

Supplementary Data

Facile, novel and efficient synthesis of new pyrazolo[3,4-b]pyridine products from condensation of pyrazole-5-amine derivatives and activated carbonyl groups

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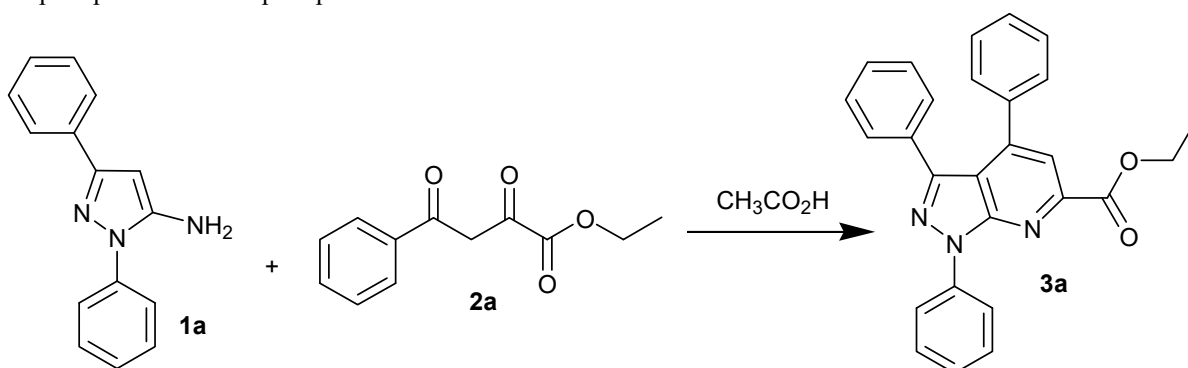
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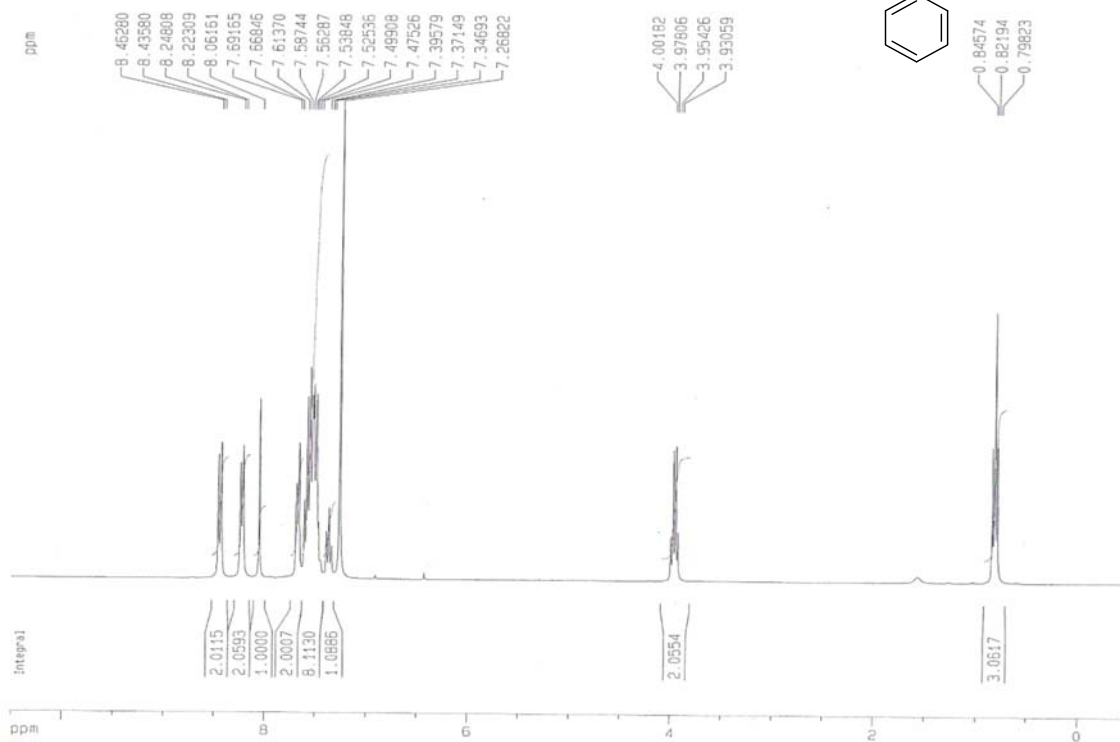
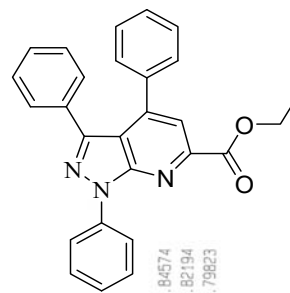
Synthesis of ethyl-1,3,4-triphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate **3a**, General Procedure

At the outset, a mixture of 1,3-diphenyl-1H-pyrazol-5-amine **1a** (1 mmol) and ethyl 2,4-dioxo-4-phenylbutanoates **2a** (1 mmol) in refluxing CH₃CO₂H (10 mL) was stirred for 5 h (Scheme S1). The progress of the reaction was monitored by TLC (ethyl acetate/*n*-hexane: 1/2). After completion, the reaction was cooled to room temperature, and the precipitated product was filtered, washed with ethanol (20 mL) and purified by crystallization to afford the pure product **3a** as a pure powder.

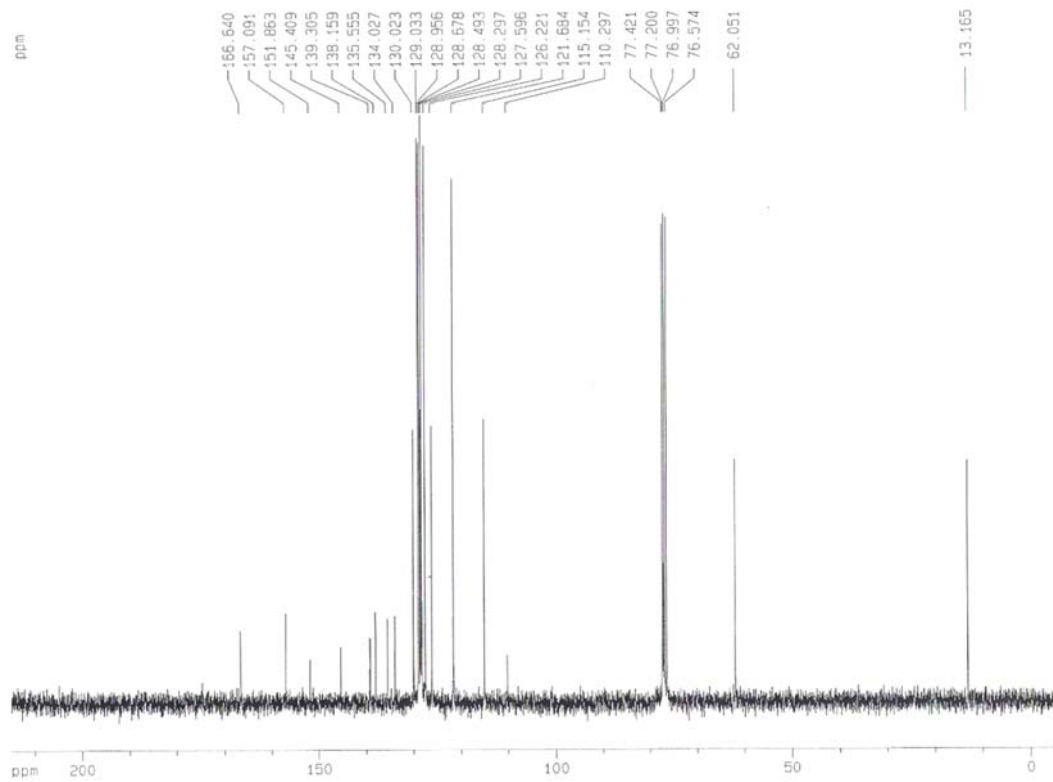


Scheme S1 Synthesis of novel pyrazolo[3,4-b]pyridine **3a**

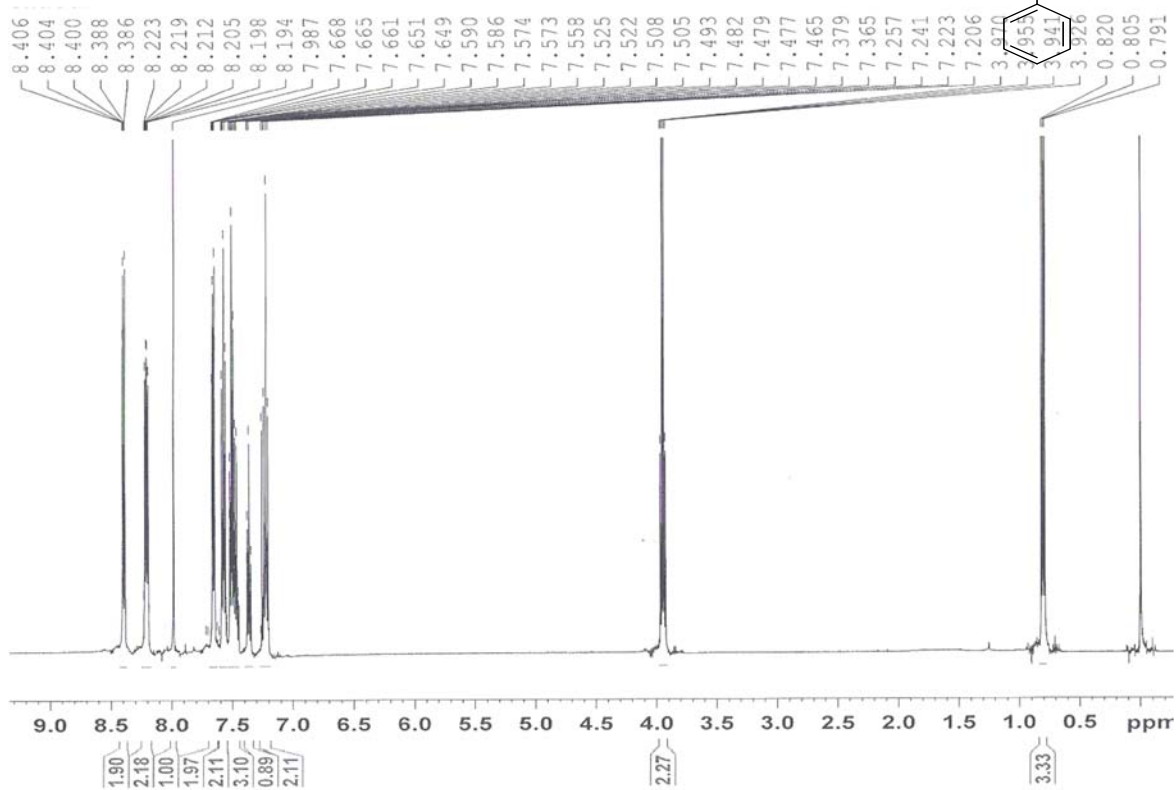
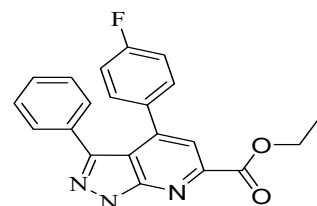
¹H NMR: Ethyl-1,3,4-triphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3a)



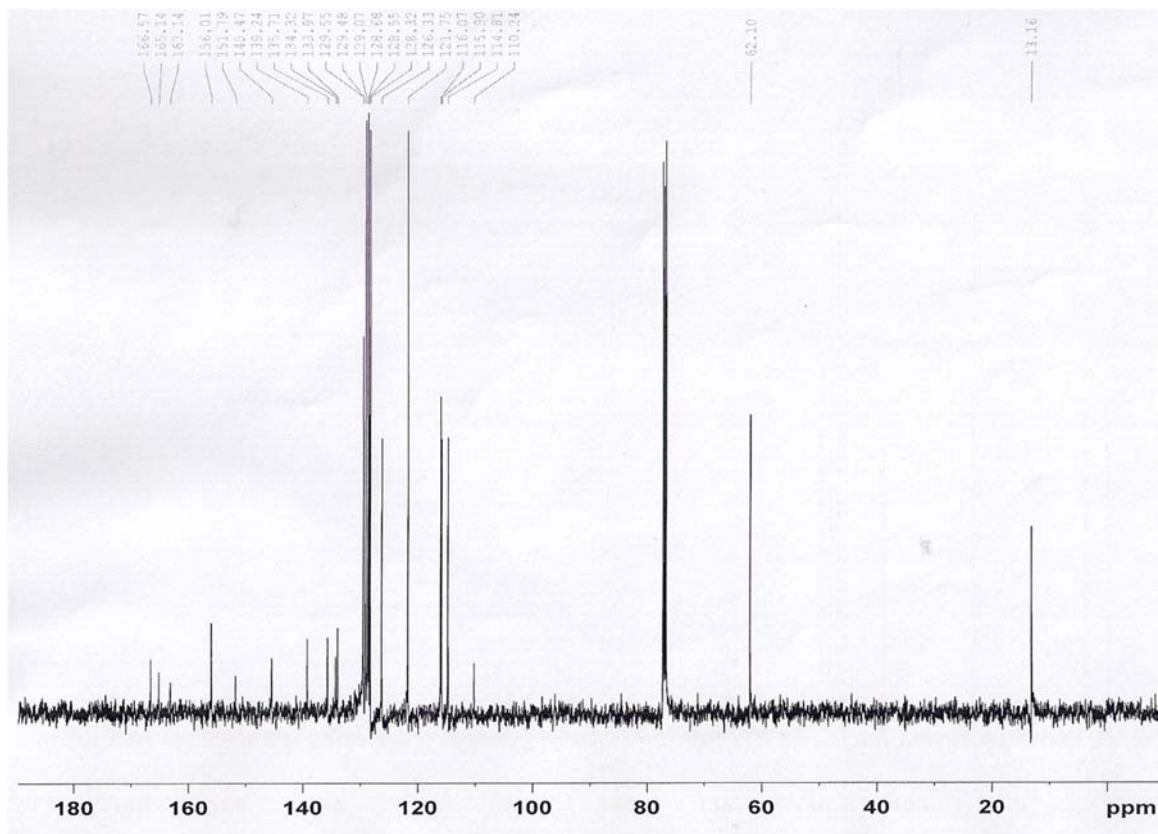
¹³C NMR (3a)



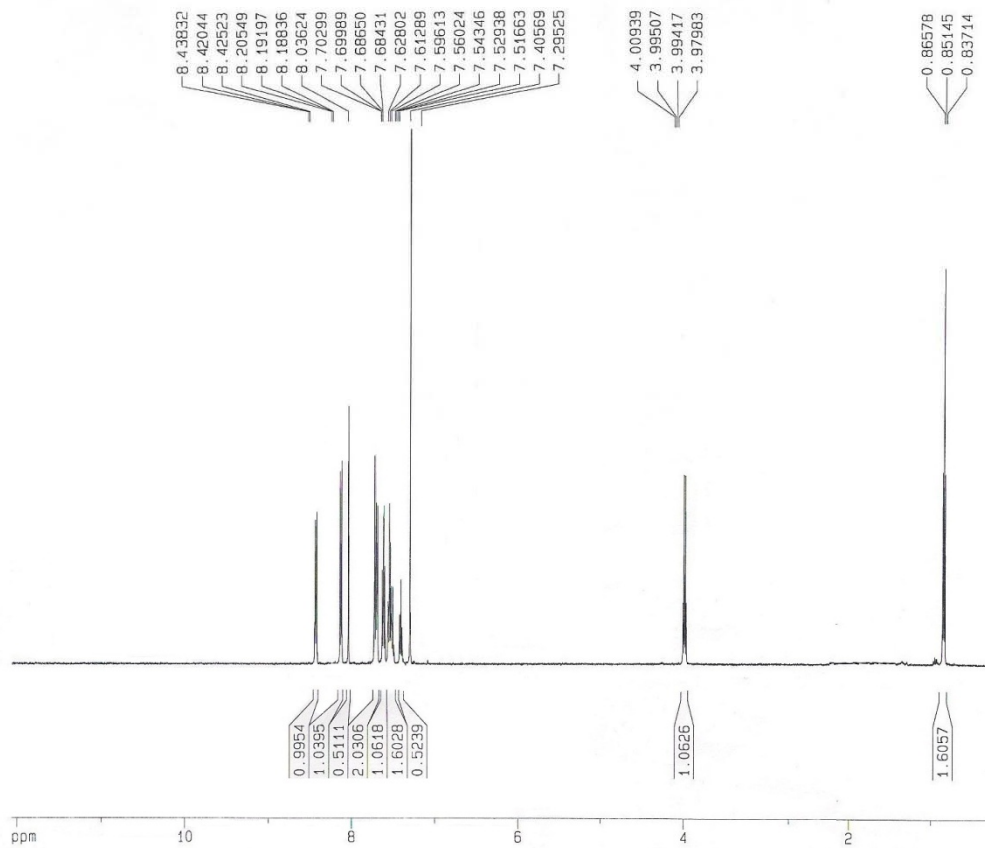
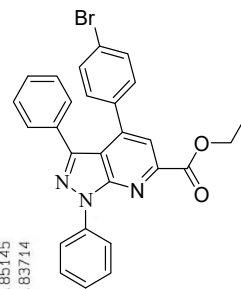
¹H NMR Ethyl-4-(4-fluorophenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3b)



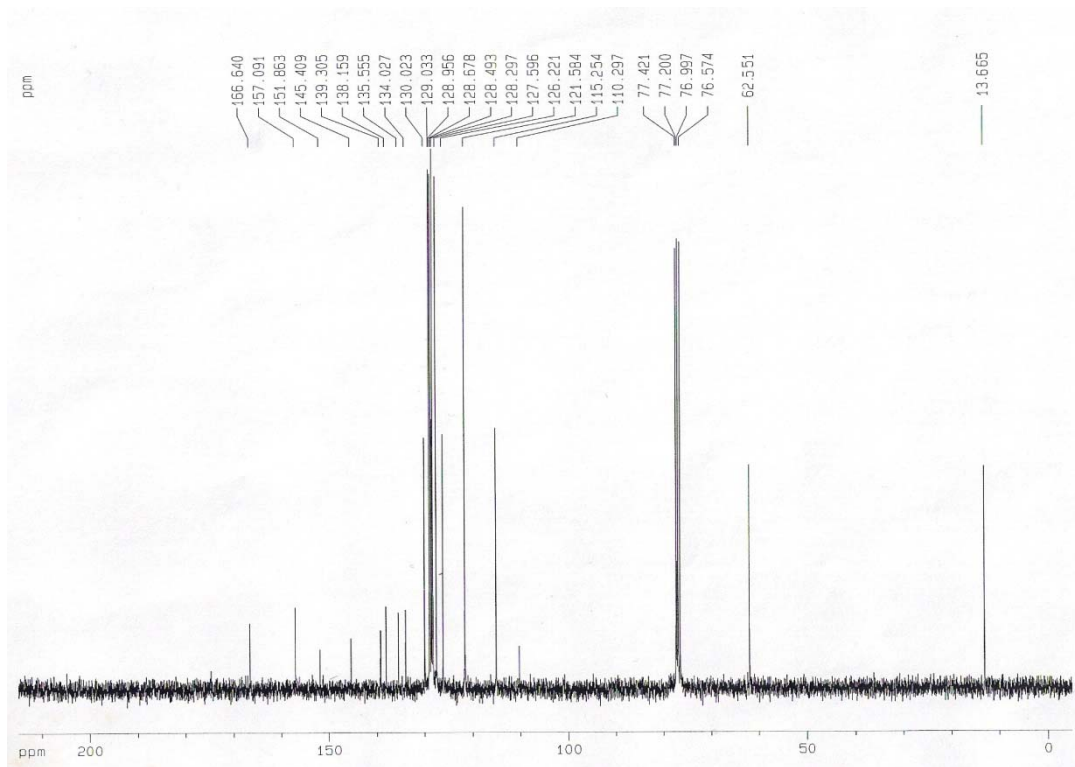
¹³C NMR (3b)



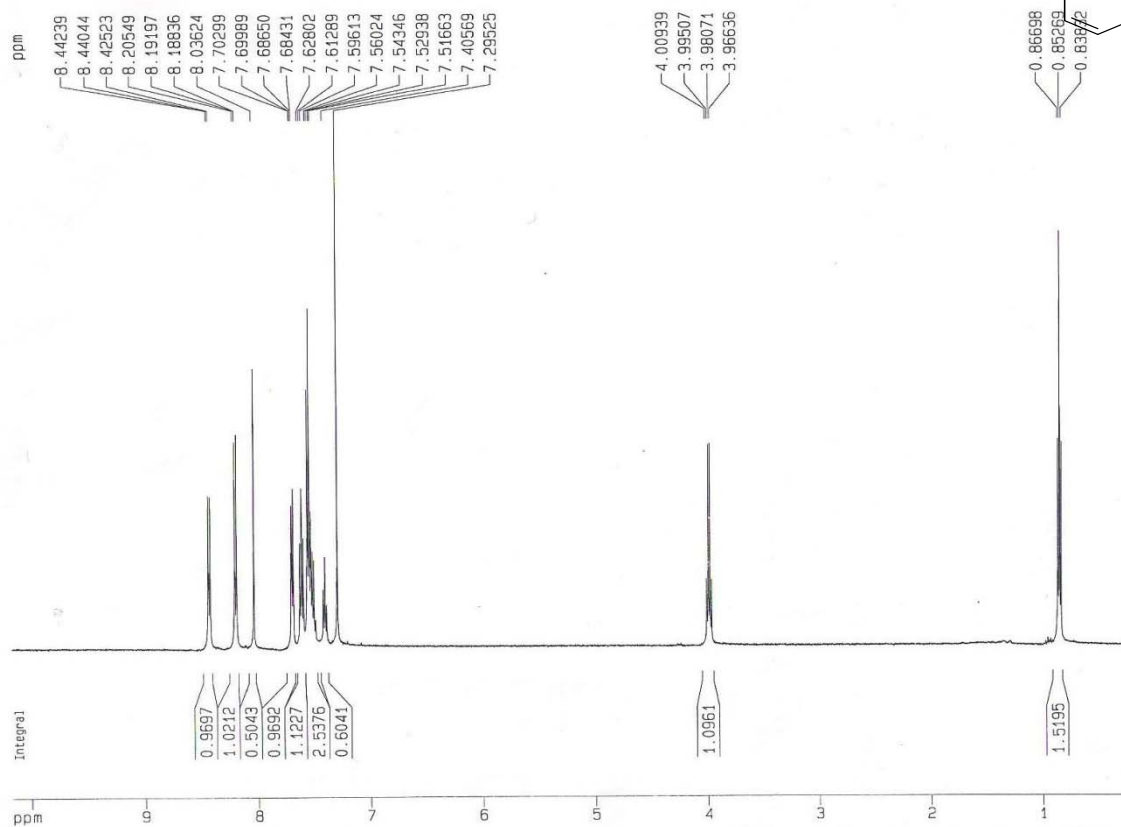
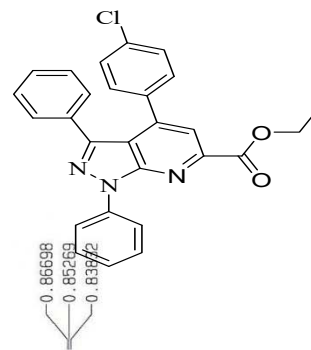
¹H NMR Ethyl-4-(4-bromophenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3c):



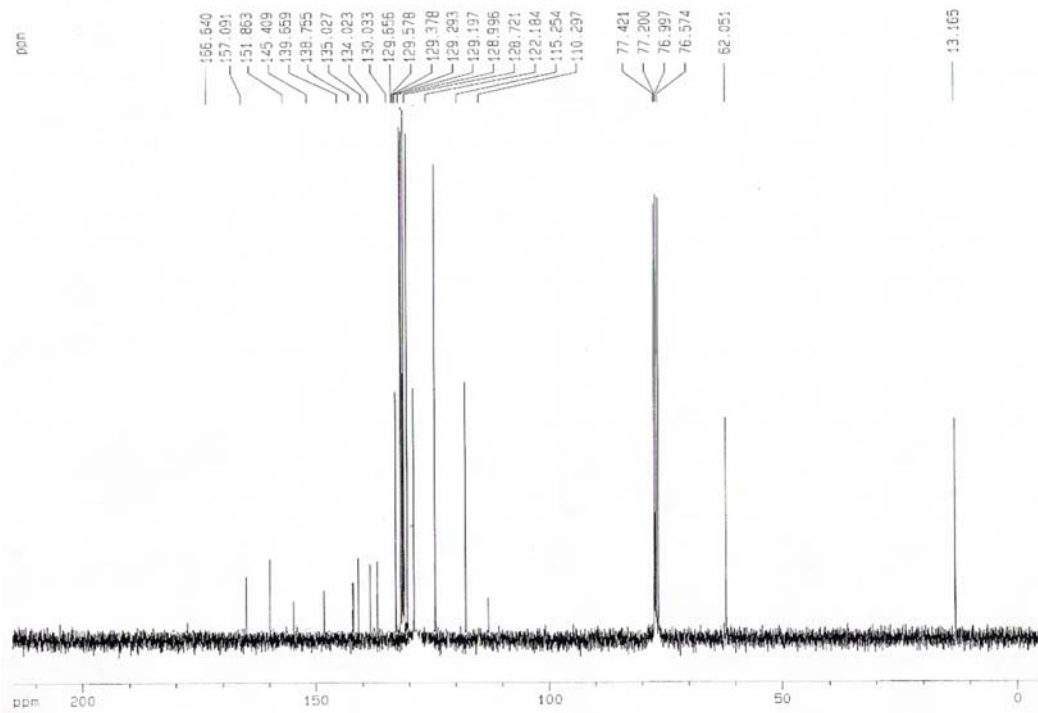
¹³C NMR (3c)



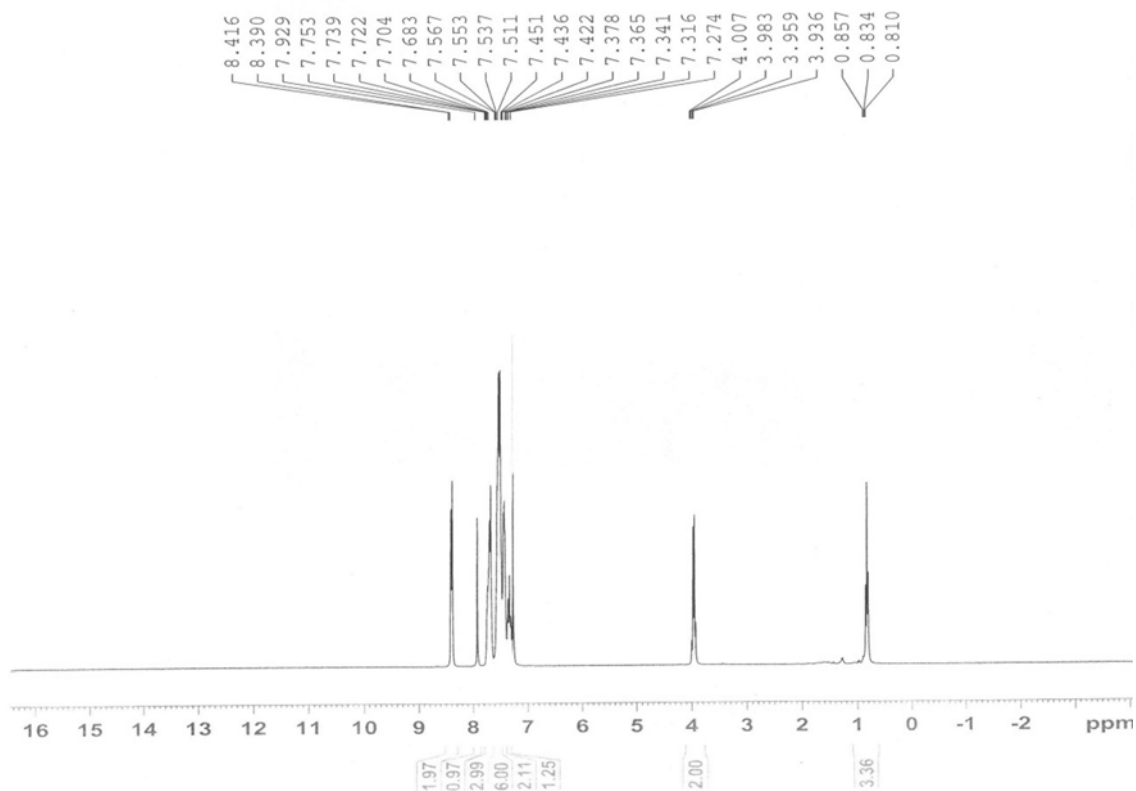
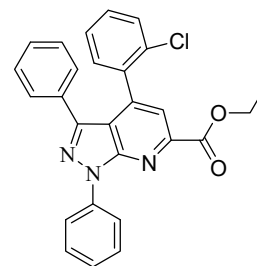
¹H NMR: Ethyl-4-(4-chlorophenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3d)



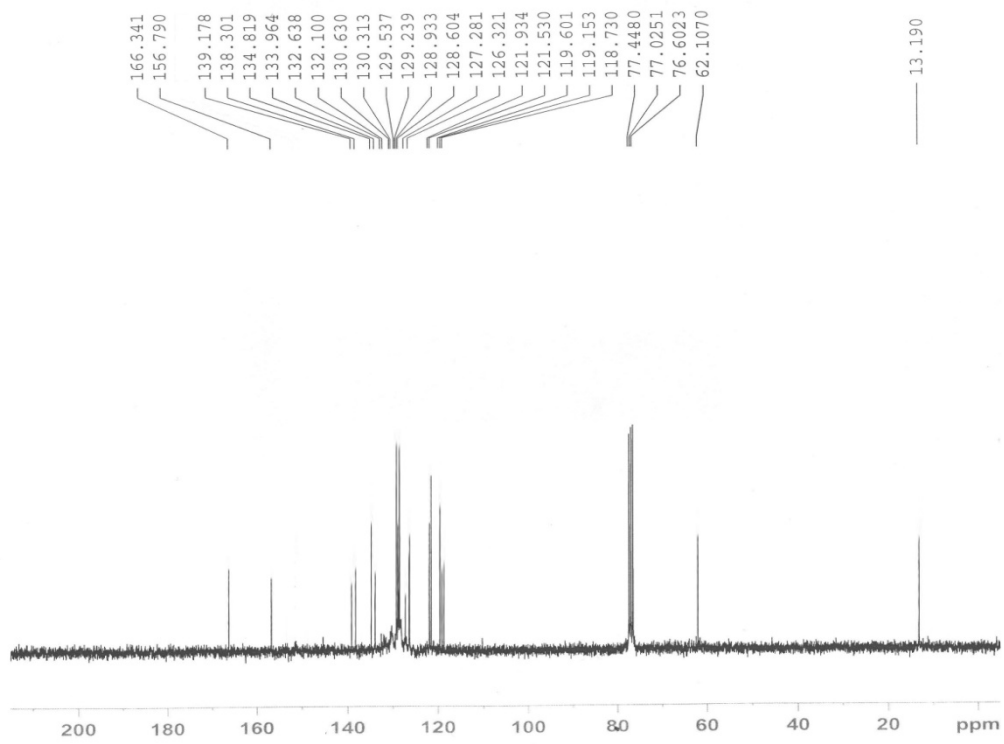
¹³C NMR (3d)



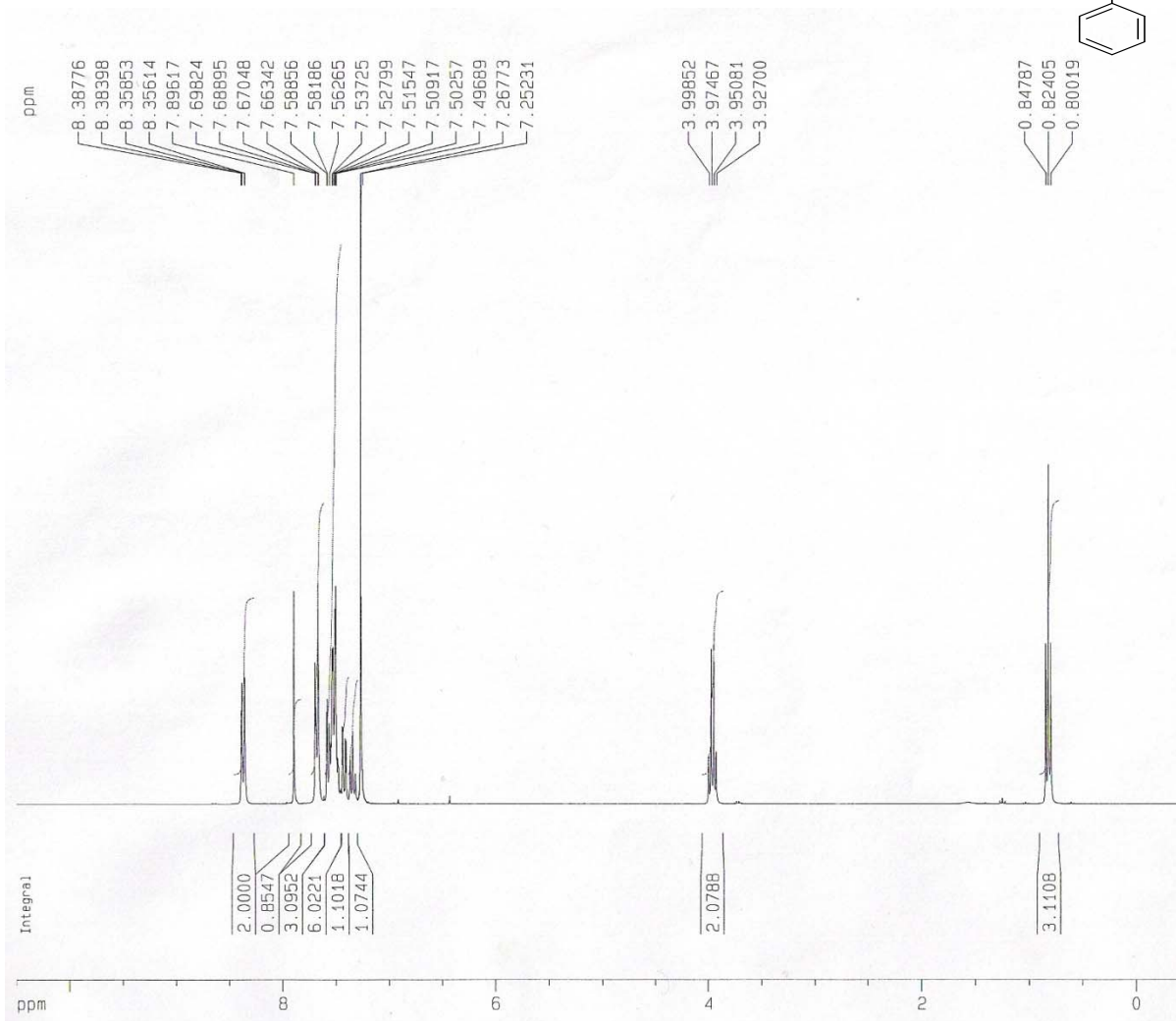
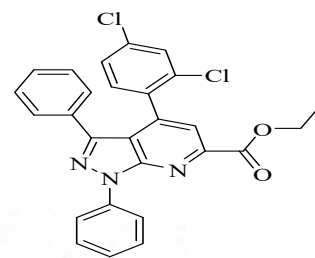
¹H NMR: Ethyl-4-(2-chlorophenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3e)



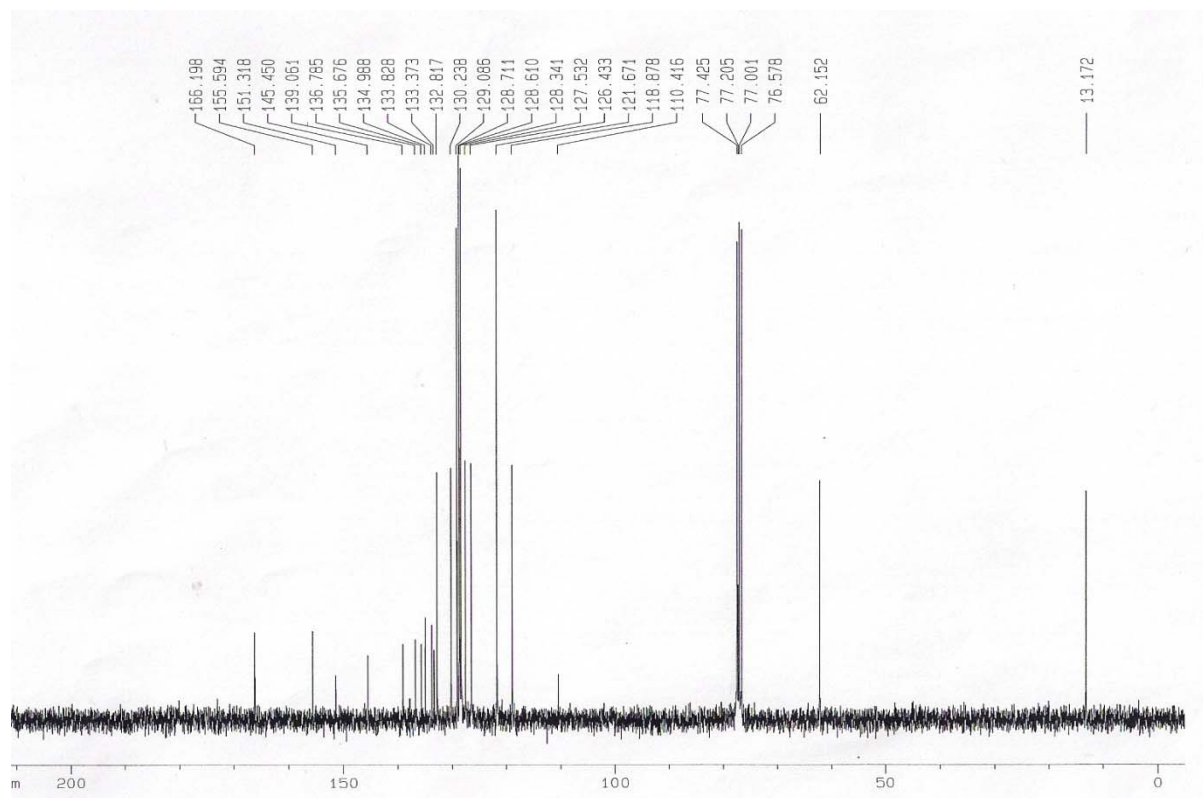
¹³C NMR (3e)



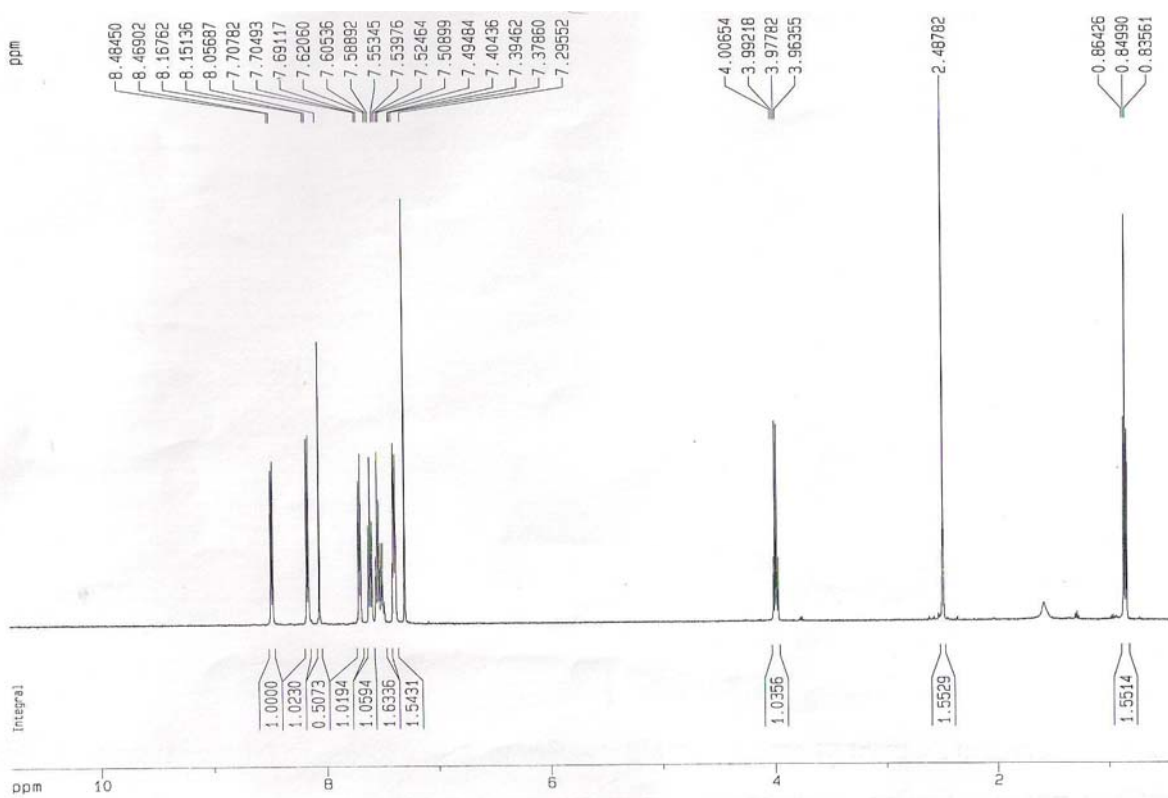
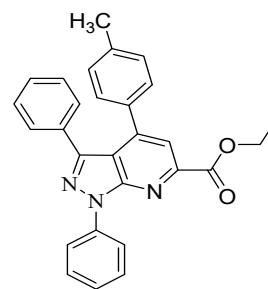
¹H NMR: Ethyl-4-(2,4-dichlorophenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3f)



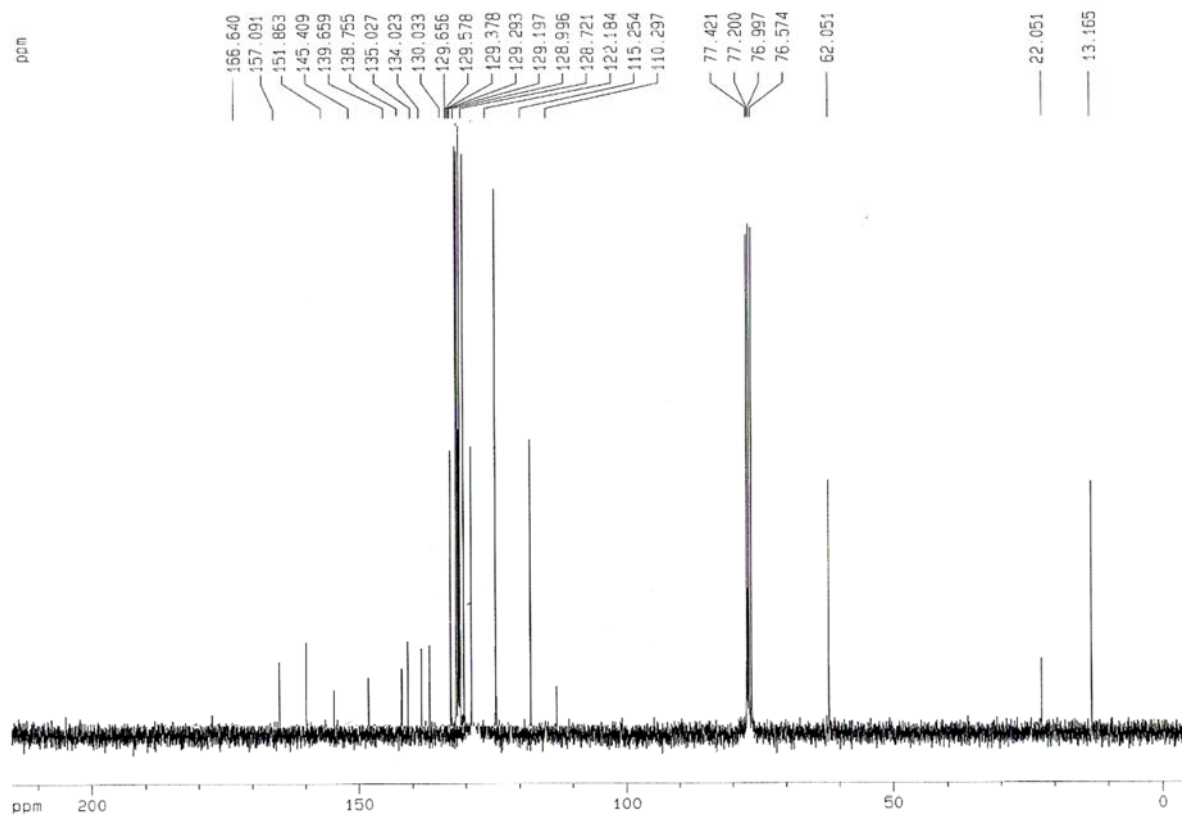
¹³C NMR (3f)



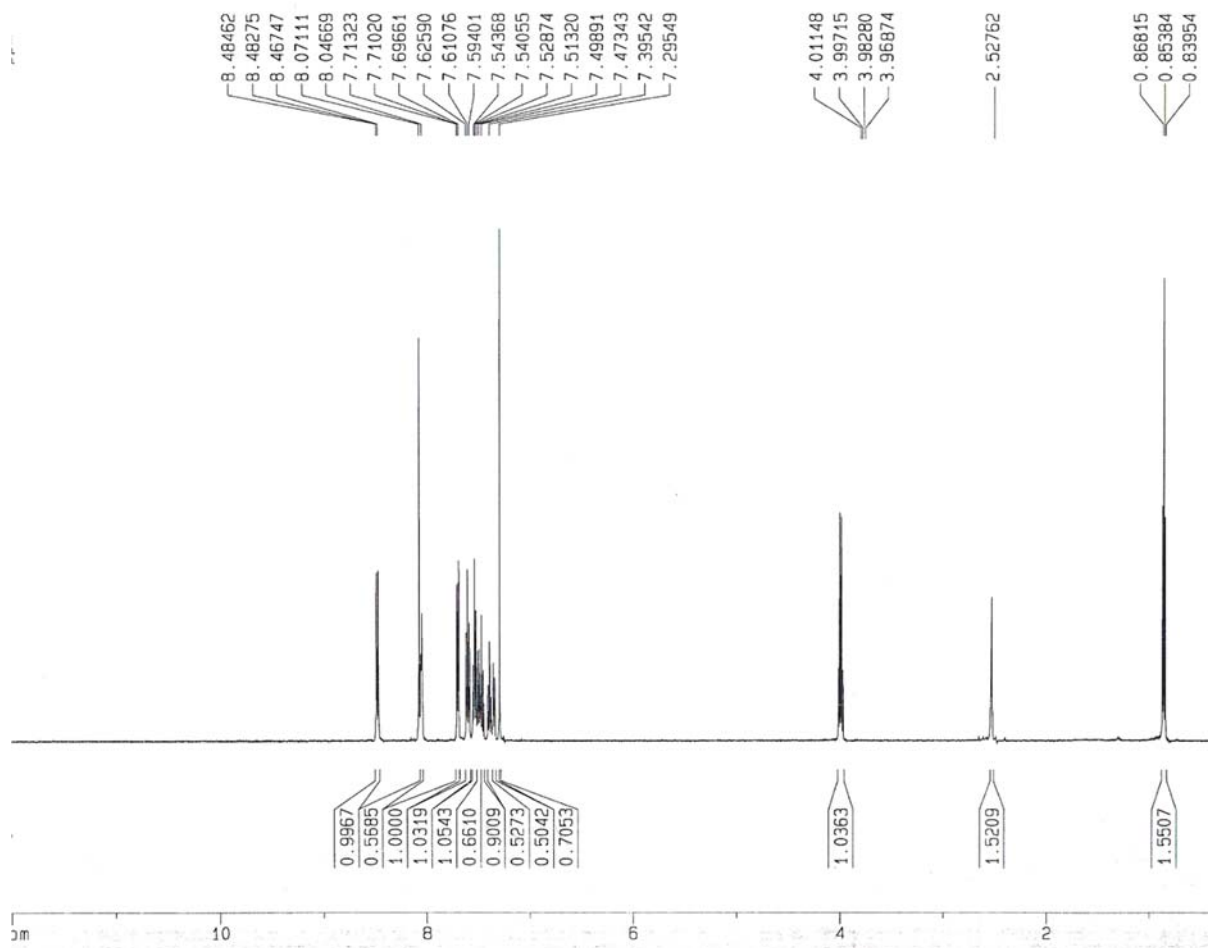
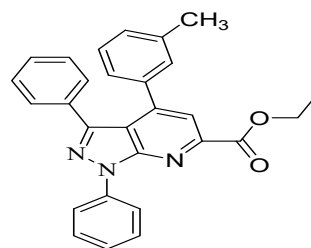
¹H NMR: Ethyl-1,3-diphenyl-4-p-tolyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3g):



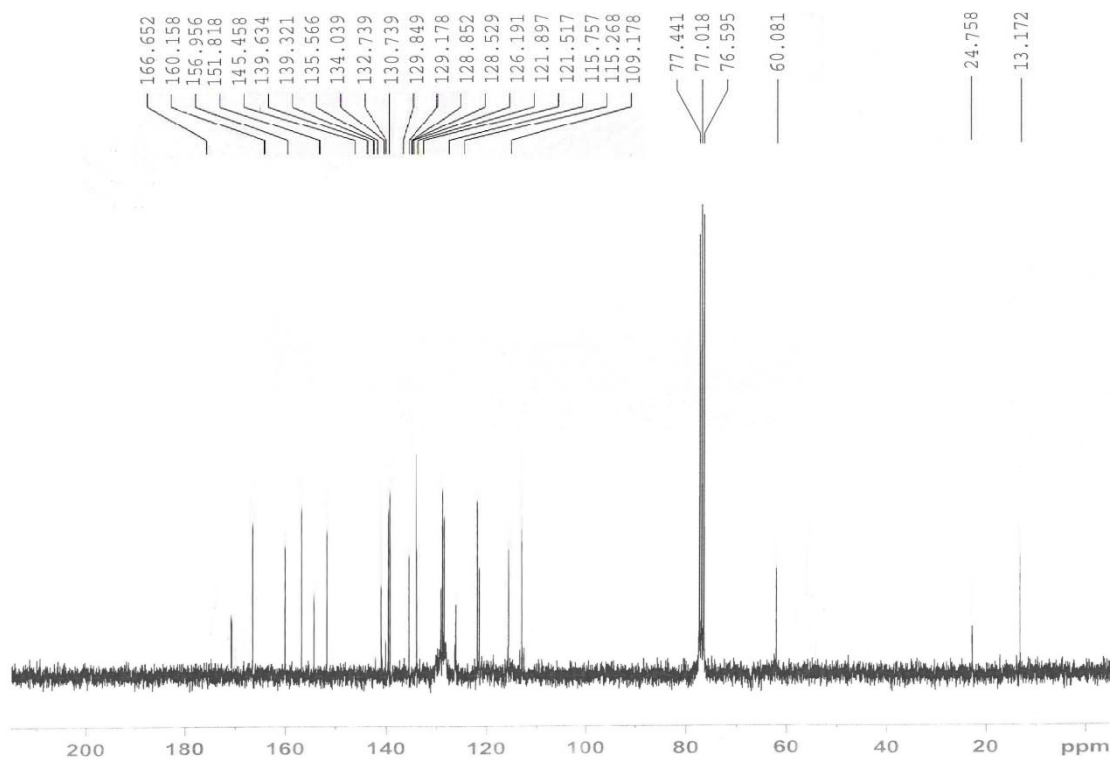
¹³CNMR (3g)



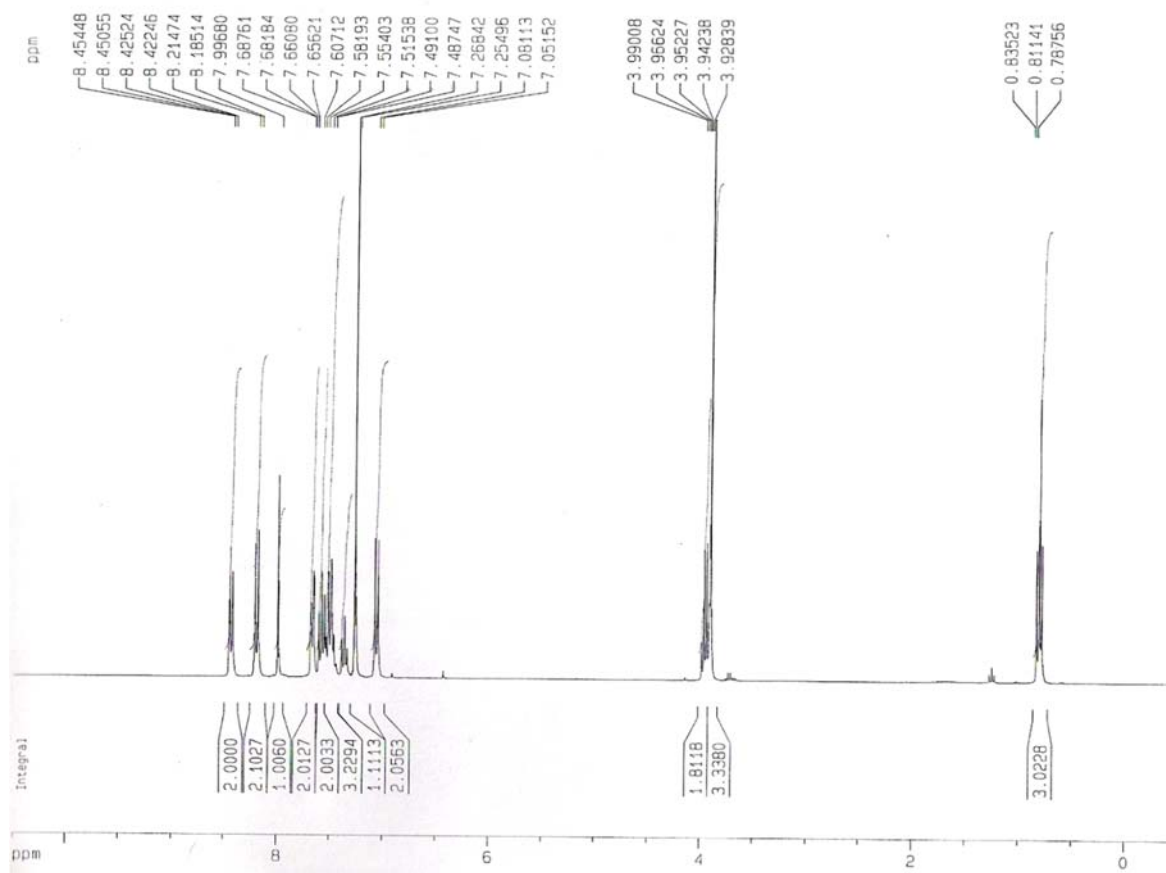
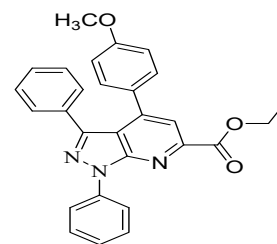
¹H NMR: Ethyl-1,3-diphenyl-4-m-tolyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3h)



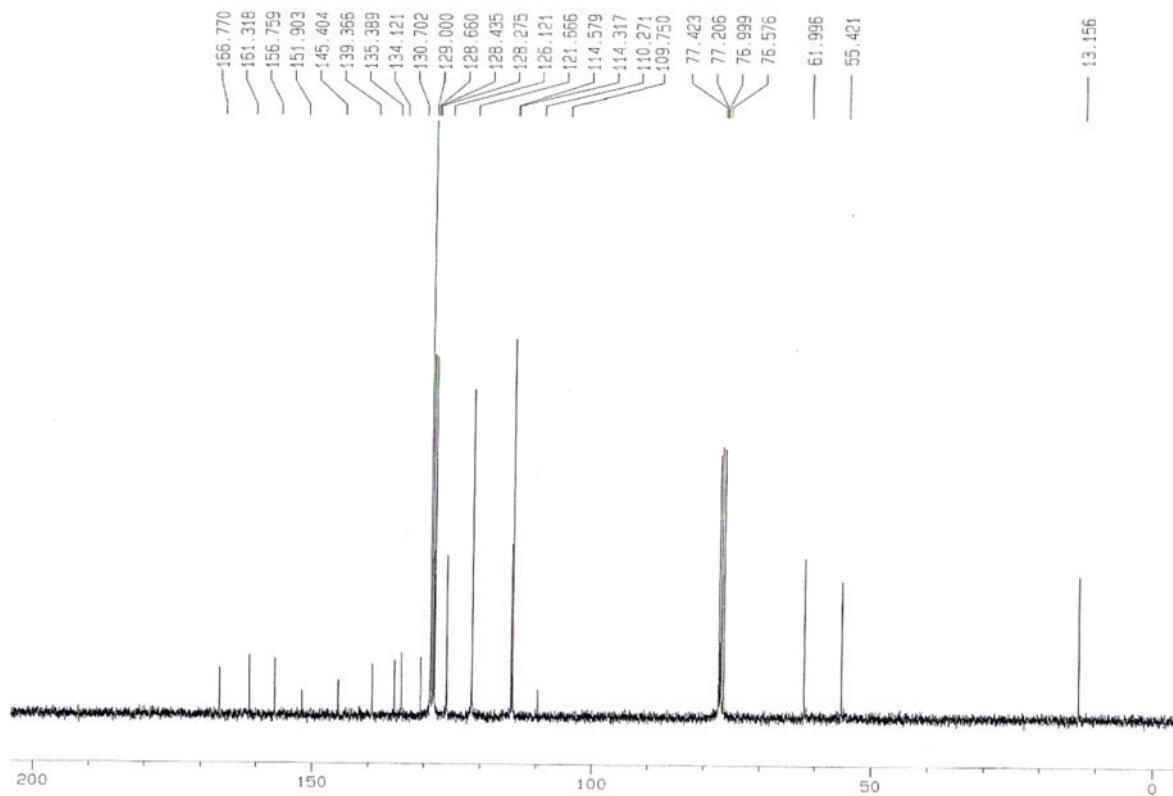
¹³C NMR (3h)



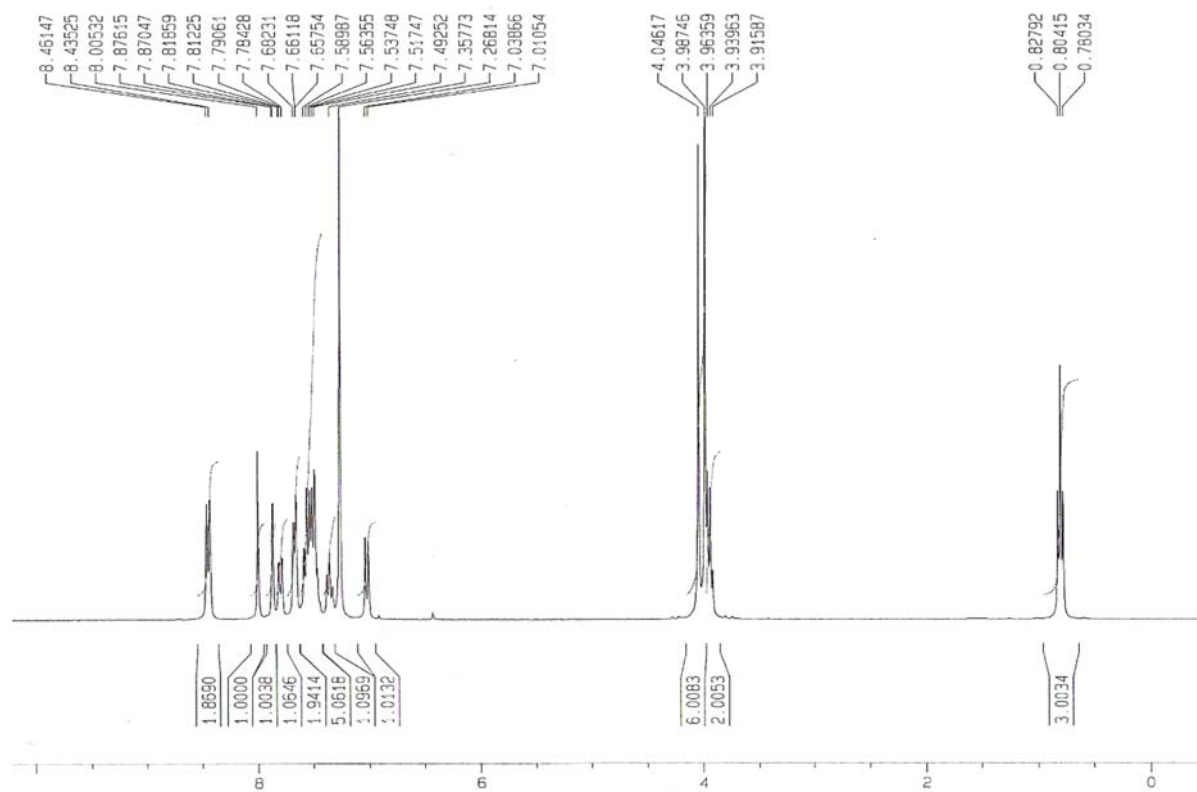
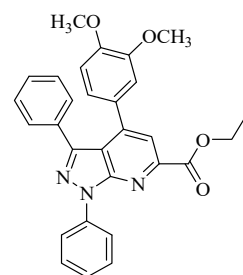
¹H NMR: Ethyl-4-(4-methoxyphenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3i)



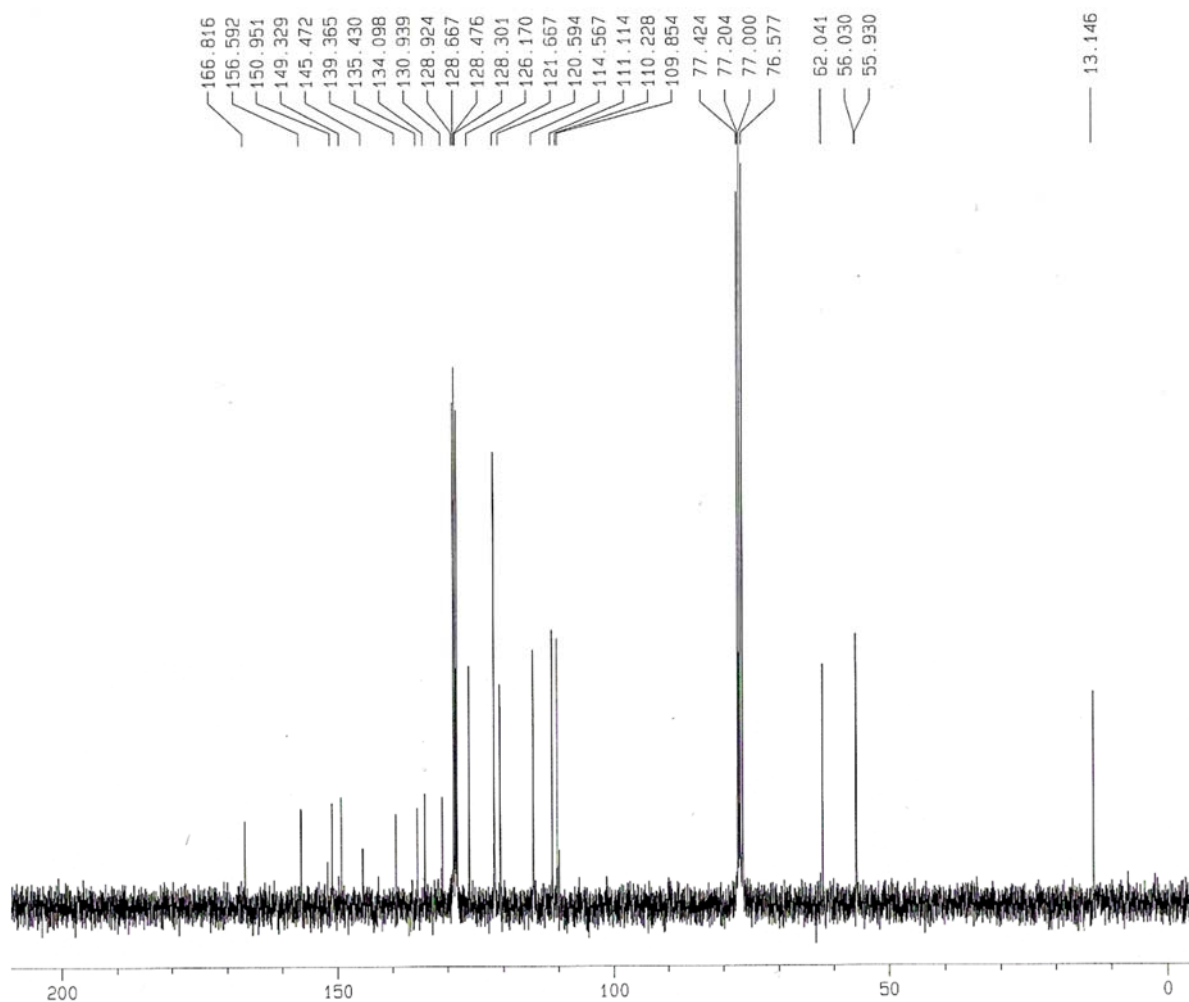
¹³C NMR (3i)



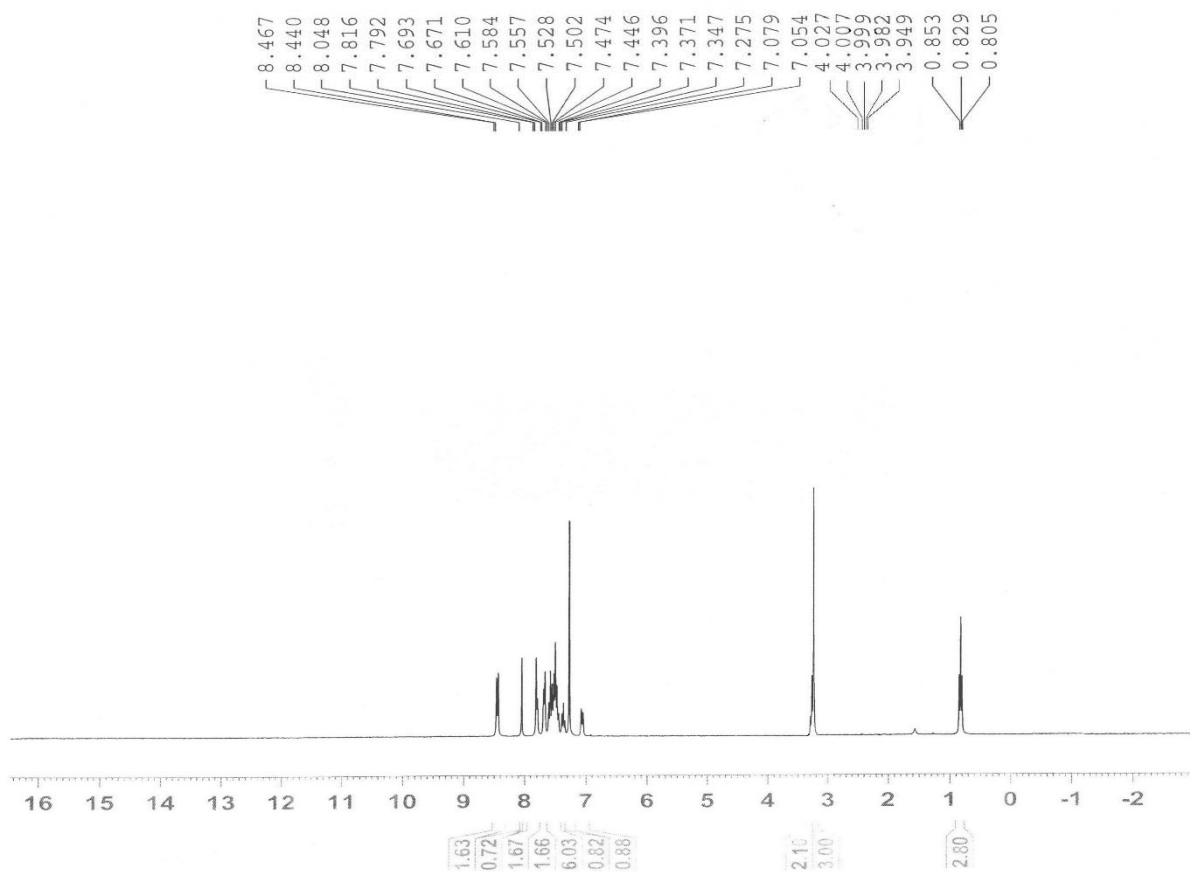
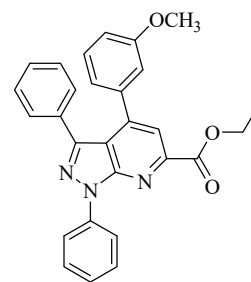
¹H NMR: Ethyl-4-(3,4-dimethoxyphenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3j)



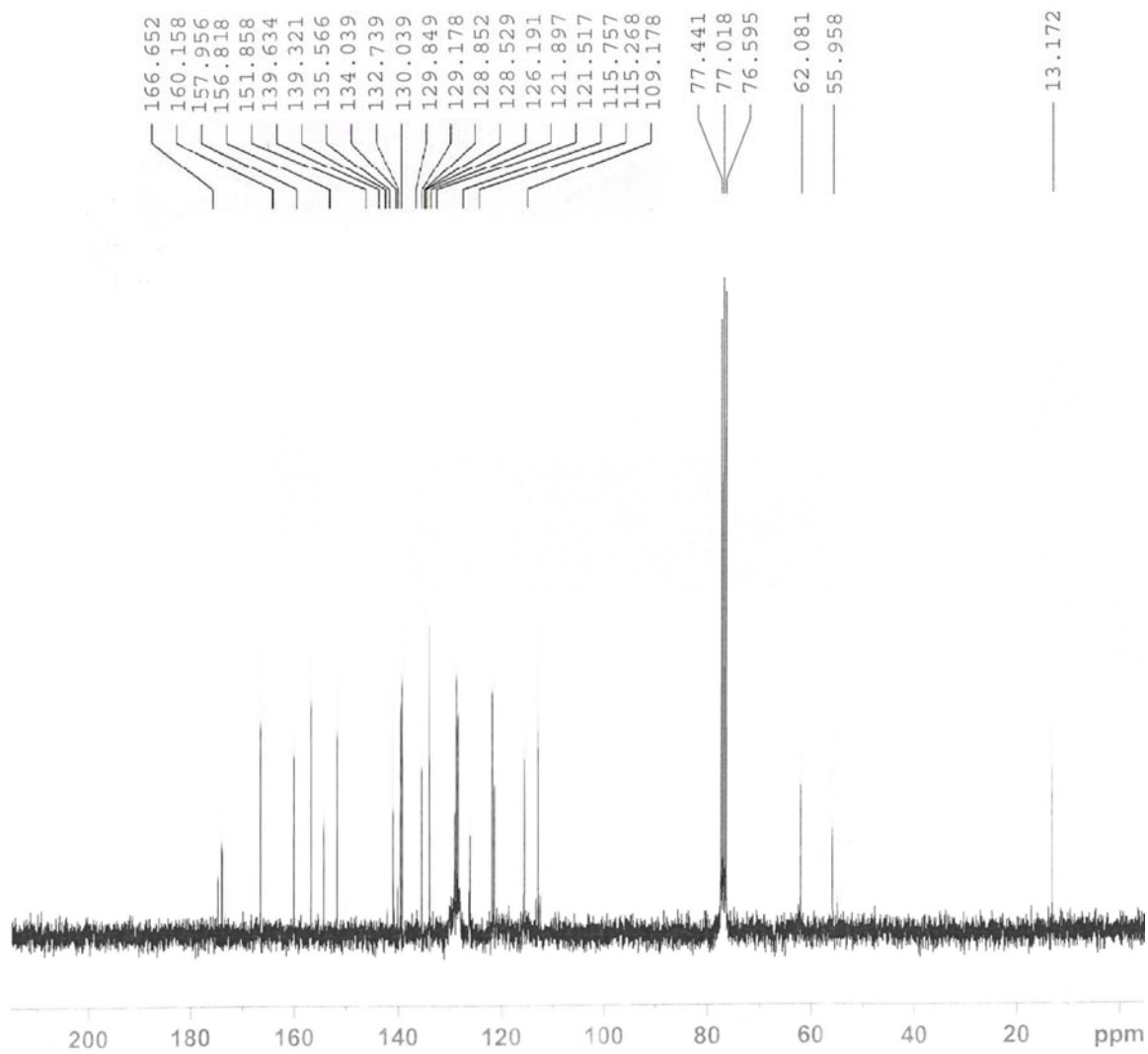
¹³C NMR: (3j)



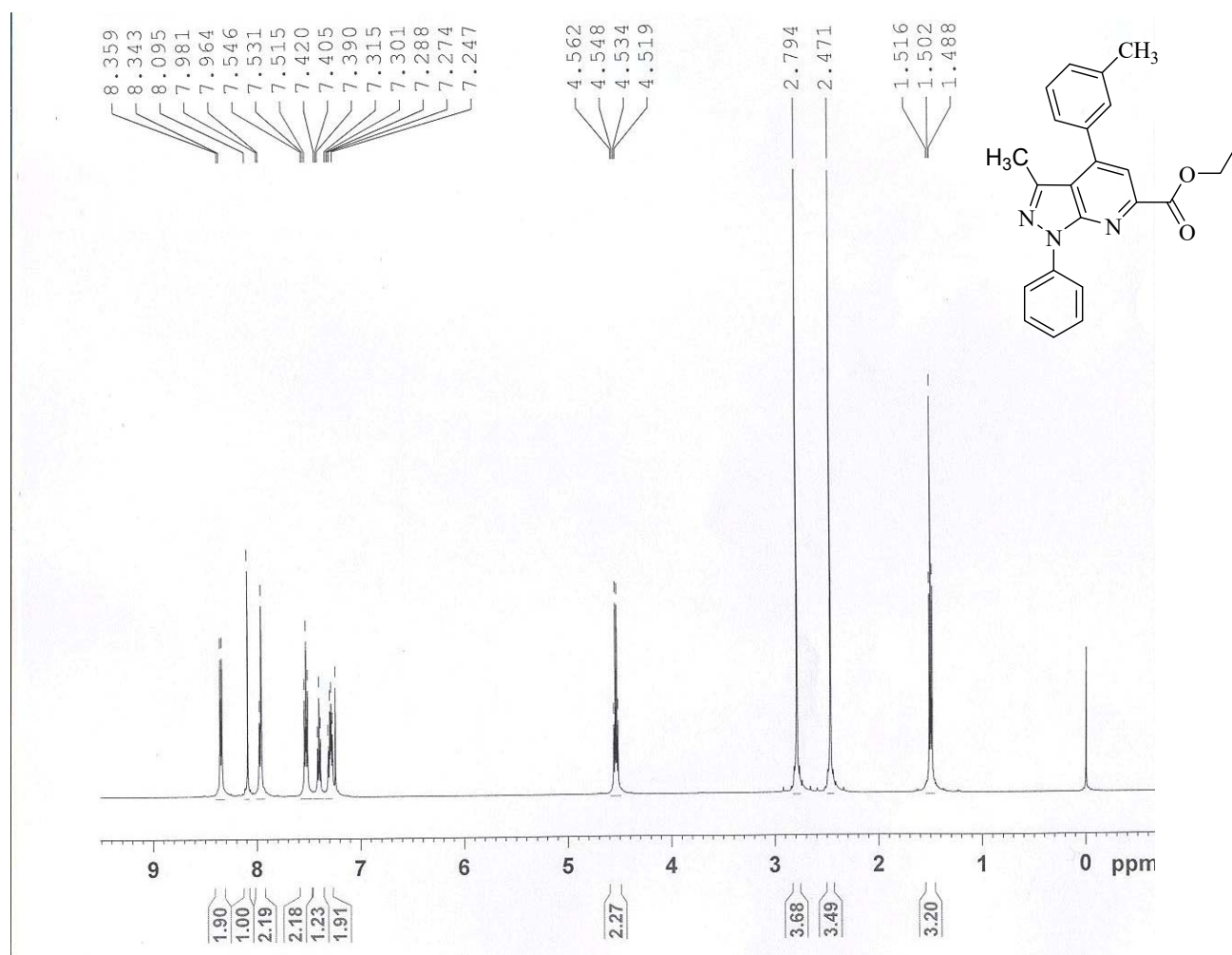
¹H NMR: Ethyl-4-(3-methoxyphenyl)-1,3-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3k)



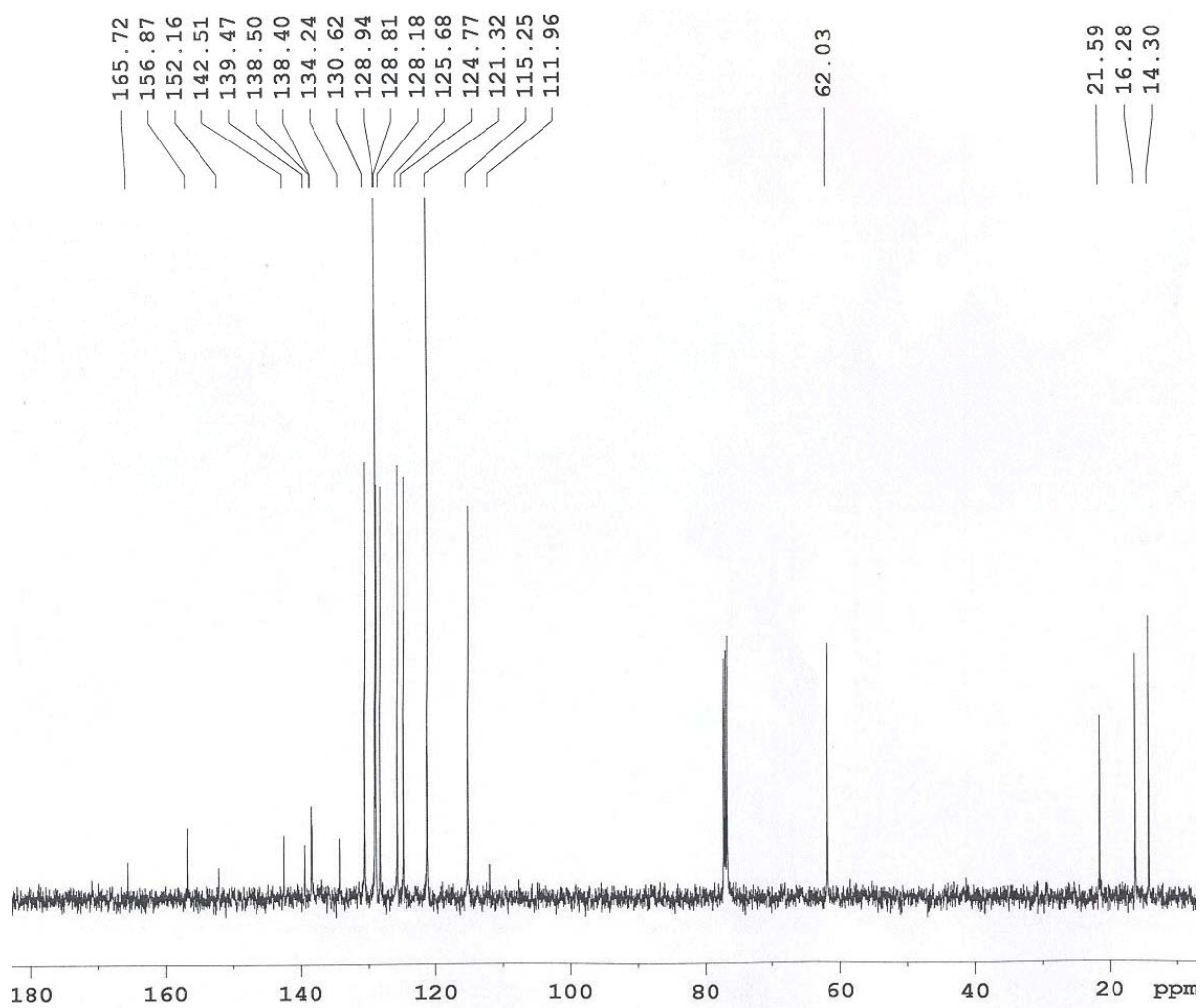
¹³C NMR: (3K)



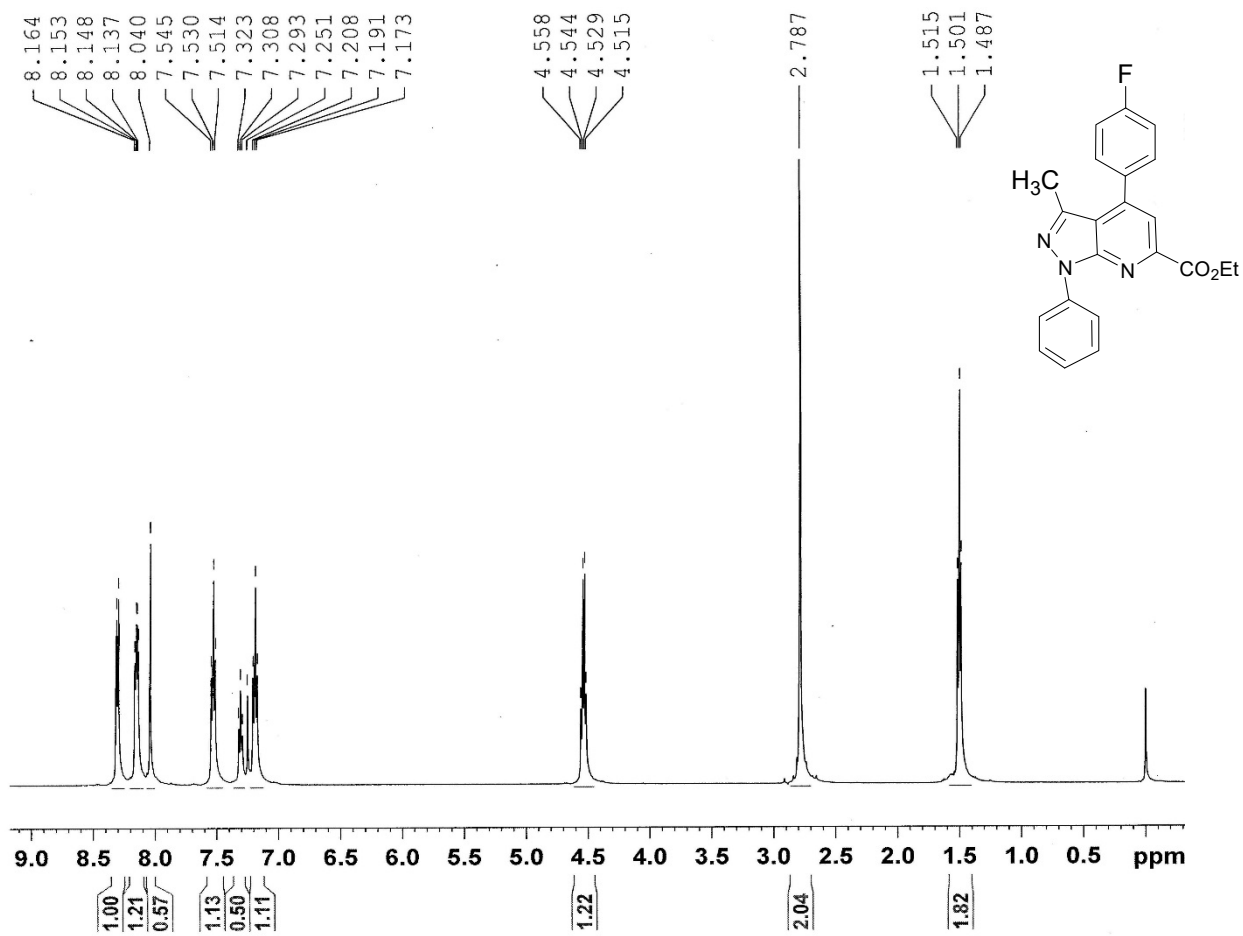
¹H NMR: Ethyl 3-methyl-1-phenyl-4-m-tolyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3m)



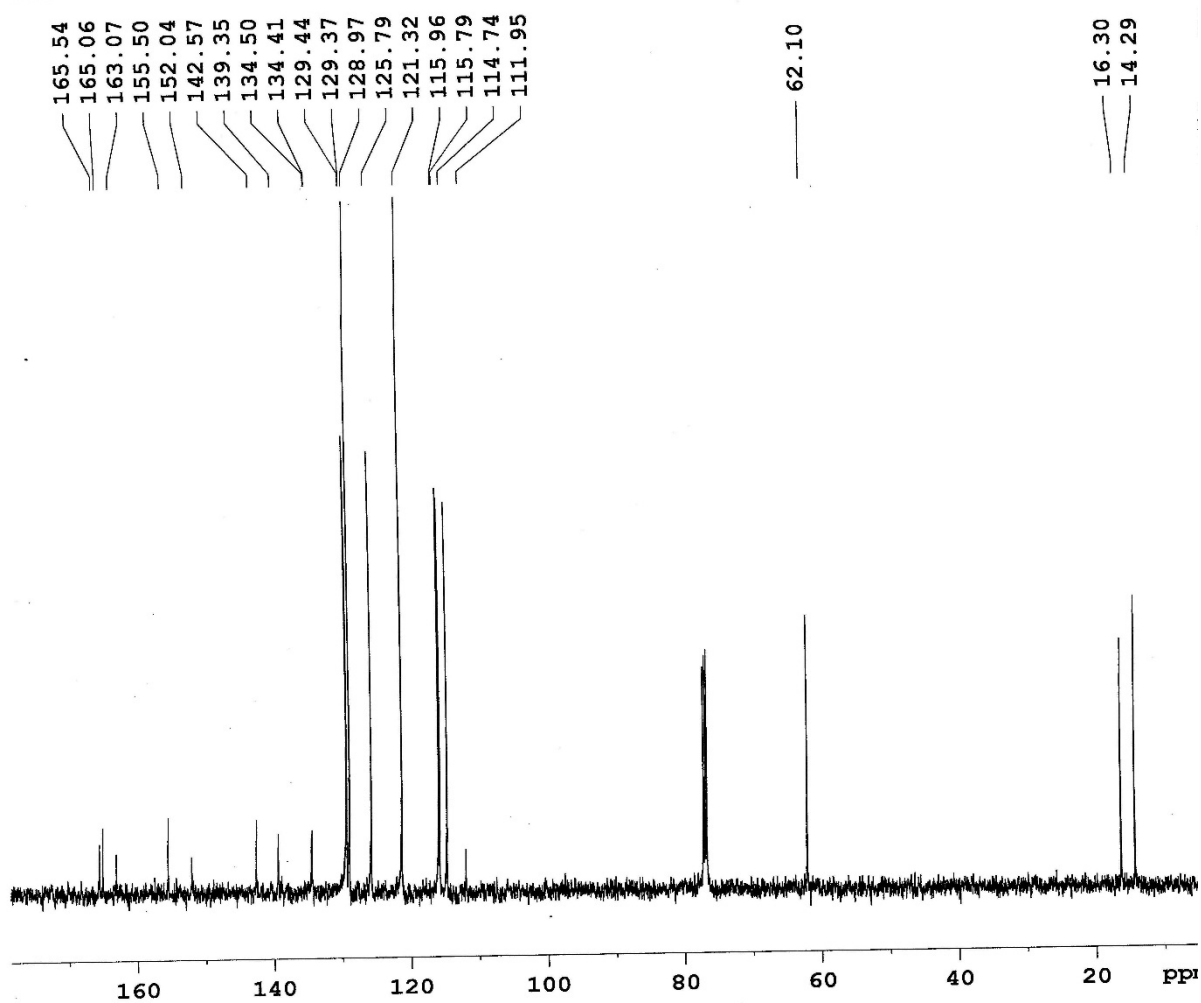
¹³C NMR (3m)



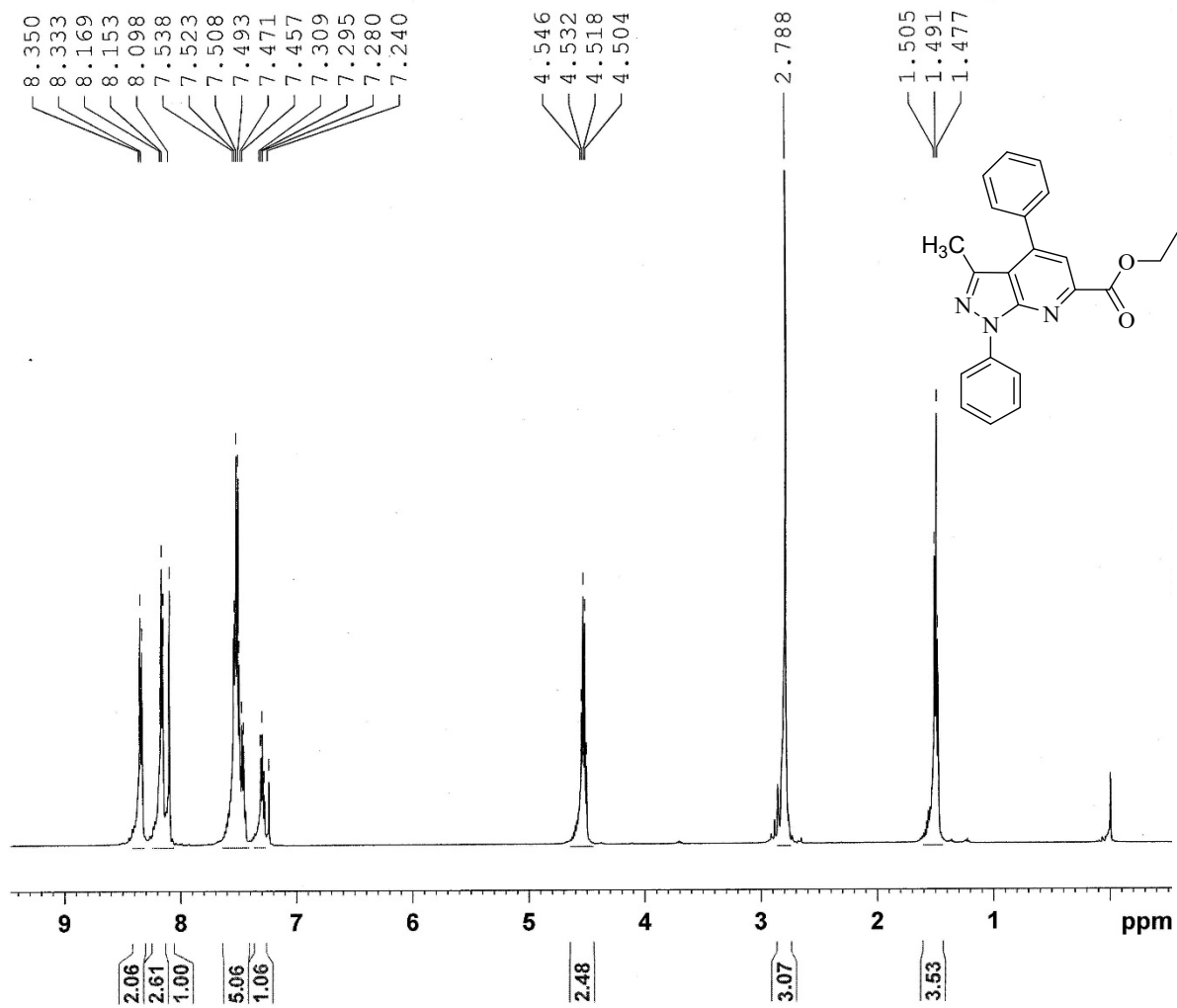
¹HNMR: Ethyl 4-(4-fluorophenyl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3n)



¹³CNMR (3n)



¹H NMR: Ethyl 3-methyl-1,4-diphenyl-1H-pyrazolo[3,4-b]pyridine-6-carboxylate (3p)



¹³CNMR (3p)

