

Supplementary Material

A novel one-pot three-component synthesis of 4-aryl-6-alkylamino/piperidinyl-1,3,5-triazine-2-amines under controlled microwave irradiation

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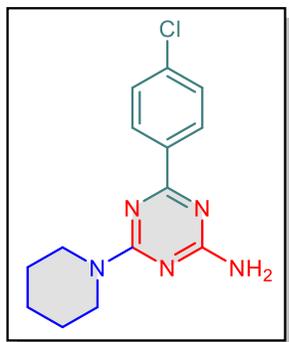
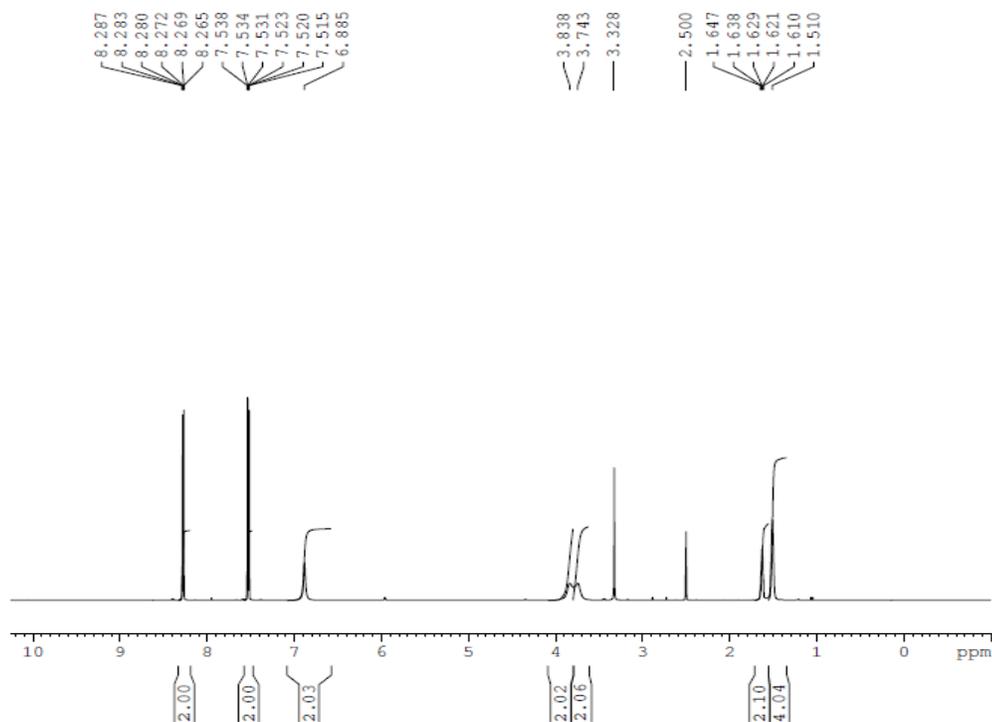
Email: kusadek@yahoo.com

Table of Contents

-Spectral Data of the Products.....	S2
4-(4-Chlorophenyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7a).....	S2
4-Phenyl-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7b).....	S4
4-(4-Tolyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7c).....	S6
4-(4-Methoxyphenyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7d).....	S8
4-(2-Thienyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7e).....	S9
6-Phenyl- <i>N</i> ² , <i>N</i> ² -dimethyl-1,3,5-triazine-2,4-diamine (8a).....	S10
6-(4-Methoxyphenyl)- <i>N</i> ² , <i>N</i> ² -dimethyl-1,3,5-triazine-2,4-diamine (8b).....	S11
6-(3-Chlorophenyl)- <i>N</i> ² , <i>N</i> ² -dimethyl-1,3,5-triazine-2,4-diamine (8c).....	S13
6-Phenyl- <i>N</i> ² -butyl-1,3,5-triazine-2,4-diamine (9a).....	S15
6-(4-tolyl)- <i>N</i> ² -butyl-1,3,5-triazine-2,4-diamine (9b).....	S16
6-(4-Methoxyphenyl)- <i>N</i> ² -1,3,5-triazine-2,4-diamine (9c).....	S18
6-(3-Nitrophenyl)- <i>N</i> ² -butyl-1,3,5-triazine-2,4-diamine (9d).....	S19

- Spectral Data of the Products

4-(4-Chlorophenyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7a).

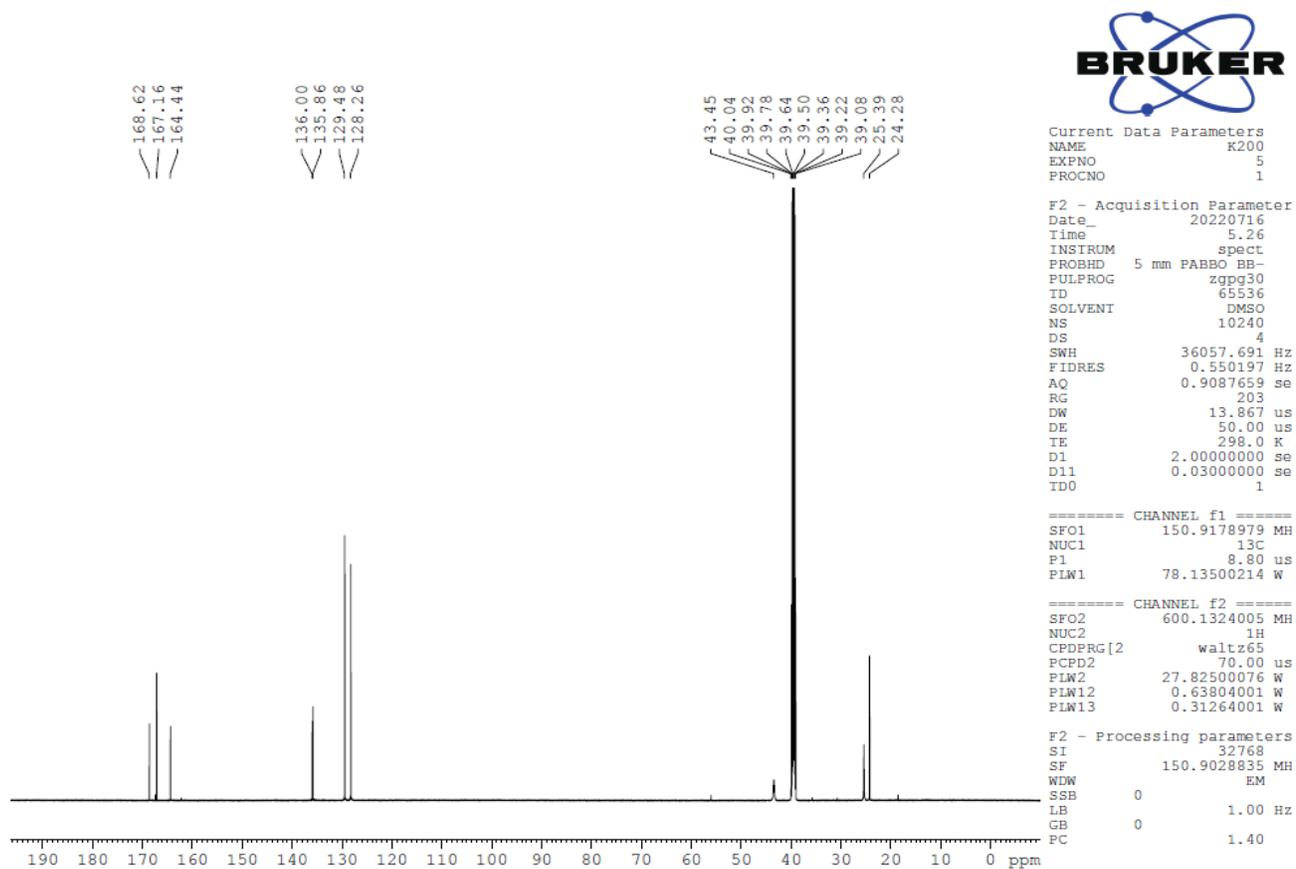
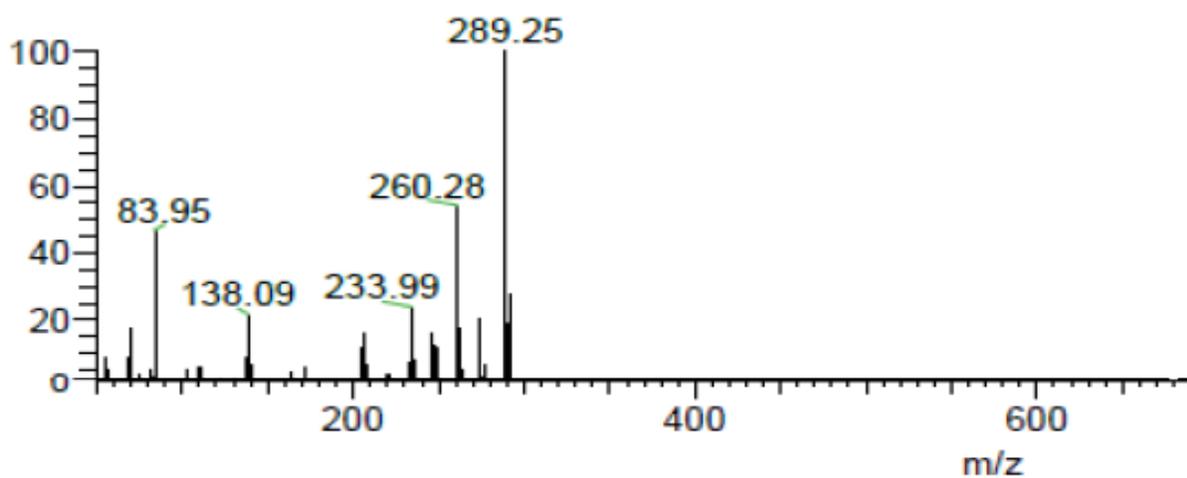
**7a** ^1H NMR (400 MHz, $\text{DMSO-}d_6$):

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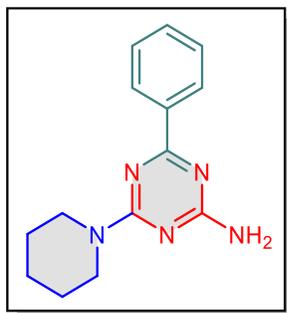
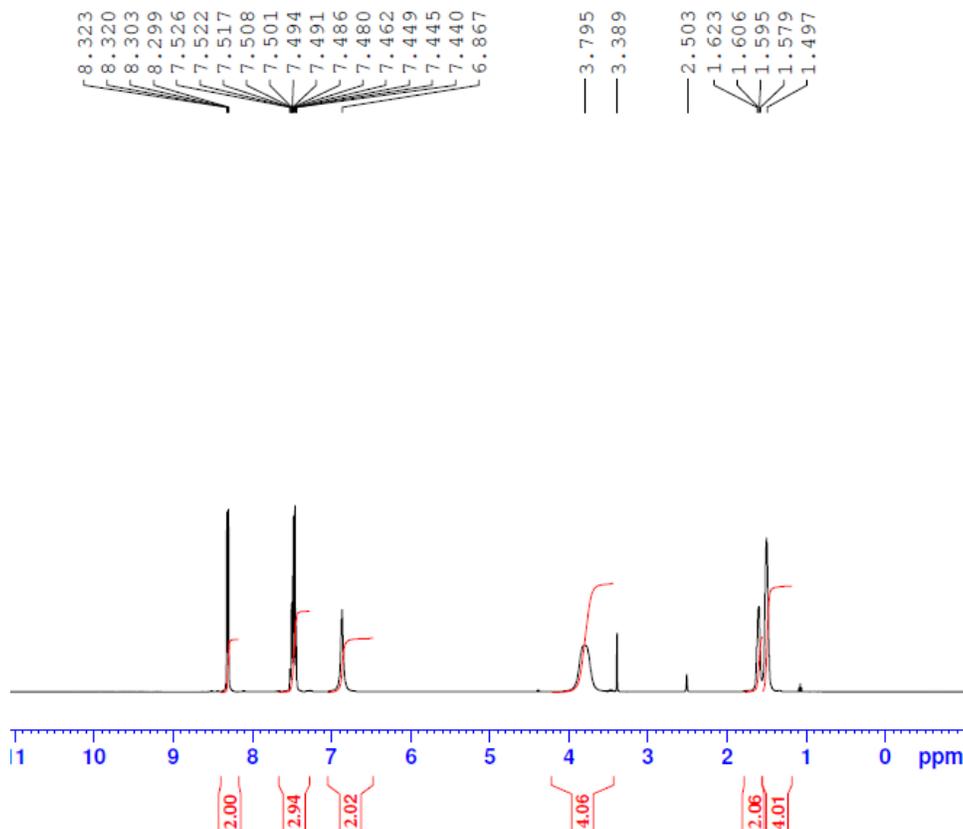
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 DS 2
 SWH 12335.526 H:
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 AQ 2.6563926 s:
 RG 203
 DW 40.533 u:
 DE 20.00 u:
 TE 298.0 K
 D1 1.0000000 s:
 TD0 1

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 NUC1 1H
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F2 - Processing parameters:
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7a ^{13}C NMR (100 MHz, DMSO- d_6):**7a** Mass spectrum

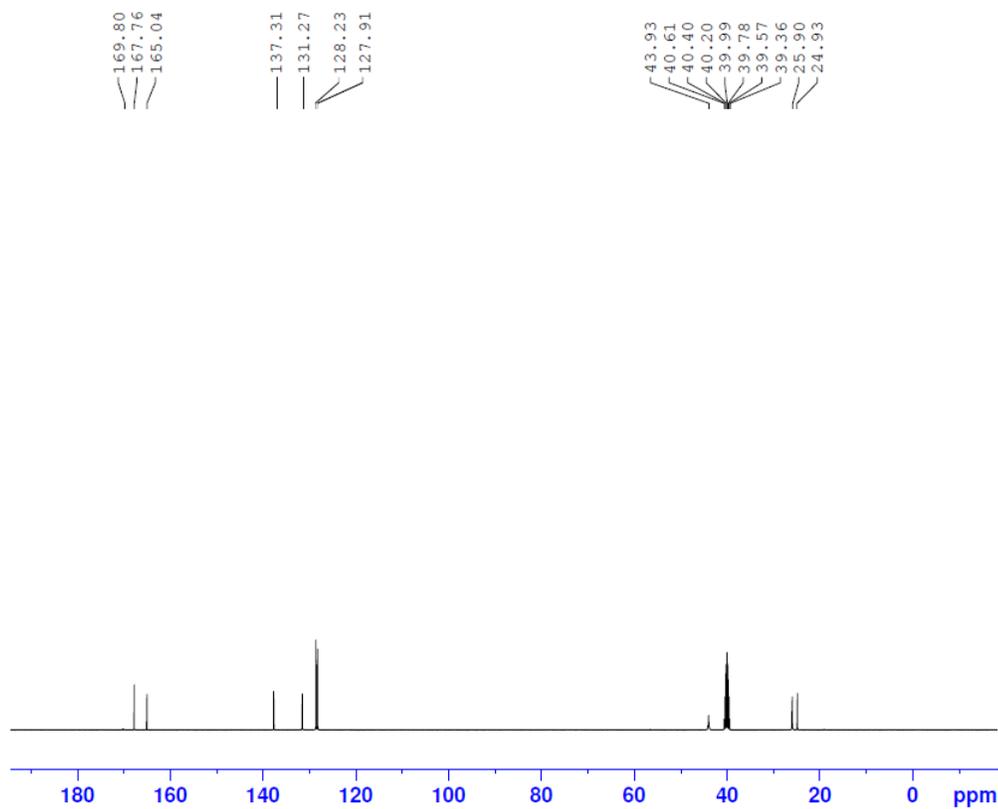
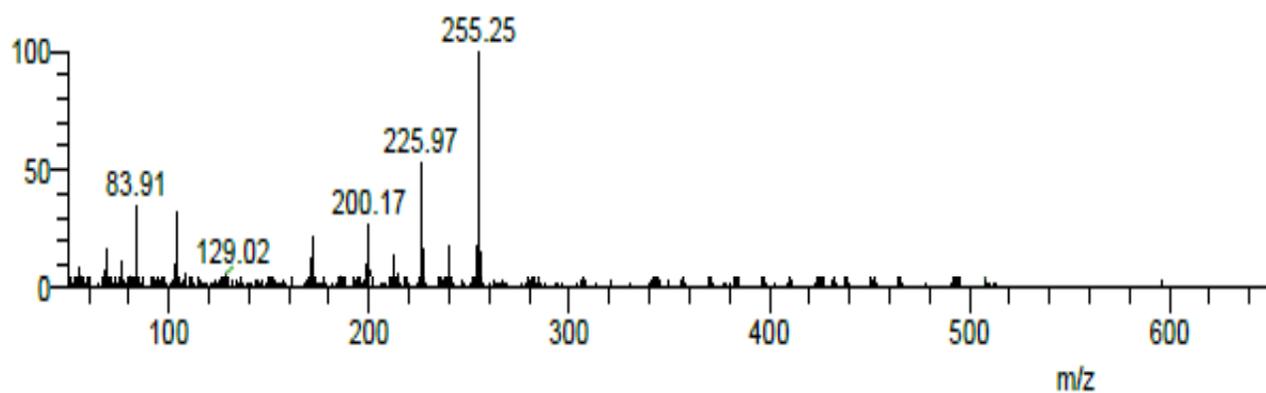
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**7b** ^1H NMR (400 MHz, $\text{DMSO-}d_6$):

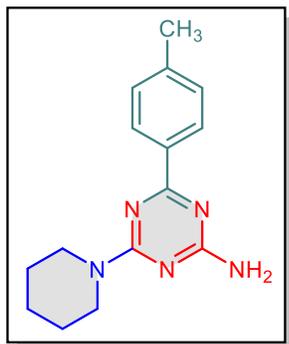
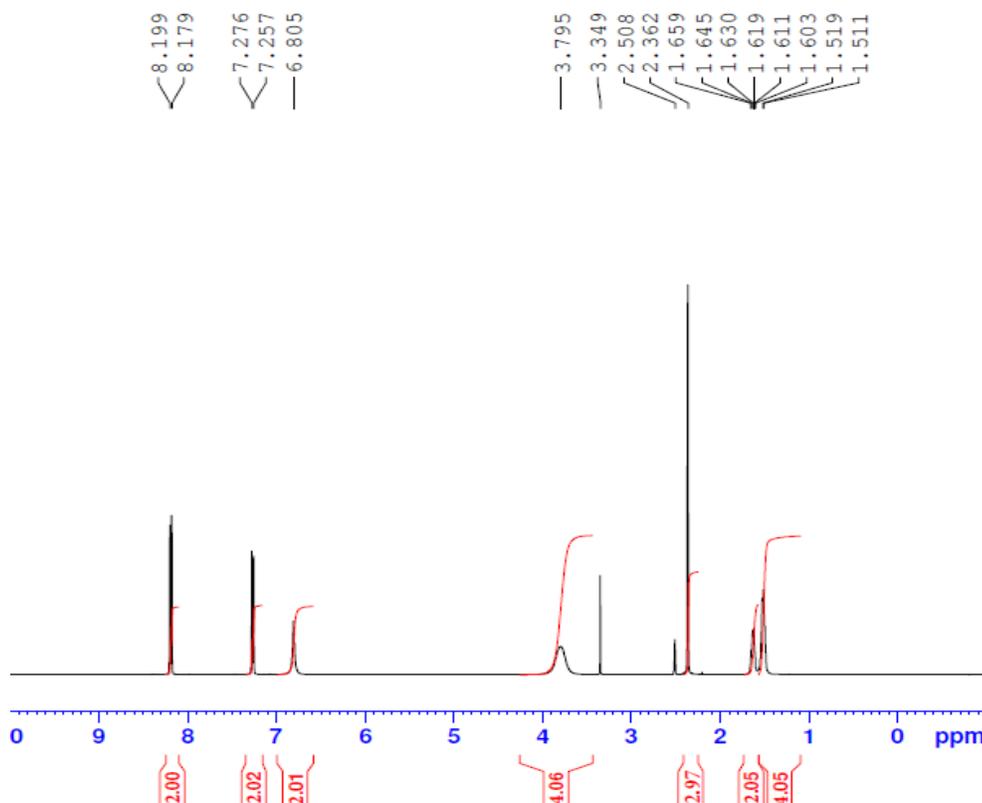
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 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 57
 DW 61.000 usec
 DE 12.86 usec
 TE 296.6 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1324708 MHz
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 P1 14.00 usec
 PLW1 17.11499977 W

F2 - Processing parameters
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7b ^{13}C NMR (100 MHz, DMSO- d_6):**7b** Mass spectrum

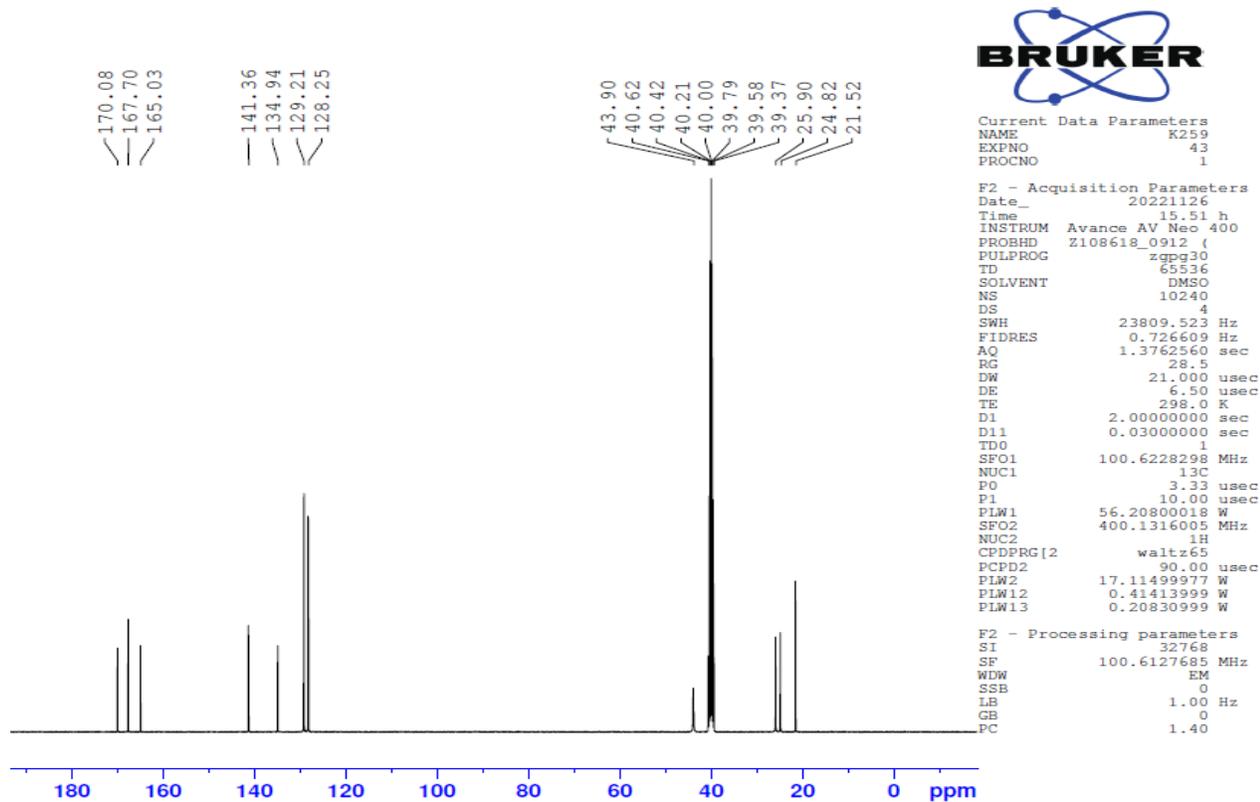
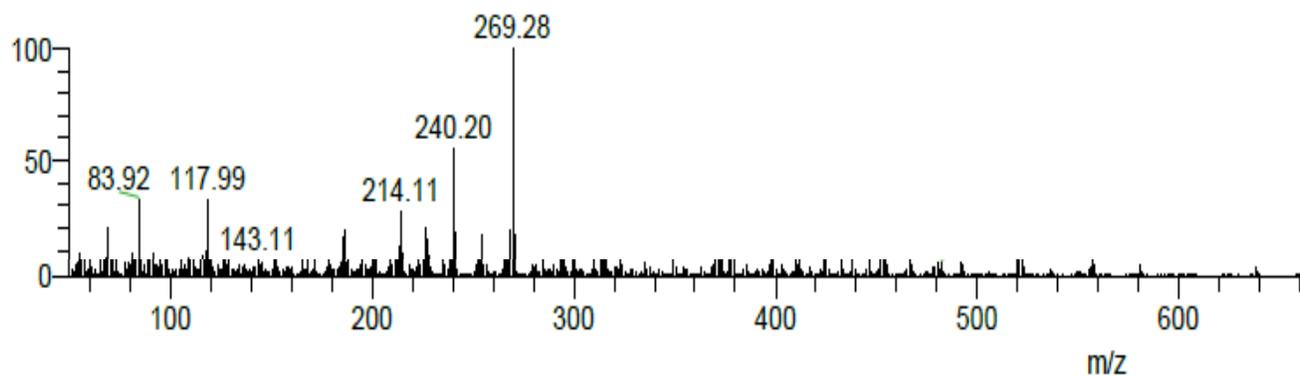
4-(4-Tolyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7c).

7c ¹H NMR (400 MHz, DMSO-d₆):

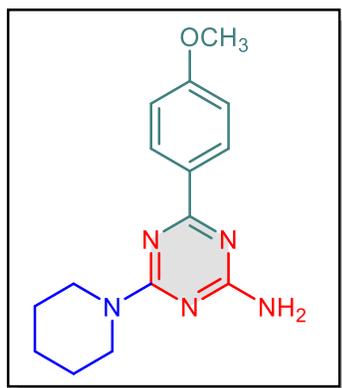
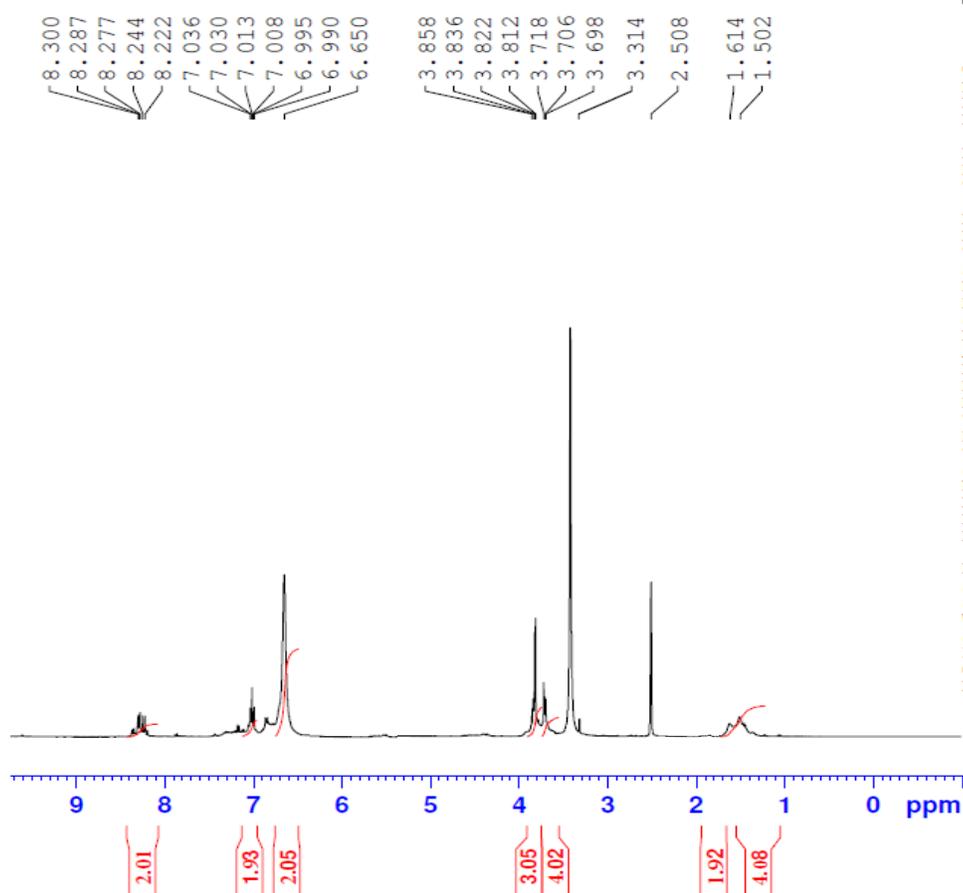
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 DS 2
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 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 12.86 usec
 TE 296.6 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 4.67 usec
 P1 14.00 usec
 PLW1 17.11499977 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7c ^{13}C NMR (100 MHz, DMSO- d_6):**7c** Mass spectrum

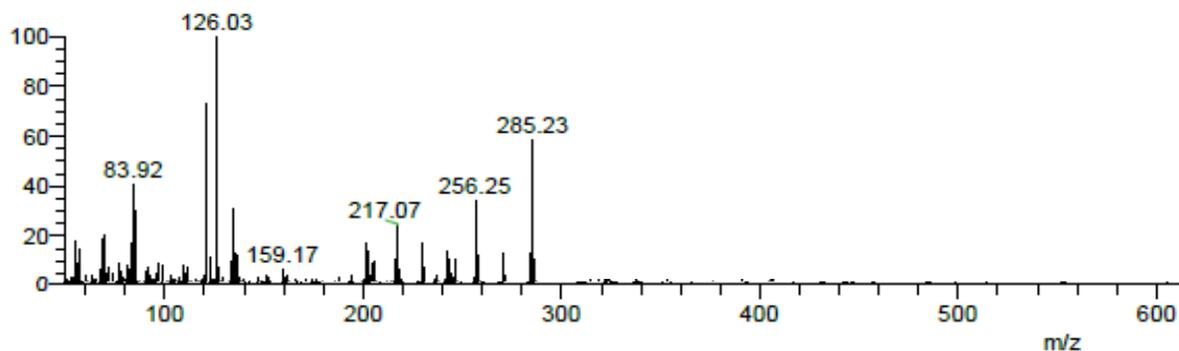
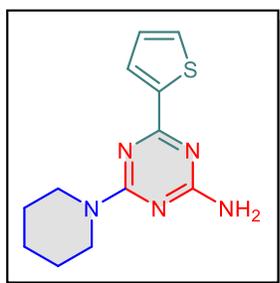
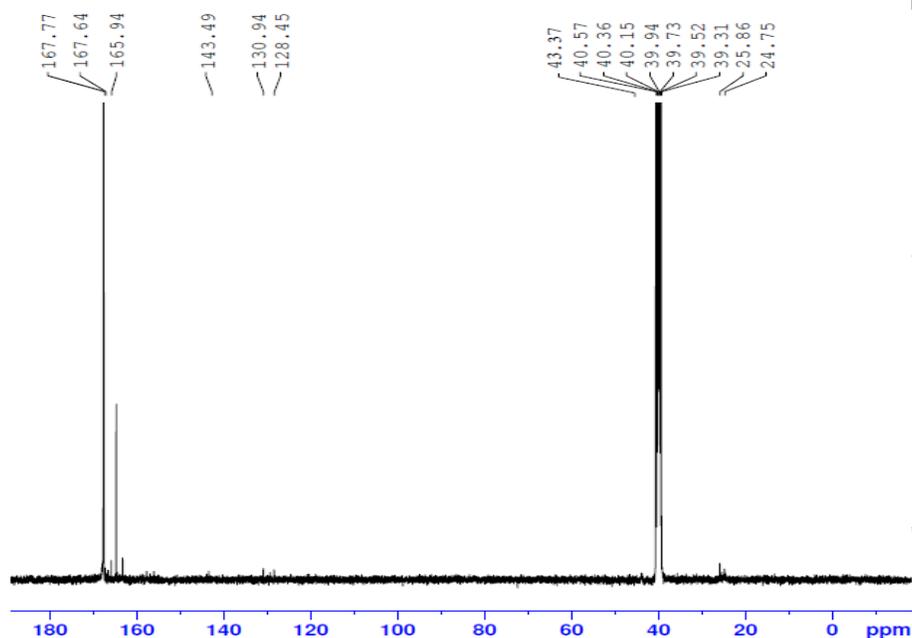
4-(4-Methoxyphenyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7d).

**7d ¹H NMR (400 MHz, DMSO-d₆):**

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 EXPNO 1
 PROCNO 1

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 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 12.86 usec
 TE 297.0 K
 D1 1.0000000 sec
 TD0 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P0 4.67 usec
 P1 14.00 usec
 PLW1 17.11499977 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7d Mass spectrum**4-(2-Thienyl)-6-(piperidine-1-yl)-1,3,5-triazine-2-amine (7e).****7e ¹³C NMR (100 MHz, DMSO-d₆):**

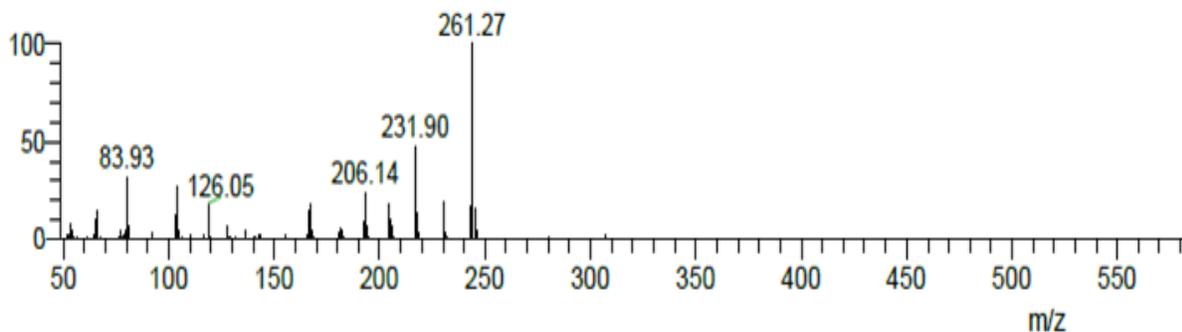
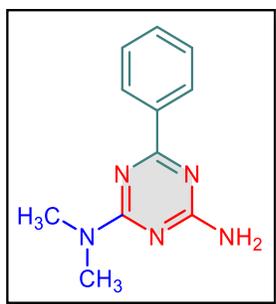
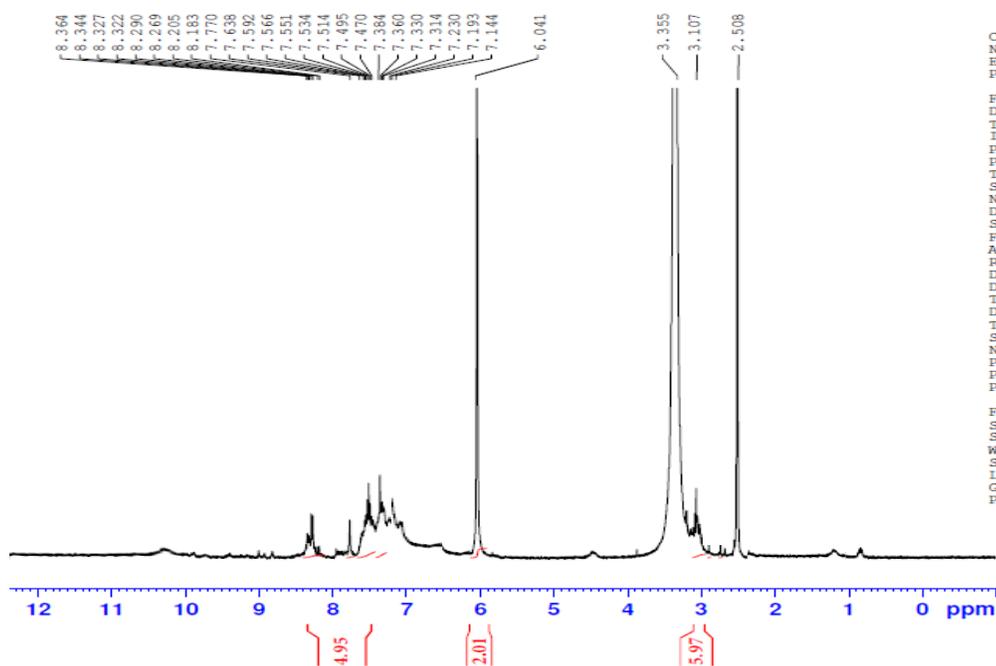
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PULPROG  zgpg30
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FIDRES   0.726609 Hz
AQ       1.3762560 sec
RG       32
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DE       6.50 usec
TE       298.4 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
PQ       3.33 usec
P1       10.00 usec
PLW1     56.20800018 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz65
PCPD2    90.00 usec
PLM2     17.11499977 W
PLW12    0.41413999 W
PLW13    0.20830999 W

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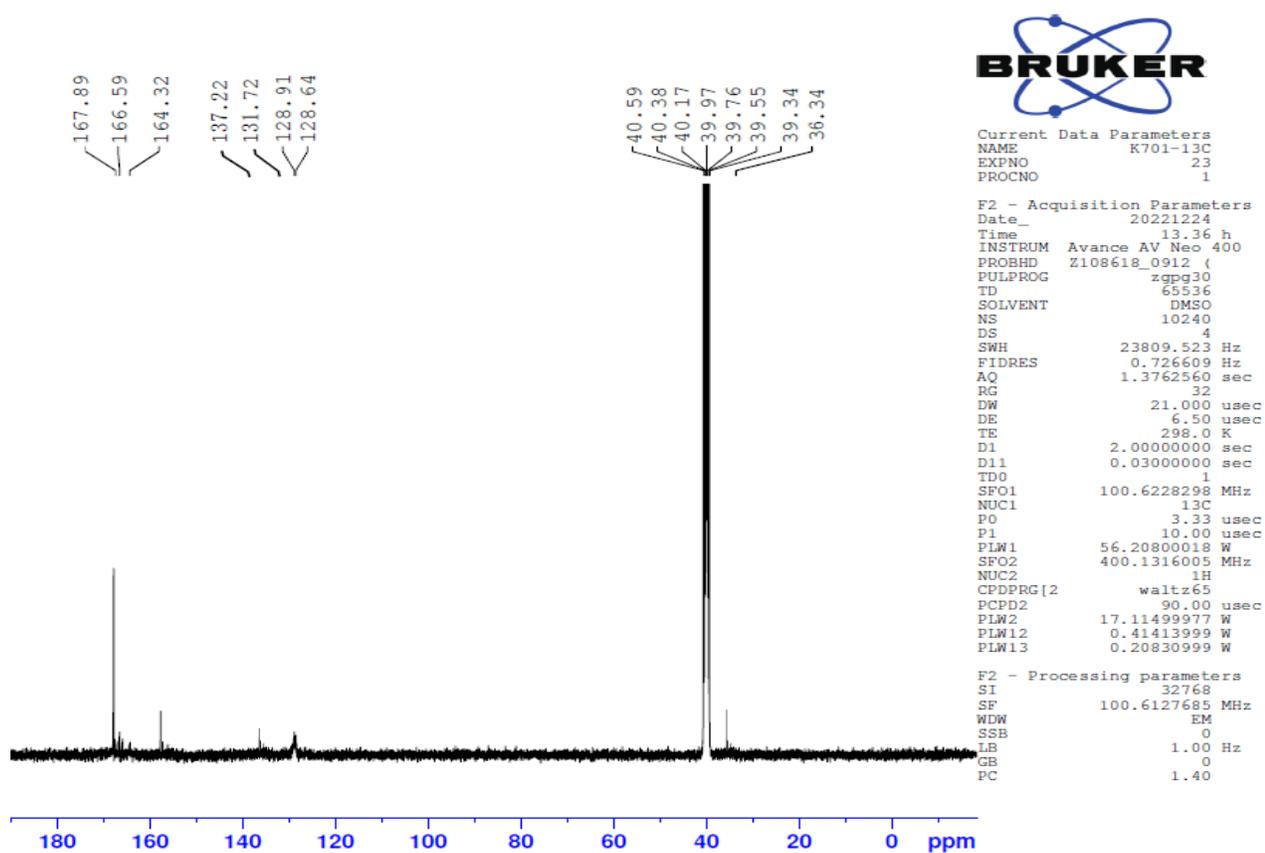
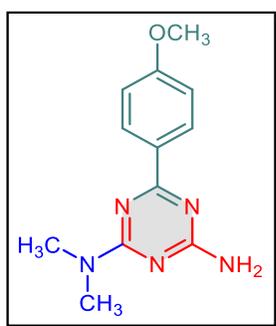
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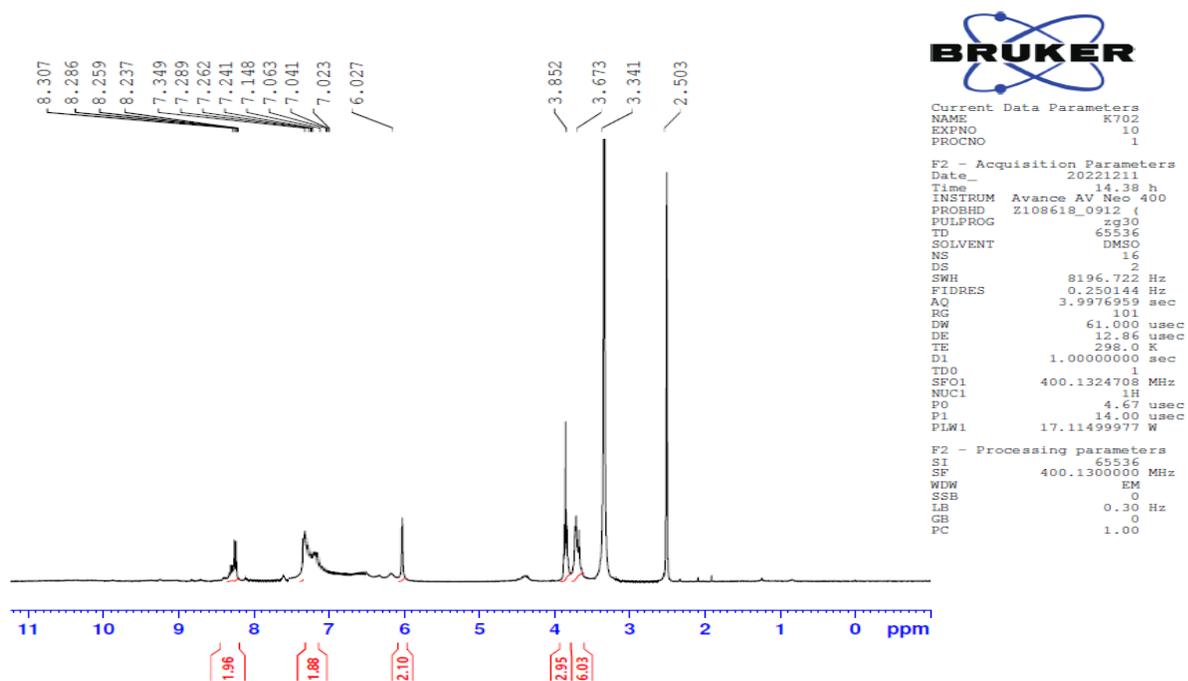
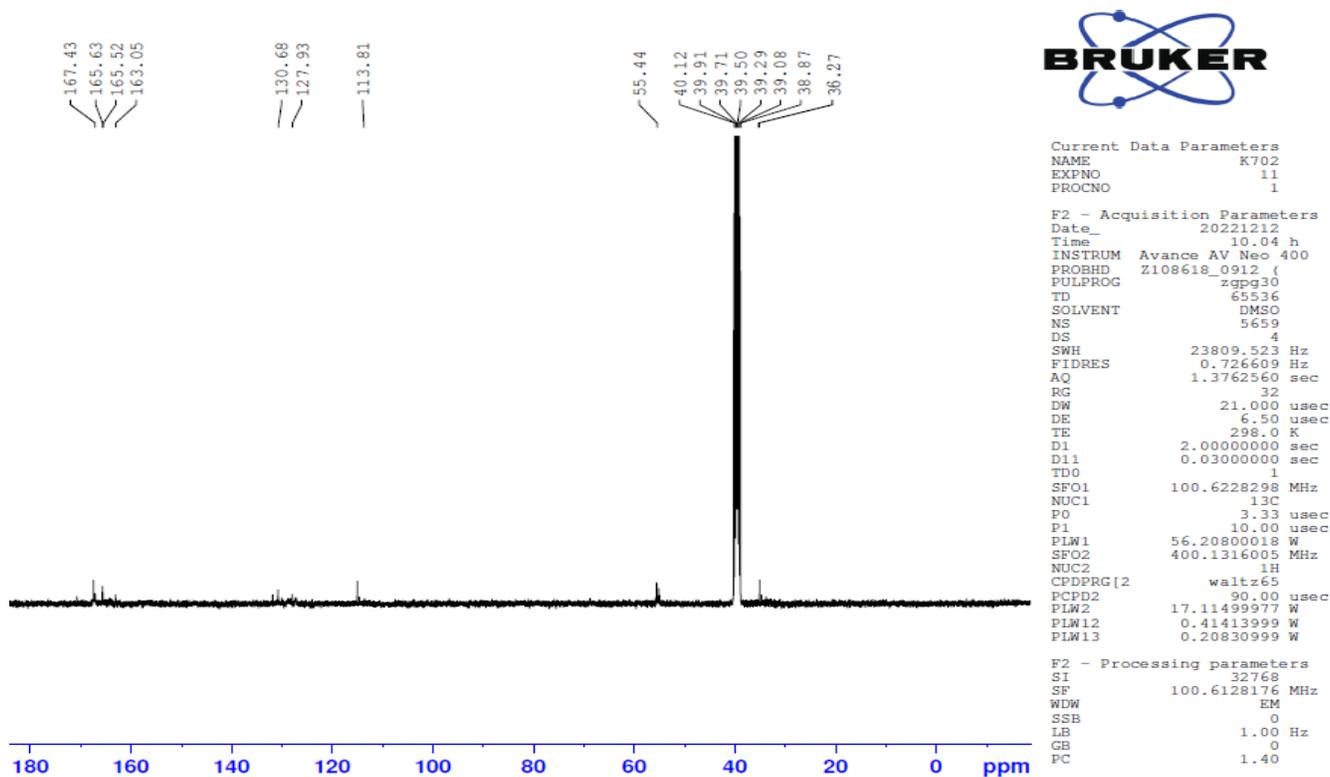
7e Mass spectrum**6-Phenyl-*N*²,*N*²-dimethyl-1,3,5-triazine-2,4-diamine (8a).****8a ¹H NMR (400 MHz, DMSO-*d*₆):**

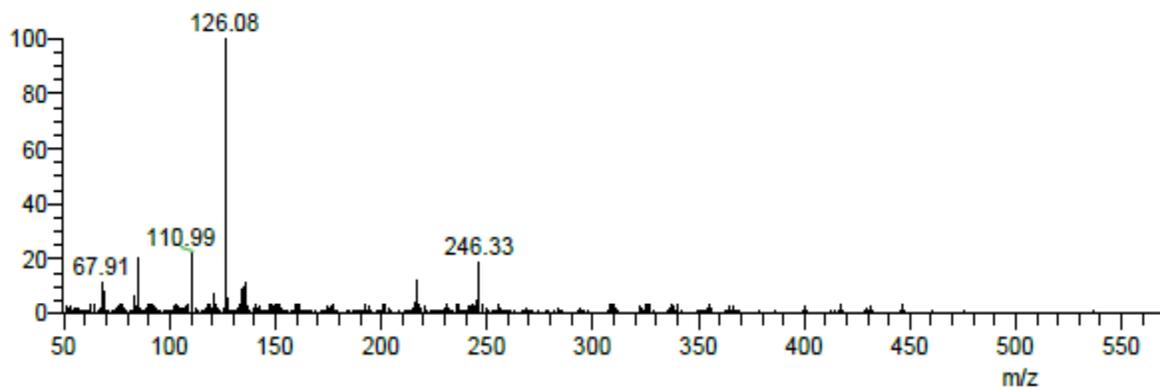
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 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 12.86 usec
 TE 298.0 K
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 TDO 1
 SFO1 400.1324708 MHz
 NUC1 1H
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 P1 14.00 usec
 PLW1 17.11499977 W

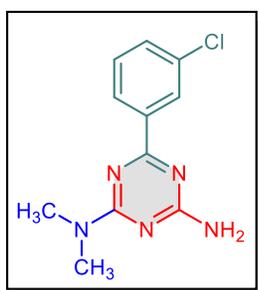
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 GB 0
 PC 1.00

8a ^{13}C NMR (100 MHz, DMSO- d_6):**6-(4-Methoxyphenyl)- N^2,N^2 -dimethyl-1,3,5-triazine-2,4-diamine (8b).**

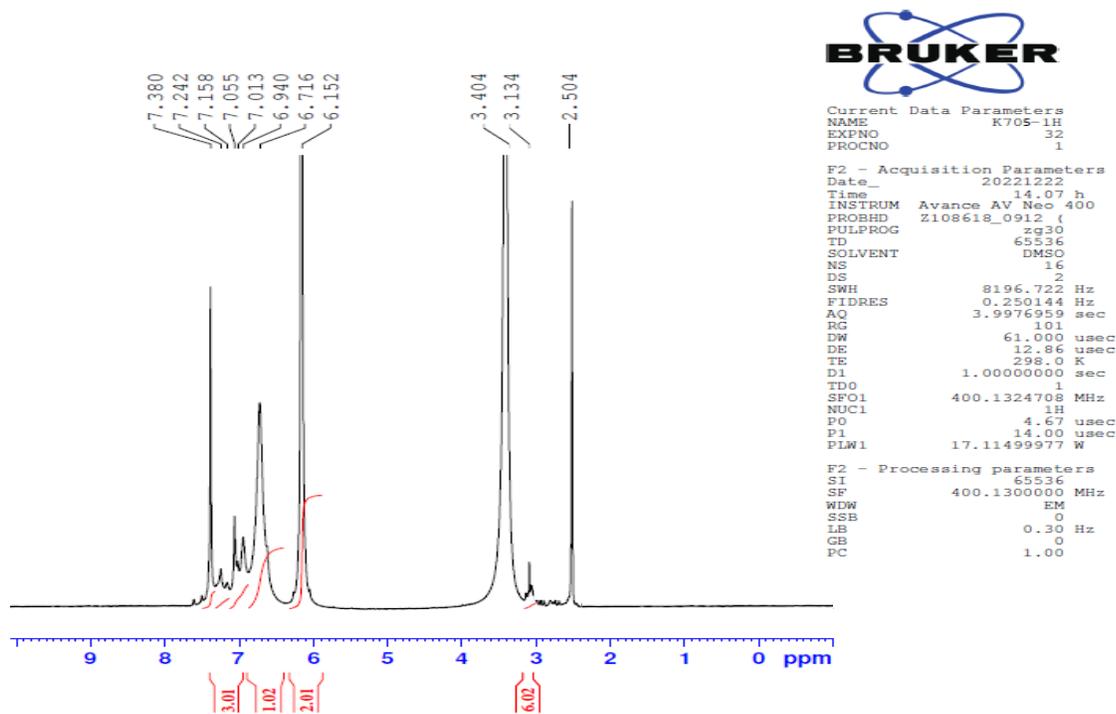
8b ^1H NMR (400 MHz, $\text{DMSO-}d_6$):**8b** ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):**8b** Mass spectrum

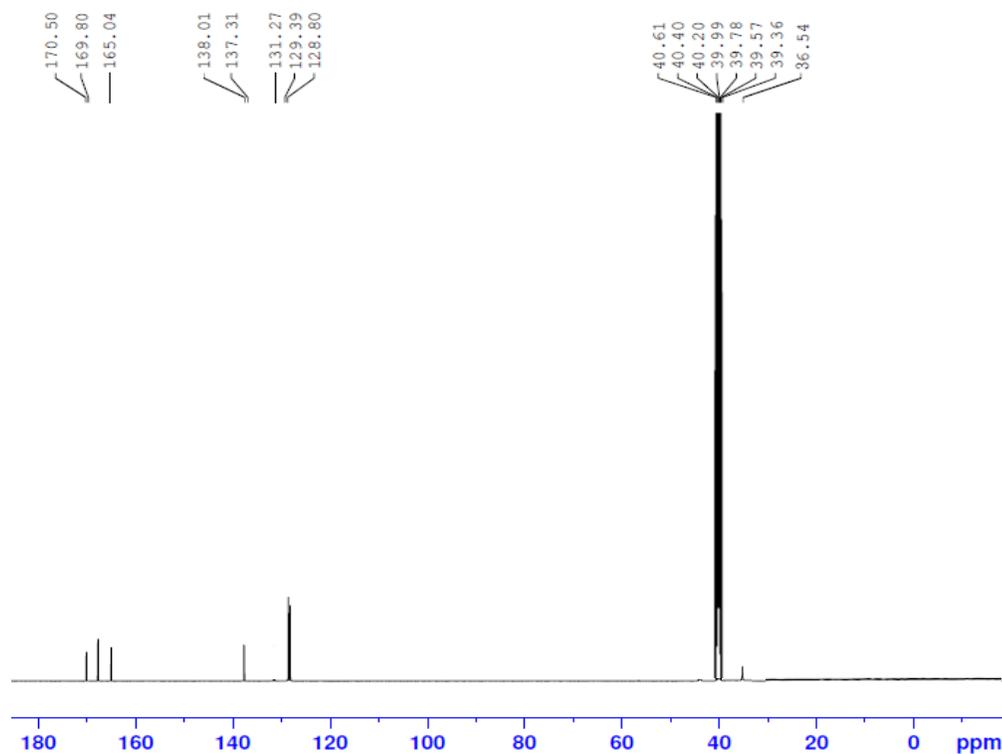
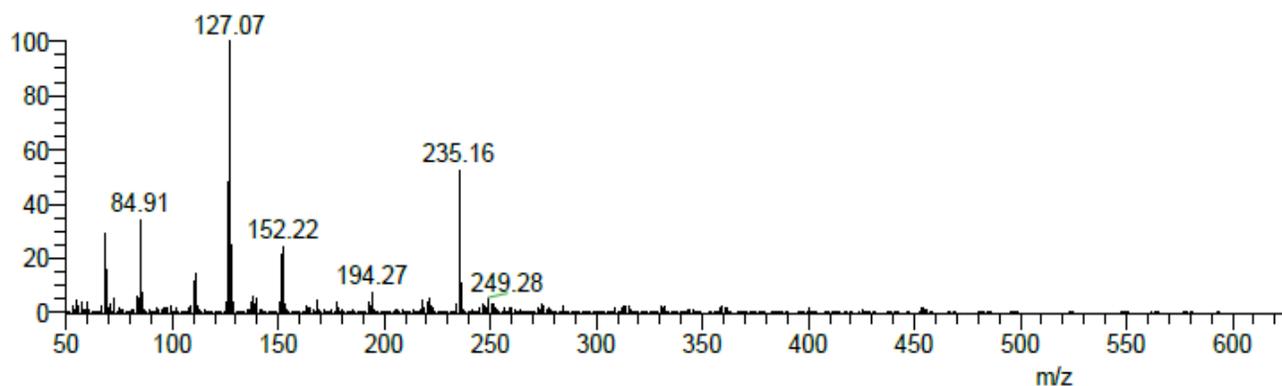


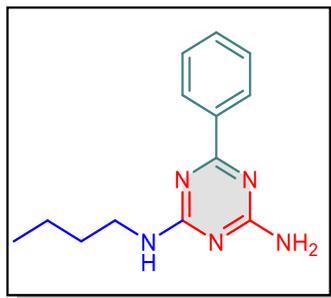
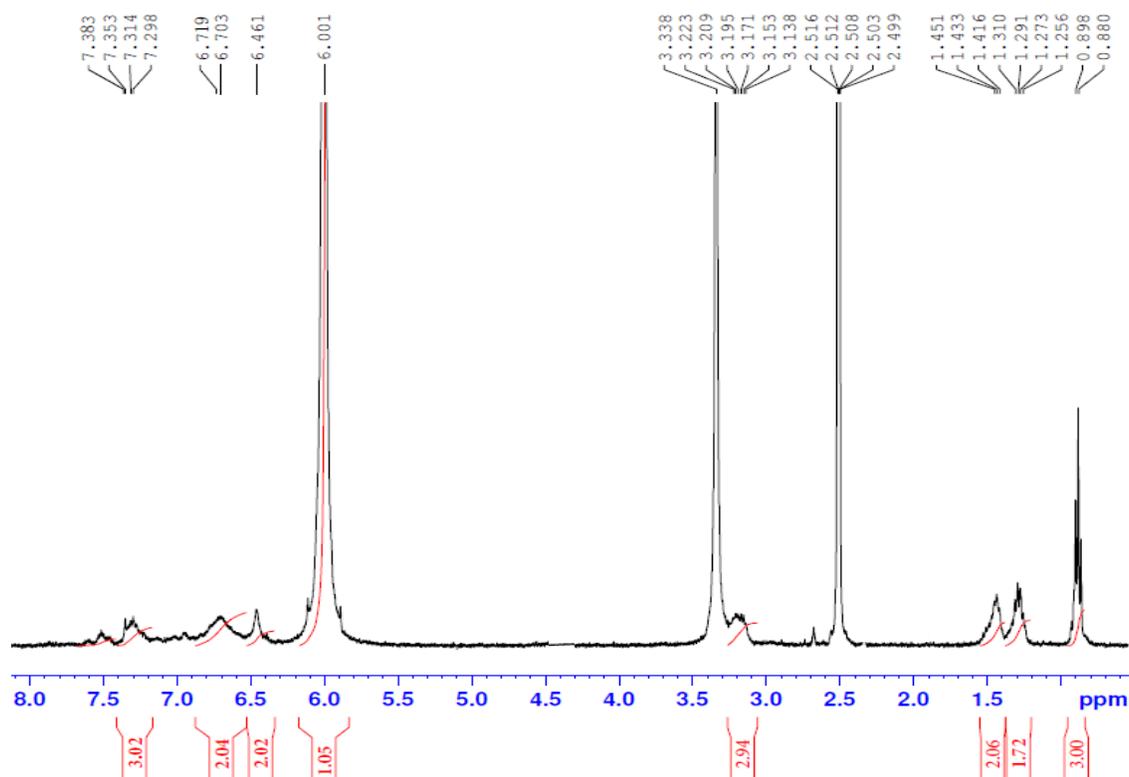
6-(3-Chlorophenyl)-*N*²,*N*²-dimethyl-1,3,5-triazine-2,4-diamine (8c).



8c ¹H NMR (400 MHz, DMSO-*d*₆):



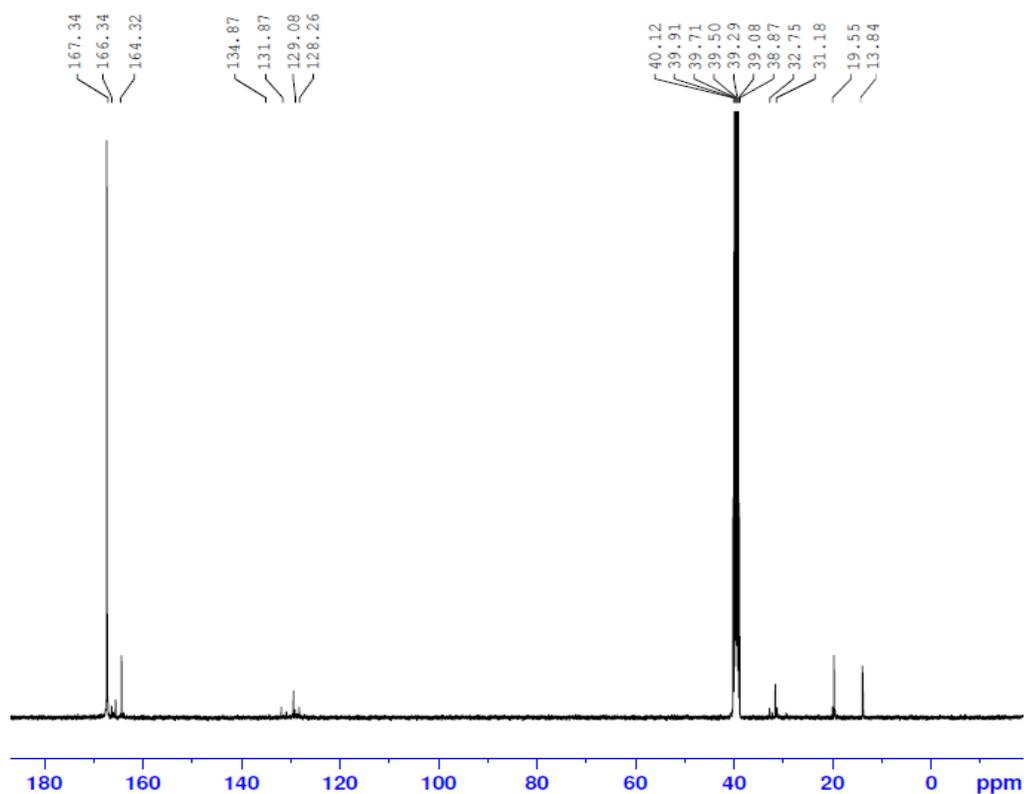
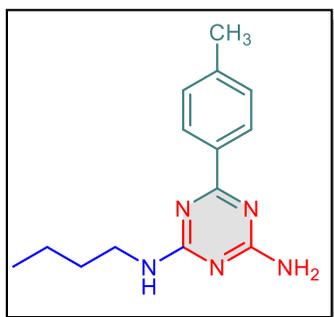
8c ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):**8c** Mass spectrum

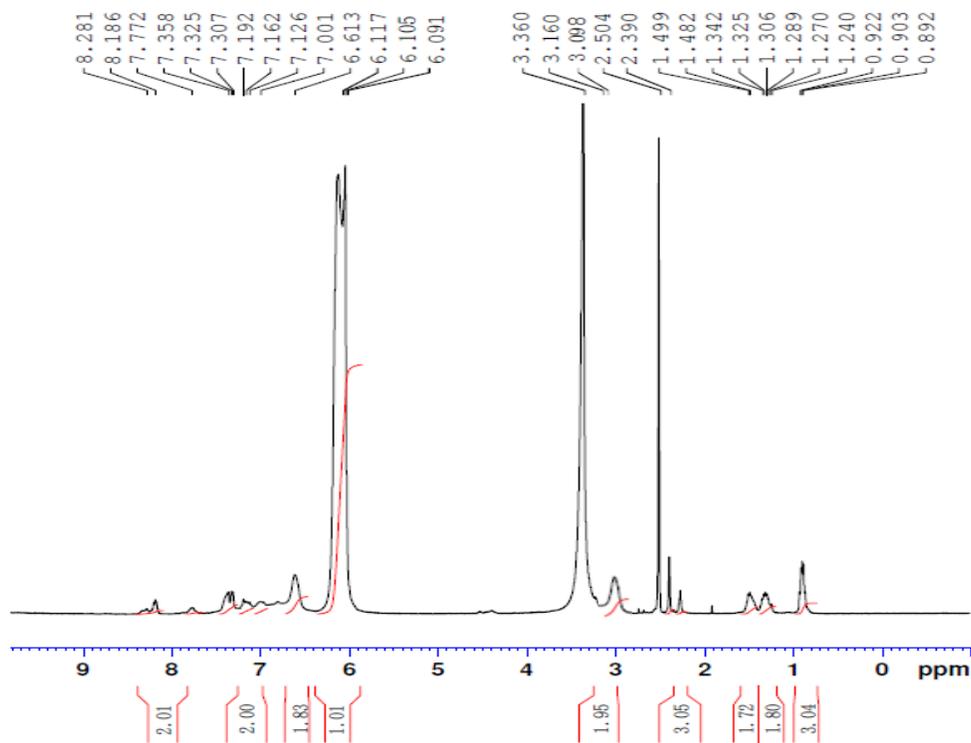
6-Phenyl-*N*²-butyl-1,3,5-triazine-2,4-diamine (9a).**9a ¹H NMR (400 MHz, DMSO-*d*₆):**

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SOLVENT DMSO
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SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
PO 4.67 usec
P1 14.00 usec
PLW1 17.11499977 W

F2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

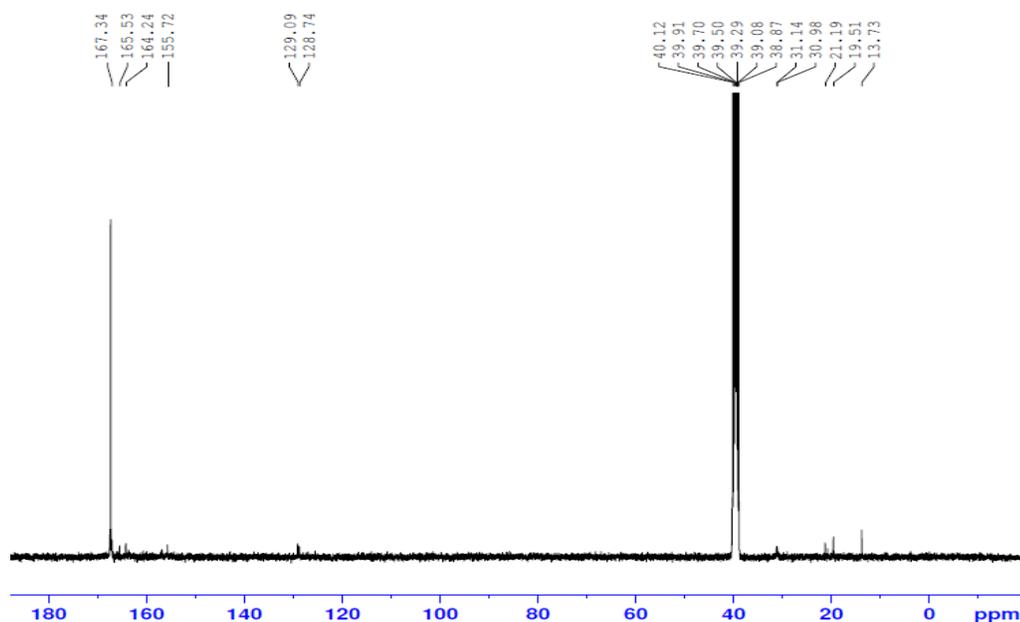
9a ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):**6-(4-tolyl)- N^2 -butyl-1,3,5-triazine-2,4-diamine (9b).**

9b ¹H NMR (400 MHz, DMSO-d₆):

Current Data Parameters
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 EXPNO 32
 PROCNO 1

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 SOLVENT DMSO
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 DS 2
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 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 12.86 usec
 TE 296.8 K
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 TD0 1
 SFO1 400.1324708 MHz
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 P1 14.00 usec
 PLW1 17.11499977 W

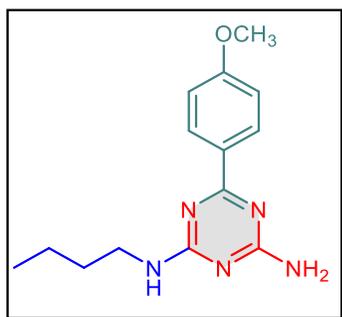
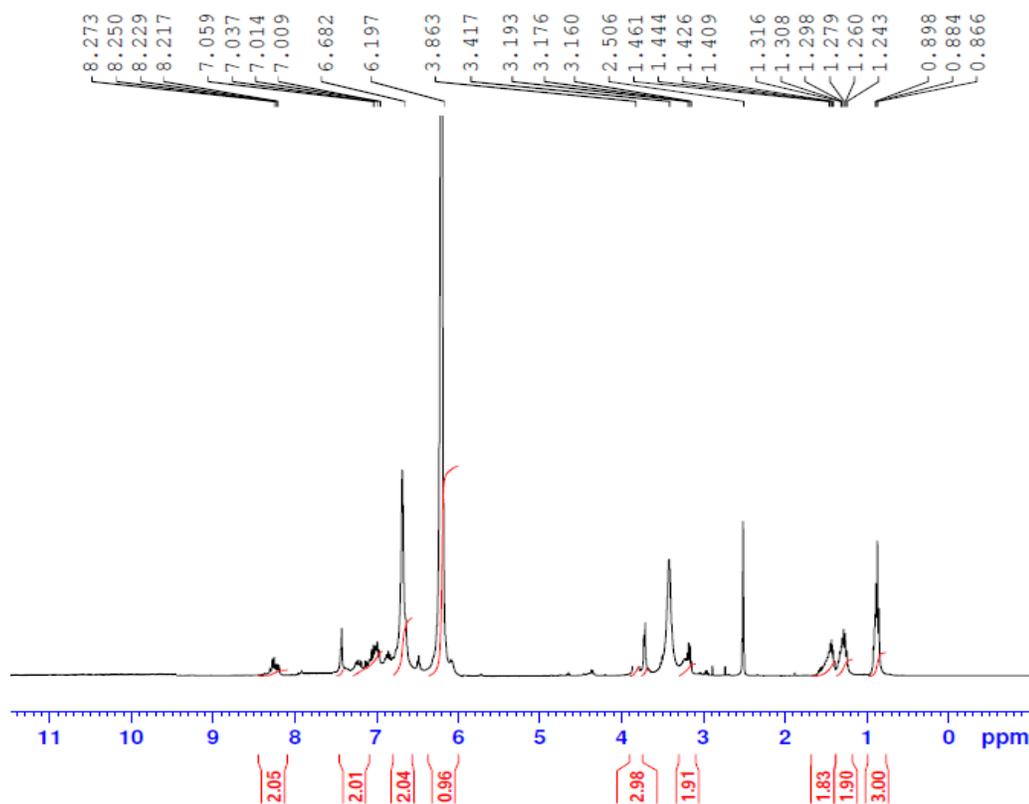
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9b ¹³C NMR (100 MHz, DMSO-d₆):

Current Data Parameters
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 EXPNO 33
 PROCNO 1

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 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 23809.523 Hz
 FIDRES 0.726609 Hz
 AQ 1.5762560 sec
 RG 32
 DW 21.000 usec
 DE 6.50 usec
 TE 297.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6228298 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 56.20800018 W
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 90.00 usec
 PLW2 17.11499977 W
 PLW12 0.41413999 W
 PLW13 0.20830999 W

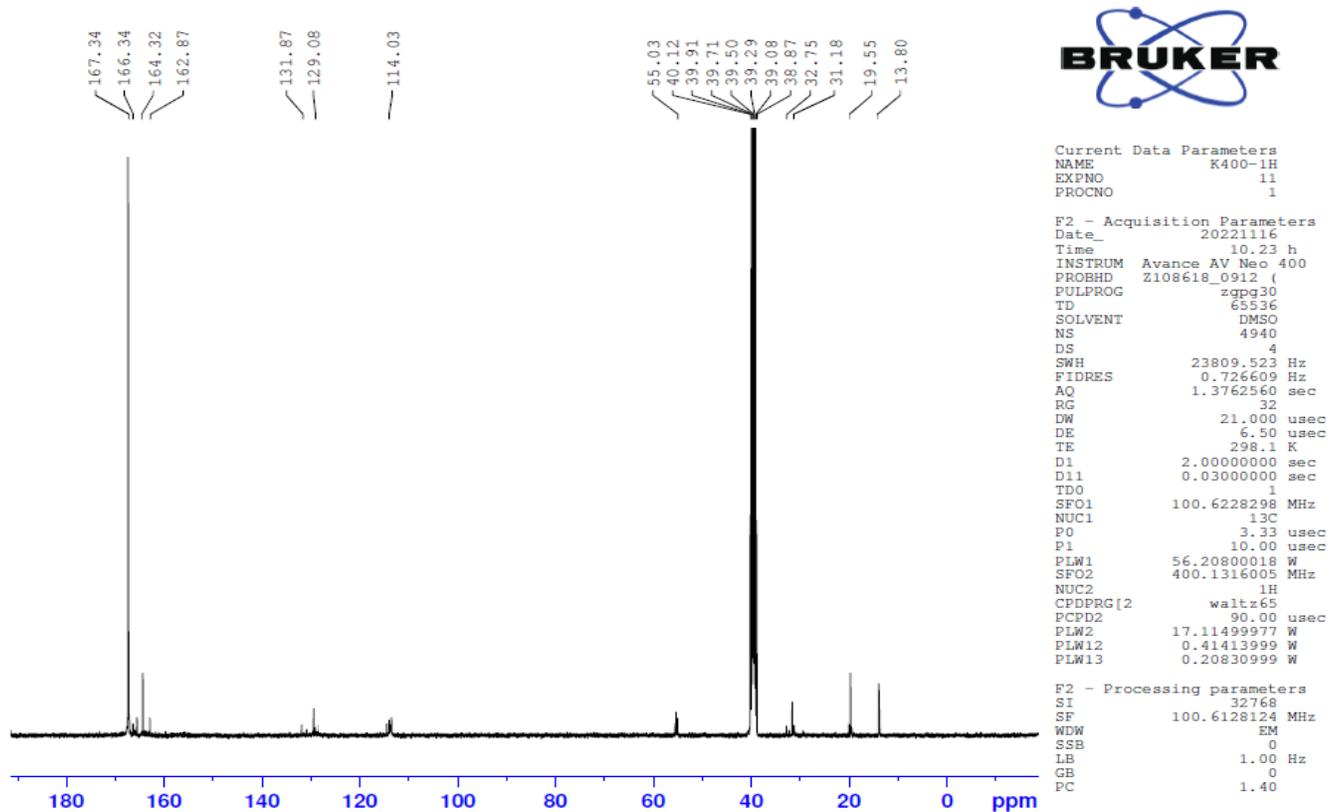
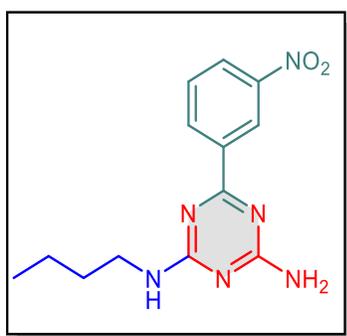
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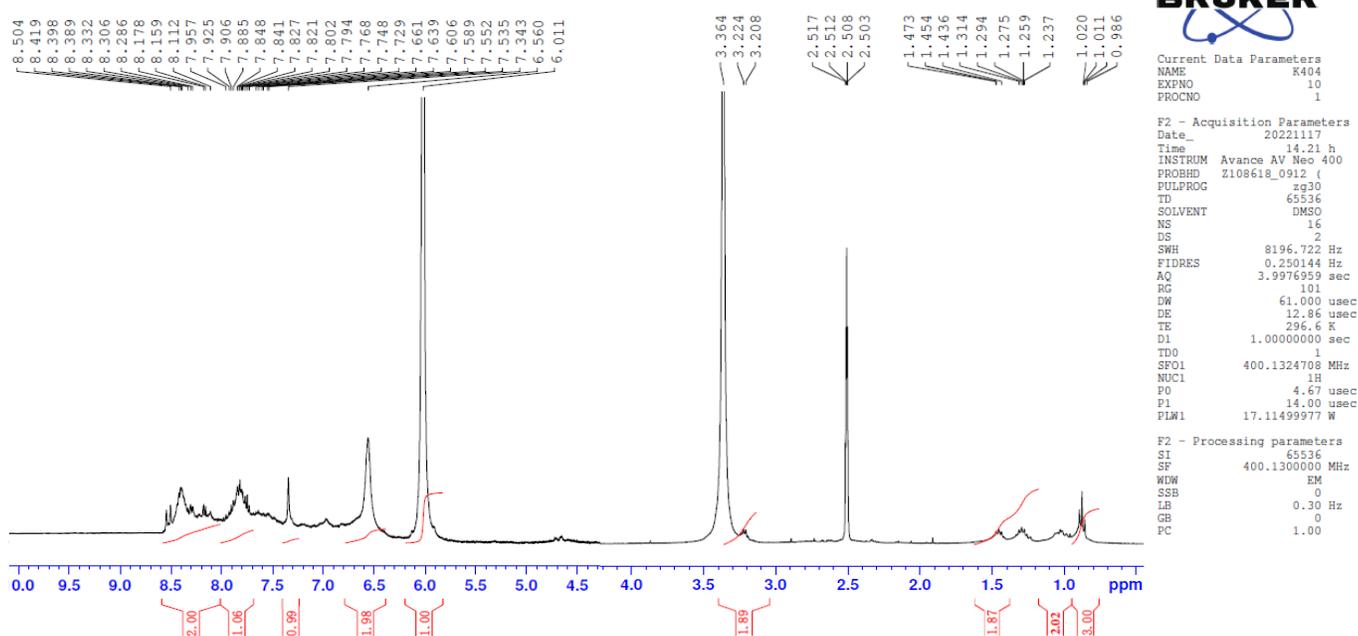
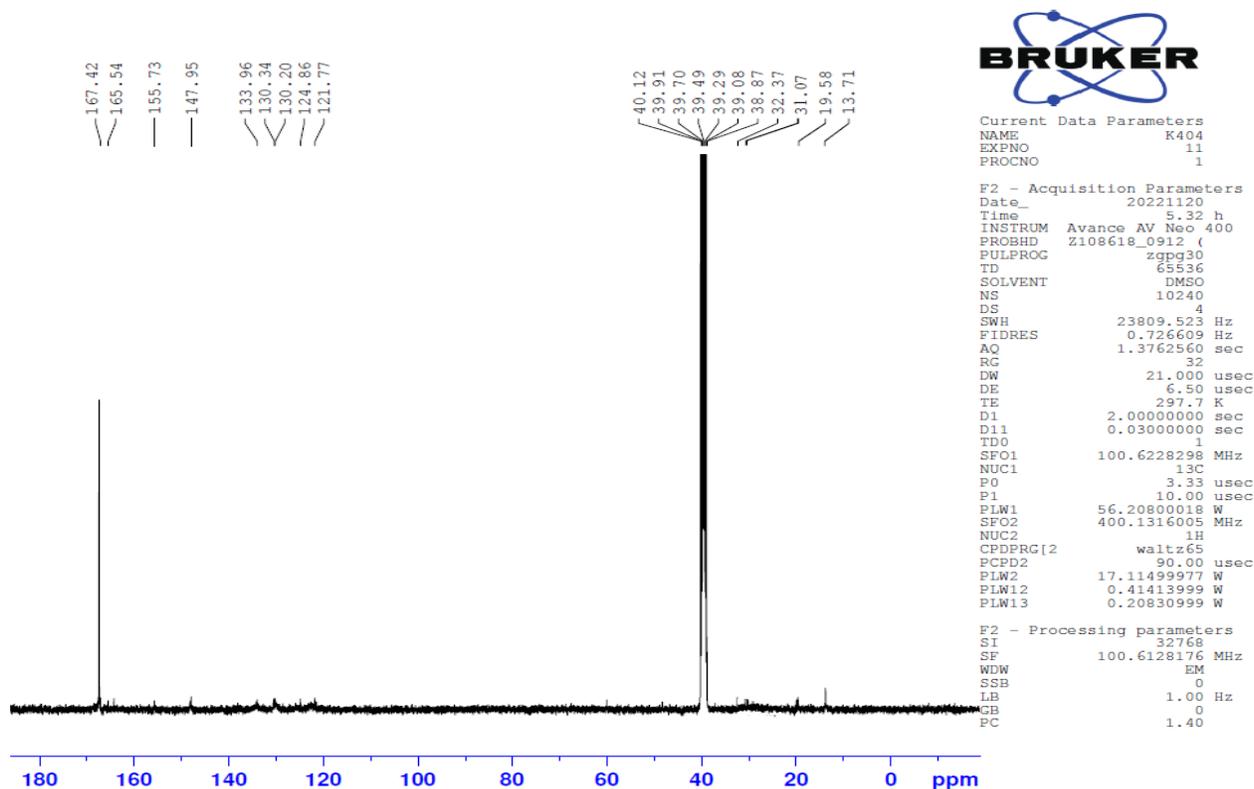
6-(4-Methoxyphenyl)-*N*²-1,3,5-triazine-2,4-diamine (9c).**9c ¹H NMR (400 MHz, DMSO-*d*₆):**

Current Data Parameters
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PROCNO 1

F2 - Acquisition Parameters
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INSTRUM Avance AV Neo 400
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 296.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 17.11499977 W

F2 - Processing parameters
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9c ^{13}C NMR (100 MHz, DMSO- d_6):**6-(3-Nitrophenyl)-N2-butyl-1,3,5-triazine-2,4-diamine (9d).**

9d ¹H NMR (400 MHz, DMSO-d₆):**9d ¹³C NMR (100 MHz, DMSO-d₆):**

9d Mass spectrum