**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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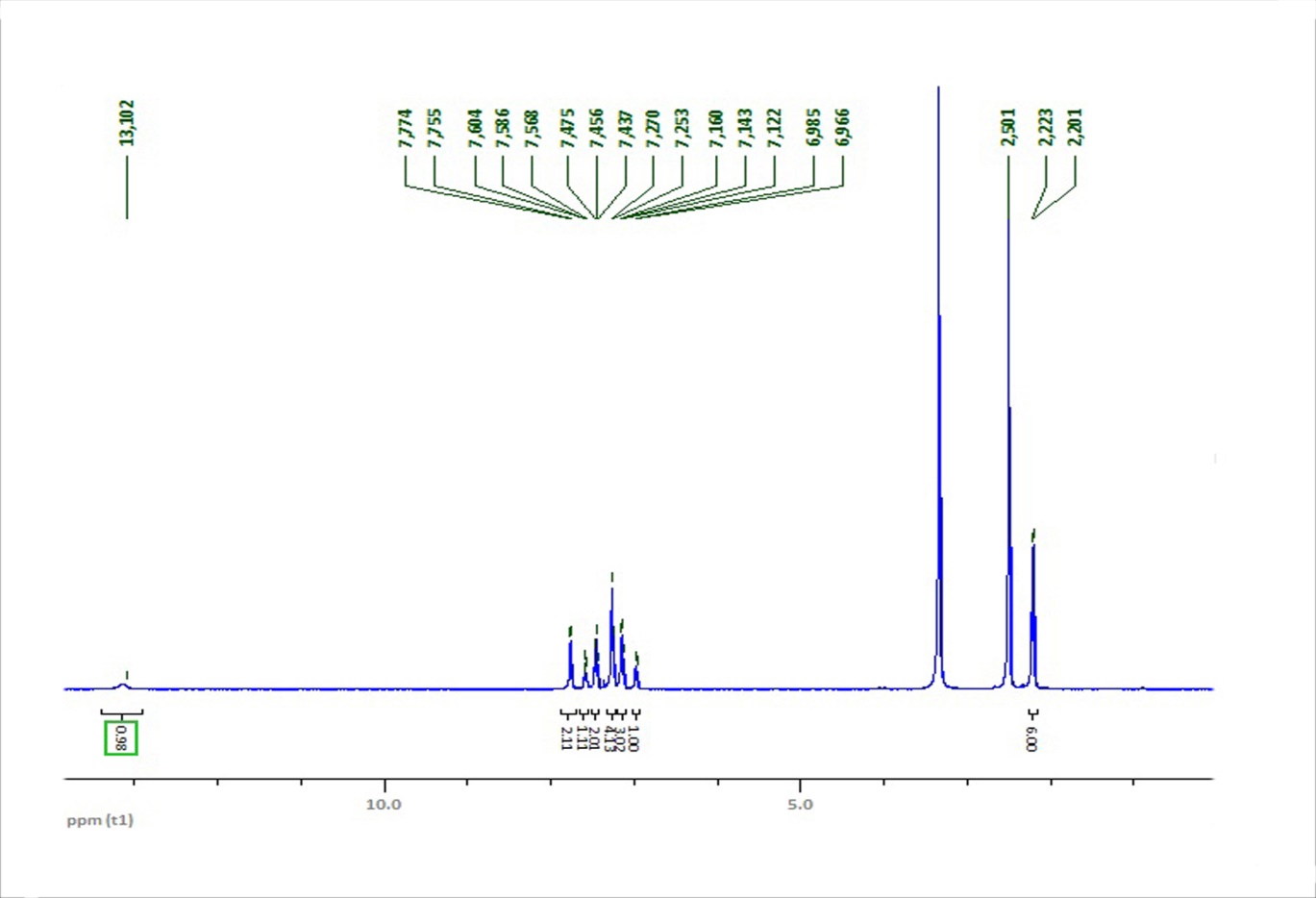
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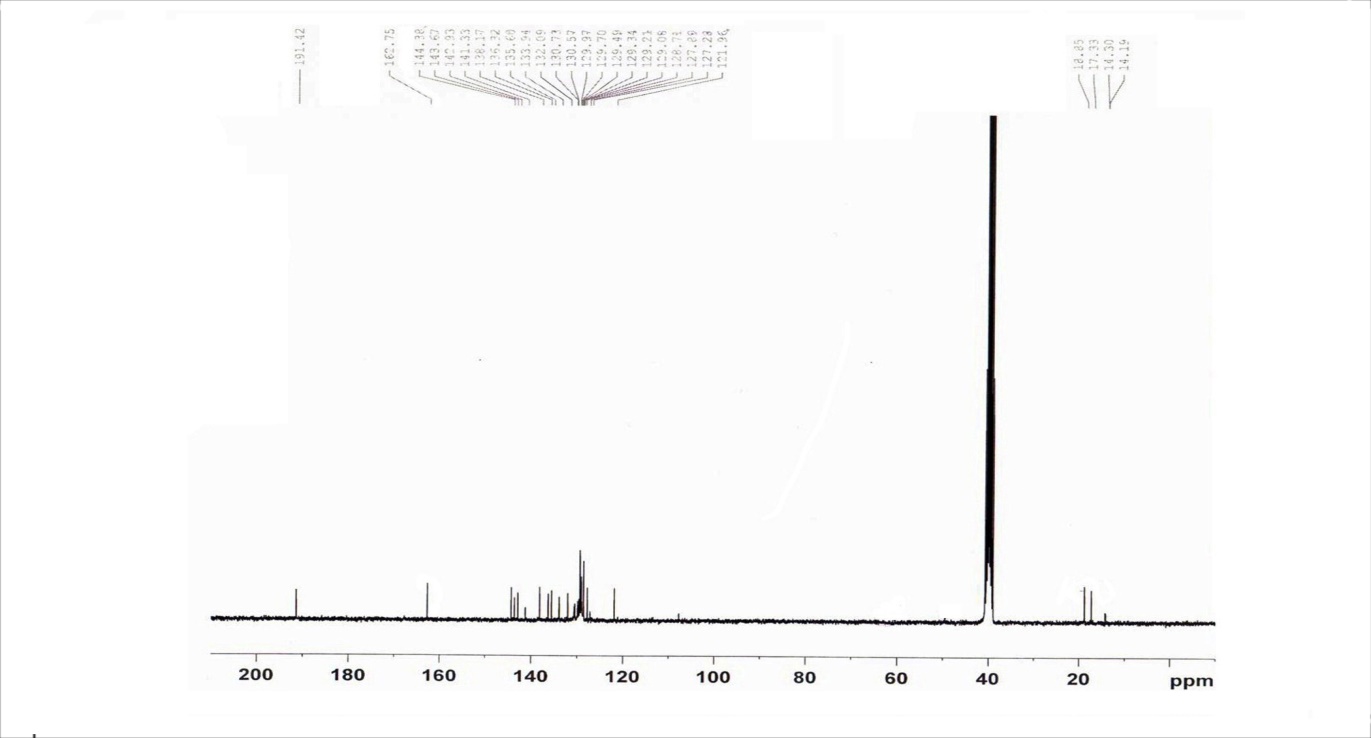
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**Figure S1.** 1H and 13C NMR Spectra of 4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-carboxylic acid **(1)**

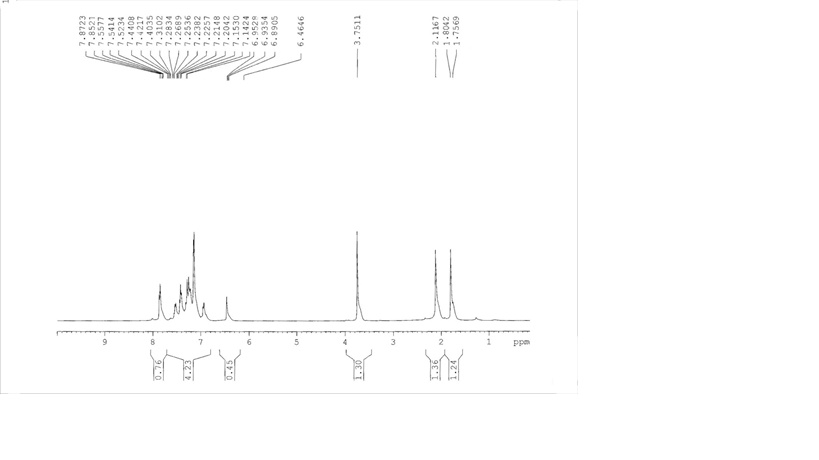
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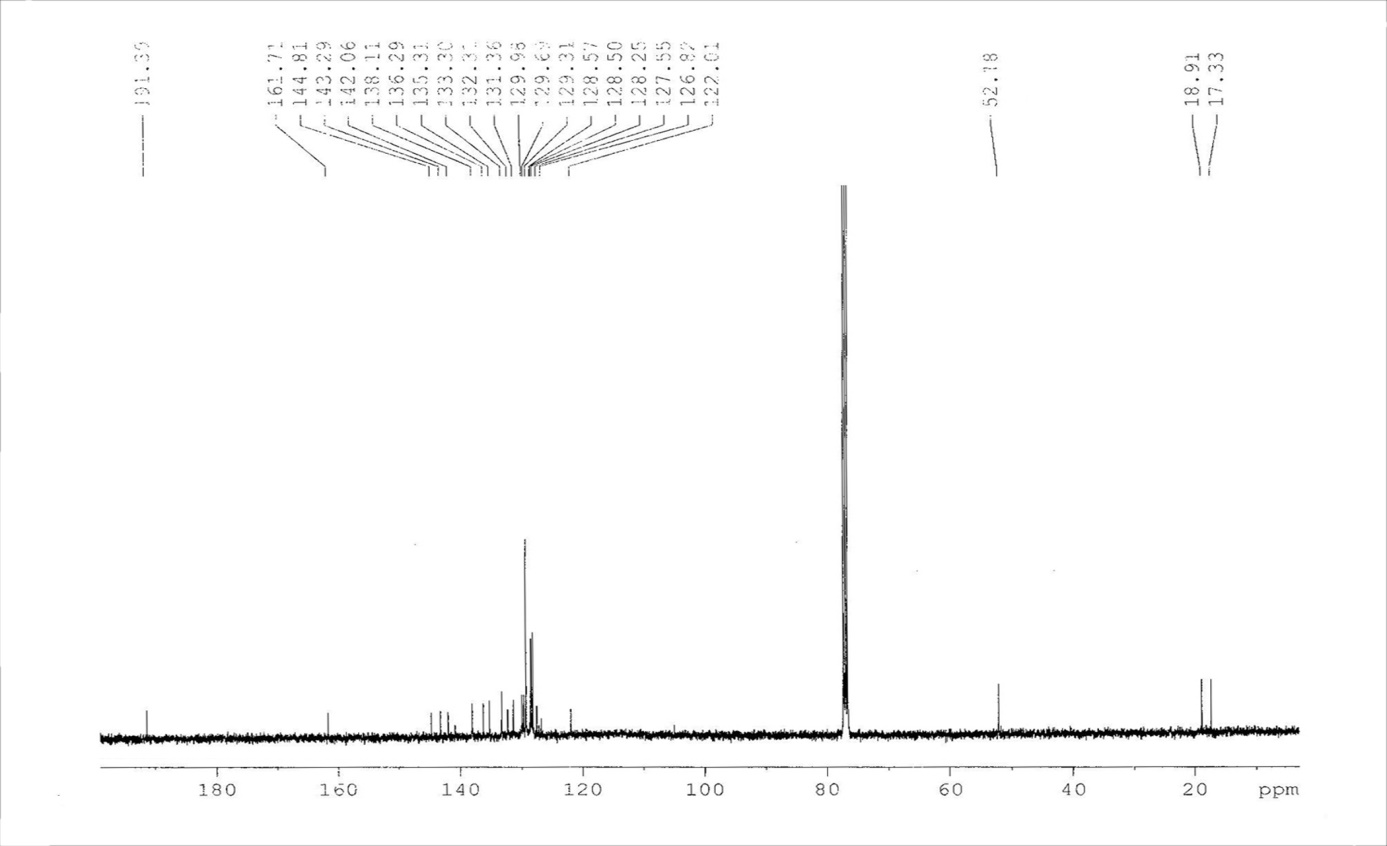
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**Figure S2.** 1H and 13C NMR Spectra of 4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3- carboxylate **(2)**

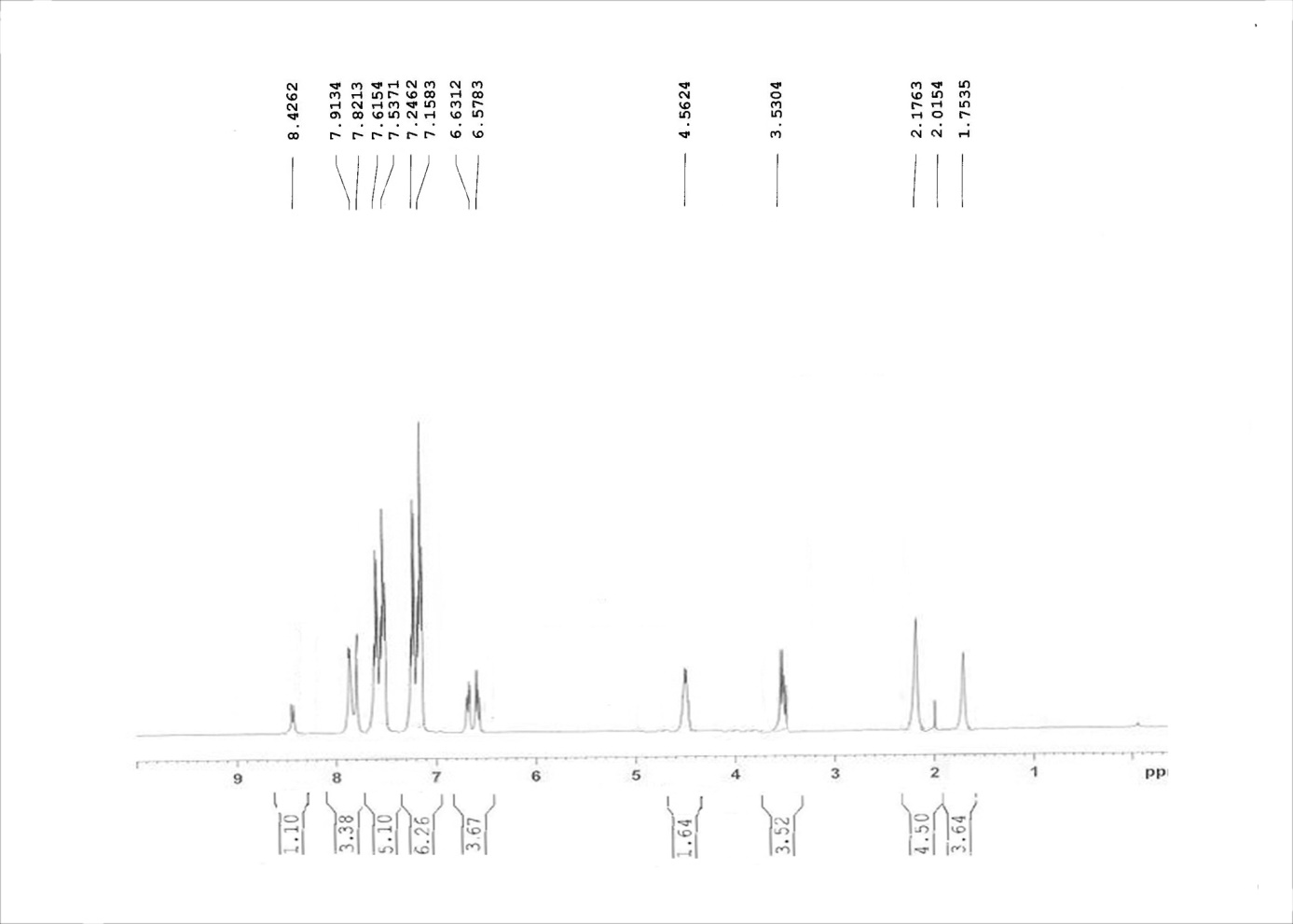
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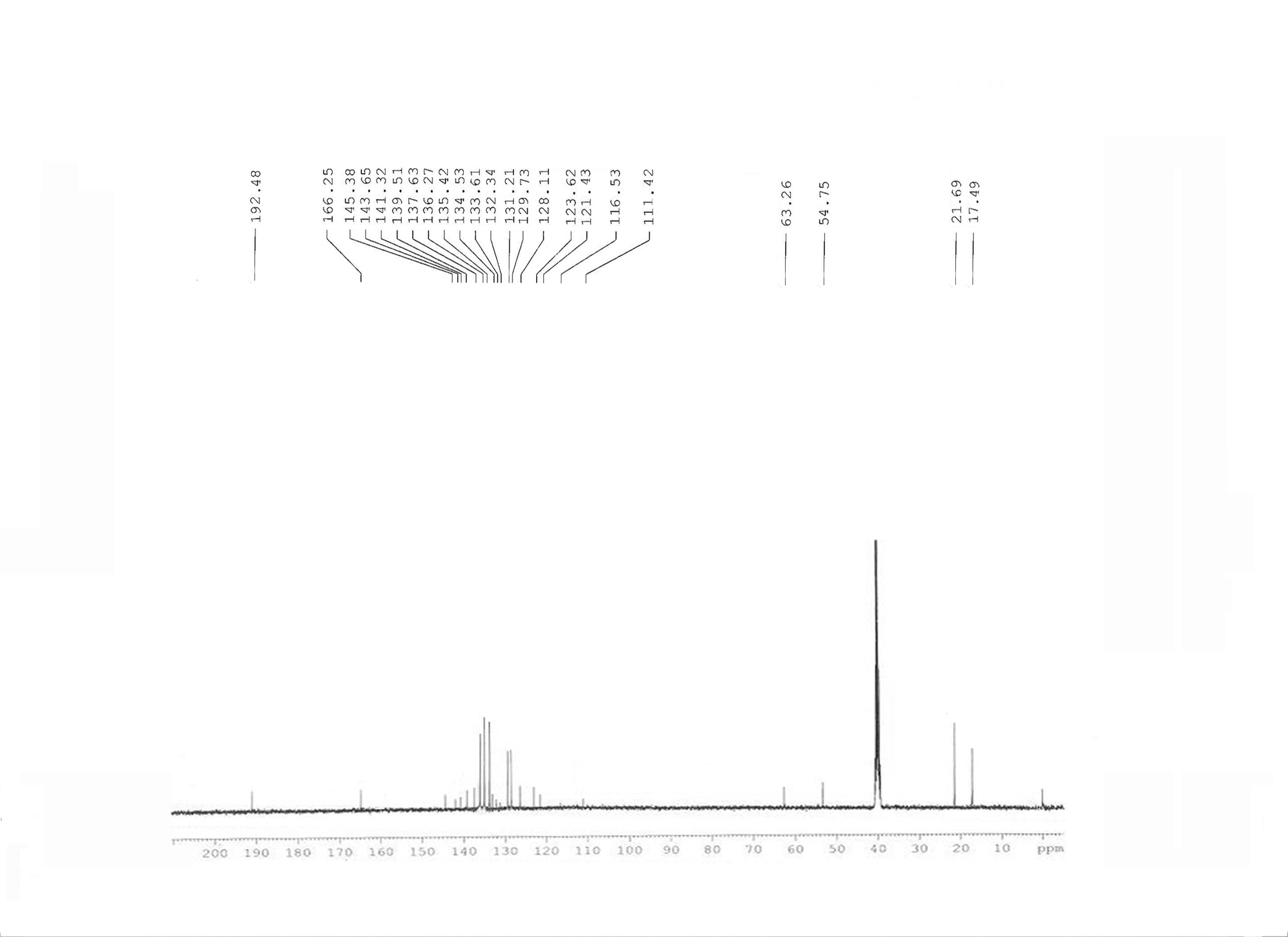




**Figure S3.** (R)-4-benzoyl-1-(2,5-dimethylphenyl)-N-(2-hydroxy-1-phenylethyl)-5-phenyl-1H-pyrazole-3-carboxamide  **(3a)**





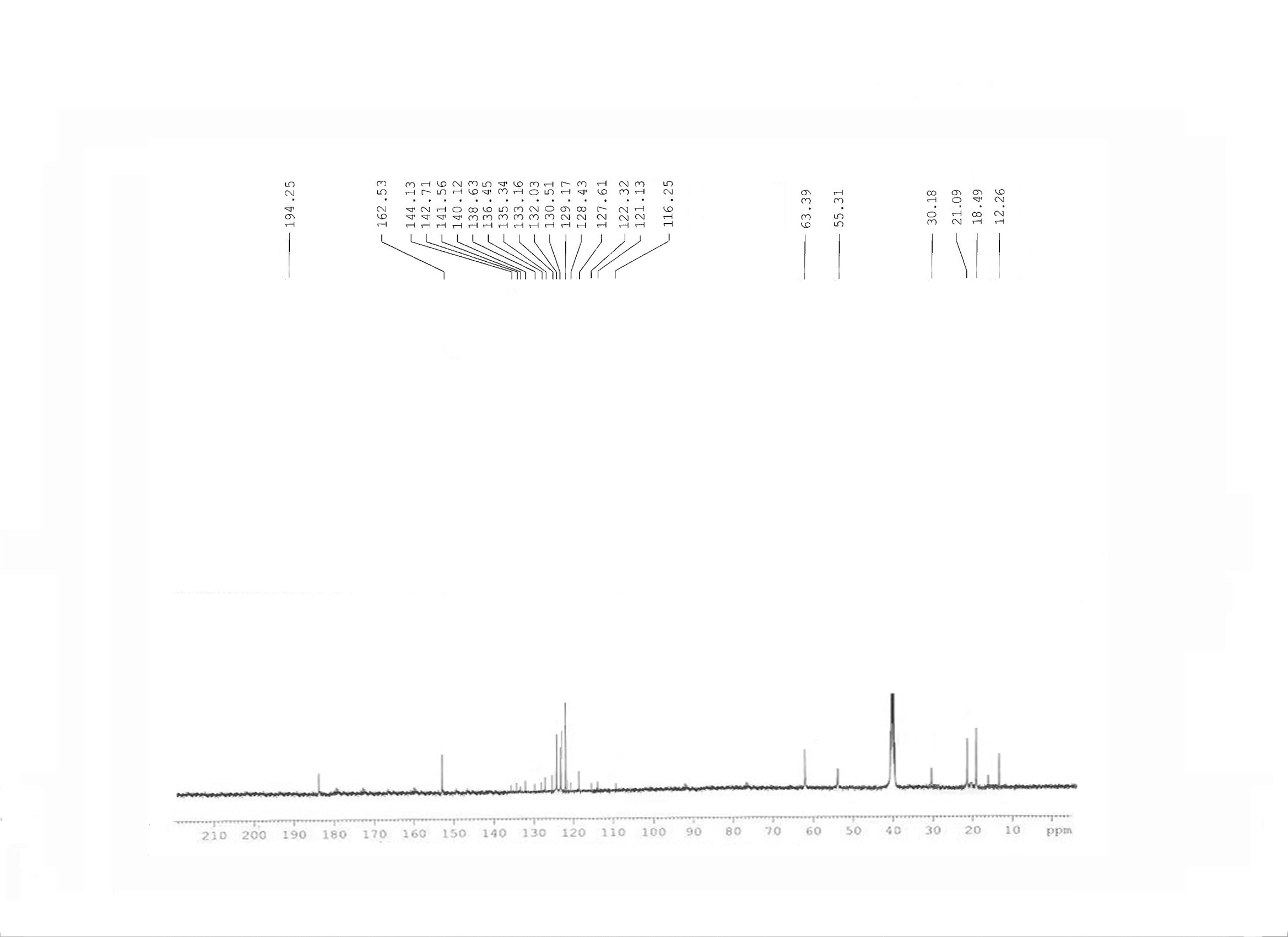




**Figure S4.** 1H and 13C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-3-methylbutan-2-yl)-5-phenyl-1*H*-pyrazole-3-carboxamide **(3b)**

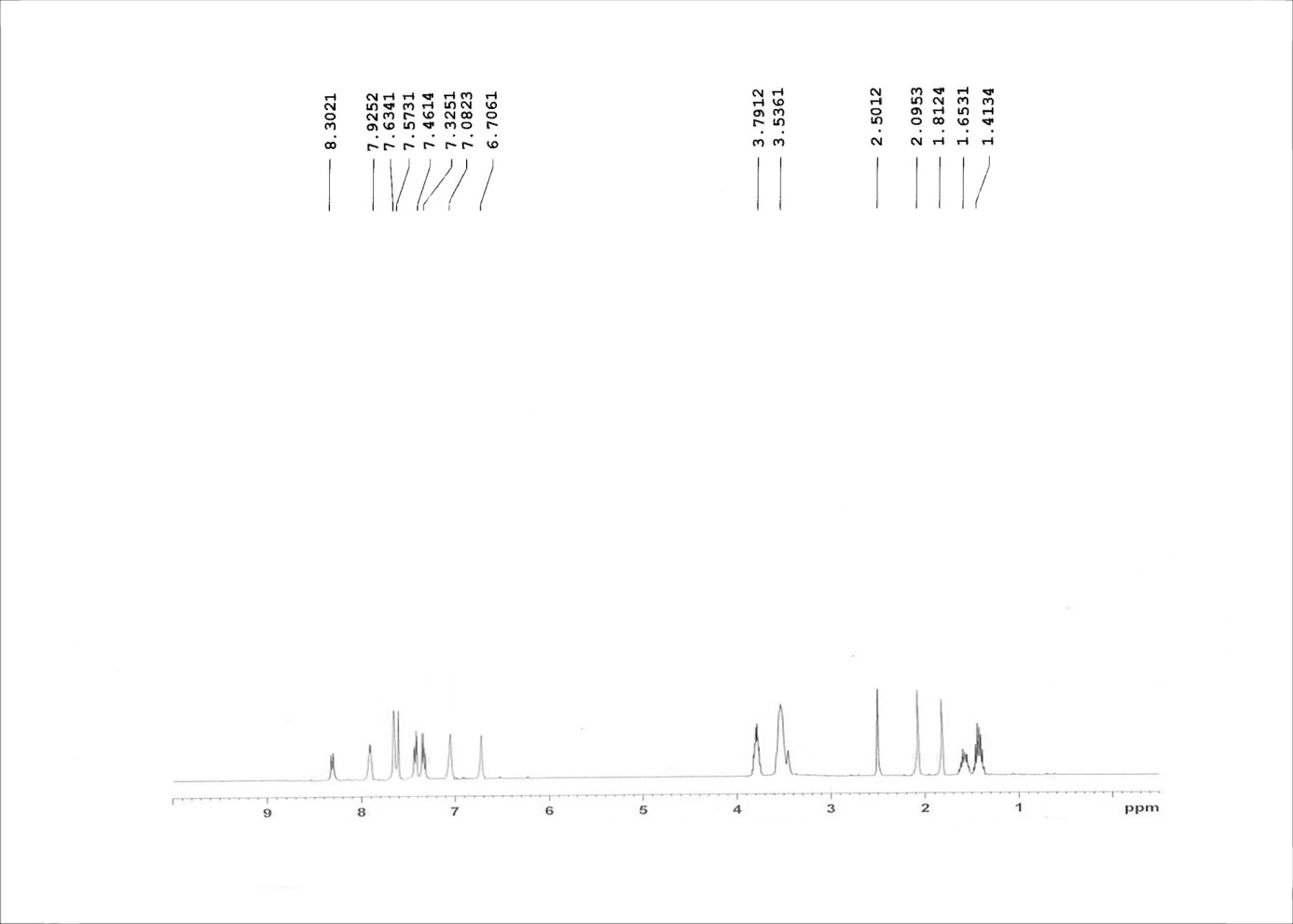




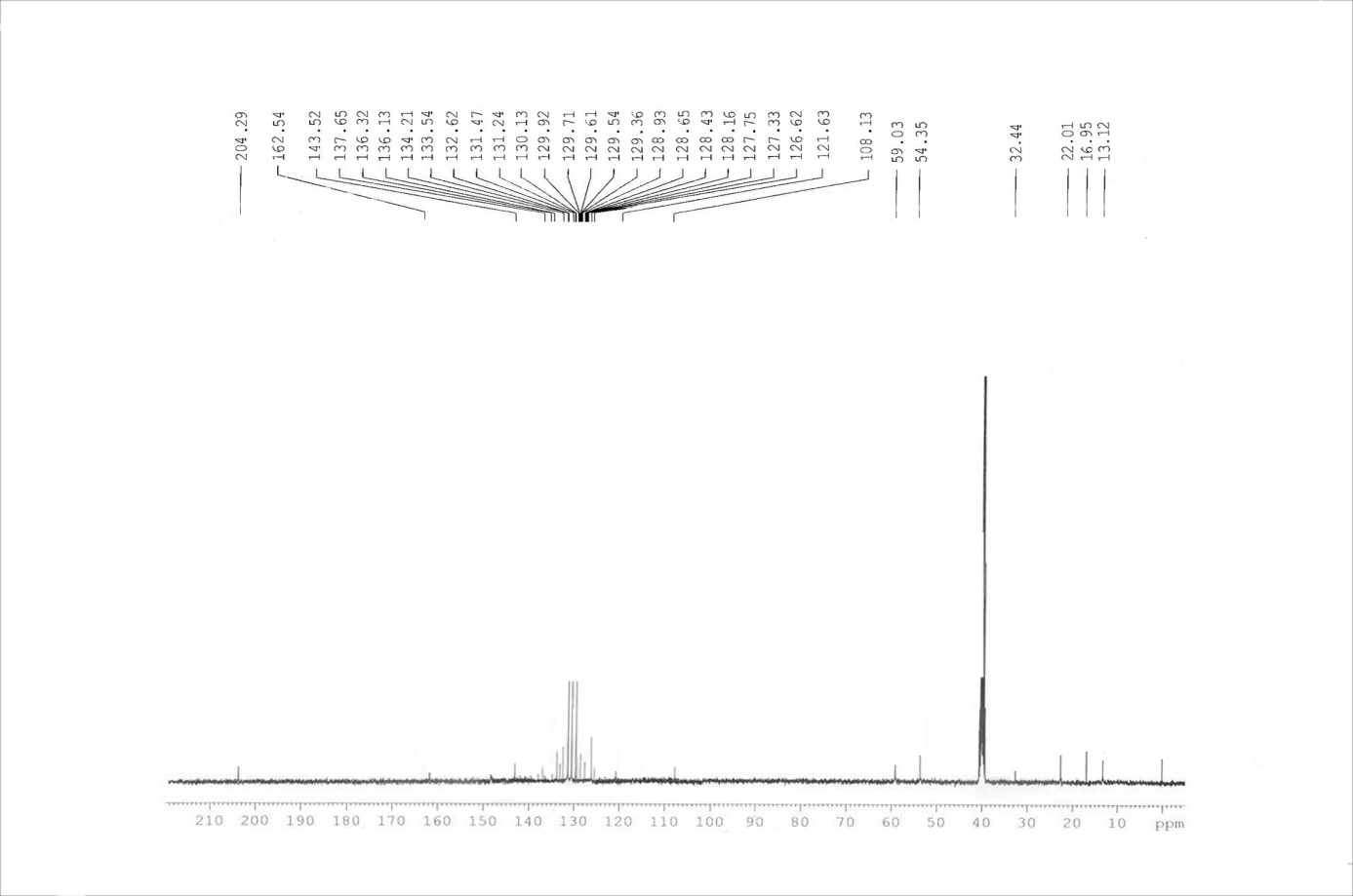




**Figure S5.** 1H and 13C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-butan-2-yl)-5-phenyl-1*H*-pyrazole-3-carboxamide **(3c)**

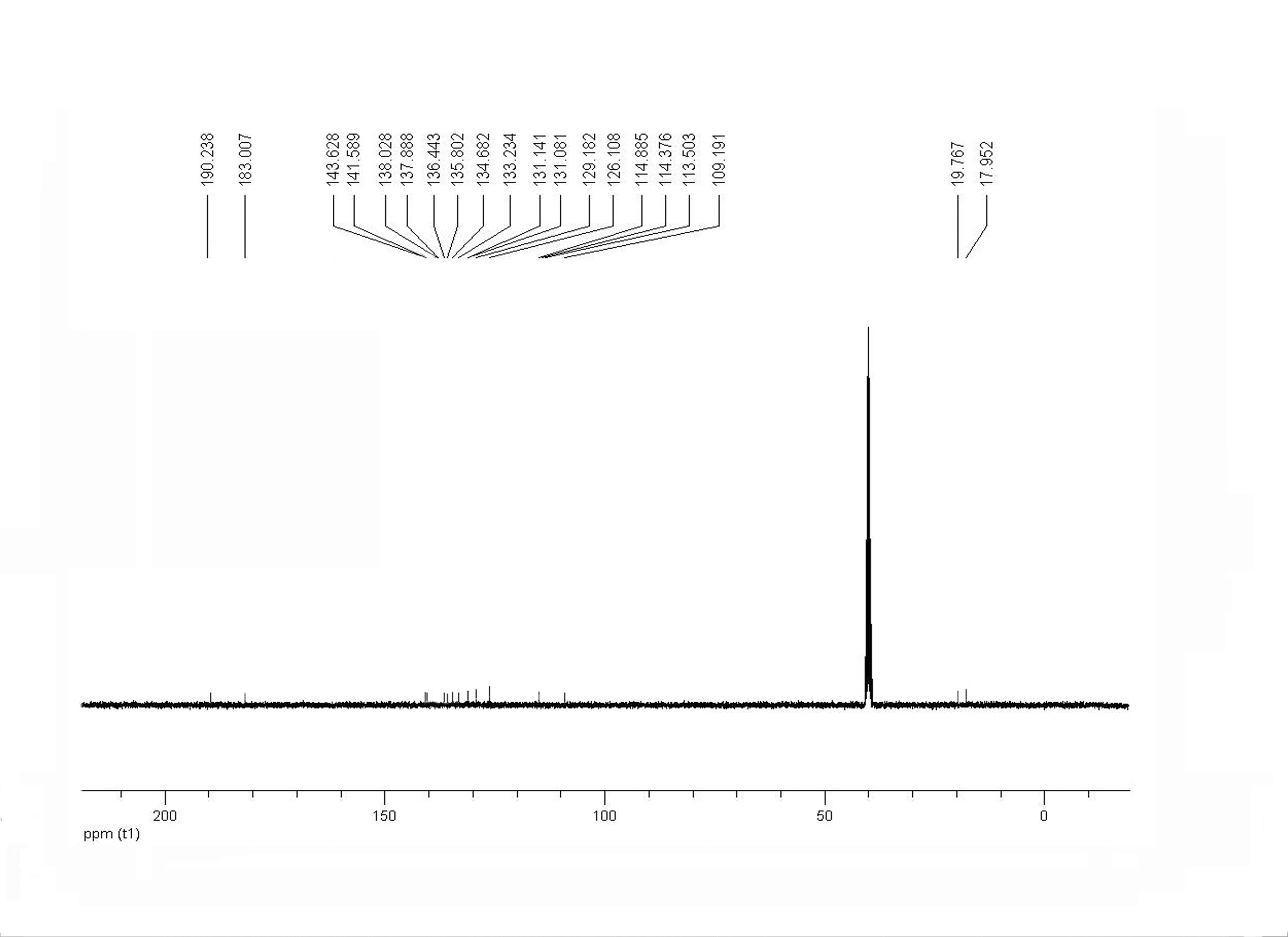
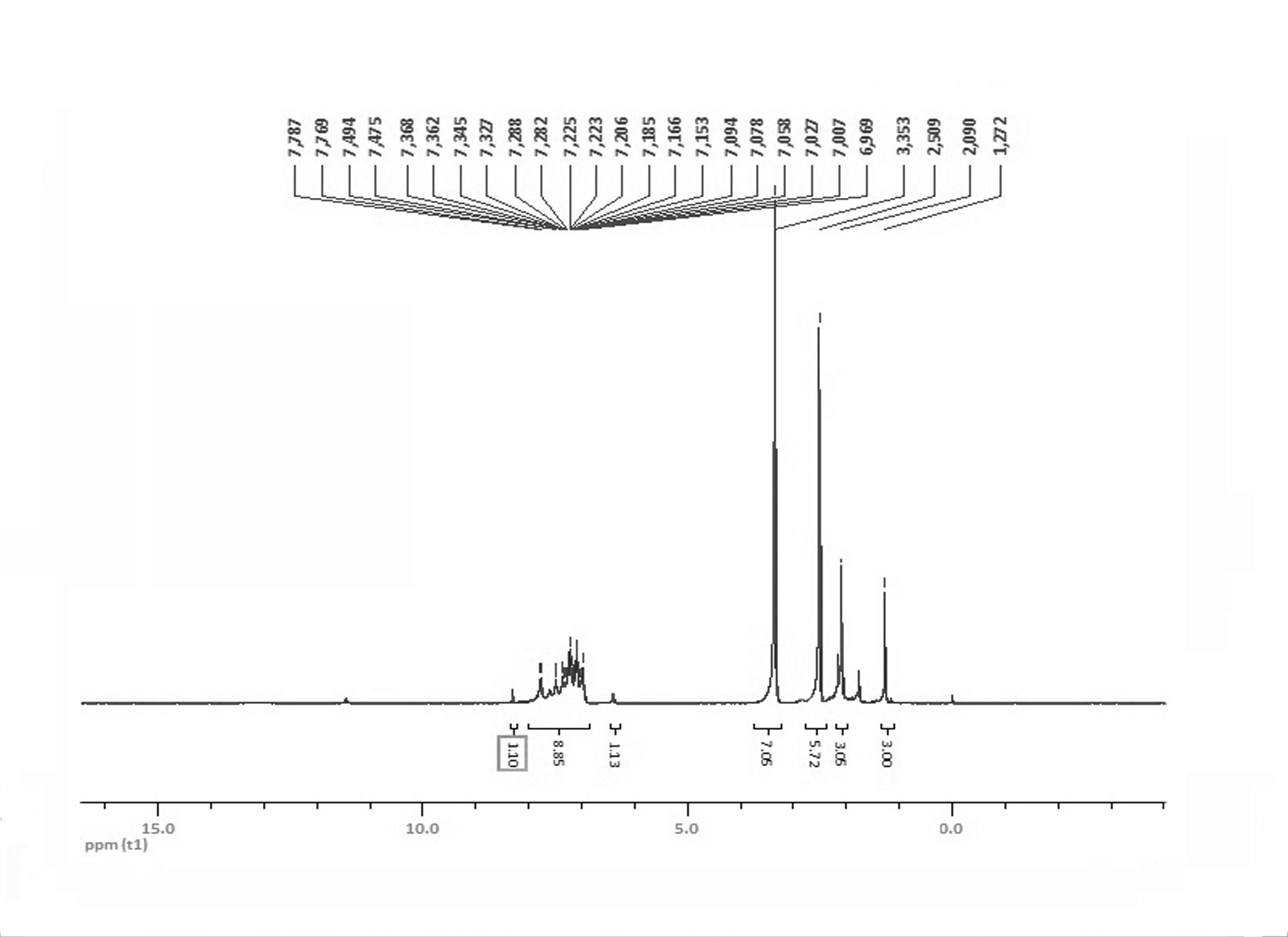
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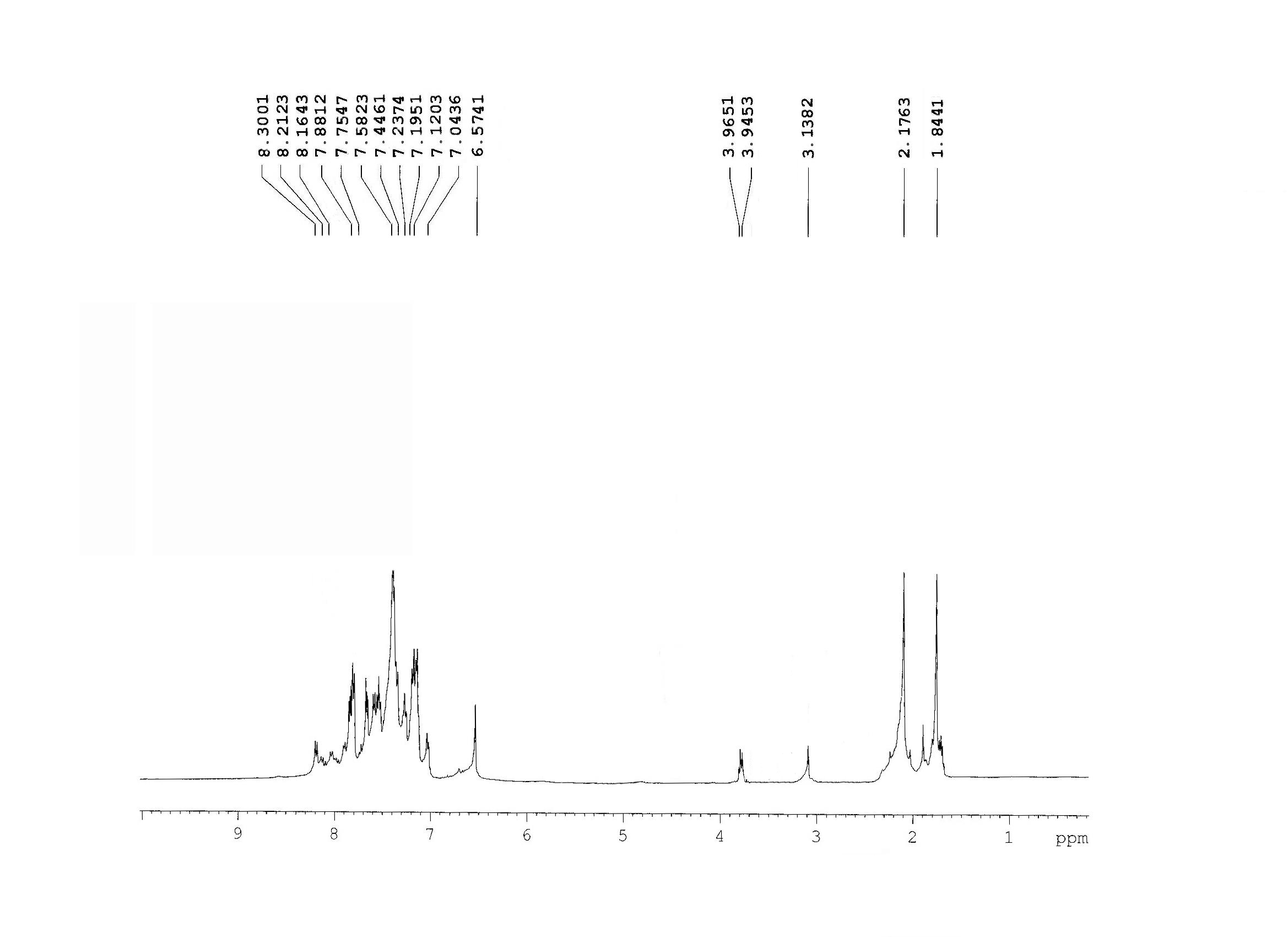
**Figure S6.** 1H and 13C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H-*pyrazole-3-carbonyl-isothiocyanate **(4)**

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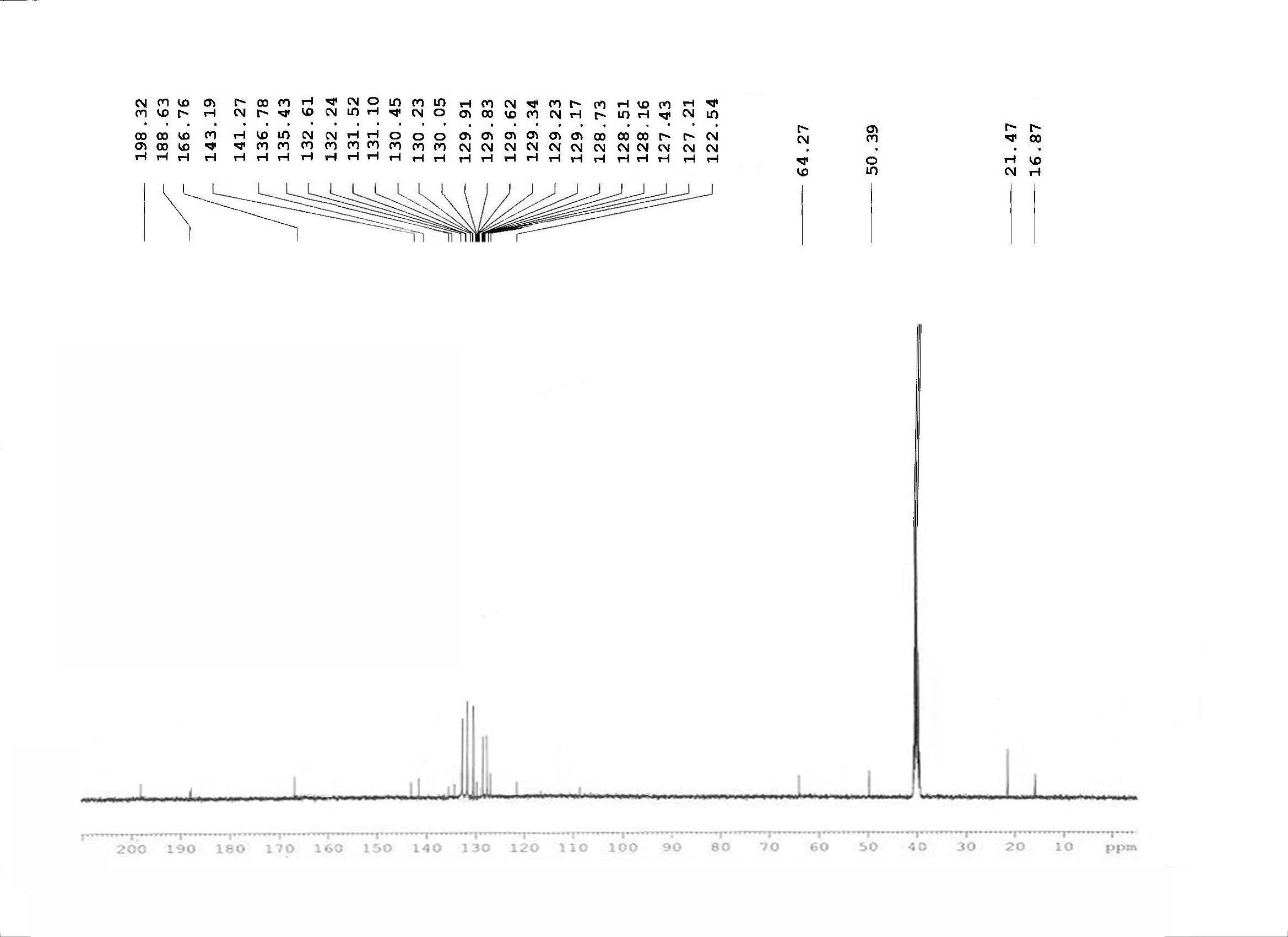




**Figure S7.** 1H and 13C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-carbonyl)-3-(2-hydroxy-1-phenylethyl)-thiourea **(5a)**

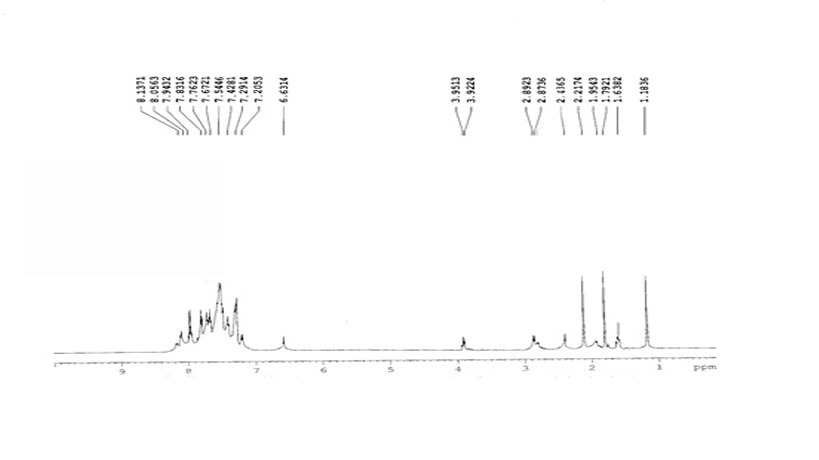
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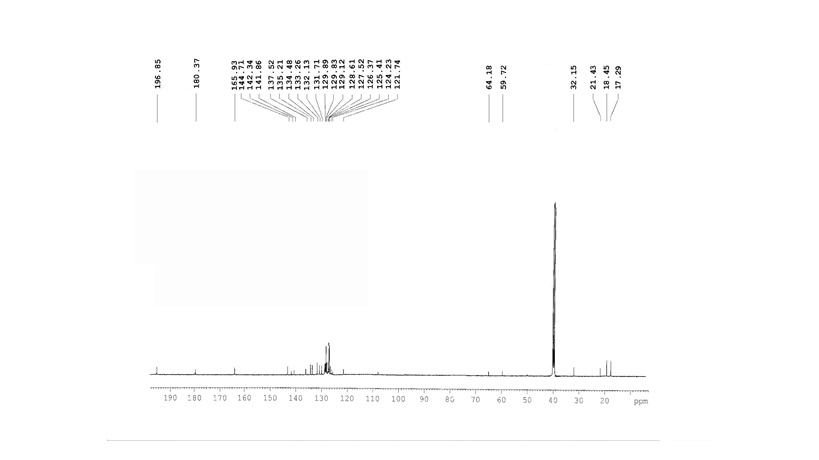
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**Figure S8.** 1H and 13C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3-carbonyl)-3-(1-hydroxy-3-methylbutan-2-yl)-thiourea **(5b)**

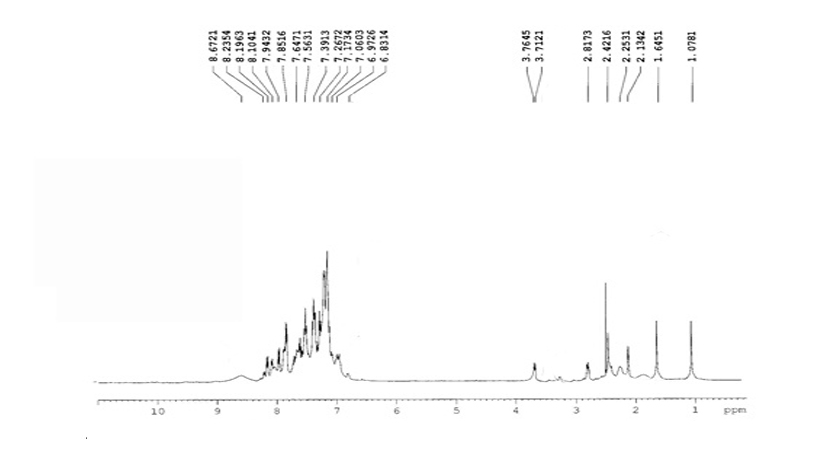
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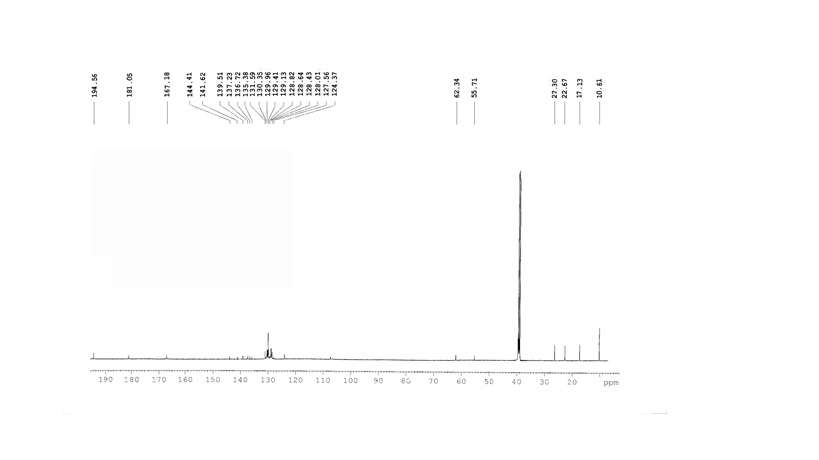
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**Figure S9.** 1H and 13C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-carbonyl)-3-(1-hydroxy propan-2-yl)-thiourea **(5c)**









**Tablo1.** Geometric optimization was done by means of Gaussian 09 with DFT/B3LYP 6-311G

Coordinates for compound 3a

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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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

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50 1 H 7.114527 0.978993 1.284788

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52 6 C 2.511389 -3.020235 0.732891

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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

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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

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68 8 O 1.188026 2.742913 2.106971

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