Electronic Supplementary Material (ESI) for ChemComm.

N-Heterocyclic Carbene-catalyzed Annulation of Ynals with Amidines: Access to 1,2,6-Trisubstituted Pyrimidin-4-ones

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Supporting Information

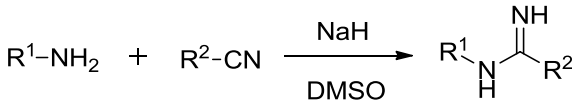
Contents:

General Information

Chemicals were purchased from commercial suppliers and used as received. Solvents were dried on alumina columns using a solvent dispensing system. Thin-layer chromatography (TLC) was conducted on plates (GF254) supplied by Yantai Chemicals (China) and visualized with a UV light at 254 nm. ^{1}H, ^{13}C NMR, ^{19}F NMR, ^{31}P NMR spectra were recorded on a Bruker 400 MHz spectrometer. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26, Acetone δ 2.05, MeOH δ 3.31), carbon (chloroform δ 77.16) or tetramethylsilane (TMS δ 0.00) was used as a reference. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), bs (broad singlet). Coupling constants were reported in Hertz (Hz). All high resolution mass spectra were obtained on Waters Xevo G2 QTof Mass Spectrometer. Flash chromatography separations were performed on Silica gel (200-300 mesh) supplied by Tsingdao Haiyang Chemicals (China).

General procedure for the synthesis of amidines [1-3]

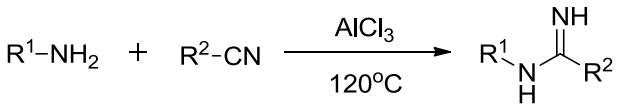
Procedure A:



A round bottom flask (25 mL in volume) was charged with NaH (60% in mineral oil) (300 mg, 7.5 mmol, 60%, 1.5 equiv). Under a stream of Ar, DMSO (2.5 mL) was added, and the resulting suspension was cooled with an ice-water bath prior to the addition of the aniline (5.5 mmol, 1.1 equiv) and the carbonitrile (5.0 mmol). The mixture was kept at 0 ℃ for 30-60 min and then stirred at room temperature until the starting material was consumed as monitored by TLC analysis. Ice-water (25 mL) was

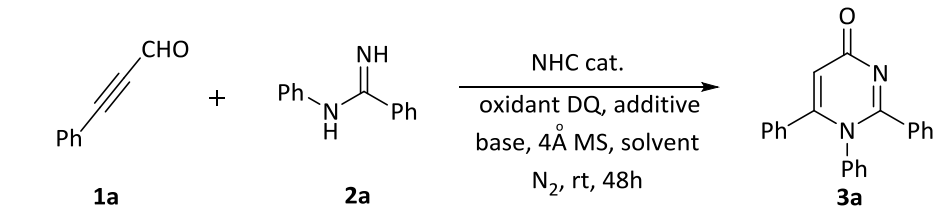
added while maintaining vigorous stirring. In the cases when the amidine precipitated upon addition of water, the solid was filtered off and dissolved in EtOAc (20 mL). In all other cases, the aqueous layer was extracted with EtOAc (3 × 20 mL). The extracts were combined and washed with water (2 × 25 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified either by silica gel chromatography or upon recrystallization to provide the corresponding amidine derivatives (R^2 = aryl).

Procedure B:



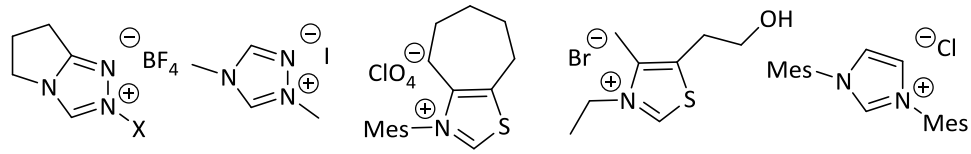
A pressure flask (50 mL in volume) equipped with a stirrer bar was charged with aniline (5.5 mmol, 1.1 equiv) and carbonitrile (5.0 mmol) under air. $AlCl_3$ (5.0 mmol, 1.0 equiv) was added in one portion. The flask was tightly sealed with a screw cap and lowered into a preheated oil bath at 120 ℃. The reaction mixture was stirred until it was completed, and taken out of the oil bath. Ice-water (25 mL) was then added to the hot mixture while maintaining vigorous stirring. If necessary, the mixture was warmed with a heat gun to obtain a homogenous aqueous solution, before it was transferred into a separatory funnel. Concentrated aqueous NaOH was added until a pH of 14 was reached, and the aqueous layer was extracted with EtOAc (3 × 20 mL). The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was either purified by silica gel chromatography or upon recrystallization to provide the corresponding amidine derivatives (R^2 = alkyl)**.**

Optimization of the reaction conditions



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

NHC cat.



A: X = Mes
B: X = C_6F_5

C **D** **E** **F**

Table S1. The effect of catalysts and additives[a]

Entry	Cat.	Additive	Yield (%)[b]
1	A	-	trace
2	B	-	trace
3	C	-	trace
4	D	-	33
5	E	-	13
6	F	-	trace
7	D	LiCl	35
8	D	$Sc(OTf)_3$	52
9	D	$Cu(OTf)_2$	43
10	D	$Mg(OTf)_2$	78
11	D	$Al(OTf)_3$	66

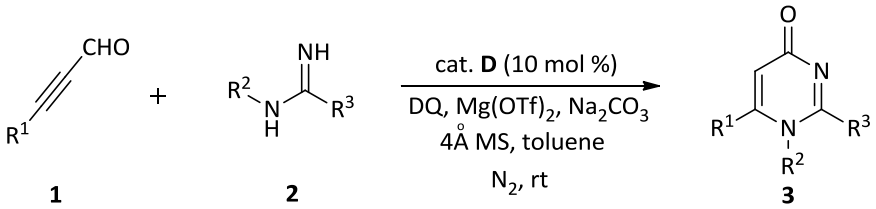
[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.1 mmol), cat. **A**-**F** (10 mol%), NaH (150 mol%), 3,3',5,5'-tetra-*tert*-butyldiphenoquinone (DQ) (0.2 mmol), additive (20 mol%), 4Å MS, toluene (1.0 mL), room temperature, 48h. [b] Isolated yield after flash chromatograph.

Table S2. The effect of base and solvent[a]

Entry	Base	Solvent	Yield (%)[b]
1	NaH	Toluene	78
2	LiO*t*-Bu	Toluene	68
3	K_2CO_3	Toluene	77
4	Na_2CO_3	Toluene	87
5	Cs_2CO_3	Toluene	84
6	$KHCO_3$	Toluene	83
7	K_2HPO_4	Toluene	84
8	Na_2HPO_4	Toluene	83
9	Et_3N	Toluene	22
10	Na_2CO_3	THF	23
11	Na_2CO_3	Et_2O	18
12	Na_2CO_3	CH_2Cl_2	16
13	Na_2CO_3	CH_3CN	12
14[c]	Na_2CO_3	Toluene	89
15[d]	Na_2CO_3	Toluene	86
16[e]	Na_2CO_3	Toluene	93
17[f]	Na_2CO_3	Toluene	82
18[g]	Na_2CO_3	Toluene	92
19[h]	Na_2CO_3	Toluene	81

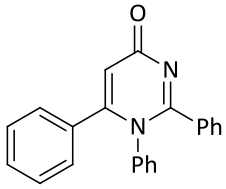
[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.1 mmol), Cat. **D** (10 mol%), base (150 mol%), DQ (200 mol%), $Mg(OTf)_2$ (20 mol%), 4Å MS, toluene (1.0 mL), room temperature, 48h. [b] Isolated yield after flash chromatograph. [c] DQ (0.15 mmol). [d] DQ (0.12 mmol). [e] DQ (0.12 mmol), **1a** (0.15 mmol). [f] DQ (0.12 mmol), **1a** (0.12 mmol). [g] DQ (0.12 mmol), **1a** (0.15 mmol), Na_2CO_3 (50 mol%). [h] DQ (0.12 mmol), **1a** (0.15 mmol), Na_2CO_3 (20 mol%).

General procedure for Thiazolium-catalyzed Annulation of Ynals with Amidines

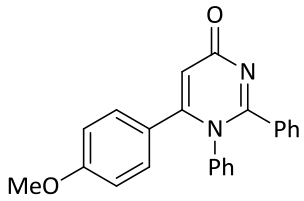


In a nitrogen-filled glovebox, to a flame-dried Schlenk tube was added amidine **2** (0.10 mmol), pre-catalyst **D** (3.7 mg, 0.01 mmol), Na_2CO_3 (5.3 mg, 0.05 mmol), $Mg(OTf)_2$ (6.4 mg, 0.02 mmol), 4 Å molecular sieves and DQ (49.0 mg, 0.12 mmol), then aldehyde **1** (0.15 mmol) in dry toluene (1.0 ml) was added. The mixture was stirred at room temperature (or indicated temperature) until the reaction was completed (monitored by TLC). The mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (DCM to DCM/MeOH = 10:1) to afford the desired product.

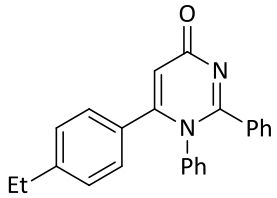
Characterization data



3a: 48 h, Yield = 92%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.6 Hz, 2H), 7.22 – 7.00 (m, 11H), 6.94-6.83 (m, 2H), 6.30 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.0, 161.2, 154.8, 138.7, 134.7, 133.3, 129.6, 129.5, 129.3, 129.3, 129.0, 128.9, 128.7, 128.2, 127.7, 112.1; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{17}N_2O$ ($[M + H]^+$) 325.1341, found: 325.1340.

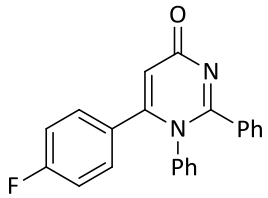


3b: 36 h, Yield = 89%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.2 Hz, 2H), 7.25 – 7.04 (m, 6H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.94-6.84 (m, 2H), 6.69 (d, *J* = 8.8 Hz, 2H), 6.31 (s, 1H), 3.73 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.2, 161.3, 160.2, 154.7, 138.9, 134.8, 130.5, 129.6, 129.5, 129.3, 128.9, 128.7, 127.8, 125.6, 113.7, 112.1, 55.3; **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O_2$ ($[M + H]^+$) 355.1447, found: 355.1445.

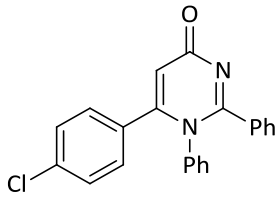


3c: 36 h, Yield = 94%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 2H), 7.11-7.04 (m, 3H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.89-6.84 (m, 2H), 6.33 (s, 1H), 2.55 (q, *J* = 7.6

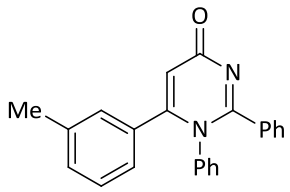
Hz, 2H), 1.15 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.1, 161.2, 154.9, 145.8, 138.9, 134.8, 130.7, 129.6, 129.6, 129.4, 129.0, 128.9, 128.7, 127.8, 127.8, 112.2, 28.6, 15.2; **HRMS** (ESI): *m/z*: calculated for $C_{24}H_{21}N_2O$ ($[M + H]^+$) 353.1654, found: 353.1656.



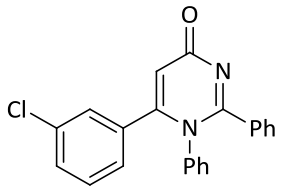
3d: 60 h, Yield = 67%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.2 Hz, 2H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.17 – 7.04 (m, 7H), 6.94-6.84 (m, 4H), 6.30 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.9, 164.2, 161.8, 161.4, 153.8, 138.7, 134.6, 131.1, 131.1, 129.7, 129.6, 129.5, 129.5, 129.4, 129.1, 128.9, 127.8, 115.7, 115.5, 112.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -110.5; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}FN_2O$ ($[M + H]^+$) 343.1247, found: 343.1245.



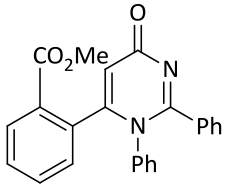
3e: 60 h, Yield = 74%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 2H), 7.25 – 7.20 (m, 1H), 7.20 – 7.07 (m, 7H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.93 – 6.86 (m, 2H), 6.30 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.8, 161.4, 153.6, 138.6, 135.8, 134.6, 131.8, 130.4, 129.8, 129.6, 129.4, 129.2, 129.1, 128.7, 127.9, 112.4; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}ClN_2O$ ($[M + H]^+$) 359.0951, found: 359.0953.



3f: 48 h, Yield = 94%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 2H), 7.09 – 7.01 (m, 5H), 6.91 – 6.80 (m, 4H), 6.33 (s, 1H), 2.20 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.3, 161.3, 155.1, 138.8, 138.1, 134.7, 133.2, 130.1, 129.7, 129.7, 129.6, 129.4, 128.9, 128.8, 128.1, 127.8, 126.1, 112.2, 21.3. **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O$ ($[M + H]^+$) 339.1497, found: 339.1493.

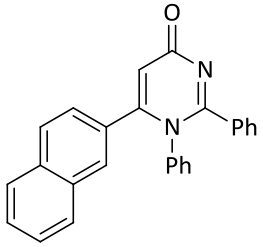


3g: 60 h, Yield = 75%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32-7.25 (m, 2H), 7.25-7.19 (m, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.14-7.07 (m, 5H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.93-6.87 (m, 2H), 6.31 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 161.4, 153.3, 138.5, 134.9, 134.5, 134.4, 129.8, 129.6, 129.5, 129.4, 129.2, 129.1, 129.1, 127.9, 127.2, 112.4; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}ClN_2O$ ($[M + H]^+$) 359.0951, found: 359.0951.

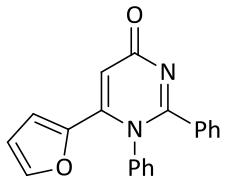


3h: 48 h, Yield = 83%, light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0, 1H), 7.46-7.39 (m, 1H), 7.37-7.29 (m, 3H), 7.28 – 7.23 (m, 1H), 7.22 – 7.15 (m, 1H), 7.12 (m, 2H), 7.04 – 6.90 (m, 4H), 6.90 – 6.79 (m, 1H), 6.18 (s, 1H), 3.80 (s, 3H);

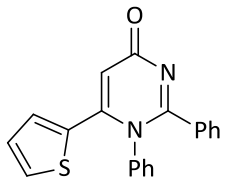
^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 165.8, 160.9, 154.9, 138.8, 134.7, 134.2, 132.2, 131.1, 130.4, 129.7, 129.6, 129.5, 129.4, 129.2, 128.7, 128.6, 128.5, 127.7, 110.8, 52.5; **HRMS** (ESI): *m/z*: calculated for $C_{24}H_{19}N_2O_3$ ($[M + H]^+$) 383.1396, found: 383.1395.



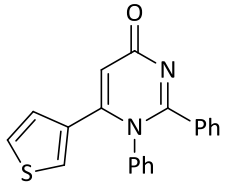
3i: 60 h, Yield = 76%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79-7.71 (m, 3H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.34 – 7.28 (m, 2H), 7.26 – 7.20 (m, 1H), 7.20-7.13 (m, 2H), 7.06 – 6.98 (m, 4H), 6.96 – 6.90 (m, 2H), 6.44 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 161.3, 154.8, 138.8, 134.7, 133.0, 132.6, 130.9, 129.7, 129.6, 129.4, 129.2, 129.0, 128.8, 128.4, 127.9, 127.8, 127.6, 127.1, 125.5, 112.7; **HRMS** (ESI): *m/z*: calculated for $C_{26}H_{19}N_2O$ ($[M + H]^+$) 375.1497, found: 375.1498.



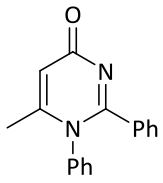
3j: 60 h, Yield = 86%, light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.36 (m, 1H), 7.36 – 7.26 (m, 3H), 7.25 – 7.17 (m, 3H), 7.17 – 7.09 (m, 4H), 6.77 (s, 1H), 6.21 (dd, *J* = 3.6, 1.8 Hz, 1H), 5.29 (d, *J* = 3.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.3, 161.6, 144.9, 144.5, 144.2, 138.9, 134.4, 130.0, 129.6, 129.5, 129.5, 129.1, 127.8, 114.9, 112.0, 109.0; **HRMS** (ESI): *m/z*: calculated for $C_{20}H_{15}N_2O_2$ ($[M + H]^+$) 315.1134, found: 315.1136.



3k: 48 h, Yield = 97%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 5.0 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.24 – 7.11 (m, 6H), 7.02 (d, *J* = 7.4 Hz, 2H), 6.87 – 6.82 (m, 1H), 6.77 (d, *J* = 3.5 Hz, 1H), 6.51 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.8, 161.6, 148.2, 138.7, 134.7, 133.7, 130.6, 129.8, 129.7, 129.6, 129.5, 129.2, 127.8, 127.2, 112.7; **HRMS** (ESI): *m/z*: calculated for $C_{20}H_{15}N_2OS$ ($[M + H]^+$) 331.0905, found: 331.0904.

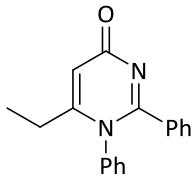


3l: 36 h, Yield = 96%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 6.8 Hz, 2H), 7.23 – 7.11 (m, 7H), 7.10-7.06 (m, 1H), 6.96 (d, *J* = 7.2 Hz, 2H), 6.55 (d, *J* = 4.8 Hz, 1H), 6.39 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 161.3, 150.1, 138.9, 134.7, 133.6, 129.6, 129.4, 129.3, 129.1, 127.8, 127.6, 127.4, 126.1, 112.0; **HRMS** (ESI): *m/z*: calculated for $C_{20}H_{15}N_2OS$ ($[M + H]^+$) 331.0905, found: 331.0902.

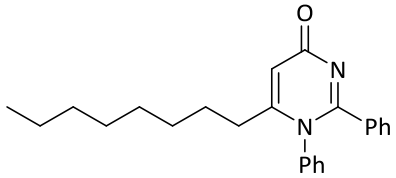


3m: 48 h, Yield = 71%, light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 3H), 7.26-7.22 (m, 2H), 7.21 – 7.15 (m, 1H), 7.15 – 7.08 (m, 4H), 6.21 (m, 1H), 1.97 (d, *J* = 0.9 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.3, 161.3, 151.8, 138.7,

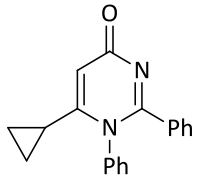
134.5, 129.7, 129.6, 129.6, 129.3, 128.9, 127.8, 111.0, 21.2.; **HRMS** (ESI): *m/z*: calculated for $C_{17}H_{15}N_2O$ ($[M + H]^+$) 263.1184, found: 263.1181.



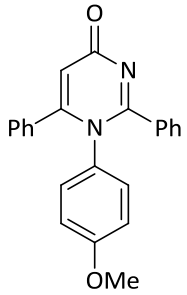
3n: 48 h, Yield = 62%, light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 3H), 7.25 – 7.21 (m, 2H), 7.20 – 7.15 (m, 1H), 7.15 – 7.09 (m, 4H), 6.25 (m, 1H), 2.27-2.15 (m, 2H), 1.09 (t, *J* = 7.4 Hz, 3H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.54, 161.41, 156.63, 138.27, 134.71, 129.61, 129.60, 129.45, 129.26, 129.21, 127.76, 108.79, 26.30, 11.42. **HRMS** (ESI): *m/z*: calculated for $C_{18}H_{17}N_2O$ ($[M + H]^+$) 277.1341, found: 277.1344.



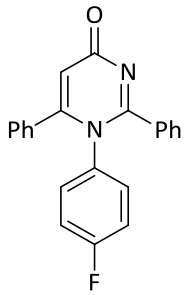
3o: 48 h, Yield = 58%, light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 3H), 7.25 – 7.20 (m, 2H), 7.21 – 7.15 (m, 1H), 7.15 – 7.08 (m, 4H), 6.23 (s, 1H), 2.24 – 2.12 (m, 2H), 1.47-1.36 (m, 2H), 1.28 – 1.09 (m, 10H), 0.85 (t, *J* = 7.0 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)δ 170.45, 161.45, 155.59, 138.27, 134.75, 129.60, 129.55, 129.44, 129.30, 129.20, 127.76, 109.68, 32.87, 31.81, 29.13, 29.07, 29.03, 27.46, 22.70, 14.18.; **HRMS** (ESI): *m/z*: calculated for $C_{24}H_{29}N_2O$ ($[M + H]^+$) 361.2280, found: 361.2283.



3p: 96 h, Yield = 67%, light brown solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37-7.28 (m, 3H), 7.25 (d, *J* = 6.4 Hz, 2H), 7.22 – 7.08 (m, 5H), 6.00 (s, 1H), 1.30-1.18 (m, 1H), 0.85-0.72 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.8, 161.4, 156.9, 138.8, 134.7, 129.5, 129.5, 129.4, 129.3, 127.8, 106.4, 14.0, 8.9; **HRMS** (ESI): *m/z*: calculated for $C_{19}H_{17}N_2O$ ($[M + H]^+$) 289.1341, found: 289.1343.

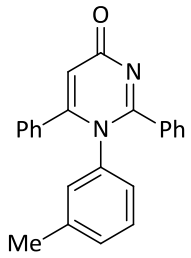


4a: 42 h, Yield = 88%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.11 (m, 8H), 7.08 (d, *J* = 7.0 Hz, 2H), 6.77 (d, *J* = 8.8 Hz, 2H), 6.54 (d, *J* = 8.8 Hz, 2H), 6.32 (s, 1H), 3.65 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.0, 161.6, 159.1, 155.1, 134.8, 133.4, 131.3, 130.5, 129.3, 129.2, 129.1, 128.9, 128.2, 127.7, 113.8, 112.0, 55.3; **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O_2$ ($[M + H]^+$) 355.1447, found: 355.1446 .

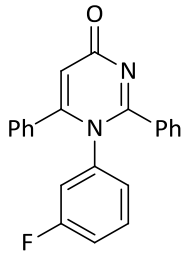


4b: 36 h, Yield = 91%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.13 (m, 8H), 7.09 (d, *J* = 6.8 Hz, 2H), 6.94-6.86 (m, 2H), 6.75 (t, *J* = 8.4 Hz, 2H), 6.31 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.9, 163.2, 161.4, 160.7, 154.8, 134.9, 134.9, 134.6, 133.2, 131.5, 131.4, 129.8, 129.5, 129.3, 129.0, 128.5, 128.0, 116.2, 115.9, 112.3; **^{19}F**

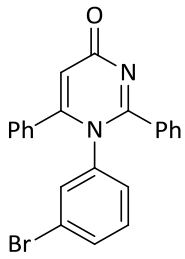
NMR (376 MHz, $CDCl_3$) δ -110.8; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}FN_2O$ ($[M + H]^+$) 343.1247, found: 343.1248.



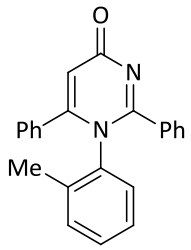
4c: 48 h, Yield = 96%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (m, 2H), 7.25 – 7.12 (m, 6H), 7.09-7.04 (m, 2H), 6.95 – 6.89 (m, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.69 – 6.63 (m, 2H), 6.32 (s, 1H), 2.07 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.1, 161.3, 154.8, 139.1, 138.6, 134.8, 133.4, 130.1, 129.6, 129.4, 129.3, 128.9, 128.6, 128.2, 127.7, 126.6, 112.2, 21.0; **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O$ ($[M + H]^+$) 339.1497, found: 339.1492.



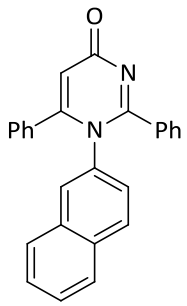
4d: 84 h, Yield = 71%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 2H), 7.27-7.24 (m, 1H), 7.24-7.14 (m, 5H), 7.13 – 7.08 (m, 2H), 7.07-6.99 (m, 1H), 6.83-6.77 (m, 1H), 6.77-6.72 (m, 1H), 6.70-6.65 (m, 1H), 6.30 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 163.4, 161.0, 160.9, 154.5, 140.1, 140.0, 134.4, 133.0, 130.1, 130.0, 129.9, 129.6, 129.2, 128.9, 128.5, 127.9, 125.8, 125.8, 117.5, 117.3, 116.2, 116.0, 112.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -110.34; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}FN_2O$ ($[M + H]^+$) 343.1247, found: 343.1246.



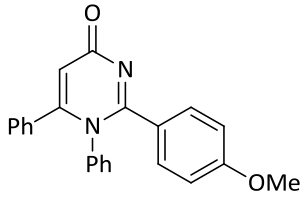
4e: 84 h, Yield = 69%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 2H), 7.27 – 7.15 (m, 7H), 7.13 – 7.06 (m, 3H), 6.93 (t, *J* = 7.8 Hz, 1H), 6.90-6.85 (m, 1H), 6.31 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 161.0, 154.5, 139.9, 134.3, 132.9, 132.8, 131.9, 130.0, 129.9, 129.7, 129.3, 129.0, 128.5, 128.4, 128.0, 122.2, 112.2; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}BrN_2O$ ($[M + H]^+$) 403.0446, found: 403.0446.



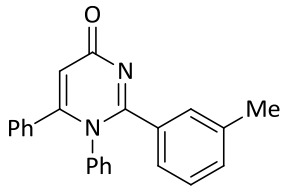
4f: 54 h, Yield = 94%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 2H), 7.25 – 7.11 (m, 6H), 7.08 – 6.87 (m, 6H), 6.35 (s, 1H), 1.96 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.2, 161.4, 154.9, 137.6, 135.4, 134.4, 133.0, 131.2, 130.7, 129.9, 129.6, 129.6, 129.2, 128.7, 128.2, 127.7, 126.4, 112.4, 18.0; **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O$ ($[M + H]^+$) 339.1497, found: 339.1495.



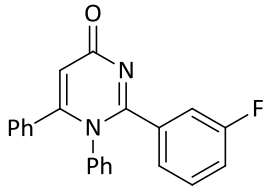
4g: 84 h, Yield = 79%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.7 Hz, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.38-7.36 (m, 1H), 7.36 – 7.30 (m, 2H), 7.17 – 7.03 (m, 8H), 6.97 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.37 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 161.5, 155.0, 136.1, 134.7, 133.4, 132.4, 132.2, 129.7, 129.4, 129.3, 129.0, 128.9, 128.9, 128.3, 128.0, 127.8, 127.8, 127.6, 127.3, 126.5, 112.3; **HRMS** (ESI) calculated for $C_{26}H_{19}N_2O$ ($[M + H]^+$) 375.1497 , found: 375.1494.



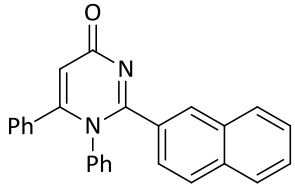
4h: 54 h, Yield = 96%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23 – 7.10 (m, 5H), 7.07 – 7.01 (m, 5H), 6.93 – 6.86 (m, 2H), 6.58 (d, *J* = 8.9 Hz, 2H), 6.23 (s, 1H), 3.66 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.1, 160.8, 160.4, 154.9, 139.0, 133.4, 131.4, 129.6, 129.1, 128.9, 128.8, 128.6, 128.1, 126.8, 113.0, 111.8, 55.2; **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O_2$ $(M + H]^+$) 355.1447, found: 355.1442 .



4i: 36 h, Yield = 82%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25 – 7.15 (m, 4H), 7.10 – 7.04 (m, 5H), 7.03-6.98 (m, 1H), 6.98 – 6.95 (m, 2H), 6.90 – 6.85 (m, 2H), 6.31 (s, 1H), 2.19 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.0, 161.4, 154.7, 138.9, 137.7, 134.6, 133.4, 130.4, 130.3, 129.6, 129.3, 129.0, 128.8, 128.7, 128.3, 127.5, 126.4, 112.2, 21.2; **HRMS** (ESI): *m/z*: calculated for $C_{23}H_{19}N_2O$ ($[M + H]^+$) 339.1497, found: 339.1500 .

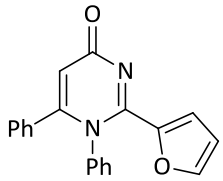


4j: 96 h, Yield = 71%, white solid; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 7.32–7.15 (m, 10H), 7.13 – 7.03 (m, 4H), 6.15 (s, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 161.9 (d, *J* = 246.0 Hz), 159.9 (d, *J* = 2.0 Hz), 154.8, 138.5, 136.6 (d, *J* = 8.0 Hz), 133.1, 129.6, 129.5, 129.5, 129.1, 129.1, 129.0, 128.3, 125.2 (d, *J* = 3.0 Hz), 116.8 (d, *J* = 21.0 Hz), 116.7(d, *J* = 24.0 Hz), 112.4; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.5; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{16}FN_2O$ ($[M + H]^+$) 343.1247, found: 343.1247.

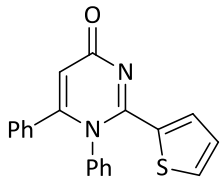


4k: 36 h, Yield = 85%, white solid; **^{1}H NMR** (400 MHz, Methanol-d_4, 50^{o}C) δ 7.92 (s, 1H), 7.75 (t, *J* = 6.2 Hz, 2H), 7.67 (d, *J* = 8.6 Hz, 1H), 7.52-7.43 (m, 2H), 7.40 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.31 – 7.20 (m, 5H), 7.19-7.12 (m, 2H), 7.07 – 7.00 (m, 3H), 6.40 (s, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.1, 161.2, 154.9, 138.8, 133.4, 133.3, 132.3, 132.0, 130.5, 129.7, 129.3, 129.0, 128.9, 128.8, 128.7, 128.3, 127.6, 127.5,

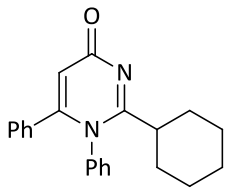
127.2, 126.6, 125.7, 112.3; **HRMS** (ESI): *m/z*: calculated for $C_{26}H_{19}N_2O$ ($[M + H]^+$) 375.1497, found: 375.1495.



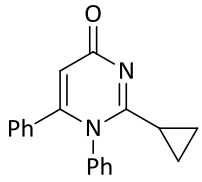
4l: 48h, Yield = 71%, white solid; **^{1}H NMR** (400 MHz, Acetone-d_6) δ 7.49 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.35 – 7.22 (m, 8H), 6.37 (dd, *J* = 3.6, 1.8 Hz, 1H), 6.09 (dd, *J* = 3.6, 0.8 Hz, 1H), 5.98 (s, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 154.6, 150.7, 146.1, 145.7, 138.5, 132.8, 129.5, 129.3, 129.2, 129.2, 129.1, 128.1, 118.5, 111.9, 111.8; **HRMS** (ESI): *m/z*: calculated for $C_{20}H_{15}N_2O_2$ ($[M + H]^+$) 315.1134, found: 315.1131.



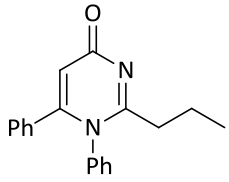
4m: 48 h, Yield = 73%, pale red solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.26 (m, 4H), 7.24 – 7.16 (m, 3H), 7.15 – 7.10 (m, 2H), 7.09-7.03 (m, 2H), 6.75 (dd, *J* = 5.1, 4.0 Hz, 1H), 6.47-6.42 (m, 1H), 6.24 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.7, 154.8, 154.5, 138.5, 137.3, 133.1, 132.9, 132.6, 130.1, 129.9, 129.7, 129.3, 129.2, 128.2, 127.5, 112.0; **HRMS** (ESI): *m/z*: calculated for $C_{20}H_{15}N_2OS$ ($[M + H]^+$) 331.0905, found: 331.0902.



4n: 24h, Yield = 95%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33-7.25 (m, 3H), 7.22-7.11 (m, 3H), 7.08 – 7.01 (m, 4H), 6.17 (s, 1H), 2.28-2.17 (m, 1H), 1.88 – 1.76 (m, 2H), 1.75-1.63 (m, 4H), 1.59-1.48 (m, 1H), 1.26 – 1.11 (m, 1H), 0.99-0.83 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.8, 167.2, 154.4, 138.2, 133.5, 129.6, 129.5, 129.2, 129.0, 128.9, 128.2, 111.3, 42.5, 31.1, 25.8, 25.4; **HRMS** (ESI): *m/z*: calculated for $C_{22}H_{23}N_2O$ ($[M + H]^+$) 331.1810, found: 331.1811.

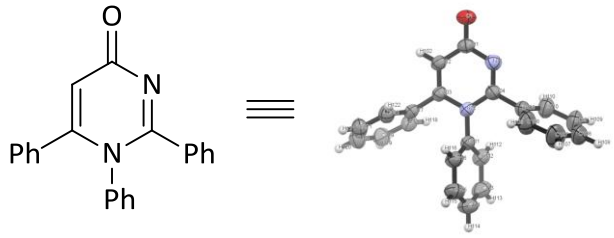


4o: 24 h, Yield = 87%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 3H), 7.22 – 7.12 (m, 5H), 7.07-7.00 (m, 2H), 6.15 (s, 1H), 1.42-1.31 (m, 3H), 0.88-0.80 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.6, 165.1, 154.3, 138.3, 133.3, 129.6, 129.5, 129.2, 129.0, 128.2, 111.2, 14.2, 11.8; **HRMS** (ESI): *m/z*: calculated for $C_{19}H_{17}N_2O$ ($[M + H]^+$) 289.1341, found: 289.1343 .



4p: 24 h, Yield = 68%, white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34-7.27 (m, 3H), 7.22 – 7.13 (m, 3H), 7.10-7.02 (m, 4H), 6.20 (s, 1H), 2.38 – 2.29 (m, 2H), 1.80 – 1.68 (m, 2H), 0.84 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.5, 163.5, 154.5, 138.3, 133.3, 129.6, 129.6, 129.3, 129.0, 129.0, 128.2, 111.3, 37.6, 20.5, 13.9; **HRMS** (ESI): *m/z*: calculated for $C_{19}H_{19}N_2O$ ($[M + H]^+$) 291.1497, found: 291.1499.

Crystal structure of 3a



Basic information pertaining to crystal parameters and structure refinement is summarized in Table S3.

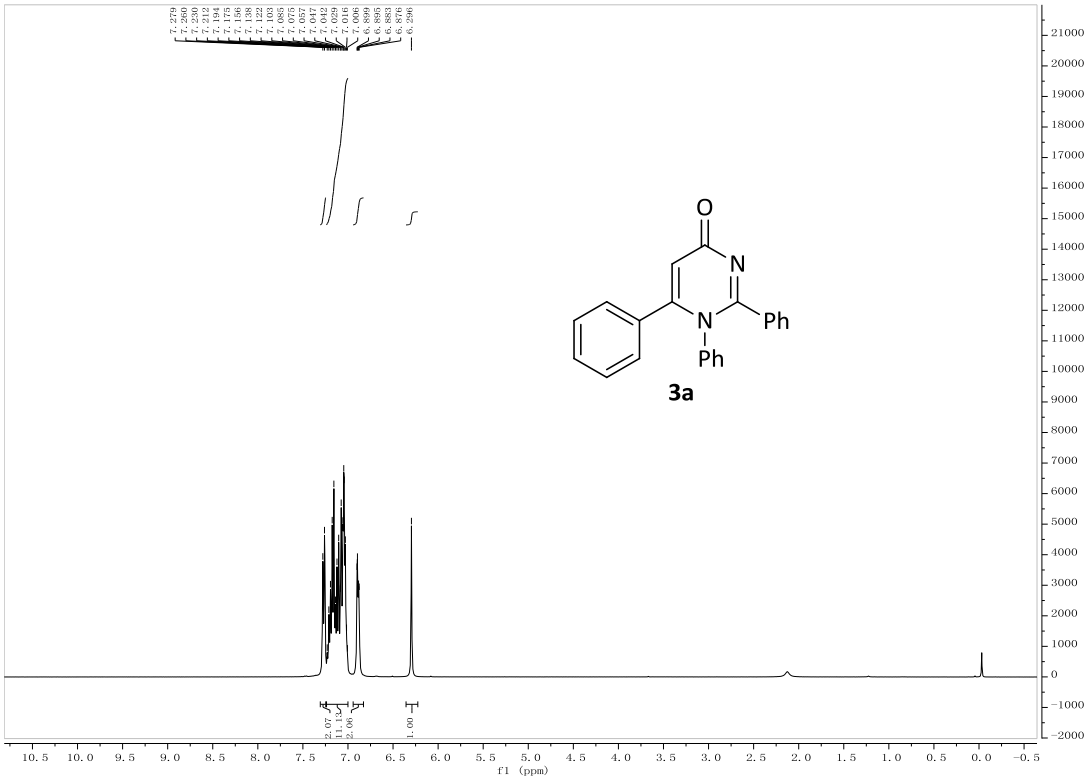
Table S3 Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{22}H_{16}N_2O$
Formula weight	324.37
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	23.5316(6)
b/Å	6.70060(10)
c/Å	24.2907(6)
α/°	90
β/°	115.166(3)
γ/°	90
Volume/Å^3	3466.50(15)
Z	8
ρ_{calc}g/cm^3	1.243
μ/mm^{-1}	0.609
F(000)	1360.0
Crystal size/mm^3	0.3 × 0.2 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.316 to 143.044
Index ranges	-27 ≤ h ≤ 28, -5 ≤ k ≤ 7, -29 ≤ l ≤ 28
Reflections collected	12227
Independent reflections	6491 [R_{int} = 0.0161, R_{sigma} = 0.0209]
Data/restraints/parameters	6491/0/451
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0461, wR_2 = 0.1213
Final R indexes [all data]	R_1 = 0.0586, wR_2 = 0.1328
Largest diff. peak/hole / e Å^{-3}	0.20/-0.18

References:

1. Digwal, C. S.; Yadav, U.; Sri Ramya, P. V.; Sana, S.; Swain, B.; Kamal, A. *J. Org. Chem.* **2017**, *82*, 7332−7345.
2. Wang, Y.; Wang, H. G.; Peng, J. L.; Zhu, Q. *Org. Lett.* **2011**, *13*, 4604–4607.
3. Ohta, Y.; Tokimizu, Y.; Oishi, S.; Fujii, N.; Ohno, H. *Org. Lett.* **2010**, *12*, 3963–3965.

NMR Spectra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7.122
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7.057
7.047
7.029
7.016
7.006
6.899
6.895
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6.876
6.296
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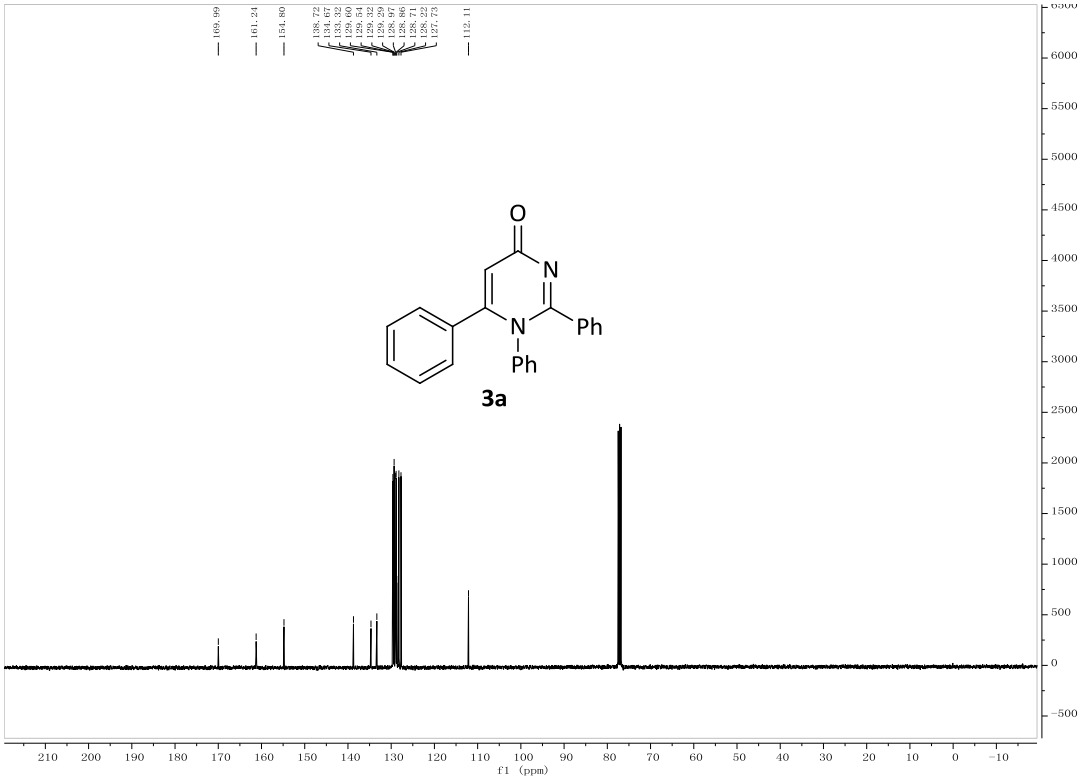
N
N
Ph
Ph
3a
2.07
1.13
2.06
1.00
f1 (ppm)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N
Ph
Ph
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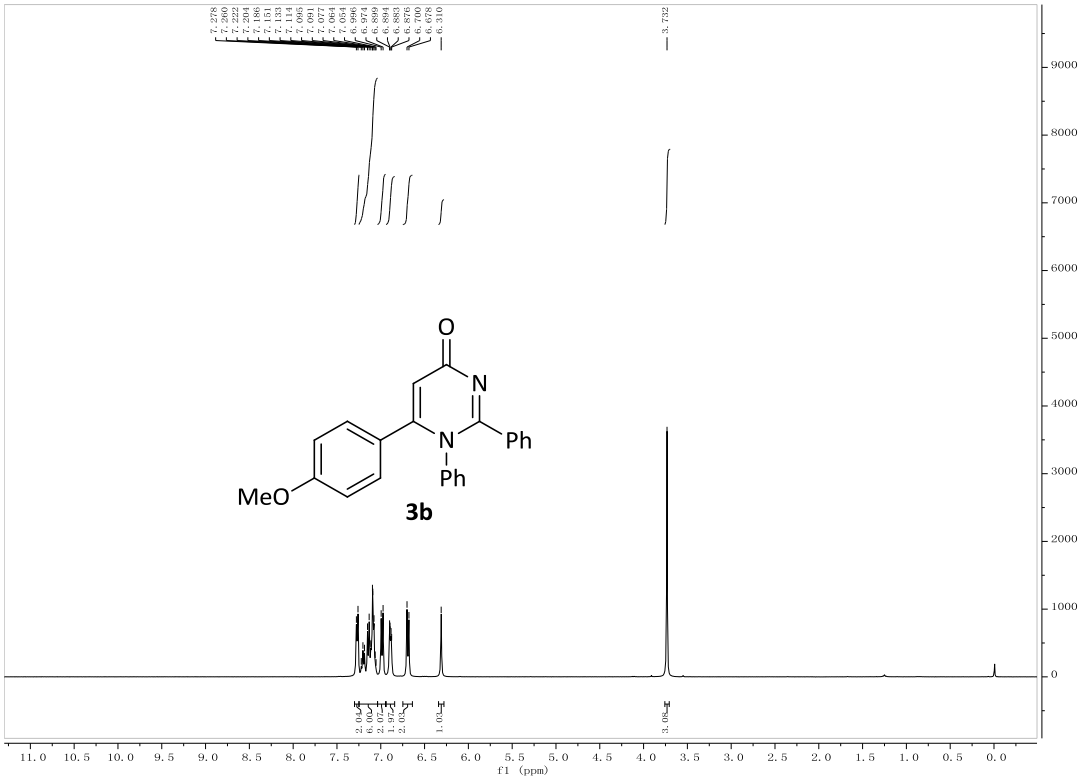
f1 (ppm)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6.954
6.889
6.884
6.883
6.878
6.700
6.678
6.310
3.732
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Ph
MeO
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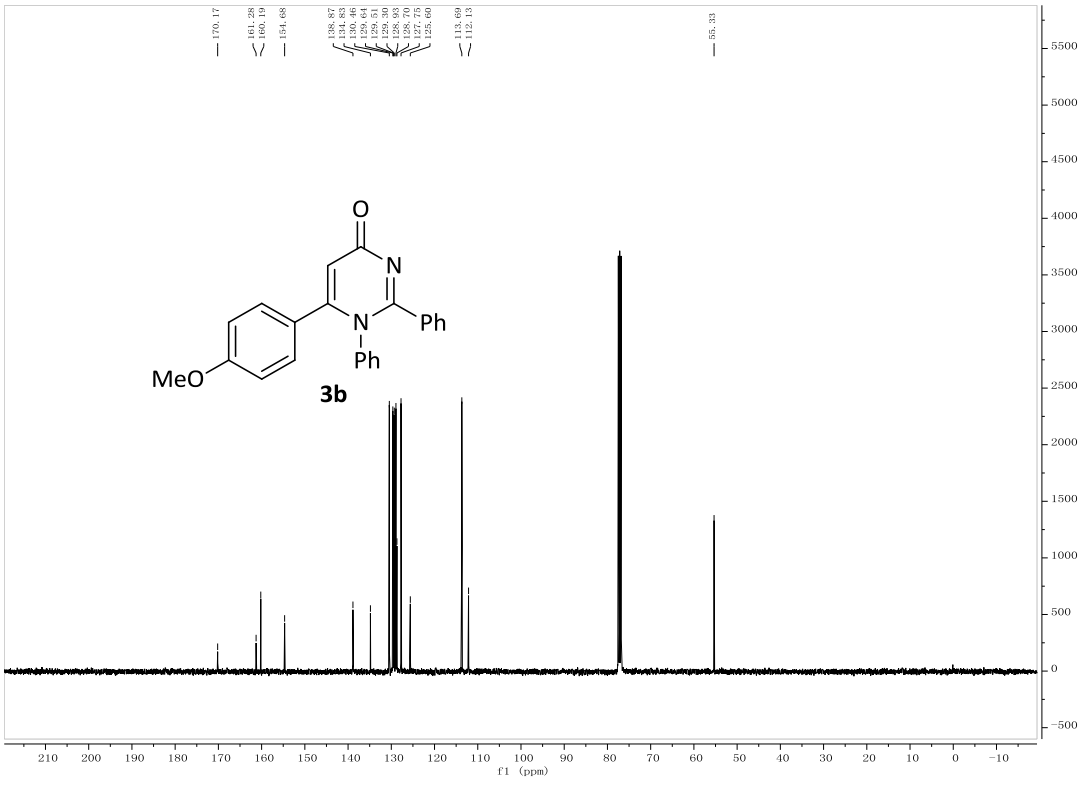
3.08
f1 (ppm)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113.69
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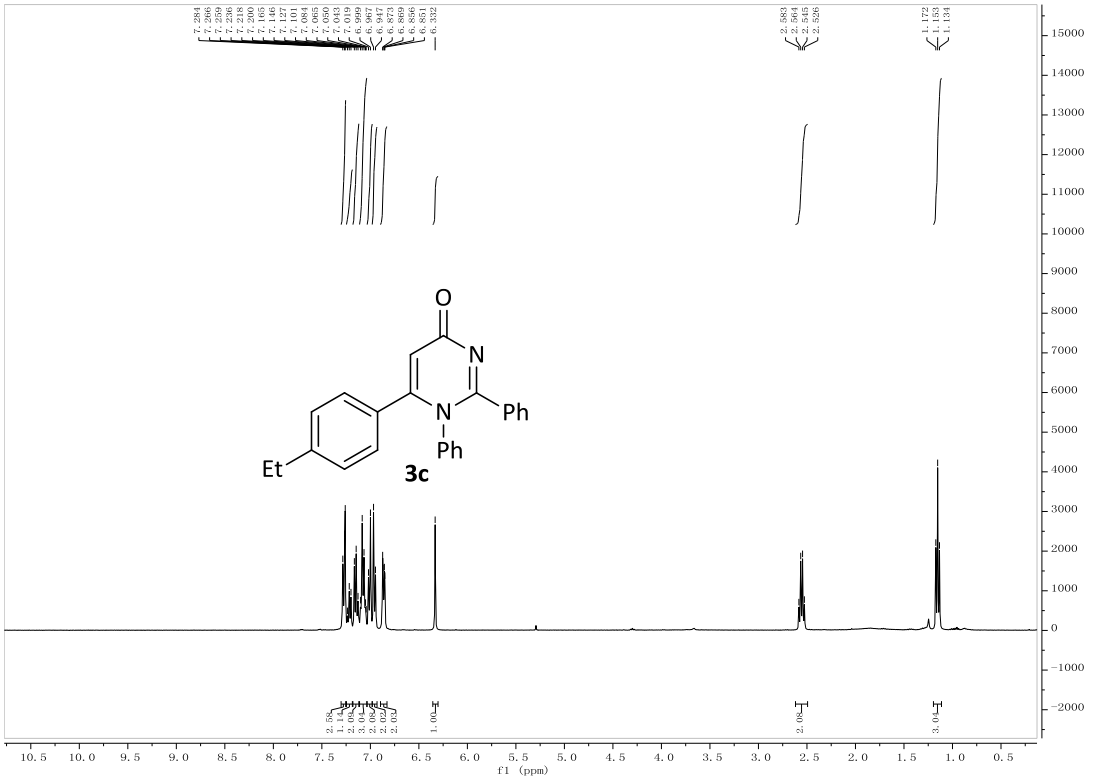
N
Ph
Ph
MeO
3b
f1 (ppm)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7.045
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6.947
6.873
6.869
6.856
6.851
6.332
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2.564
2.545
2.526
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1.153
1.134
O
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N
Ph
Ph
Et
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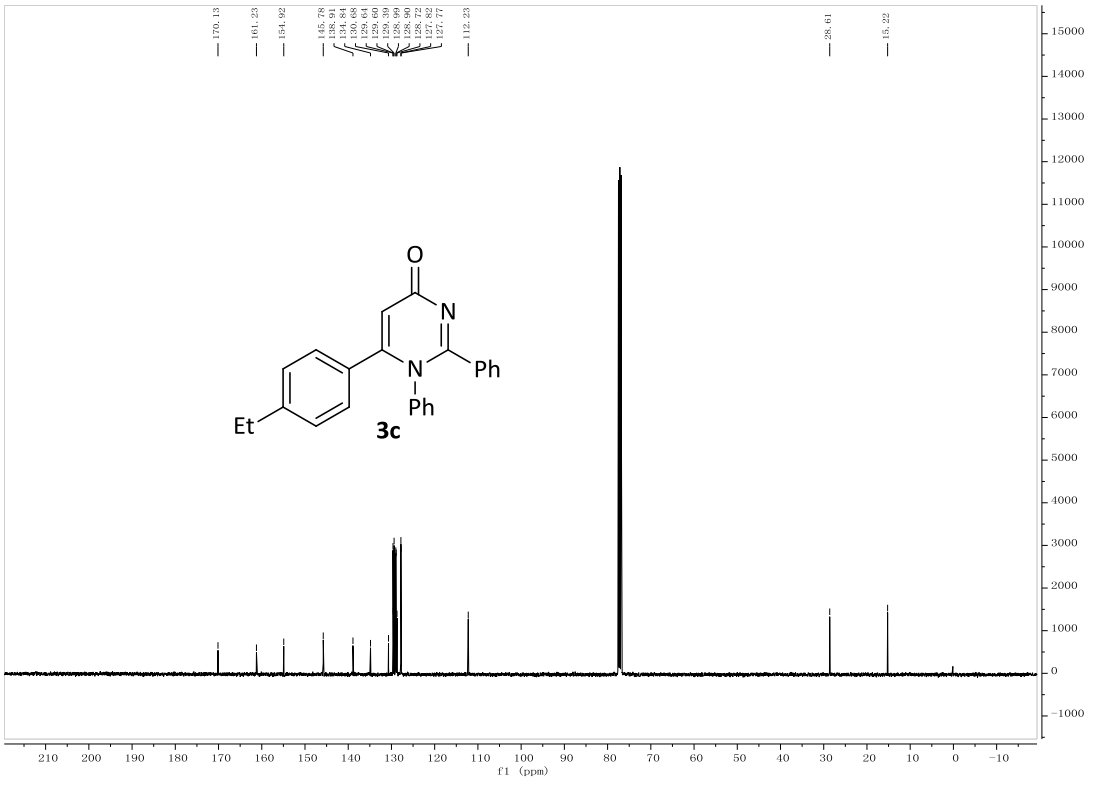
f1 (ppm)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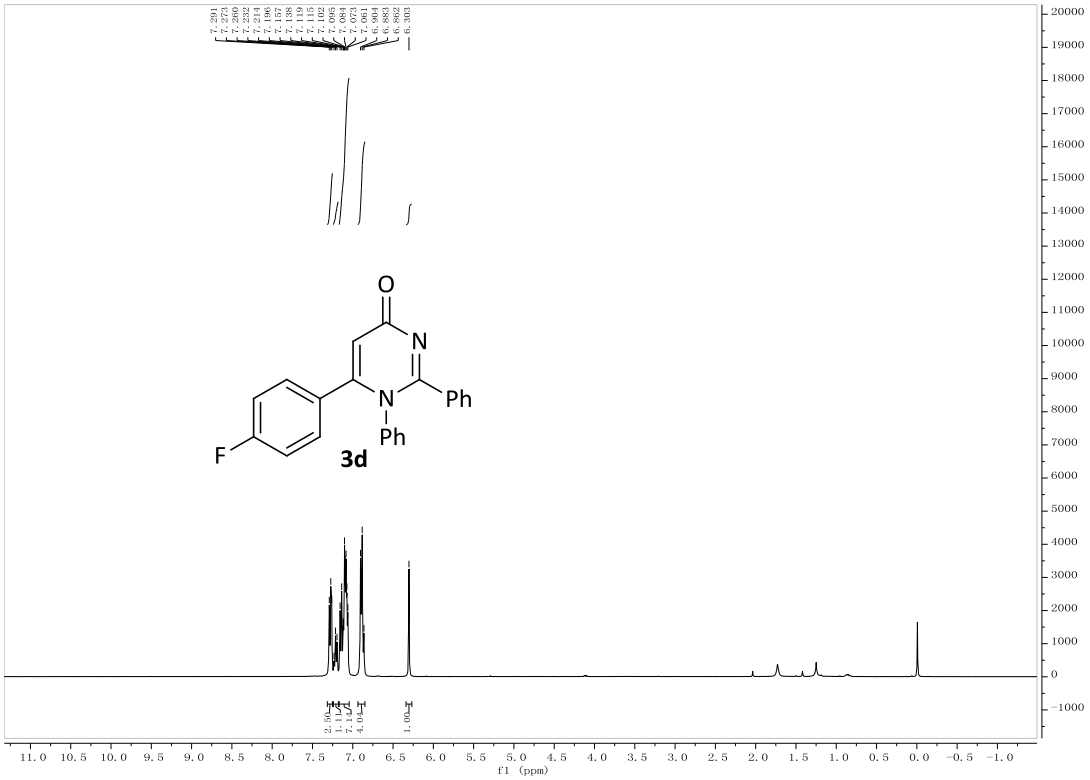
N
Ph
Ph
Et
3c
f1 (ppm)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7.073
7.061
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6.883
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N
Ph
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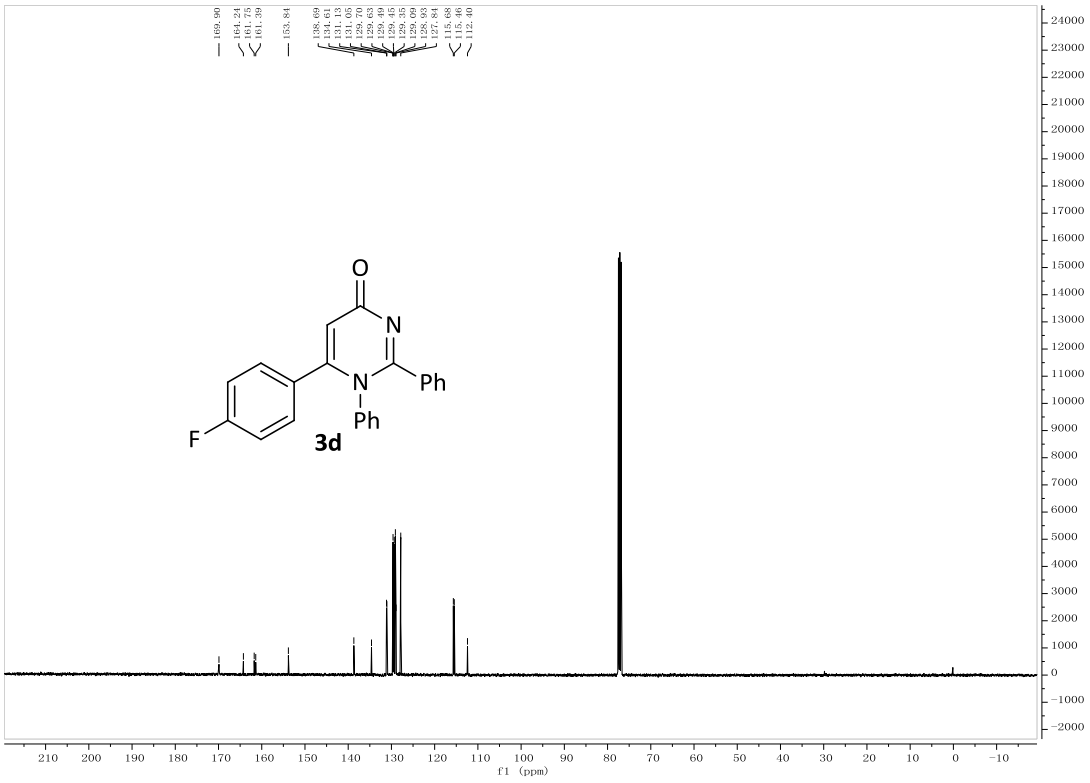
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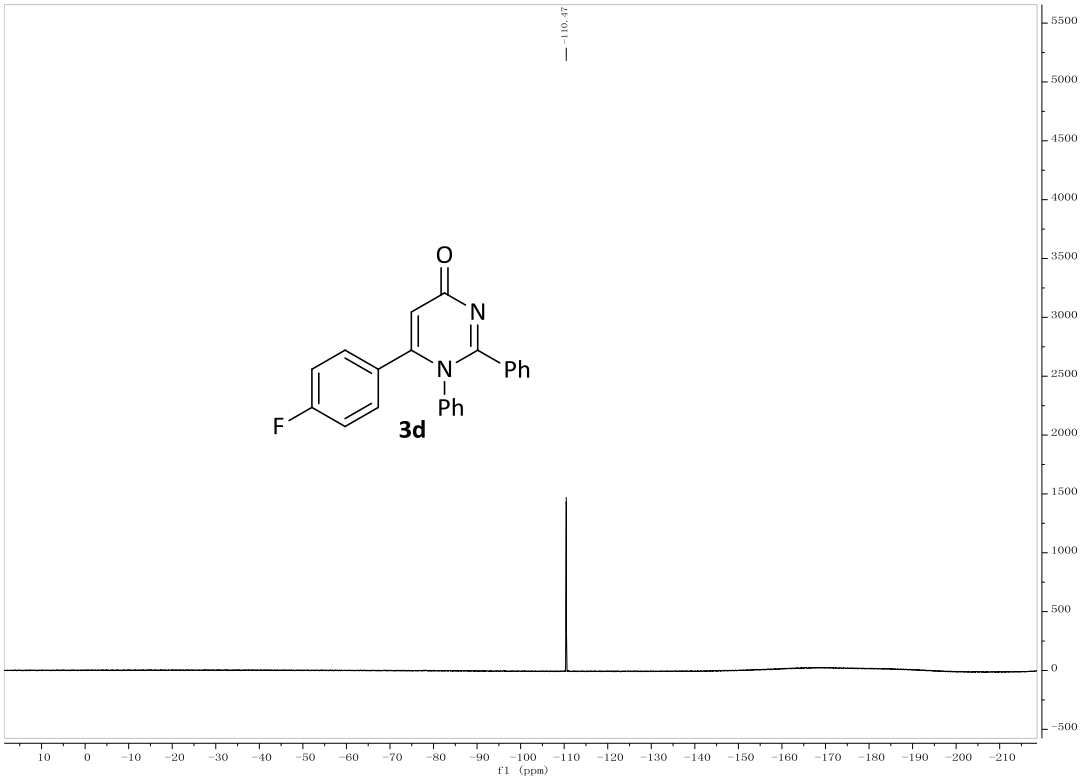
3d
f1 (ppm)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Ph
F
3d
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3000
2500
2000
1500
1000
500
0
−500
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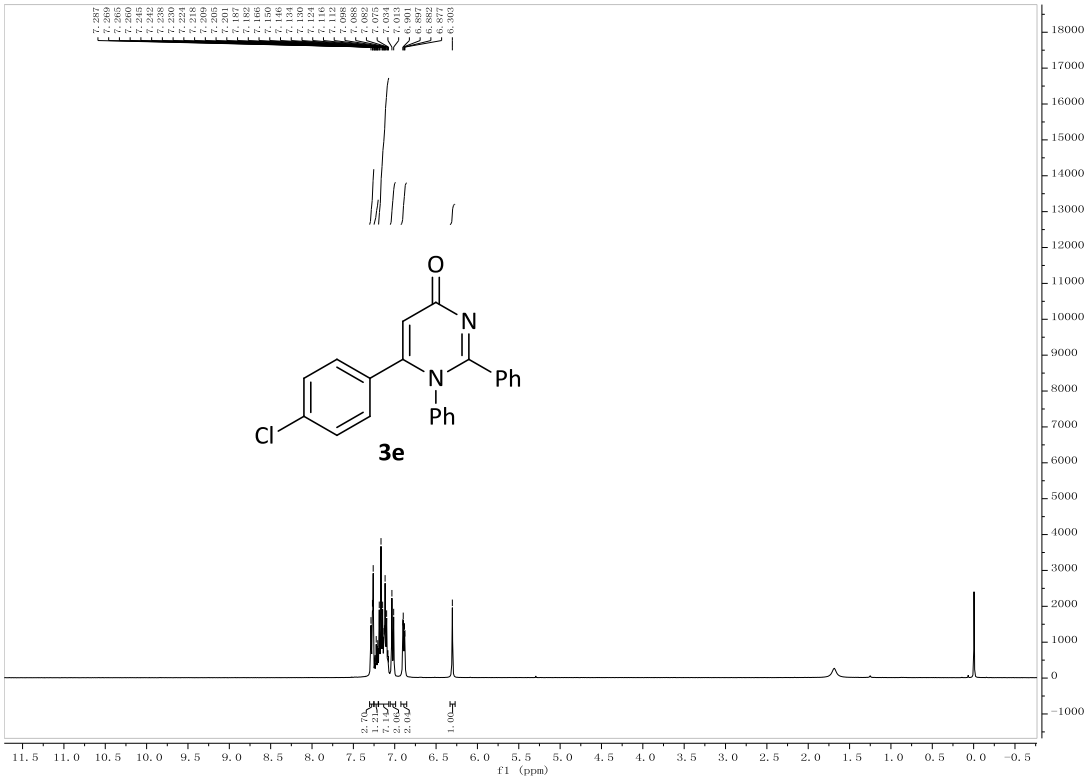
f1 (ppm)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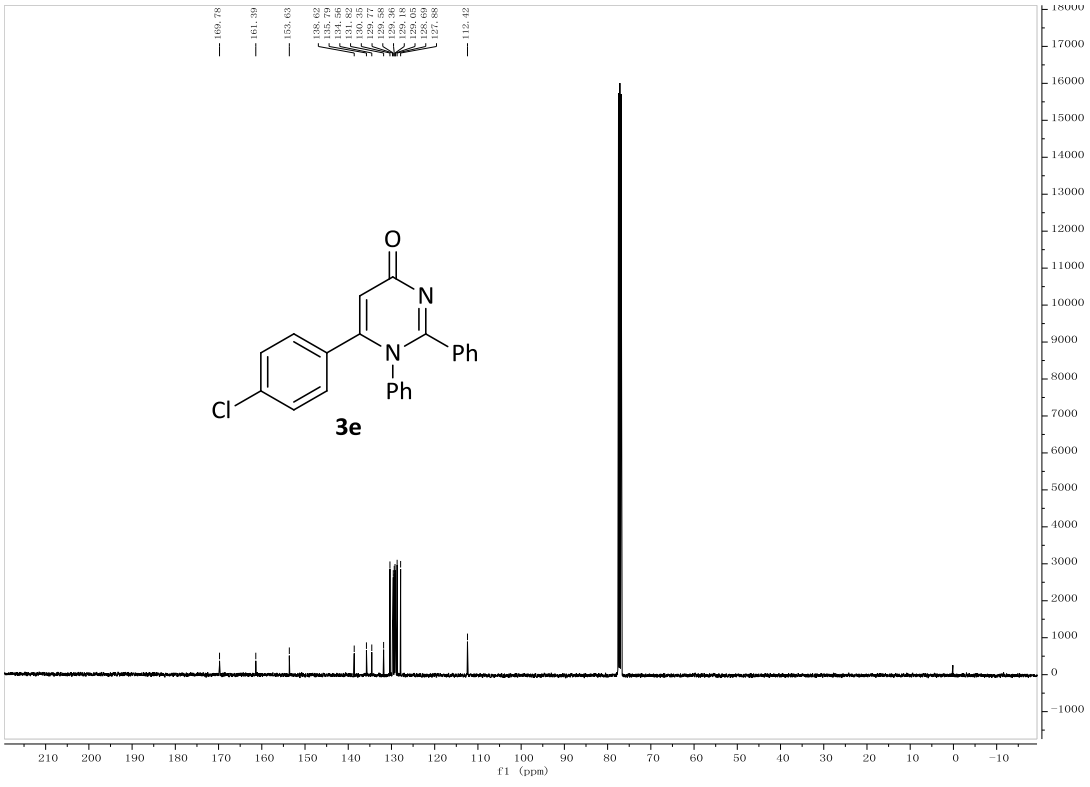
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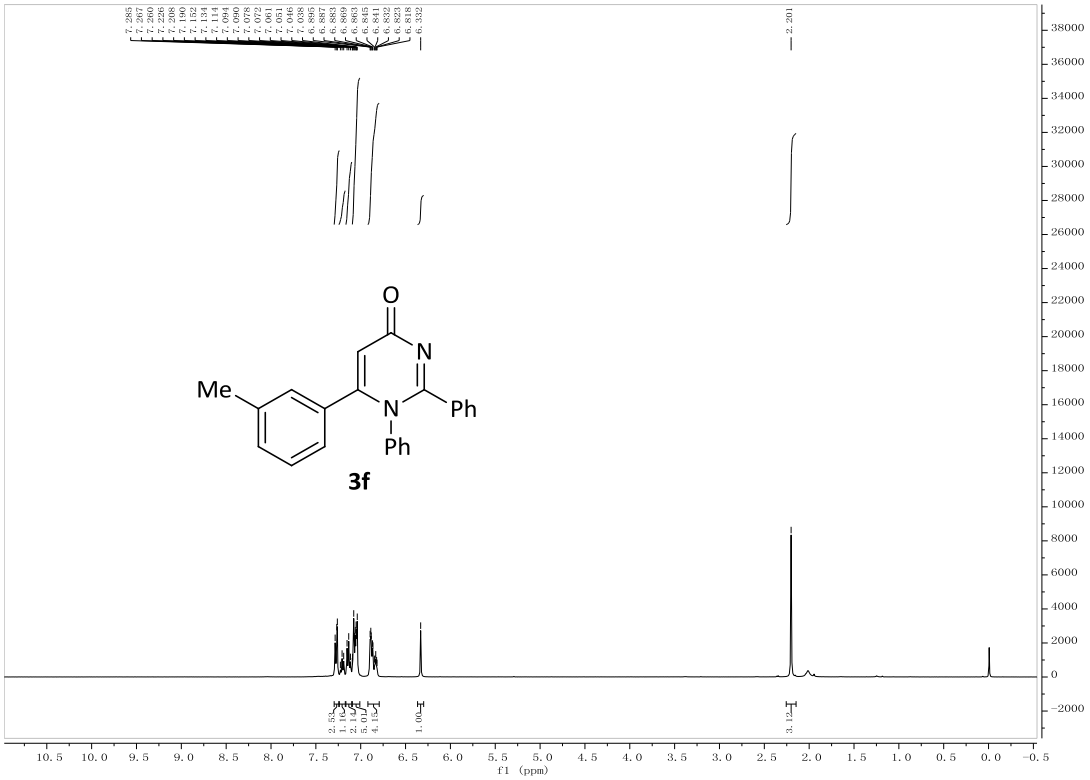
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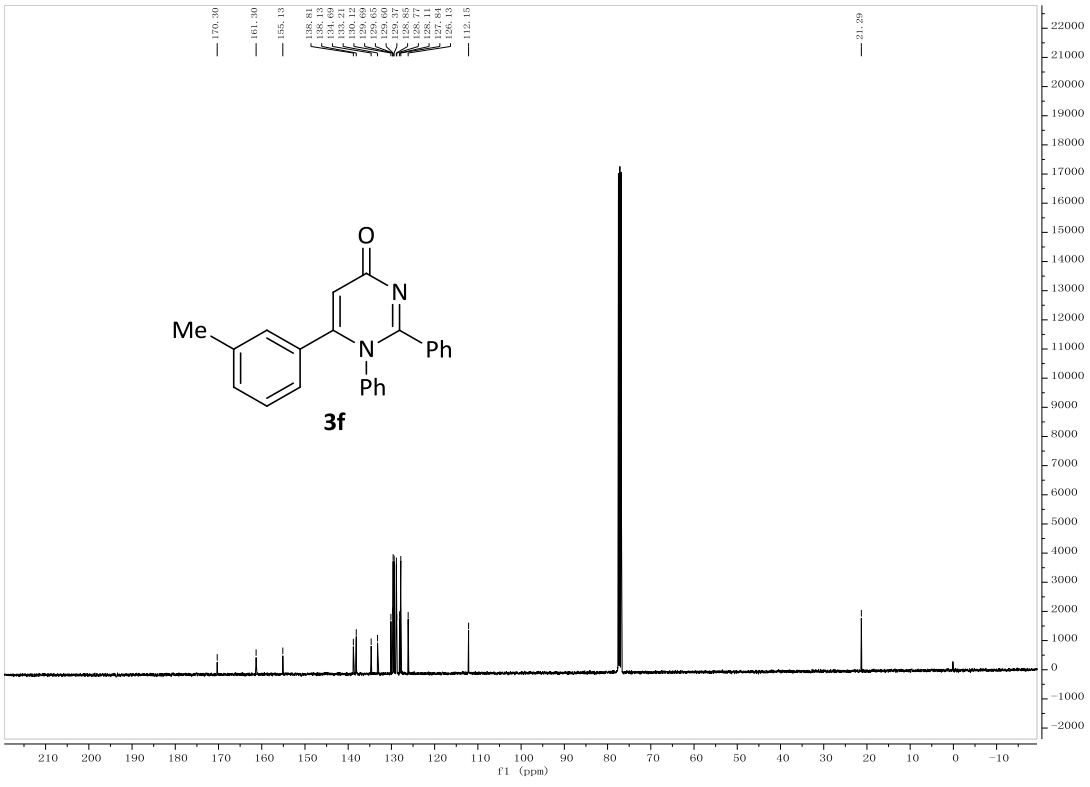
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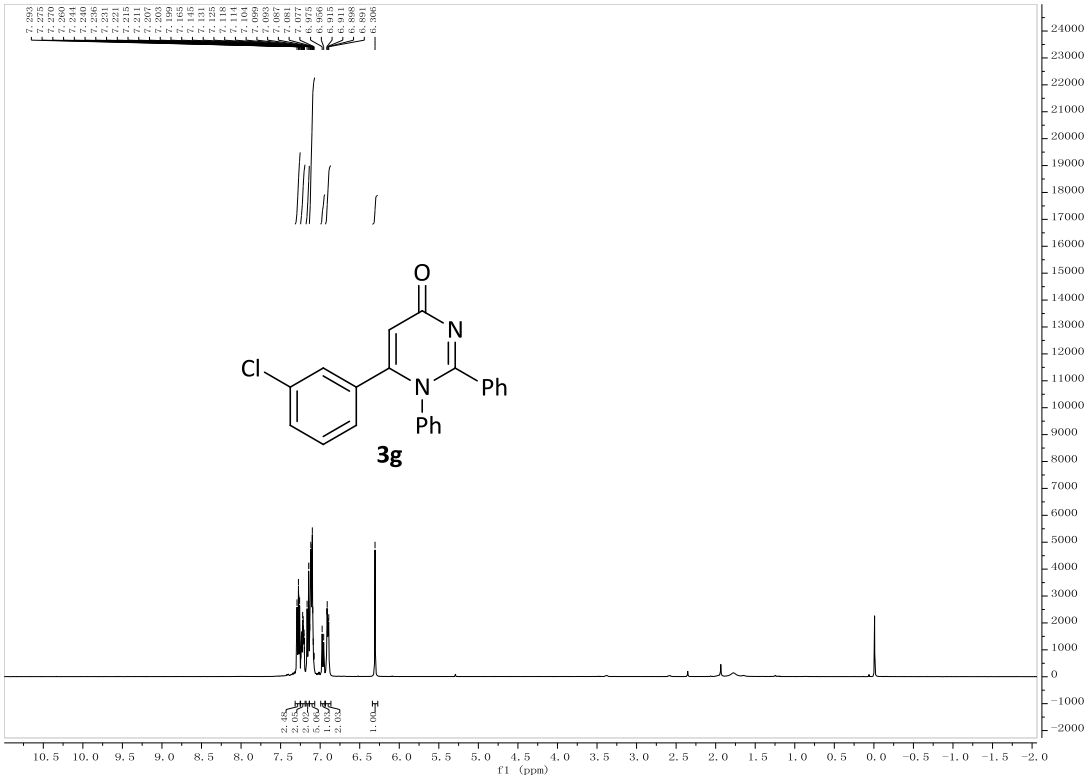
Ph
3f
f1 (ppm)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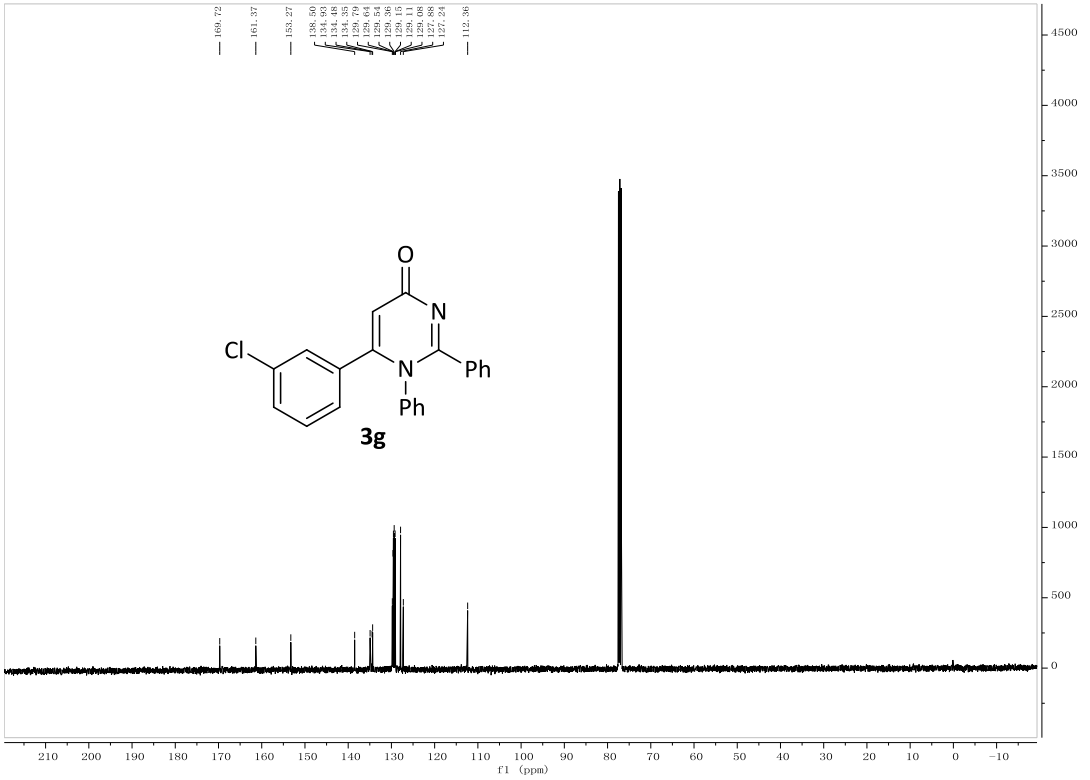
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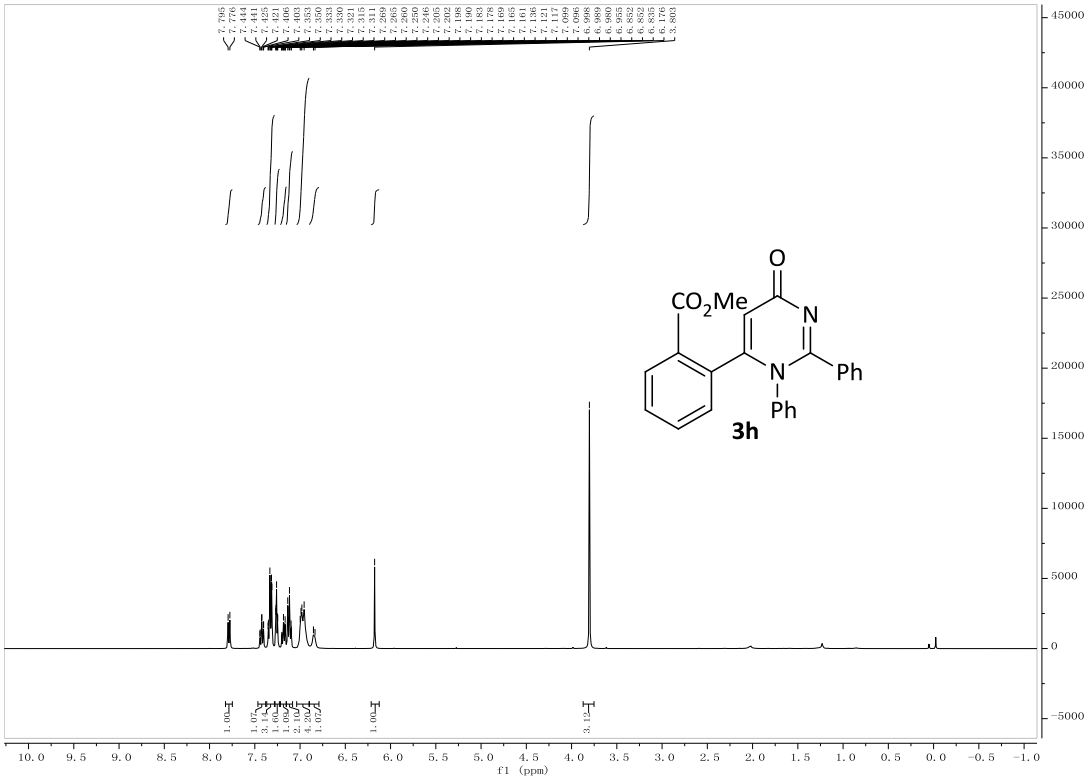
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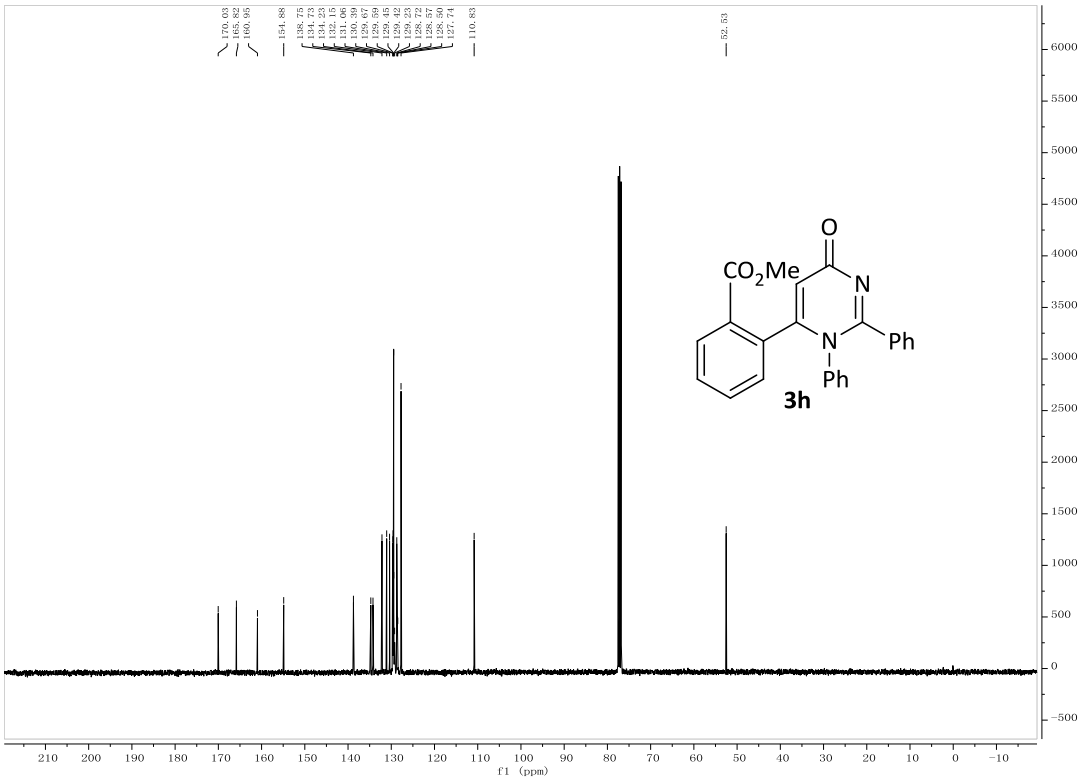
CO2Me
O
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Ph
Ph
3h
f1 (ppm)


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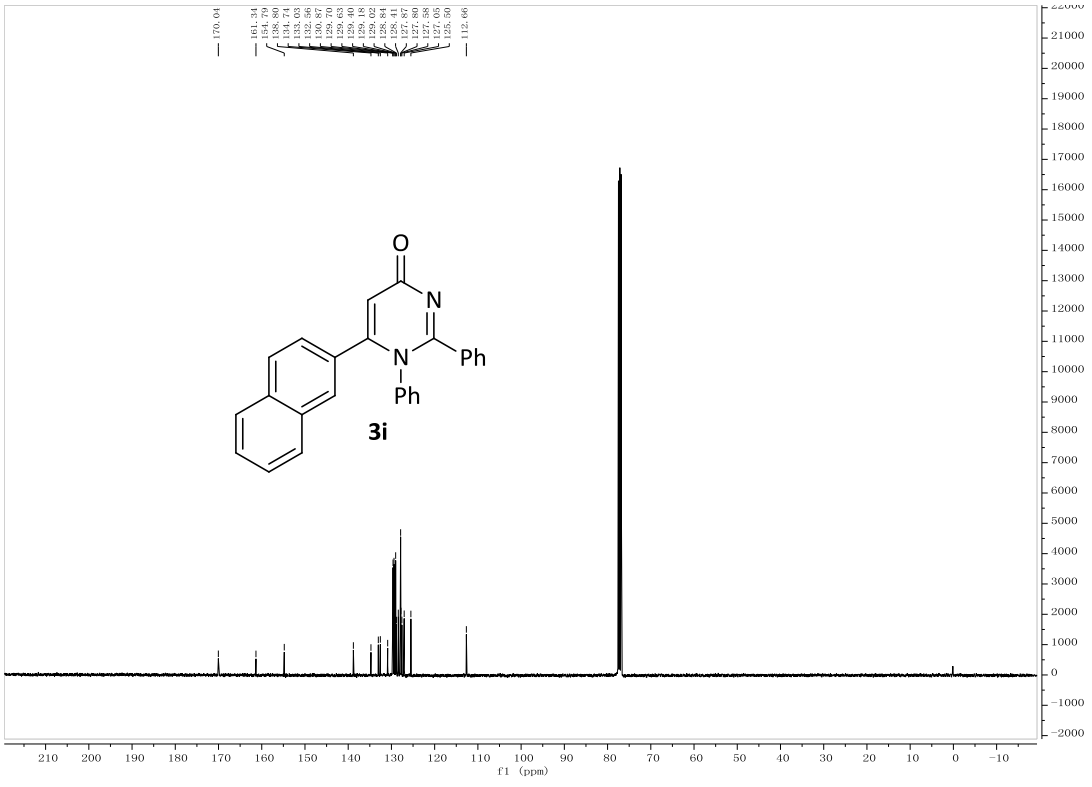
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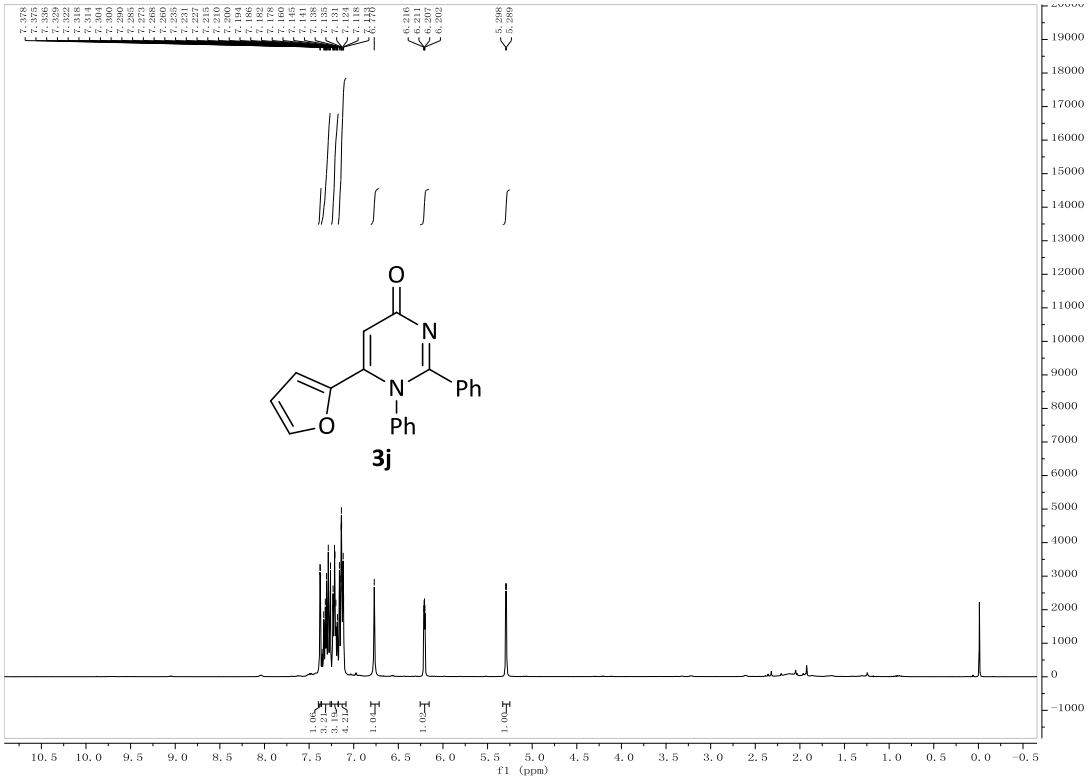
f1 (ppm)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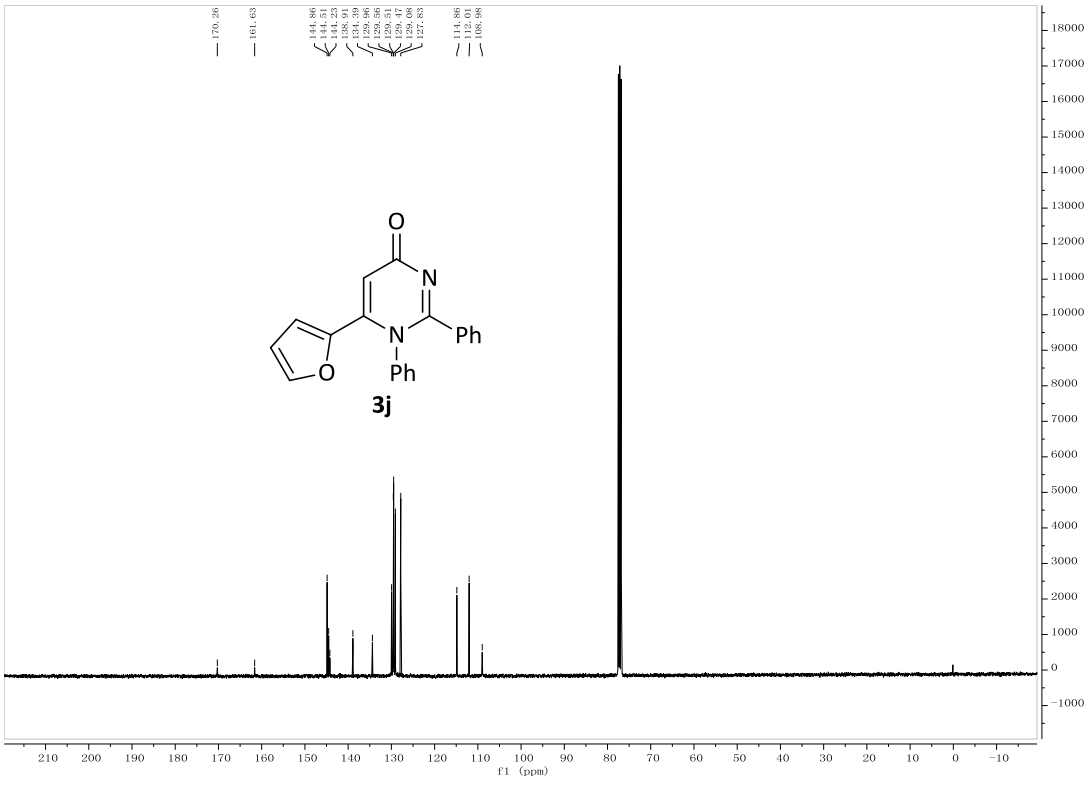
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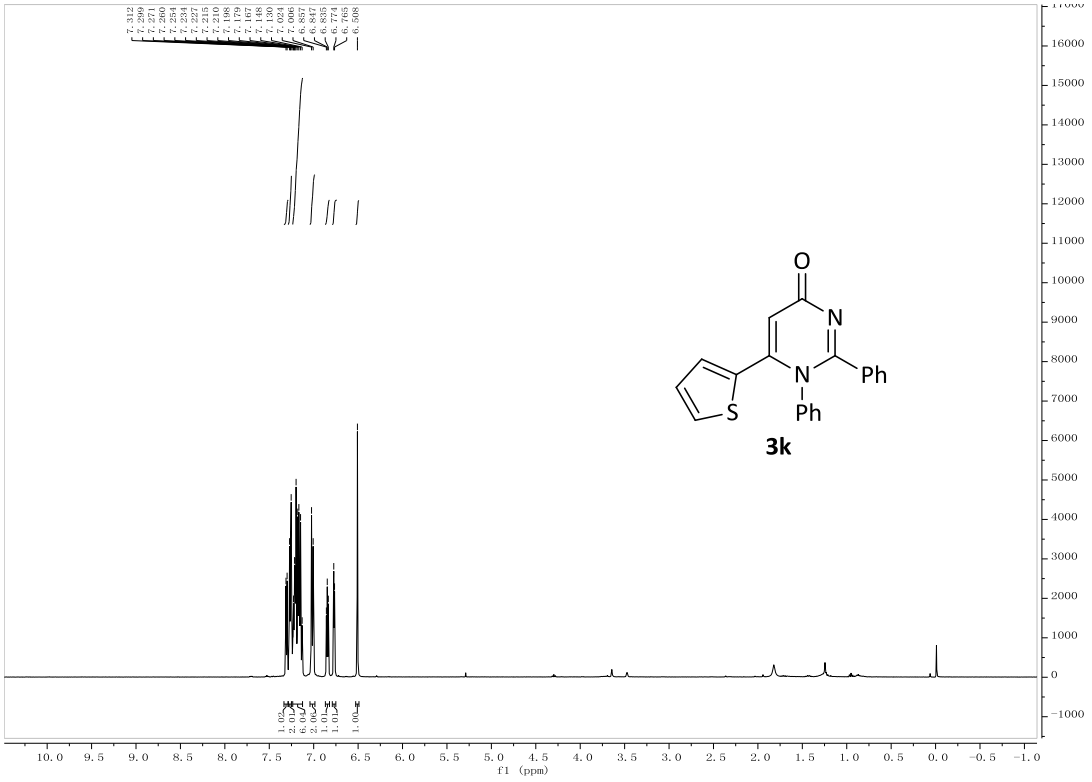
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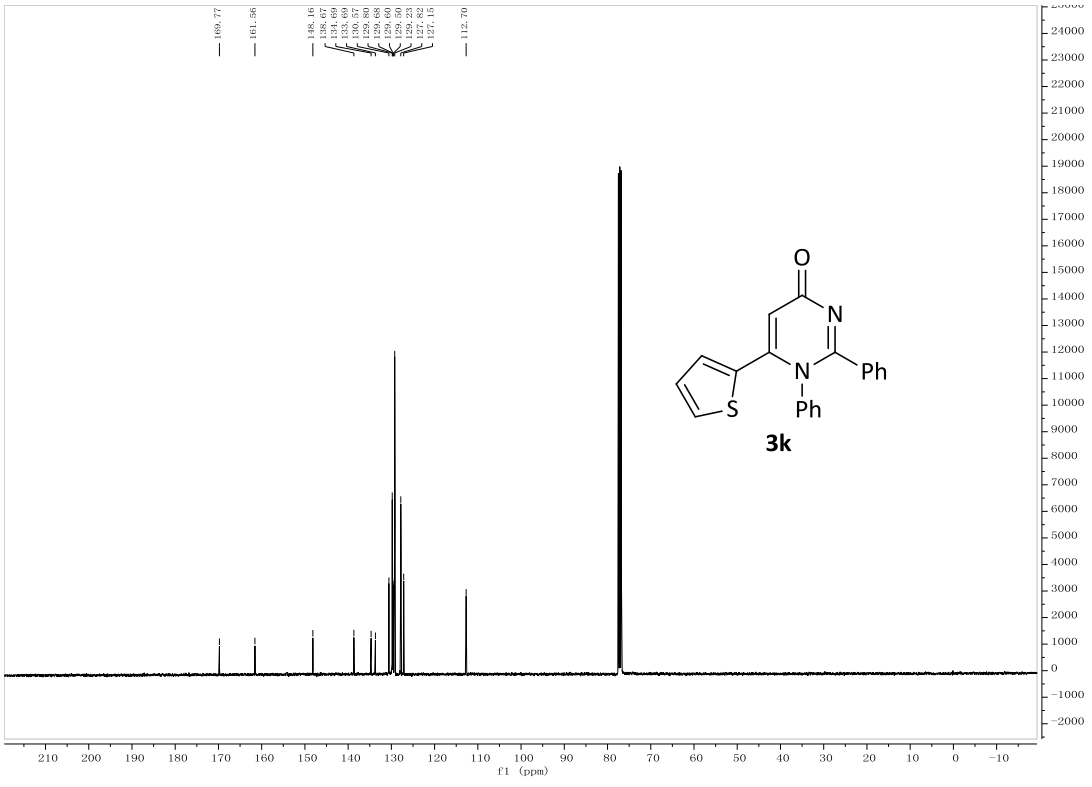
Ph
S
3k
f1 (ppm)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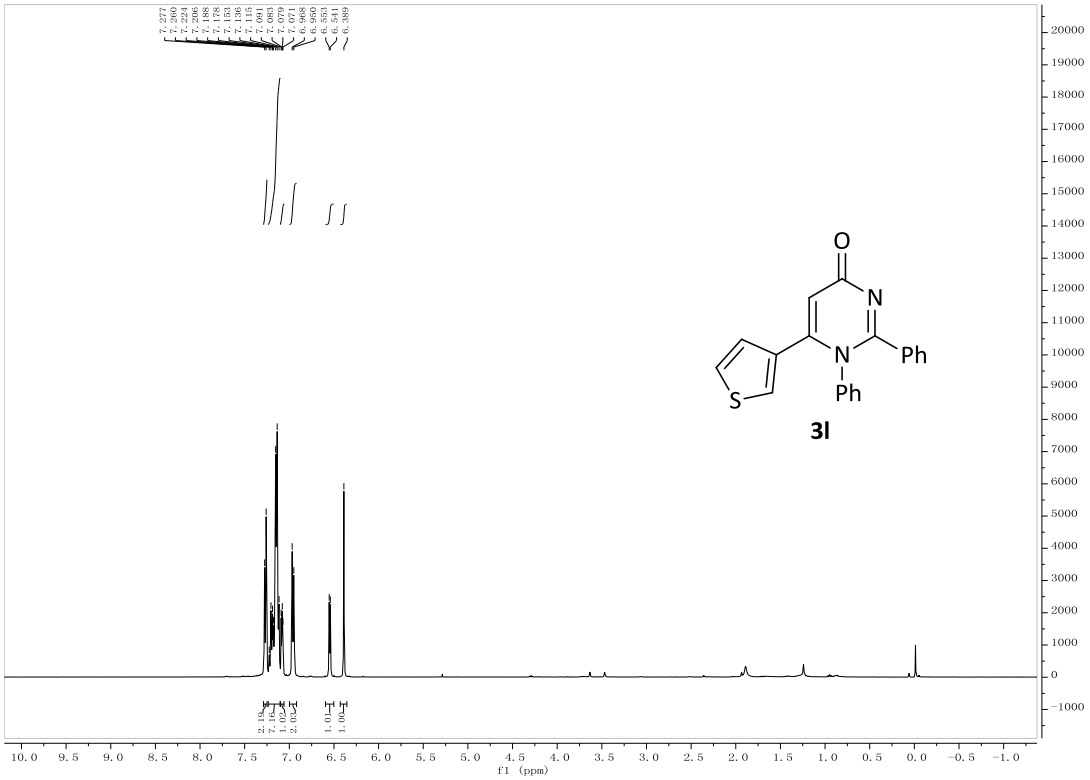
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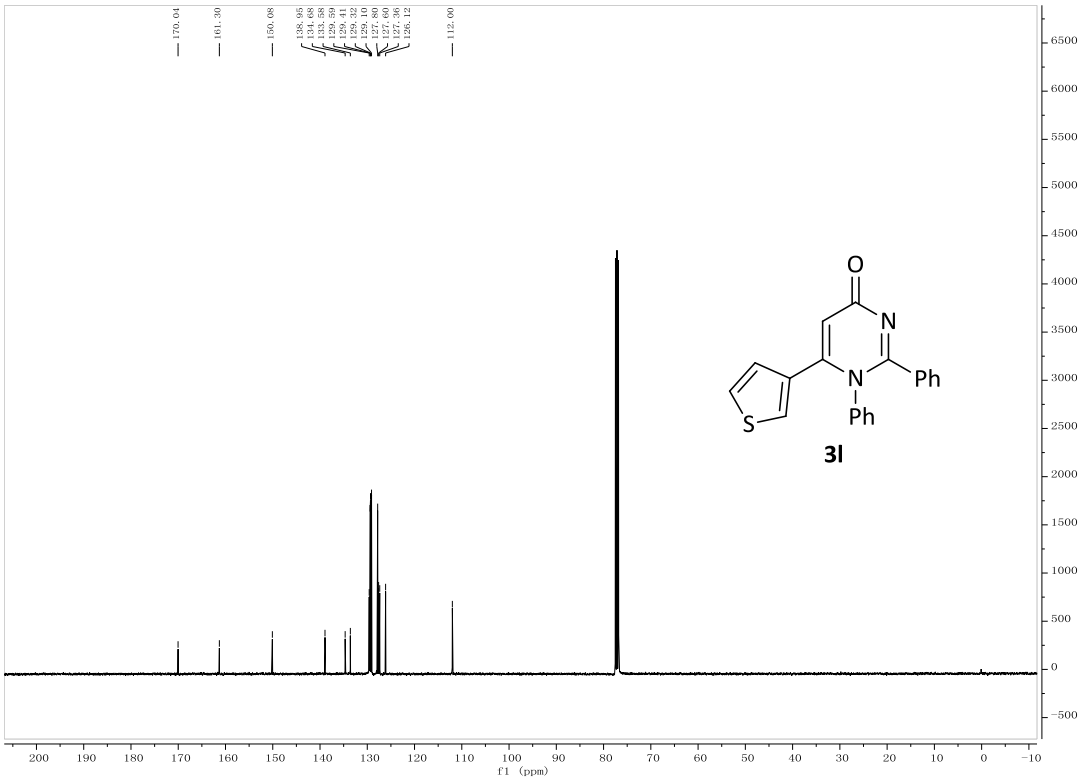
f1 (ppm)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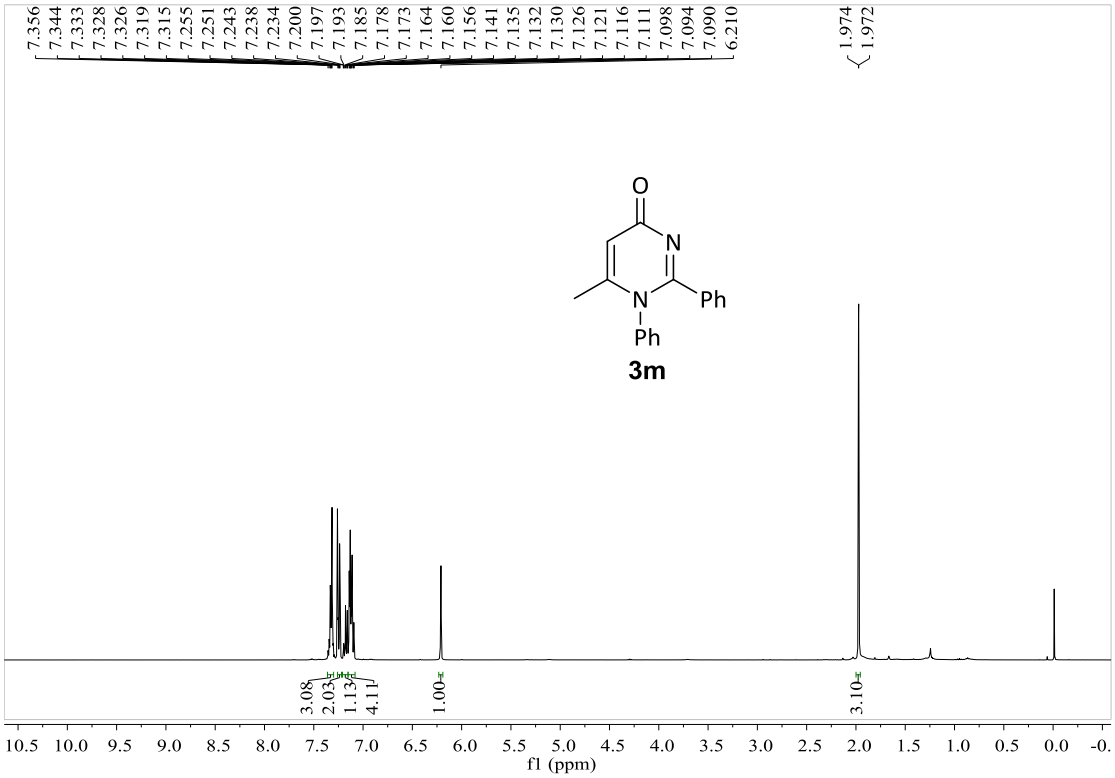
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7.090
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Ph
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2.03
1.13
4.11
1.00
3.10
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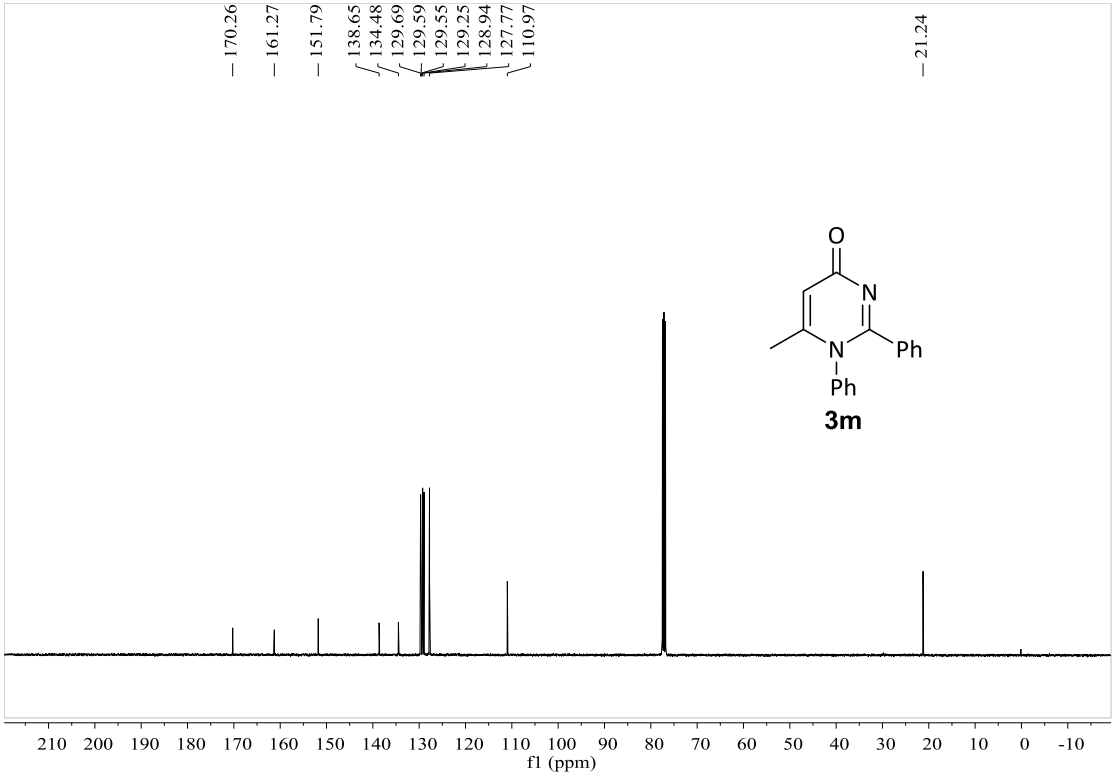
f1 (ppm)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Ph
Ph
3m
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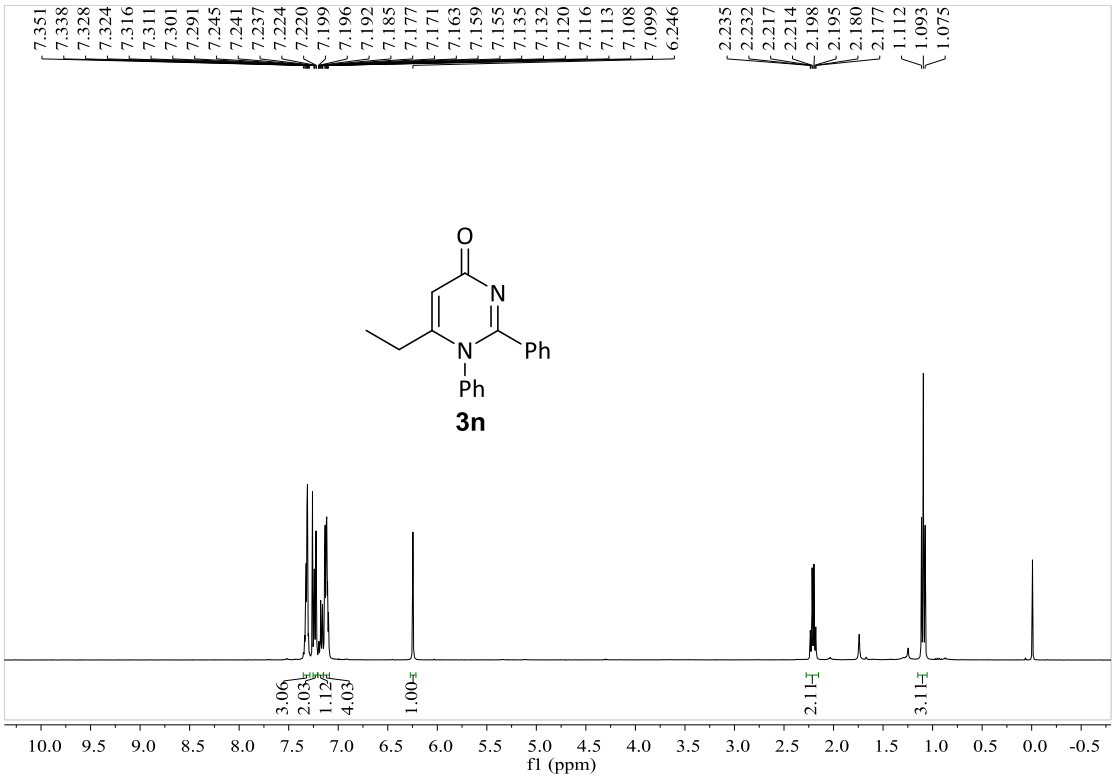
f1 (ppm)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7.159
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7.113
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N
Ph
Ph
3n
3.06
2.03
1.12
4.03
1.00
2.11
3.11
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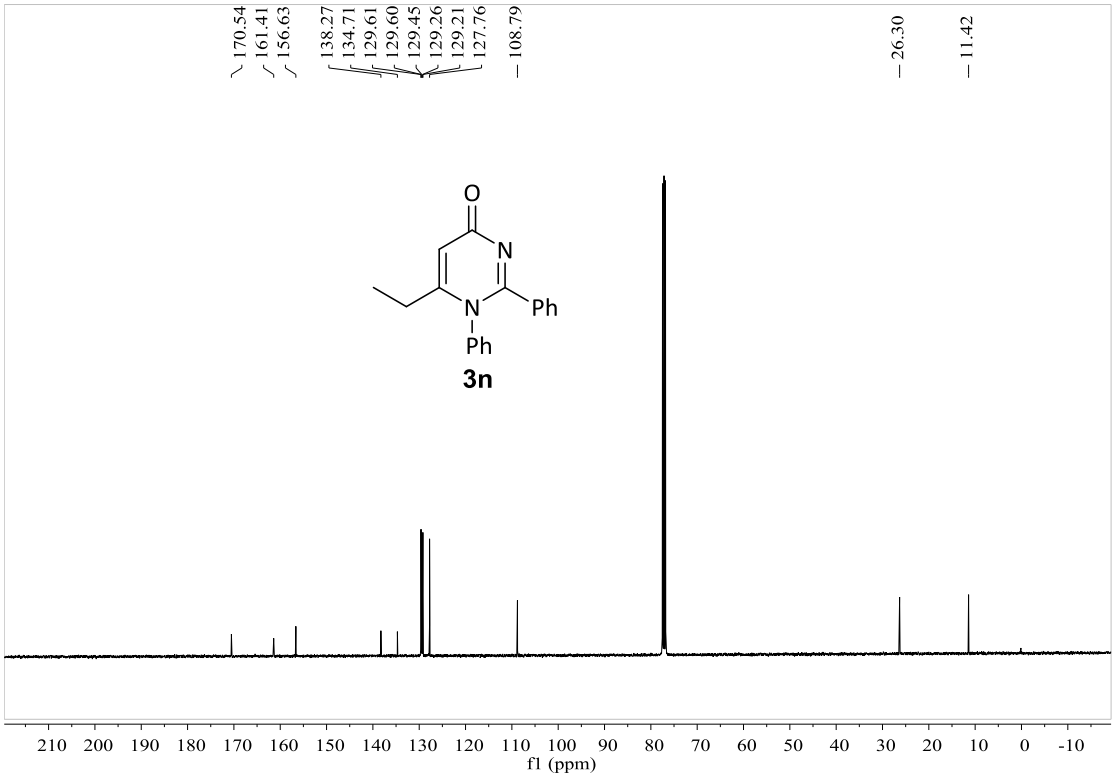
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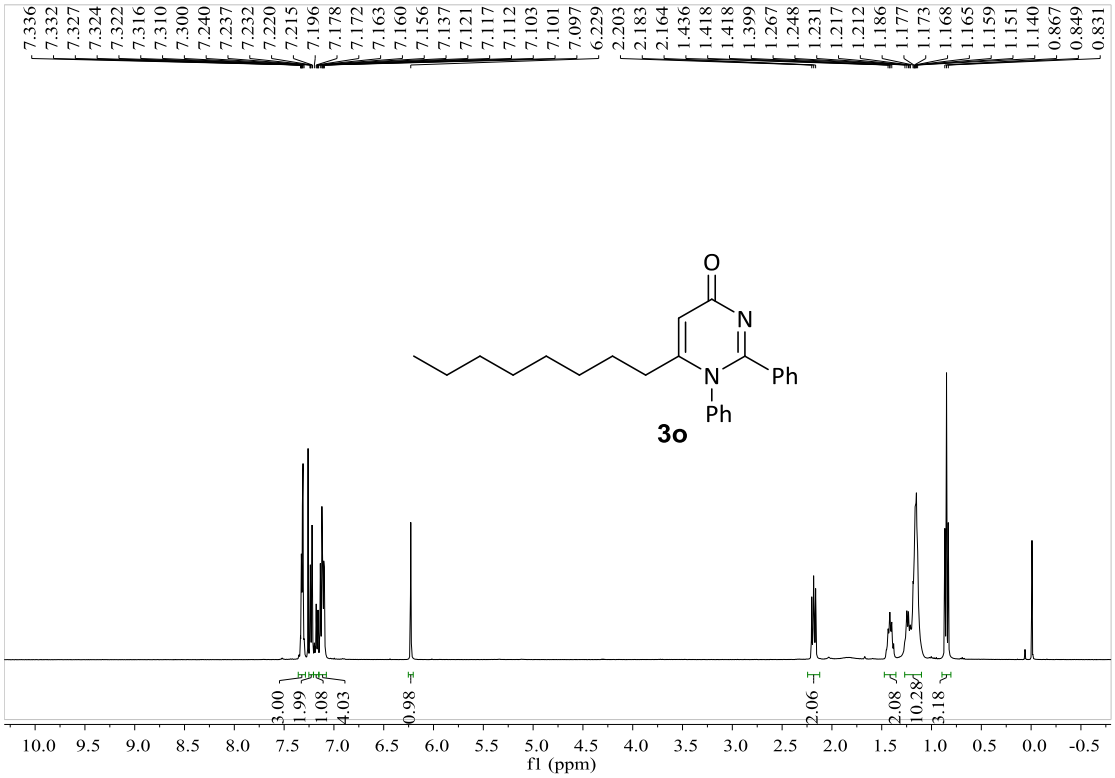
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.327
7.324
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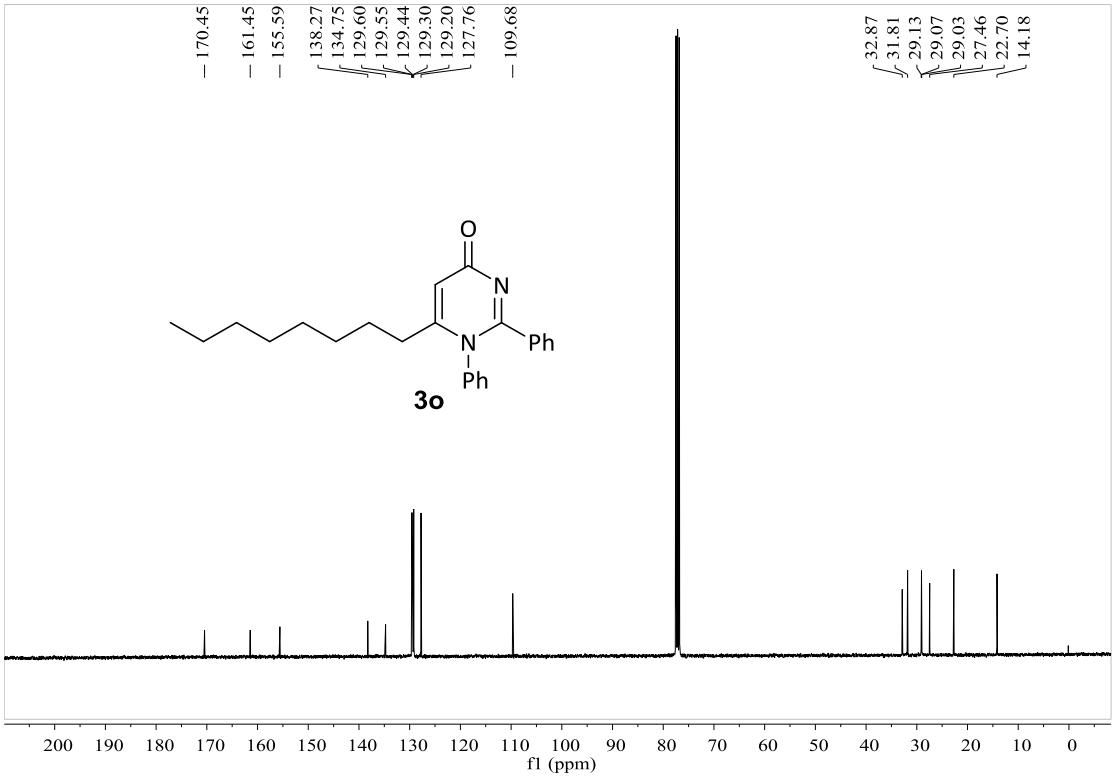
7.316
7.310
7.300
7.240
7.237
7.232
7.220
7.215
7.196
7.178
7.172
7.163
7.160
7.156
7.137
7.121
7.117
7.112
7.103
7.101
7.097
6.229
2.203
2.183
2.164
1.436
1.418
1.418
1.399
1.267
1.248
1.231
1.217
1.212
1.186
1.177
1.173
1.168
1.165
1.159
1.151
1.140
0.867
0.849
0.831
O
N
N
Ph
Ph
3o
3.00
1.99
1.08
4.03
0.98
2.06
2.08
10.28
3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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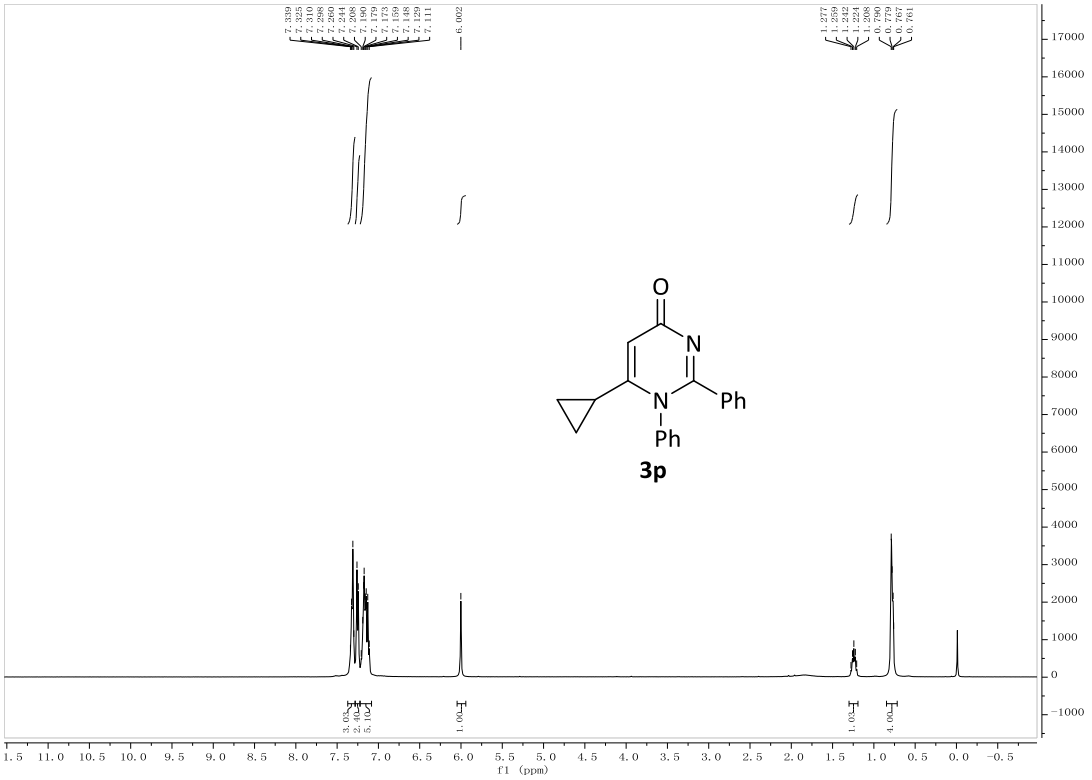
161.45
155.59
138.27
134.75
129.60
129.55
129.44
129.30
129.20
127.76
109.68
32.87
31.81
29.13
29.07
29.03
27.46
22.70
14.18
O
N
N
Ph
Ph
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.244
7.198
7.196
7.179
7.173
7.159
7.148
7.129
7.111
6.002
1.277
1.259
1.242
1.224
1.208
0.790
0.779
0.767
0.761
O
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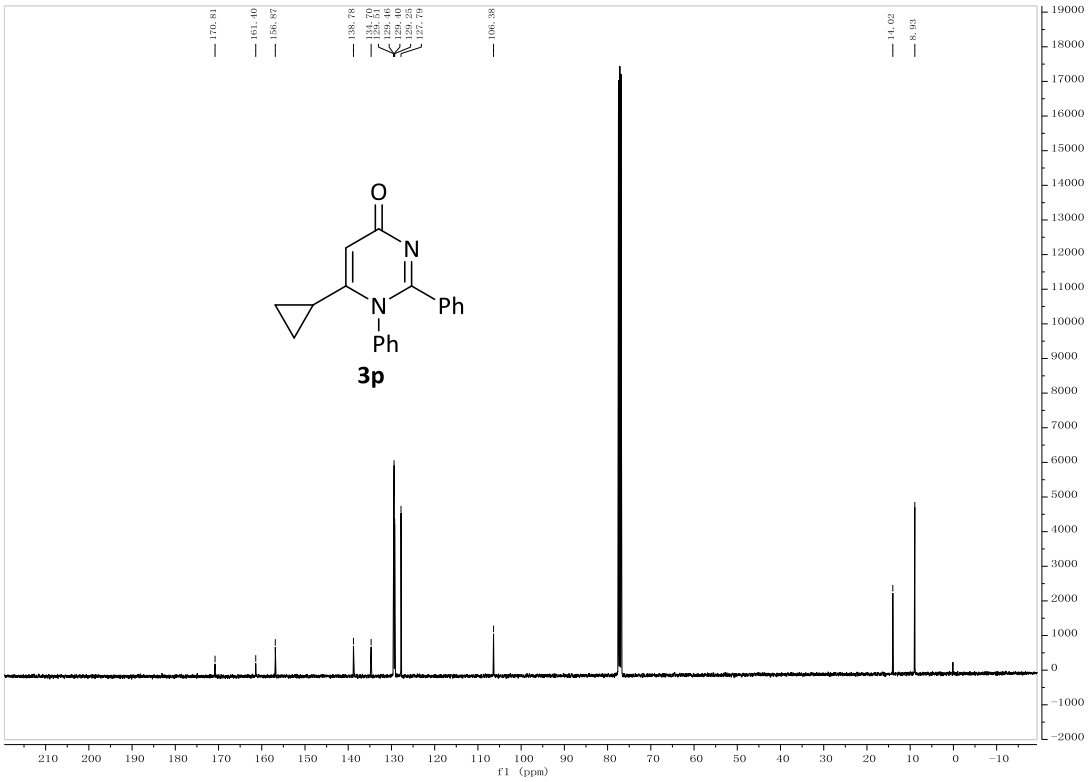
N
Ph
Ph
3p
3.03
2.46
5.10
1.00
1.03
4.06
f1 (ppm)


170.81
161.40
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134.70
130.15
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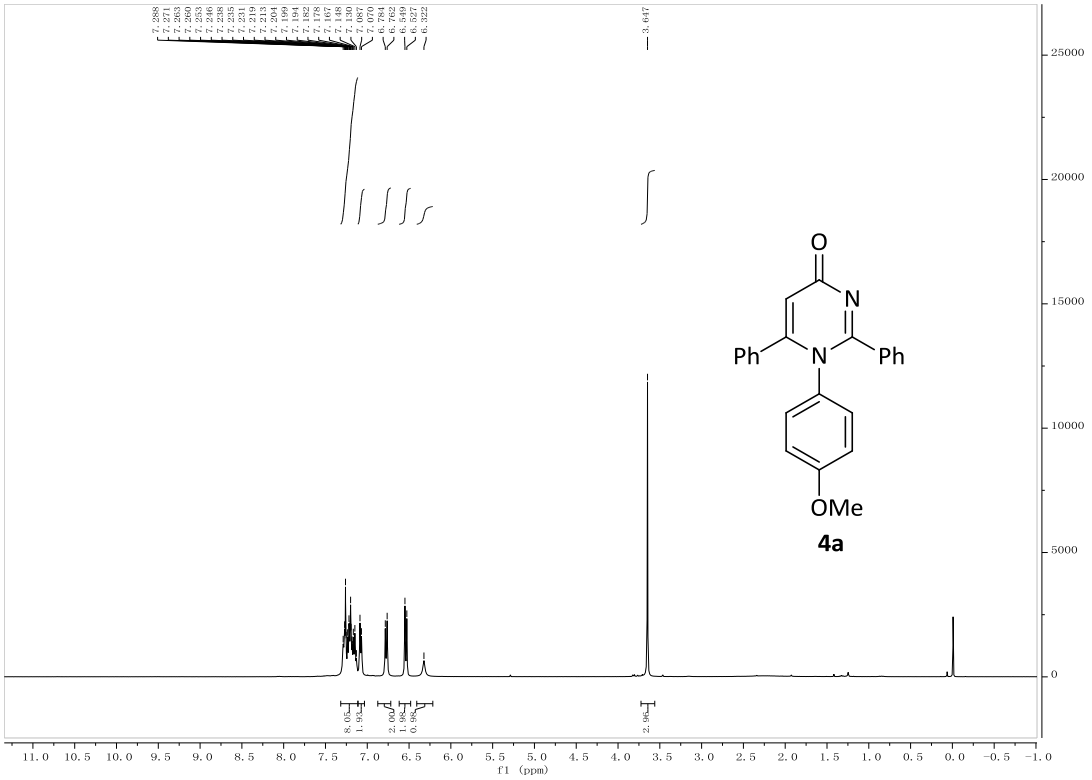
129.40
129.35
127.79
106.38
14.02
8.93
O
N
N
Ph
Ph
3p
f1 (ppm)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7.235
7.231
7.218
7.213
7.204
7.199
7.184
7.182
7.178
7.167
7.148
7.140
7.087
7.070
6.784
6.762
6.549
6.527
6.322
3.647
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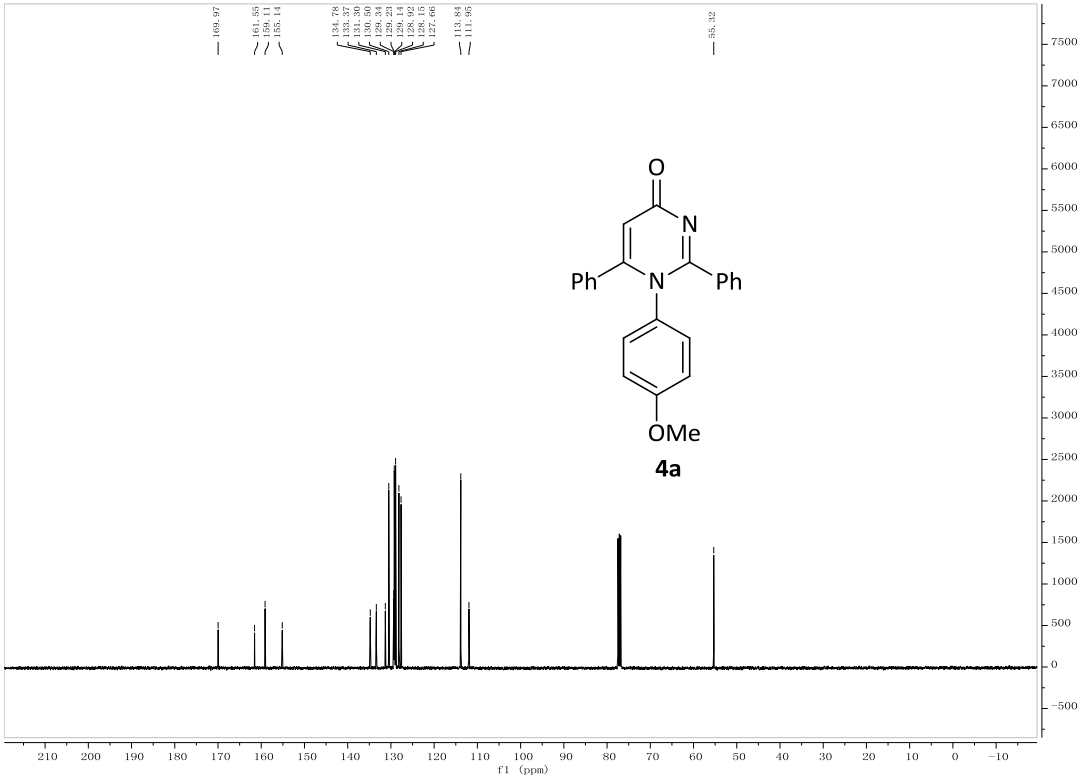
N
Ph
N
Ph
OMe
4a
8.05
1.95
2.06
1.98
0.98
2.96
f1 (ppm)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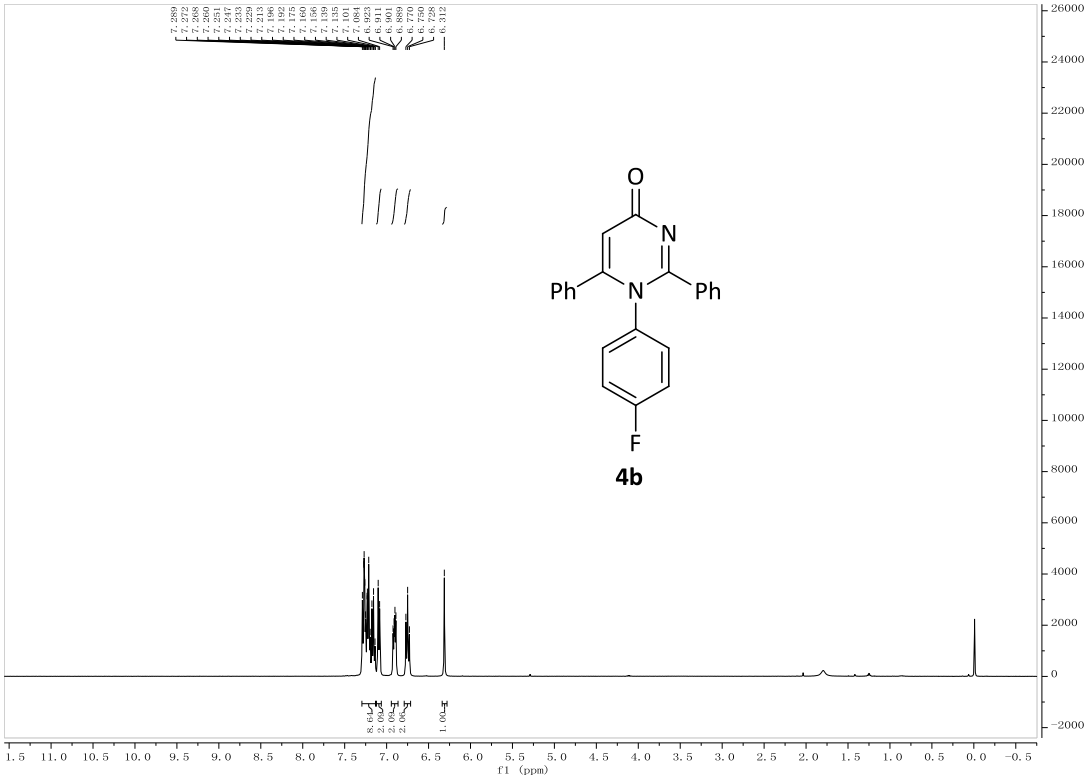
133.37
130.50
129.34
129.23
129.14
128.92
128.15
127.66
113.84
111.95
55.32
O
N
Ph
N
Ph
OMe
4a
f1 (ppm)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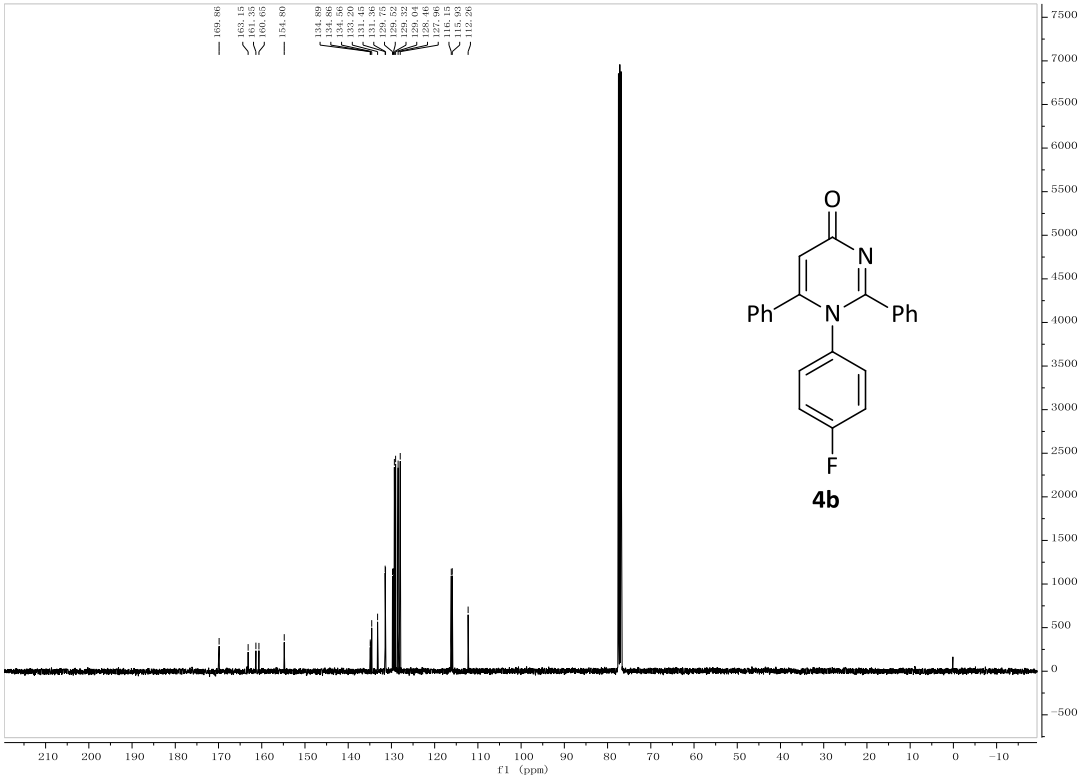
Ph
N
Ph
F
4b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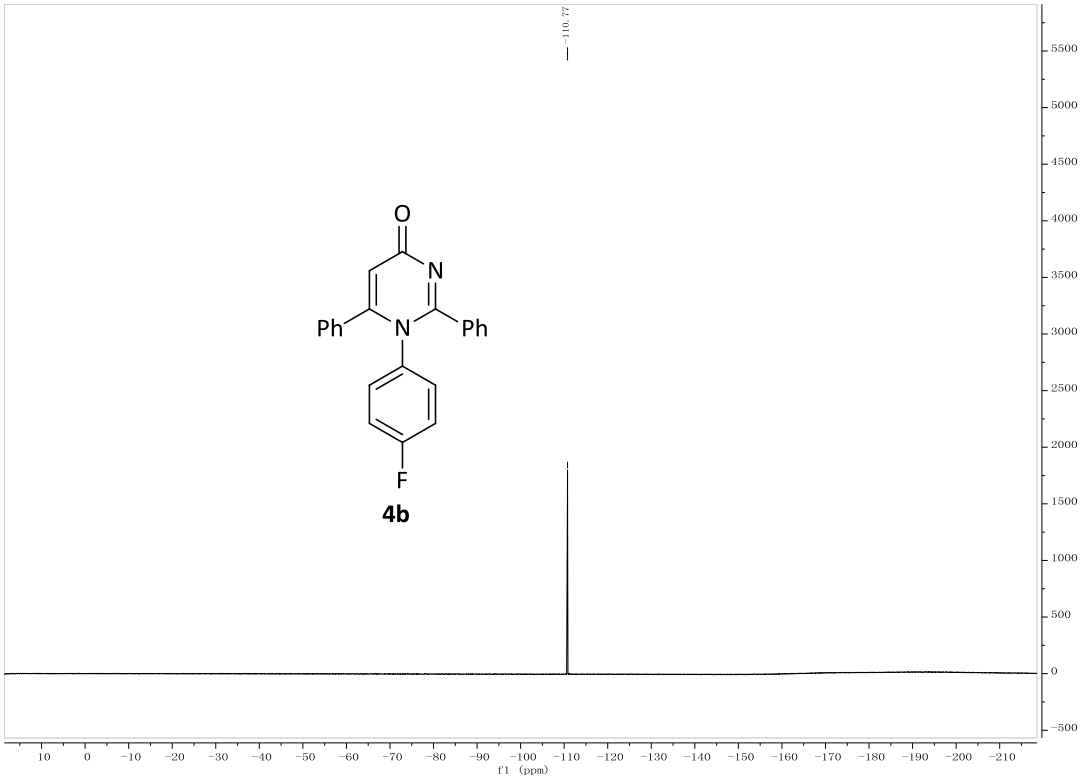
Ph
N
Ph
F
4b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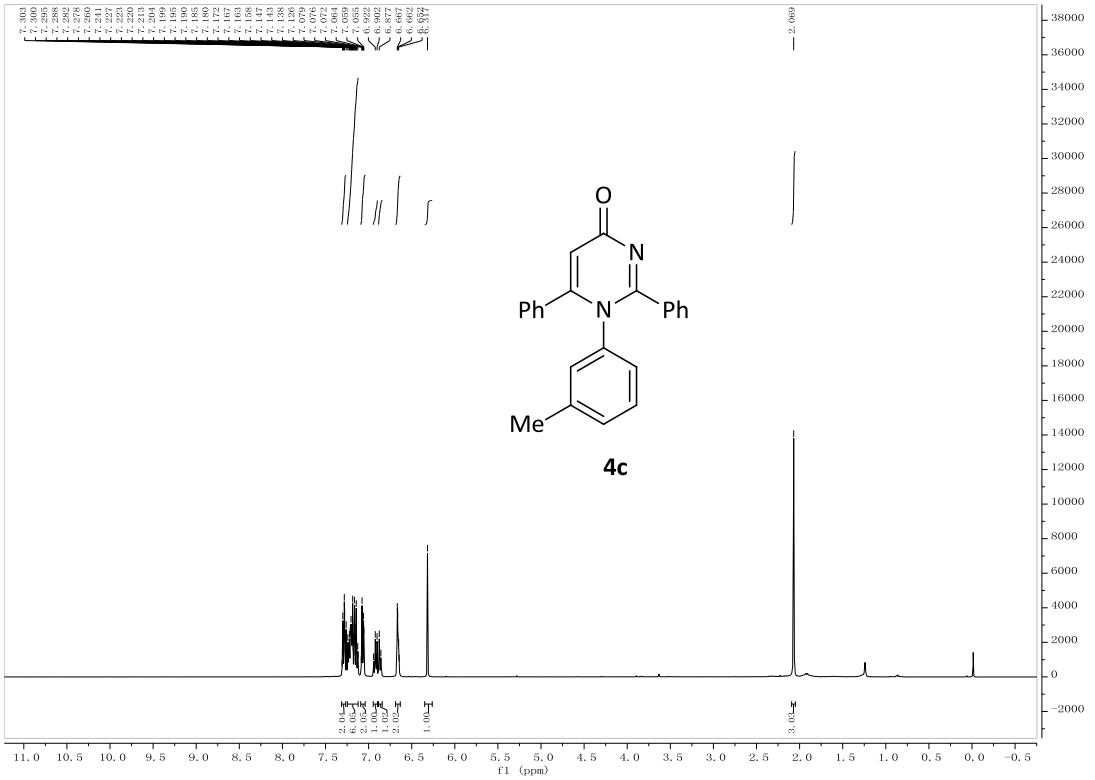
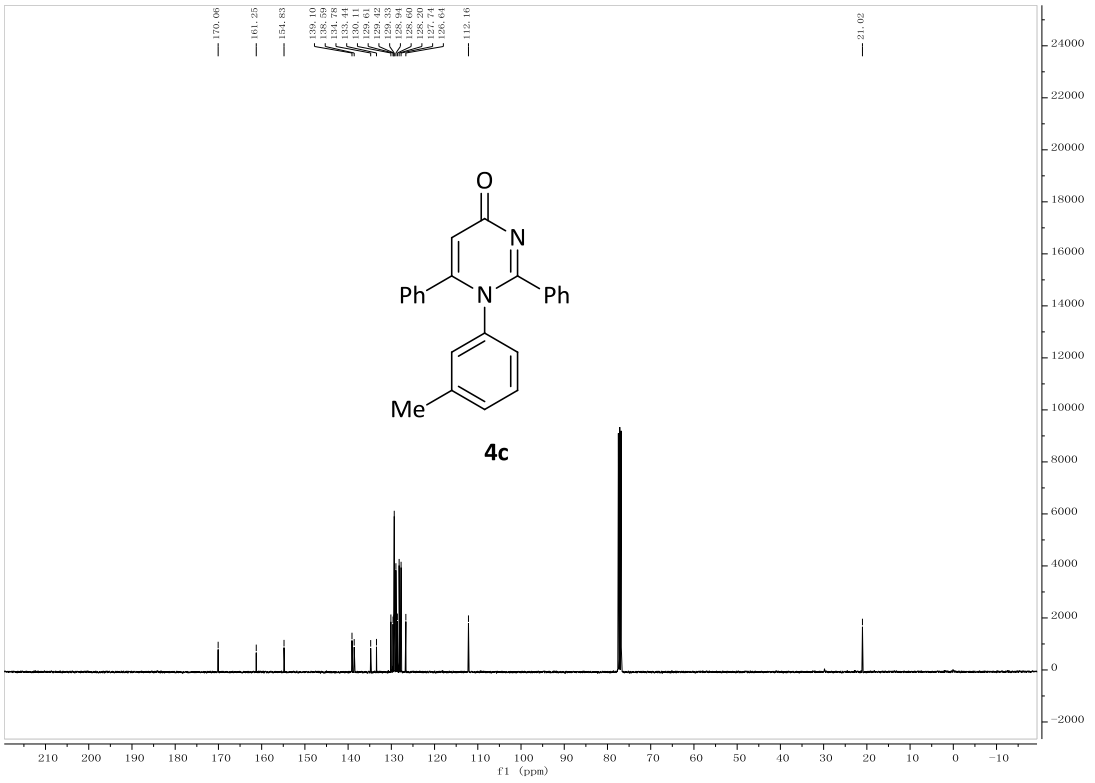
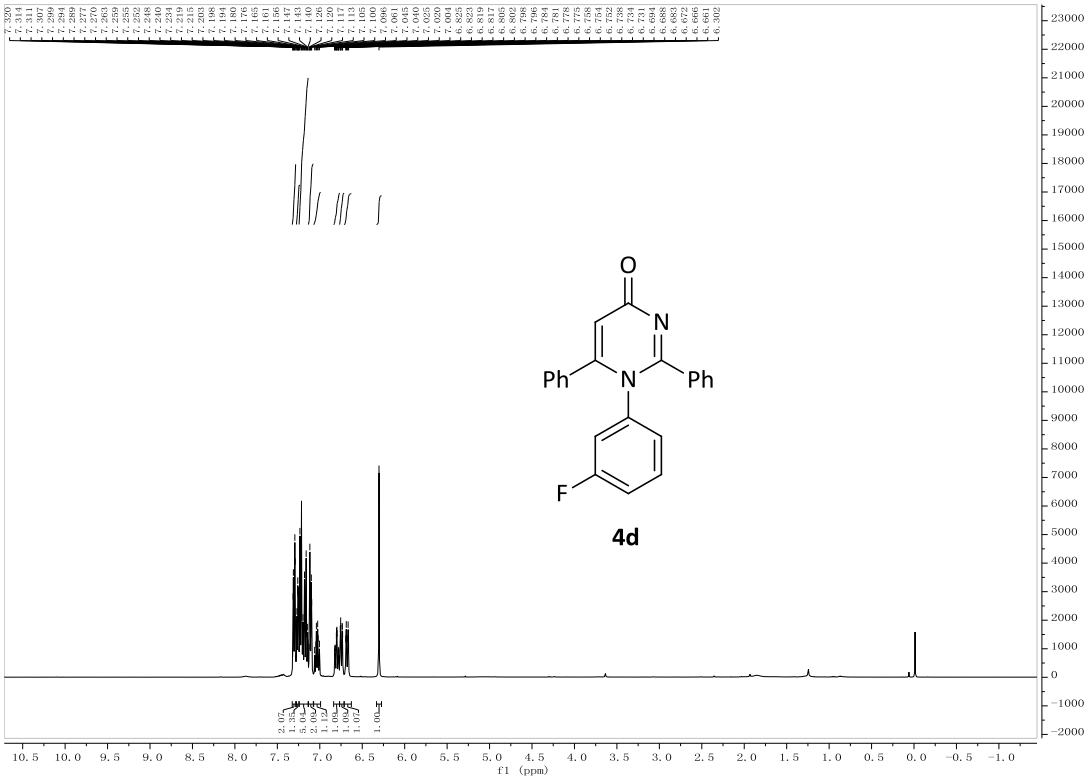
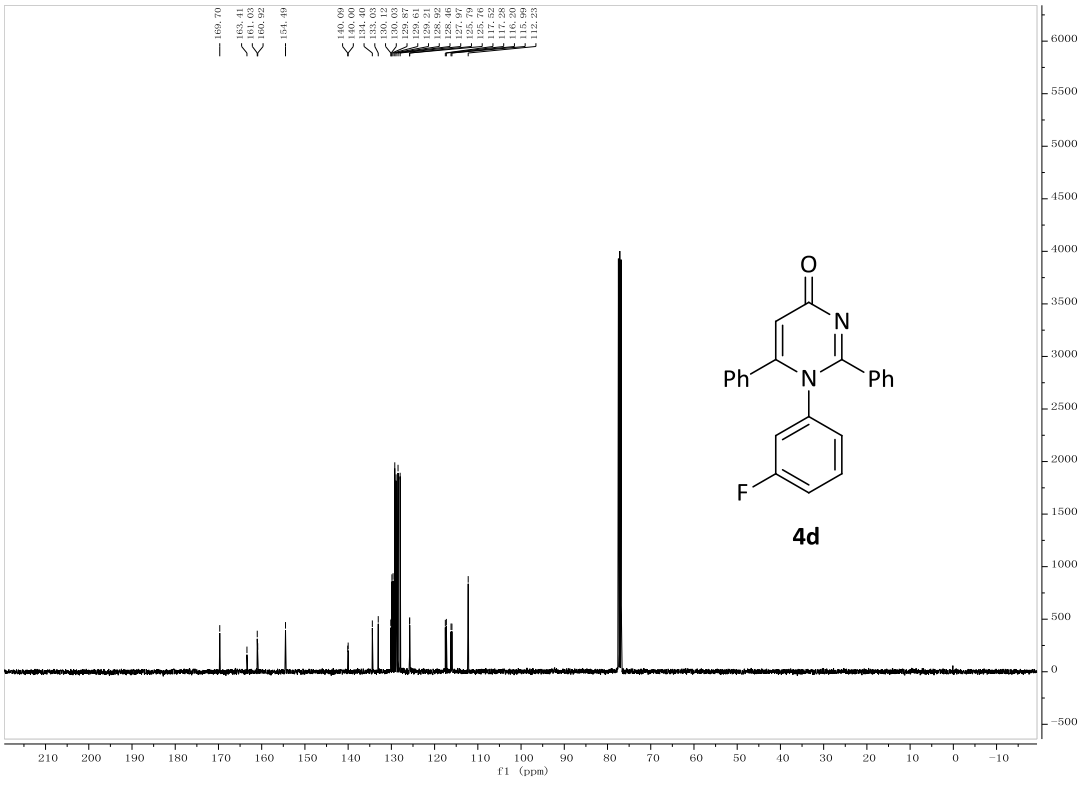
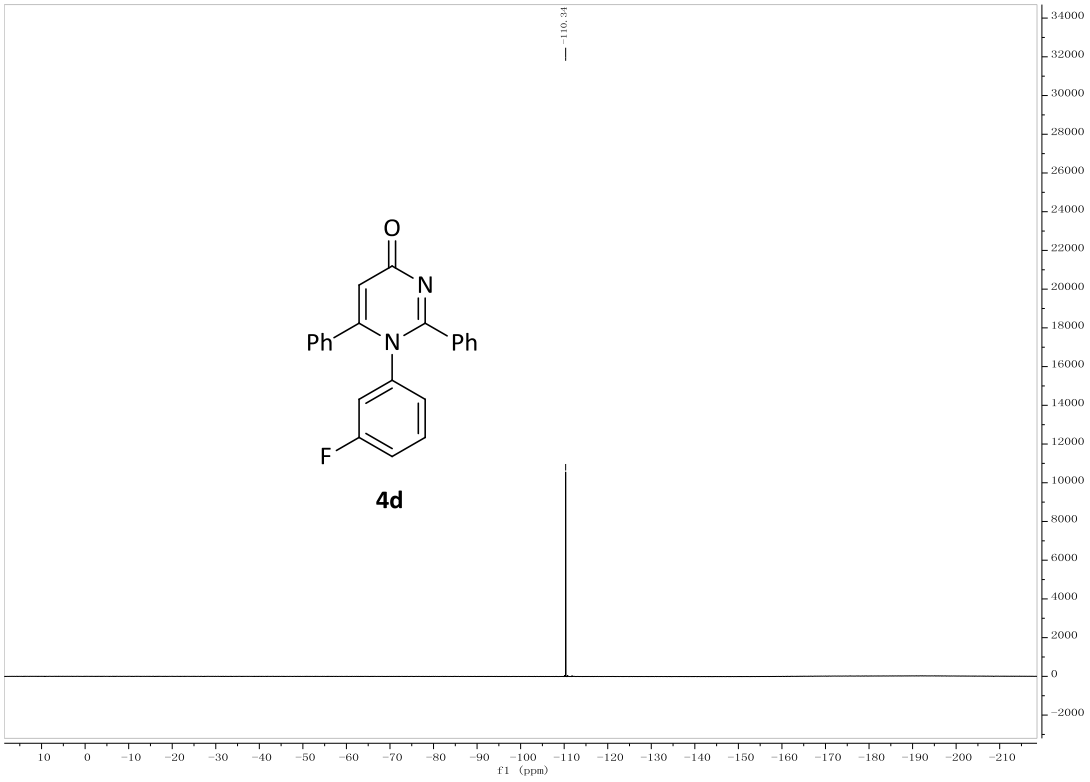
Ph
N
Ph
F
4b
-110.77
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


O
N
Ph
N
Ph
Me
4c
f1 (ppm)


O
N
Ph
N
Ph
Me
4c
f1 (ppm)


O
N
Ph
N
Ph
F
4d
f1 (ppm)


O
N
Ph
N
Ph
F
4d
f1 (ppm)


-110.34
O
N
Ph
N
Ph
F
4d
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32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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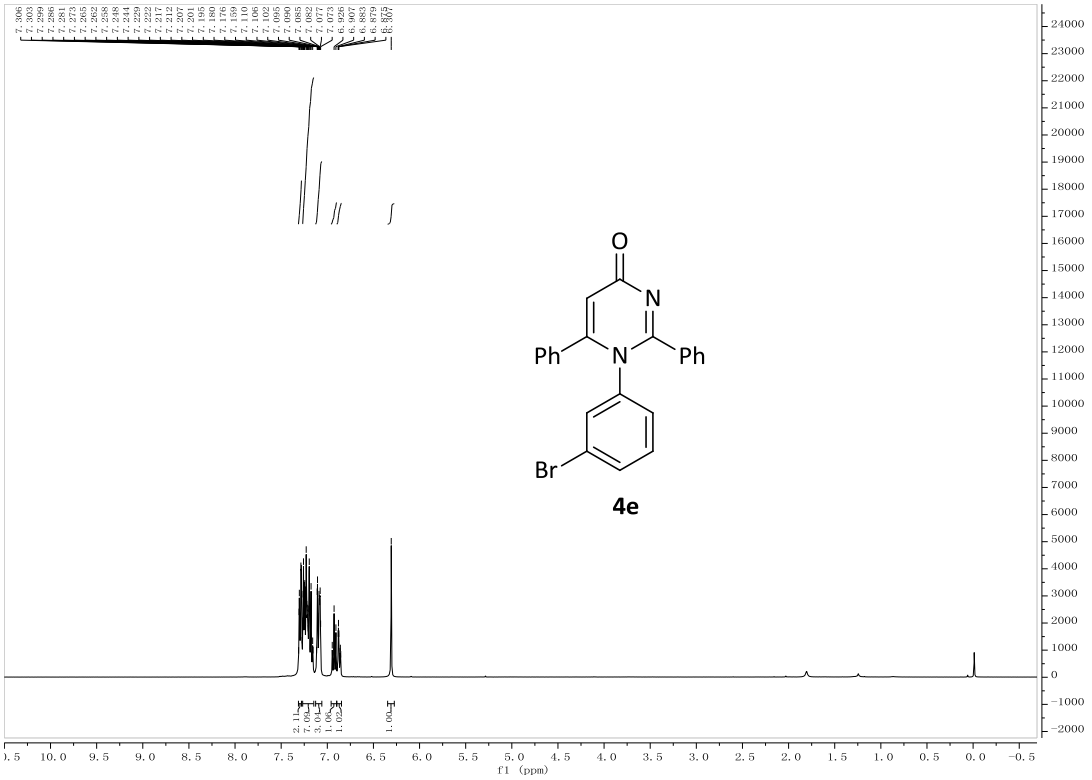
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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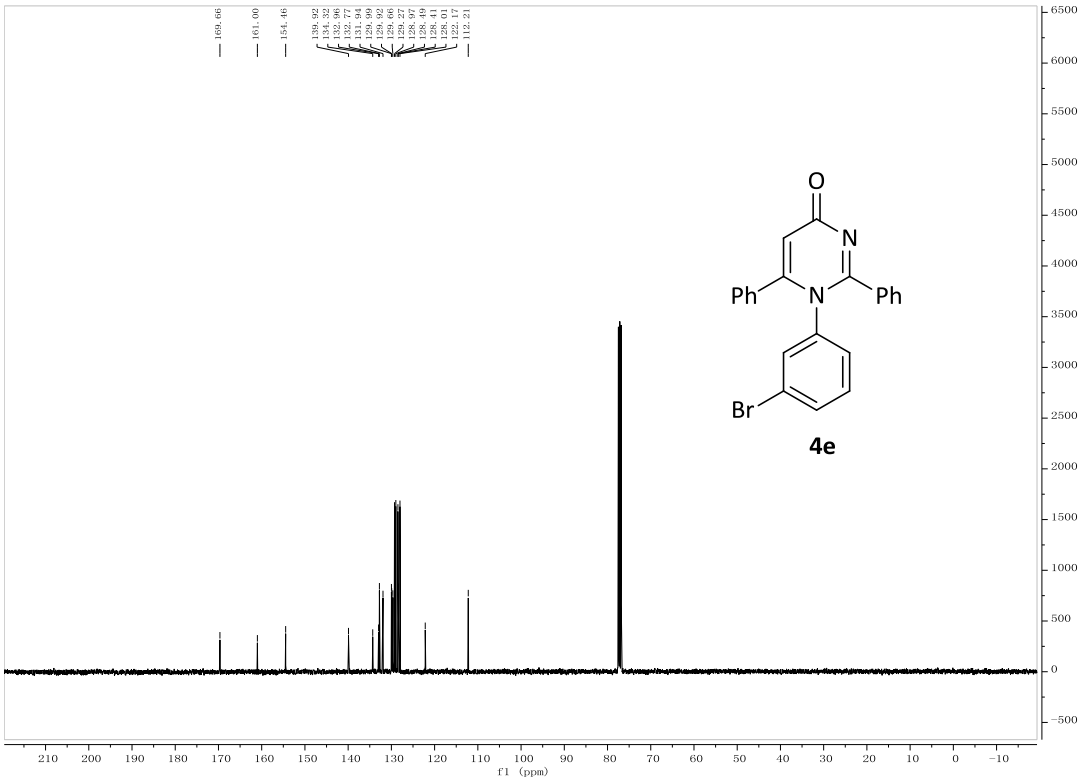
Ph
N
Ph
Br
4e
f1 (ppm)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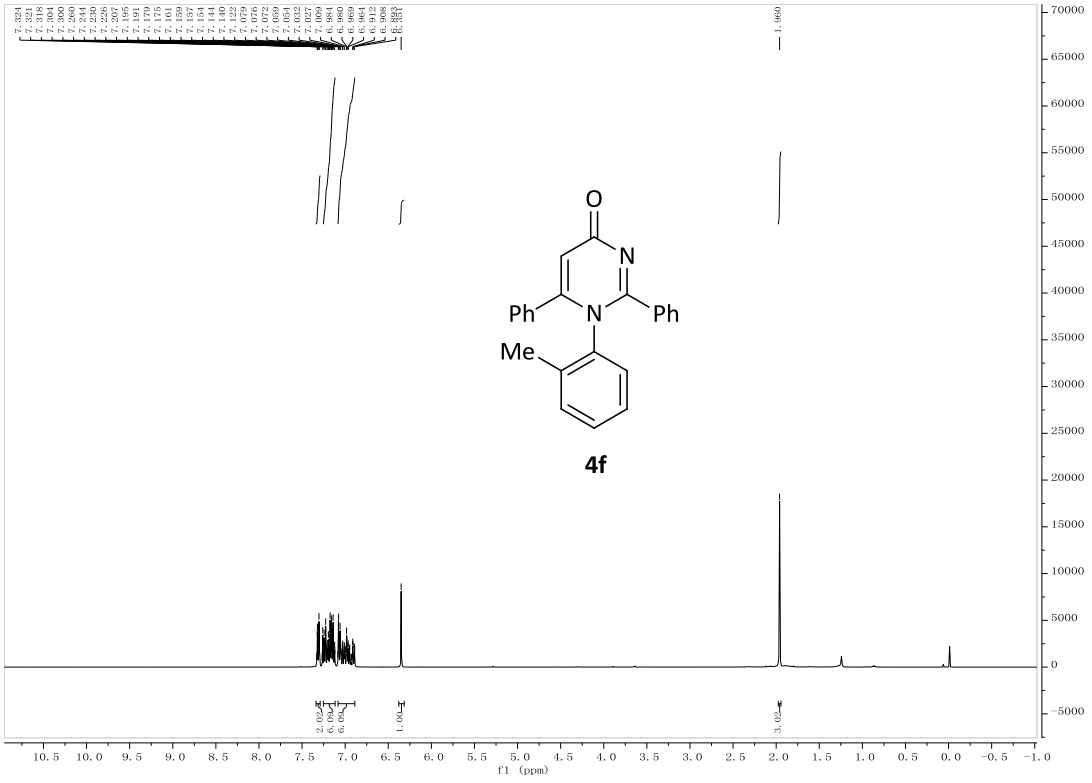
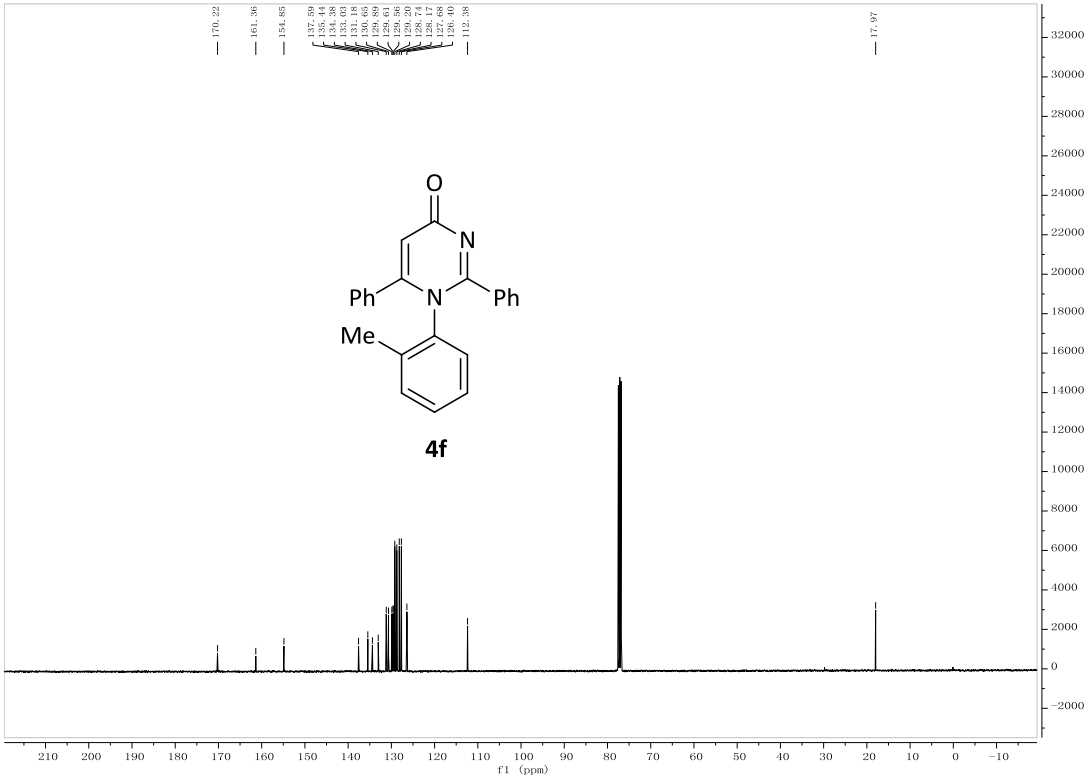
N
Ph
N
Ph
Br
4e
f1 (ppm)


O
N
Ph
N
Ph
Me
4f
f1 (ppm)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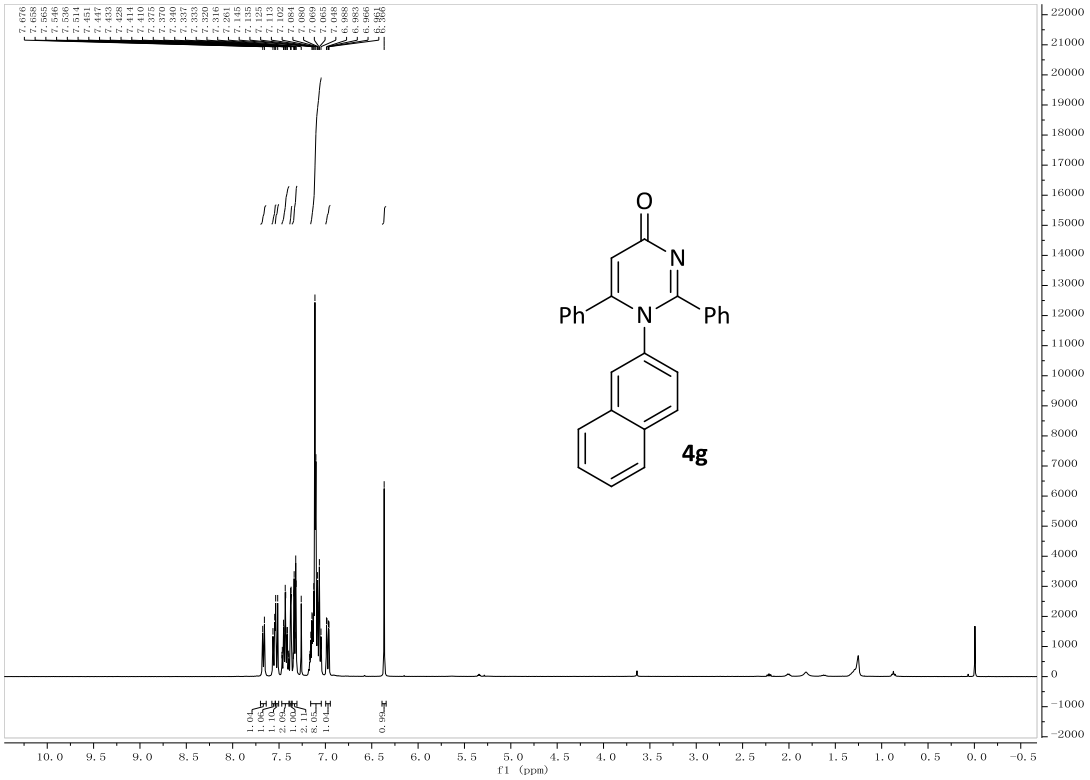
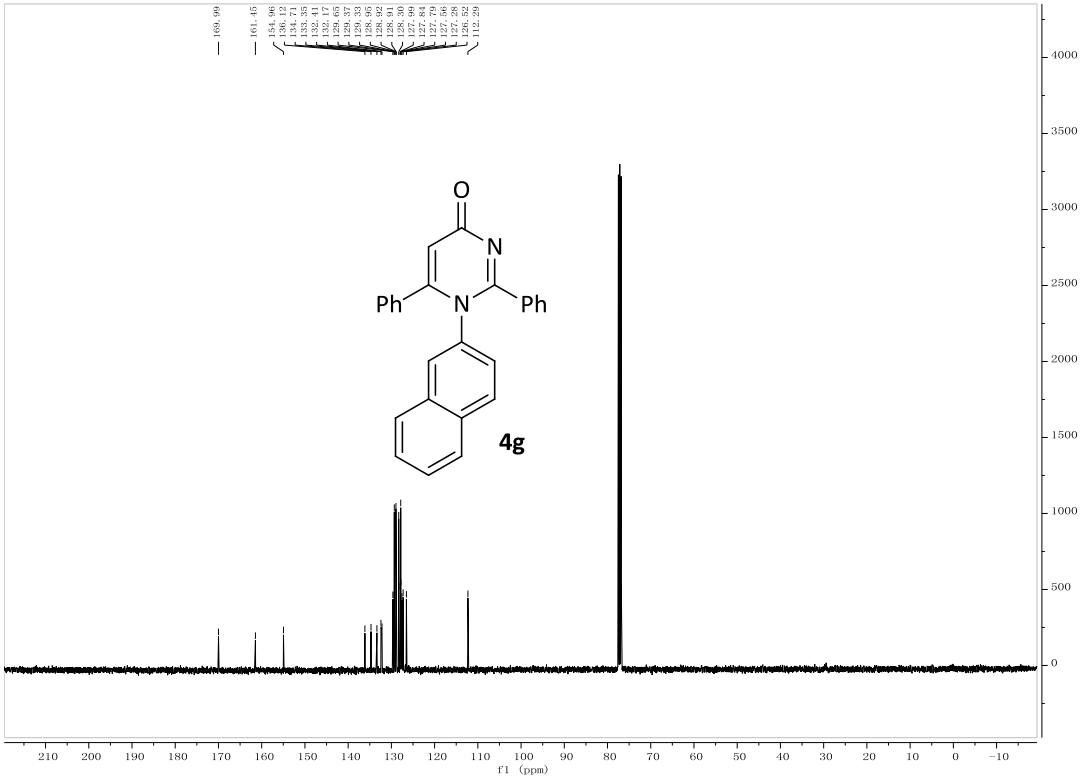
N
Ph
N
Ph
Me
4f
f1 (ppm)


O
N
Ph
N
Ph
4g
f1 (ppm)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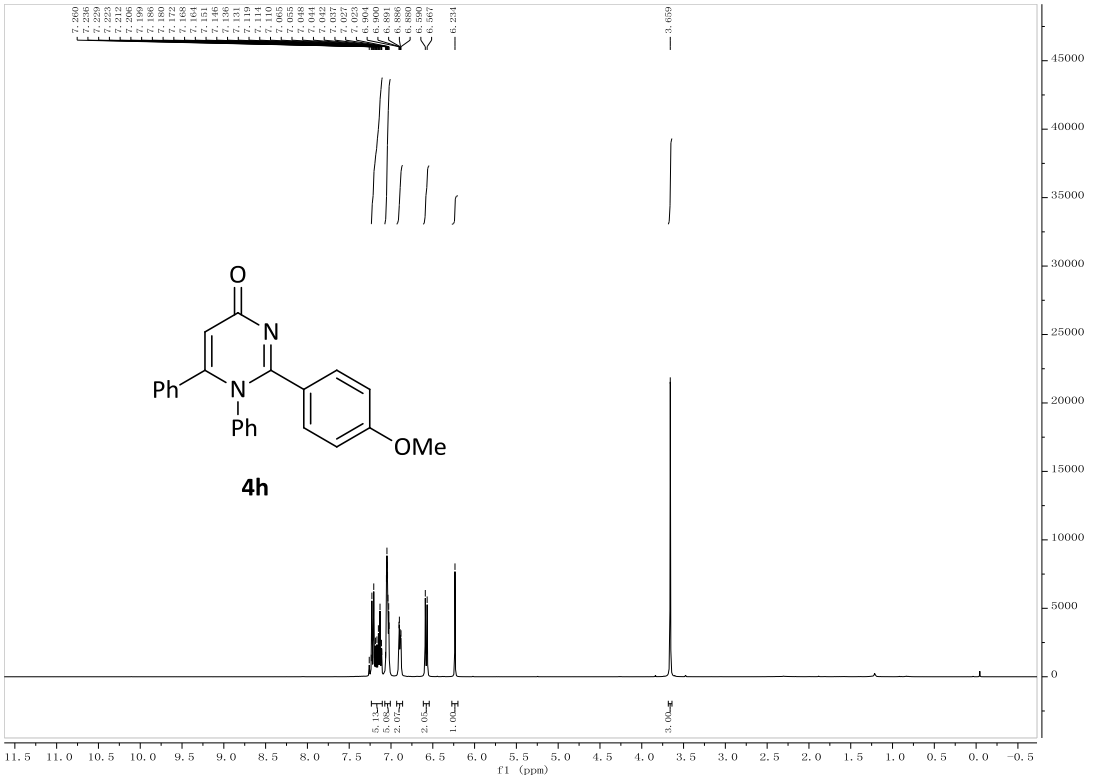
N
Ph
N
Ph
4g
f1 (ppm)


7.260
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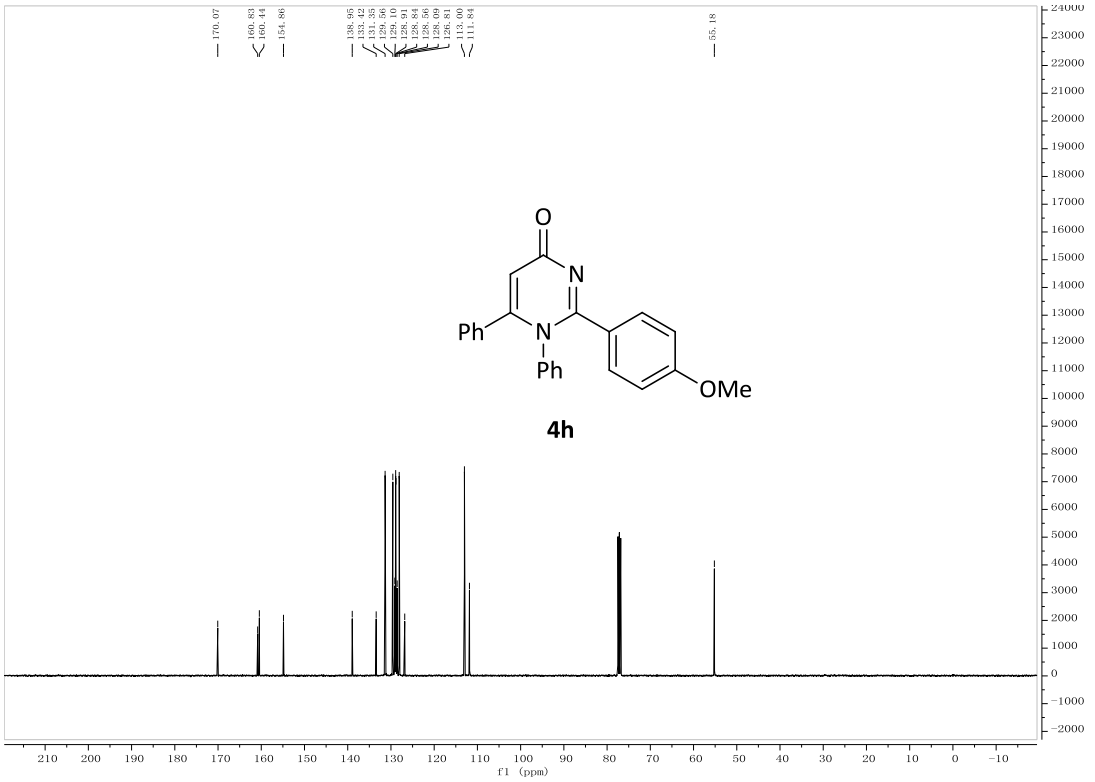
7.229
7.223
7.212
7.205
7.194
7.186
7.180
7.172
7.168
7.164
7.151
7.146
7.136
7.131
7.119
7.114
7.110
7.065
7.055
7.048
7.044
7.042
7.037
7.027
7.023
6.904
6.900
6.891
6.886
6.880
6.590
6.587
6.234
3.659
O
N
Ph
N
Ph
OMe
4h
5.13
5.08
2.07
2.05
1.00
3.00
f1 (ppm)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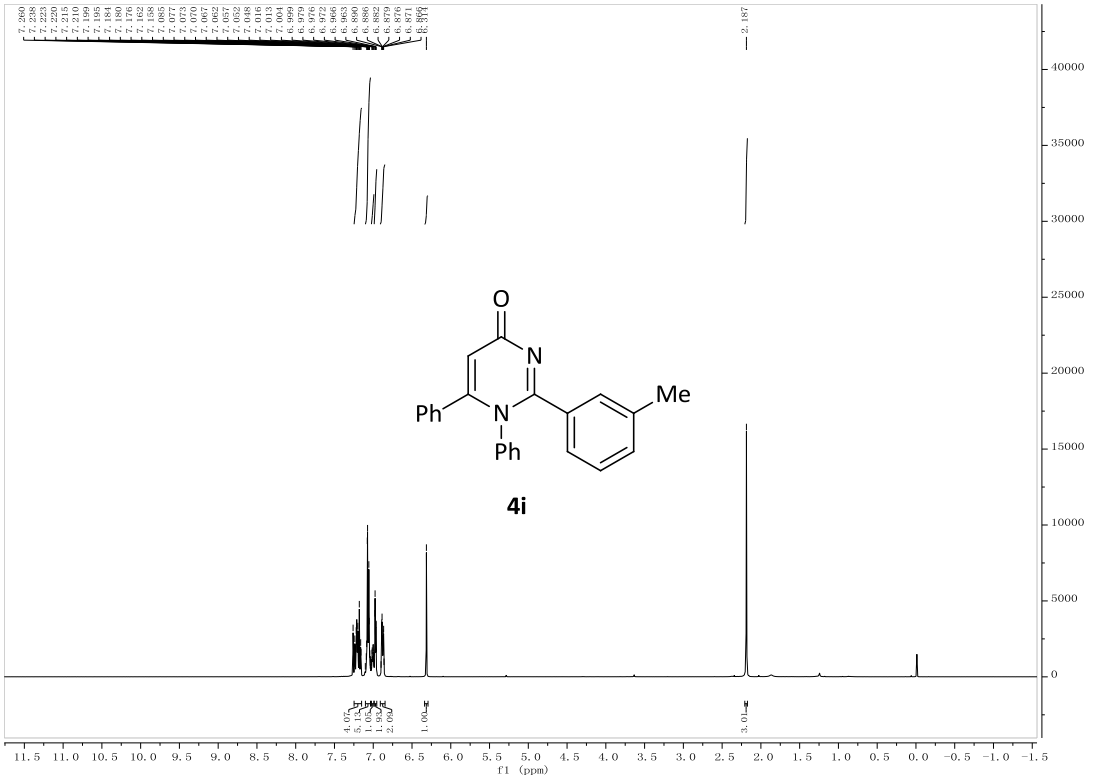
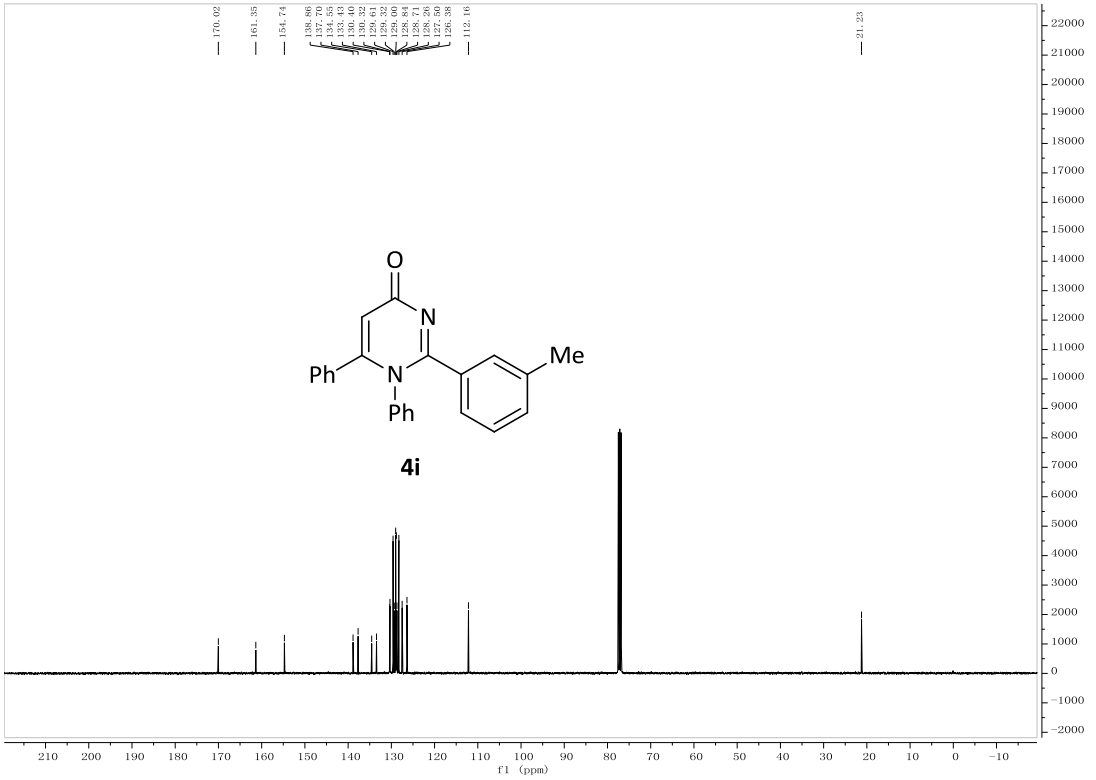
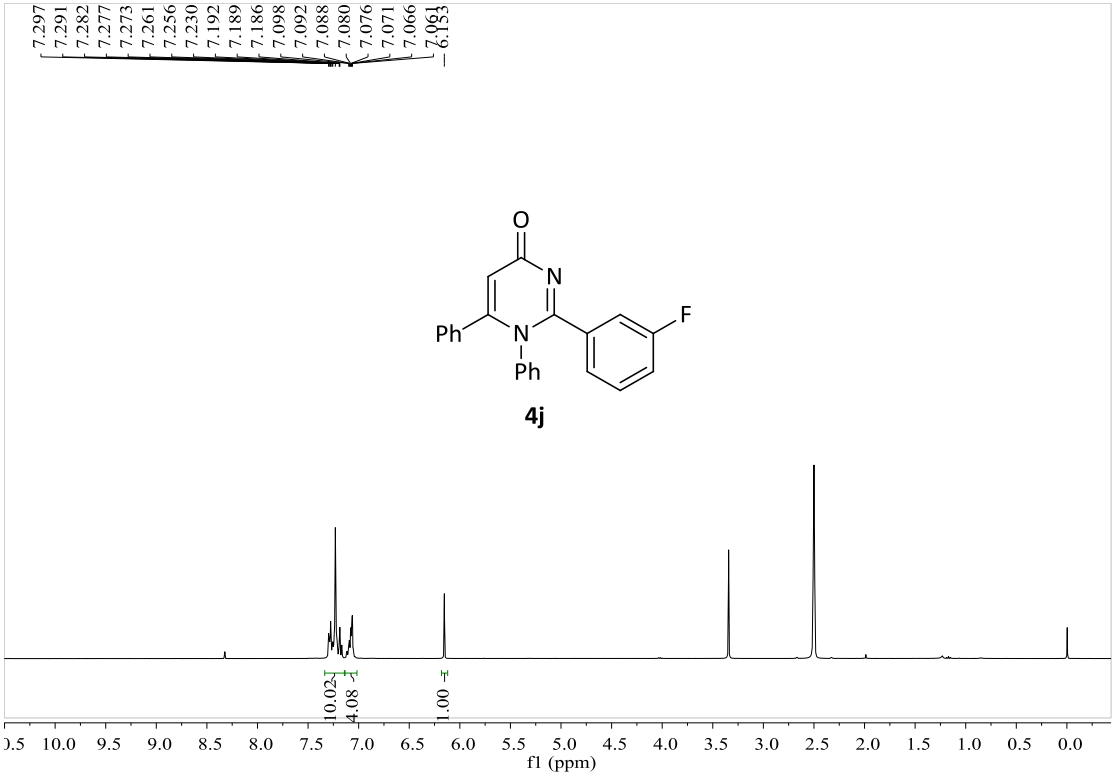
160.83
160.44
154.86
138.95
133.42
131.35
129.56
129.10
128.91
128.84
128.56
128.09
126.81
113.00
111.84
55.18
O
N
Ph
N
Ph
OMe
4h
f1 (ppm)


O
N
Ph
N
Me
Ph
4i
f1 (ppm)


O
N
Ph
N
Me
Ph
4i
f1 (ppm)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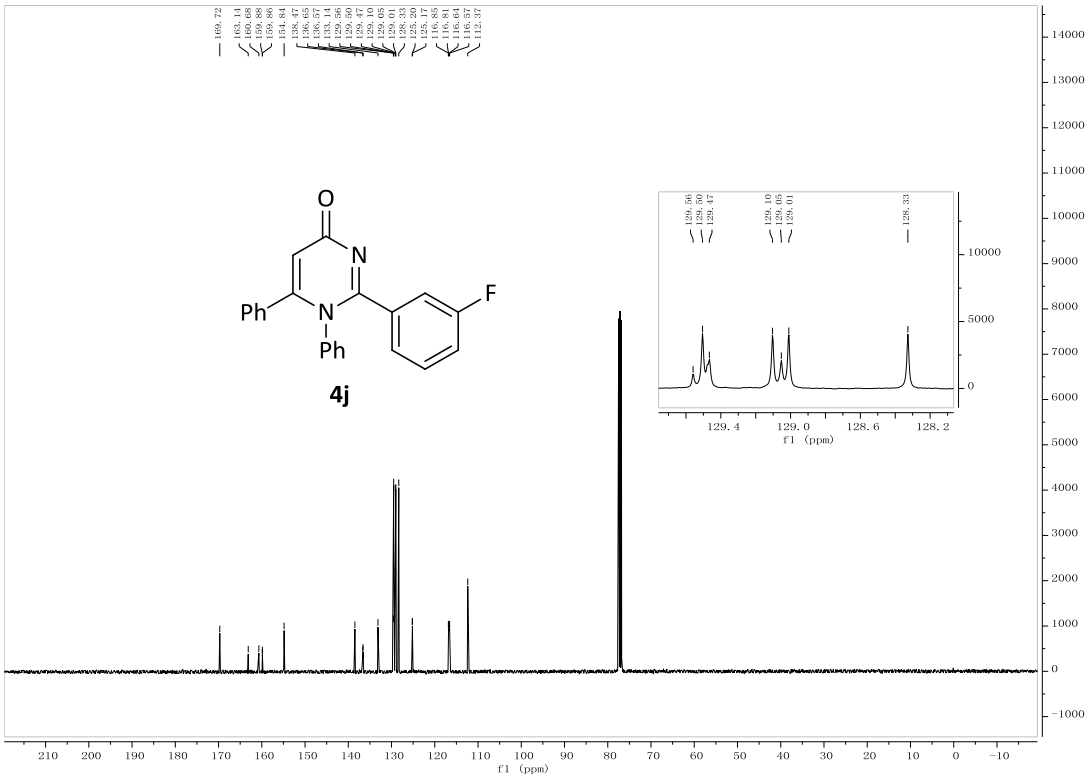
7.277
7.273
7.261
7.256
7.230
7.192
7.189
7.186
7.098
7.092
7.088
7.080
7.076
7.071
7.066
7.061
6.133
O
N
F
Ph
N
Ph
4j
10.02
4.08
1.00
f1 (ppm)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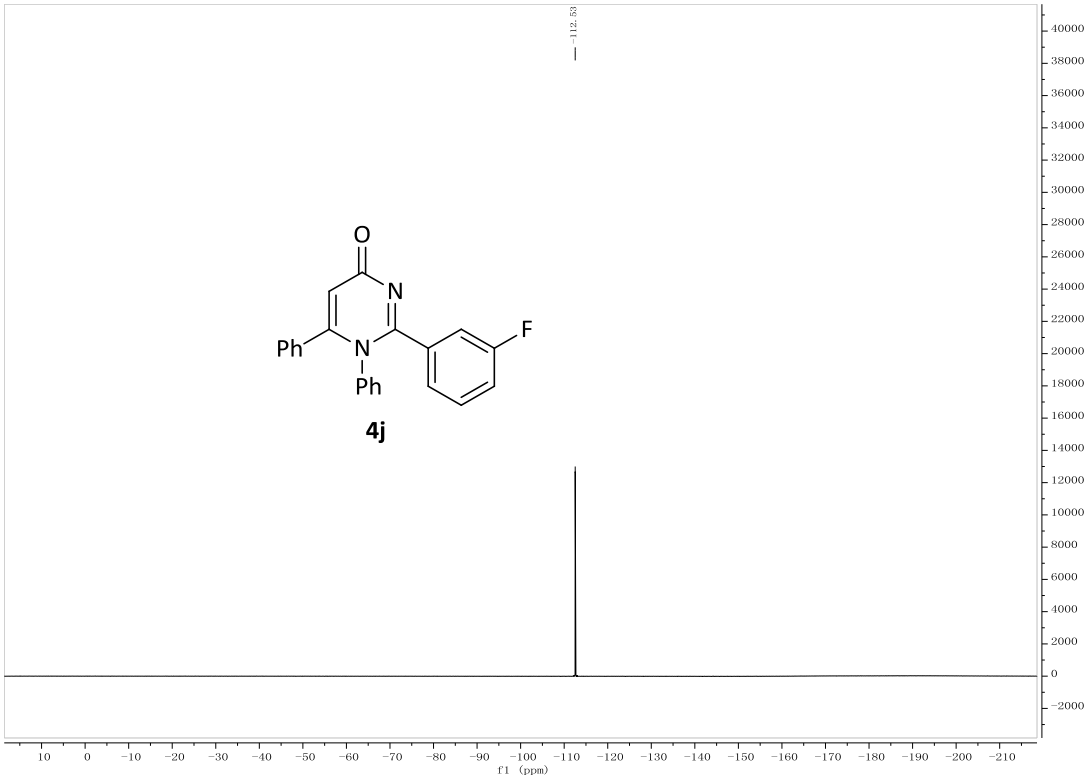
154.47
136.65
136.57
133.14
129.55
129.50
129.47
129.10
129.05
129.01
128.33
125.20
125.17
116.85
116.81
116.64
116.57
112.37
O
N
F
Ph
N
Ph
4j
129.56
129.50
129.47
129.10
129.05
129.01
128.33
f1 (ppm)
f1 (ppm)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N
F
Ph
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30000
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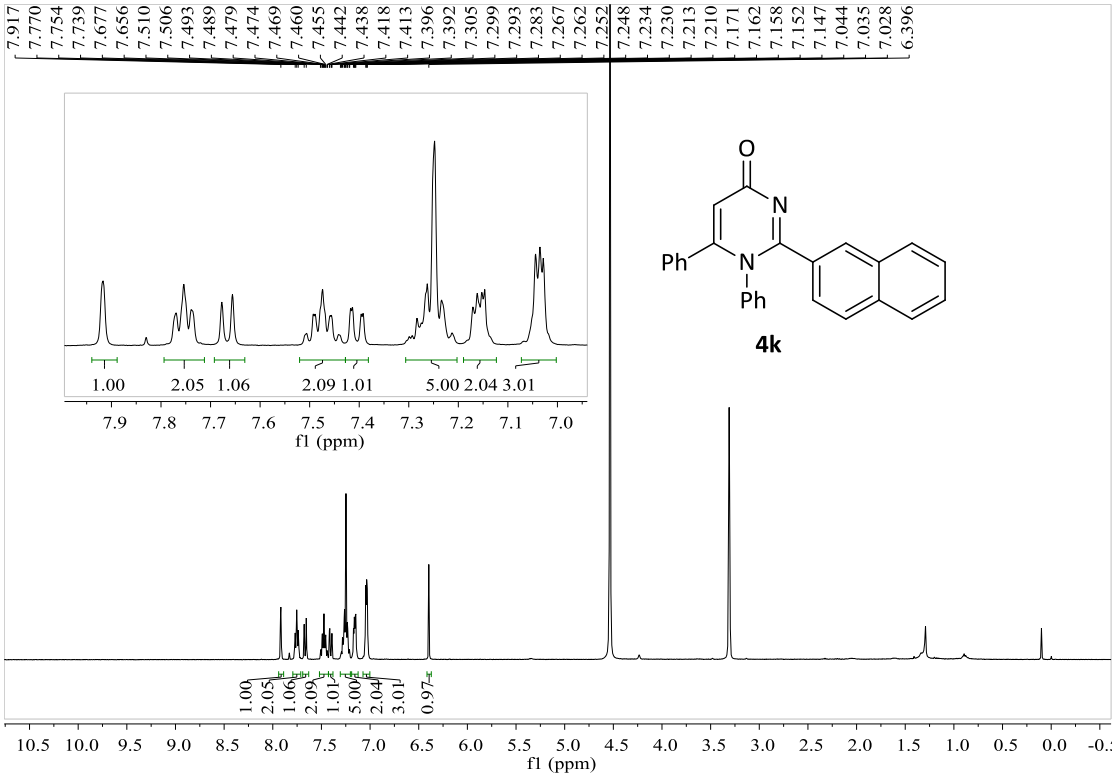
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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7.506
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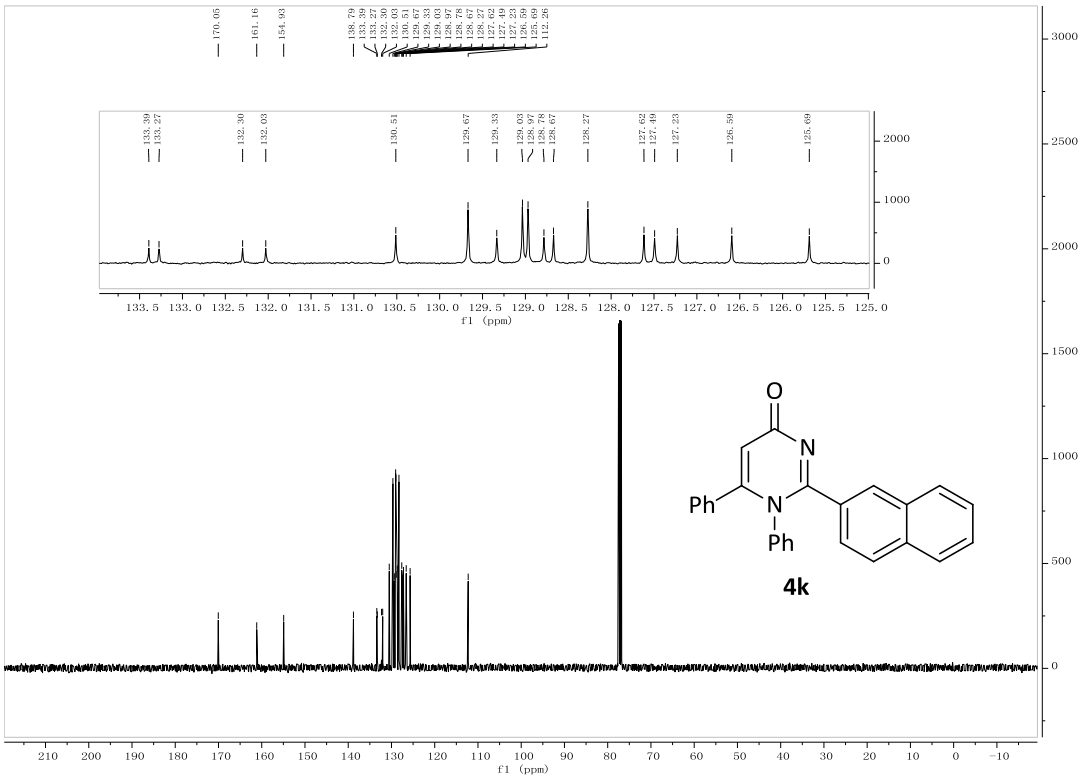
7.489
7.479
7.474
7.469
7.460
7.455
7.442
7.438
7.418
7.413
7.396
7.392
7.305
7.299
7.293
7.283
7.267
7.262
7.252
7.248
7.234
7.230
7.213
7.210
7.171
7.162
7.158
7.152
7.147
7.044
7.035
7.028
6.396
1.00 2.05 1.06 2.09 1.01 5.00 2.04 3.01
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
O
N
Ph
N
Ph
4k
1.00 2.05 1.06 2.09 1.01 5.00 2.04 3.01 0.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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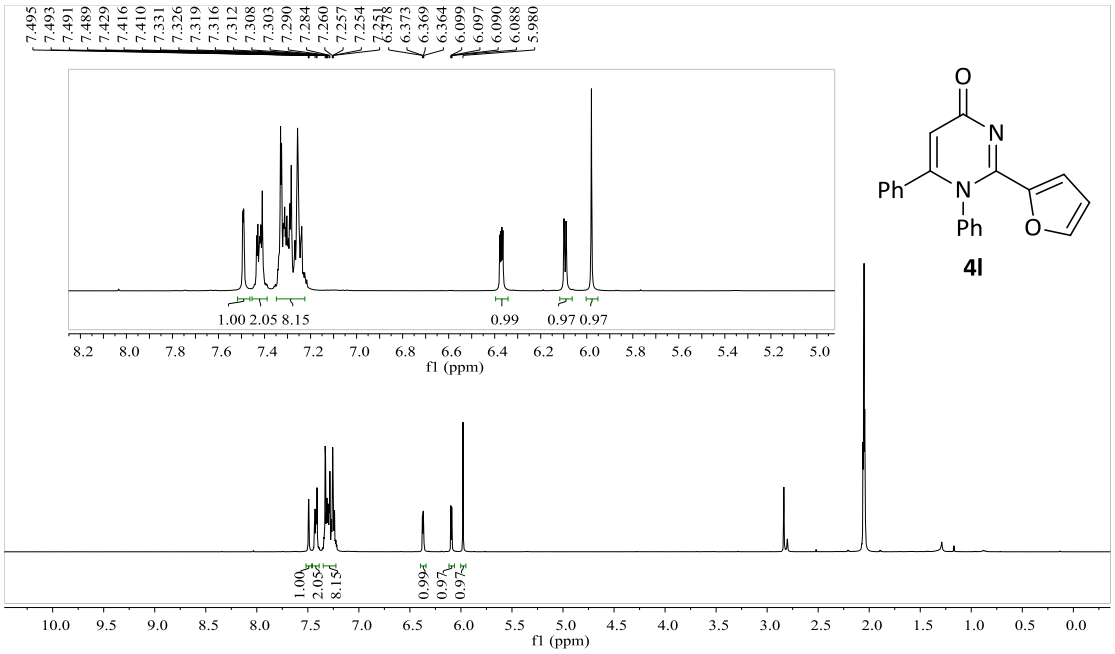
129.33
129.03
128.97
128.78
128.67
128.27
127.62
127.49
127.23
126.59
125.69
112.96
133.39
133.27
132.30
132.03
130.51
129.67
129.33
129.03
128.97
128.78
128.67
128.27
127.62
127.49
127.23
126.59
125.69
f1 (ppm)
f1 (ppm)
O
N
Ph
N
Ph
4k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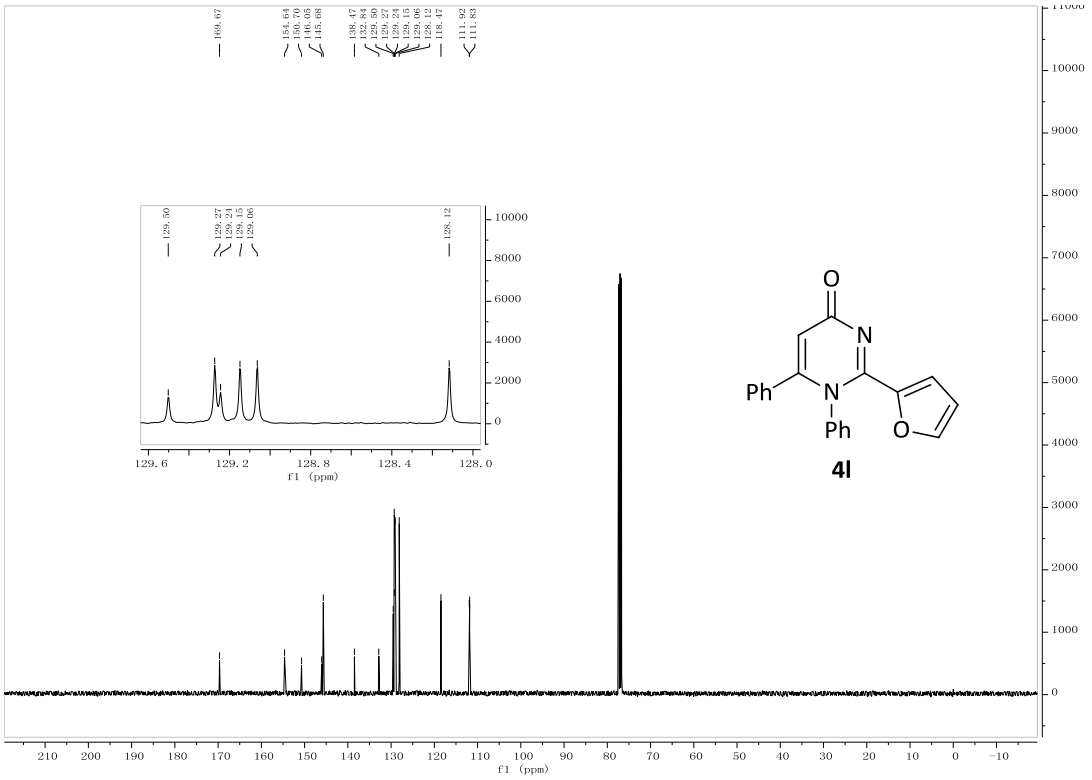
7.308
7.303
7.290
7.284
7.260
7.257
7.254
7.251
6.378
6.373
6.369
6.364
6.099
6.097
6.090
6.088
5.980
1.00 2.05 8.15
0.99
0.97 0.97
f1 (ppm)
O
N
Ph
N
Ph
O
4l
1.00
2.05
8.15
0.99
0.97
0.97
f1 (ppm)


169.67
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151.70
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145.68
138.47
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129.50
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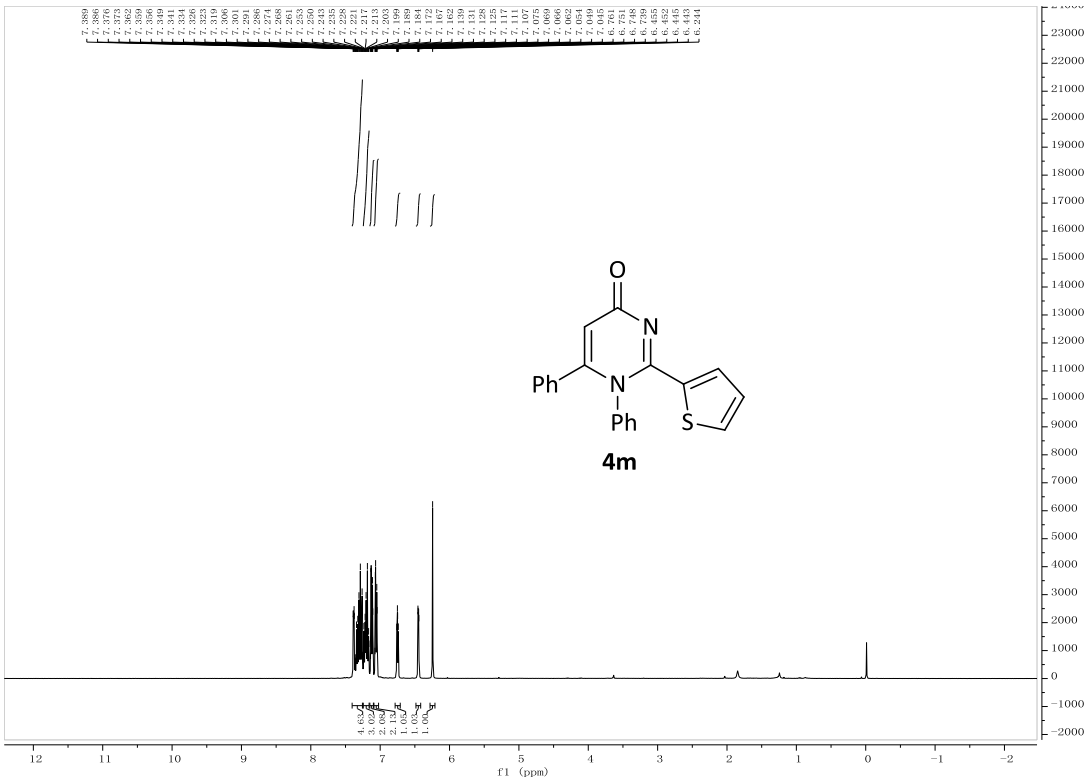
129.24
129.15
129.06
128.12
118.47
111.92
111.83
129.50
129.27
129.24
129.15
129.06
128.12
f1 (ppm)
O
N
Ph
N
Ph
O
4l
f1 (ppm)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7.319
7.306
7.301
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7.274
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7.213
7.203
7.199
7.189
7.184
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7.125
7.117
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7.107
7.075
7.069
7.066
7.062
7.054
7.049
7.045
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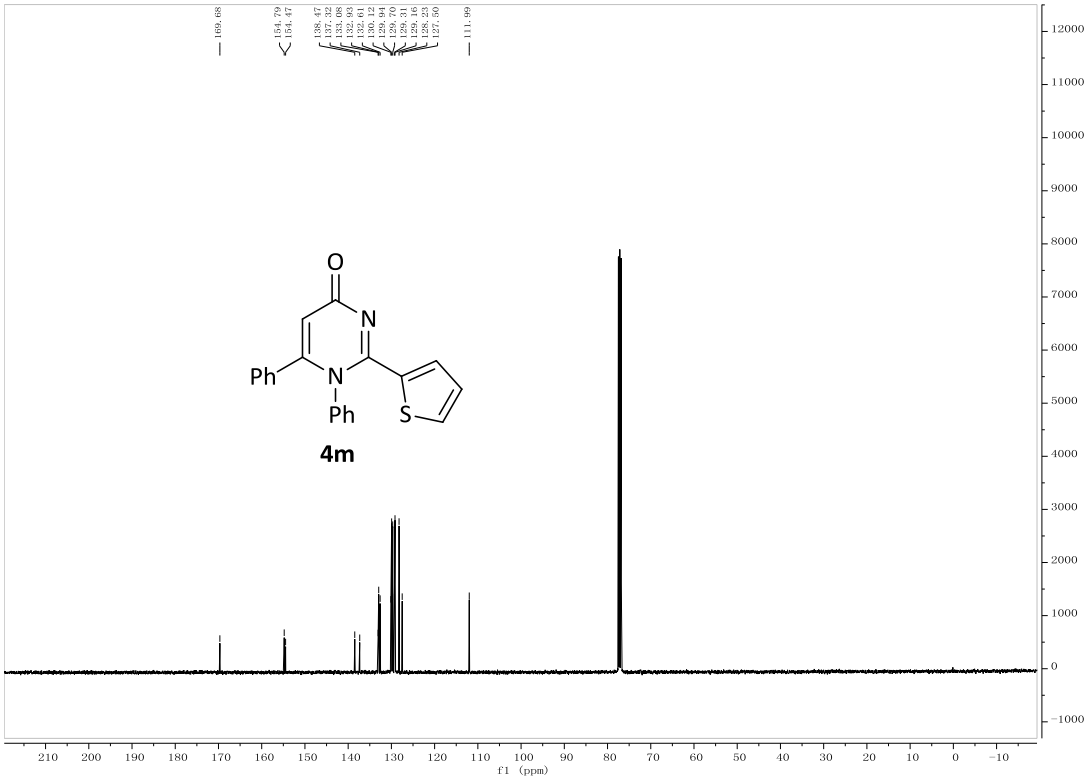
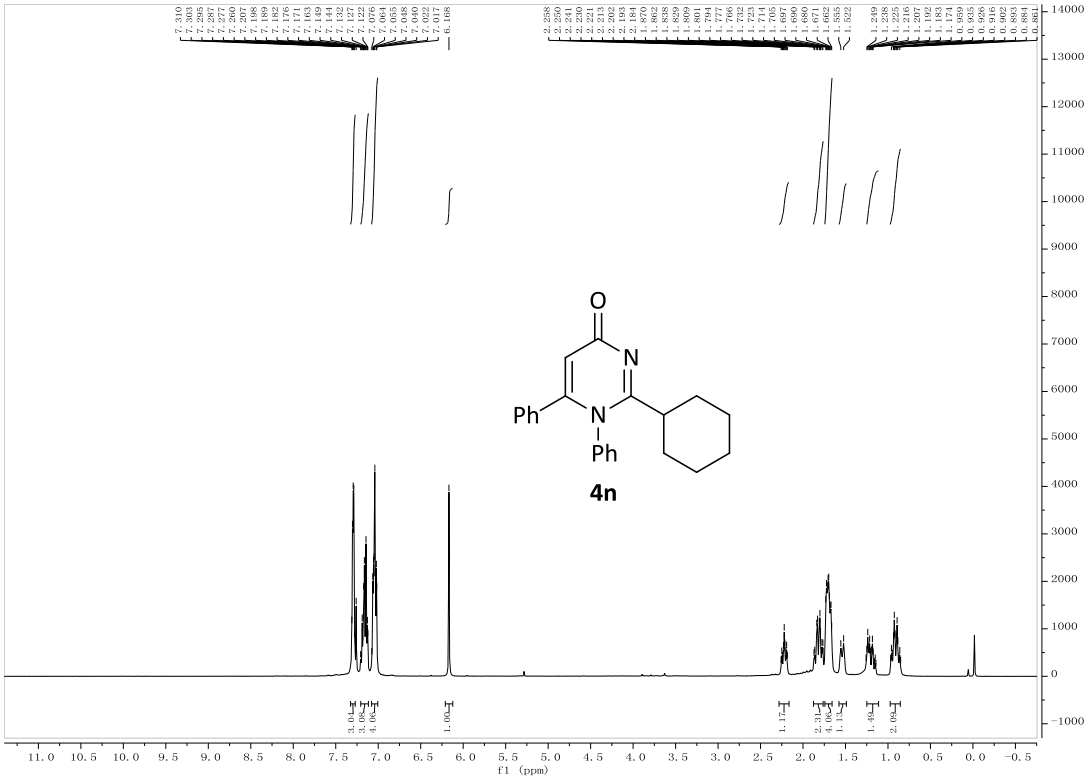
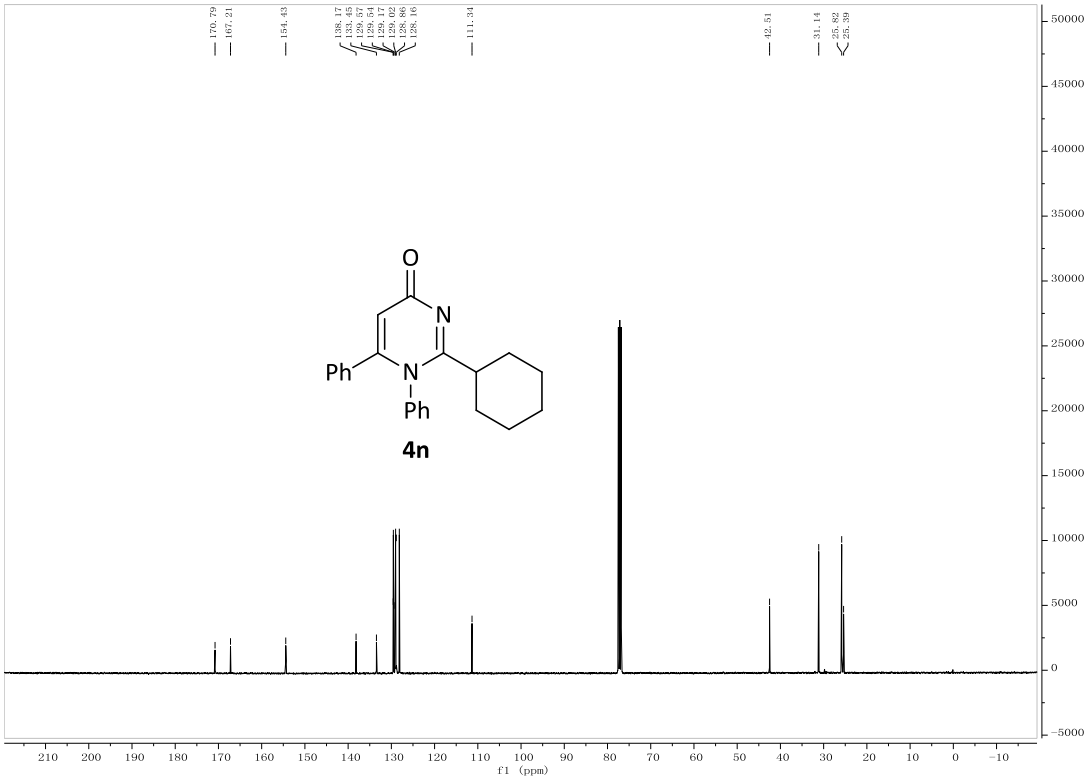
6.751
6.748
6.739
6.455
6.452
6.445
6.441
6.244
O
N
Ph
N
Ph
S
4m
f1 (ppm)


169.68
154.79
154.47
138.47
137.32
133.08
132.85
132.61
130.12
129.94
129.70
129.31
129.16
128.23
127.50
111.99
O
N
Ph
N
Ph
S
4m
f1 (ppm)


7.310
7.303
7.295
7.287
7.277
7.260
7.207
7.189
7.188
7.182
7.176
7.171
7.155
7.149
7.144
7.132
7.127
7.122
7.076
7.064
7.055
7.048
7.040
7.022
7.017
6.168
2.258
2.250
2.241
2.230
2.221
2.213
2.202
2.193
2.184
1.870
1.862
1.838
1.829
1.809
1.801
1.794
1.777
1.766
1.732
1.723
1.714
1.705
1.697
1.690
1.680
1.671
1.662
1.555
1.522
1.249
1.238
1.225
1.216
1.207
1.192
1.184
1.174
0.959
0.935
0.926
0.916
0.902
0.893
0.884
0.881
O
N
Ph
N
Ph
4n
3.04
3.08
4.00
1.00
1.17
2.31
4.06
1.12
1.49
2.09
f1 (ppm)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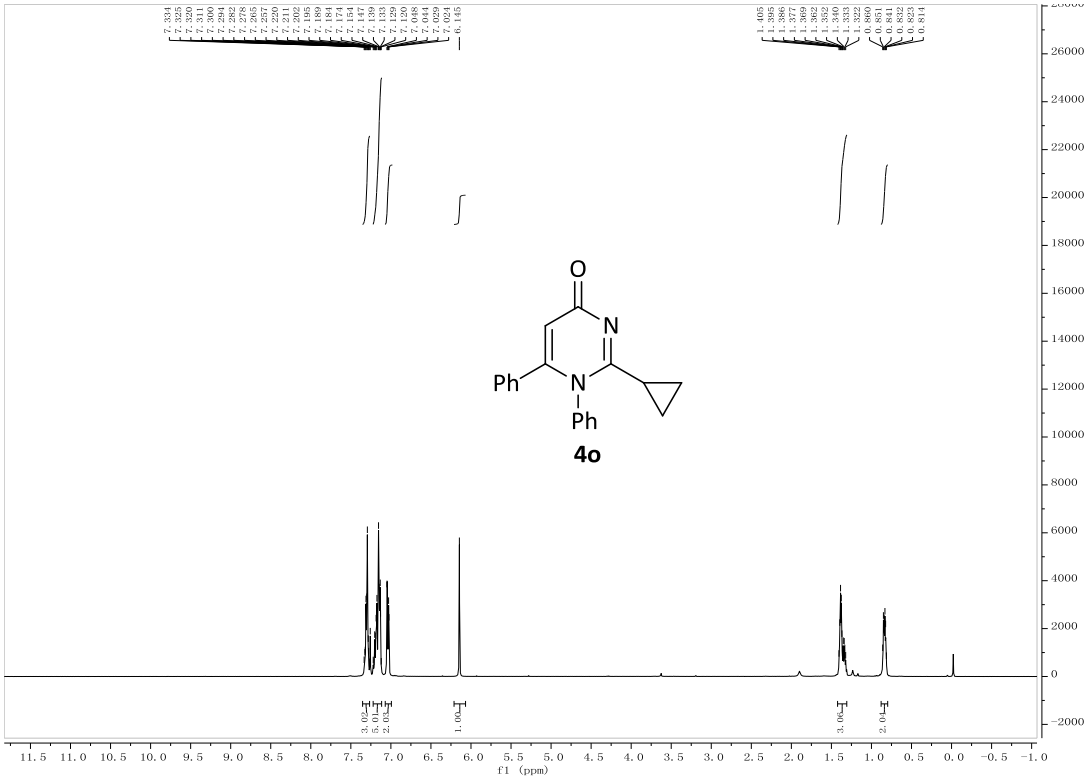
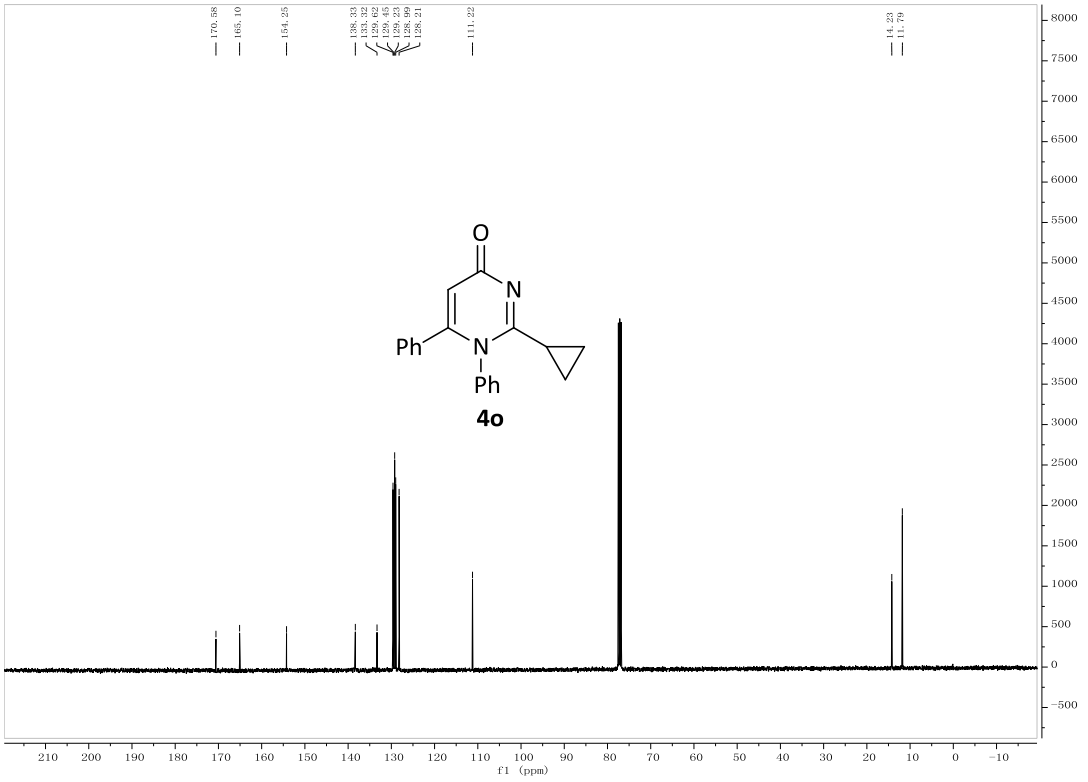
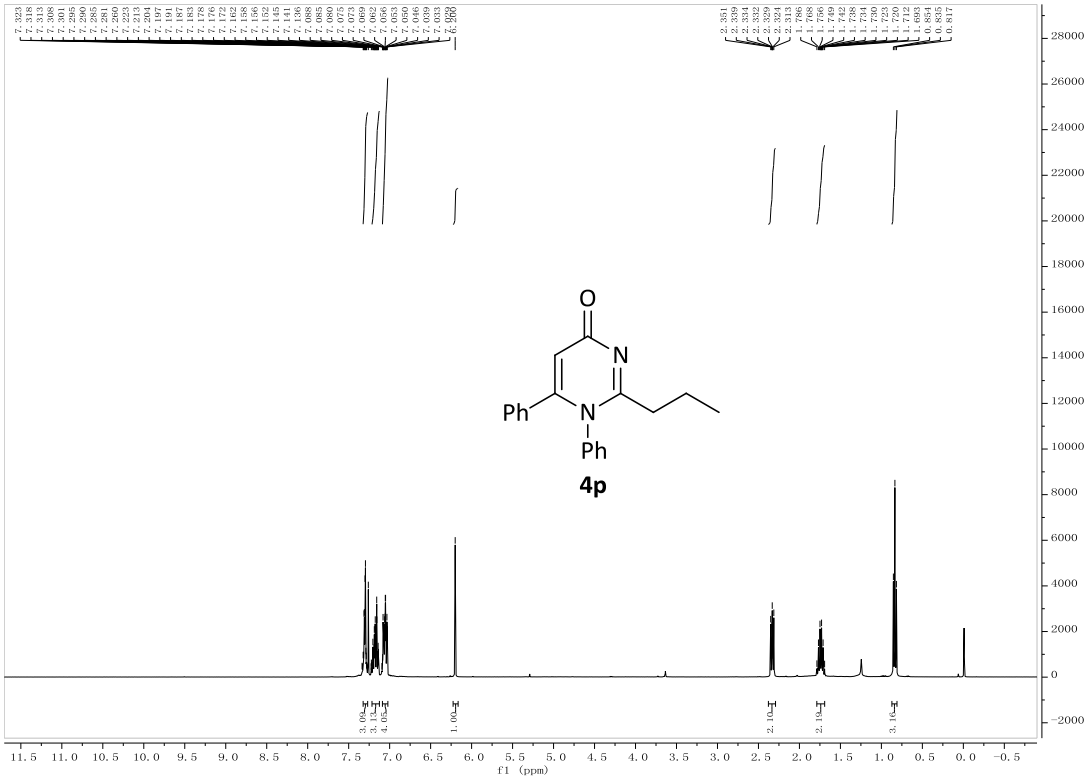
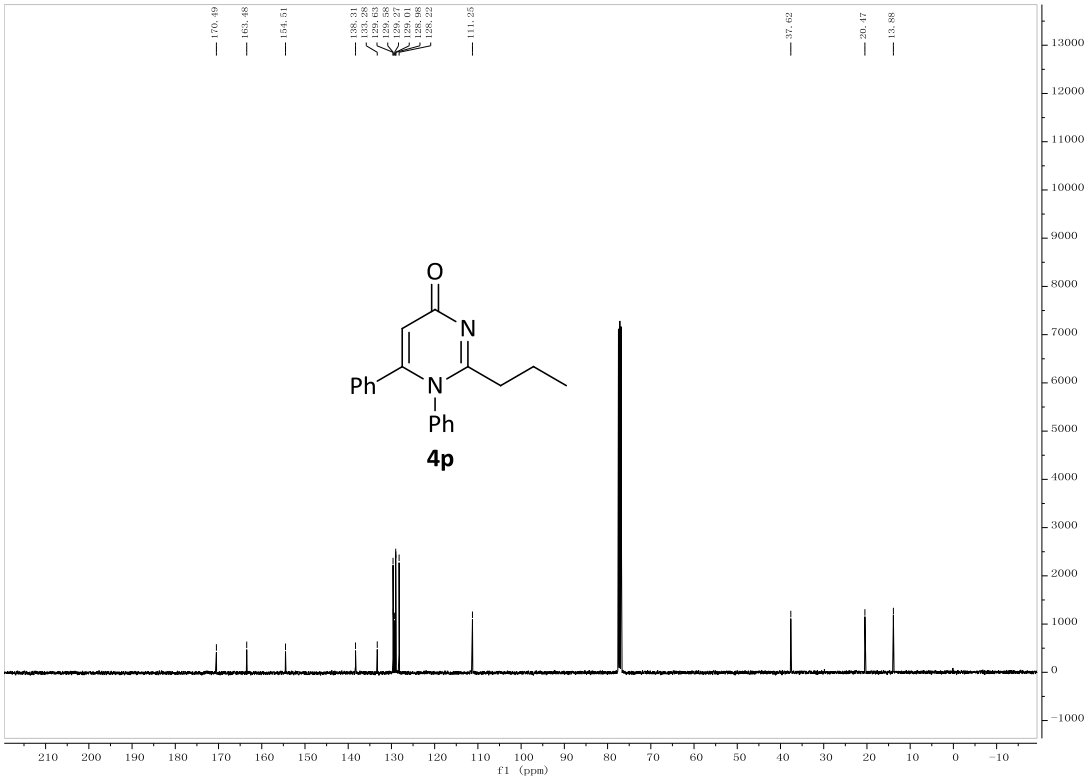
167.21
154.43
138.17
133.45
129.57
129.54
129.17
128.92
128.86
128.16
111.34
42.51
31.14
25.82
25.39
O
N
Ph
N
Ph
4n
f1 (ppm)


7.334
7.325
7.320
7.311
7.300
7.294
7.282
7.278
7.265
7.257
7.220
7.211
7.202
7.195
7.189
7.184
7.174
7.154
7.147
7.139
7.133
7.124
7.120
7.048
7.044
7.029
7.024
6.145
1.405
1.395
1.386
1.377
1.369
1.362
1.352
1.340
1.333
1.322
1.310
0.860
0.851
0.841
0.832
0.824
0.814
O
N
Ph
N
Ph
4o
3.02
5.01
2.03
1.00
3.06
2.04
f1 (ppm)


170.38
165.10
154.25
138.33
133.32
129.62
129.45
129.23
128.99
128.21
111.22
14.23
11.79
O
N
Ph
N
Ph
4o
f1 (ppm)


O
N
Ph
N
Ph
4p
f1 (ppm)


170.49
163.48
154.51
138.34
135.26
129.63
129.58
129.57
129.01
128.98
128.22
111.25
37.62
20.47
13.88
O
N
Ph
N
Ph
4p
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
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)