Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Photocatalyzed Cascade Oxidative Annulation of Propargylamines and Phosphine Oxides

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1. General information

1.1 Materials and measurement.

Commercially available reagents were used as received without purification. Raw Materials were purchased from Sigma–Aldrich. Column chromatography was carried out on silica gel (300–400 mesh). Analytical thin–layer chromatography was performed on glass plates of Silica Gel GF–254 with detection by UV. ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded on a Bruker AVANCE 400M spectrometer. The chemical shift references were as follows: ^{1}H NMR ($CDCl_3$) 7.26 ppm; ^{13}C NMR ($CDCl_3$) 77.00 ppm. HRMS spectra were carried out on Micromass GCT (ESI). Melting point determination was taken on a Melt–Temp apparatus (X-4) from Beijing Fukai Electro–optic Instrument Plant. Absorption and photoluminescence spectra were measured on a UV-3100 spectrophotometer and a Hitachi F-4600 photoluminescence spectrophotometer, respectively. Cyclic voltammetry measurements were conducted on a MPI-A multifunctional electrochemical and chemiluminescent system (Xi'an Remex Analytical Instrument Ltd. Co., China) at room temperature, with a polished Pt plate as the working electrode, platinum thread as the counter electrode and Ag-$AgNO_3$ (0.1 M) in CH_3CN as the reference electrode, *tetra*-n-butylammonium perchlorate (0.1 M) was used as the supporting electrolyte, using Fc^+/Fc as the internal standard, the scan rate was 0.1 V/s.

1.2 Fabrication and measurements of OLEDs.

Indium-tin-oxide (ITO) coated glass with a sheet resistance of 10 Ω sq^{-1} was used as the anode substrate. Prior to film deposition, patterned ITO substrates were cleaned with detergent, rinsed in deionized water, dried in an oven, and finally treated with oxygen plasma for 5 minutes at a pressure of

10 Pa to enhance the surface work function of ITO anode (from 4.7 to 5.1 eV). All the organic layers were deposited with the rate of 0.1 nm s^{-1} under high vacuum ($\leq 2\times10^{-5}$ Pa). The doped layers were prepared by co-evaporating dopant and host material from two individual sources, and the doping concentrations were modulated by controlling the evaporation rate of dopant. MoO_3, LiF and Al were deposited in another vacuum chamber ($\leq 8.0\times10^{-5}$ Pa) with the rates of 0.01, 0.01 and 1 nm s^{-1}, respectively, without being exposed to the atmosphere. The thicknesses of these deposited layers and the evaporation rate of individual materials were monitored in vacuum with quartz crystal monitors. A shadow mask was used to define the cathode and to make ten emitting dots (with the active area of 10 mm^2) on each substrate. Device performances were measured by using a programmable Keithley source measurement unit (Keithley 2400 and Keithley 2000) with a silicon photodiode. The EL spectra were measured with a calibrated Hitachi F−7000 fluorescence spectrophotometer. Based on the uncorrected EL fluorescence spectra, the Commission Internationale de l'Eclairage (CIE) coordinates were calculated using the test program of Spectrascan PR650 spectrophotometer. The EQE of EL devices were calculated based on the photo energy measured by the photodiode, the EL spectrum, and the current pass through the device.

2. Experimental Section

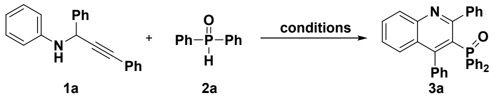
2.1 Synthesis of propargylamines following reported procedures (*J. Org. Chem.* **2006**, *71*, 2064-2070; *Org. Lett.* **2006**, *8*, 2405-2408; *Tetrahedron*, **2014**, *70*, 3134-3140).

2.2 General procedure for the preparation of 3-phosphorylated quinolines.

A dry and argon-flushed *Schlenk*-flask, equipped with a magnetic stirring bar is charged with propargylamine (0.3 mmol), diphenylphosphine oxide (0.6 mmol), $Ir(ppy)_3$ (0.009 mmol), iodobenzene diacetate (0.6 mmol), sodium bicarbonate (0.45 mmol). Then dry DMF (3.0 mL) is added and the reaction mixture is irradiated with a green LED lamp (5 W). After stirring for 36 h at room temperature, the crude mixture was purified by flash column chromatography to afford the target product.

3. Supplementary data

Table S1. Optimization of the reaction conditions[a].



entry	additive (equiv)	solvent	T (℃)/t (h)	yield (%)[b]
1	AgOAc (3.0)	DMF	100/12	63
2	CF_3COOAg (3.0)	DMF	100/12	trace
3	AgOTf (3.0)	DMF	100/12	trace
4	$AgBF_4$ (3.0)	DMF	100/12	trace
5	$AgNO_3$ (3.0)	DMF	100/12	trace
6	Ag_2CO_3 (3.0)	DMF	100/12	57
7	Ag_2O (3.0)	DMF	100/12	55
8	$Cu(OAc)_2$ (3.0)	DMF	100/12	NR
9	$K_2S_2O_8$ (3.0)	DMF	100/12	23
10	TBHP (3.0)	DMF	100/12	trace
11	AgOAc (3.0)	DMAc	100/12	35
12	AgOAc (3.0)	DMSO	100/12	26
13	AgOAc (3.0)	NMP	100/12	42
14	AgOAc (3.0)	MeOH	100/12	37
15	AgOAc (3.0)	CH_3CN	100/12	68
16	AgOAc (3.0)	THF	100/12	20
17	AgOAc (3.0)	toluene	100/12	trace
18	AgOAc (3.0)	DCE	100/12	51
19	AgOAc (0.2)/$K_2S_2O_8$ (3.0)	CH_3CN	100/12	trace
20	AgOAc (0.2)/$Mg(NO_3)_2 \cdot 6H_2O$ (0.5)	CH_3CN	100/12	trace
21	AgOAc (3.0)/KOAc (3.0)	CH_3CN	100/12	69
22	AgOAc (3.0)/Na_2CO_3 (3.0)	CH_3CN	100/12	60
23	AgOAc (3.0)/DIPEA (3.0)	CH_3CN	100/12	27
24	AgOAc (3.0)/DBU (3.0)	CH_3CN	100/12	trace
25	**AgOAc (3.0)/DABCO (3.0)**	**CH_3CN**	100/12	**76**
26	AgOAc (3.0)/DABCO (3.0)	CH_3CN	120/12	73
27	AgOAc (3.0)/DABCO (3.0)	CH_3CN	80/12	60
28	AgOAc (3.0)/DABCO (3.0)	CH_3CN	100/24	73
29	AgOAc (2.0)/DABCO (3.0)	CH_3CN	100/12	45
30[c]	AgOAc (3.0)/DABCO (3.0)	CH_3CN	100/12	75

[a]Reaction condition: Propargylamine (0.3 mmol), diphenylphosphine oxide (0.6 mmol), solvent (3.0 mL), under an ambient atmosphere. [b]Isolated yield. [c]Under argon.

Scheme S1. Sequential model for the synthesis of phosphorylated quinoline

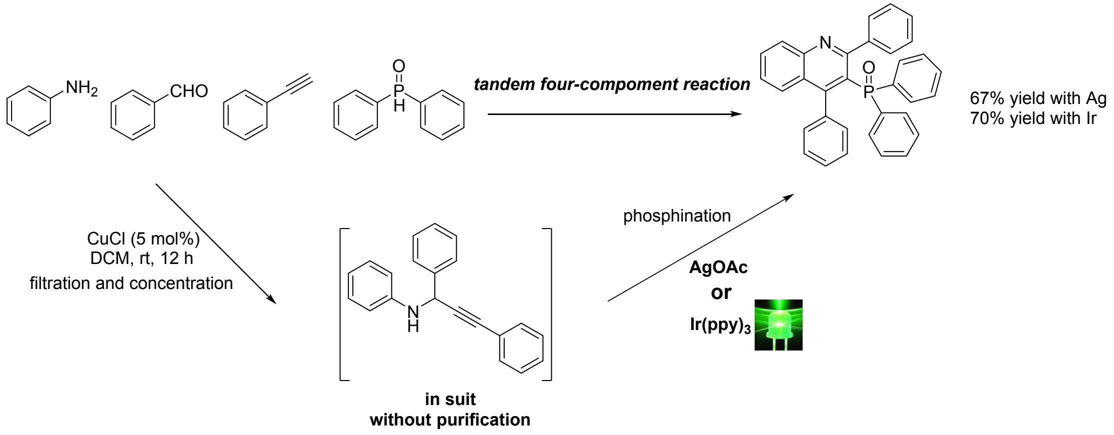
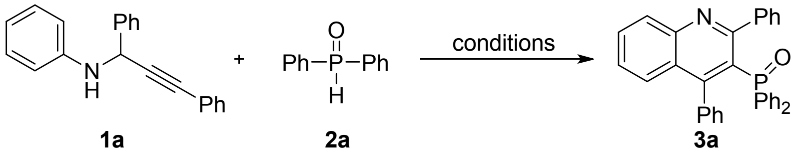


Table S2. Optimization of the photocatalyzed reaction conditions[a].



entry	photocatalyst	oxidant	base	solvent	light source	yield[b]
1	$Ru(bpy)_3 \cdot 6H_2O$	PIDA (2.0 eqv)	--------------	DMF	G-LED	Trace
2	$(dfppy)_2Ir(dtbpy)PF_6$	PIDA (2.0 eqv)	--------------	DMF	G-LED	13%
3	$Ir(mppy)_3$	PIDA (2.0 eqv)	--------------	DMF	G-LED	44%
4	$Ir(ppy)_3$	PIDA (2.0 eqv)	--------------	DMF	G-LED	53%
5	FIrpic	PIDA (2.0 eqv)	--------------	DMF	G-LED	37%
6	EosinY	PIDA (2.0 eqv)	--------------	DMF	G-LED	15%
7	$Ir(ppy)_3$	PIDA (2.0 eqv)	Na_2HPO_4 (1.5 eqv)	DMF	G-LED	50%
8	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	62%
9	$Ir(ppy)_3$	PIDA (2.0 eqv)	LiOAc (1.5 eqv)	DMF	G-LED	42%
10	$Ir(ppy)_3$	PIDA (2.0 eqv)	K_2CO_3 (1.5 eqv)	DMF	G-LED	31%
11	$Ir(ppy)_3$	PIDA (2.0 eqv)	DABCO (1.5 eqv)	DMF	G-LED	Trace
12	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.0 eqv)	DMF	G-LED	55%
13	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (2.0 eqv)	DMF	G-LED	47%
14	$Ir(ppy)_3$	PIFA	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	trace
15	$Ir(ppy)_3$	$Ph_2I^+OTf^-$	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	32%
16	$Ir(ppy)_3$	TBHP	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	trace
17	$Ir(ppy)_3$	BQ	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	NR
18	$Ir(ppy)_3$	CBr_4	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	NR
19	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMSO	G-LED	40%
20	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	NMP	G-LED	45%
21	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	CH_3CN	G-LED	15%
22	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	Acetone	G-LED	Trace
23	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMF	B-LED	39
24	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMF	W-LED	45
25	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMF	W-CFL	40
26	$Ir(ppy)_3$	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMF	Dark	NR
27	--------	PIDA (2.0 eqv)	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	Trace
28	$Ir(ppy)_3$	---------	$NaHCO_3$ (1.5 eqv)	DMF	G-LED	Trace

29	Ir(ppy)$_3$	PIDA (3.0 eqv)	NaHCO$_3$ (1.5 eqv)	DMF	G-LED	50%
30[c]	Ir(ppy)$_3$	PIDA (2.0 eqv)	NaHCO$_3$ (1.5 eqv)	DMF	G-LED	61%
31[d]	**Ir(ppy)$_3$**	**PIDA (2.0 eqv)**	**NaHCO$_3$ (1.5 eqv)**	**DMF**	**G-LED**	**78%**
32[e]	Ir(ppy)$_3$	PIDA (2.0 eqv)	NaHCO$_3$ (1.5 eqv)	DMF	G-LED	NR

[a]Reaction condition: Propargylamine (0.3 mmol), diphenylphosphine oxide (0.6 mmol), photocatalyst (3 mol%), oxidant (0.6 mmol), base (0.45 mmol), solvent (3.0 mL), under an ambient atmosphere for 36 h. [b]Isolated yield. [c]diphenylphosphine oxide (0.9 mmol). [d]Under argon. [e]Under oxygen.

Table S3. Physical property data of QDPO (**3a**).

Compound	T_d [a)] [°C]	λ_{abs} [b)] [nm]	λ_{em} [b)] [nm]	E$_g$ [eV]	HOMO/LUMO [c)] [eV]
QDPO	370	245/345	405	3.85	6.65/2.80

[a)] T_d: decomposition temperature; [b)]Measured at RT in CH$_2$Cl$_2$ (10^{-5} M); [c)] HOMO/LUMO energy levels calculated using the cyclic voltammetry (CV) diagram with ferrocene as the internal standard and the absorption spectra of QDPO for E$_g$. $E_{HOMO} = E_{ox} - E^{+}_{Fc/Fc} + 4.8$; $E_{LUMO} = E_{HOMO} - E_g$.

Table S4. The relevant data values for HOMO/LUMO levels of QDPO.

Compound	$\Delta E_{ox\text{-}Ferrocene}$ [a)] [eV]	$\Delta E_{ox\text{-}complexes}$ [a)] [eV]	HOMO[b)] [eV]	λ_{ab} [nm]	E$_g$ [eV]	LUMO [eV]
QDPO	0.18	2.03	-6.65	322	3.85	-2.80

$E_{HOMO} = E_{ox} - E^{+}_{Fc/Fc} + 4.8$; $E_{LUMO} = E_{HOMO} - E_g$; initial absorption spectra of QDPO for E$_g$.

$E_{HOMO} = E_{ox} - E^{+}_{Fc/Fc} + 4.8 = 2.03 - 0.18 + 4.8 = 6.65$ eV;

$E_g = 1240/322 = 3.85$ eV;

$E_{LUMO} = E_{HOMO} - E_g = 6.65 - 3.85 = 2.80$ eV

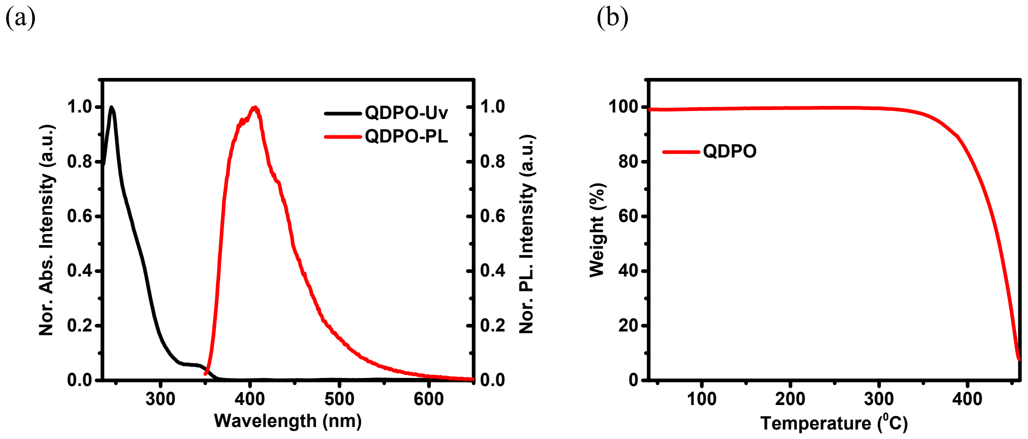


Figure S1. (a) UV−vis absorption and photoluminescence spectra of QDPO in CH$_2$Cl$_2$ (10^{-5} M) solution at room temperature; (b) The TGA curves of QDPO recorded at a heating rate of 10 °C min^{-1}.

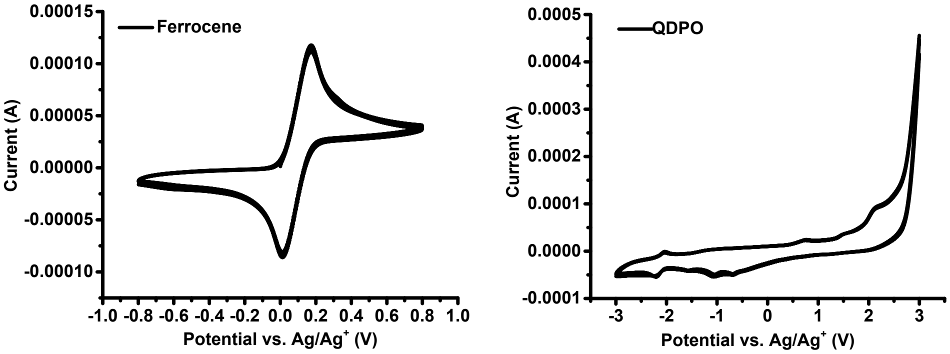


Figure S2. Cyclovoltammety (CV) diagrams of QDPO in acetonitrile and CV of ferrocene is shown for the calibration.

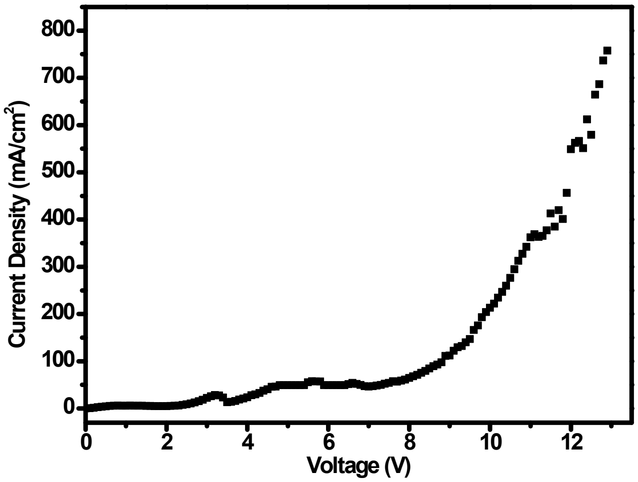


Figure S3. Current density versus voltage characteristics of the electron-only device based on QDPO compound.

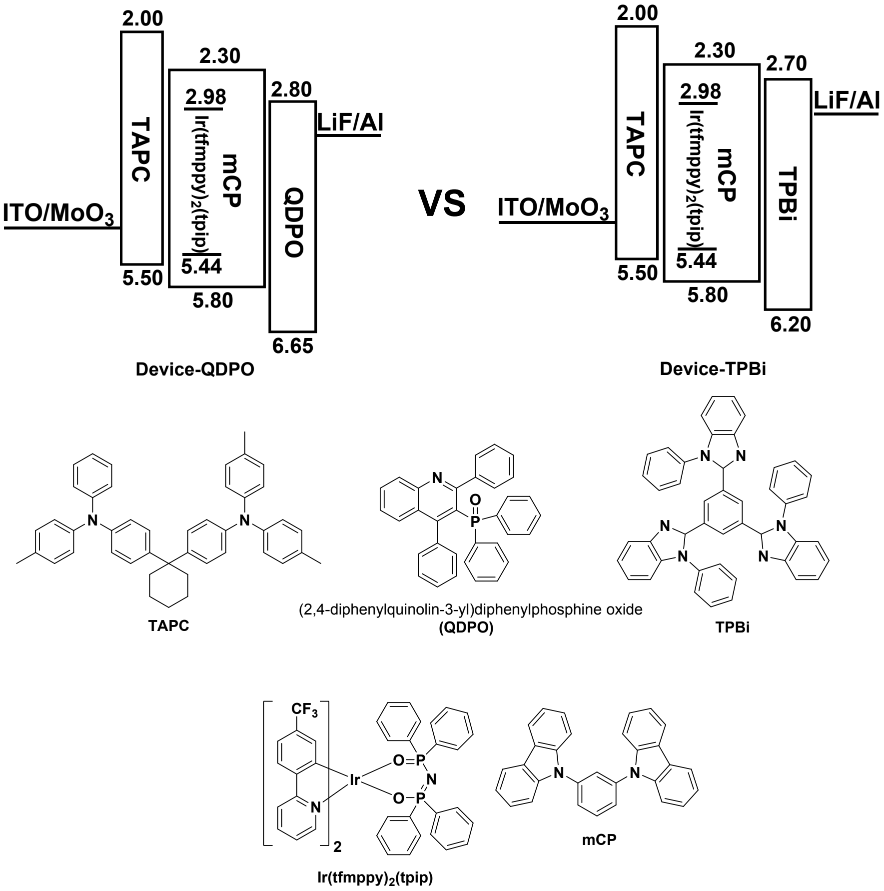


Figure S4. Energy level diagram of HOMO and LUMO levels for materials and their molecular structures.

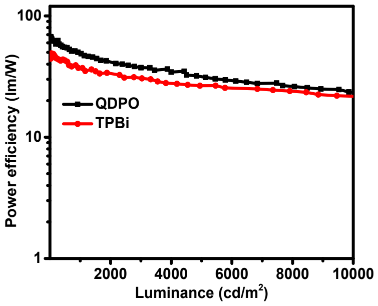
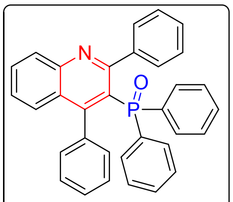


Figure S5. Power efficiency versus luminance curves of the devices.

4. Characterization data

(All the compounds are new except for **3d**).



3a

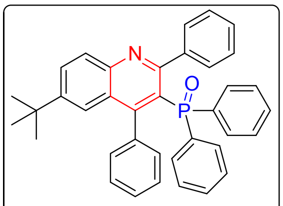
(2,4-diphenylquinolin-3-yl)diphenylphosphine oxide (3a): White solid. Melting point: 238-240 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.2 Hz, 1H), 7.81 (t, *J* = 7.4 Hz, 1H), 7.71 (d, *J* = 4.3 Hz, 3H), 7.52 – 7.44 (m, 1H), 7.30 – 7.19 (m, 7H), 7.15 – 7.05 (m, 7H), 6.98 (d, *J* = 4.7 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.98 (d, *J* = 11.3 Hz), 158.24 (s), 147.85 (s), 141.90 (s), 136.08 (s), 135.72 (d, *J* = 6.0 Hz), 135.03 (s), 132.22 (s), 131.53 (s), 130.62 – 130.08 (m), 129.84 (d, *J* = 2.6 Hz), 129.59 (s), 129.21 (s), 128.51 (d, *J* = 5.7 Hz), 128.18 (s), 127.68 (dd, *J* = 21.4, 9.1 Hz), 126.79 (d, *J* = 20.4 Hz), 126.65 – 126.58 (m), 125.68 – 125.25 (m), 124.57 (s), 113.94 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 19.98.

HRMS (ESI) *m/z* calcd for $C_{33}H_{24}NOPH$ [M+H]: 482.1674, found: 482.1671.



3b

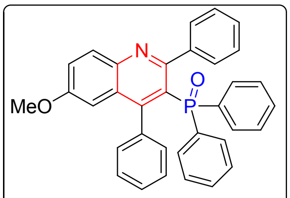
(6-(tert-butyl)-2,4-diphenylquinolin-3-yl)diphenylphosphine oxide (3b): White solid. Melting point: 280-282 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 1.6 Hz, 1H), 7.73 – 7.65 (m, 3H), 7.58 (dd, *J* = 9.0, 1.9 Hz, 1H), 7.30 (s, 2H), 7.28 – 7.23 (m, 4H), 7.21 (d, *J* = 7.4 Hz, 1H), 7.17 – 7.07 (m, 7H), 6.98 (td, *J* = 7.6, 3.1 Hz, 4H), 1.46 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.18 (d, *J* = 11.3 Hz), 157.68 (d, *J* = 9.0 Hz), 155.27 (s), 148.20 (s), 142.14 (s), 136.17 (s), 135.90 (d, *J* = 5.8 Hz), 135.12 (s), 132.11 (s), 130.75 – 130.10 (m), 129.78 (s), 128.36 (d, *J* = 10.3 Hz), 127.65 (dd, *J* = 23.0, 10.8 Hz), 126.30 (s), 125.84 (s), 124.90 (d, *J* = 26.3 Hz), 123.76 (s), 123.39 (d, *J* = 8.3 Hz), 35.33 (s), 31.03 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.18.

HRMS (ESI) *m/z* calcd for $C_{37}H_{32}NOPH$ [M+H]: 538.2300, found: 538.2292.



3c

(6-methoxy-2,4-diphenylquinolin-3-yl)diphenylphosphine oxide (3c): Light yellow solid.

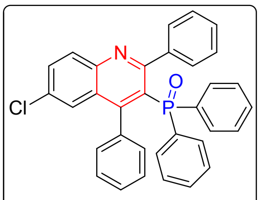
Melting point: 185-187 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 9.2 Hz, 1H), 7.68 (dd, J = 7.6, 1.8 Hz, 2H), 7.46 (dd, J = 9.2, 2.8 Hz, 1H), 7.29 (s, 2H), 7.25 – 7.21 (m, 3H), 7.19 (d, J = 7.3 Hz, 1H), 7.16 – 7.03 (m, 8H), 7.00 – 6.93 (m, 5H), 3.70 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.77 (d, J = 11.5 Hz), 158.07 (s), 156.45 (d, J = 9.1 Hz), 144.21 (s), 142.03 (s), 136.39 – 135.80 (m), 135.16 (s), 132.03 (s), 131.10 (s), 130.59 – 130.17 (m), 129.78 (d, J = 2.7 Hz), 128.46 (s), 128.21 (s), 127.68 (dd, J = 16.3, 4.1 Hz), 126.39 (d, J = 8.5 Hz), 124.64 (s), 124.00 (s), 104.27 (s), 55.40 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.32.

HRMS (ESI) *m/z* calcd for $C_{34}H_{26}NO_2PNa$ [M+Na]: 534.1599, found: 534.1597.



3d

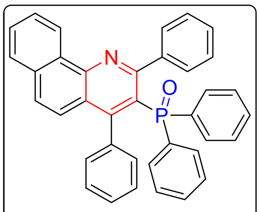
(6-chloro-2,4-diphenylquinolin-3-yl)diphenylphosphine oxide (3d): White solid. Melting point: 235-237 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.9 Hz, 1H), 7.76 – 7.66 (m, 4H), 7.26 – 7.20 (m, 6H), 7.12 (ddd, J = 22.6, 11.8, 7.3 Hz, 8H), 6.98 (td, J = 7.5, 3.0 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.25 (d, J = 11.0 Hz), 157.36 (d, J = 8.8 Hz), 146.25 (s), 141.58 (s), 135.77 (s), 135.15 (d, J = 6.0 Hz), 134.71 (s), 132.88 (s), 132.37 (s), 132.10 (s), 131.19 (s), 130.71 – 130.11 (m), 129.98 (d, J = 2.4 Hz), 128.77 (d, J = 15.9 Hz), 127.80 (dd, J = 12.1, 2.2 Hz), 126.64 (s), 126.16 (d, J = 8.3 Hz), 125.65 (s), 125.37 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.06.

HRMS (ESI) *m/z* calcd for $C_{33}H_{23}ClNOPH$ [M+H]: 516.1284, found: 516.1282.



3e

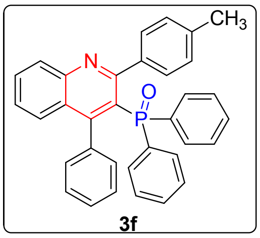
(2,4-diphenylbenzo[*h*]quinolin-3-yl)diphenylphosphine oxide (3e): White solid. Melting point: 250-252 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.51 – 9.30 (m, 1H), 8.00 – 7.83 (m, 3H), 7.79 – 7.64 (m, 3H), 7.55 (d, J = 9.2 Hz, 1H), 7.26 (dd, J = 14.3, 5.3 Hz, 6H), 7.16 (dt, J = 23.8, 7.4 Hz, 6H), 7.06 (t, J = 7.2 Hz, 2H), 7.01 – 6.91 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.17 (d, J = 11.0 Hz), 157.04 (d, J = 9.1 Hz), 146.63 (s), 142.34 (s), 136.44 – 135.94 (m), 135.19 (s), 134.24 (s), 132.44 (s), 131.04 (d, J = 10.6 Hz), 130.35 (d, J = 8.7 Hz), 129.80 (d, J = 2.4 Hz), 129.27 (s), 128.65 (s), 128.32 (s), 127.61 (dd, J = 17.2, 13.7 Hz), 127.23 (s), 125.61 (d, J = 14.2 Hz), 124.54 (s), 123.08 – 122.66 (m).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.32.

HRMS (ESI) *m/z* calcd for $C_{37}H_{26}NOPH$ [M+H]: 532.1830, found: 532.1829.



3f

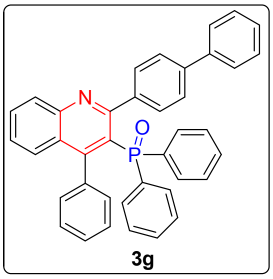
diphenyl(4-phenyl-2-(p-tolyl)quinolin-3-yl)phosphine oxide (3f): Light yellow solid. Melting point: 243-245 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.21 (d, *J* = 8.4 Hz, 1H), 7.79 (t, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.40 (m, 1H), 7.27 – 7.17 (m, 7H), 7.13 – 7.04 (m, 4H), 6.95 (ddd, *J* = 18.7, 11.6, 5.4 Hz, 6H), 2.23 (s, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 163.05 (d, *J* = 11.2 Hz), 158.05 (d, *J* = 8.9 Hz), 147.99 (s), 139.24 (s), 138.29 (s), 136.16 (s), 135.77 (d, *J* = 5.9 Hz), 135.11 (s), 132.24 (s), 131.42 (s), 130.56 – 130.03 (m), 130.03 – 129.31 (m), 128.46 (s), 127.84 – 127.18 (m), 126.68 (s), 125.66 – 125.11 (m), 124.46 (s), 21.19 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 20.19.

HRMS (ESI) *m/z* calcd for $C_{34}H_{26}NOPNa$ [M+Na]: 518.1650, found: 518.1642.



3g

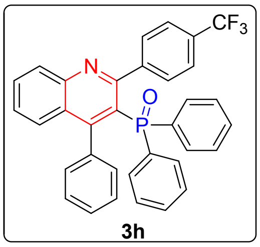
(2-([1,1'-biphenyl]-4-yl)-4-phenylquinolin-3-yl)diphenylphosphine oxide (3g): White solid. Melting point: 282-284 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.25 (d, *J* = 8.2 Hz, 1H), 7.88 – 7.67 (m, 4H), 7.54 – 7.41 (m, 5H), 7.36 – 7.23 (m, 9H), 7.20 (d, *J* = 6.9 Hz, 1H), 7.16 – 7.04 (m, 4H), 6.98 (d, *J* = 4.8 Hz, 4H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 162.63 (d, *J* = 11.1 Hz), 158.18 (d, *J* = 8.7 Hz), 147.95 (s), 141.19 (s), 140.92 (s), 136.06 (s), 135.69 (d, *J* = 6.1 Hz), 135.01 (s), 132.24 (s), 131.58 (s), 130.83 (s), 130.39 (d, *J* = 8.7 Hz), 129.87 (d, *J* = 2.5 Hz), 129.62 (s), 128.76 (s), 128.56 (s), 127.55 (dd, *J* = 27.3, 14.5 Hz), 127.25 – 126.54 (m), 125.81 – 125.33 (m), 124.69 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 20.03.

HRMS (ESI) *m/z* calcd for $C_{39}H_{28}NOPNa$ [M+Na]: 580.1806, found: 580.1803.



3h

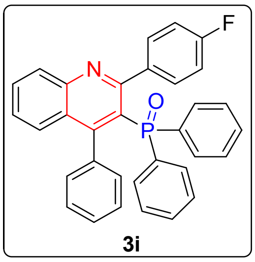
diphenyl(4-phenyl-2-(4-(trifluoromethyl)phenyl)quinolin-3-yl)phosphine oxide (3h): White solid. Melting point: 227-229 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.27 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.80 (m, 3H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.24 (m, 7H), 7.14 (dd, *J* = 16.1, 7.7 Hz, 4H), 7.01 (td, *J* = 7.5, 2.9 Hz, 4H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 161.48 (s), 158.28 (s), 147.85 (s), 145.21 (s), 135.48 (s), 132.11 (s), 131.97 (d, *J* = 28.4 Hz), 130.76 (s), 130.47 (s), 130.36 – 129.48 (m), 128.72 (s), 127.89 (d, *J* = 9.9 Hz), 127.52 (d, *J* = 19.6 Hz), 126.81 (s), 125.70 (s), 125.43 (s), 124.57 (d, *J* = 3.5 Hz), 122.72 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 19.93.

HRMS (ESI) *m/z* calcd for $C_{34}H_{23}F_3NOPH$ [M+H]: 550.1548, found: 550.1540.



3i

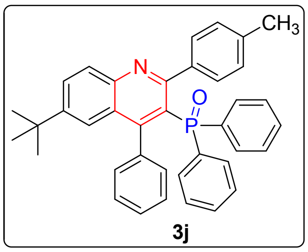
(2-(4-fluorophenyl)-4-phenylquinolin-3-yl)diphenylphosphine oxide (3i): White solid. Melting point: 260-262 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.21 (d, *J* = 8.4 Hz, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.71 (dd, *J* = 11.5, 6.5 Hz, 3H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.29 – 7.18 (m, 7H), 7.11 (dd, *J* = 14.8, 7.4 Hz, 4H), 7.04 – 6.95 (m, 4H), 6.81 (t, *J* = 8.6 Hz, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 164.22 (s), 161.81 (d, *J* = 12.6 Hz), 158.19 (d, *J* = 8.8 Hz), 147.87 (s), 138.15 (s), 135.97 (s), 135.65 (d, *J* = 5.9 Hz), 134.92 (s), 132.55 – 131.98 (m), 131.63 (s), 130.28 (d, *J* = 8.8 Hz), 130.00 (d, *J* = 2.6 Hz), 129.54 (s), 128.61 (s), 127.93 – 127.45 (m), 127.00 (s), 126.70 (s), 125.41 (d, *J* = 8.8 Hz), 124.47 (s), 114.77 (s), 114.55 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 20.13.

HRMS (ESI) *m/z* calcd for $C_{33}H_{23}FNOPH$ [M+H]: 500.1580, found: 550.1575.



3j

(6-(tert-butyl)-4-phenyl-2-(p-tolyl)quinolin-3-yl)diphenylphosphine oxide (3j): White solid. Melting point: 278-280 °C.

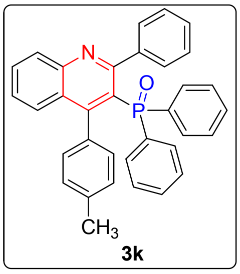
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.95 – 7.84 (m, 1H), 7.64 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 2H), 7.30 – 7.18 (m, 7H), 7.16 – 7.04 (m, 4H), 7.02 – 6.87 (m, 6H), 2.23 (s, 3H), 1.27 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 162.52 (d, *J* = 11.5 Hz), 158.00 (s), 149.60 (s), 146.45 (s), 139.19

(s), 138.17 (s), 136.31 (s), 136.30 – 135.61 (m), 135.24 (s), 132.24 (s), 130.76 – 130.10 (m), 129.68 (d, *J* = 2.4 Hz), 129.02 (s), 128.43 (s), 127.80 – 127.19 (m), 125.34 (s), 124.86 (d, *J* = 8.4 Hz), 124.33 (s), 121.55 (s), 35.15 (s), 31.02 (s), 21.17 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 20.18.

HRMS (ESI) *m/z* calcd for $C_{38}H_{34}NOPH$ [M+H]: 552.2456, found: 552.2452.



3k

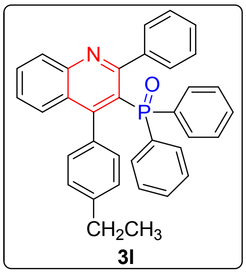
diphenyl(2-phenyl-4-(p-tolyl)quinolin-3-yl)phosphine oxide (3k): White solid. Melting point: 218-220 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H), 7.84 – 7.67 (m, 4H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.20 (m, 4H), 7.18 – 7.04 (m, 7H), 6.96 (td, *J* = 7.6, 3.0 Hz, 4H), 6.89 (d, *J* = 7.8 Hz, 2H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 163.03 (d, *J* = 11.5 Hz), 158.26 (d, *J* = 8.9 Hz), 147.90 (s), 142.02 (s), 138.47 (s), 136.19 (s), 135.14 (s), 132.89 (d, *J* = 6.0 Hz), 132.16 (s), 131.42 (s), 130.54 – 130.20 (m), 129.86 – 129.41 (m), 128.30 (d, *J* = 17.8 Hz), 127.86 – 127.27 (m), 126.76 (s), 125.76 – 125.34 (m), 124.65 (s), 21.29 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 20.08.

HRMS (ESI) *m/z* calcd for $C_{34}H_{26}NOPH$ [M+H]: 496.1830, found: 496.1826.



3l

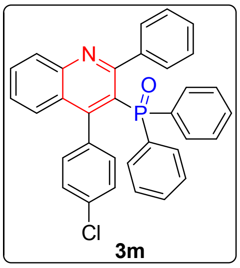
(4-(4-ethylphenyl)-2-phenylquinolin-3-yl)diphenylphosphine oxide (3l): White solid. Melting point: 230-232 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H), 7.85 – 7.66 (m, 4H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.18 (m, 6H), 7.14 – 7.03 (m, 5H), 7.00 – 6.90 (m, 6H), 2.61 (q, *J* = 7.5 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 163.04 (d, *J* = 11.2 Hz), 158.34 (d, *J* = 9.0 Hz), 147.91 (s), 144.61 (s), 142.01 (s), 136.22 (s), 135.17 (s), 133.10 (d, *J* = 6.1 Hz), 132.29 (s), 131.43 (s), 130.55 – 130.02 (m), 129.98 – 129.35 (m), 128.40 (s), 127.90 – 127.43 (m), 127.06 (s), 126.79 (d, *J* = 3.0 Hz), 125.50 (d, *J* = 8.6 Hz), 124.54 (s), 28.68 (s), 15.43 (s).

^{31}P NMR (162 MHz, CDCl$_3$) δ 20.06.

HRMS (ESI) *m/z* calcd for $C_{35}H_{28}NOPH$ [M+H]: 510.1987, found: 510.1985.



3m

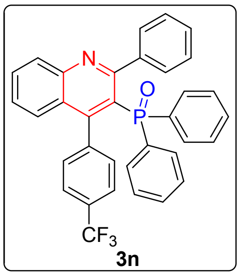
(4-(4-chlorophenyl)-2-phenylquinolin-3-yl)diphenylphosphine oxide (3m): Light yellow solid. Melting point: 262-264 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.86 – 7.78 (m, 1H), 7.70 (dd, *J* = 7.3, 2.1 Hz, 2H), 7.64 (d, *J* = 8.3 Hz, 1H), 7.48 (dd, *J* = 11.2, 4.0 Hz, 1H), 7.29 – 7.18 (m, 6H), 7.16 – 7.05 (m, 7H), 7.01 (td, *J* = 7.6, 3.1 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.88 (d, *J* = 11.1 Hz), 156.64 (d, *J* = 8.7 Hz), 147.93 (s), 141.84 (s), 135.88 (s), 134.90 (d, *J* = 15.6 Hz), 134.12 (d, *J* = 6.1 Hz), 133.37 (s), 131.68 (s), 130.50 – 129.94 (m), 129.77 (s), 128.56 (s), 127.76 (dd, *J* = 11.9, 1.2 Hz), 127.12 (s), 126.25 (s), 125.77 (s), 125.09 (d, *J* = 8.2 Hz), 124.78 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.10.

HRMS (ESI) *m/z* calcd for $C_{33}H_{23}ClNOPH$ [M+H]: 516.1284, found: 516.1280.



3n

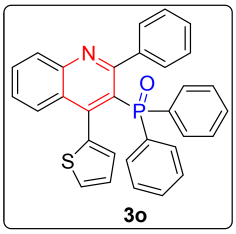
diphenyl(2-phenyl-4-(4-(trifluoromethyl)phenyl)quinolin-3-yl)phosphine oxide (3n): White solid. Melting point: 250-252 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.4 Hz, 1H), 7.84 (t, *J* = 7.2 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.57 (d, *J* = 8.2 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.43 – 7.35 (m, 4H), 7.29 – 7.21 (m, 4H), 7.12 (dd, *J* = 13.1, 6.4 Hz, 5H), 6.99 (td, *J* = 7.5, 2.9 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.84 (d, *J* = 10.9 Hz), 156.22 (d, *J* = 8.6 Hz), 147.91 (s), 141.72 (s), 139.23 (d, *J* = 5.6 Hz), 135.72 (s), 134.67 (s), 132.40 (s), 131.82 (s), 130.77 – 129.96 (m), 129.82 (s), 128.64 (s), 128.14 – 127.73 (m), 127.30 (s), 126.12 (s), 125.84 (s), 125.25 (s), 124.87 (d, *J* = 7.9 Hz), 124.31 (d, *J* = 3.7 Hz), 122.55 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.01.

HRMS (ESI) *m/z* calcd for $C_{34}H_{23}F_3NOPNa$ [M+Na]: 572.1367, found: 572.1362.



3o

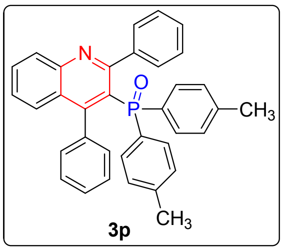
diphenyl(2-phenyl-4-(thiophen-2-yl)quinolin-3-yl)phosphine oxide (3o): Light yellow solid. Melting point: 228-230 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.3 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 7.68 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 3.0 Hz, 1H), 7.34 – 7.26 (m, 5H), 7.16 – 7.08 (m, 5H), 7.01 (td, *J* = 7.5, 3.1 Hz, 4H), 6.90 (dd, *J* = 4.9, 3.7 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.05 (d, *J* = 11.4 Hz), 150.28 (s), 148.02 (s), 141.80 (s), 136.38 (d, *J* = 6.8 Hz), 135.78 (s), 134.72 (s), 134.31 (s), 131.61 (s), 130.43 (t, *J* = 10.6 Hz), 129.78 (d, *J* = 21.8 Hz), 129.53 – 129.21 (m), 128.54 (s), 127.76 (d, *J* = 12.1 Hz), 127.25 (s), 127.09 (d, *J* = 19.3 Hz), 126.56 (d, *J* = 27.8 Hz), 125.76 (d, *J* = 8.1 Hz).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.28.

HRMS (ESI) *m/z* calcd for $C_{31}H_{22}NOPSH$ [M+H]: 488.1238, found: 488.1235.



3p

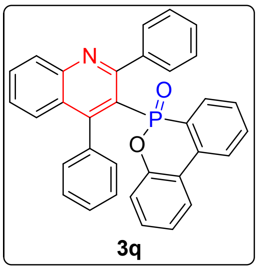
(2,4-diphenylquinolin-3-yl)di-p-tolylphosphine oxide (3p): White solid. Melting point: 235-237 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.3 Hz, 1H), 7.83 – 7.75 (m, 1H), 7.72 – 7.63 (m, 3H), 7.49 – 7.40 (m, 1H), 7.26 – 7.19 (m, 3H), 7.16 – 7.07 (m, 9H), 6.76 (dd, *J* = 8.0, 2.6 Hz, 4H), 2.17 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.09 (d, *J* = 11.4 Hz), 157.86 (s), 147.81 (s), 142.10 (s), 139.91 (d, *J* = 2.8 Hz), 135.93 (d, *J* = 5.8 Hz), 132.89 (s), 132.12 (s), 131.81 (s), 131.34 (s), 130.31 (d, *J* = 8.8 Hz), 129.58 (s), 128.39 (t, *J* = 10.4 Hz), 127.54 (s), 127.23 (s), 126.72 (d, *J* = 8.5 Hz), 126.23 (s), 125.45 (d, *J* = 8.3 Hz), 21.23 (s).

^{31}P NMR (162 MHz, $CDCl_3$) δ 20.61.

HRMS (ESI) *m/z* calcd for $C_{35}H_{28}NOPNa$ [M+Na]: 532.1806, found: 532.1802.



3q

6-(2,4-diphenylquinolin-3-yl)-6H-dibenzo[*c*,*e*][1,2]oxaphosphinine 6-oxide (3q): Light yellow solid. Melting point: 240-242 °C.

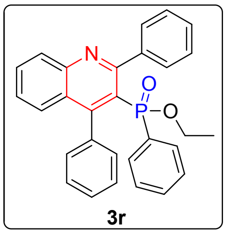
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.2 Hz, 1H), 7.85 (s, 2H), 7.76 – 7.68 (m, 1H), 7.62 – 7.49 (m, 2H), 7.39 (t, *J* = 11.8 Hz, 8H), 7.22 (dd, *J* = 18.0, 10.6 Hz, 2H), 7.16 – 7.01 (m, 4H), 6.92 (d, *J* = 6.9 Hz, 1H), 6.61 (d, *J* = 7.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.12 (d, *J* = 10.4 Hz), 156.76 (d, *J* = 12.0 Hz), 148.03 (d, *J* =

8.2 Hz), 147.75 (s), 141.85 (s), 136.20 (d, *J* = 5.8 Hz), 134.59 (d, *J* = 7.1 Hz), 131.80 (d, *J* = 10.5 Hz), 131.31 – 130.55 (m), 129.92 (d, *J* = 9.8 Hz), 129.58 (d, *J* = 15.8 Hz), 128.64 (d, *J* = 16.7 Hz), 128.38 – 127.60 (m), 126.90 (t, *J* = 14.0 Hz), 125.85 (d, *J* = 10.5 Hz), 125.42 (s), 124.20 (s), 123.33 (d, *J* = 10.3 Hz), 122.66 – 122.08 (m), 120.84 (d, *J* = 6.5 Hz).

^{31}P NMR (162 MHz, CDCl$_3$) δ 23.14.

HRMS (ESI) *m/z* calcd for $C_{33}H_{22}NO_2PNa$ [M+Na]: 518.1286, found: 518.1279.



3r

ethyl (2,4-diphenylquinolin-3-yl)(phenyl)phosphinate (3r): White solid. Melting point: 75-77 °C.

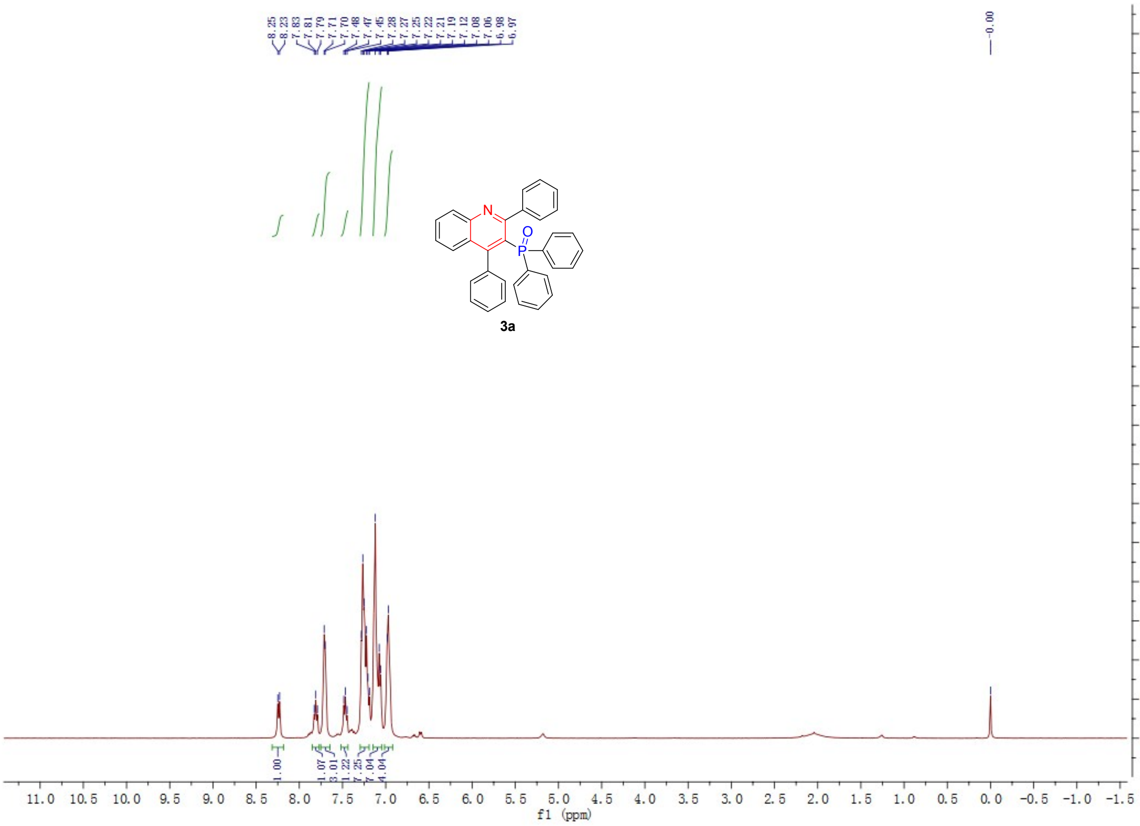
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.20 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 6.8 Hz, 2H), 7.76 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.49 (td, *J* = 7.6, 0.7 Hz, 1H), 7.45 – 7.36 (m, 4H), 7.35 – 7.31 (m, 1H), 7.23 – 7.16 (m, 1H), 7.05 – 6.98 (m, 5H), 6.84 (d, *J* = 7.7 Hz, 1H), 3.20 (dd, *J* = 13.7, 7.0 Hz, 2H), 0.51 (t, *J* = 7.1 Hz, 3H).

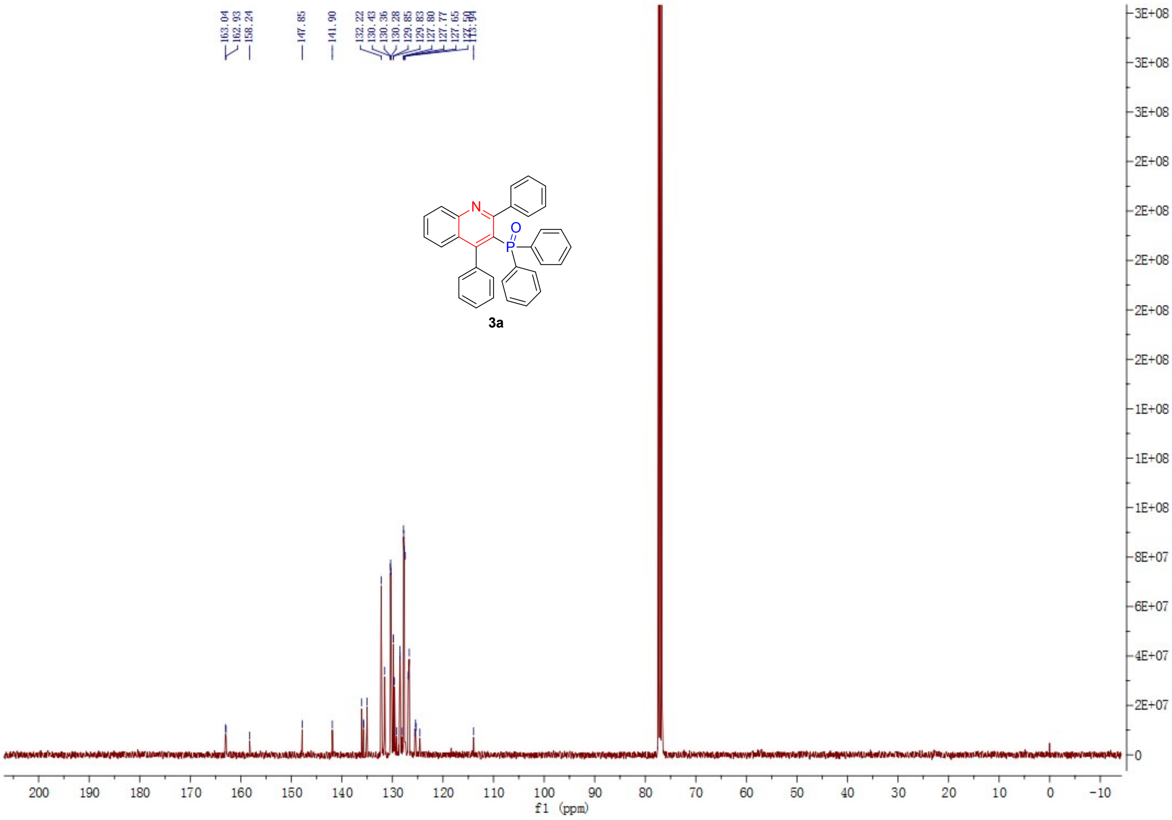
^{13}C NMR (101 MHz, CDCl$_3$) δ 161.74 (d, *J* = 10.3 Hz), 155.88 (d, *J* = 11.1 Hz), 147.63 (s), 143.29 (s), 136.59 (d, *J* = 6.1 Hz), 133.89 (s), 132.53 (s), 131.69 (s), 131.49 – 131.01 (m), 130.77 – 130.43 (m), 129.54 (d, *J* = 4.3 Hz), 128.90 (s), 128.20 (d, *J* = 8.2 Hz), 127.75 (dd, *J* = 23.5, 9.8 Hz), 126.77 (d, *J* = 7.4 Hz), 125.56 (d, *J* = 10.3 Hz), 124.77 (s), 124.06 (s), 123.39 (s), 119.90 (s), 59.80 (d, *J* = 5.6 Hz), 15.25 (d, *J* = 7.1 Hz).

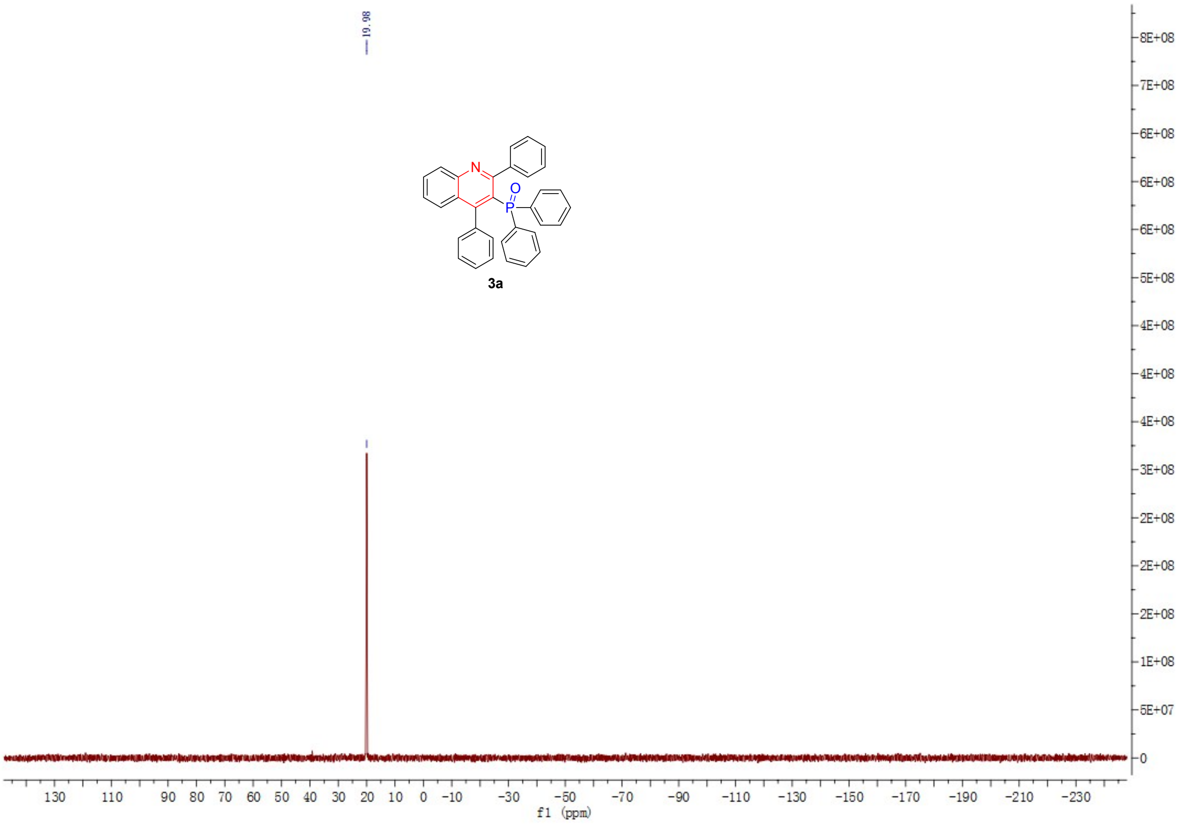
^{31}P NMR (162 MHz, CDCl$_3$) δ 30.99 (d, *J* = 7.5 Hz).

HRMS (ESI) *m/z* calcd for $C_{29}H_{24}NO_2PNa$ [M+Na]: 472.1442, found: 472.1443.

5. ^{1}H, ^{13}C and ^{31}P NMR Spectra

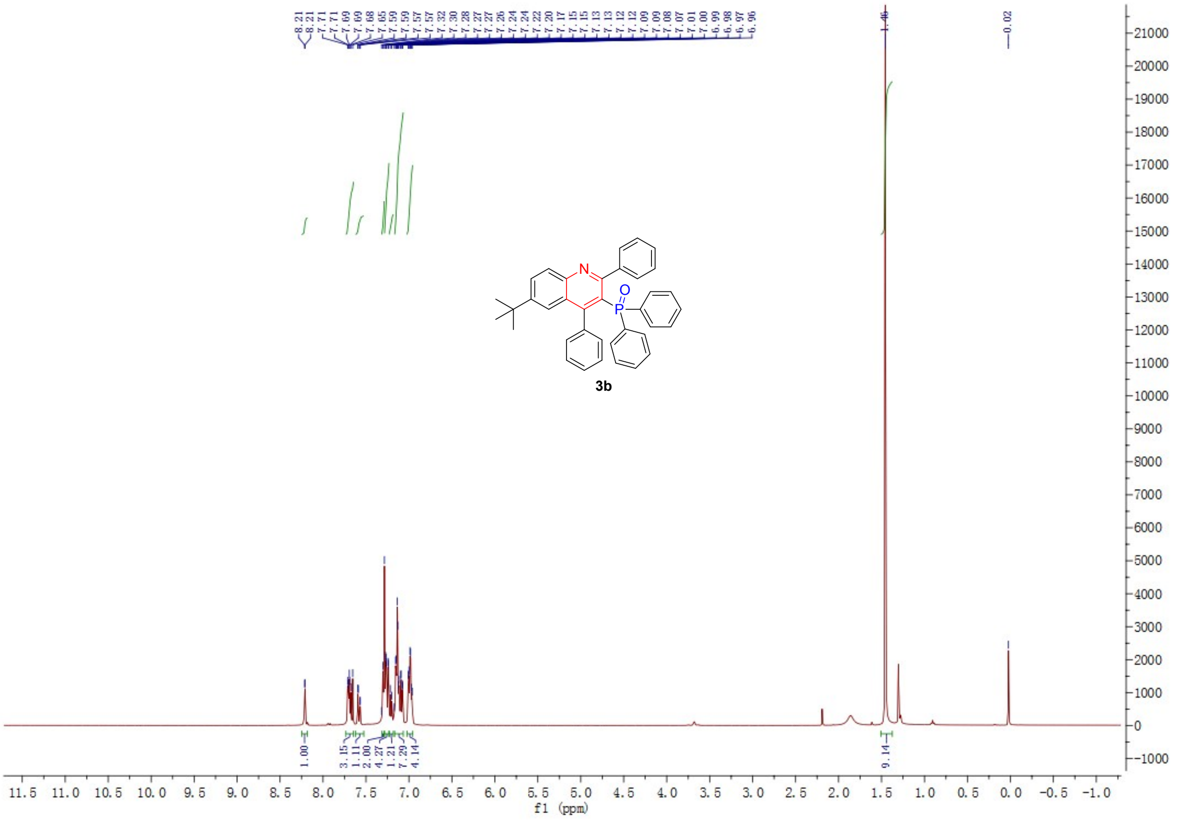






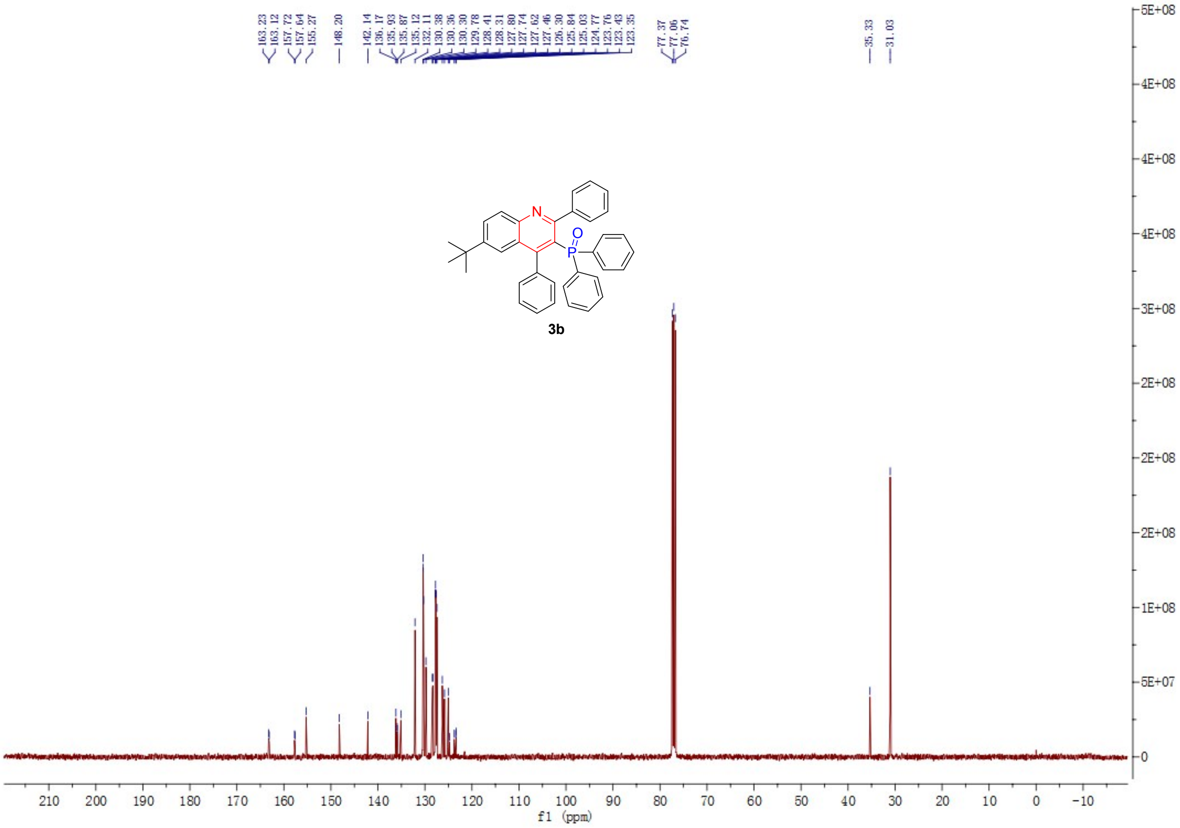
3a

19.98
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)
N
O
P

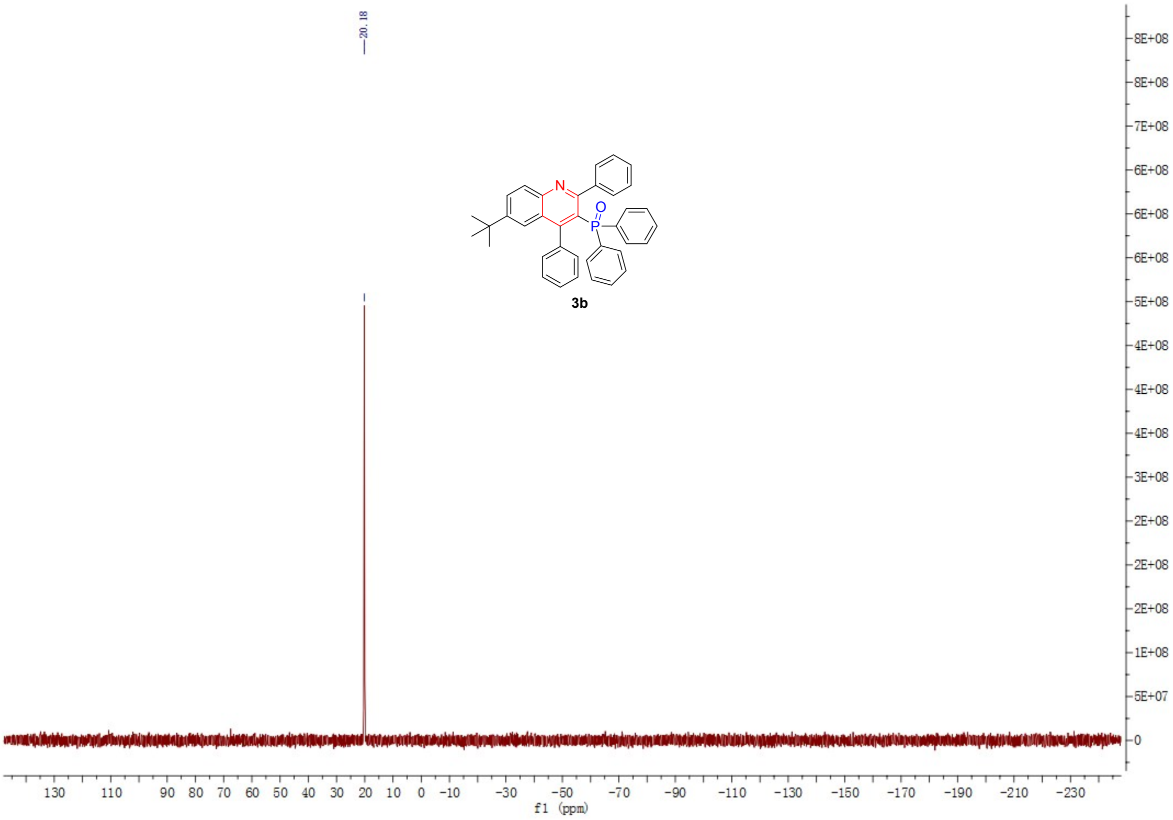


3b

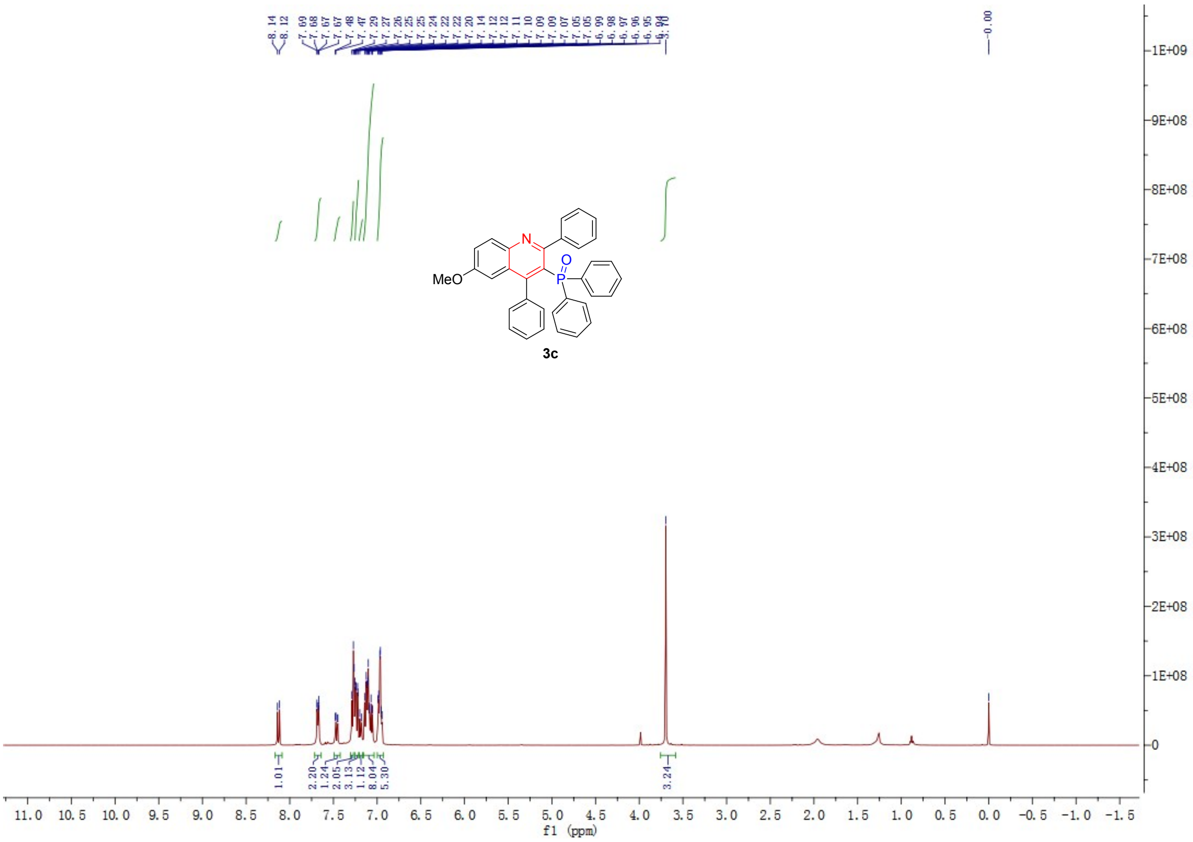
8.21
8.21
7.71
7.71
7.69
7.69
7.68
7.65
7.59
7.59
7.57
7.57
7.32
7.30
7.28
7.27
7.27
7.26
7.24
7.24
7.22
7.20
7.17
7.15
7.15
7.13
7.13
7.12
7.12
7.09
7.09
7.08
7.07
7.01
7.00
6.99
6.98
6.97
6.96
1.46
0.02
1.00
3.15
1.11
2.00
4.27
1.21
7.29
4.14
9.14
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
11.5
11.0
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
-0.5
-1.0
f1 (ppm)
N
O
P

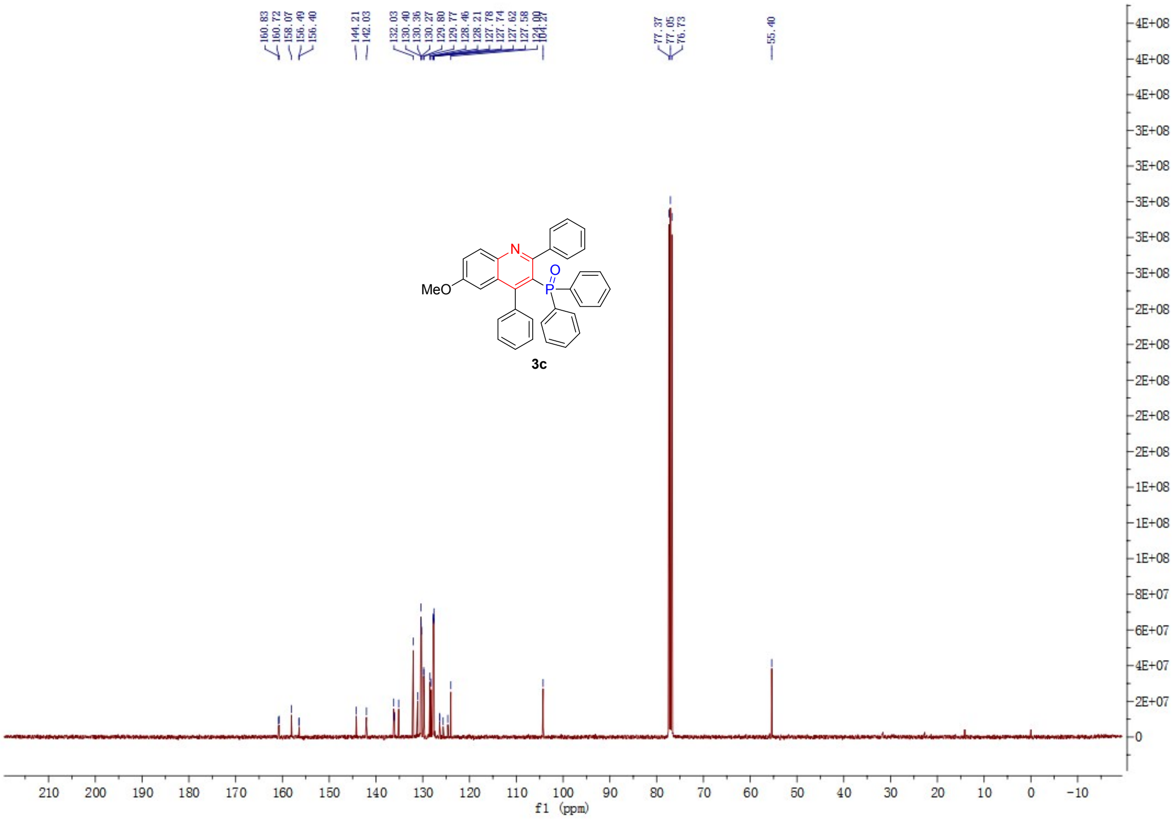


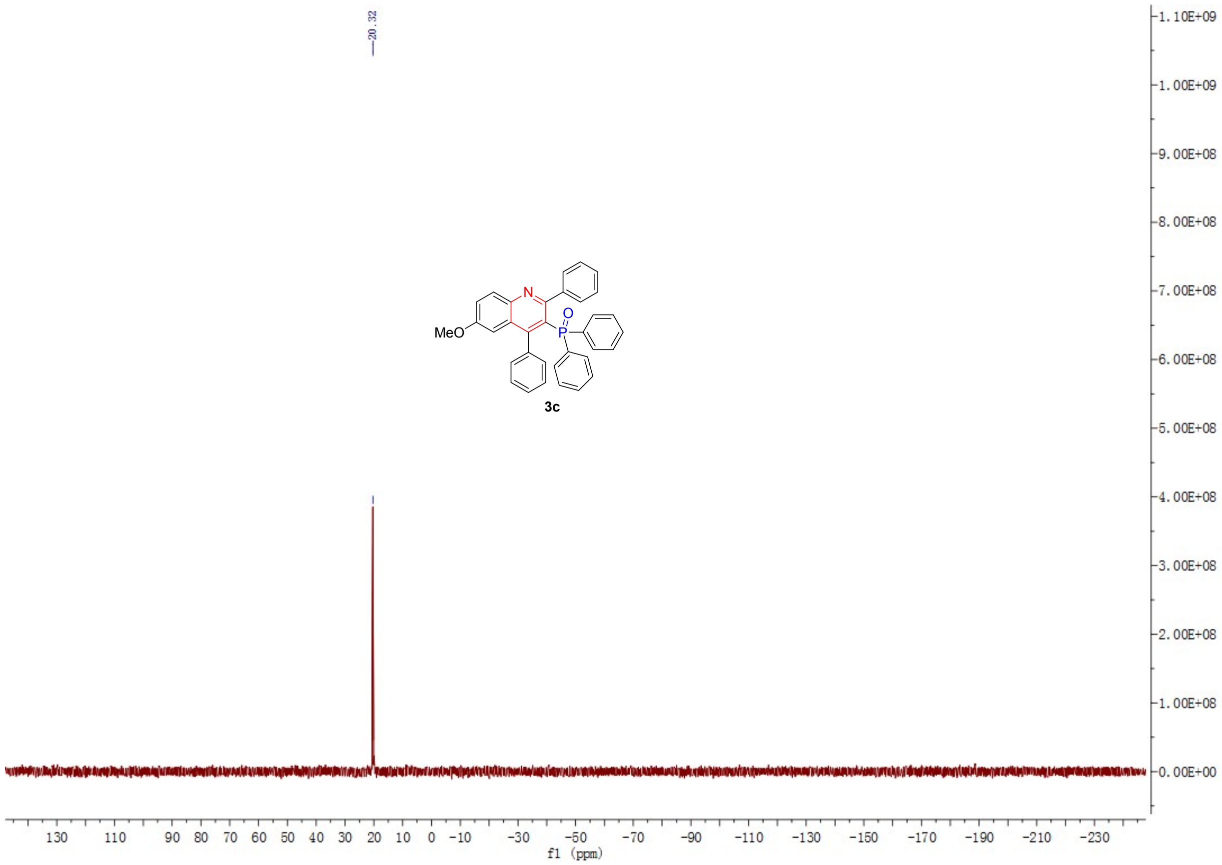
163.23
163.12
157.72
157.64
155.27
148.20
142.14
136.17
135.93
135.87
135.12
132.11
130.38
130.36
130.30
129.78
128.41
128.31
127.80
127.74
127.62
127.46
126.30
125.84
125.03
124.77
123.76
123.43
123.35
77.37
77.06
76.74
35.33
31.03
N
O
P
3b
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
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)



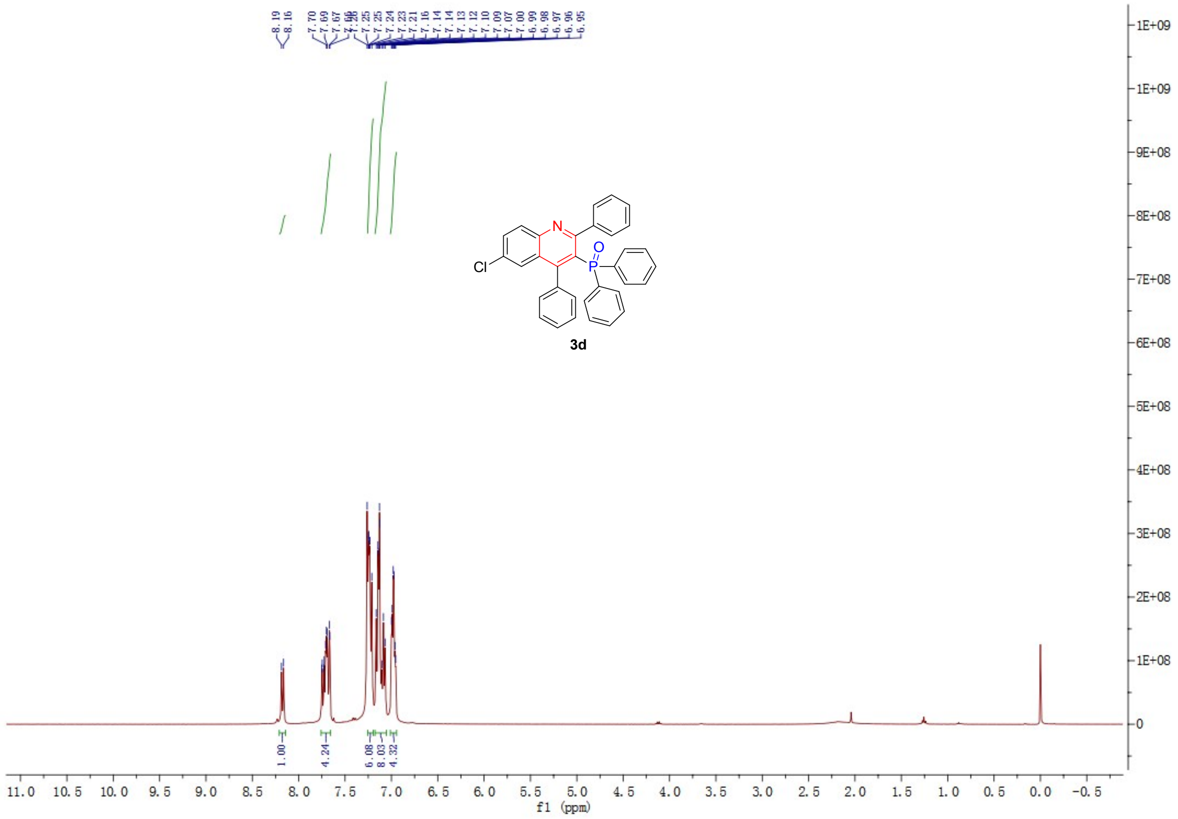
20.18
N
O
P
3b
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


8.14
8.12
7.69
7.68
7.67
7.67
7.48
7.47
7.29
7.27
7.26
7.25
7.25
7.24
7.22
7.22
7.20
7.14
7.12
7.12
7.11
7.10
7.09
7.09
7.07
7.05
7.05
6.99
6.98
6.97
6.96
6.95
6.94
3.70
0.00
1.01
2.20
1.24
2.05
3.13
1.12
8.04
5.30
3.24
MeO
N
P
O
3c
11.0
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
-0.5
-1.0
-1.5
f1 (ppm)
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0

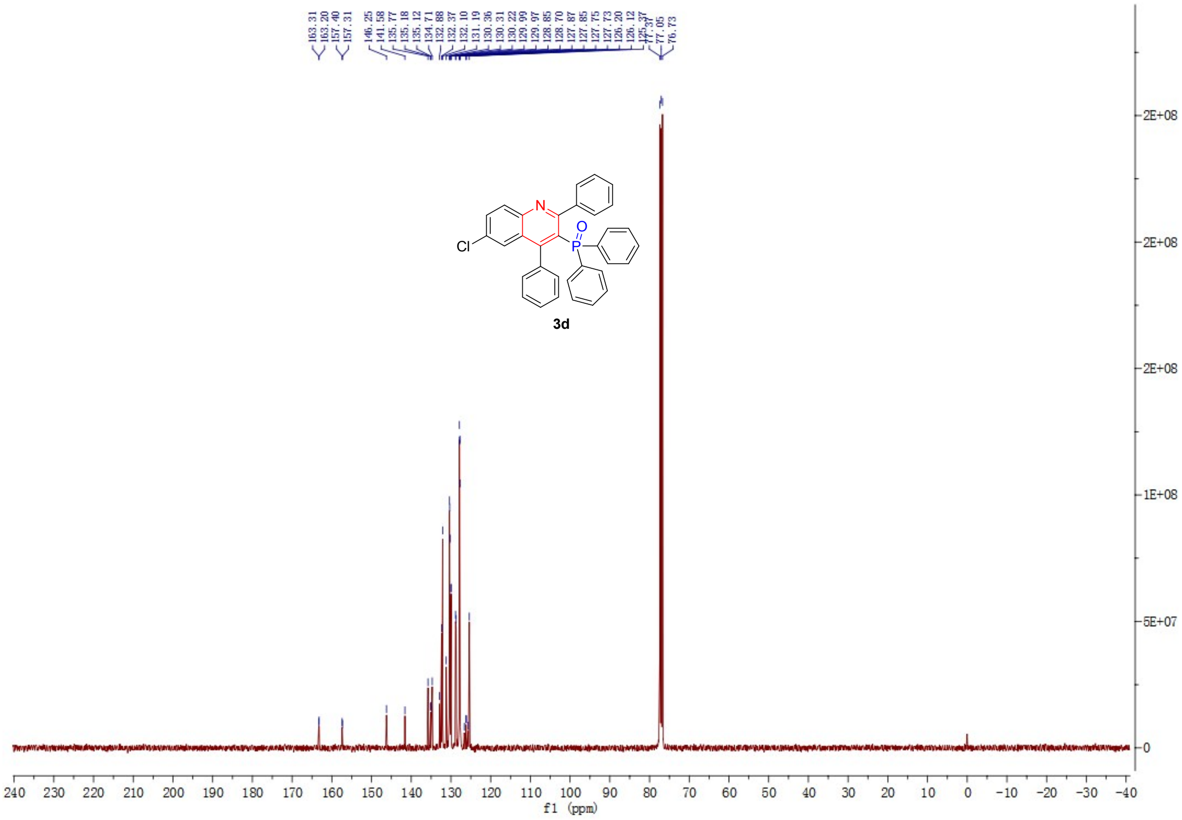

160.83
160.72
158.07
156.49
156.40
144.21
142.03
132.03
130.40
130.36
130.27
129.80
129.77
128.46
128.21
127.78
127.74
127.62
127.58
124.09
104.27
77.37
77.05
76.73
55.40
MeO
N
P
O
3c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
4E+08
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0

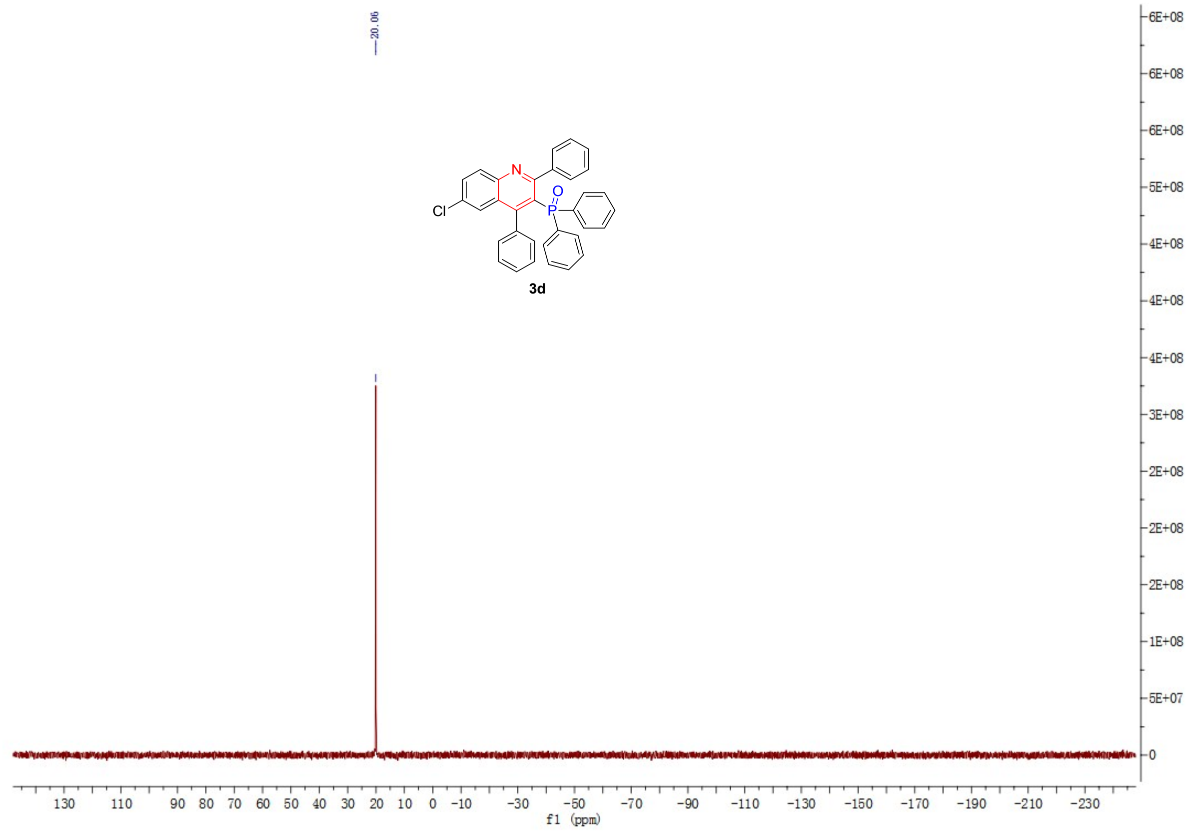

20.32
MeO
N
P
O
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

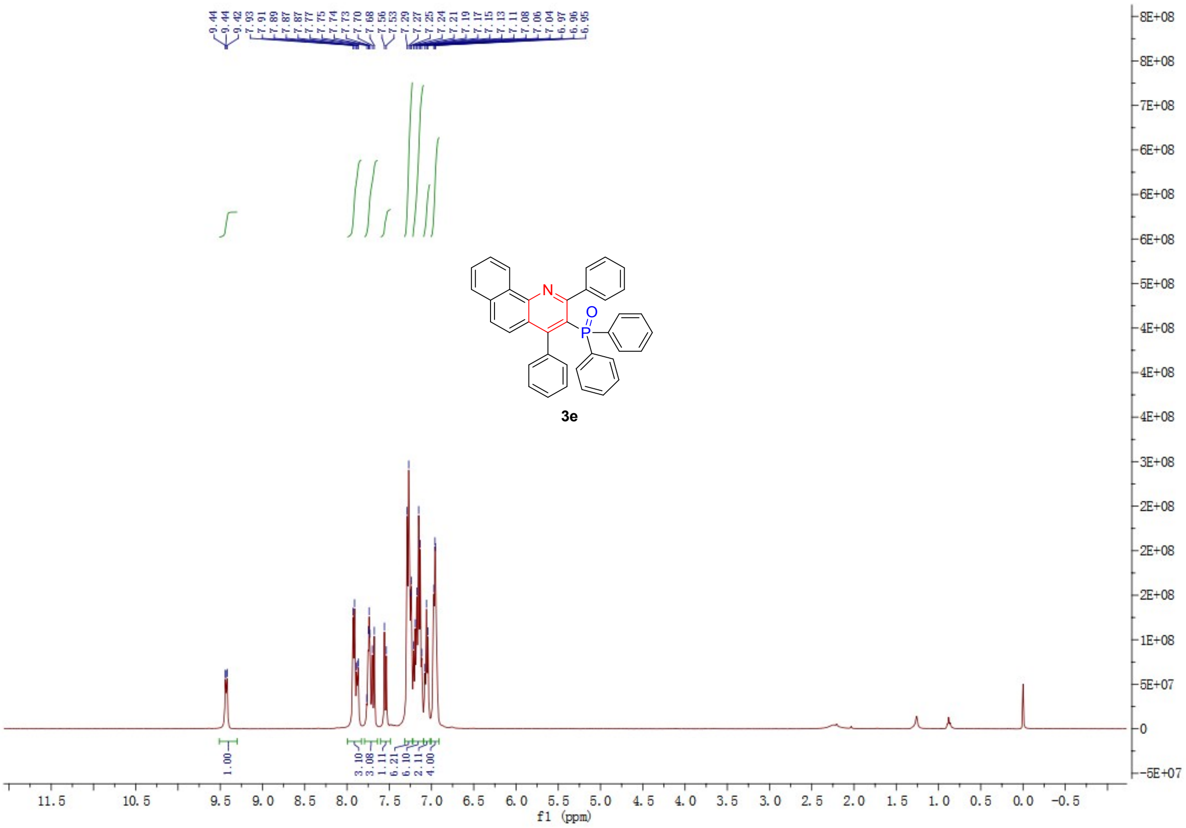
3c

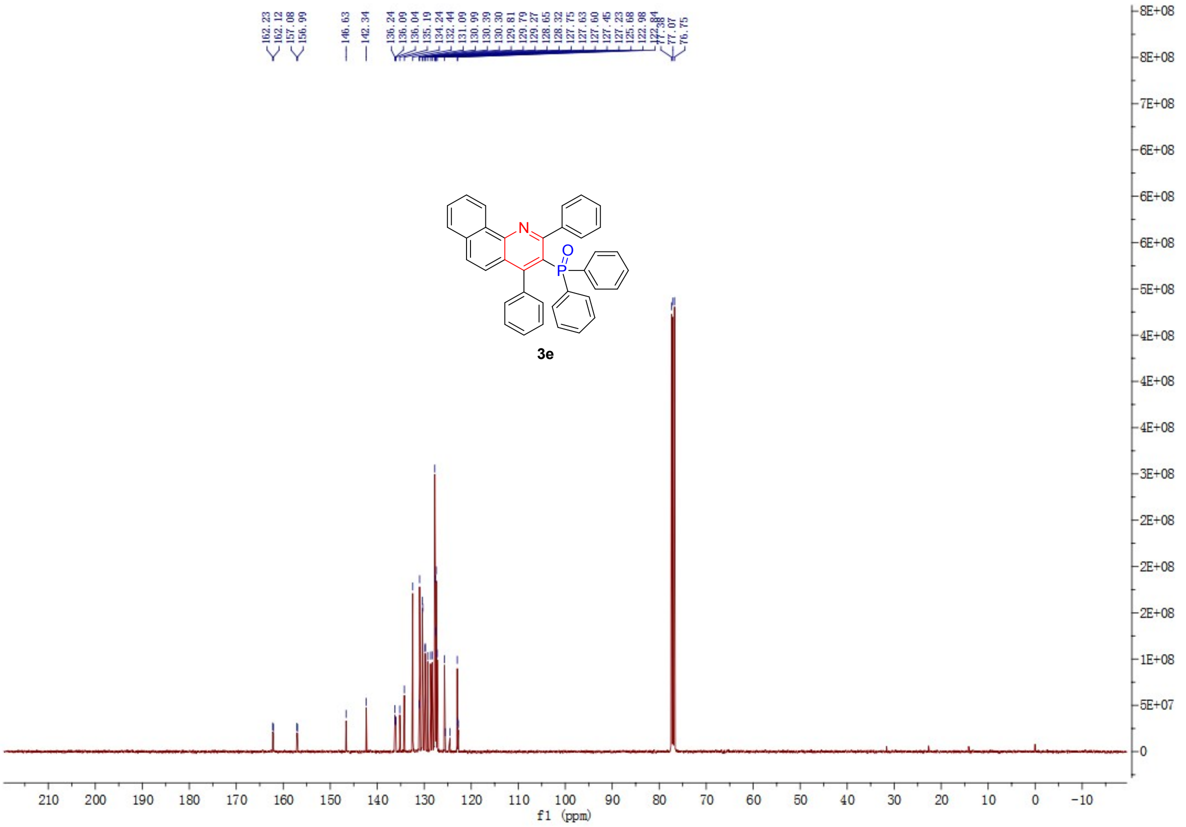

8.19
8.16
7.70
7.69
7.67
7.66
7.26
7.25
7.25
7.24
7.23
7.21
7.16
7.14
7.14
7.13
7.12
7.10
7.09
7.07
7.00
6.99
6.98
6.97
6.96
6.95
Cl
N
P
O
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
1.00
4.24
6.08
8.03
4.32
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

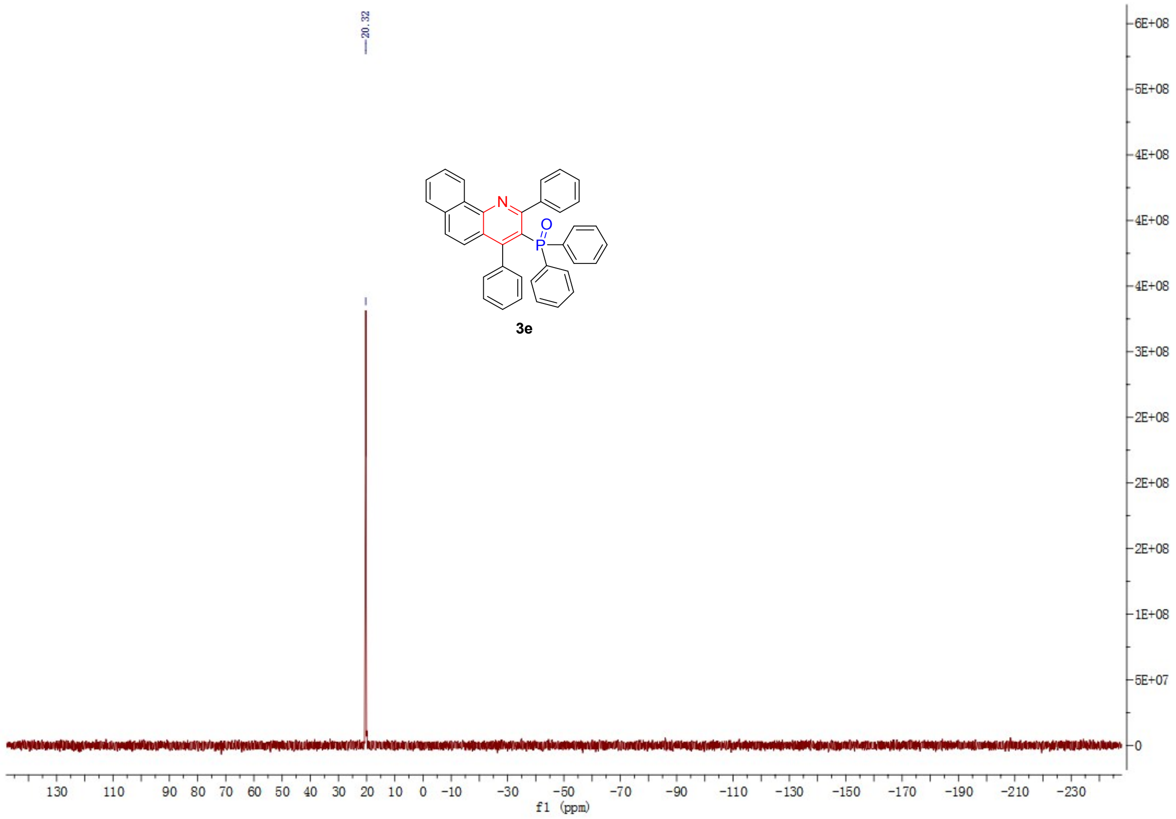
3d


163.31
163.20
157.40
157.31
146.25
141.58
135.77
135.18
135.12
134.71
132.88
132.37
132.10
131.19
130.36
130.31
130.22
129.99
129.97
128.85
128.70
127.87
127.85
127.75
127.73
126.20
126.12
125.37
77.37
77.05
76.73
N
O
P
Cl
3d
2E+08
2E+08
2E+08
1E+08
5E+07
0
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)

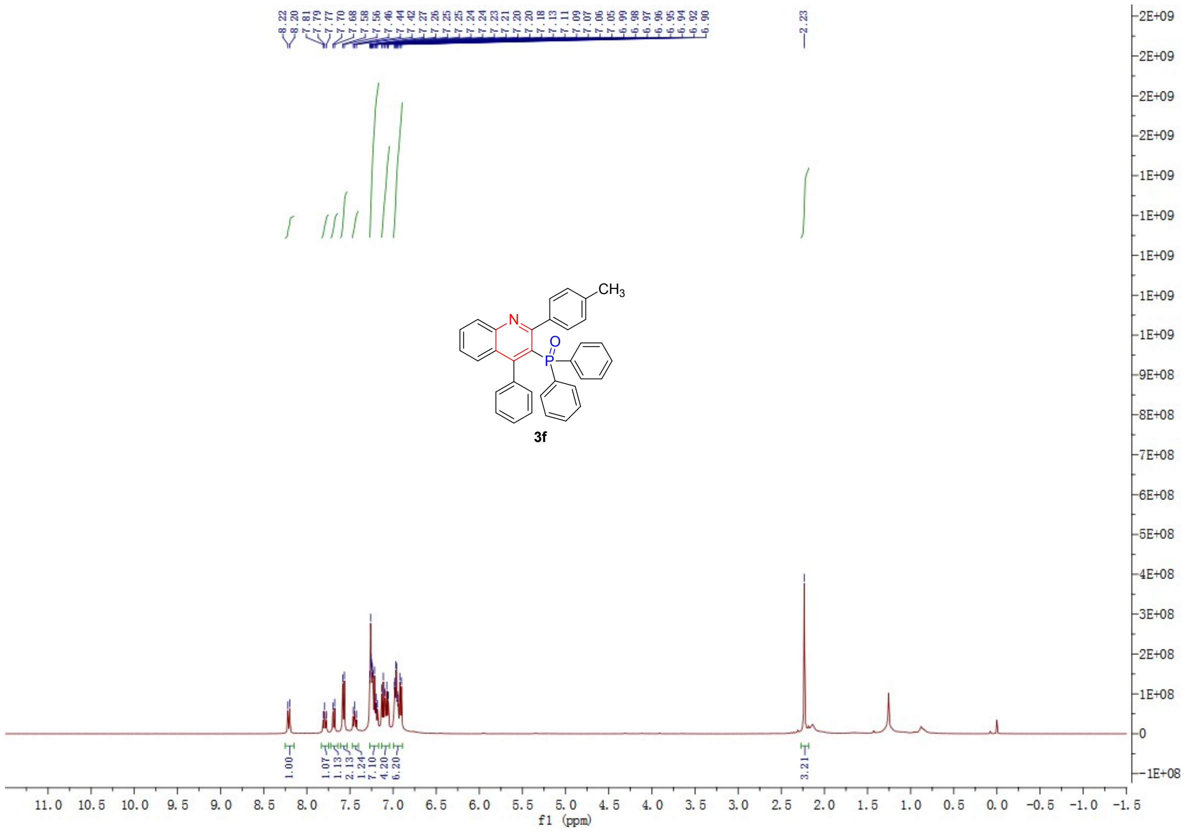

20.06
N
O
P
Cl
3d
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)


9.44
9.44
9.42
7.93
7.91
7.89
7.87
7.87
7.77
7.75
7.74
7.73
7.70
7.68
7.56
7.53
7.29
7.27
7.25
7.24
7.21
7.19
7.17
7.15
7.13
7.11
7.08
7.06
7.04
6.97
6.96
6.95
N
O
P
3e
1.00
3.10
3.08
1.11
6.21
6.10
2.11
4.00
8E+08
8E+08
7E+08
6E+08
6E+08
5E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
11.5
10.5
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)

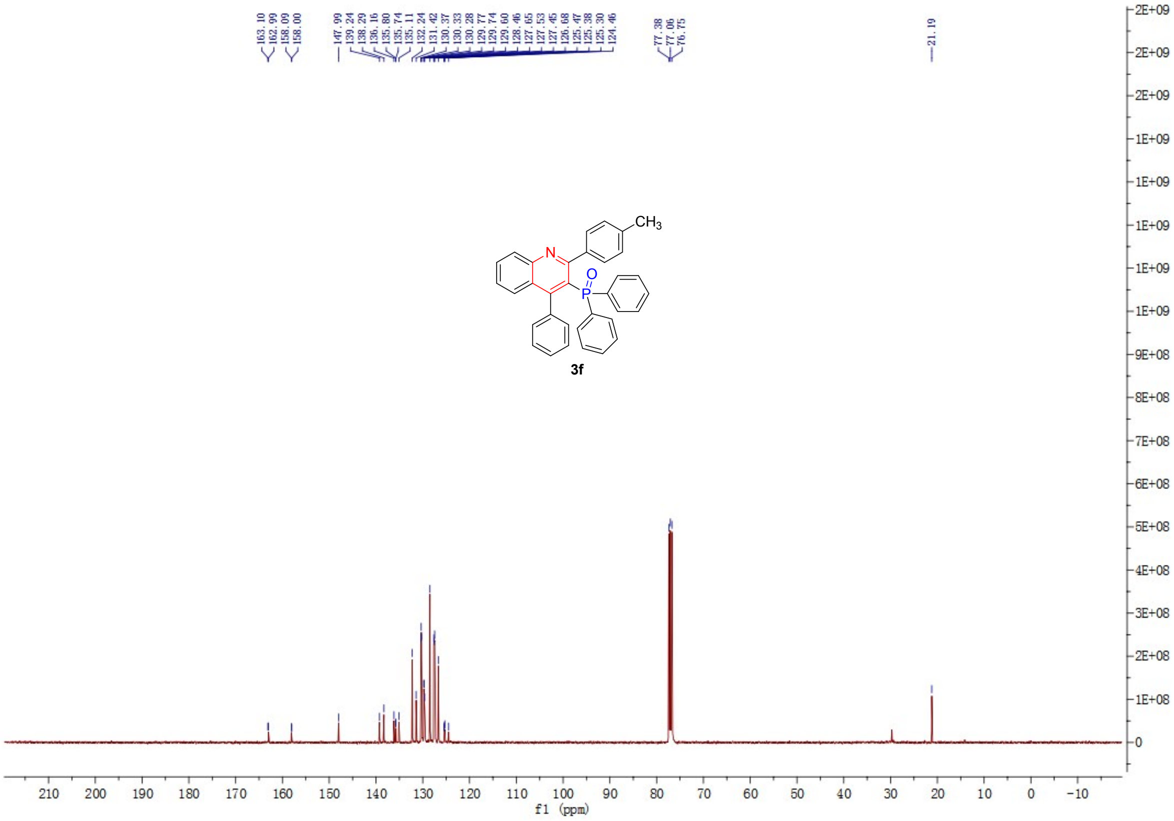

162.23
162.12
157.08
156.99
146.63
142.34
136.24
136.09
136.04
135.19
134.24
132.44
131.09
130.99
130.39
130.30
129.81
129.79
129.27
128.65
128.32
127.75
127.63
127.60
127.45
127.23
125.68
122.98
122.84
77.38
77.07
76.75
N
O
P
3e
8E+08
8E+08
7E+08
6E+08
6E+08
5E+08
4E+08
4E+08
3E+08
2E+08
2E+08
1E+08
5E+07
0
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)

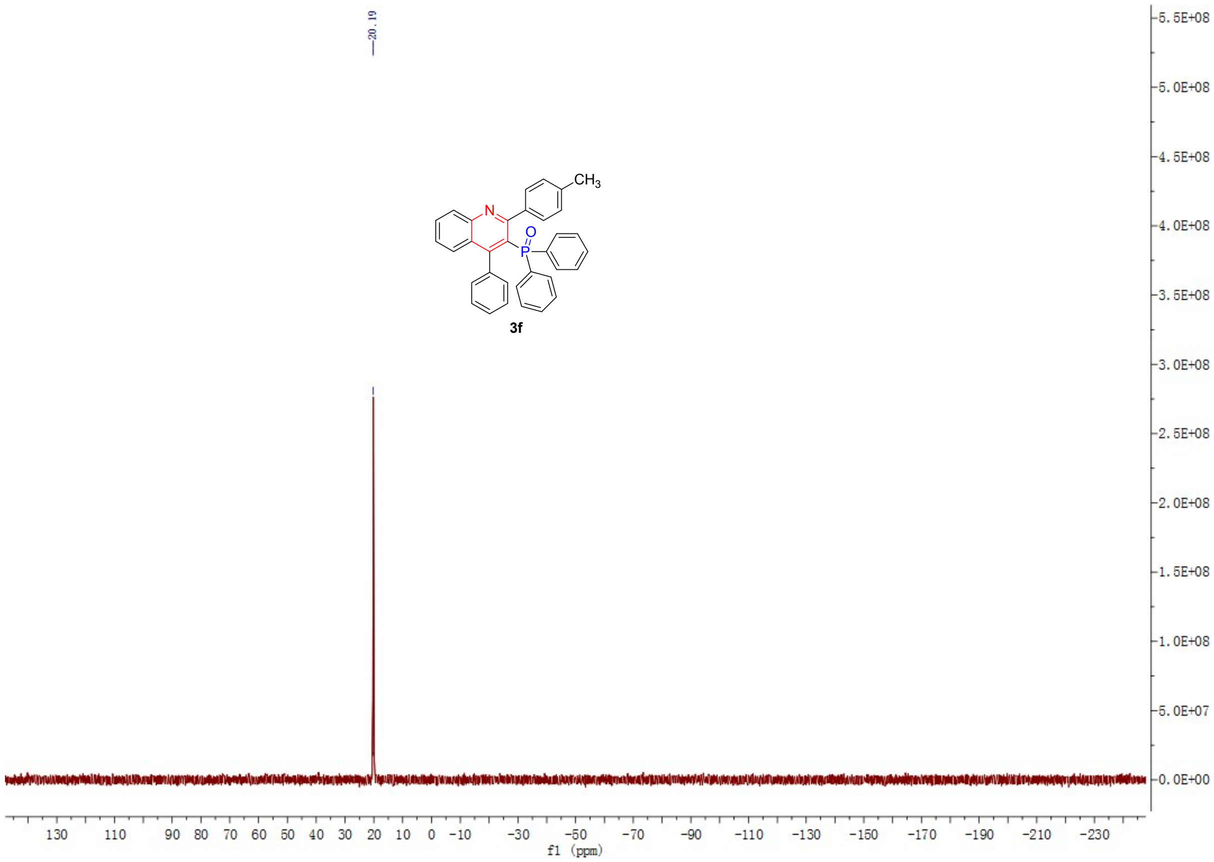


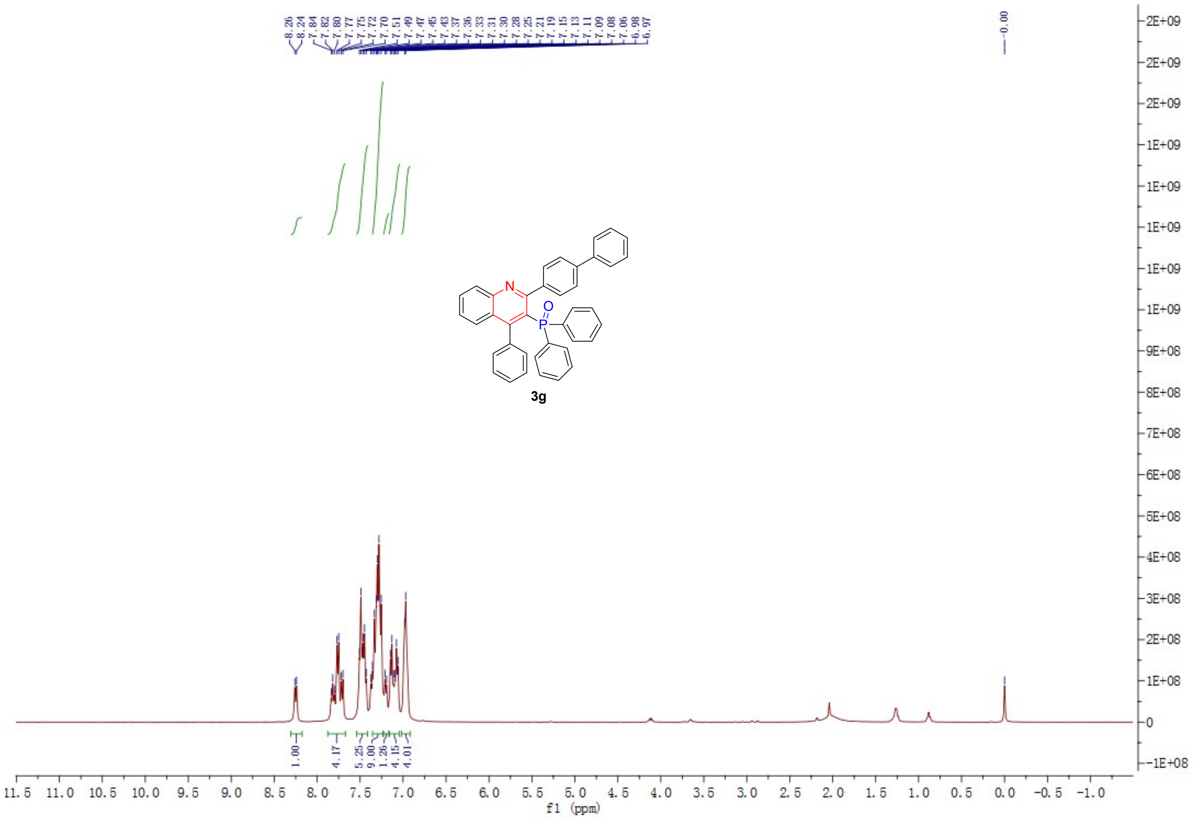
20.32
N
O
P
3e
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130 110 90 80 70 60 50 40 30 20 10 0 −10 −30 −50 −70 −90 −110 −130 −150 −170 −190 −210 −230
f1 (ppm)

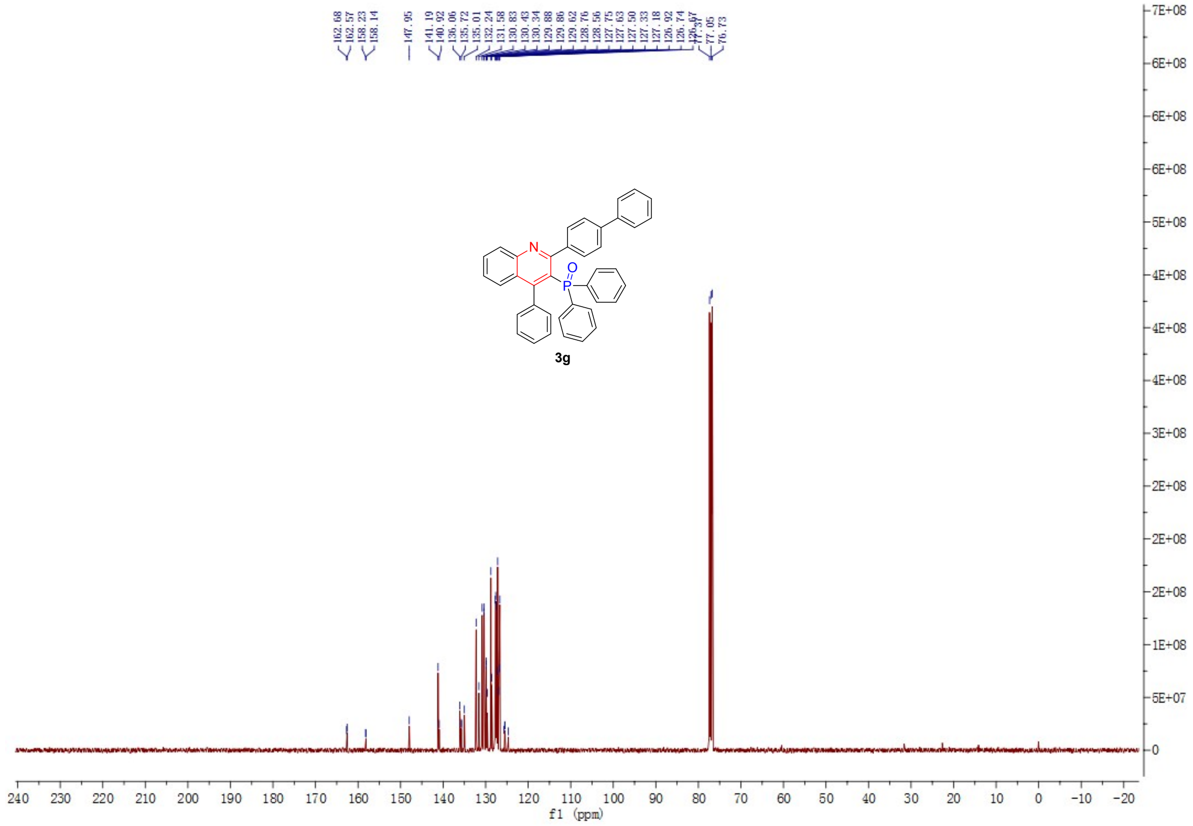


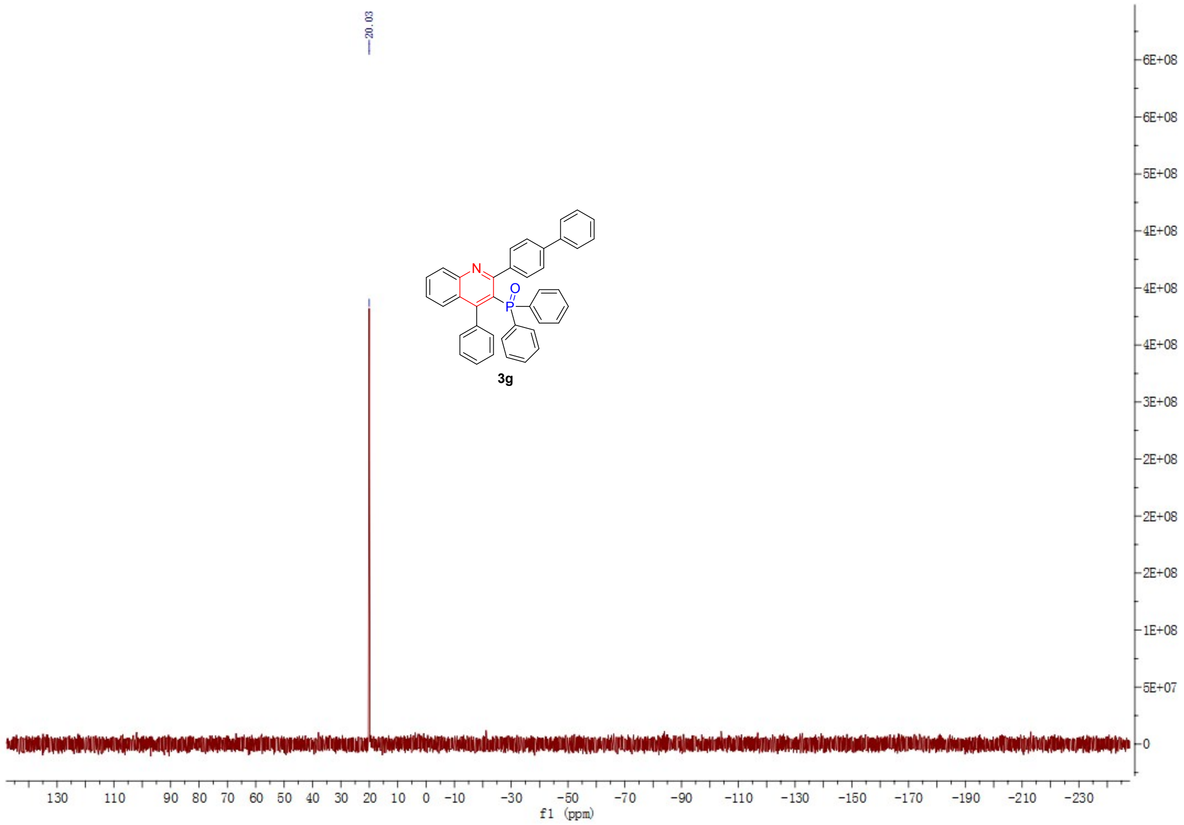
8.22
8.20
7.81
7.79
7.77
7.70
7.68
7.58
7.56
7.46
7.44
7.42
7.27
7.26
7.25
7.25
7.24
7.24
7.23
7.21
7.20
7.20
7.18
7.13
7.11
7.09
7.07
7.06
6.99
6.98
6.97
6.96
6.95
6.94
6.92
6.90
2.23
N
O
P
CH3
3f
1.00
1.07
1.13
2.13
1.24
7.10
4.20
6.20
3.21
2E+09
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
−1E+08
11.0 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 −0.5 −1.0 −1.5
f1 (ppm)

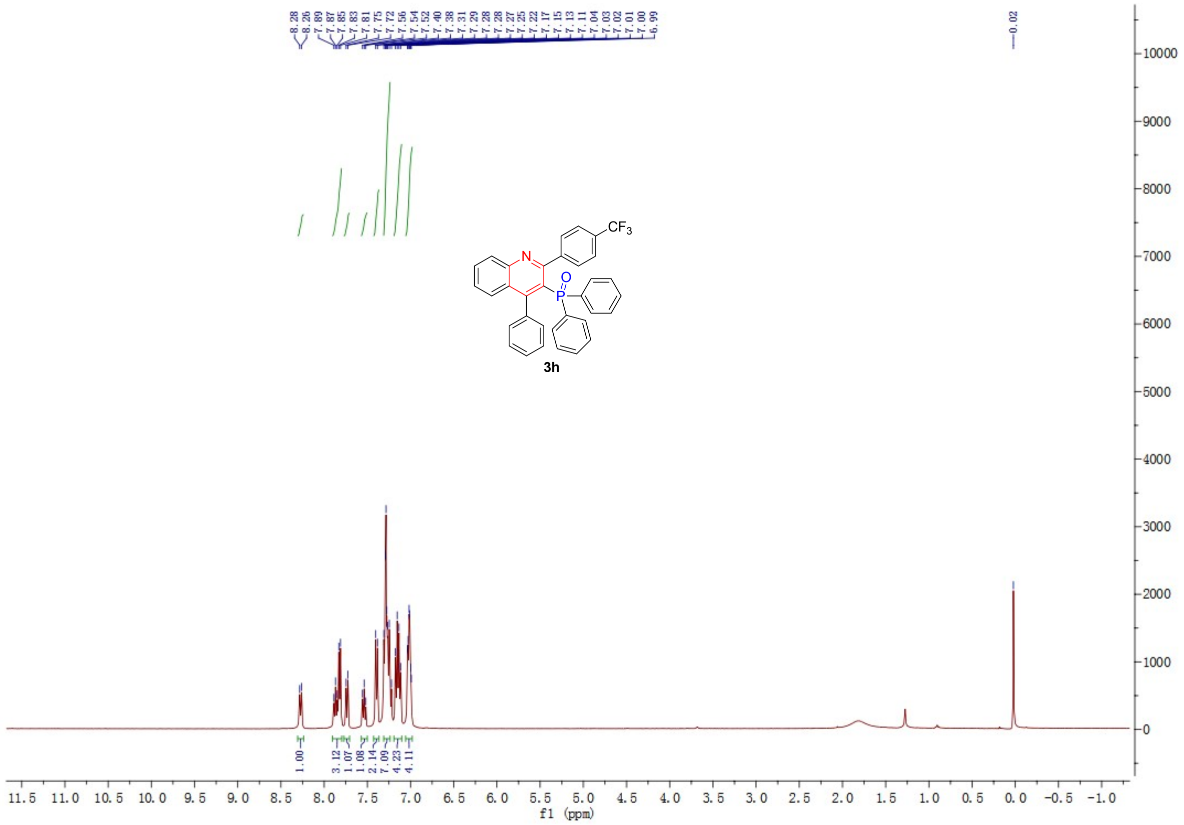

163.10
162.99
158.09
158.00
147.99
139.24
138.29
136.16
135.80
135.74
135.11
132.24
131.42
130.37
130.33
130.28
129.77
129.74
129.60
128.46
127.65
127.53
127.45
126.68
125.47
125.38
125.30
124.46
77.38
77.06
76.75
21.19
CH3
N
O
P
3f
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
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)

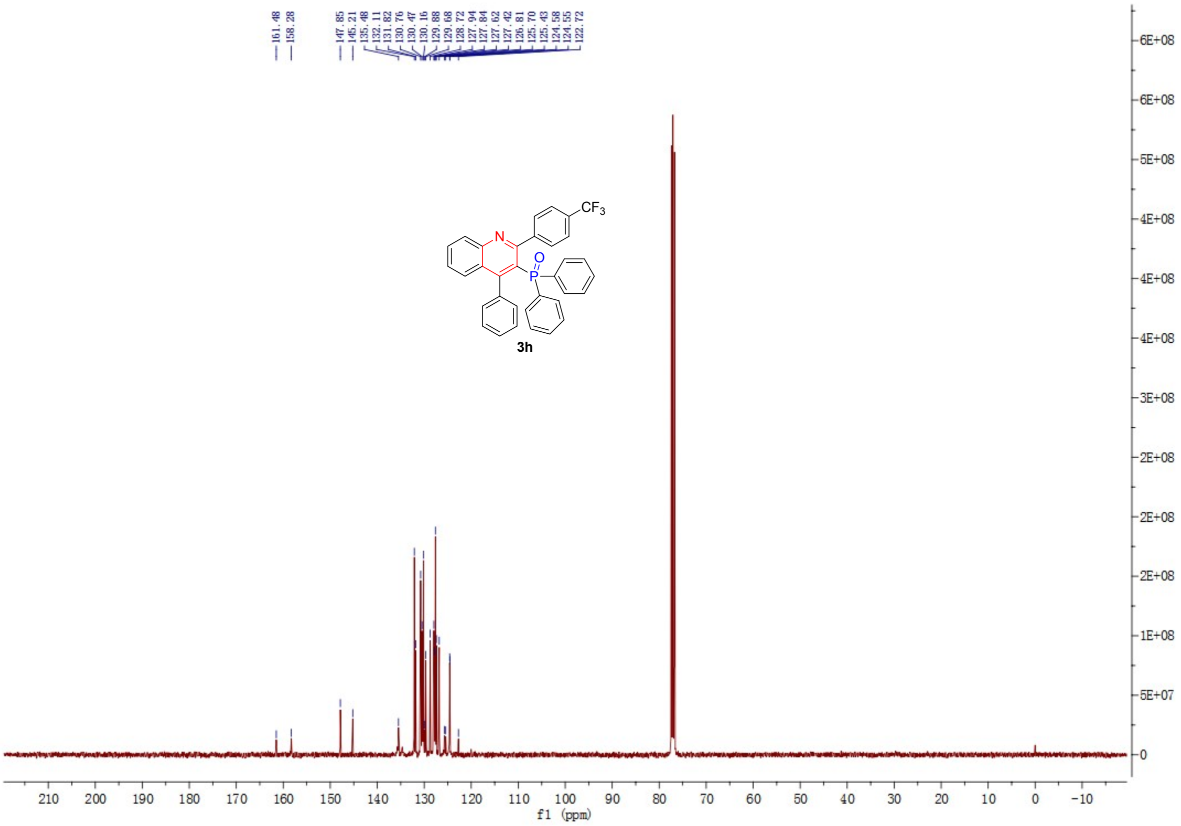

20.19
CH3
N
O
P
3f
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)

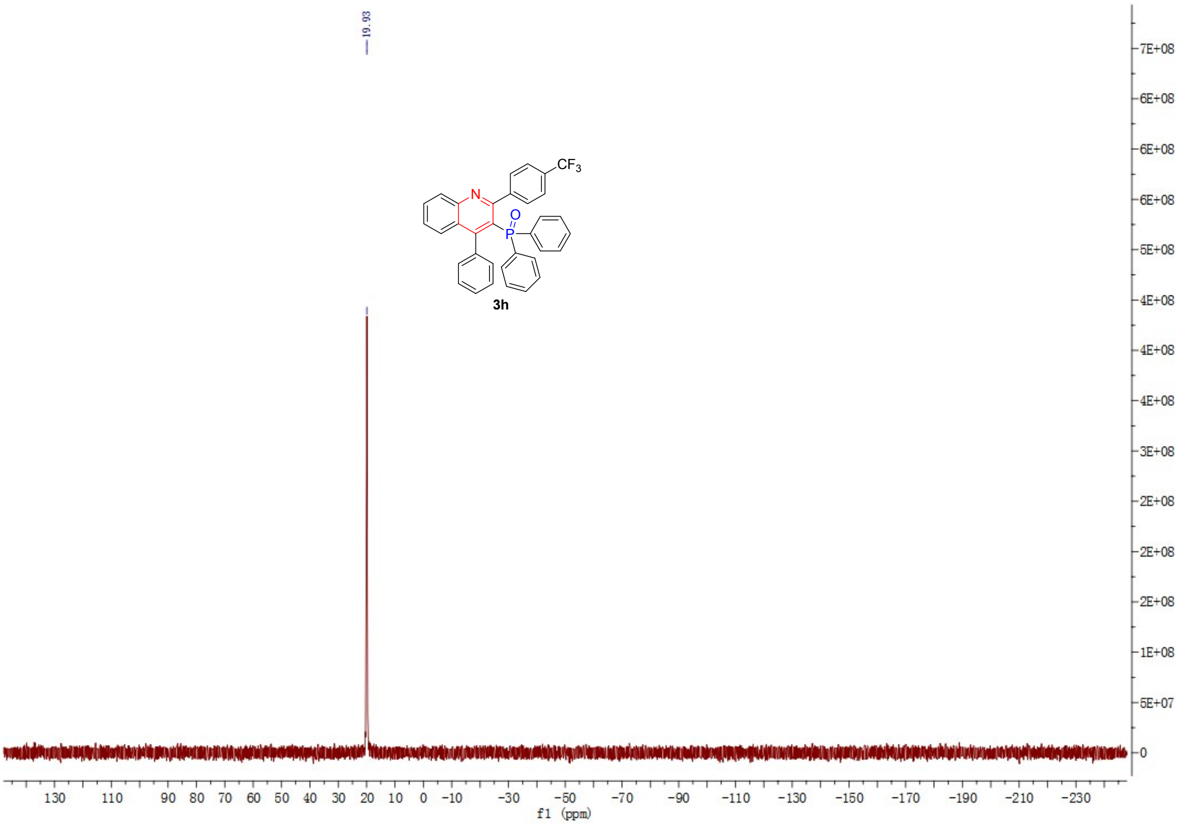

8.26
8.24
7.84
7.82
7.80
7.77
7.75
7.72
7.70
7.51
7.49
7.47
7.45
7.43
7.37
7.36
7.33
7.31
7.30
7.28
7.25
7.21
7.19
7.15
7.13
7.11
7.09
7.08
7.06
6.98
6.97
0.00
N
O
P
3g
1.00
4.17
5.25
9.00
1.26
4.15
4.01
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
2E+09
2E+09
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08

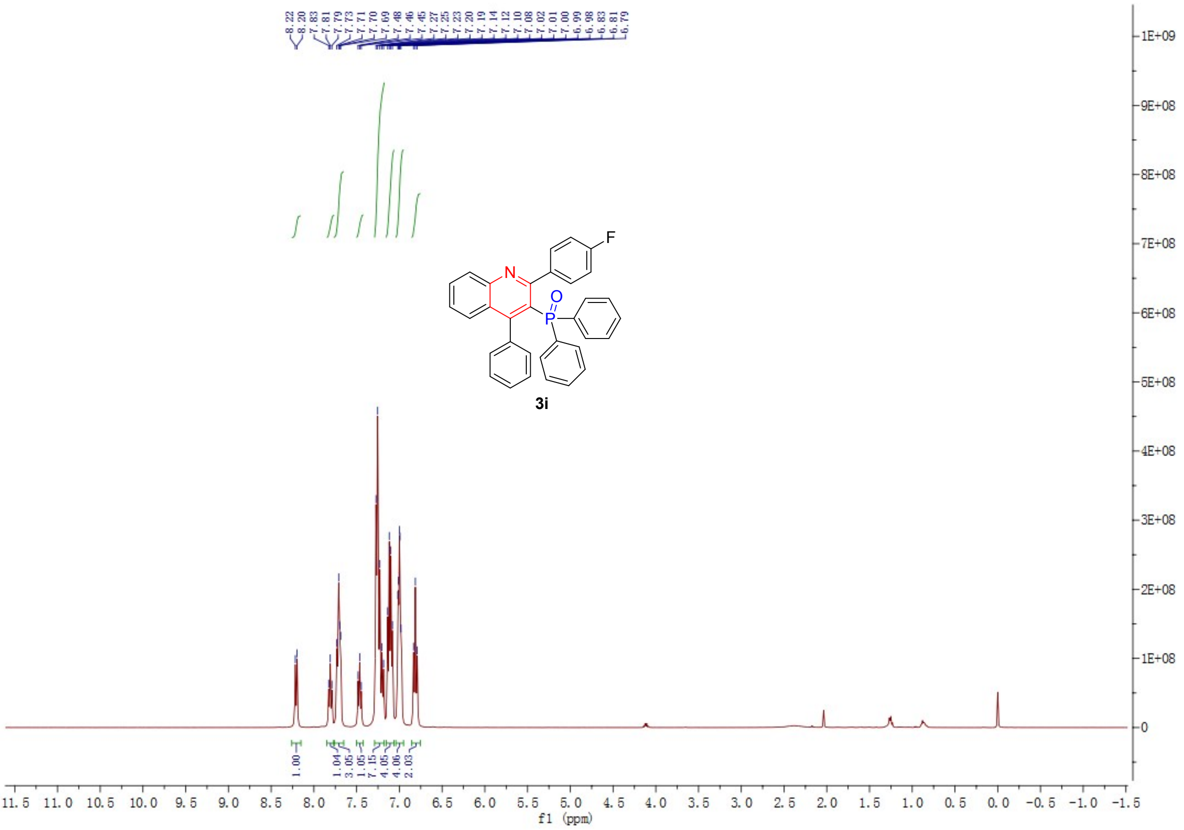

162.68
162.57
158.23
158.14
147.95
141.19
140.92
136.06
135.72
135.01
132.24
131.58
130.83
130.43
130.34
129.88
129.86
129.62
128.76
128.56
127.75
127.63
127.50
127.33
127.18
126.92
126.74
126.67
77.37
77.05
76.73
N
O
P
3g
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0

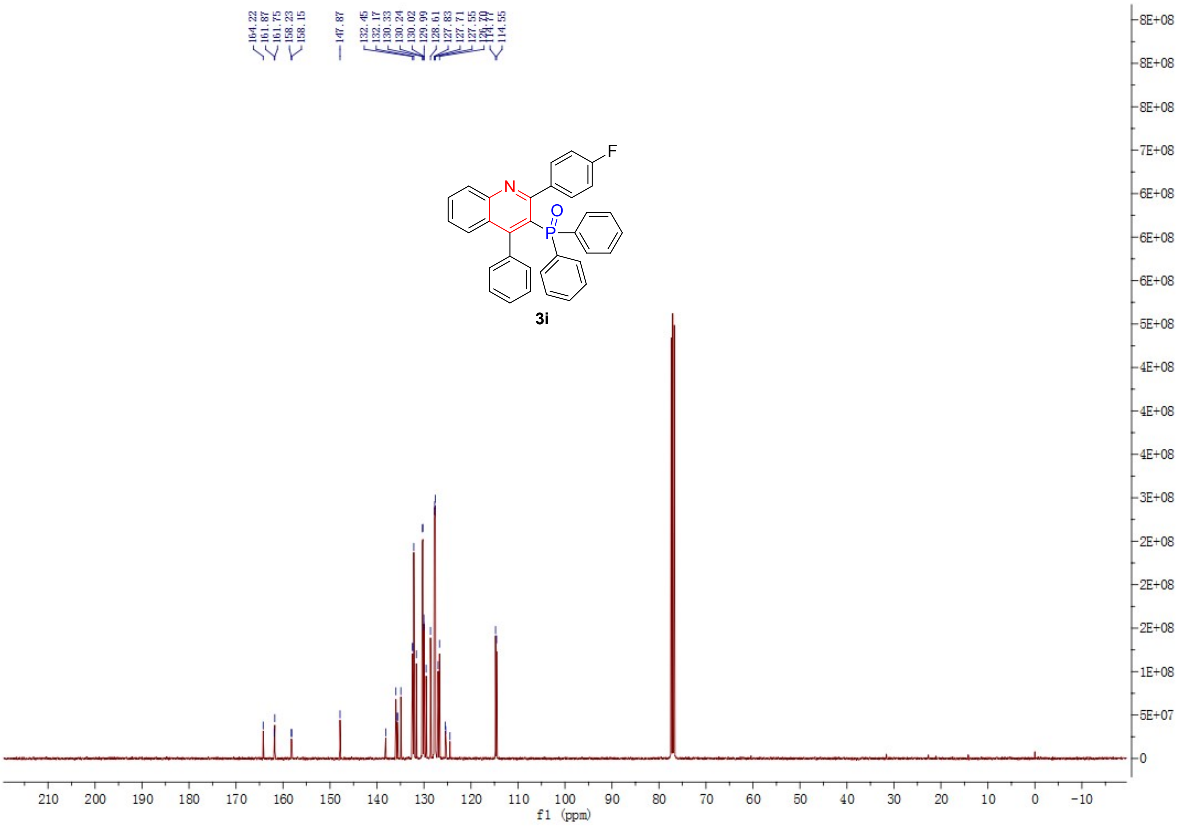

20.03
3g
O
P
N
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)

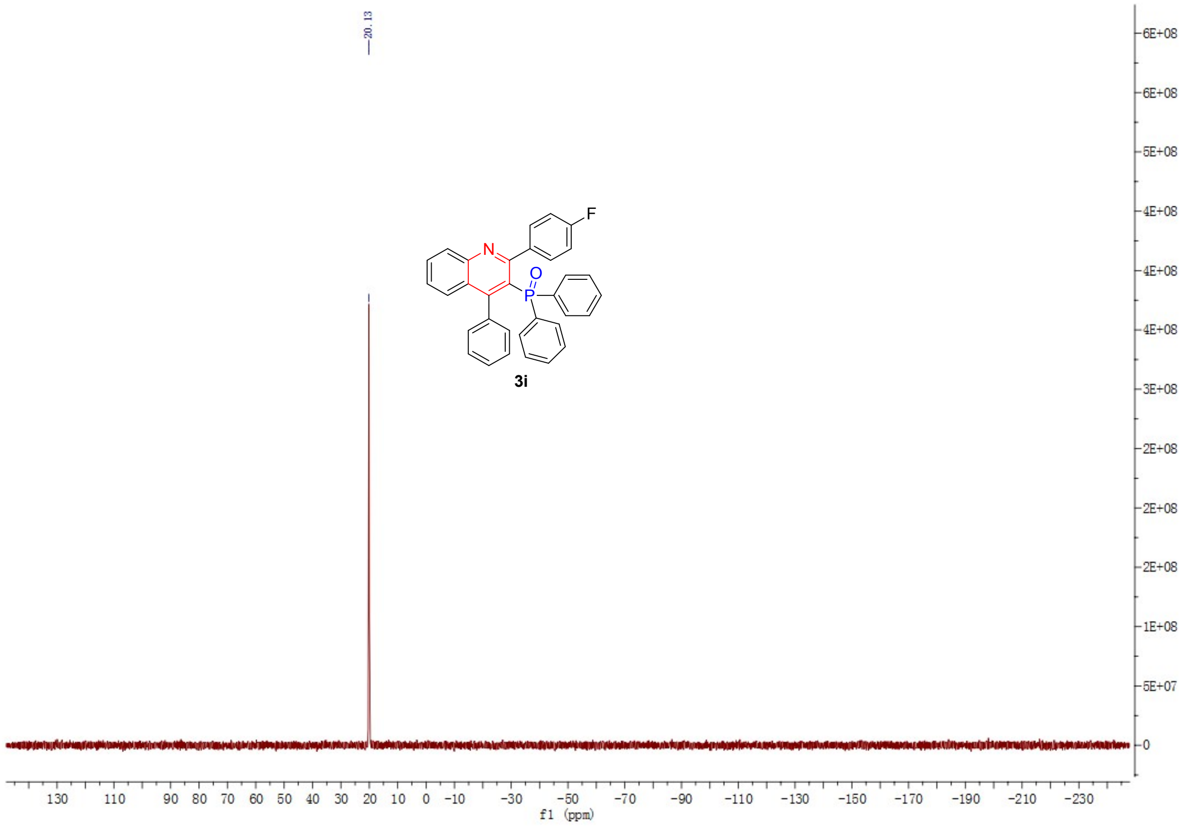

8.28
8.26
7.89
7.87
7.85
7.83
7.81
7.75
7.72
7.56
7.54
7.52
7.40
7.38
7.31
7.29
7.28
7.28
7.27
7.25
7.22
7.17
7.15
7.13
7.11
7.04
7.03
7.02
7.01
7.00
6.99
0.02
CF$_3$
N
O
P
3h
1.00
3.12
1.07
1.08
2.14
7.09
4.23
4.11
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
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
-0.5
-1.0
f1 (ppm)


161.48
158.28
147.85
145.21
135.48
132.11
131.82
130.76
130.47
130.16
129.88
129.68
128.72
127.94
127.84
127.62
127.42
126.81
125.70
125.43
124.58
124.55
122.72
N
O
P
CF3
3h
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
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)

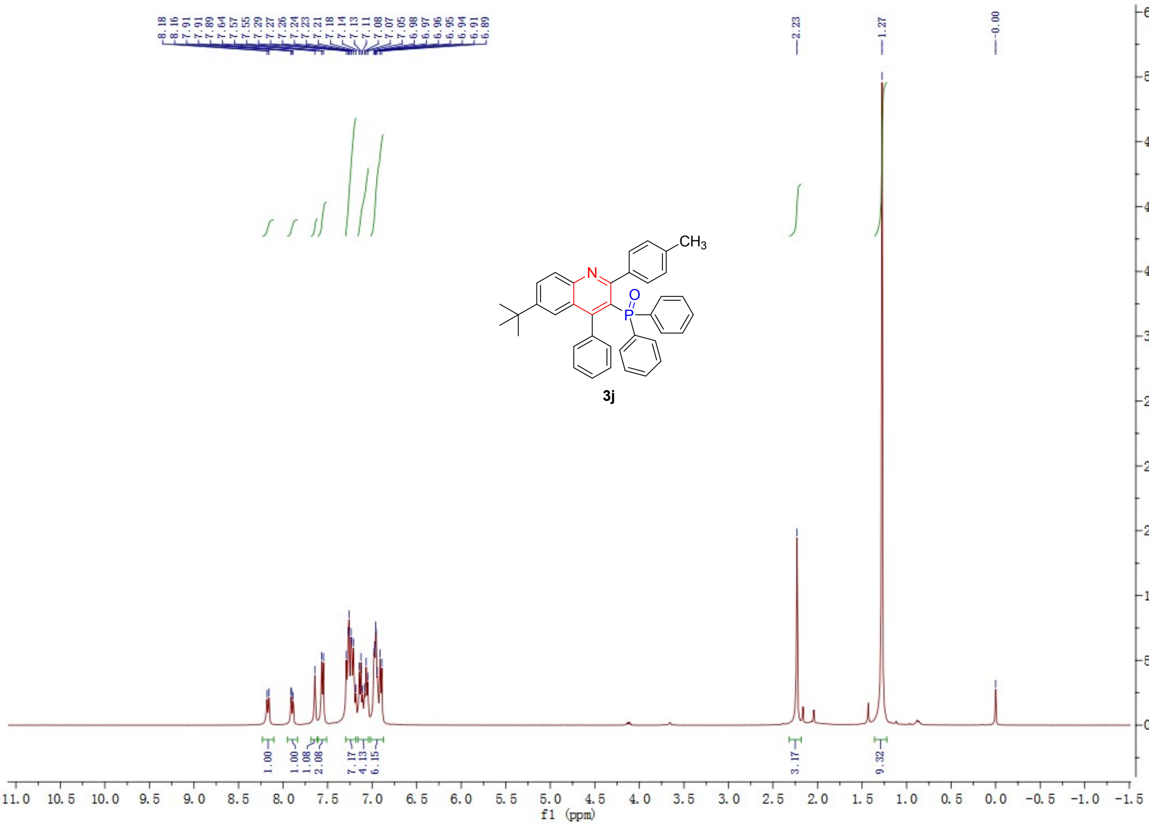

19.93
N
O
P
CF3
3h
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


8.22
8.20
7.83
7.81
7.79
7.73
7.71
7.70
7.69
7.48
7.46
7.45
7.27
7.25
7.23
7.20
7.19
7.14
7.12
7.10
7.08
7.02
7.01
7.00
6.99
6.98
6.83
6.81
6.79
N
O
P
F
3i
1.00
1.04
3.05
1.05
1.15
7.15
4.05
4.06
2.03
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
11.5 11.0 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 -0.5 -1.0 -1.5
f1 (ppm)

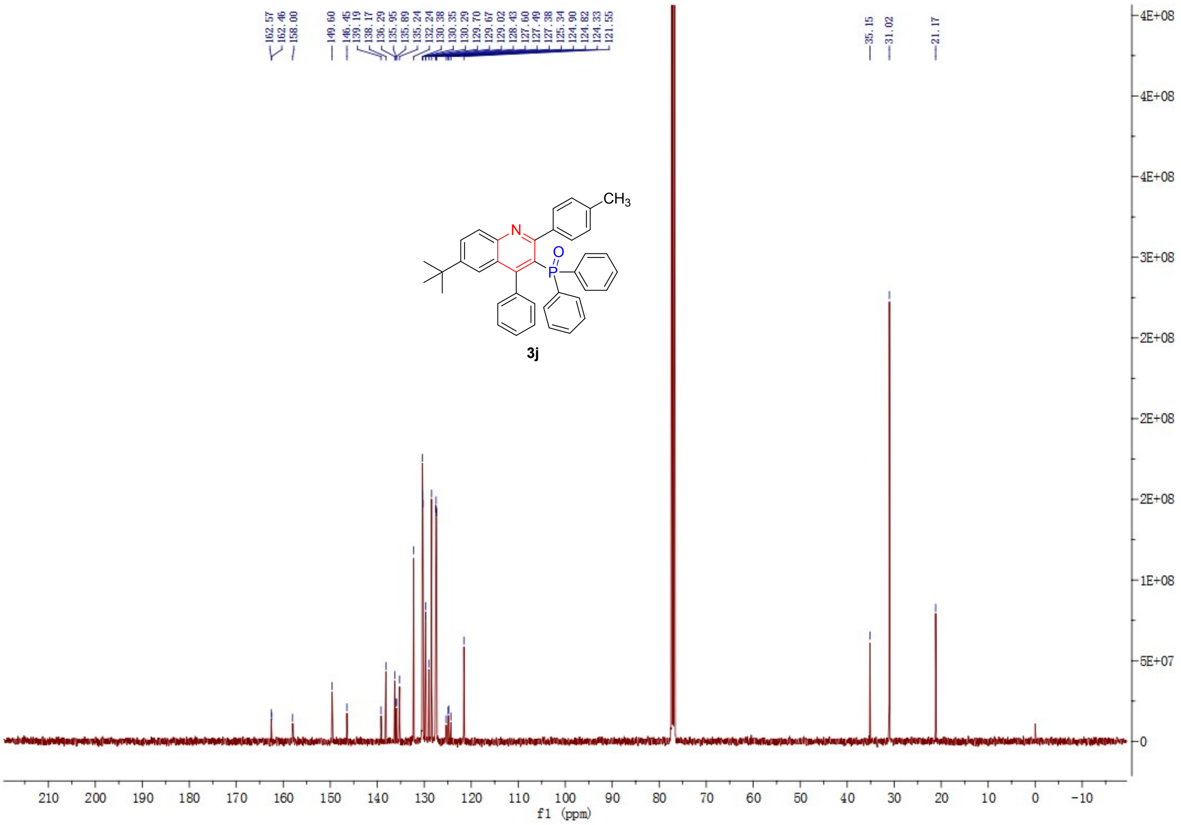

164.22
161.87
161.75
158.23
158.15
147.87
132.45
132.17
130.33
130.24
130.02
129.99
128.61
127.83
127.71
127.55
126.70
114.77
114.55
N
O
P
F
3i
8E+08
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


20.13
F
N
O
P
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

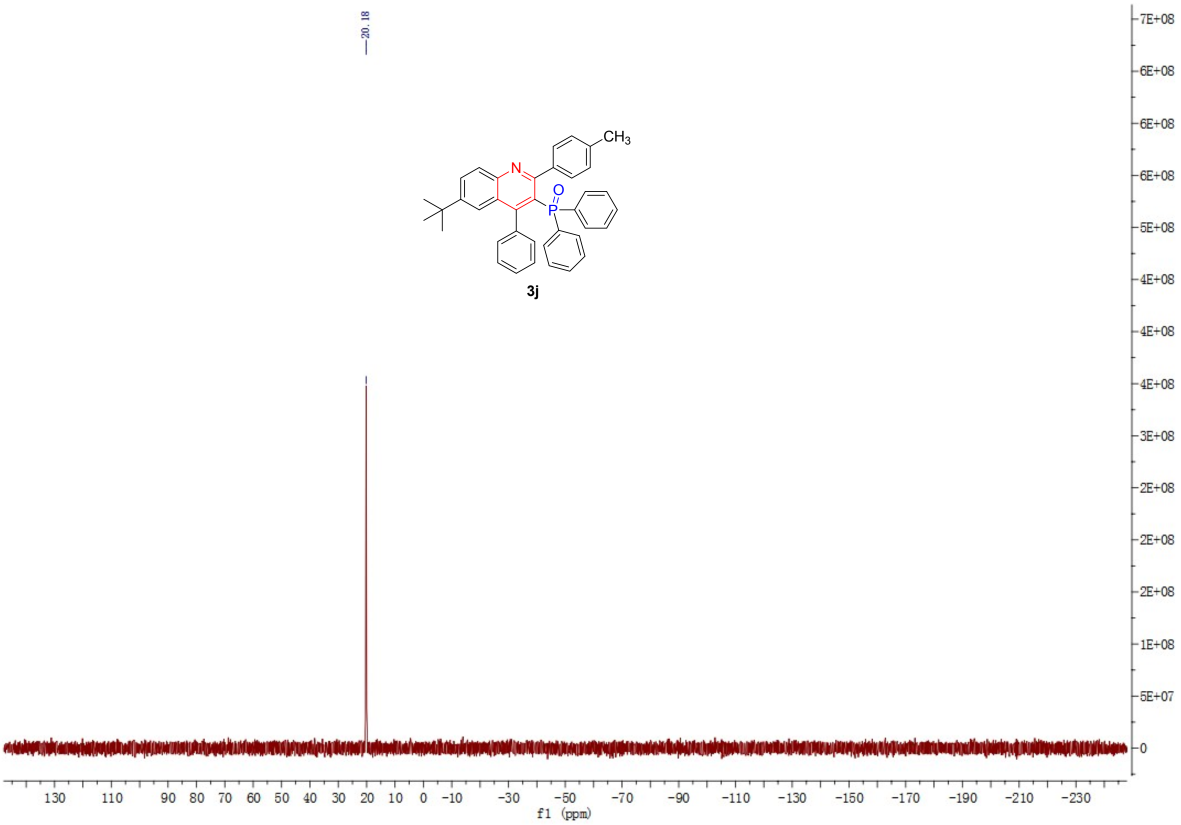
3i


8.18
8.16
7.91
7.89
7.64
7.57
7.55
7.29
7.27
7.26
7.24
7.23
7.21
7.18
7.14
7.13
7.11
7.08
7.07
7.05
6.98
6.97
6.96
6.95
6.94
6.91
6.89
2.23
1.27
0.00
CH3
N
O
P
1.00
1.00
1.08
2.08
7.17
4.13
6.15
3.17
9.32
6E+08
5E+08
4E+08
4E+08
3E+08
2E+08
2E+08
1E+08
5E+07
0
11.0 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 -0.5 -1.0 -1.5
f1 (ppm)

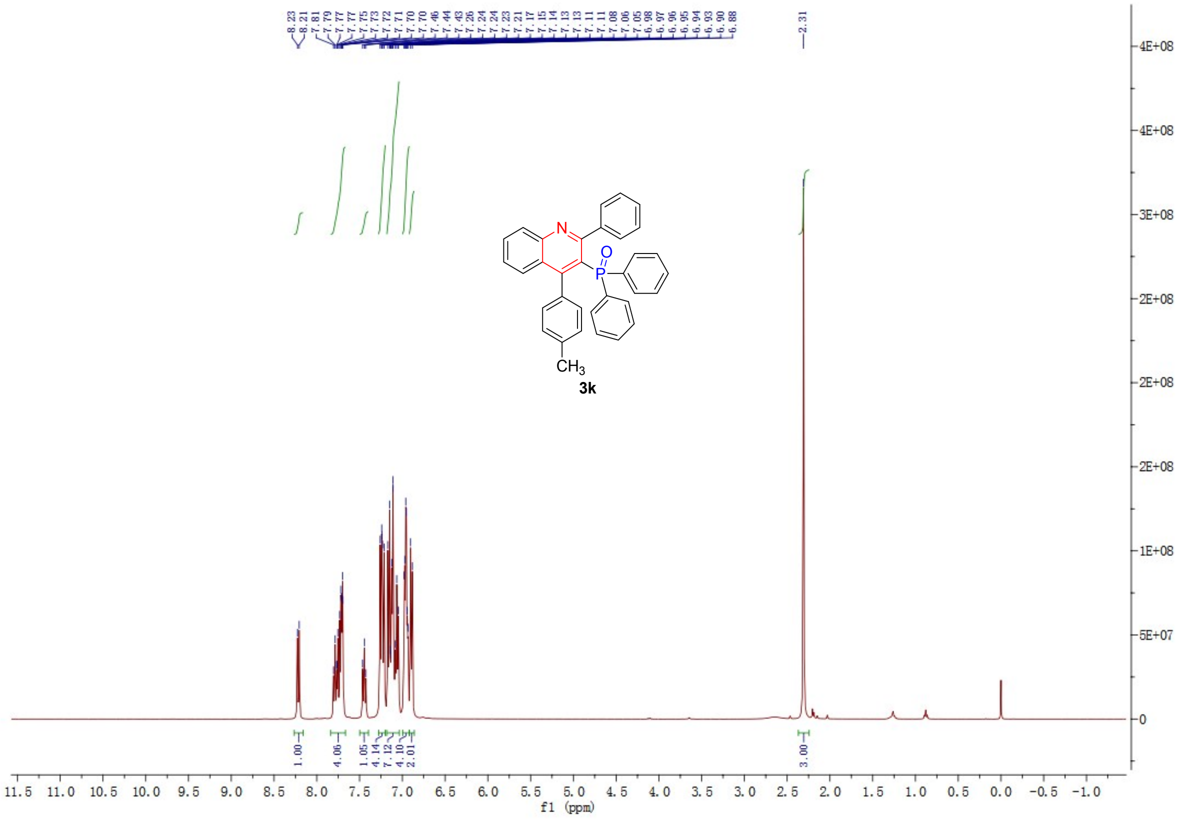
3j

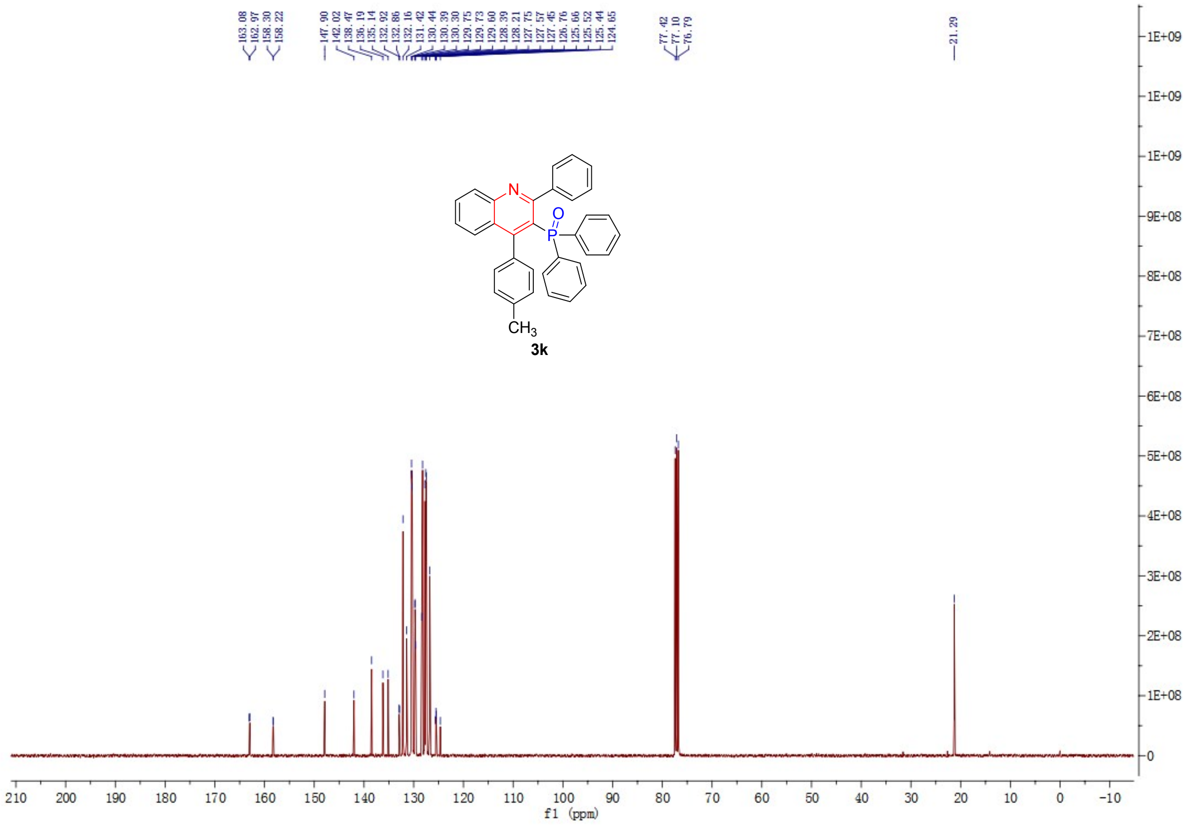

162.57
162.46
158.00
149.60
146.45
139.19
138.17
136.29
135.95
135.89
135.24
132.24
130.38
130.35
130.29
129.70
129.67
129.02
128.43
127.60
127.49
127.38
125.34
124.90
124.82
124.33
121.55
35.15
31.02
21.17
CH3
N
O
P
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

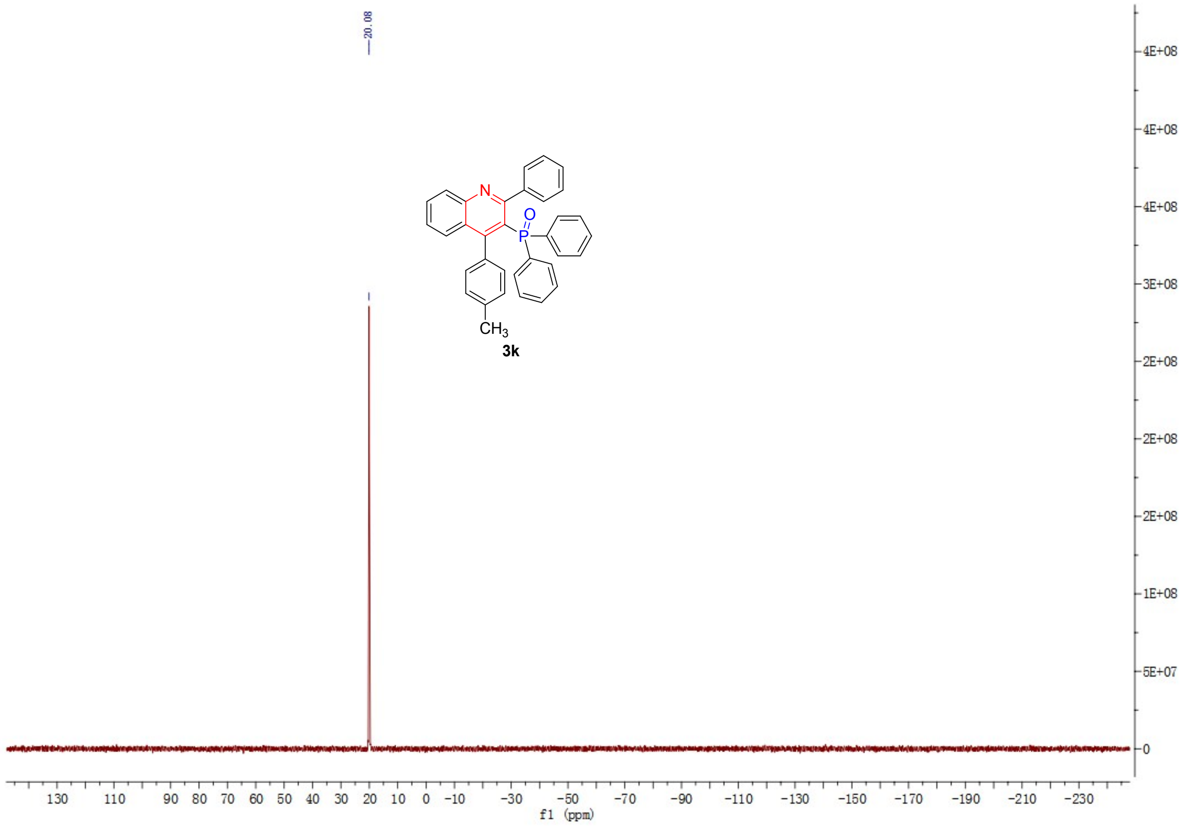
3j


20.18
CH3
N
O
P
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

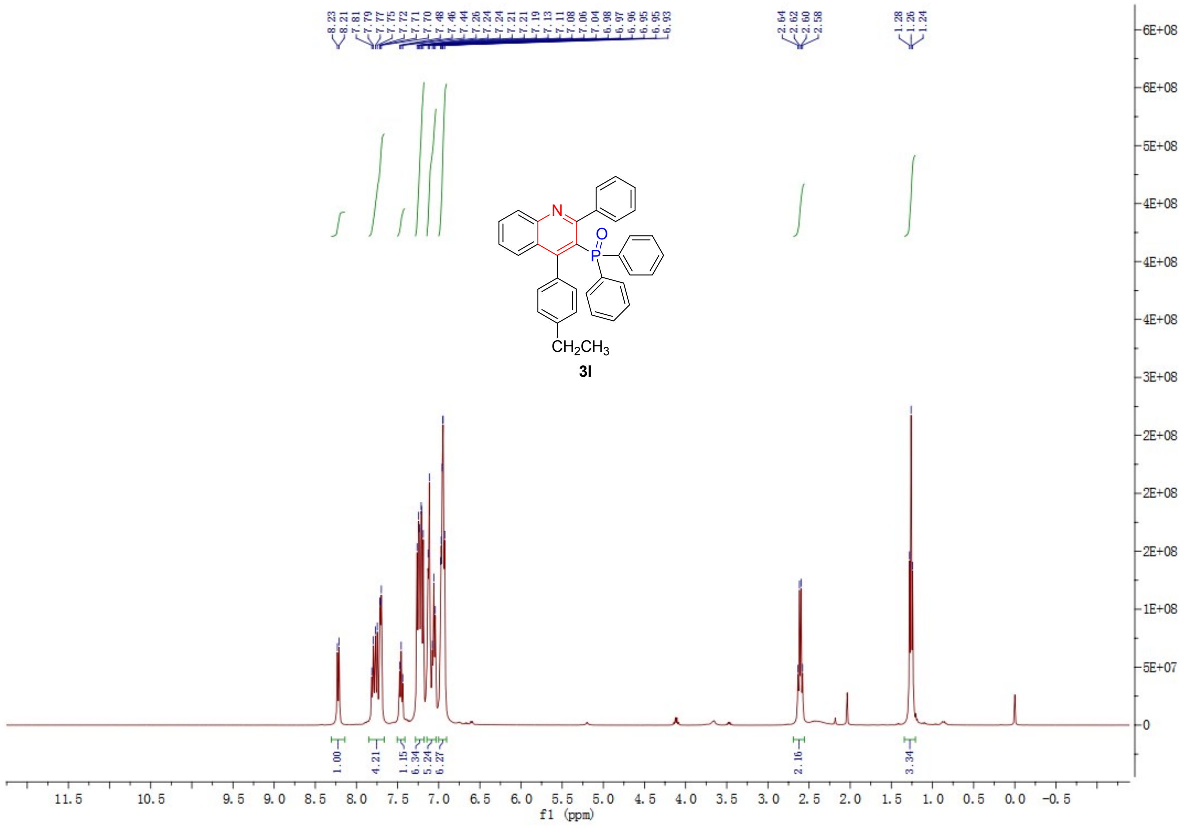
3j


8.23
8.21
7.81
7.79
7.77
7.77
7.75
7.73
7.72
7.71
7.70
7.70
7.46
7.44
7.43
7.26
7.24
7.24
7.23
7.21
7.17
7.15
7.14
7.13
7.13
7.11
7.11
7.08
7.06
7.05
6.98
6.97
6.96
6.95
6.94
6.93
6.90
6.88
2.31
1.00
4.06
1.05
4.14
7.12
4.10
2.01
3.00
N
O
P
CH3
3k
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.5 11.0 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 -0.5 -1.0
f1 (ppm)

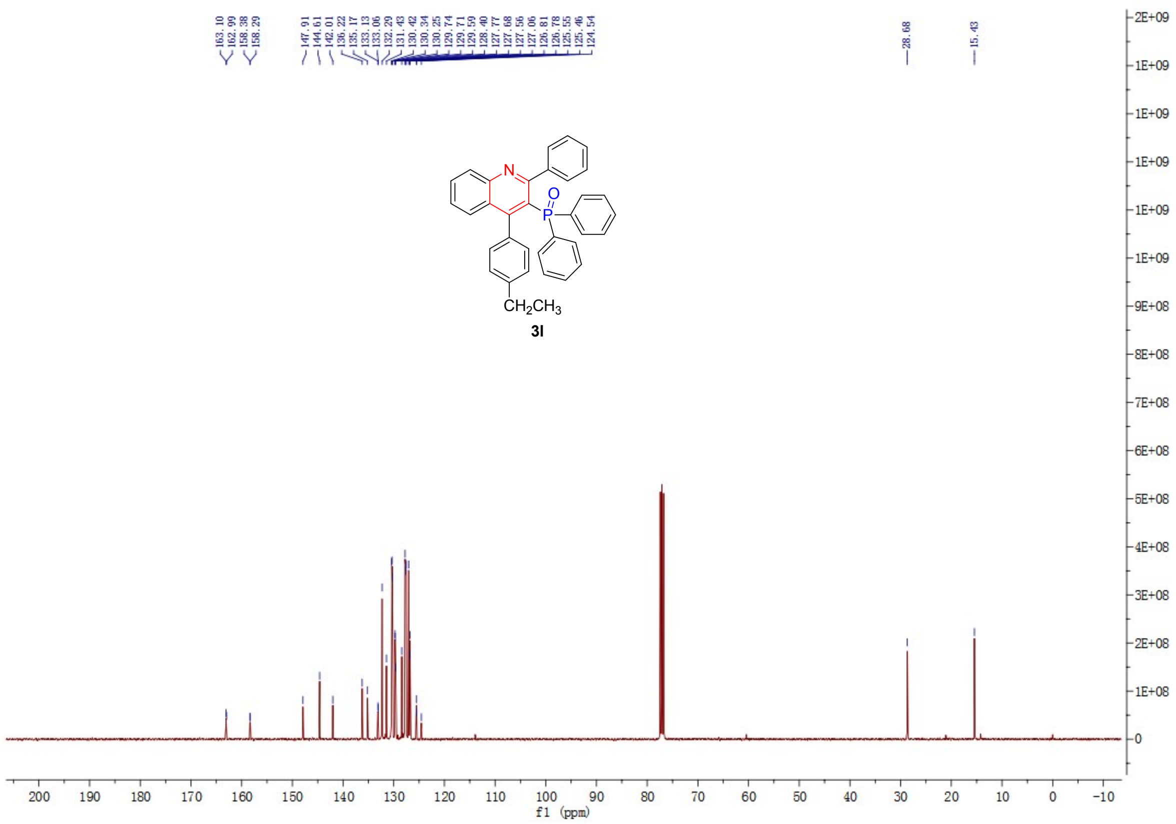

163.08
162.97
158.30
158.22
147.90
142.02
138.47
136.19
135.14
132.92
132.86
132.16
131.42
130.44
130.39
130.30
129.75
129.73
129.60
128.39
128.21
127.75
127.57
127.45
126.76
126.66
125.52
125.44
124.65
77.42
77.10
76.79
21.29
N
O
P
CH3
3k
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
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)

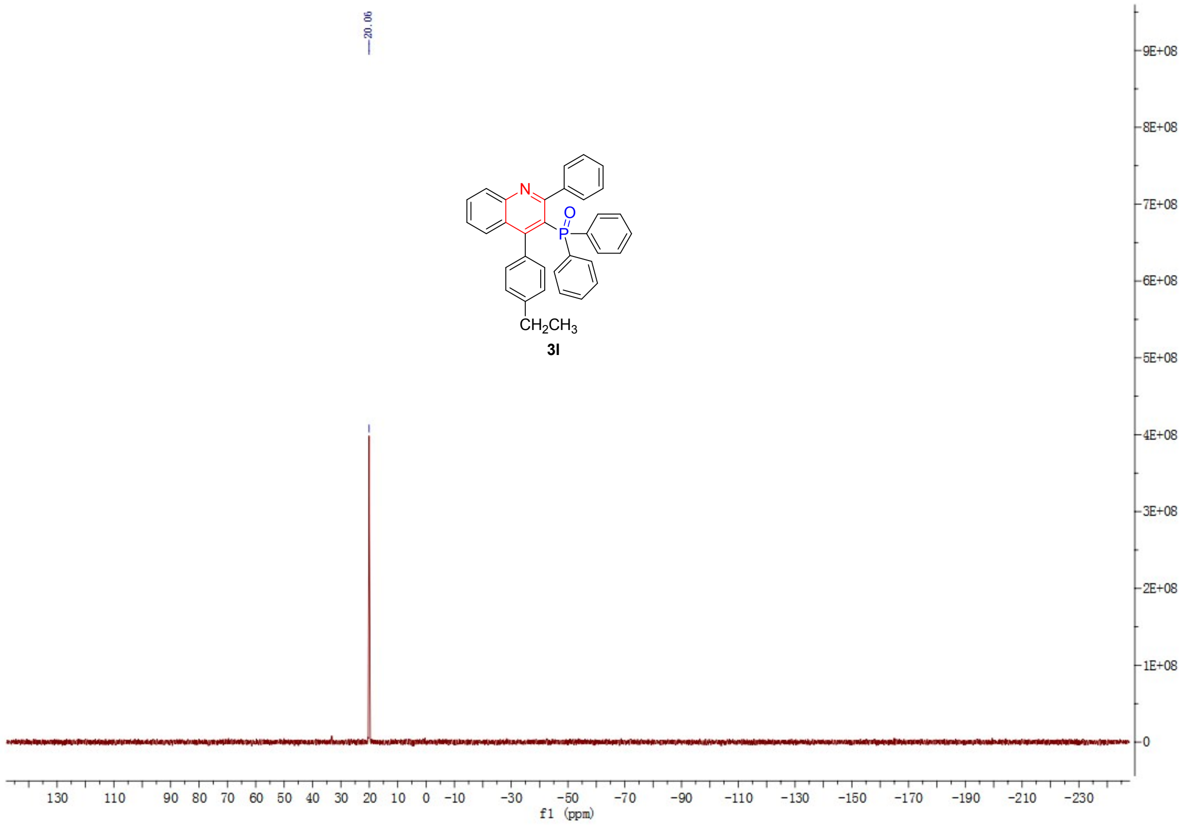

20.08
N
O
P
CH3
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

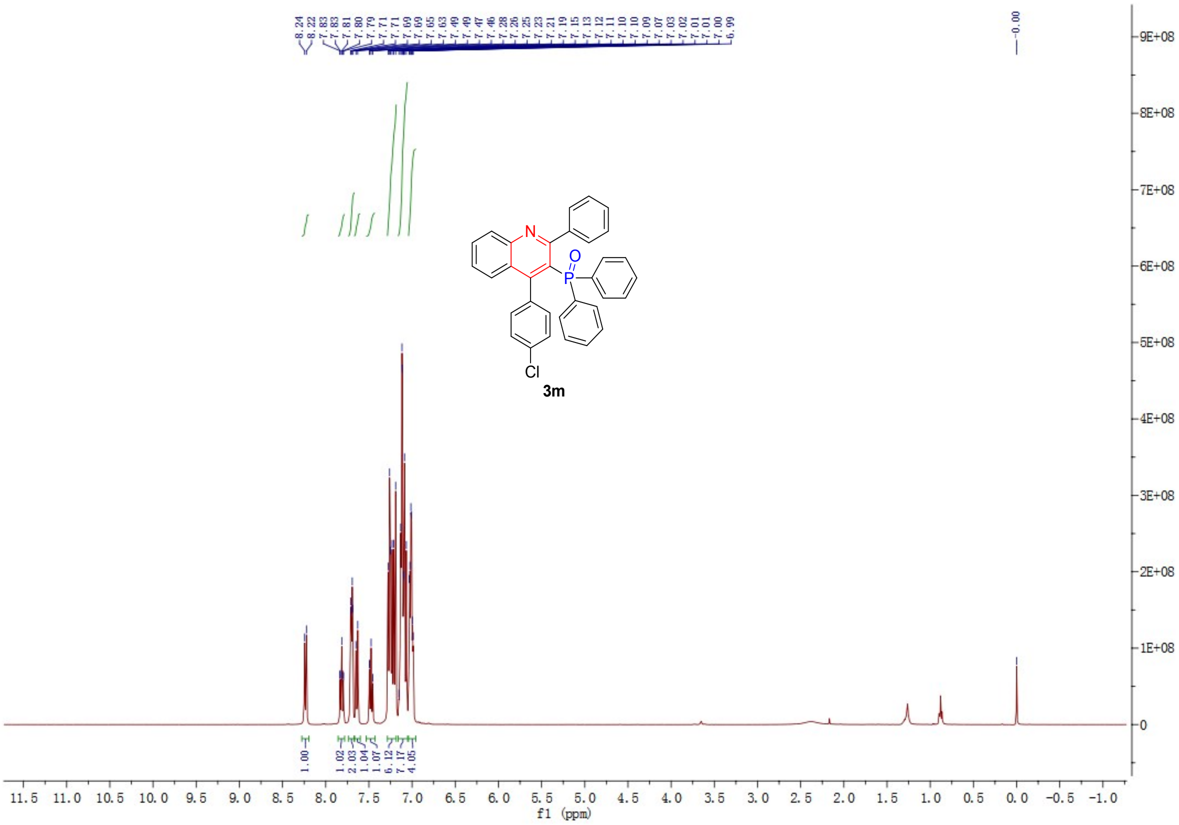
3k


8.23
8.21
7.81
7.79
7.77
7.75
7.72
7.71
7.70
7.48
7.46
7.44
7.26
7.24
7.24
7.21
7.21
7.19
7.13
7.11
7.08
7.06
7.04
6.98
6.97
6.96
6.95
6.95
6.93
2.64
2.62
2.60
2.58
1.28
1.26
1.24
N
O
P
CH2CH3
1.00
4.21
1.15
6.34
5.24
6.27
2.16
3.34
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.5 10.5 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)

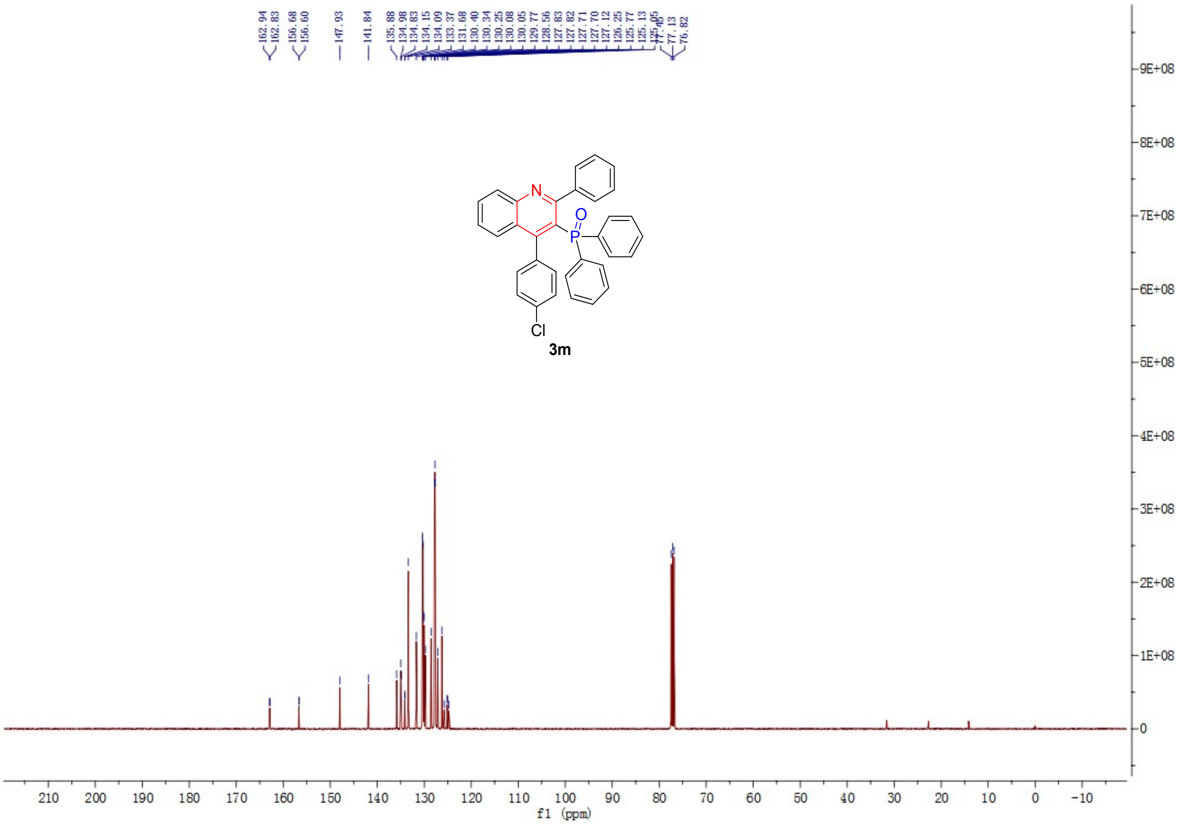
3l


163.10
162.99
158.38
158.29
147.91
144.61
142.01
136.22
135.17
133.13
133.06
132.29
131.43
130.42
130.34
130.25
129.74
129.71
129.59
128.40
127.77
127.68
127.56
127.06
126.81
126.78
125.55
125.46
124.54
28.68
15.43
N
O
P
CH2CH3
3l
2E+09
1E+09
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

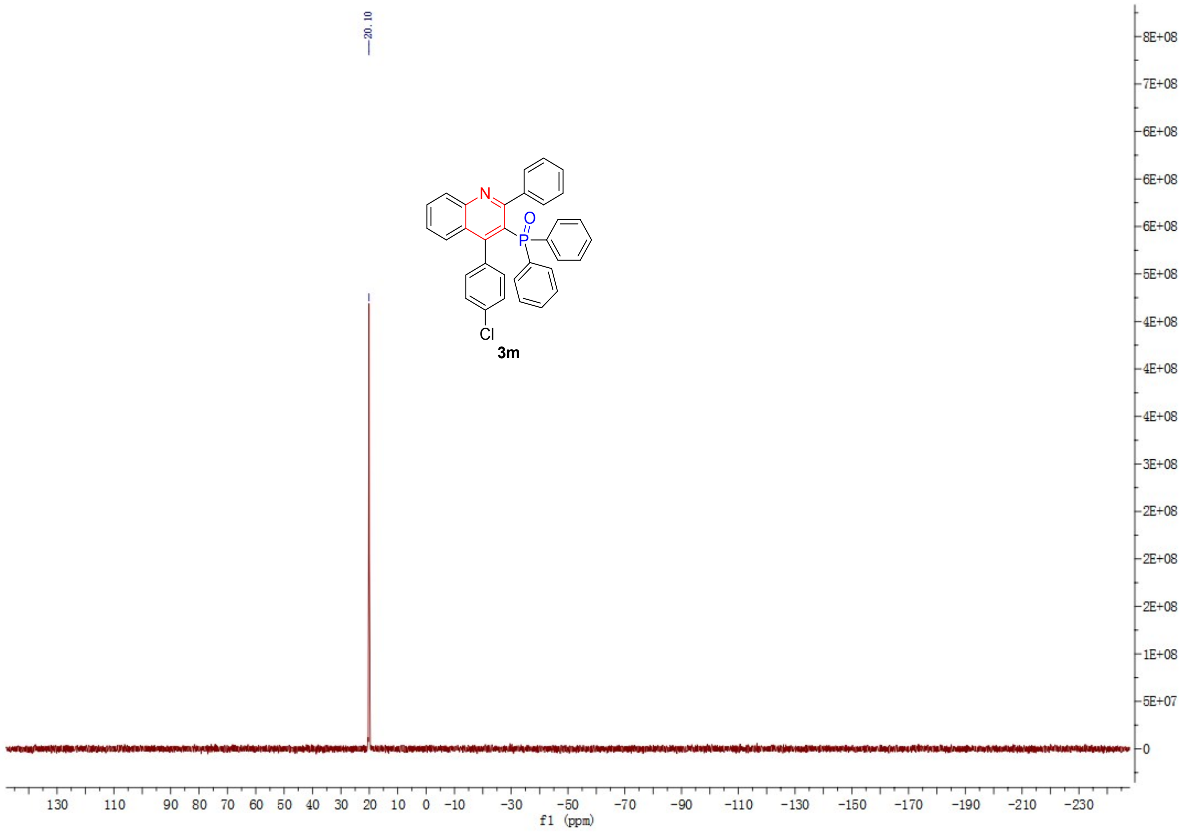

20.06
N
O
P
CH2CH3
3l
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


8.24
8.22
7.83
7.83
7.81
7.80
7.79
7.71
7.71
7.69
7.69
7.65
7.63
7.49
7.49
7.47
7.46
7.28
7.26
7.25
7.23
7.21
7.19
7.15
7.13
7.12
7.11
7.10
7.10
7.09
7.07
7.03
7.02
7.01
7.01
7.00
6.99
0.00
N
O
P
Cl
1.00
1.02
2.03
1.04
1.07
6.12
7.17
4.05
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
11.5
11.0
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
-0.5
-1.0
f1 (ppm)

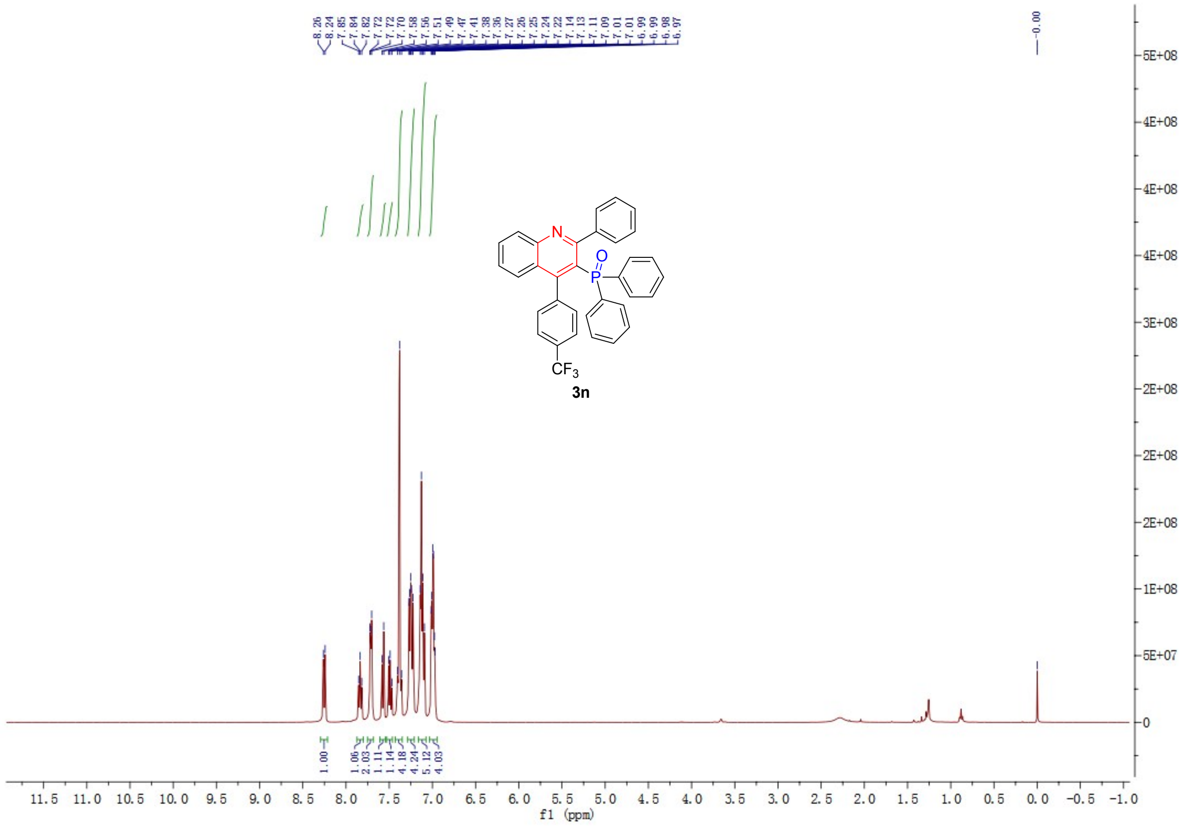
3m


162.94
162.83
156.68
156.60
147.93
141.84
135.88
134.98
134.83
134.15
134.09
133.37
131.68
130.40
130.34
130.25
130.08
130.05
129.77
128.56
127.83
127.82
127.71
127.70
127.12
126.25
125.77
125.13
125.05
77.45
77.13
76.82
N
O
P
Cl
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
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)

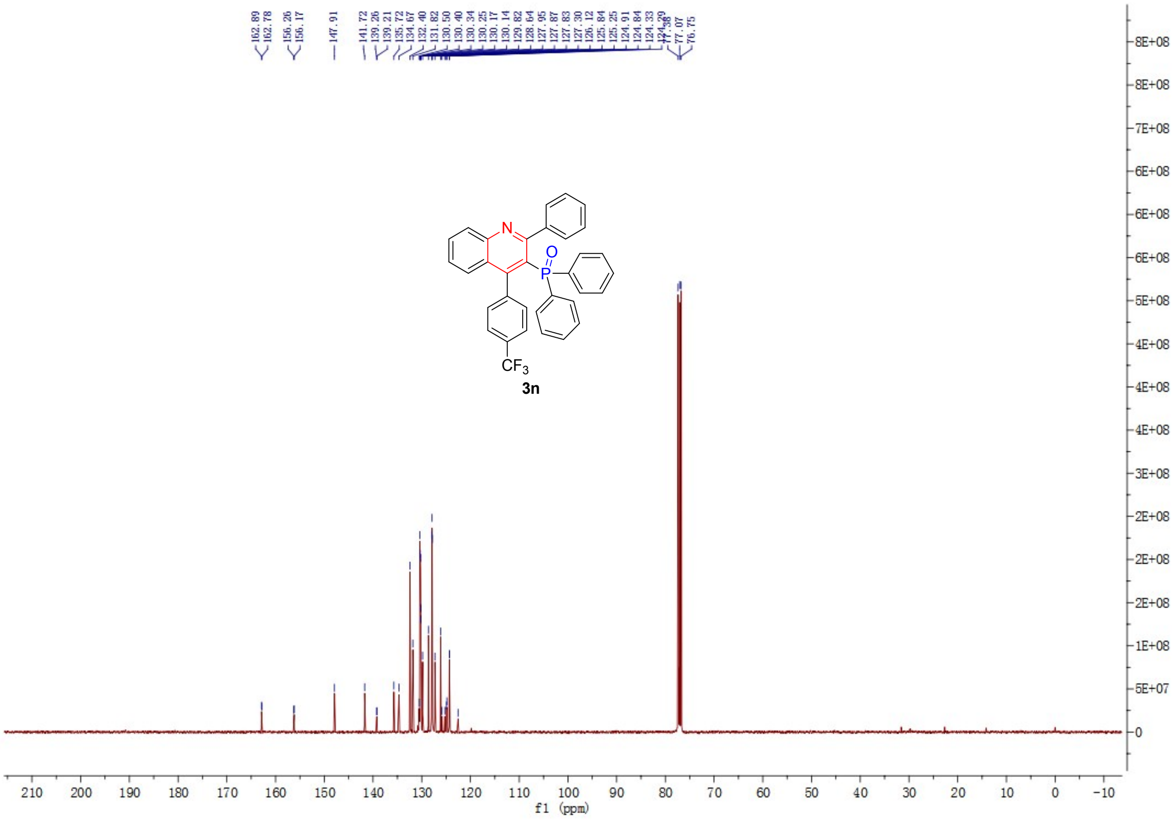
3m

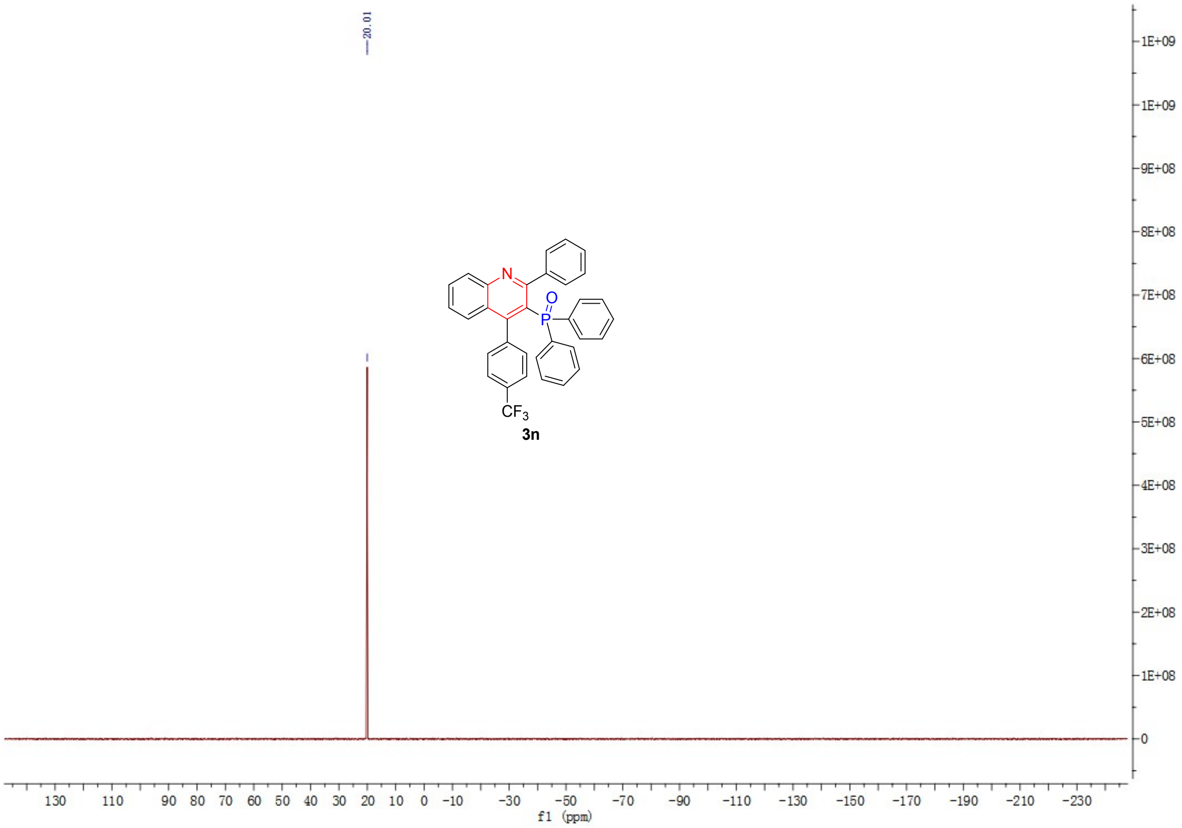

20.10
N
O
P
Cl
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

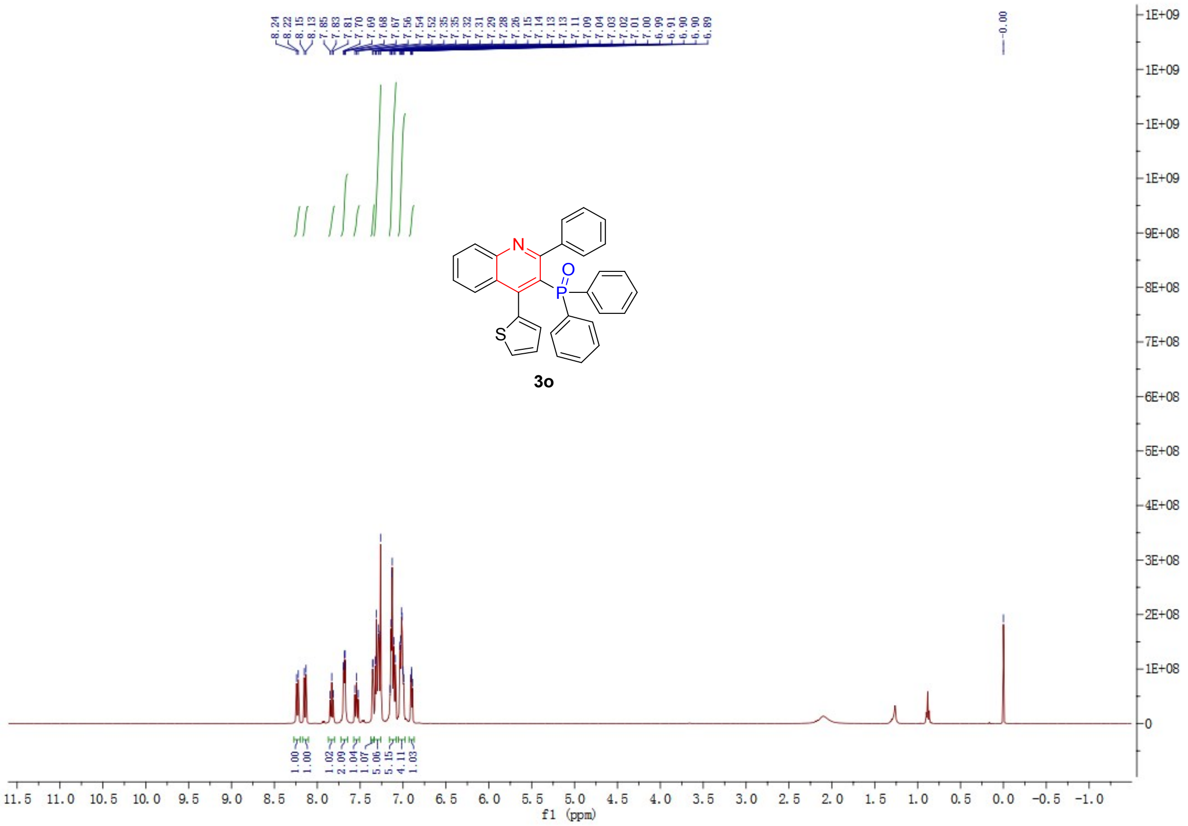
3m


8.26
8.24
7.85
7.84
7.82
7.72
7.72
7.70
7.58
7.56
7.51
7.49
7.47
7.41
7.38
7.36
7.27
7.26
7.25
7.24
7.22
7.14
7.13
7.11
7.09
7.01
7.01
6.99
6.99
6.98
6.97
0.00
N
O
P
CF3
1.00
1.06
2.03
1.11
1.14
4.18
4.24
5.12
4.03
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.5 11.0 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 -0.5 -1.0
f1 (ppm)

3n

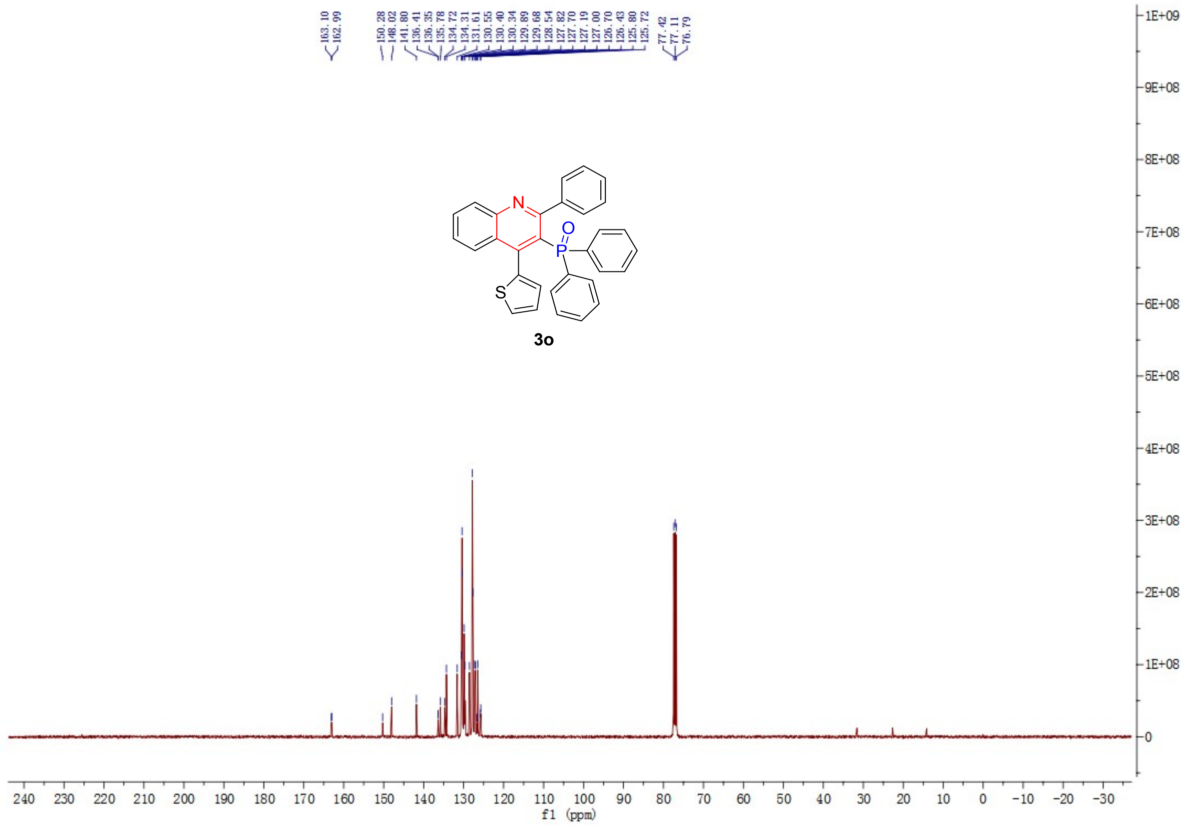

162.89
162.78
156.26
156.17
147.91
141.72
139.26
139.21
135.72
134.67
132.40
131.82
130.50
130.40
130.34
130.25
130.17
130.14
129.82
128.64
127.95
127.87
127.83
127.30
126.12
125.84
125.25
124.91
124.84
124.33
124.29
77.38
77.07
76.75
N
O
P
CF3
3n
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
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)


20.01
N
O
P
CF3
3n
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)



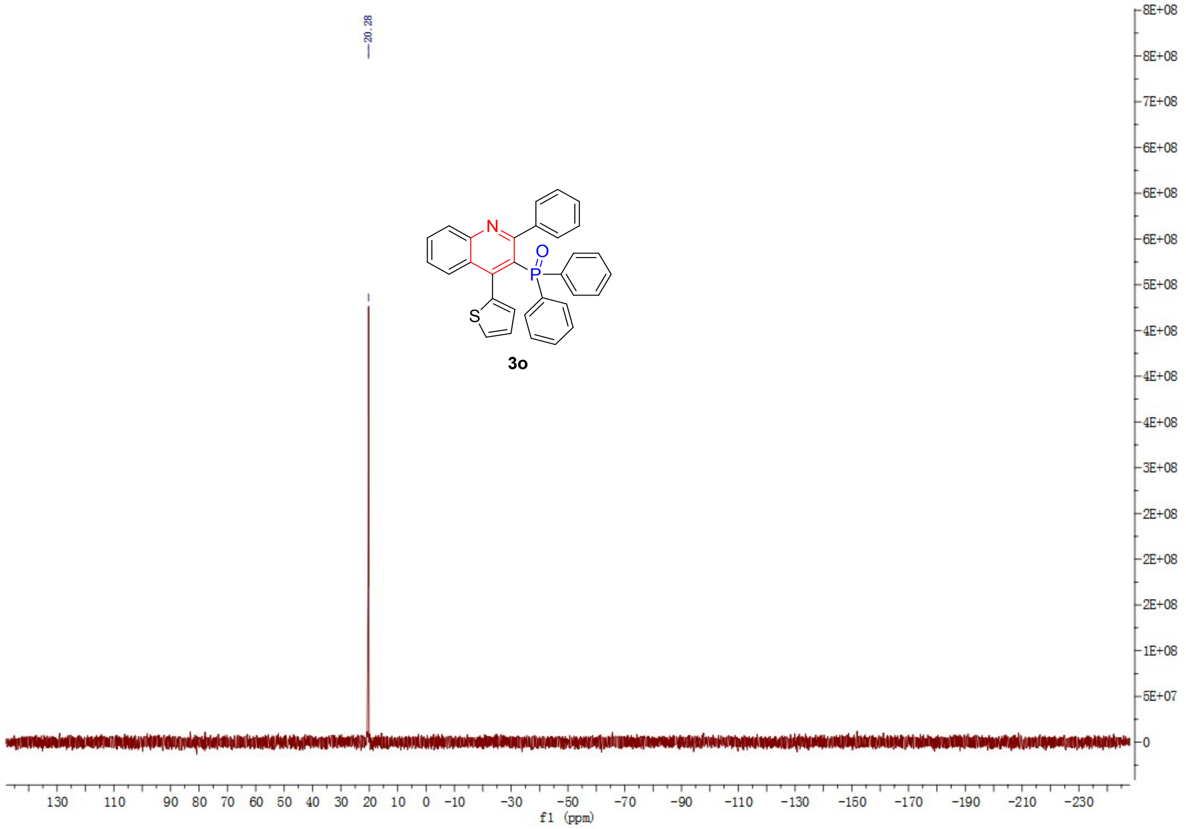
3o

8.24
8.22
8.15
8.13
7.85
7.83
7.81
7.70
7.69
7.68
7.67
7.56
7.54
7.52
7.35
7.35
7.32
7.31
7.29
7.28
7.26
7.15
7.14
7.13
7.13
7.11
7.09
7.04
7.03
7.02
7.01
7.00
6.99
6.91
6.90
6.90
6.89
0.00
N
O
P
S
1.00
1.00
1.02
2.09
1.04
1.07
5.06
5.15
4.11
1.03
11.5
11.0
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
-0.5
-1.0
f1 (ppm)
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0

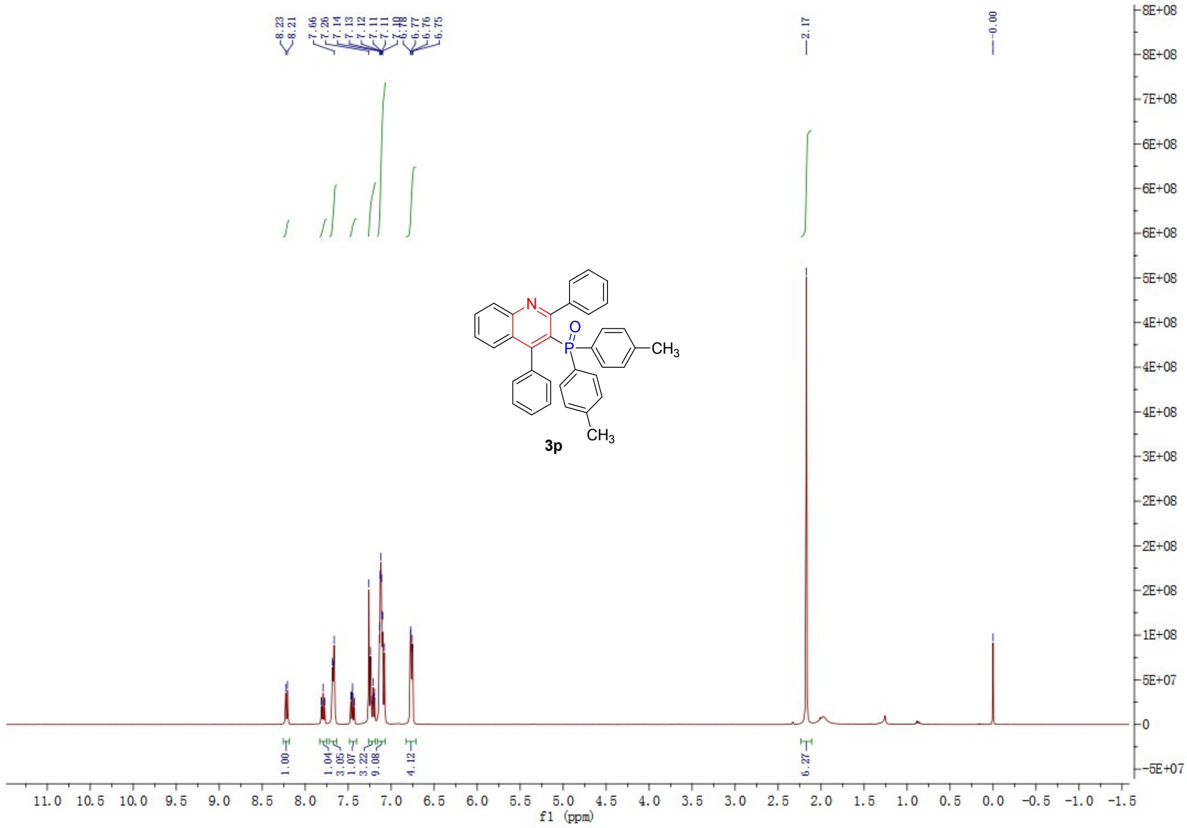


3o

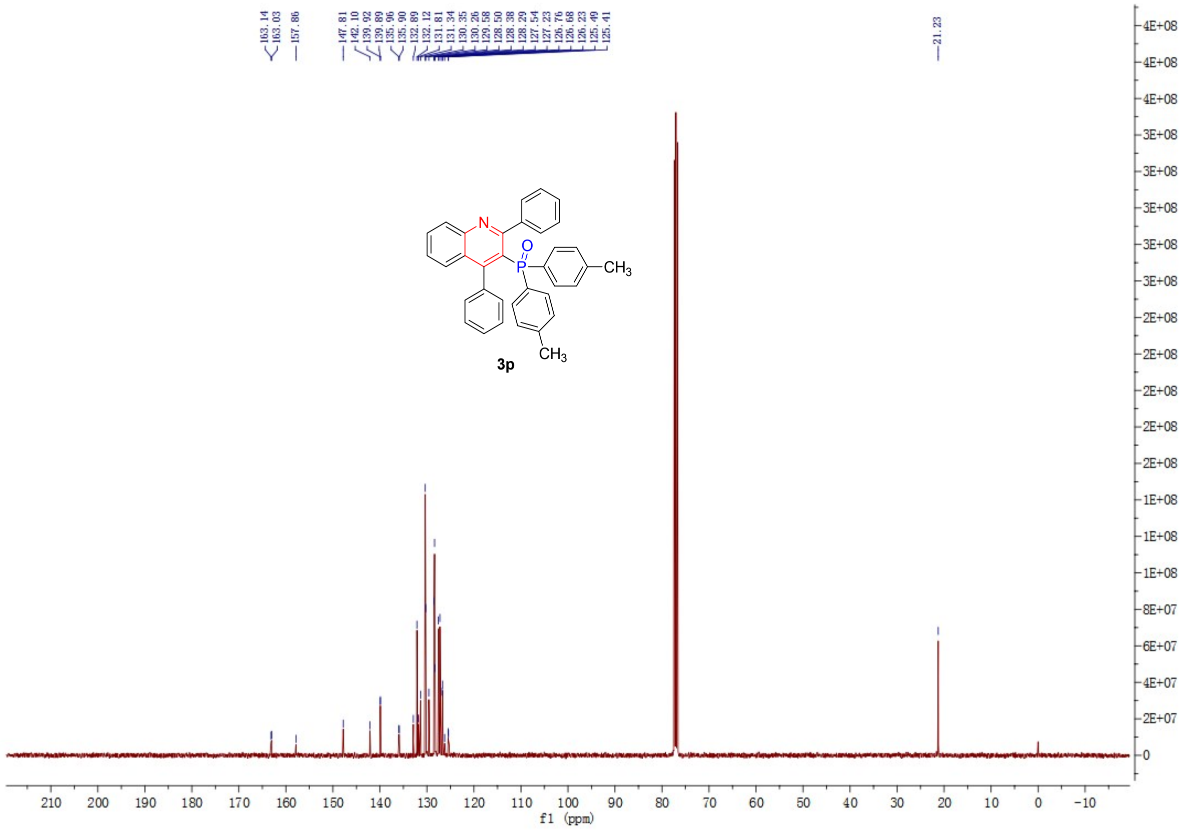
163.10
162.99
150.28
148.02
141.80
136.41
136.35
135.78
134.72
134.31
131.61
130.55
130.40
130.34
129.89
129.68
128.54
127.82
127.70
127.19
127.00
126.70
126.43
125.80
125.72
77.42
77.11
76.79
N
O
P
S
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
f1 (ppm)
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0

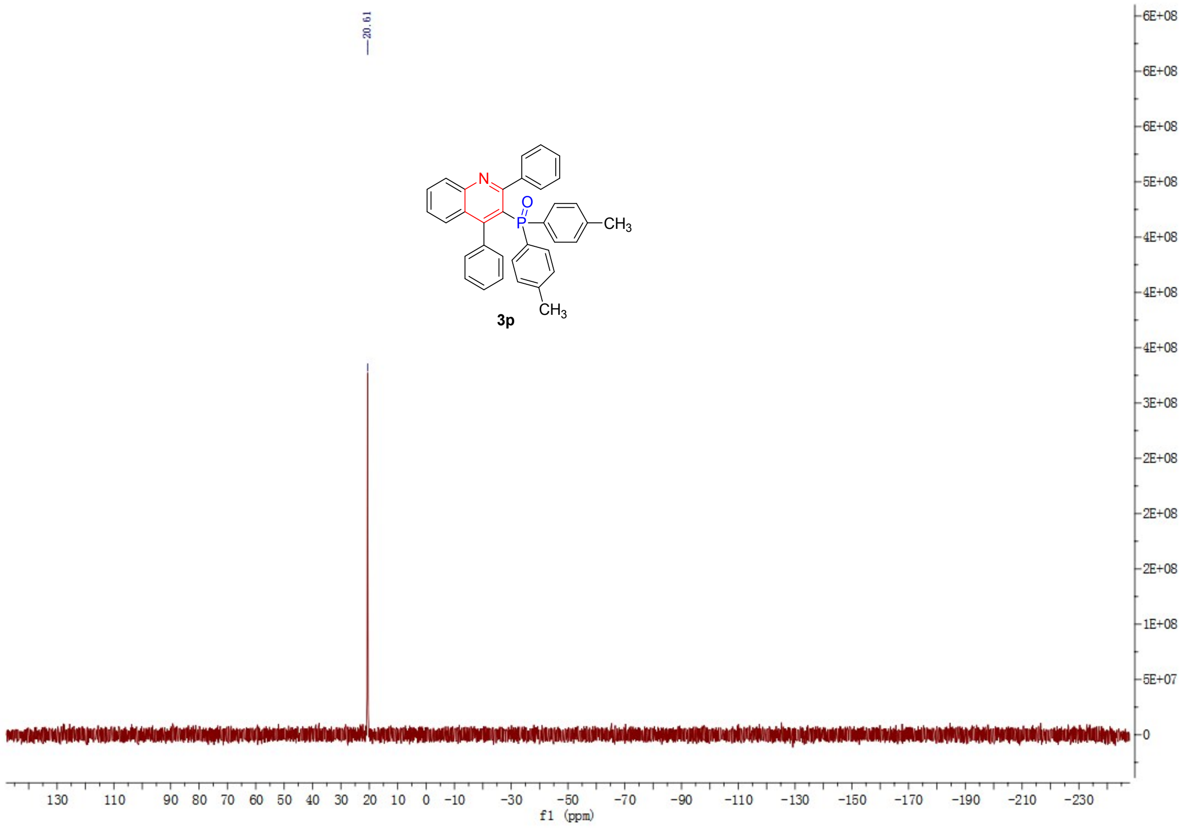

20.28
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)
N
O
P
S

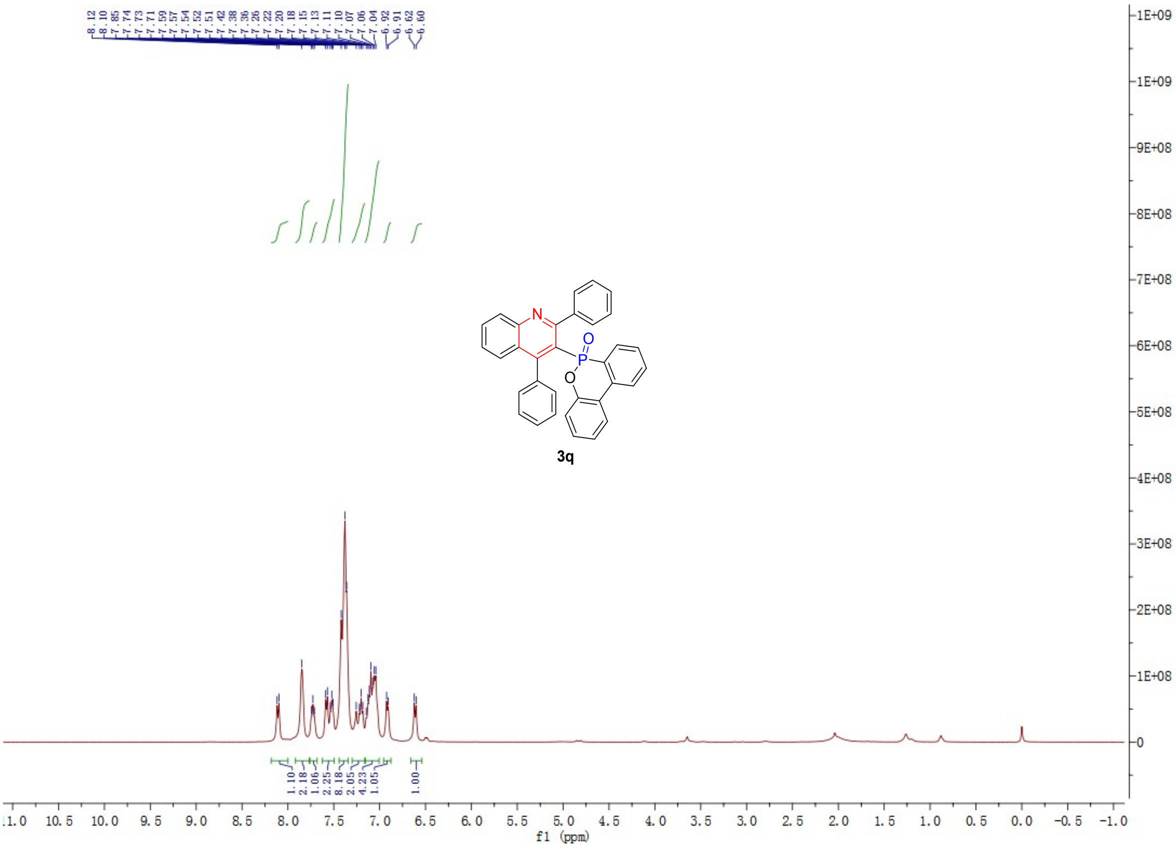
3o

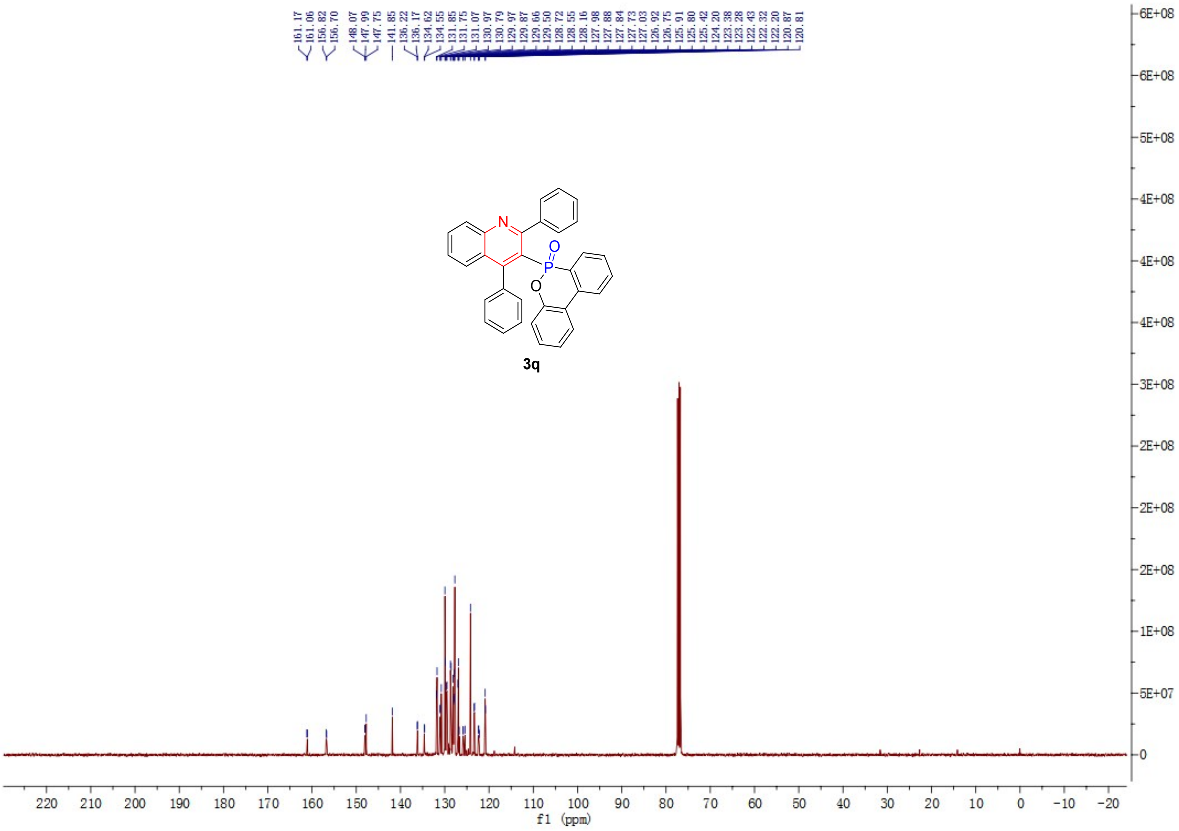

8.23
8.21
7.66
7.26
7.14
7.13
7.12
7.11
7.11
7.10
6.78
6.77
6.76
6.75
2.17
0.00
8E+08
8E+08
7E+08
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
1.00
1.04
3.05
1.07
3.22
9.08
4.12
6.27
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)
N
O
P
CH_3
CH_3

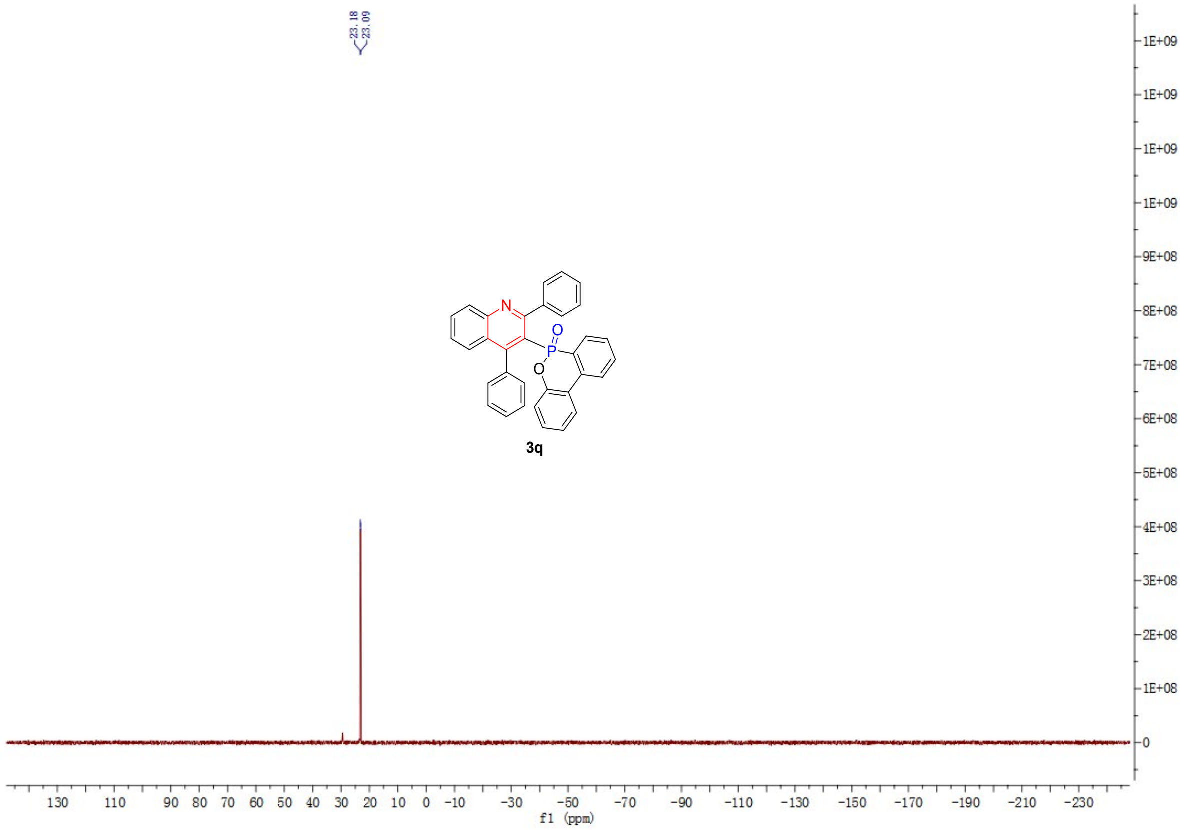
3p


163.14
163.03
157.86
147.81
142.10
139.92
139.89
135.96
135.90
132.89
132.12
131.81
131.34
130.35
130.26
129.58
128.50
128.38
128.29
127.54
127.23
126.76
126.68
126.23
125.49
125.41
21.23
N
O
P
CH3
CH3
3p
4E+08
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
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)

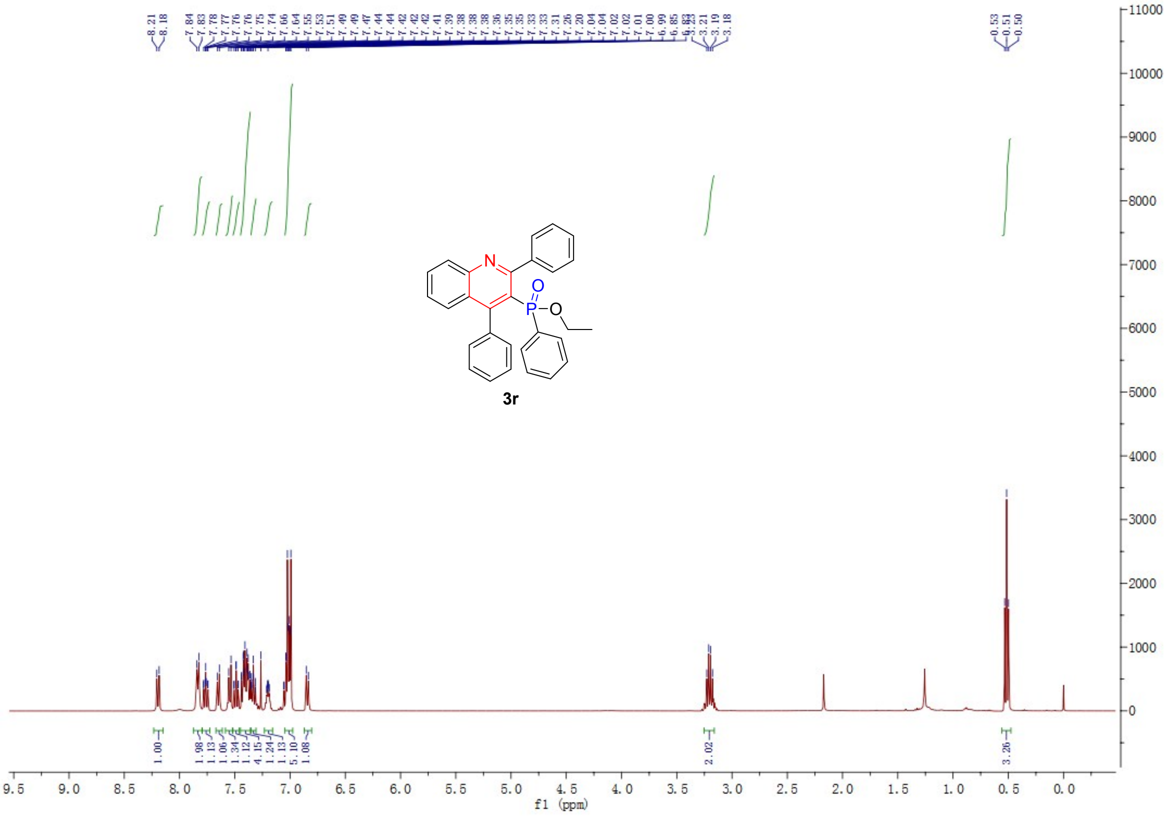

20.61
N
O
P
CH3
CH3
3p
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


8.12
8.10
7.85
7.74
7.73
7.71
7.59
7.57
7.54
7.52
7.51
7.42
7.38
7.36
7.26
7.22
7.20
7.18
7.15
7.13
7.11
7.10
7.07
7.06
7.04
6.92
6.91
6.62
6.60
N
P
O
O
3q
1.10
2.18
1.06
2.25
8.18
2.05
4.23
1.05
1.00
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
11.0
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
-0.5
-1.0
f1 (ppm)

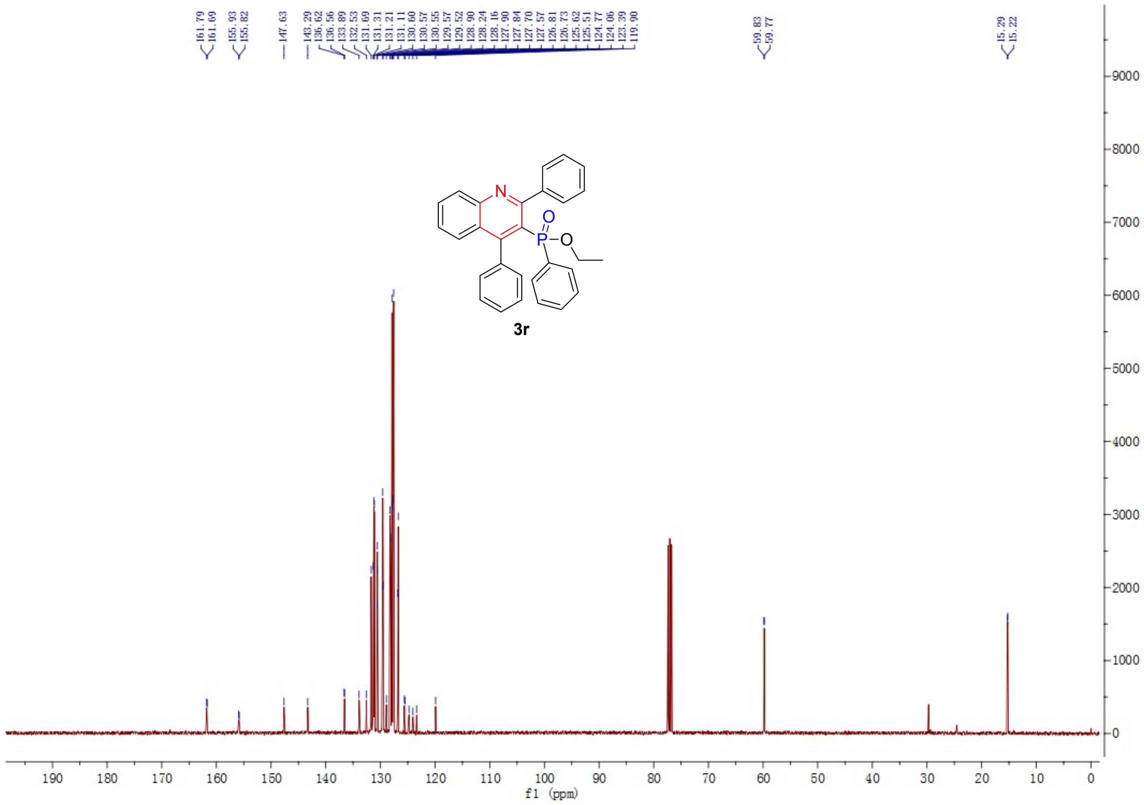

161.17
161.06
156.82
156.70
148.07
147.99
147.75
141.85
136.22
136.17
134.62
134.55
131.85
131.75
131.07
130.97
130.79
129.97
129.87
129.66
129.50
128.72
128.55
128.16
127.98
127.88
127.84
127.73
127.03
126.92
126.75
125.91
125.80
125.42
124.20
123.38
123.28
122.43
122.32
122.20
120.87
120.81
N
P
O
O
3q
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

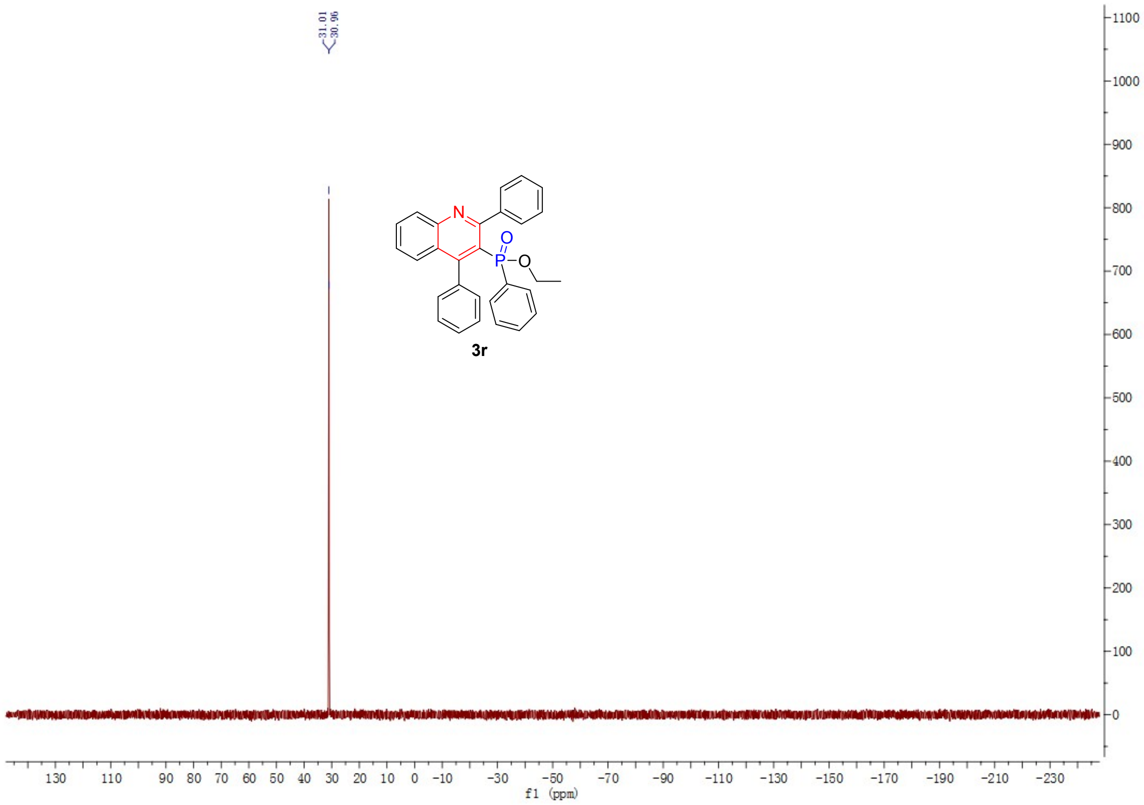

23.18
23.09
N
P
O
O
1E+09
1E+09
1E+09
1E+09
9E+08
8E+08
7E+08
6E+08
5E+08
4E+08
3E+08
2E+08
1E+08
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)

3q


8.21
8.18
7.84
7.83
7.78
7.77
7.76
7.76
7.75
7.74
7.66
7.64
7.55
7.53
7.51
7.49
7.49
7.47
7.44
7.44
7.42
7.42
7.42
7.41
7.39
7.38
7.38
7.38
7.36
7.35
7.35
7.33
7.33
7.31
7.26
7.20
7.04
7.04
7.02
7.02
7.01
7.00
6.99
6.85
6.83
3.23
3.21
3.19
3.18
0.53
0.51
0.50
N
P
O
O
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1.00
1.98
1.13
1.06
1.34
1.12
4.15
1.24
1.13
5.10
1.08
2.02
3.26
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)

3r


161.79
161.69
155.93
155.82
147.63
143.29
136.62
136.56
133.89
132.53
131.69
131.31
131.21
131.11
130.60
130.57
130.55
129.57
129.52
128.90
128.24
128.16
127.90
127.84
127.70
127.57
126.81
126.73
125.62
125.51
124.77
124.06
123.39
119.90
59.83
59.77
15.29
15.22
N
P
O
O
3r
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


31.01
30.96
N
P
O
O
3r
1100
1000
900
800
700
600
500
400
300
200
100
0
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230
f1 (ppm)