

## **Supplementary data**

### **Synthesis and in vitro anticancer activity of novel 4-aryl-3-(4-methoxyphenyl)-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridines arrest cell cycle and induce cell apoptosis by inhibiting CDK2 and/or CDK9**

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**Keywords:** Pyrazolo[3,4-*b*]pyridines; Antiproliferative; Cell cycle; Apoptosis; CDK2; CDK9

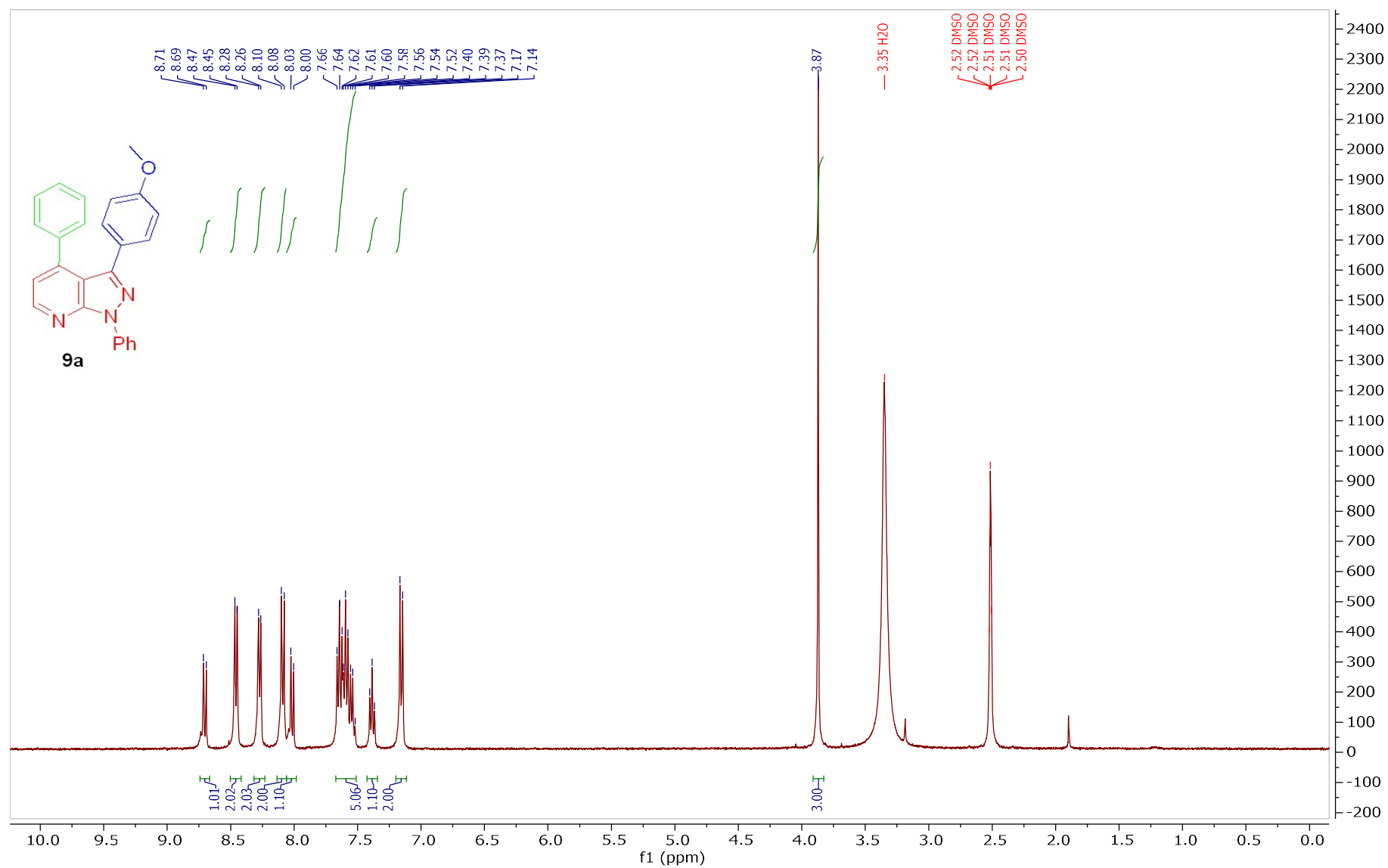
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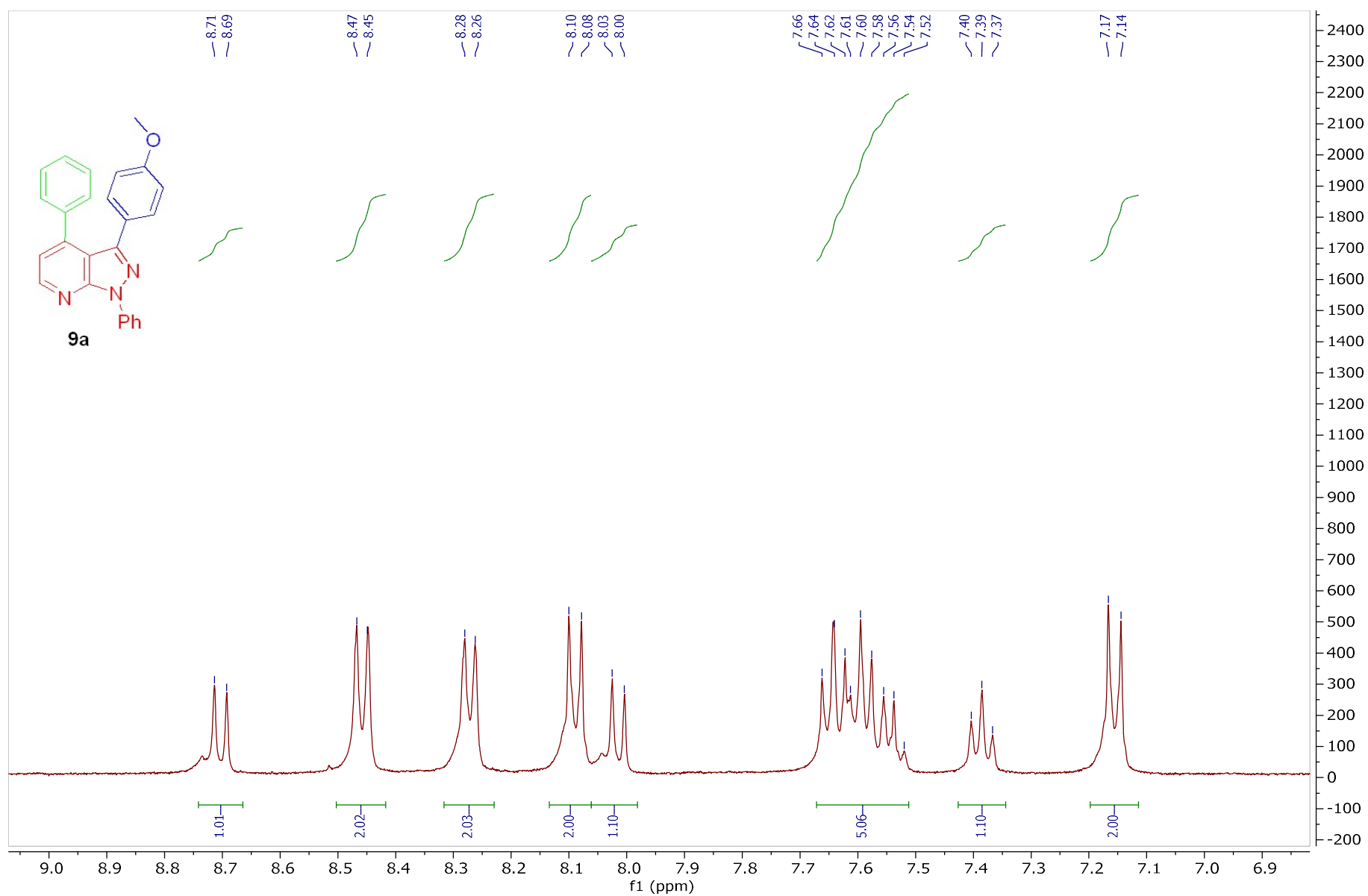
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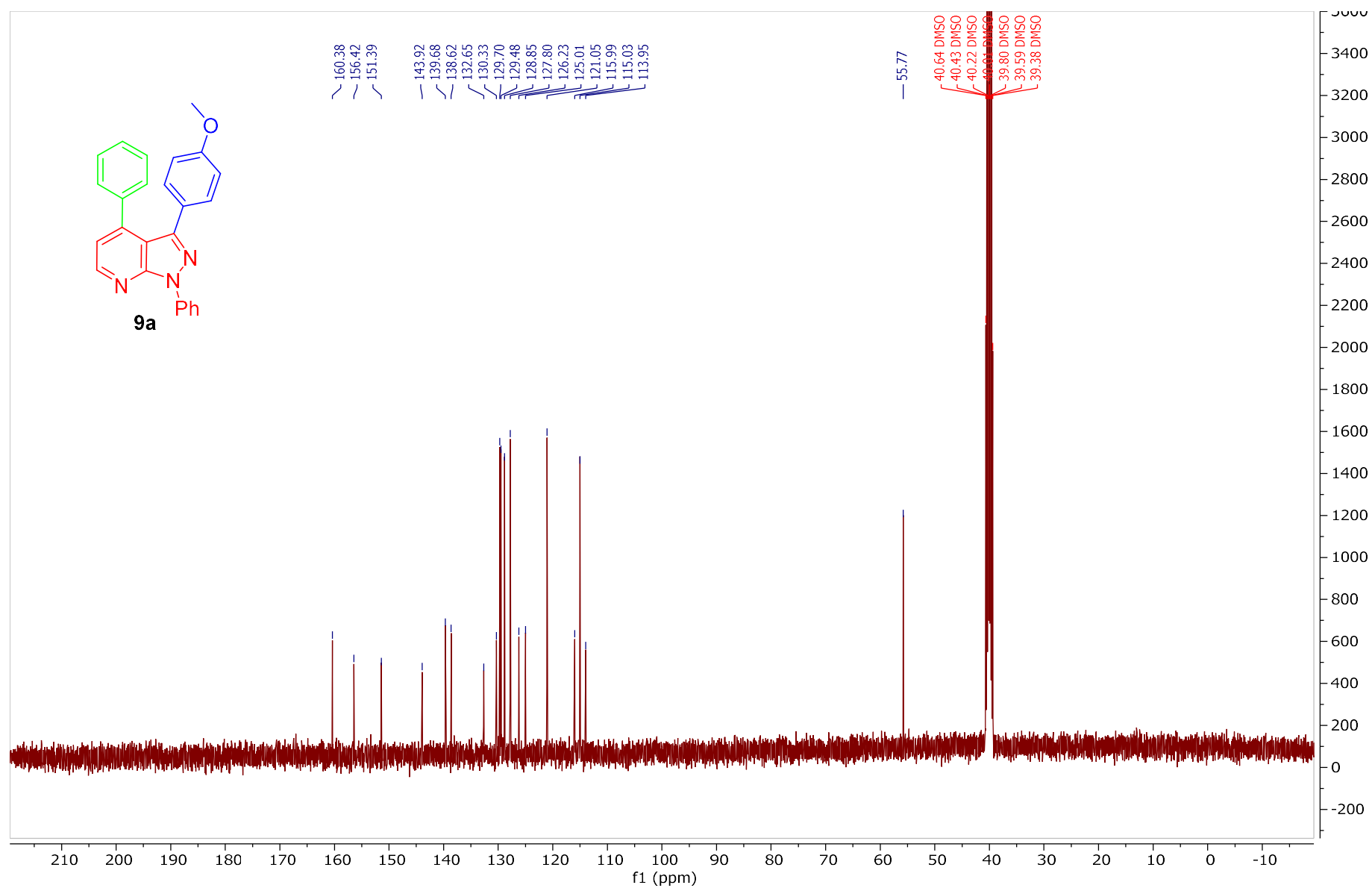
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**Figure S1.** <sup>1</sup>H NMR of compound **9a**, full spectrum

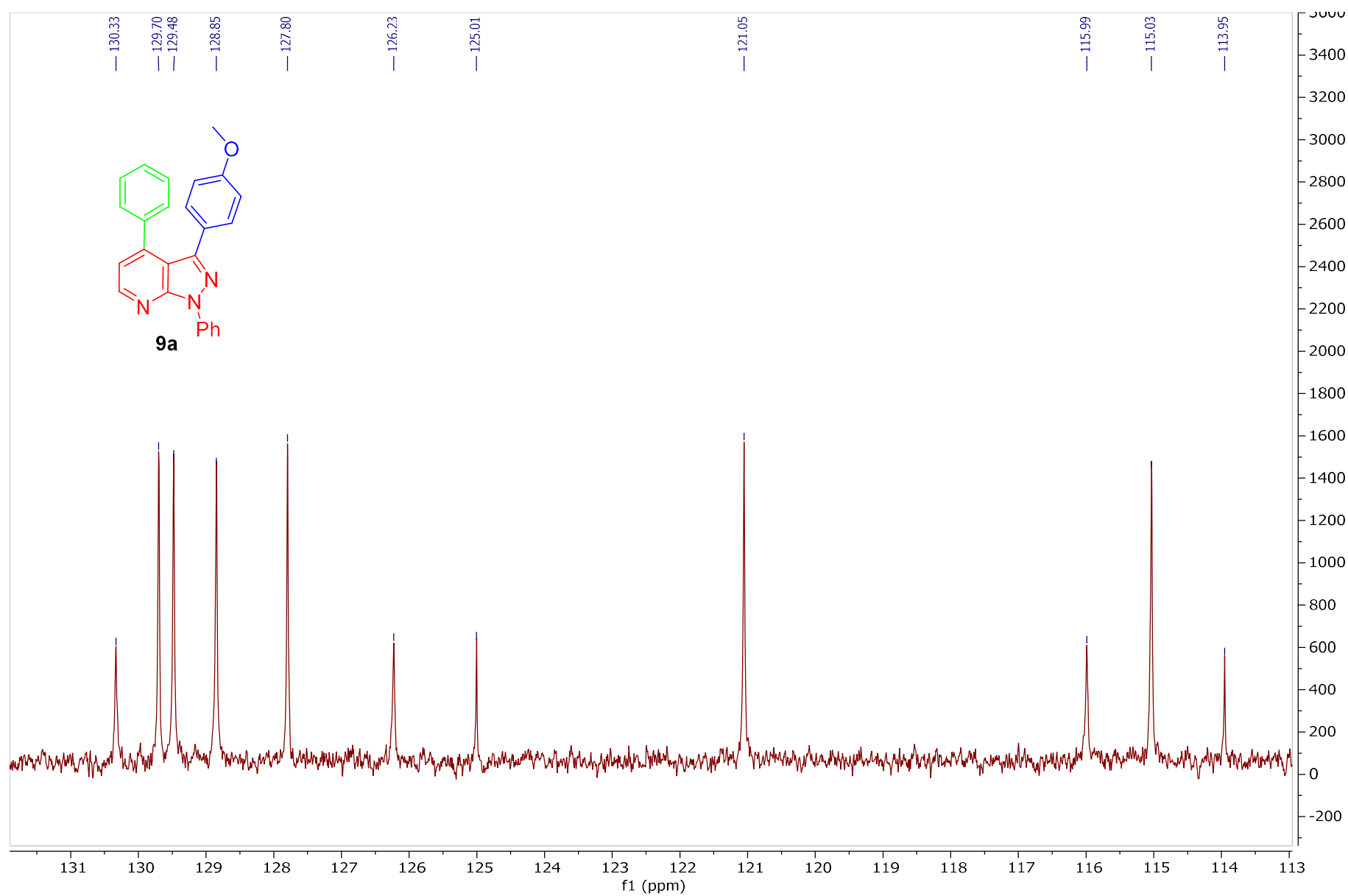


**Figure S2.** <sup>1</sup>H NMR of compound **9a**, aromatic region

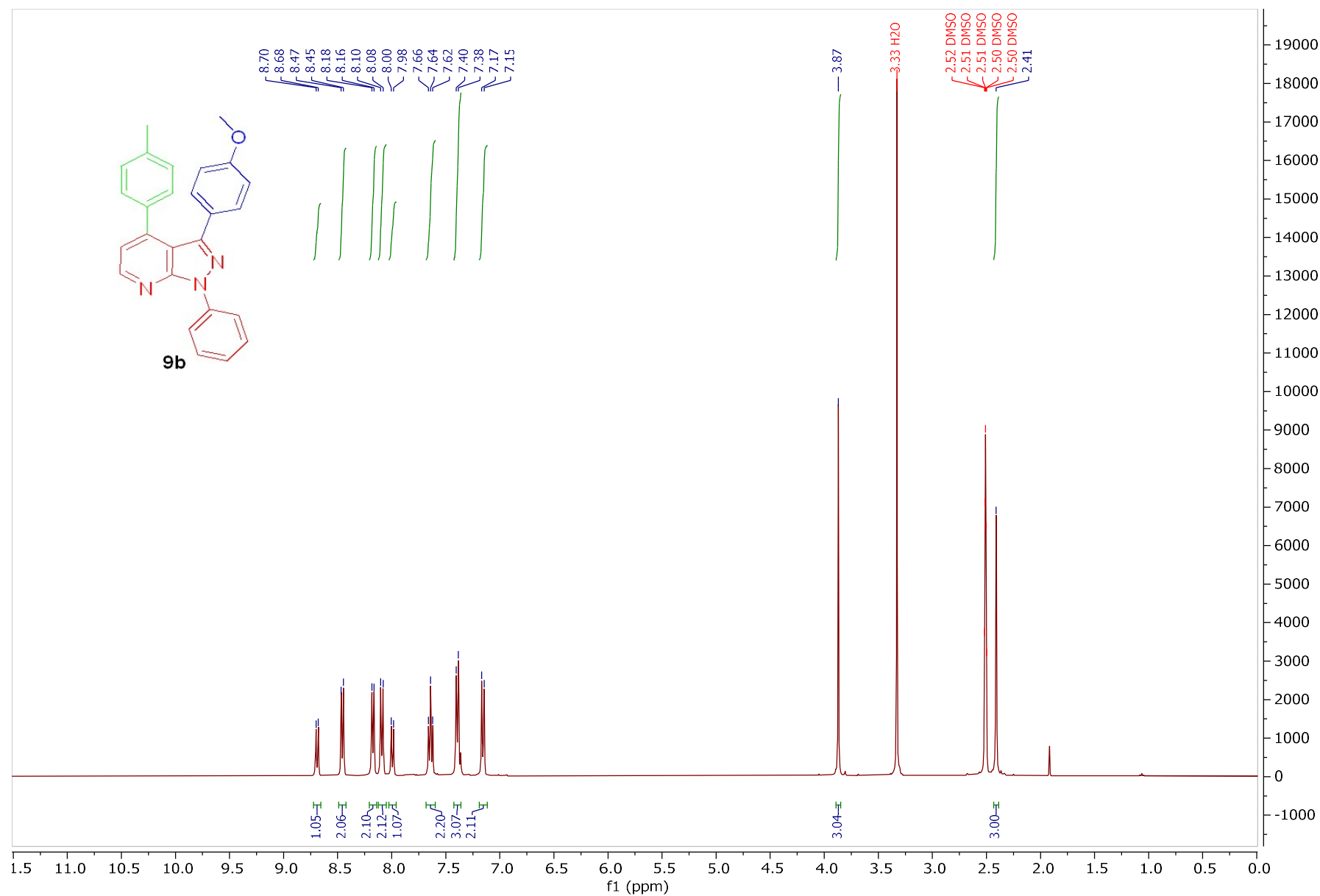


**Figure S3.**  $^{13}\text{C}$  NMR of compound **9a**, full spectrum

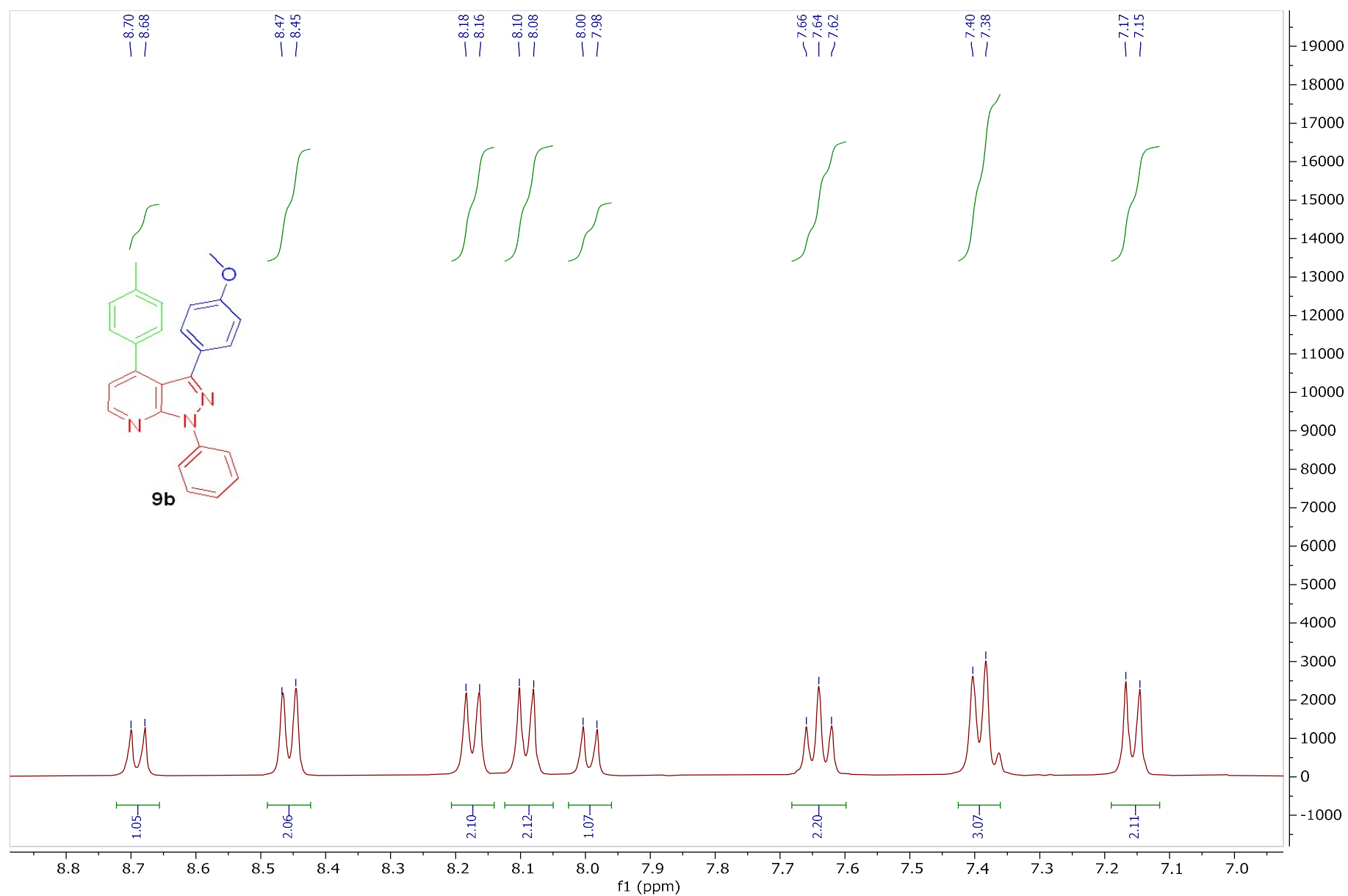




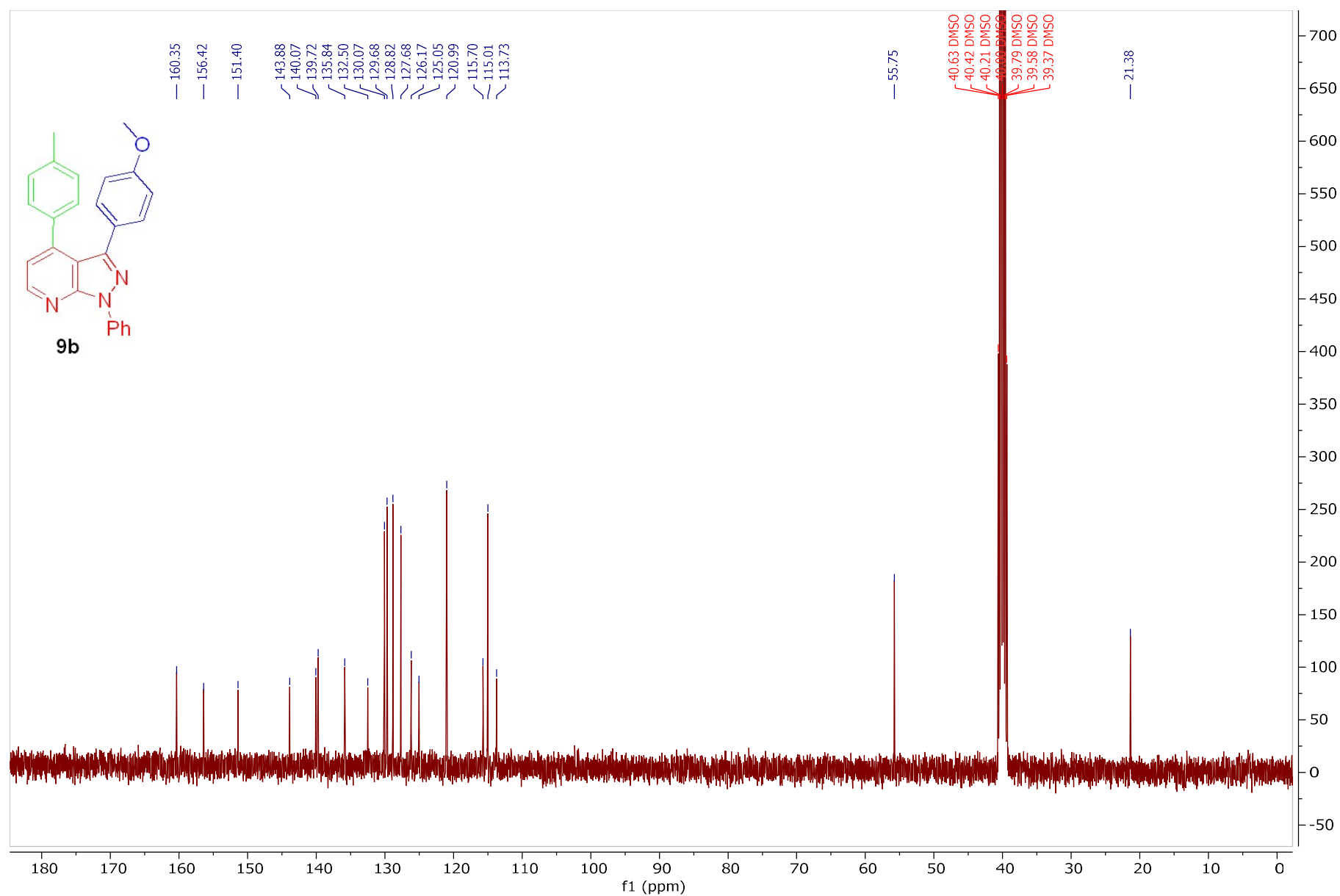
**Figure S4.**  $^{13}\text{C}$  NMR of compound **9a**, aromatic region



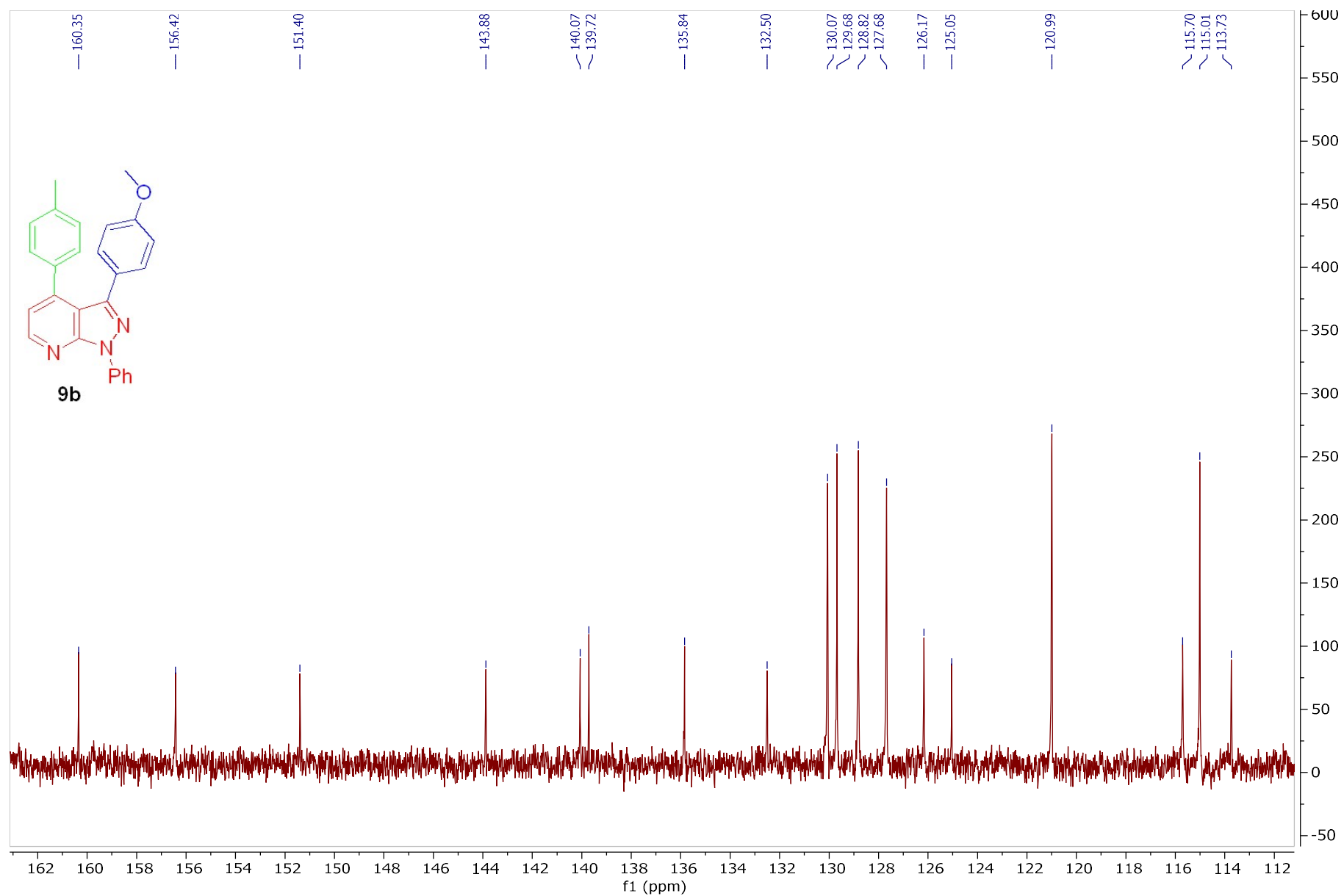
**Figure S5.** <sup>1</sup>H NMR of compound **9b**, full spectrum



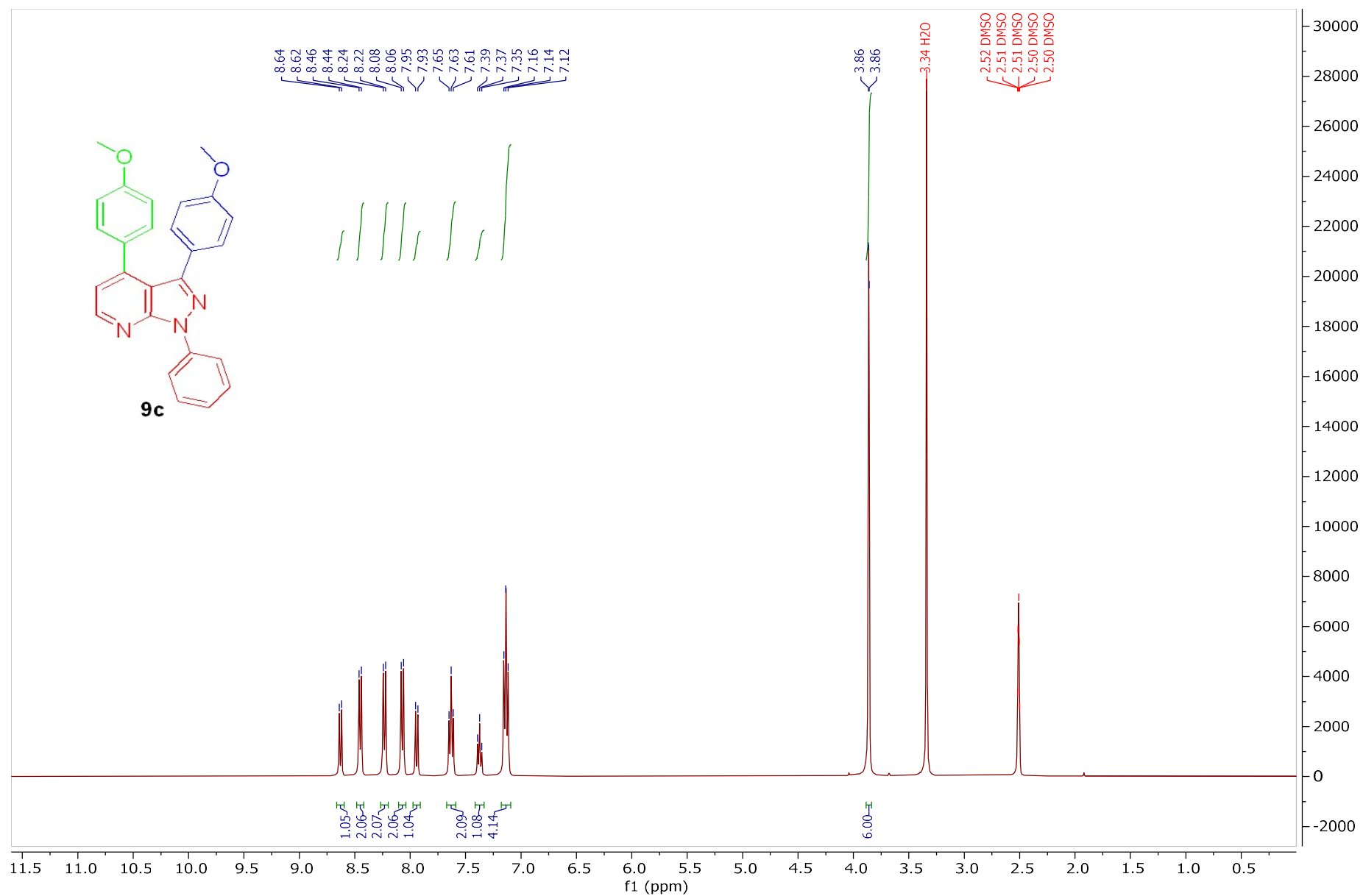
**Figure S6.** <sup>1</sup>H NMR of compound **9b**, aromatic region



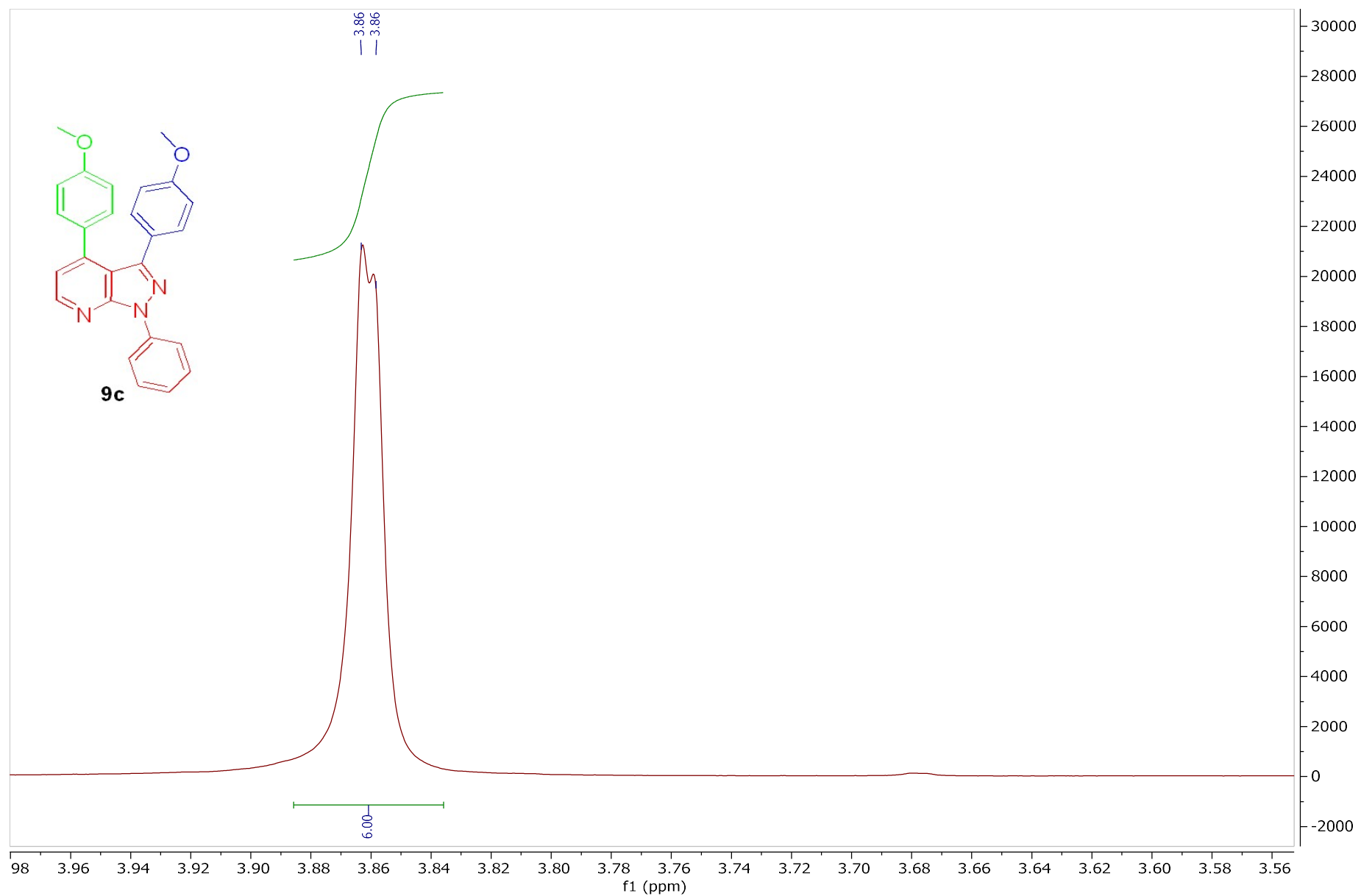
**Figure S7.**  $^{13}\text{C}$  NMR of compound **9b**, full spectrum



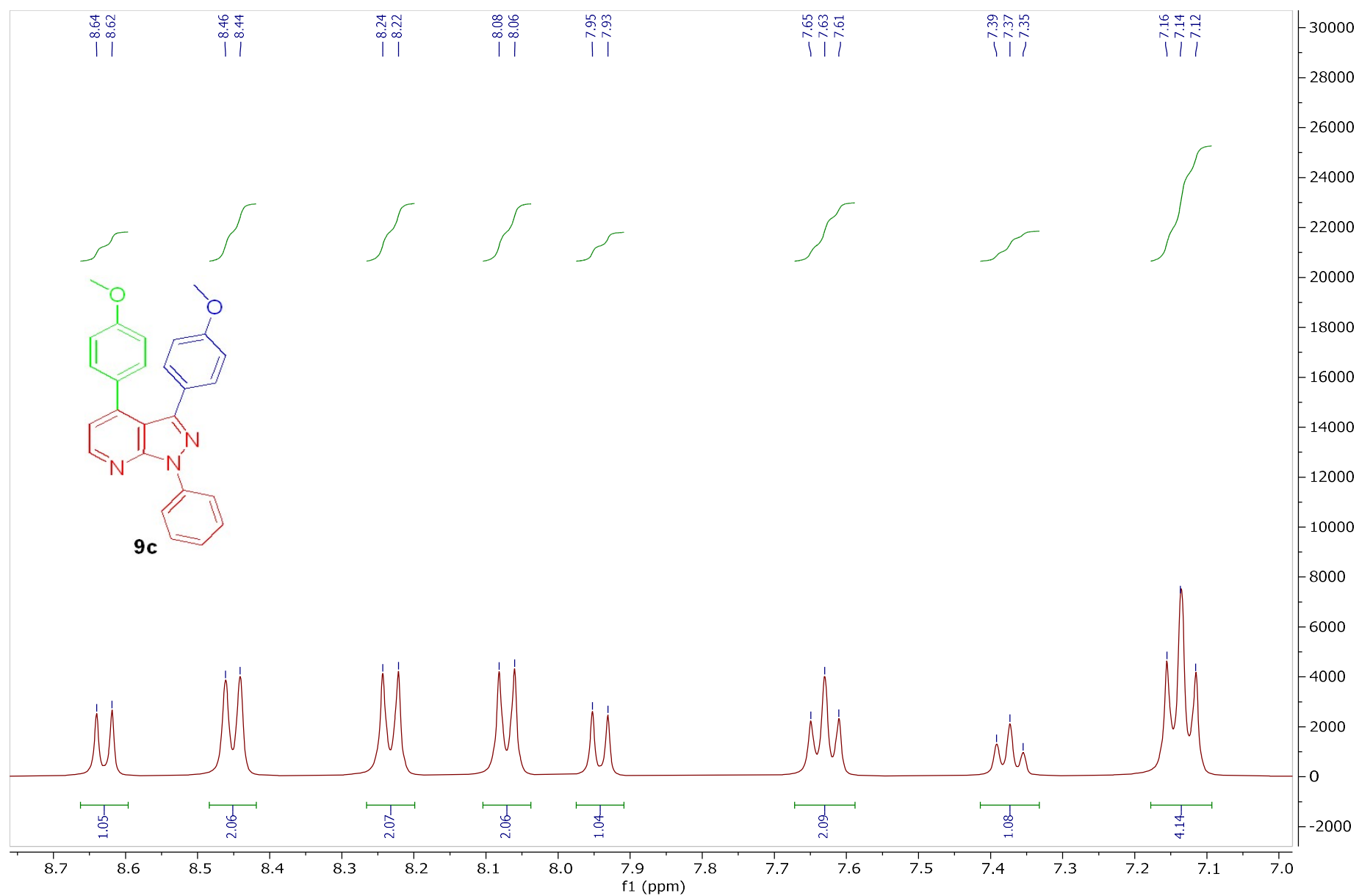
**Figure S8.**  $^{13}\text{C}$  NMR of compound **9b**, aromatic region



**Figure S9.** <sup>1</sup>H NMR of compound **9c**, full spectrum

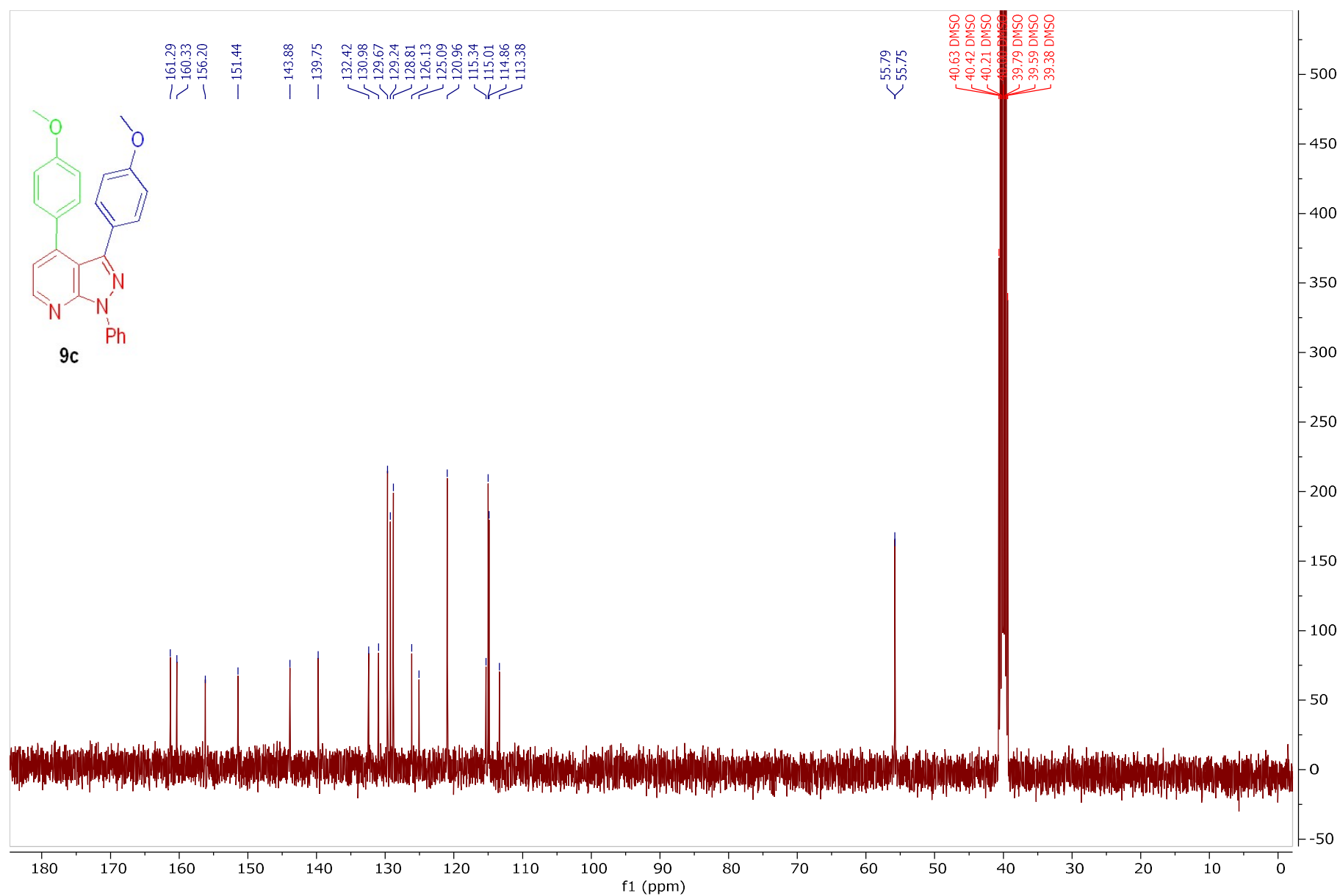


**Figure S10.**  $^1\text{H}$  NMR of compound **9c**, aliphatic region

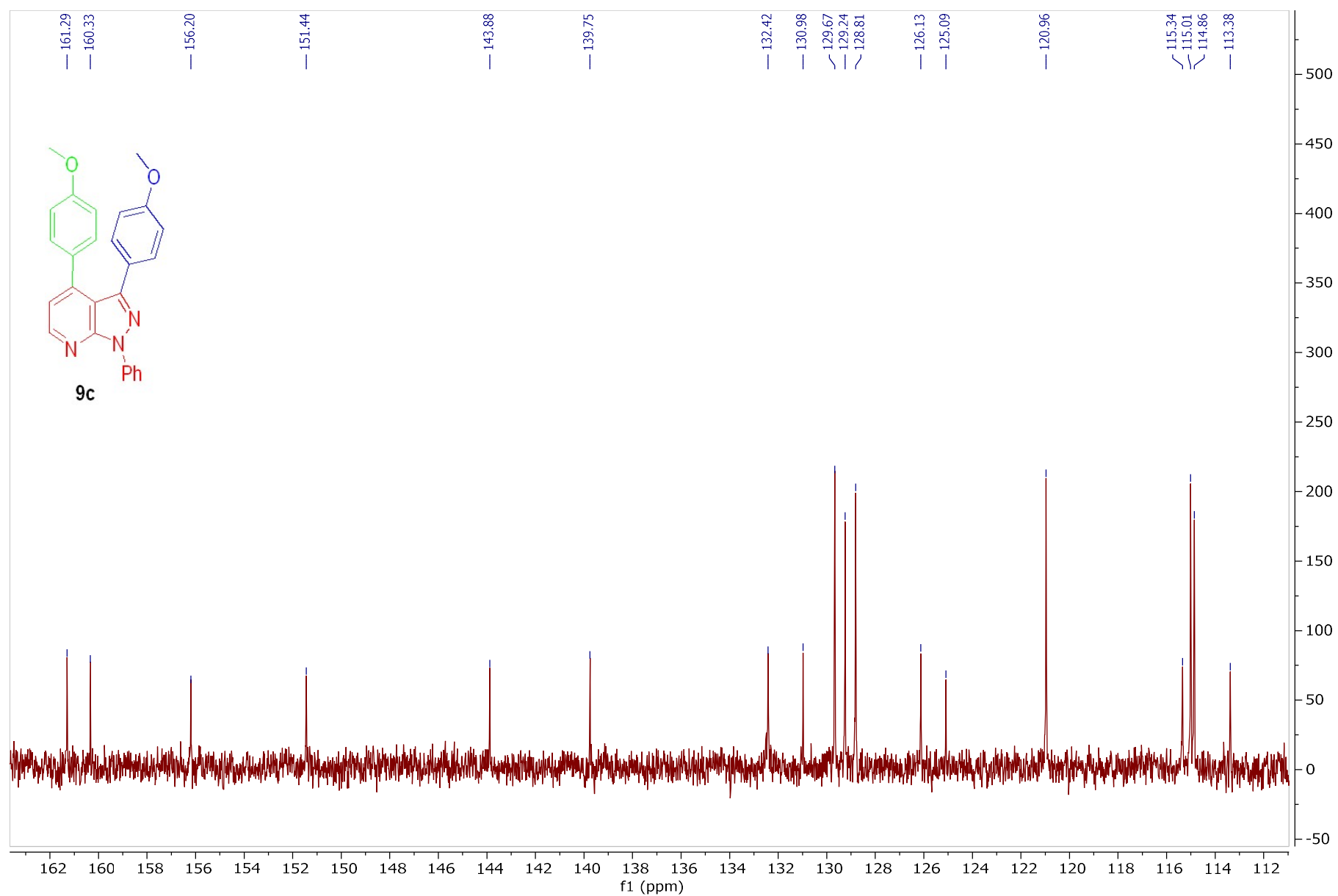


**Figure S11.**  $^1\text{H}$  NMR of compound **9c**, aromatic region

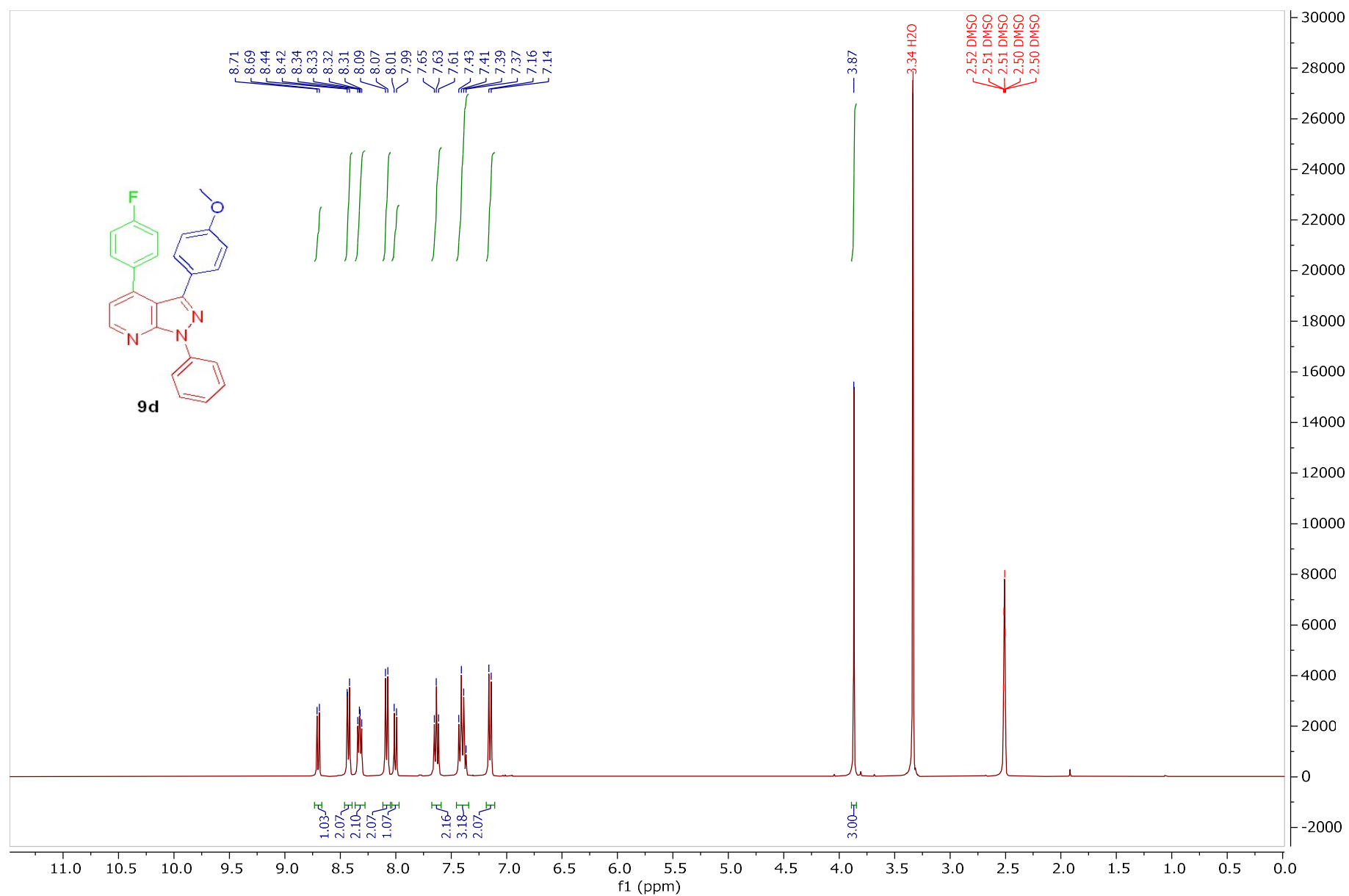




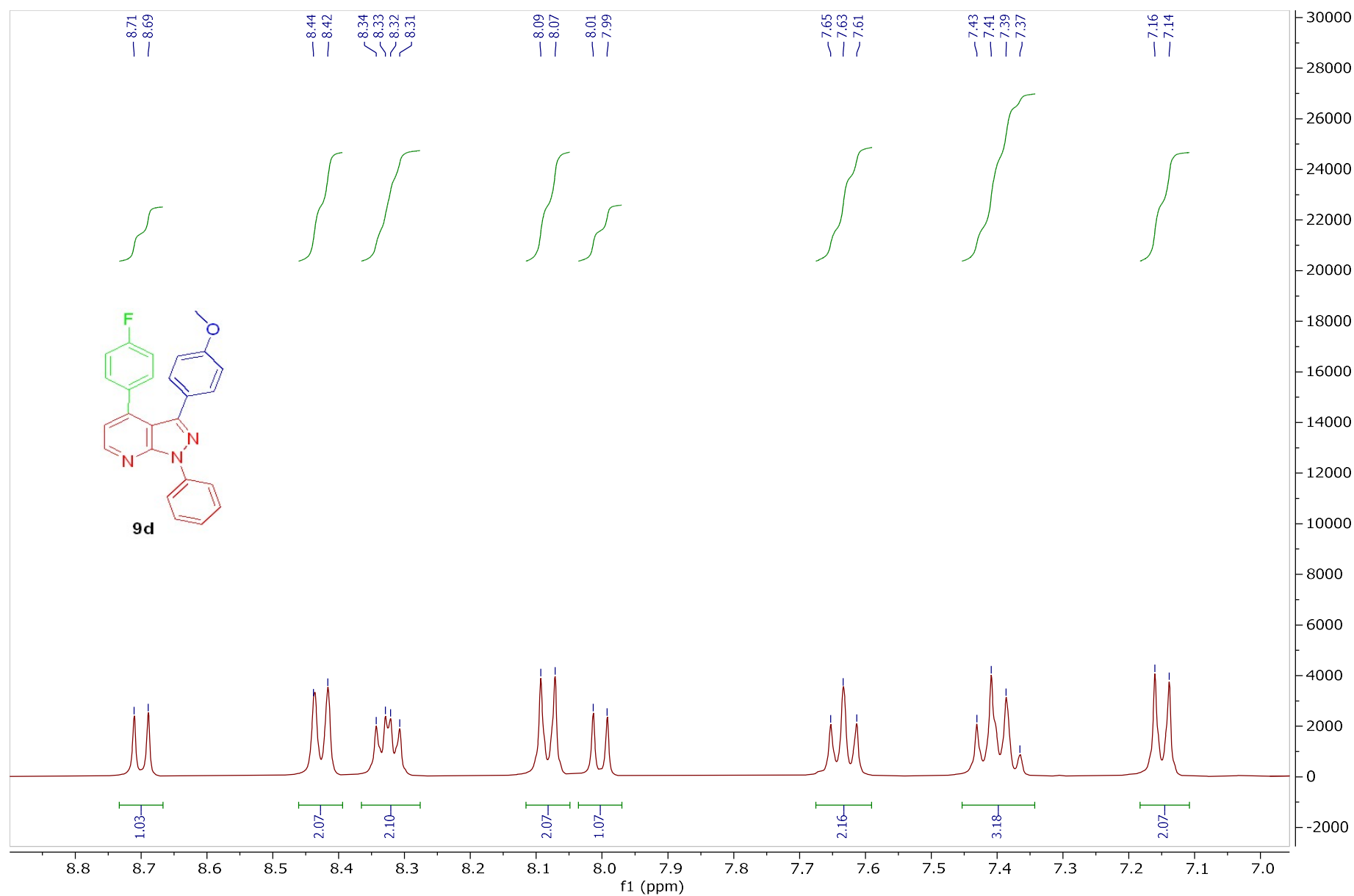
**Figure S12.**  $^{13}\text{C}$  NMR of compound **9c**, full spectrum



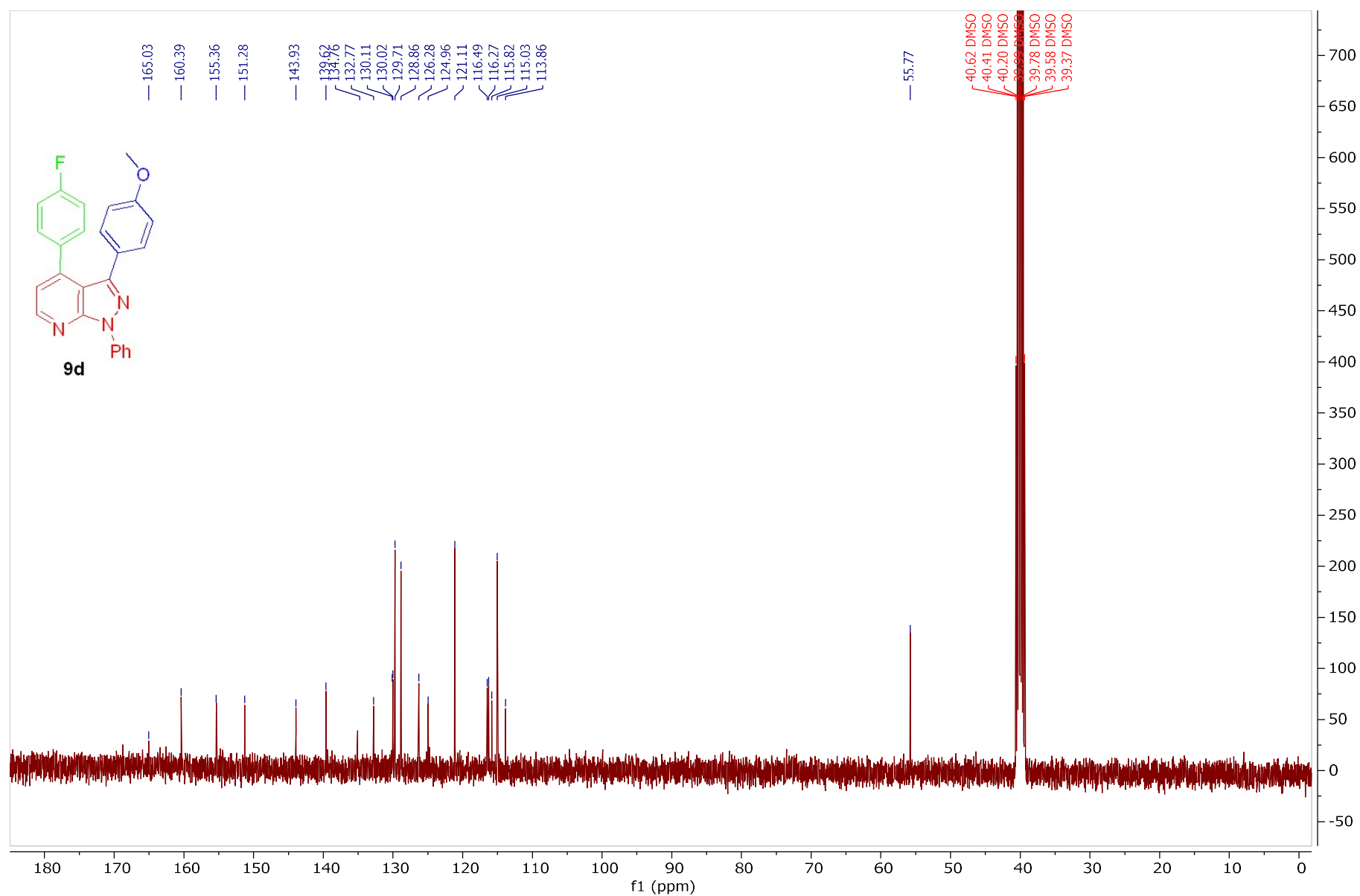
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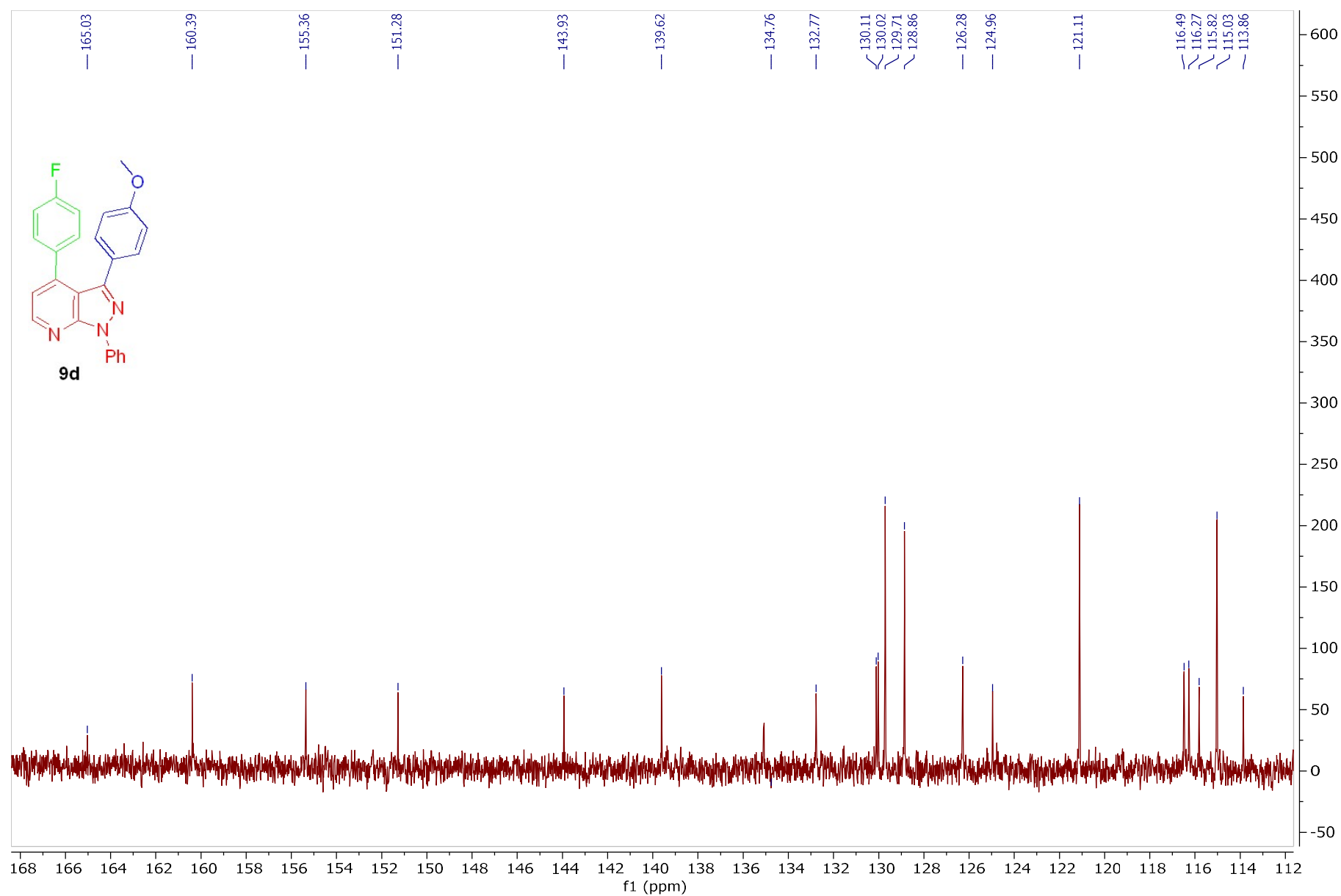
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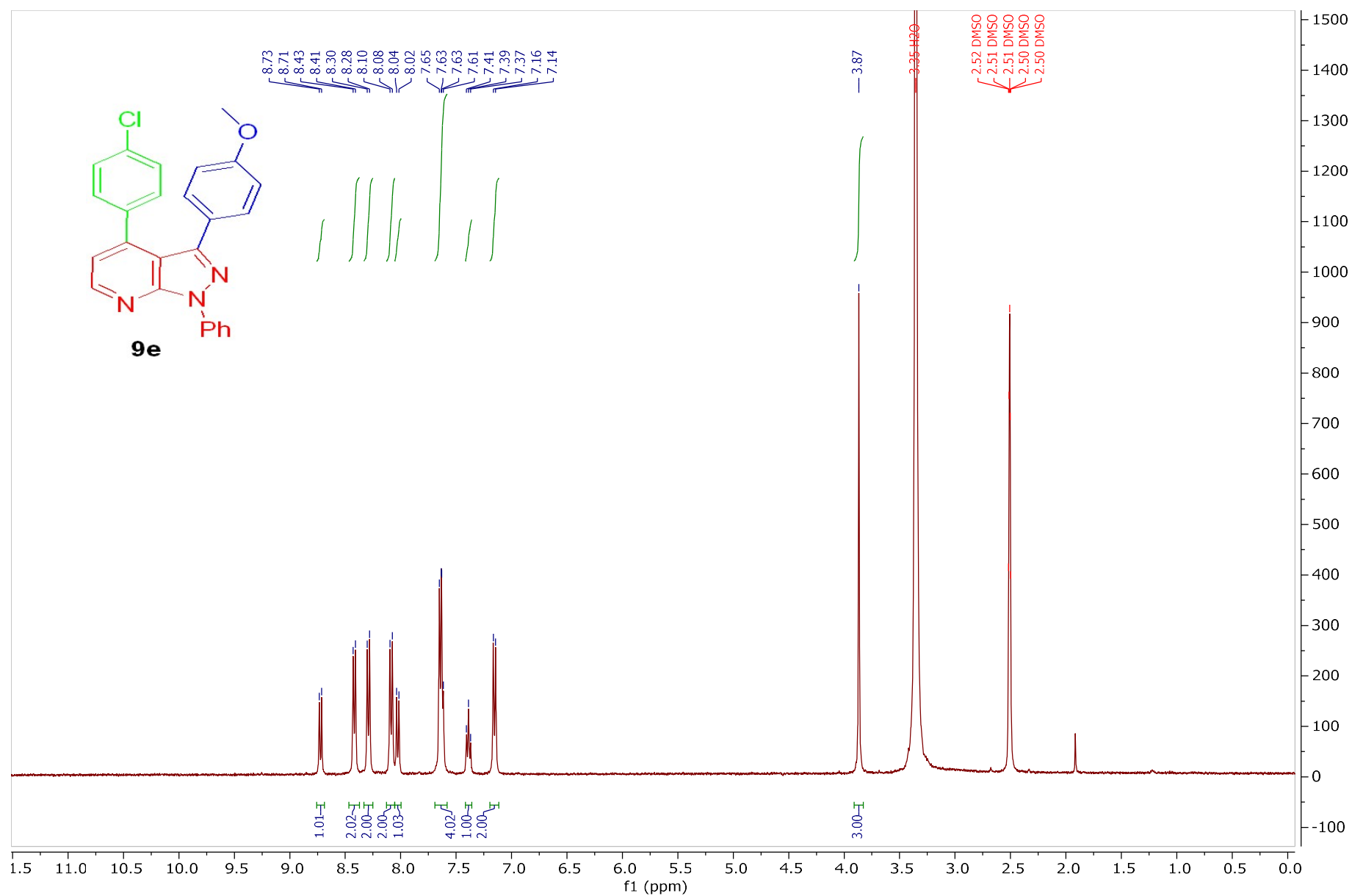
**Figure S15.**  $^1\text{H}$  NMR of compound **9d**, aromatic region



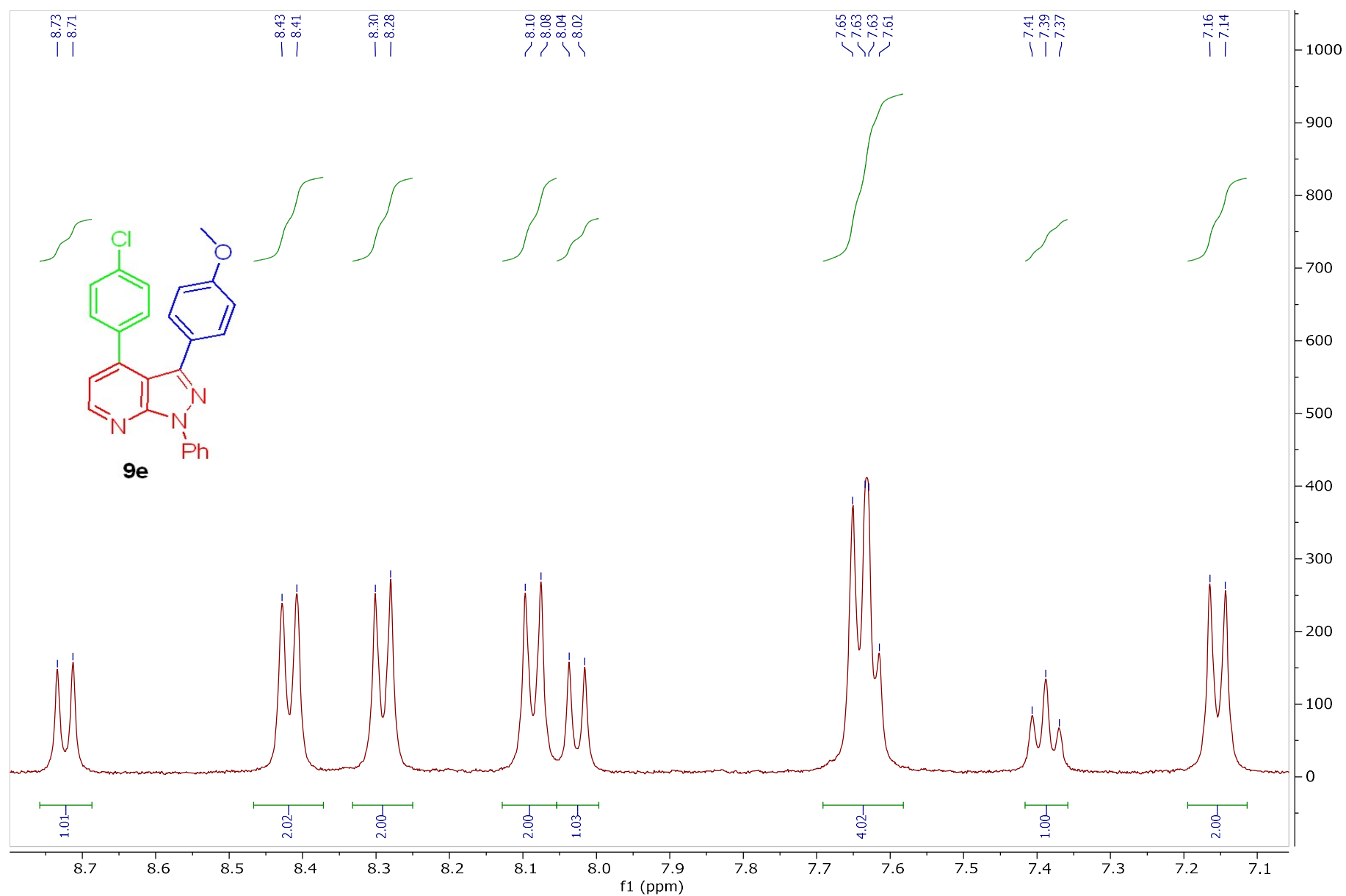
**Figure S16.**  $^{13}\text{C}$  NMR of compound **9d**, full spectrum



**Figure S17.**  $^{13}\text{C}$  NMR of compound **9d**, aromatic region

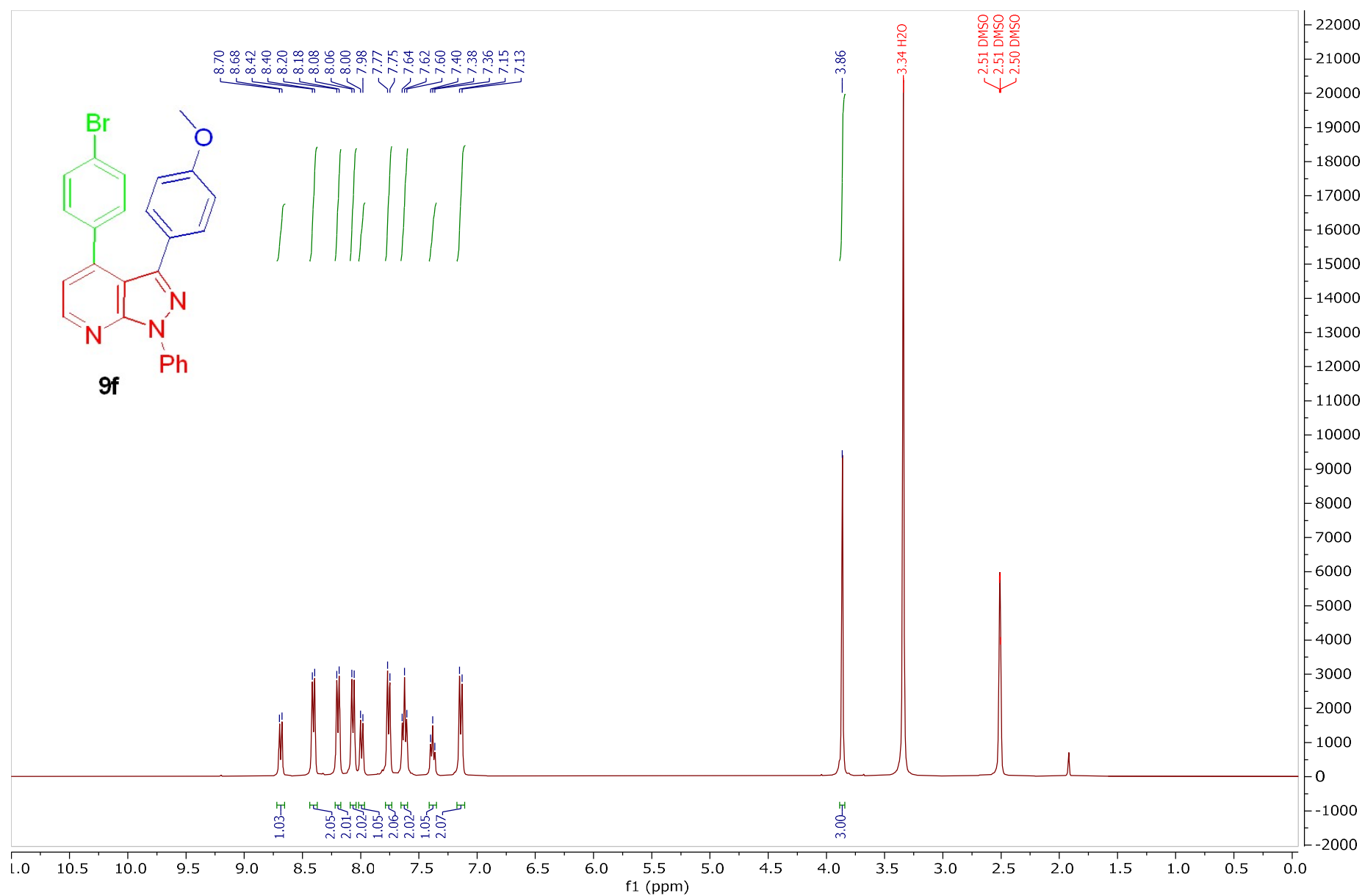


**Figure S18.** <sup>1</sup>H NMR of compound **9e**, full spectrum

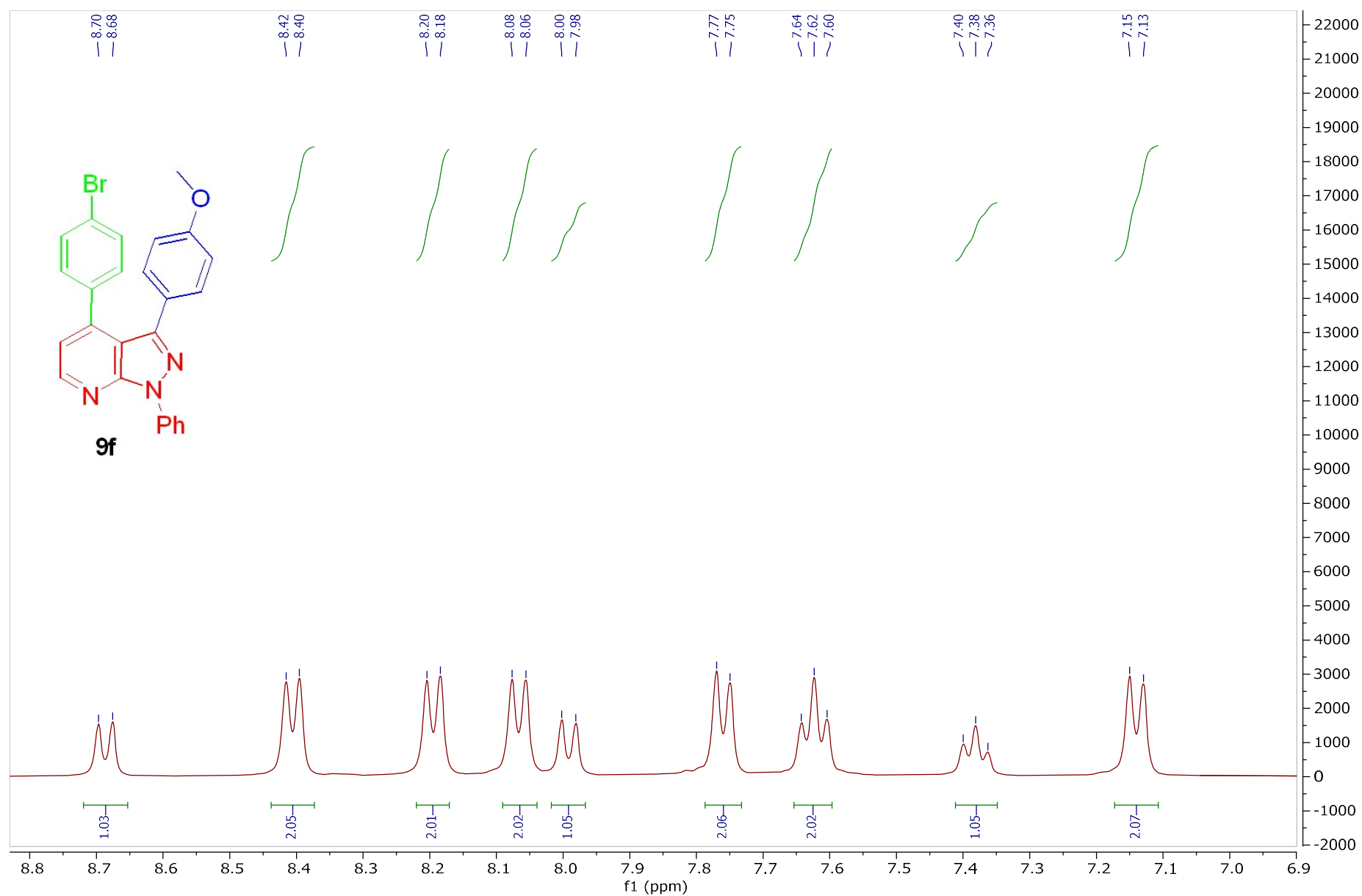


**Figure S19.** <sup>1</sup>H NMR of compound **9e**, aromatic region





**Figure S20.** <sup>1</sup>H NMR of compound **9f**, full spectrum



**Figure S21.** <sup>1</sup>H NMR of compound **9f**, aromatic region

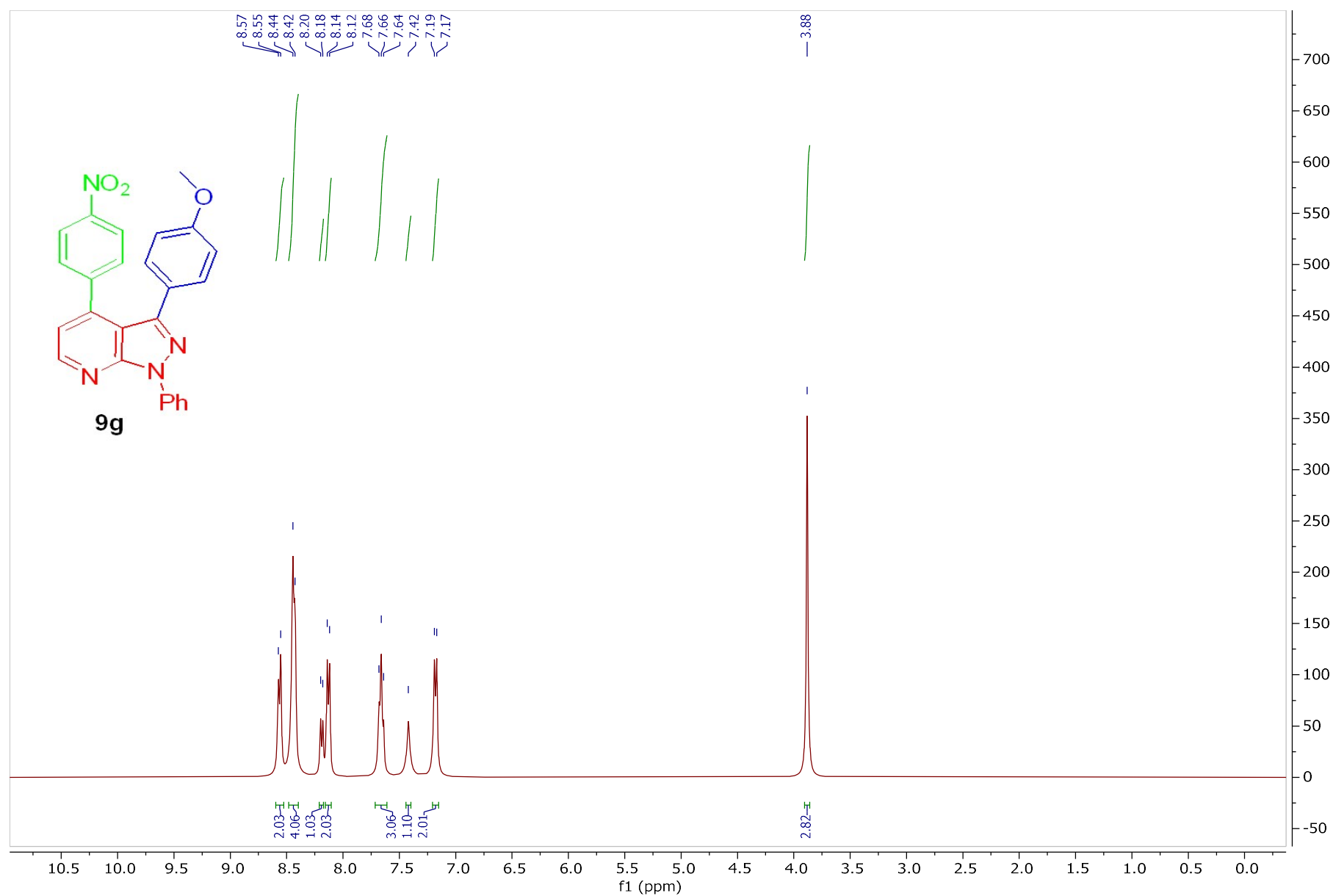
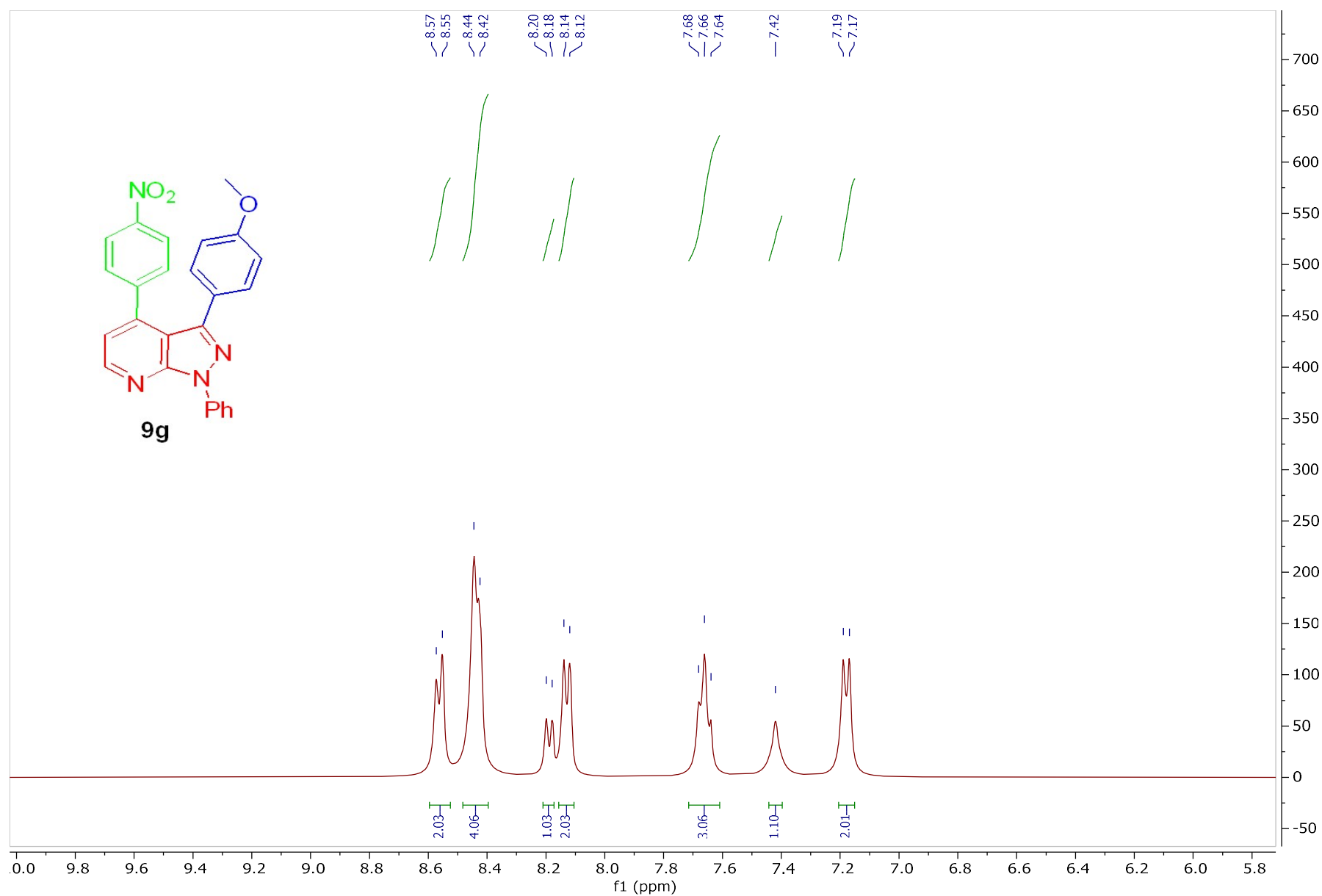
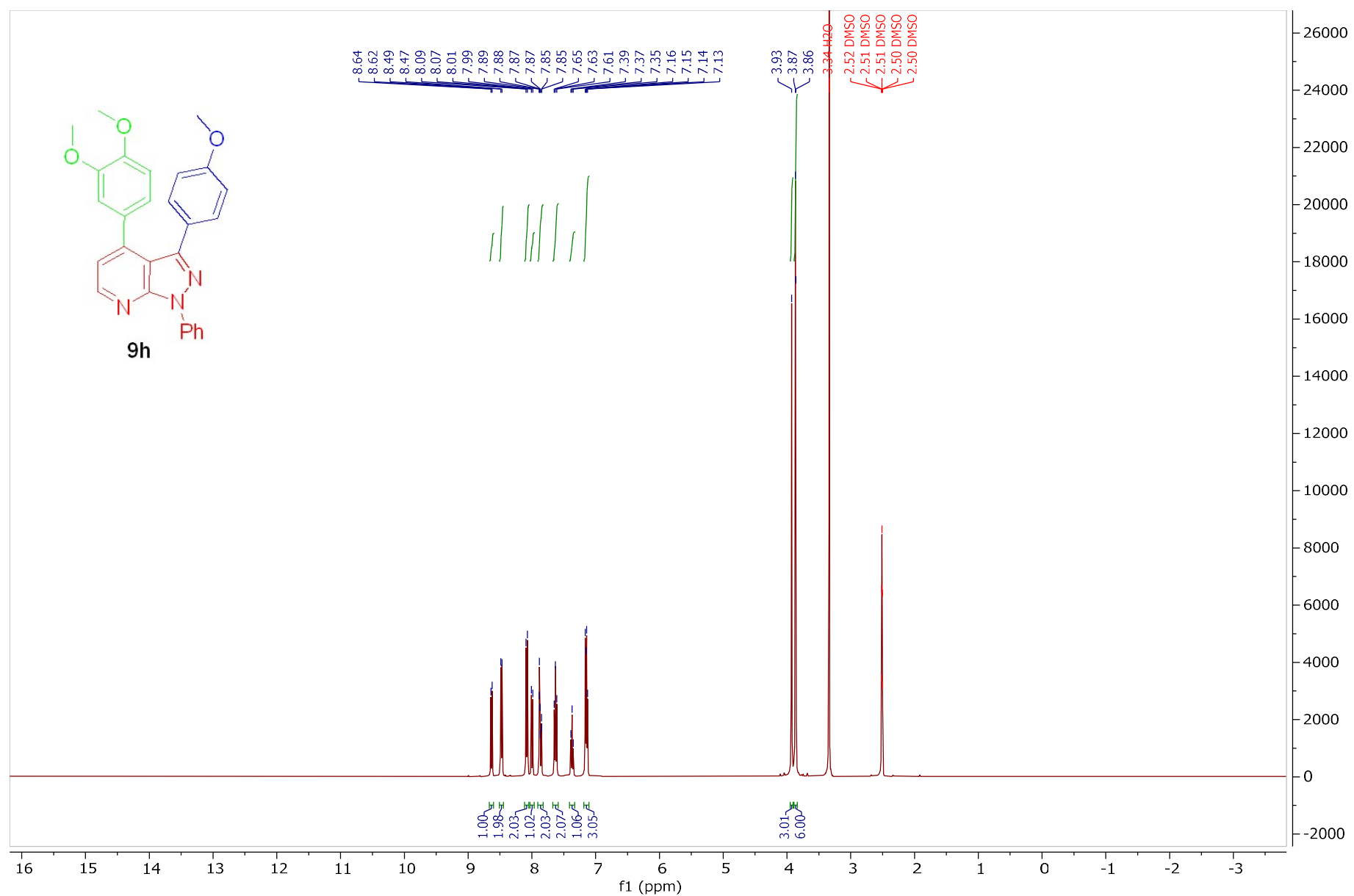


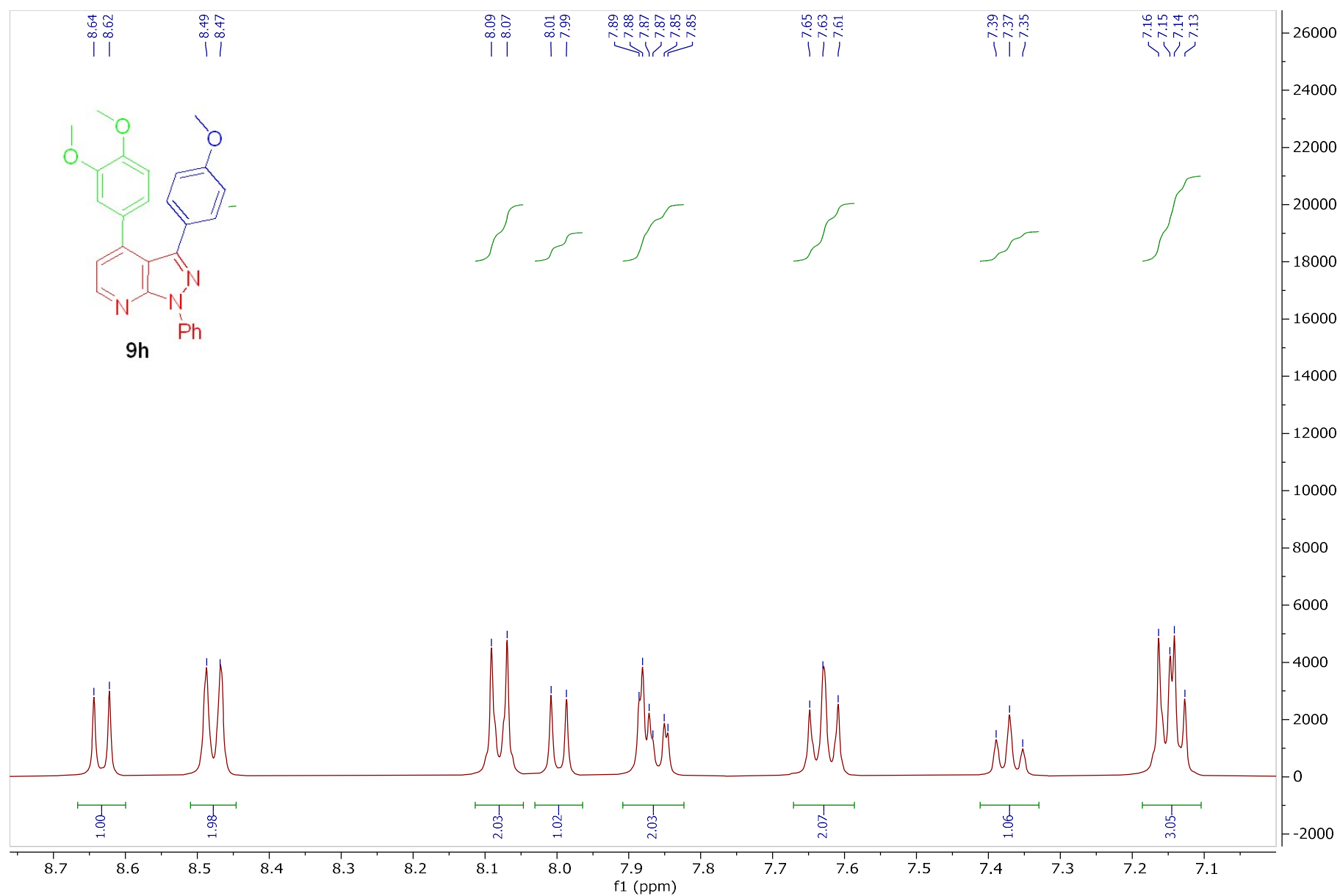
Figure S22.  $^1\text{H}$  NMR of compound **9g**, full spectrum



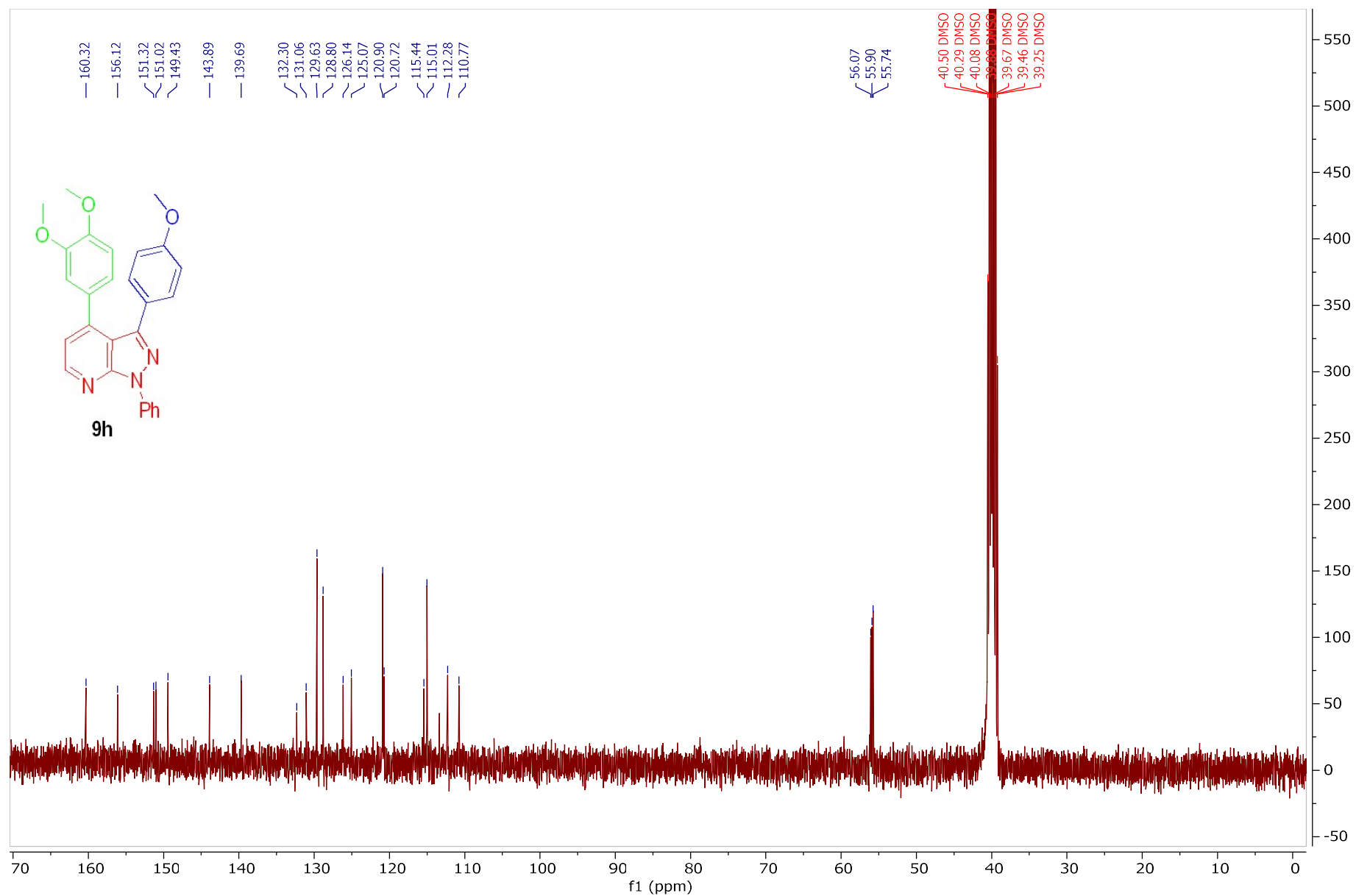
**Figure S23.** <sup>1</sup>H NMR of compound **9g**, aromatic region



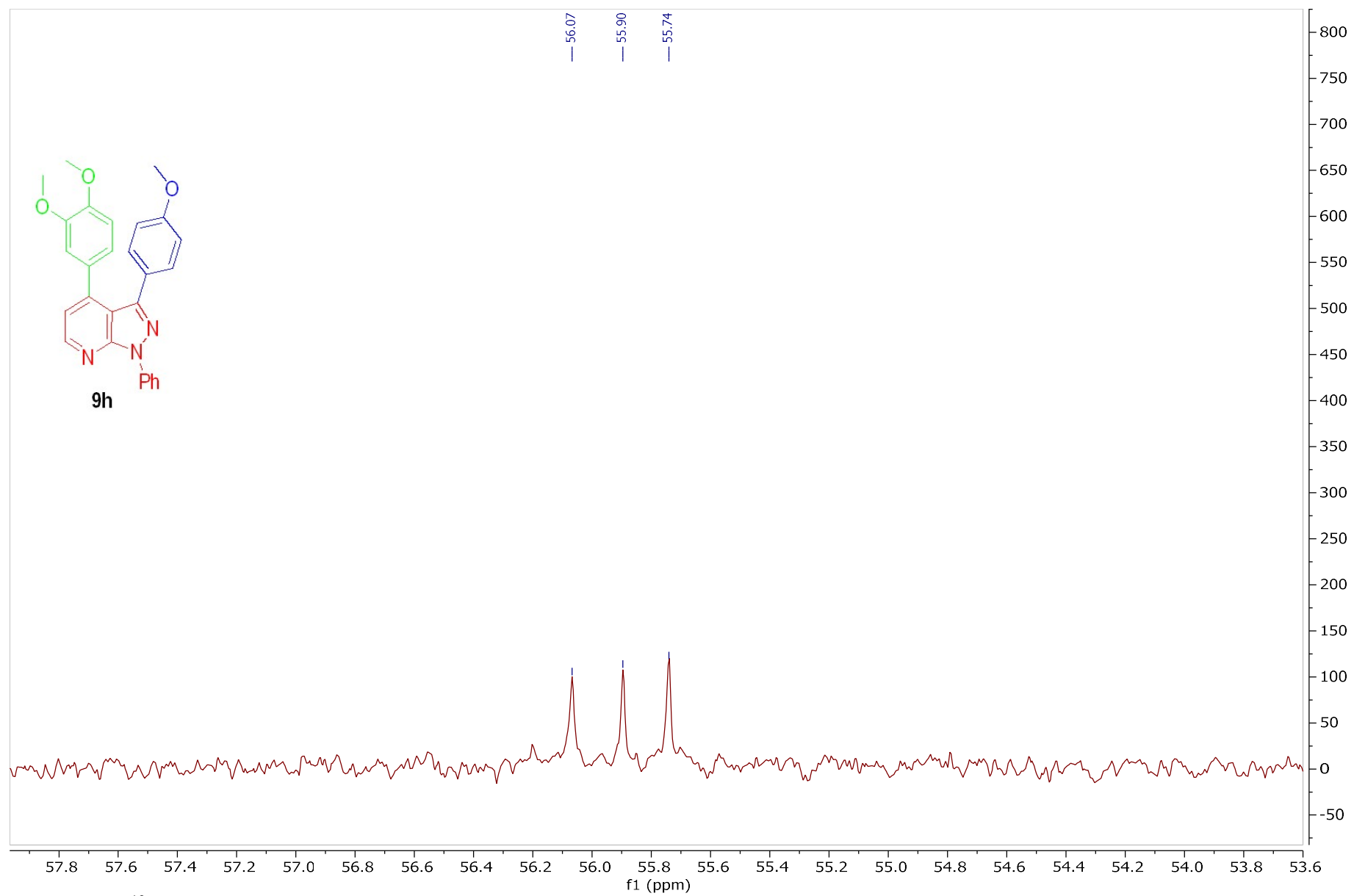
**Figure S24.** <sup>1</sup>H NMR of compound **9h**, full spectrum



**Figure S25.**  $^1\text{H}$  NMR of compound **9h**, aromatic region

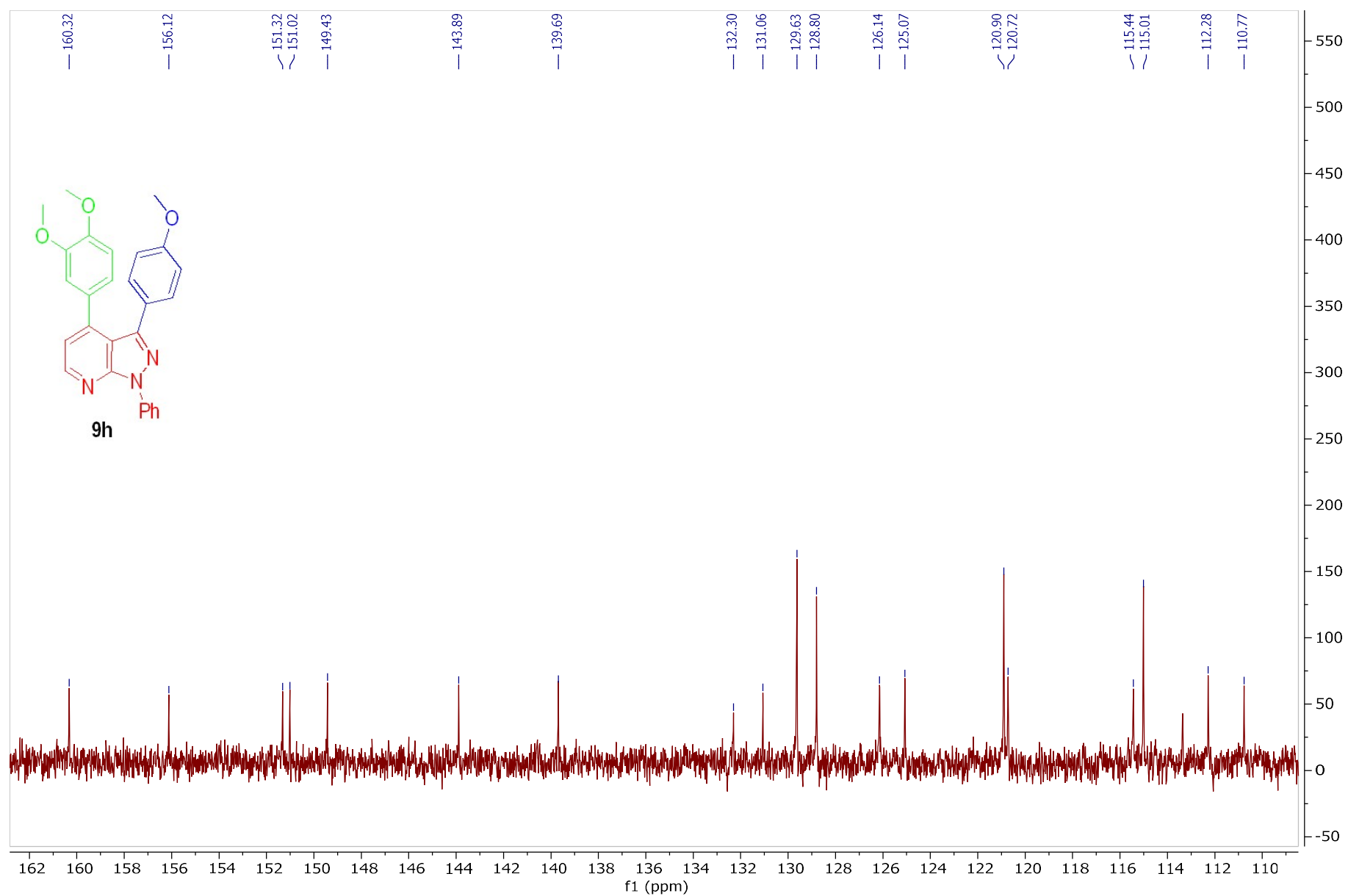


**Figure S26.**  $^{13}\text{C}$  NMR of compound **9h**, full spectrum

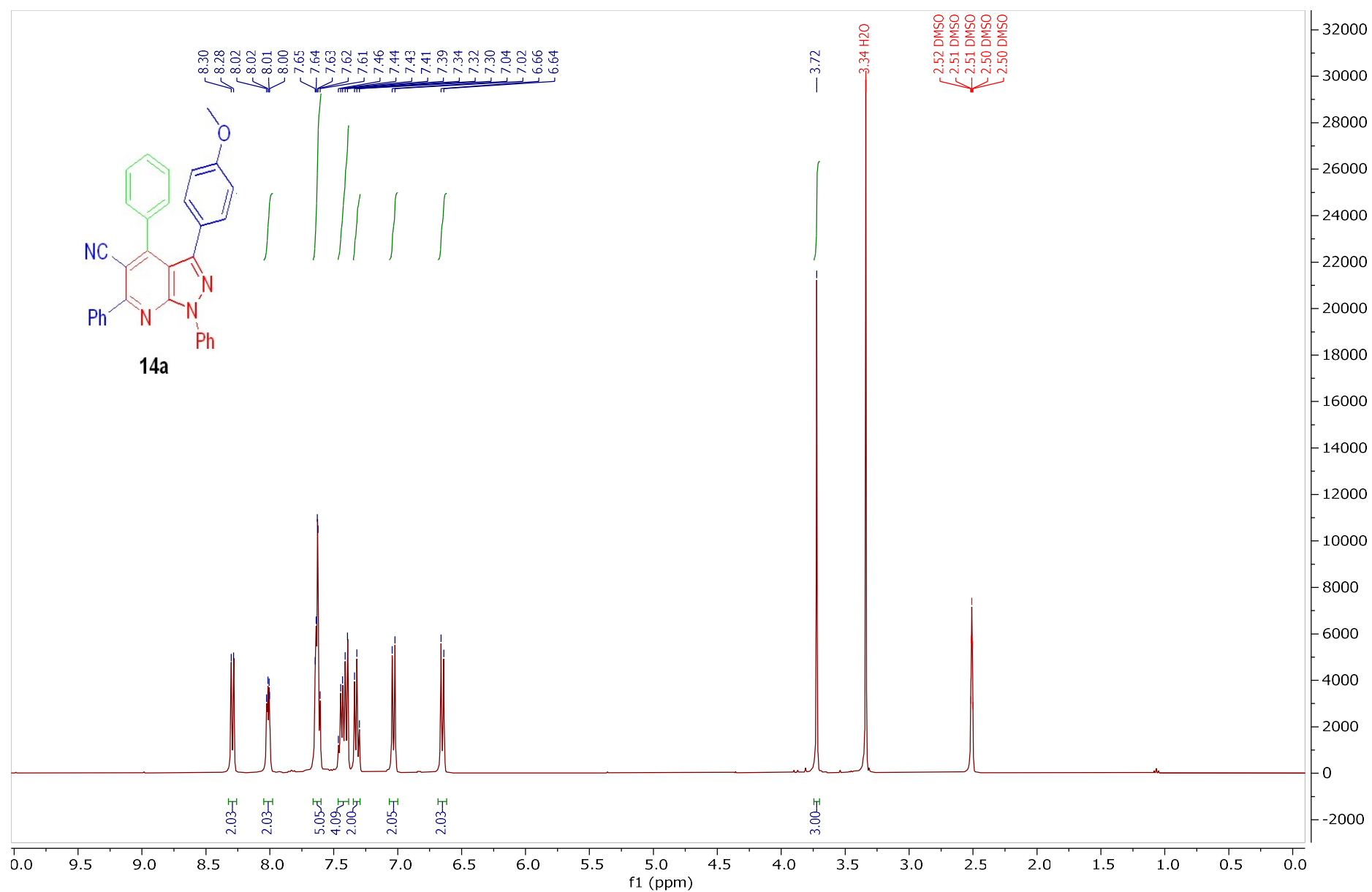


**Figure S27.**  $^{13}\text{C}$  NMR of compound **9h**, aliphatic region

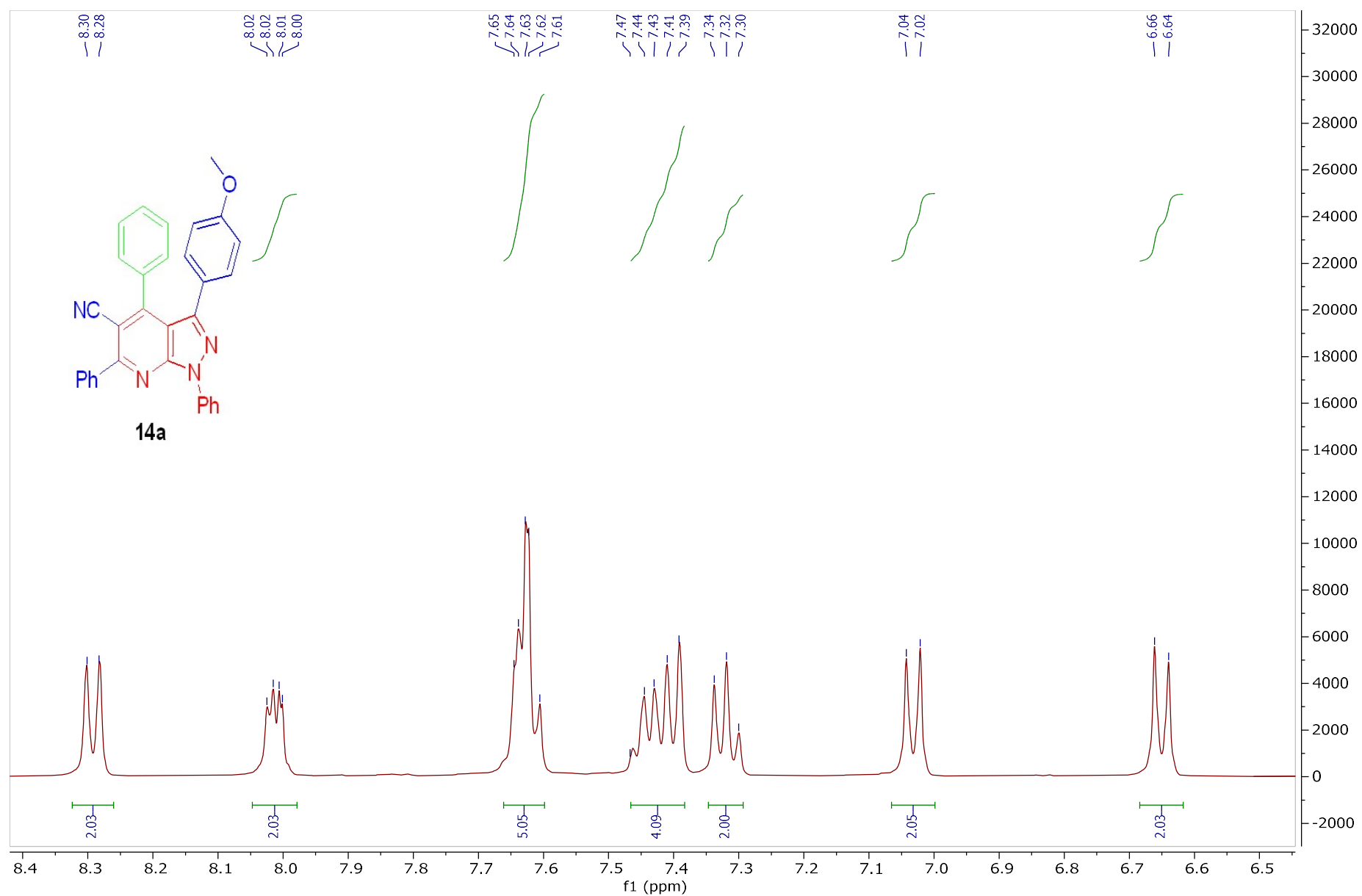




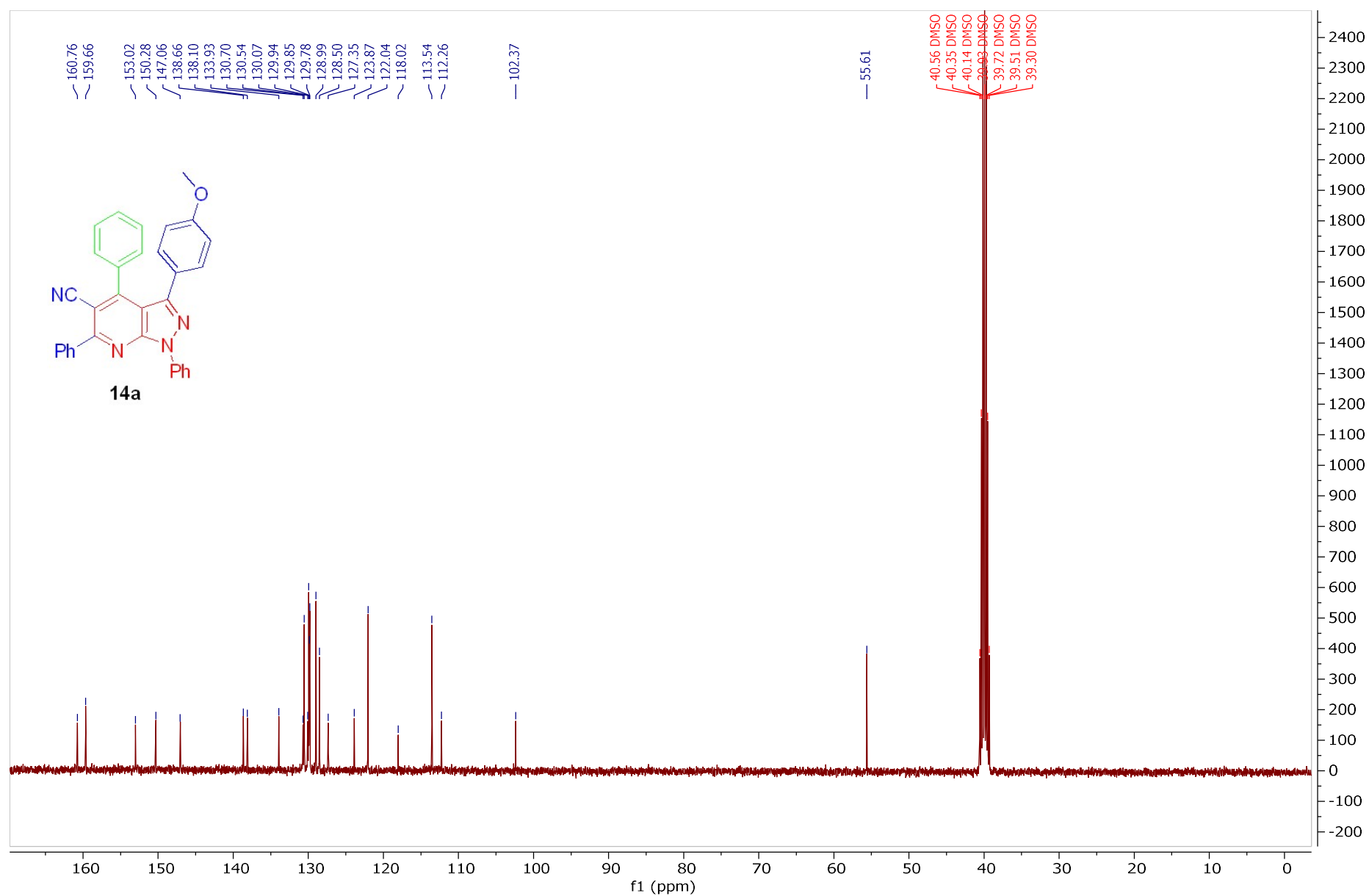
**Figure S28.**  $^{13}\text{C}$  NMR of compound **9h**, aromatic region



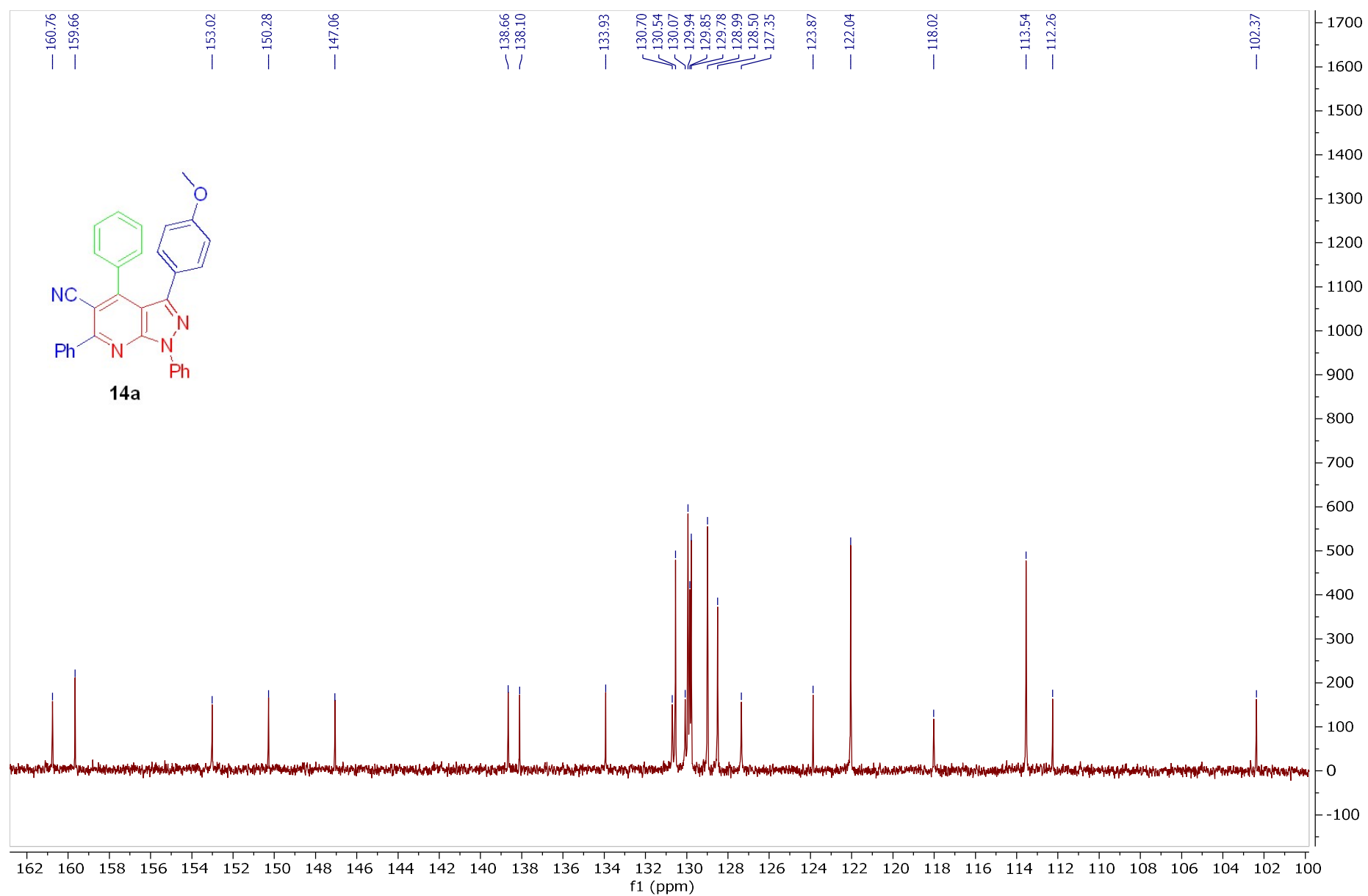
**Figure S29.** <sup>1</sup>H NMR of compound **14a**, full spectrum



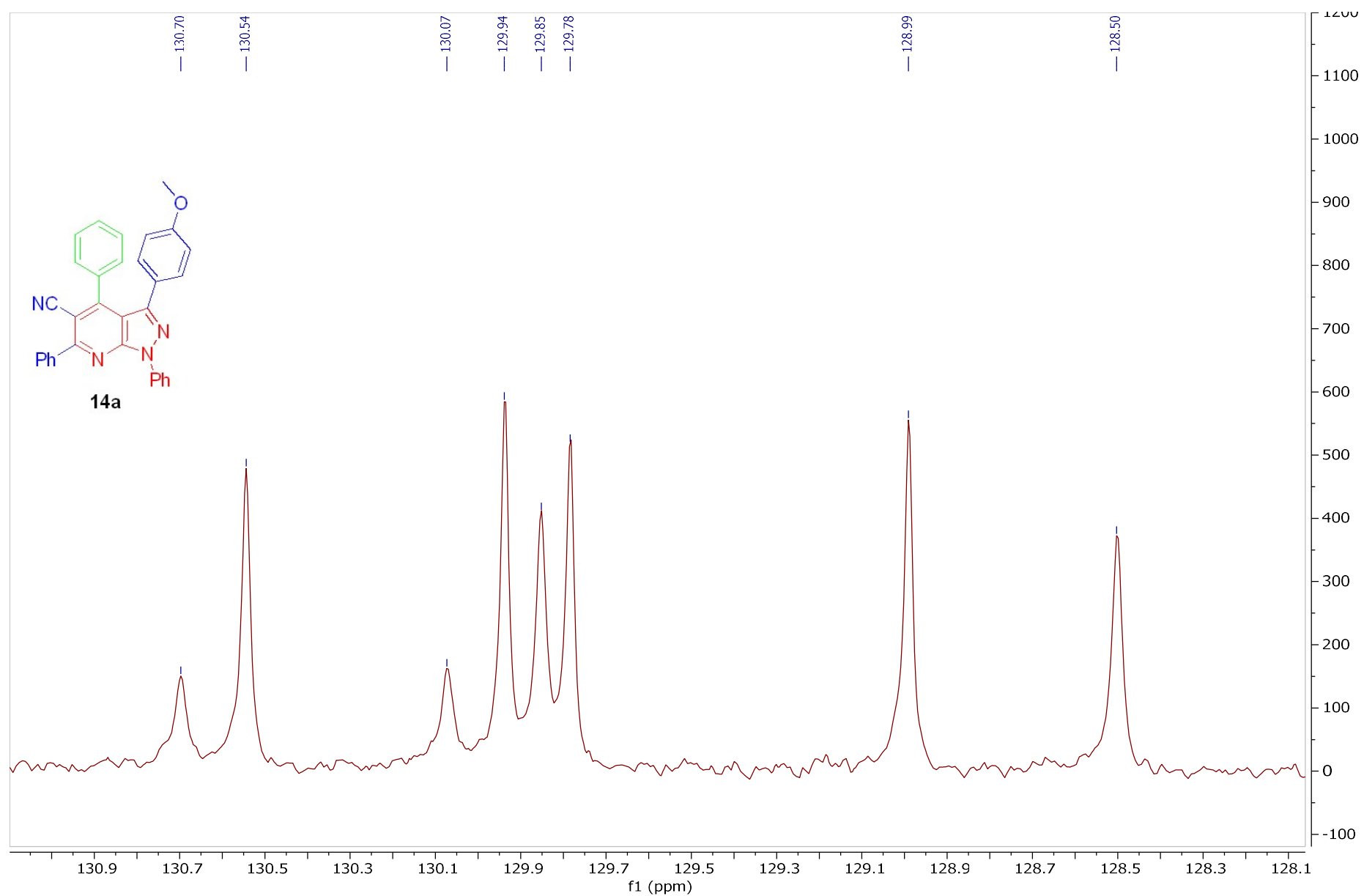
**Figure S30.** <sup>1</sup>H NMR of compound **14a**, aromatic region



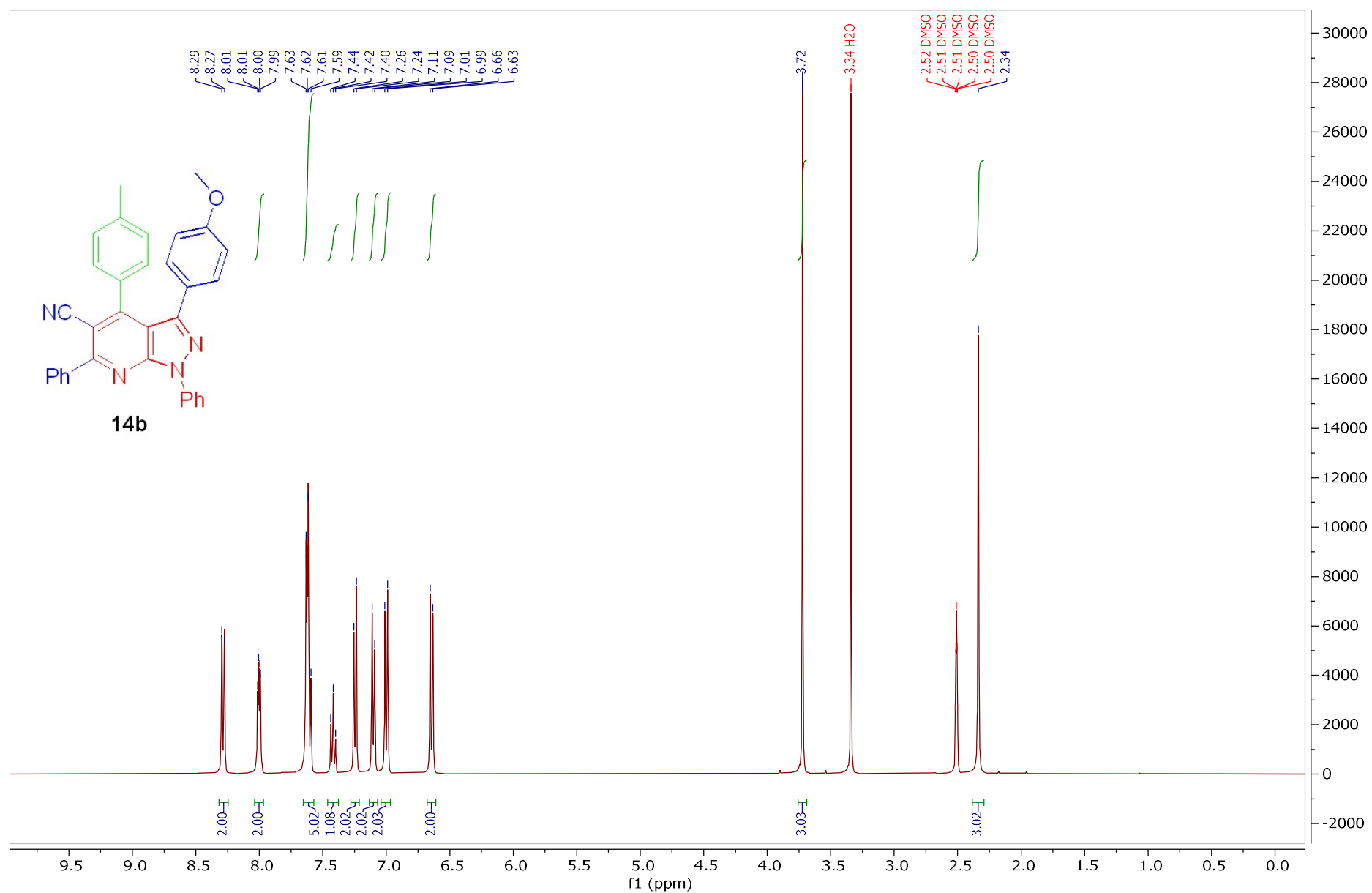
**Figure S31.**  $^{13}\text{C}$  NMR of compound **14a**, full spectrum



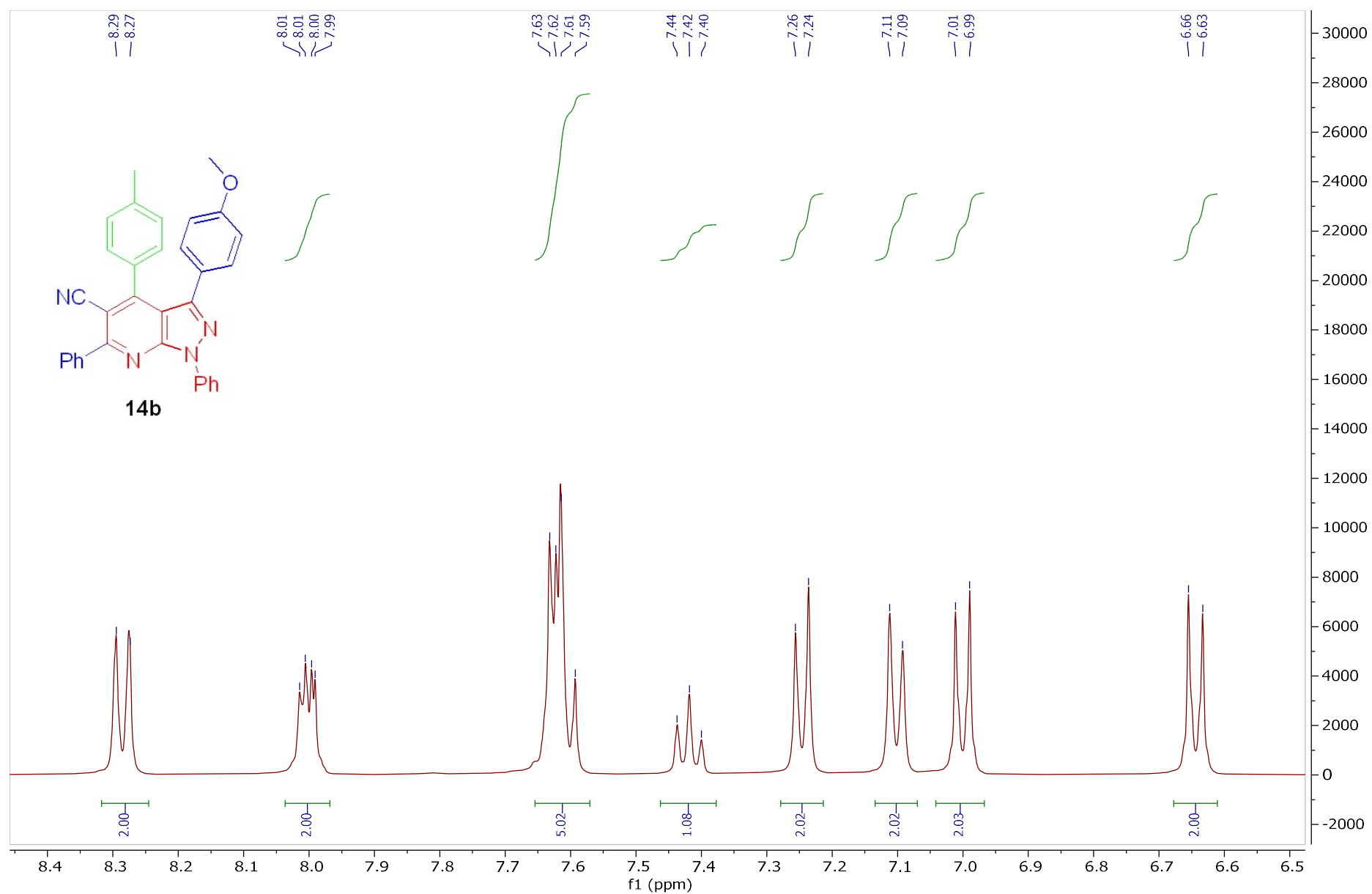
**Figure S32.**  $^{13}\text{C}$  NMR of compound **14a**, aromatic region



**Figure S33.**  $^{13}\text{C}$  NMR of compound **14a**, aromatic region 128-131 *ppm*



**Figure S34.** <sup>1</sup>H NMR of compound **14b**, full spectrum



**Figure S35.** <sup>1</sup>H NMR of compound **14b**, aromatic region



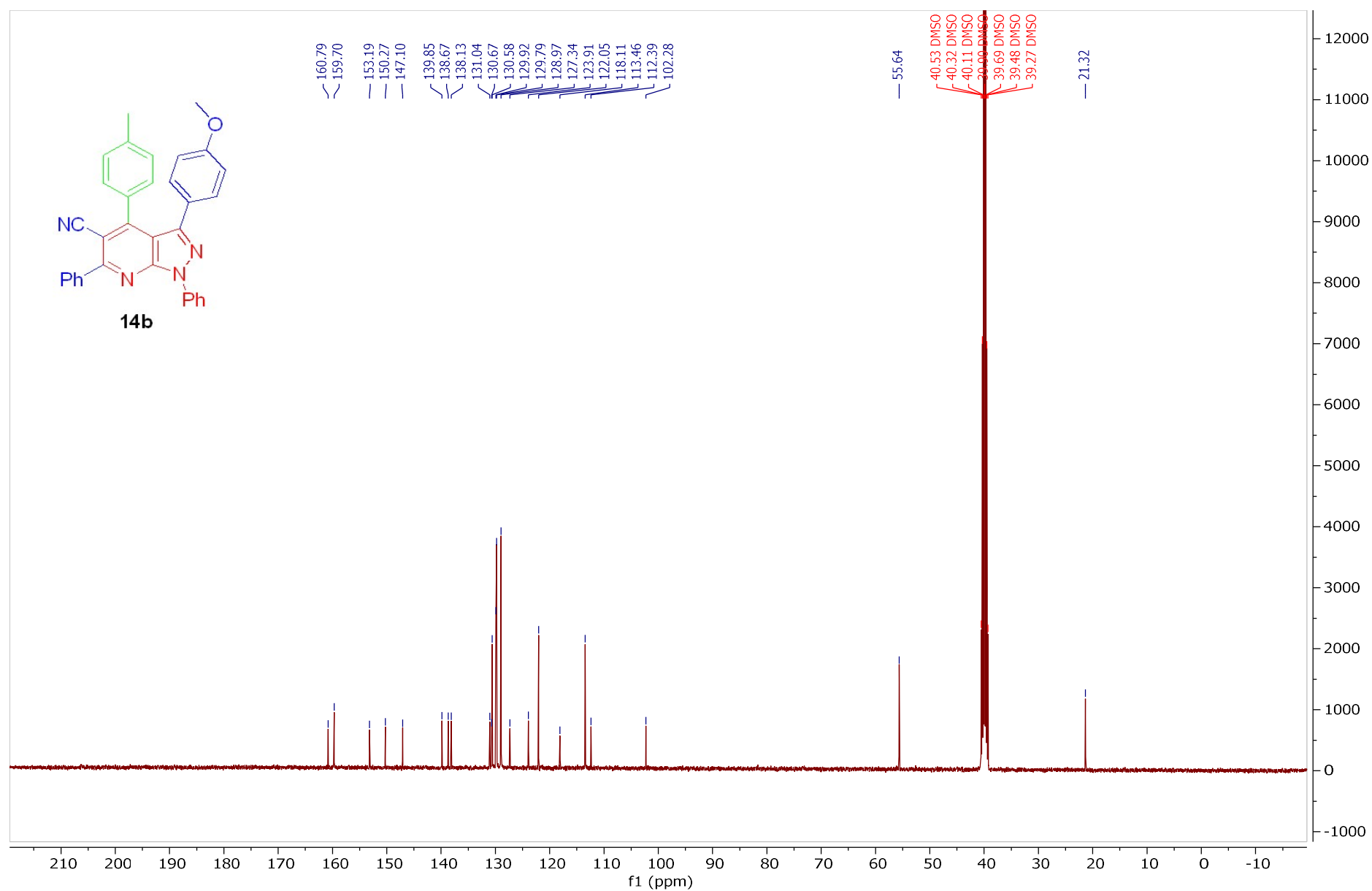
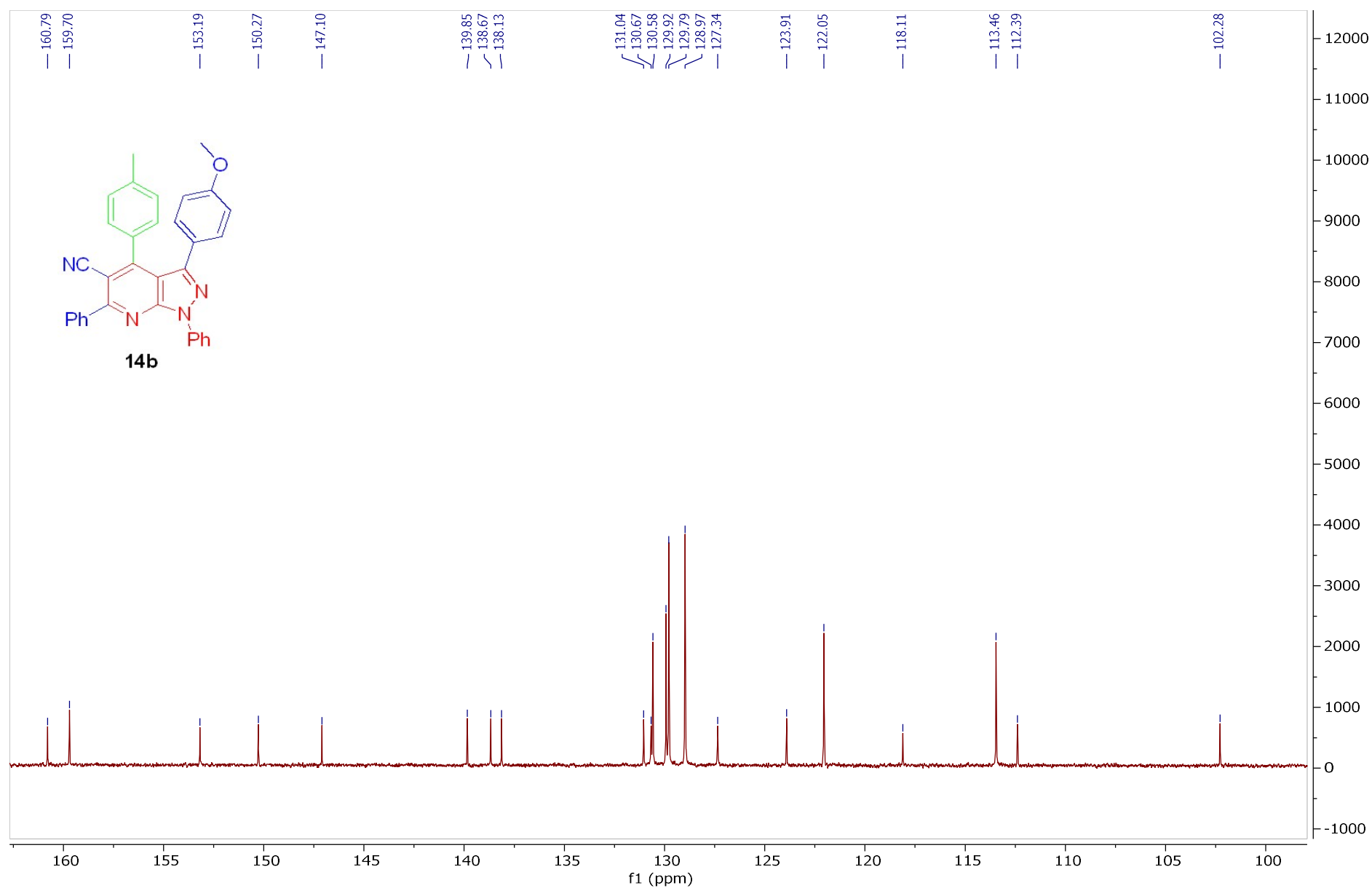
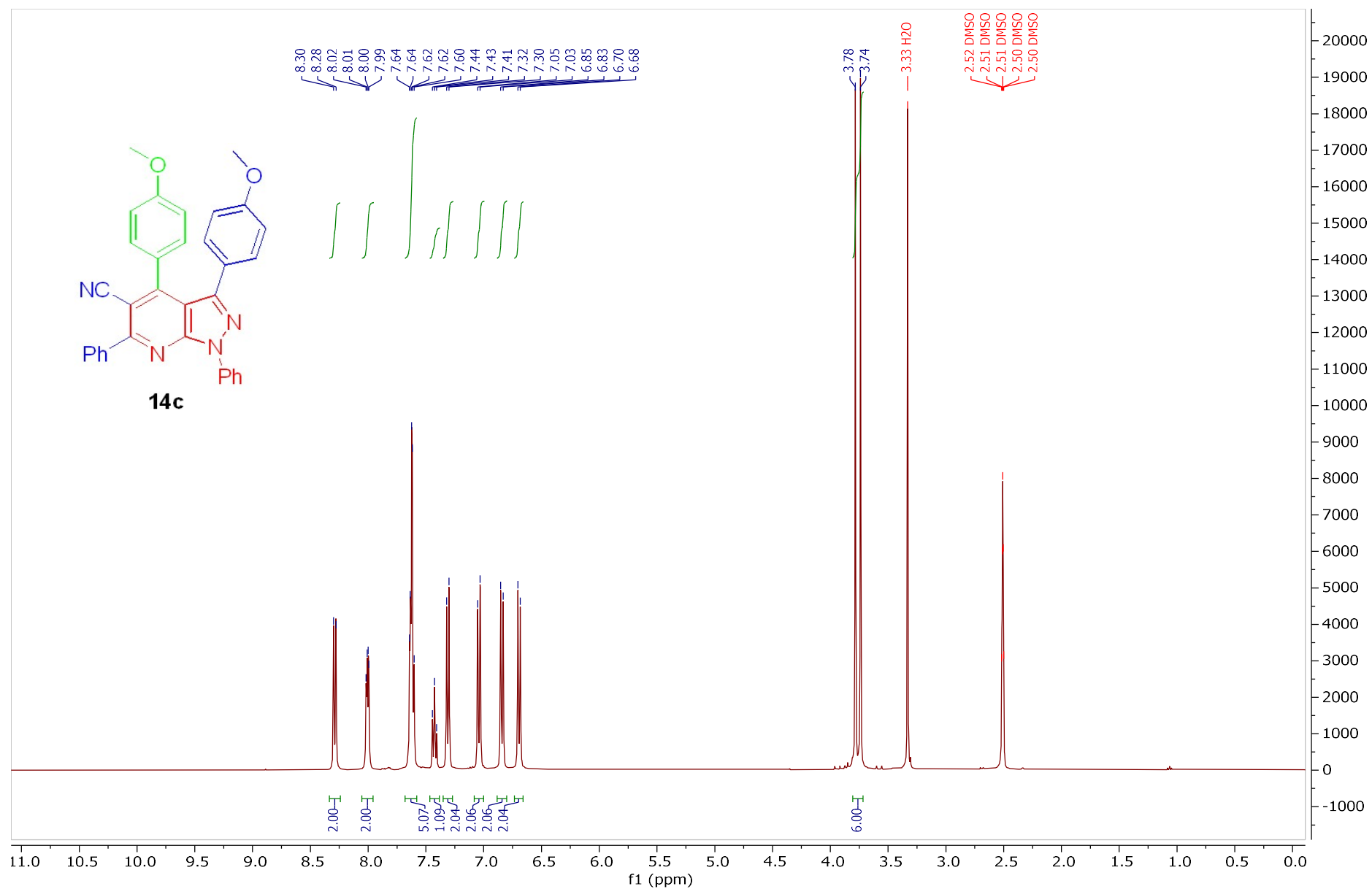


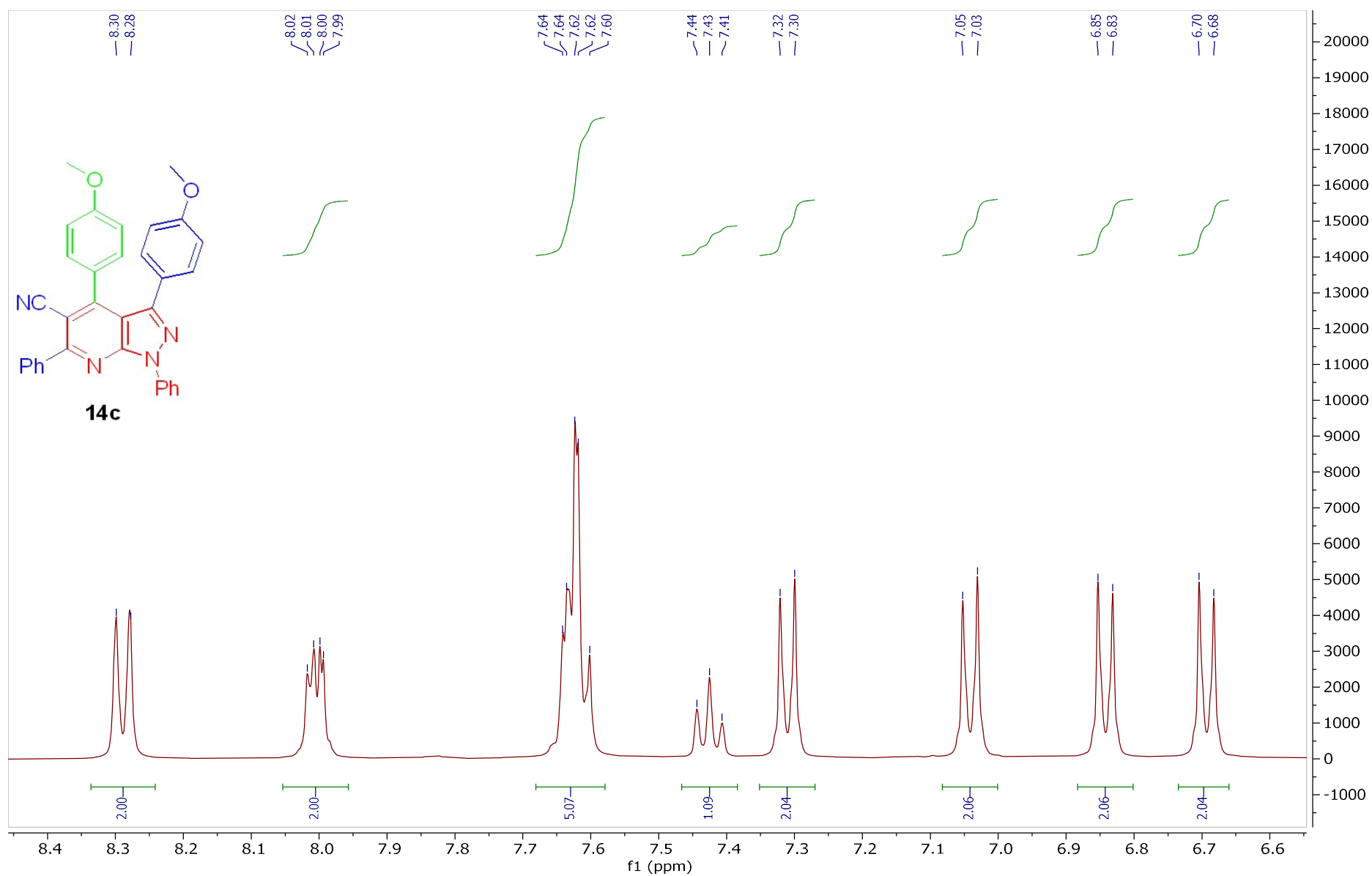
Figure S36.  $^{13}\text{C}$  NMR of compound **14b**, full spectrum



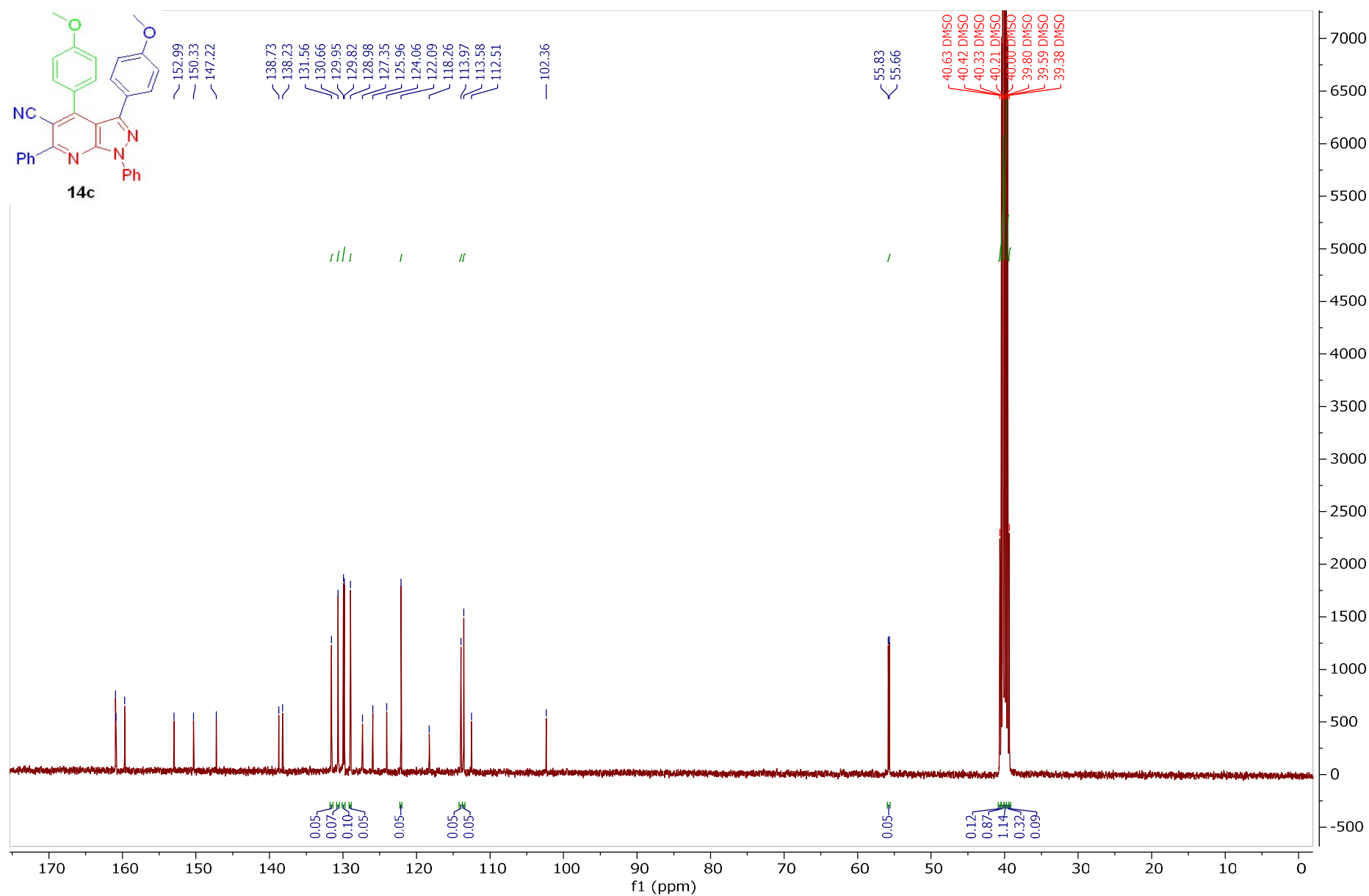
**Figure S37.**  $^{13}\text{C}$  NMR of compound **14b**, aromatic region



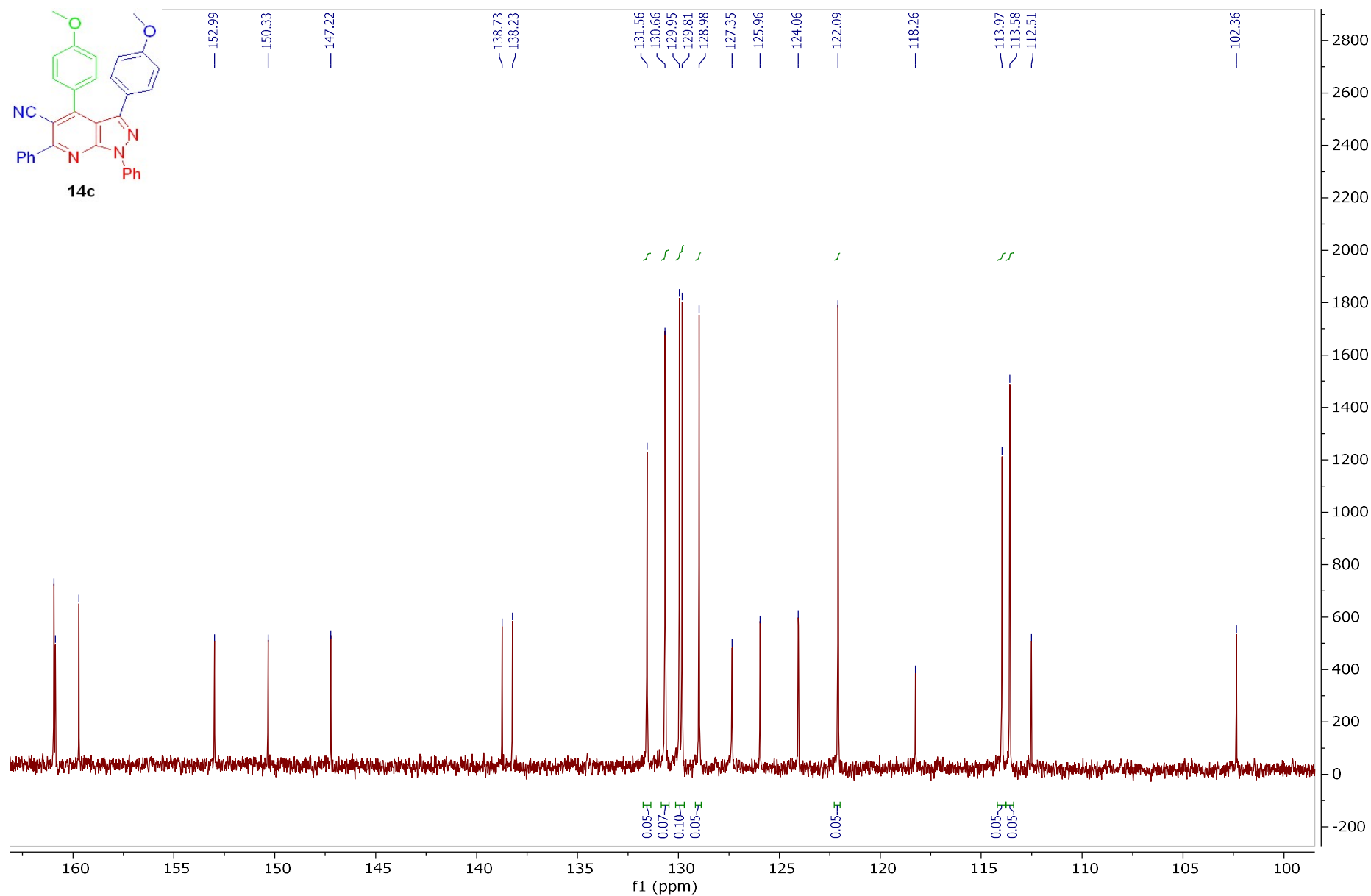
**Figure S38.** <sup>1</sup>H NMR of compound **14c**, full spectrum



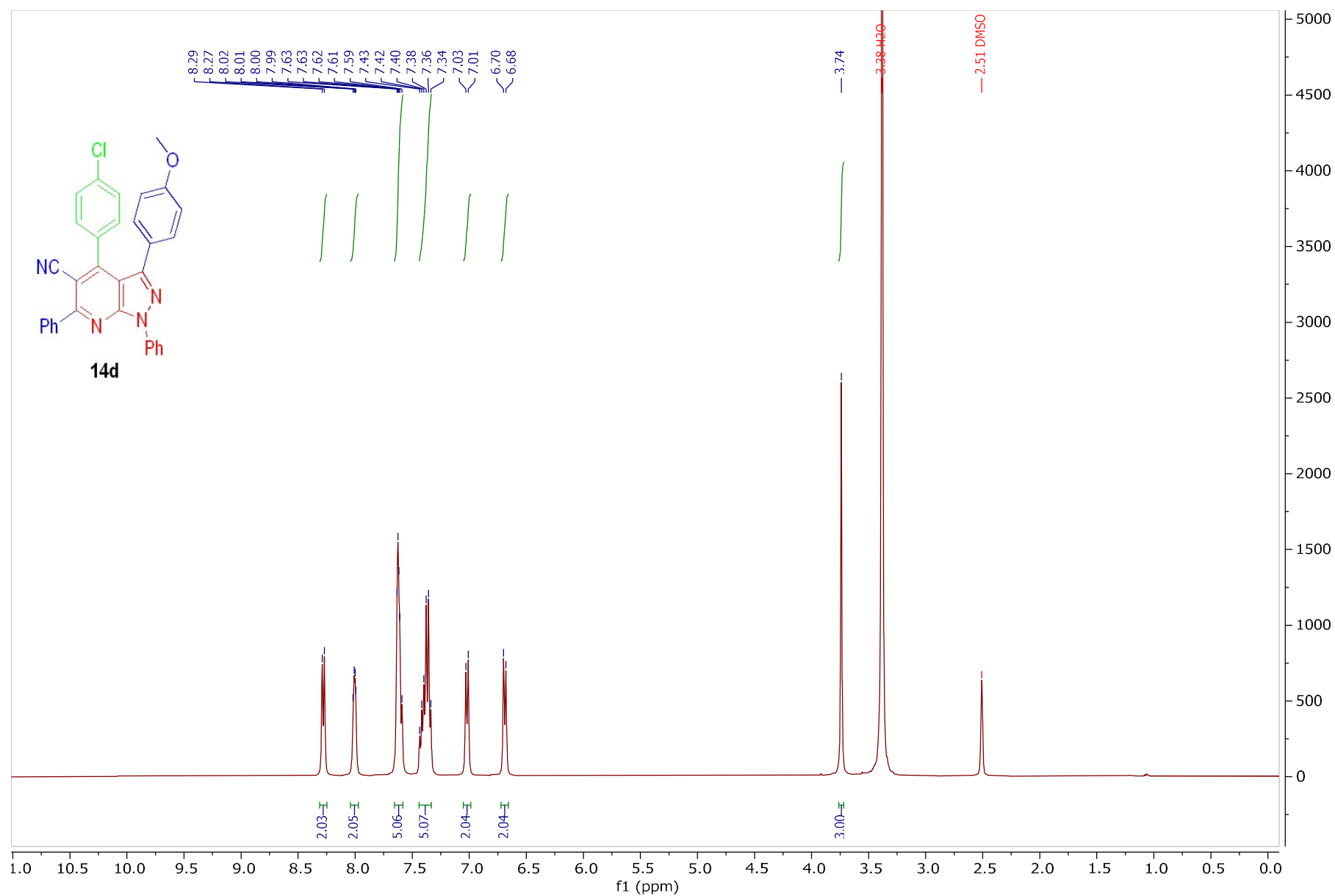
**Figure S39.** <sup>1</sup>H NMR of compound **14c**, aromatic region



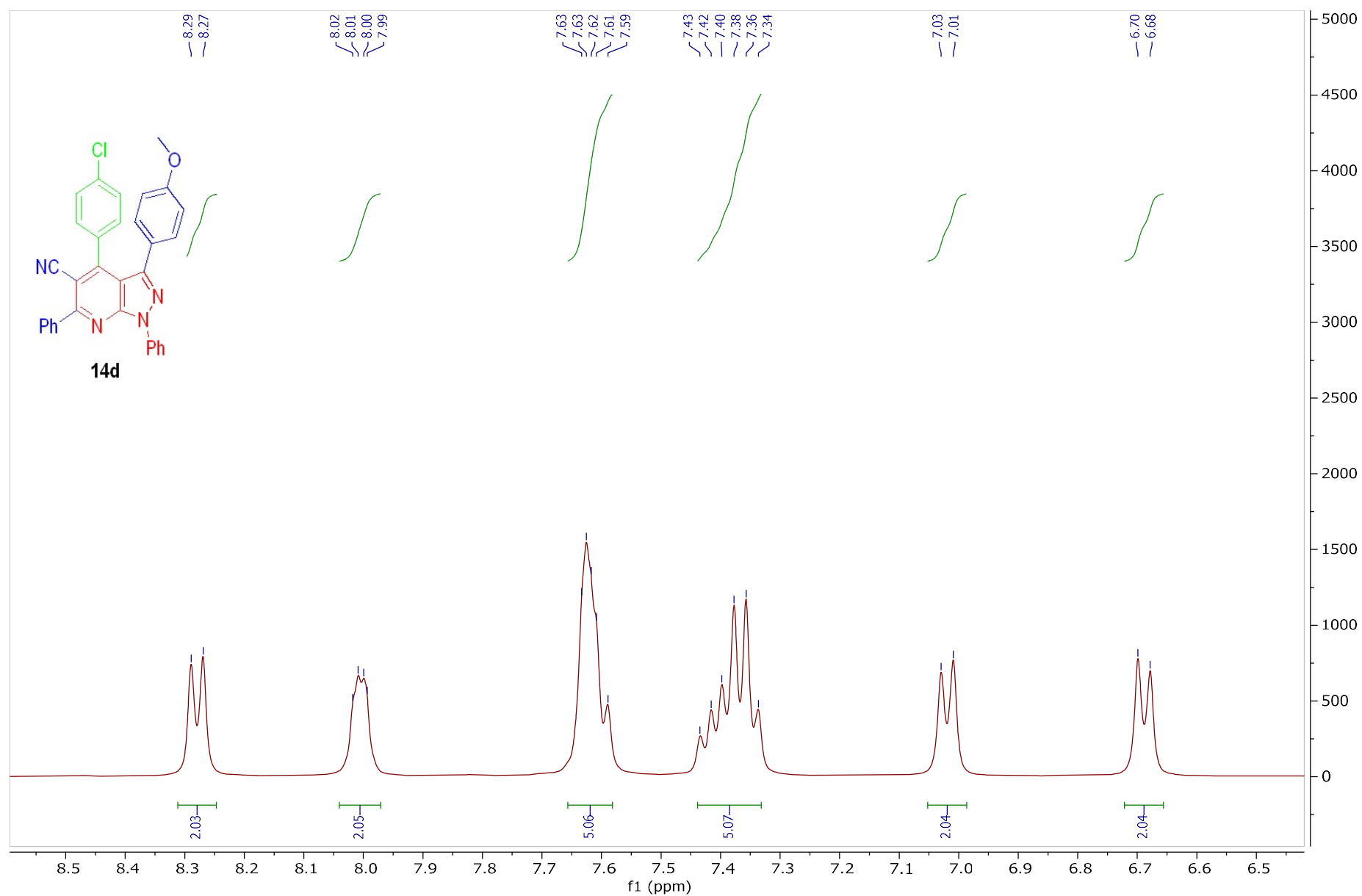
**Figure S40.**  $^{13}\text{C}$  NMR of compound **14c**, full spectrum



**Figure S41.** <sup>13</sup>C NMR of compound **14c**, aromatic region

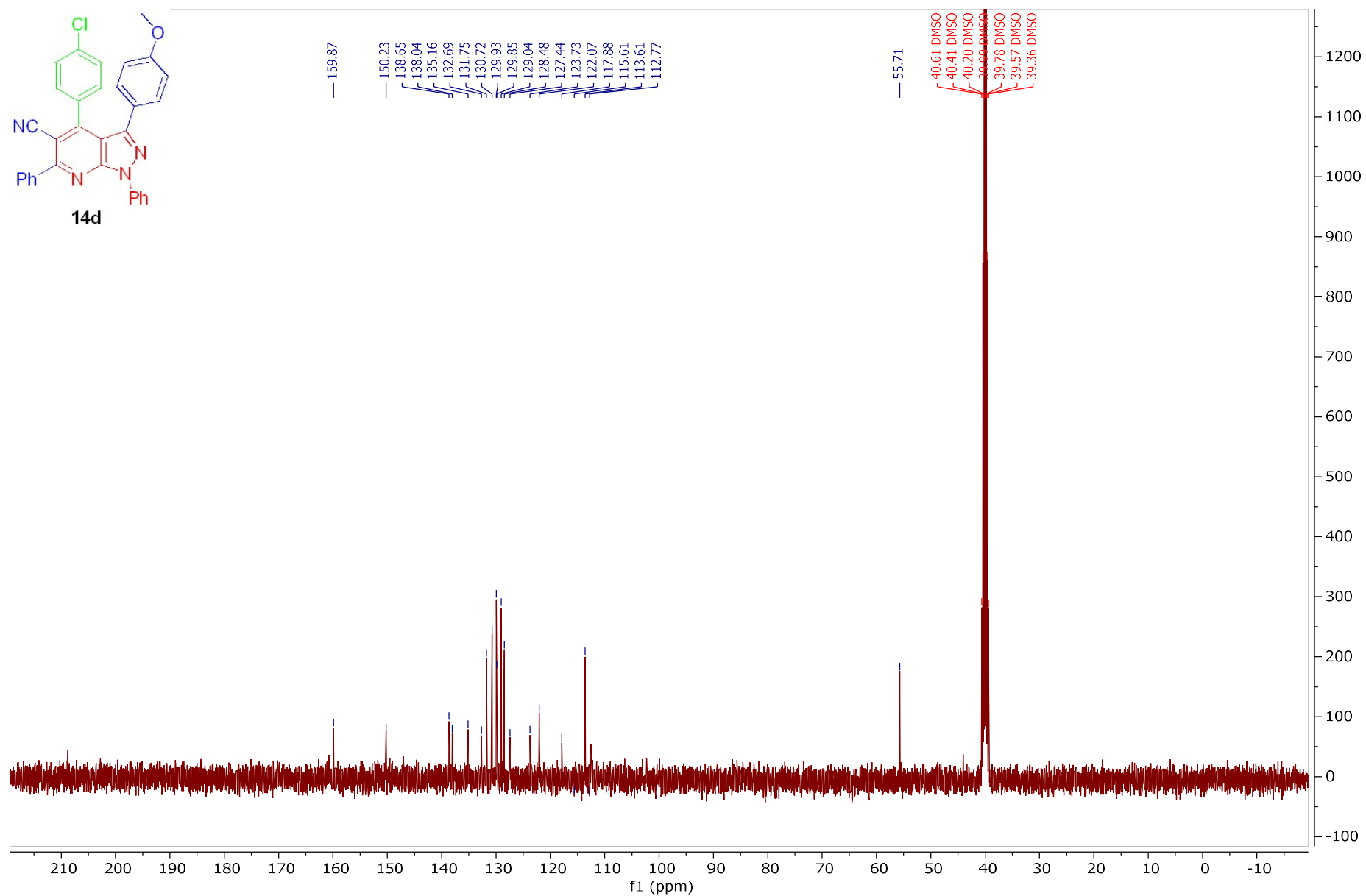


**Figure S42.** <sup>1</sup>H NMR of compound **14d**, full spectrum

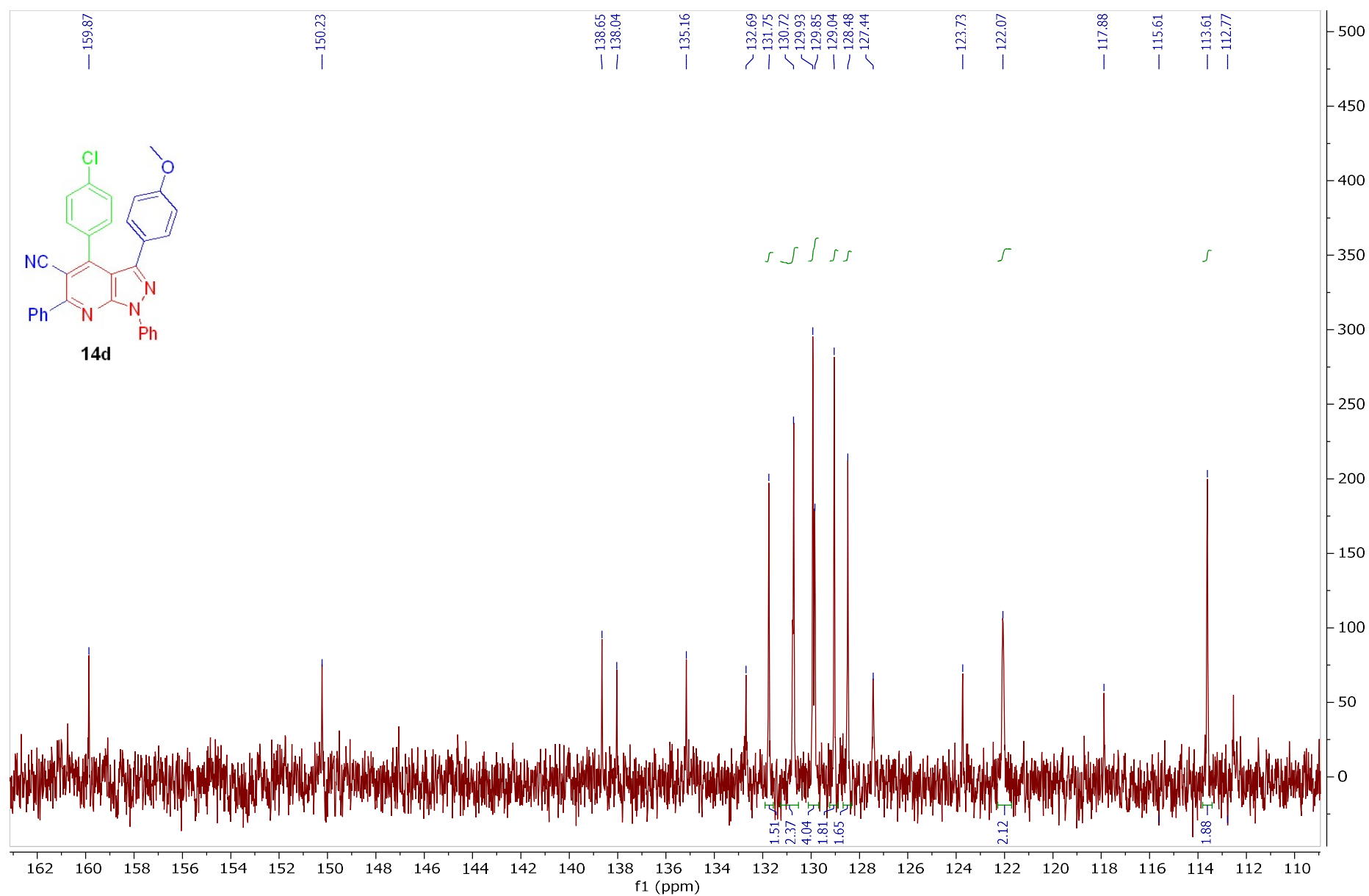


**Figure S43.**  $^1\text{H}$  NMR of compound **14d**, aromatic region

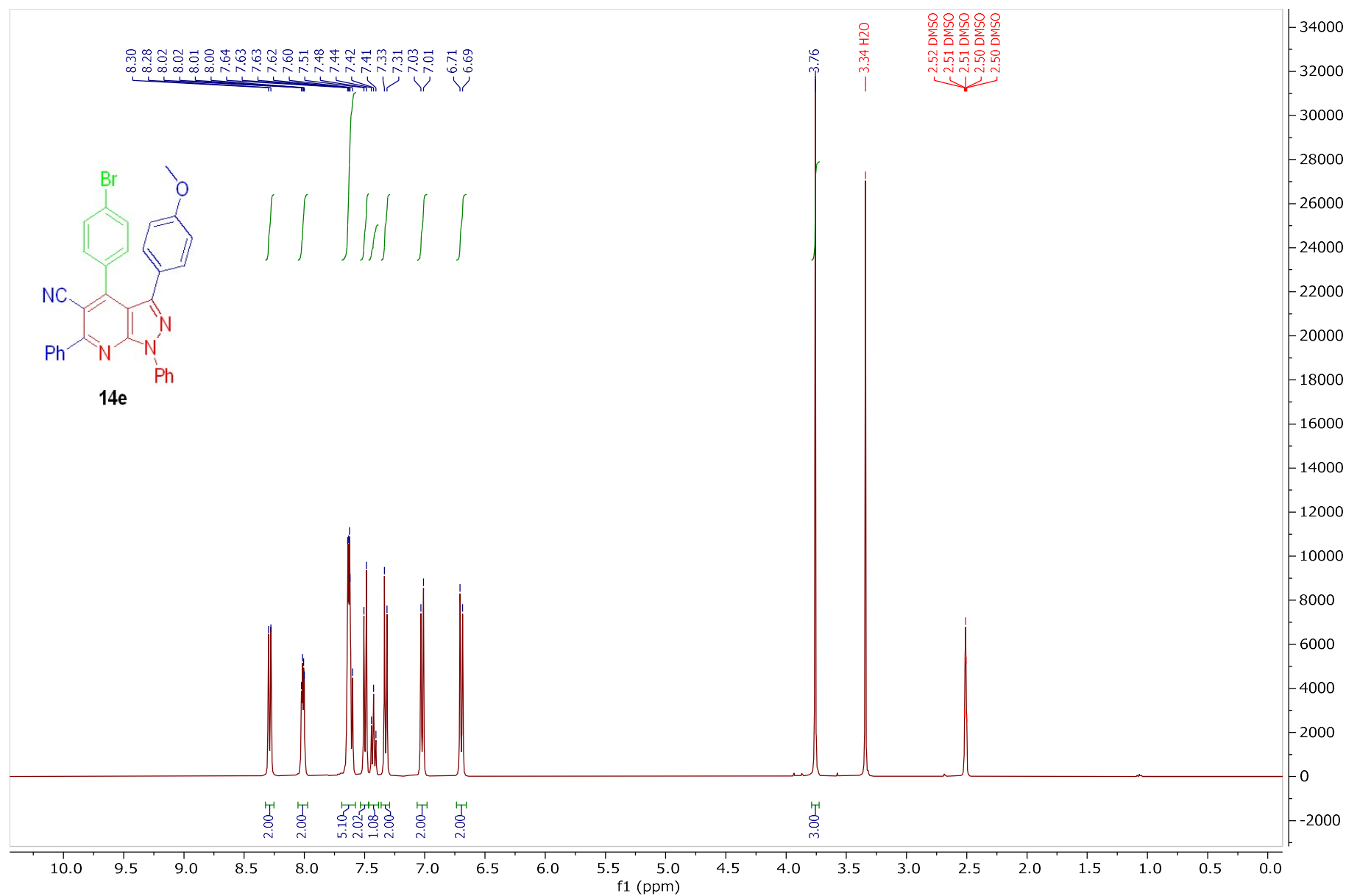




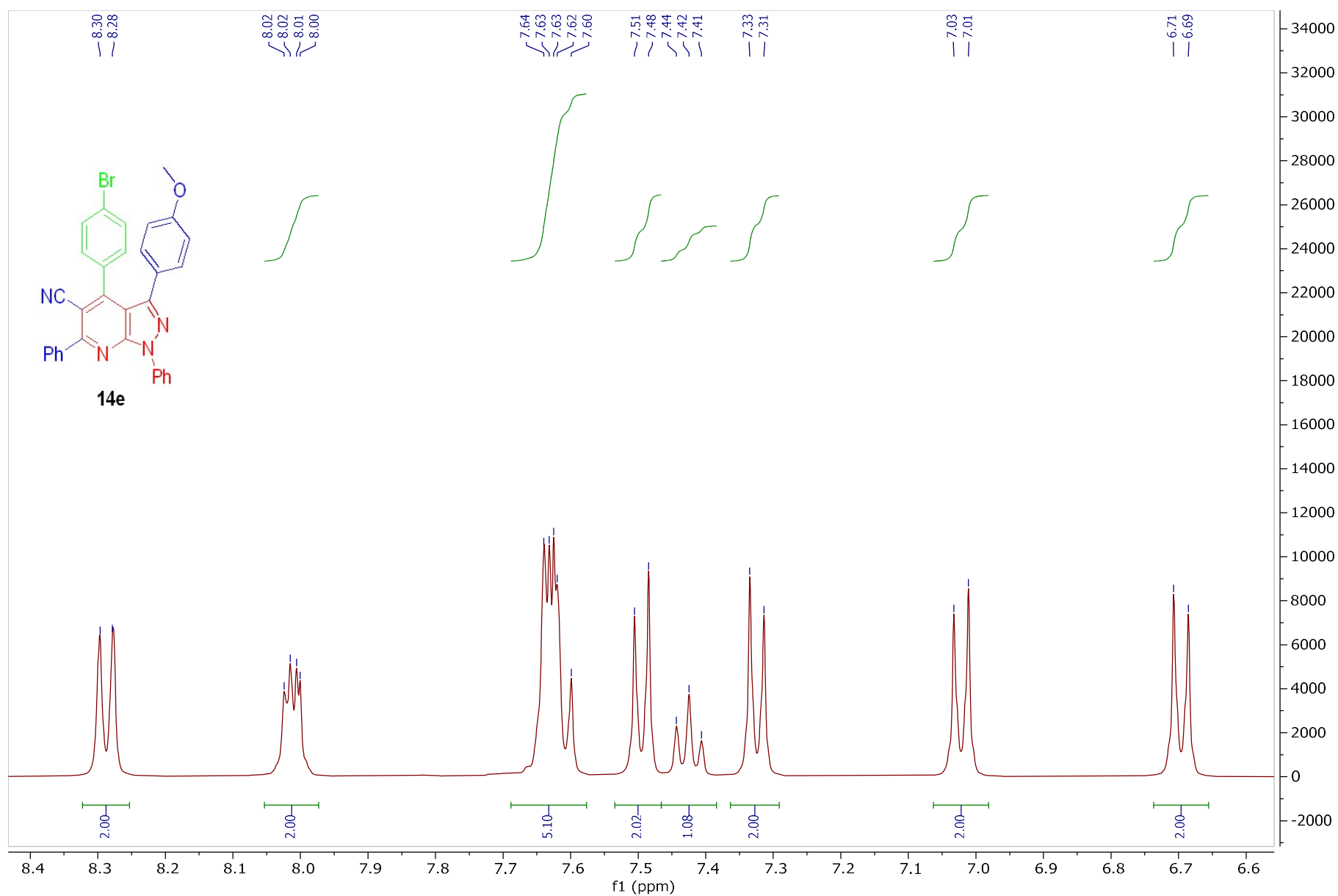
**Figure S44.**  $^{13}\text{C}$  NMR of compound **14d**, full spectrum



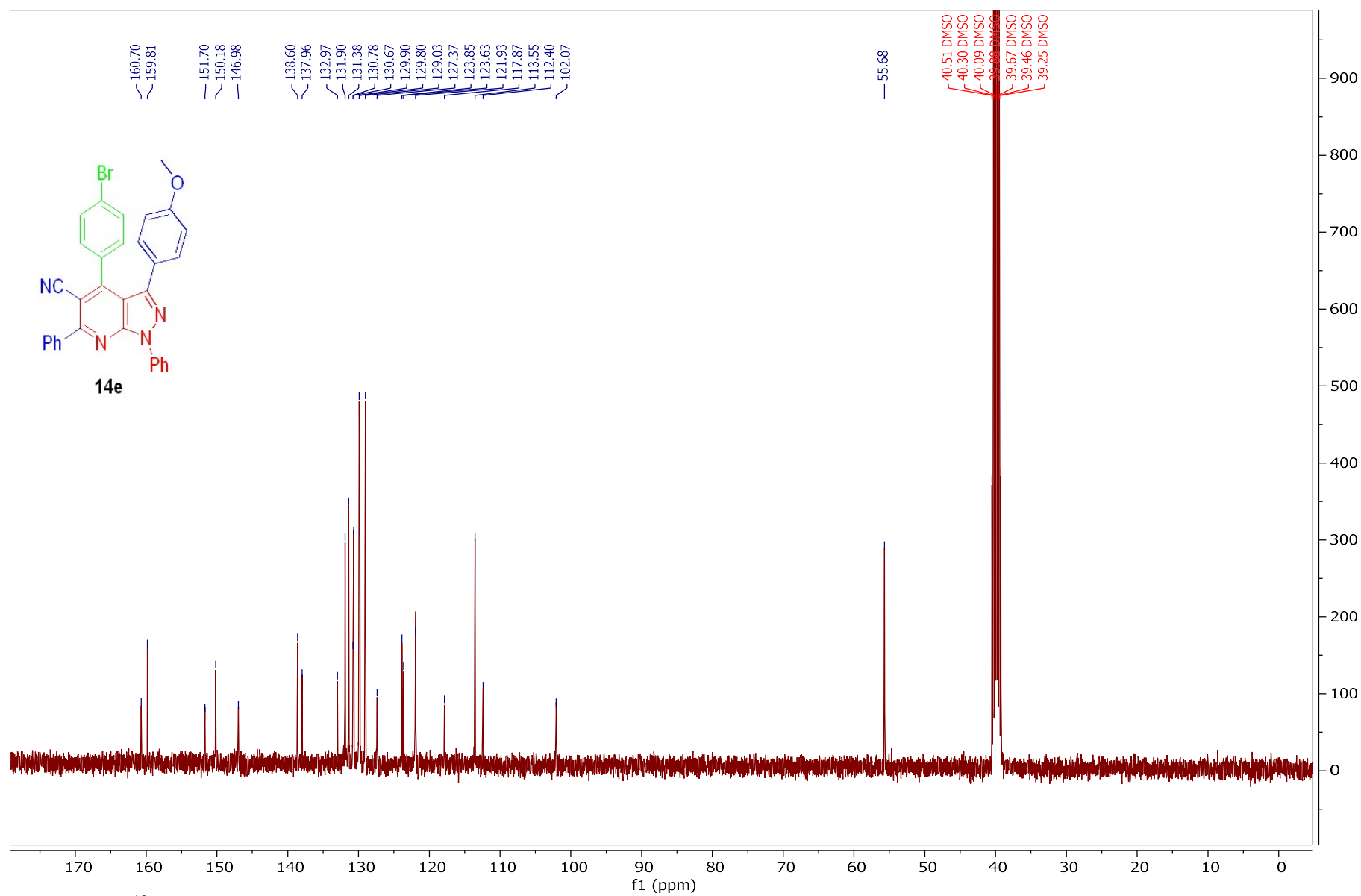
**Figure S45.**  $^{13}\text{C}$  NMR of compound **14d**, aromatic region



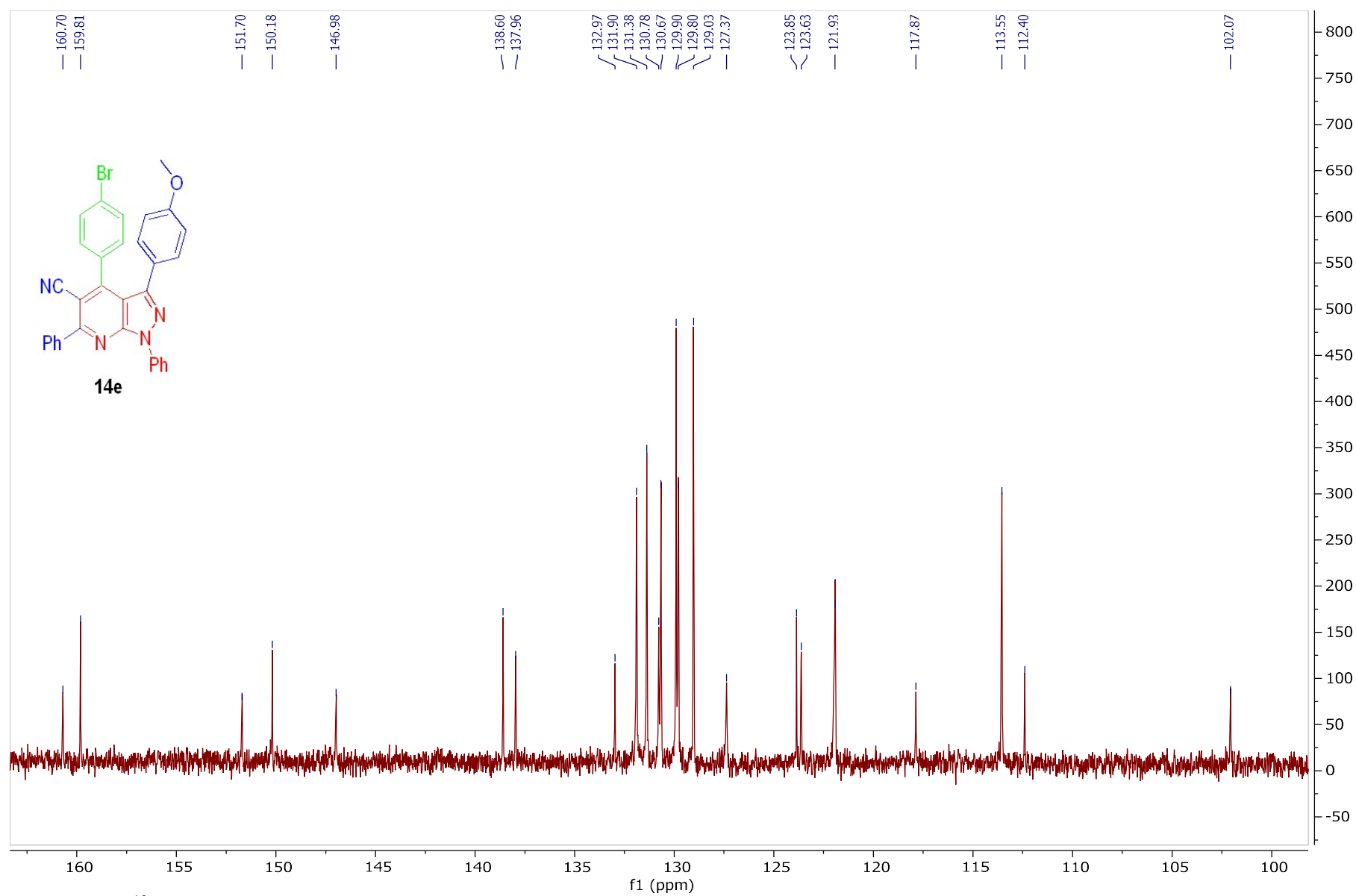
**Figure S46.** <sup>1</sup>H NMR of compound **14e**, full spectrum



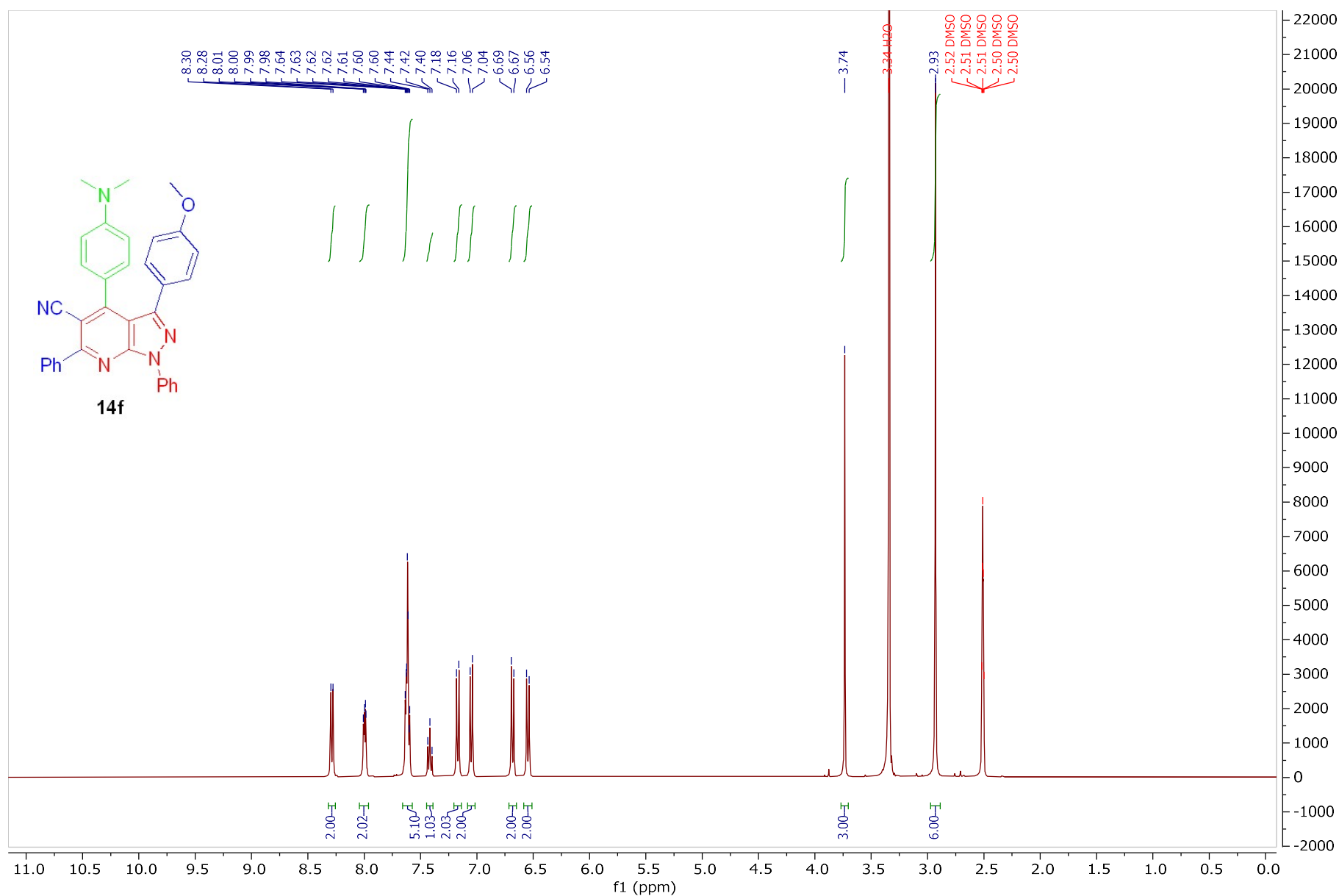
**Figure S47.** <sup>1</sup>H NMR of compound **14e**, aromatic region



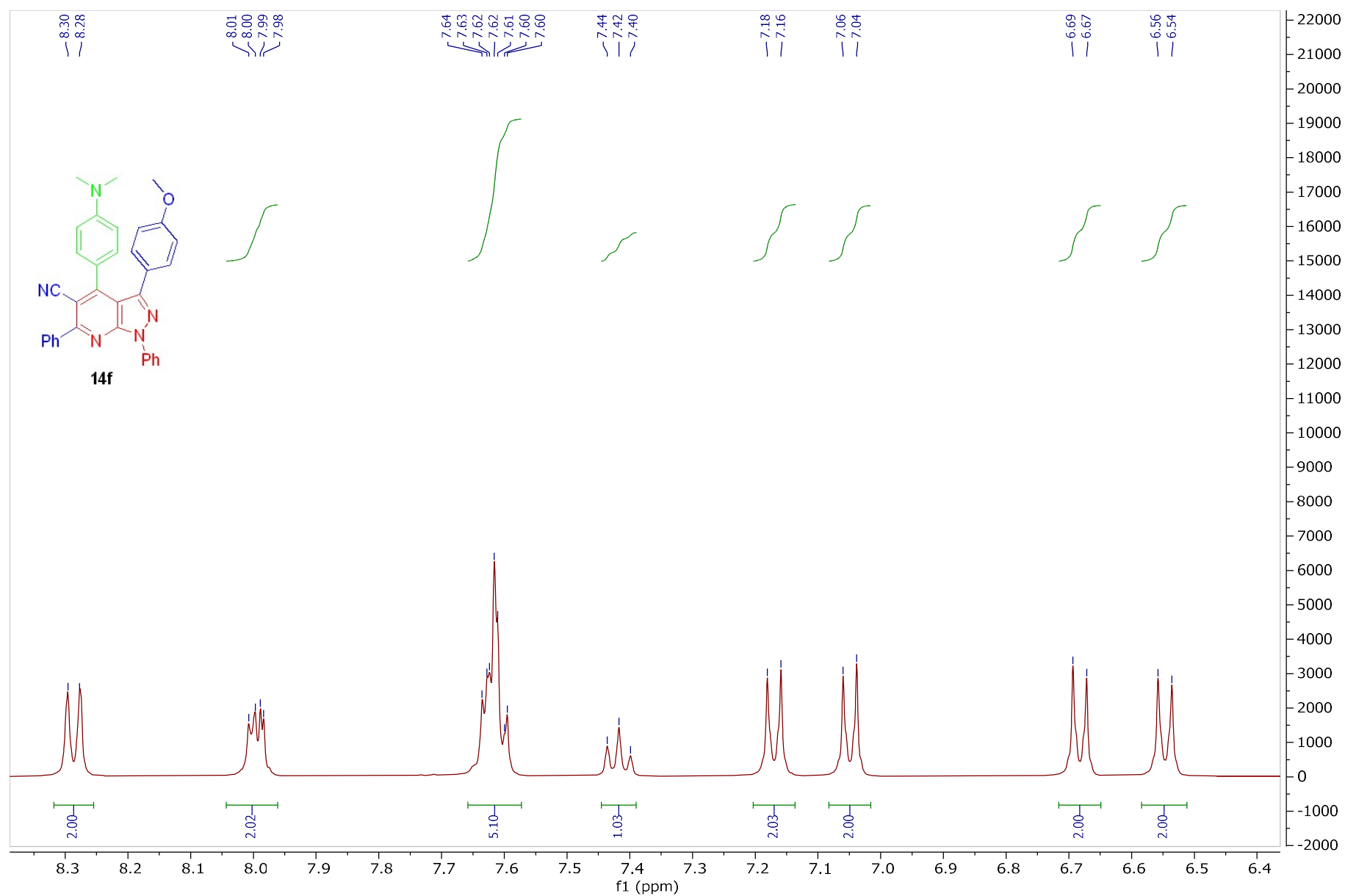
**Figure S48.** <sup>13</sup>C NMR of compound **14e**, full spectrum



**Figure S49.** <sup>13</sup>C NMR of compound **14e**, aromatic region



**Figure S50.** <sup>1</sup>H NMR of compound **14f**, full spectrum



**Figure S51.** <sup>1</sup>H NMR of compound **14f**, aromatic region



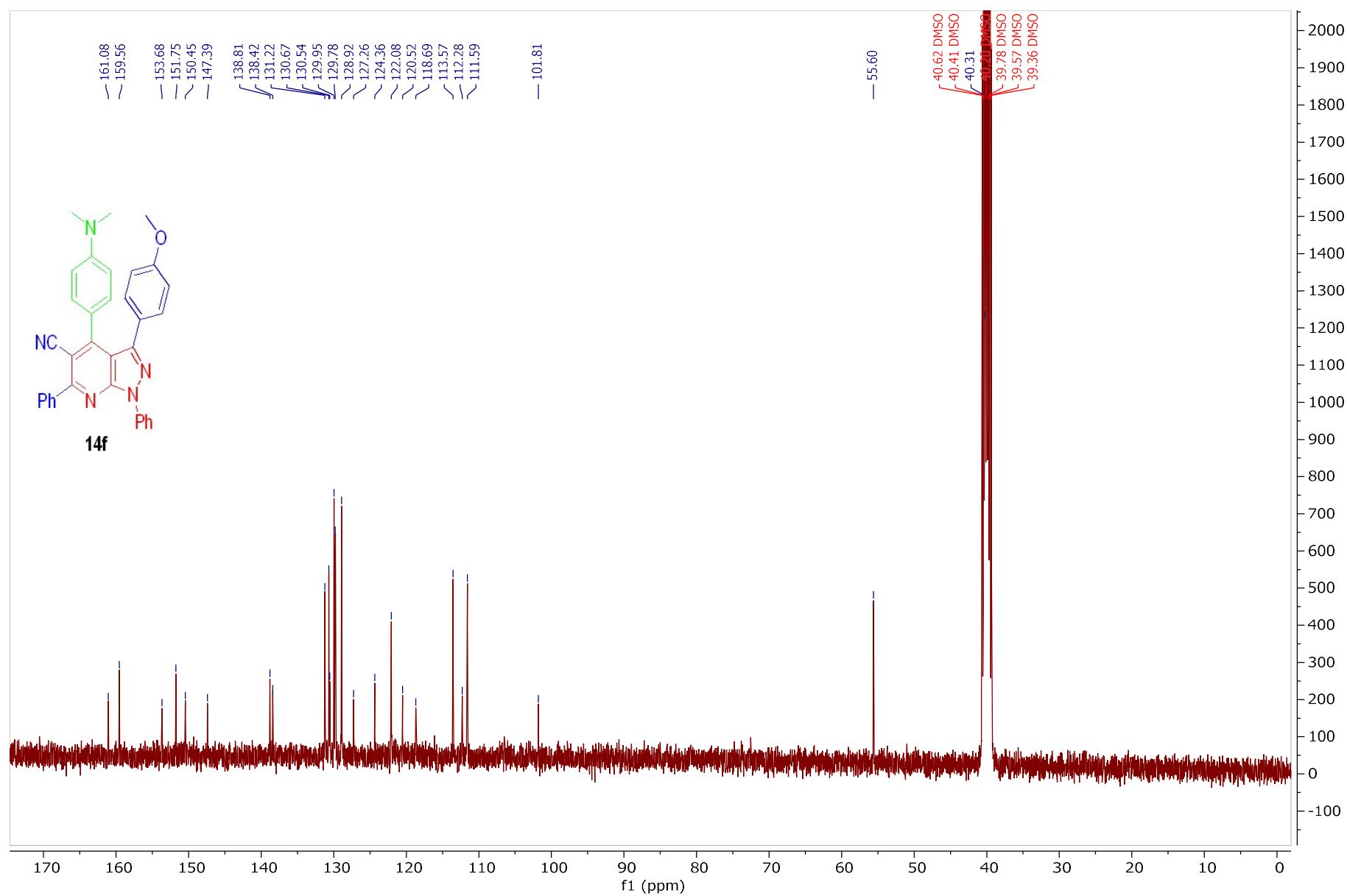
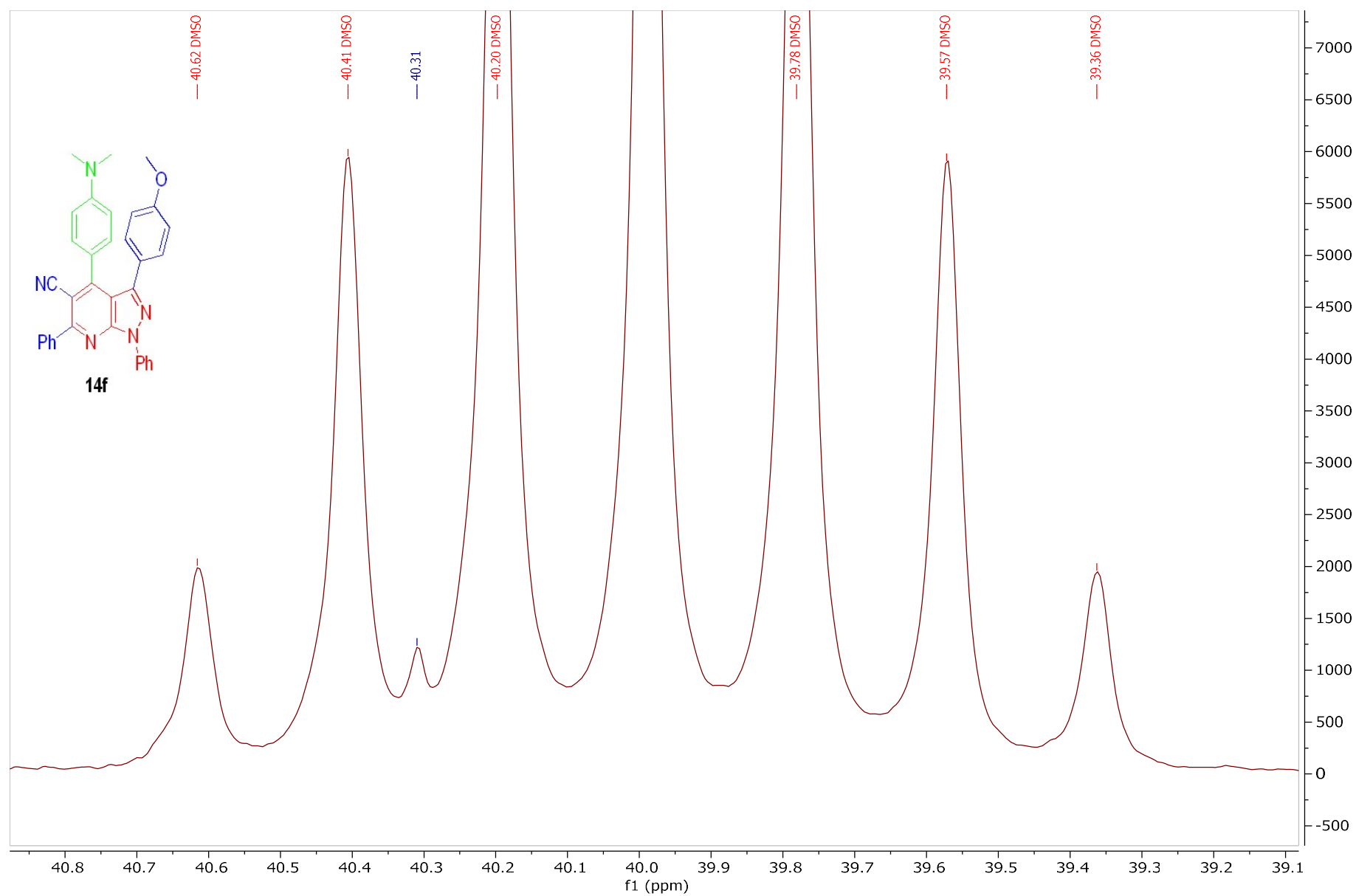


Figure S52.  $^{13}\text{C}$  NMR of compound **14f**, full spectrum



**Figure S53.** <sup>13</sup>C NMR of compound **14f**, aliphatic region

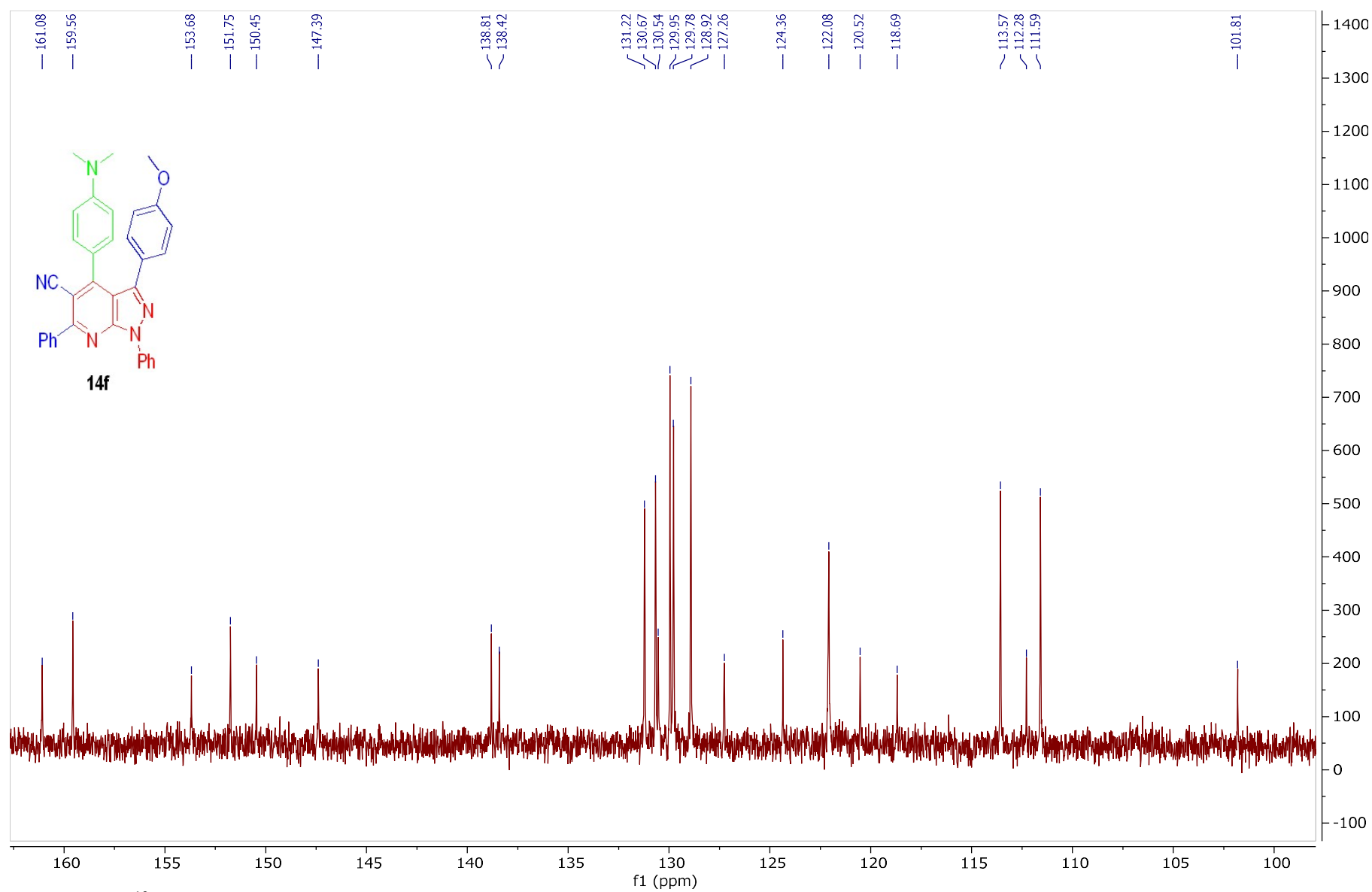
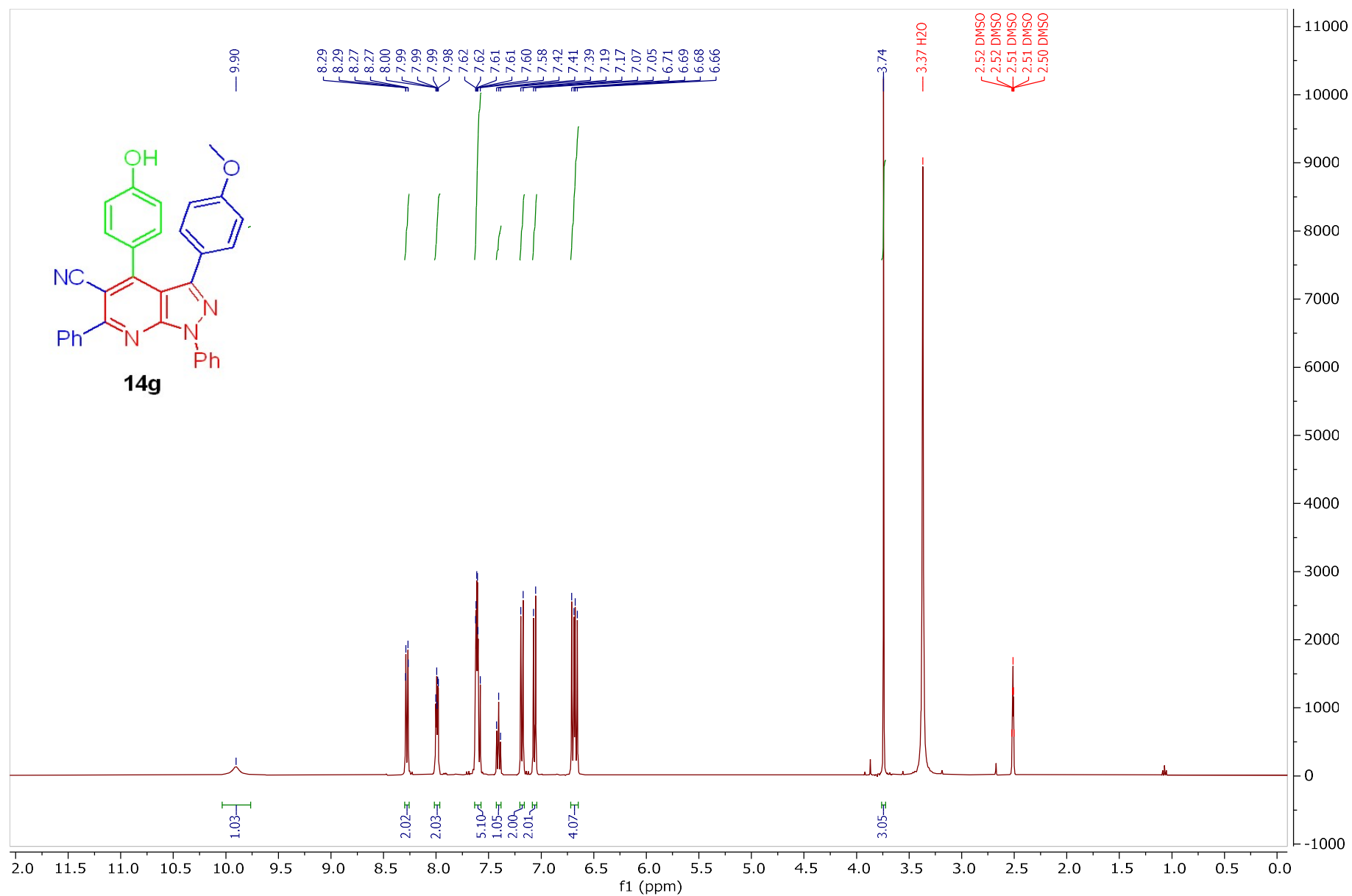
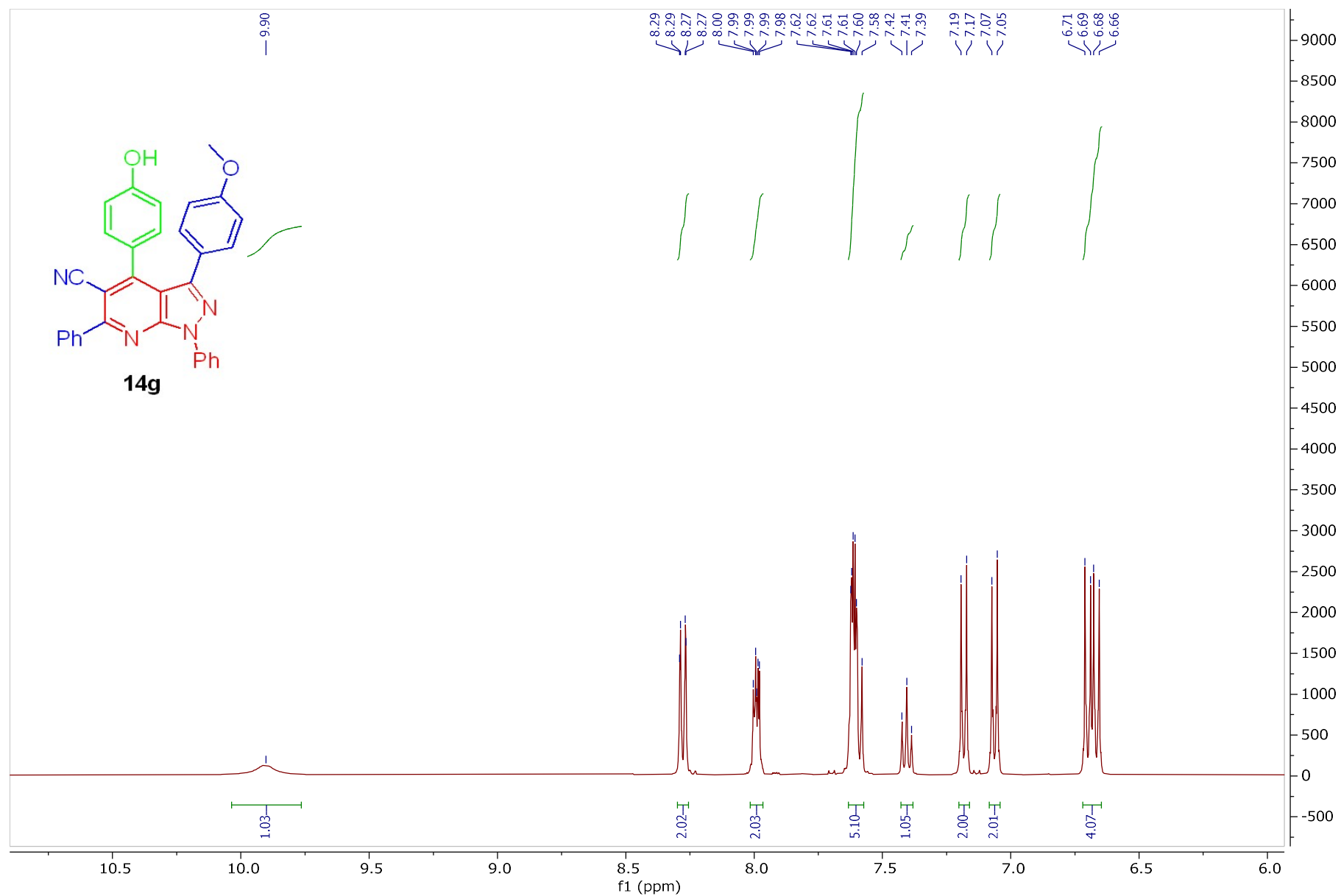


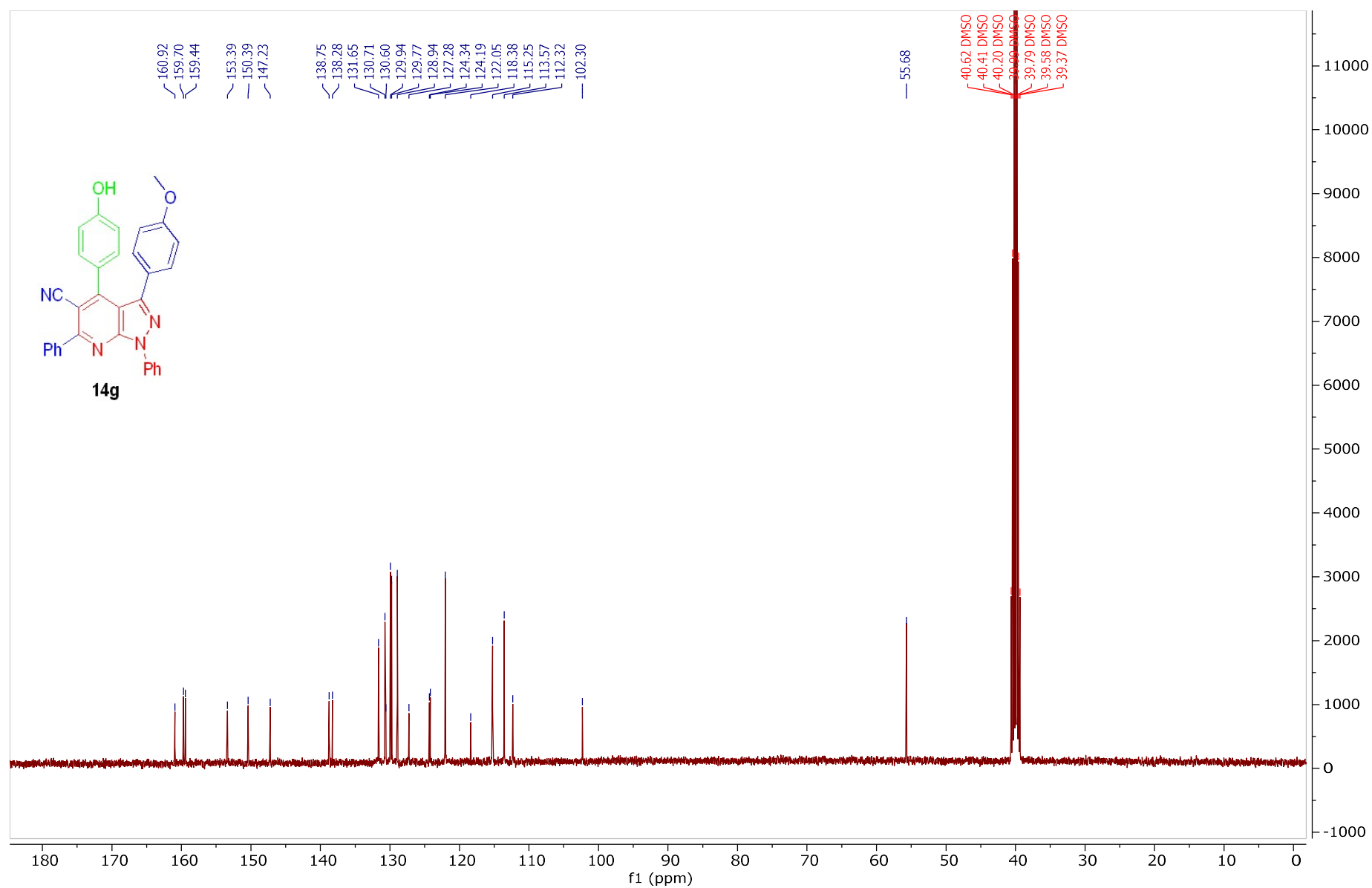
Figure S54. <sup>13</sup>C NMR of compound **14f**, aromatic region



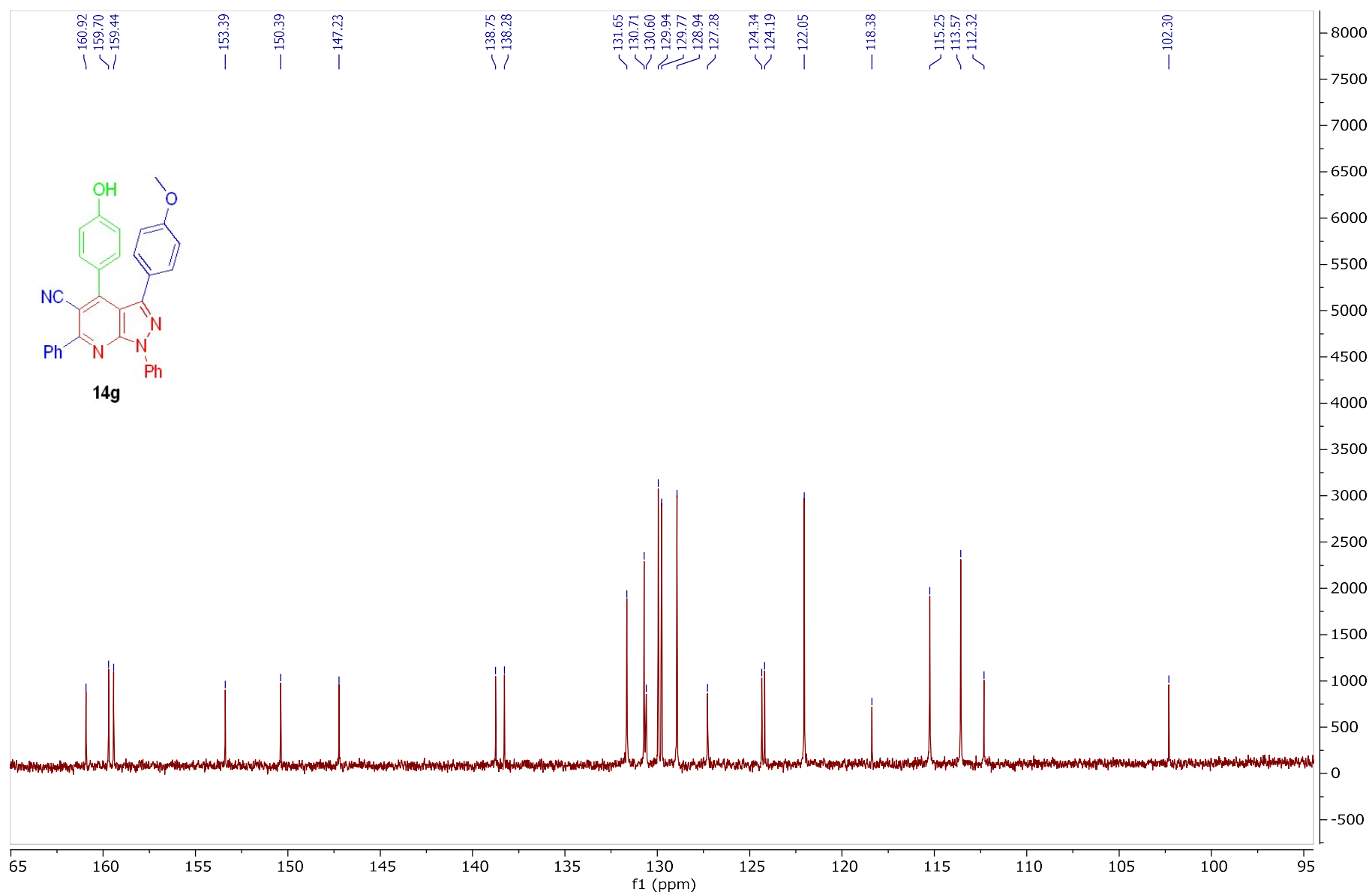
**Figure S55.**  $^1\text{H}$  NMR of compound **14g**, full spectrum



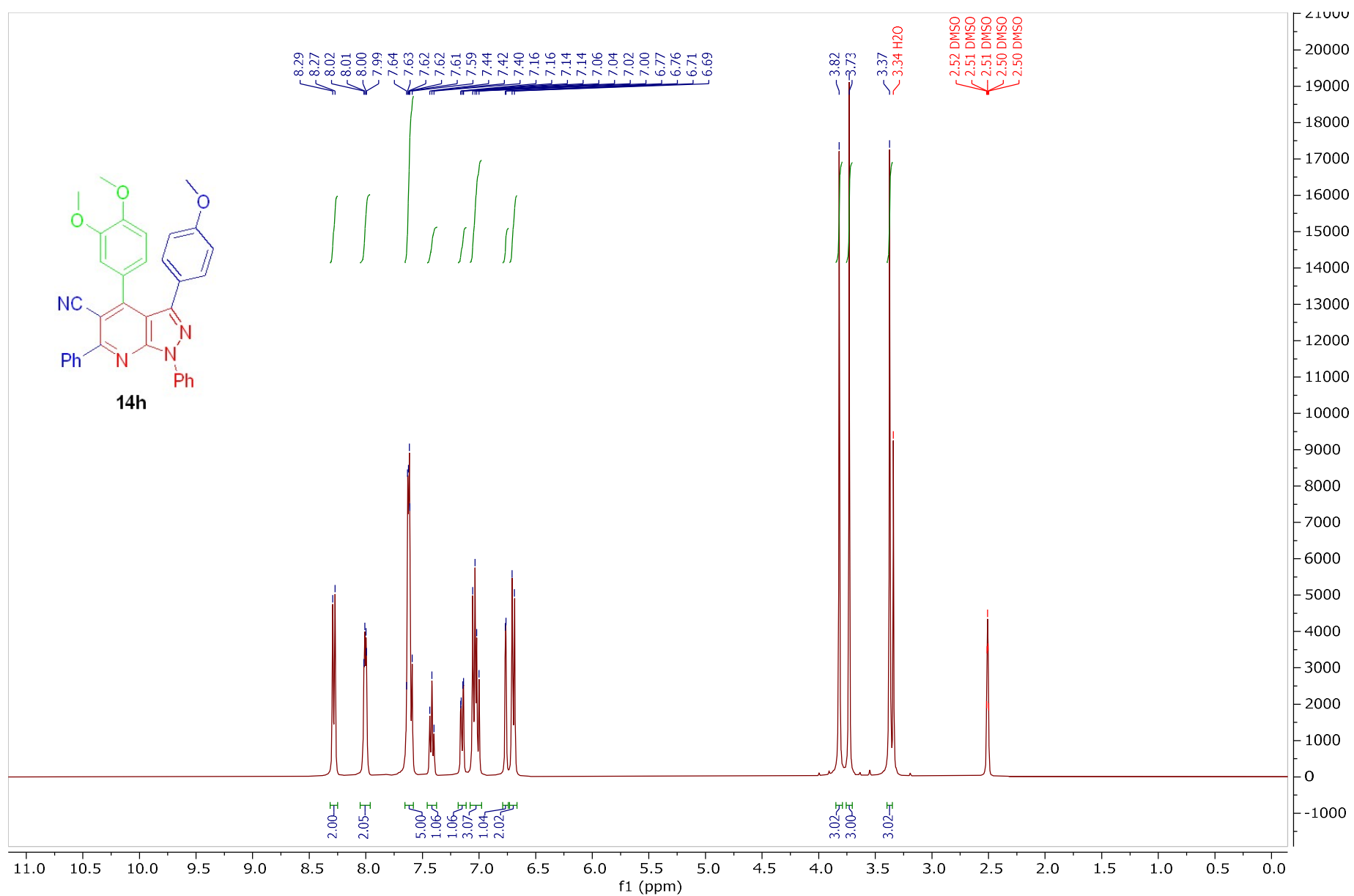
**Figure S56.** <sup>1</sup>H NMR of compound **14g**, aromatic region



**Figure S57.**  $^{13}\text{C}$  NMR of compound **14g**, full spectrum

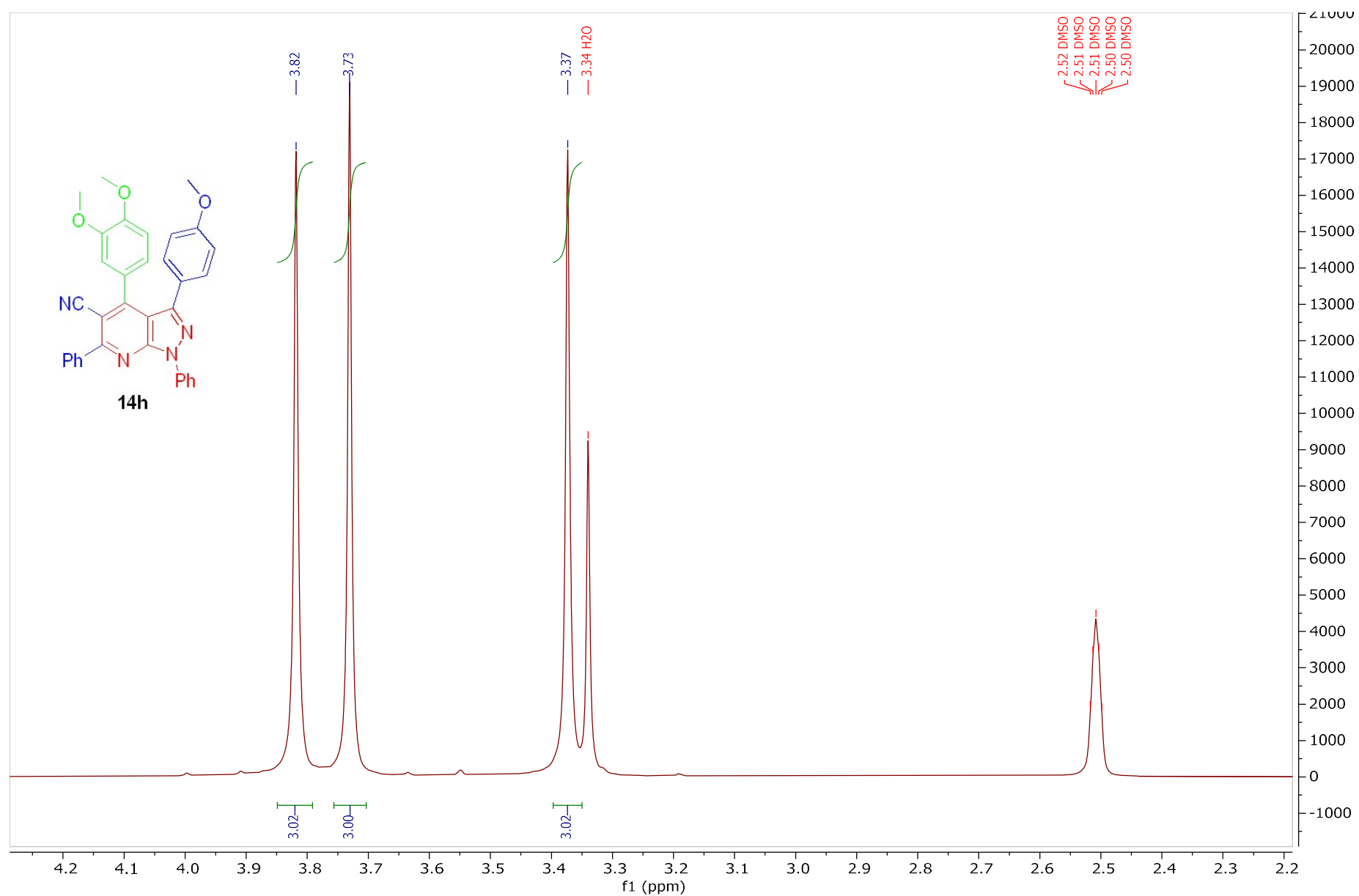


**Figure S58.** <sup>13</sup>C NMR of compound **14g**, aromatic region

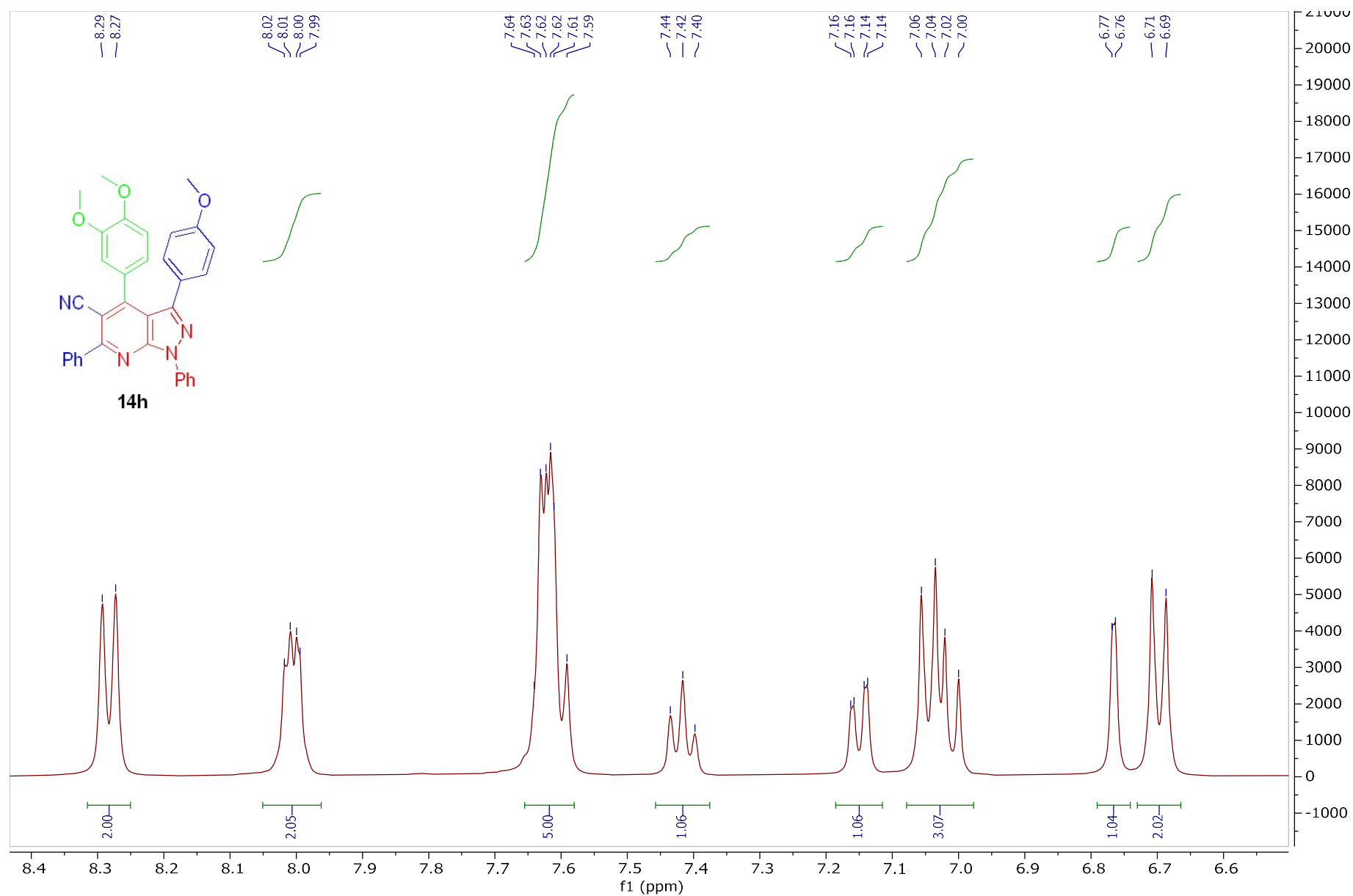


**Figure S59.**  $^1\text{H}$  NMR of compound **14h**, full spectrum

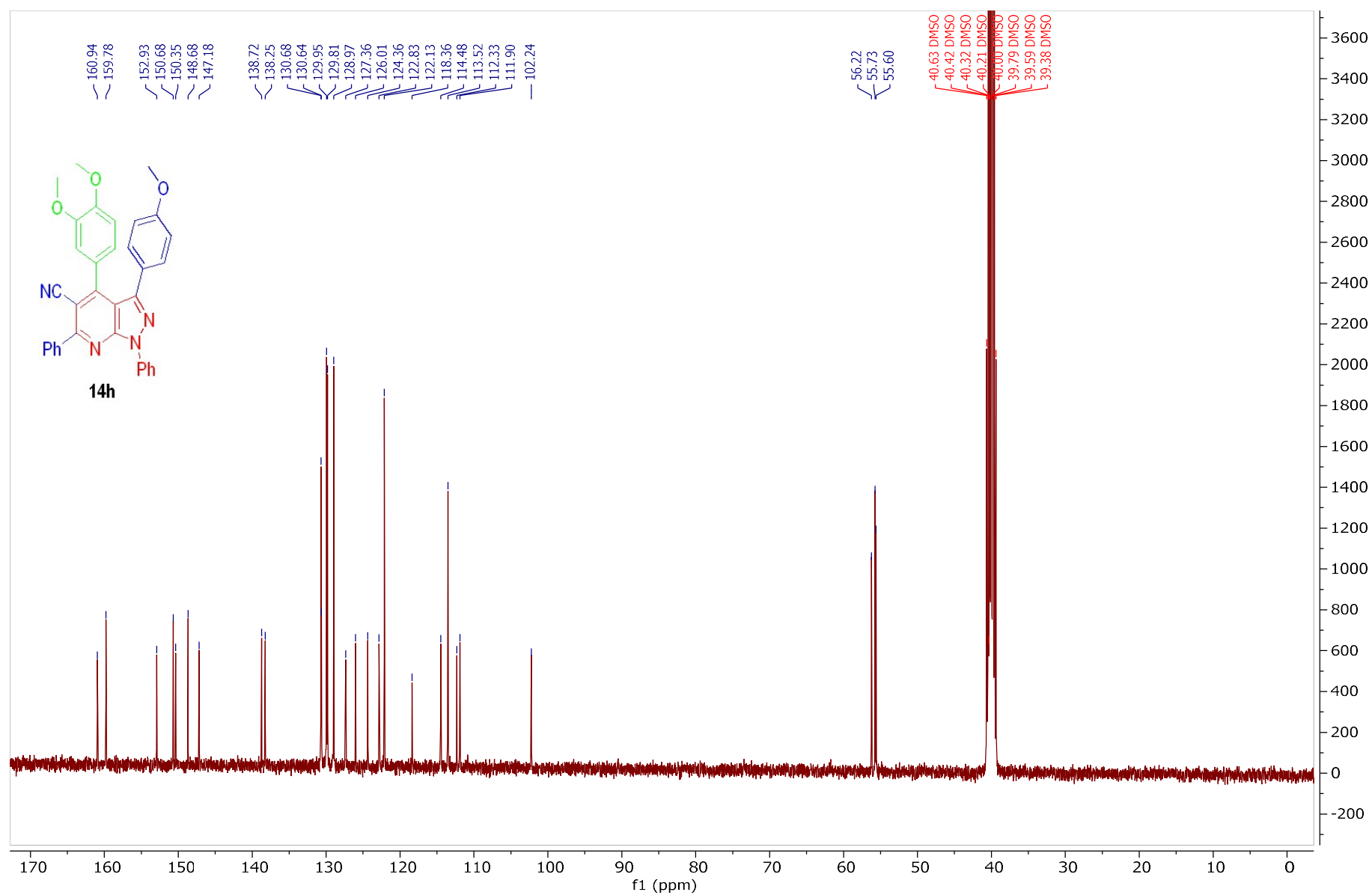




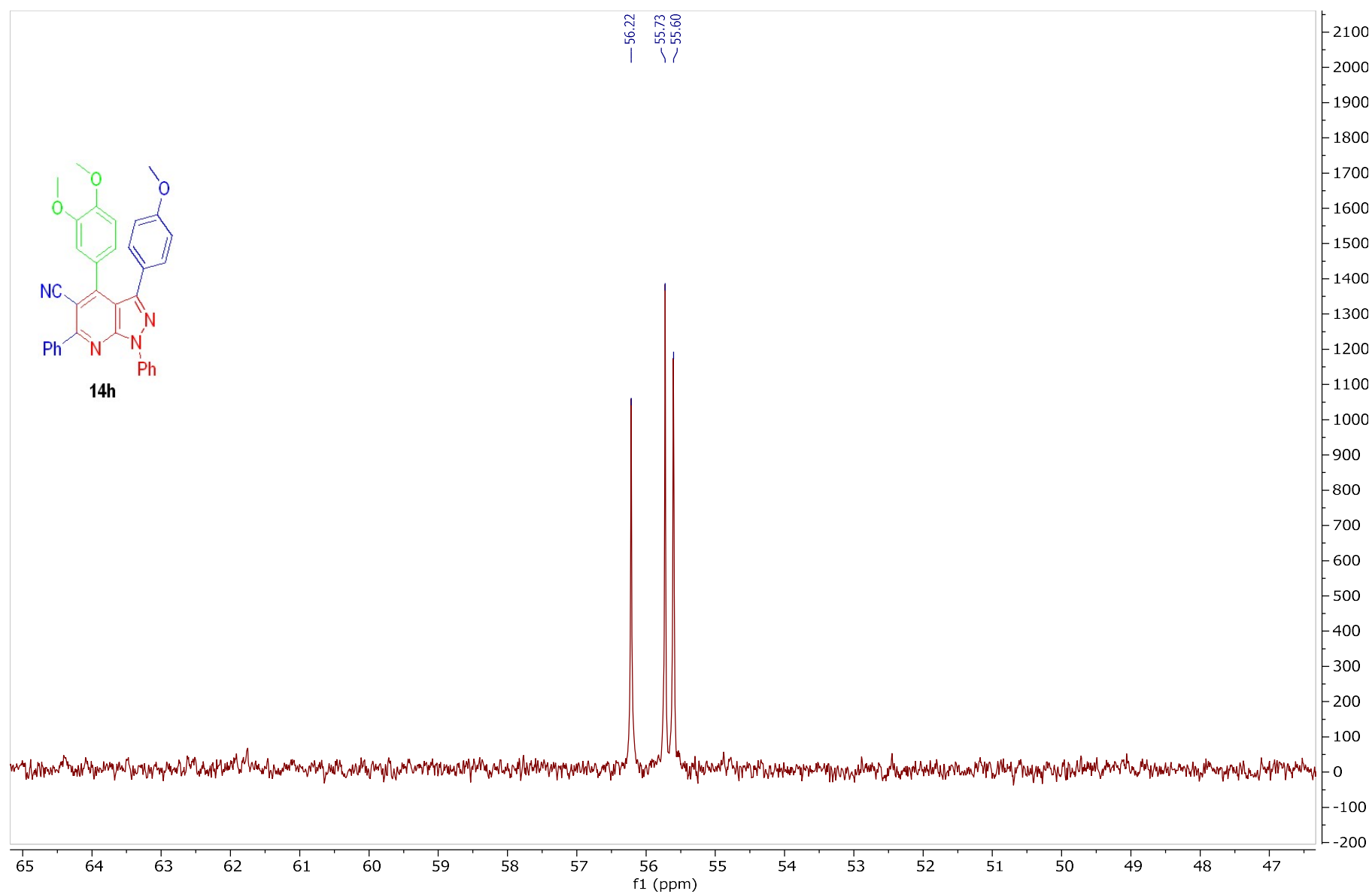
**Figure S60.** <sup>1</sup>H NMR of compound **14h**, aliphatic region



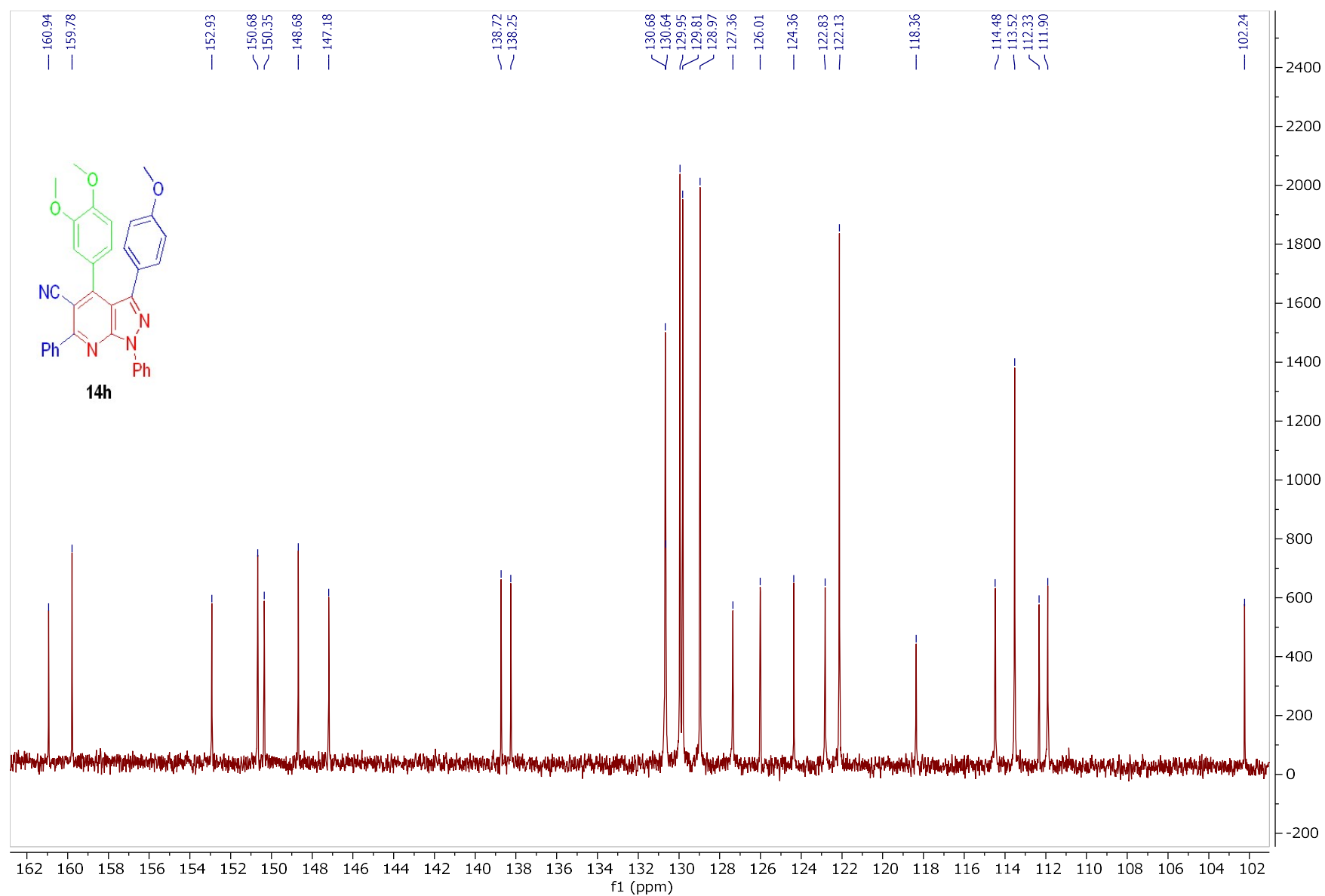
**Figure S61.** <sup>1</sup>H NMR of compound **14h**, aromatic region



**Figure S62.**  $^{13}\text{C}$  NMR of compound **14h**, full spectrum



**Figure S63.**  $^{13}\text{C}$  NMR of compound **14h**, aliphatic region



**Figure S64.**  $^{13}\text{C}$  NMR of compound **14h**, aromatic region

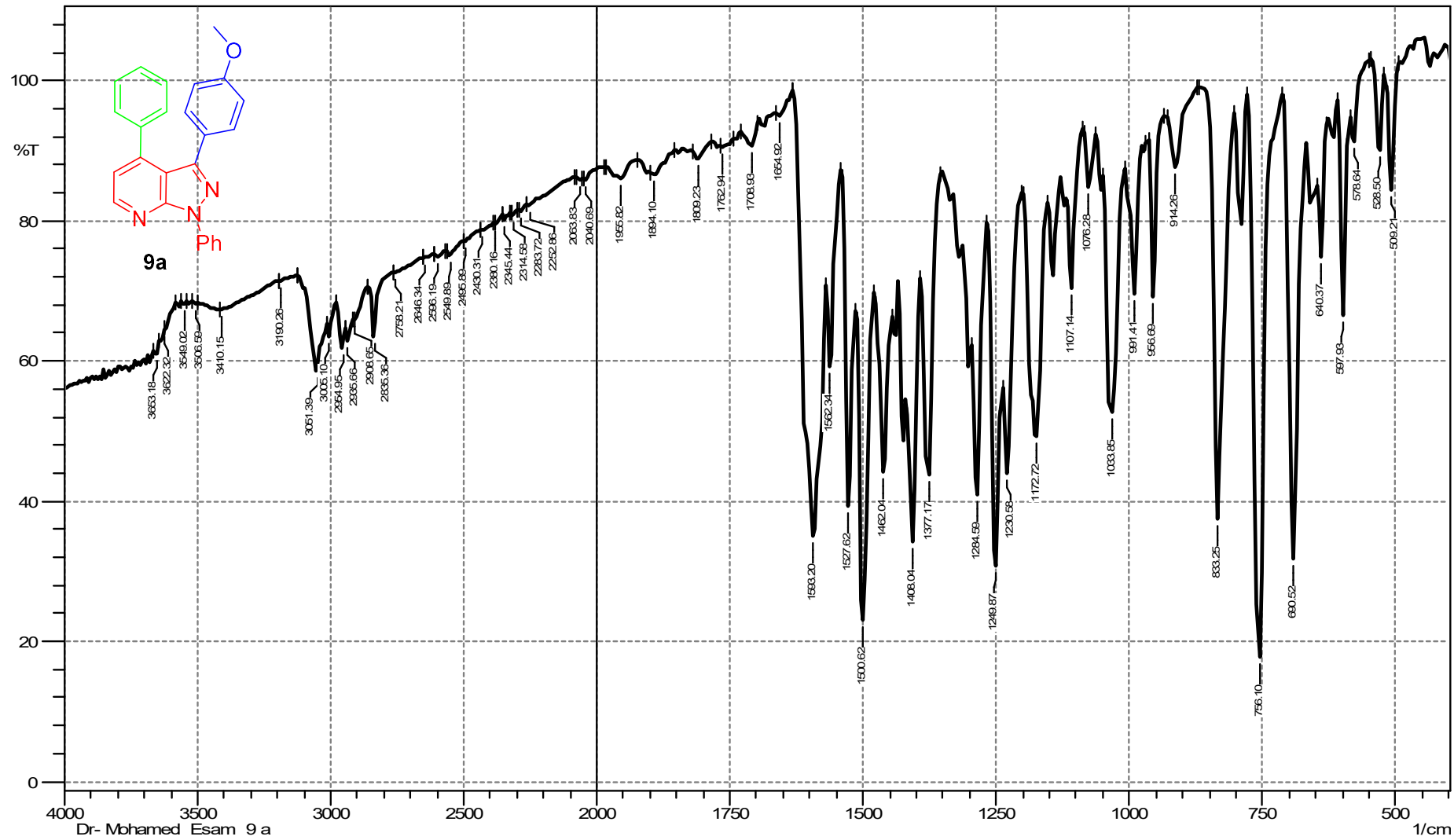


Figure S65. IR of compound 9a

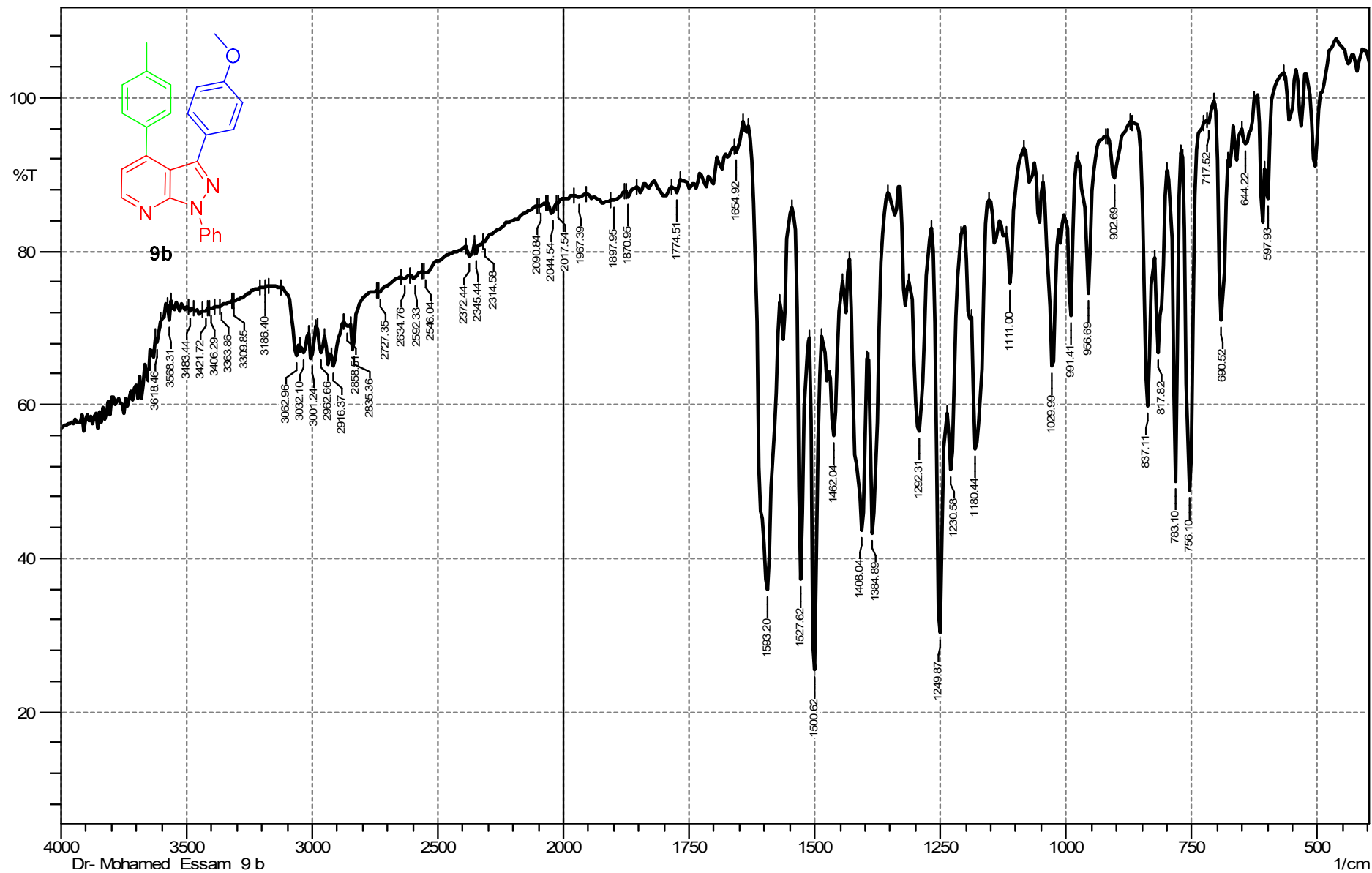
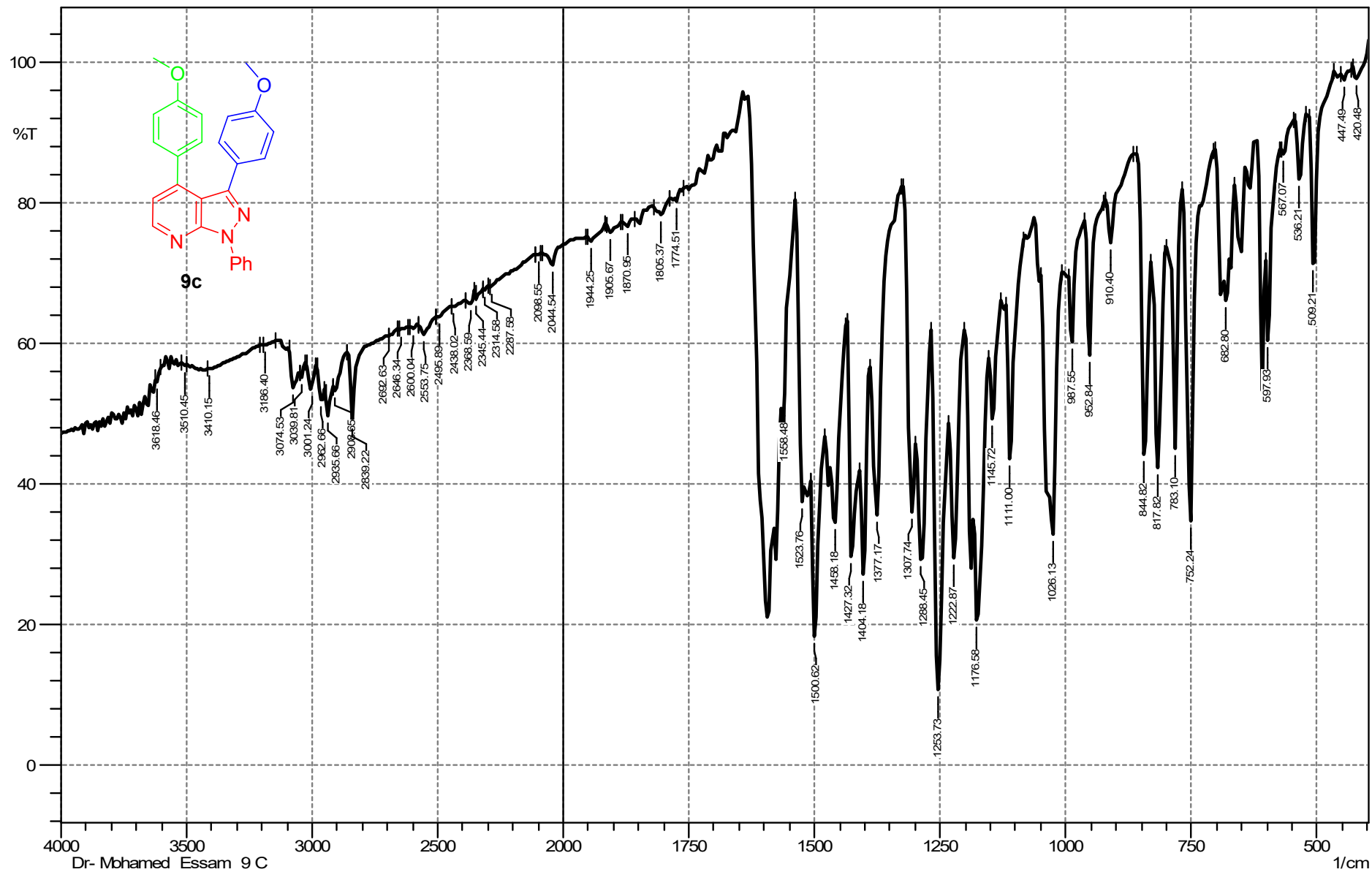


Figure S66. IR of compound **9b**



Dr- Mohamed Essam 9 C  
Figure S67. IR of compound 9c



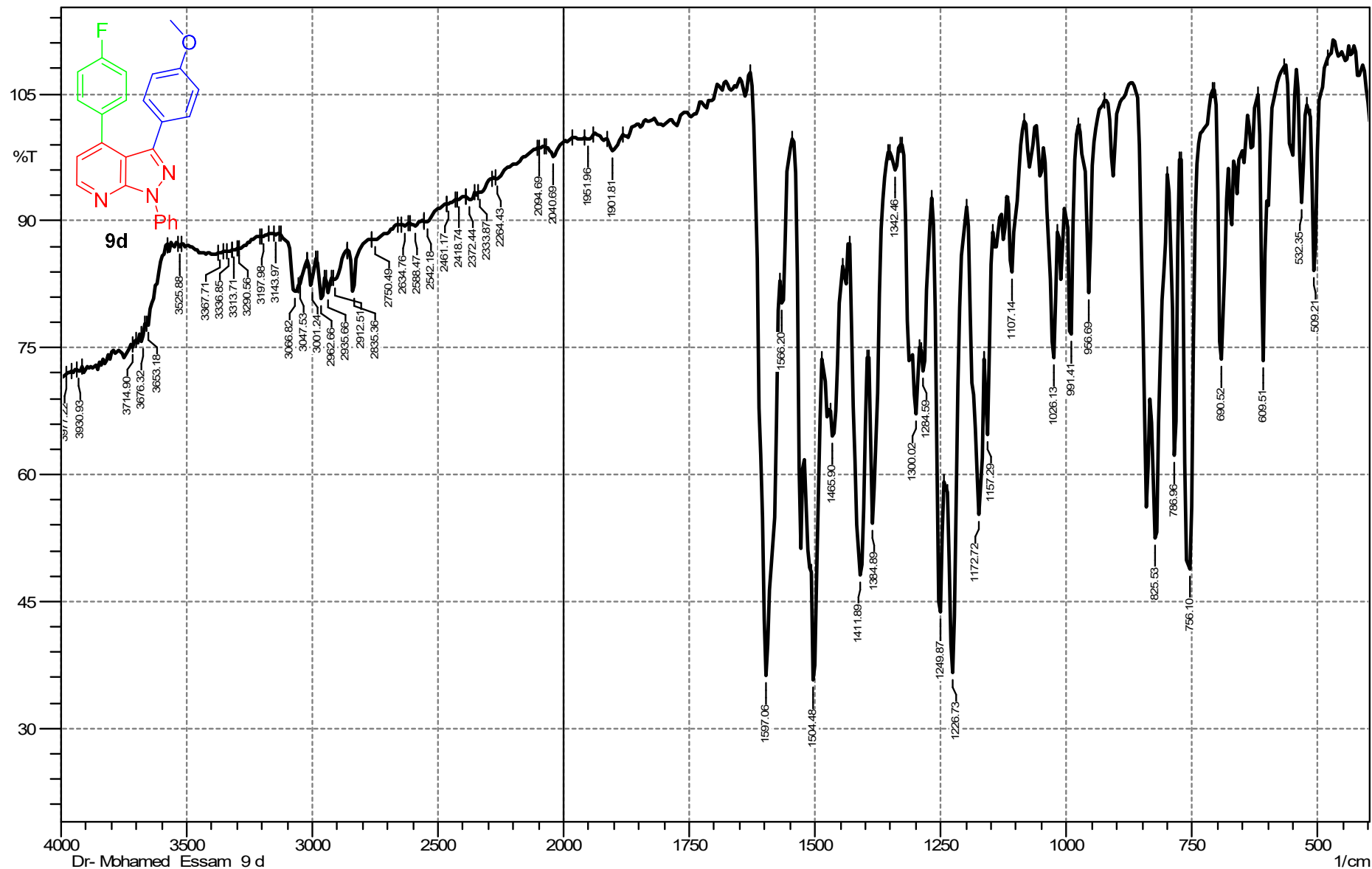


Figure S68. IR of compound 9d

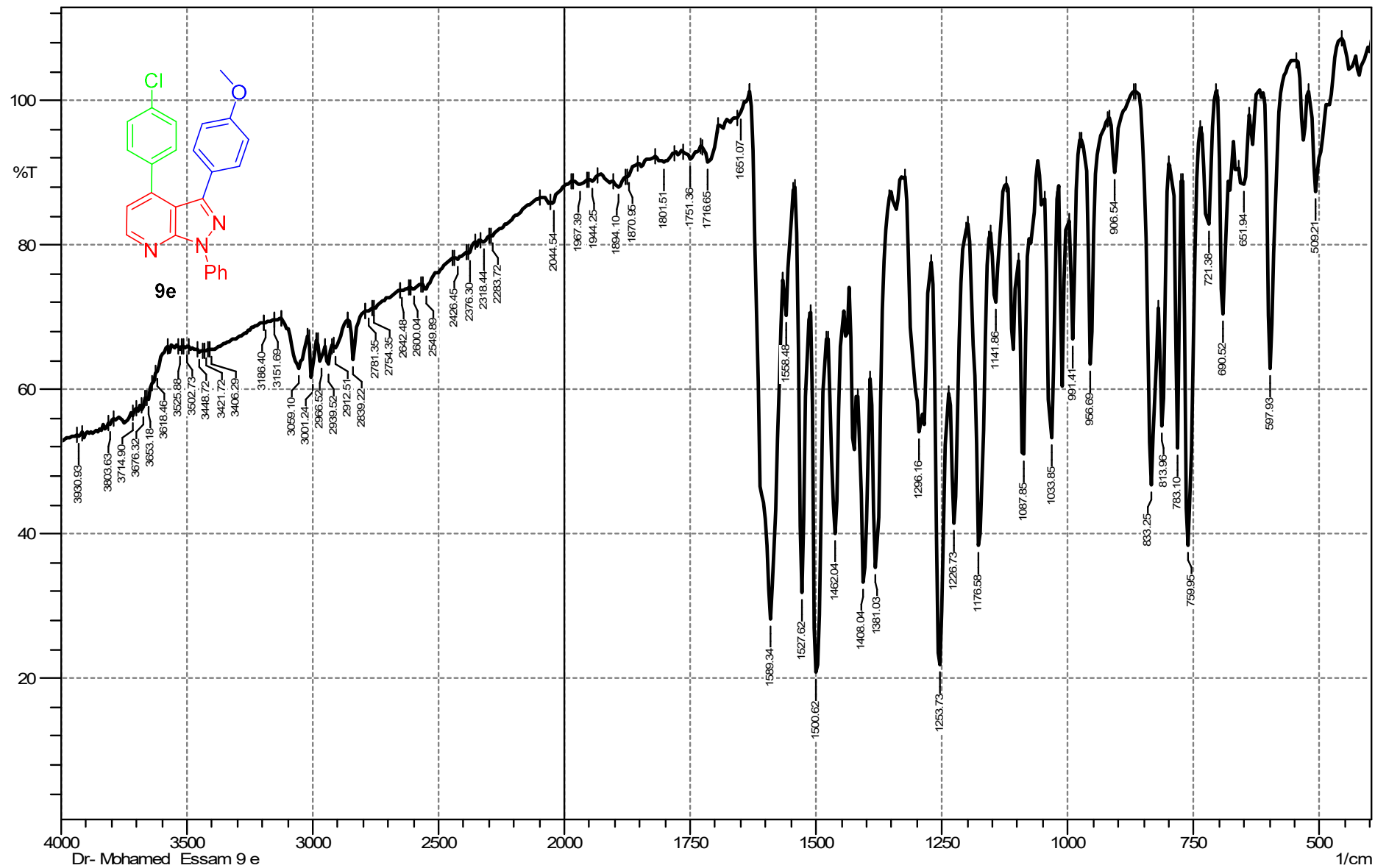


Figure S69. IR of compound **9e**

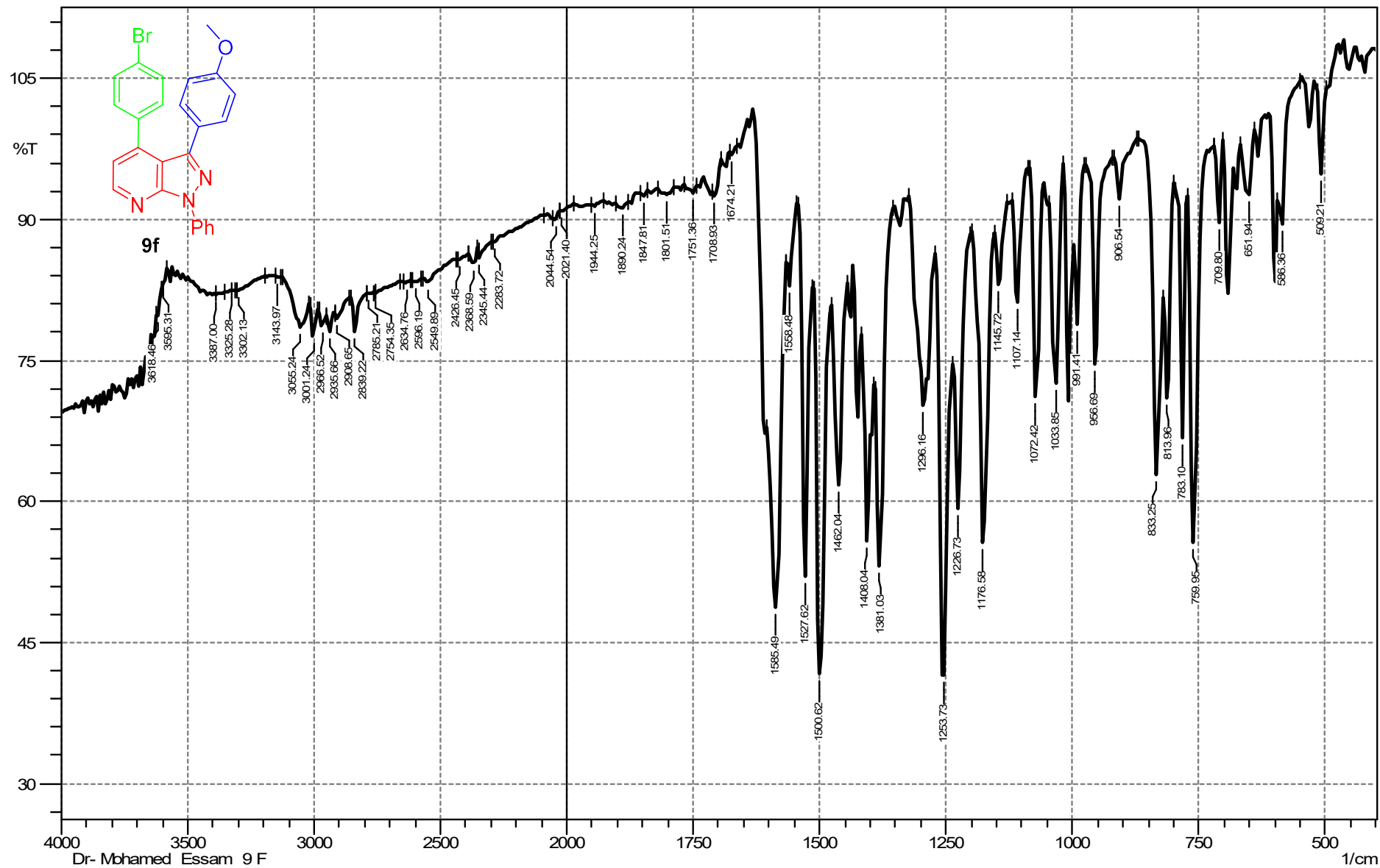


Figure S70. IR of compound 9f

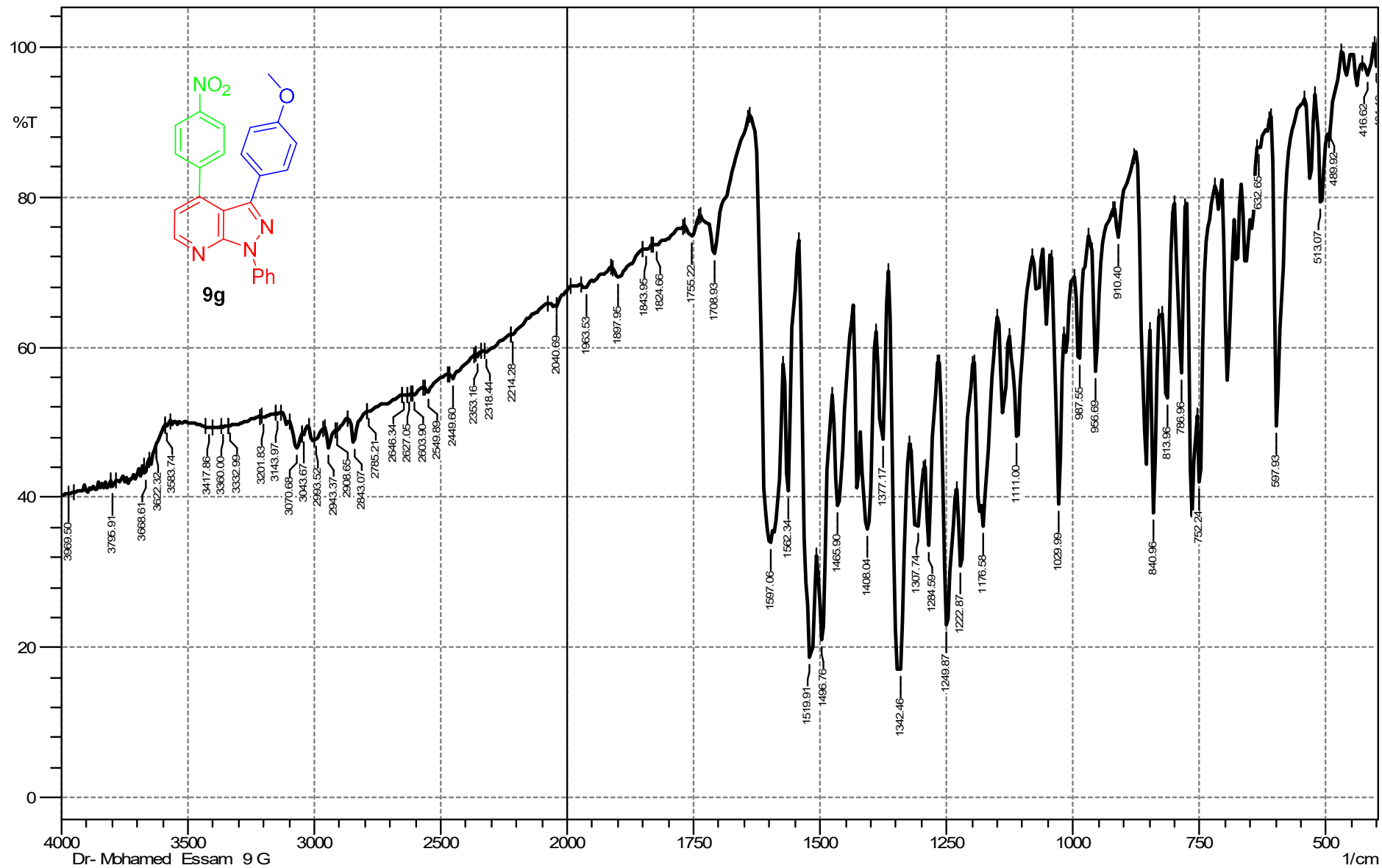


Figure S71. IR of compound **9g**

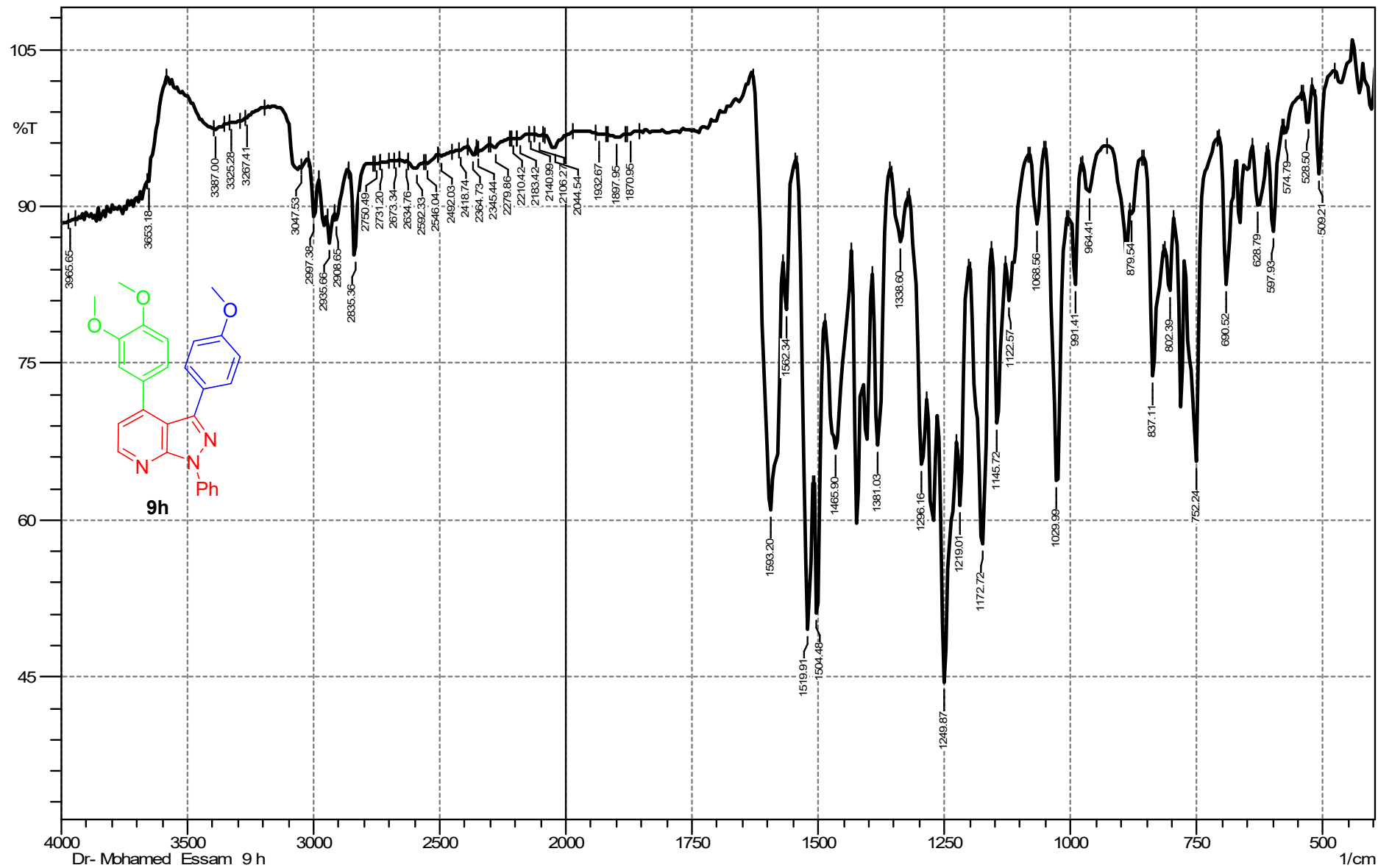
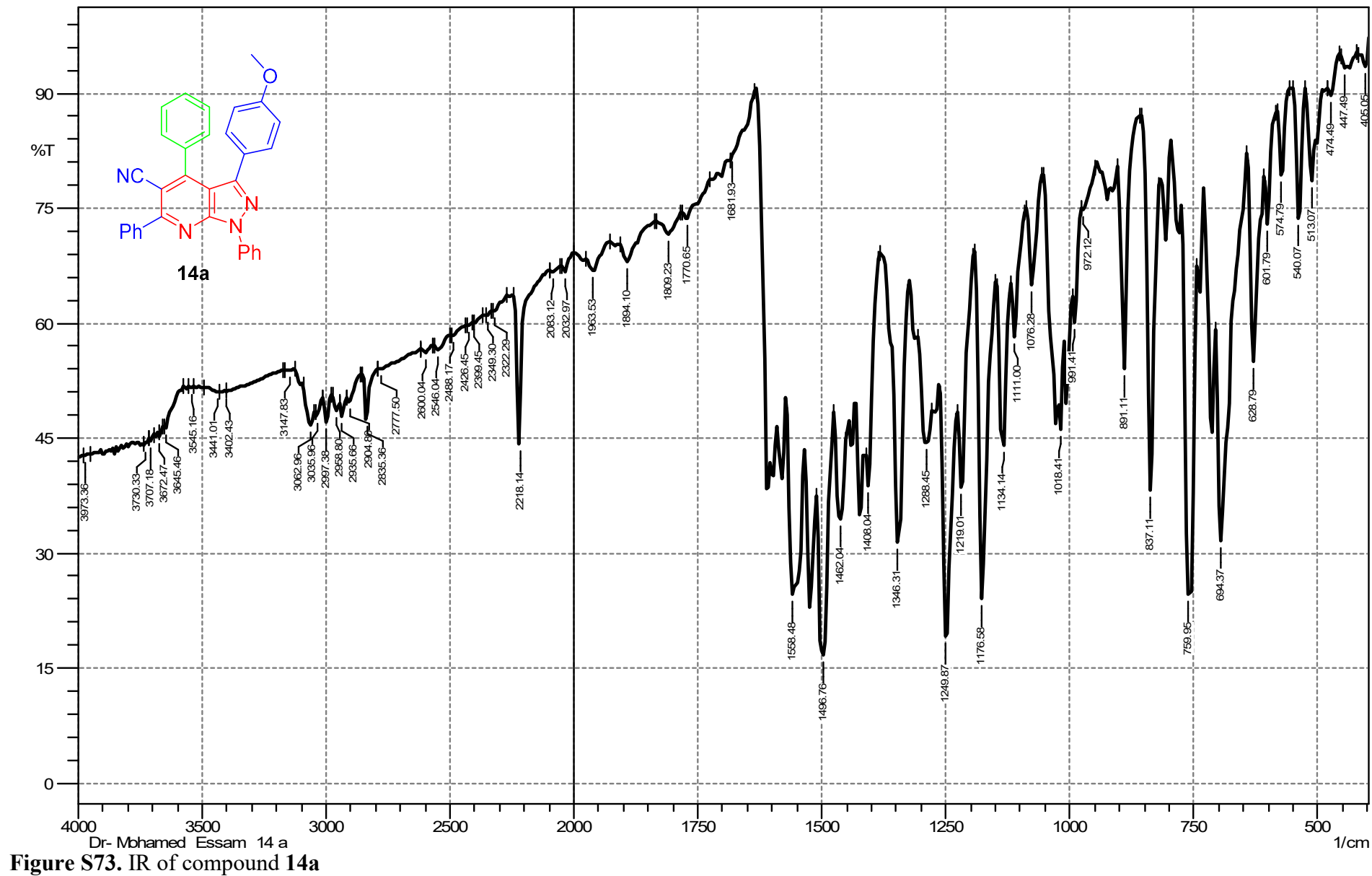


Figure S72. IR of compound 9h



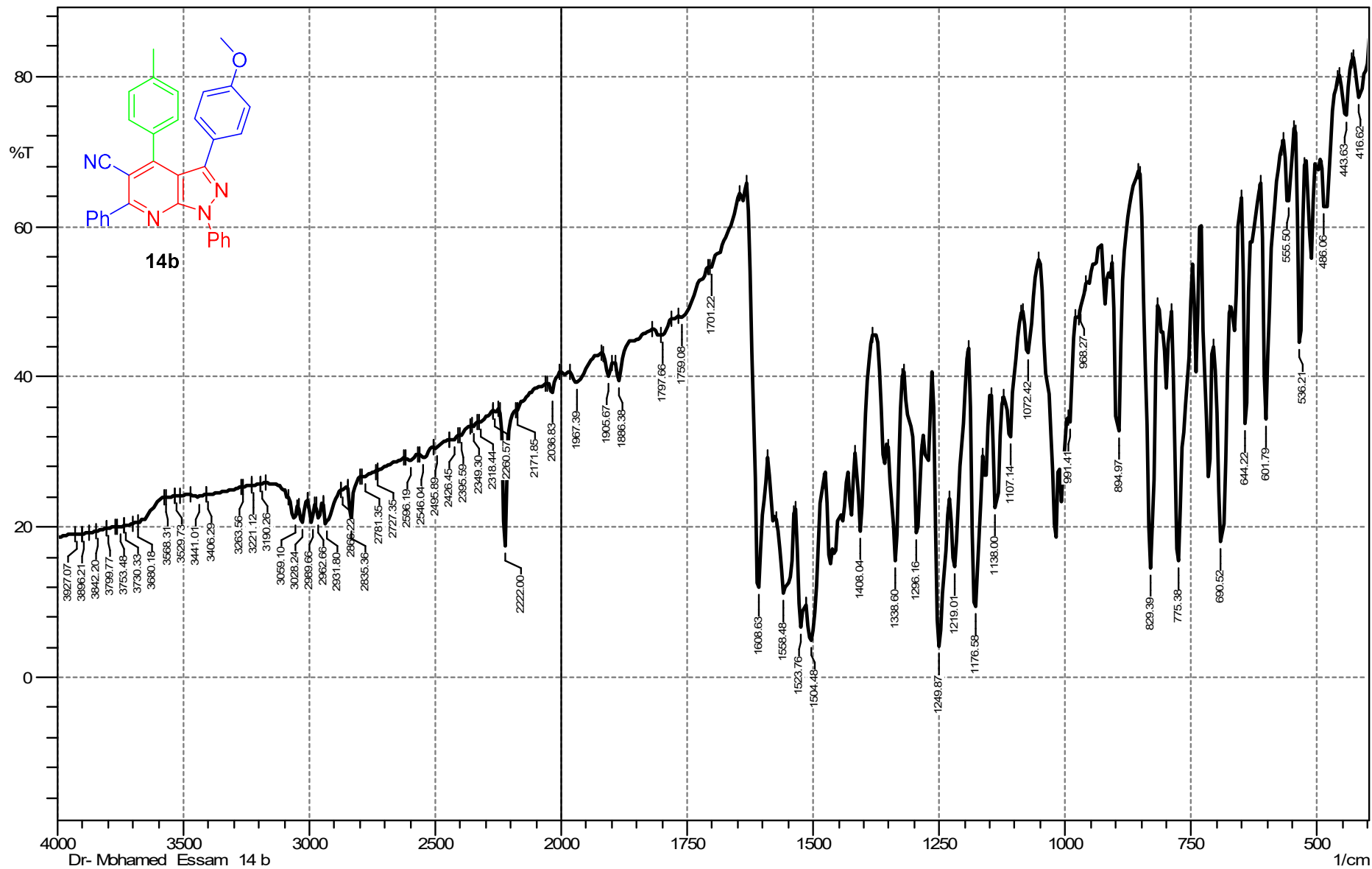


Figure S74. IR of compound 14b

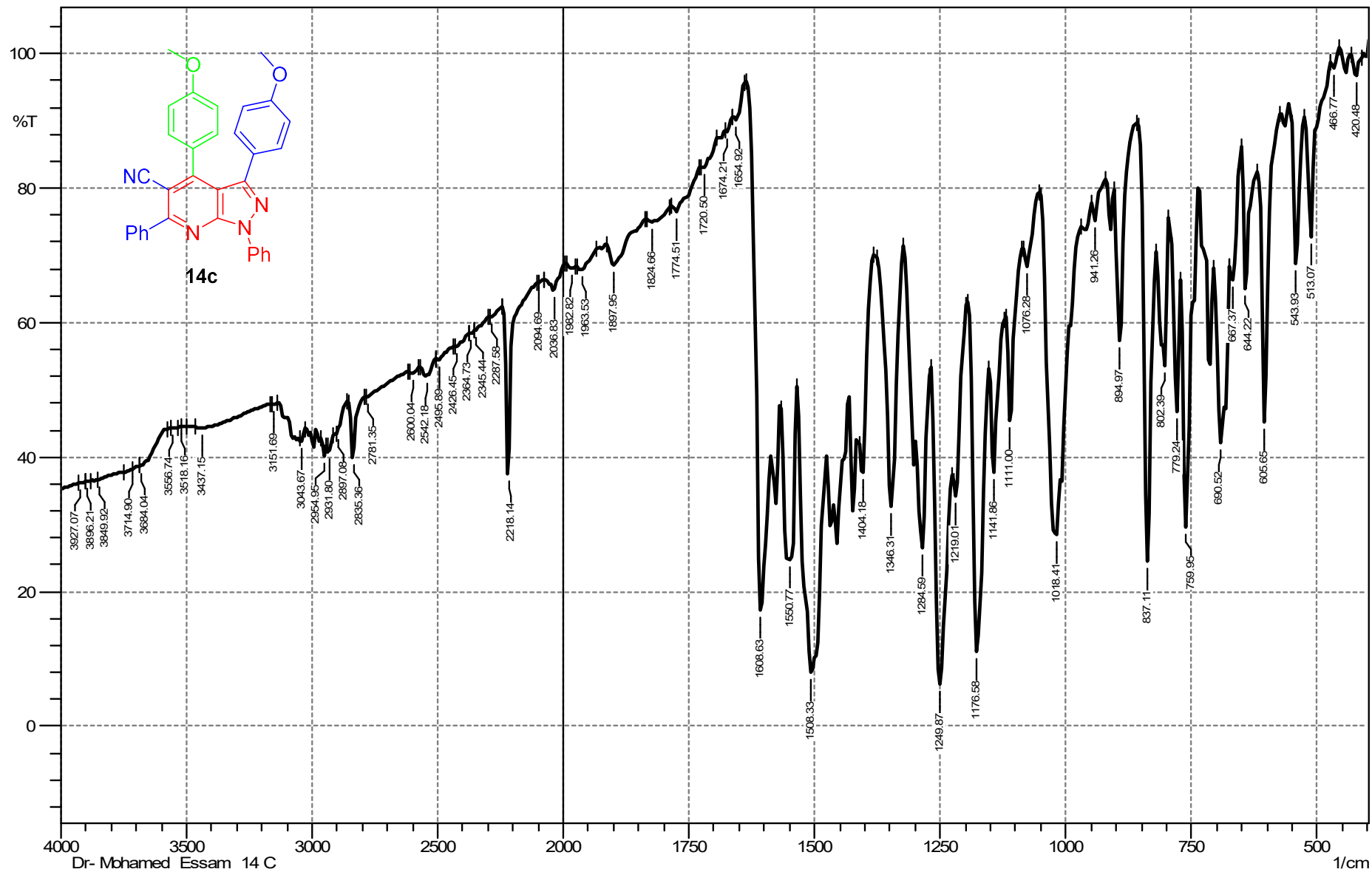


Figure S75. IR of compound 14c



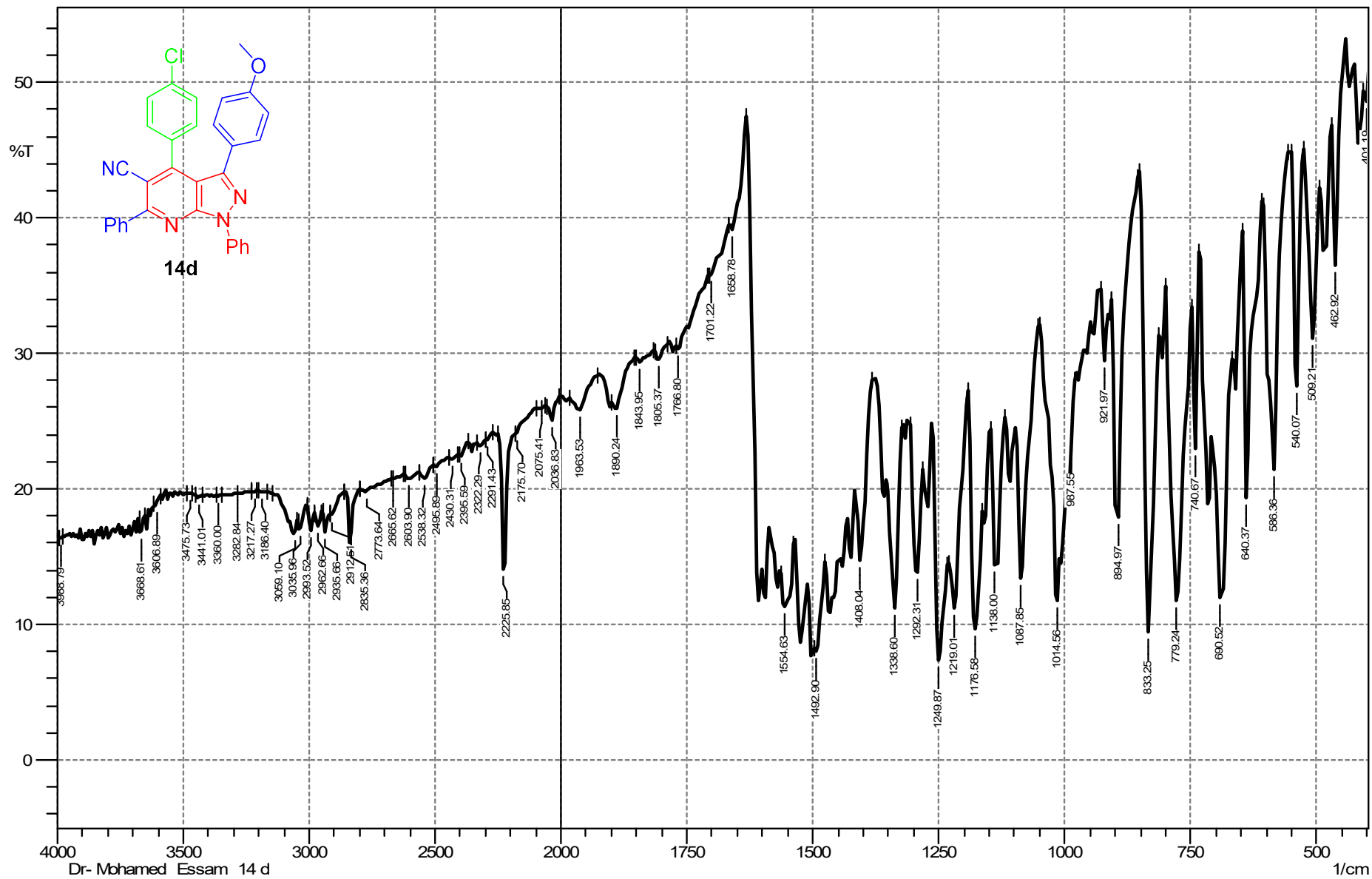


Figure S76. IR of compound **14d**

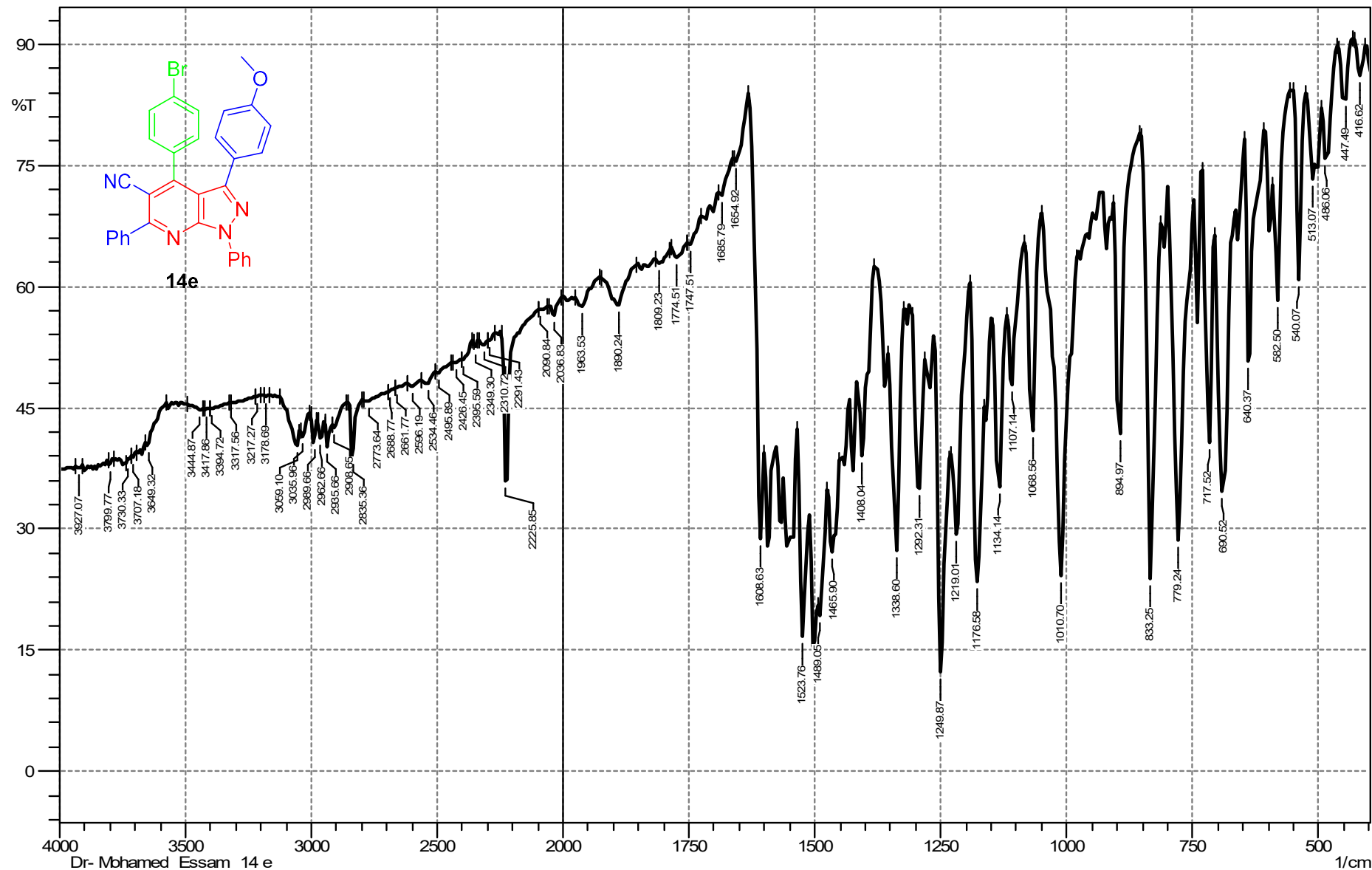


Figure S77. IR of compound 14e

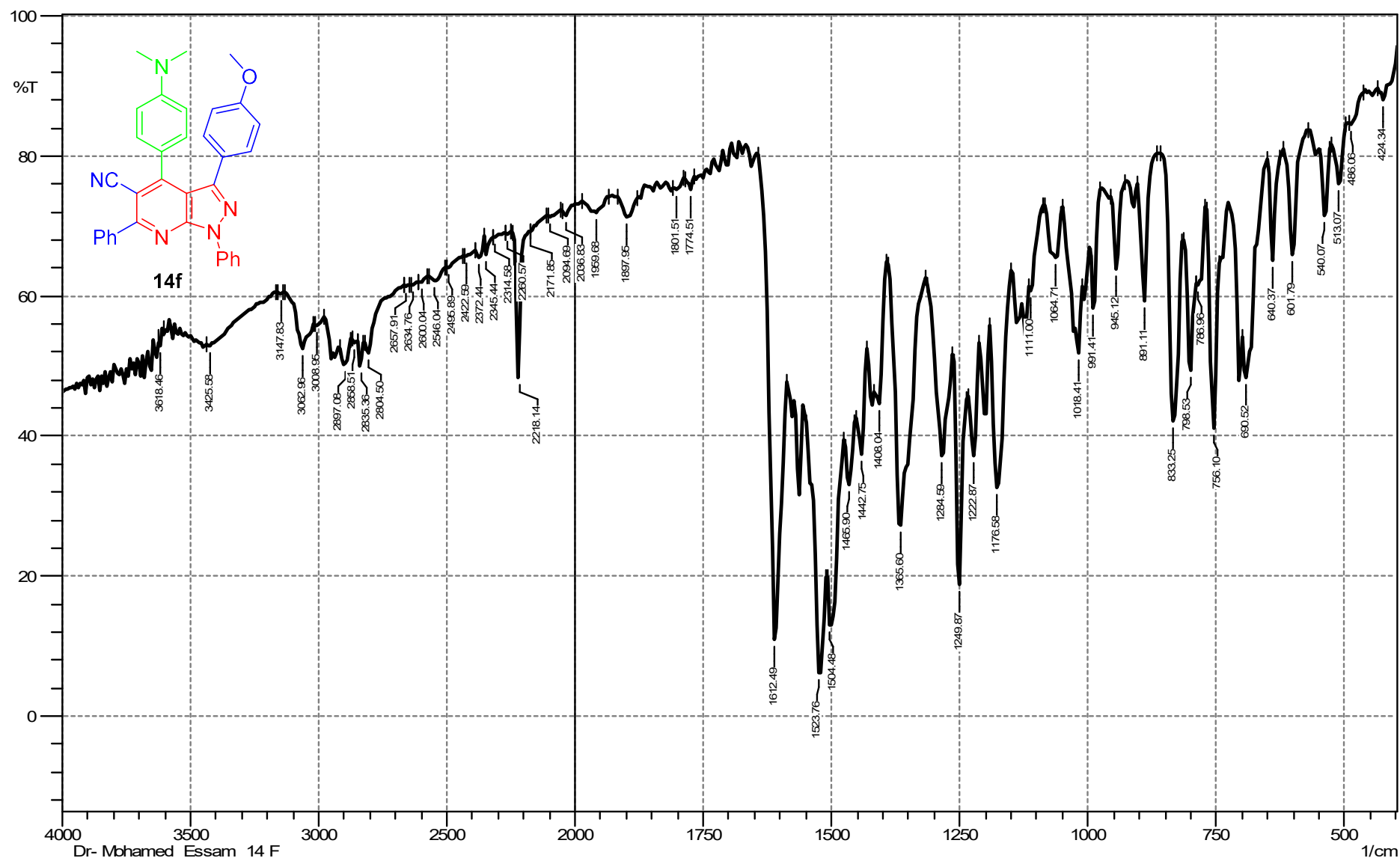


Figure S78. IR of compound **14f**

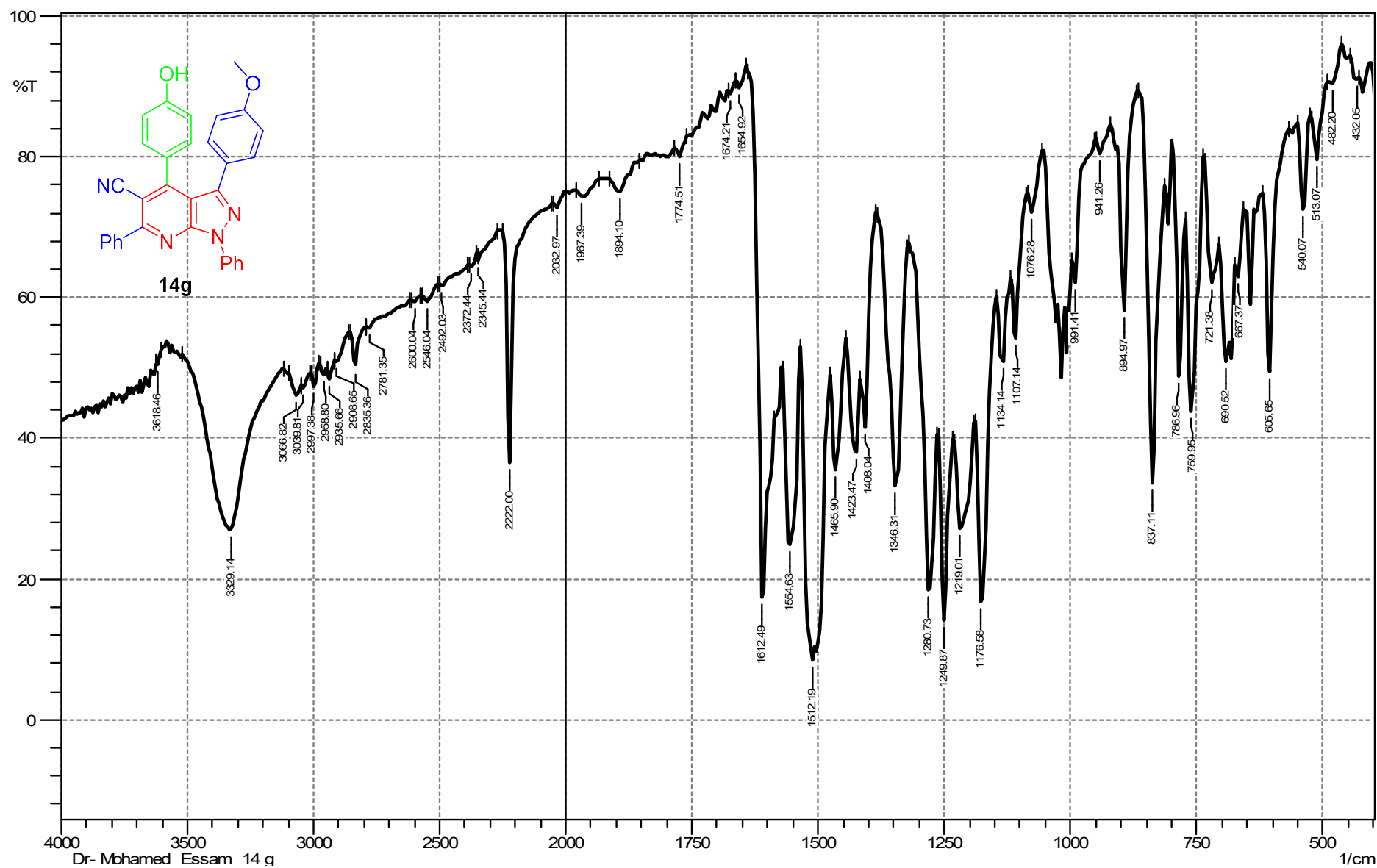


Figure S79. IR of compound **14g**

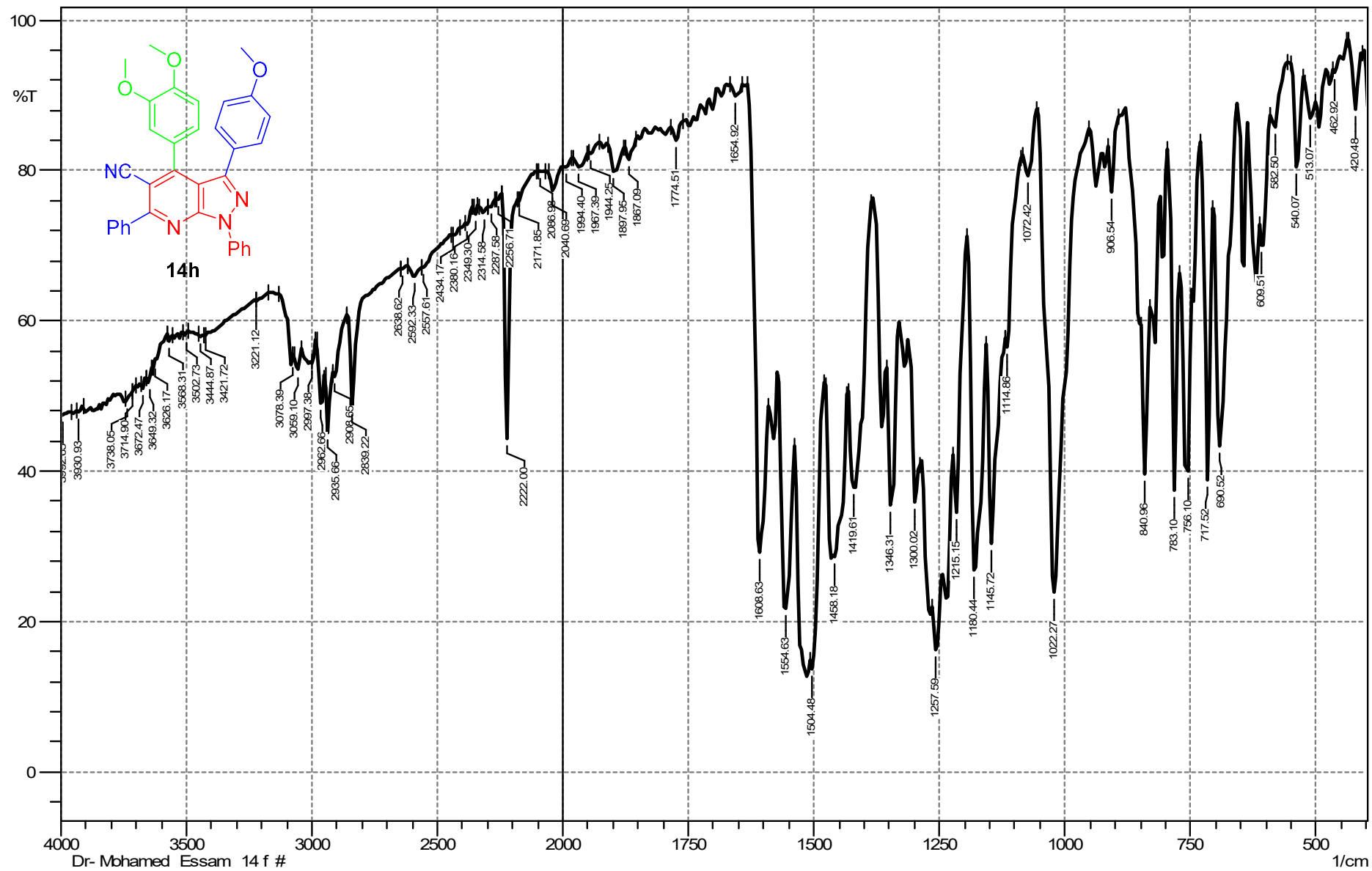


Figure S80. IR of compound 14h

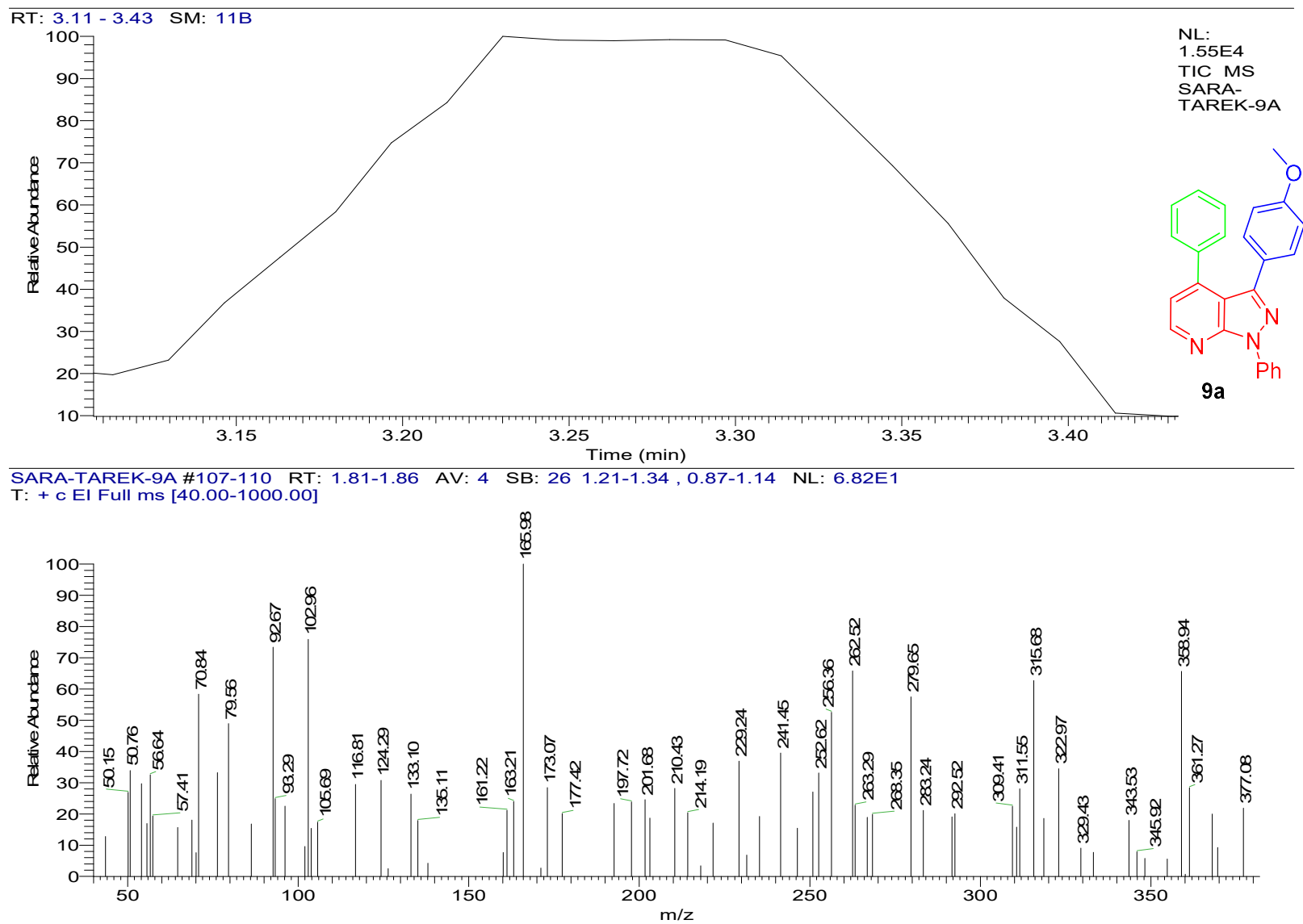


Figure S81. Mass of compound **9a**

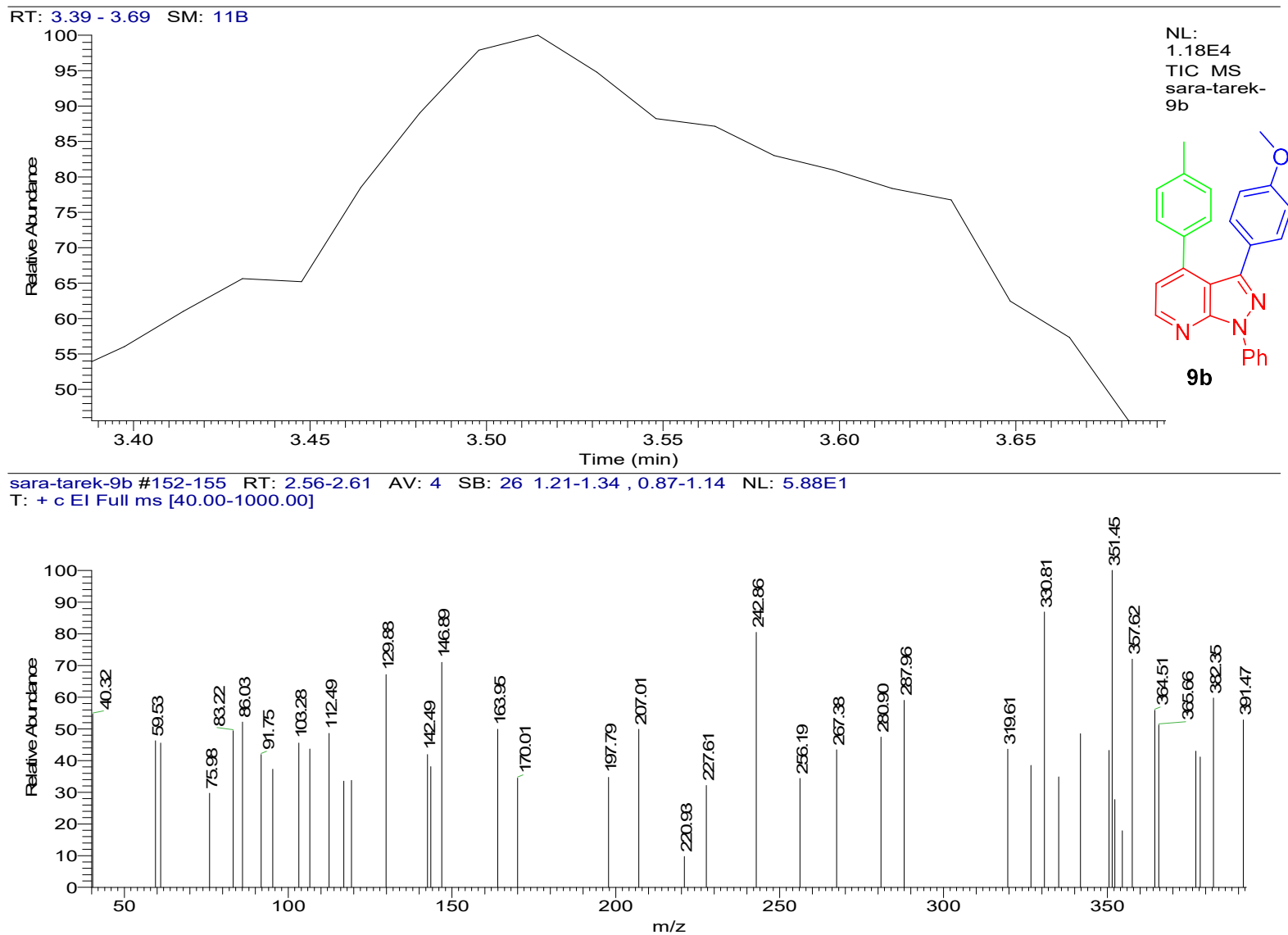


Figure S82. Mass of compound 9b

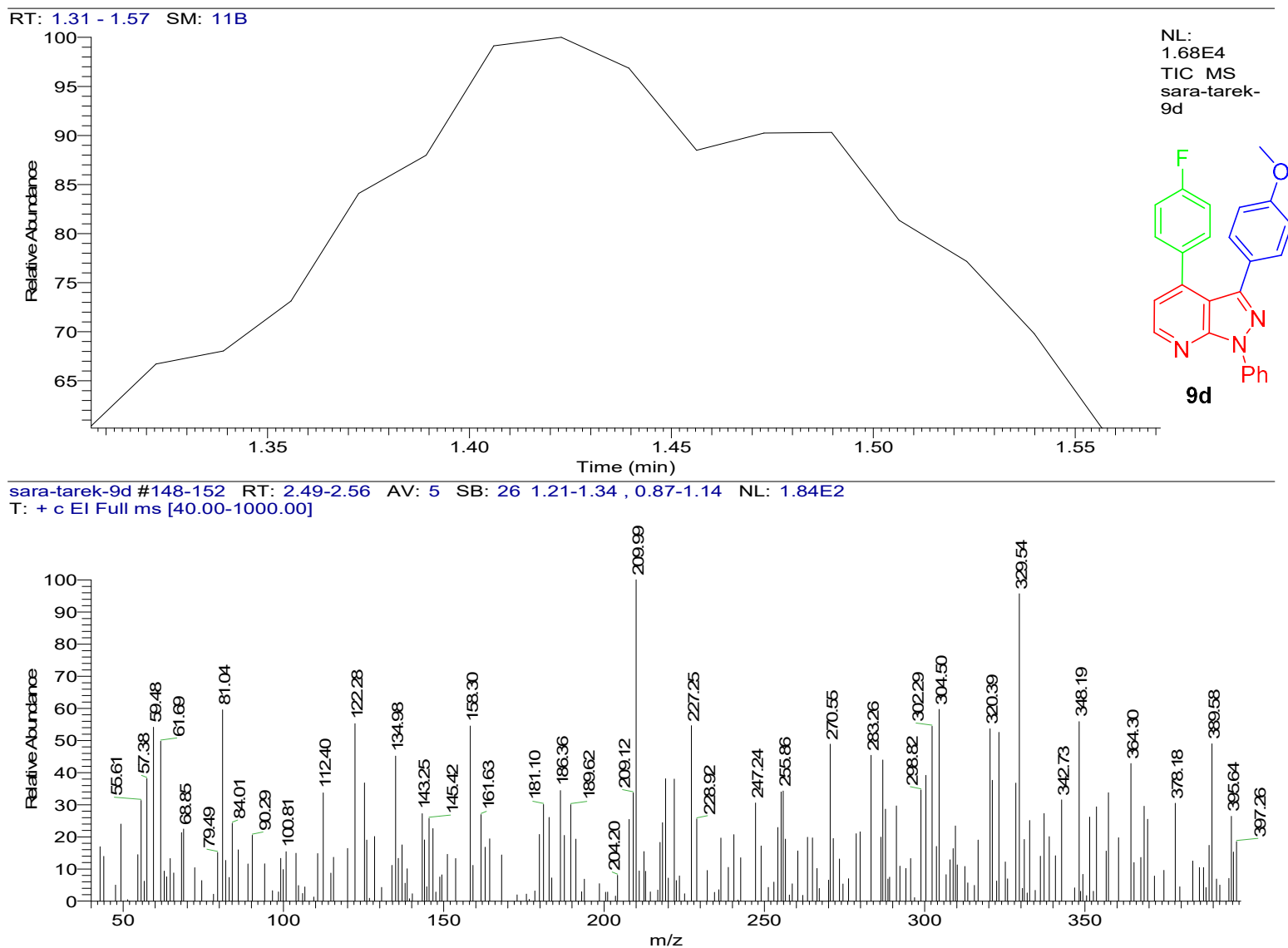


Figure S83. Mass of compound 9d



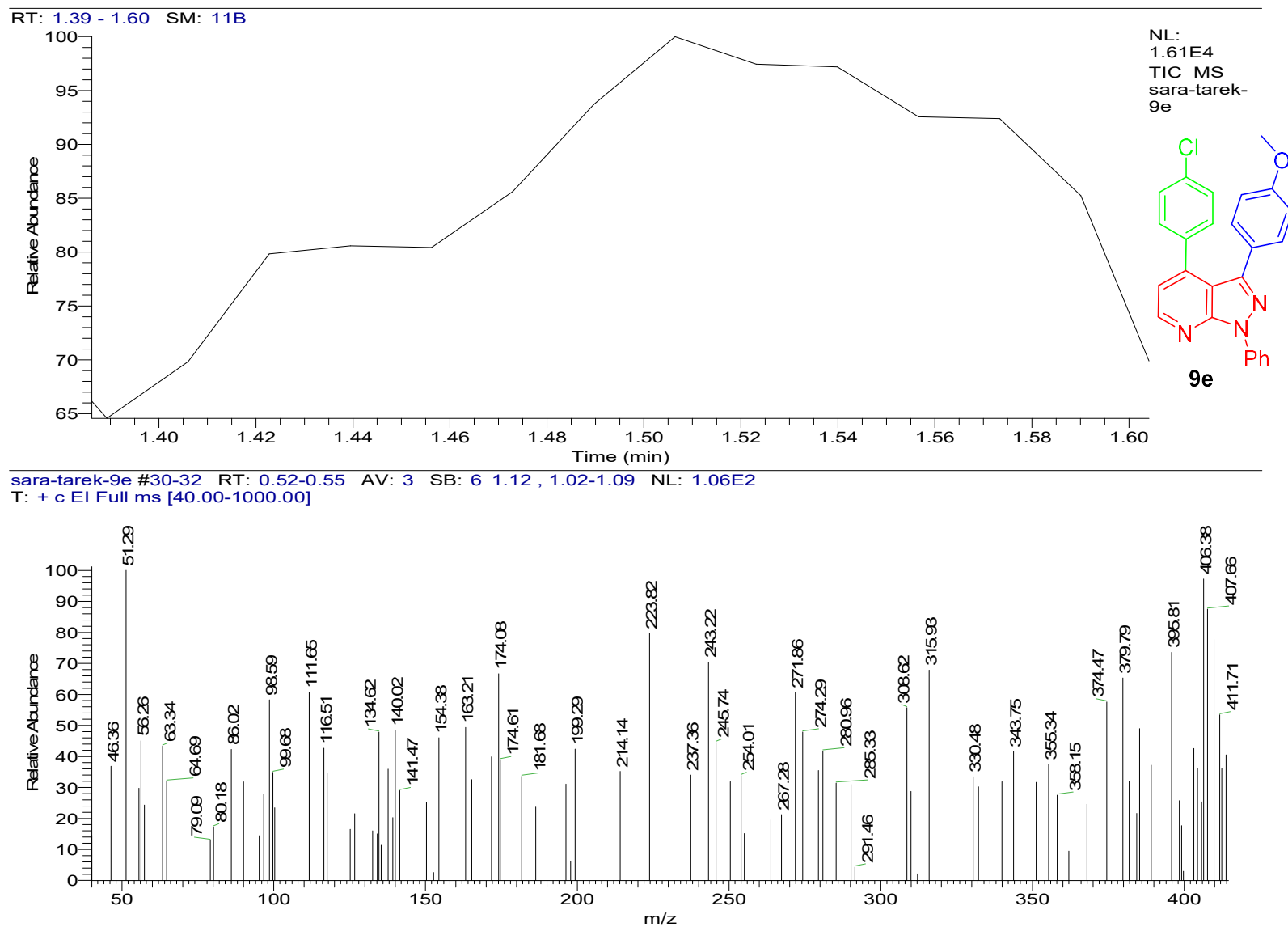


Figure S84. Mass of compound 9e

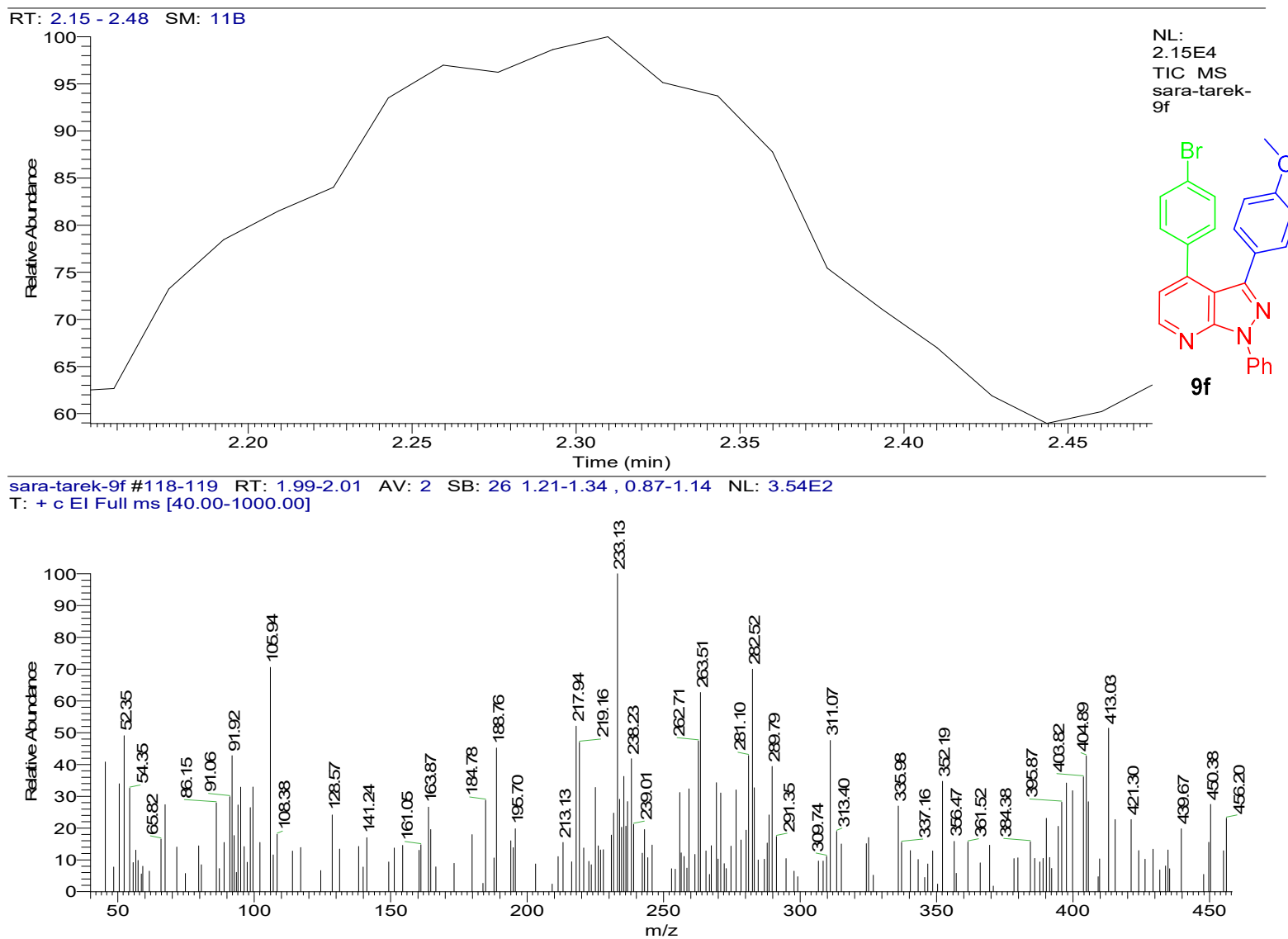


Figure S85. Mass of compound 9f

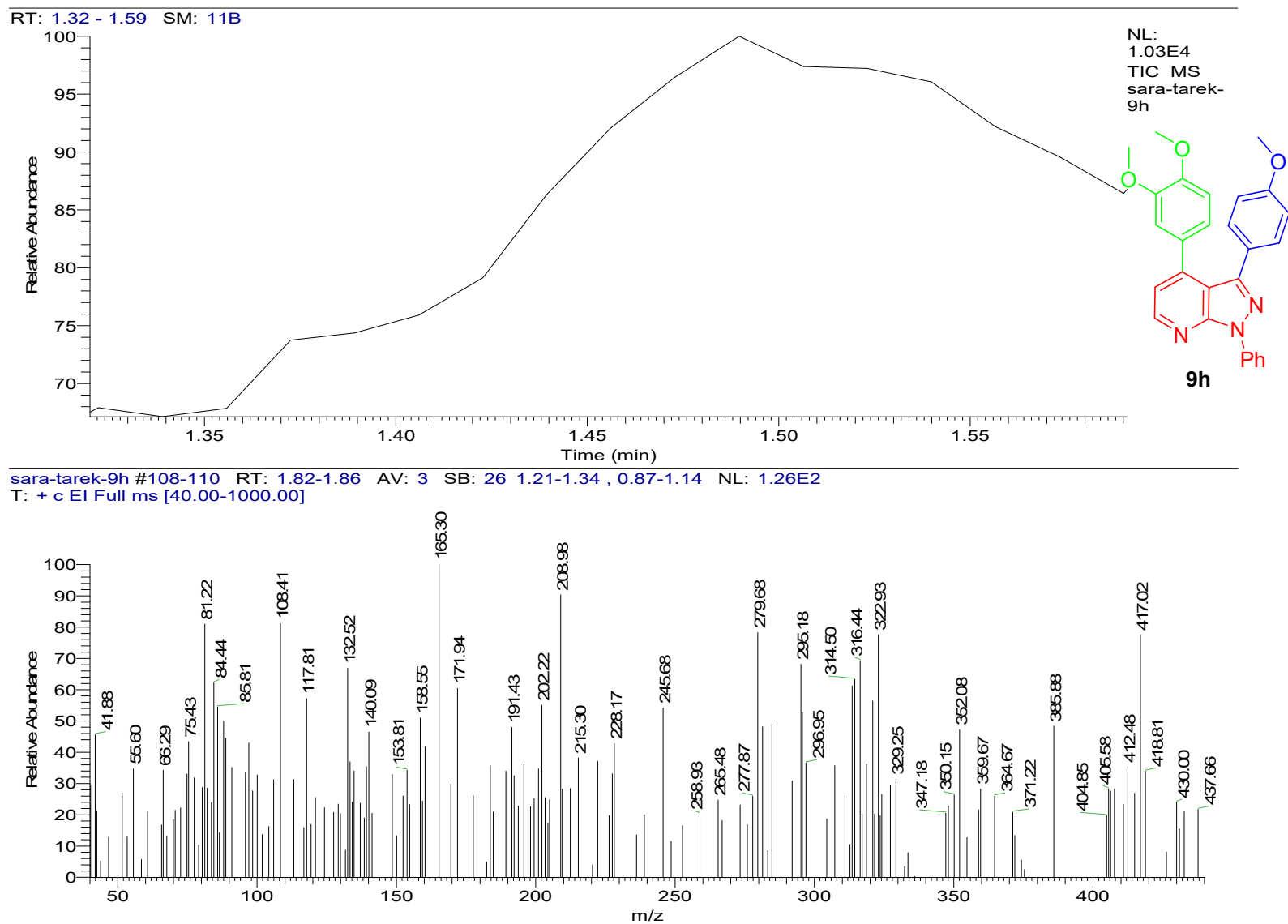
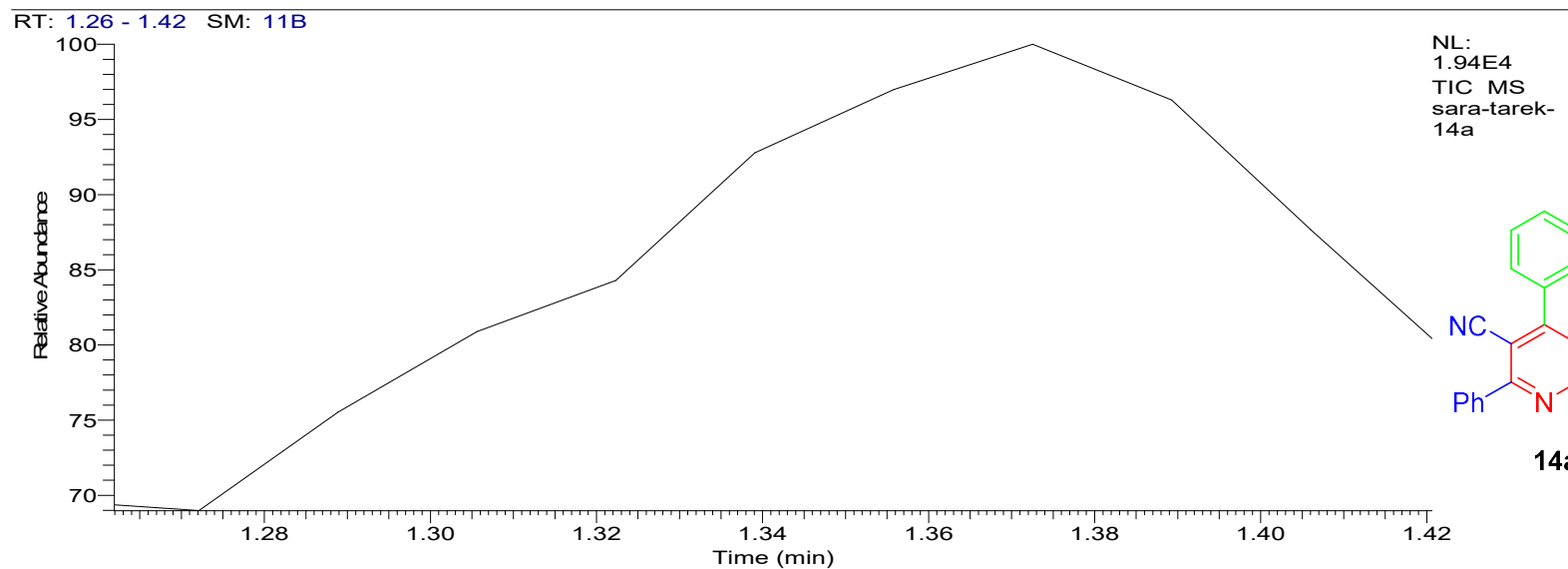


Figure S86. Mass of compound 9h



sara-tarek-14a #100-103 RT: 1.69-1.74 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.75E2  
T: + c EI Full ms [40.00-1000.00]

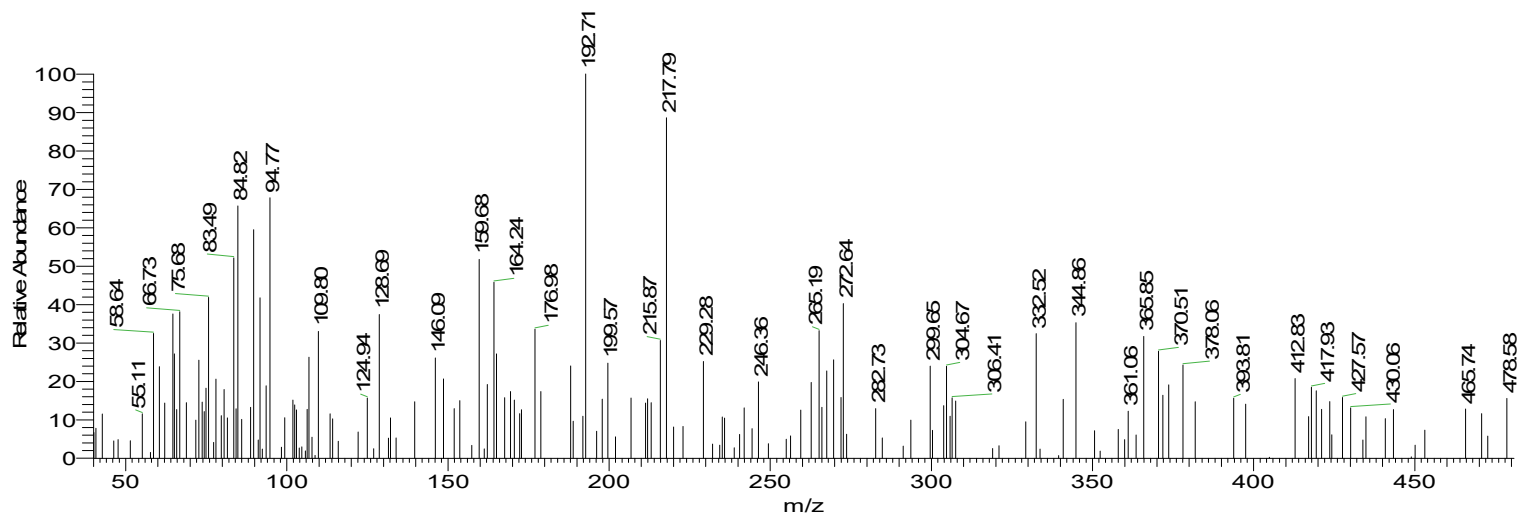


Figure S87. Mass of compound 14a

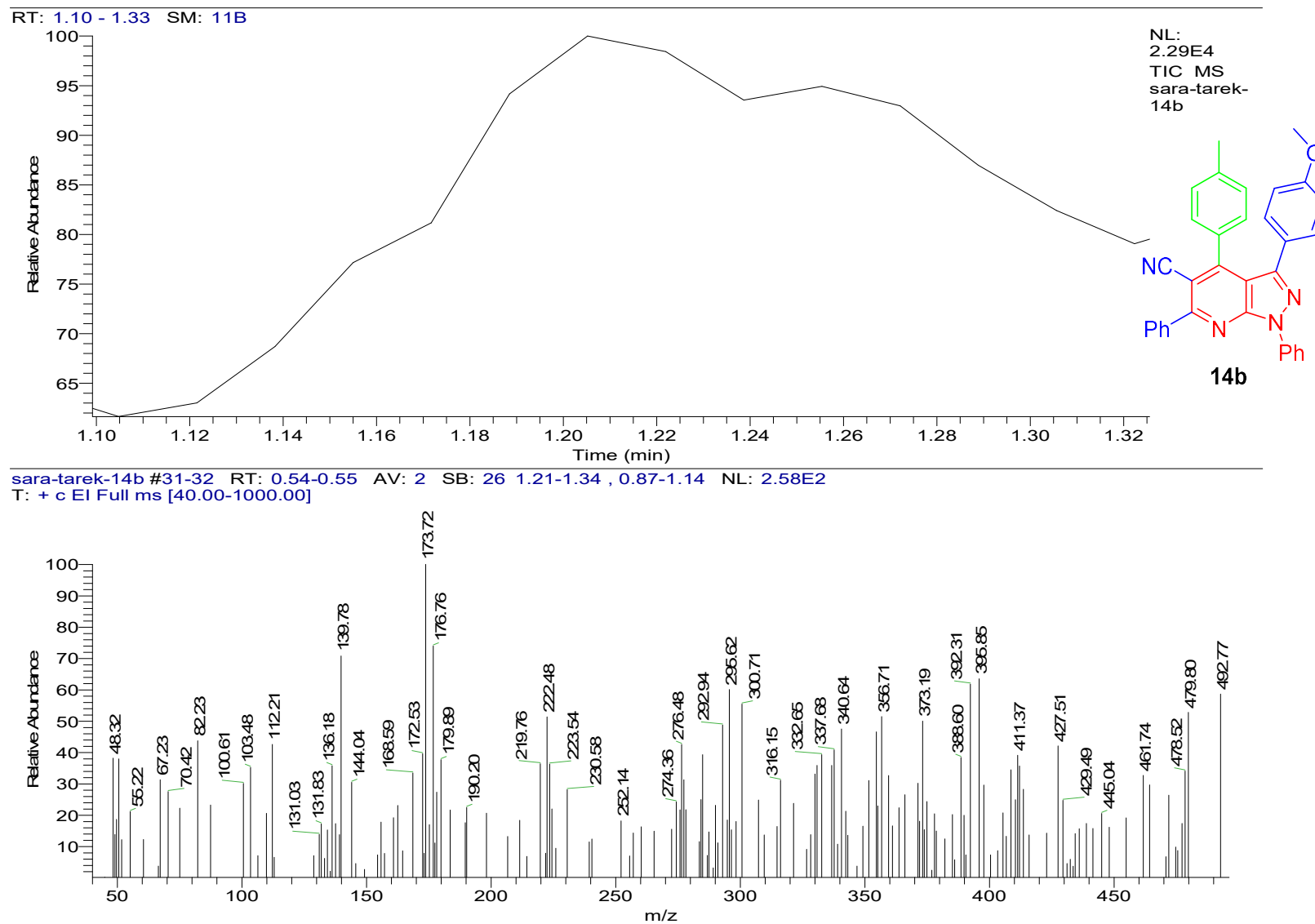


Figure S88. Mass of compound **14b**

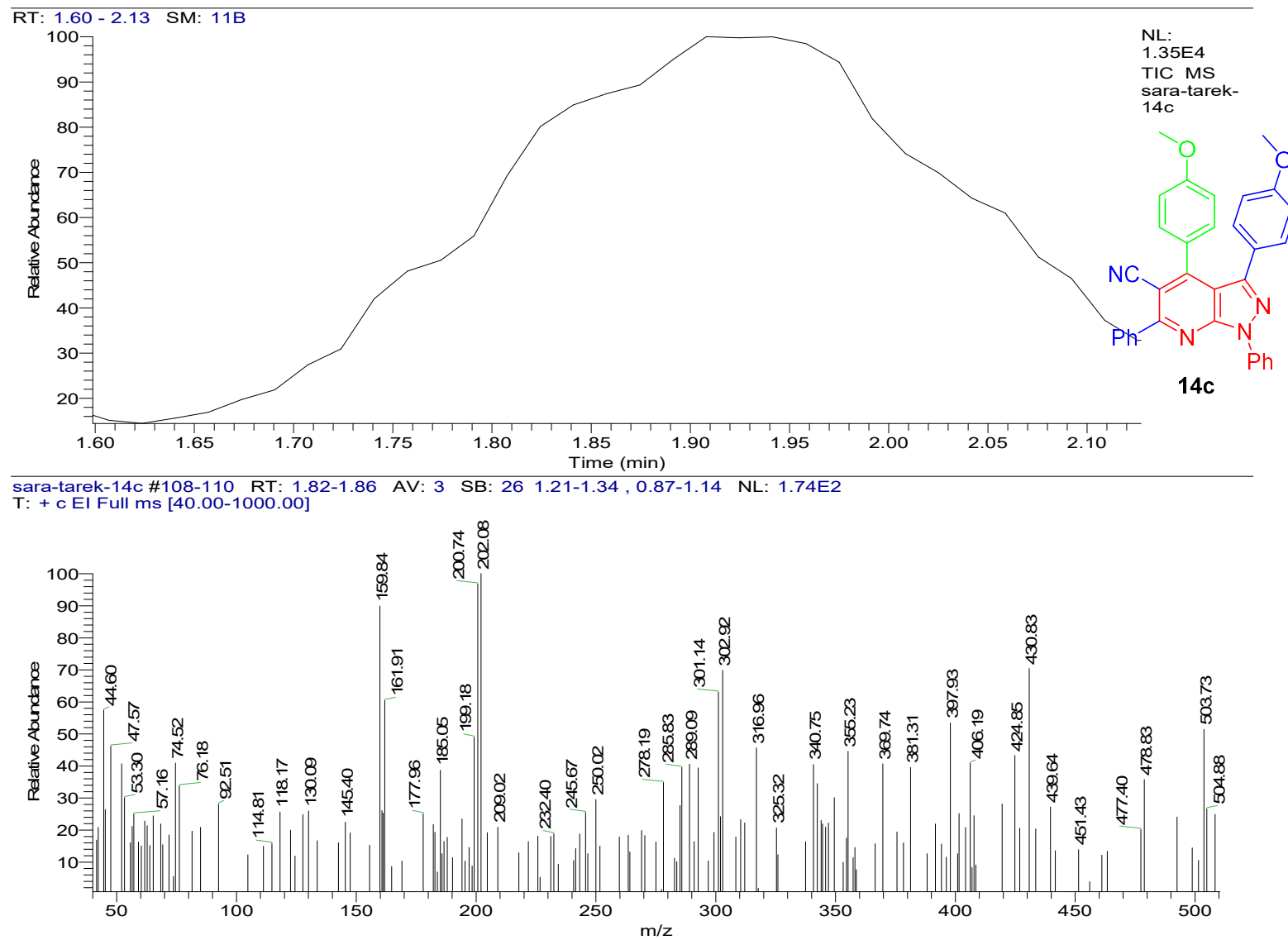


Figure S89. Mass of compound 14c

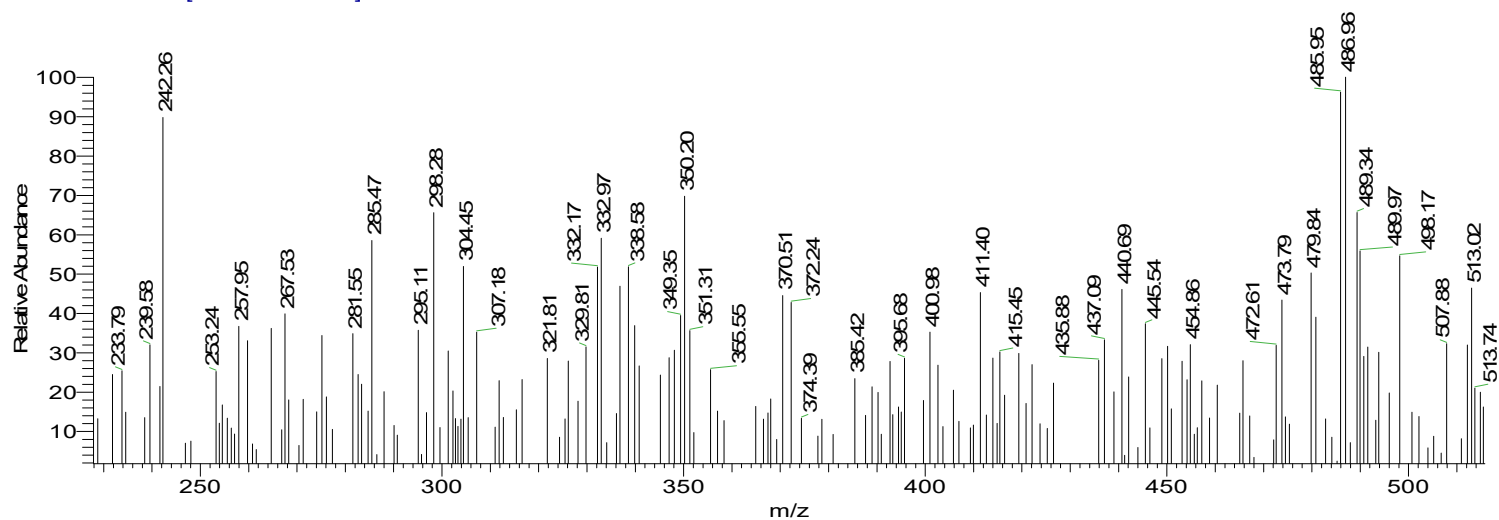
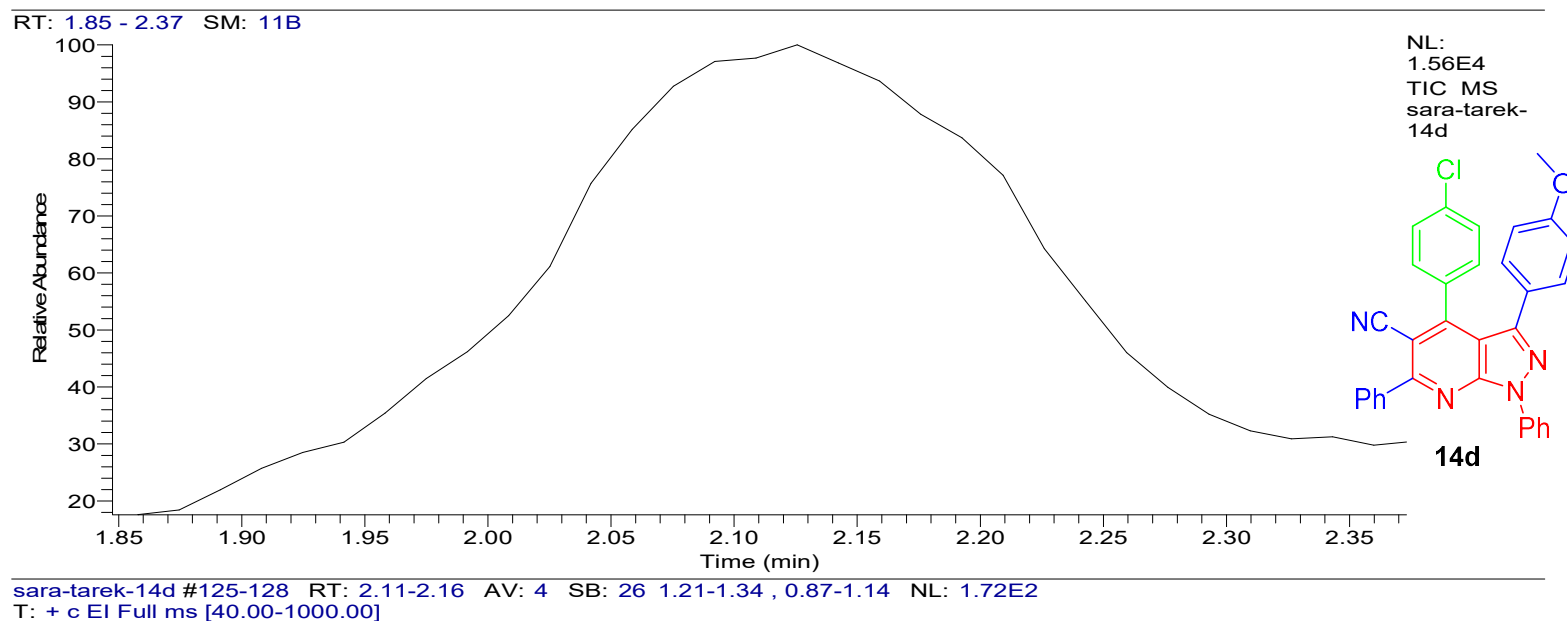


Figure S90. Mass of compound **14d**

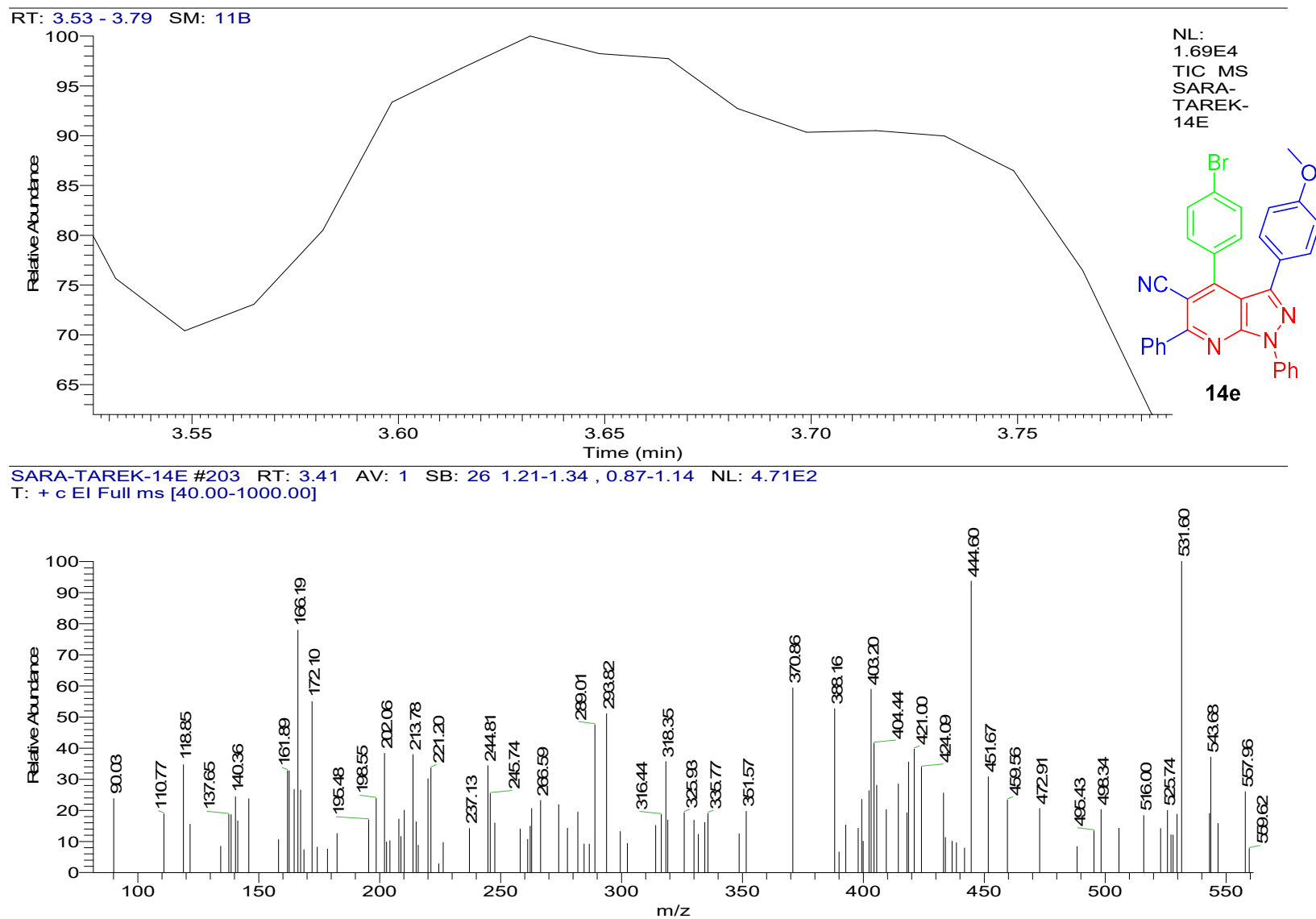


Figure S91. Mass of compound 14e



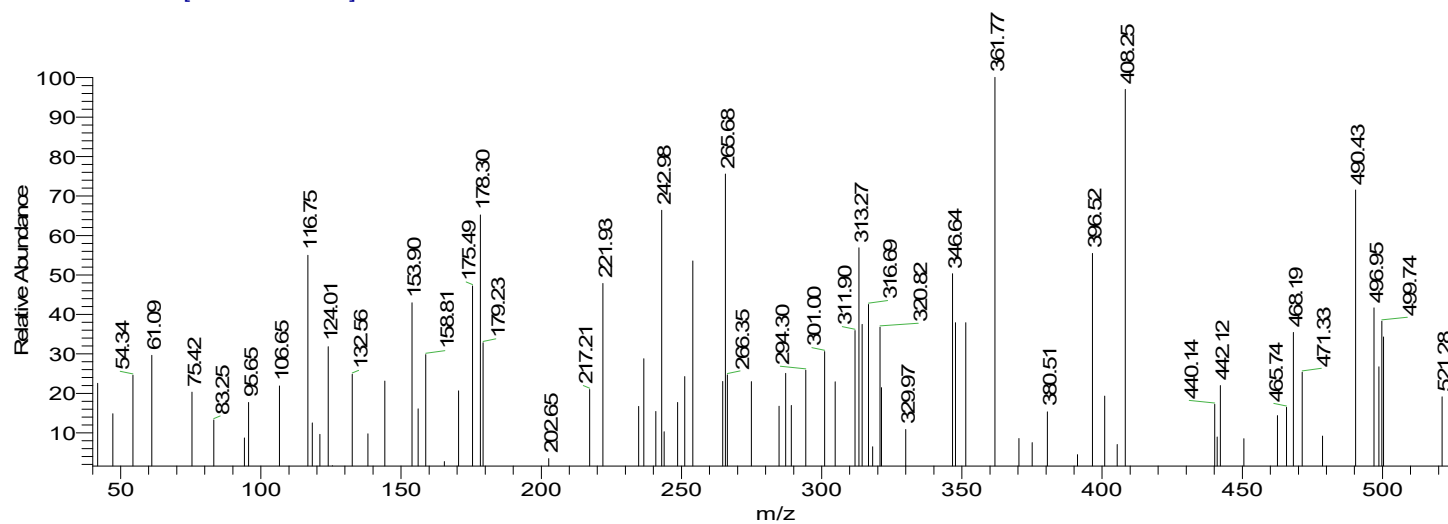
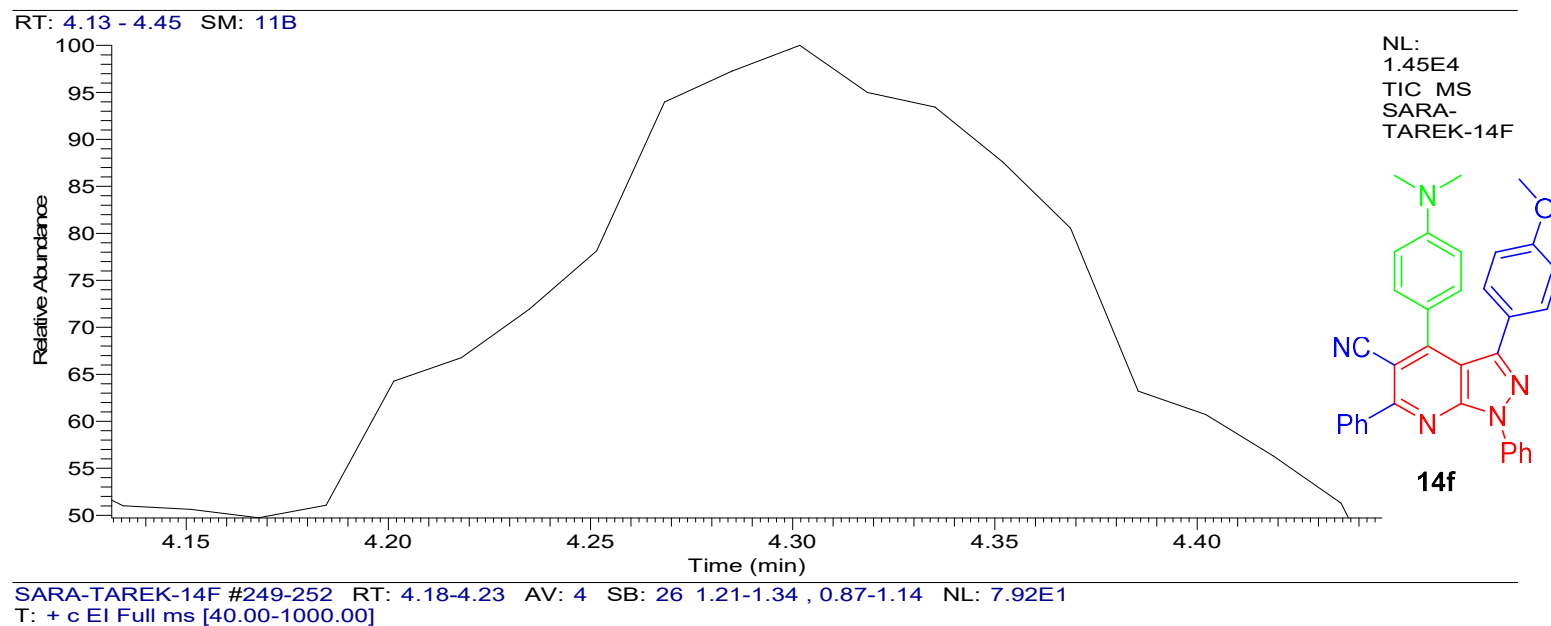


Figure S92. Mass of compound **14f**

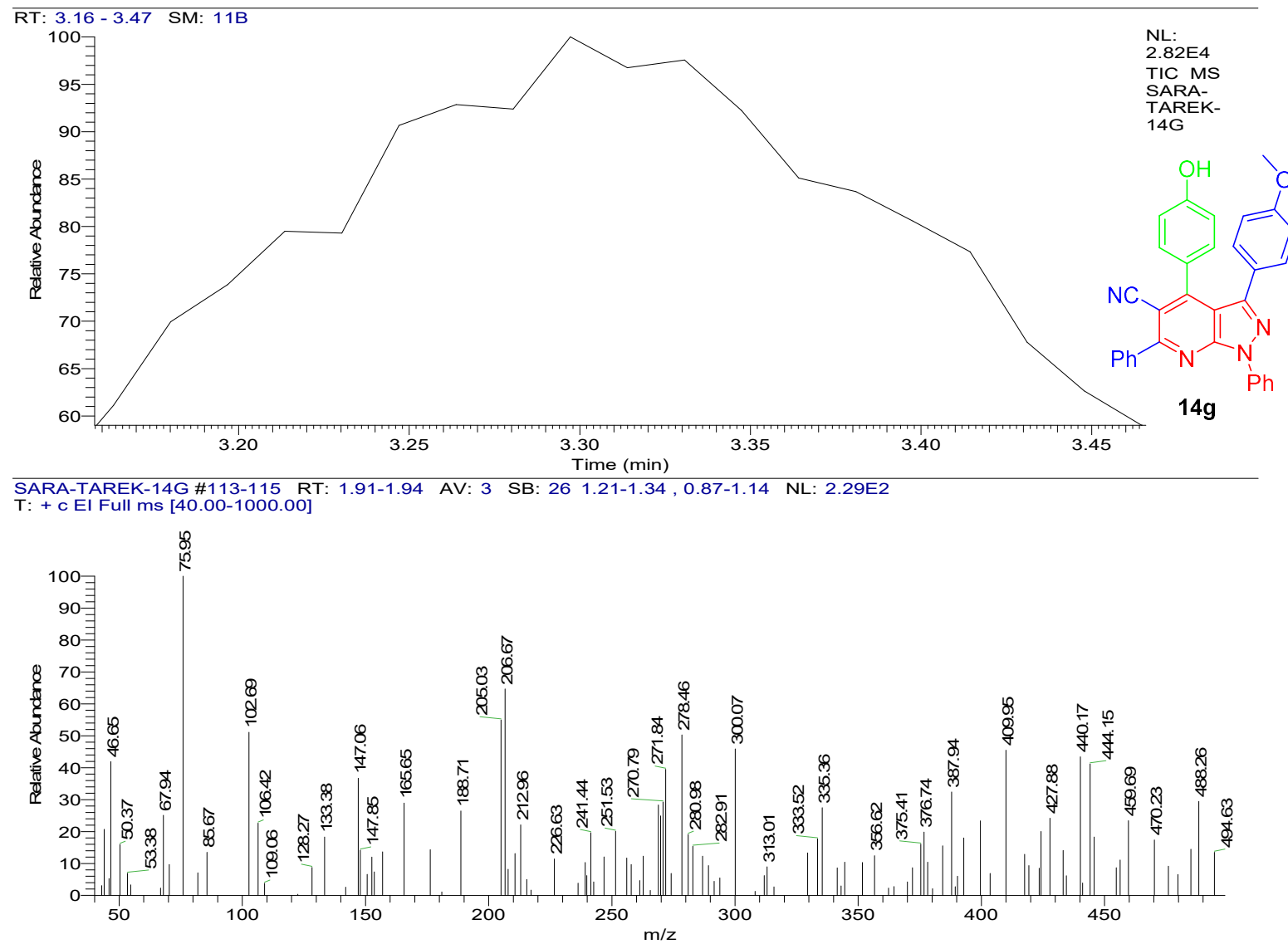


Figure S93. Mass of compound 14g

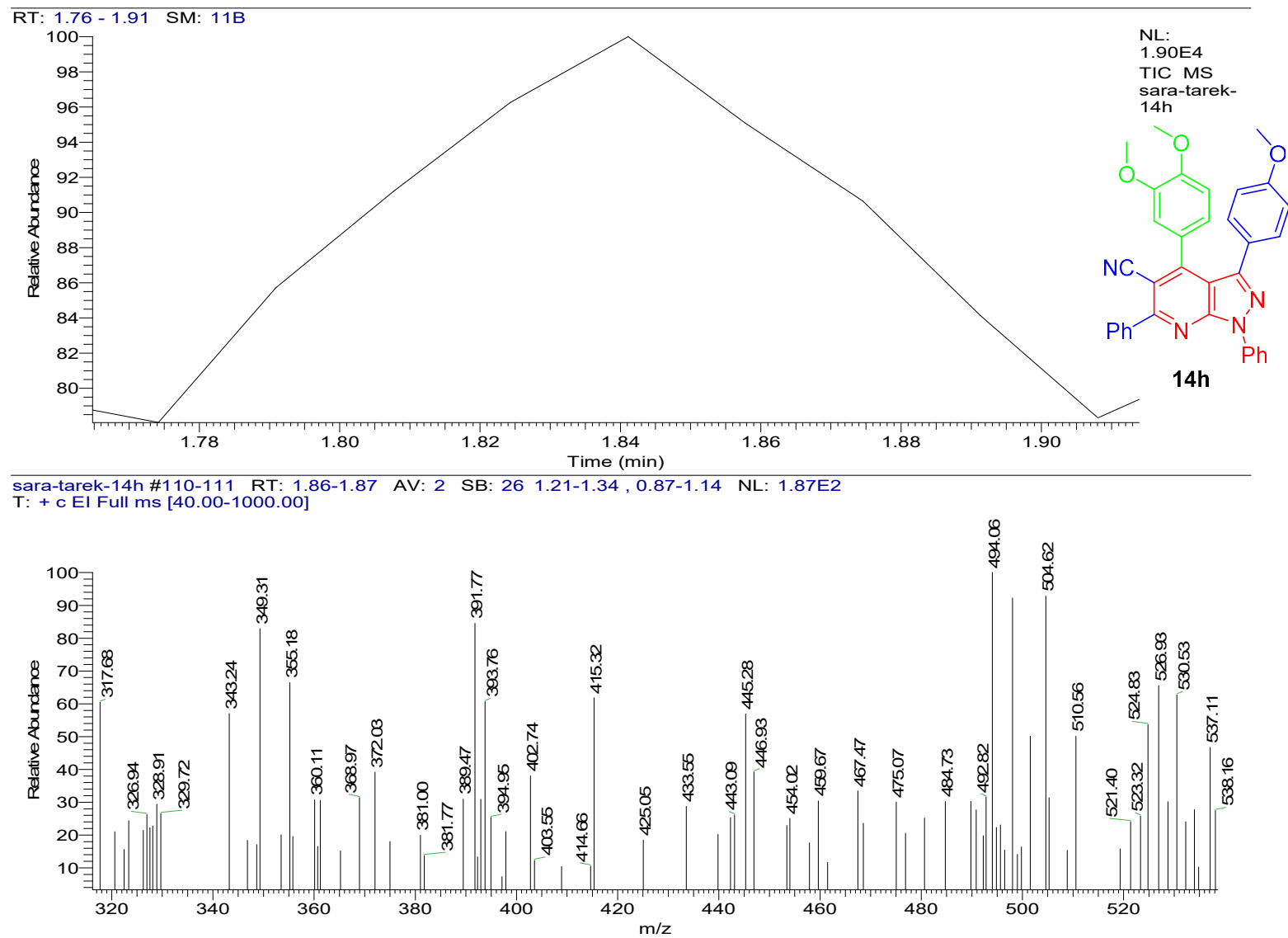


Figure S94. Mass of compound 14h

## **Characterization instruments**

# A Stuart melting point apparatus was used for detection the melting points ( $^{\circ}\text{C}$ , uncorrected).

# Bruker alpha 2 ATR/FTIR spectrometer recorded all the IR spectra (KBr).

# BRUKER 400 MHz NMR spectrometers recorded the NMR spectra.

Chemical shifts were recorded in parts per million ( $\delta$ ), and the coupling constants (J) were stated in Hertz.

TMS was used as the internal standard.  $^1\text{H}$  and  $^{13}\text{C}$  spectra were run at 400 and 100 MHz, respectively.

DMSO- $d_6$  is used as solvent and  $\text{D}_2\text{O}$  is used to predict the exchangeable protons.

# Electron impact mass spectra were measured on Direct probe controller inlet part to single quadropole mass analyzer in THERMO SCIENTIFIC GCMS model (ISQ LT) using THERMO X-CALIBUR SOFTWARE.