Electronic Supplementary Material (ESI) for ChemComm.

Base-controlled [3+3] cycloaddition of isoquinoline *N*-oxides with azaoxyallyl cations

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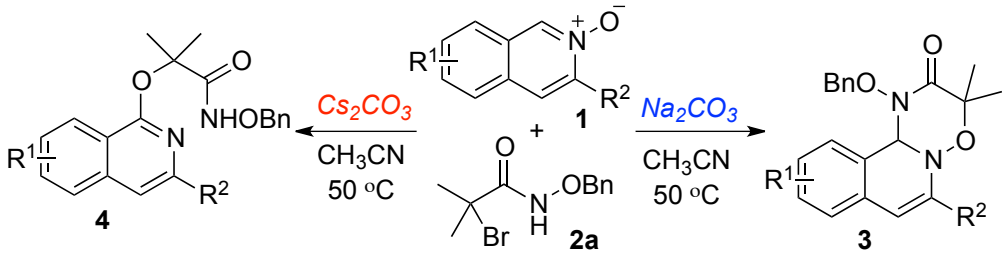
Supporting Information

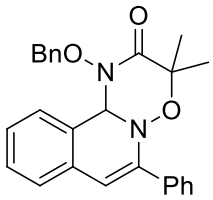
General experimental methods:

All reactions were performed in reaction tubes under air atmosphere. Unless otherwise stated, all commercial reagents were used as received. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

*General experimental procedure for the [3+3] cycloaddition of isoquinoline N-oxides **1** with azaoxyallyl cations **2**.*

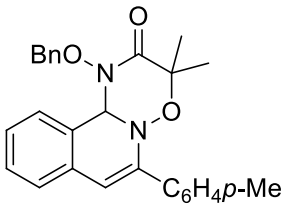


In a reaction tube, isoquinoline *N*-oxides **1** (0.2 mmol) was combined with azaoxyallyl cation **2a** (0.3 mmol, 1.5 equiv.) and base. Then CH_3CN (2.0 mL) was added, and the solution was stirred at 50 °C under air atmosphere for 8-12 hours. After completion of the reaction as indicated by TLC, the mixture was purified directly by flash column chromatography on silica gel (PE: EA, 8:1 or 4:1) to give the desired product **3** and **4**.



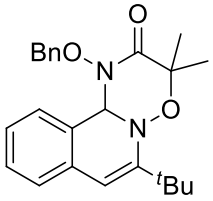
1-(Benzyloxy)-3,3-dimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 3H), 1.64 (s, 3H), 5.19 (d, *J* = 9.7 Hz, 1H), 5.25-5.28 (m, 1H), 5.41 (s, 1H), 6.82 (s, 1H), 7.28-7.30 (m, 1H), 7.34-7.43 (m, 8H), 7.51 (d, *J* = 6.8 Hz, 2H), 7.63-7.65 (m, 1H), 7.73 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 24.7, 76.4, 77.2, 82.3, 125.9, 126.2, 127.1, 128.4, 128.6, 128.7, 128.8, 129.0, 129.1, 130.0, 130.5, 130.7, 134.4, 135.3, 141.9, 169.2; HRMS (ESI) calcd for $C_{26}H_{24}N_2O_3$: 413.1860 ($M + H^+$), found: 413.1859.



1-(Benzyloxy)-3,3-dimethyl-6-(*p*-tolyl)-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3b**)

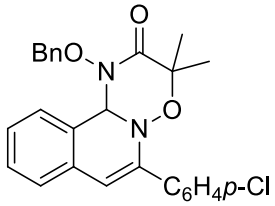
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 3H), 1.65 (s, 3H), 2.39 (s, 3H), 5.19 (d, *J* = 9.7 Hz, 1H), 5.26 (d, *J* = 9.9 Hz, 1H), 5.38 (s, 1H), 6.78 (s, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.25-7.27 (m, 2H), 7.33-7.39 (m, 5H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.63 (d, *J* = 8.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 23.5, 24.7, 76.3, 77.2, 82.2, 117.2, 124.3, 125.8, 126.0, 127.1, 127.8, 128.6, 128.6, 129.2, 130.0, 130.4, 130.8, 132.5, 134.5, 139.1, 141.9, 169.2; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_3$: 427.2016 ($M + H^+$), found: 427.2015.



1-(Benzyloxy)-6-(*tert*-butyl)-3,3-dimethyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3c**)

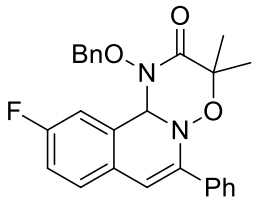
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16 (s, 9H), 1.18 (s, 3H), 1.73 (s, 3H), 4.93 (s, 1H), 5.15 (d,

J = 10.8 Hz, 1H), 5.26 (d, *J* = 10.8 Hz, 1H), 6.42 (s, 1H), 7.13 (dd, J_1 = 5.7 Hz, J_2 = 3.0 Hz, 1H), 7.28 (dd, J_1 = 5.5 Hz, J_2 = 3.3 Hz, 2H), 7.34-7.36 (m, 3H), 7.46-7.49 (m, 2H), 7.55-7.57 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 25.0, 29.0, 36.0, 76.4, 78.2, 82.1, 118.4, 125.4, 126.0, 128.4, 128.5, 128.6, 129.1, 130.1, 130.2, 131.6, 134.7, 152.5, 168.6; HRMS (ESI) calcd for $C_{24}H_{28}N_2O_3$: 393.2173 ($M + H^+$), found: 393.2162.



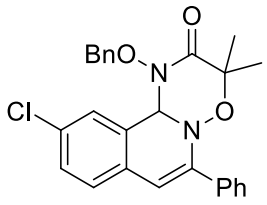
1-(Benzyloxy)-6-(4-chlorophenyl)-3,3-dimethyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 3H), 1.63 (s, 3H), 5.19 (d, *J* = 9.9 Hz, 1H), 5.26 (d, *J* = 10.0 Hz, 1H), 5.38 (s, 1H), 6.80 (s, 1H), 7.28 (dd, J_1 = 5.2 Hz, J_2 = 3.4 Hz, 1H), 7.36-7.39 (m, 7H), 7.50-7.52 (m, 2H), 7.64 (t, *J* = 7.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 24.7, 76.4, 77.0, 82.3, 118.3, 125.9, 126.3, 128.3, 128.6, 128.6, 128.7, 129.1, 129.1, 130.0, 130.4, 133.9, 134.4, 134.9, 140.8, 169.0; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_3$: 447.1470 ($M + H^+$), found: 447.1468.



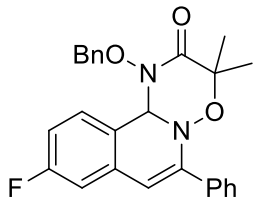
1-(Benzyloxy)-10-fluoro-3,3-dimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.19 (s, 3H), 1.65 (s, 3H), 5.22 (d, *J* = 10.2 Hz, 1H), 5.28 (d, *J* = 7.2 Hz, 2H), 6.80 (s, 1H), 7.04 (dd, J_1 = 8.2 Hz, J_2 = 6.7 Hz, 1H), 7.24 (dd, J_1 = 8.1 Hz, J_2 = 5.3 Hz, 1H), 7.38-7.41 (m, 7H), 7.52 (d, *J* = 6.3 Hz, 2H), 7.71 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 24.7, 76.4, 77.1, 82.3, 113.7 (d, $^2J_{CF}$ = 24.1 Hz), 115.6, (d, $^2J_{CF}$ = 22.2 Hz), 126.8, 127.0, 127.9 (d, $^3J_{CF}$ = 8.0 Hz), 128.5, 128.6, 129.1, 129.3, 130.0, 133.1 (d, $^3J_{CF}$ = 6.9 Hz), 134.3, 135.2, 141.2, 163.2 (d, $^1J_{CF}$ = 249.6 Hz), 169.0; HRMS (ESI) calcd for $C_{26}H_{23}FN_2O_3$: 431.1765 ($M + H^+$), found: 431.1778.



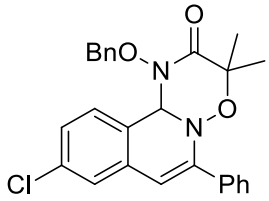
1-(Benzyloxy)-10-chloro-3,3-dimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.19 (s, 3H), 1.64 (s, 3H), 5.18 (d, *J* = 10.1 Hz, 1H), 5.26 (s, 1H), 5.29 (d, *J* = 10.3 Hz, 1H), 6.76 (s, 1H), 7.19 (d, *J* = 8.1 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.36-7.41 (m, 6H), 7.52 (d, *J* = 6.3 Hz, 2H), 7.65 (s, 1H), 7.69 (d, *J* = 6.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 24.7, 76.5, 77.0, 82.4, 117.0, 126.2, 127.1, 127.3, 128.5, 128.6, 128.9, 129.2, 129.3, 130.1, 132.2, 134.3, 134.6, 135.0, 142.2, 169.0; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_3$: 447.1470 ($M + H^+$), found: 447.1450.



1-(Benzyloxy)-9-fluoro-3,3-dimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*] isoquinolin-2(3*H*)-one (**3g**)

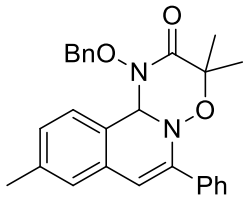
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17 (s, 3H), 1.63 (s, 3H), 5.13 (d, *J* = 9.0 Hz, 1H), 5.23 (d, *J* = 10.3 Hz, 1H), 5.41 (s, 1H), 6.69 (s, 1H), 6.95-7.03 (m, 2H), 7.36-7.41 (m, 6H), 7.49 (d, *J* = 6.0 Hz, 2H), 7.58 (dd, J_1 = 7.9 Hz, J_2 = 5.6 Hz, 1H), 7.71 (d, *J* = 6.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 24.7, 76.5, 76.8, 82.6, 112.7 (d, $^{2}J_{CF}$ = 22.8 Hz), 115.1, (d, $^{2}J_{CF}$ = 21.8 Hz), 116.4, 125.9, 127.3, 127.9 (d, $^{3}J_{CF}$ = 8.0 Hz), 128.5, 128.6, 129.2, 129.4, 130.0, 132.8 (d, $^{3}J_{CF}$ = 8.5 Hz), 134.4, 135.0, 143.3, 163.0 (d, $^{1}J_{CF}$ = 246.5 Hz), 169.1; HRMS (ESI) calcd for $C_{26}H_{23}FN_2O_3$: 431.1765 ($M + H^+$), found: 431.1764.



1-(Benzyloxy)-9-chloro-3,3-dimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*] isoquinolin-2(3*H*)-one (**3h**)

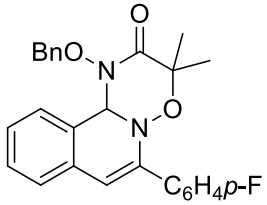
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17 (s, 3H), 1.63 (s, 3H), 5.16 (d, *J* = 9.7 Hz, 1H), 5.24 (d,

J = 8.3 Hz, 1H), 5.36 (s, 1H), 6.69 (s, 1H), 7.24 (s, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.36-7.41 (m, 6H), 7.49 (d, *J* = 5.9 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.4, 24.6, 76.5, 76.8, 82.6, 116.4, 125.9, 127.3, 127.4, 128.5, 128.6, 129.2, 129.4, 130.0, 132.5, 134.3, 134.6, 134.9, 143.2, 169.0; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_3$: 447.1470 (M + H^+), found: 447.1461.



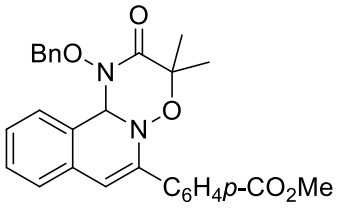
1-(Benzyloxy)-3,3,9-trimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17 (s, 3H), 1.64 (s, 3H), 2.36 (s, 3H), 5.17 (d, *J* = 9.5 Hz, 1H), 5.23 (d, *J* = 7.2 Hz, 1H), 5.40 (s, 1H), 6.76 (s, 1H), 7.09 (s, 1H), 7.16 (d, *J* = 7.7 Hz, 1H), 7.34-7.42 (m, 6H), 7.49-7.53 (m, 3H), 7.72 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 23.5, 24.7, 76.3, 77.1, 82.3, 118.0, 125.8, 126.9, 127.1, 127.7, 128.4, 128.6, 129.0, 129.1, 129.5, 130.0, 130.6, 134.5, 135.5, 138.5, 141.9, 169.2; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_3$: 427.2016 (M + H^+), found: 427.2026.



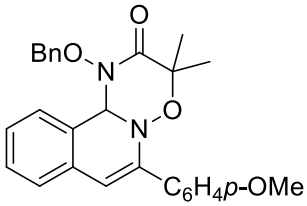
1-(Benzyloxy)-6-(4-fluorophenyl)-3,3-dimethyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 3H), 1.62 (s, 3H), 5.19 (d, *J* = 9.7 Hz, 1H), 5.26 (d, *J* = 6.4 Hz, 1H), 5.38 (s, 1H), 6.75 (s, 1H), 7.10 (t, *J* = 8.6 Hz, 2H), 7.25-7.28 (m, 1H), 7.35-7.38 (m, 5H), 7.50 (d, *J* = 5.5 Hz, 2H), 7.62-7.64 (m, 1H), 7.70 (dd, J_1 = 8.6 Hz, J_2 = 5.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 24.7, 76.4, 77.2, 82.3, 115.4 (d, $^2J_{CF}$ = 21.7 Hz), 117.8, 125.9, 126.1, 128.6, 128.7, 128.9, 129.0, 129.1, 130.0, 130.3, 130.5, 131.5, 134.4, 140.9, 163.3, 169.1 (d, $^1J_{CF}$ = 249.2 Hz), 169.1; HRMS (ESI) calcd for $C_{26}H_{23}FN_2O_3$: 431.1765 (M + H^+), found: 431.1766.



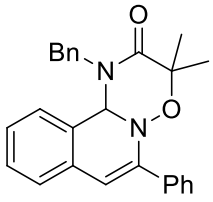
Methyl 4-(1-(benzyloxy)-3,3-dimethyl-2-oxo-1,2,3,11b-tetrahydro-[1,2,4]oxadiazino [3,2-*a*]isoquinolin-6-yl)benzoate (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17 (s, 3H), 1.64 (s, 3H), 3.93 (s, 3H), 5.18 (d, *J* = 9.8 Hz, 1H), 5.27 (d, *J* = 10.0 Hz, 1H), 5.42 (s, 1H), 6.92 (s, 1H), 7.29-7.31 (m, 1H), 7.36-7.40 (m, 5H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.64-7.66 (m, 1H), 7.79 (d, *J* = 8.4 Hz, 2H), 8.08 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 24.7, 52.2, 76.4, 77.2, 82.4, 119.7, 126.0, 126.5, 126.8, 128.6, 128.8, 129.2, 129.4, 129.7, 130.0, 130.2, 130.3, 130.7, 134.4, 139.7, 140.8, 166.7, 168.9; HRMS (ESI) calcd for $C_{28}H_{26}N_2O_5$: 471.1914 ($M + H^+$), found: 471.1915.



1-(Benzyloxy)-6-(4-methoxyphenyl)-3,3-dimethyl-1,11b-dihydro-[1,2,4]oxadiazino[3, 2-*a*]isoquinolin-2(3*H*)-one (**3l**)

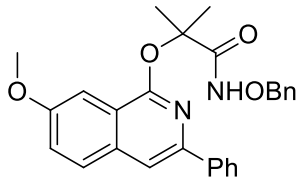
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 3H), 1.65 (s, 3H), 3.85 (s, 3H), 5.23 (dd, J_1 = 22.9 Hz, J_2 = 10.0 Hz, 2H), 5.38 (s, 1H), 6.72 (s, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 5.4 Hz, 1H), 7.33-7.41 (m, 5H), 7.50-7.52 (m, 2H), 7.61-7.63 (m, 1H), 7.67 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 23.5, 24.7, 55.3, 76.3, 77.2, 82.2, 113.8, 116.4, 125.8, 125.9, 127.9, 128.4, 128.5, 128.6, 128.6, 129.1, 130.0, 130.9, 134.4, 141.6, 160.4, 169.2. HRMS (ESI) calcd for $C_{27}H_{26}N_2O_4$: 443.1965 ($M + H^+$), found: 443.1959.



1-Benzyl-3,3-dimethyl-6-phenyl-1,11b-dihydro-[1,2,4]oxadiazino[3,2-*a*]isoquinolin-2(3*H*)-one (**3m**)

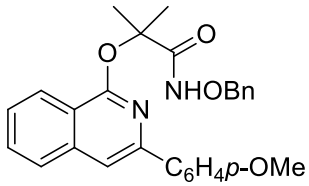
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.91 (s, 6H), 4.42 (d, *J* = 5.8 Hz, 2H), 6.42 (t, *J* = 4.8 Hz,

1H), 6.96-7.04 (m, 5H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 3H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.77 (d, *J* = 9.1 Hz, 2H), 8.13 (d, *J* = 7.6 Hz, 2H), 8.19 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.5, 43.4, 81.4, 110.7, 119.2, 124.0, 126.5, 126.6, 126.9, 127.0, 127.4, 128.3, 128.5, 128.8, 130.7, 138.3, 138.5, 139.1, 147.5, 157.5, 174.2; HRMS (ESI) calcd for $C_{26}H_{24}N_2O_2$: 397.1911 ($M + H^+$), found: 397.1909.



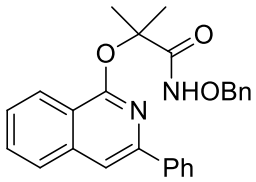
N-(Benzyloxy)-2-((7-methoxy-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamide (**4a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.85 (s, 6H), 3.89 (s, 3H), 4.69 (s, 2H), 6.98 (d, J = 7.2 Hz, 2H), 7.05 (t, J = 7.4 Hz, 2H), 7.13 (d, *J* = 7.1 Hz, 1H), 7.29-7.34 (m, 3H), 7.48 (t, J = 7.6 Hz, 2H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.74(s, 1H), 8.13(d, *J* = 7.6 Hz, 2H), 8.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.6, 55.5, 78.0, 80.6, 102.2, 110.9, 120.0, 123.2, 126.2, 128.2, 128.3, 128.3, 128.4, 128.9, 128.9, 134.5, 135.2, 138.5, 145.4, 156.6, 158.3, 172.2; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_4$: 443.1965 ($M + H^+$), found: 443.1954.



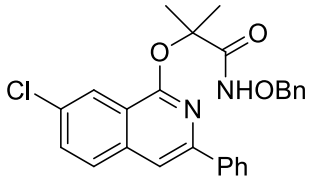
N-(Benzyloxy)-2-((3-(4-methoxyphenyl)isoquinolin-1-yl)oxy)-2-methylpropanamide (**4b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 3.84 (s, 3H), 4.70 (s, 2H), 6.99-7.07 (m, 6H), 7.13 (d, *J* = 7.1 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.69(s, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 8.10 (d, *J* = 8.8 Hz, 2H), 8.71 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 55.3, 78.1, 80.7, 109.7, 114.3, 118.7, 123.9, 126.2, 126.6, 127.8, 128.2, 128.3, 128.9, 130.8, 131.0, 135.2, 139.3, 147.3, 157.3, 160.2, 172.1; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_4$: 443.1965 ($M + H^+$), found: 443.1974.



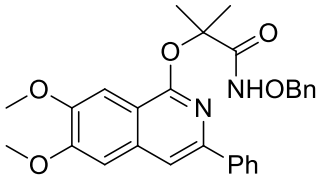
N-(Benzyloxy)-2-methyl-2-((3-phenylisoquinolin-1-yl)oxy)propanamide (**4c**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (s, 6H), 4.71 (s, 2H), 7.01 (d, *J* = 7.2 Hz, 2H), 7.06 (t, *J* = 7.3 Hz, 2H), 7.14 (d, *J* = 7.0 Hz, 1H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.49 (dd, J_1 = 13.1 Hz, J_2 = 6.7 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 8.9 Hz, 2H), 8.07 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 7.6 Hz, 2H), 8.74 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 78.1, 80.9, 111.0, 119.2, 123.9, 126.5, 126.7, 126.8, 128.2, 128.3, 128.7, 128.9, 130.9, 135.2, 138.3, 139.2, 147.4, 157.5, 172.0; HRMS (ESI) calcd for $C_{26}H_{24}N_2O_3$: 435.1679 (M + Na^+), found: 435.1666.



N-(Benzyloxy)-2-((7-chloro-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamide (**4d**)

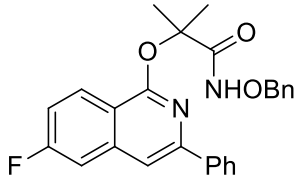
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 4.69 (s, 2H), 7.00 (d, *J* = 7.0 Hz, 2H), 7.07 (t, *J* = 7.2 Hz, 2H), 7.13 (d, *J* = 7.0 Hz, 1H), 7.38 (d, *J* = 7.1 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 8.7 Hz, 2H), 8.07 (s, 1H), 8.13 (d, *J* = 7.5 Hz, 2H), 8.69 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 78.0, 80.9, 110.4, 119.6, 123.2, 126.5, 128.2, 128.3, 128.4, 128.8, 128.9, 131.7, 132.2, 135.1, 137.4, 137.9, 147.9, 156.6, 171.7; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_3$: 447.1470 (M + H^+), found: 447.1464.



N-(Benzyloxy)-2-((6,7-dimethoxy-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamid e (**4e**)

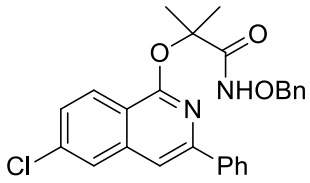
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.83 (s, 6H), 3.95 (d, *J* = 2.9 Hz, 6H), 4.73 (s, 2H), 7.04 (d, *J* = 7.1 Hz, 3H), 7.09 (t, *J* = 7.3 Hz, 2H), 7.14 (d, *J* = 7.0 Hz, 1H), 7.29 (s, 1H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.67 (s, 1H), 8.12 (d, *J* = 7.6 Hz, 2H), 9.00 (s, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 25.6, 55.9, 56.0, 77.9, 80.5, 102.4, 105.4, 110.2, 113.9, 126.3, 128.2, 128.2, 128.3, 128.8, 128.9, 135.4, 135.7, 138.6, 146.2, 149.7, 153.1, 156.4, 172.4; HRMS (ESI) calcd for $C_{28}H_{28}N_2O_5$: 473.2071 ($M + H^+$), found: 473.2067.



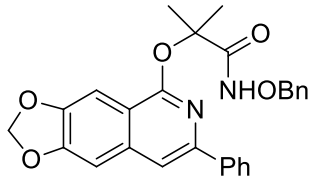
N-(Benzyloxy)-2-((6-fluoro-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamide (**4f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 4.71 (s, 2H), 7.02 (d, *J* = 7.2 Hz, 2H), 7.08 (t, *J* = 7.3 Hz, 2H), 7.13-7.21 (m, 2H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.70 (s, 1H), 8.08 (dd, J_1 = 8.8 Hz, J_2 = 5.8 Hz, 1H), 8.12 (d, *J* = 7.6 Hz, 2H), 8.74 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.8, 71.4, 78.2, 111.4, 118.3, 123.7, 126.5, 126.7, 128.3, 128.5, 128.6, 128.8, 129.0, 129.5, 131.0, 134.8, 138.5, 139.1, 147.4, 158.2, 169.3; HRMS (ESI) calcd for $C_{26}H_{23}FN_2O_3$: 431.1765 ($M + H^+$), found: 431.1771.



N-(Benzyloxy)-2-((6-chloro-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamide (**4g**)

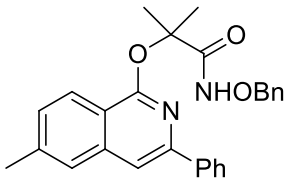
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 4.71 (s, 2H), 7.02 (d, *J* = 7.2 Hz, 2H), 7.09 (t, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 7.1 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 2H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.67 (s, 1H), 7.76 (s, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 8.12 (d, *J* = 7.6 Hz, 2H), 8.68 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 78.0, 81.0, 110.0, 117.3, 125.6, 125.7, 126.6, 127.4, 128.2, 128.3, 128.9, 128.9, 129.0, 135.1, 137.1, 137.9, 140.1, 148.8, 157.5, 171.8; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_3$: 447.1470 ($M + H^+$), found: 447.1464.



N-(Benzyloxy)-2-methyl-2-((7-phenyl-[1,3]dioxolo[4,5-*g*]isoquinolin-5-yl)oxy)propanamide (**4h**)

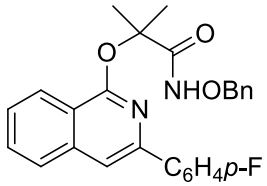
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.81 (s, 6H), 4.72 (s, 2H), 6.02 (s, 2H), 7.04 (t, *J* = 6.0 Hz,

3H), 7.10 (t, *J* = 7.3 Hz, 2H), 7.14-7.18 (m, 1H), 7.35 (d, *J* =10.1 Hz, 2H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.62 (s, 1H), 8.09 (d, *J* = 7.5Hz, 2H), 8.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.5, 78.0, 80.7, 100.5, 101.6, 103.2, 111.0, 115.3, 126.3, 128.2, 128.3, 128.4, 128.8, 128.9, 135.3, 137.3, 138.4, 146.6, 148.0, 151.2, 156.8, 172.4; HRMS (ESI) calcd for $C_{27}H_{24}N_2O_5$: 457.1758 ($M + H^+$), found: 457.1764.



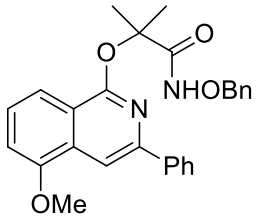
N-(Benzyloxy)-2-methyl-2-((6-methyl-3-phenylisoquinolin-1-yl)oxy)propanamide (**4i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 2.53 (s, 3H), 4.71 (s, 2H), 7.02 (d, *J* = 7.1 Hz, 2H), 7.08 (t, *J* = 7.4 Hz, 2H), 7.15 (t, *J* = 7.1 Hz, 1H), 7.31 (d, *J* =8.5 Hz, 1H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.57 (s, 1H), 7.71 (s, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 7.5 Hz, 2H), 8.80 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.9, 25.5, 78.0, 80.8, 110.7, 117.4, 123.7, 126.0, 126.5, 128.2, 128.3, 128.6, 128.8, 128.9, 135.2, 138.5, 139.5, 141.2, 147.5, 157.5, 172.2; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_3$: 427.2016 ($M + H^+$), found: 427.2017.



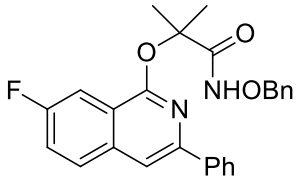
N-(Benzyloxy)-2-((3-(4-fluorophenyl)isoquinolin-1-yl)oxy)-2-methylpropanamide (**4j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 4.70 (s, 2H), 7.01 (d, *J* = 7.2 Hz, 2H), 7.07 (t, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 8.3 Hz, 3H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.71 (s, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 8.10-8.14 (m, 2H), 8.65 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 78.1, 80.7, 110.6, 115.8 (d, $^2J_{CF}$ = 21.5 Hz), 119.0, 123.9, 126.8, 128.3, 128.3, 128.4, 128.9, 131.0, 134.6, 135.1, 139.2, 146.5, 157.5, 163.3 (d, $^1J_{CF}$ = 248.2 Hz), 172.1; HRMS (ESI) calcd for $C_{26}H_{23}FN_2O_3$: 431.1765 ($M + H^+$), found: 431.1759.



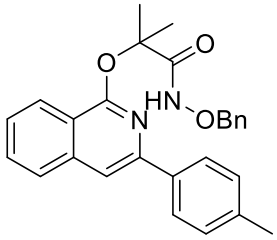
N-(Benzyloxy)-2-((5-methoxy-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamide (**4k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.85 (s, 6H), 4.02 (s, 3H), 4.71 (s, 2H), 7.01 (dd, J_1 = 13.8 Hz, J_2 = 7.6 Hz, 3H), 7.08 (t, *J* = 7.2 Hz, 2H), 7.12-7.16 (m, 1H), 7.37 (q, *J* = 8.1 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 3H), 8.78 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 55.7, 78.1, 80.8, 105.5, 108.4, 115.6, 119.9, 126.5, 126.7, 128.2, 128.3, 128.5, 128.8, 128.9, 131.5, 135.2, 138.6, 146.8, 154.9, 157.3, 172.1; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_4$: 443.1965 ($M + H^+$), found: 443.1972.



N-(Benzyloxy)-2-((7-fluoro-3-phenylisoquinolin-1-yl)oxy)-2-methylpropanamide (**4l**)

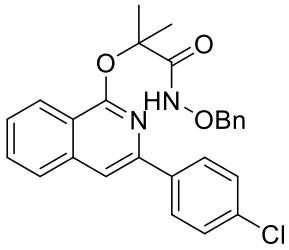
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 4.71 (s, 2H), 7.01 (d, *J* = 6.4 Hz, 2H), 7.07 (t, *J* = 6.9 Hz, 2H), 7.12 (d, *J* = 6.6 Hz, 1H), 7.34-7.44 (m, 2H), 7.48 (t, *J* = 7.0 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.76-7.80 (m, 2H), 8.12 (d, *J* = 7.3 Hz, 2H), 8.73 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 78.0, 80.9, 108.1 (d, $^{2}J_{CF}$ = 22.2 Hz), 110.5, 119.7 (d, $^{3}J_{CF}$ = 8.4 Hz), 121.1 (d, $^{2}J_{CF}$ = 25.0 Hz), 126.4, 128.2, 128.3, 128.7, 128.8, 128.9, 129.3, 129.3, 135.1, 136.1, 138.1, 147.0, 157.1 (d, $^{4}J_{CF}$ = 5.0 Hz), 160.7 (d, $^{1}J_{CF}$ = 284.4 Hz), 171.8; HRMS (ESI) calcd for $C_{26}H_{23}FN_2O_3$: 431.1765 ($M + H^+$), found: 431.1758.



N-(benzyloxy)-2-methyl-2-((3-(p-tolyl)isoquinolin-1-yl)oxy)propanamide (**4m**)

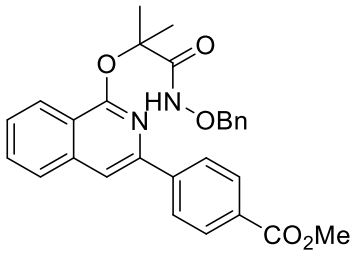
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.85 (s, 6H), 2.39 (s, 3H), 4.71 (s, 2H), 7.00 (d, *J* = 7.1 Hz,

2H), 7.06 (t, *J* = 7.2 Hz, 2H), 7.13 (t, *J* = 6.8 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.75 (s, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 7.5 Hz, 3H), 8.76 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 25.4, 78.1, 80.8, 110.4, 119.0, 123.9, 126.4, 126.7, 128.2, 128.3, 128.9, 129.6, 130.8, 135.2, 135.6, 138.6, 139.3, 147.5, 157.4, 172.1; HRMS (ESI) calcd for $C_{27}H_{26}N_2O_3$: 427.2016 (M + H^+), found: 427.2014.



N-(benzyloxy)-2-((3-(4-chlorophenyl)isoquinolin-1-yl)oxy)-2-methylpropanamide (**4n**)

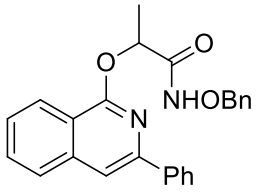
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.84 (s, 6H), 4.71 (s, 2H), 7.02 (d, *J* = 7.3 Hz, 2H), 7.08 (t, *J* = 7.4 Hz, 2H), 7.15 (t, *J* = 7.1 Hz, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.75 (s, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 8.07 (d, *J* = 8.5 Hz, 3H), 8.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 78.1, 80.7, 111.0, 119.2, 123.9, 126.8, 126.9, 127.8, 128.3, 128.4, 128.9, 129.0, 131.0, 134.6, 135.1, 136.9, 139.1, 146.2, 157.5, 172.0; HRMS (ESI) calcd for $C_{26}H_{23}ClN_2O_3$: 447.1470 (M + H^+), found: 447.1467.



Methyl 4-(1-((1-((benzyloxy)amino)-2-methyl-1-oxopropan-2-yl)oxy)isoquinolin-3-yl)benzoate (**4o**)

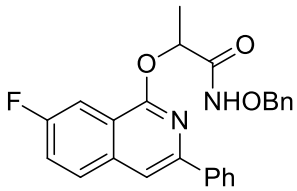
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (s, 6H), 3.93 (s, 3H), 4.73 (s, 2H), 7.03 (d, *J* = 7.3 Hz, 2H), 7.09 (t, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 7.1 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.5 Hz, 1H), 7.84 (d, *J* = 10.2 Hz, 1H), 8.09 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 2H), 8.21 (d, *J* = 8.4 Hz, 2H), 8.68 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.4, 52.1, 78.1, 80.9, 112.2, 119.5, 124.0, 126.3, 127.0, 127.3, 128.2, 128.3, 128.9, 129.9, 130.2,

131.1, 135.1, 138.9, 142.6, 146.1, 157.6, 166.9, 172.0; HRMS (ESI) calcd for $C_{28}H_{26}N_2O_5$: 471.1914 (M + H^+), found: 471.1908.



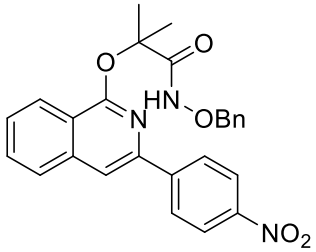
N-(Benzyloxy)-2-((3-phenylisoquinolin-1-yl)oxy)propanamide (**4p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.72 (d, *J* = 6.7 Hz, 3H), 4.75 (d, *J* = 11.2 Hz, 1H), 4.87 (d, *J* = 11.3 Hz, 1H), 5.85 (d, *J* = 6.5 Hz, 1H), 7.05-7.10 (m, 5H), 7.37 (t, *J* = 7.0 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 3H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.71 (s, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 8.07 (d, *J* = 7.7 Hz, 2H), 9.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.8, 71.4, 78.2, 111.4, 118.3, 123.6, 126.5, 126.8, 128.4, 128.5, 128.7, 128.8, 129.1, 131.0, 134.7, 138.5, 139.1, 147.4, 158.2, 169.3; HRMS (ESI) calcd for $C_{25}H_{22}N_2O_3$: 339.1703 (M + H^+), found: 339.1703.



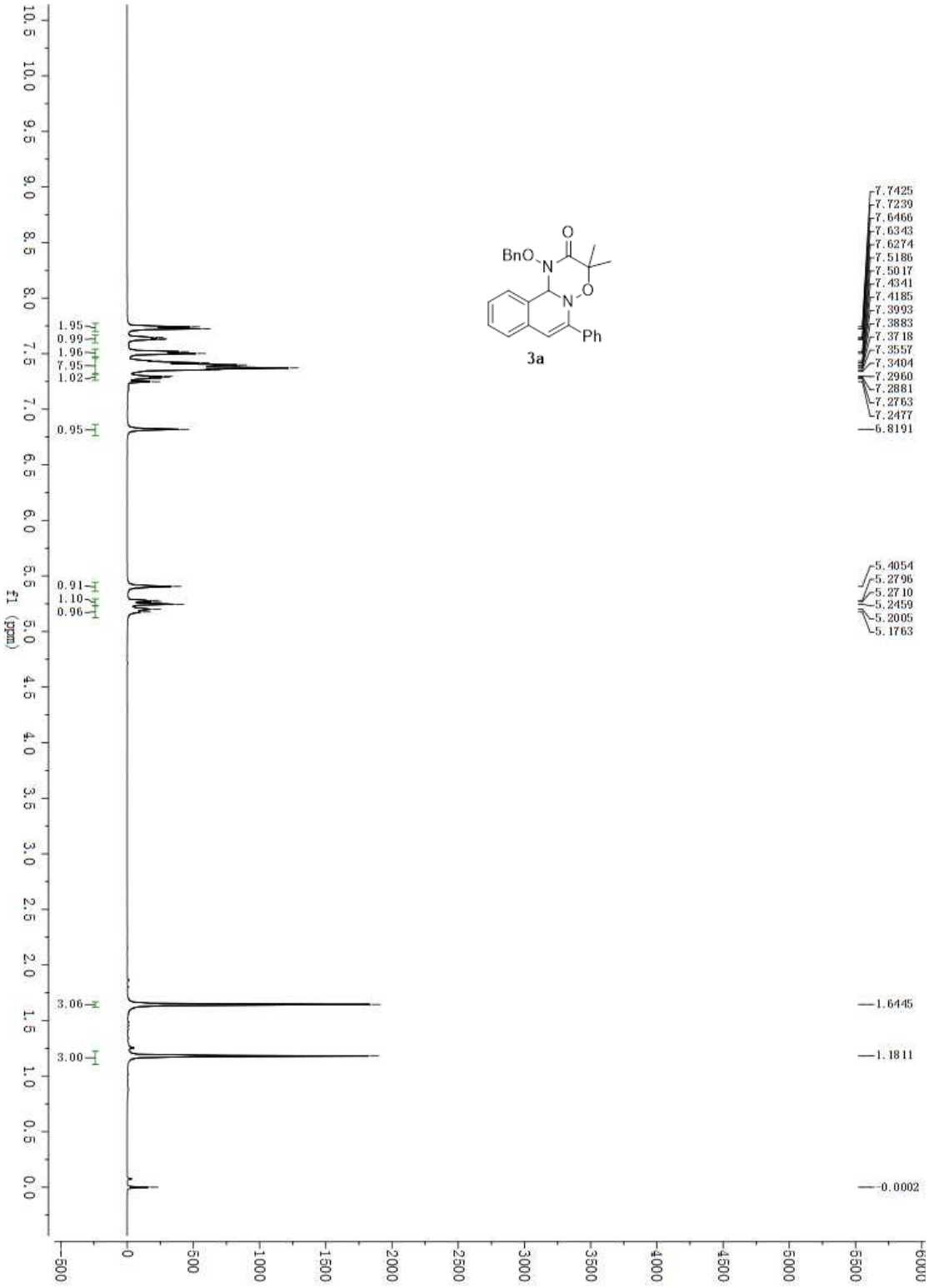
N-(Benzyloxy)-2-((7-fluoro-3-phenylisoquinolin-1-yl)oxy)propanamide (**4q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.72 (d, *J* = 6.7 Hz, 3H), 4.76 (d, *J* = 11.2 Hz, 1H), 4.87 (d, *J* = 11.2 Hz, 1H), 5.82 (d, *J* = 11.2 Hz, 1H), 7.08-7.25 (m, 6H), 7.39 (t, *J* = 7.1 Hz, 2H), 7.46 (t, *J* = 7.1 Hz, 2H), 7.64 (s, 1H), 8.05 (d, *J* = 7.4 Hz, 3H), 8.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.7, 71.4, 78.2, 110.4 (d, $^2J_{CF}$ = 21.1 Hz), 110.9, 111.0, 115.2, 116.6 (d, $^2J_{CF}$ = 25.0 Hz), 126.6, 126.8 (d, $^3J_{CF}$ = 9.5 Hz), 128.3, 128.8, 129.0, 134.7, 138.1, 140.9 (d, $^3J_{CF}$ = 10.4 Hz), 148.8, 158.2, 164.0 (d, $^1J_{CF}$ = 252.1 Hz), 169.1; HRMS (ESI) calcd for $C_{25}H_{21}FN_2O_3$: 417.1609 (M + H^+), found: 417.1617.



N-(benzyloxy)-2-methyl-2-((3-(4-nitrophenyl)isoquinolin-1-yl)oxy)propanamide (**4r**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.86 (s, 6H), 4.75 (s, 2H), 7.07 (d, *J* = 7.1 Hz, 2H), 7.12 (t, *J* = 7.3 Hz, 2H), 7.19 (t, *J* = 7.0 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 9.7 Hz, 2H), 8.13 (d, *J* = 8.2 Hz, 1H), 8.26-8.32 (m, 4H), 8.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.3, 78.2, 80.8, 113.0, 119.7, 124.0, 124.1, 127.1, 127.2, 127.9, 128.3, 128.5, 128.9, 131.3, 135.1, 138.7, 144.5, 144.8, 147.7, 157.7, 172.0.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O
N
O
Ph
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7.6466
7.6343
7.6274
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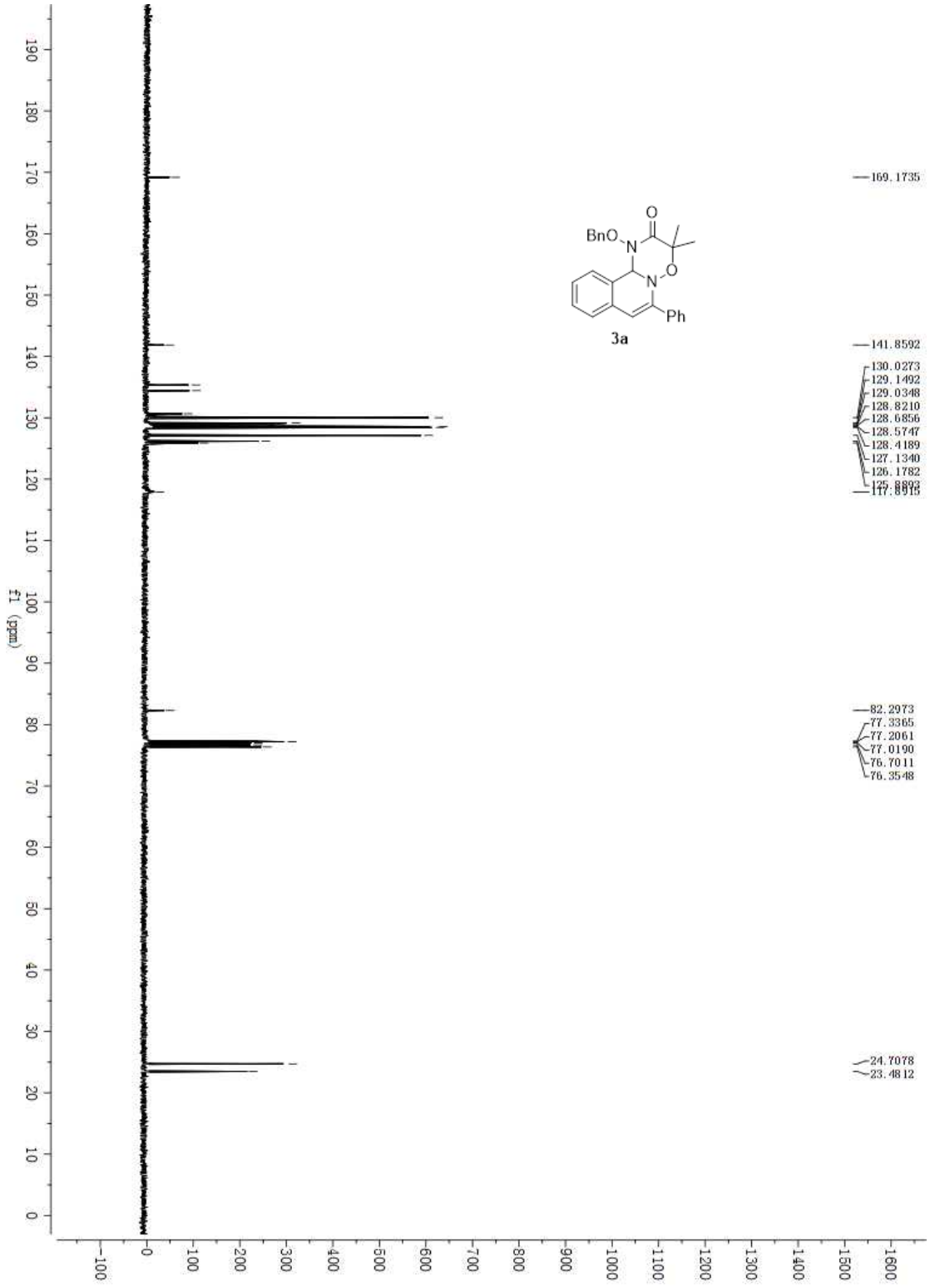
7.5017
7.4341
7.4185
7.3993
7.3883
7.3718
7.3557
7.3404
7.2960
7.2881
7.2763
7.2477
6.8191
5.4054
5.2796
5.2710
5.2459
5.2005
5.1763
1.6445
1.1811
0.0002
1.95
0.99
1.96
7.95
1.02
0.95
0.91
1.10
0.96
3.06
3.00
f1 (ppm)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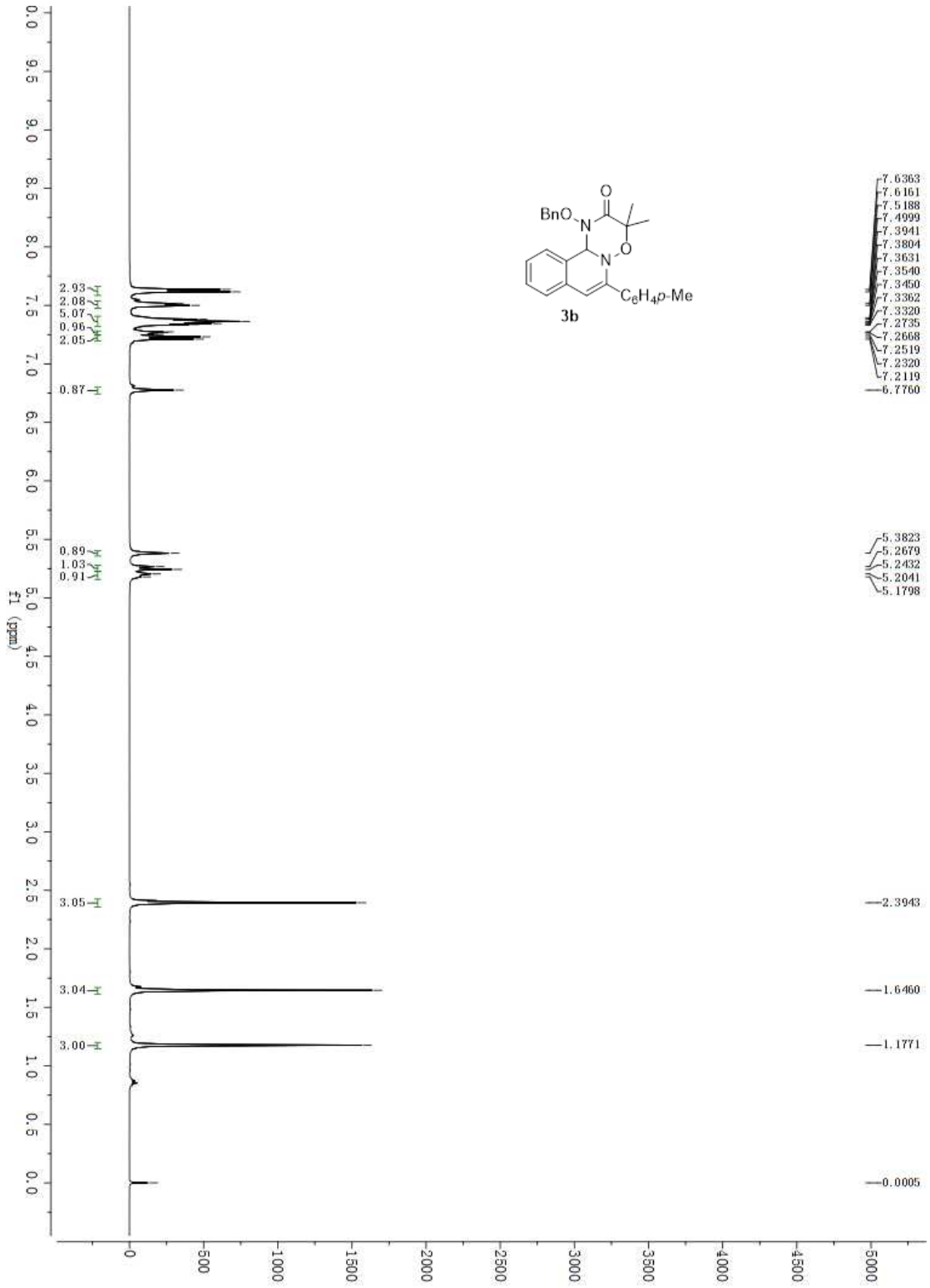
130.0273
129.1492
129.0348
128.8210
128.6856
128.5747
128.4189
127.1340
126.1782
125.8803
117.8915
82.2973
77.3365
77.2061
77.0190
76.7011
76.3548
24.7078
23.4812
BnO
N
O
O
N
Ph
3a
f1 (ppm)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O
N
O
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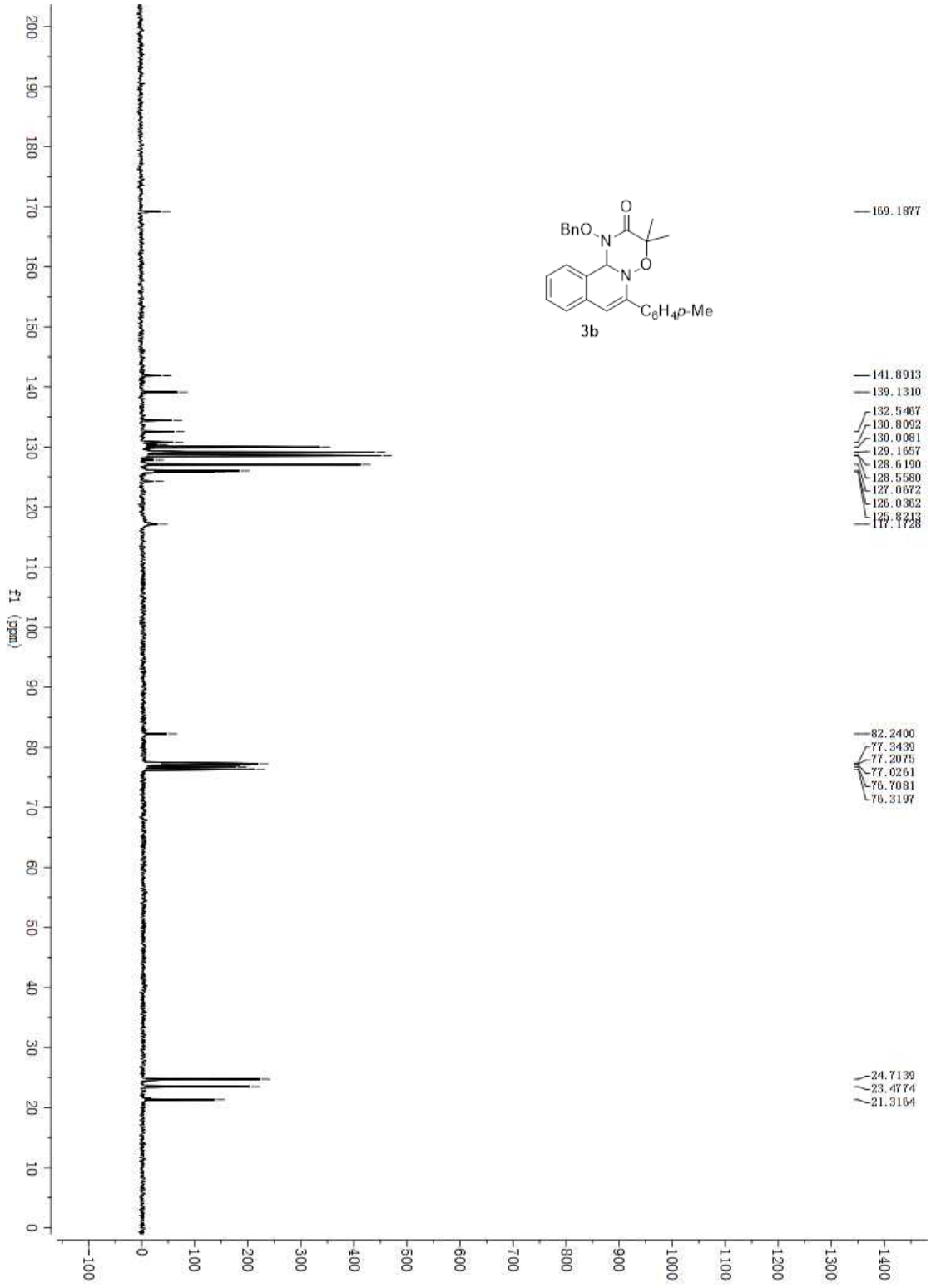
7.5188
7.4999
7.3941
7.3804
7.3631
7.3540
7.3450
7.3362
7.3320
7.2735
7.2668
7.2519
7.2320
7.2119
6.7760
5.3823
5.2679
5.2432
5.2041
5.1798
2.3943
1.6460
1.1771
0.0005
2.93
2.08
5.07
0.96
2.05
0.87
0.89
1.03
0.91
3.05
3.04
3.00
f1 (ppm)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N
O
N
O
C6H4p-Me
3b
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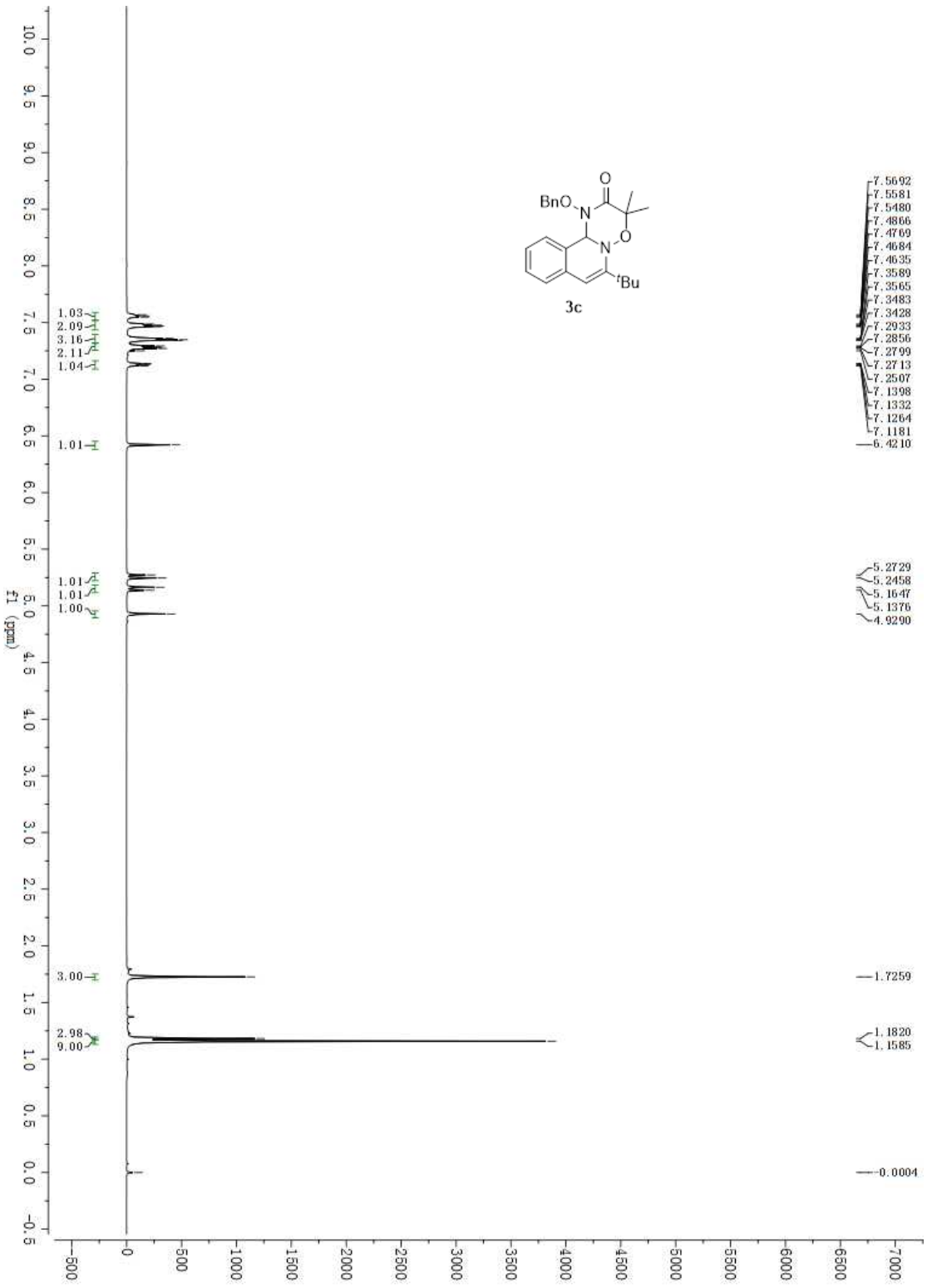
141.8913
139.1310
132.5467
130.8092
130.0081
129.1657
128.6190
128.5580
127.0672
126.0362
125.8213
117.1728
82.2400
77.3439
77.2075
77.0261
76.7081
76.3197
24.7139
23.4774
21.3164
f1 (ppm)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O
N
O
tBu
3c
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7.5480
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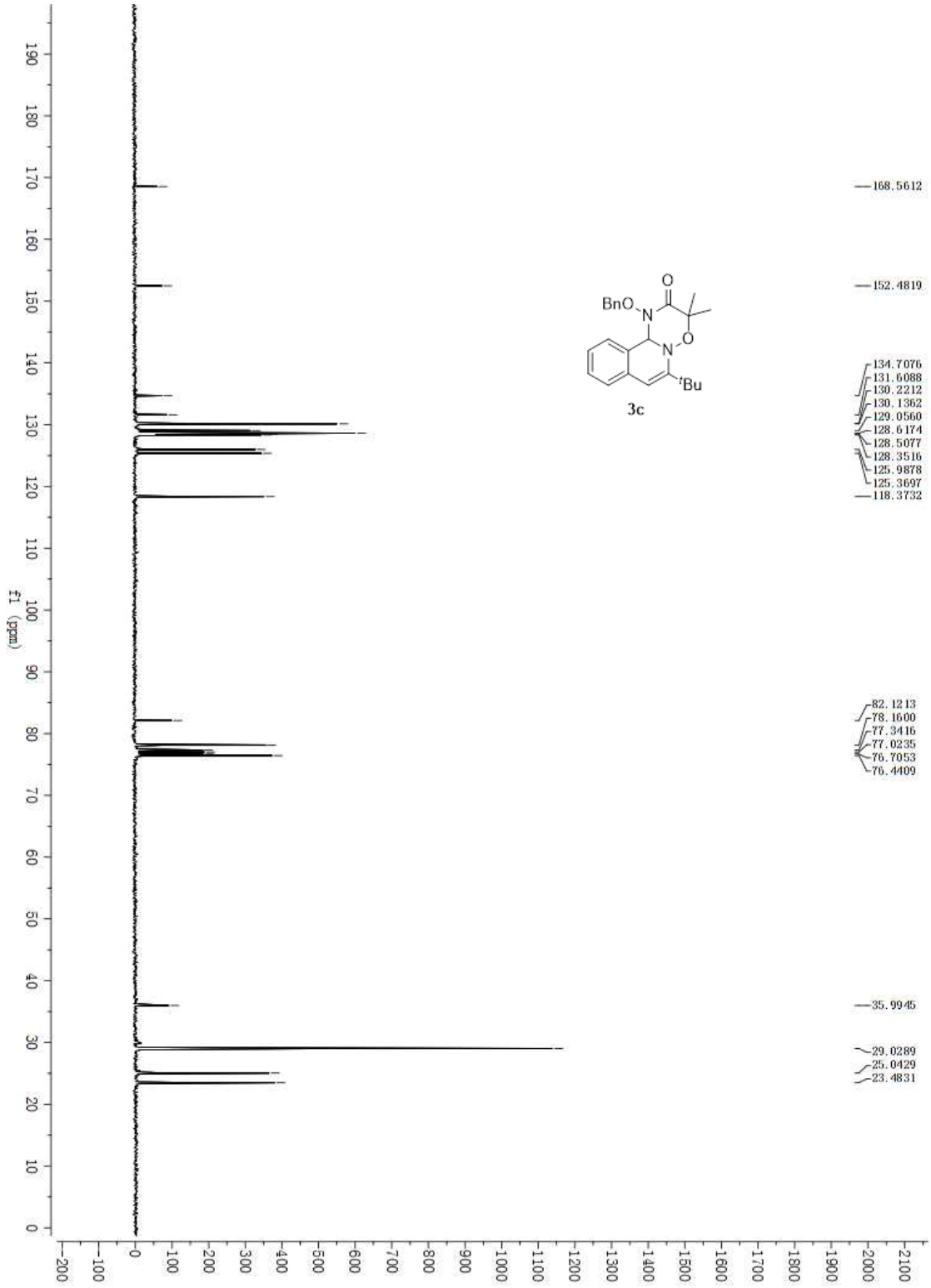
7.4769
7.4684
7.4635
7.3589
7.3565
7.3483
7.3428
7.2933
7.2856
7.2799
7.2713
7.2507
7.1398
7.1332
7.1264
7.1181
6.4210
5.2729
5.2458
5.1647
5.1376
4.9290
1.7259
1.1820
1.1585
0.0004
1.03
2.09
3.16
2.11
1.04
1.01
1.01
1.01
1.00
3.00
2.98
9.00
f1 (ppm)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130.2212
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128.5077
128.3516
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78.1600
77.3416
77.0235
76.7053
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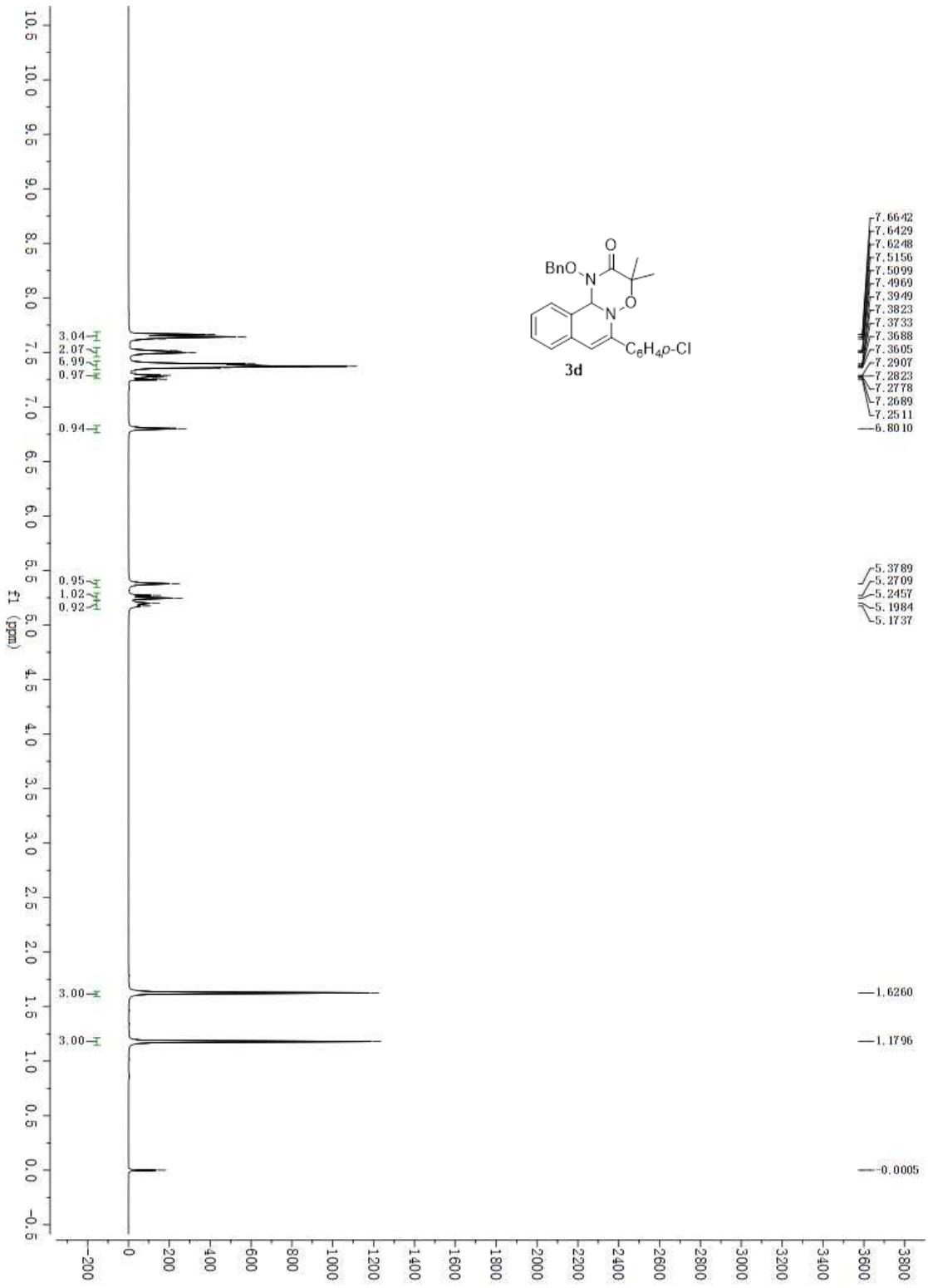
29.0289
25.0429
23.4831
BnO
N
O
N
O
tBu
3c
f1 (ppm)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O
O
N
C6H4p-Cl
3d
f1 (ppm)
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2.07
6.99
0.97
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0.95
1.02
0.92
3.00
3.00
7.6642
7.6429
7.6248
7.5156
7.5099
7.4969
7.3949
7.3823
7.3733
7.3688
7.3605
7.2907
7.2823
7.2778
7.2689
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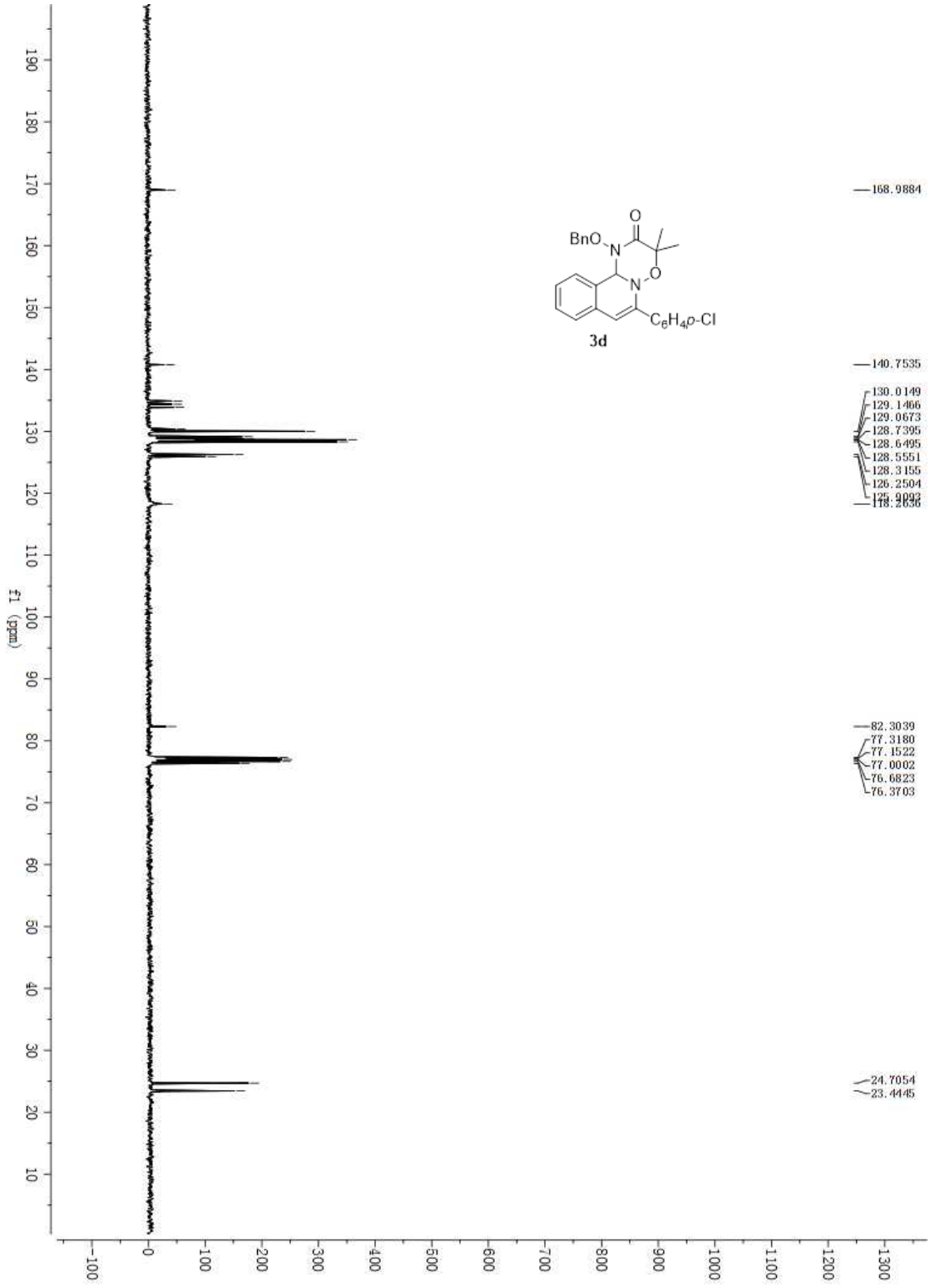
5.2709
5.2457
5.1984
5.1737
1.6260
1.1796
0.0005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O
N
O
C6H4p-Cl
3d
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129.1466
129.0673
128.7395
128.6495
128.5551
128.3155
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77.1522
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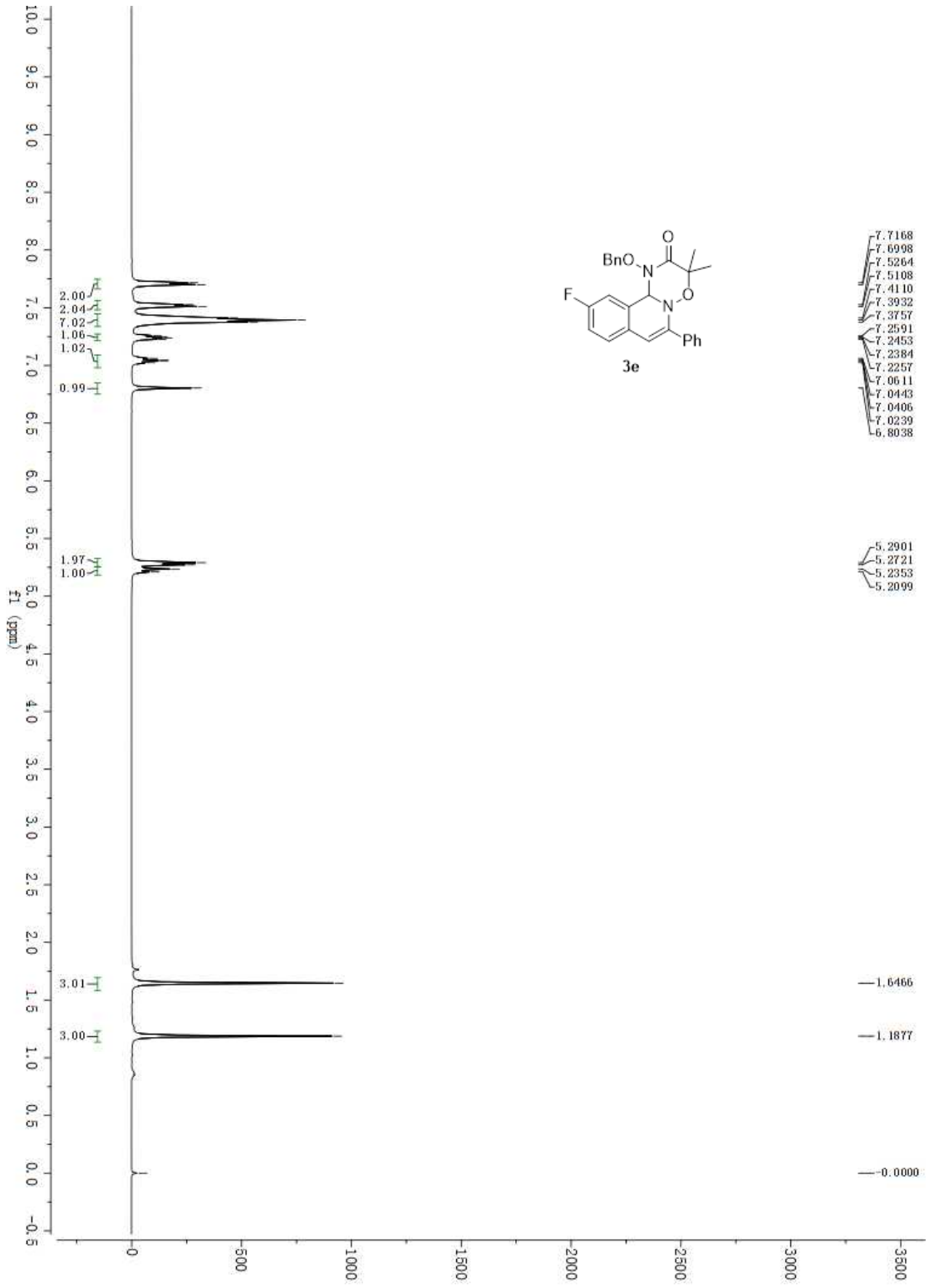
76.6823
76.3703
24.7054
23.4445
f1 (ppm)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O
F
N
O
Ph
3e
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7.5108
7.4110
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7.0406
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5.2901
5.2721
5.2353
5.2099
1.6466
1.1877
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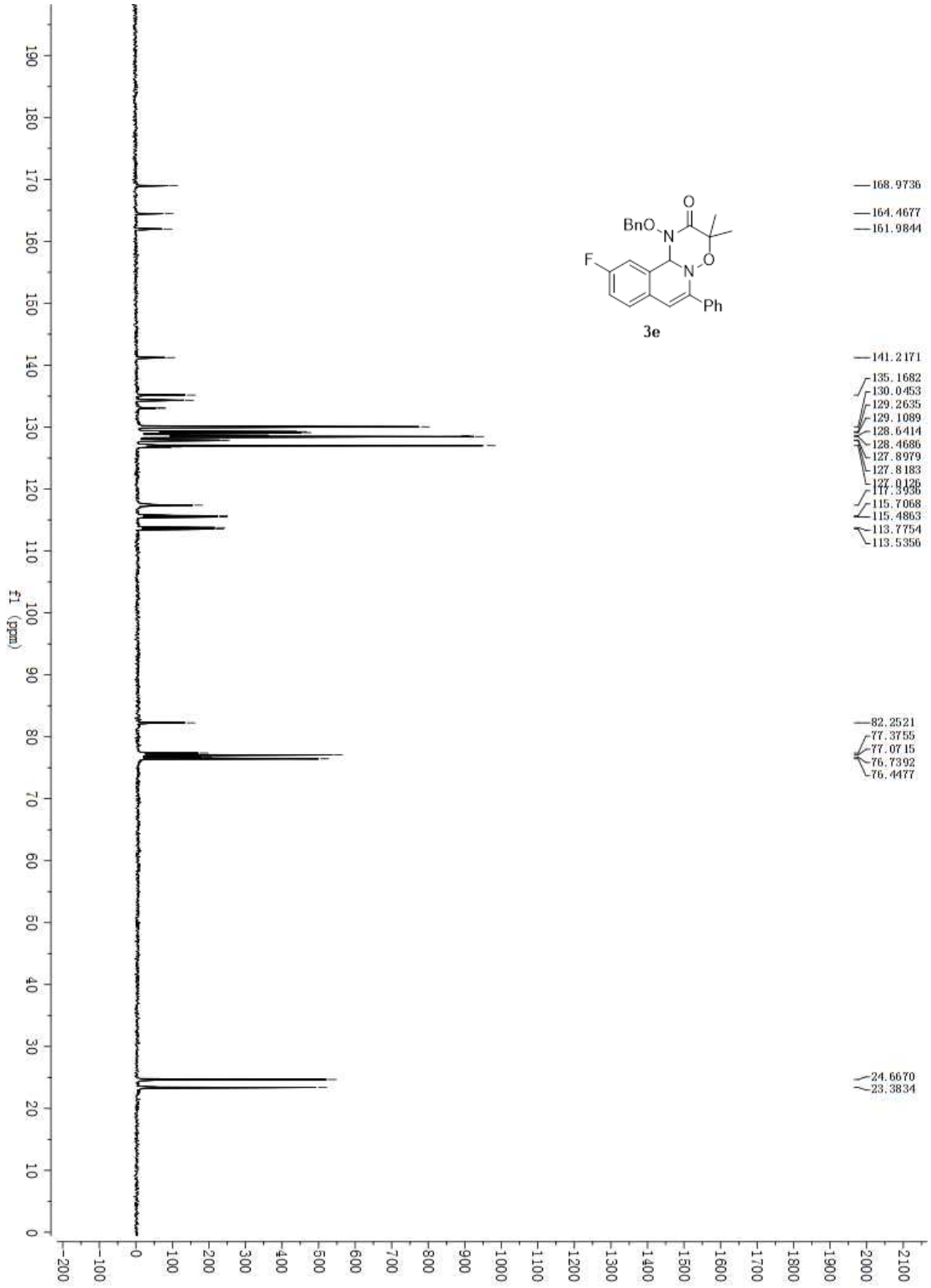
7.02
1.06
1.02
0.99
1.97
1.00
3.01
3.00
f1 (ppm)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127.8183
127.0136
117.3936
115.7068
115.4863
113.7754
113.5356
82.2521
77.3755
77.0715
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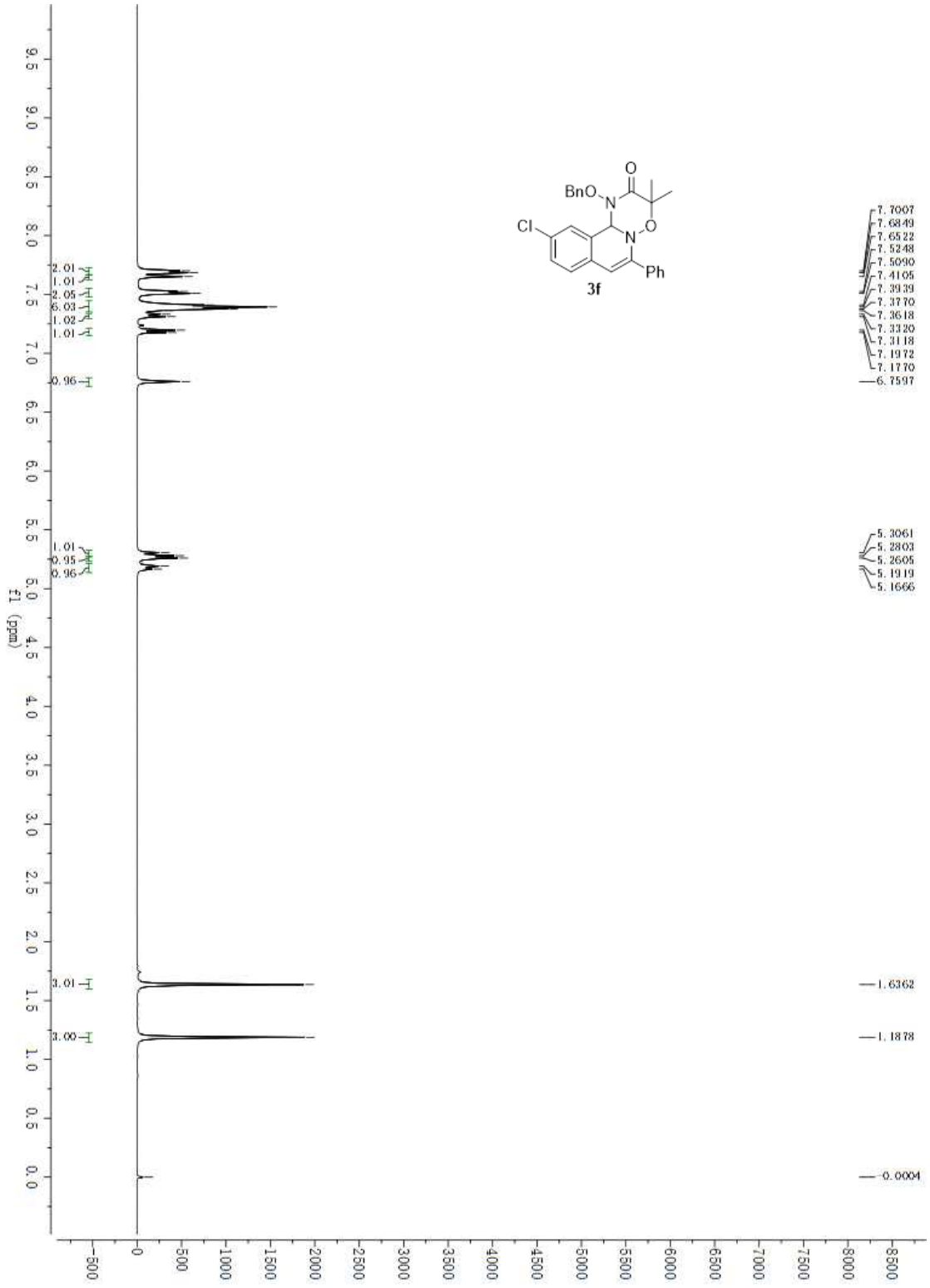
76.4477
24.6670
23.3834
BnO
N
O
F
N
O
Ph
3e
f1 (ppm)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O
Cl
N
O
Ph
3f
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7.5248
7.5090
7.4105
7.3939
7.3770
7.3618
7.3320
7.3118
7.1972
7.1770
6.7597
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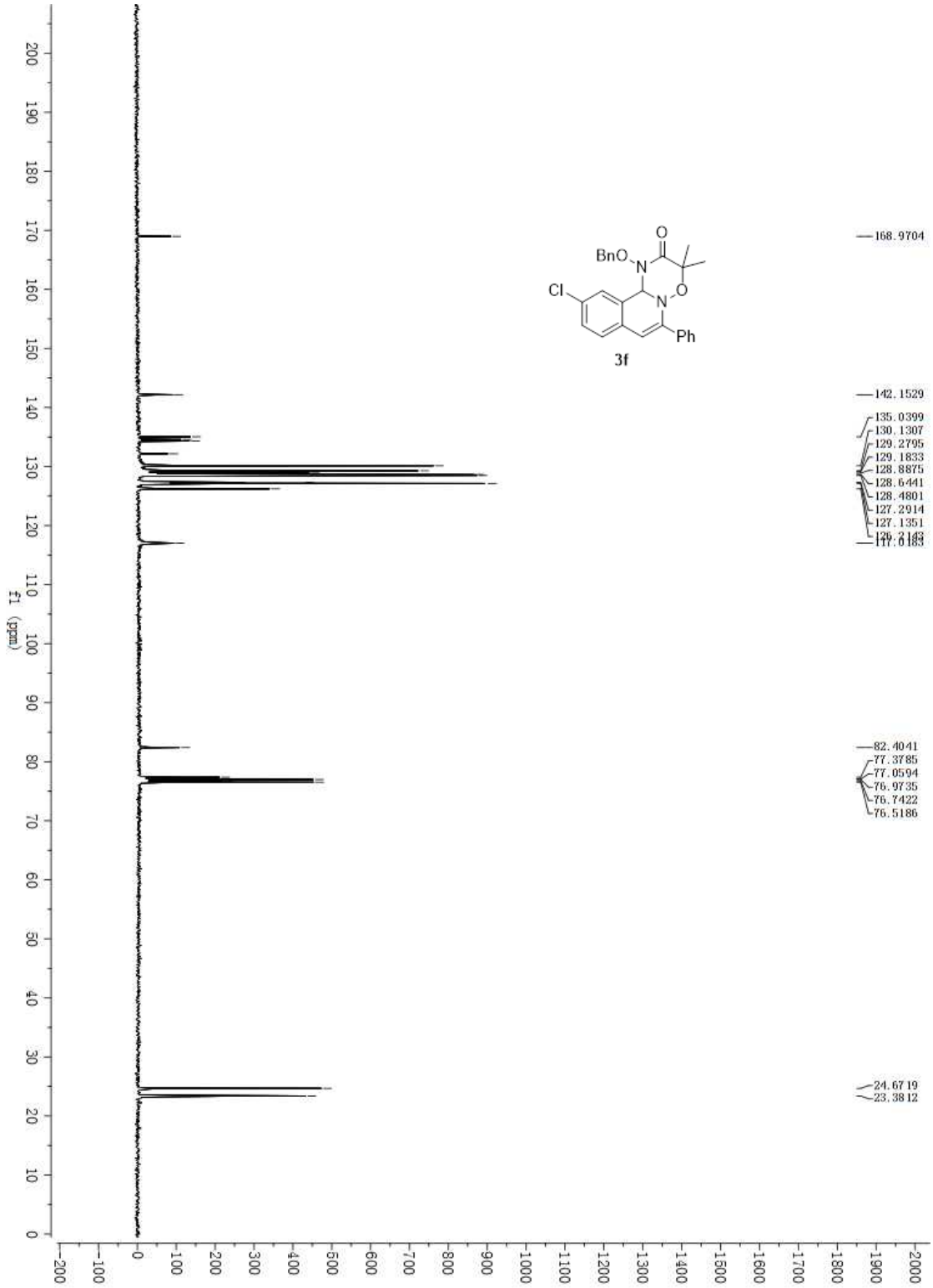
5.2803
5.2605
5.1919
5.1666
1.6362
1.1878
0.0004
f1 (ppm)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127.1351
82.4041
77.3785
77.0594
76.9735
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24.6719
23.3812
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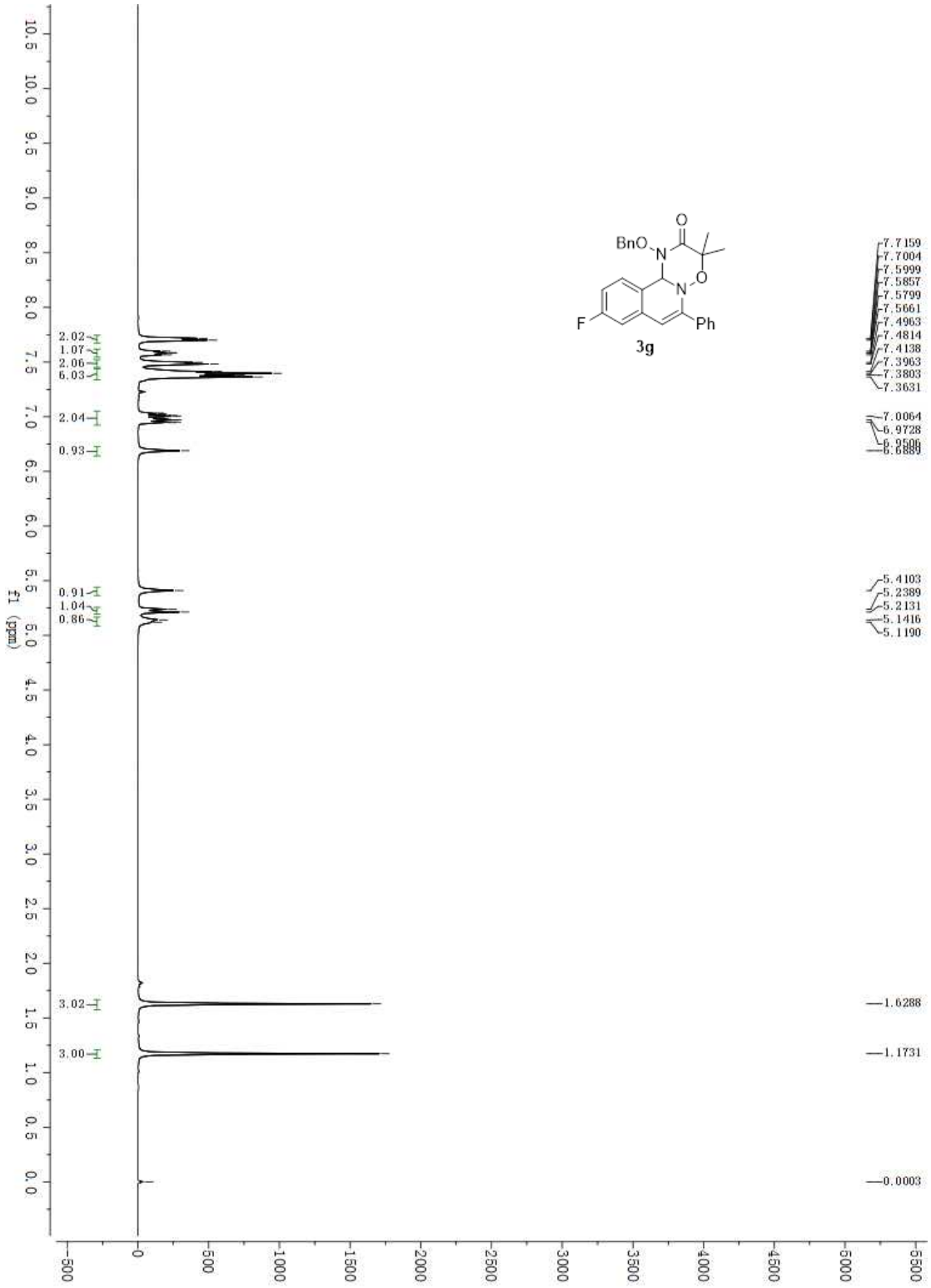
N
O
Cl
N
O
Ph
3f
f1 (ppm)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N
O
F
Ph
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7.5857
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7.4963
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7.4138
7.3963
7.3803
7.3631
7.0064
6.9728
6.9506
6.6889
5.4103
5.2389
5.2131
5.1416
5.1190
1.6288
1.1731
0.0003
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1.07
2.06
6.03
2.04
0.93
0.91
1.04
0.86
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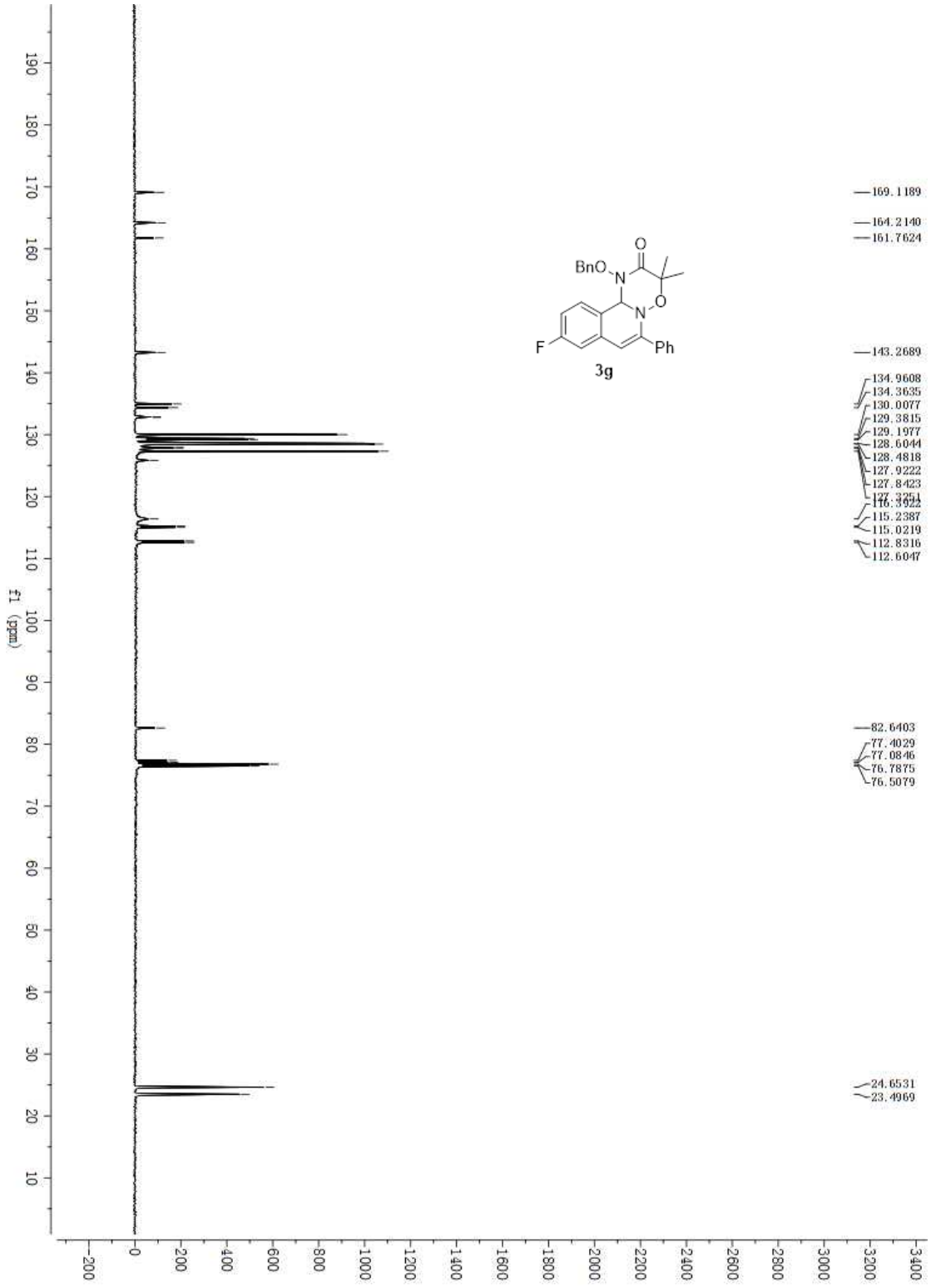
3.00
f1 (ppm)


BnO
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O
O
N
F
Ph
3g
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143.2689
134.9608
134.3635
130.0077
129.3815
129.1977
128.6044
128.4818
127.9222
127.8423
127.3251
116.3922
115.2387
115.0219
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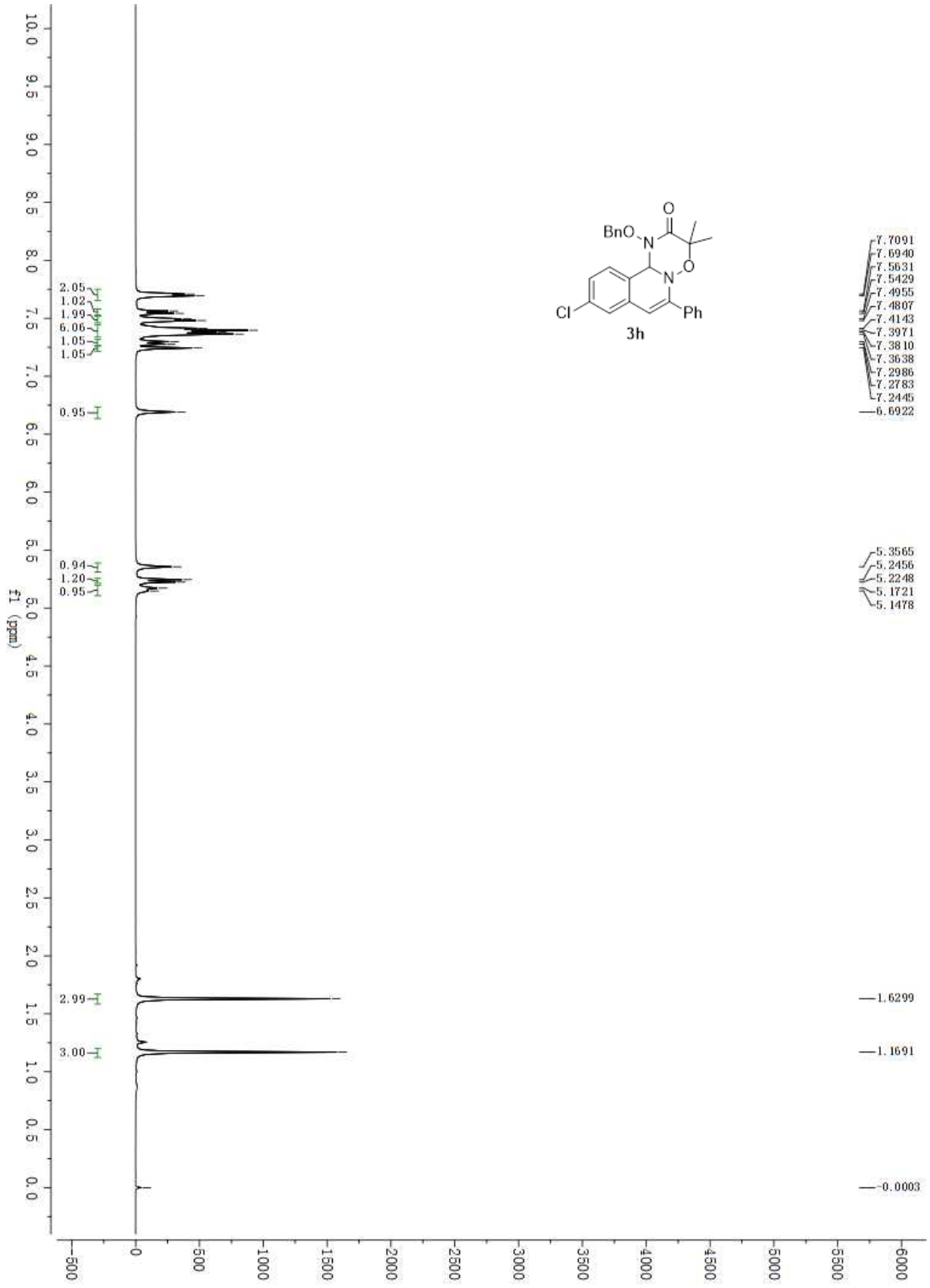
82.6403
77.4029
77.0846
76.7875
76.5079
24.6531
23.4969
f1 (ppm)


BnO
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O
O
N
Cl
Ph
3h
f1 (ppm)
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1.02
1.99
6.06
1.05
1.05
0.95
0.94
1.20
0.95
2.99
3.00
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7.6940
7.5631
7.5429
7.4955
7.4807
7.4143
7.3971
7.3810
7.3638
7.2986
7.2783
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5.3565
5.2456
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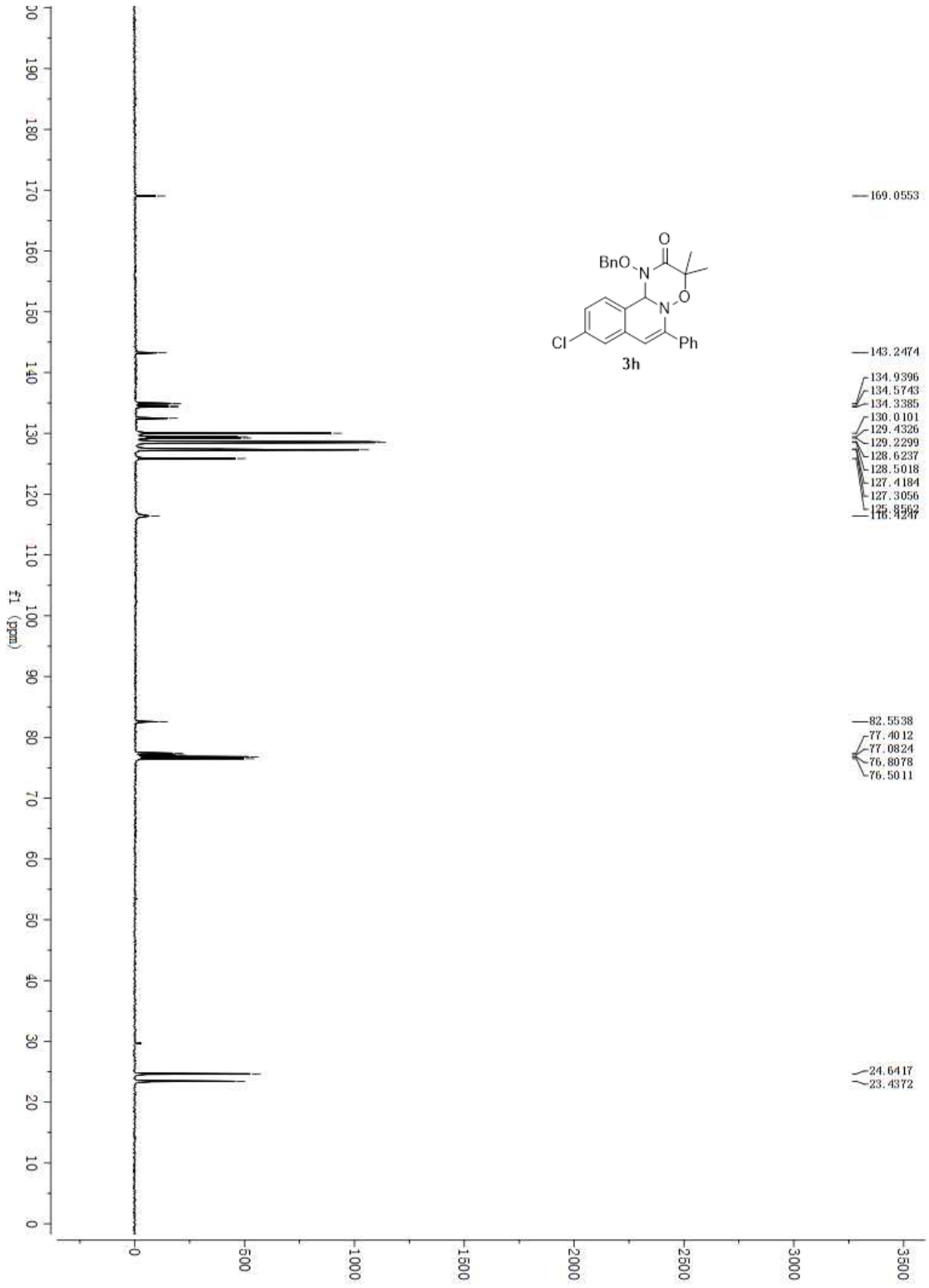
5.1721
5.1478
1.6299
1.1691
0.0003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125.8562
116.4247
82.5538
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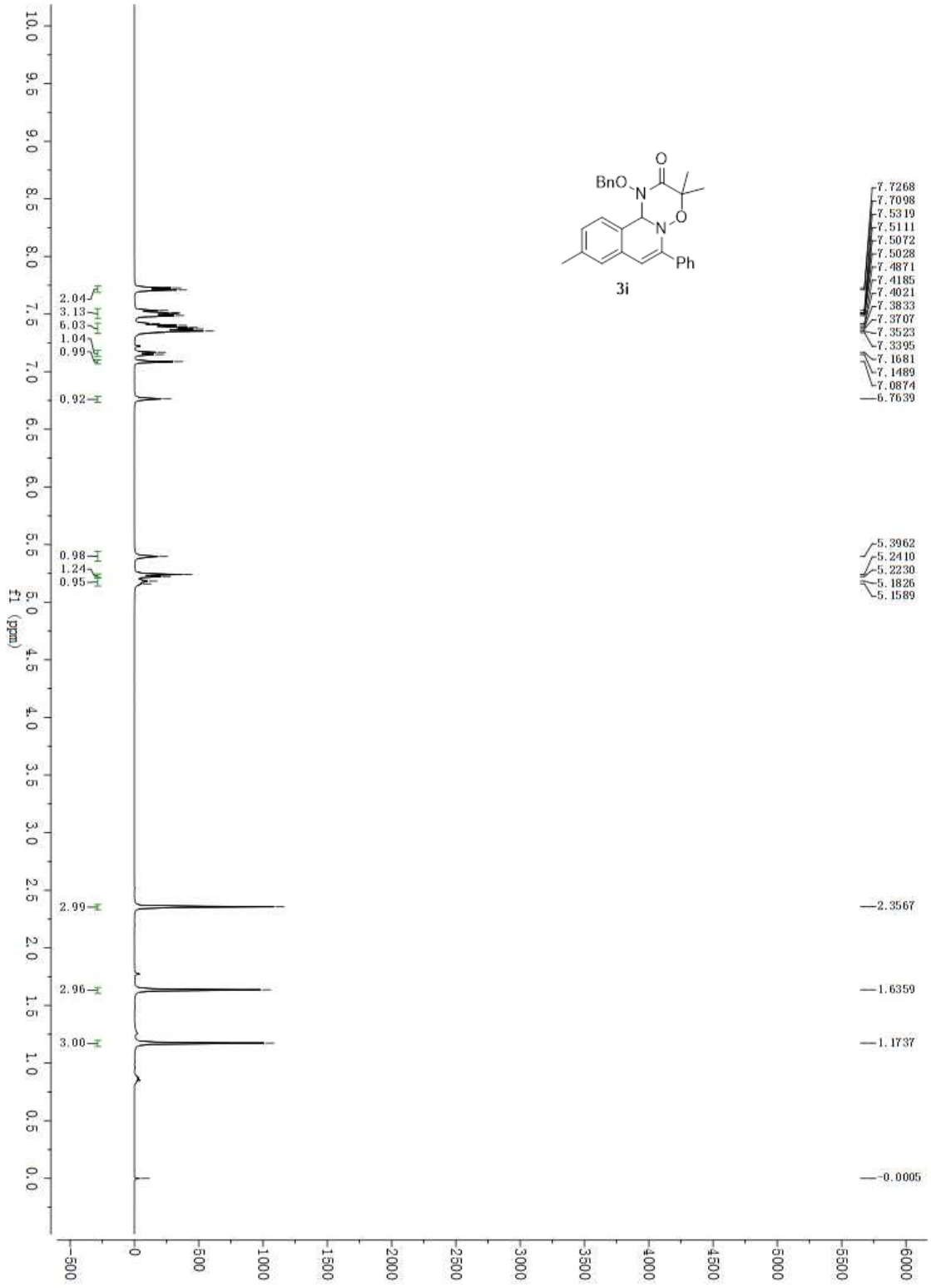
77.0824
76.8078
76.5011
24.6417
23.4372
BnO
N
O
O
N
Cl
Ph
3h
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
0
500
1000
1500
2000
2500
3000
3500


BnO
N
O
N
O
Ph
3i
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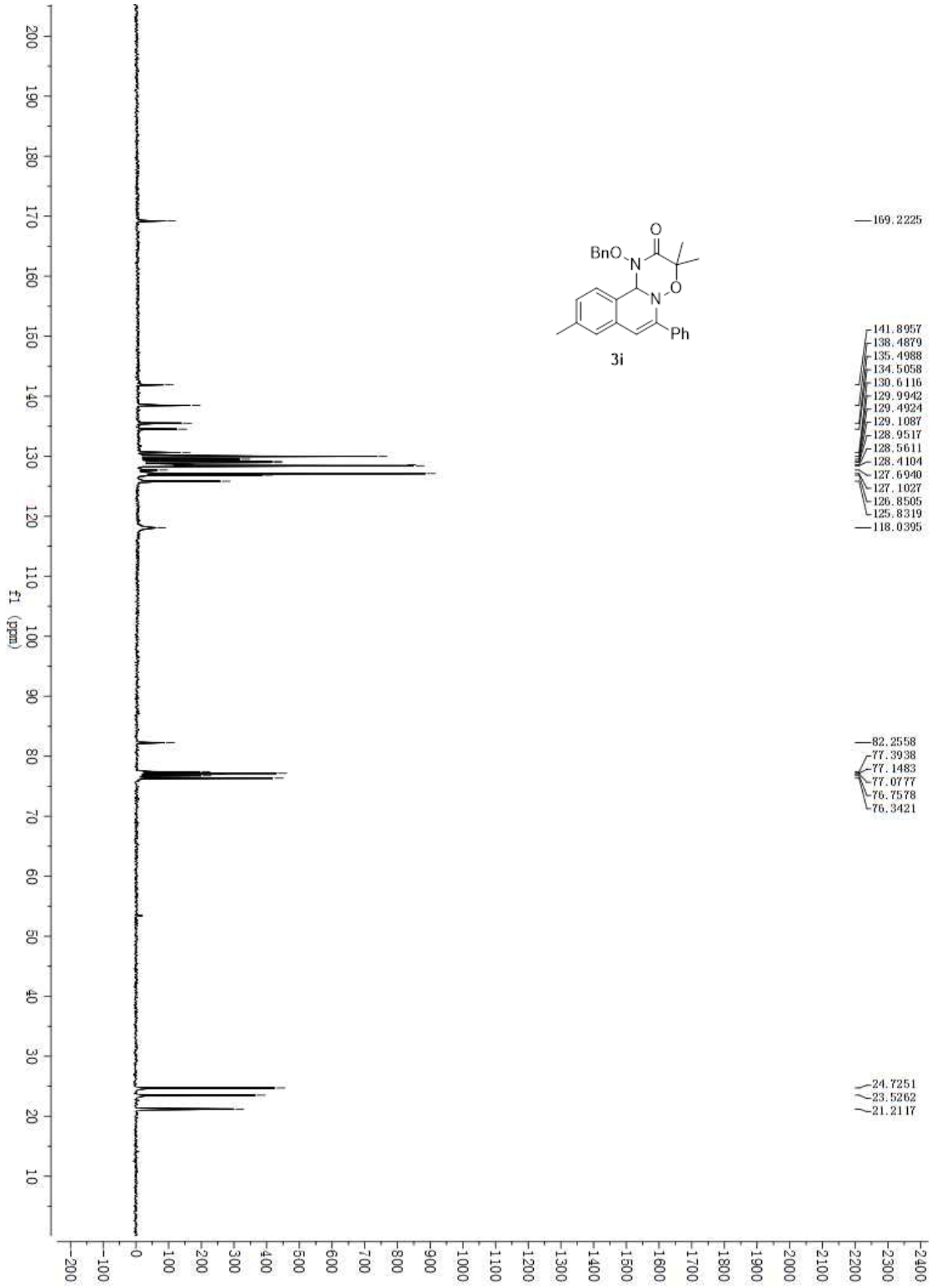
7.5319
7.5111
7.5072
7.5028
7.4871
7.4185
7.4021
7.3833
7.3707
7.3523
7.3395
7.1681
7.1489
7.0874
6.7639
5.3962
5.2410
5.2230
5.1826
5.1589
2.3567
1.6359
1.1737
-0.0005
2.04
3.13
6.03
1.04
0.99
0.92
0.98
1.24
0.95
2.99
2.96
3.00
f1 (ppm)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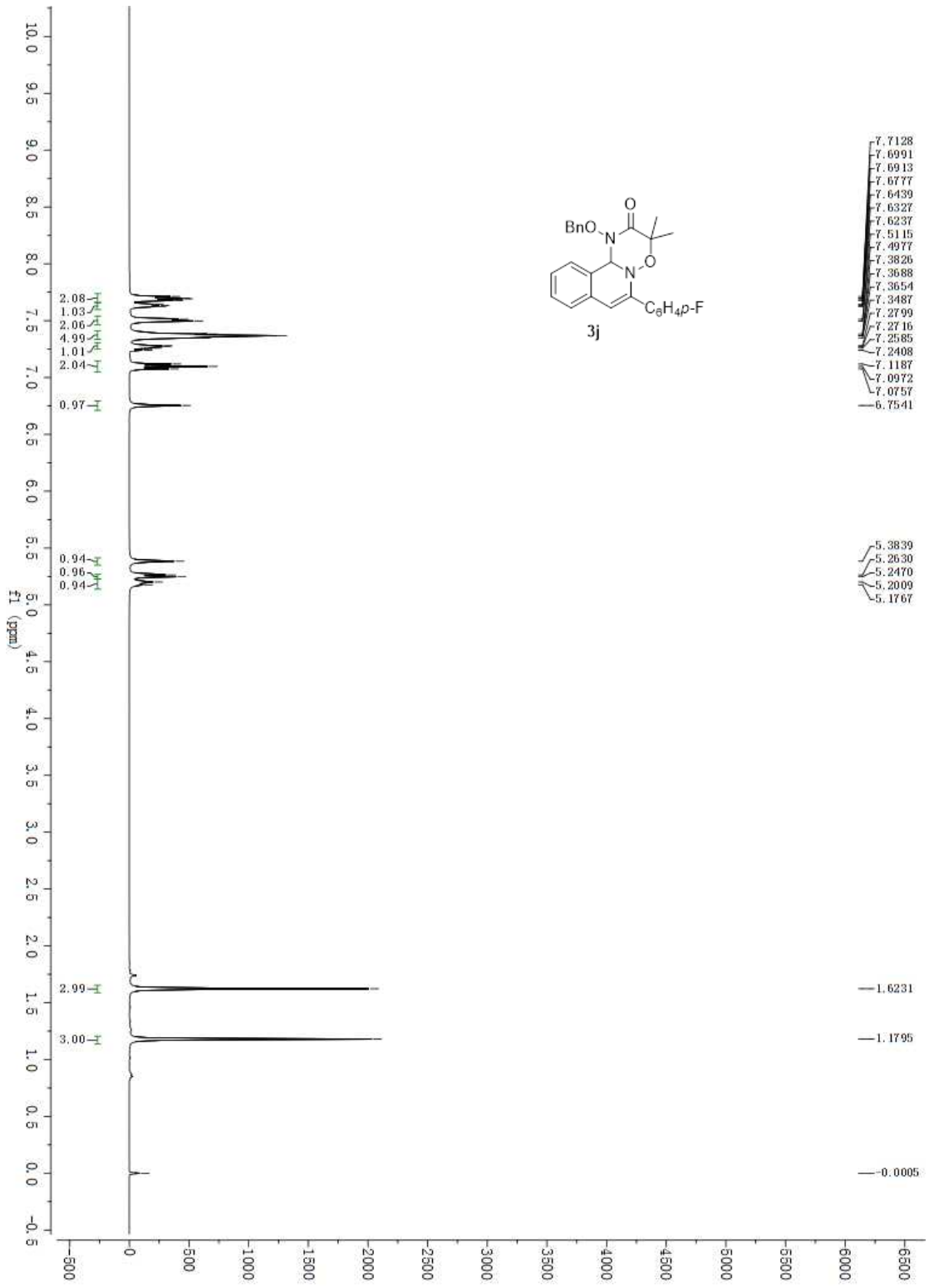
128.4104
127.6940
127.1027
126.8505
125.8319
118.0395
82.2558
77.3938
77.1483
77.0777
76.7578
76.3421
24.7251
23.5262
21.2117
f1 (ppm)
BnO
N
O
N
O
Ph
3i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O
O
N
C6H4p-F
3j
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7.6777
7.6439
7.6327
7.6237
7.5115
7.4977
7.3826
7.3688
7.3654
7.3487
7.2799
7.2716
7.2585
7.2408
7.1187
7.0972
7.0757
6.7541
5.3839
5.2630
5.2470
5.2009
5.1767
1.6231
1.1795
0.0005
2.08
1.03
2.06
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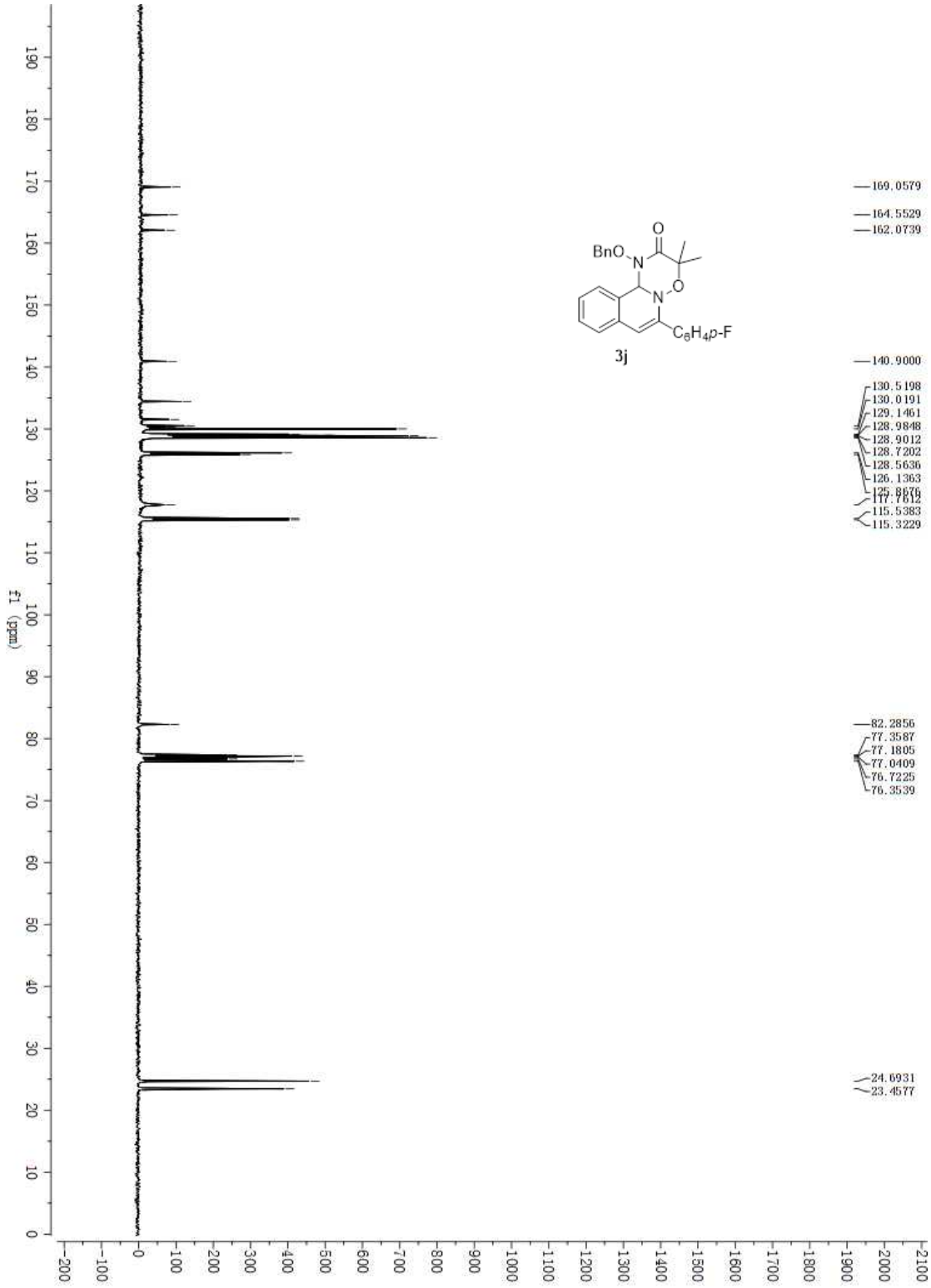
1.01
2.04
0.97
0.94
0.96
0.94
2.99
3.00
f1 (ppm)


BnO
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O
N
O
C6H4p-F
3j
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125.8676
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115.3229
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77.3587
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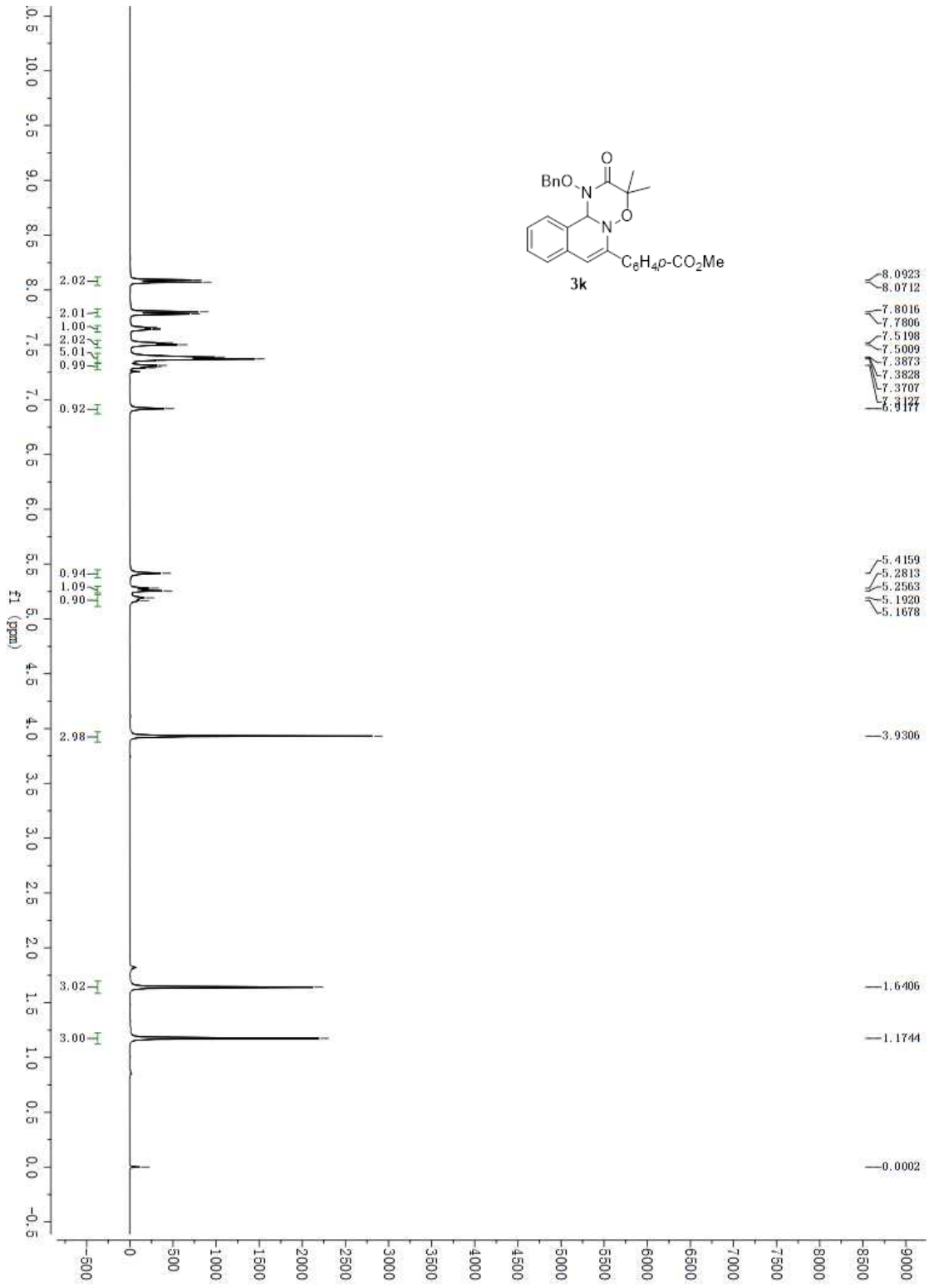
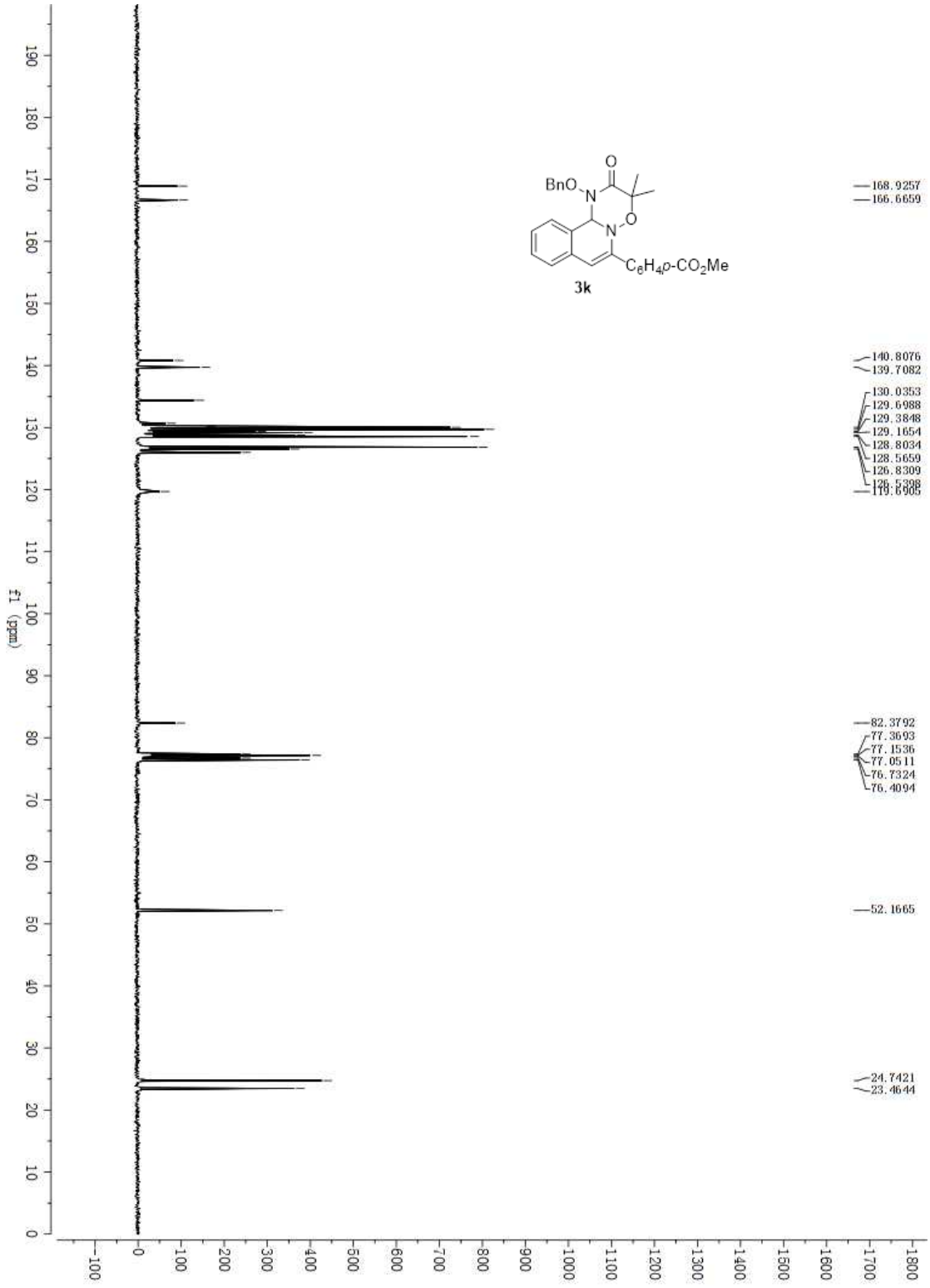
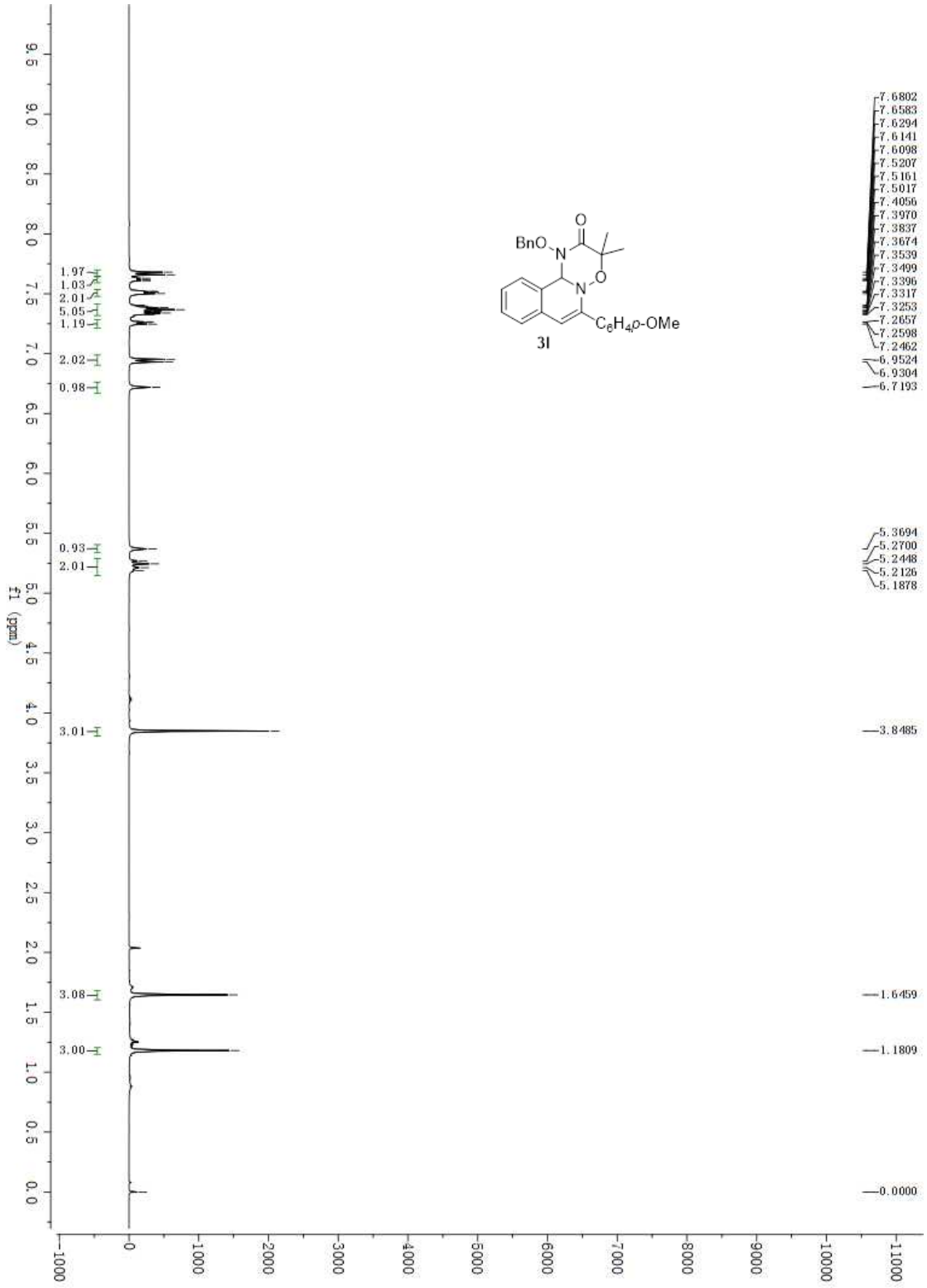
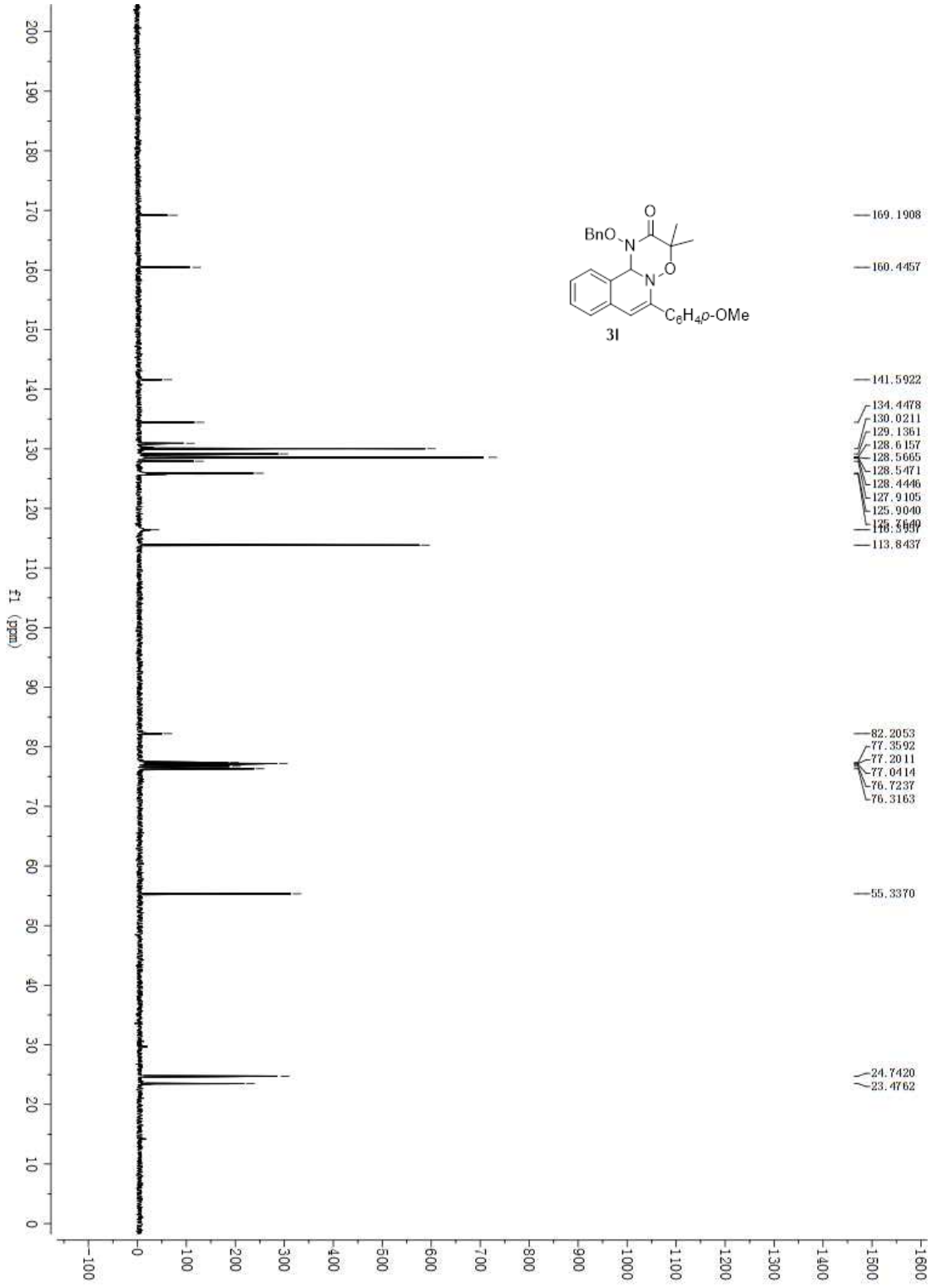
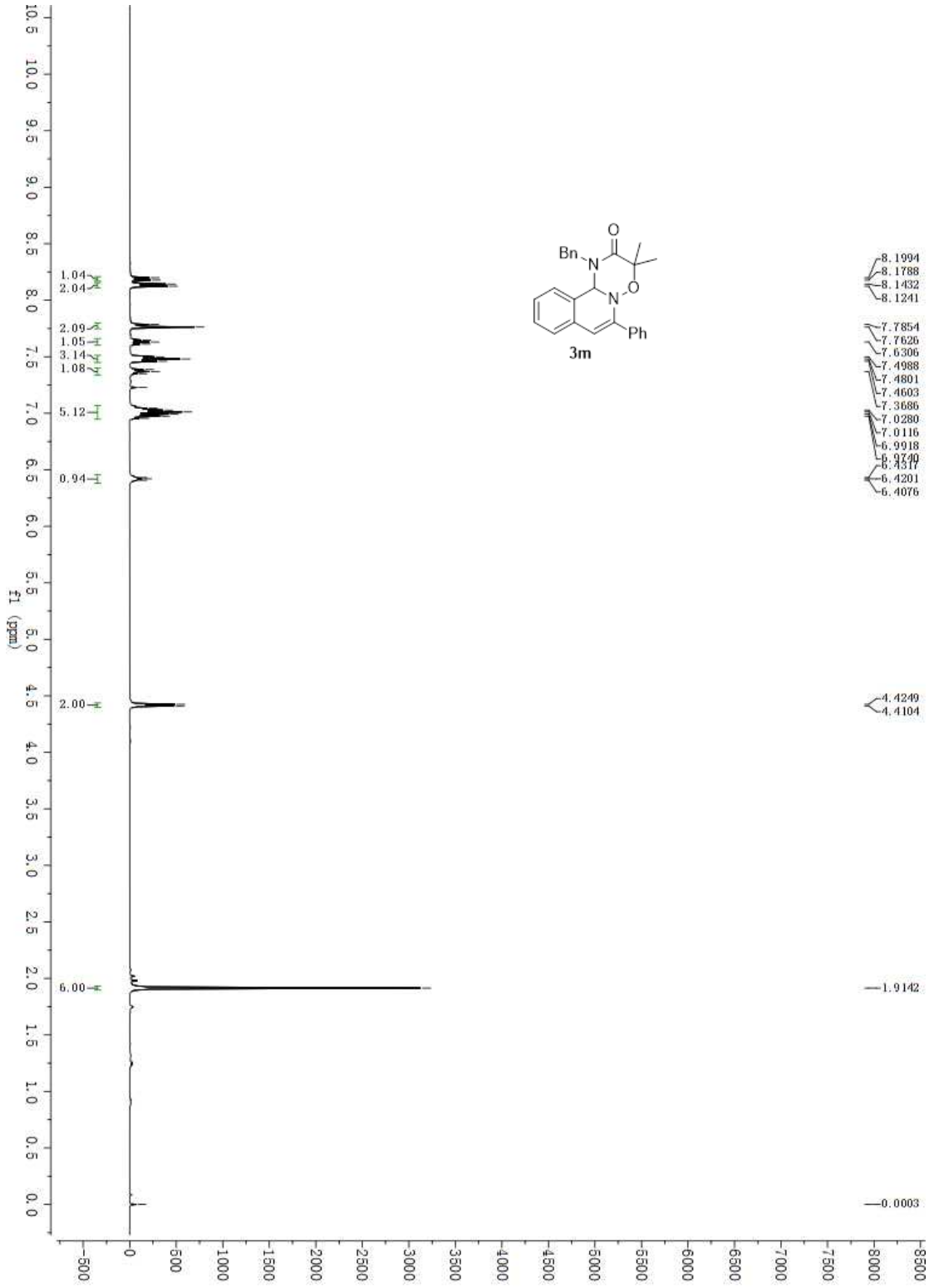
76.7225
76.3539
24.6931
23.4577
f1 (ppm)

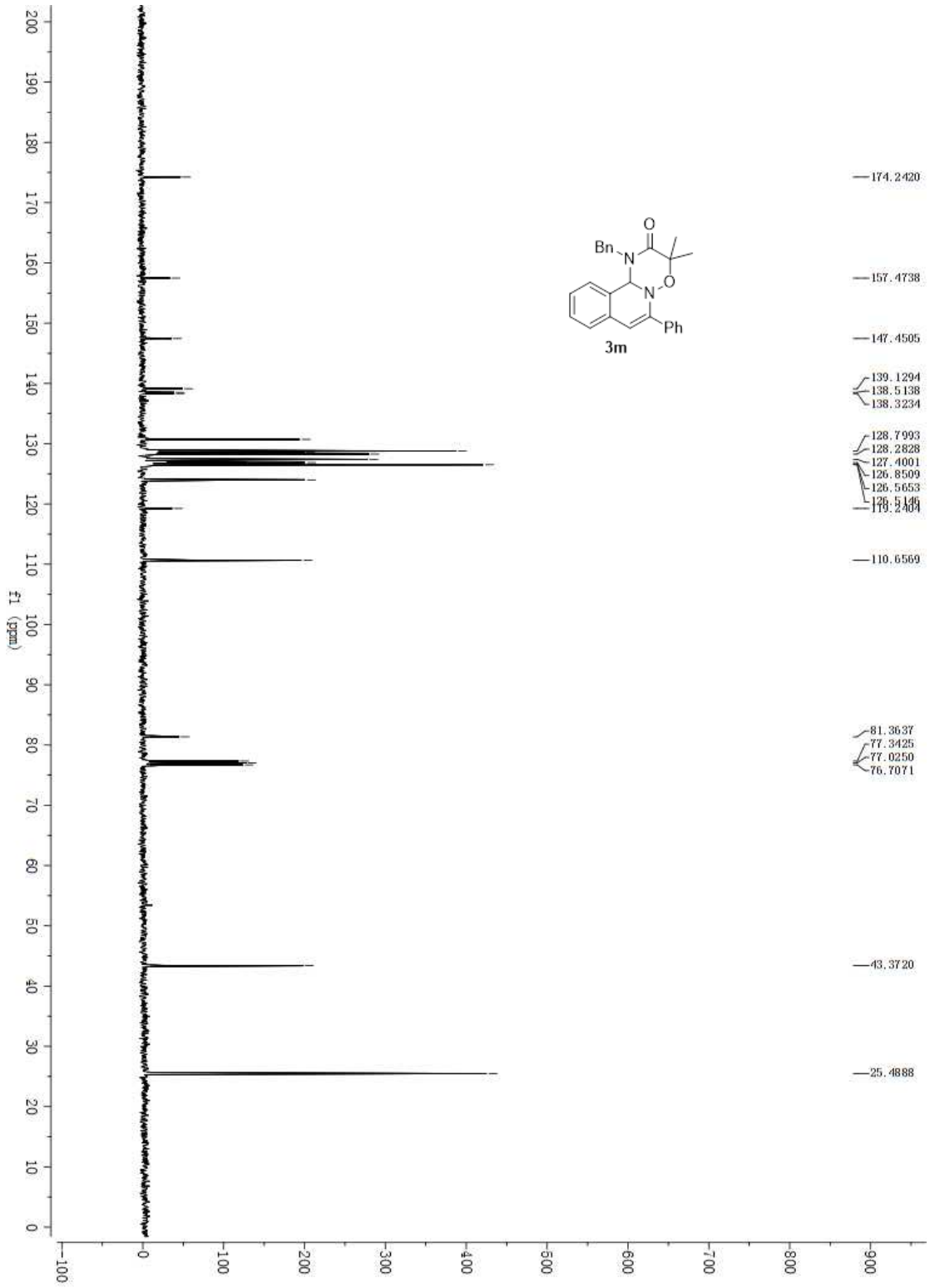

BnO
N
O
N
O
C6H4p-CO2Me
3k
f1 (ppm)
2.02
2.01
1.00
2.02
5.01
0.99
0.92
0.94
1.09
0.90
2.98
3.02
3.00
8.0923
8.0712
7.8016
7.7806
7.5198
7.5009
7.3873
7.3828
7.3707
5.4159
5.2813
5.2563
5.1920
5.1678
3.9306
1.6406
1.1744
0.0002

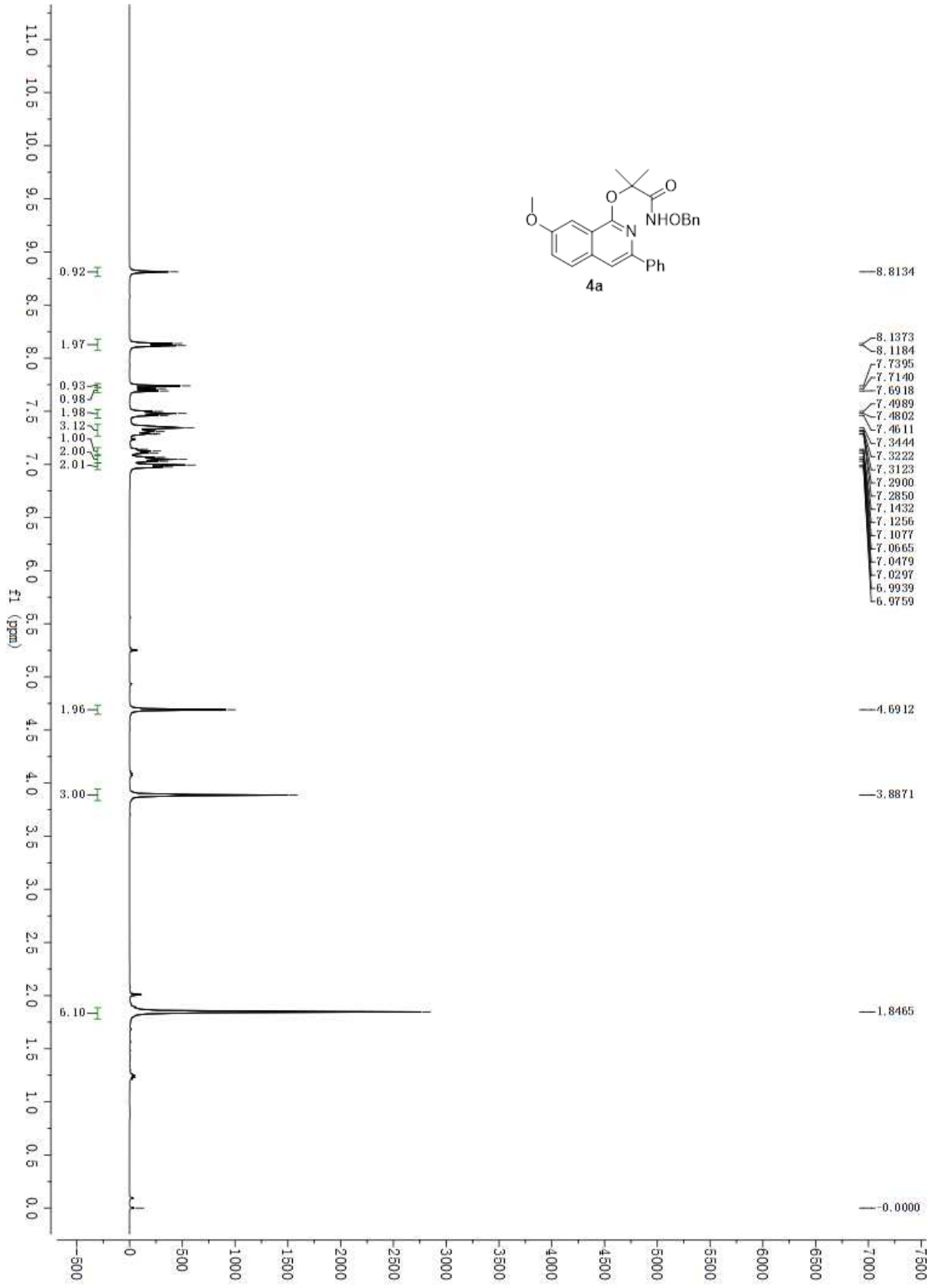

BnO
N
O
N
O
C6H4p-CO2Me
3k
168.9257
166.6659
140.8076
139.7082
130.0353
129.6988
129.3848
129.1654
128.8034
128.5659
126.8309
126.5398
119.6905
82.3792
77.3693
77.1536
77.0511
76.7324
76.4094
52.1665
24.7421
23.4644
f1 (ppm)

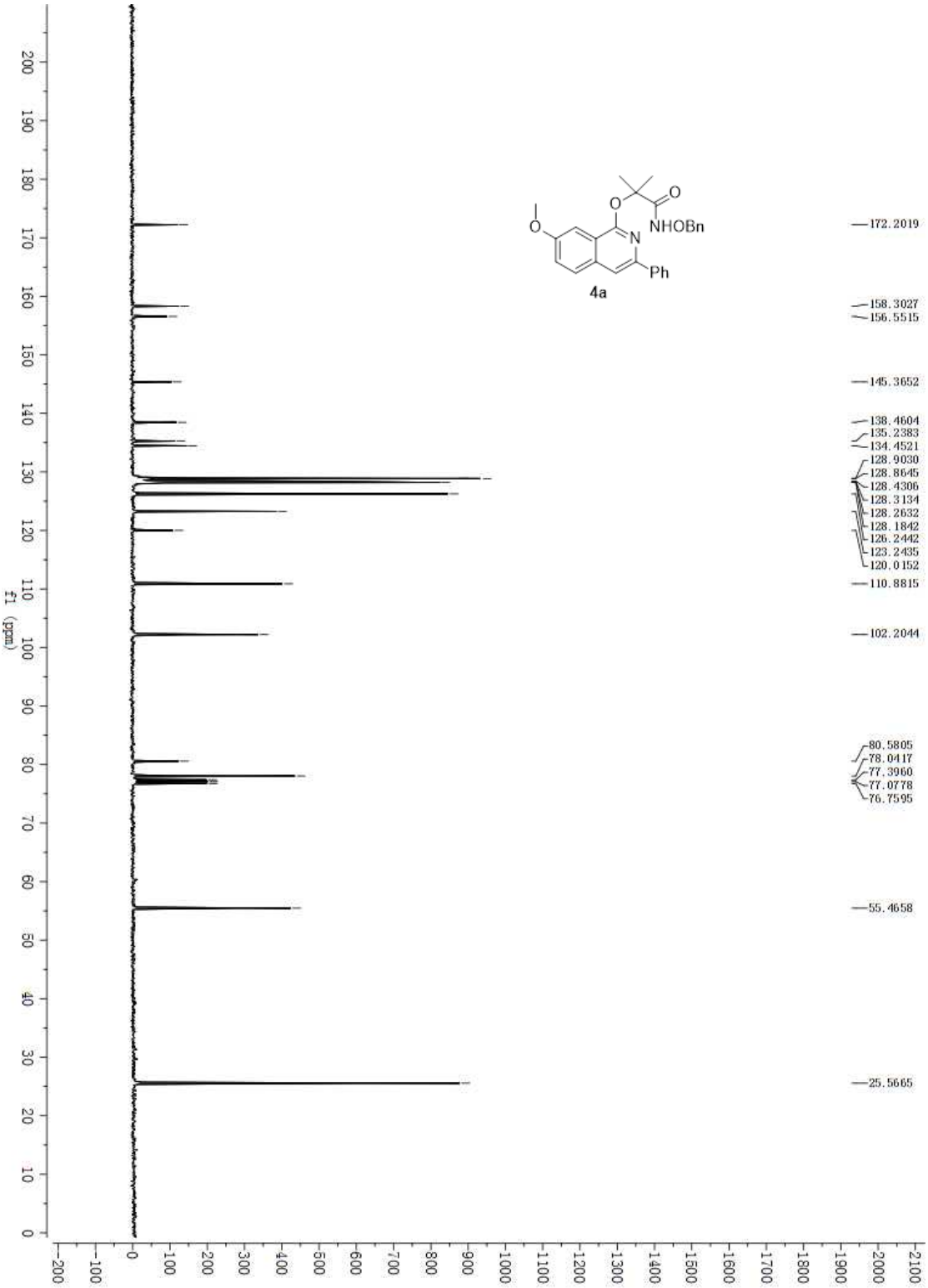

BnO
N
O
N
O
C6H4p-OMe
3l
7.6802
7.6583
7.6294
7.6141
7.6098
7.5207
7.5161
7.5017
7.4056
7.3970
7.3837
7.3674
7.3539
7.3499
7.3396
7.3317
7.3253
7.2657
7.2598
7.2462
6.9524
6.9304
6.7193
5.3694
5.2700
5.2448
5.2126
5.1878
3.8485
1.6459
1.1809
0.0000
1.97
1.03
2.01
5.05
1.19
2.02
0.98
0.93
2.01
3.01
3.08
3.00
f1 (ppm)

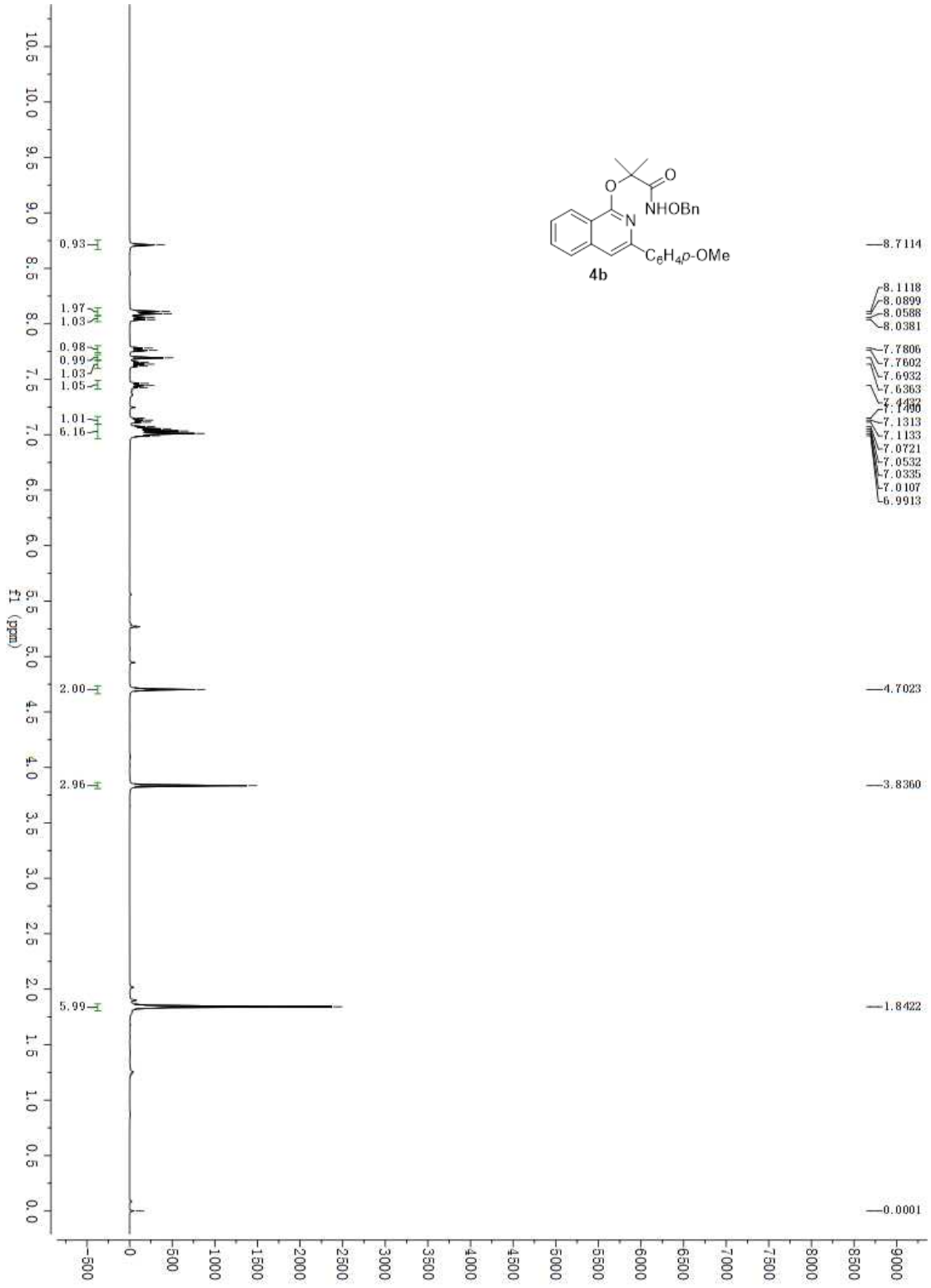

BnO
N
O
O
N
C6H4p-OMe
3l
169.1908
160.4457
141.5922
134.4478
130.0211
129.1361
128.6157
128.5665
128.5471
128.4446
127.9105
125.9040
113.8437
82.2053
77.3592
77.2011
77.0414
76.7237
76.3163
55.3370
24.7420
23.4762
f1 (ppm)

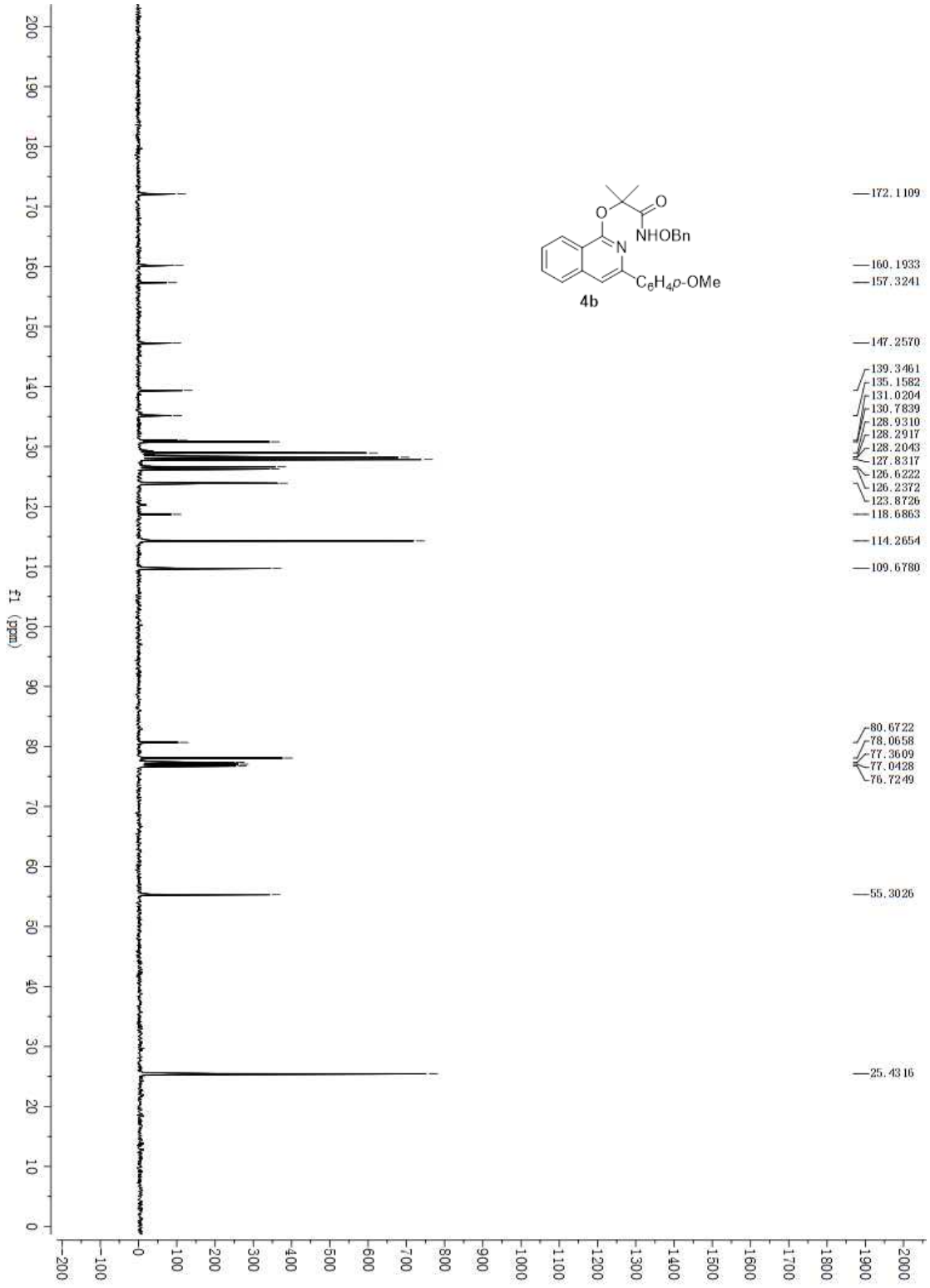

Bn
N
O
N
O
Ph
3m
8.1994
8.1788
8.1432
8.1241
7.7854
7.7626
7.6306
7.4988
7.4801
7.4603
7.3686
7.0280
7.0116
6.9918
6.9740
6.4317
6.4201
6.4076
4.4249
4.4104
1.9142
0.0003
1.04
2.04
2.09
1.05
3.14
1.08
5.12
0.94
2.00
6.00
f1 (ppm)

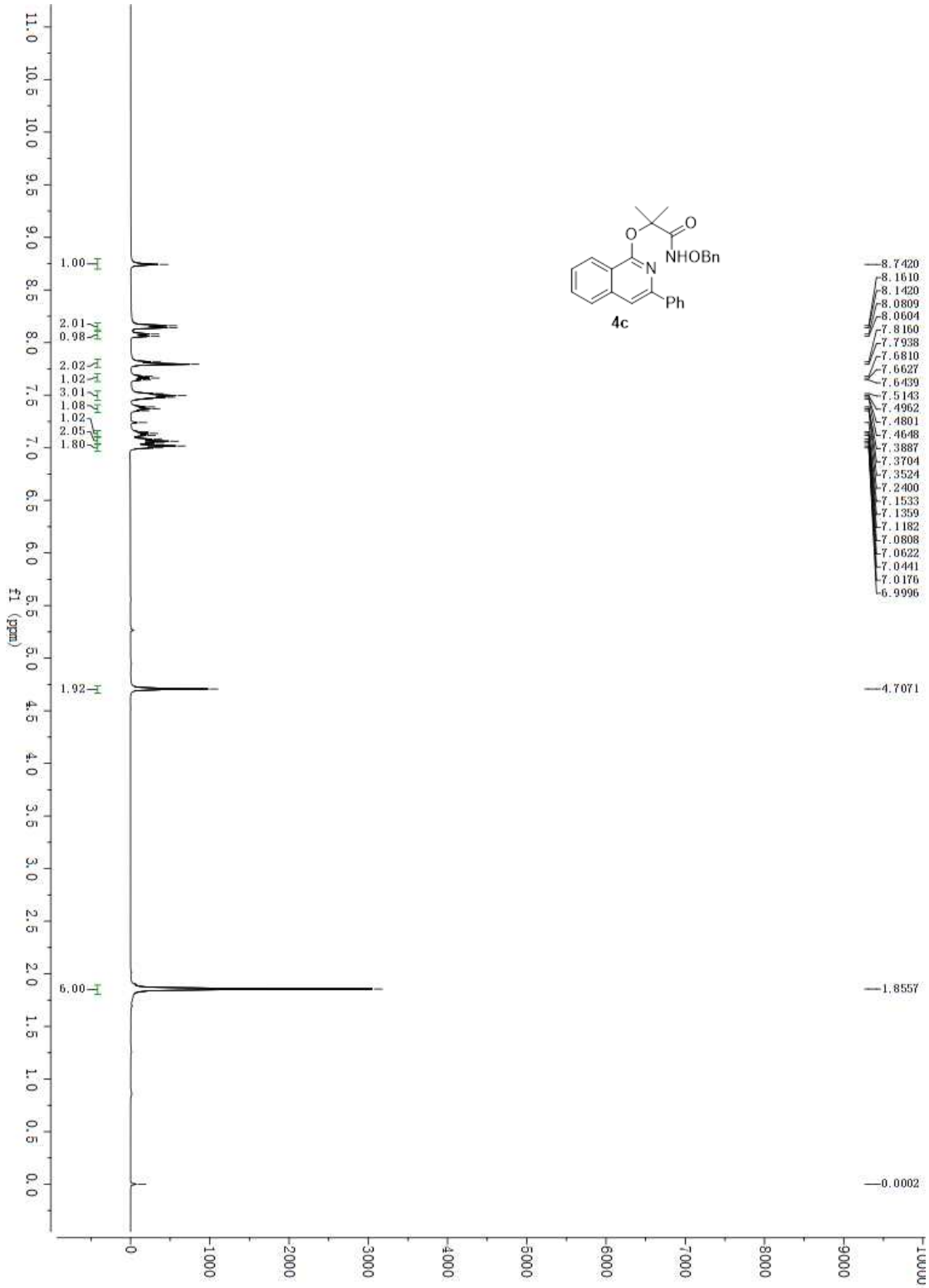

174.2420
157.4738
147.4505
139.1294
138.5138
138.3234
128.7993
128.2828
127.4001
126.8509
126.5653
126.5146
119.2404
110.6569
81.3637
77.3425
77.0250
76.7071
43.3720
25.4888
f1 (ppm)
Bn
N
O
N
O
Ph
3m

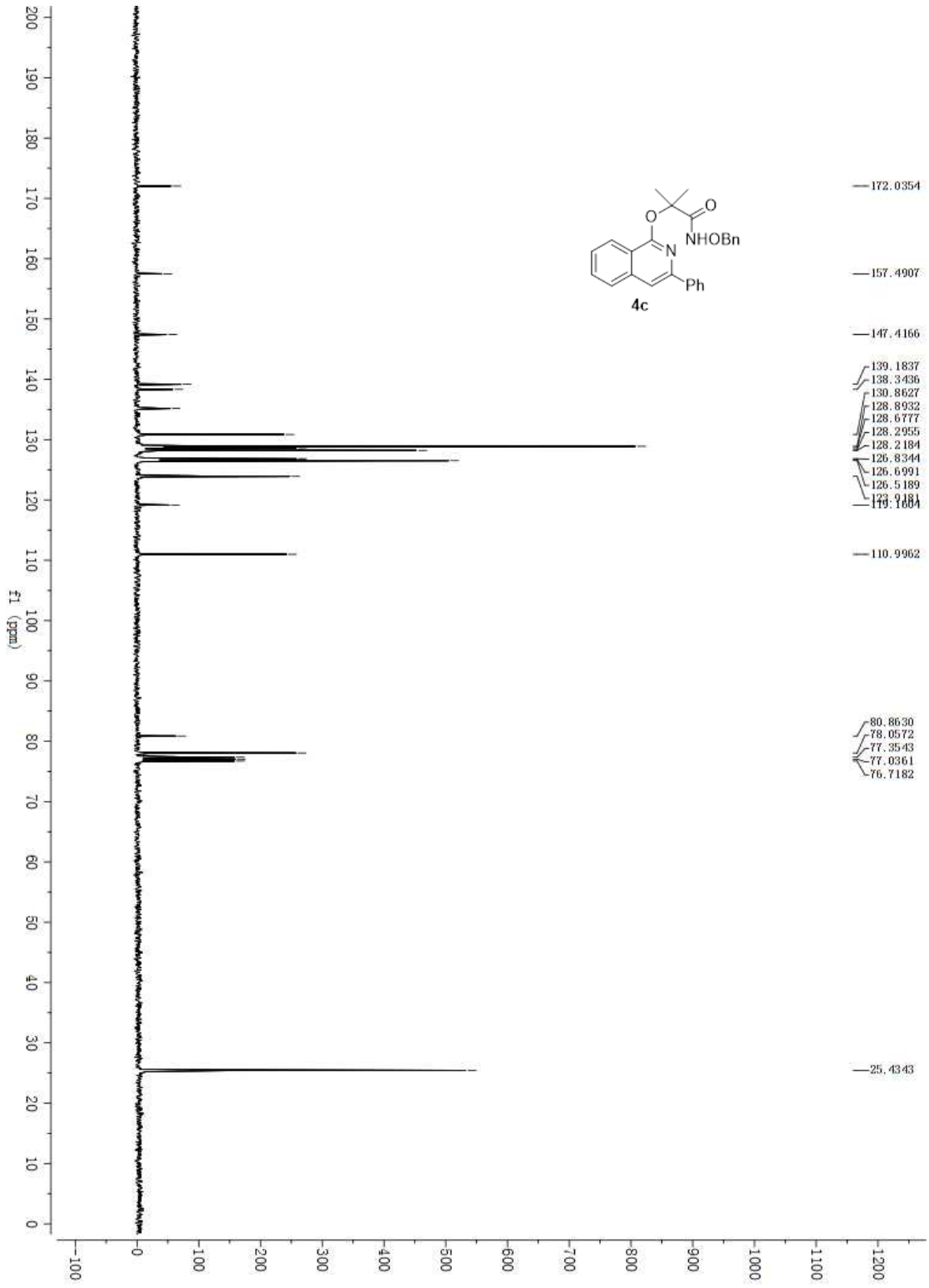

4a
0.92
1.97
0.93
0.98
1.98
3.12
1.00
2.00
2.01
1.96
3.00
6.10
8.8134
8.1373
8.1184
7.7395
7.7140
7.6918
7.4989
7.4802
7.4611
7.3444
7.3222
7.3123
7.2900
7.2850
7.1432
7.1256
7.1077
7.0665
7.0479
7.0297
6.9939
6.9759
4.6912
3.8871
1.8465
0.0000
f1 (ppm)

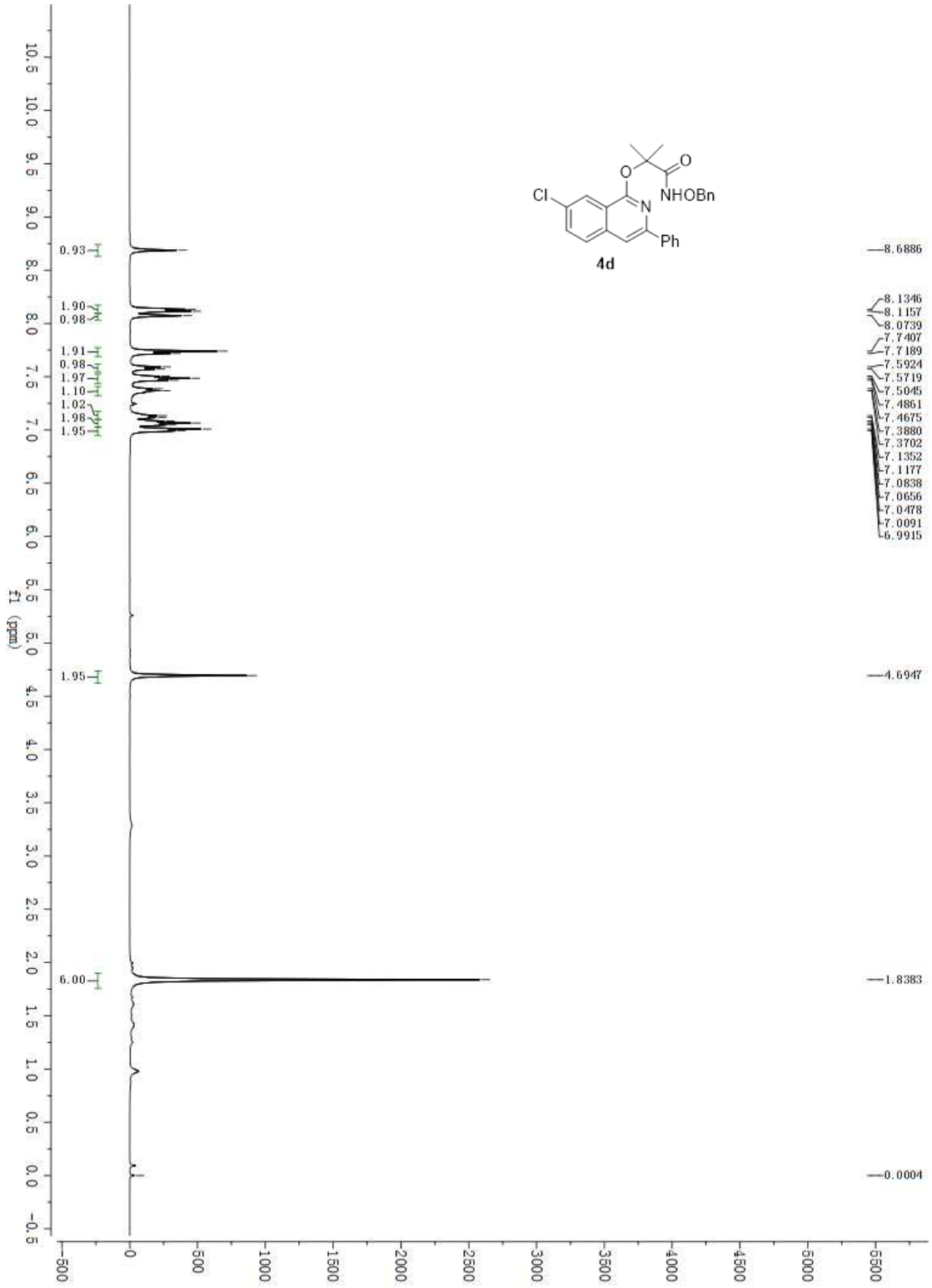

O
O
NHOBn
O
N
Ph
4a
172.2019
158.3027
156.5515
145.3652
138.4604
135.2383
134.4521
128.9030
128.8645
128.4306
128.3134
128.2632
128.1842
126.2442
123.2435
120.0152
110.8815
102.2044
80.5805
78.0417
77.3960
77.0778
76.7595
55.4658
25.5665
f1 (ppm)

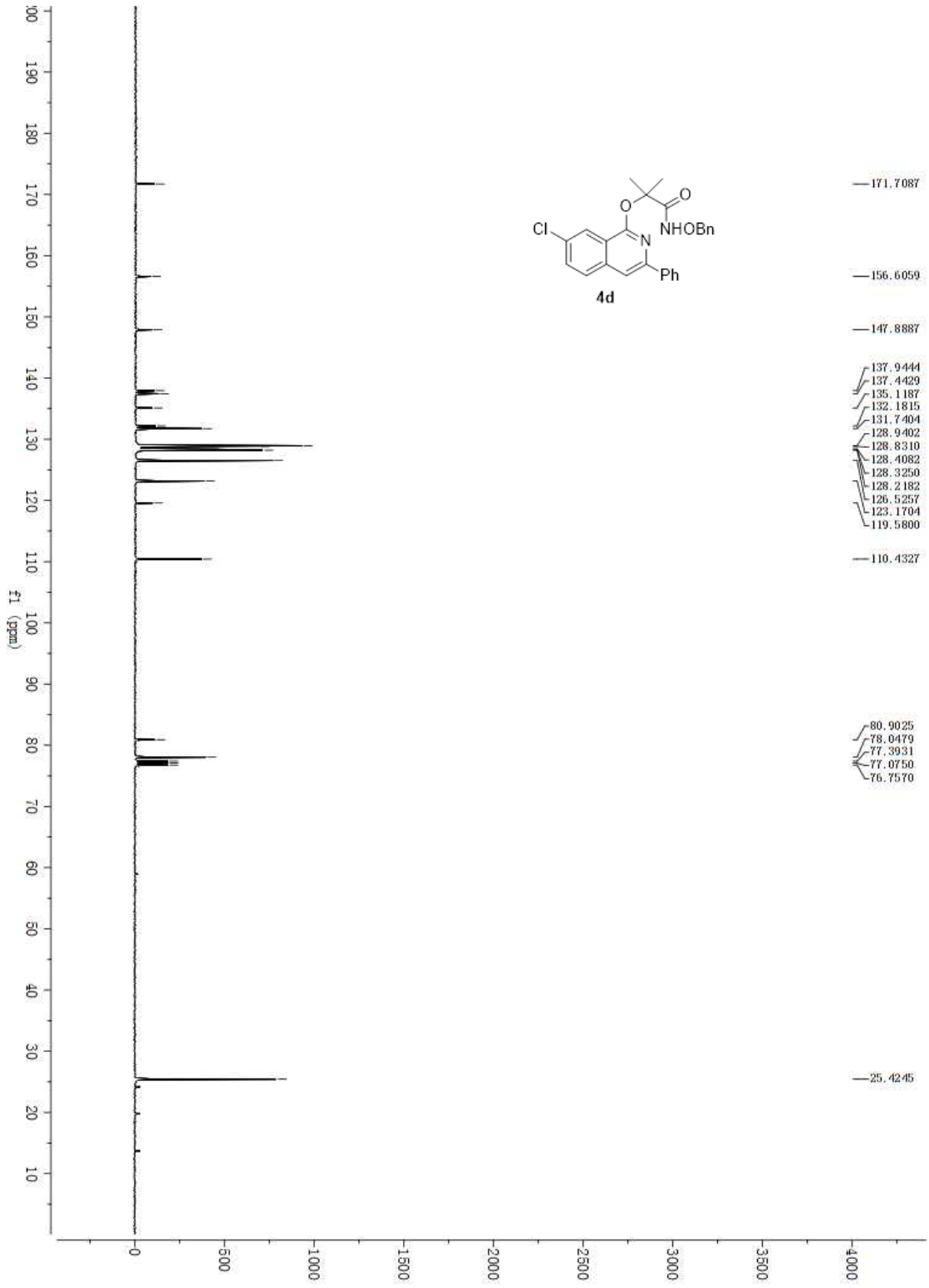

4b
NHOBn
C6H4p-OMe
f1 (ppm)
0.93
1.97
1.03
0.98
0.99
1.03
1.05
1.01
6.16
2.00
2.96
5.99
8.7114
8.1118
8.0899
8.0588
8.0381
7.7806
7.7602
7.6932
7.6363
7.1313
7.1133
7.0721
7.0532
7.0335
7.0107
6.9913
4.7023
3.8360
1.8422
0.0001

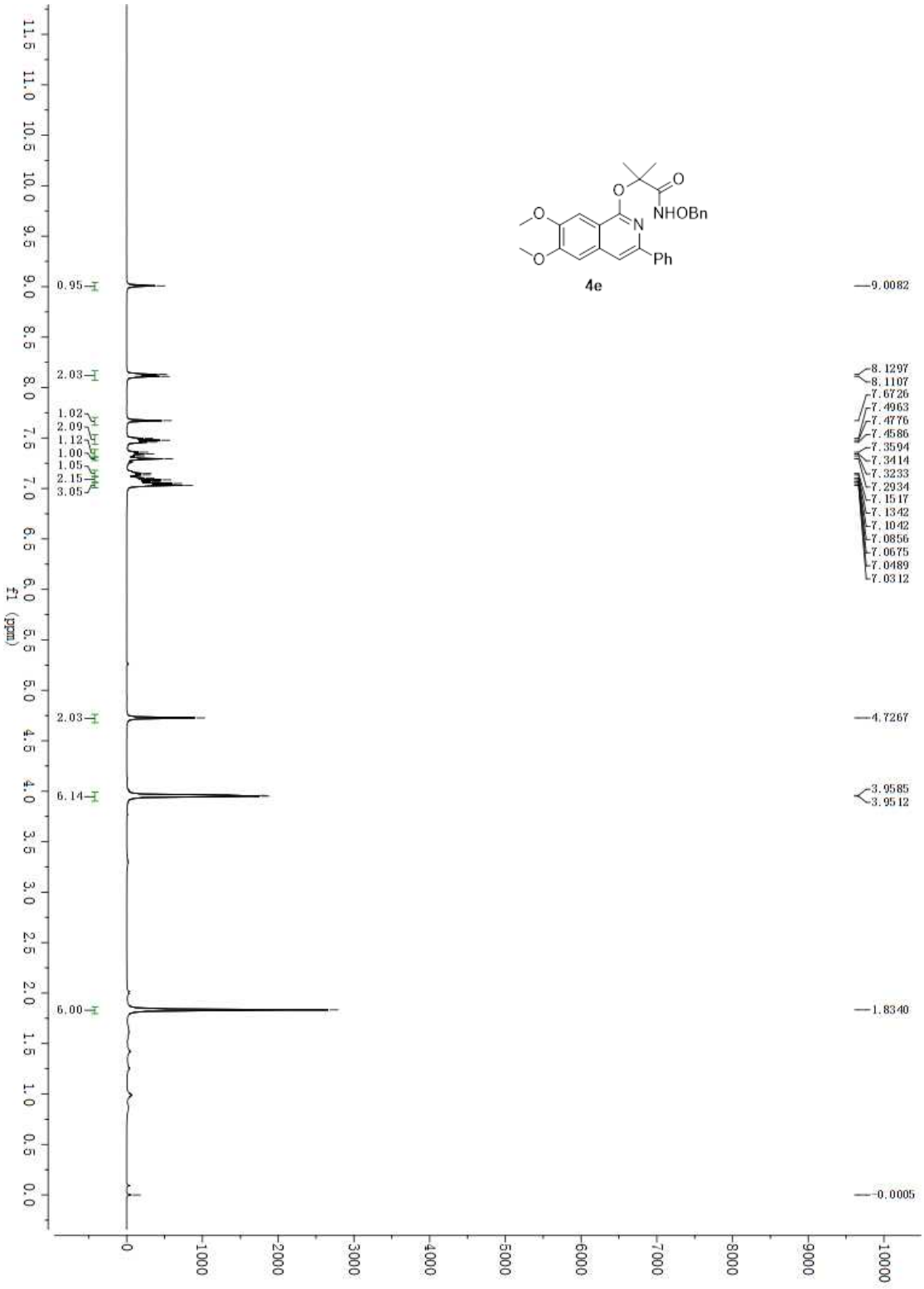

O
O
NHOBn
N
C6H4p-OMe
4b
172.1109
160.1933
157.3241
147.2570
139.3461
135.1582
131.0204
130.7839
128.9310
128.2917
128.2043
127.8317
126.6222
126.2372
123.8726
118.6863
114.2654
109.6780
80.6722
78.0658
77.3609
77.0428
76.7249
55.3026
25.4316
f1 (ppm)

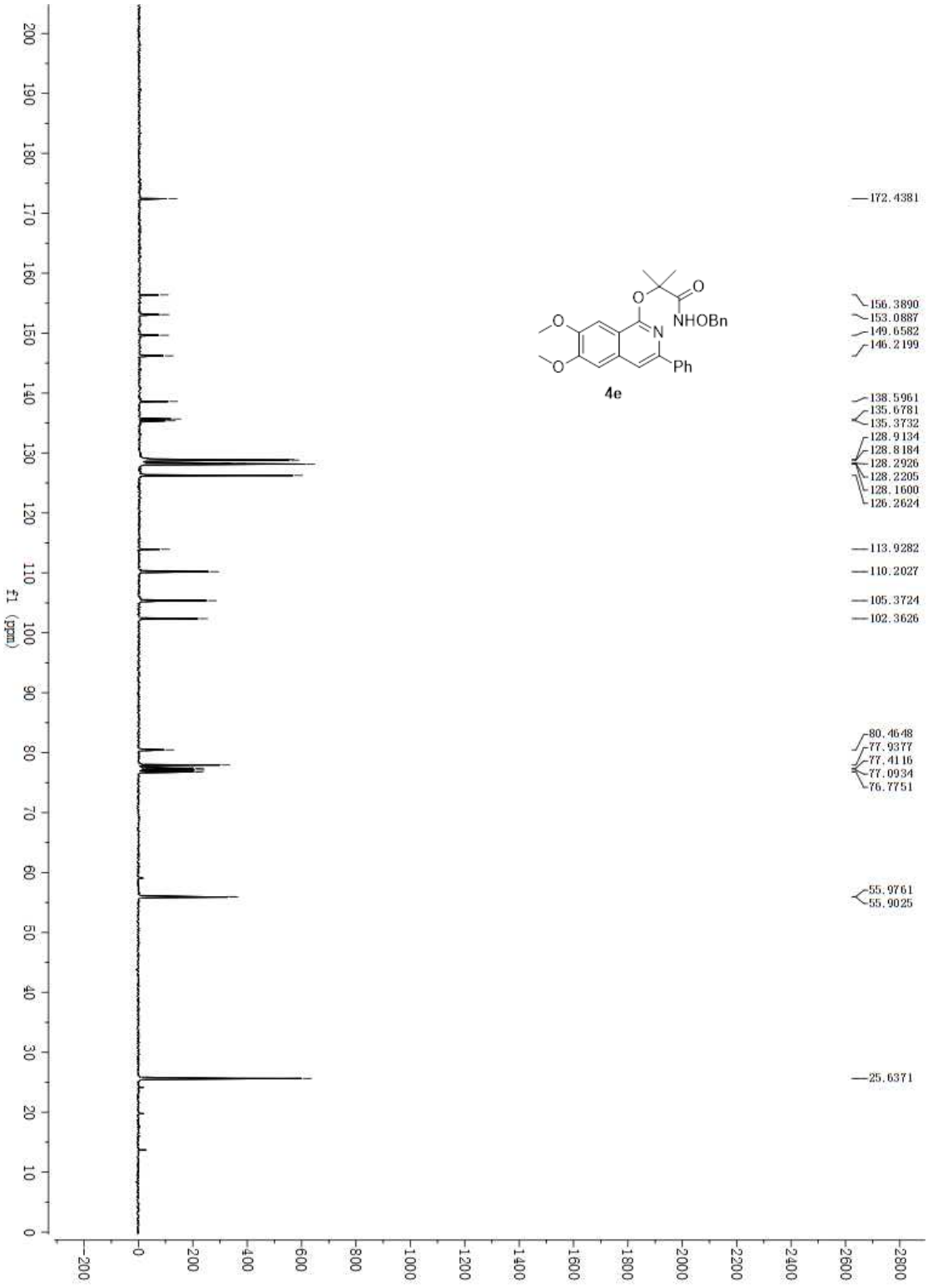

4c
NHOBn
Ph
f1 (ppm)
1.00
2.01
0.98
2.02
1.02
3.01
1.08
1.02
2.05
1.80
1.92
6.00
8.7420
8.1610
8.1420
8.0809
8.0604
7.8160
7.7938
7.6810
7.6627
7.6439
7.5143
7.4962
7.4801
7.4648
7.3887
7.3704
7.3524
7.2400
7.1533
7.1359
7.1182
7.0808
7.0622
7.0441
7.0176
6.9996
4.7071
1.8557
0.0002

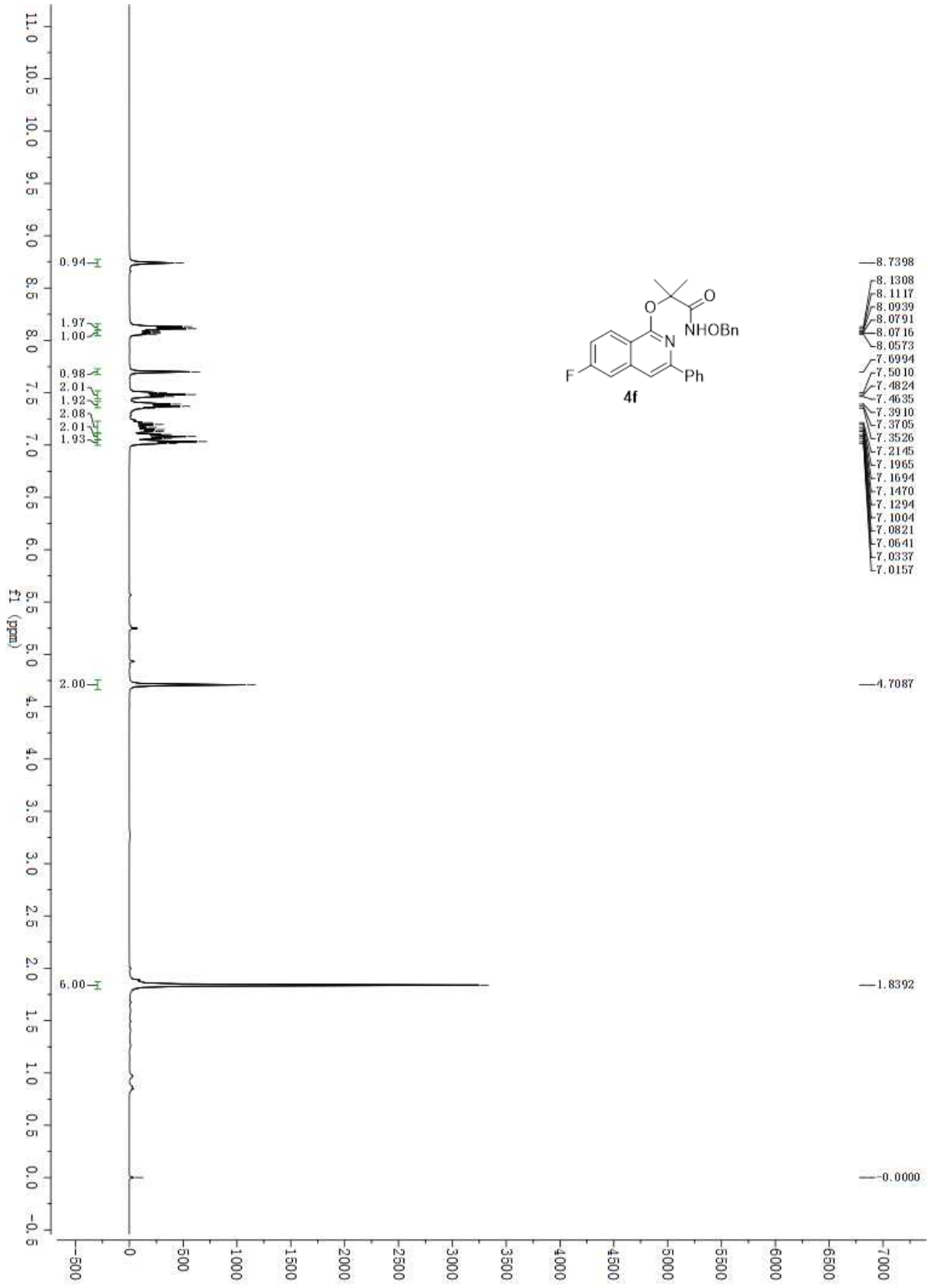

172.0354
157.4907
147.4166
139.1837
138.3436
130.8627
128.8932
128.6777
128.2955
128.2184
126.8344
126.6991
126.5189
123.9181
119.1604
110.9962
80.8630
78.0572
77.3543
77.0361
76.7182
25.4343
f1 (ppm)
NHOBn
Ph
4c

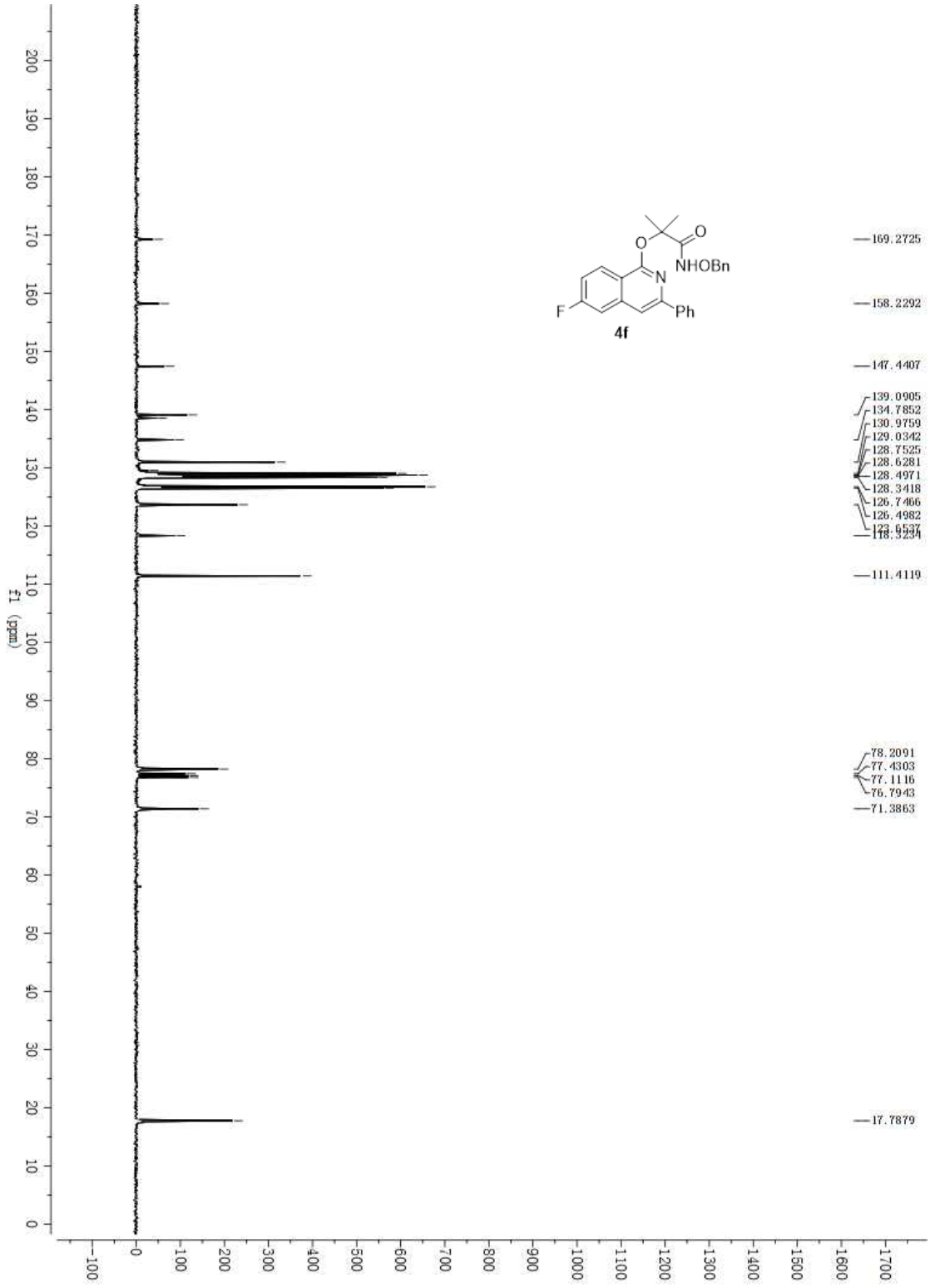

Cl
O
O
NHOBn
N
Ph
4d
0.93
1.90
0.98
1.91
0.98
1.97
1.10
1.02
1.98
1.95
1.95
6.00
8.6886
8.1346
8.1157
8.0739
7.7407
7.7189
7.5924
7.5719
7.5045
7.4861
7.4675
7.3880
7.3702
7.1352
7.1177
7.0838
7.0656
7.0478
7.0091
6.9915
4.6947
1.8383
0.0004
f1 (ppm)

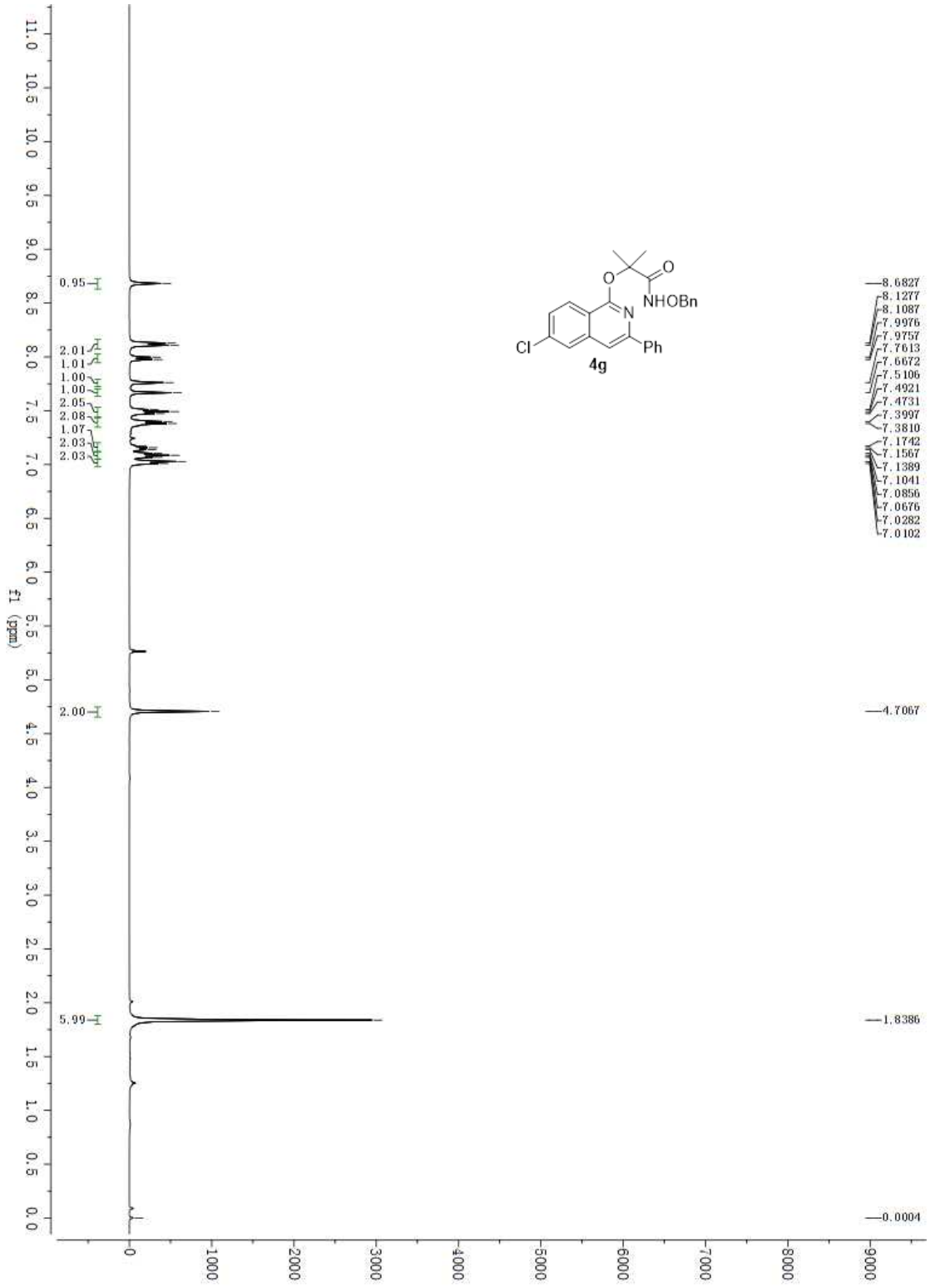

Cl
O
O
NHOBn
N
Ph
4d
171.7087
156.6059
147.8887
137.9444
137.4429
135.1187
132.1815
131.7404
128.9402
128.8310
128.4082
128.3250
128.2182
126.5257
123.1704
119.5800
110.4327
80.9025
78.0479
77.3931
77.0750
76.7570
25.4245
f1 (ppm)

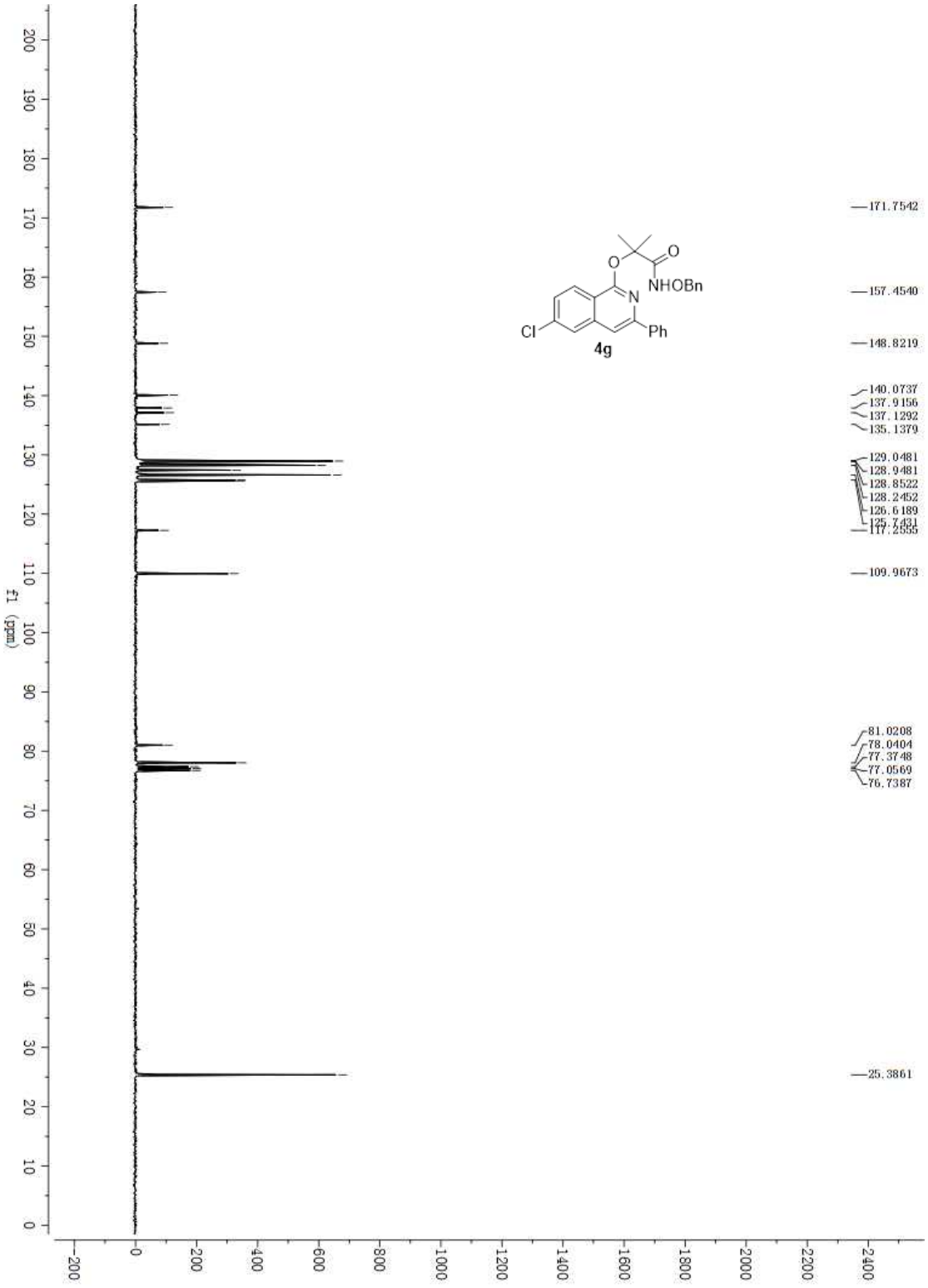

4e
NHOBn
Ph
f1 (ppm)
0.95
2.03
1.02
2.09
1.12
1.00
1.05
2.15
3.05
2.03
6.14
6.00
9.0082
8.1297
8.1107
7.6726
7.4963
7.4776
7.4586
7.3594
7.3414
7.3233
7.2934
7.1517
7.1342
7.1042
7.0856
7.0675
7.0489
7.0312
4.7267
3.9585
3.9512
1.8340
0.0005

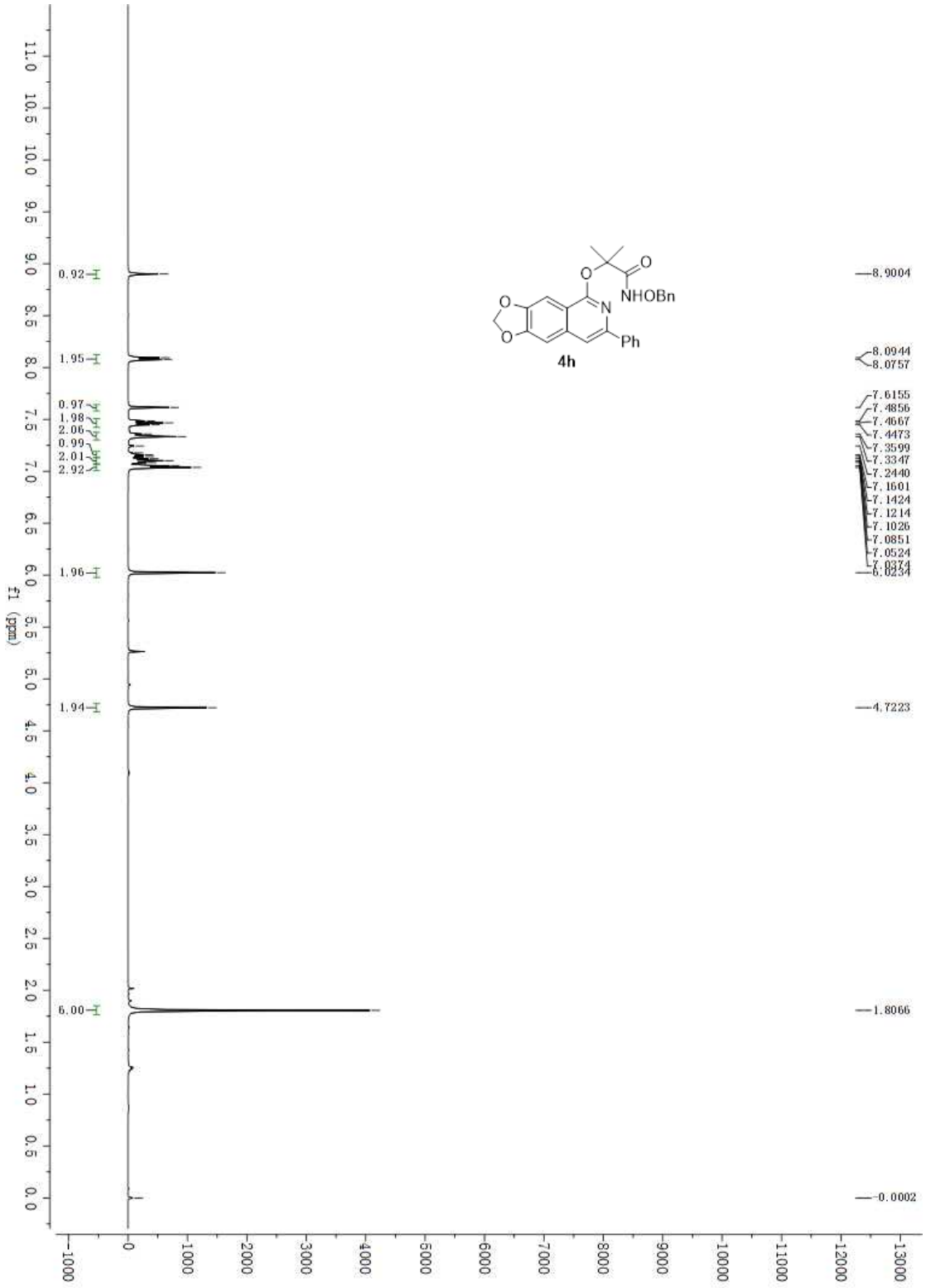

172.4381
156.3890
153.0887
149.6582
146.2199
138.5961
135.6781
135.3732
128.9134
128.8184
128.2926
128.2205
128.1600
126.2624
113.9282
110.2027
105.3724
102.3626
80.4648
77.9377
77.4116
77.0934
76.7751
55.9761
55.9025
25.6371
f1 (ppm)
NHOBn
Ph
4e

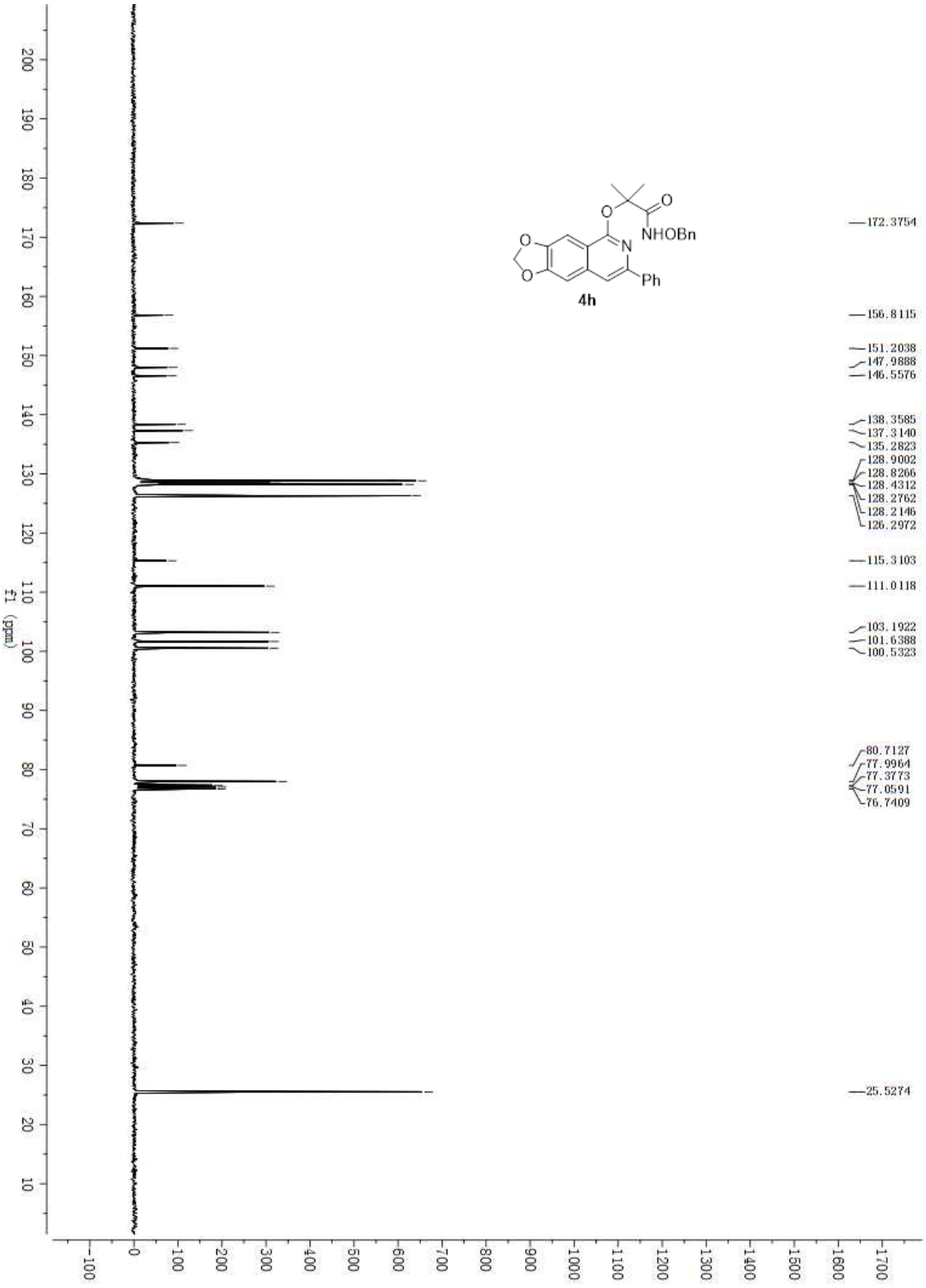

0.94
1.97
1.00
0.98
2.01
1.92
2.08
2.01
1.93
2.00
6.00
f1 (ppm)
8.7398
8.1308
8.1117
8.0939
8.0791
8.0716
8.0573
7.6994
7.5010
7.4824
7.4635
7.3910
7.3705
7.3526
7.2145
7.1965
7.1694
7.1470
7.1294
7.1004
7.0821
7.0641
7.0337
7.0157
4.7087
1.8392
0.0000
O
O
NHOBn
N
F
Ph
4f

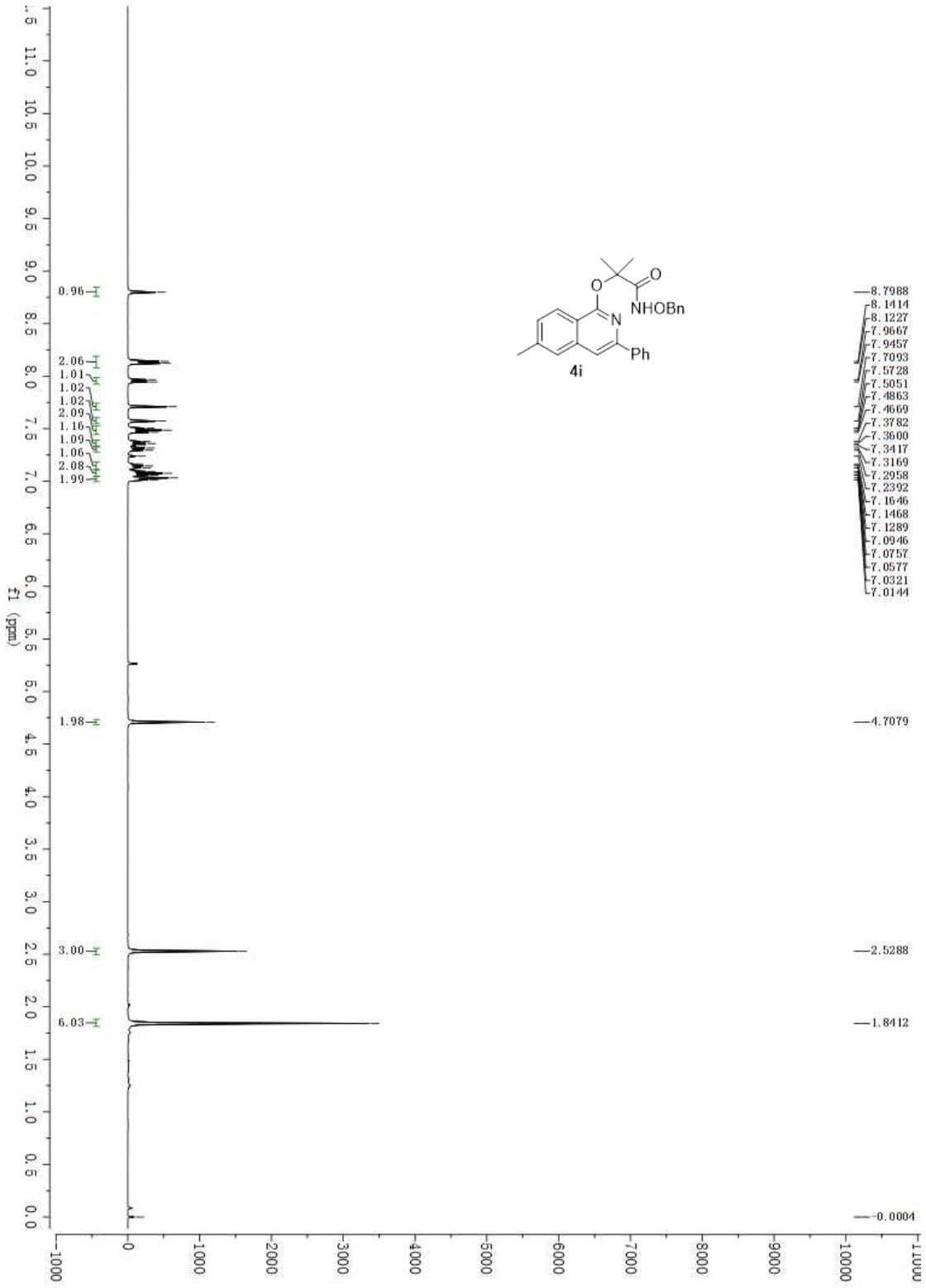

O
NHOBn
N
F
Ph
4f
169.2725
158.2292
147.4407
139.0905
134.7852
130.9759
129.0342
128.7525
128.6281
128.4971
128.3418
126.7466
126.4982
123.6537
118.3234
111.4119
78.2091
77.4303
77.1116
76.7943
71.3863
17.7879
f1 (ppm)

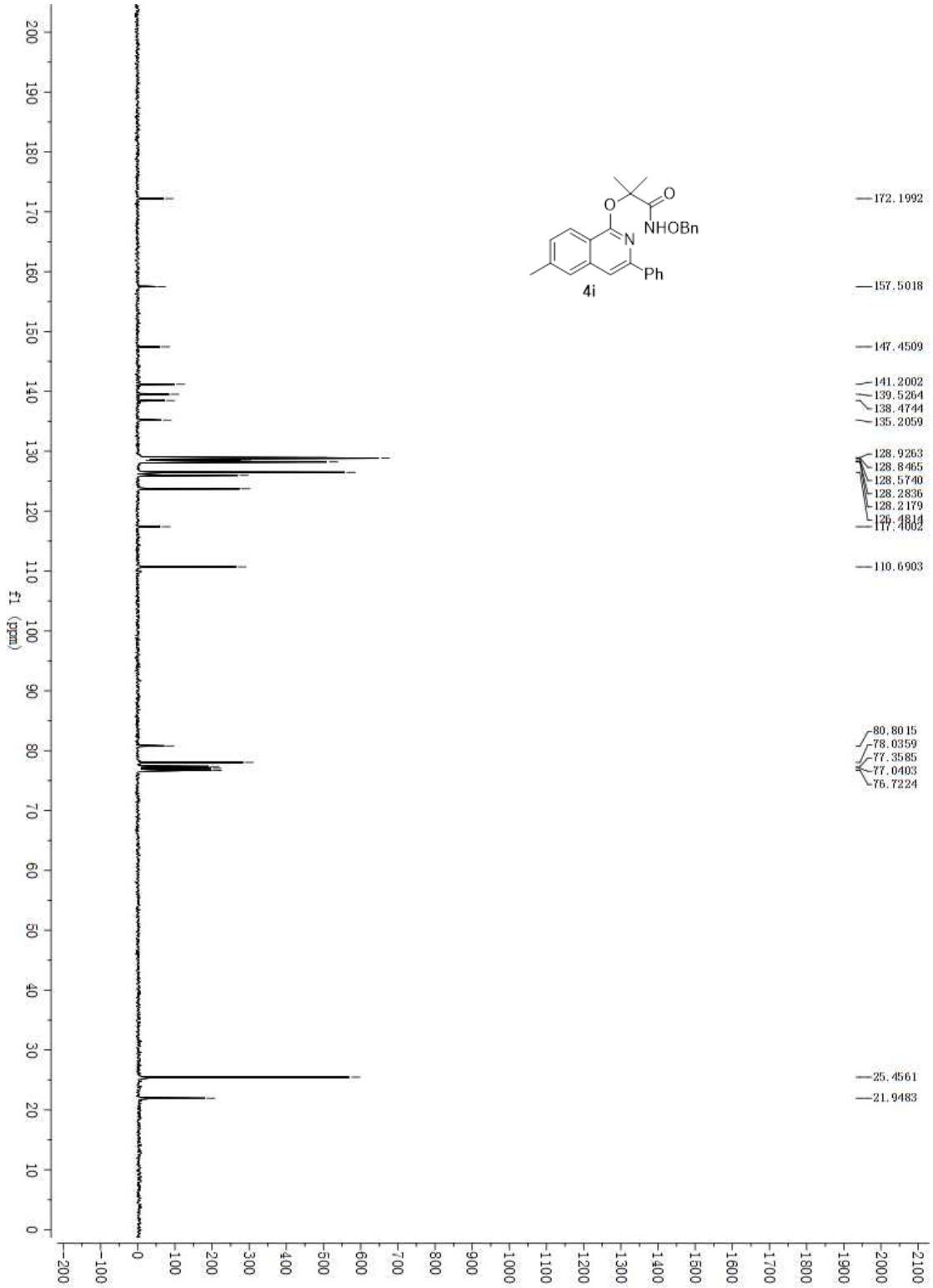

O
O
NHOBn
N
Cl
Ph
4g
f1 (ppm)
0.95
2.01
1.01
1.00
1.00
2.05
2.08
1.07
2.03
2.03
2.00
5.99
8.6827
8.1277
8.1087
7.9976
7.9757
7.7613
7.6672
7.5106
7.4921
7.4731
7.3997
7.3810
7.1742
7.1567
7.1389
7.1041
7.0856
7.0676
7.0282
7.0102
4.7067
1.8386
0.0004

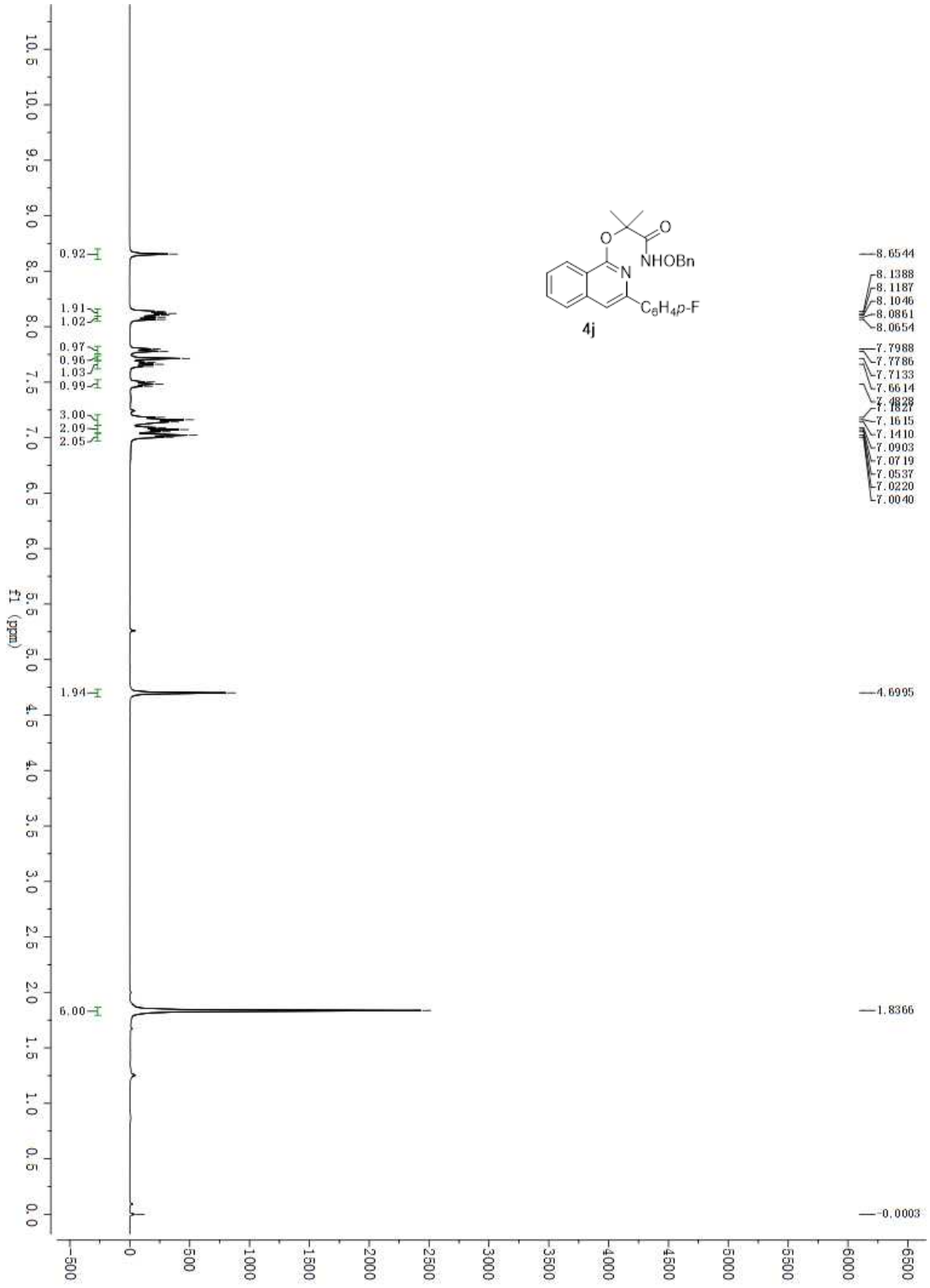

171.7542
157.4540
148.8219
140.0737
137.9156
137.1292
135.1379
129.0481
128.9481
128.8522
128.2452
126.6189
125.7431
117.2555
109.9673
81.0208
78.0404
77.3748
77.0569
76.7387
25.3861
f1 (ppm)
O
O
NHOBn
N
Cl
Ph
4g

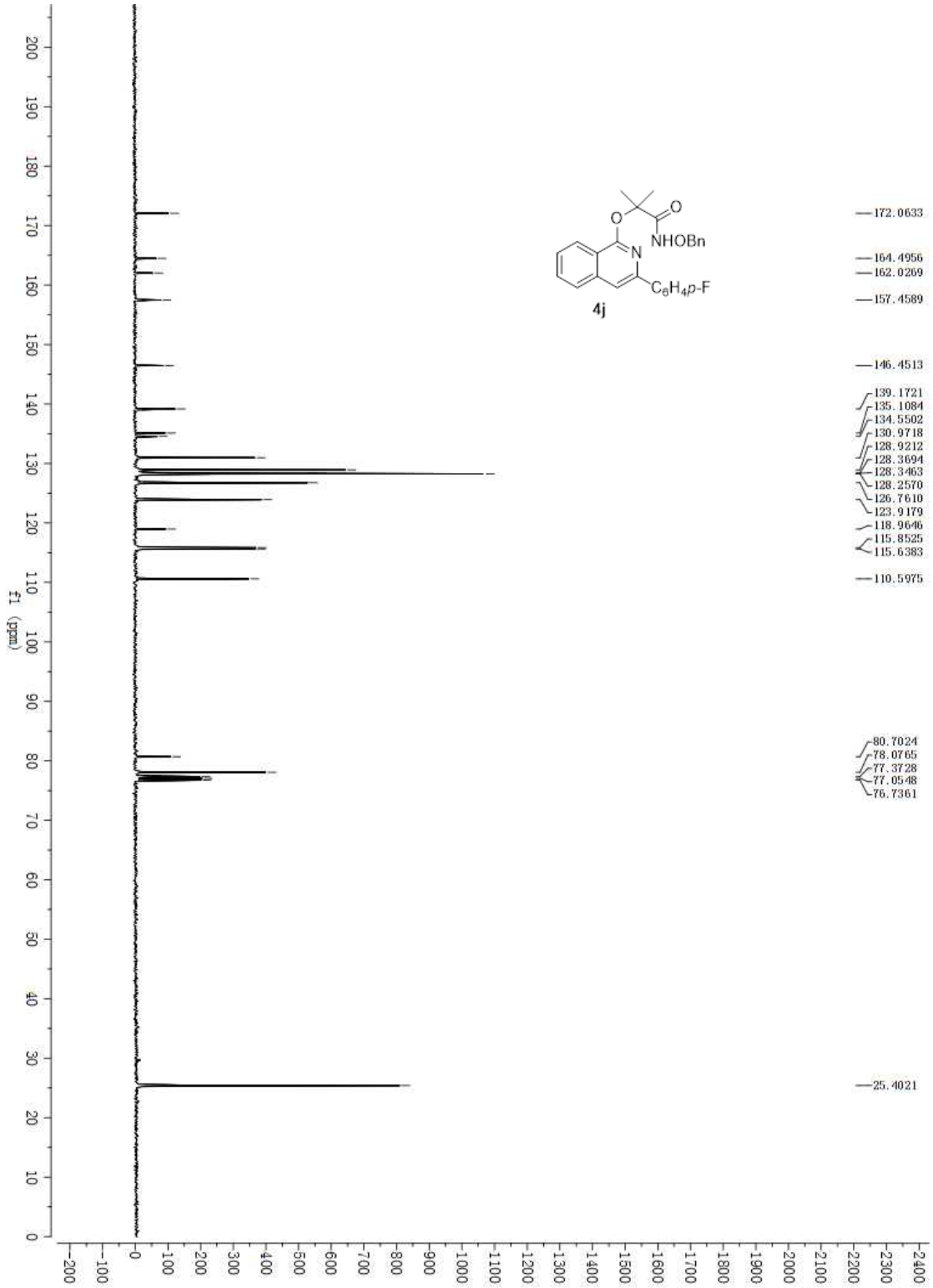

4h
NHOBn
Ph
f1 (ppm)
0.92
1.95
0.97
1.98
2.06
0.99
2.01
2.92
1.96
1.94
6.00
8.9004
8.0944
8.0757
7.6155
7.4856
7.4667
7.4473
7.3599
7.3347
7.2440
7.1601
7.1424
7.1214
7.1026
7.0851
7.0524
7.0374
6.0234
4.7223
1.8066
0.0002

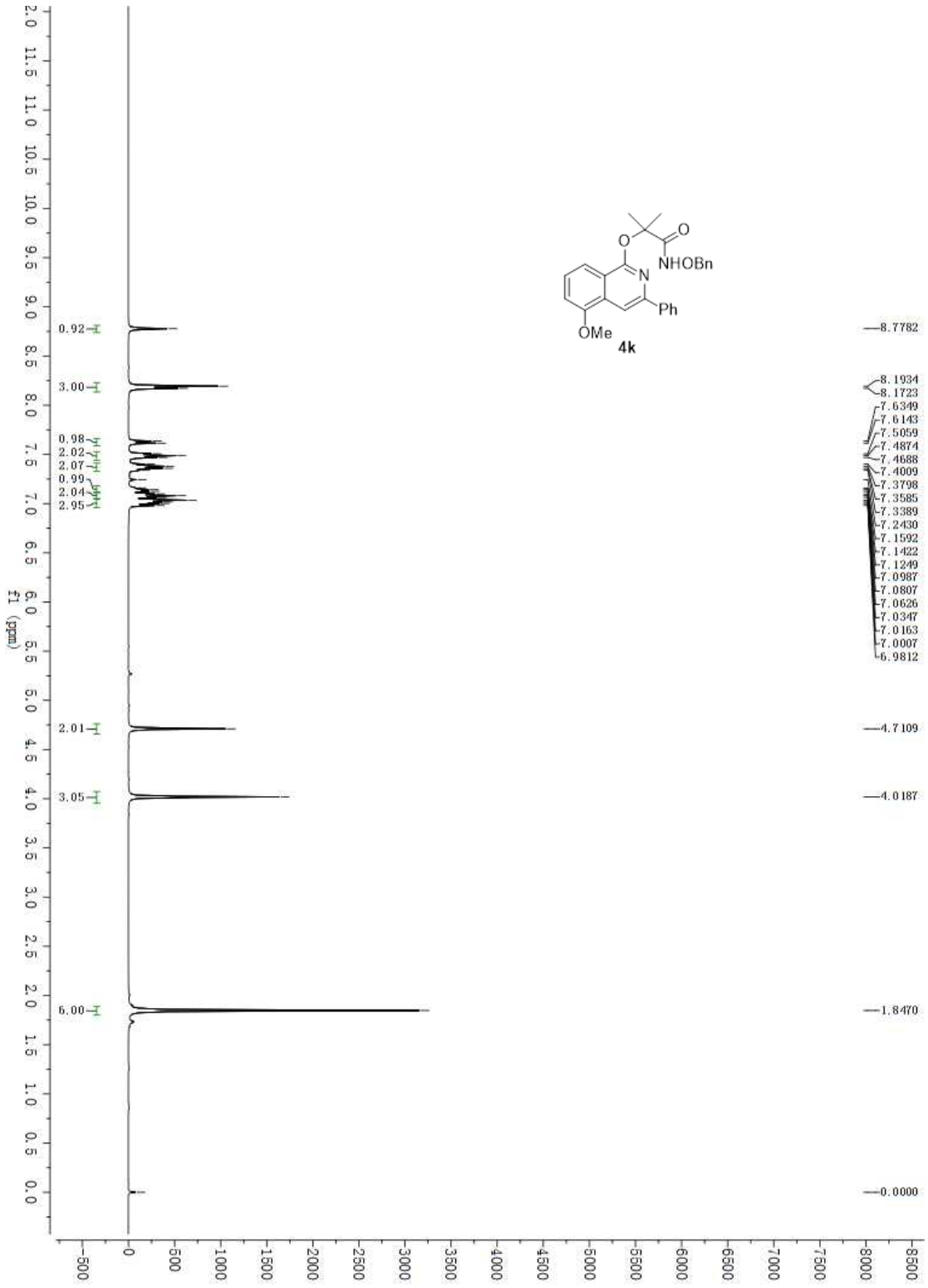

O
O
NHOBn
O
N
Ph
4h
172.3754
156.8115
151.2038
147.9888
146.5576
138.3585
137.3140
135.2823
128.9002
128.8266
128.4312
128.2762
128.2146
126.2972
115.3103
111.0118
103.1922
101.6388
100.5323
80.7127
77.9964
77.3773
77.0591
76.7409
25.5274
f1 (ppm)

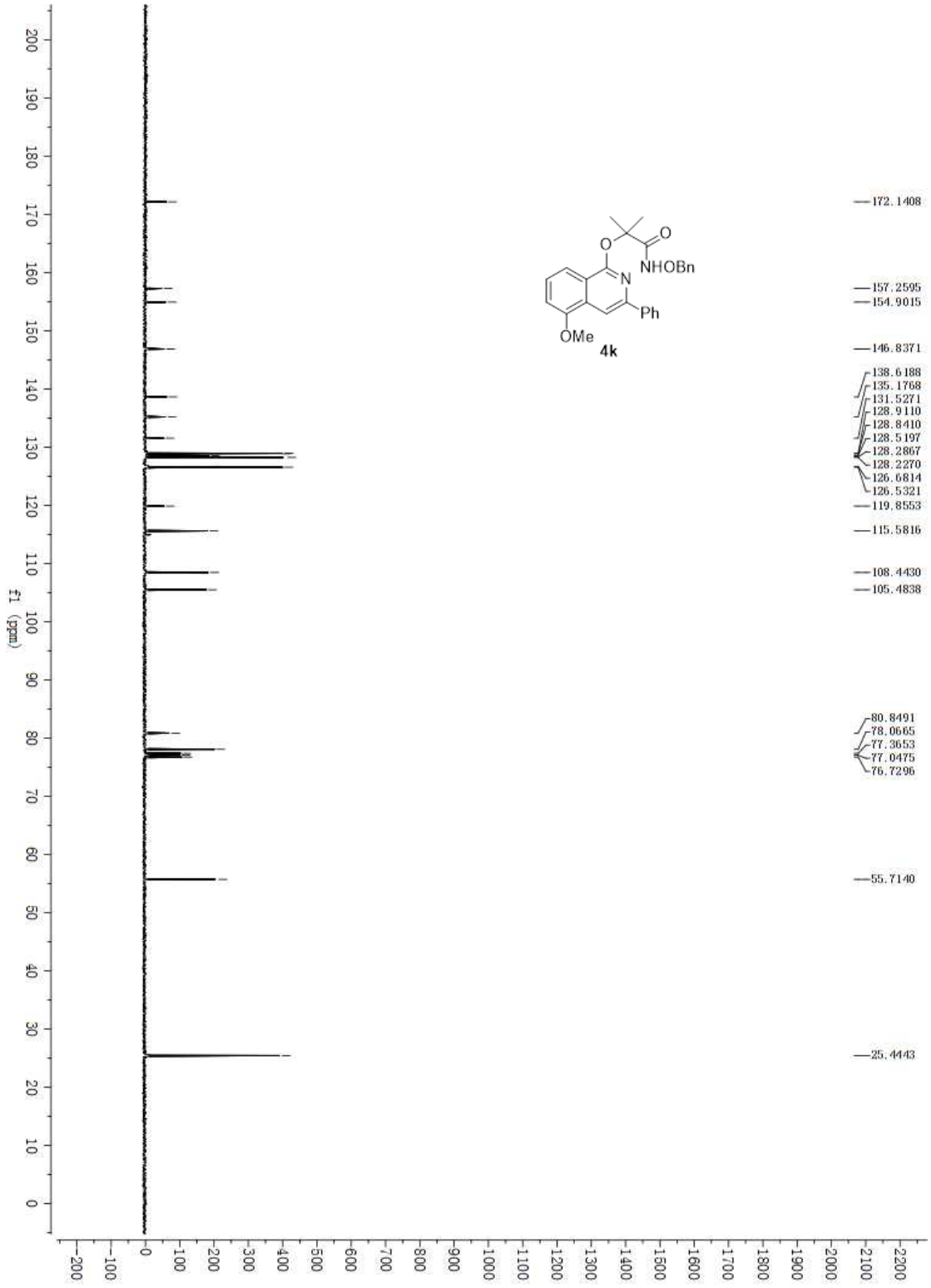

O
O
NHOBn
N
Ph
4i
f1 (ppm)
0.96
2.06
1.01
1.02
1.02
2.09
1.16
1.09
1.06
2.08
1.99
1.98
3.00
6.03
8.7988
8.1414
8.1227
7.9667
7.9457
7.7093
7.5728
7.5051
7.4863
7.4669
7.3782
7.3600
7.3417
7.3169
7.2958
7.2392
7.1646
7.1468
7.1289
7.0946
7.0757
7.0577
7.0321
7.0144
4.7079
2.5288
1.8412
0.0004

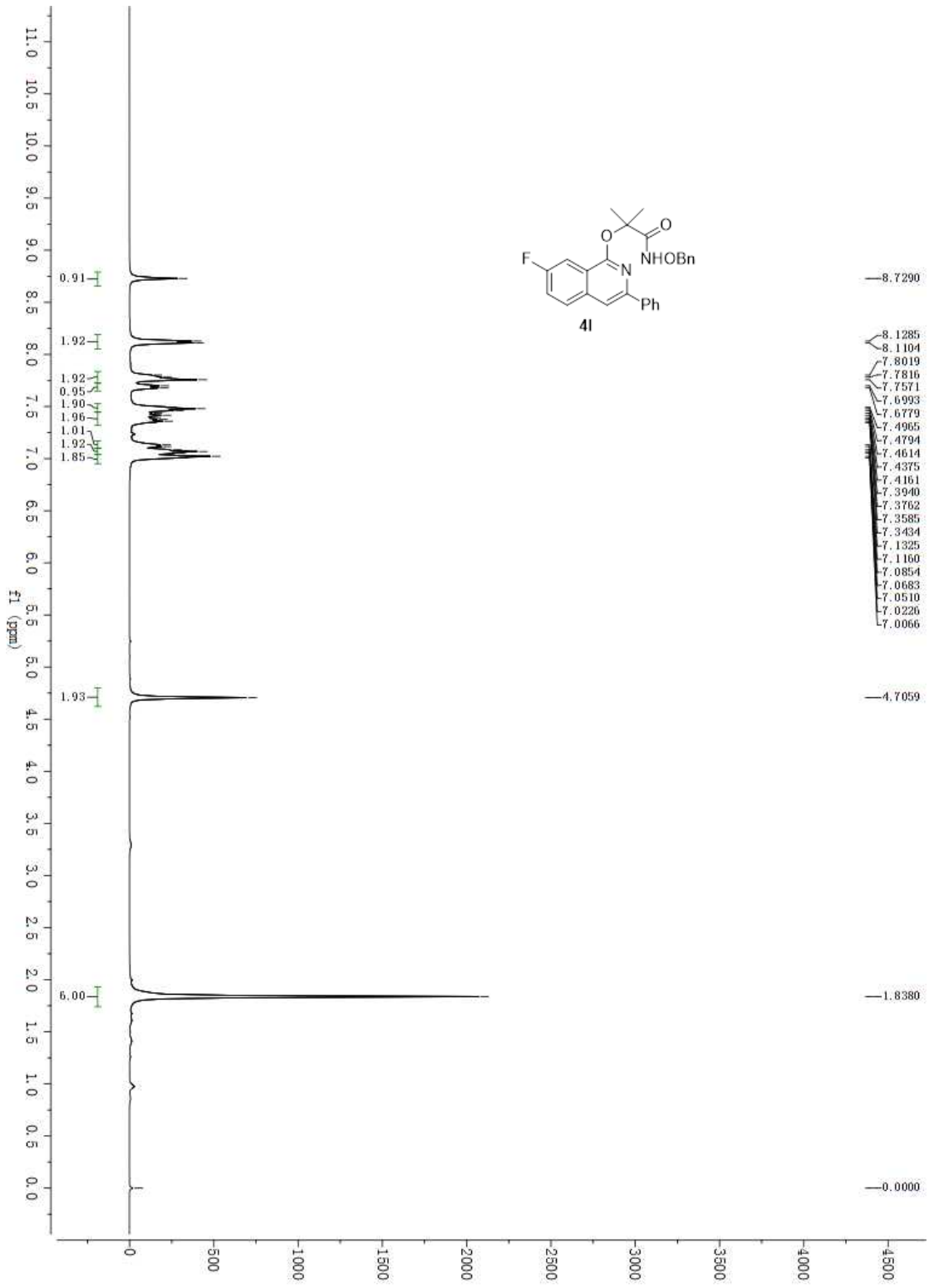

O
O
NHOBn
N
Ph
4i
172.1992
157.5018
147.4509
141.2002
139.5264
138.4744
135.2059
128.9263
128.8465
128.5740
128.2836
128.2179
126.4814
117.4002
110.6903
80.8015
78.0359
77.3585
77.0403
76.7224
25.4561
21.9483
f1 (ppm)

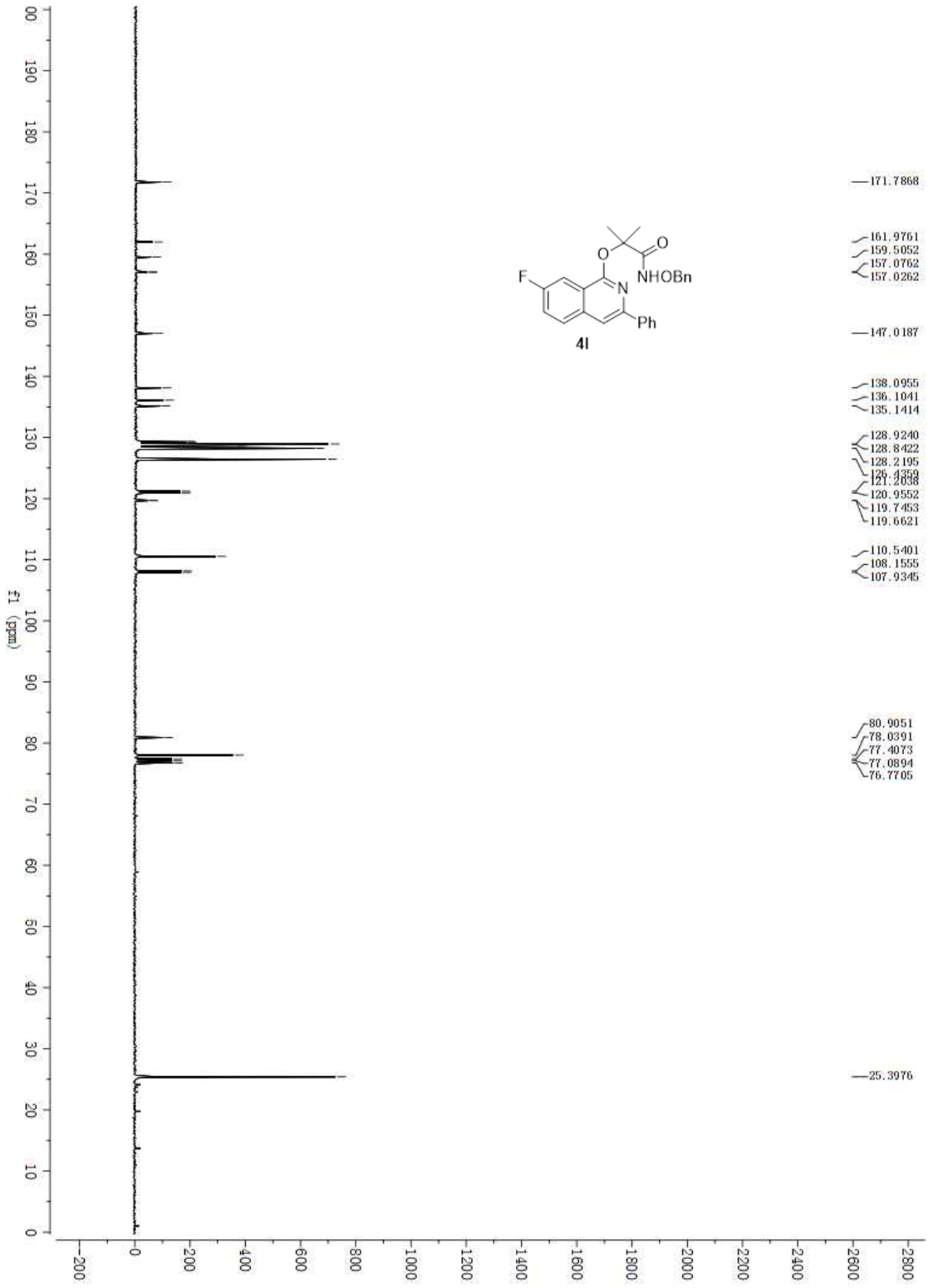

O
O
NHOBn
N
C6H4p-F
4j
f1 (ppm)
0.92
1.91
1.02
0.97
0.96
1.03
0.99
3.00
2.09
2.05
1.94
6.00
8.6544
8.1388
8.1187
8.1046
8.0861
8.0654
7.7988
7.7786
7.7133
7.6614
7.4829
7.1821
7.1615
7.1410
7.0903
7.0719
7.0537
7.0220
7.0040
4.6995
1.8366
0.0003

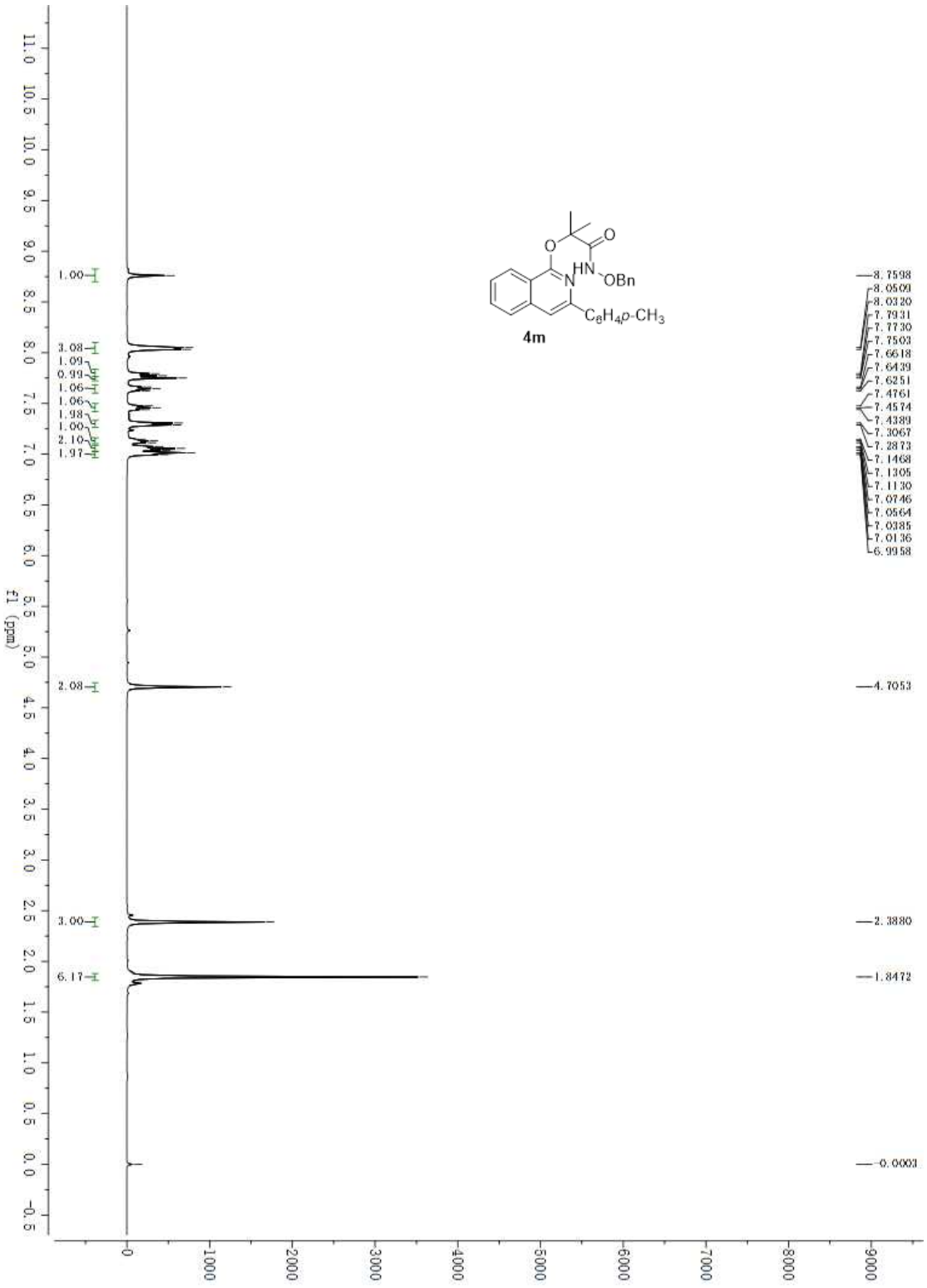

O
O
NHOBn
N
C6H4p-F
4j
172.0633
164.4956
162.0269
157.4589
146.4513
139.1721
135.1084
134.5502
130.9718
128.9212
128.3694
128.3463
128.2570
126.7610
123.9179
118.9646
115.8525
115.6383
110.5975
80.7024
78.0765
77.3728
77.0548
76.7361
25.4021
f1 (ppm)

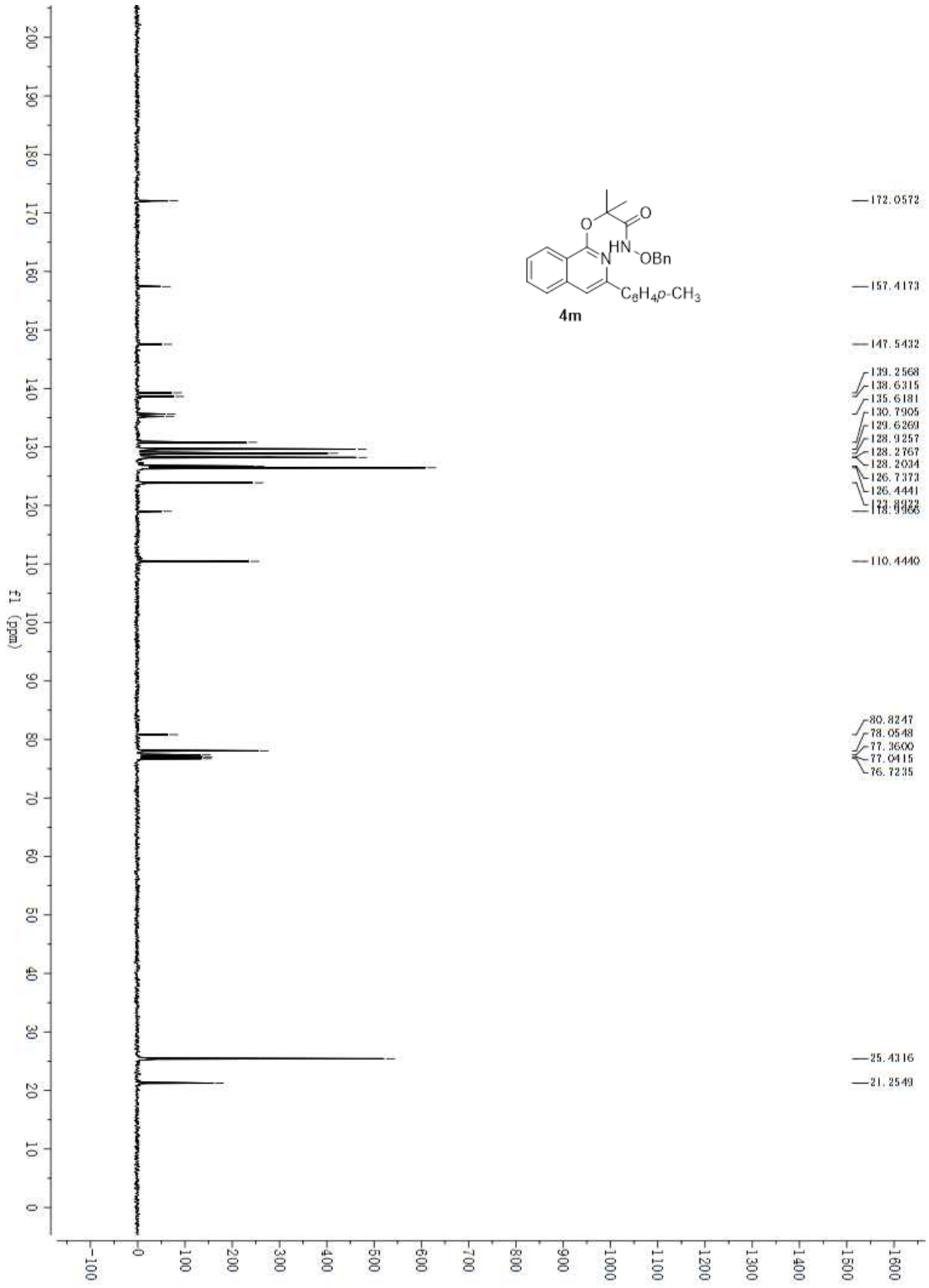

O
O
NHOBn
N
Ph
OMe
4k
0.92
3.00
0.98
2.02
2.07
0.99
2.04
2.95
2.01
3.05
6.00
8.7782
8.1934
8.1723
7.6349
7.6143
7.5059
7.4874
7.4688
7.4009
7.3798
7.3585
7.3389
7.2430
7.1592
7.1422
7.1249
7.0987
7.0807
7.0626
7.0347
7.0163
7.0007
6.9812
4.7109
4.0187
1.8470
0.0000
f1 (ppm)

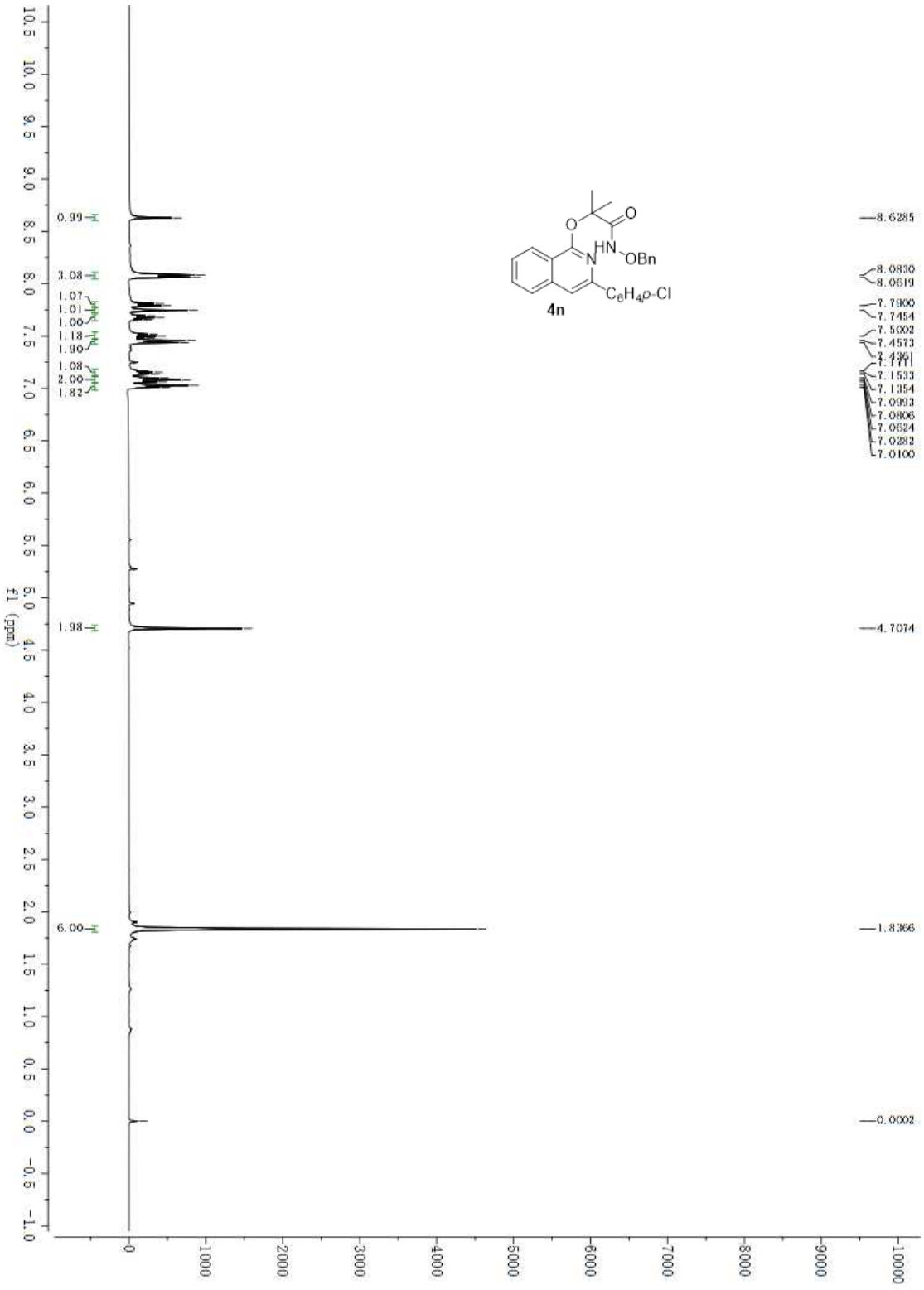

172.1408
157.2595
154.9015
146.8371
138.6188
135.1768
131.5271
128.9110
128.8410
128.5197
128.2867
128.2270
126.6814
126.5321
119.8553
115.5816
108.4430
105.4838
80.8491
78.0665
77.3653
77.0475
76.7296
55.7140
25.4443
NHOBn
Ph
OMe
4k
f1 (ppm)

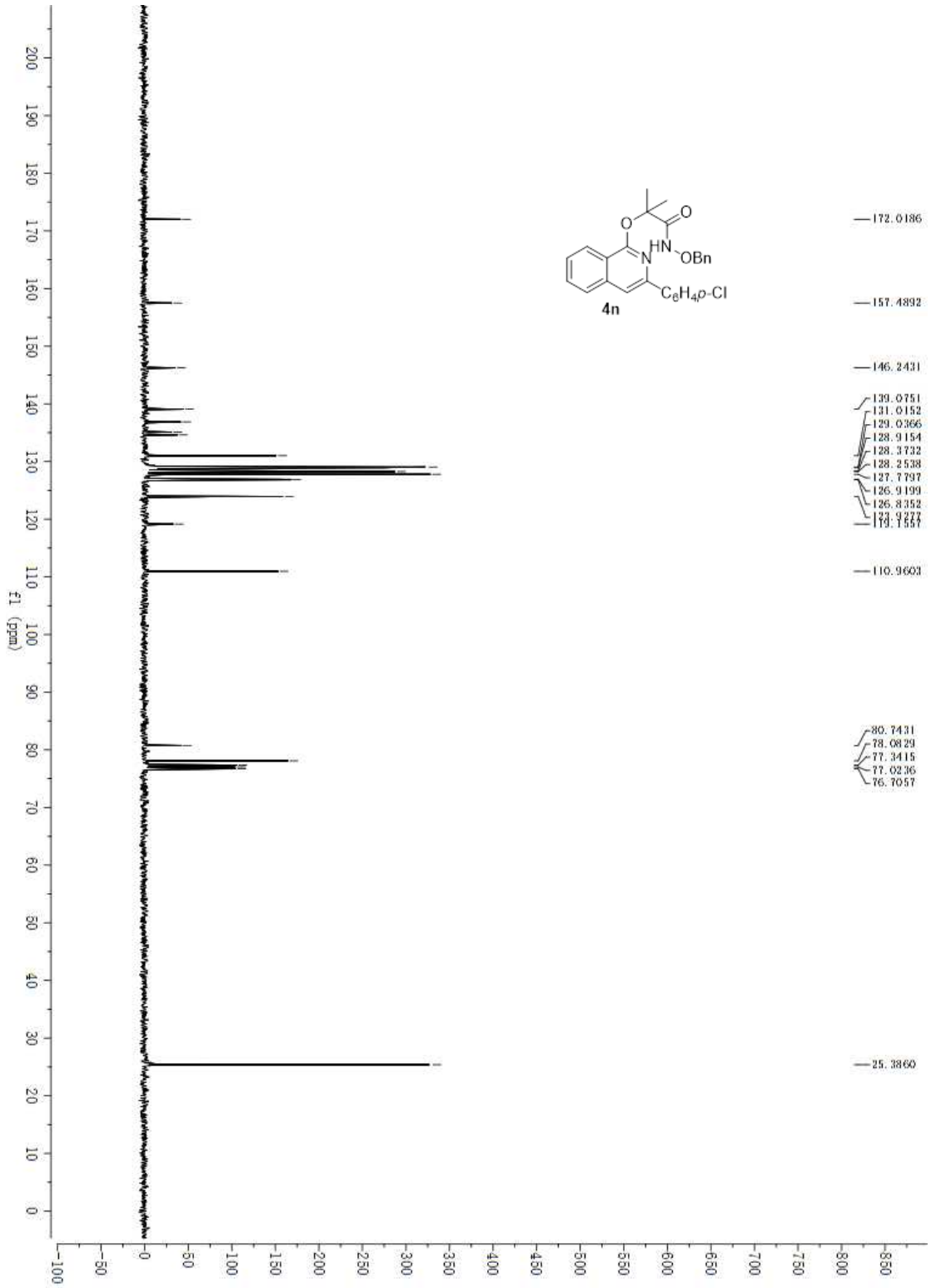

F
O
O
NHOBn
N
Ph
4l
f1 (ppm)
0.91
1.92
1.92
0.95
1.90
1.96
1.01
1.92
1.85
1.93
6.00
8.7290
8.1285
8.1104
7.8019
7.7816
7.7571
7.6993
7.6779
7.4965
7.4794
7.4614
7.4375
7.4161
7.3940
7.3762
7.3585
7.3434
7.1325
7.1160
7.0854
7.0683
7.0510
7.0226
7.0066
4.7059
1.8380
0.0000

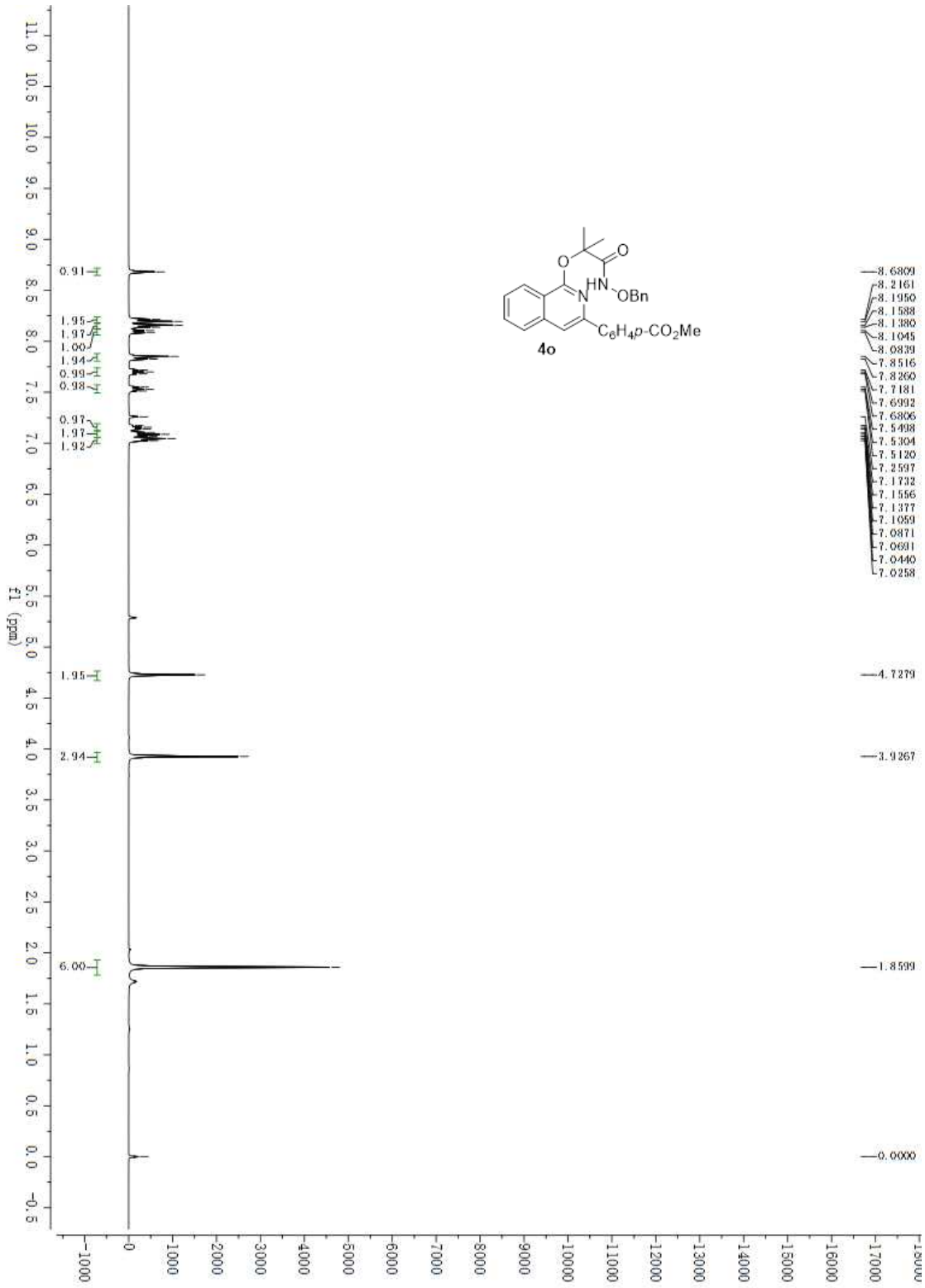

171.7868
161.9761
159.5052
157.0762
157.0262
147.0187
138.0955
136.1041
135.1414
128.9240
128.8422
128.2195
120.4359
121.2038
120.9552
119.7453
119.6621
110.5401
108.1555
107.9345
80.9051
78.0391
77.4073
77.0894
76.7705
25.3976
O
O
NHOBn
N
F
Ph
4l
f1 (ppm)

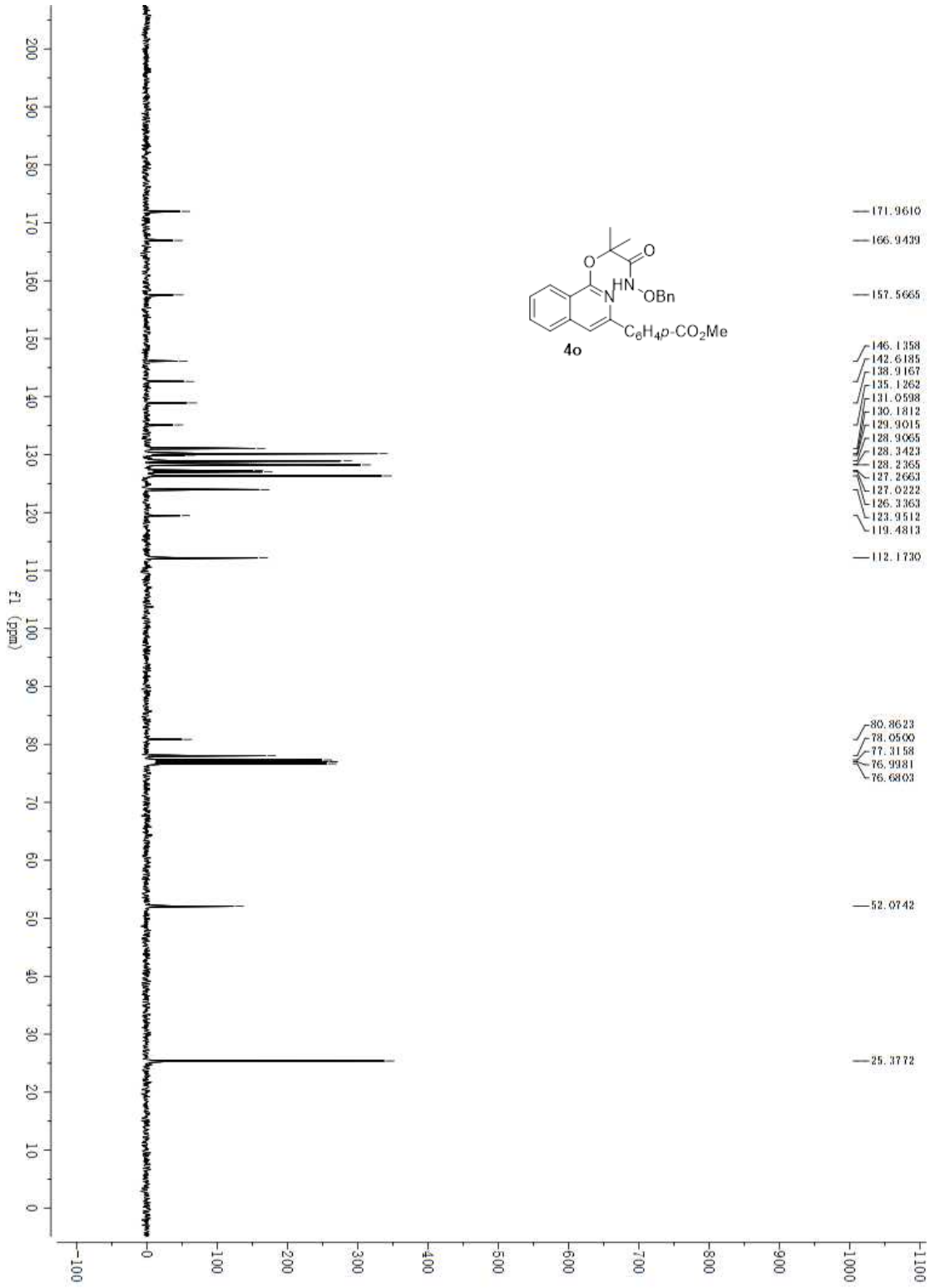

4m
C8H4p-CH3
OBn
HN
O
N
f1 (ppm)
1.00
3.08
1.09
0.99
1.06
1.06
1.98
1.00
2.10
1.97
2.08
3.00
6.17
8.7598
8.0509
8.0320
7.7931
7.7730
7.7503
7.6618
7.6439
7.6251
7.4761
7.4574
7.4389
7.3067
7.2873
7.1468
7.1305
7.1130
7.0746
7.0564
7.0385
7.0136
6.9958
4.7053
2.3880
1.8472
0.0000

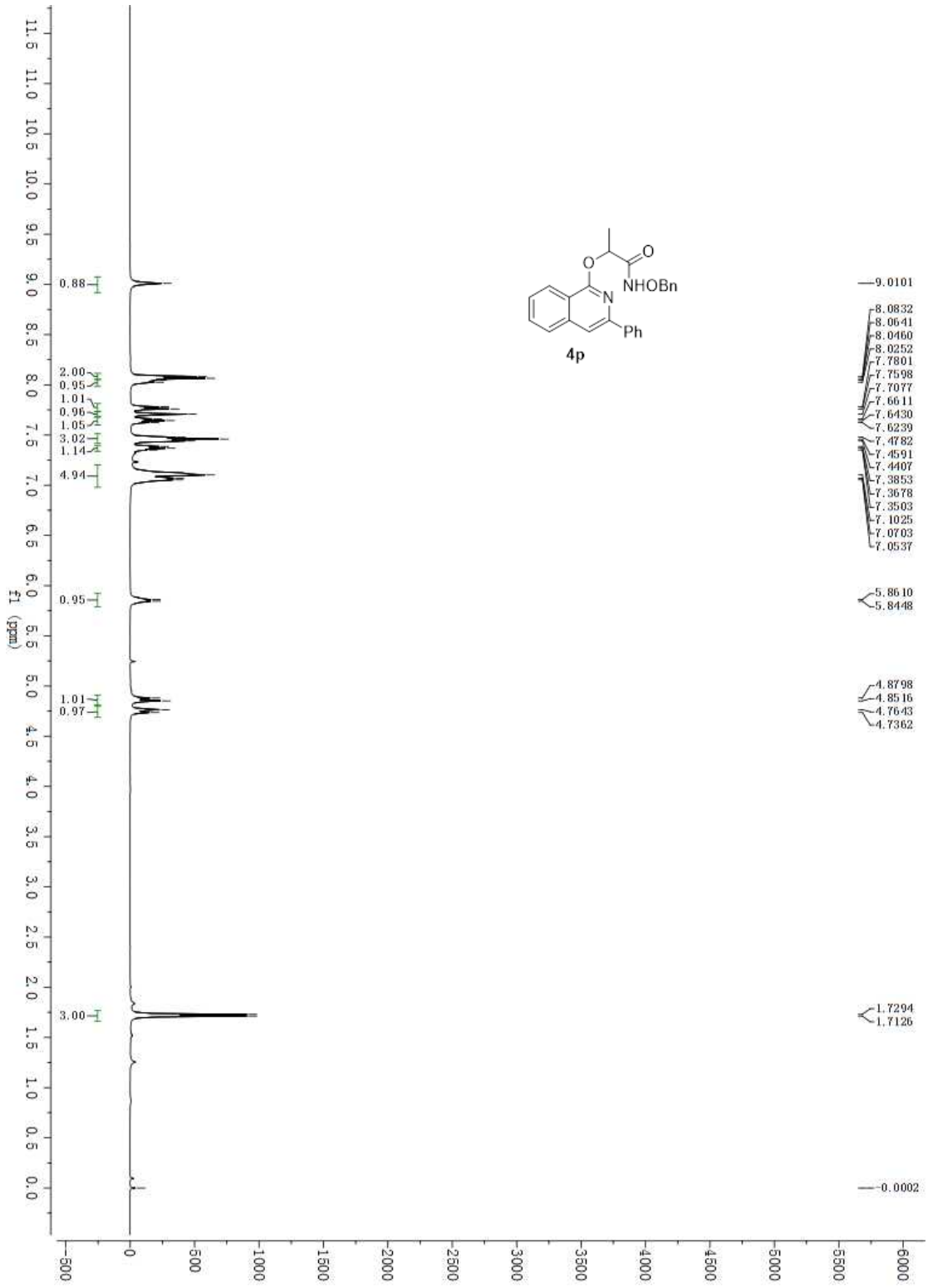

4m
172.0572
157.4173
147.5432
139.2568
138.6315
135.6181
130.7905
129.6269
128.9257
128.2767
128.2034
126.7373
126.4441
110.4440
80.8247
78.0548
77.3600
77.0415
76.7235
25.4316
21.2549
f1 (ppm)

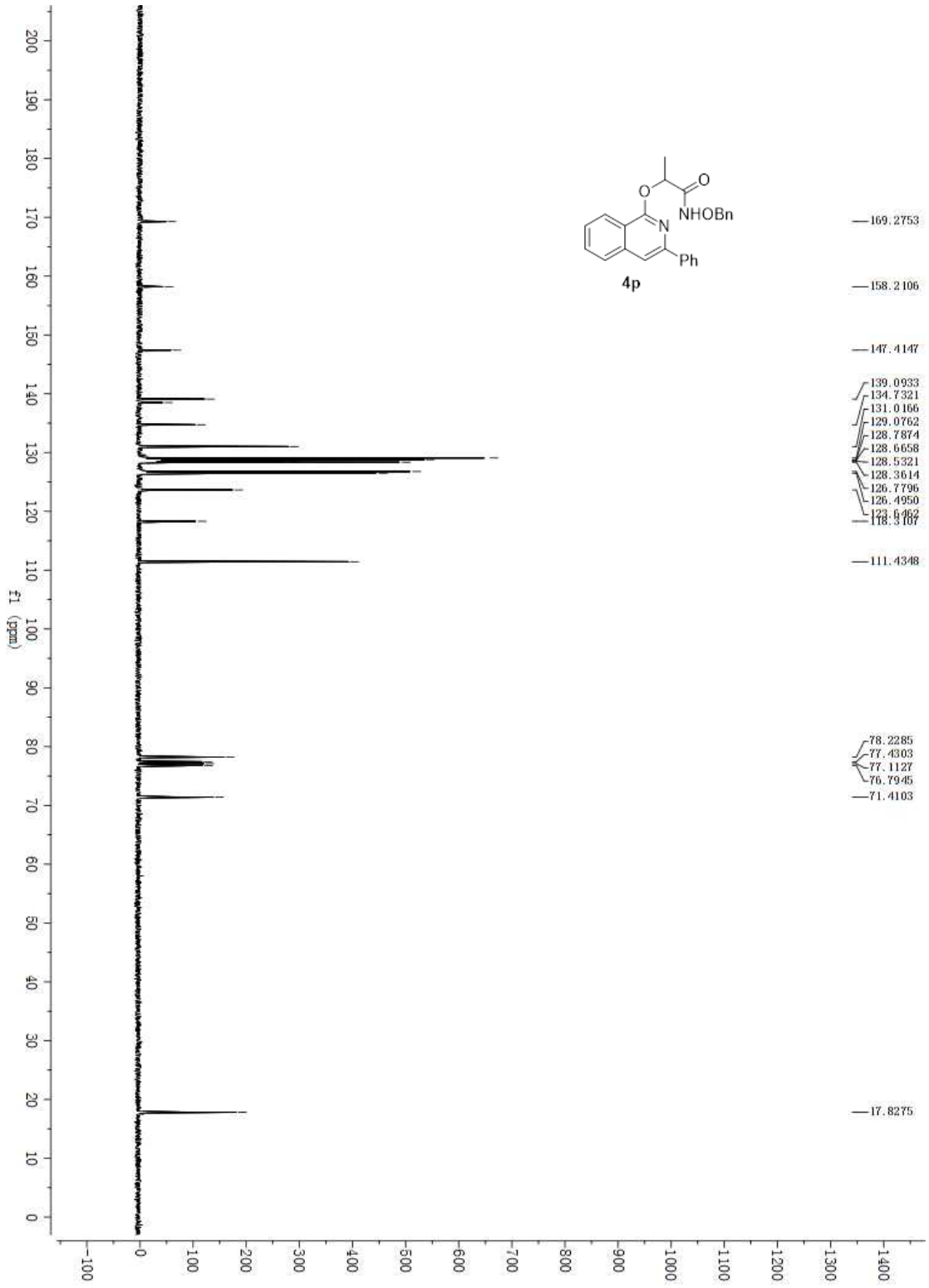

4n
f1 (ppm)
0.99
3.08
1.07
1.01
1.00
1.18
1.90
1.08
2.00
1.82
1.98
6.00
8.6285
8.0830
8.0619
7.7900
7.7454
7.5002
7.4573
7.1533
7.1354
7.0993
7.0806
7.0624
7.0282
7.0100
4.7074
1.8366
0.0002

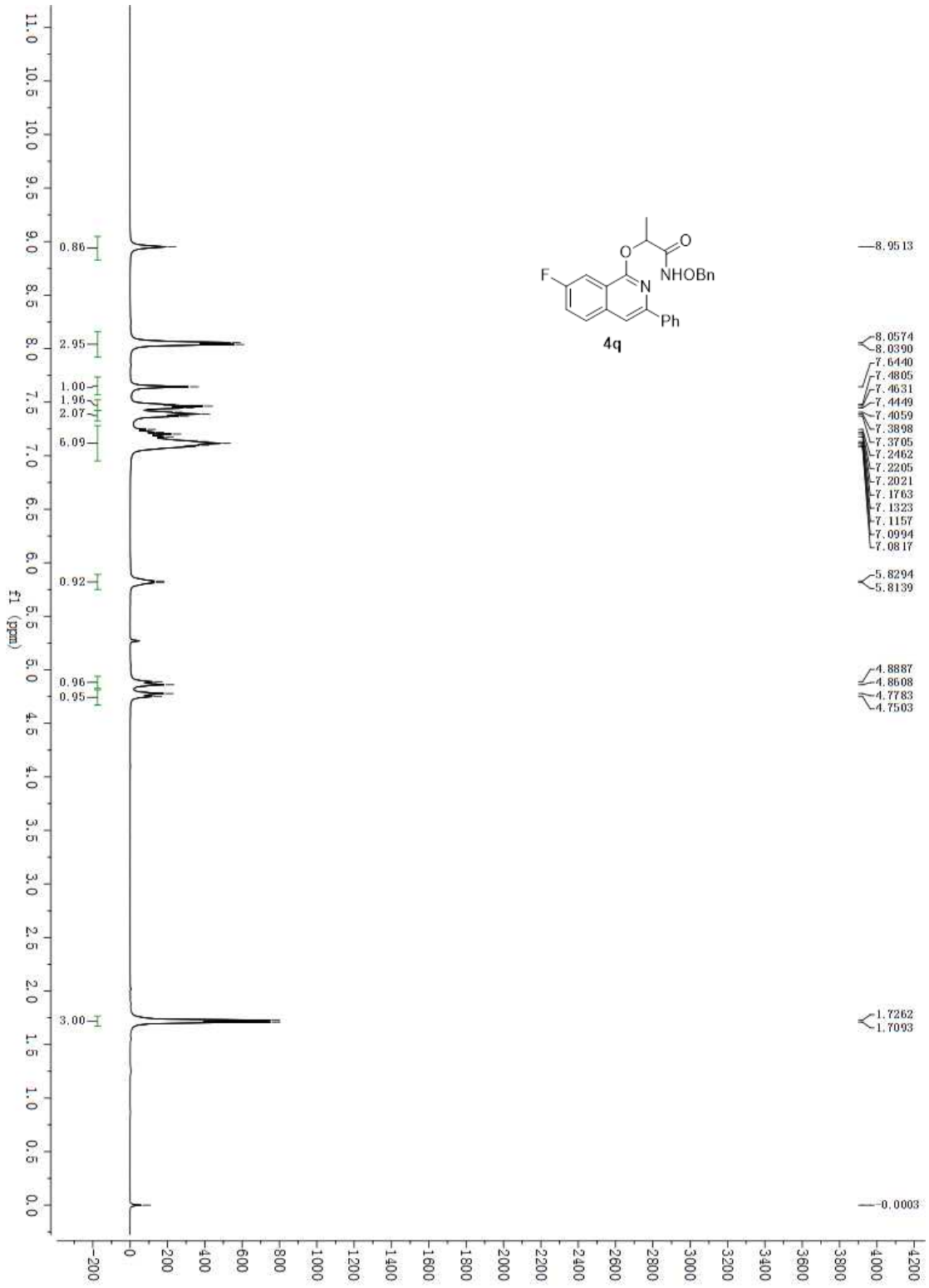

4n
172.0186
157.4892
146.2431
139.0751
131.0152
129.0366
128.9154
128.3732
128.2538
127.7797
126.9199
126.8352
123.9277
119.1557
110.9603
80.7431
78.0829
77.3415
77.0236
76.7057
25.3860
f1 (ppm)

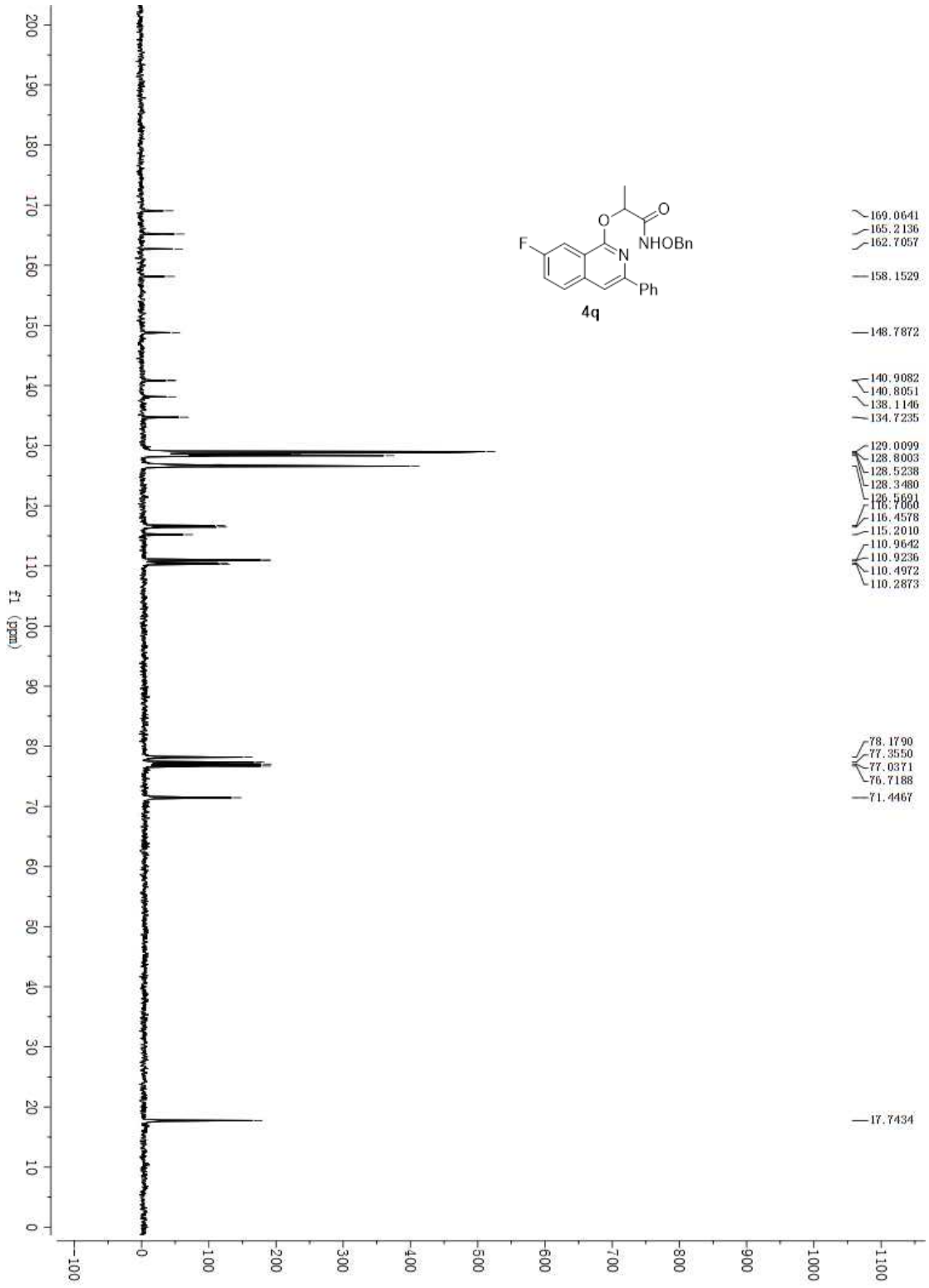

4o
f1 (ppm)
0.91
1.95
1.97
1.00
1.94
0.99
0.98
0.97
1.97
1.92
1.95
2.94
6.00
8.6809
8.2161
8.1950
8.1588
8.1380
8.1045
8.0839
7.8516
7.8260
7.7181
7.6992
7.6806
7.5498
7.5304
7.5120
7.2597
7.1732
7.1556
7.1377
7.1059
7.0871
7.0691
7.0440
7.0258
4.7279
3.9267
1.8599
0.0000

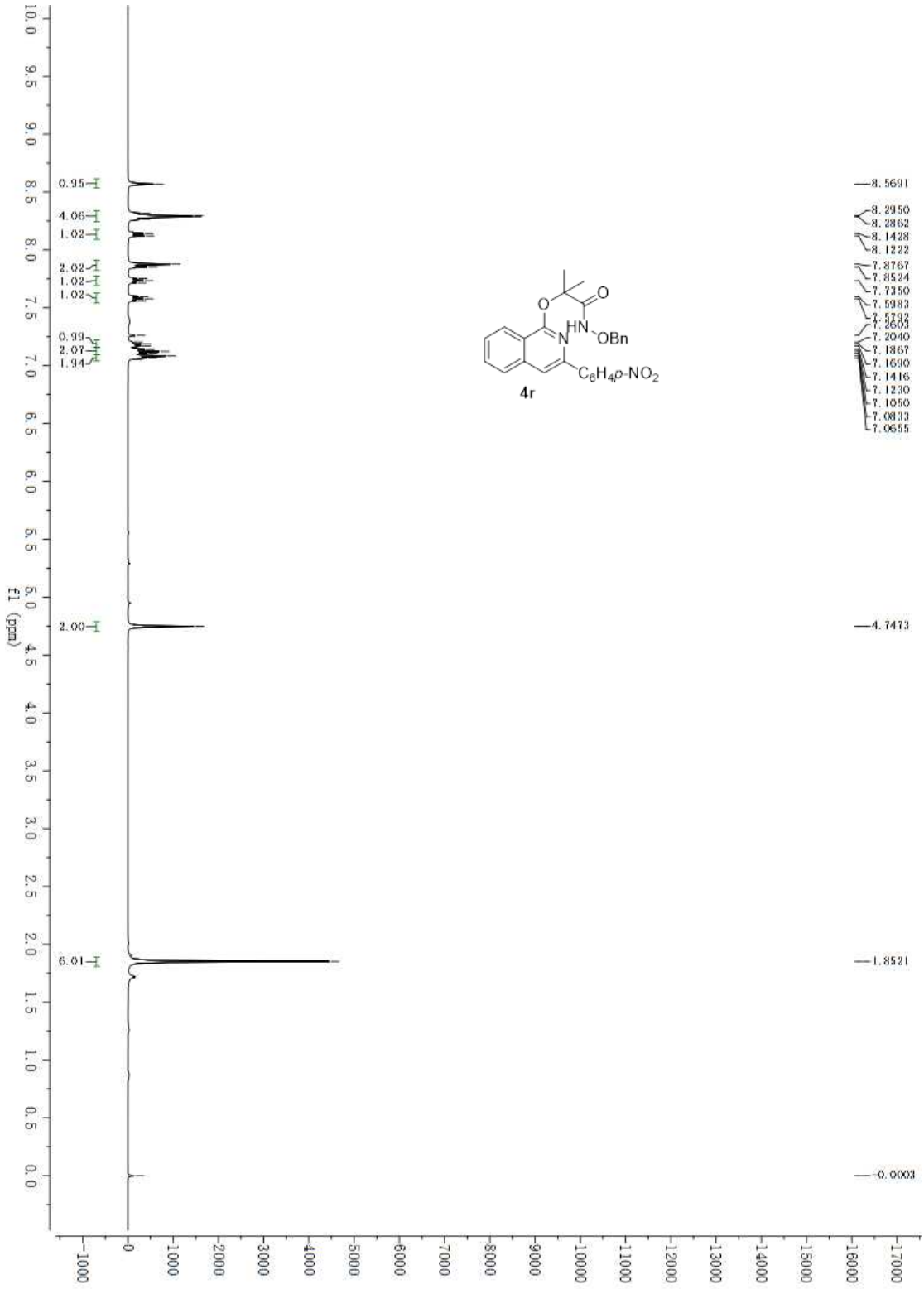

171.9610
166.9439
157.5665
146.1358
142.6185
138.9167
135.1262
131.0598
130.1812
129.9015
128.9065
128.3423
128.2365
127.2663
127.0222
126.3363
123.9512
119.4813
112.1730
80.8623
78.0500
77.3158
76.9981
76.6803
52.0742
25.3772
f1 (ppm)
4o


4p
NHOBn
Ph
f1 (ppm)
0.88
2.00
0.95
1.01
0.96
1.05
3.02
1.14
4.94
0.95
1.01
0.97
3.00
9.0101
8.0832
8.0641
8.0460
8.0252
7.7801
7.7598
7.7077
7.6611
7.6430
7.6239
7.4782
7.4591
7.4407
7.3853
7.3678
7.3503
7.1025
7.0703
7.0537
5.8610
5.8448
4.8798
4.8516
4.7643
4.7362
1.7294
1.7126
0.0002

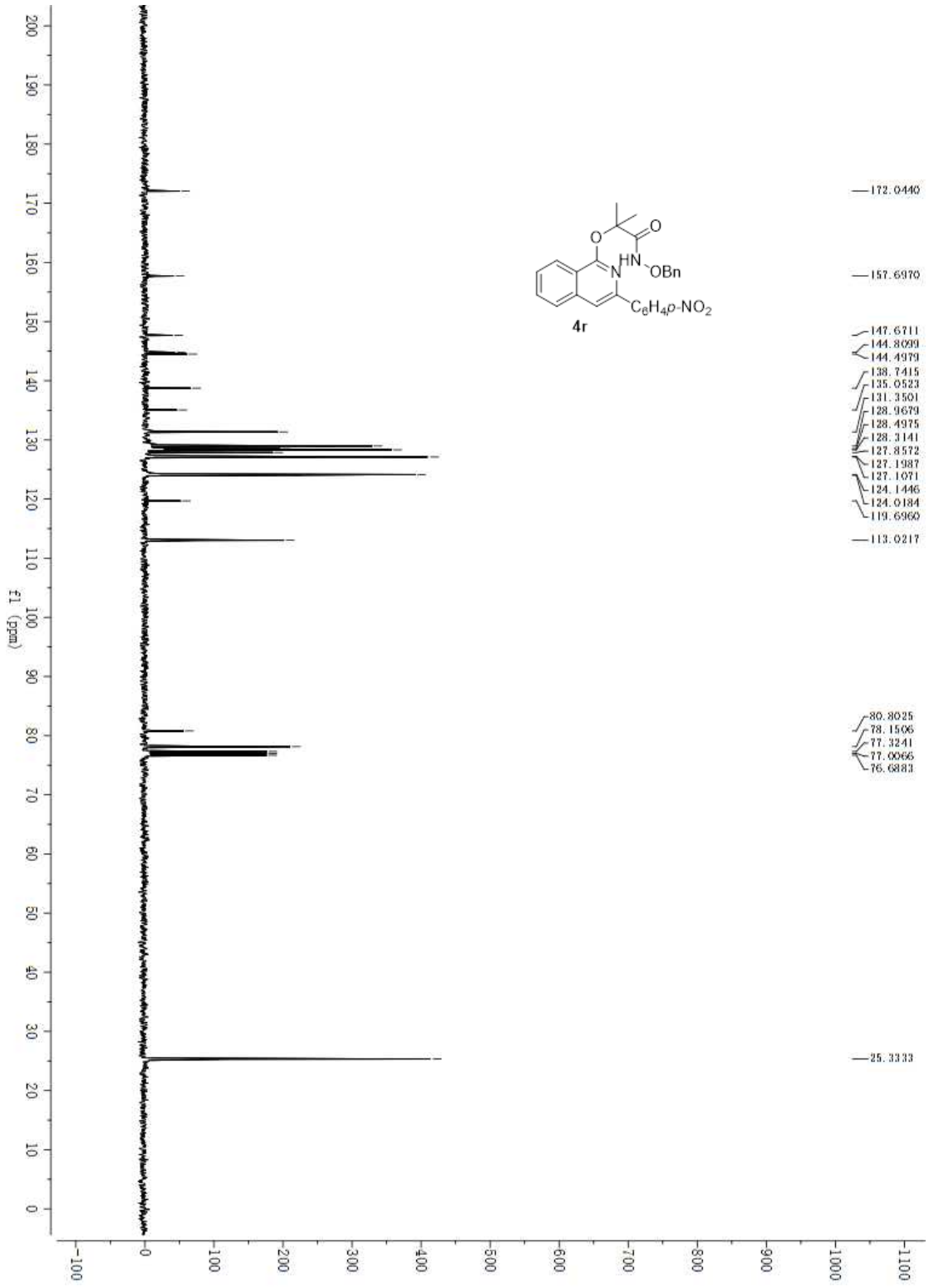

O
NHOBn
N
Ph
4p
169.2753
158.2106
147.4147
139.0933
134.7321
131.0166
129.0762
128.7874
128.6658
128.5321
128.3614
126.7796
126.4950
123.6462
118.3107
111.4348
78.2285
77.4303
77.1127
76.7945
71.4103
17.8275
f1 (ppm)


F
O
O
NHOBn
N
Ph
4q
0.86
2.95
1.00
1.96
2.07
6.09
0.92
0.96
0.95
3.00
8.9513
8.0574
8.0390
7.6440
7.4805
7.4631
7.4449
7.4059
7.3898
7.3705
7.2462
7.2205
7.2021
7.1763
7.1323
7.1157
7.0994
7.0817
5.8294
5.8139
4.8887
4.8608
4.7783
4.7503
1.7262
1.7093
0.0003
f1 (ppm)


F
O
O
NHOBn
N
Ph
4q
169.0641
165.2136
162.7057
158.1529
148.7872
140.9082
140.8051
138.1146
134.7235
129.0099
128.8003
128.5238
128.3480
126.5691
116.7060
116.4578
115.2010
110.9642
110.9236
110.4972
110.2873
78.1790
77.3550
77.0371
76.7188
71.4467
17.7434
f1 (ppm)


0.95
4.06
1.02
2.02
1.02
1.02
0.99
2.07
1.94
2.00
6.01
8.5691
8.2950
8.2862
8.1428
8.1222
7.8767
7.8524
7.7350
7.5983
7.5732
7.2603
7.2040
7.1867
7.1690
7.1416
7.1230
7.1050
7.0833
7.0655
4.7473
1.8521
0.0000
f1 (ppm)
O
O
HN
OBn
N
C6H4p-NO2

4r


172.0440
157.6970
147.6711
144.8099
144.4979
138.7415
135.0523
131.3501
128.9679
128.4975
128.3141
127.8572
127.1987
127.1071
124.1446
124.0184
119.6960
113.0217
80.8025
78.1506
77.3241
77.0066
76.6883
25.3333
4r
f1 (ppm)