Supplementary Materials

A metal-free synthesis of pyrimidines from amidines with α, β-unsaturated ketones *via* tandem [3+3] annulation and visible light enabled photo-oxidation

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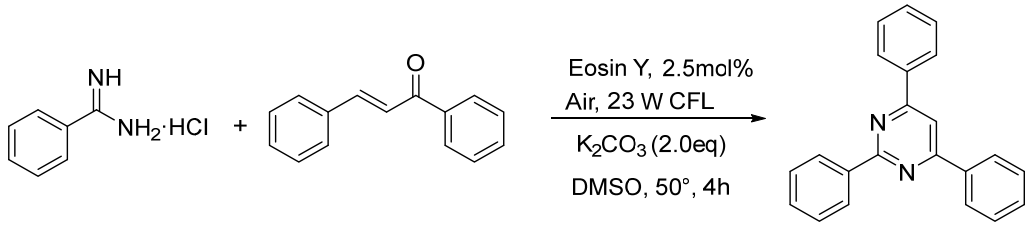
Contents

1. General information

All chemicals were purchased from commercial suppliers and used without further purification unless specially noted. Thin-layer chromatography (TLC) was performed using silica gel GF254 plates. Column chromatography was performed on silica gel (300 ~ 400 mesh) with petroleum ether/ethyl acetate for the gradient elution. All melting points were measured without correction. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III HD 600 or HD 500 spectrometer at 600/500 MHz (^{1}H NMR) and 151/125 MHz (^{13}C NMR) respectively. The chemical shifts are reported relative to $CHCl_3$ (δ = 7.26 for ^{1}H NMR and δ = 77.16 for ^{13}C NMR).

2. Typical procedure for **3a**

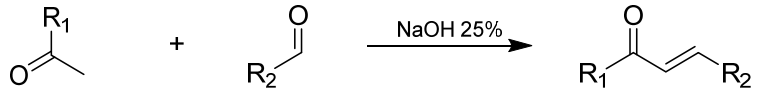


1a **2a** **3a**

A mixture of benzamidine hydrochloride **1a** (15.6 mg, 0.10 mmol)，chalcone **2a** (42.0 mg, 0.20 mmol) and K_2CO_3 (13.6 mg, 0.10 mmol) was dissolved in DMSO (4.0 mL) and put in a reaction vessel open to air and stirred at 50 °C for 3 h until the full consumption of **1a** by TLC monitoring (eluent chloroform: methanol: TEA = 50: 16: 5). Then Eosin Y (1.70 mg, 0.0025 mmol) was added in and irradiated under four 23 W CFLs at 40 °C for 1 h to complete the transformation. The mixture was then diluted with 10 mL de-ionized water (turn orange) and extracted by 20 mL EtOAc for three times. The organic phase was combined, dried over Na_2SO_4 and filtered. The solvent was removed under vacuum and the residue was put on silica gel chromatography and eluted with EA/PE (0.5:100) to give **3a** as a white solid (25.0 mg, 81%).

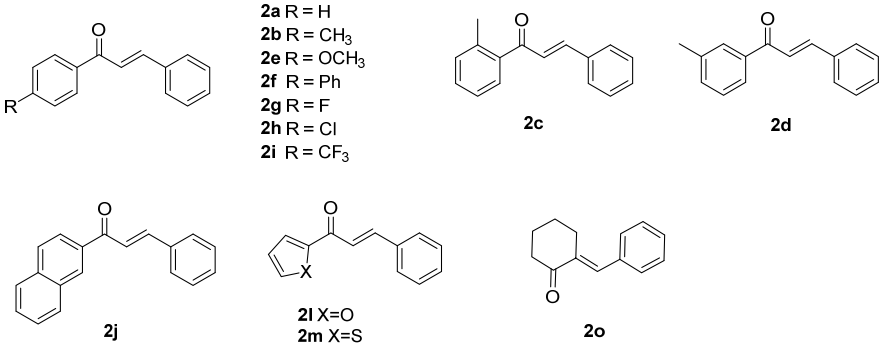
3. Syntheses of starting materials

3.1 Synthesis of unsaturated ketones[1]

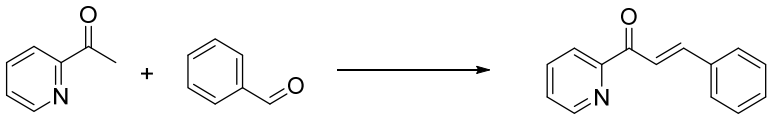


Preparation of chalcone

To a solution of suitable ketone (25 mmol) and aldehyde (30 mmol) in ethanol (15 mL), aqueous sodium hydroxide (25 mL, 2.5 M) was added dropwisely at 0 ℃. The reaction mixture was further stirred at room temperature until the completion of reaction (detected by TLC). The reaction mixture was then filtered and washed with ethanol-water solution (1/1) and dried. The precipitate was recrystallized in methanol to obtain pure unsaturated ketone product. The unsaturated ketones (**2a**-**2j**, **2l**-**2o**) were synthesized using this method.



Synthesis of (*E*)-3-phenyl-1-(pyridin-2-yl)prop-2-en-1-one (**2k**) [2]

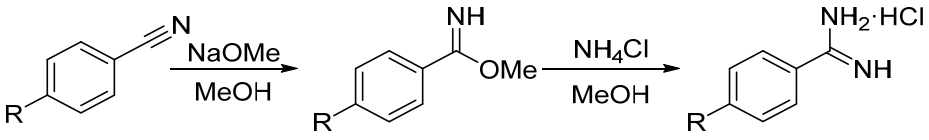


2k

Seventeen millimoles of the 2-acetylpyridine and 16.5 mmol of the benzaldehyde were introduced in 100 mL of water at temperatures below 5 °C. The mixture was shaken thoroughly in order to obtain a finely dispersed emulsion. Ten milliliters of a 10% sodium hydroxide solution were added. The mixture was again shaken and left overnight undisturbed at 4 °C. The solution should not be stirred since this results in a phase separation and lower yields. The product was separated as an oil that solidified upon shaking. Filtration and washing with water gave the almost pure product **2k** in 95%

yield.

3.2 Synthesis of benzamidine hydrochlorides[3]



R=H, CH_3, OCH_3, Cl, CF_3, F

Synthesis of benzamidine hydrochlorides.

To a 250 mL round-bottom flask charged with 100 mL of CH_3OH, 0.4 g sodium was added. After the dissolution of sodium, 0.1 mol of the appropriate nitrile was added in. The contents of the flask were protected from moisture and stirred magnetically for 48 h at room temperature. Then, 0.1 mol of NH_4C1 was added and stirring was continued for 24 h. Unreacted NH_4C1 was filtered, and methanol was stripped from the filtrate to afford the crude products. The product was then washed free of unreacted arylnitriles with ether and dried to give arylamidine hydrochloride in 60-80% yield.

4. Mehchanistic study

4.1 Fluorescence quenching experiment

The fluorescence spectrum of the Eosin Y was recorded on a spectrofluorimeter (RF-6000, SHIMADZU). Emission and excitation spectra were corrected for source intensity (lamp and grating) by standard correction curves. The excitation wavelength was fixed at 540 nm. In the blank experiment, Eosin Y solution of DMSO was recorded in the concentration of 1×10^{-5} M. Subsequently, different mounts of dihydropyrimidine **4a** was dissolved in the solution, and the resulting changes in fluorescence intensity in the concentrations of 6×10^{-5} M, 12×10^{-5} M, 18×10^{-5} M, 24×10^{-5} M were collected, please see Figure S1. The Stern-Volmer plot gives a K_{sv} of 11934 M^{-1} (Figure S2). According to the results, the dihydropyrimidine **4a** exhibited evident quenching effect to the fluorescent emission intensity of Eosin Y, supporting that dihydropyrimidine was the energy acceptor of excited Eosin Y during the reported photocatalytic reactions.

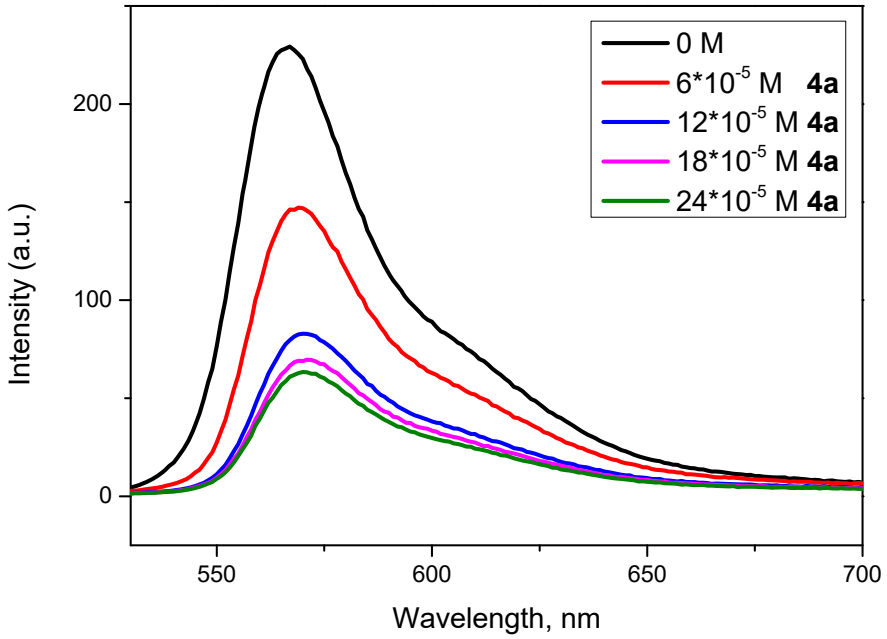


Figure S1

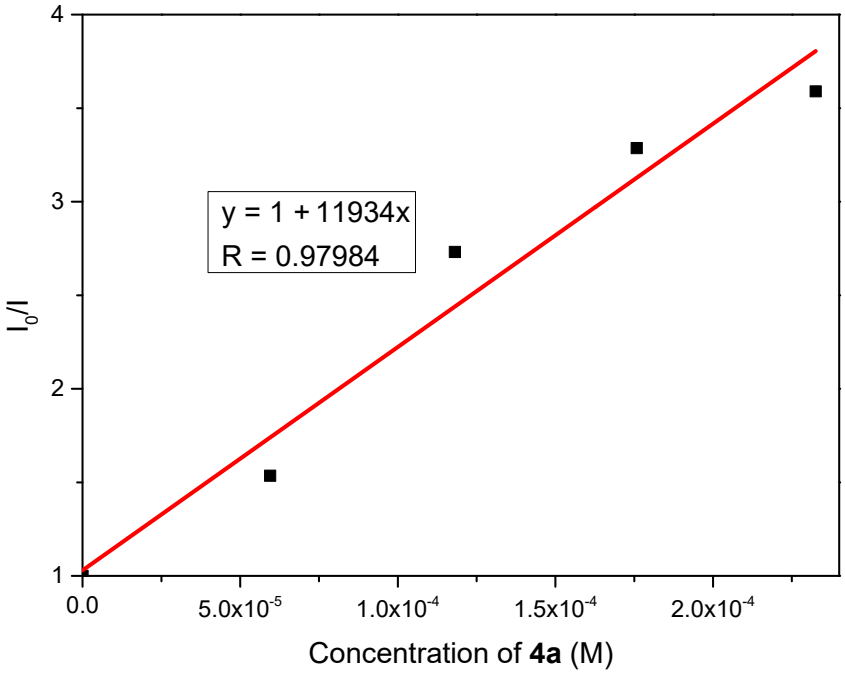


Figure S2 Stern-Volmer plot of the fluorescence quenching of Eosin Y by **4a** in DMSO.

4.2 Benzylic radical capture

Benzylic radical IV in Scheme 3 could be captured by TEMPO and gave a weak signal in HRMS at 465.2731 which was assigned to M^+ (Calculated for $C_{31}H_{35}N_3O^+$: 465.2780).

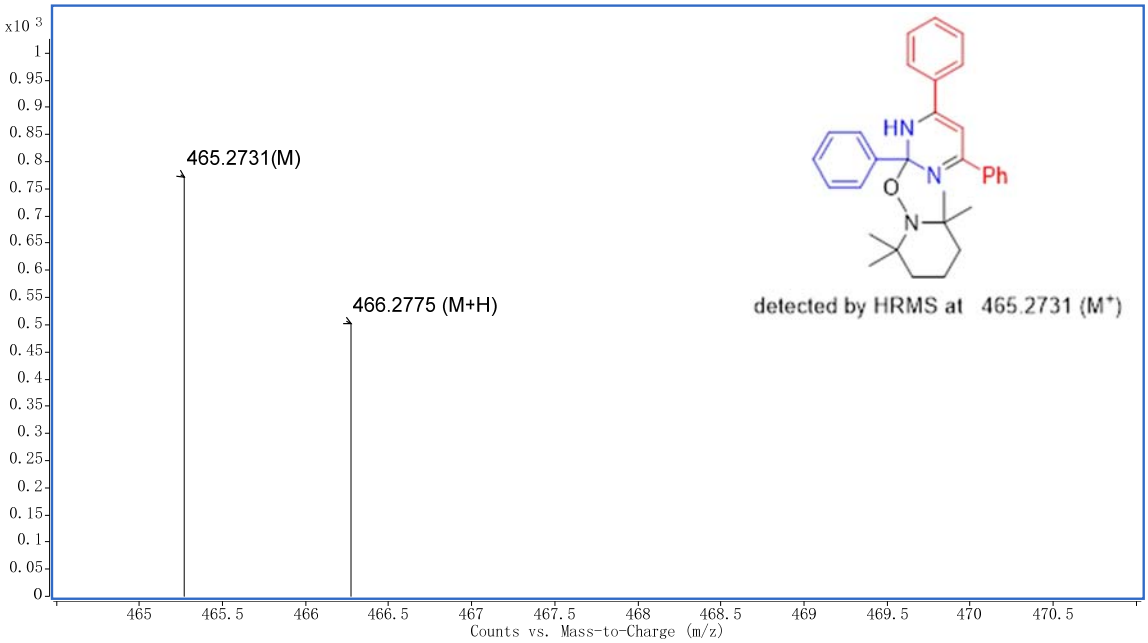
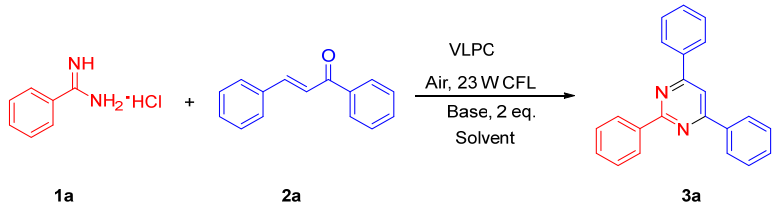


Figure S4

5. Conditions optimization and reaction scope details

Table S1 Conditions screening for the synthesis of 2,4,6-triphenylpyrimidine (**3a**).



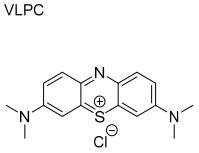
1a **2a** **3a**

Entry	VLPC, 5 mol%	Base	Solvent	Light source	Temp, °C	Time, h	Yield, % [a, b]
1	Eosin Y	K_2CO_3	DMF	23 W CFLs	35	5	21
2	Eosin Y	K_2CO_3	DMF	23 W CFLs	40	6	36
3	Eosin Y	K_2CO_3	DMF	23 W CFLs	45	5	47
4	Eosin Y	K_2CO_3	DMF	23 W CFLs	50	4	56
5	Eosin Y	K_2CO_3	DMF	23 W CFLs	55	4	51
6	Eosin Y	KOH	DMF	23 W CFLs	50	4.5	57
7	Eosin Y	KO^tBu	DMF	23 W CFLs	50	4	53
8	Eosin Y	Na_2CO_3	DMF	23 W CFLs	50	5	10
9	Eosin Y	K_3PO_4	DMF	23 W CFLs	50	5	8
10	Eosin Y	/	DMF	23 W CFLs	50	4	NR
11	Methylene Blue	K_2CO_3	DMF	23 W CFLs	50	4	56
12	Rose Bengal	K_2CO_3	DMF	23 W CFLs	50	4.5	50
13	TPP	K_2CO_3	DMF	23 W CFLs	50	5	51
14	TXO	K_2CO_3	DMF	24 W blue LEDs	50	5	50
15	$Co(dmgH)_2Cl_2$	K_2CO_3	DMF	24 W blue LEDs	50	5	21
16	Eosin Y	K_2CO_3	MeOH	23 W CFLs	50	8	24
17 [c]	Eosin Y	K_2CO_3	MeCN+H_2O	23 W CFLs	50	6	19
18	Eosin Y	K_2CO_3	DMSO	23 W CFLs	50	4	75
19	Eosin Y	K_2CO_3	DMF	In dark.	50	4.5	17
20	Eosin Y	K_2CO_3	DMSO	In dark.	50	4	20
21 [d]	Eosin Y	K_2CO_3	DMSO	23 W CFLs	50	4	16
22	Eosin Y	/	DMSO	23 W CFLs	50	4	NR
23	/	K_2CO_3	DMSO	23 W CFLs	50	4	16
24	Eosin Y, 1 mol%	K_2CO_3	DMSO	23 W CFLs	50	4	20
25	Eosin Y, 2.5 mol%	K_2CO_3	DMSO	23 W CFLs	50	4	75
26	Eosin Y, 10 mol%	K_2CO_3	DMSO	23 W CFLs	50	4	76
27 [e]	Eosin Y, 2.5 mol%	K_2CO_3	DMSO	23 W CFLs	50	4	78
28 [f]	Eosin Y, 2.5 mol%	K_2CO_3	DMSO	23 W CFLs	50	4+1	81
29 [e,f]	Eosin Y, 2.5 mol%	K_2CO_3	DMSO	23 W CFLs	50	4+0.2	80

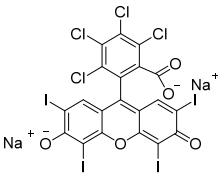
[a] Reagents and conditions: benzenamidine hydrochloride (0.1 mmol), chalcone (0.2 mmol), base (2 eq) and 0.005 mmol VLPC were dissolved in 4 mL solvent and irradiated under four 23w CFLs at 50 °C open to air until the reaction was completed by TLC monitoring. TXO: Thioxanthen-9-one. TPP: 2,4,6-Triphenylpyrylium. NR =

No reaction. [b] Isolated yield. [c] MeCN 4.0 mL and H_2O 0.3 mL was used. [d] Under argon. [e] Under oxygen. [f] The reaction mixture was stirred for about 4 h until the benzamidine hydrochloride was consumed, then irradiated at ambient temperature (40 °C) for about 1 h to complete the transformation.

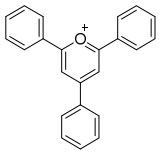
VLPC



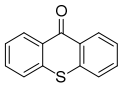
Methylene blue



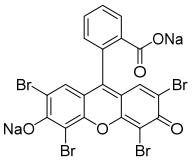
Rose Bengal



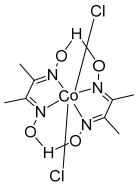
TPP



TXO

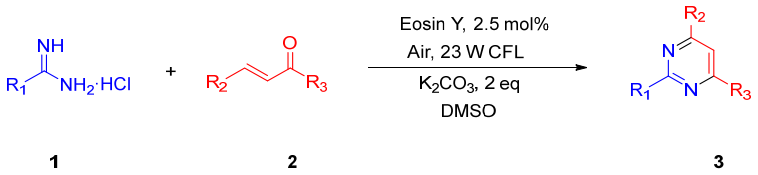


Eosin Y

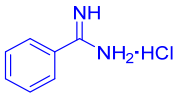
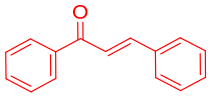
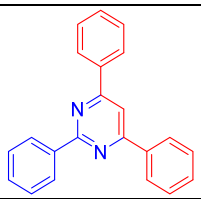
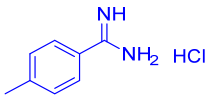
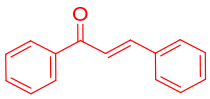
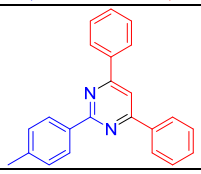


$Co(dmgH)_2Cl_2$

Table S2 Scope of substrates.



1 **2** **3**

entry	Amidine (**1**)	Chalcone (**2**)	Product (**3**)	Method and time[a]	Yield, % [a, b]
1				A, 4 h, 50 °C	75
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	81
2				A, 4 h, 50 °C	72
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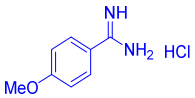
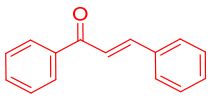
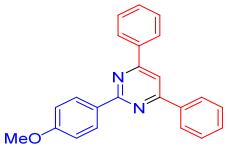
3				A, 4 h, 50°C	47
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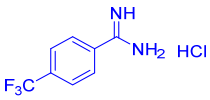
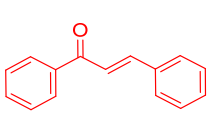
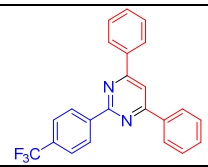
4				A, 4 h, 50 °C, using 2 eq $NaHCO_3$ as base	40
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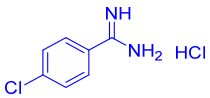
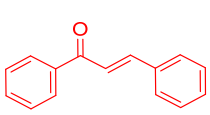
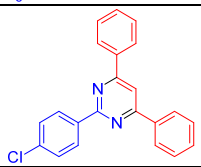
5				A, 4 h, 50 °C	71
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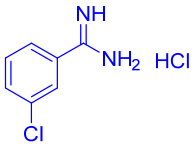
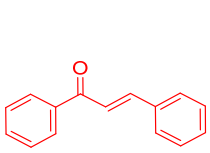
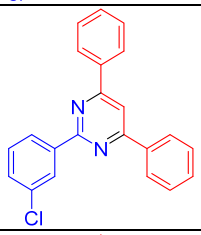
6				A, 4 h, 50 °C	74
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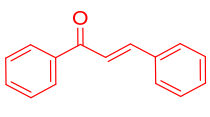
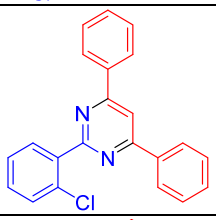
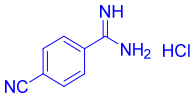
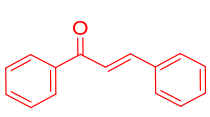
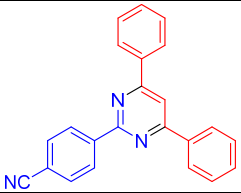
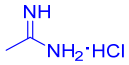
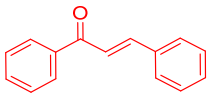
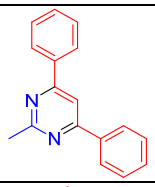
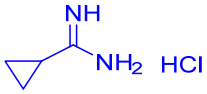
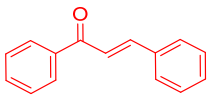
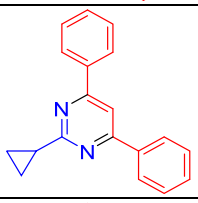
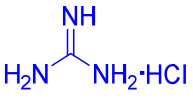
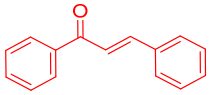
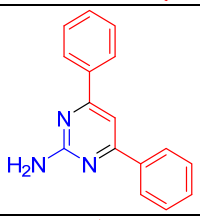
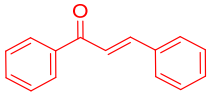
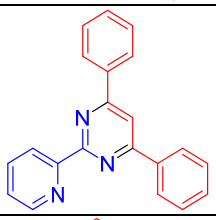
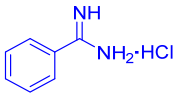
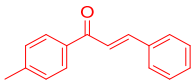
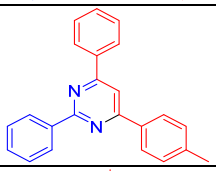
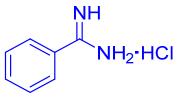
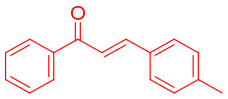
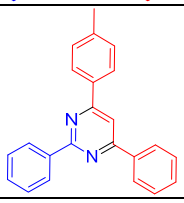
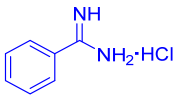
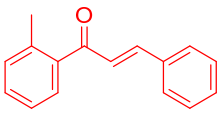
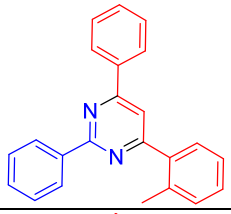
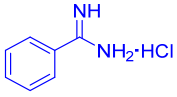
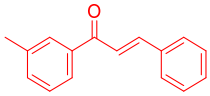
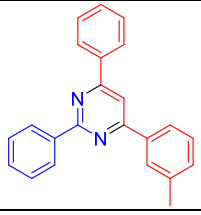
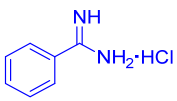
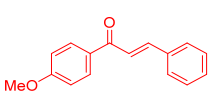
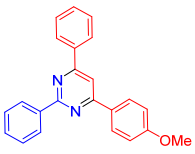
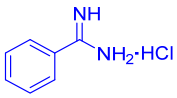
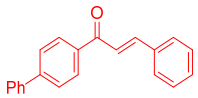
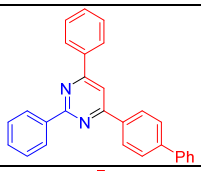
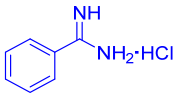
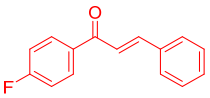
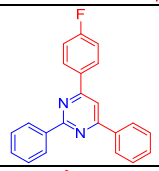
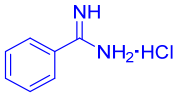
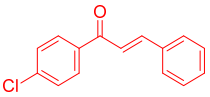
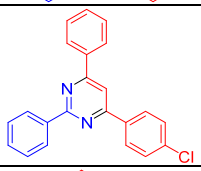
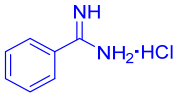
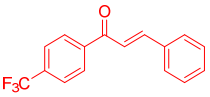
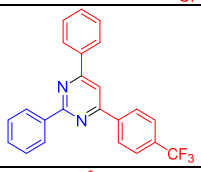
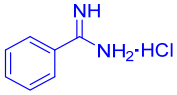
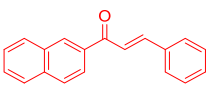
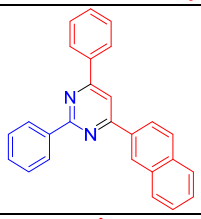
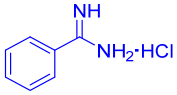
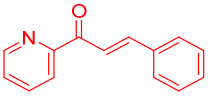
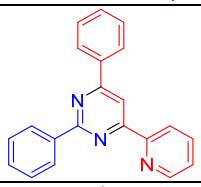
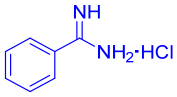
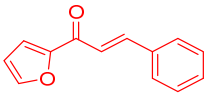
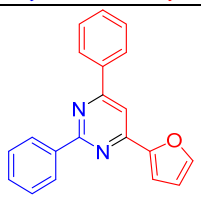
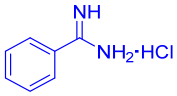
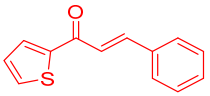
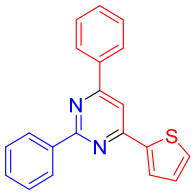
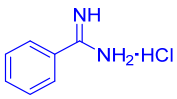
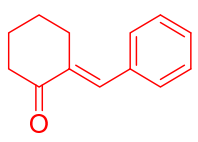
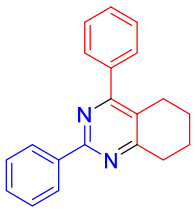
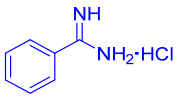
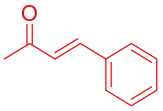
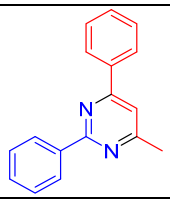
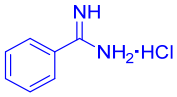
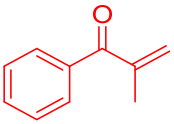
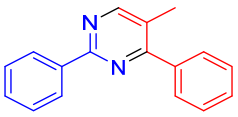
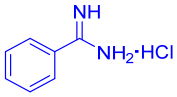
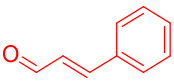
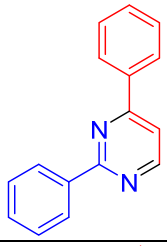
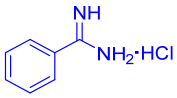
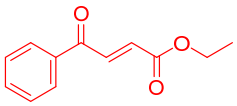
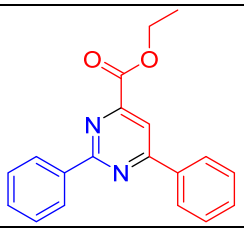
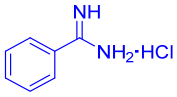
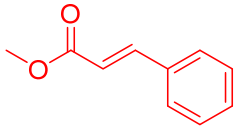
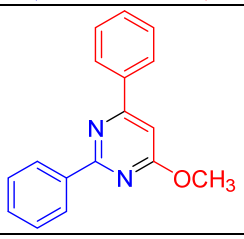
7				A, 4 h, 50 °C	72
				B: 2 h (in dark, 50 °C), 2 h (irradiation, 40 °C)	67
8				A, 4 h, 50 °C	40
				B: 3 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	51

9				A, 3 h, 50 °C	41
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	65
10				A, 3 h, 50 °C	76
				B: 2 h (in dark, 50 °C), 2 h (irradiation, 40 °C)	80
11				A, 4 h, 50 °C	71
				B: 3 h (in dark, 50 °C), 2 h (irradiation, 40 °C)	77
12				A, 28 h, 50 °C	65
				B: 5 h (in dark, 50 °C), 5 h (irradiation, 40 °C),	52
13				A: 4.5 h, 50 °C	65
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	70
14				A: 4.5 h, 50 °C	65
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	62
15				A: 4.5 h, 60 °C	67
				B: 4 h (in dark, 60 °C), 1 h (irradiation, 40 °C)	52
16				A: 4 h, 50 °C	67
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	78
17				A: 5 h, 60 °C	76
				B: 4 h (in dark, 60 °C), 1 h (irradiation, 40 °C)	80

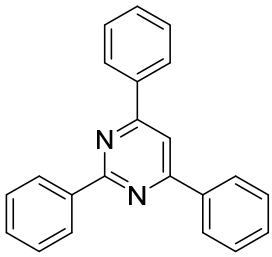
18				A: 3 h, 50 °C	63
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	74
19				A: 4 h, 50 °C	80
				B: 2 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	90
20				A: 4 h, 50 °C	79
				B: 4 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	88
21				A: 4 h, 50 °C	75
				B: 3 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	83
22				A: 4 h, 50 °C	33
				B: 3 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	84
23				A: 4 h, 50 °C	94
				B: 4 h (in dark, 50 °C), 4 h (irradiation, 40 °C)	82
24				A: 2 h, 50 °C	28
				B: 2 h (in dark, 75 °C), 2 h (irradiation, 40 °C)	73
25				A: 4 h, 50 °C	71
				B: 4 h (in dark, 50 °C), 1 h (irradiation, 40 °C)	74
26				A: 4 h, 50 °C	Trace
				B: 4 h (in dark, 100 °C), 2 h (irradiation, 43 °C),	32
				B: 4 h (in dark, 100 °C), 2 h (irradiation, 43 °C), using 2 eq KOH as base	45

27				A: 4 h, 50°C	37
				B: 4 h (in dark, 75 °C), 1h (irradiation, 40 °C)	57
28				A: 4 h, 50 °C	Trace
				B: 4 h (in dark, 70 °C), 2 h (irradiation, 40 °C)	44
29				A: 4 h, 50 °C using 2 eq $NaHCO_3$ as base	44.8
				B: 2 h (in dark, 85 °C), 1 h (irradiation, 40 °C)	67
30				5 h (in dark, 50 °C), 2 h (irradiation, 40 °C)	36
31				4 h (in dark, 50 °C), 2 h (irradiation, 40 °C)	Trace

[a] Reagents and conditions: benzamidine hydrochloride (0.1 mmol), chalcone (0.2 mmol), K_2CO_3 (2 eq) were dissolved in 4 mL DMSO. To the reaction mixture, Eosin Y (0.0025 mmol) was added and irradiated under four 23 w CFLs at 50 °C open to air until the reaction was completed by TLC monitoring (Method A). Otherwise, the reaction mixture was stirred at 50 °C or specified temperature until the benzamidine hydrochloride was consumed, and then VLPC was added and irradiated at ambient temperature (40 °C) for about 1 h to complete the transformation (Method B). [b] Isolated yield.

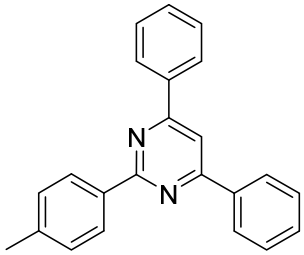
6. The spectral data

All the reported compounds' spectral data (^{1}H NMR, ^{13}C NMR) agree with the cited references. New compound **3f** and dihydropyrimidine intermediate **4a** was characterized by ^{1}H NMR, ^{13}C NMR and HRMS.



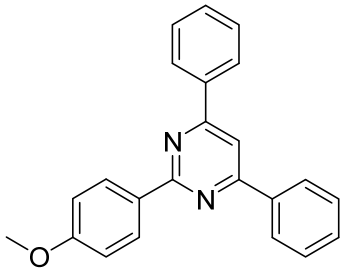
2,4,6-Triphenylpyrimidine (3a) [4]

Yield: 25.0 mg, 80%. White solid, m.p. 190-191 °C (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (dd, *J* = 7.9, 1.6 Hz, 2H), 8.30 (dd, *J* = 7.8, 1.7 Hz, 4H), 8.03 (s, 1H), 7.61 – 7.49 (m, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 164.7, 138.3, 137.7, 130.9, 130.8, 129.1, 128.62, 128.59, 127.4, 110.5. IR(KBr) υ_{max}: 3095, 3065, 3032, 2923, 2852, 1589, 1570, 1530, 1496, 1361, 738, 681, 630 cm^{-1}.



4,6-Diphenyl-2-(*p*-tolyl) pyrimidine (3b) [5]

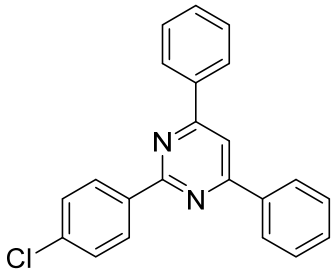
Yield: 27.0 mg, 84%. White solid, m.p. 179-182 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.1 Hz, 2H), 8.30 (dd, *J* = 8.0, 1.5 Hz, 4H), 7.99 (s, 1H), 7.61 – 7.52 (m, 6H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.47 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.83, 164.75, 141.0, 137.8, 135.6, 130.8, 129.4, 129.0, 128.6, 127.4, 110.2, 21.7. IR(KBr) υ_{max}: 3084, 3057, 3030, 2949, 2916, 1586, 1566, 1529, 1494, 1360, 758, 685 cm^{-1}.



2-(4-Methoxyphenyl)-4,6-diphenylpyrimidine (3c) [6]

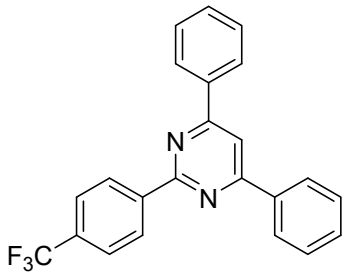
Yield: 25.4 mg, 75%. White solid, m.p. 140-141 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.8 Hz, 2H), 8.33 – 8.25 (m,

4H), 7.96 (s, 1H), 7.61 – 7.50 (m, 6H), 7.06 (d, *J* = 8.8 Hz, 2H), 3.91 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 164.4, 162.0, 137.8, 131.1, 130.8, 130.2, 129.0, 127.4, 113.9, 109.8, 55.5. IR(KBr) υ_{max}: 3052, 2958, 2933, 2839, 1607, 1588, 1567, 1532, 1360, 1248, 764, 685 cm^{-1}.



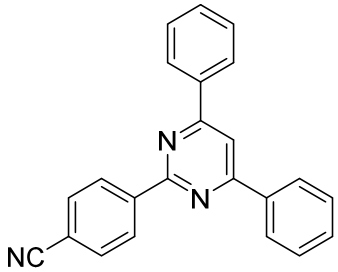
2-(4-Chlorophenyl)-4,6-diphenylpyrimidine (3d) [5]

Yield: 25.0 mg, 73%. White solid, m.p. 219-221 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.5 Hz, 2H), 8.31 – 8.23 (m, 4H), 8.01 (s, 1H), 7.60 – 7.53 (m, 6H), 7.50 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 163.7, 137.5, 137.0, 136.8, 131.0, 130.0, 129.1, 128.8, 127.4, 110.6. IR(KBr) υ_{max}: 3087, 3067, 3038, 1586, 1565, 1526, 1361, 759, 683 cm^{-1}.



4,6-Diphenyl-2-(4-(trifluoromethyl) phenyl) pyrimidine (3e) [7]

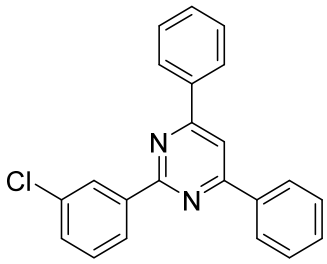
Yield: 22.8 mg, 60%. White solid, m.p. 205-206 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.1 Hz, 2H), 8.33 – 8.24 (m, 4H), 8.05 (s, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 7.63 – 7.52 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 163.2, 141.4, 137.2, 132.2 (q, *J* = 32.2 Hz), 131.0, 129.0, 128.7, 127.3, 125.4 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 272.1 Hz), 111.0. ^{19}F NMR (565 MHz, $CDCl_3$) δ -63.14. IR(KBr) υ_{max}: 3065, 2926, 1595, 1567, 1534, 1497, 1329, 1116, 1068, 766, 685 cm^{-1}.



4-(4,6-Diphenyl-2-pyrimidinyl) benzonitrile (3f)

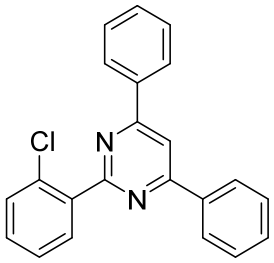
Yield: 18.0 mg, 54%. White solid, m.p. 240-242 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.1 Hz, 2H), 8.27 (dd, *J* = 6.3, 2.7 Hz, 4H), 8.07 (s, 1H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.58 (dd, *J* = 5.0, 1.7 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.20, 162.82, 142.37, 137.13, 132.41, 131.28, 129.18,

129.06, 127.42, 119.11, 113.99, 111.30. IR(KBr) υ_{max}: 3058, 2221, 1586, 1576, 1561, 1528, 1360, 765, 687 cm^{-1}. HRMS calcd for $C_{23}H_{16}N_3^+$ $(M+H)^+$: 334.13387, found: 334.13324.



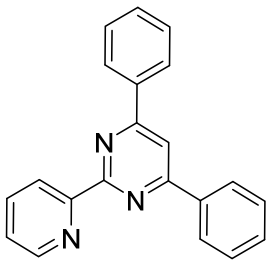
2-(3-Chlorophenyl)-4,6-diphenylpyrimidine (3g) [8]

Yield: 30.5 mg, 89%. White solid, m.p. 156-160 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.71 (d, *J* = 1.7 Hz, 1H), 8.63 (dt, *J* = 6.7, 1.7 Hz, 1H), 8.31 – 8.27 (m, 4H), 8.05 (s, 1H), 7.61 – 7.54 (m, 6H), 7.51 – 7.46 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 163.4, 140.2, 137.4, 134.7, 131.1, 130.7, 129.8, 129.1, 128.6, 127.4, 126.7, 110.9. IR(KBr) υ_{max}: 3091, 3063, 3040, 1586, 1567, 1526, 1360, 759, 732, 686 cm^{-1}.



2-(2-Chlorophenyl)-4,6-diphenylpyrimidine (3h) [9]

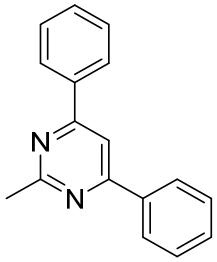
Yield: 23.0 mg, 67%. White solid, m.p. 72-74 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, CDCl3) δ 8.26 (dd, *J* = 7.6, 1.9 Hz, 4H), 8.08 (s, 1H), 8.05 – 8.00 (m, 1H), 7.59 – 7.51 (m, 7H), 7.45 – 7.38 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.6, 165.0, 138.2, 137.4, 133.3, 132.3, 131.0, 130.9, 130.5, 129.1, 127.6, 126.9, 110.6. IR(KBr) υ_{max}: 3063, 3046, 1586, 1574, 1527, 1495, 1364, 744, 682 cm^{-1}.



4,6-Diphenyl-2-(pyridin-2-yl)pyrimidine (3i) [5]

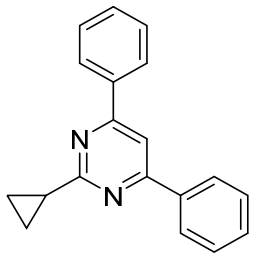
Yield: 16.7 mg, 54%. Yellow solid, m.p. 144-146 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (dt, *J* = 4.7, 1.4 Hz, 1H), 8.73 (dt, *J* = 7.9, 1.1 Hz, 1H), 8.34 – 8.25 (m, 4H), 8.12 (s, 1H), 7.90 (td, *J* = 7.7, 1.8 Hz, 1H), 7.60

– 7.50 (m, 6H), 7.43 (ddd, *J* = 7.5, 4.7, 1.2 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.6, 164.1, 155.7, 150.2, 137.4, 136.9, 131.0, 129.1, 127.6, 124.8, 124.3, 112.0. IR(KBr) υ_{max}: 3054, 3003, 1575, 1564, 1528, 1362, 752, 689 cm^{-1}. HRMS calcd for $C_{21}H_{16}N_3^+$ $(M+H)^+$: 310.13387, found: 310.13339.



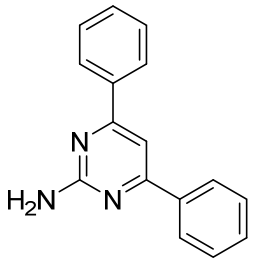
2-Methyl-4,6-diphenylpyrimidine (3j) [7]

Yield: 16.0 mg, 65%. White solid, m.p. 90–92 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.13 (dd, *J* = 7.6, 1.9 Hz, 4H), 7.89 (s, 1H), 7.56 – 7.49 (m, 6H), 2.87 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.7, 165.0, 137.7, 130.8, 129.1, 127.4, 110.2, 26.6. IR(KBr) υ_{max}: 3052, 3038, 2960, 2928, 2856, 1584, 1574, 1531, 1367, 745, 686 cm^{-1}.



2-Cyclopropyl-4,6-diphenylpyrimidine (3k) [5]

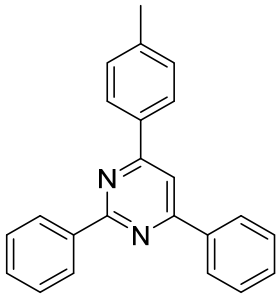
Yield: 21.9 mg, 80%. White solid, m.p. 89-90 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR ($CDCl_3$, 600 MHz): δ 8.16-8.13 (m, 4H), 7.85 (s, 1H), 7.55-7.51 (m, 6H), 2.45-2.38 (m, 1H), 1.34-1.31 (m, 2H), 1.14-1.09 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.3, 164.5, 137.8, 130.7, 129.0, 127.3, 109.6, 18.7, 10.8. IR(KBr) υ_{max}:3087, 3061, 3009, 2964, 2930, 1586, 1575, 1536, 1365, 761, 686 cm^{-1}.



4,6-Diphenylpyrimidin-2-amine (3l) [10]

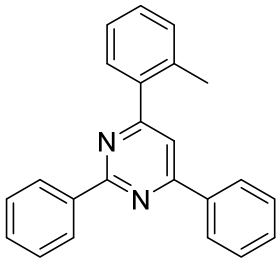
Yield: 19.0 mg, 77%. White solid, m.p. 140-142 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 – 8.04 (m, 4H), 7.53 – 7.48 (m, 6H),

7.47 (s, 1H), 5.33 (d, J = 21.0 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.4, 163.7, 137.9, 130.6, 128.9, 127.3, 104.5. IR(KBr) υ_{max}: 3468, 3318, 3067, 3042, 1603, 1566, 1543, 1364, 765, 692 cm^{-1}.



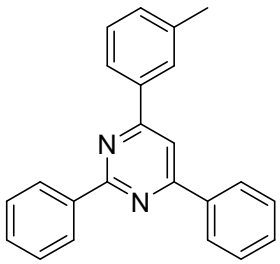
2,4-Diphenyl-6-(*p*-tolyl)pyrimidine (3ab) [11]

Yield: 22.6mg, 70%. White solid, m.p. 167-170 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74 (d, J = 6.8 Hz, 2H), 8.30 (d, J = 6.6 Hz, 2H), 8.21 (d, J = 8.1 Hz, 2H), 8.00 (s, 1H), 7.62 – 7.50 (m, 6H), 7.37 (d, J = 7.9 Hz, 2H), 2.47 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 164.8, 164.6, 141.3, 138.4, 137.8, 134.9, 130.8, 130.7, 129.8, 129.0, 128.6, 128.6, 127.4, 127.3, 110.1, 21.6. IR(KBr) υ_{max}: 3063, 3030, 2914, 1589, 1569, 1527, 1510, 1496, 1361, 748, 687 cm^{-1}.



2,4-Diphenyl-6-(*o*-tolyl)pyrimidine (3ac) [11]

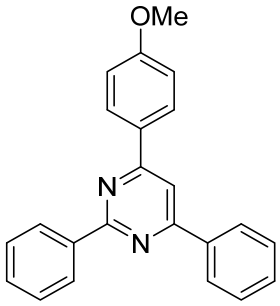
Yield: 16.7mg, 52%. Yellow liquid (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.68 (dd, J = 7.7, 1.9 Hz, 2H), 8.28 (dd, J = 7.7, 1.9 Hz, 2H), 7.75 (s, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.54 (dd, J = 21.4, 7.3 Hz, 6H), 7.43 – 7.34 (m, 3H), 2.58 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.3, 164.3, 164.2, 138.8, 138.2, 137.5, 136.6, 131.4, 130.9, 130.8, 129.8, 129.5, 129.1, 128.6, 127.4, 126.3, 114.5, 20.9. IR(KBr) υ_{max}: 3057, 2919, 1533, 1489, 1444, 1390, 1006, 756, 691 cm^{-1}.



2,4-Diphenyl-6-(*m*-tolyl)pyrimidine (3ad) [11]

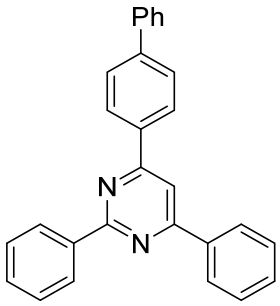
Yield: 25.3mg, 78%. White solid, m.p. 127-129 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 – 8.70 (m, 2H), 8.31 (dd, J = 7.8, 1.6

Hz, 2H), 8.11 (s, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 8.01 (s, 1H), 7.60 – 7.51 (m, 6H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 2.52 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.1, 164.8, 164.6, 138.8, 138.4, 137.74, 137.68, 131.7, 130.9, 130.8, 129.05, 128.97, 128.62, 128.59, 128.0, 127.4, 124.6, 110.6, 21.8. IR(KBr) υ_{max}: 3054, 3030, 2919, 2856, 1588, 1571, 1531, 1353, 748, 686 cm^{-1}.



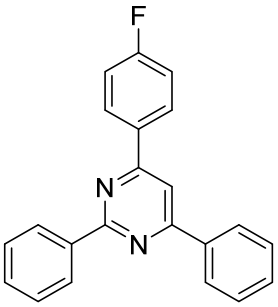
4-(4-Methoxyphenyl)-2,6-diphenylpyrimidine (3ae) [11]

Yield: 27.0 mg, 80%. White solid, m.p. 139-140 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (500 MHz, $CDCl_3$)34 δ 8.72 (dt, *J* = 8.4, 2.2 Hz, 2H), 8.31 – 8.26 (m, 4H), 7.96 (s, 1H), 7.59 – 7.51 (m, 6H), 7.10 – 7.05 (m, 2H), 3.91 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.6, 164.5, 164.4, 162.1, 138.4, 137.9, 130.8, 130.7, 130.1, 129.0, 128.9, 128.58, 128.55, 127.4, 114.4, 109.6, 55.6. IR(KBr) υ_{max}: 3052, 3003, 2923, 2848, 1612, 1588, 1528, 1513, 1366, 1171, 755, 689 cm^{-1}.



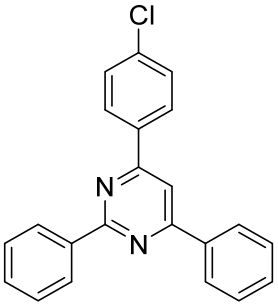
4-([1,1'-Biphenyl]-4-yl)-2,6-diphenylpyrimidine (3af) [11]

Yield: 28.5 mg, 74%. White solid, m.p. 177-179 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.82 – 8.70 (m, 2H), 8.43 – 8.36 (m, 2H), 8.32 (dt, *J* = 8.4, 2.2 Hz, 2H), 8.06 (s, 1H), 7.85 – 7.76 (m, 2H), 7.75 – 7.64 (m, 2H), 7.62 – 7.52 (m, 6H), 7.53 – 7.47 (m, 2H), 7.45 – 7.39 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 164.7, 164.5, 143.7, 140.5, 138.3, 137.7, 136.5, 130.9, 130.8, 129.1, 128.63, 128.61, 128.0, 127.9, 127.8, 127.4, 127.3, 110.3. IR(KBr) υ_{max}: 3089, 3061, 3030, 1589, 1570, 1526, 1362, 748, 687 cm^{-1}.



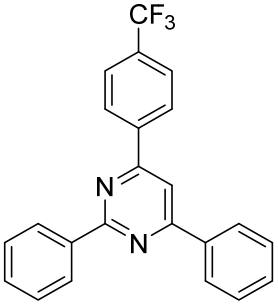
4-(4-Fluorophenyl)-2,6-diphenylpyrimidine (3ag) [11]

Yield: 29.3 mg, 90%. White solid, m.p. 164-166 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 – 8.69 (m, 2H), 8.30 (qd, *J* = 8.7, 6.4 Hz, 4H), 7.97 (d, *J* = 1.1 Hz, 1H), 7.61 – 7.50 (m, 6H), 7.28 – 7.22 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 164.7 (d, *J* = 251.1 Hz), 164.7, 163.8, 138.2, 137.6, 133.8 (d, *J* = 2.9 Hz) , 131.0, 130.9, 129.4 (d, *J* = 8.7 Hz), 129.1 128.6, 128.6, 127.4, 116.1 (d, *J* = 21.8 Hz), 110.0. ^{19}F NMR (565 MHz, $CDCl_3$) δ -110.41 IR(KBr) υ_{max}: 3052, 3029, 2962, 2925, 1572, 1530, 1361, 1231, 834, 750, 687 cm^{-1}.



4-(4-Chlorophenyl)-2,6-diphenylpyrimidine (3ah) [11]

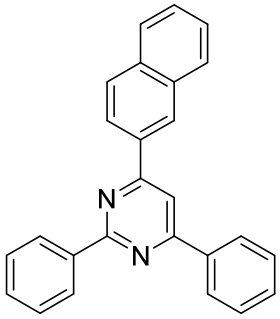
Yield: 30.0 mg, 88%. White solid, m.p. 165-166 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 6.5 Hz, 2H), 8.29 (d, *J* = 6.9 Hz, 2H), 8.25 (d, *J* = 8.3 Hz, 2H), 7.98 (s, 1H), 7.59 – 7.51 (m, 8H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 164.6, 163.5, 138.0, 137.4, 137.0, 136.0, 130.9, 130.8, 129.2, 129.0, 128.6, 128.49, 128.47, 127.3, 110.0. IR(KBr) υ_{max}: 3063, 3046, 1586, 1574, 1527, 1495, 1364, 744, 682 cm^{-1}.



2,4-Diphenyl-6-(4-(trifluoromethyl)phenyl)pyrimidine (3ai) [12]

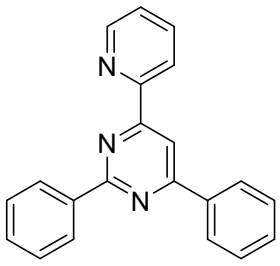
Yield: 31.4 mg, 83%. White solid, m.p. 136-140 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.75 – 8.66 (m, 2H), 8.38 (d, *J* = 8.1 Hz, 2H), 8.33 – 8.24 (m, 2H), 8.01 (s, 1H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.63 – 7.50 (m, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 165.4, 164.9, 163.4, 141.1, 137.9, 137.3, 132.6 (q, *J* = 32.6 Hz), 131.2, 131.0, 129.1, 128.7, 128.6, 127.8, 127.5, 126.0 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 272.4Hz), 110.7. ^{19}F NMR (565 MHz, $CDCl_3$) δ -63.26. IR(KBr) υ_{max}: 3066, 3038, 2940, 1591, 1570, 1530, 1518, 1364, 1323, 1118, 739 cm^{-1}.



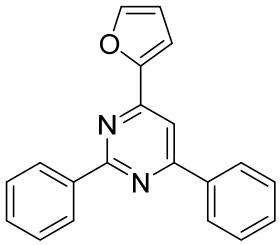
4-(Naphthalen-2-yl)-2,6-diphenylpyrimidine (3aj) [11]

Yield: 29.9 mg, 83.5%. White solid, m.p. 157-159 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 (d, *J* = 6.9 Hz, 2H), 8.77(s, 1H), 8.40 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.37 – 8.29 (m, 2H), 8.14 (s, 1H), 8.06 – 8.03 (m, 1H), 8.02 (d, *J* = 8.6 Hz, 1H), 7.95 – 7.89 (m, 1H), 7.65 – 7.42 (m, 8H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.9, 164.8, 164.7, 138.4, 137.7, 135.0, 134.8, 133.5, 130.9, 130.8, 129.2, 129.1, 128.8, 128.7, 128.6, 127.9, 127.6, 127.47, 127.46, 126.7, 124.4, 110.7. IR(KBr) υ_{max}: 3061, 3038, 1589, 1570, 1531, 1496, 1372, 853, 756, 692 cm^{-1}.



2,4-Diphenyl-6-(pyridin-2-yl)pyrimidine (3ak) [13]

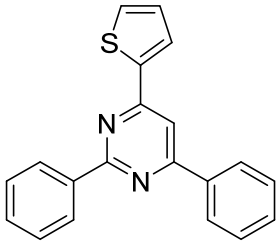
Yield: 25.4 mg, 82%. White solid, m.p. 144-146 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 – 8.70 (m, 5H), 8.44 – 8.35 (m, 2H), 7.92 (td, *J* = 7.7, 1.8 Hz, 1H), 7.61 – 7.50 (m, 6H), 7.47 – 7.38 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.3, 164.4, 163.7, 154.8, 149.6, 138.2, 137.5, 137.2, 131.0, 130.8, 129.0, 128.63, 128.55, 127.6, 125.4, 122.1, 110.7. IR(KBr) υ_{max}: 3091, 3058, 3034, 3007, 1574, 1566, 1533, 1364, 743, 686 cm^{-1}.



4-(Furan-2-yl)-2,6-diphenylpyrimidine (3al) [14]

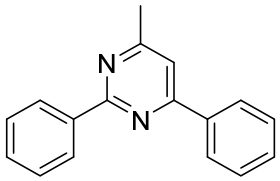
Yield: 21.9 mg, 73%. White solid, m.p. 158-160 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (dt, *J* = 4.0, 2.2 Hz, 2H), 8.30 (dt, *J* =

4.2, 2.3 Hz, 2H), 7.95 (s, 1H), 7.65 (d, *J* = 0.9 Hz, 1H), 7.59 – 7.50 (m, 6H), 7.46 (dd, *J* = 3.4, 0.5 Hz, 1H), 6.64 (dd, *J* = 3.4, 1.7 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.8, 164.6, 156.5, 152.8, 144.9, 138.1, 137.5, 131.0, 130.8, 129.0, 128.6, 128.5, 127.4, 112.6, 112.2, 108.2. IR(KBr) υ_{max}: 3061, 3036, 1601, 1558, 1531, 1482, 748, 698, 684 cm^{-1}.



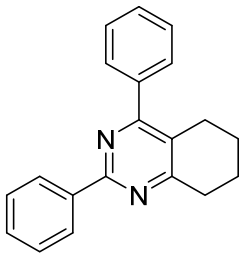
2,4-Diphenyl-6-(thiophen-2-yl)pyrimidine (3am) [12]

Yield: 22.2 mg, 74%. White solid, m.p. 160-164 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (500 MHz, $CDCl_3$) 8.73 – 8.63 (m, 2H), 8.30 – 8.22 (m, 2H), 7.93 (dd, *J* = 3.7, 1.0 Hz, 1H), 7.86 (s, 1H), 7.60 – 7.45 (m, 7H), 7.21 (dd, *J* = 5.0, 3.7 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 164.6, 159.8, 143.5, 137.9, 137.5, 131.0, 130.9, 129.9, 129.0, 128.6, 128.4, 127.4, 127.2, 108.6. IR(KBr) υ_{max}: 3071, 3038, 2926, 2852, 1586, 1568, 1524, 1494, 1364, 748, 687 cm^{-1}.



4-Methyl-2,6-diphenylpyrimidine (3an) [15]

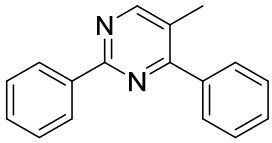
Yield: 14.1 mg, 57%. White solid, m.p. 93-94 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, CDCl3) δ 8.60 (dd, J = 7.9, 1.6 Hz, 2H), 8.22 (dd, J = 7.7, 1.8 Hz, 2H), 7.56 – 7.49 (m, 6H), 7.48 (s, 1H), 2.66 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.9, 164.5, 163.8, 138.3, 137.4, 130.8, 130.6, 129.0, 128.6, 128.5 127.3, 114.1, 24.8. IR(KBr) υ_{max}: 3061, 3034, 2919, 1590, 1571, 1533, 1366, 749, 690 cm^{-1}.



2,4-Diphenyl-5,6,7,8-tetrahydroquinazoline (3ao) [16]

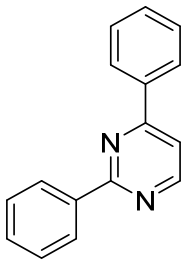
Yield: 12.8 mg, 45%. White solid, m.p. 103-105 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 8.0, 1.8 Hz, 2H), 7.69 – 7.63 (m, 2H), 7.53 – 7.41 (m, 6H), 3.04 (t, *J* = 6.6 Hz, 2H), 2.80 (t, *J* = 6.2 Hz, 2H), 2.00 – 1.92 (m, 2H), 1.79 (dtd, *J* = 9.2, 6.1, 3.0 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.9,

165.2, 161.6, 138.8, 138.3, 130.1, 129.2, 129.1, 128.5, 128.3, 128.2, 125.6, 32.9, 27.1, 23.1, 22.6. IR(KBr) υ_{max}: 3089, 3065, 3030, 2944, 2926, 2858, 1538, 1497, 1394, 750, 695 cm^{-1}.



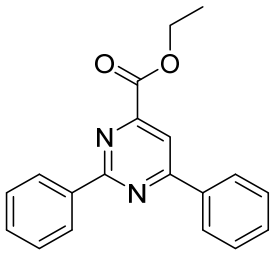
5-Methyl-2,4-diphenylpyrimidine (3ap) [17]

Yield: 10.8 mg, 44%. White solid, m.p. 83-84 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (s, 1H), 8.51 (dd, *J* = 10.5, 8.7 Hz, 2H), 7.74 (d, *J* = 6.9 Hz, 2H), 7.55 – 7.44 (m, 6H), 2.43 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.0, 162.6, 159.3, 138.6, 137.9, 130.4, 129.4, 129.2, 128.6, 128.5, 128.2, 125.7, 17.2. IR(KBr) υ_{max}: 3058, 3028, 2973, 2923, 2856, 1562, 1534, 1491, 1421, 756, 691 cm^{-1}.



2,4-Diphenylpyrimidine (3aq) [18]

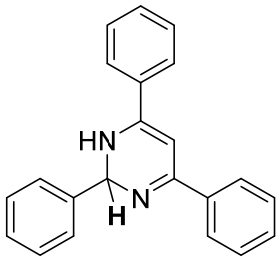
Yield: 15.5 mg, 67%. Yellow solid, m.p. 63-65 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.85 (d, *J* = 5.2 Hz, 1H), 8.59 (dd, *J* = 7.7, 2.0 Hz, 2H), 8.24 (dd, *J* = 7.3, 2.4 Hz, 2H), 7.61 (d, *J* = 5.2 Hz, 1H), 7.57 – 7.49 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 164.0, 158.0, 138.0, 137.1, 131.1, 130.8, 129.1, 128.7, 128.4, 127.3, 114.7. IR(KBr) υ_{max}: 3054, 3036, 1591, 1561, 1542, 1424, 1378, 747, 688 cm^{-1}.



Ethyl 2,6-diphenylpyrimidine-4-carboxylate (3ar) [19]

Yield: 11.0 mg, 36%. White solid, m.p. 94-95 ℃ (petroleum ether/dichloromethane = 2:1, V/V). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.66 (dd, *J* = 6.4, 3.2 Hz, 2H), 8.31 (dd, *J* = 6.5, 3.1 Hz, 2H), 8.29 (s, 1H), 7.61 – 7.55 (m, 3H), 7.53 (dd, *J* = 5.1, 2.0 Hz, 3H), 4.55 (q, *J* = 7.1 Hz, 2H), 1.51 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.2, 165.4, 165.1, 156.4, 137.3, 136.5, 131.6, 131.3, 129.2, 128.8, 128.7, 127.6, 114.2,

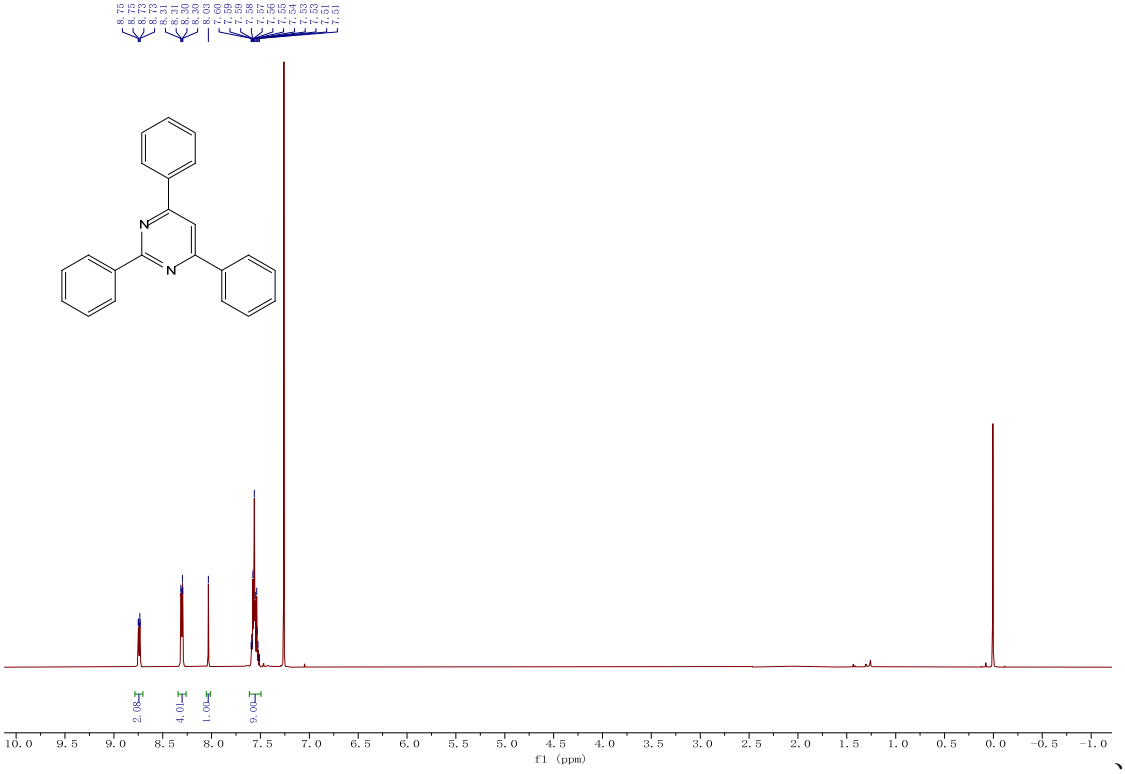
62.6, 14.4. IR(KBr) υ_{max}: 3057, 2984, 2906, 1744, 1569, 1541, 1376, 1250, 740, 691 cm^{-1}.

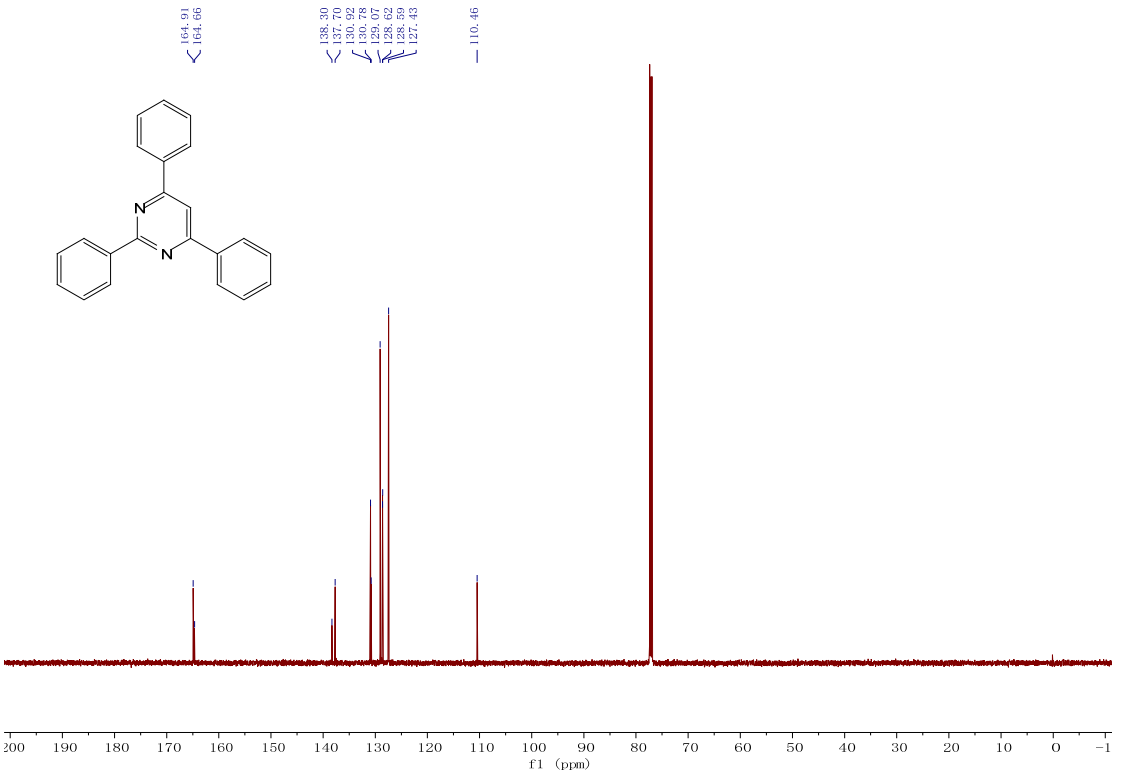


2,4,6-Triphenyl-1,2-dihydropyrimidine (**4a**).
Yield: 23.3 mg, 75%. Yellow solid, ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.5 Hz, 4H), 7.50 – 7.42 (m, 5H), 7.42 – 7.36 (m, 4H), 7.32 (t, *J* = 6.9 Hz, 2H), 5.77 – 5.33 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.0, 135.6, 130.8, 129.1, 128.7, 128.4, 128.4, 128.1, 127.2, 126.6, 125.5. IR(KBr) υ_{max}: 3410, 3054, 3026, 1567, 1527, 1362, 748, 691 cm^{-1}. HRMS calcd for $C_{22}H_{19}N_2^+$ $(M+H)^+$: 311.15428, found: 311.15381.

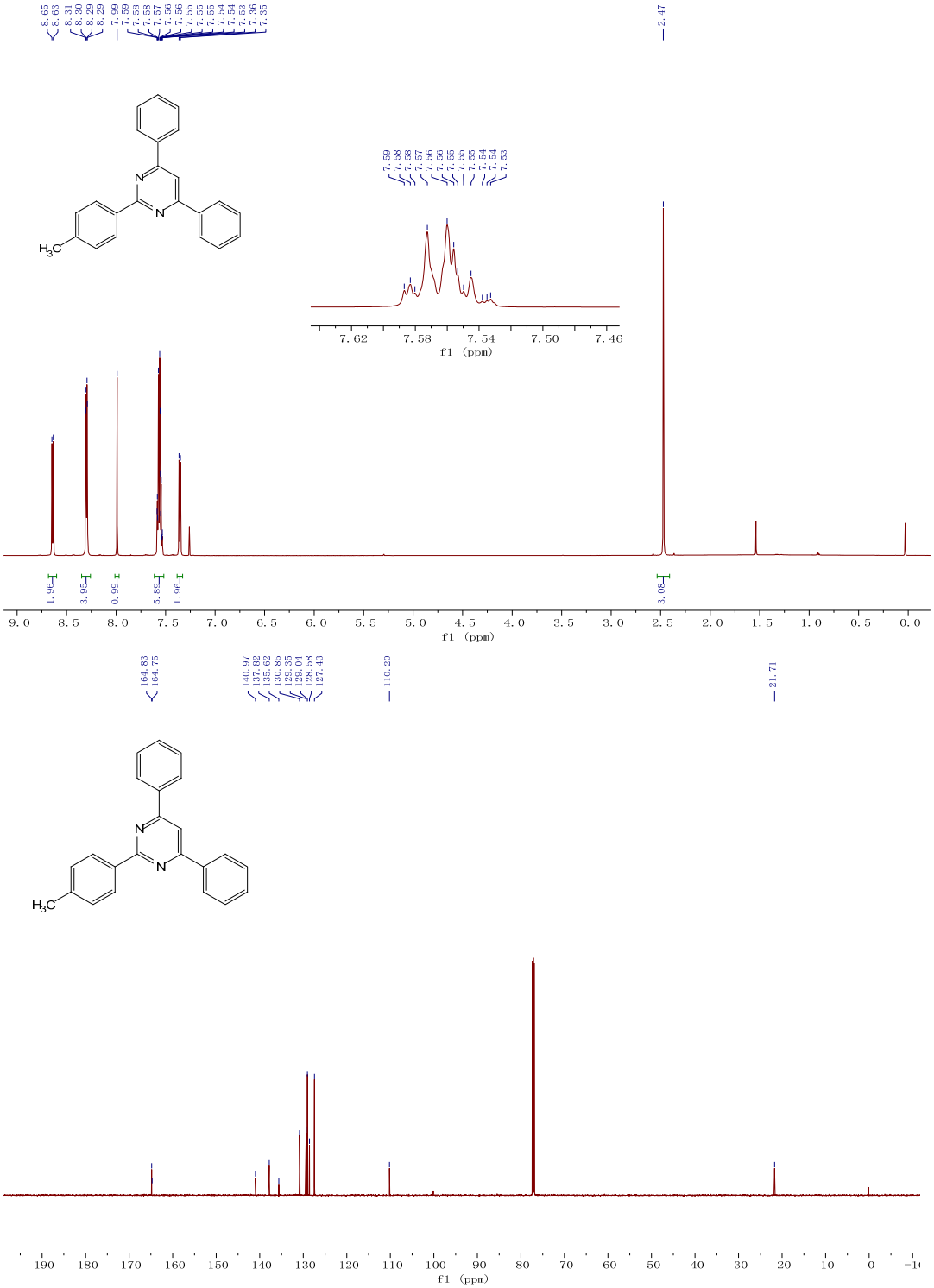
7. The NMR Charts

2,4,6-Triphenylpyrimidine (**3a**)

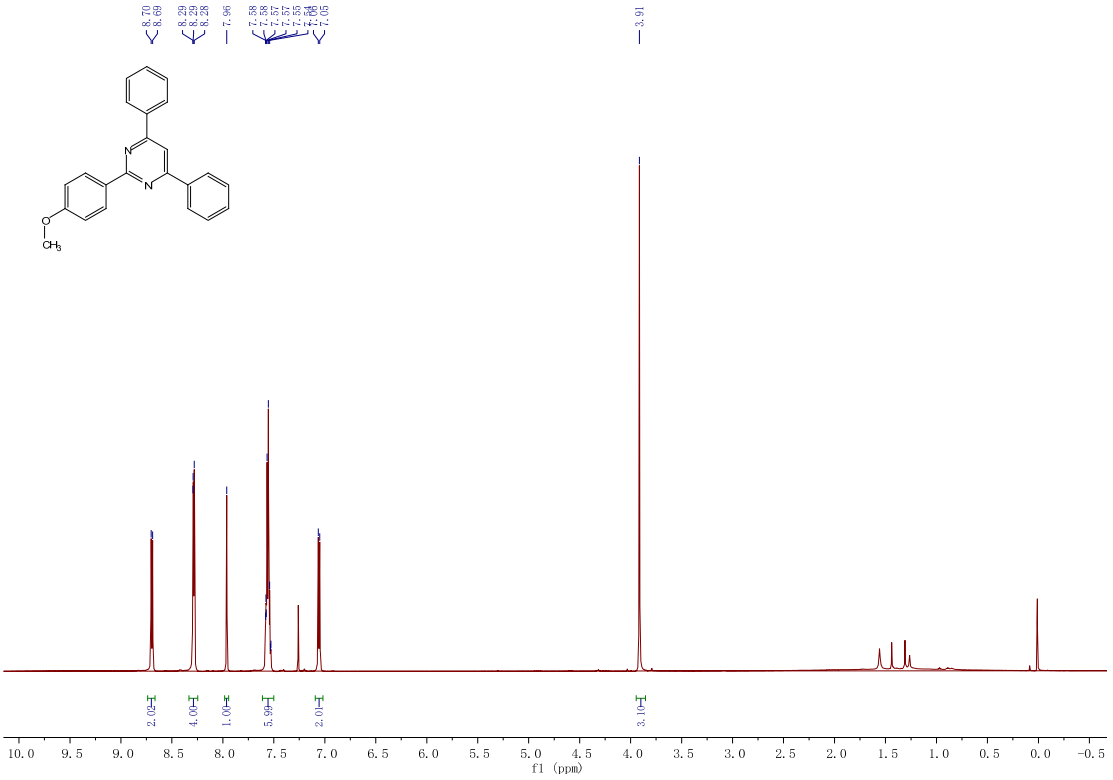


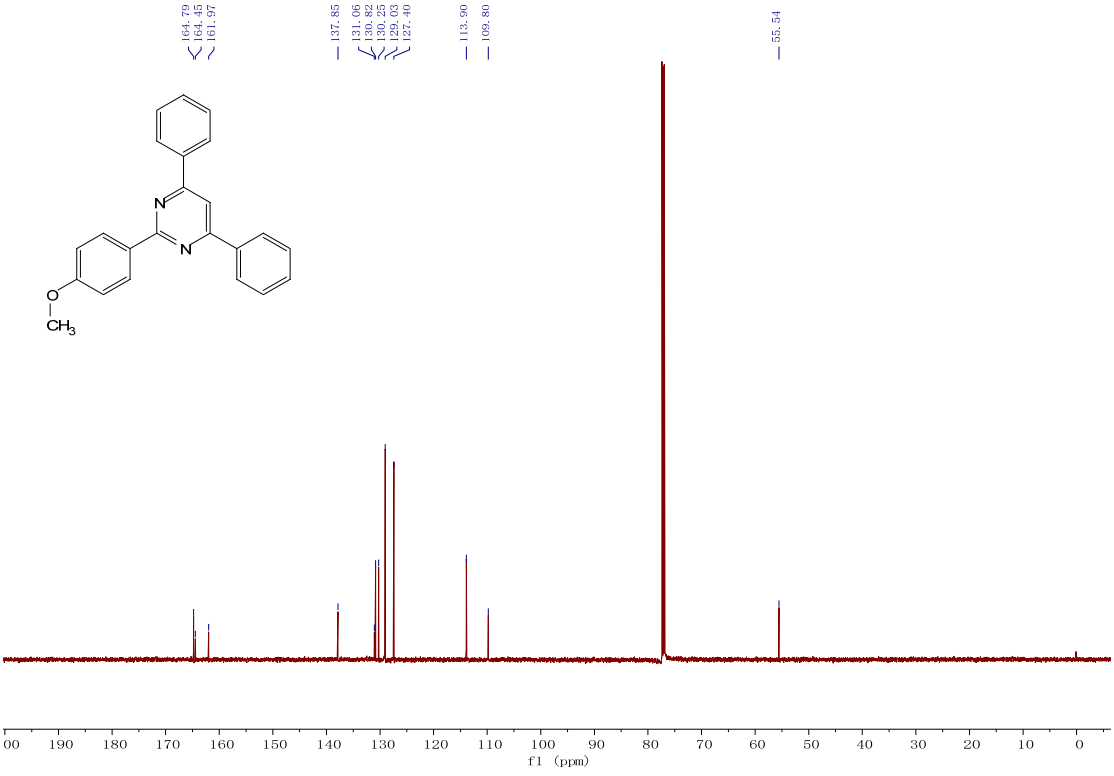


4,6-Diphenyl-2-(p-tolyl) pyrimidine (**3b**)

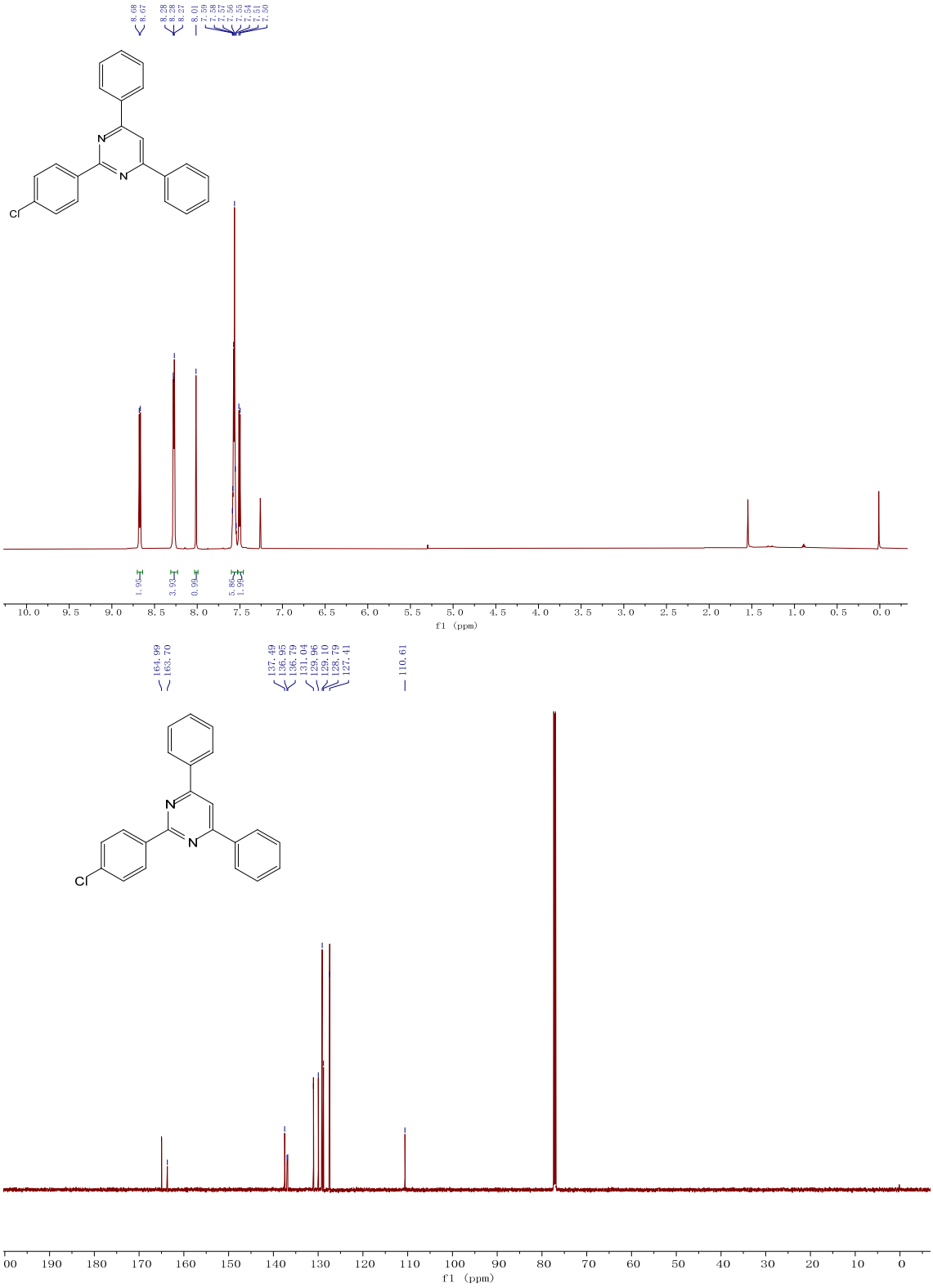


2-(4-Methoxyphenyl)-4,6-diphenylpyrimidine (**3c)**





2-(4-Chlorophenyl)-4,6-diphenylpyrimidine (**3d**)



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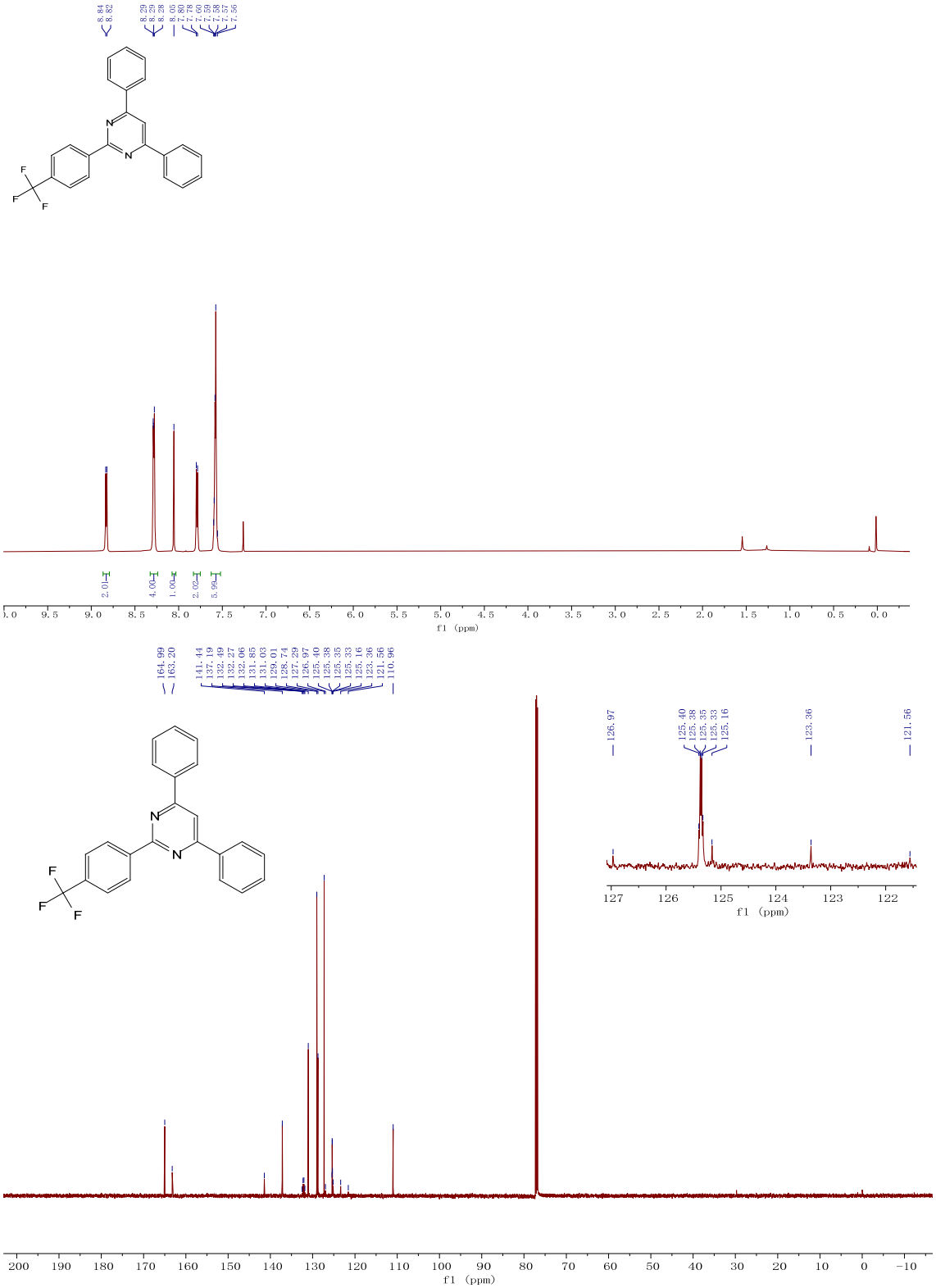
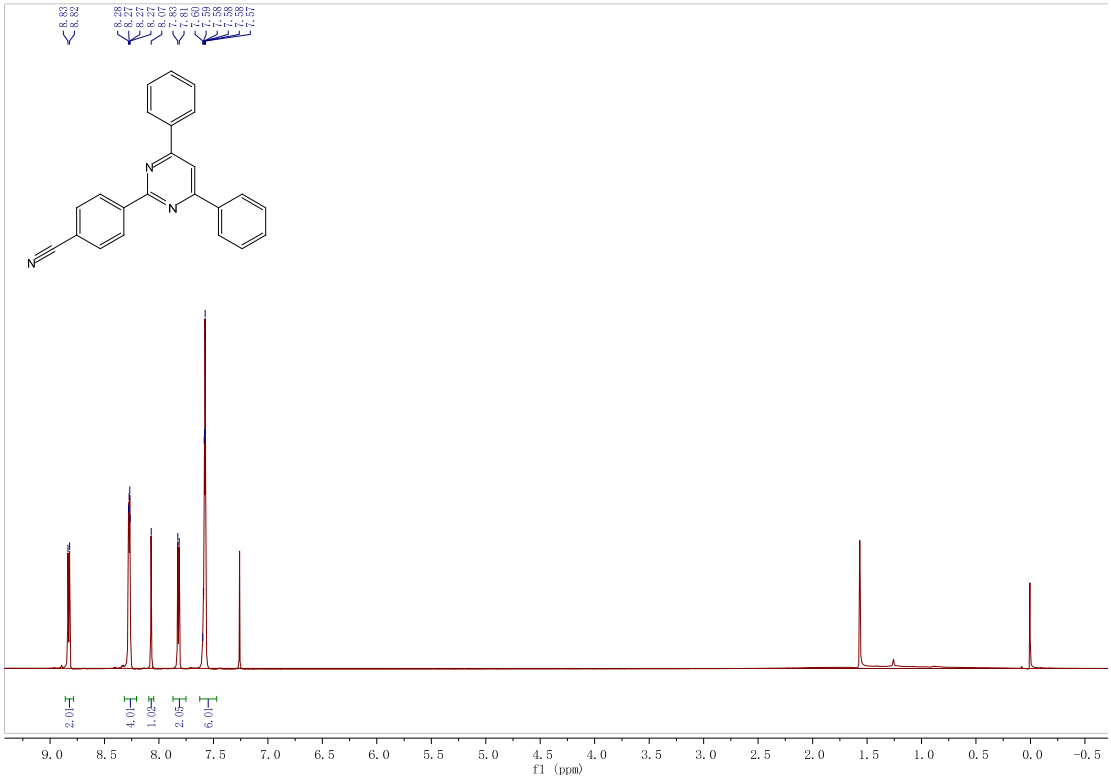
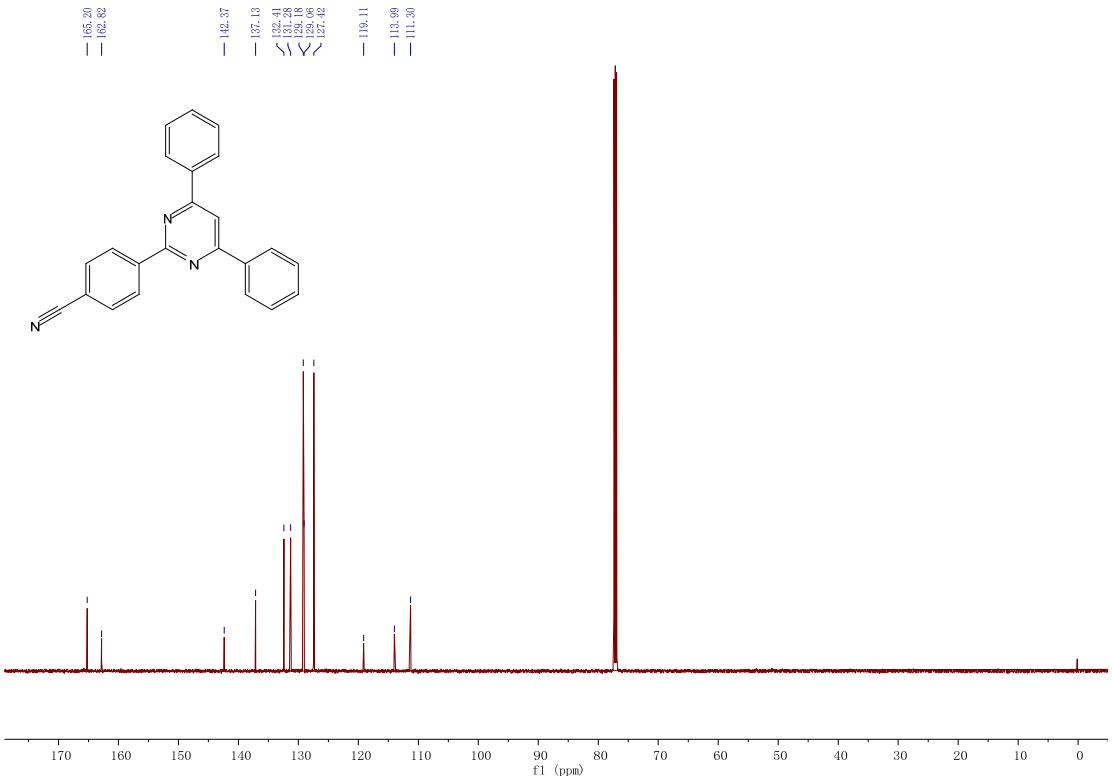
4,6-Diphenyl-2-(4-(trifluoromethyl) phenyl) pyrimidine (**3e)**

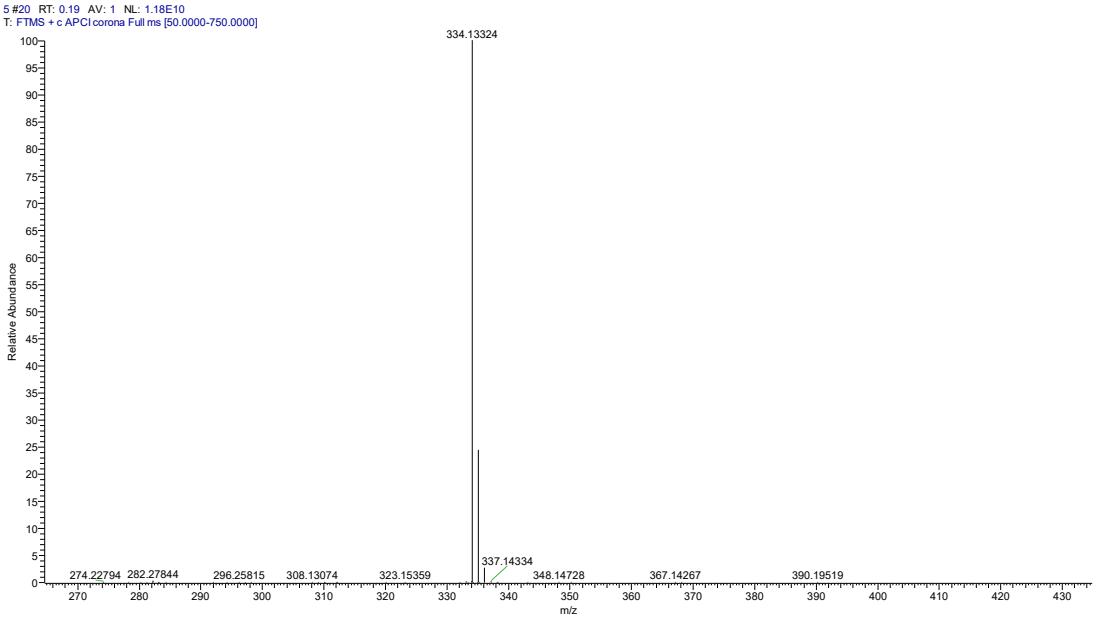


4-(4,6-Diphenyl-2-pyrimidinyl) benzonitrile (**3f**)

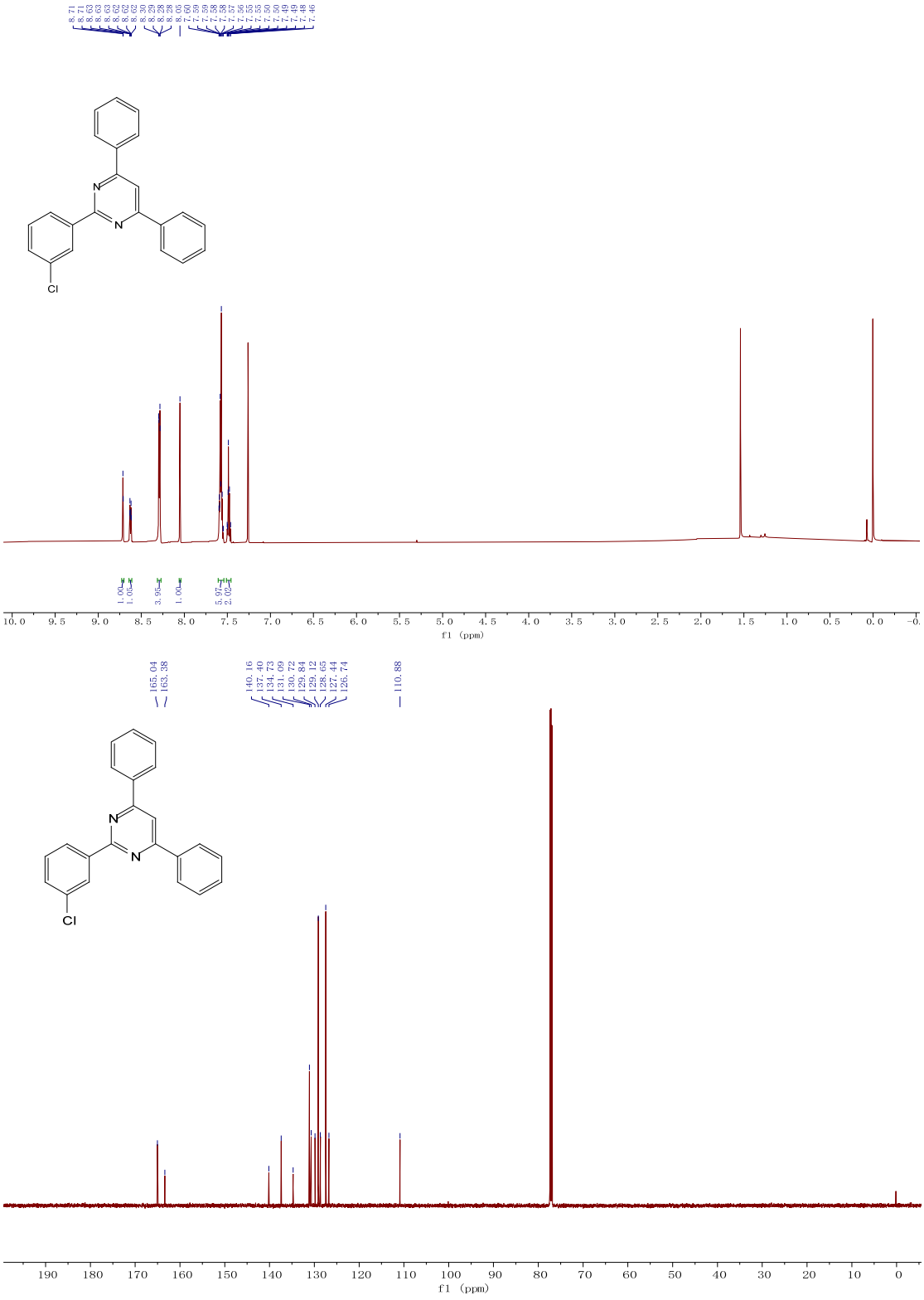



165.20
162.82
142.37
137.13
132.41
131.28
129.18
128.96
122.42
119.11
113.99
111.30
N
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

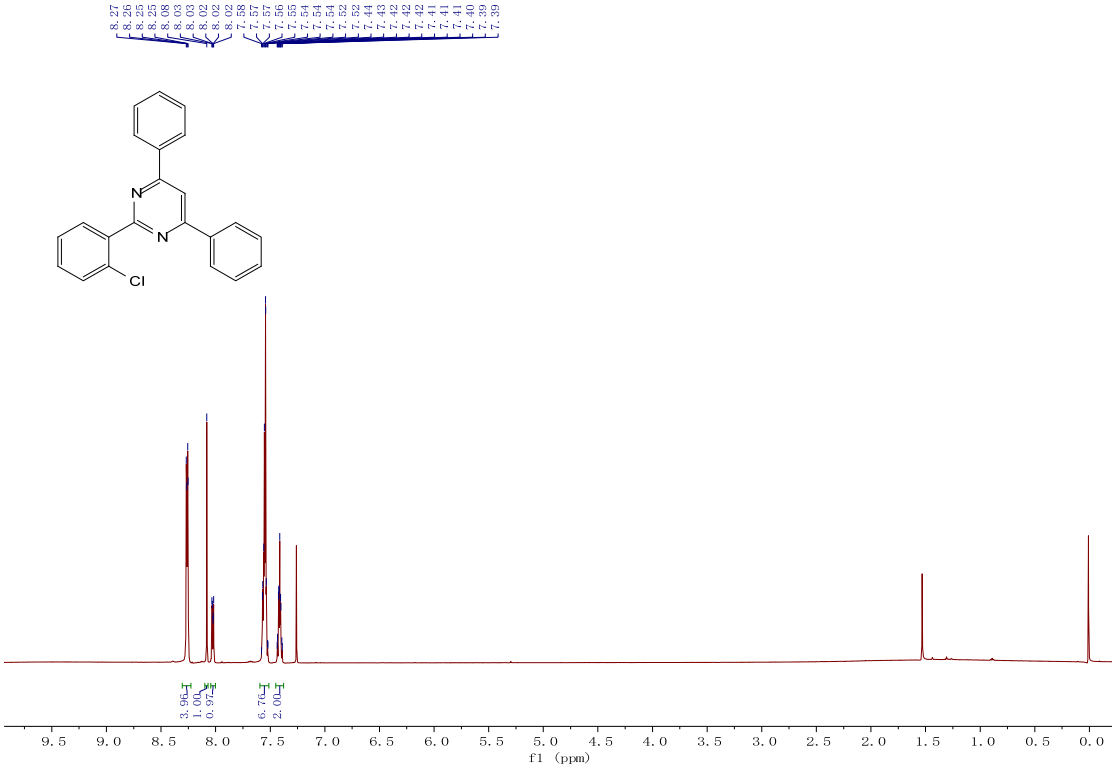
HRMS

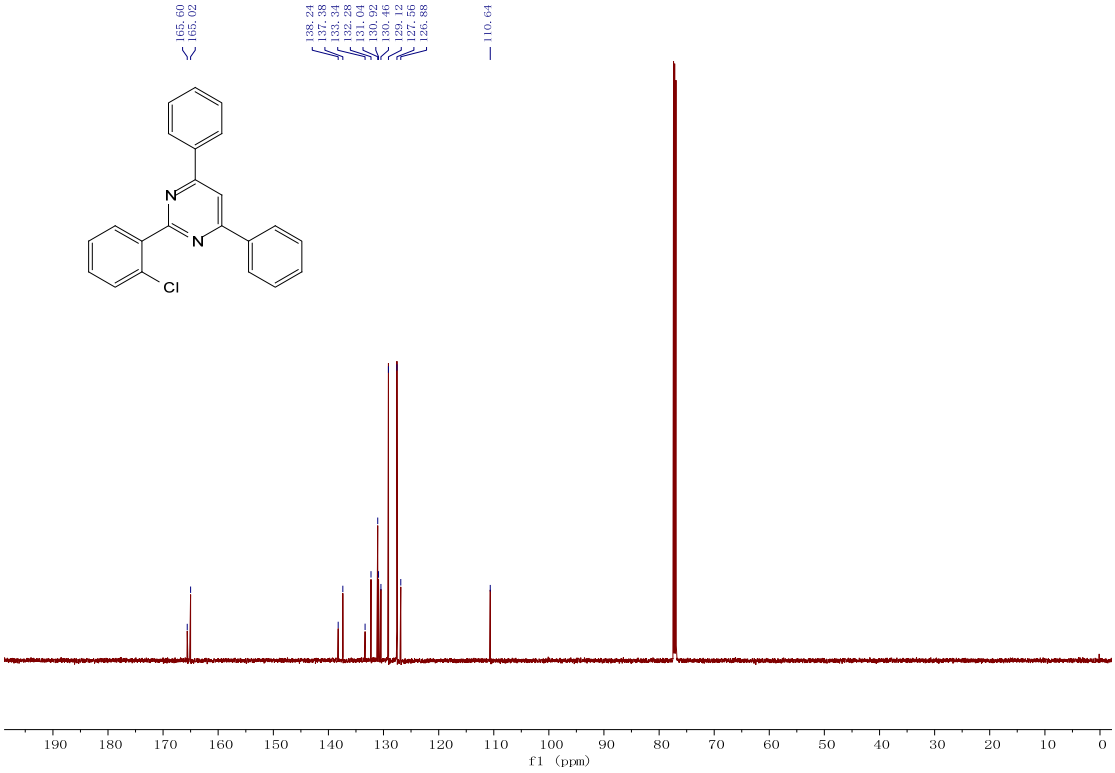

5 #20 RT: 0.19 AV: 1 NL: 1.18E10
T: FTMS + c APCI corona Full ms [50.0000-750.0000]
334.13324
337.14334
274.22794
282.27844
296.25815
308.13074
323.15359
348.14728
367.14267
390.19519
Relative Abundance
m/z

2-(3-Chlorophenyl)-4,6-diphenylpyrimidine (**3g)**

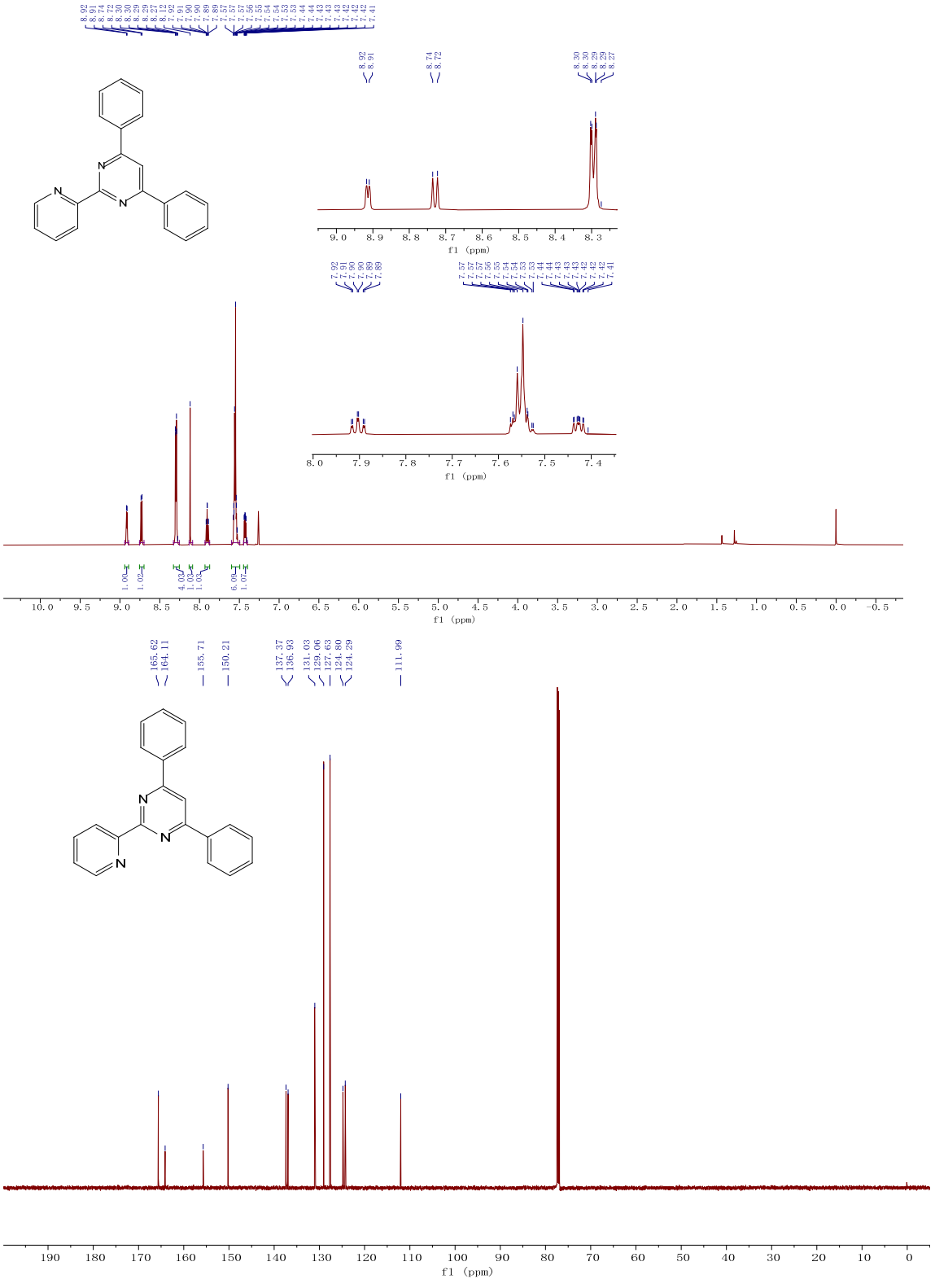


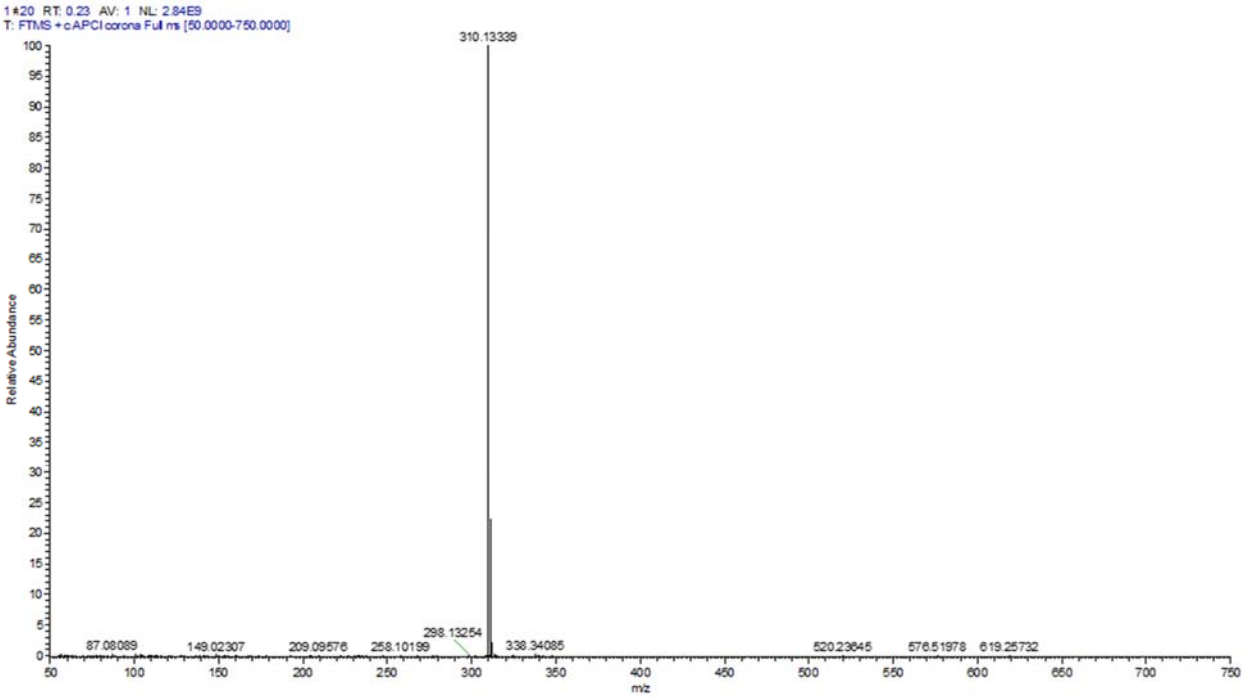
2-(2-Chlorophenyl)-4,6-diphenylpyrimidine (**3h**)



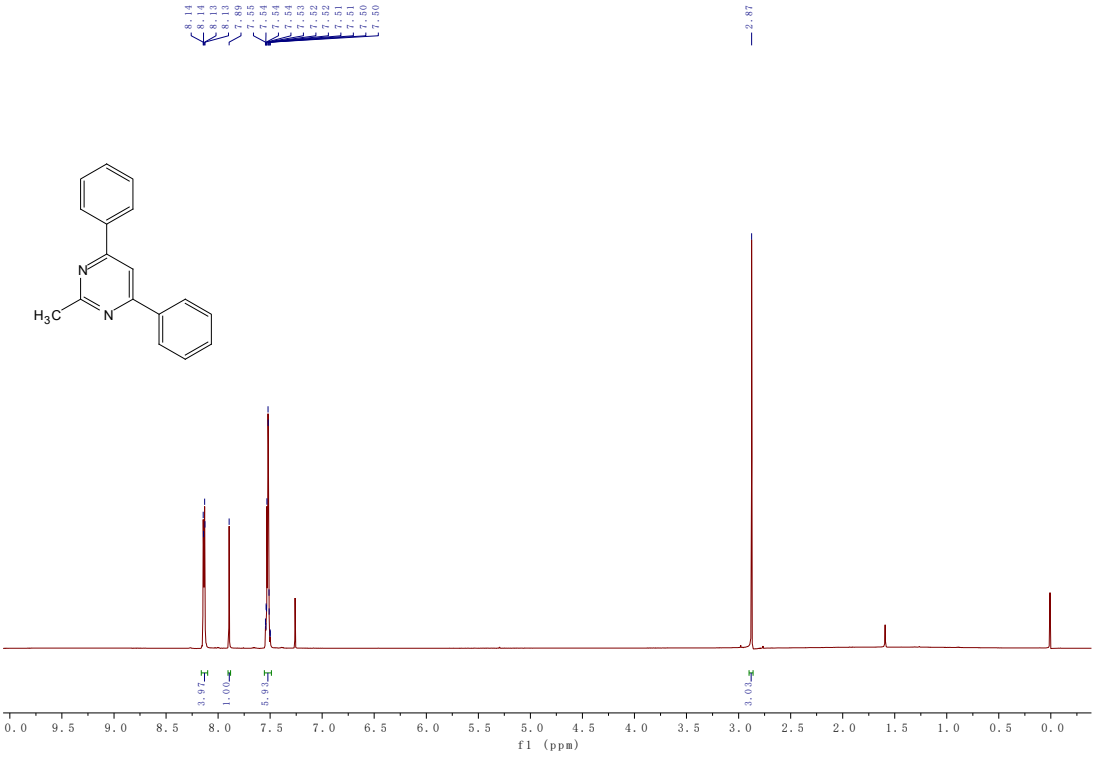


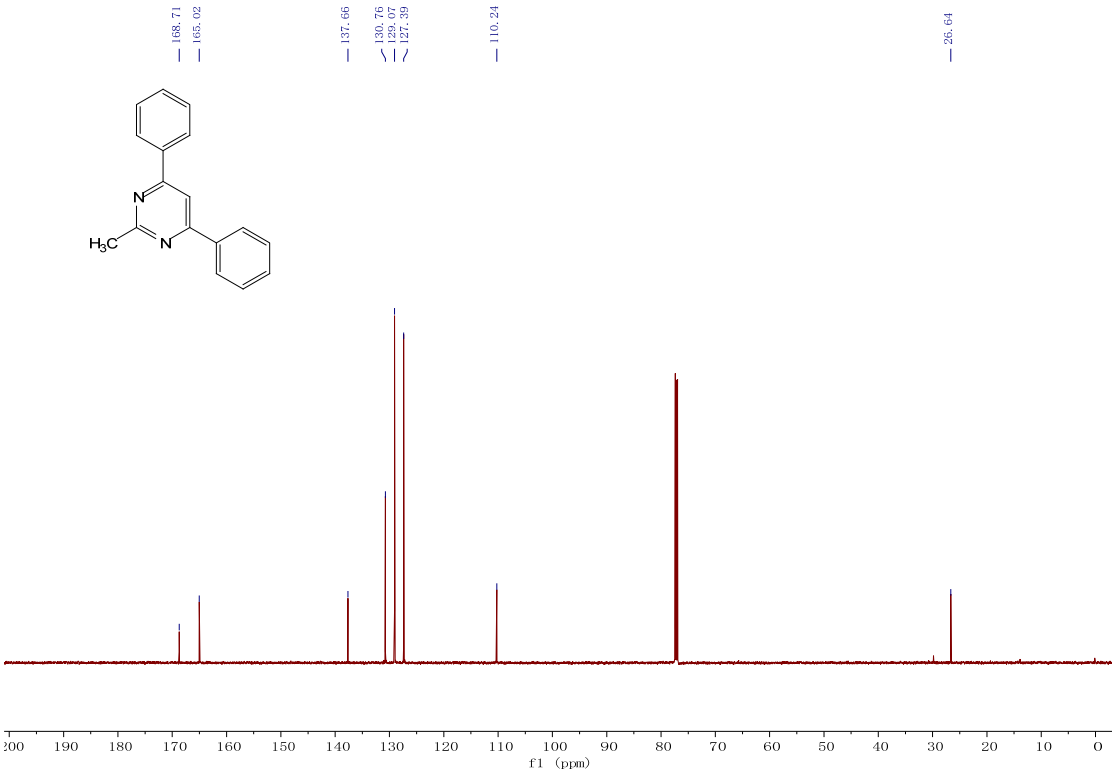
4,6-Diphenyl-2-(pyridin-2-yl)pyrimidine（**3i**）



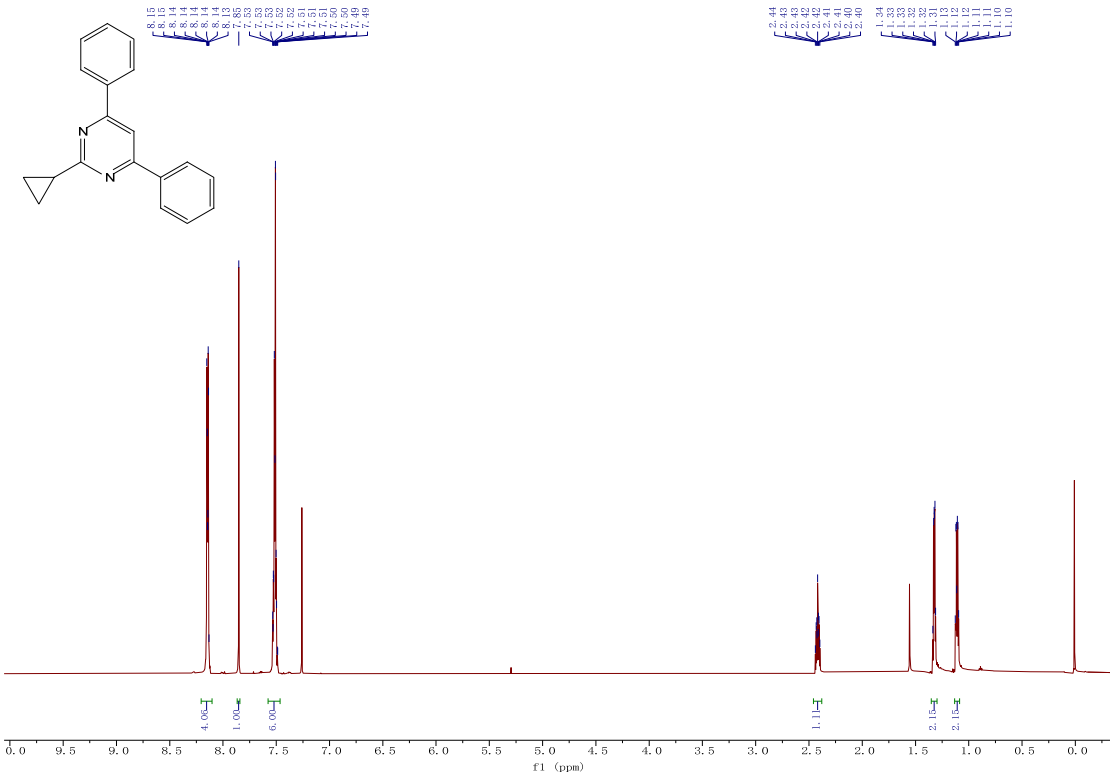


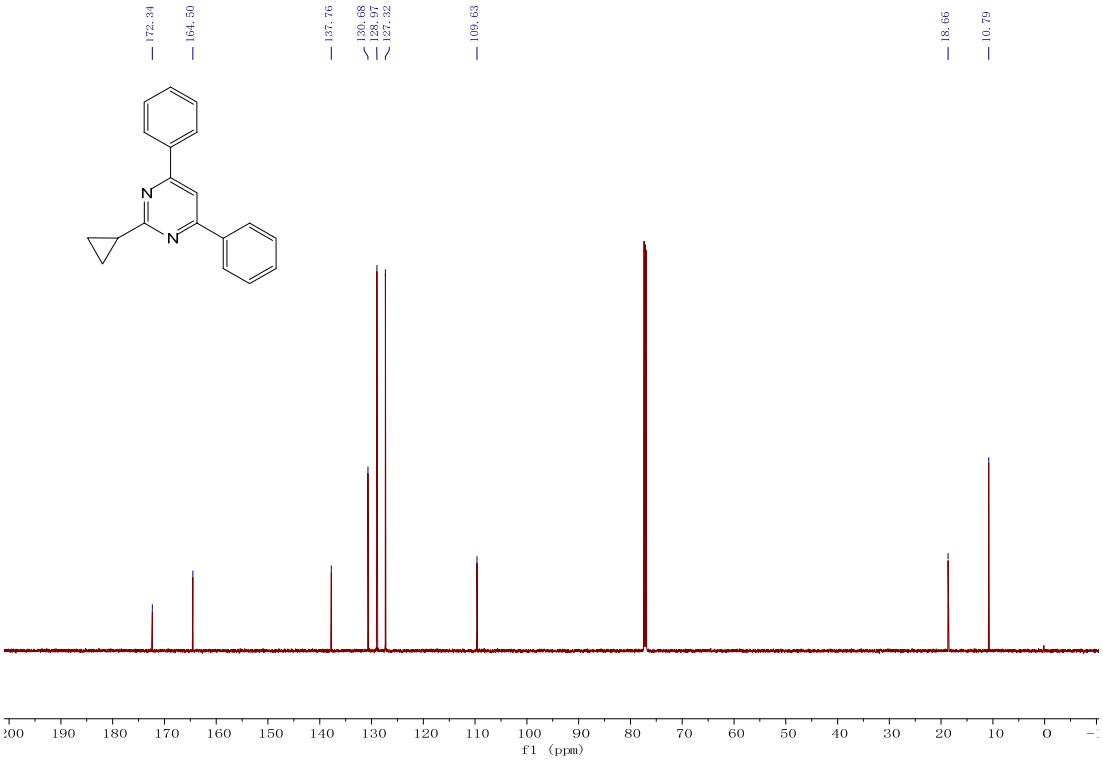
2-Methyl-4,6-diphenylpyrimidine (**3j**)



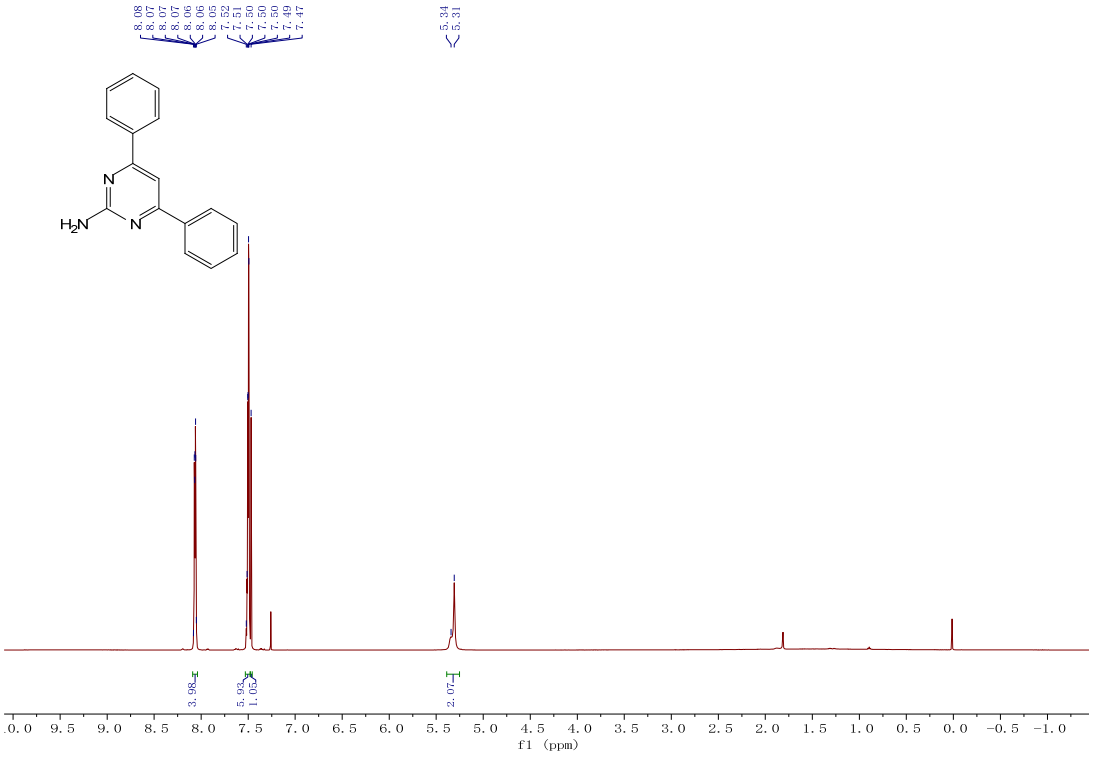


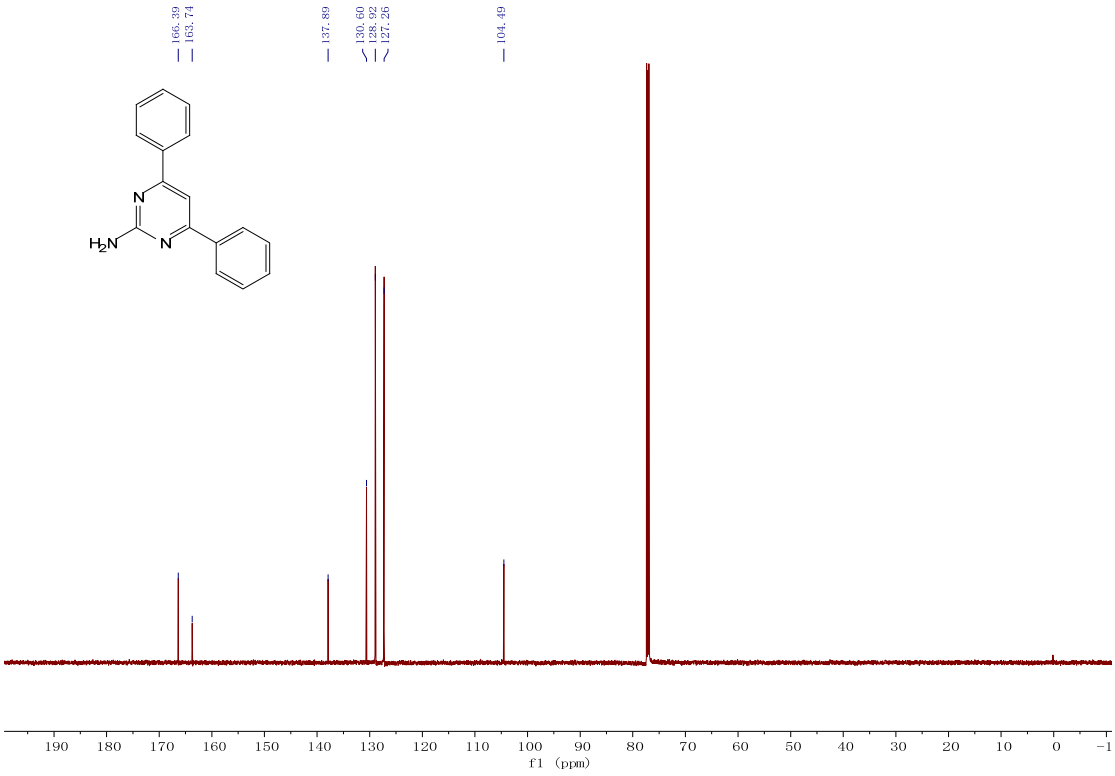
2-Cyclopropyl-4,6-diphenylpyrimidine (**3k**)



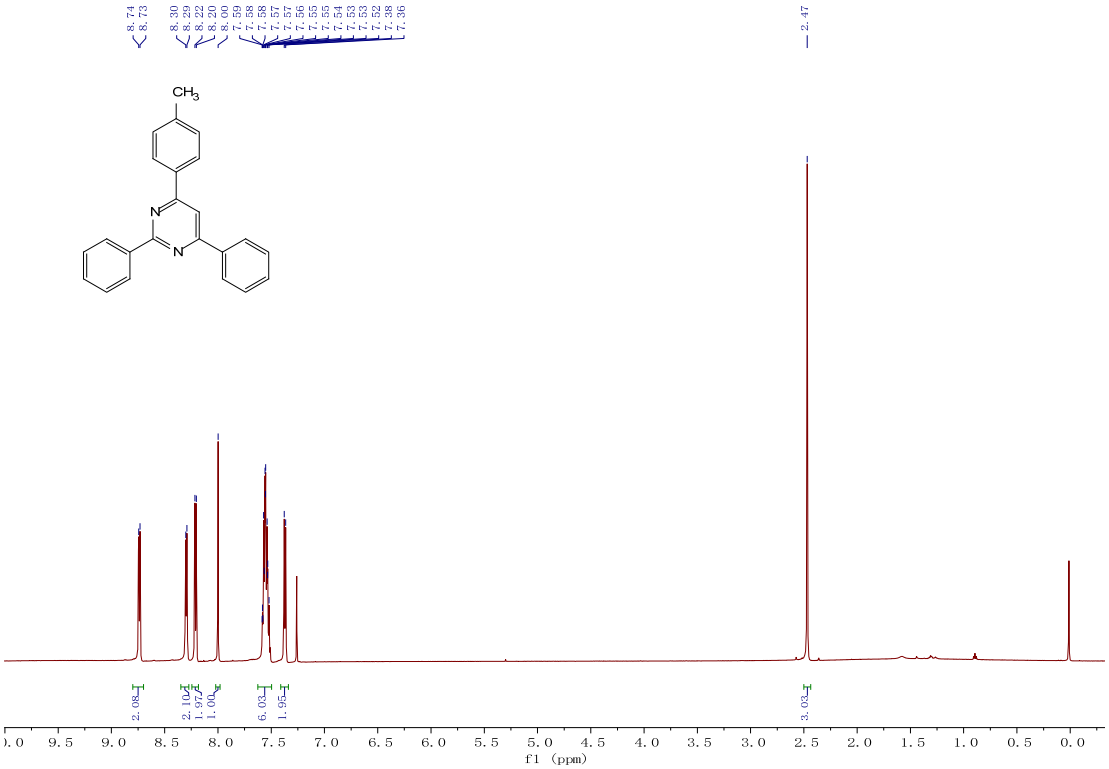


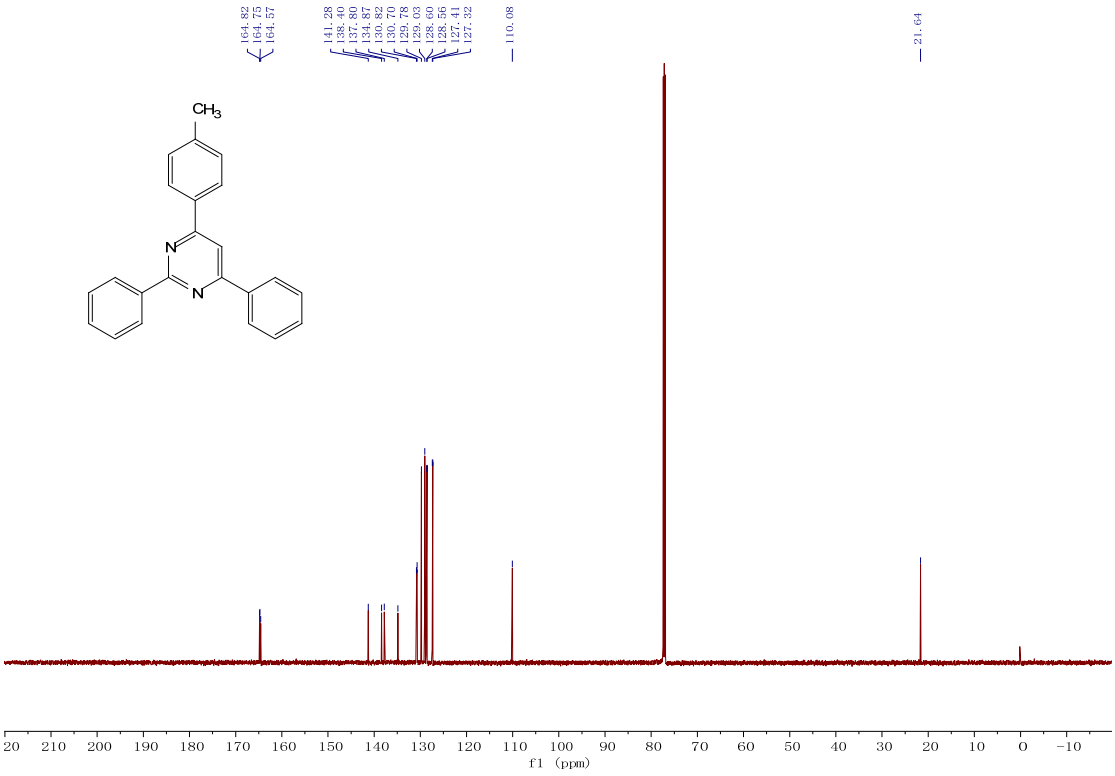
4,6-Diphenylpyrimidin-2-amine (**3l**)



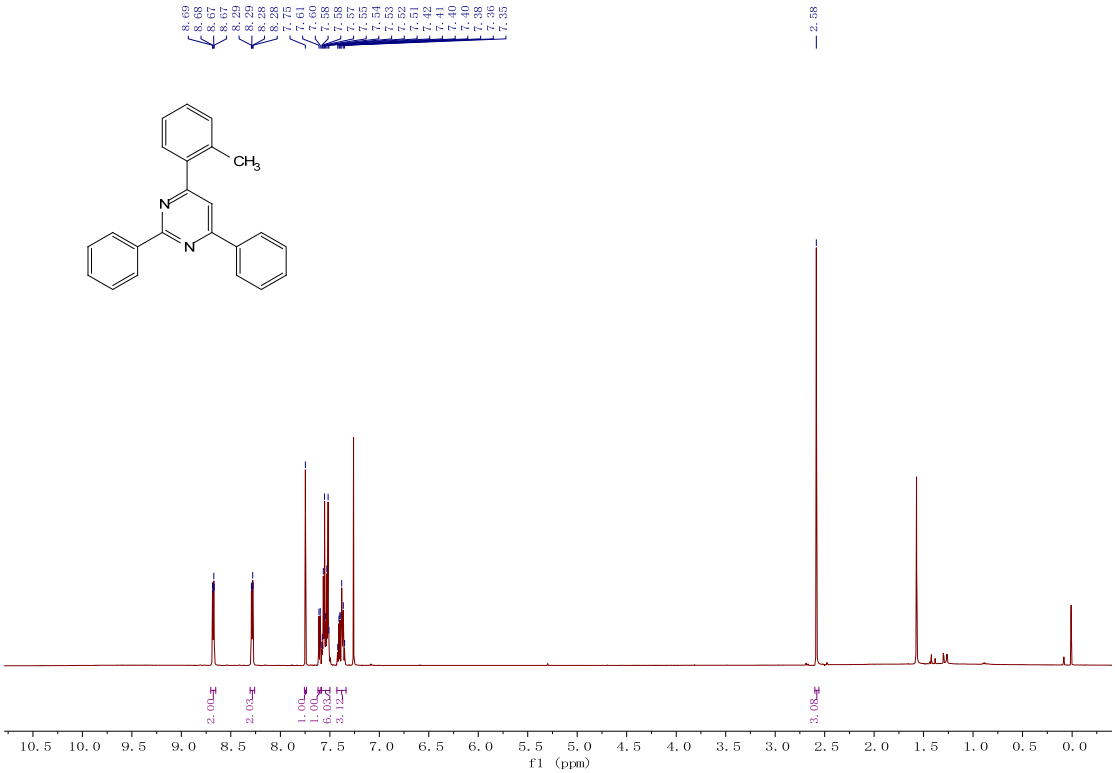


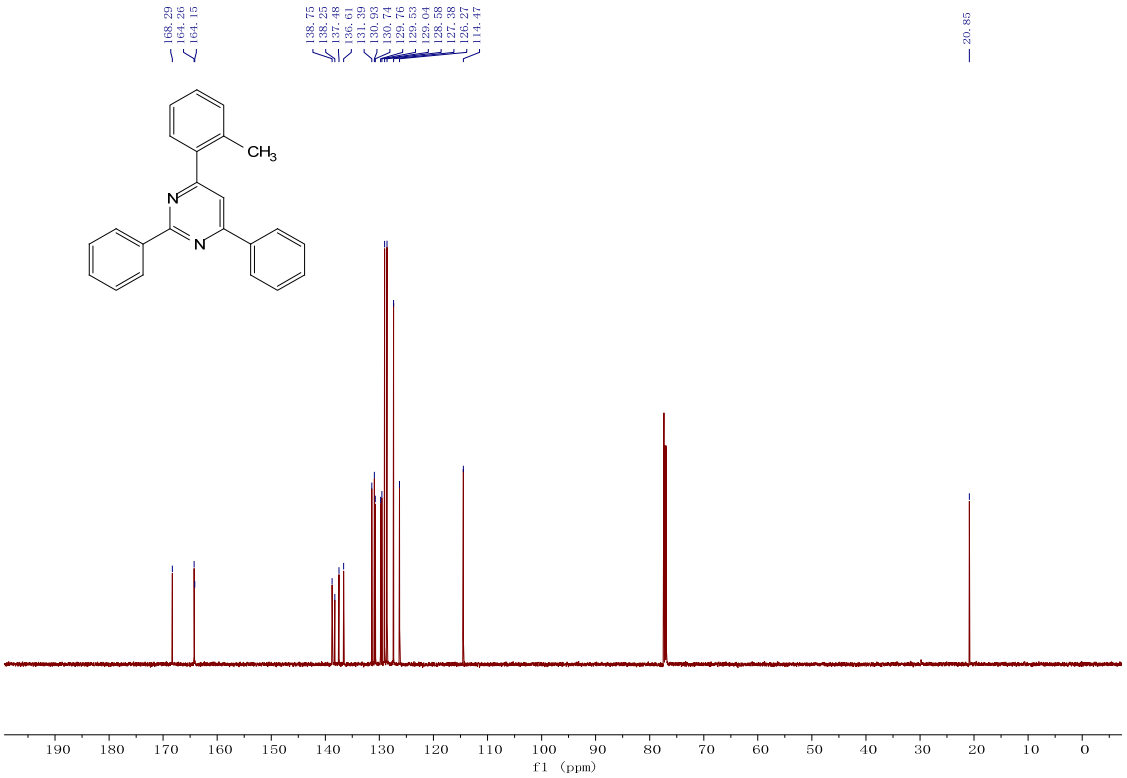
2,4-Diphenyl-6-(*p*-tolyl)pyrimidine (**3ab)**



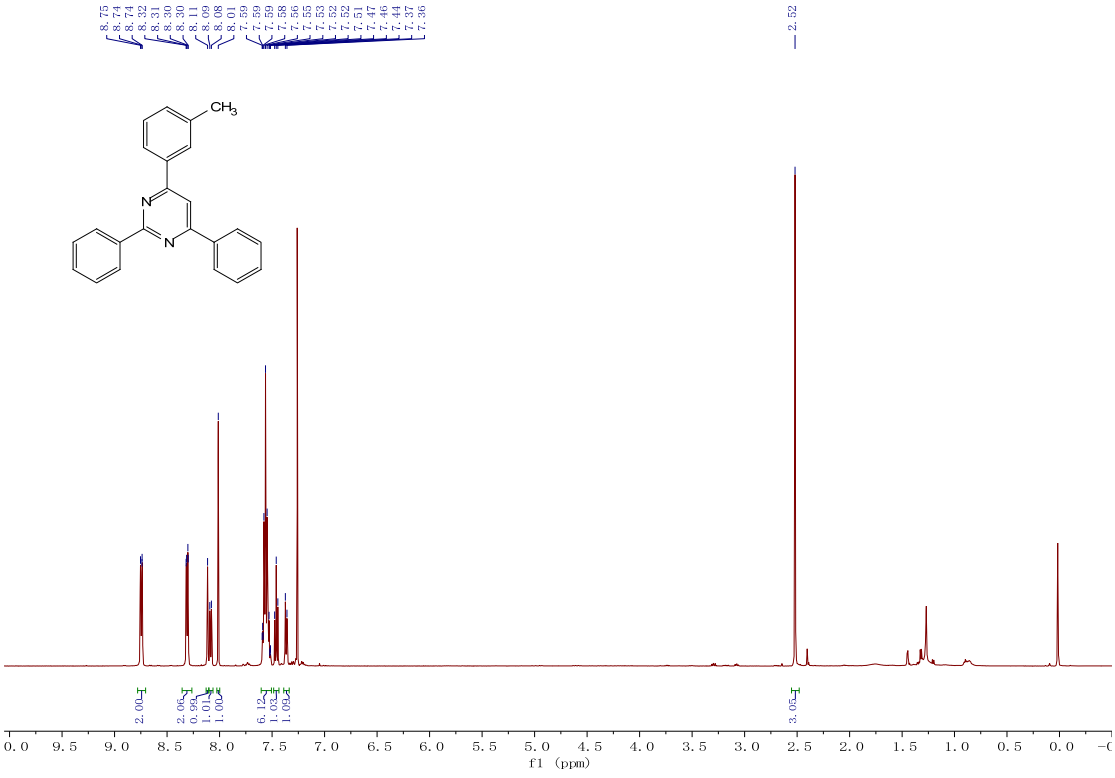


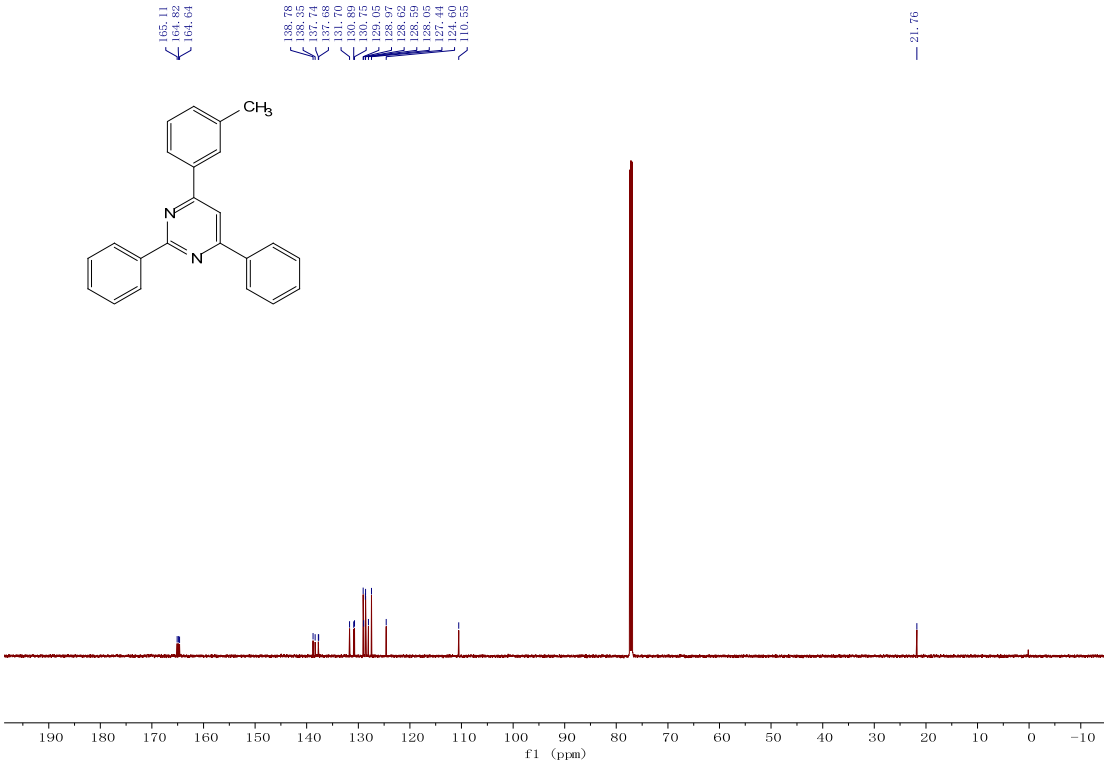
2,4-Diphenyl-6-(*o*-tolyl)pyrimidine (**3ac)**



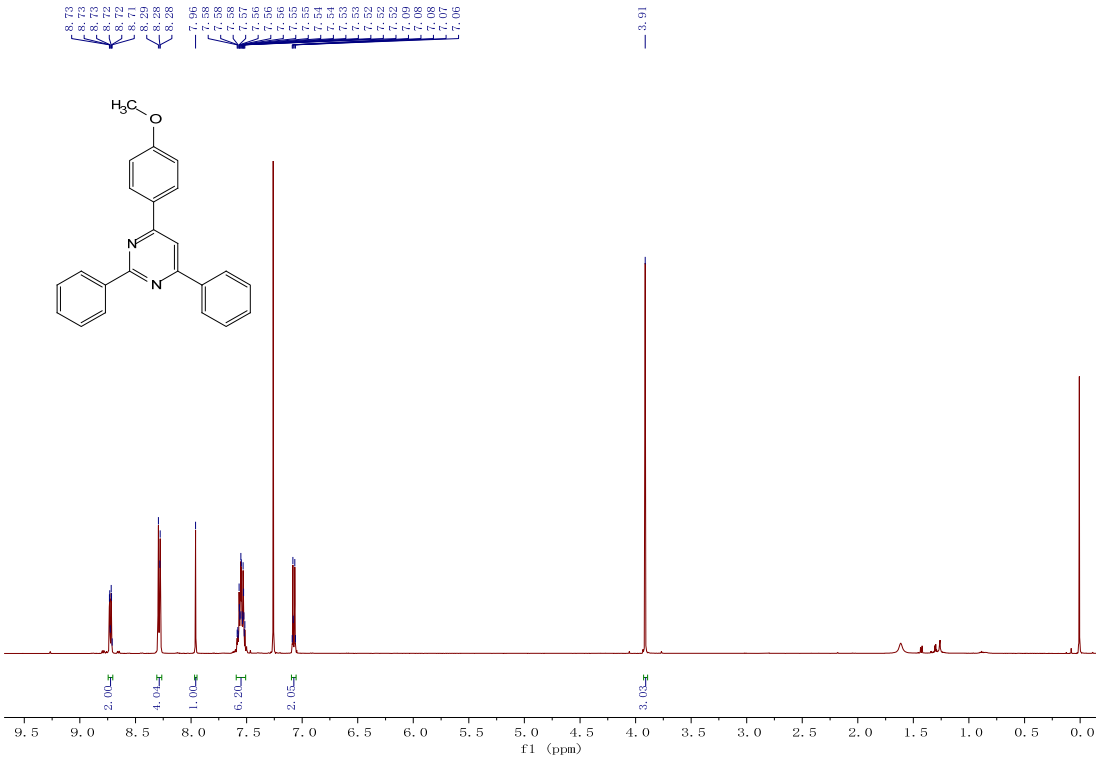


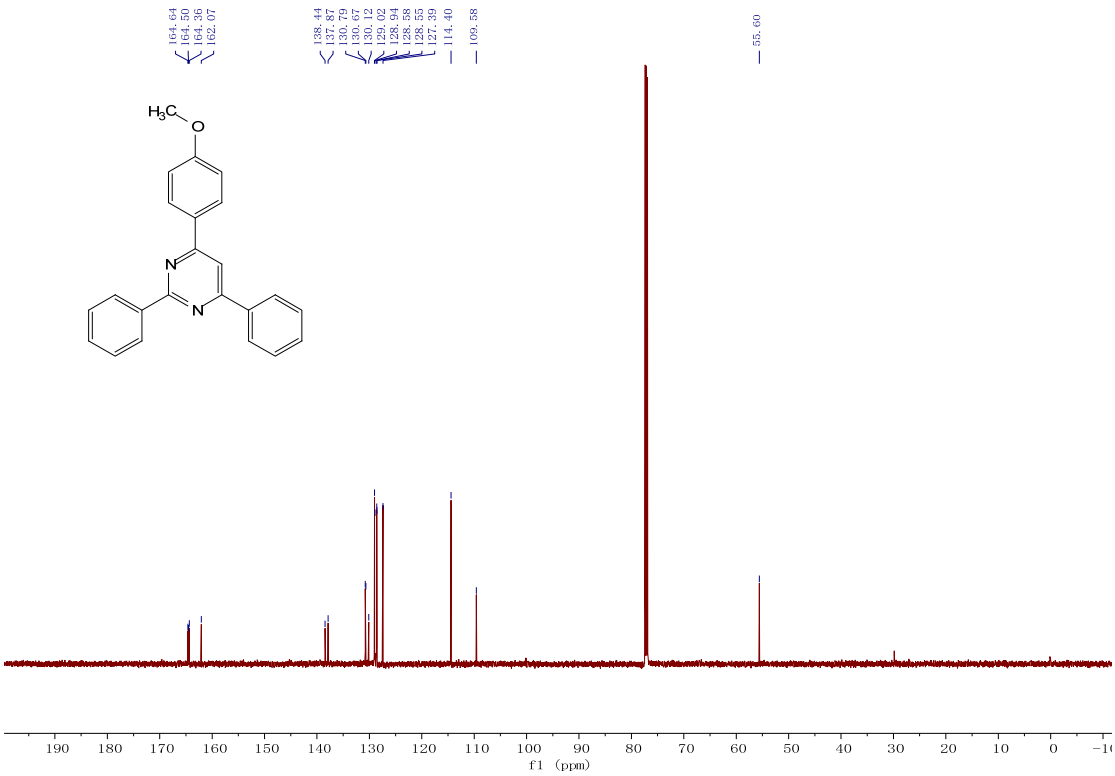
2,4-Diphenyl-6-(*m*-tolyl)pyrimidine (**3ad**)



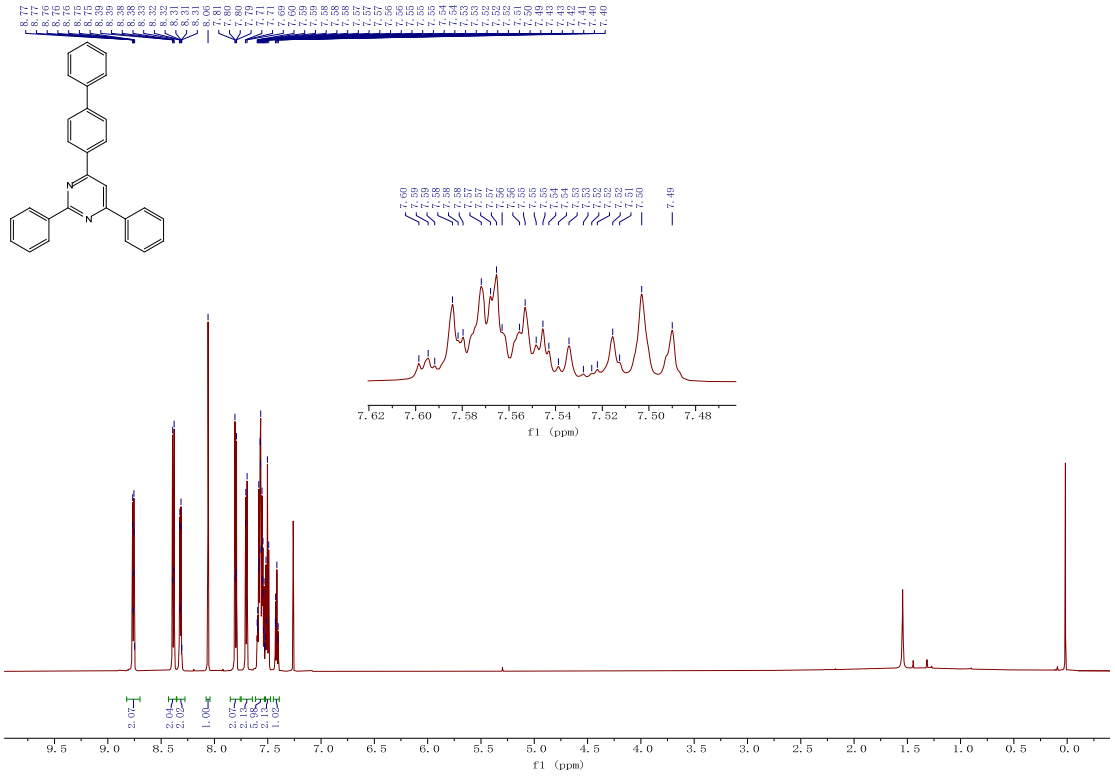


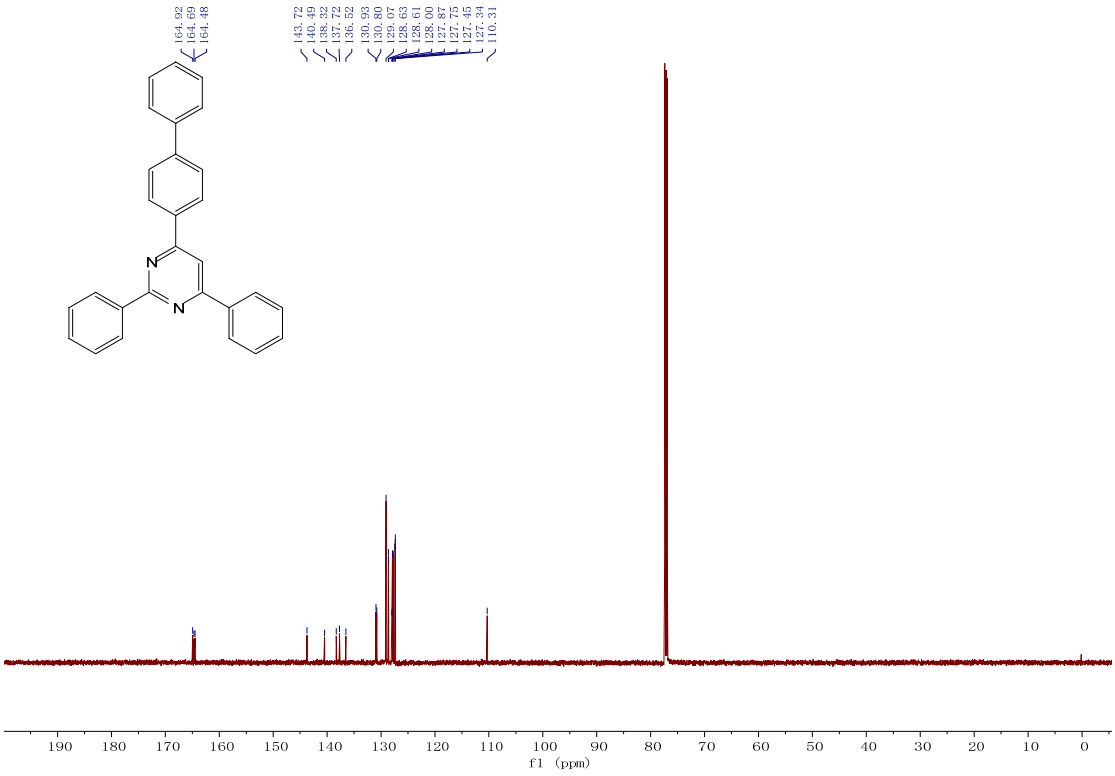
4-(4-Methoxyphenyl)-2,6-diphenylpyrimidine (**3ae**)



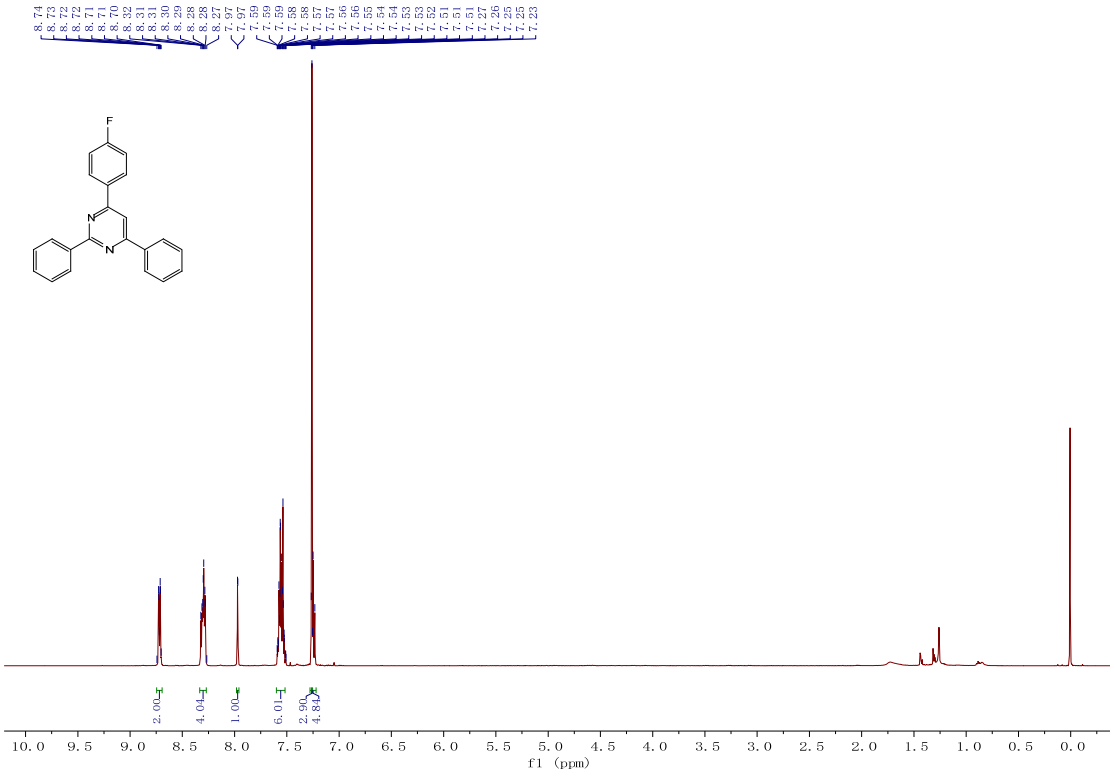


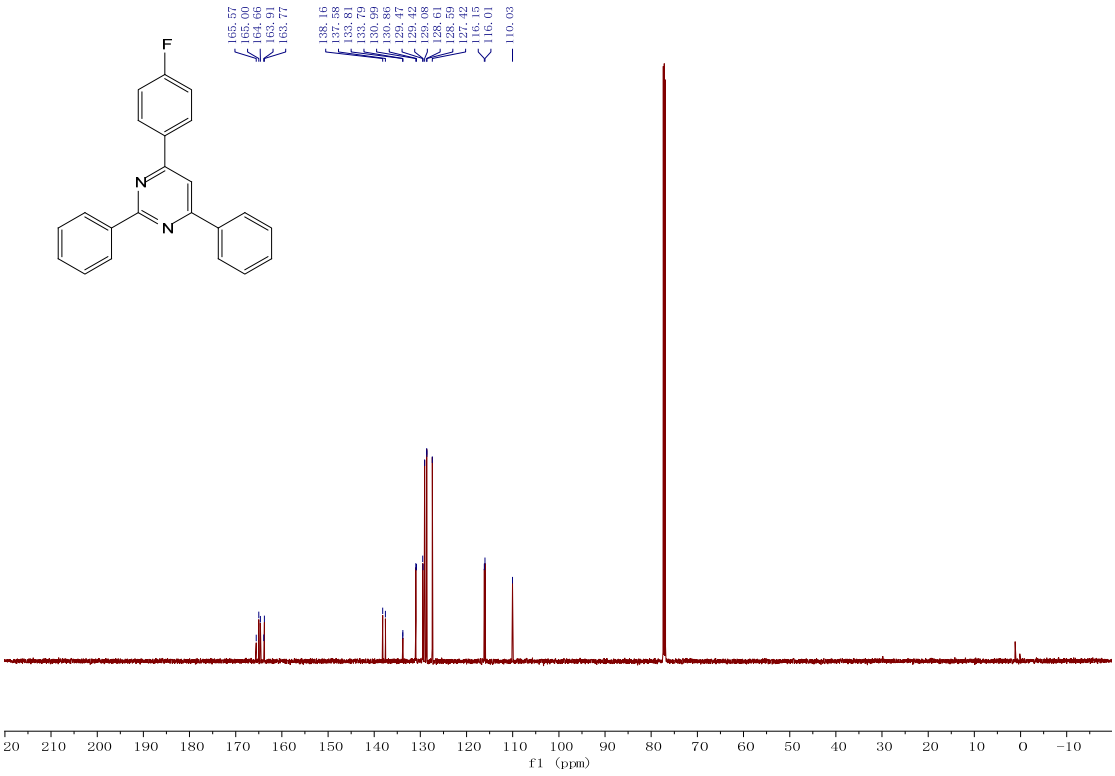
4-([1,1'-Biphenyl]-4-yl)-2,6-diphenylpyrimidine (**3af**)





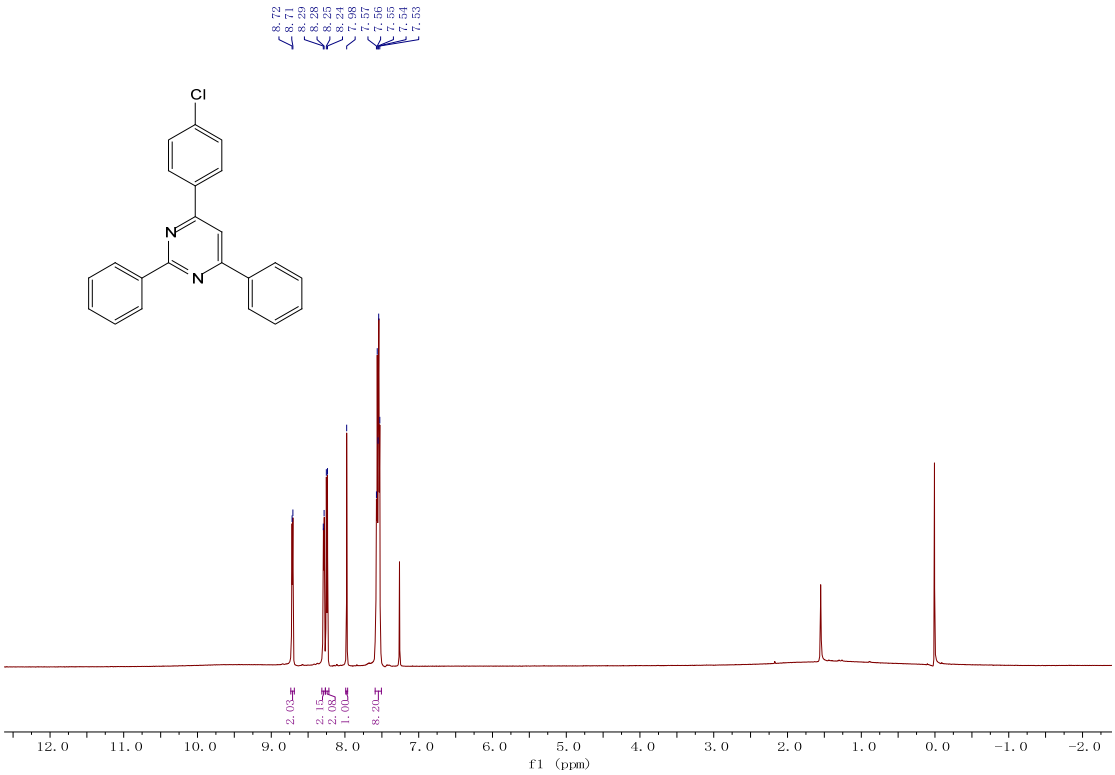
4-(4-Fluorophenyl)-2,6-diphenylpyrimidine (**3ag**)

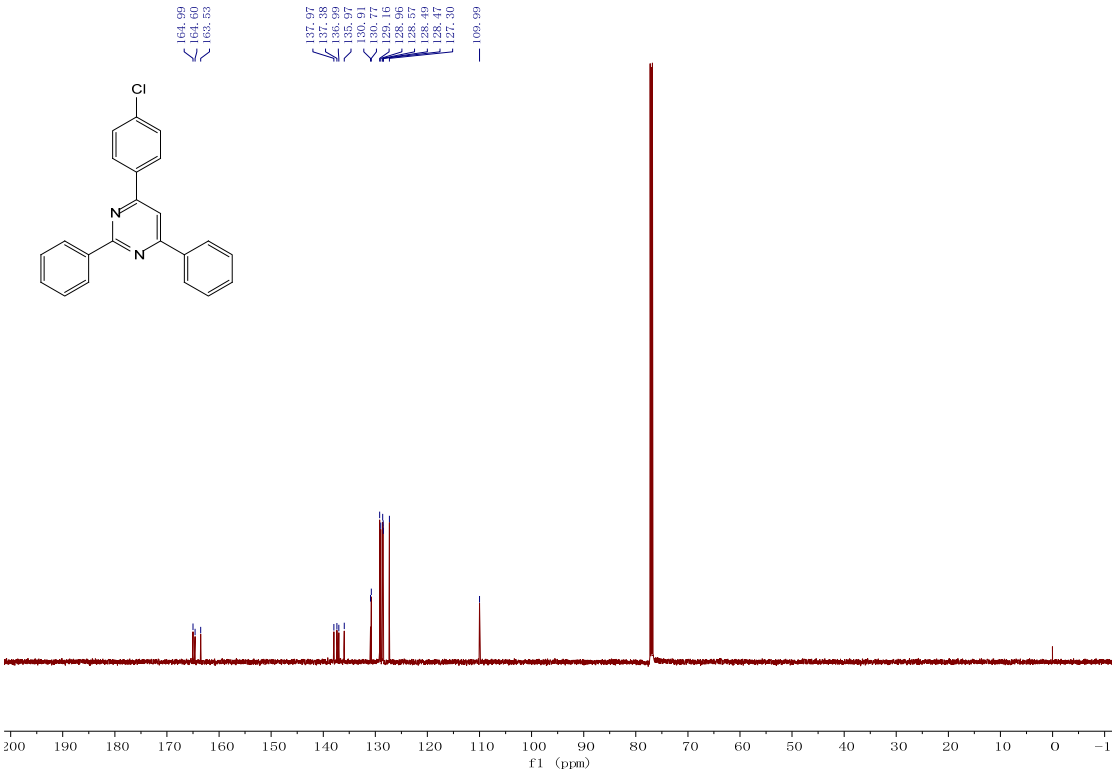



F
N
N
165.57
165.00
164.66
163.91
163.77
138.16
137.58
133.81
133.79
130.99
130.86
129.47
129.42
129.08
128.61
128.59
127.42
116.15
116.01
110.03
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

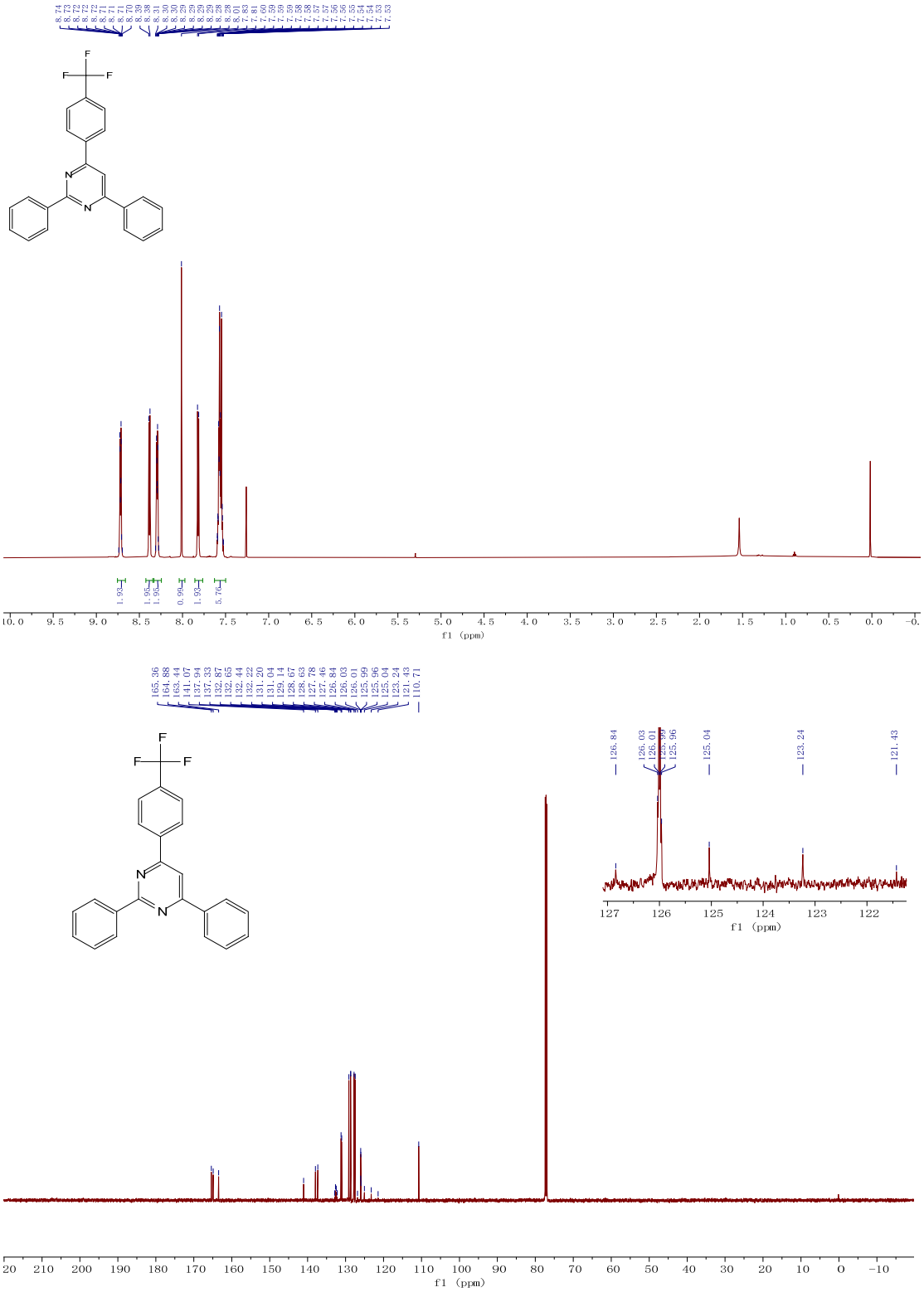

F
N
N
-110.41
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

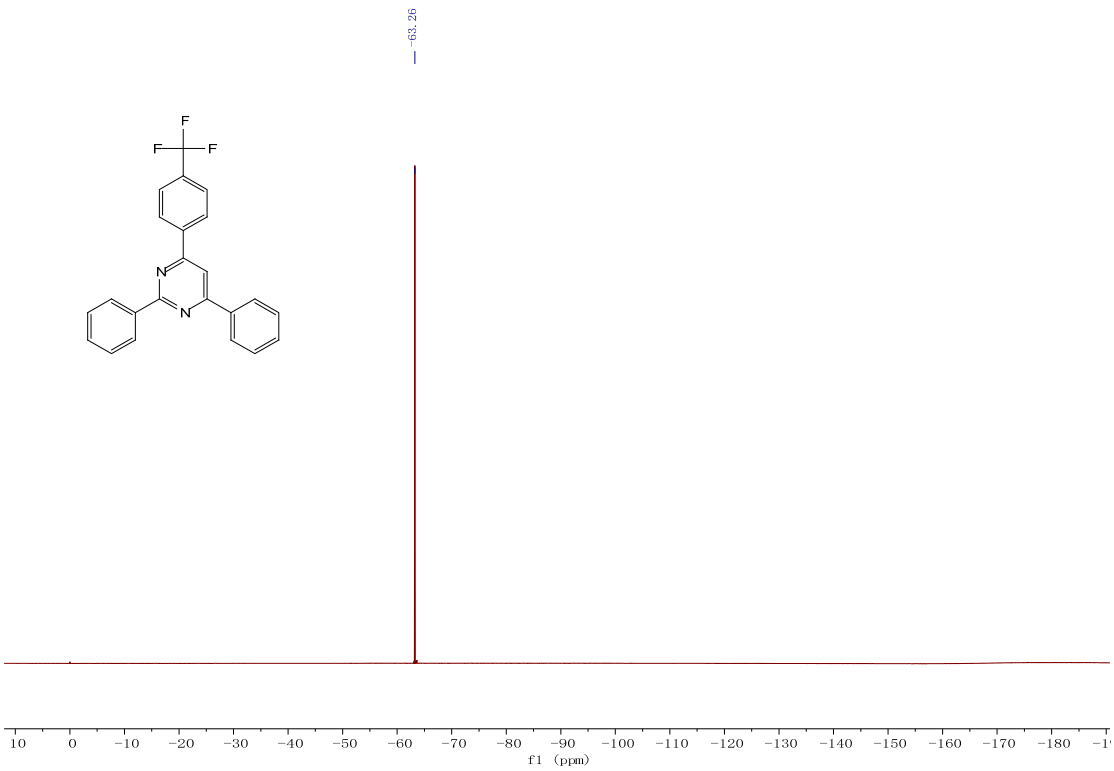
4-(4-Chlorophenyl)-2,6-diphenylpyrimidine (**3ah**)



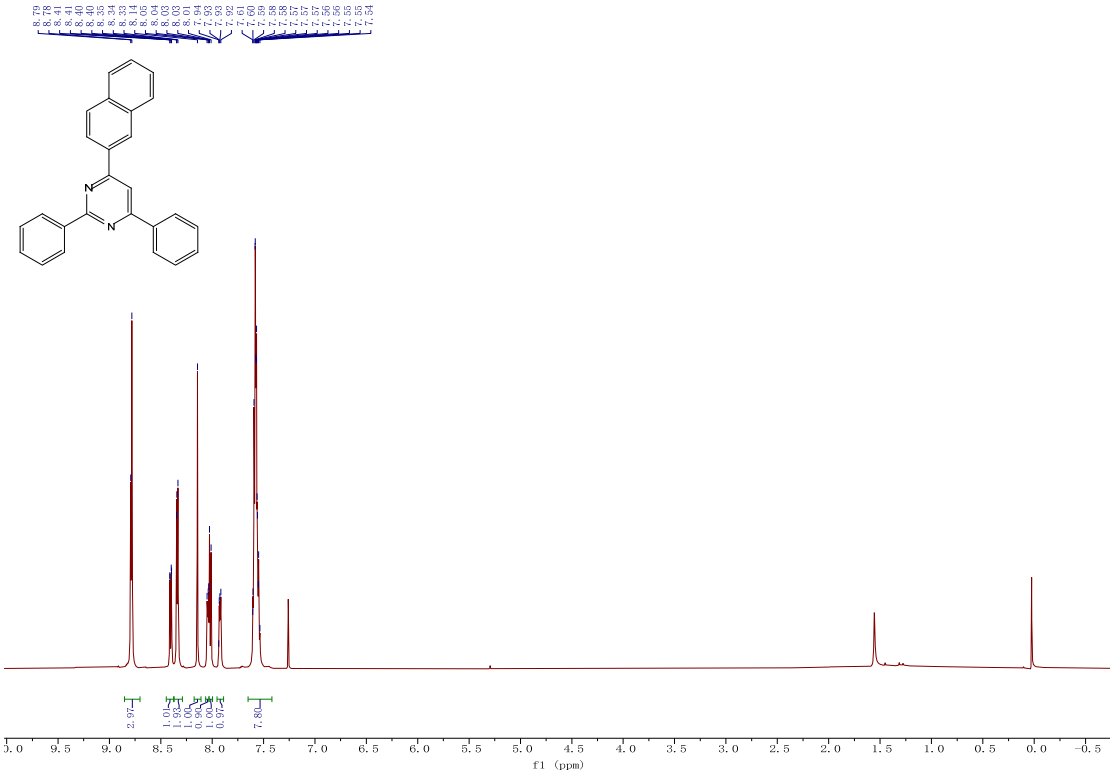


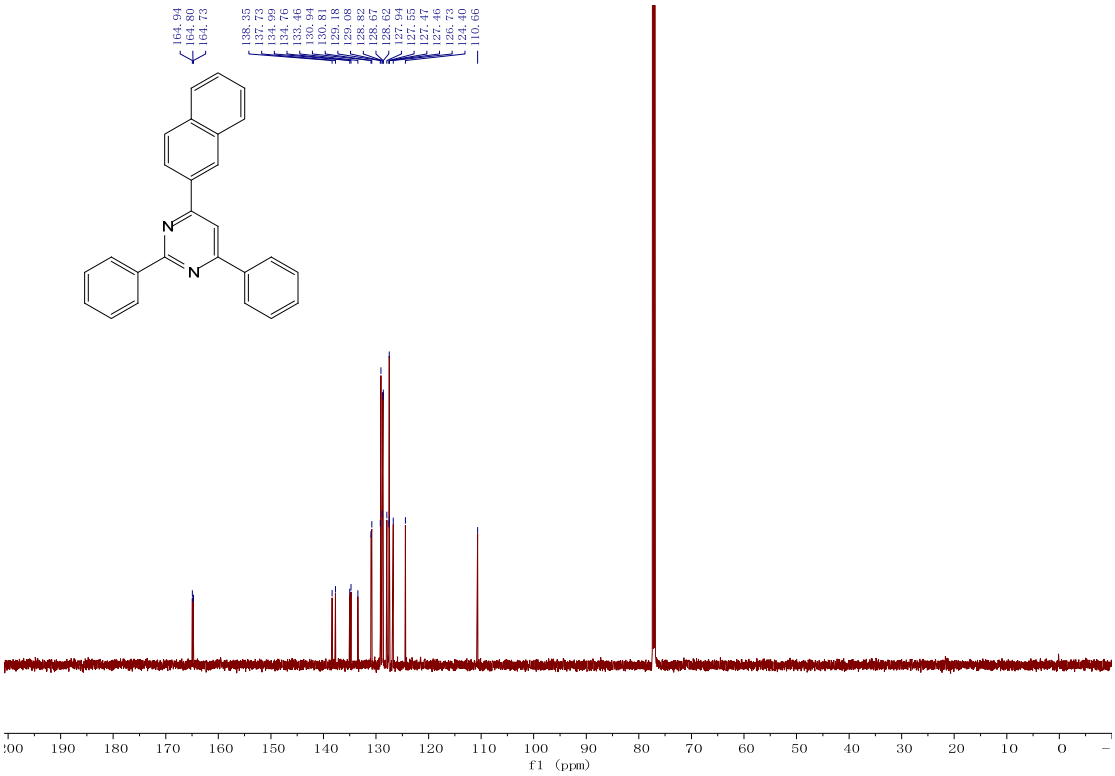
2,4-Diphenyl-6-(4-(trifluoromethyl)phenyl)pyrimidine (**3ai**)



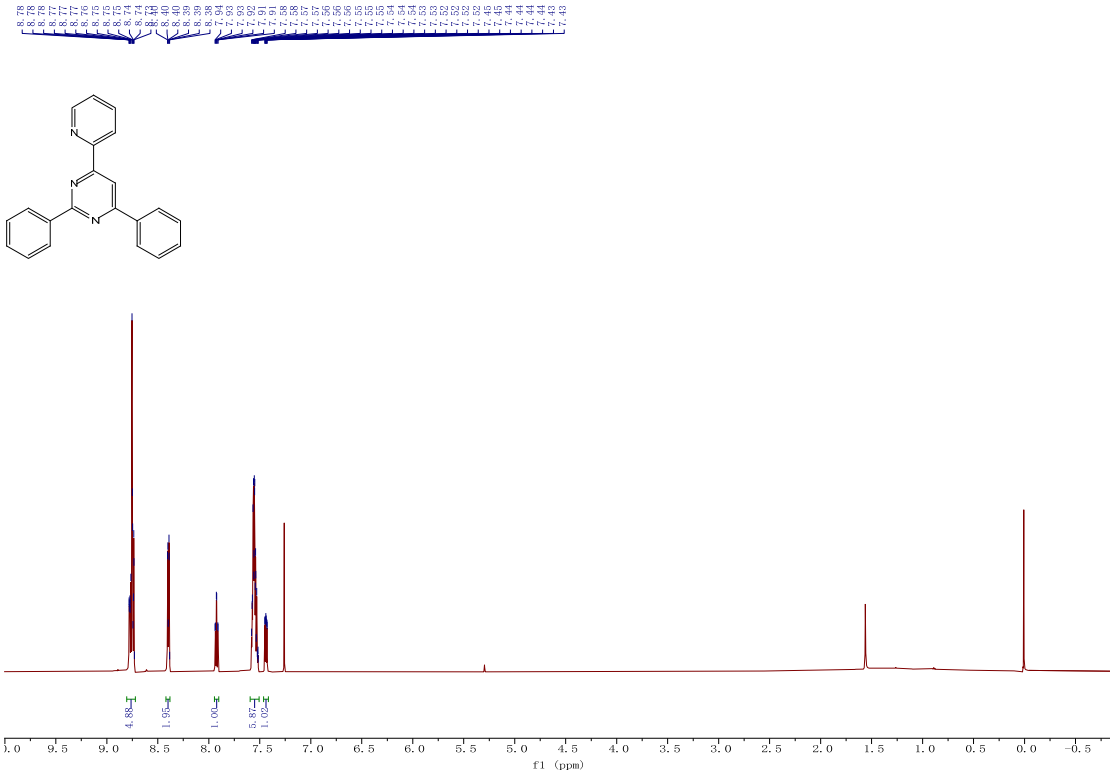


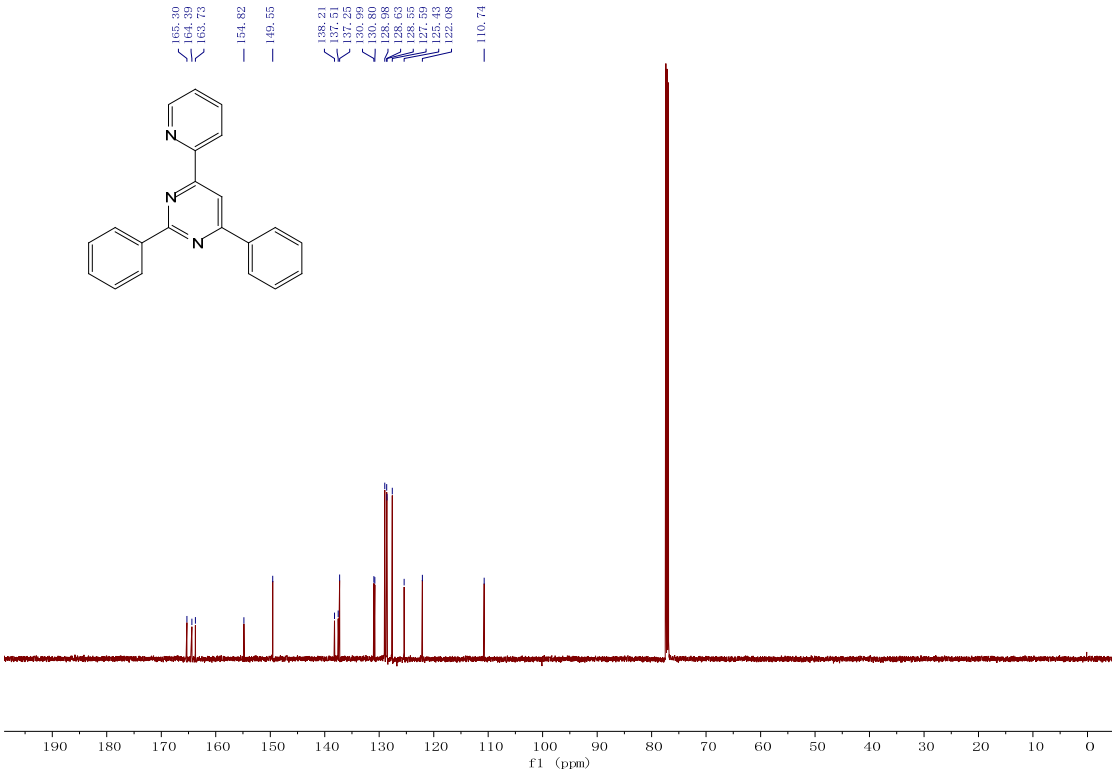
4-(Naphthalen-2-yl)-2,6-diphenylpyrimidine (**3aj**)



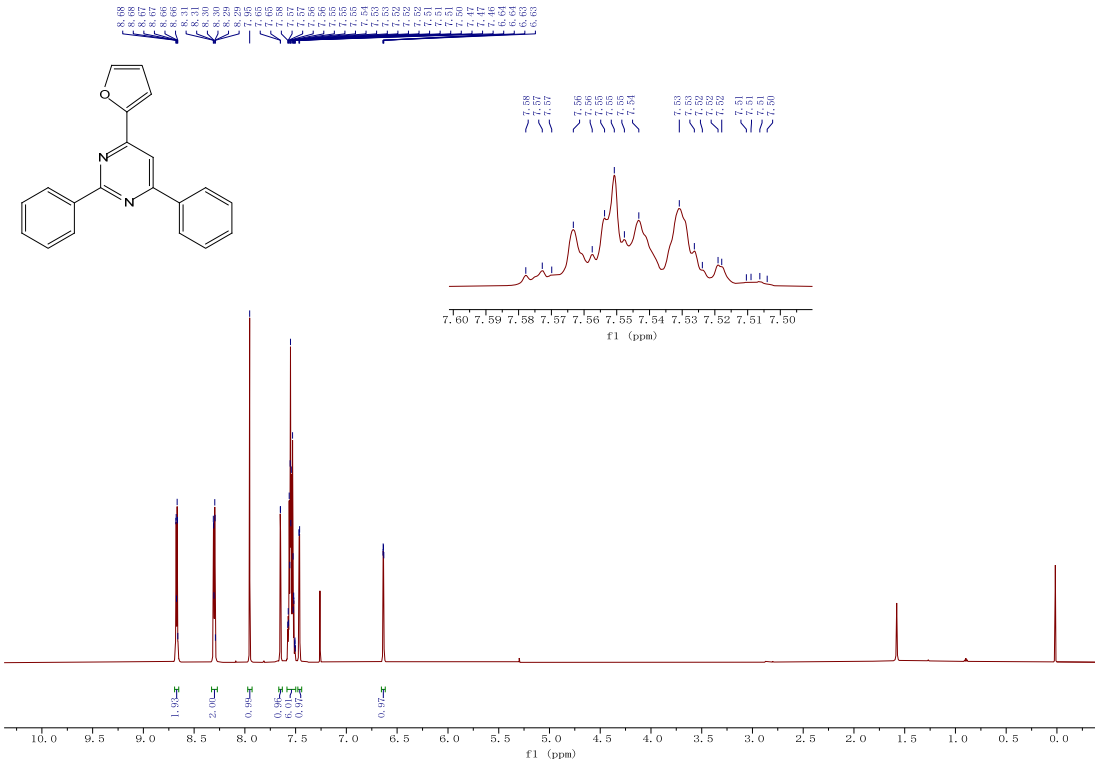


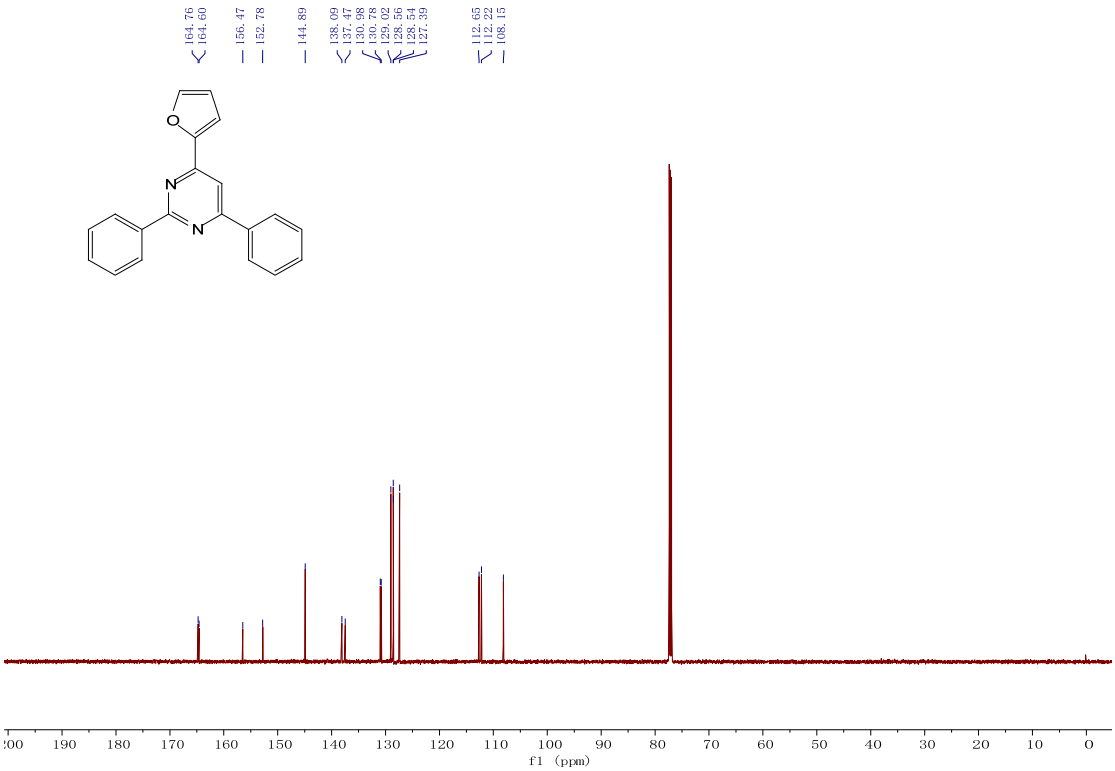
2,4-Diphenyl-6-(pyridin-2-yl)pyrimidine (**3ak**)



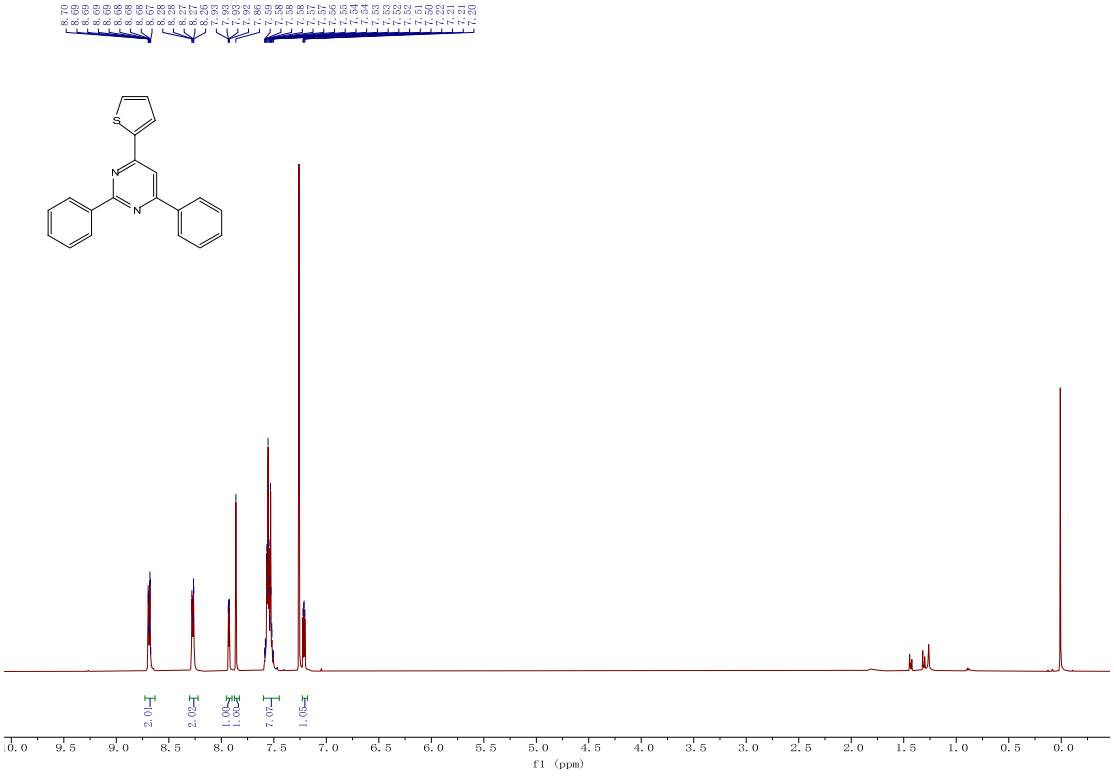


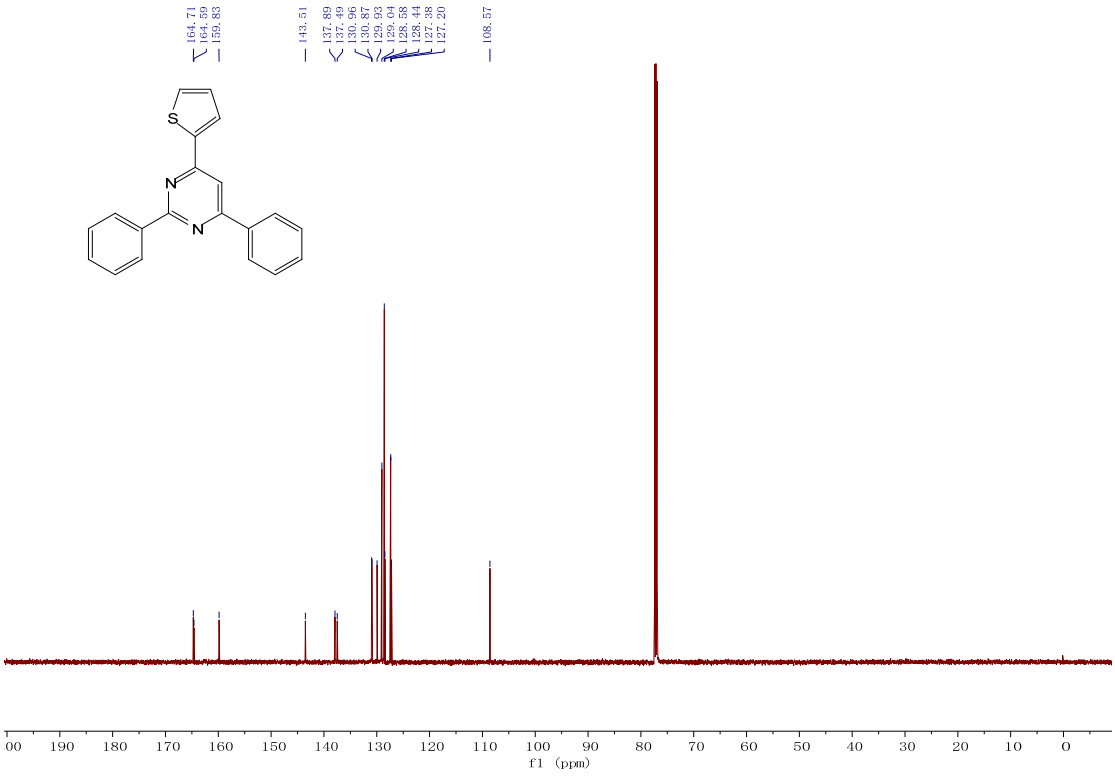
4-(Furan-2-yl)-2,6-diphenylpyrimidine (**3al**)



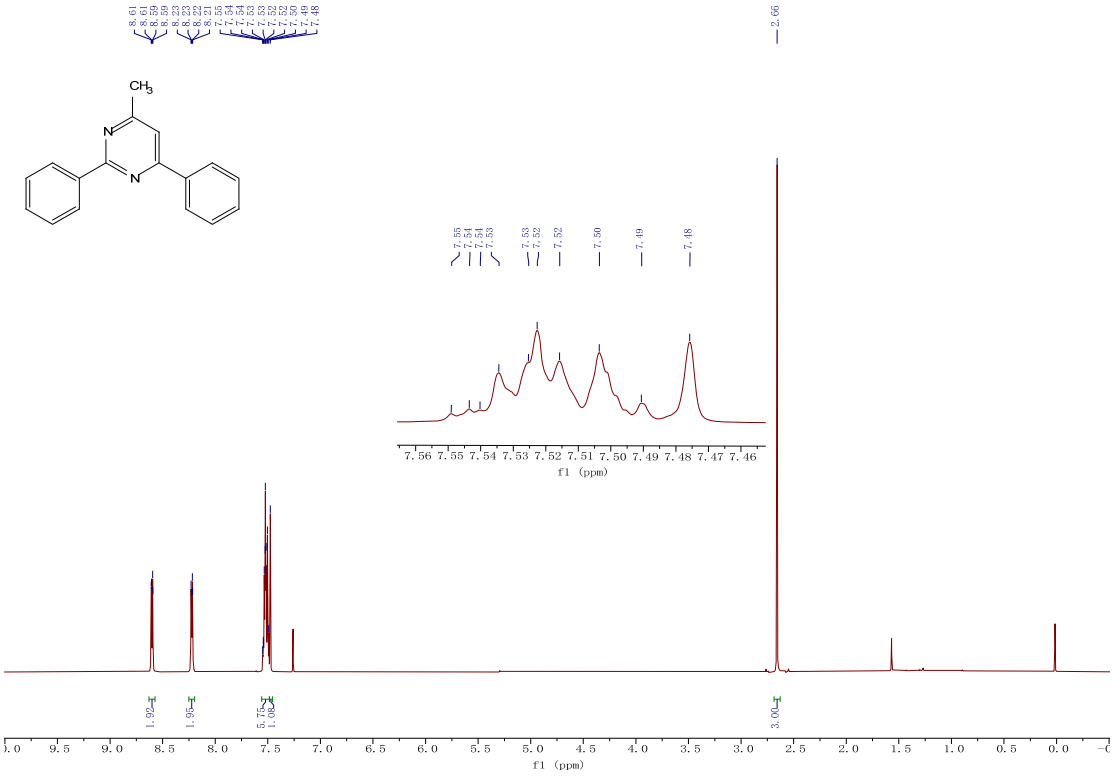


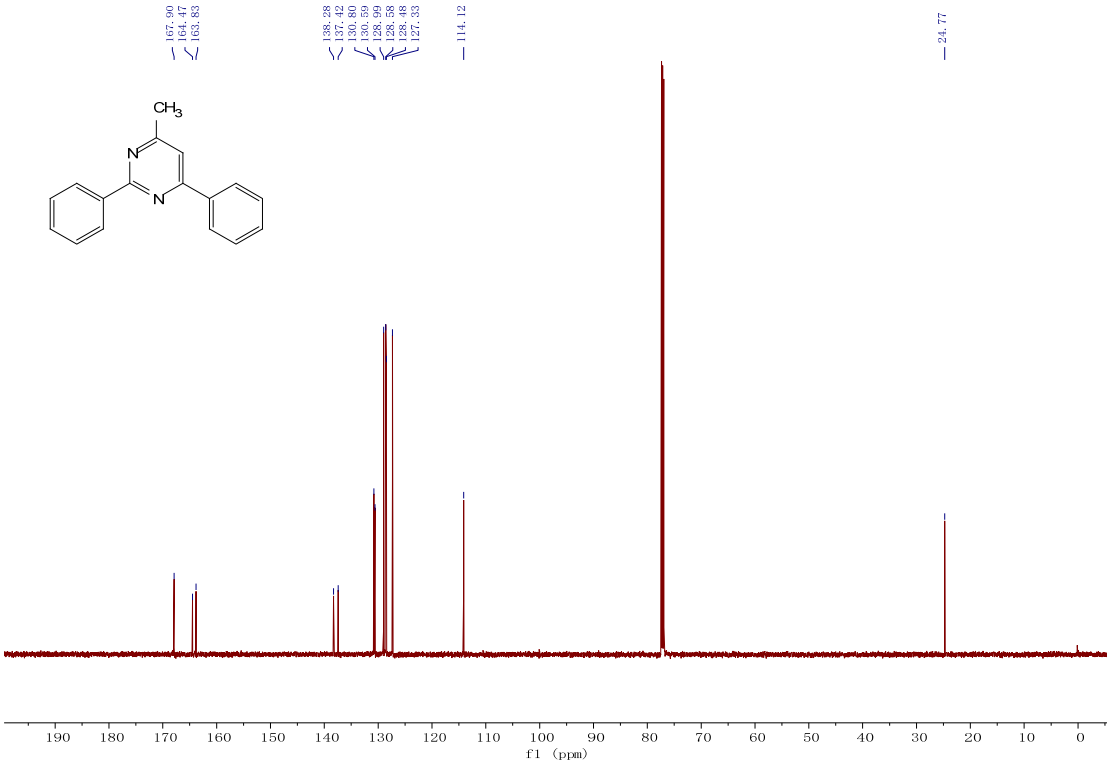
2,4-Diphenyl-6-(thiophen-2-yl)pyrimidine (**3am**)



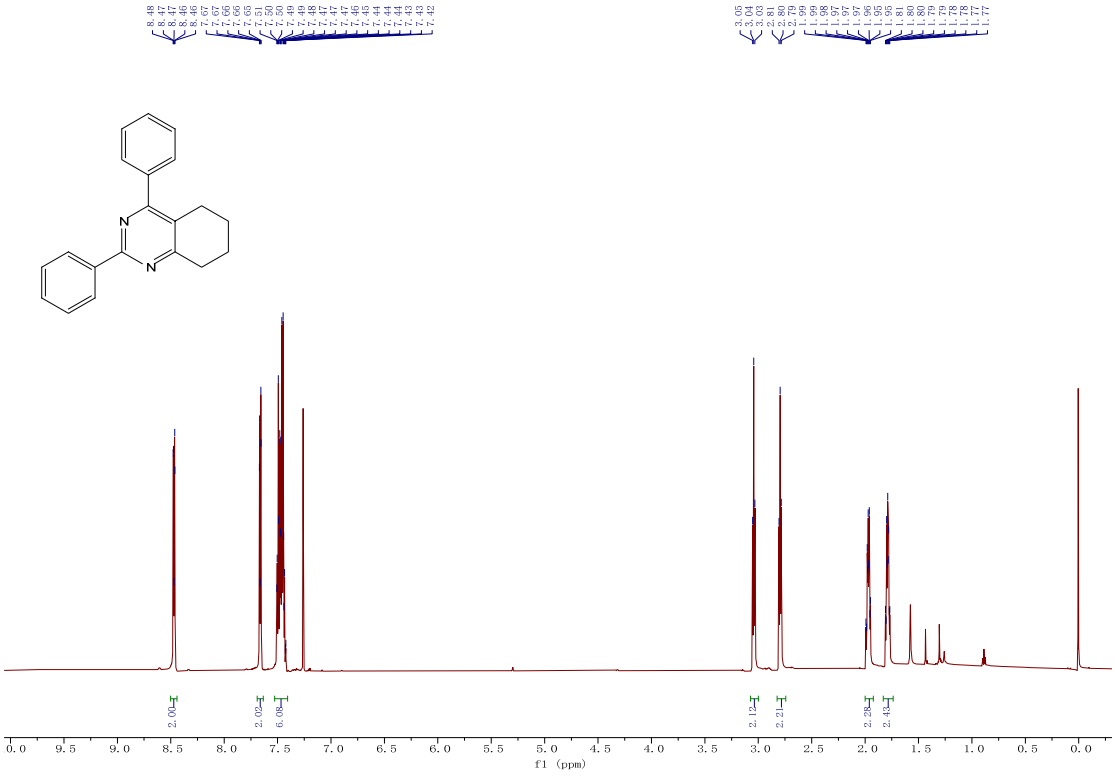


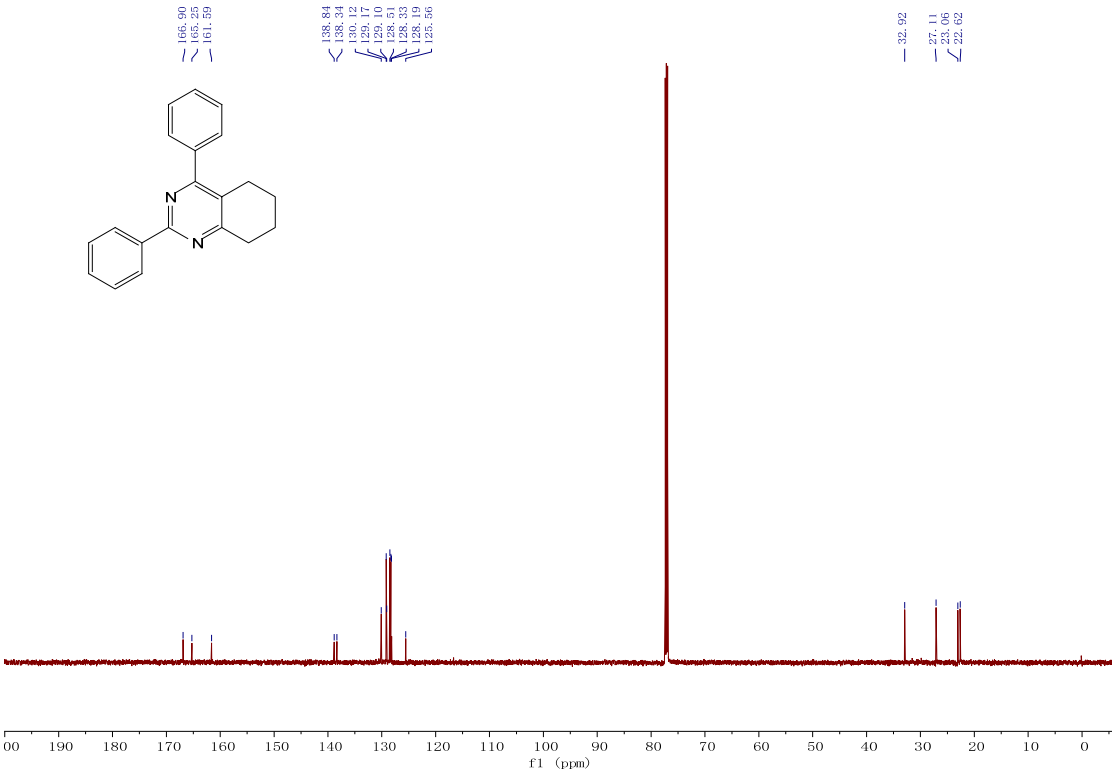
4-Methyl-2,6-diphenylpyrimidine (**3an**)



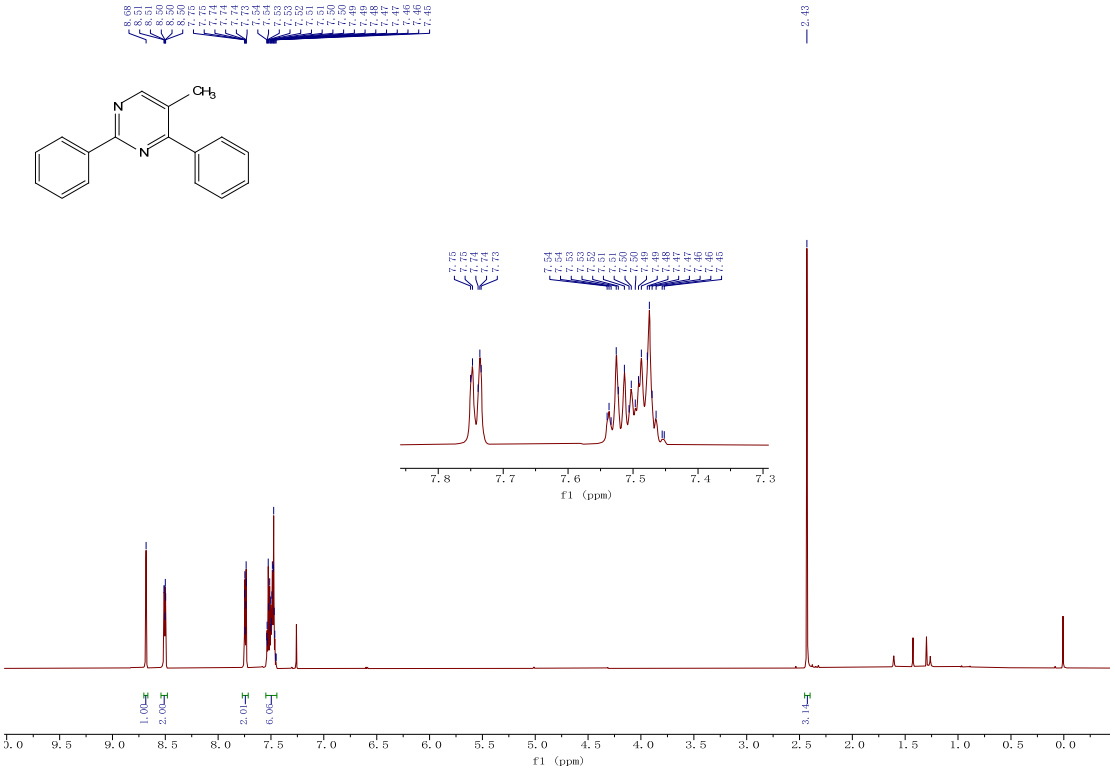


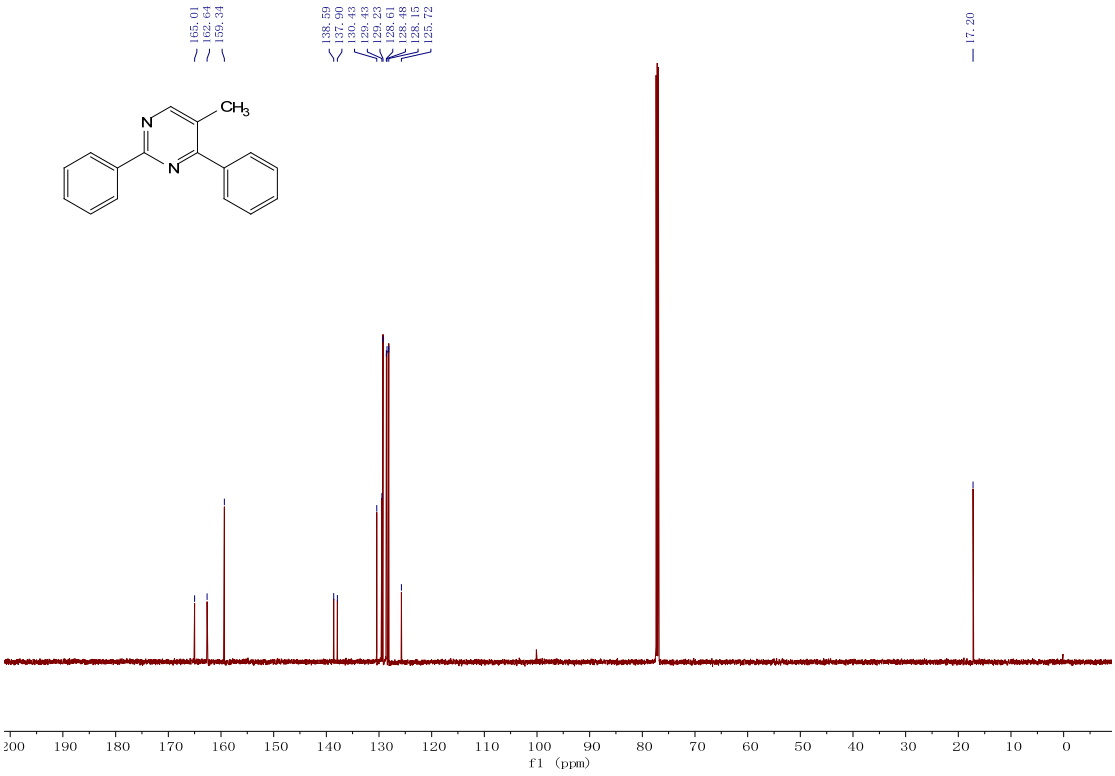
2,4-Diphenyl-5,6,7,8-tetrahydroquinazoline (**3ao**)



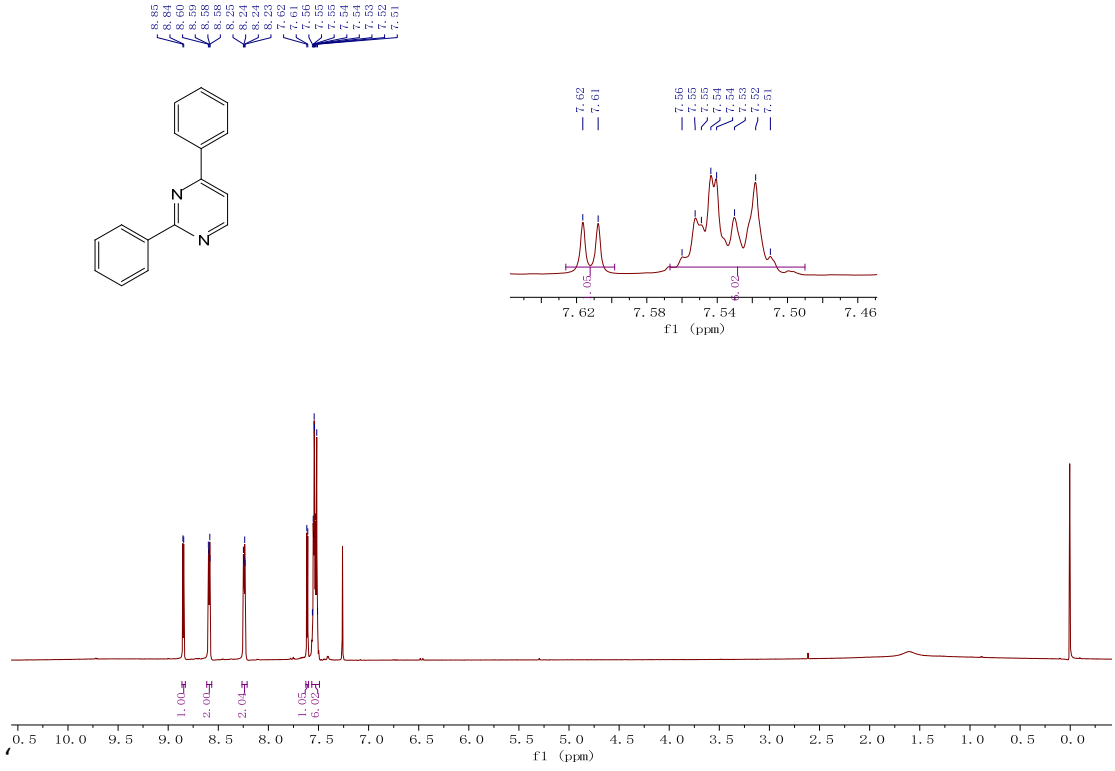


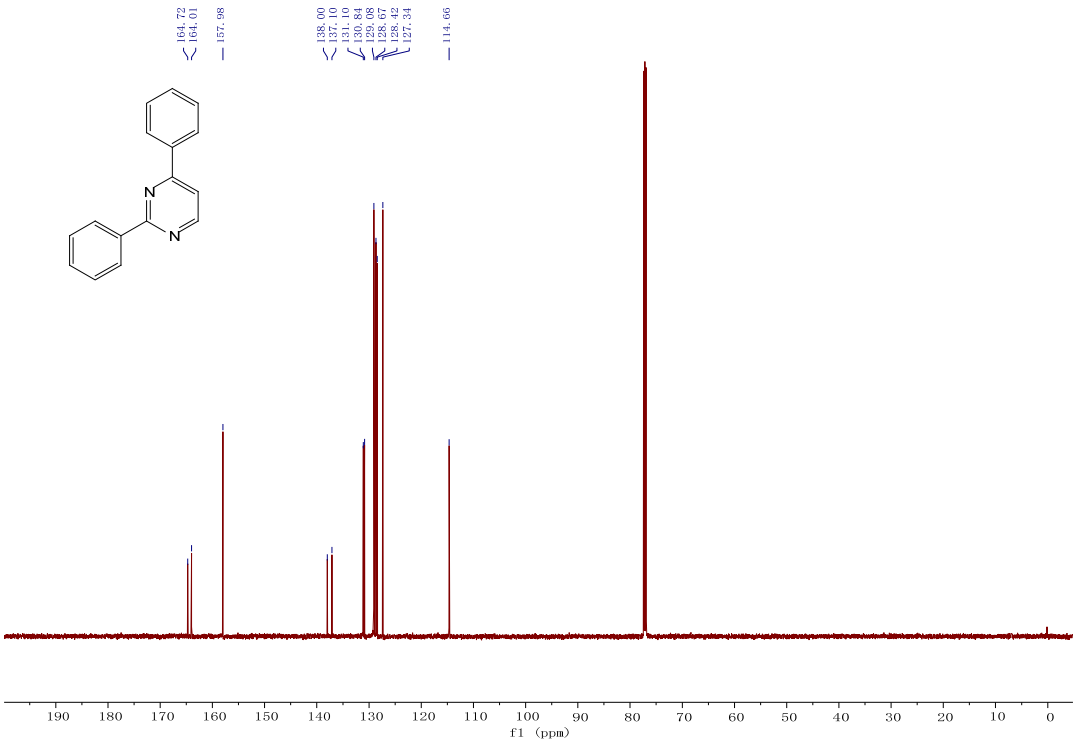
5-Methyl-2,4-diphenylpyrimidine (**3ap**)



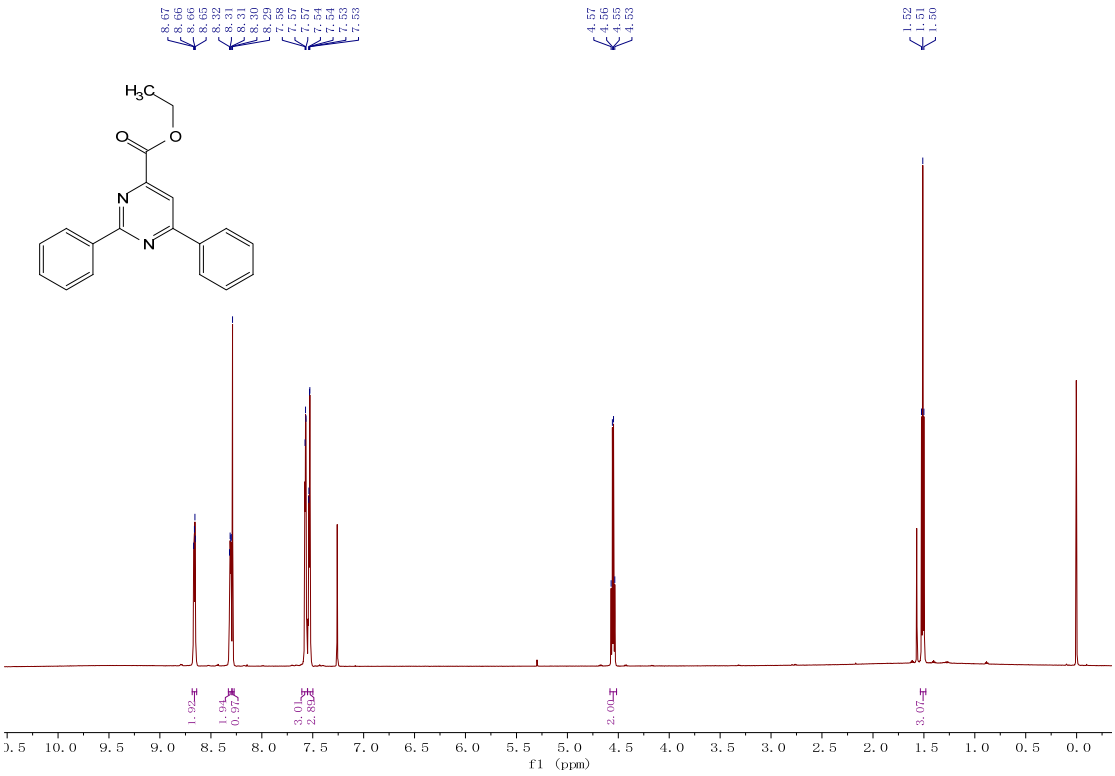


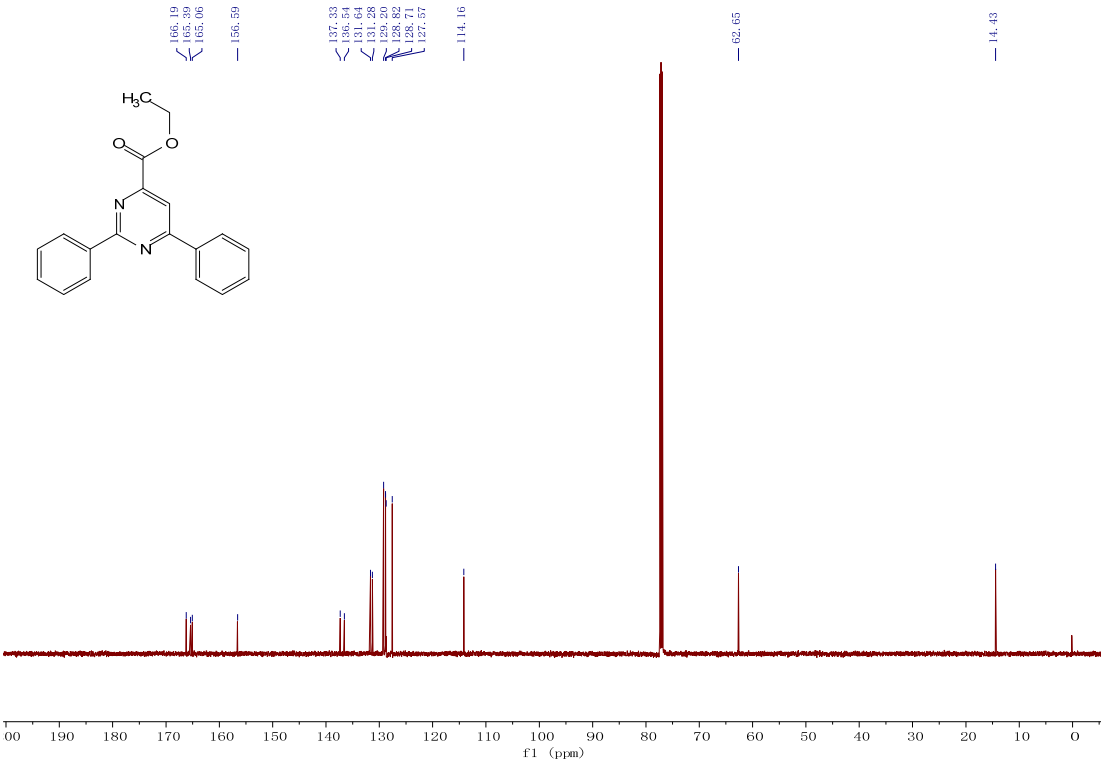
2,4-Diphenylpyrimidine (**3aq**)



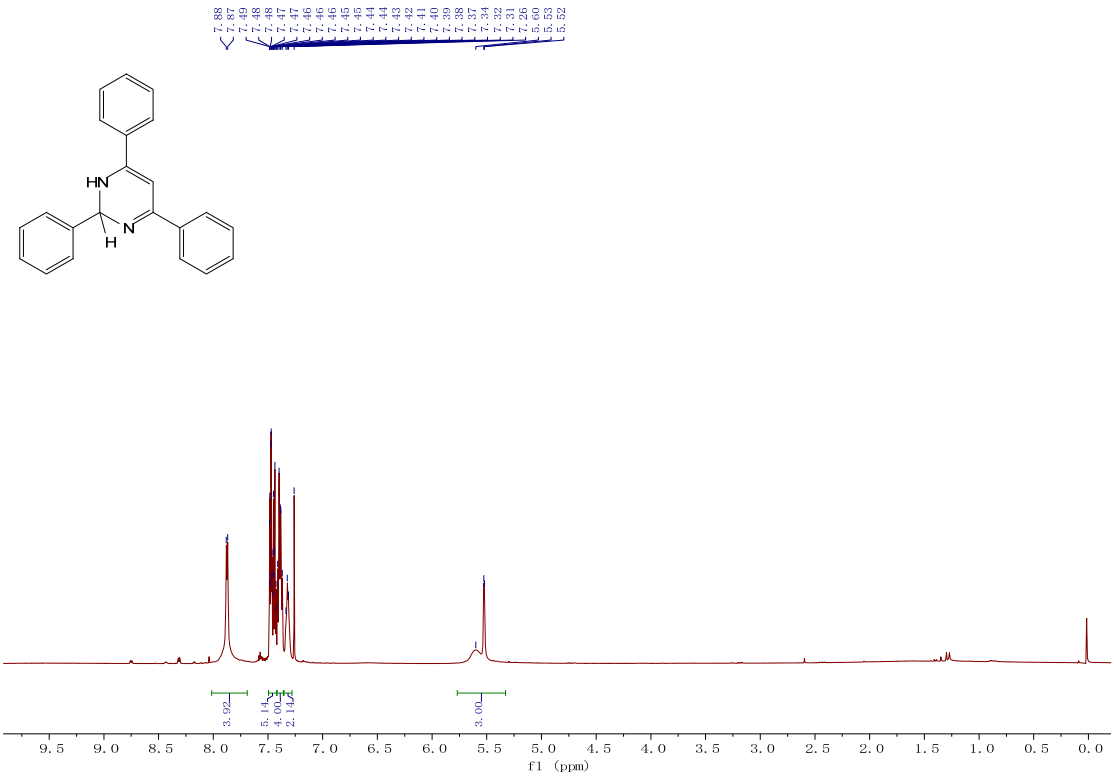


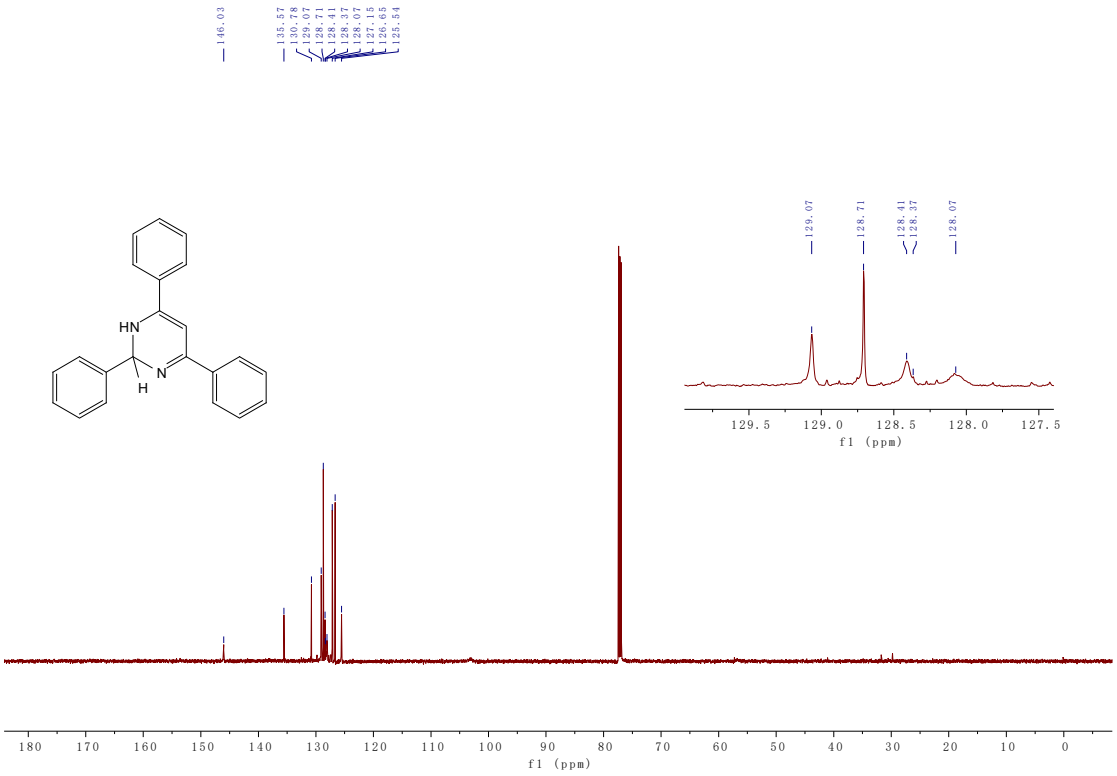
Ethyl 2,6-diphenylpyrimidine-4-carboxylate (**3ar**)

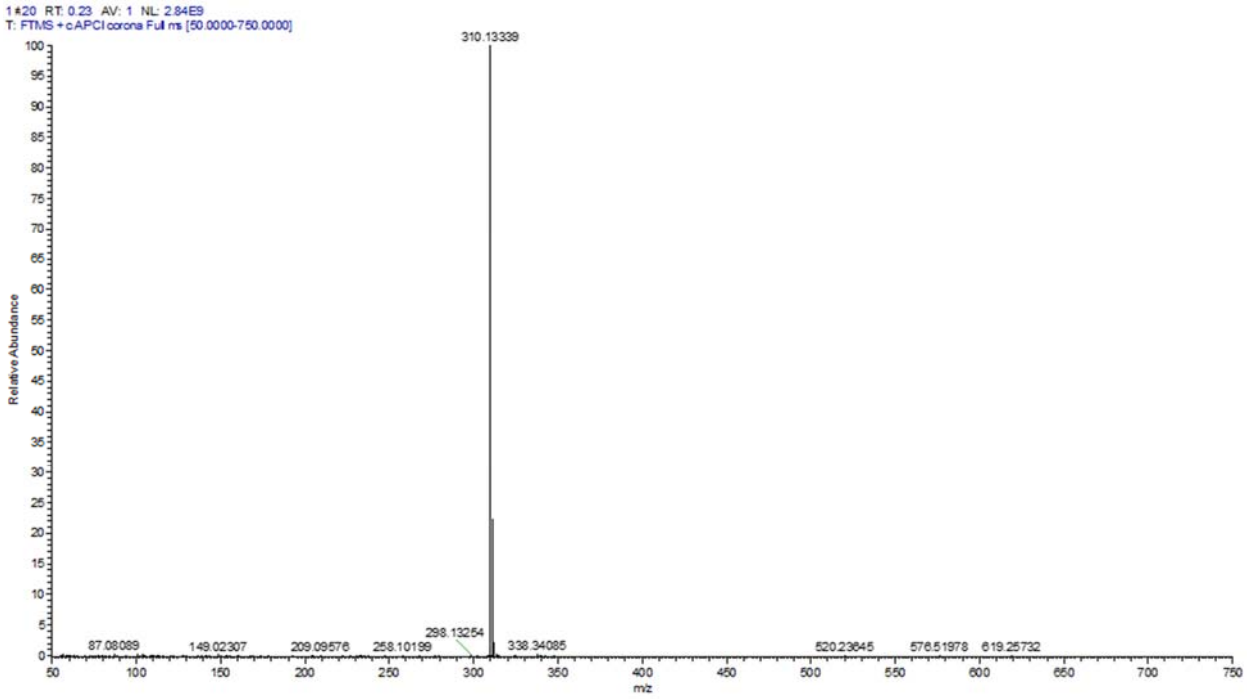




2,4,6-Triphenyl-1,2-dihydropyrimidine (**4a**).




146.03
135.57
130.78
129.07
128.71
128.41
128.37
128.07
127.15
126.65
125.54
HN
N
H
129.07
128.71
128.41
128.37
128.07
129.5
129.0
128.5
128.0
127.5
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1 #20 RT: 0.23 AV: 1 NL: 2.84E9
T: FTMS + cAPCI corona Full ms [50.0000-750.0000]
310.13339
Relative Abundance
87.08089
149.02307
209.09576
258.10199
298.13254
338.34085
520.23645
576.51978
619.25732
m/z

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