

Electronic Supplementary Information

for

Synthesis and SAR Studies of Pyrazole-3-Carboxamides and -Thioureides Including Chiral Moiety: Novel Candidates as Antibacterial Agents

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CONTENTS

Figure 1. ¹ H and ¹³ C NMR Spectra of 4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carboxylic acid (1)	2
Figure 2. ¹ H and ¹³ C NMR Spectra of 4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carboxylate (2)	3
Figure 3. (R)-4-benzoyl-1-(2,5-dimethylphenyl)-N-(2-hydroxy-1-phenylethyl)-5-phenyl-1H-pyrazole-3-carboxamide (3a)	4
Figure 4. (R)-4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-3-methylbutan-2-yl)-5-phenyl-1H-pyrazole-3-carboxamide (3b)	5
Figure 5. (R)-4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-butan-2-yl)-5-phenyl-1H-pyrazole-3-carboxamide (3c)	6
Figure 6. 4-benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl chloride (4)	7
Figure 7. 4-benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl-isothiocyanate (5)	8
Figure 8. (R)-1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl)-3-(2-hydroxy-1-phenylethyl)-thiourea (6a).....	9
Figure 9. (R)-1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl)-3-(1-hydroxy-3-methylbutan-2-yl)-thiourea (6b).....	10
Figure 10. (R)-1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl)-3-(1-hydroxypropan-2-yl)-thiourea (6c).....	11
Tablo1. Geometric optimization was done by means of Gaussian 09 with DFT/B3LYP 6-311G Coordinates for compound 3a	12

Chemical structure: CC1=CC=C(C=C1C2=CC=CC=C2C3=CC(=O)C(=O)O)N3C(=O)C4=CC=CC=C4

¹H NMR spectrum (ppm [t1]):

- 13.102 (broad, integration 1.00)
- 7.774, 7.755, 7.604, 7.586, 7.568, 7.475, 7.456, 7.437, 7.270, 7.253, 7.160, 7.143, 7.122 (multiplet, integration 1.12)
- 6.985, 6.966 (multiplet, integration 1.11)
- 2.501 (singlet, integration 3.00)
- 2.223, 2.201 (singlet, integration 3.00)

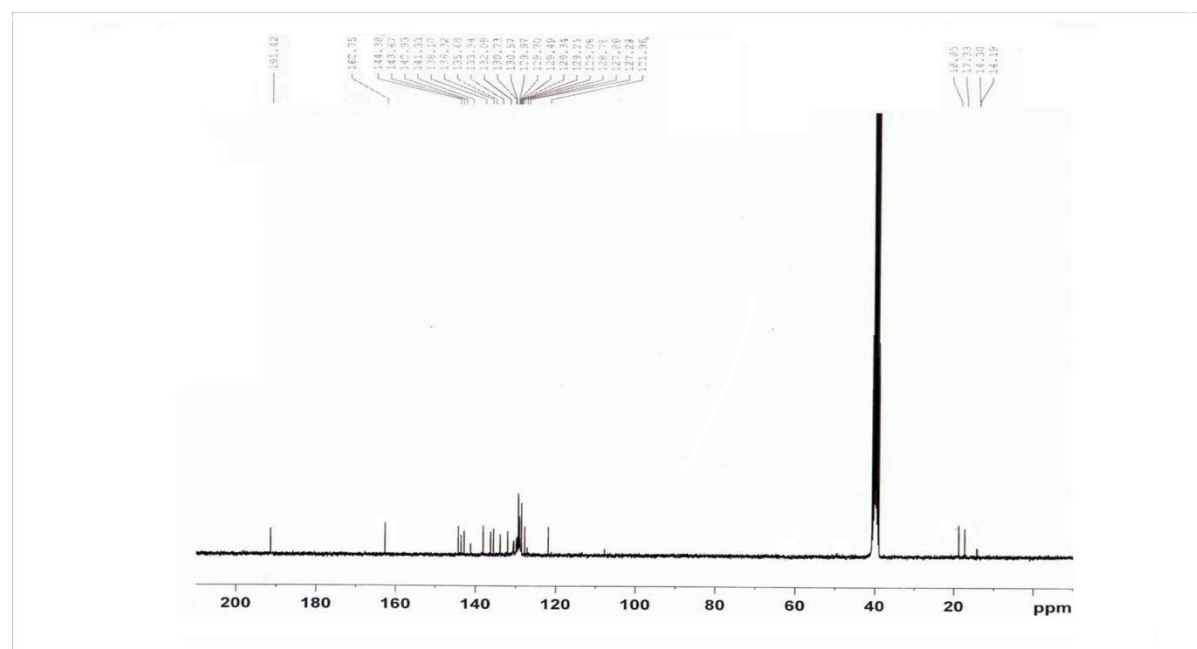


Figure 2. ^1H and ^{13}C NMR Spectra of 4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3- carboxylate (2)

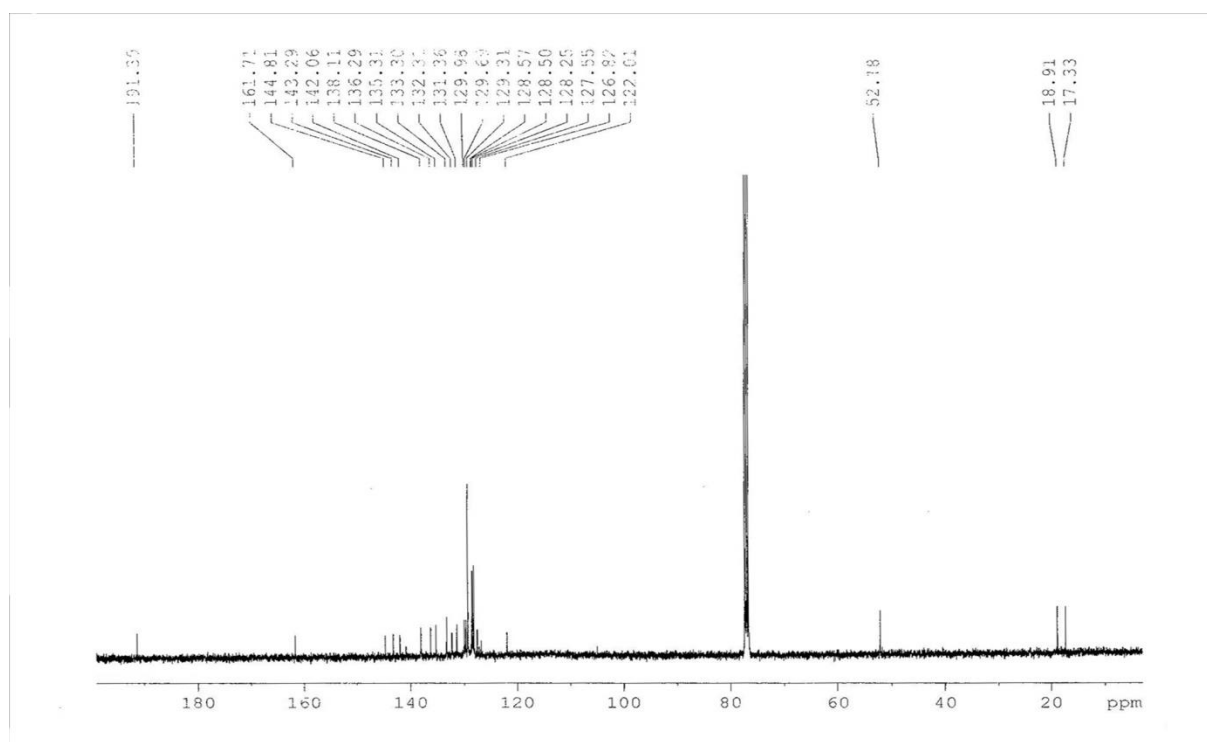
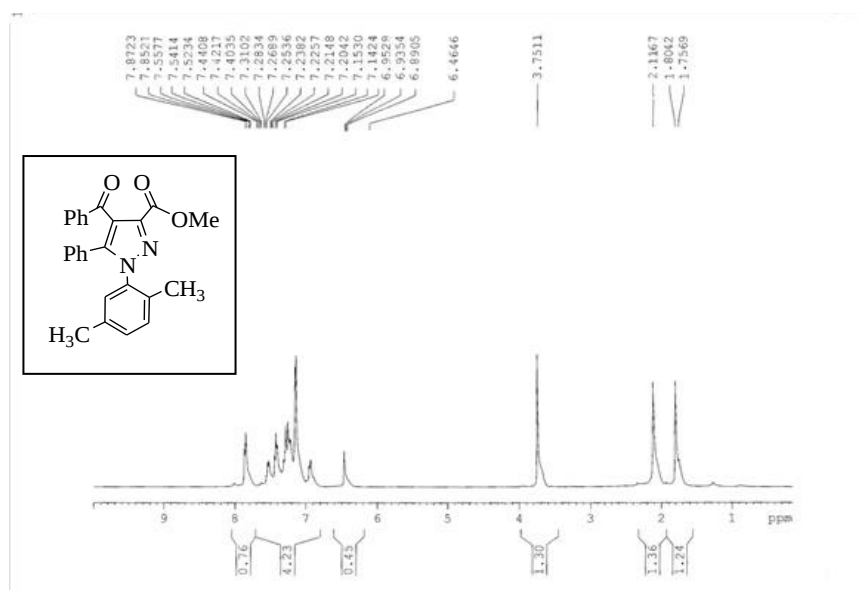


Figure 3. (R)-4-benzoyl-1-(2,5-dimethylphenyl)-N-(2-hydroxy-1-phenylethyl)-5-phenyl-1H-pyrazole-3-carboxamide (**3a**)

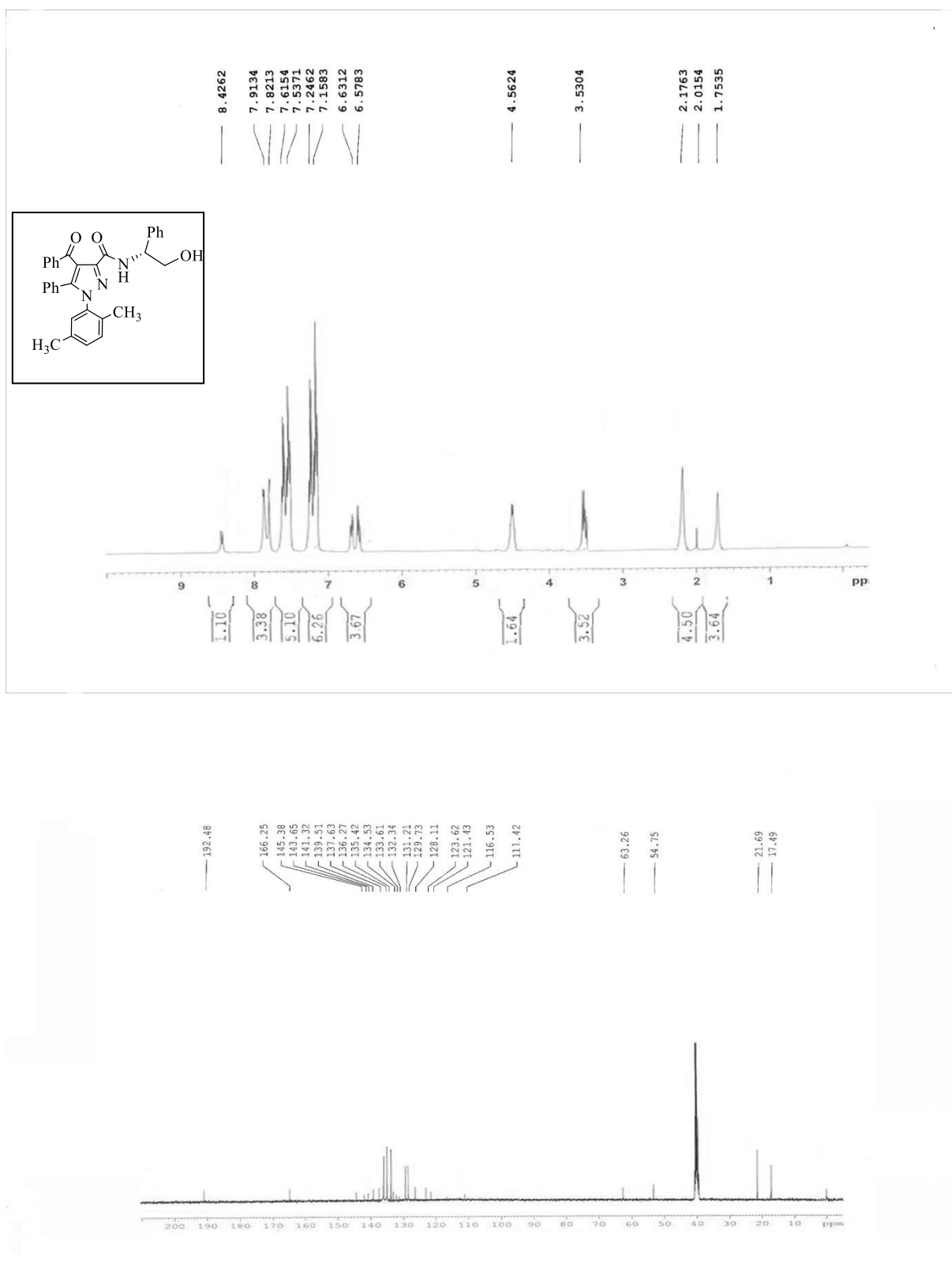


Figure 4. ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-3-methylbutan-2-yl)-5-phenyl-1*H*-pyrazole-3-carboxamide (**3b**)

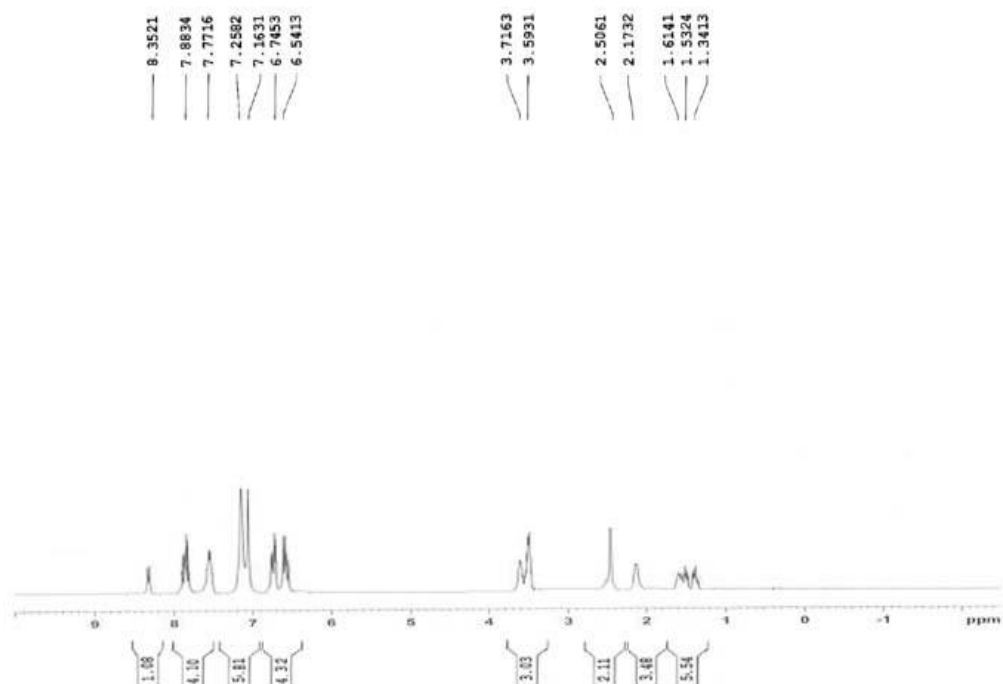
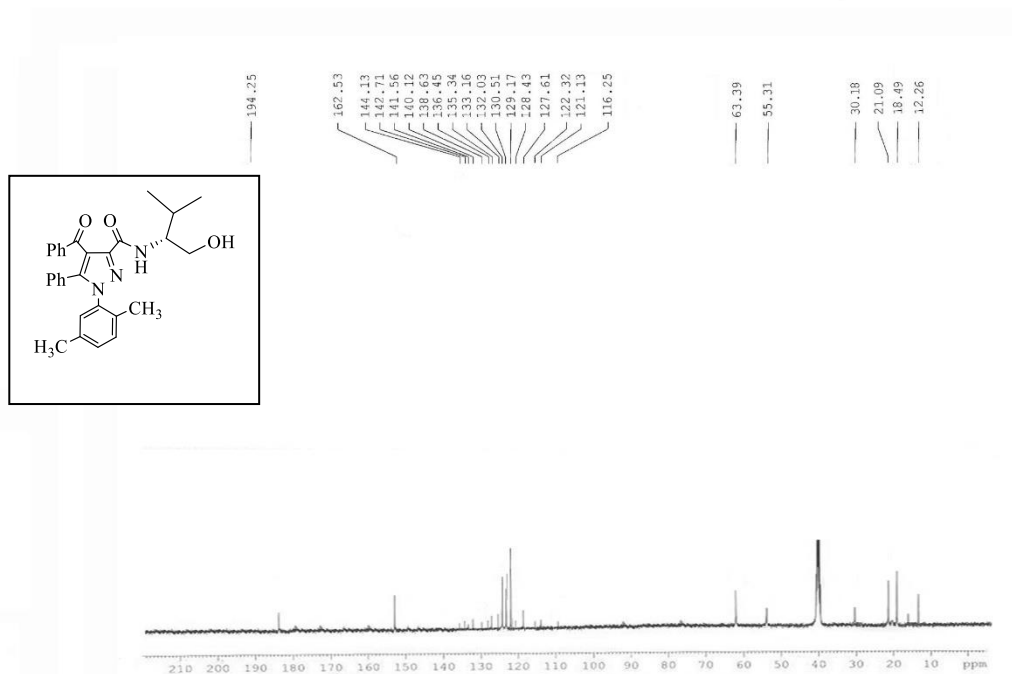


Figure 5. ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-butan-2-yl)-5-phenyl-1*H*-pyrazole-3-carboxamide (**3c**)

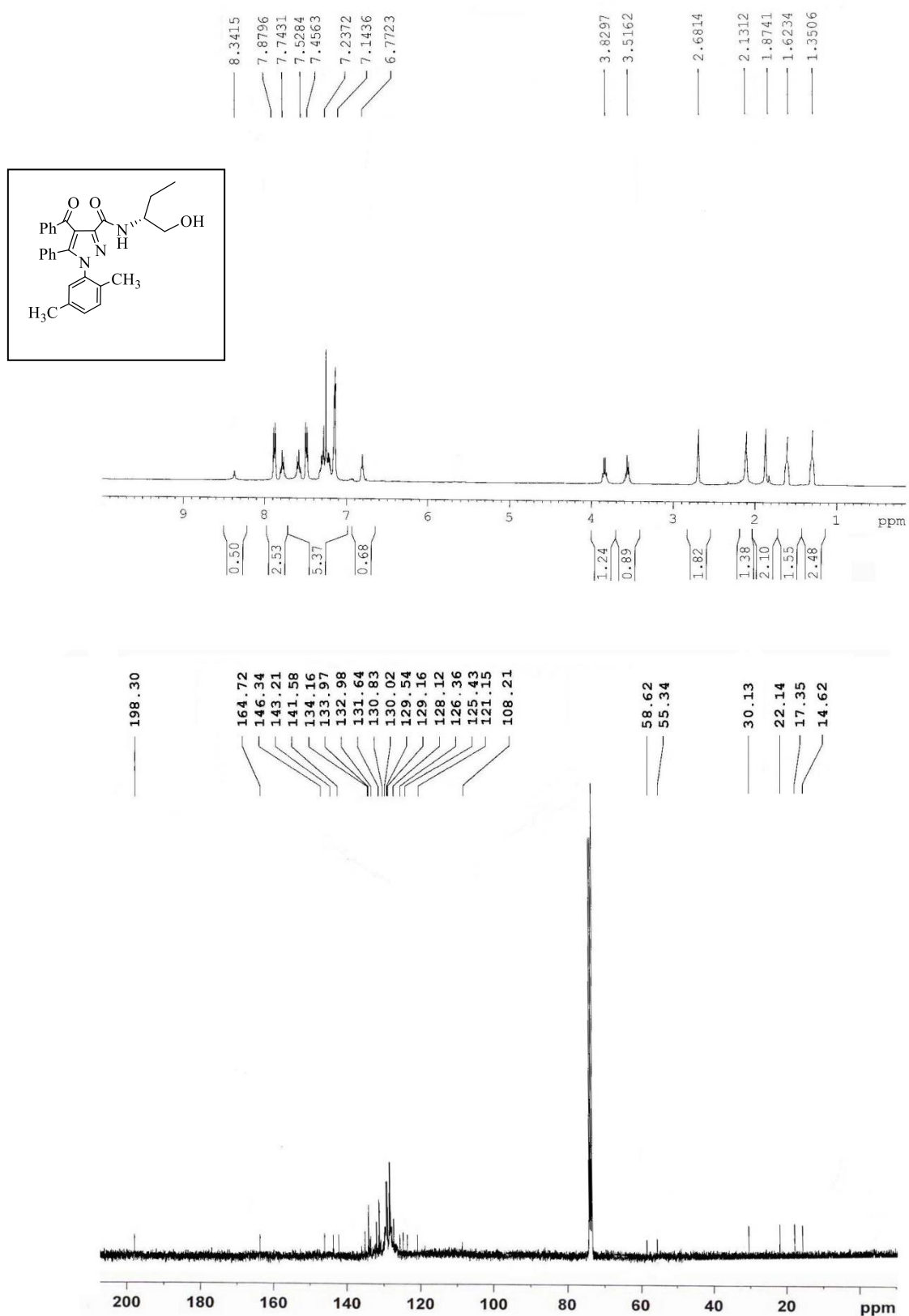


Figure 6. ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl chloride (**4**)

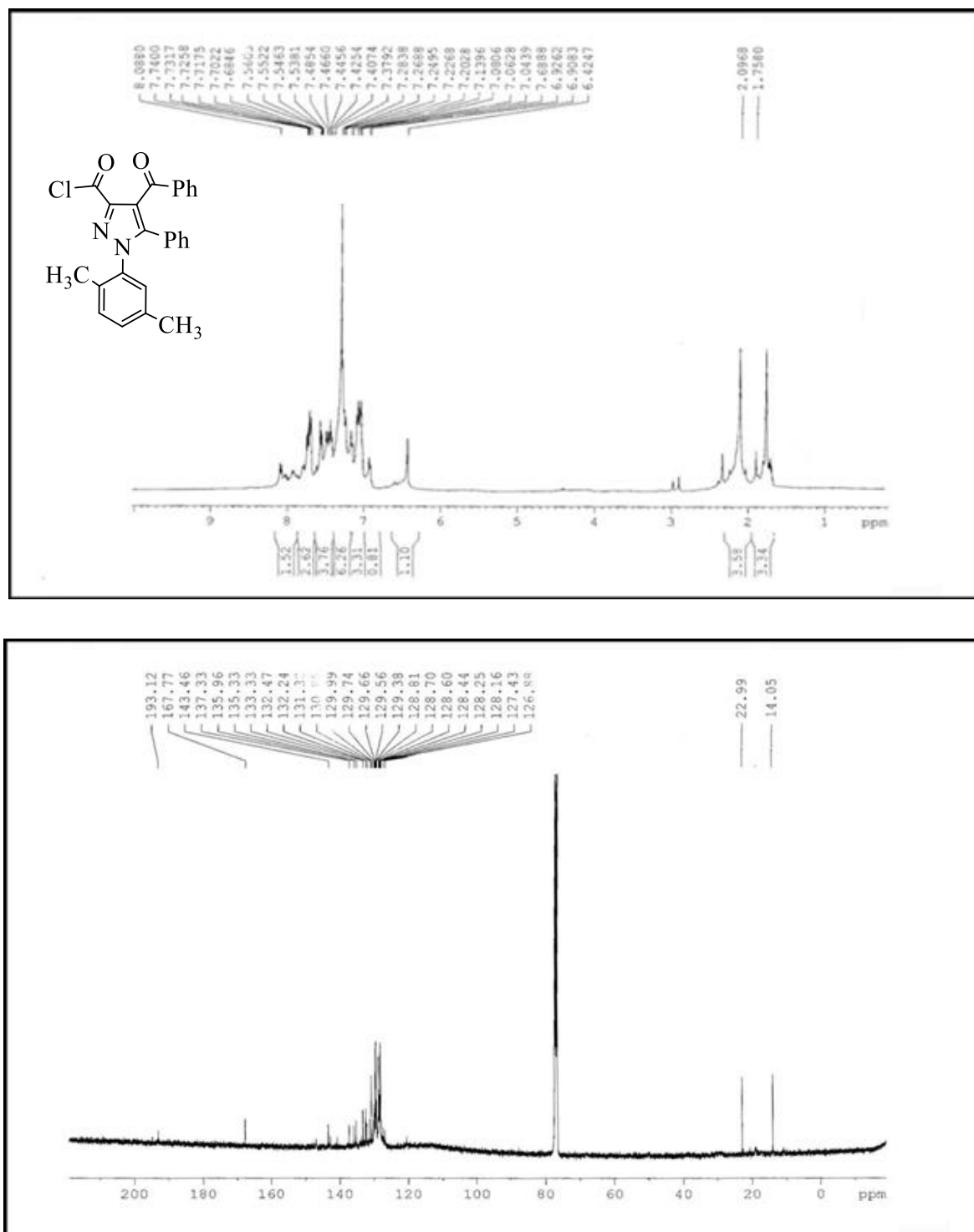
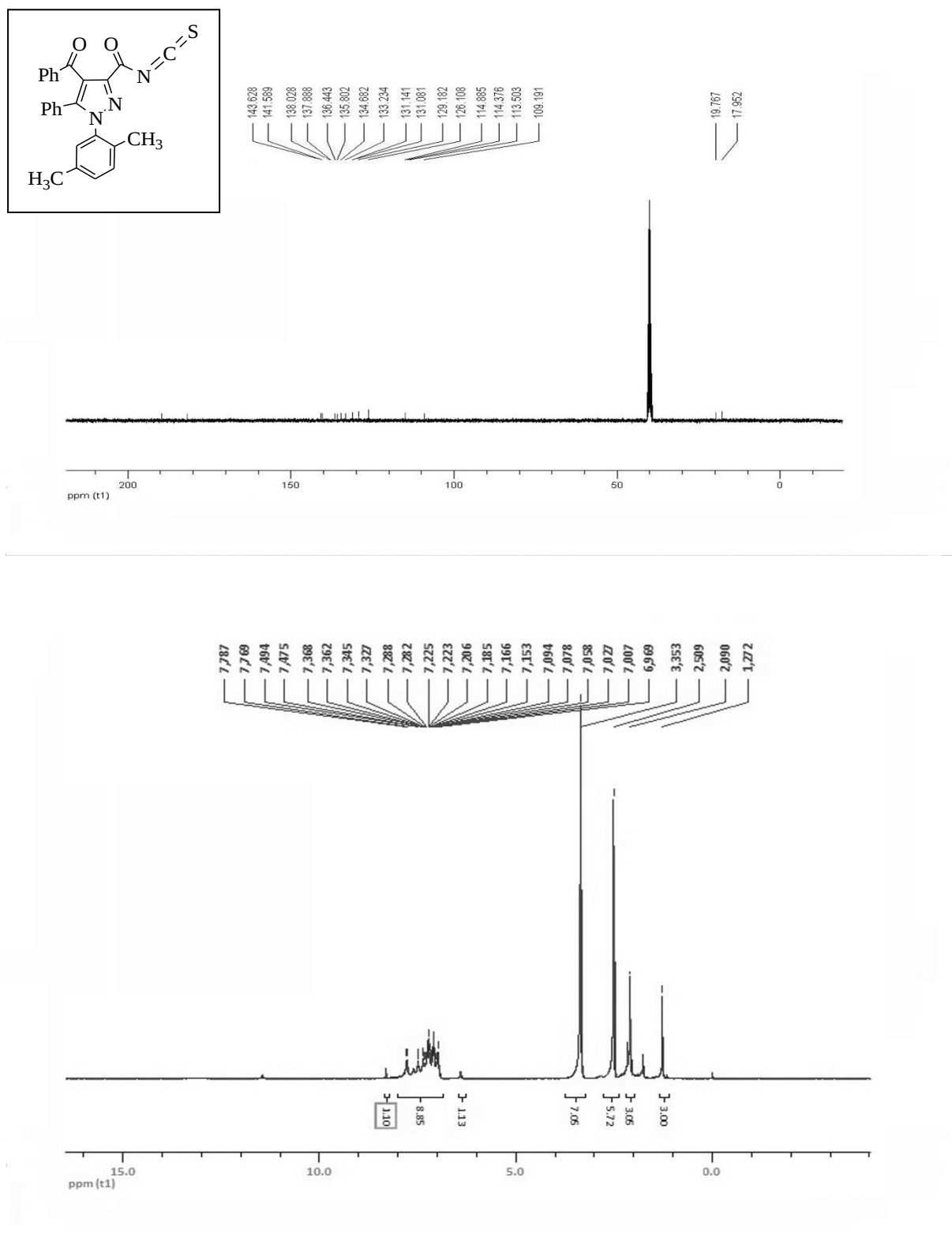


Figure 7. ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-carbonyl-isothiocyanate (**5**)



[illegible]

Figure 9. ^1H and ^{13}C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl)-3-(1-hydroxy-3-methylbutan-2-yl)-thiourea (**6b**)

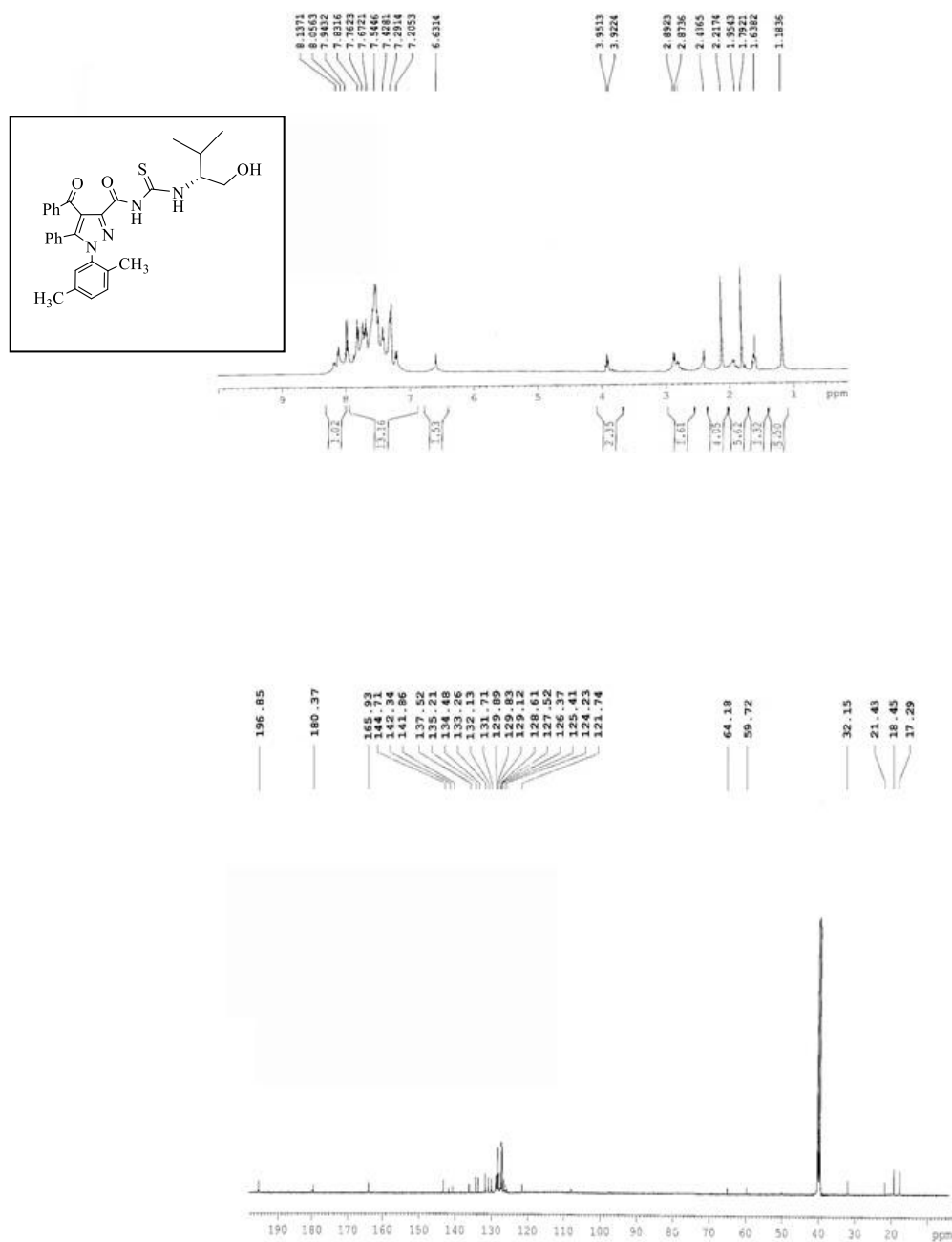


Figure 10. ^1H and ^{13}C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-carbonyl)-3-(1-hydroxy propan-2-yl)-thiourea (**6c**)

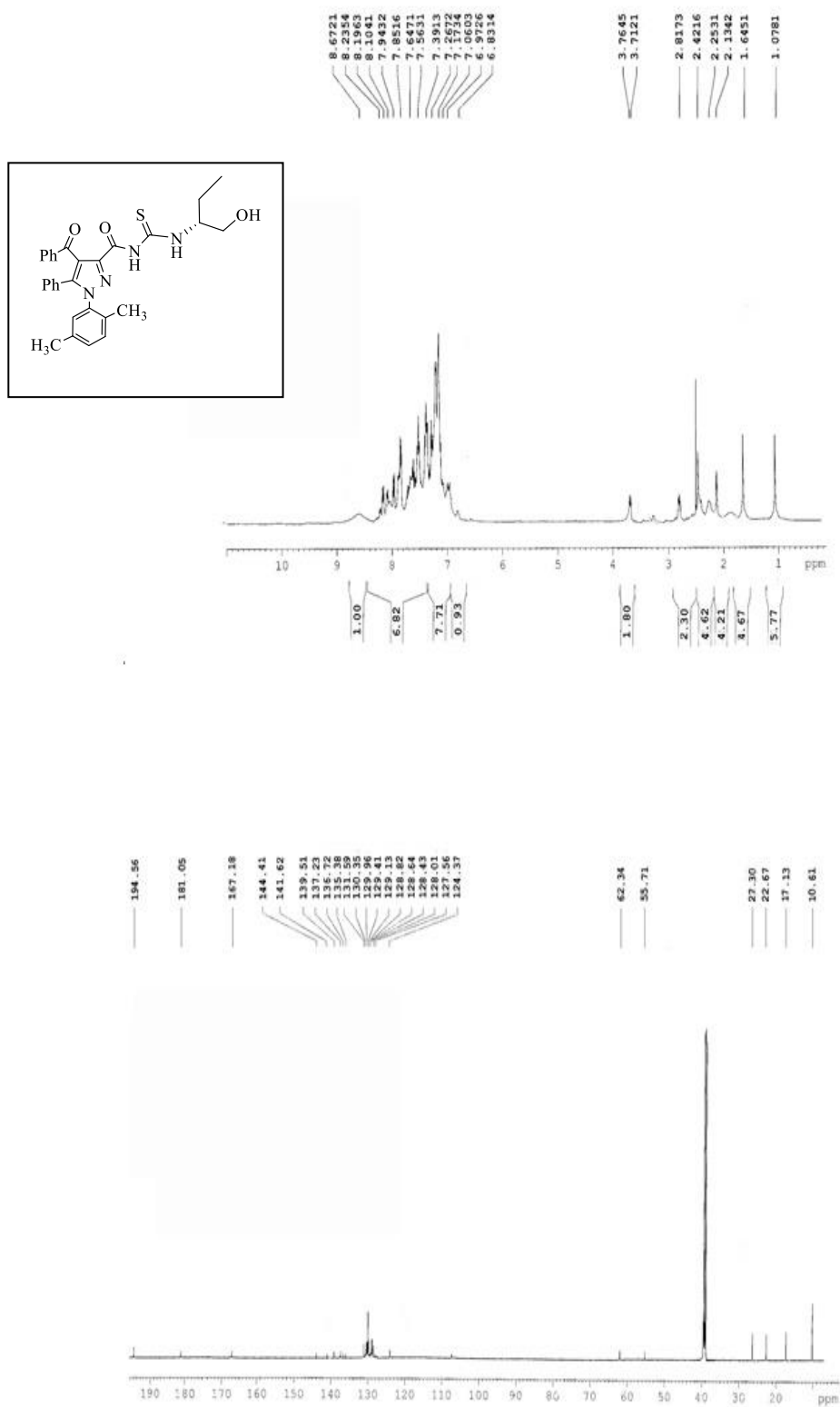


Table 1. Geometric optimization was done by means of Gaussian 09 with DFT/B3LYP 6-311G Coordinates for compound **3a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	C	1.886164	0.182310	0.387761
2	6	C	0.815864	1.067826	0.490730
3	6	C	-0.311698	0.321007	0.073428
4	7	N	1.352732	-1.001579	0.074996
5	7	N	0.020381	-0.922917	0.257937
6	6	C	-1.733583	0.771618	0.058274
7	7	N	-2.601688	-0.142755	0.461464
8	1	H	-2.204126	-1.019508	0.767333
9	6	C	-4.038832	0.068571	0.513621
10	1	H	-4.197588	1.096045	0.179523
11	6	C	-4.489919	-0.009421	1.984974
12	1	H	-4.402315	-1.047914	2.336405
13	1	H	-3.810929	0.617868	2.576822
14	8	O	-5.829246	0.456676	2.077350
15	1	H	-6.166408	0.241696	2.950967
16	6	C	-4.824462	-0.873797	0.394263
17	6	C	-4.273670	-2.055062	0.897675
18	6	C	-6.148309	-0.560315	0.726002
19	6	C	-5.027405	-2.908686	1.702377
20	1	H	-3.240996	-2.308568	0.688846
21	6	C	-6.901028	-1.411384	1.529307
22	1	H	-6.588670	0.350302	0.340795
23	6	C	-6.344504	-2.591568	2.019560
24	1	H	-4.578337	-3.818053	2.086572
25	1	H	-7.923228	-1.148303	1.778727
26	1	H	-6.929760	-3.252410	2.649274
27	8	O	-2.054630	1.869538	0.484301
28	6	C	0.858672	2.492137	0.961191
29	6	C	0.549206	3.584426	0.009477
30	6	C	0.395199	4.886137	0.483962
31	6	C	0.456673	3.358701	1.386761
32	6	C	0.142197	5.939544	0.383868
33	1	H	0.474180	5.043631	1.552193
34	6	C	0.213594	4.417021	2.257364
35	1	H	0.582518	2.356515	1.777708
36	6	C	0.052275	5.707100	1.757413
37	1	H	0.013837	6.943088	0.005783
38	1	H	0.148526	4.235807	3.324333
39	1	H	-0.143434	6.530682	2.435263
40	6	C	3.326781	0.388513	0.630504
41	6	C	3.757209	1.005177	1.815445
42	6	C	4.285059	-0.005154	0.315680
43	6	C	5.114068	1.215109	2.044587
44	1	H	3.022101	1.326393	2.541334
45	6	C	5.639292	0.205689	0.078958
46	1	H	3.969905	-0.466895	1.242860
47	6	C	6.058517	0.814305	1.102551
48	1	H	5.431324	1.693881	2.963977
49	1	H	6.367133	-0.100175	0.821931

50	1	H	7.114527	0.978993	1.284788
51	6	C	2.006901	-2.257865	0.325938
52	6	C	2.511389	-3.020235	0.732891
53	6	C	2.070626	-2.700751	1.647262
54	6	C	3.119652	-4.235089	0.393891
55	6	C	2.668428	-3.916626	1.970104
56	1	H	1.638241	-2.078773	2.422823
57	6	C	3.202307	-4.673704	0.921021
58	1	H	3.523617	-4.854024	1.187999
59	1	H	3.678602	-5.625078	1.135985
60	6	C	2.399505	-2.586885	2.171709
61	1	H	1.420332	-2.151899	2.383183
62	1	H	3.151851	-1.833663	2.422297
63	1	H	2.545113	-3.439158	2.837537
64	6	C	2.733450	-4.407195	3.396130
65	1	H	2.145558	-5.321255	3.525555
66	1	H	3.761621	-4.638945	3.689139
67	1	H	2.345910	-3.661276	4.092470
68	8	O	1.188026	2.742913	2.106971
