

**Synthesis, spectral characterization and molecular docking studies of some thiocarbohydrazide-based Schiff bases  
with pyrazole moiety as potential anti-inflammatory agents**

Mokhtar A. Abd ul-Malik<sup>a\*</sup>, Aly Abdou<sup>b</sup>, Mohamed R. Fouad<sup>c</sup>, Ahmed S. N. Alkamali<sup>a</sup> and Shaban A. A. Abdel-Raheem<sup>d</sup>

<sup>a</sup> *Department of Chemistry, Faculty of Applied Science, Taiz University, Taiz, Yemen*

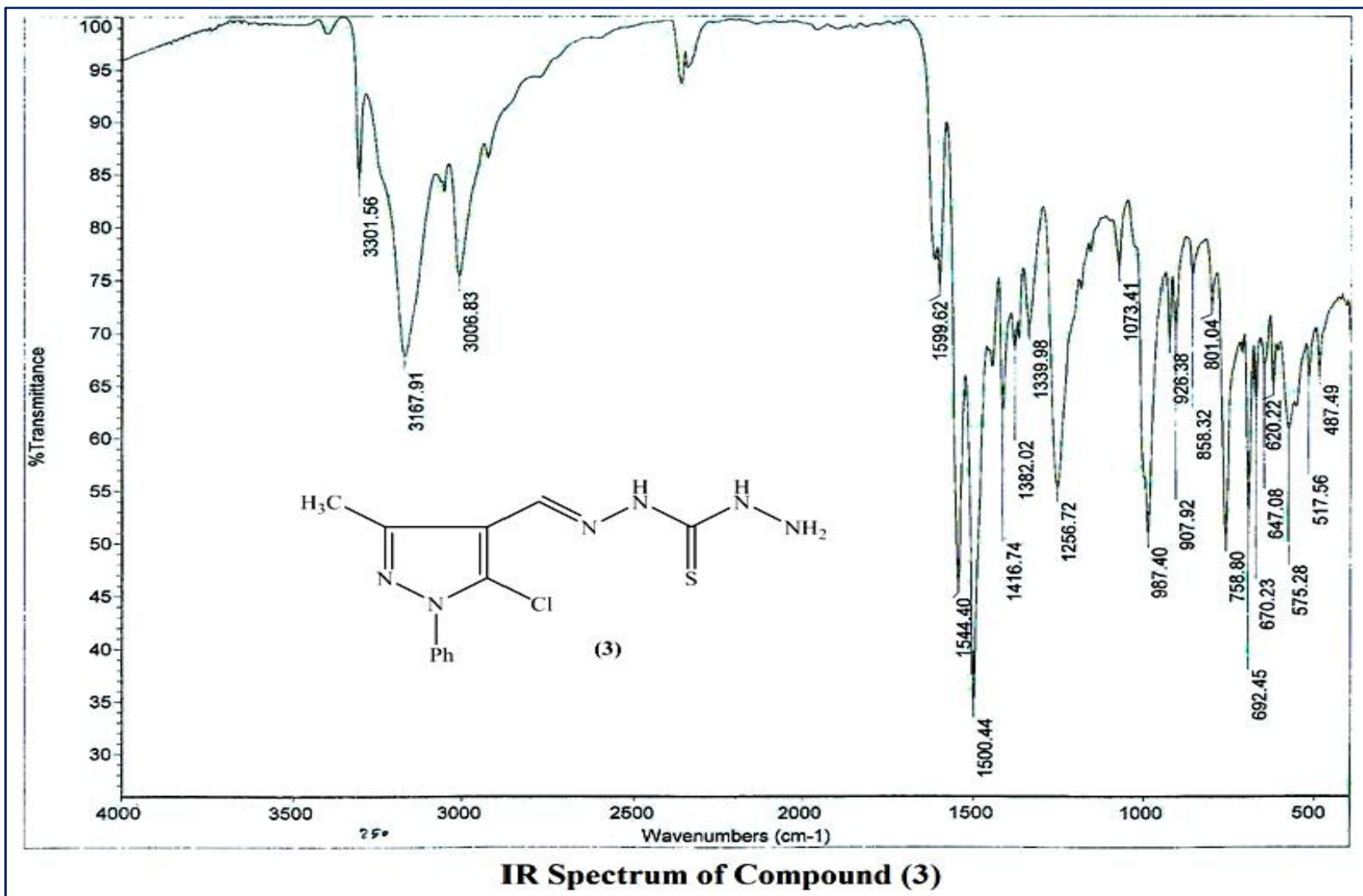
<sup>b</sup> *Department of Chemistry, Faculty of Science, Sohag University, Sohag 82524, Egypt*

<sup>c</sup> *Department of Pesticide Chemistry and Technology, Faculty of Agriculture, Alexandria University, Aflaton St., 21545, El-Shatby, Alexandria, Egypt*

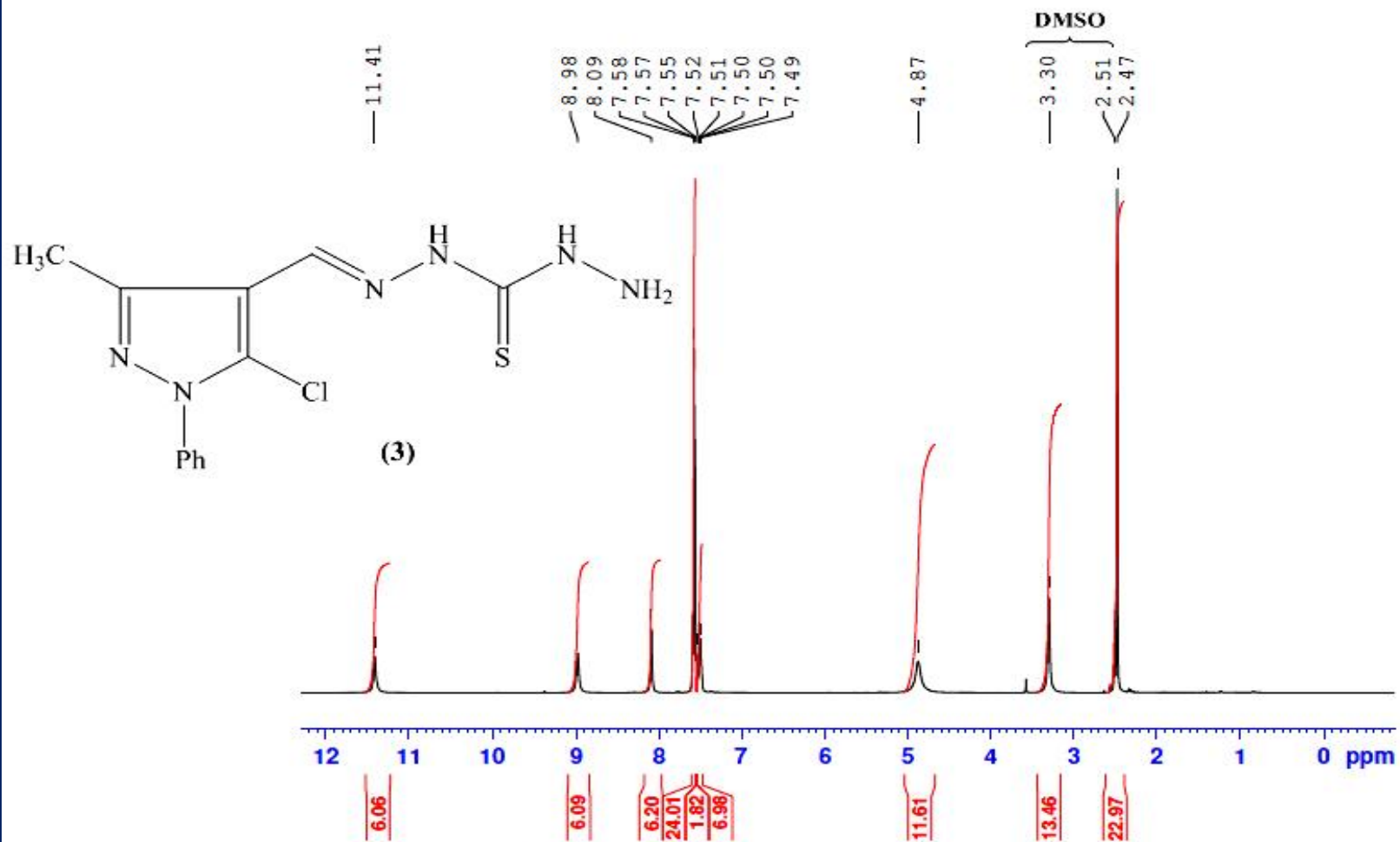
<sup>d</sup> *Soils, Water, and Environment Research Institute, Agricultural Research Center, Giza 12112, Egypt*

*\* Corresponding author: E-mail address: mokh.amin@taiz.edu.ye*

Spectral Analysis of Compound (3) including FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass Spectra.

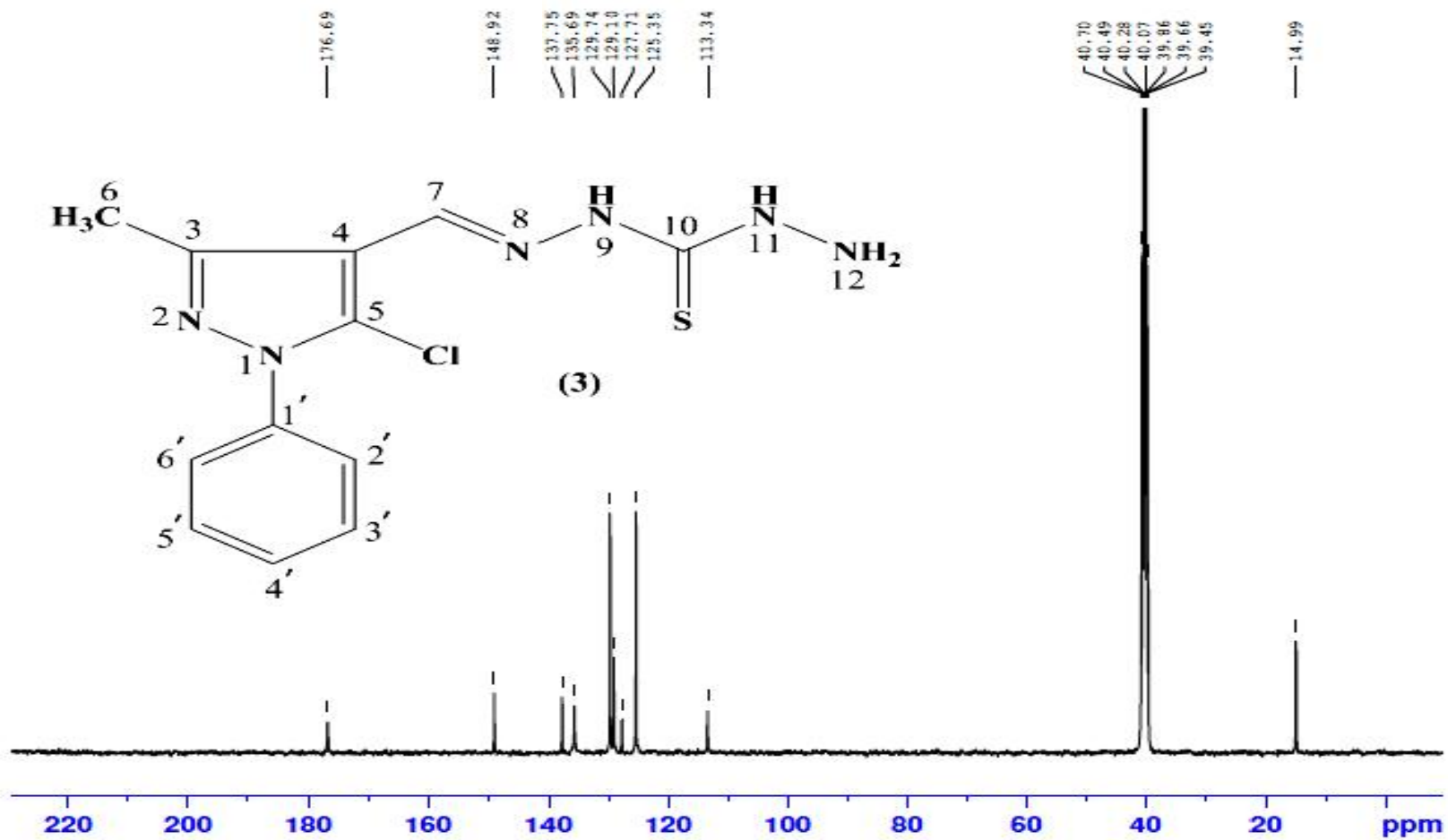


MS-1  
proton\_su DMSO (C:\nmr-data) Student 18



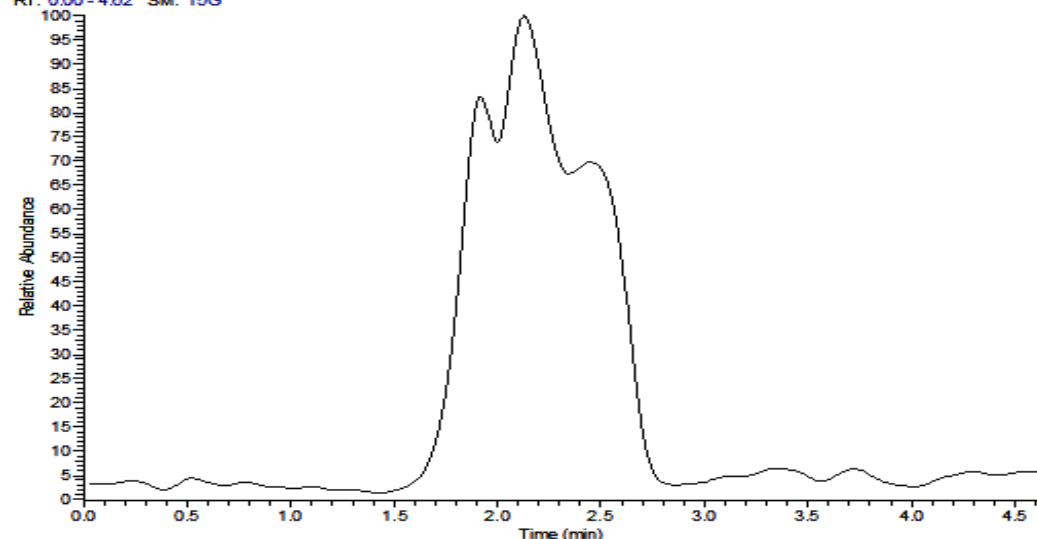
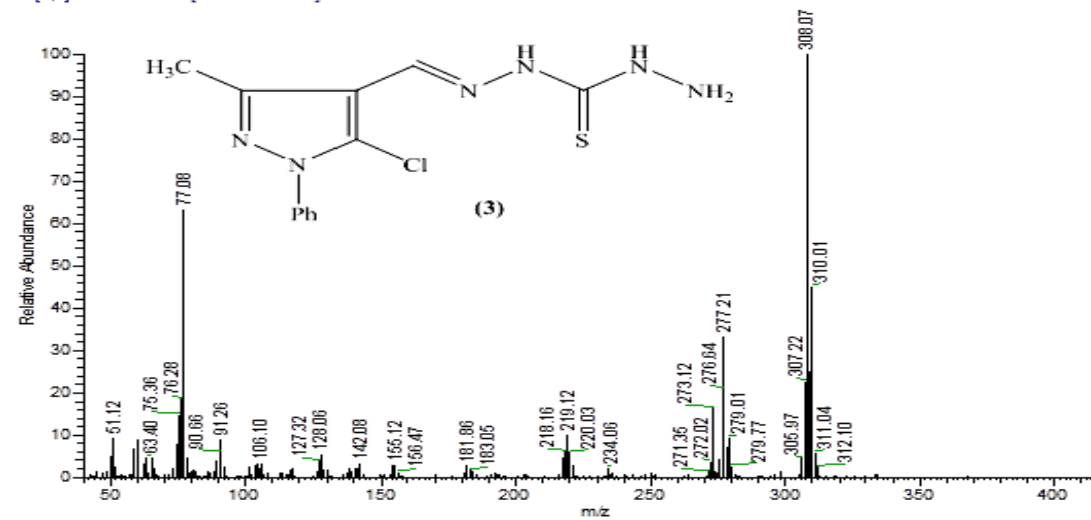
**<sup>1</sup>H-NMR Spectrum of Compound (3)**

MS-1  
c13\_su DMSO (C:\nmr-data) Student 18

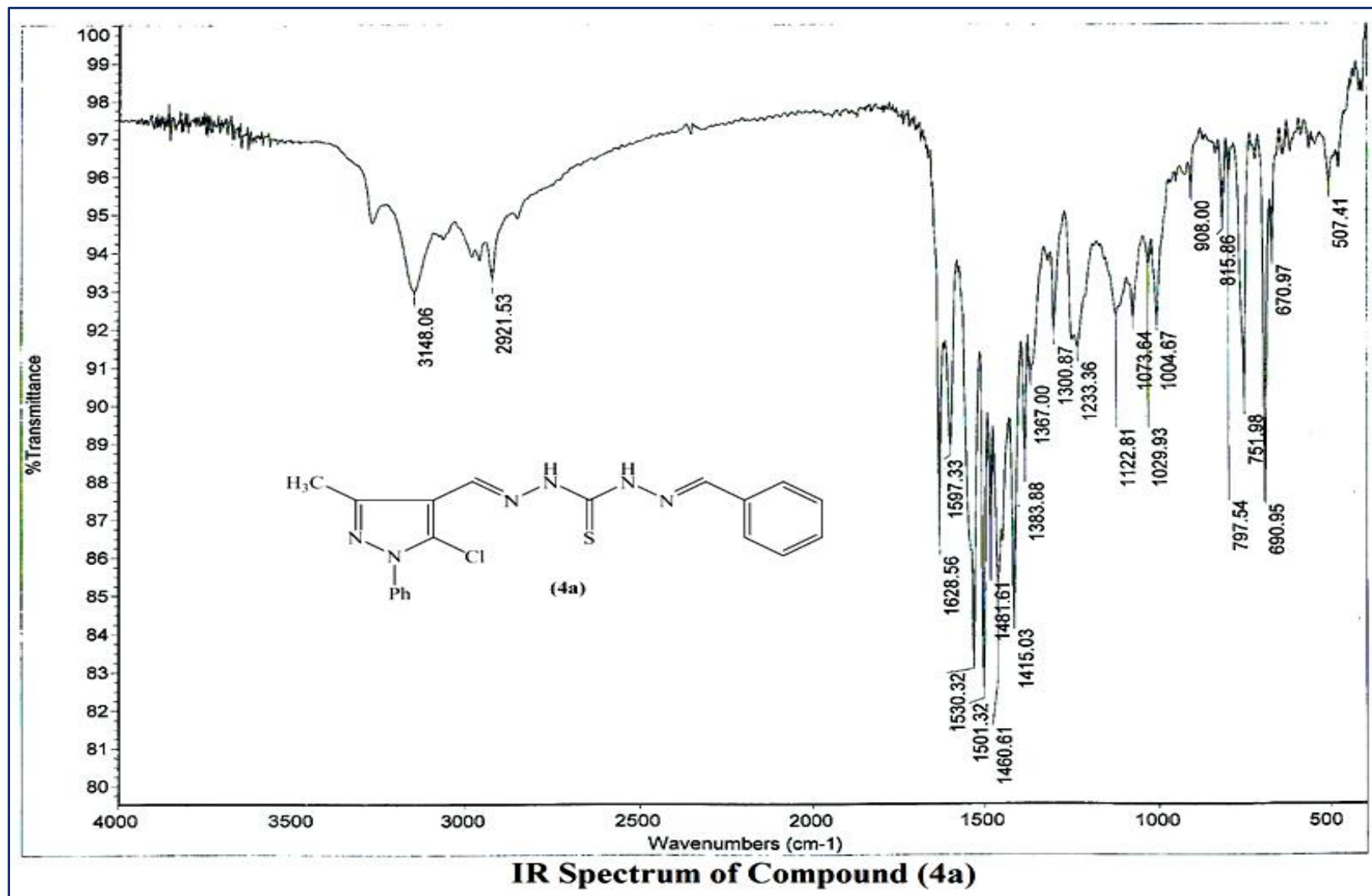


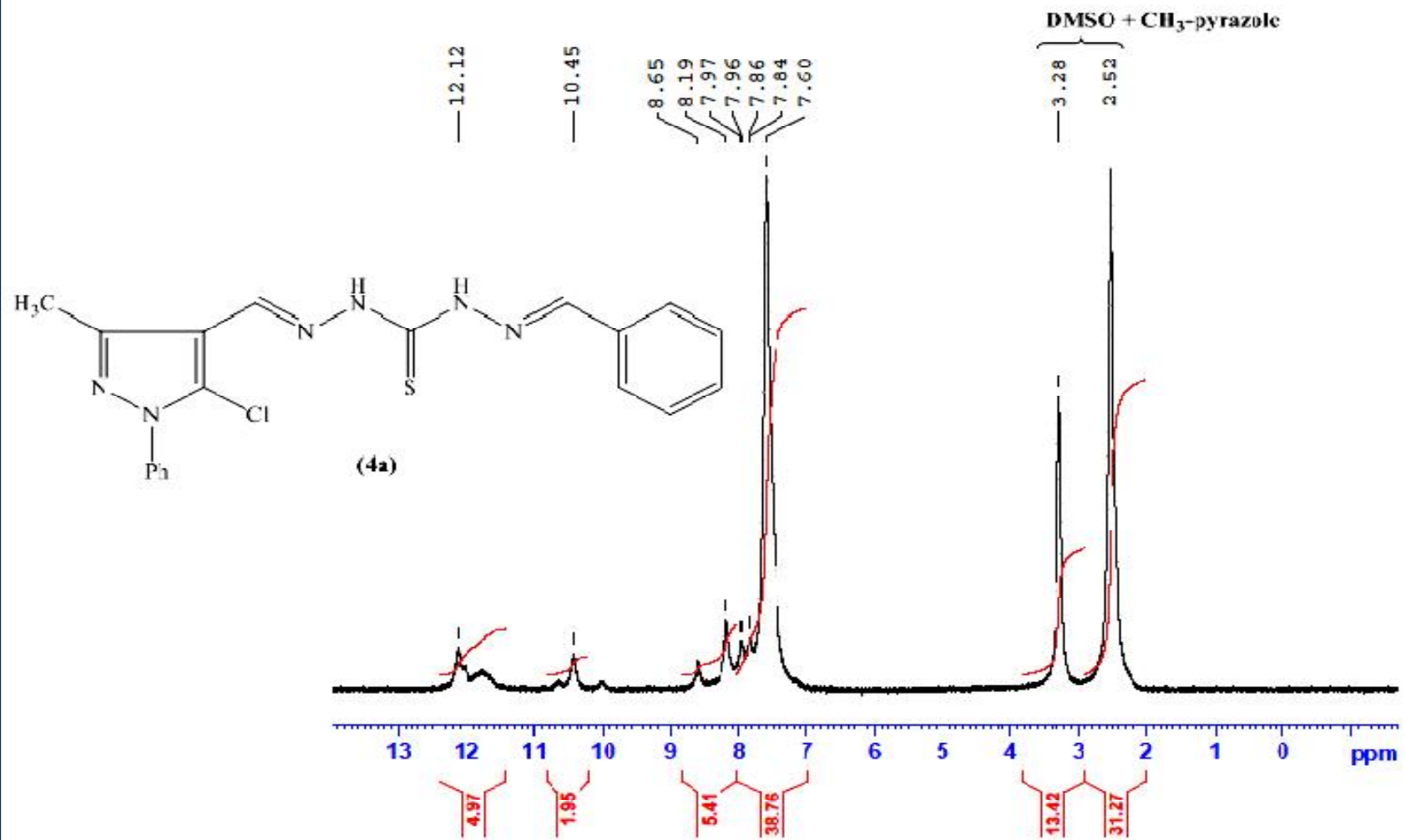
$^{13}\text{C}$ -NMR Spectrum of Compound (3)

RT: 0.00 - 4.62 SM: 15G

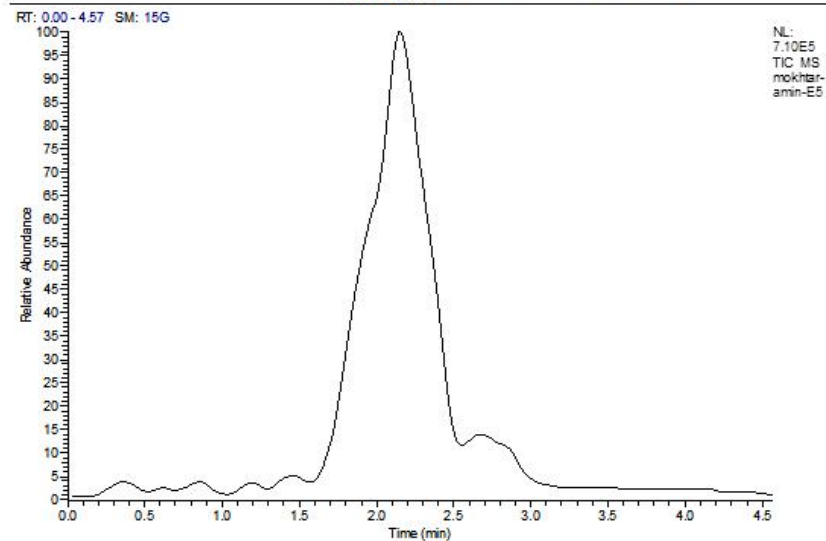
NL:  
8.14E5  
TIC MS  
mokhtar-  
amin-Emokhtar-amin-E #127 RT: 2.14 AV: 1 SB: 2 4.55 , 4.59 NL: 8.84E4  
T: (0,0) +c EI Full ms [40.00-1000.00]**Mass Spectrum of Compound (3)**

Spectral Analysis of Compound (4a) including FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass Spectra.

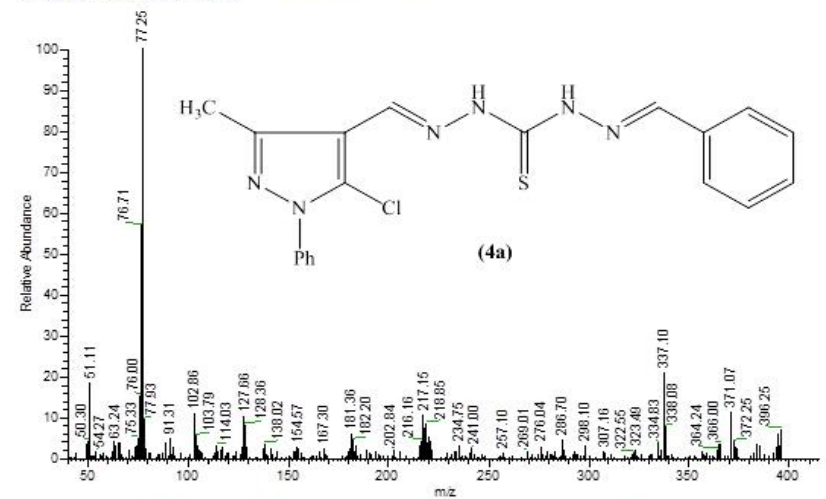




**<sup>1</sup>H-NMR Spectrum of Compound (4a)**



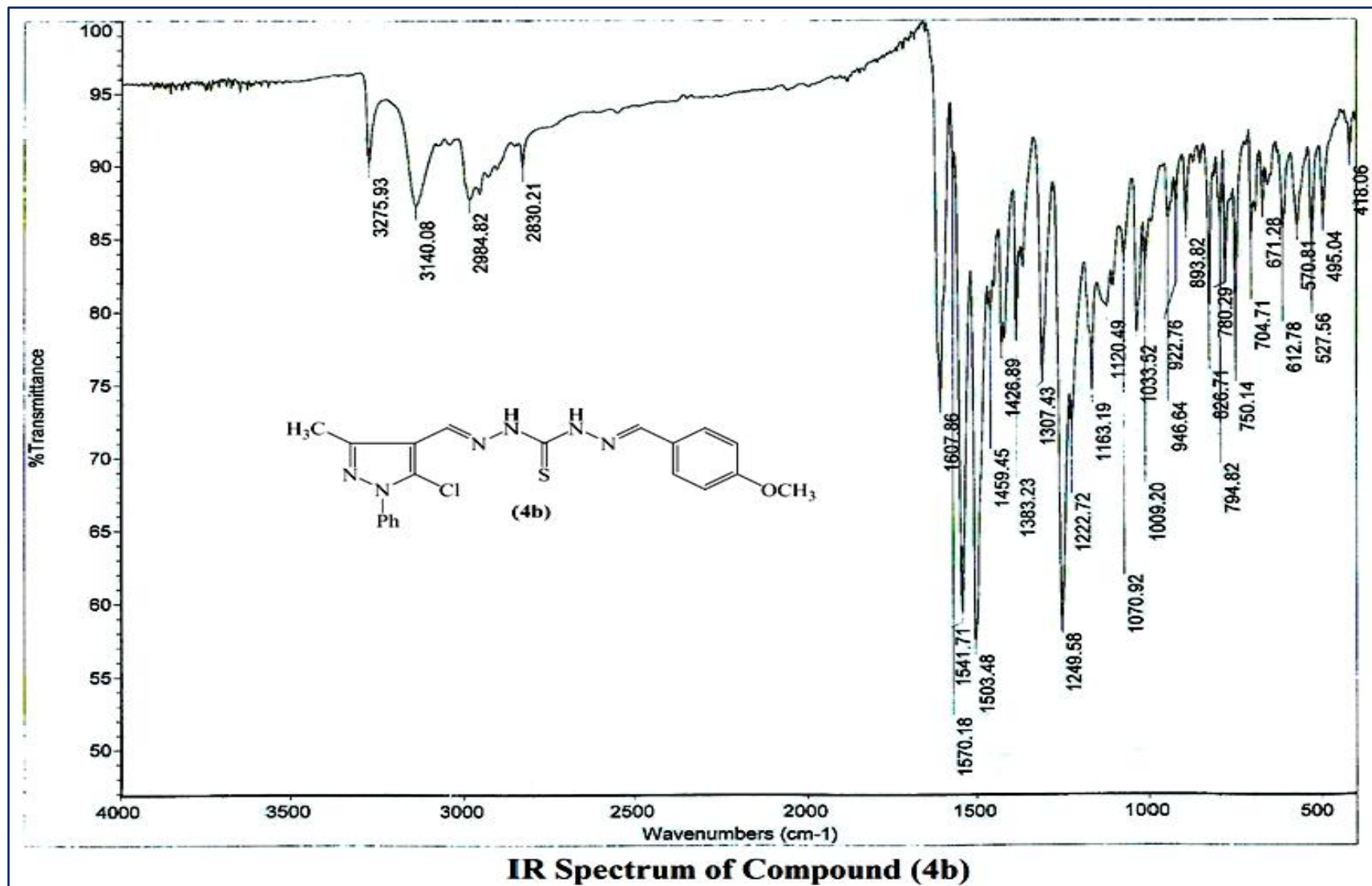
mokhtar-amin-E5 #129 RT: 2.18 AV: 1 SB: 2 4.55, 4.57 NL: 3.74E4  
T: (0,0) + e EI Full ms [40.00-1000.00]



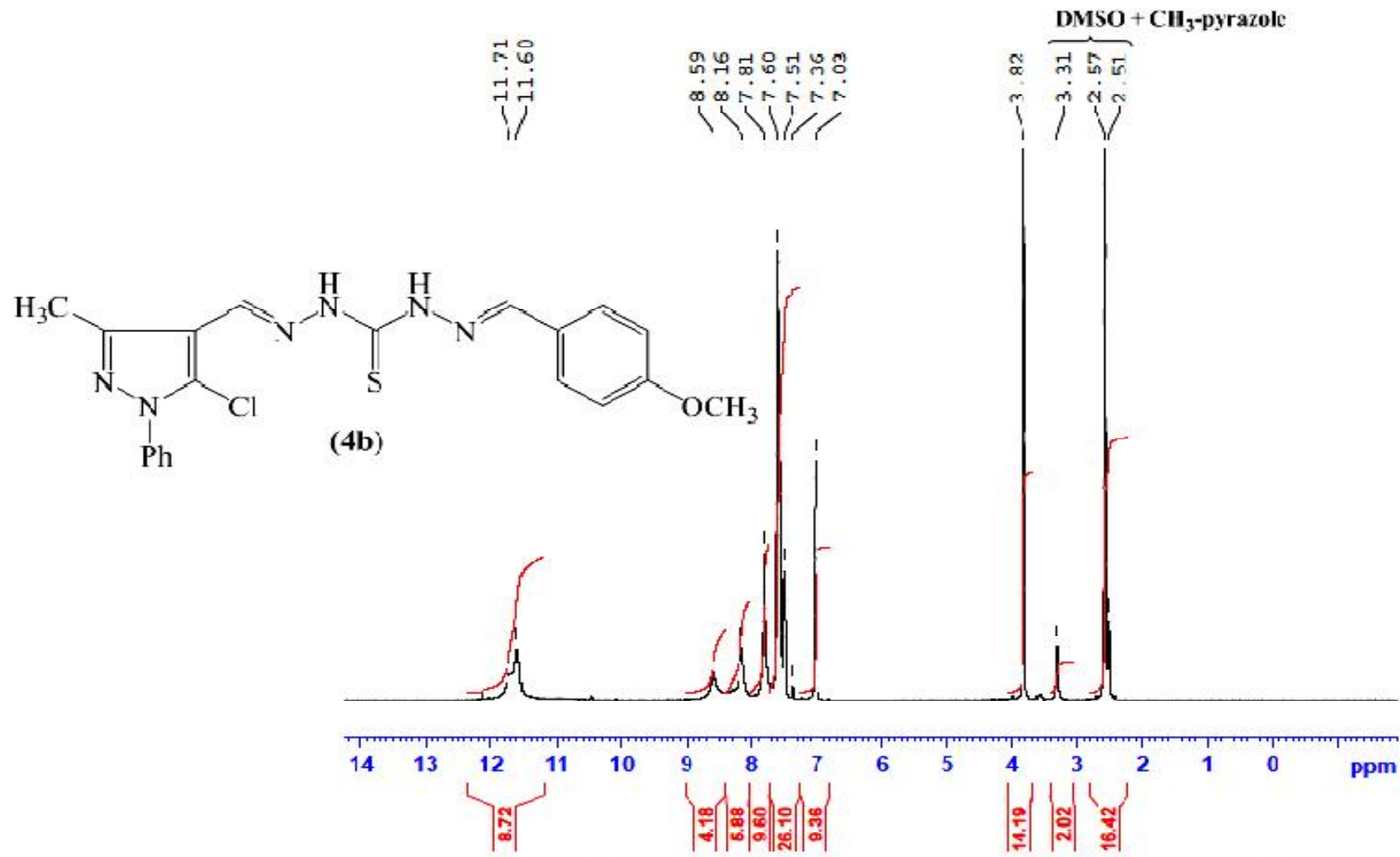
**Mass Spectrum of Compound (4a)**



Spectral Analysis of Compound (4b) including FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass Spectra.

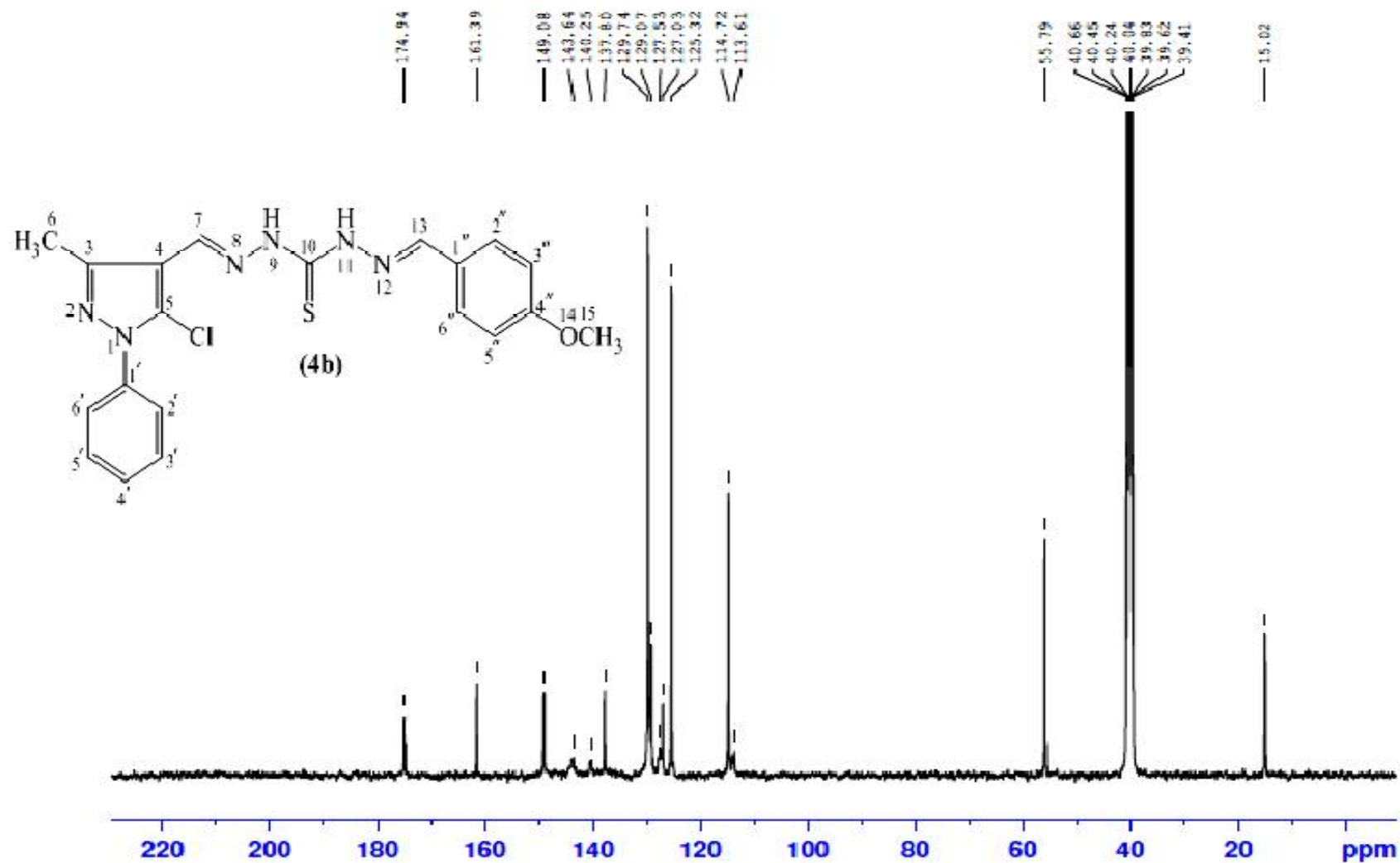


3-3  
proton\_su DMSO {C:\nmr-data} Student 6

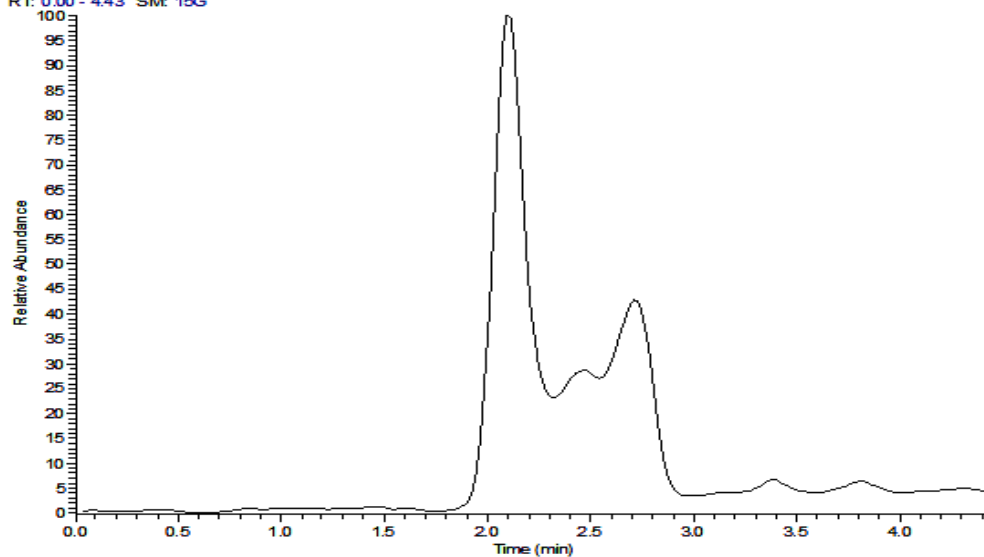
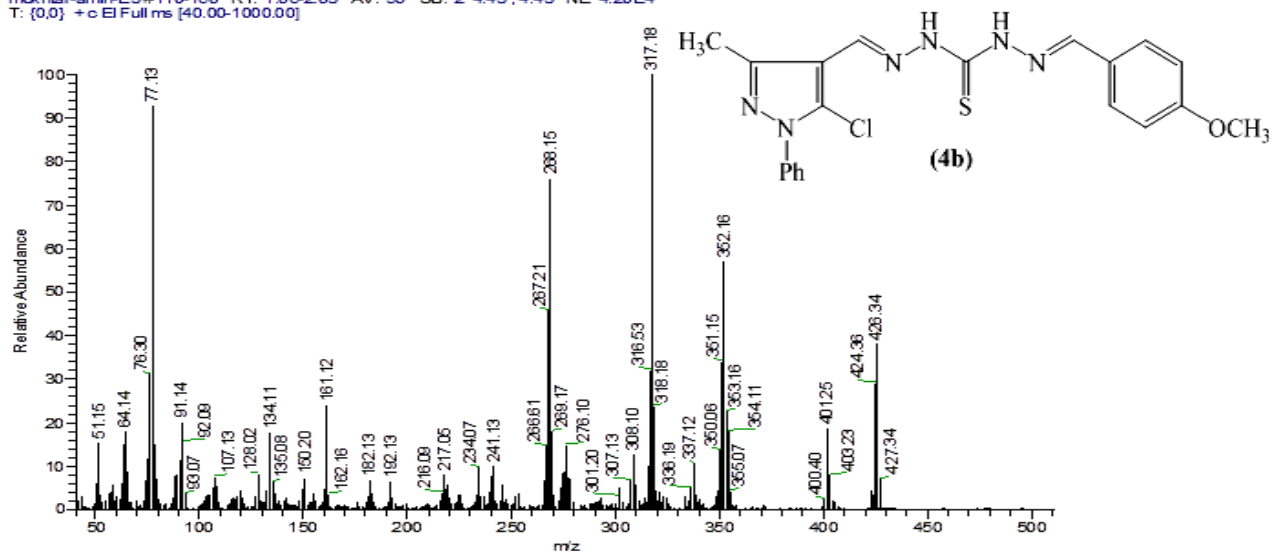


**<sup>1</sup>H-NMR Spectrum of Compound (4b)**

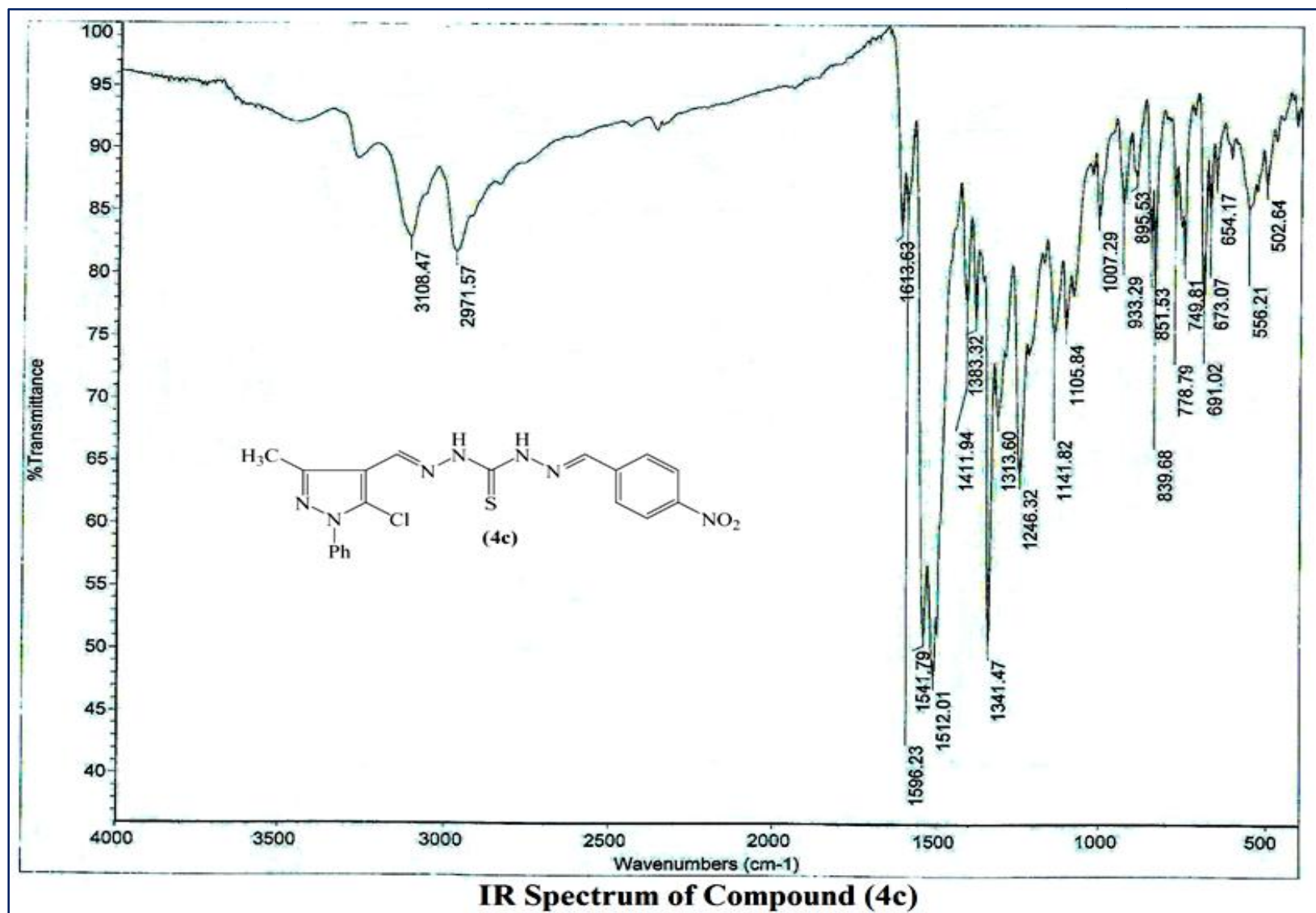
E-3  
c13\_su DMSO (C:\nmr-data) Student 12



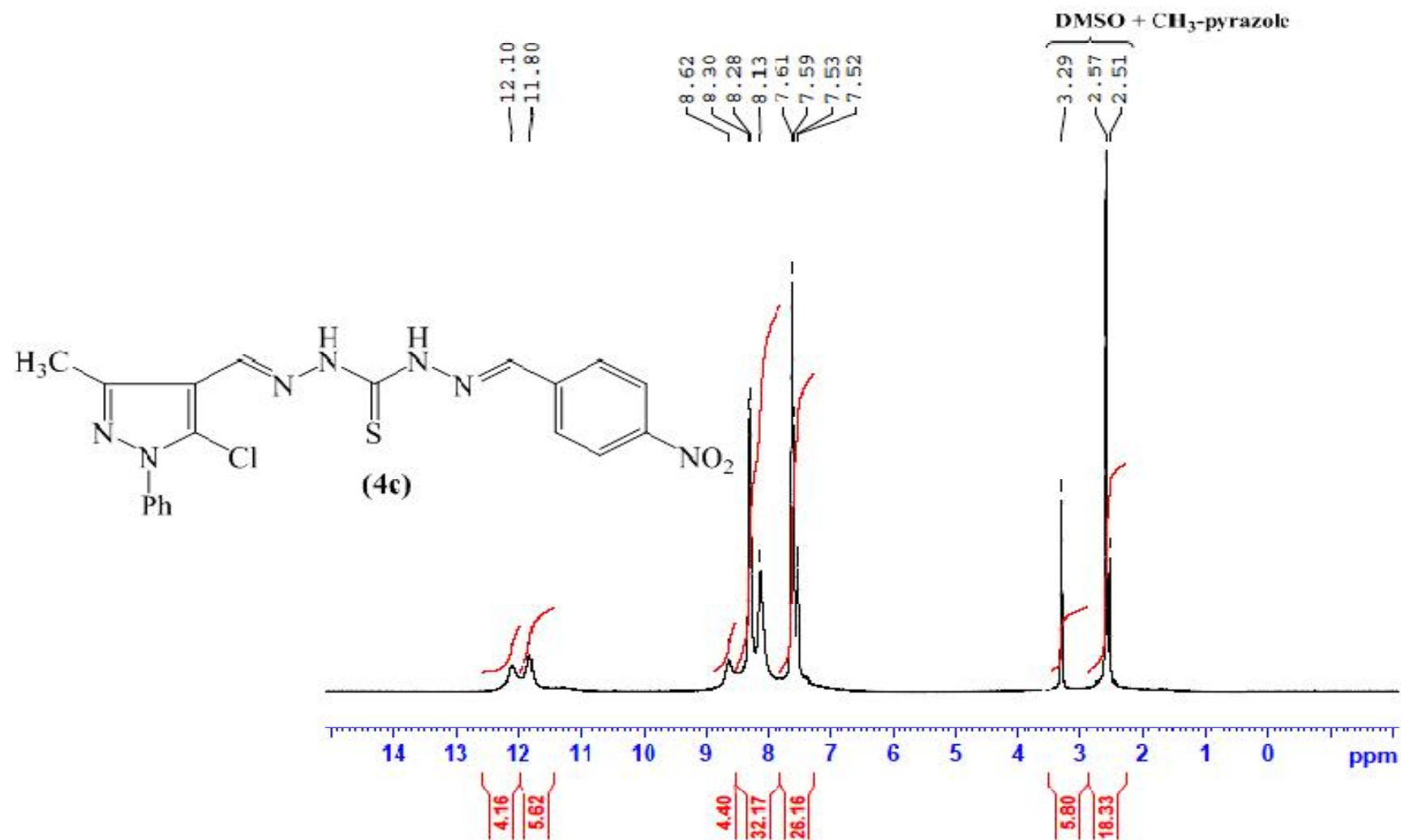
RT: 0.00 - 4.43 SM: 15G

NL:  
1.98E6  
TIC MS  
mokhtar-  
amin-E3mokhtar-amin-E3#110:168 RT: 1.86-2.83 AV: 59 SB: 2 4.43, 4.43 NL: 4.20E4  
T: [0,0] +c EI Full ms [40.00-1000.00]

Spectral Analysis of Compound (4c) including FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass Spectra.

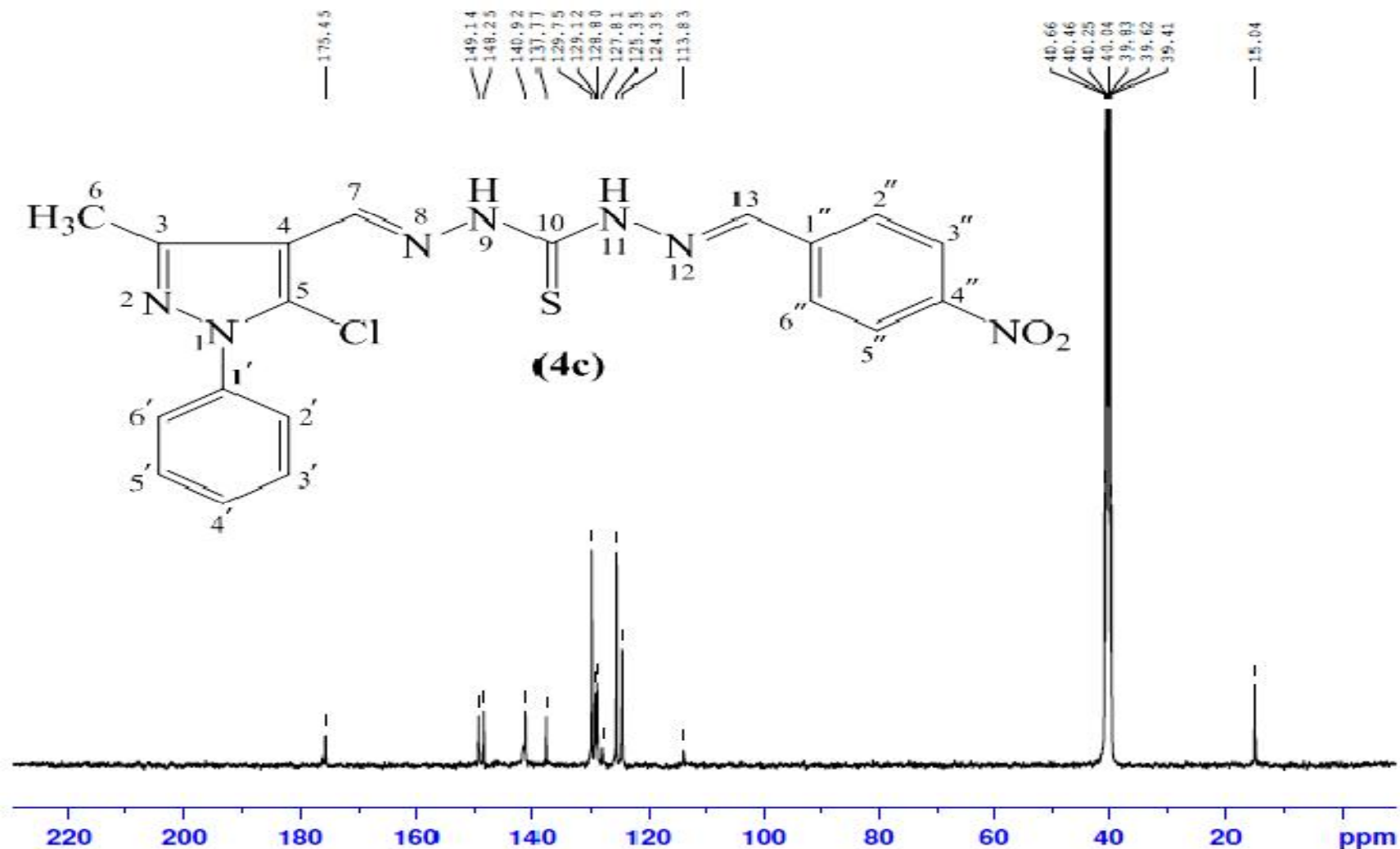


E-1  
proton\_su DMSO {C:\nmr-data} Student 4

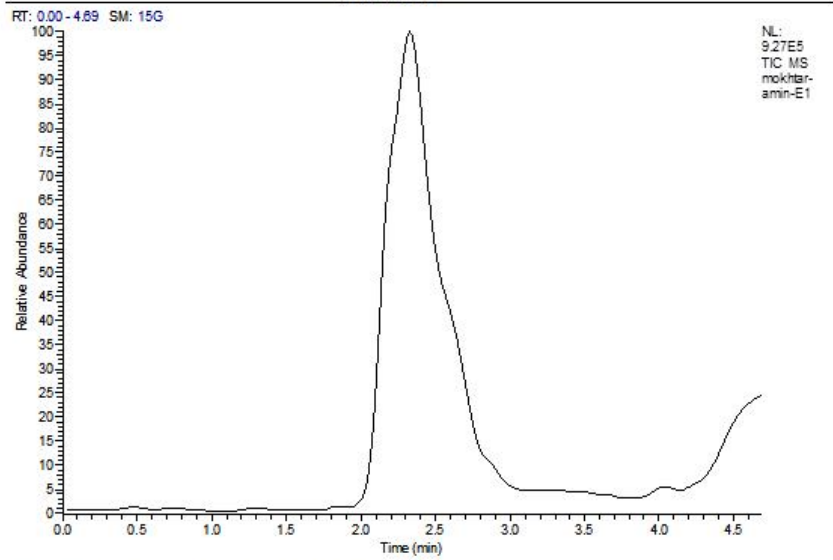


**<sup>1</sup>H-NMR Spectrum of Compound (4c)**

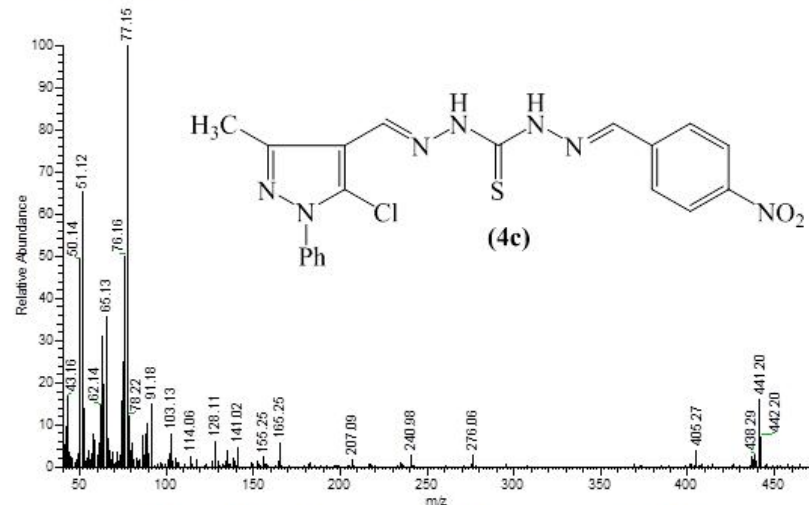
E-1  
c13\_su DMSO (C:\nmr-data) Student 10



**$^{13}\text{C}$ -NMR Spectrum of Compound (4c)**

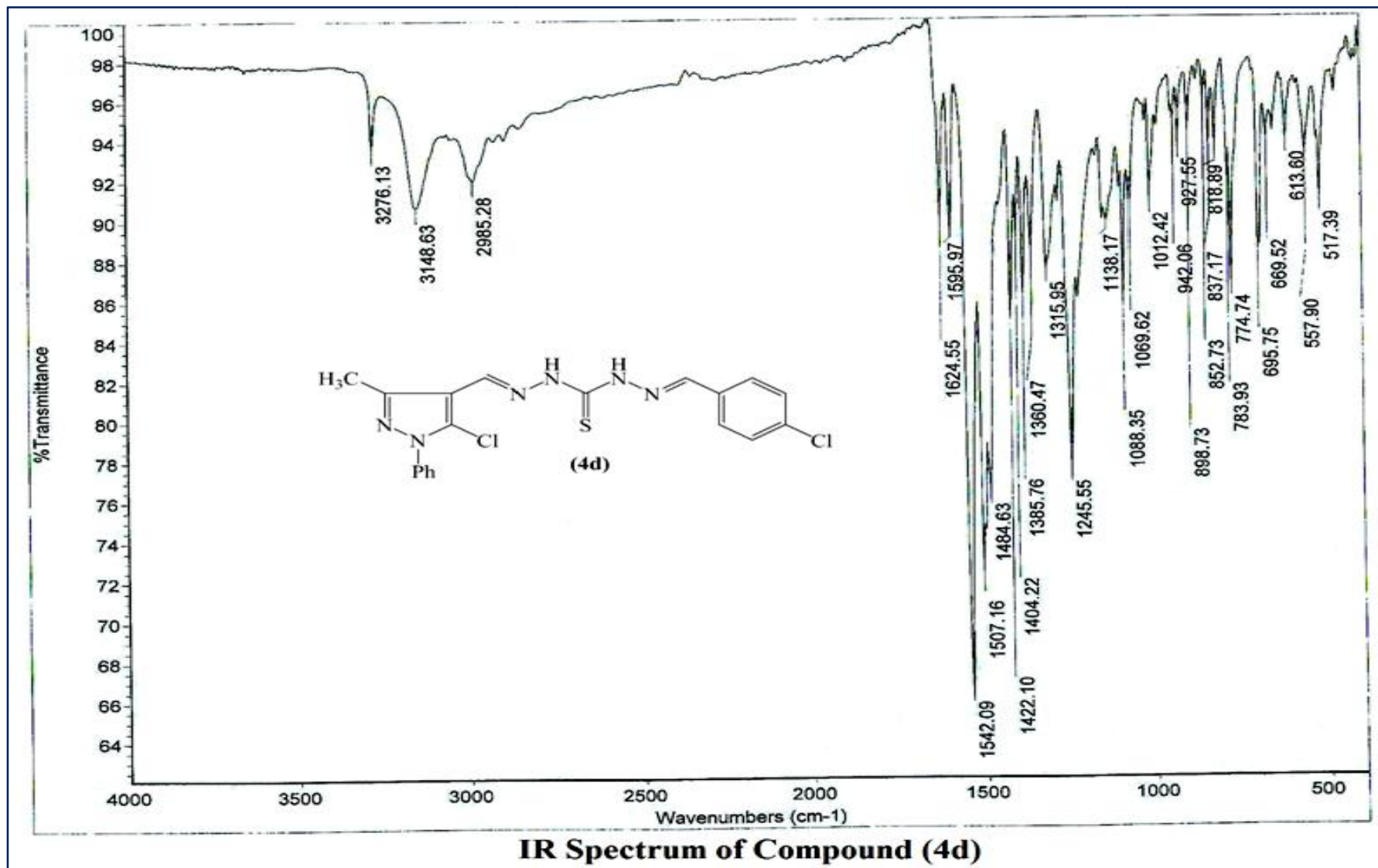


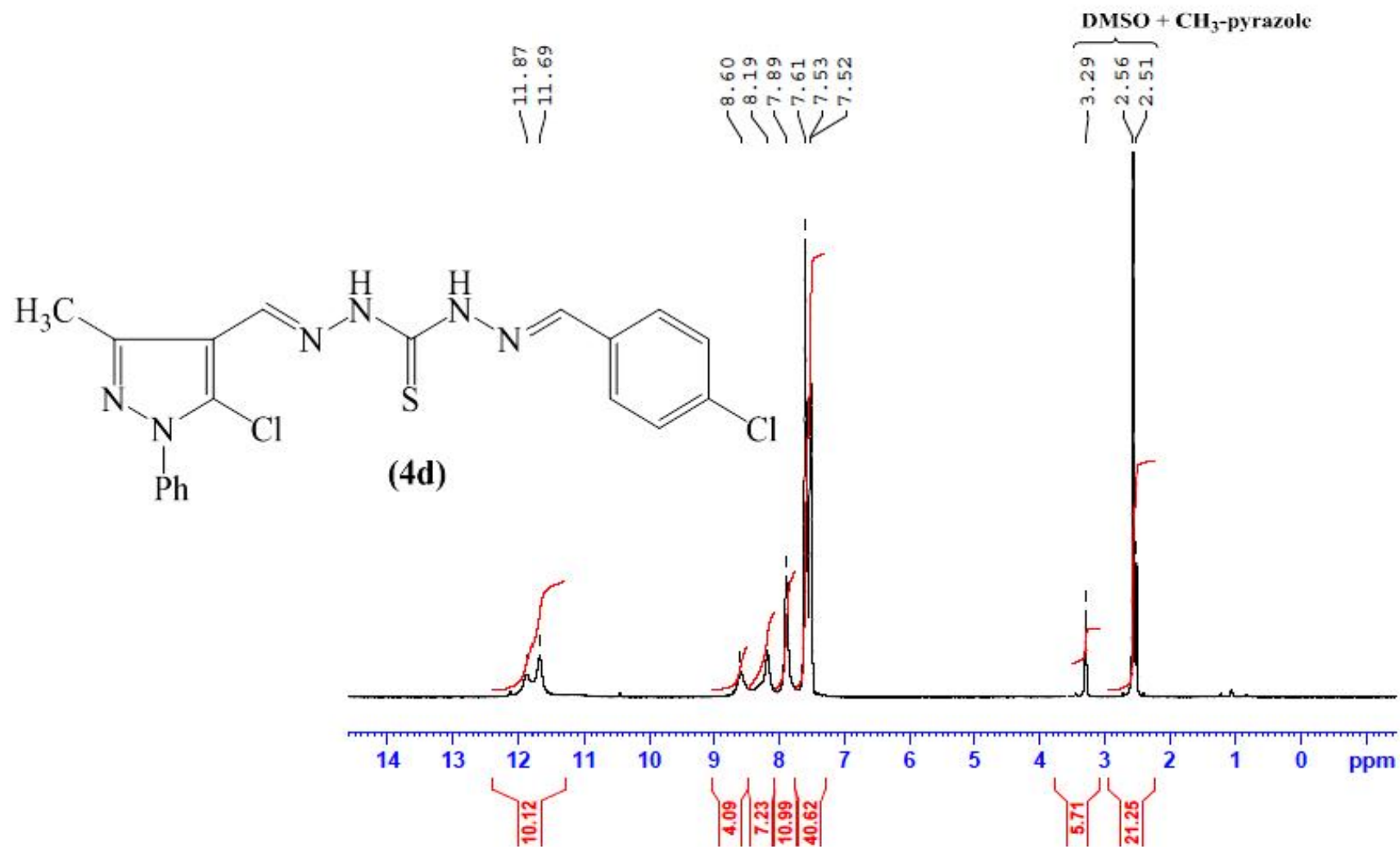
mokter-amin-E1#131 RT: 2.21 AV: 1 SB: 2 4.55, 4.59 NL: 7.89E4  
 T: (0,0) +o EI Full ms [40.00-1000.00]





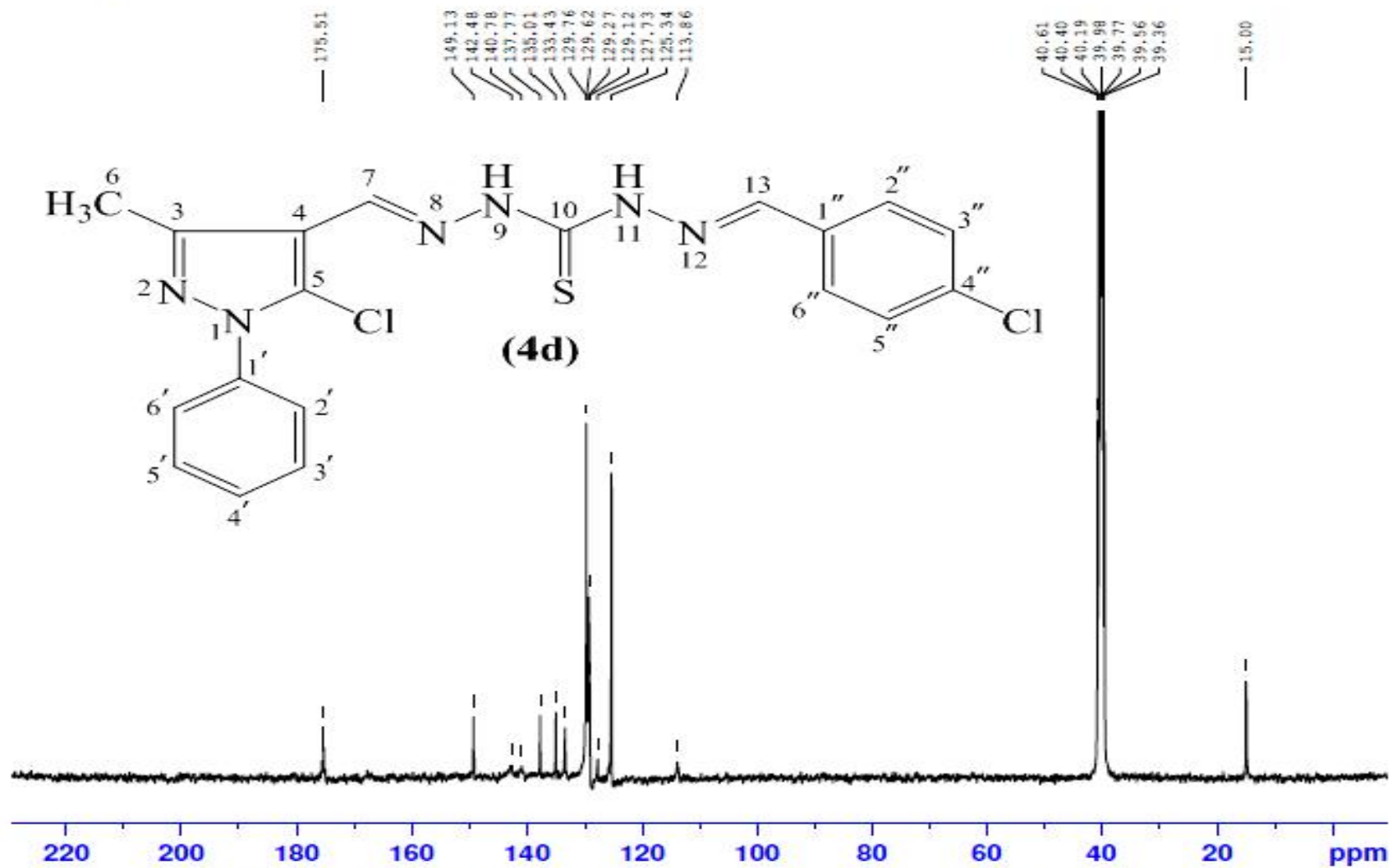
Spectral Analysis of Compound (4d) including FT-IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass Spectra.

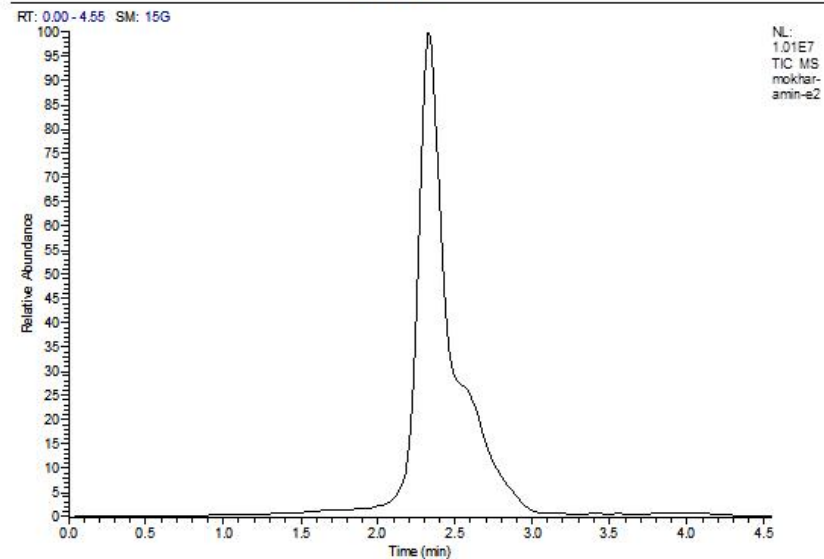




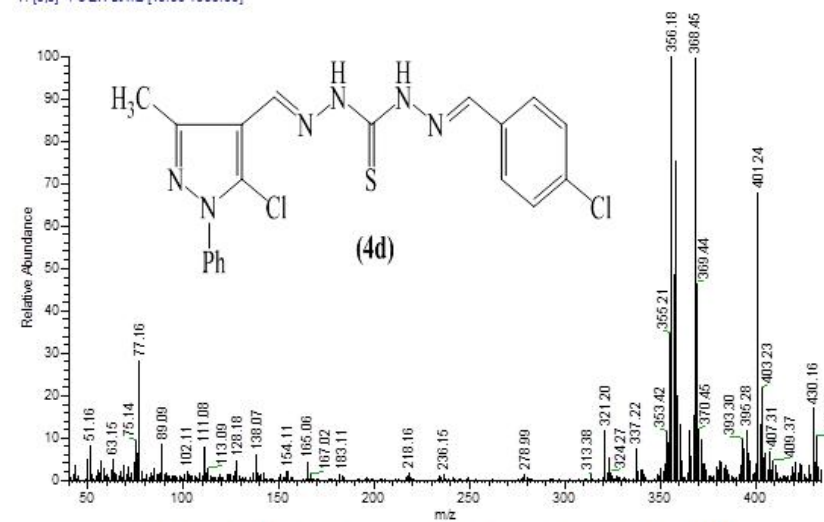
**<sup>1</sup>H-NMR Spectrum of Compound (4d)**

E-2  
c13\_su DMSO (C:\nmr-data) Student 11





mokhar-amin-e2 #135 RT: 2.28 AV: 1 SB: 2 4.55, 4.55 NL: 2.59E5  
T: (0,0) +eI Full ms [40.00-1000.00]



**Mass Spectrum of Compound (4d)**