Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Rhodium-catalyzed synthesis of substituted isoquinolones *via* selective decarbonylation/alkyne insertion cascade of phthalimides

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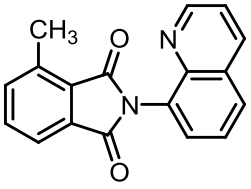
1. General Information

Unless otherwise noted, all the reactions were carried out in a glassware under an air atmosphere. The commercially available chemicals and solvents were used as received without further purification. Phthalimides were prepared according to the published procedure.[S1-S5] The reactions were monitored by TLC using UV-light or by staining with iodine. Column chromatography was performed on silica gel (200-300 mesh). Single-crystal X-ray data in this work were collected on an Agilent Technologies SuperNova Single Crystal Diffractometer at different temperatures equipped with graphite-monochromatic Mo Kα or Cu Kα radiation (λ = 0.71073 Å or 1.54184 Å). The structures were solved by SHELXS (direct methods) and refined by SHELXL (full matrix least-squares techniques) in the Olex2 package.[S6] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to carbon were placed in geometrically idealized positions and refined using a riding model. ^{1}H, ^{13}C, and ^{19}F NMR were recorded on a 400 MHz Bruker NMR spectrometer in $CDCl_3$ (7.26 ppm for ^{1}H and 77.16 ppm for ^{13}C) using tetramethylsilane (TMS) as the internal standard(s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet).

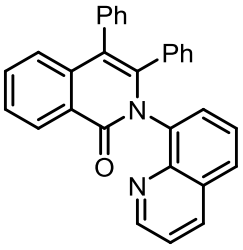
2. General Procedure

A mixture of $Rh(PPh_3)_2(CO)Cl$ (5 mol%), 2-(quinolin-8-yl)isoindoline-1,3-dione **1a** (0.125 mmol), 1,2-diphenylethyne **2a** (1.3 equiv), PhCl (2 mL) was reflux for 24 h. After cooling the reaction to room temperature, the solvent was removed under vacuum and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate = 10:1-4:1 to afford desired products **3aa-3ia** and **3aa-3am**.

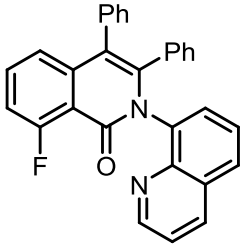
3. Characterization of Phthalimides and Products



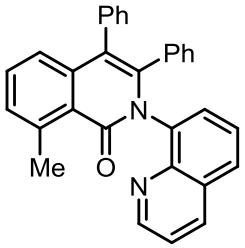
4-methyl-2-(quinolin-8-yl)isoindoline-1,3-dione (1c). white solid, mp 109.5-111.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.87 (dd, *J*=4.2, 1.7, 1H), 8.23 (dd, *J*=8.3, 1.7, 1H), 7.96 (dd, *J*=8.2, 1.5, 1H), 7.83 (d, *J*=7.3, 1H), 7.74 (dd, *J*=7.3, 1.5, 1H), 7.70 – 7.62 (m, 2H), 7.55 (d, *J*=7.7, 1H), 7.44 (dd, *J*=8.3, 4.2, 1H), 2.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 168.7, 168.0, 151.0, 144.5, 138.6, 136.6, 136.2, 133.7, 132.9, 130.3, 130.0, 129.5, 129.3, 129.2, 126.2, 121.9, 121.5, 17.8.



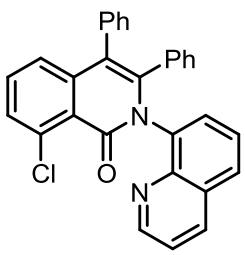
3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3aa). white solid (93 %), mp 123.9-125.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.58 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.05 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.65 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.56 – 7.46 (m, 2H), 7.41 – 7.33 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.27 – 7.10 (m, 5H), 6.97 (d, *J* = 7.7 Hz, 1H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.78 – 6.67 (m, 2H), 6.49 (dd, *J* = 11.0, 4.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.7, 150.7, 144.7, 141.8, 138.1, 137.7, 136.6, 136.0, 134.9, 132.4, 131.8, 131.7, 130.9, 130.8, 129.8, 128.7, 128.5, 128.4, 128.0, 127.8, 127.2, 126.7, 126.64, 126.62, 126.4, 125.8, 125.6, 125.6, 121.5, 118.5.



8-fluoro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ba). white solid (88 %), mp164.5-165.9°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (dd, *J*=4.2, 1.7, 1H), 8.43 (dd, *J*=8.0, 0.9, 1H), 8.03 (dd, *J*=8.3, 1.6, 1H), 7.64 (dd, *J*=8.2, 1.2, 1H), 7.47 (ddd, *J*=11.4, 6.0, 3.0, 2H), 7.41 – 7.32 (m, 2H), 7.28 (ddd, *J*=12.2, 7.9, 1.3, 1H), 7.20 (ddd, *J*=8.3, 6.3, 4.6, 2H), 7.16 – 7.11 (m, 1H), 7.11 – 7.04 (m, 2H), 6.93 (d, *J*=7.6, 1H), 6.85 – 6.77 (m, 1H), 6.72 – 6.65 (m, 2H), 6.49 – 6.41 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.67 (d, *J* = 3.1 Hz), 158.53 (d, *J* = 255.0 Hz), 150.8, 144.4, 143.2, 138.42 (d, *J* = 3.4 Hz), 137.4, 136.0, 134.4, 130.84 (dd, *J* = 13.5, 3.2 Hz), 130.8, 129.8, 128.71, 128.68, 127.80 (d, *J* = 2.5 Hz), 127.3, 127.2, 127.1, 126.75 (d, *J* = 9.0 Hz), 126.41 (d, *J* = 18.9 Hz), 126.3, 125.7, 124.61 (d, *J* = 3.9 Hz), 121.5, 119.45 (d, *J* = 22.3 Hz) 114.3.



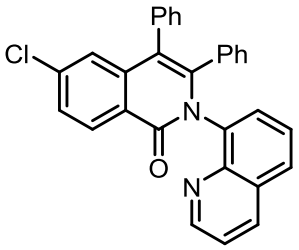
8-methyl-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ca). white solid (51%), mp 161.2-162.7°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.91 (dd, *J*=4.2, 1.7, 1H), 8.56 (dd, *J*=5.8, 3.8, 1H), 8.02 (dd, *J*=8.3, 1.7, 1H), 7.62 (dd, *J*=8.2, 1.3, 1H), 7.47 (dd, *J*=7.3, 1.3, 1H), 7.44 – 7.39 (m, 2H), 7.37 – 7.31 (m, 2H), 7.21 – 7.13 (m, 2H), 7.12 – 7.00 (m, 3H), 6.90 (d, *J*=7.7, 1H), 6.78 (t, *J*=7.3, 1H), 6.69 – 6.59 (m, 2H), 6.42 (td, *J*=7.6, 0.8, 1H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.9, 150.7, 144.6, 142.5, 140.0, 137.8, 136.8, 136.0, 135.9, 135.3, 135.2, 132.3, 132.2, 131.1, 130.9, 130.0, 128.7, 128.5, 127.4, 127.3, 127.0, 126.9, 126.6, 126.5, 126.3, 126.1, 125.7, 121.5, 118.2, 112.0, 23.9.



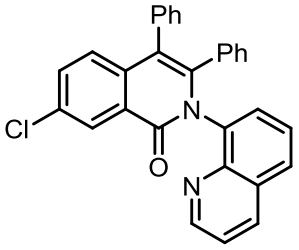
8-chloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3da). white solid (42%), mp 164.4-166.1°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ =

8.92 (dd, *J*=4.2, 1.7, 1H), 8.61 (dd, *J*=8.0, 1.5, 1H), 8.04 (dd, *J*=8.3, 1.7, 1H), 7.66 (ddd, *J*=14.1, 8.0, 1.4, 2H), 7.50 – 7.40 (m, 2H), 7.40 – 7.31 (m, 2H), 7.15 (dt, *J*=7.4, 3.3, 2H), 7.11 – 6.98 (m, 3H), 6.91 (d, *J*=7.7, 1H), 6.80 (dd, *J*=11.0, 4.1, 1H), 6.67 (tdd, *J*=3.6, 2.2, 1.2, 2H), 6.46 – 6.38 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162., 150.8, 144.4, 144.1, 138.3, 137.4, 136.3, 136.0, 134.7, 134.3, 132.3, 132.2, 131.1, 130.9, 130.8, 129.8, 128.7, 128.7, 128.4, 128.1, 127.2, 127.1, 127.0, 127.0, 126.44, 126.40, 126.2, 125.7, 121.6, 116.6.

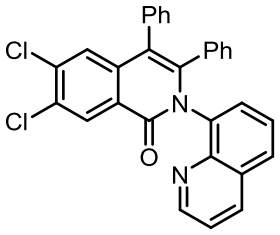
6-chloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ea). white solid (49%), mp 175.0-176.9°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (dd, *J*=4.2, 1.7, 1H), 8.50 (d, *J*=8.6, 1H), 8.05 (dd, *J*=8.3, 1.6, 1H), 7.66 (dd, *J*=8.2, 1.2, 1H), 7.52 – 7.42 (m, 2H), 7.40 – 7.31 (m, 2H), 7.31 – 7.12 (m, 6H), 6.95 (d, *J*=7.8, 1H), 6.83 (td, *J*=7.7, 1.2, 1H), 6.78 – 6.67 (m, 2H), 6.49 (dd, *J*=11.3, 3.9, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.2, 150.8, 144.6, 143.4, 139.5, 139.2, 137.4, 136.0, 135.8, 134.6, 131.7, 131.5, 130.8, 130.6, 130.3, 129.6, 128.8, 128.7, 128.2, 128.0, 127.4, 127.2, 127.1, 126.7, 126.5, 125.7, 125.0, 124.0, 121.6, 117.7.



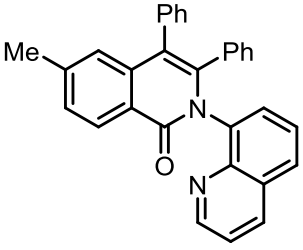
7-chloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ea'). white solid (41%), mp 121.5-123.3°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (dd, *J*=4.2, 1.7, 1H), 8.54 (d, *J*=2.3, 1H), 8.06 (dd, *J*=8.3, 1.7, 1H), 7.67 (dd, *J*=8.2, 1.3, 1H), 7.53 (dd, *J*=8.7, 2.3, 1H), 7.48 (dd, *J*=7.3, 1.3, 1H), 7.42 – 7.33 (m, 2H), 7.27 – 7.19 (m, 3H), 7.19 – 7.12 (m, 3H), 6.96 (d, *J*=7.7, 1H), 6.83 (t, *J*=7.5, 1H), 6.77 – 6.66 (m, 2H), 6.49 (dd, *J*=11.1, 4.1, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.7, 150.8, 144.6, 142.2, 137.4, 136.6, 136.1, 136.0, 134.6, 132.8, 132.7, 131.8, 131.5, 130.8, 130.7, 129.7, 128.8, 128.7, 128.1, 127.9, 127.8, 127.4, 127.4, 127.0, 126.7, 126.7, 126.5, 125.8, 121.6, 118.1.



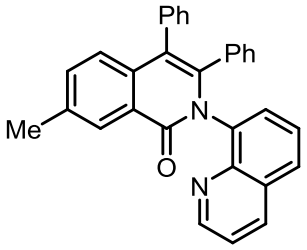
6,7-dichloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3fa). white solid (32%), mp 154.7-156.4°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (dd, *J*=4.2, 1.7, 1H), 8.63 (s, 1H), 8.06 (dd, *J*=8.3, 1.6, 1H), 7.67 (dd, *J*=8.2, 1.3, 1H), 7.47 (dd, *J*=7.3, 1.3, 1H), 7.42 – 7.34 (m, 3H), 7.29 – 7.22 (m, 1H), 7.22 – 7.09 (m, 4H), 6.95 (d, *J*=7.7, 1H), 6.84 (td, *J*=7.6, 0.7, 1H), 6.72 (ddd, *J*=21.7, 10.9, 4.5, 2H), 6.53 – 6.44 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.2, 150.9, 144.5, 143.6, 137.7, 137.4, 137.2, 136.1, 135.5, 134.4, 131.7, 131.4, 131.1, 130.7, 130.5, 130.1, 129.5, 128.8, 128.8, 128.3, 128.1, 127.5, 127.2, 127.2, 126.8, 126.5, 125.7, 125.0, 121.6, 117.2.



6-methyl-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ga'). white solid (46 %), mp 155.6-157.5°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (dd, *J*=4.2, 1.7, 1H), 8.47 (d, *J*=8.2, 1H), 8.04 (dd, *J*=8.3, 1.7, 1H), 7.65 (dd, *J*=8.2, 1.3, 1H), 7.49 (dd, *J*=7.3, 1.3, 1H), 7.40 – 7.31 (m, 3H), 7.29 – 7.20 (m, 3H), 7.21 – 7.10 (m, 3H), 6.95 (d, *J*=7.7, 1H), 6.82 (t, *J*=7.2, 1H), 6.76 – 6.66 (m, 2H), 6.47 (td, *J*=7.6, 0.8, 1H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.7, 150.7, 144.8, 143.0, 141.9, 138.2, 137.8, 136.7, 135.9, 135.0, 131.9, 131.7, 130.9, 130.8, 129.8, 128.7, 128.5, 128.3, 128.0, 127.7, 127.1, 126.7, 126.6, 126.4, 125.7, 125.3, 123.4, 121.4, 118.4, 22.1.

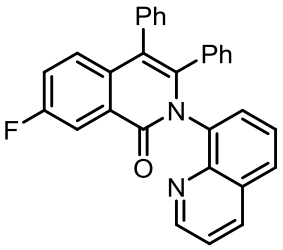


7-methyl-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ga).



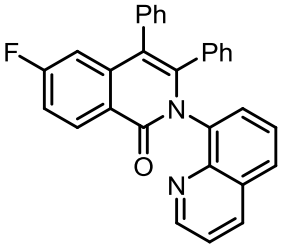
white solid (50%), mp 160.7-162.5°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.92 (dd, *J*=4.2, 1.7, 1H), 8.38 (s, 1H), 8.05 (dd, *J*=8.3, 1.7, 1H), 7.65 (dd, *J*=8.2, 1.2, 1H), 7.48 (dd, *J*=7.3, 1.3, 1H), 7.42 (dd, *J*=8.3, 1.7, 1H), 7.39 – 7.32 (m, 2H), 7.25 – 7.18 (m, 3H), 7.18 – 7.10 (m, 3H), 6.96 (d, *J*=7.7, 1H), 6.82 (t, *J*=7.5, 1H), 6.71 (td, *J*=7.6, 1.1, 2H), 6.48 (dt, *J*=7.6, 3.8, 1H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.7, 150.7, 144.8, 140.9, 137.9, 136.8, 136.7, 136.0, 135.9, 135.0, 133.9, 131.9, 131.7, 130.9, 129.9, 128.7, 128.5, 128.0, 128.0, 127.7, 127.1, 126.7, 126.6, 126.4, 125.7, 125.6, 125.5, 121.4, 118.5, 21.4.

7-fluoro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ha).



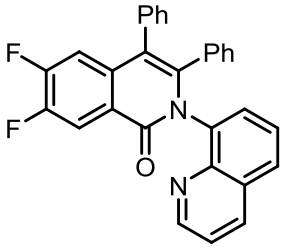
white solid (44%), mp 119.5-121.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.29 – 8.14 (m, 1H), 8.06 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.67 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.49 (dd, *J* = 7.3, 1.2 Hz, 1H), 7.41 – 7.28 (m, 4H), 7.25 – 7.20 (m, 2H), 7.19 – 7.08 (m, 3H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.82 (dd, *J* = 11.7, 4.2 Hz, 1H), 6.78 – 6.67 (m, 2H), 6.48 (dd, *J* = 11.0, 4.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.87 (d, *J* = 3.5 Hz), 161.50 (d, *J* = 247.4 Hz), 150.8, 144.5, 141.1, 137.4, 136.3, 136.1, 134.79 (d, *J* = 2.1 Hz), 134.6, 131.64 (d, *J* = 21.3 Hz), 130.8, 129.8, 128.74, 128.68, 128.23 (d, *J* = 7.7 Hz), 127.99 (d, *J* = 24.5 Hz), 127.3, 127.18 (d, *J* = 8.1 Hz), 126.9, 126.57 (d, *J* = 22.7 Hz), 125.8, 121.5, 121.00 (d, *J* = 23.3 Hz), 118.1, 113.39 (d, *J* = 22.8 Hz).^{19}F NMR (376 MHz, $CDCl_3$) δ = -113.79.

6-fluoro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ha').



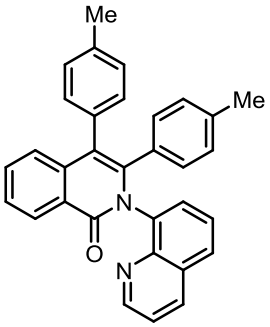
white solid (37%), mp 170.2-171.9°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.58 (dd, *J* = 8.9, 6.0 Hz, 1H), 8.06 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.67 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.49 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.41 – 7.33 (m, 2H), 7.26 – 7.10 (m, 6H), 6.99 – 6.89 (m, 2H), 6.83 (dd, *J* = 11.8, 4.3 Hz, 1H), 6.73 (td, *J* = 7.4, 1.3 Hz, 2H), 6.53 – 6.44 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 165.59 (d, *J* = 251.7 Hz), 162.0, 150.8, 144.6, 143.2, 140.68 (d, *J* = 10.1 Hz), 137.4, 136.1, 136.0, 134.6, 131.67 (d, *J* = 10.0 Hz), 131.58 (d, *J* = 22.5 Hz), 131.58 (d, *J* = 22.5 Hz), 130.9, 130.6, 129.6, 128.7, 128.7, 128.08 (d, *J* = 22.7 Hz), 127.19 (d, *J* = 35.2 Hz), 126.58 (d, *J* = 22.5 Hz), 125.8, 122.2, 121.5, 118.04 (d, *J* = 3.2 Hz), 115.19 (d, *J* = 23.5 Hz), 110.82 (d, *J* = 23.2 Hz).

6,7-difluoro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ia)

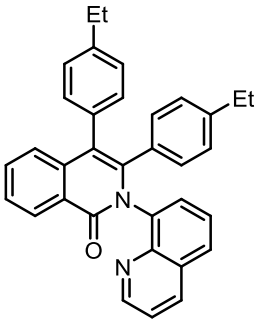


white solid (24%), mp 105.9-107.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.93 (dd, *J*=4.2, 1.7, 1H), 8.33 (dd, *J*=10.7, 8.3, 1H), 8.07 (dd, *J*=8.3, 1.6, 1H), 7.67 (dd, *J*=8.2, 1.3, 1H), 7.48 (dd, *J*=7.3, 1.4, 1H), 7.44 – 7.35 (m, 2H), 7.29 – 7.22 (m, 1H), 7.22 – 7.12 (m, 4H), 7.06 (dd, *J*=11.7, 7.5, 1H), 6.95 (d, *J*=7.7, 1H), 6.84 (t, *J*=7.2, 1H), 6.77 – 6.68 (m, 2H), 6.52 – 6.43 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -129.40 (d, *J* = 22.0 Hz), -137.59 (d, *J* = 22.0 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.28 (d, *J* = 3.7 Hz), 153.96 (dd, *J* = 255.1, 14.1 Hz), 150.84, 149.84 (dd, *J* = 250.9, 14.2 Hz), 144.49, 142.68 (d, *J* = 2.2 Hz), 137.26, 136.27 (d, *J* = 2.7 Hz), 136.19 (d, *J* = 2.5 Hz), 136.11, 135.87, 134.43, 131.49 (d, *J* = 25.2 Hz), 130.76, 130.11 (d, *J* = 99.2 Hz),, 128.80, 128.78, 128.20 (d, *J* = 21.7 Hz), 127.34 (d, *J* = 26.3 Hz), 126.64 (d, *J* = 23.0 Hz),

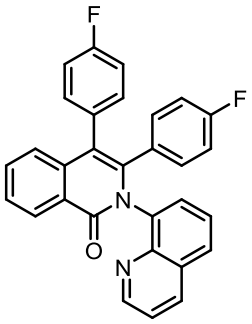
125.76, 122.64 (dd, *J* = 6.2, 2.0 Hz), 121.61, 117.58, 116.46 (dd, *J* = 18.7, 1.9 Hz), 113.48 (d, *J* = 19.2 Hz).



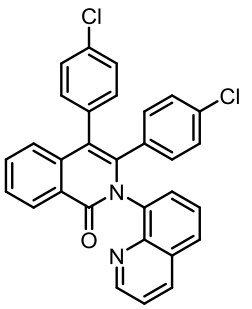
2-(quinolin-8-yl)-3,4-di-p-tolylisoquinolin-1(2H)-one (3ab). white solid (95 %), mp 173.1-174.9°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.91 (dd, *J*=4.2, 1.7, 1H), 8.56 (dd, *J*=7.9, 1.1, 1H), 7.63 (dd, *J*=8.2, 1.3, 1H), 7.60 – 7.53 (m, 1H), 7.52 – 7.42 (m, 2H), 7.39 – 7.27 (m, 3H), 7.13 (dd, *J*=7.9, 1.6, 1H), 7.04 (dd, *J*=7.9, 1.7, 2H), 6.96 (d, *J*=8.0, 1H), 6.84 (dd, *J*=7.8, 1.7, 1H), 6.66 – 6.57 (m, 2H), 6.27 (d, *J*=8.0, 1H), 2.25 (s, 3H), 1.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.8, 150.7, 144.8, 142.0, 138.5, 137.9, 136.7, 136.1, 136.0, 133.7, 132.3, 132.1, 131.7, 131.5, 130.8, 130.7, 129.6, 128.8, 128.7, 128.5, 128.4, 128.3, 127.4, 127.2, 126.5, 125.8, 125.7, 125.6, 121.4, 118.5, 21.2, 21.0.



3,4-bis(4-ethylphenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ac). white solid (97%), mp 143.9-145.7°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.57 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.05 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.69 – 7.54 (m, 2H), 7.54 – 7.42 (m, 2H), 7.40 – 7.29 (m, 3H), 7.15 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.09 – 7.01 (m, 2H), 6.98 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.84 (dd, *J* = 7.8, 1.7 Hz, 1H), 6.63 (td, *J* = 7.8, 1.3 Hz, 2H), 6.29 (dd, *J* = 7.9, 1.4 Hz, 1H), 2.56 (q, *J* = 7.6 Hz, 2H), 2.23 (q, *J* = 7.6 Hz, 2H), 1.17 (t, *J* = 7.6 Hz, 3H), 0.88 (dd, *J* = 9.1, 6.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.8, 150.6, 144.7, 142.9, 142.4, 142.0, 138.4, 137.9, 136.0, 133.8, 132.3, 131.7, 131.5, 130.8, 130.7, 129.7, 128.7, 128.3, 127.4, 127.1, 126.4, 126.0, 125.8, 125.8, 125.7, 125.5, 121.4, 118.5, 28.5, 28.2, 15.4, 15.0.



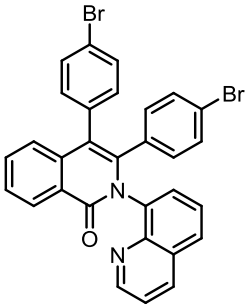
3,4-bis(4-fluorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ad). white solid (89 %), mp 152.5-154.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.58 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.09 (d, *J* = 8.2 Hz, 1H), 7.71 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.66 – 7.58 (m, 1H), 7.53 (ddd, *J* = 15.1, 7.9, 1.2 Hz, 2H), 7.45 – 7.33 (m, 2H), 7.27 (d, *J* = 6.7 Hz, 1H), 7.20 – 7.11 (m, 2H), 6.99 – 6.84 (m, 3H), 6.79 – 6.71 (m, 1H), 6.55 (td, *J* = 8.6, 2.7 Hz, 1H), 6.21 (td, *J* = 8.6, 2.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.68, 161.66 (d, *J* = 246.4 Hz), 161.44 (d, *J* = 248.0 Hz), 150.70, 144.41, 141.11, 137.93, 137.37, 136.28, 132.62, 130.93, 133.24 (dd, *J* = 27.8, 8.0 Hz), 132.30 (d, *J* = 3.5 Hz), 132.01 (dd, *J* = 76.8, 8.3 Hz), 130.85 (d, *J* = 3.6 Hz), 130.85 (d, *J* = 3.6 Hz), 128.85, 125.90, 125.67, 128.65 (d, *J* = 30.1 Hz), 126.94, 125.43, 115.11 (d, *J* = 3.4 Hz), 115.11 (d, *J* = 39.3 Hz), 113.83, 113.8 (d, *J* = 42.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ = -113.24, -115.05.



3,4-bis(4-chlorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ae). white solid (87%), mp 174.4-175.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.57 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.71 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.65 – 7.57 (m, 1H), 7.57 – 7.47 (m, 2H), 7.44 – 7.32 (m, 2H), 7.28 – 7.07 (m, 6H), 6.87 (ddd, *J* = 24.1, 8.2, 2.1 Hz, 2H), 6.70 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.50 (dd, *J* = 8.3, 2.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.6, 150.8, 144.4, 140.8, 137.6, 137.2, 136.2, 134.8, 133.4,

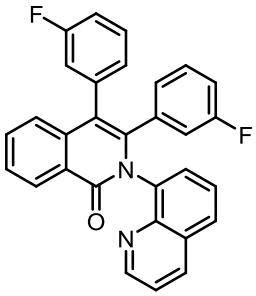
133.13, 133.07, 133.0, 132.8, 132.7, 131.9, 131.1, 130.8, 128.9, 128.8, 128.5, 128.3, 127.2, 127.1, 127.0, 125.9, 125.7, 125.4, 121.6, 117.5.

3,4-bis(4-bromophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3af).



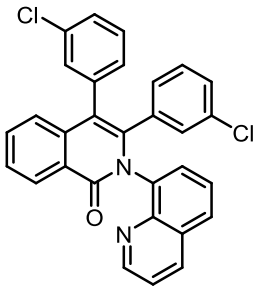
white solid (83%), mp 176.3-178.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.91 (dd, *J*=4.2, 1.5, 1H), 8.56 (dd, *J*=7.9, 1.0, 1H), 8.11 (d, *J*=7.5, 1H), 7.73 (dd, *J*=8.2, 1.2, 1H), 7.66 – 7.58 (m, 1H), 7.58 – 7.47 (m, 2H), 7.46 – 7.32 (m, 4H), 7.24 (d, *J*=7.7, 1H), 7.08 (ddd, *J*=7.5, 5.3, 1.9, 2H), 7.00 (d, *J*=8.3, 1H), 6.84 (d, *J*=8.2, 1H), 6.66 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.6, 150.8, 144.5, 140.7, 137.8, 137.2, 136.2, 135.3, 133.6, 133.4, 133.2, 132.7, 132.1, 131.5, 131.3, 130.8, 130.1, 129.9, 129.0, 128.8, 128.5, 127.1, 125.9, 125.7, 125.4, 121.8, 121.7, 121.3, 117.4.

3,4-bis(3-fluorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ag).



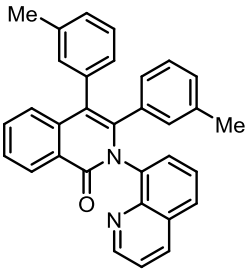
white solid (86%), mp 136.0-137.8°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.96 – 8.86 (m, 1H), 8.58 (dd, *J*=8.0, 1.0, 1H), 8.07 (dd, *J*=8.1, 3.6, 1H), 7.69 (d, *J*=8.2, 1H), 7.66 – 7.58 (m, 1H), 7.58 – 7.48 (m, 2H), 7.45 – 7.34 (m, 2H), 7.30 – 7.11 (m, 2H), 7.06 – 6.74 (m, 4H), 6.73 – 6.54 (m, 1H), 6.49 (ddd, *J*=21.8, 9.3, 4.6, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.43 (ddd, *J* = 246.3, 11.9, 3.3 Hz), 161.15 (ddd, *J* = 246.4, 13.8, 3.4 Hz), 162.54, 150.93 (d, *J* = 4.8 Hz), 150.77 (d, *J* = 4.9 Hz), 144.54, 144.50, 140.57, 138.46 (ddd, *J* = 7.4, 5.2, 2.1 Hz), 137.50, 137.21 (d, *J* = 1.5 Hz), 136.49 (dd, *J* = 11.4, 6.0 Hz), 136.15, 132.70, 130.88, 130.83, 130.77, 129.77, 129.69, 129.54 (dd, *J* = 10.6, 2.0 Hz), 129.39, 128.91, 128.85, 128.82, 128.54, 128.44, 128.34 (d, *J* = 1.9 Hz), 128.27 (d, *J* = 4.6 Hz), 128.20 (d, *J* = 2.2 Hz),, 128.11, 127.63, 127.60, 127.57, 127.40 (dd, *J* = 2.7, 1.2 Hz), 127.11, 126.58 (d, *J* = 2.4 Hz), 125.90 (d, *J* = 5.0 Hz), 125.77 (d, *J* = 3.4 Hz), 125.72 (d, *J* = 2.8 Hz),, 125.41, 121.73 (d, *J* = 2.6 Hz), 118.77 (d, *J* = 2.0 Hz), 118.55, 118.34, 117.64 (d, *J* = 22.0 Hz), 117.46 (d, *J* = 1.8 Hz), 117.44, 117.42, 116.91 (d, *J* = 22.6 Hz), 114.35 (ddd, *J* = 24.1, 21.0, 3.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ = -113.34 (dd, *J*=104.7, 101.2), -114.00 (dd, *J*=108.6, 14.0).

3,4-bis(3-chlorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ah).

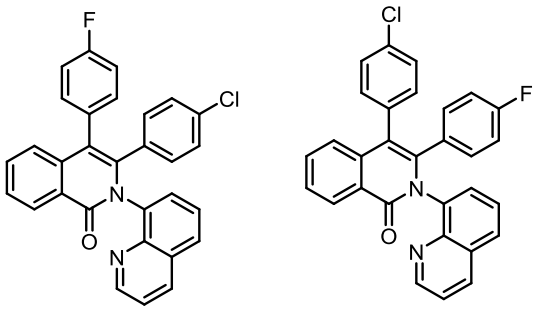


white solid (85%), mp 153.5-155.2°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.02 – 8.81 (m, 1H), 8.58 (d, *J*=7.9, 1H), 8.18 – 7.97 (m, 1H), 7.71 (d, *J*=8.2, 1H), 7.65 (dd, *J*=11.1, 4.0, 1H), 7.60 – 7.34 (m, 4H), 7.29 – 7.24 (m, 2H), 7.14 (m, *J*=17.6, 16.0, 9.5, 5.1, 3H), 7.04 – 6.70 (m, 3H), 6.51 (ddd, *J*=41.1, 15.8, 7.8, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.54 (d, *J* = 2.5 Hz), 150.92 (d, *J* = 4.1 Hz), 150.75 (d, *J* = 4.8 Hz), 144.46, 140.68, 140.64, 140.55, 138.04, 137.45, 137.18, 137.09, 136.23, 136.14, 136.13, 136.09, 136.05, 133.92 (dd, *J* = 19.1, 16.6 Hz), 132.76, 132.57 (d, *J* = 3.2 Hz), 131.67 (d, *J* = 20.1 Hz), 131.59 (d, *J* = 21.2 Hz), 130.96, 130.72 (d, *J* = 3.8 Hz), 130.62 (d, *J* = 8.5 Hz), 130.09, 130.06, 129.97, 129.80 (d, *J* = 7.5 Hz), 129.58, 129.39 (d, *J* = 4.0 Hz),, 129.22, 128.96 (d, *J* = 7.0 Hz), 128.88, 128.86, 128.75 (d, *J* = 5.6 Hz), 128.56, 128.13 (d, *J* = 5.6 Hz), 127.93 (d, *J* = 3.0 Hz), 127.91 (d, *J* = 17.3 Hz), 127.71 (dd, *J* = 4.3, 1.3 Hz), 127.37, 127.17 (d, *J* = 2.1 Hz), 125.97, 125.85 (d, *J* = 6.2 Hz), 125.73, 125.72, 125.69, 125.41, 121.74, 121.72, 121.62, 121.60, 117.50, 117.42 (dd, *J* = 9.6, 5.1 Hz)., 117.35.

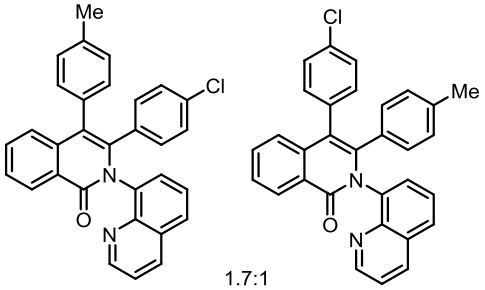
2-(quinolin-8-yl)-3,4-di-m-tolylisoquinolin-1(2H)-one (3ai). white solid (79%), mp132.6-134.5°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (ddd, *J* = 16.7, 4.2, 1.6 Hz, 1H), 8.64 – 8.47 (m, 1H), 8.07 (dd, *J* = 10.5, 3.9 Hz, 1H), 7.71 – 7.54 (m, 2H), 7.54 – 7.28 (m, 5H), 7.17 – 6.90 (m, 4H), 6.82 – 6.65 (m, 2H), 6.53 (t, *J* = 15.7 Hz, 2H), 6.37 (td, *J* = 7.6, 2.8 Hz, 1H), 2.33 – 2.14 (m, 3H), 1.81 (dd, *J* = 158.3, 5.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.7, 150.5, 141.8, 138.2, 137.9, 137.4, 137.1, 137.0, 136.5, 136.4, 136.1, 135.9, 135.9, 135.8, 135.7, 134.7, 132.6, 132.5, 132.4, 132.3, 131.6, 131.5, 130.9, 130.6, 130.6, 128.9, 128.8, 128.7, 128.7, 128.4, 128.3, 127.8, 127.8, 127.5, 127.5, 127.4, 127.4, 127.0, 126.9, 126.5, 126.40, 126.38, 126.2, 126.1, 125.9, 125.7, 125.5, 121.41, 121.39, 121.3, 118.5, 21.32, 21.25, 21.00, 20.56.



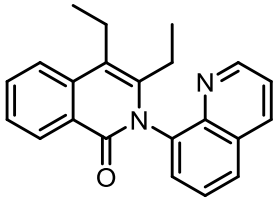
3-(4-chlorophenyl)-4-(4-fluorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3aj) and 4-(4-chlorophenyl)-3-(4-fluorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ak). white solid (82%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.57 (dd, *J* = 7.9, 0.8 Hz, 1H), 8.12 – 8.02 (m, 1H), 7.71 (ddd, *J* = 8.2, 4.2, 1.3 Hz, 1H), 7.65 – 7.57 (m, 1H), 7.57 – 7.46 (m, 2H), 7.45 – 7.34 (m, 2H), 7.29 – 7.09 (m, 4H), 6.98 – 6.86 (m, 2H), 6.83 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.77 – 6.67 (m, 1H), 6.59 – 6.46 (m, 1H), 6.22 (td, *J* = 8.6, 2.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.69 (d, *J* = 246.5 Hz), 161.49 (d, *J* = 248.2 Hz), 162.7, 162.6, 150.8, 144.4, 141.0, 140.9, 137.9, 137.7, 137.34, 137.29, 136.2, 134.9, 133.4, 133.3, 133.13, 133.10, 133.05, 132.89, 132.87, 132.6, 132.36 (d, *J* = 8.3 Hz), 132.13 (d, *J* = 3.5 Hz), 131.9, 131.60 (d, *J* = 8.2 Hz), 131.1, 130.8, 130.70 (d, *J* = 3.5 Hz), 128.9, 128.8, 128.8, 128.49 (d, *J* = 8.4 Hz), 128.5, 128.3, 126.99 (d, *J* = 19.6 Hz), 127.0, 125.9, 125.76 (d, *J* = 20.9 Hz), 125.4, 125.3, 121.6, 117.7, 117.6, 115.4, 115.17 (d, *J* = 3.0 Hz), 115.0, 114.1, 113.89 (d, *J* = 1.5 Hz) 113.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ = -113.02, -114.85.



3-(4-chlorophenyl)-2-(quinolin-8-yl)-4-(p-tolyl)isoquinolin-1(2H)-one (3al) and 4-(4-chlorophenyl)-2-(quinolin-8-yl)-3-(p-tolyl)isoquinolin-1(2H)-one (3am). white solid (90%), ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.97 – 8.87 (m, 1H), 8.56 (dd, *J*=8.0, 1.4, 1H), 8.06 (ddd, *J*=7.2, 5.5, 1.6, 1H), 7.67 (ddd, *J*=12.3, 8.2, 1.2, 1H), 7.59 (ddd, *J*=8.4, 4.0, 2.0, 1H), 7.55 – 7.44 (m, 2H), 7.43 – 7.32 (m, 2H), 7.30 (d, *J*=7.6, 1H), 7.22 (dd, *J*=8.5, 2.1, 1H), 7.20 – 7.14 (m, 1H), 7.12 (dd, *J*=11.4, 1.8, 1H), 7.10 – 6.97 (m, 3H), 6.91 (dd, *J*=8.3, 2.0, 1H), 6.84 – 6.77 (m, 1H), 6.71 (dd, *J*=8.3, 2.0, 1H), 6.65 (d, *J*=7.7, 1H), 6.59 (dd, *J*=7.9, 1.7, 1H), 6.47 (dd, *J*=8.3, 2.1, 1H), 6.30 (d, *J*=7.7, 1H), 2.28 (s, 2H), 1.95 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.7, 162.6, 150.8, 150.7, 144.6, 142.3, 140.5, 138.2, 137.9, 137.6, 137.5, 137.0, 136.5, 136.1, 136.0, 135.3, 133.6, 133.2, 133.1, 133.0, 132.97, 132.6, 132.5, 132.5, 132.0, 131.6, 131.5, 131.3, 131.2, 130.8, 130.76, 130.5, 129.4, 128.9, 128.81, 128.79, 128.7, 128.52, 128.49, 128.4, 128.3, 128.1, 127.6, 127.3, 126.9, 126.8, 126.7, 126.7, 125.8, 125.8, 125.6, 125.5, 125.2, 121.6, 121.5, 118.7, 117.2, 21.2, 21.0.



3,4-diethyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3an). white solid (79%), mp 122.4-124.0°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.46 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.24 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.96 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.75 – 7.63 (m, 3H), 7.49 – 7.35 (m, 2H), 2.87 (q, *J* = 7.5 Hz, 2H), 2.57 (dd, *J* = 14.9, 7.5 Hz, 1H), 2.08 (dd, *J* = 14.8, 7.5 Hz, 1H), 1.33 (t, *J* = 7.5 Hz, 3H), 0.88 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 163.2, 151.3, 144.8, 141.7, 137.44, 137.38, 136.3, 134.2, 132.4, 130.4, 129.3, 129.1, 128.7, 126.2, 125.62, 125.55, 123.9, 122.8, 121.8, 114.6, 23.6, 20.7, 14.9, 14.1.



4. References

(S1) L. Zeng, H. Li, S. Tang, X. Gao, Y. Deng, G. Zhang, C.-W. Pao, J.-L. Chen, J.-F. Lee and A. Lei, *ACS Catalysis*, 2018, **8**, 5448.
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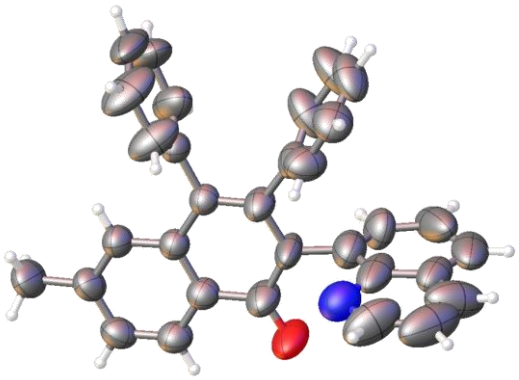
(S3) B. Khan, A. A. Khan, R. Kant and D. Koley, *Adv. Synth. Catal.*, 2016, **358**, 3753.
(S4) T. Shiba, T. Kurahashi and S. Matsubara, *J. Am. Chem. Soc.*, 2013, **135**, 13636.
(S5) Y. Kajita, S. Matsubara and T. Kurahashi, *J. Am. Chem. Soc.*, 2008, **130**, 6058.
(S6) Sheldrick, G. M. *SHELXTL-97*, *Program for X-ray Crystal Structure Solution*; University of Göttingen: Göttingen, Germany, **1997**.

5. Single-Crystal X-Ray Crystallography

5.1 Crystal structure of targeted isoquinolone 3ga'. The displacement ellipsoids are drawn at the 30% probability.



3ga'

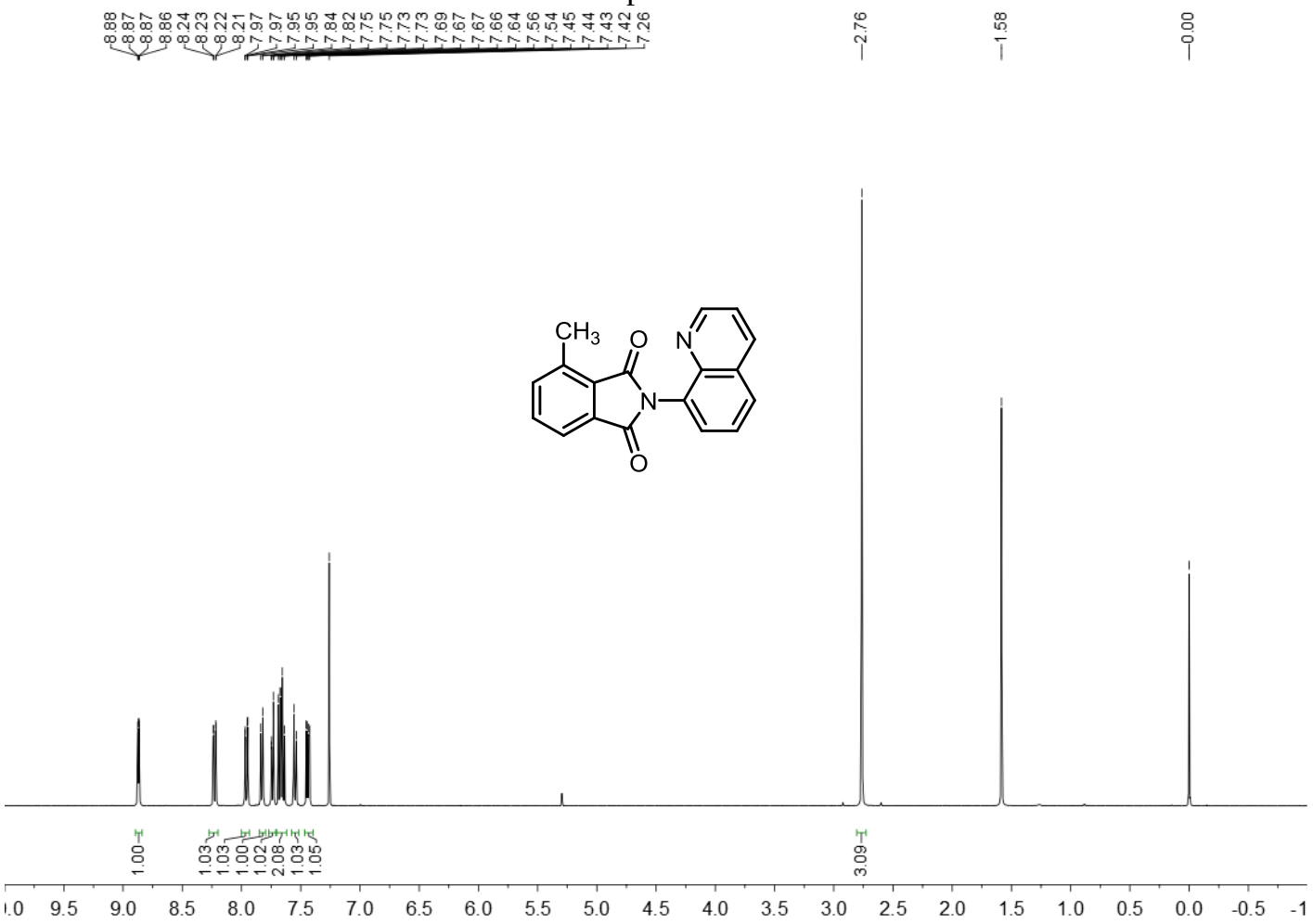
Table S1. Crystal data and structure refinement details for targeted **3ga'**.

	3ga'
Empirical formula	$C_{12.8}H_{8.8}N_{0.4}O_{0.4}$
Formula weight	174.60
Crystal system	triclinic
Space group	P-1
a / Å	9.6741(10)
b / Å	10.8198(12)
c / Å	12.5635(11)
α / °	69.234(9)
β / °	89.878(8)
γ / °	72.178(10)
Volume / $Å^3$	1162.2(2)
Z	5
D / g cm^{-3}	1.247
μ / mm^{-1}	0.580
F (000)	458.0
R_{int}	0.0334
Goodness-of-fit on F^2	2.237
$R_1{}^a$ / $wR_2{}^b$ [I >2σ(I)]	0.1657/0.4066
$R_1{}^a$ / $wR_2{}^b$ (all data)	0.1907/0.4291
CCDC number	2026038

^{a} $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. ^{b} $wR_2 = |\Sigma w(|F_o|^2 - |F_c|^2)|/\Sigma|w(F_o)^2|^{1/2}$, where $w = 1/[\sigma^2(F_o{}^2) + (aP)^2 + bP]$. $P = (F_o{}^2 + 2F_c{}^2)/3$.

6. Copy of NMR (^{1}H, ^{13}C, ^{19}F) Spectra

Compound **1c**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8.24
8.23
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8.21
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7.97
7.95
7.95
7.84
7.82
7.75
7.75
7.73
7.73
7.69
7.67
7.67
7.66
7.64
7.56
7.54
7.45
7.44
7.43
7.42
7.26
2.76
1.58
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CH3
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N
N
O
O
1.00
1.03
1.03
1.00
1.02
2.08
1.03
1.05
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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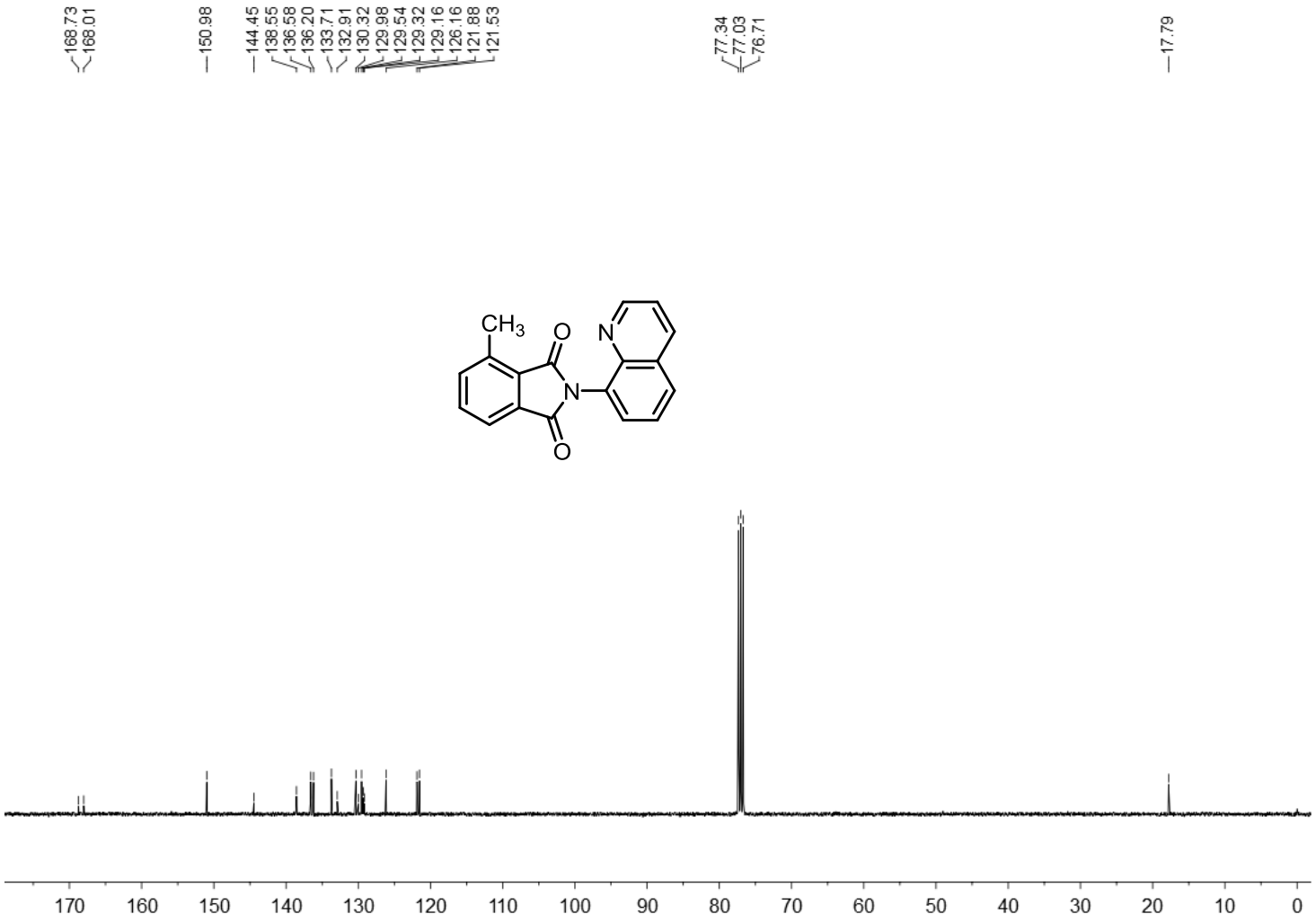
0.0
-0.5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138.55
136.58
136.20
133.71
132.91
130.32
129.98
129.54
129.32
129.16
126.16
121.88
121.53
77.34
77.03
76.71
17.79
CH3
O
N
N
O
O
170
160
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120
110
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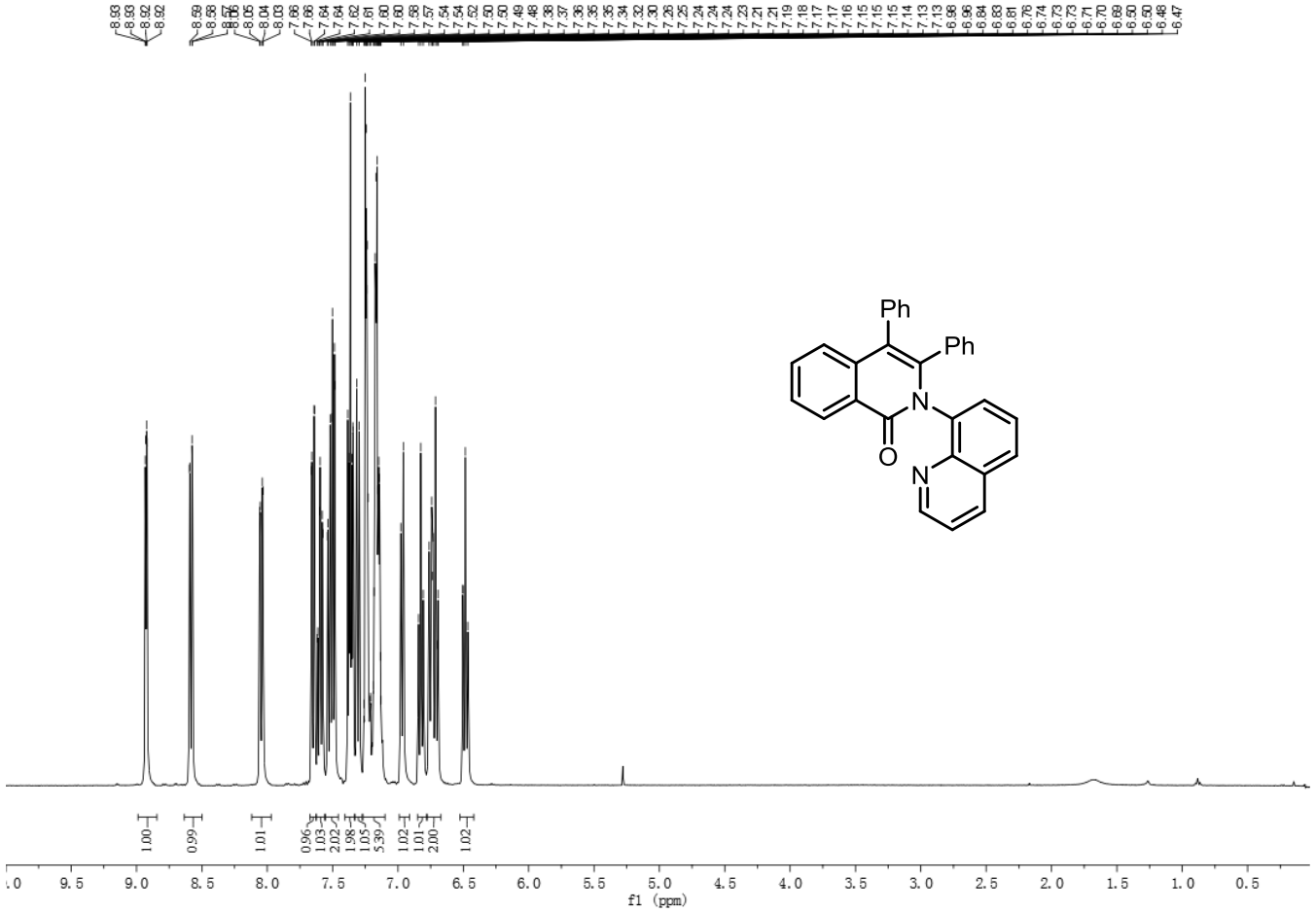
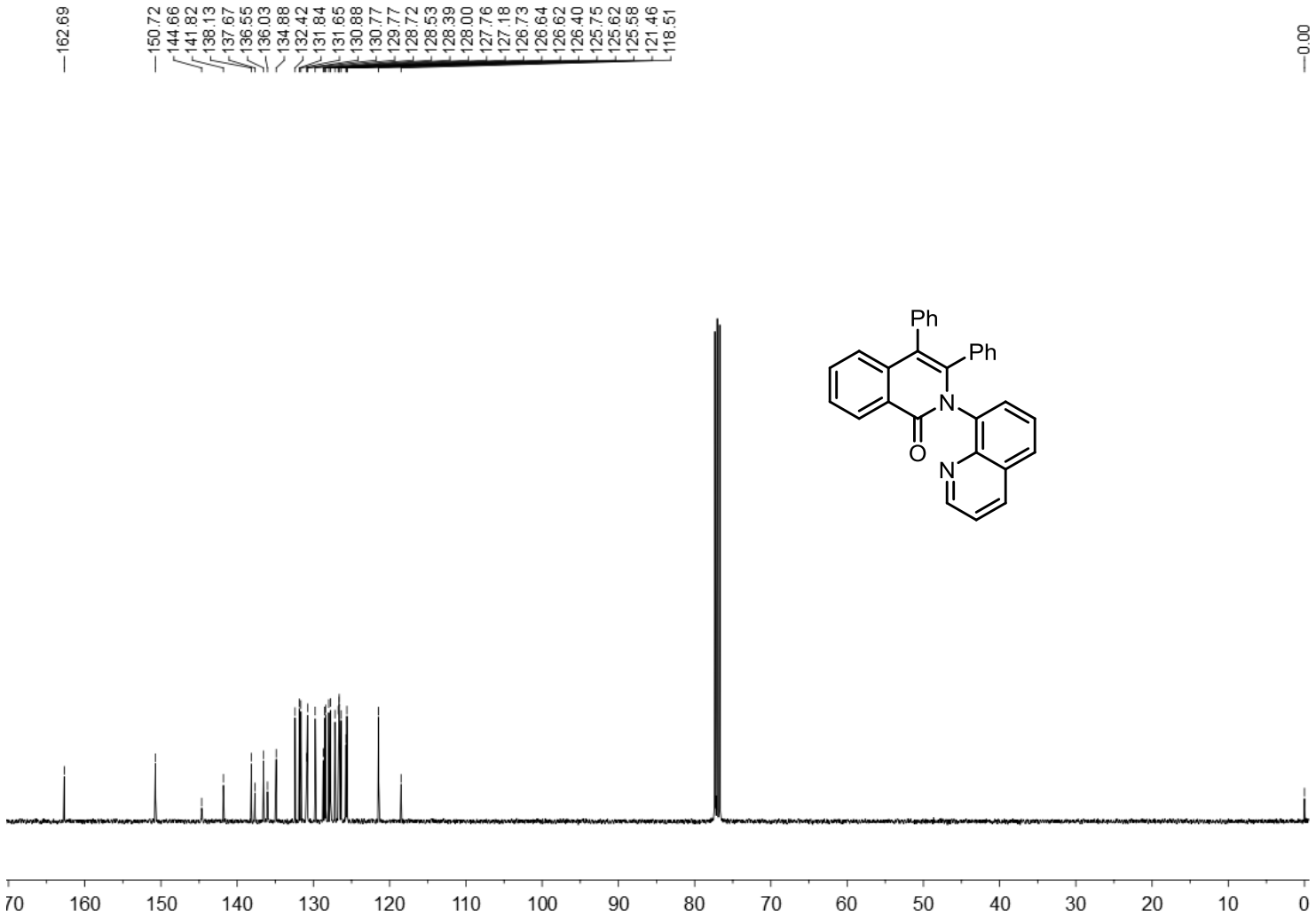
90
80
70
60
50
40
30
20
10
0

Compound **3aa**

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138.13
137.67
136.55
136.03
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130.77
129.77
128.72
128.53
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127.18
126.73
126.64
126.62
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125.75
125.62
125.58
121.46
118.51
0.00
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Ph
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O
N
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110
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90
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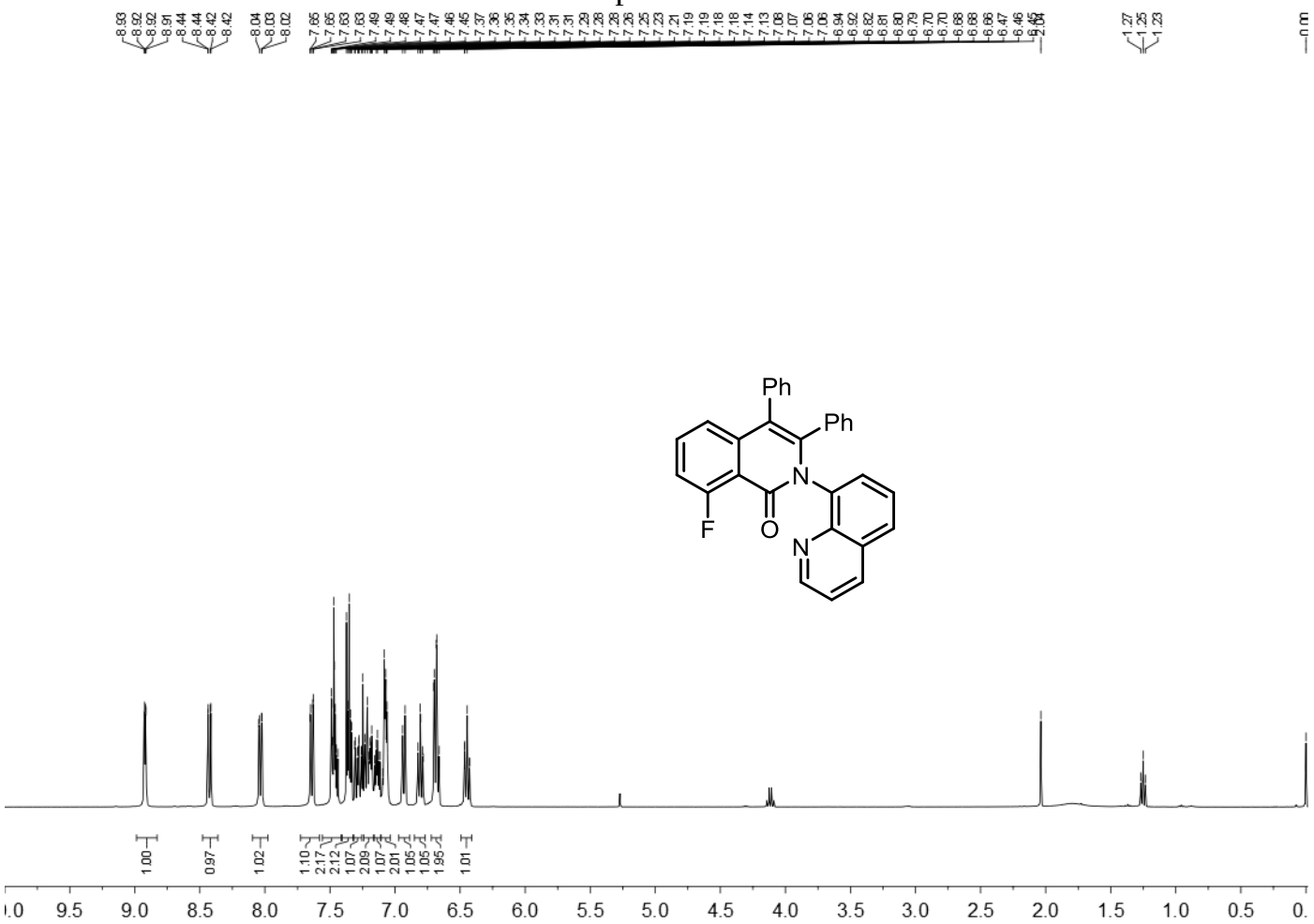
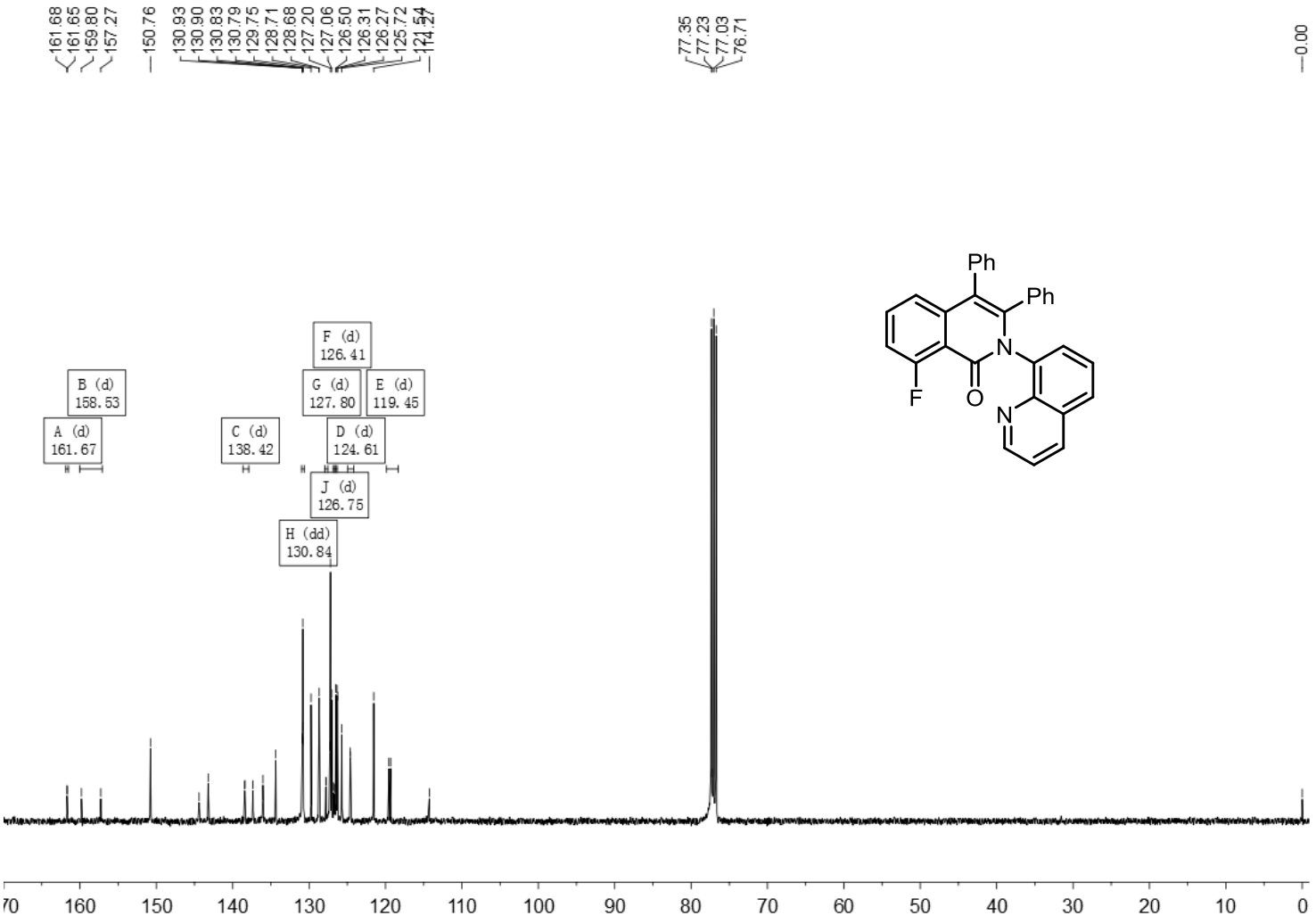
10
0

Compound **3ba**

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126.31
126.27
125.72
77.35
77.23
77.03
76.71
0.00
A (d)
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B (d)
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C (d)
138.42
D (d)
124.61
E (d)
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F (d)
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G (d)
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H (dd)
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O
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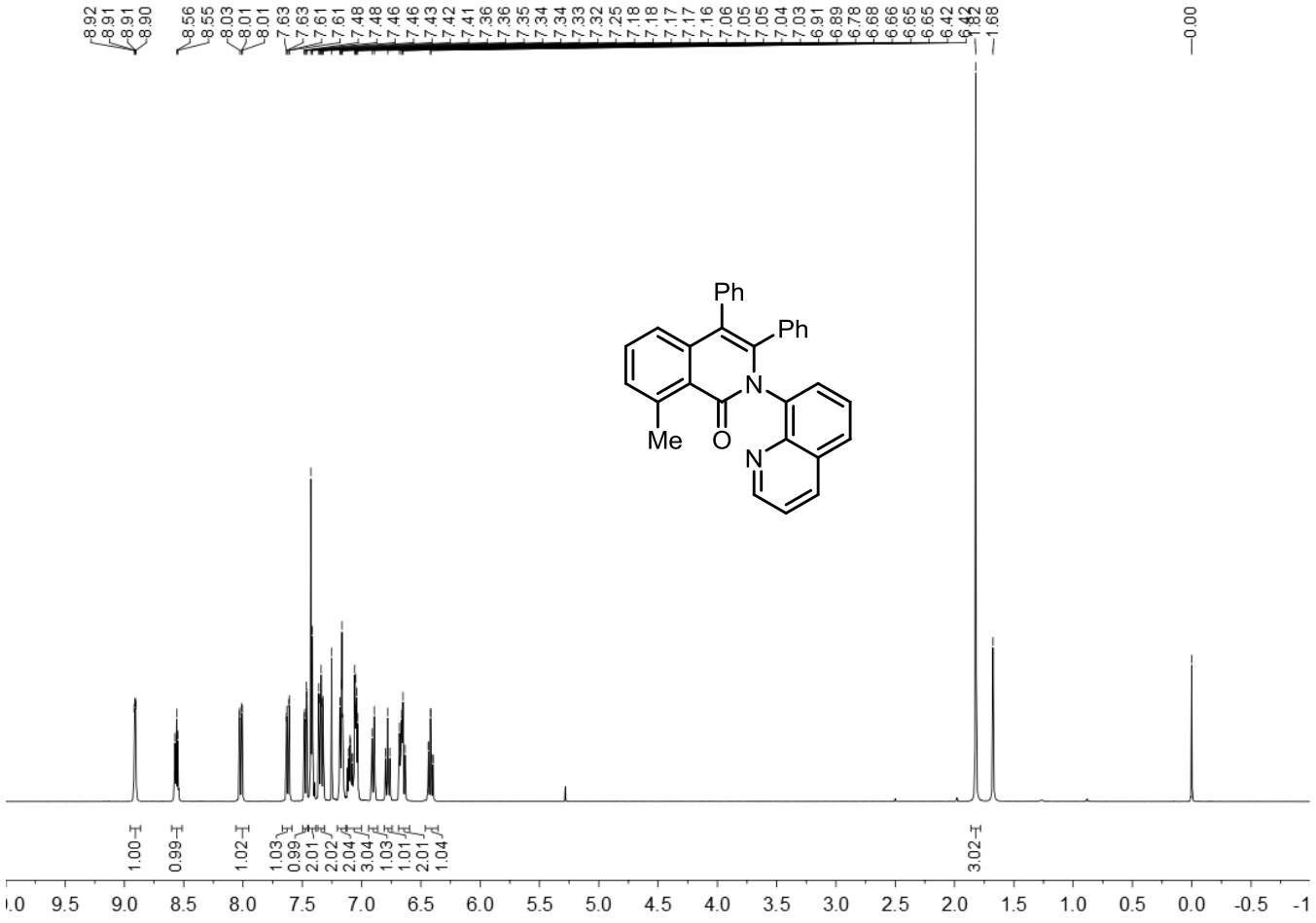

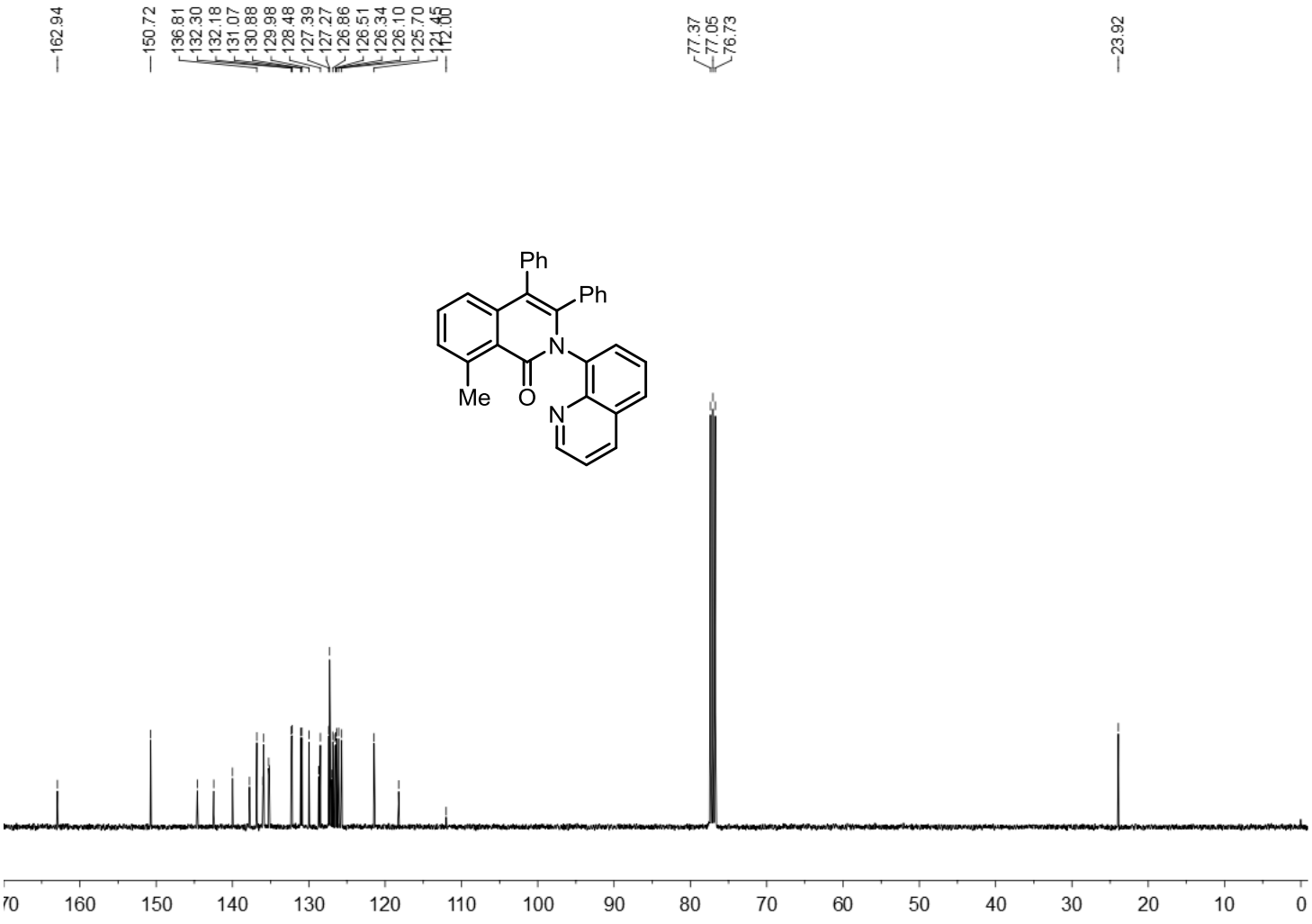
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Ph
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Me
O
N
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50
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30
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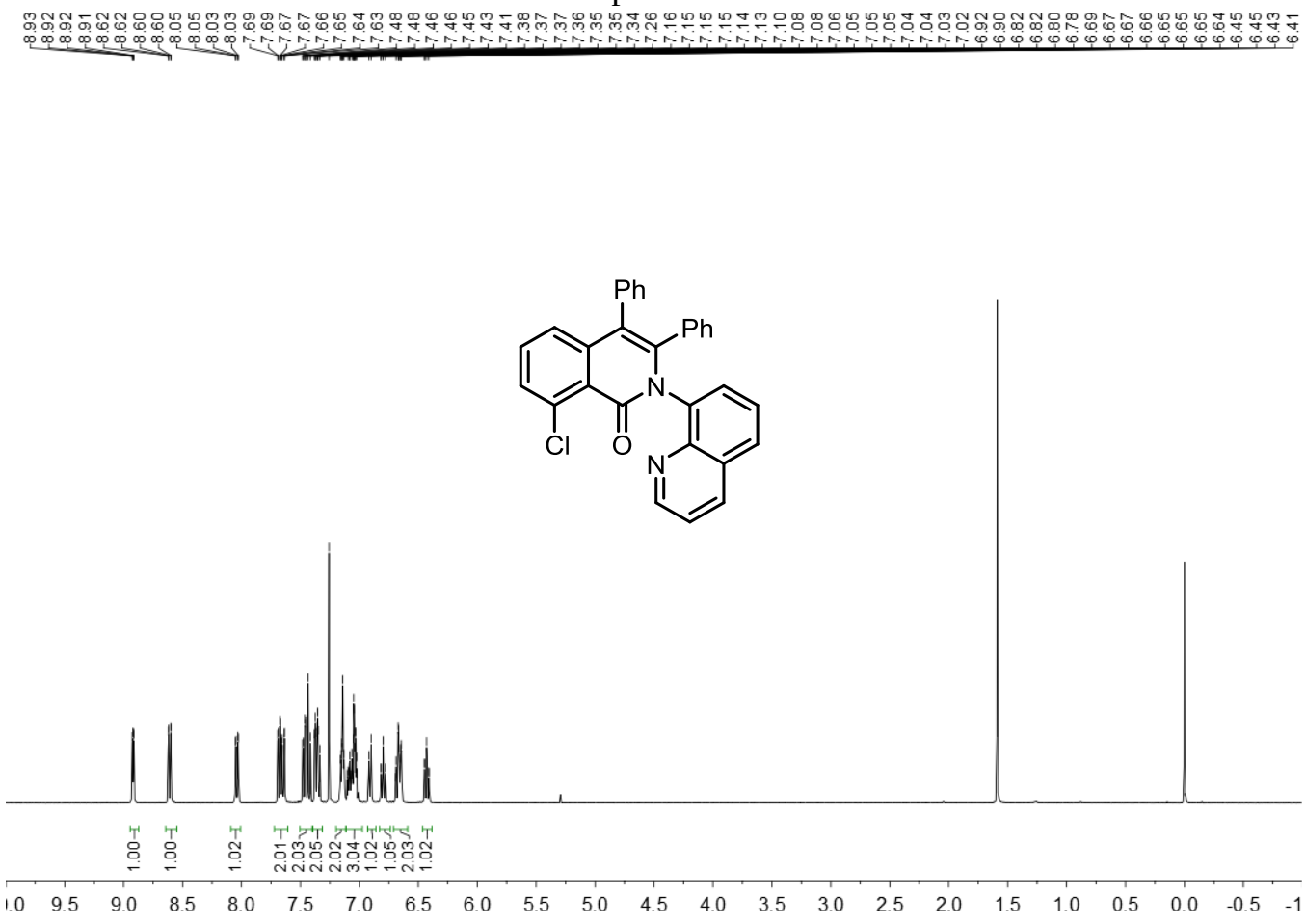
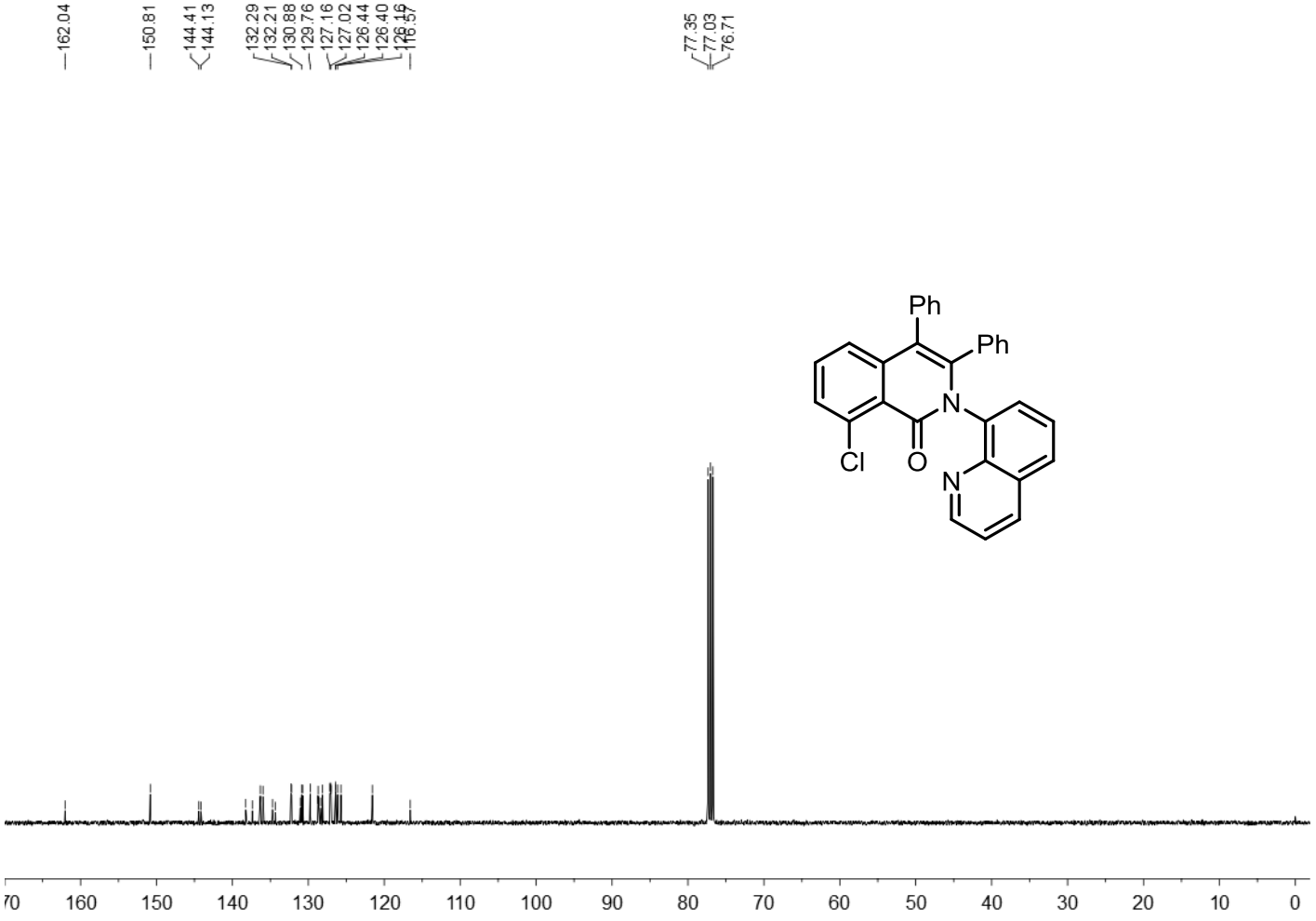
Compound **3da**

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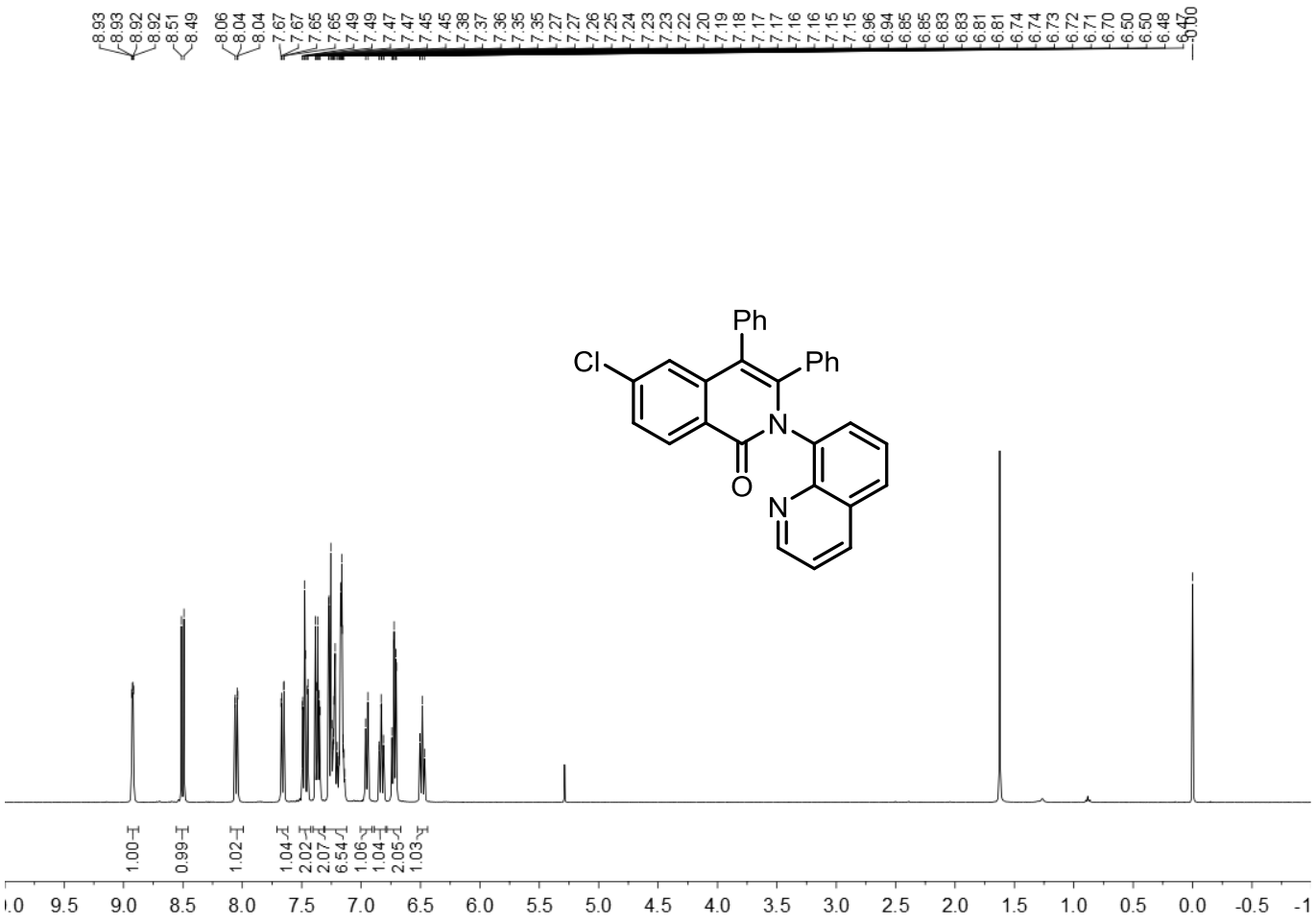
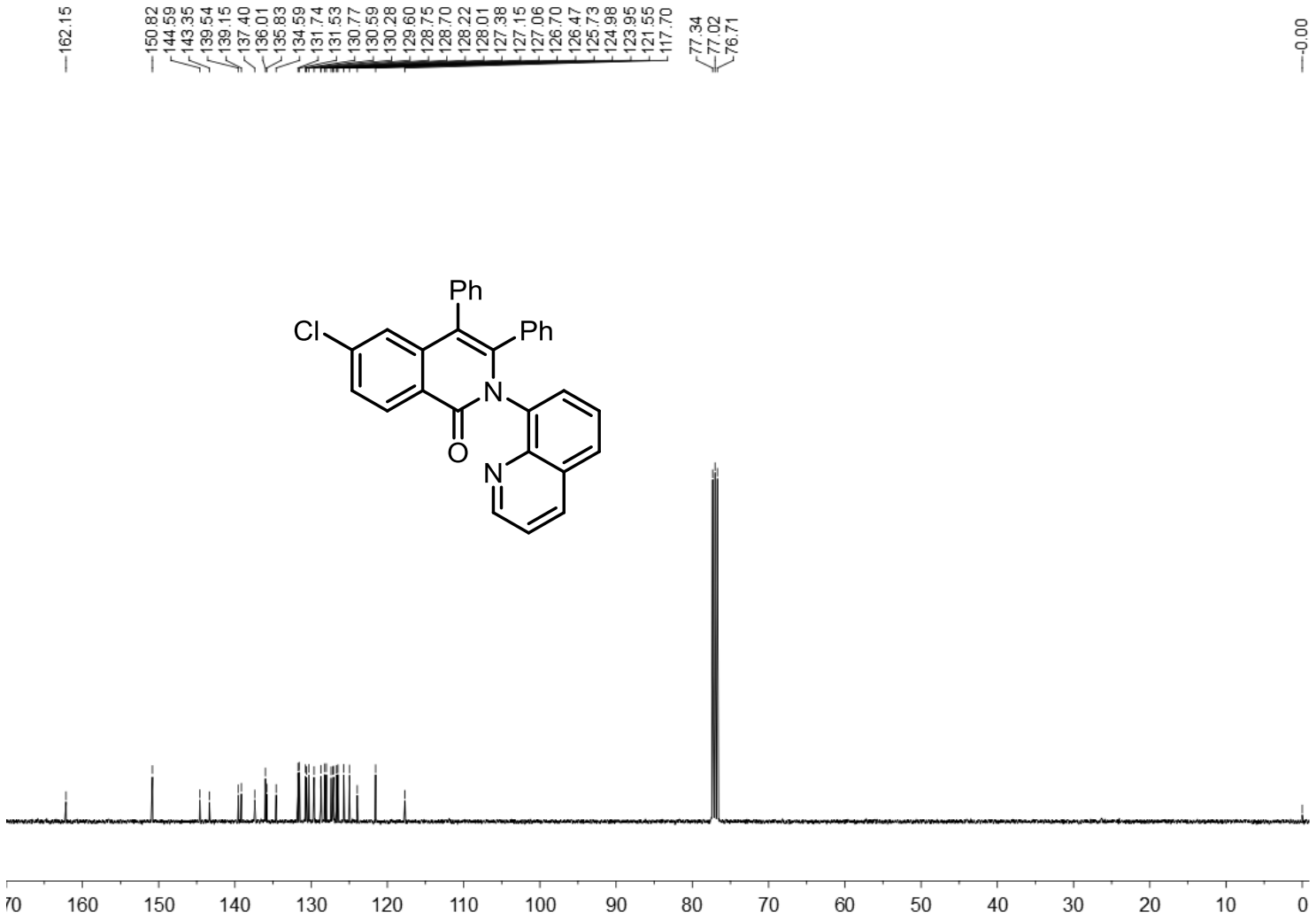
Compound **3ea**

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Cl
Ph
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O
N
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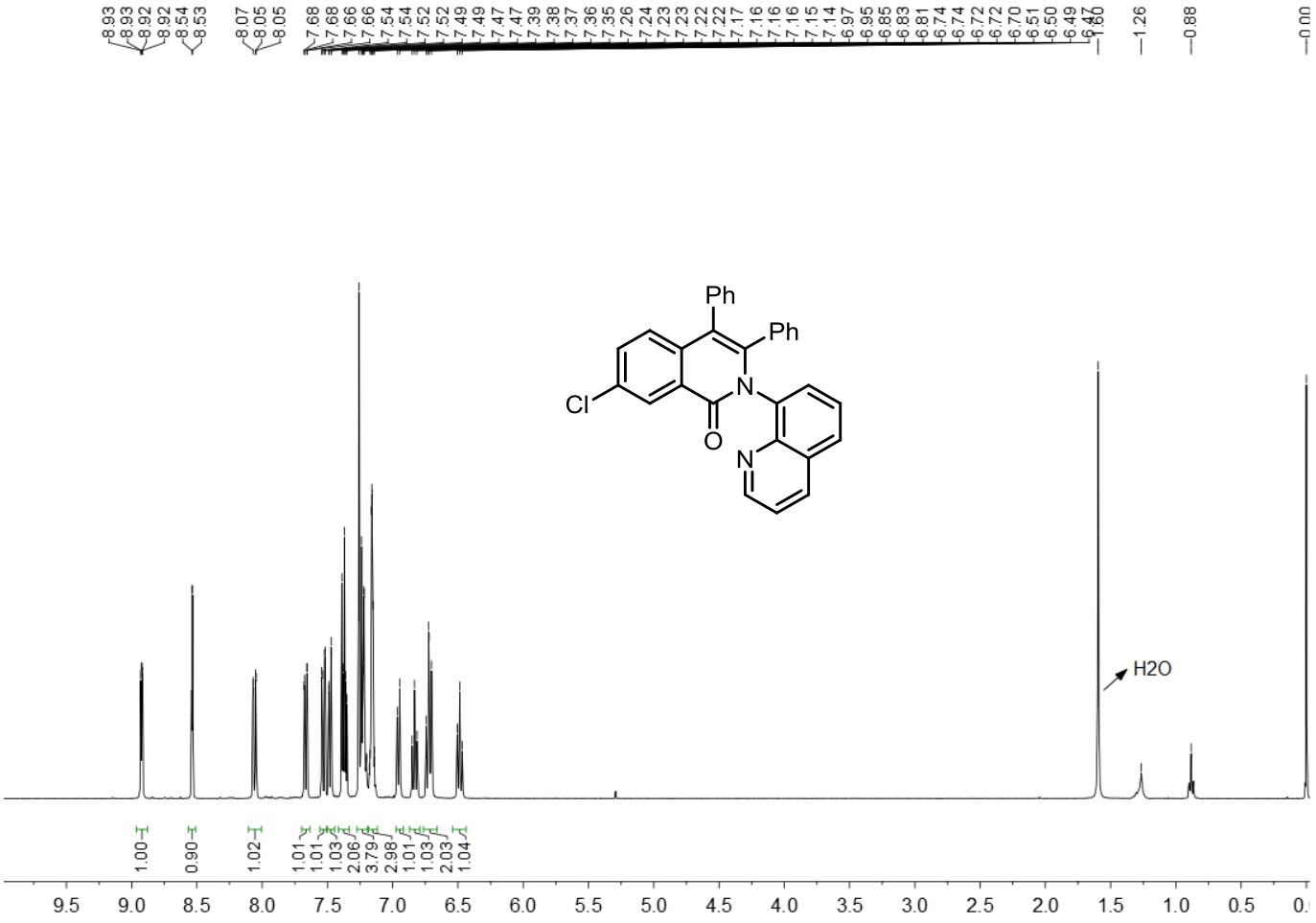
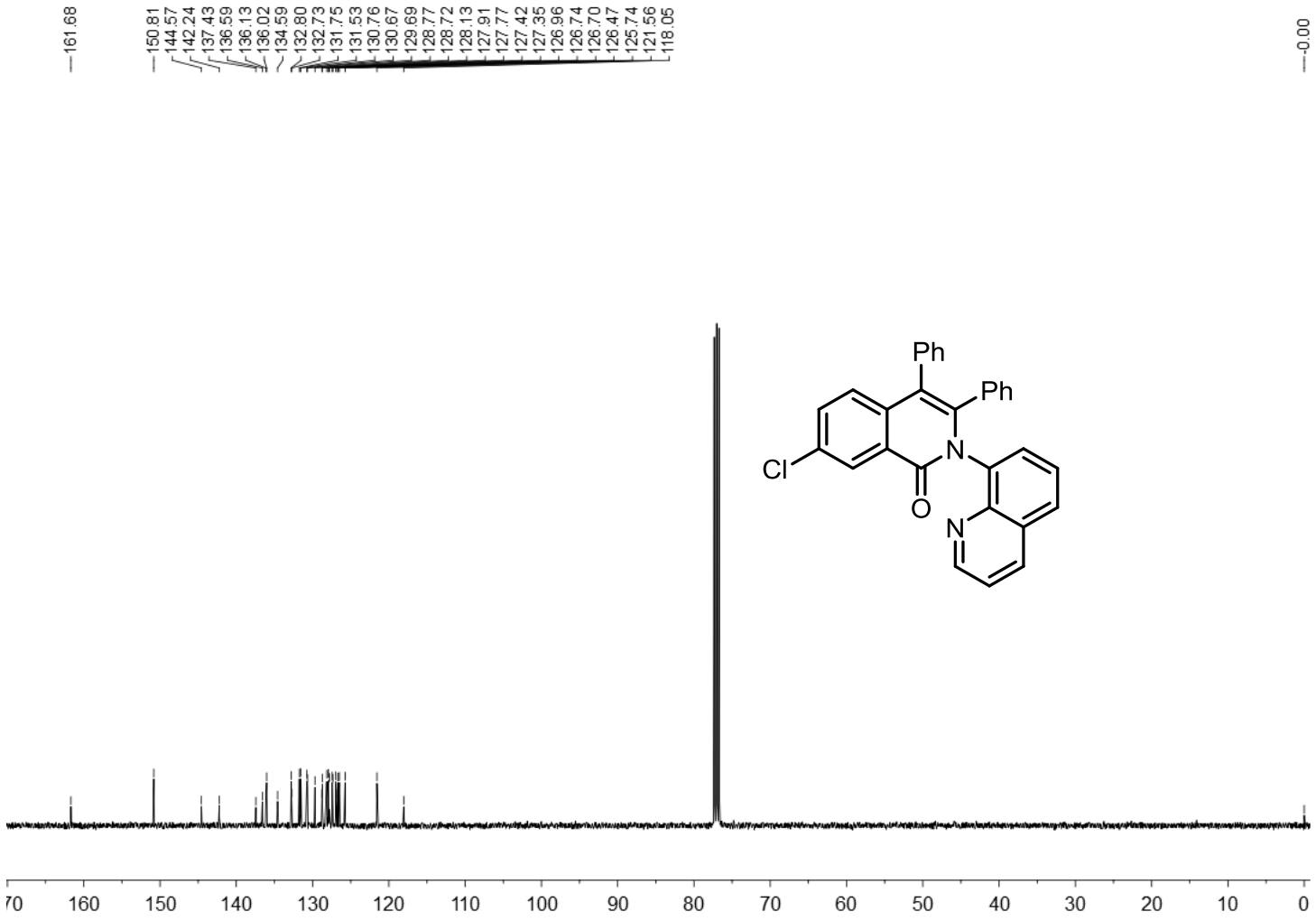
Compound **3ea'**

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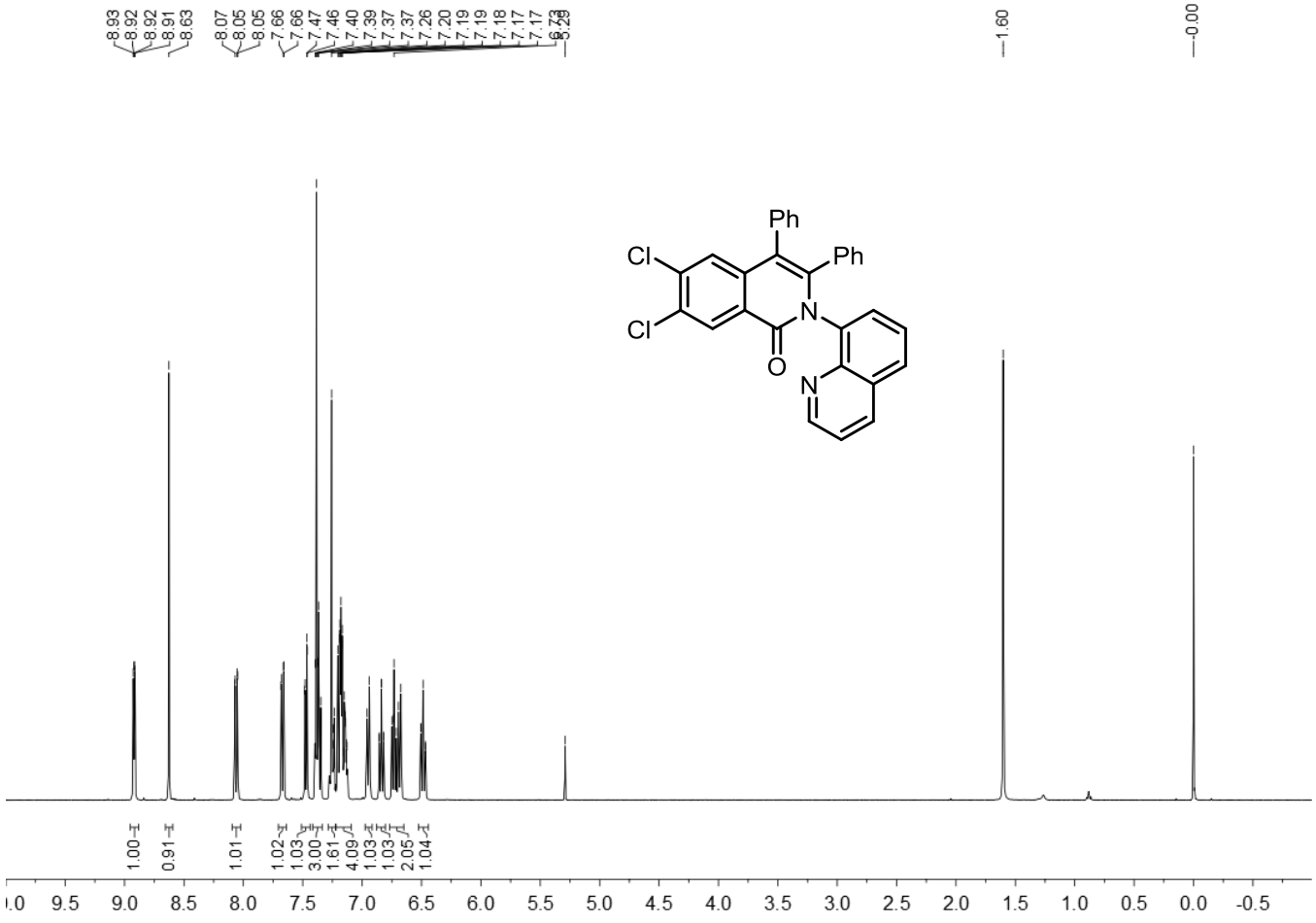
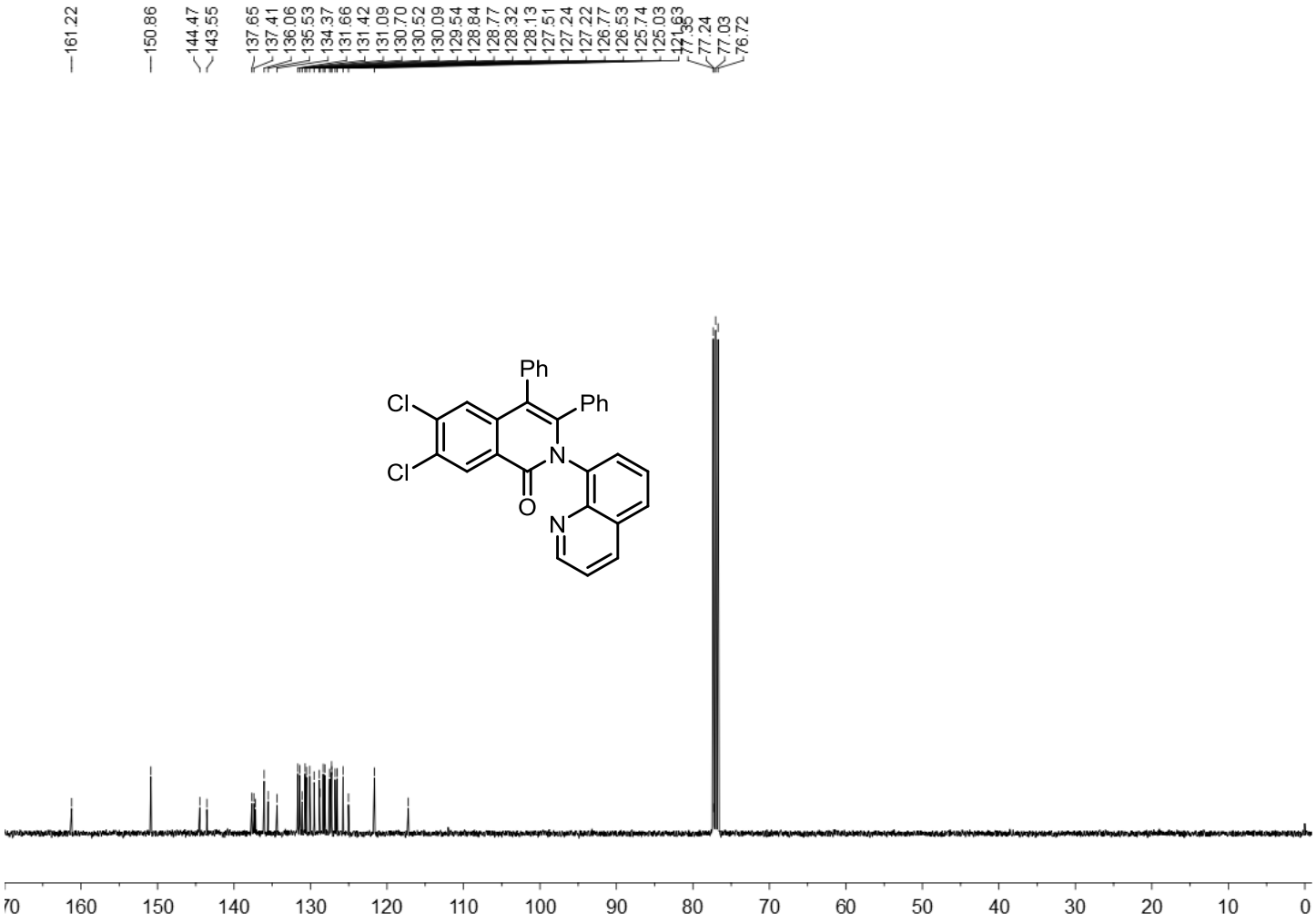
Compound **3fa**

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Cl
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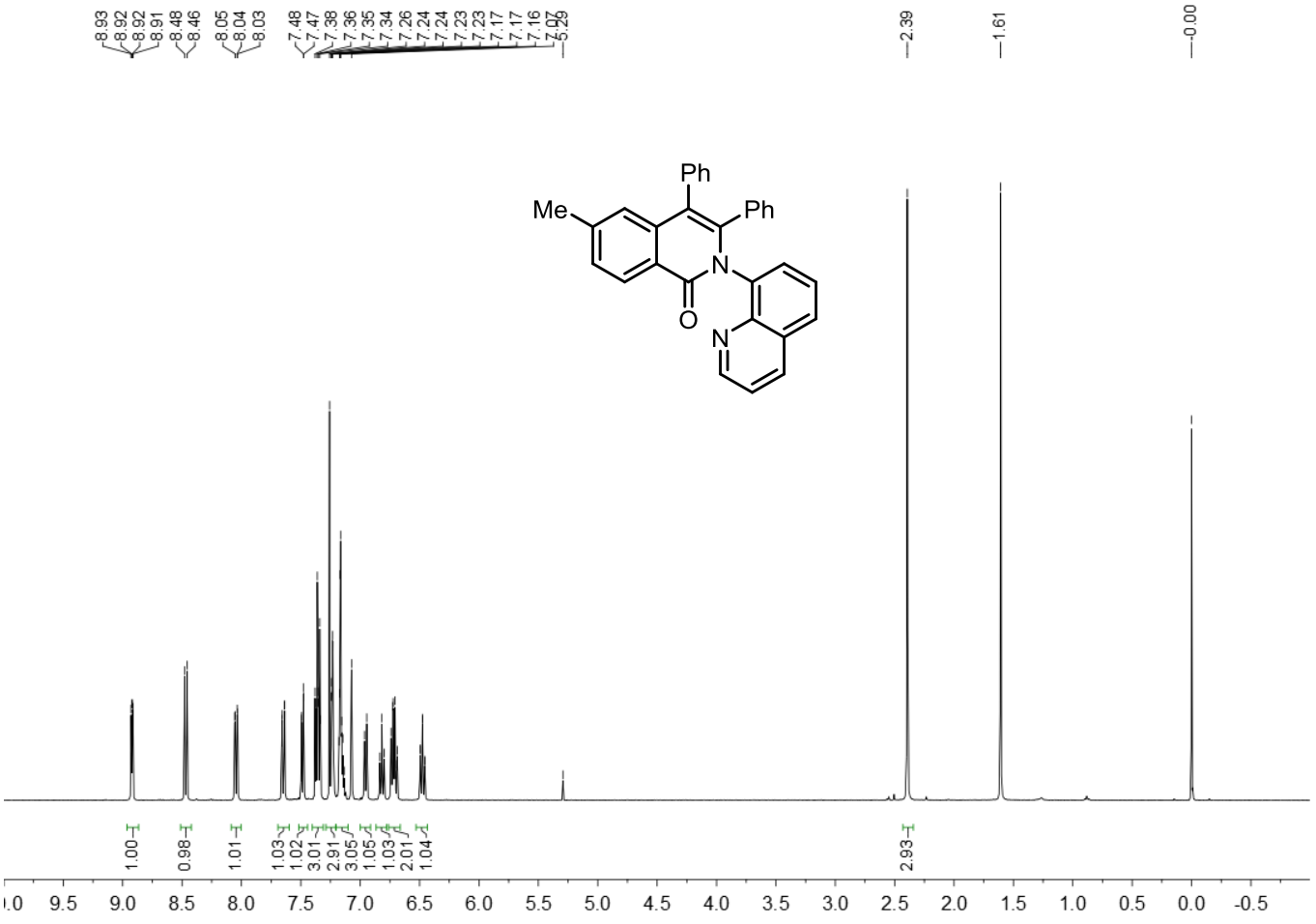
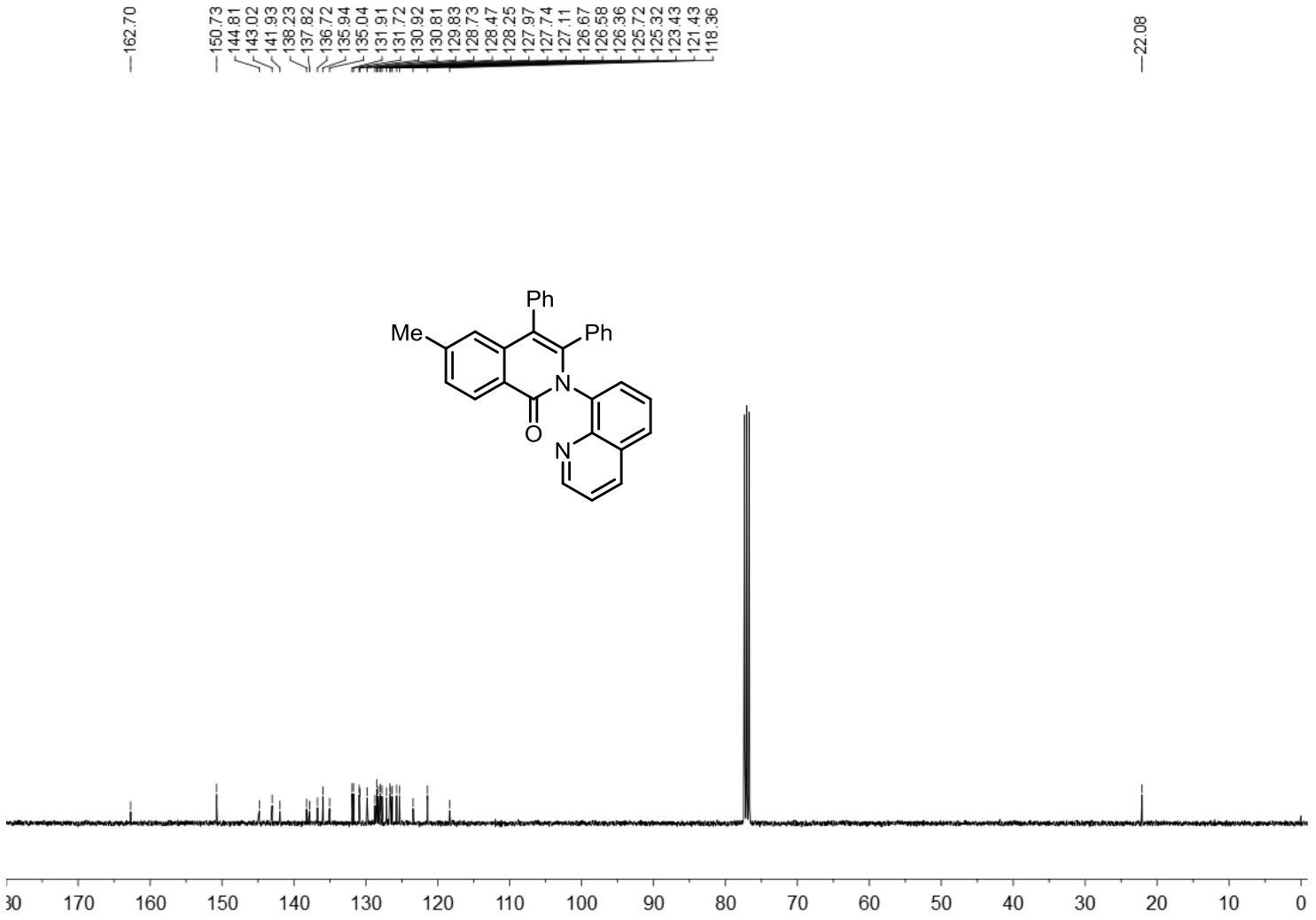
Compound **3ga'**

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Me
Ph
N
O
N
30
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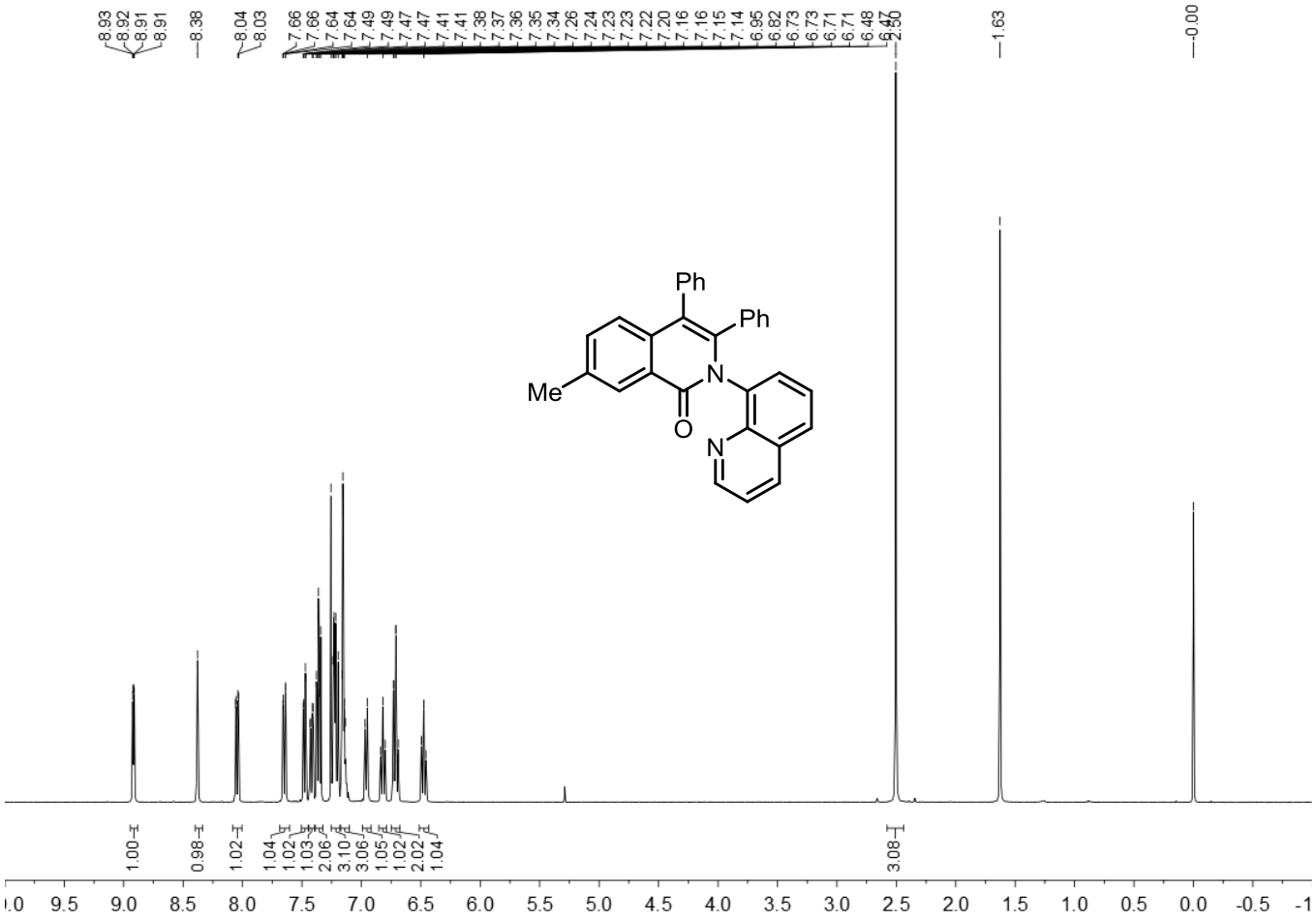
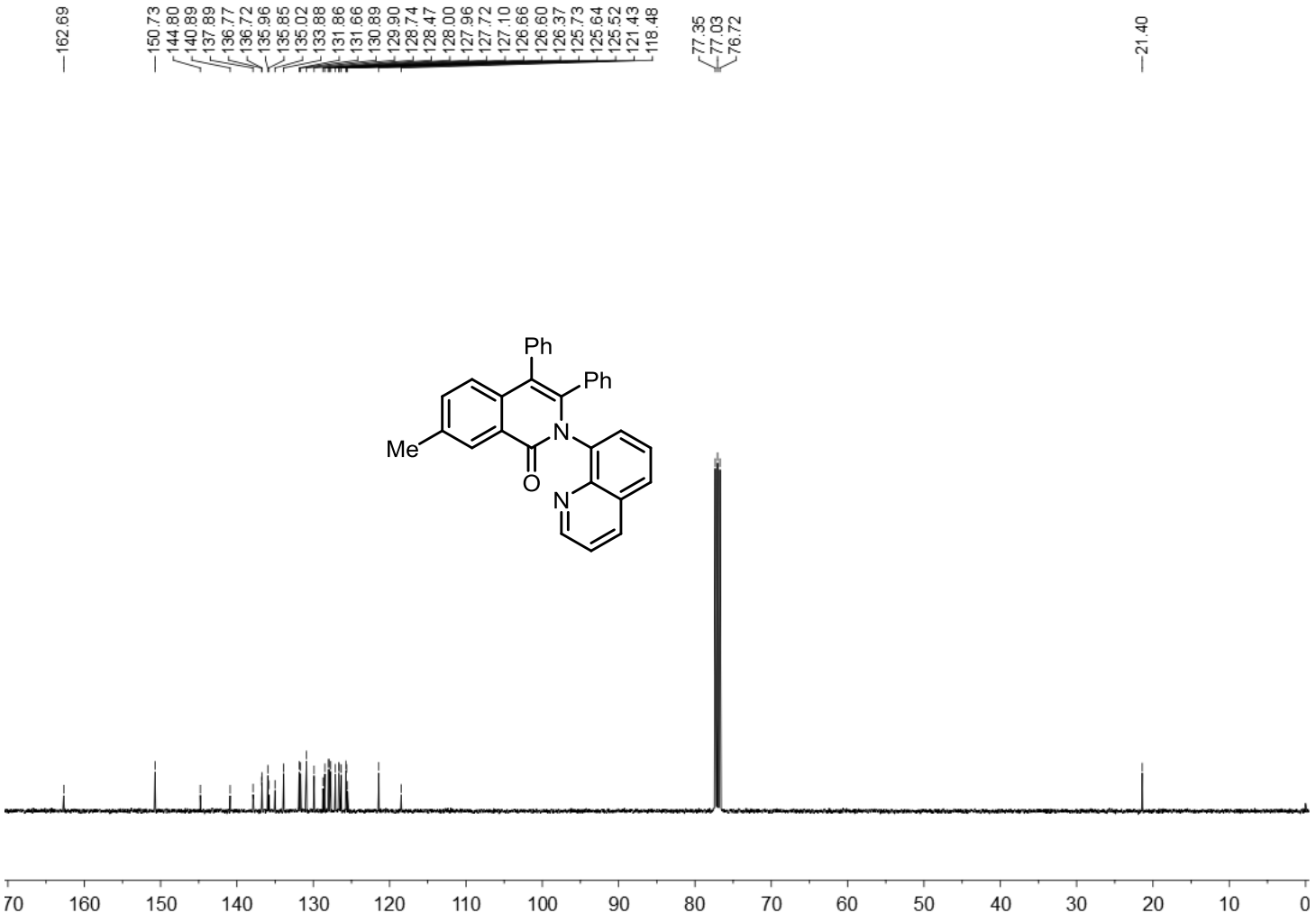
Compound **3ga**

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Ph
Me
O
N
N
70
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90
80
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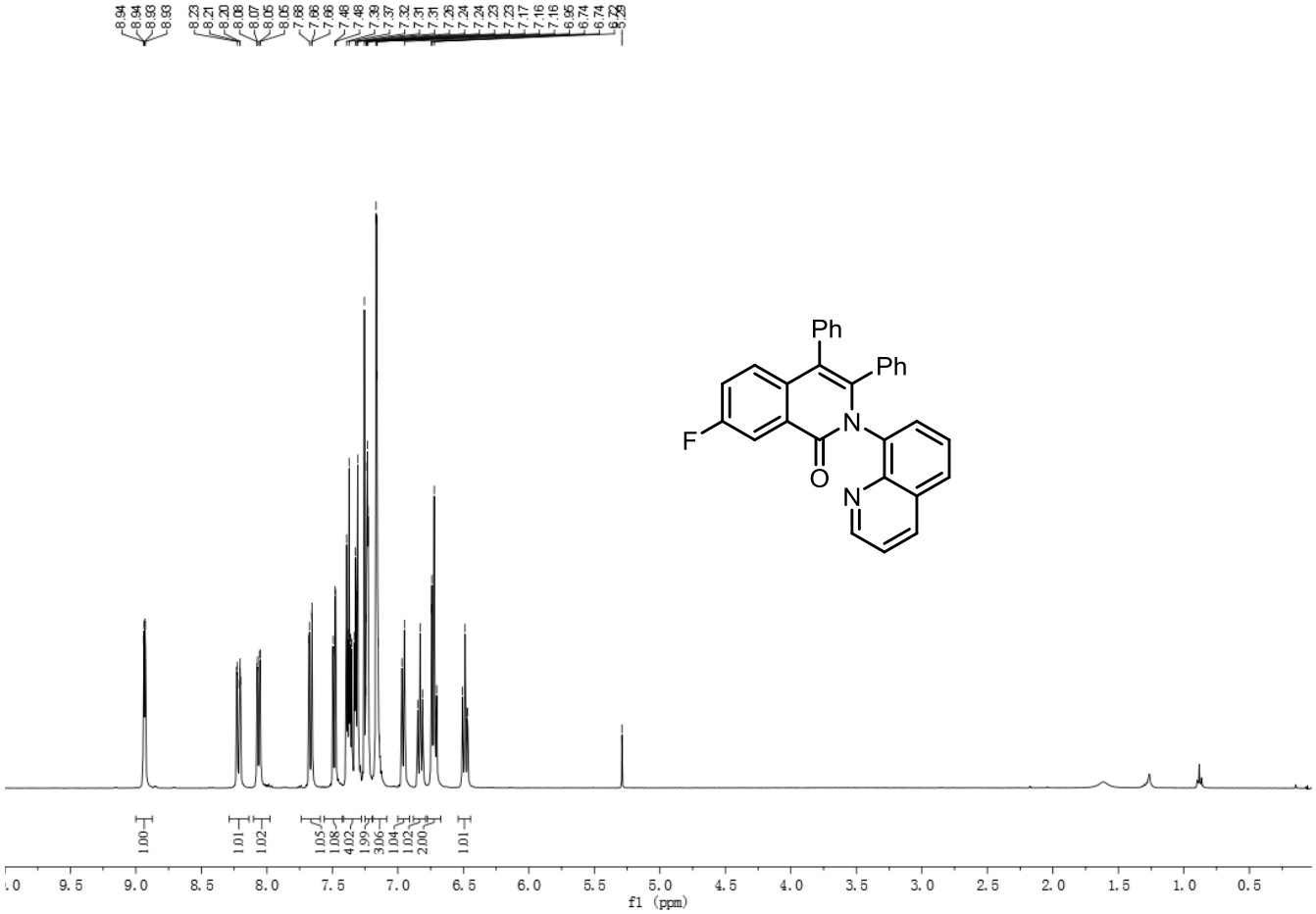
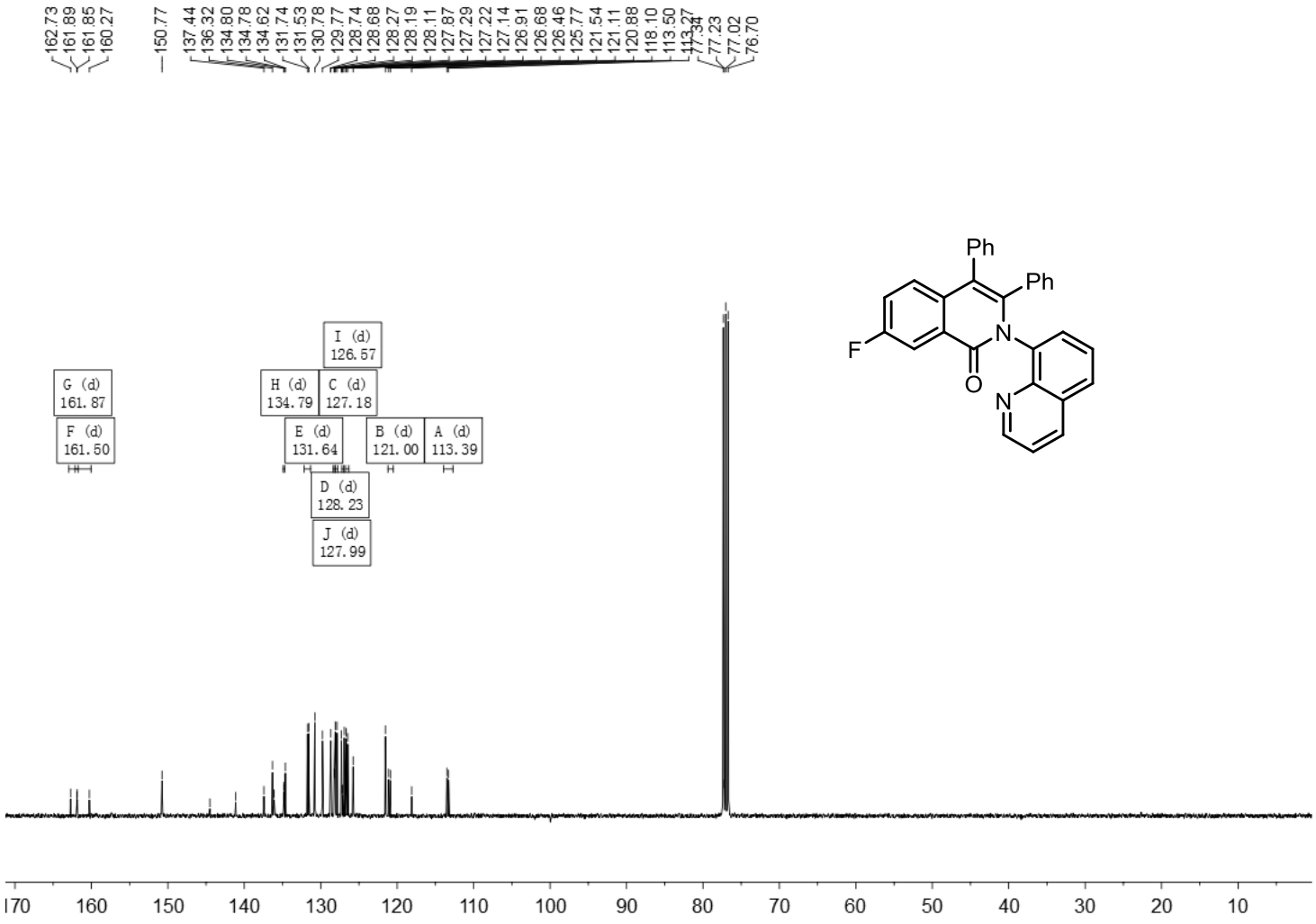
0

Compound **3ha**

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77.34
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77.02
76.70
G (d) 161.87
F (d) 161.50
I (d) 126.57
H (d) 134.79
C (d) 127.18
E (d) 131.64
B (d) 121.00
A (d) 113.39
D (d) 128.23
J (d) 127.99
Ph
Ph
F
N
O
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


-113.79
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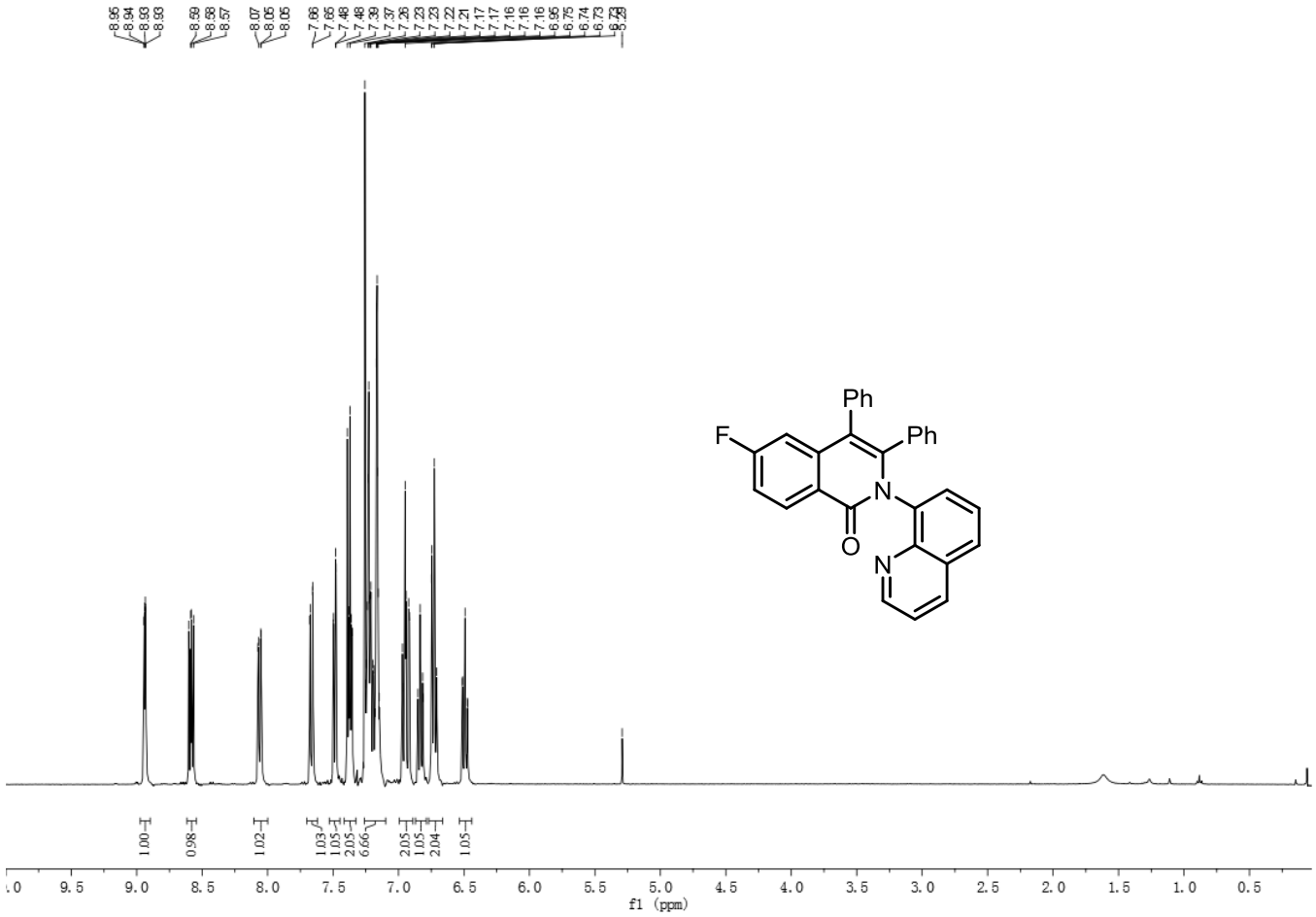
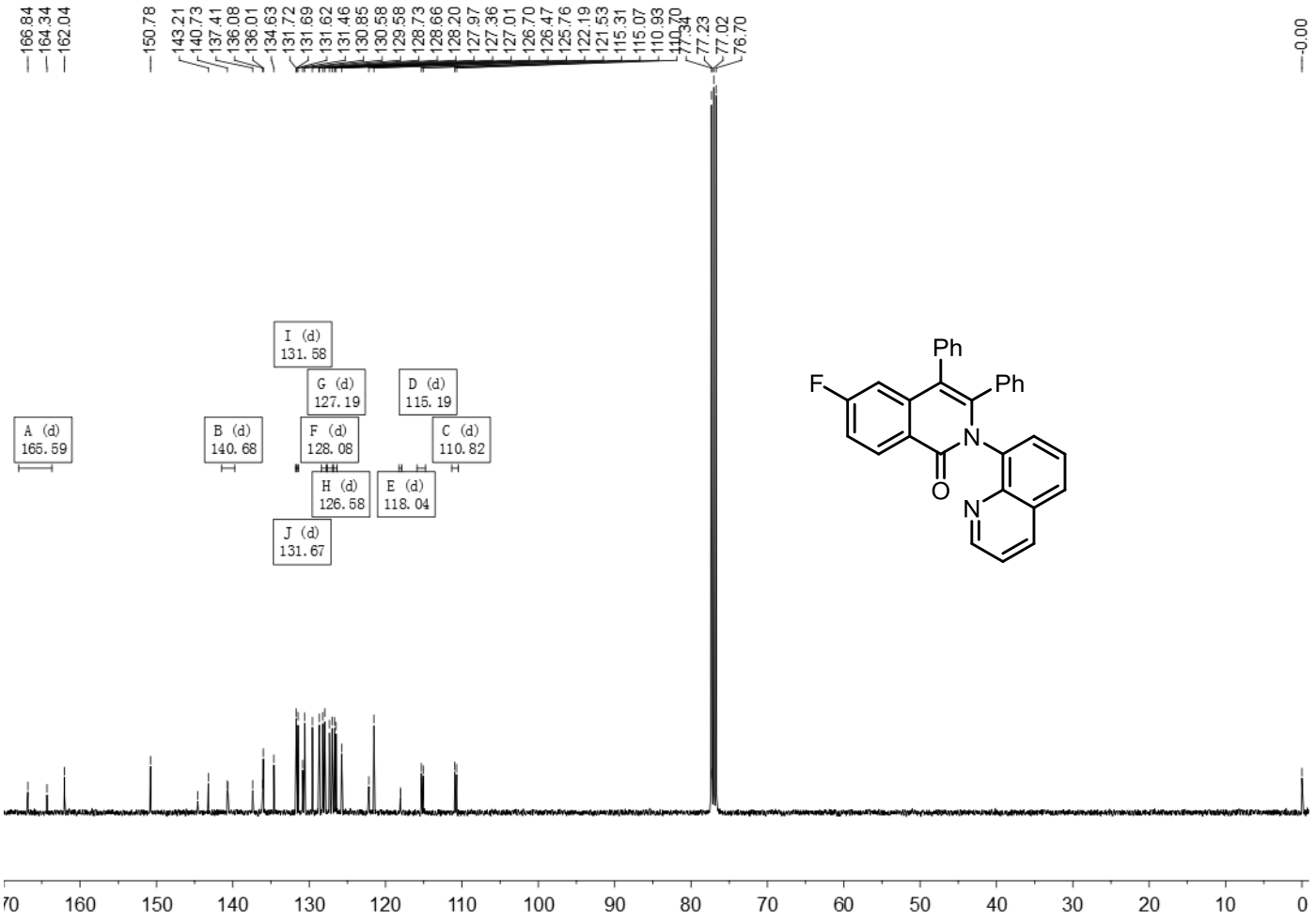
Compound **3ha'**

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125.76
122.19
121.53
115.31
115.07
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I (d) 131.58
G (d) 127.19
D (d) 115.19
A (d) 165.59
B (d) 140.68
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70
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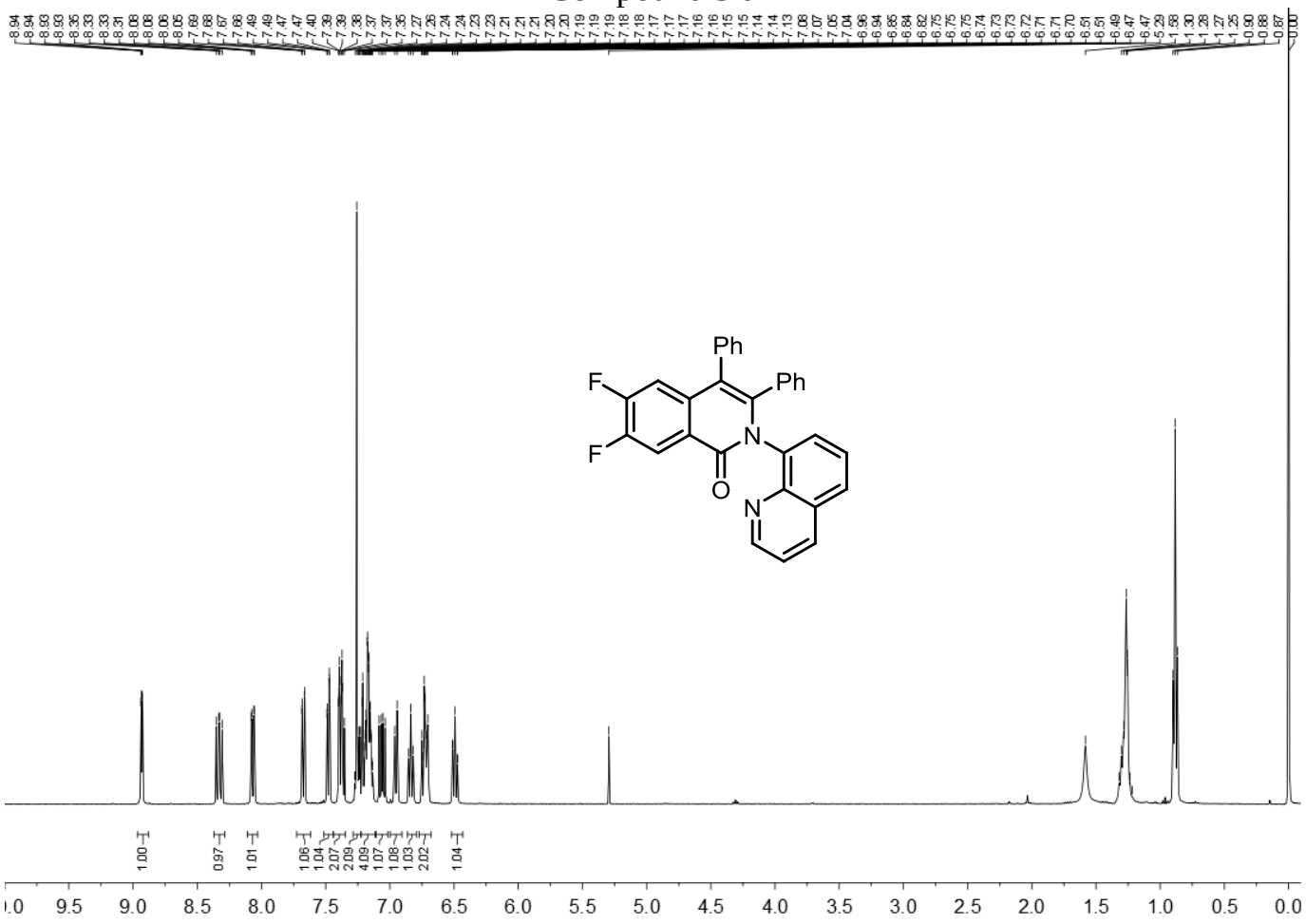
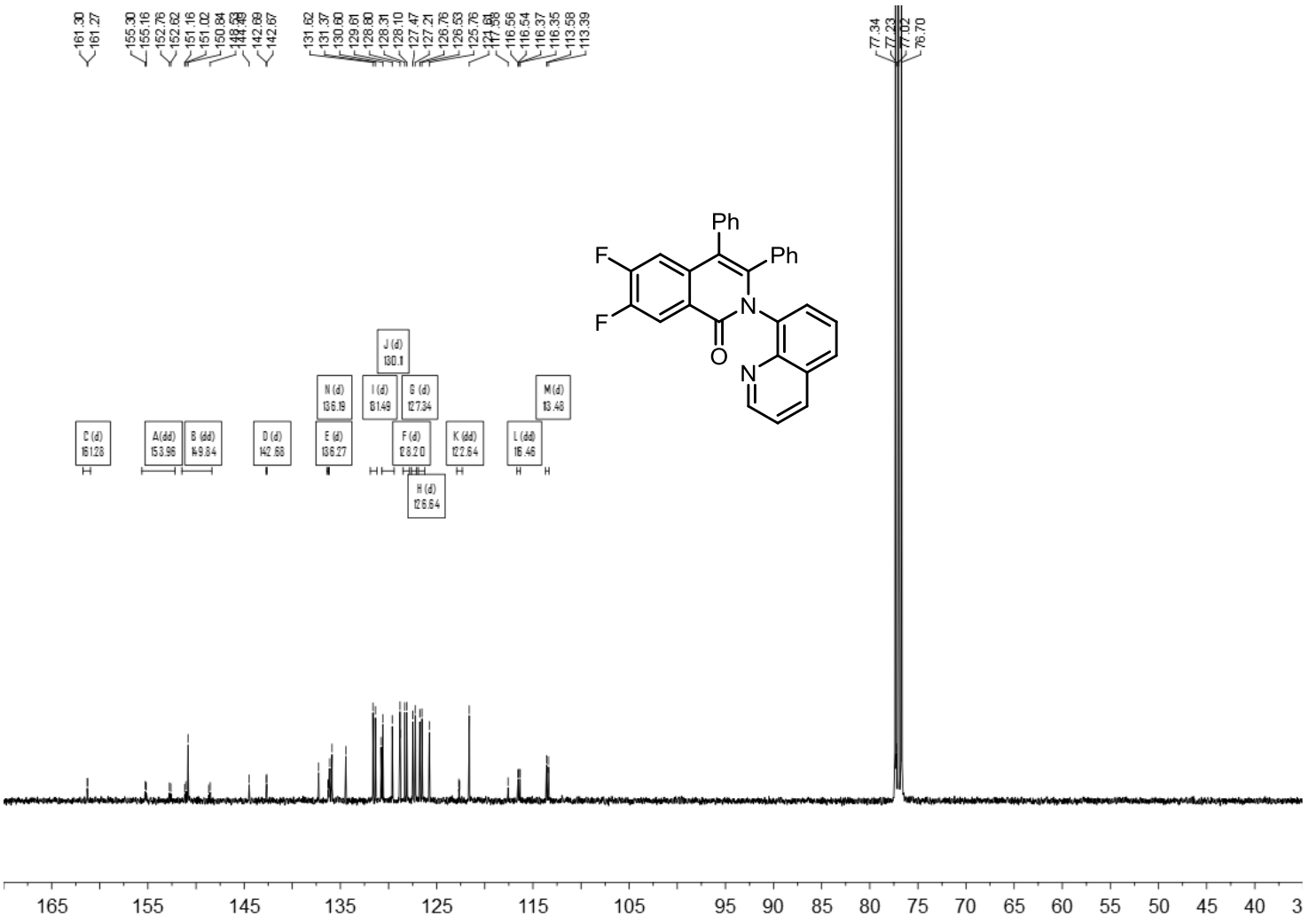
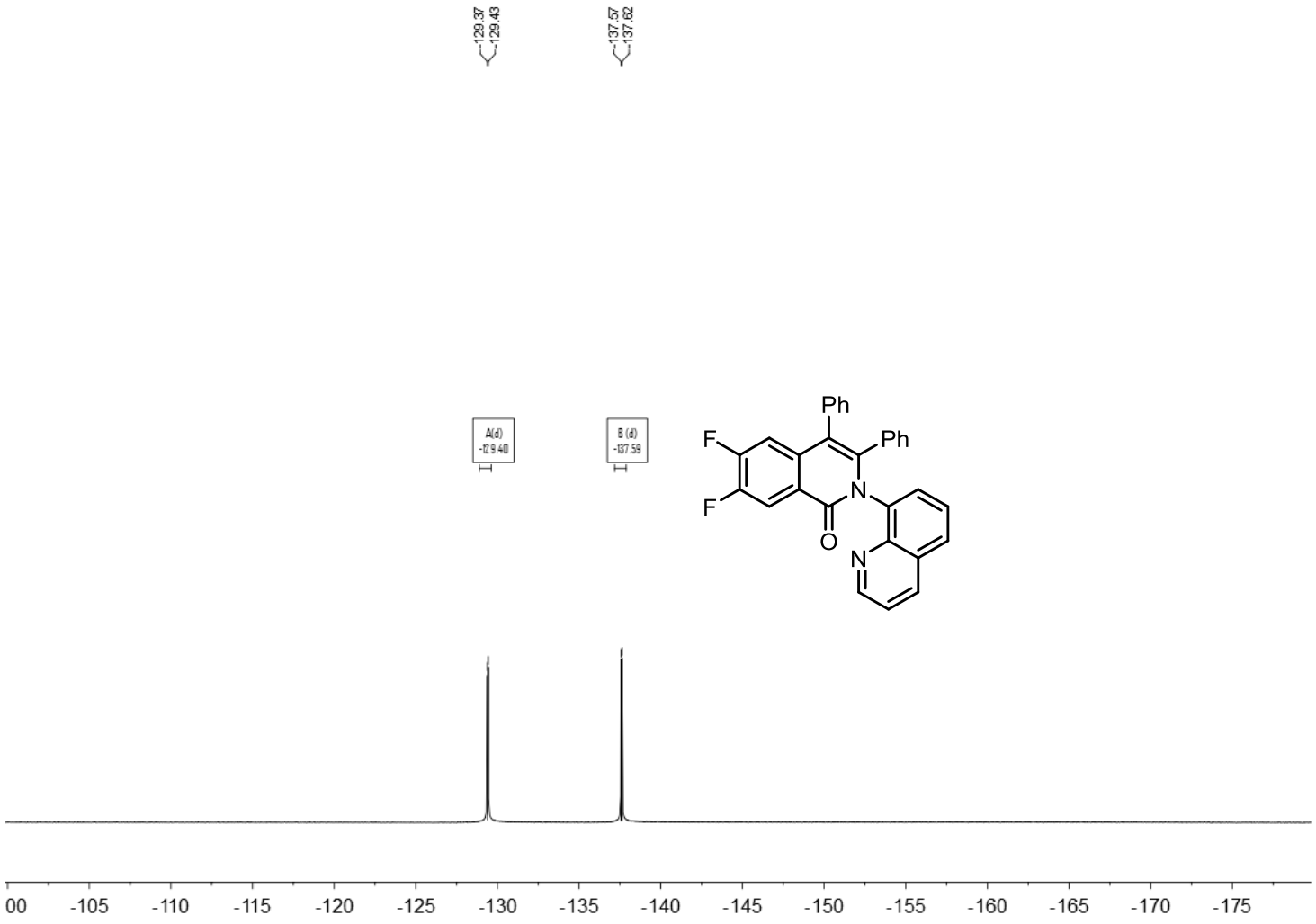
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

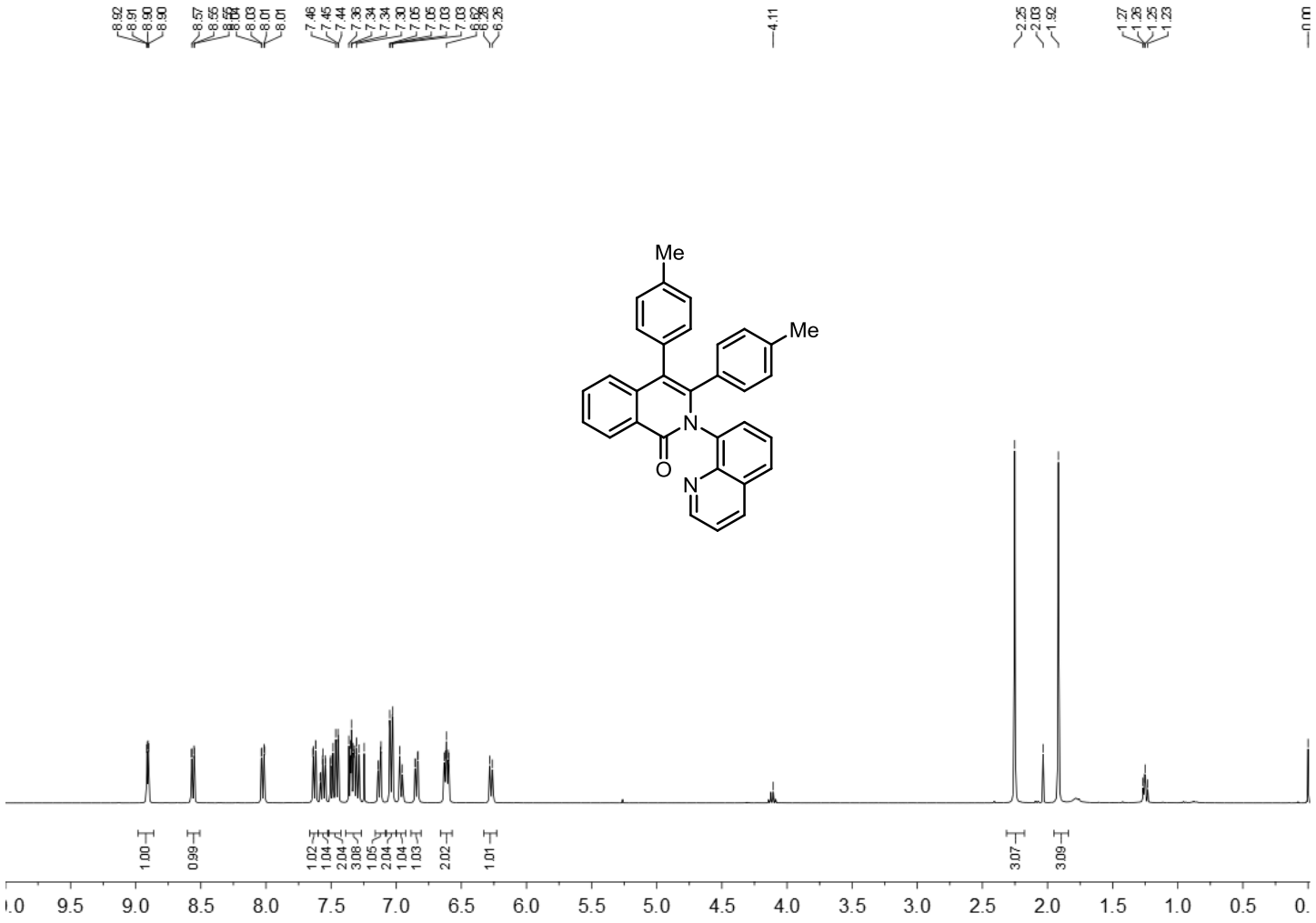
Compound **3ia**

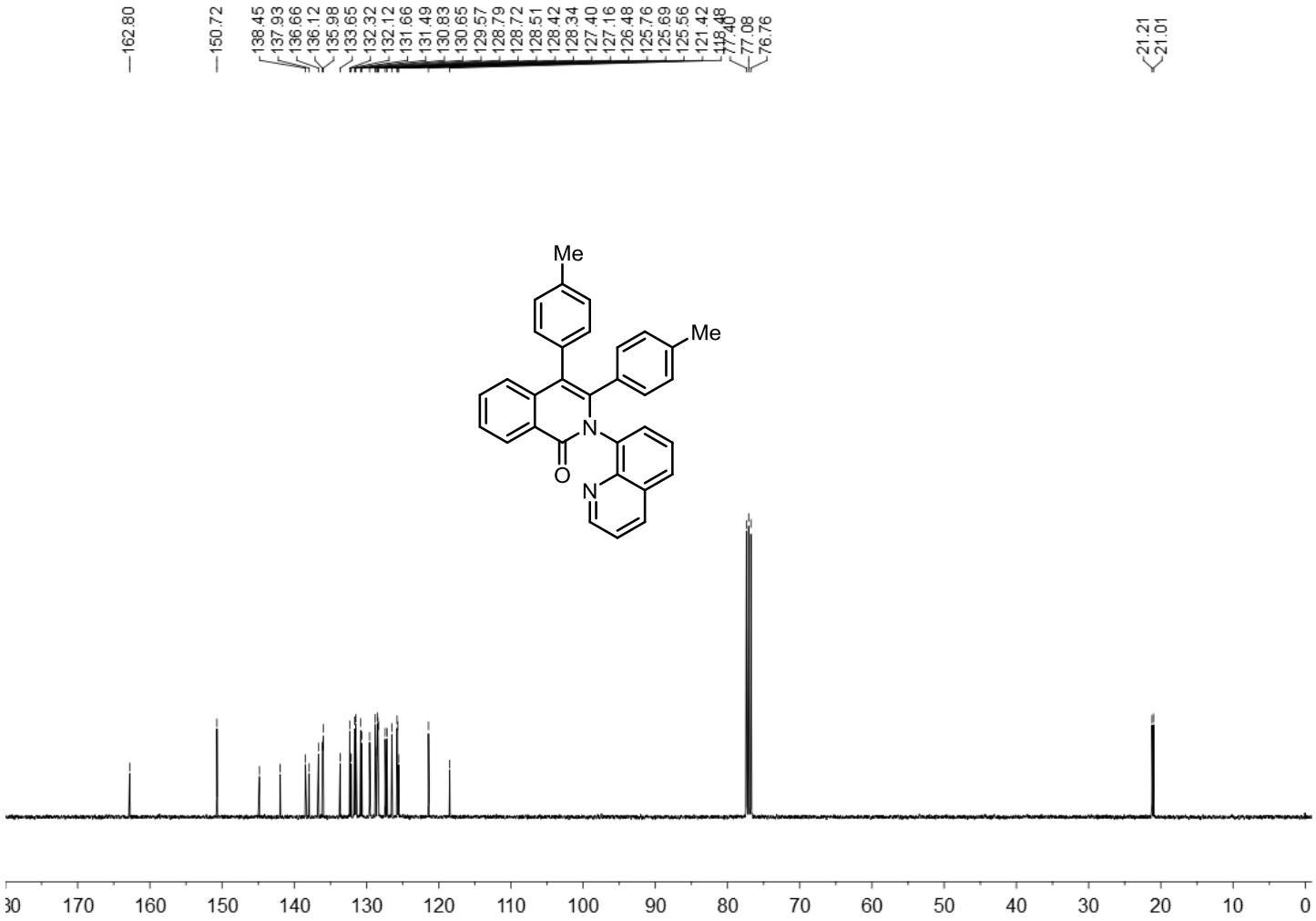



161.30
161.27
155.30
155.16
152.76
152.62
151.16
151.02
150.84
142.89
142.67
131.62
131.37
130.60
129.61
128.80
128.31
128.10
127.47
127.21
126.76
126.53
125.76
116.56
116.54
116.37
116.35
113.58
113.39
77.34
77.23
77.02
76.70
C (d) 161.28
A(dd) 153.96
B (dd) 149.84
D (d) 142.68
N (d) 136.19
E (d) 136.27
I (d) 131.49
J (d) 130.11
G (d) 127.34
F (d) 126.20
H (d) 126.64
K (dd) 122.64
L (dd) 116.46
M (d) 113.48
Ph
Ph
F
F
N
O
N
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
3

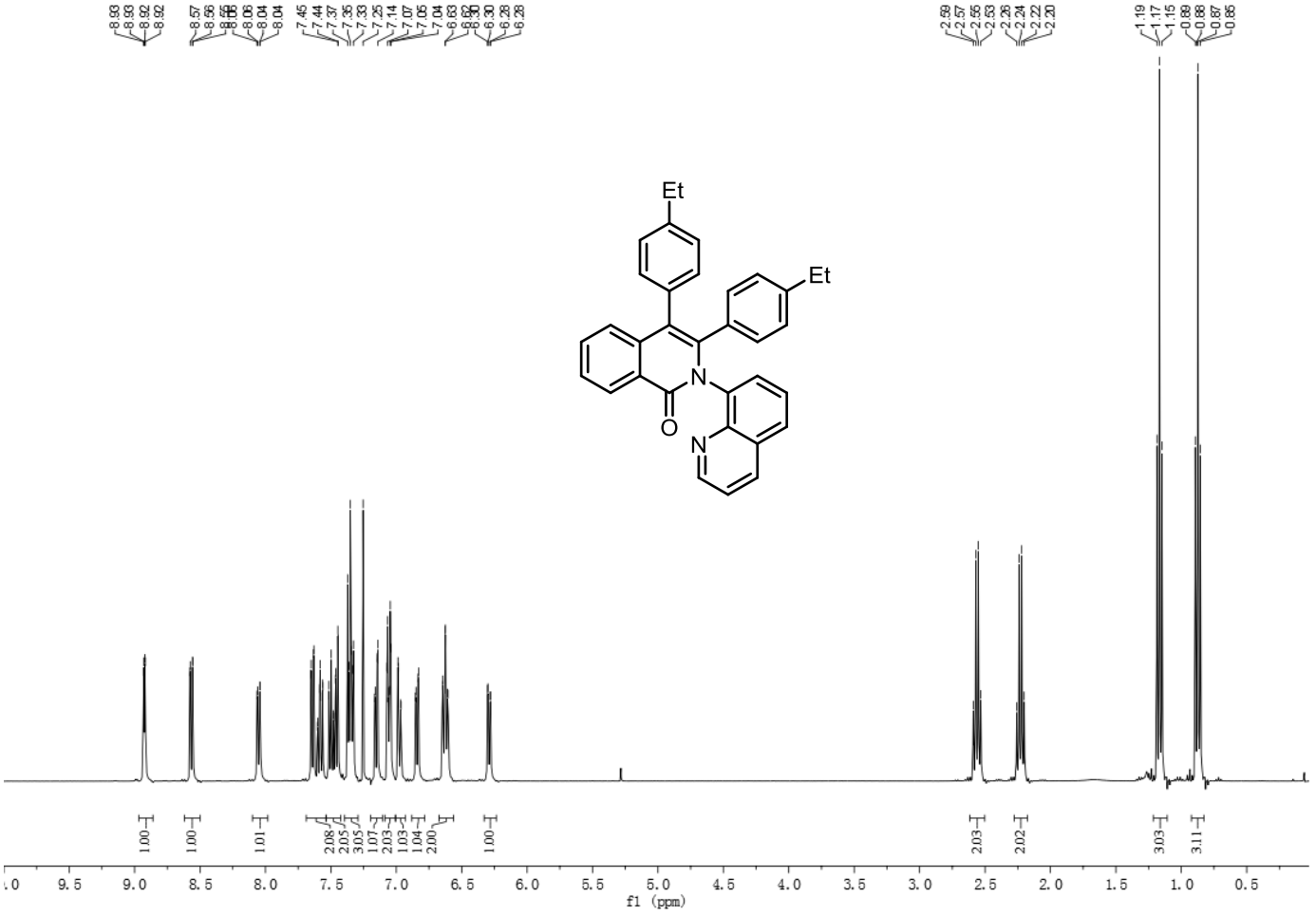

-129.37
-129.43
-137.57
-137.62
A(d)
-129.40
B (d)
-137.59
Ph
Ph
F
F
N
O
N
00
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175

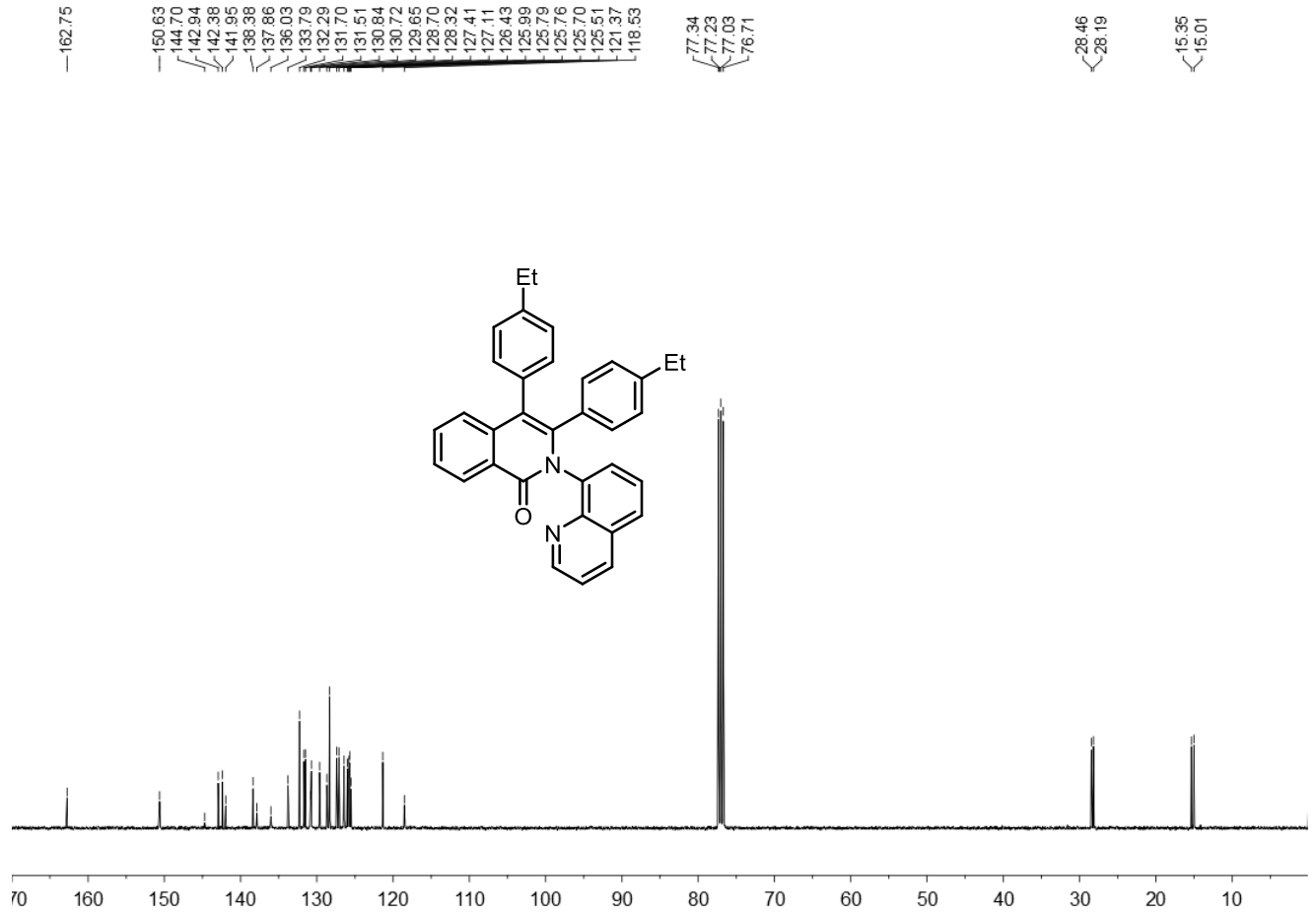
Compound **3ab**



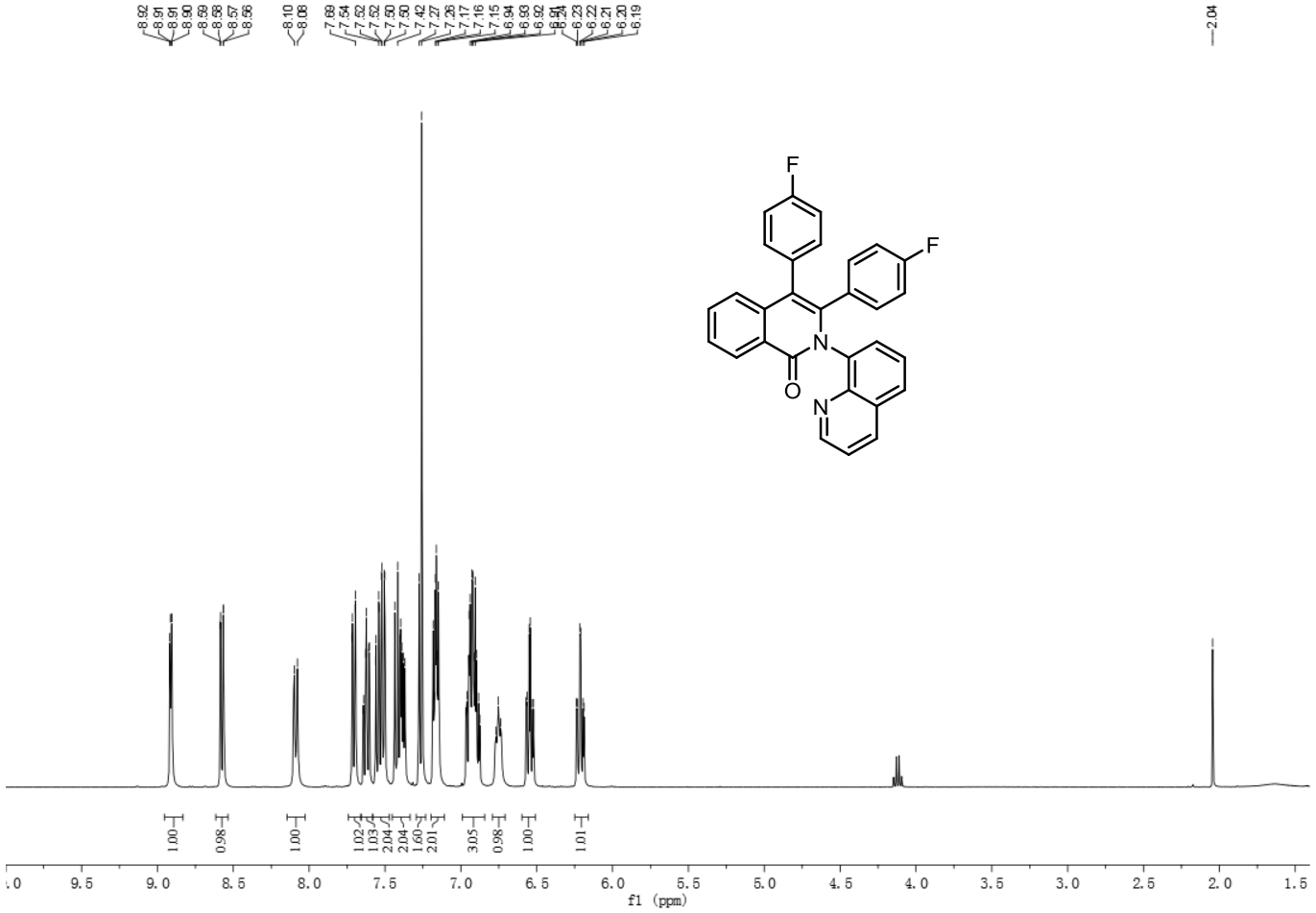

162.80
150.72
138.45
137.93
136.66
136.12
135.98
133.65
132.32
132.12
131.66
131.49
130.83
130.65
129.57
128.79
128.72
128.51
128.42
128.34
127.40
127.16
126.48
125.76
125.69
125.56
121.42
118.48
77.40
77.08
76.76
21.21
21.01
Me
Me
N
O
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

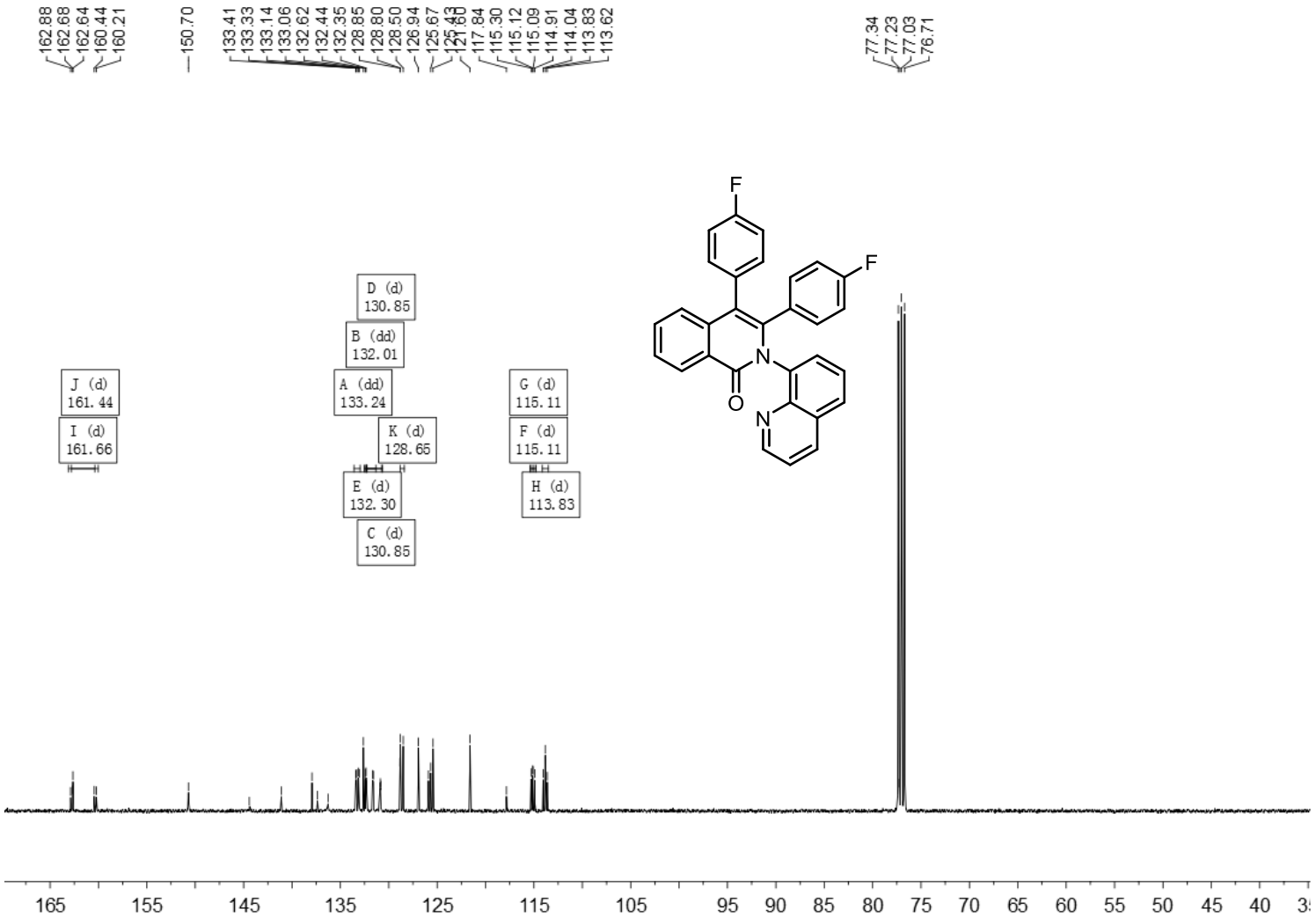
Compound **3ac**

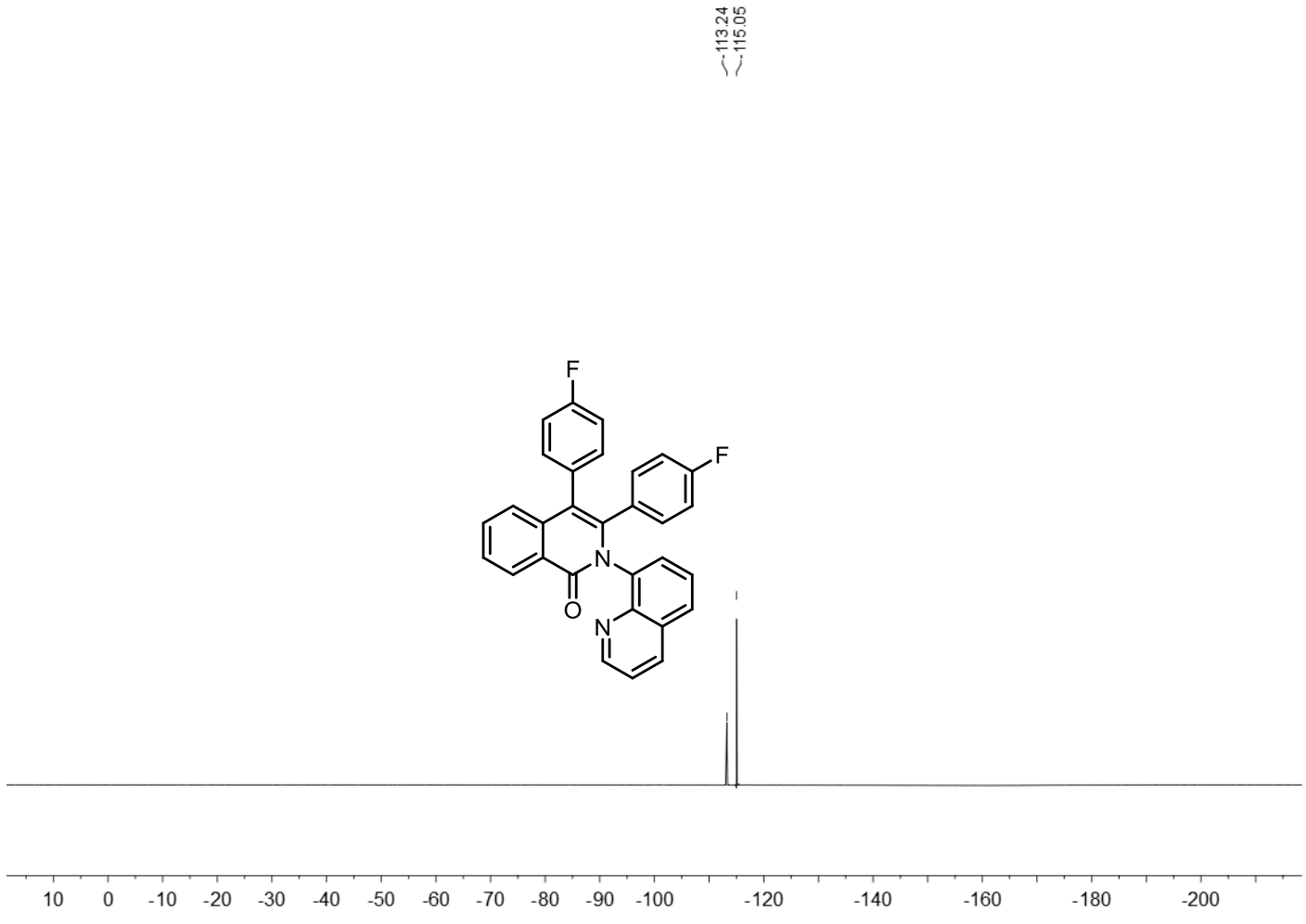



162.75
150.63
144.70
142.94
142.38
141.95
138.38
137.86
136.03
133.79
132.29
131.70
131.51
130.84
130.72
129.65
128.70
128.32
127.41
127.11
126.43
125.99
125.79
125.76
125.70
125.51
121.37
118.53
77.34
77.23
77.03
76.71
28.46
28.19
15.35
15.01
Et
Et
N
O
N
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

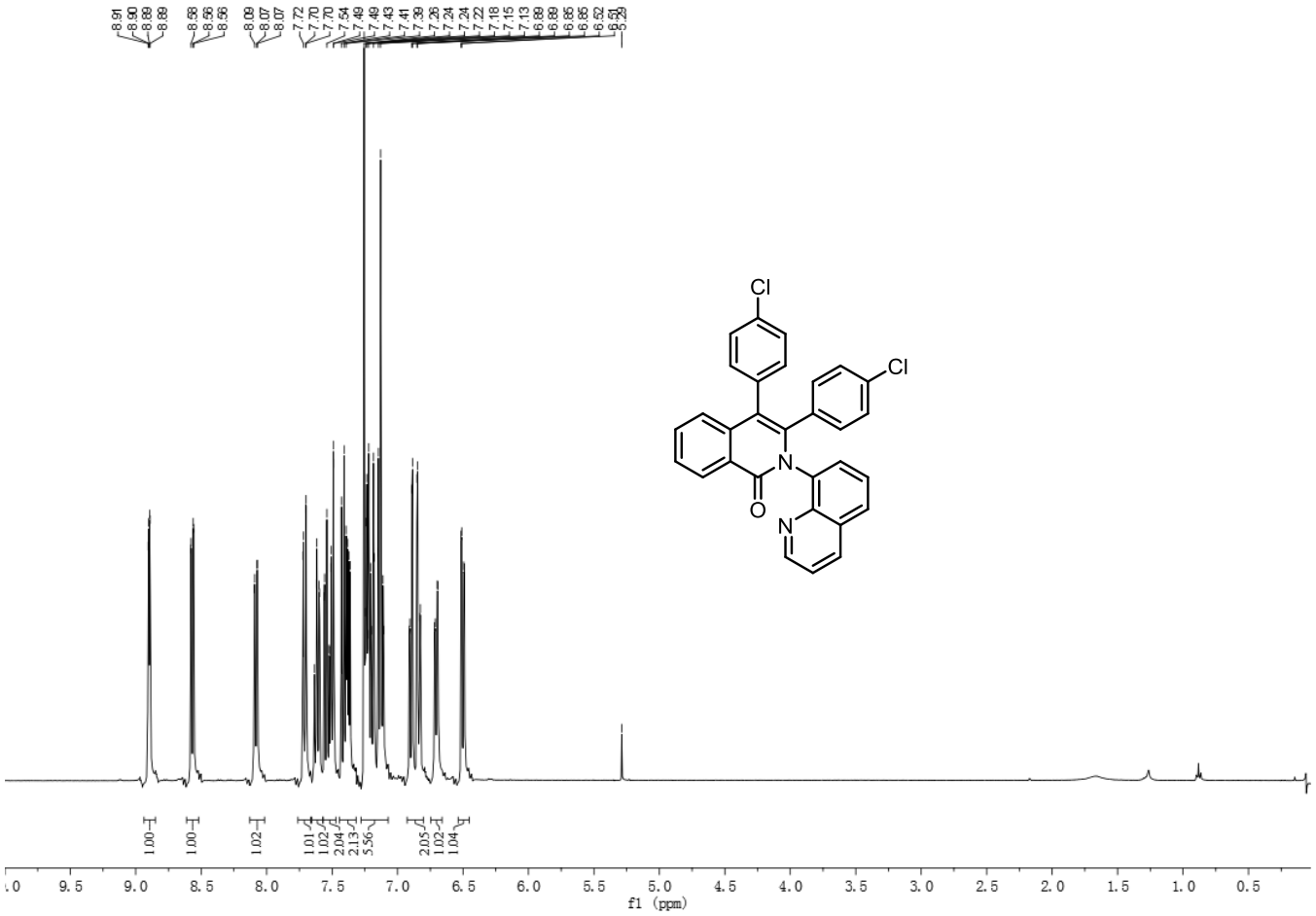
Compound **3ad**

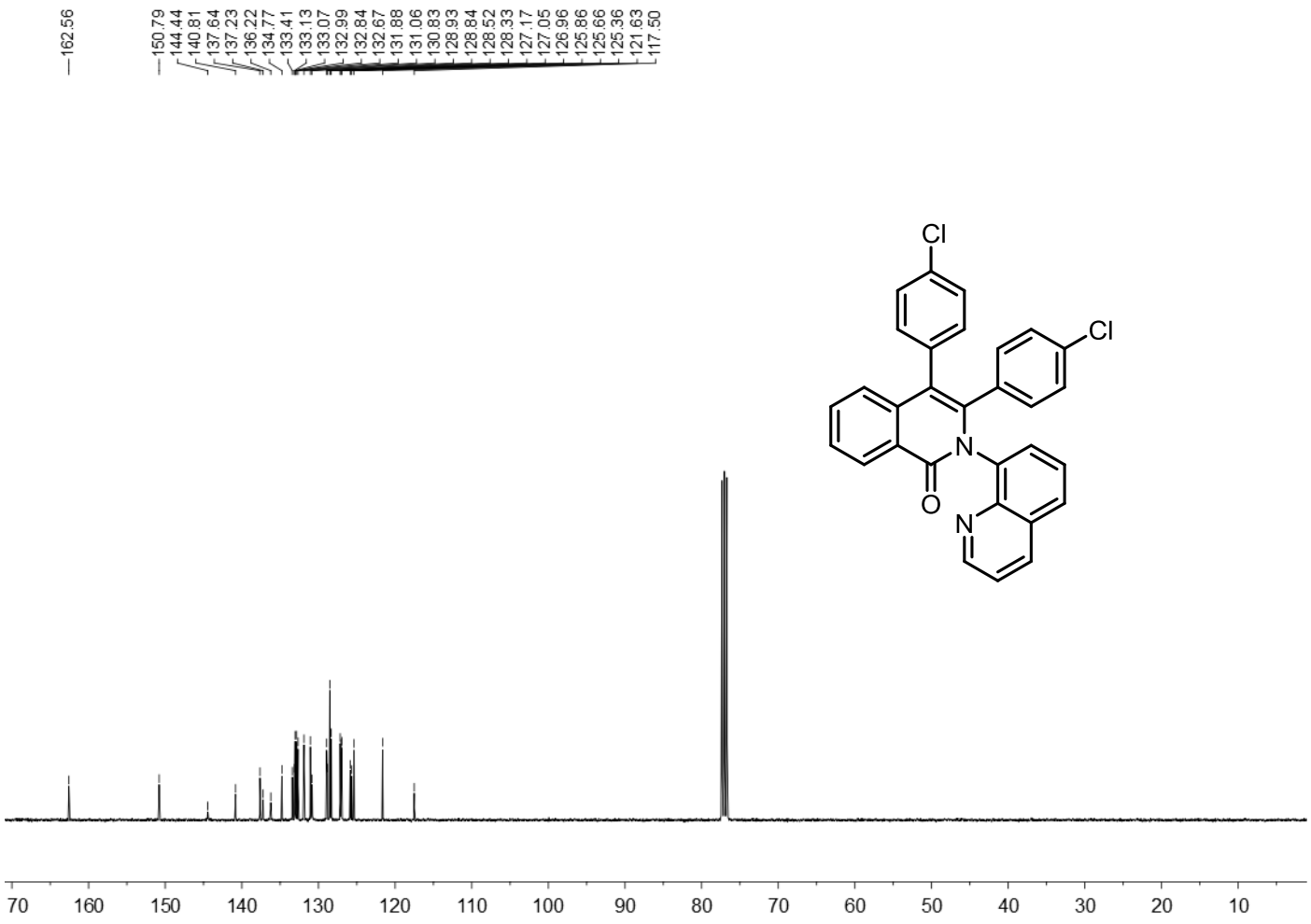



162.88
162.68
162.64
160.44
160.21
150.70
133.41
133.33
133.14
133.06
132.62
132.44
132.35
128.85
128.80
128.50
126.94
125.67
117.84
115.30
115.12
115.09
114.91
114.04
113.83
113.62
77.34
77.23
77.03
76.71
J (d)
161.44
I (d)
161.66
D (d)
130.85
B (dd)
132.01
A (dd)
133.24
K (d)
128.65
E (d)
132.30
C (d)
130.85
G (d)
115.11
F (d)
115.11
H (d)
113.83
F
F
N
O
N
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40

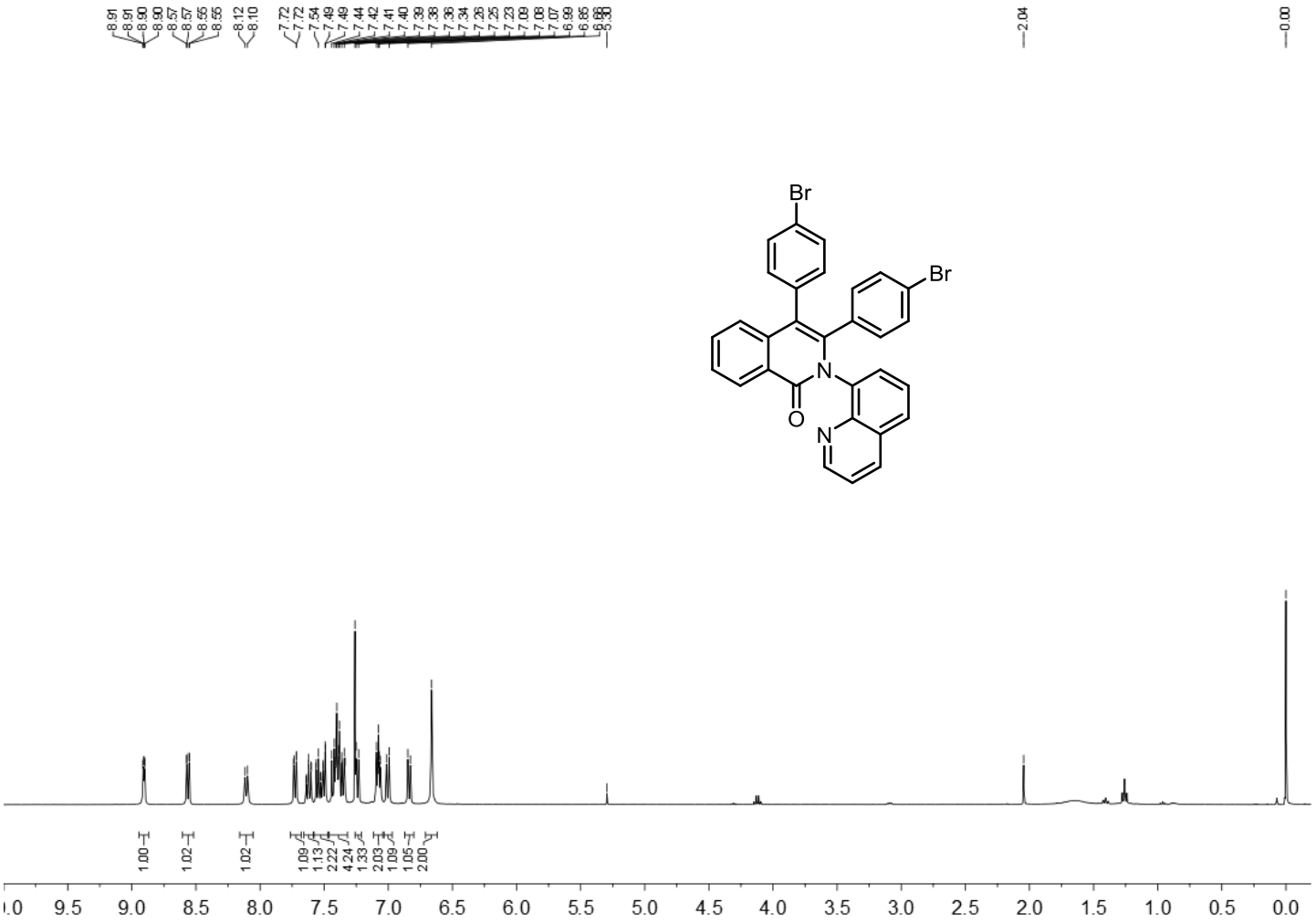

-113.24
-115.05
F
F
N
O
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200

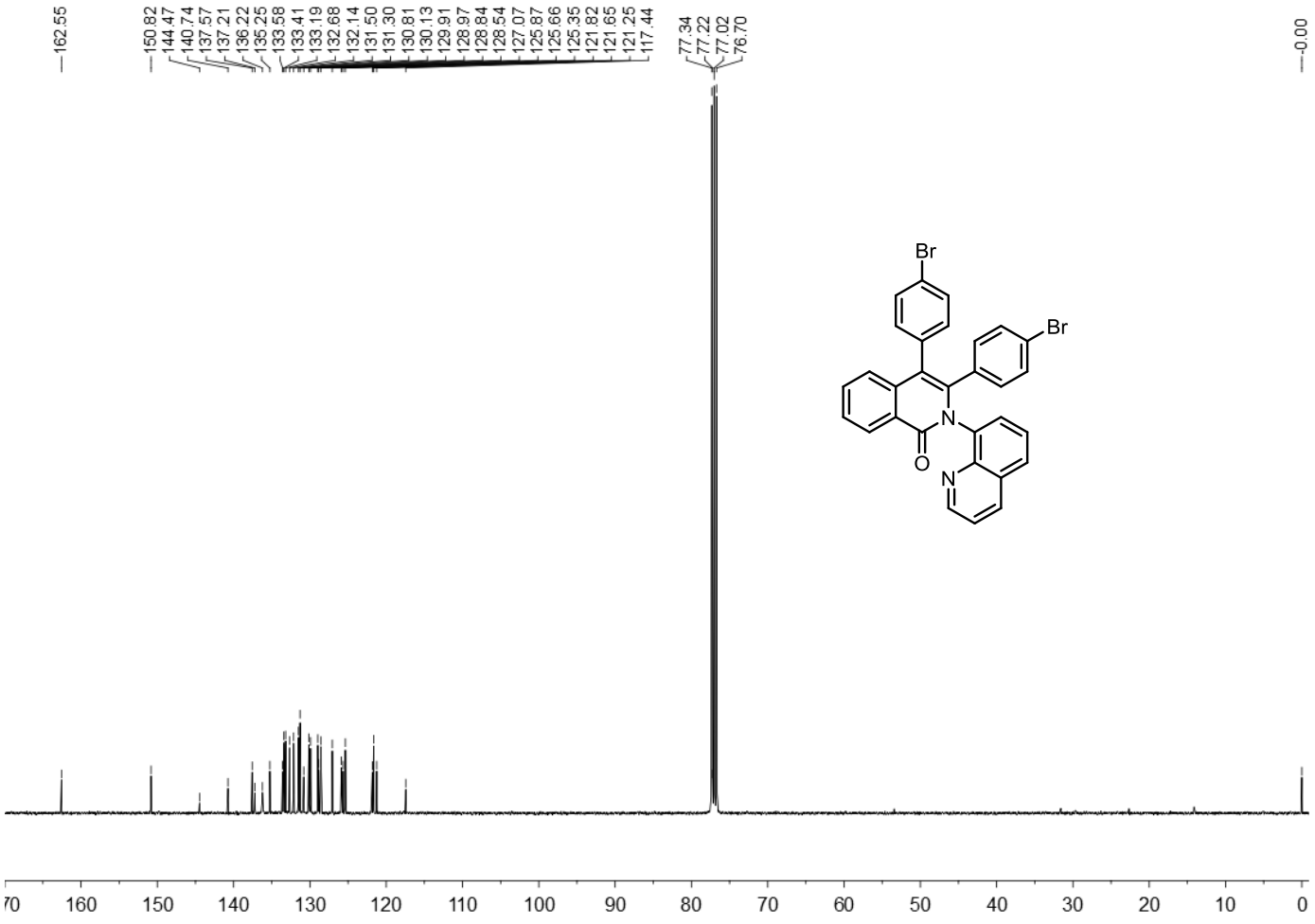
Compound **3ae**



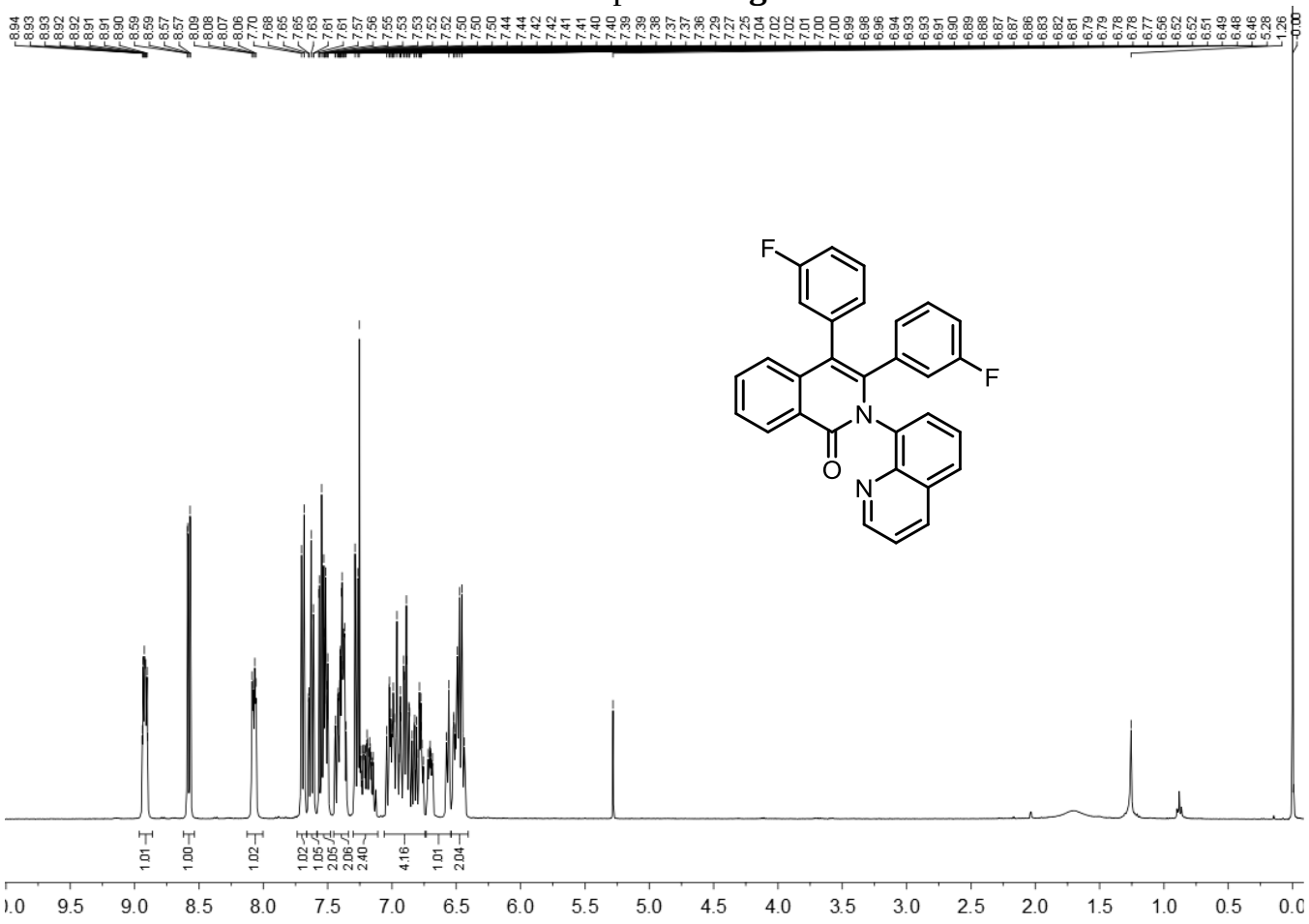

162.56
150.79
144.44
140.81
137.64
137.23
136.22
134.77
133.41
133.13
133.07
132.99
132.84
132.67
131.88
131.06
130.83
128.93
128.84
128.52
128.33
127.17
127.05
126.96
125.86
125.66
125.36
121.63
117.50
Cl
Cl
N
O
N
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

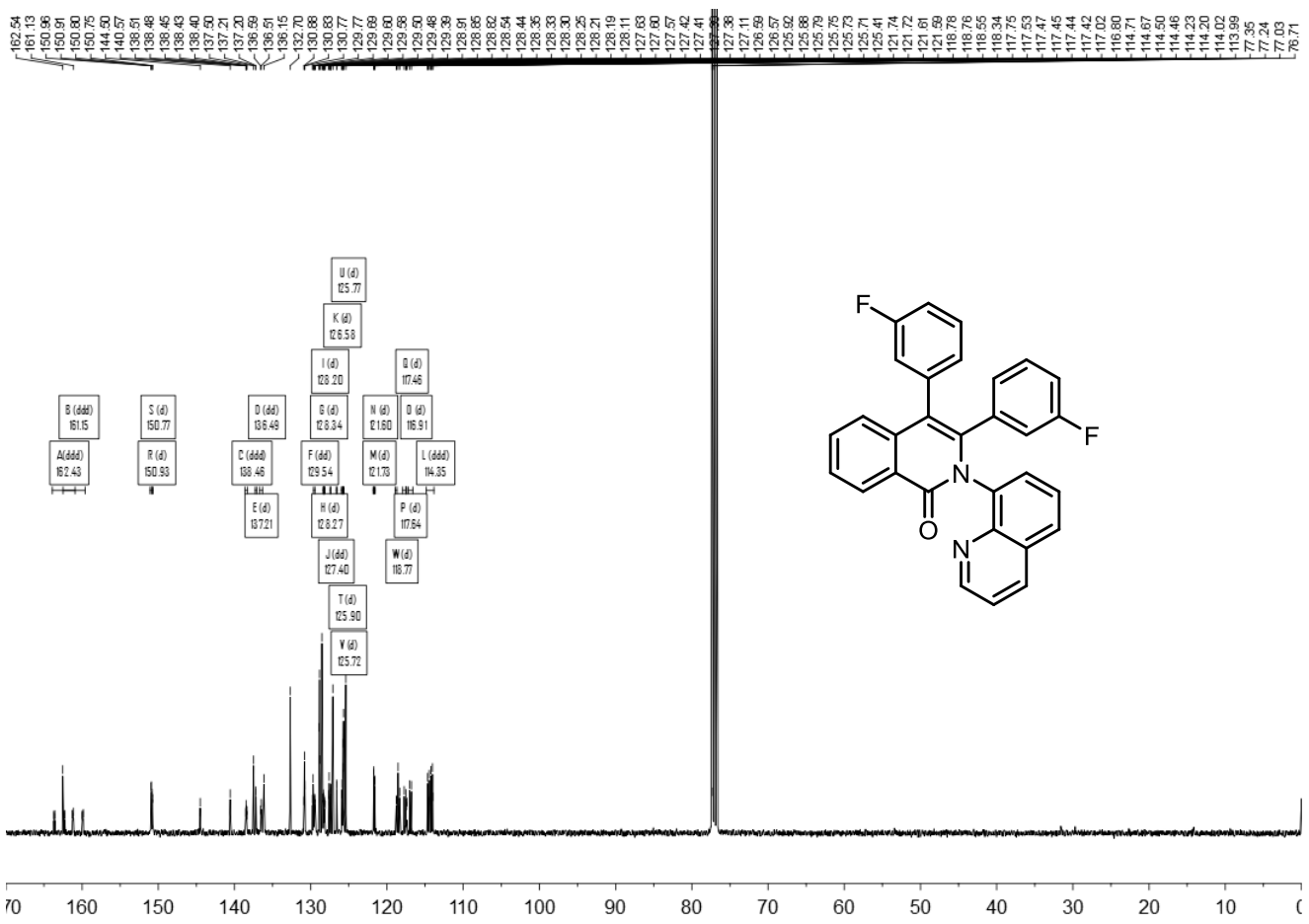
Compound **3af**




162.55
150.82
144.47
140.74
137.57
137.21
136.22
135.25
133.58
133.41
133.19
132.68
132.14
131.50
131.30
130.81
130.13
129.91
128.97
128.84
128.54
127.07
125.87
125.66
125.35
121.82
121.65
121.25
117.44
77.34
77.22
77.02
76.70
0.00
Br
Br
N
O
N
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

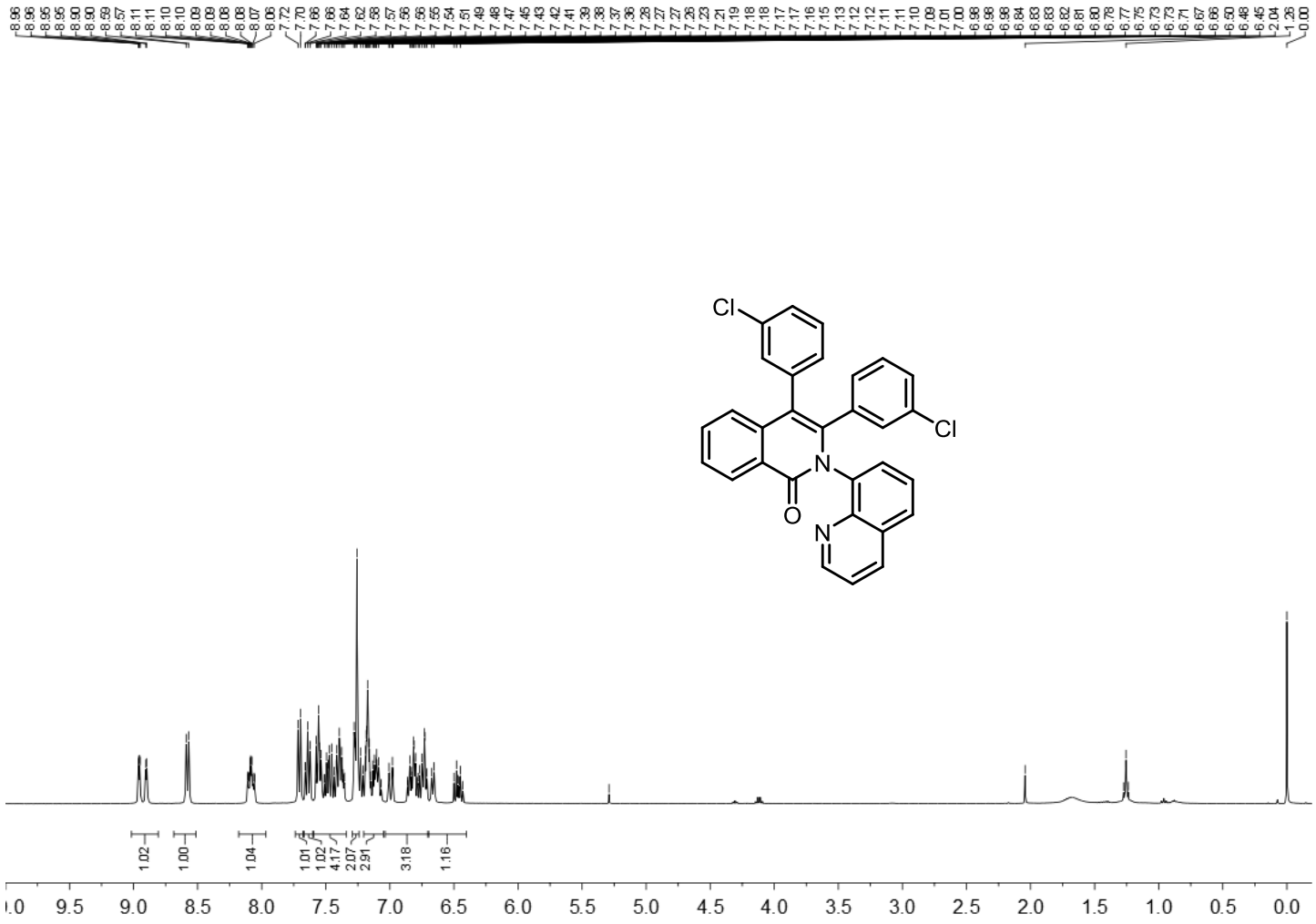
Compound **3ag**

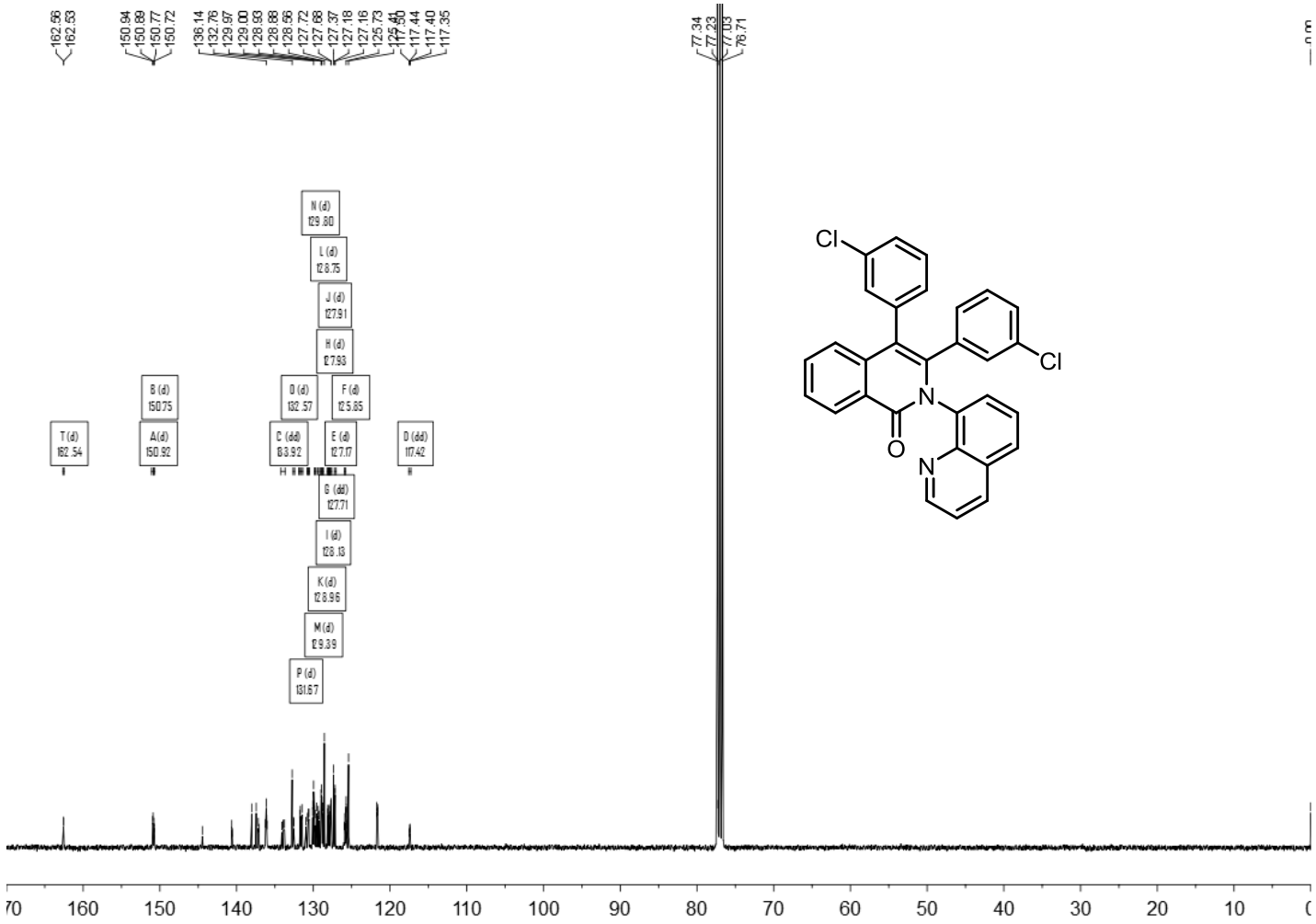



F
F
N
O
N

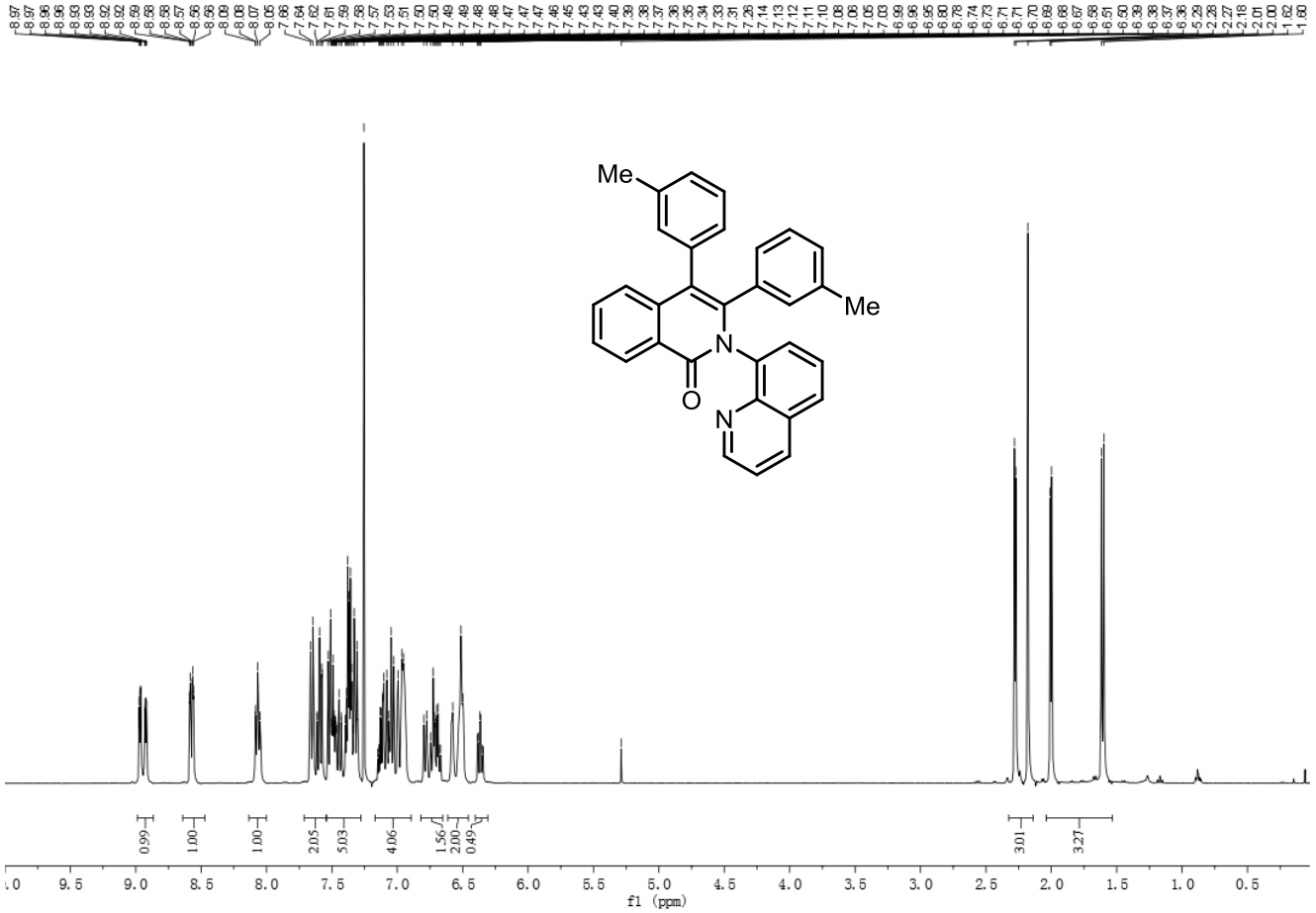

-113.06
-113.33
-113.34
-113.61
-113.84
-113.88
-114.13
-114.16
F
F
N
O
N
B (dd)
-113.34
A(dd)
-114.00
-110.6
-111.2
-111.8
-112.4
-113.0
-113.6
-114.2
-114.8
-115.4
-116.0

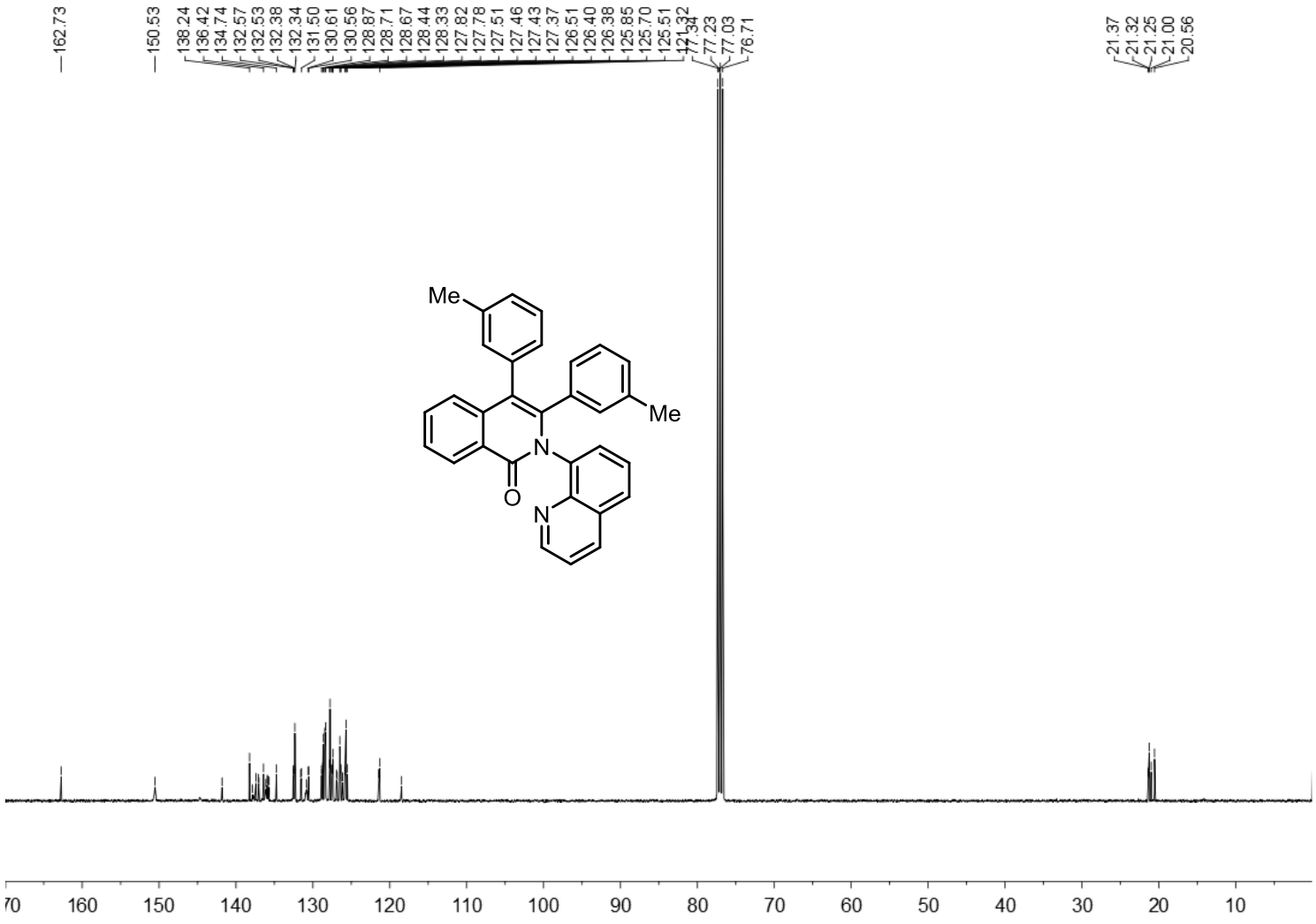
Compound **3ah**



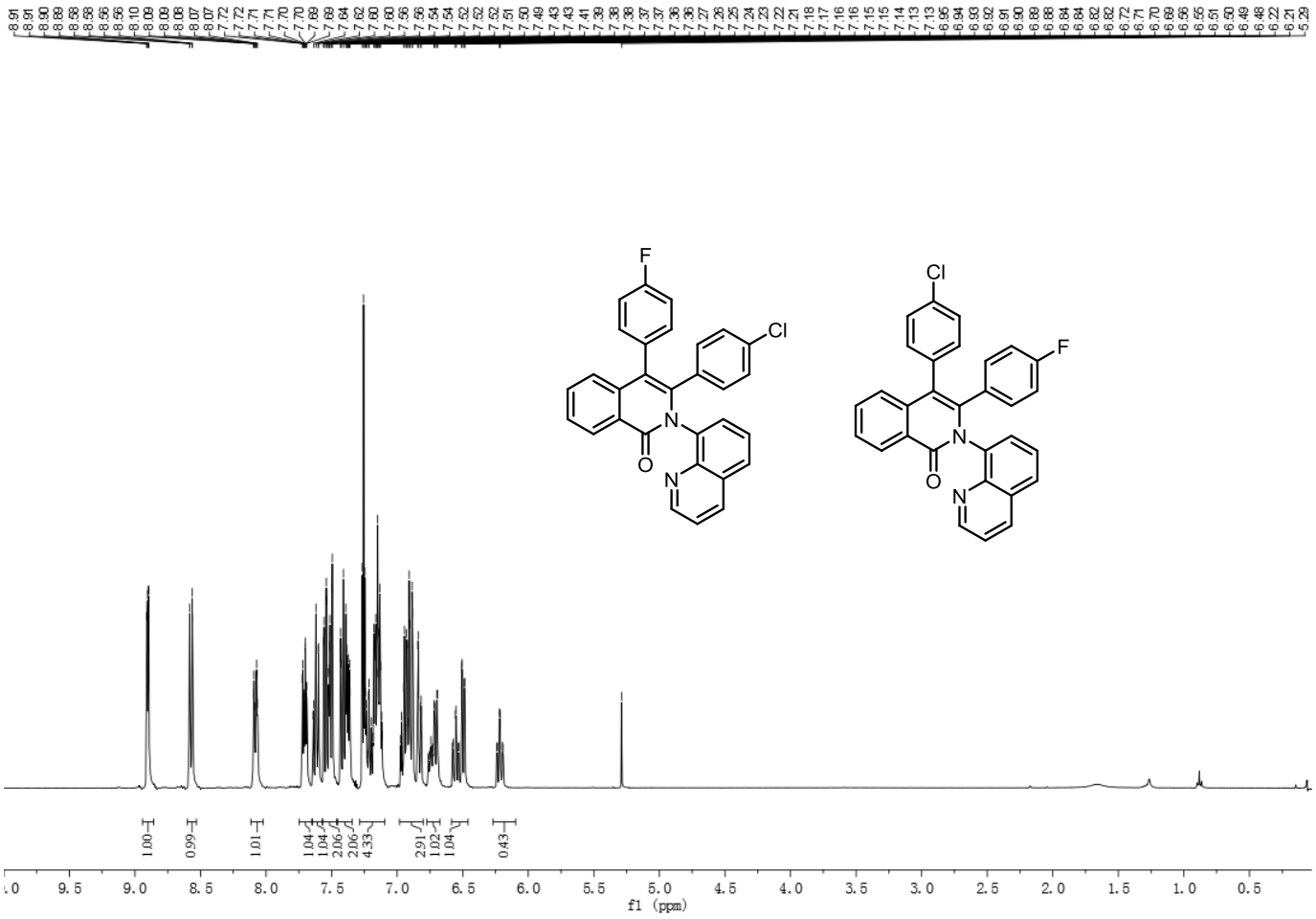

162.56
162.53
150.94
150.89
150.77
150.72
136.14
132.76
129.97
129.00
128.93
128.88
128.56
127.72
127.68
127.37
127.18
127.16
125.73
125.41
117.50
117.44
117.40
117.35
77.34
77.23
77.03
76.71
N (d)
129.80
L (d)
128.75
J (d)
127.91
H (d)
127.93
B (d)
150.75
D (d)
132.57
F (d)
125.85
T (d)
162.54
A (d)
150.92
C (dd)
133.92
E (d)
127.17
D (dd)
117.42
G (dd)
127.71
I (d)
128.13
K (d)
128.96
M (d)
129.39
P (d)
131.67
Cl
Cl
N
O
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

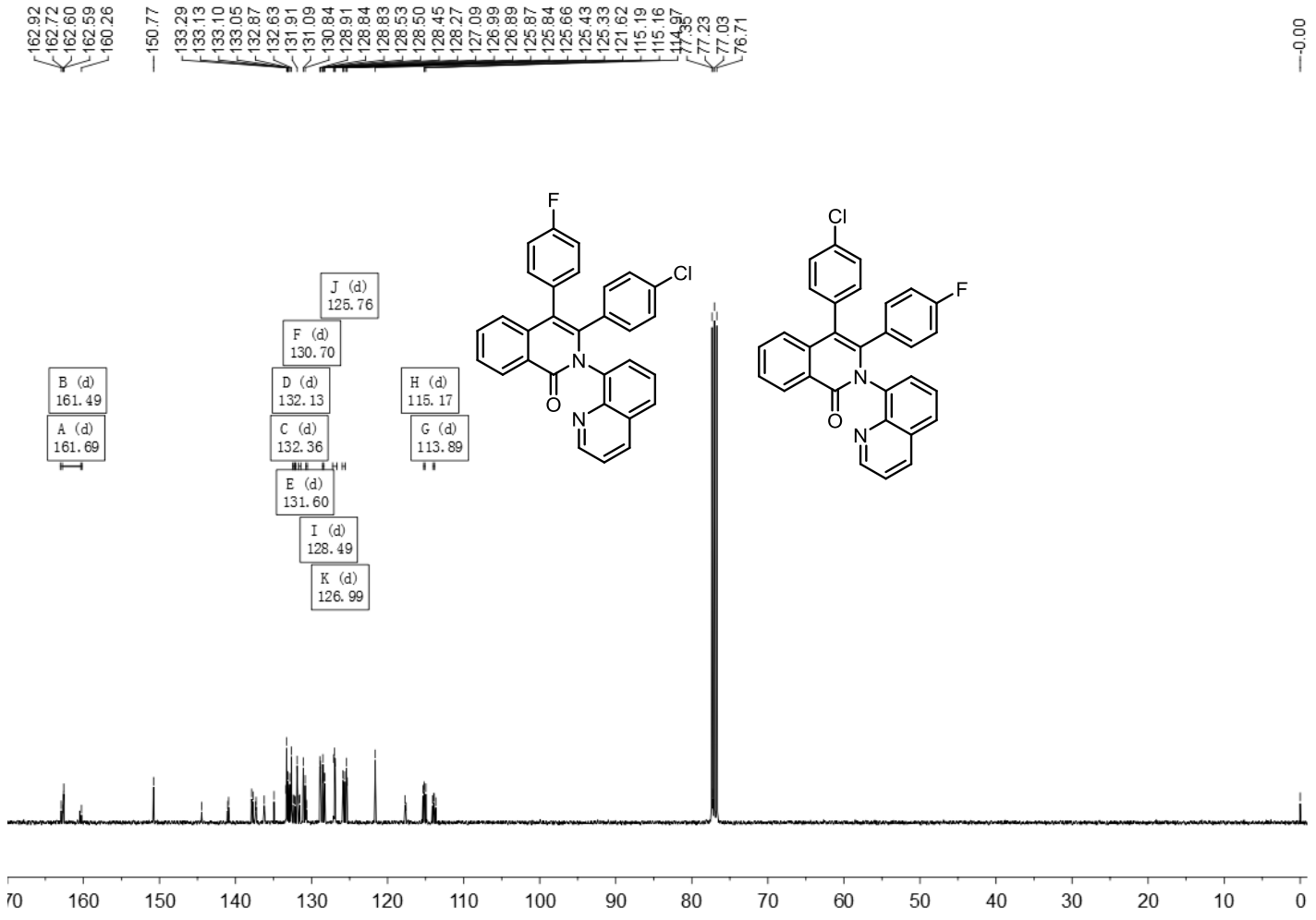
Compound **3ai**

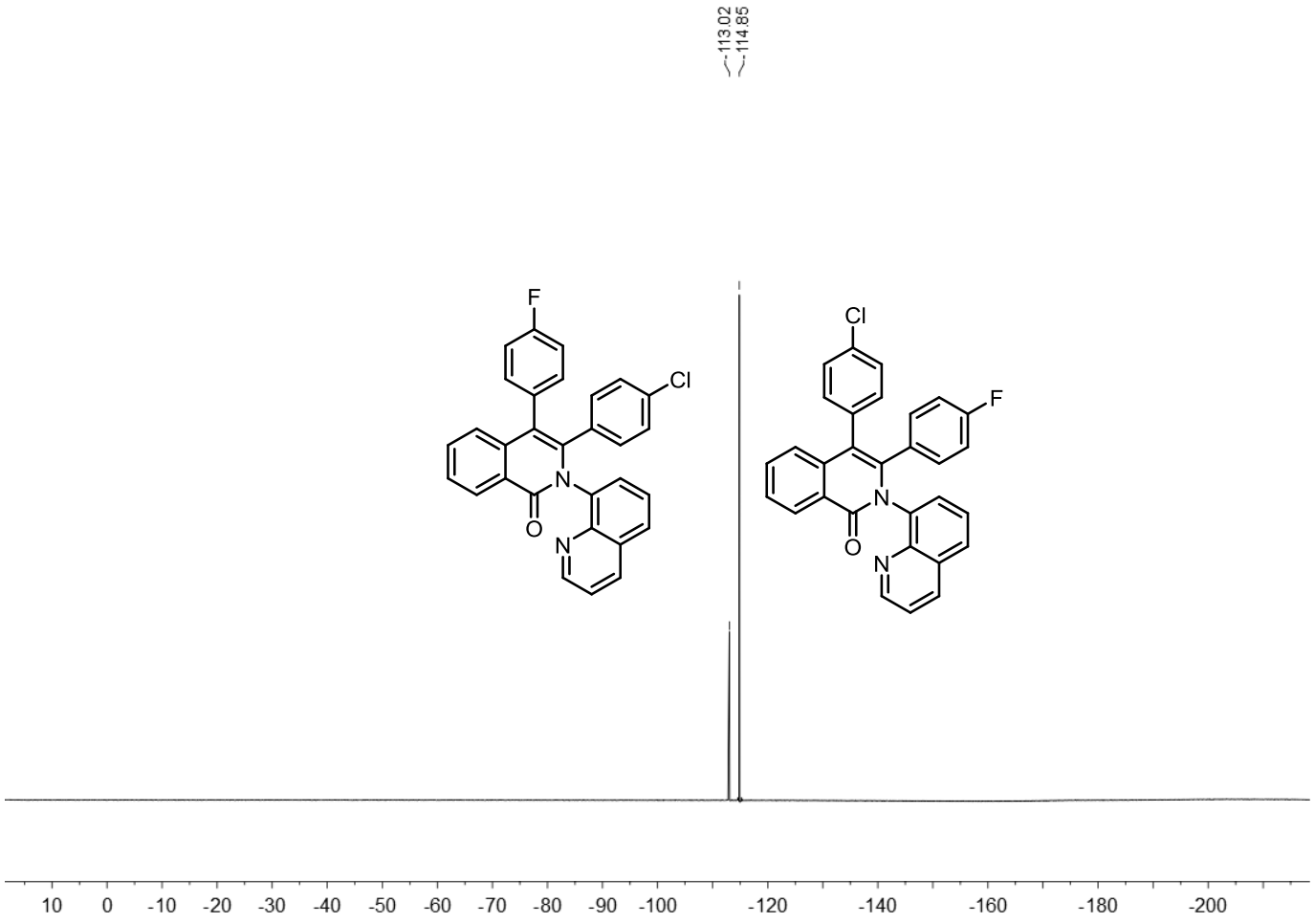



162.73
150.53
138.24
136.42
134.74
132.57
132.53
132.38
132.34
131.50
130.61
130.56
128.87
128.71
128.67
128.44
128.33
127.82
127.78
127.51
127.46
127.43
127.37
126.51
126.40
126.38
125.85
125.70
125.51
121.32
77.34
77.23
77.03
76.71
21.37
21.32
21.25
21.00
20.56
Me
Me
N
O
N
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

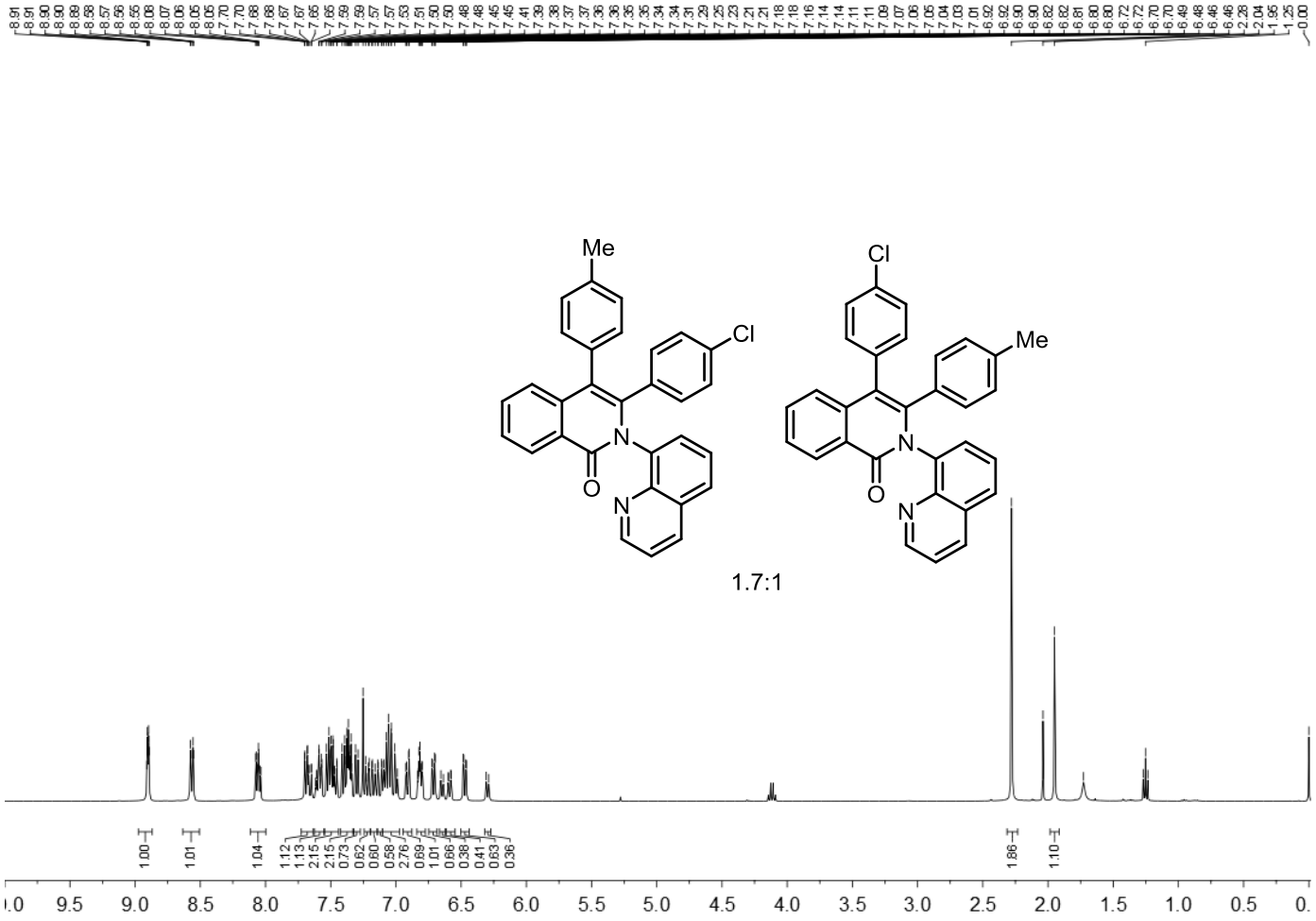
Compound **3aj** and **3ak**

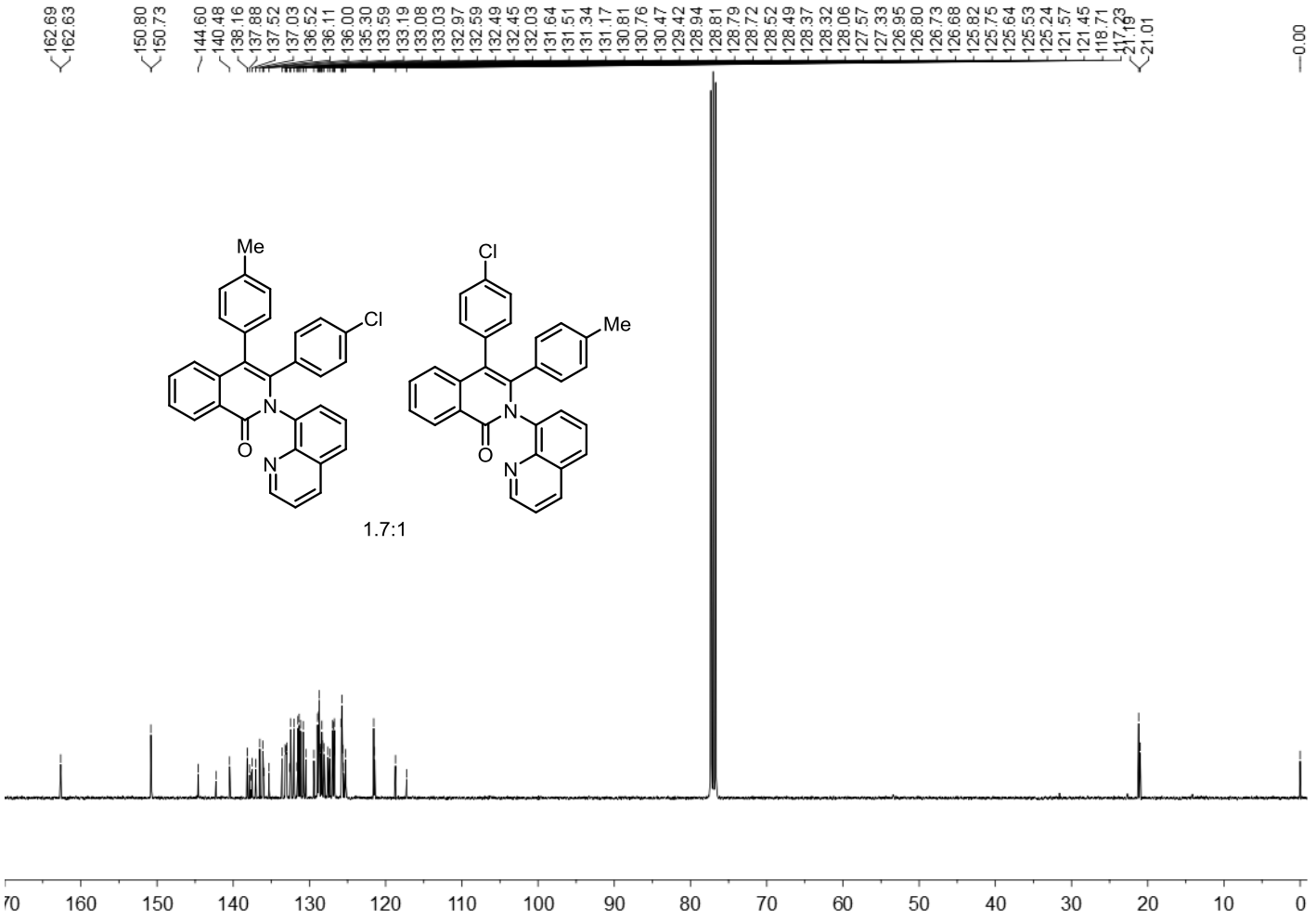



162.92
162.72
162.60
162.59
160.26
150.77
133.29
133.13
133.10
133.05
132.87
132.63
131.91
131.09
130.84
128.91
128.84
128.83
128.53
128.50
128.45
128.27
127.09
126.99
126.89
125.87
125.84
125.66
125.43
125.33
121.62
115.19
115.16
114.97
77.35
77.23
77.03
76.71
0.00
B (d) 161.49
A (d) 161.69
J (d) 125.76
F (d) 130.70
D (d) 132.13
C (d) 132.36
E (d) 131.60
I (d) 128.49
K (d) 126.99
H (d) 115.17
G (d) 113.89
F
Cl
O
N
Cl
F
O
N
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

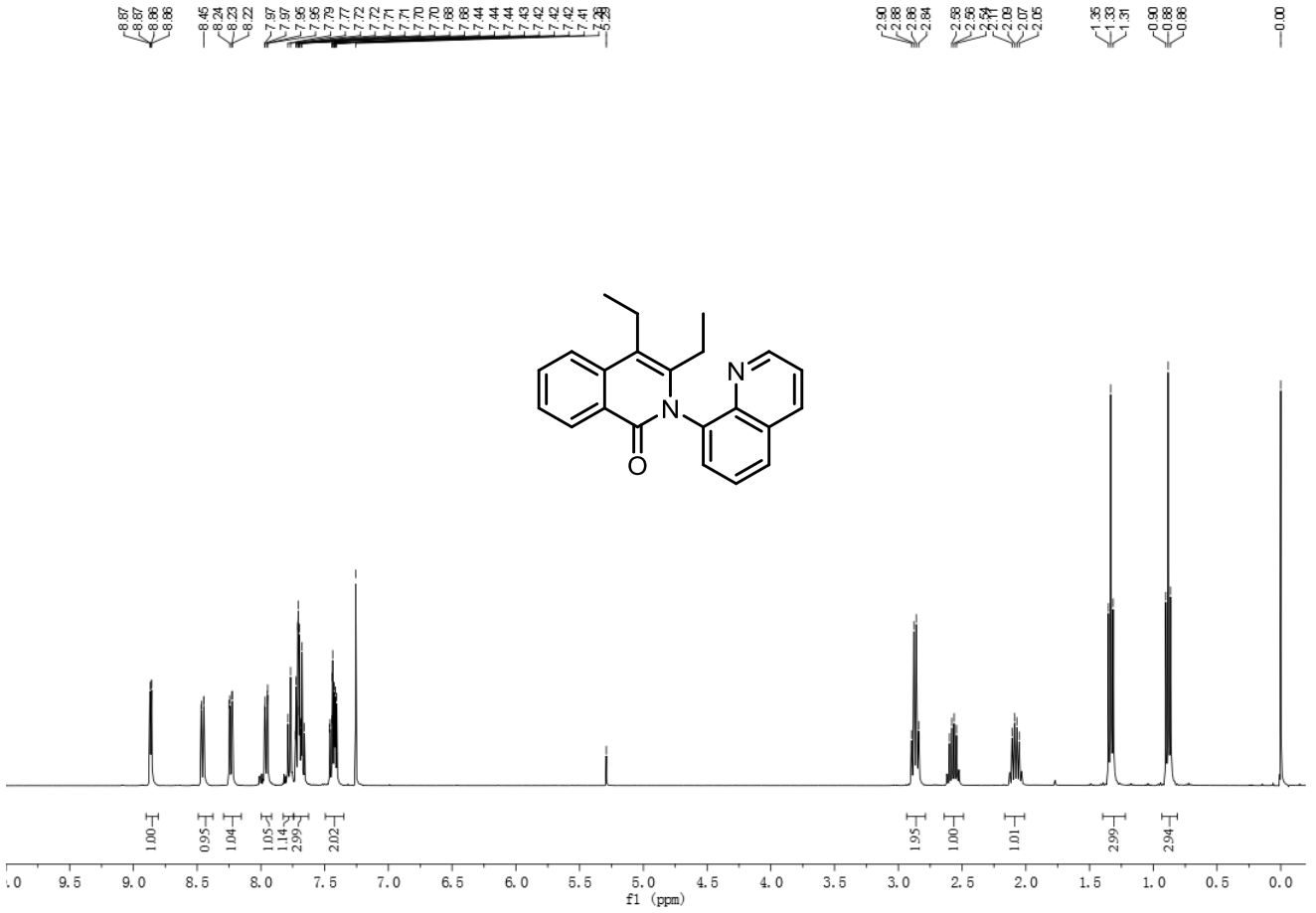

-113.02
-114.85
F
Cl
N
O
N
Cl
F
N
O
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200

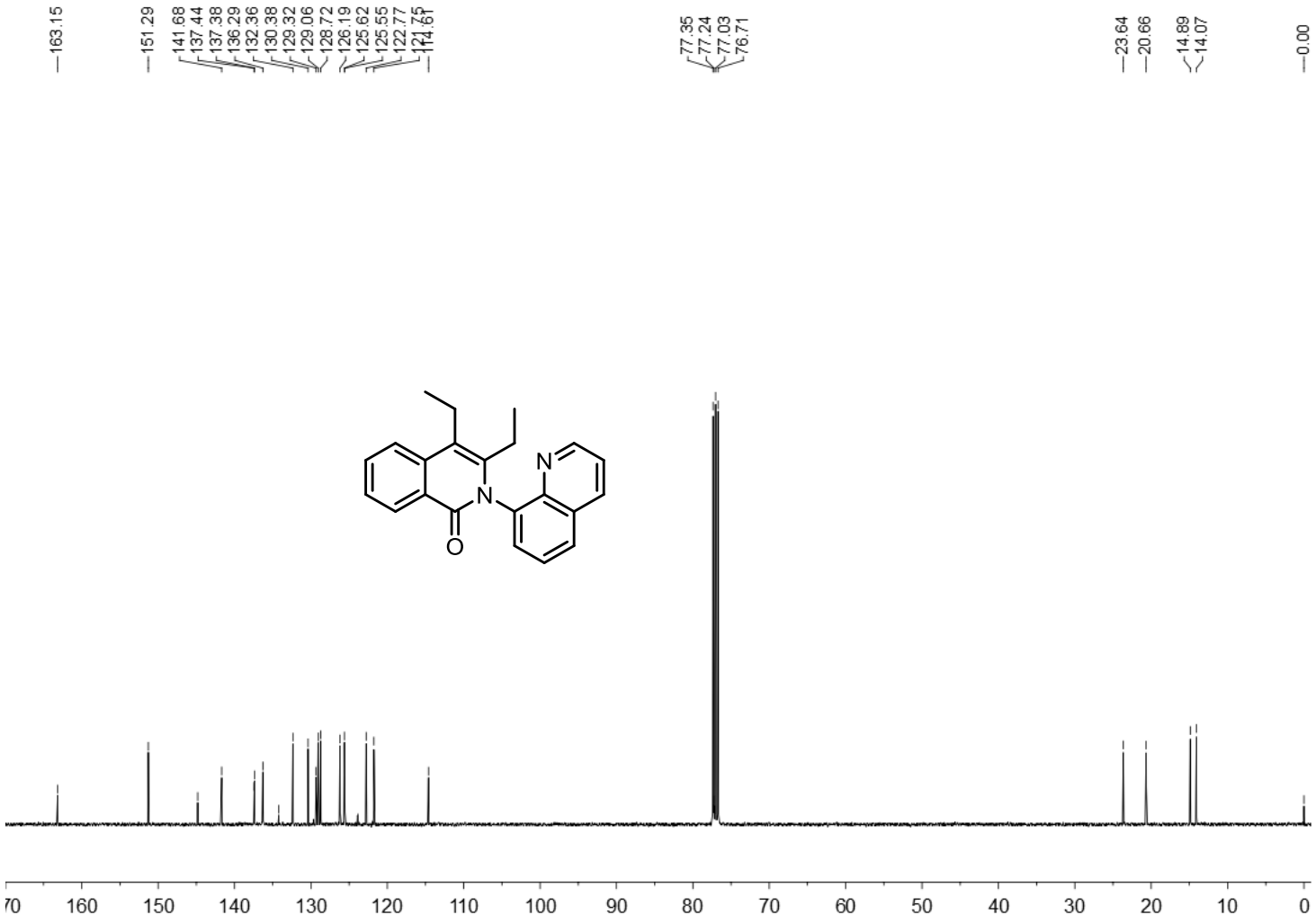
Compound **3al** and **3am**




162.69
162.63
150.80
150.73
144.60
140.48
138.16
137.88
137.52
137.03
136.52
136.11
136.00
135.30
133.59
133.19
133.08
133.03
132.97
132.59
132.49
132.45
132.03
131.64
131.51
131.34
131.17
130.81
130.76
130.47
129.42
128.94
128.81
128.79
128.72
128.52
128.49
128.37
128.32
128.06
127.57
127.33
126.95
126.80
126.73
126.68
125.82
125.75
125.64
125.53
125.24
121.57
121.45
118.71
117.23
21.19
21.01
0.00
Me
Cl
Cl
Me
1.7:1
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound **3an**




163.15
151.29
141.68
137.44
137.38
136.29
132.36
130.38
129.32
129.06
128.72
126.19
125.62
125.55
122.77
121.75
114.61
77.35
77.24
77.03
76.71
23.64
20.66
14.89
14.07
0.00
N
N
O
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0