

A practical and cost-effective approach to polysubstituted pyrimidine derivatives via DBU mediated redox isomerization of propargyl alcohol and subsequent N-C-N fragment condensation

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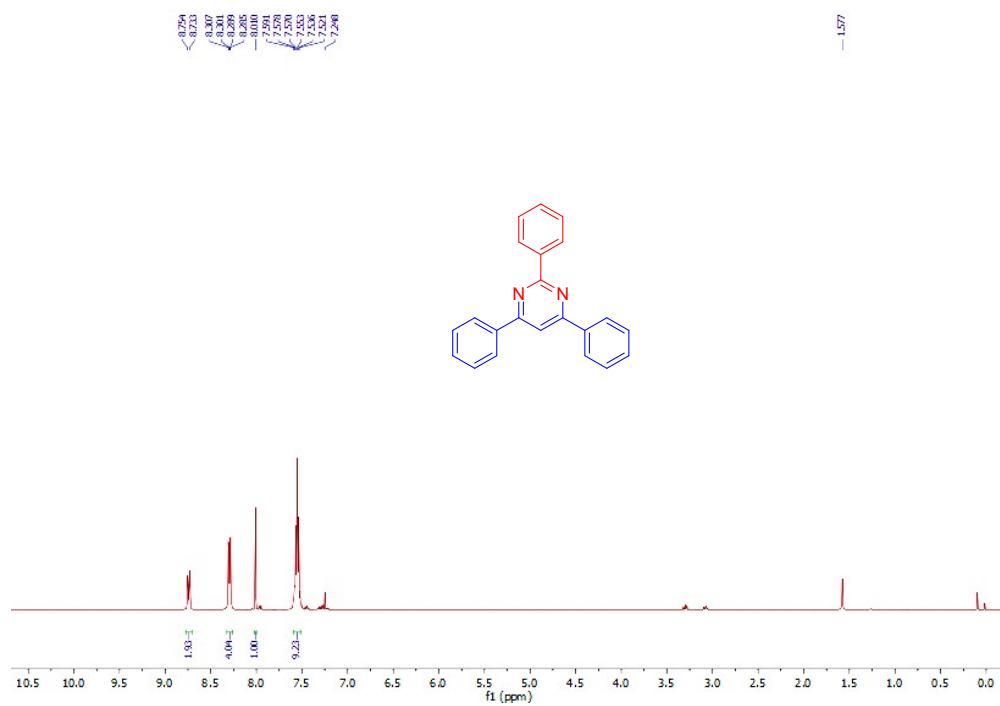
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Supporting information

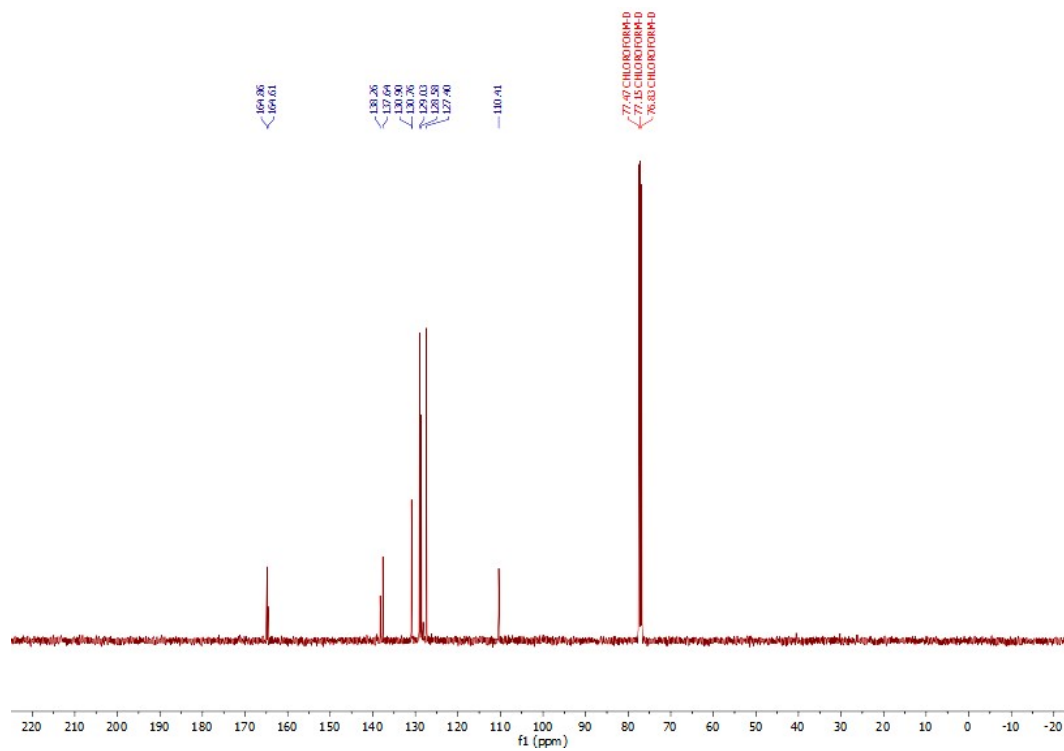
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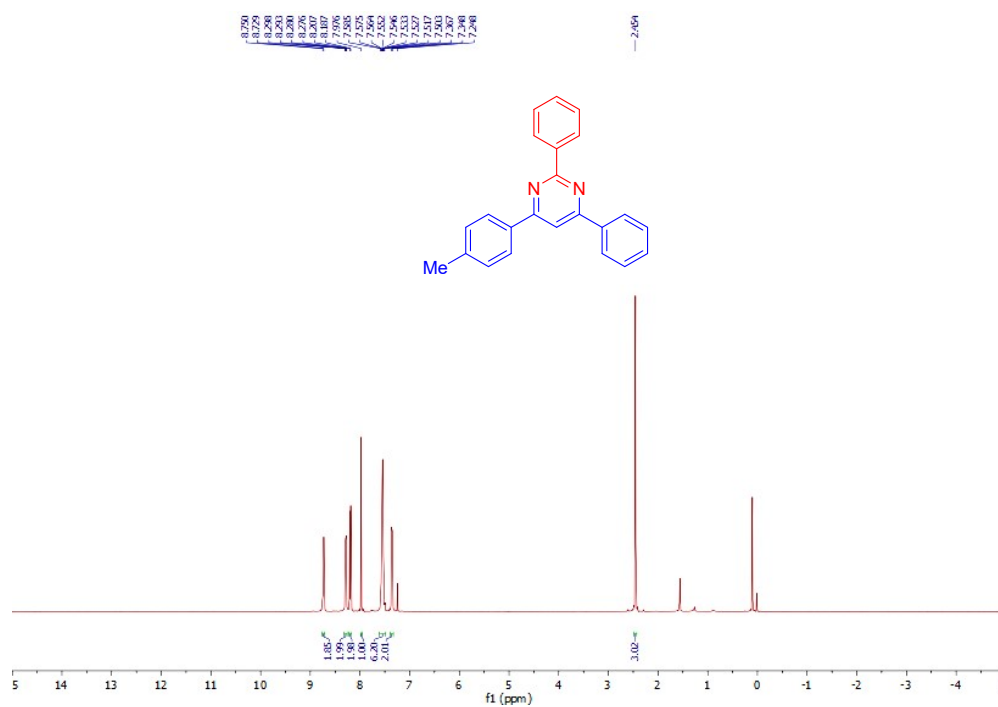
¹H NMR (400 MHz) of 2, 4, 6-triphenylpyrimidine (3a):



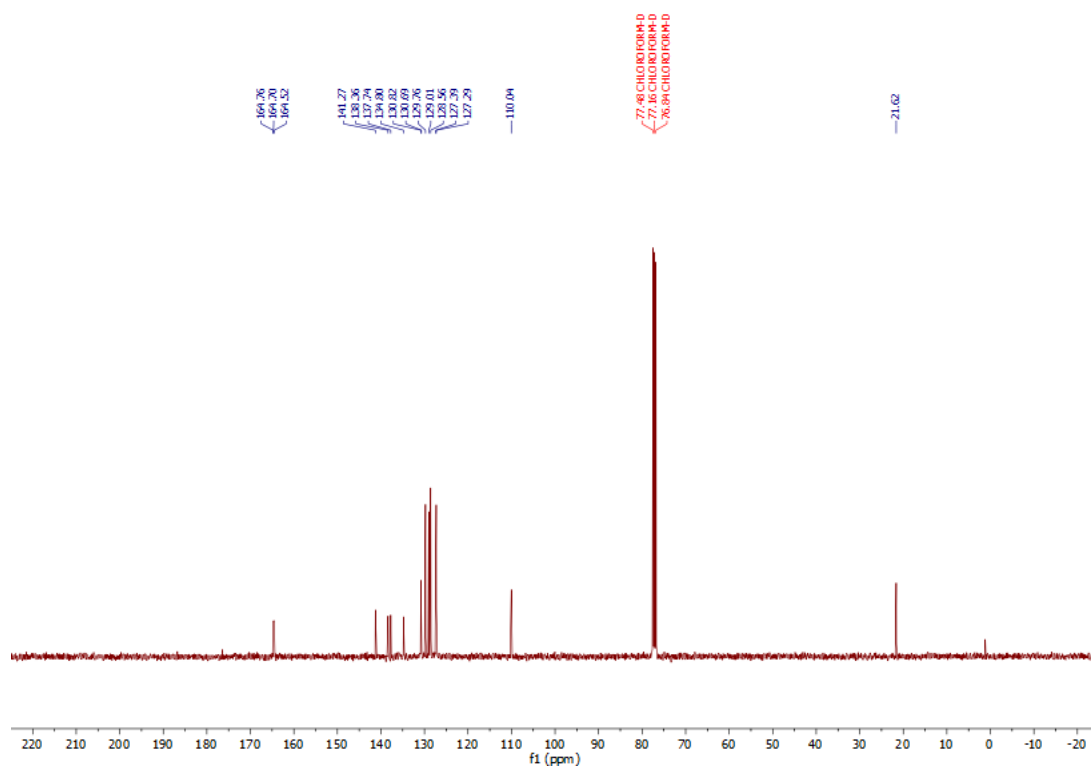
¹³C NMR (100 MHz) of 2, 4, 6-triphenylpyrimidine (3a):



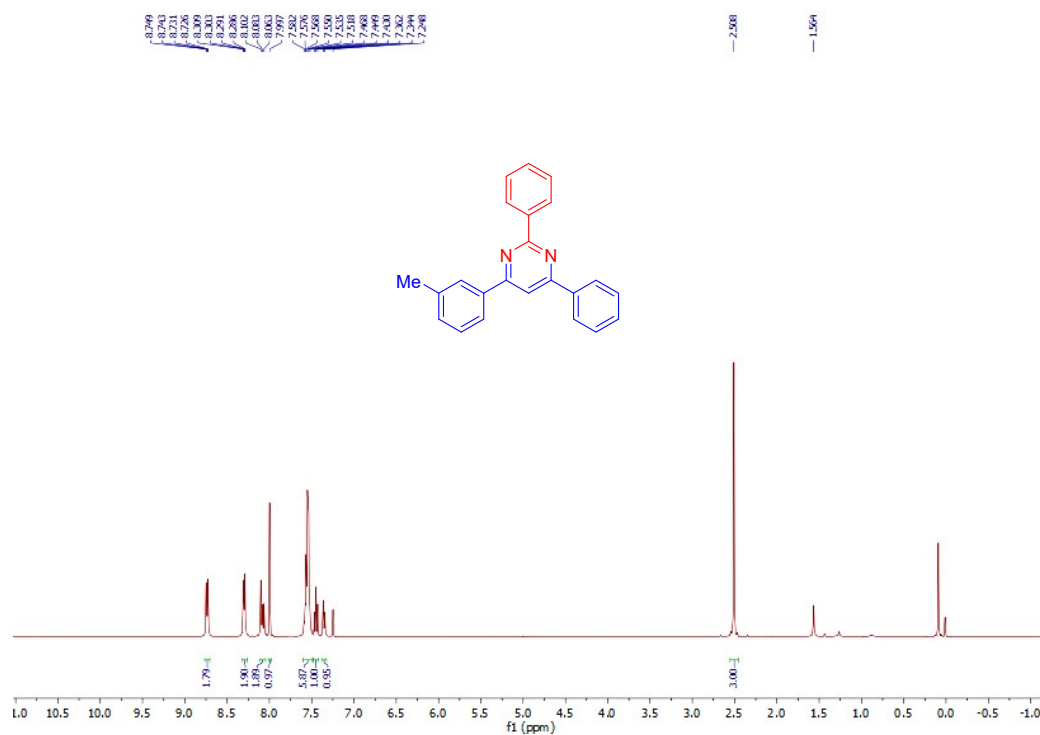
¹H NMR (400 MHz) of 2, 4-diphenyl-6-(p-tolyl)pyrimidine (3b):



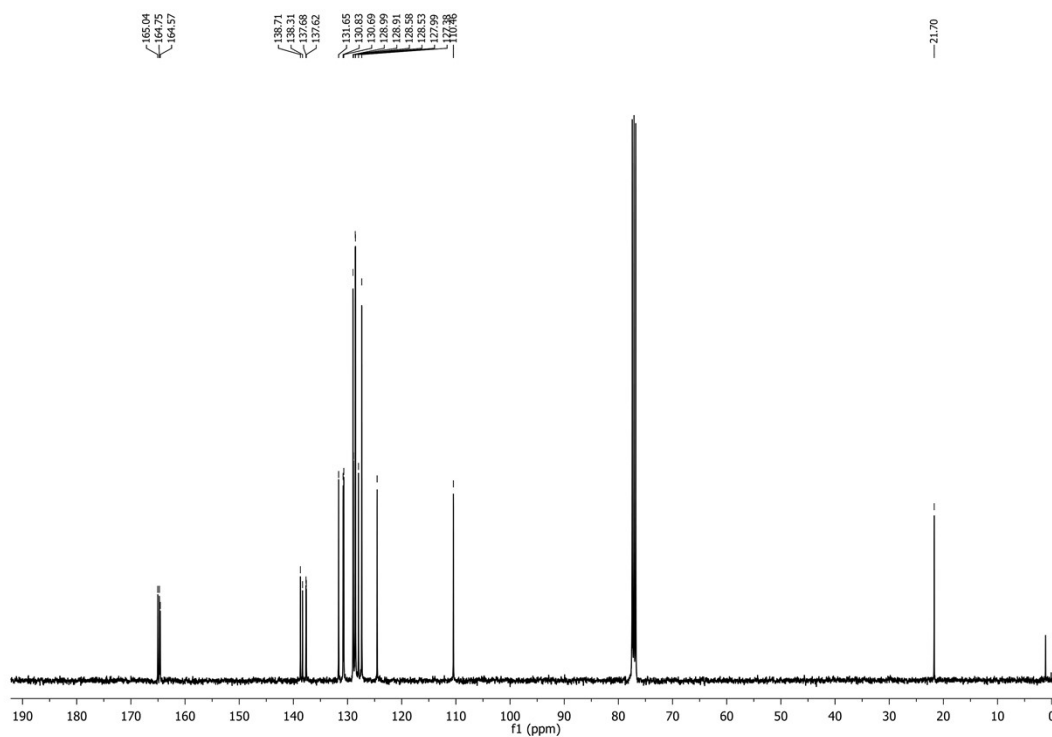
¹³C NMR (100 MHz) of 2, 4-diphenyl-6-(p-tolyl) pyrimidine (3b):



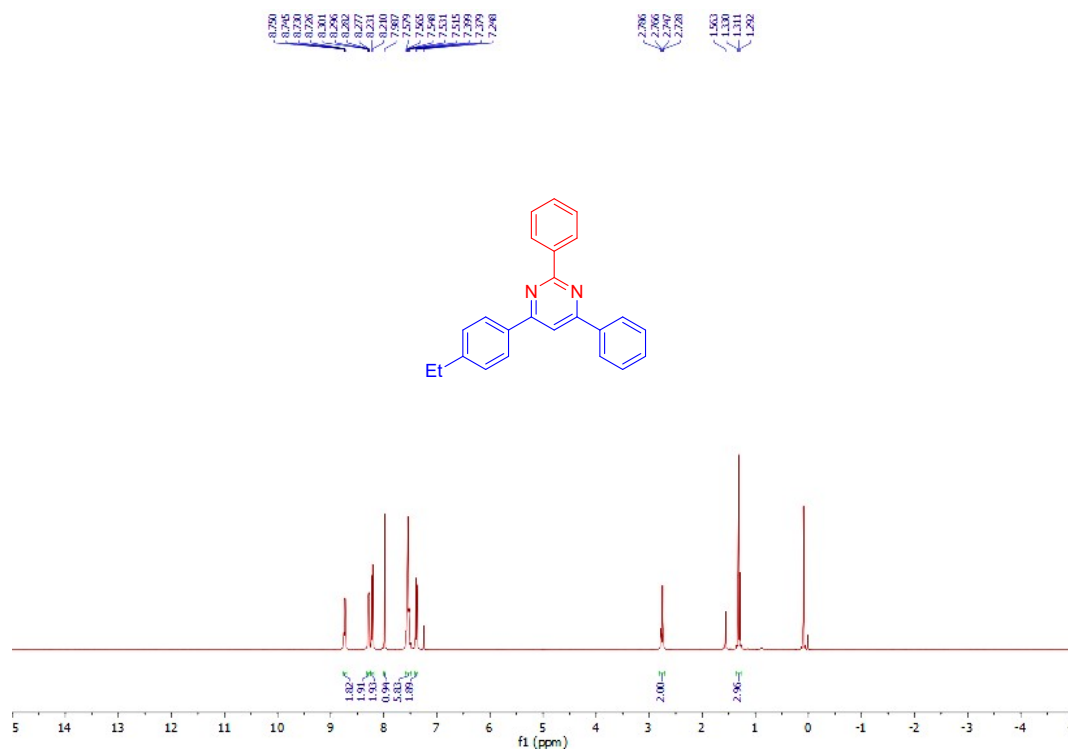
¹H NMR (400 MHz) of 2, 4-diphenyl-6-(m-tolyl) pyrimidine (3c):



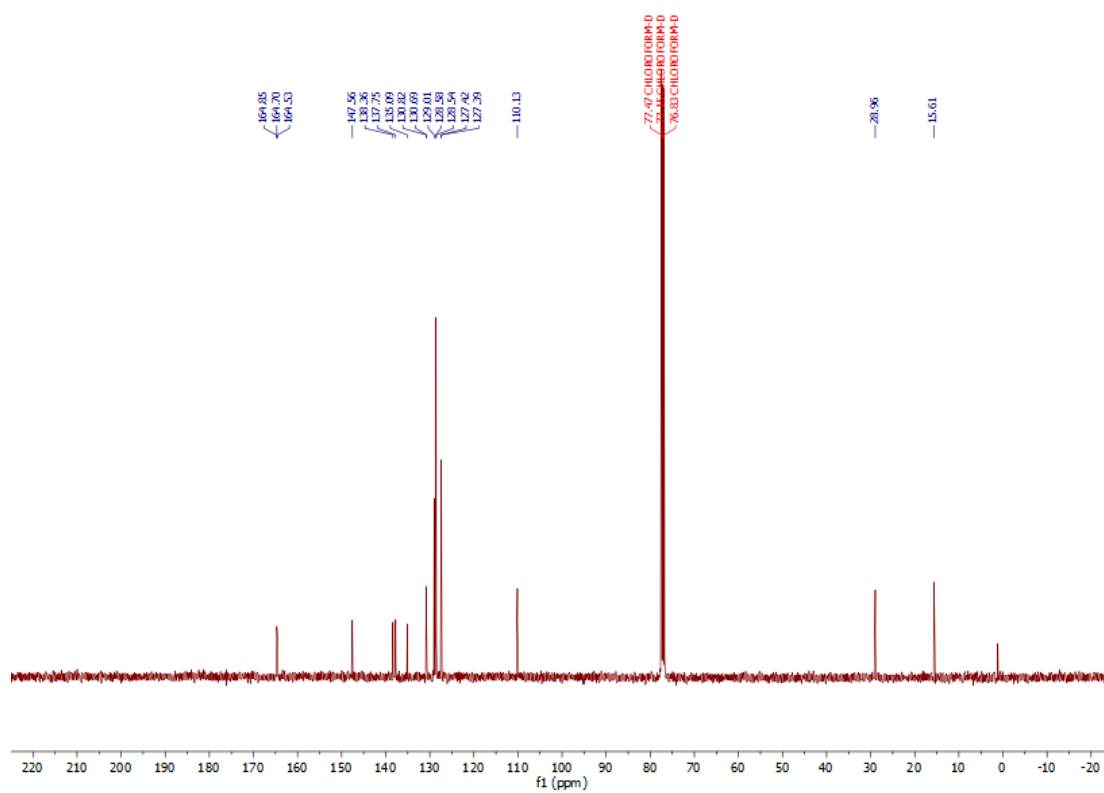
¹³C NMR (100 MHz) of 2, 4-diphenyl-6-(m-tolyl) pyrimidine (3c):



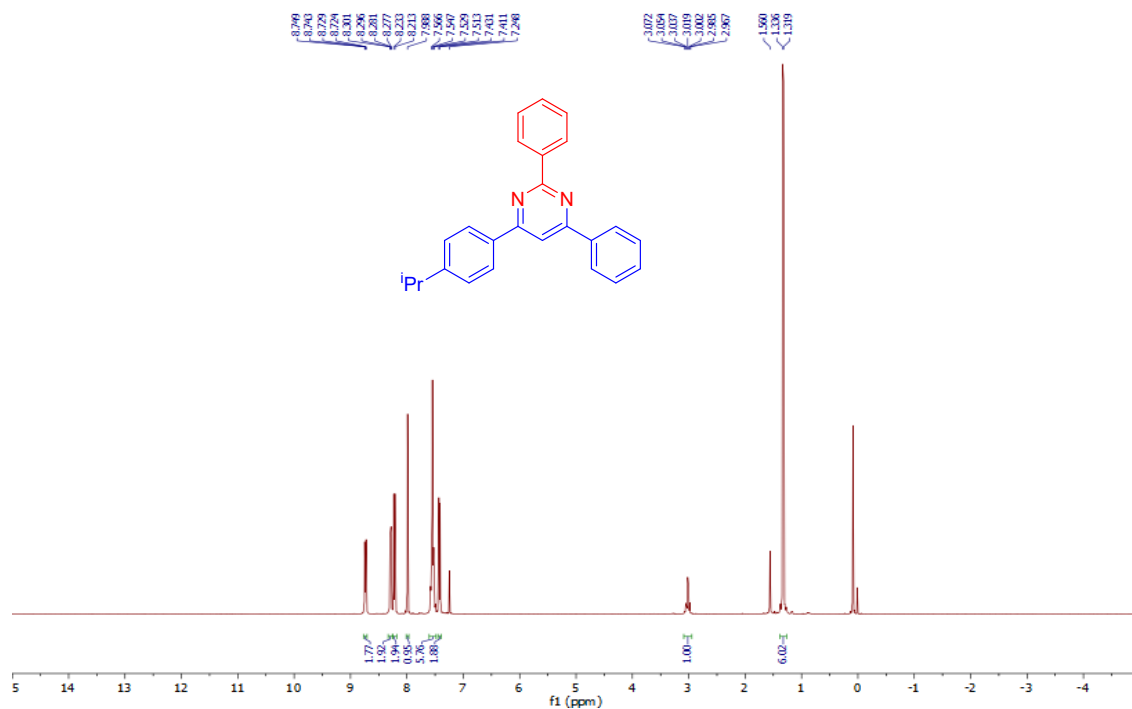
¹H NMR (400 MHz) of 4-(4-ethylphenyl)-2,6-diphenylpyrimidine (3d):



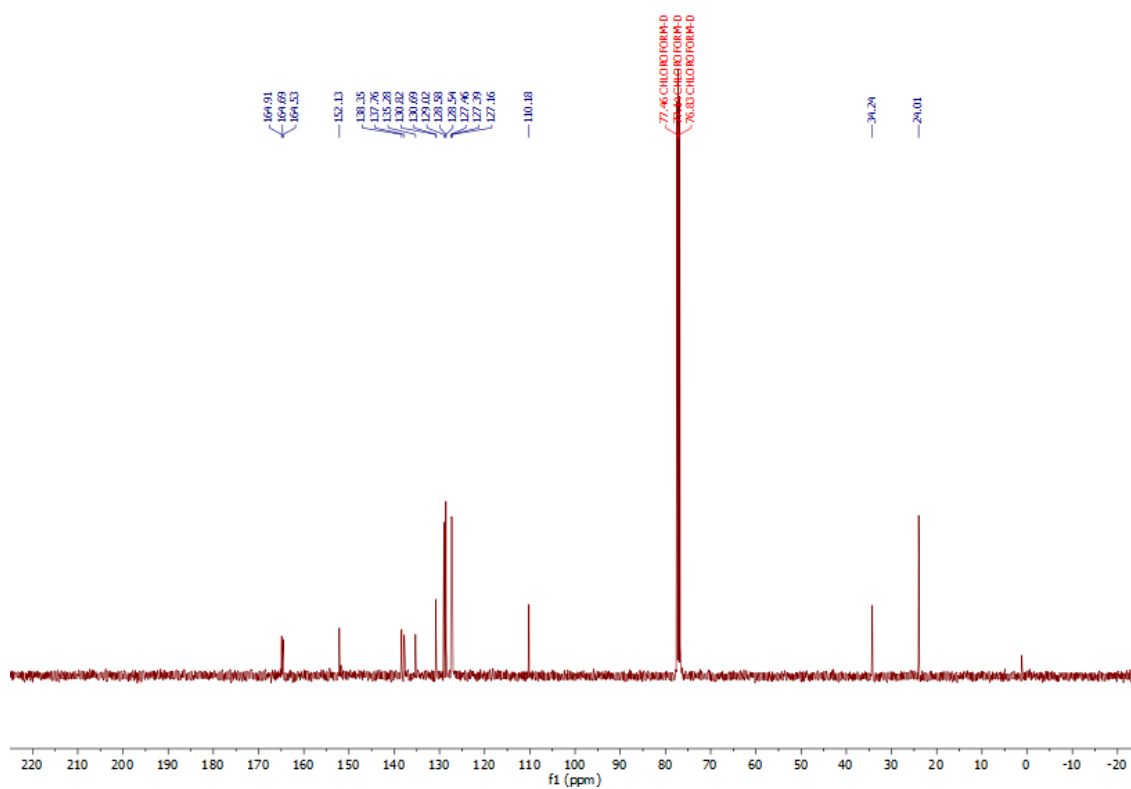
¹³C NMR (100 MHz) of 4-(4-ethylphenyl)-2,6-diphenylpyrimidine (3d):



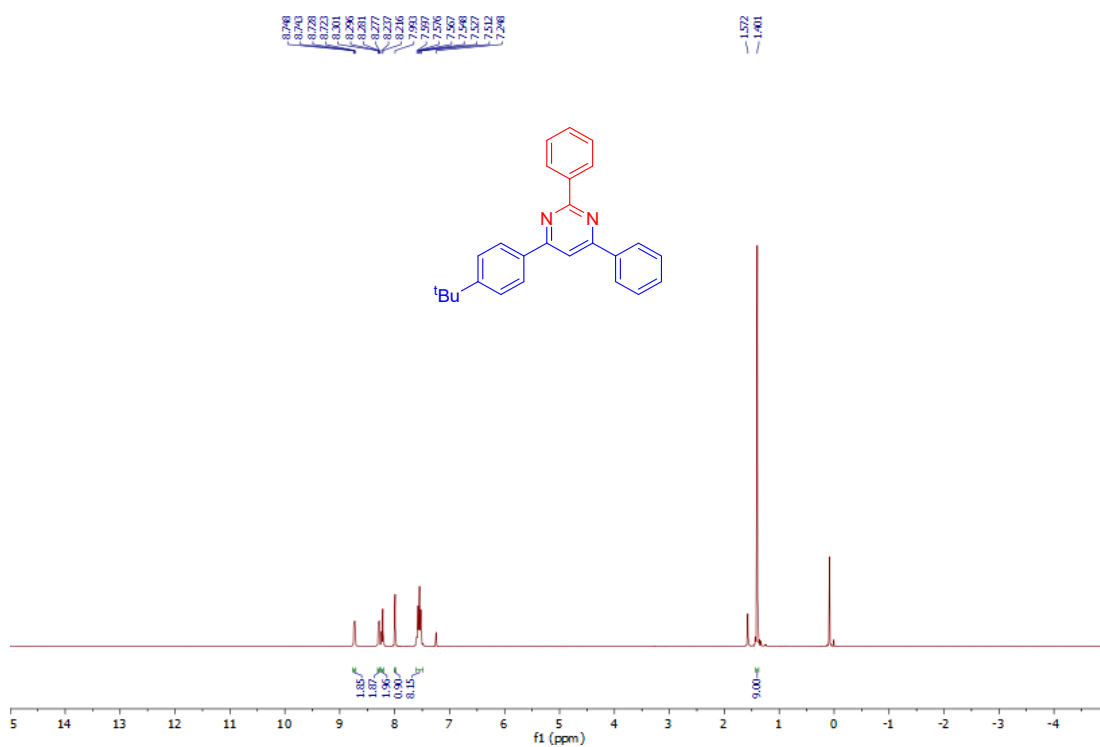
¹H NMR (400 MHz) of 4-(4-isopropylphenyl)-2,6-diphenylpyrimidine (3e):



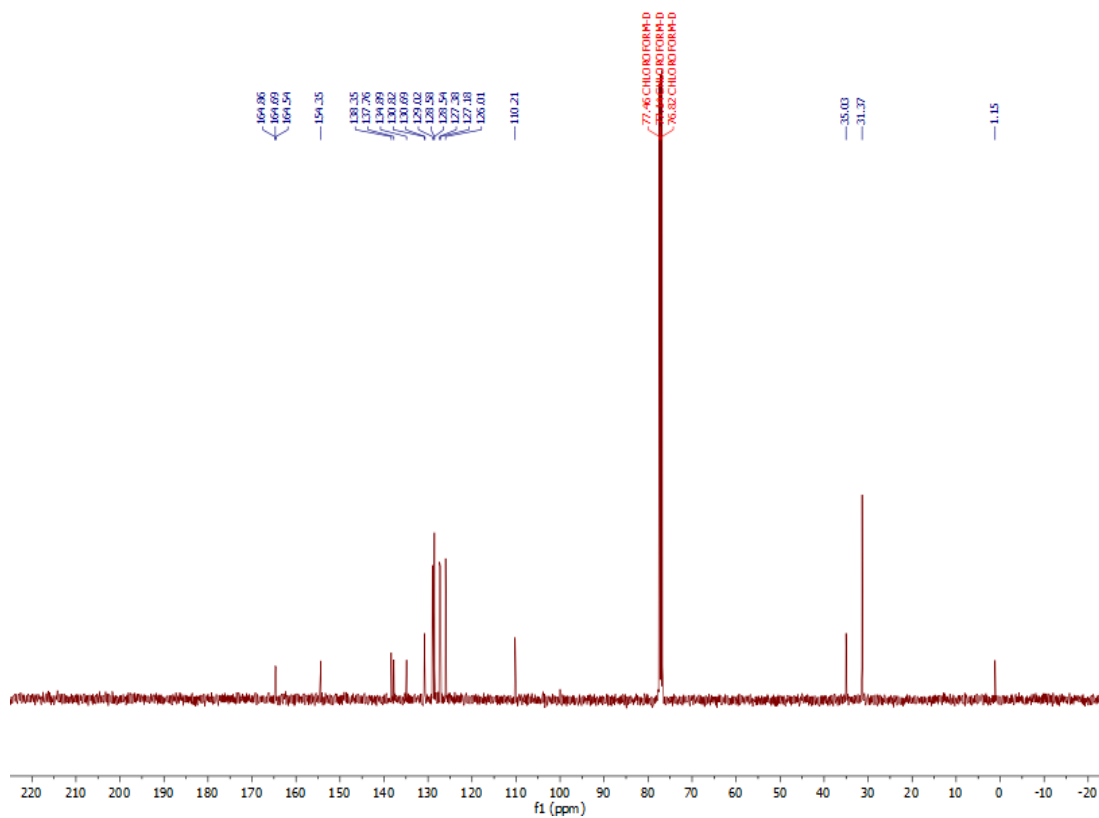
¹³C NMR (100 MHz) of 4-(4-isopropylphenyl)-2,6-diphenylpyrimidine (3e):



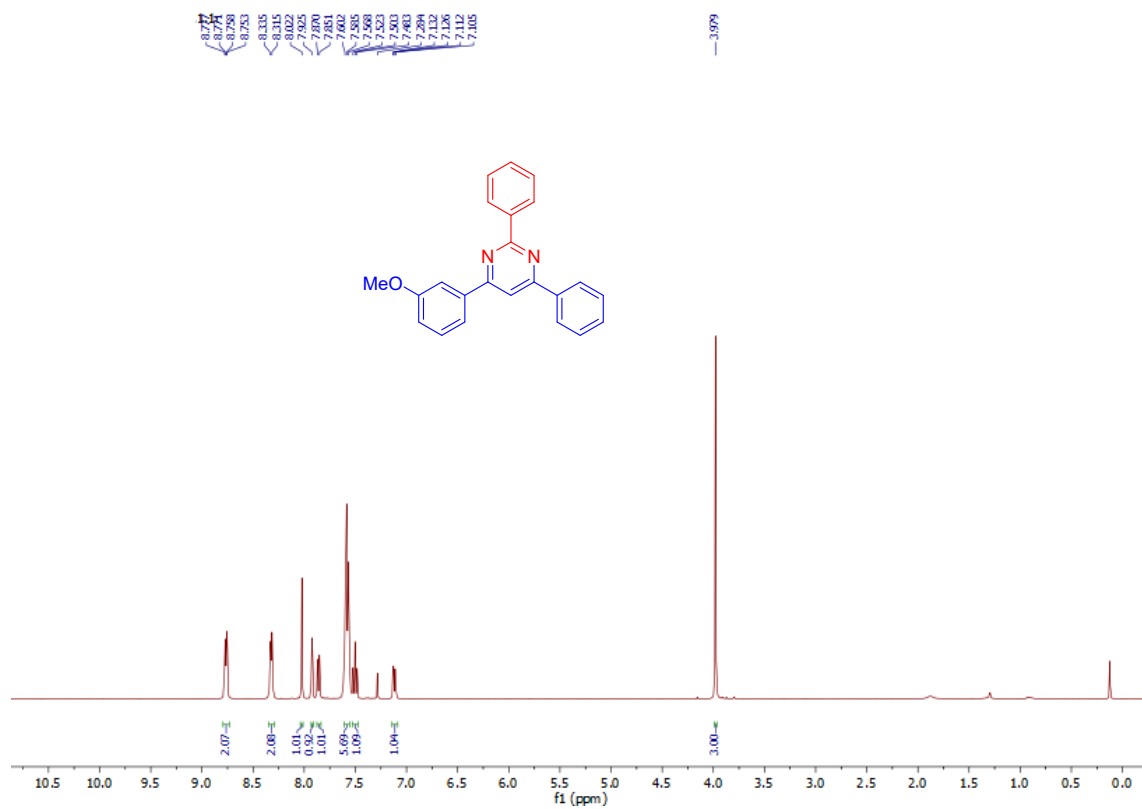
¹H NMR (400 MHz) of 4-(4-(tert-butyl)phenyl)-2,6-diphenylpyrimidine (3f):



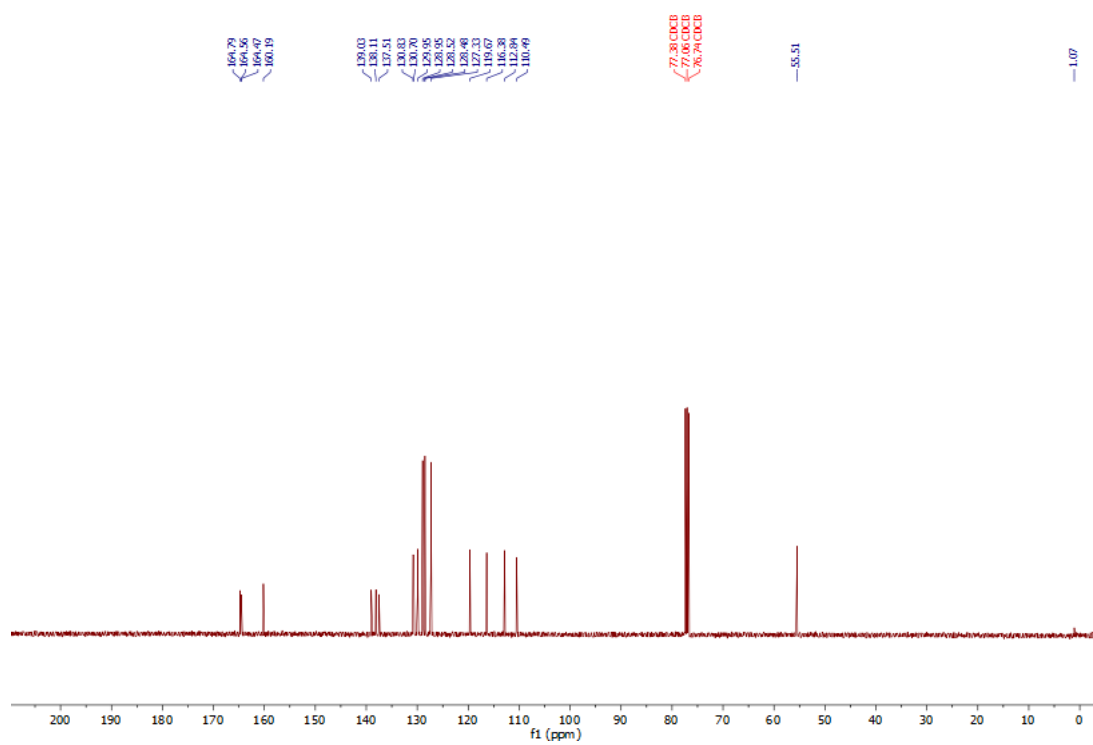
¹³C NMR (100 MHz) of 4-(4-(tert-butyl) phenyl)-2,6-diphenylpyrimidine (3f):



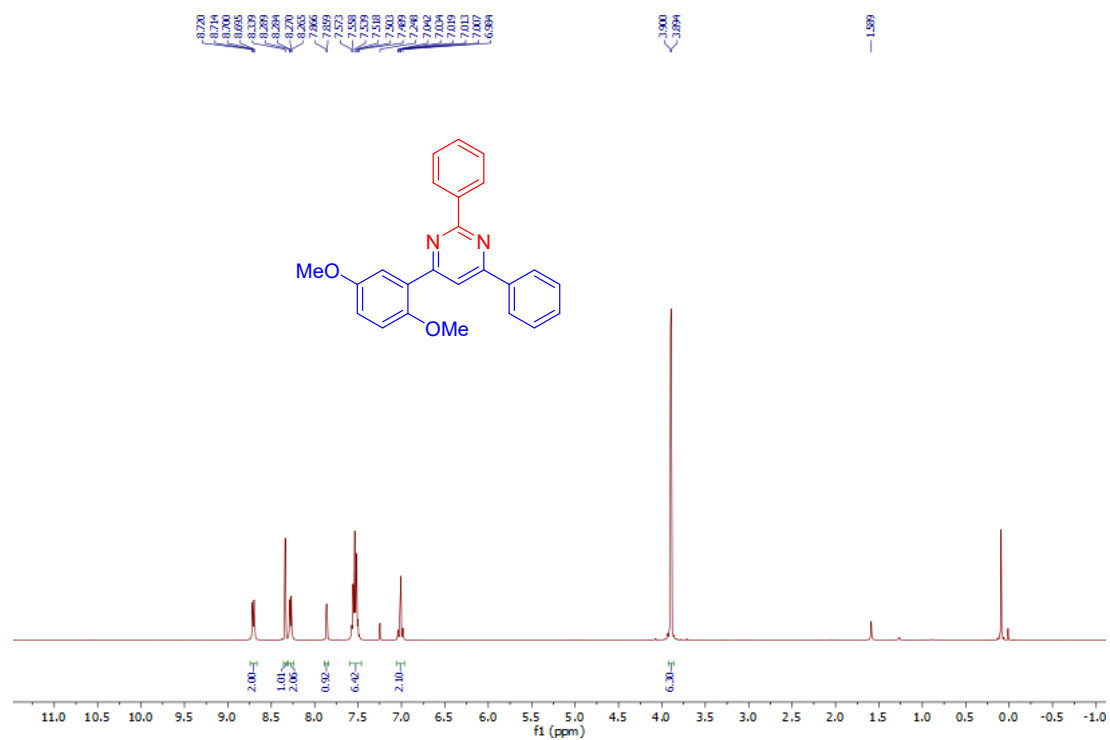
¹H NMR (400 MHz) of 4-(3-methoxyphenyl)-2,6-diphenylpyrimidine (3h):



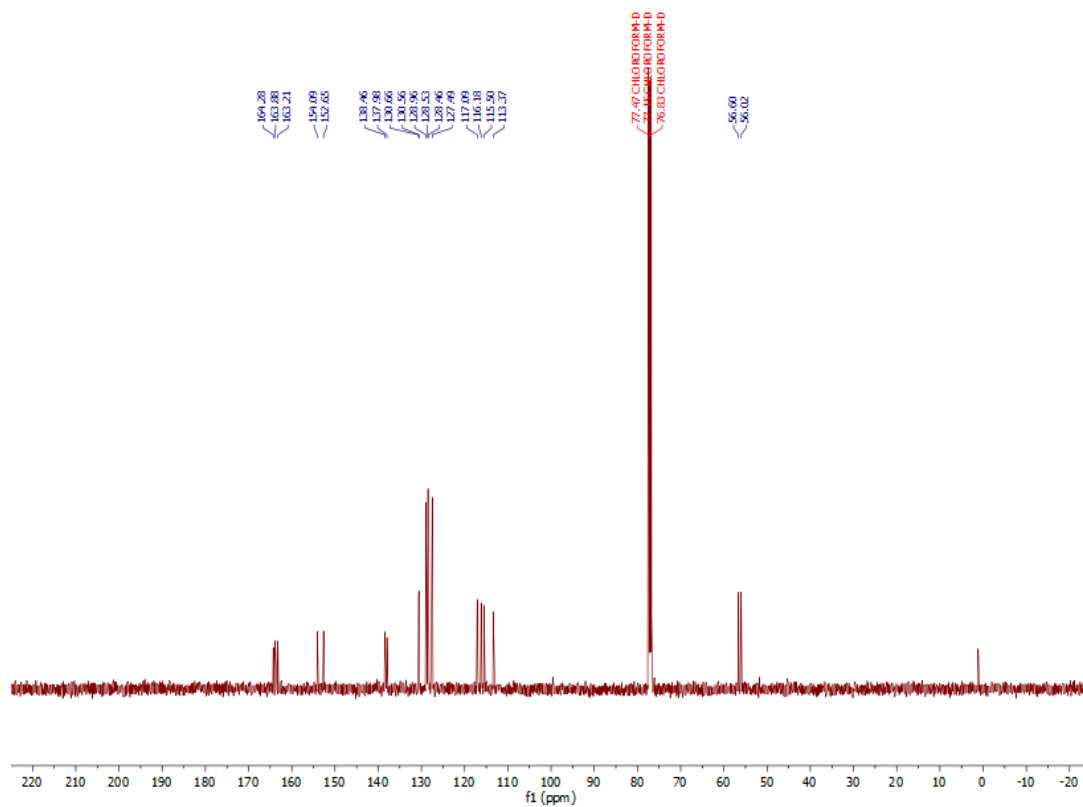
¹³C NMR (100 MHz) of 4-(3-methoxyphenyl)-2,6-diphenylpyrimidine (3h):



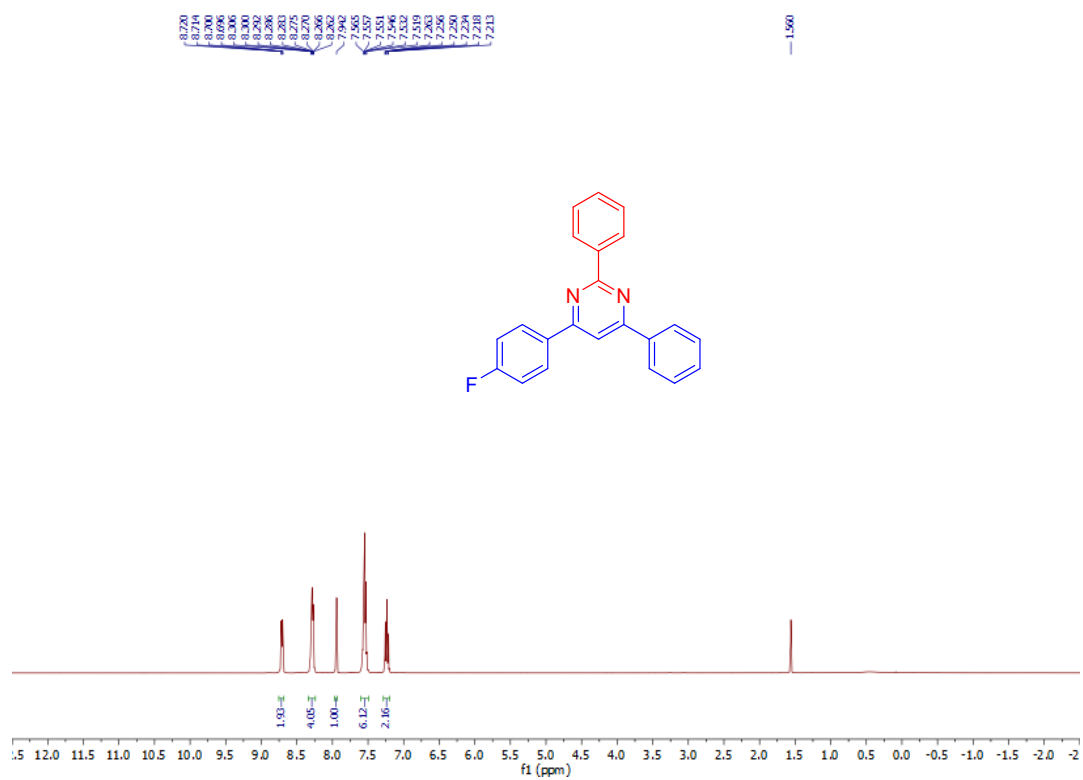
¹H NMR (400 MHz) of 4-(2,5-dimethoxyphenyl)-2,6-diphenylpyrimidine (3i):



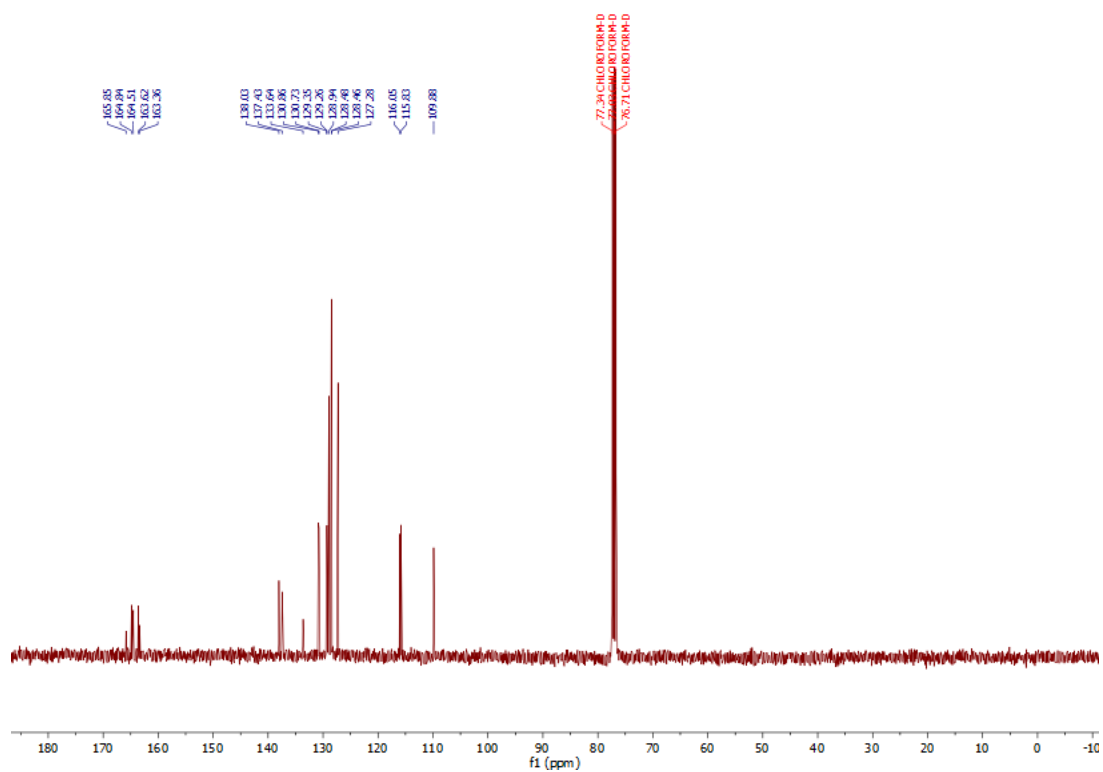
¹³C NMR (100 MHz) of 4-(2,5-dimethoxyphenyl)-2,6-diphenylpyrimidine (3i):



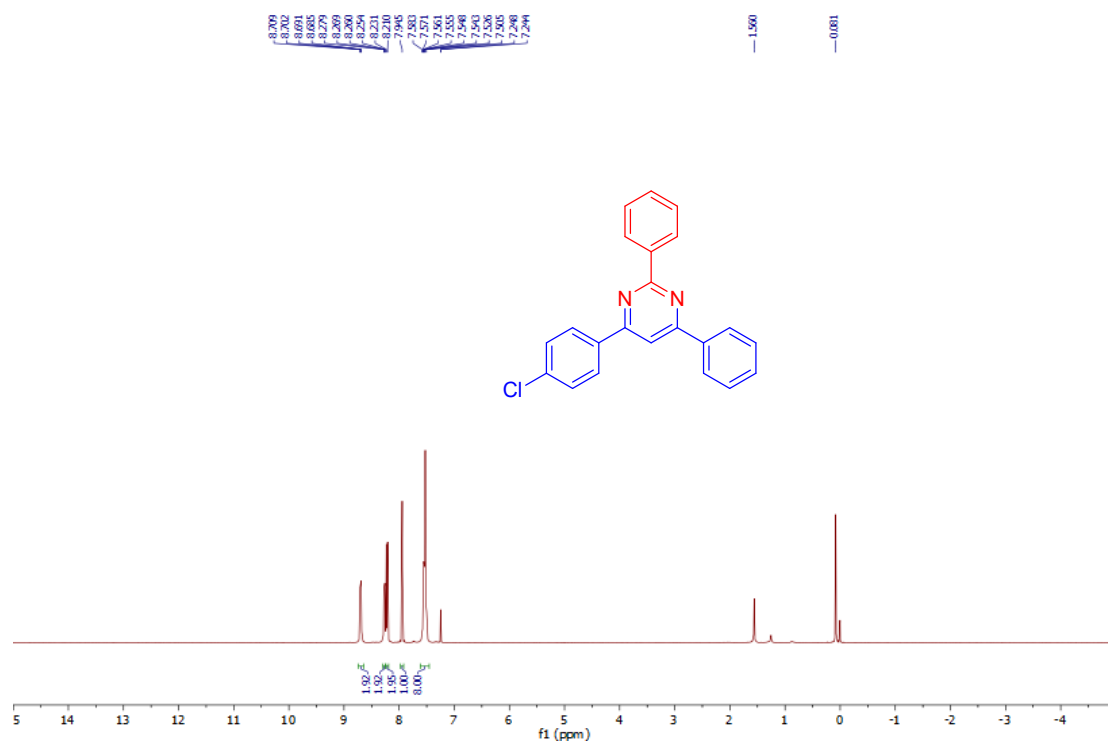
¹H NMR (400 MHz) of 4-(4-fluorophenyl)-2,6-diphenylpyrimidine (3j):



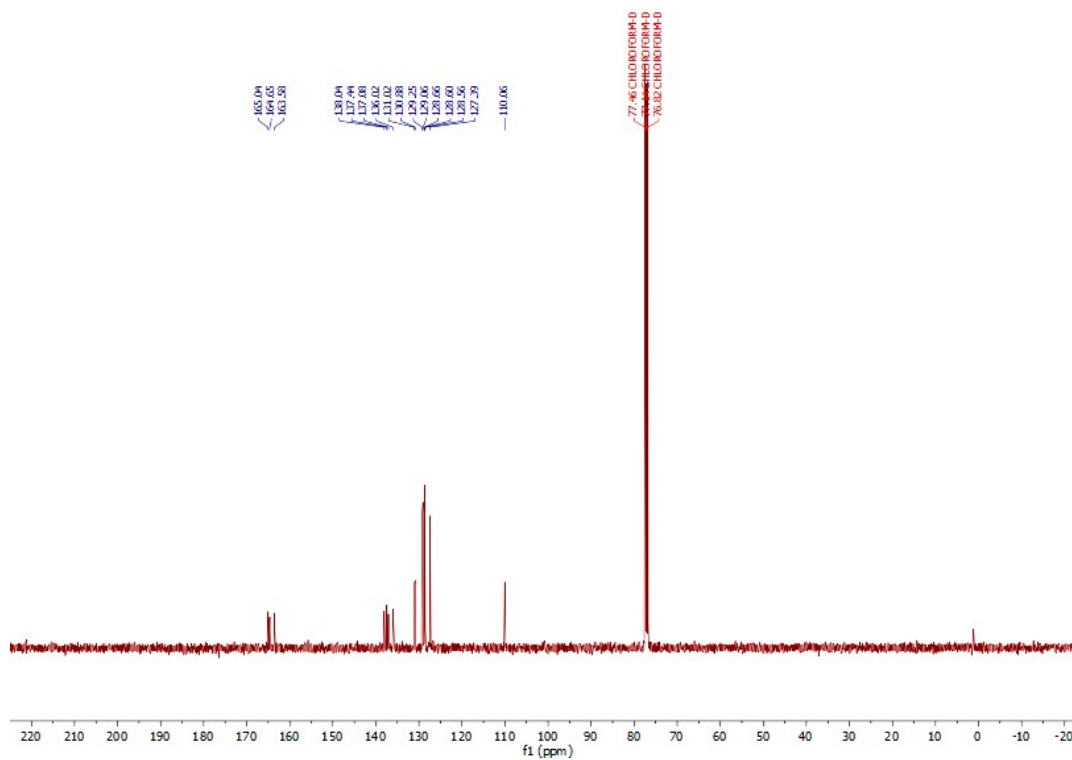
¹³C NMR (100 MHz) of 4-(4-fluorophenyl)-2,6-diphenylpyrimidine (3j):



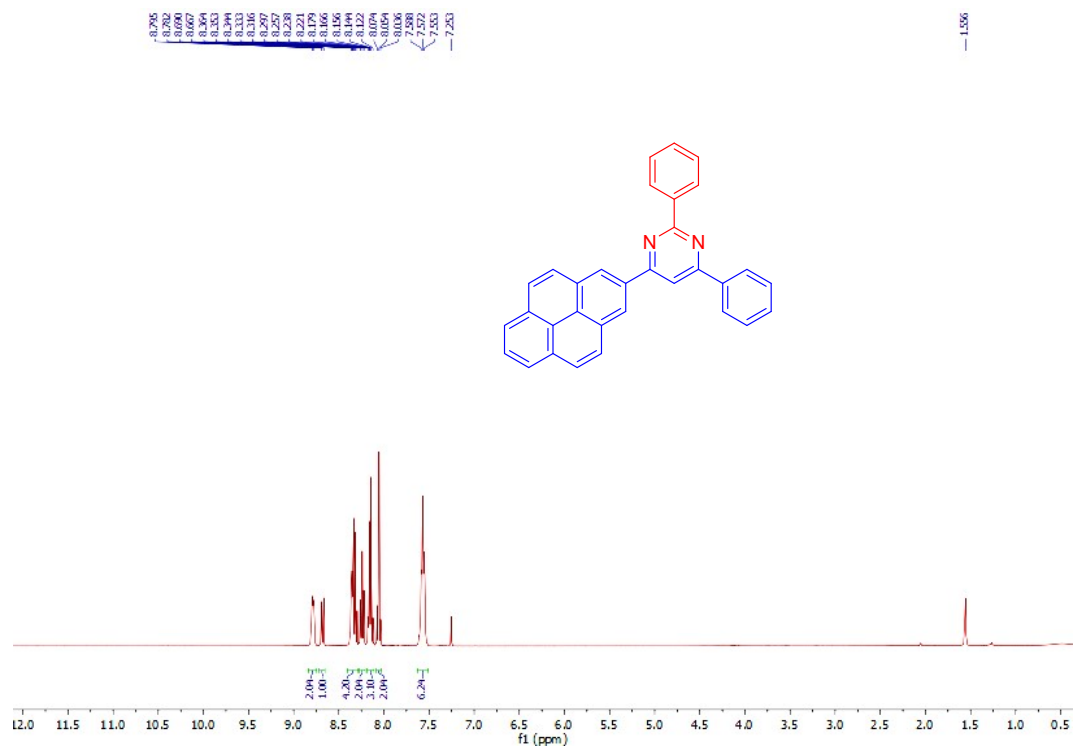
¹H NMR (400 MHz) of 4-(4-chlorophenyl)-2,6-diphenylpyrimidine (3k):



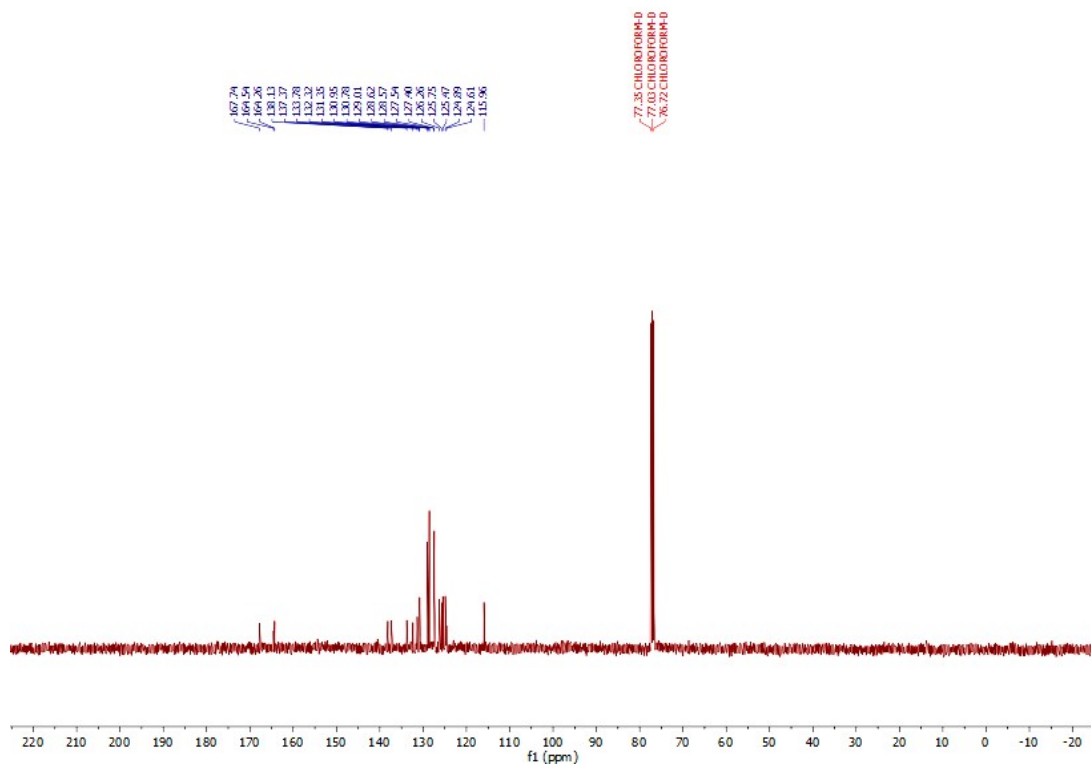
¹³C NMR (100 MHz) of 4-(4-chlorophenyl)-2,6-diphenylpyrimidine (3k):



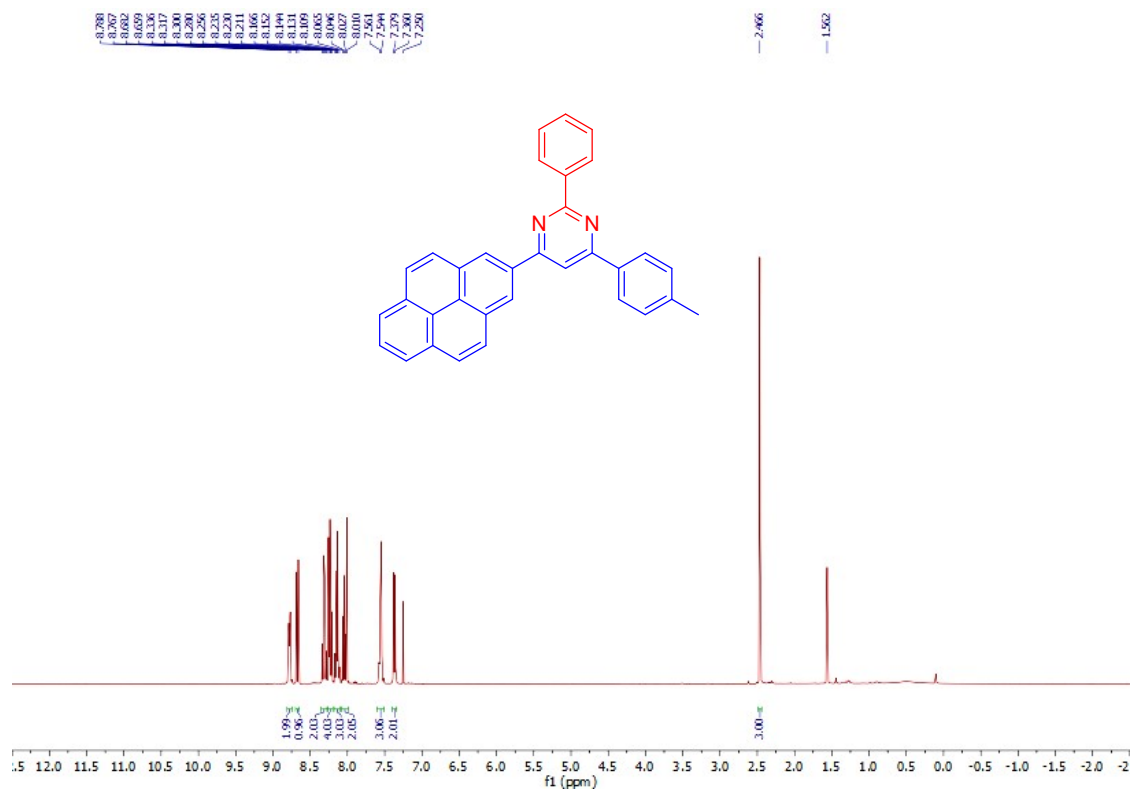
¹H NMR (400 MHz) of 2,4-diphenyl-6-(pyren-2-yl) pyrimidine (3n):



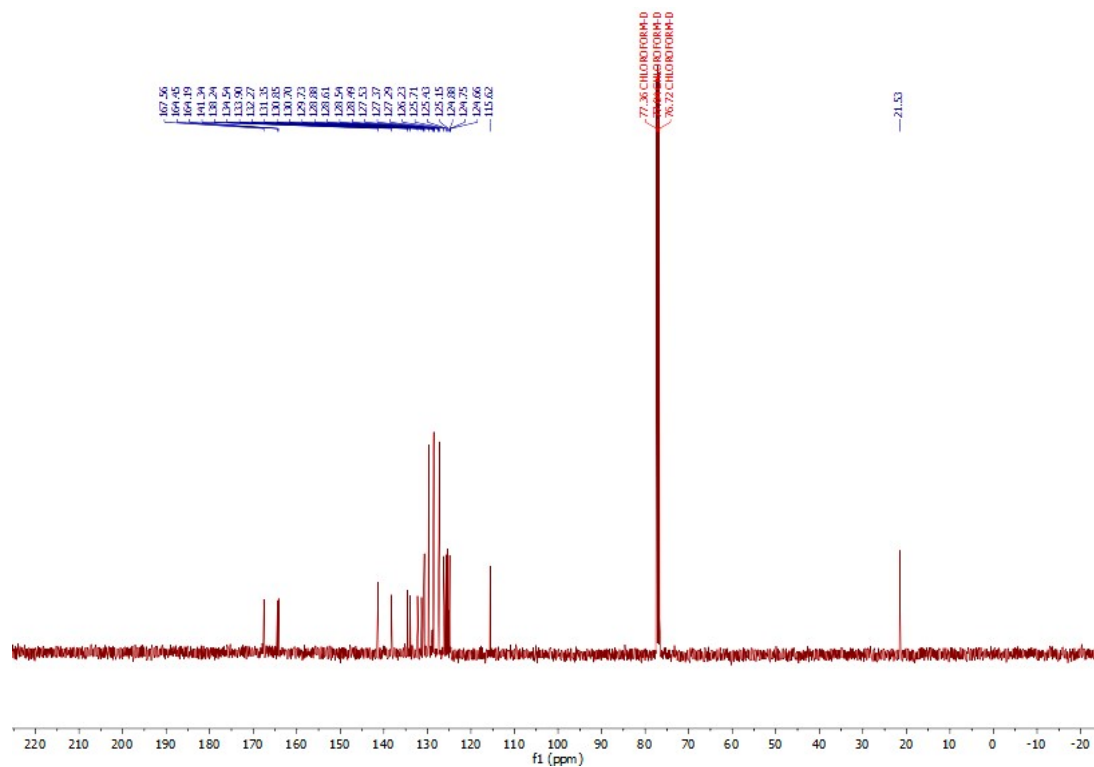
¹³C NMR (100 MHz) of 2,4-diphenyl-6-(pyren-2-yl) pyrimidine (3n):



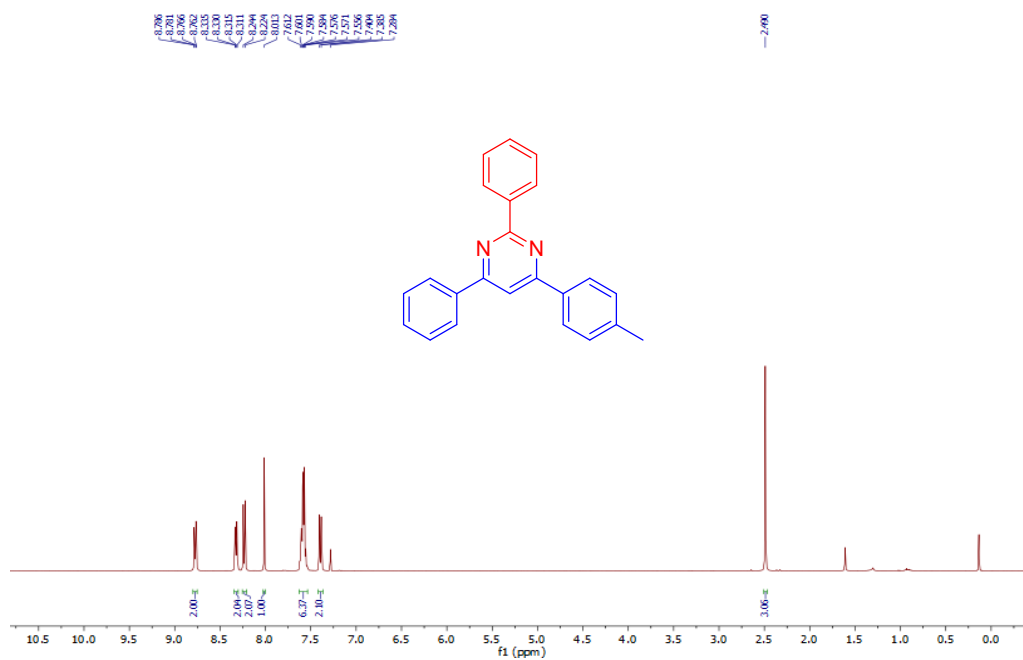
¹H NMR (400 MHz) of 2-phenyl-4-(pyren-2-yl)-6-(p-tolyl) pyrimidine (3o):



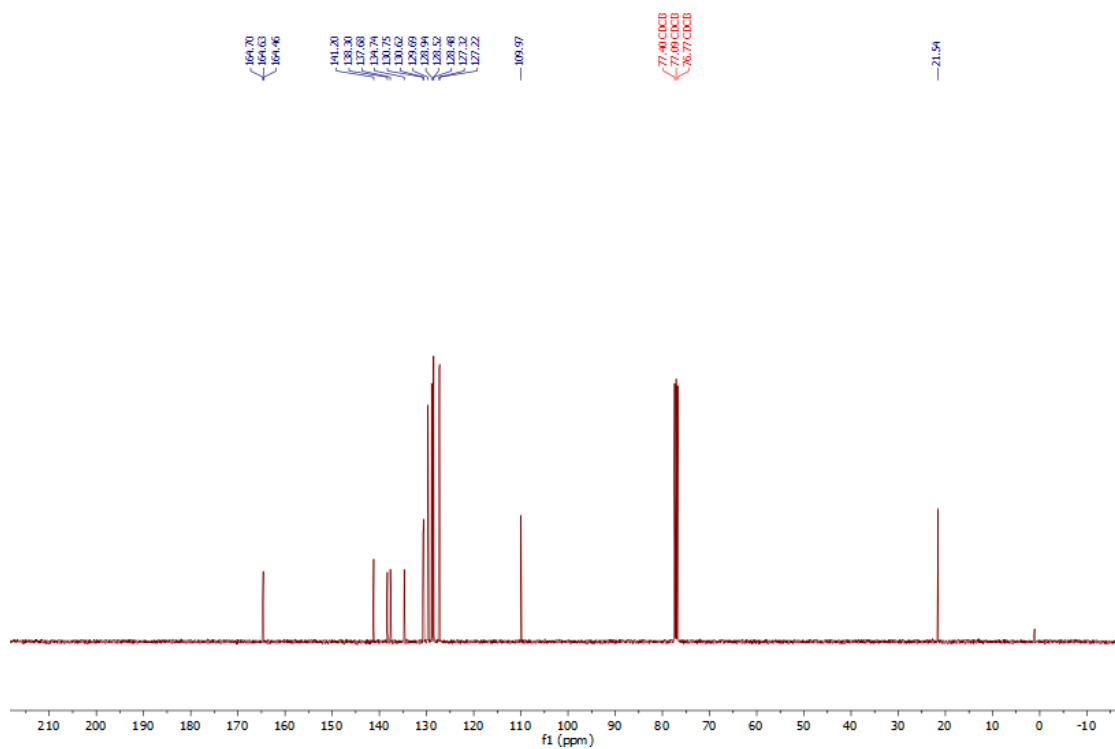
¹³C NMR (100 MHz) of 2-phenyl-4-(pyren-2-yl)-6-(p-tolyl) pyrimidine (3o):



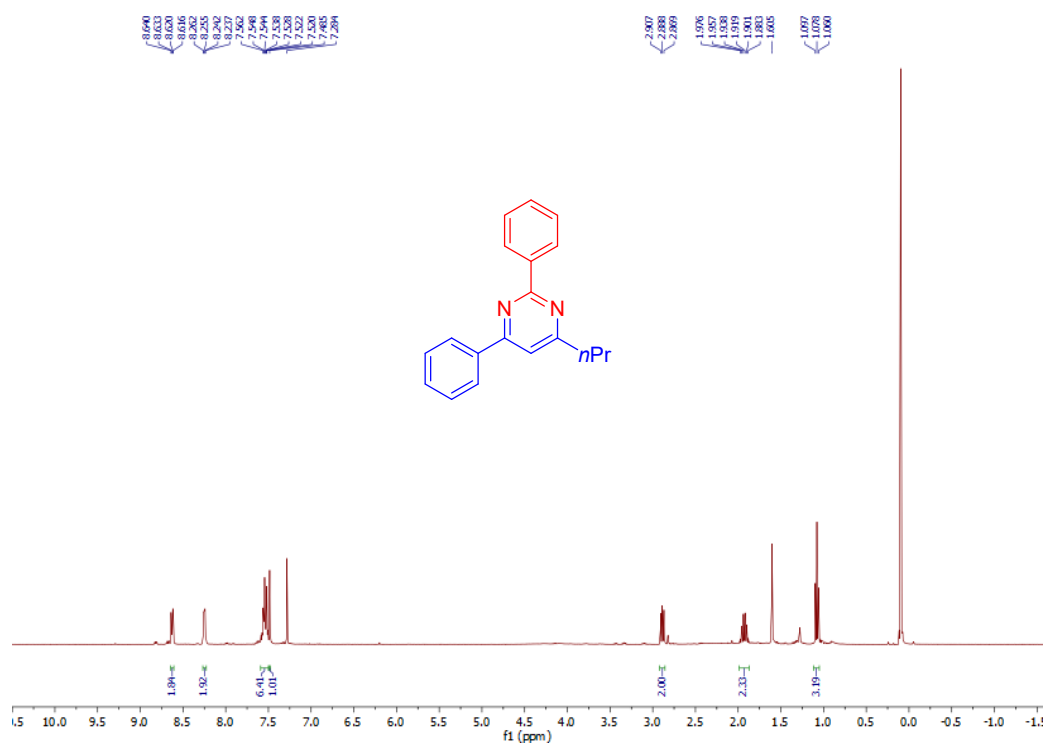
¹H NMR (400 MHz) of 2,4-diphenyl-6-(p-tolyl)pyrimidine (3p):



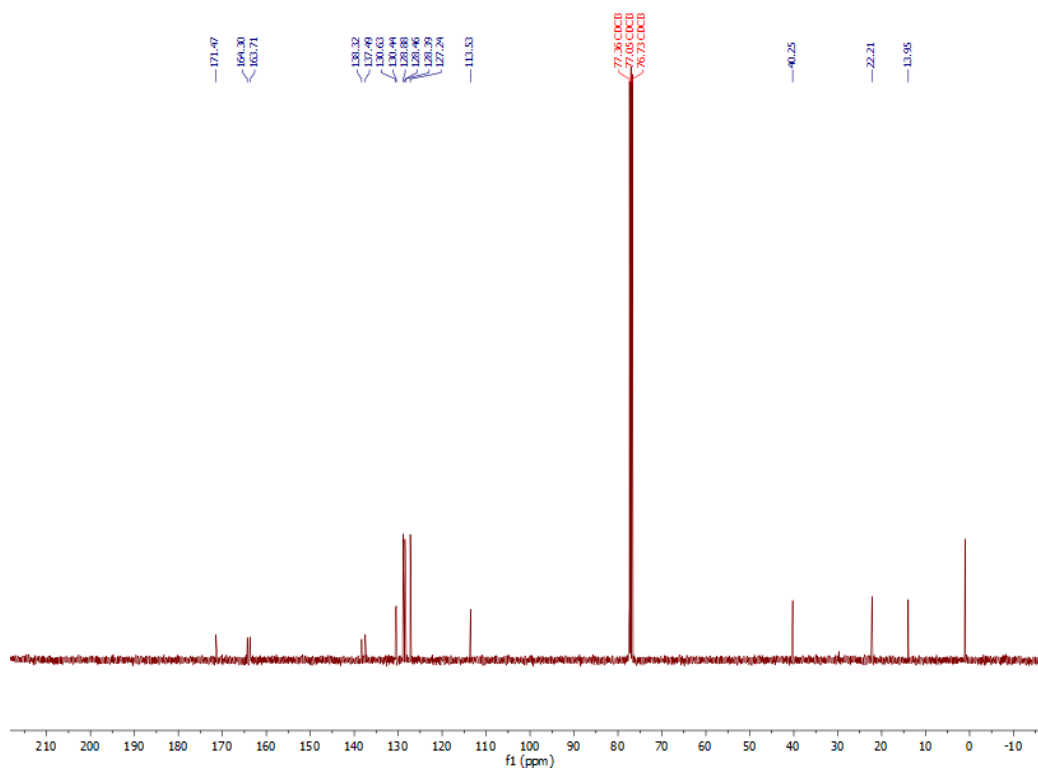
¹³C NMR (100 MHz) of 2,4-diphenyl-6-(p-tolyl)pyrimidine (3p):



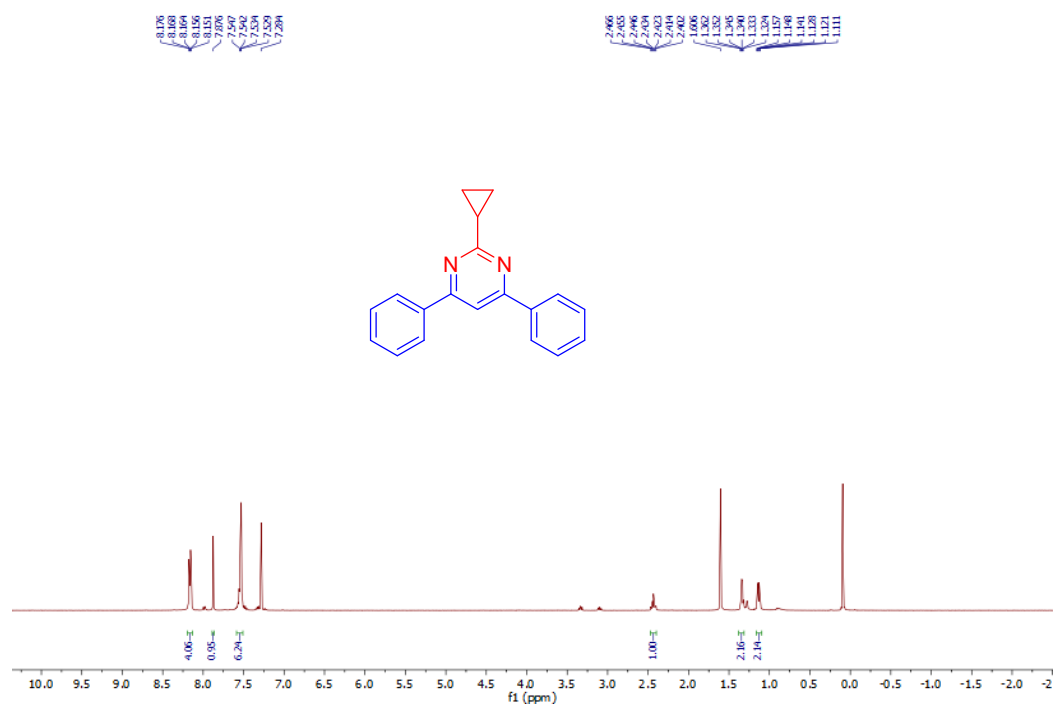
¹H NMR (400 MHz) of 2,4-diphenyl-6-propylpyrimidine (3q):



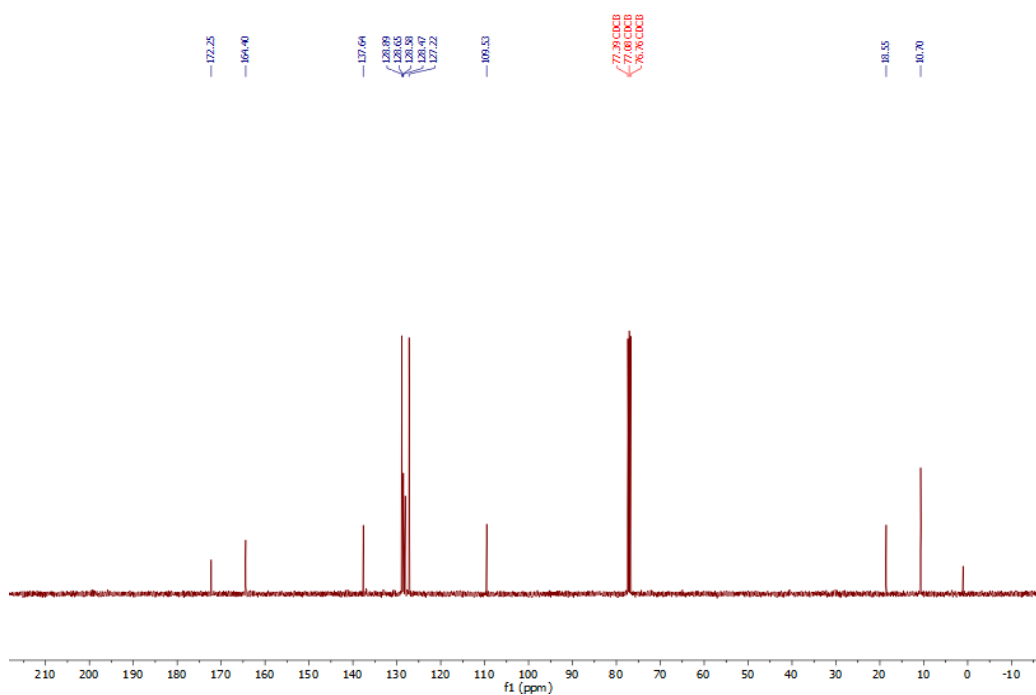
¹³C NMR (100 MHz) of 2,4-diphenyl-6-propylpyrimidine (3q):



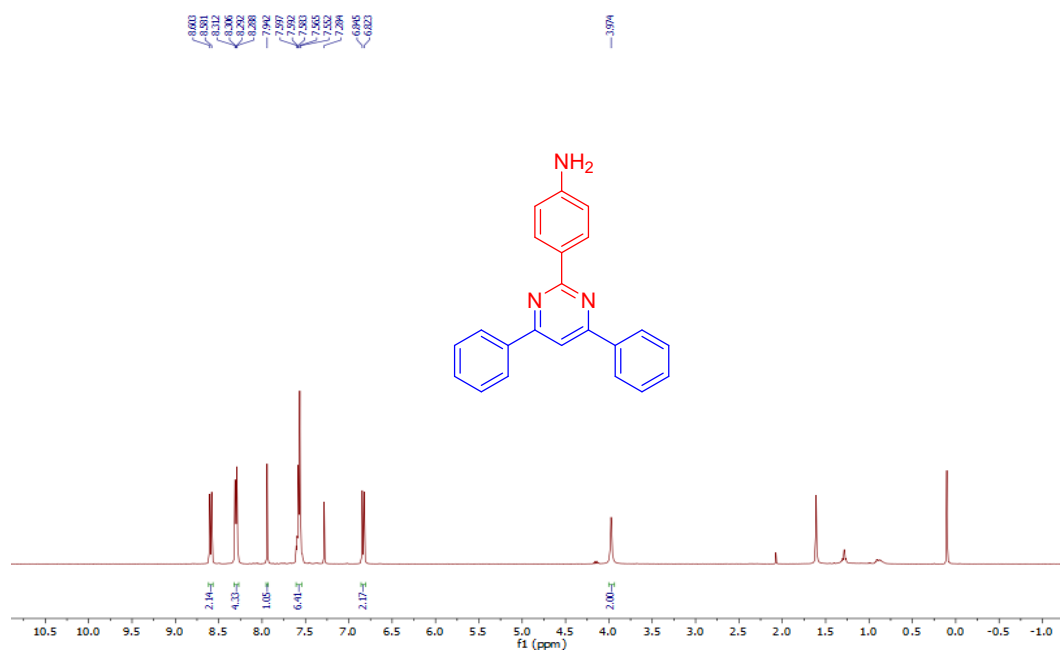
¹H NMR (400 MHz) of 2-cyclopropyl-4,6-diphenylpyrimidine (3r):



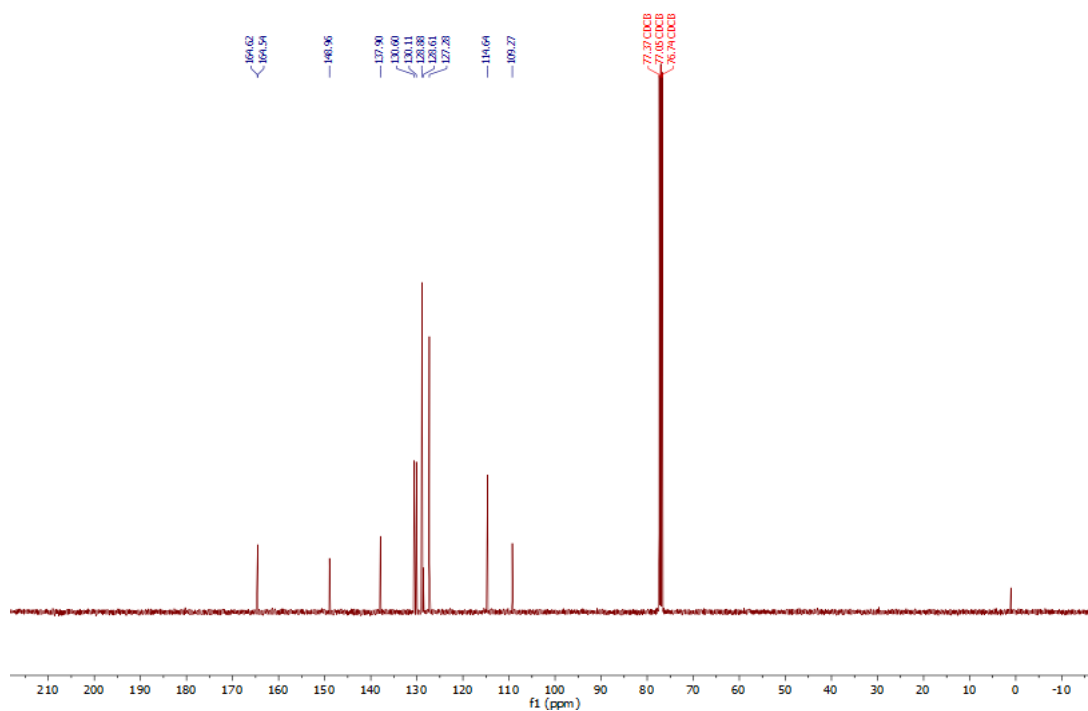
¹³C NMR (100 MHz) of 2-cyclopropyl-4,6-diphenylpyrimidine (3r):



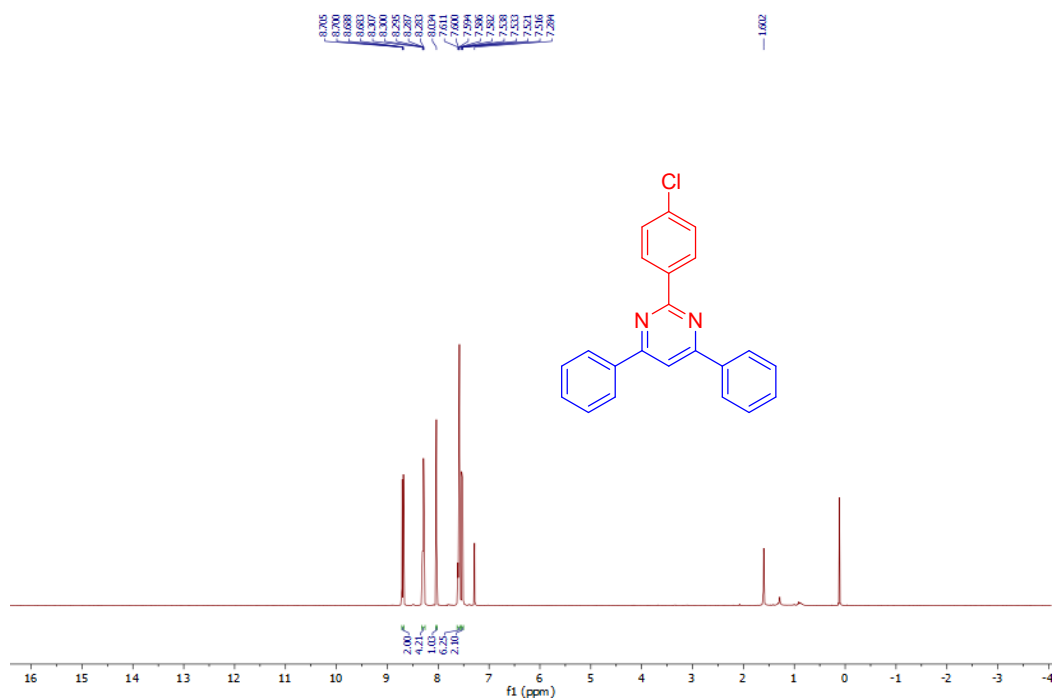
¹H NMR (400 MHz) of 4-(4,6-diphenylpyrimidin-2-yl)aniline (3s):



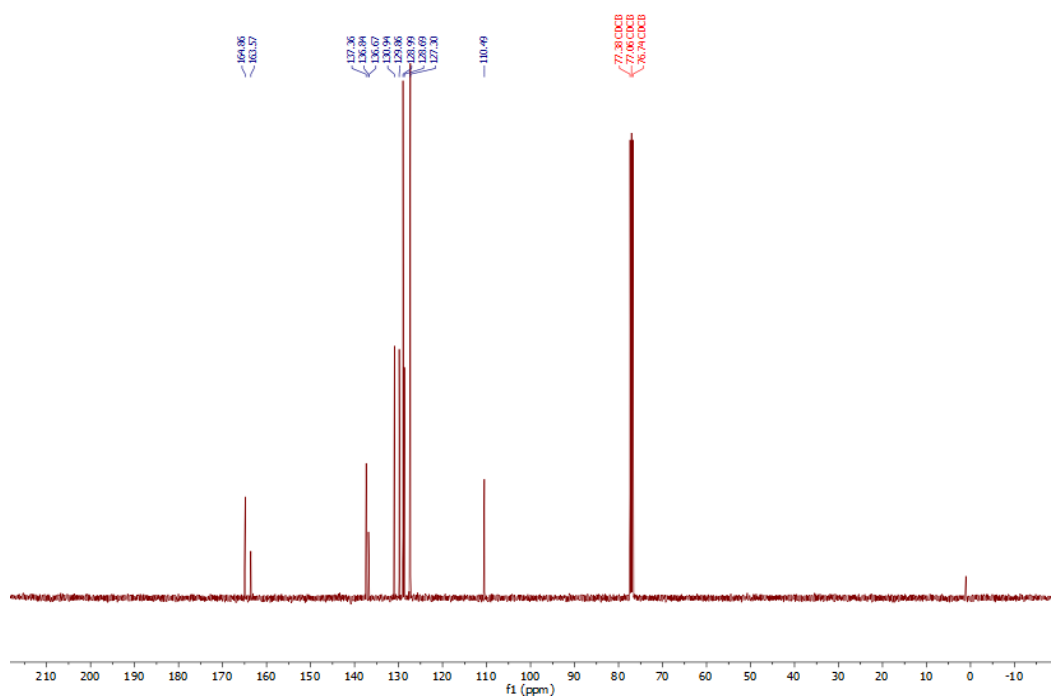
¹³C NMR (100 MHz) of 4-(4,6-diphenylpyrimidin-2-yl)aniline (3s):



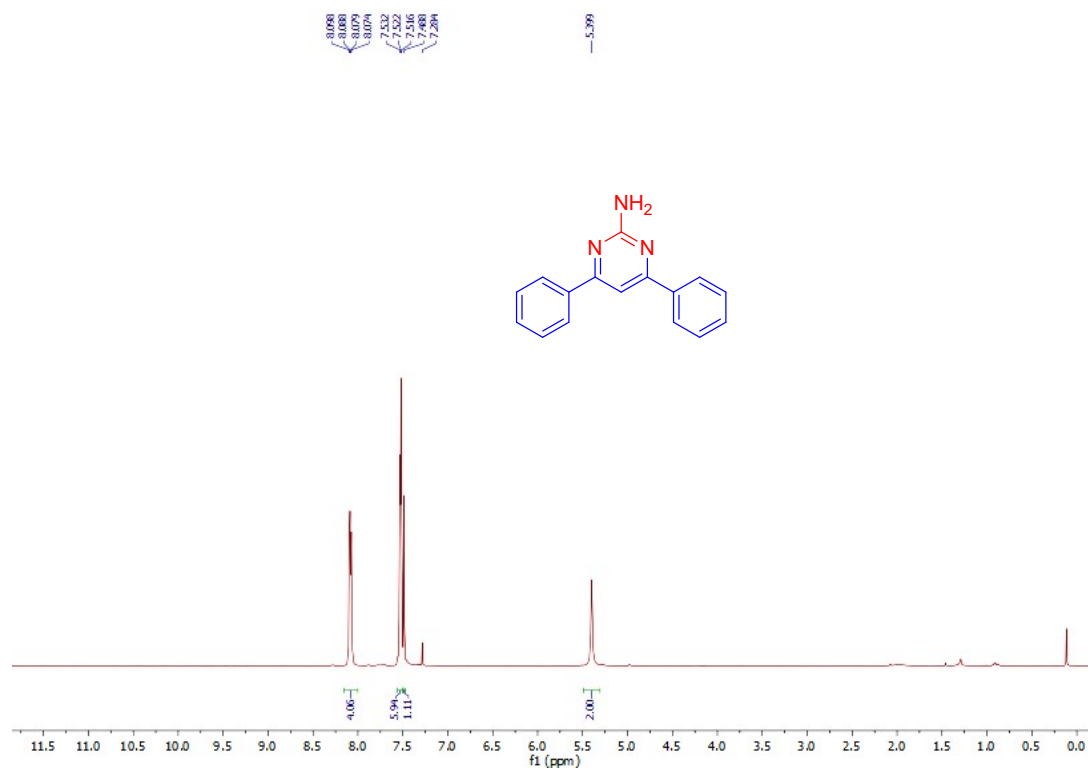
¹H NMR (400 MHz) of 2-(4-chlorophenyl)-4,6-diphenylpyrimidine (3t):



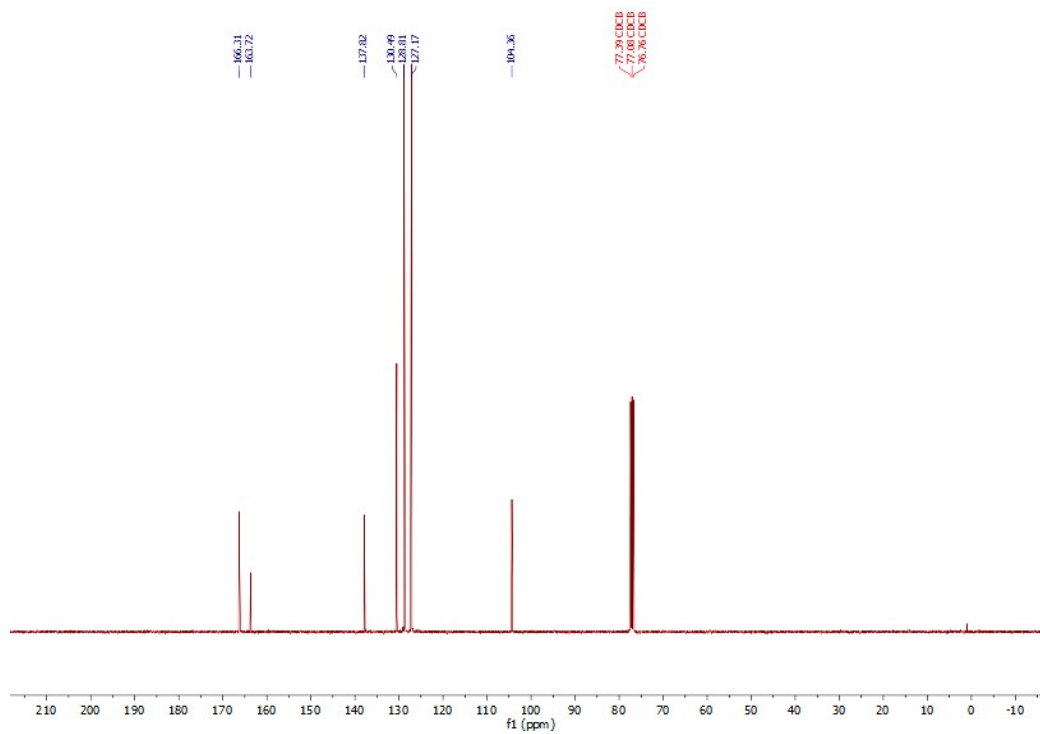
¹³C NMR (100 MHz) of 2-(4-chlorophenyl)-4,6-diphenylpyrimidine (3t):



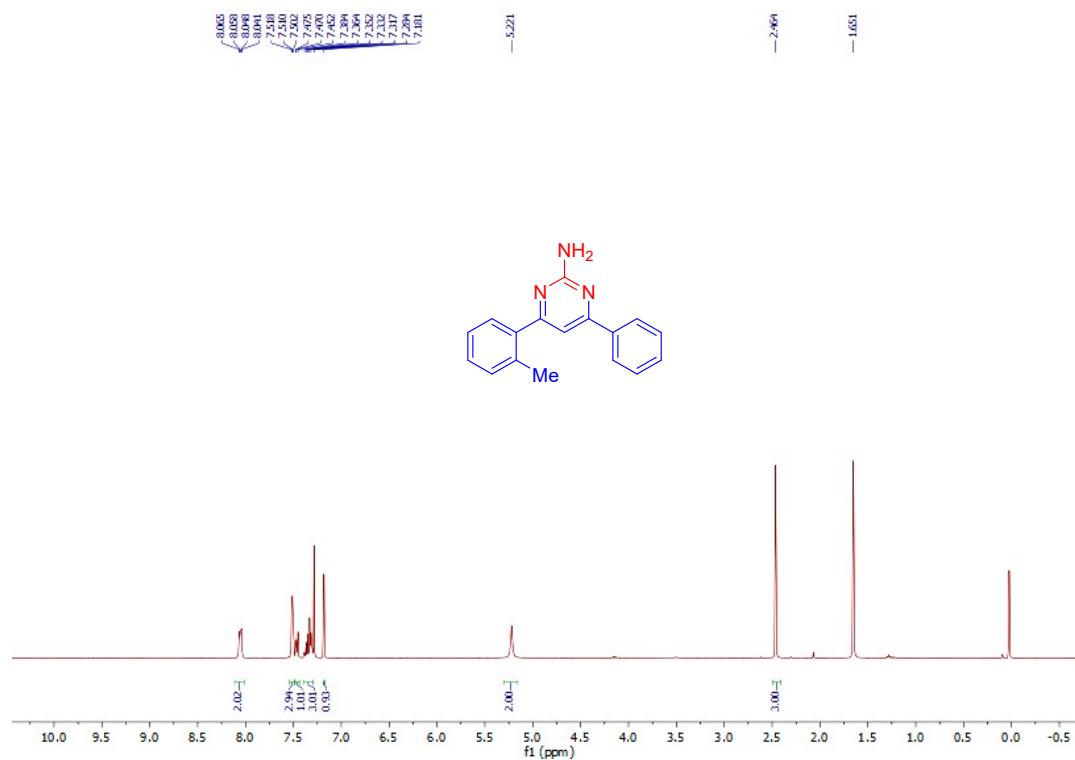
¹H NMR (400 MHz) of 4,6-diphenylpyrimidin-2-amine (5a):



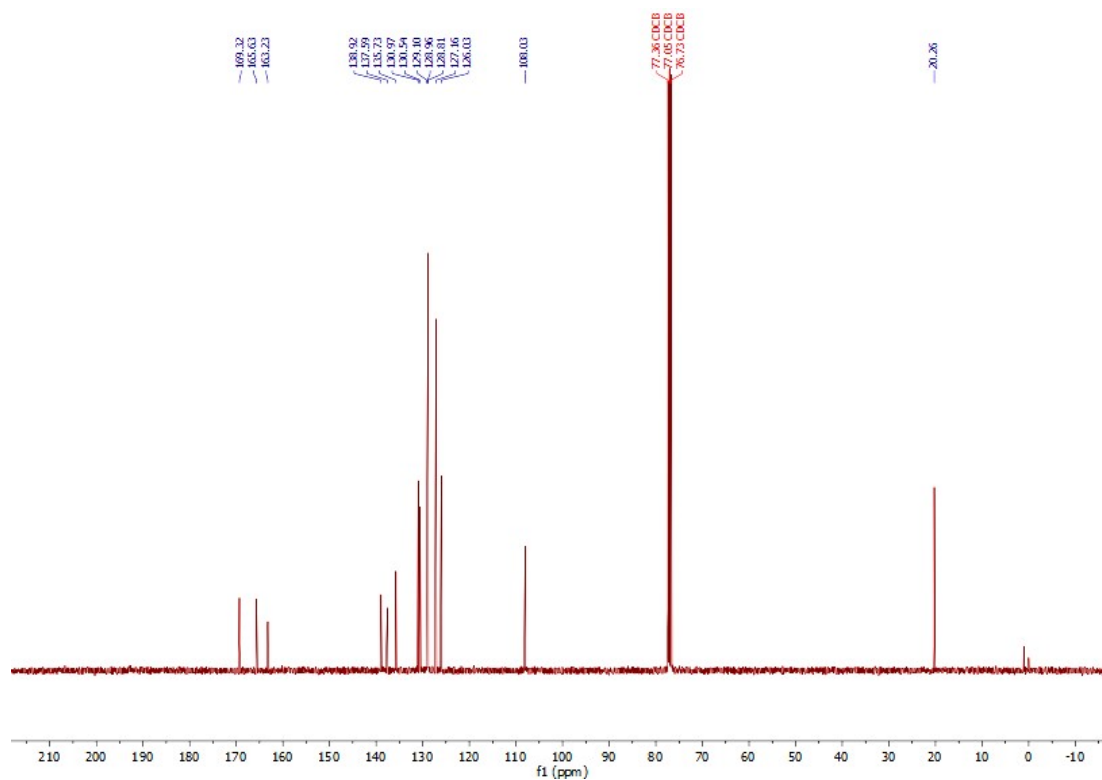
¹³C NMR (100 MHz) of 4,6-diphenylpyrimidin-2-amine (5a):



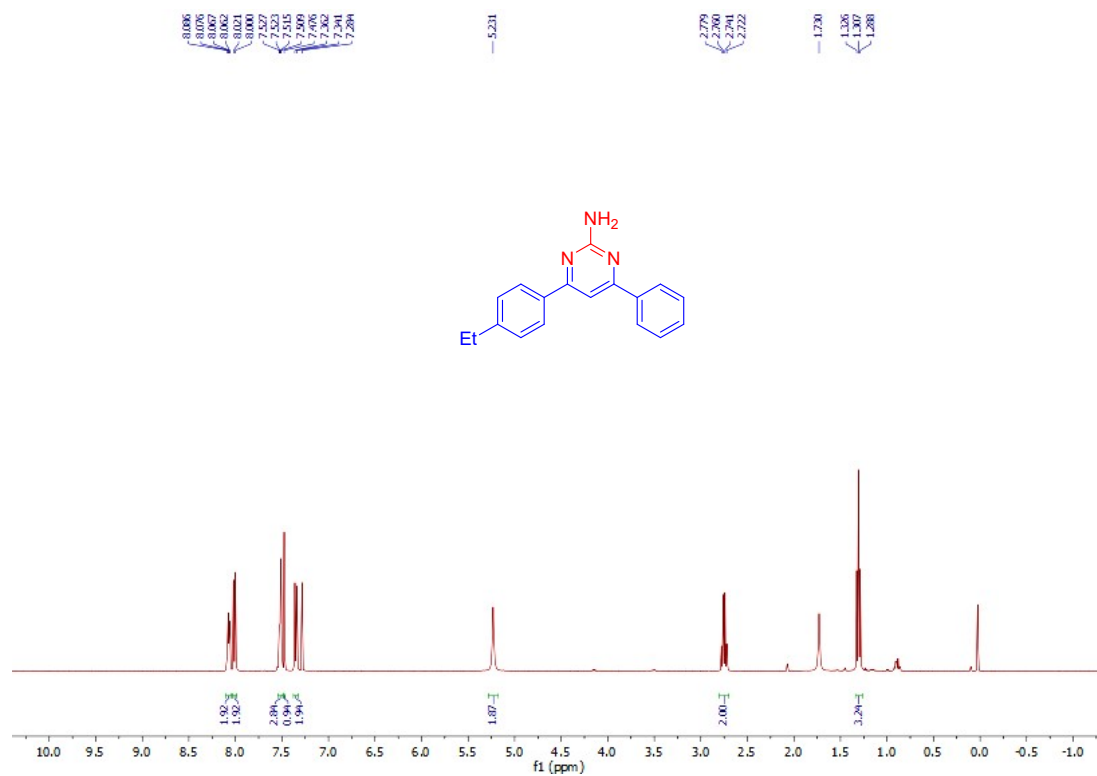
¹H NMR (400 MHz) of 4-phenyl-6-(o-tolyl)pyrimidin-2-amine (5b):



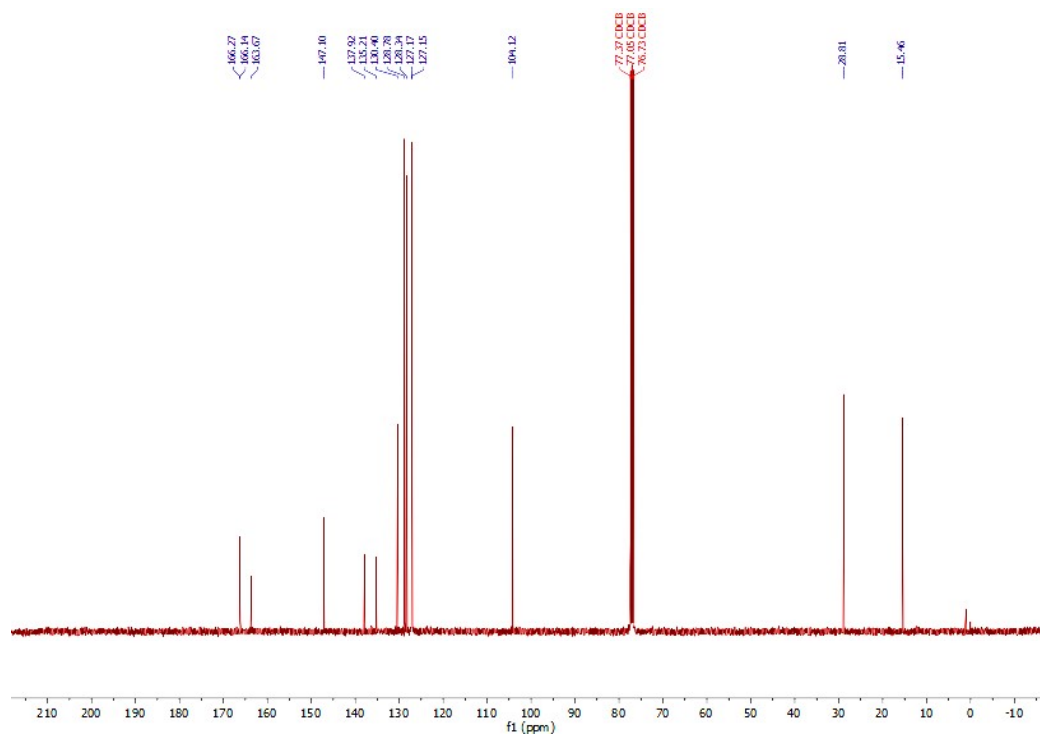
¹³C NMR (100 MHz) of 4-phenyl-6-(o-tolyl) pyrimidin-2-amine (5b):



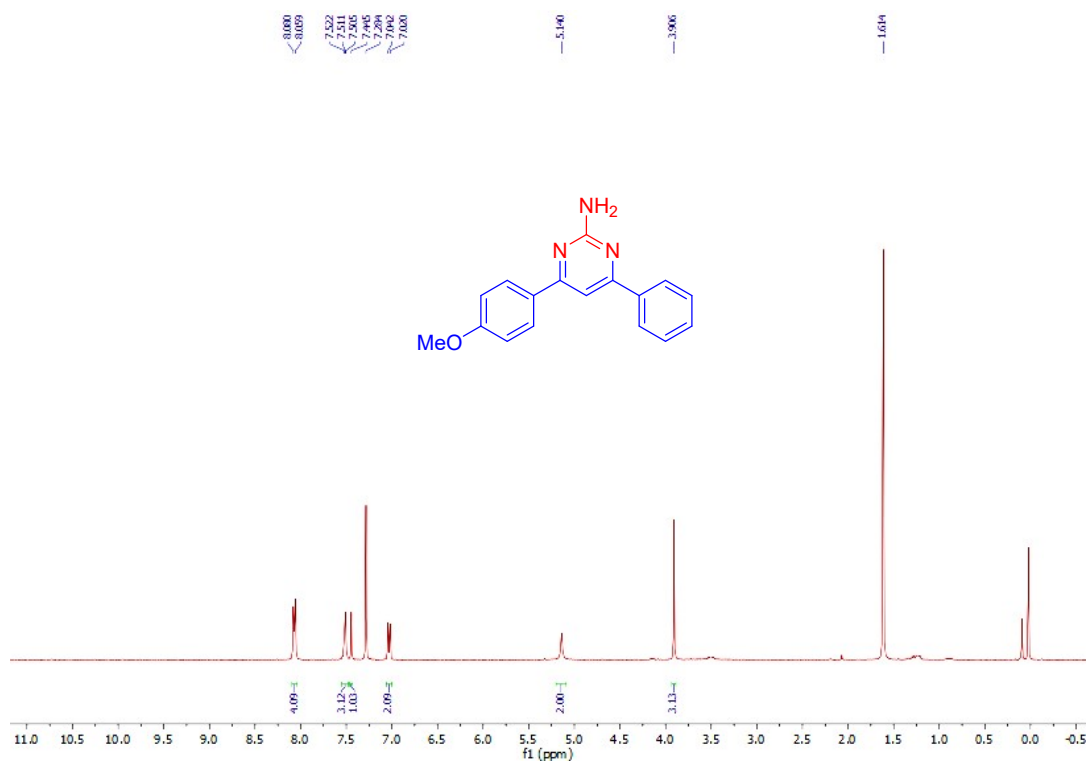
¹H NMR (400 MHz) of 4-(4-ethylphenyl)-6-phenylpyrimidin-2-amine (5c):



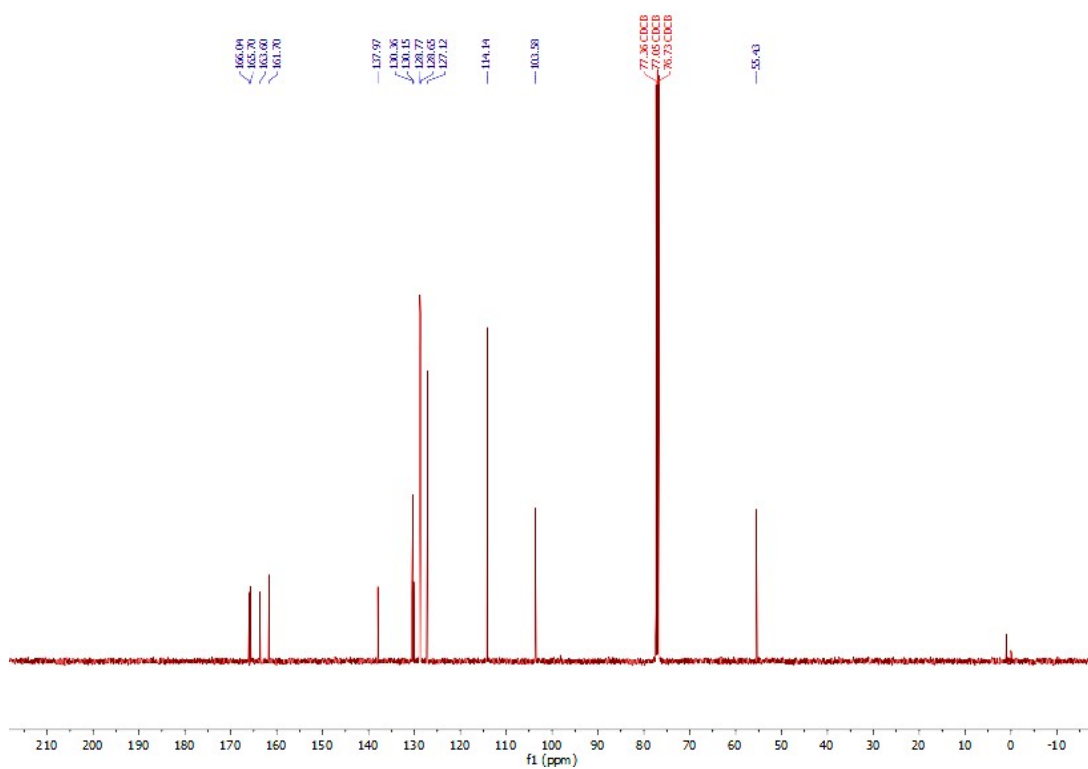
¹³C NMR (100 MHz) of 4-(4-ethylphenyl)-6-phenylpyrimidin-2-amine (5c):



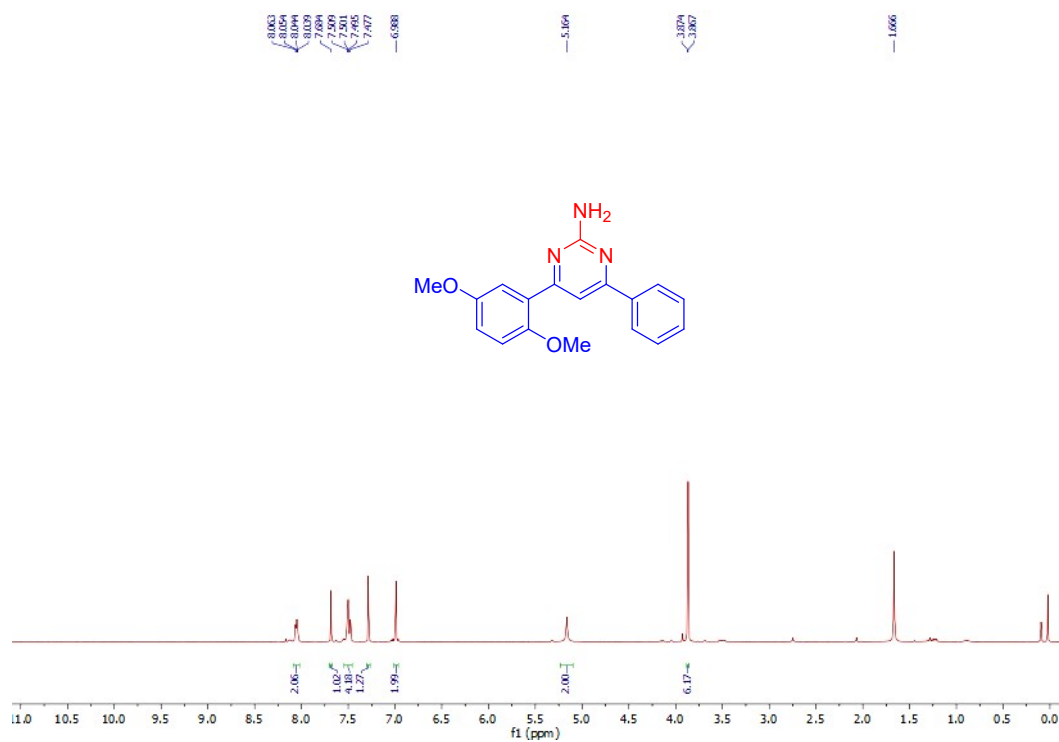
¹H NMR (400 MHz) of 4-(4-methoxyphenyl)-6-phenylpyrimidin-2-amine (5d):



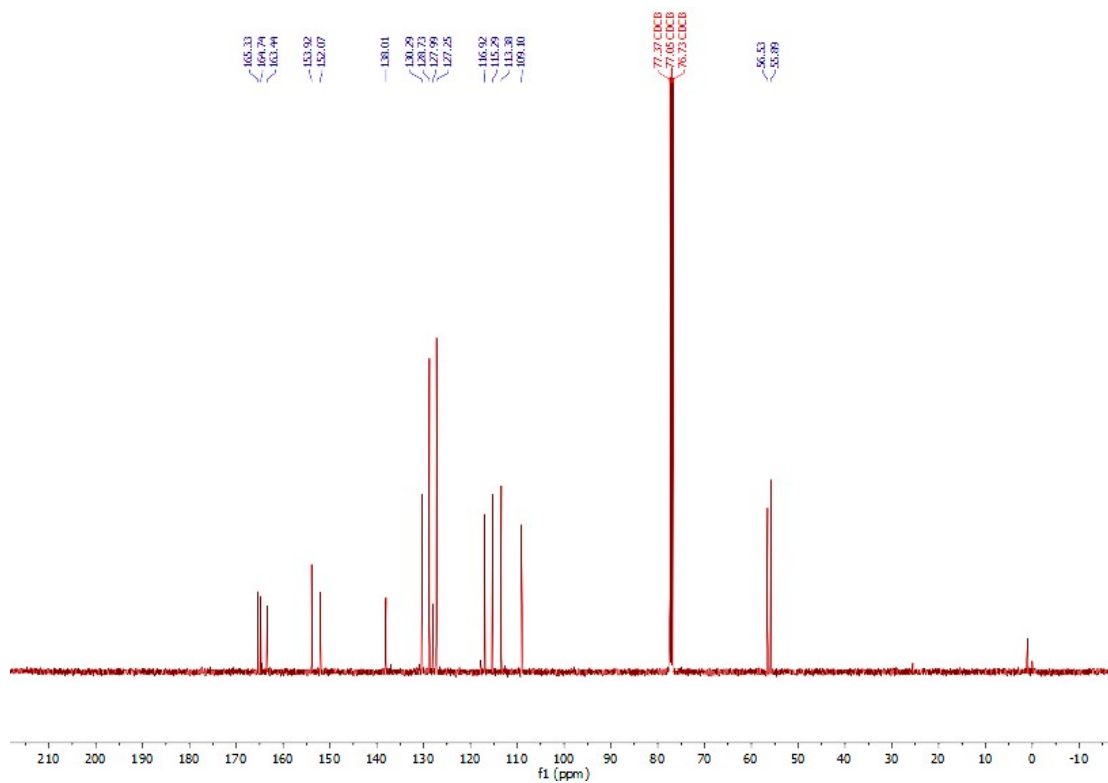
¹³C NMR (100 MHz) of 4-(4-methoxyphenyl)-6-phenylpyrimidin-2-amine (5d):



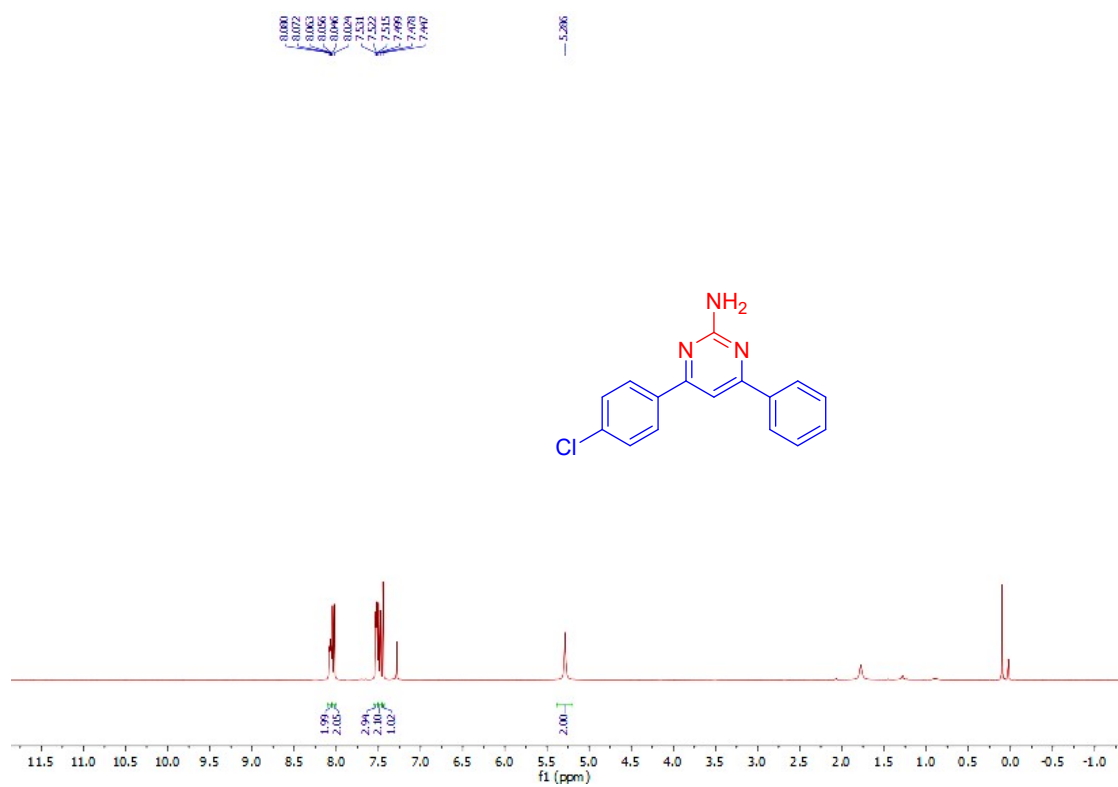
¹H NMR (400 MHz) of 4-(2,5-dimethoxyphenyl)-6-phenylpyrimidin-2-amine (5e):



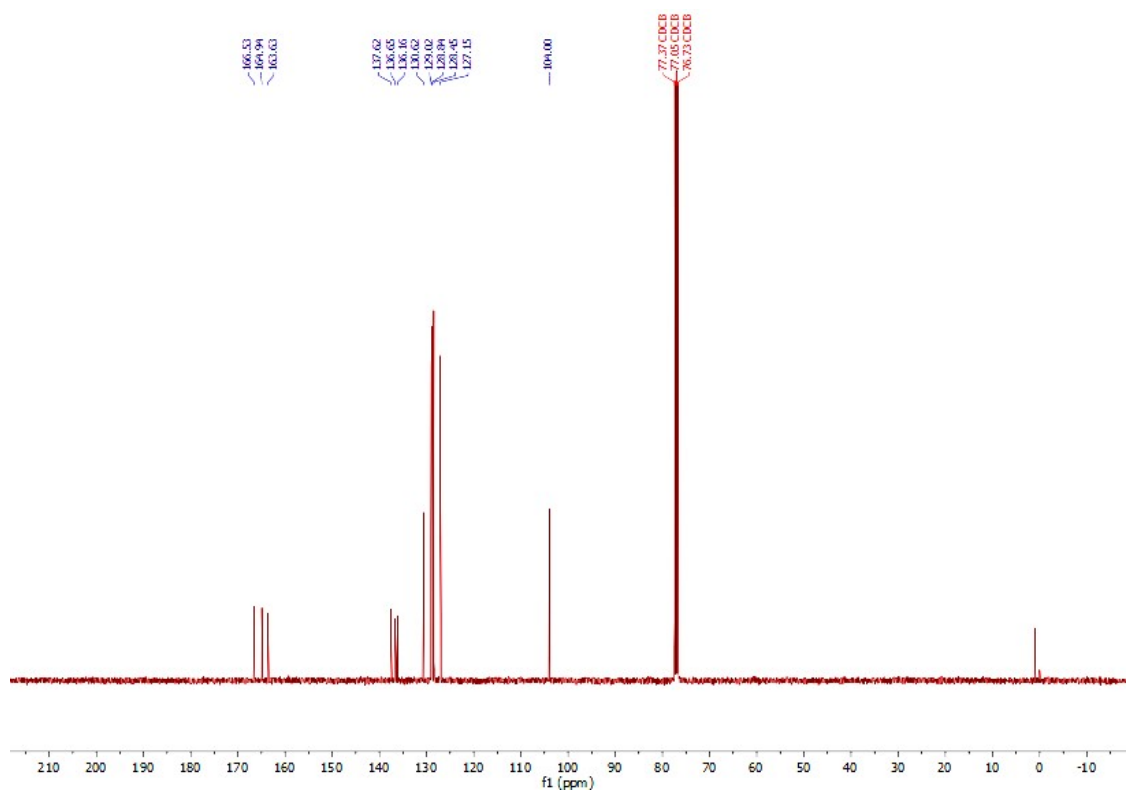
¹³C NMR (100 MHz) of 4-(2,5-dimethoxyphenyl)-6-phenylpyrimidin-2-amine (5e):



¹H NMR (400 MHz) of 4-(4-chlorophenyl)-6-phenylpyrimidin-2-amine (5f):



¹³C NMR (100 MHz) of 4-(4-chlorophenyl)-6-phenylpyrimidin-2-amine (5f):



Crystallographic data analysis of compound **3o**:

We have attempted for crystallization of some compound and we have got crystal from compound **3o** in ethyl acetate-hexane solvent mixture by slow evaporation. A yellow colored, needle shaped crystal was obtained. The single-crystal X-ray diffraction (SC-XRD) at low temperature indicates the triclinic system with space group P-1. The crystallographic details are given in table 3.

Table 3. Crystallographic details of **3o**

Parameters	Compound 3o
Formula	C ₃₃ H ₂₂ N ₂
Formula Weight	446.53
Crystal System	Triclinic
Space group	P1
a (Å)	8.036 (1)
b(Å)	10.55(2)
c (Å)	13.26(3)
α(°)	93.56(5)
β(°)	96.81(4)
γ(°)	94.96(5)
V (Å³)	1109(4)
Z	2
D(calc) (g.cm⁻³)	1.337
μ Mo K_α (mm⁻¹)	0.078
F (000)	468.0
Temperature (K)	297
Radiation Mo K_α (Å)	0.71073
θMax (°)	25.213
Nref, Npar	4012, 318
R, wR2, S	0.0805(3031), 0.2891(3989), 1.127
CCDC No.	2087550