Supplementary Material

New pyrazole derivatives of potential biological activity

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Dedicated to Professor Keith Smith on the occasion of his 65th anniversary

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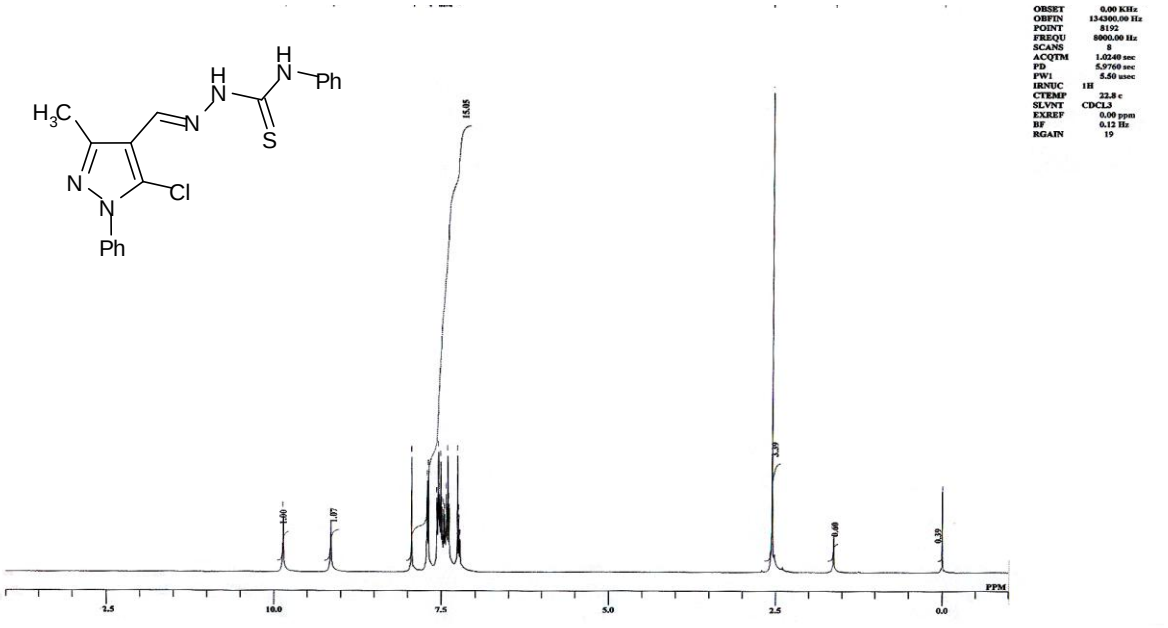
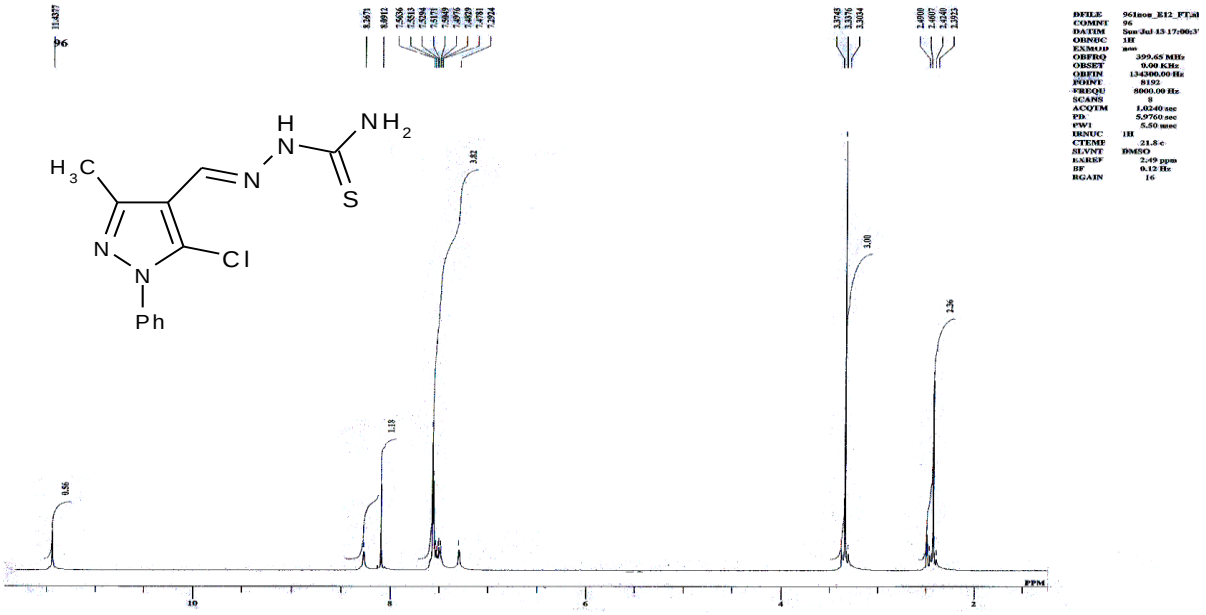
General Information

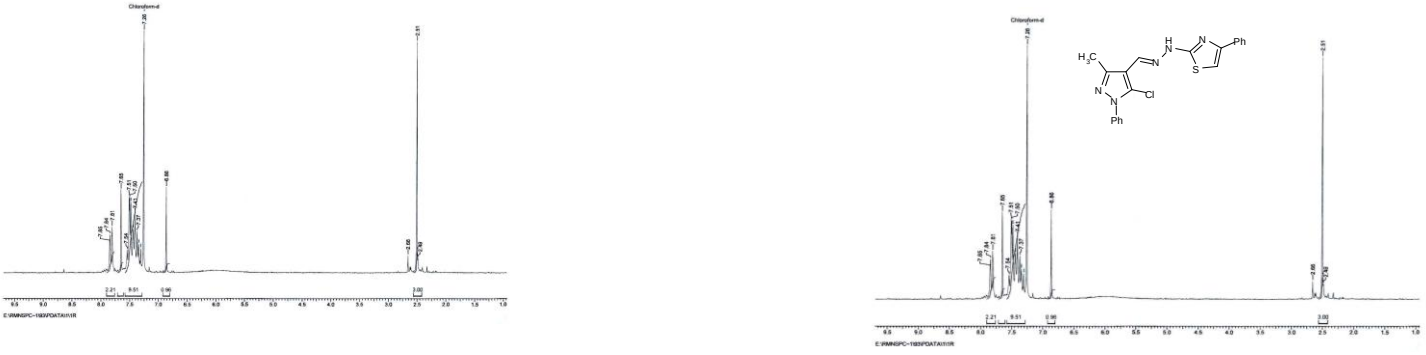
Melting points were measured on Stuart melting point apparatus (Bibby Scientific) SMP3. The IR spectra were recorded on a Shimadzu 470 IR-Spectrophotometer using KBr wafer technique. The ^{1}H NMR spectra were recorded on a Bruker ARX 200 spectrometer (200 MHz for ^{1}H and 50 MHz for ^{13}C) at the Faculty of Pharmacy, University of Aix Marseille, France, and on a Jeol LA 400 MHz (400 MHz for ^{1}H, 100 MHz for the ^{13}C) at Assiut university, ^{1}H and ^{13}C NMR chemical shifts (δ) were reported in parts per million (ppm) and were referenced to the solvent peak; $CDCl_3$ (7.26 ppm for ^{1}H and 76.90 ppm for ^{13}C) and DMSO-d_6 (2.50 ppm for ^{1}H and 39.70 ppm for ^{13}C). Multiplicities are represented by s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). Coupling constants (*J*) are reported in Hertz (Hz). Mass spectra were obtained with a Jeol JMS-600 mass spectrometer (Assiut University). Elemental analyses were carried out using a Perkin-Elmer 240C Microanalyzer (Microanalytical Laboratory), Faculty of Science, Assiut University and the results were in an acceptable range (±0.4%). All other solvents, reagents and chemicals were used as purchased unless stated otherwise.



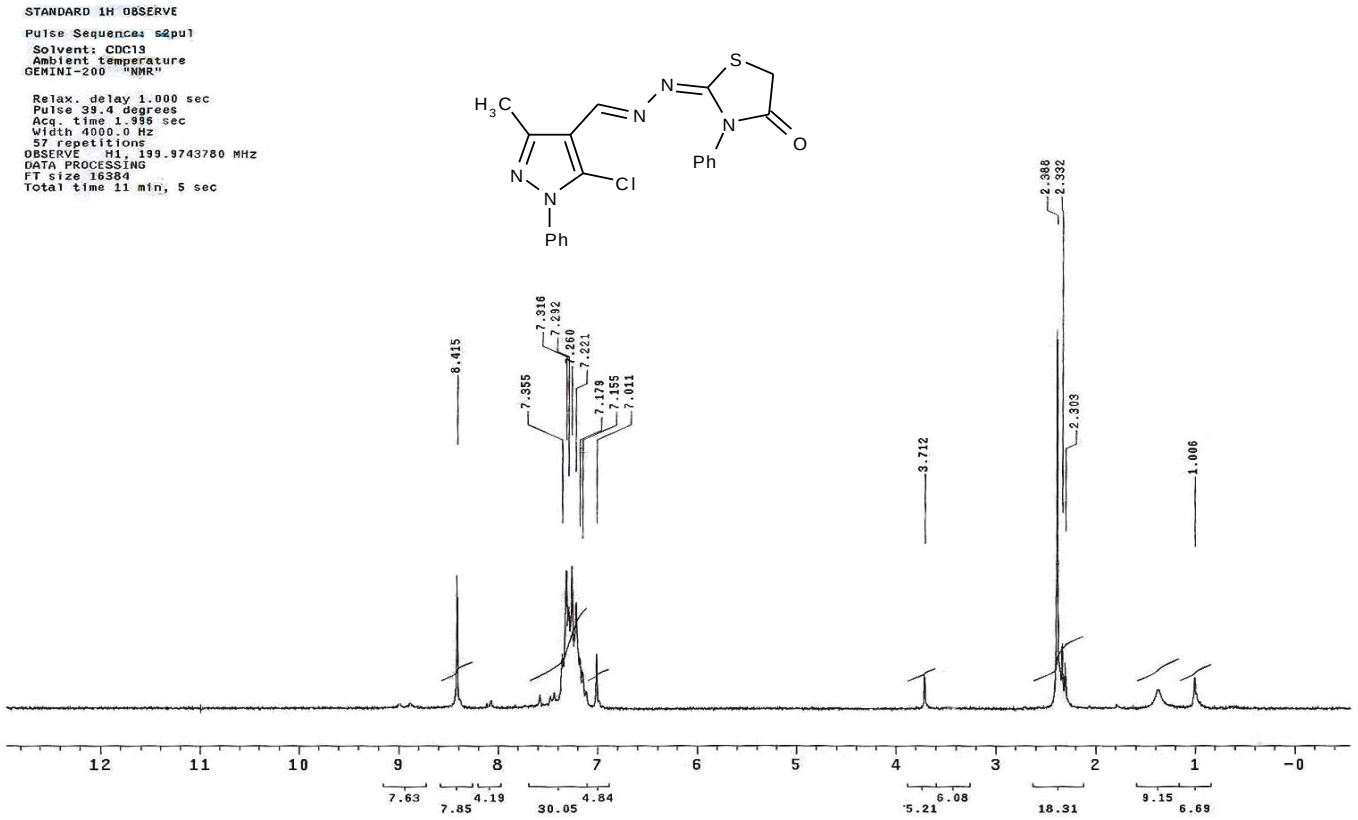
N^1-((5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylene)-N^4-phenylthiosemicarbazone (3)



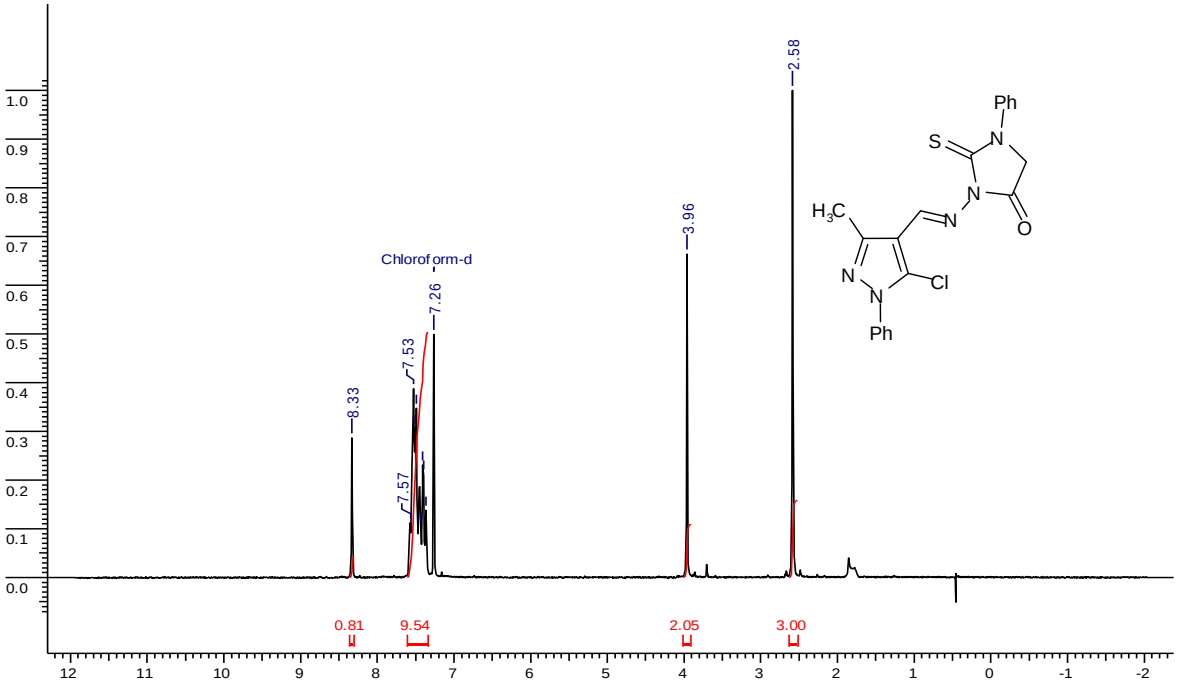
N^1-((5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylene)thiosemicarbazone (4)



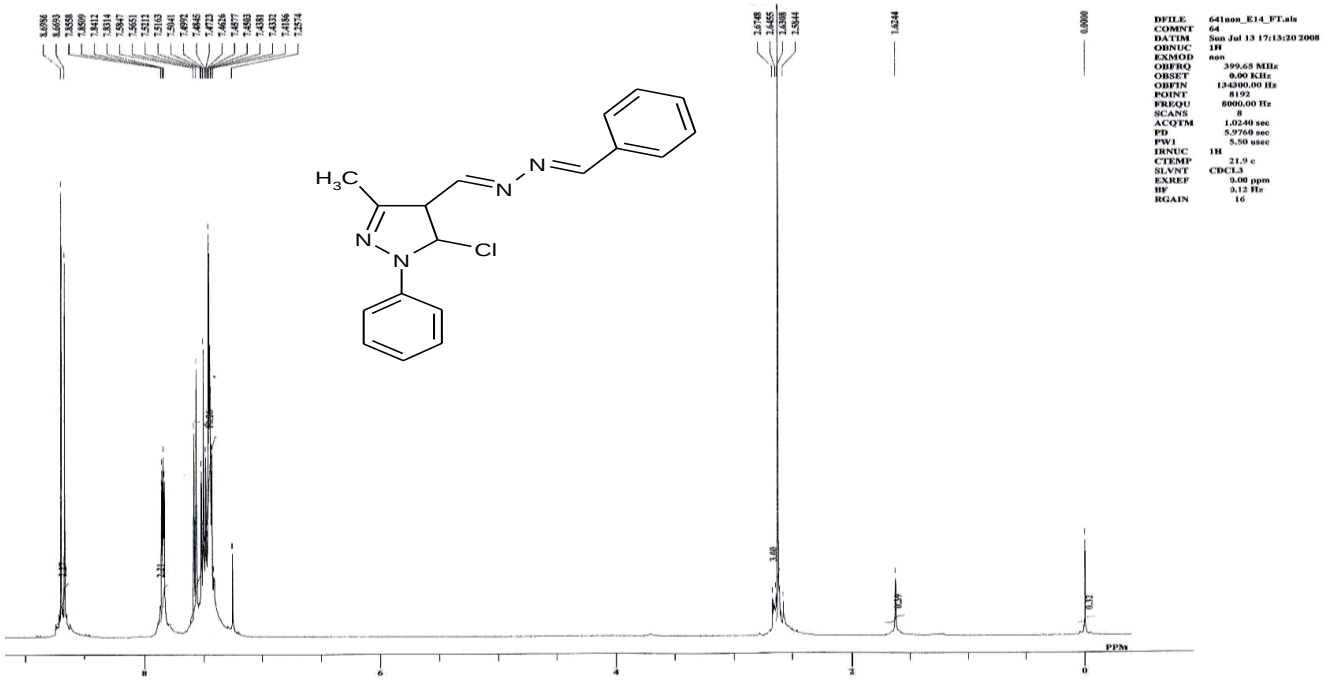
2-(2-((5-chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylene)hydrazino)-4-phenyl-1,3-thiazole (5)



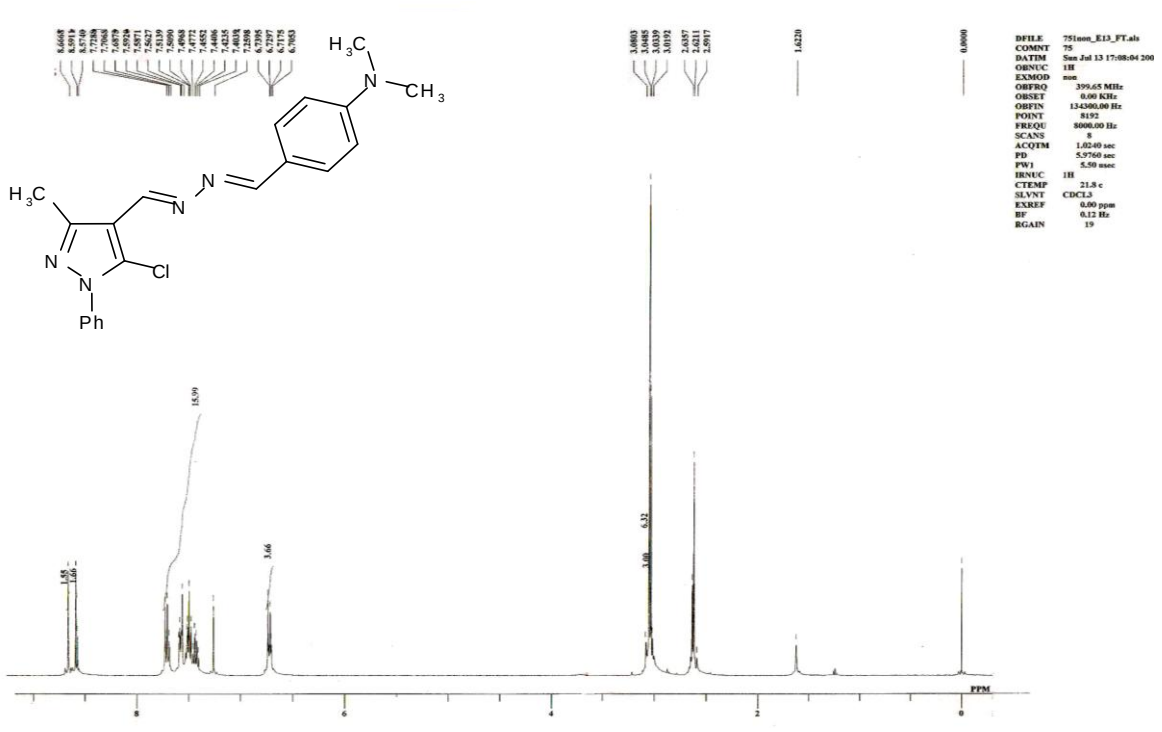
2-((5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylenehydrazono)-3-phenylthiazolidin -4-one (6)



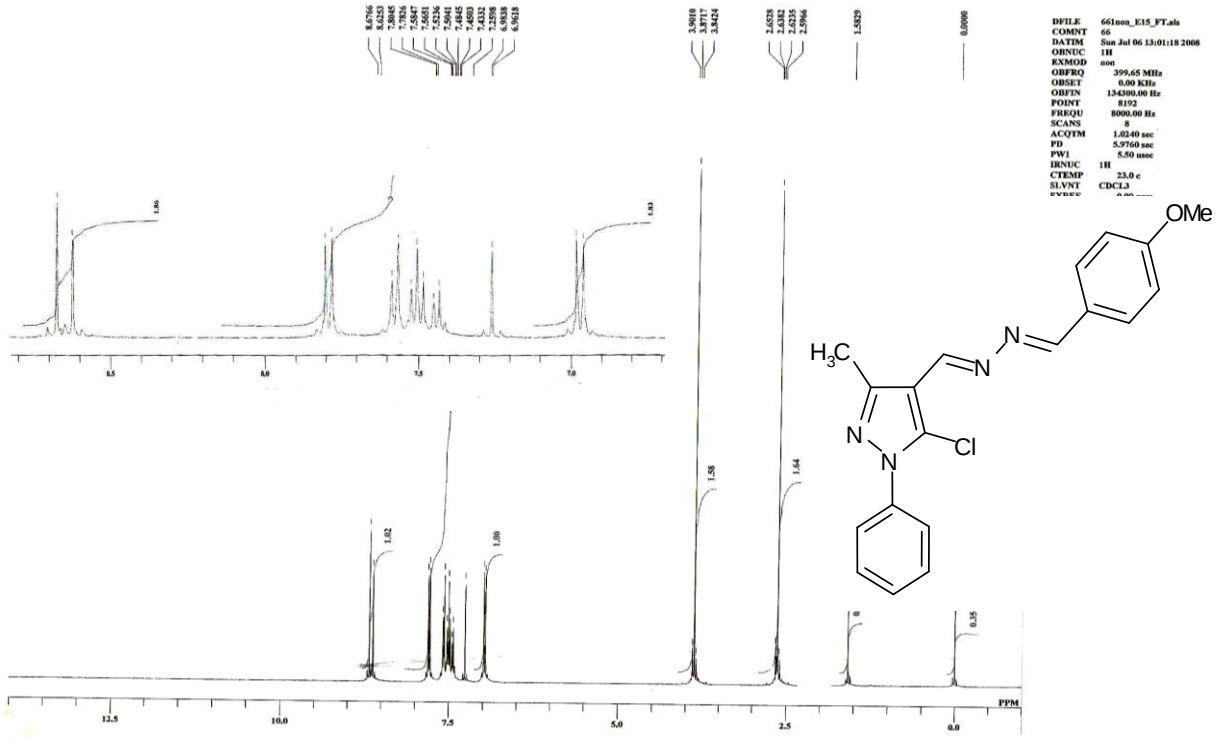
3-((5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methyleneamino)-1-phenyl-2-thioxo-imidazolidin-4-one (7)



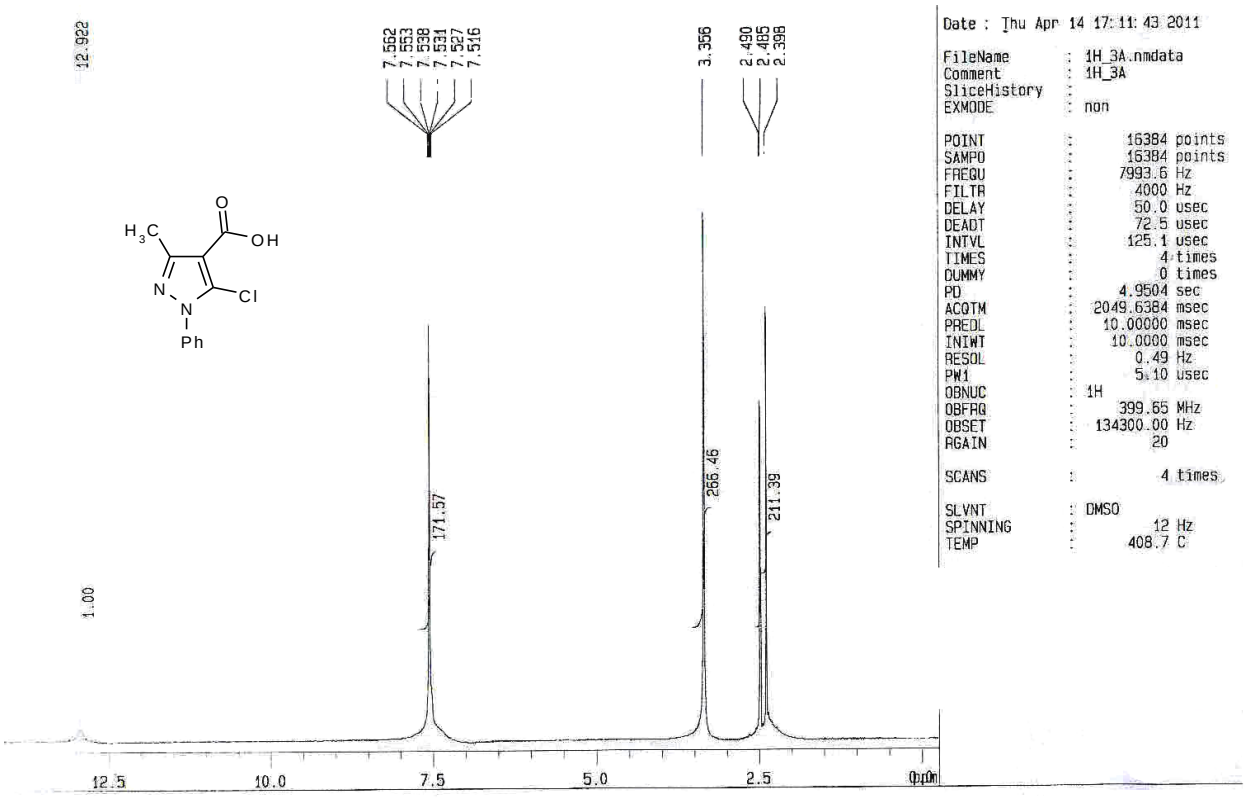
_N_-((5-Chloro-3-methyl-1-phenyl-1_H_-pyrazol-4-yl)methylene)-_N'_-benzylidenehydrazine (8a)



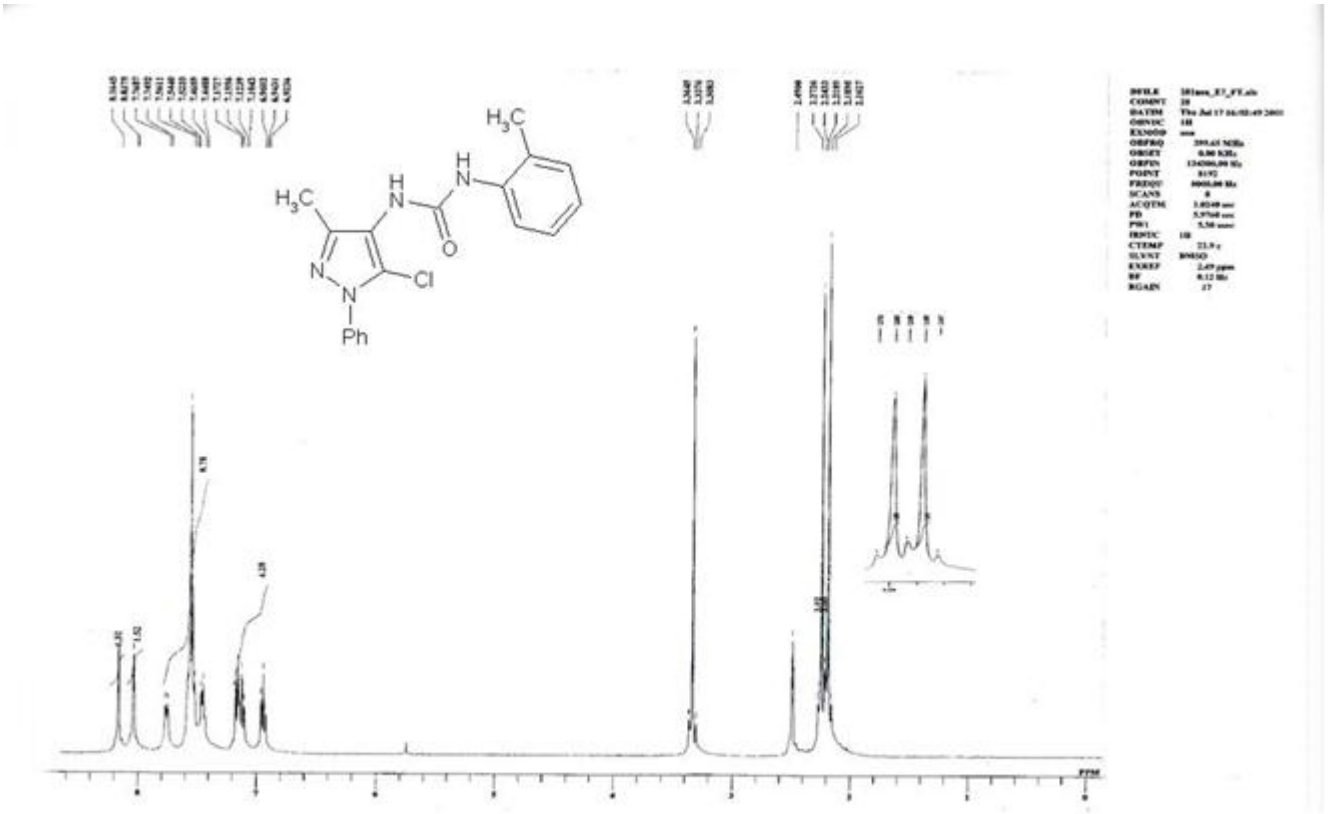
_N_-((5-Chloro-3-methyl-1-phenyl-1_H_-pyrazol-4-yl)methylene)-_N_'-(4-dimethylaminobenzylid- ene)hydrazine (8c)



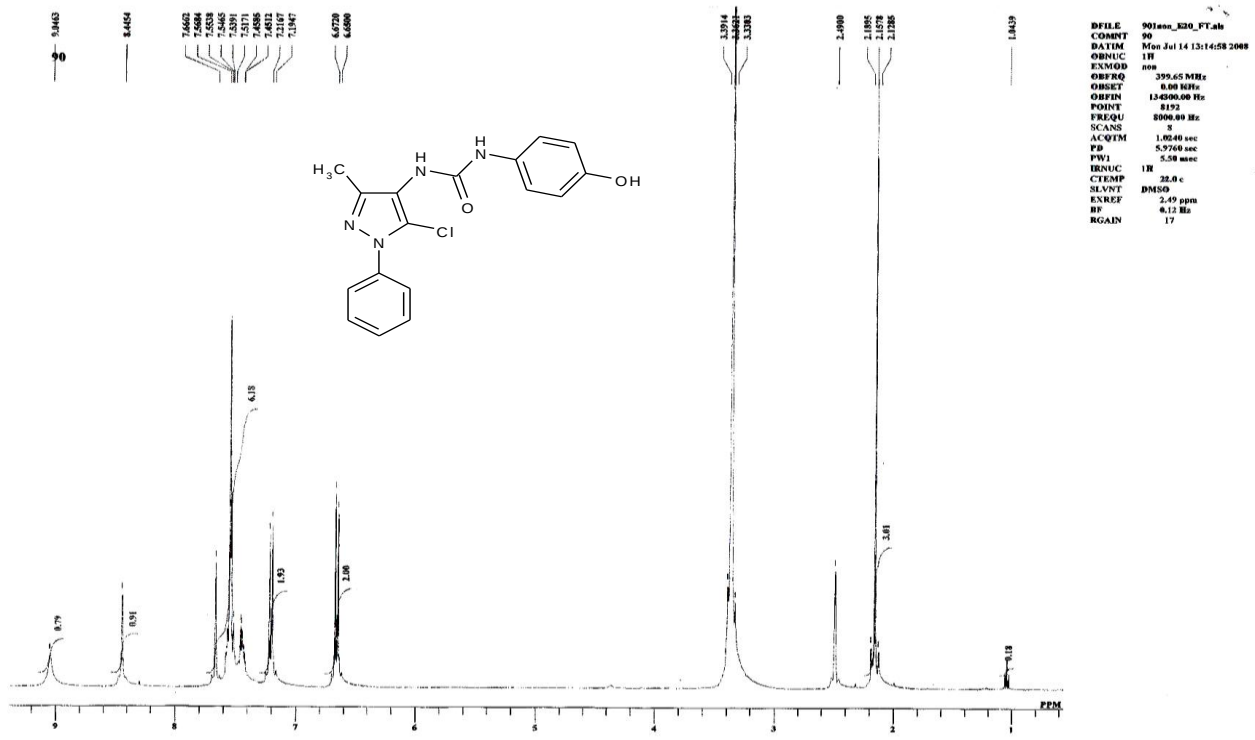
_N_-((5-Chloro-3-methyl-1-phenyl-1_H_-pyrazol-4-yl)methylene)-_N_'-(4-methoxybenzylidene)-hydrazine (8d)



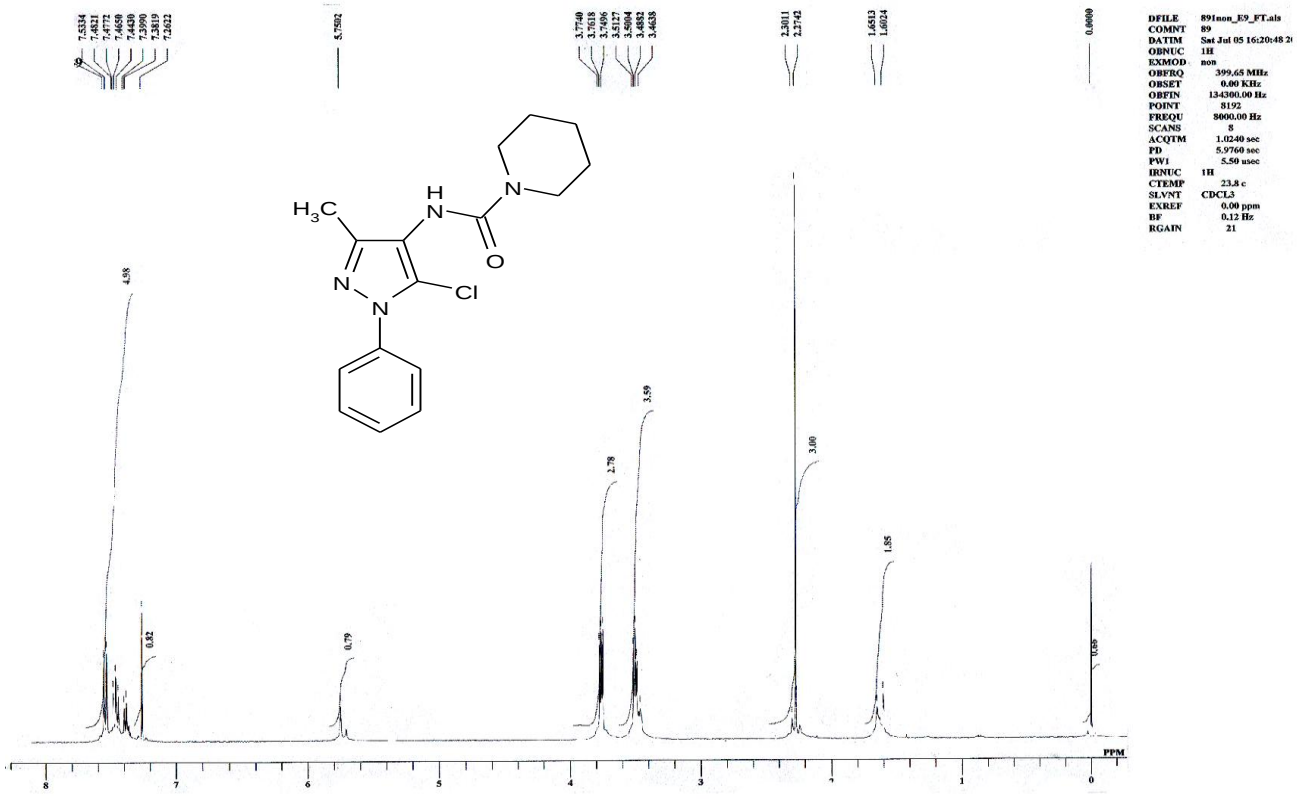
5-Chloro-3-methyl-1-phenyl-1*H*-pyrazole-4-carboxylic acid (9)



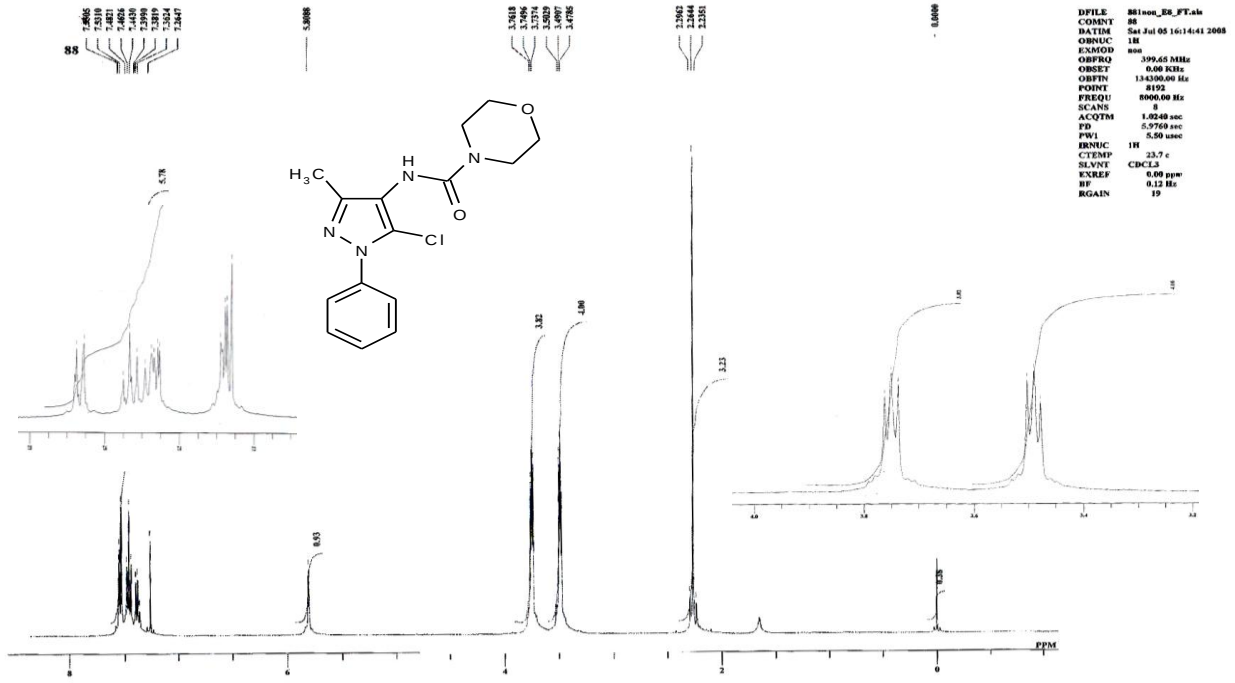
***N*¹-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)-*N*³-(2-methylphenyl)urea (13c).**



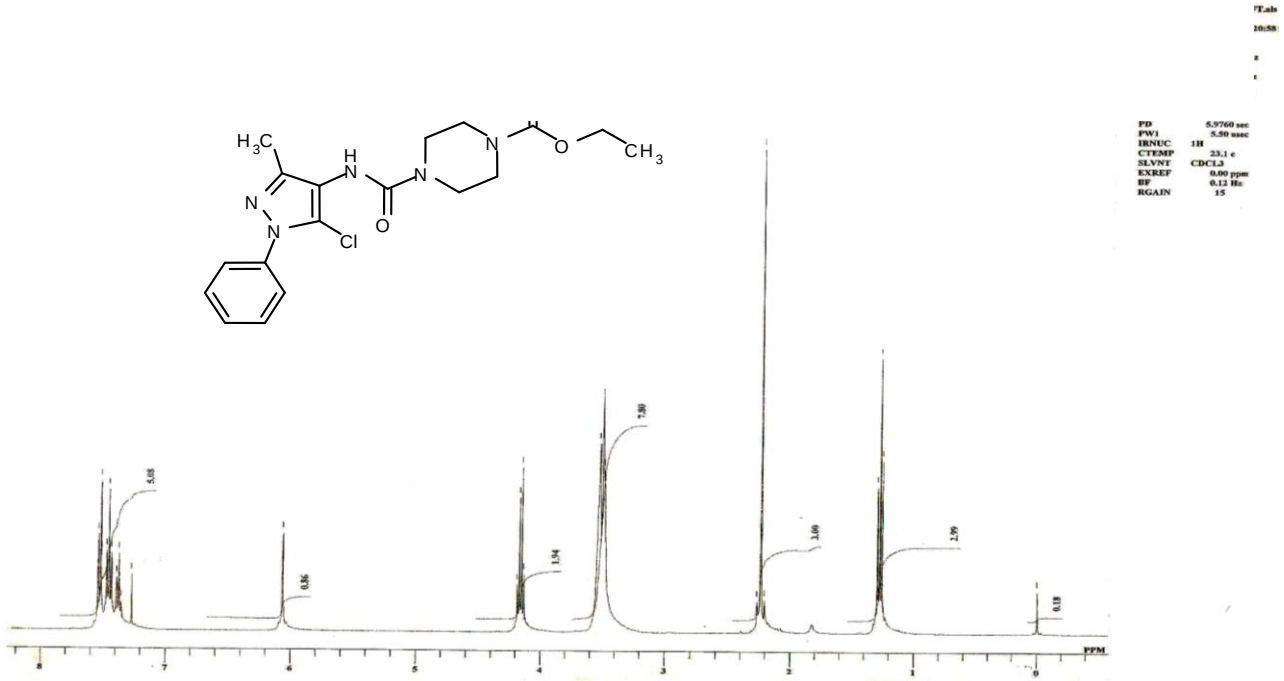
N^1-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)-N^3-(4-hydroxyphenyl)urea (13d)



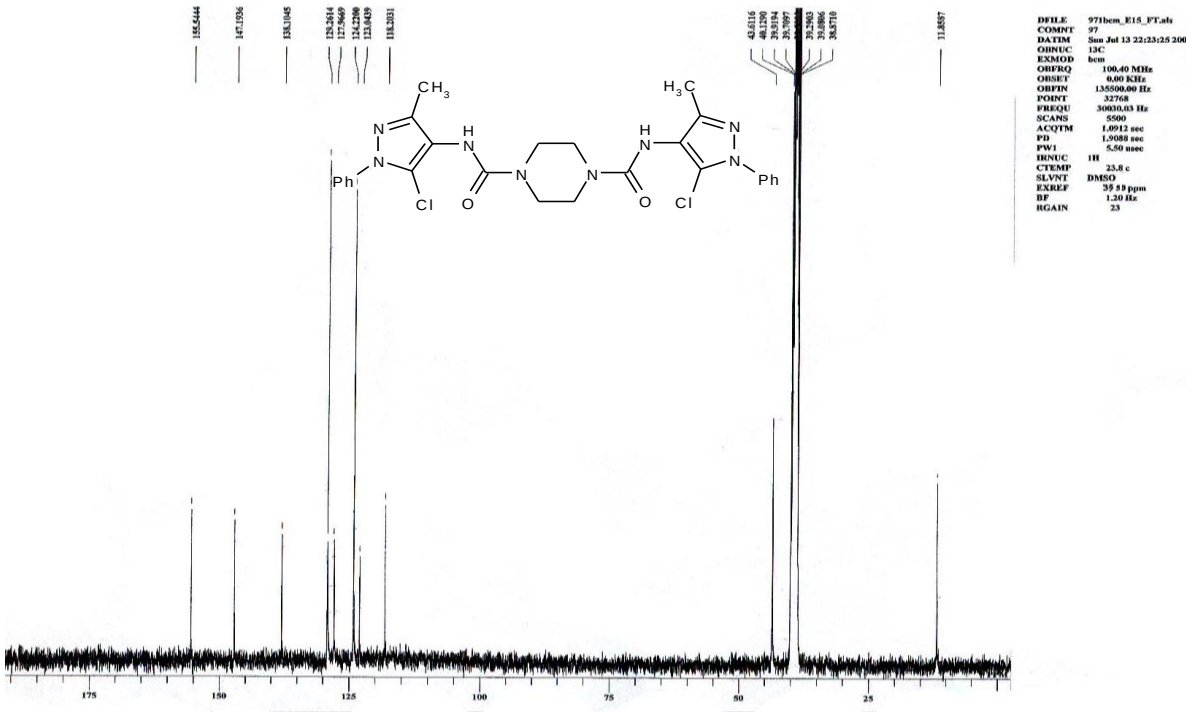
5-Chloro-3-methyl-1-phenyl-1*H*-4-(piperidinocarbonylamino)pyrazole (14a)



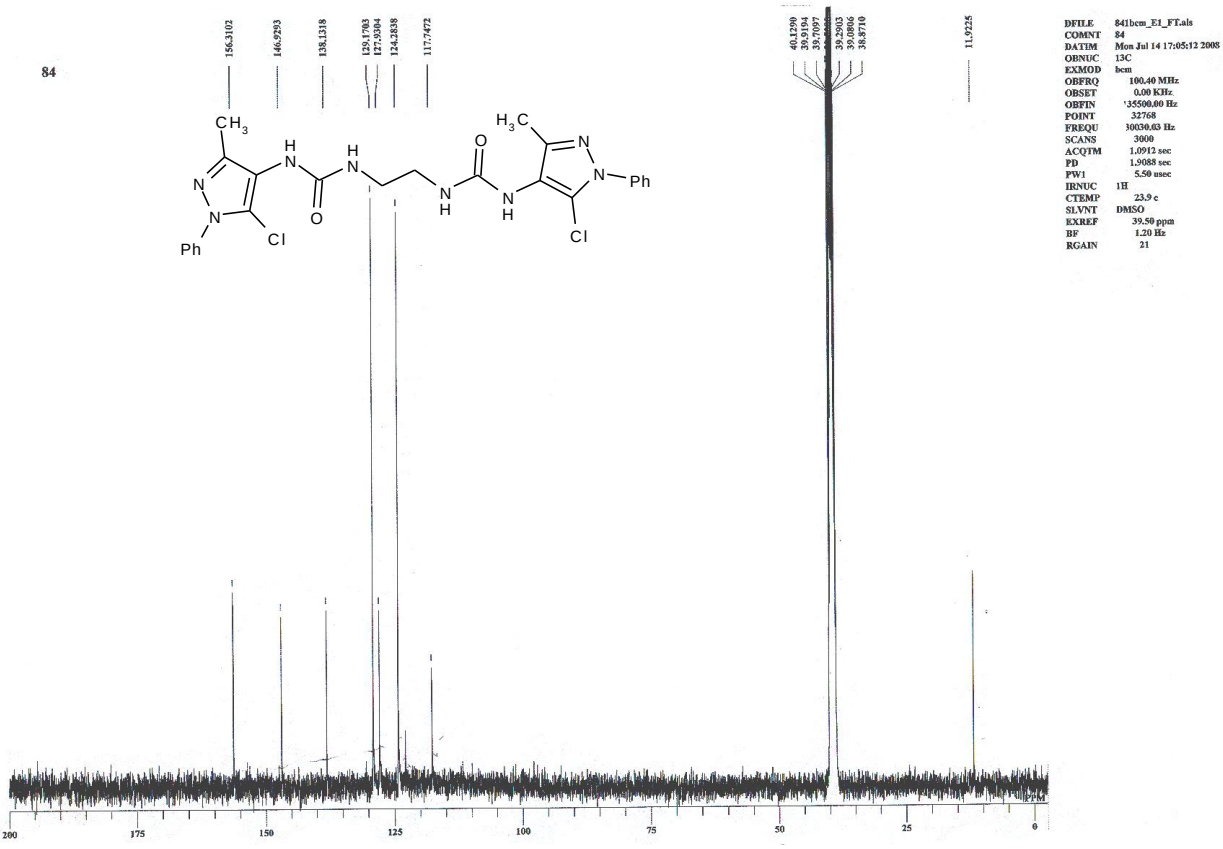
5-Chloro-3-methyl-1-phenyl-1*H*-4-(morpholinocarbonylamino)pyrazole (14b).



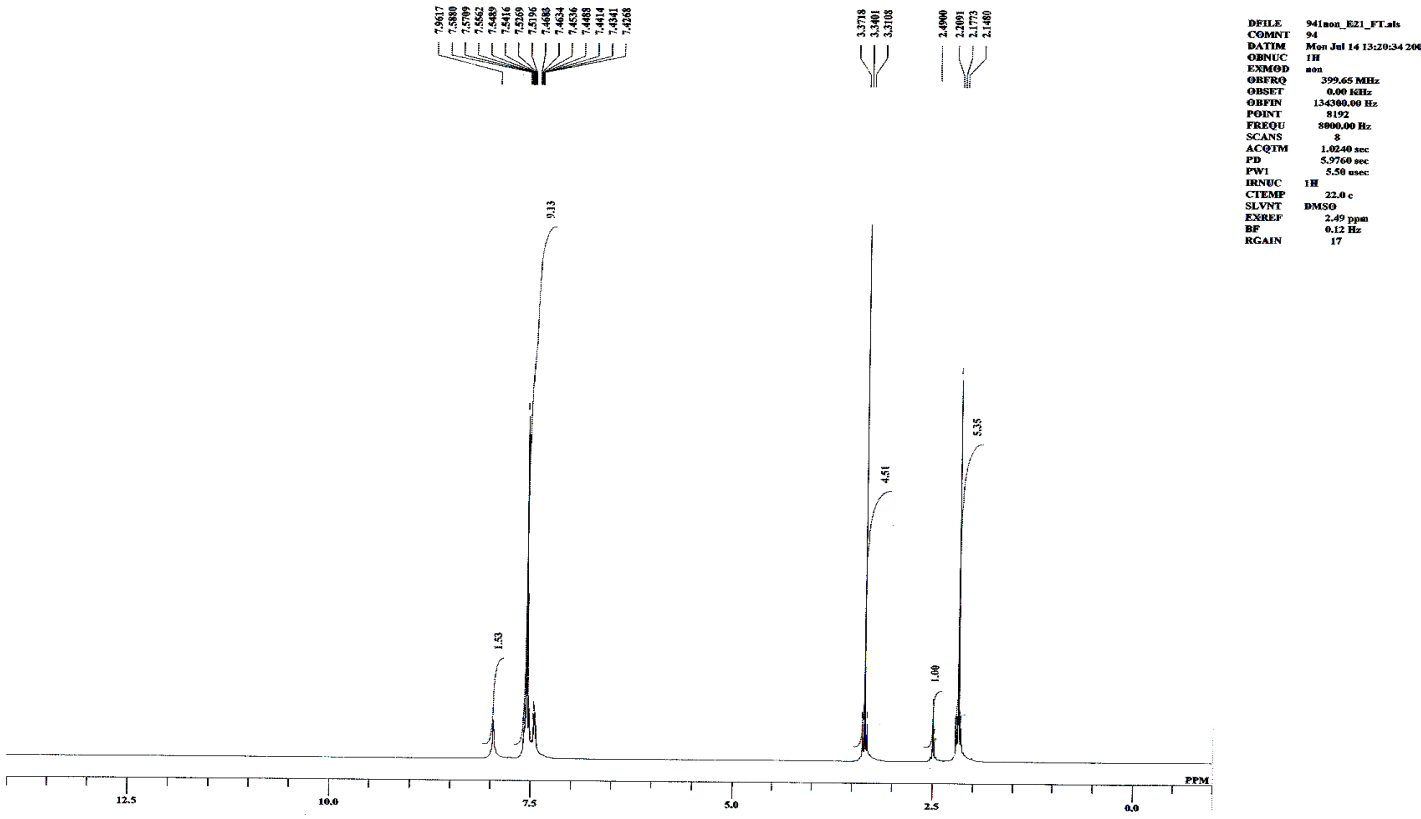
Ethyl 4-(5-chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-ylcarbamoyl)piperazine-1-carboxylate (14c)



N^1,N^4-Bis-(5-chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)piperazine-1,4-dicarboxamide (15)



1,4-Di(3-(5-chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)ureido)ethane (17)



***N*[1],*N*[3]-Bis(5-chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)urea (18)**

