

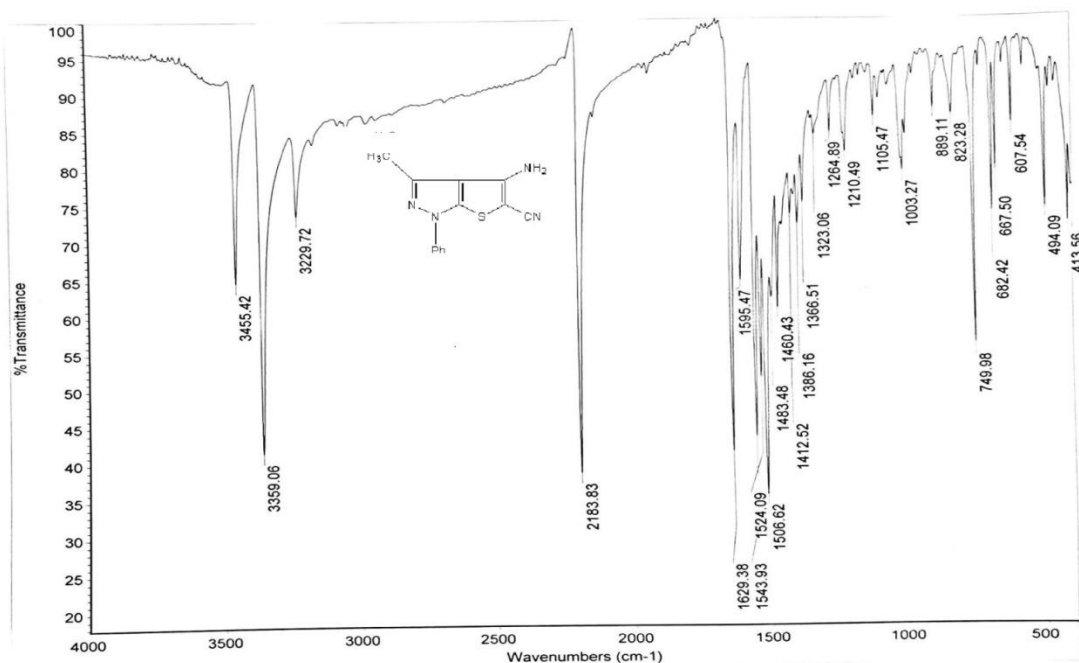
## Supplementary Information

### A Convenient Synthesis, Reactions and Biological Activity of Some New 6H-Pyrazolo[4',3':4,5]thieno[3,2-d][1,2,3]triazine Compounds as Antibacterial, Anti-Fungal and Anti-Inflammatory Agents

Remon M. Zaki,\*<sup>a</sup> Adel M. Kamal El-Dean,<sup>a</sup> Shaban M. Radwan<sup>a</sup> and Ahmed F. Saber<sup>a</sup>

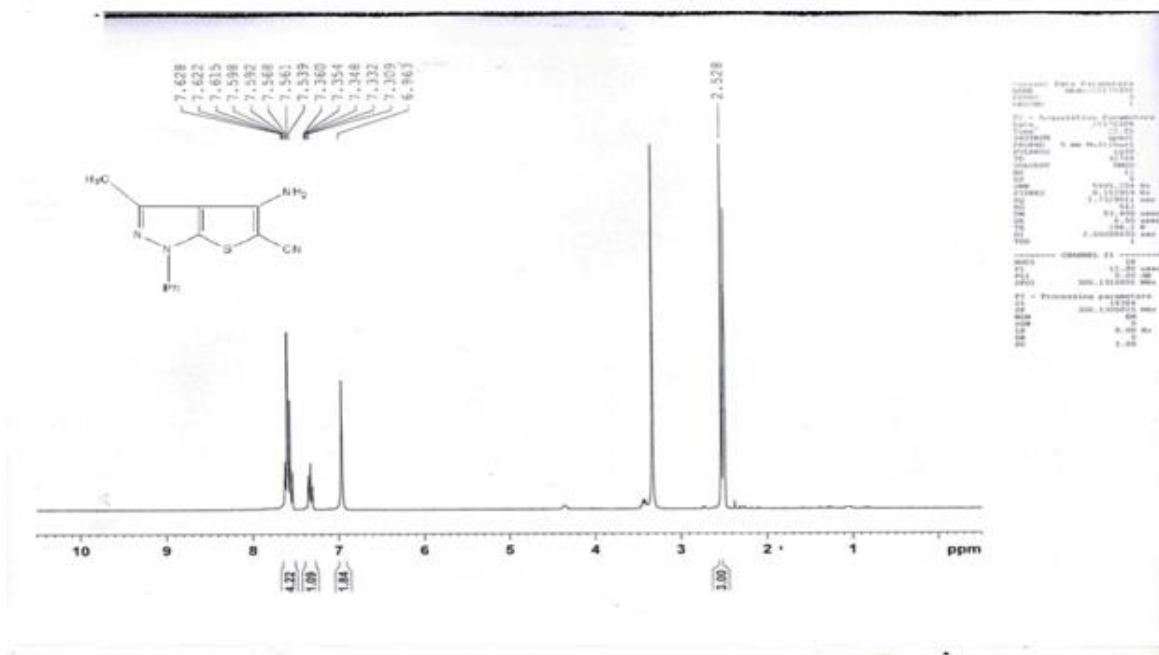
<sup>a</sup>Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt

Spectral analyses

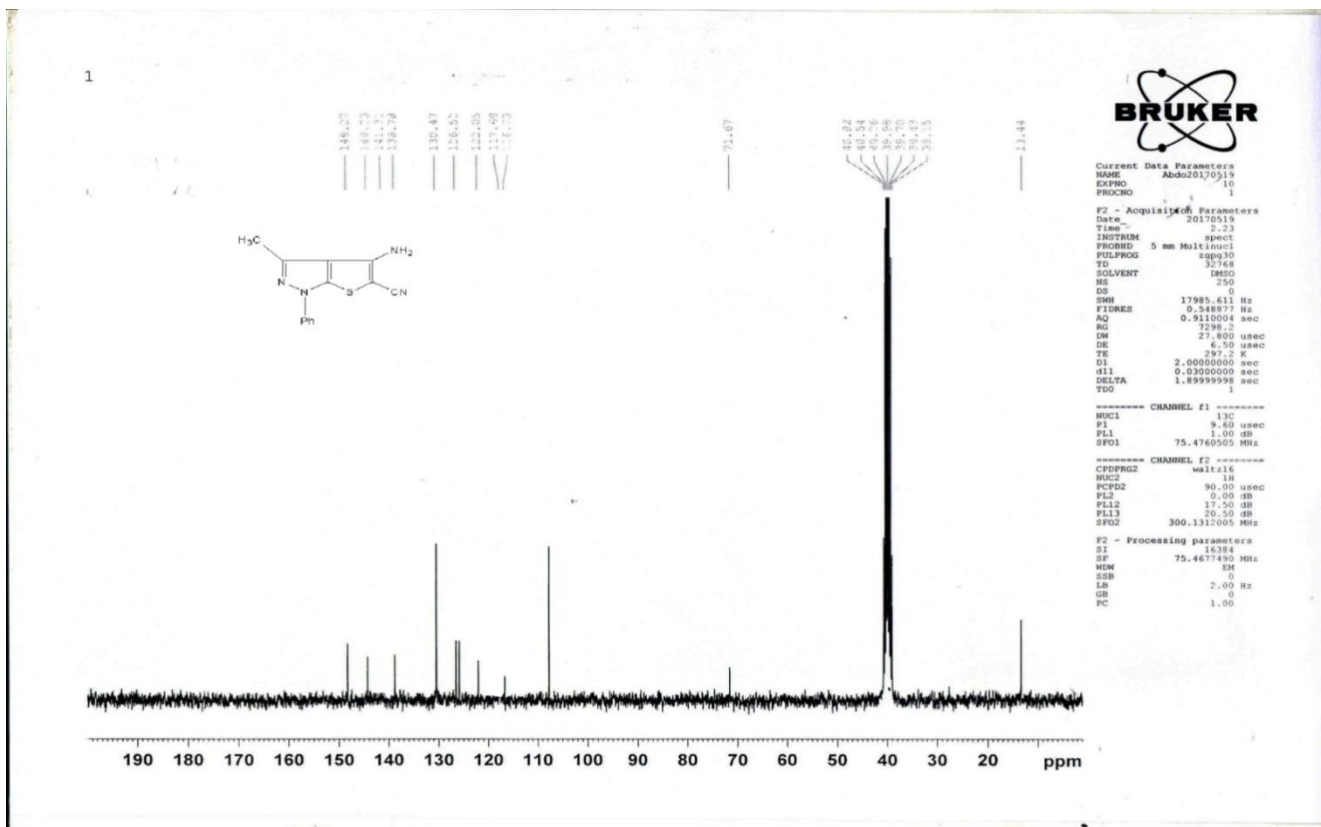


**Figure S1.** FTIR spectrum (KBr) of amino thienopyrazolecarbonitrile compound 5.

\*e-mail: remonch2003@yahoo.com, remon.asal2015@gmail.com

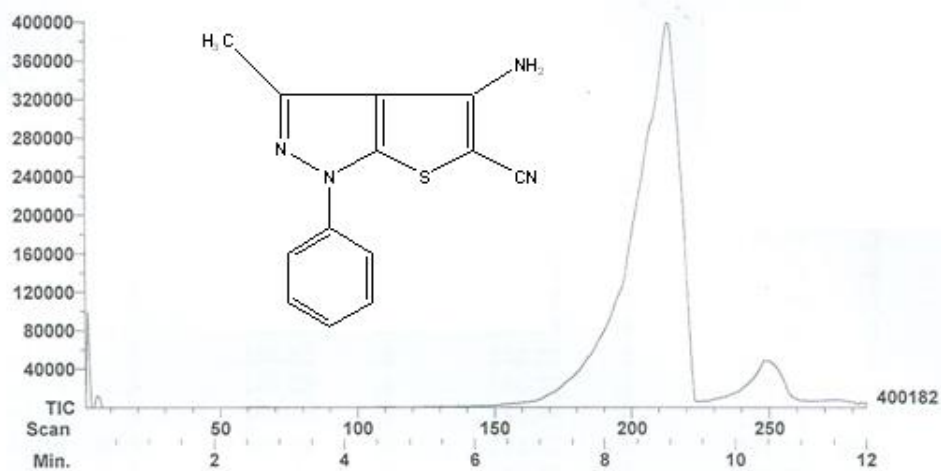


**Figure S2.** <sup>1</sup>H NMR spectrum (300 MHz, DMSO-d<sub>6</sub>) of amino thienopyrazole carbonitrile compound 5.

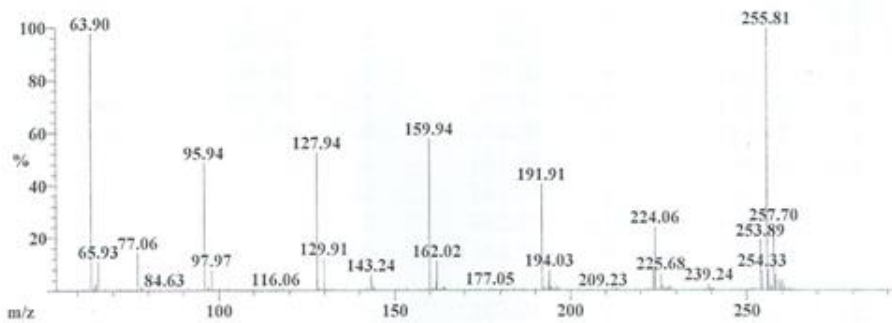


**Figure S3.** <sup>13</sup>C NMR spectrum (300 MHz, DMSO-d<sub>6</sub>) of amino thienopyrazole carbonitrile compound 5.

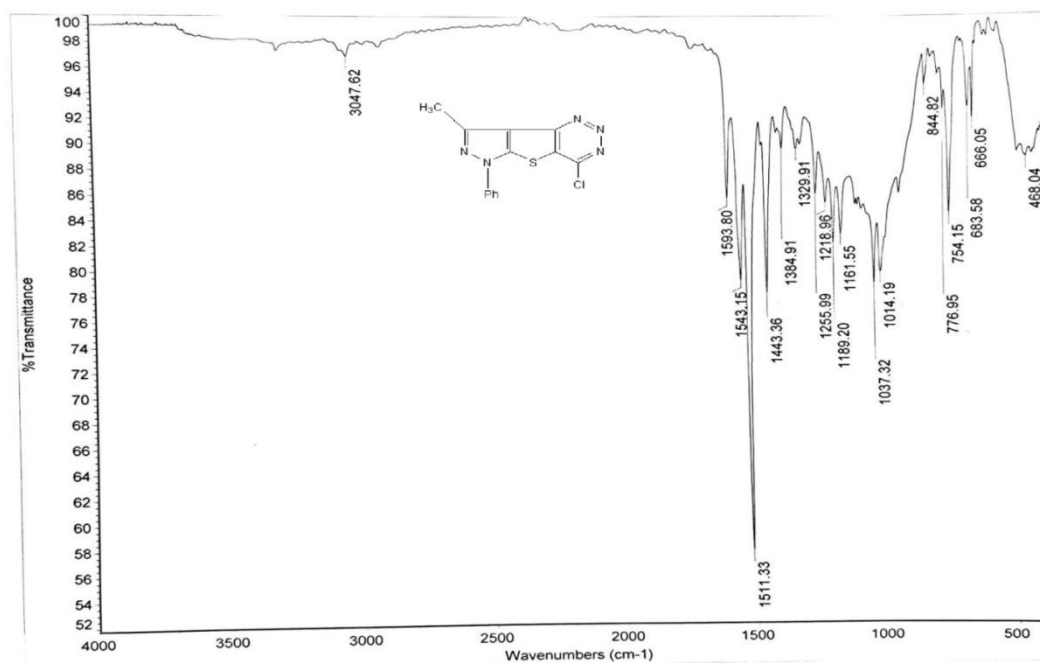
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 Sample: Dr/AdelKamal Run By: Souzan  
 Instrument: JEOL JMS600 Printed by: Souzan  
 Inlet: My Inlet Ionization mode: EI+



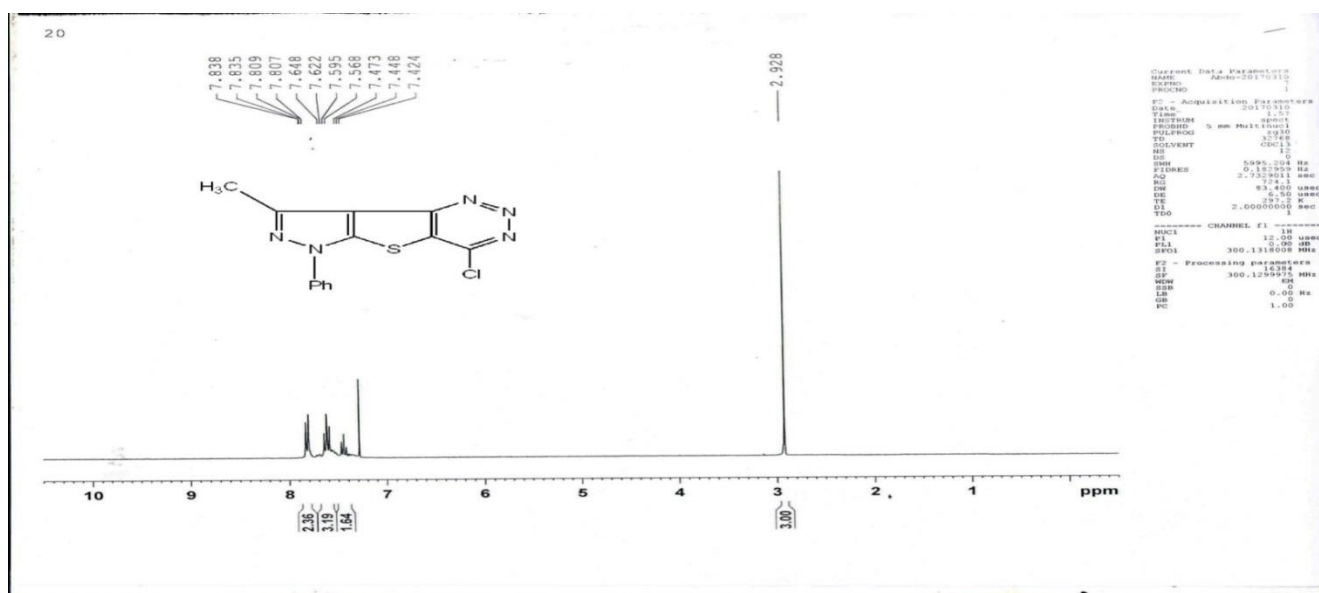
Scan: 148-276 (224-228) R.T.: 8:55.326  
 Base: m/z 256; .9%FS TIC: 64315 #Ions: 429



**Figure S4.** Mass spectrum of the o-amino carbonitrile compound 5.



**Figure S5.** FTIR spectrum (KBr) of chlorotriazine compound compound 6.



**Figure S6.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CDCl}_3$ ) of chlorotriazine compound 6.

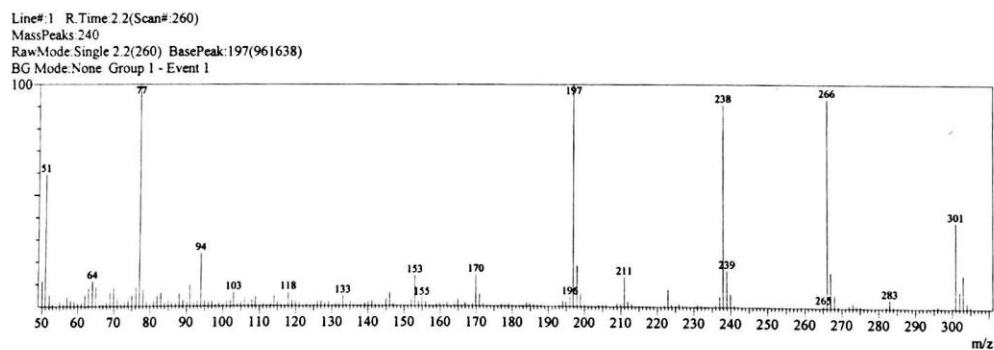
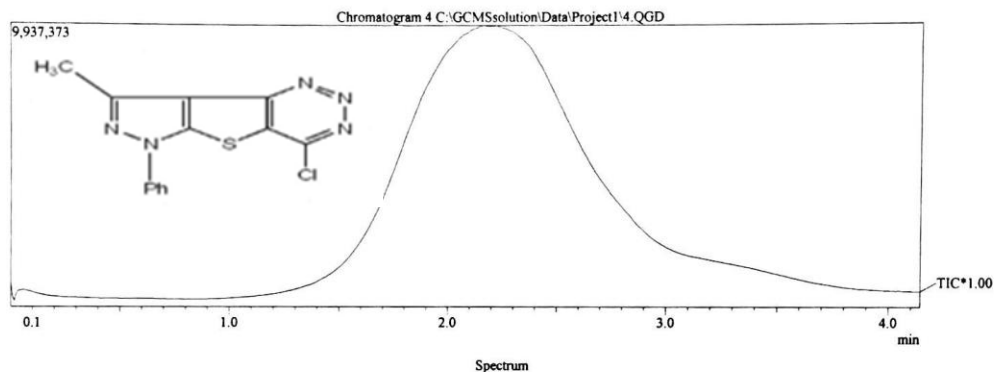
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Micro Analytical Center**

**DI Analysis  
Shimadzu Qp-2010 Plus**



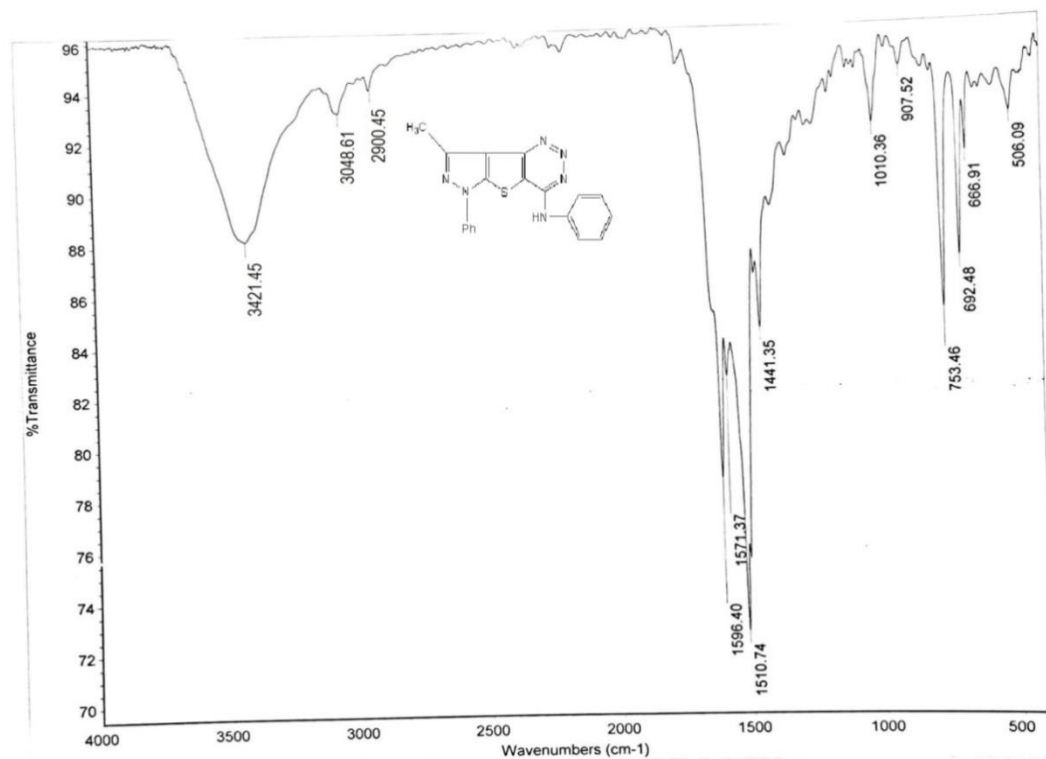
|                           |                                                     |                              |
|---------------------------|-----------------------------------------------------|------------------------------|
| <b>Sample Information</b> |                                                     | <b>Method</b>                |
| Analyzed by               | : Dr. Mai Younis                                    | ==== Analytical Line 1 ===== |
| Analyzed                  | : 19/04/2017 09:52:54                               | IonSourceTemp :250.00 °C     |
| Sample Name               | : 4                                                 | [MS Table]                   |
| Sample ID                 | :                                                   | --Group 1 - Event 1--        |
| Customer Name             | : Dr. Ahmed Fathy - Science - Asyot                 | Start Time :0.00min          |
| Data File                 | : C:\GCMSsolution\Data\Project1\4.QGD               | End Time :10.00min           |
| Org Data File             | : C:\GCMSsolution\Data\Project1\4.QGD               | ACQ Mode :Scan               |
| Method File               | : C:\GCMSsolution\Data\Project1\High Temperature Op | Event Time :0.50sec          |
| Org Method File           | : C:\GCMSsolution\Data\Project1\High Temperature Op | Scan Speed :1000             |
| Report File               | :                                                   | Start m/z :50.00             |
| Tuning File               | : C:\GCMSsolution\System\Tune1\_default.qgt         | End m/z :500.00              |
| SEndIfSModified by        | : Dr. Mai Younis                                    |                              |
| Modified                  | : 19/04/2017 09:57:05                               |                              |
|                           |                                                     | Electron Voltage : 70 eV     |
|                           |                                                     | Ionization Mode : EI         |

C:\GCMSsolution\Data\Project1\4.QGD

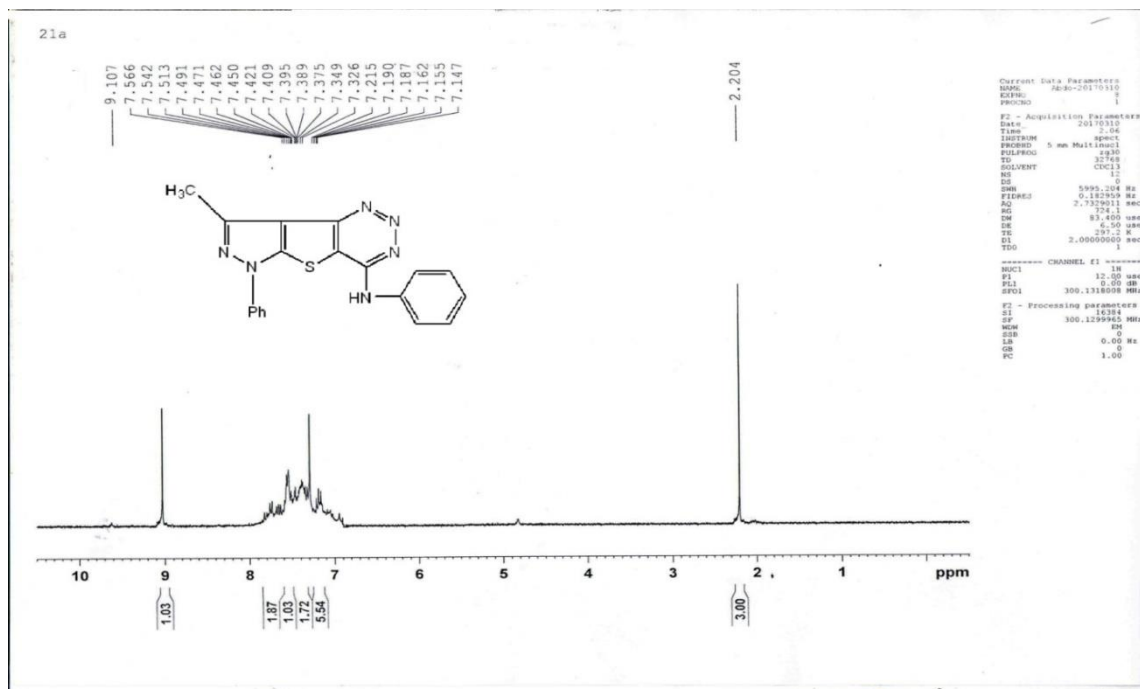


Mass Table  
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MassPeaks:240  
RawMode:Single 2.2(260) BasePeak:197(961638)

**Figure S7.** Mass spectrum of the chlorotriazine compound **6**.



**Figure S8.** FTIR spectrum (KBr) of the phenylaminotriazine compound 7a.



**Figure S9.** <sup>1</sup>H NMR spectrum (300 MHz, CDCl<sub>3</sub>) of the phenylamino-triazine compound 7a.

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**DI Analysis  
Shimadzu Qp-2010 Plus**

Sample Information  
 Analyzed by : Noha Bagato  
 Analyzed : 17/07/2017 12:53:40  
 Sample Name :  
 Sample ID :  
 Customer Name : جامعة اسوط - د احمد قتيبي  
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 Modified : 17/07/2017 01:03:43

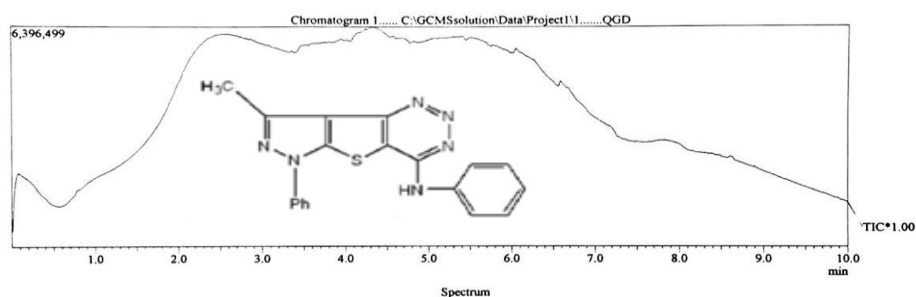
Method

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 Event Time : 0.50sec  
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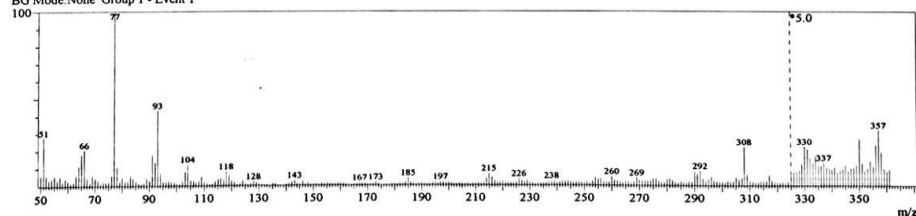
Electron Voltage : 70 eV  
 Ionization Mode : EI



C:\GCMSolution\Data\Project1\1\.....QGD



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 RawMode:Single 7.8(934) BasePeak:77(232892)  
 BG Mode:None Group 1 - Event 1



Mass Table

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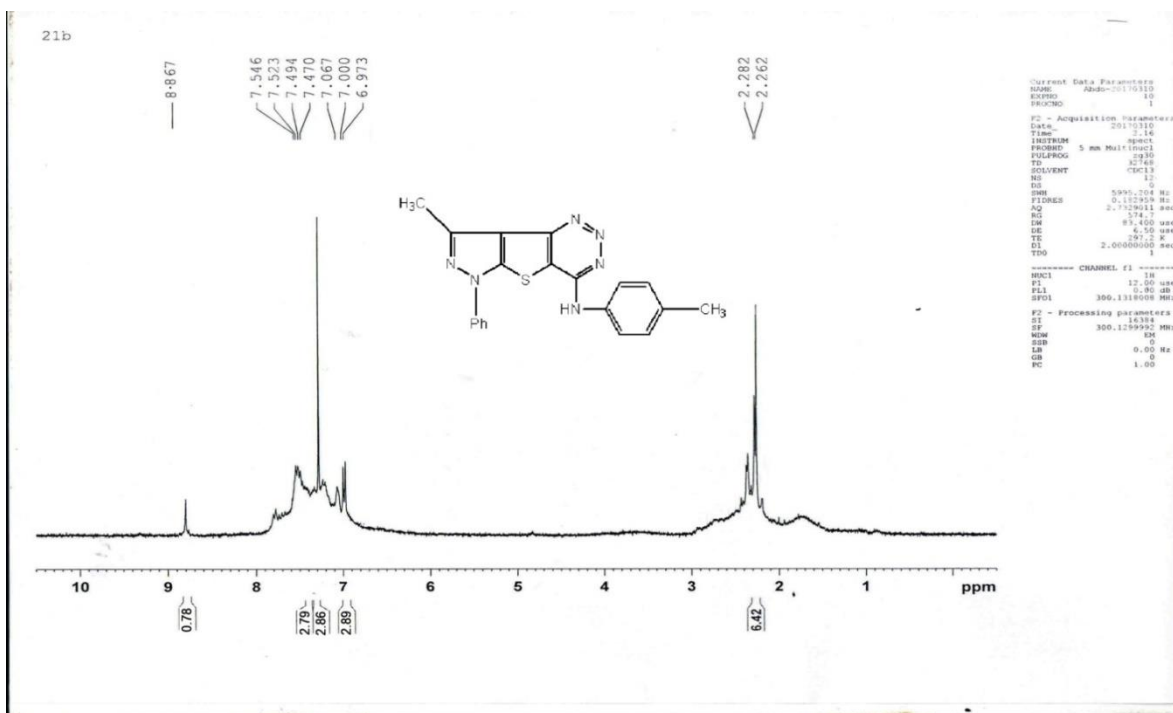
MassPeaks:302

RawMode:Single 7.8(934) BasePeak:77(232892)

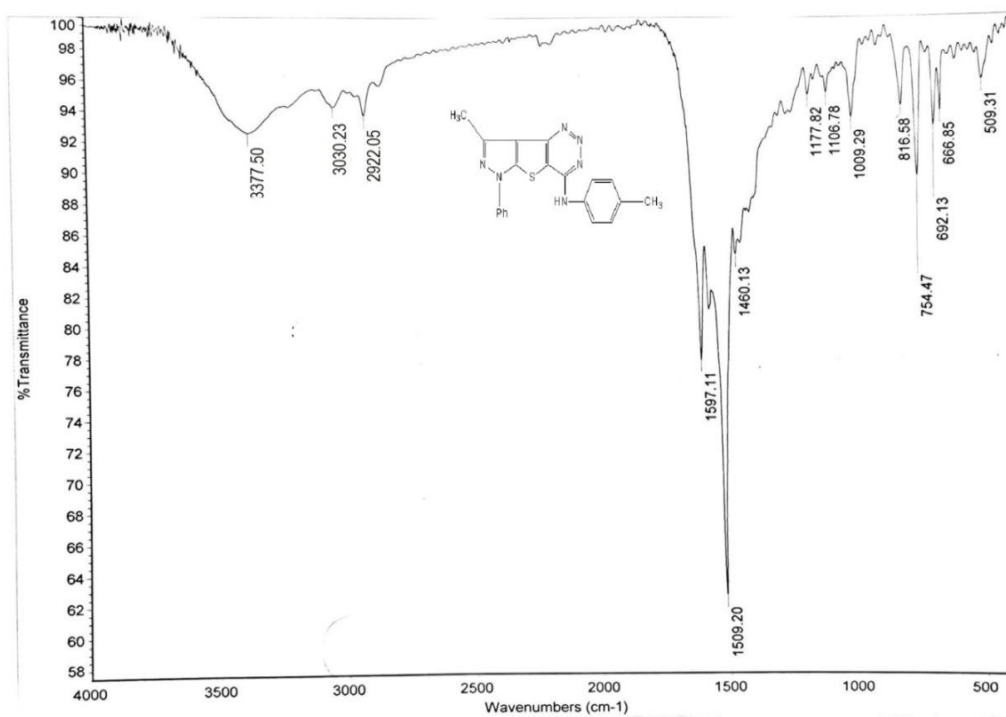
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| # | m/z   | Abs. In | Rel. Int. | # | m/z   | Abs. In | Rel. Int. | # | m/z   | Abs. In | Rel. Int. |
|---|-------|---------|-----------|---|-------|---------|-----------|---|-------|---------|-----------|
| 1 | 50.05 | 13757   | 5.91      | 4 | 53.00 | 7743    | 3.32      | 7 | 56.00 | 7580    | 3.25      |
| 2 | 51.00 | 64678   | 27.77     | 5 | 54.00 | 9346    | 4.01      | 8 | 57.00 | 13214   | 5.67      |
| 3 | 52.00 | 14281   | 6.13      | 6 | 55.00 | 13207   | 5.67      | 9 | 58.00 | 5647    | 2.42      |

**Figure S10.** Mass spectrum of the phenylaminotriazine compound **7a**.

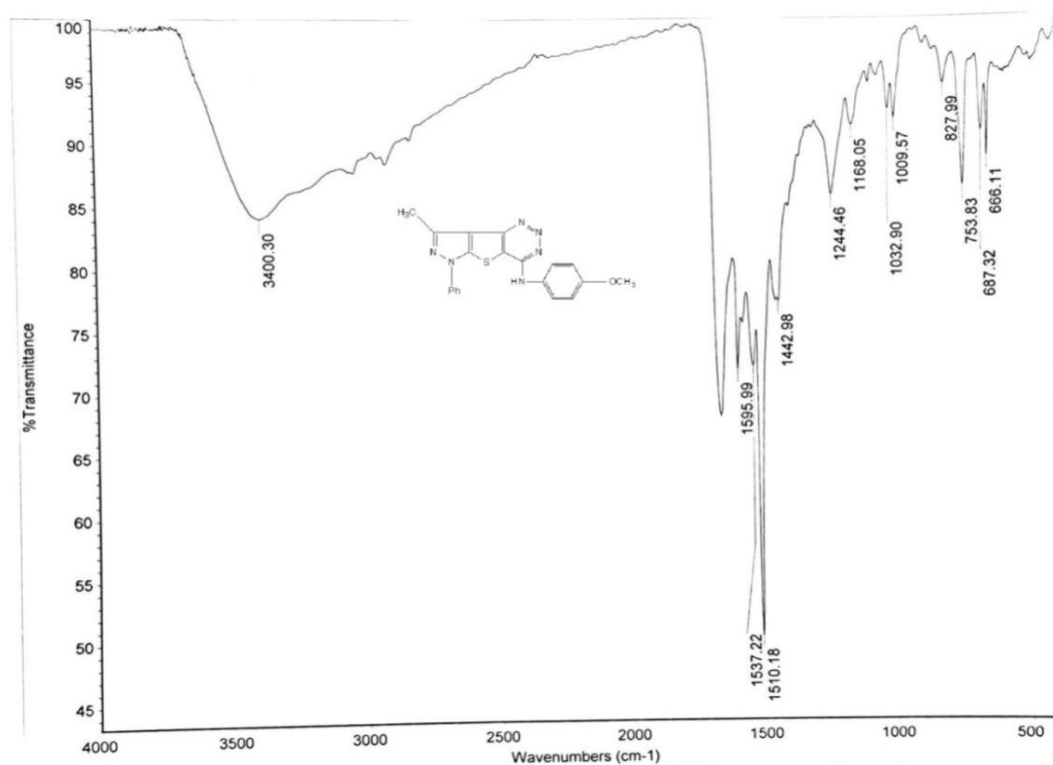


**Figure S11.** FTIR spectrum (KBr) of the *p*-tolylamino-triazine compound **7b**.

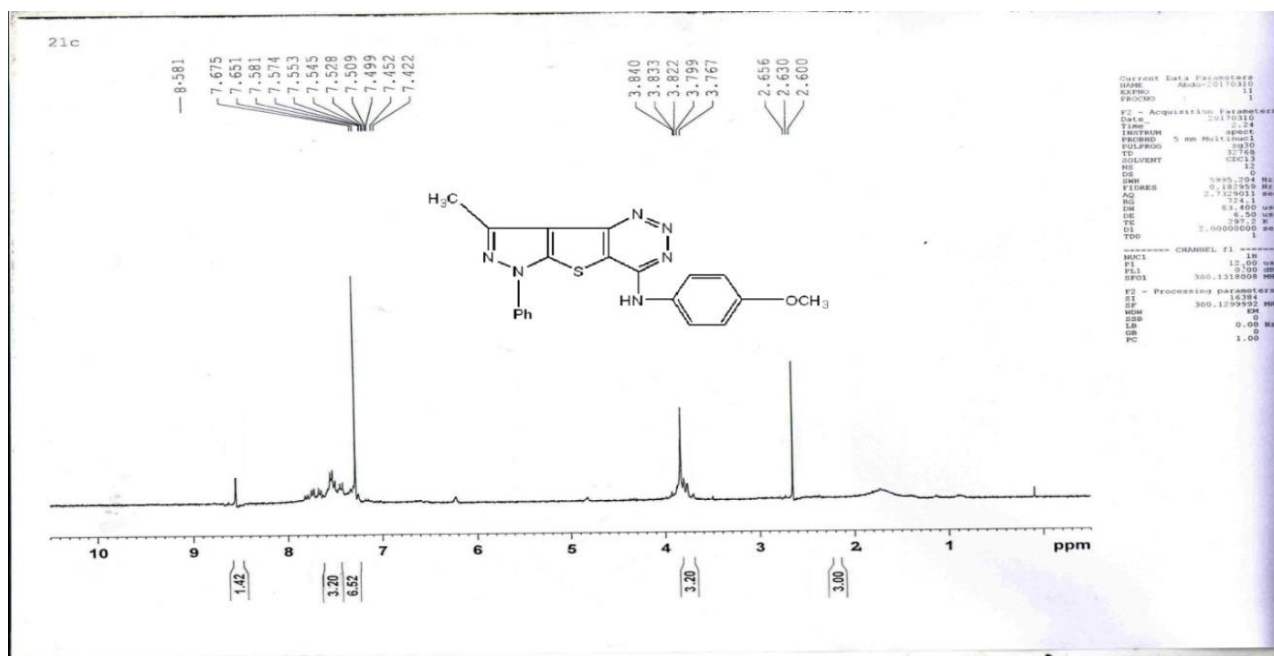


**Figure S12.** <sup>1</sup>H NMR spectrum (300 MHz, CDCl<sub>3</sub>) of the *p*-tolylamino-triazine compound **7b**.





**Figure S13.** FTIR spectrum (KBr) of the *p*-anisylamino-triazine compound **7c**.



**Figure S14.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CDCl}_3$ ) of the *p*-anisylamino-triazine compound **7c**.

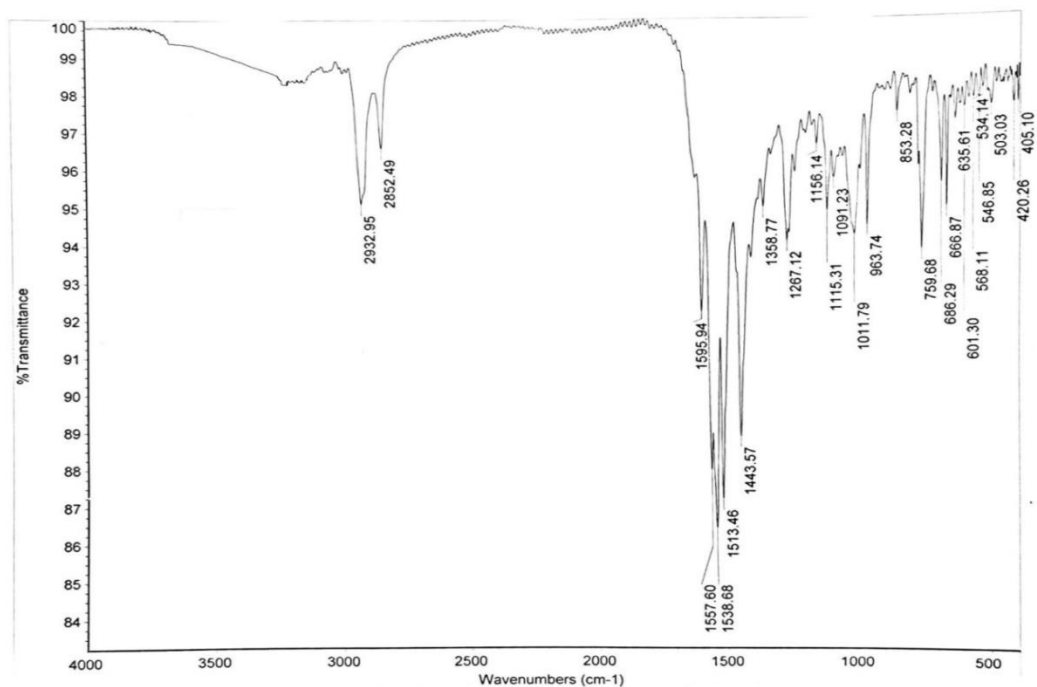


Figure S15. FTIR spectrum (KBr) of the piperidinyl compound **8a**.

(1)  
proton\_su CDCl3 {C:\nmr-data} Student 18

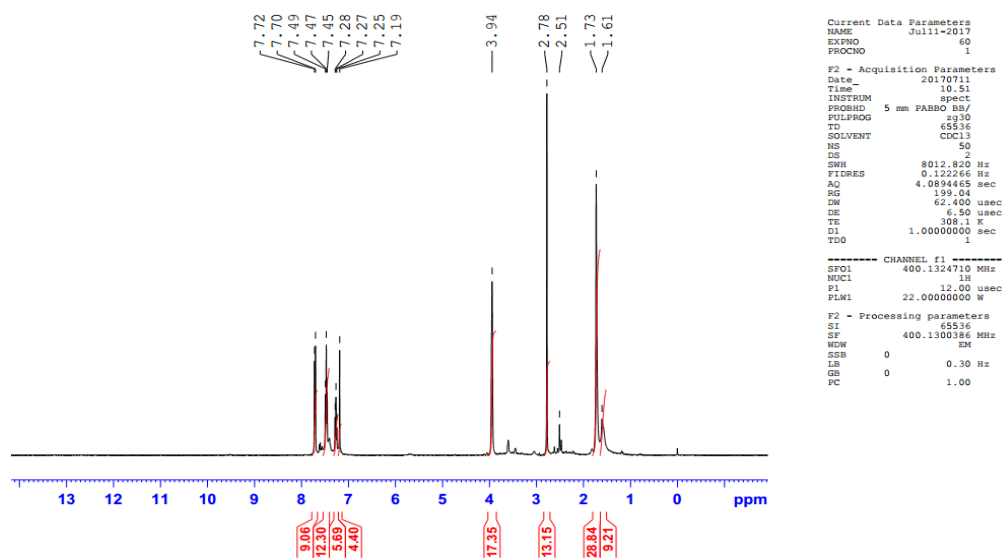
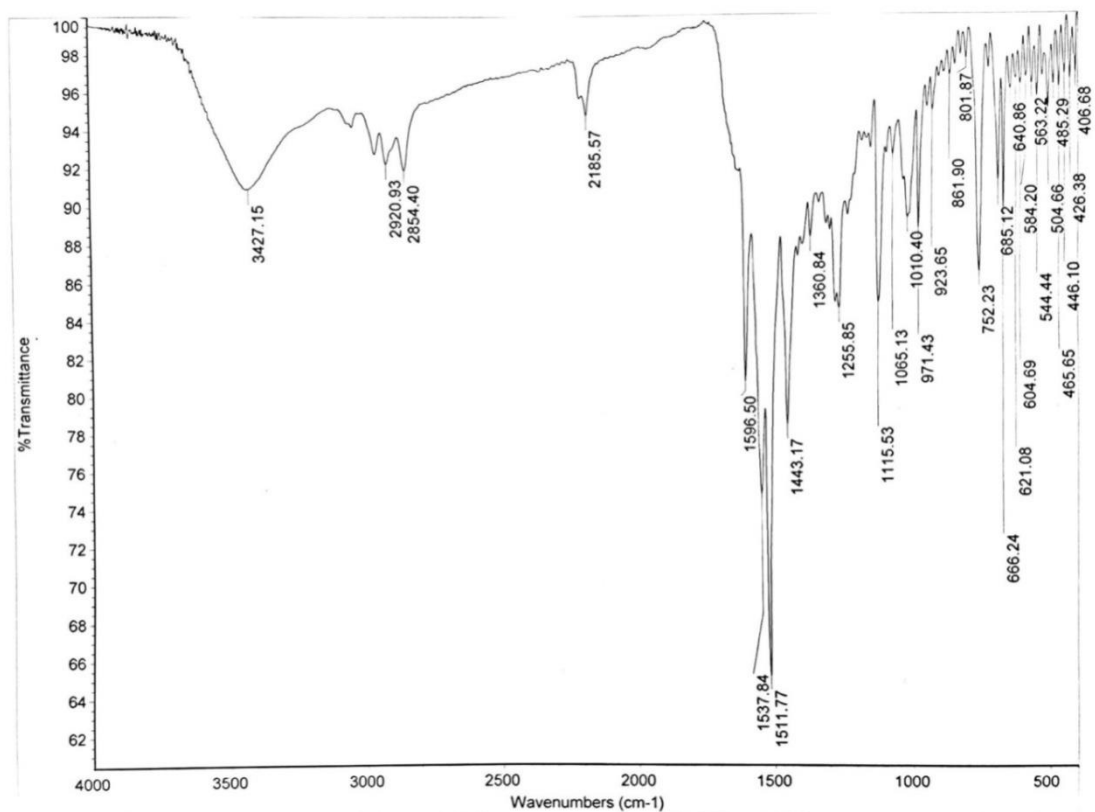


Figure S16.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of the piperidinyl compound **8a**.



**Figure S17.** FTIR spectrum (KBr) of the morpholinyl compound **8b**.

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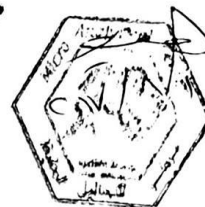
## DI Analysis Shimadzu Qp-2010 Plus

Sample Information  
Analyzed by : Noha Bagato  
Analyzed : 17/07/2017 12:30:29  
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Sample ID :  
Customer Name : جامعة اسبوط - د. احمد قنص  
Data File : C:\GCMSsolution\Data\Project1\2.QGD  
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Method File : C:\GCMSsolution\Data\Project1\High Temperature Op  
Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op  
Report File :  
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\$EndIf\$Modified by : Noha Bagato  
Modified : 17/07/2017 12:38:12

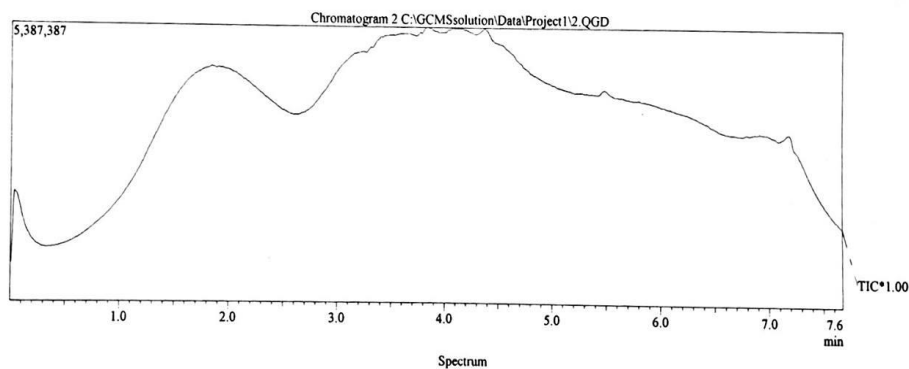
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End Time : 10.00min  
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Event Time : 0.50sec  
Scan Speed : 1000  
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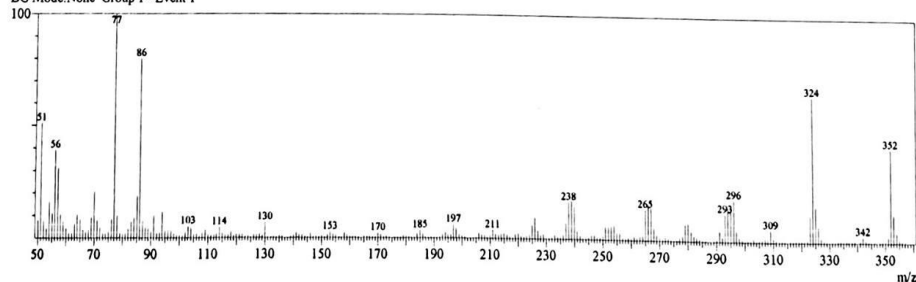
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Ionization Mode : EI



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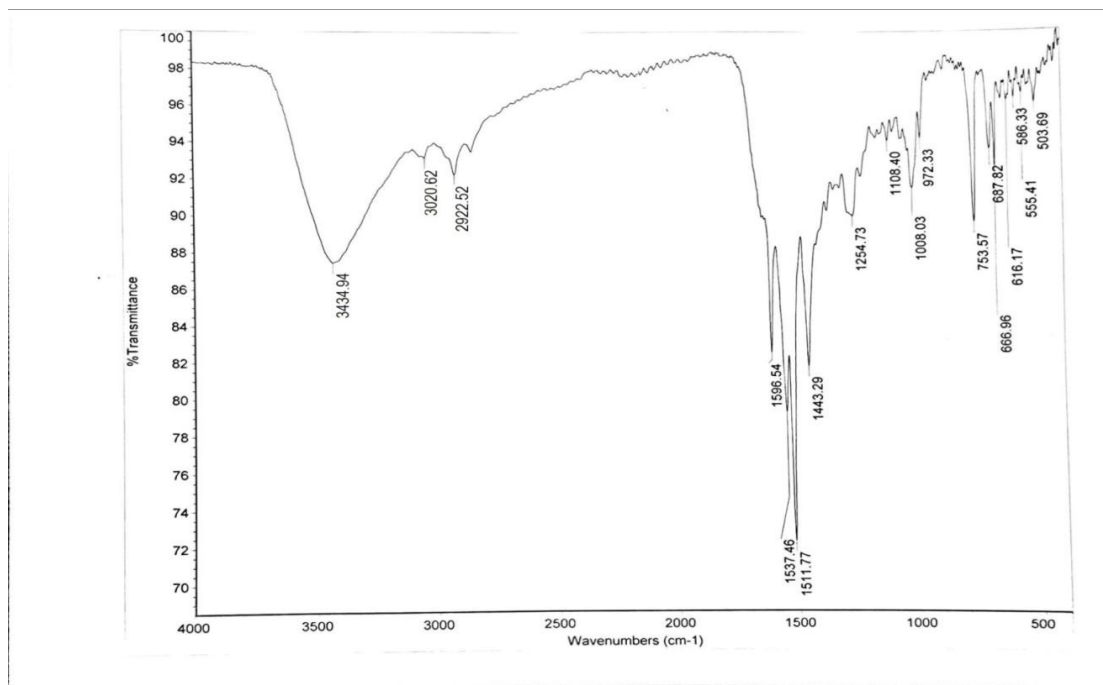
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BG Mode:None Group 1 - Event 1



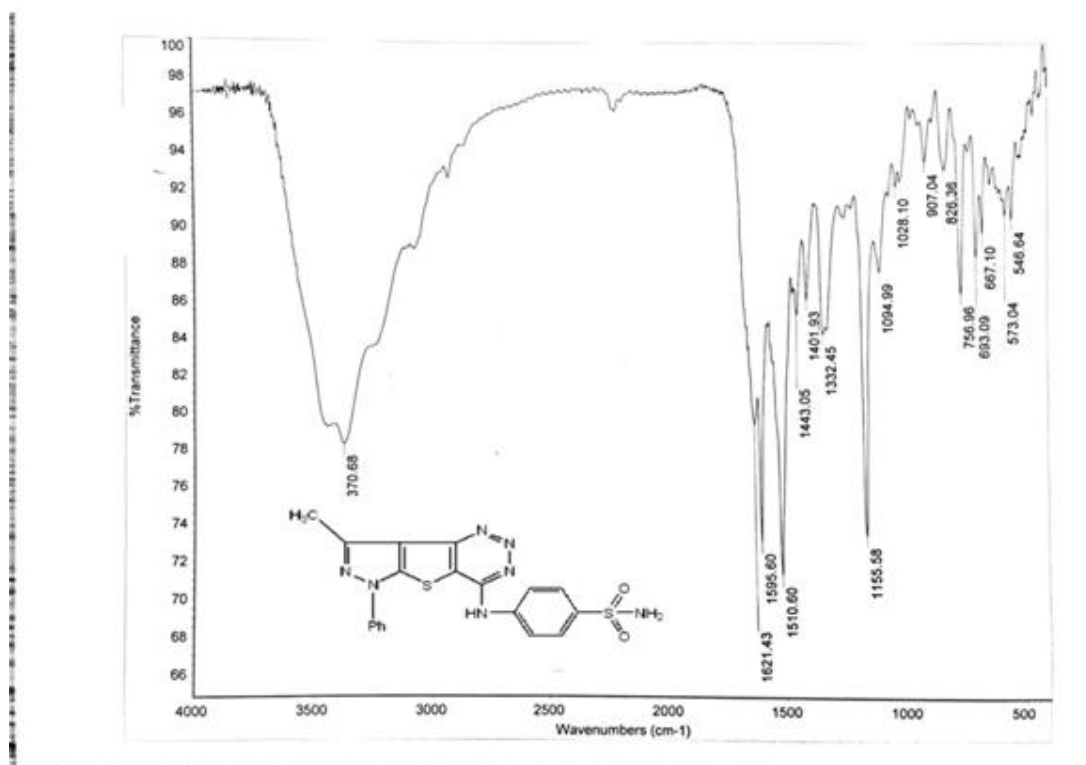
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BG Mode:None Group 1 - Event 1

| # | m/z   | Abs. In | Rel. Int. | # | m/z   | Abs. In | Rel. Int. | # | m/z   | Abs. In | Rel. Int. |
|---|-------|---------|-----------|---|-------|---------|-----------|---|-------|---------|-----------|
| 1 | 50.05 | 30652   | 7.72      | 4 | 53.05 | 17186   | 4.33      | 7 | 56.00 | 155103  | 39.05     |
| 2 | 50.95 | 202774  | 51.05     | 5 | 54.00 | 63633   | 16.02     | 8 | 57.00 | 123482  | 31.08     |
| 3 | 52.00 | 30740   | 7.74      | 6 | 55.05 | 43375   | 10.92     | 9 | 58.00 | 41745   | 10.51     |

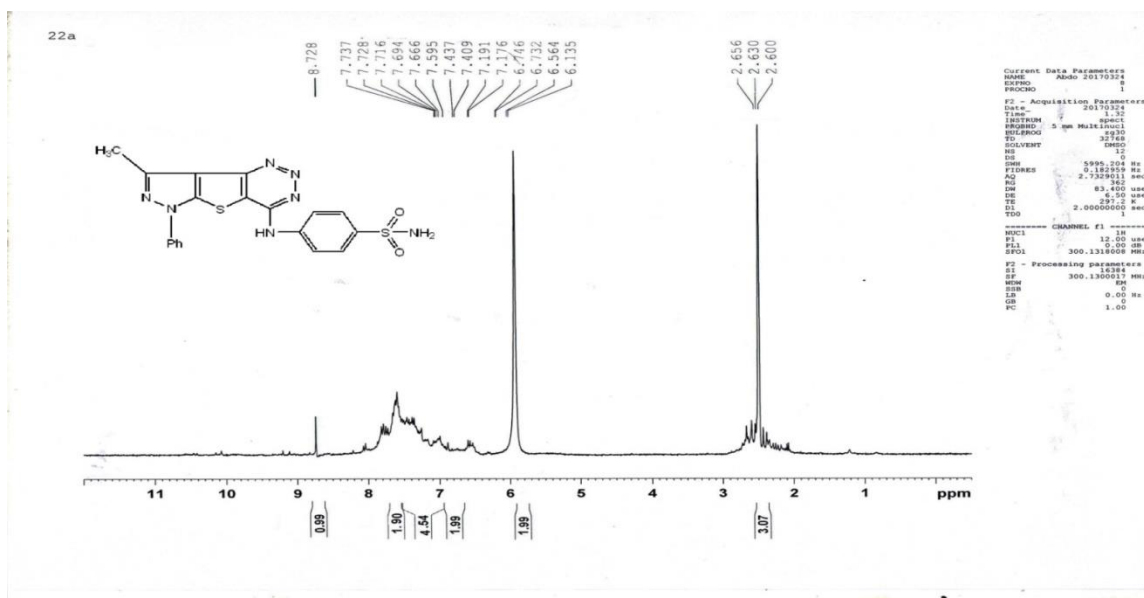
Figure S18. Mass spectrum of the morpholiny compound **8b**.



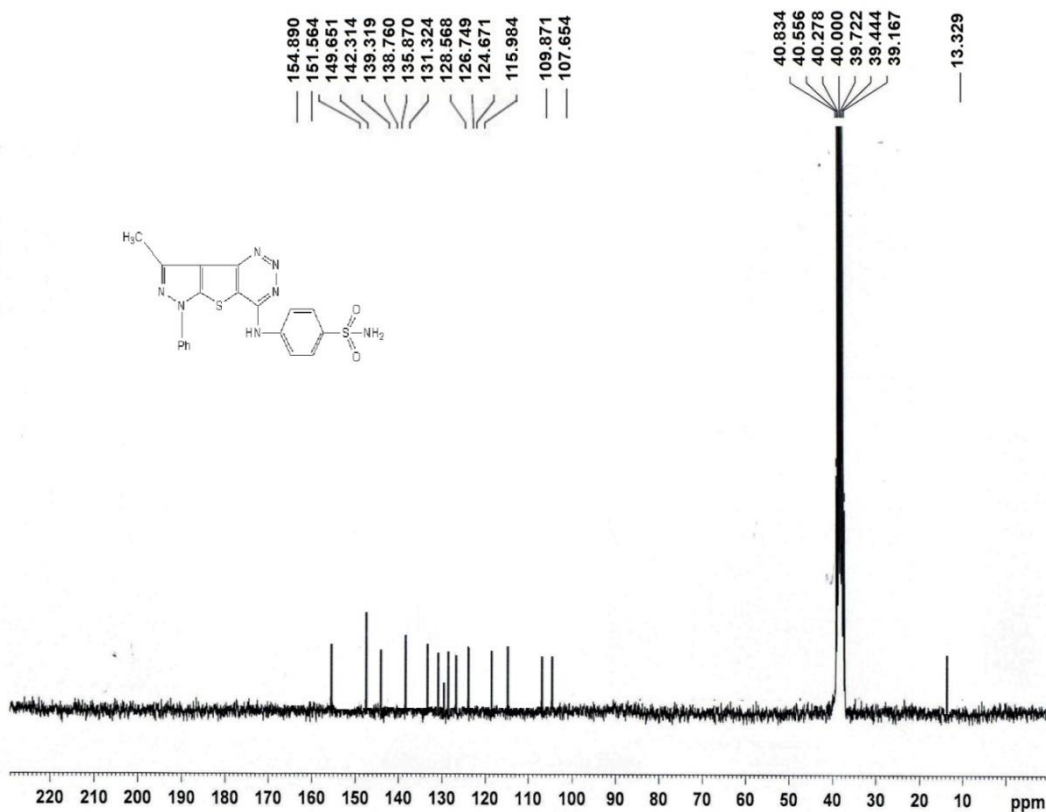
**Figure S19.** FTIR spectrum (KBr) of the piperazinyl compound **8c**.



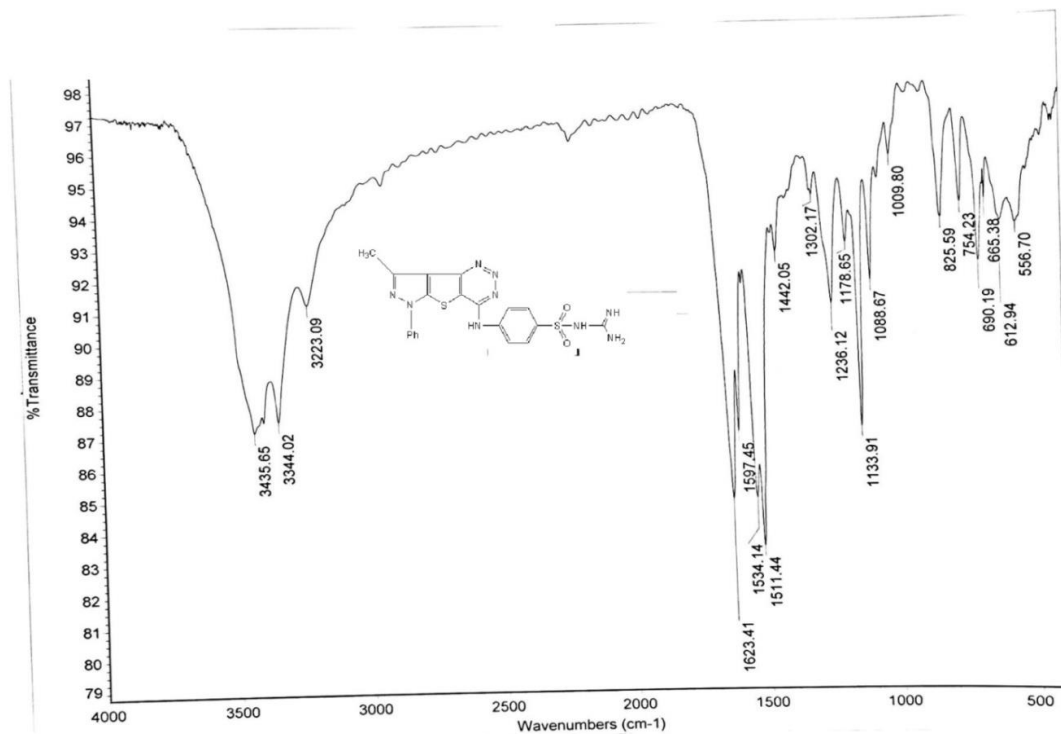
**Figure S20.** FTIR spectrum (KBr) of the thiazinylaminobenzene sulfonamide derivative **9a**.



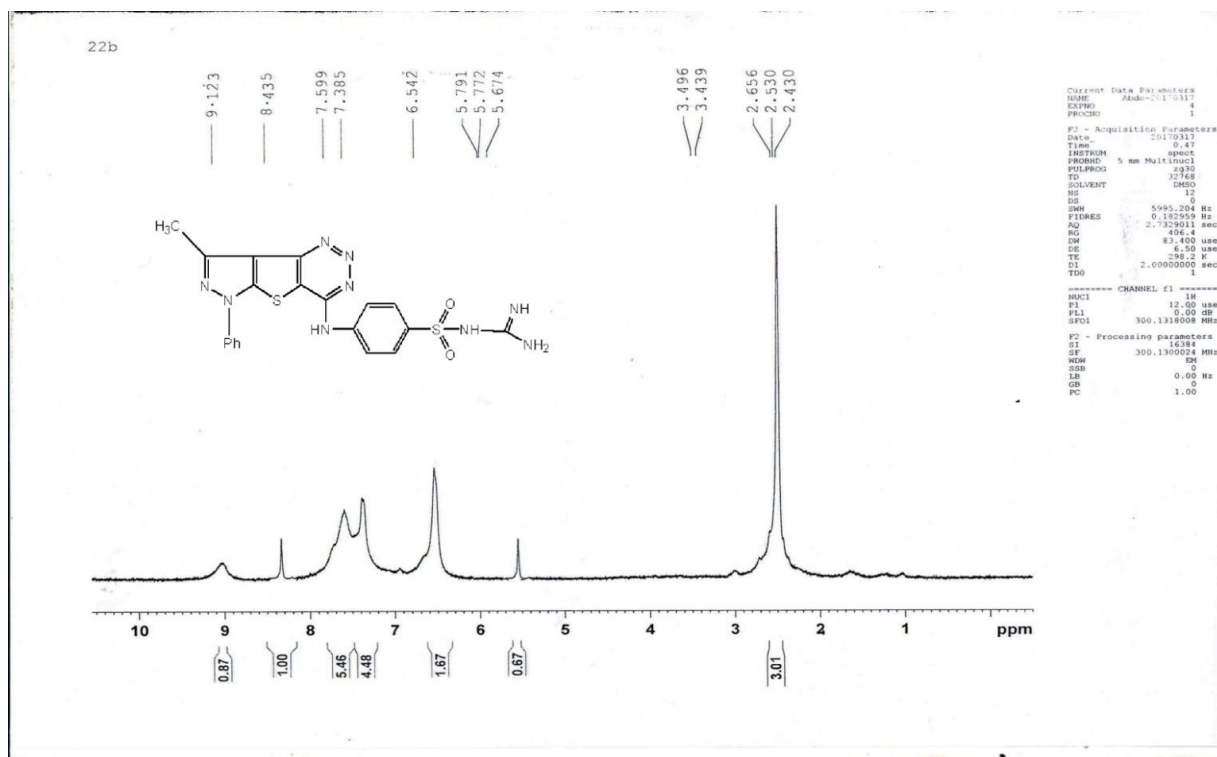
**Figure S21.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{CDCl}_3$ ) of the triazinylaminobenzene sulfonamide **9a**.



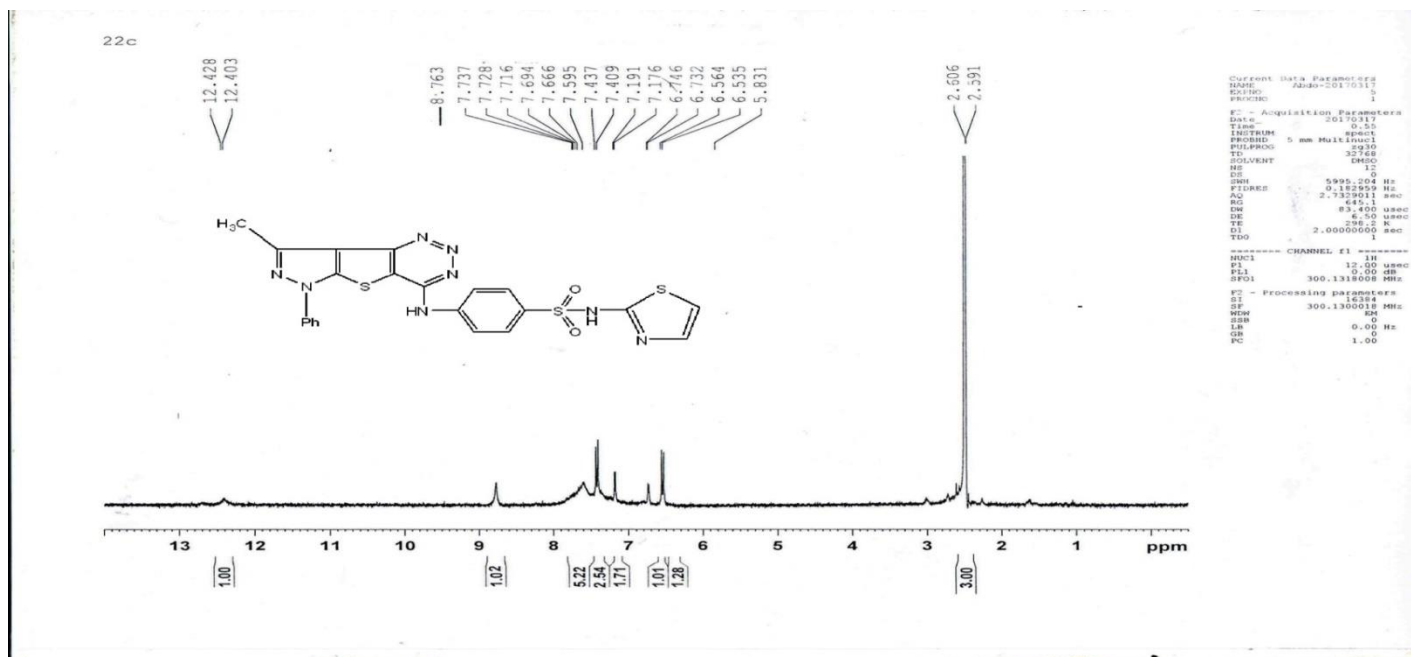
**Figure S22.**  $^{13}\text{C}$  NMR spectrum (300 MHz,  $\text{DMSO}-d_6$ ) of triazinylaminobenzene sulfonamide compound **9a**.



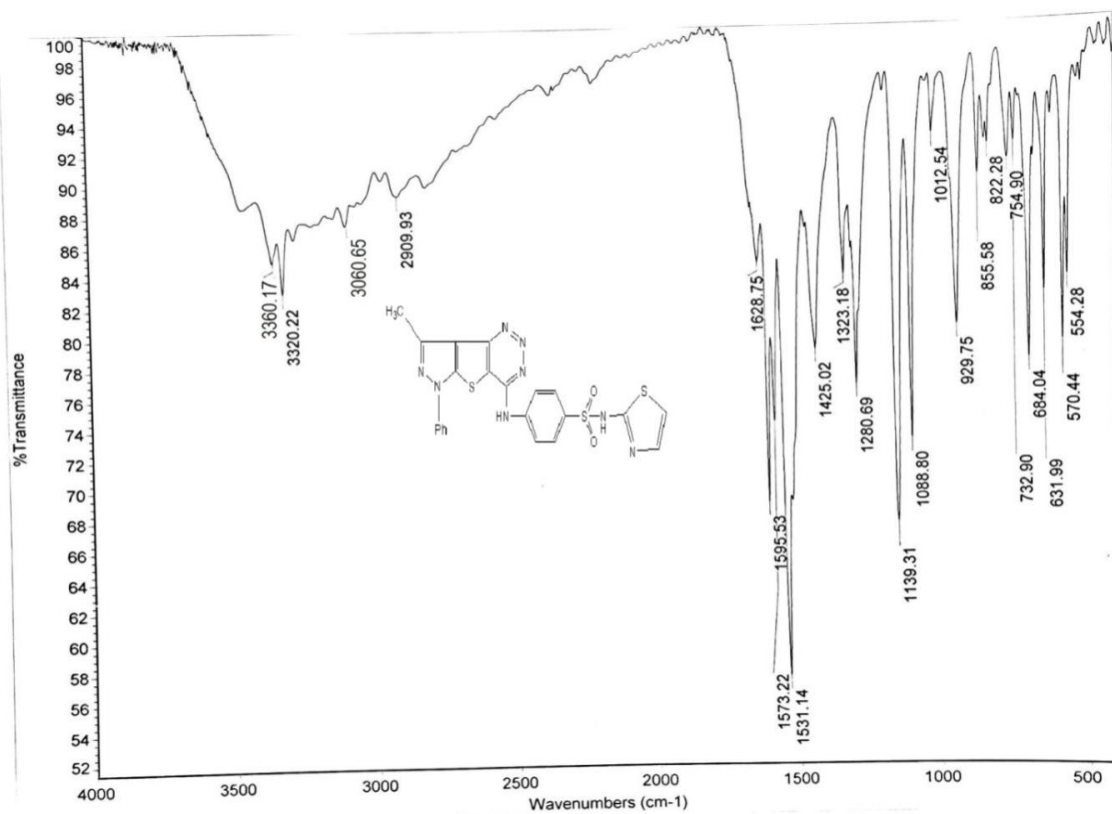
**Figure S23.** FTIR spectrum (KBr) of the *N*-carbamimidoyl benzene sulfonamide **9b**.



**Figure S24.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{DMSO}-d_6$ ) of the *N*-carbamimidoyl benzene sulfonamide **9b**.

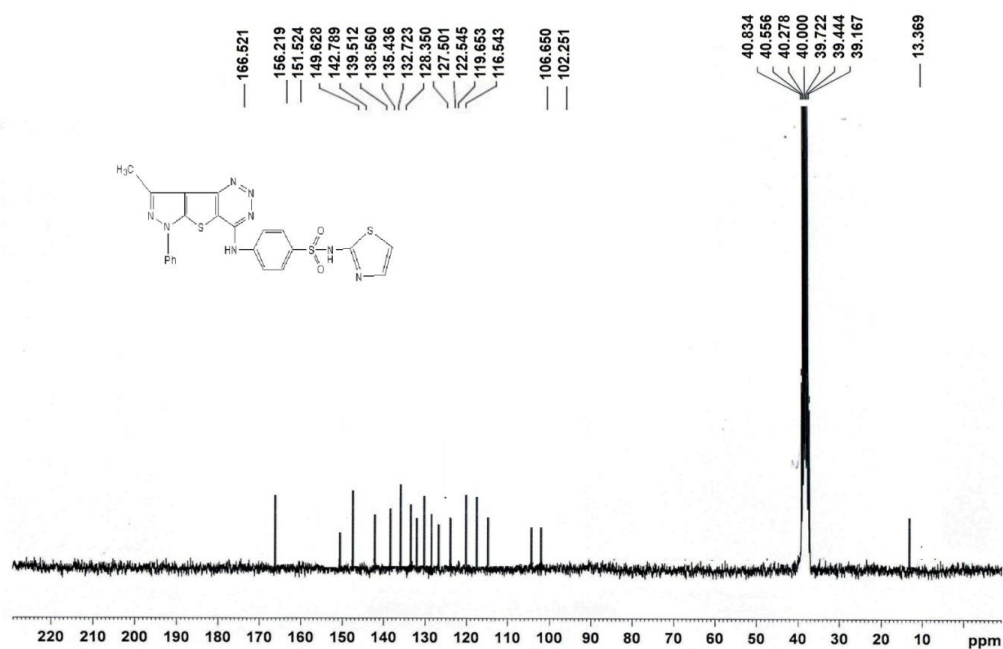


**Figure S25.** FTIR spectrum (KBr) of the *N*-thiazolyl benzene sulfonamide **9c**.

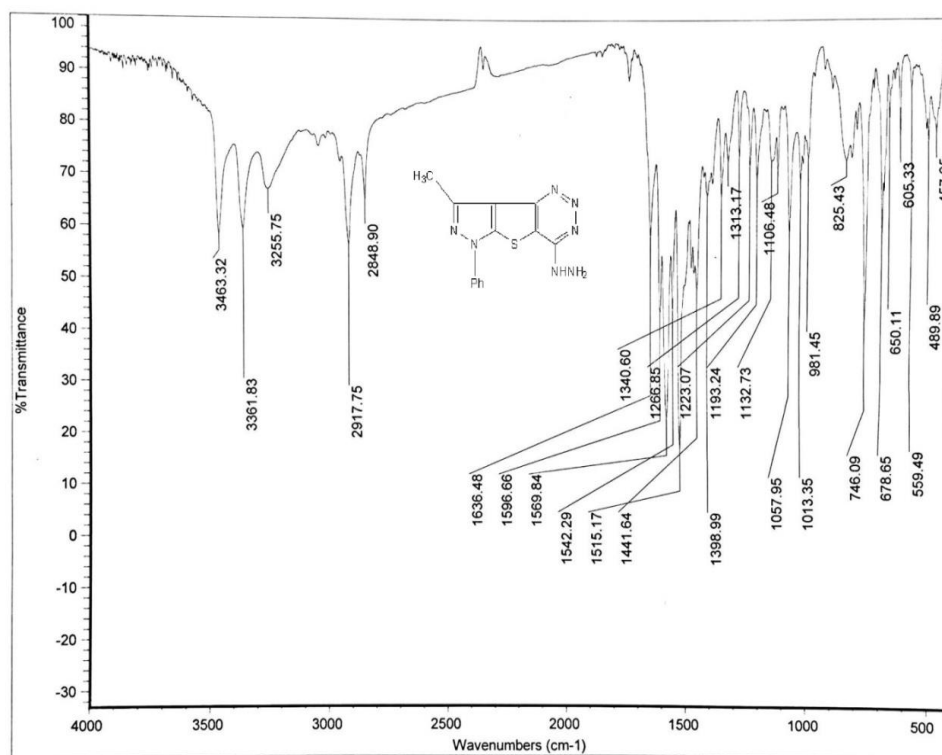


**Figure S26.** <sup>1</sup>H NMR spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of the *N*-thiazolyl benzene sulfonamide **9c**.

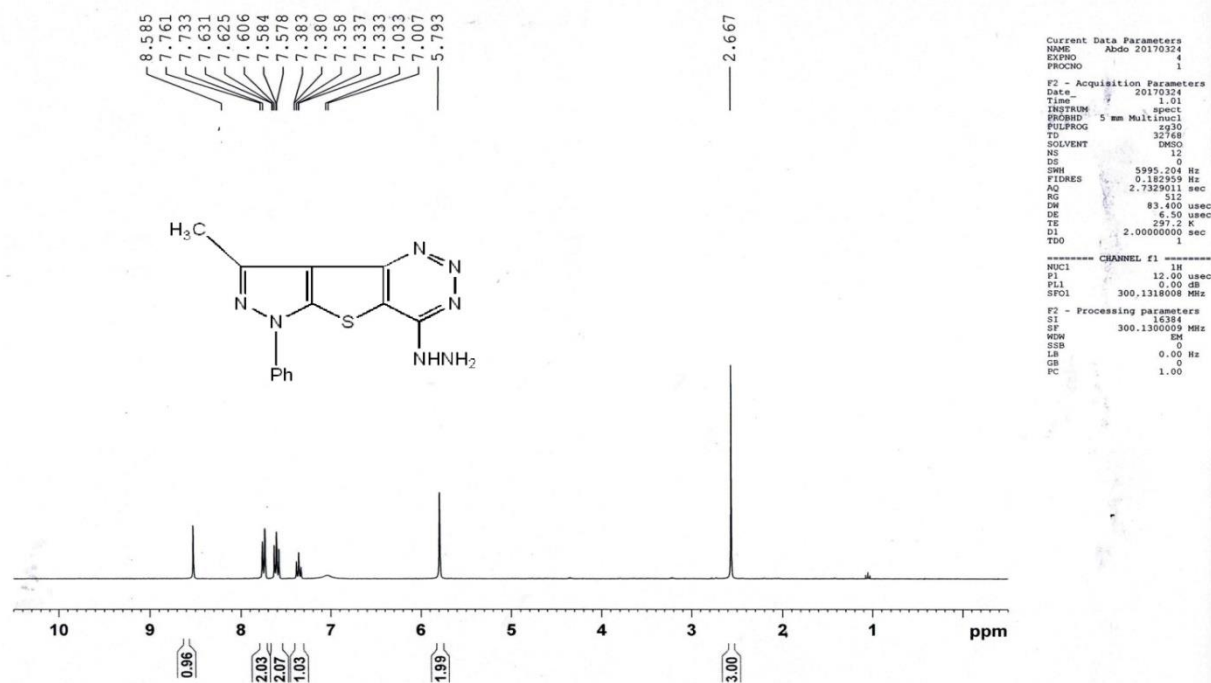




**Figure S27.** <sup>13</sup>C NMR spectrum (300 MHz, DMSO-*d*<sub>6</sub>) spectrum the *N*-thiazolyl benzene sulfonamide **9c**.



**Figure S28.** FTIR spectrum (KBr) of the hydrazinotriazine compound **10**.



**Figure S29.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{DMSO-}d_6$ ) of the hydrazinotriazine compound **10**.

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**DI Analysis  
Shimadzu Qp-2010 Plus**

Sample Information  
 Analyzed by : Noha Bagato  
 Analyzed : 18/07/2017 03:41:44 م  
 Sample Name : sample 3  
 Sample ID :  
 Customer Name : جامعة اسبوط - د. احمد فتحي  
 Data File : C:\GCMSsolution\Data\Project1\sample 3 QGD  
 Org Data File : C:\GCMSsolution\Data\Project1\sample 3 QGD  
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op  
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op  
 Report File :  
 Tuning File : C:\GCMSsolution\System\Tune1\\_default.qgt  
 \$EndIf\$Modified by : Noha Bagato  
 Modified : 18/07/2017 03:48:57 م

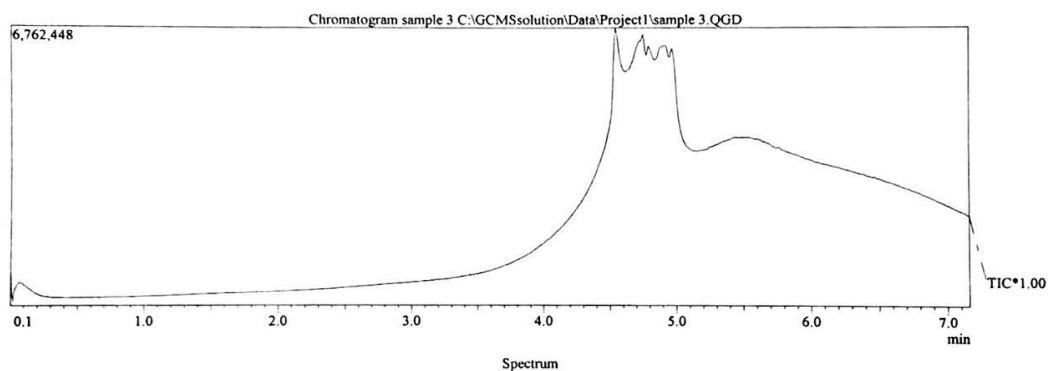
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 End Time : 10.00min  
 ACQ Mode : Scan  
 Event Time : 0.50sec  
 Scan Speed : 1000  
 Start m/z : 50.00  
 End m/z : 500.00

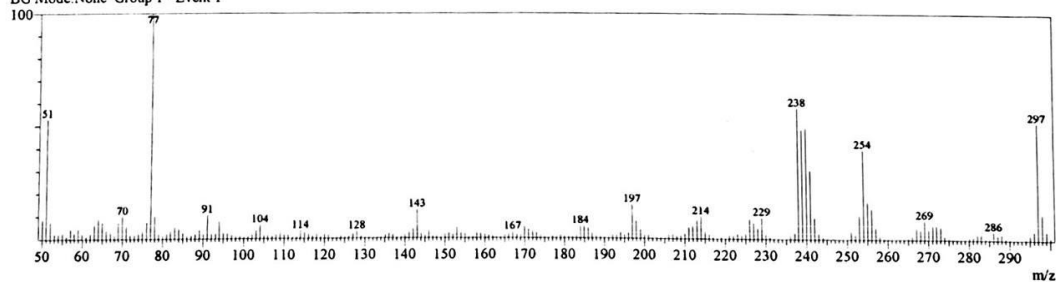
Electron Voltage : 70 eV  
 Ionization Mode : EI



C:\GCMSsolution\Data\Project1\sample 3 QGD



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Mass Table

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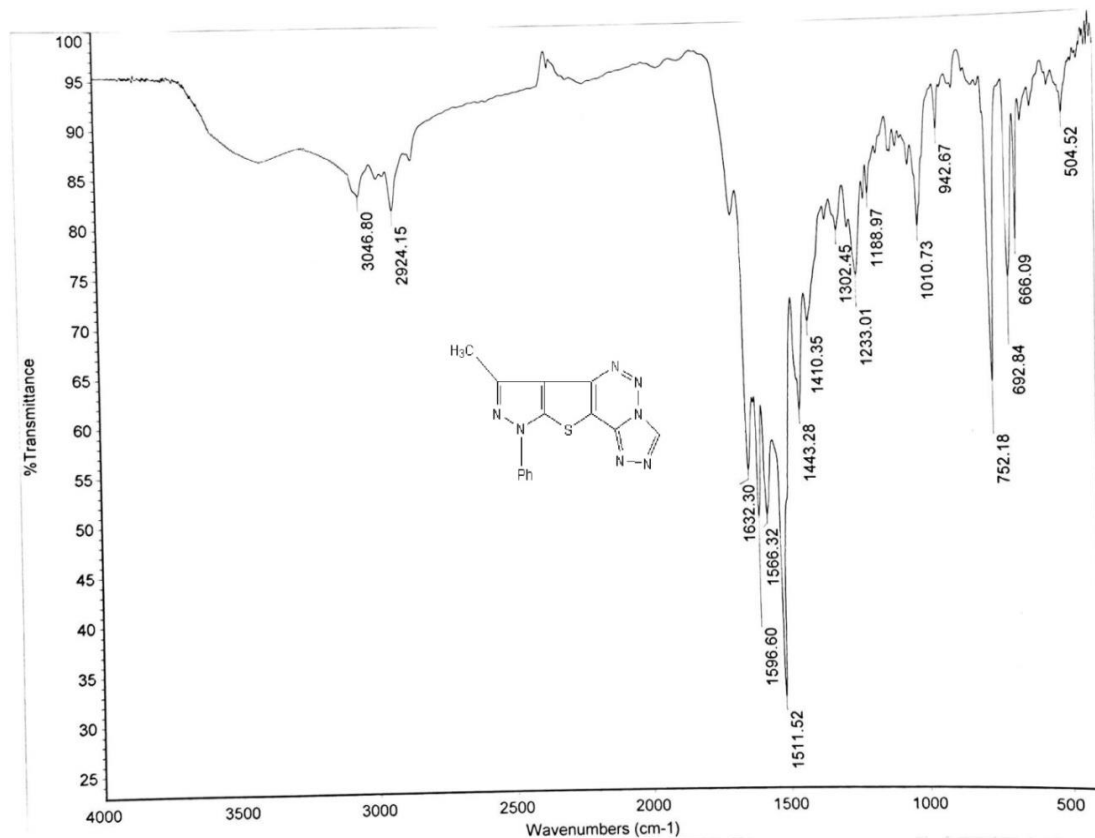
MassPeaks:245

RawMode:Single 4.9(590) BasePeak:77(568764)

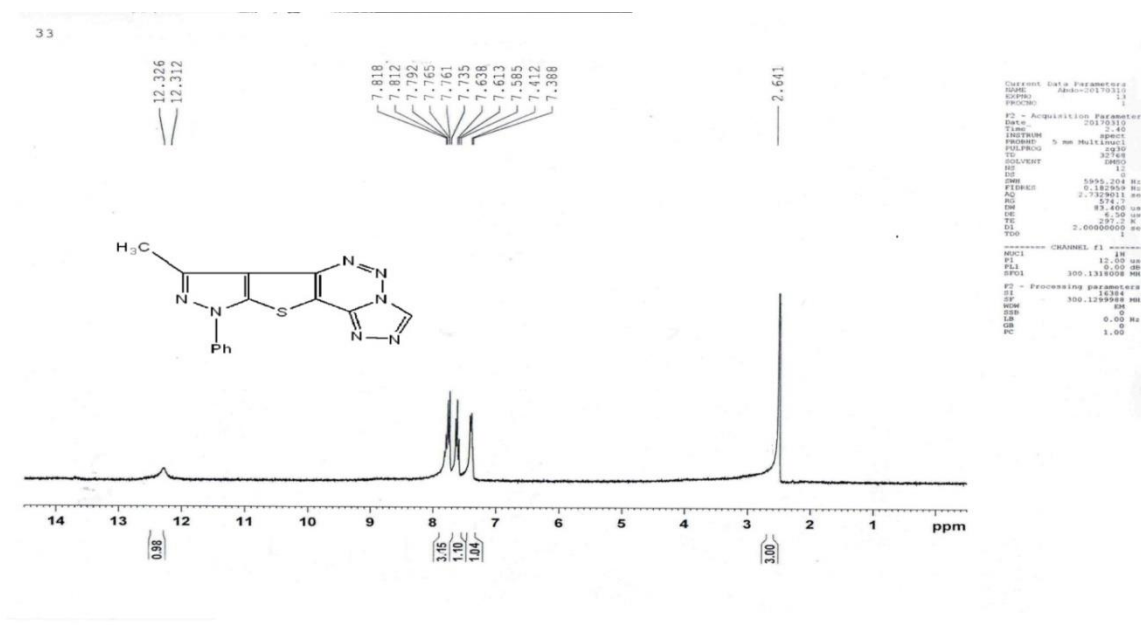
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| 2 | 50.95 | 301491  | 53.01     | 5 | 54.00 | 13444   | 2.36      |
| 3 | 51.95 | 42383   | 7.45      | 6 | 55.00 | 17108   | 3.01      |
|   |       |         |           | 7 | 56.00 | 6273    | 1.10      |
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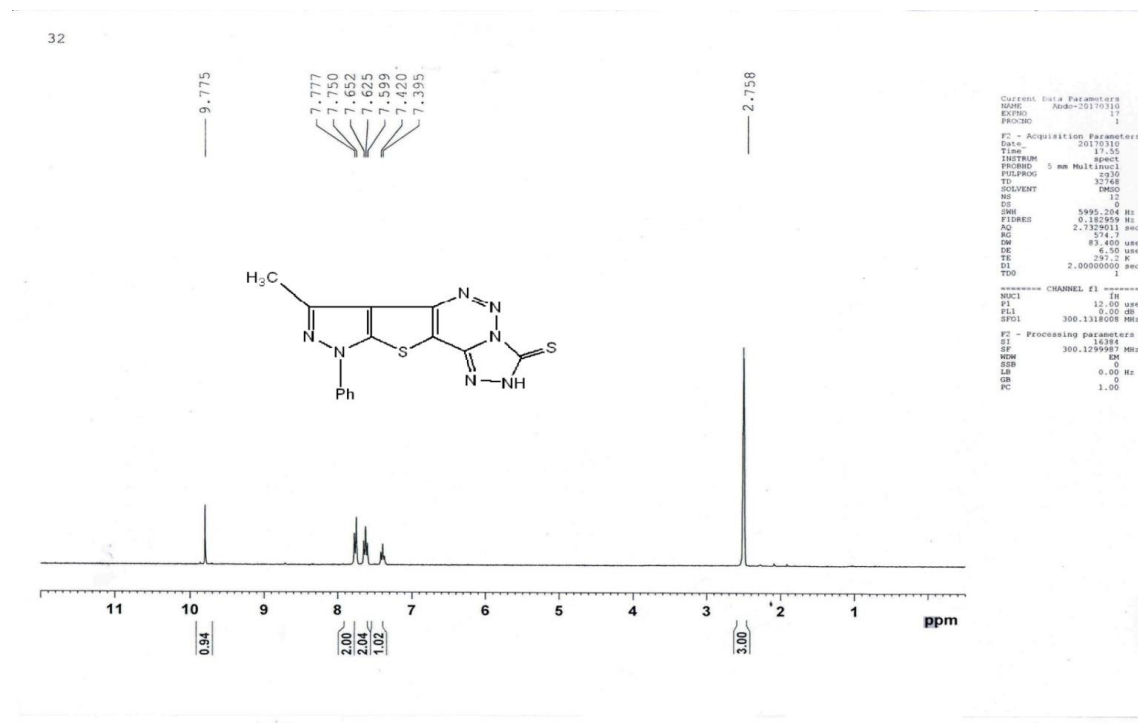
**Figure S30.** Mass spectrum of the hydrazinotriazine compound **10**.



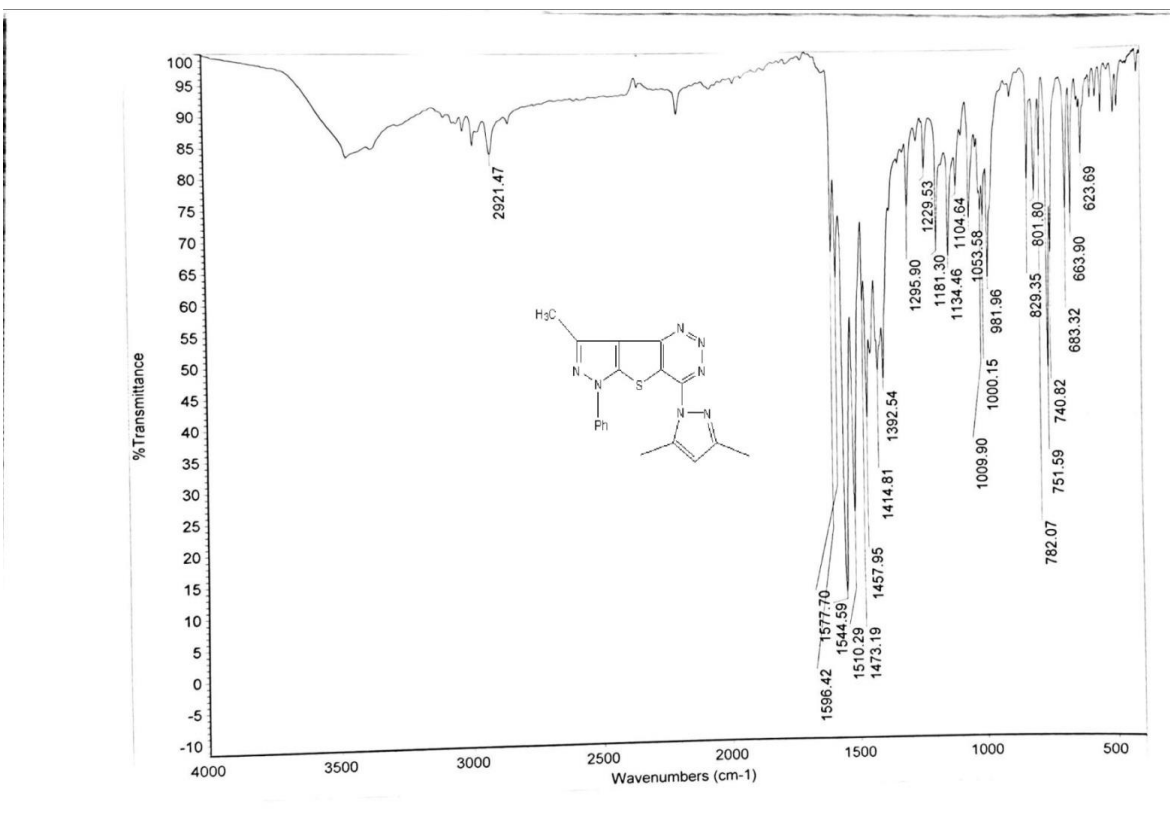
**Figure S31.** FTIR spectrum (KBr) of the triazolotriazine compound **11**.



**Figure S32.** <sup>1</sup>H NMR spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of the triazolotriazine compound **11**.



**Figure S33.** <sup>1</sup>H NMR spectrum (300 MHz, DMSO-d<sub>6</sub>) of the triazolotriazinethione compound **12**.



**Figure S34.** FTIR spectrum (KBr) of the dimethyl pyrazolyl compound **13**.

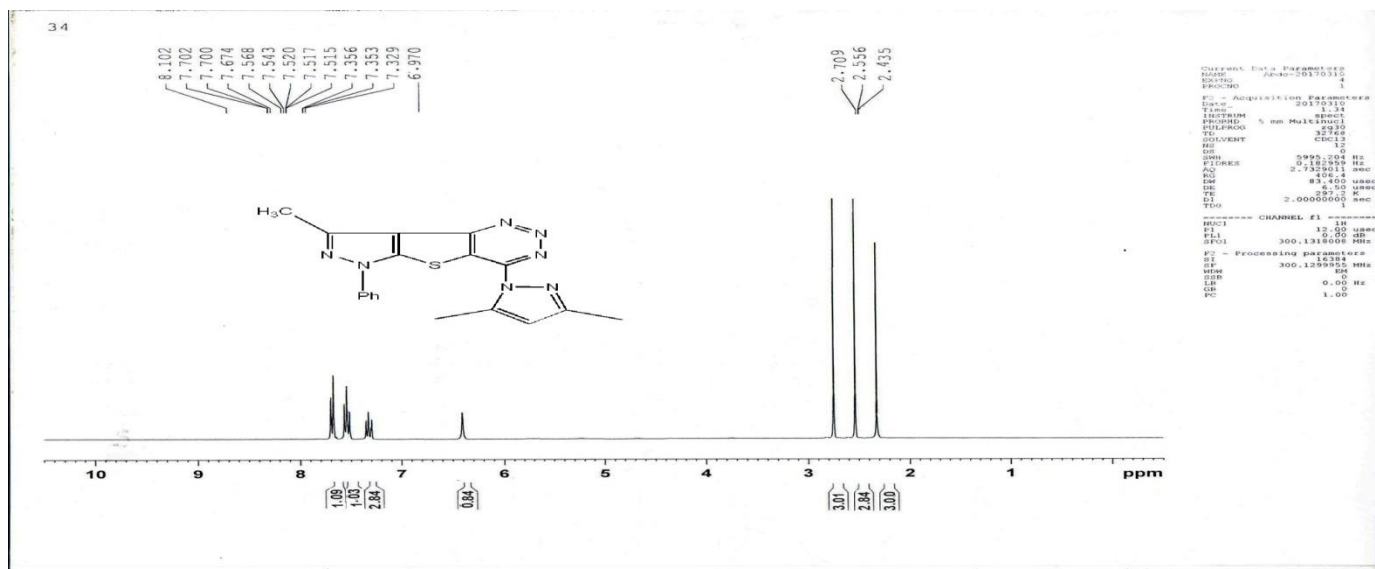


Figure S35. <sup>1</sup>H NMR spectrum (300 MHz, CDCl<sub>3</sub>) of the dimethyl pyrazolyl compound 13.

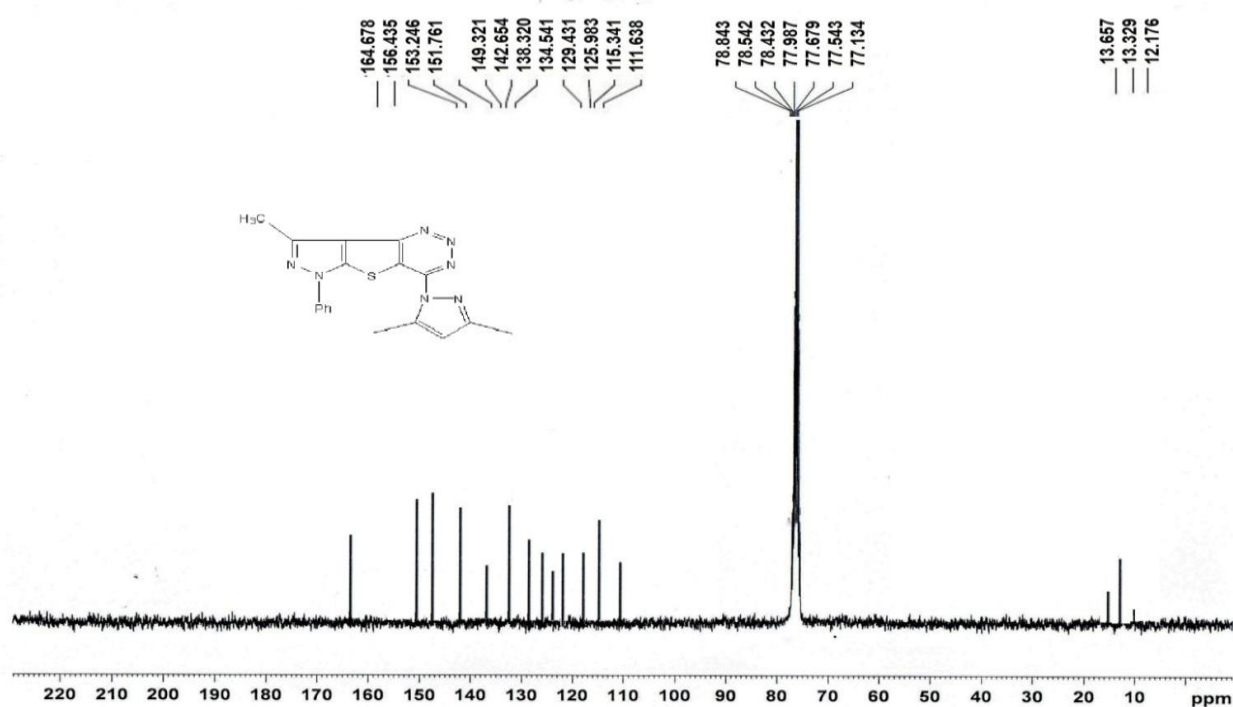
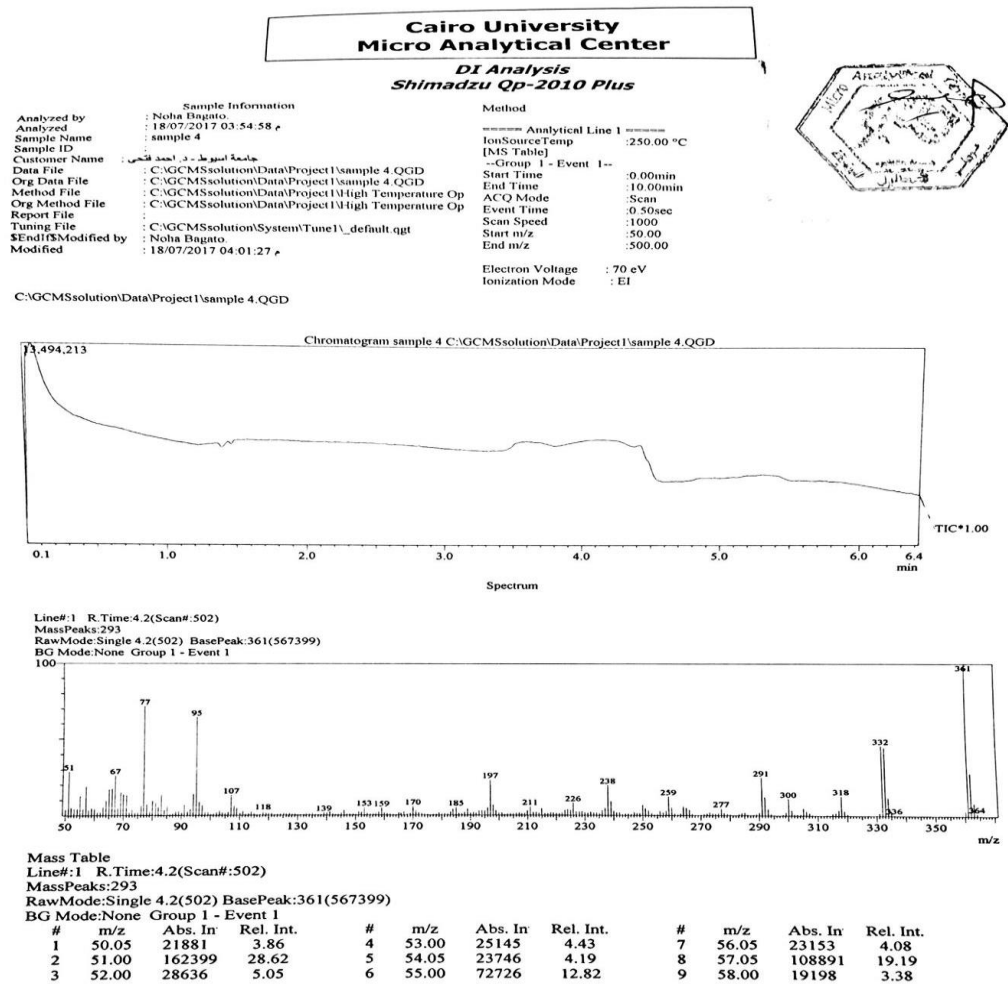
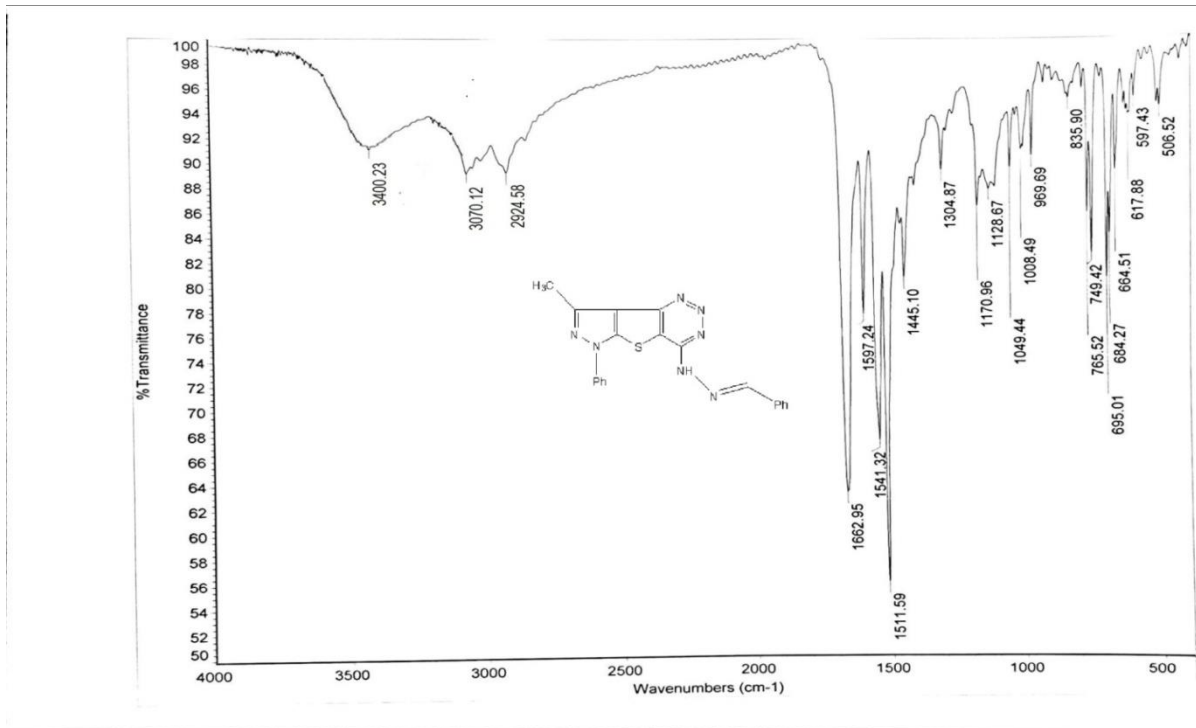


Figure S36. <sup>13</sup>C NMR spectrum (300 MHz, CDCl<sub>3</sub>) of the dimethyl pyrazolyl compound 13.

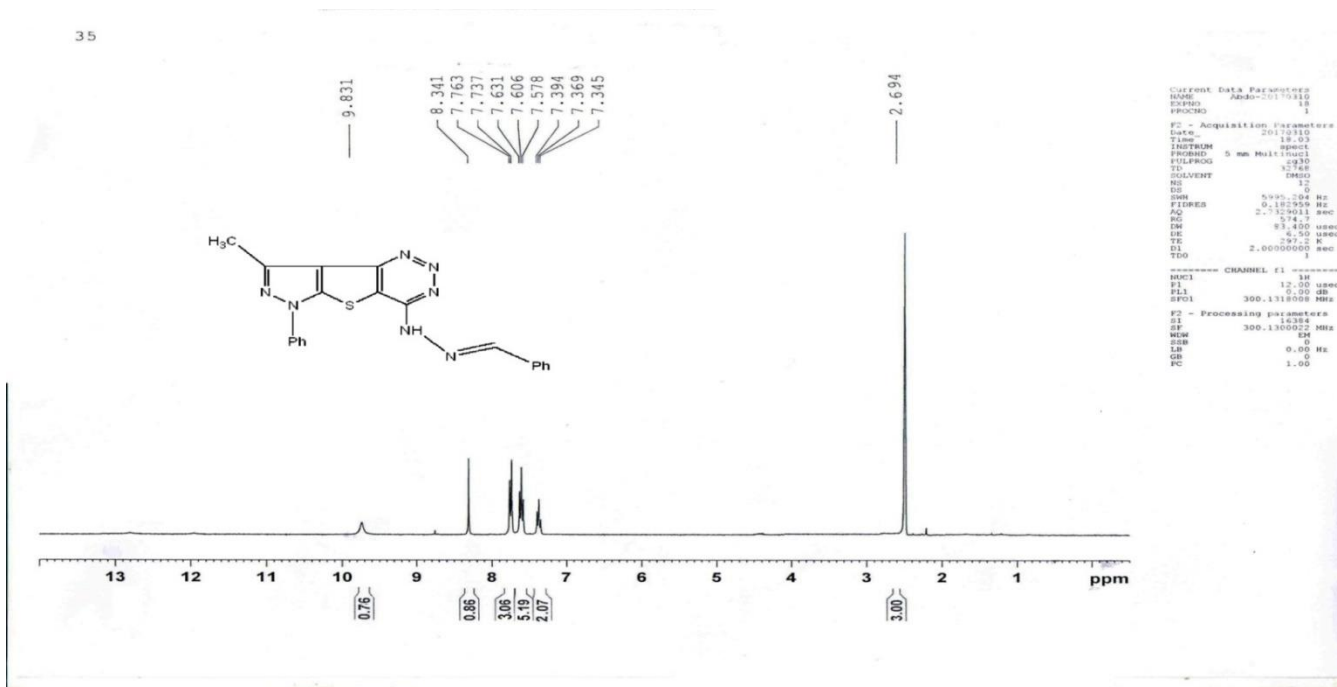


1 / 3

**Figure S37.** Mass spectrum of the dimethyl pyrazolyl compound **13**.

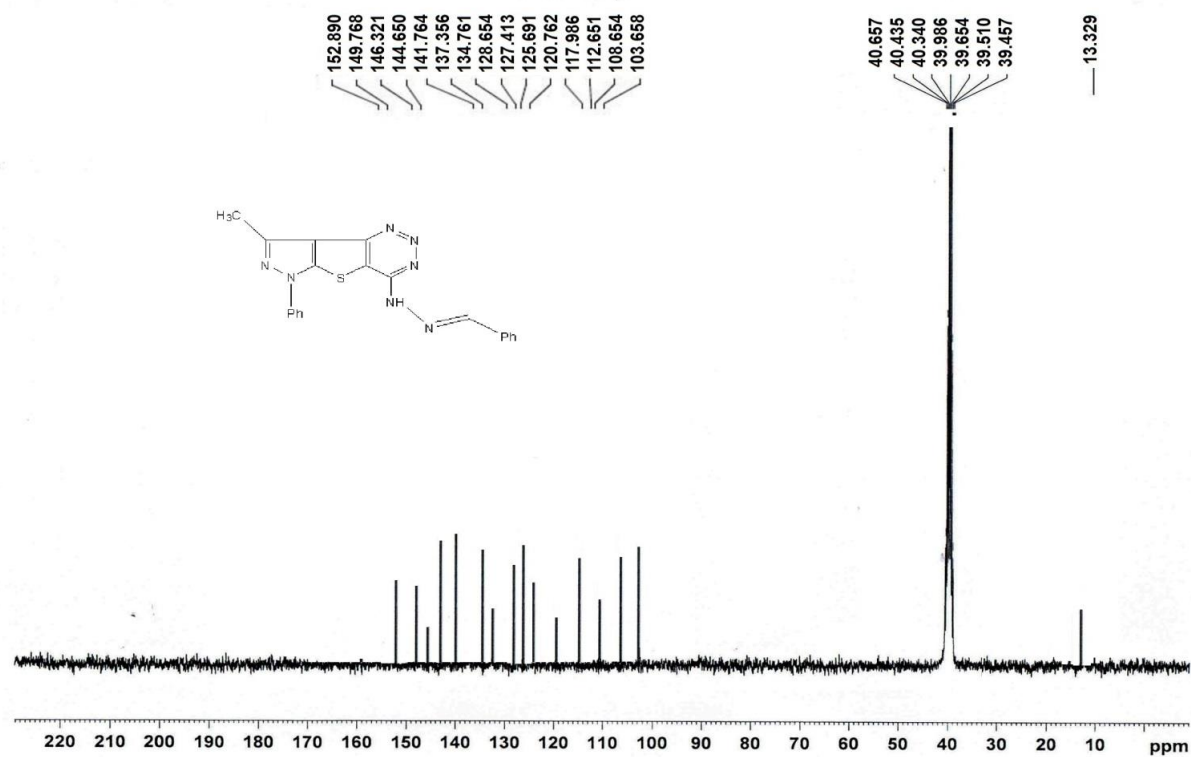


**Figure S38.** FTIR spectrum (KBr) of the benzylidenehydrazino compound **14**.



**Figure S39.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{DMSO}-d_6$ ) of the benzylidenehydrazino compound **14**.





**Figure S40.** <sup>13</sup>C NMR spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of the benzylidenehydrazino compound **14**.