



Supporting Information

for

Microwave-assisted efficient one-pot synthesis of N^2 -(tetrazol-5-yl)-6-aryl/heteroaryl-5,6-dihydro-1,3,5-triazine-2,4-diamines

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Saleh Mohammed Al-Mousawi, Mohamed Abd-Elmonem, Hesham El-Zorba,
Afaf Mohamed Abdel Hameed, Tahany Mahmoud Mohamed and Kamal Usef Sadek

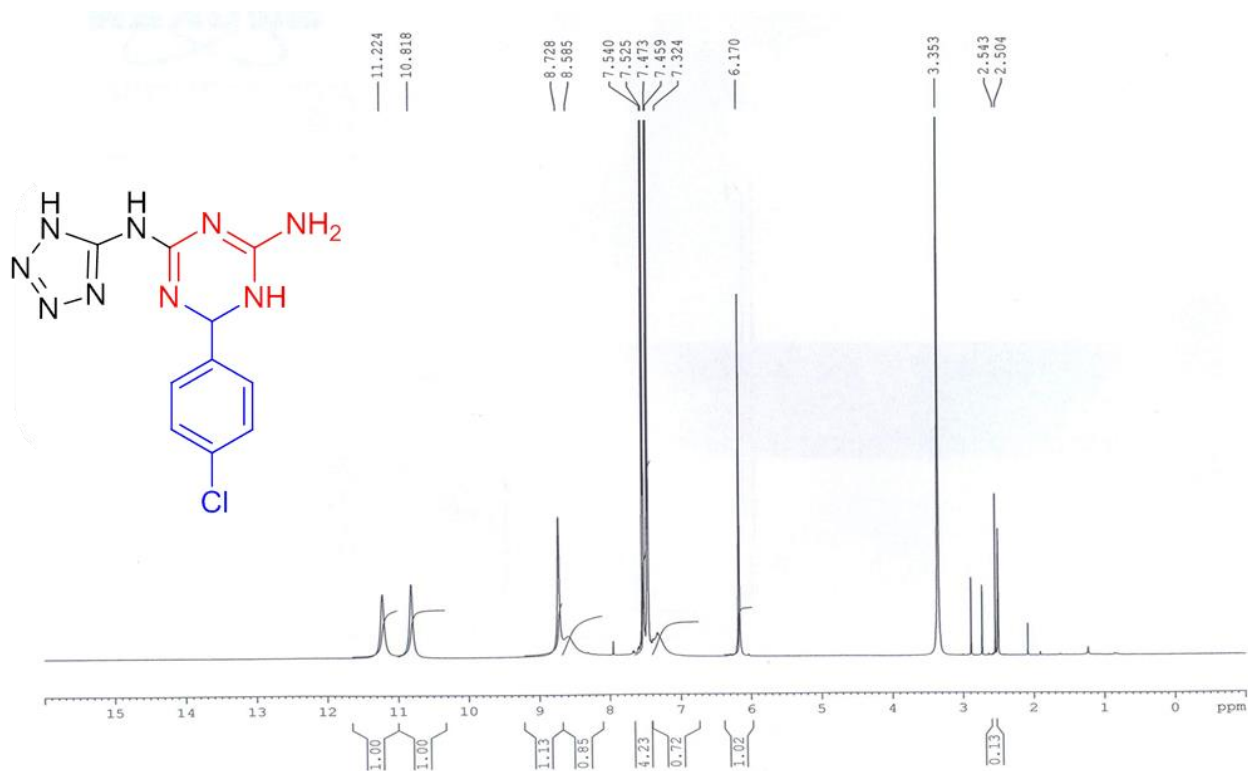
Beilstein J. Org. Chem. **2020**, *16*, 1706–1712. [doi:10.3762/bjoc.16.142](https://doi.org/10.3762/bjoc.16.142)

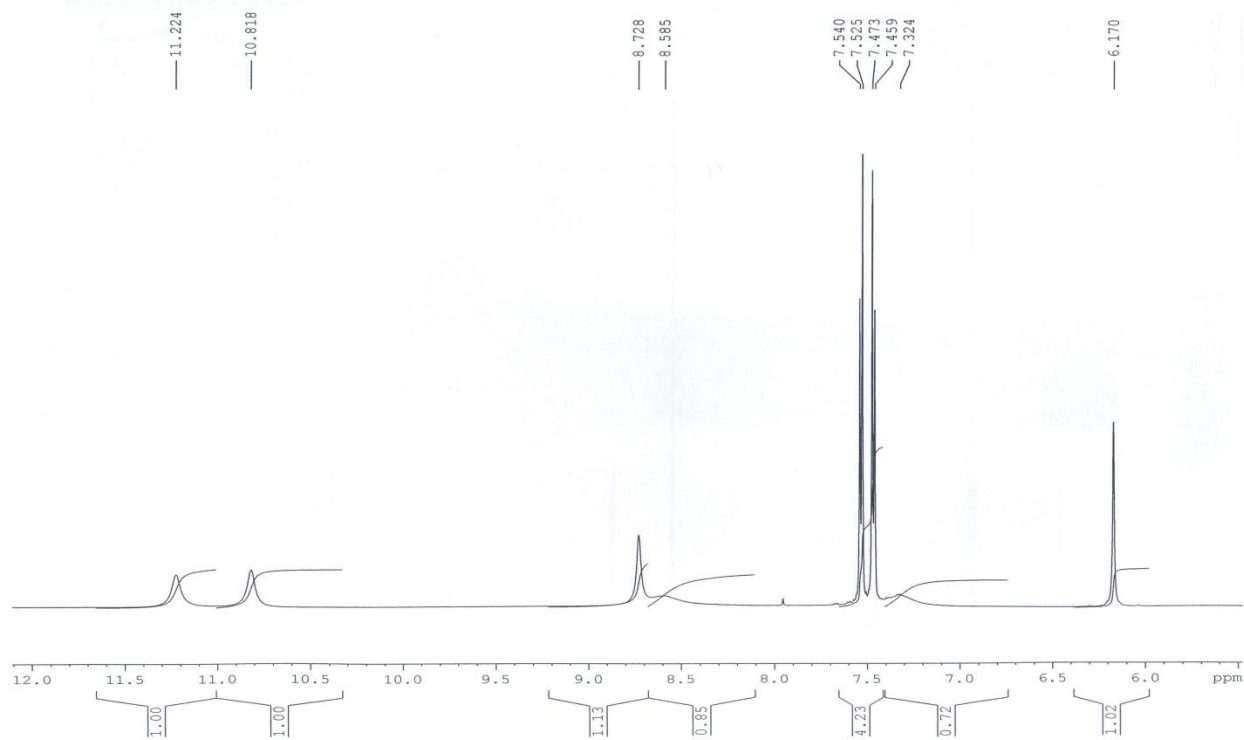
NMR and mass spectra

6-(4-Chlorophenyl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4a).

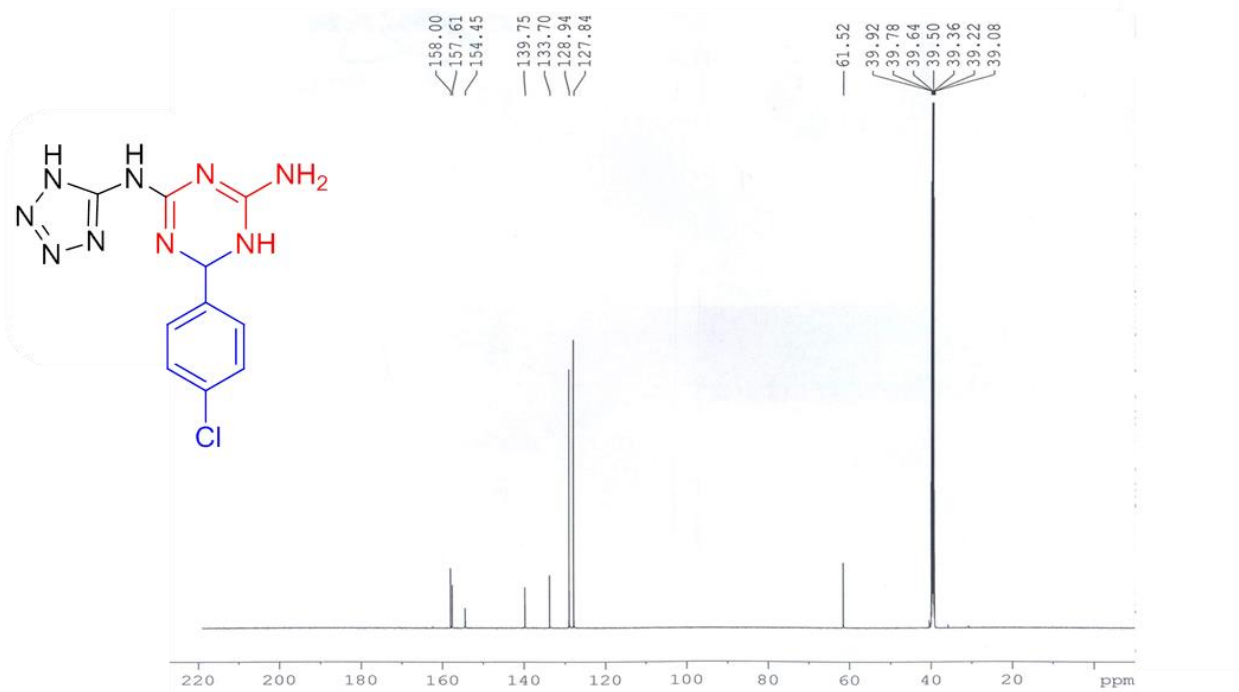
This compound is novel.

4a ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



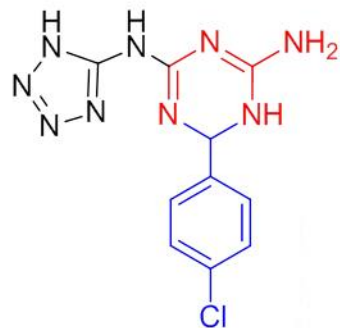
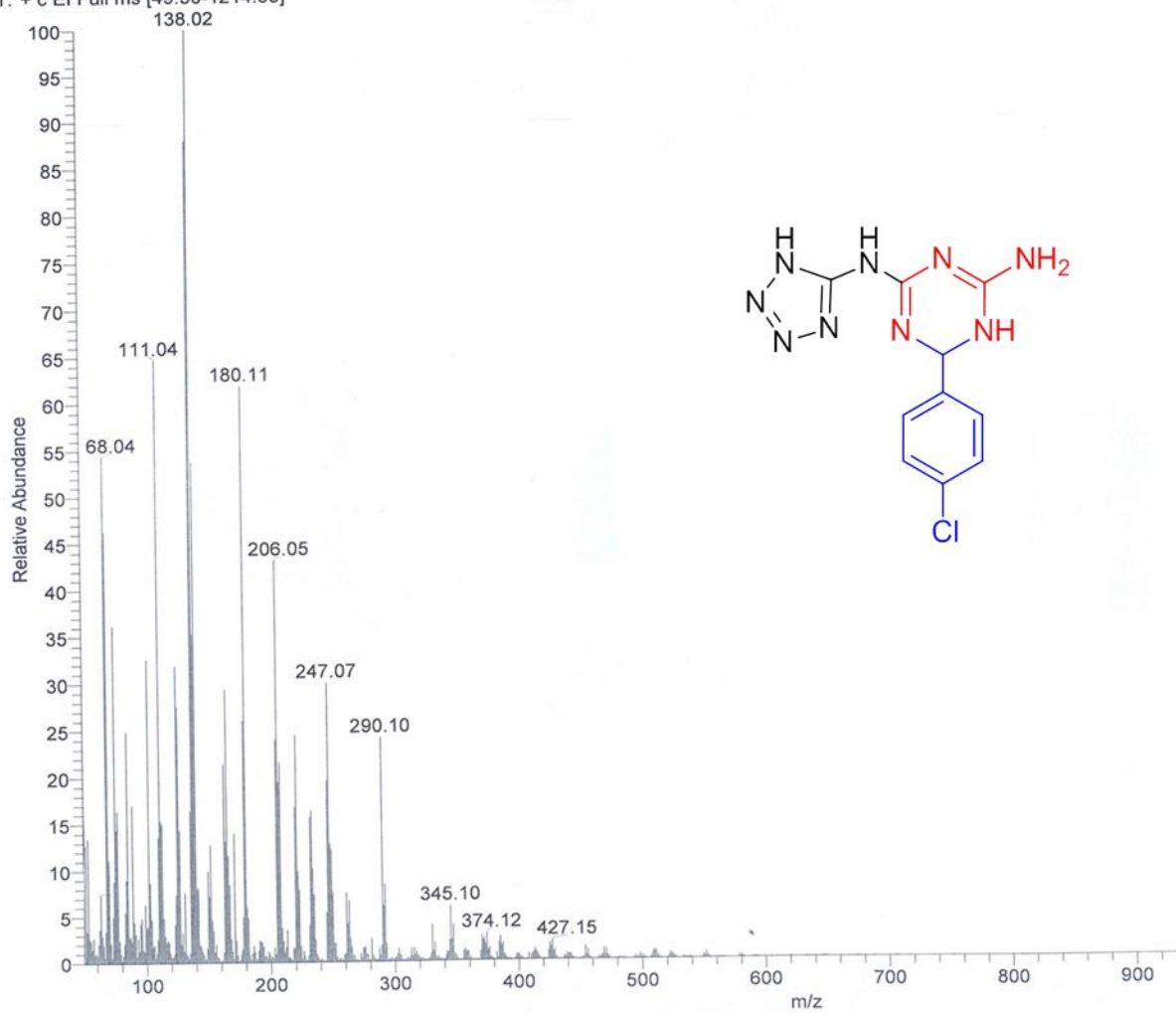


4a ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$).



4a Mass spectrum.

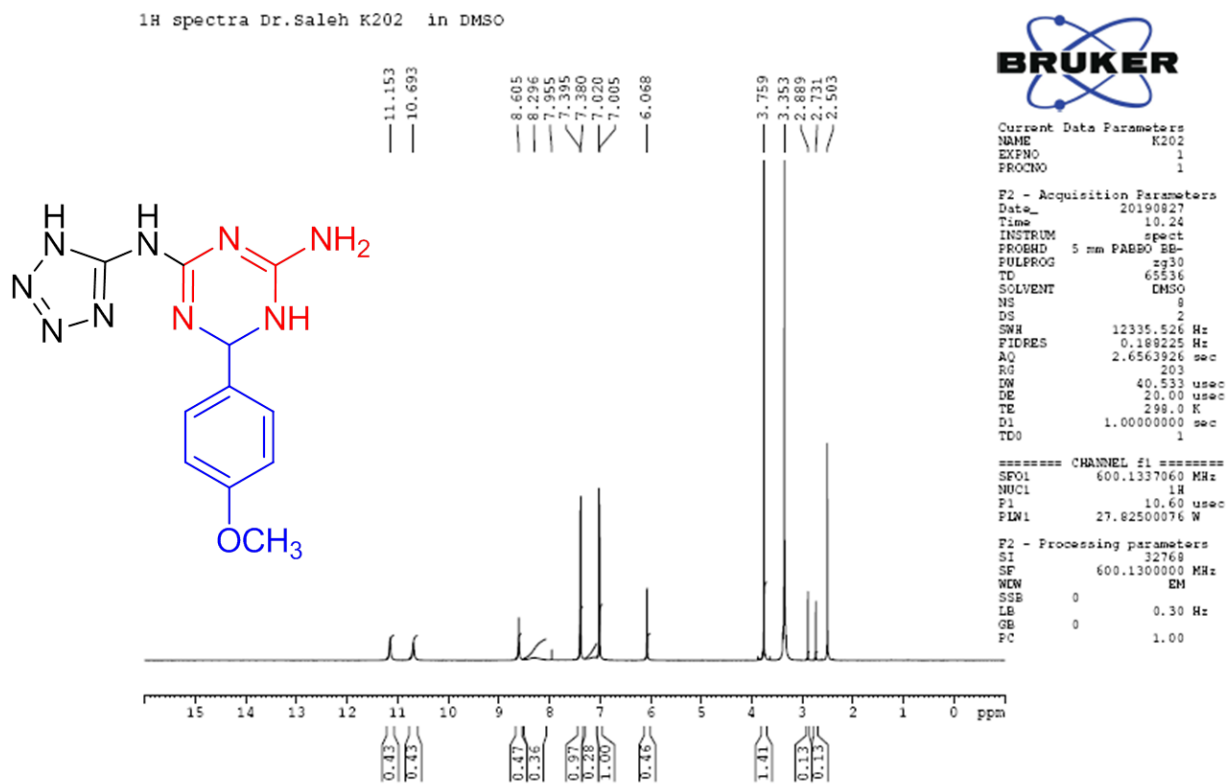
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T: + c EI Full ms [49.50-1214.53]



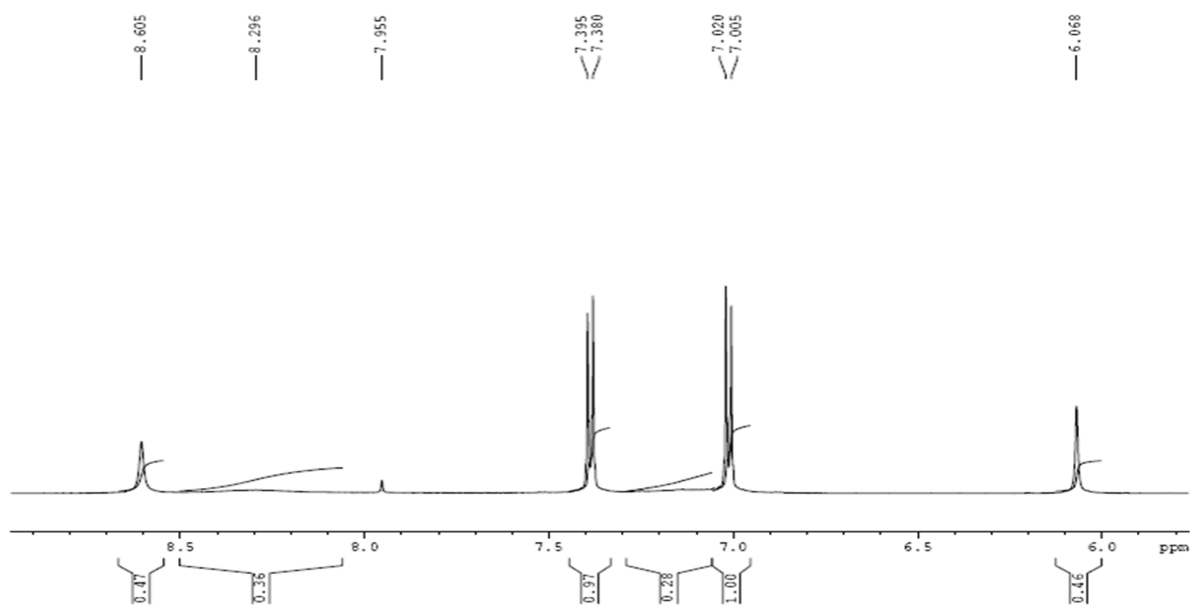
6-(4-Methoxyphenyl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4b).

This compound is novel.

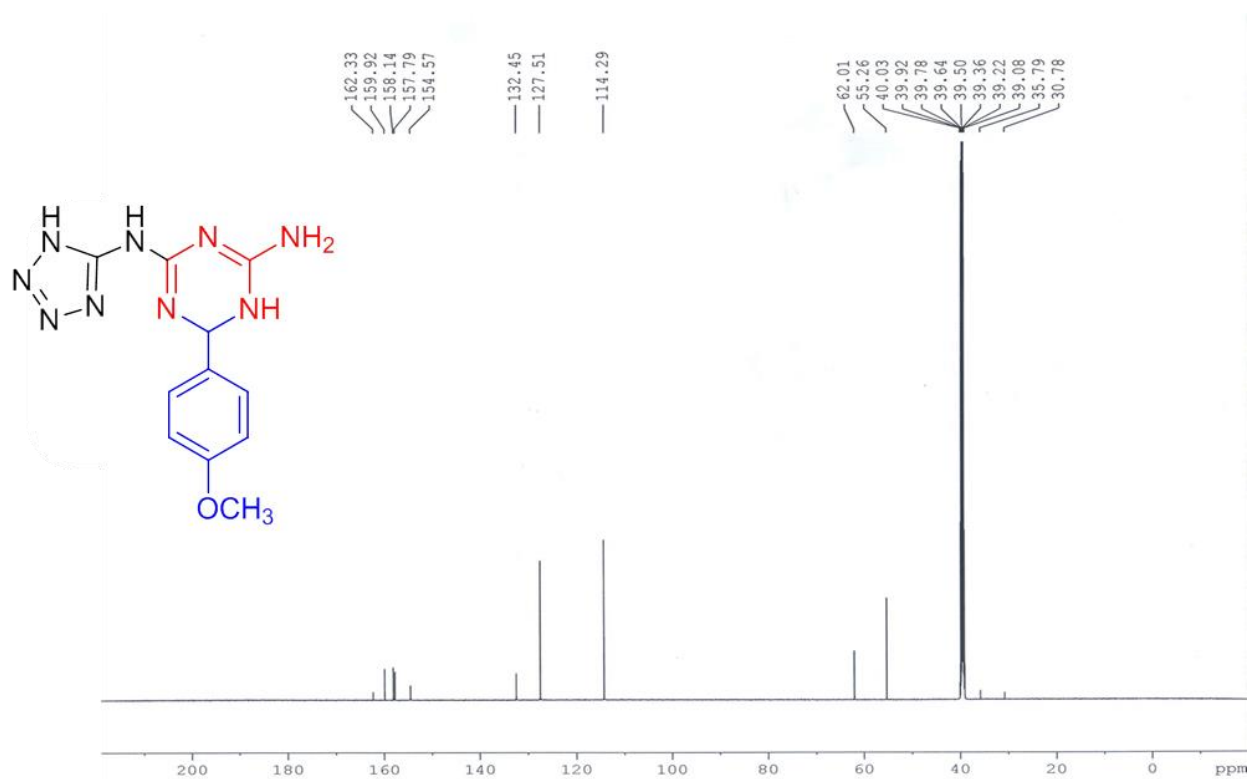
4b ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



¹H spectra Dr.Saleh K202 in DMSO

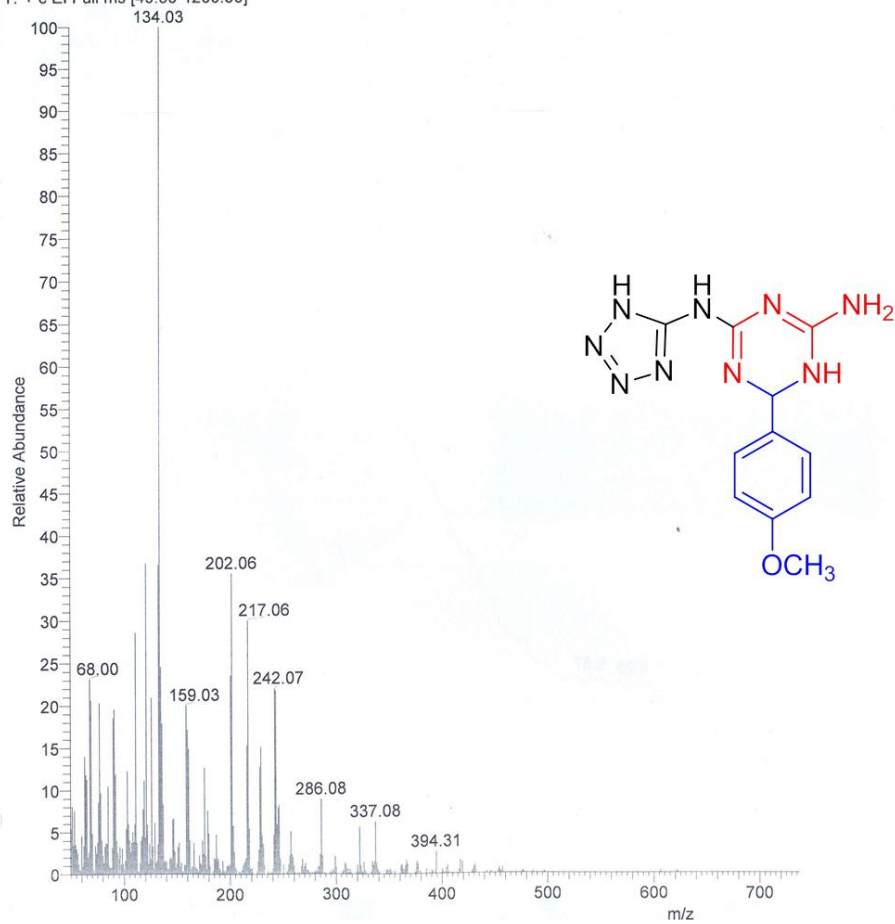


4b ¹³C NMR spectrum (150 MHz, DMSO-*d*₆).



4b Mass spectrum.

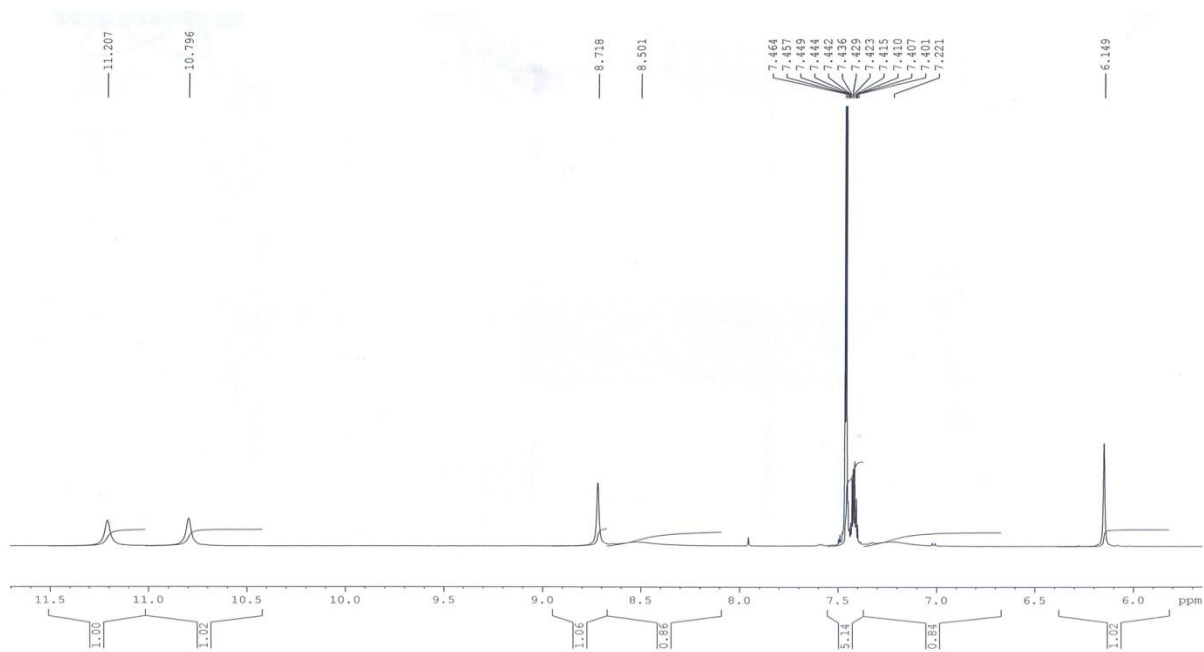
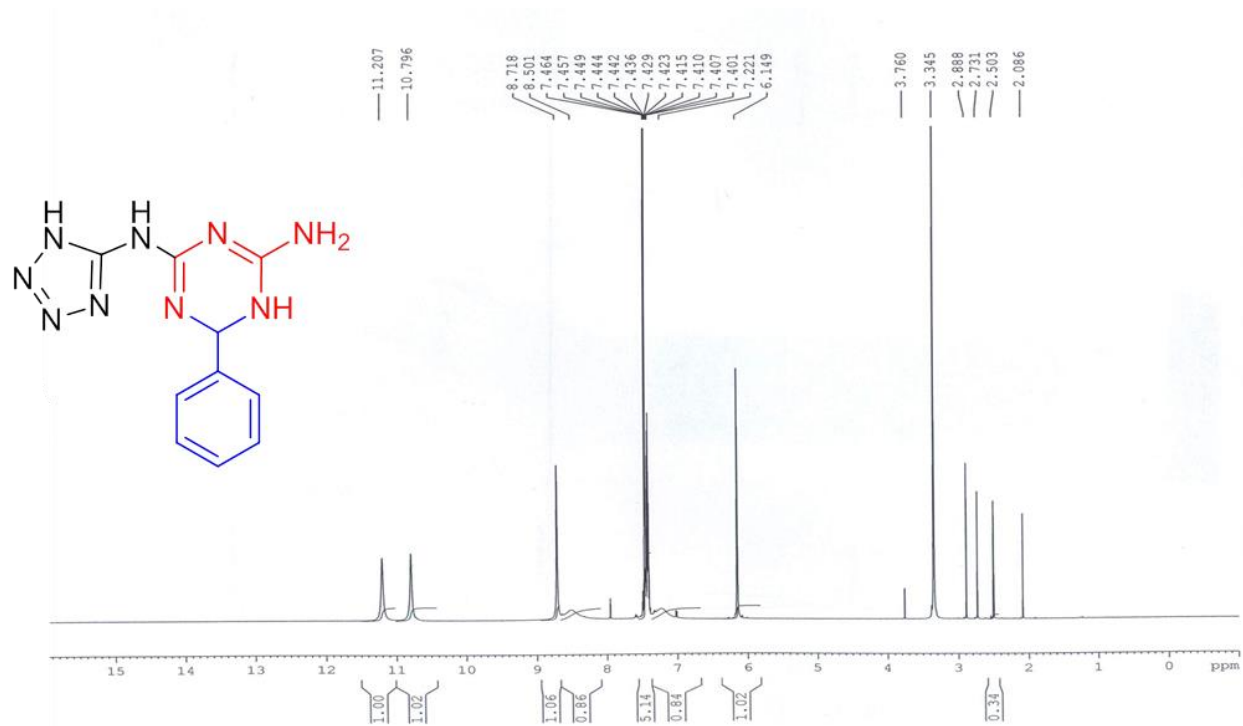
K202 #307 RT: 14.87 AV: 1 SB: 147 0.49-5.15 , 2.14-4.52 NL: 6.26E5
T: + c EI Full ms [49.50-1200.50]



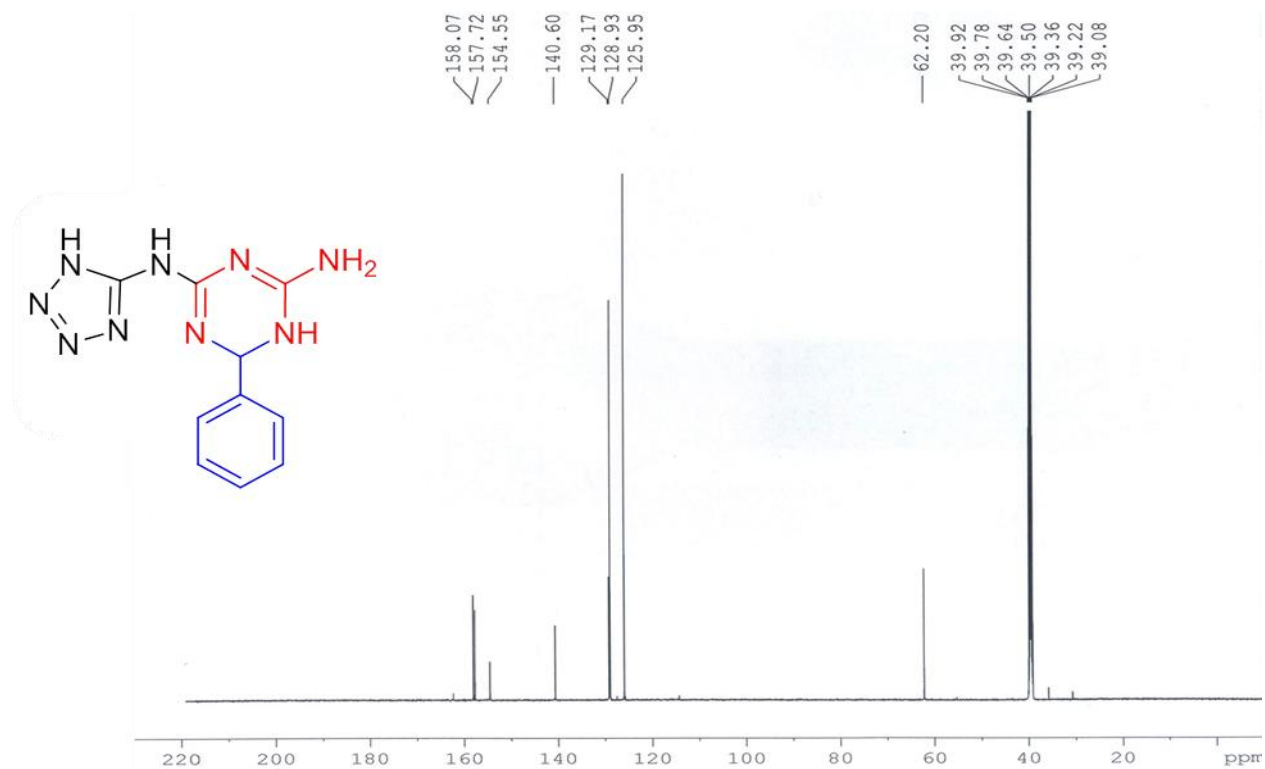
6-Phenyl-*N*²-(5*H*-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4c).

This compound is novel.

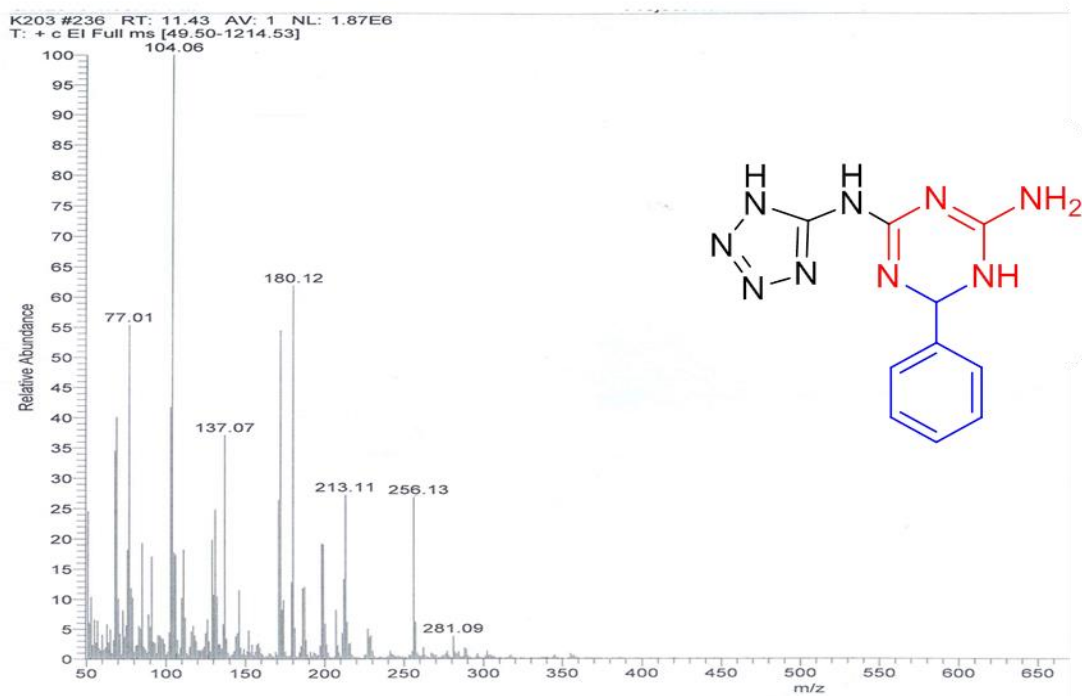
4c ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



4c ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$).



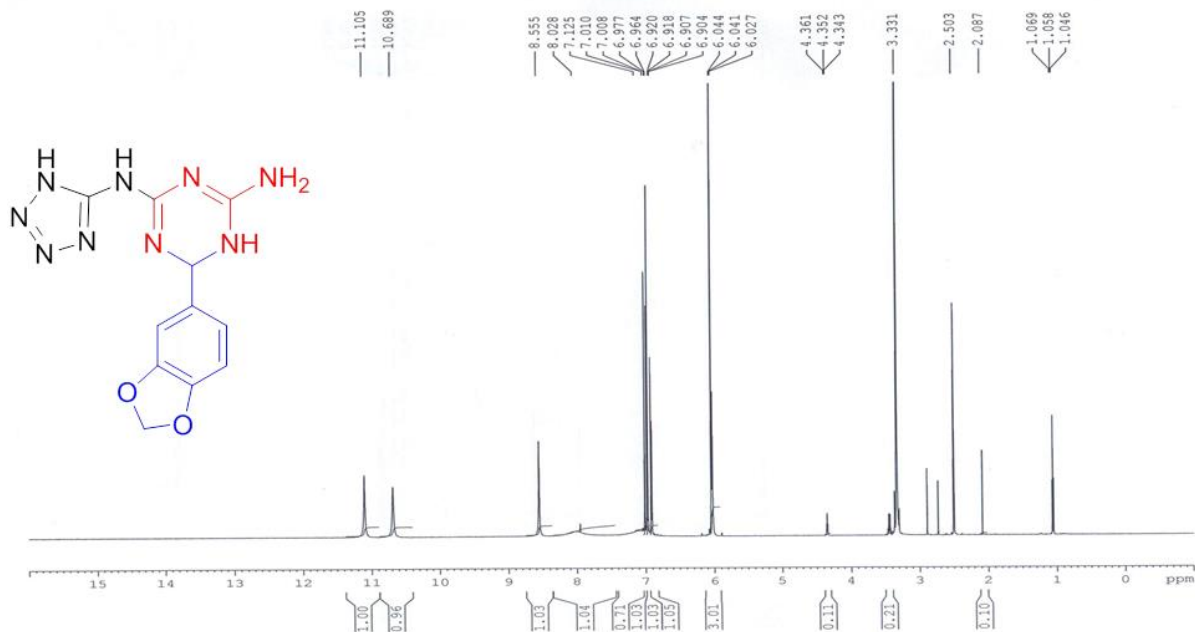
4c Mass spectrum.



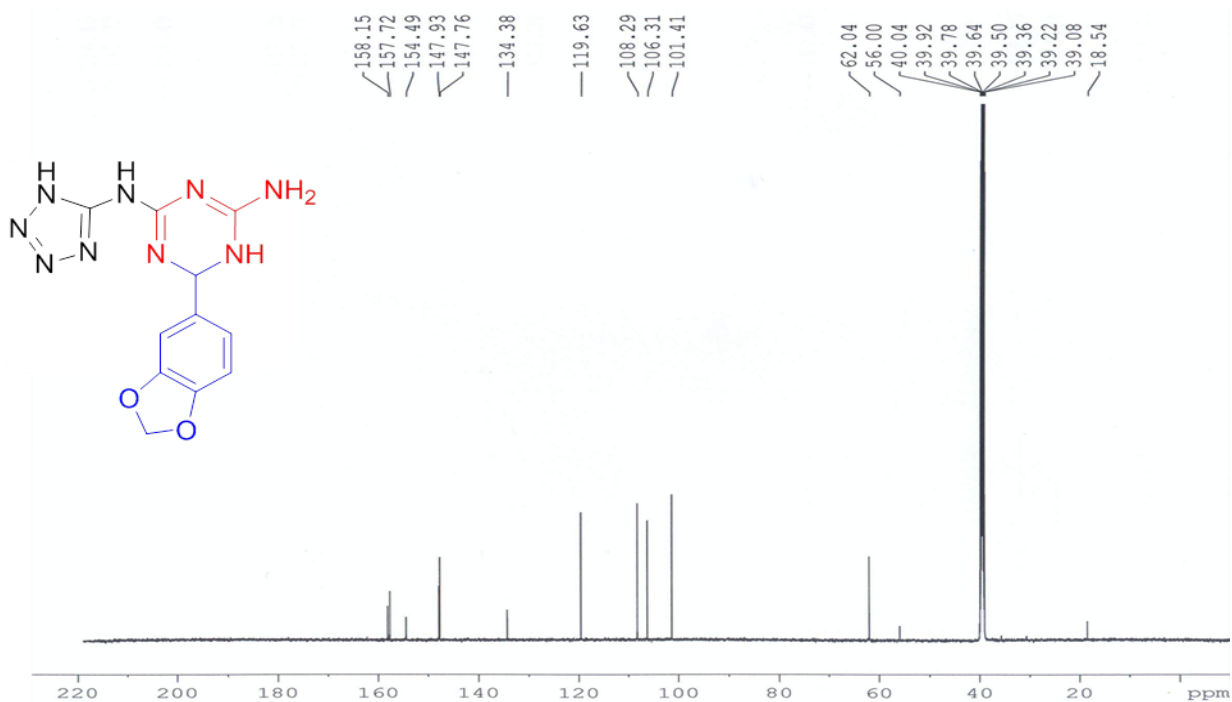
6-(Benzo[d][1,3]dioxol-5-yl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4d).

This compound is novel.

4d ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



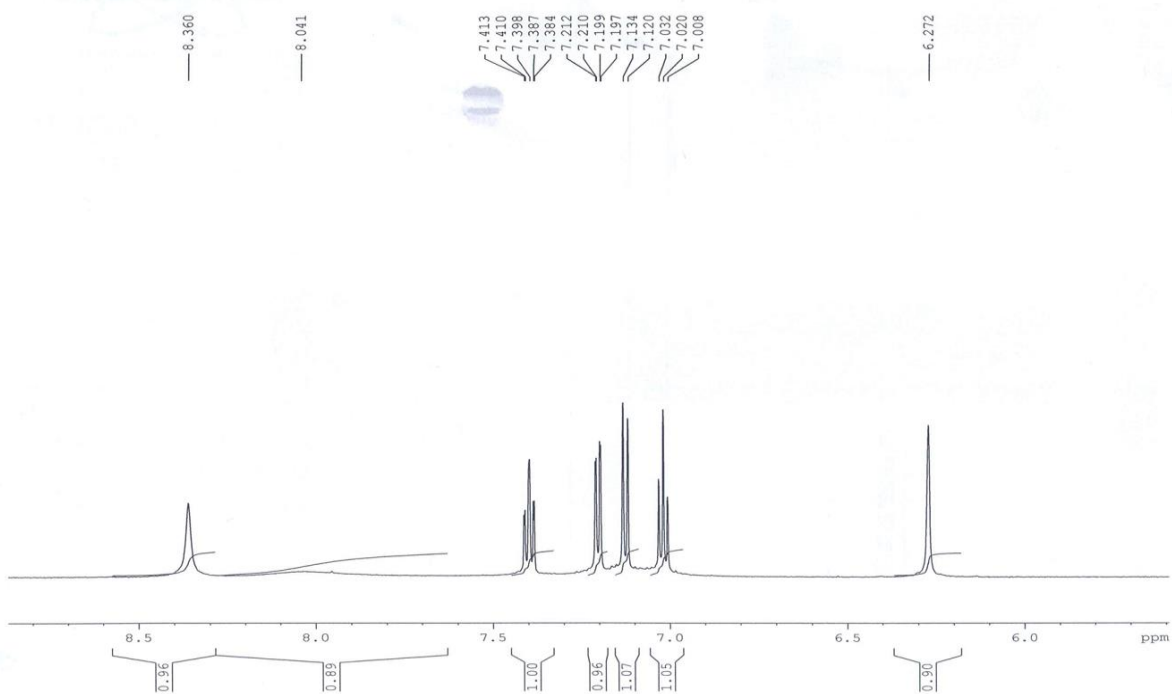
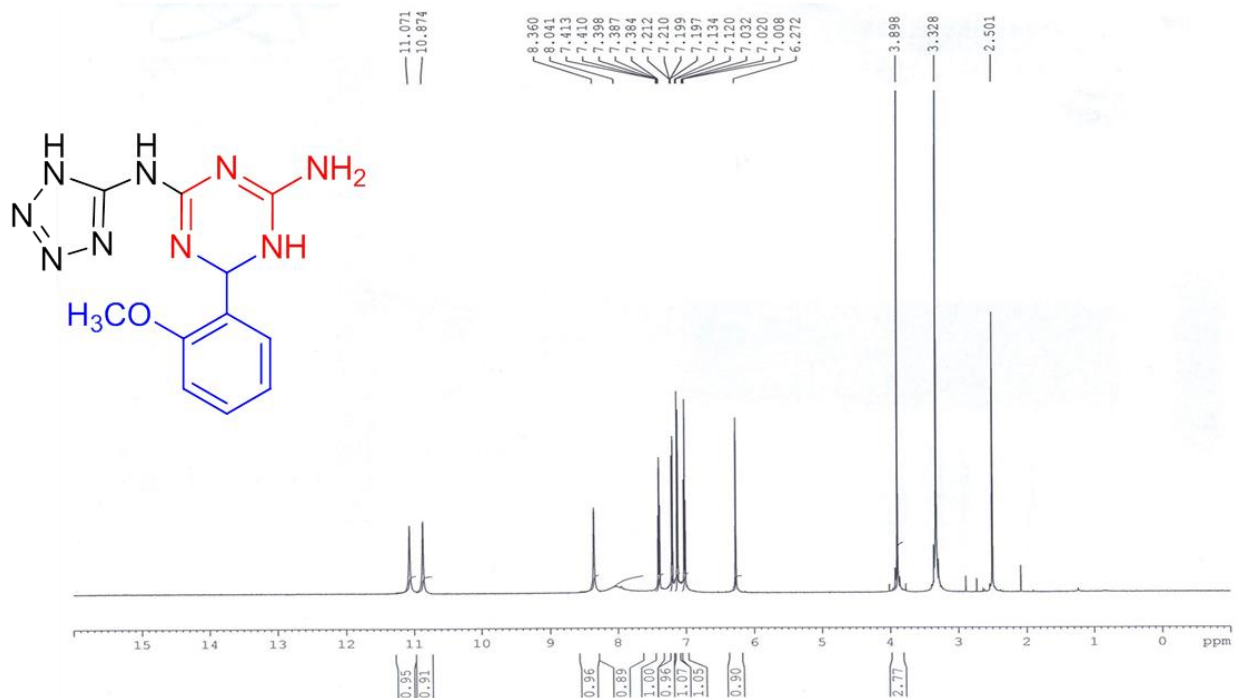
4d ¹³C NMR spectrum (150 MHz, DMSO-*d*₆).



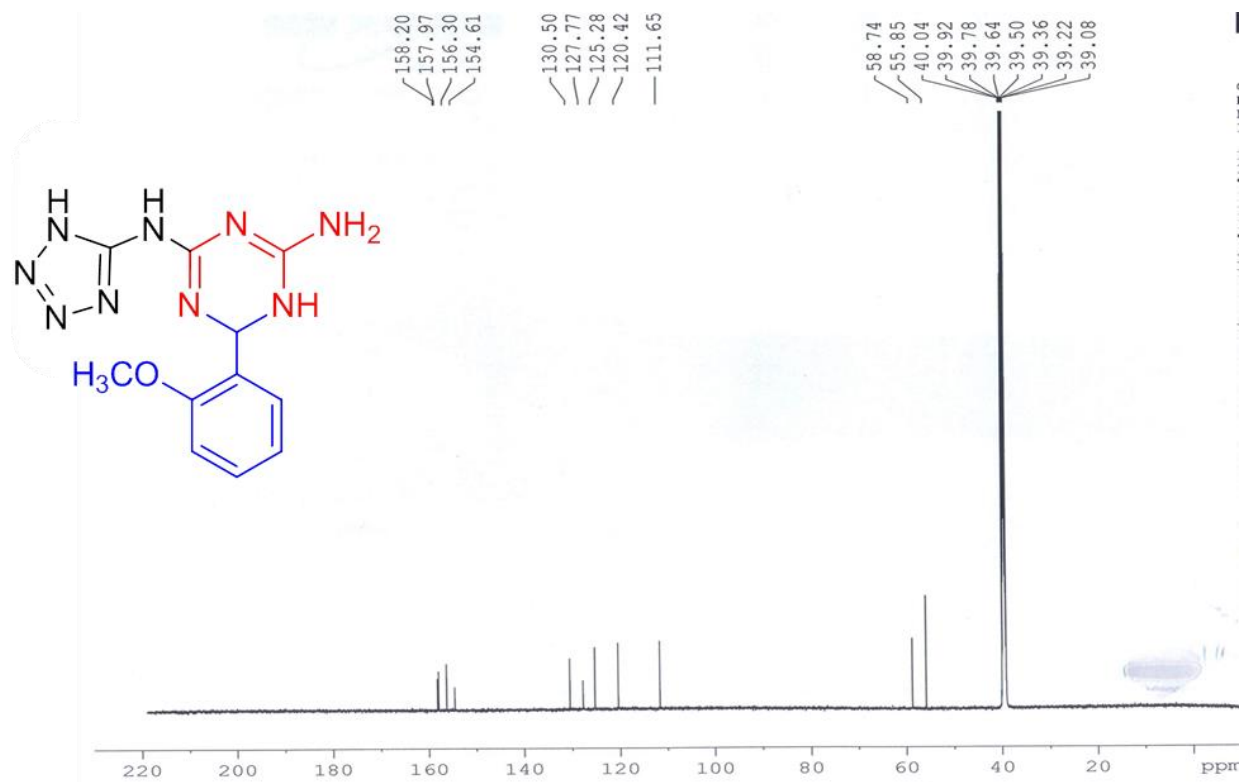
6-(2-Methoxyphenyl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4e).

This compound is novel.

4e ¹H NMR spectrum (600 MHz, DMSO-*d*₆).

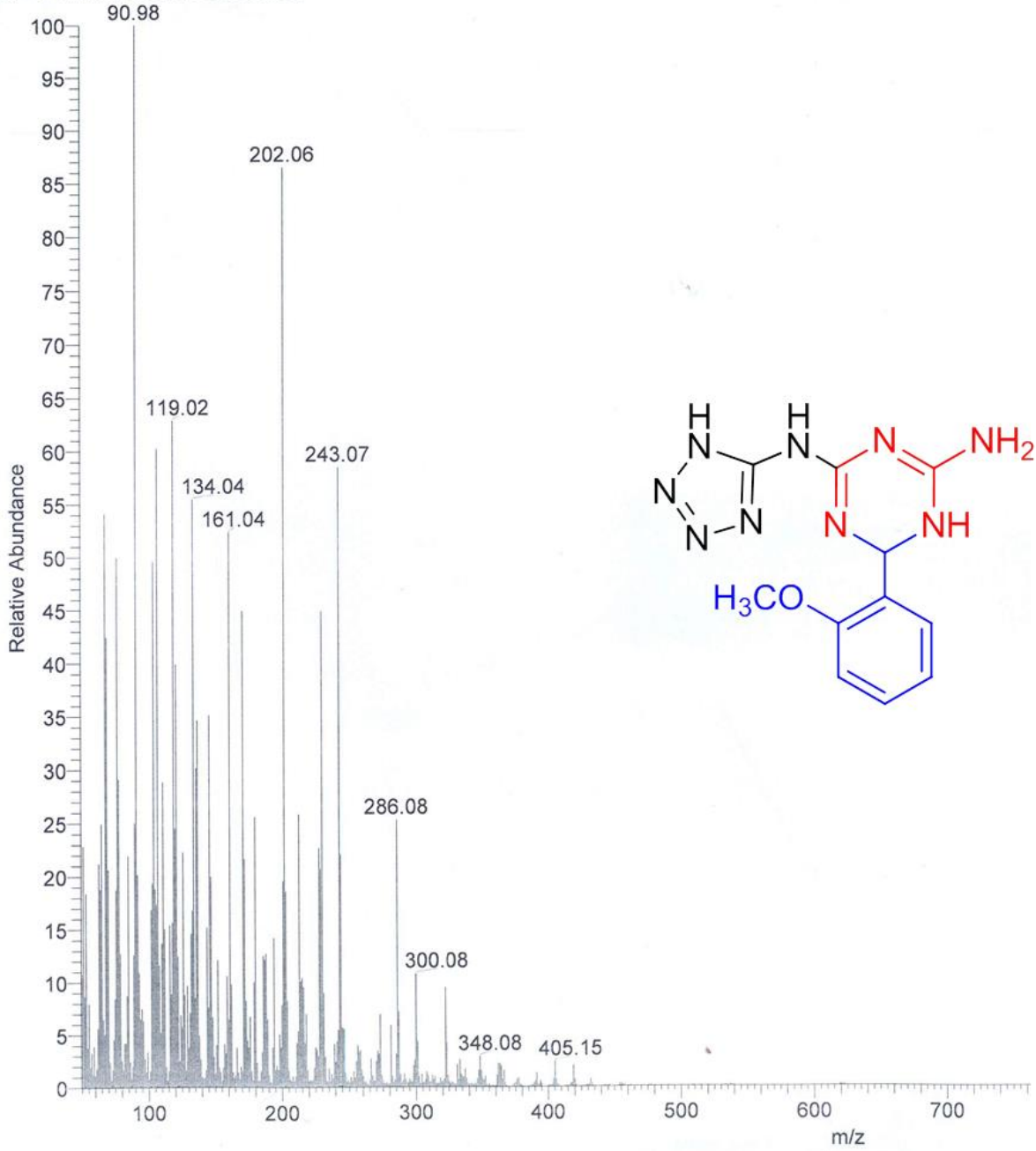


4e ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$).



4e Mass spectrum.

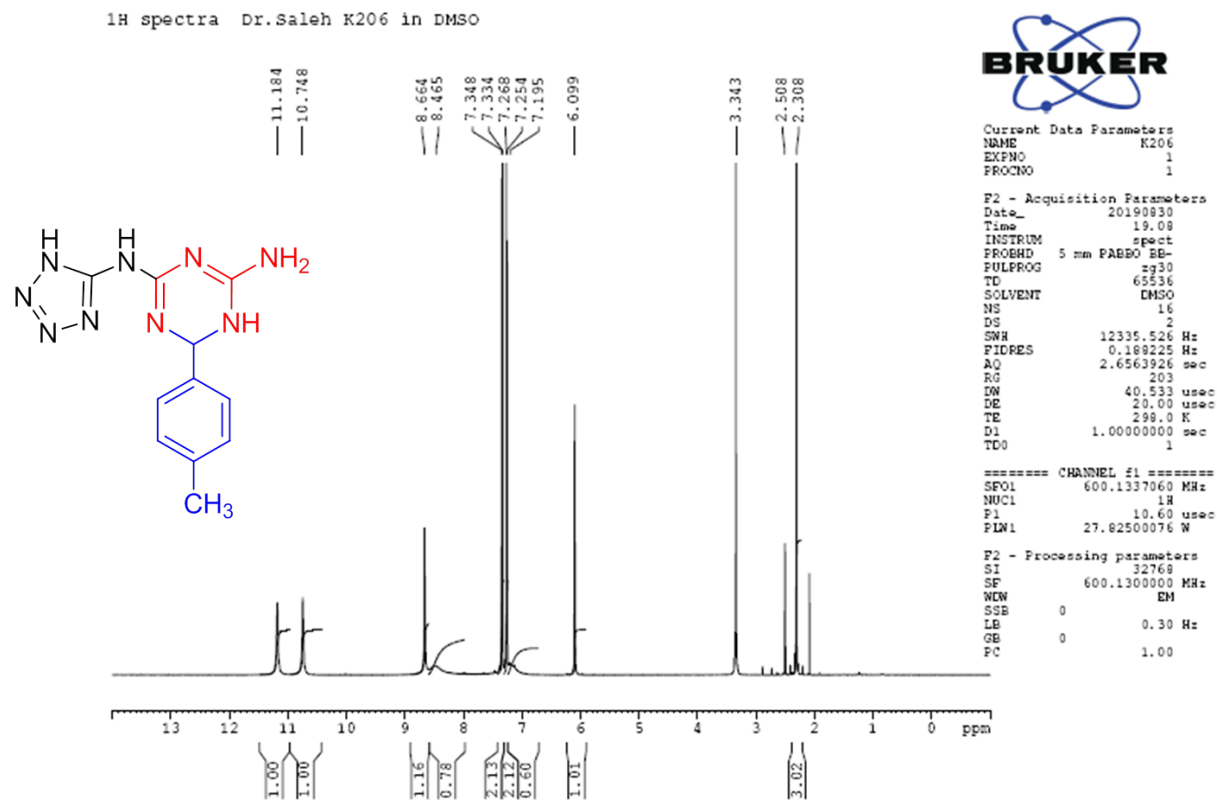
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T: + c EI Full ms [49.50-1200.50]

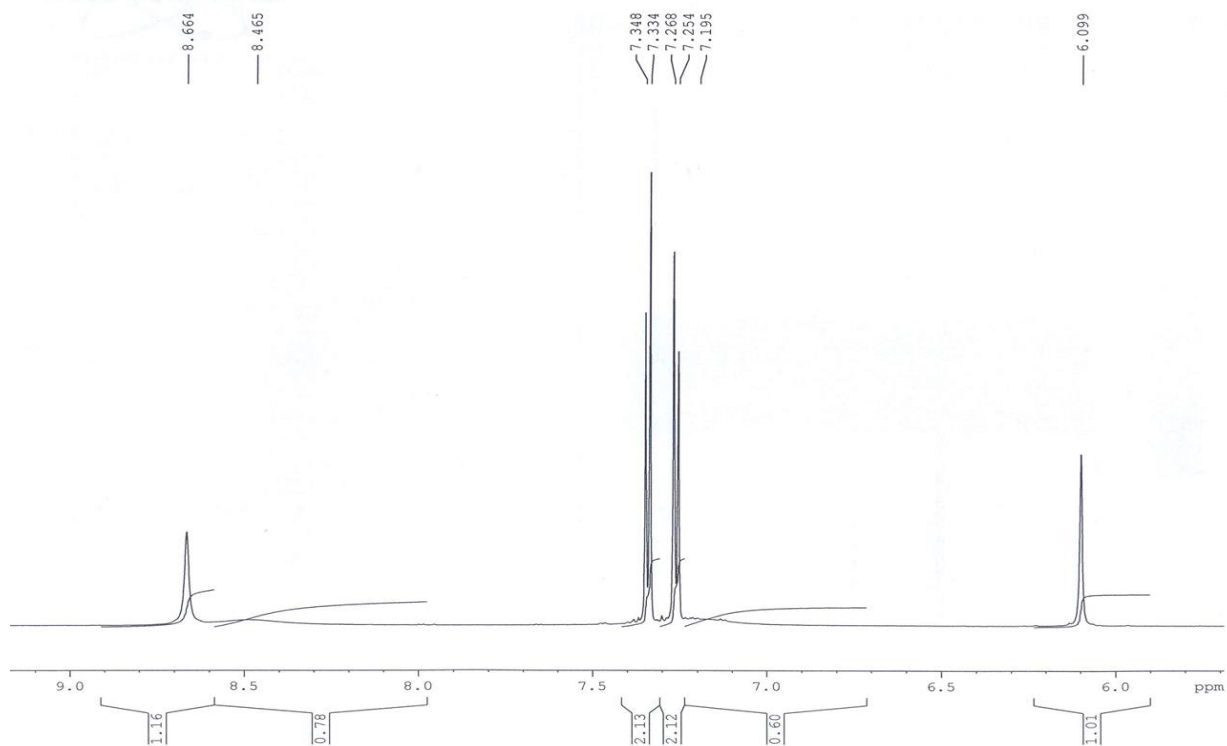


6-(4-Methylphenyl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4f).

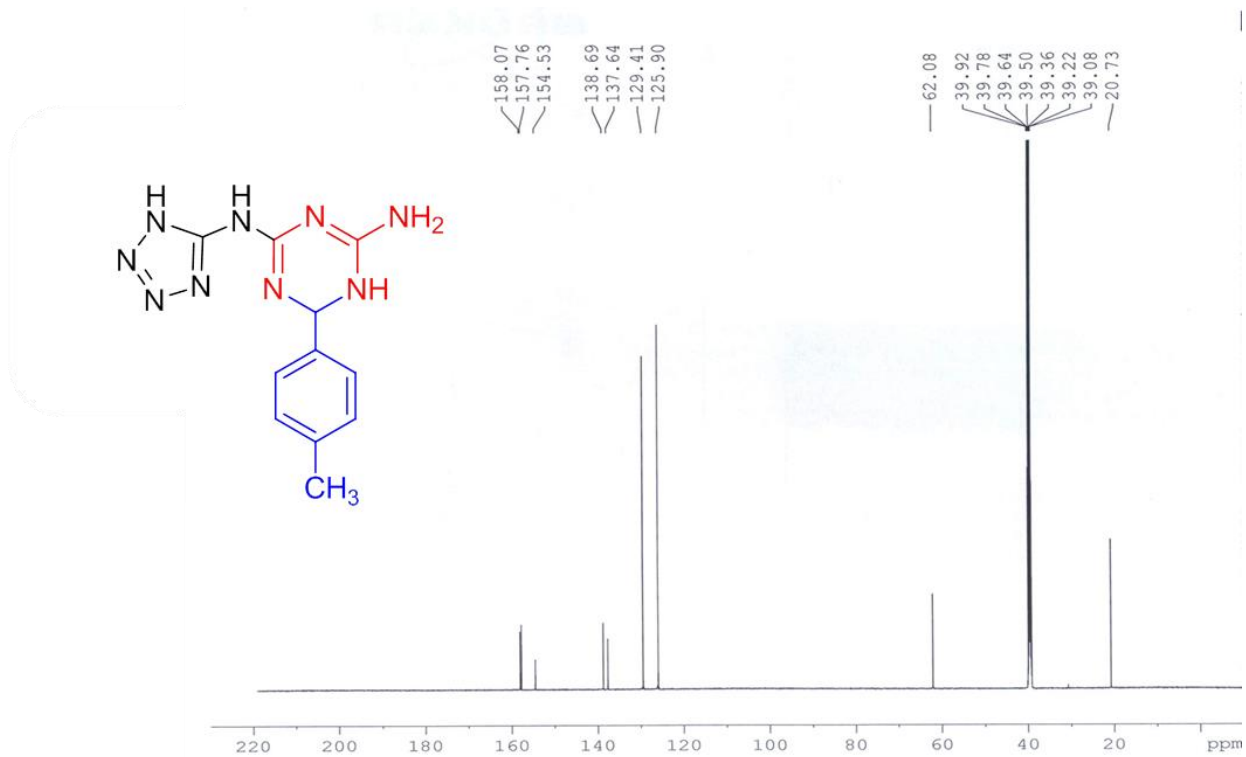
This compound is novel.

4f ¹H NMR spectrum (600 MHz, DMSO-*d*₆).





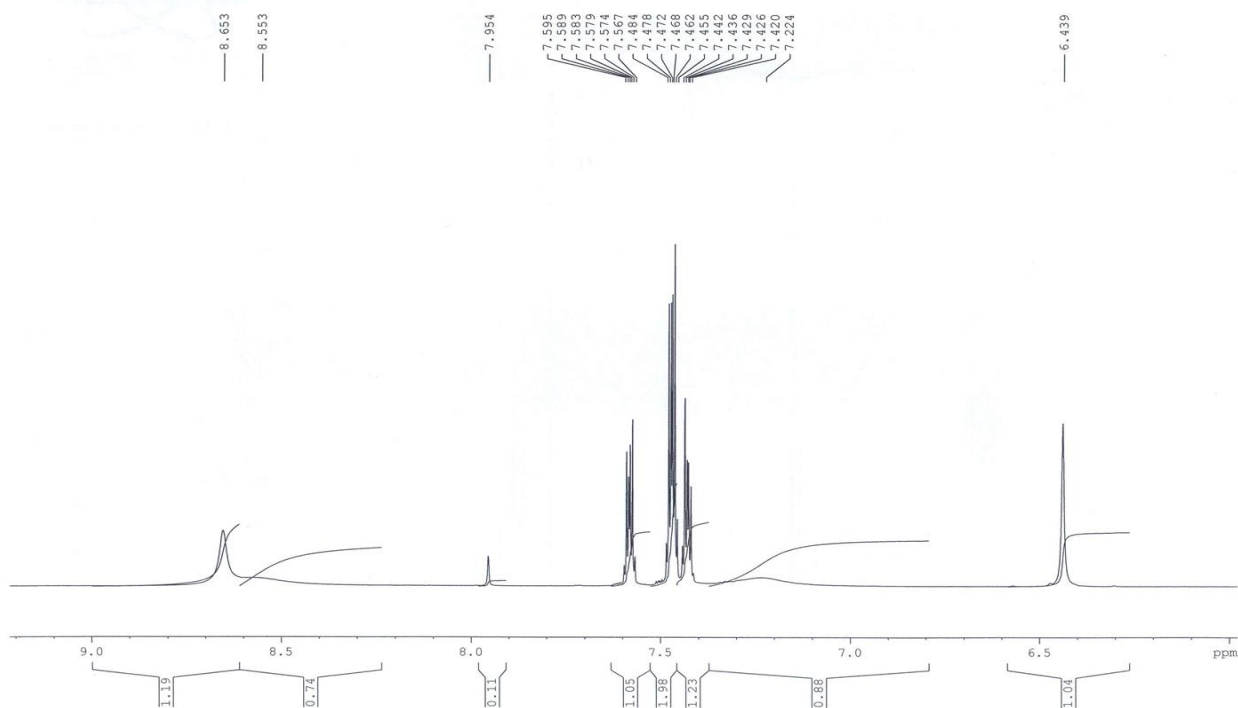
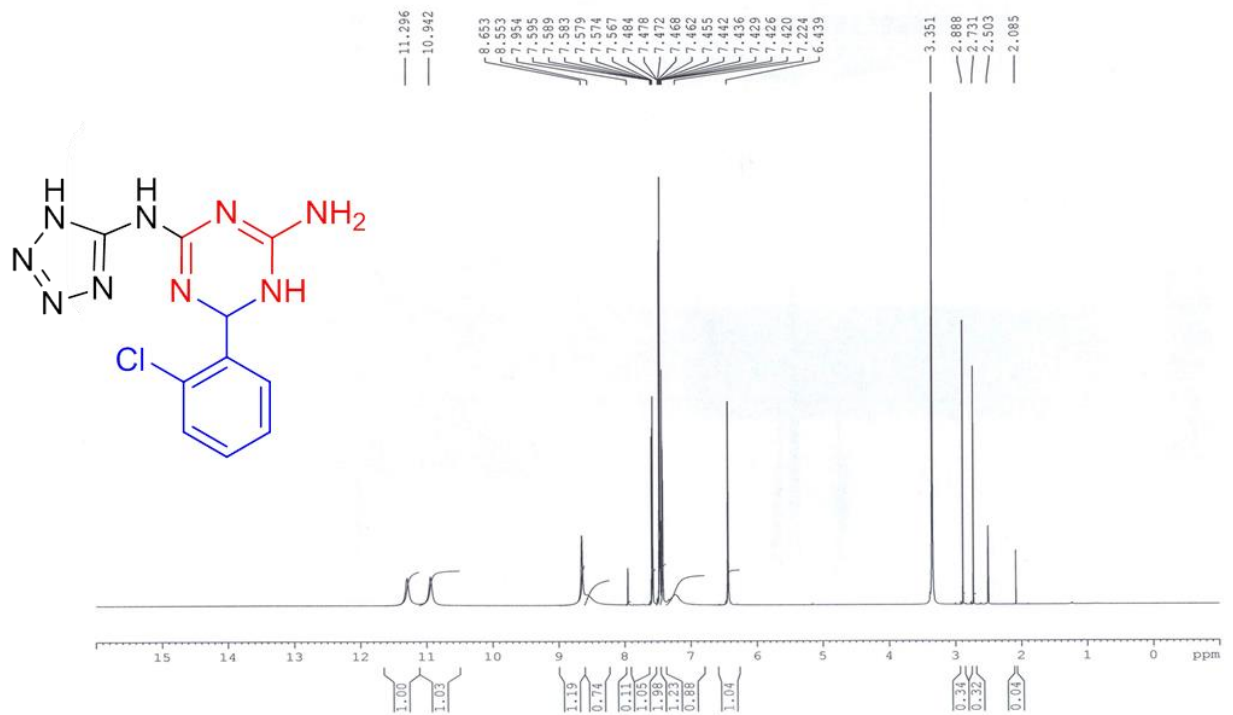
4f ^{13}C NMR spectrum (150 MHz, DMSO-d_6).



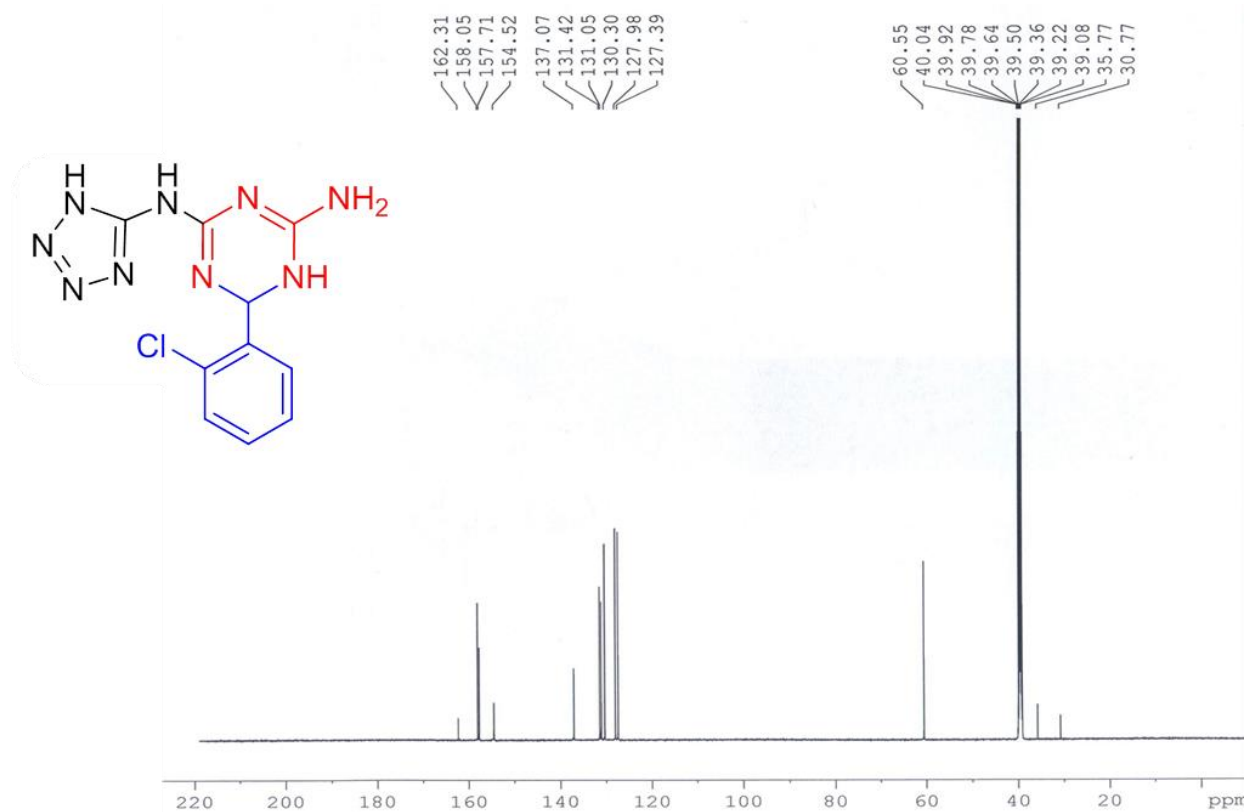
6-(2-Chlorophenyl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4g).

This compound is novel.

4g ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



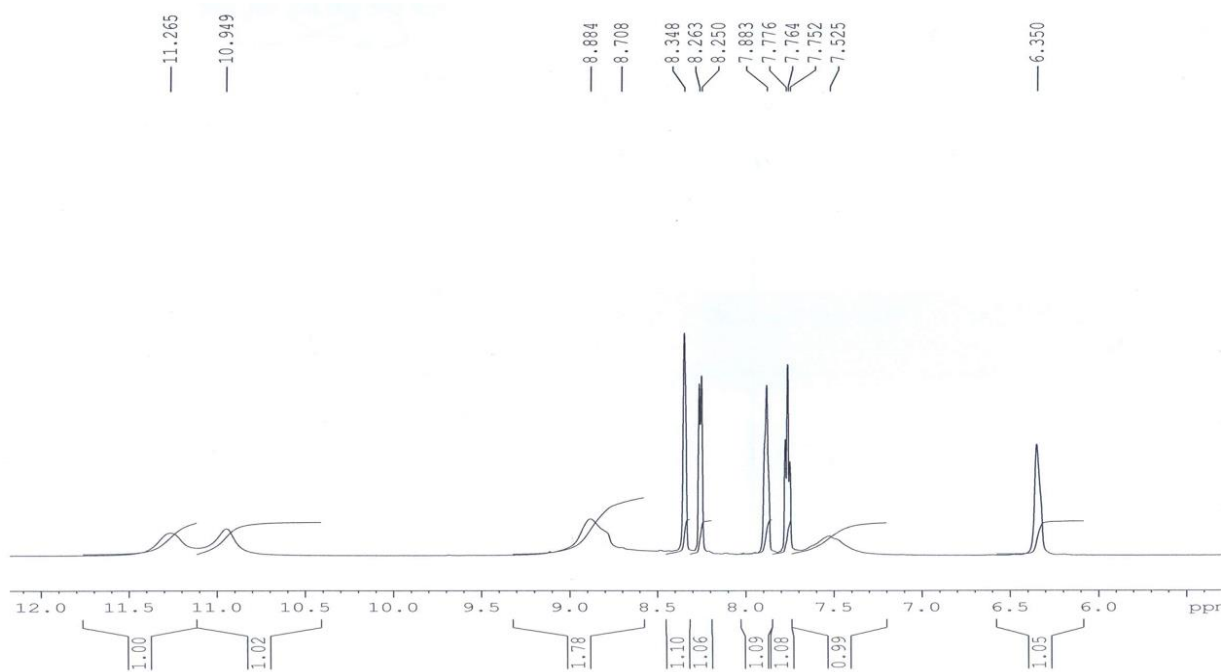
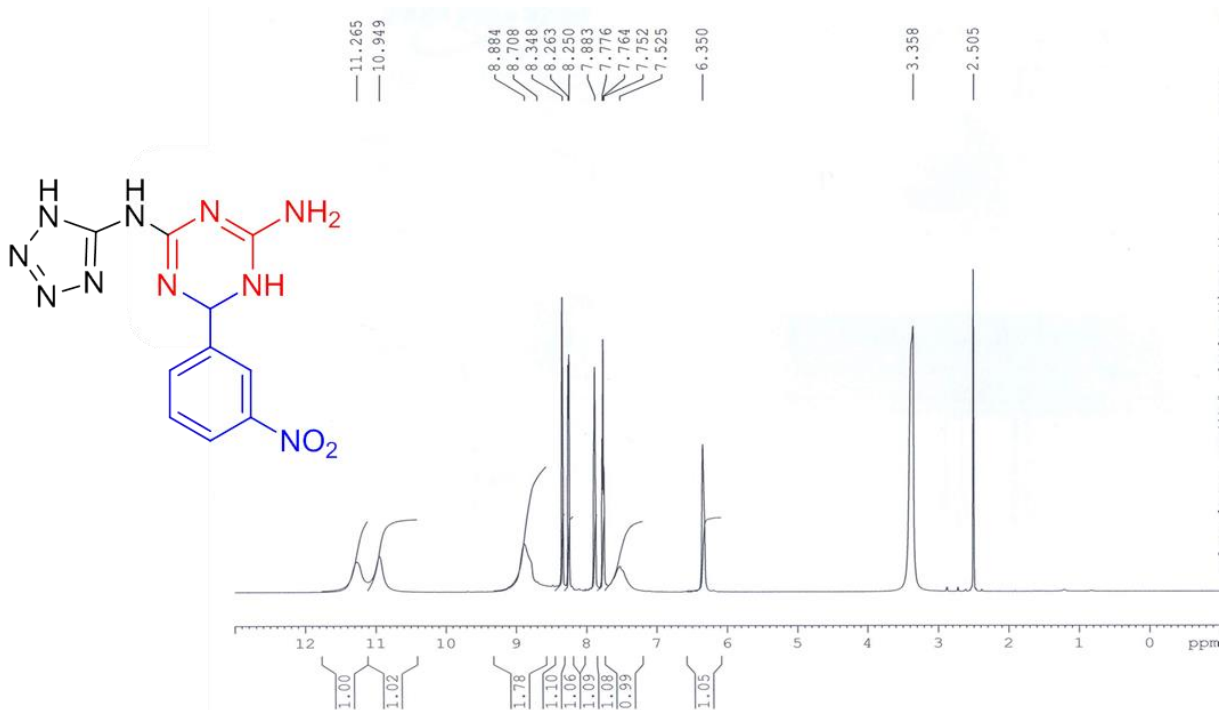
4g ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$).



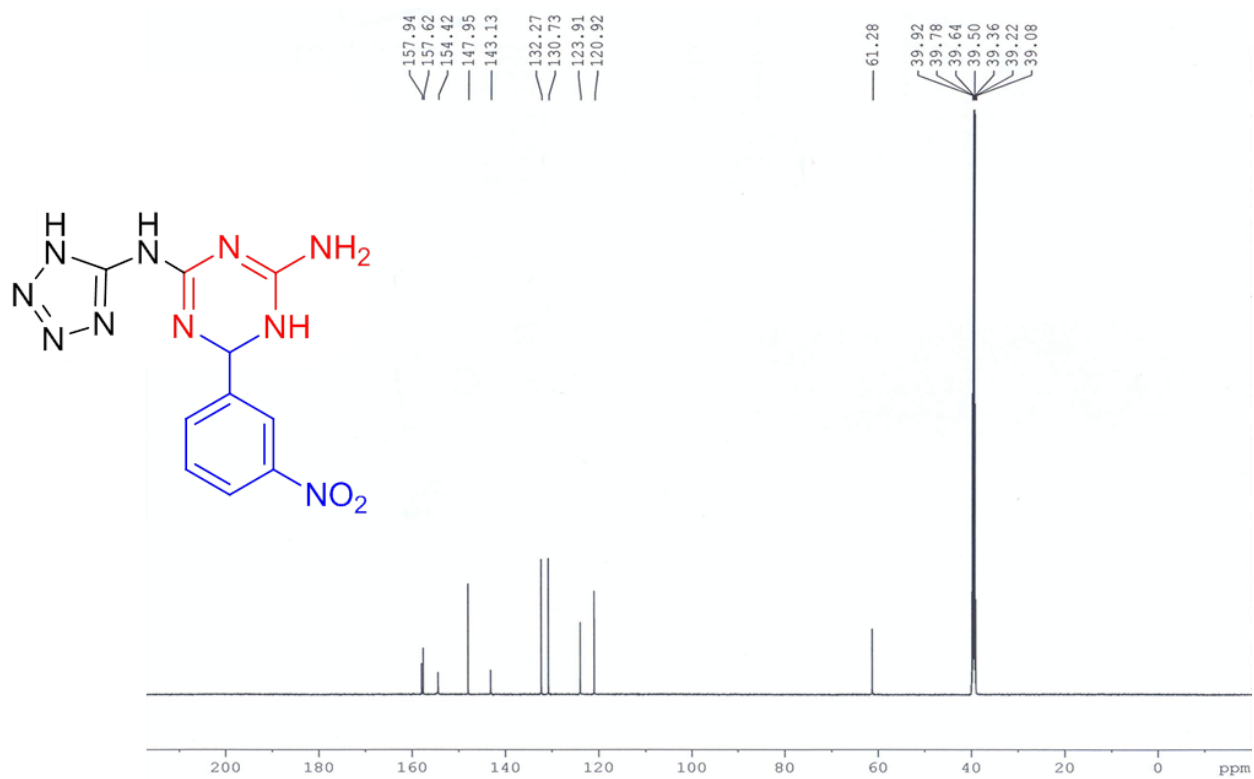
6-(3-Nitrophenyl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4h).

This compound is novel.

4h ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



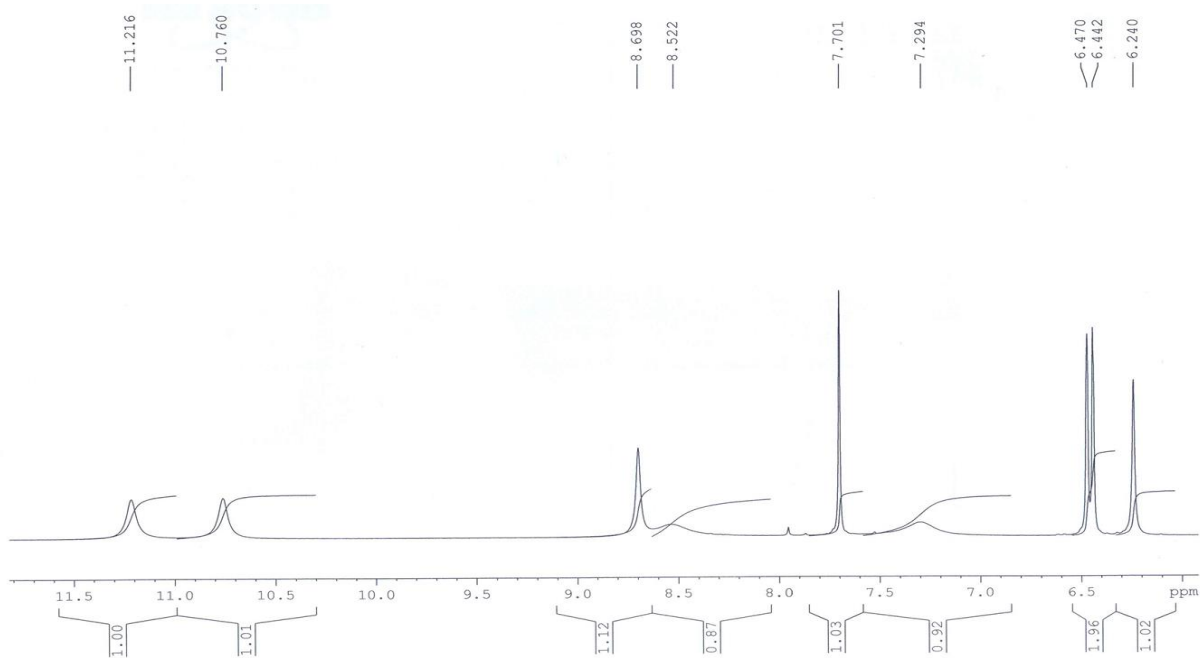
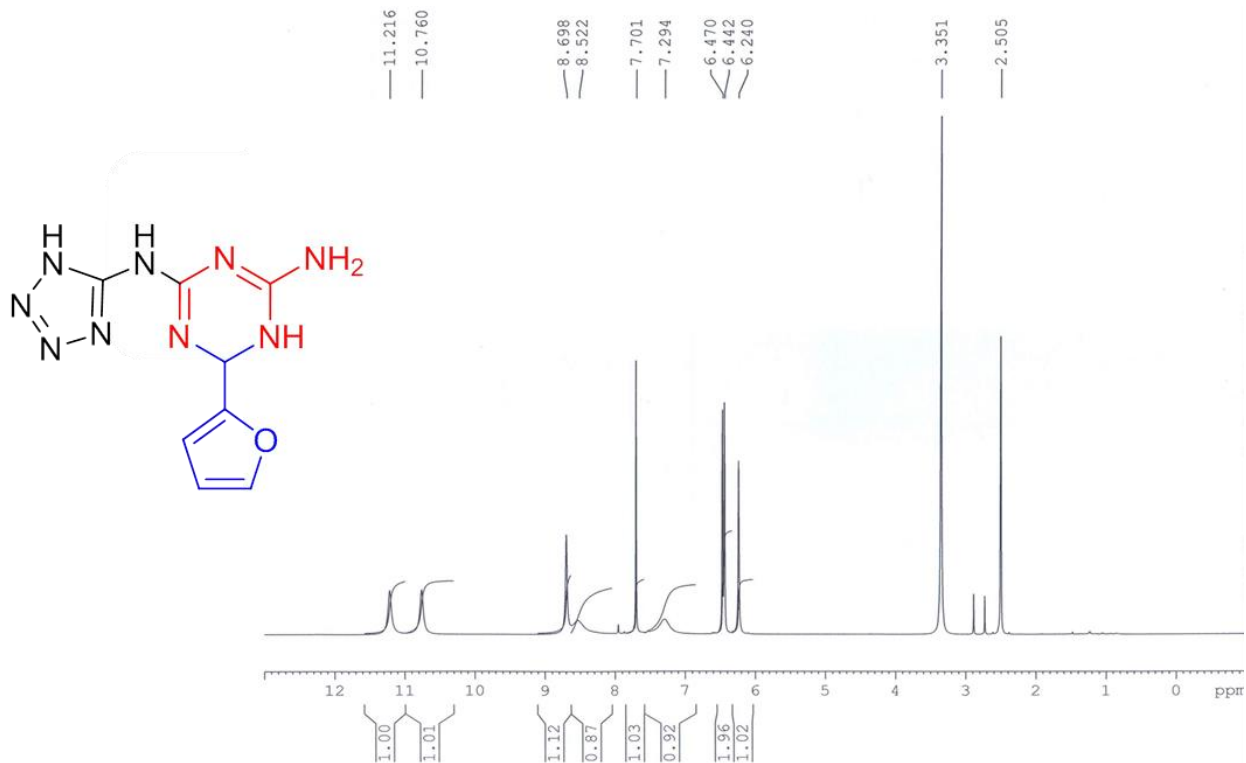
4h ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$).



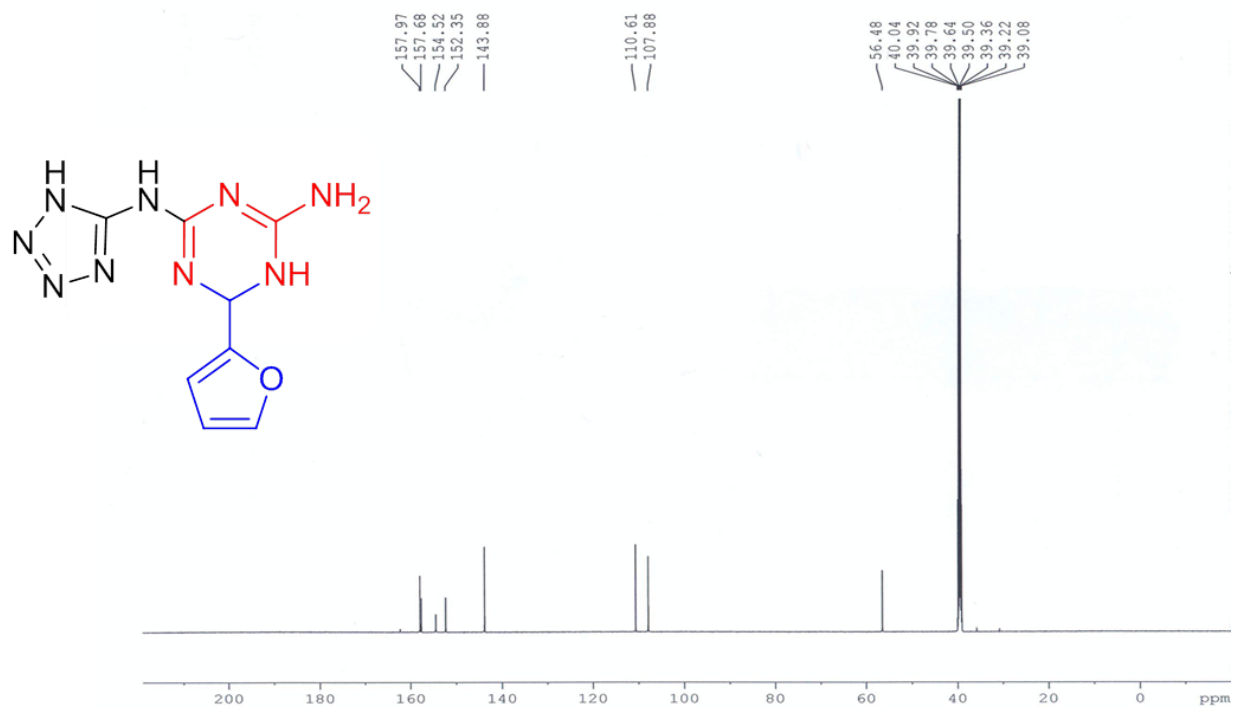
6-(Furan-2-yl)-N²-(5H-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4i).

This compound is novel.

4i ¹H NMR spectrum (600 MHz, DMSO-*d*₆).

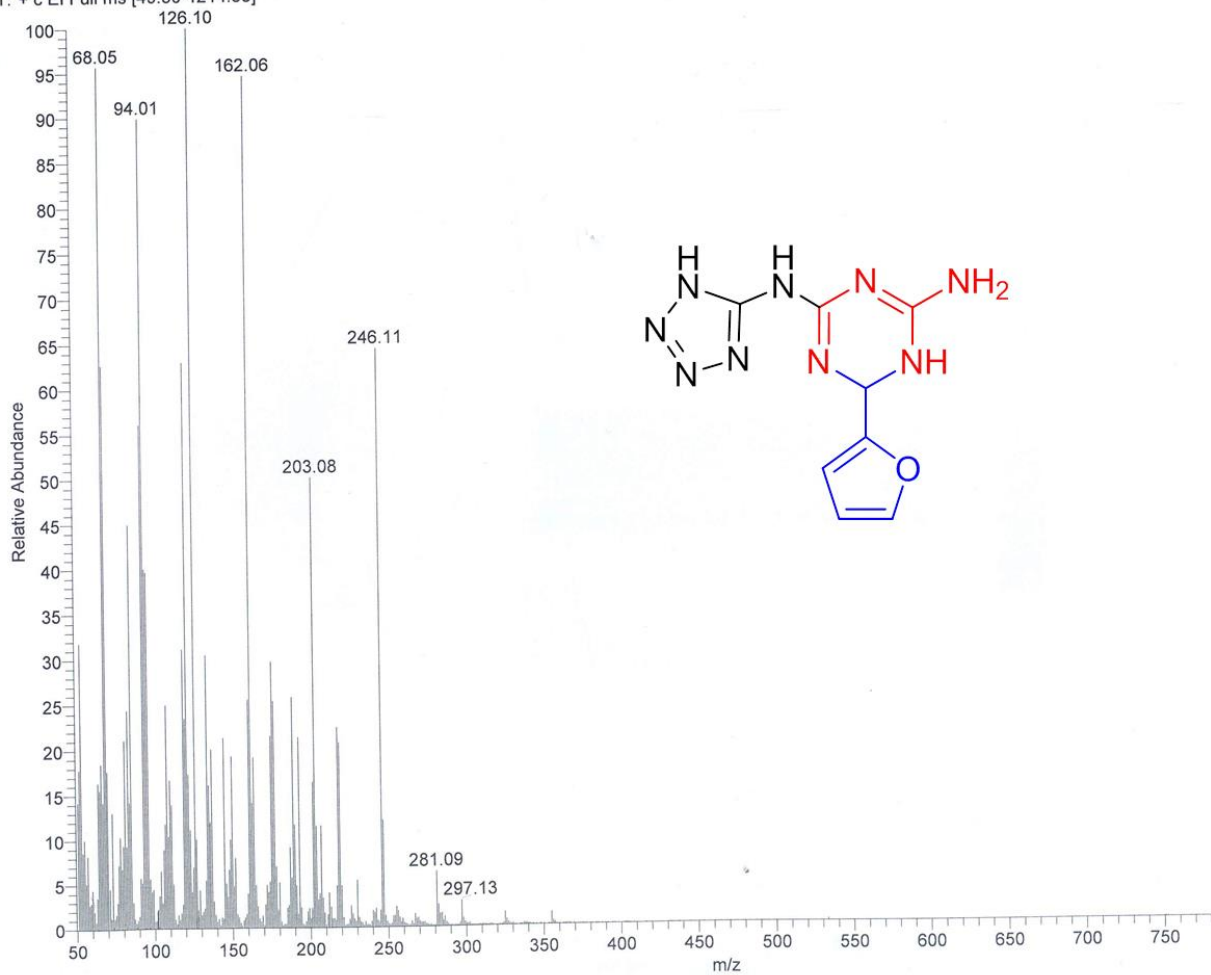


4i ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$).



4i Mass spectrum

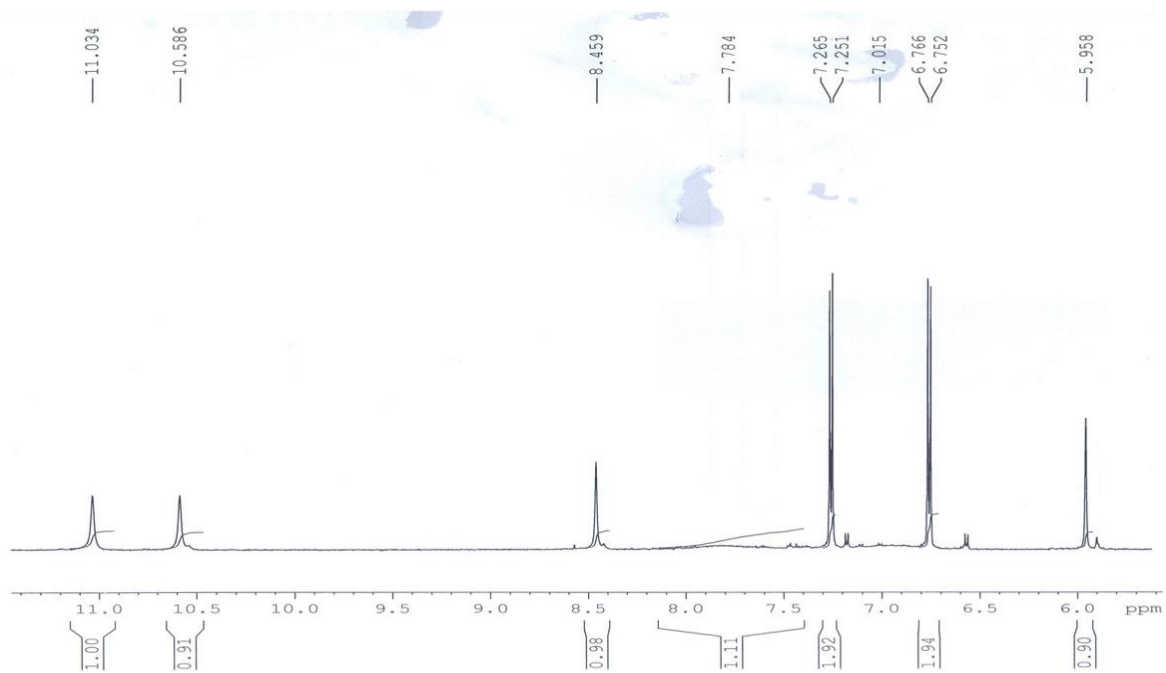
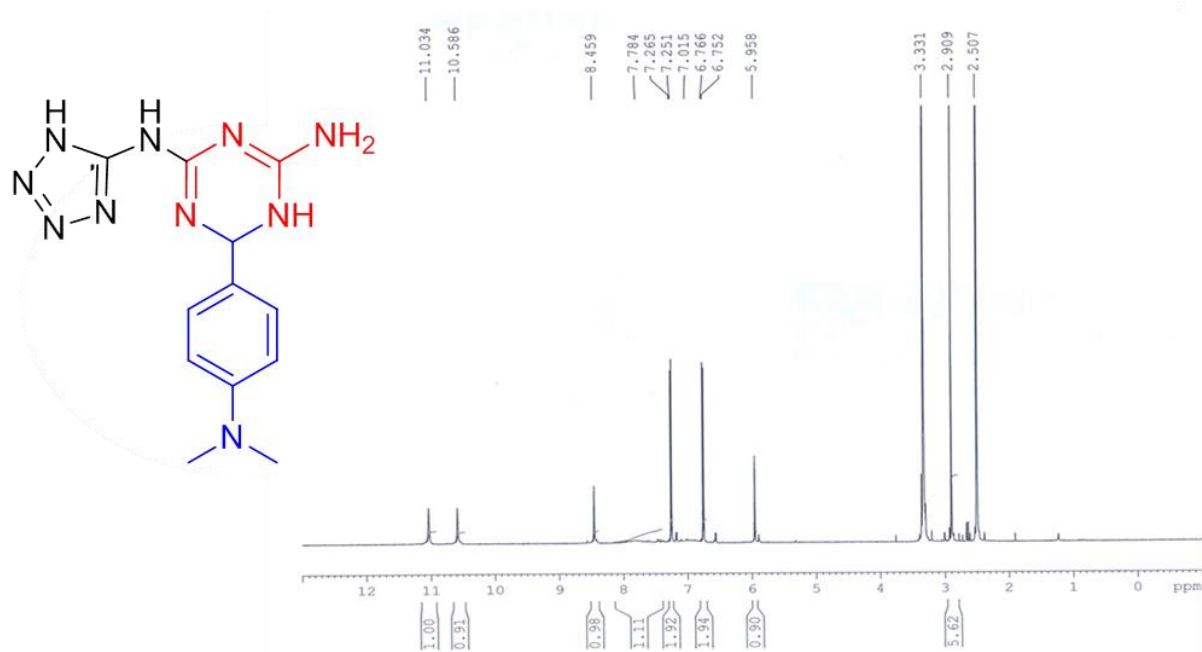
K10 #243 RT: 11.77 AV: 1 NL: 1.15E6
T: + c EI Full ms [49.50-1214.53]



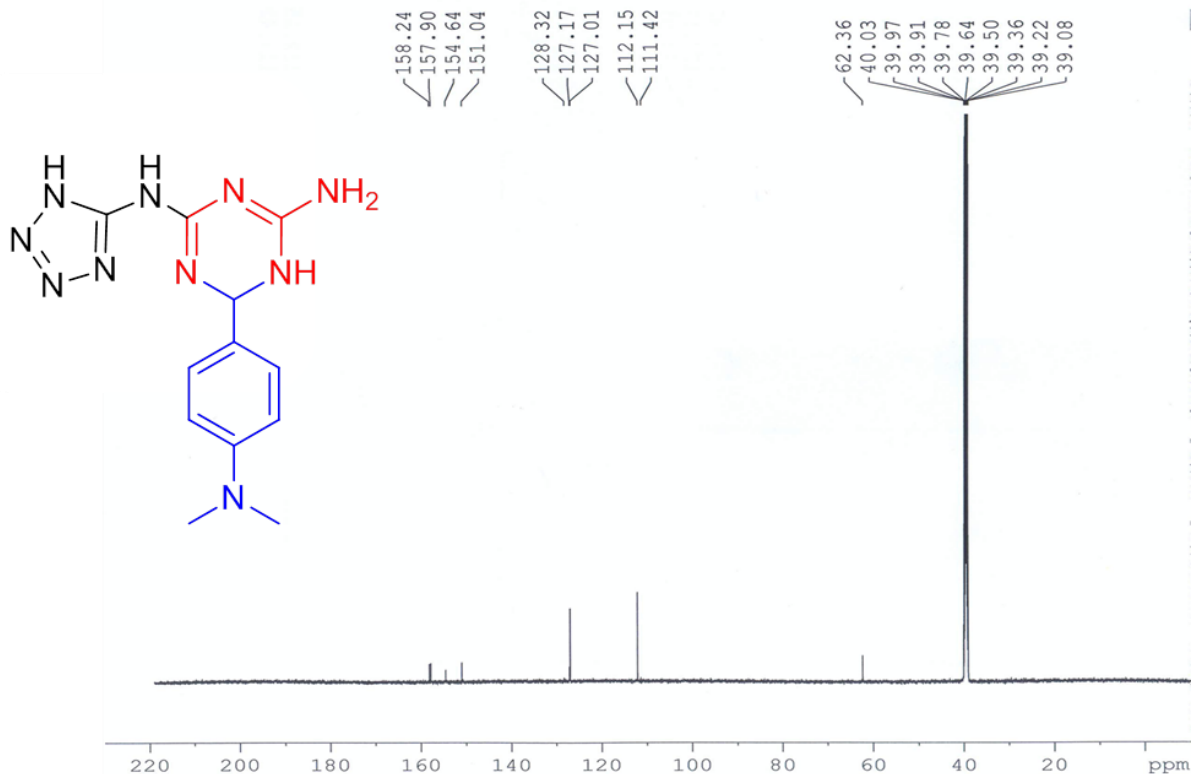
6-(4-*N,N*-Dimethylaminophenyl)-*N*²-(5*H*-tetrazol-5-yl)-5,6-dihydro-1,3,5-triazine-2,4-diamine (4j).

This compound is novel.

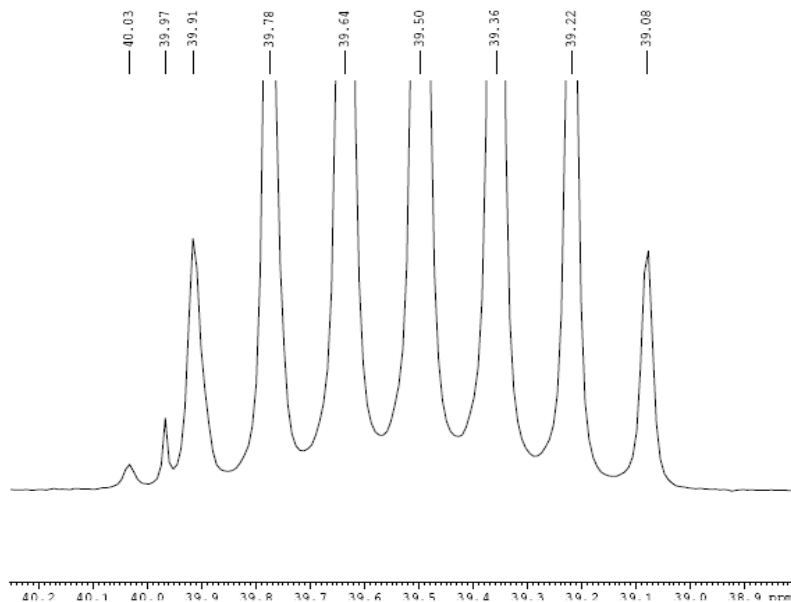
4j ¹H NMR spectrum (600 MHz, DMSO-*d*₆).



4j ¹³C NMR spectrum (150 MHz, DMSO-d₆).



¹³C decoupled spectra Dr.Saleh K211 in DMSO



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Current Data Parameters
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EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20190829
Time     9.42
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PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       10240
DS       4
SWH      36057.691 Hz
FIDRES   0.550197 Hz
AQ       0.9087659 sec
RG       203
DM       13.867 usec
DE       60.00 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0

===== CHANNEL f1 =====
SF01    150.9178979 MHz
NUC1    13C
P1      8.80 usec
PLW1    78.13500214 W

===== CHANNEL f2 =====
SF02    600.1324005 MHz
NUC2    1H
CPDPRG2 waltz65
PCPD2   70.00 usec
PLW2    27.82500076 W
PLW12   0.63804001 W
PLW13   0.31264001 W

F2 - Processing parameters
SI      32768
SF      150.9028824 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
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¹³C decoupled spectra Dr.Saleh K211 in DMSO

