RSC Advances

ELECTRONIC SUPPLEMENTARY INFORMATION

A one-pot synthesis of N^2,6-diaryl-5,6-dihydro-1,3,5-triazine-2,4-diamines and systematic evaluation of their ability to host ethanol in crystals

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Table S1. Key geometric parameters (Å, °) for **1b**.EtOH and **1f**.EtOH

Parameter		Parameter		Parameter		Parameter	
1b – molecule 1		**1b – molecule 2**		**1f – molecule 1**		**1f – molecule 2**	
C1–N1	1.447(6)	C17–N6	1.471(6)	C1–N1	1.448(6)	C16–N6	1.463(6)
C1–N3	1.470(6)	C17–N8	1.452(6)	C1–N3	1.474(6)	C16–N8	1.452(6)
C2–N1	1.305(6)	C18–N6	1.312(7	C2–N1	1.301(7)	C17–N6	1.297(7)
C2–N2	1.373(6)	C18–N7	1.366(6)	C2–N2	1.379(6)	C17–N7	1.388(6)
C3–N2	1.339(6)	C19–N7	1.340(6)	C3–N2	1.338(6)	C18–N7	1.318(6)
C3–N3	1.334(6)	C19–N8	1.342(7)	C3–N3	1.324(7)	C18–N8	1.336(7)
C1–N1–C2	115.1(4)	C17–N6–C18	113.3(4)	C1–N1–C2	115.6(4)	C16–N6–C18	114.6(4)
C2–N2–C3	114.0(4)	C18–N7–C19	115.1(4)	C2–N2–C3	113.6(4)	C17–N7–C18	114.9(4)
C1–N3–C3	117.6(4)	C17–N8–C19	117.8(4)	C1–N3–C3	118.4(4)	C16–N8–C18	118.2(4)
N1–C1–N3	110.5(4)	N6–C17–N8	110.0(4)	N1–C1–N3	110.5(4)	N6–C16–N8	111.0(4)
N1–C2–N2	127.8(4)	N6–C18–N7	127.4(4)	N1–C2–N2	128.1(4)	N6–C17–N7	126.9(4)
N2–C3–N3	122.5(4)	N7–C19–N8	121.0(4)	N2–C3–N3	123.3(4)	N7–C18–N8	122.6(4)

Table S2. Least-squares plane data for **1b**.EtOH and **1f**.EtOH.

1b	
N1-molecule	
r.m.s. deviation (N1-N3, C2 and C3)	0.042
deviation of C1	0.477(6)
Dihedral angles	
(N1-N3, C1-C3)/(C4-C9)	89.07(13)
(N1-N3, C1-C3)/(C11-C16)	19.2(3)
(C4-C9)/(C11-C16)	70.43(15)
N6-molecule	
r.m.s. deviation (N6-N8, C17 and C8)	0.043
deviation of C16	0.529(6)
Dihedral angles	
(N6-N8, C16-C18)/(C20-C25)	74.56(17)
(N6-N8, C16-C18)/(C27-C32)	13.6(3)
(C20-C25)/(C27-C32)	63.38(17)
1f	
N1-molecule	
r.m.s. deviation (N1-N3, C2 and C3)	0.030
deviation of C1	0.441(6)
Dihedral angles	
(N1-N3, C1-C3)/(C4-C9)	88.31(16)
(N1-N3, C1-C3)/(C10-C15)	18.3(2)
(C4-C9)/(C10-C15)	75.81(17)
N6-molecule	
r.m.s. deviation (N6-N8, C17 and C8)	0.032
deviation of C16	0.467(6)
Dihedral angles	
(N6-N8, C16-C18)/(C19-C24)	72.61(18)
(N6-N8, C16-C18)/(C25-C30)	19.3(3)
(C19-C24)/(C25-C30)	57.61(18)

Table S3 Geometric parameters (Å, °) characterizing the intermolecular interactions occurring in the crystal of **1b**.EtOH

A	H	B	A–H	H···B	A···B	A–H···B	Symmetry operation
N3	H3n	N7	0.88(4)	2.08(4)	2.932(6)	161(4)	1-*x*, ½+*y*, 1-*z*
N8	H8n	N2	0.88(4)	2.08(3)	2.929(6)	161(5)	1-*x*, ½+*y*, 1-*z*
N4	H4na	Cg(C27-C32)	0.88(4)	2.59(5)	137(4)	3.290(5)	*x*, *y*, 1+*z*
N9	H9na	Cg(C11-C16)	0.88(5)	2.72(5)	134(4)	3.389(5)	*x*, *y*, *z*
C22	H22	Cg(C11-C16)	0.95	2.76	3.565(6)	143	1-*x*, 1/2+*y*, 1-*z*
O3	H3o	N1	0.88(5)	1.86(5)	2.712(5)	162(5)	*x*, *y*, *z*
O4	H4o	N6	0.87(5)	1.88(5)	2.732(5)	167(5)	*x*, *y*, 1+*z*
N5	H5n	O3	0.88(4)	2.05(4)	2.916(6)	167(5)	1-*x*, -½+*y*, 1-*z*
N9	H9Nb	O3	0.88(5)	2.03(5)	2.861(6)	158(6)	*x*, *y*, *z*
N4	H4nb	O4	0.88(5)	2.02(5)	2.883(6)	170(5)	*x*, *y*, *z*
N10	H10n	O4	0.88(4)	2.07(4)	2.912(6)	163(5)	1-*x*, -½+*y*, 1-*z*
C15	H15	O2	0.95	2.44	3.275(7)	147	-1+ *x*, *y*, *z*
C29	H29	O1	0.95	2.42	3.342(7)	165	1-*x*, ½+*y*, -*z*
C33	H33a	Cl2	0.99	2.80	3.551(7)	133	1-*x*, ½+*y*, -*z*

Table S4 Geometric parameters (Å, °) characterizing the intermolecular interactions occurring in the crystal of **1f**.EtOH

A	H	B	A–H	H···B	A···B	A–H···B	Symmetry operation
N3	H3n	N7	0.88(3)	2.04(3)	2.911(6)	168(4)	1-*x*, -½+*y*, 1-*z*
N8	H8n	N2	0.88(4)	2.10(4)	2.943(6)	161(5)	1-*x*, -½+*y*, 1-*z*
N4	H4na	Cg(C25-C30)	0.89(4)	2.58(6)	136(4)	3.279(5)	*x*, *y*, 1+*z*
N9	H9na	Cg(C10-C15)	0.88(3)	2.65(6)	127(5)	3.257(6)	*x*, *y*, *z*
C22	H22	Cg(C4-C9)	0.95	2.75	3.611(6)	152	*x*, *y*, 1+*z*
O1	H1o	N1	0.84(5)	1.89(5)	2.728(5)	175(5)	*x*, *y*, *z*
O2	H2o	N6	0.83(5)	1.88(5)	2.708(5)	173(7)	*x*, *y*, *z*
N5	H5n	O1	0.88(5)	2.02(5)	2.890(5)	172(5)	1-*x*, ½+*y*, 1-*z*
N9	H9nb	O1	0.88(5)	2.00(5)	2.878(6)	177(6)	*x*, *y*, *z*
N4	H4nb	O2	0.87(5)	2.02(5)	2.885(6)	173(4)	*x*, *y*, 1+*z*
N10	H10n	O2	0.88(5)	2.03(5)	2.894(6)	170(5)	1-*x*, ½+*y*, *z*
C7	H7	Br1	0.95	2.92	3.682(7)	138	-*x*, -½+*y*, 1-*z*

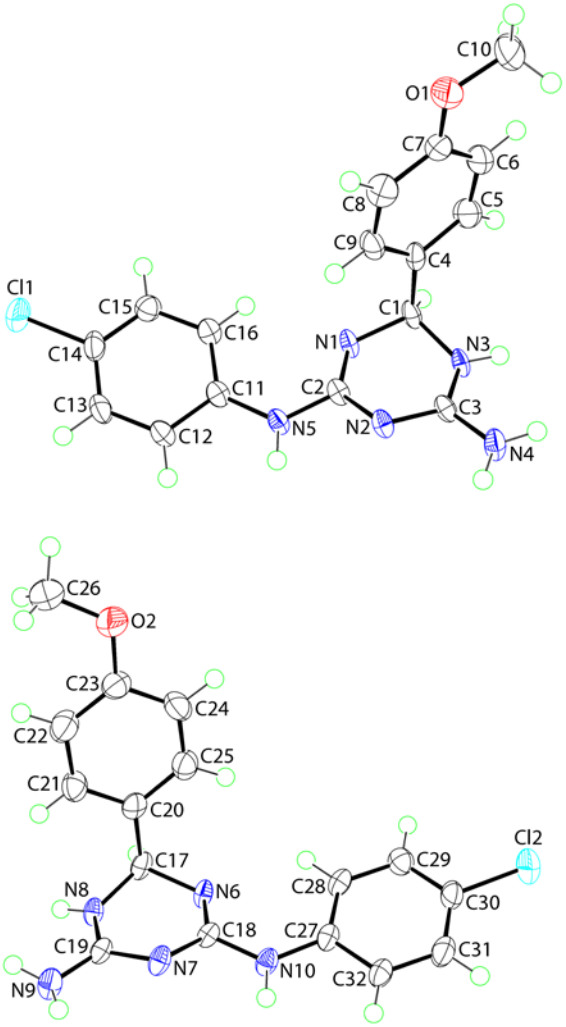


Figure S1. The molecular structures of the two independent molecules of **1b** comprising the asymmetric unit of **1b**.EtOH, showing atom labelling scheme and displacement ellipsoids at the 70% probability level.

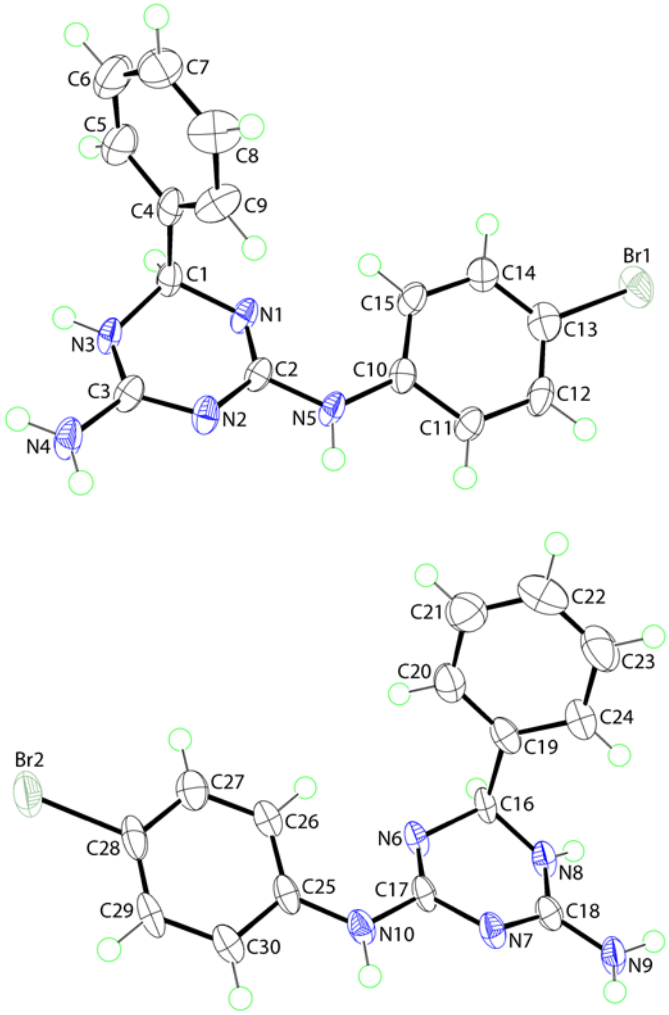
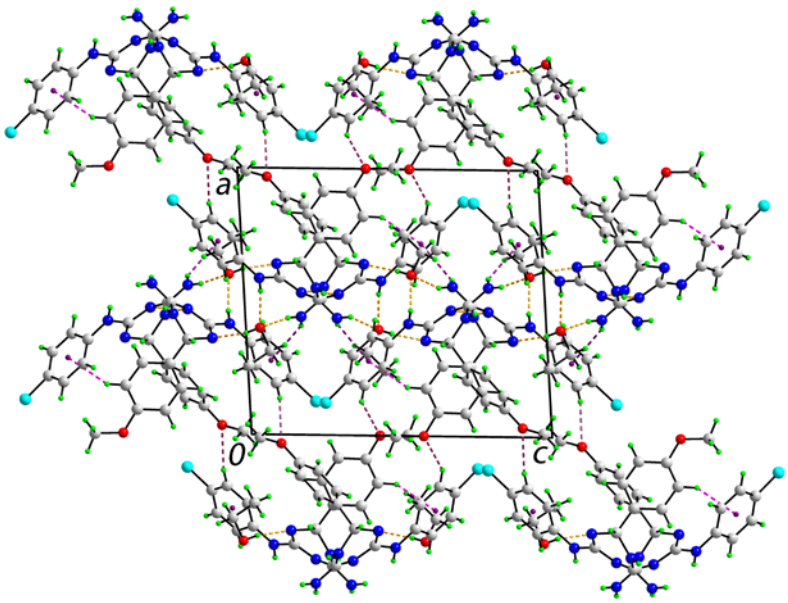


Figure S2. The molecular structures of the two independent molecules of **1e** comprising the asymmetric unit of **1e**.EtOH, showing atom labelling scheme and displacement ellipsoids at the 70% probability level.



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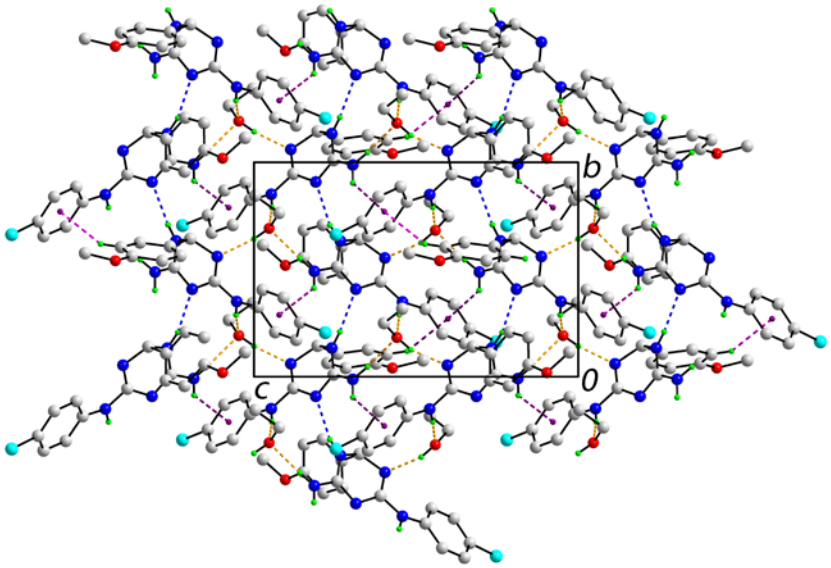


(b)

Figure S3. Molecular packing in **1b**.EtOH: (a) view of the unit cell contents in projection down the *a*-axis highlighting the stacking of layers and (b) a plan view of the layer (non-participating hydrogen atoms are omitted for reasons of clarity). The N–H···N, N–H···π, C–H···π and C–H···O interactions are shown as blue, purple, pink and plum dashed lines, respectively. The hydrogen-bonding involving the ethanol molecules are shown as orange dashed lines.

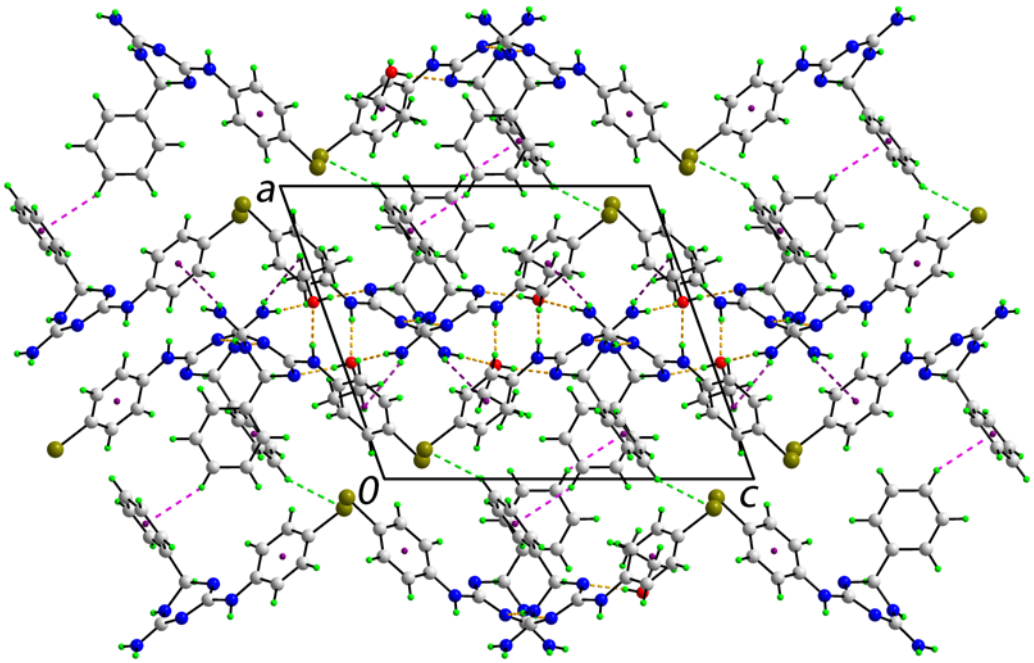
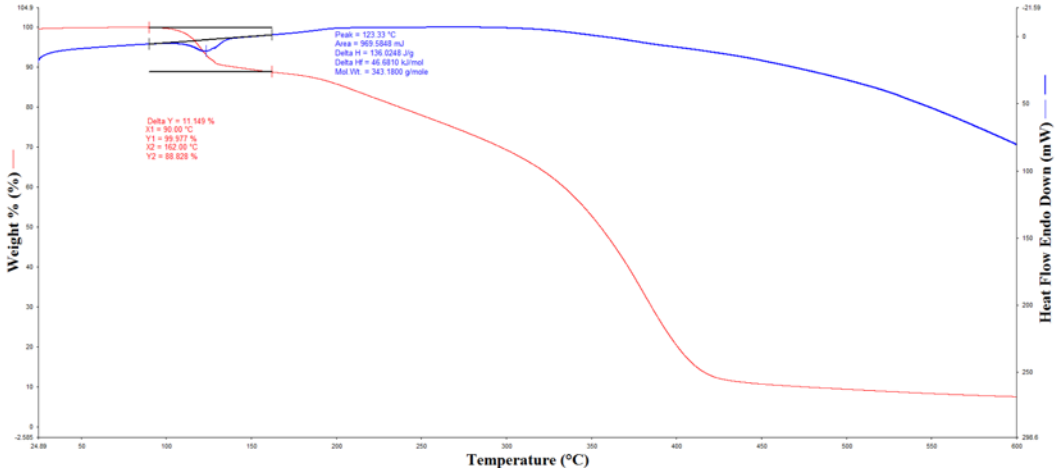


Figure S4. Molecular packing in **1f**.EtOH: view of the unit cell contents in projection down the *b*-axis highlighting the stacking of layers. The N–H···N, N–H···π, C–H···π and C–H···Br interactions are shown as blue, purple, pink and green dashed lines, respectively. Hydrogen-bonding involving the ethanol molecules are shown as orange dashed lines.



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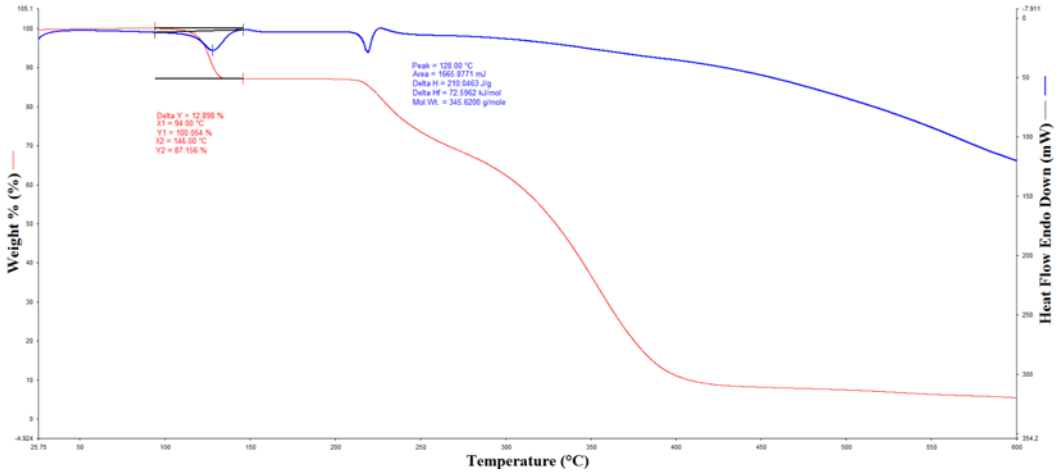
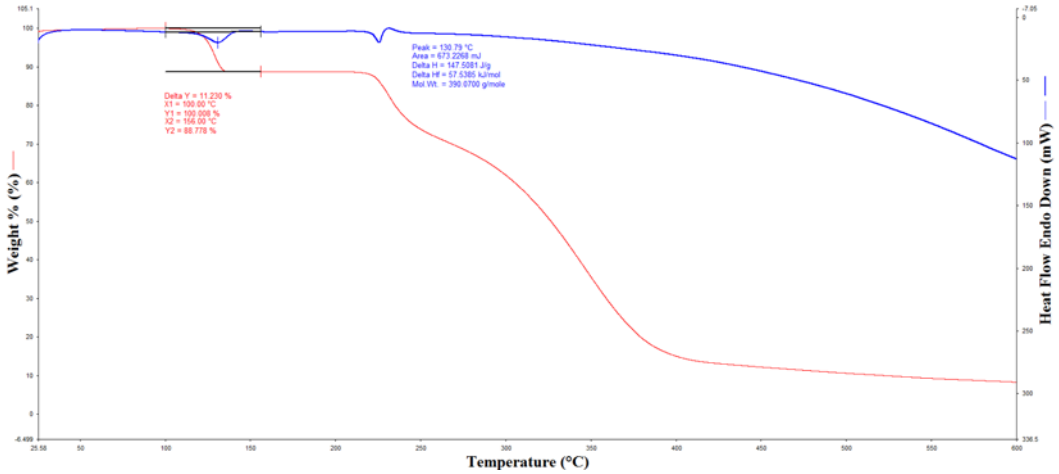


(b)



(c)

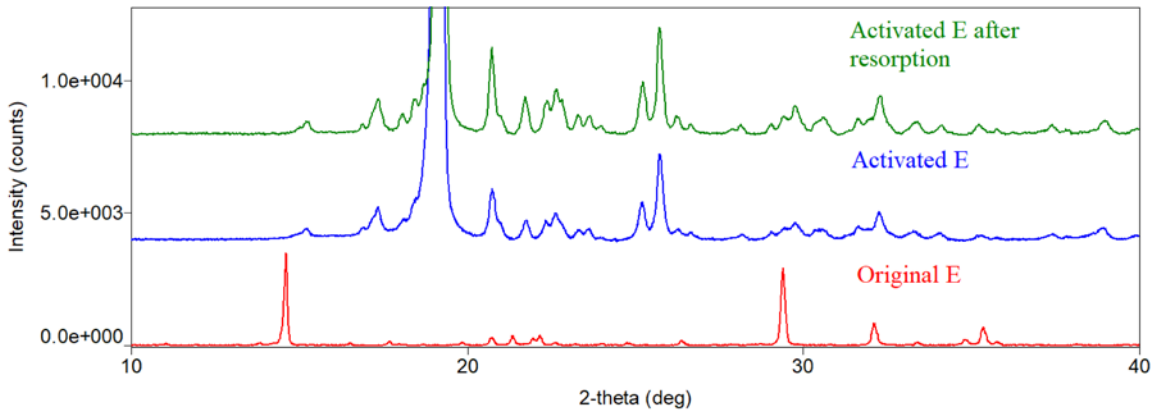
Figure S5. Traces for the STA conducted on (a) **1b**, (b) **1e** and (c) **1f**.

Data for the first weight loss (first exothermic process):

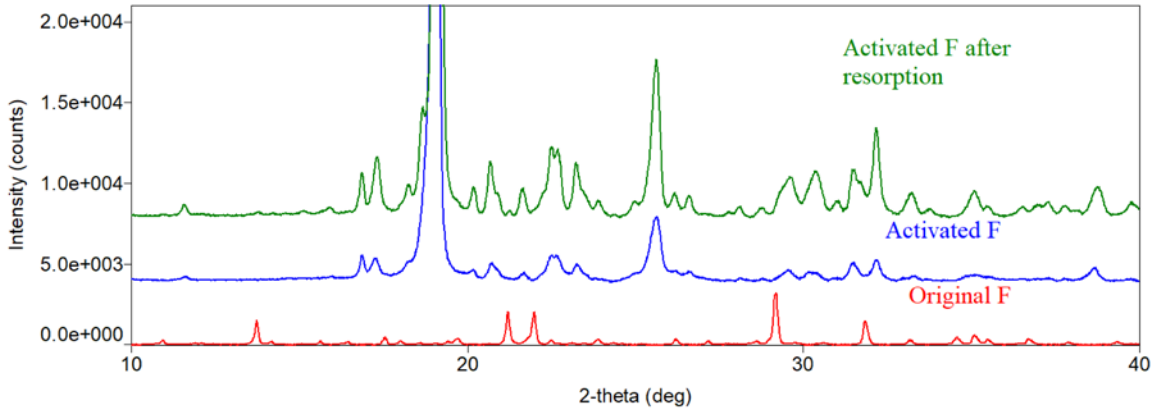
	Temp. range (°C)	Expt'l wght loss (%)	calcd wght loss (%)	$\Delta H_{desolvation}$ (kJ/mol)
1b.EtOH	90 – 162	88.8	86.6	46.7
1e.EtOH	94 – 146	87.2	86.7	72.6
1f.EtOH	100 – 156	88.8	88.2	57.5

Data for the second exothermic process:

	Temp. range (°C)	Peak temp. (°C)	$\Delta H_{melting}$ (kJ/mol)
1e.EtOH	204 – 227	219.4	29.2
1f.EtOH	211 – 232	225.9	27.6



(a)

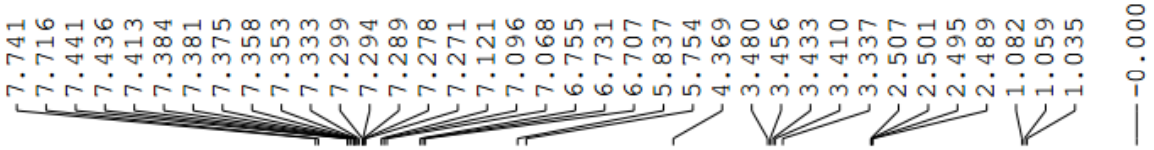


(b)

Figure S6. Experimental powder X-ray diffraction patterns for (a) **1e** and (b) **1f**. The red trace is of the original materials, *i.e*. **1e**.EtOH and **1f**.EtOH. The blue traces are of the desolvated materials as per the STA analyses, showing that the crystal structures are different. The green traces are measurements taken after exposing the desolvated materials to EtOH vapour overnight, showing no reversion to the original structures of **1e**.EtOH and **1f**.EtOH had occurred.

Copies of NMR spectra of prepared products **1a-k · EtOH** and **1a**

N²,6-Diphenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1a · EtOH)



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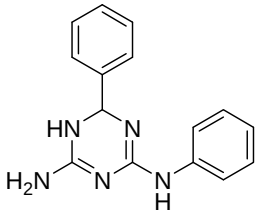

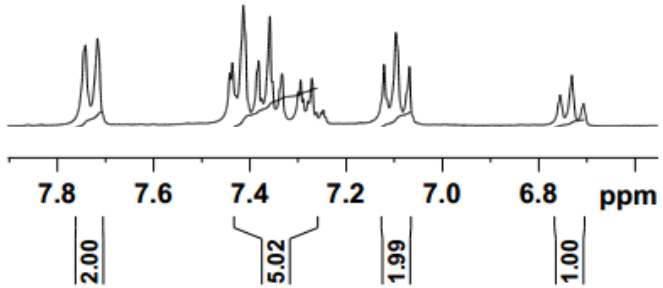

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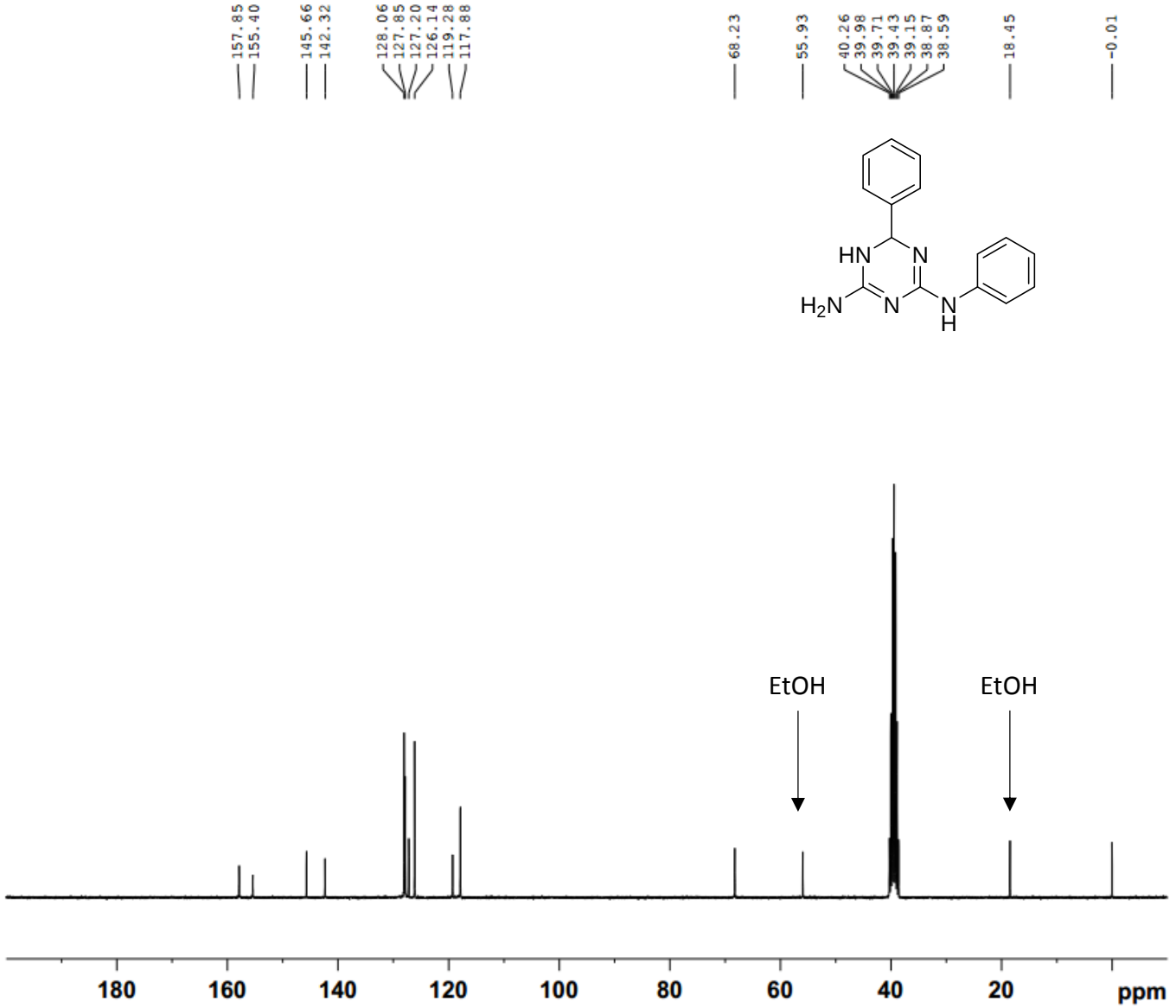

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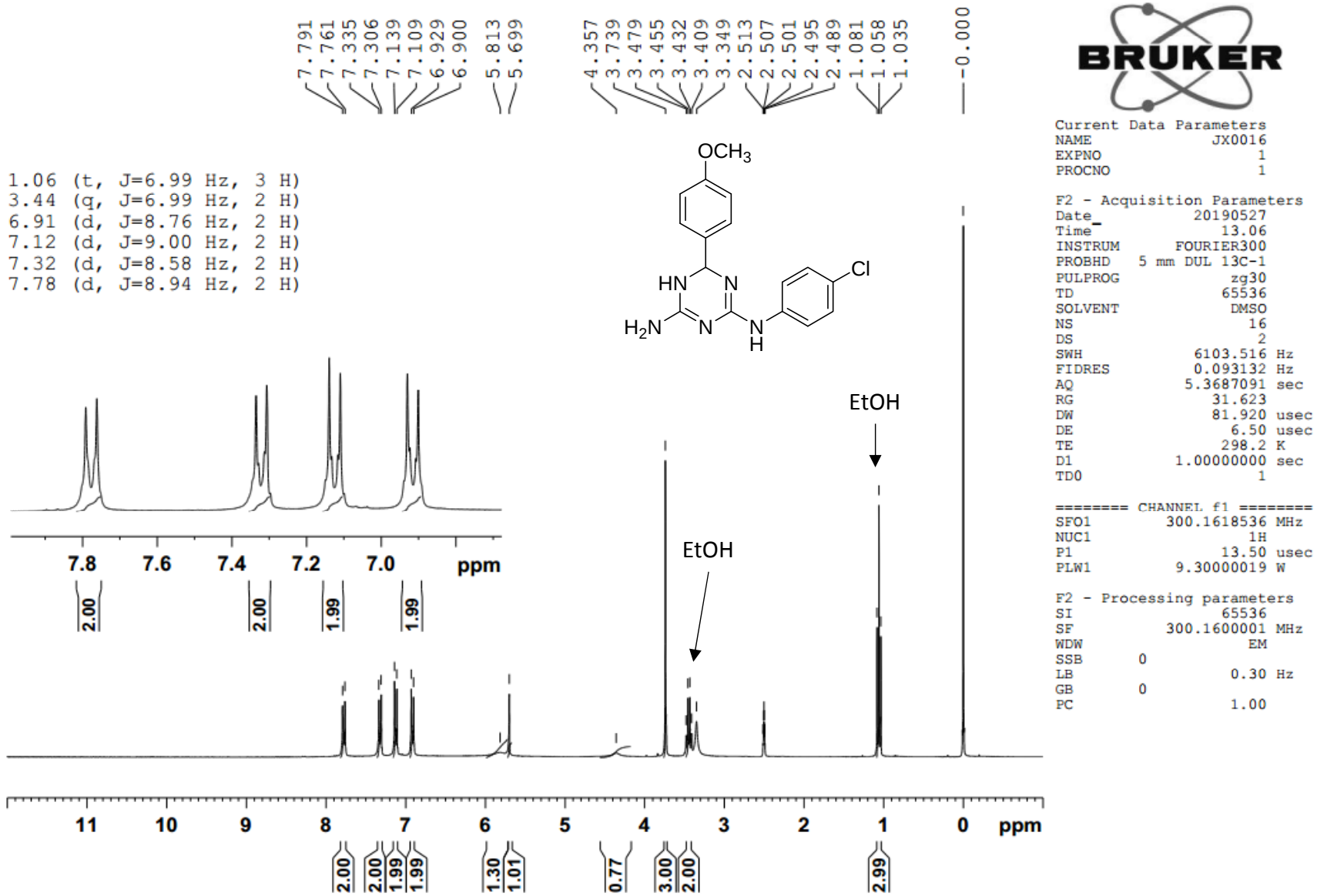

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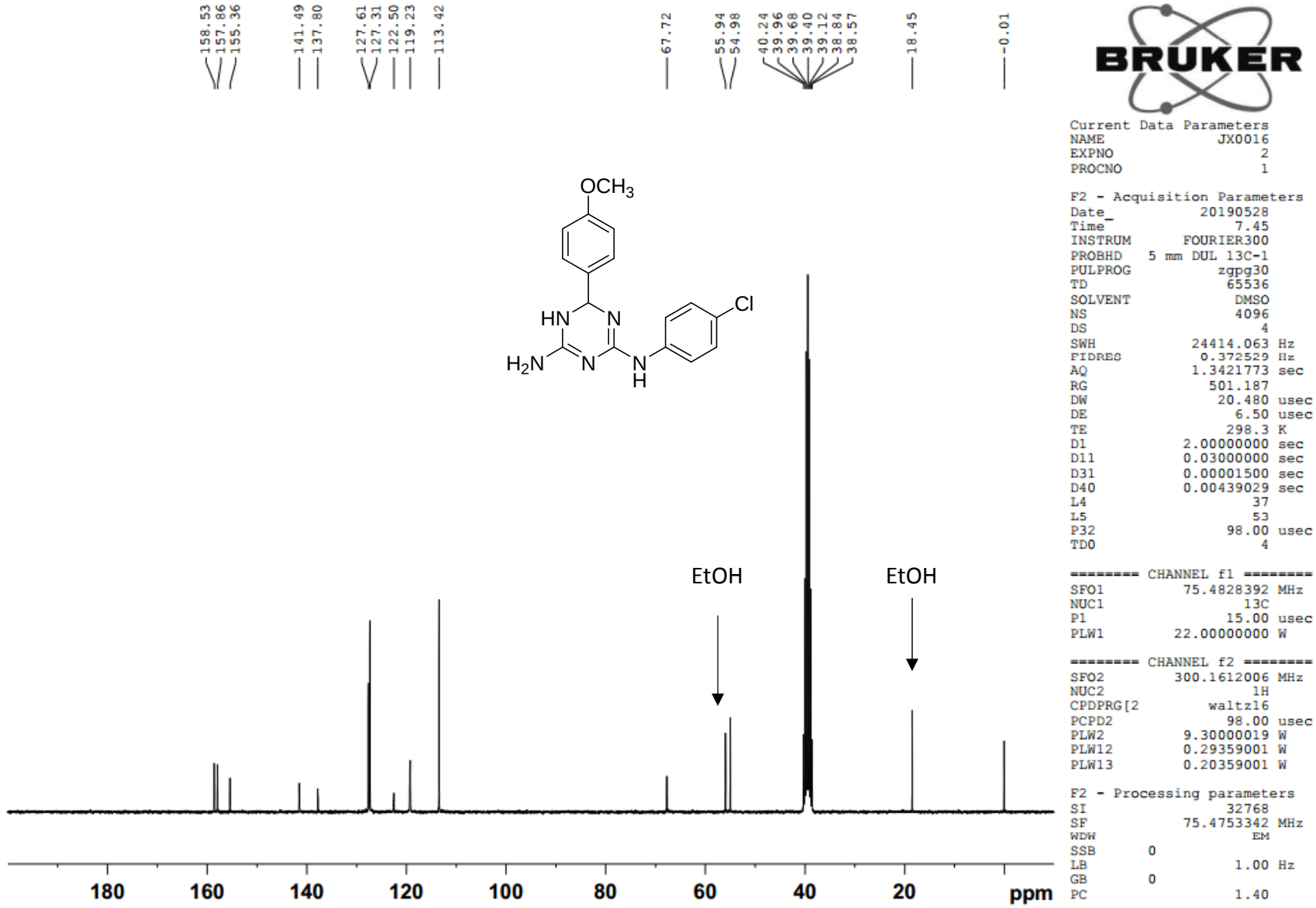

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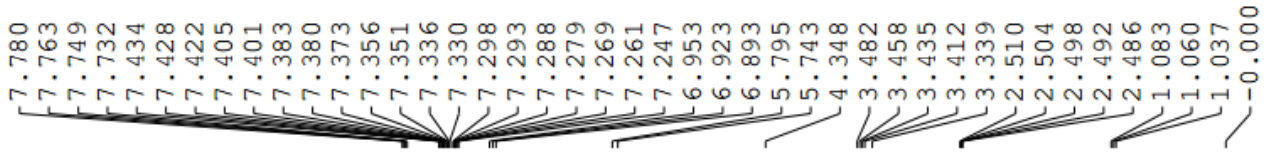
N²-(4-Fluorophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1c · EtOH)



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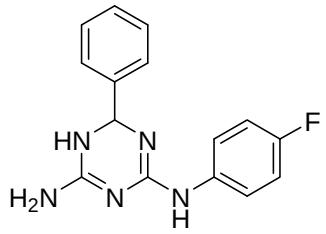

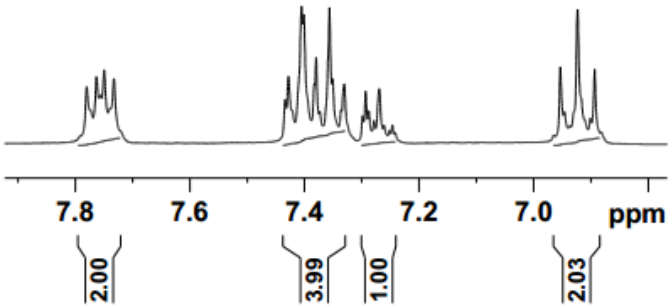


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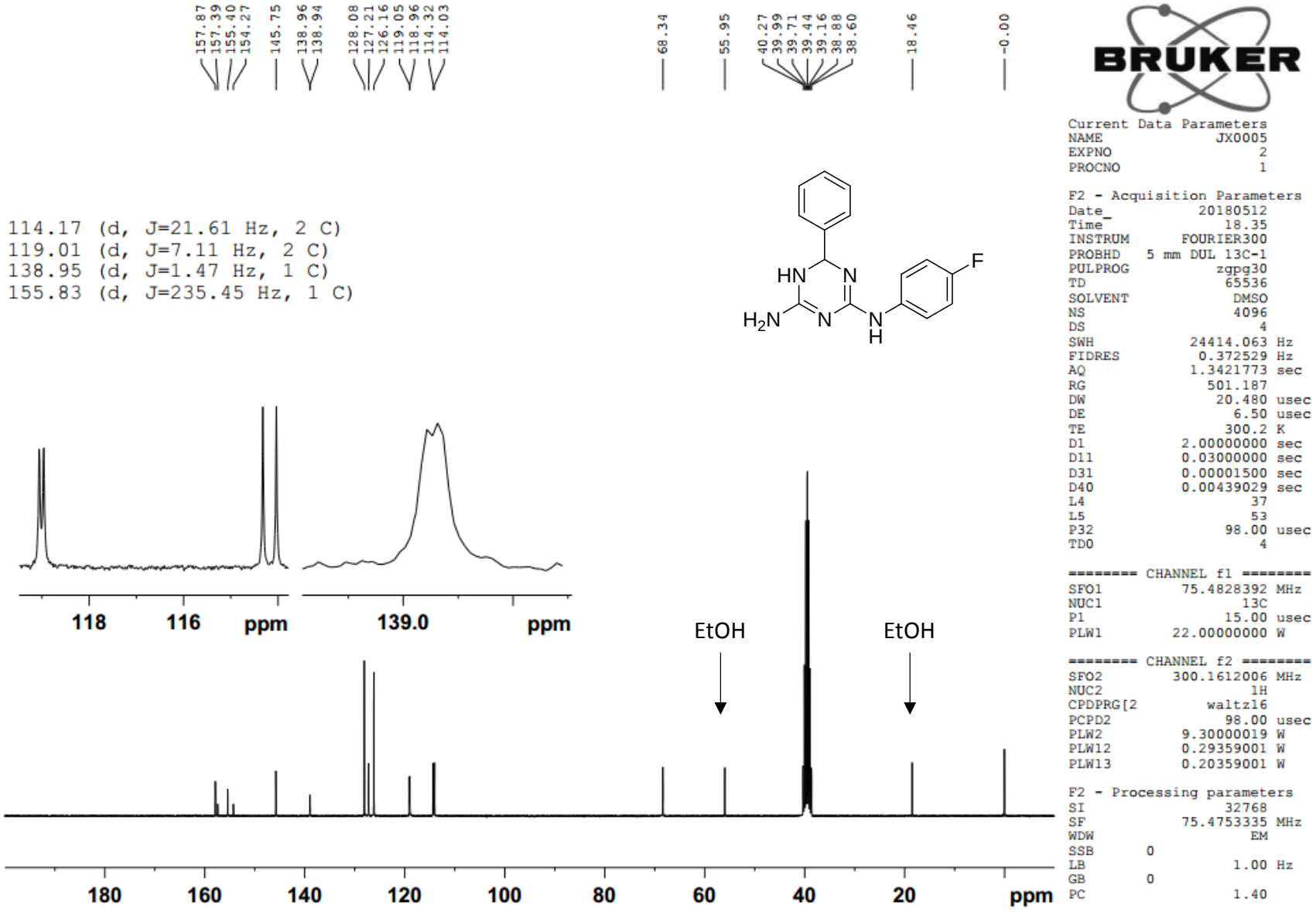
F2 - Acquisition Parameters
Date_              20180512
Time                   2.42
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                6103.516 Hz
FIDRES             0.093132 Hz
AQ                 5.3687091 sec
RG                    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               300.1600020 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N²-(4-Fluorophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1c · EtOH)




```
Current Data Parameters
NAME                  JX0005
EXPNO                      2
PROCNO                     1

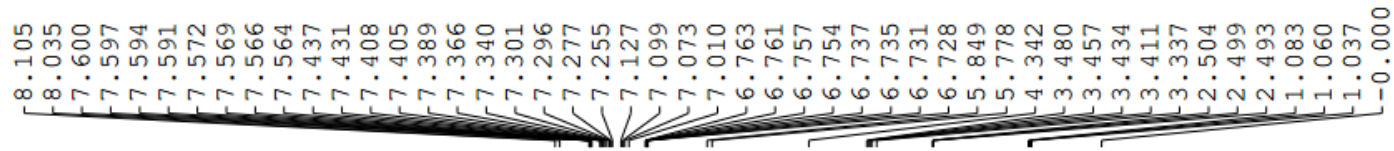
F2 - Acquisition Parameters
Date_              20180512
Time                  18.35
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    4096
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.2 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                      4

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

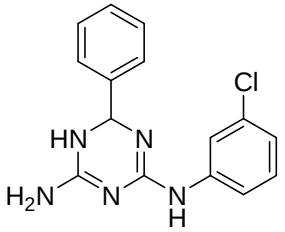
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

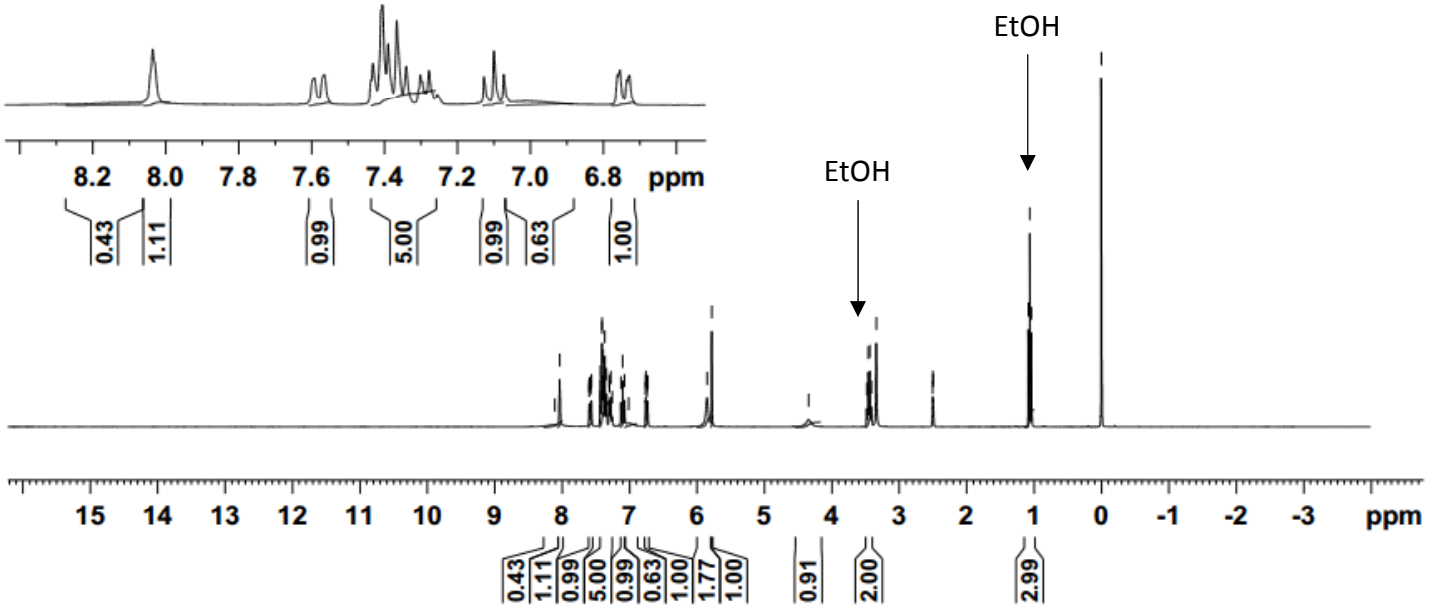
F2 - Processing parameters
SI                    32768
SF              75.4753335 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

N²-(3-Chlorophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1d · EtOH)



1.06 (t, J=6.99 Hz, 3 H)
3.45 (q, J=6.97 Hz, 2 H)
6.75 (ddd, J=0.84, 2.01, 7.86 Hz, 1 H)
7.10 (dd, J=8.09, 8.09 Hz, 1 H)
7.58 (ddd, J=0.86, 1.55, 8.55 Hz, 1 H)





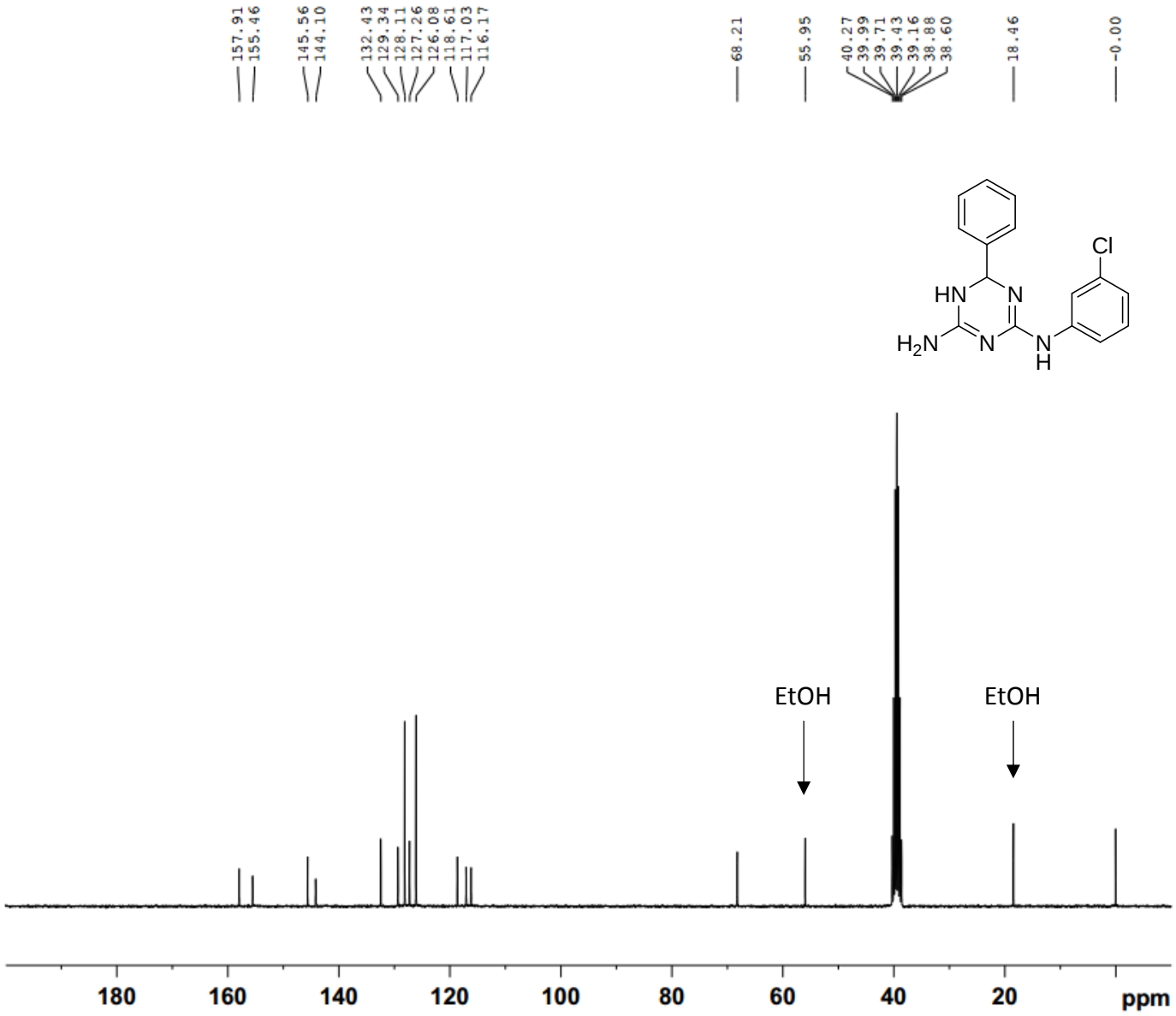

```
Current Data Parameters
NAME                  JX0008
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180516
Time                  15.57
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               300.1600016 MHz
WDW                         EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N²-(3-Chlorophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1d · EtOH)




```
Current Data Parameters
NAME                  JX0008
EXPNO                      3
PROCNO                     1

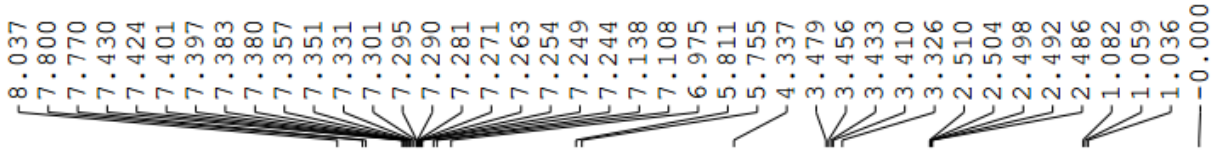
F2 - Acquisition Parameters
Date_              20180516
Time                  18.05
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     4096
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.1 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                       4

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

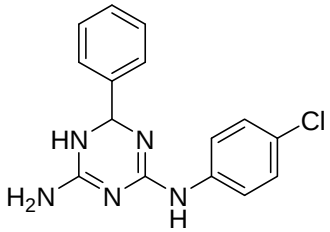
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

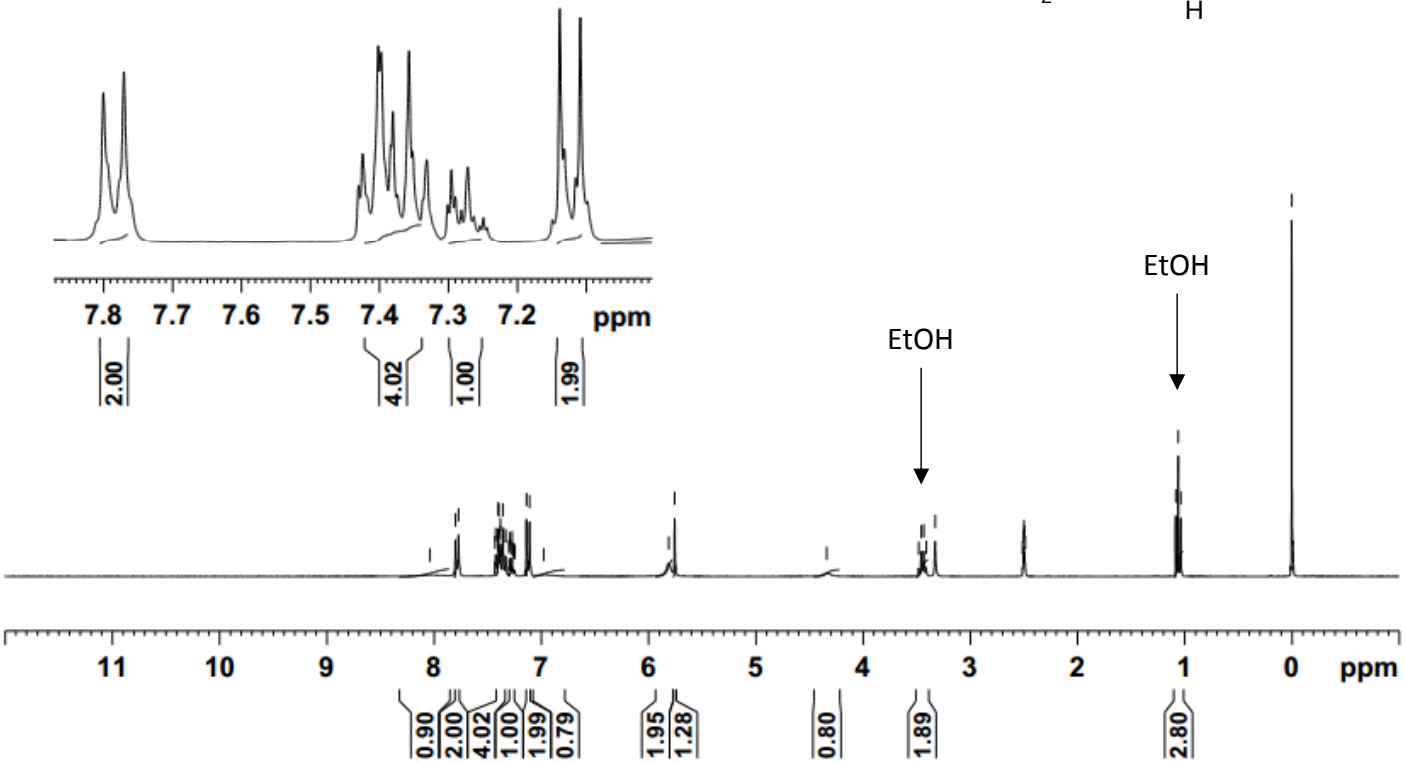
F2 - Processing parameters
SI                    32768
SF              75.4753342 MHz
WDW                      EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

N²-(4-Chlorophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1e · EtOH)



1.06 (t, J=6.99 Hz, 3 H)
3.44 (q, J=6.97 Hz, 2 H)
7.12 (d, J=8.97 Hz, 2 H)
7.78 (d, J=8.94 Hz, 2 H)





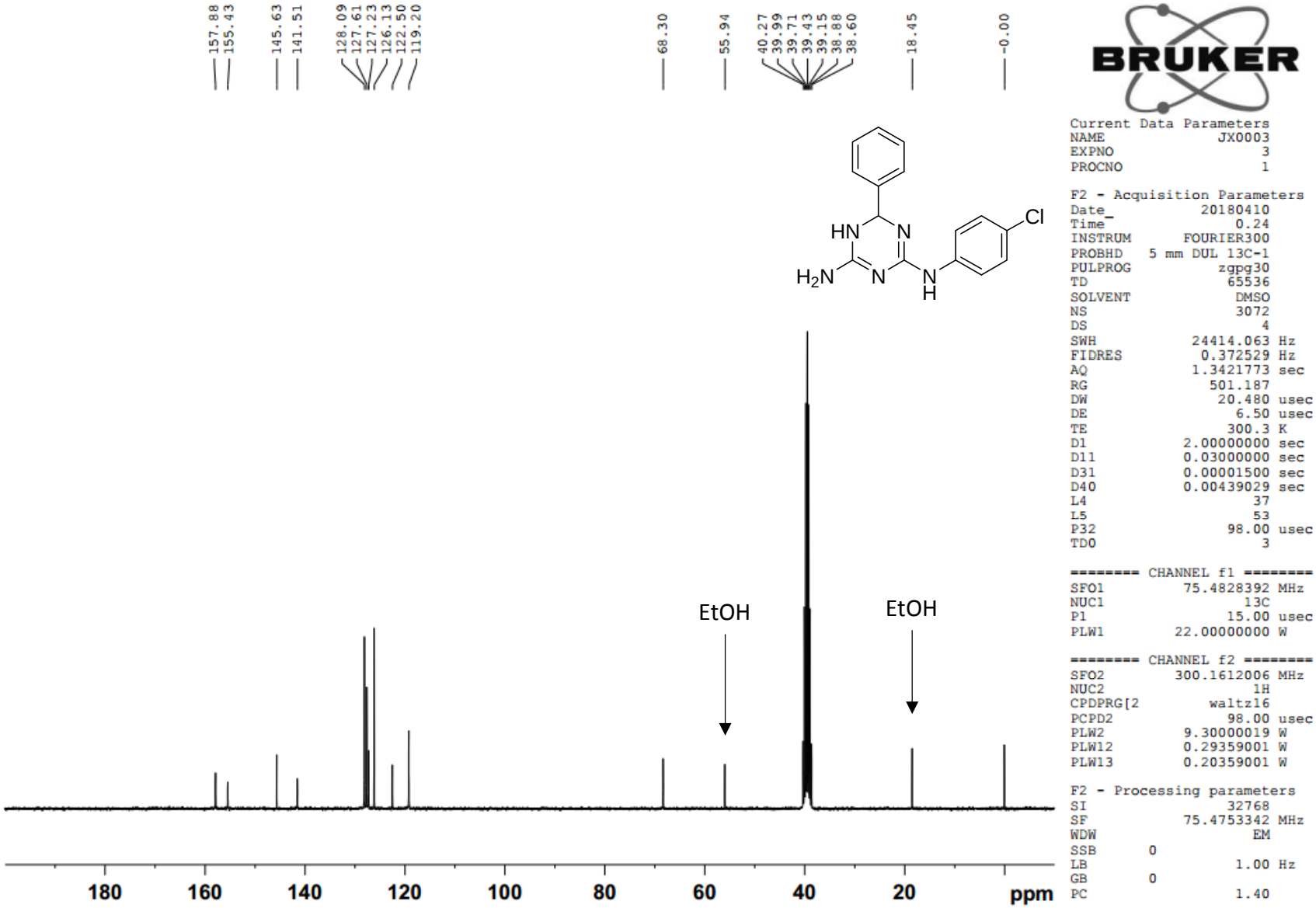

```
Current Data Parameters
NAME                  JX0003
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180404
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                   60.5742
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                300.1600016 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N²-(4-Chlorophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1e · EtOH)



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```
Current Data Parameters
NAME                  JX0003
EXPNO                      3
PROCNO                     1

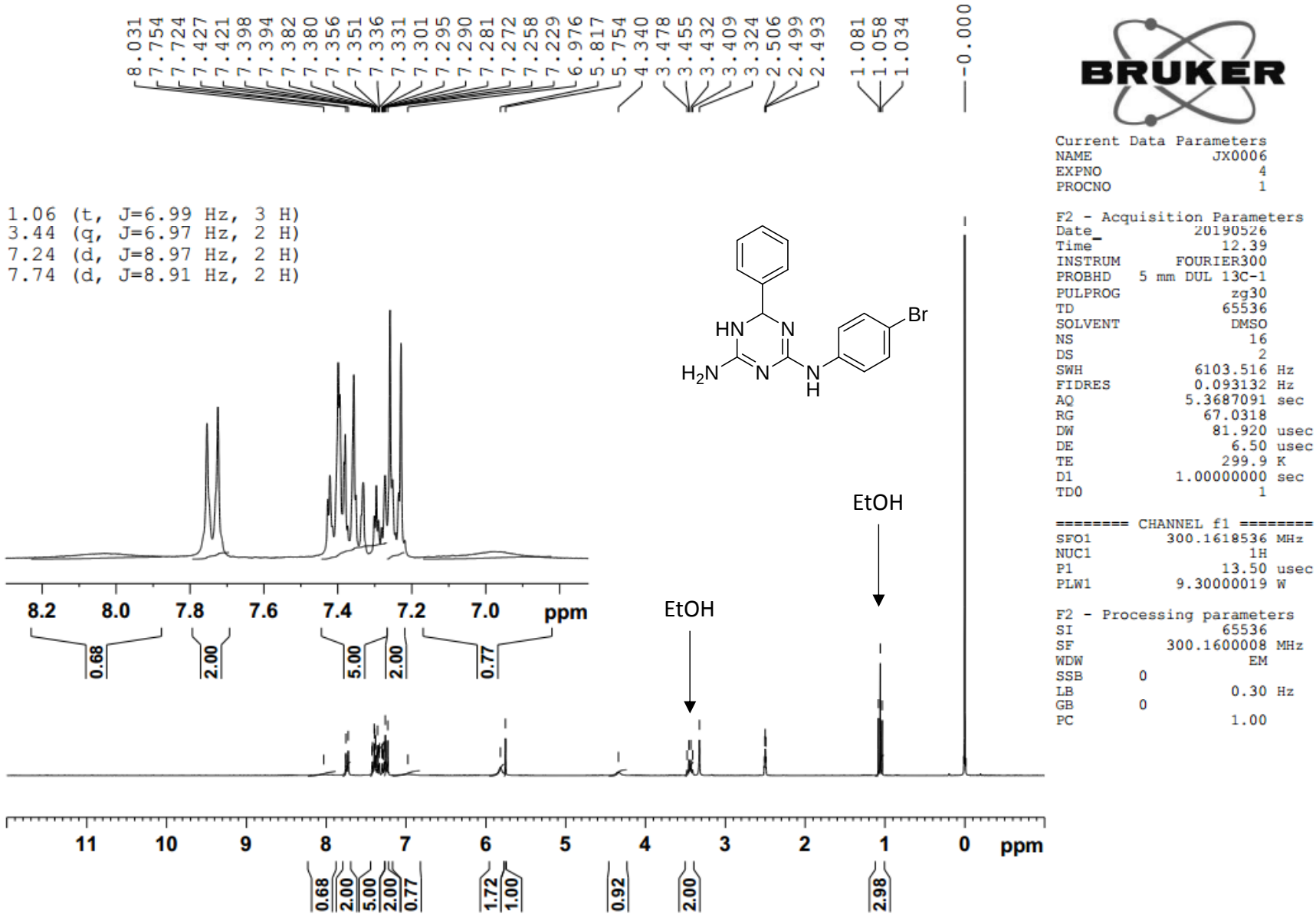
F2 - Acquisition Parameters
Date_              20180410
Time                   0.24
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH              24414.063 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               75.4753342 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

N²-(4-Bromophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1f · EtOH)



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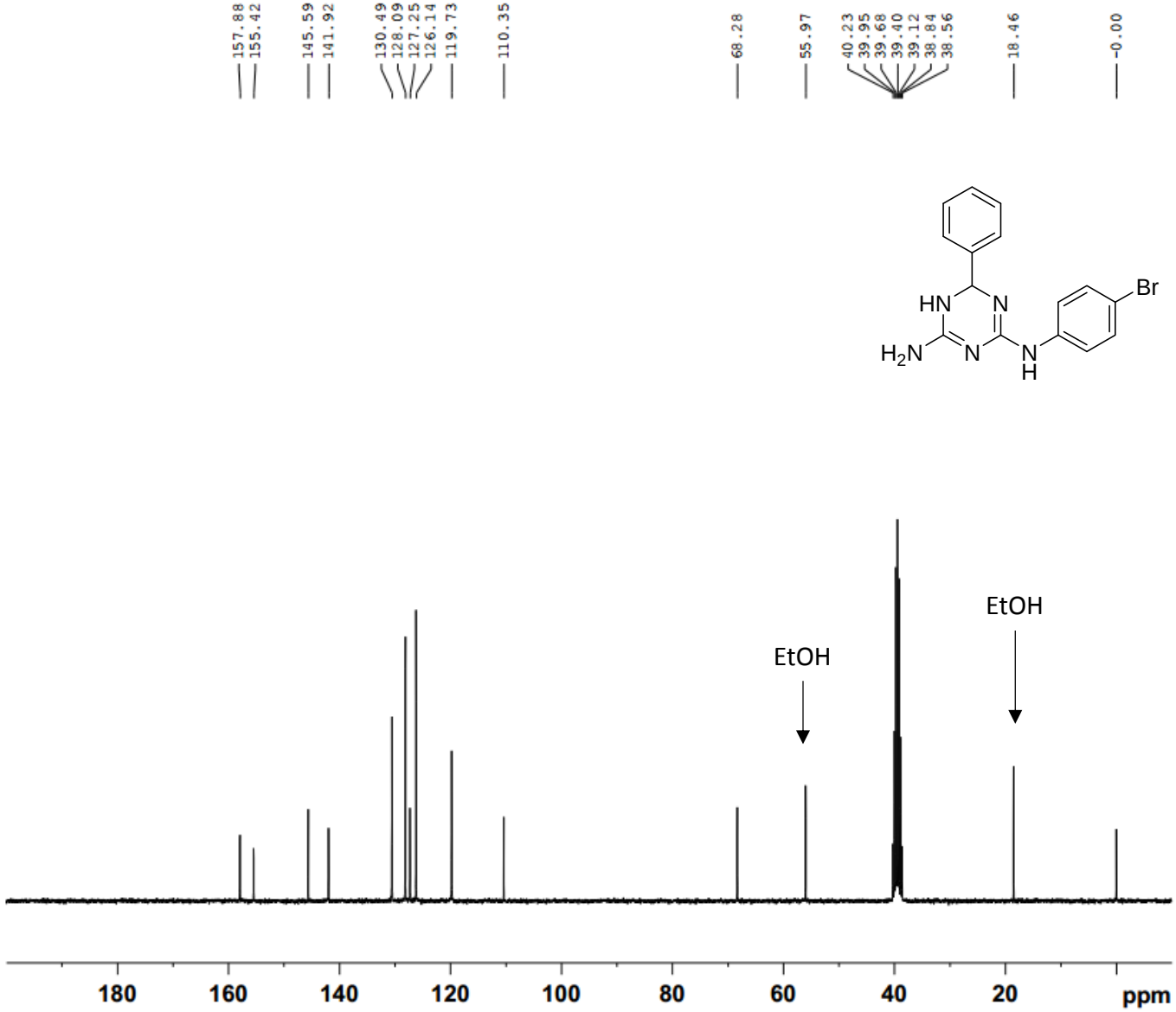
```
Current Data Parameters
NAME                  JX0006
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190526
Time                  12.39
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                  67.0318
DW                  81.920 usec
DE                    6.50 usec
TE                   299.9 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             300.1600008 MHz
WDW                       EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

N²-(4-Bromophenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1f · EtOH)




```
Current Data Parameters
NAME                  JX0006
EXPNO                      5
PROCNO                     1

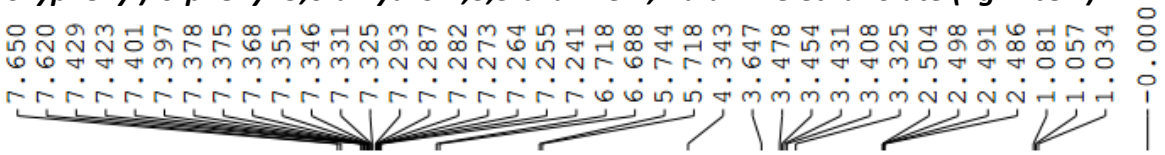
F2 - Acquisition Parameters
Date_              20190528
Time                  15.46
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                       774
DS                         4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
D31                0.00001500 sec
D40                0.00439029 sec
L4                        37
L5                        53
P32                   98.00 usec
TD0                        3

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

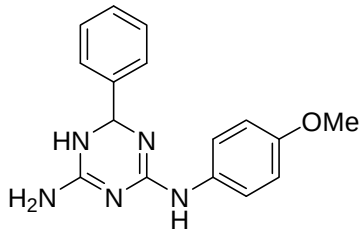
======== CHANNEL f2 ========
SFO2              300.1612006 MHz
NUC2                       1H
CPDPRG[2               waltz16
PCPD2                 98.00 usec
PLW2               9.30000019 W
PLW12              0.29359001 W
PLW13              0.20359001 W

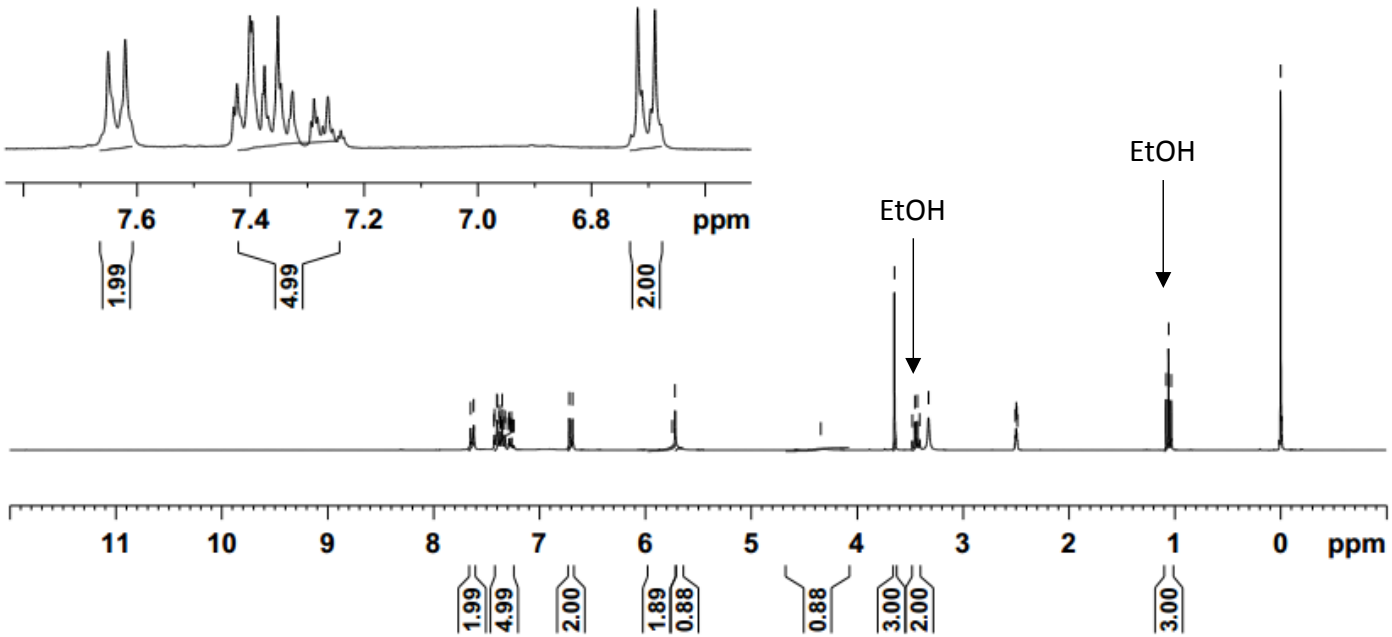
F2 - Processing parameters
SI                        32768
SF                 75.4753342 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

N²-(4-Methoxyphenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1g · EtOH)



1.06 (t, J=6.99 Hz, 3 H)
3.44 (q, J=7.00 Hz, 2 H)
6.70 (d, J=9.12 Hz, 2 H)
7.64 (d, J=9.03 Hz, 2 H)





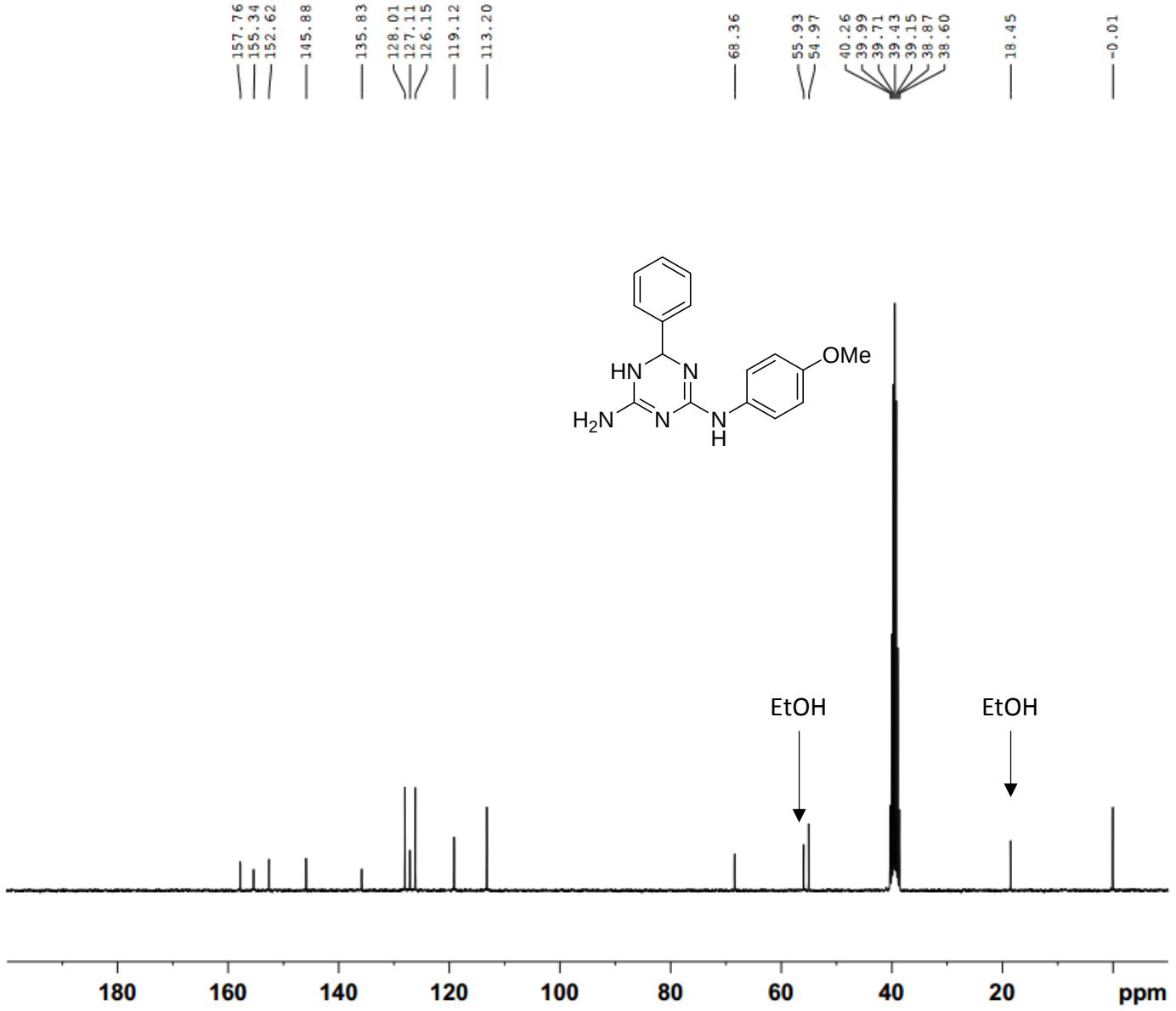

```
Current Data Parameters
NAME                  JX0004
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180516
Time                 16.01
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  58.3985
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             300.1600017 MHz
WDW                    EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```

N²-(4-Methoxyphenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1g · EtOH)




```
Current Data Parameters
NAME                  JX0004
EXPNO                      3
PROCNO                     1

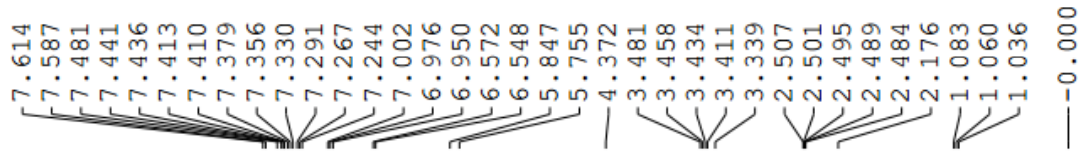
F2 - Acquisition Parameters
Date_              20180516
Time                  22.00
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     4096
DS                        4
SWH              24414.063 Hz
FIDRES               0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.2 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                       4

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

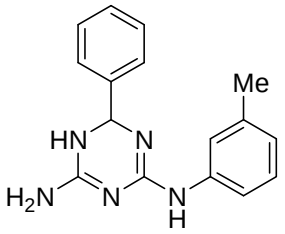
======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

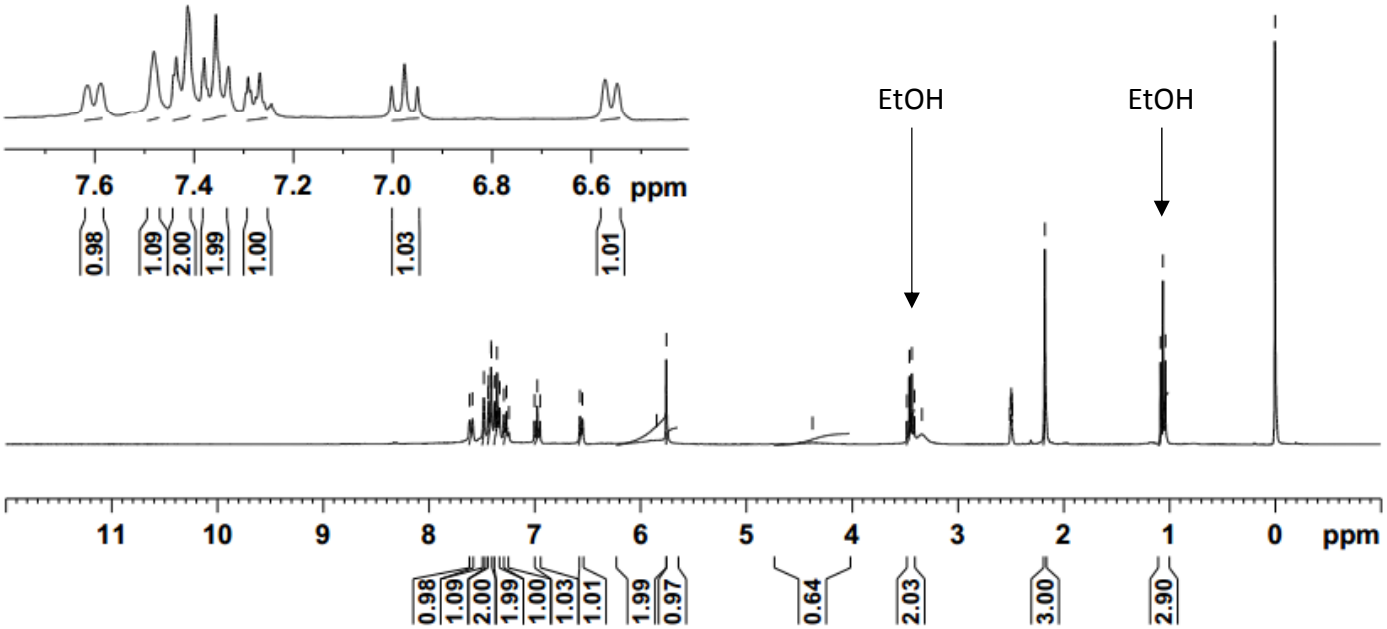
F2 - Processing parameters
SI                    32768
SF              75.4753350 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

N²-(3-Methylphenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1h · EtOH)



1.06 (t, J=6.99 Hz, 3 H)
3.45 (q, J=6.99 Hz, 2 H)
6.56 (d, J=7.35 Hz, 1 H)
6.98 (dd, J=7.79, 7.79 Hz, 1 H)
7.27 (t, J=7.05 Hz, 1 H)
7.36 (dd, J=7.29, 7.29 Hz, 2 H)
7.42 (dd, J=1.16, 8.06 Hz, 2 H)
7.60 (d, J=8.13 Hz, 1 H)





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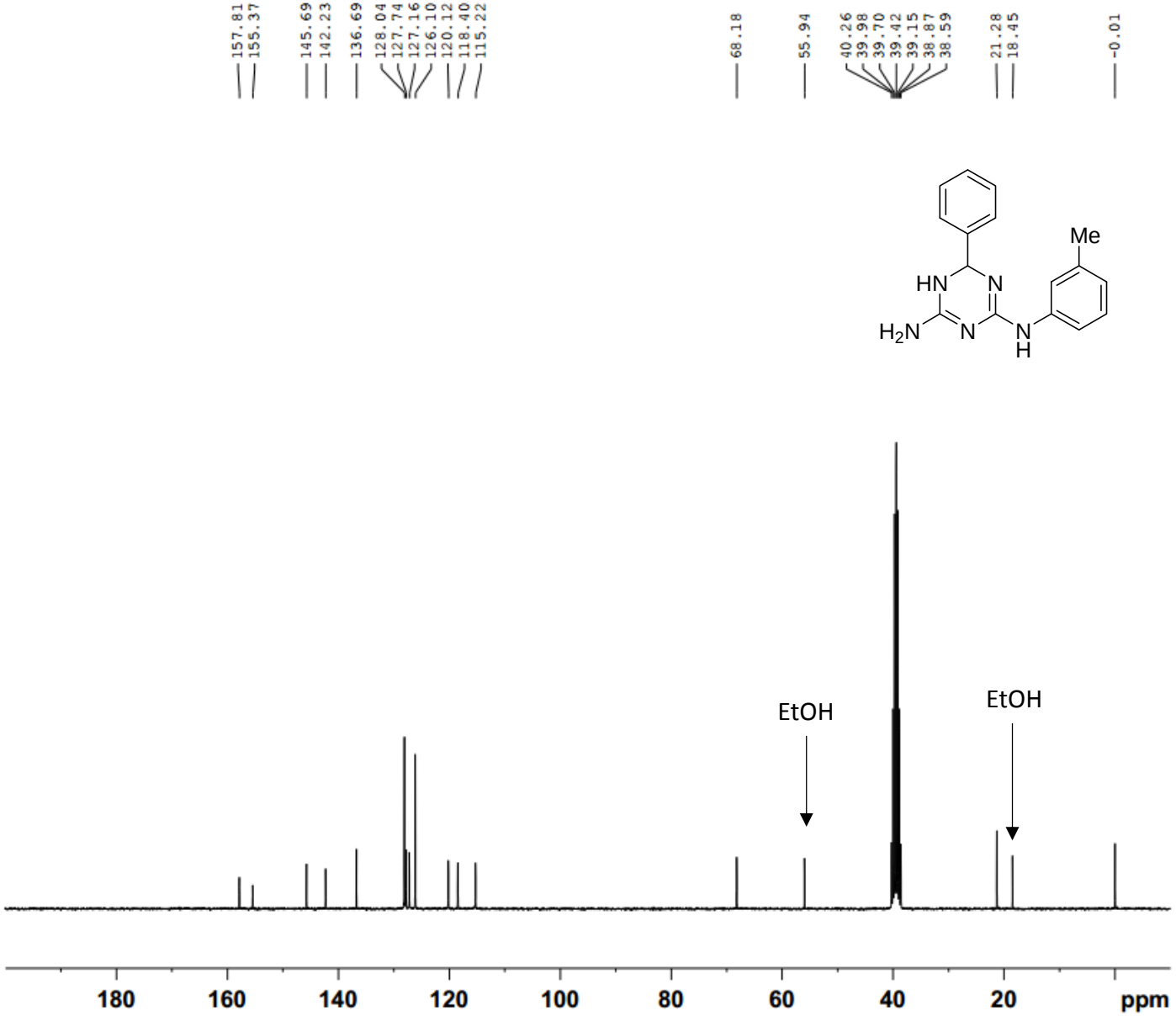
```
Current Data Parameters
NAME                  JX0007
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180513
Time                 14.36
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                    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             300.1600025 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

N^2-(3-Methylphenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1h · EtOH)




```
Current Data Parameters
NAME                  JX0007
EXPNO                      2
PROCNO                     1

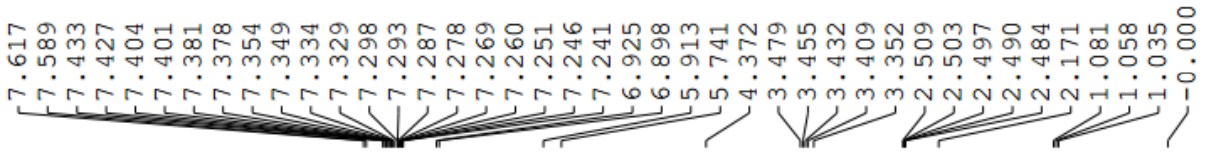
F2 - Acquisition Parameters
Date_              20180513
Time                  18.44
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                      4096
DS                         4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    300.2 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                        4

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

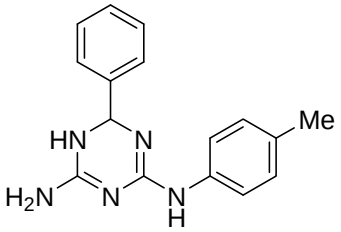
======== CHANNEL f2 ========
SFO2             300.1612006 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 98.00 usec
PLW2               9.30000019 W
PLW12              0.29359001 W
PLW13              0.20359001 W

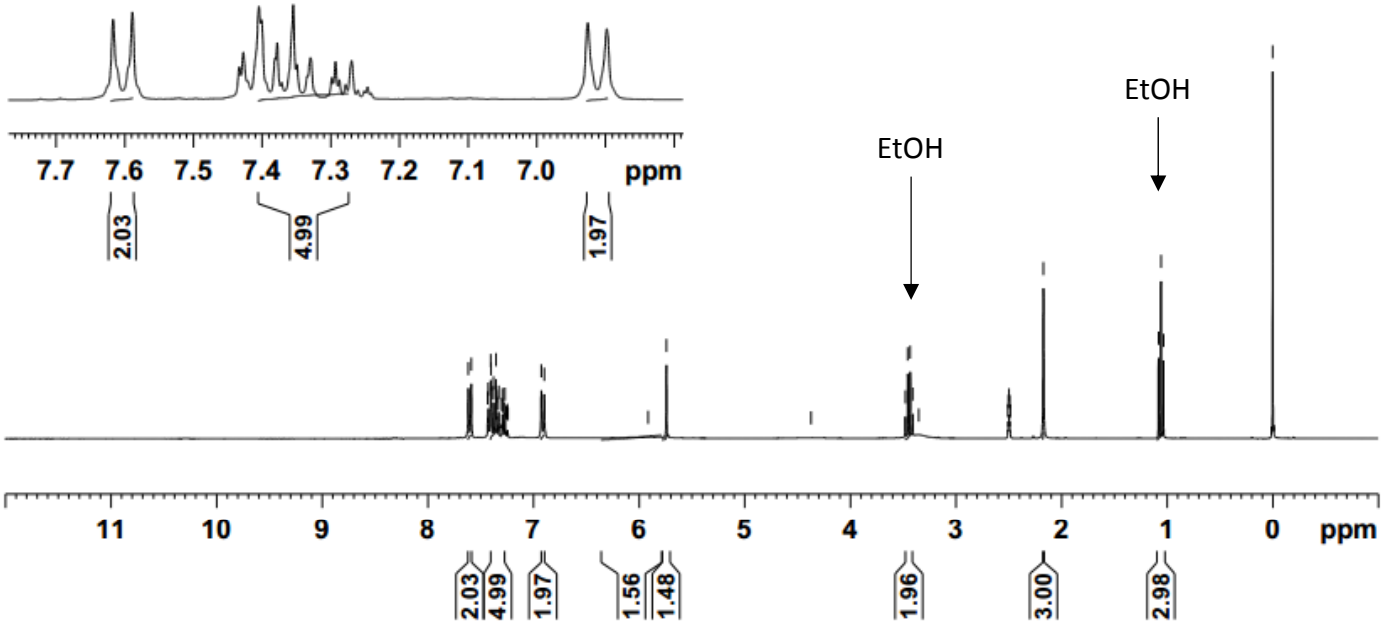
F2 - Processing parameters
SI                        32768
SF                75.4753350 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB          0
PC                     1.40
```

N²-(4-Methylphenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1i · EtOH)



1.06 (t, J=6.99 Hz, 3 H)
3.44 (q, J=6.99 Hz, 2 H)
6.91 (d, J=8.31 Hz, 2 H)
7.60 (d, J=8.43 Hz, 2 H)





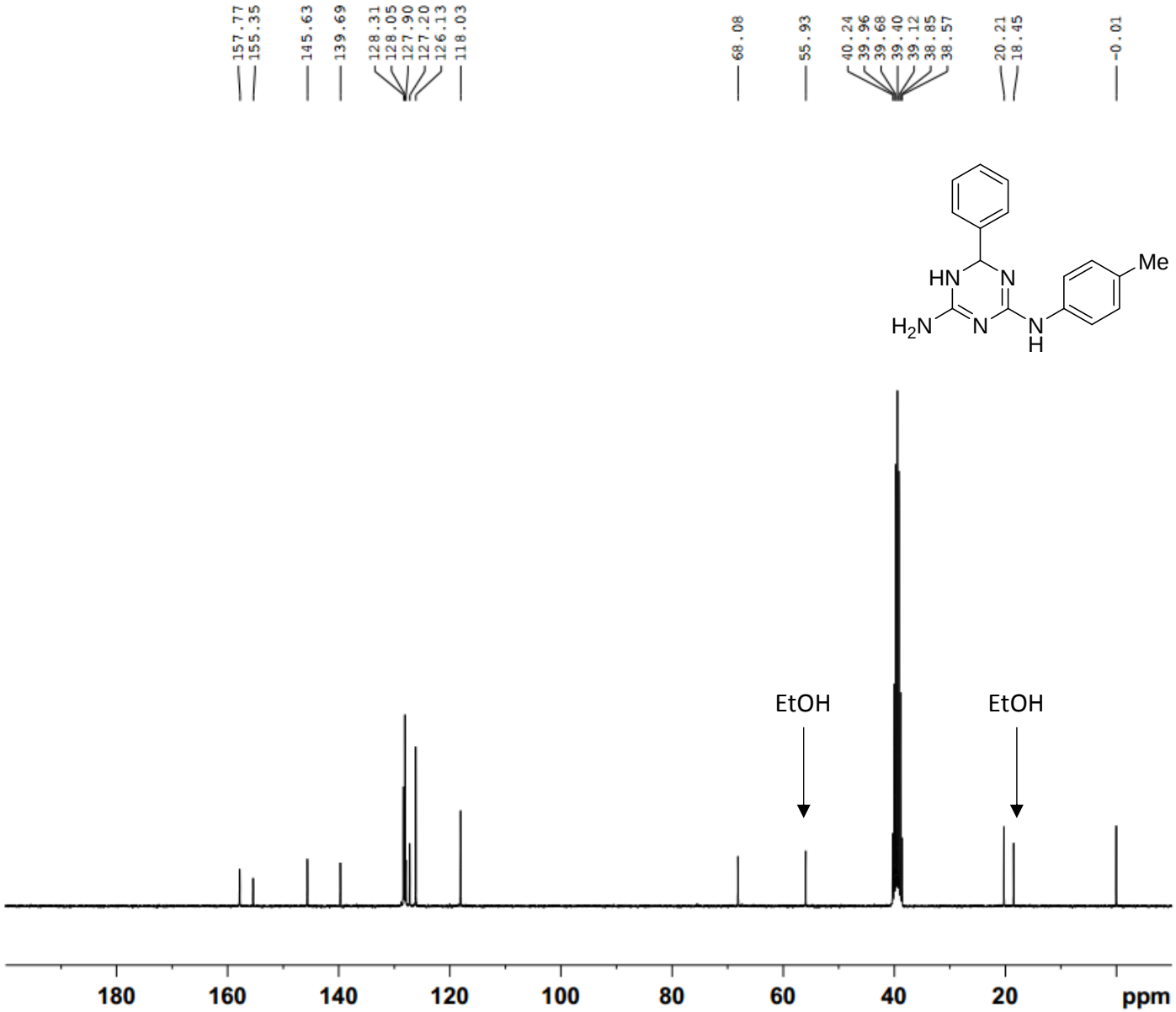
Current Data Parameters
NAME JX0002
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190527
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 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 300.1600016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N²-(4-Methylphenyl)-6-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1i · EtOH)




```
Current Data Parameters
NAME                  JX0002
EXPNO                      4
PROCNO                     1

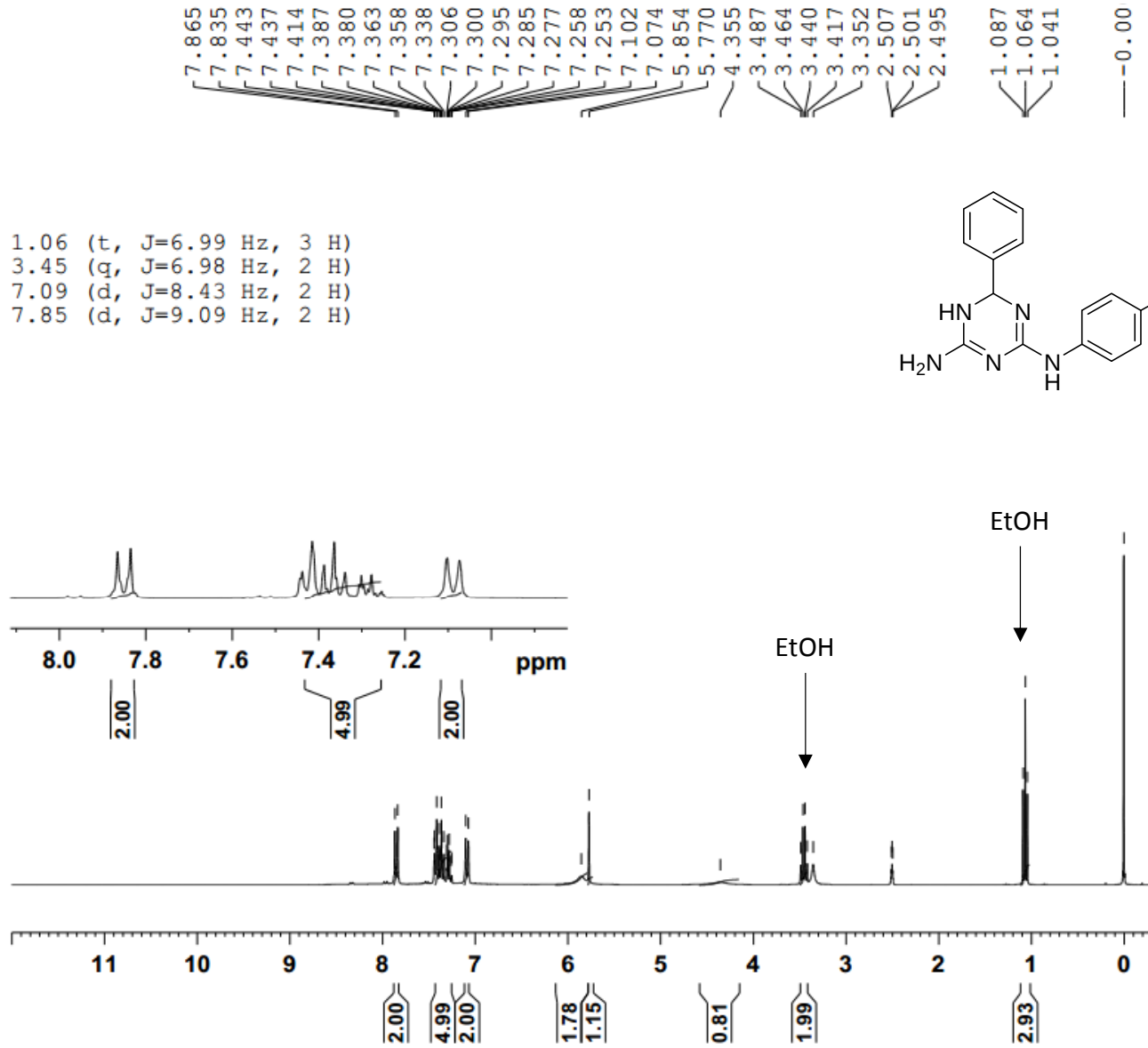
F2 - Acquisition Parameters
Date_              20190528
Time                  11.41
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     4096
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  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                       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              75.4753350 MHz
WDW                       EM
SSB          0
LB                   1.00 Hz
GB           0
PC                    1.40
```

6-Phenyl-N²-(4-(trifluoromethoxy)phenyl)-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1j · EtOH)



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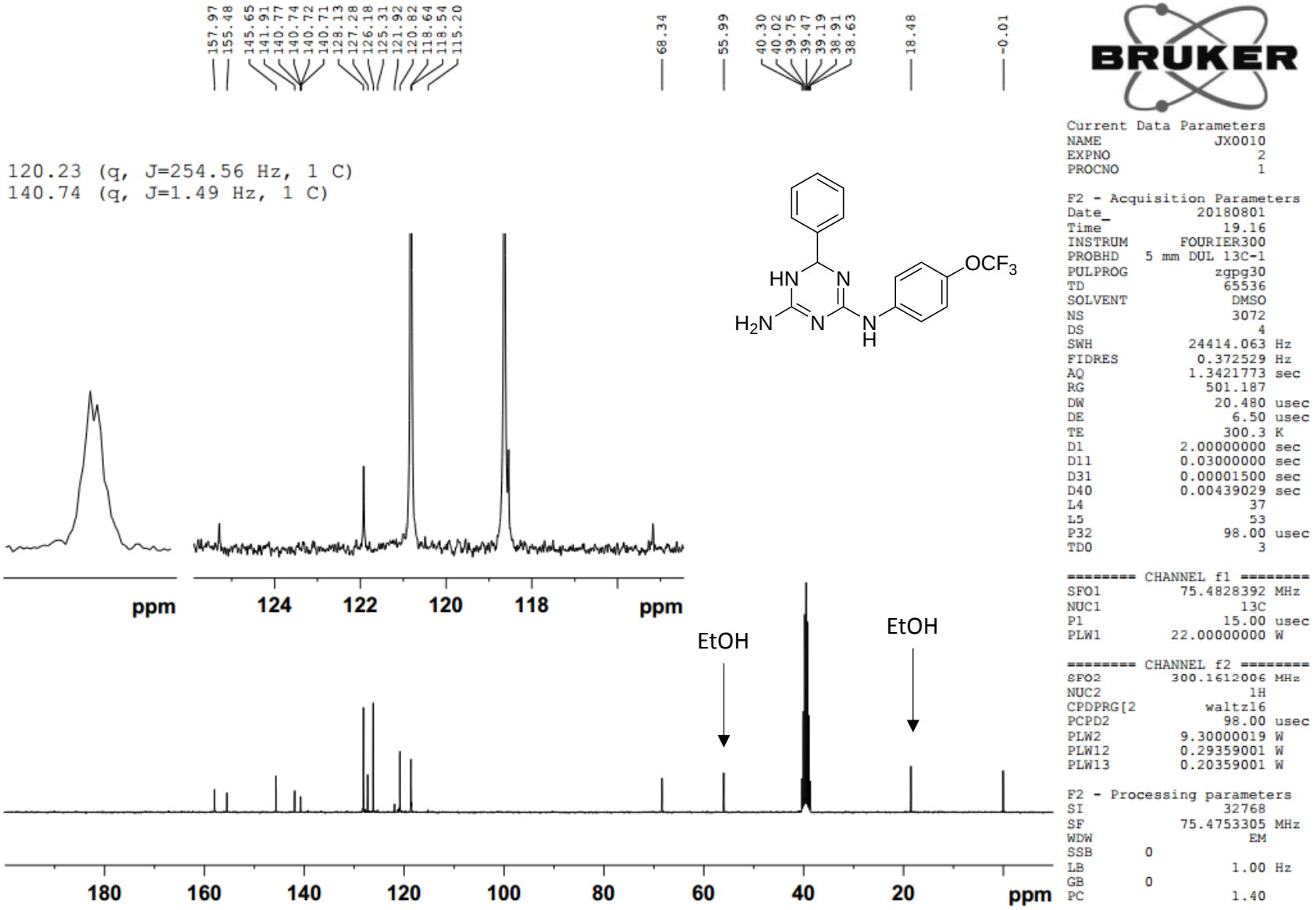
```
Current Data Parameters
NAME                  JX0010
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180801
Time                  16.05
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                    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               300.1600002 MHz
WDW                       EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

6-Phenyl-N²-(4-(trifluoromethoxy)phenyl)-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1j · EtOH)




```
Current Data Parameters
NAME                  JX0010
EXPNO                      2
PROCNO                     1

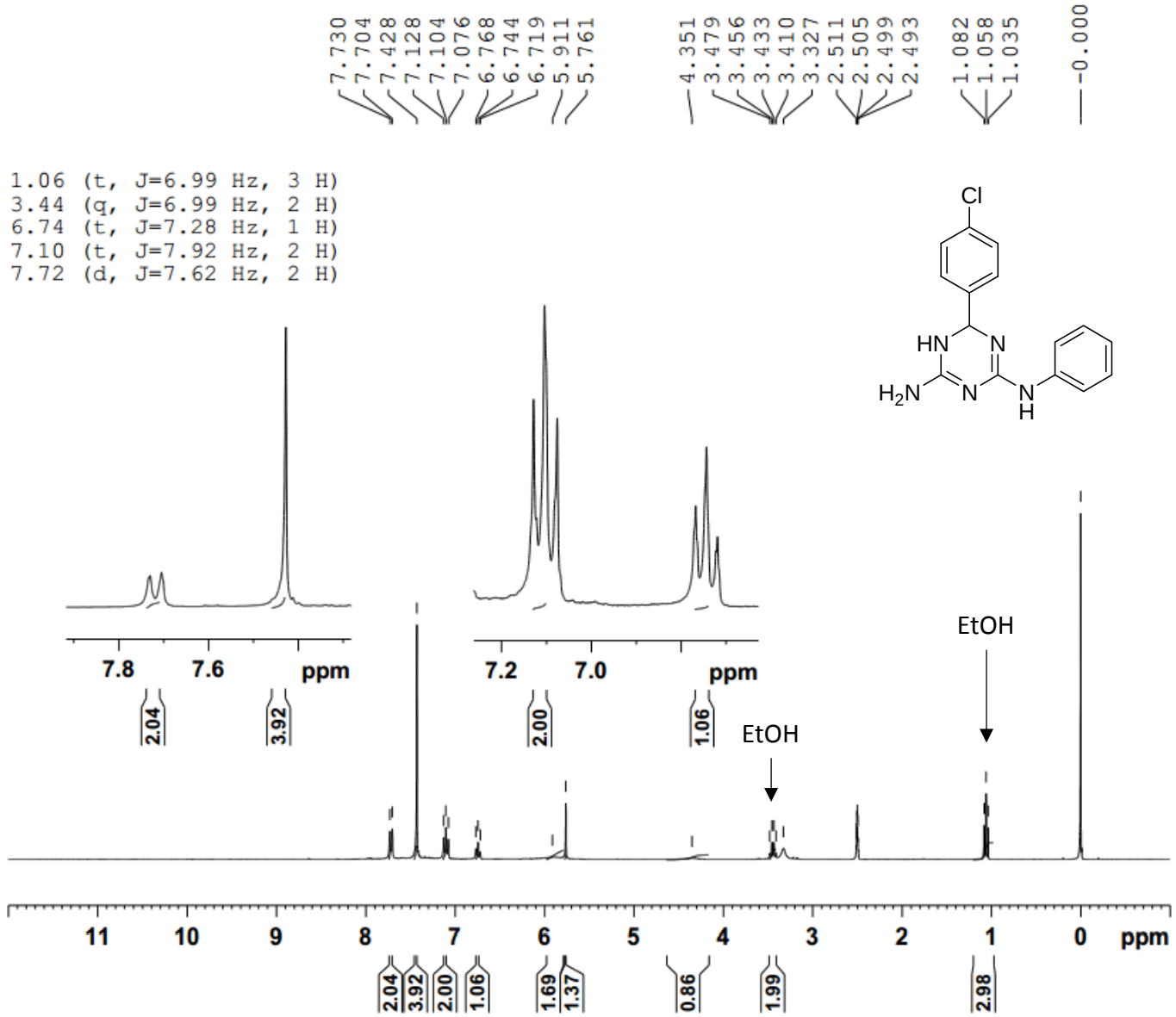
F2 - Acquisition Parameters
Date_              20180801
Time                  19.16
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    3072
DS                       4
SWH              24414.063 Hz
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                    1.00 Hz
GB        0
PC                    1.40
```

6-(4-Chlorophenyl)-N²-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1k · EtOH)



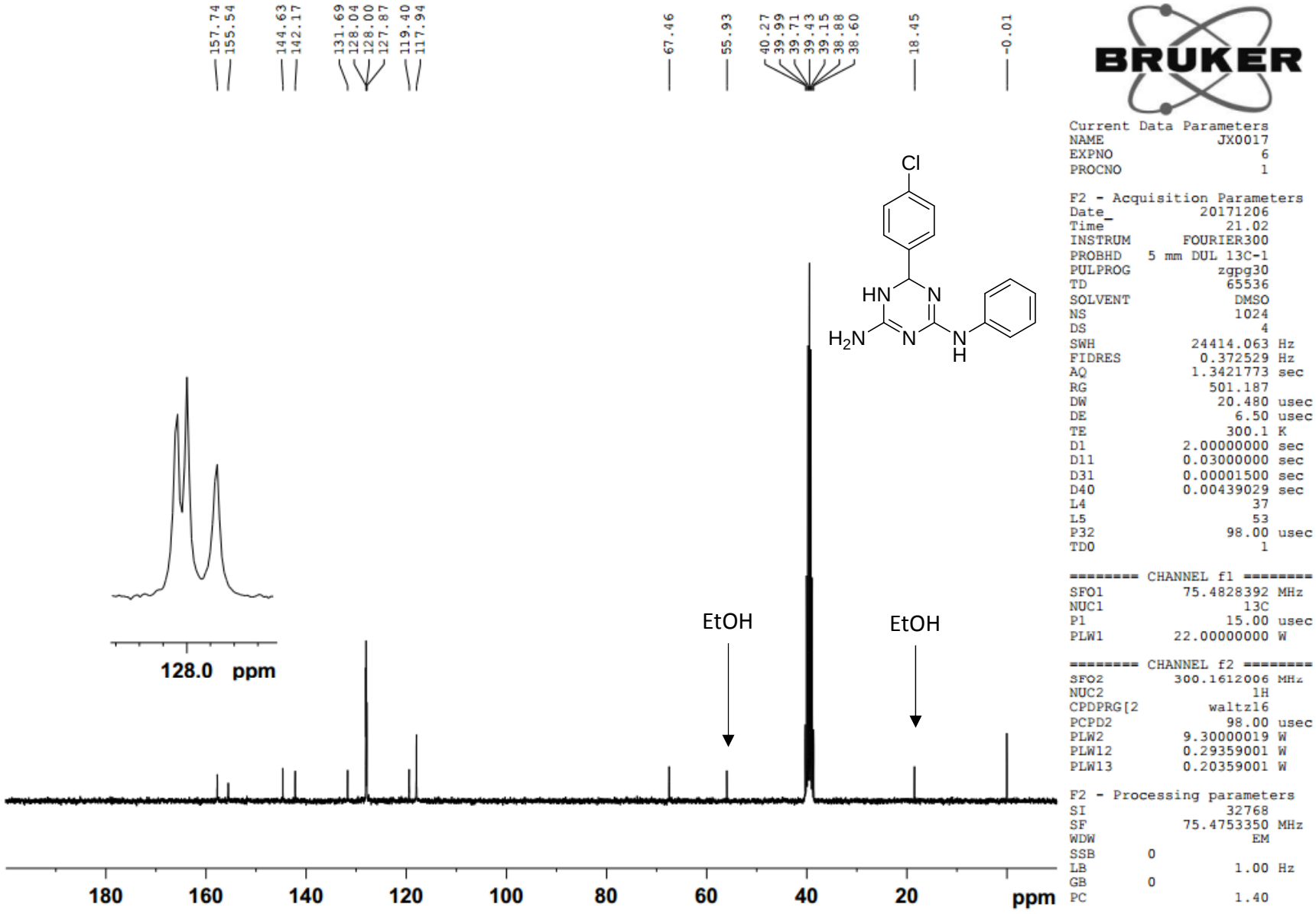

```
Current Data Parameters
NAME                  JX0017
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171206
Time                  11.16
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                   75.1903
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               300.1600009 MHz
WDW                         EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

6-(4-Chlorophenyl)-N²-phenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine ethanolate (1k · EtOH)



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```
Current Data Parameters
NAME                  JX0017
EXPNO                      6
PROCNO                     1

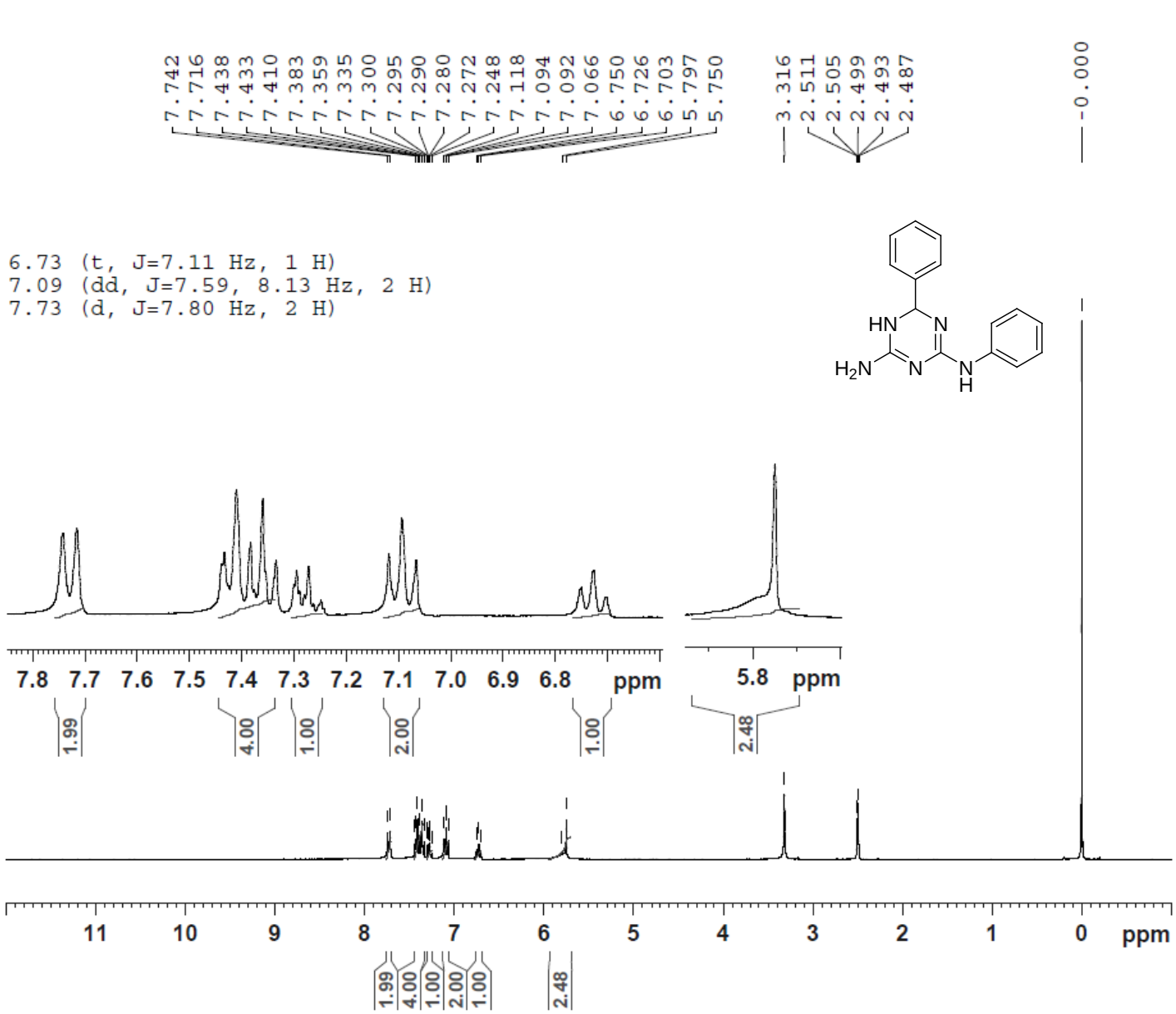
F2 - Acquisition Parameters
Date_              20171206
Time                 21.02
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH              24414.063 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              75.4753350 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

N²,6-Diphenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine (1a)



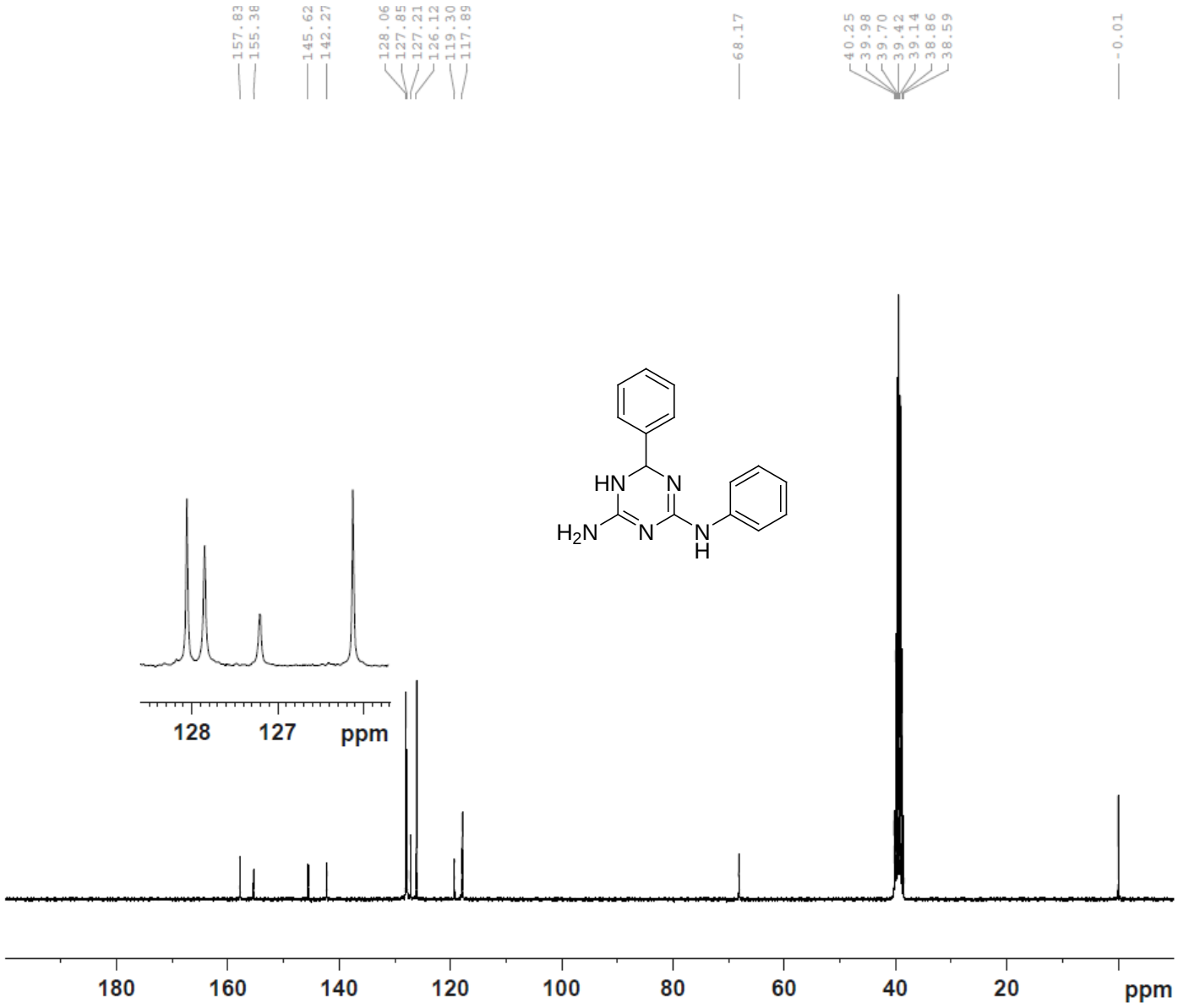

```
Current Data Parameters
NAME                  JX00001
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20191112
Time                    11.22
INSTRUM            FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                 zg30
TD                     65536
SOLVENT             Dioxane
NS                         16
DS                          2
SWH                 6103.516 Hz
FIDRES              0.093132 Hz
AQ                  5.3687091 sec
RG                     53.813
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               300.1603126 MHz
WDW                           EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

N²,6-Diphenyl-5,6-dihydro-1,3,5-triazine-2,4-diamine (1a)



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```
Current Data Parameters
NAME                  JX0001
EXPNO                      7
PROCNO                     1

F2 - Acquisition Parameters
Date_              20191111
Time                  16.07
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                  300.1 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                       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               75.4753357 MHz
WDW                       EM
SSB          0
LB                   1.00 Hz
GB           0
PC                   1.40
```