Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# Copper-Catalyzed Direct C-H Phosphorylation of N-iminoisoquinolinium ylides with H-Phosphonates

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# Supporting Information

## Contents

# Ⅰ General Methods:

Chemicals were either purchased or purified by standard techniques. $^{1}H$ NMR and $^{13}C$ NMR spectra were measured on a Bruker ADVANCE-500 spectrometer ($^{1}H$ at 500 MHz, $^{13}C$ at 125 MHz), using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as an internal standard at room temperature. Chemical shifts are given in $\delta$ relative to $CDCl_3$, the coupling constants J are given in hertz. High resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometry. All reactions under nitrogen atmosphere were conducted using standard Schlenk techniques. Melting points were measured on X-4 melting point apparatus (Beijing Tech. Instrument) and uncorrected. Infrared data was measured by infrared ($cm^{-1}$). Column chromatography was performed using EM Silica gel 60 (300-400 mesh).

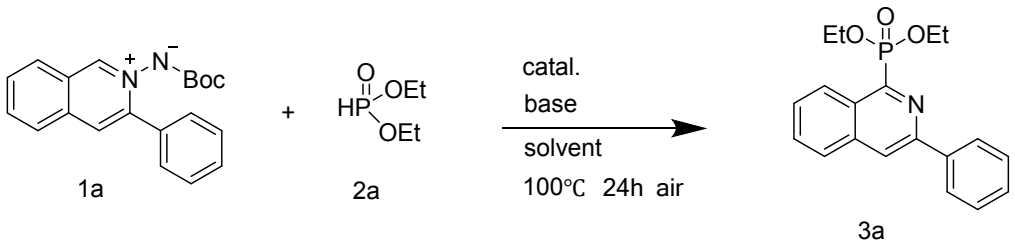
**Synthesis of N-iminoisoquinolinium ylides**. All the isoquinoline N-amides was prepared by previously reported procedure. [1]

# II Optimization of reaction conditions:

1) Synthesis of compounds **3**

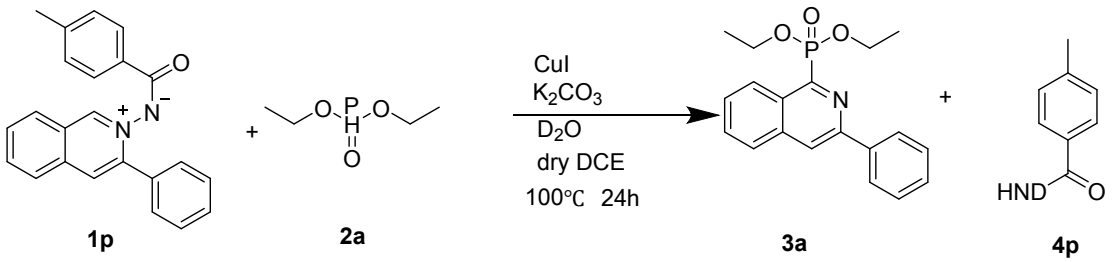
To an oven dried 10 mL vial was added (tert-butoxycarbonyl) (3-phenylisoquinolin-2-ium-2-yl) amide (**1a**, 0.1 mmol, 1.0 equiv) and diethyl phosphonate (**2a**, 0.2 mmol, 2.0 equiv) in 2 mL solvent, followed by addition of the catalyst (10 mol%) and base (0.2 mmol, 2.0 equiv), the reaction was stirred at 100 °C (oil bath temperature) for 24 h and then cooled to room temperature. The reaction mixture was concentrated under reduced pressure and the resulting residue was purified by flash chromatography (solvent degreaser / ethyl acetate = 5:1) to provide **3a**.

2) Control experiments

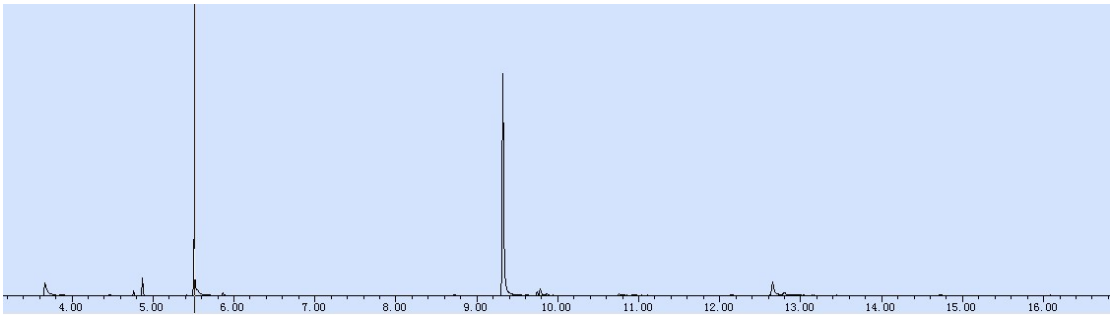


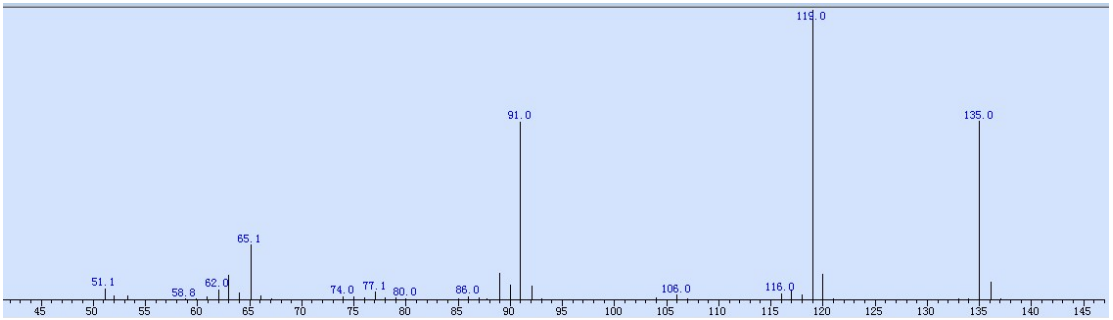

1a 2a 3a

To an oven dried 10 mL vial was added (4-methylbenzoyl) (3-phenylisoquinolin-2-ium-2-yl)amide (**1p**, 0.1 mmol, 1.0 equiv) and diethyl phosphonate (**2a**, 0.2 mmol, 2.0 equiv) in 2 mL solvent, followed by addition of the catalyst (10 mol%) and base (0.2 mmol, 2.0 equiv), the reaction was stirred at 100 °C (oil bath temperature) for 24 h and then cooled to room temperature. Then capture **4p** through GC-MS analysis.




**1p** **2a** **3a** **4p**



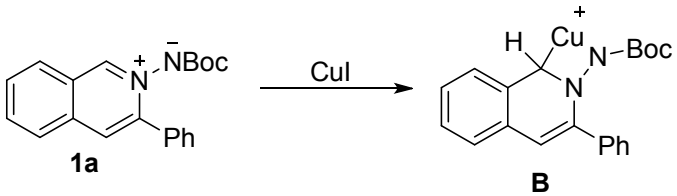




| Entry | m/z | Abundance | Entry | m/z | Abundance |
|---|---|---|---|---|---|
| 1 | 50.10 | 4.0 | 24 | 86.00 | 1.0 |
| 2 | 51.00 | 5.0 | 25 | 87.00 | 1.0 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 52.10 | 2.0 | 26 | 87.90 | 0.0 |
| 4 | 53.20 | 1.0 | 27 | 89.00 | 10.0 |
| 5 | 58.70 | 0.0 | 28 | 90.10 | 6.0 |
| 6 | 60.00 | 0.0 | 29 | 91.10 | 68.0 |
| 7 | 61.00 | 1.0 | 30 | 92.10 | 6.0 |
| 8 | 62.00 | 4.0 | 31 | 93.10 | 0.0 |
| 9 | 63.00 | 10.0 | 32 | 104.00 | 1.0 |
| 10 | 64.00 | 3.0 | 33 | 105.00 | 0.0 |
| 11 | 65.10 | 21.0 | 34 | 106.00 | 2.0 |
| 12 | 66.10 | 1.0 | 35 | 107.10 | 0.0 |
| 13 | 67.00 | 0.0 | 36 | 116.00 | 2.0 |
| 14 | 67.80 | 0.0 | 37 | 117.00 | 3.0 |
| 15 | 73.10 | 0.0 | 38 | 118.00 | 2.0 |
| 16 | 74.00 | 1.0 | 39 | 119.00 | 100.0 |
| 17 | 75.00 | 1.0 | 40 | 120.00 | 9.0 |
| 18 | 76.10 | 1.0 | 41 | 121.00 | 1.0 |
| 19 | 77.00 | 3.0 | 42 | 134.10 | 0.0 |
| 20 | 78.10 | 1.0 | 43 | 135.10 | 60.0 |
| 21 | 79.00 | 1.0 | 44 | 136.00 | 6.0 |
| 22 | 80.00 | 0.0 | 45 | 137.00 | 0.0 |
| 23 | 85.00 | 1.0 | | | |

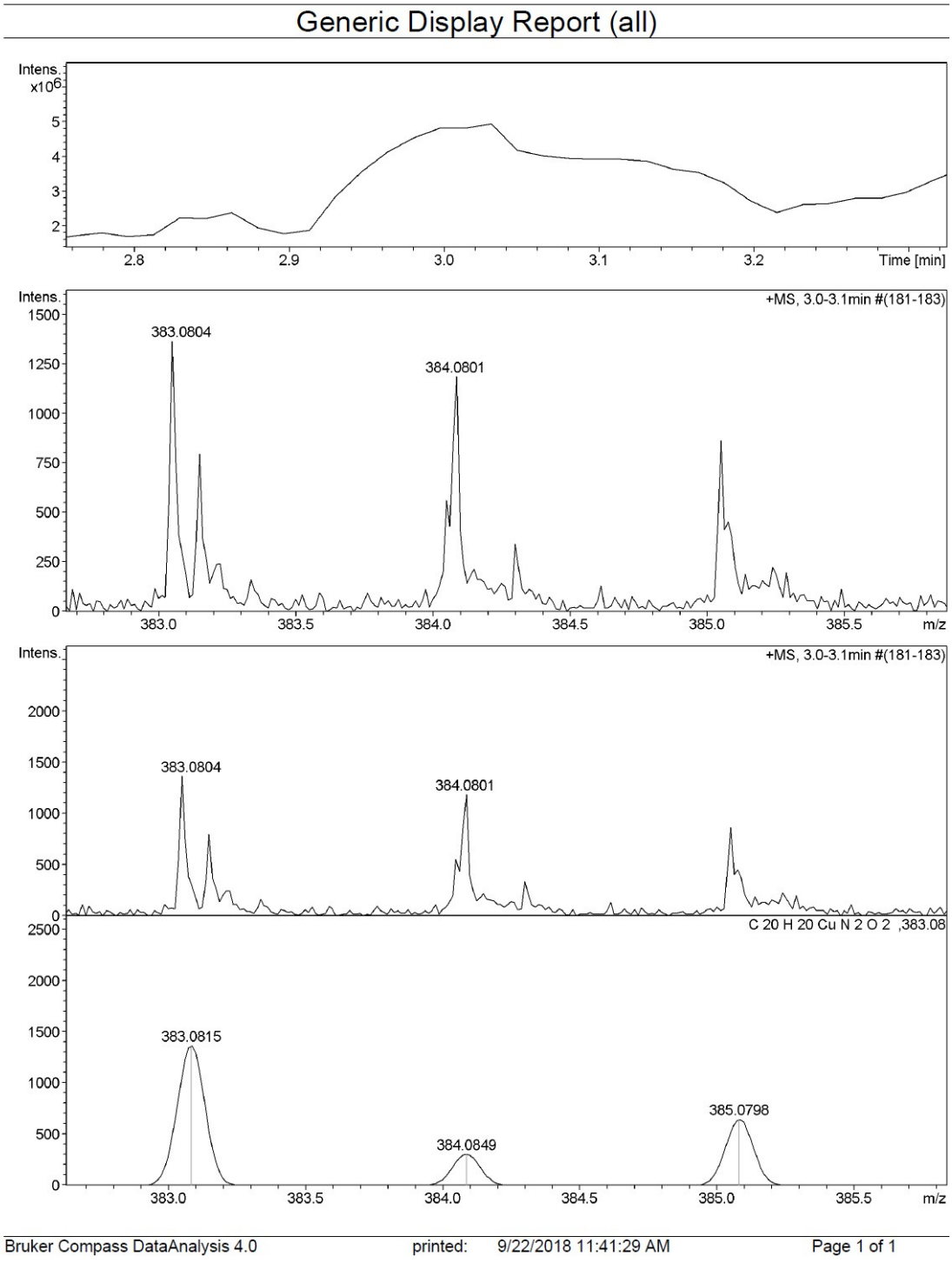
3) HRMS (ESI) studies on copper complex **B**

To an oven dried 10 mL vial was added (tert-butoxycarbonyl) (3-phenylisoquinolin-2-ium-2-yl) amide (**1a**, 0.1 mmol, 1.0 equiv) and diethyl phosphonate (**2a**, 0.2 mmol, 2.0 equiv) in 2 mL solvent, followed by addition of the catalyst (10 mol%) and base (0.2 mmol, 2.0 equiv), the reaction was stirred at 100 °C (oil bath temperature) for 1h. Then 0.01 mL of the solution was dilute from the vial, and subjected to run ESI analysis.



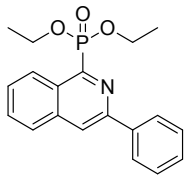

**1a** **B**

**HRMS (ESI) Calcd for $C_{20}H_{20}CuN_2O_2^+$ ($[B]^+$) 383.0804, Found: 383.0815.**



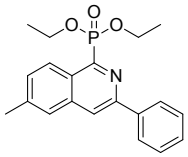

# Ⅲ Characterization of products:

***diethyl (3-phenylisoquinolin-1-yl)phosphonate*** **(3a)**[2]



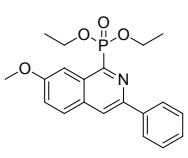
Yellow oil ( 28.0 mg, 82% yield ); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.92 (d, $J$ = 8.5 Hz, 1H), 8.14–8.16 (m, 3H), 7.86 (d, $J$ = 8.0 Hz, 1H), 7.66 (t, $J$ = 7.0 Hz, 1H), 7.66 (t, $J$ = 8.0 Hz, 1H), 7.49 (t, $J$ = 7.5 Hz, 2H), 7.40 (t, $J$ = 7.5 Hz, 1H), 4.37–4.43 (m, 4H), 1.42 (t, $J$ = 7.5 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 152.4 (d, $^{1}J_{c\text{-}p}$= 222.5 Hz), 149.8 (d, $^{3}J_{c\text{-}p}$ = 25.0 Hz), 138.7 (s), 137.1 (d, $^{3}J_{c\text{-}p}$ = 10.0 Hz), 130.6 (s), 128.9 (d, $^{3}J_{c\text{-}p}$ = 28.8 Hz), 128.8 (s), 128.8 (s), 128.1 (s), 127.7 (d, $^{4}J_{c\text{-}p}$ = 2.5 Hz), 127.1 (s), 126.9 (s), 119.2 (d, $^{3}J_{c\text{-}p}$ = 5.0 Hz), 63.5 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 16.5 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{19}H_{21}N_3OP^+$ ([M + H]$^+$) 342.1254, Found: 342.1254.

***diethyl (6-methyl-3-phenylisoquinolin-1-yl)phosphonate*** **(3b)**



Yellow oil (26.6 mg, 75% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.80 (d, $J$ = 9.0 Hz, 1H), 8.15 (d, $J$ = 8.5 Hz, 2H), 8.09 (s, 1H), 7.65 (s, 1H), 7.46–7.51 (m, 3H), 7.41 (t, $J$ = 8.0 Hz, 1H), 4.52–4.25 (m, 4H), 2.53 (s, 3H), 1.41 (t, $J$ = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 151.9 (d, $^{1}J_{c\text{-}p}$ = 225.0 Hz), 149.9 (d, $^{3}J_{c\text{-}p}$ = 25.0 Hz), 141.1 (s), 138.9 (s), 137.5 (d, $^{3}J_{c\text{-}p}$ = 11.3 Hz), 130.5 (s), 128.8 (s), 128.8 (s), 127.4 (d, $^{2}J_{c\text{-}p}$ = 30.0 Hz), 126.9 (s), 126.8 (s), 126.5 (d, $^{4}J_{c\text{-}p}$ = 2.5 Hz), 118.7 (d, $^{3}J_{c\text{-}p}$ = 3.8 Hz), 63.5 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 21.9 (s), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{23}NO_4P^+$ ([M + H]$^+$) 372.1359, Found: 372.1387.

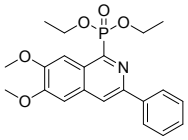
***diethyl (7-methoxy-3-phenylisoquinolin-1-yl)phosphonate*** **(3c)**



Yellow oil (23.7 mg, 64% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.16 – 8.10 (m, 3H), 7.77 (d, $J$ = 8.5 Hz, 1H), 7.48 (t, $J$ = 7.5 Hz, 2H), 7.39 (t, $J$ =7.5 Hz, 1H), 7.34 (d, $J$ = 9.0 Hz, 1H), 4.45–4.33 (m, 4H), 3.99 (s, 3H), 1.42 (t, $J$ = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 159.1 (s), 149.9 (d, $^{1}J_{c\text{-}p}$ = 222.5 Hz), 148.3 (d,

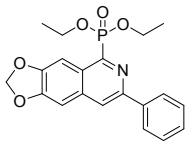
$^{3}J_{c\text{-}p}$ = 25.0 Hz), 138.8 (s), 132.9 (d, $^{3}J_{c\text{-}p}$ = 11.3 Hz), 130.5 (d, $^{2}J_{c\text{-}p}$ = 28.8 Hz), 129.2 (d, $^{4}J_{c\text{-}p}$= 3.8 Hz), 128.8 (s), 128.5 (s), 126.6 (s), 124.2 (s), 119.2 (d, $^{3}J_{c\text{-}p}$ = 5.0 Hz), 104.3 (s), 63.4 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 55.6 (s), 16.5 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{21}H_{25}NO_5P^+$ ([M + H]$^+$) 402.1465, Found: 402.1475.

***diethyl (6,7-dimethoxy-3-phenylisoquinolin-1-yl)phosphonate*** **(3d)**



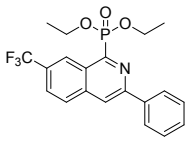
Yellow oil (22.5 mg, 56% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 8.04 (s, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.12 (s, 1H), 4.40–4.35(m, 4H), 4.08 (s, 3H), 4.01 (s, 3H), 1.41 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 153.15 (s), 150.9 (s), 148.8 (d, $^{3}J_{c\text{-}p}$ = 25.0 Hz), 148.8 (d, $^{1}J_{c\text{-}p}$ = 221.2 Hz), 139.0 (s), 134.3 (d, $^{3}J_{c\text{-}p}$ = 10.0 Hz), 128.7 (s), 128.4 (s), 126.5 (s), 125.8 (d, $^{2}J_{c\text{-}p}$ = 31.3 Hz), 118.0 (d, $^{3}J_{c\text{-}p}$ = 3.8 Hz), 105.3 (d, $^{4}J_{c\text{-}p}$ = 2.5 Hz), 105.1 (s), 63.4 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 56.1 (s), 56.0 (s), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{21}H_{25}NO_5P^+$ ([M + H]$^+$) 402.1465, Found: 402.1475.

***diethyl (7-phenyl-[1,3]dioxolo[4,5-g]isoquinolin-5-yl)phosphonate*** **(3e)**



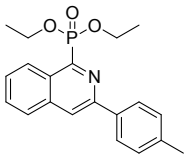
Yellow oil (34.1 mg, 92% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.26 (s, 1H), 8.10 (d, *J* = 7.5 Hz, 2H), 7.98 (d, *J* = 2.0 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.40 (t, *J* = 7.0 Hz, 1H), 7.10 (d, *J* = 2.0 Hz, 1H), 6.08 (s, 2H), 4.39–4.35 (m, 4H), 1.41 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 151.0 (s), 149.3 (s), 148.6 (d, $^{1}J_{c\text{-}p}$ = 222.5 Hz), 149.1 (s), 138.8 (s), 136.0 (d, $^{3}J_{c\text{-}p}$ = 11.3 Hz), 128.7 (s), 128.6 (s), 126.9 (d, $^{2}J_{c\text{-}p}$ = 28.8Hz), 126.6 (s), 118.9 (d, $^{4}J_{c\text{-}p}$ = 3.8 Hz), 103.1 (d, $^{3}J_{c\text{-}p}$ = 5.0 Hz), 101.9 (s), 63.4 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 29.7 (s), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{21}NO_5P^+$ ([M + H]$^+$) 386.1152, Found: 386.1168.

***diethyl (3-phenyl-7-(trifluoromethyl)isoquinolin-1-yl)phosphonate*** **(3f)**



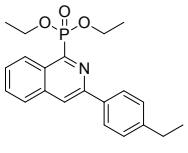
Yellow solid(17.2 mg, 42% yield); mp 110–112 °C; $^{1}$H NMR (500 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.24 (d, *J* = 1.5 Hz, 1H), 8.19 (d, *J* = 8.0 Hz, 2H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.5 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.0 Hz, 1H), 4.47–4.38 (m, 4H), 1.45 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 154.0 (d, $^{1}J_{c\text{-}p}$ = 222.5Hz), 151.9 (d, $^{3}J_{c\text{-}p}$ = 23.8 Hz), 138.3 (d, $^{3}J_{c\text{-}p}$ = 10.0 Hz), 138.0 (s), 129.5 (s), 129.5 (s), 129.0 (s), 128.9 (d, $^{3}J_{c\text{-}p}$ = 2.5 Hz), 127.6 (d, $^{2}J_{c\text{-}p}$ = 28.8 Hz), 127.1 (s), 126.3 (d, $^{4}J_{c\text{-}p}$ = 2.5Hz), 125.4–125.1 (m), 124.8 (s), 122.7 (s), 118.6 (s), 63.8 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{20}F_3NO_3P^+$ ([M + H]$^+$) 410.1127, Found: 410.1127

***diethyl (3-(p-tolyl)isoquinolin-1-yl)phosphonate*** **(3g)**



Yellow oil (30.2 mg, 85% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.91 (d, *J* = 8.5 Hz, 1H), 8.13 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.0 Hz, 1H), 7.64 (d, *J* = 7.5 Hz, 1H), 7.30 (d, *J* = 7.5 Hz, 2H), 4.59–4.22 (m, 4H), 2.41 (s, 3H), 1.41 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 152.3 (d, $^{1}J_{c\text{-}p}$ = 221.2 Hz), 150.0 (d, $^{3}J_{c\text{-}p}$ = 25.0 Hz), 138.8 (s), 137.1 (d, $^{3}J_{c\text{-}p}$ = 10.0 Hz), 136.0 (s), 130.5 (s), 129.6 (s), 128.8 (d, $^{2}J_{c\text{-}p}$ = 30.0 Hz), 127.9 (s), 127.6 (d, $^{4}J_{c\text{-}p}$ = 2.5 Hz), 127.1 (s), 126.8 (s), 118.7 (d, $^{3}J_{c\text{-}p}$ = 3.8 Hz), 63.5 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 21.2 (s), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{23}NO_3P^+$ ([M + H]$^+$) 356.1410, Found: 356.1426.

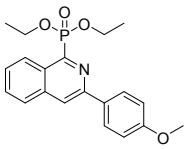
***diethyl (3-(4-ethylphenyl)isoquinolin-1-yl)phosphonate*** **(3h)**



Yellow oil (25.5 mg, 67% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.90 (d, *J* = 8.5 Hz, 1H), 8.17 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.70 (t, *J* = 7.0 Hz, 1H), 7.64 (t, *J* = 7.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 4.58–4.30 (m, 4H), 2.73 (q,

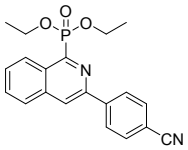
*J* = 7.5 Hz, 2H), 1.42 (t, *J* = 7.0 Hz, 6H), 1.30 (t, *J* = 8.0 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 152.3 (d, $^1J_{c\text{-}p}$ = 221.3 Hz), 150.0 (d, $^3J_{c\text{-}p}$ = 25.0 Hz), 145.2 (s), 137.1 (d, $^3J_{c\text{-}p}$ = 11.3 Hz), 136.2 (s), 130.6 (s), 128.8 (d, $^2J_{c\text{-}p}$ = 30.0 Hz), 128.4 (s), 128.0 (s), 127.6 (d, $^4J_{c\text{-}p}$ = 2.5 Hz), 127.1 (s), 126.9 (s), 118.8 (d, $^3J_{c\text{-}p}$ = 3.8 Hz), 63.5 (d, $^2J_{c\text{-}p}$ = 5.0 Hz), 28.7 (s), 16.4 (d, $^3J_{c\text{-}p}$ = 6.3 Hz), 15.5 (s); HRMS (ESI) Calcd for $C_{21}H_{25}NO_3P^+$ ([M + H]$^+$) 370.1567, Found: 370.1570.

***diethyl (3-(4-methoxyphenyl)isoquinolin-1-yl)phosphonate*** **(3i)**[2]



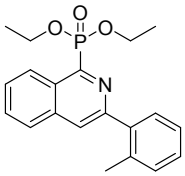
Yellow oil (34.1 mg, 92% yield); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.90 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 2H), 8.07 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.65 (t, *J* = 7.0 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 2H), 4.58–4.27 (m, 4H), 3.84 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 6H); $^{13}$C NMR (125MHz, $CDCl_3$) δ 160.4 (s), 152.2 (d, $^1J_{c\text{-}p}$ = 221.2 Hz), 149.7 (d, $^3J_{c\text{-}p}$ = 25.0 Hz), 137.2 (d, $^3J_{c\text{-}p}$ = 11.2 Hz), 131.3 (s), 130.5 (s), 128.6 (d, $^2J_{c\text{-}p}$ = 28.7 Hz), 128.1 (s), 127.7 (s), 127.5 (d, $^4J_{c\text{-}p}$ = 2.5 Hz), 127.0 (s), 118.0 (d, $^3J_{c\text{-}p}$ = 3.7 Hz), 114.2 (s), 63.4 (d, $^2J_{c\text{-}p}$ = 6.3 Hz), 55.3 (s), 16.4 (d, $^3J_{c\text{-}p}$ = 6.3 Hz).

**diethyl (3-(4-cyanophenyl)isoquinolin-1-yl)phosphonate (3j)**



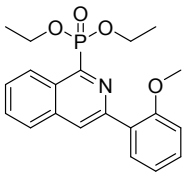
Yellow solid (7.7 mg, 21% yield); mp 137–140 $^o$C; $^1$H NMR (500 MHz, $CDCl_3$) δ 8.93 (d, *J* = 8.4 Hz, 1H), 8.48–8.18 (m, 3H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.81–7.74 (m, 3H), 7.73 (t, *J* = 7.5 Hz, 1H), 4.69–4.25 (m, 4H), 1.44 (t, *J* = 7.0 Hz, 6H).$^{13}$C NMR (125 MHz, $CDCl_3$) δ 153.13 (d, $^1J_{c\text{-}p}$ = 223.2 Hz), 147.57 (d, $^3J_{c\text{-}p}$ = 25.0 Hz), 142.88 (s), 136.83 (d, $^3J_{c\text{-}p}$ = 11.3 Hz), 132.63 (s), 131.12 (s), 129.27 (d, $^2J_{c\text{-}p}$ = 28.8 Hz), 129.07 (s), 127.93 (d, $^4J_{c\text{-}p}$ = 2.5 Hz), 127.33 (s), 127.27 (s), 120.41 (d, $^3J_{c\text{-}p}$ = 3.8 Hz), 118.80 (s), 112.26 (s), 63.53 (d, $^2J_{c\text{-}p}$ = 6.3 Hz), 16.46 (d, $^3J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{20}N_2O_3P^+$ ([M + H]$^+$) 367.1206, Found: 370.1570.

***diethyl (3-(o-tolyl)isoquinolin-1-yl)phosphonate*** **(3k)**



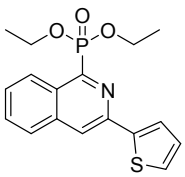
Yellow oil (16.0 mg, 45% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.24 (s, 1H), 8.19 (d, *J* = 7.5 Hz, 2H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.5 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.0 Hz, 1H), 4.47–4.38 (m, 4H), 1.45 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 154.0 (d, $^{1}J_{c\text{-}p}$ = 222.5 Hz), 151.9 (d, $^{3}J_{c\text{-}p}$ = 23.8 Hz), 138.3 (d, $^{3}J_{c\text{-}p}$ = 10.0 Hz), 138.0 (s), 129.5 (s), 129.0 (s), 128.9 (d, $^{3}J_{c\text{-}p}$ = 2.5 Hz), 127.6 (d, $^{2}J_{c\text{-}p}$ = 28.8 Hz), 127.1 (s), 126.3 (d, $^{3}J_{c\text{-}p}$ = 2.5 Hz), 125.3 (d, $^{3}J_{c\text{-}p}$ = 5.0 Hz), 124.8 (s), 122.7 (s), 118.6 (d, $^{4}J_{c\text{-}p}$ = 3.7 Hz), 63.8 (d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 29.7 (s), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{23}NO_3P^+$ ([M + H]$^+$) 356.1410, Found: 356.1417.

***diethyl (3-(2-methoxyphenyl)isoquinolin-1-yl)phosphonate*** **(3l)**



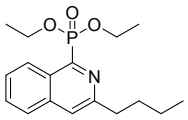
Yellow oil (19.3 mg, 52% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.91 (d, *J* = 8.5 Hz, 1H), 8.44 (s, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.71–7.56 (m, 2H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 4.63–4.22 (m, 4H), 3.87 (s, 3H), 1.39 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 157.4 (s), 151.8 (d, $^{1}J_{c\text{-}p}$ = 222.5 Hz), 147.9 (d, $^{3}J_{c\text{-}p}$ = 25.0 Hz), 136.6 (d, $^{3}J_{c\text{-}p}$ = 11.3 Hz), 131.5 (s), 130.3 (s), 129.8 (s), 128.5 (d, $^{2}J_{c\text{-}p}$ = 30.0 Hz), 128.1 (s), 128.0 (s), 127.9 (d, $^{4}J_{c\text{-}p}$= 2.5 Hz), 126.8 (s), 124.3 (d, $^{3}J_{c\text{-}p}$ = 3.8 Hz), 121.0 (s), 111.6 (s), 63.4 (d, $^{2}J_{c\text{-}p}$= 6.3 Hz), 55.6 (s), 16.4 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{20}H_{23}NO_4P^+$ ([M + H]$^+$) 372.1359, Found: 372.1386.

***diethyl (3-(thiophen-2-yl)isoquinolin-1-yl)phosphonate*** **(3m)**



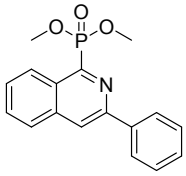
Black oil (25.6 mg, 65% yield); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.86 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 2.5 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.66–7.69 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 5.0 Hz, 1H), 7.14 (d, *J* = 4.5 Hz, 1H), 4.57–4.30 (m, 4H), 1.44 (t, *J* = 7.0 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 152.6 (d, $^1J_{c\text{-}p}$ = 220.0 Hz), 145.5 (d, $^3J_{c\text{-}p}$ = 25.0 Hz), 144.6 (s), 136.9 (d, $^3J_{c\text{-}p}$ = 10.0 Hz), 130.9 (s), 128.8 (d, $^2J_{c\text{-}p}$ = 28.8 Hz), 128.2 (s), 127.9 (s), 127.4 (d, $^4J_{c\text{-}p}$ = 2.5 Hz), 127.4 (s), 127.3 (s), 124.2 (s), 117.0 (d, $^3J_{c\text{-}p}$ = 3.8 Hz), 63.8 (d, $^2J_{c\text{-}p}$ = 6.3 Hz), 16.5 (d, $^3J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{17}H_{19}NO_3PS^+$ ([M + H]$^+$) 348.0818, Found: 348.0826.

***diethyl (3-butylisoquinolin-1-yl)phosphonate*** **(3n)**



Yellow oil (25.7 mg, 80% yield); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 7.0 Hz, 1H), 7.61–7.56 (m, 2H), 4.60–4.23 (m, 4H), 2.99 (t, *J* = 7.5 Hz, 2H), 2.00–1.56 (m, 2H), 1.42–1.38 (m, 8H), 0.95 (t, *J* = 7.5 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 154.9 (d, $^3J_{c\text{-}p}$ = 25.0 Hz), 151.8 (d, $^1J_{c\text{-}p}$ = 221.3 Hz), 136.8 (d, $^3J_{c\text{-}p}$ = 11.3 Hz), 130.2 (s), 128.3 (d, $^2J_{c\text{-}p}$ = 28.8 Hz), 127.3 (s), 126.9 (s), 126.8 (d, $^4J_{c\text{-}p}$ = 2.5 Hz), 121.2 (d, $^3J_{c\text{-}p}$ = 4.1 Hz), 63.2 (d, $^2J_{c\text{-}p}$ = 6.3 Hz), 37.4 (s), 31.8 (s), 22.3 (s), 16.3 (d, $^3J_{c\text{-}p}$ = 6.3 Hz), 13.9 (s); (ESI) Calcd for $C_{17}H_{24}NO_3P^+$ ([M + H]$^+$) 322.1567, Found: 322.1582.

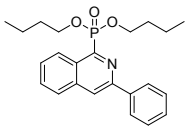
***dimethyl (3-phenylisoquinolin-1-yl)phosphonate*** **(3o)**



Yellow oil (23.2 mg, 74% yield); $^1$H NMR (500 MHz, $CDCl_3$) δ 8.86 (d, *J* = 8.0 Hz, 1H), 8.26–8.12 (m, 3H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.68 (t, *J* = 7.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.0 Hz, 2H), 7.42 (t, *J* = 7.0 Hz, 1H), 4.03 (s, 3H), 4.01 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 151.6 (d, $^1J_{c\text{-}p}$ = 222.5 Hz), 149.9 (d, $^3J_{c\text{-}p}$ = 25.0 Hz), 138.6 (s), 137.1 (d, $^3J_{c\text{-}p}$ = 11.3 Hz), 130.8 (s), 128.9 (s), 128.9 (s), 128.4 (d, $^2J_{c\text{-}p}$ = 30.0 Hz), 128.3 (s), 127.7 (d, $^4J_{c\text{-}p}$ = 2.5 Hz), 126.9 (s), 126.9 (s), 119.4 (d, $^3J_{c\text{-}p}$ =5.0

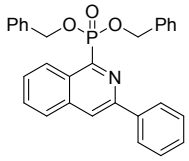
Hz), 54.1 (d, $^{2}J_{c\text{-}p}$ =6.3 Hz); HRMS (ESI) Calcd for $C_{17}H_{17}NO_3P^+$ ([M + H]$^+$) 314.0941, Found: 314.0936.

***dibutyl (3-phenylisoquinolin-1-yl)phosphonate*** **(3p)**



Yellow oil (34.6 mg, 87% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.92 (d, *J* = 8.5 Hz, 1H), 8.16–8.17 (m, 3H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 7.0 Hz, 1H), 7.64 (t, *J* = 8.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 4.49–4.15 (m, 4H), 2.04–1.62 (m, 4H), 1.45 (dq, *J* = 15.0, 7.5 Hz, 4H), 0.91 (t, *J* = 7.5 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 152.6 (d, $^{1}J_{c\text{-}p}$ = 221.3 Hz), 149.9 (d, $^{2}J_{c\text{-}p}$ = 23.8 Hz), 138.7 (s), 137.1 (d, $^{3}J_{c\text{-}p}$ = 11.3 Hz), 130.6 (s), 129.1 (s), 128.8 (s), 128.8 (s), 128.1 (s), 127.7 (d, $^{4}J_{c\text{-}p}$ = 2.5 Hz), 127.2 (s), 126.9 (s), 119.1 (d, $^{3}J_{c\text{-}p}$ = 3.8 Hz), 67.2(d, $^{2}J_{c\text{-}p}$ = 6.3 Hz), 32.6 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz), 18.8 (s), 13.6 (s); HRMS (ESI) Calcd for $C_{23}H_{29}NO_3P^+$ ([M + H]$^+$) 396.1880, Found: 398.1896.

***dibenzyl (3-phenylisoquinolin-1-yl)phosphonate*** **(3q)**



Yellow oil (39.1 mg, 84% yield); $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.89 (d, *J* = 8.5 Hz, 1H), 8.18 (s, 1H), 8.10 (d, *J* = 7.0 Hz, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 7.0 Hz, 1H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.0 Hz, 2H), 7.43–7.35 (m, 5H), 7.30–7.27 (m, 6H), 5.41–5.32 (m, 4H); $^{13}$C NMR (125 MHz, $CDCl_3$) δ 152.1 (d, $^{1}J_{c\text{-}p}$ = 225.5 Hz), 150.0 (d, $^{3}J_{c\text{-}p}$ = 25.0 Hz), 138.6 (s), 137.1 (d, $^{3}J_{c\text{-}p}$ = 10.8 Hz), 136.2 (d, $^{3}J_{c\text{-}p}$ = 6.6 Hz), 130.7 (s), 129.1 (s), 128.9 (s), 128.8 (s), 128.5 (s), 128.3 (s), 128.2 (s), 127.9 (s), 127.7 (d, $^{4}J_{c\text{-}p}$ = 2.5 Hz), 127.1 (s), 127.0 (s), 119.4 (d, $^{3}J_{c\text{-}p}$ = 3.8 Hz), 68.9 (d, $^{3}J_{c\text{-}p}$ = 6.3 Hz); HRMS (ESI) Calcd for $C_{29}H_{25}NO_3P^+$ ([M + H]$^+$) 466.1567, Found: 466.1576.

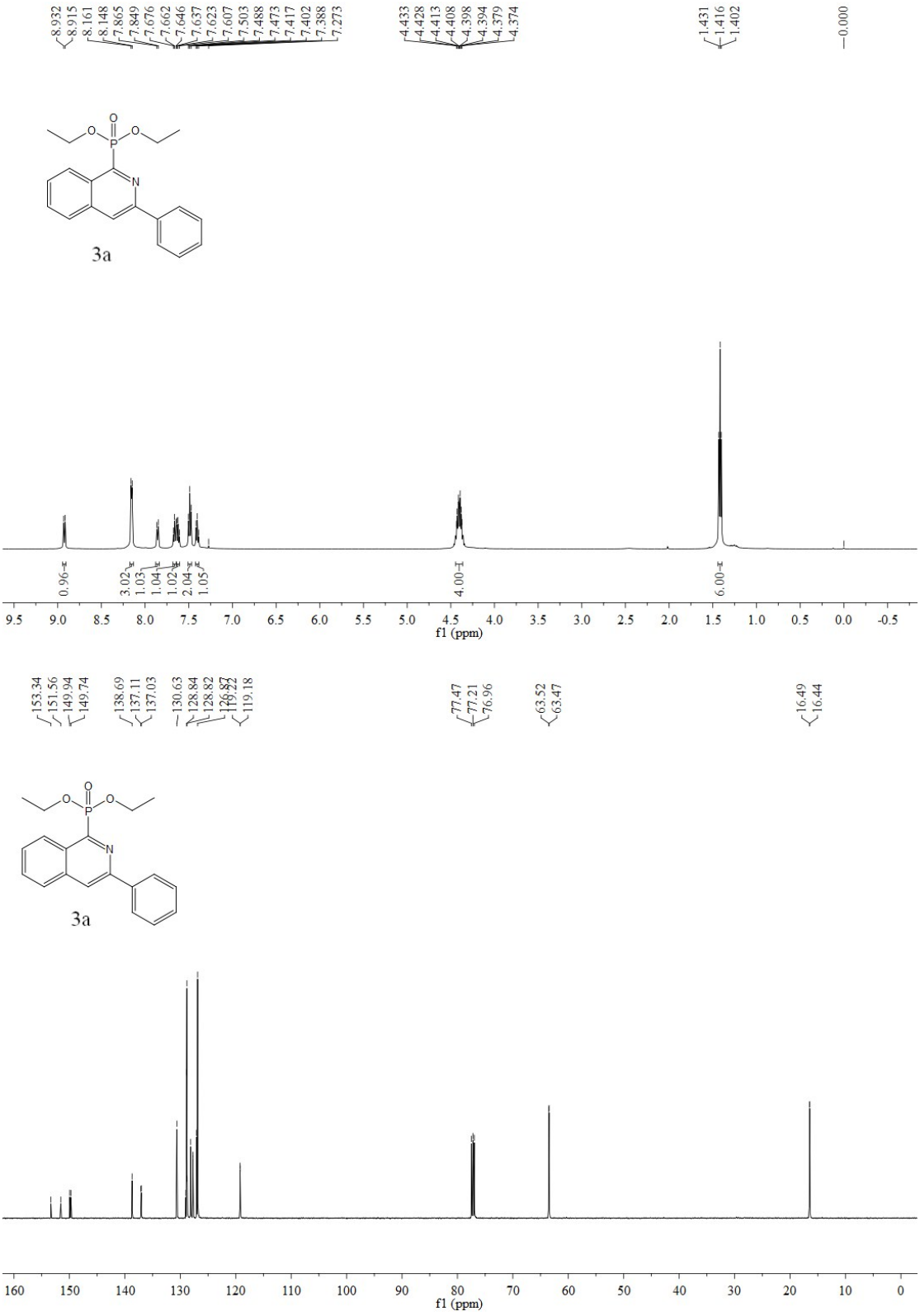
## Ⅳ References:

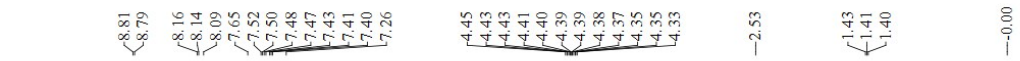
1. (a) V.-A. Peshkov, O.-P. Pereshivko, V.-H. Sofie, D.-S. Ermolat, V.-V. Erik,

*synthesis,*. 2011, **20**, 3371–3374. (b) Z. -L. Zhou, Y. -L. Liu, J. -L. Song and C. -L. Deng, *Synthesis.*, 2016, **48**, 2057-2064.

2. X.-X. Yu, Q.-P. Ding, Z.-Y Chen, J. Wu, *Tetrahedron Letters*,. 2009, **50** 4279–4282

# V $^{1}$H and $^{13}$C NMR Spectra:




8.81
8.79
8.16
8.14
8.09
7.65
7.52
7.50
7.48
7.47
7.43
7.41
7.40
7.26
4.45
4.43
4.43
4.41
4.40
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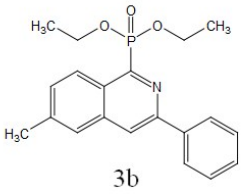
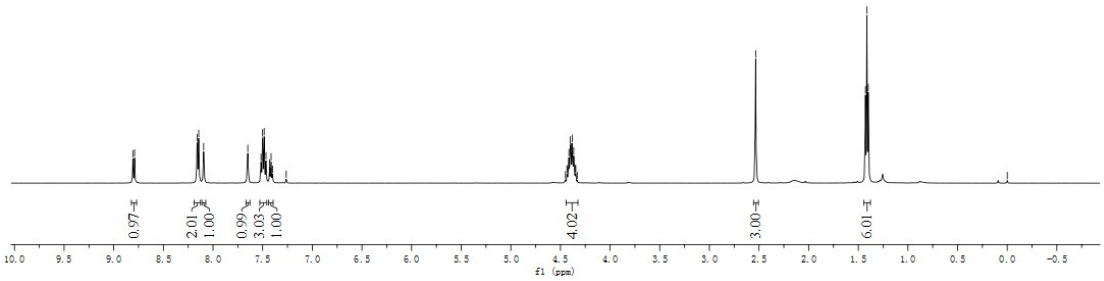
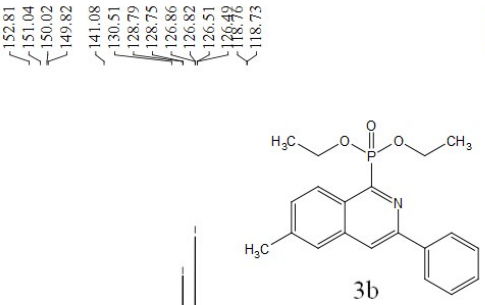
4.33
2.53
1.43
1.41
1.40
0.00


H3C
O
P
O
CH3
N
H3C

3b


0.97
2.01
1.00
0.99
3.03
1.00
4.02
3.00
6.01
f1 (ppm)


152.81
151.04
150.02
149.82
141.08
130.51
128.79
128.75
126.86
126.82
126.51
118.76
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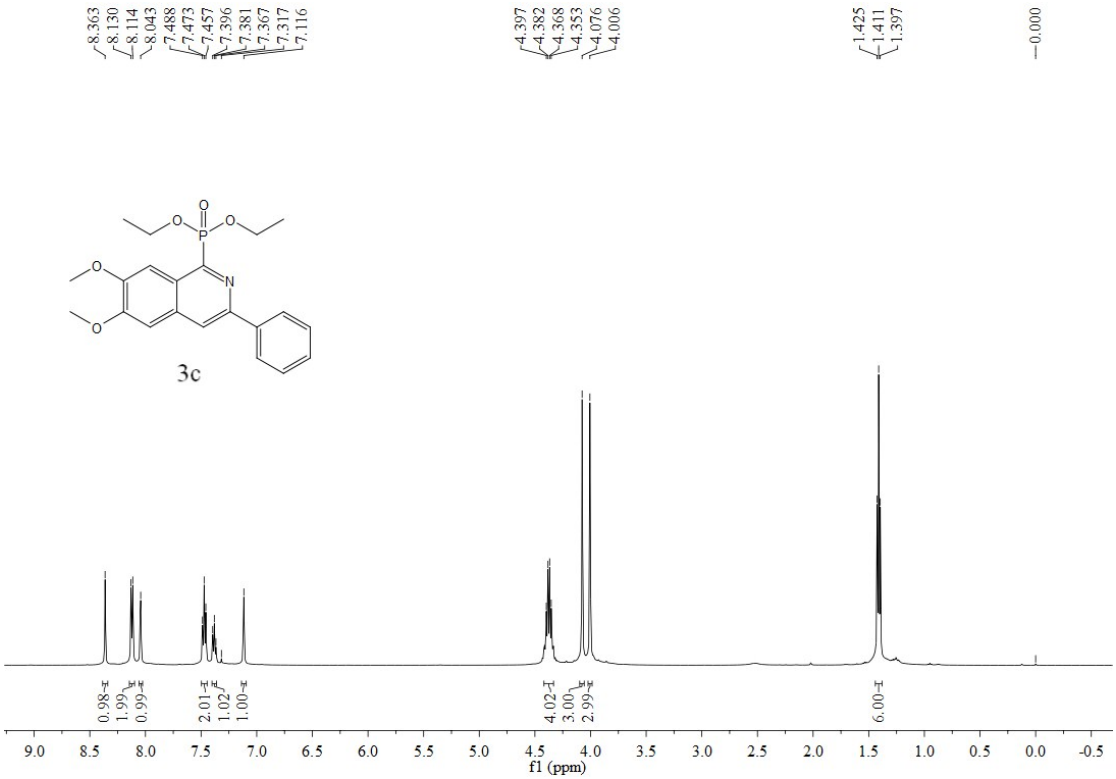
77.35
77.10
76.85
63.49
63.44
21.92
16.47
16.42
H3C
O
P
O
CH3
N
H3C
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3b


8.363
8.130
8.114
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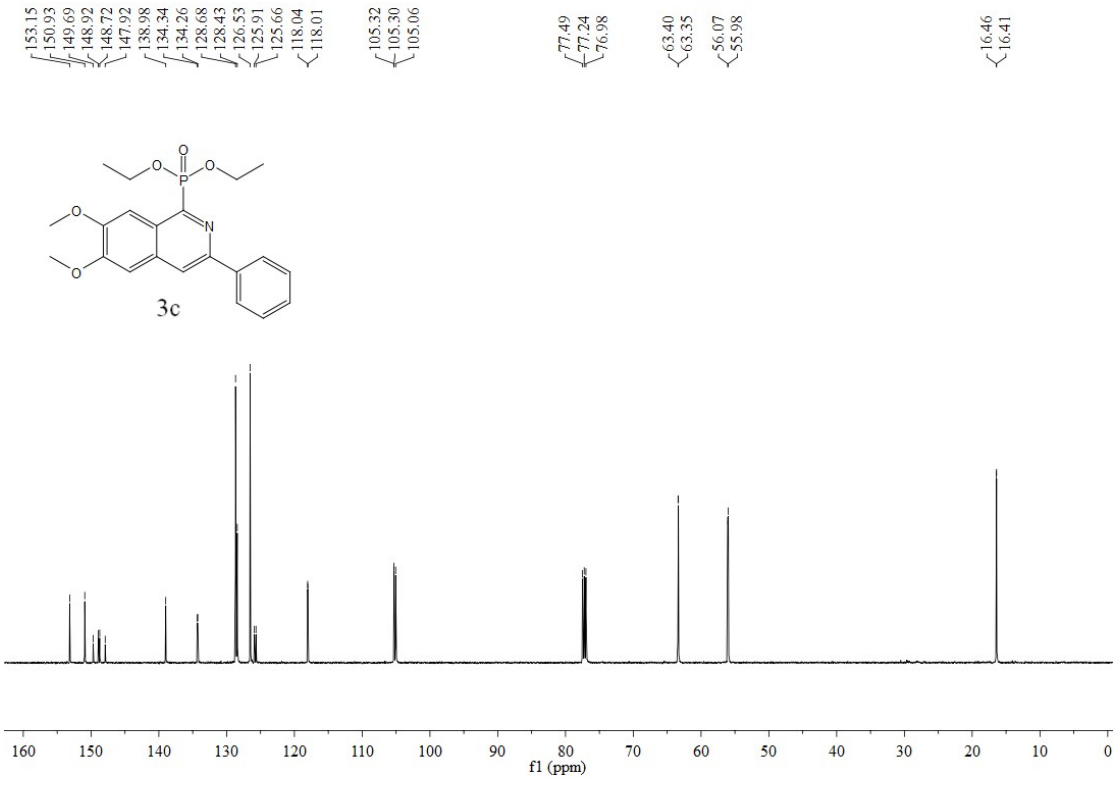
7.488
7.473
7.457
7.396
7.381
7.367
7.317
7.116
4.397
4.382
4.368
4.353
4.076
4.006
1.425
1.411
1.397
0.000
3c
0.98
1.99
0.99
2.01
1.02
1.00
4.02
3.00
2.99
6.00
f1 (ppm)


153.15
150.93
149.69
148.92
148.72
147.92
138.98
134.34
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128.68
128.43
126.53
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125.66
118.04
118.01
105.32
105.30
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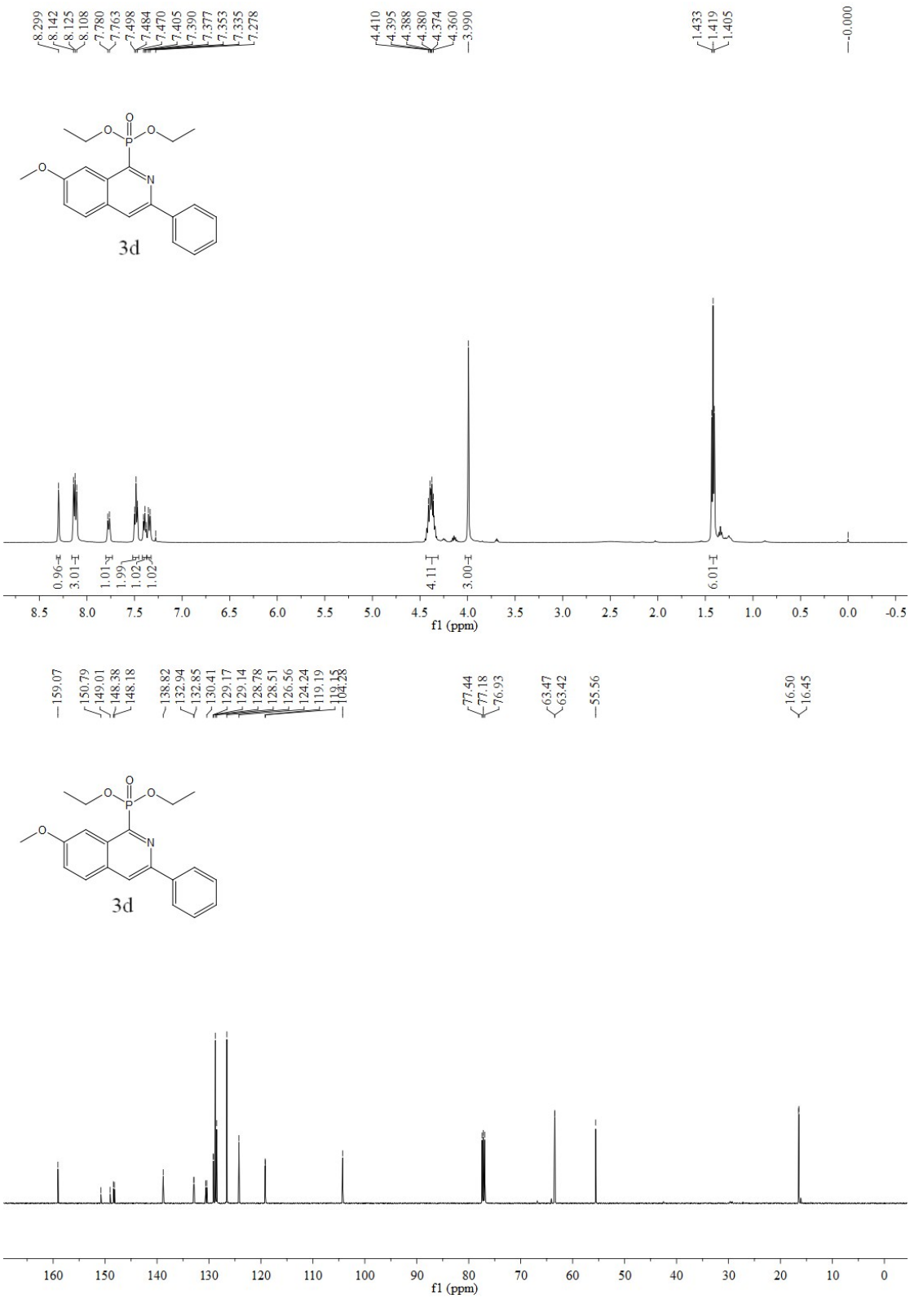
55.98
16.46
16.41
3c
f1 (ppm)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8.108
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7.484
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7.405
7.390
7.377
7.353
7.335
7.278
4.410
4.395
4.388
4.380
4.374
4.360
3.990
1.433
1.419
1.405
0.000
3d
0.96
3.01
1.01
1.99
1.02
1.02
4.11
3.00
6.01
f1 (ppm)
159.07
150.79
149.01
148.38
148.18
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55.56
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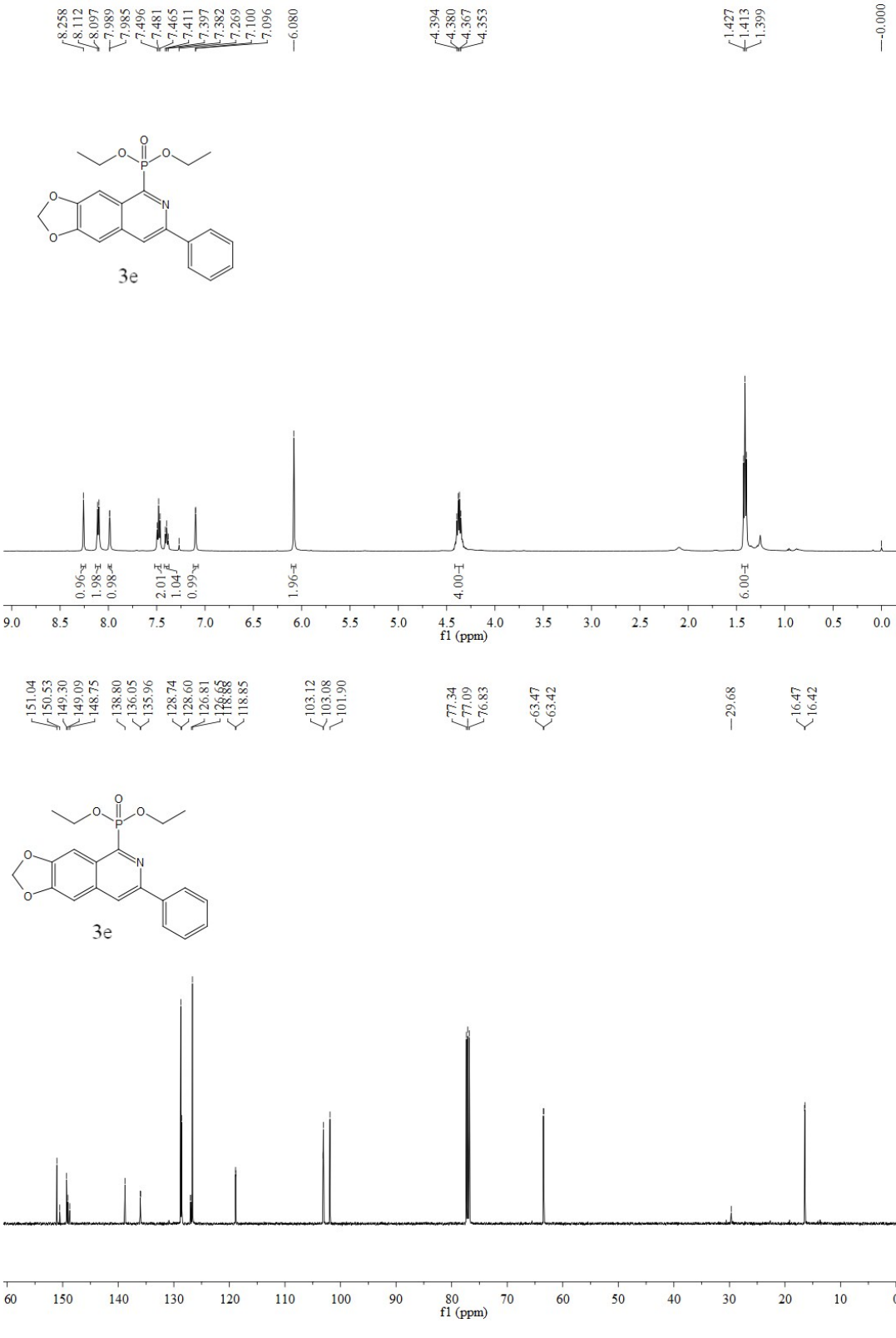
16.45
3d
f1 (ppm)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8.112
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7.496
7.481
7.465
7.411
7.397
7.382
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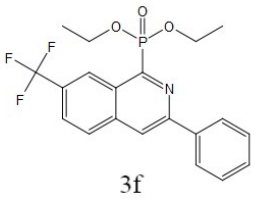
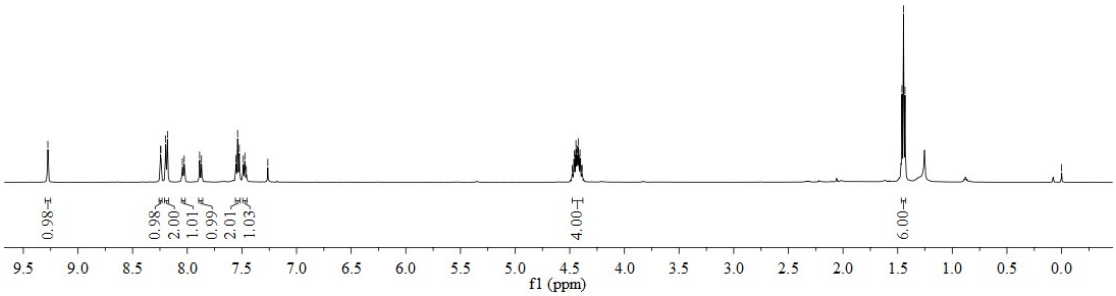
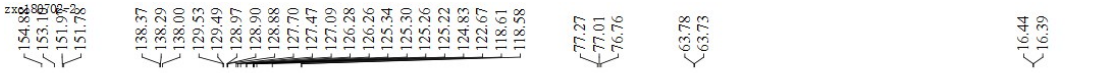
7.100
7.096
6.080
4.394
4.380
4.367
4.353
1.427
1.413
1.399
0.000
3e
0.96
1.98
0.98
2.01
1.04
0.99
1.96
4.00
6.00
f1 (ppm)
151.04
150.53
149.30
149.09
148.75
138.80
136.05
135.96
128.74
128.60
126.81
118.88
118.85
103.12
103.08
101.90
77.34
77.09
76.83
63.47
63.42
29.68
16.47
16.42
3e
f1 (ppm)

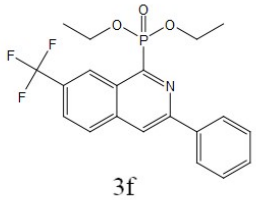

zxc180702-2
9.276
8.244
8.241
8.197
8.181
8.044
8.028
7.887
7.870
7.554
7.539
7.524
7.487
7.473
7.460
7.263
4.478
4.472
4.463
4.458
4.449
4.443
4.435
4.429
4.421
4.415
4.407
4.401
4.392
4.386
1.461
1.447
1.433
0.000


O
O
O
P
F
F
F
N

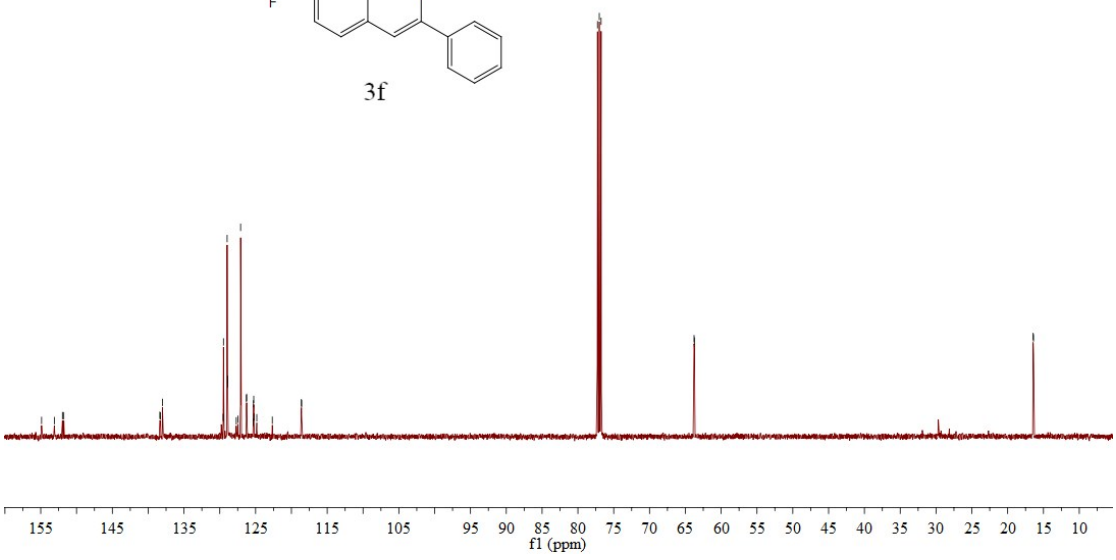
3f

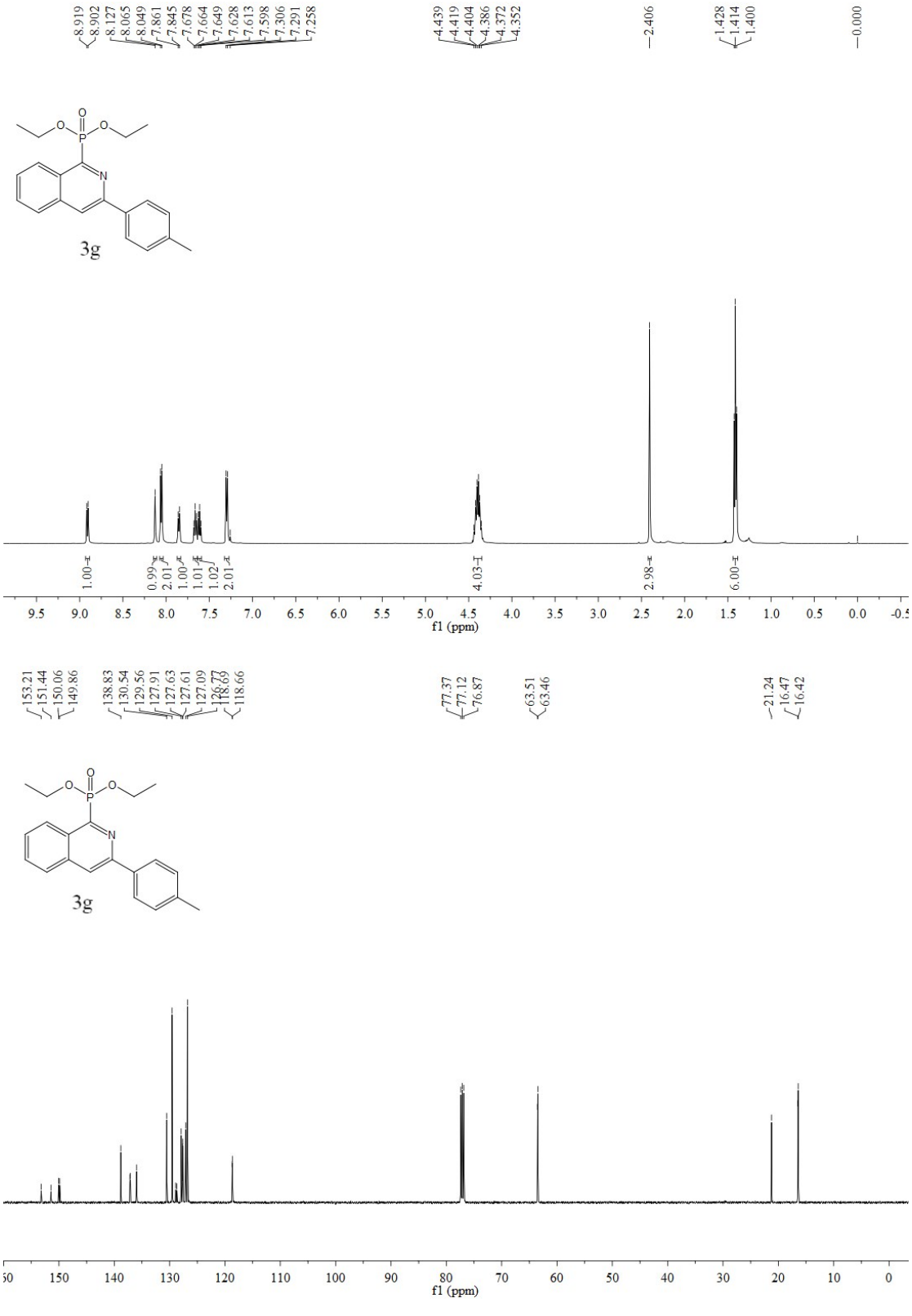

0.98
0.98
2.00
1.01
0.99
2.01
1.03
4.00
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

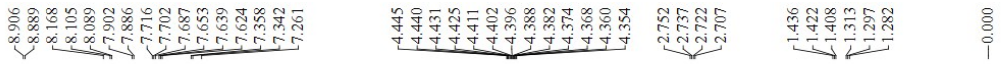

zxc180702-2
154.88
153.11
151.98
151.78
138.37
138.29
138.00
129.53
129.49
128.97
128.90
128.88
127.70
127.47
127.09
126.28
126.26
125.34
125.30
125.26
125.22
124.83
122.67
118.61
118.58
77.27
77.01
76.76
63.78
63.73
16.44
16.39

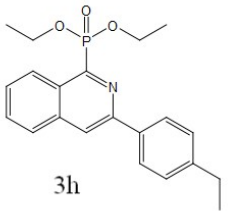

O
O
O
P
F
F
F
N

3f

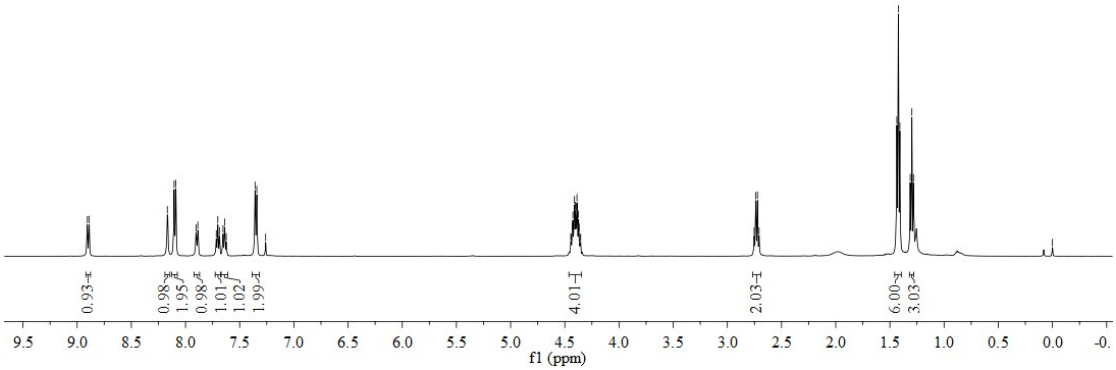

155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)


8.919
8.902
8.127
8.065
8.049
7.861
7.845
7.678
7.664
7.649
7.628
7.613
7.598
7.306
7.291
7.258
4.439
4.419
4.404
4.386
4.372
4.352
2.406
1.428
1.414
1.400
0.000
3g
1.00
0.99
2.01
1.00
1.01
1.02
2.01
4.03
2.98
6.00
f1 (ppm)
153.21
151.44
150.06
149.86
138.83
130.54
129.56
127.91
127.63
127.61
127.09
126.77
118.63
118.66
77.37
77.12
76.87
63.51
63.46
21.24
16.47
16.42
3g
f1 (ppm)

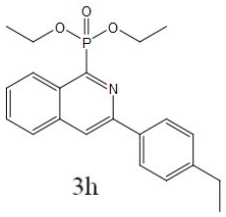

8.906
8.889
8.168
8.105
8.089
7.902
7.886
7.716
7.702
7.687
7.653
7.639
7.624
7.358
7.342
7.261
4.445
4.440
4.431
4.425
4.411
4.402
4.396
4.388
4.382
4.374
4.368
4.360
4.354
2.752
2.737
2.722
2.707
1.436
1.422
1.408
1.313
1.297
1.282
0.000


O
O
O
P
N

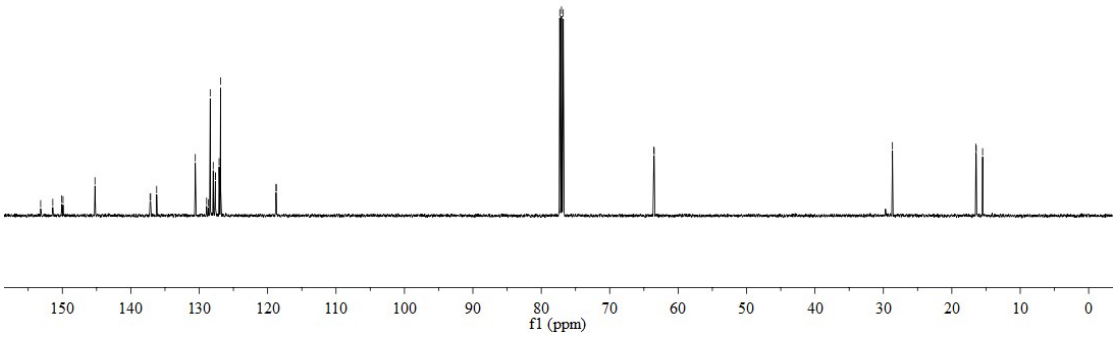
3h

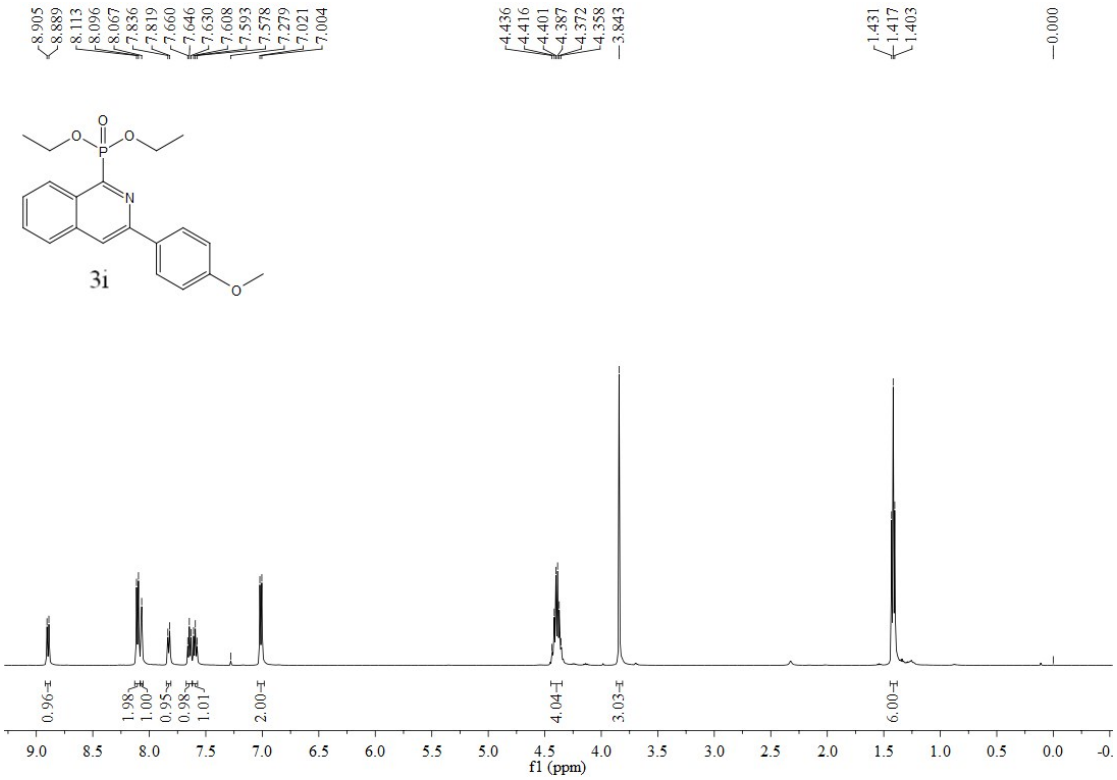

0.93
0.98
1.95
0.98
1.01
1.02
1.99
4.01
2.03
6.00
3.03
f1 (ppm)

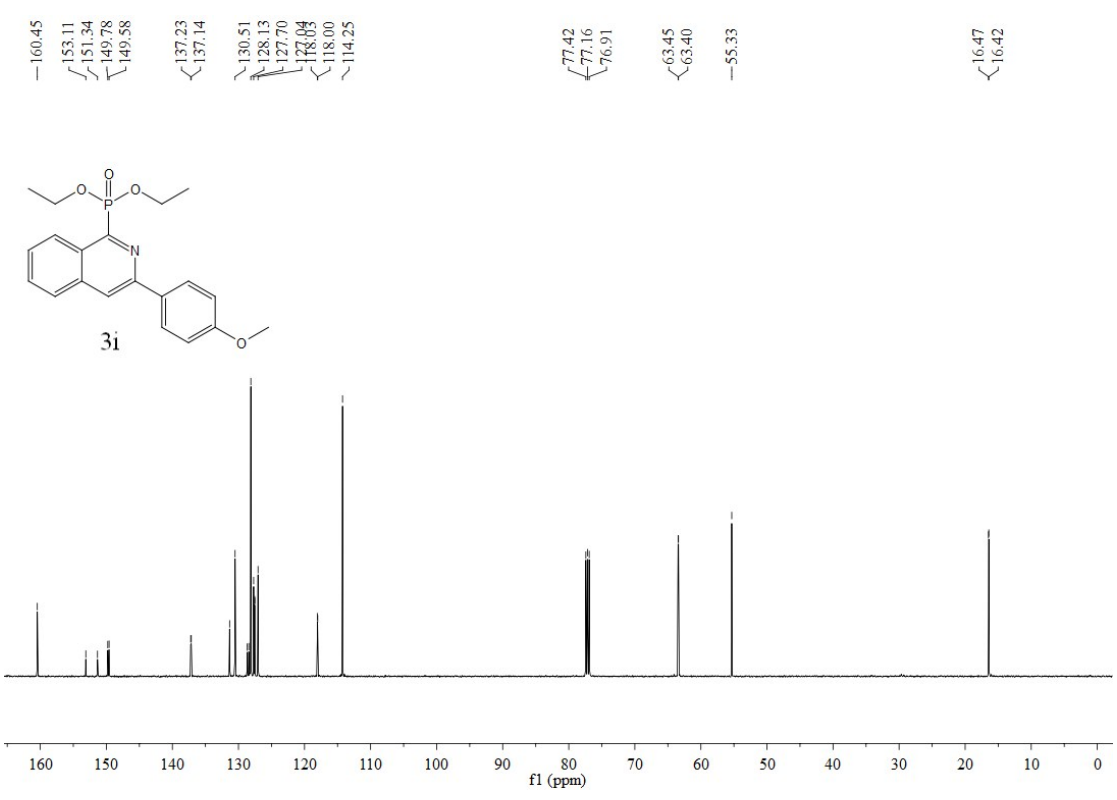

153.17
151.40
150.10
149.90
145.23
137.19
137.10
136.22
130.57
128.39
127.09
118.73
77.30
77.05
76.79
63.55
63.49
28.68
16.48
16.43
15.50

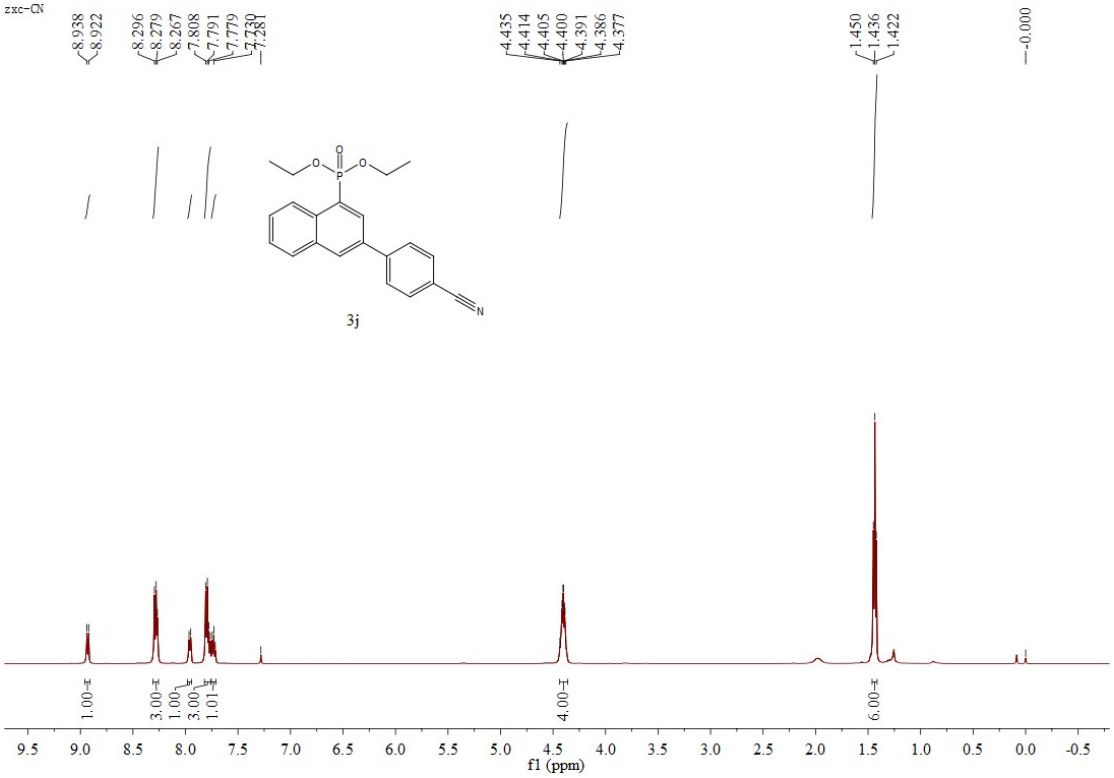

O
O
O
P
N

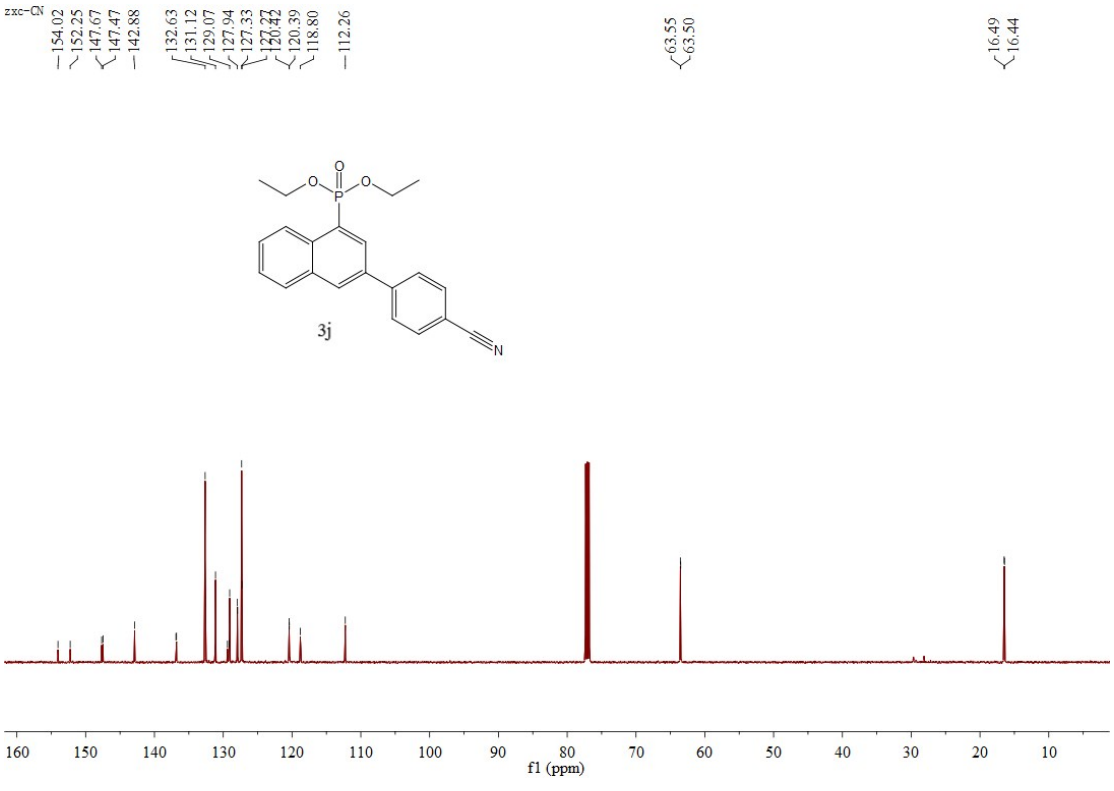
3h

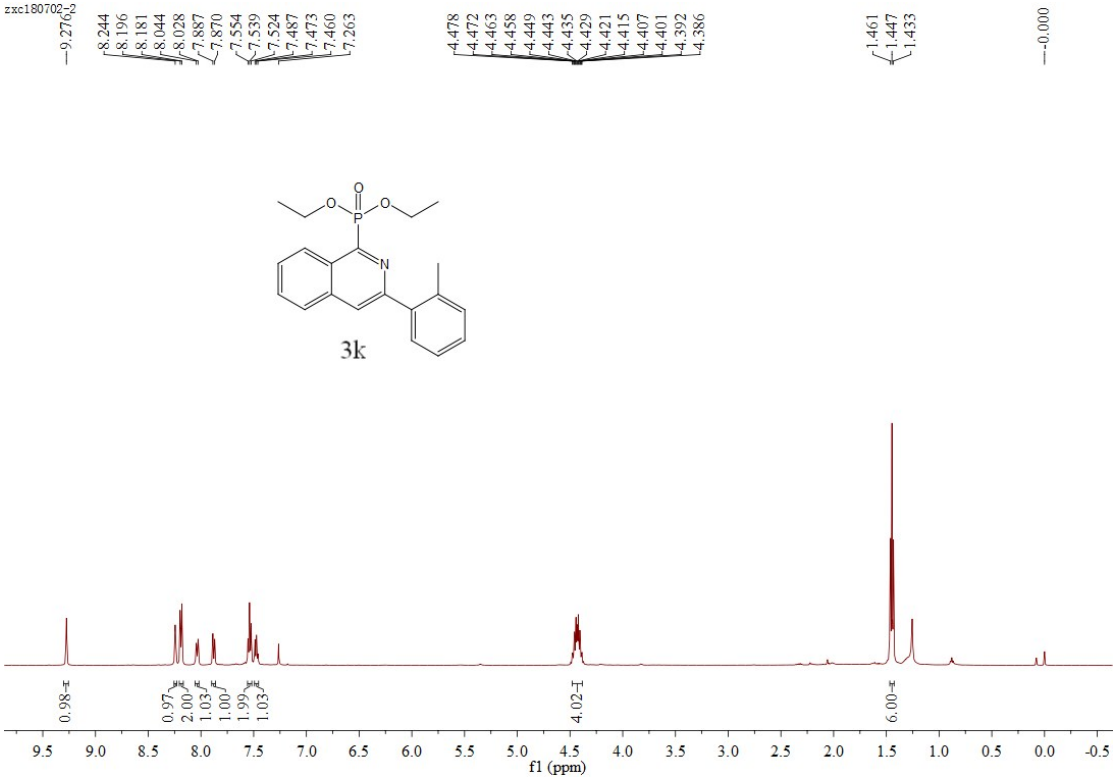

f1 (ppm)

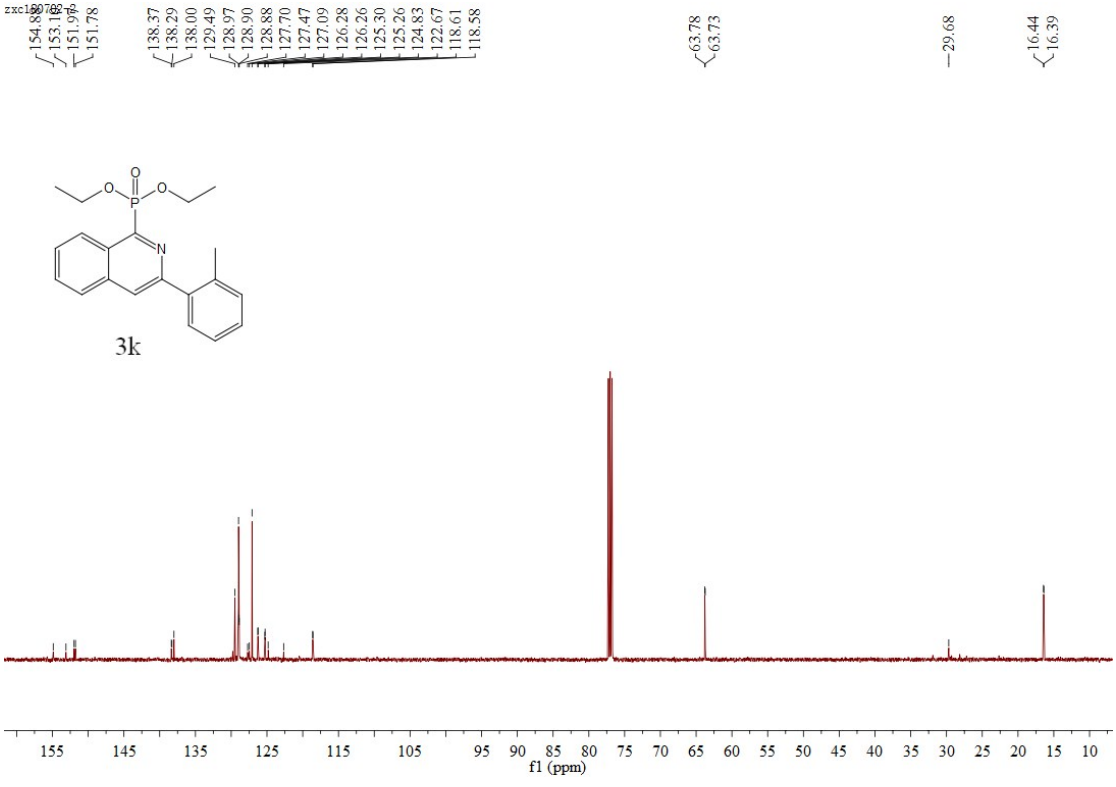

8.905
8.889
8.113
8.096
8.067
7.836
7.819
7.660
7.646
7.630
7.608
7.593
7.578
7.279
7.021
7.004
4.436
4.416
4.401
4.387
4.372
4.358
3.843
1.431
1.417
1.403
0.000
3i
0.96
1.98
1.00
0.95
0.98
1.01
2.00
4.04
3.03
6.00
f1 (ppm)

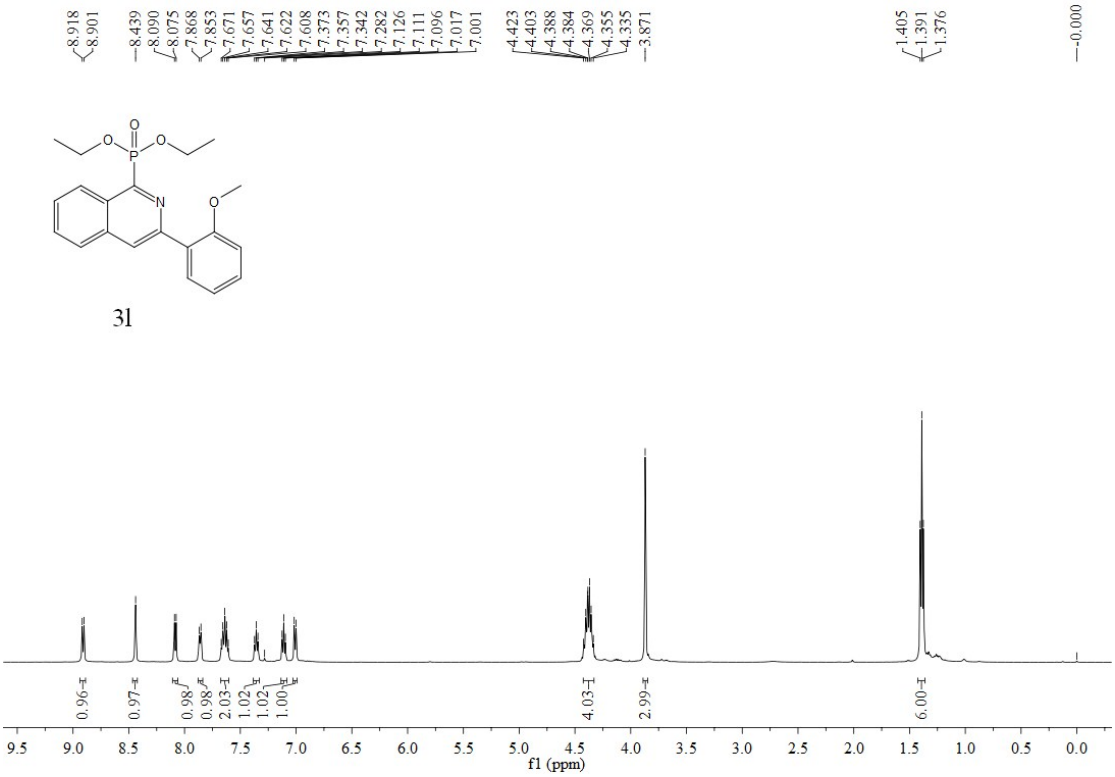

160.45
153.11
151.34
149.78
149.58
137.23
137.14
130.51
128.13
127.70
118.03
118.00
114.25
77.42
77.16
76.91
63.45
63.40
55.33
16.47
16.42
3i
f1 (ppm)


zxc-CN
8.938
8.922
8.296
8.279
8.267
7.808
7.791
7.779
7.730
7.281
4.435
4.414
4.405
4.400
4.391
4.386
4.377
1.450
1.436
1.422
-0.000
3j
1.00
3.00
1.00
3.00
1.01
4.00
6.00
f1 (ppm)

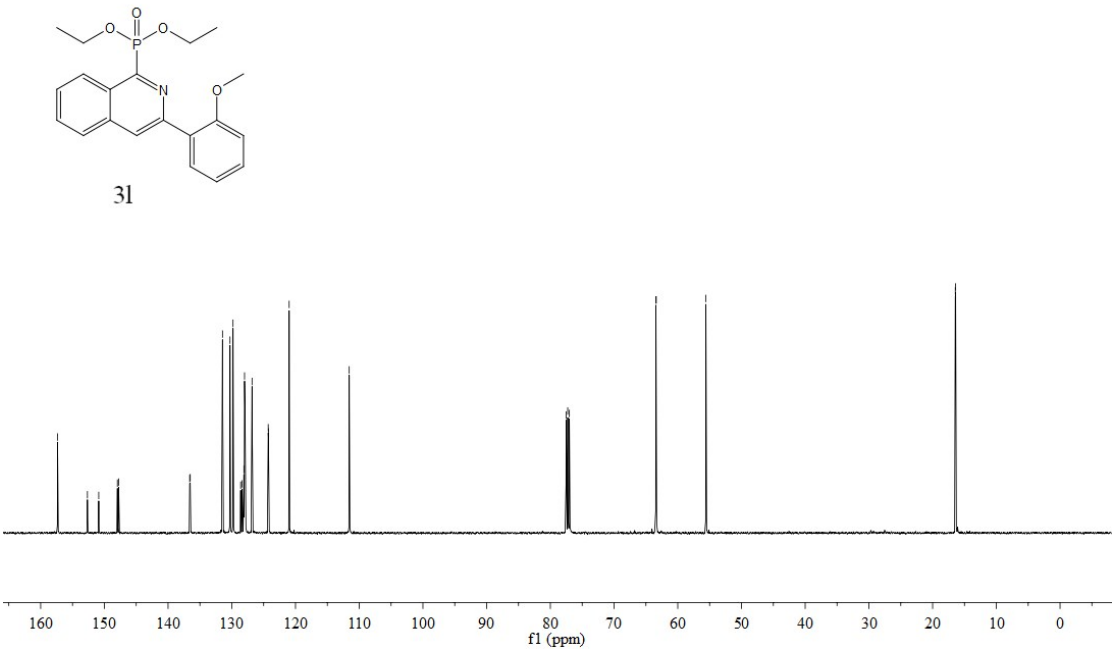

zxc-CN
154.02
152.25
147.67
147.47
142.88
132.63
131.12
129.07
127.94
127.33
120.42
120.39
118.80
112.26
63.55
63.50
16.49
16.44
3j
f1 (ppm)


zxc180702-2
9.276
8.244
8.196
8.181
8.044
8.028
7.887
7.870
7.554
7.539
7.524
7.487
7.473
7.460
7.263
4.478
4.472
4.463
4.458
4.449
4.443
4.435
4.429
4.421
4.415
4.407
4.401
4.392
4.386
1.461
1.447
1.433
0.000
3k
0.98
0.97
2.00
1.03
1.00
1.99
1.03
4.02
6.00
f1 (ppm)


154.88
153.11
151.99
151.78
138.37
138.29
138.00
129.49
128.97
128.90
128.88
127.70
127.47
127.09
126.28
126.26
125.30
125.26
124.83
122.67
118.61
118.58
63.78
63.73
29.68
16.44
16.39
3k
f1 (ppm)

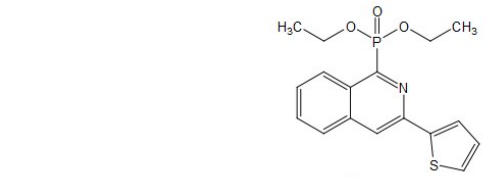

8.918
8.901
8.439
8.090
8.075
7.868
7.853
7.671
7.657
7.641
7.622
7.608
7.373
7.357
7.342
7.282
7.126
7.111
7.096
7.017
7.001
4.423
4.403
4.388
4.384
4.369
4.355
4.335
3.871
1.405
1.391
1.376
-0.000
0.96
0.97
0.98
0.98
2.03
1.02
1.00
4.03
2.99
6.00
f1 (ppm)

31

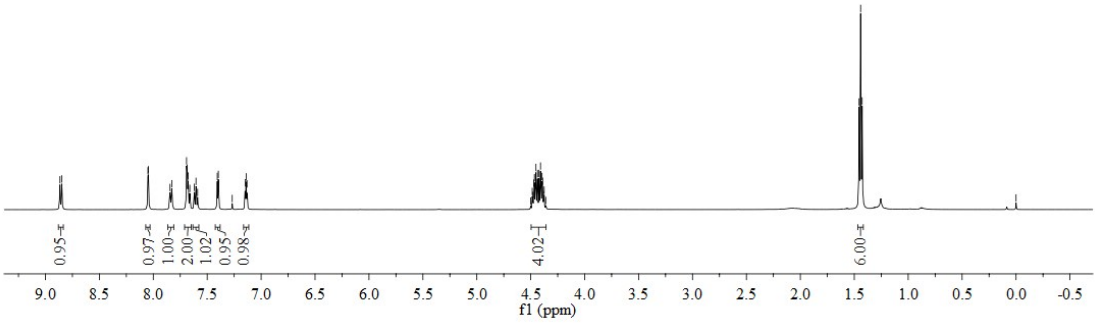

157.35
152.66
150.88
147.96
147.76
131.46
130.28
129.81
128.00
127.92
127.90
126.82
124.28
124.25
77.53
77.27
77.02
63.43
63.38
55.59
16.44
16.39
f1 (ppm)

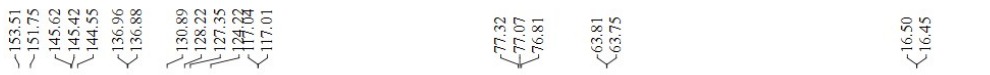
31

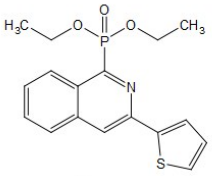

8.865
8.848
8.050
8.045
7.845
7.828
7.692
7.686
7.677
7.661
7.619
7.604
7.589
7.407
7.397
7.148
7.139
4.500
4.486
4.480
4.472
4.466
4.457
4.452
4.437
4.423
4.409
4.404
4.395
4.389
4.381
4.375
4.361
1.455
1.441
1.427
0.000


H3C
O
P
O
CH3
N
S

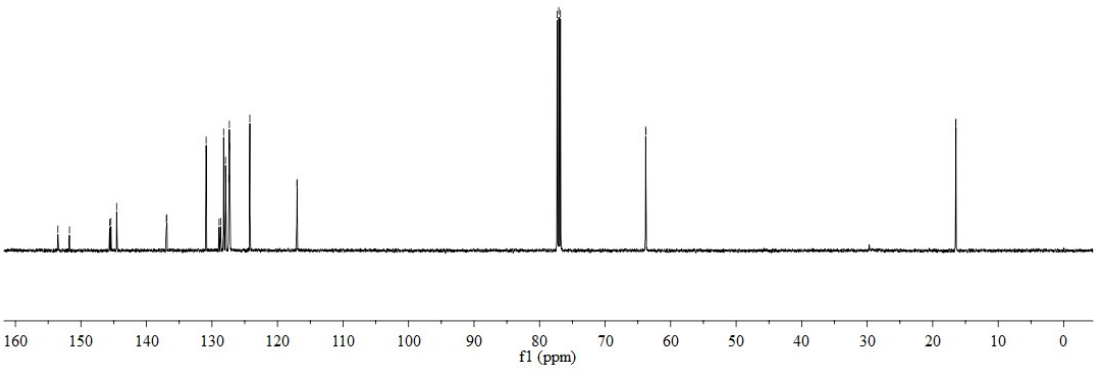
3m

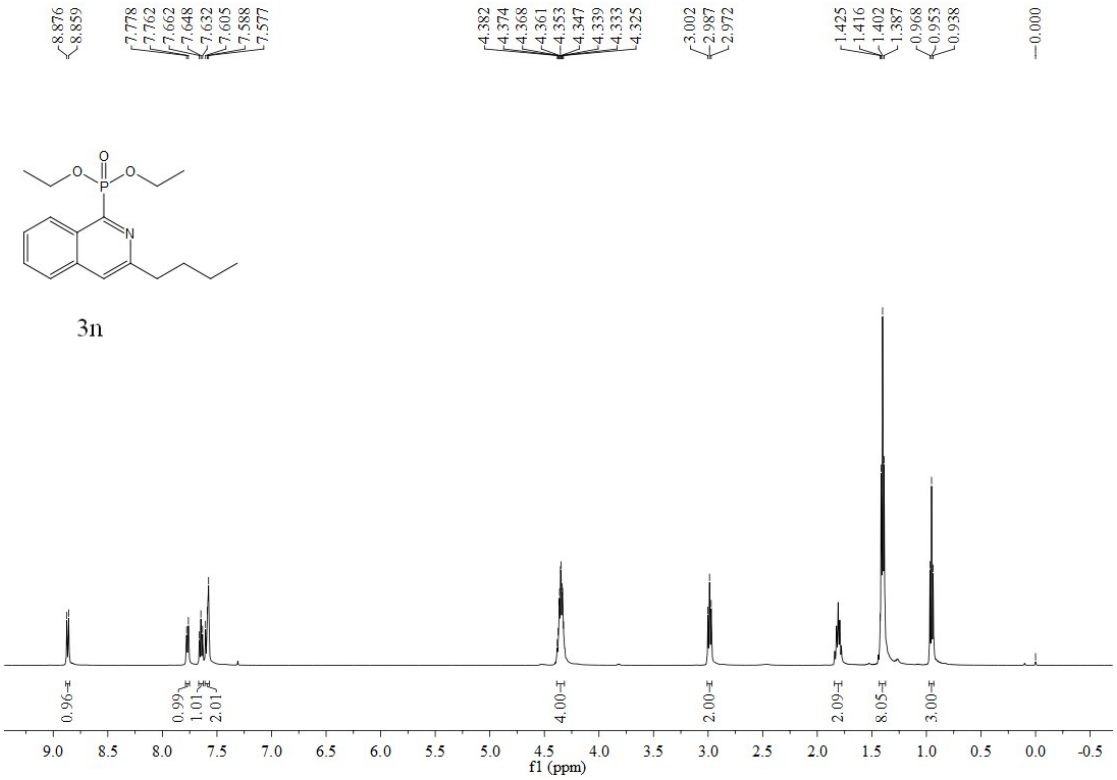

0.95
0.97
1.00
2.00
1.02
0.95
0.98
4.02
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


153.51
151.75
145.62
145.42
144.55
136.96
136.88
130.89
128.22
127.35
124.22
124.04
117.01
77.32
77.07
76.81
63.81
63.75
16.50
16.45

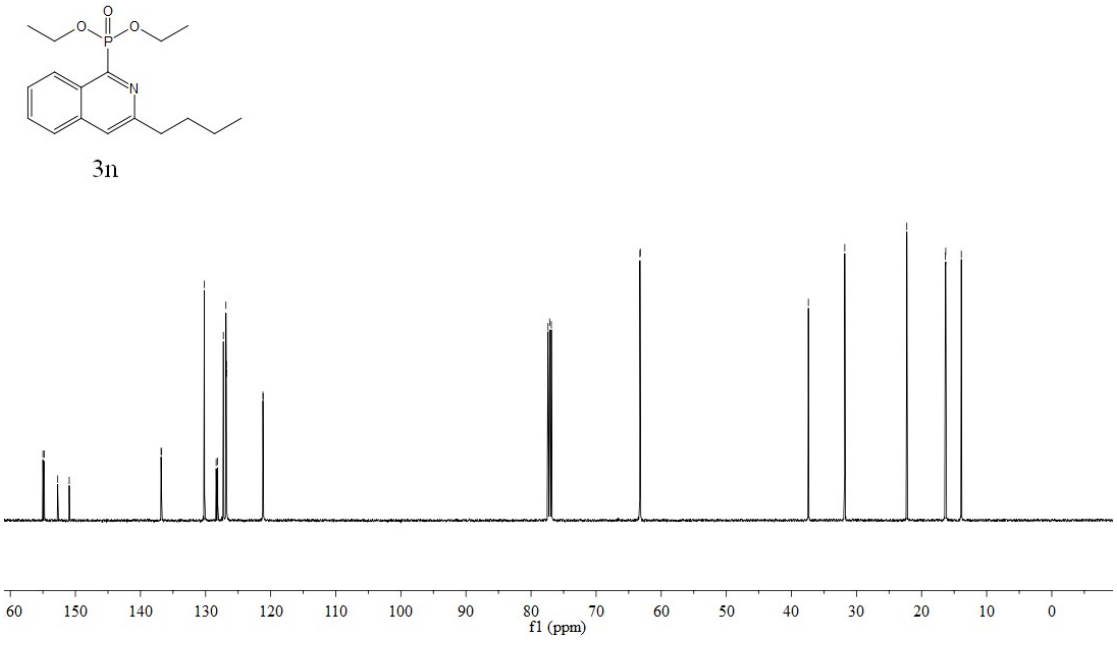

H3C
O
P
O
CH3
N
S

3m

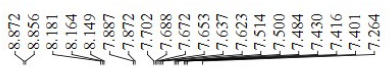

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

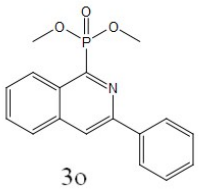

8.876
8.859
7.778
7.762
7.662
7.648
7.632
7.605
7.588
7.577
4.382
4.374
4.368
4.361
4.353
4.347
4.339
4.333
4.325
3.002
2.987
2.972
1.425
1.416
1.402
1.387
0.968
0.953
0.938
0.000
0.96
0.99
1.01
2.01
4.00
2.00
2.09
8.05
3.00
f1 (ppm)

3n

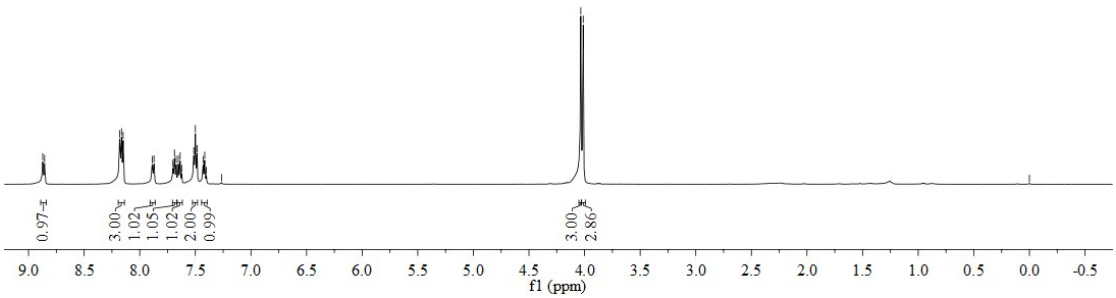

154.99
154.79
152.72
150.95
136.84
136.75
130.19
128.37
128.14
127.27
126.87
126.80
126.78
121.19
121.15
77.39
77.14
76.88
63.27
63.22
37.39
31.80
22.27
16.34
16.29
13.90
f1 (ppm)

3n


8.872
8.856
8.181
8.164
8.149
7.887
7.872
7.702
7.688
7.672
7.653
7.637
7.623
7.514
7.500
7.484
7.430
7.416
7.401
7.264
4.034
4.012
-0.000



3o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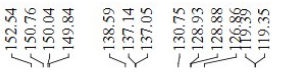
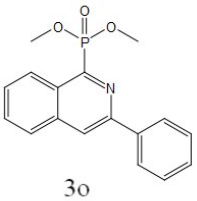
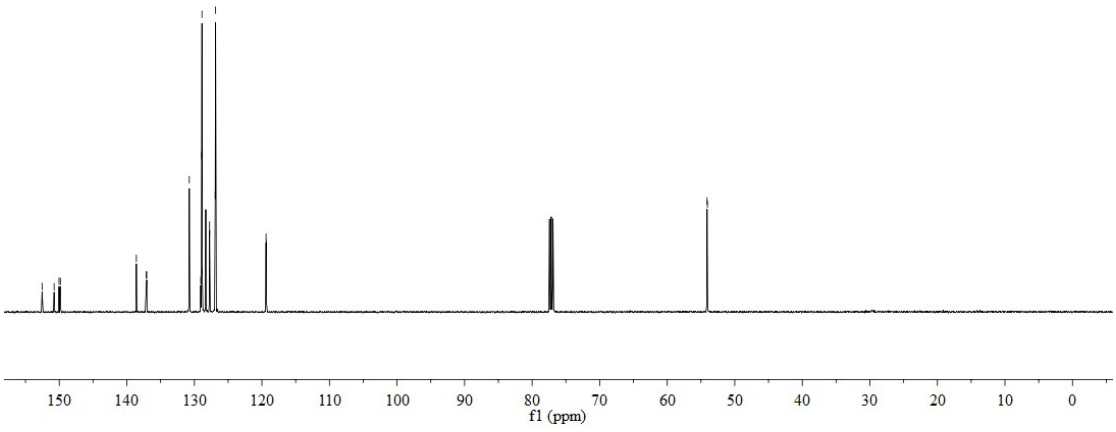
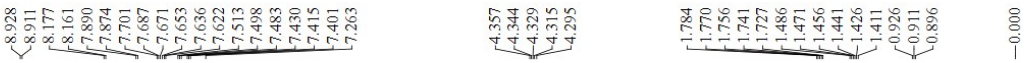
3.00
1.02
1.05
1.02
2.00
0.99
3.00
2.86
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


152.54
150.76
150.04
149.84
138.59
137.14
137.05
130.75
128.93
128.88
126.86
119.39
119.35
54.10
54.05



3o


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.911
8.177
8.161
7.890
7.874
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7.687
7.671
7.653
7.636
7.622
7.513
7.498
7.483
7.430
7.415
7.401
7.263
4.357
4.344
4.329
4.315
4.295
1.784
1.770
1.756
1.741
1.727
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1.471
1.456
1.441
1.426
1.411
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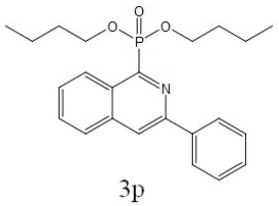
0.911
0.896
0.000



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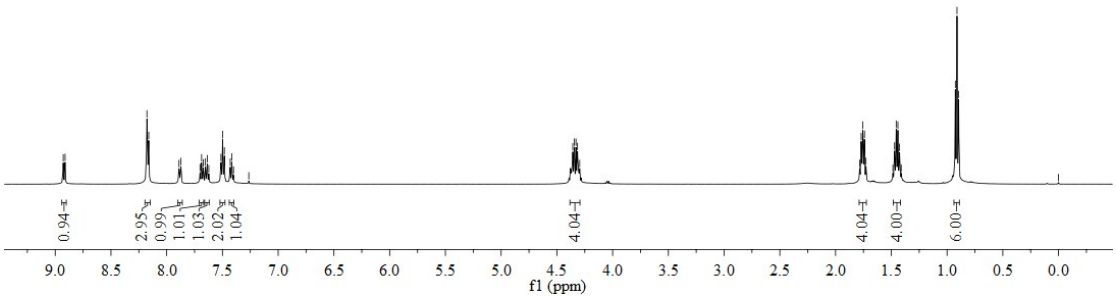
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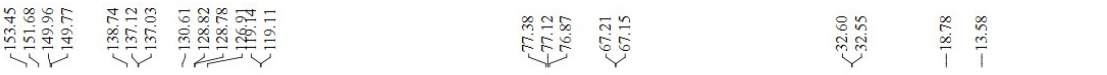
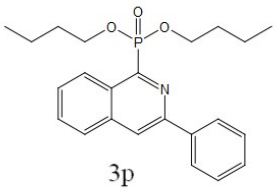
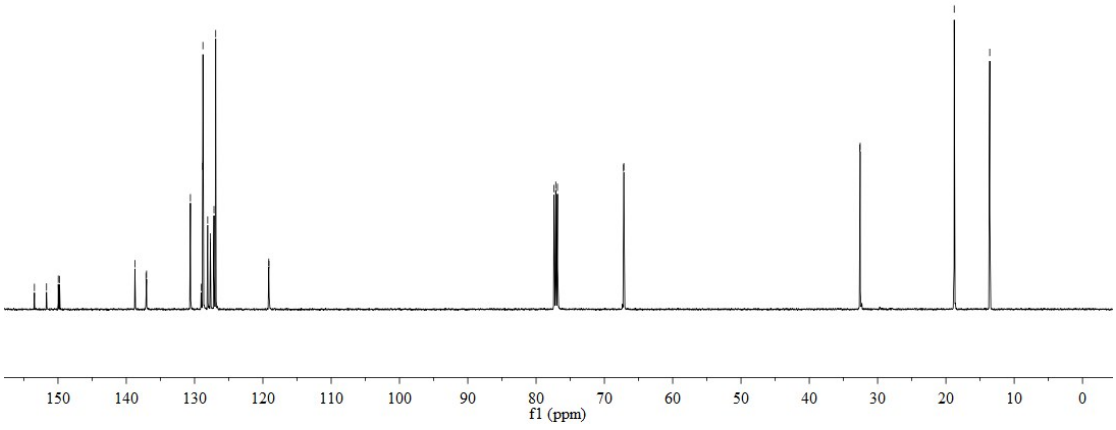
2.95
0.99
1.01
1.03
2.02
1.04
4.04
4.04
4.00
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.45
151.68
149.96
149.77
138.74
137.12
137.03
130.61
128.82
128.78
126.91
119.14
119.11
77.38
77.12
76.87
67.21
67.15
32.60
32.55
18.78
13.58



3p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130
120
110
100
90
80
70
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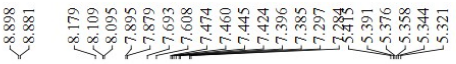
50
40
30
20
10
0
f1 (ppm)


8.898
8.881
8.179
8.109
8.095
7.895
7.879
7.693
7.608
7.474
7.460
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7.424
7.396
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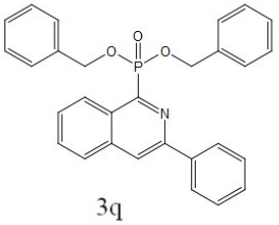
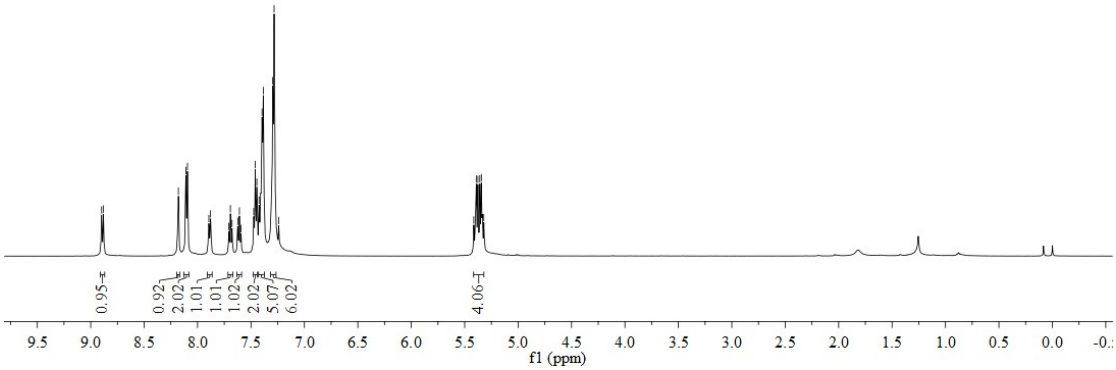
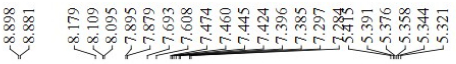
7.284
5.391
5.376
5.358
5.344
5.321


O
P
O
O
N

3q


0.95
0.92
2.02
1.01
1.01
1.02
2.02
5.07
6.02
4.06
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)


8.898
8.881
8.179
8.109
8.095
7.895
7.879
7.693
7.608
7.474
7.460
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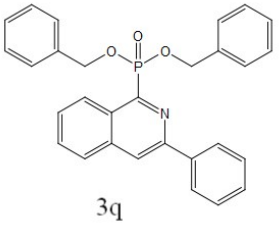
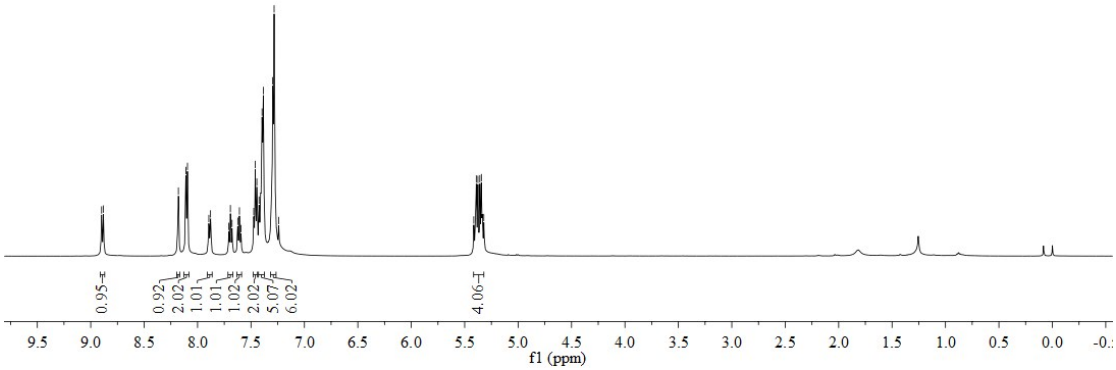
7.284
5.391
5.376
5.358
5.344
5.321


O
P
O
O
N

3q


0.95
0.92
2.02
1.01
1.01
1.02
2.02
5.07
6.02
4.06
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)