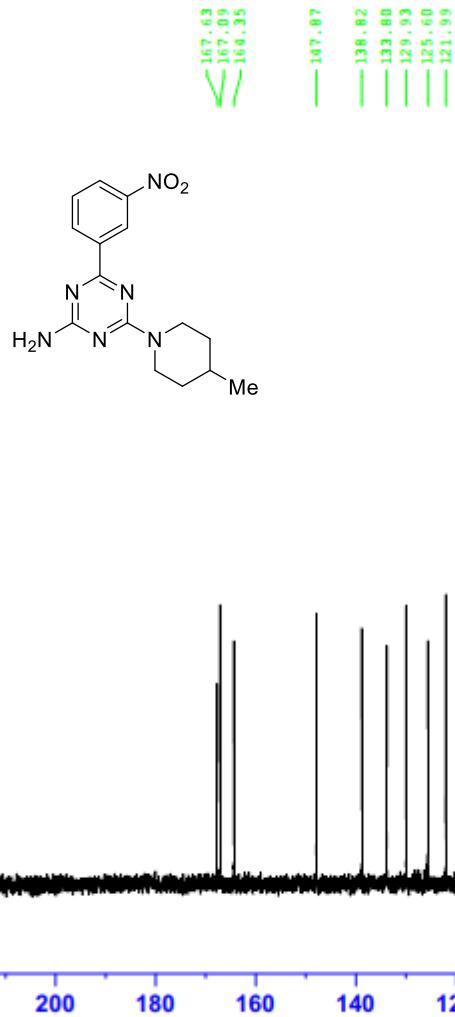
```
===== CHANNEL f1 =====
SFO1      300.1618536 MHz
NUC1          1H
P1           13.50 usec
PLW1      9.300000019 u
```

```

P2 - Processing parameters
SI          65536
SF        300.1599976 MHz
NDW           EM
SSB          0
LB          0.30 Hz
GB          0
PC          1.00

```

4-(4-Methylpiperidino)-6-(3-nitrophenyl)-1,3,5-triazine-2-amine (**9{3,10}**)



Current Data Parameters
NAME MS157
EXPNO 2
PROCNO 1

```

P2 - Acquisition Parameters
Date_          20190518
Time_          5.48
INSTRUM_        FOURIER300
PROBHD_        5 mm DUL 13C-1
PULPROG_       zgpp30
TD_            65536
SOLVENT_        DMso
NS_             6144
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_          0.03000000 sec
D31_          0.00001500 sec
D40_          0.00439029 sec
L4_             37
L5_              53
R32_           0.0010000 sec

```

----- CHANNEL f1 -----
SF01 75.4828392 MHz
NUC1 13C
P1 15.00 used
PWR1 22.0000000 W

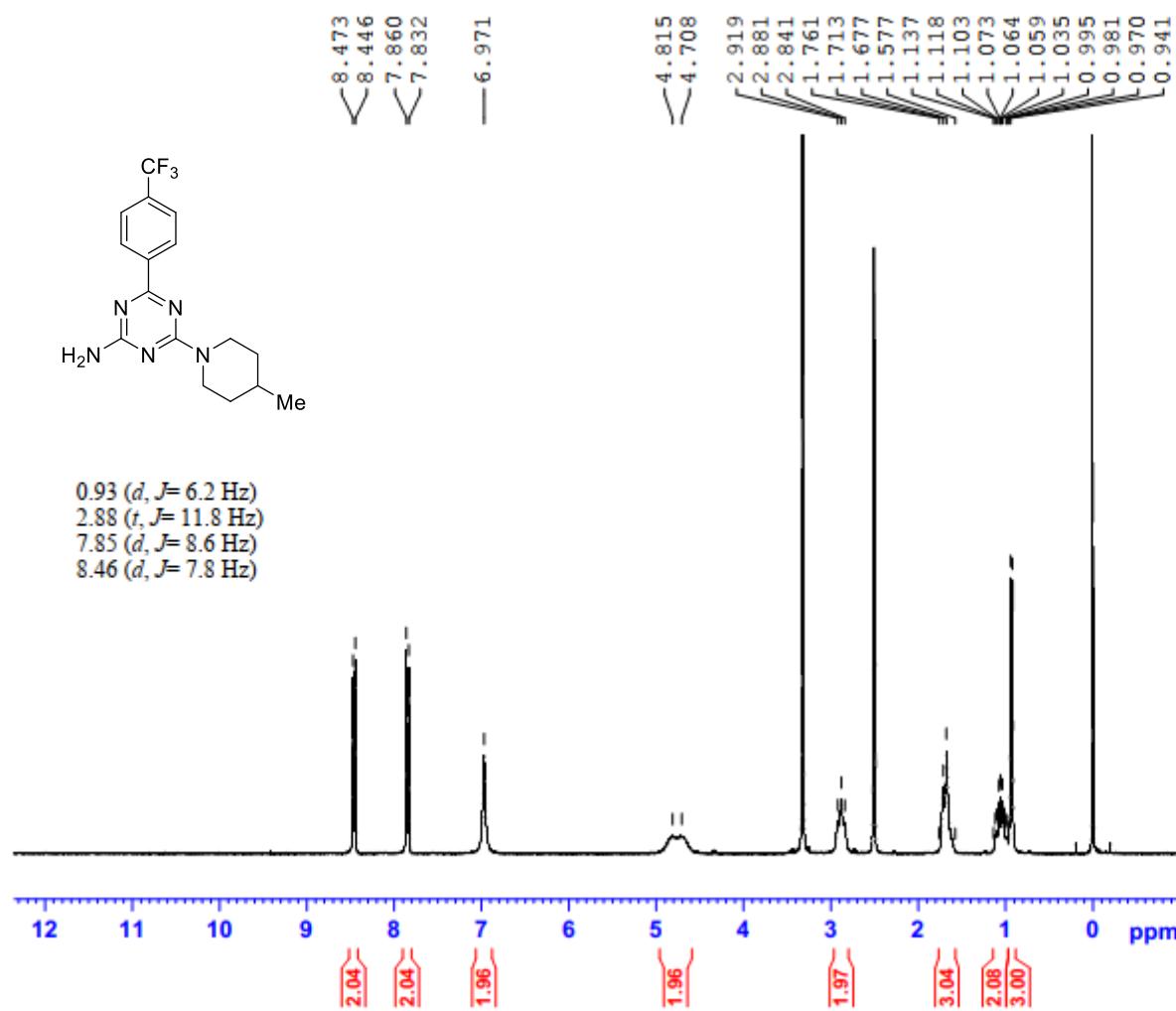
----- CHANNEL f2 -----
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 98.00 used
PLN2 9.30000019 W
PLN12 0.29359001 W
PLN13 0.29359001 W

```

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

```

6-[4-(Trifluoromethyl)phenyl]-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,11}**)



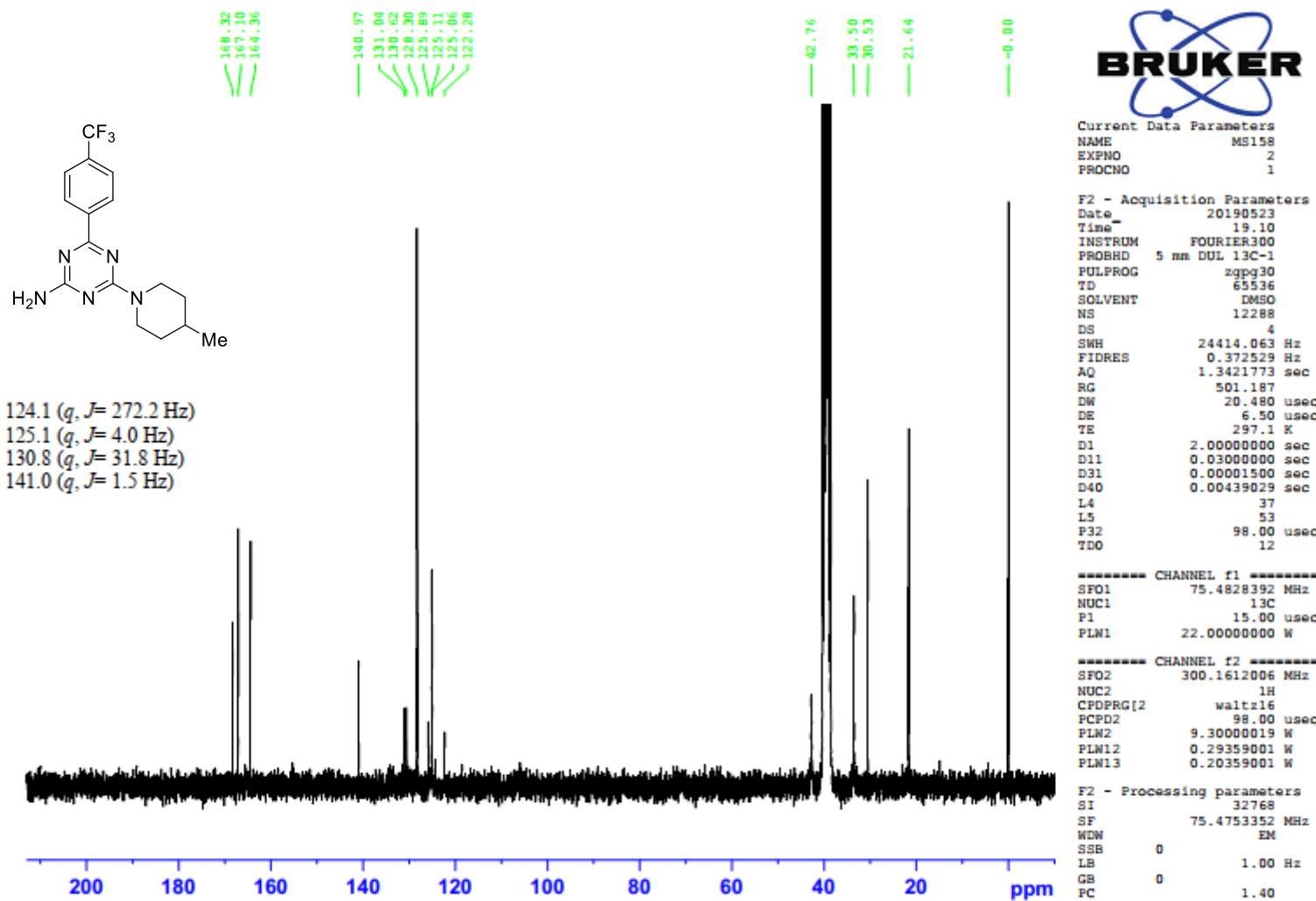
Current Data Parameters
NAME MS158
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20190521
Time 13.19
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 107.255
DW 81.920 usec
DE 6.50 usec
TE 300.1 K
D1 1.0000000 sec
TDO 1

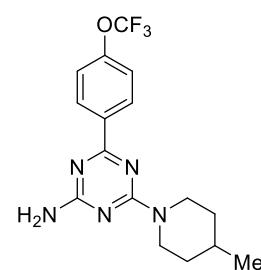
===== CHANNEL f1 =====
SFO1 300.1618536 MHz
NUC1 1H
PI 13.50 usec
PLW1 9.30000019 W

F2 - Processing parameters
SI 65536
SF 300.1599994 MHz
WDW EM
SSB 0
LB 0 0.30 Hz
GB 0
PC 1.00

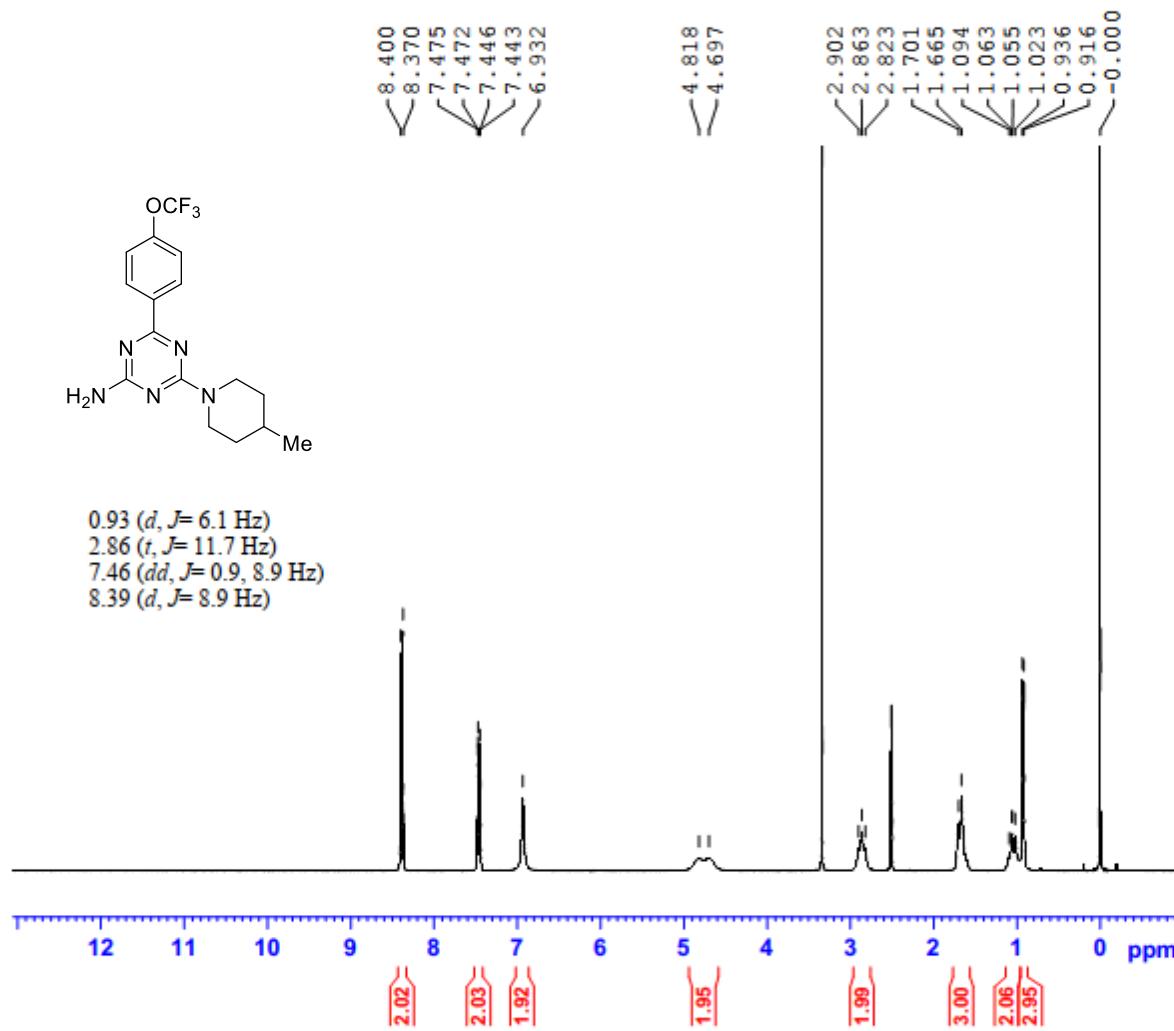
6-[4-(Trifluoromethyl)phenyl]-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,11}**)



6-[4-(Trifluoromethoxy)phenyl]-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,12}**)



0.93 (*d*, $J = 6.1$ Hz)
 2.86 (*t*, $J = 11.7$ Hz)
 7.46 (*dd*, $J = 0.9, 8.9$ Hz)
 8.39 (*d*, $J = 8.9$ Hz)



Current Data Parameters
NAME MS156
EXPNO 1
PROCNO 1

```

P2 - Acquisition Parameters
Date_           20190514
Time            14.34
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              67.8511
DW              81.920 usec
DE              6.50 usec
TE              296.7 k
D1              1.0000000 sec
TD0              1

```

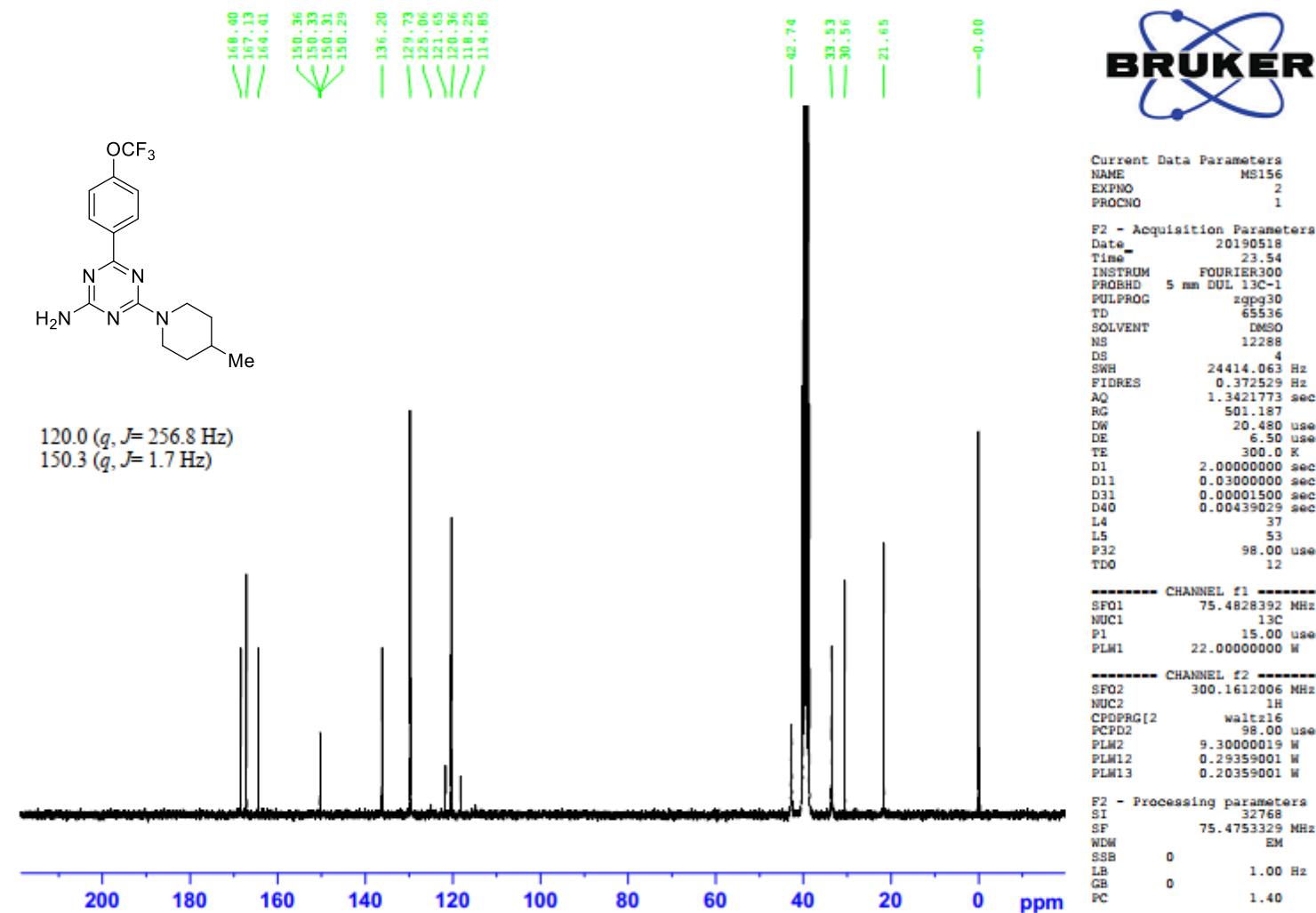
```
===== CHANNEL f1 =====
SFO1      300.1618536 MHz
NUC1          1H
P1           13.50 usec
PLW1      9.300000019 W
```

```

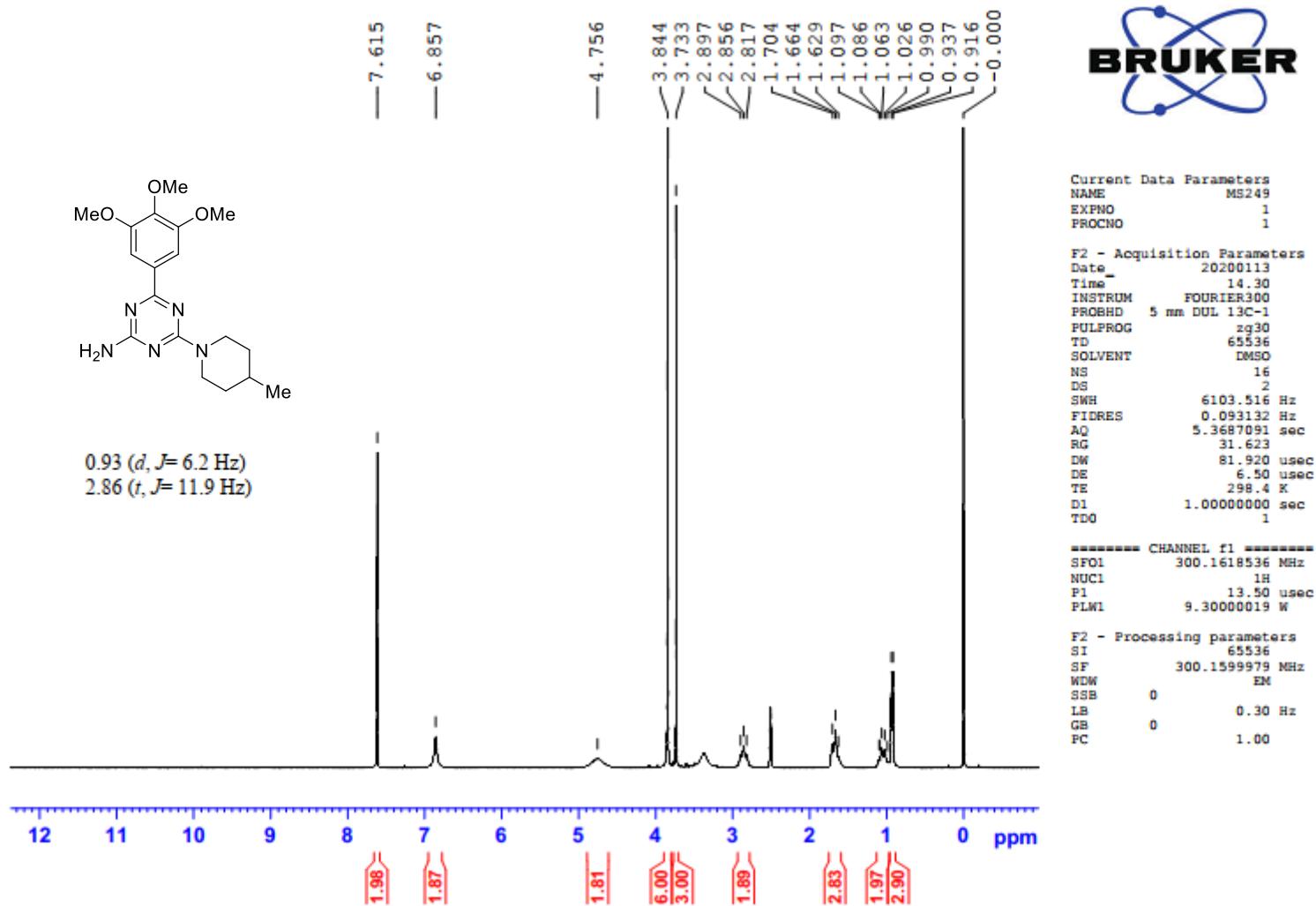
P2 - Processing parameters
SI           65536
SF          300.1599977 MHz
WDW           EM
SSB            0
LB             0.30 Hz
GB            0
PC           1.00

```

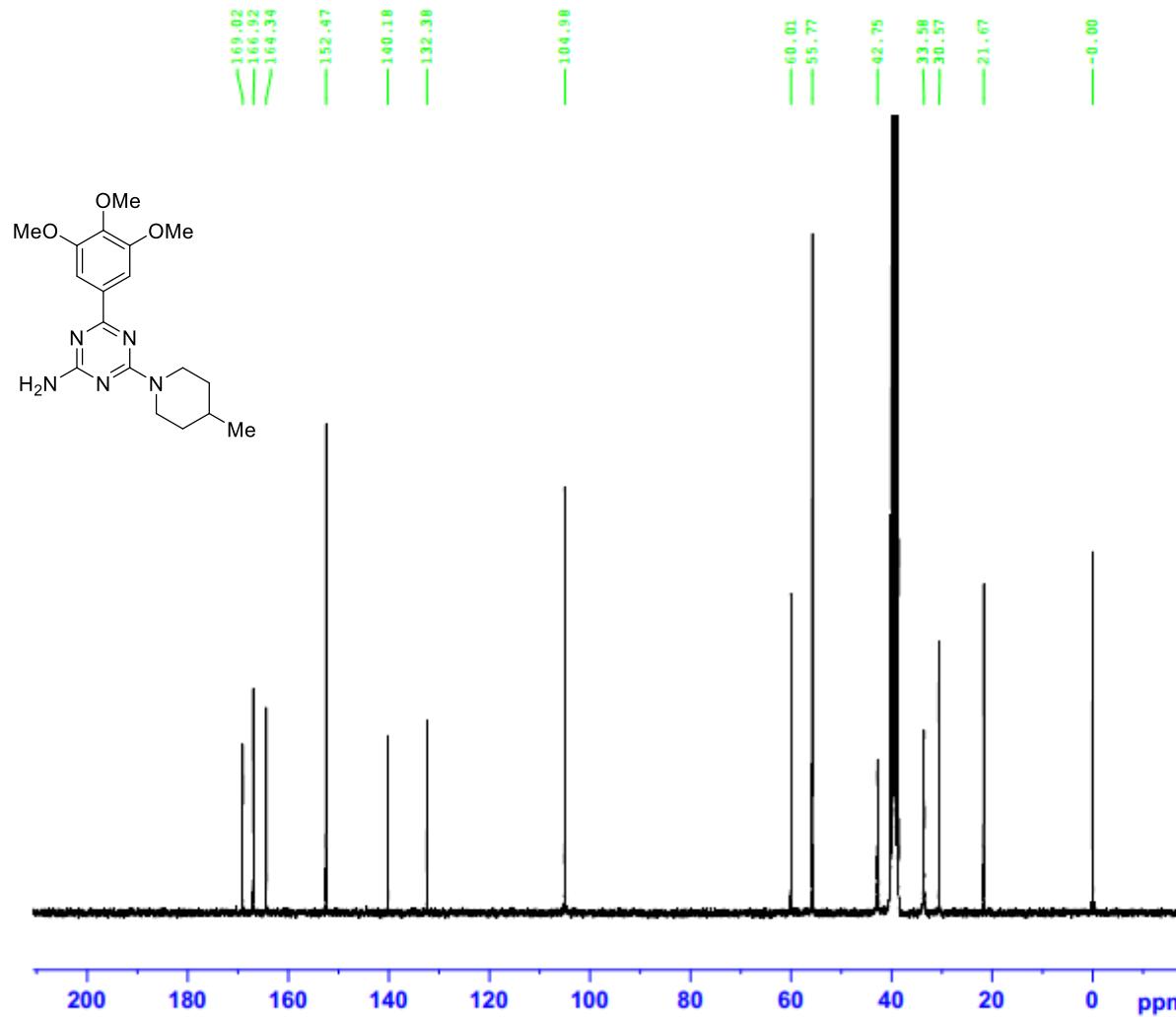
6-[4-(Trifluoromethoxy)phenyl]-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,12}**)



6-(3,4,5-Trimethoxyphenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,17}**)



6-(3,4,5-Trimethoxyphenyl)-4-(4-methylpiperidino)-1,3,5-triazine-2-amine (**9{3,17}**)



BRUKER

Current Data Parameter
NAME MS24
EXPNO
PROCNO

```

P2 - Acquisition Parameters
Date _ 20200114
Time _ 18.05
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpp30
TD 65536
SOLVENT DMSO
NS 12288
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 298.1 K
D1 2.0000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D40 0.00439029 sec
L4 37
L5 53
P32 98.00 usec
TDD 13

```

----- CHANNEL f1 -----
SFO1 75.4828392 MHz
NUC1 13C
P1 15.00 usec
RIM1 22.0000000 M

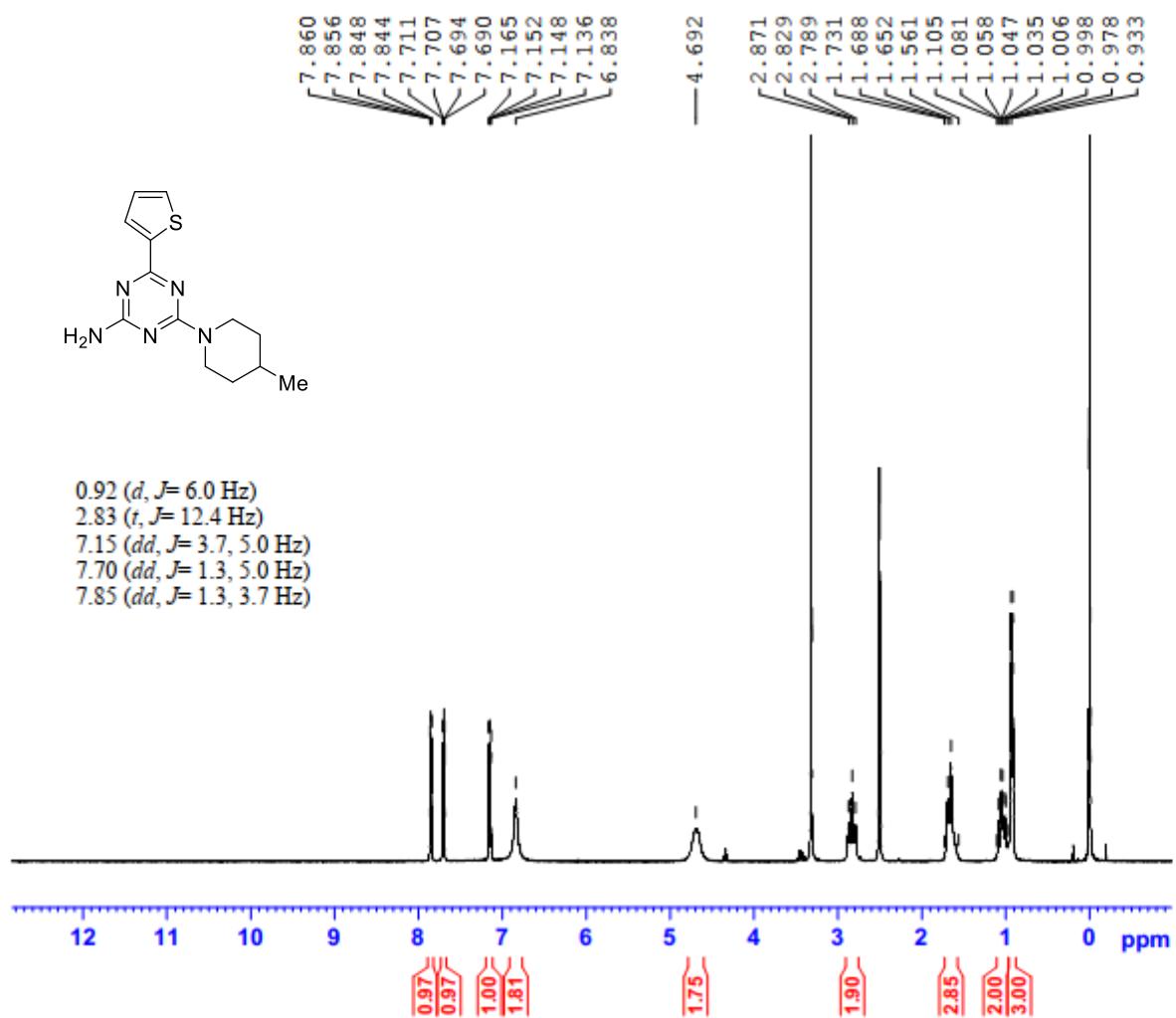
----- CHANNEL f2 -----
SFO2 300.1612006 MHz
NUC2 1H
CPDPBRC[2] waltz16
PCFD2 98.00 usec
PLW2 9.30000019 W
PLW12 0.29359001 W
PLW13 0.21211000 W

```

P2 - Processing parameters
SI           32768
SF          75.4753335 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB           0
PC           1.40

```

4-(4-Methylpiperidino)-6-(2-thienyl)-1,3,5-triazine-2-amine (**9{3,18}**)



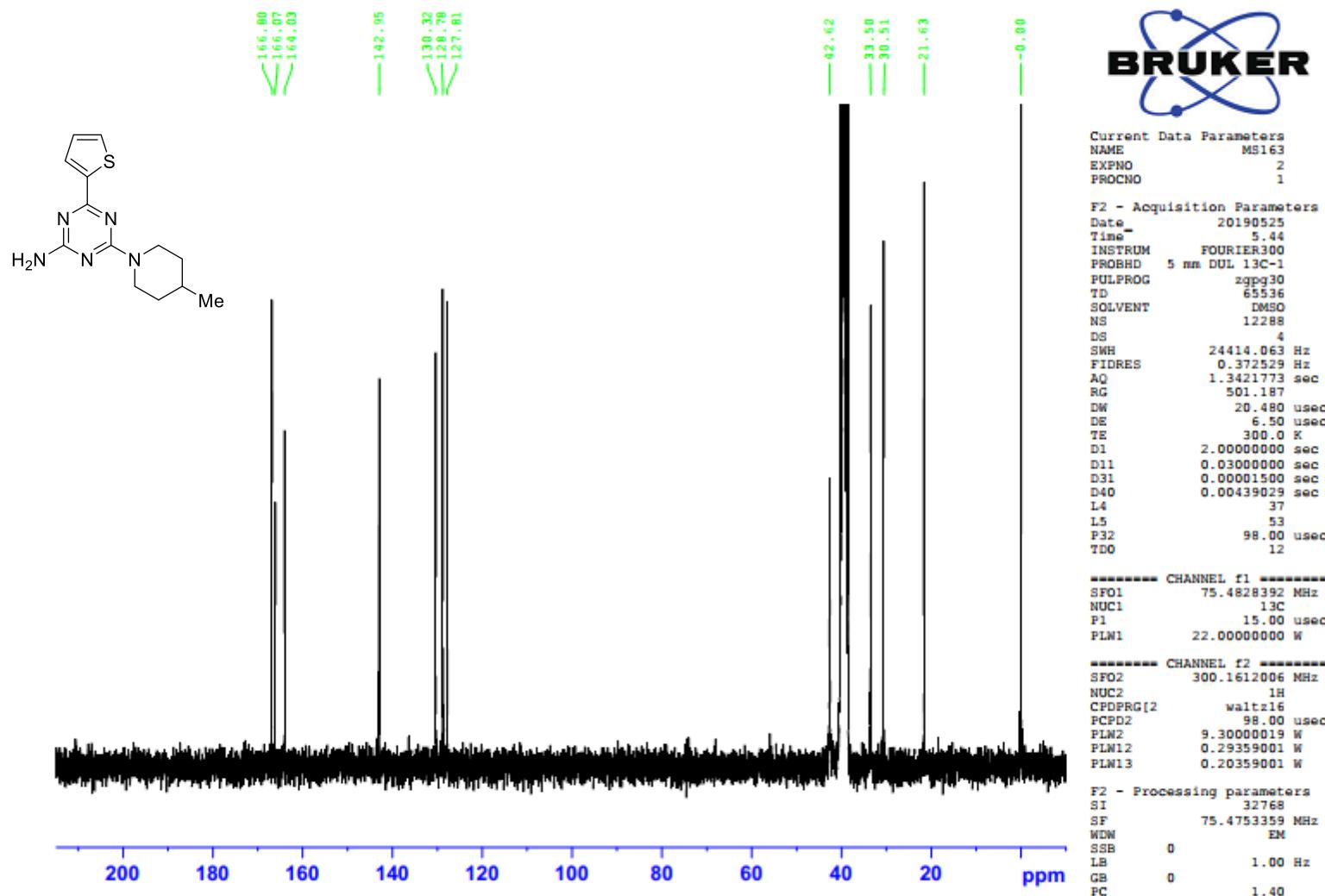
Current Data Parameters
 NAME MS163
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20190521
 Time 13.27
 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 98.4753
 DW 81.920 usec
 DE 6.50 usec
 TE 300.1 K
 D1 1.0000000 sec
 TD0 1

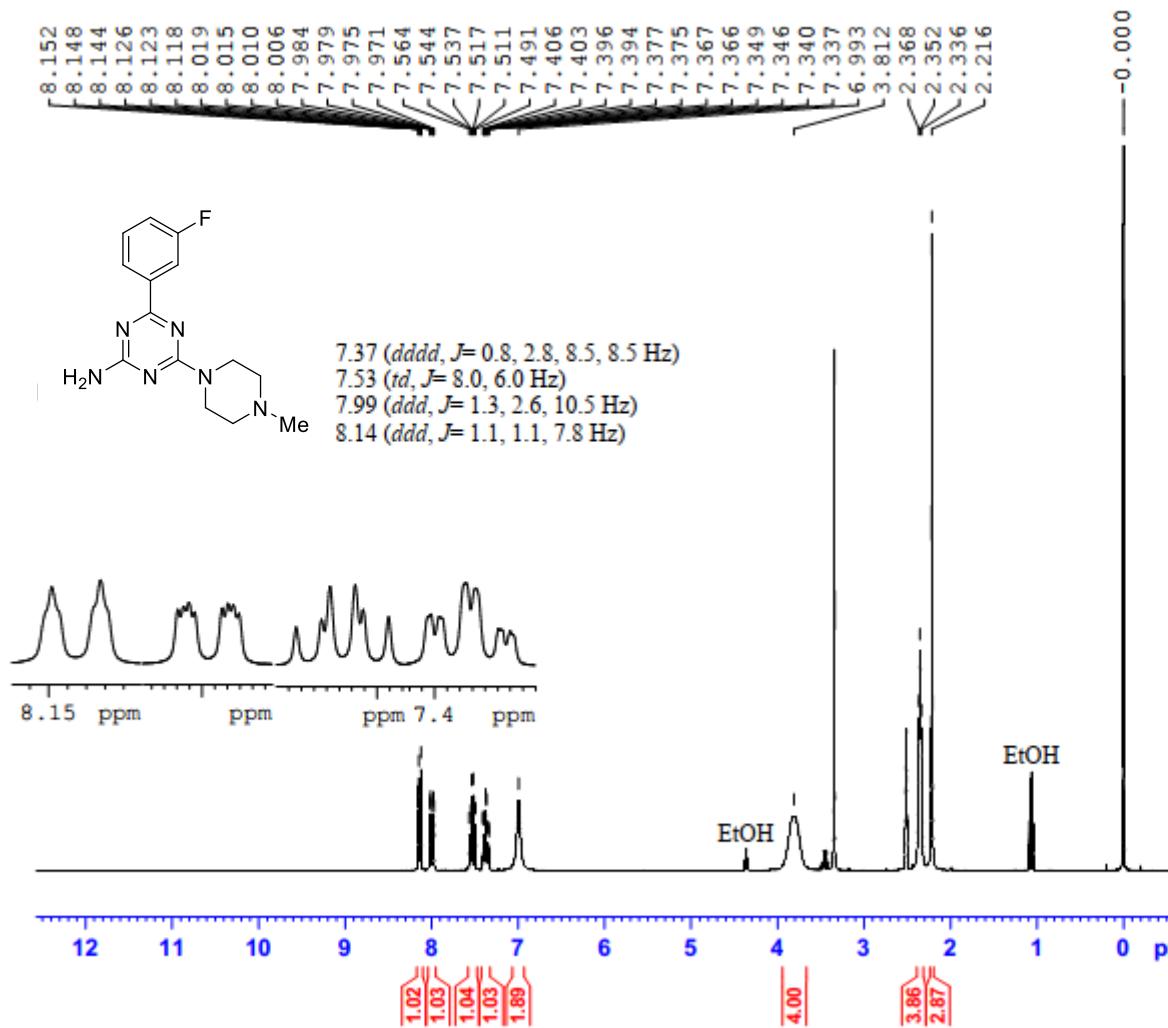
===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

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

4-(4-Methylpiperidino)-6-(2-thienyl)-1,3,5-triazine-2-amine (**9{3,18}**)



6-(3-Fluorophenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,2}**)



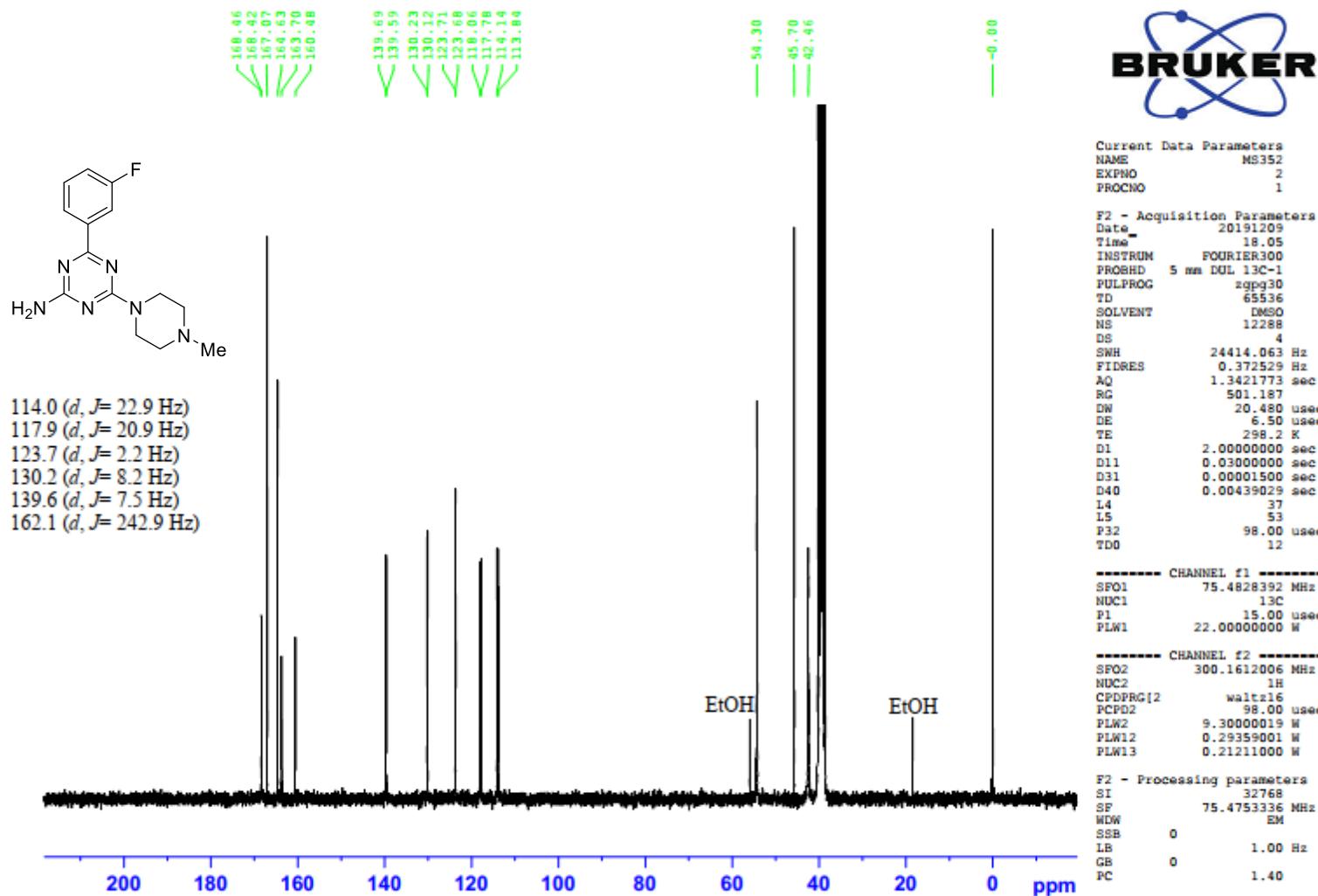
Current Data Parameters
NAME MS352
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20191206
Time 14.34
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 297.7 K
D1 1.0000000 sec
TD0 1

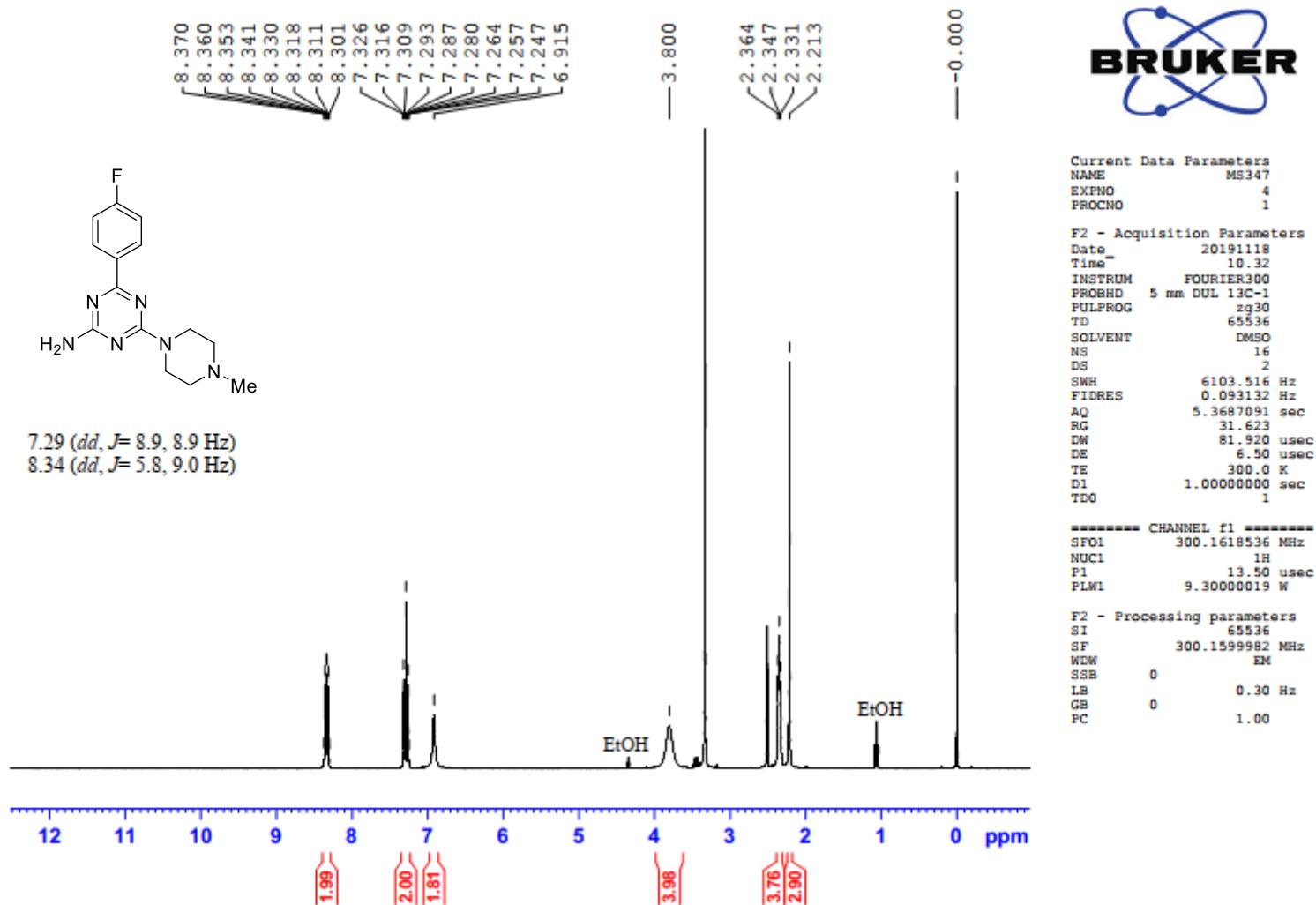
===== CHANNEL f1 =====
SF01 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

F2 - Processing parameters
SI 65536
SF 300.1599968 MHz
WDW EM
SSB 0 0.30 Hz
LB 0
GB 0 1.00
PC

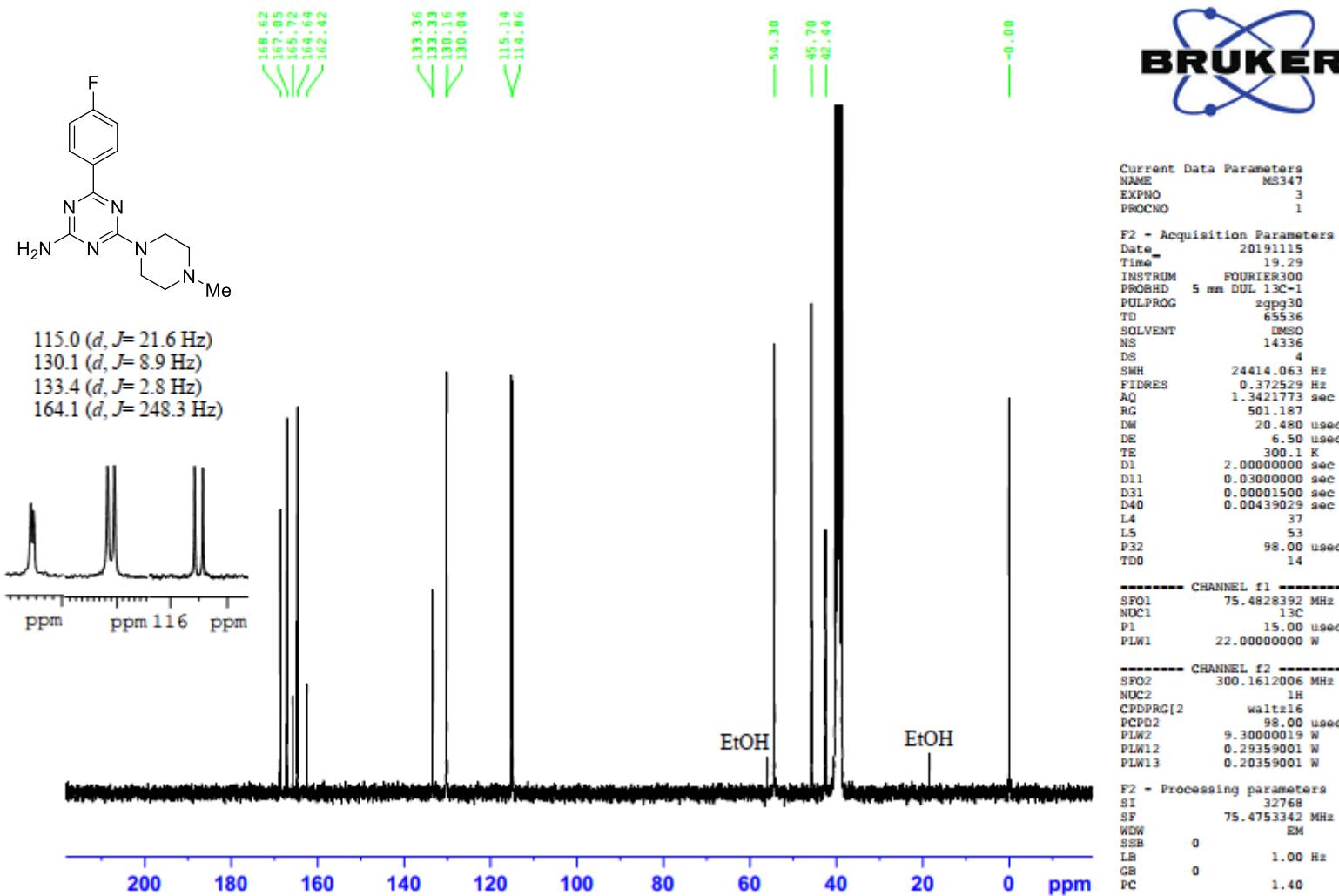
6-(3-Fluorophenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,2}**)



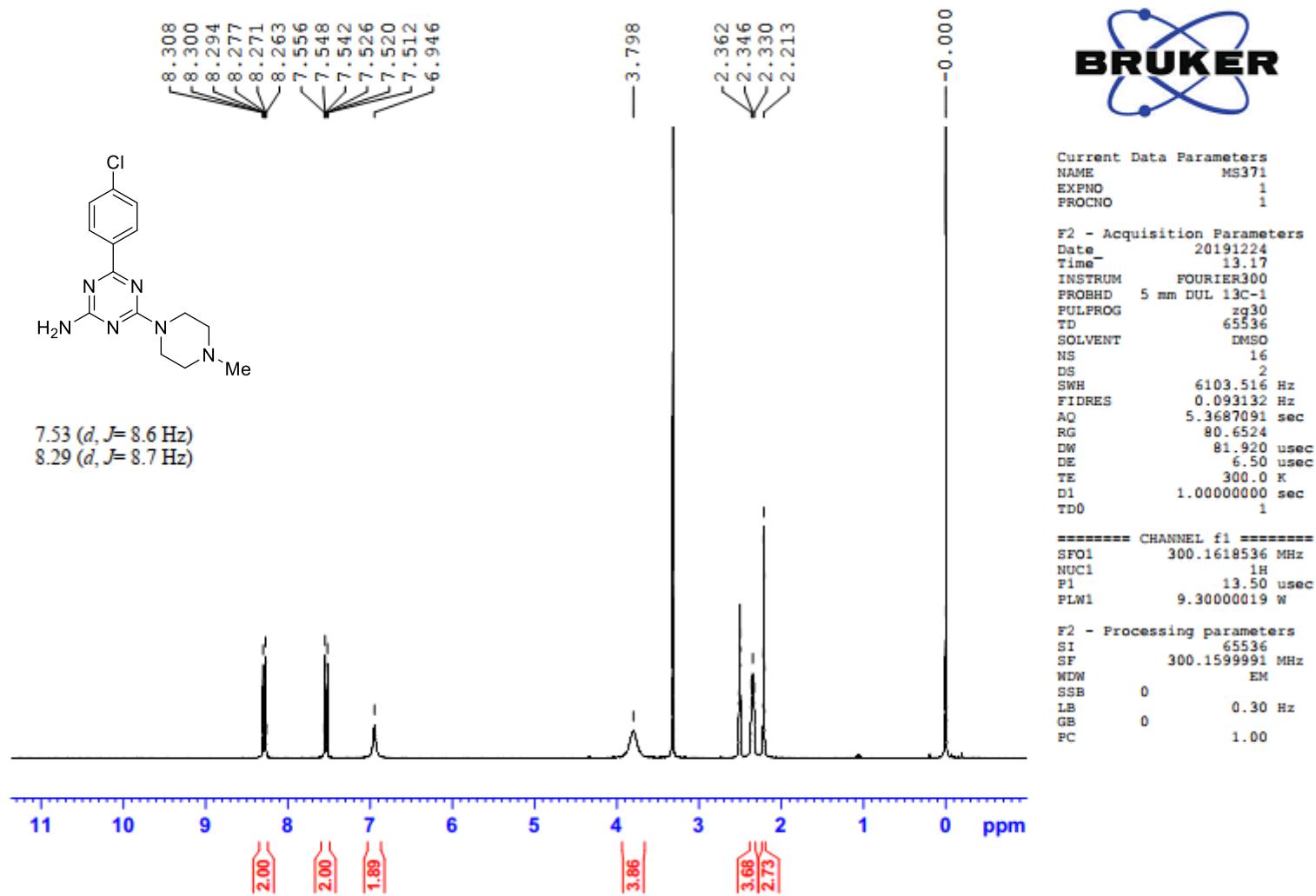
6-(4-Fluorophenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,3}**)



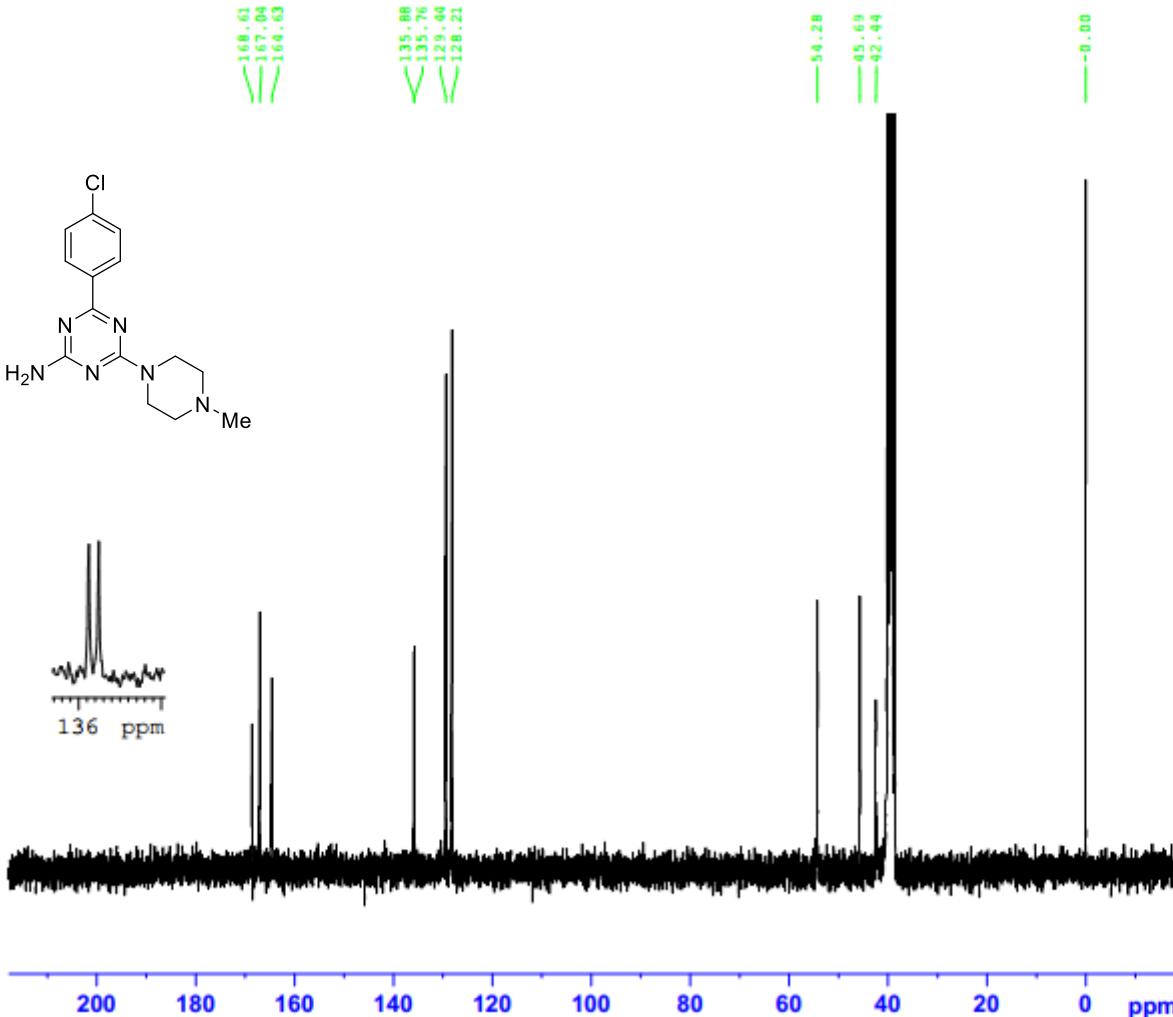
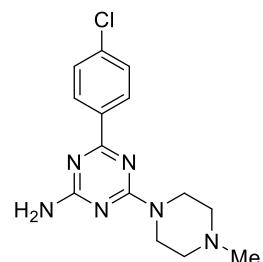
6-(4-Fluorophenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,3}**)



6-(4-Chlorophenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,4}**)



6-(4-Chlorophenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,4}**)



BRUKER

Current Data Parameters
NAME M9371
EXPNO 2
PROCNO 1

```

F2 - Acquisition Parameters
Date_      20191227
Time       22.13
INSTRUM   FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG  zappr30
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        300.1 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
PDD       .4

```

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

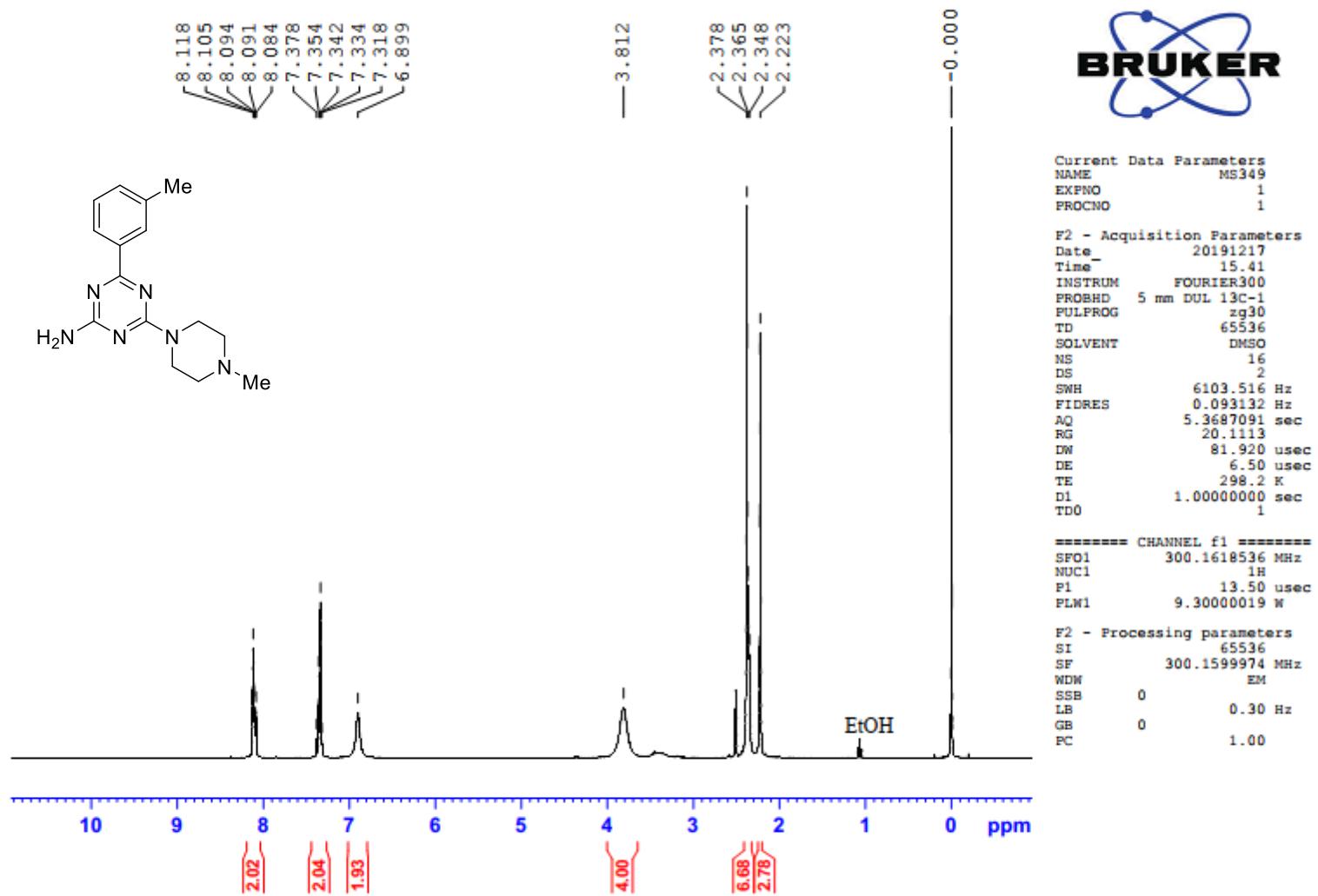
----- CHANNEL f2 -----
SF02 300.1612006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 98.00 use
PLM2 9.30000019 W
PLM12 0.29359001 W
PLM13 0.21211000 W

```

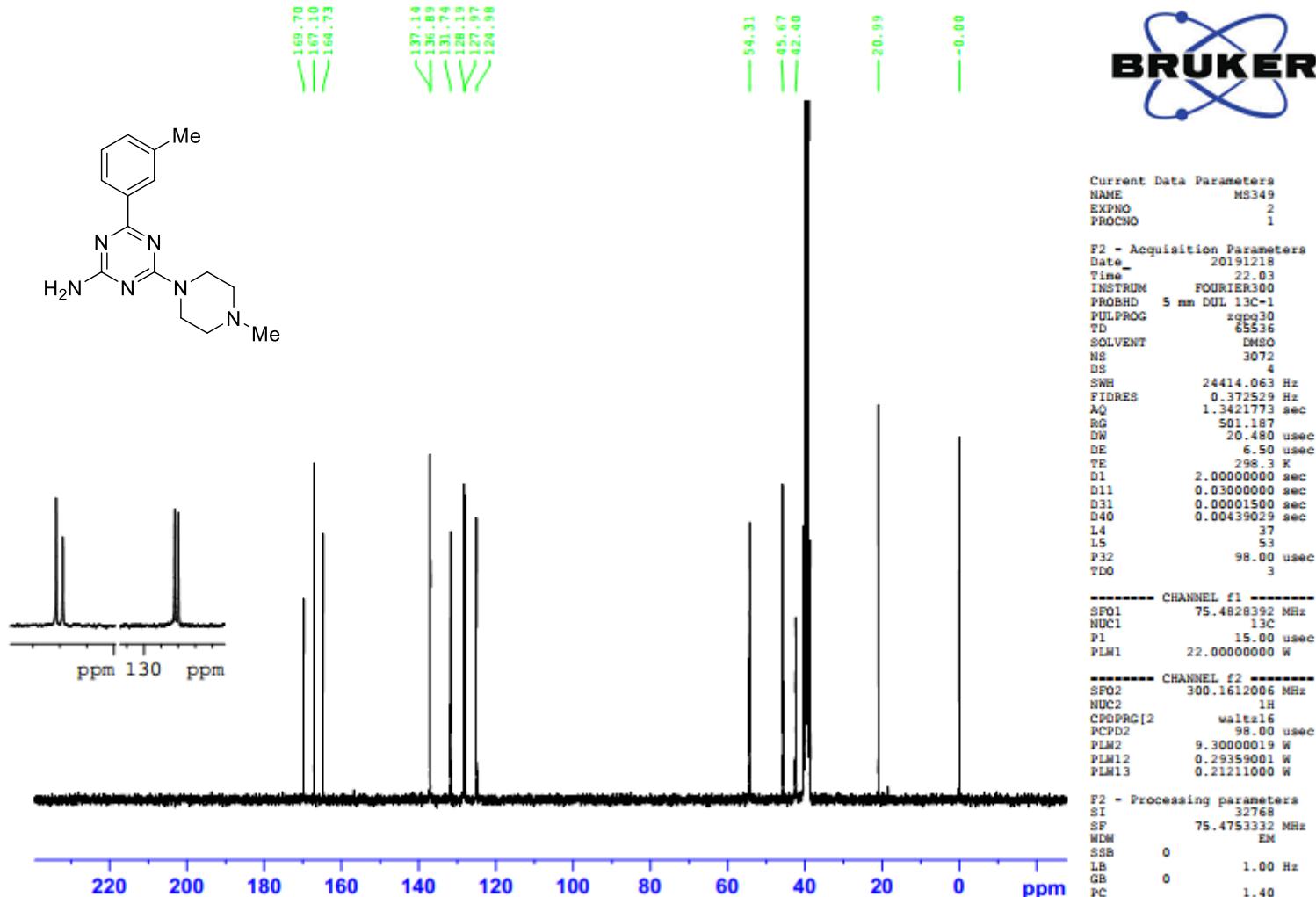
F2 - Processing parameters
SI          32768
SF          75.4753350 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB          0
PC          1.40

```

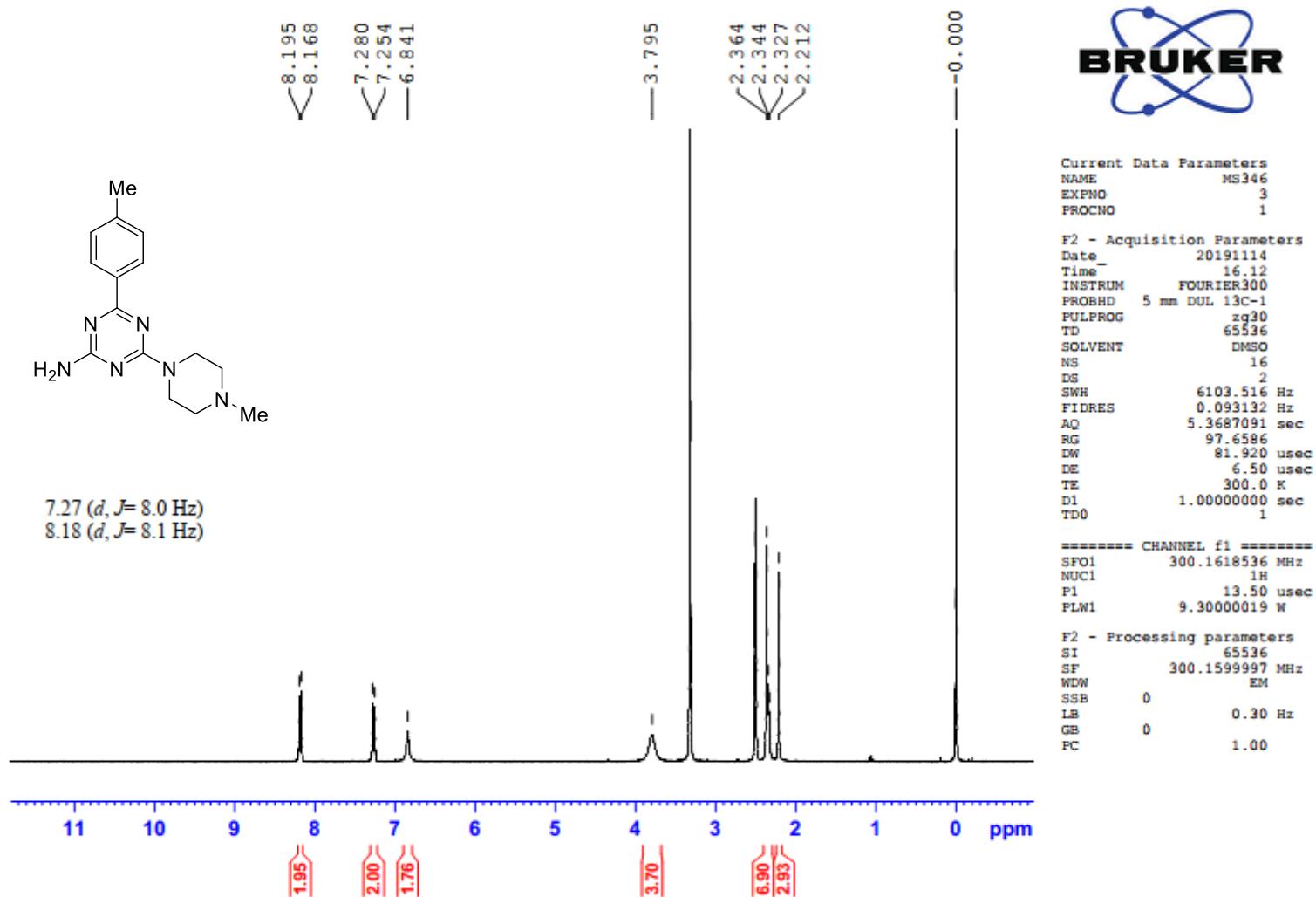
6-(3-Methylphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,5}**)



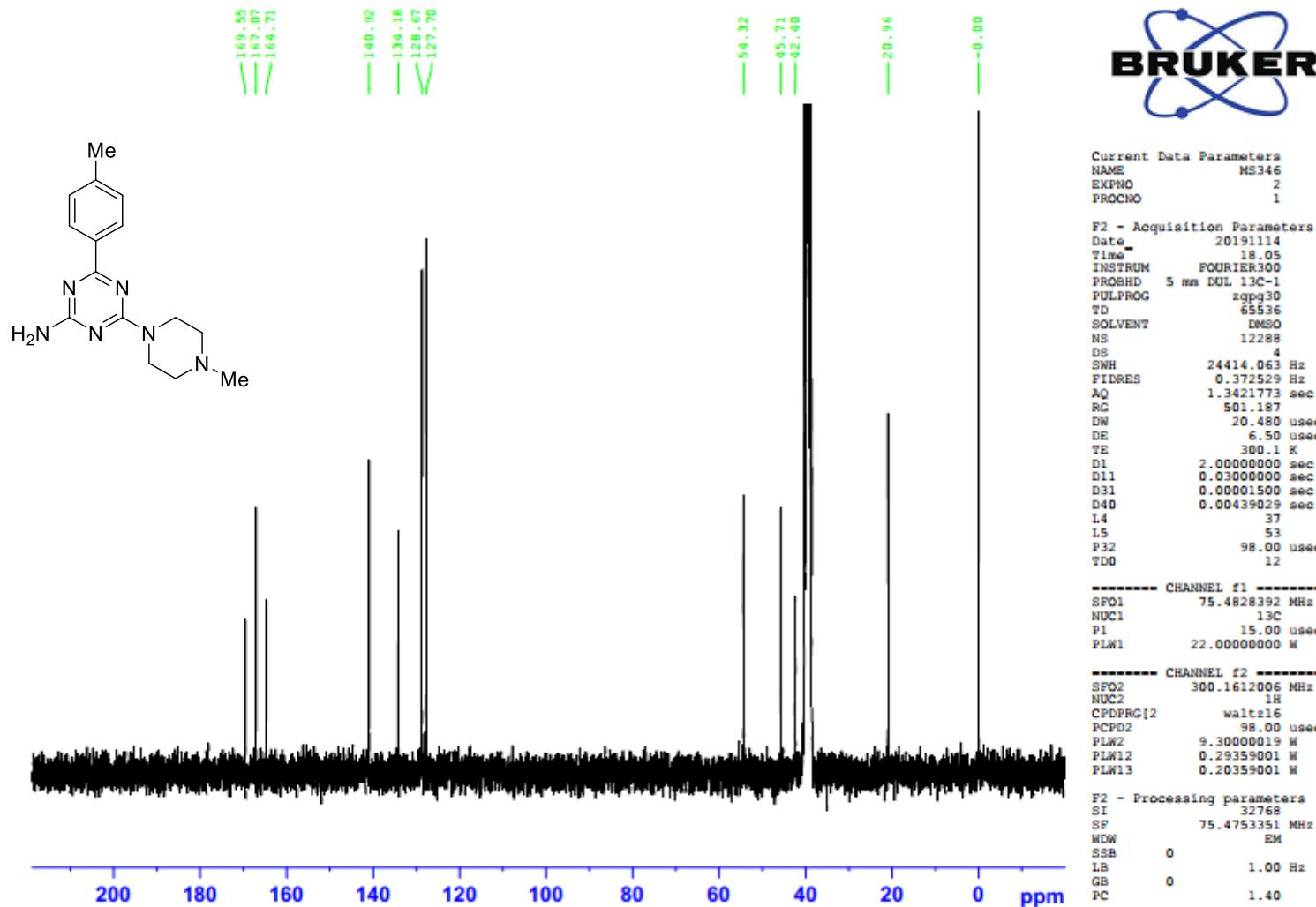
6-(3-Methylphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,5}**)



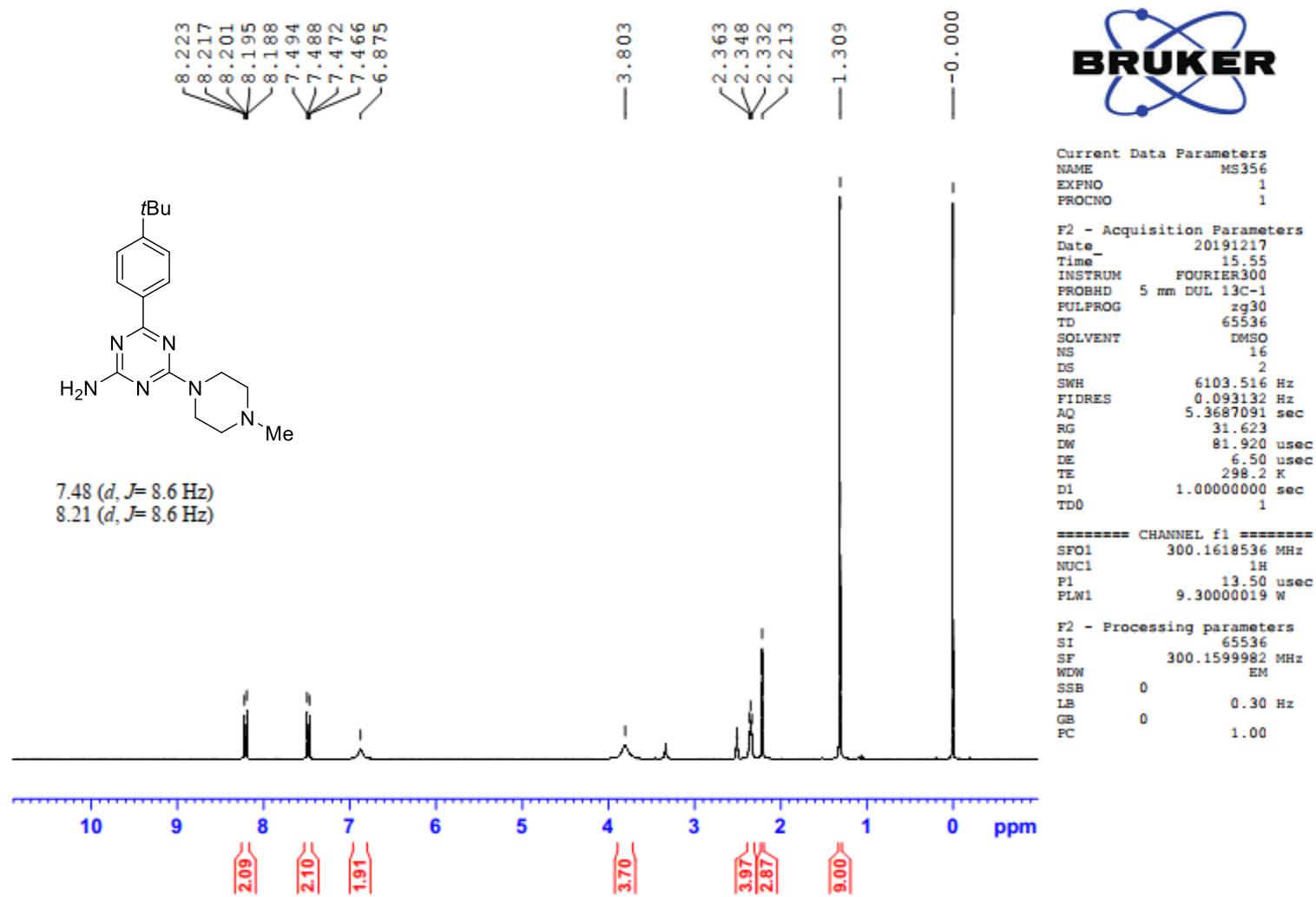
6-(4-Methylphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,6}**)



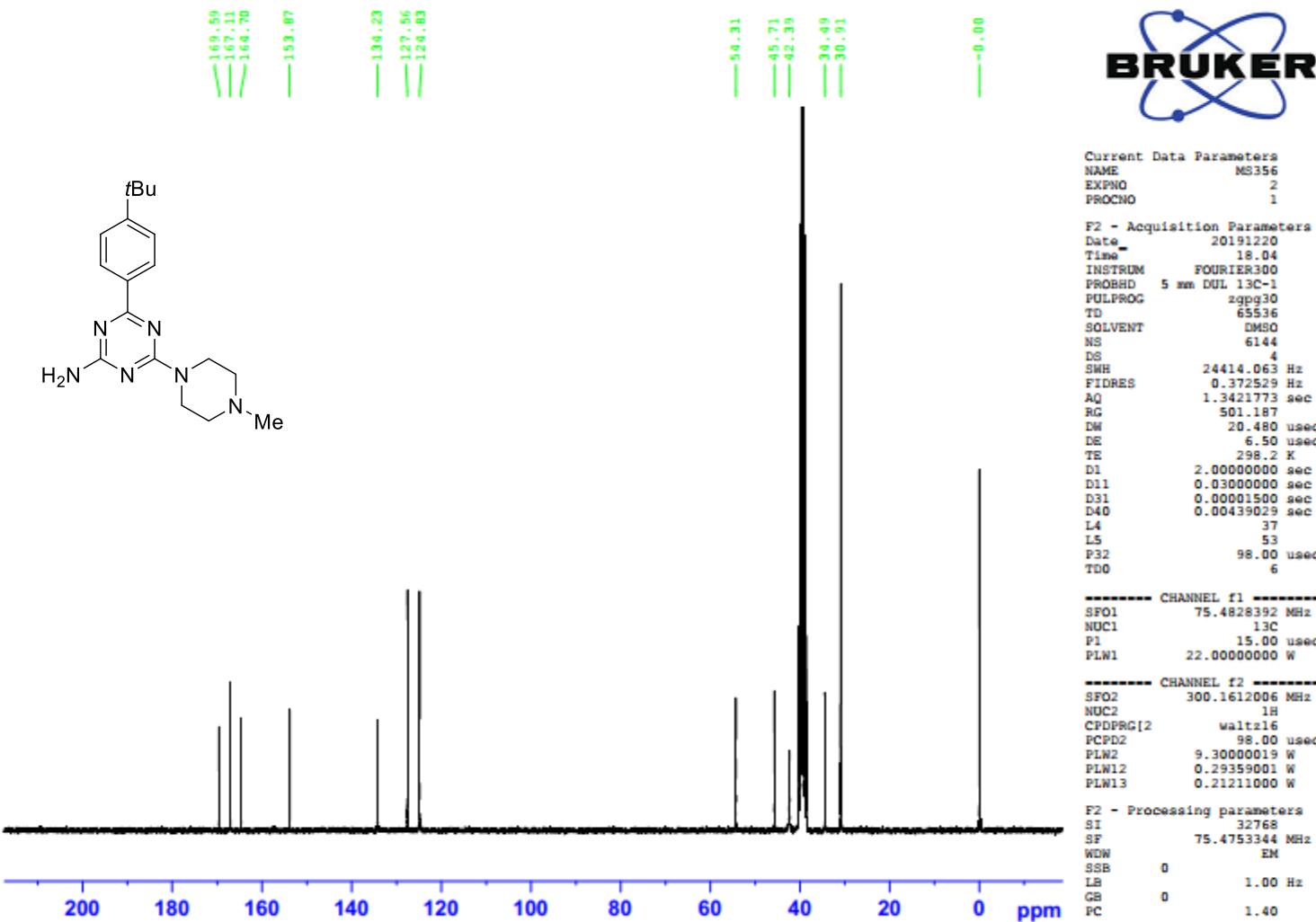
6-(4-Methylphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,6}**)



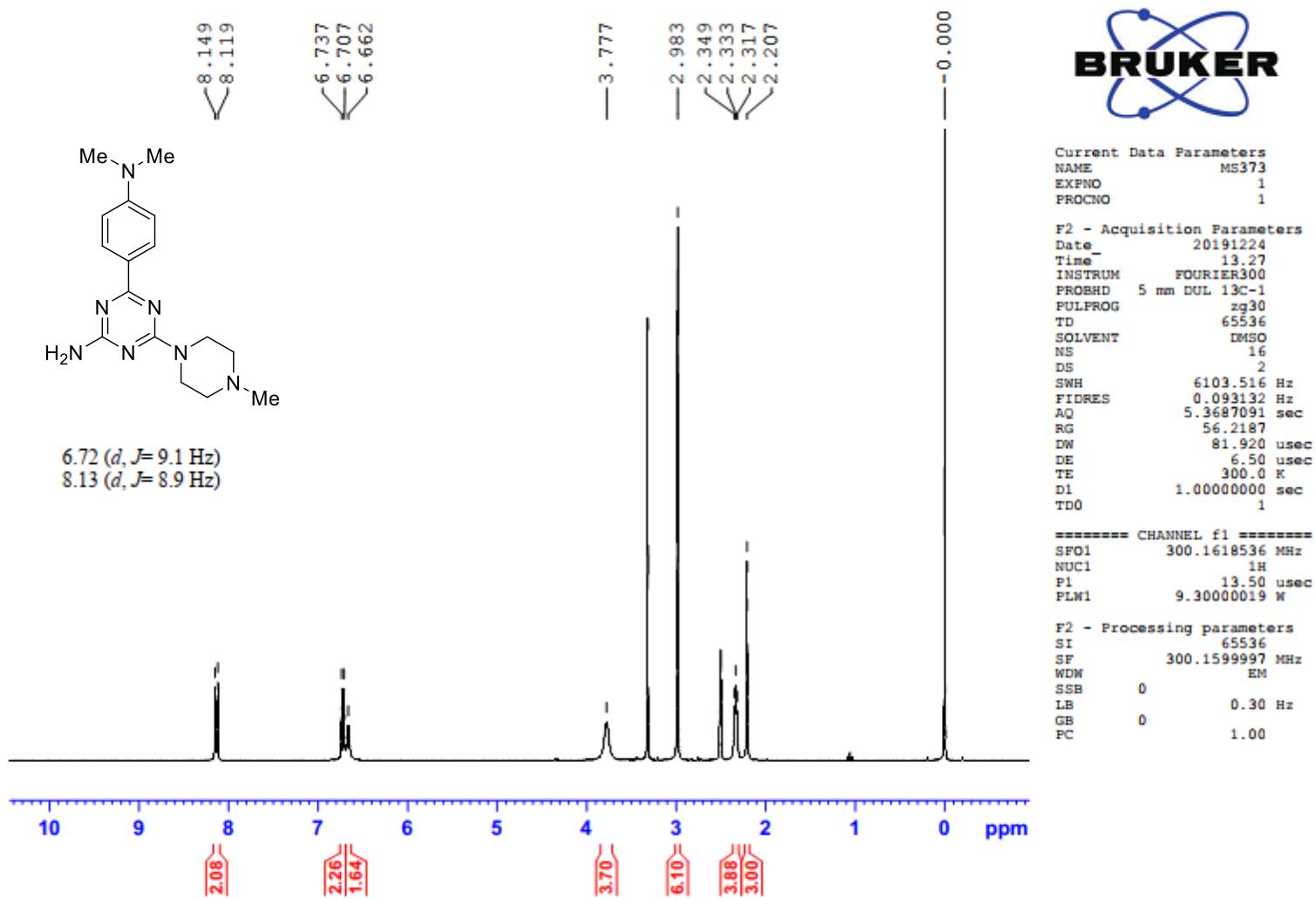
6-[4-(*tert*-Butyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,7}**)



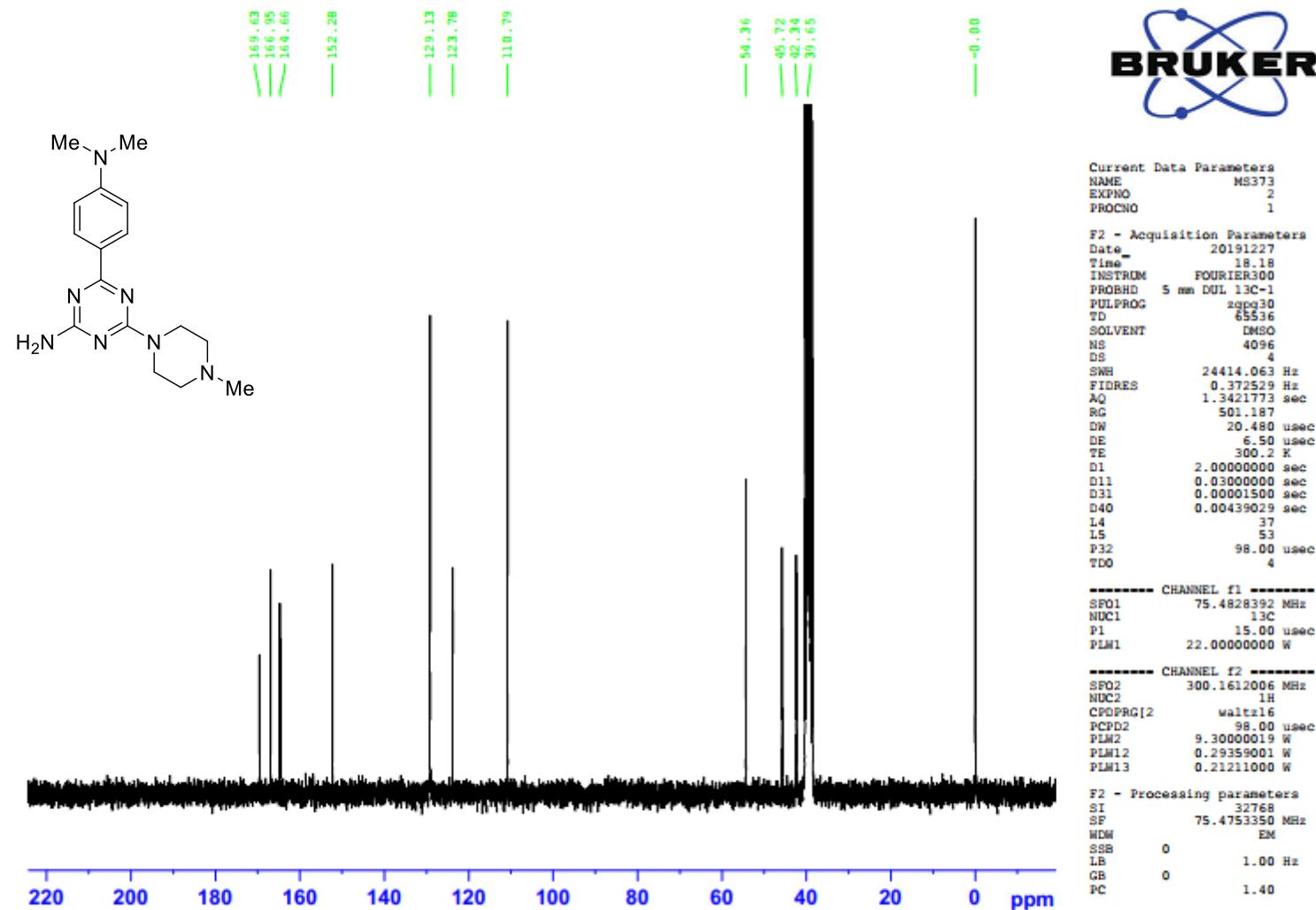
6-[4-(*tert*-Butyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,7}**)



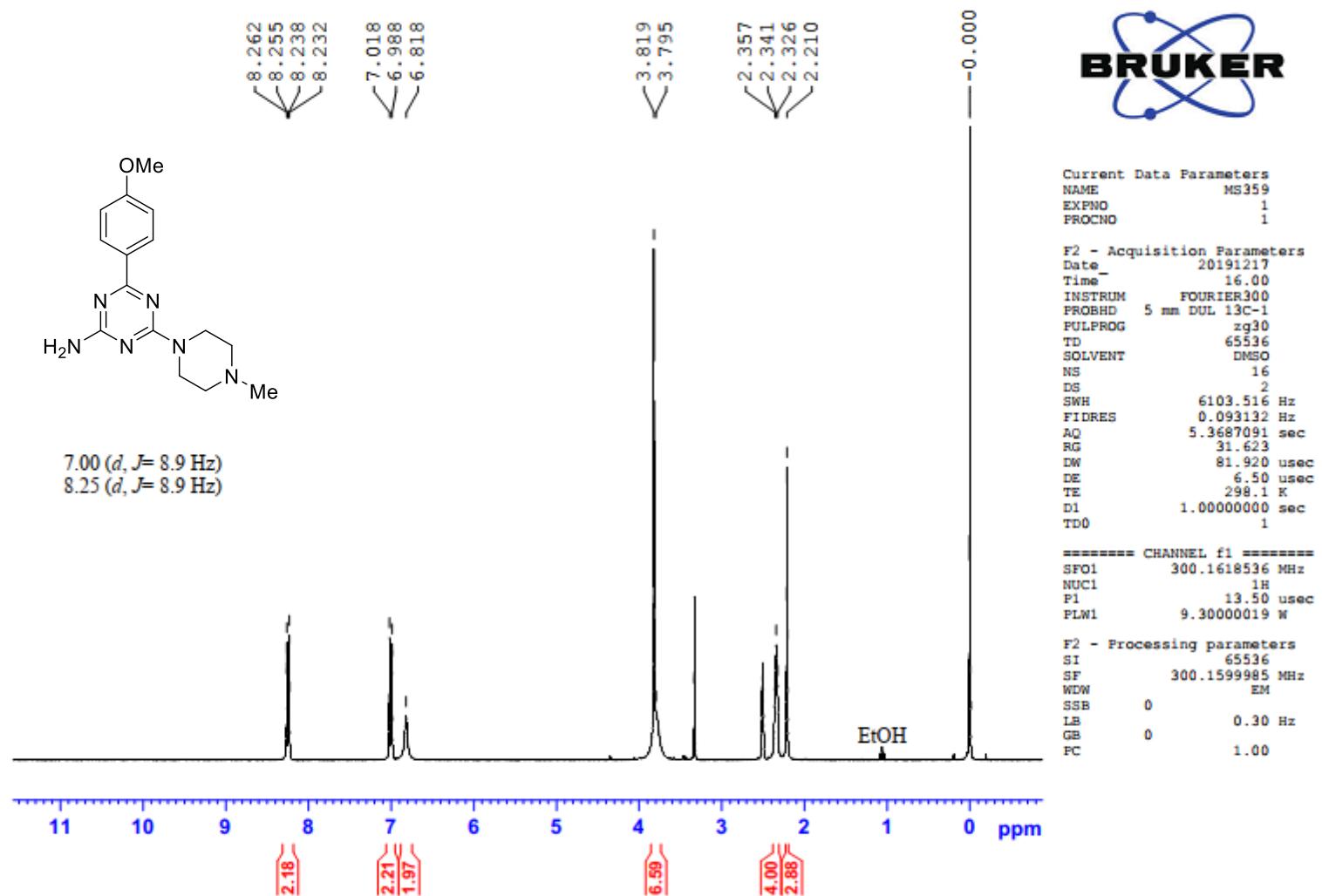
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,8}**)



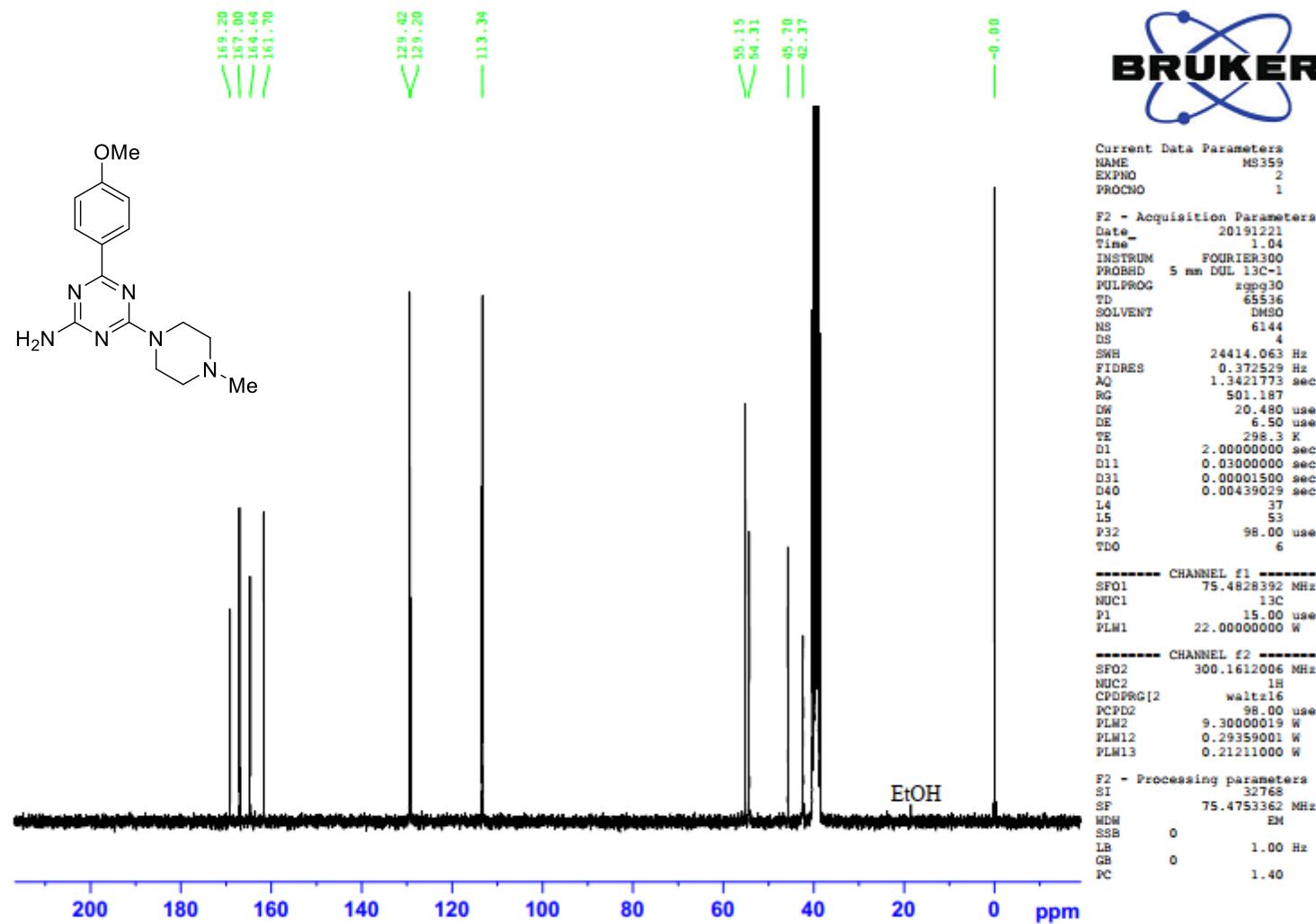
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,8}**)



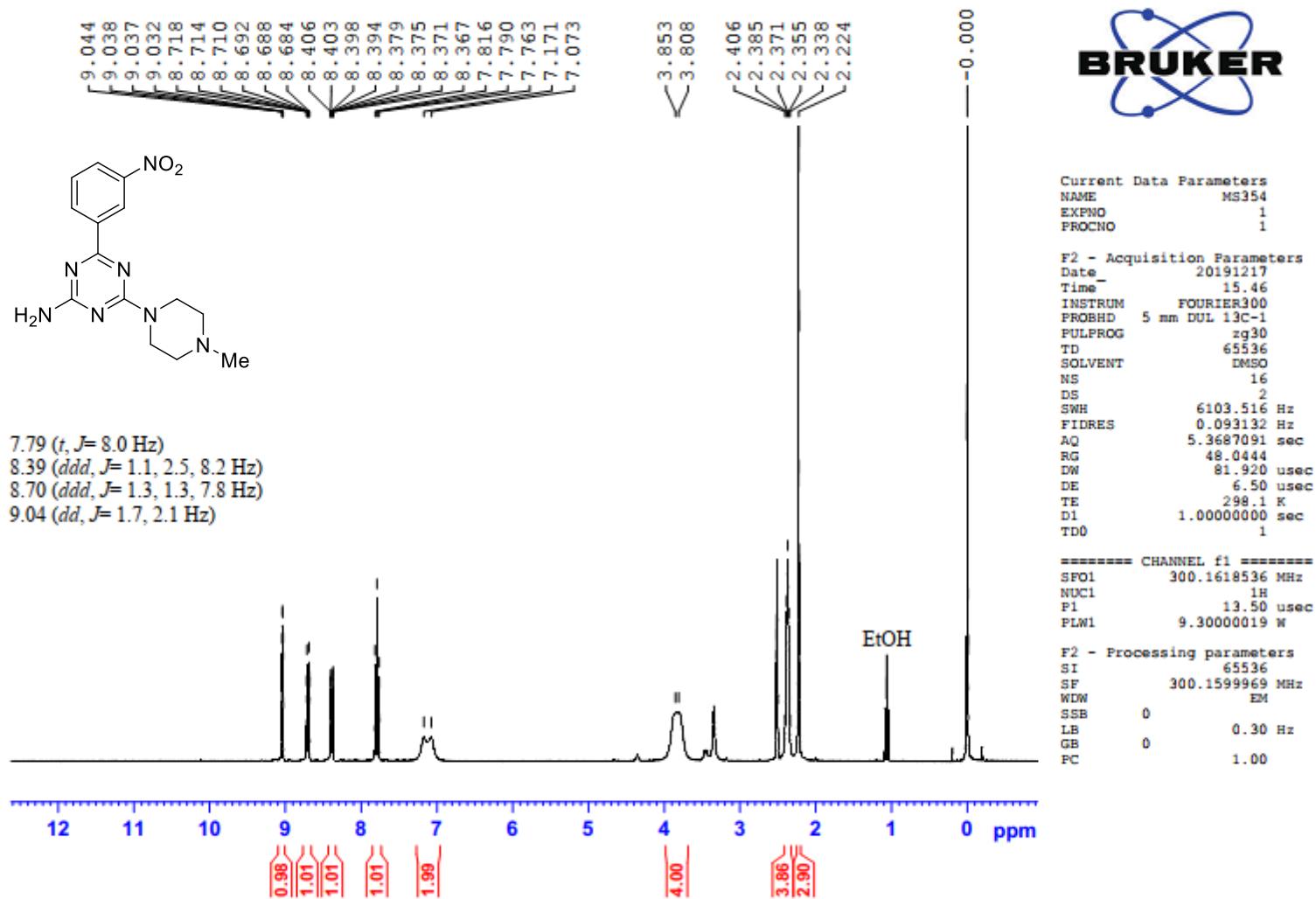
6-(4-Methoxyphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,9}**)



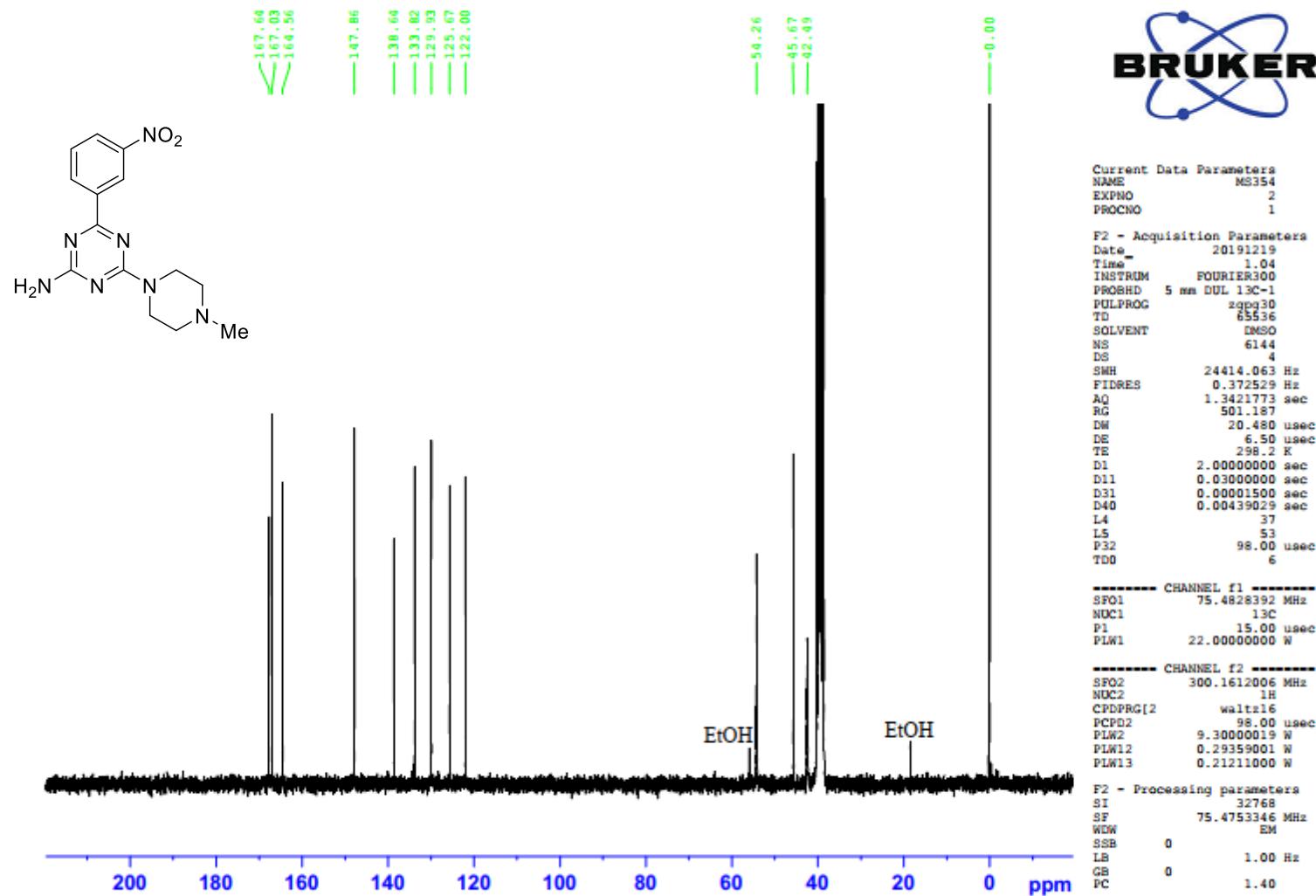
6-(4-Methoxyphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,9}**)



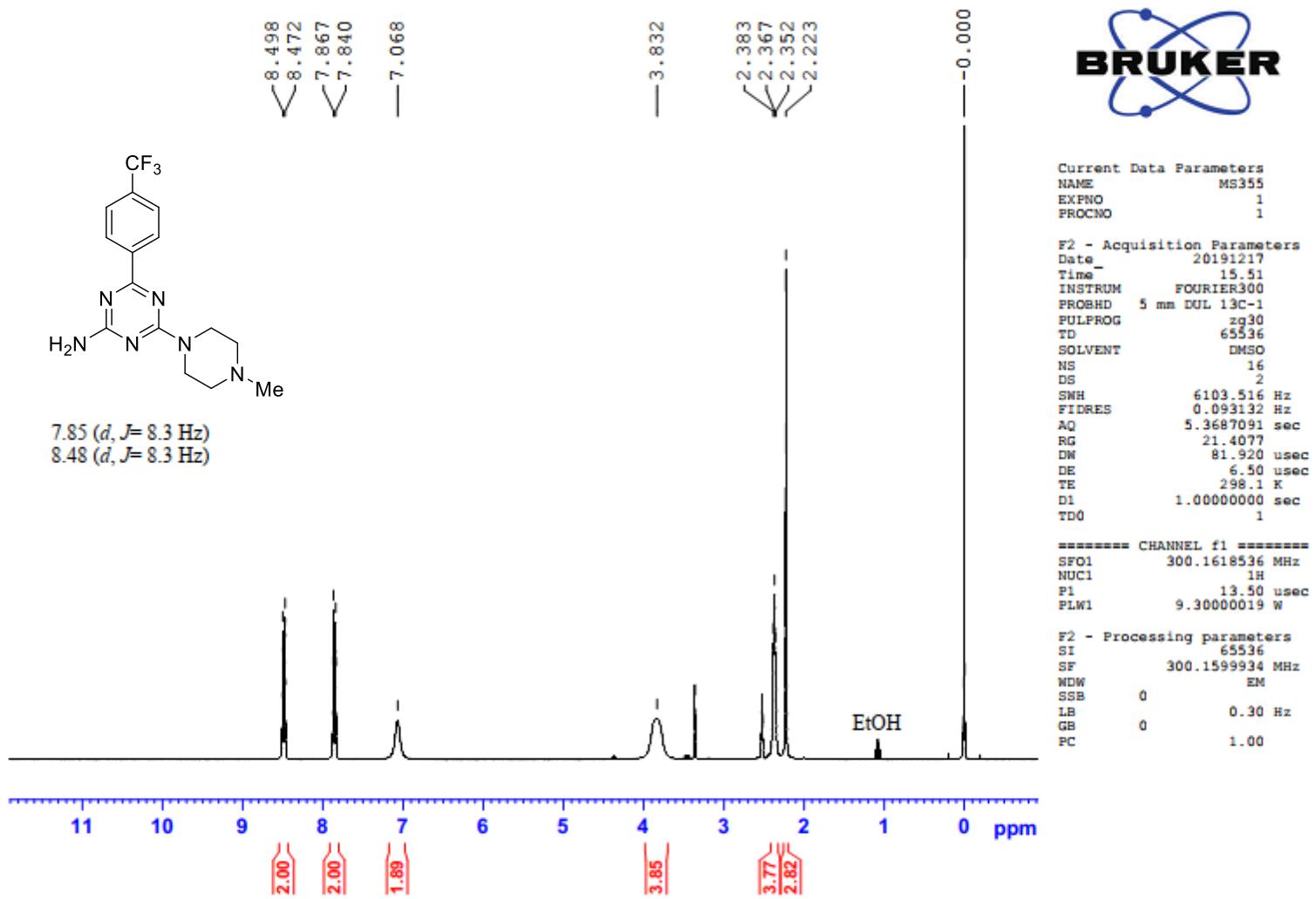
4-(4-Methylpiperazino)-6-(3-nitrophenyl)-1,3,5-triazine-2-amine (**9{4,10}**)



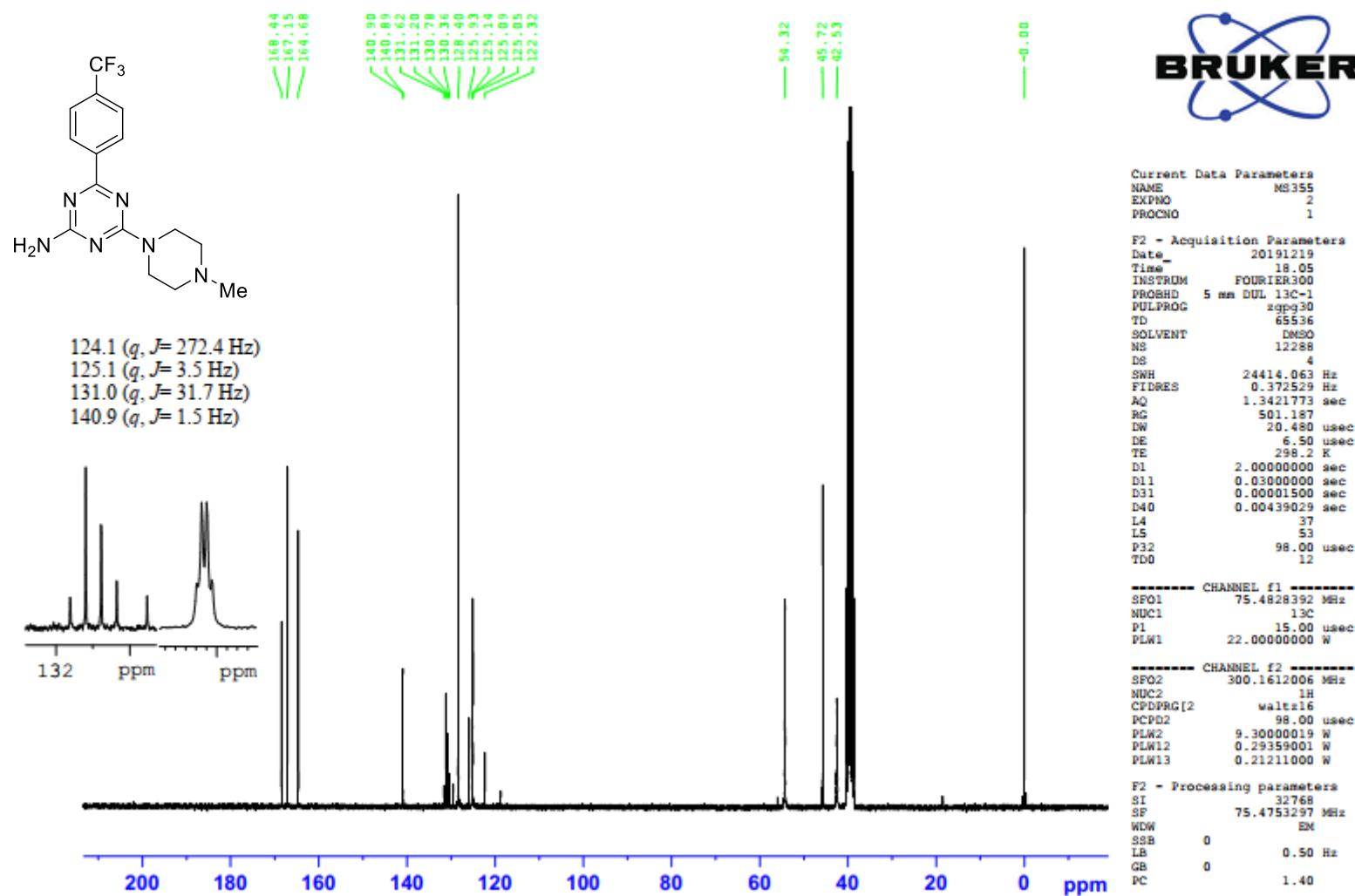
4-(4-Methylpiperazino)-6-(3-nitrophenyl)-1,3,5-triazine-2-amine (**9{4,10}**)



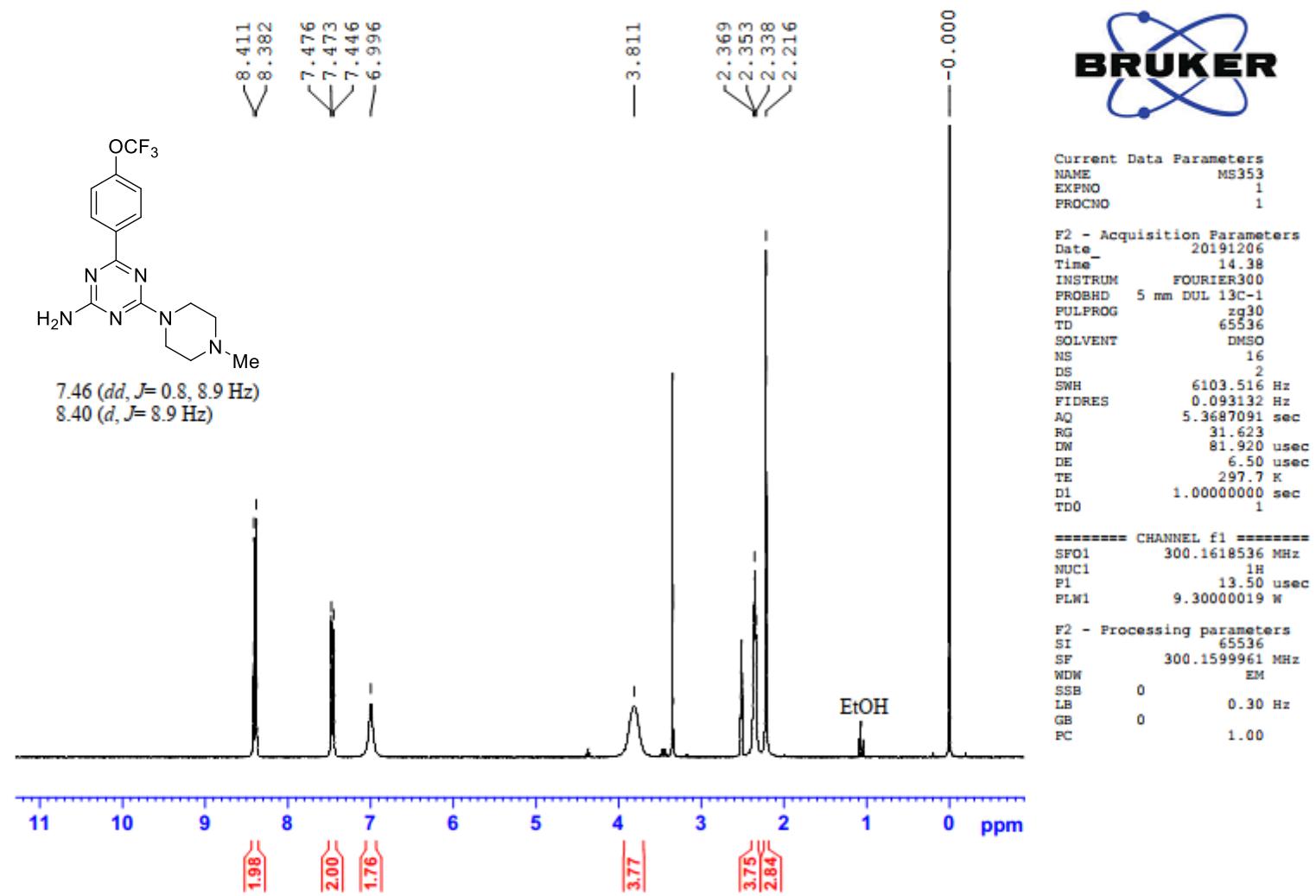
6-[4-(Trifluoromethyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,11}**)



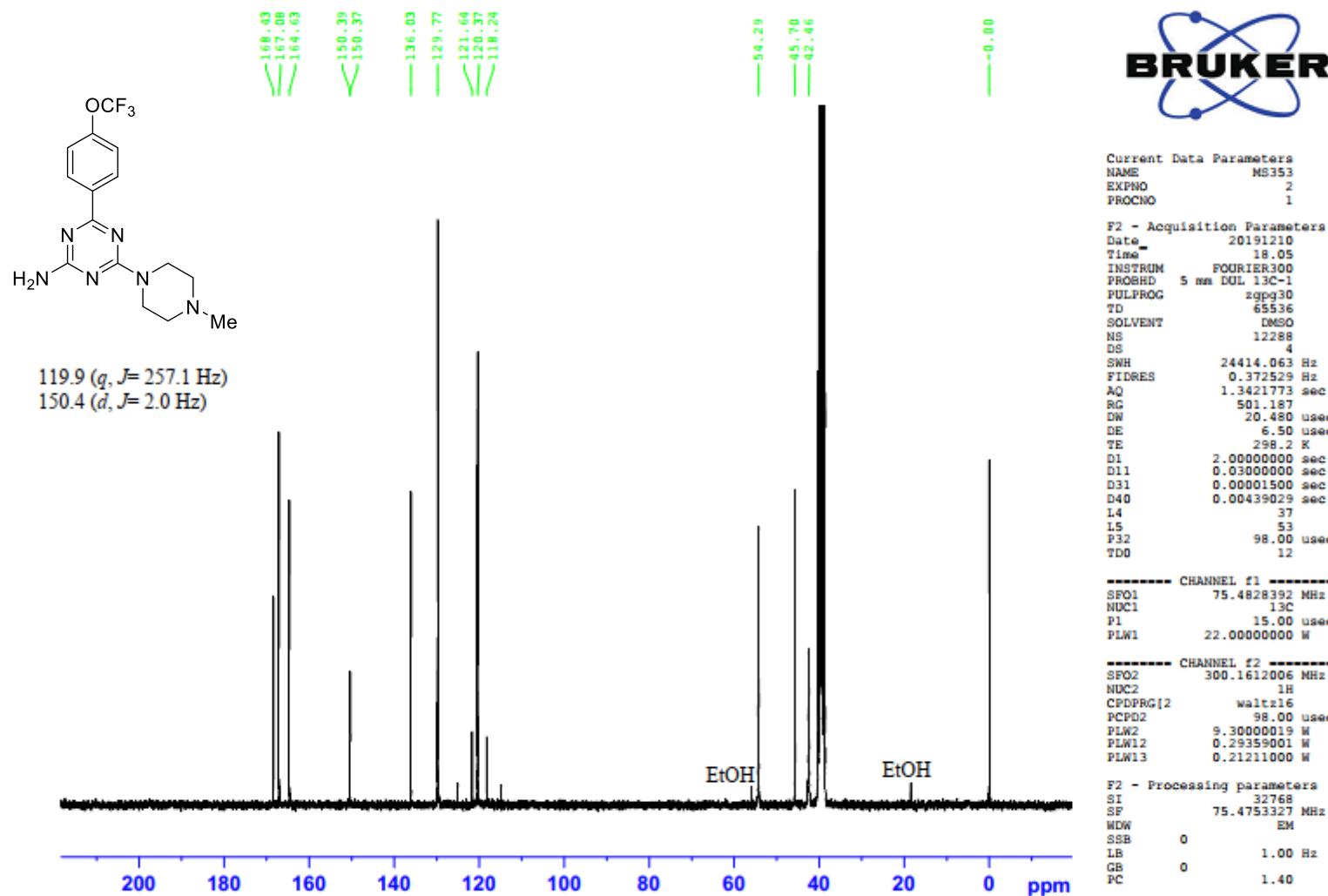
6-[4-(Trifluoromethyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,11}**)



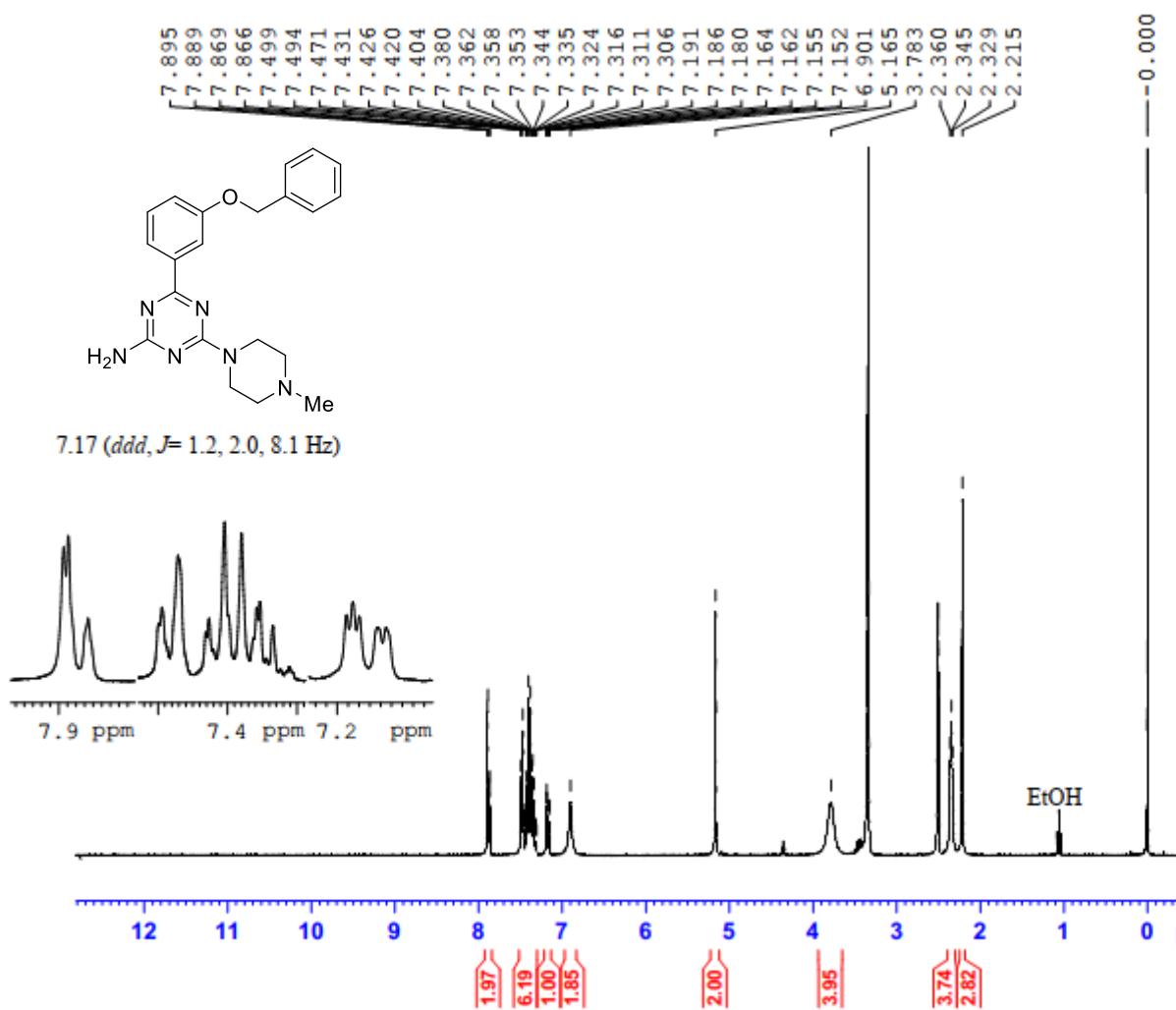
6-[4-(Trifluoromethoxy)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9**{4,12})



6-[4-(Trifluoromethoxy)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,12}**)



6-[3-(Benzyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9**{4,14})



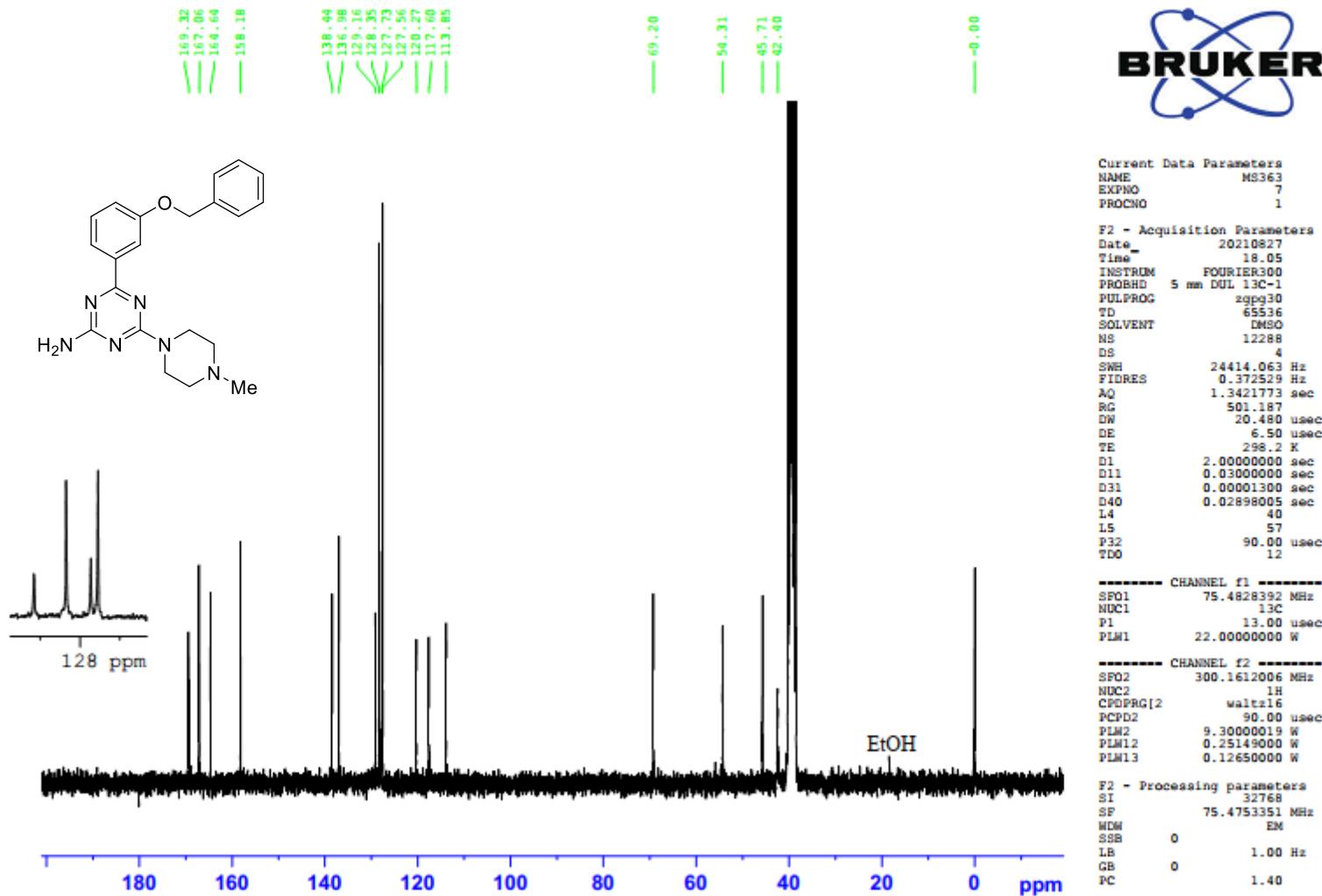
Current Data Parameters
 NAME MS363
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date 20210826
 Time 10.10
 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 76.3575
 DW 81.920 usec
 DE 6.50 usec
 TE 299.2 K
 D1 1.0000000 sec
 TDO 1

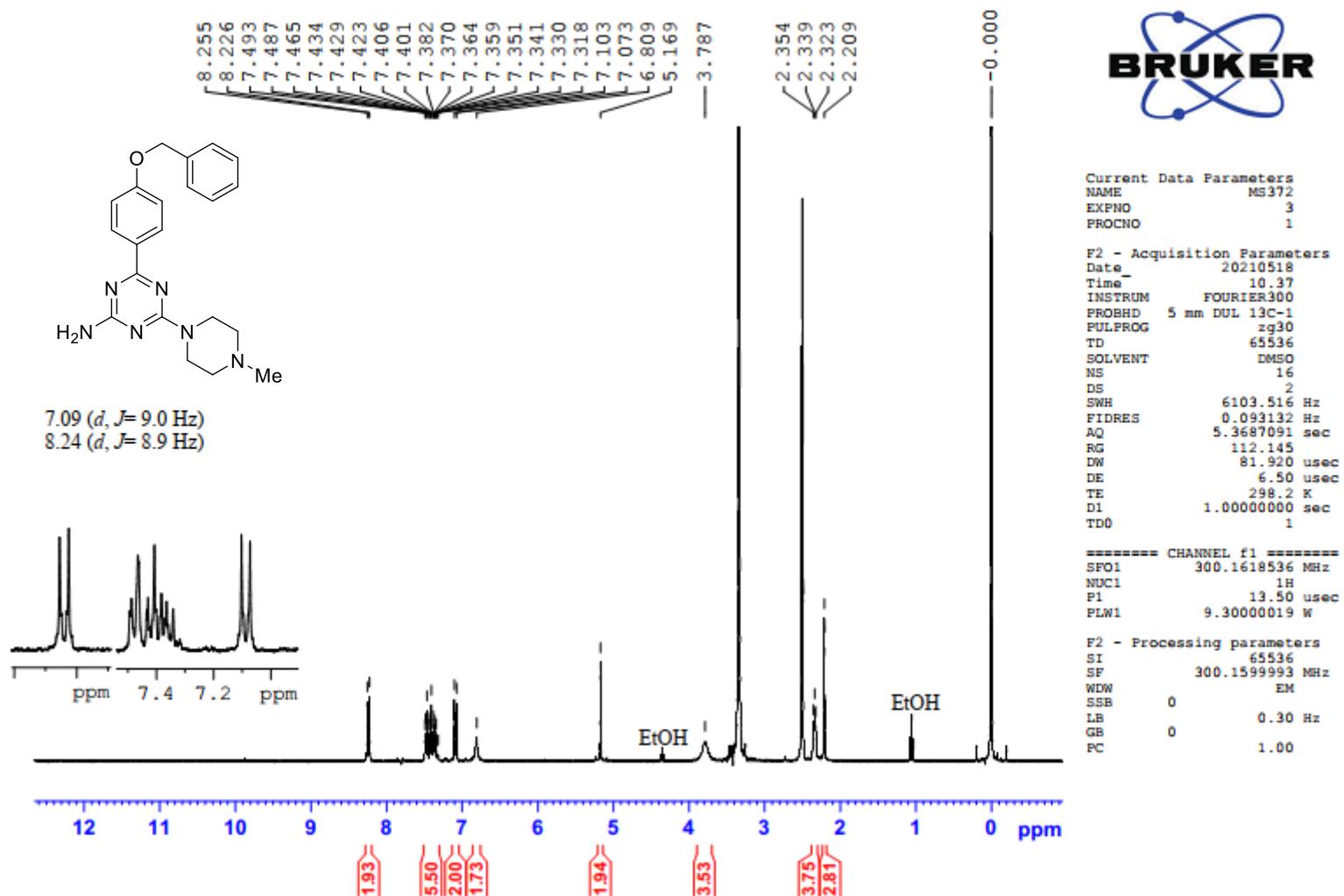
===== CHANNEL f1 =====
 SFO1 300.1618536 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 9.30000019 W

F2 - Processing parameters
 SI 65536
 SF 300.1599987 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

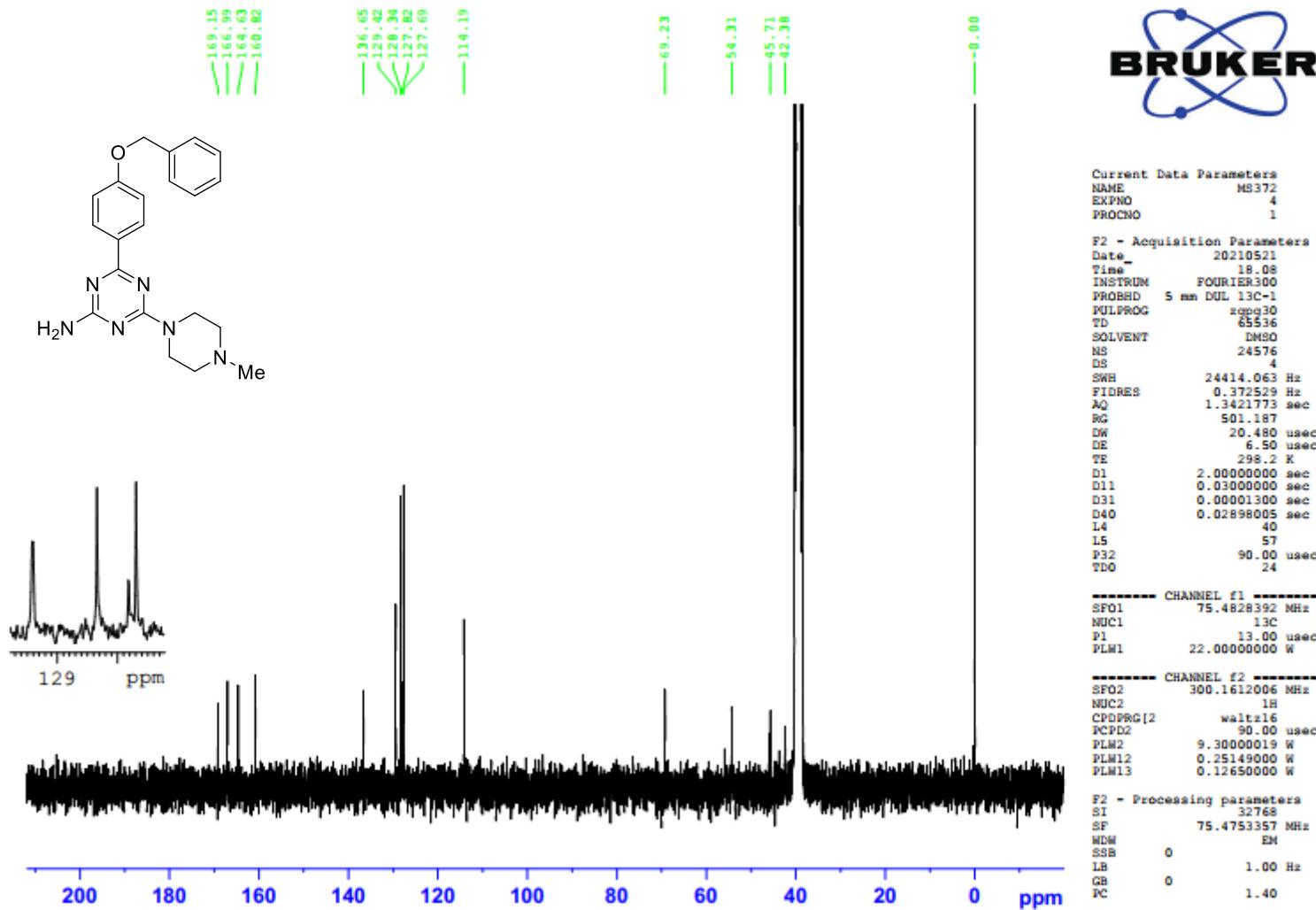
6-[3-(Benzyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,14}**)



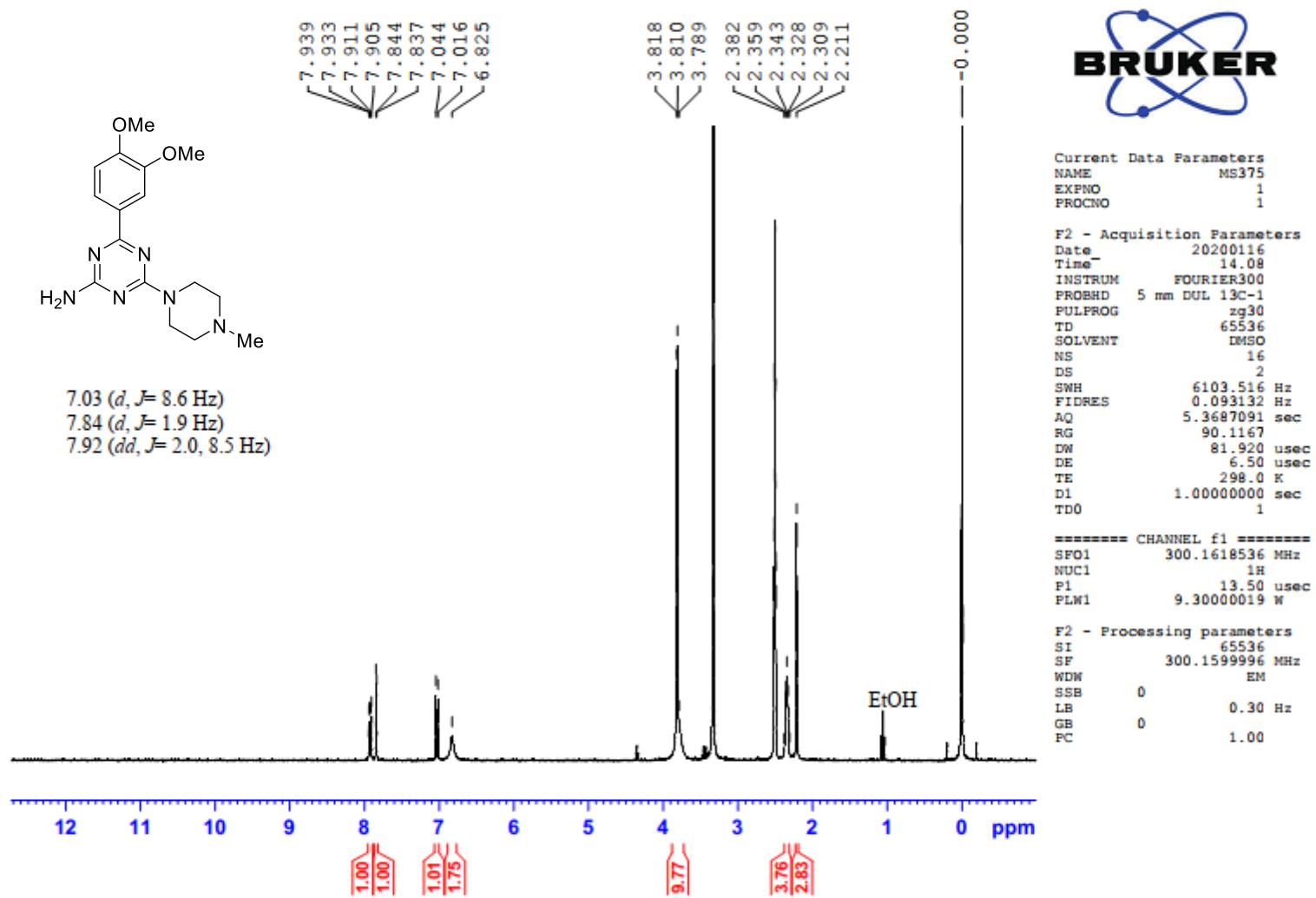
6-[4-(Benzyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,15}**)



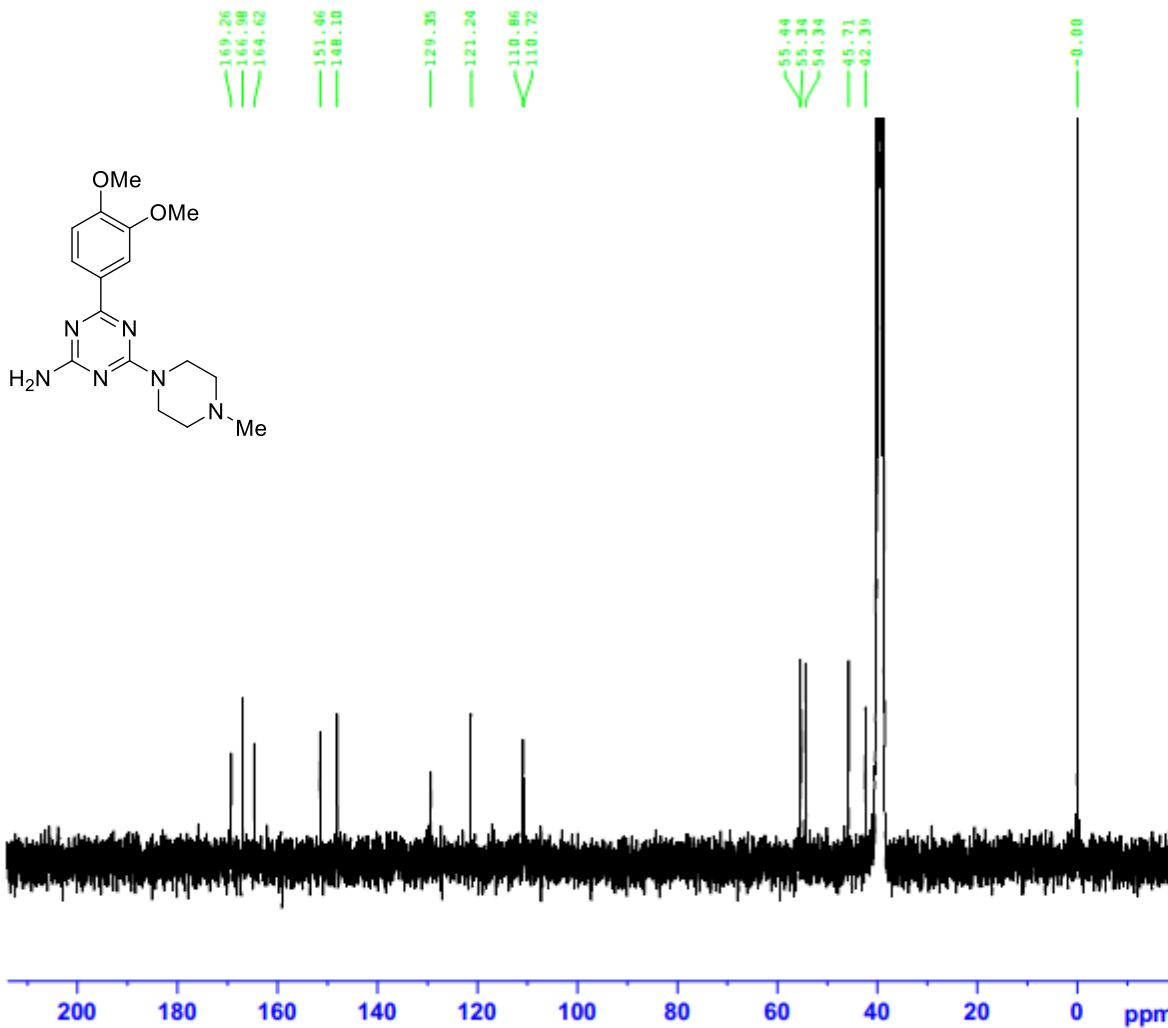
6-[4-(Benzyl)phenyl]-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,15}**)



6-(3,4-Dimethoxyphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,16}**)



6-(3,4-Dimethoxyphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,16}**)



BRUKER

Current Data Parameters
NAME MS375
EXPNO 2
PROCNO 1

```

F2 - Acquisition Parameters
Date       20200117
Time       18.06
INSTRUM   FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG  zgpg30
TD        65536
SOLVENT   DMso
NS        12288
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        298.1 K
D1        2.0000000 sec
D11       0.03000000 sec
D31       0.00001500 sec
D40       0.00439029 sec
L4        37
L5        53
P32       98.00 usec
TDDO      12

```

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

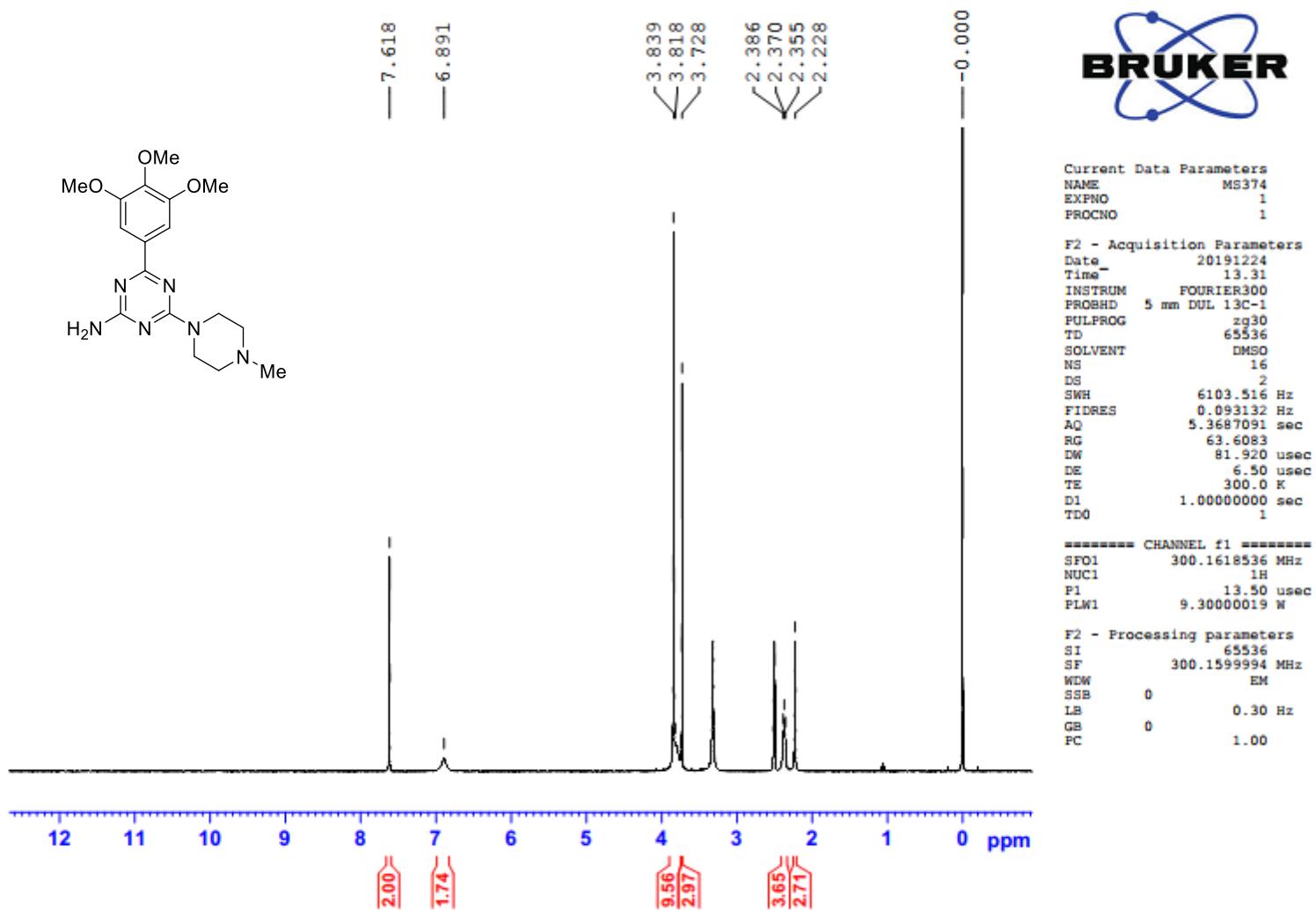
----- CHANNEL f2 -----
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 98.00 usec
PLW2 9.30000019 W
PLW12 0.293359001 W
PLW13 0.212111000 W

```

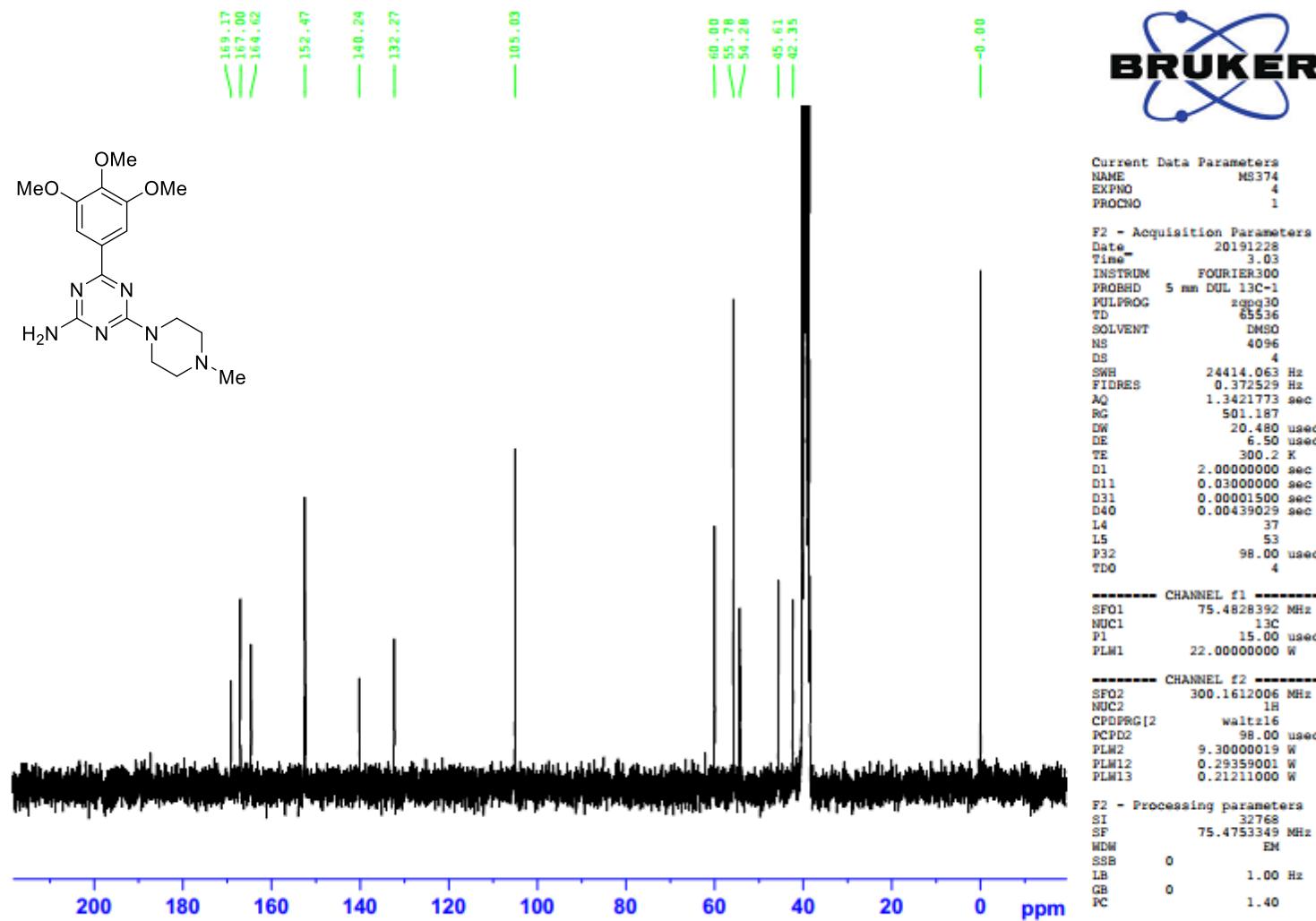
F2 - Processing parameters
SI           32768
SF          75.4753357 MHz
WDW           EM
SSB           0
LB           1.00 Hz
GB           0
PC           1.40

```

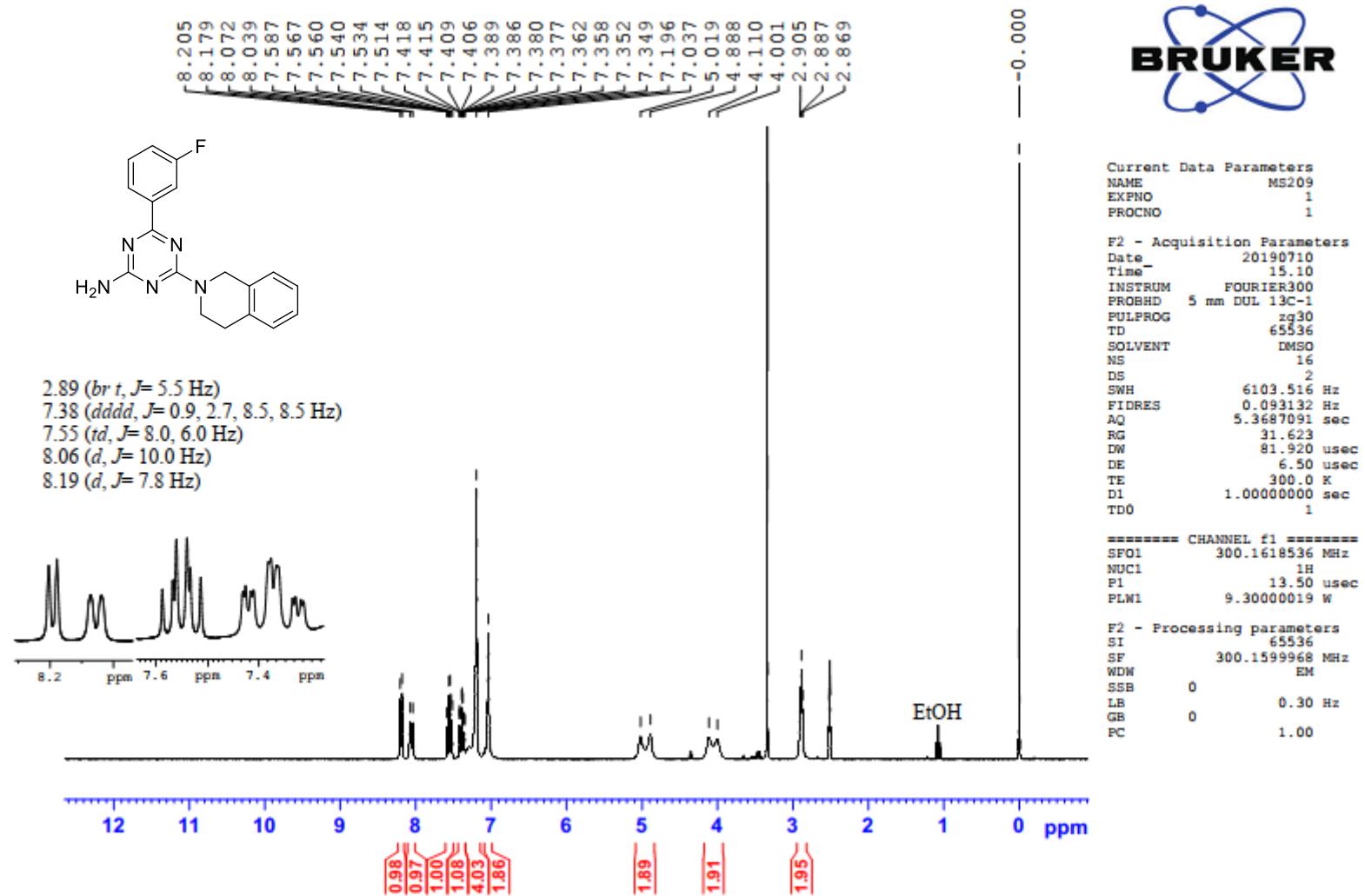
6-(3,4,5-Trimethoxyphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9**{4,17})



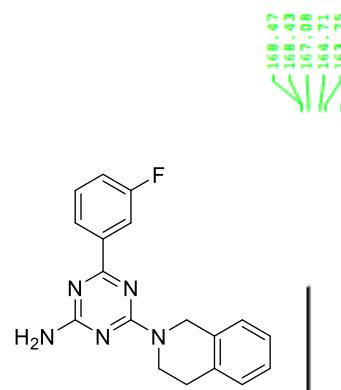
6-(3,4,5-Trimethoxyphenyl)-4-(4-methylpiperazino)-1,3,5-triazine-2-amine (**9{4,17}**)



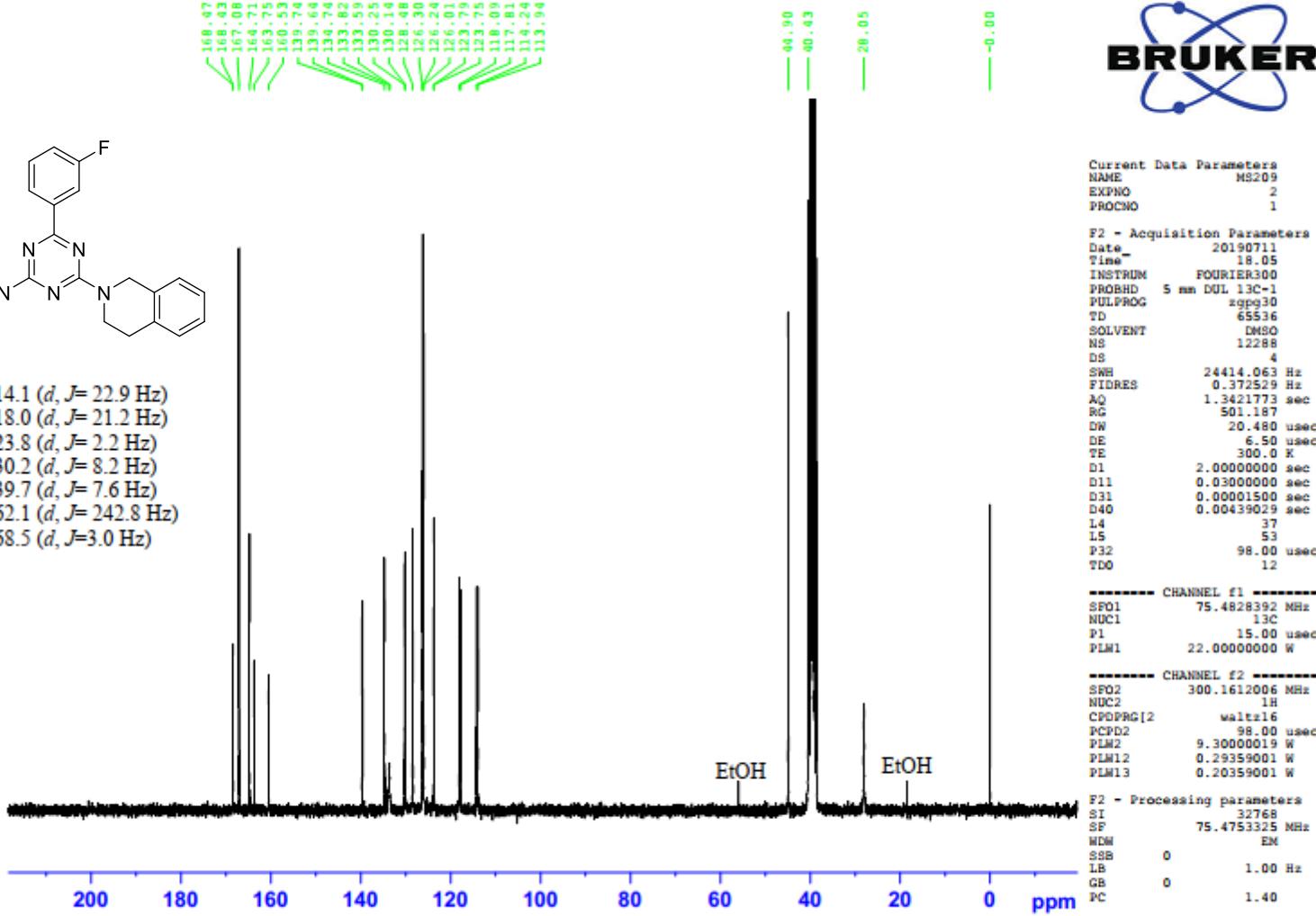
6-(3-Fluorophenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,2}**)



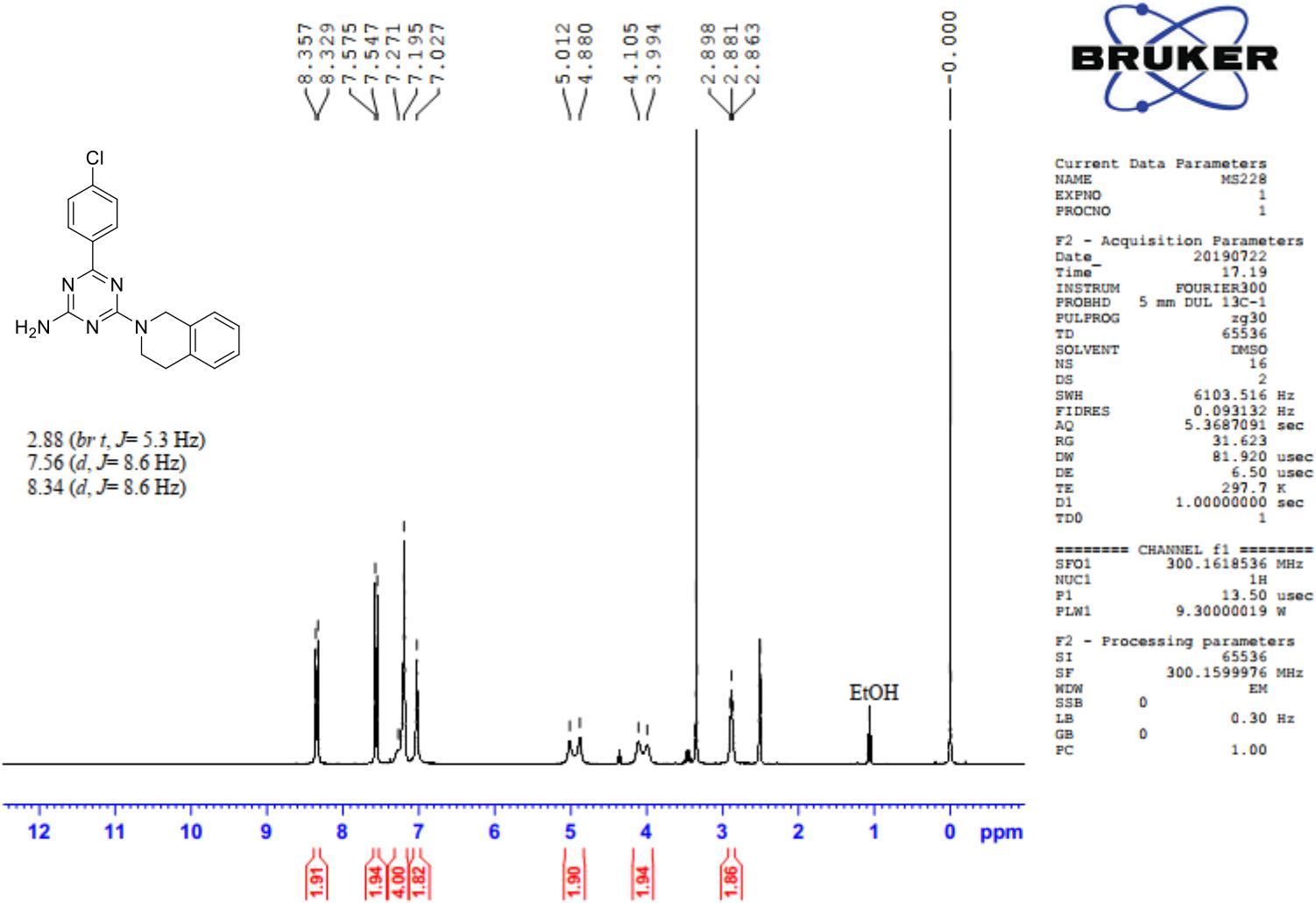
6-(3-Fluorophenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,2}**)



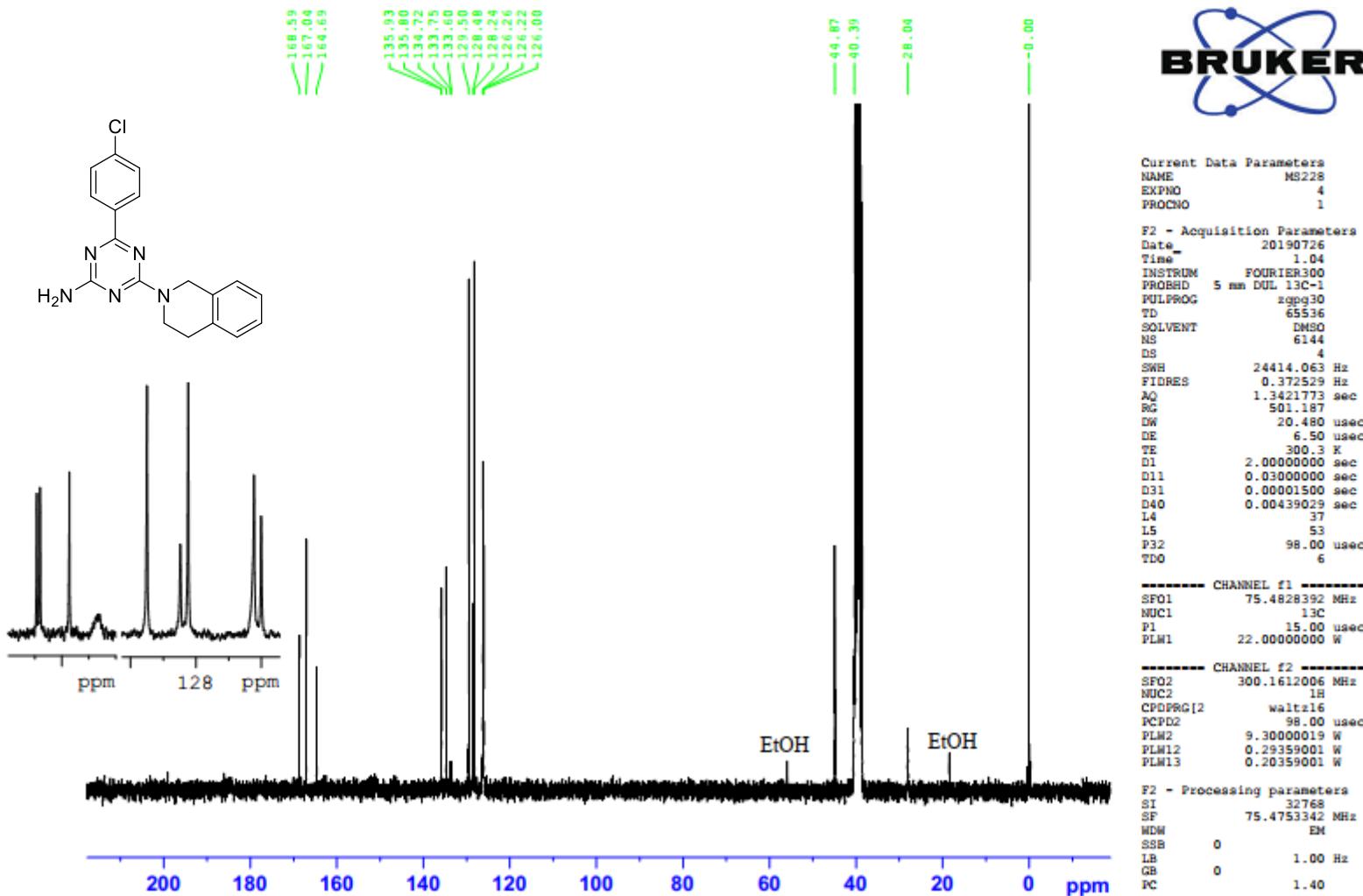
114.1 (d , $J = 22.9$ Hz)
 118.0 (d , $J = 21.2$ Hz)
 123.8 (d , $J = 2.2$ Hz)
 130.2 (d , $J = 8.2$ Hz)
 139.7 (d , $J = 7.6$ Hz)
 162.1 (d , $J = 242.8$ Hz)
 168.5 (d , $J = 3.0$ Hz)



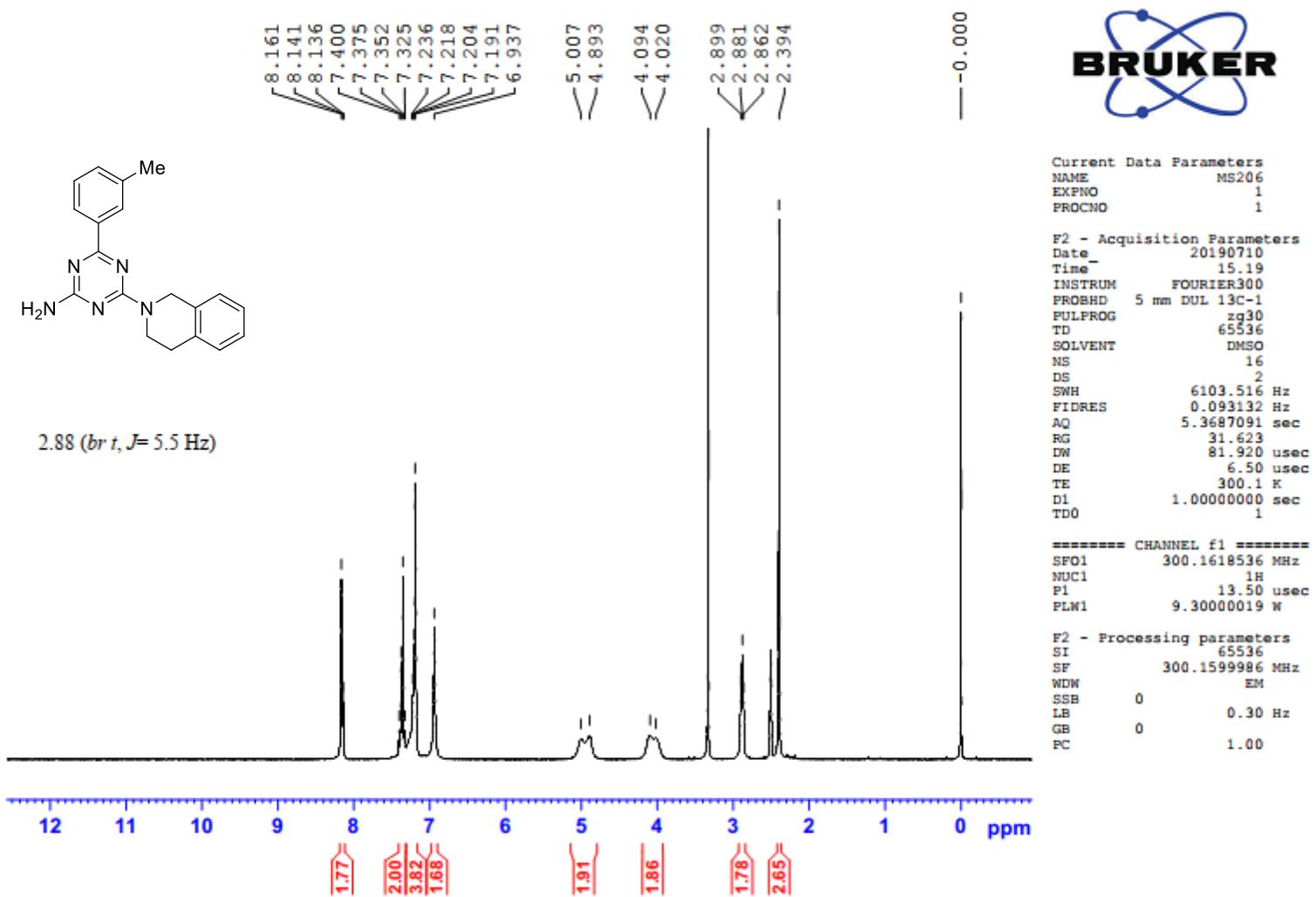
6-(4-Chlorophenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,4}**)



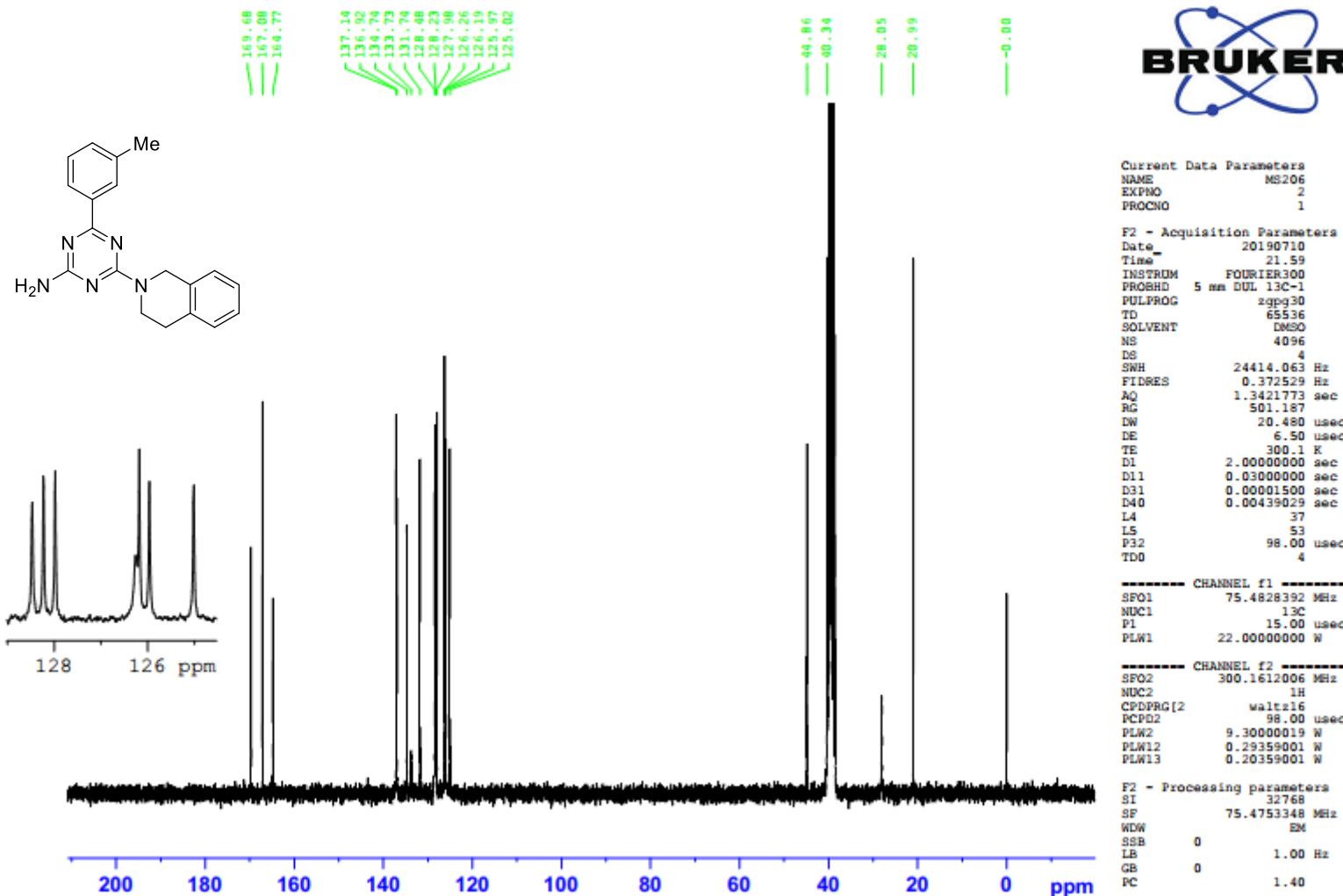
6-(4-Chlorophenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,4}**)



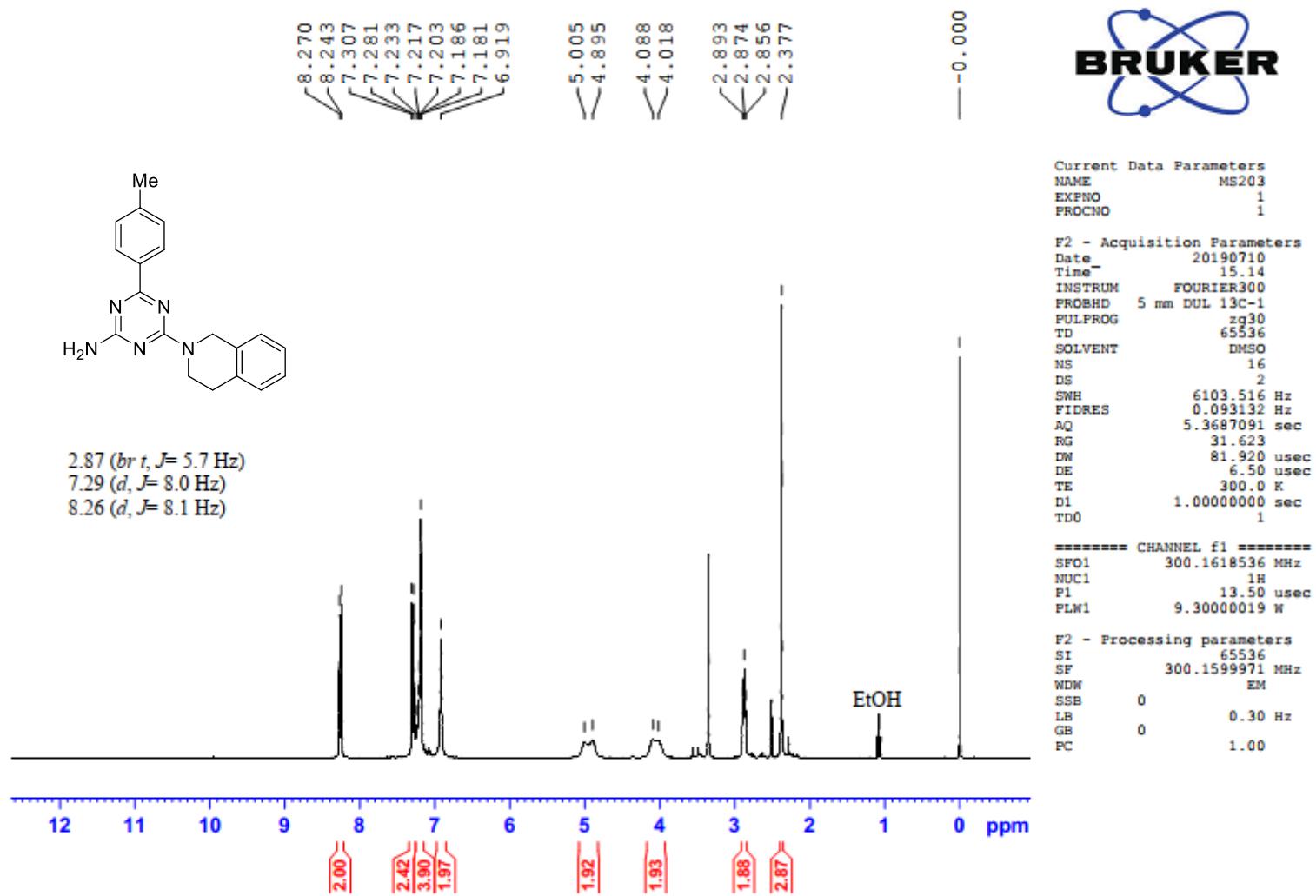
6-(3-Methylphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,5}**)



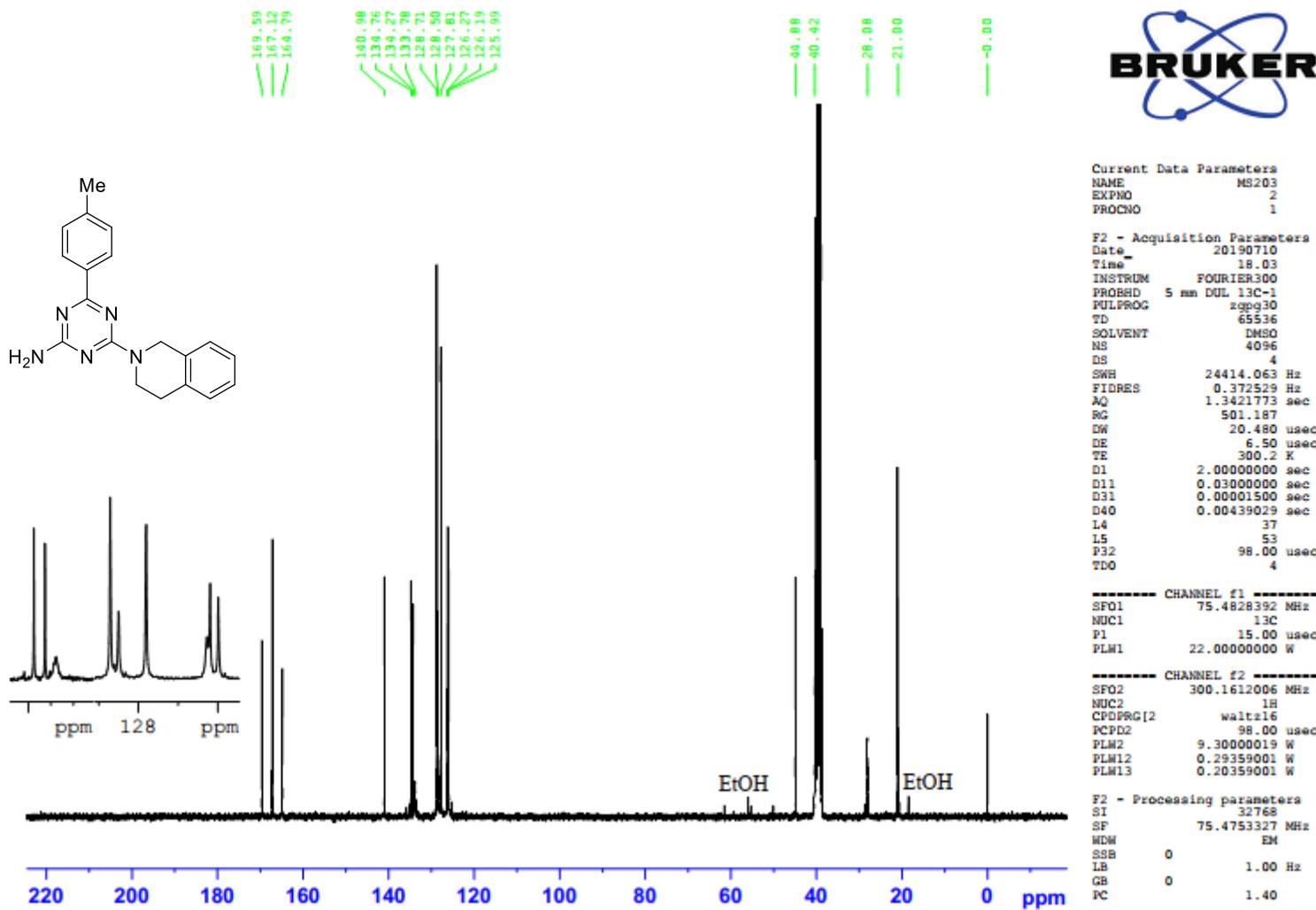
6-(3-Methylphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,5}**)



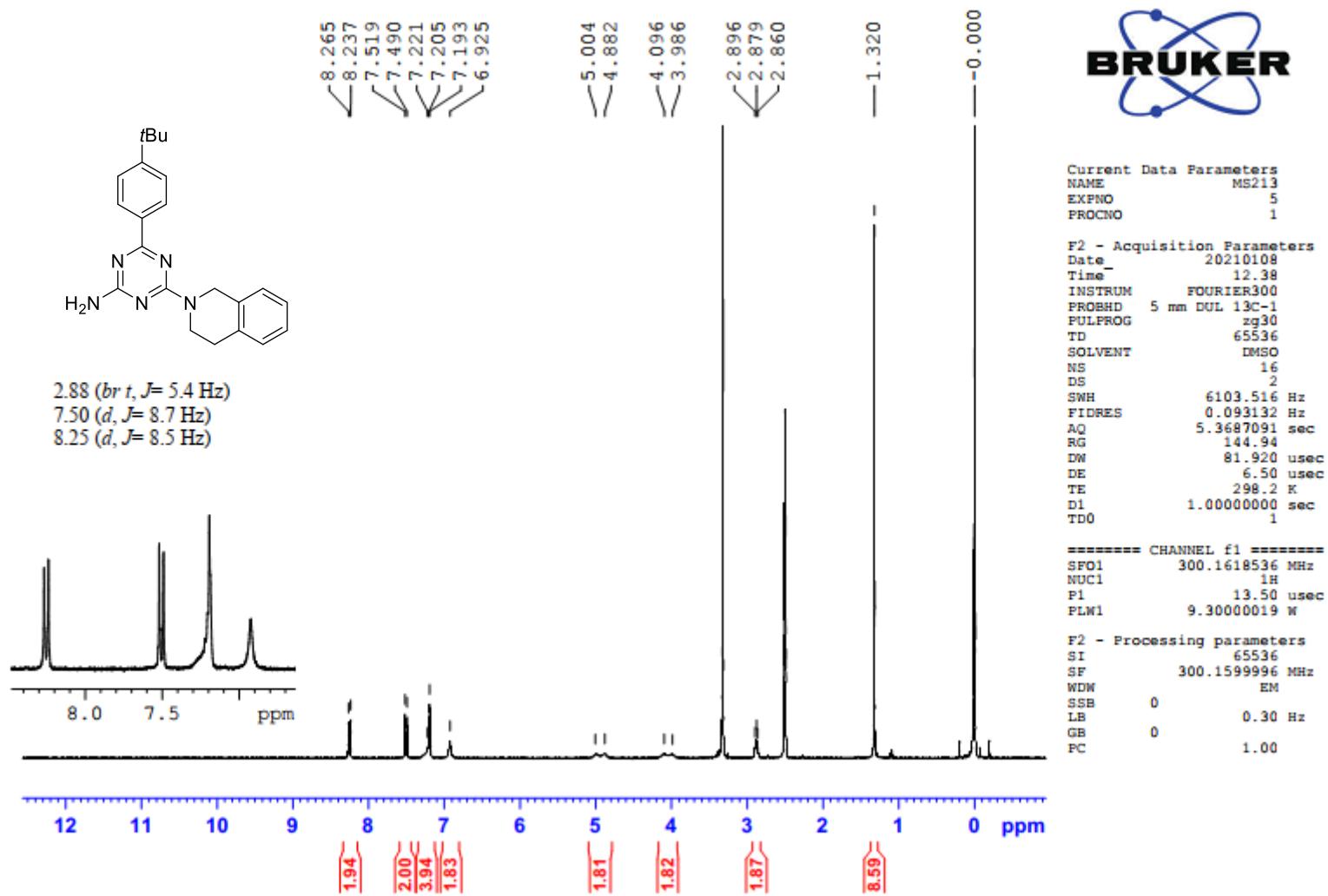
6-(4-Methylphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,6}**)



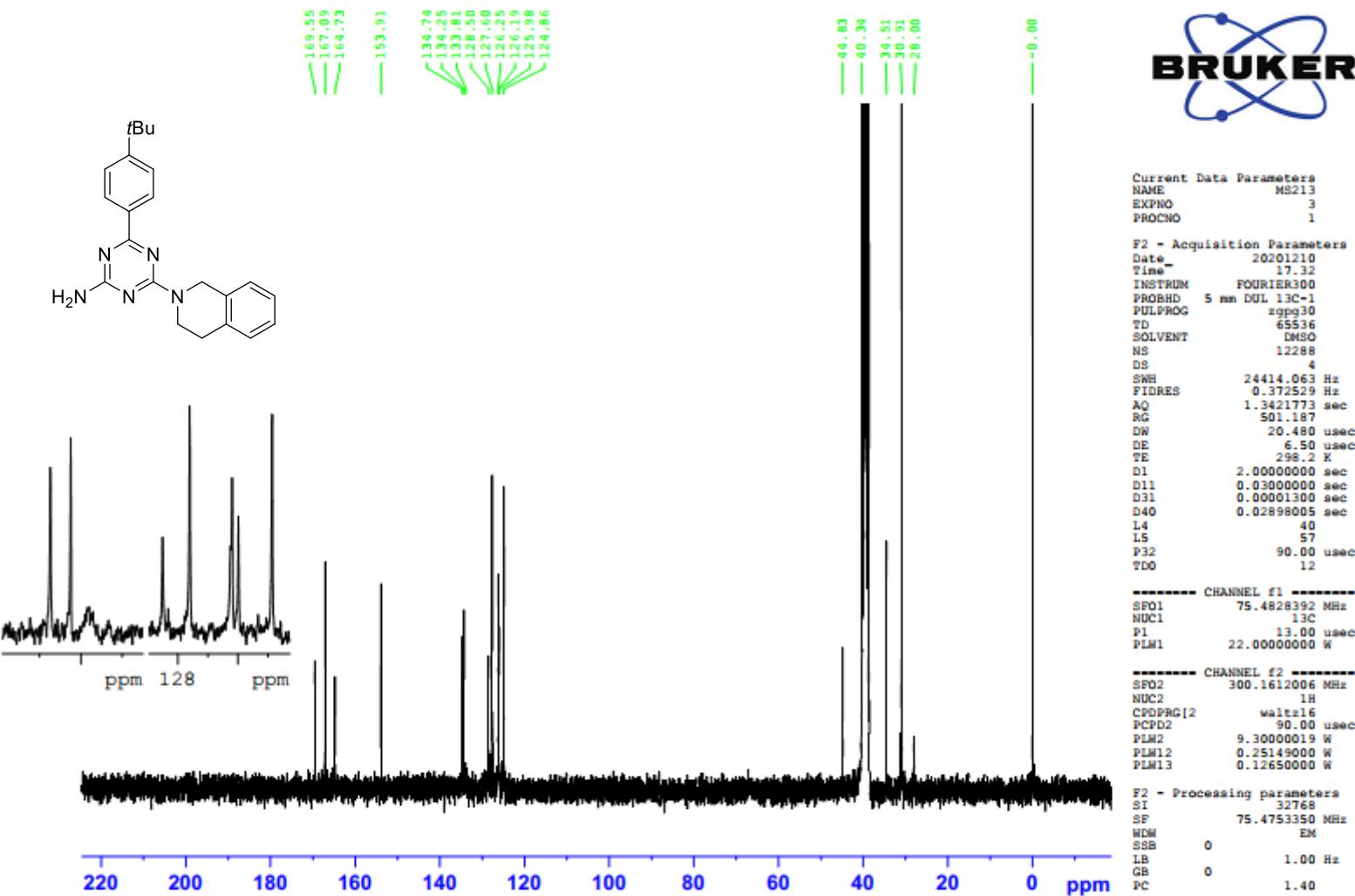
6-(4-Methylphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,6}**)



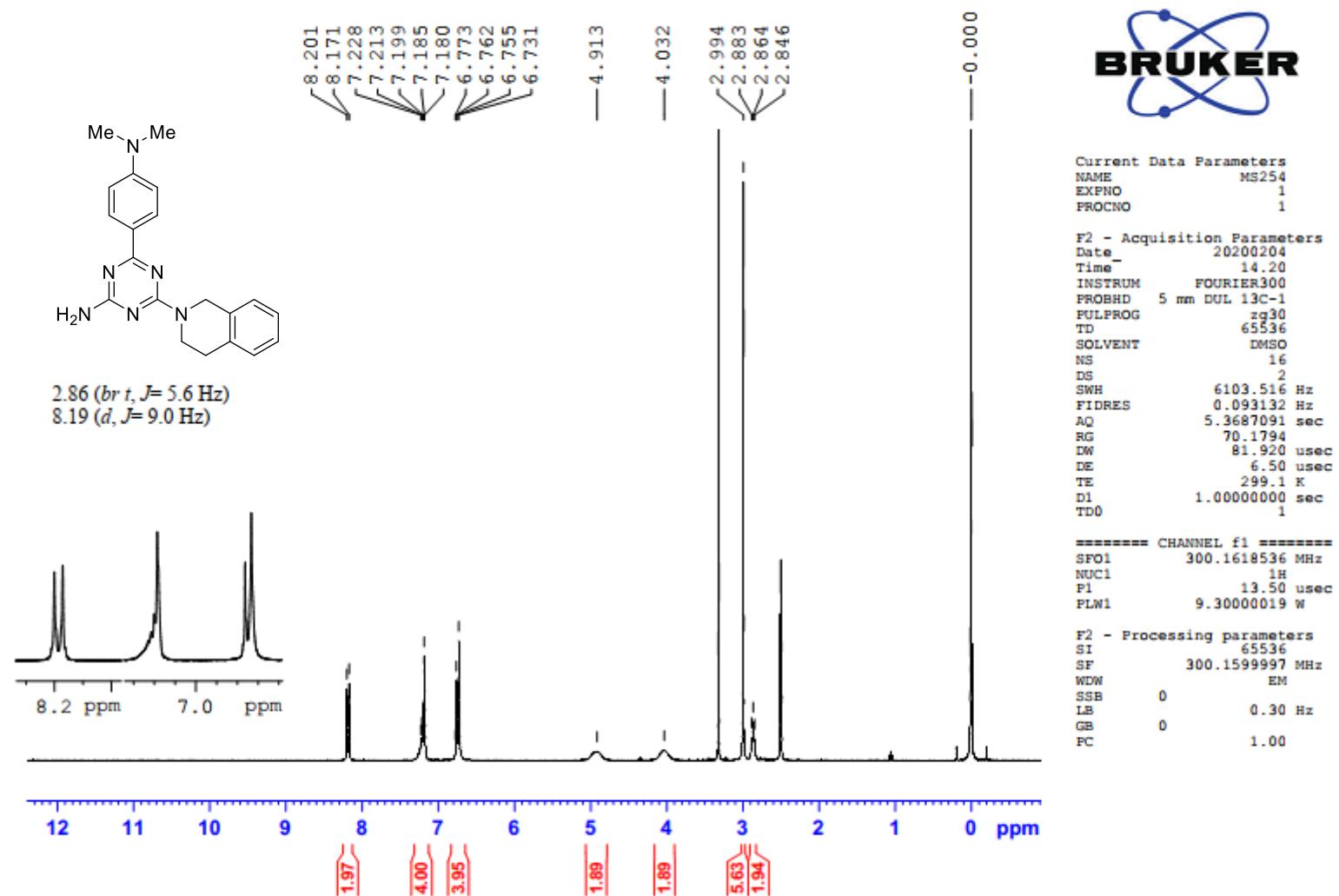
6-[4-(*tert*-Butyl)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,7}**)



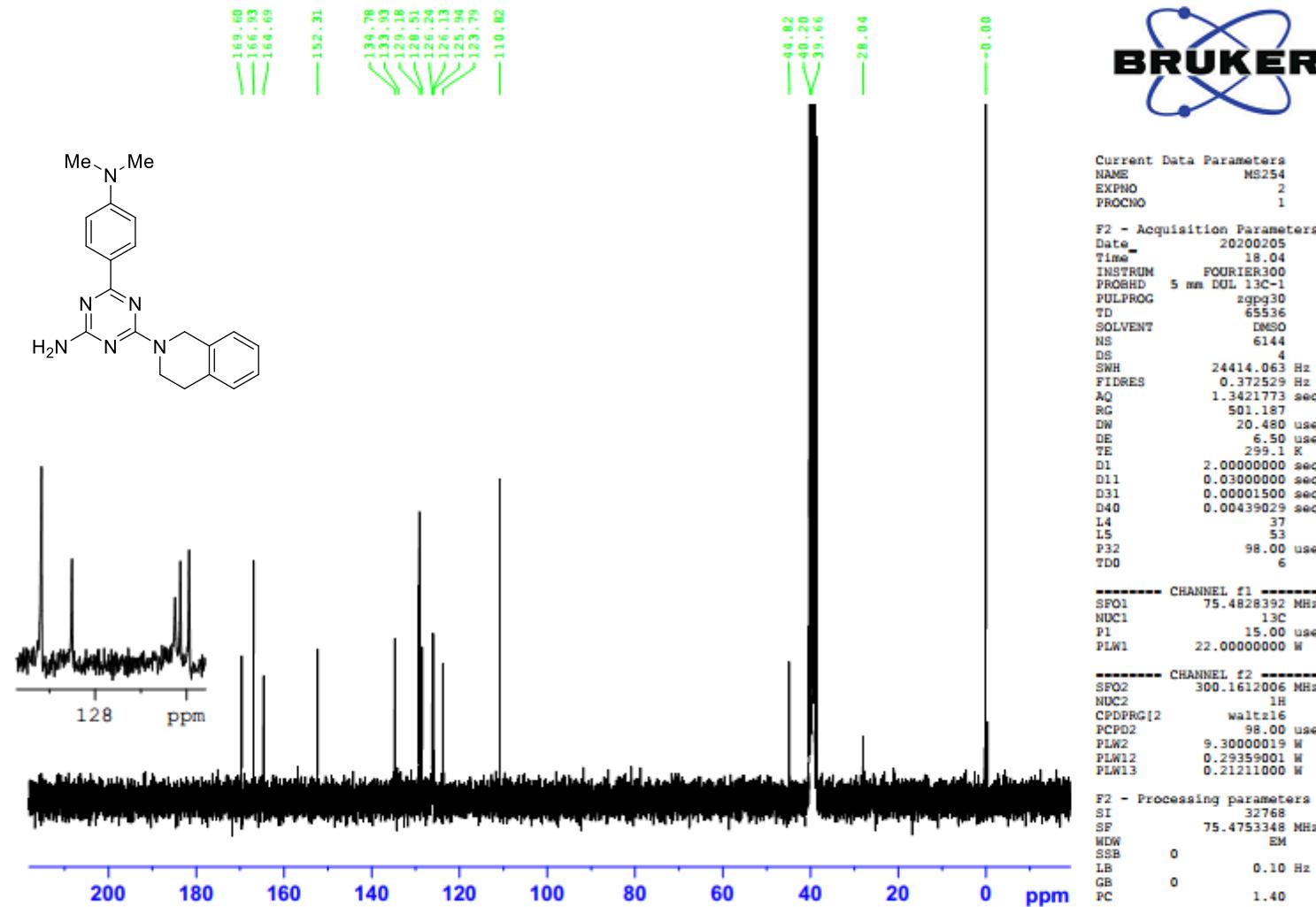
6-[4-(*tert*-Butyl)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,7}**)



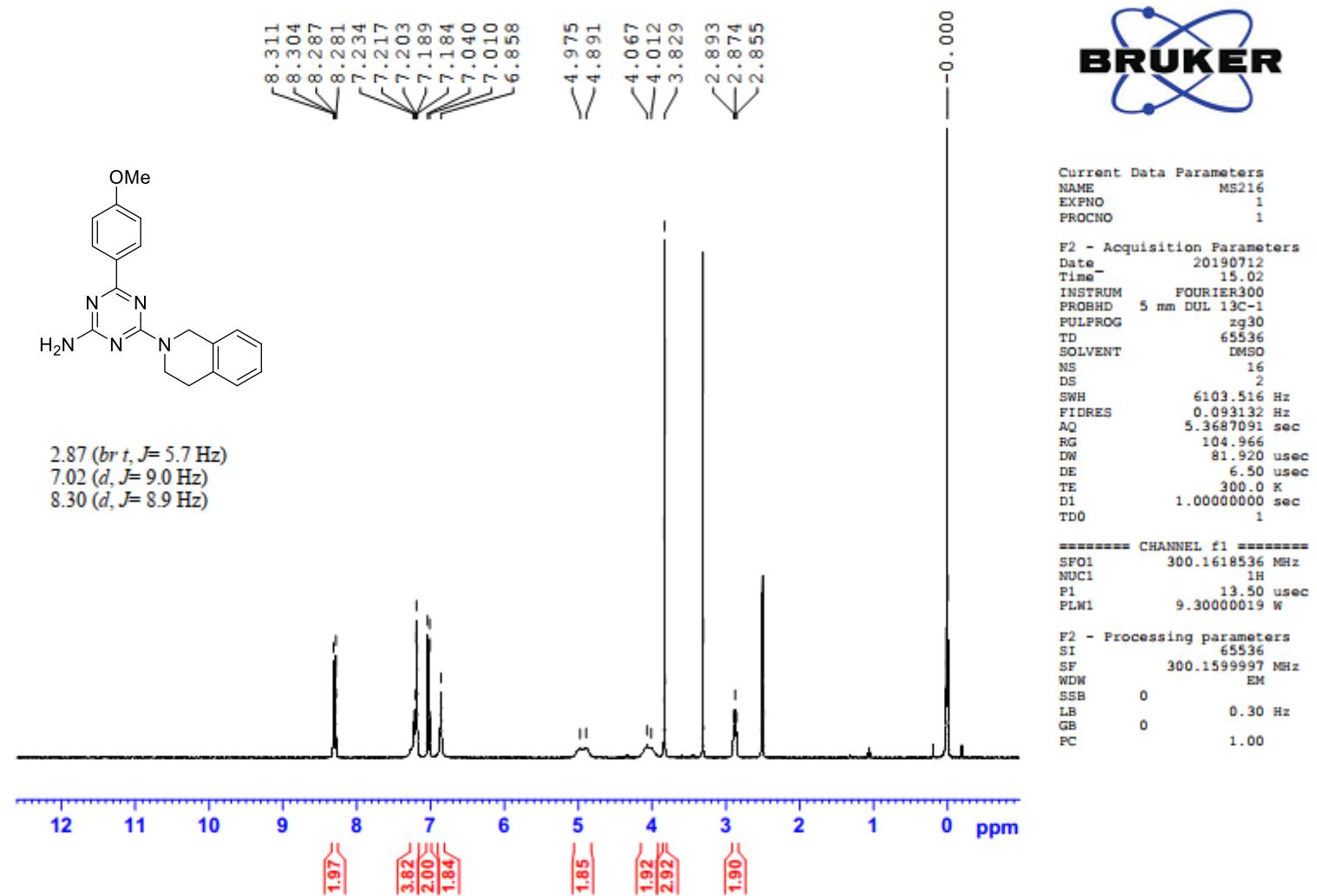
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,8}**)



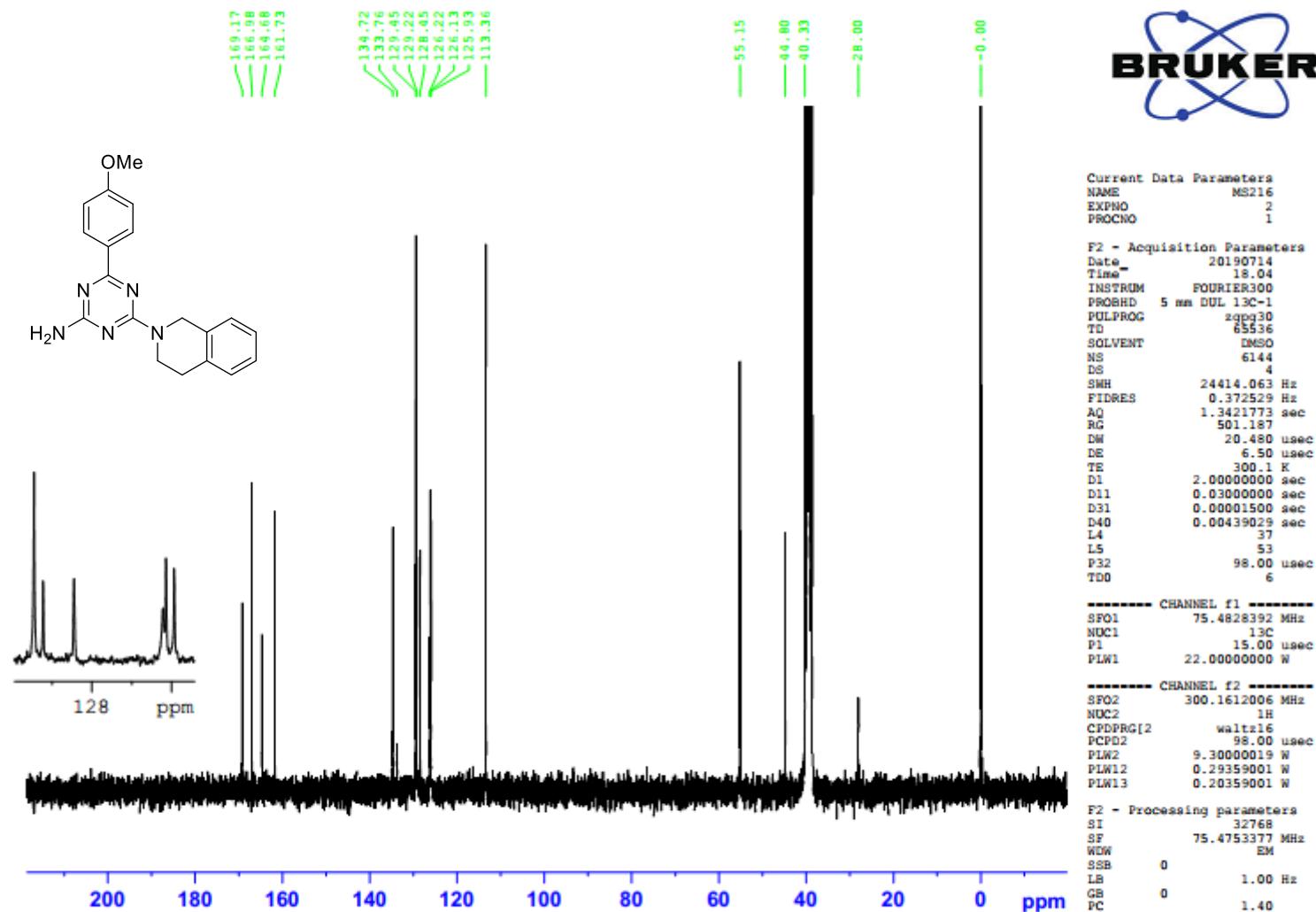
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,8}**)



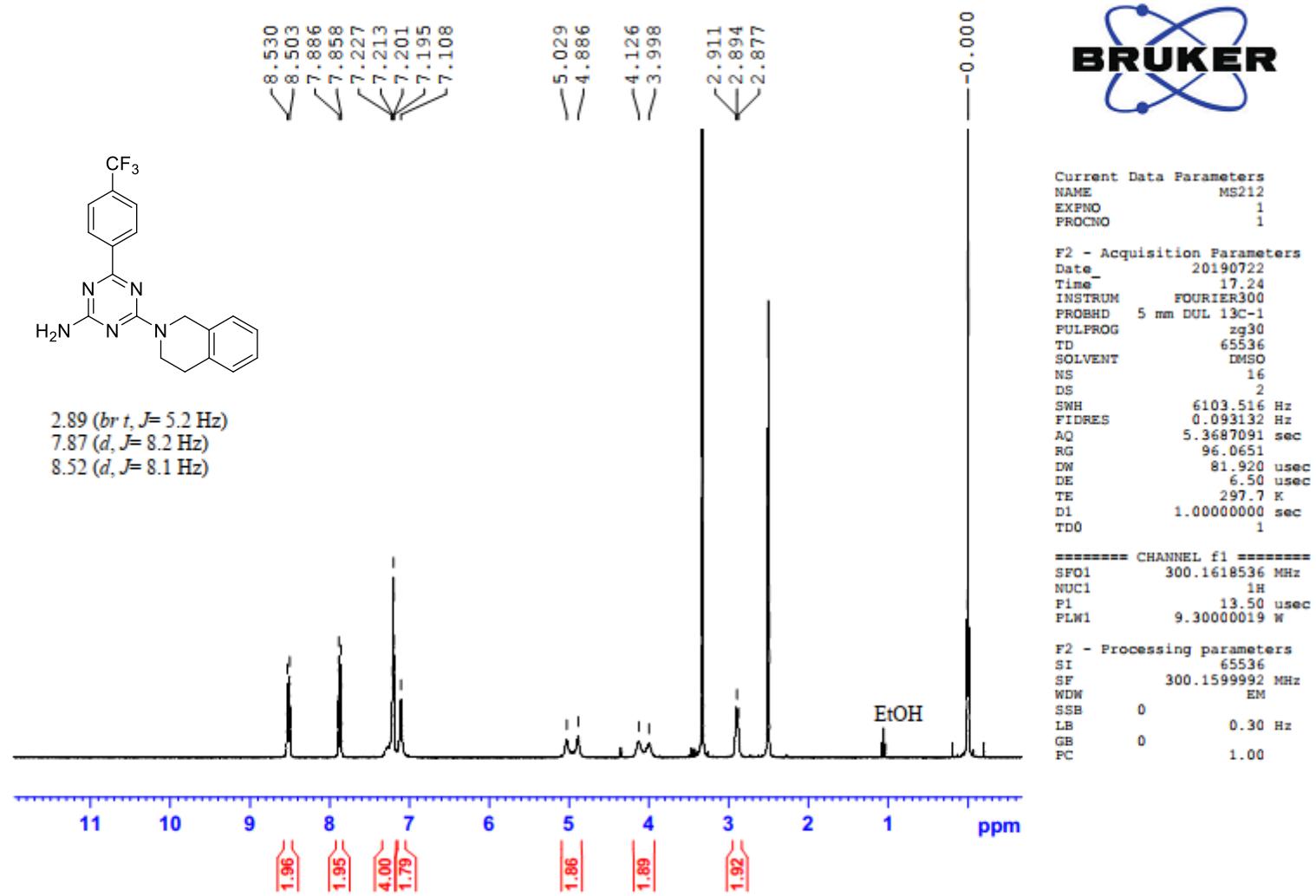
6-(4-Methoxyphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,9}**)



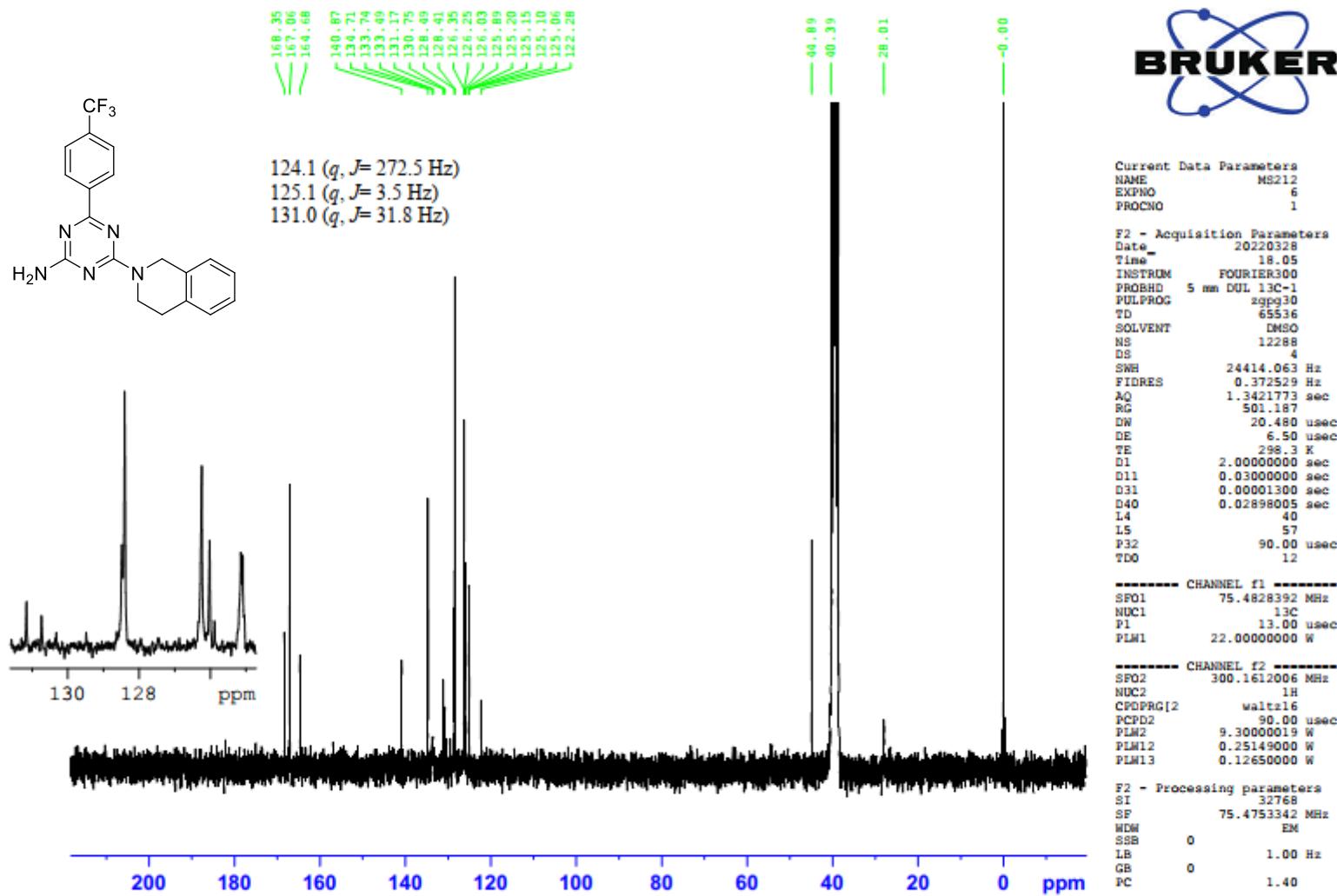
6-(4-Methoxyphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,9}**)



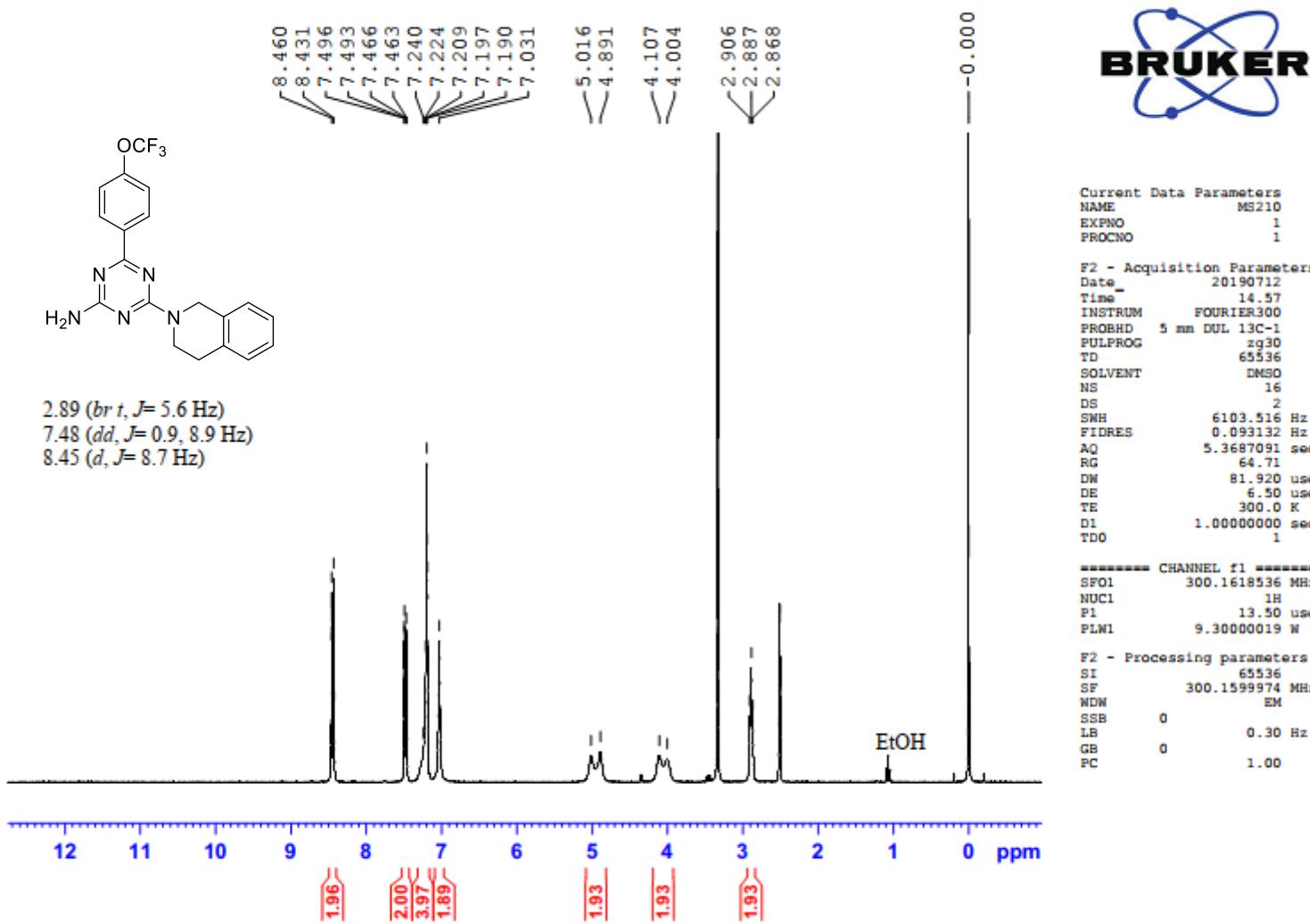
6-[4-(Trifluoromethyl)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,11}**)



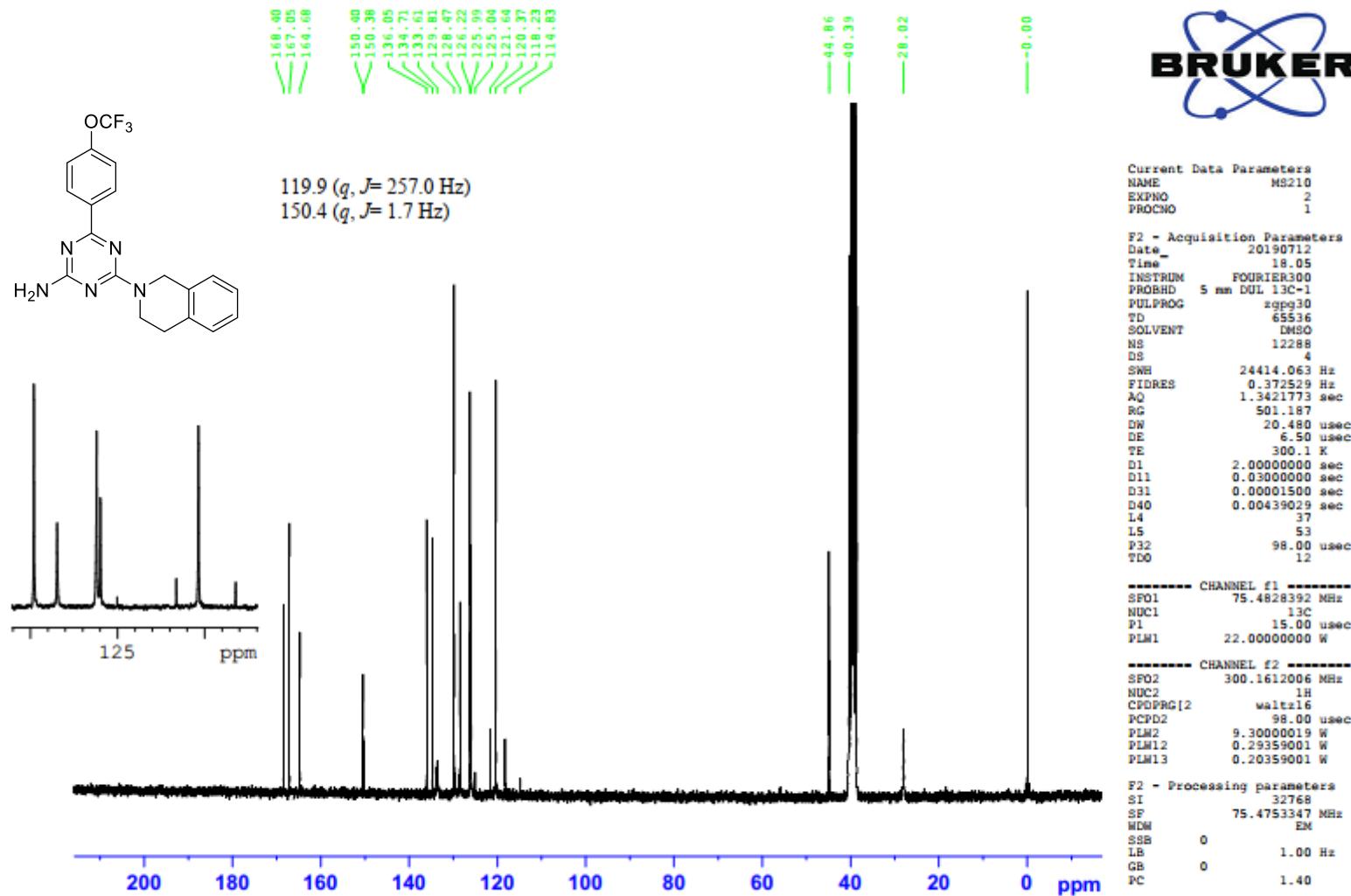
6-[4-(Trifluoromethyl)phenyl]-4-(3,4-dihydroisoquinolin-2(1H)-yl)-1,3,5-triazine-2-amine (**9{6,11}**)



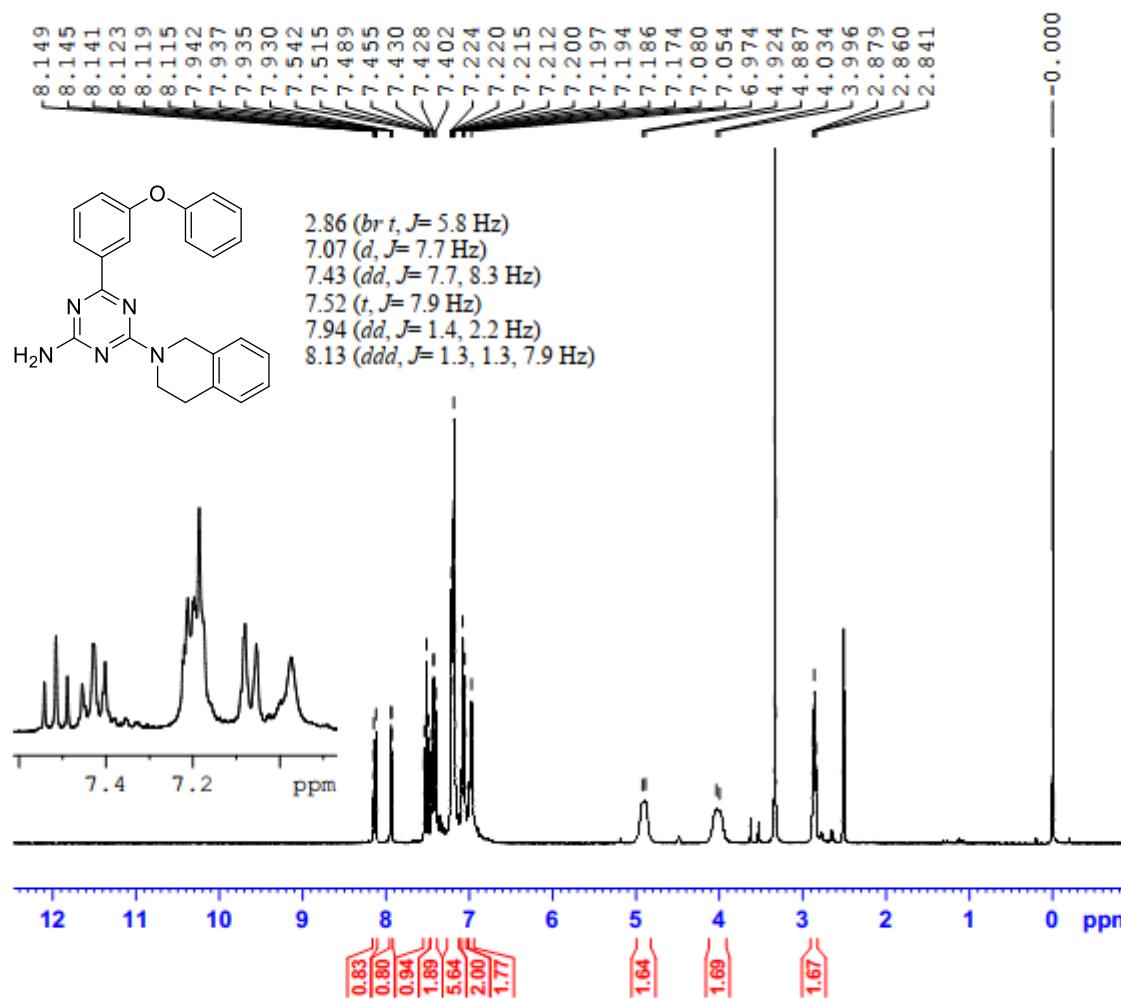
6-[4-(Trifluoromethoxy)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,12}**)



6-[4-(Trifluoromethoxy)phenyl]-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,12}**)



4-(3,4-Dihydroisoquinolin-2(1*H*)-yl)-6-(3-phenoxyphenyl)-1,3,5-triazine-2-amine (**9{6,13}**)



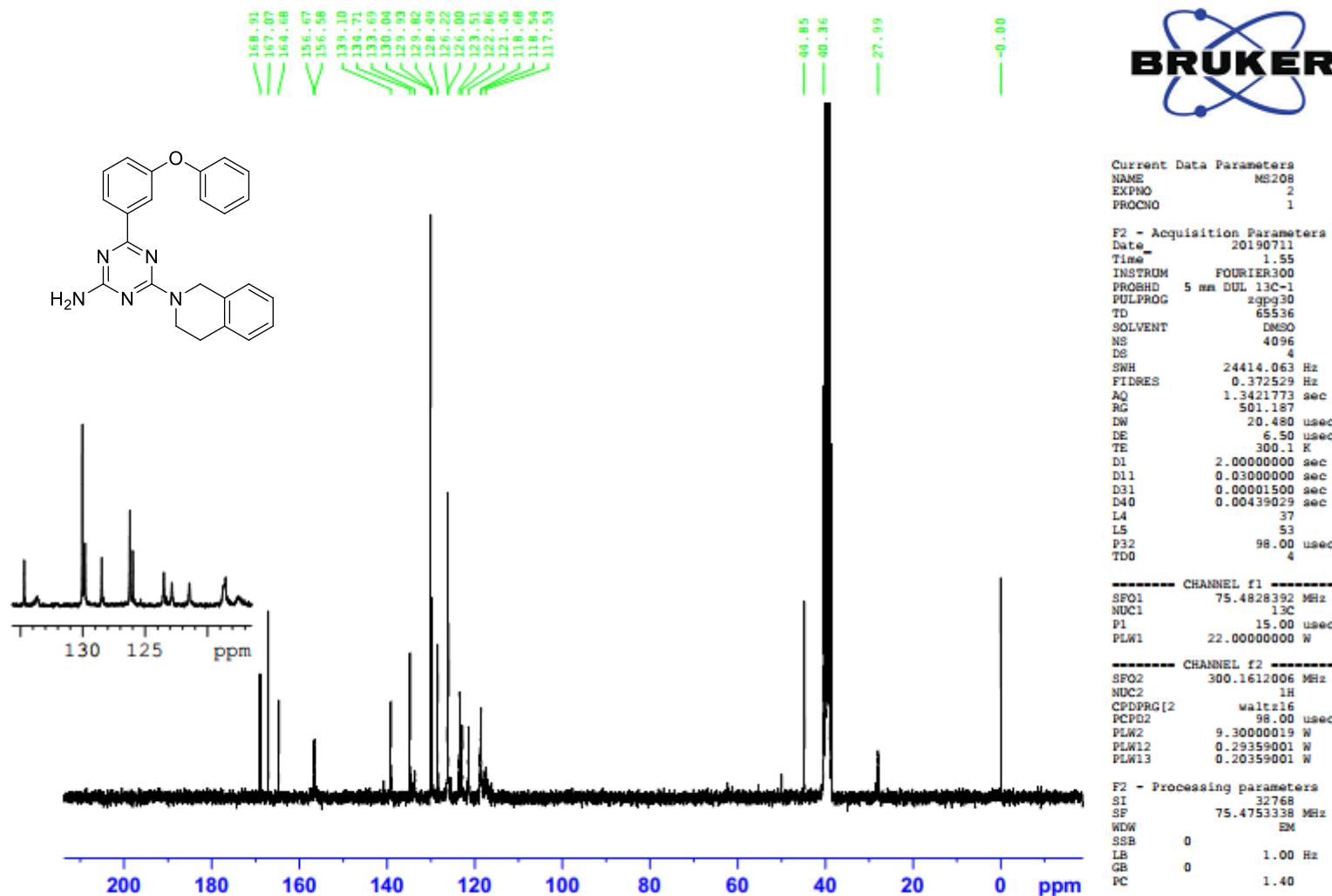
Current Data Parameters
NAME MS208
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20190710
Time 15.24
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 1.0000000 sec
TD0 1

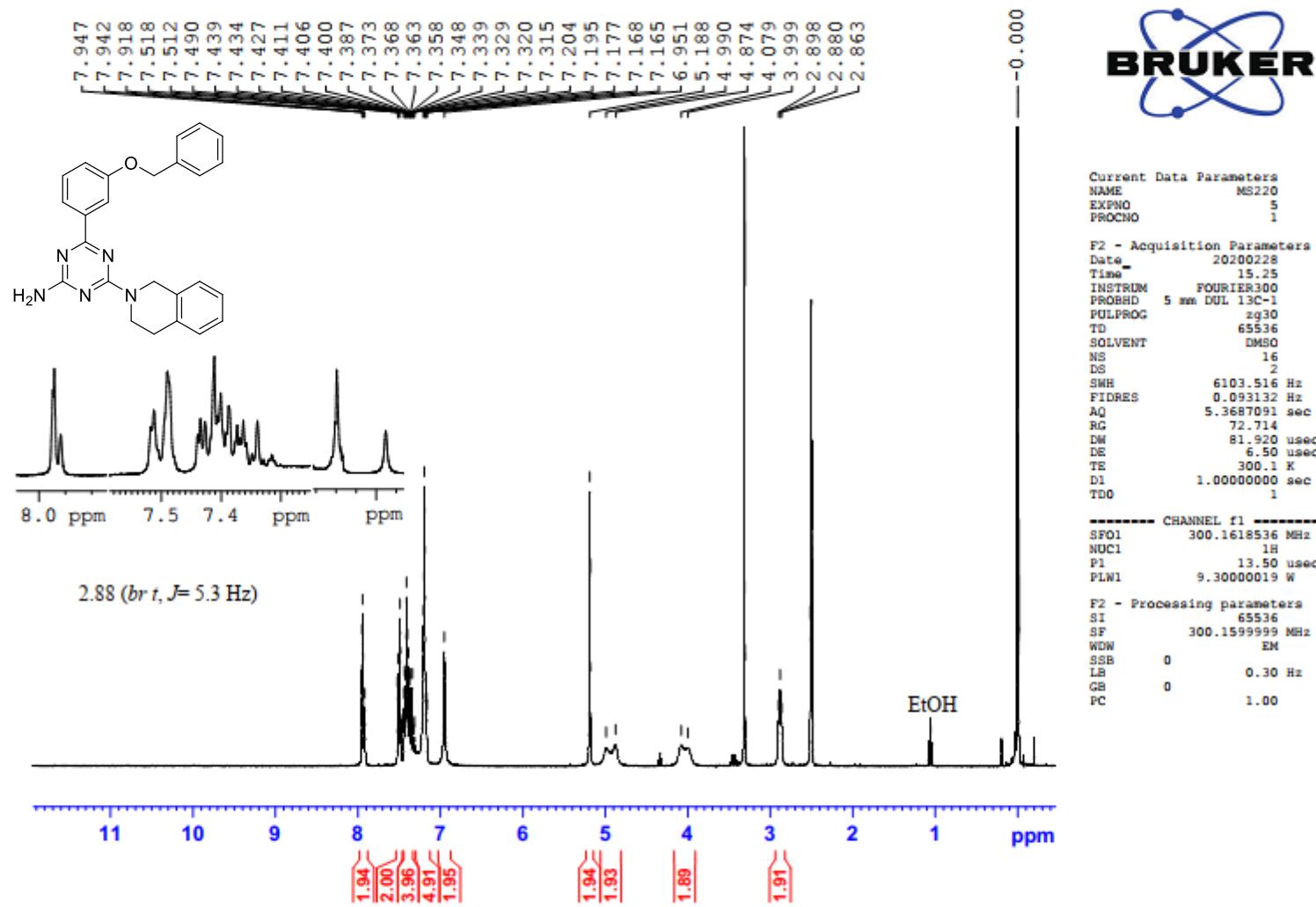
===== CHANNEL f1 =====
SF01 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

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

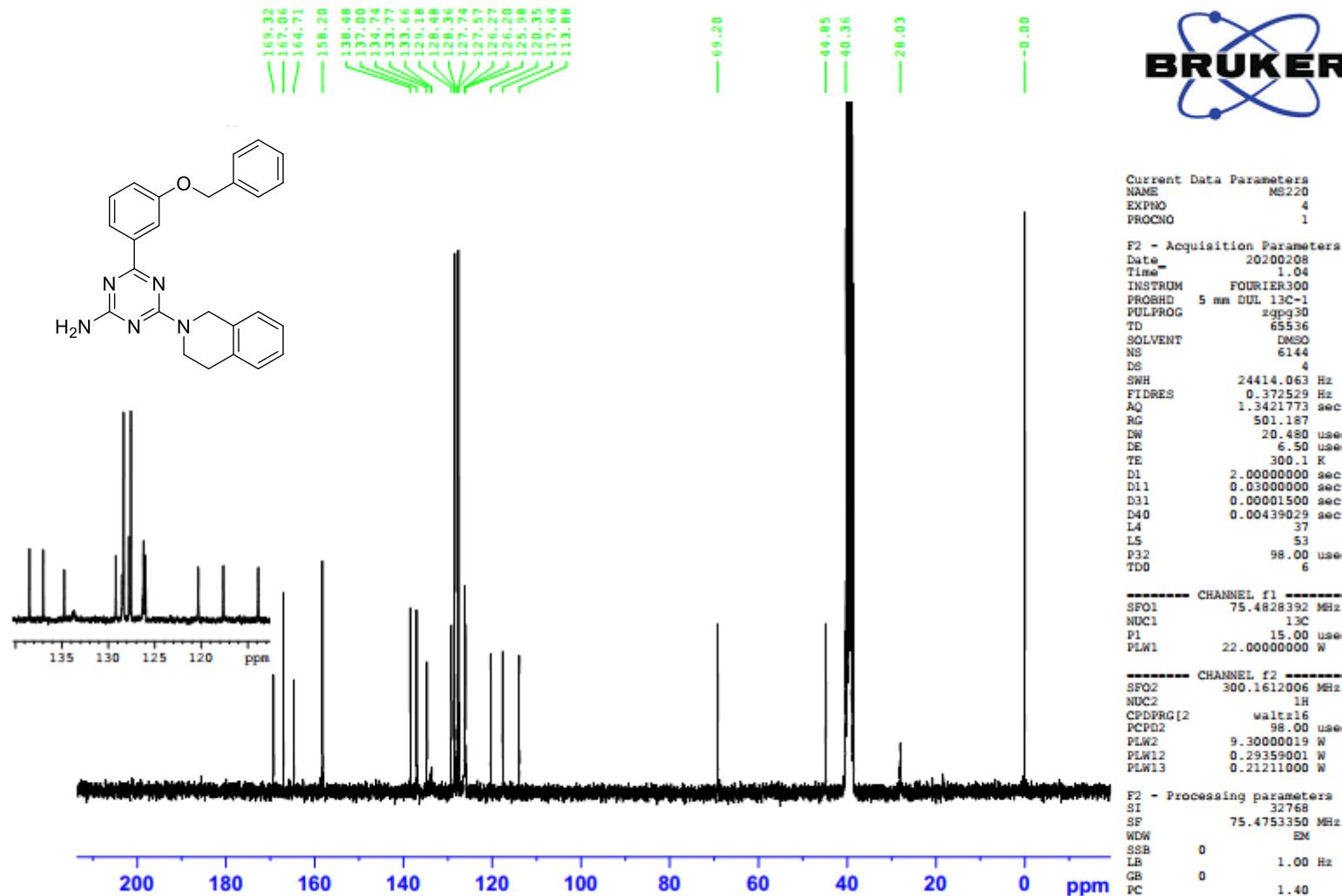
4-(3,4-Dihydroisoquinolin-2(1*H*)-yl)-6-(3-phenoxyphenyl)-1,3,5-triazine-2-amine (**9{6,13}**)



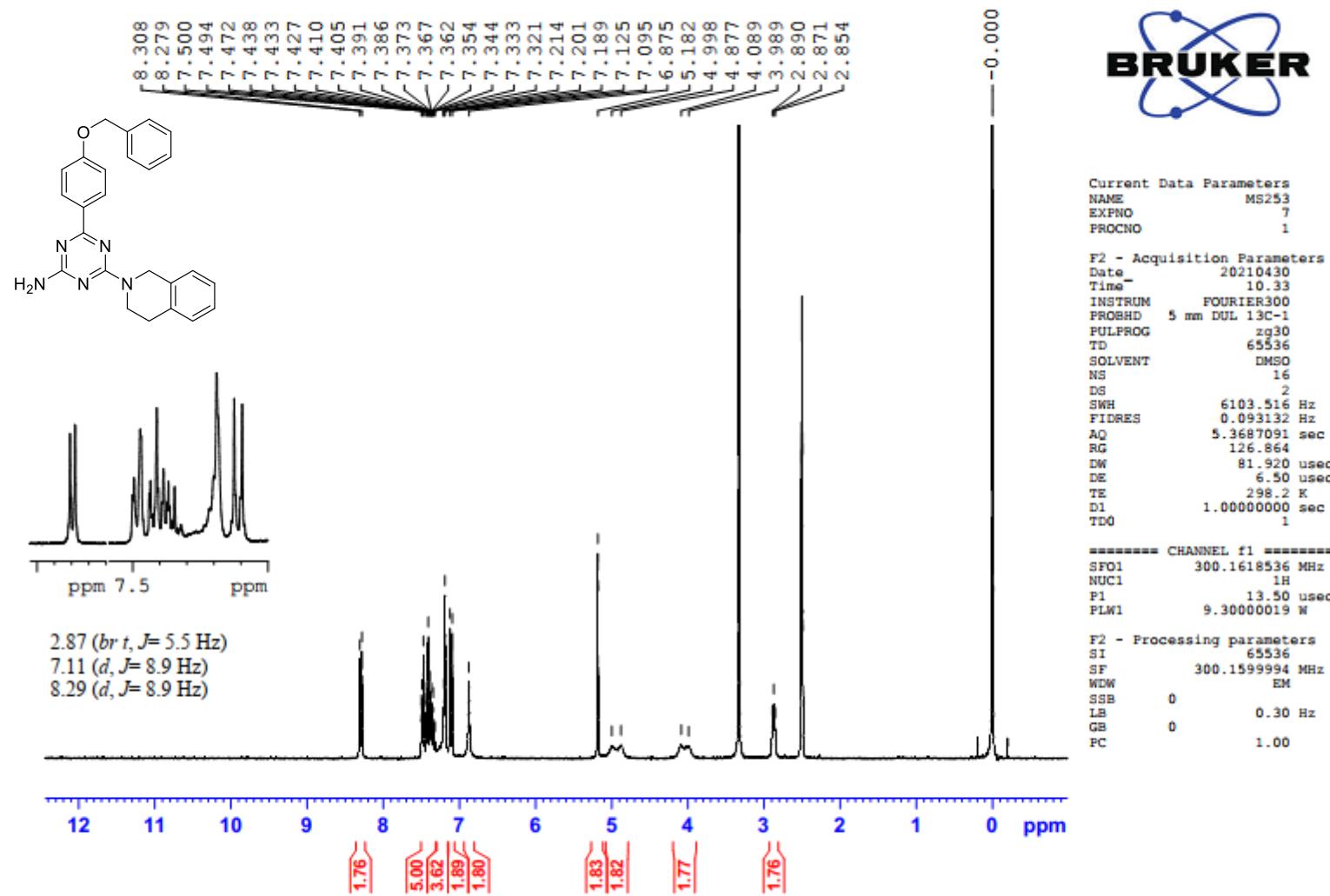
6-(3-(BenzylOxy)phenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,14}**)



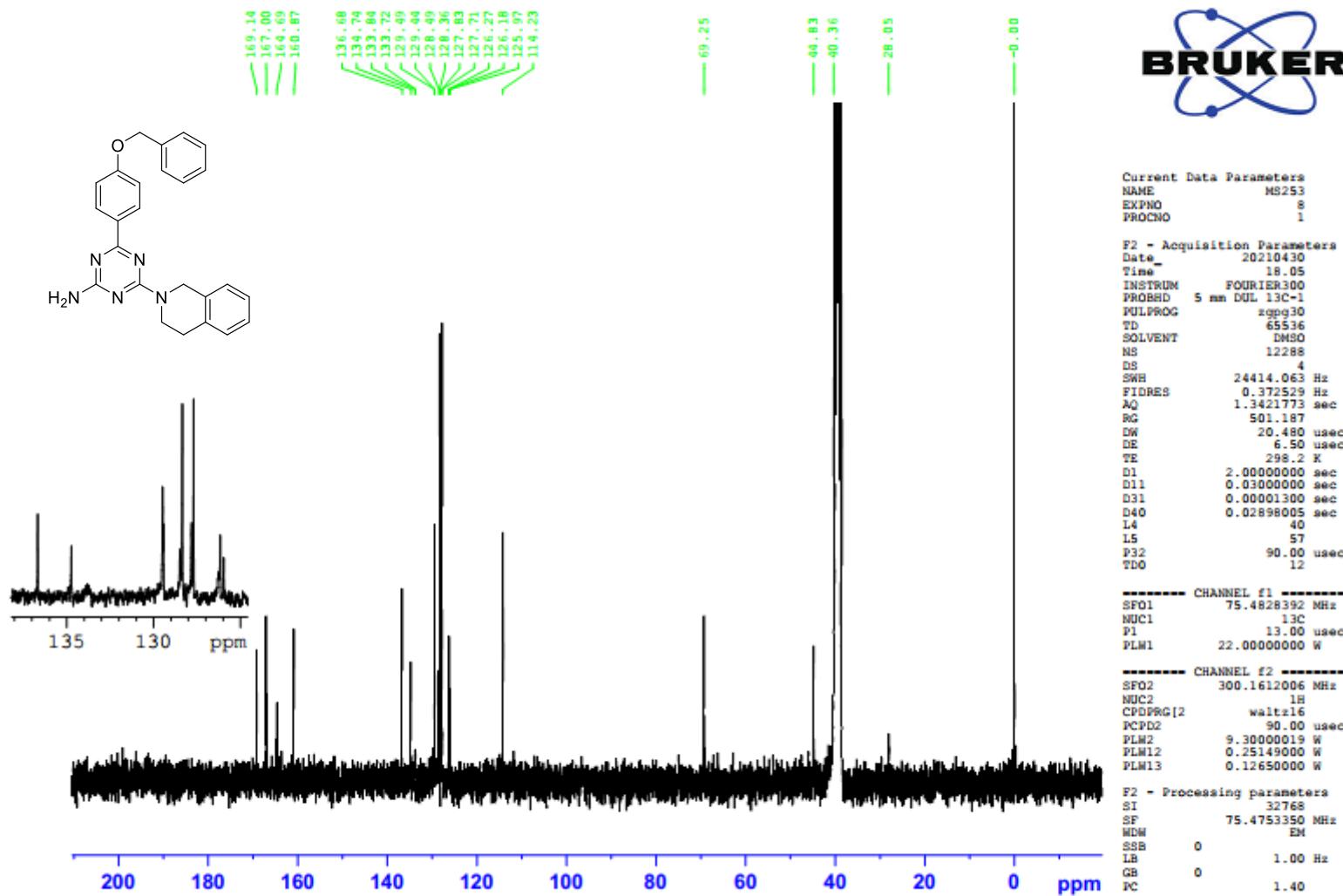
6-(3-(Benzyl)phenyl)-4-(3,4-dihydroisoquinolin-2(1H)-yl)-1,3,5-triazine-2-amine (**9{6,14}**)



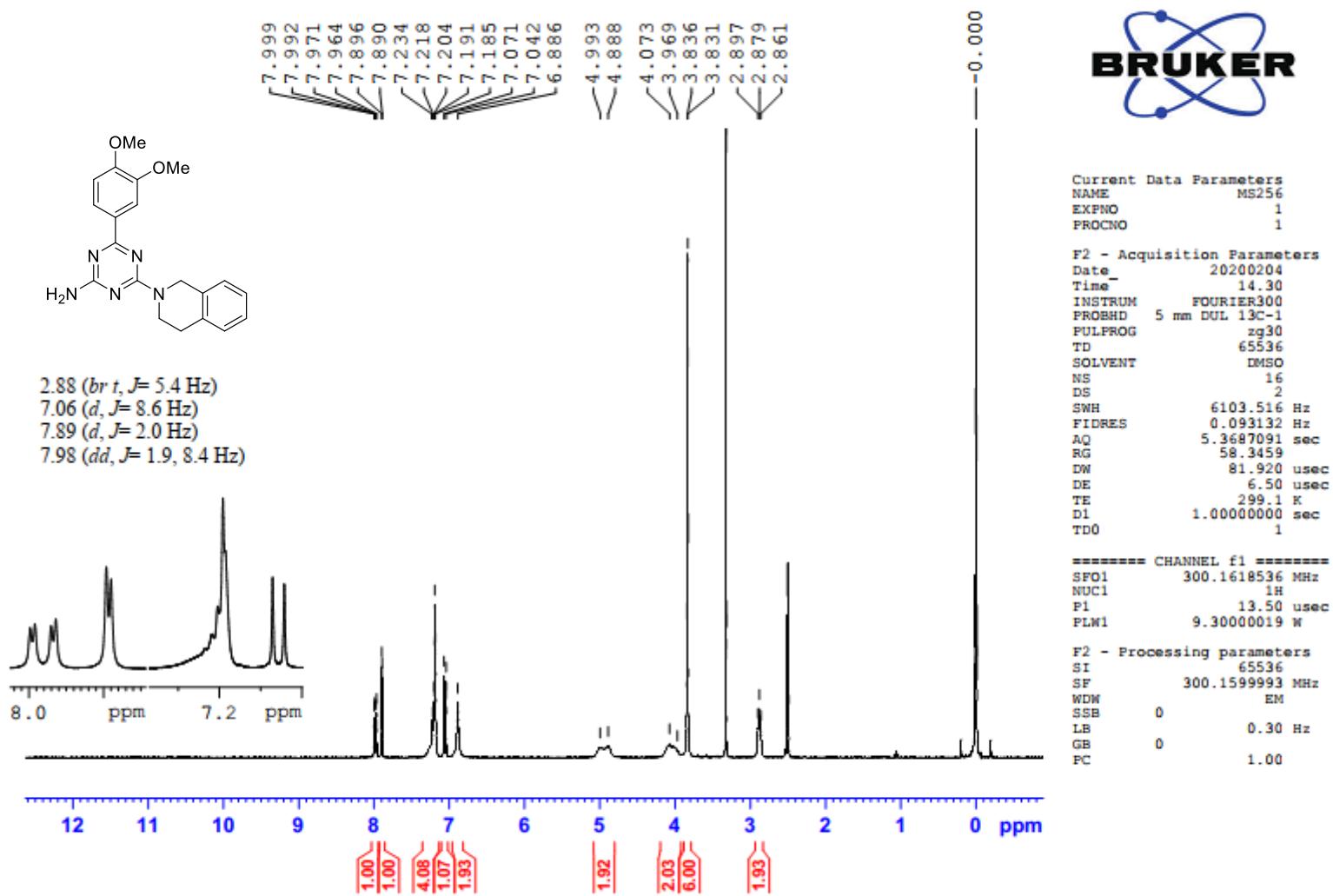
6-(4-(Benzyl)phenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,15}**)



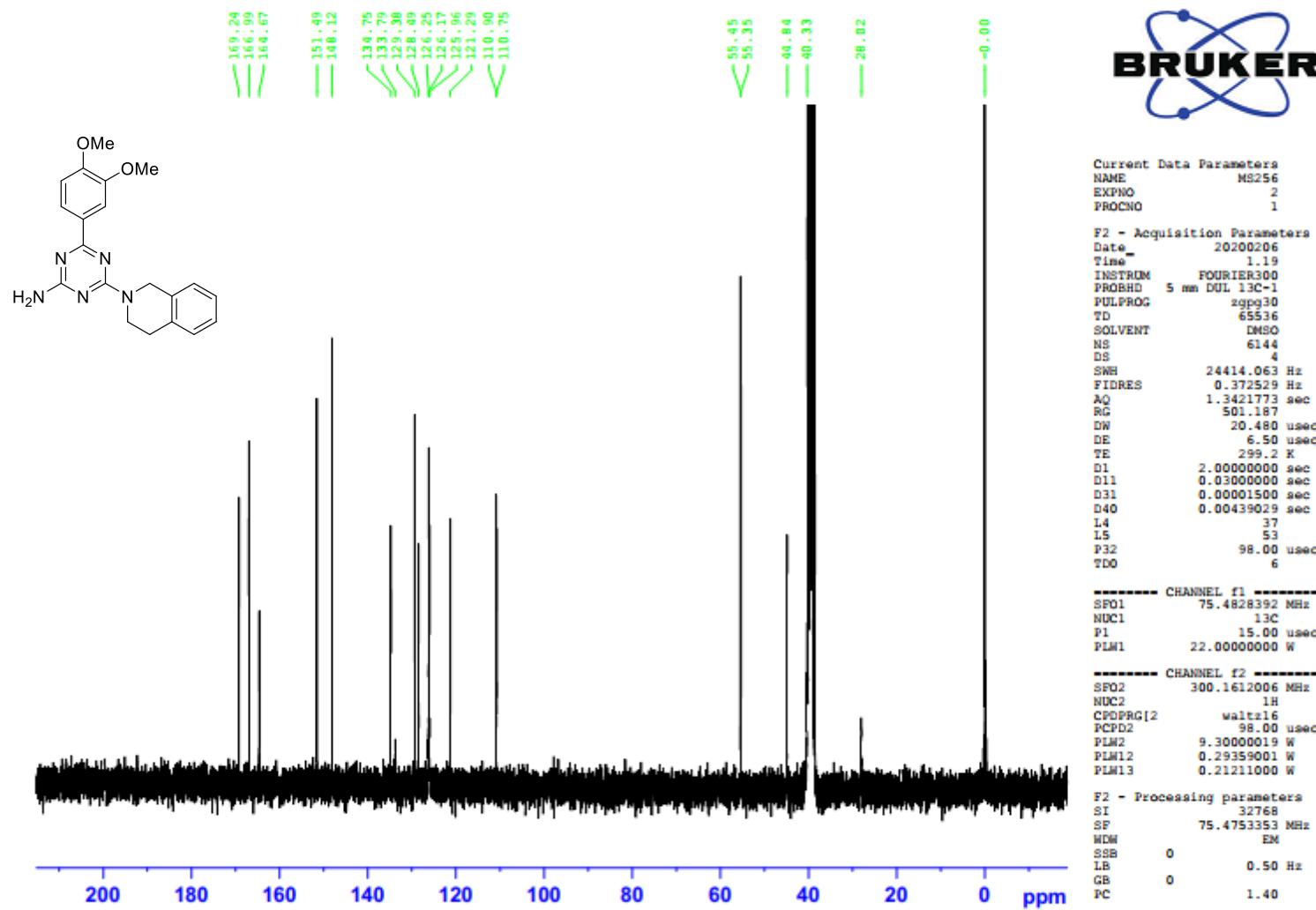
6-(4-(Benzyl)phenyl)-4-(3,4-dihydroisoquinolin-2(1H)-yl)-1,3,5-triazine-2-amine (**9{6,15}**)



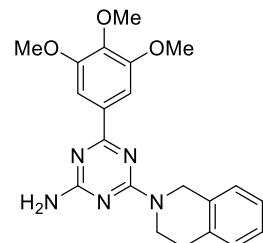
6-(3,4-Dimethoxyphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazin-2-amine (**9{6,16}**)



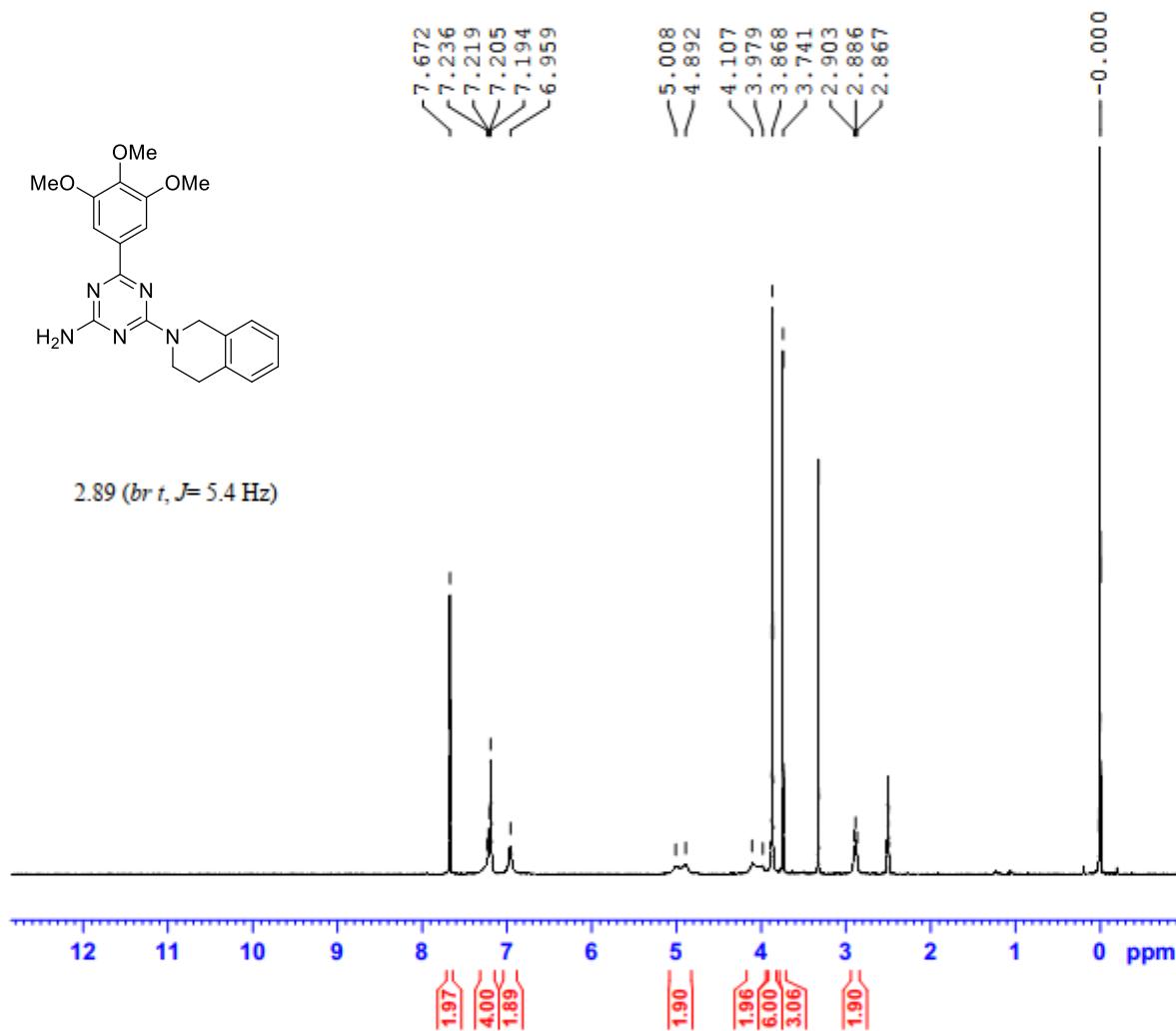
6-(3,4-Dimethoxyphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazin-2-amine (**9{6,16}**)



6-(3,4,5-Trimethoxyphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,17}**)



2.89 (*br t*, $J = 5.4$ Hz)



Current Data Parameters	
NAME	MS255
EXPNO	1
PROCNO	1

```

F2 - Acquisition Parameters
Date       20200204
Time       14.25
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 used
DE        6.50 used
TE        299.1 K
D1        1.0000000 sec
TD0       1

```

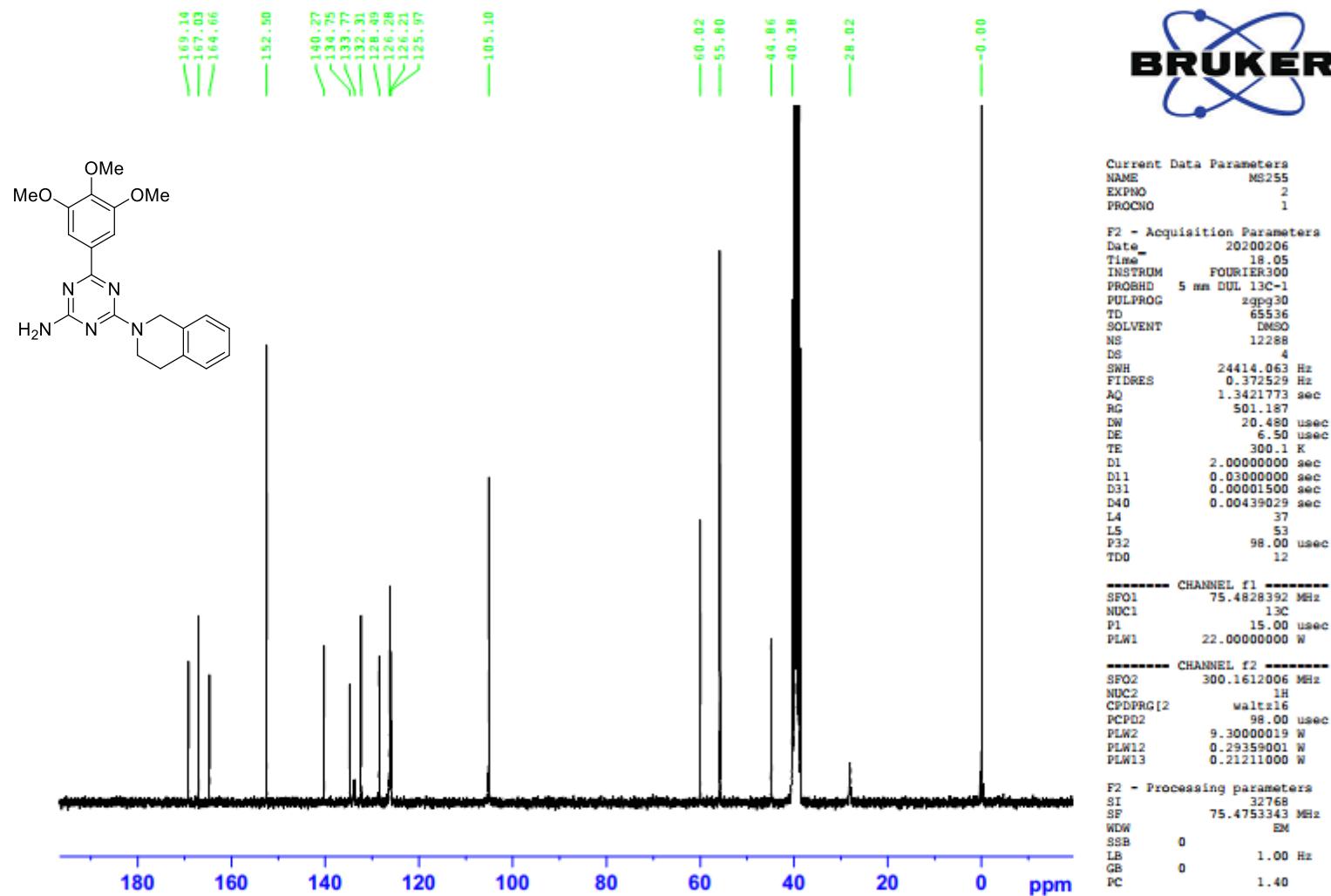
===== CHANNEL f1 =====
SFO1 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.300000019 u

```

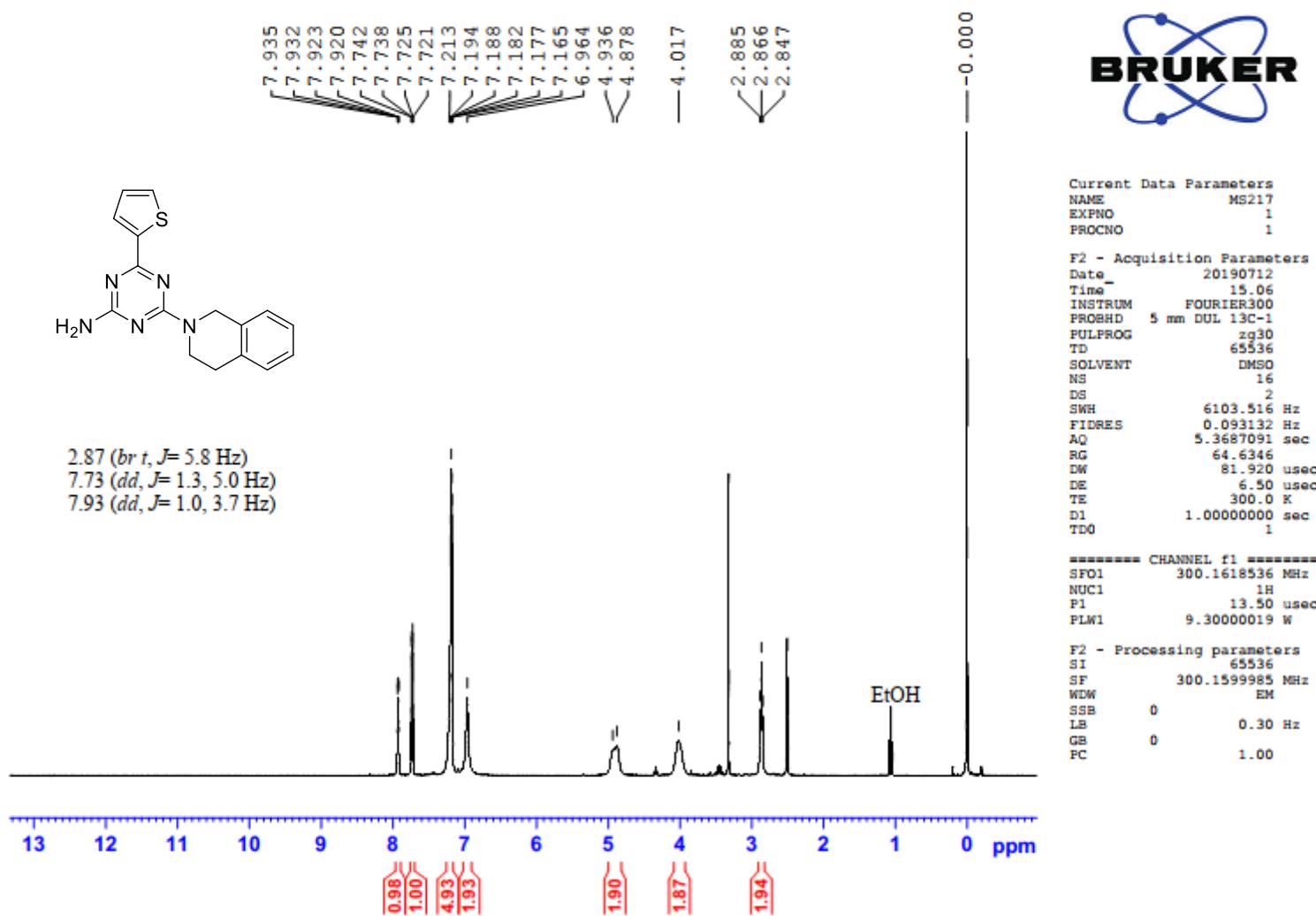
P2 - Processing parameters
SI           65536
SF          300.1599989 MHz
WDW           EM
SSB            0
LB             0.30 Hz
GB            0
PC            1.00

```

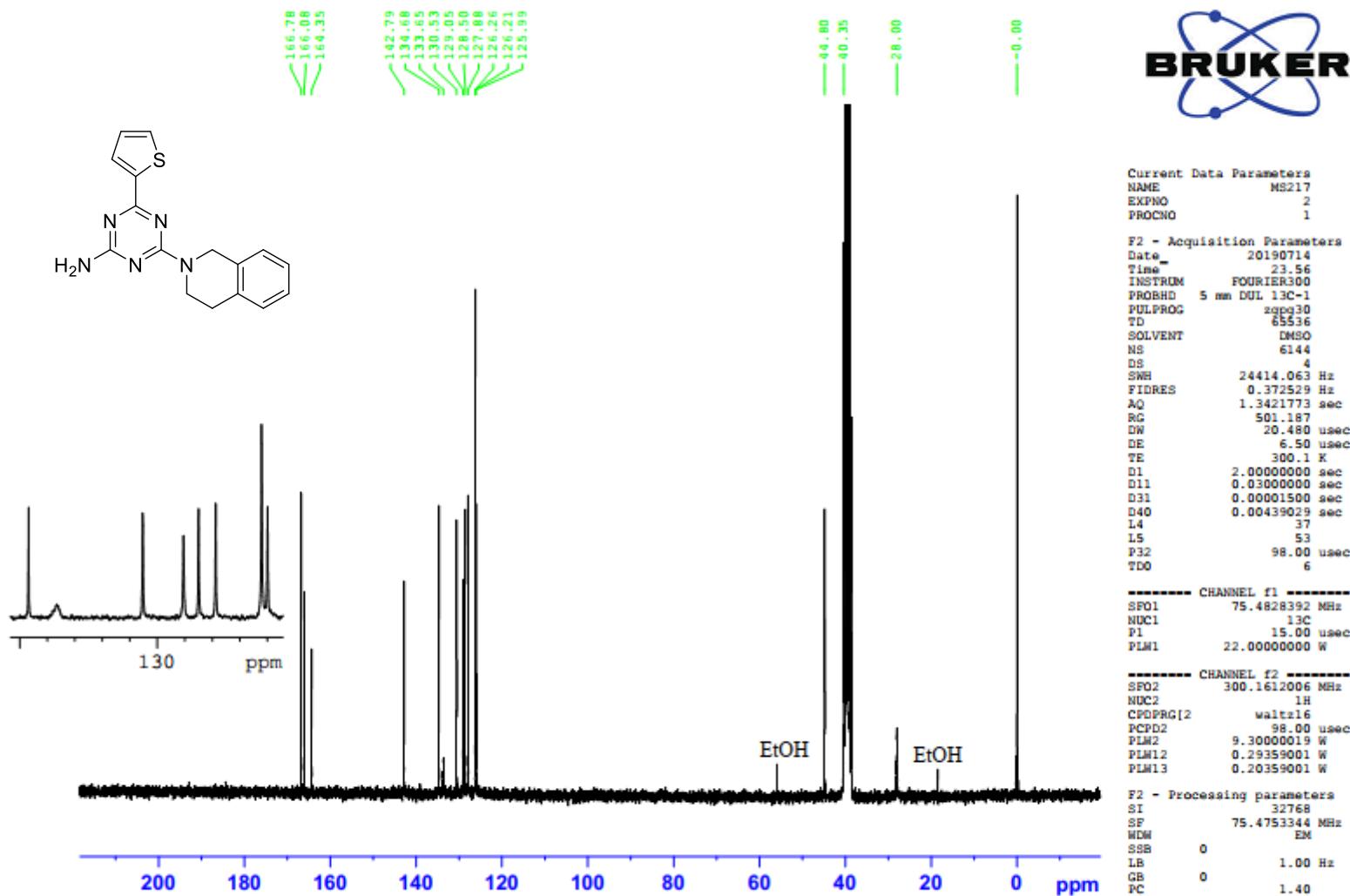
6-(3,4,5-Trimethoxyphenyl)-4-(3,4-dihydroisoquinolin-2(1*H*)-yl)-1,3,5-triazine-2-amine (**9{6,17}**)



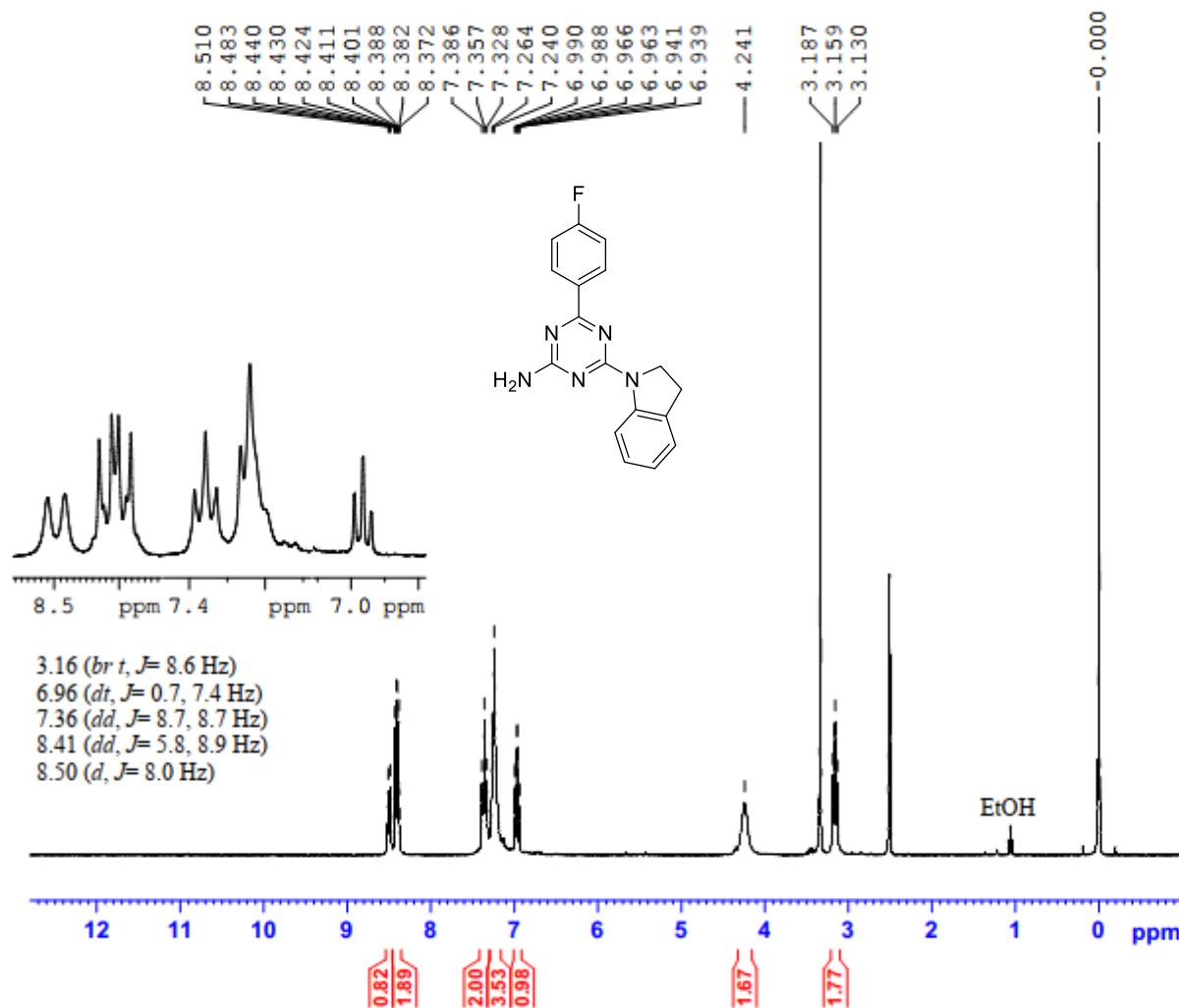
4-(3,4-Dihydroisoquinolin-2(1*H*)-yl)-6-(2-thienyl)-1,3,5-triazine-2-amine (**9{6,18}**)



4-(3,4-Dihydroisoquinolin-2(1*H*)-yl)-6-(2-thienyl)-1,3,5-triazine-2-amine (**9{6,18}**)



6-(4-Fluorophenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,3}**)



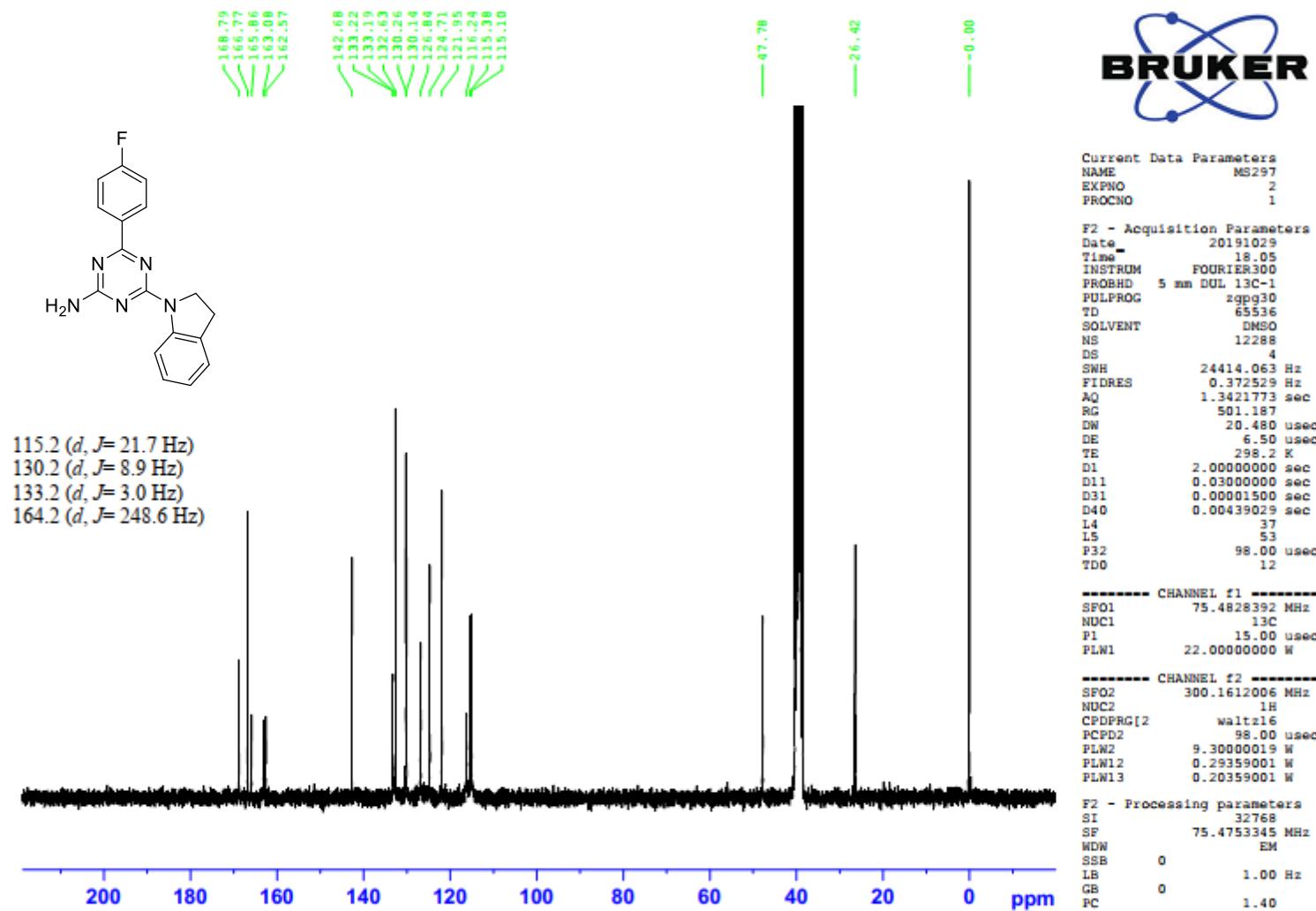
Current Data Parameters
NAME MS297
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20191023
Time 14.55
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 54.7609
DW 81.920 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

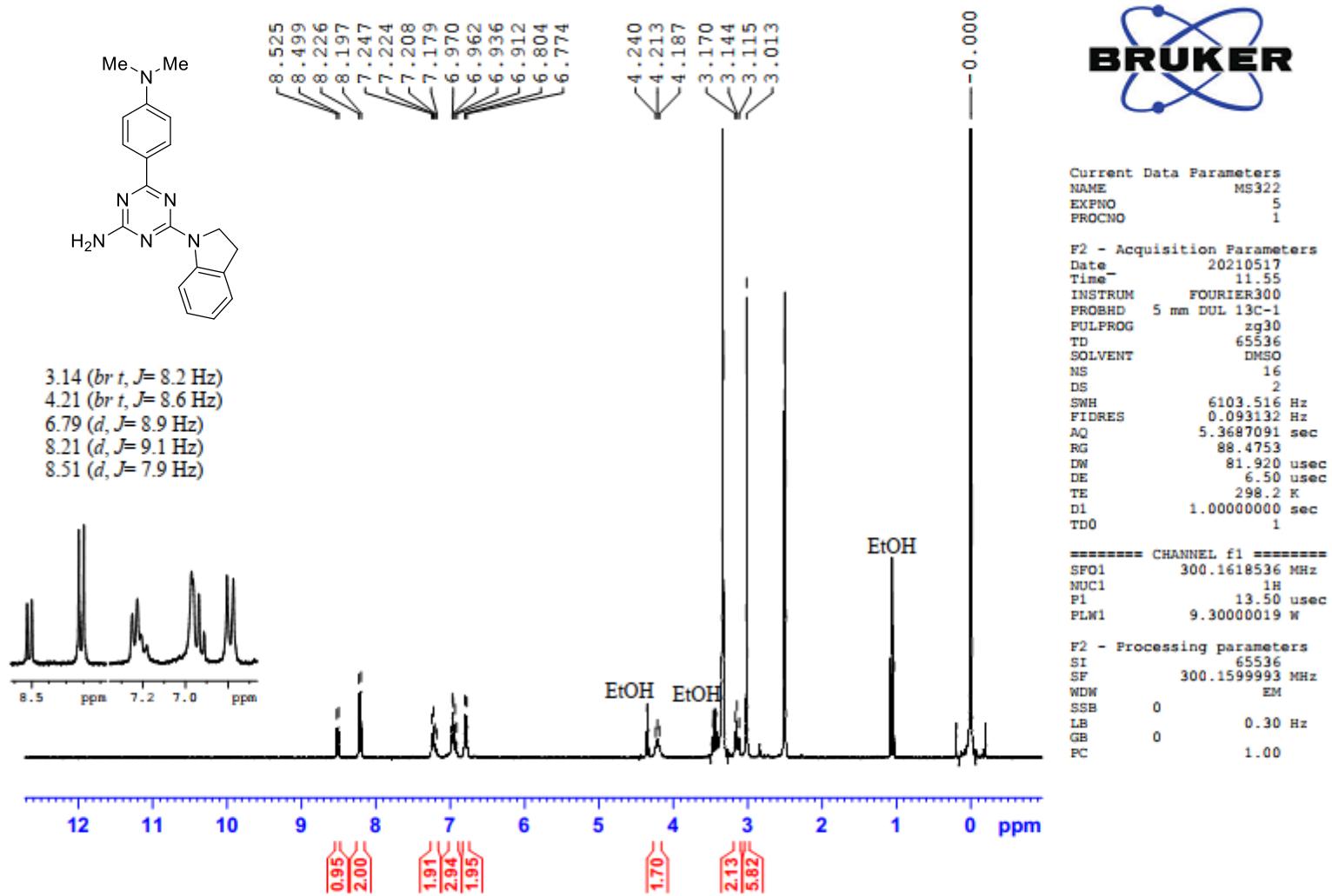
===== CHANNEL f1 =====
SFO1 300.1618536 MHz
NUC1 1H
P1 13.50 usec
PLW1 9.30000019 W

F2 - Processing parameters
SI 65536
SF 300.1599985 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

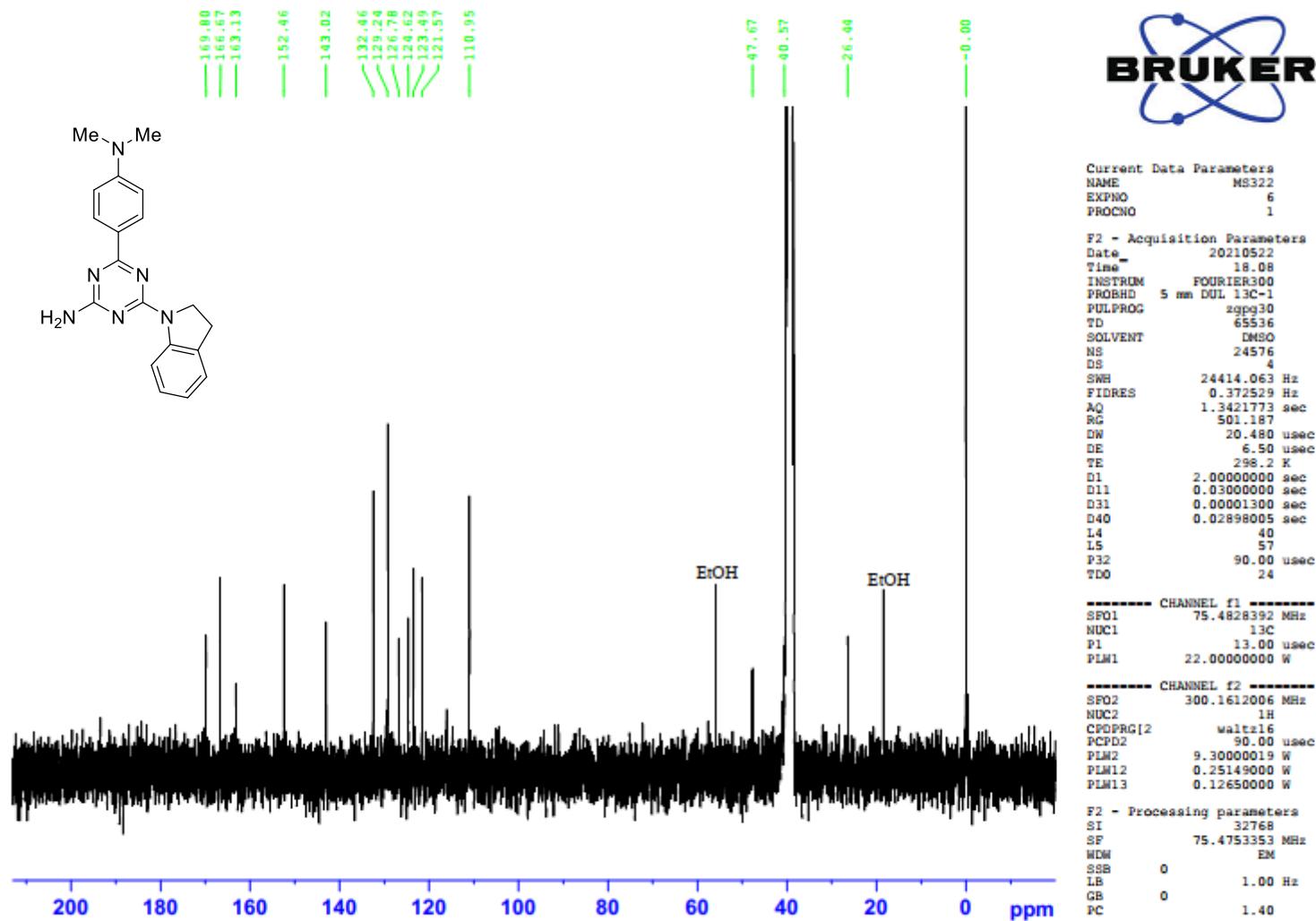
6-(4-Fluorophenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,3}**)



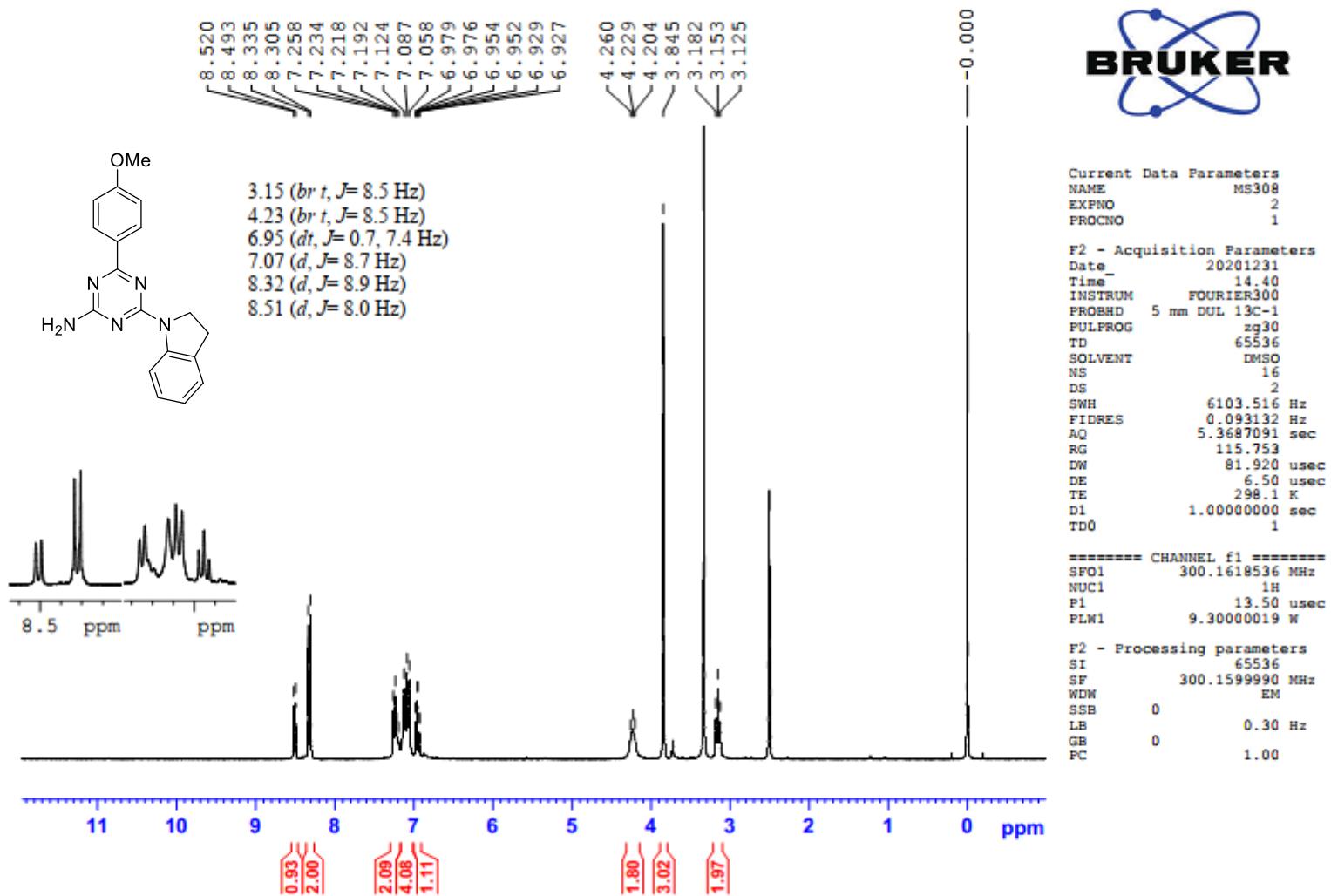
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,8}**)



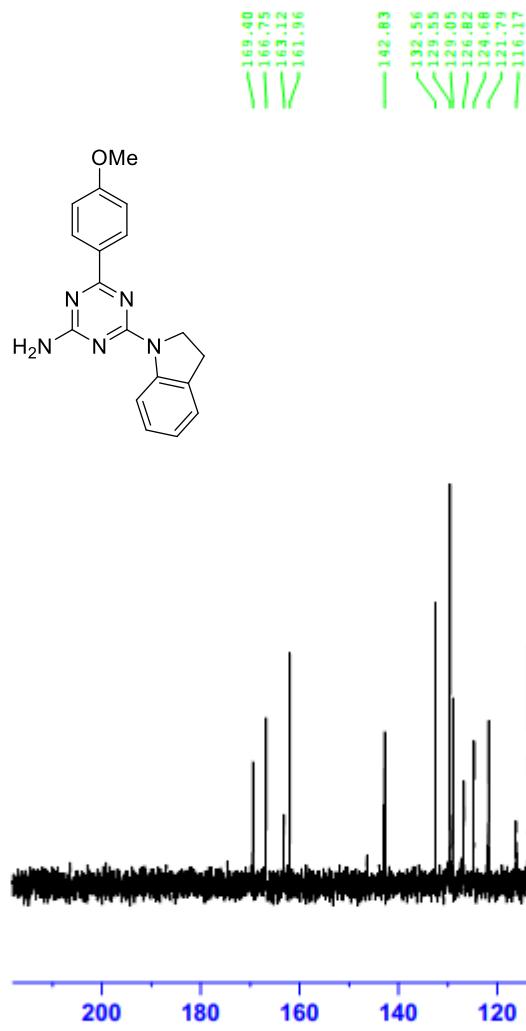
6-[4-(*N,N*-Dimethylamino)phenyl]-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,8}**)



6-(4-Methoxyphenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,9}**)



6-(4-Methoxyphenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,9}**)



Current Data Parameters
NAME MS308
EXPNO 5
PROCNO 1

```

F2 - Acquisition Parameters
Date_      20210427
Time       18.05
INSTRUM   FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG  zgpp30
TD        65536
SOLVENT   DMso
NS        12288
DS         4
SWH      24414.063 Hz
FIDRES   0.372529 Hz
AQ        1.3421773 sec
RG        501.187
DW        20.480 used
DE        6.50 used
TE        298.2 K
D1        2.0000000 sec
D11       0.03000000 sec
D31       0.00001300 sec
D40       0.02898005 sec
L4        40
L5        57
P32      90.00 used
PSSB     0.00

```

----- CHANNEL f1 -----
SFO1 75.4828392 MHz
NUC1 13C
P1 13.00 used
PLW1 22.00000000 N

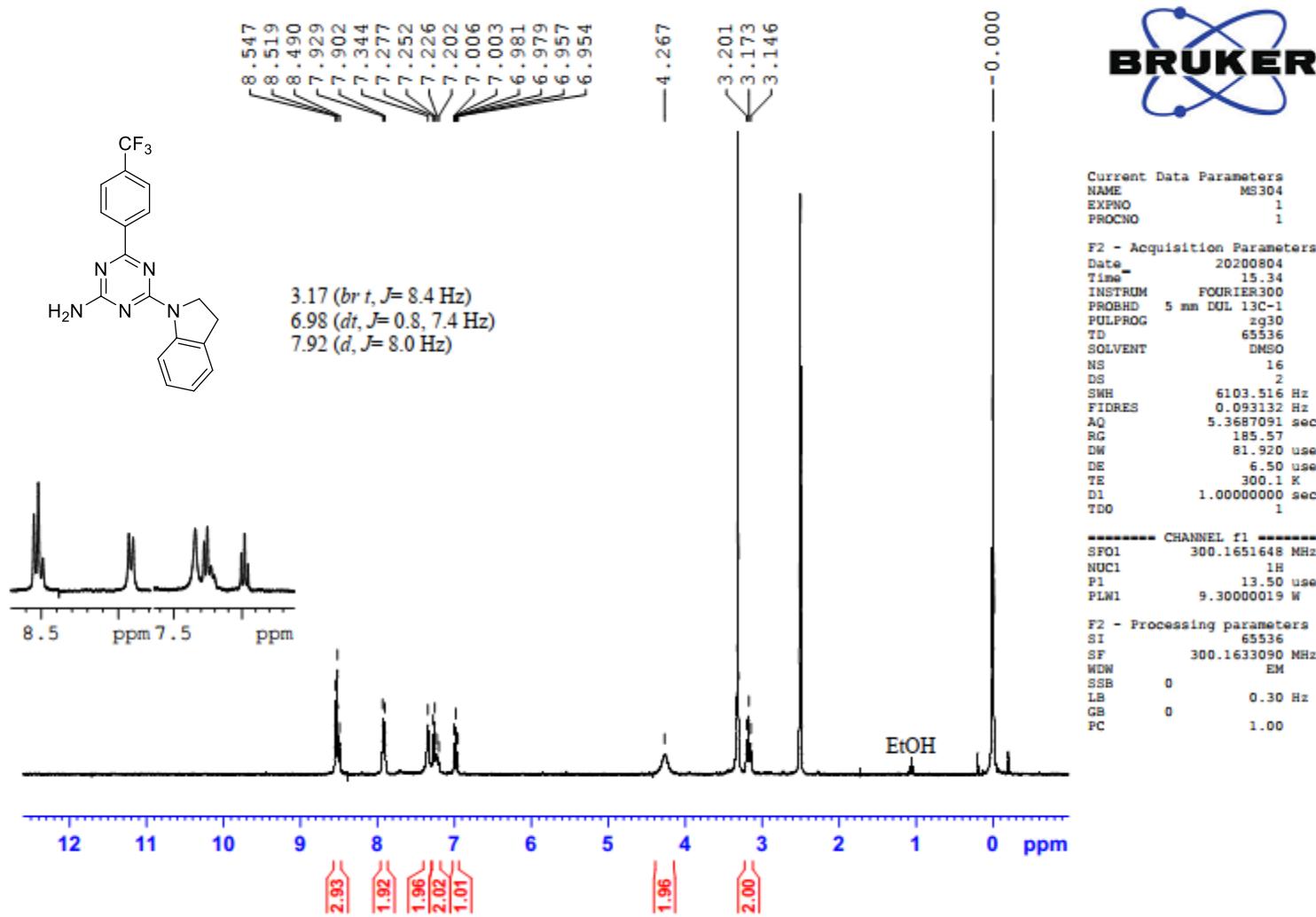
----- CHANNEL f2 -----
SFQ2 300.1612006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 used
PLM2 9.30000019 W
PLW12 0.25149000 W
PLW13 0.12650000 W

```

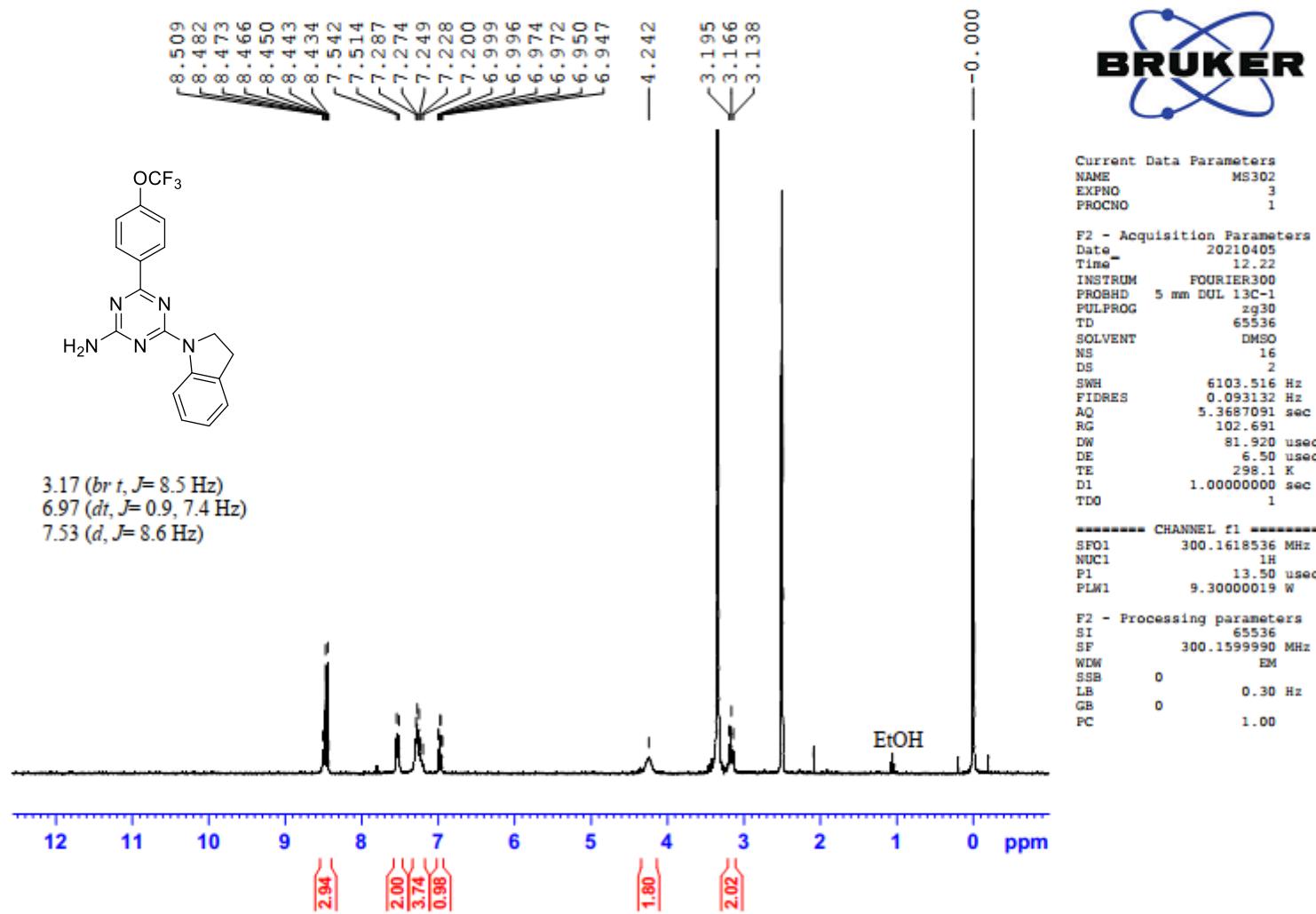
F2 - Processing parameters
SI          32768
SF        75.4753350 MHz
MDW          EM
SSB          0
LB           1.00 Hz
GB          0
PC          1.40

```

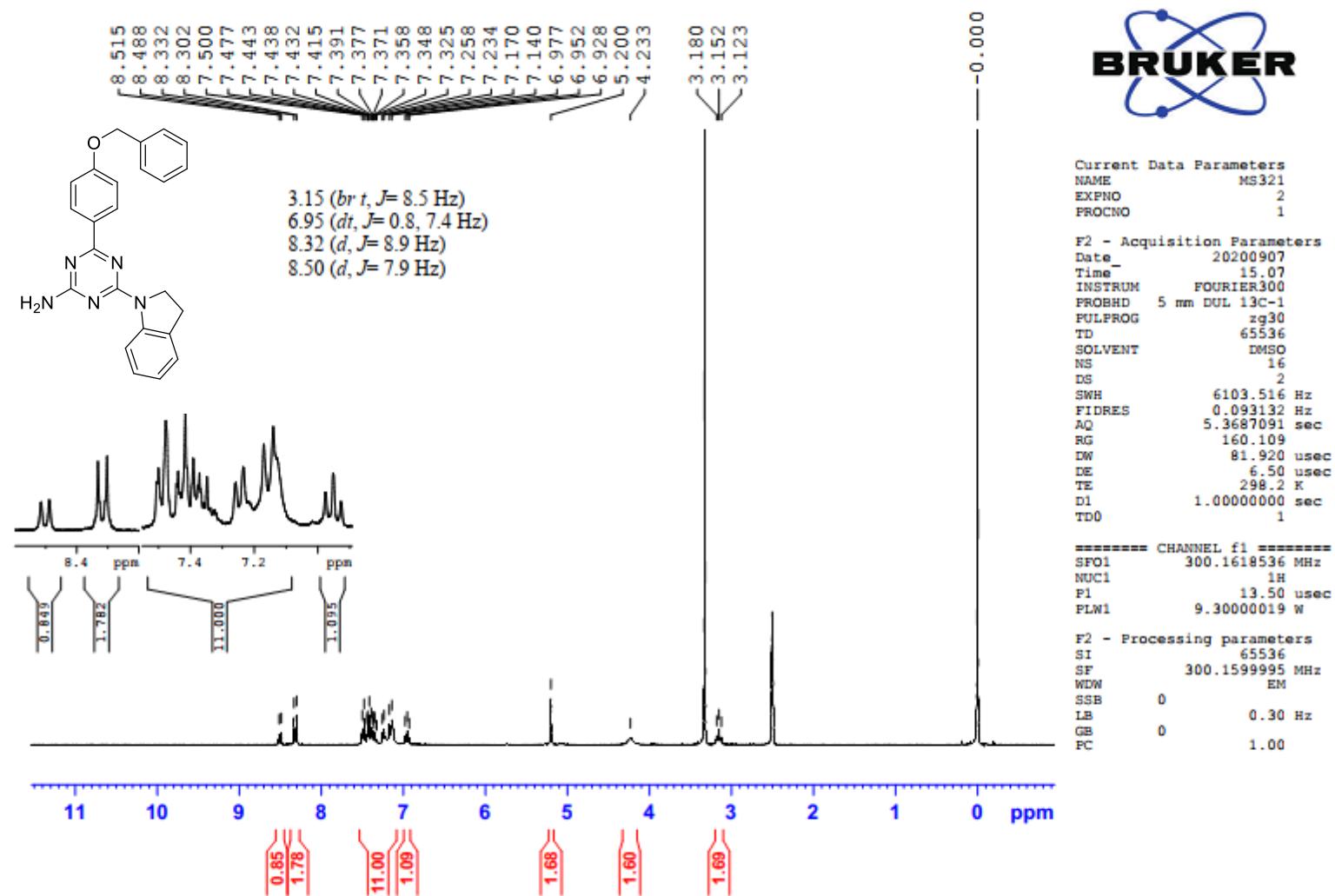
6-[4-(Trifluoromethyl)phenyl]-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,11}**)



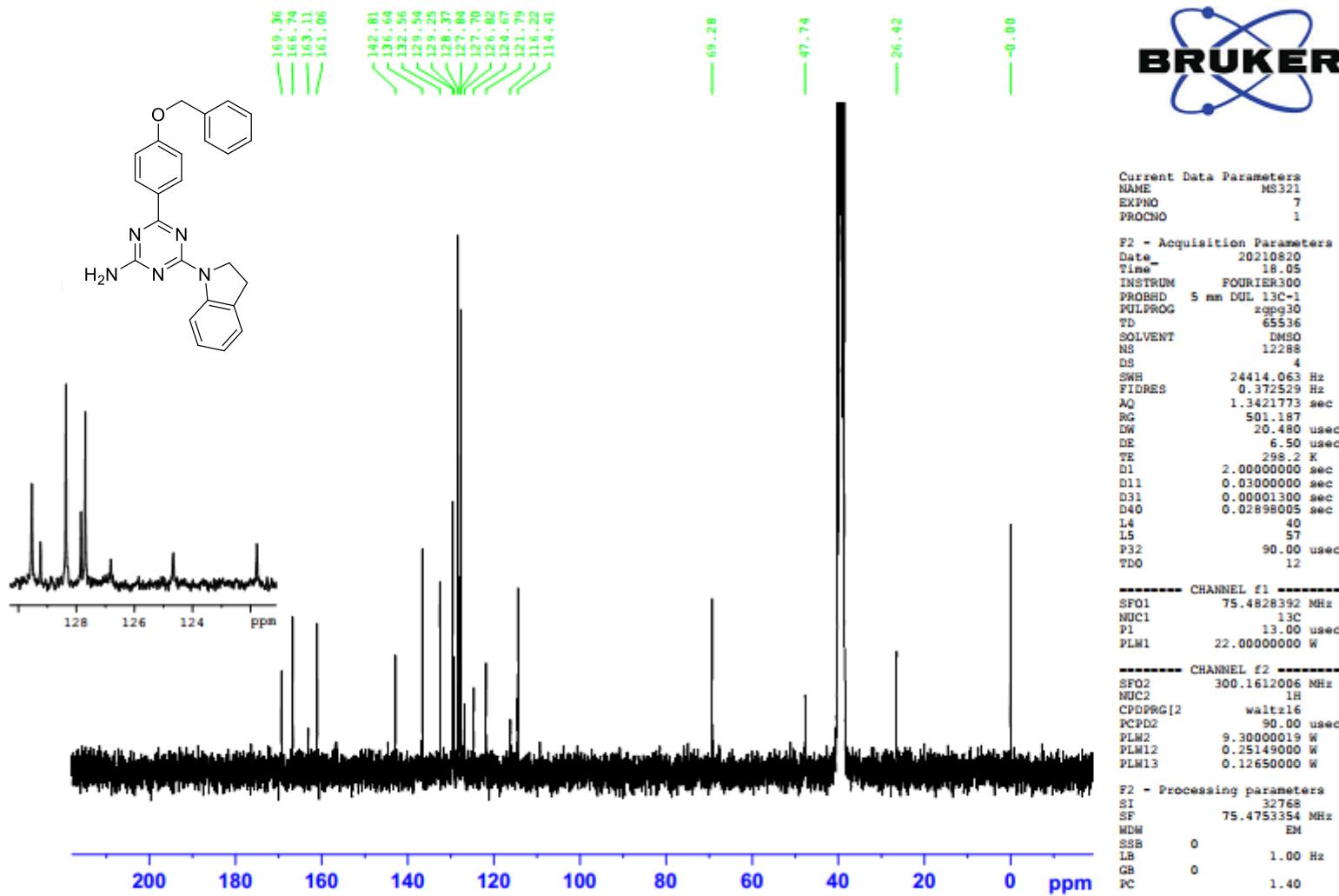
6-[4-(Trifluoromethoxy)phenyl]-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,12}**)



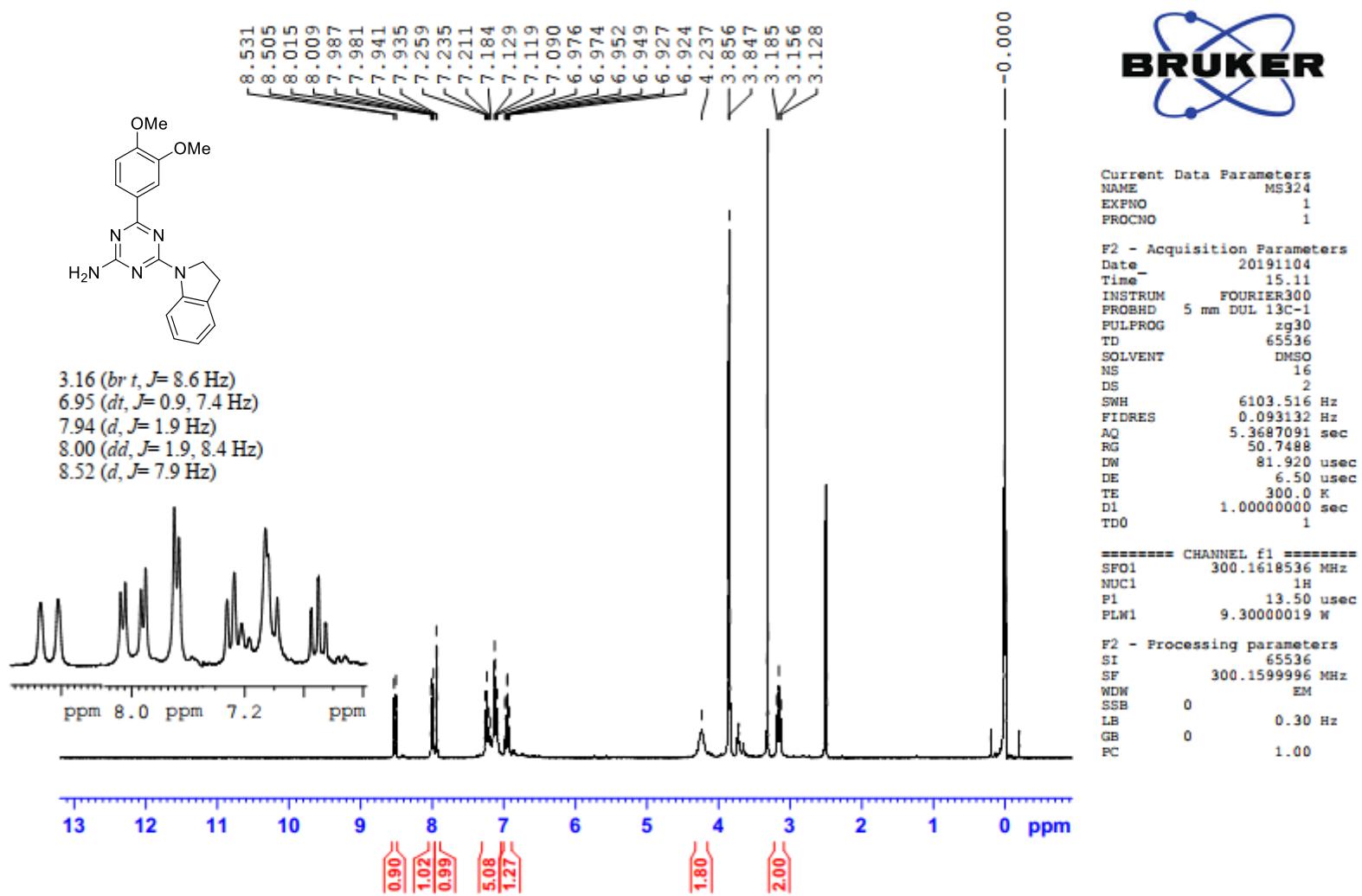
6-(4-(Benzylloxy)phenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,15}**)



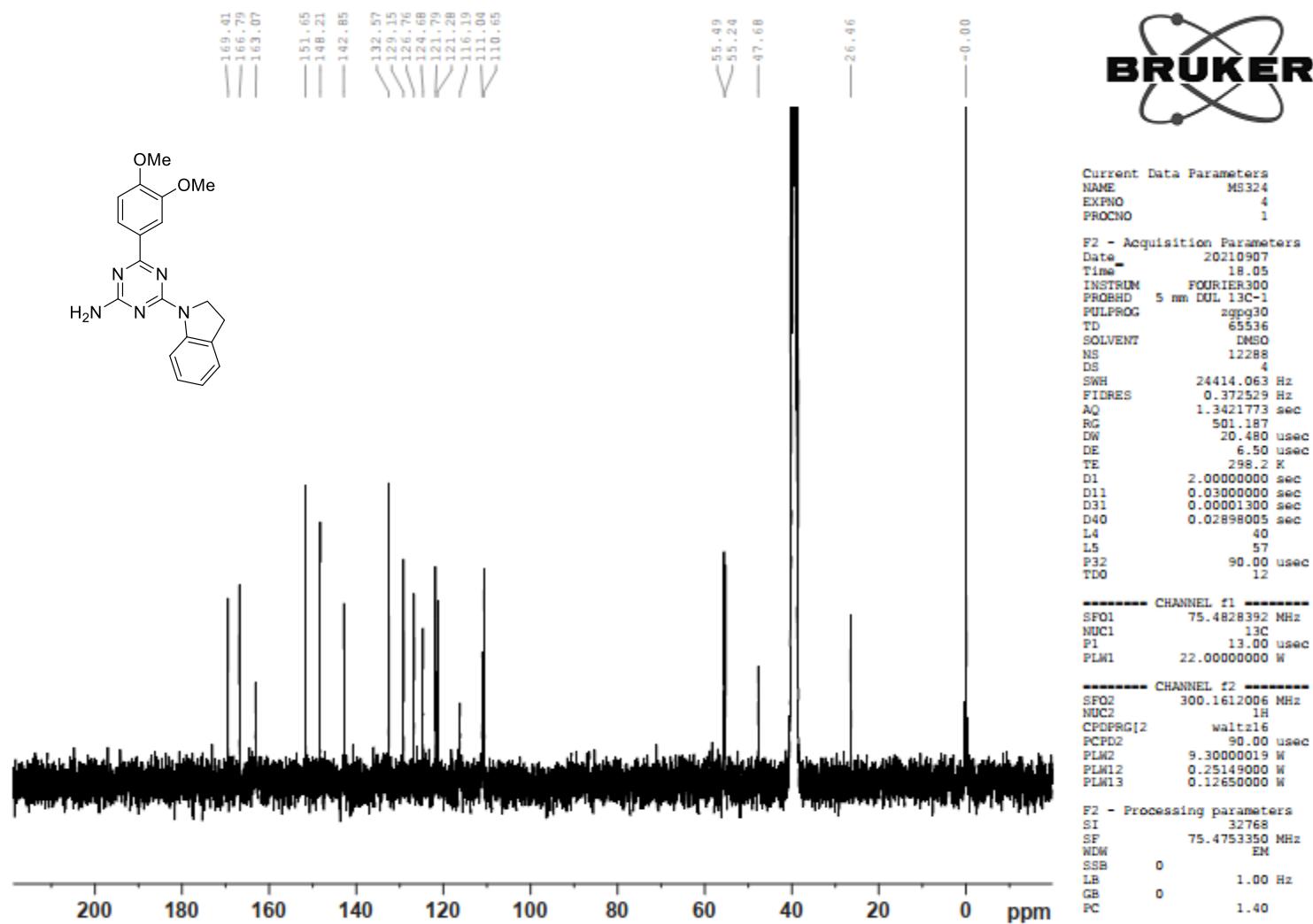
6-(4-(Benzyl)phenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,15}**)



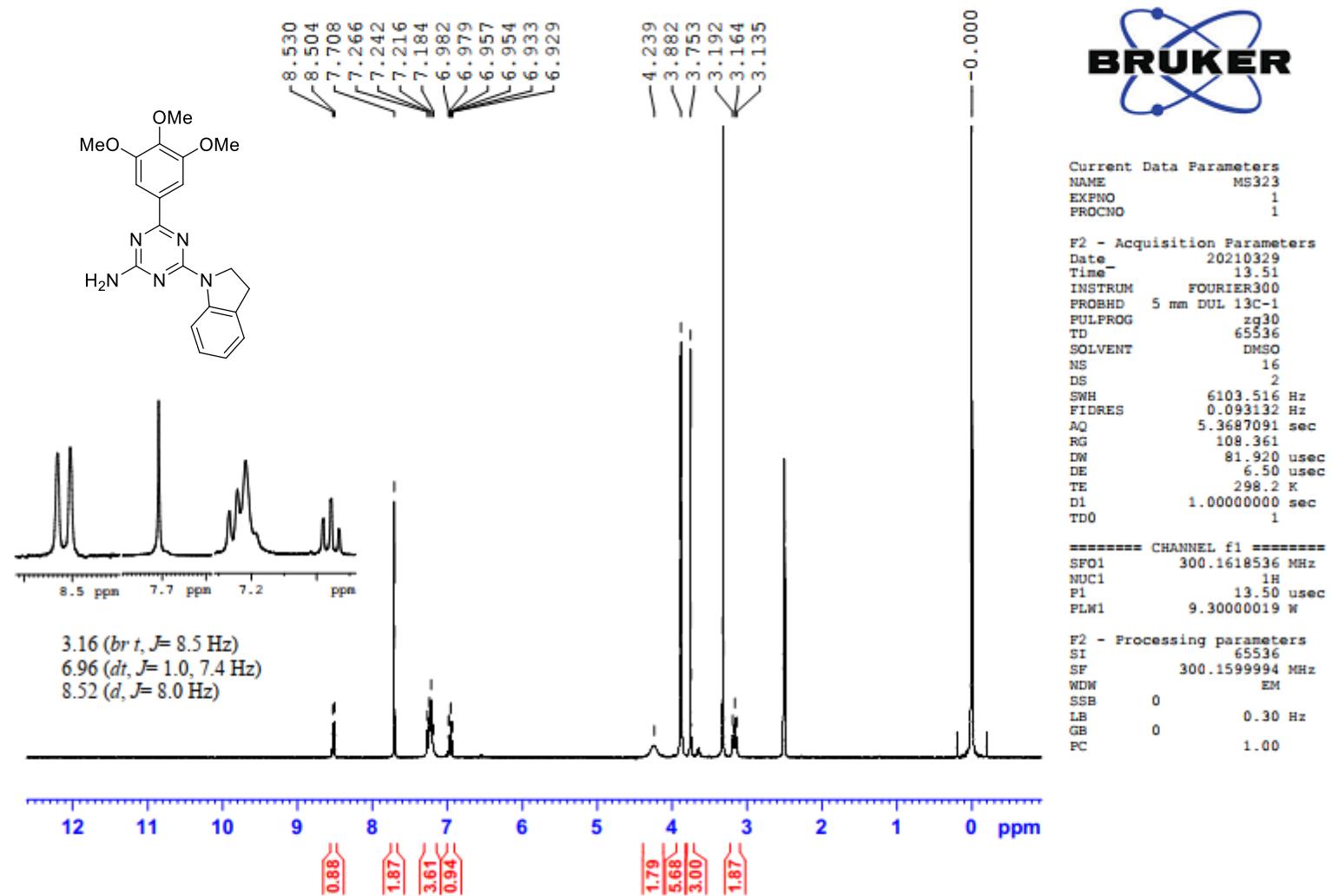
6-(3,4-Dimethoxyphenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,16}**)



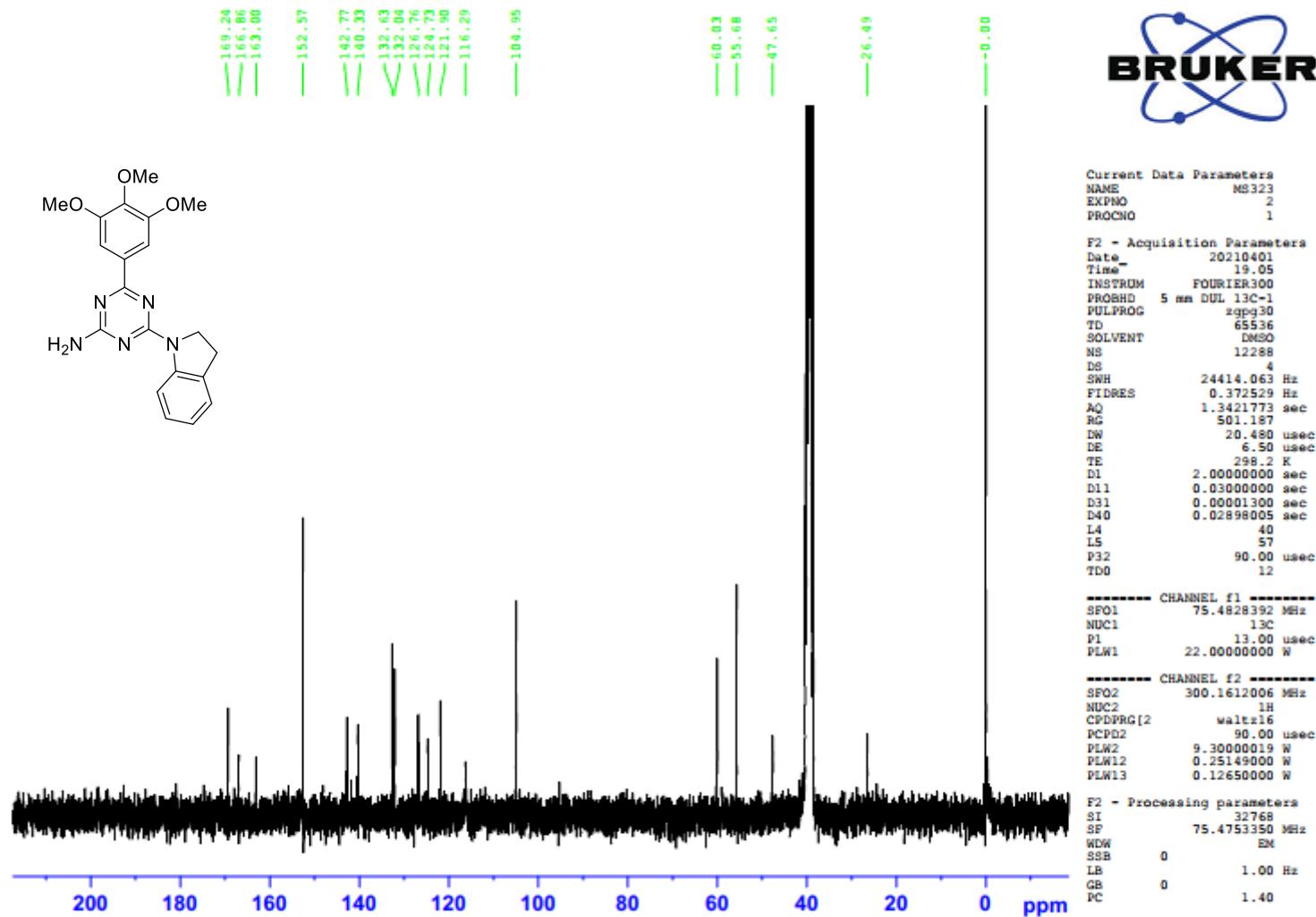
6-(3,4-Dimethoxyphenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,16}**)



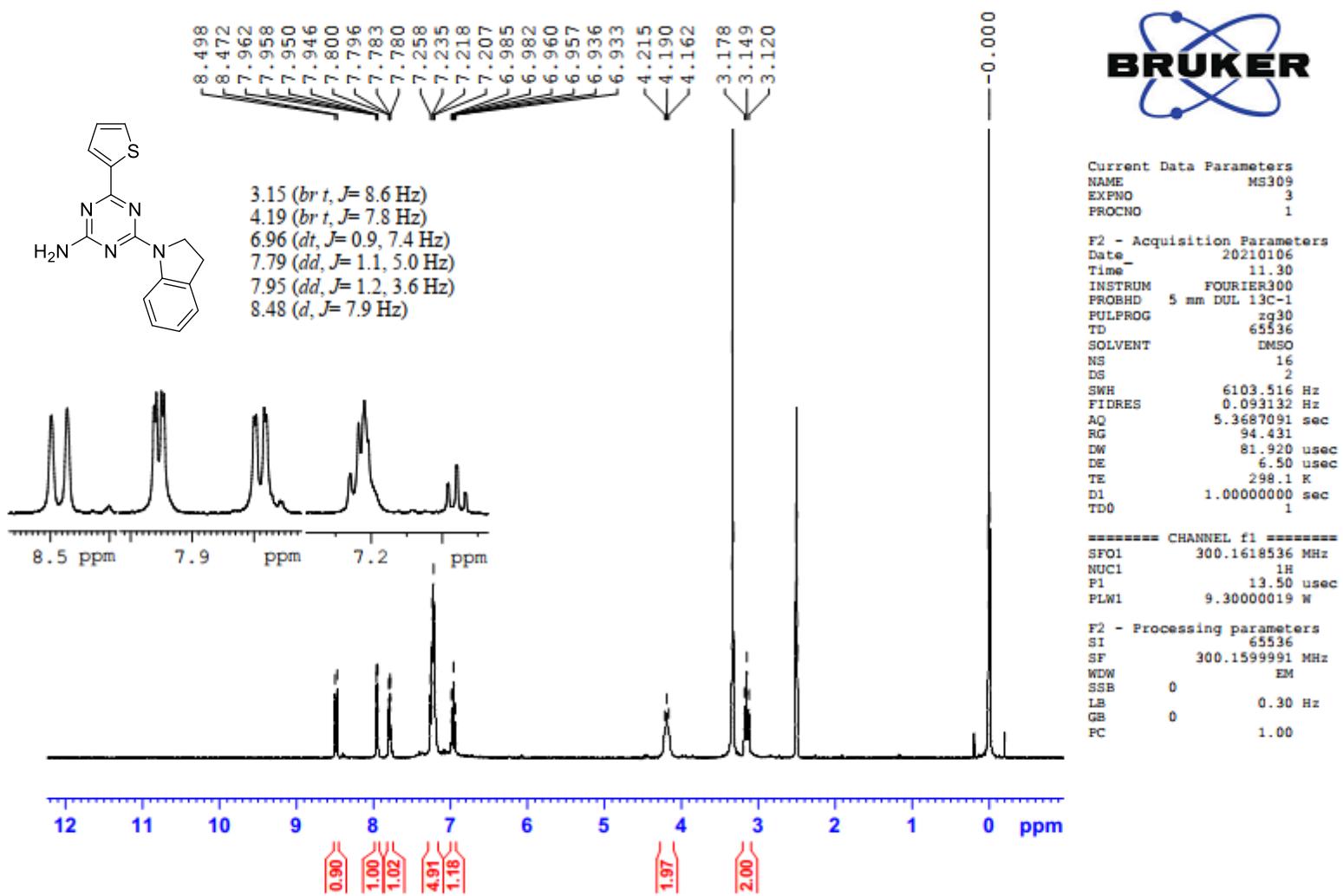
6-(3,4,5-Trimethoxyphenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,17}**)



6-(3,4,5-Trimethoxyphenyl)-4-(indolin-1-yl)-1,3,5-triazine-2-amine (**9{7,17}**)



4-(Indolin-1-yl)-6-(2-thienyl)-1,3,5-triazine-2-amine (**9**{7,18})



4-(Indolin-1-yl)-6-(2-thienyl)-1,3,5-triazine-2-amine (9{7,18})

