Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Transition Metal Free Oxygenation of 8-Aminoquinoline Amides in Water

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1. General experimental information

Unless otherwise noted, all reactions were carried out without exclusion of air or moisture. Commercial solvents and reagents were used without further purification. Analytical thin layer chromatography (TLC) was performed using silica gel GF254 plates. Chemical yields refer to pure isolated substances. Column chromatography was performed using silica gel (300-400 mesh) eluting with petroleum ether and ethyl acetate. Nuclear magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded with a Bruker DPX (^{1}H at 400 MHz, ^{13}C at 100 MHz). Unless otherwise noted, all spectra were acquired in $CDCl_3$. Chemical shifts are reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ =0.00ppm) and are referenced to residual solvent (CDCl3, δ =7.26 ppm (^{1}H) and 77.00 ppm (^{13}C)). Coupling constants were reported in hertz (Hz). Data for ^{1}H NMR spectra were reported as follows: chemical shift (ppm, referenced to protium; s =singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). All products were characterized by their NMR spectra.

2. General experimental procedure

2.1 synthesis of 8- aminoquinoline amides

To a 50 mL single neck flask charged with CH_2Cl_2 (20 mL) was added 8-aminoquinoline (10 mmol) and triethylamine (11 mmol) and stirred at room temperature for 5 min, then the reaction solution was cooled in an ice bath. The acid chloride (12 mmol) was added dropwise. The reaction solution was stirred 6 h. When the reaction was completed (monitored by TLC), the mixture was filtered through a pad of Celite, the solid was washed with ethyl acetate (30 mL), and the organic layer was washed with 1 M $NaHCO_3$ aqueous solution (3 × 15 mL), then the organic layer was dried with Na_2SO_4, filtered, and the solvent was removed under reduced pressure. The product was finally obtained by column chromatography on silica gel.

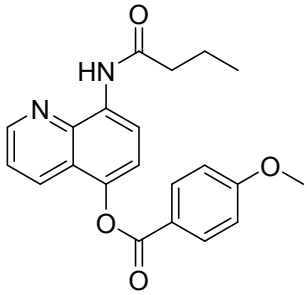
2.2 synthesis of aryl acylperoxide.

In a round-bottomed flask, the solution of acid chloride (5 mmol) in diethyl ether (2.5 mL) was cooled to 0 °C in an ice-bath. Then, hydrogen peroxide (0.294 g, 30 wt.% in H_2O, 2.86 mmol) was added dropwise over 10 minutes to the cold solution. This was followed by the dropwise addition of an aqueous solution of NaOH (0.252g, 6.32 mmol, 2 mL) over 20 minutes. The resulting white precipitate was collected by filtration. After washing with water (3×5 mL) and diethyl ether (3×5 mL), the solid was crystallized from a cold acetone/water mixture (v/v = 1/3) to give the pure aryl acylperoxide.

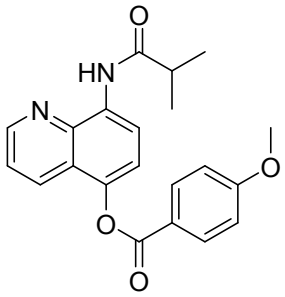
2.3 general experimental procedure for the oxygenation of 8-aminoquinoline amides

Amide derivatives (0.1 mmol), catalyst (20 mmol%), were combined in H_2O (1 mL) in a 10mL vial. the vial was stirred in 80° C oil bath for 0.5 hours. benzoyl peroxides (2 equiv.) was injected into the vial. The vial was then stirred at 80° C for 24 hours without an inert gas atmosphere. After cooled down to the room temperature, the mixture was then extracted with ethyl acetate (3 x 5mL). The residue was purified by silica-gel column chromatography to afford the corresponding product.

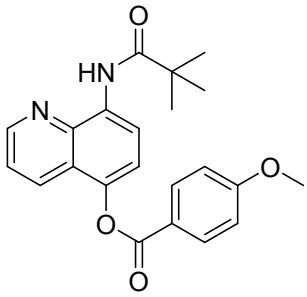
3. Characterization data of all products



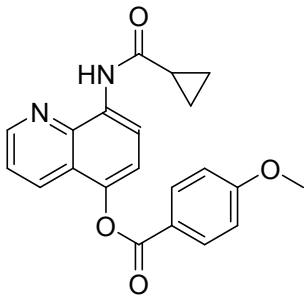
8-butyramidoquinolin-5-yl 4-methoxybenzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.91 – 8.77 (m, 2H), 8.31 – 8.17 (m, 3H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.08 – 6.97 (m, 2H), 3.92 (s, 3H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.94 – 1.79 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.82, 165.12, 164.32, 148.55, 140.88, 138.69, 132.87, 132.60, 130.84, 122.36, 121.87, 121.27, 119.68, 116.02, 114.17, 55.71, 40.25, 19.26, 13.95. HRMS: Calcd for $C_{21}H_{20}N_2O_4Na$[M+Na] =387.1321, found 387.1269



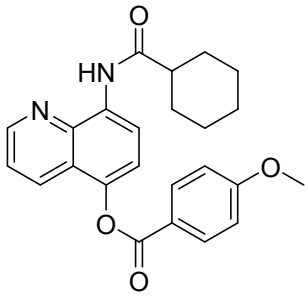
8-isobutyramidoquinolin-5-yl 4-methoxybenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.90 – 8.77 (m, 2H), 8.30 – 8.18 (m, 3H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.07 – 7.00 (m, 2H), 3.92 (s, 3H), 2.85 – 2.71 (m, 1H), 1.40 – 1.32 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.81, 165.16, 164.34, 148.63, 140.89, 138.92, 133.00, 132.62, 130.79, 122.38, 121.89, 121.32, 119.68, 115.98, 114.19, 55.73, 37.25, 19.86. HRMS: Calcd for $C_{21}H_{20}N_2O_4$ Na[M+Na] =387.1321, found 387.1277



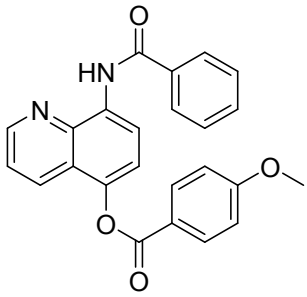
8-pivalamidoquinolin-5-yl 4-methoxybenzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 8.92 – 8.77 (m, 2H), 8.34 – 8.15 (m, 3H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.08 – 7.00 (m, 2H), 3.93 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.32, 165.17, 164.34, 148.72, 140.87, 139.24, 133.10, 132.63, 130.76, 122.40, 121.87, 121.38, 119.68, 115.79, 114.20, 55.74, 40.48, 27.88. HRMS Calcd for $C_{22}H_{22}N_2O_4$ Na[M+Na] =401.1477, found: 401.1474



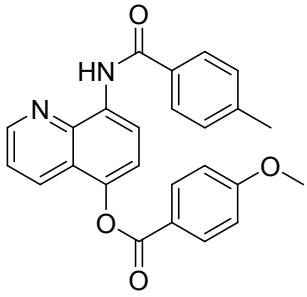
8-(cyclopropanecarboxamido) quinolin-5-yl 4-methoxybenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.94 – 8.68 (m, 2H), 8.26 – 8.13 (m, 3H), 7.47 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.38 (dd, *J* = 18.2, 8.2 Hz, 3H), 2.48 (s, 3H), 1.86 – 1.76 (m, 1H), 1.19 – 1.13 (m, 2H), 0.97 – 0.88 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.34, 165.48, 148.59, 145.05, 140.71, 138.66, 133.14, 130.74, 130.50, 129.63, 126.32, 122.30, 121.92, 119.67, 115.92, 21.96, 16.39, 8.34. HRMS Calcd for $C_{21}H_{18}N_2O_4$ Na[M+Na] =385.1164, found: 385.1171



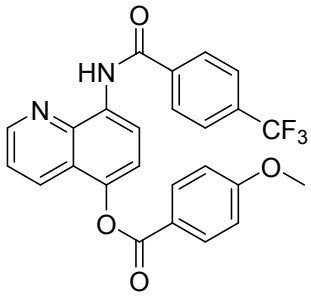
8-(cyclohexanecarboxamido) quinolin-5-yl 4-methoxybenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.83 (s, 1H), 8.87 – 8.80 (m, 2H), 8.29 – 8.19 (m, 3H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 1H), 7.07 – 7.00 (m, 2H), 3.92 (s, 3H), 2.54 – 2.43 (m, 1H), 2.09 (dd, *J* = 13.5, 1.9 Hz, 2H), 1.95 – 1.84 (m, 2H), 1.79 – 1.65 (m, 2H), 1.36 (dddd, *J* = 18.8, 12.5, 9.3, 3.2 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.94, 165.16, 164.34, 148.61, 140.85, 138.94, 133.04, 132.62, 130.80, 122.39, 121.88, 121.34, 119.70, 115.99, 114.19, 55.73, 47.02, 29.89, 25.90. HRMS Calcd for $C_{24}H_{24}N_2O_4$Na[M+Na] =427.1634, found 427.1643



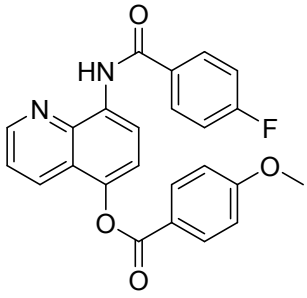
8-benzamidoquinolin-5-yl 4-methoxybenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 10.71 (s, 1H), 9.00 (d, *J* = 8.5 Hz, 1H), 8.90 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.36 – 8.21 (m, 3H), 8.11 (dd, *J* = 7.9, 1.5 Hz, 2H), 7.61 – 7.47 (m, 5H), 7.10 – 7.00 (m, 2H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 165.68 (s), 165.09 (s), 164.42 (s), 148.50 (s), 141.35 (s), 138.79 (s), 135.10 (s), 132.67 (s), 132.09 (s), 131.50 (s), 128.95 (s), 127.55 (s), 122.64 (s), 121.97 (s), 121.25 (s), 119.97 (s), 116.96 (s), 114.24 (s), 55.76 (s). HRMS Calcd for $C_{24}H_{18}N_2O_4$ K[M+K]=437.0904, found 437.0917



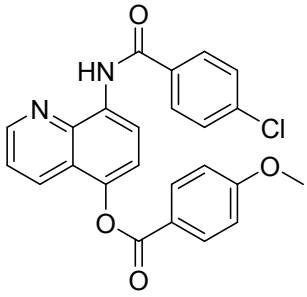
8-(4-methylbenzamido) quinolin-5-yl 4-methoxybenzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 8.99 (d, *J* = 8.5 Hz, 1H), 8.89 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.32 – 8.22 (m, 3H), 7.99 (d, *J* = 8.2 Hz, 2H), 7.52 – 7.44 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 9.0 Hz, 2H), 3.93 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.65, 165.27, 164.50, 148.88, 142.66, 141.26, 133.21, 132.76, 132.54, 130.98, 129.74, 127.58, 122.62, 122.10, 121.50, 119.88, 116.22, 114.34, 55.85, 21.81. HRMS Calcd for $C_{25}H_{20}N_2O_4Na$[M+Na] =435.1321, found 435.1334



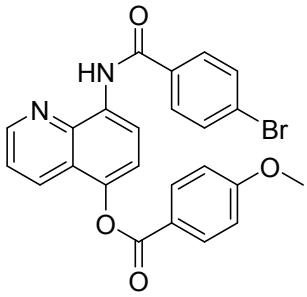
8-(4-(trifluoromethyl) benzamido) quinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, $cdcl_3$) δ 10.73 (s, 1H), 8.98 (d, *J* = 8.5 Hz, 1H), 8.90 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.32 – 8.23 (m, 3H), 8.20 (d, *J* = 8.1 Hz, 2H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.55 – 7.46 (m, 2H), 7.08 – 7.02 (m, 2H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $cdcl_3$) δ 164.40, 164.13, 148.96, 141.62, 139.17, 138.44, 132.57, 131.01, 127.91, 126.05, 122.54, 122.19, 121.18, 119.73, 116.40, 114.23, 55.77. HRMS Calcd for $C_{25}H_{17}F_3N_2O_4$[M+H] =466.1140, found 466.1141



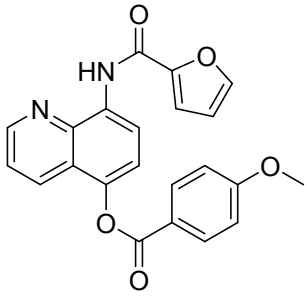
8-(4-fluorobenzamido) quinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 9.07 – 8.75 (m, 2H), 8.33 – 8.20 (m, 3H), 8.17 – 8.02 (m, 2H), 7.57 – 7.39 (m, 2H), 7.30 – 7.16 (m, 3H), 7.11 – 6.98 (m, 2H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.43, 165.12, 164.40, 163.92, 148.84, 141.35, 139.21, 132.73, 131.42, 130.95, 129.82, 122.53, 122.07, 121.30, 119.74, 116.16, 115.92, 114.23, 55.75. HRMS Calcd for $C_{24}H_{17}FN_2O_4$[M+H] =416.1172, found 416.1174



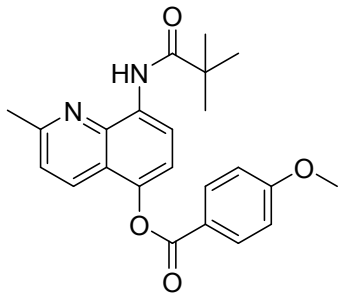
8-(4-chlorobenzamido) quinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, cdcl$_3$) δ 10.66 (s, 1H), 8.97 (d, *J* = 8.5 Hz, 1H), 8.89 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.27 (dd, *J* = 9.4, 2.2 Hz, 3H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.58 – 7.44 (m, 5H), 7.05 (d, *J* = 8.9 Hz, 2H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 164.40, 148.87, 139.18, 138.33, 133.57, 132.67, 130.96, 129.24, 128.88, 122.52, 122.11, 121.25, 119.74, 118.06, 116.25, 114.23, 55.76. HRMS Calcd for $C_{24}H_{17}ClN_2O_4$[M+H] = 432.0877, found 432.0879



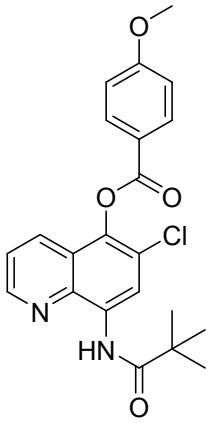
8-(4-bromobenzamido) quinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, cdcl$_3$) δ 10.66 (s, 1H), 9.01 – 8.85 (m, 1H), 8.33 – 8.21 (m, 2H), 8.14 – 8.06 (m, 2H), 7.96 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.55 – 7.41 (m, 1H), 7.00 (dt, *J* = 14.4, 5.8 Hz, 3H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 165.11, 164.69, 164.44, 162.42, 148.88, 141.43, 139.17, 134.03, 132.97, 132.65, 132.21, 129.04, 122.11, 121.40, 119.73, 116.25, 114.24, 55.75. HRMS Calcd for $C_{24}H_{17}BrN_2O_4$[M+H] = 476.0372, found 476.0376



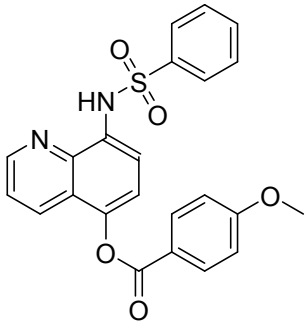
8-(furan-2-carboxamido) quinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, cdcl$_3$) δ 10.73 (s, 1H), 8.93 (d, *J* = 8.6 Hz, 2H), 8.26 (d, *J* = 8.6 Hz, 3H), 7.64 (s, 1H), 7.55 – 7.40 (m, 2H), 7.31 (d, *J* = 3.4 Hz, 1H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.69 – 6.45 (m, 1H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 165.11, 164.36, 156.44, 148.93, 148.40, 144.69, 141.33, 139.12, 132.59, 130.79, 122.49, 122.05, 121.28, 119.67, 116.27, 115.36, 114.20, 112.62, 55.74. HRMS Calcd for $C_{22}H_{16}N_2O_5$[M+H] =388.1059, found 388.1065



2-methyl-8-pivalamidoquinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, cdcl$_3$) δ 10.29 (s, 1H), 8.79 (d, *J* = 8.5 Hz, 1H), 8.24 (d, *J* = 8.9 Hz, 2H), 8.09 (dd, *J* = 8.7, 6.1 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.00 (dd, *J* = 19.3, 8.9 Hz, 2H), 3.92 (s, 3H), 2.75 (s, 3H), 1.43 (d, *J* = 6.7 Hz, 9H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 177.15, 165.18, 164.26, 157.65, 140.98, 138.68, 132.97, 132.50, 130.85 (s), 122.63, 121.45, 120.44, 118.61, 115.72, 114.20, 110.15, 55.73, 40.49, 27.85, 25.56. HRMS Calcd for $C_{23}H_{24}N_2O_4$[M+H] =392.1736, found 392.1739

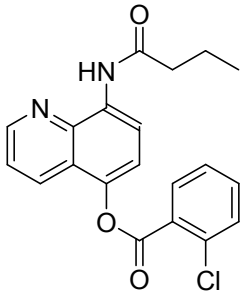


6-chloro-8-pivalamidoquinolin-5-yl 4-methoxybenzoate white solid ^{1}H NMR (400 MHz, cdcl$_3$) δ 10.19 (s, 1H), 8.98 (s, 1H), 8.83 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.33 – 8.22 (m, 2H), 8.16 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.48 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.12 – 6.99 (m, 2H), 3.93 (s, 3H), 1.43 (s, 9H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 177.42 (s), 164.52 (s), 164.08 (s), 148.63 (s), 137.92 (s), 137.03 (s), 133.68 (s), 132.88 (s), 130.58 (s), 125.73 (s), 123.37 (s), 122.71 (s), 120.65 (s), 117.22 (s), 114.24 (s), 55.76 (s), 40.50 (s), 27.78 (s). HRMS Calcd for $C_{22}H_{21}ClN_2O_4$[M+H] =412.1190, found 412.1196

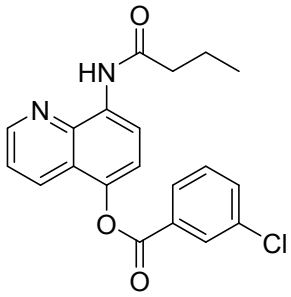


8-(phenylsulfonamido) quinolin-5-yl 4-methoxybenzoate white solid, ^{1}H NMR (400 MHz, CDCl$_3$) δ 9.15 (s, 1H), 8.78 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.25 – 8.11 (m, 3H), 7.98 – 7.82 (m, 3H), 7.50 – 7.29 (m, 5H), 7.08 – 6.97 (m, 2H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 164.48, 149.23, 141.82, 139.48, 139.05, 133.15, 132.62, 131.91, 130.82, 129.12, 127.35, 122.72, 122.27, 121.15, 119.25, 114.86, 114.27,

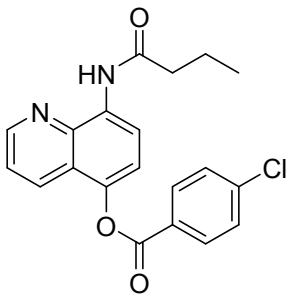
100.14, 77.42, 77.16, 76.84, 55.75. HRMS Calcd for $C_{23}H_{18}N_2O_5SNa$[M+Na] =457.0834, found 457.0937



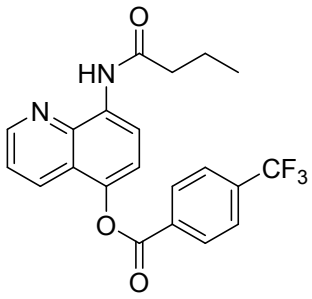
8-butyramidoquinolin-5-yl 2-chlorobenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.86 (dd, *J* = 4.9, 3.5 Hz, 2H), 8.31 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.18 (d, *J* = 7.4 Hz, 1H), 7.64 – 7.40 (m, 5H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.93 – 1.80 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.86, 164.35, 148.70, 140.52, 138.76, 134.68, 133.71, 133.24, 132.28, 131.70, 130.79, 128.96, 127.07, 122.08, 119.56, 115.87, 40.27, 19.26, 13.96. HRMS Calcd for $C_{20}H_{17}ClN_2O_3$[M+Na] =391.0825, found 391.0826



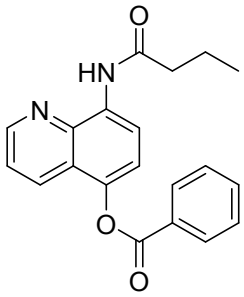
8-butyramidoquinolin-5-yl 3-chlorobenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.87 (dd, *J* = 5.0, 3.4 Hz, 2H), 8.42 (d, *J* = 8.1 Hz, 2H), 8.20 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.49 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.44 (d, *J* = 8.5 Hz, 1H), 2.57 (t, *J* = 7.5 Hz, 2H), 1.93 – 1.81 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.93, 164.27, 148.78, 140.36, 138.78, 133.38, 130.88, 130.43, 126.02, 122.11, 119.64, 115.89, 40.29, 19.28, 13.97. HRMS Calcd for $C_{20}H_{17}ClN_2O$ Na[M+Na] =391.0825, found 391.0831



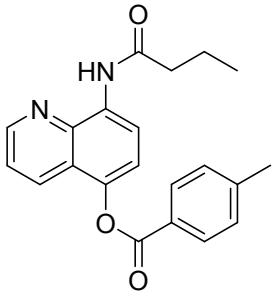
8-butyramidoquinolin-5-yl 4-chlorobenzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.89 – 8.79 (m, 2H), 8.22 (ddd, *J* = 10.1, 7.6, 1.8 Hz, 3H), 7.57 – 7.52 (m, 2H), 7.48 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 2.59 – 2.53 (m, 2H), 1.85 (dd, *J* = 14.7, 7.3 Hz, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.92 (s), 164.62 (s), 148.73 (s), 140.76 (s), 140.53 (s), 138.78 (s), 133.21 (s), 131.83 (s), 130.56 (s), 129.34 (s), 127.53 (s), 122.09 (d, *J* = 9.9 Hz), 119.65 (s), 115.94 (s), 40.28 (s), 19.29 (s), 13.96 (s). HRMS Calcd for $C_{20}H_{17}ClN_2O_3Na$[M+Na] =391.0825, found 391.0828



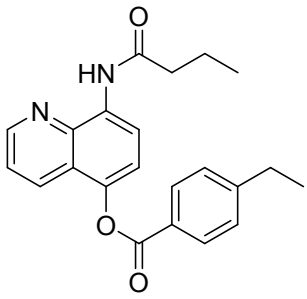
8-butyramidoquinolin-5-yl 4-(trifluoromethyl) benzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.90 – 8.81 (m, 2H), 8.28 (t, *J* = 1.8 Hz, 1H), 8.24 – 8.14 (m, 2H), 7.67 (ddd, *J* = 8.0, 2.1, 1.1 Hz, 1H), 7.56 – 7.45 (m, 2H), 7.42 (d, *J* = 8.5 Hz, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.92 – 1.81 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.90, 164.28, 148.75, 140.45, 138.77, 135.15, 134.17, 133.28, 130.86, 130.64, 130.18, 128.59, 122.07, 119.63, 115.90, 40.29, 19.28, 13.97. HRMS Calcd for $C_{21}H_{17}F_3N_2O_3K$[M+K] =441.1908, found 441.1914



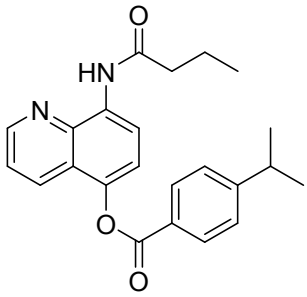
8-butyramidoquinolin-5-yl benzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.85 (dd, *J* = 9.4, 5.1 Hz, 2H), 8.34 – 8.28 (m, 2H), 8.24 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.70 (dd, *J* = 9.3, 5.4 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 2H), 7.48 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.93 – 1.80 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.87, 165.41, 148.58, 140.73, 138.65, 134.14, 133.01, 130.82, 130.46, 128.99, 122.25, 121.95, 119.70, 116.06, 40.26, 19.27, 13.96. HRMS Calcd for $C_{20}H_{18}N_2O_3$[M+H] = 334.1317, found 334.1319



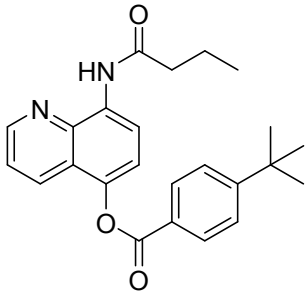
8-butyramidoquinolin-5-yl 4-methylbenzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.87 – 8.82 (m, 2H), 8.21 (ddd, *J* = 8.2, 7.5, 1.7 Hz, 3H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.60 – 2.52 (m, 2H), 2.49 (s, 3H), 1.93 – 1.80 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.86, 165.49, 148.64, 145.07, 140.87, 132.99, 130.77, 130.52, 129.65, 126.34, 122.33, 121.92, 119.68, 116.02, 40.29, 21.97, 19.29, 13.96. HRMS Calcd for $C_{21}H_{20}N_2O_3$[M+H] =348.1474, found 348.1475



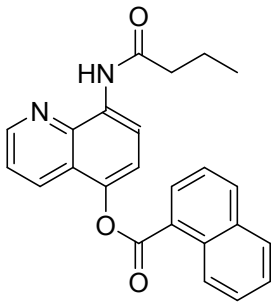
8-butyramidoquinolin-5-yl 4-ethylbenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.94 – 8.75 (m, 2H), 8.22 (ddd, *J* = 5.4, 4.6, 1.7 Hz, 3H), 7.43 (ddd, *J* = 18.9, 9.4, 6.3 Hz, 4H), 2.78 (q, *J* = 7.6 Hz, 2H), 2.60 – 2.49 (m, 2H), 1.93 – 1.80 (m, 2H), 1.31 (t, *J* = 7.6 Hz, 3H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.83, 165.48, 151.24, 148.63, 140.86, 138.79, 132.98, 130.70, 128.47, 126.52, 122.32, 121.91, 119.67, 115.98, 40.28, 29.24, 19.28, 15.40, 13.96. HRMS Calcd for $C_{22}H_{22}N_2O_3Na$[M+Na] =385.1528, found 385.1529



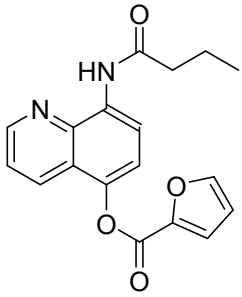
8-butyramidoquinolin-5-yl 4-isopropylbenzoate white solid,^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.89 – 8.79 (m, 2H), 8.28 – 8.16 (m, 3H), 7.44 (ddd, *J* = 11.7, 8.5, 3.8 Hz, 4H), 3.04 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.56 (t, *J* = 7.5 Hz, 2H), 1.87 (dd, *J* = 14.9, 7.4 Hz, 2H), 1.32 (d, *J* = 6.9 Hz, 6H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.84, 155.81, 148.63, 140.86, 138.79, 132.98, 130.73, 127.07, 126.65, 122.33, 121.92, 119.68, 115.98, 40.29, 34.56, 23.86, 19.29, 13.97. HRMS Calcd for $C_{23}H_{24}N_2O_3$[M+H] =376.1787, found 376.1789



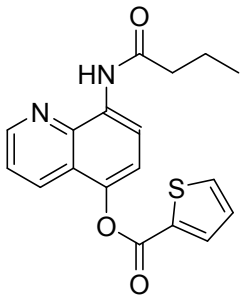
8-butyramidoquinolin-5-yl 4-(tert-butyl) benzoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.92 – 8.75 (m, 2H), 8.29 – 8.17 (m, 3H), 7.64 – 7.54 (m, 2H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 2.63 – 2.50 (m, 2H), 1.93 – 1.80 (m, 2H), 1.39 (s, 9H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.85 165.43, 158.04 148.63, 140.86, 138.80, 132.98, 130.78, 130.40, 126.27, 125.94, 122.33, 121.92, 119.68, 115.99, 40.29, 35.44, 31.26, 19.29, 13.97. HRMS Calcd for $C_{24}H_{26}N_2O_3$[M+H] =390.1943, found 390.1951



8-butyramidoquinolin-5-yl 1-naphthoate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 9.07 (d, *J* = 8.7 Hz, 1H), 8.94 – 8.82 (m, 2H), 8.67 (dd, *J* = 7.3, 1.2 Hz, 1H), 8.30 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.18 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.6 Hz, 1H), 7.71 – 7.55 (m, 3H), 7.54 – 7.43 (m, 2H), 2.62 – 2.51 (m, 2H), 1.95 – 1.81 (m, 2H), 1.09 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.88, 165.92, 148.69, 140.86, 135.01, 134.16, 133.11, 132.00, 131.67, 130.80, 128.95, 128.62, 126.74, 125.85, 125.17, 124.74, 122.43, 122.03, 119.82, 116.02, 40.31, 19.30, 13.98. HRMS Calcd for $C_{24}H_{20}N_2O_3$[M+H] =384.1474, found 384.1475



8-butyramidoquinolin-5-yl furan-2-carboxylate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.92 – 8.68 (m, 2H), 8.27 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.08 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.74 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.24 (dd, *J* = 5.0, 3.8 Hz, 1H), 2.62 – 2.48 (m, 2H), 1.94 – 1.79 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.87, 160.78, 148.69, 140.31, 138.73, 135.31, 134.12, 133.15, 132.27, 130.72, 128.45, 122.2, 122.02, 119.68, 115.88, 40.29, 19.28, 13.97. HRMS Calcd for $C_{18}H_{16}N_2O_4$[M+H] =324.1110, found 324.1111

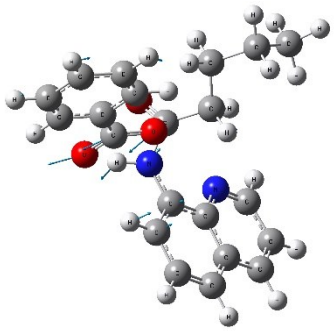


8-butyramidoquinolin-5-yl thiophene-2-carboxylate white solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.88 – 8.79 (m, 2H), 8.27 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.08 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.73 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.24 (dd, *J* = 5.0, 3.8 Hz, 1H), 2.55 (t, *J* = 7.5 Hz, 2H), 1.92 – 1.76 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.84, 160.76, 148.68, 140.30, 138.72, 135.30, 134.12, 133.15, 132.26, 130.70, 128.44, 122.21, 122.01, 119.67, 115.86, 40.28, 19.27, 13.96. HRMS Calcd for $C_{18}H_{16}N_2O_3SNa$[M+Na] =363.0779, found 363.0781

4. Computational methods

In this study, all calculations were performed using Gaussian 09 program package [1]. The geometric optimization of reactants, transition states, intermediates and products were performed by well-tested M06-2X [2] function connection with 6-31+G(*d,p*) basis set. Harmonic vibration frequencies were also calculated at the same level to characterize each molecule, with no imaginary frequencies as a minima or only one imaginary frequency as a saddle point, as well as evaluate the zero-point vibration energy (ZPVE) with the scale factor at 0.967[3]. To investigate the solvent effect of water (H_2O, ε=78.4), single point energy calculations were conducted in the framework of SMD continuum solvation model [4] implemented in Gaussian 09 program package. The unrestricted open-shelled approach is applied for all radical species. The spin contaminations of all radical species are not significant, $<S^2>$ ranging from 0.76 to 0.78. Therefore, the spin contamination will not bias found reaction energy.

Computed Structures, Cartesian Coordinates and Energy



Transition State A-B

Cartesian Coordinates and Energy

Energy: -1147.6045359 a.u.

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

--

1	6	0	2.408116	-1.751970	-1.810887
2	6	0	3.029259	-0.543972	-1.627004
3	6	0	2.526594	0.359008	-0.656402
4	6	0	1.368775	-0.040325	0.062470
5	6	0	1.282449	-2.062817	-1.008571
6	1	0	4.035141	1.887027	-0.924992
7	1	0	2.767510	-2.470023	-2.539473
8	1	0	3.908513	-0.269138	-2.203599
9	6	0	3.151972	1.597804	-0.362508
10	6	0	0.840811	0.846620	1.060995
11	1	0	0.788563	-3.026518	-1.116376
12	6	0	1.504082	2.033113	1.352916
13	6	0	2.654943	2.404799	0.635815
14	1	0	1.094831	2.677333	2.125591
15	1	0	3.141570	3.345541	0.869783
16	7	0	0.780687	-1.248930	-0.107629

17	7	0	-0.281248	0.519085	1.790941
18	1	0	-0.354646	0.922756	2.745856
19	6	0	-1.393277	-0.328020	1.429972
20	8	0	-1.907601	-0.955529	2.318687
21	6	0	-1.935460	-0.241280	0.025302
22	1	0	-1.388272	0.514891	-0.546734
23	1	0	-1.767814	-1.213738	-0.444586
24	6	0	-3.433741	0.087588	0.064569
25	1	0	-3.574124	1.008012	0.639133
26	1	0	-3.953259	-0.714583	0.601041
27	6	0	-4.031146	0.255135	-1.333968
28	1	0	-5.085709	0.533502	-1.226101
29	1	0	-3.540040	1.097017	-1.839241
30	6	0	-3.928876	-0.997371	-2.204758
31	1	0	-4.355189	-1.864846	-1.688588
32	1	0	-4.468726	-0.868846	-3.147122
33	1	0	-2.889761	-1.234955	-2.453769
34	6	0	-2.487490	4.015279	2.962251
35	6	0	-3.319767	4.520723	1.961699
36	6	0	-4.127171	5.624233	2.225609
37	6	0	-4.103221	6.220098	3.486638
38	6	0	-3.271491	5.712930	4.485301

39	6	0	-2.462224	4.610461	4.224500
40	1	0	-3.324016	4.043016	0.987147
41	1	0	-4.775129	6.020136	1.449801
42	1	0	-4.734539	7.079565	3.691475
43	1	0	-3.257211	6.175394	5.467376
44	1	0	-1.809583	4.190906	4.982981
45	6	0	-1.604791	2.817987	2.709370
46	8	0	-0.864301	2.392476	3.614720
47	8	0	-1.679034	2.311869	1.532384

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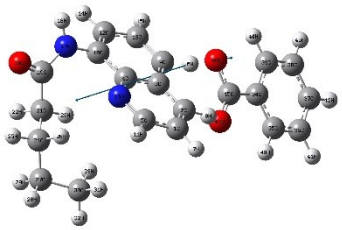


Transition State C-D

Energy: -1147.5792393 a.u.

-

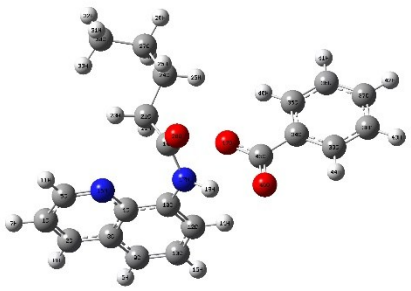
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

-

1	6	0	1.046088	1.701824	2.088186
2	6	0	0.070148	0.921366	1.527687
3	6	0	0.446418	-0.269151	0.854176
4	6	0	1.837772	-0.576220	0.769375
5	6	0	2.397963	1.291095	1.976038
6	1	0	-1.641046	-1.029954	0.381210
7	1	0	0.802719	2.620790	2.609613
8	1	0	-0.979508	1.195525	1.559080
9	6	0	-0.454542	-1.190980	0.281478
10	6	0	2.259133	-1.751007	0.059579
11	1	0	3.186604	1.891275	2.427196
12	6	0	1.320280	-2.594274	-0.489082
13	6	0	-0.065906	-2.322183	-0.370767
14	1	0	1.654594	-3.475919	-1.027365
15	1	0	-0.797633	-2.997610	-0.801542
16	7	0	2.783975	0.209799	1.342142
17	7	0	3.627709	-2.081135	-0.022502
18	1	0	3.927816	-2.943083	0.417428
19	6	0	4.683593	-1.266060	-0.387869
20	8	0	5.825125	-1.613507	-0.144037

21	6	0	4.381158	-0.024010	-1.200195
22	1	0	4.661324	-0.270595	-2.233321
23	1	0	3.313378	0.201103	-1.204612
24	6	0	5.207076	1.172986	-0.725537
25	1	0	6.266117	0.925292	-0.843024
26	1	0	5.031510	1.318873	0.347619
27	6	0	4.864473	2.458141	-1.482704
28	1	0	5.631839	3.212073	-1.272989
29	1	0	4.908023	2.267751	-2.563399
30	6	0	3.494704	3.028912	-1.112050
31	1	0	3.463892	3.290904	-0.048654
32	1	0	3.269023	3.932424	-1.685742
33	1	0	2.687427	2.311727	-1.295911
34	6	0	-4.906185	0.136405	-0.176866
35	6	0	-5.493545	1.390523	-0.355869
36	6	0	-6.864984	1.483040	-0.569480
37	6	0	-7.645529	0.327160	-0.602704
38	6	0	-7.055546	-0.923694	-0.423725
39	6	0	-5.683555	-1.024079	-0.209851
40	1	0	-4.862362	2.272426	-0.327548
41	1	0	-7.325303	2.455636	-0.710406
42	1	0	-8.715774	0.401438	-0.769064

43	1	0	-7.664299	-1.821606	-0.449752
44	1	0	-5.216537	-1.992912	-0.069200
45	6	0	-3.419366	0.106596	0.051029
46	8	0	-2.974334	-1.128997	0.249773
47	8	0	-2.725977	1.101935	0.058990



Intermediate A

Energy: -1147.6046256 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.376716	-0.370856	-0.277974
2	6	0	-4.839105	-1.452231	-0.925003
3	6	0	-3.469946	-1.770501	-0.735990
4	6	0	-2.715889	-0.914477	0.111312

5	6	0	-4.539439	0.393269	0.573603
6	1	0	-3.449422	-3.550429	-1.966163
7	1	0	-6.420447	-0.100719	-0.393293
8	1	0	-5.445131	-2.079690	-1.573231
9	6	0	-2.857566	-2.907648	-1.320740
10	6	0	-1.331654	-1.213158	0.329574
11	1	0	-4.949722	1.241587	1.118204
12	6	0	-0.773069	-2.351051	-0.226517
13	6	0	-1.540058	-3.195684	-1.053096
14	1	0	0.272286	-2.566658	-0.028139
15	1	0	-1.073024	-4.072560	-1.488577
16	7	0	-3.266078	0.139074	0.766204
17	7	0	-0.550460	-0.412720	1.159051
18	1	0	0.137105	-0.891492	1.757913
19	6	0	-0.656185	0.996716	1.409419
20	8	0	-0.325116	1.388599	2.499726
21	6	0	-1.002392	1.900791	0.252590
22	1	0	-1.101952	1.317833	-0.669069
23	1	0	-1.972201	2.352720	0.475822
24	6	0	0.074535	2.982479	0.096784
25	1	0	1.048212	2.494893	-0.012808
26	1	0	0.110926	3.573109	1.019206

27	6	0	-0.182620	3.897451	-1.102175
28	1	0	0.648373	4.608205	-1.177073
29	1	0	-0.163190	3.301746	-2.024178
30	6	0	-1.498656	4.670985	-1.018267
31	1	0	-1.565370	5.221836	-0.073419
32	1	0	-1.585180	5.393425	-1.834705
33	1	0	-2.365400	4.005272	-1.078086
34	6	0	3.578013	-0.552066	0.048524
35	6	0	3.866094	0.296813	-1.022038
36	6	0	5.177813	0.417860	-1.473562
37	6	0	6.197839	-0.306030	-0.856288
38	6	0	5.907465	-1.152682	0.213740
39	6	0	4.597286	-1.277777	0.667107
40	1	0	3.060842	0.852975	-1.491222
41	1	0	5.405551	1.076475	-2.305857
42	1	0	7.220180	-0.208946	-1.209057
43	1	0	6.702899	-1.712388	0.695845
44	1	0	4.341799	-1.924687	1.499905
45	6	0	2.171532	-0.709791	0.571421
46	8	0	1.932437	-1.474869	1.512714
47	8	0	1.284545	-0.002662	-0.049110

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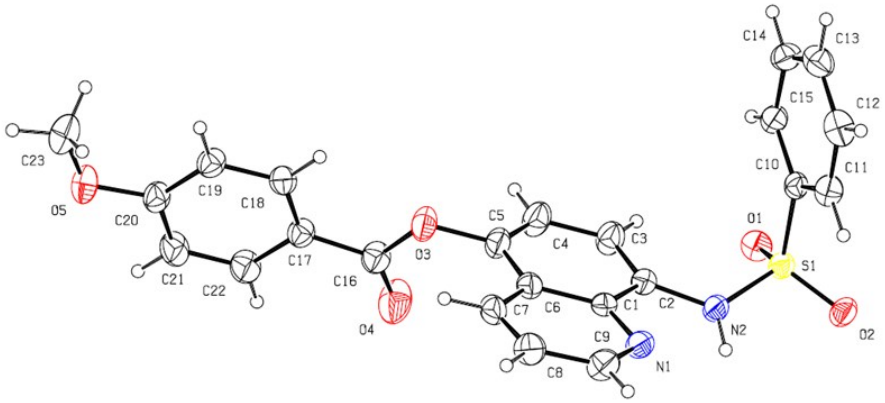
5. X-ray Crystallographic Data of Compound 3h



$C_{23}H_{18}N_2O_5S$	$Z = 2$
$M_r = 434.45$	$F(000) = 452$
Triclinic, $P\bar{1}$	$D_x = 1.406$ Mg m^{-3}
$a = 9.1495$ (7) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.0385$ (8) Å	Cell parameters from 2746 reflections
$c = 11.775$ (1) Å	$\theta = 3.8$–$28.2°$
$\alpha = 68.418$ (7)°	$\mu = 0.20$ mm^{-1}
$\beta = 81.041$ (7)°	$T = 293$ K
$\gamma = 68.191$ (7)°	0.35 × 0.3 × 0.25 mm
$V = 1026.46$ (16) Å^3	

Xcalibur, Eos diffractometer	4187 independent reflections
Radiation source: Enhance (Mo) X-ray Source	3151 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.021$
Detector resolution: 16.0874 pixels mm^{-1}	$\theta_{max} = 26.4°$, $\theta_{min} = 3.0°$

ω scans	h = -9→11
Absorption correction: multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	k = -12→13
T_{min} = 0.805, T_{max} = 1.000	l = -14→14
8234 measured reflections	

Refinement on F^2	Primary atom site location: iterative
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.120	$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.2602P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4187 reflections	$\Delta\rangle_{max}$ = 0.34 e Å^{-3}
281 parameters	$\Delta\rangle_{min}$ = -0.32 e Å^{-3}
0 restraints	

	x	y	z	U_{iso}*/U_{eq}
S1	1.12004 (6)	0.64209 (5)	0.01503 (5)	0.04225 (16)
O1	1.13147 (18)	0.77682 (15)	-0.02870 (13)	0.0515 (4)
O2	1.08928 (18)	0.59029 (16)	-0.06981 (13)	0.0530 (4)
O3	0.8626 (2)	0.82355 (15)	0.51737 (14)	0.0581 (4)
O4	0.6806 (3)	1.0185 (2)	0.40980 (18)	0.0928 (7)
O5	0.6149 (2)	1.10288 (17)	0.92133 (16)	0.0663 (5)
N1	0.8385 (2)	0.51528 (18)	0.32160 (16)	0.0481 (4)
N2	0.9761 (2)	0.64040 (18)	0.11626 (16)	0.0471 (4)
H2	0.9059	0.6101	0.1076	0.056*
C1	0.8798 (2)	0.6213 (2)	0.32252 (18)	0.0395 (5)
C2	0.9591 (2)	0.6854 (2)	0.21711 (19)	0.0436 (5)
C3	1.0094 (3)	0.7878 (2)	0.2177 (2)	0.0582 (6)

H3	1.0658	0.8272	0.1508	0.070*
C4	0.9763 (3)	0.8335 (3)	0.3187 (2)	0.0619 (7)
H4	1.0112	0.9030	0.3178	0.074*
C5	0.8954 (3)	0.7784 (2)	0.4161 (2)	0.0505 (6)
C6	0.8455 (2)	0.6688 (2)	0.42391 (18)	0.0435 (5)
C7	0.7668 (3)	0.6013 (2)	0.5255 (2)	0.0519 (6)
H7	0.7419	0.6291	0.5937	0.062*
C8	0.7276 (3)	0.4957 (3)	0.5232 (2)	0.0592 (6)
H8	0.6753	0.4503	0.5896	0.071*
C9	0.7667 (3)	0.4555 (3)	0.4196 (2)	0.0586 (6)
H9	0.7401	0.3817	0.4201	0.070*
C10	1.2910 (2)	0.5239 (2)	0.09555 (18)	0.0395 (5)
C11	1.3157 (3)	0.3836 (2)	0.1343 (2)	0.0505 (5)
H11	1.2434	0.3521	0.1171	0.061*
C12	1.4486 (3)	0.2913 (2)	0.1986 (2)	0.0597 (6)
H12	1.4658	0.1967	0.2261	0.072*
C13	1.5565 (3)	0.3385 (3)	0.2225 (2)	0.0593 (6)
H13	1.6466	0.2754	0.2655	0.071*
C14	1.5317 (3)	0.4780 (3)	0.1833 (2)	0.0554 (6)
H14	1.6054	0.5090	0.1993	0.066*
C15	1.3978 (3)	0.5722 (2)	0.12029 (19)	0.0454 (5)
H15	1.3795	0.6669	0.0948	0.055*
C16	0.7496 (3)	0.9507 (2)	0.5026 (2)	0.0533 (6)
C17	0.7263 (3)	0.9878 (2)	0.6134 (2)	0.0459 (5)
C18	0.8126 (3)	0.9049 (2)	0.7176 (2)	0.0463 (5)
H18	0.8946	0.8239	0.7174	0.056*
C19	0.7791 (3)	0.9402 (2)	0.8218 (2)	0.0488 (5)
H19	0.8377	0.8829	0.8916	0.059*
C20	0.6586 (3)	1.0608 (2)	0.8225 (2)	0.0491 (5)
C21	0.5733 (3)	1.1468 (2)	0.7170 (2)	0.0616 (7)
H21	0.4938	1.2294	0.7164	0.074*
C22	0.6059 (3)	1.1104 (2)	0.6146 (2)	0.0595 (6)

H22	0.5473	1.1679	0.5449	0.071*
C23	0.6953 (4)	1.0136 (3)	1.0329 (2)	0.0724 (8)
H23A	0.8056	1.0003	1.0206	0.109*
H23B	0.6806	0.9256	1.0578	0.109*
H23C	0.6535	1.0549	1.0952	0.109*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0430 (3)	0.0532 (3)	0.0366 (3)	-0.0223 (2)	0.0032 (2)	-0.0176 (2)
O1	0.0532 (9)	0.0502 (8)	0.0485 (9)	-0.0219 (7)	0.0022 (7)	-0.0109 (7)
O2	0.0578 (10)	0.0776 (11)	0.0395 (8)	-0.0353 (8)	0.0057 (7)	-0.0277 (8)
O3	0.0714 (11)	0.0521 (9)	0.0480 (9)	-0.0060 (8)	-0.0081 (8)	-0.0265 (7)
O4	0.1152 (18)	0.0765 (13)	0.0578 (12)	0.0122 (12)	-0.0306 (12)	-0.0249 (10)
O5	0.0838 (13)	0.0583 (10)	0.0661 (12)	-0.0206 (9)	0.0054 (10)	-0.0379 (9)
N1	0.0481 (11)	0.0600 (11)	0.0440 (10)	-0.0249 (9)	0.0008 (8)	-0.0202 (9)
N2	0.0444 (10)	0.0684 (12)	0.0433 (10)	-0.0299 (9)	0.0090 (8)	-0.0285 (9)
C1	0.0324 (10)	0.0460 (11)	0.0391 (11)	-0.0096 (9)	-0.0046 (8)	-0.0157 (9)
C2	0.0403 (11)	0.0537 (12)	0.0414 (12)	-0.0170 (10)	0.0011 (9)	-0.0210 (10)
C3	0.0693 (16)	0.0707 (15)	0.0507 (14)	-0.0398 (13)	0.0130 (12)	-0.0281 (12)
C4	0.0783 (18)	0.0647 (15)	0.0613 (16)	-0.0361 (14)	0.0055 (14)	-0.0330 (13)
C5	0.0563 (14)	0.0535 (13)	0.0430 (13)	-0.0116 (11)	-0.0051 (11)	-0.0234 (10)
C6	0.0384 (11)	0.0470 (12)	0.0394 (12)	-0.0056 (9)	-0.0049 (9)	-0.0159 (9)
C7	0.0466 (13)	0.0630 (14)	0.0393 (12)	-0.0096 (11)	0.0006 (10)	-0.0198 (10)
C8	0.0597 (15)	0.0746 (16)	0.0416 (13)	-0.0298 (13)	0.0063 (11)	-0.0139 (11)
C9	0.0660 (16)	0.0689 (15)	0.0495 (14)	-0.0370 (13)	0.0023 (12)	-0.0169 (12)
C10	0.0420 (11)	0.0469 (11)	0.0336 (10)	-0.0191 (9)	0.0064 (9)	-0.0172 (9)
C11	0.0590 (14)	0.0505 (13)	0.0475 (13)	-0.0269 (11)	0.0072 (11)	-0.0176 (10)
C12	0.0675 (17)	0.0473 (13)	0.0538 (15)	-0.0173 (12)	0.0083 (13)	-0.0115 (11)
C13	0.0501 (14)	0.0670 (16)	0.0445 (14)	-0.0102 (12)	0.0008 (11)	-0.0115 (11)
C14	0.0500 (14)	0.0748 (16)	0.0476 (13)	-0.0259 (12)	-0.0024 (11)	-0.0226 (12)
C15	0.0492 (13)	0.0504 (12)	0.0429 (12)	-0.0220 (10)	0.0020 (10)	-0.0187 (10)
C16	0.0600 (15)	0.0449 (12)	0.0506 (14)	-0.0113 (11)	-0.0061 (12)	-0.0160 (11)
C17	0.0507 (13)	0.0410 (11)	0.0467 (13)	-0.0142 (10)	-0.0032 (10)	-0.0163 (9)

C18	0.0462 (12)	0.0377 (11)	0.0548 (13)	-0.0101 (9)	-0.0027 (10)	-0.0190 (10)
C19	0.0546 (14)	0.0426 (12)	0.0496 (13)	-0.0141 (10)	-0.0074 (11)	-0.0161 (10)
C20	0.0561 (14)	0.0437 (12)	0.0571 (14)	-0.0215 (10)	0.0038 (11)	-0.0250 (11)
C21	0.0615 (16)	0.0425 (12)	0.0714 (17)	0.0001 (11)	-0.0052 (13)	-0.0257 (12)
C22	0.0612 (15)	0.0452 (12)	0.0605 (15)	-0.0013 (11)	-0.0122 (12)	-0.0177 (11)
C23	0.101 (2)	0.0741 (17)	0.0543 (16)	-0.0381 (16)	0.0040 (15)	-0.0290 (14)

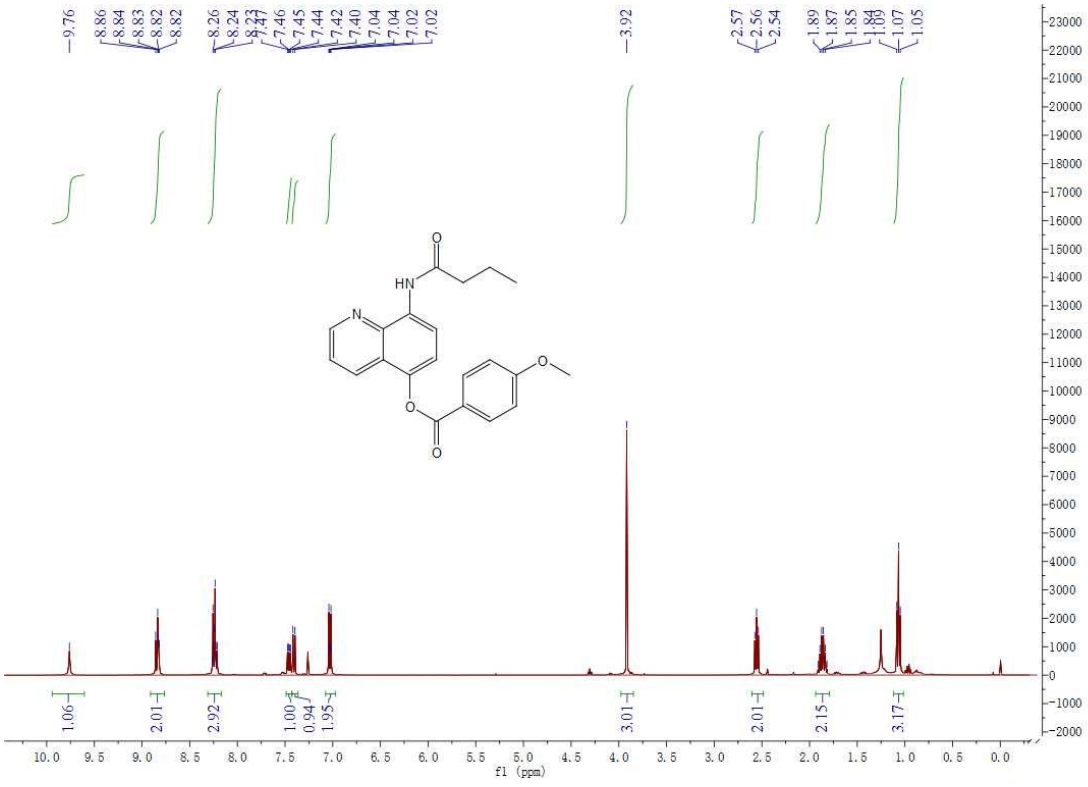
S1—O1	1.4225 (15)	C9—H9	0.9300
S1—O2	1.4253 (14)	C10—C11	1.382 (3)
S1—N2	1.6336 (17)	C10—C15	1.383 (3)
S1—C10	1.756 (2)	C11—H11	0.9300
O3—C5	1.405 (2)	C11—C12	1.374 (3)
O3—C16	1.367 (3)	C12—H12	0.9300
O4—C16	1.190 (3)	C12—C13	1.379 (4)
O5—C20	1.358 (2)	C13—H13	0.9300
O5—C23	1.431 (3)	C13—C14	1.374 (3)
N1—C1	1.360 (2)	C14—H14	0.9300
N1—C9	1.313 (3)	C14—C15	1.379 (3)
N2—H2	0.8600	C15—H15	0.9300
N2—C2	1.414 (2)	C16—C17	1.468 (3)
C1—C2	1.422 (3)	C17—C18	1.380 (3)
C1—C6	1.422 (3)	C17—C22	1.395 (3)
C2—C3	1.372 (3)	C18—H18	0.9300
C3—H3	0.9300	C18—C19	1.378 (3)
C3—C4	1.406 (3)	C19—H19	0.9300
C4—H4	0.9300	C19—C20	1.379 (3)
C4—C5	1.338 (3)	C20—C21	1.392 (3)
C5—C6	1.413 (3)	C21—H21	0.9300
C6—C7	1.407 (3)	C21—C22	1.364 (3)
C7—H7	0.9300	C22—H22	0.9300
C7—C8	1.351 (3)	C23—H23A	0.9600
C8—H8	0.9300	C23—H23B	0.9600

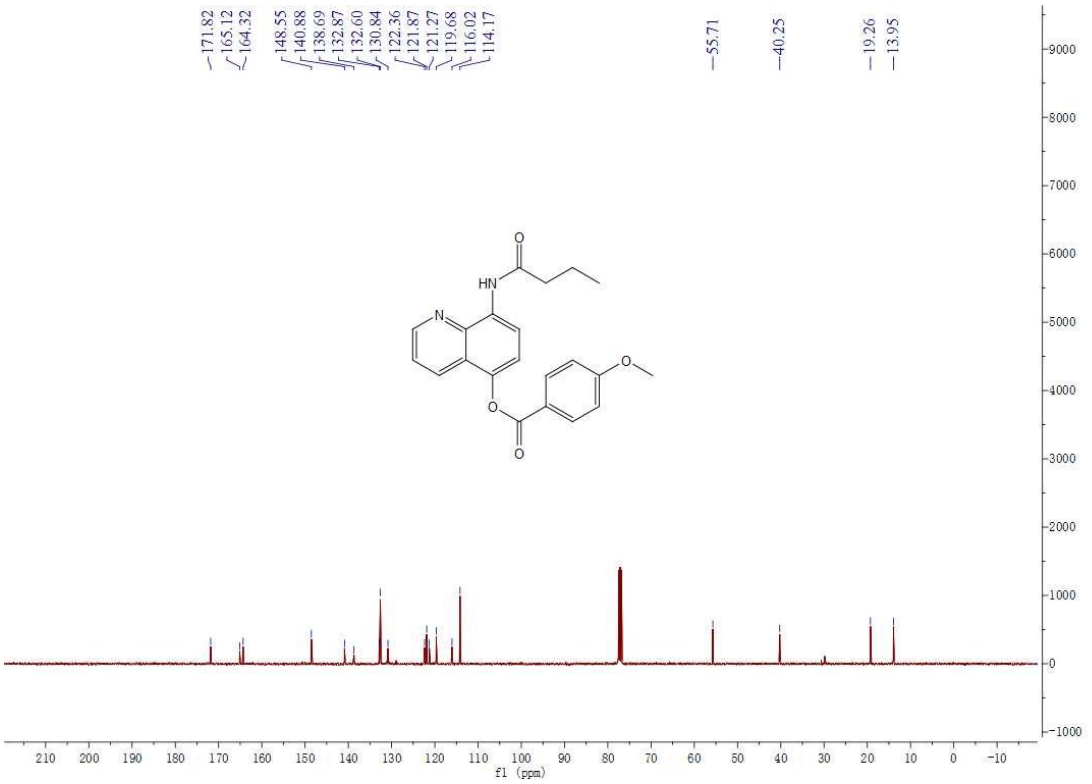
C8—C9	1.399 (3)	C23—H23C	0.9600
O1—S1—O2	118.74 (10)	C10—C11—H11	120.5
O1—S1—N2	108.24 (9)	C12—C11—C10	119.1 (2)
O1—S1—C10	108.56 (10)	C12—C11—H11	120.5
O2—S1—N2	105.42 (9)	C11—C12—H12	119.9
O2—S1—C10	109.67 (9)	C11—C12—C13	120.2 (2)
N2—S1—C10	105.39 (9)	C13—C12—H12	119.9
C16—O3—C5	116.41 (17)	C12—C13—H13	119.8
C20—O5—C23	117.73 (18)	C14—C13—C12	120.4 (2)
C9—N1—C1	117.55 (19)	C14—C13—H13	119.8
S1—N2—H2	117.8	C13—C14—H14	120.0
C2—N2—S1	124.42 (14)	C13—C14—C15	120.1 (2)
C2—N2—H2	117.8	C15—C14—H14	120.0
N1—C1—C2	117.73 (18)	C10—C15—H15	120.5
N1—C1—C6	122.25 (19)	C14—C15—C10	119.1 (2)
C6—C1—C2	120.02 (18)	C14—C15—H15	120.5
N2—C2—C1	116.43 (18)	O3—C16—C17	111.73 (19)
C3—C2—N2	124.5 (2)	O4—C16—O3	121.8 (2)
C3—C2—C1	119.07 (19)	O4—C16—C17	126.4 (2)
C2—C3—H3	119.7	C18—C17—C16	123.42 (19)
C2—C3—C4	120.5 (2)	C18—C17—C22	118.6 (2)
C4—C3—H3	119.7	C22—C17—C16	118.0 (2)
C3—C4—H4	119.5	C17—C18—H18	119.5
C5—C4—C3	120.9 (2)	C19—C18—C17	121.09 (19)
C5—C4—H4	119.5	C19—C18—H18	119.5
O3—C5—C6	117.3 (2)	C18—C19—H19	120.1
C4—C5—O3	121.1 (2)	C18—C19—C20	119.8 (2)
C4—C5—C6	121.6 (2)	C20—C19—H19	120.1
C5—C6—C1	117.70 (19)	O5—C20—C19	124.1 (2)
C7—C6—C1	117.4 (2)	O5—C20—C21	116.3 (2)
C7—C6—C5	124.9 (2)	C19—C20—C21	119.5 (2)

C6—C7—H7	120.2	C20—C21—H21	119.9
C8—C7—C6	119.5 (2)	C22—C21—C20	120.3 (2)
C8—C7—H7	120.2	C22—C21—H21	119.9
C7—C8—H8	120.4	C17—C22—H22	119.7
C7—C8—C9	119.2 (2)	C21—C22—C17	120.7 (2)
C9—C8—H8	120.4	C21—C22—H22	119.7
N1—C9—C8	124.1 (2)	O5—C23—H23A	109.5
N1—C9—H9	117.9	O5—C23—H23B	109.5
C8—C9—H9	117.9	O5—C23—H23C	109.5
C11—C10—S1	119.13 (17)	H23A—C23—H23B	109.5
C11—C10—C15	121.1 (2)	H23A—C23—H23C	109.5
C15—C10—S1	119.80 (16)	H23B—C23—H23C	109.5
S1—N2—C2—C1	-151.42 (16)	C4—C5—C6—C1	-2.0 (3)
S1—N2—C2—C3	30.6 (3)	C4—C5—C6—C7	176.8 (2)
S1—C10—C11—C12	-179.20 (16)	C5—O3—C16—O4	1.3 (4)
S1—C10—C15—C14	-179.81 (16)	C5—O3—C16—C17	-179.43 (19)
O1—S1—N2—C2	-51.2 (2)	C5—C6—C7—C8	-178.7 (2)
O1—S1—C10—C11	-172.29 (15)	C6—C1—C2—N2	-174.49 (18)
O1—S1—C10—C15	8.36 (19)	C6—C1—C2—C3	3.6 (3)
O2—S1—N2—C2	-179.24 (17)	C6—C7—C8—C9	0.2 (3)
O2—S1—C10—C11	-41.09 (18)	C7—C8—C9—N1	-0.9 (4)
O2—S1—C10—C15	139.56 (16)	C9—N1—C1—C2	179.3 (2)
O3—C5—C6—C1	-179.25 (17)	C9—N1—C1—C6	-1.0 (3)
O3—C5—C6—C7	-0.5 (3)	C10—S1—N2—C2	64.78 (19)
O3—C16—C17—C18	1.9 (3)	C10—C11—C12—C13	-0.8 (3)
O3—C16—C17—C22	-175.3 (2)	C11—C10—C15—C14	0.9 (3)
O4—C16—C17—C18	-178.9 (3)	C11—C12—C13—C14	0.5 (3)
O4—C16—C17—C22	4.0 (4)	C12—C13—C14—C15	0.5 (3)

O5—C20—C21—C22	-177.9 (2)	C13—C14—C15—C10	-1.1 (3)
N1—C1—C2—N2	5.2 (3)	C15—C10—C11—C12	0.1 (3)
N1—C1—C2—C3	-176.7 (2)	C16—O3—C5—C4	73.8 (3)
N1—C1—C6—C5	179.18 (18)	C16—O3—C5—C6	-109.0 (2)
N1—C1—C6—C7	0.3 (3)	C16—C17—C18—C19	-175.7 (2)
N2—S1—C10—C11	71.94 (17)	C16—C17—C22—C21	176.6 (2)
N2—S1—C10—C15	-107.41 (17)	C17—C18—C19—C20	-0.6 (3)
N2—C2—C3—C4	174.9 (2)	C18—C17—C22—C21	-0.7 (4)
C1—N1—C9—C8	1.3 (4)	C18—C19—C20—O5	178.7 (2)
C1—C2—C3—C4	-3.1 (4)	C18—C19—C20—C21	-0.9 (3)
C1—C6—C7—C8	0.1 (3)	C19—C20—C21—C22	1.7 (4)
C2—C1—C6—C5	-1.1 (3)	C20—C21—C22—C17	-0.9 (4)
C2—C1—C6—C7	180.00 (19)	C22—C17—C18—C19	1.4 (3)
C2—C3—C4—C5	0.0 (4)	C23—O5—C20—C19	-2.5 (3)
C3—C4—C5—O3	179.8 (2)	C23—O5—C20—C21	177.1 (2)
C3—C4—C5—C6	2.6 (4)		

6 ^{1}H and ^{13}C NMR spectra of all products

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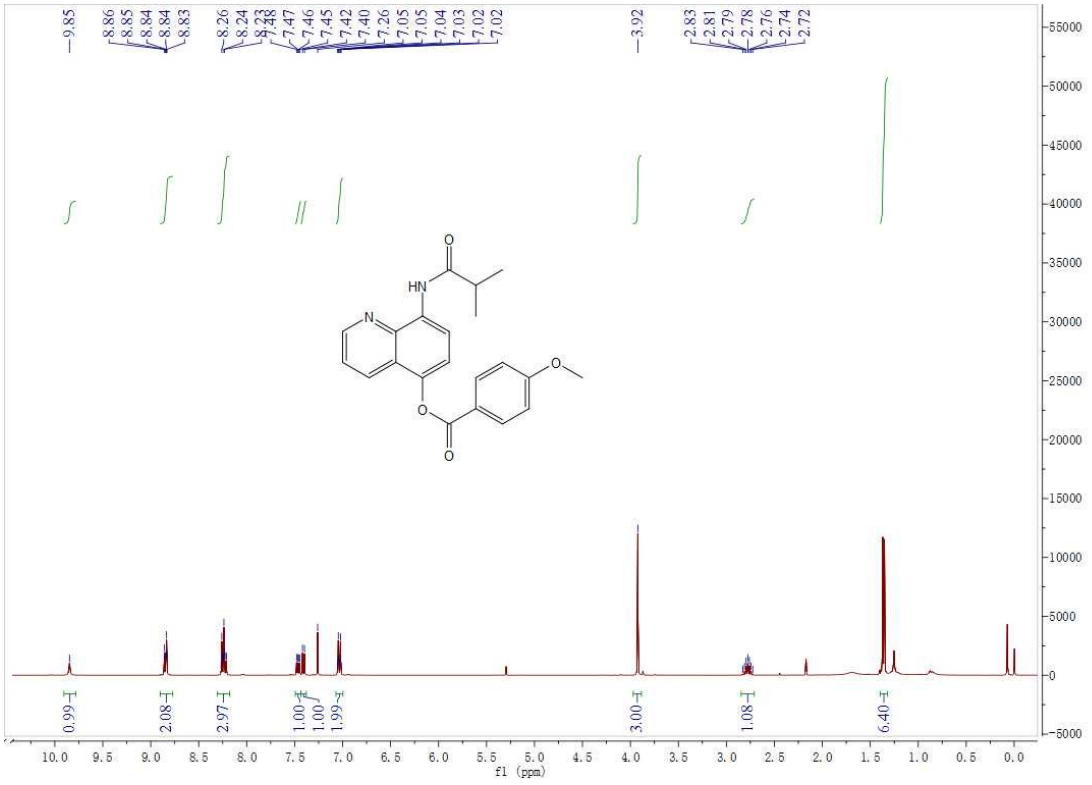
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7.26
7.05
7.05
7.04
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7.02
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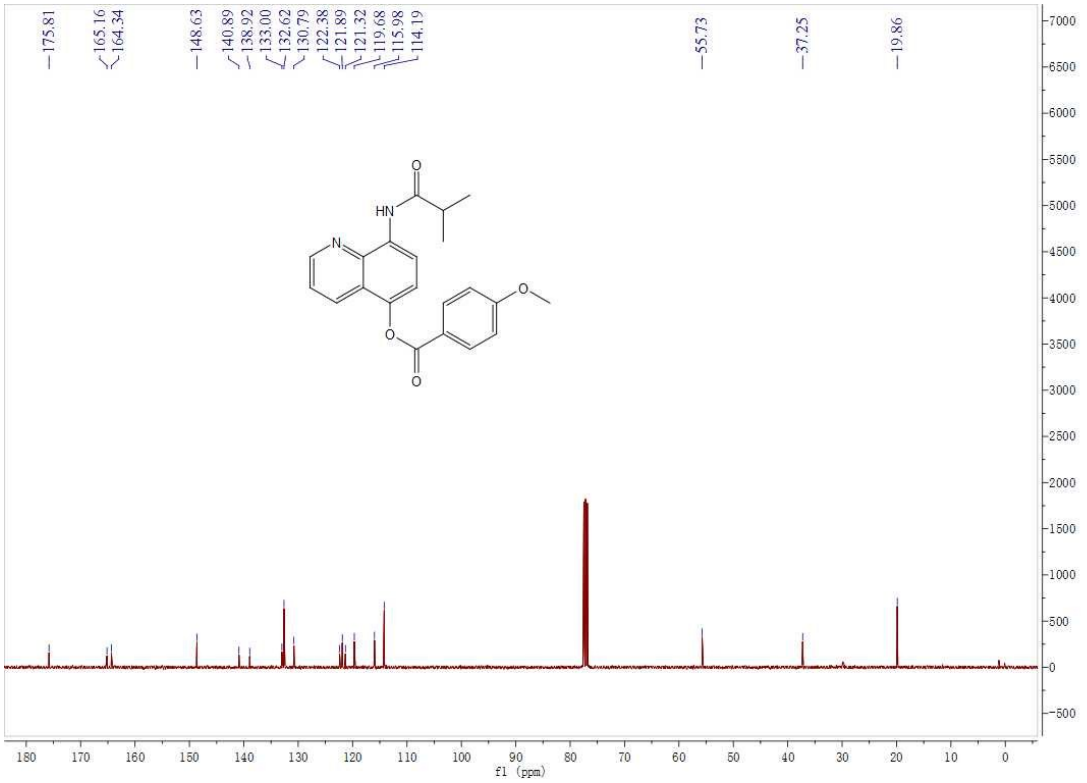
f1 (ppm)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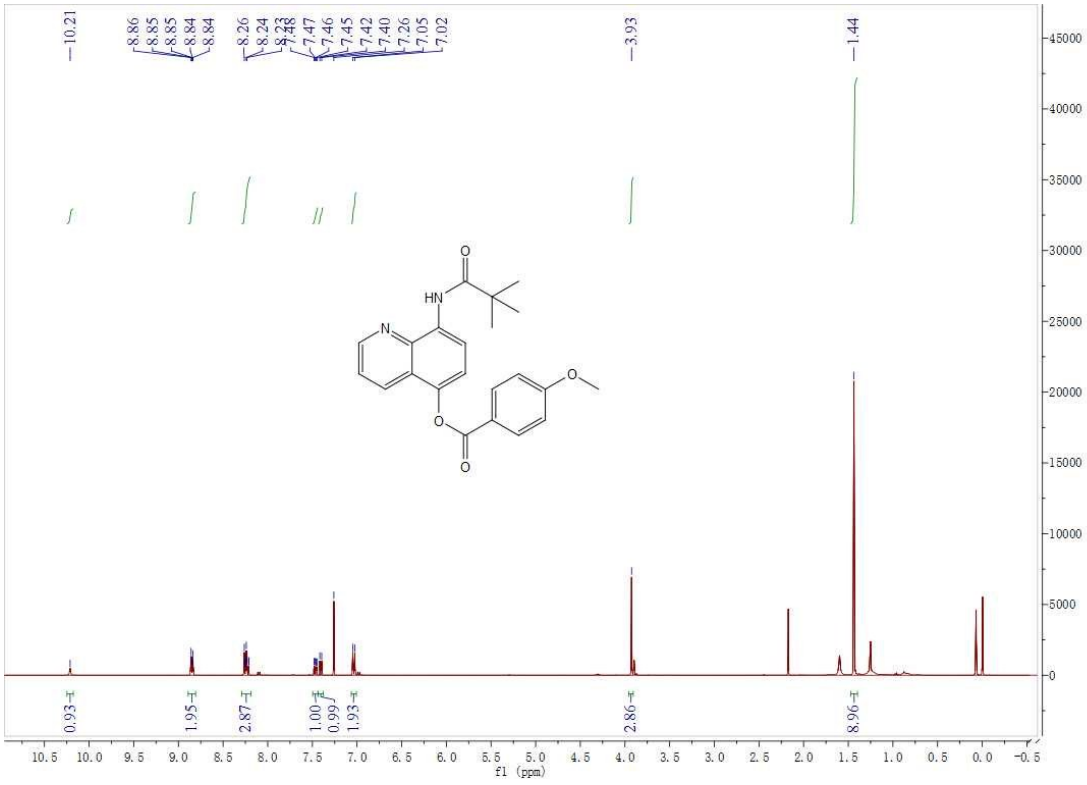
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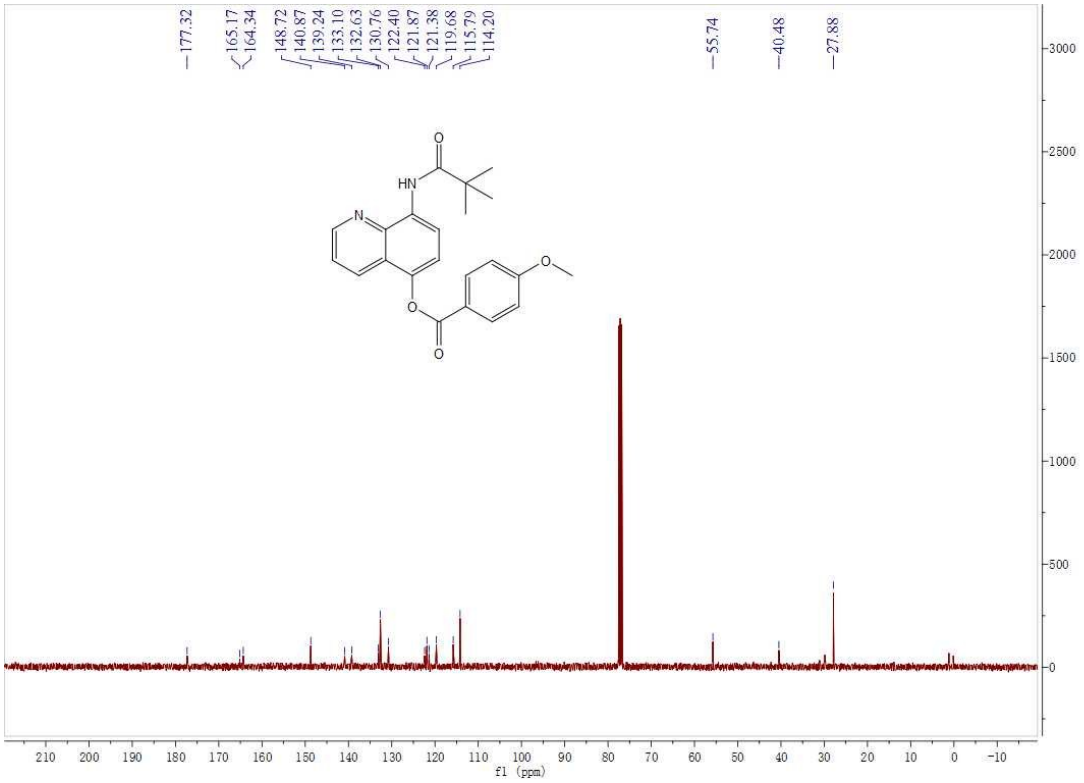
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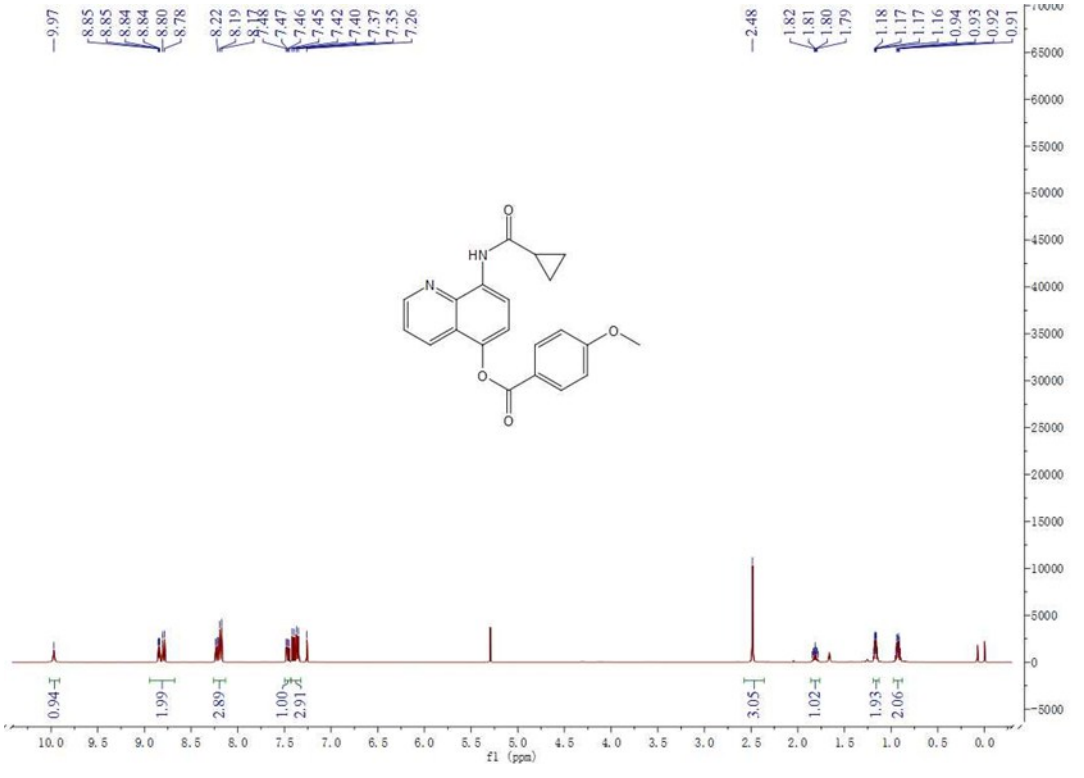
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0.93
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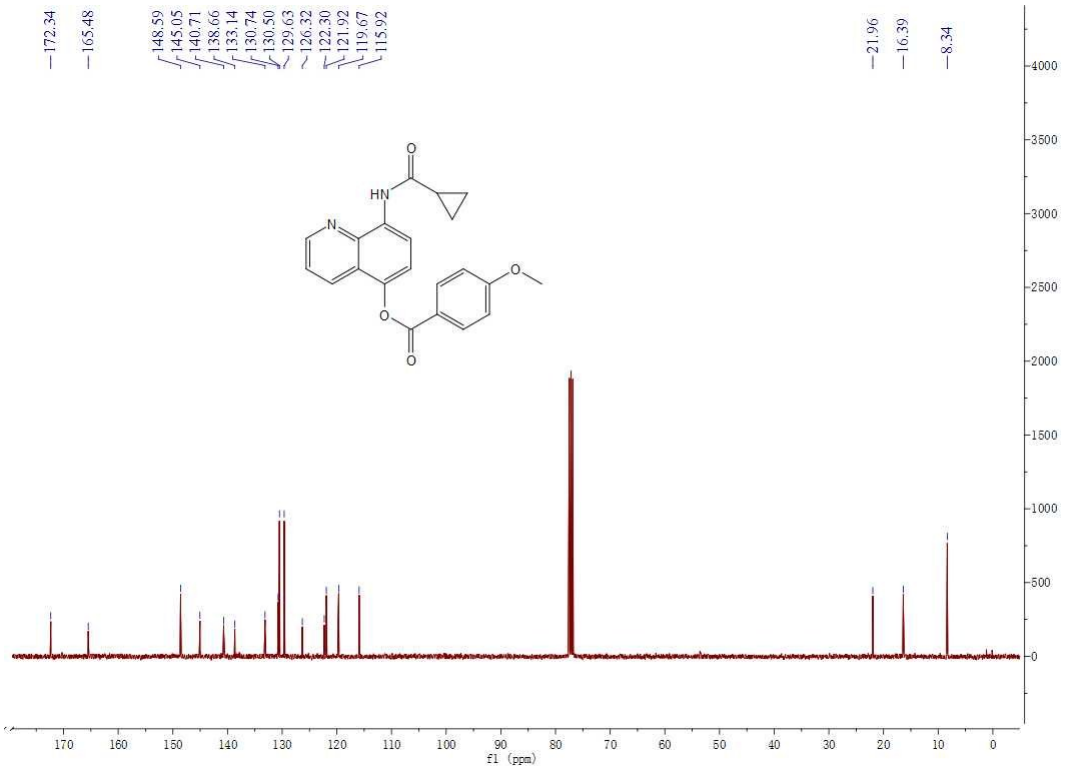
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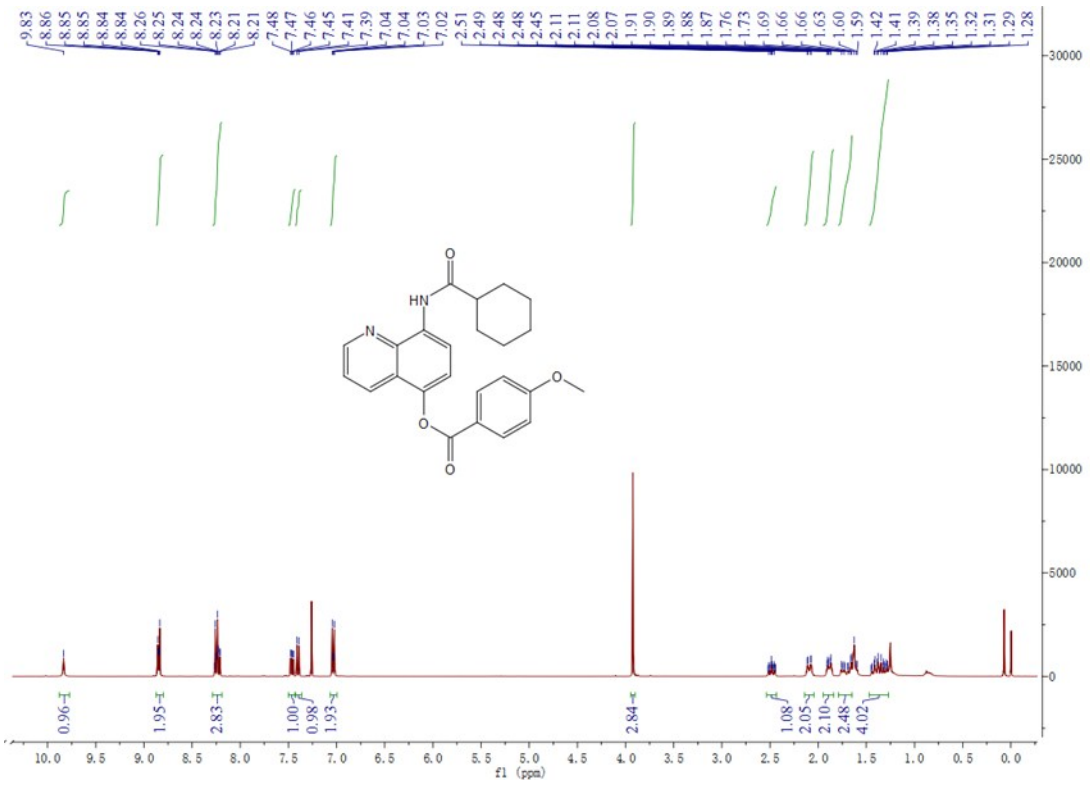
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2.08
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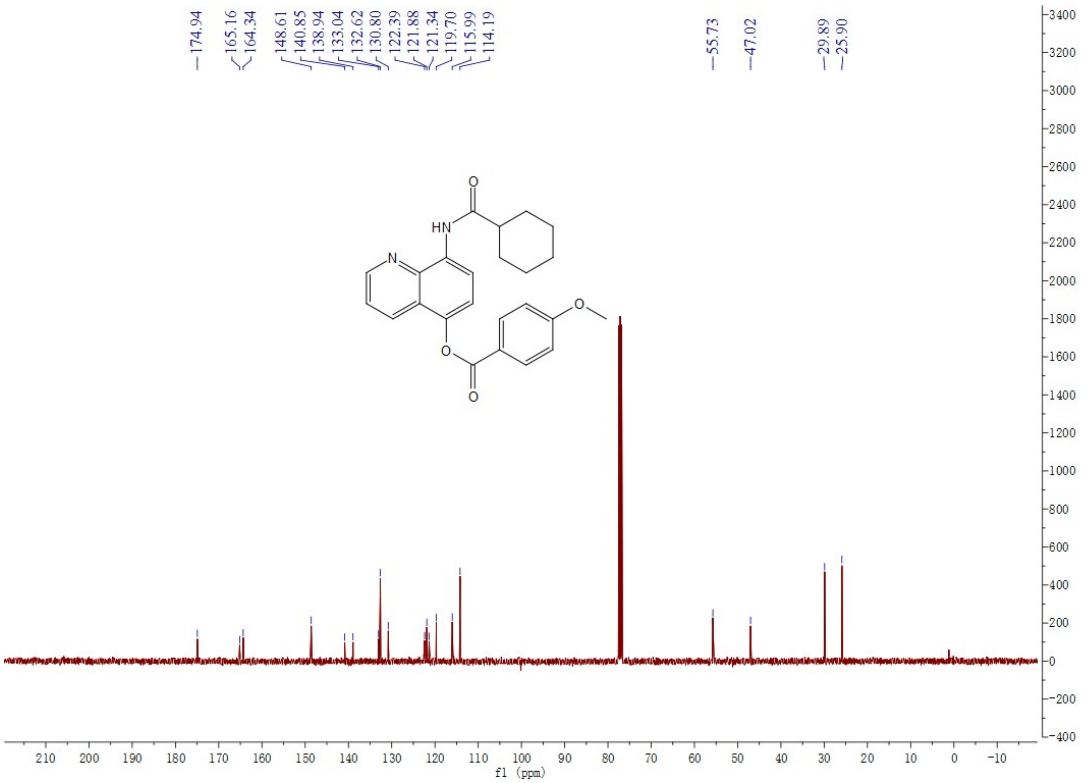
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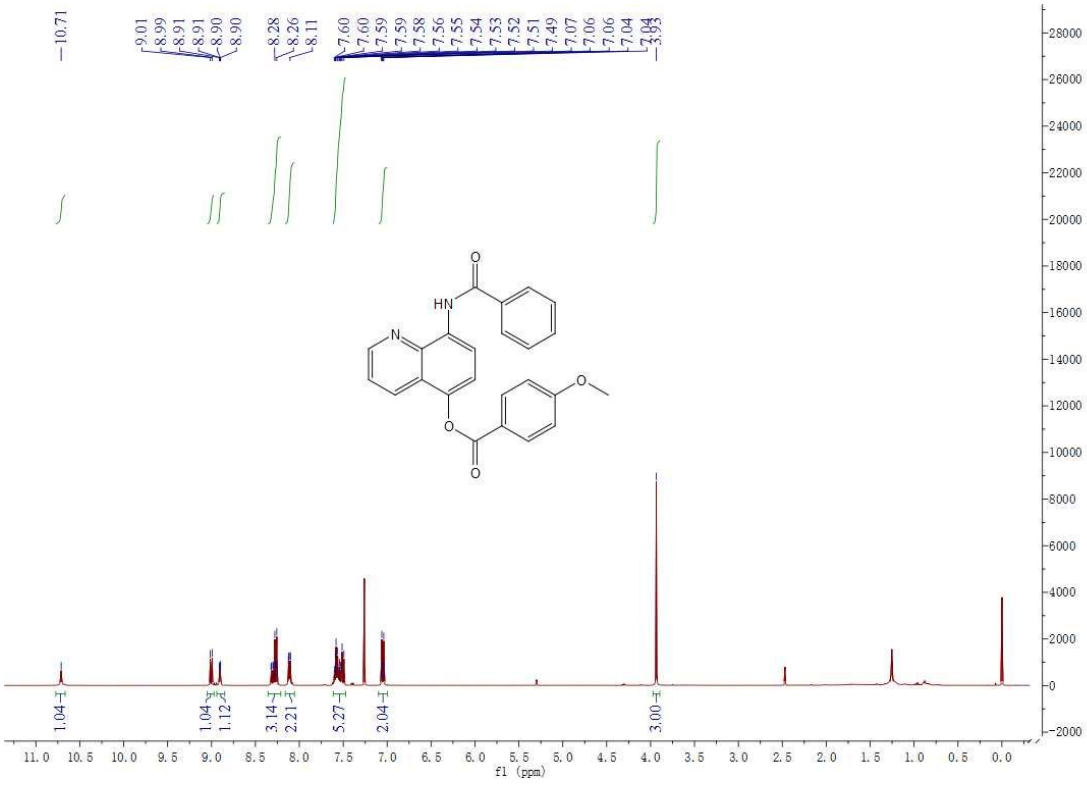
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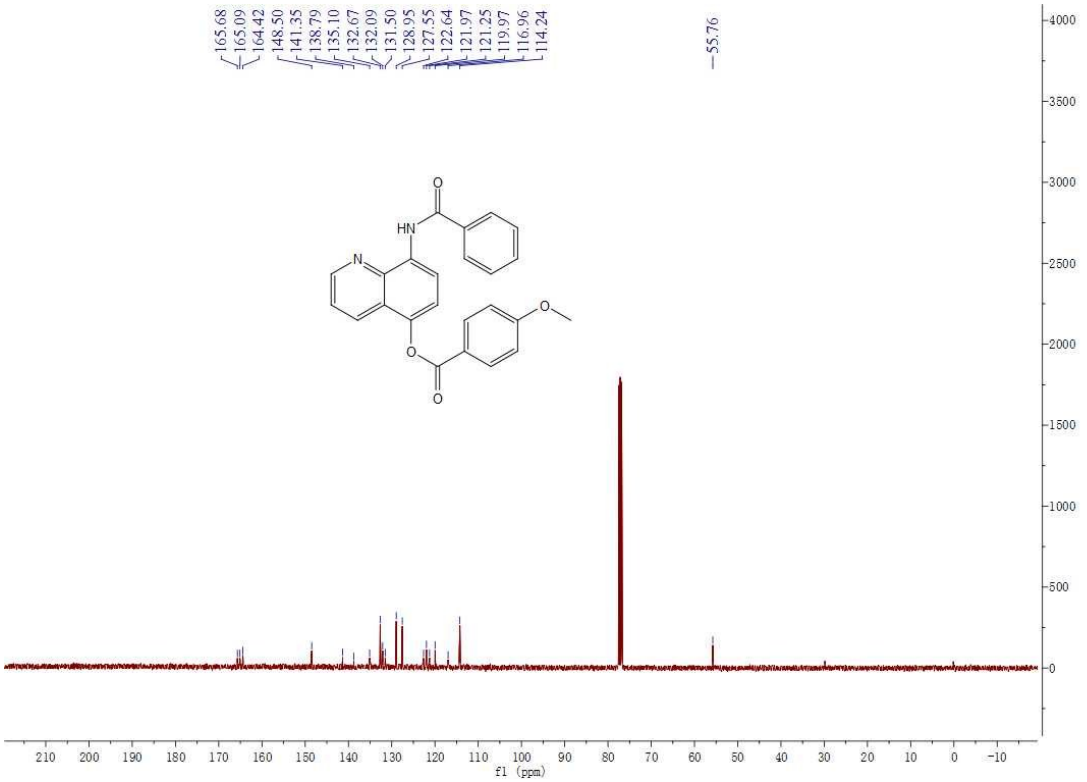
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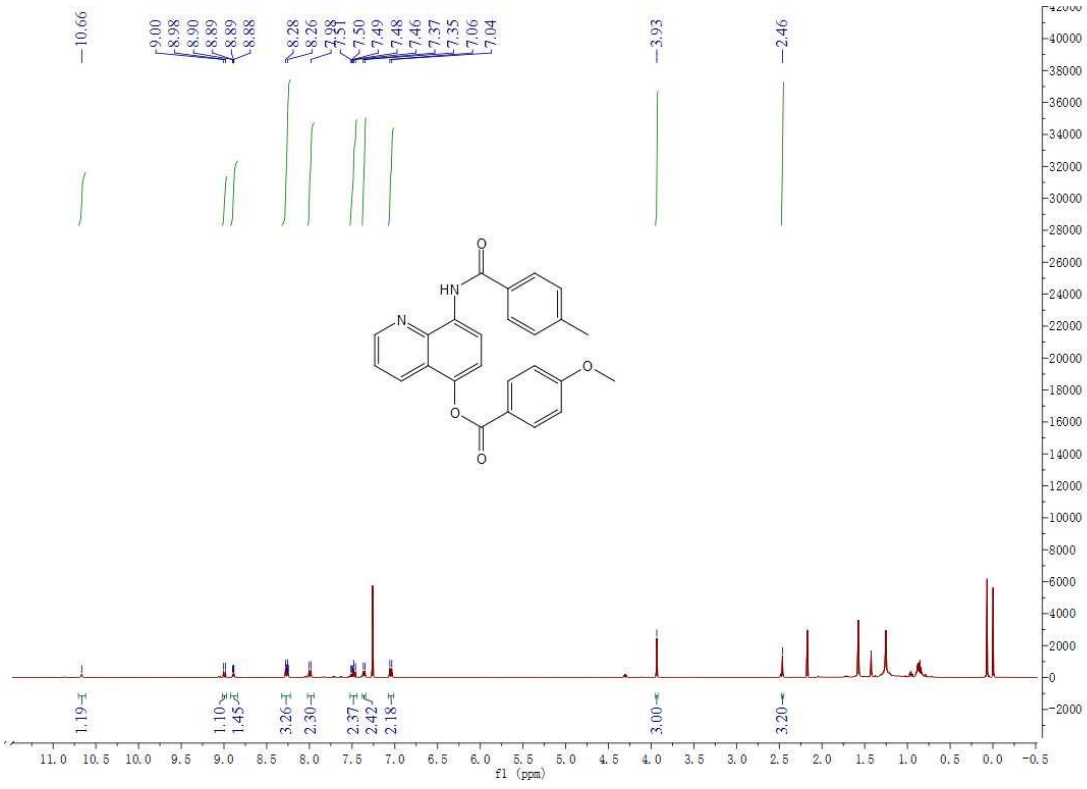
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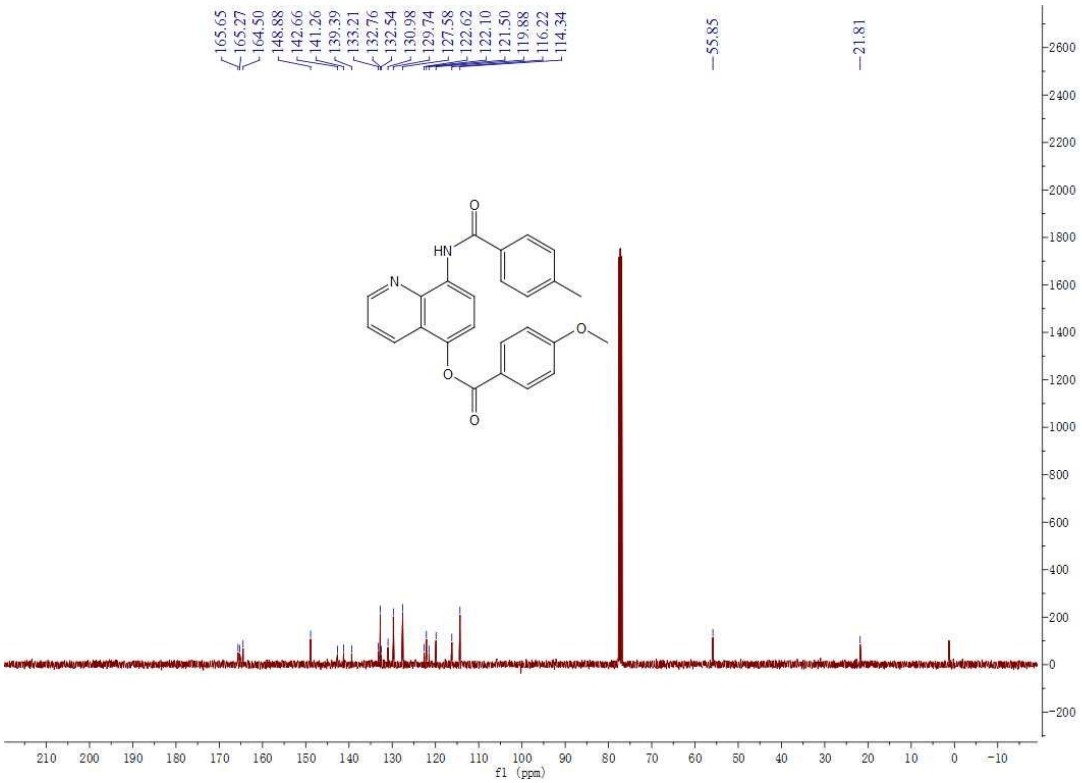
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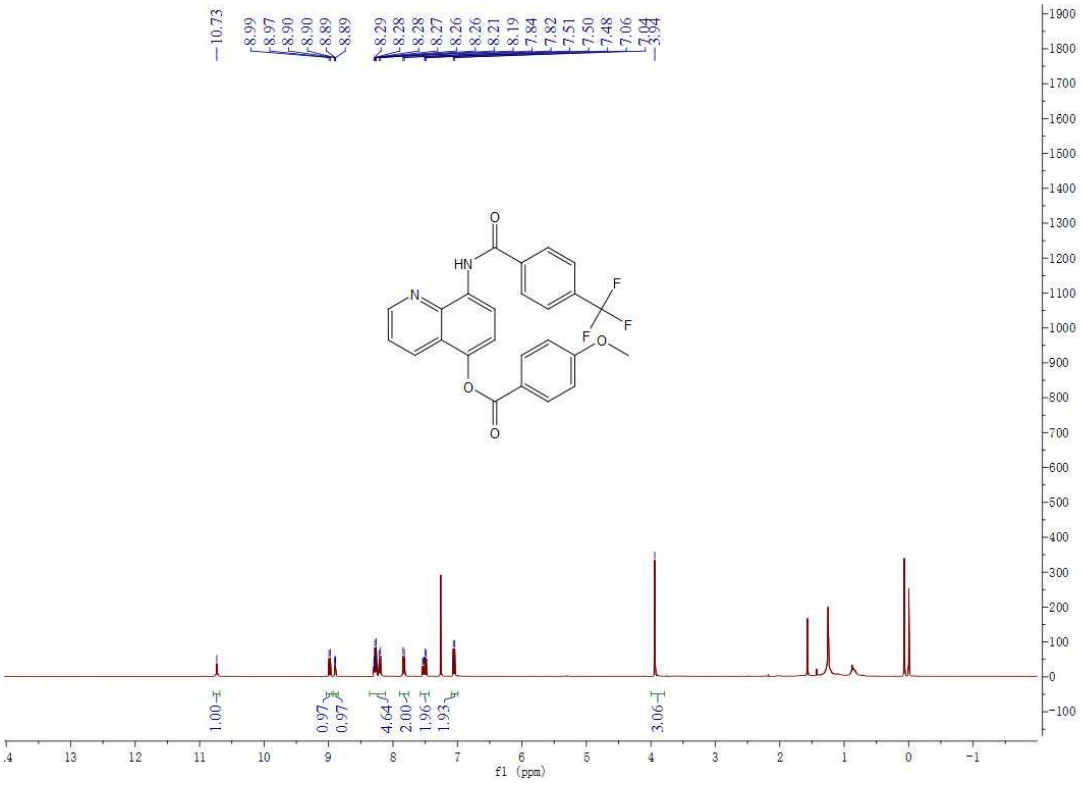
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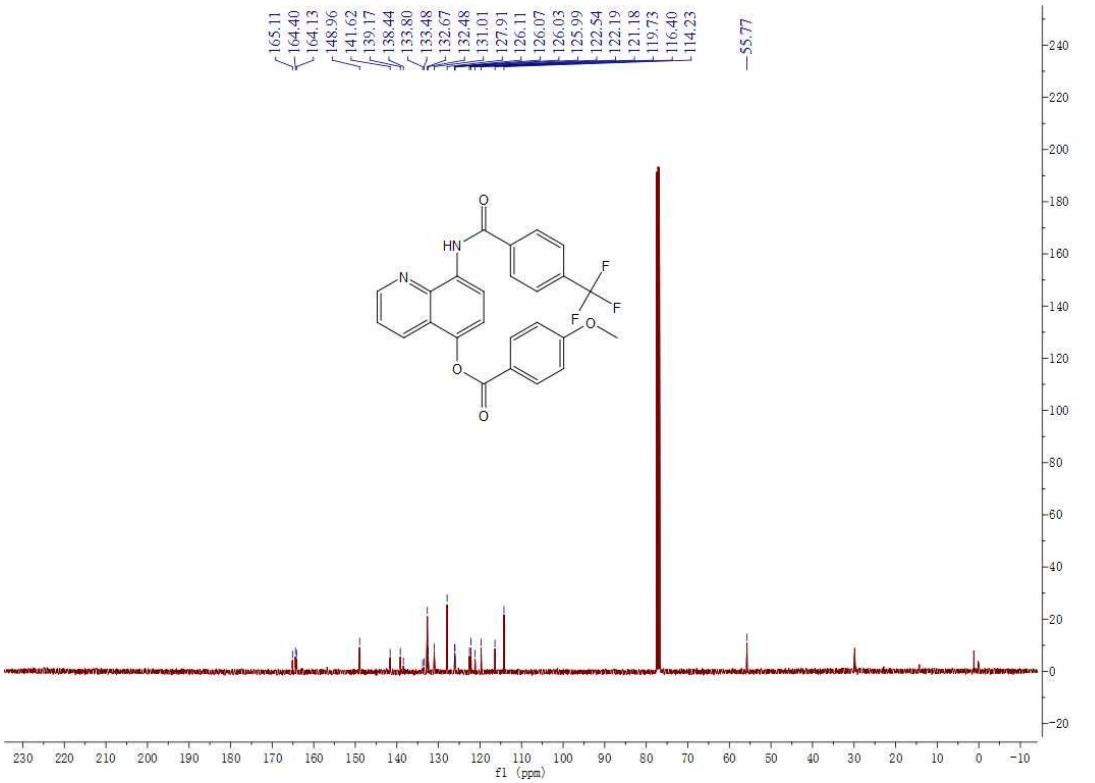
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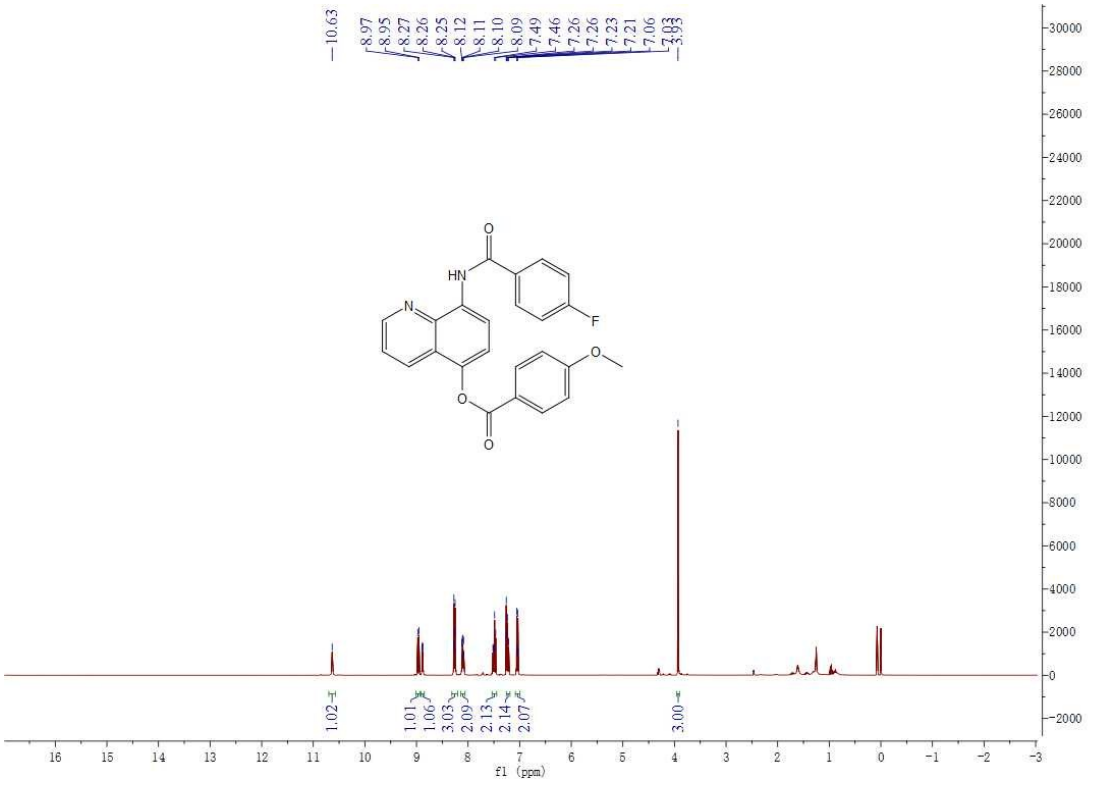
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F
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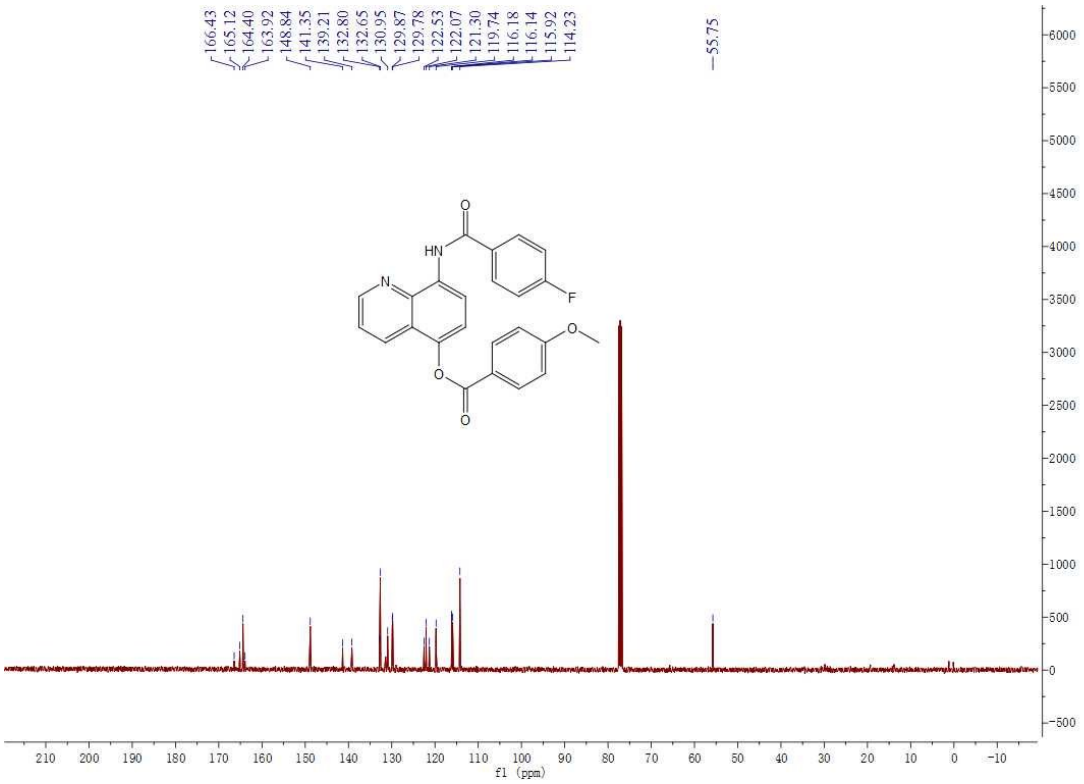
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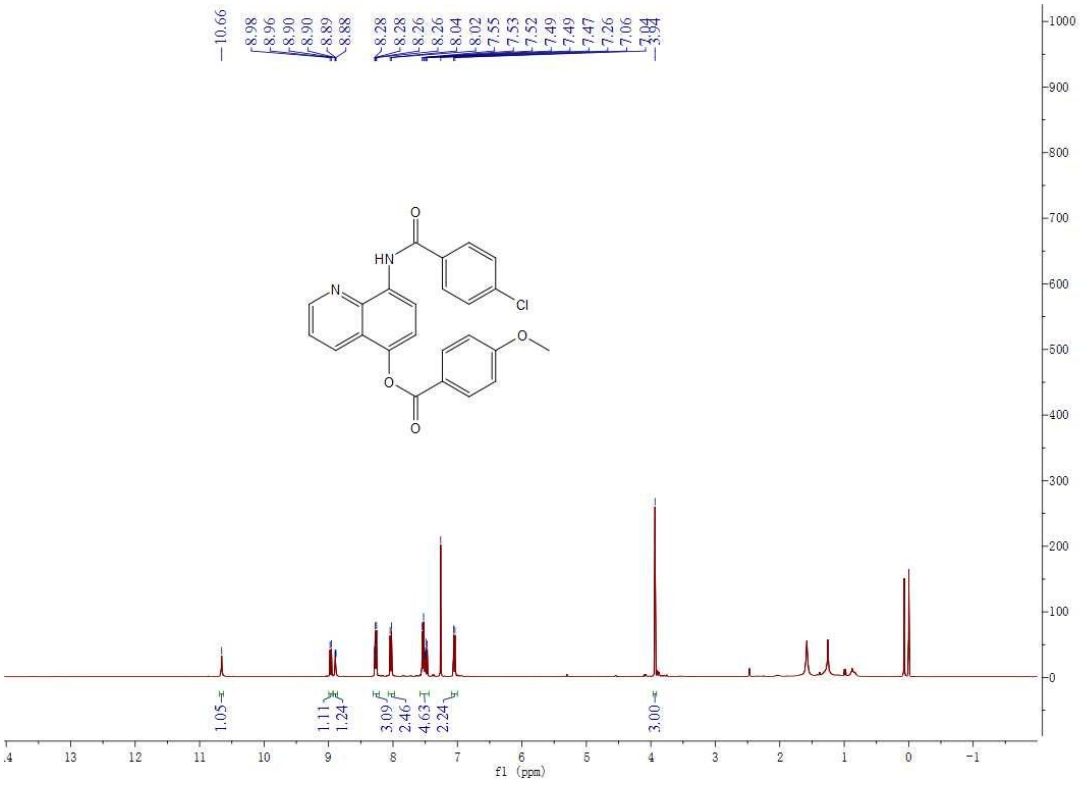
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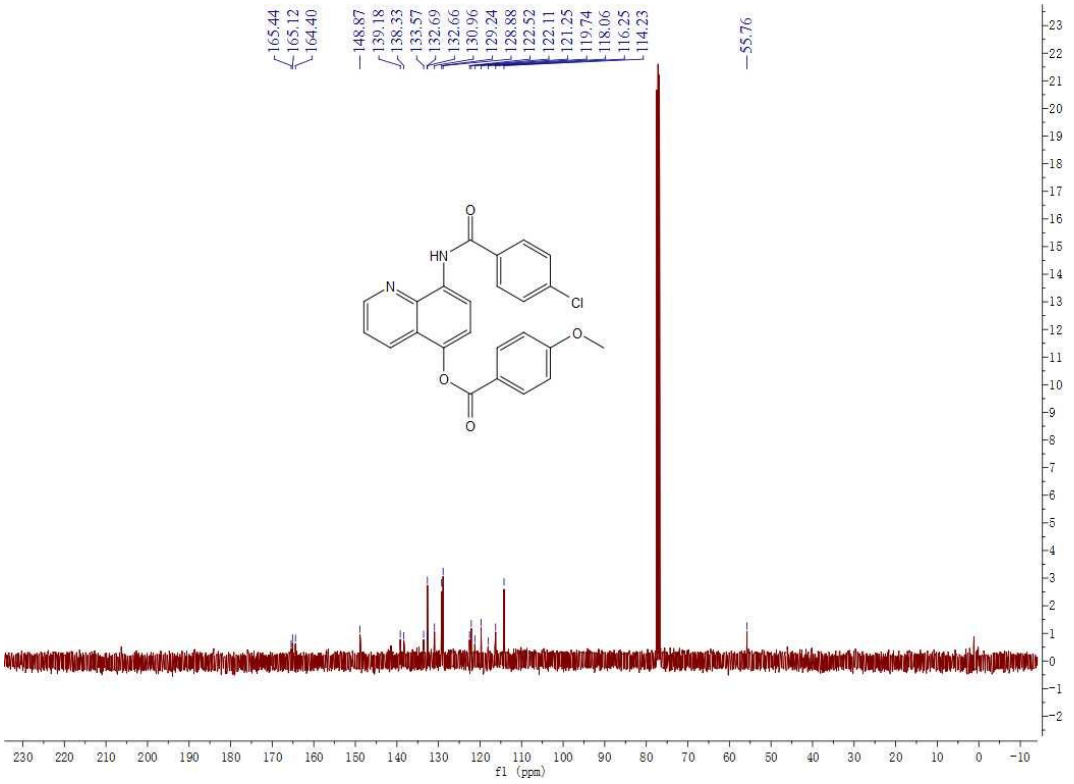
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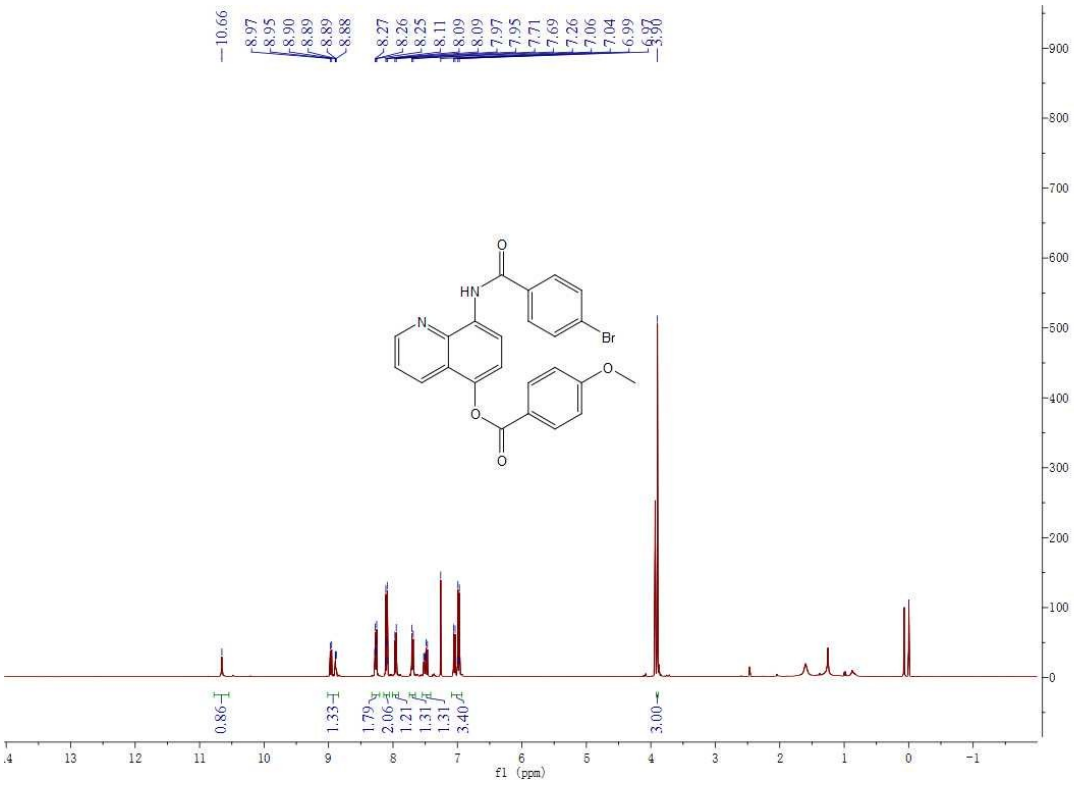
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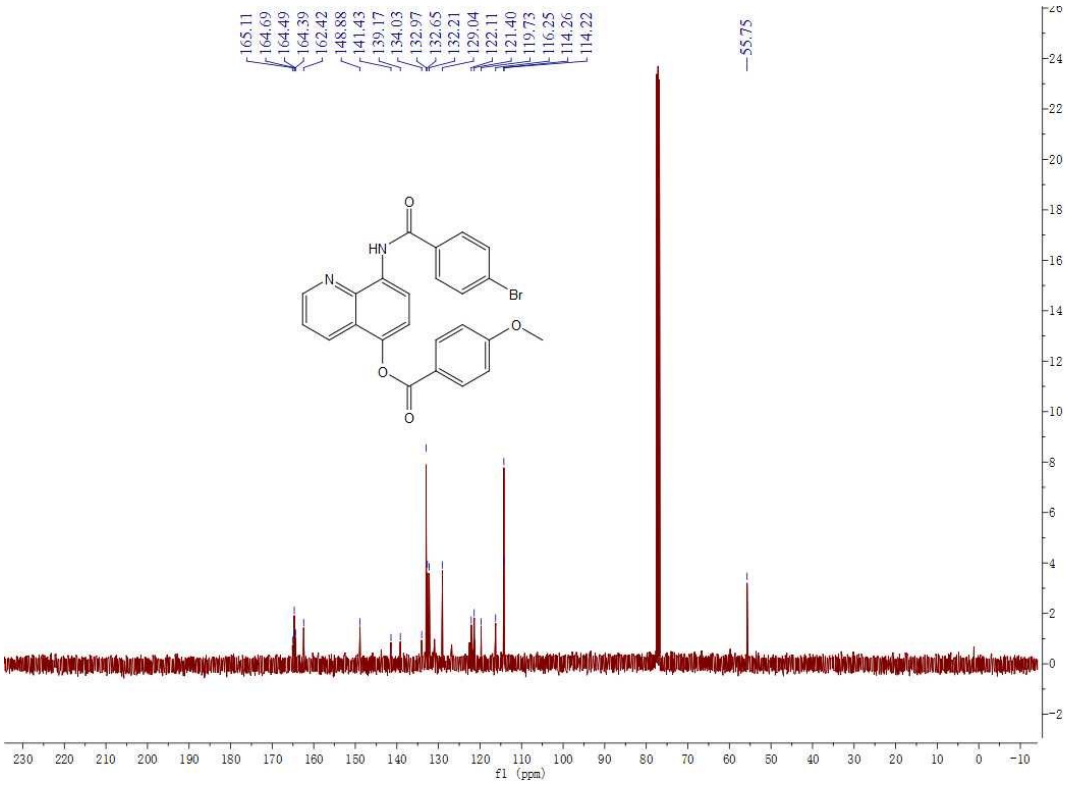
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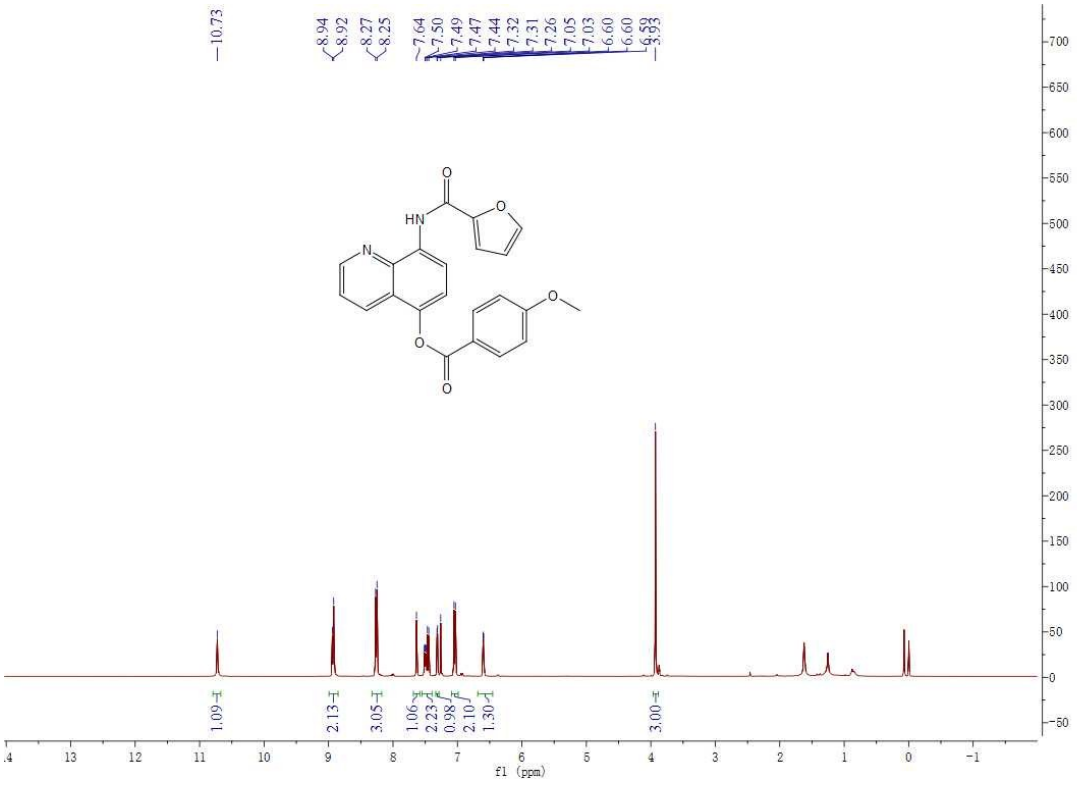
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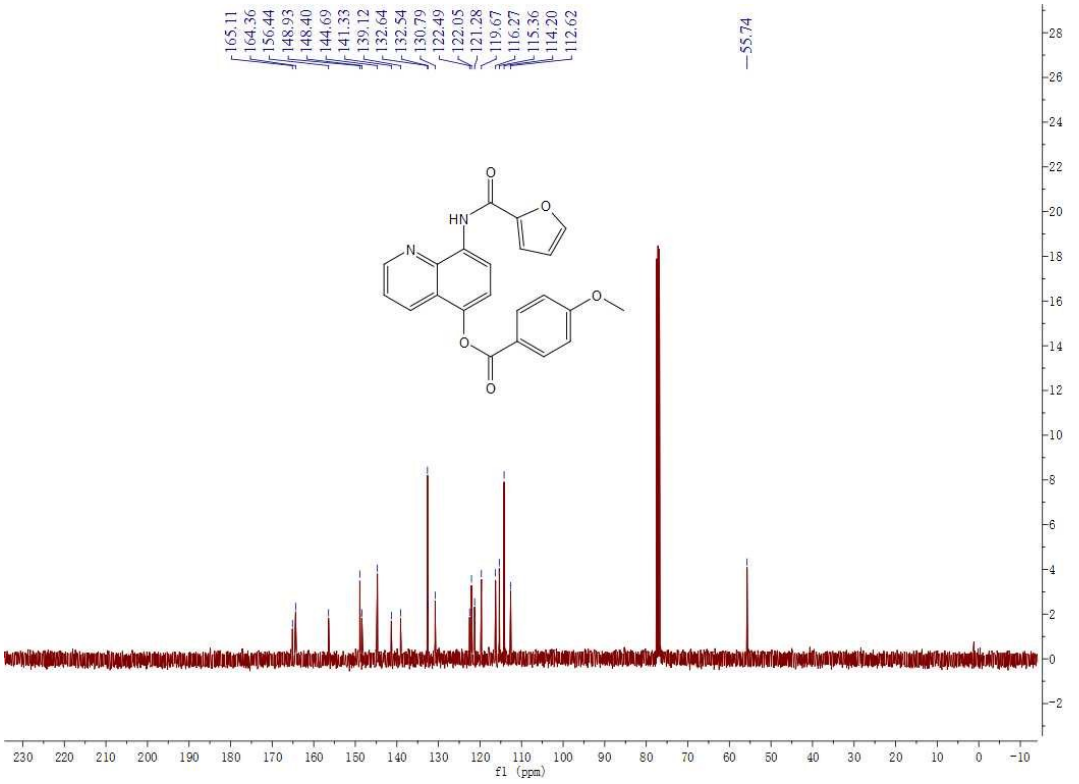
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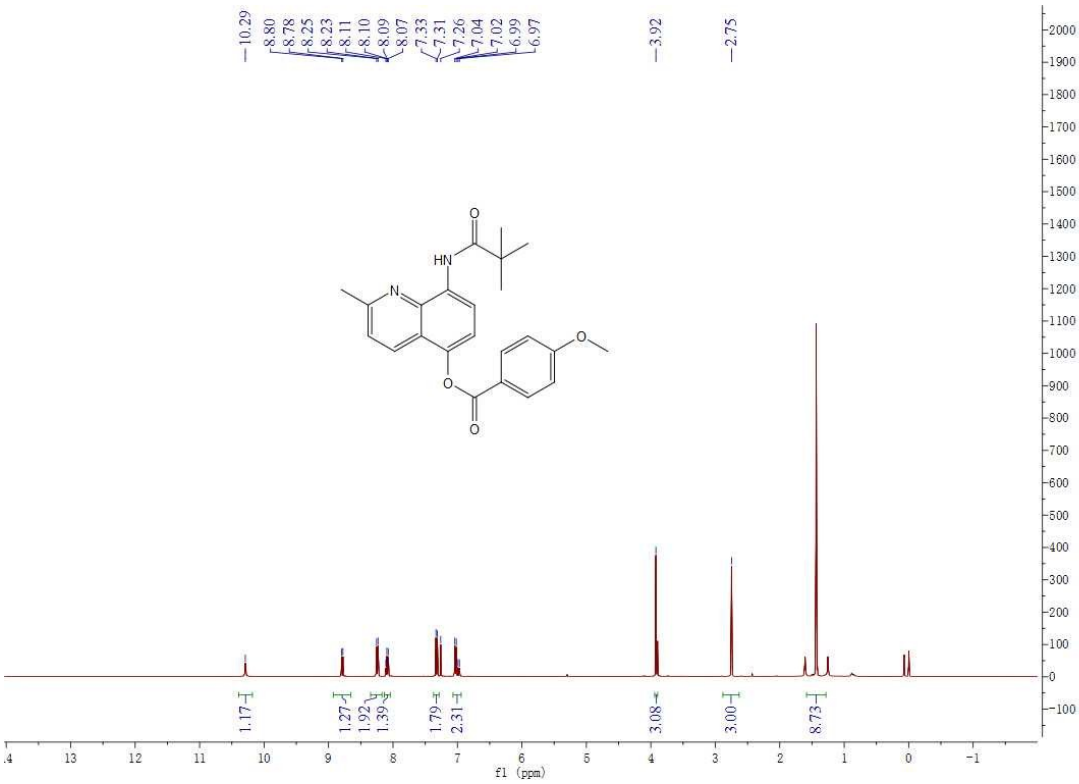
f1 (ppm)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6.97
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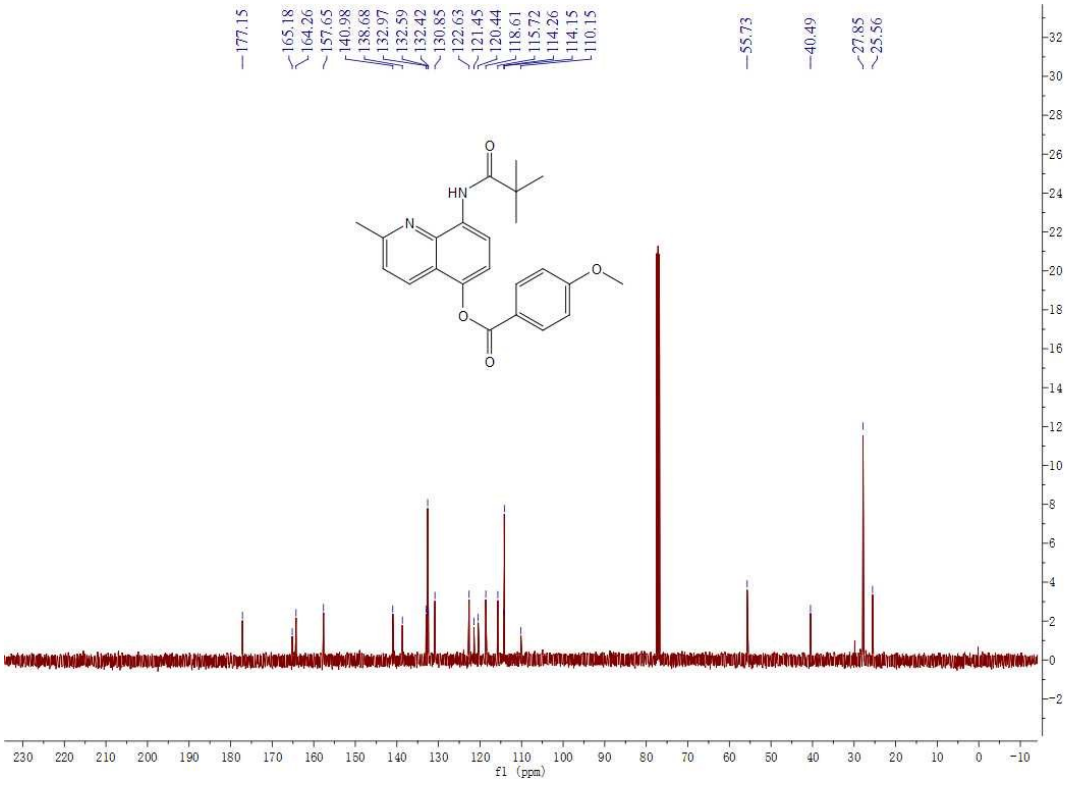
1.27
1.92
1.39
1.79
2.31
3.08
3.00
8.73
f1 (ppm)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118.61
115.72
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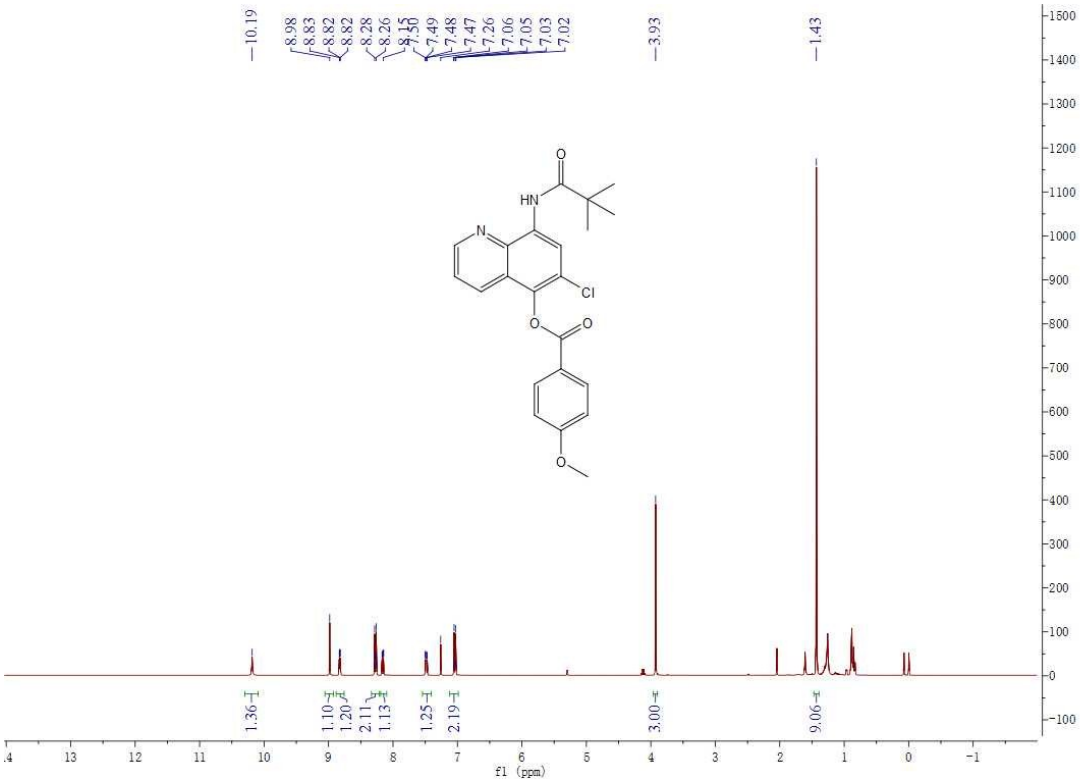
f1 (ppm)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7.03
7.02
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2.19
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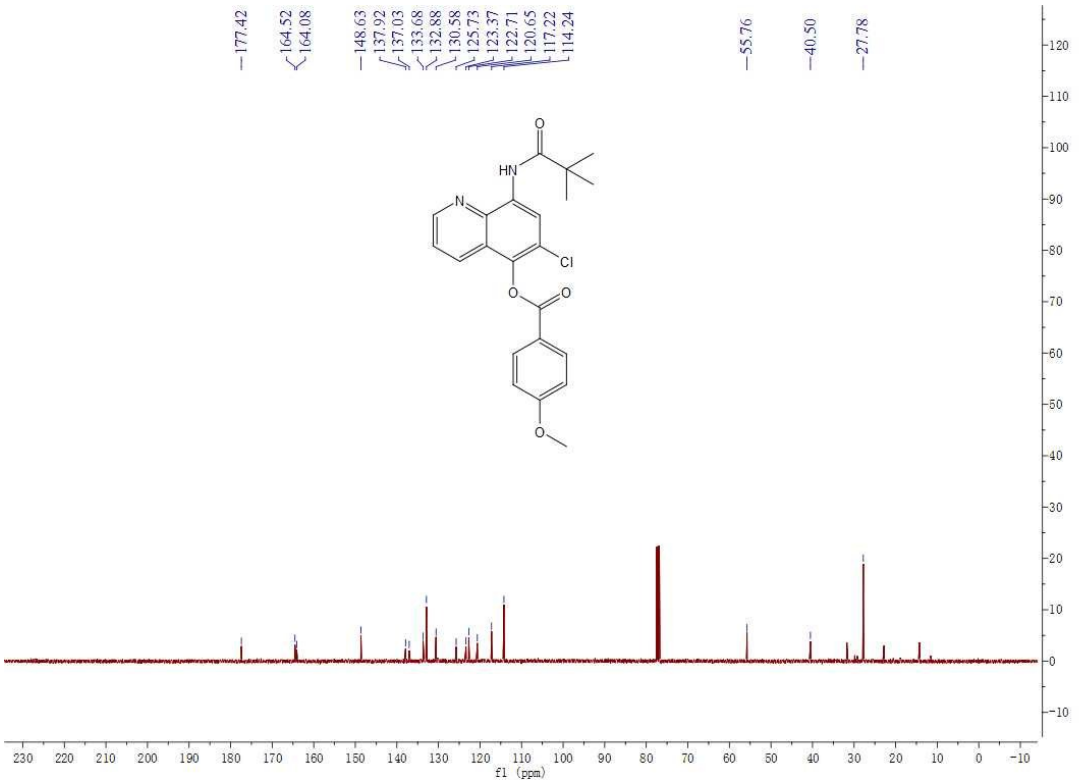
f1 (ppm)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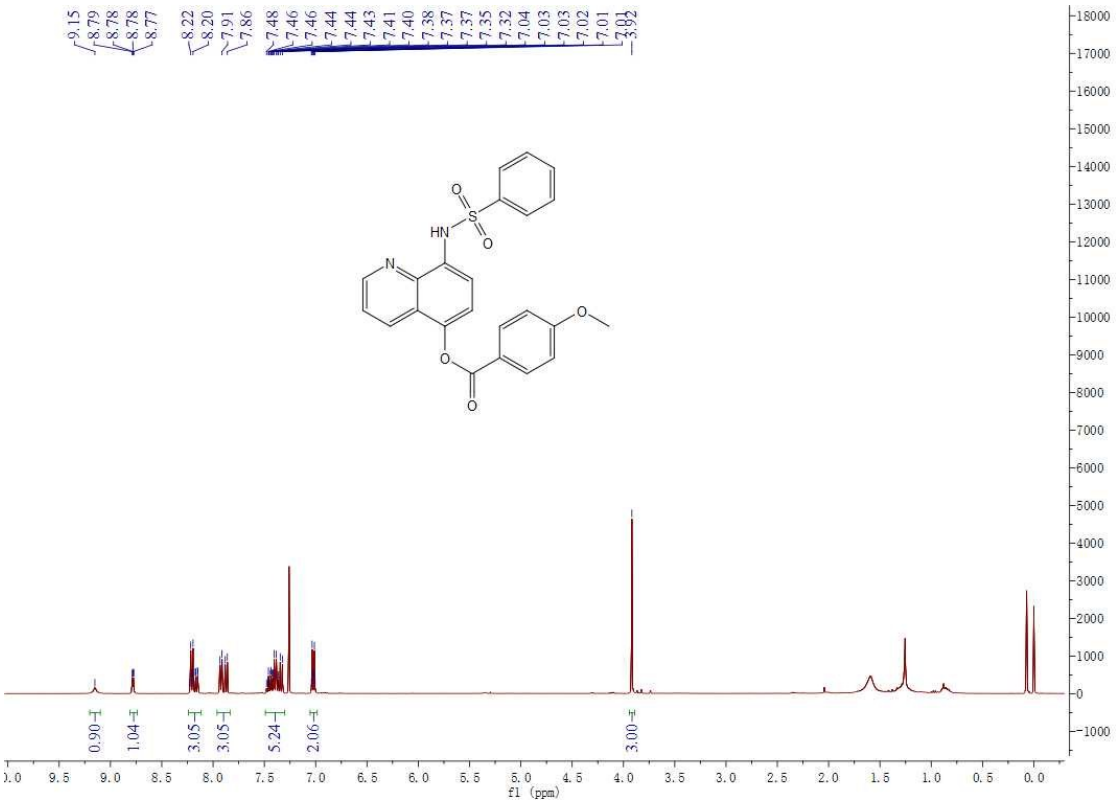
O
f1 (ppm)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7.40
7.38
7.37
7.37
7.35
7.32
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7.03
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3.05
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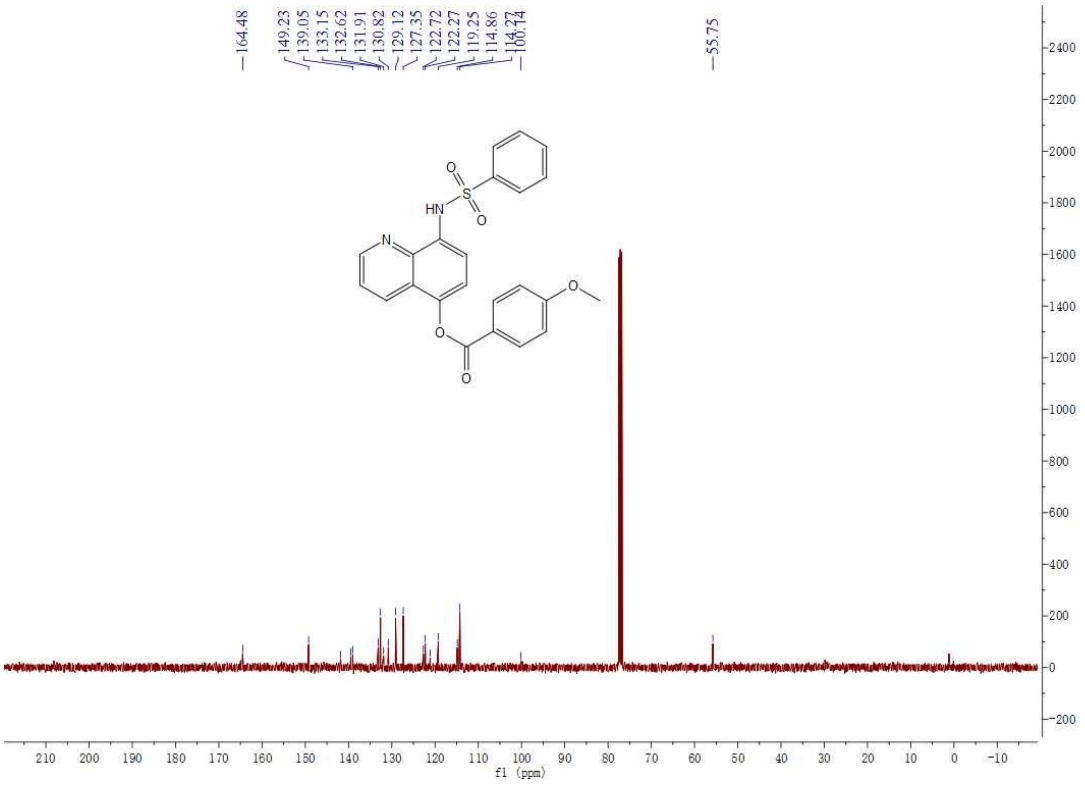
2.06
3.00
f1 (ppm)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114.27
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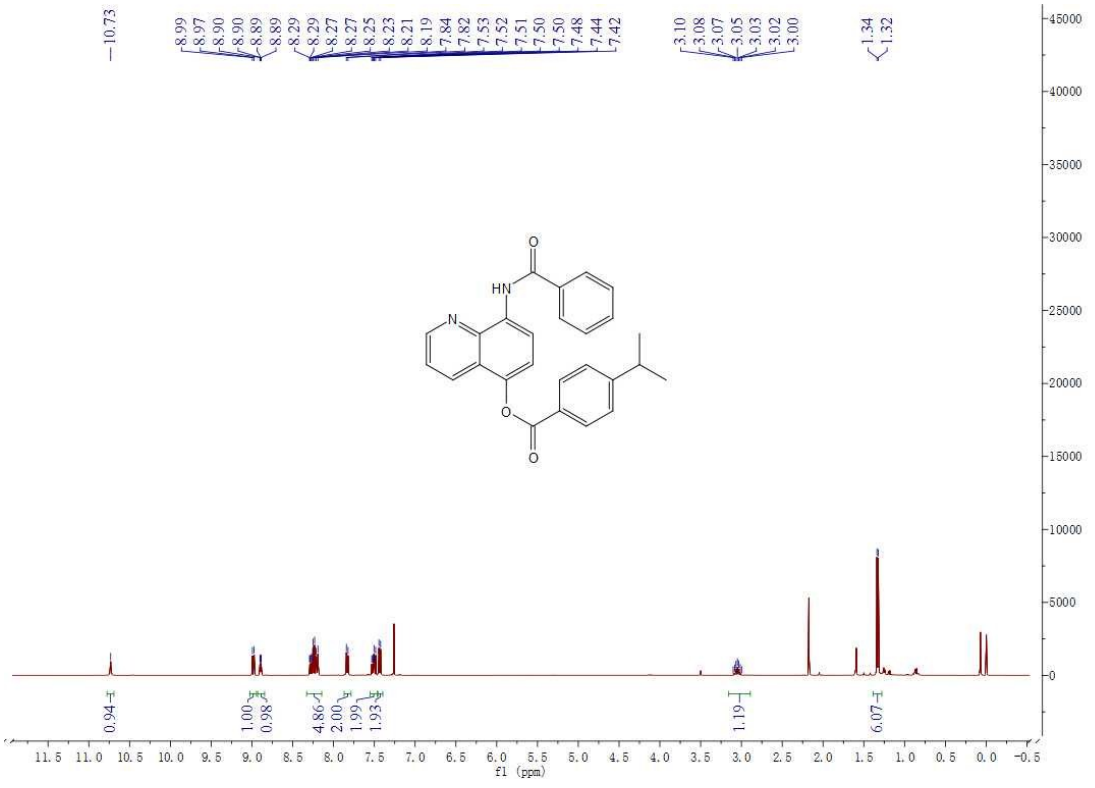
55.75
f1 (ppm)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7.51
7.50
7.50
7.48
7.44
7.42
3.10
3.08
3.07
3.05
3.03
3.02
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1.32
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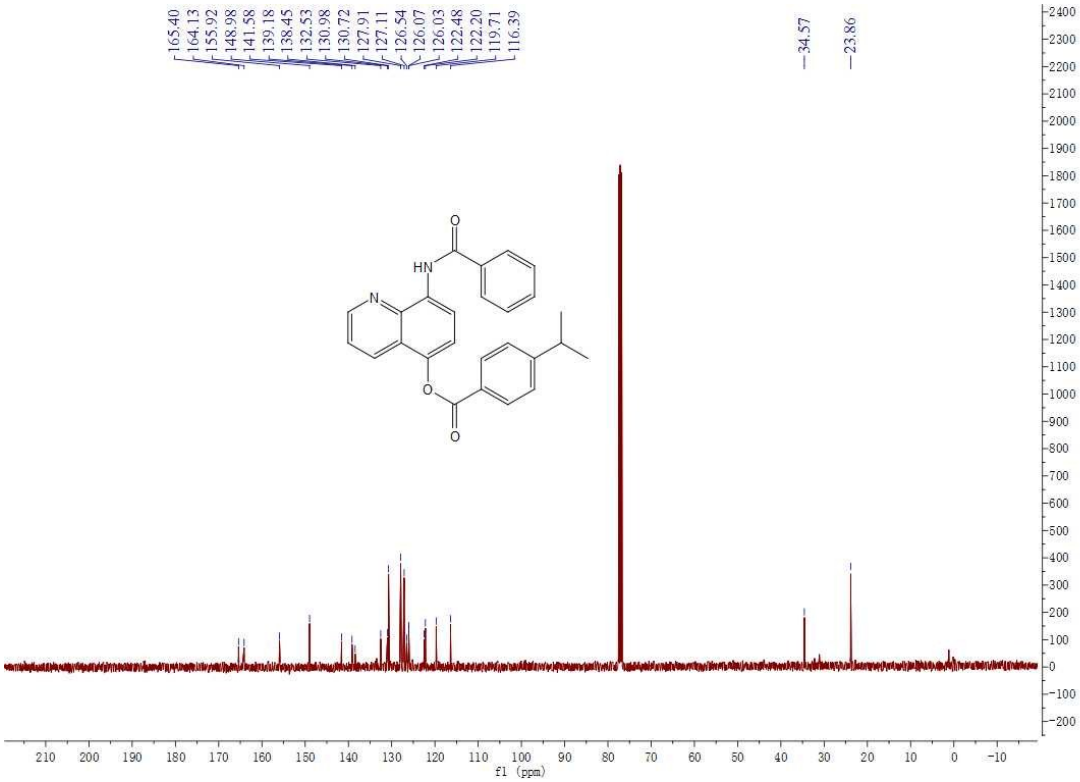
6.07
f1 (ppm)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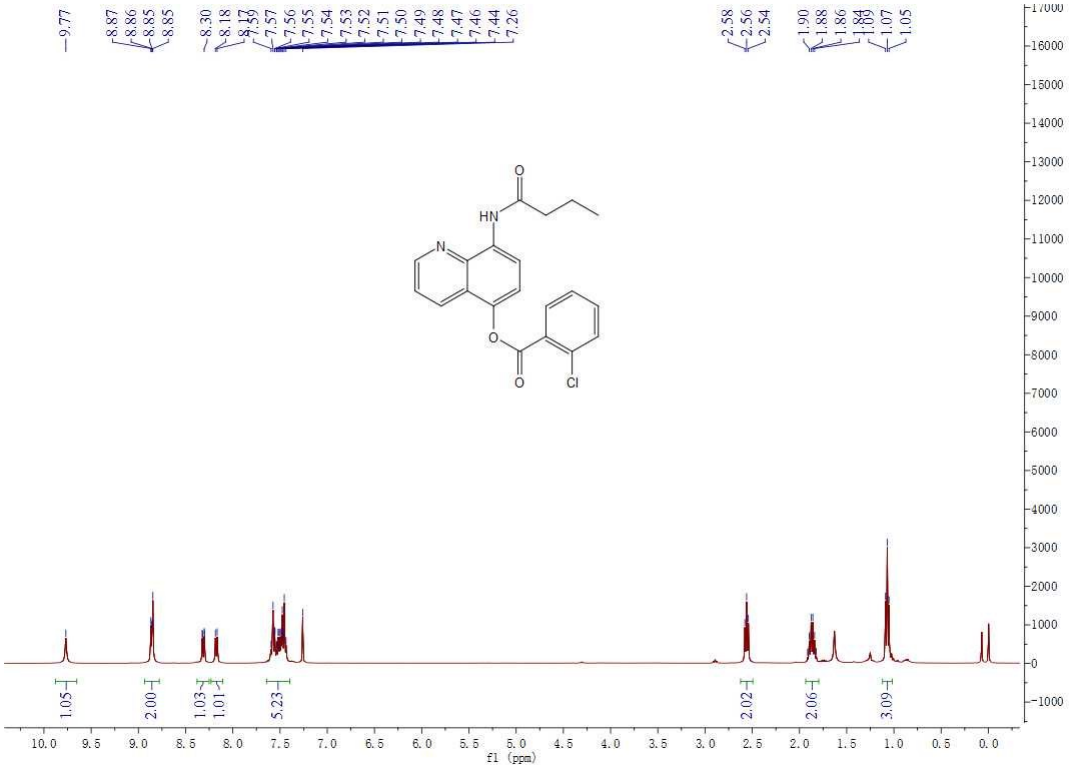
f1 (ppm)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1.07
1.05
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1.01
5.23
2.02
2.06
3.09
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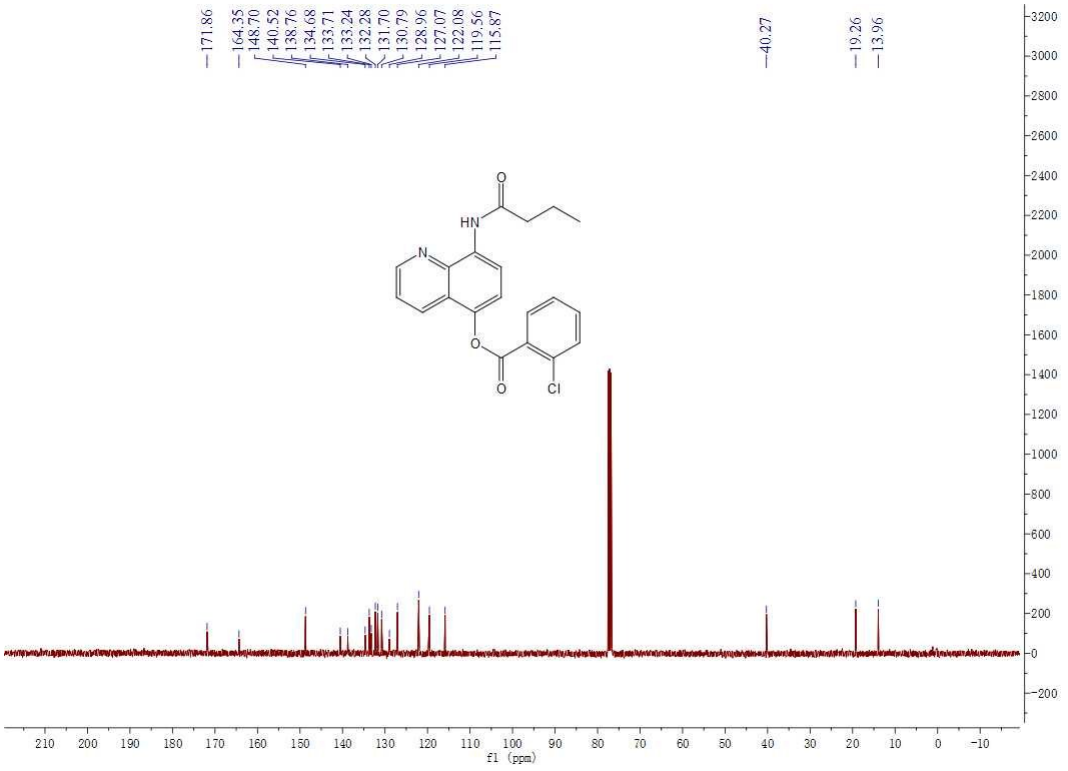
O
Cl
f1 (ppm)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19.26
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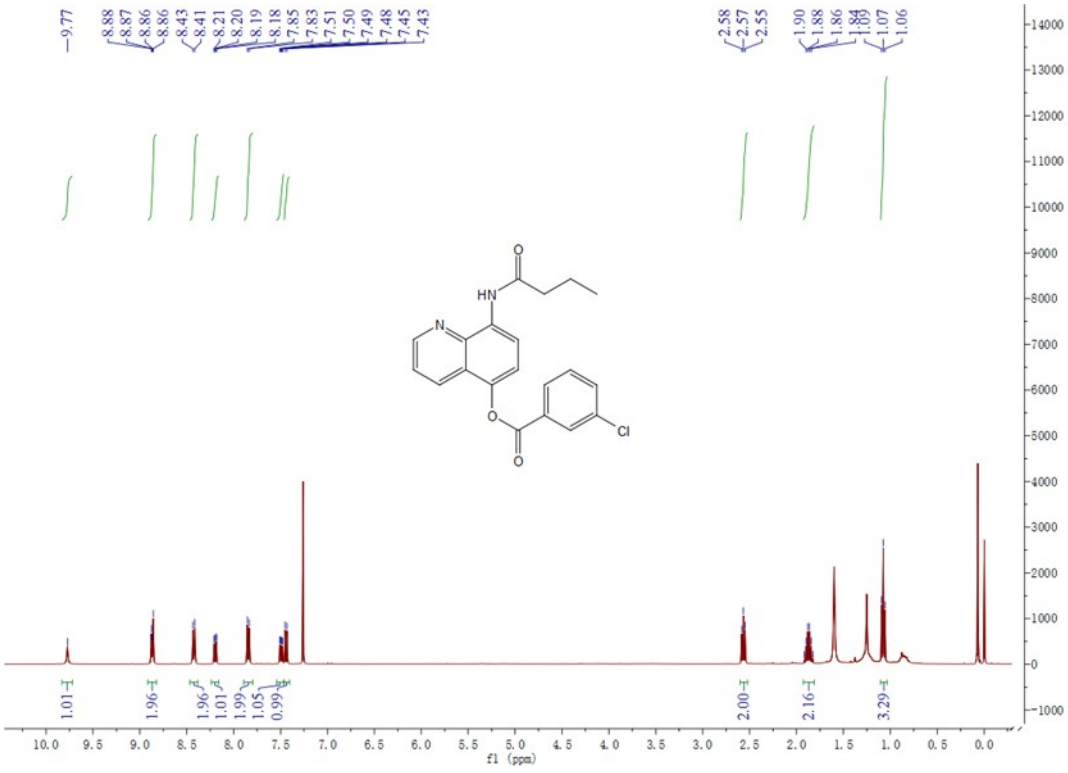
O
Cl
f1 (ppm)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2.55
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1.88
1.86
1.07
1.06
1.01
1.96
1.96
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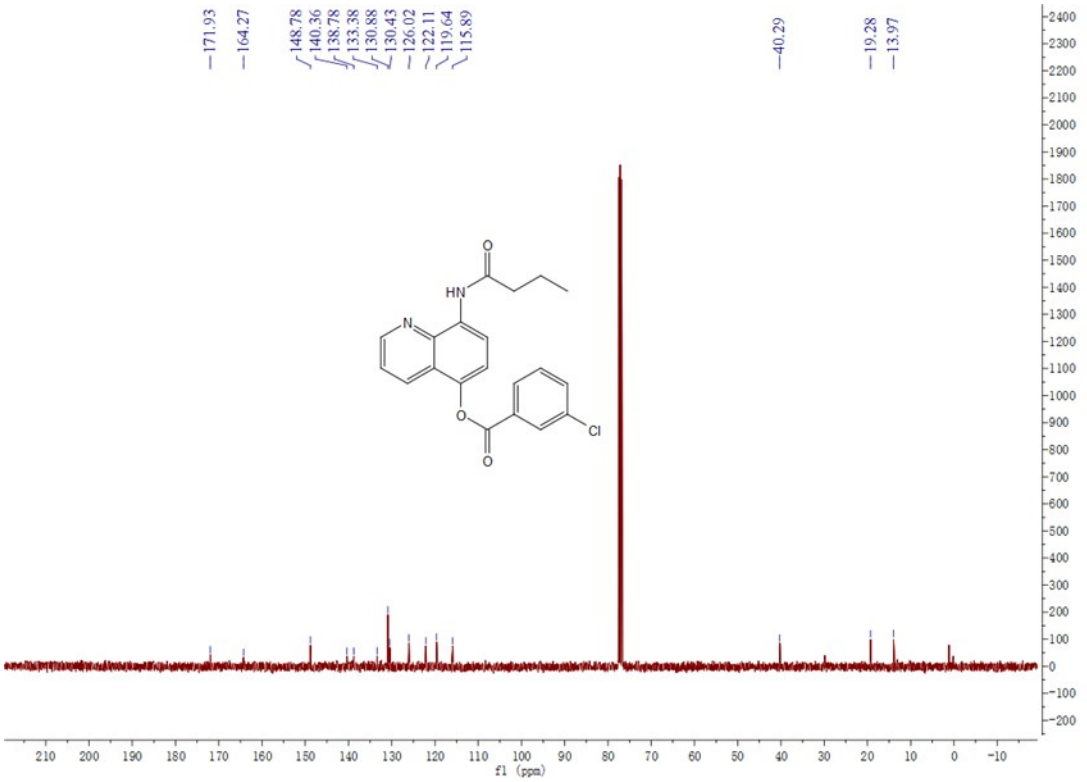
O
Cl
f1 (ppm)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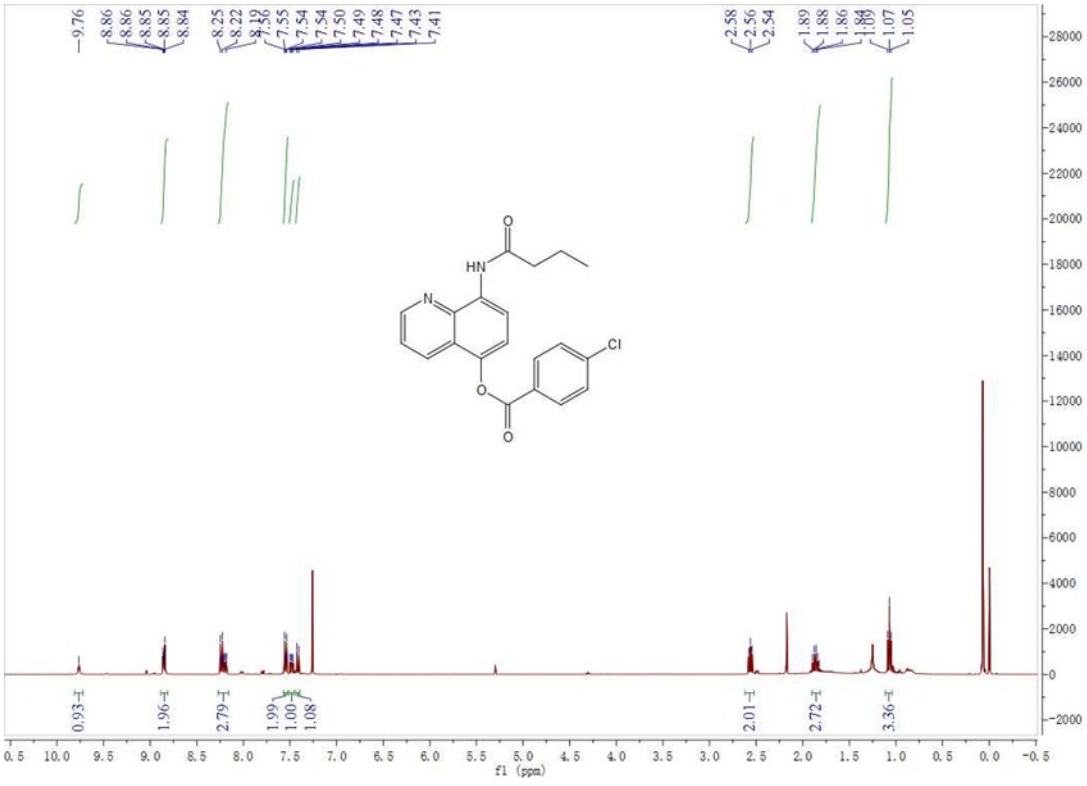
O
Cl
f1 (ppm)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7.41
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2.56
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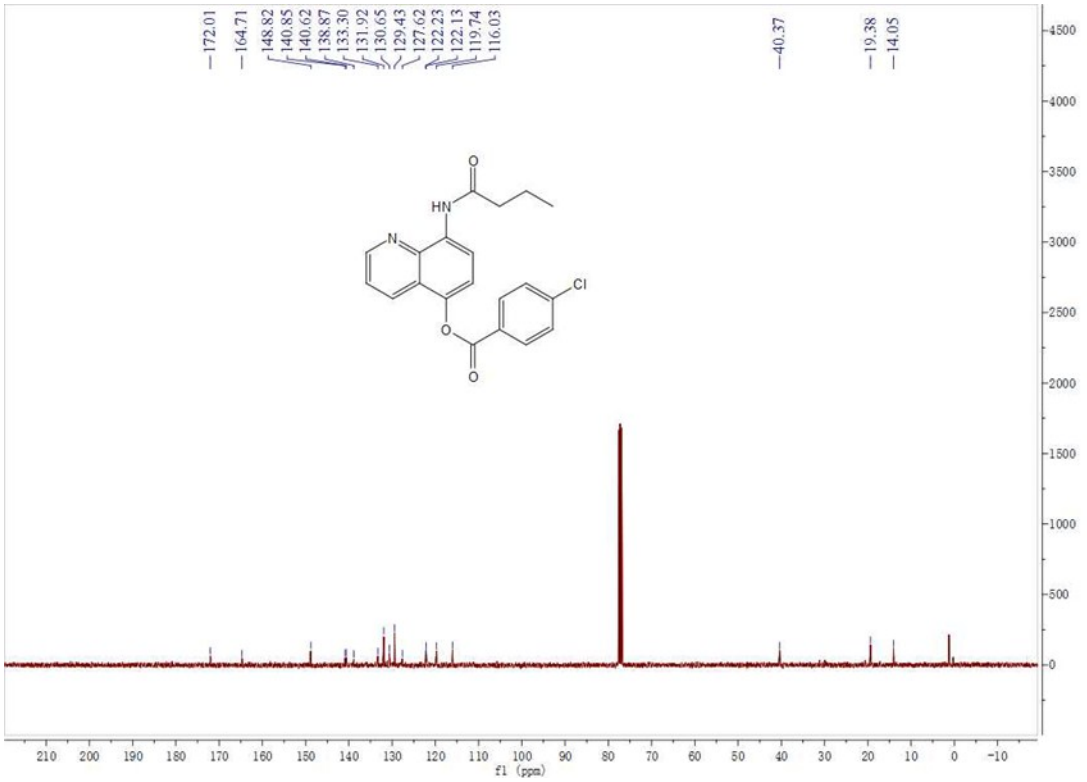
Cl
f1 (ppm)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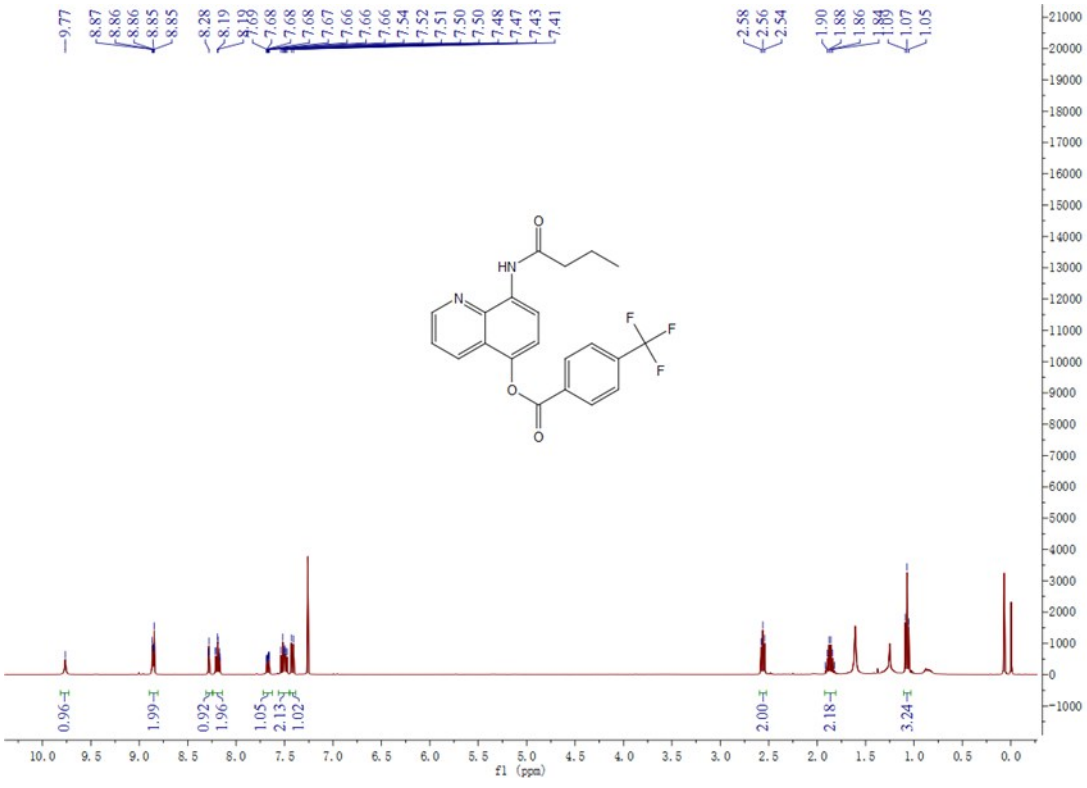
f1 (ppm)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1.07
1.05
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O
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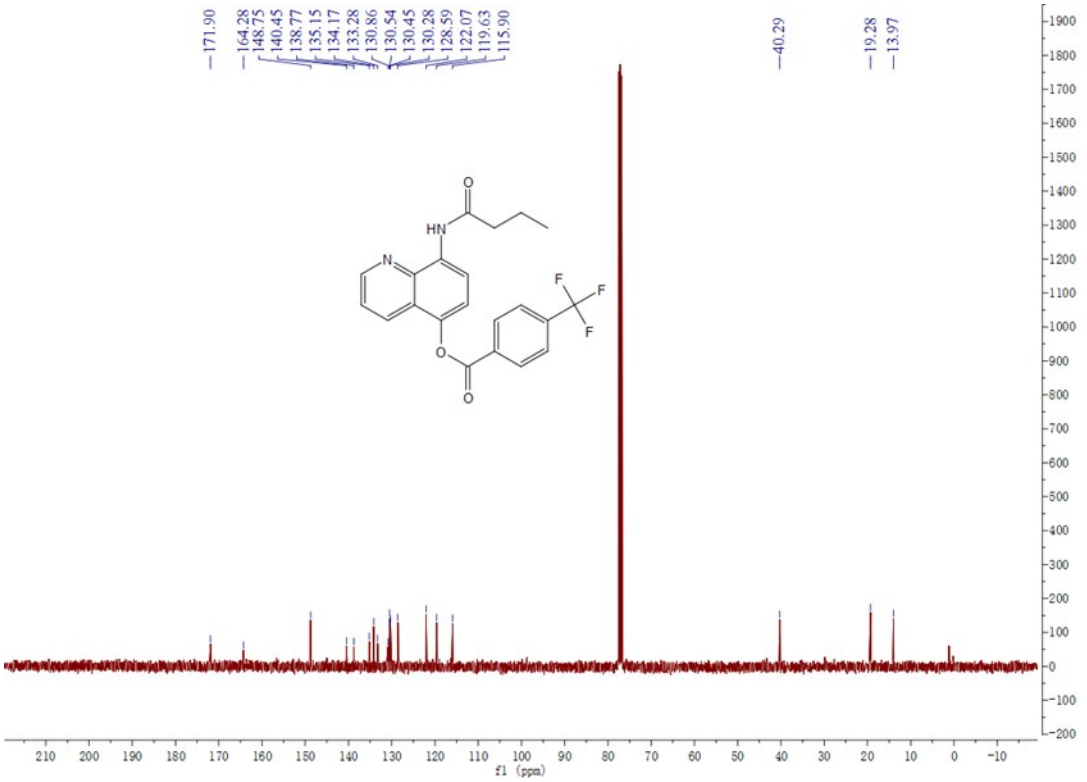
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19.28
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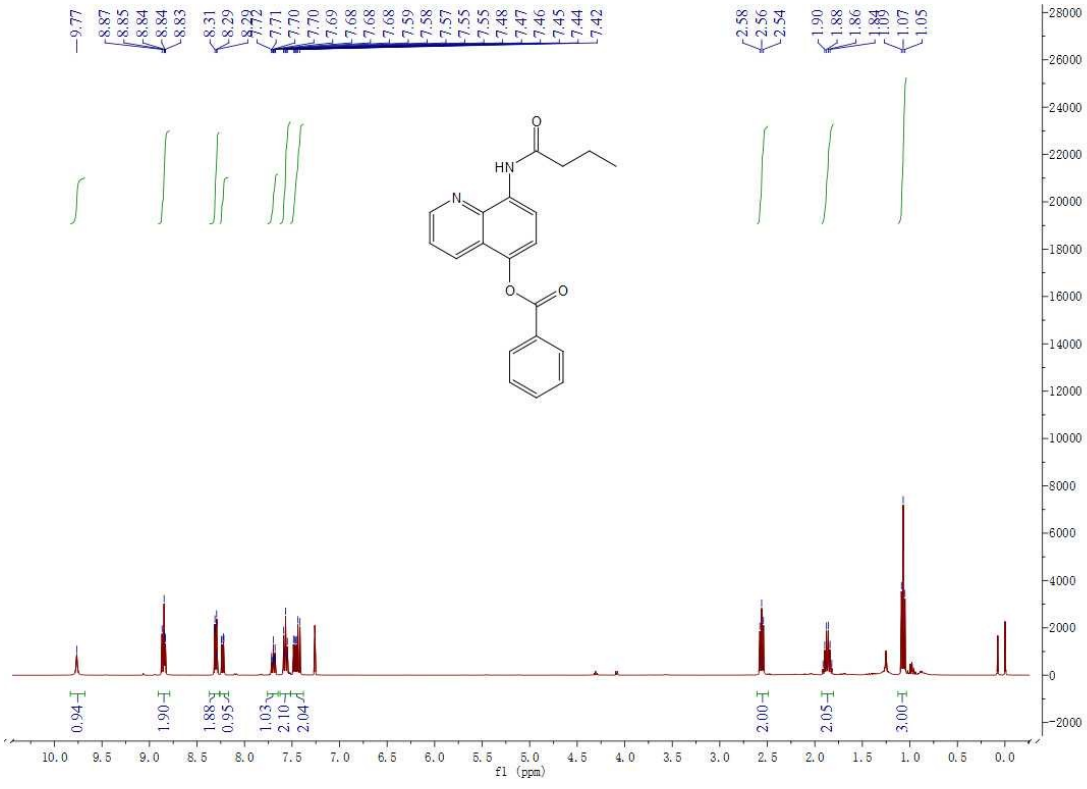
F
F
F
f1 (ppm)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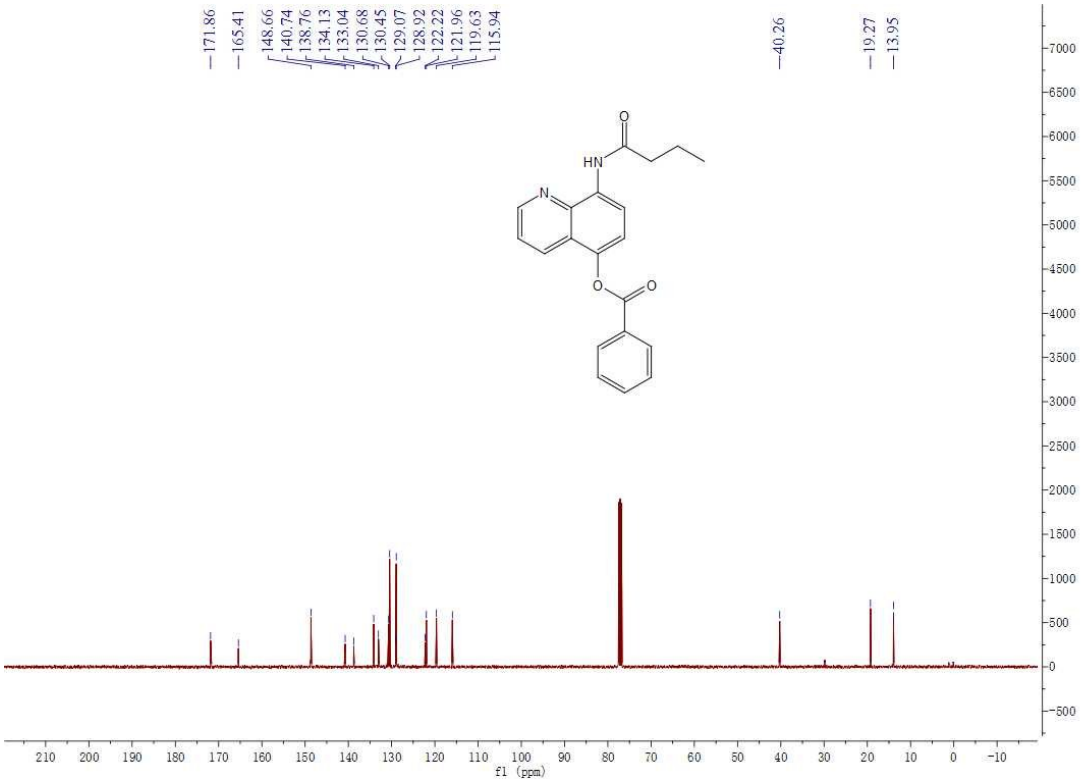
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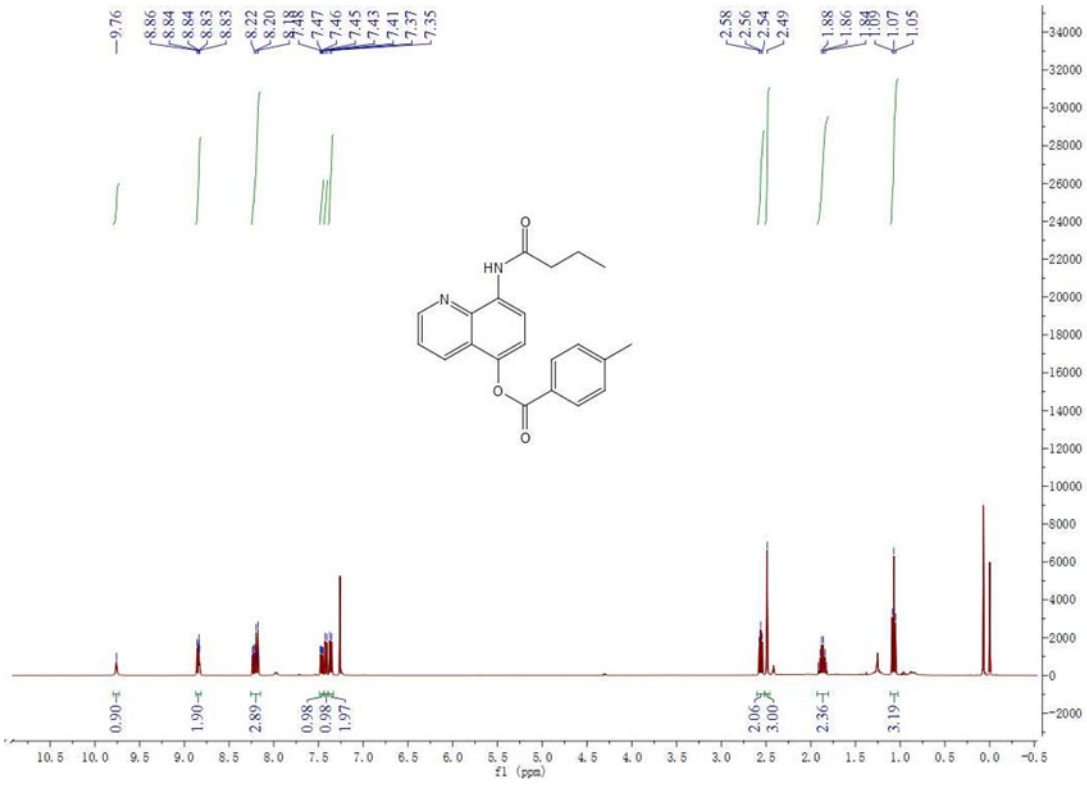
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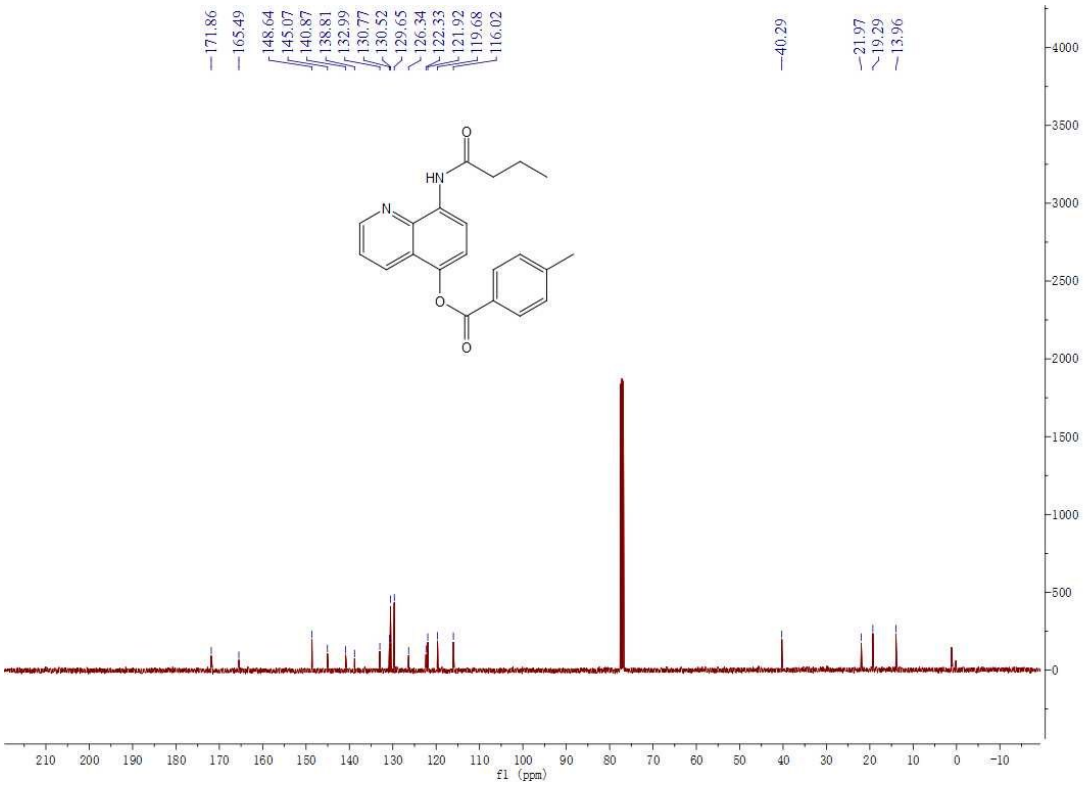
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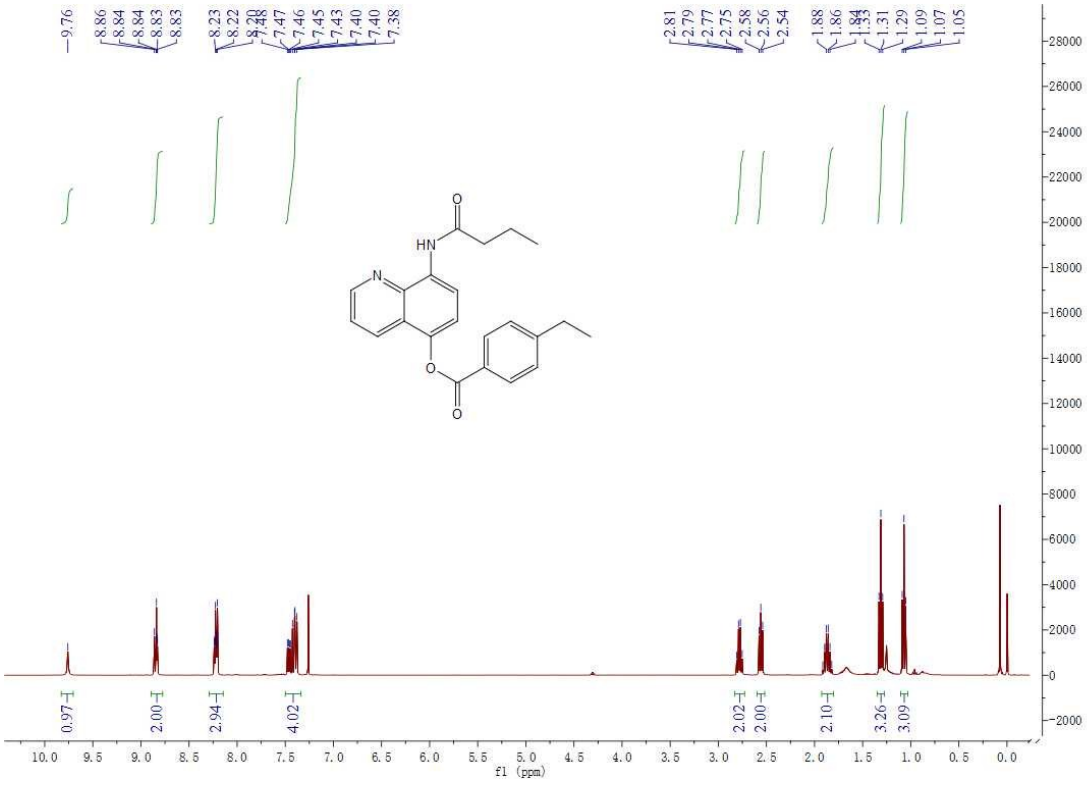
f1 (ppm)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1.07
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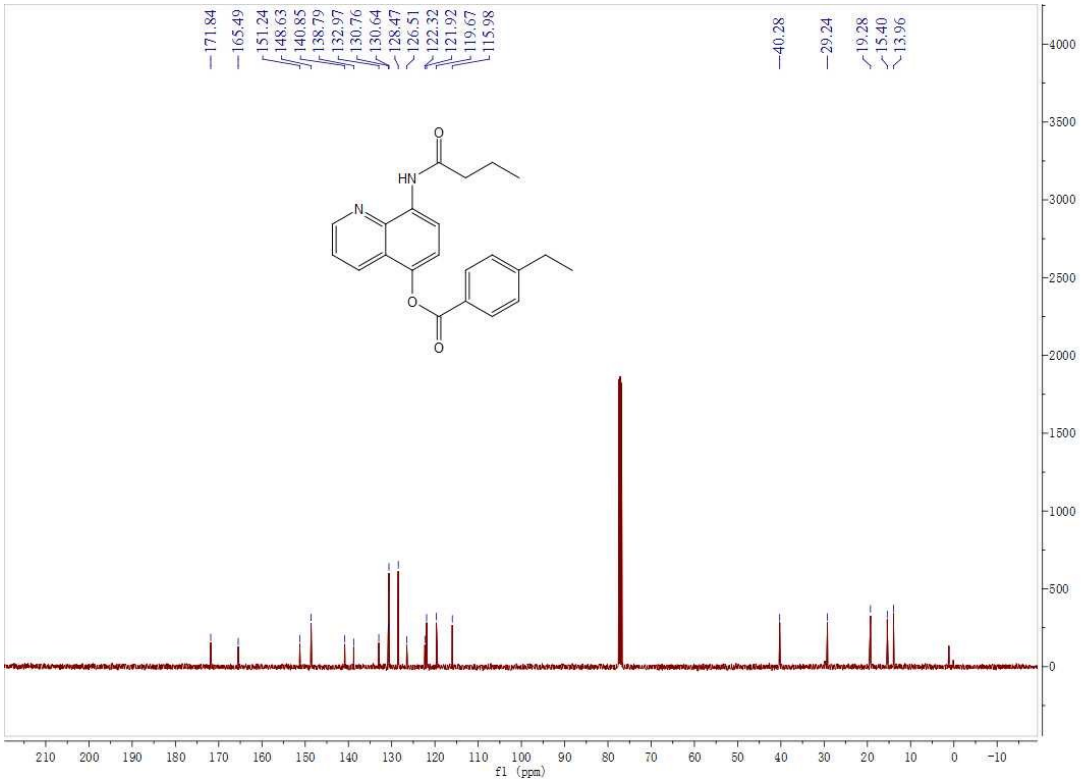
f1 (ppm)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O
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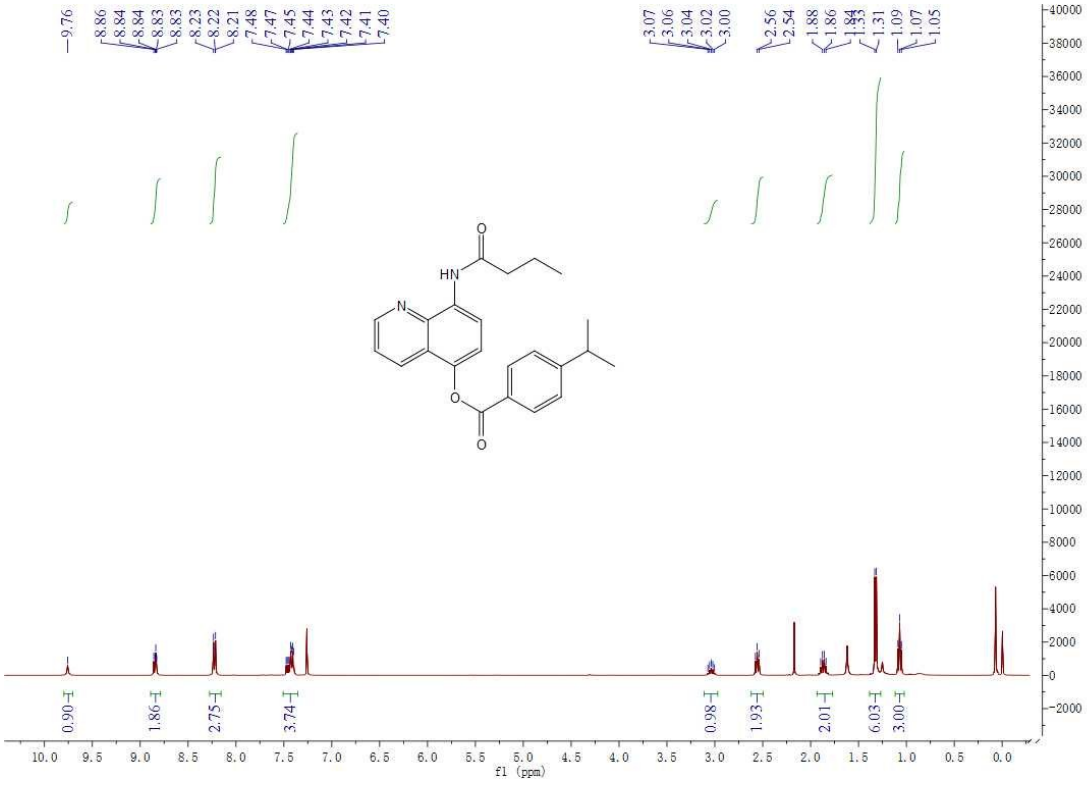
f1 (ppm)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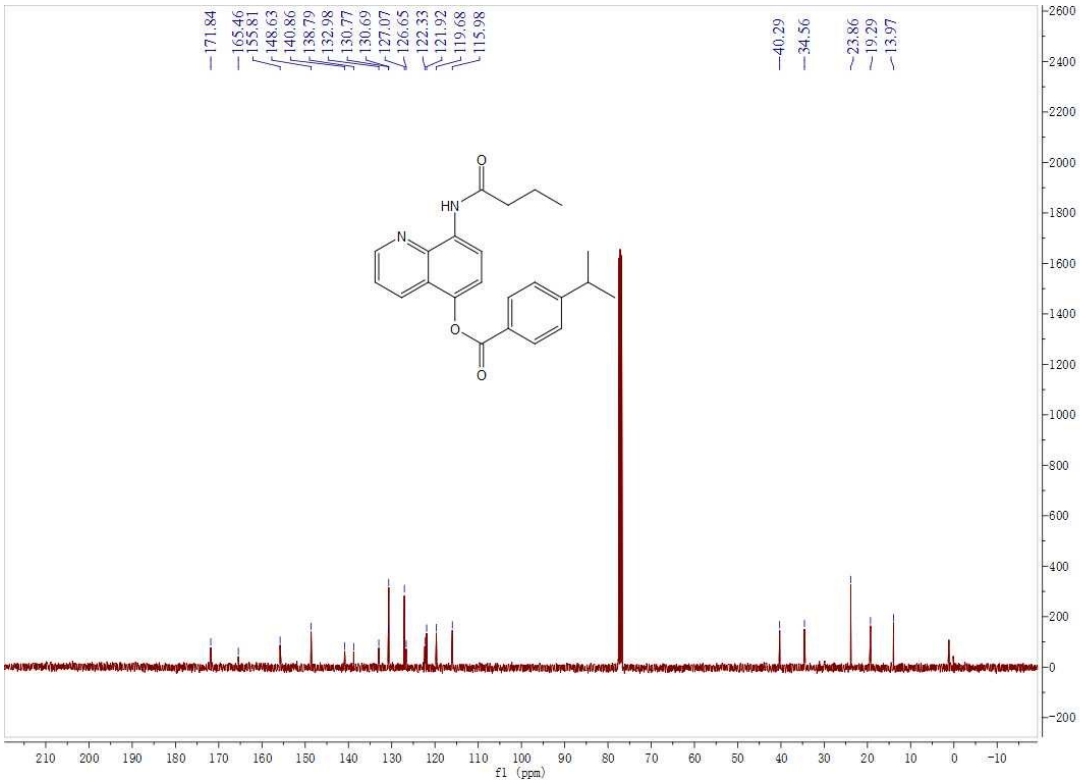
O
O
f1 (ppm)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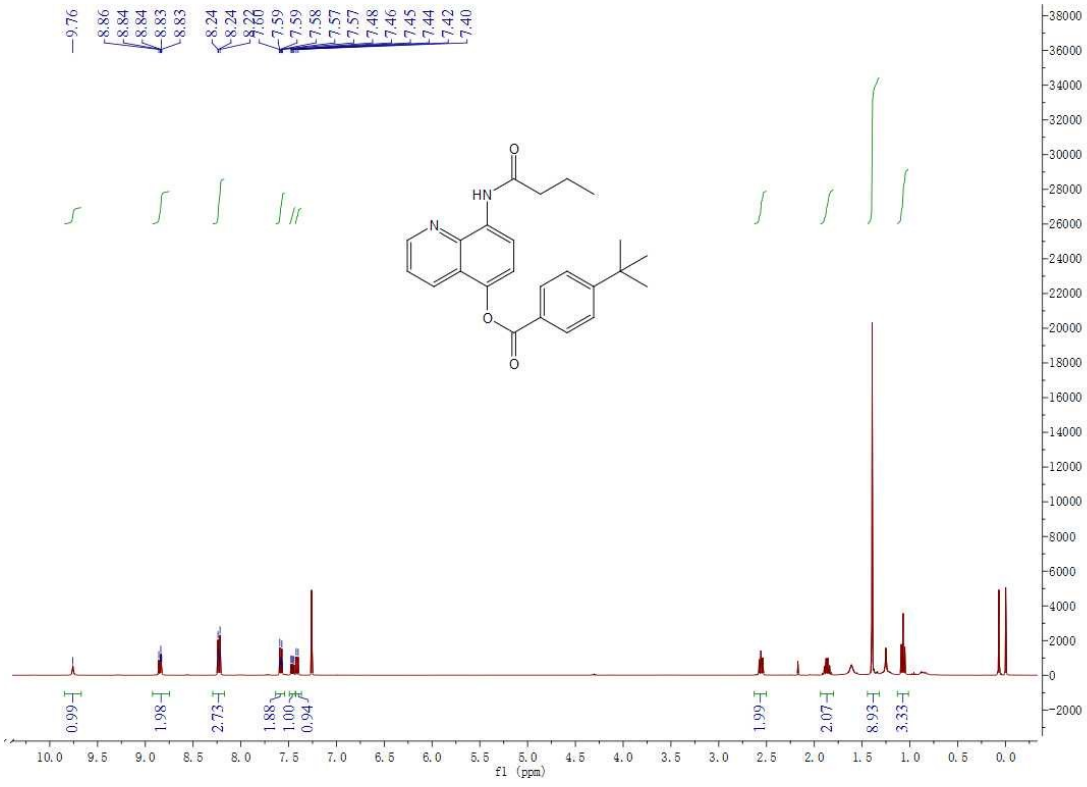
f1 (ppm)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7.44
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2.07
8.93
3.33
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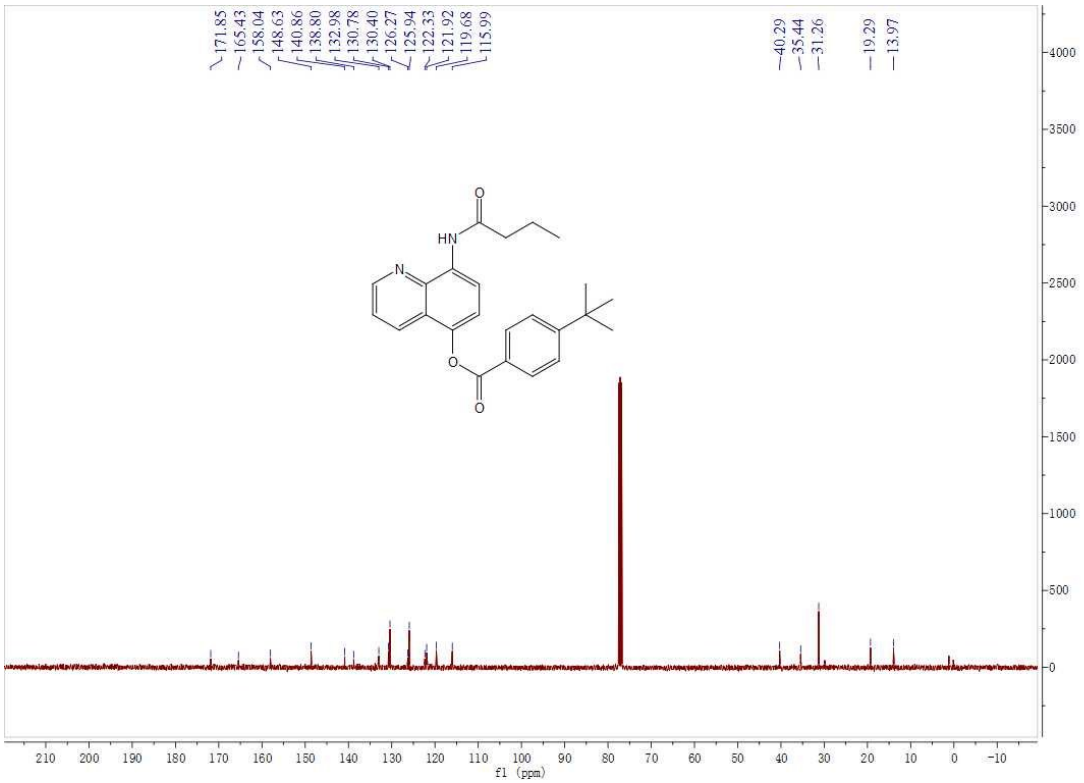
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19.29
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HN
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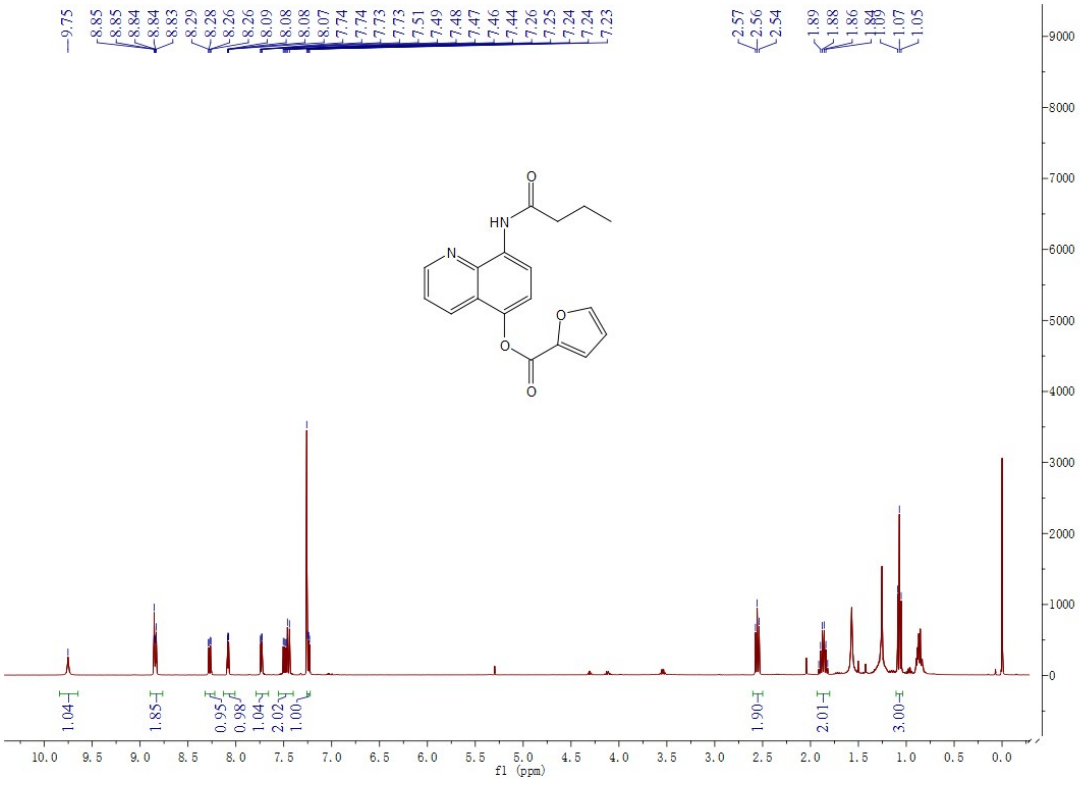
O
O
f1 (ppm)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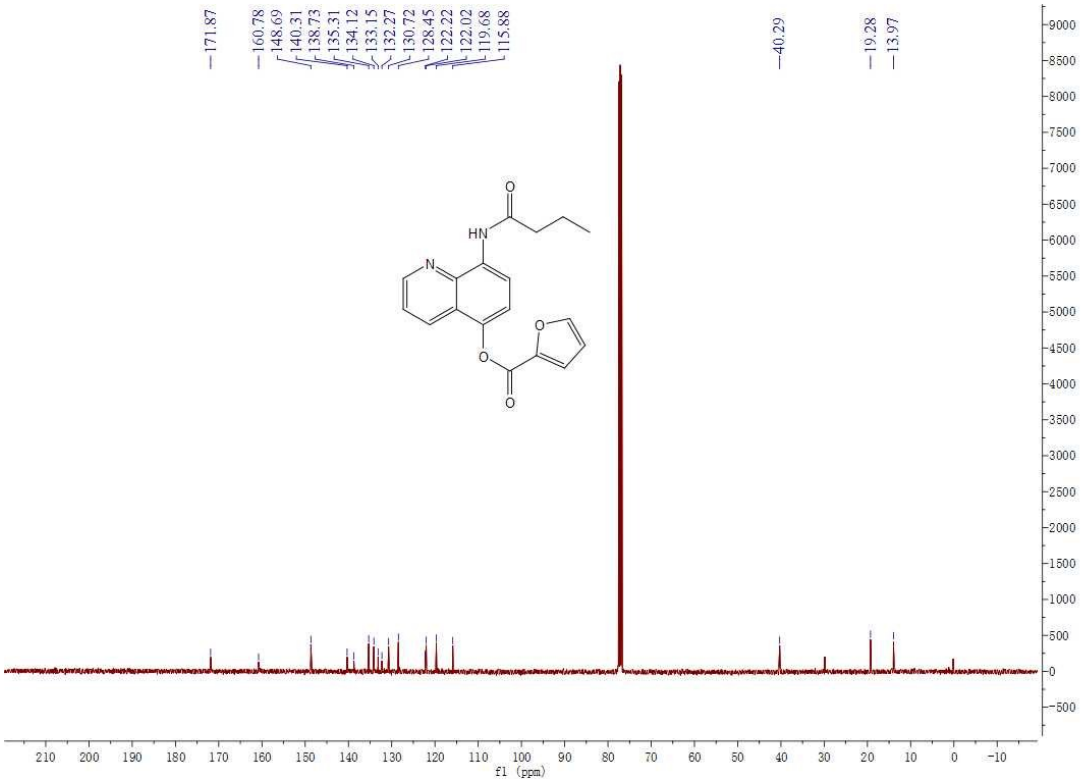
f1 (ppm)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115.88
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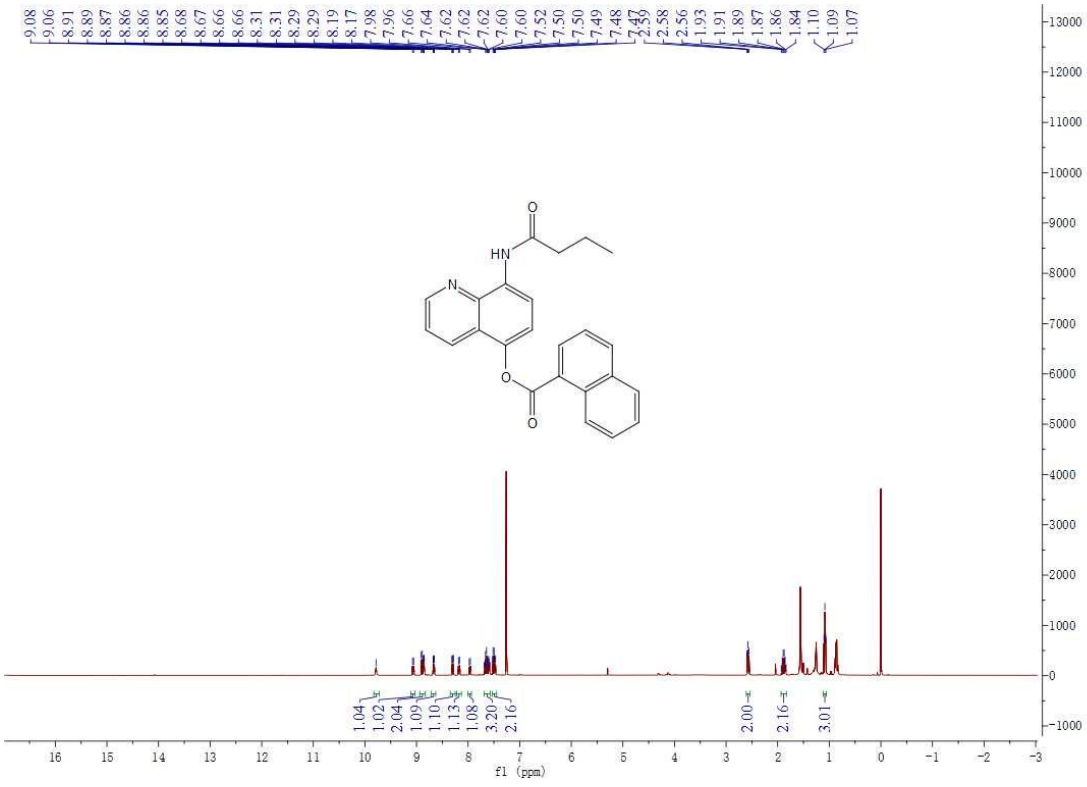
O
O
f1 (ppm)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7.62
7.62
7.62
7.60
7.60
7.52
7.50
7.50
7.49
7.48
2.58
2.56
1.93
1.91
1.89
1.87
1.86
1.84
1.10
1.09
1.07
HN
N
O
O
O
1.04
1.02
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1.13
1.08
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2.16
3.01
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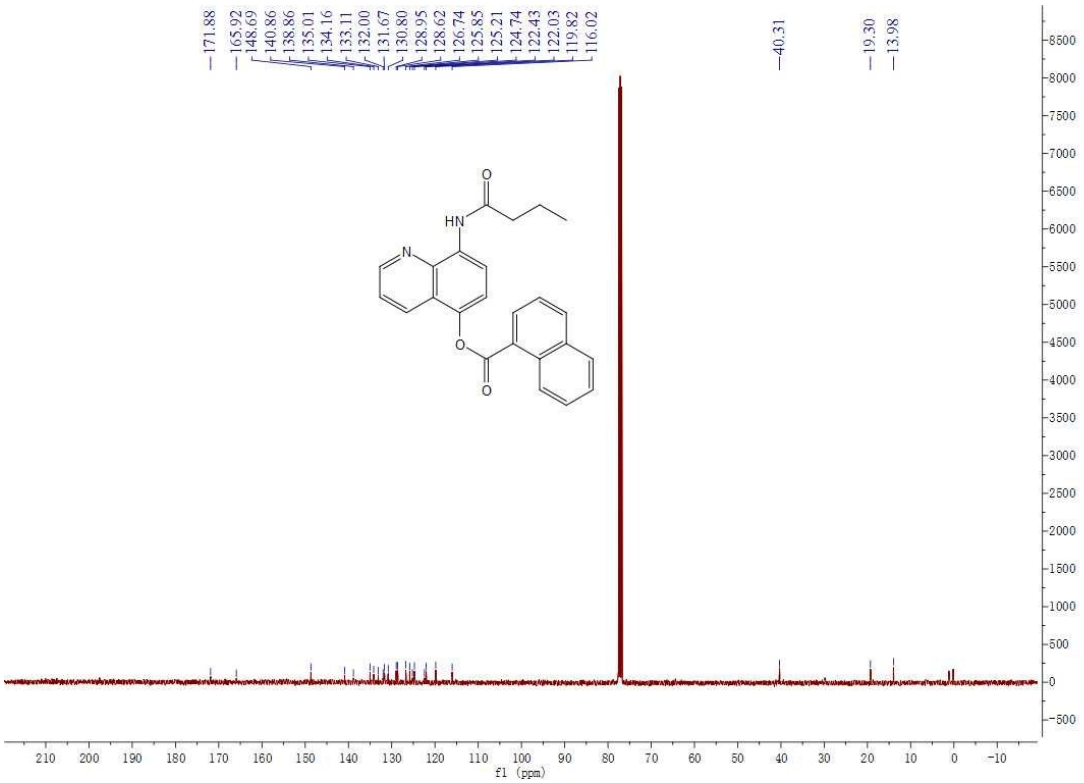
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134.16
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126.74
125.85
125.21
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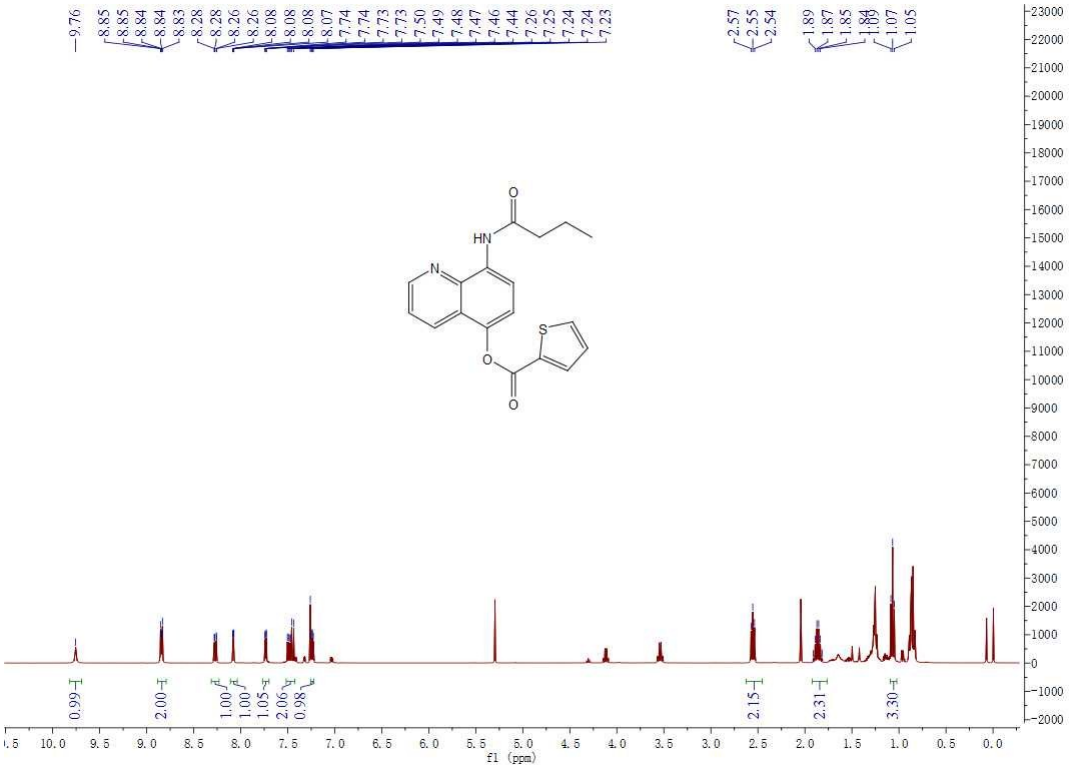
116.02
40.31
19.30
13.98
HN
N
O
O
O
f1 (ppm)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8.08
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7.47
7.46
7.44
7.26
7.25
7.24
7.23
2.57
2.55
2.54
1.89
1.87
1.85
1.84
1.07
1.05
0.99
2.00
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1.05
2.06
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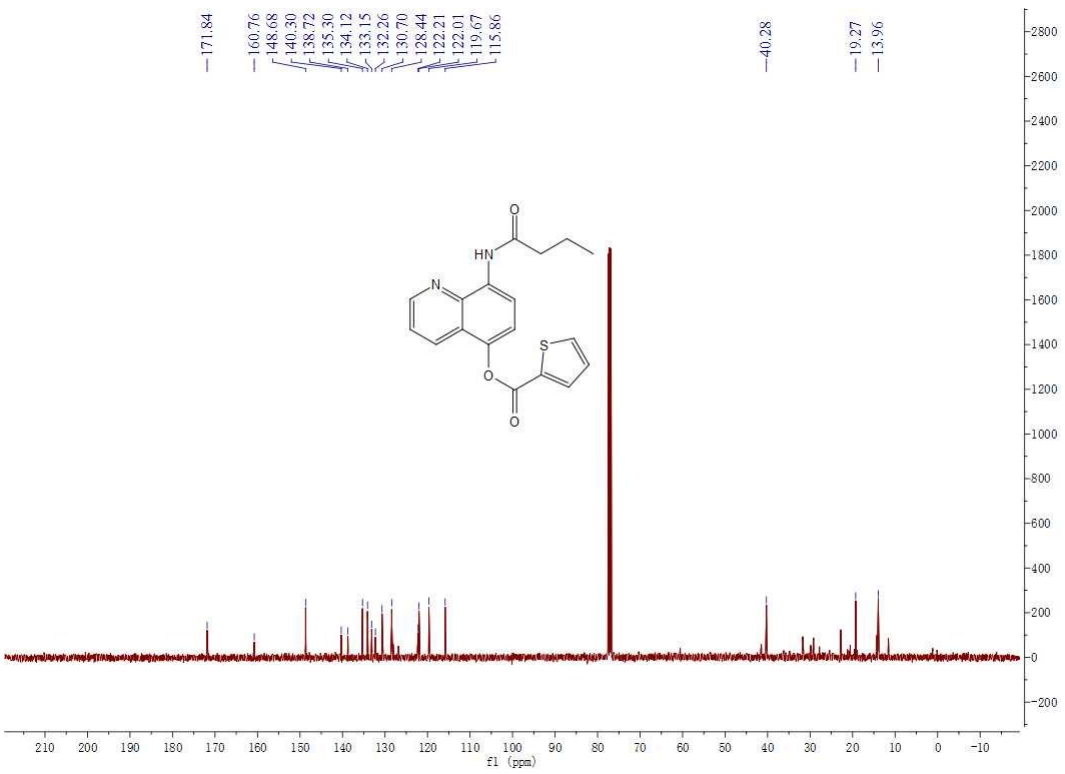
2.15
2.31
3.30
HN
N
S
O
O
f1 (ppm)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132.26
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119.67
115.86
40.28
19.27
13.96
HN
N
S
O
O
O
f1 (ppm)