

Antibiofilm and anti-quorum sensing activities of novel pyrazole and pyrazolo[1,5-*a*]pyrimidine derivatives as carbonic anhydrase I and II inhibitors: Design, synthesis, radio-sterilization, and molecular docking studies

Ahmed Ragab^{1,*}, Sawsan A. Fouad², Yousry A. Ammar¹, Dina S. Aboul-Magd³, and Moustafa S. Abusaif^{1,*}

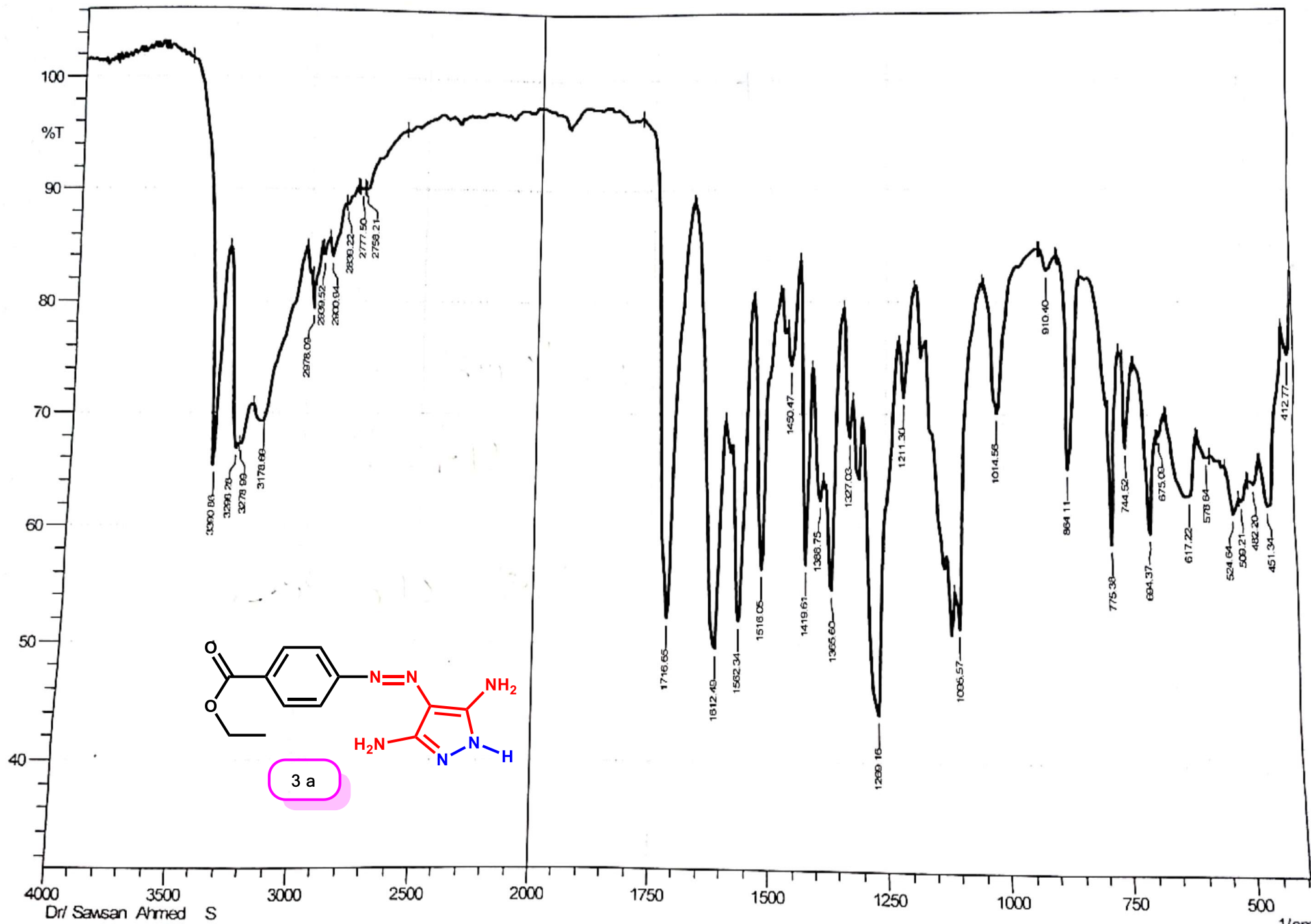
¹ Department of Chemistry, Faculty of Science (Boys), Al-Azhar University, Nasr City, 11884, Cairo, Egypt

² Department of Chemistry, Faculty of Science (Girls), Al-Azhar University, Nasr City, Cairo, Egypt

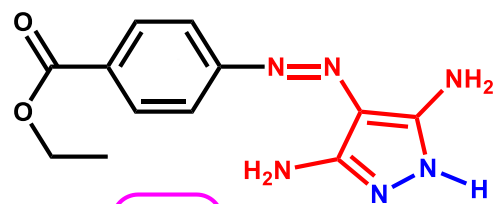
³ Drug Radiation Research Department, National Center for Radiation Research and Technology (NCRRT), Egyptian Atomic Energy Authority, Egypt

***Correspondence:** Ahmed Ragab E-mail: ahmed_ragab7@ymail.com; ahmed_ragab@azhar.edu.eg Tel.: (0201009341359) and

Yousry A. Ammar (yossry@yahoo.com)



HNMR- DMSO- 3a



3 a

0.81

2.33

2.00

2.03

1.96

2.09

3.00

10.65

7.92

7.90

7.61

7.60

6.43

5.95

4.28

4.26

4.25

4.24

3.33

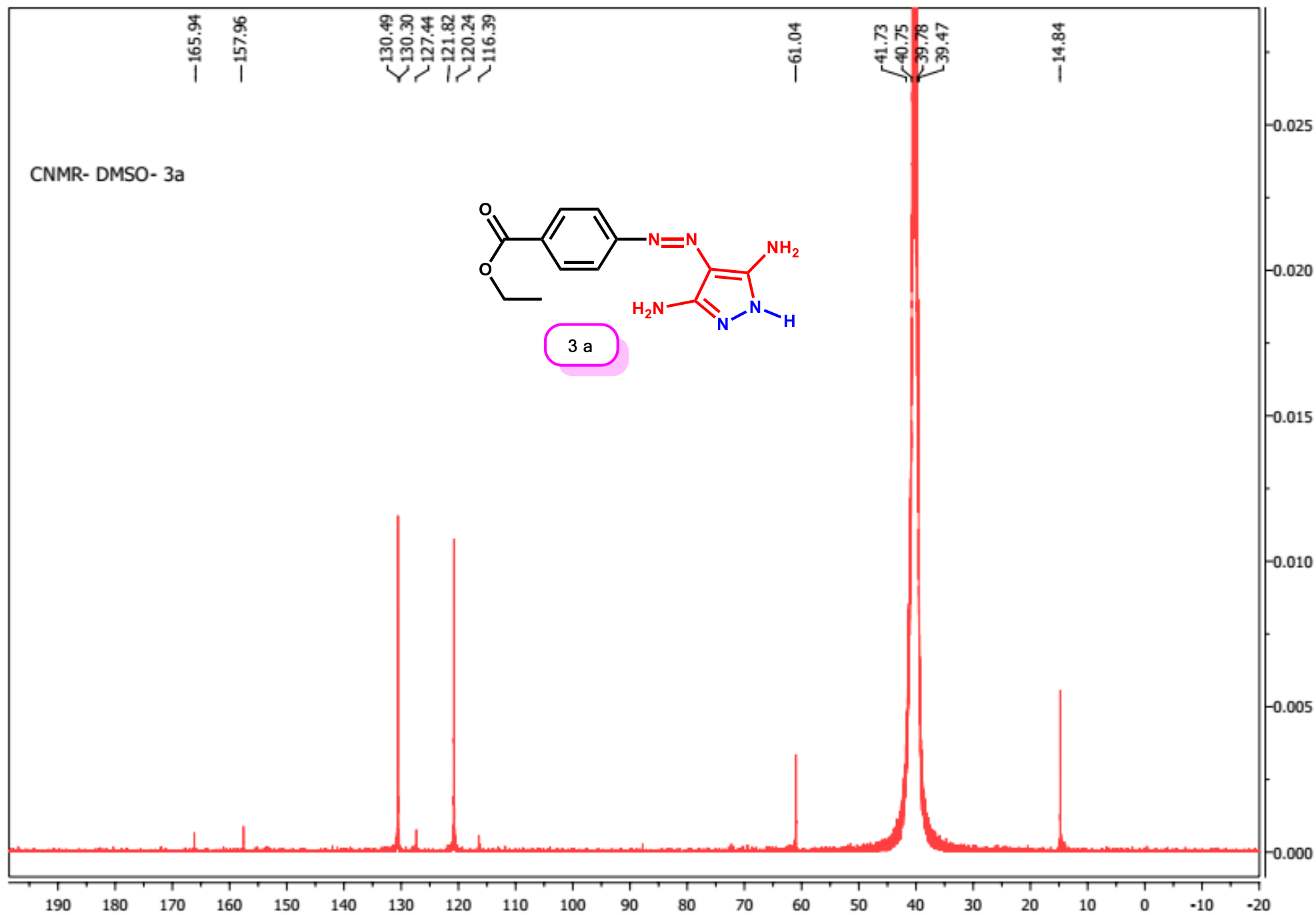
2.47

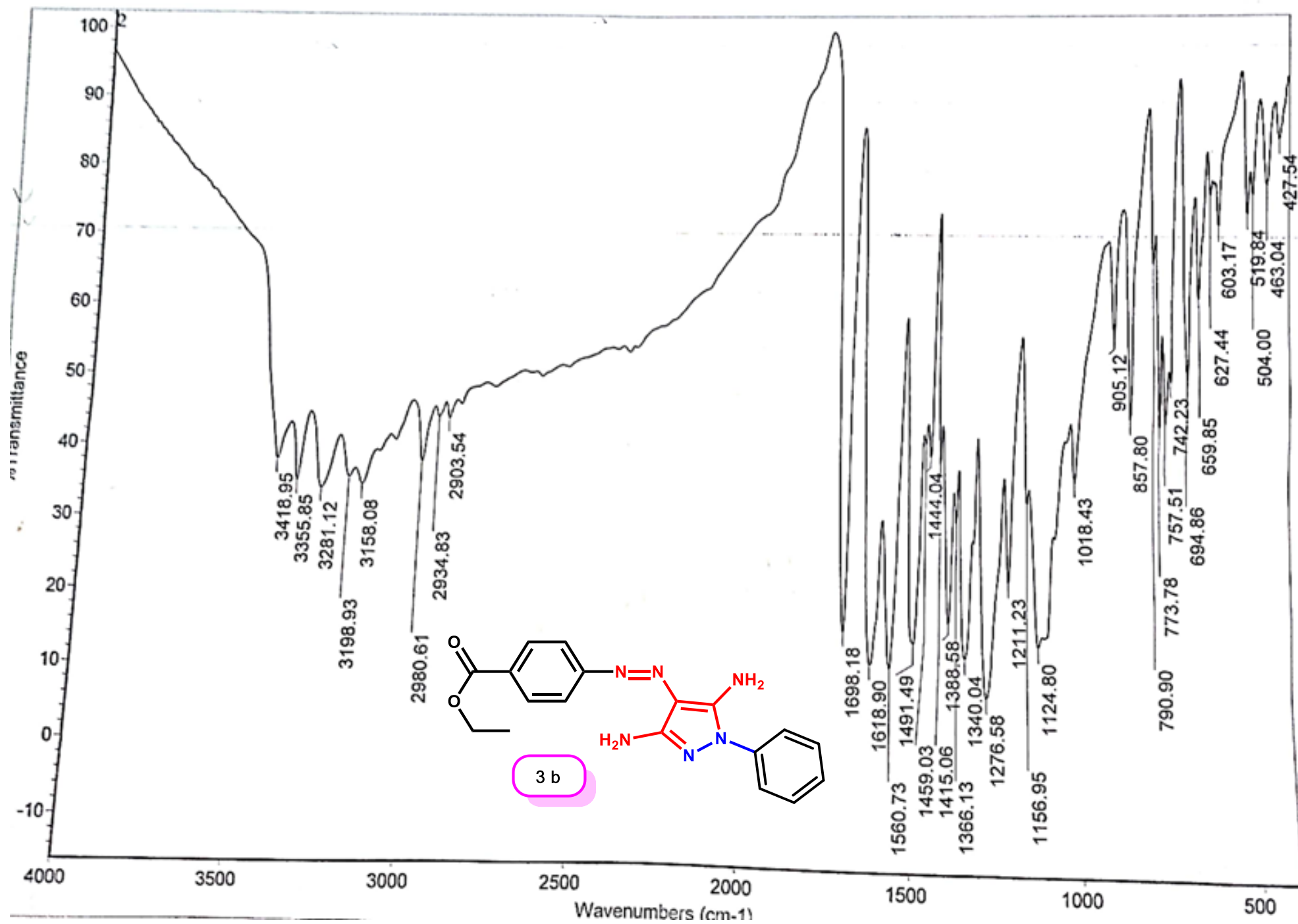
1.29

1.28

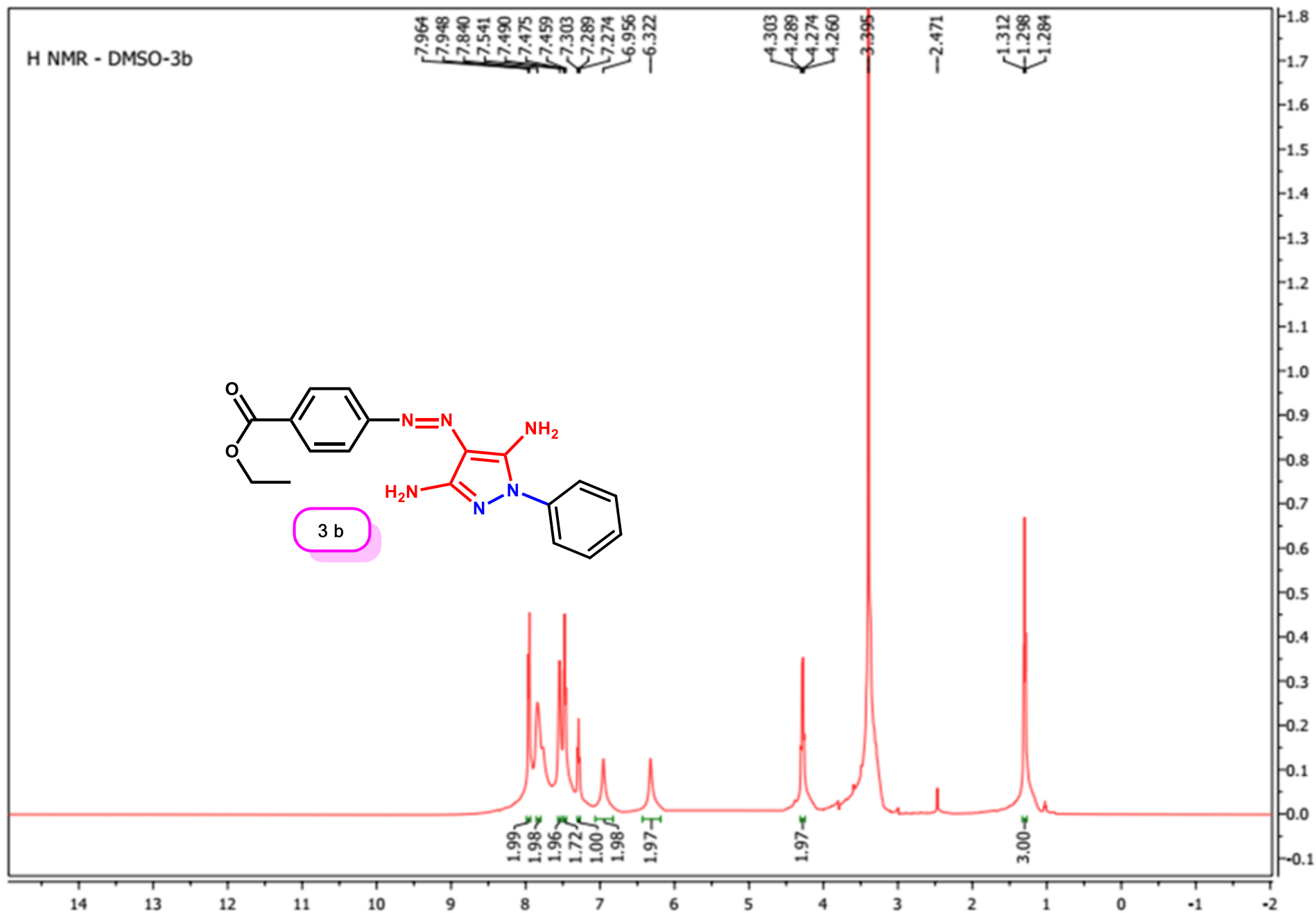
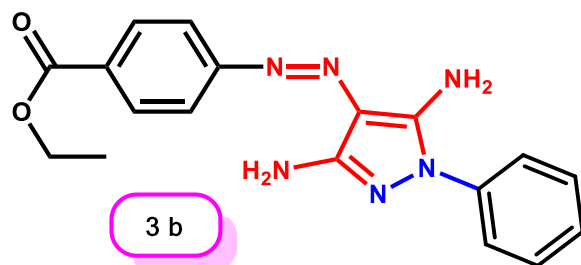
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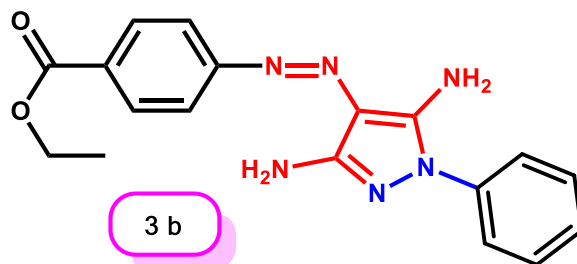
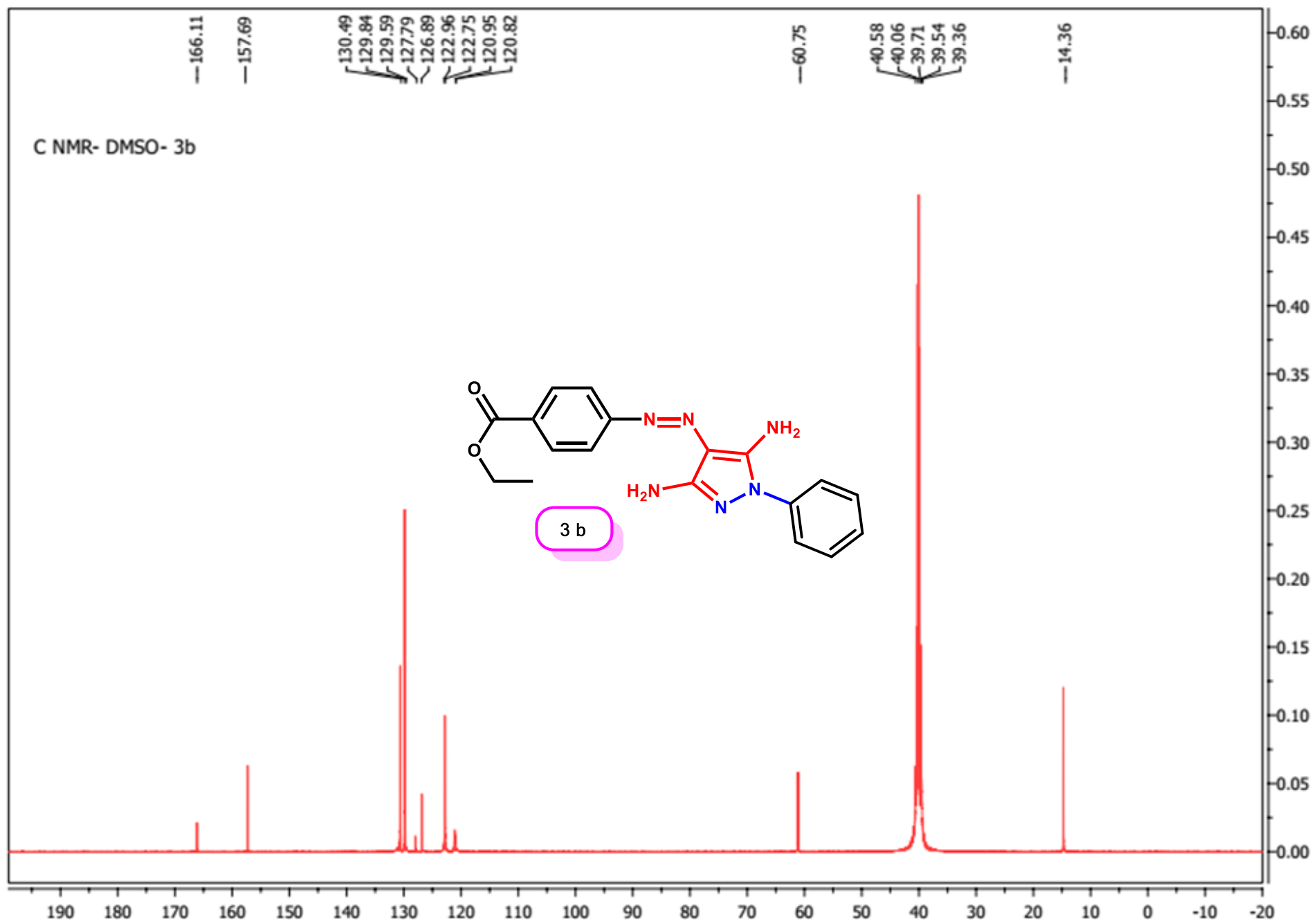
f1 (ppm)

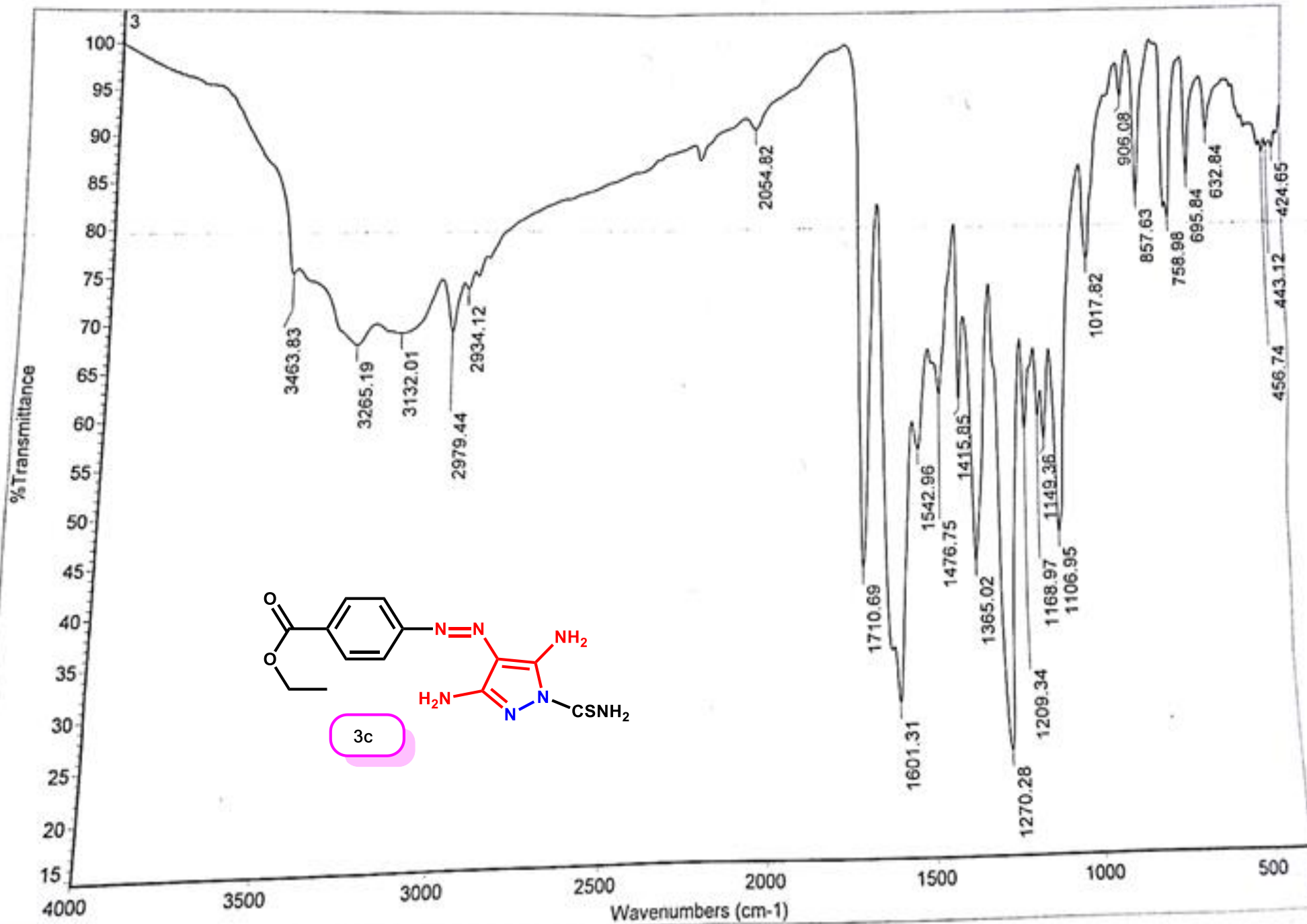


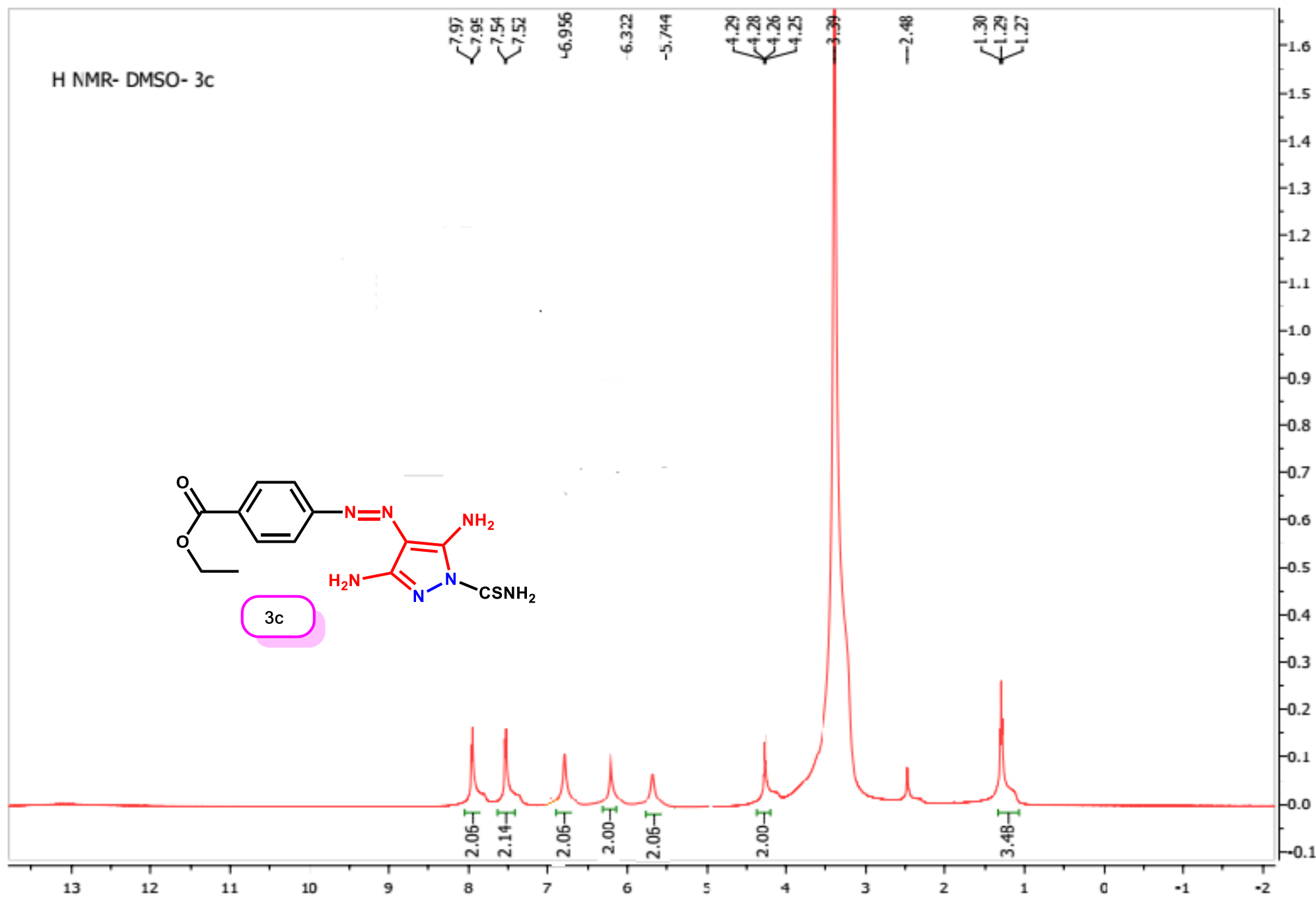


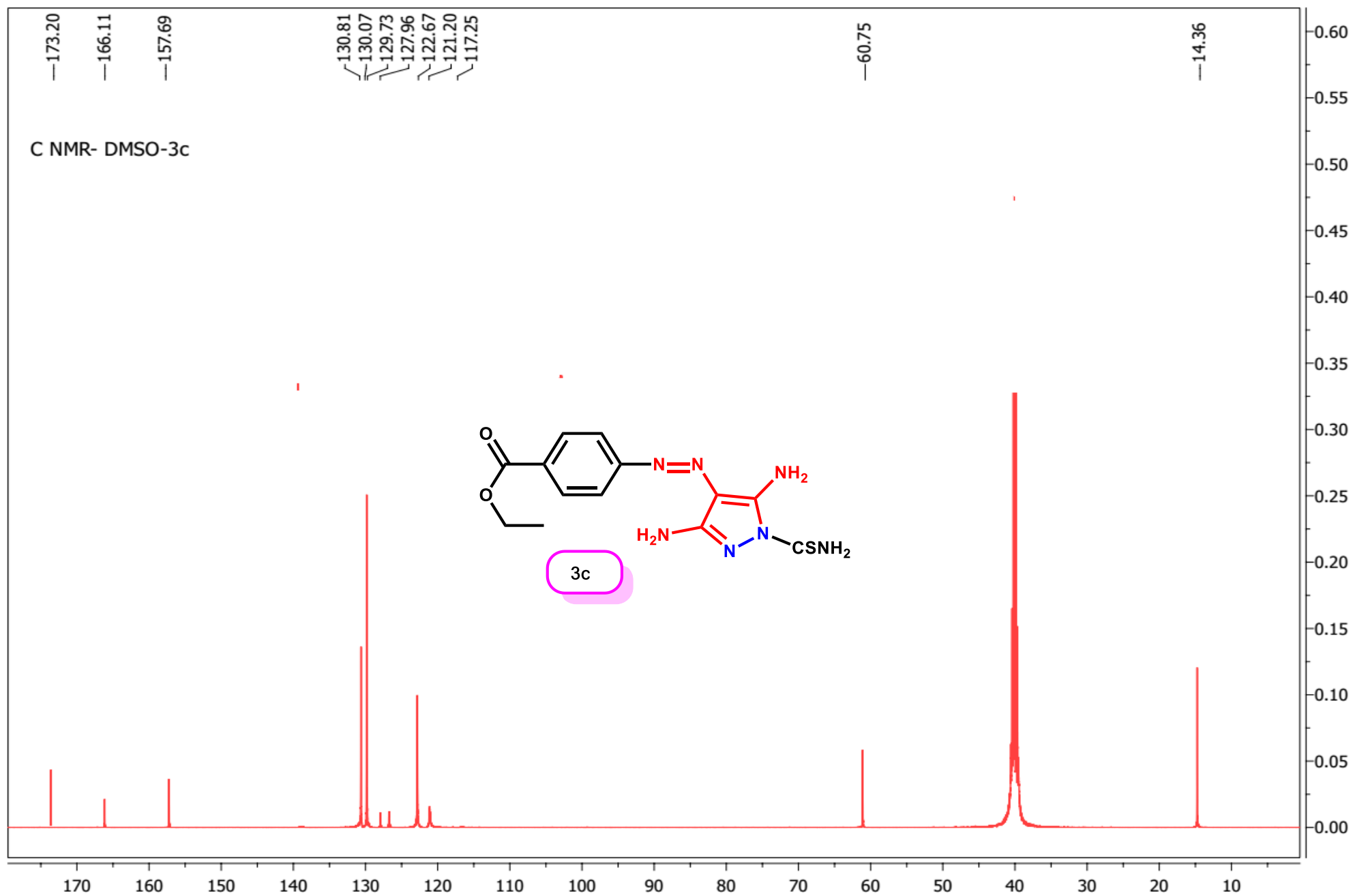
H NMR - DMSO-3b

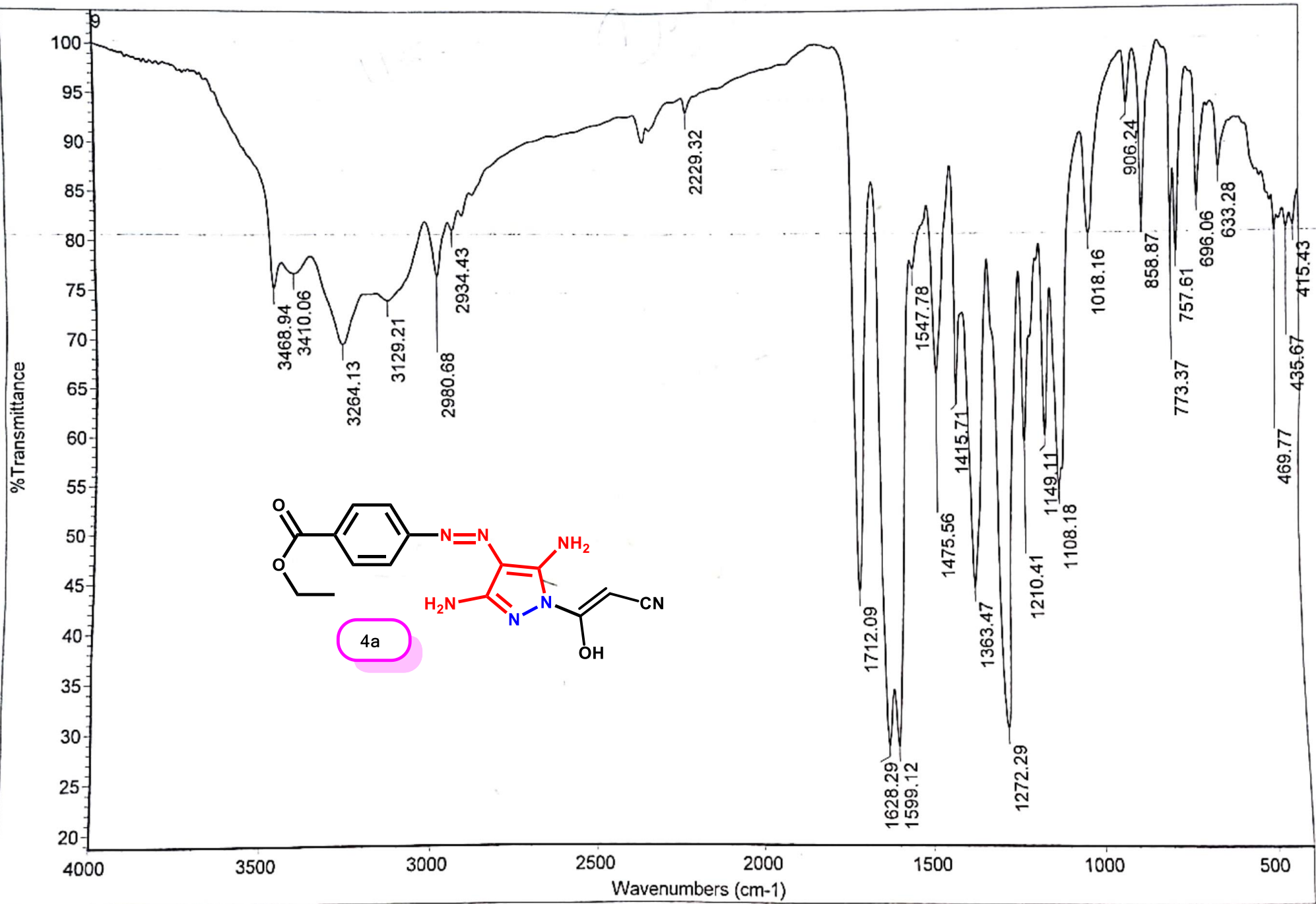


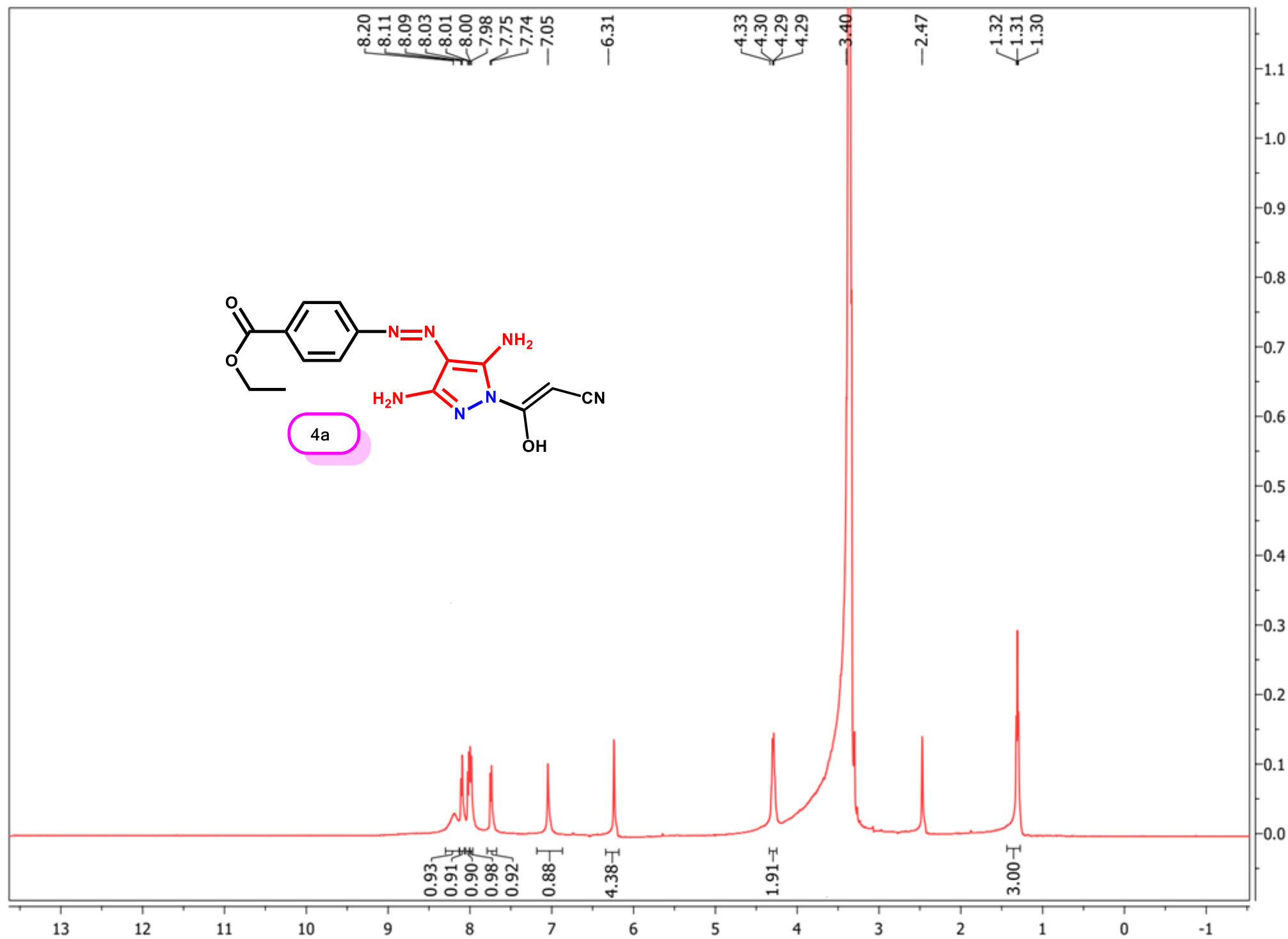


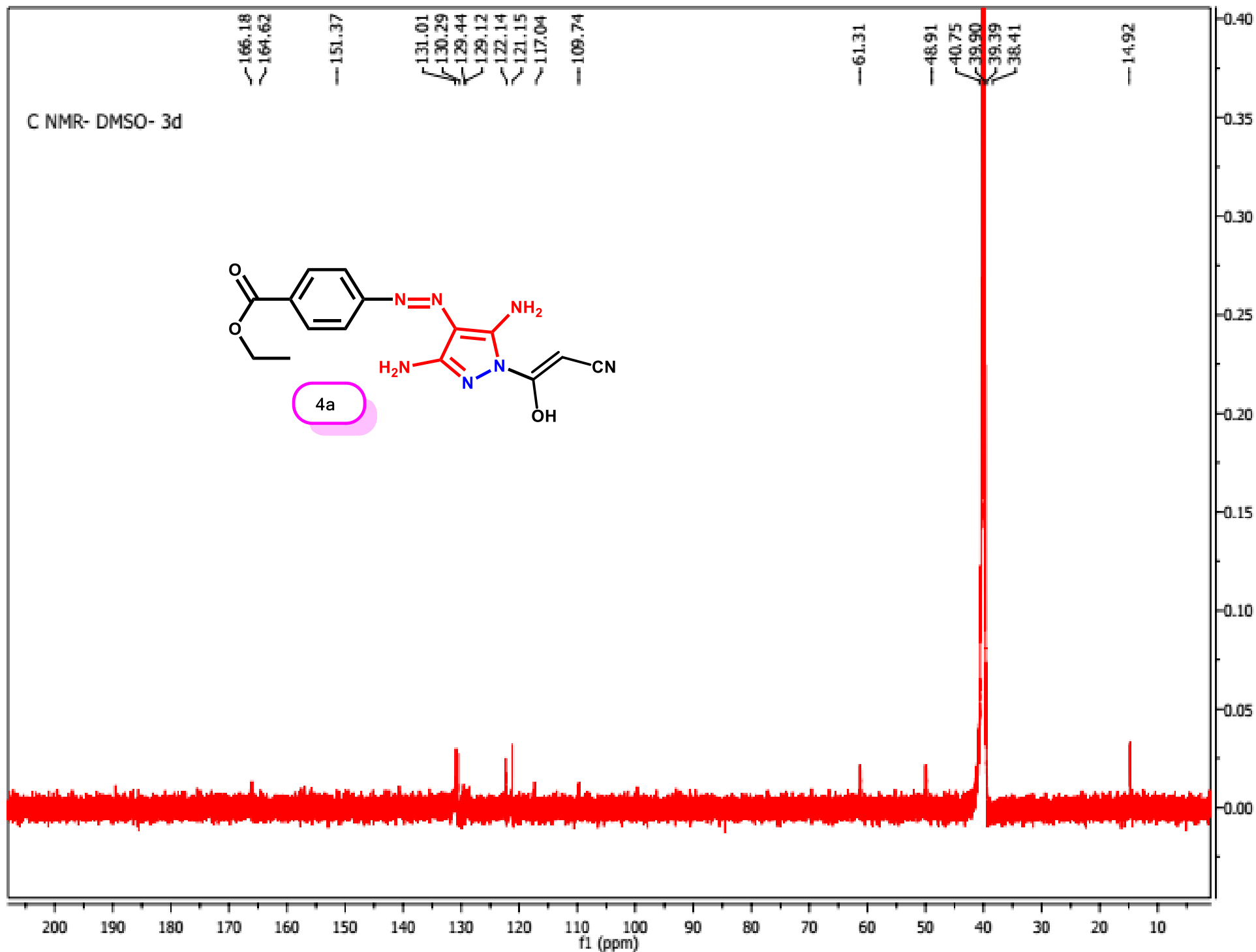


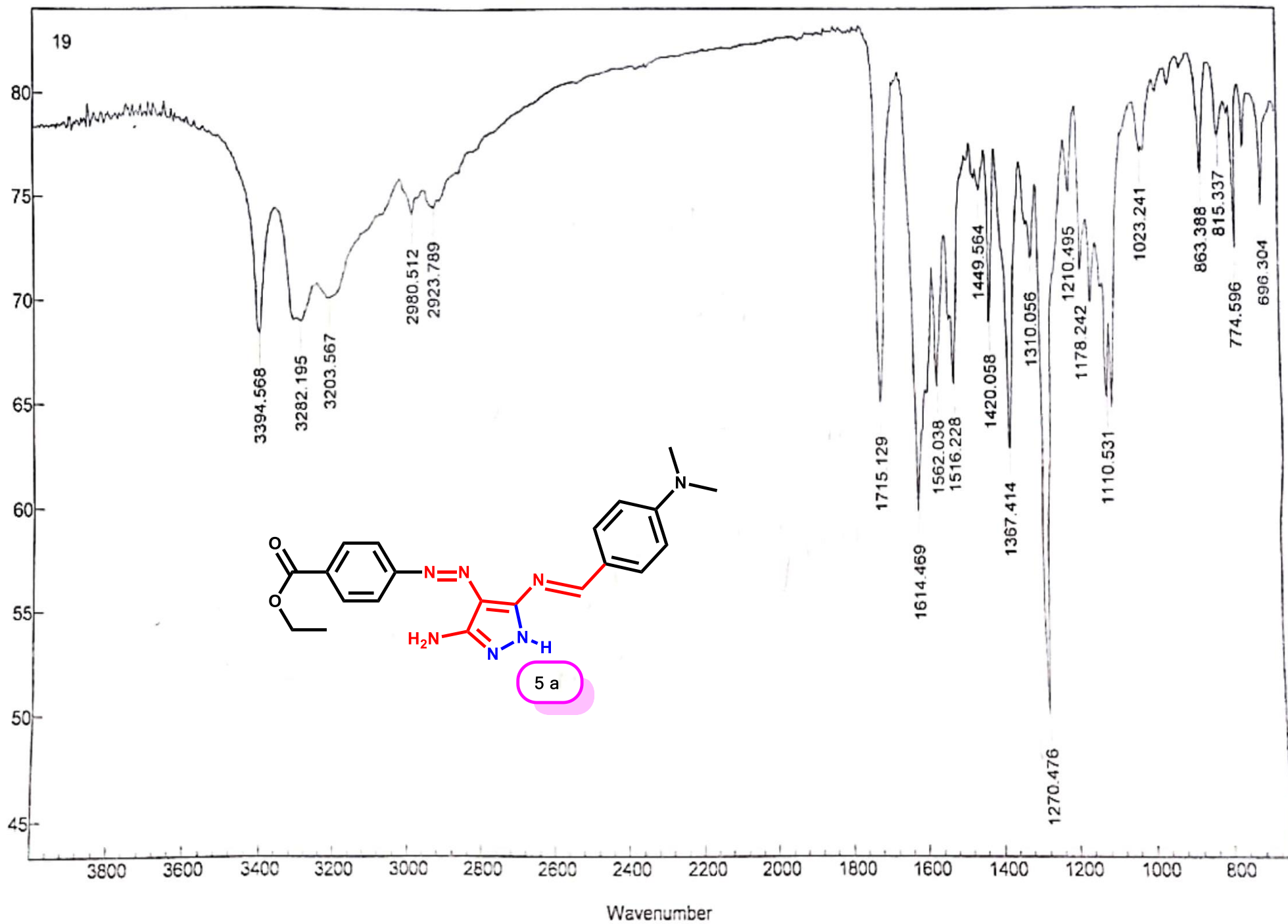


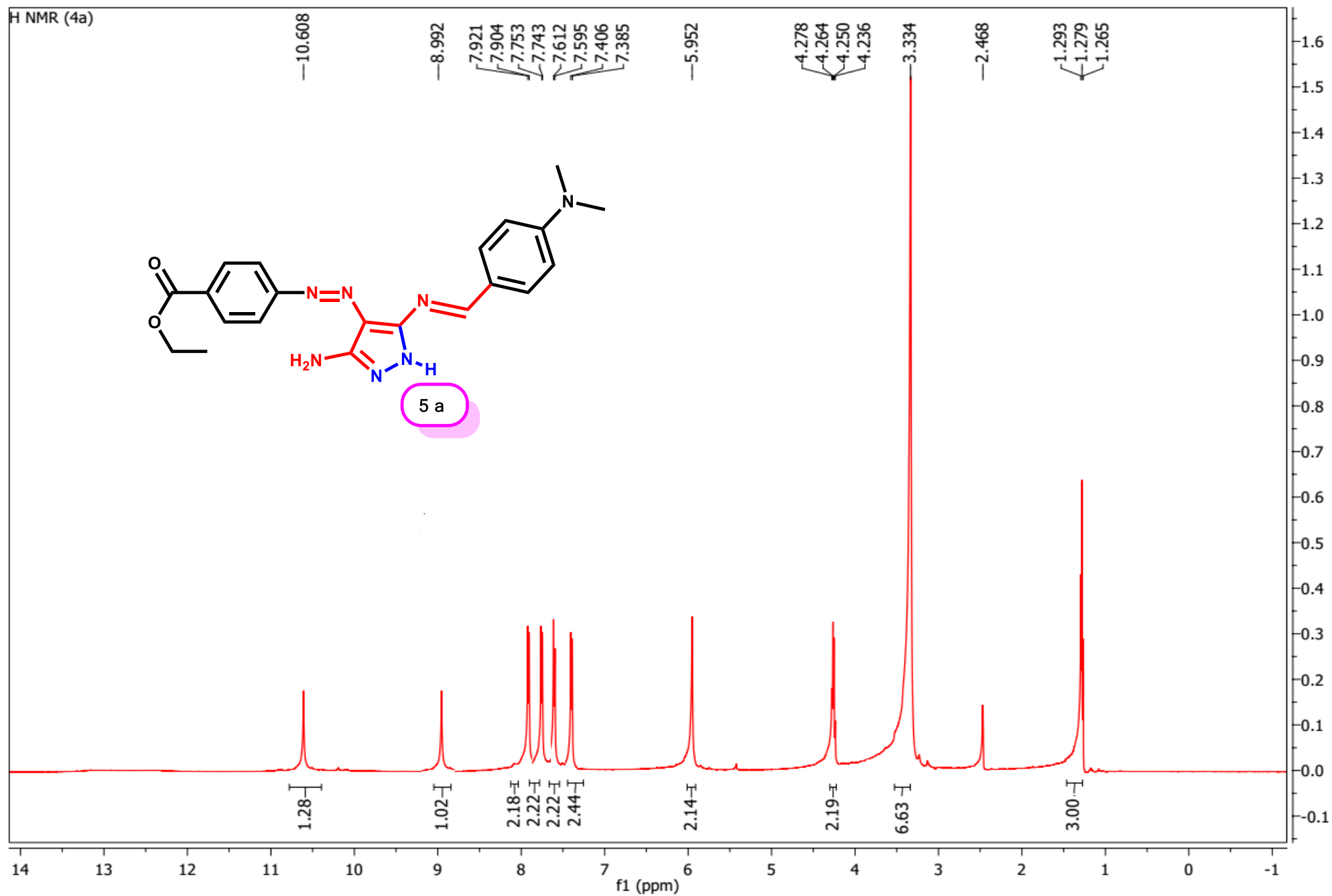


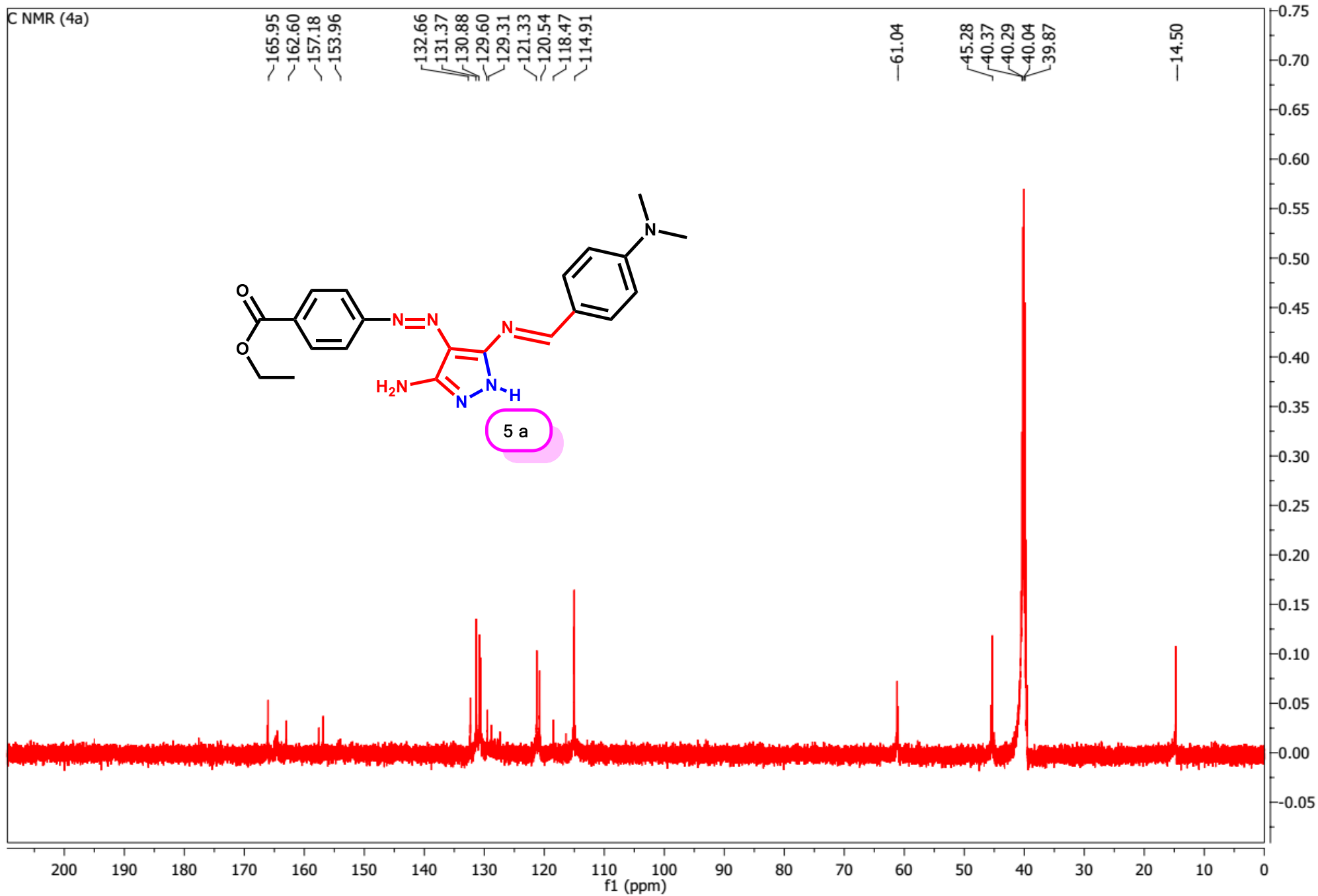


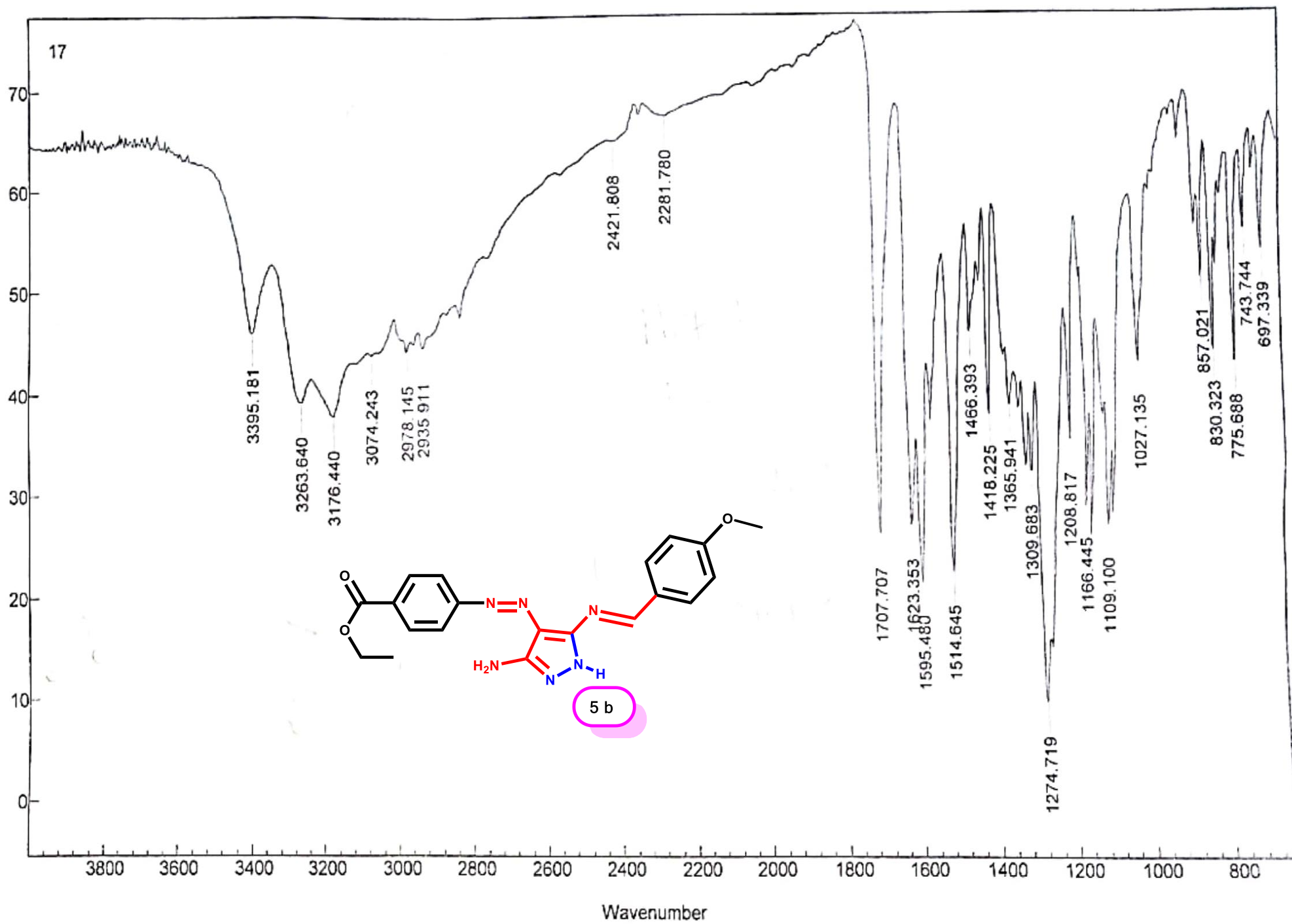




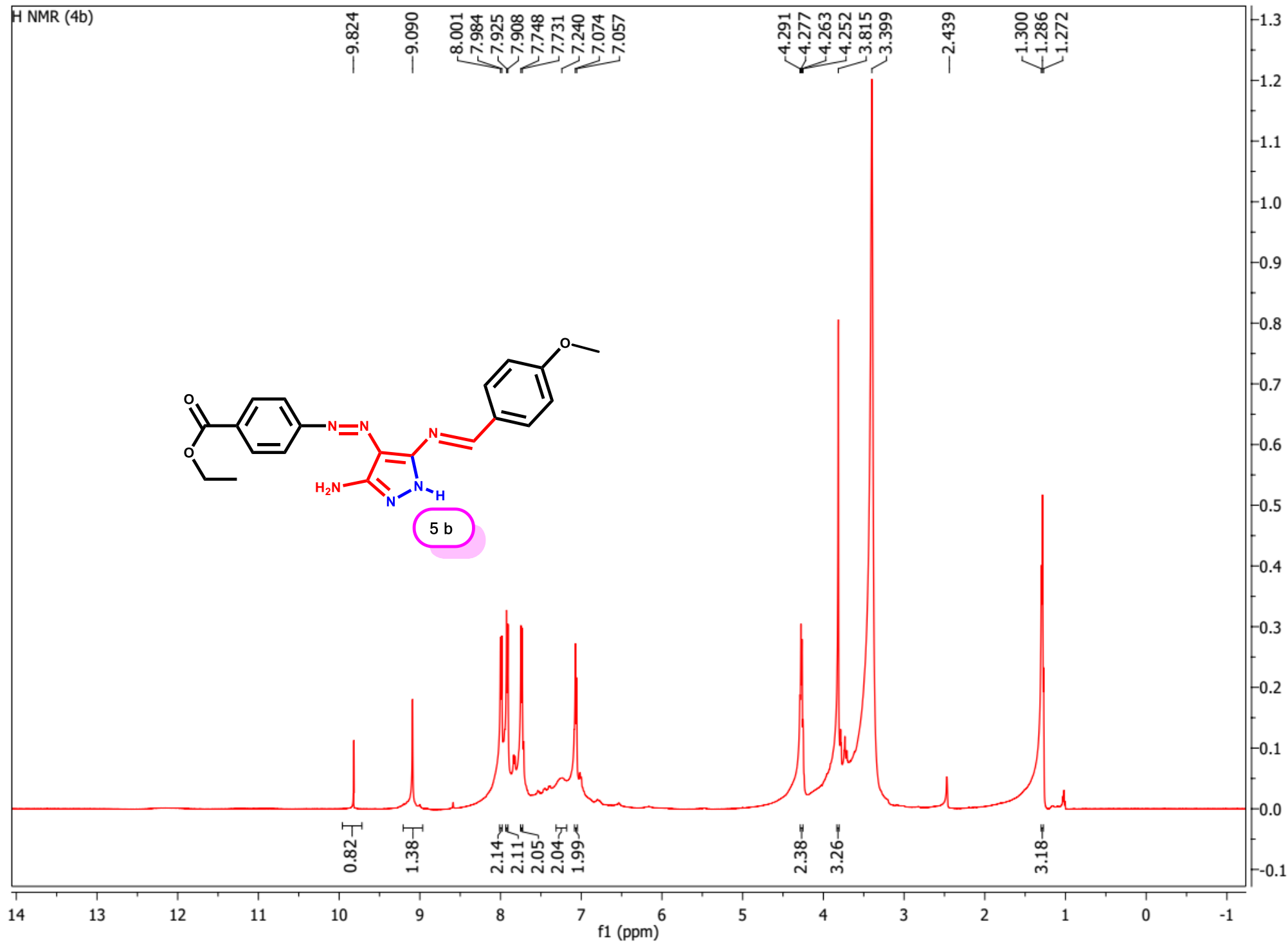
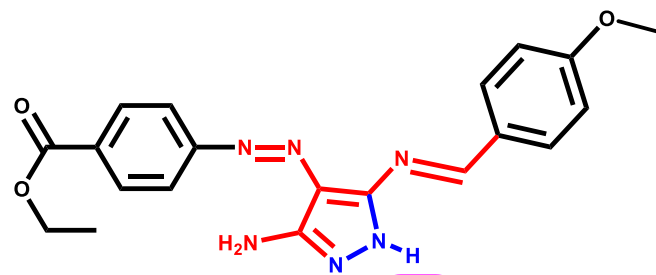


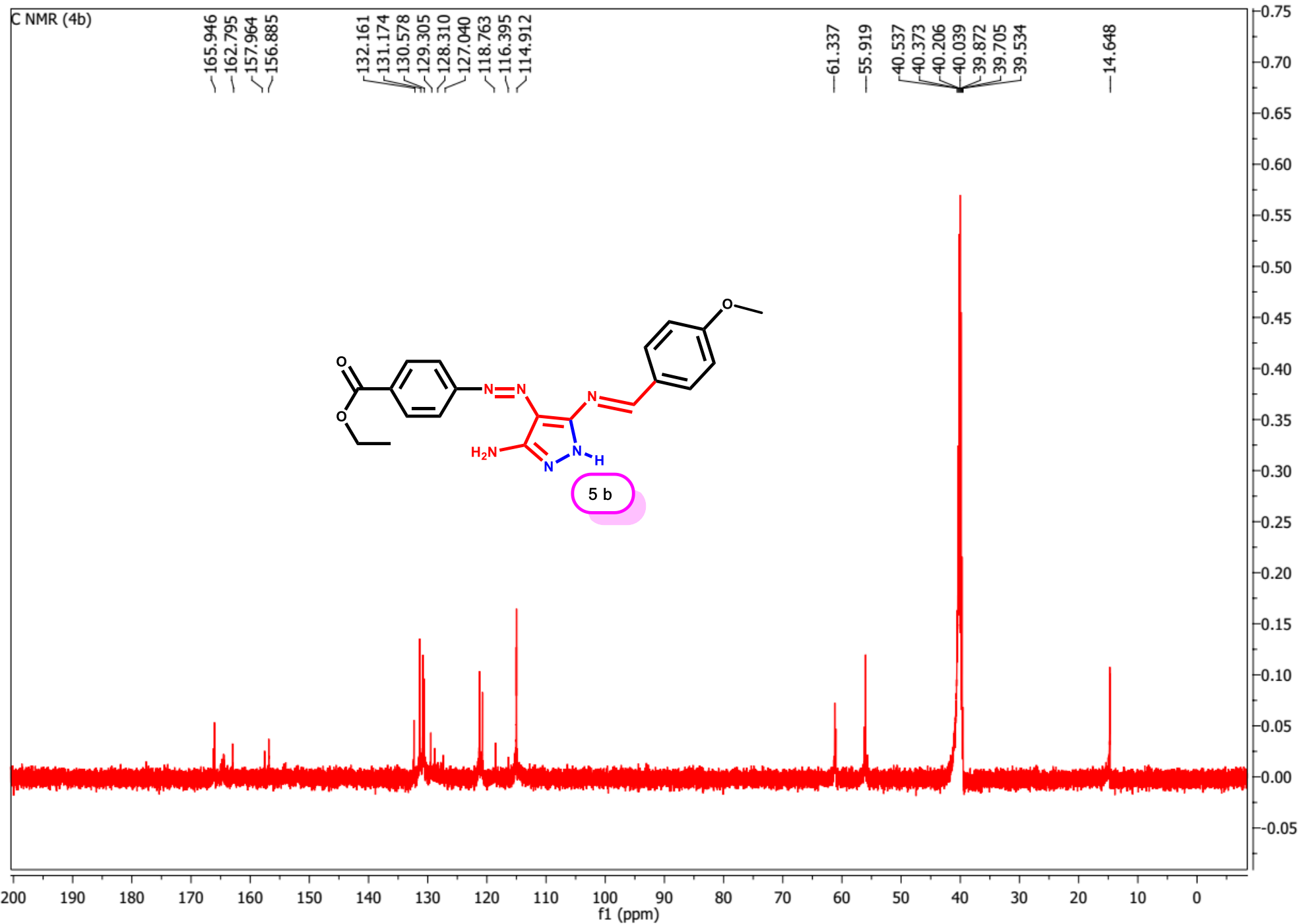


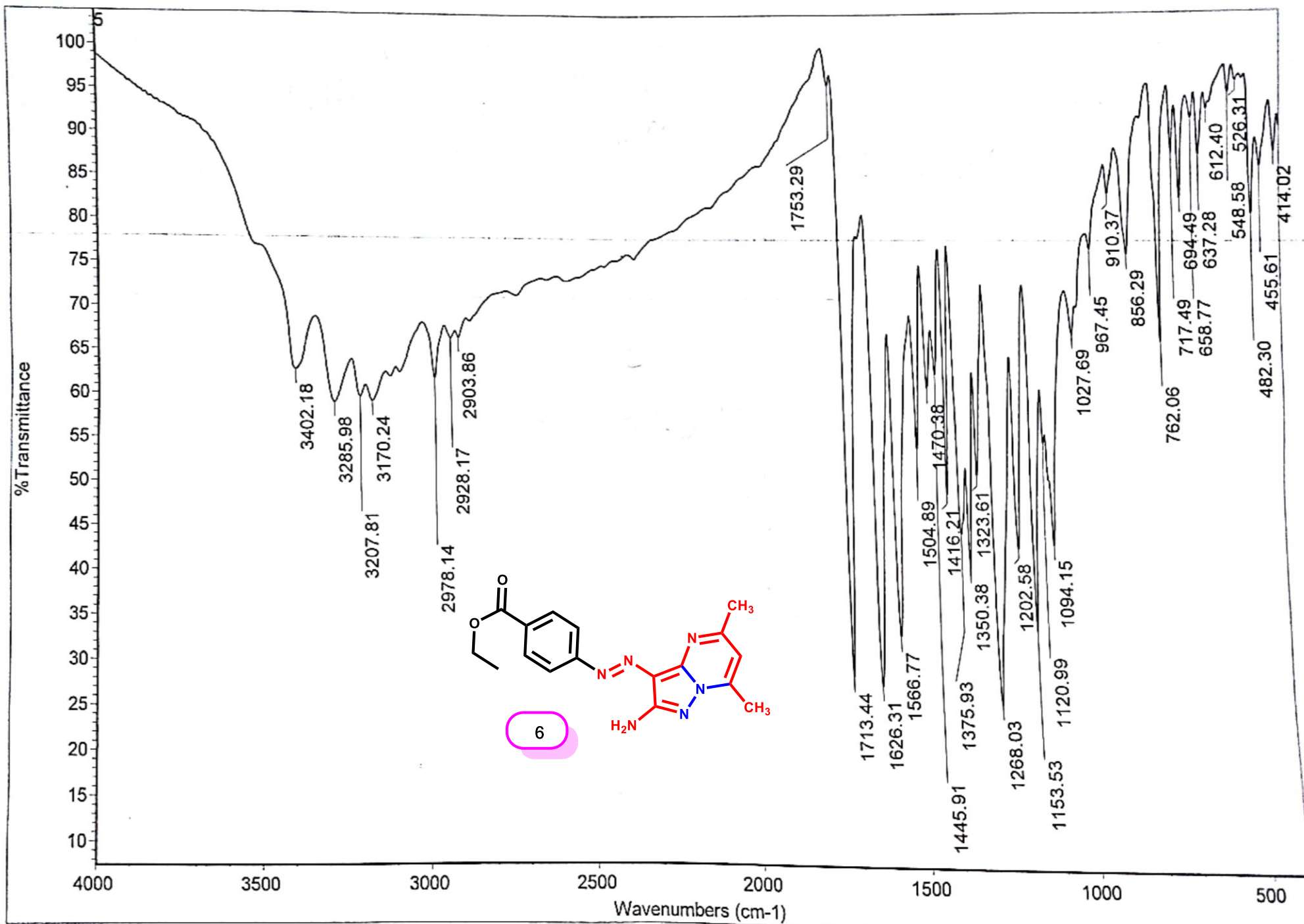


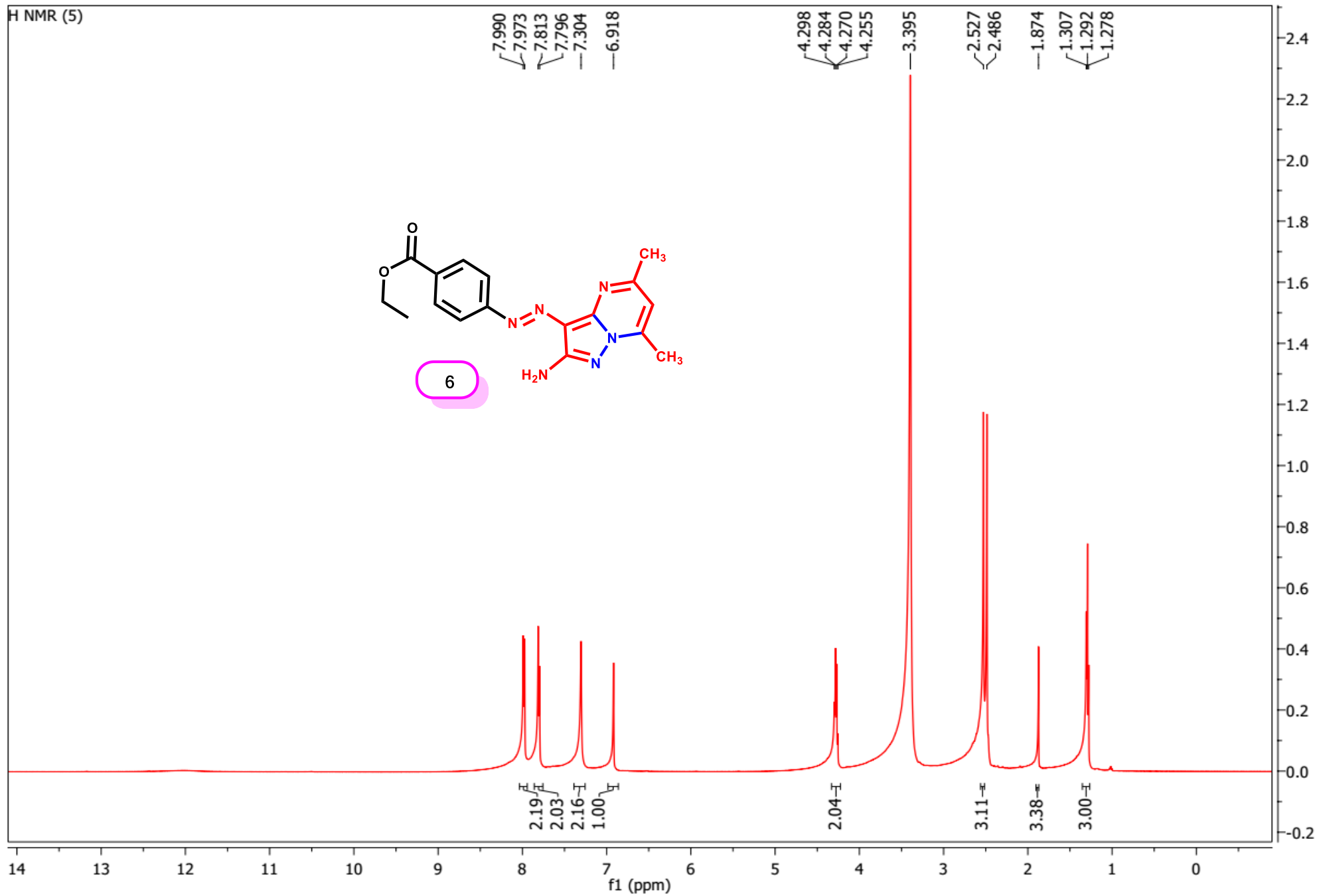


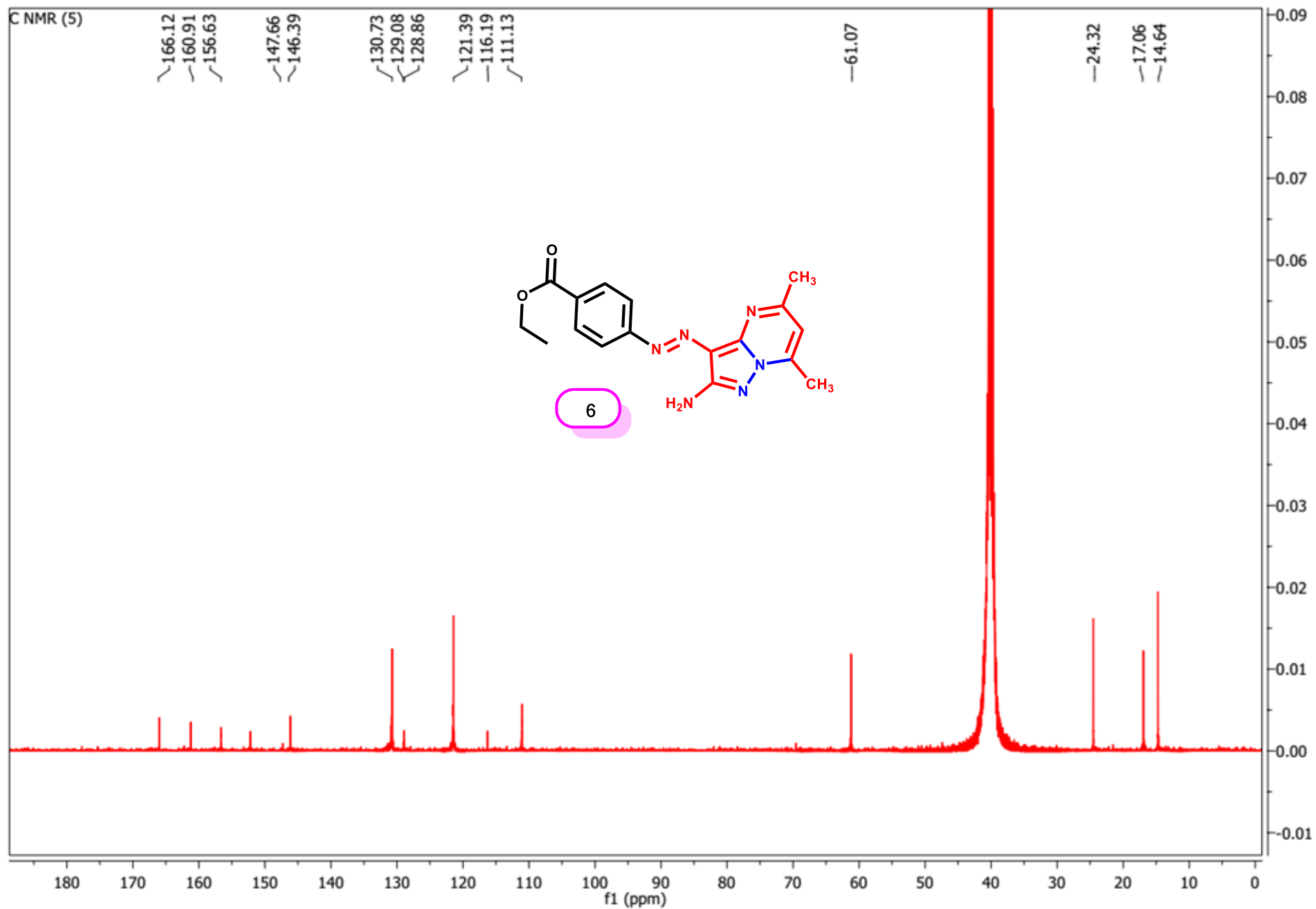
¹H NMR (4b)

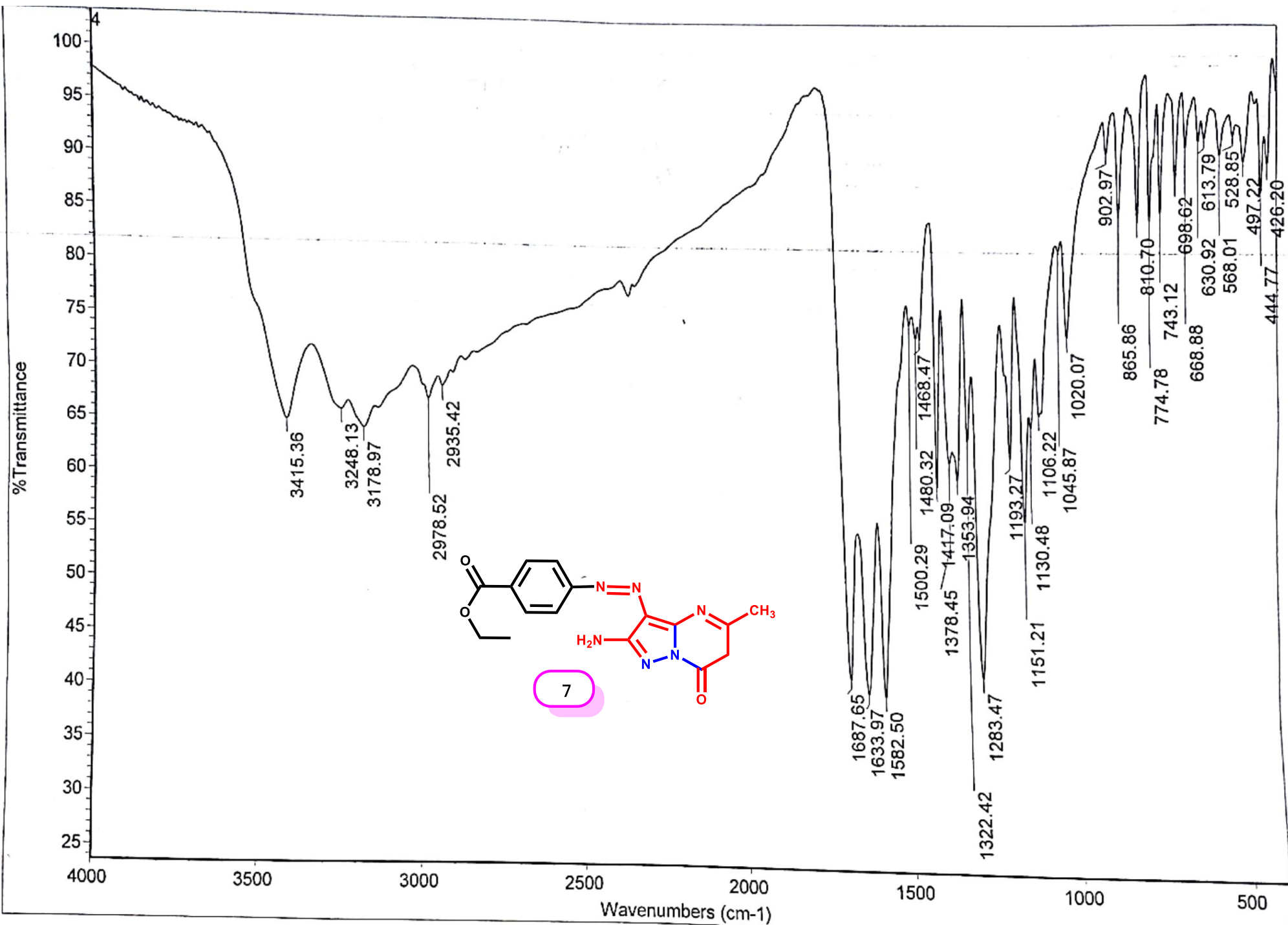


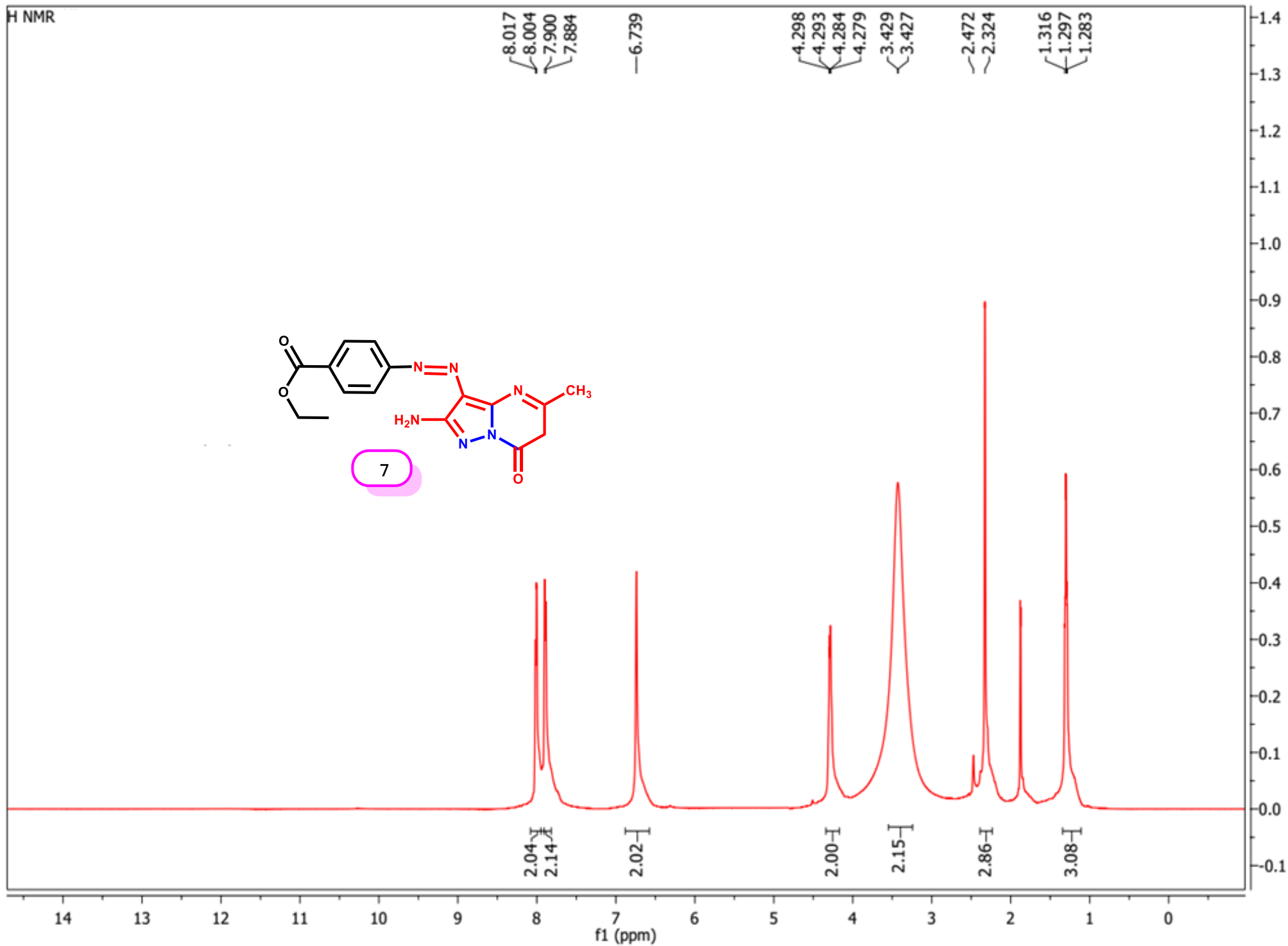


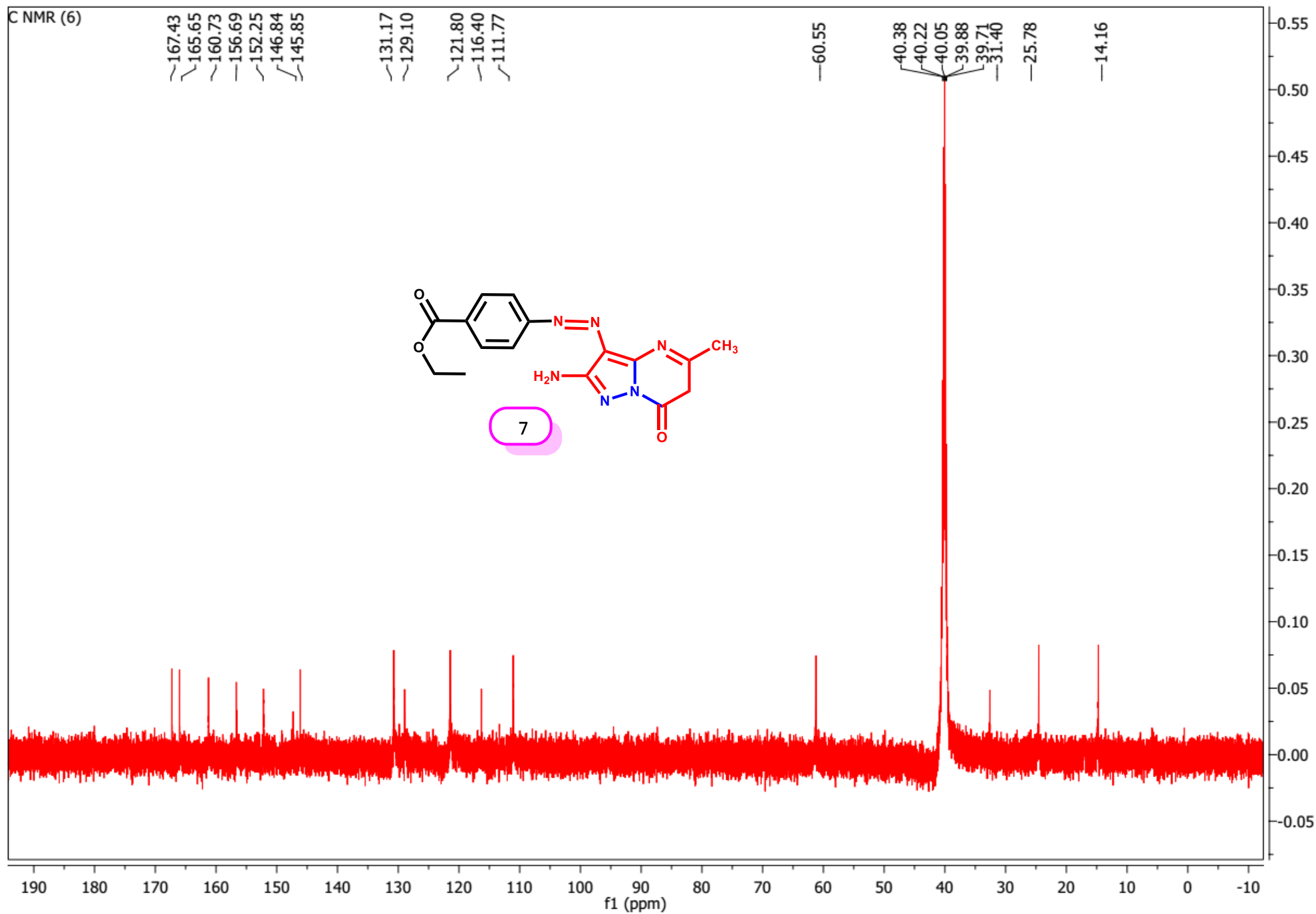


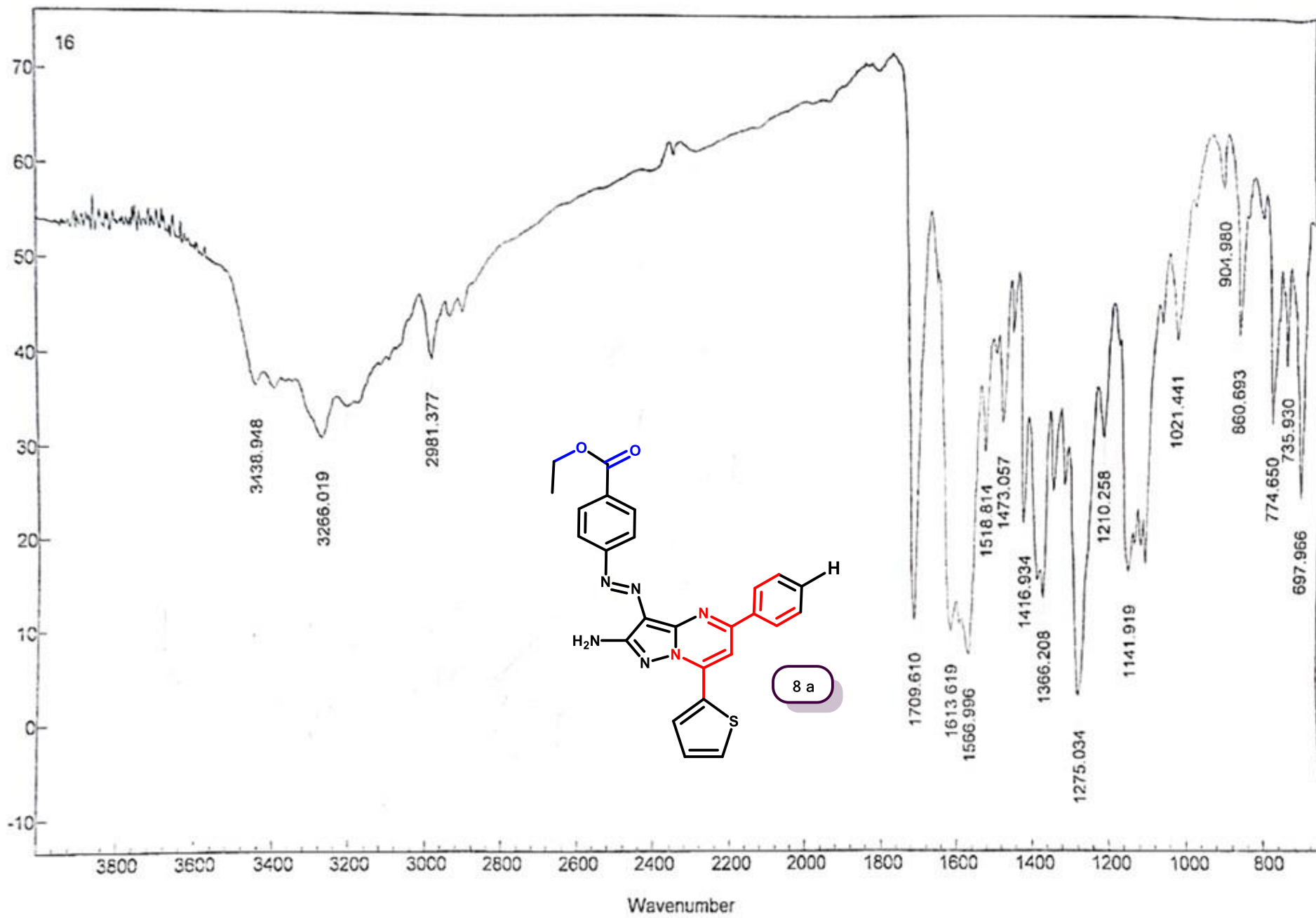


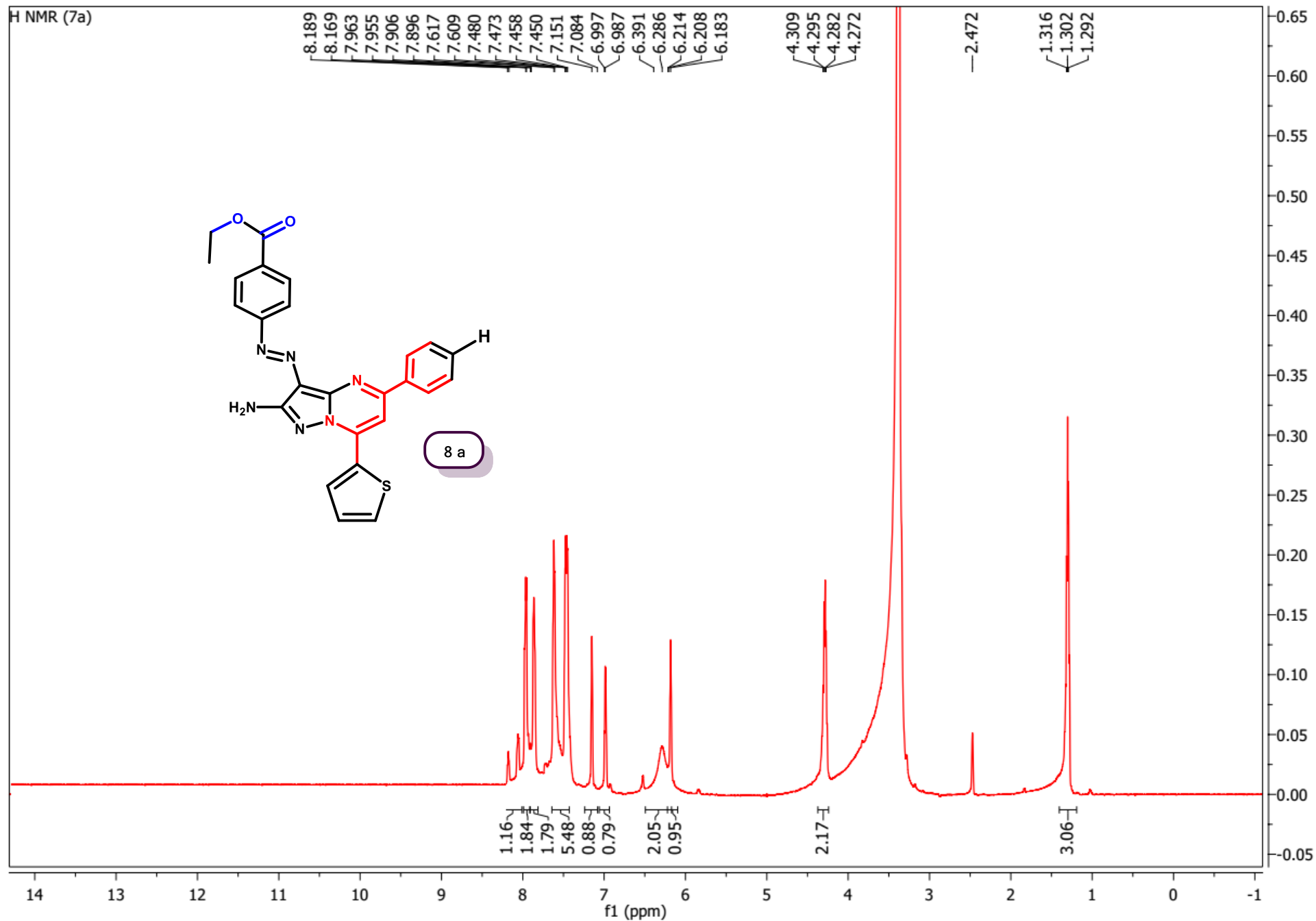


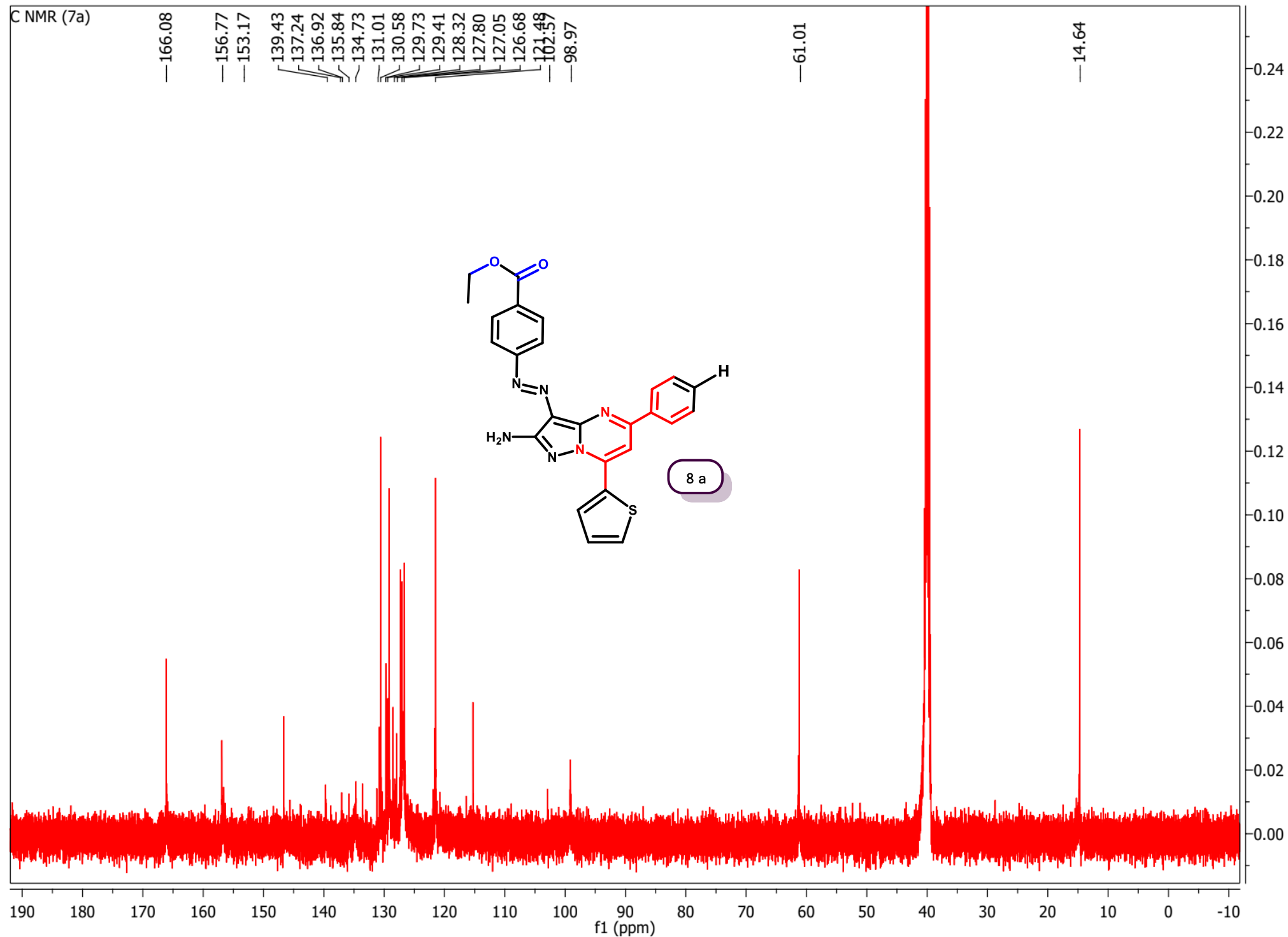


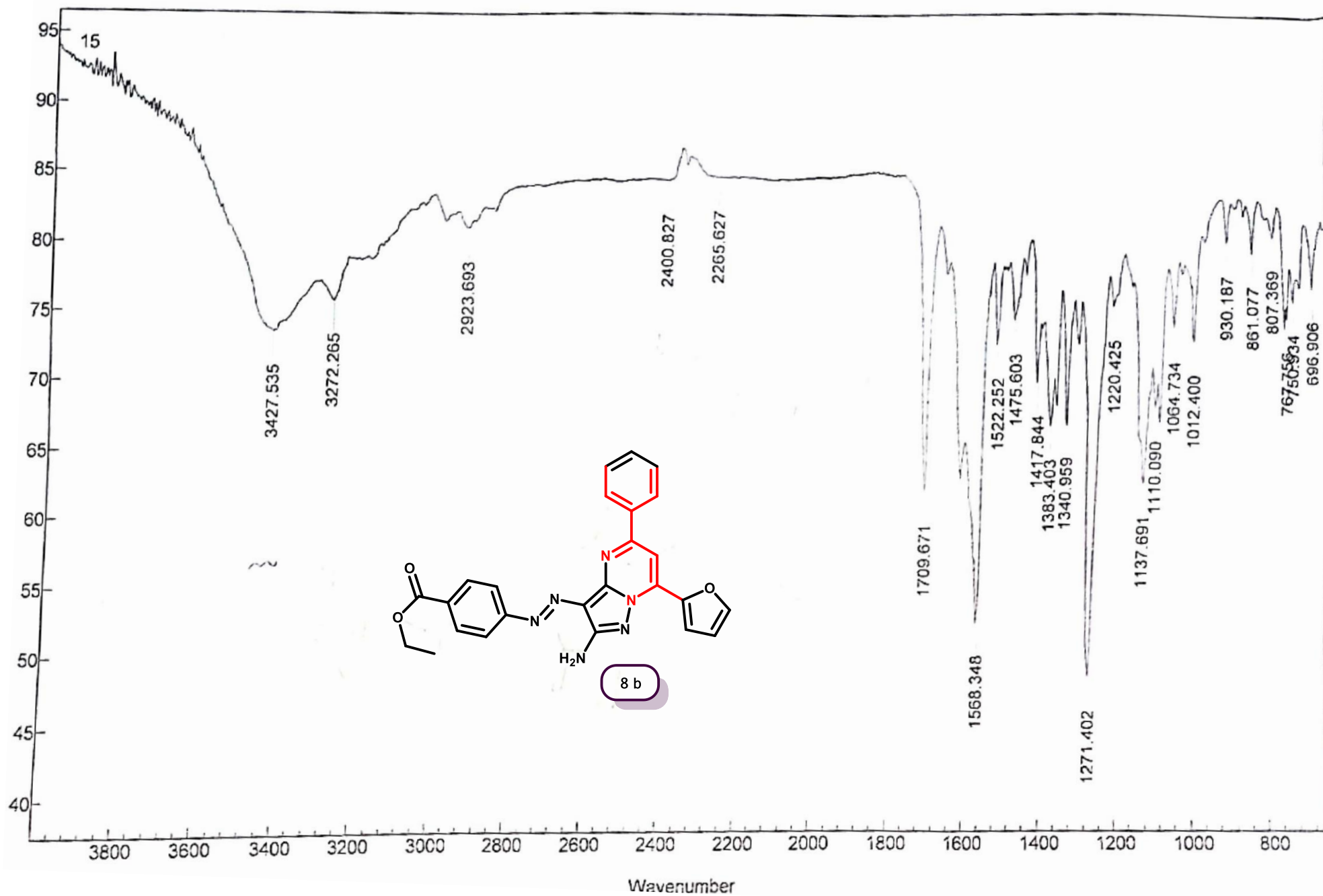




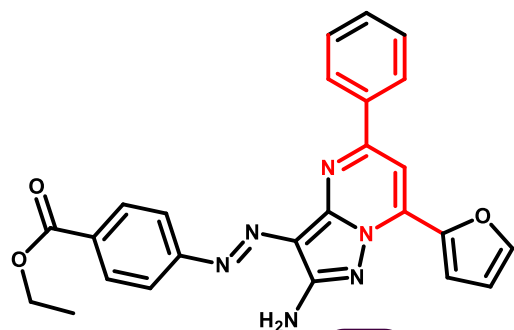








¹H NMR (7b)



8 b

8.22
8.21
8.06
8.05
7.98
7.97
7.95
7.92
7.87
7.74
7.73
7.71
7.61
7.60
7.47
7.45
7.44
6.45
6.43
6.41
6.27

4.31
4.30
4.29
4.27

—2.47

1.32
1.31
1.29

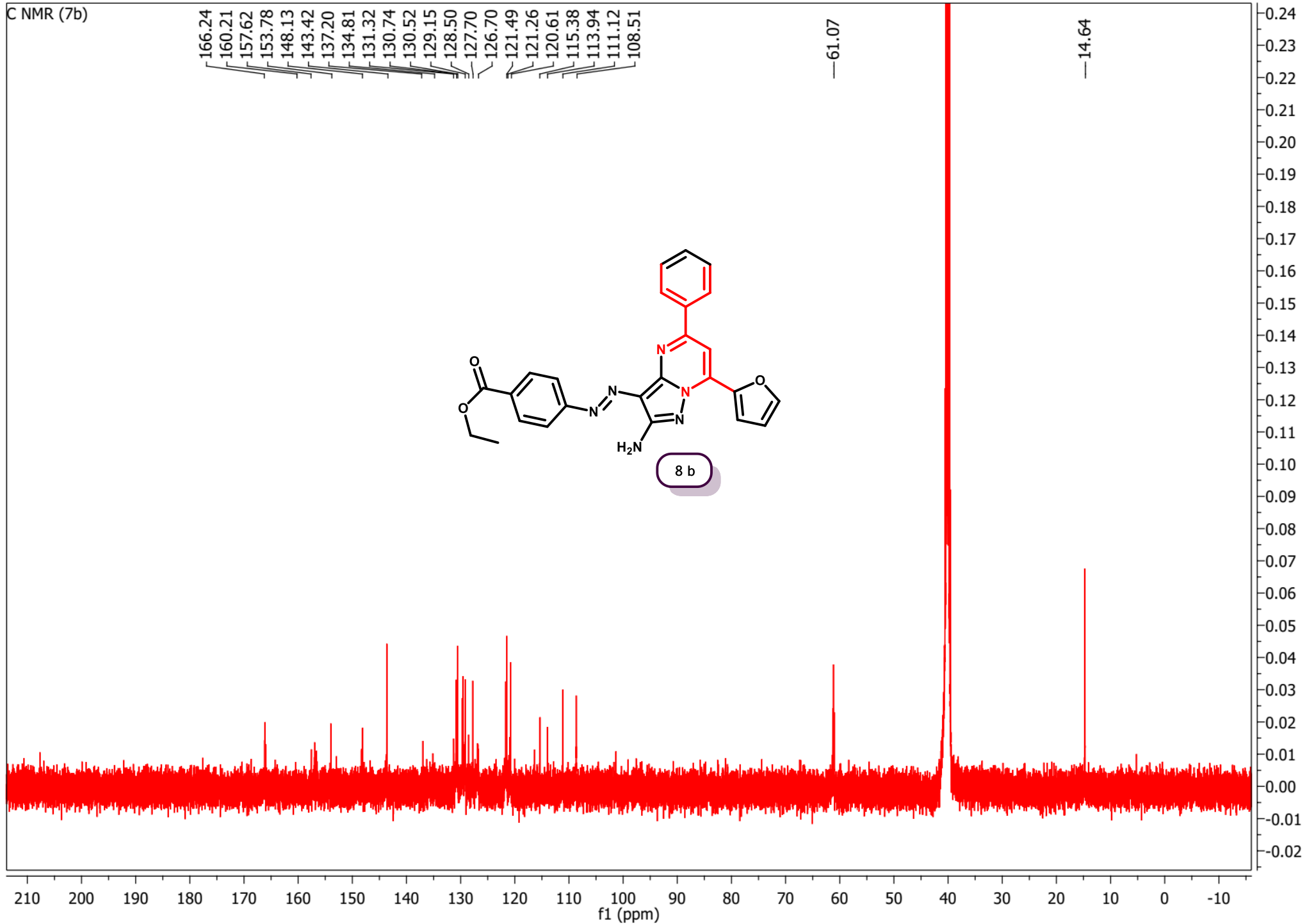
1.03
0.89
3.97
1.99
0.94
1.82
1.99

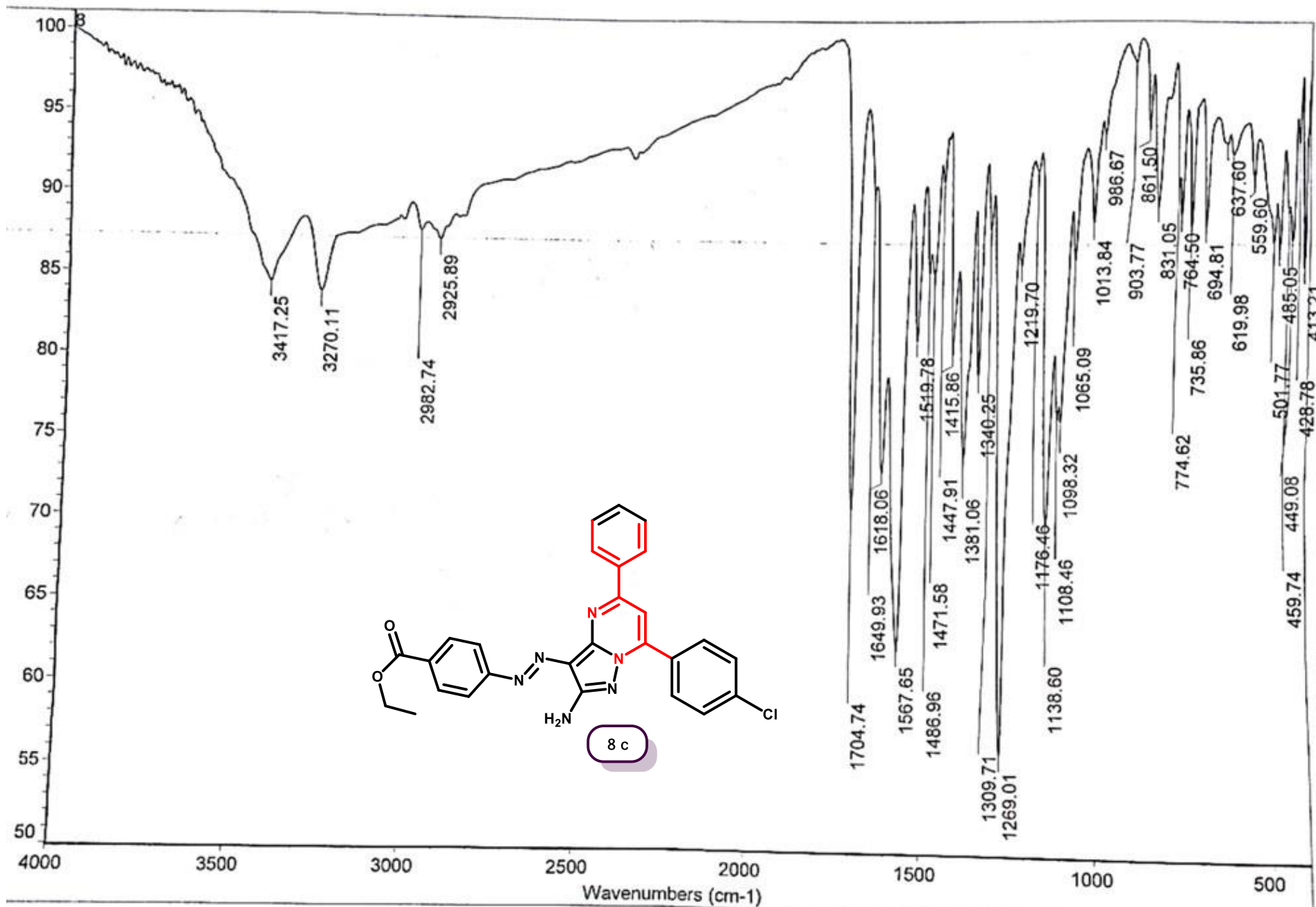
1.01
1.66

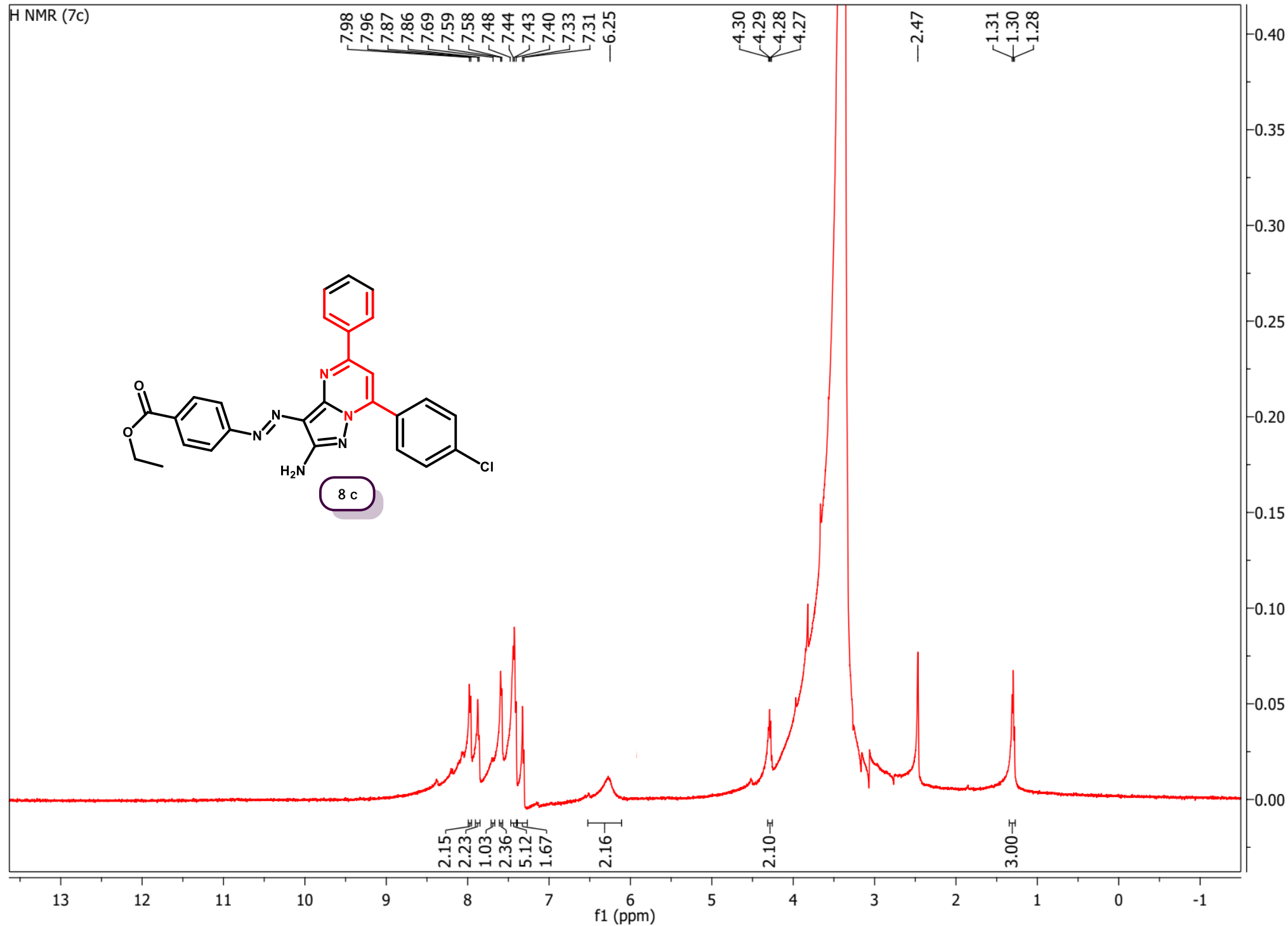
1.90

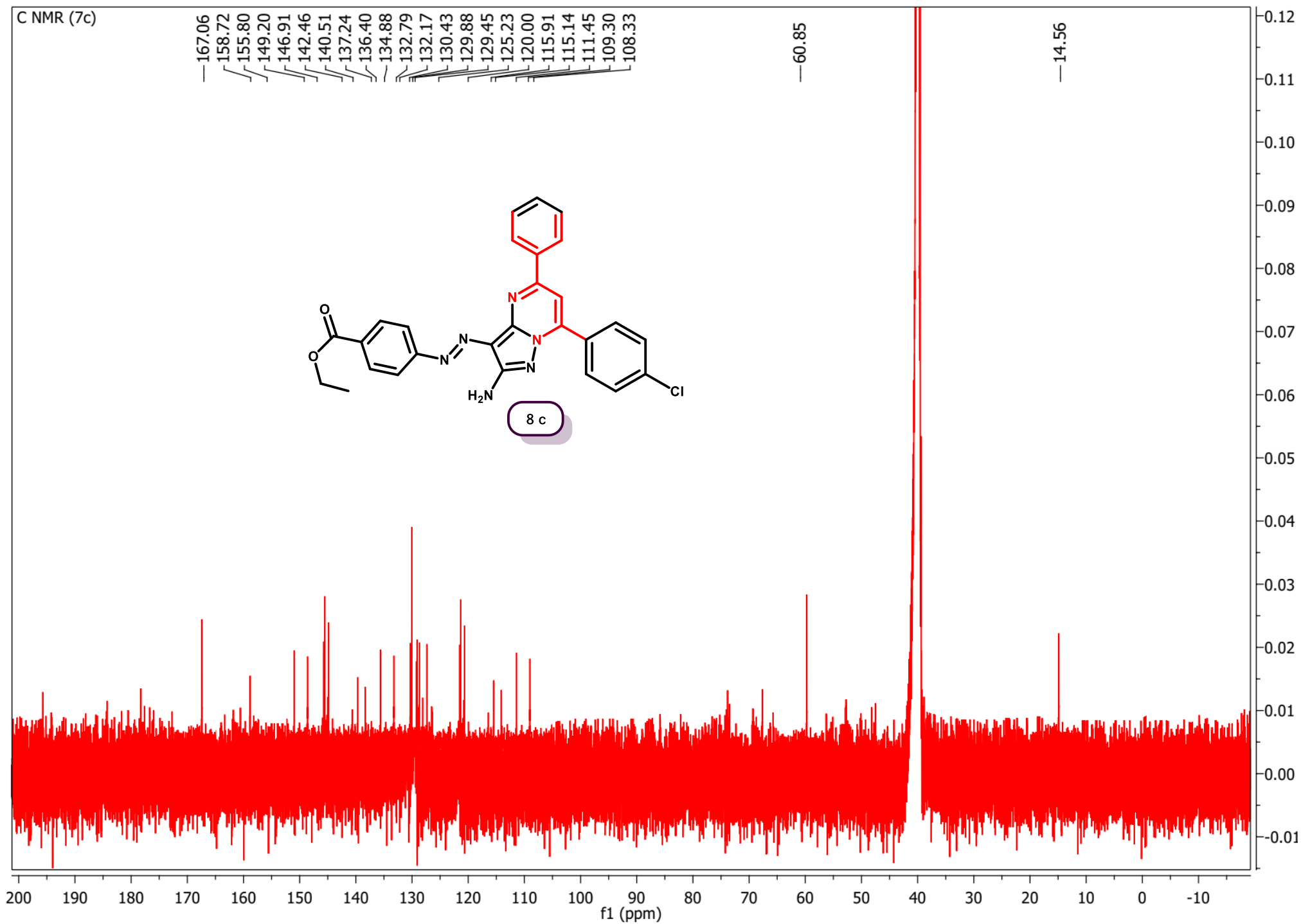
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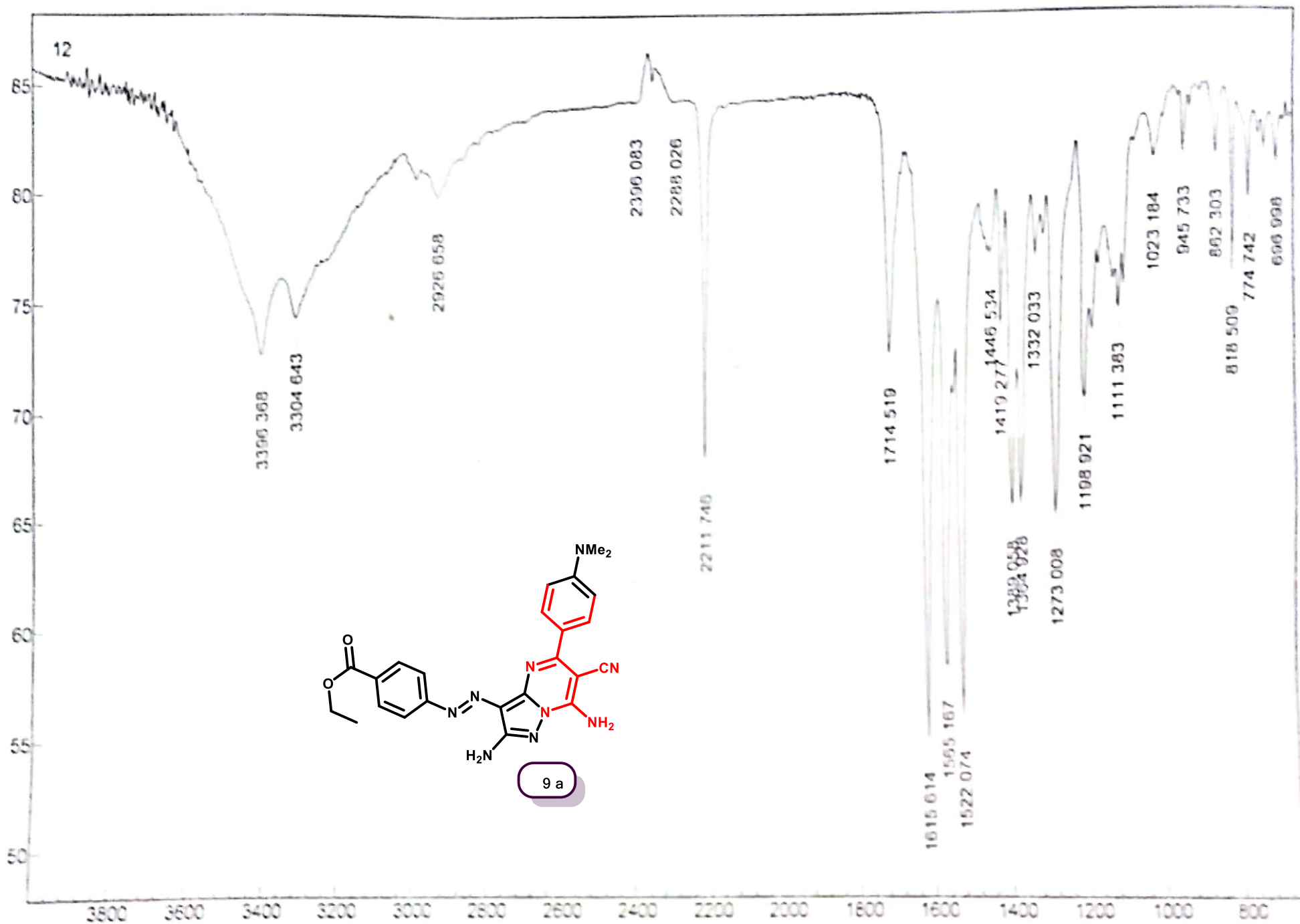
f1 (ppm)

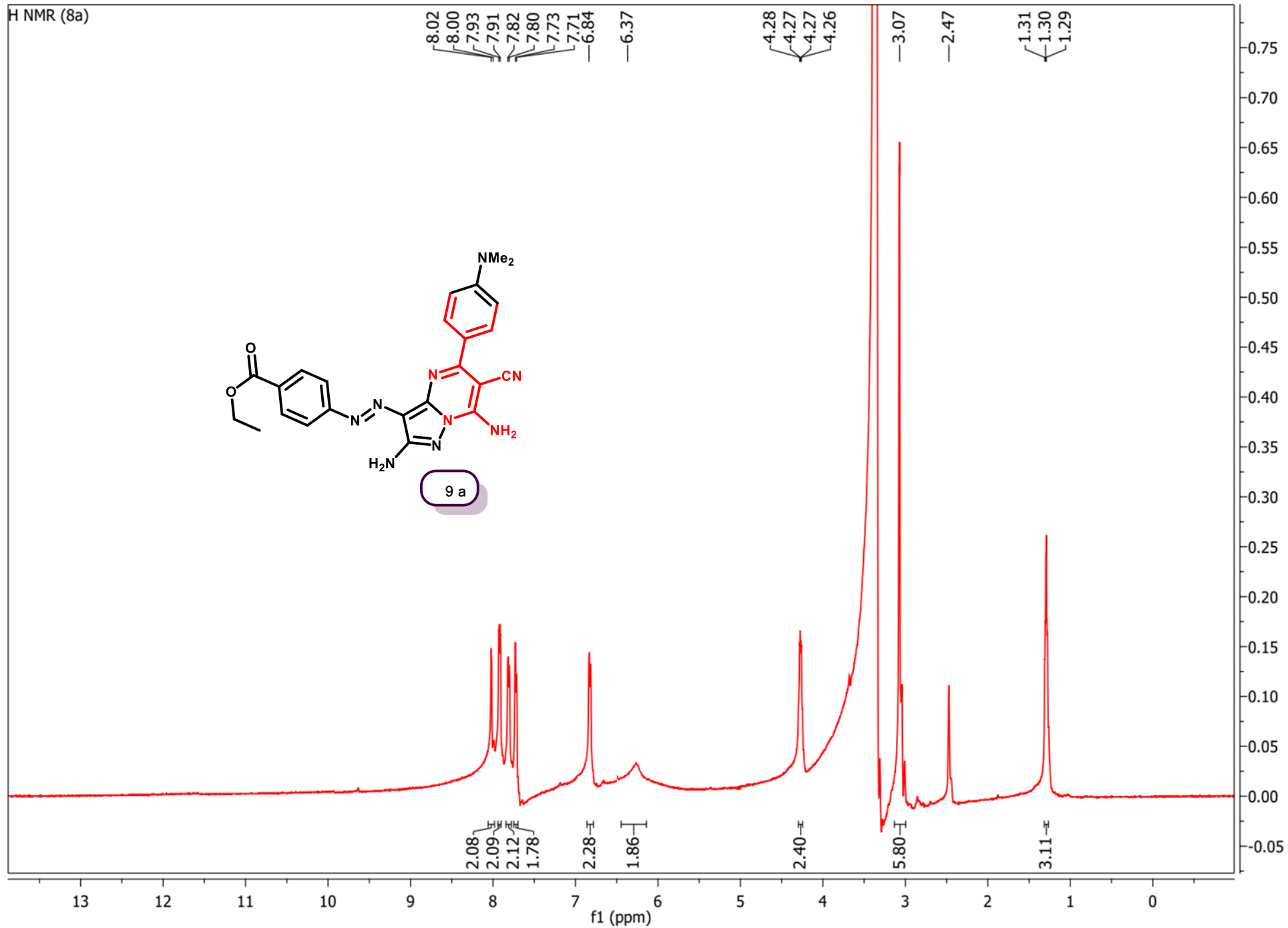


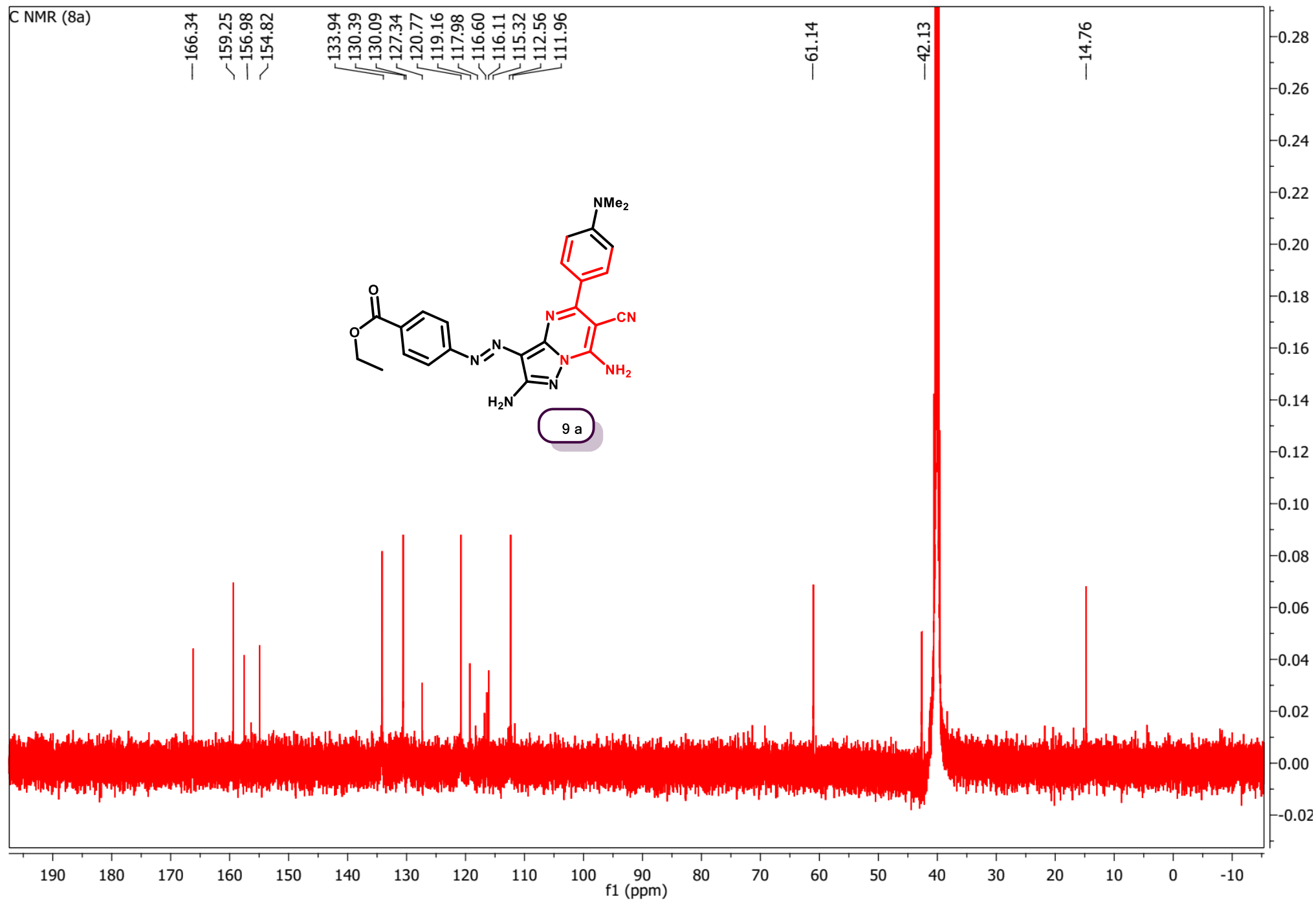


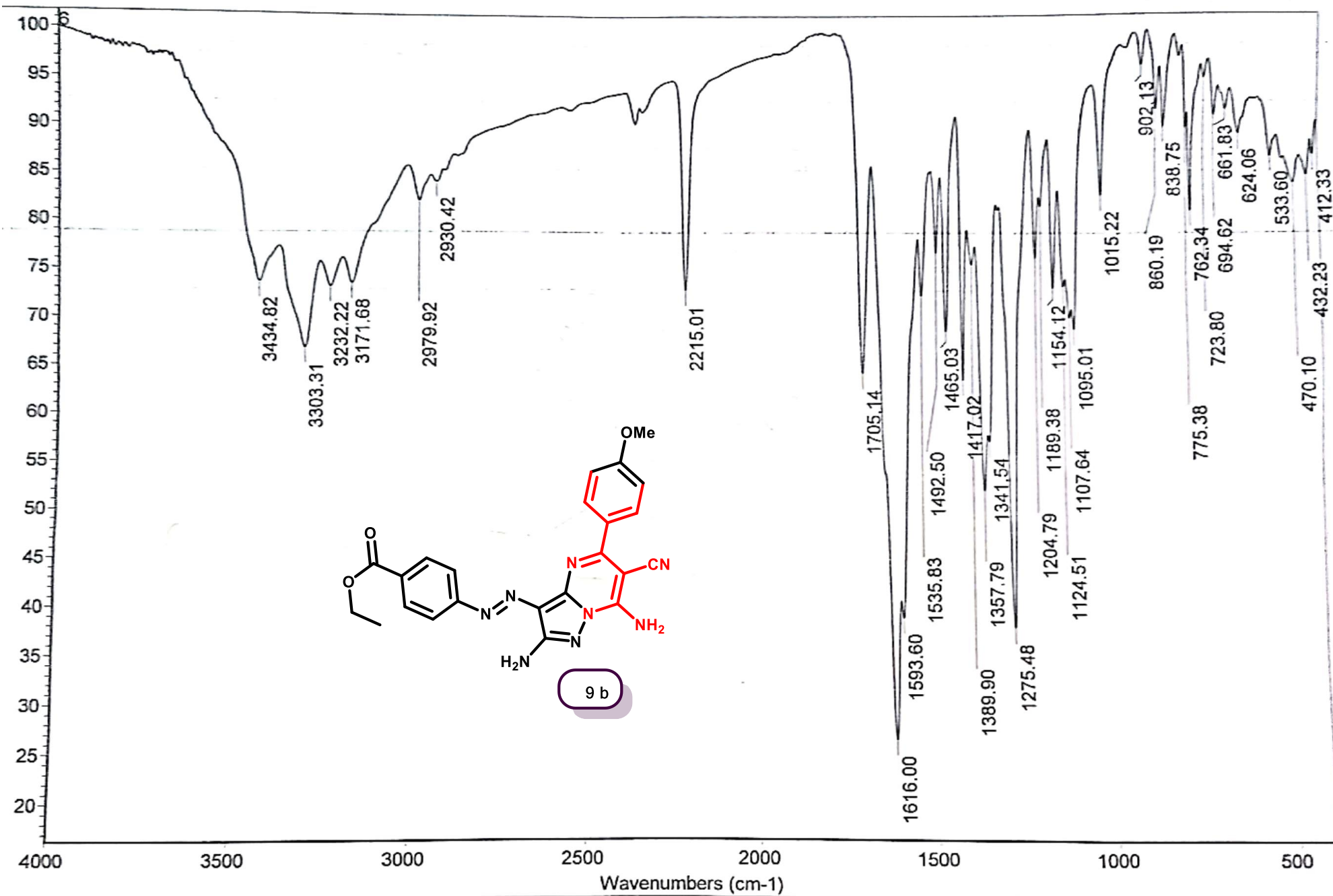


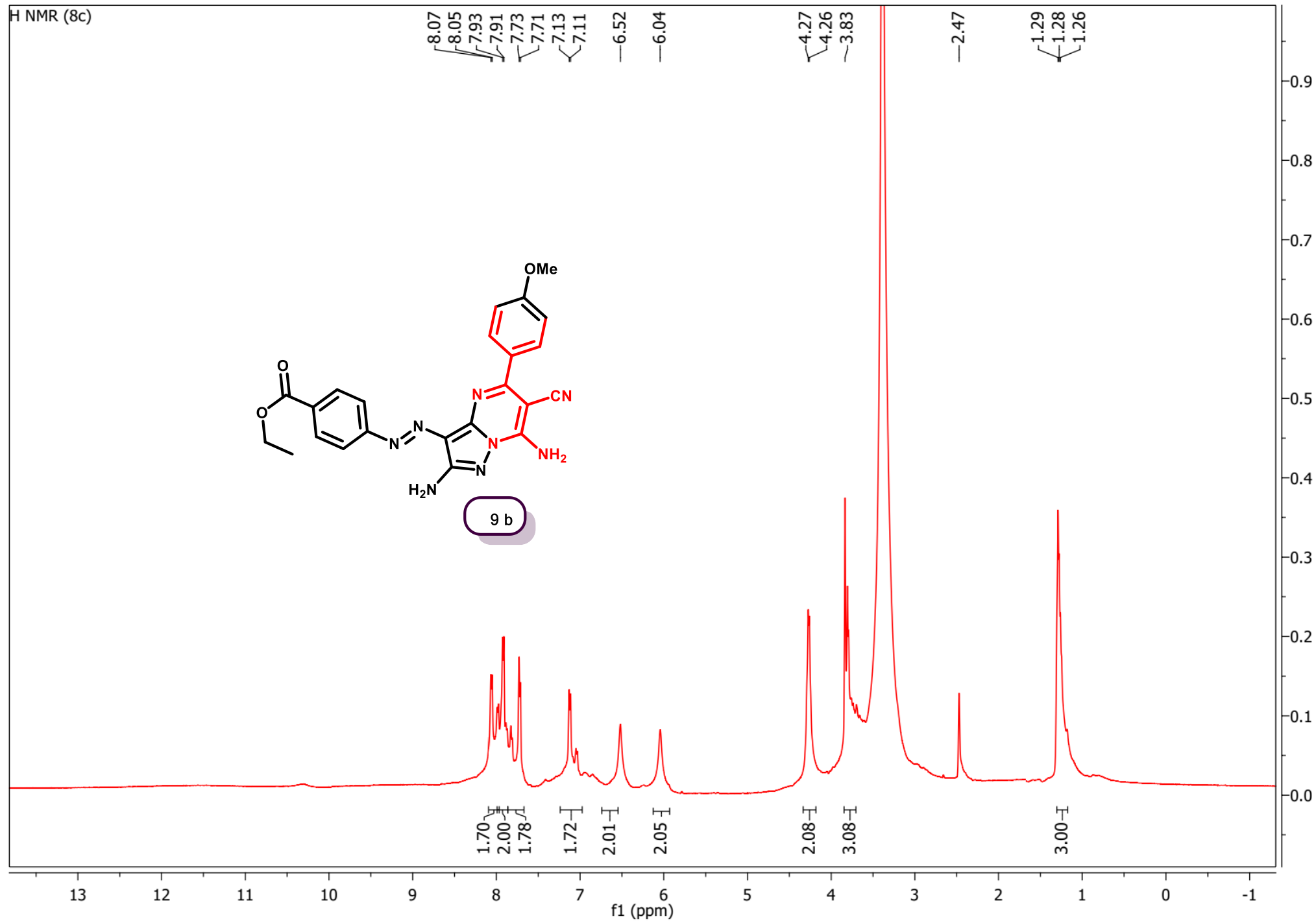


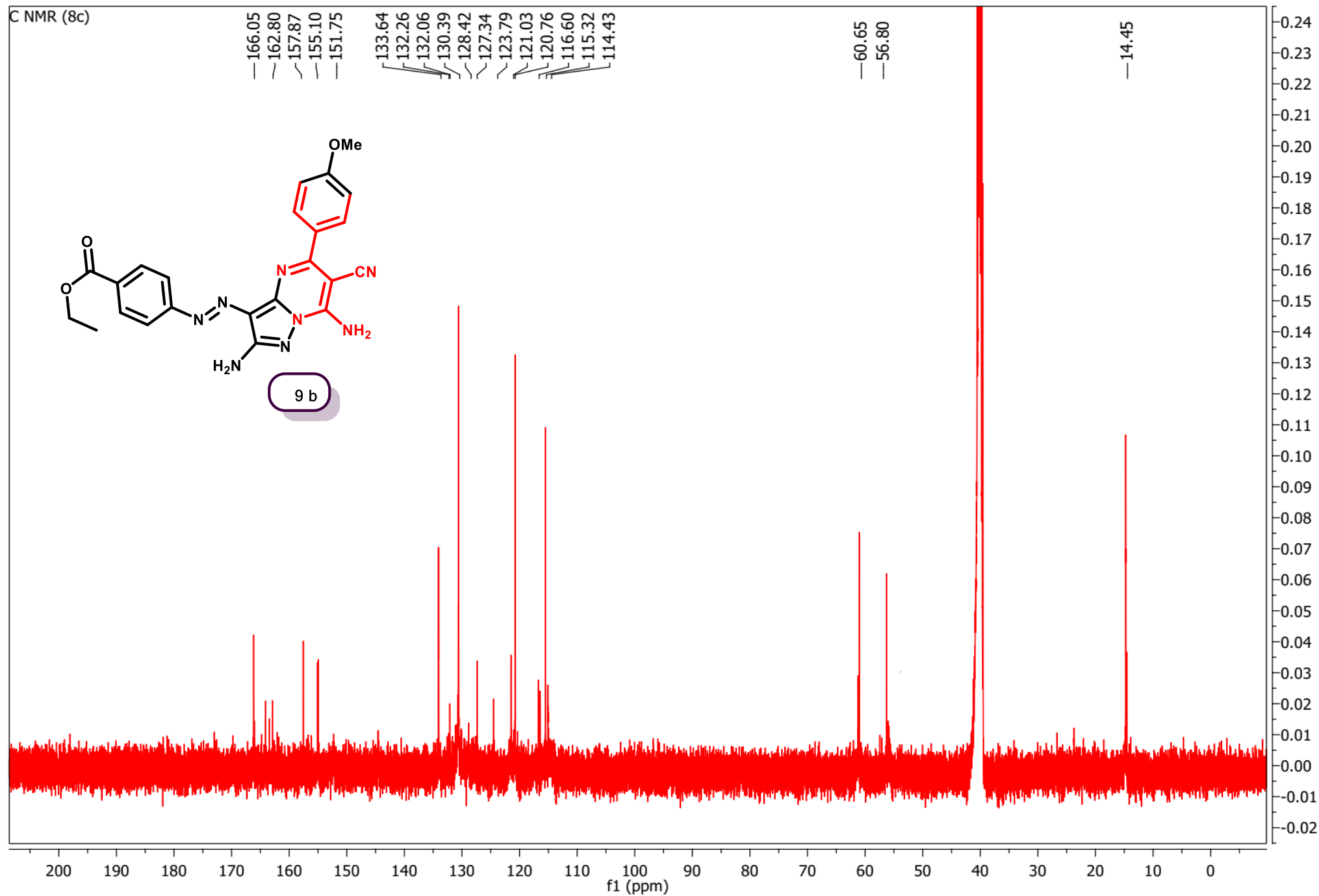


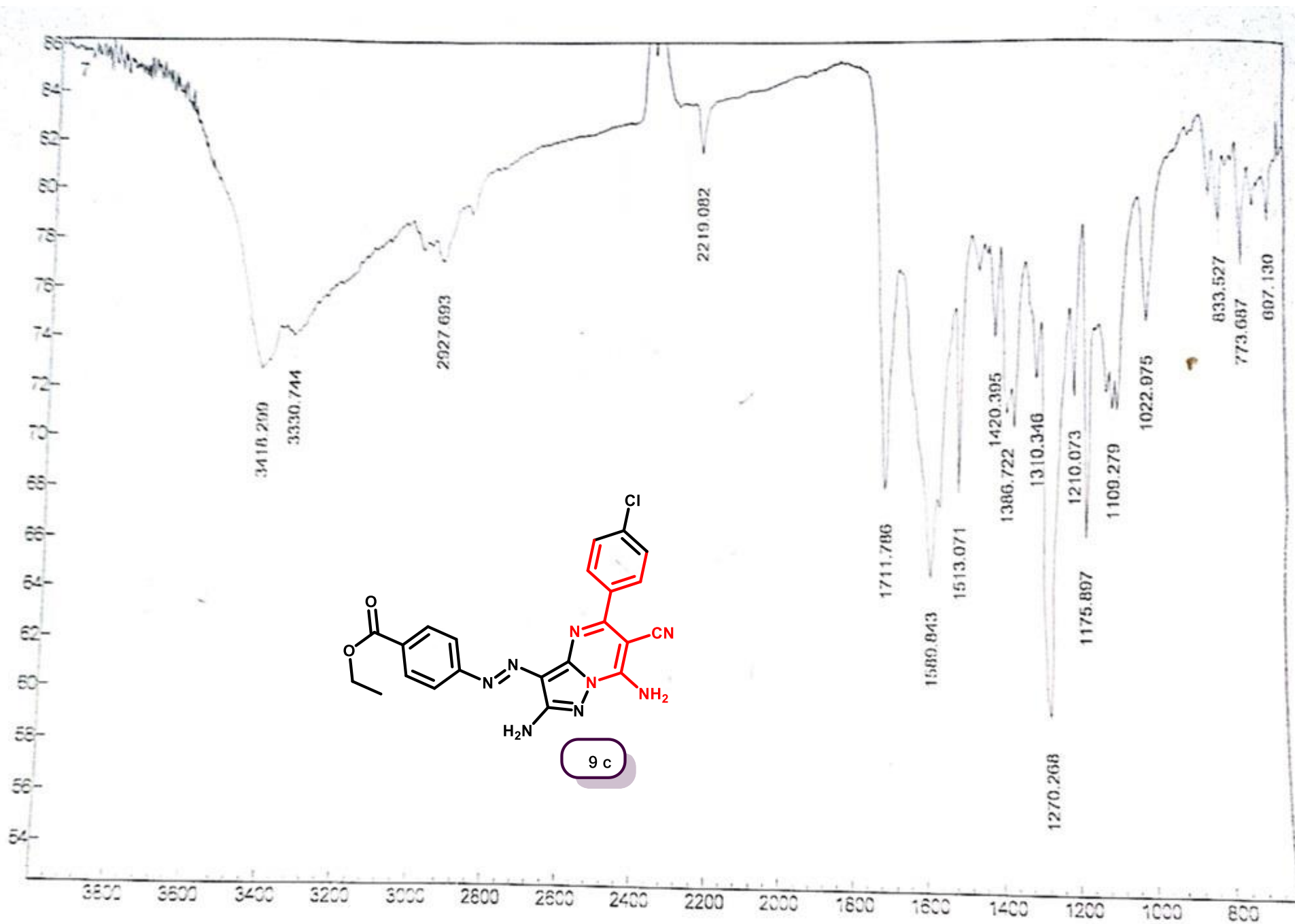




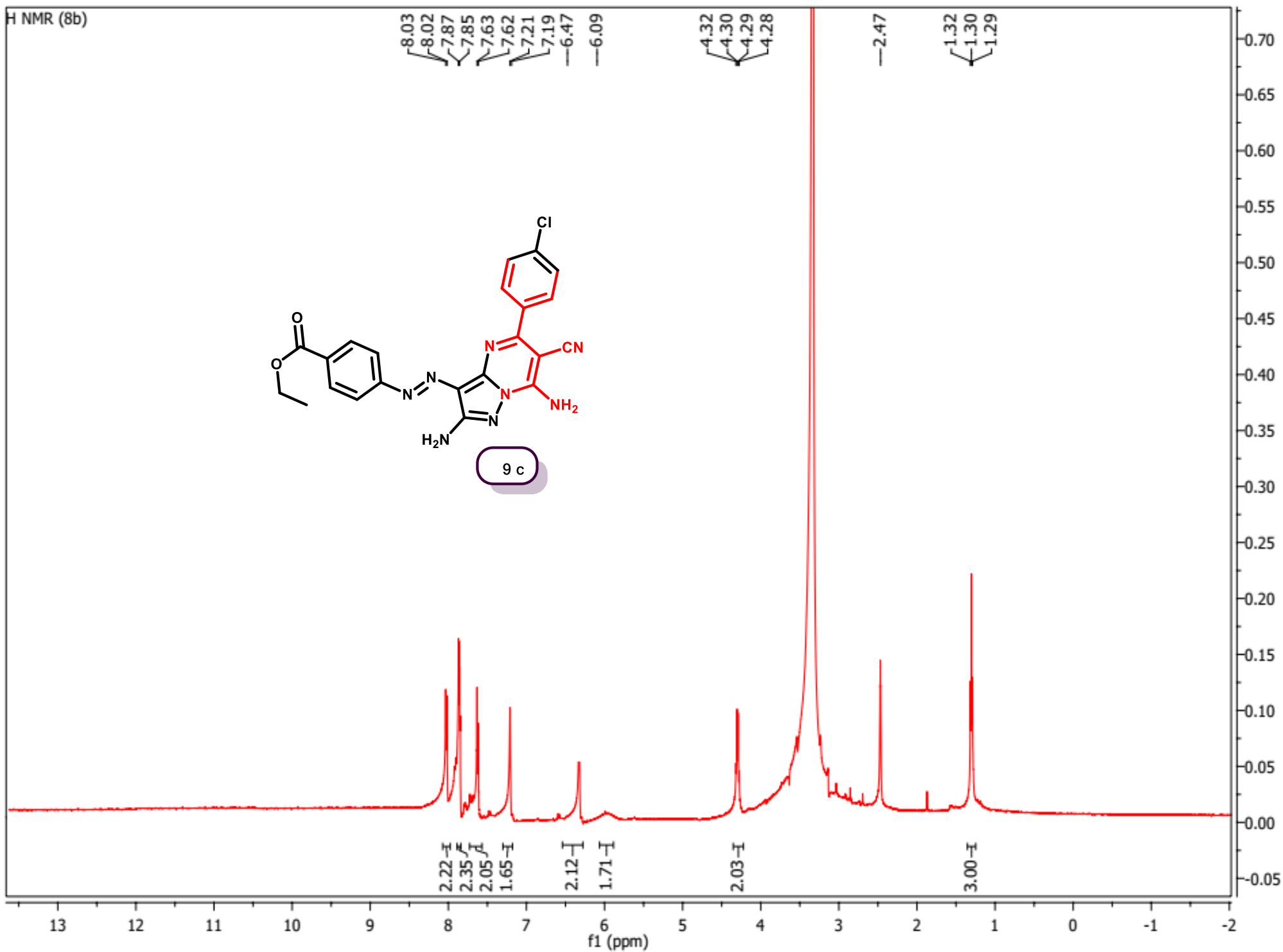
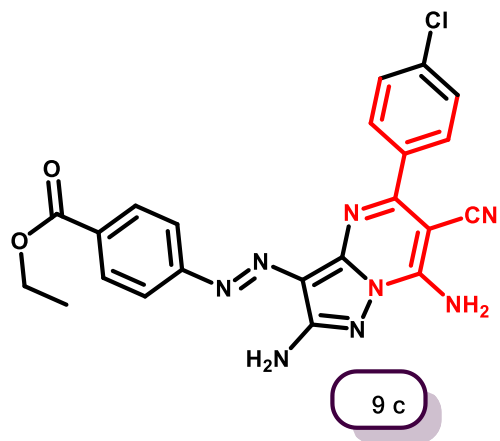








¹H NMR (8b)

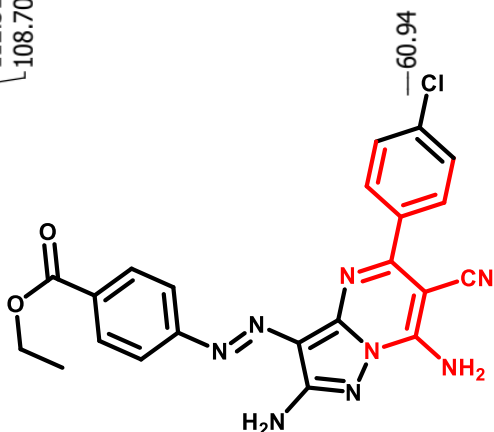


C NMR (8b)

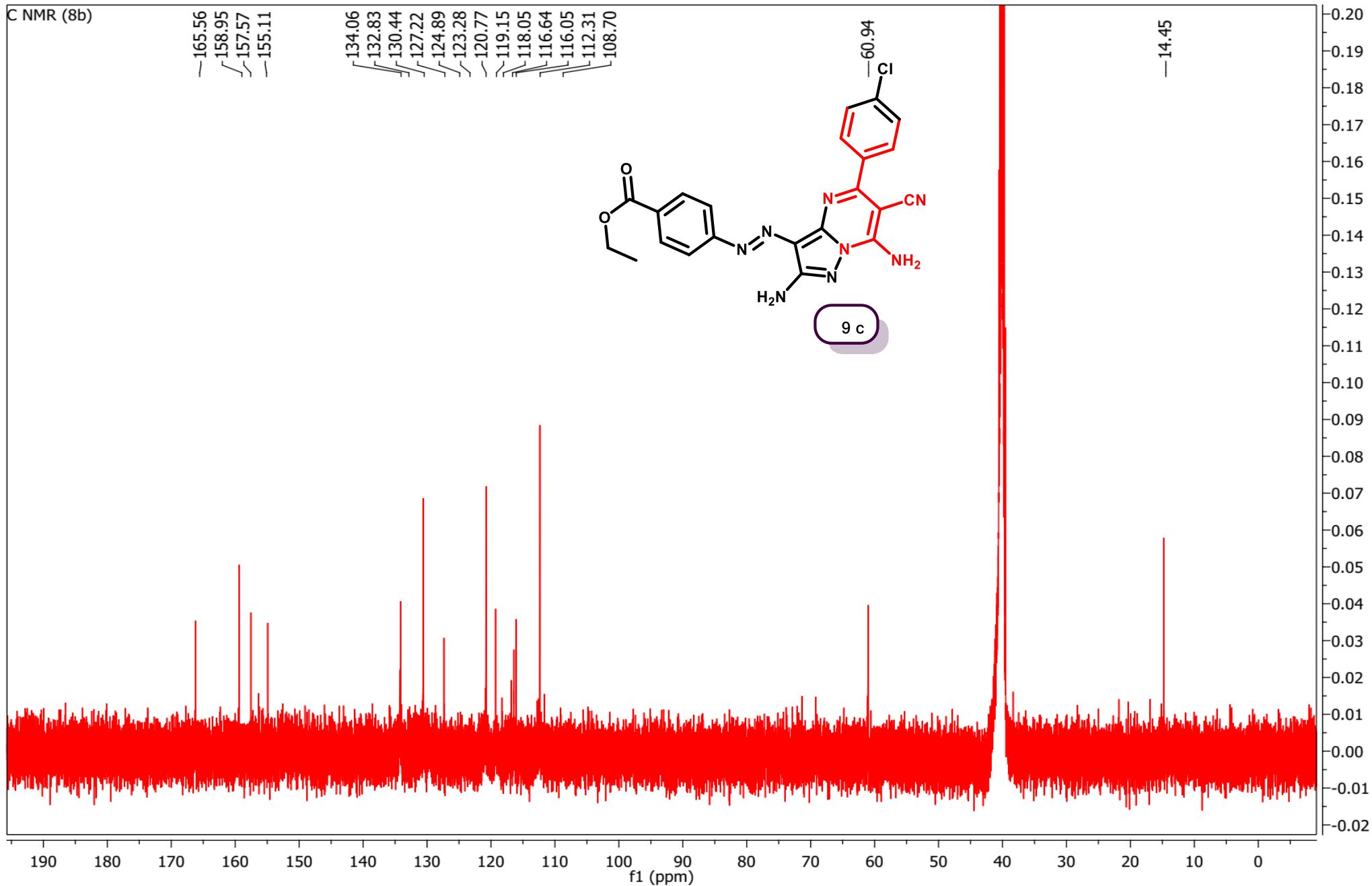
165.56
158.95
157.57
155.11

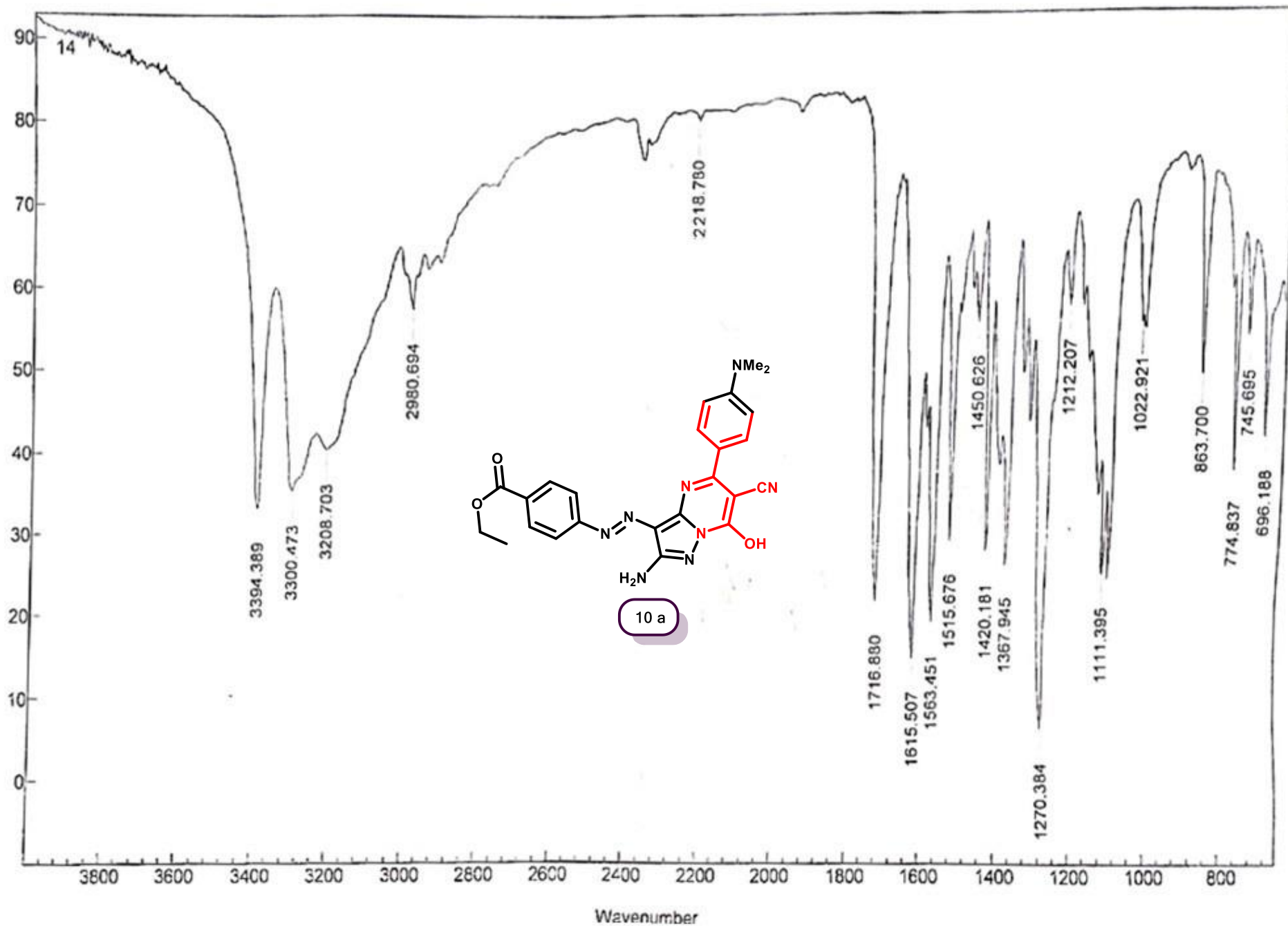
134.06
132.83
130.44
127.22
124.89
123.28
120.77
119.15
118.05
116.64
116.05
112.31
108.70

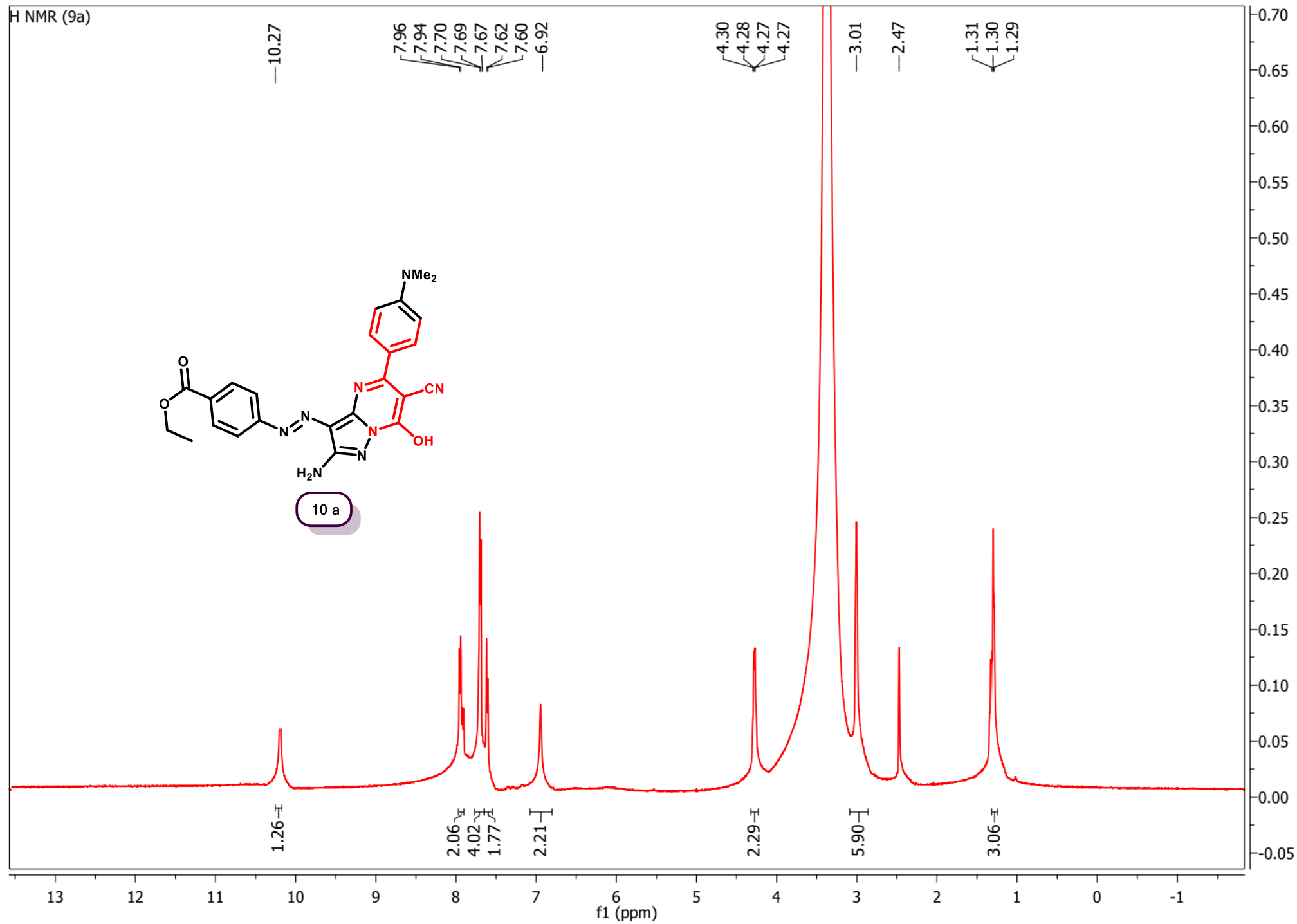
14.45

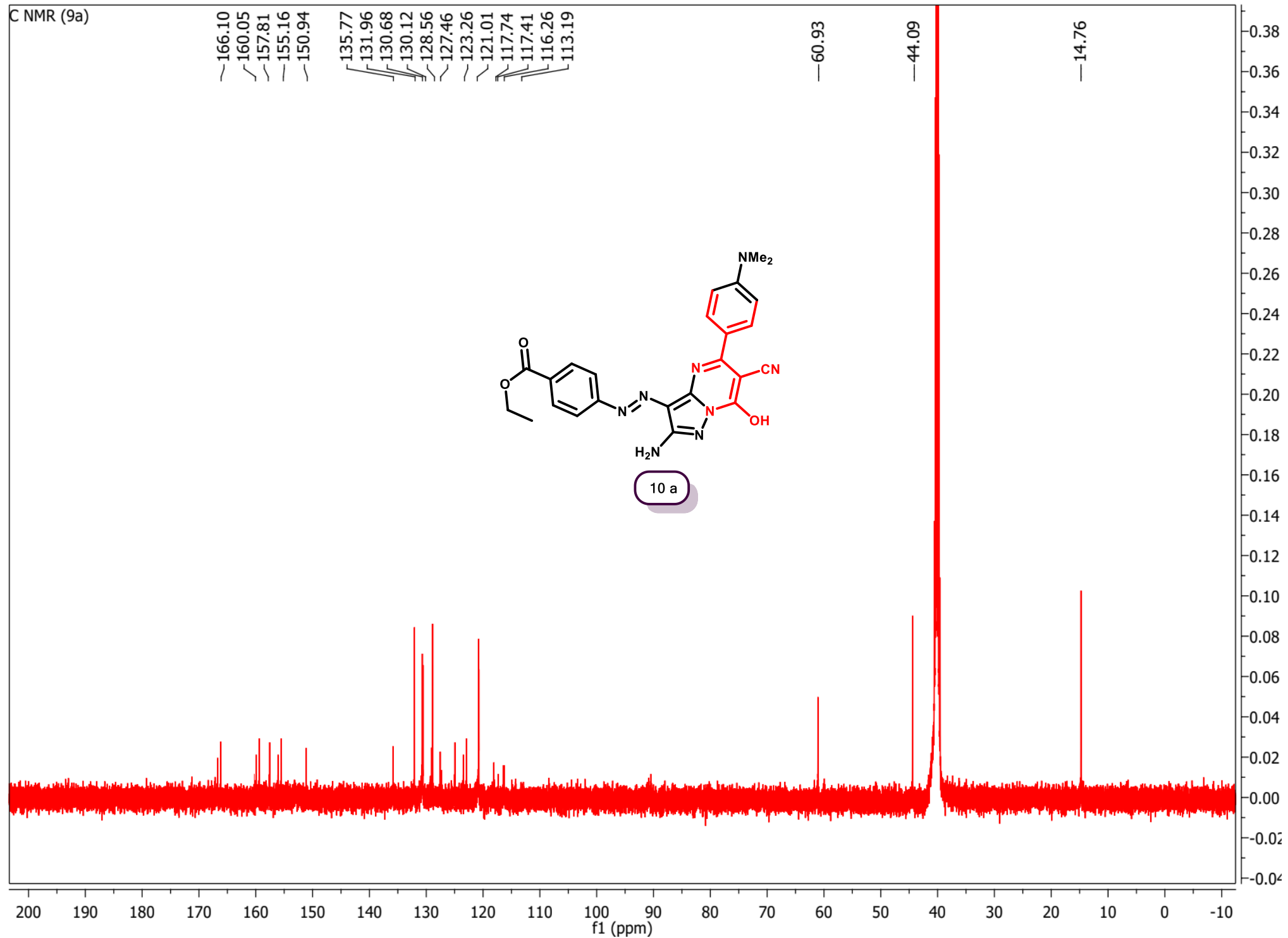


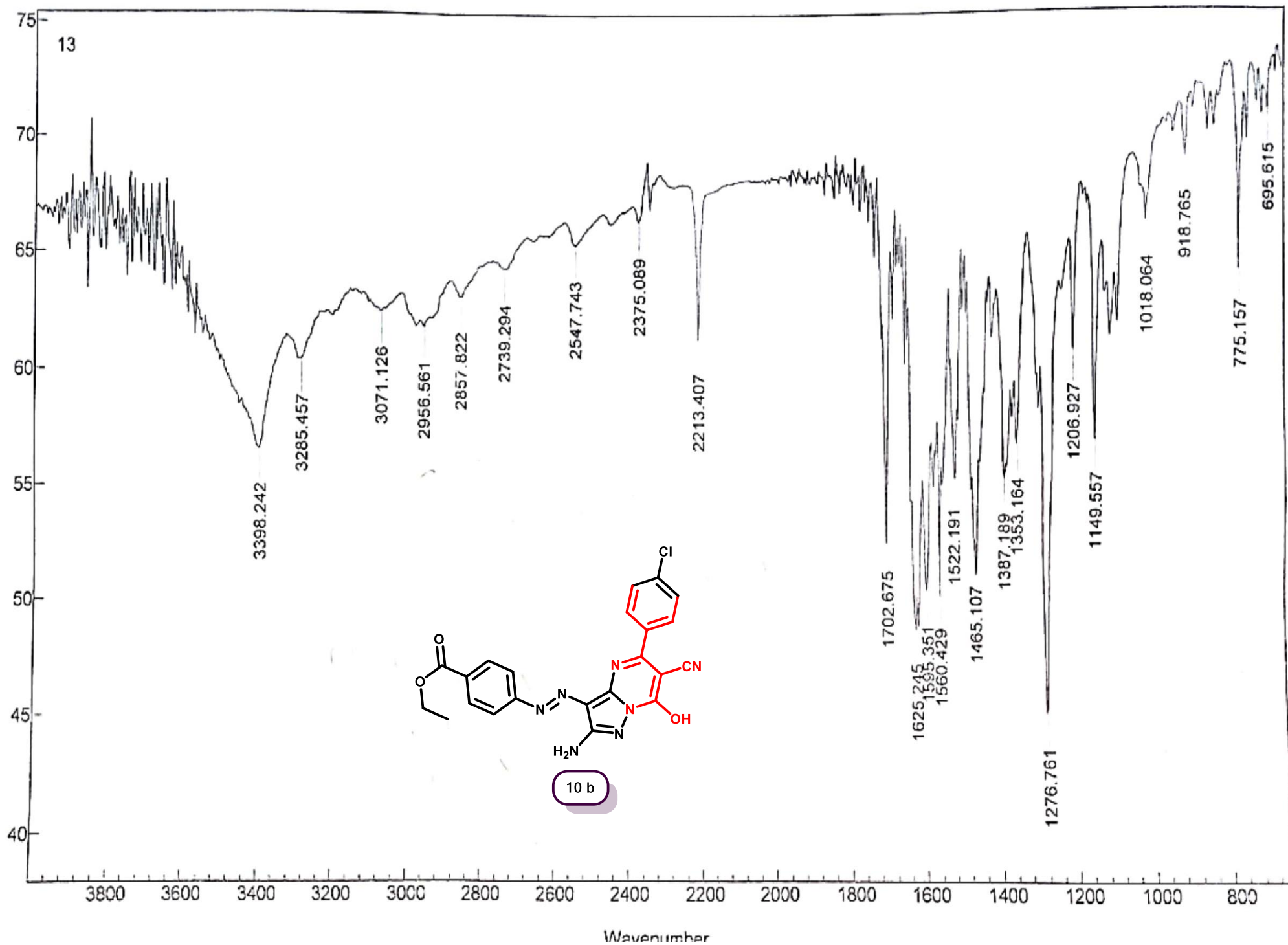
9 c

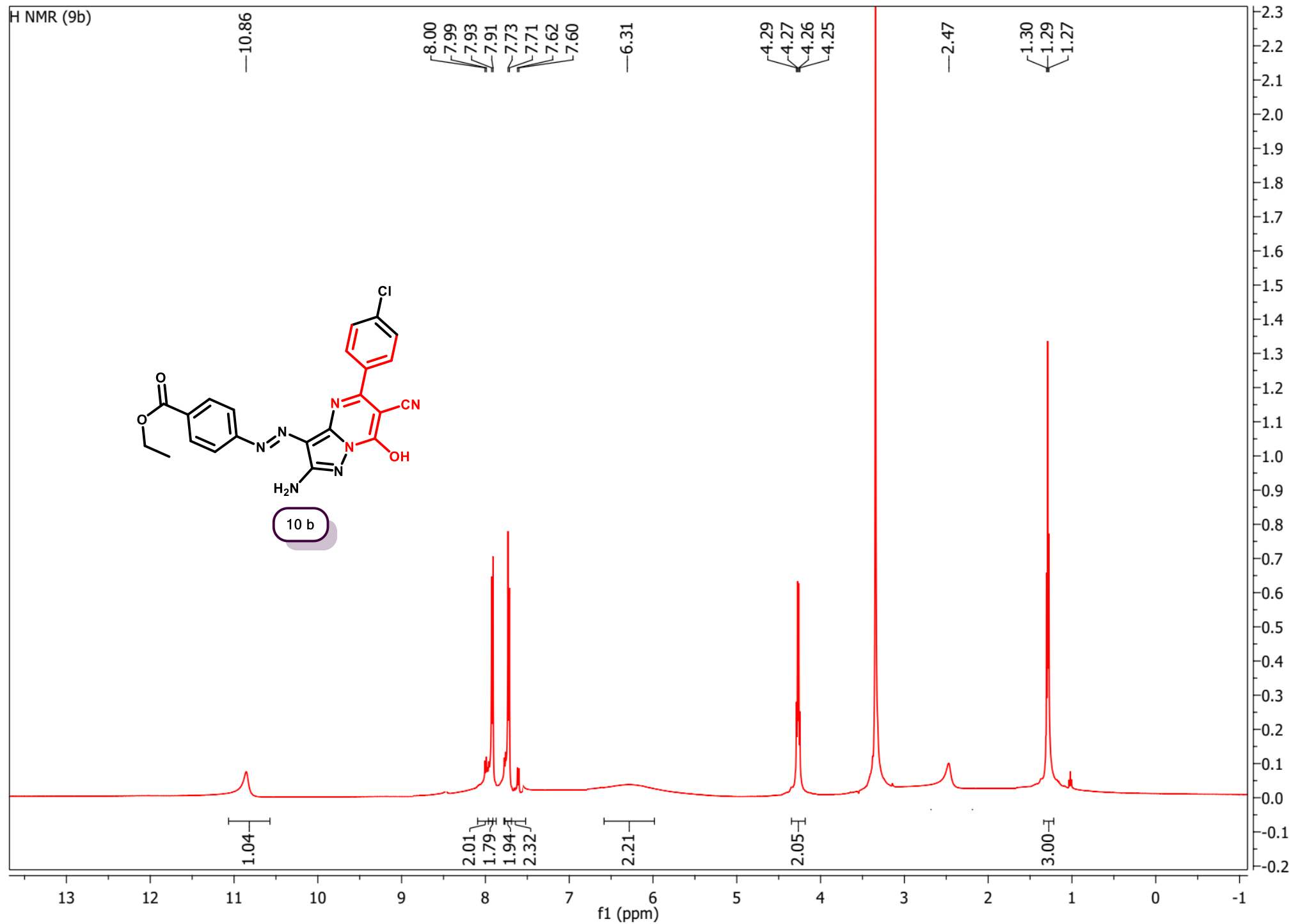


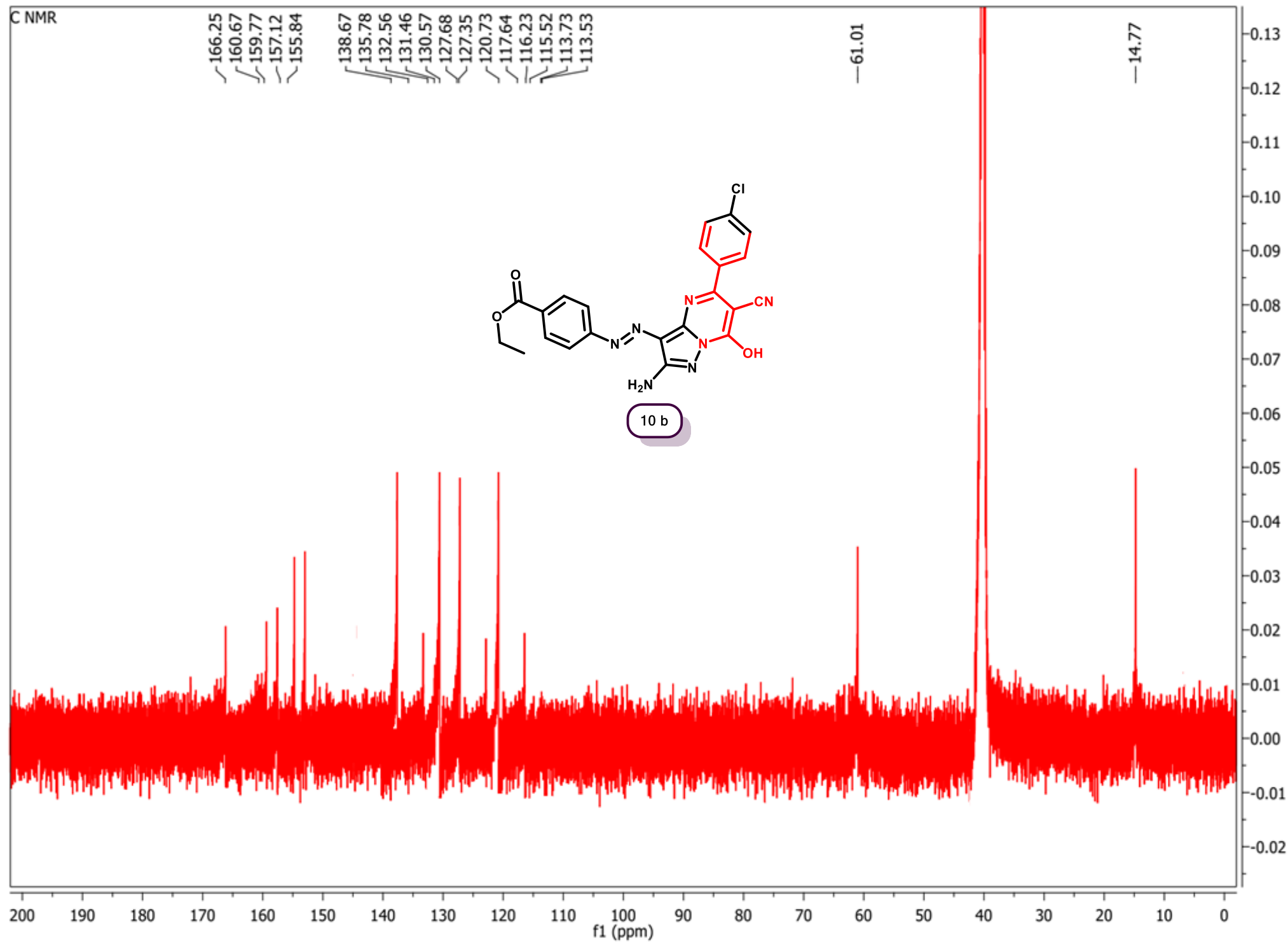


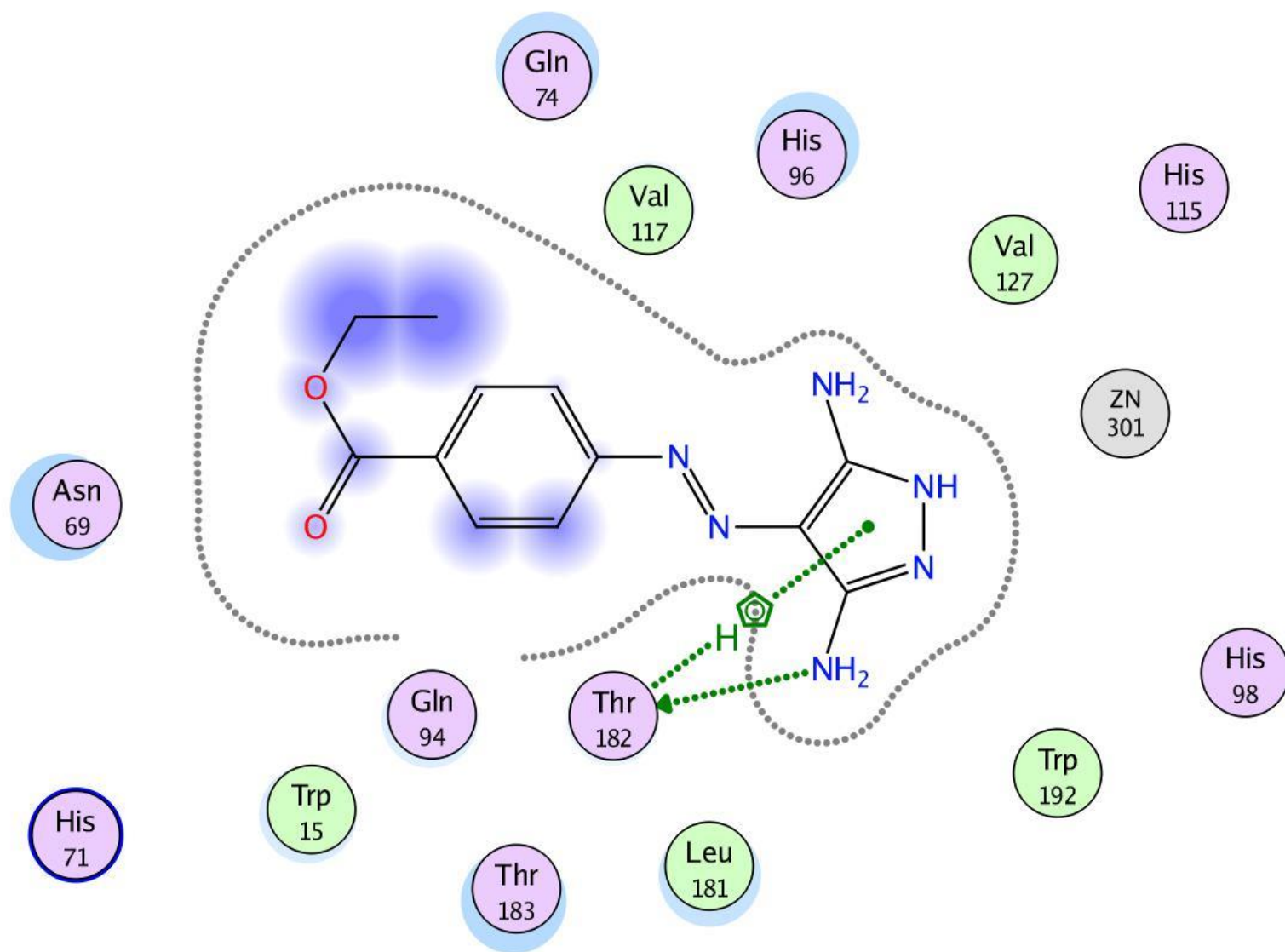




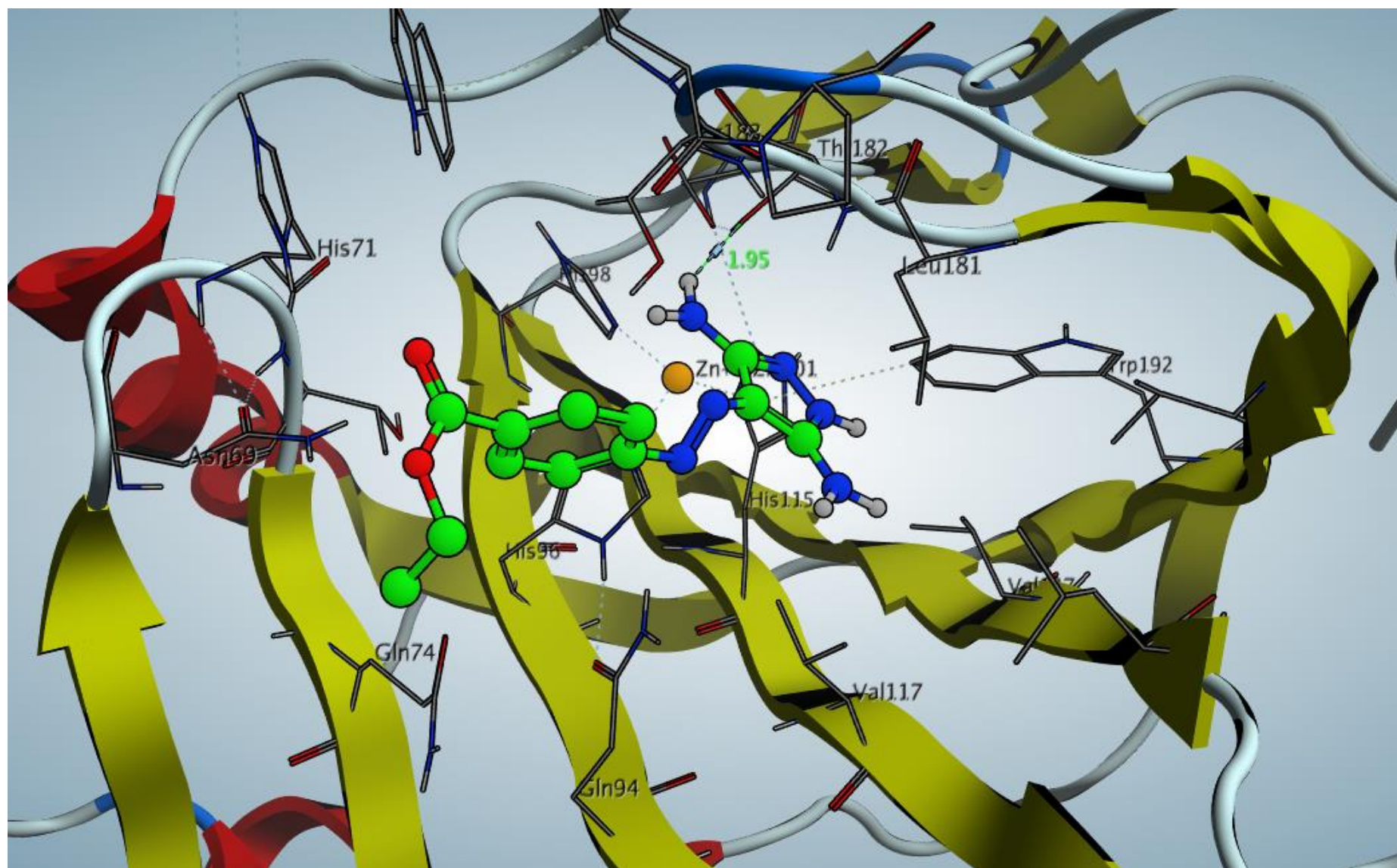




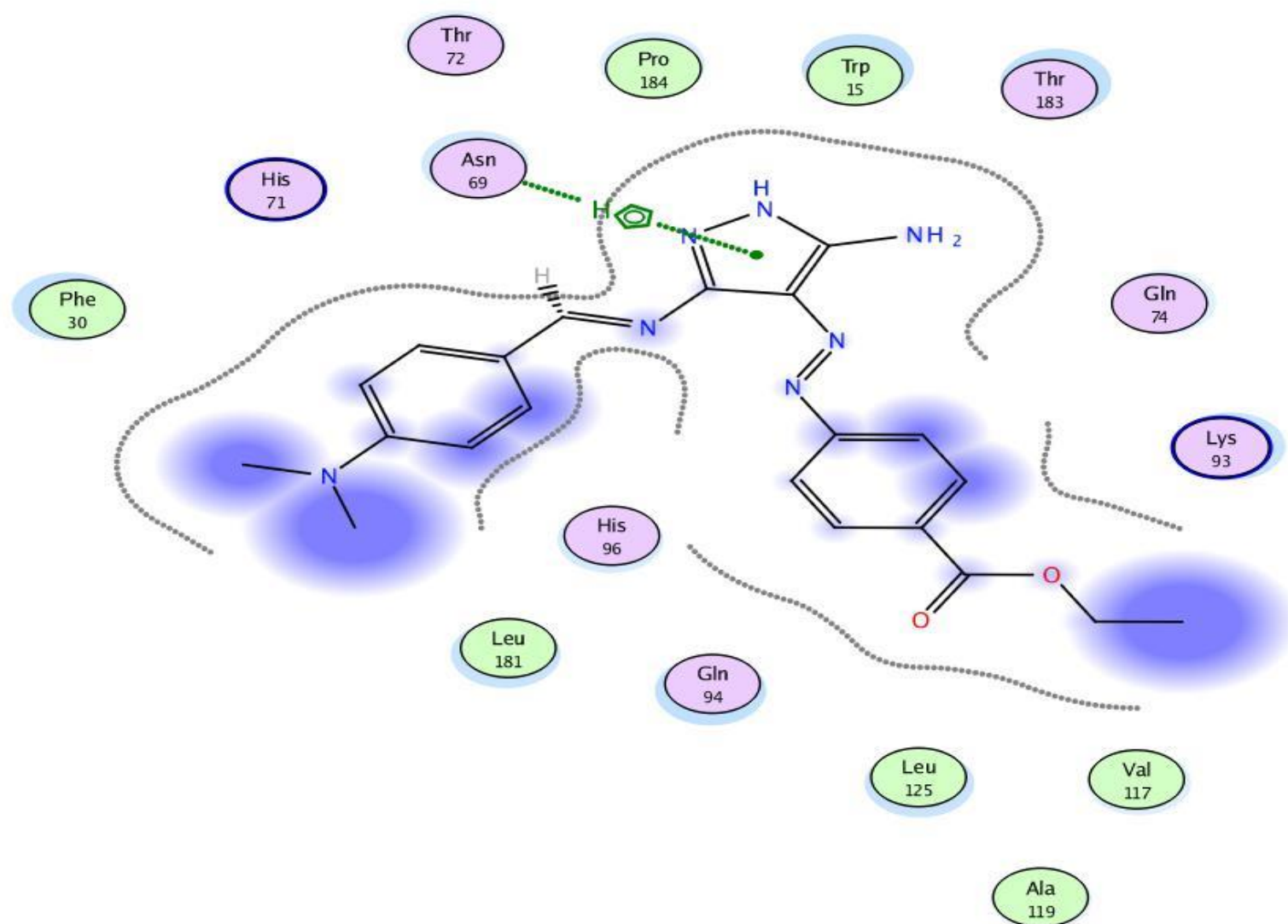




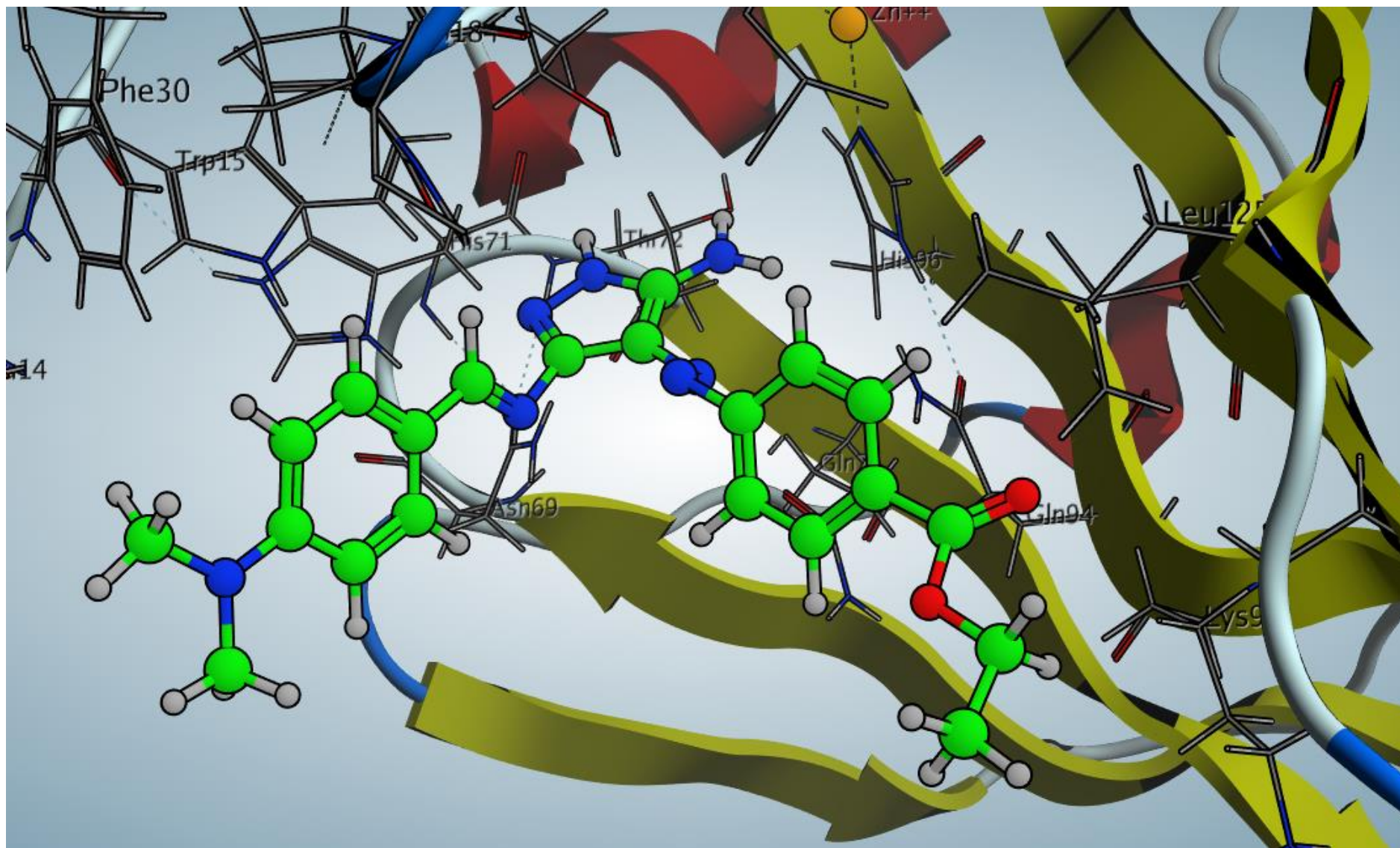
2D enzyme-ligand interaction of compounds **3a** inside the active site of alpha CA (PDB: 5HPJ)



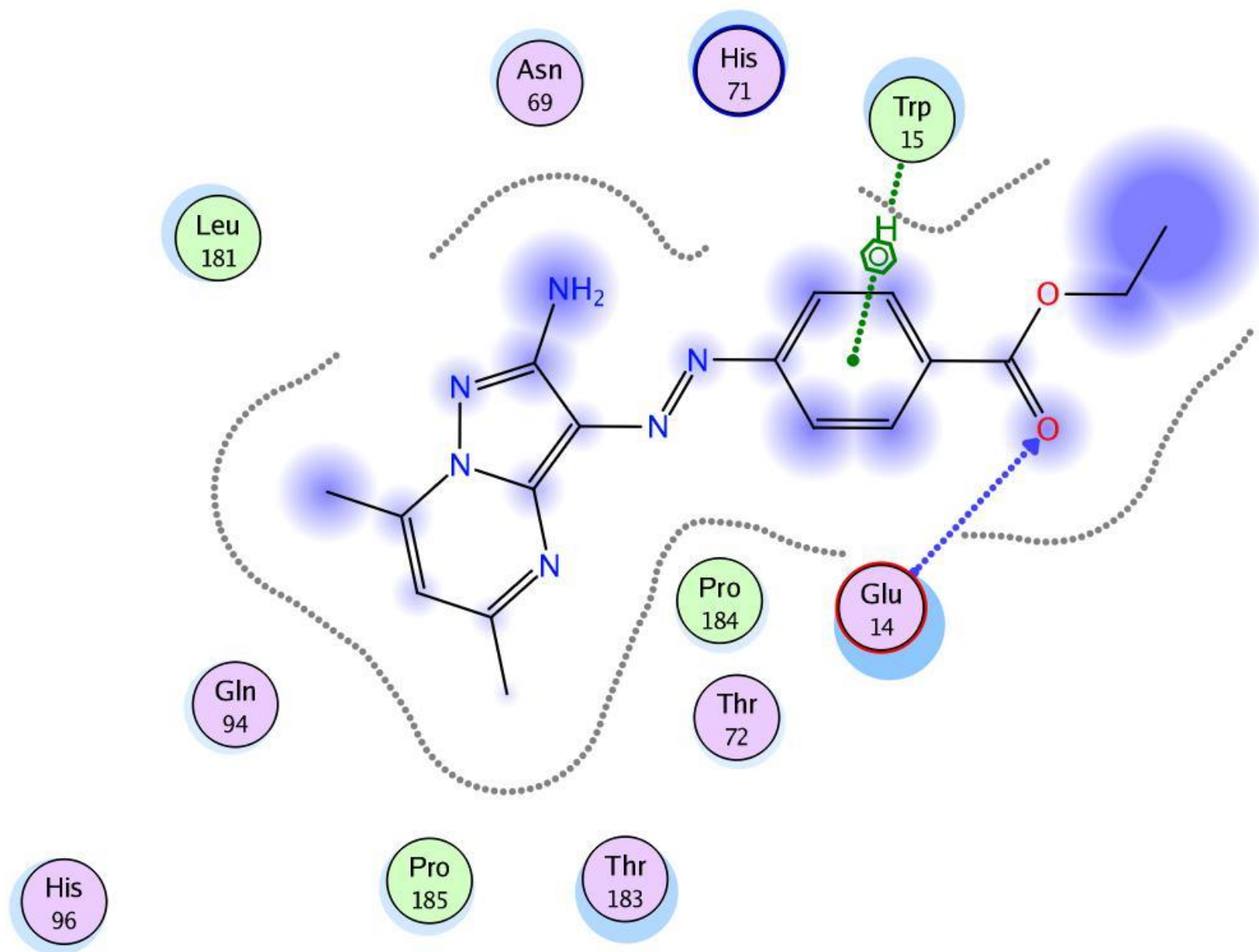
3D enzyme-ligand interaction of compounds **3a** inside the active site of alpha CA (PDB: 5HPJ)



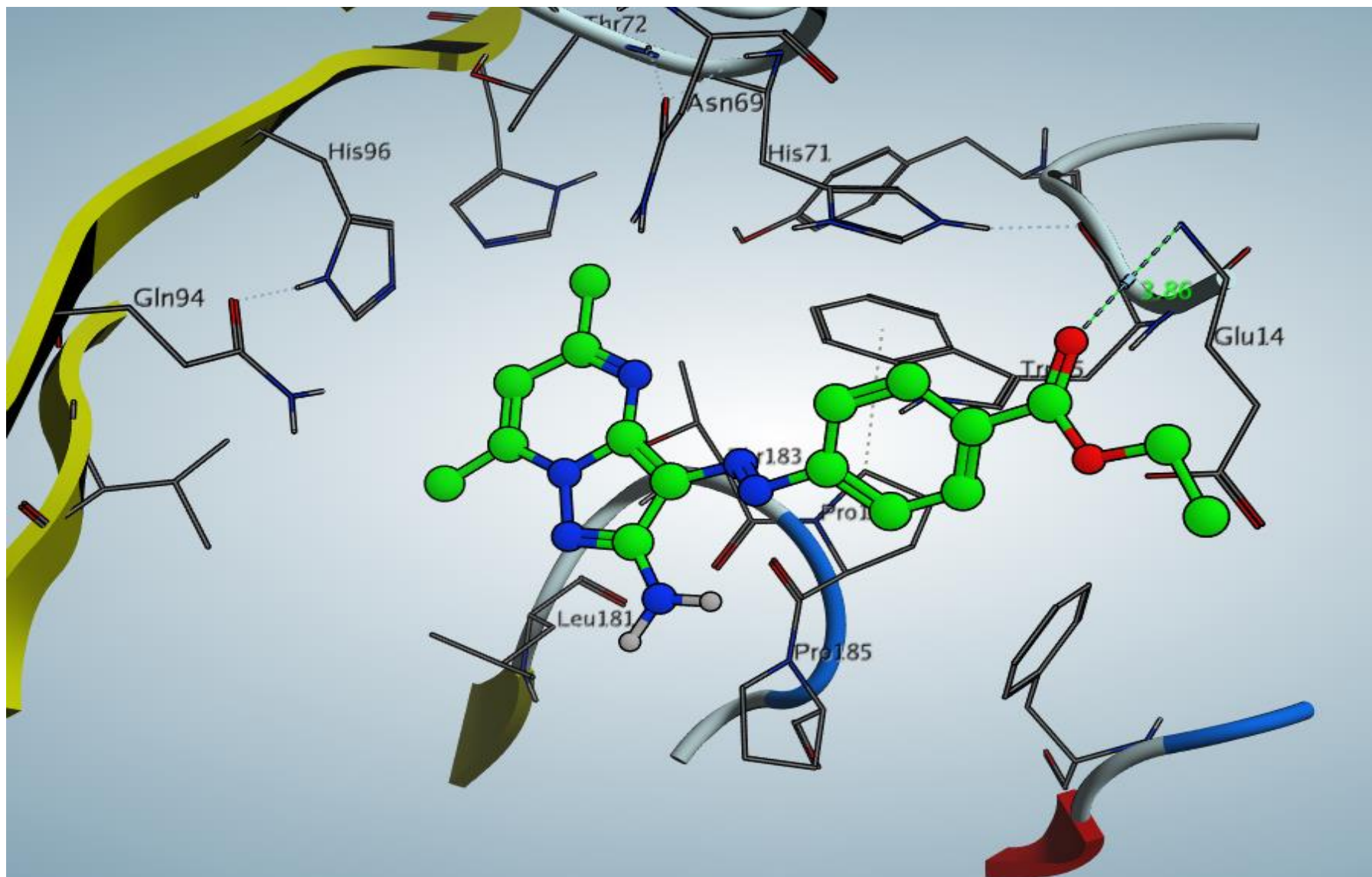
2D enzyme-ligand interaction of compounds **5a** inside the active site of alpha CA (PDB: 5HPJ)



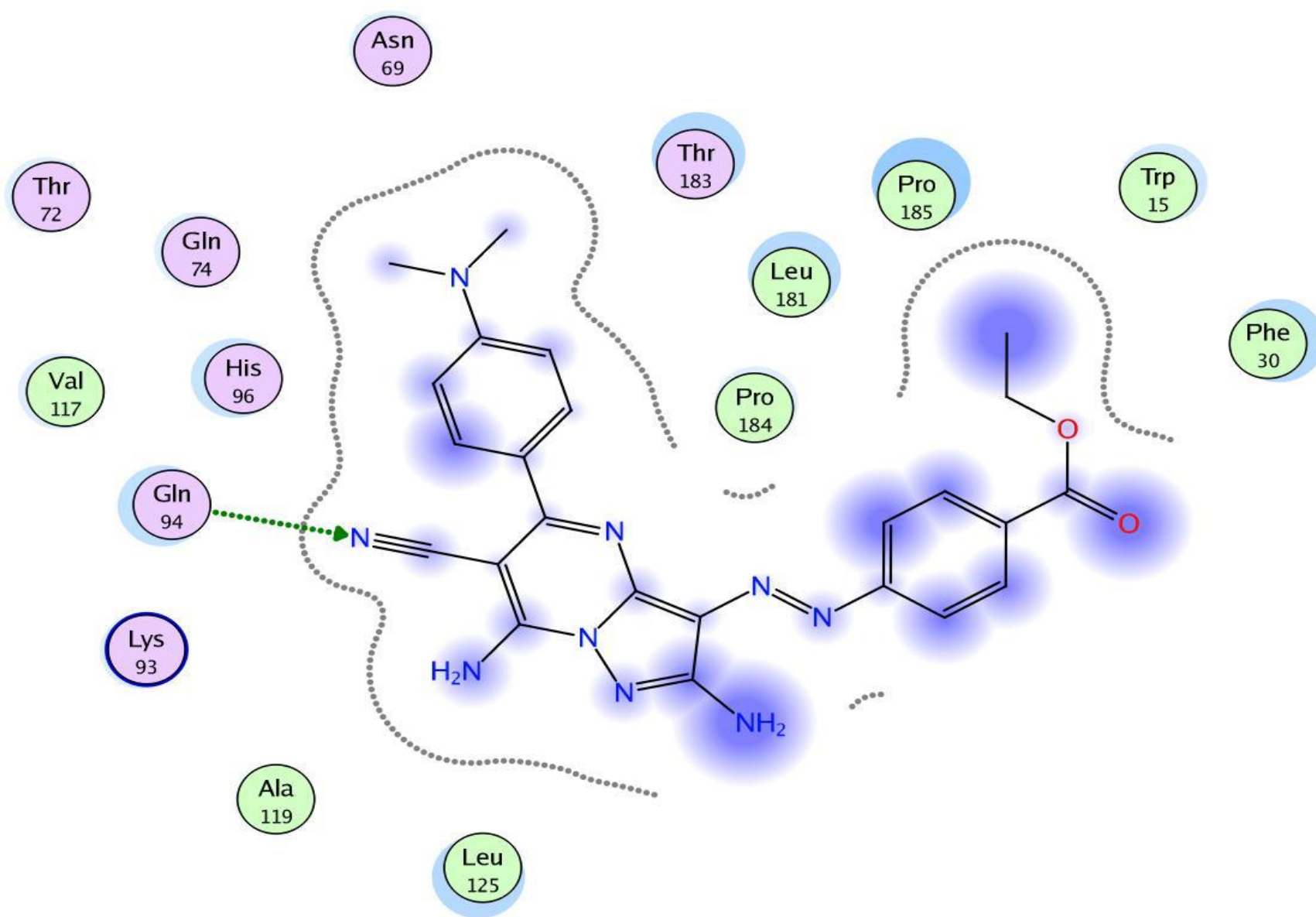
3D enzyme-ligand interaction of compounds **5a** inside the active site of alpha CA (PDB: 5HPJ)



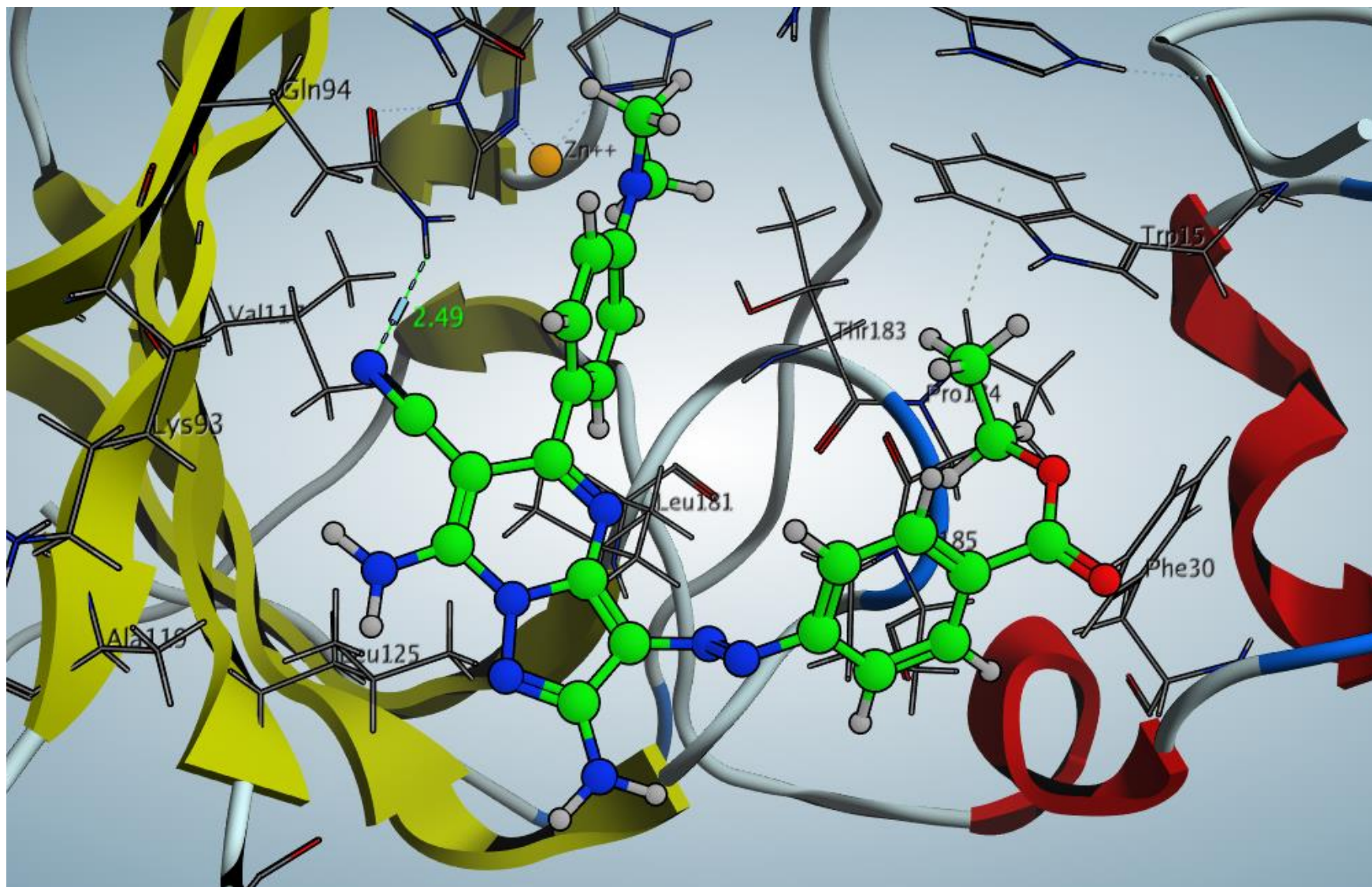
2D enzyme-ligand interaction of compounds **6** inside the active site of alpha CA (PDB: 5HPJ)



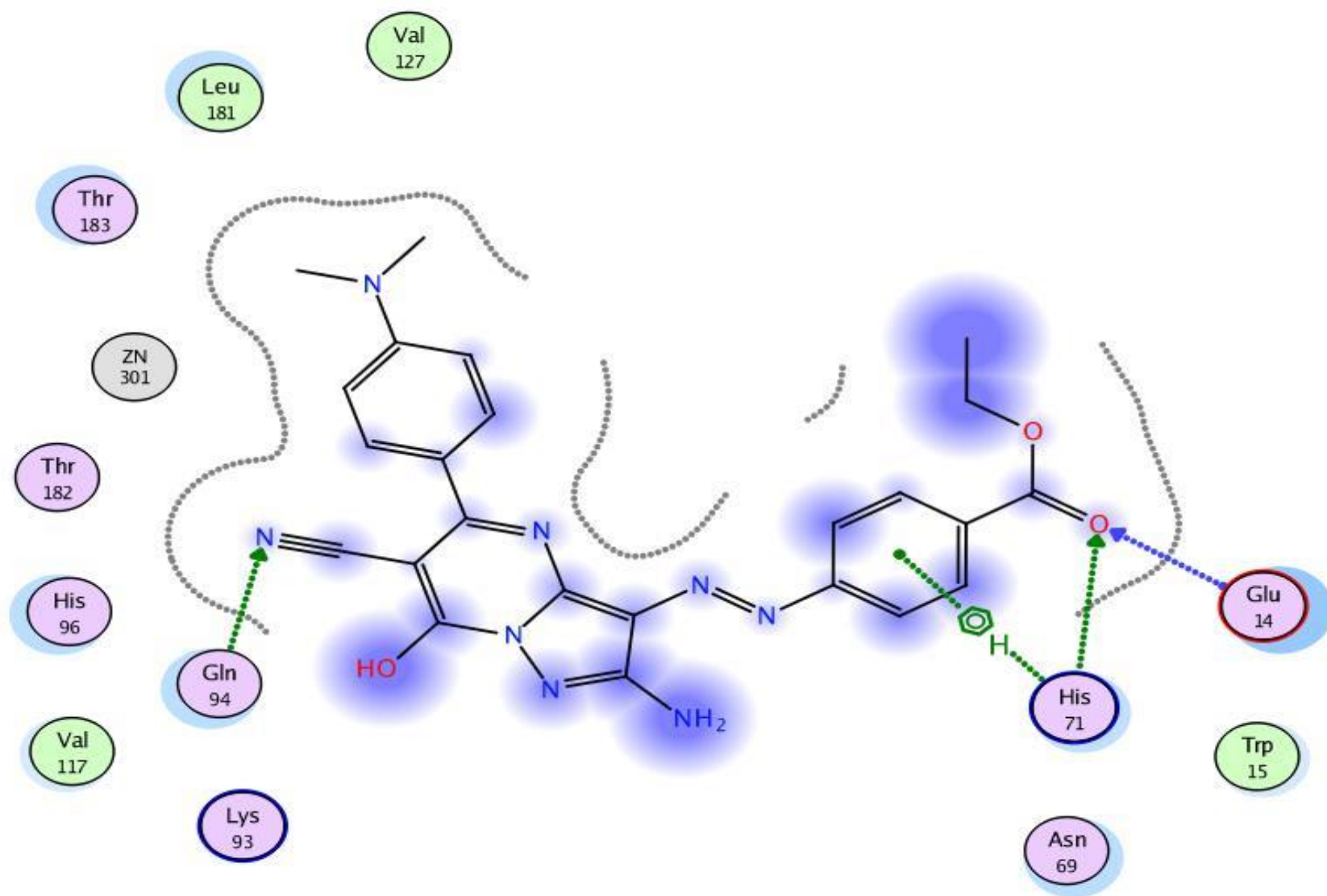
3D enzyme-ligand interaction of compounds 6 inside the active site of alpha CA (PDB: 5HPJ)



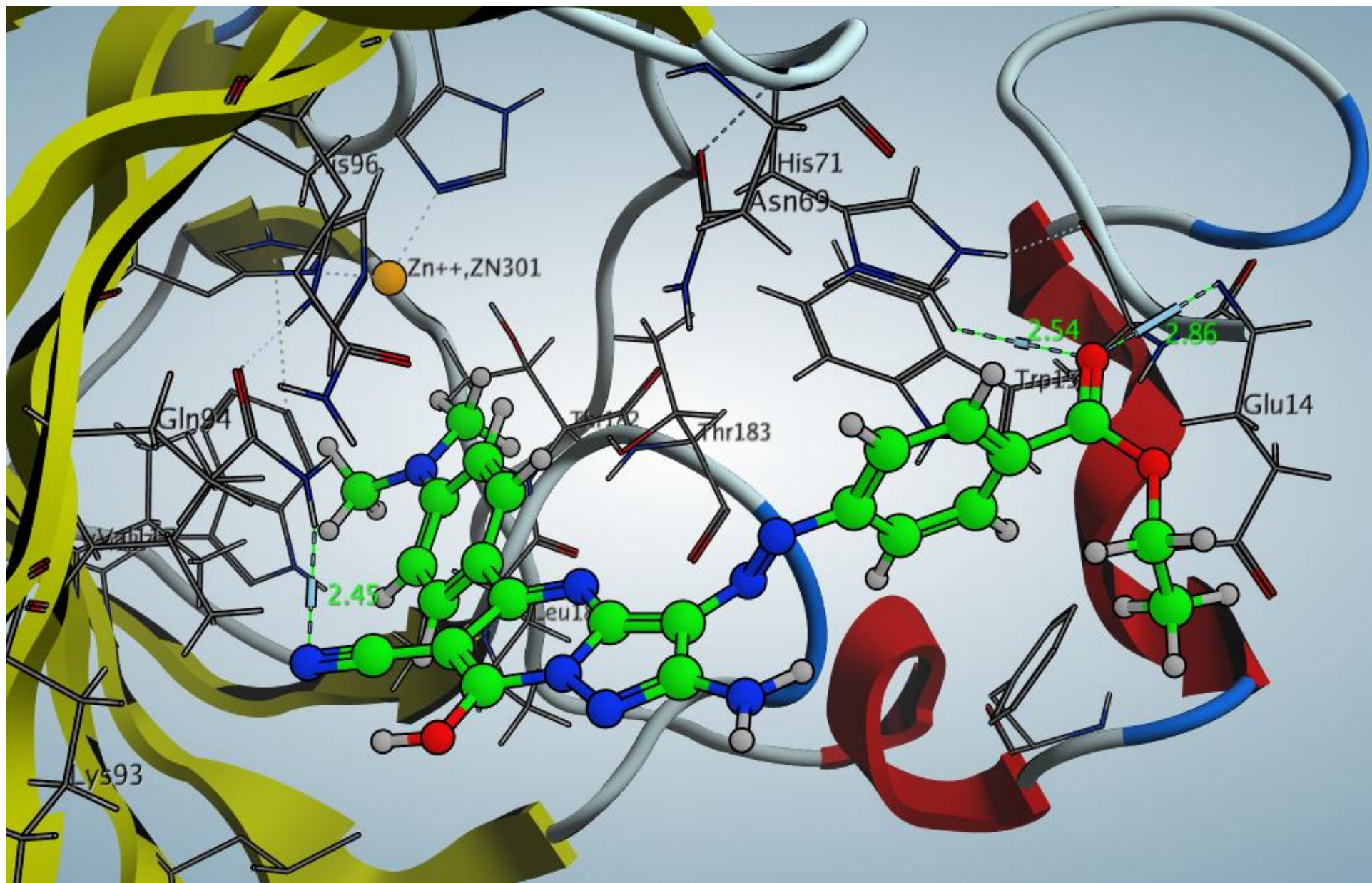
2D enzyme-ligand interaction of compounds **9a** inside the active site of alpha CA (PDB: 5HPJ)



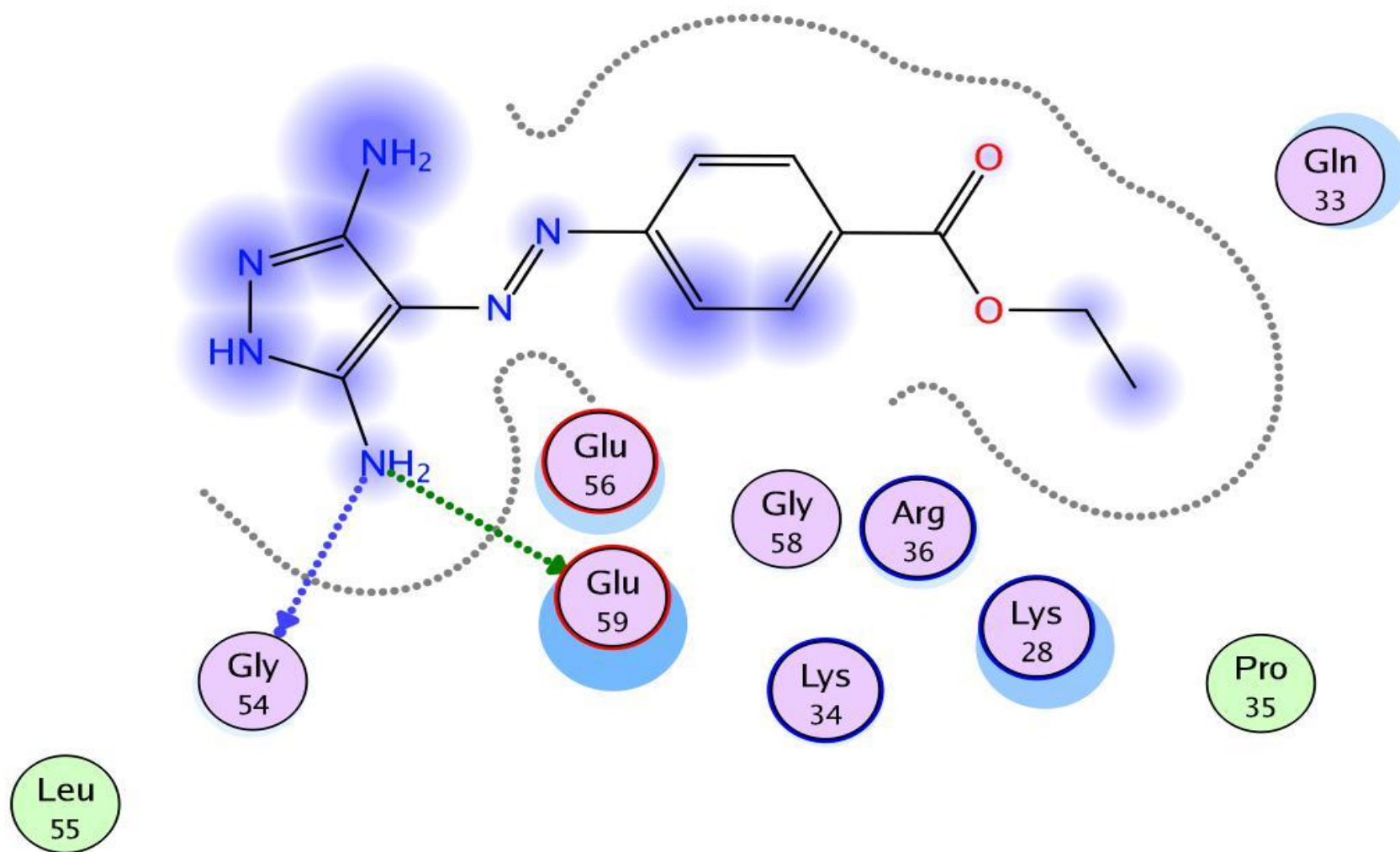
3D enzyme-ligand interaction of compounds **9a** inside the active site of alpha CA (PDB: 5HPJ)



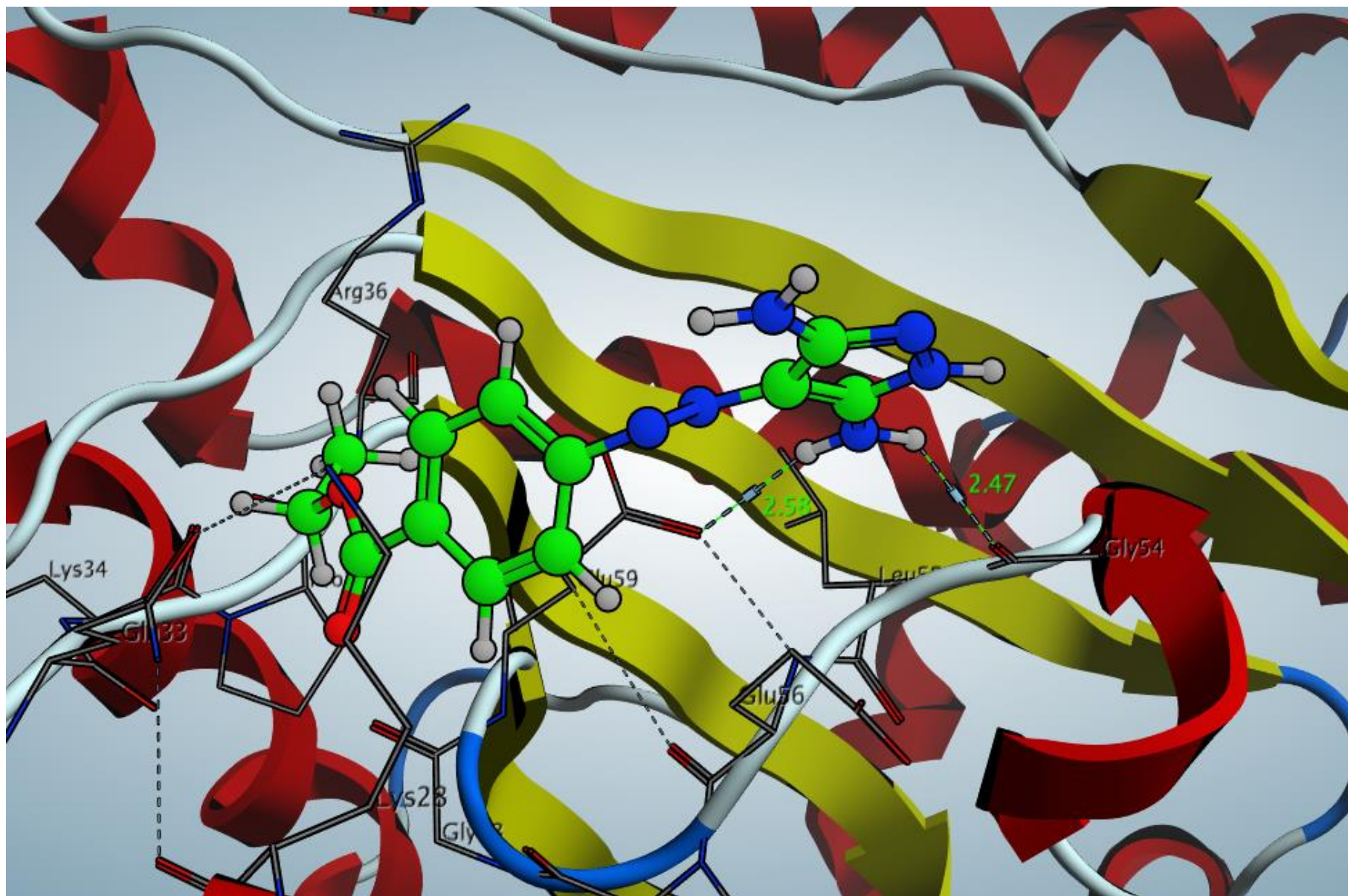
2D enzyme-ligand interaction of compounds **10a** inside the active site of alpha CA (PDB: 5HPJ)



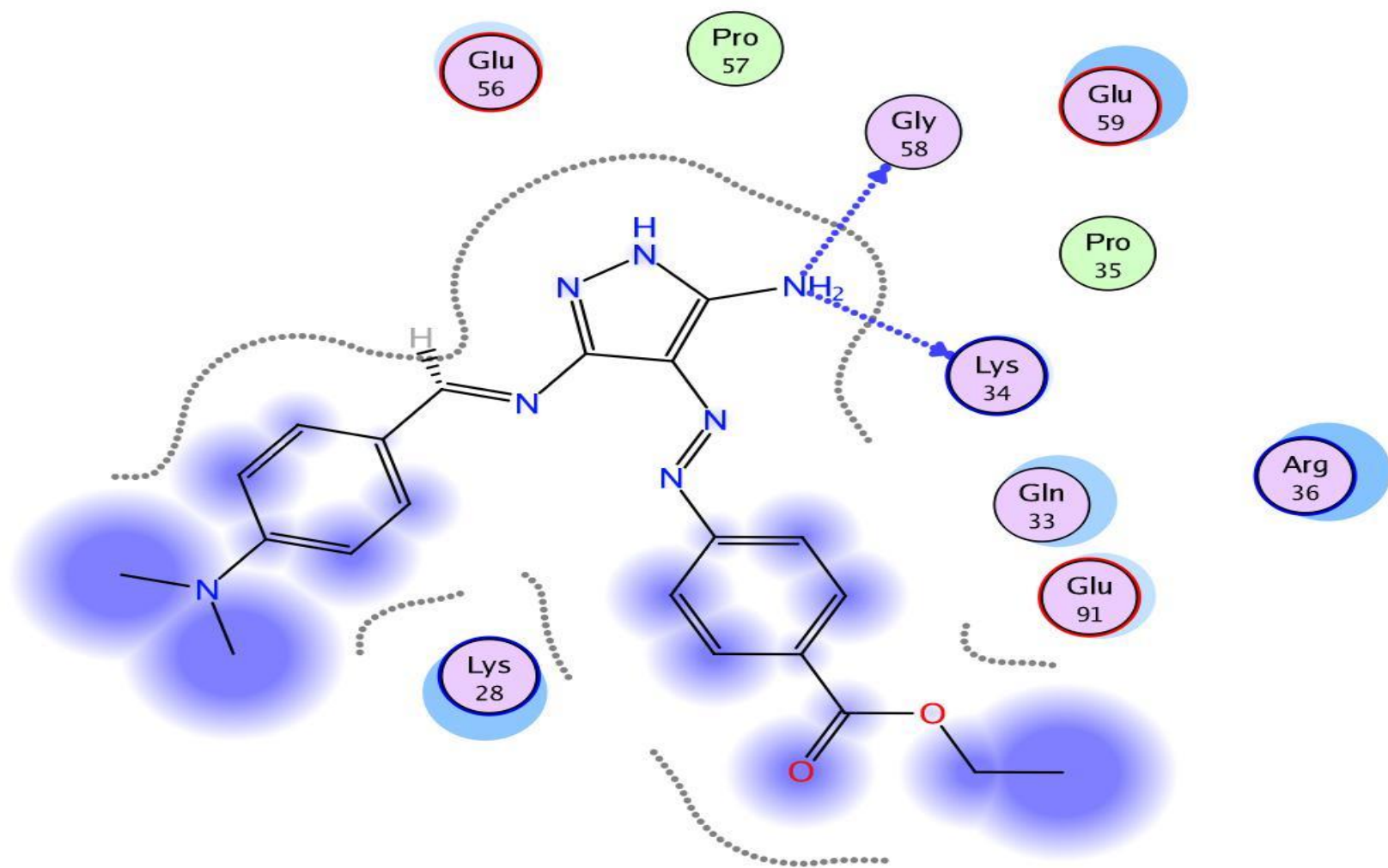
3D enzyme-ligand interaction of compounds **10a** inside the active site of alpha CA (PDB: 5HPJ)



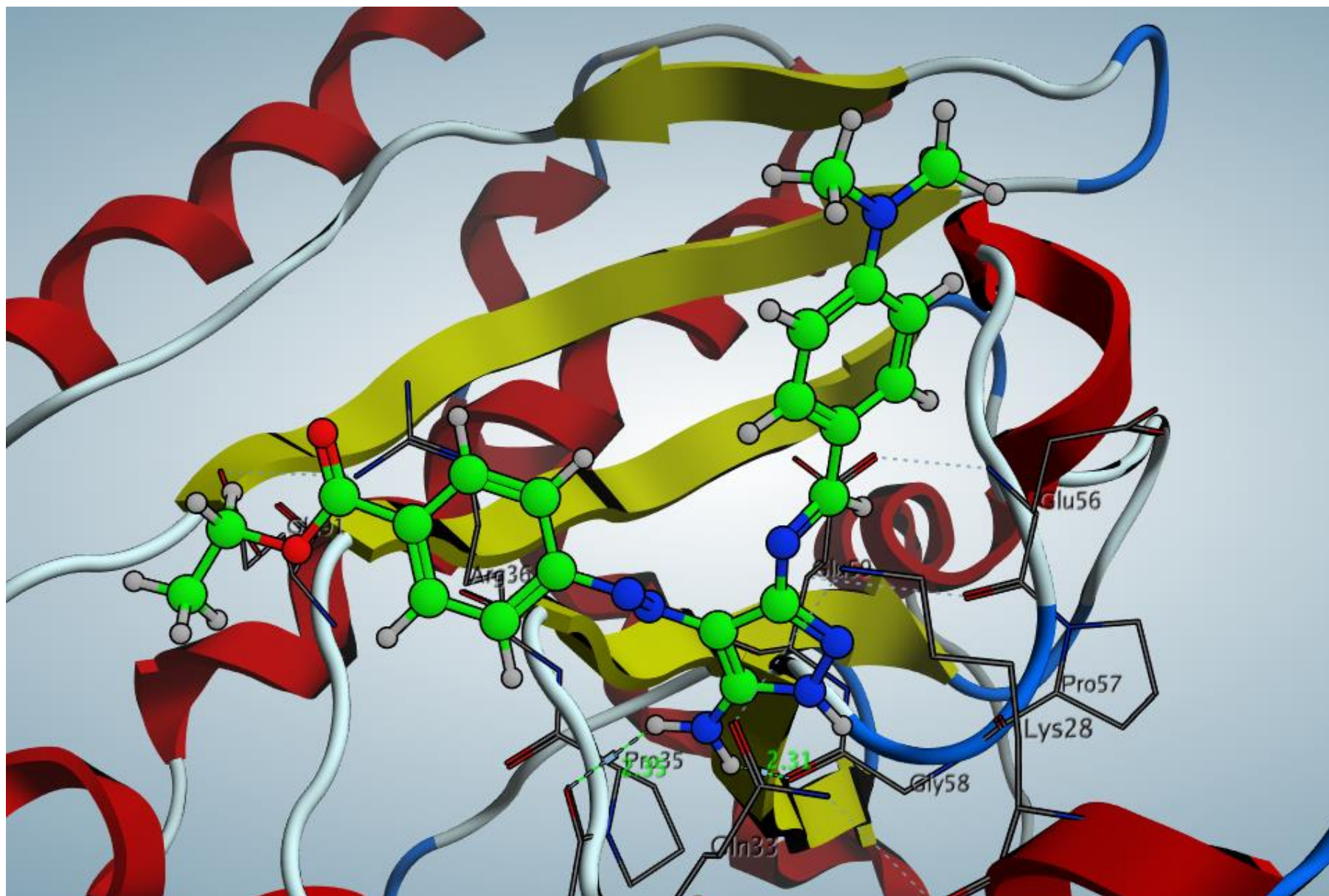
2D enzyme-ligand interaction of compounds 3a inside the active site of beta CA (PDB: 1I6P)



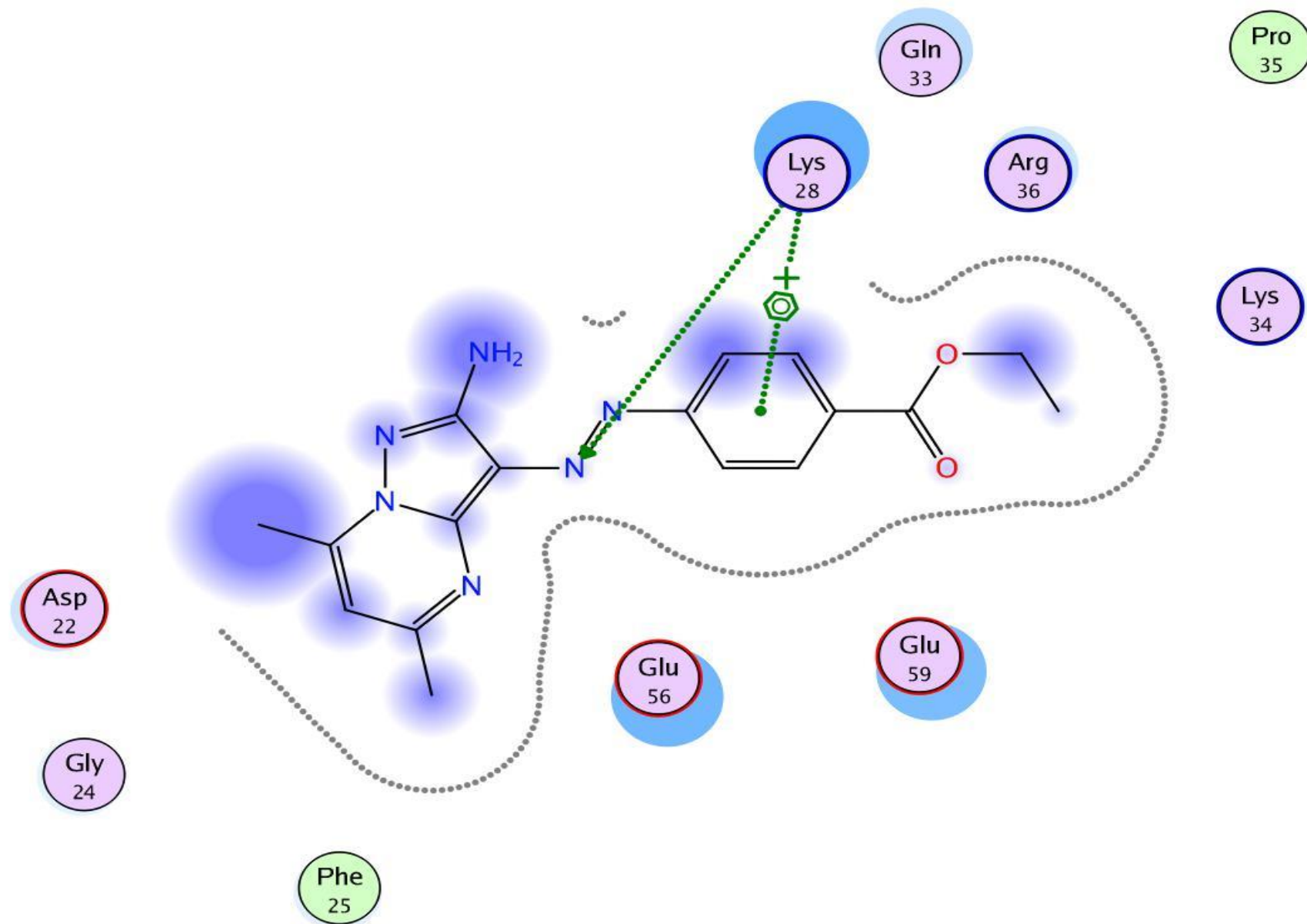
3D enzyme-ligand interaction of compounds 3a inside the active site of beta CA (PDB: 1I6P)



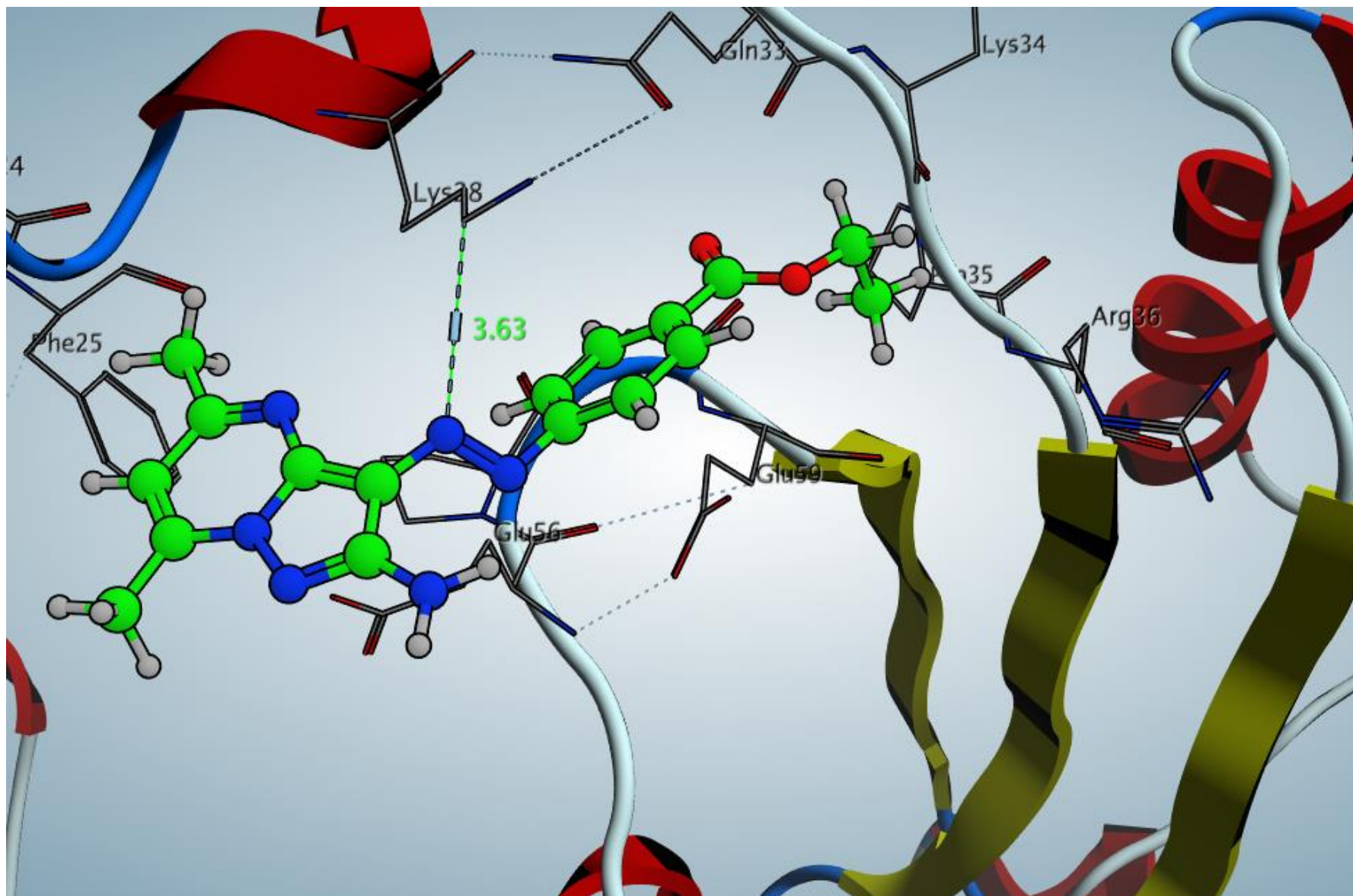
2D enzyme-ligand interaction of compounds 5a inside the active site of beta CA (PDB: 1I6P)



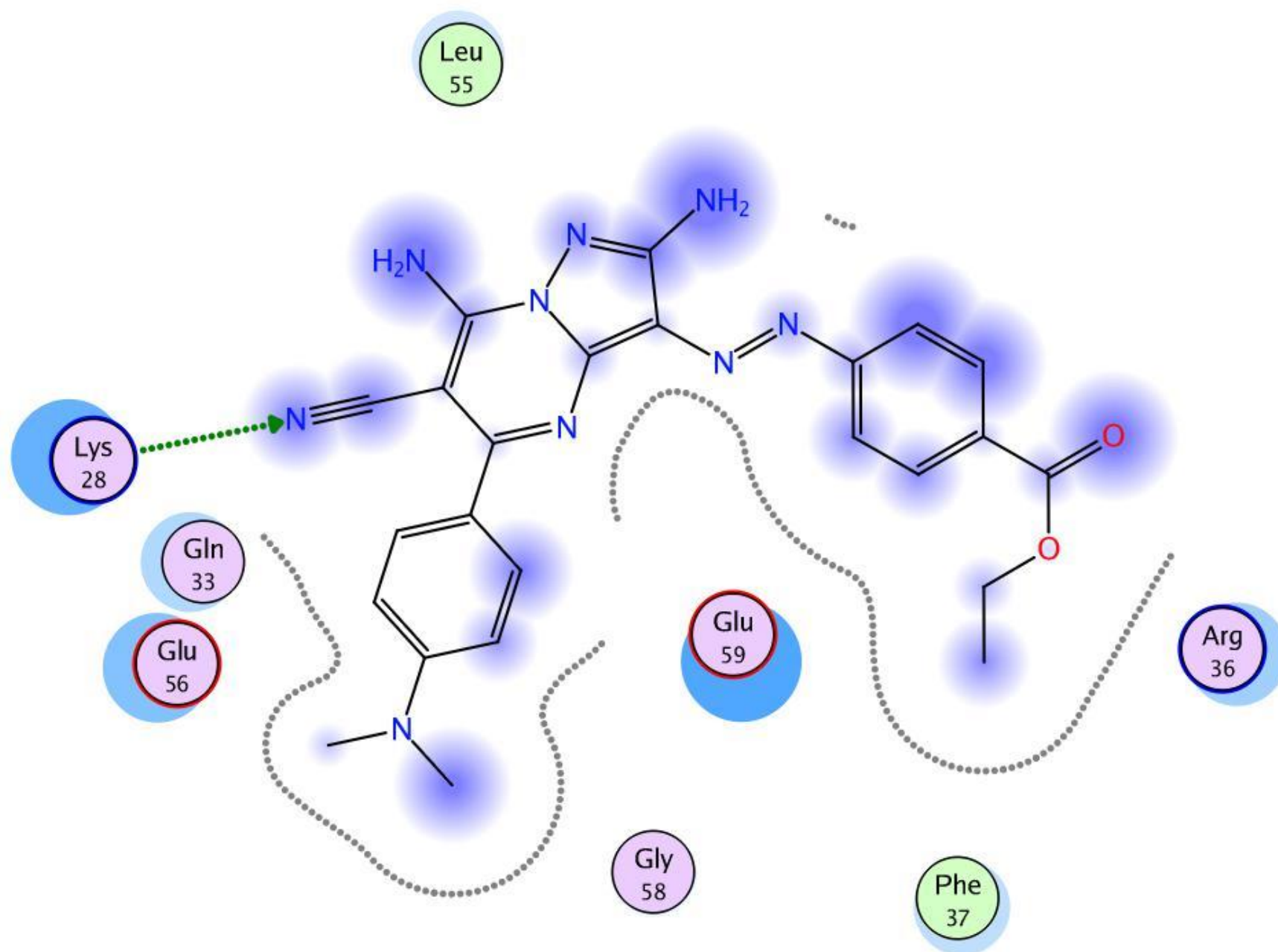
3D enzyme-ligand interaction of compounds 5a inside the active site of beta CA (PDB: 1I6P)



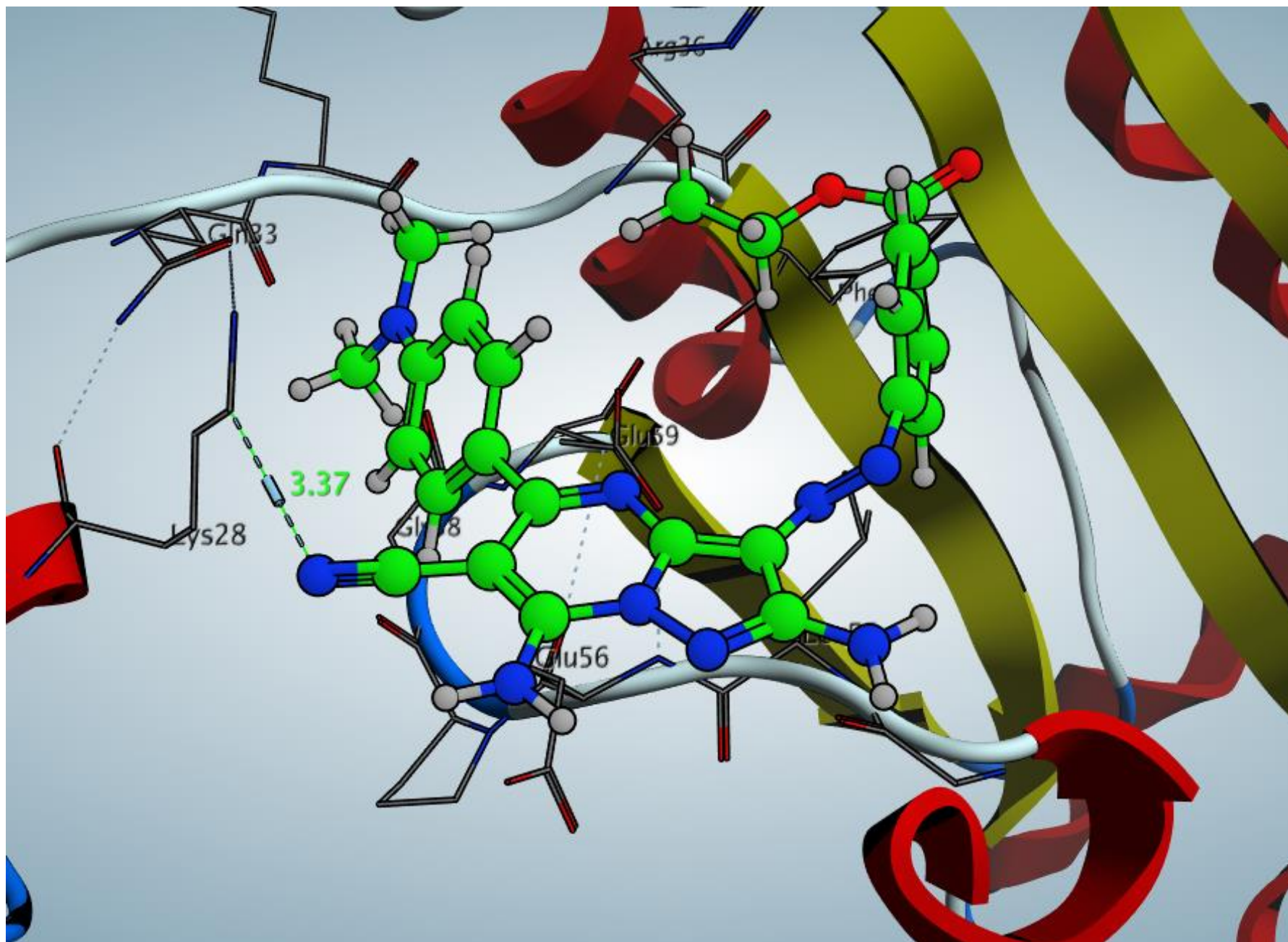
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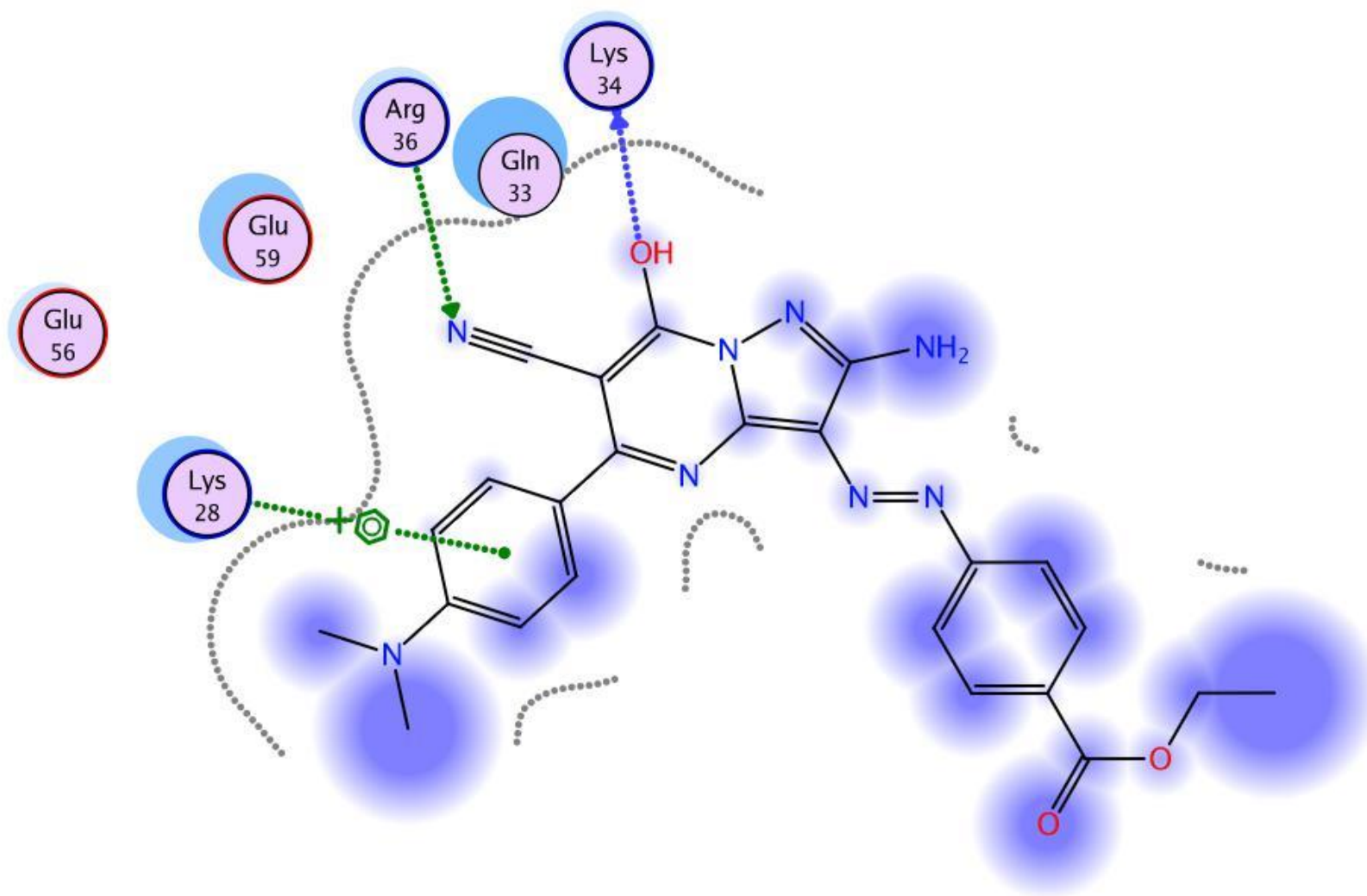
3D enzyme-ligand interaction of compounds 6 inside the active site of beta CA (PDB: 1I6P)



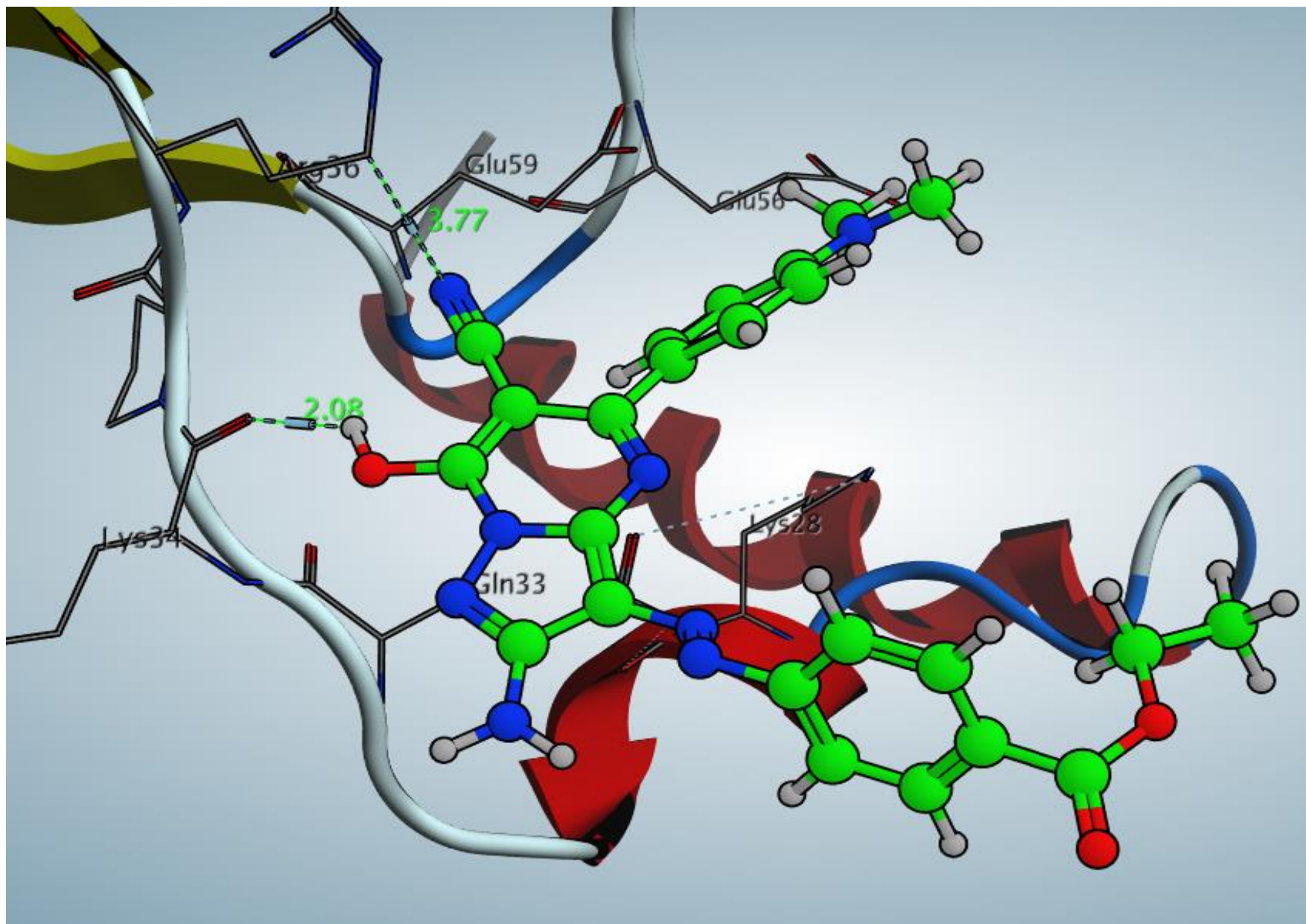
2D enzyme-ligand interaction of compounds 9a inside the active site of beta CA (PDB: 1I6P)



3D enzyme-ligand interaction of compounds 9a inside the active site of beta CA (PDB: 1I6P)



2D enzyme-ligand interaction of compounds 10a inside the active site of beta CA (PDB: 1I6P)



3D enzyme-ligand interaction of compounds **10a** inside the active site of beta CA (PDB: 1I6P)