Generation of diverse isoquinoline *N*-oxides in Aqueous System

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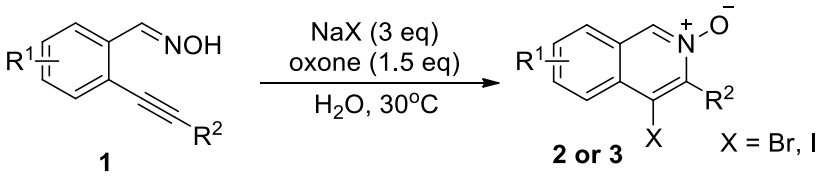
Supporting Information

General experimental methods:

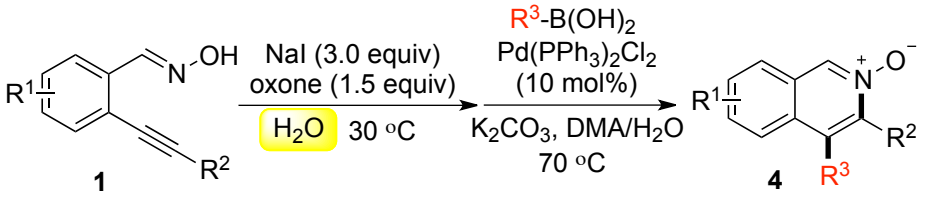
All reactions were performed in tubes in air. Unless otherwise stated, all commercial reagents were used as received. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated 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 procedure of generation of 4-bromo-isoquinoline N-oxides or 4-iodo-isoquinoline N-oxides via an electrophilic cyclization of 2-alkynylbenzaldehyde oximes **1** with halogen generated in situ in water.*

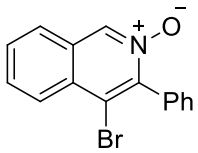


2-Alkynylbenzaldoxime **1** (0.30 mmol) was added to a mixture of sodium bromide or sodium iodide (2 equiv, 0.6 mmol) and oxone (1.5 equiv, 0.45 mmol) in water (3.0 mL). The mixture was stirred under 30 °C. After completion of the reaction (12 hours), the mixture was extracted by EtOAc (2 × 5.0 mL) and dried by anhydrous Na_2SO_4. Evaporation of the solvent followed by purification on silica gel provided the product **2** or **3**.

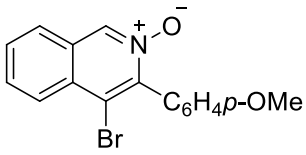
General procedure of one-pot synthesis of functionalized isoquinoline N-oxides via an electrophilic cyclization of 2-alkynylbenzaldehyde oxime ***1*** *followed by the palladium-catalyzed Suzuki coupling in aqueous system.*



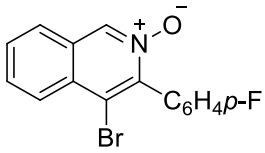
2-Alkynylbenzaldoxime **1** (0.30 mmol) was added to a mixture of sodium bromide or sodium iodide (2 equiv, 0.6 mmol) and oxone (1.5 equiv, 0.45 mmol) in water (3.0 mL). The mixture was stirred under 30 °C. After 12 hours, $Pd(PPh_3)Cl_2$ (10 mol %, 0.03 mmol), K_2CO_3 (4.0 equiv, 1.2 mmol), arylboronic acid (1.5 equiv, 0.45 mmol) and DMA (4.0 mL) were added. The mixture was stirred under 70 °C for another 20 hours. After the completion of the reaction, the mixture was diluted by saturated brine, extracted by EtOAc (2 × 5.0 mL), and dried by anhydrous Na_2SO_4. Evaporation of the solvent followed by purification on silica gel provided the product **4**.



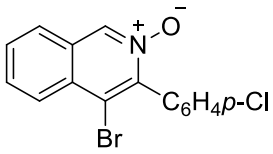
4-Bromo-3-phenylisoquinoline 2-oxide (**2a**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.2 Hz, 2H), 7.48-7.58 (m, 3H), 7.66-7.71 (m, 3H), 8.16 (d, J = 7.6 Hz, 1H), 8.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 122.2, 125.1, 127.3, 128.6, 129.1, 129.5, 129.8, 123.0, 123.1 133.5, 136.2, 147.7.



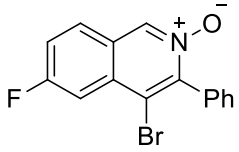
4-Bromo-3-(4-methoxyphenyl)isoquinoline 2-oxide (**2b**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) 3.90 (s, 3H), 7.09 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 7.62-7.67 (m, 3H), 8.08 (d, J = 8.0 Hz, 1H), 8.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.3, 102.4, 114.1, 125.1, 128.4, 129.5, 129.7, 130.2, 131.2, 131.7, 132.6, 136.7, 151.0, 160.3.



4-Bromo-3-phenylisoquinoline 2-oxide (**2c**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.25 (m, 2H), 7.43-7.46 (m, 2H), 7.64-7.75 (m, 3H), 8.16 (d, J = 8.4 Hz, 1H), 8.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.8 (d, $^2J_{CF}$ = 22.0 Hz), 122.5, 125.1, 127.4, 128.6, 129.1, 129.2, 130.1, 132.0, 132.1, 136.2, 146.8, 163.2 (d, $^1J_{CF}$ = 248.0 Hz); HRMS (ESI) calcd for $C_{15}H_{10}BrFNO$: 317.9924 ($M + H^+$), found: 317.9939.

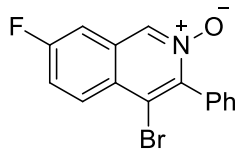


4-Bromo-3-(4-chlorophenyl)isoquinoline 2-oxide (**2d**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 8.0 Hz, 2H), 7.67-7.75 (m, 3H), 8.16 (d, J = 8.0 Hz, 1H), 8.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 122.3, 125.1, 127.4, 128.7, 129.0, 129.1, 130.2, 131.4, 131.7, 135.6, 136.3, 146.6; HRMS (ESI) calcd for $C_{15}H_{10}BrClNO$: 333.9629 ($M + H^+$), found: 333.9640.

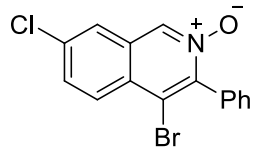


4-Bromo-6-fluoro-3-phenylisoquinoline 2-oxide (**2e**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.45 (m, 3H), 7.53-7.55 (m, 3H), 7.75 (s, 1H), 7.83 (d, J = 9.6 Hz, 1H), 8.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 112.1 (d, $^2J_{CF}$ = 25.0 Hz), 120.6 (d, $^2J_{CF}$ = 26.0 Hz), 121.2, 125.7, 128.0, 128.1, 128.7, 129.7, 130.7 (d, $^3J_{CF}$ = 10.0 Hz), 133.2, 136.0, 148.7, 163.1 (d,

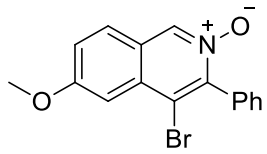
$^{1}J_{CF}$ = 252.0 Hz); HRMS (ESI) calcd for $C_{15}H_{10}BrFNO$: 317.9924 (M + H^{+}), found: 317.9937.



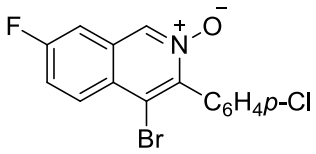
4-Bromo-7-fluoro-3-phenylisoquinoline 2-oxide (**2f**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.44 (m, 4H), 7.50-7.56 (m, 3H), 8.18 (d, *J* = 8.0 Hz, 1H), 8.85 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.5 (d, $^{2}J_{CF}$ = 22.0 Hz), 120.0 (d, $^{2}J_{CF}$ = 25.0 Hz), 122.1, 126.0, 128.7, 129.6, 129.8, 130.3, 130.5 (d, $^{3}J_{CF}$ = 8.0 Hz), 133.2, 135.4, 147.4, 162.7 (d, $^{1}J_{CF}$ = 252.0 Hz).



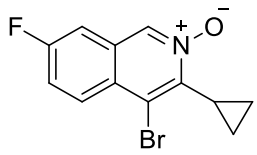
4-Bromo-7-chloro-3-phenylisoquinoline 2-oxide (**2g**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.6 Hz, 1H), 7.50-7.59 (m, 4H), 7.70 (s, 1H), 8.09 (d, *J* = 9,2 Hz, 1H), 8.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 122.1, 123.5, 127.3, 128.7, 129.1, 129.3, 129.6, 129.7, 130.6, 133.1, 135.2, 136.2, 148.2; HRMS (ESI) calcd for $C_{15}H_{10}BrClNO$: 333.9629 (M + H^{+}), found: 333.9616.



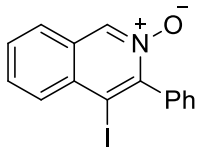
4-Bromo-6-methoxy-3-phenylisoquinoline 2-oxide (**2h**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.99 (s, 3H), 7.29 (d, *J* = 9.2 Hz, 1H), 7.44-7.45 (m, 3H), 7.50-7.56 (m, 3H), 7.69 (d, *J* = 9.2 Hz, 1H), 8.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 105.9, 120.7, 123.0, 123.8, 127.2, 128.6, 129.4, 129.7, 131.3, 133.7, 136.3, 147.7, 161.3.



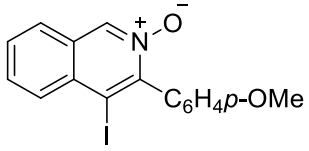
4-Bromo-3-(4-chlorophenyl)-7-fluoroisoquinoline 2-oxide (**2i**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.38 (m, 3H), 7.45 (t, J = 8.8 Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 8.19 (dd, J = 2.4, 9.2 Hz, 1H), 8.82 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 108.7 (d, $^{2}J_{CF}$ = 23.0 Hz), 120.3 (d, $^{2}J_{CF}$ = 25.0 Hz), 122.2, 126.1, 129.0, 129.7, 129.8, 130.5, 130.6, 131.4, 135.6, 135.7, 146.2, 162.8 (d, $^{1}J_{CF}$ = 252.0 Hz); HRMS (ESI) calcd for $C_{15}H_9BrClFNO$: 351.9535 (M + H^+), found: 351.9545.



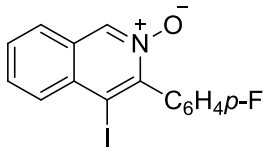
4-Bromo-3-cyclopropyl-7-fluoroisoquinoline 2-oxide (**2j**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13-1.17 (m, 2H), 1.27-1.32 (m, 1H), 2.04-2.22 (m, 1H), 7.26-7.29 (m, 1H), 7.32-7.37 (m, 1H), 8.13 (dd, J = 5.2, 9.2 Hz, 1H), 8.71 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.7, 13.6, 108.1 (d, $^{2}J_{CF}$ = 28.9 Hz), 119.8 (d, $^{2}J_{CF}$ = 25.0 Hz), 123.6, 126.3, 128.5 (d, $^{3}J_{CF}$ = 10.0 Hz), 129.8 (d, $^{3}J_{CF}$ = 9.0 Hz), 135.4 (d, $^{3}J_{CF}$ = 5.0 Hz), 147.9, 162.2 (d, $^{1}J_{CF}$ = 251.0 Hz). HRMS (ESI) calcd for $C_{12}H_{10}BrFNO$: 281.9924 (M + H^+), found: 281.9915.



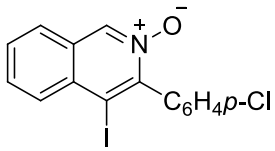
4-Iodo-3-phenylisoquinoline 2-oxide (**3a**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38(s, 1H), 7.48-7.52 (m, 3H), 7.53-7.57 (m, 3H), 8.07 (d, J = 8.0 Hz, 1H), 8.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.9, 125.2, 128.5, 128.7, 129.5, 129.6, 129.8, 130.3, 131.7, 132.6, 136.8, 137.3, 151.2.



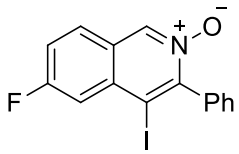
4-Iodo-3-(4-methoxyphenyl)isoquinoline 2-oxide (**3b**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.88 (s, 3H), 7.06 (d, J = 8.8 Hz, 2H), 7.33 (d, J = 8.8 Hz, 2H), 7.58-7.65 (m, 3H), 8.05 (d, J = 8.4Hz, 1H), 8.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.3, 102.4, 114.1, 125.1, 128.4, 129.6, 129.7, 130.2, 131.2, 131.7, 132.7, 136.7, 151.1, 160.3.



3-(4-Fluorophenyl)-4-iodoisoquinoline 2-oxide (**3c**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (t, J = 8.8 Hz, 2H), 7.36-7.39 (m, 2H), 7.61-7.66 (m, 3H), 8.05 (d, J = 8.0 Hz, 1H), 8.83 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 102.1, 115.9 (d, $^{2}J_{CF}$ = 22.0 Hz), 125.2, 128.5, 129.9, 130.4, 131.6, 131.9 (d, $^{3}J_{CF}$ = 9.0 Hz), 132.6, 133.2, 136.7, 150.2, 163.2 (d, $^{1}J_{CF}$ = 248.0 Hz); HRMS (ESI) calcd for $C_{15}H_{10}FINO$: 365.9786 ($M + H^+$), found: 365.9752.

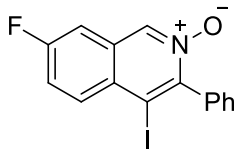


3-(4-Chlorophenyl)-4-iodoisoquinoline 2-oxide (**3d**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.60-7.68 (m, 3H), 8.05 (d, J = 8.0 Hz, 1H), 8.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.9, 125.3, 128.5, 129.1, 130.0, 133.5, 131.3, 131.6, 132.6, 135.6, 136.8, 150.5; HRMS (ESI) calcd for $C_{15}H_{10}ClINO$: 381.9490 ($M + H^+$), found: 381.9466.



6-Fluoro-4-iodo-3-phenylisoquinoline 2-oxide (**3e**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.40 (m, 3H), 7.47-7.56 (m, 3H), 7.69-7.73 (m, 1H), 7.77 (dd, J = 2.0, 10.0 Hz, 1H), 8.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 100.4, 117.3 (d, $^{2}J_{CF}$ = 24.0 Hz), 120.3 (d, $^{2}J_{CF}$ = 26.0 Hz), 125.5, 128.3 (d, $^{3}J_{CF}$ = 9.0 Hz), 128.8, 129.5, 129.6, 133.3 (d, $^{3}J_{CF}$ = 10.0

Hz), 136.5, 137.1, 152.0, 163.4 (d, $^{1}J_{CF}$ = 252.0 Hz); HRMS (ESI) calcd for $C_{15}H_{10}FINO$: 365.9786 (M + H^{+}), found: 365.9786.



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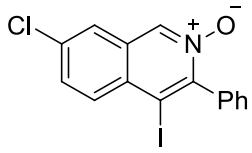
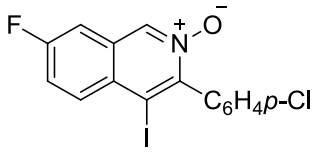
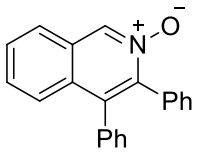
7-Fluoro-4-iodo-3-phenylisoquinoline 2-oxide (**3f**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.40 (m, 4H), 7.48-7.56 (m, 3H), 8.10 (dd, *J* = 5.2, 9.6 Hz, 1H), 8.79 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.4, 108.4 (d, $^{2}J_{CF}$ = 22.0 Hz), 120.1 (d, $^{2}J_{CF}$ = 25.0 Hz), 128.8, 129.5, 129.6, 135.6, 135.7, 135.8, 135.9, 150.8, 162.6 (d, $^{1}J_{CF}$ =252.0 Hz); HRMS (ESI) calcd for $C_{15}H_{10}FINO$: 365.9786 (M + H^{+}), found: 365.9795.



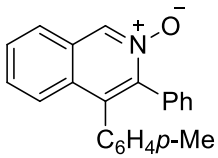
7-Chloro-4-iodo-3-phenylisoquinoline 2-oxide (**3g**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.0 Hz, 2H), 7.49-7.56 (m, 2H), 7.64-7.65 (m, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 8.75 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.4, 123.5, 128.8, 129.0, 129.5, 129.6, 129.9, 130.8, 134.3, 135.7, 136.0, 137.0, 151.6; HRMS (ESI) calcd for $C_{15}H_{10}ClINO$: 381.9490 (M + H^{+}), found: 381.9480.



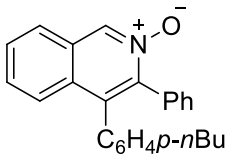
3-(4-Chlorophenyl)-7-fluoro-4-iodoisoquinoline 2-oxide (**3h**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.32 (m, 3H), 7.36-7.41 (m, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 8.09 (dd, *J* = 5.2, 9.2 Hz, 1H), 8.77 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 101.3, 108.4 (d, $^{2}J_{CF}$ = 23.0 Hz), 120.3 (d, $^{2}J_{CF}$ = 25.0 Hz), 128.6, 129.1, 129.3 (d, $^{3}J_{CF}$ = 10.0 Hz), 131.3, 135.3, 135.7, 135.8, 136.0, 149.6, 161.8 (d, $^{1}J_{CF}$ = 253.0 Hz); HRMS (ESI) calcd for $C_{15}H_9ClFINO$: 399.9396 (M + H^{+}), found: 399.9402.



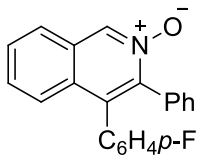
3,4-Diphenylisoquinoline 2-oxide (**4a**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12-7.14 (m, 2H), 7.22-7.28 (m, 8H), 7.45-7.46 (m, 1H), 7.57-7.61 (m, 1H), 7.64-7.71 (m, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 8.98 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.7, 126.3, 127.7, 127.8, 128.2, 128.3, 128.8, 129.0, 129.1, 130.4, 130.7, 132.1, 132.2, 135.0, 136.0, 137.0, 146.2.



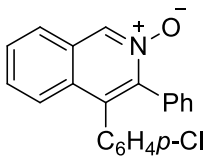
3-Phenyl-4-(p-tolyl)isoquinoline 2-oxide (**4b**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.31 (s, 3H), 7.00 (d, *J* = 8.0 Hz, 2H), 7.08 (m, *J* = 8.0 Hz, 2H), 7.25-7.26 (m, 5H), 7.47-7.48 (m, 2H), 7.57-7.62 (m, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 9.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 125.0, 126.4, 137.8, 128.3, 128.5, 128.9, 129.0, 129.1, 130.3, 130.8, 131.8, 132.1, 132.2, 136.3, 137.2, 137.6, 146.0.



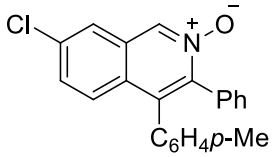
4-(4-(*tert*-Butyl)phenyl)-3-phenylisoquinoline 2-oxide (**4c**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (s, 9H), 7.03 (d, *J* = 8.4, 2H), 7.23-7.29 (m, 7H), 7.45-7.50 (m, 2H), 7.57-7.61 (m, 1H), 7.64-7.71 (m, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 8.98 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.3, 124.7, 125.0, 126.5, 127.7, 128.2, 128.6, 130.0, 130.1, 130.8, 131.8, 132.0, 132.1, 132.2, 132.3, 135.9, 150.8.



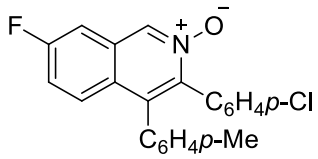
4-(4-Fluorophenyl)-3-phenylisoquinoline 2-oxide (**4d**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (t, *J* = 8.4 Hz, 2H), 7.08-7.12 (m, 2H), 7.21-7.26 (m, 4H), 7.41-7.49 (m, 3H), 7.59-7.62 (m, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 8.99 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 115.4 (d, $^{2}J_{CF}$ = 22.0 Hz), 124.9, 126.0, 128.0, 128.5, 128.6, 128.9, 129.0, 129.2, 129.4, 130.7, 131.0 (d, $^{3}J_{CF}$ = 7.0 Hz), 132.2 (d, $^{3}J_{CF}$ = 8.0 Hz), 136.0, 136.3, 146.4, 162.2 (d, $^{1}J_{CF}$ = 247.0 Hz).



4-(4-Chlorophenyl)-3-phenylisoquinoline 2-oxide (**4e**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.4 Hz, 2H), 7.21-7.27 (m, 6H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.48-7.52 (m, 1H), 7.60-7.70 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 8.98 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 125.0, 125.9, 128.0, 128.5, 128.6, 128.9, 129.2, 129.3, 130.7, 131.8, 132.1, 132.2, 133.4, 134.0, 135.8, 136.5, 146.2.



7-Chloro-3-phenyl-4-(p-tolyl)isoquinoline 2-oxide (**4f**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.3 (s, 3H), 6.98 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.24-7.25 (m, 5H), 7.34 (dd, *J* = 2.0, 9.2 Hz, 1H), 7.40 (d, *J* = 9.2 Hz, 1H), 7.72 (d, *J* = 2.0 Hz, 1H), 8.87 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 123.1, 127.7, 127.9, 128.2, 128.4, 129.0, 129.3, 129.7, 130.2, 130.7, 131.5, 131.9, 134.9, 135.1, 137.1, 137.9, 146.6.



3-(4-Chlorophenyl)-7-fluoro-4-(*p*-tolyl)isoquinoline 2-oxide (**4g**).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 7.6 Hz, 2H), 7.16-7.23 (m, 4H), 7.37 (dd,

J = 2.4, 8.8 Hz, 1H), 7.45-7.47 (m, 2H), 7.64-7.67 (m, 1H), 8.88 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 108.1 (d, $^2J_{CF}$ = 23.0 Hz), 118.9 (d, $^2J_{CF}$ = 25.0 Hz), 126.4, 128.2, 128.5, 128.6, 129.2, 129.4, 130.1, 130.5, 131.4, 132.0, 132.1 (d, $^3J_{CF}$ = 10.0 Hz), 135.2 (d, $^3J_{CF}$ = 6.0 Hz), 138.2, 144.5, 162.3 (d, $^1J_{CF}$ = 251.0 Hz).

Reference:

1. Q. Ding and J. Wu, *Adv. Synth. Catal.*, 2008, **350**, 1850.

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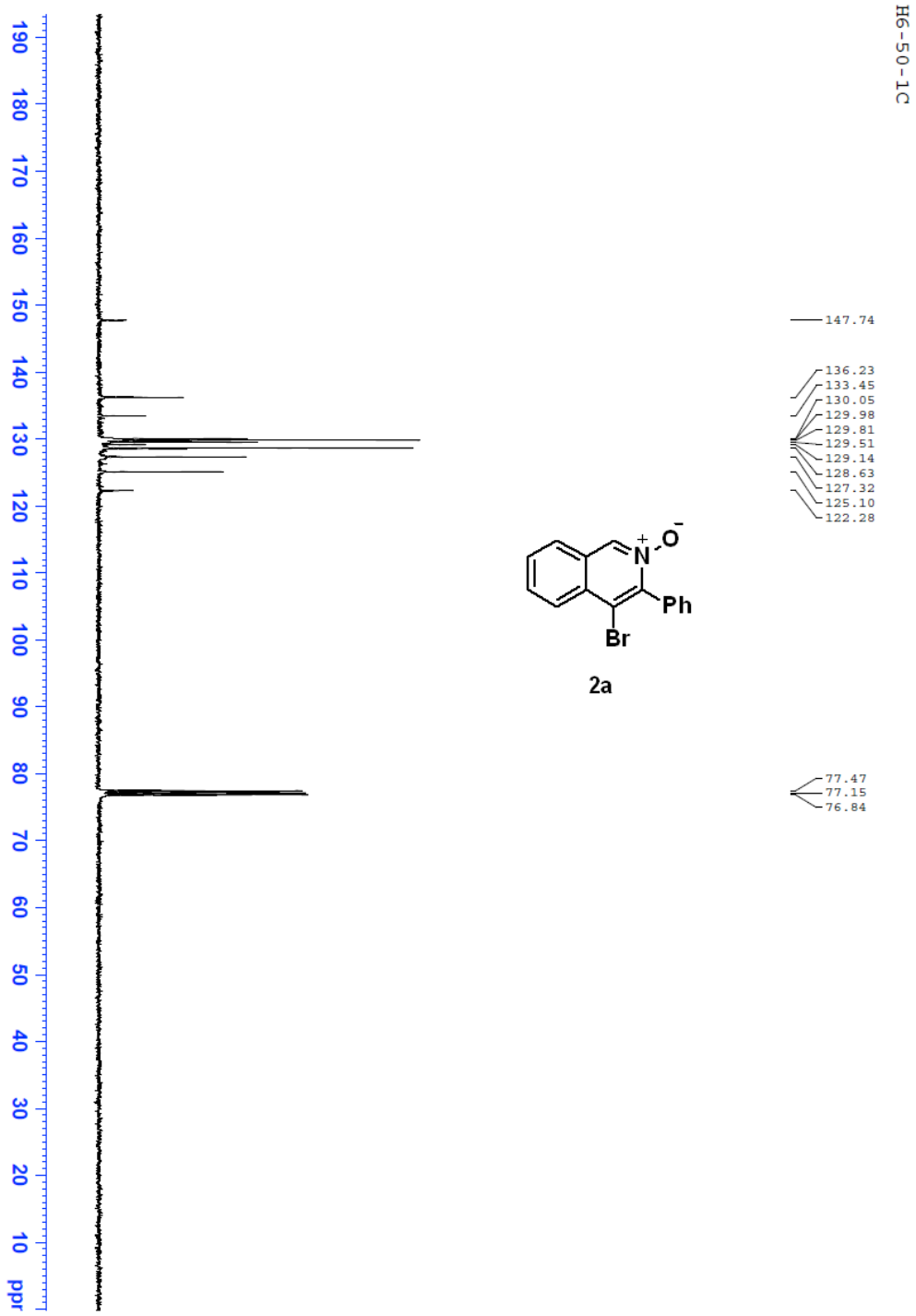

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7.451
7.443
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1.00
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DE 6.50 usec
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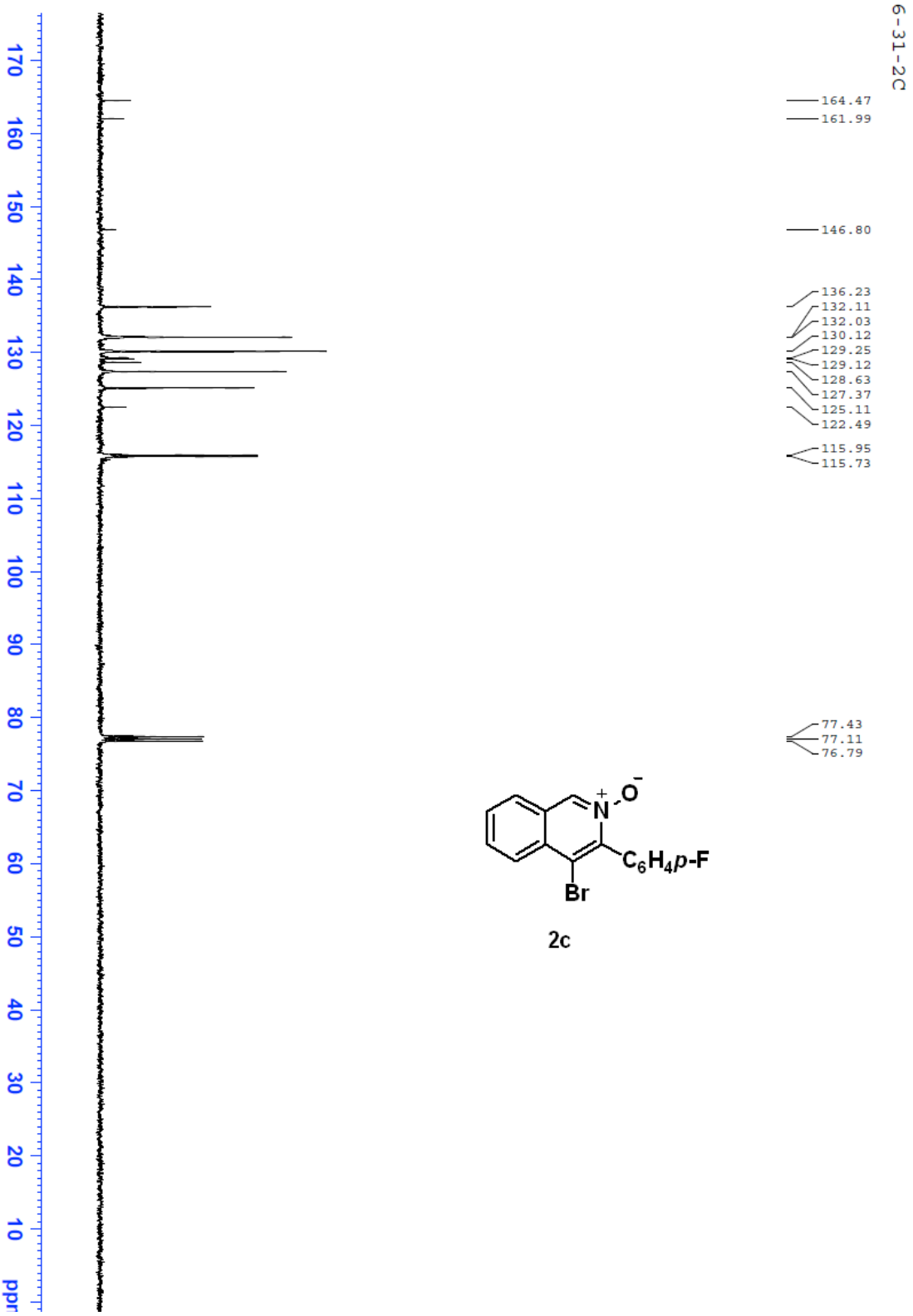

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3.11
2.07
2.13
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C6H4p-Cl
2d
BRUKER
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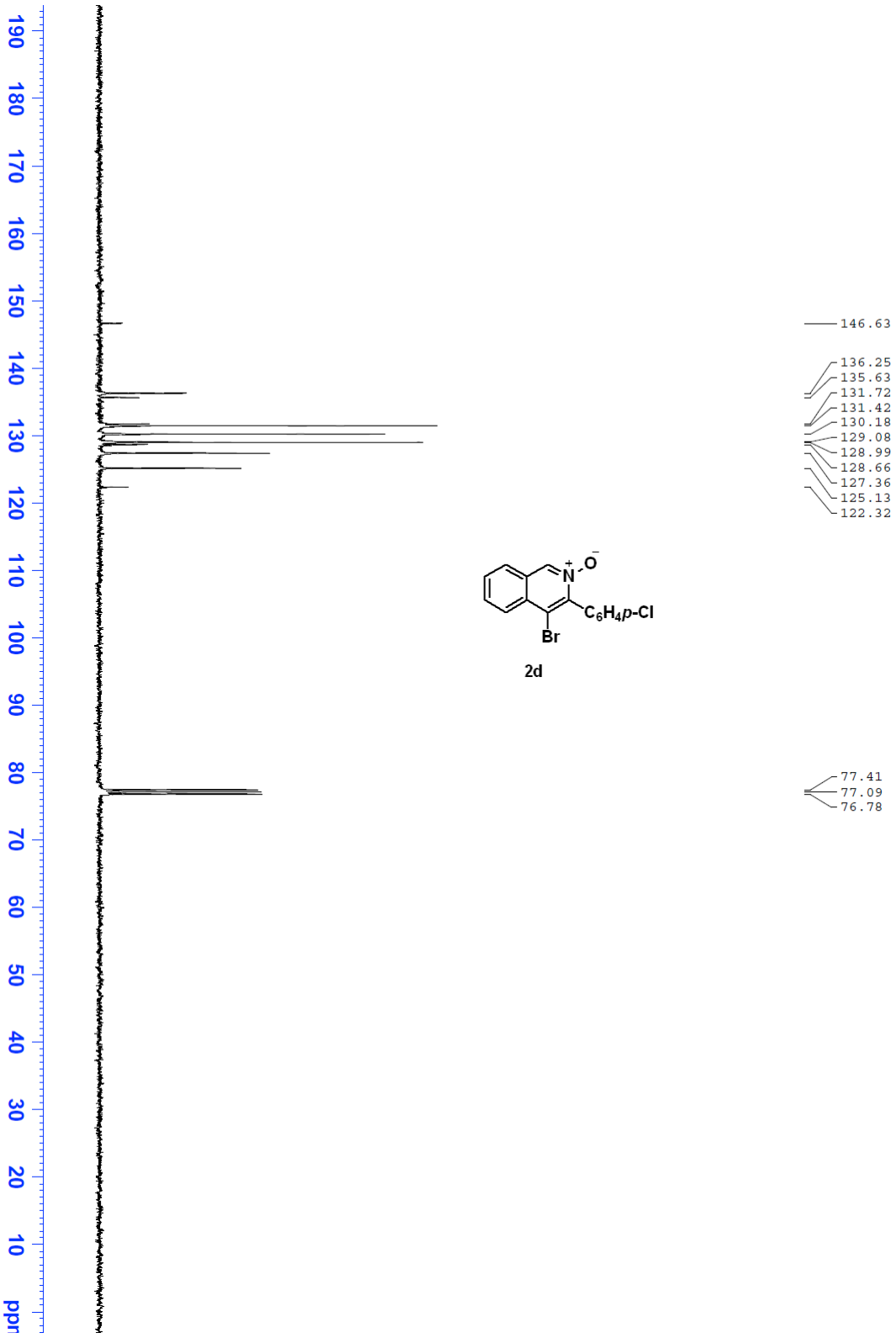
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O
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Br
2d
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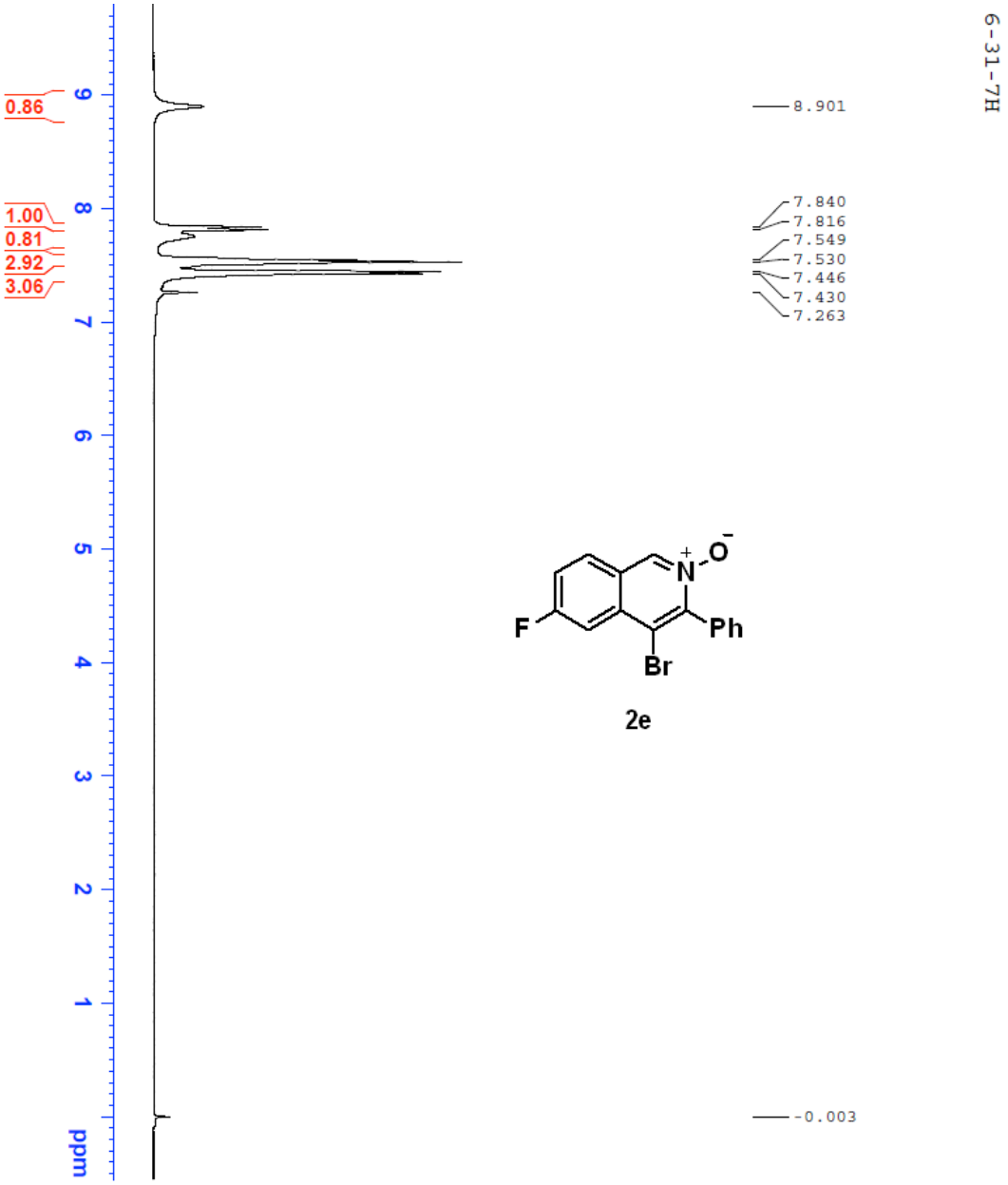

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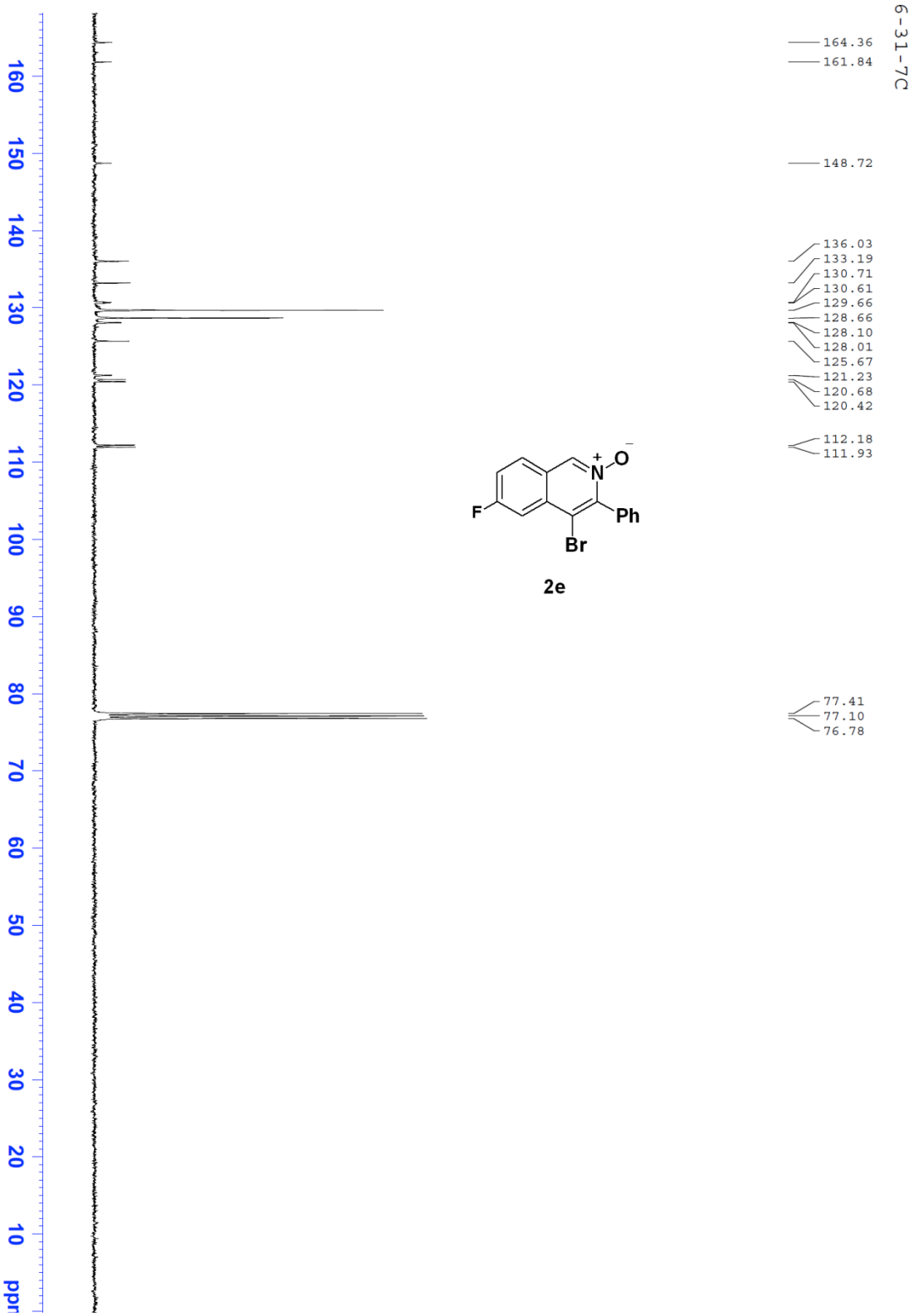
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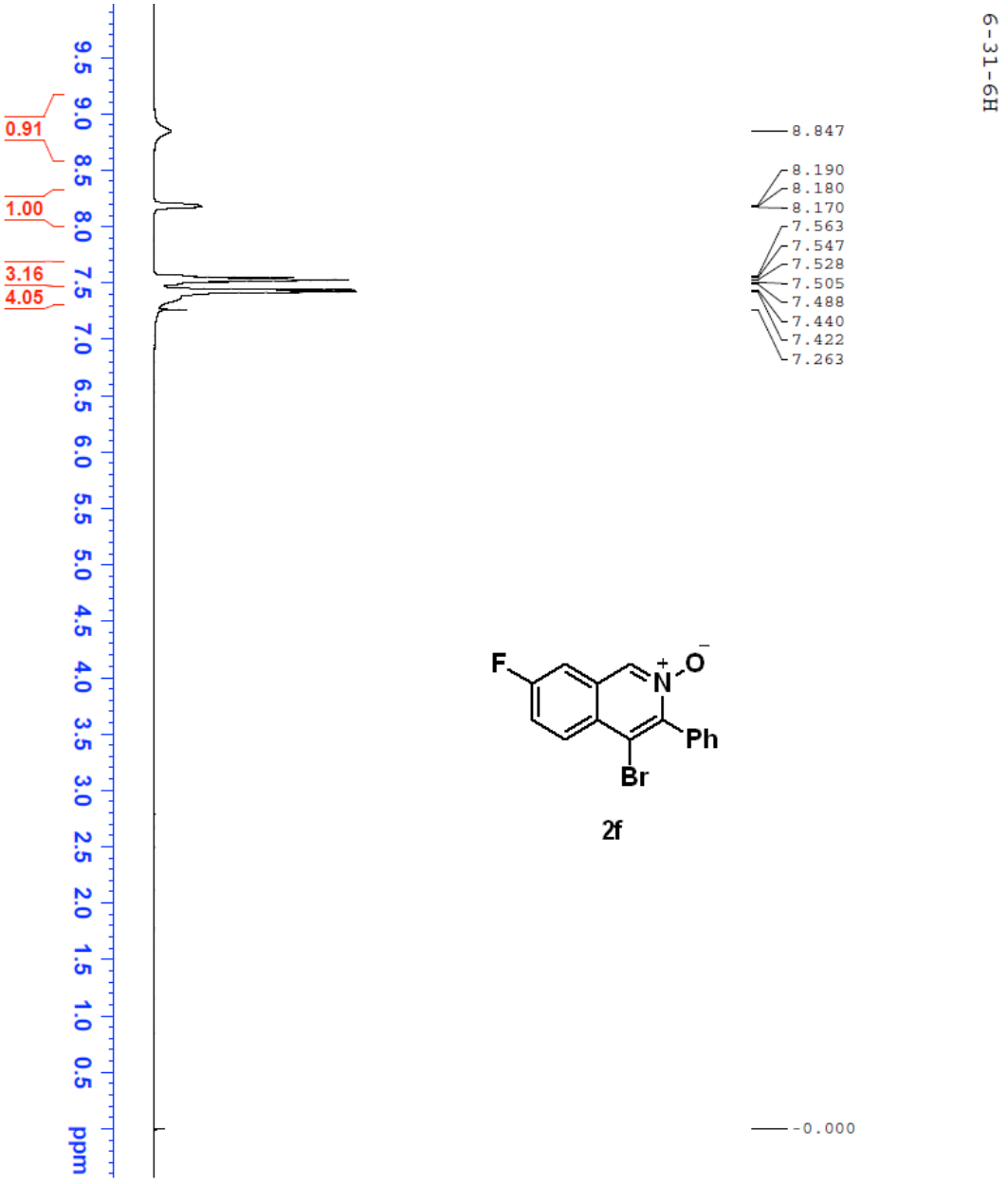
Ph
Br

2e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Br
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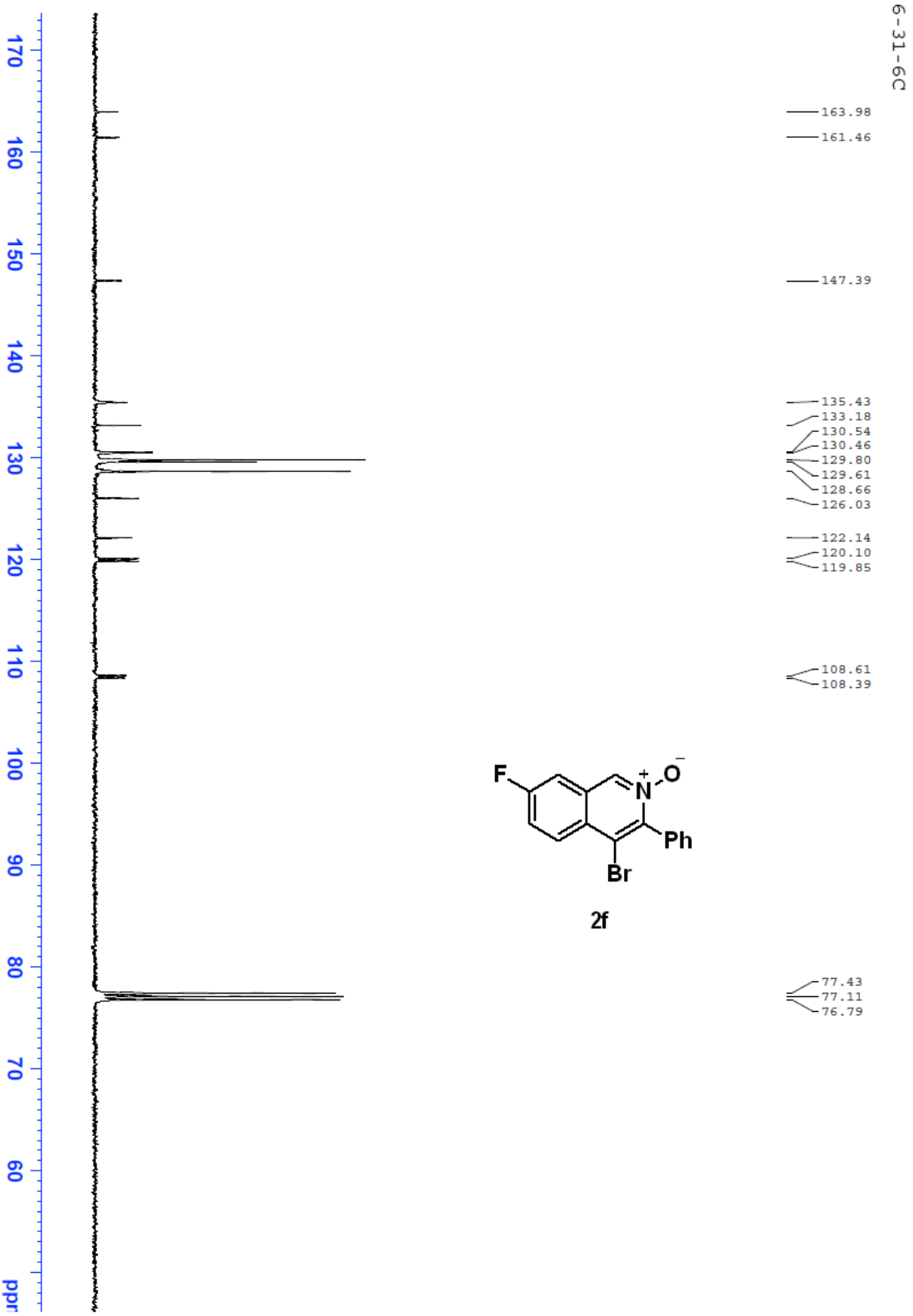
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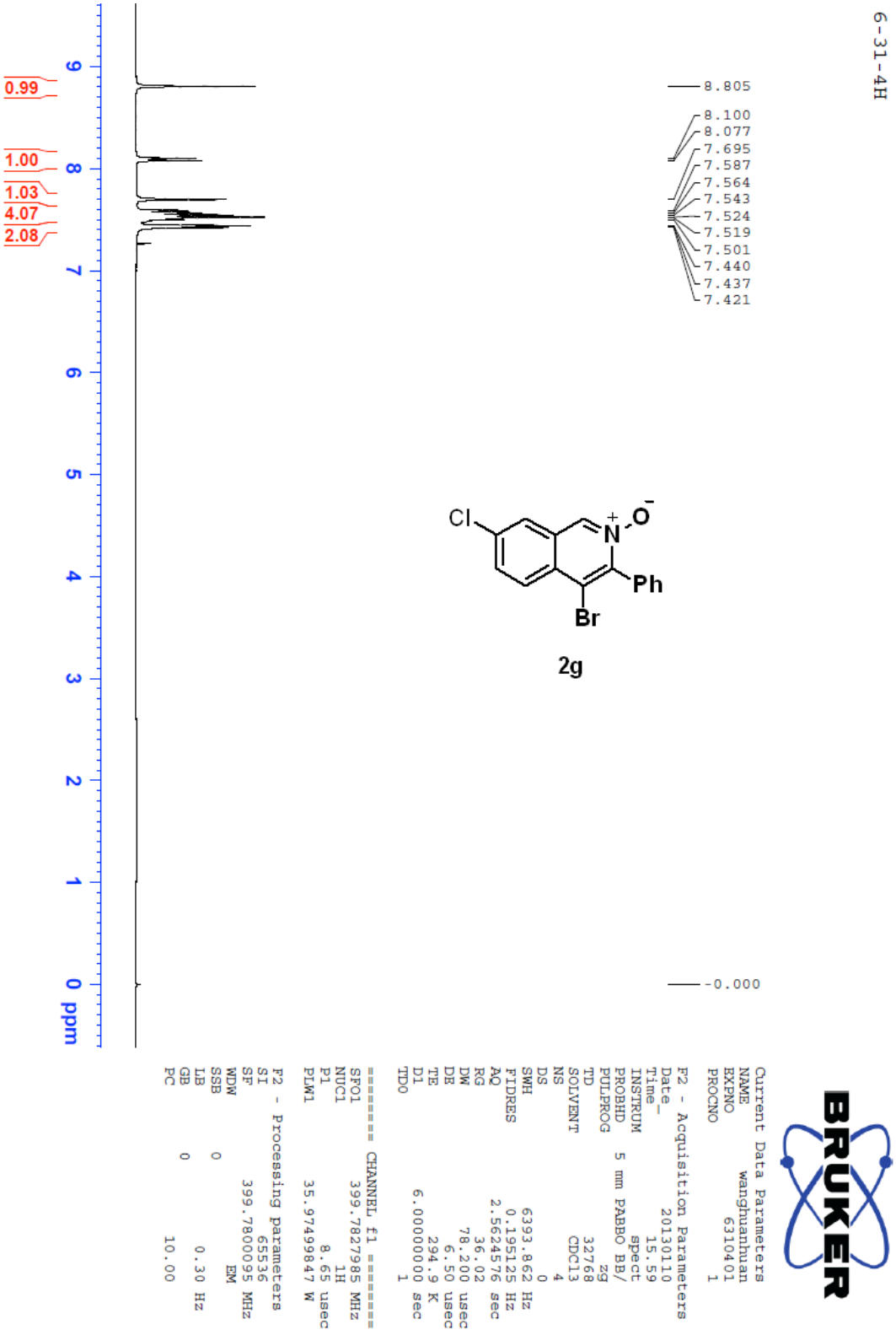
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6
5
4
3
2
1
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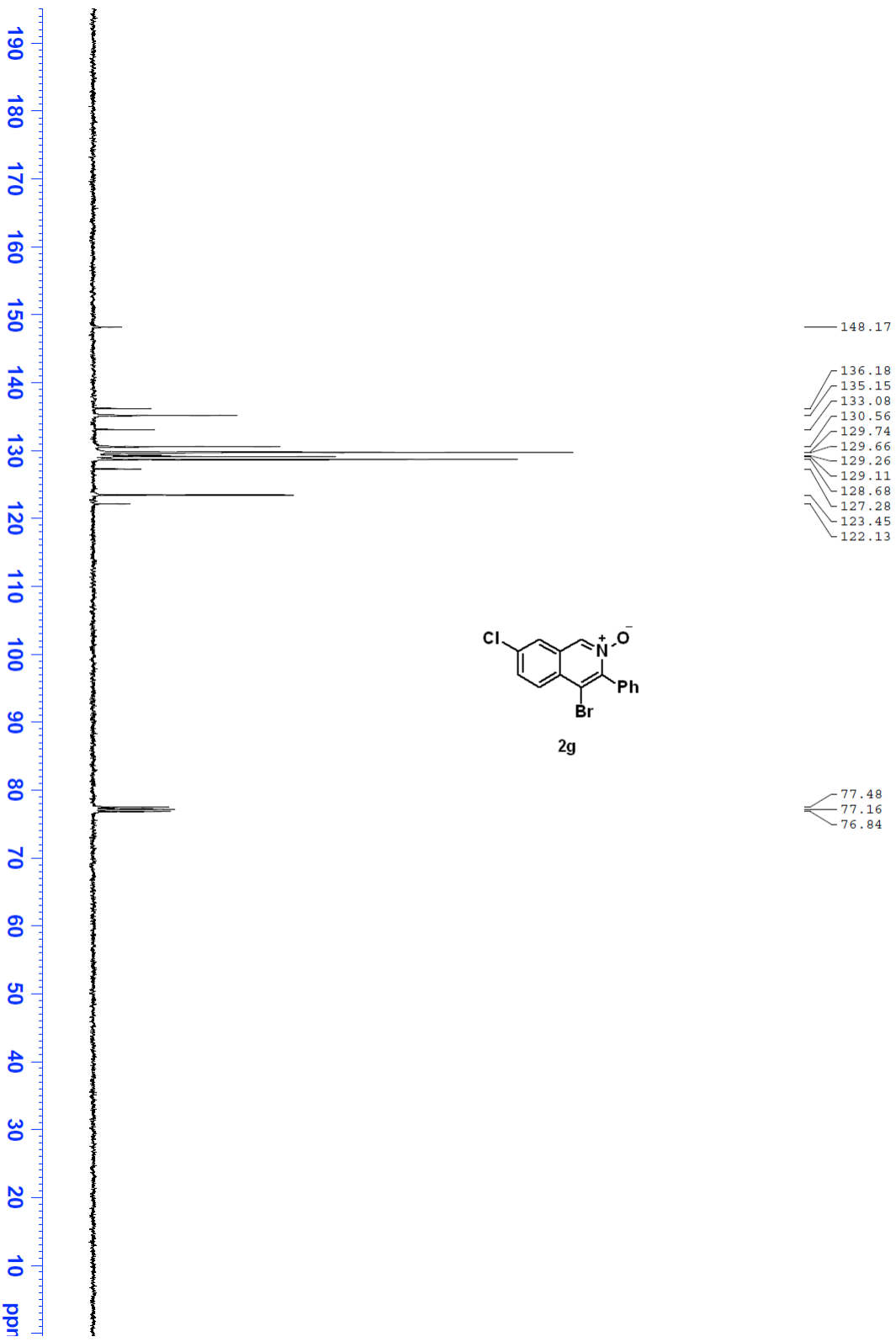

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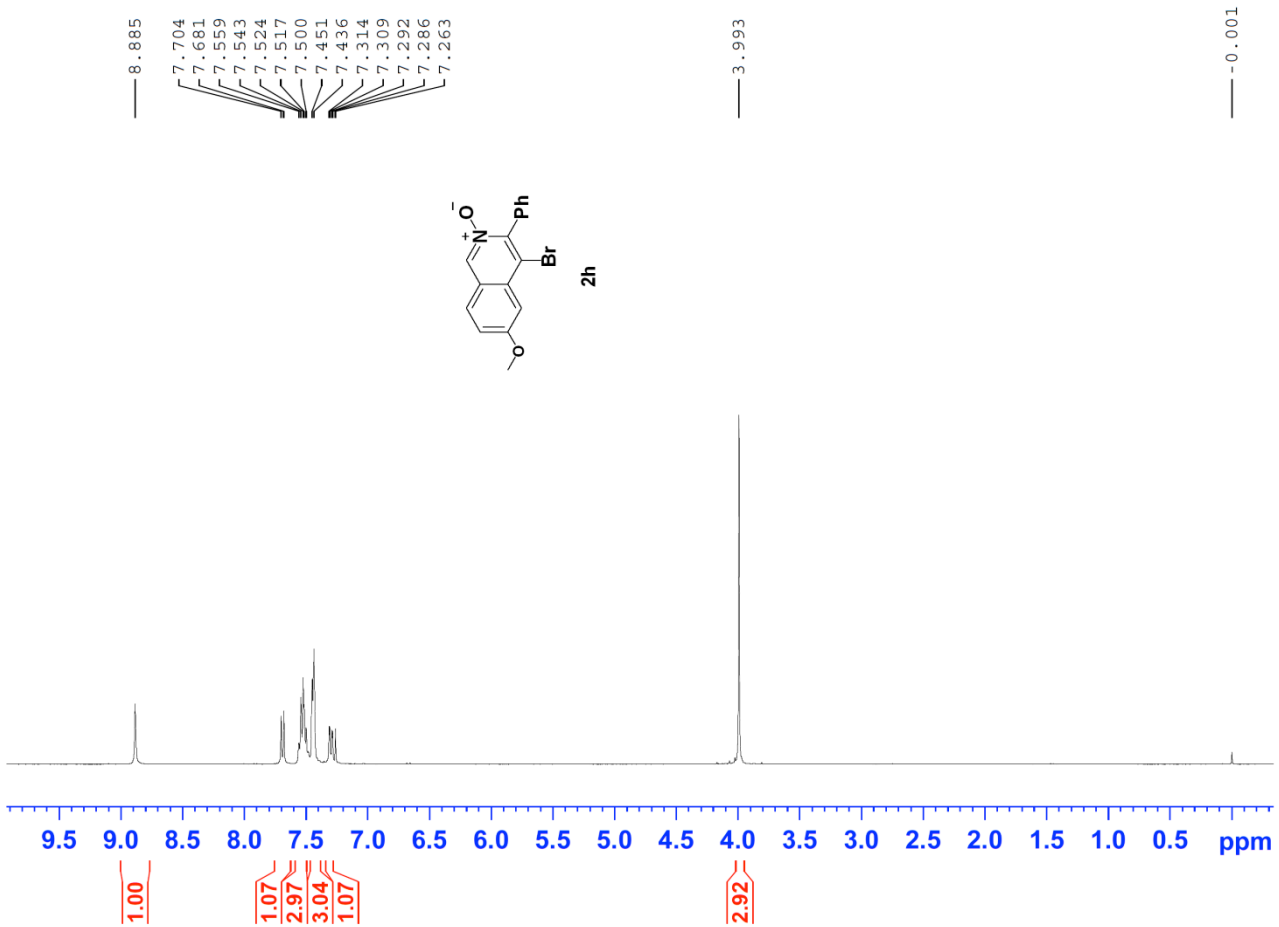

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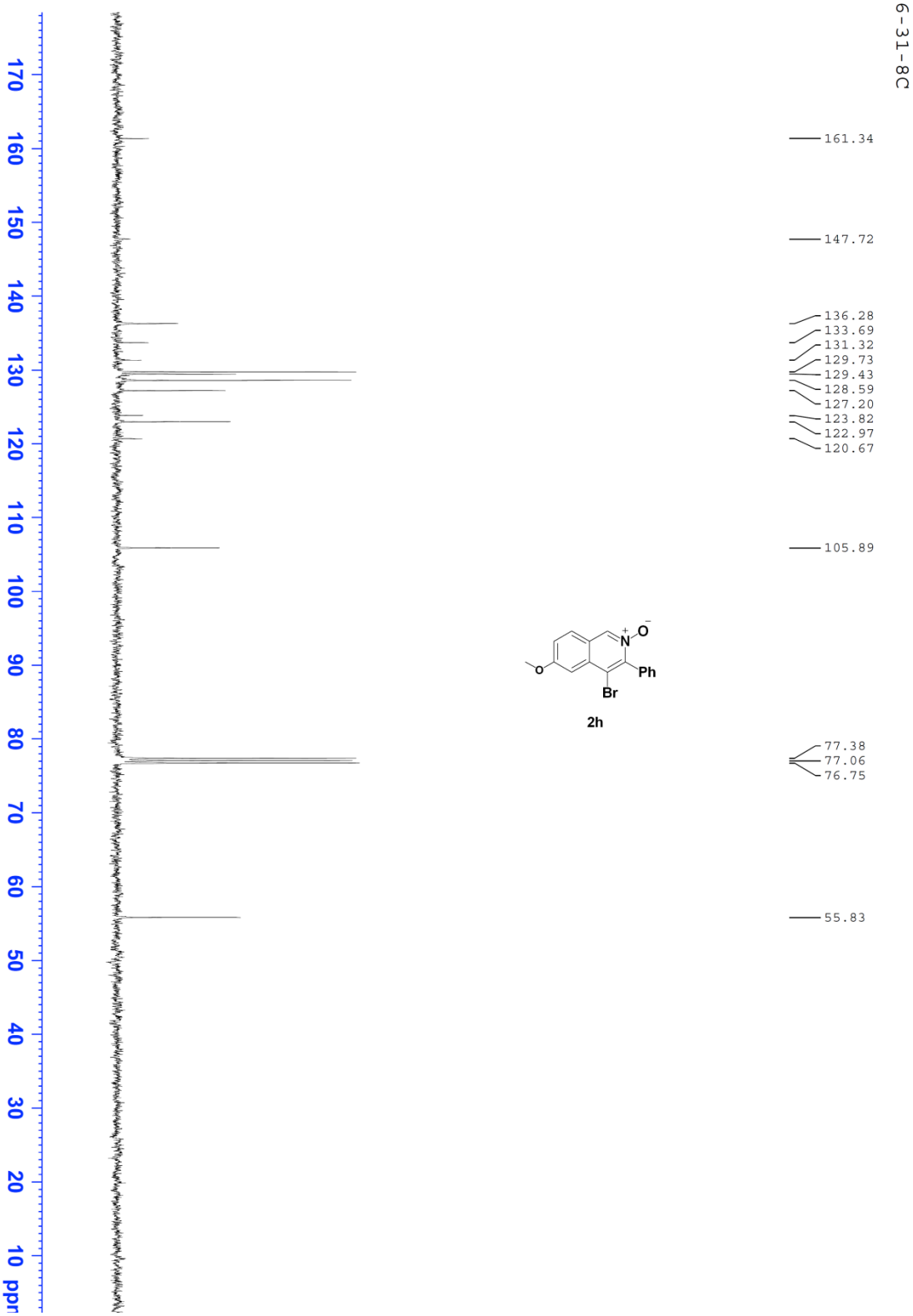

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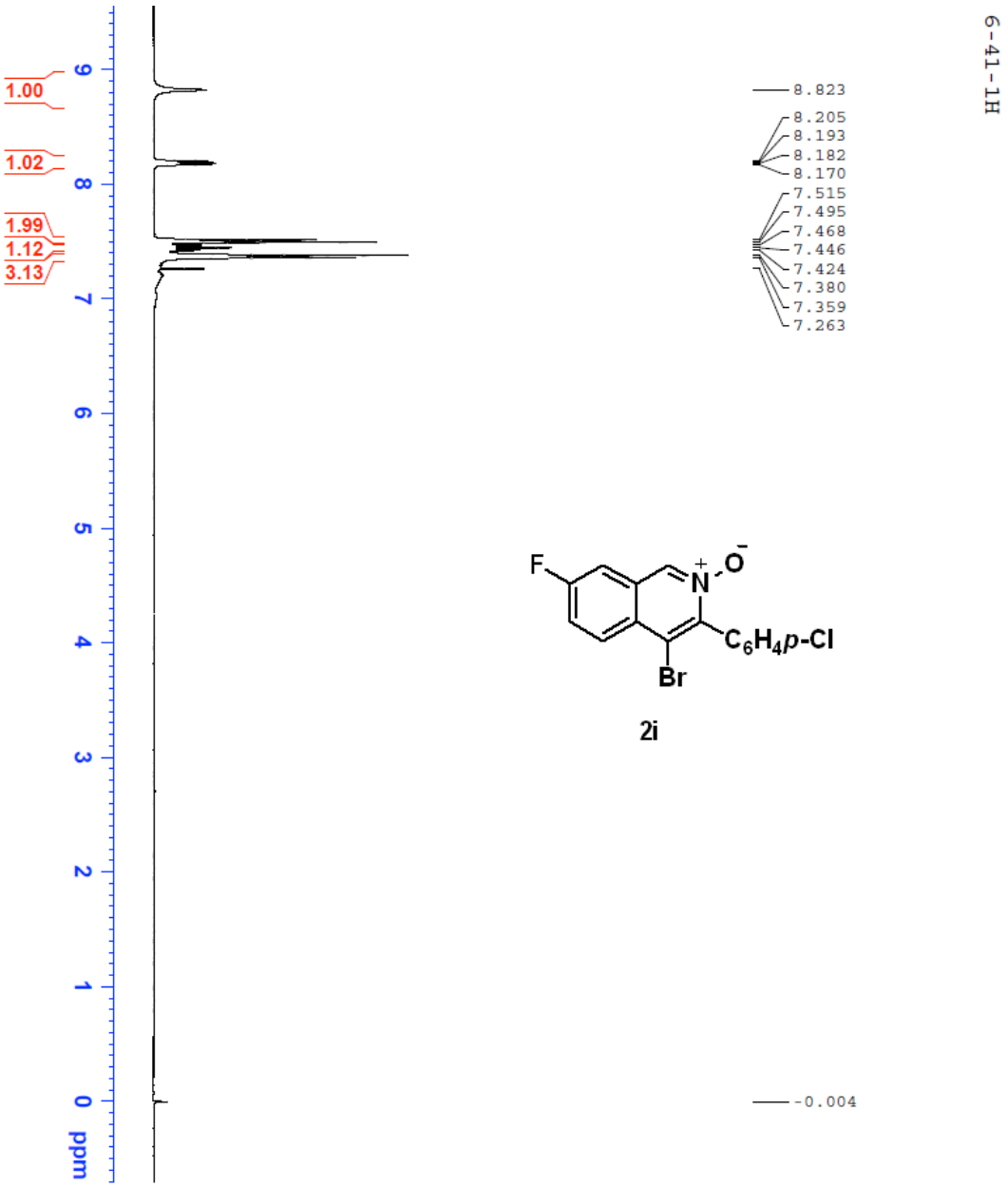
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N
O
Br
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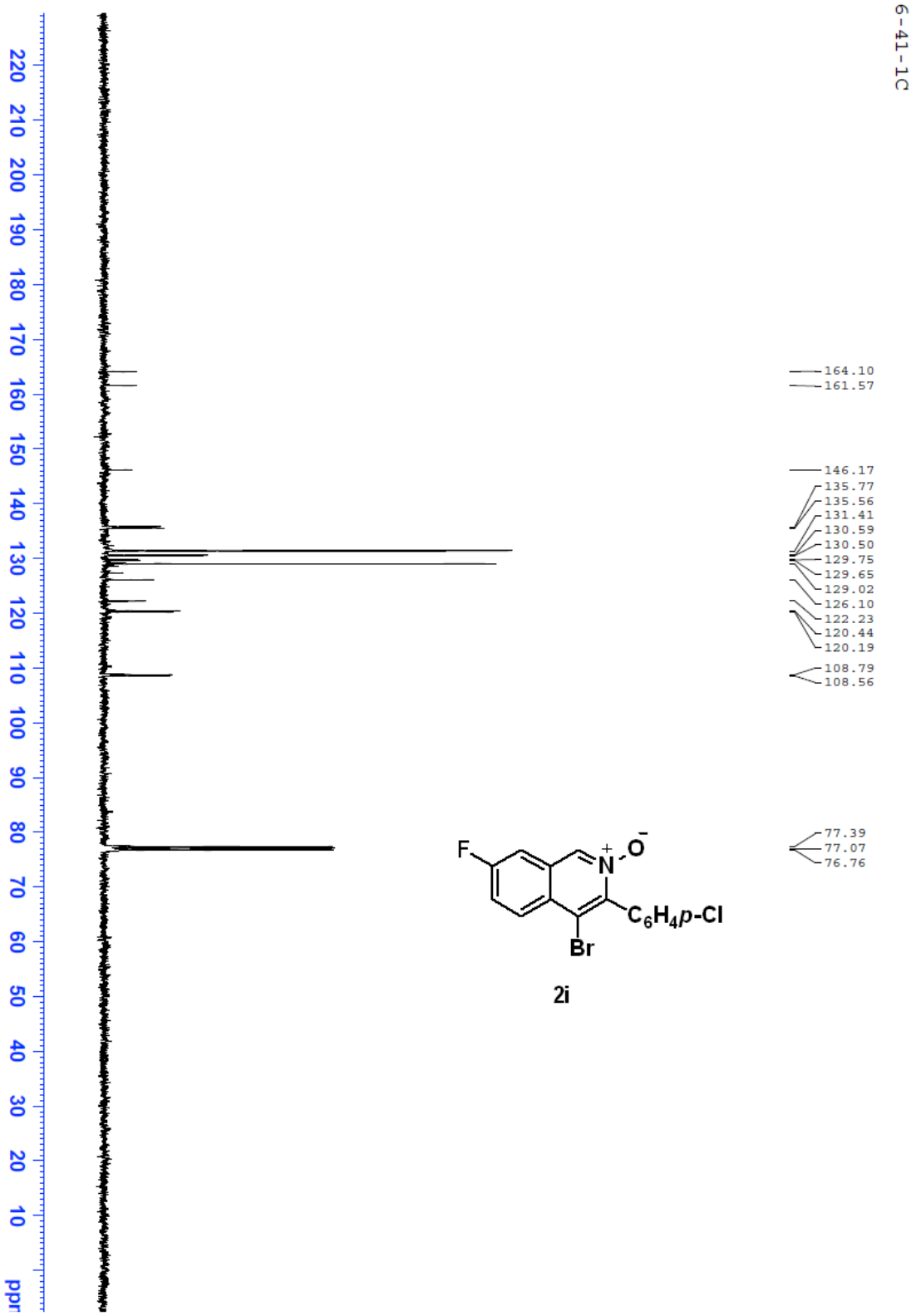
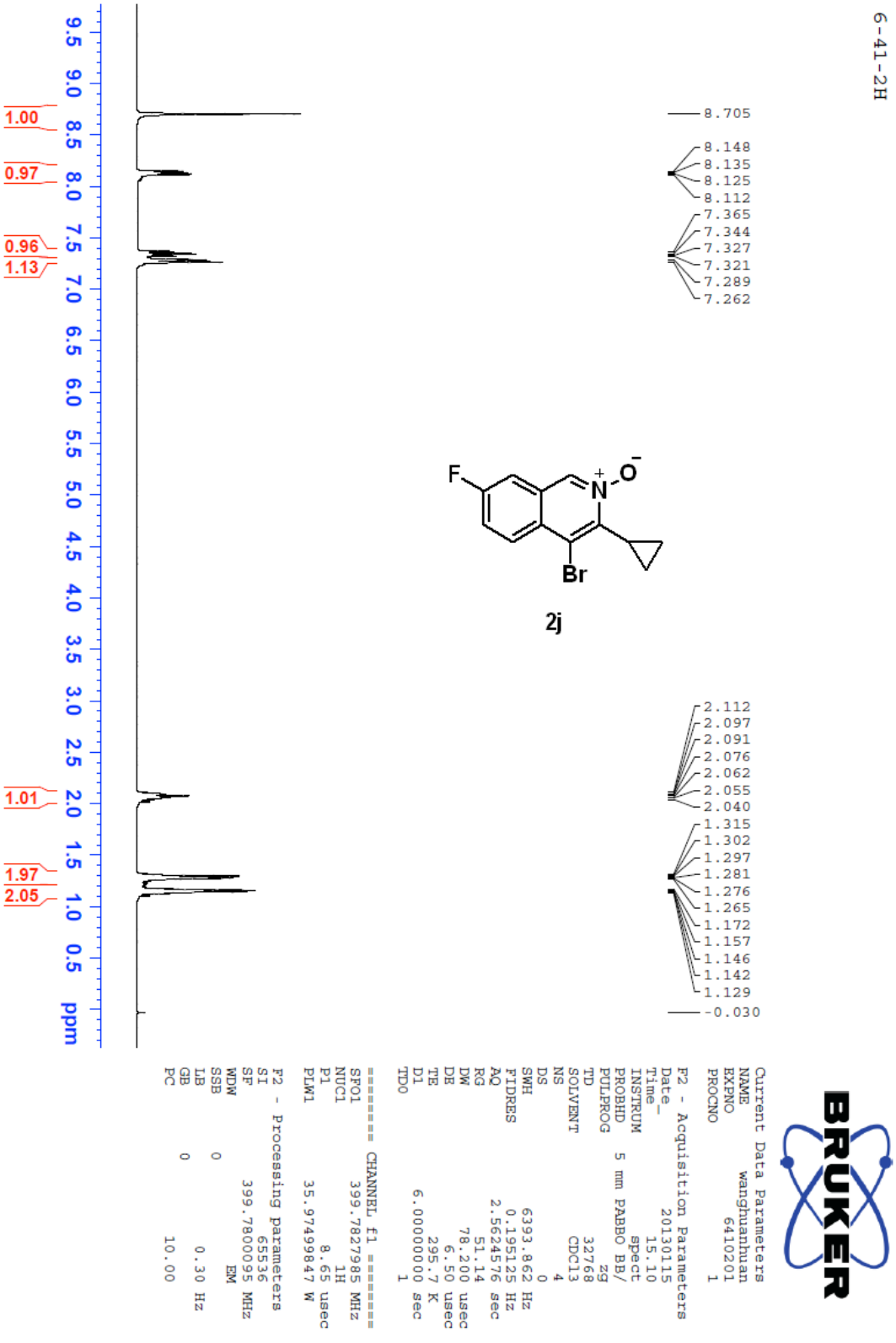
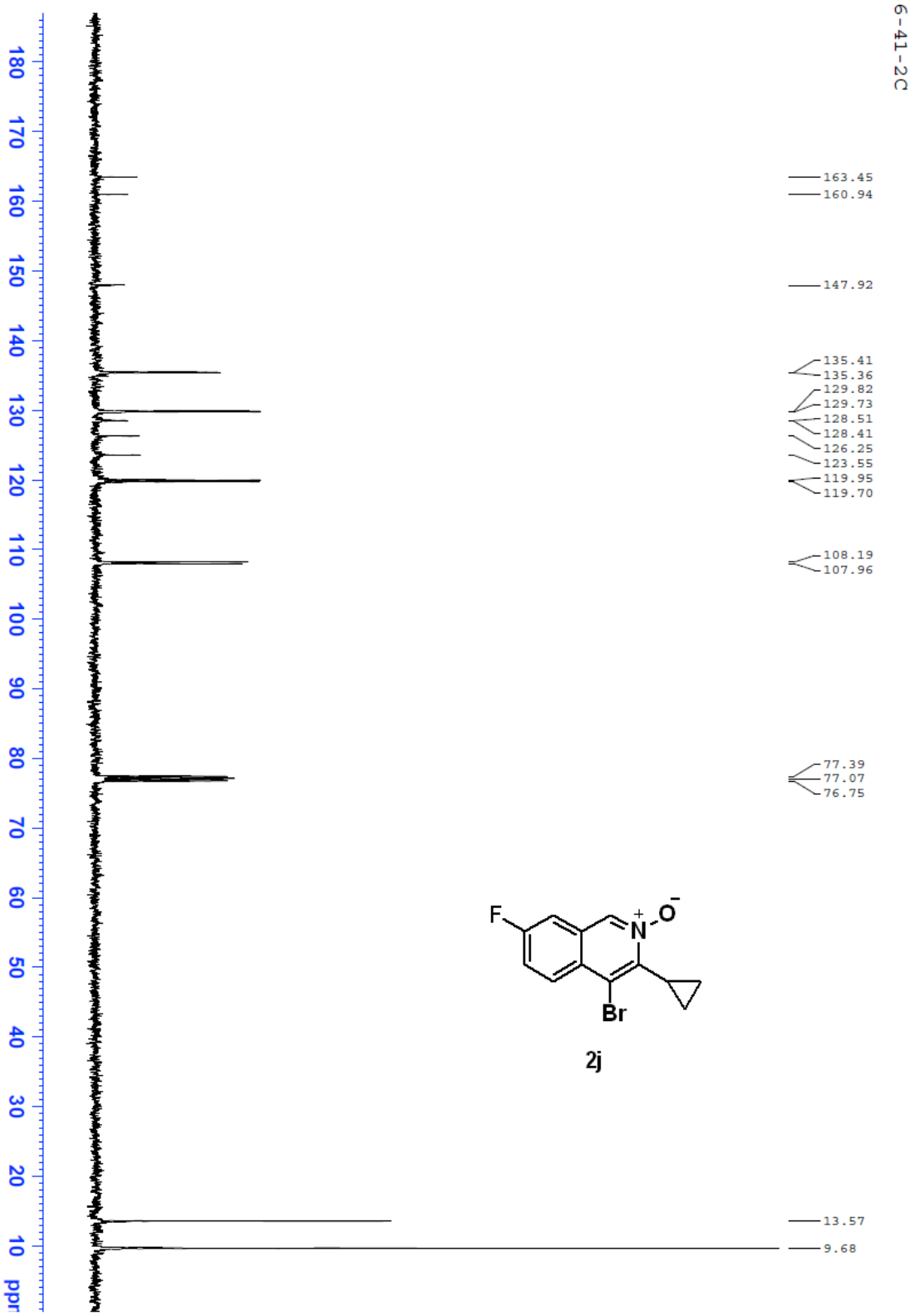
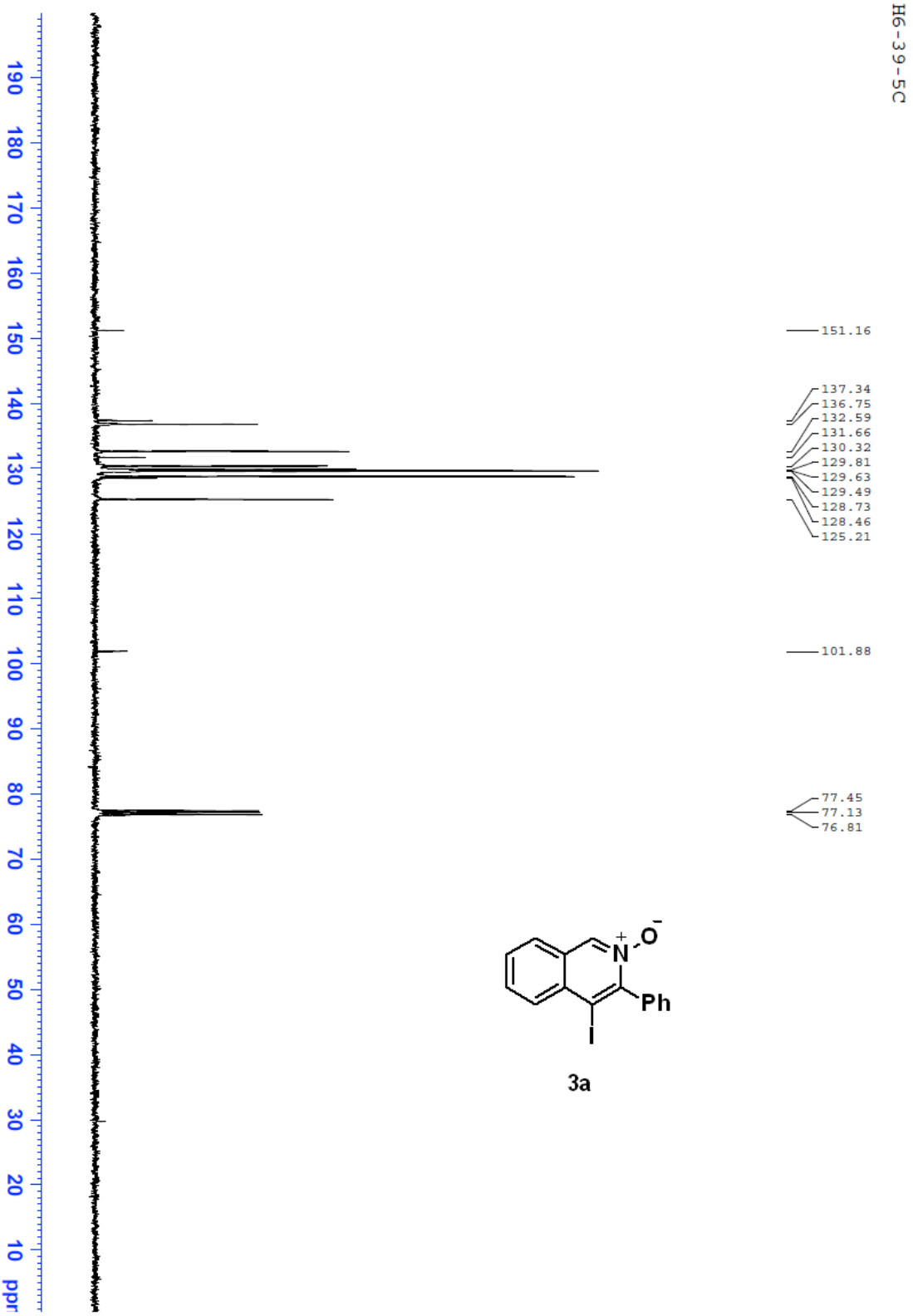
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 51.14
DW 78.200 usec
DE 6.50 usec
TE 298.0 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00


6-41-1C
164.10
161.57
146.17
135.77
135.56
131.41
130.59
130.50
129.75
129.65
129.02
126.10
122.23
120.44
120.19
108.79
108.56
77.39
77.07
76.76
F
N
O
C6H4p-Cl
Br
2i
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

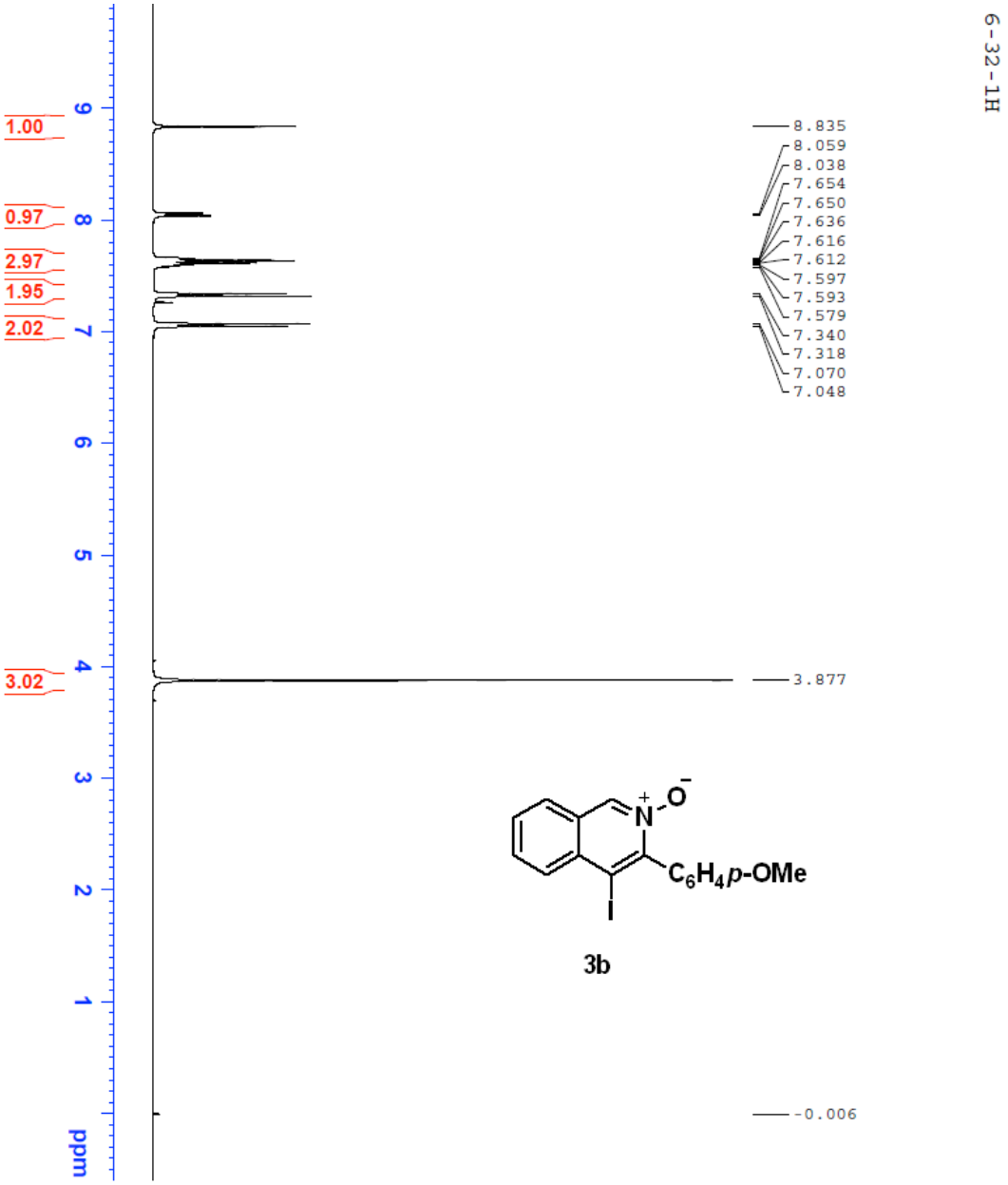

6-41-2H
8.705
8.148
8.135
8.125
8.112
7.365
7.344
7.327
7.321
7.289
7.262
F
N
O
Br
2j
2.112
2.097
2.091
2.076
2.062
2.055
2.040
1.315
1.302
1.297
1.281
1.276
1.265
1.172
1.157
1.146
1.142
1.129
-0.030
1.00
0.97
0.96
1.13
1.01
1.97
2.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
Current Data Parameters
NAME wanghuanhuan
EXPNO 6410201
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130115
Time_ 15.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 51.14
DW 78.200 usec
DE 6.50 usec
TE 295.7 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00

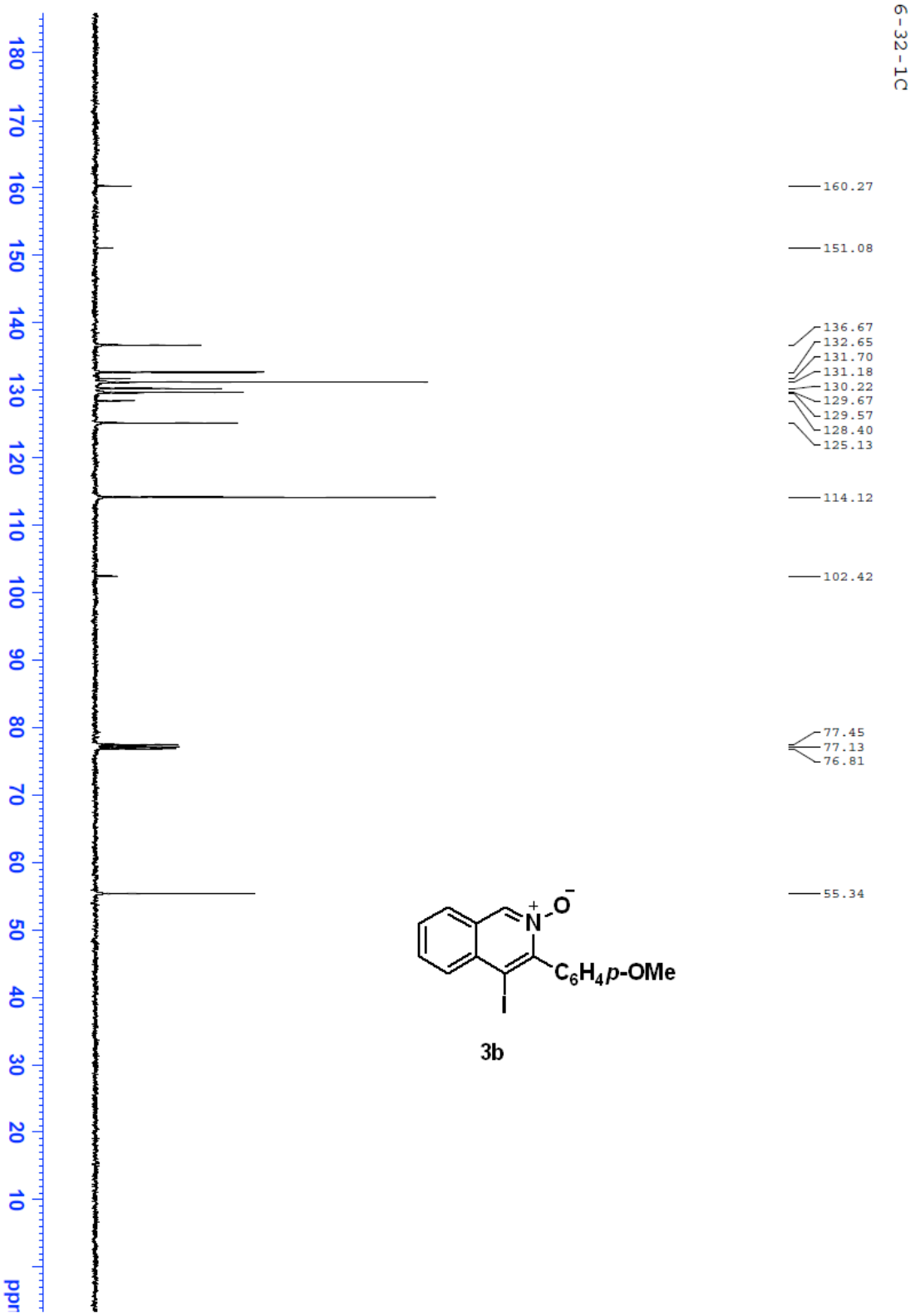

6-41-2C
163.45
160.94
147.92
135.41
135.36
129.82
129.73
128.51
128.41
126.25
123.55
119.95
119.70
108.19
107.96
77.39
77.07
76.75
13.57
9.68
F
N
O
Br
2j
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

H6-39-5H
8.856
8.075
8.055
7.675
7.657
7.637
7.615
7.570
7.553
7.534
7.519
7.501
7.482
7.400
7.396
7.380
7.263
0.001
1.00
0.99
3.01
3.07
2.05
ppm
9
8
7
6
5
4
3
2
1
Ph
3a
Current Data Parameters
NAME wanghuanhuan
EXPNO 6390501
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130322
Time_ 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 38.64
DW 78.200 use
DE 6.50 use
TE 293.6 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 =======
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 use
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00



3a


6-32-1H
8.835
8.059
8.038
7.654
7.650
7.636
7.616
7.612
7.597
7.593
7.579
7.340
7.318
7.070
7.048
3.877
-0.006
1.00
0.97
2.97
1.95
2.02
3.02
ppm
3b
Current Data Parameters
NAME wanghuanhuan
EXPNO 6320101
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130115
Time_ 15.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 51.14
DW 78.200 usec
DE 6.50 usec
TE 295.7 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00



3b

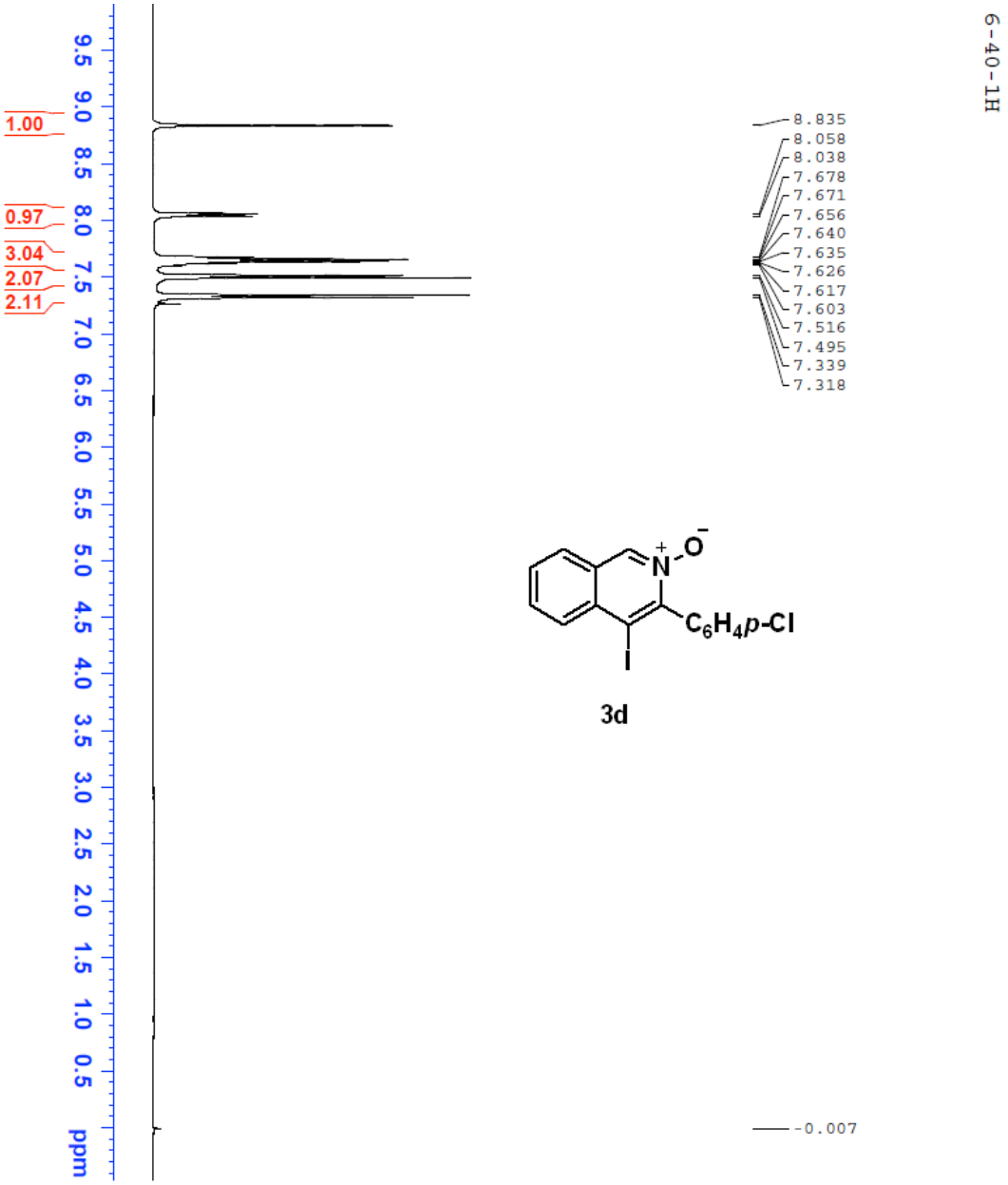
6-40-5H
8.829
8.060
8.040
7.663
7.649
7.632
7.627
7.619
7.609
7.390
7.385
7.377
7.368
7.355
7.237
7.215
7.193
1.00
0.98
3.00
2.01
2.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
-0.006
Current Data Parameters
NAME wanghuanhuan
EXPNO 6400501
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130121
Time_ 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 23.07
DW 78.200 usec
DE 6.50 usec
TE 302.0 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00

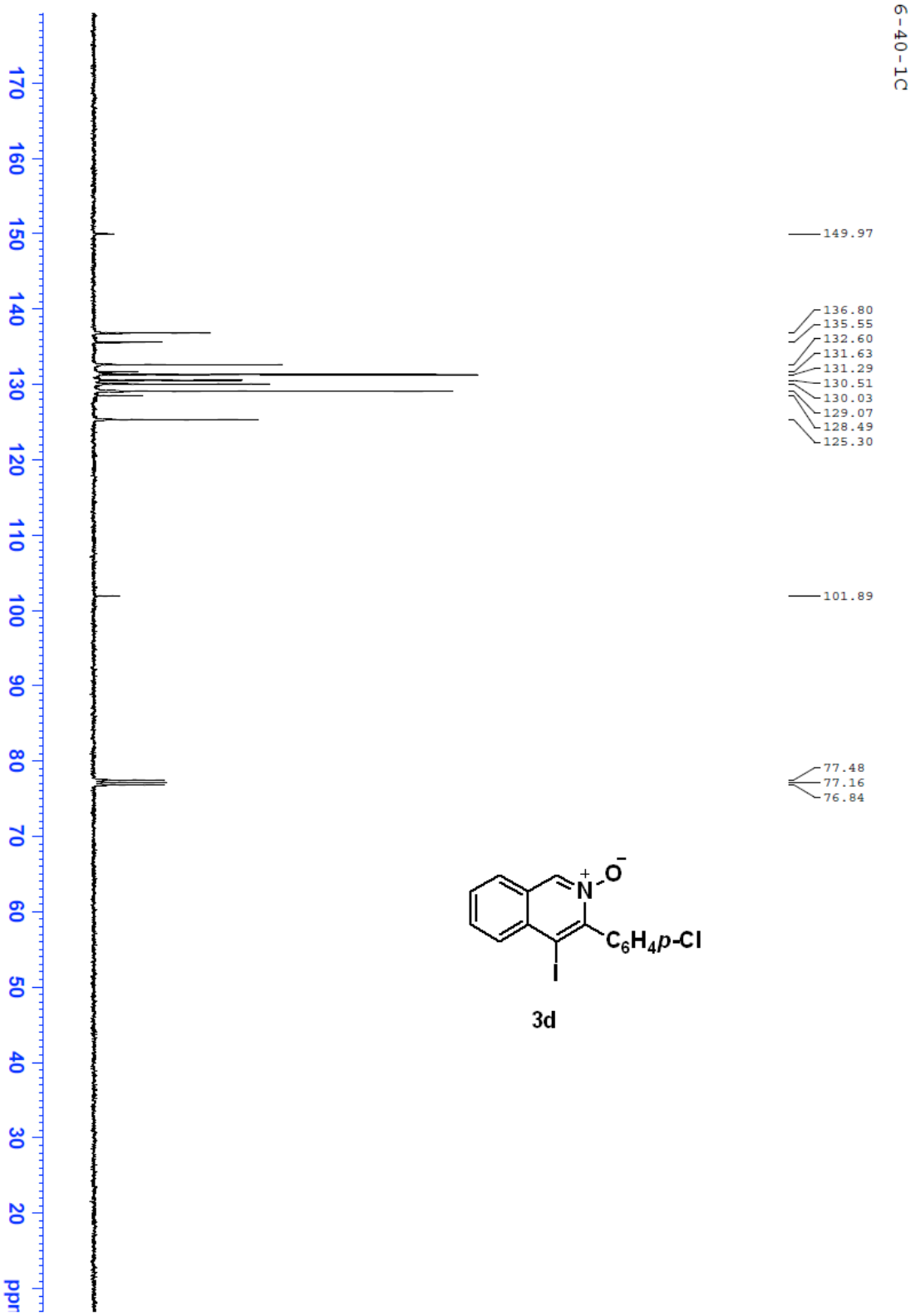
N
O
C6H4p-F
I

3c

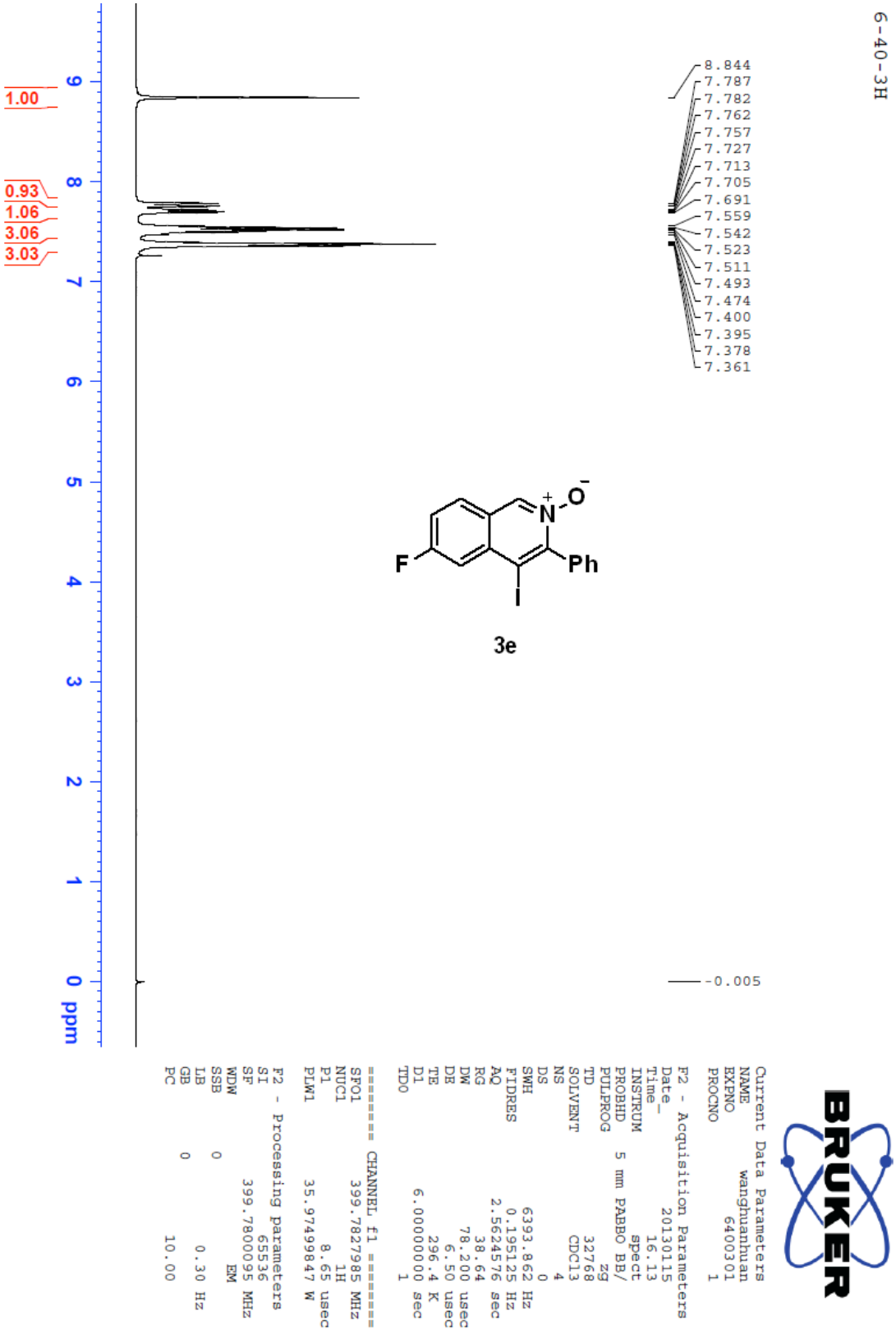

6-40-5C
164.45
161.97
150.20
136.72
133.20
132.63
131.96
131.87
131.63
130.40
129.93
128.51
125.22
116.00
115.78
102.12
77.45
77.13
76.82
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
N
O
C6H4p-F
I

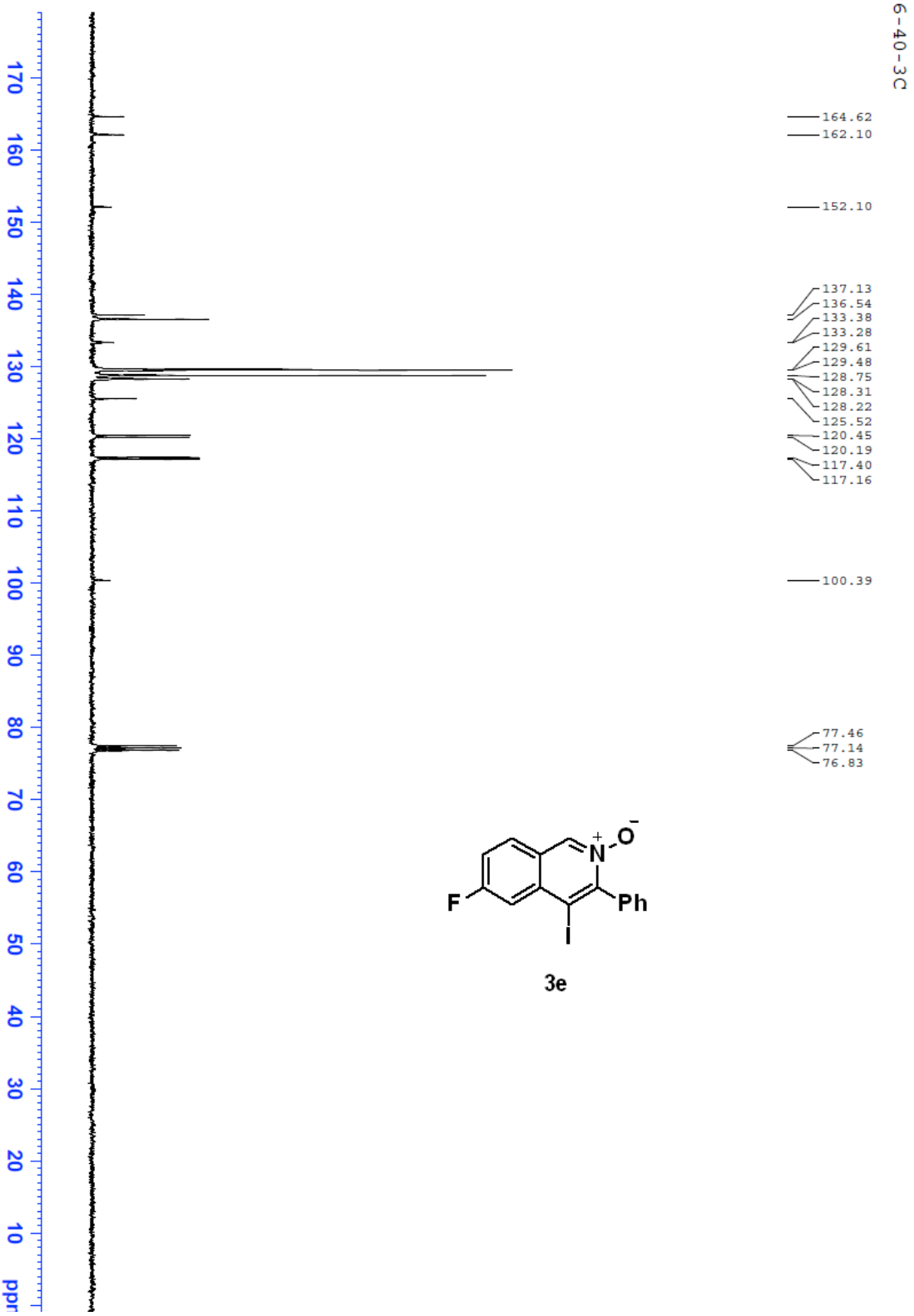
3c


6-40-1H
8.835
8.058
8.038
7.678
7.671
7.656
7.640
7.635
7.626
7.617
7.603
7.516
7.495
7.339
7.318
1.00
0.97
3.04
2.07
2.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
-0.007
C_6H_4p-Cl
3d
Current Data Parameters
NAME wanghuanhuan
EXPNO 6400101
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130115
Time_ 16.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 36.02
DW 78.200 usec
DE 6.50 usec
TE 296.3 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00


6-40-1C
149.97
136.80
135.55
132.60
131.63
131.29
130.51
130.03
129.07
128.49
125.30
101.89
77.48
77.16
76.84
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
N
O
C6H4p-Cl
I

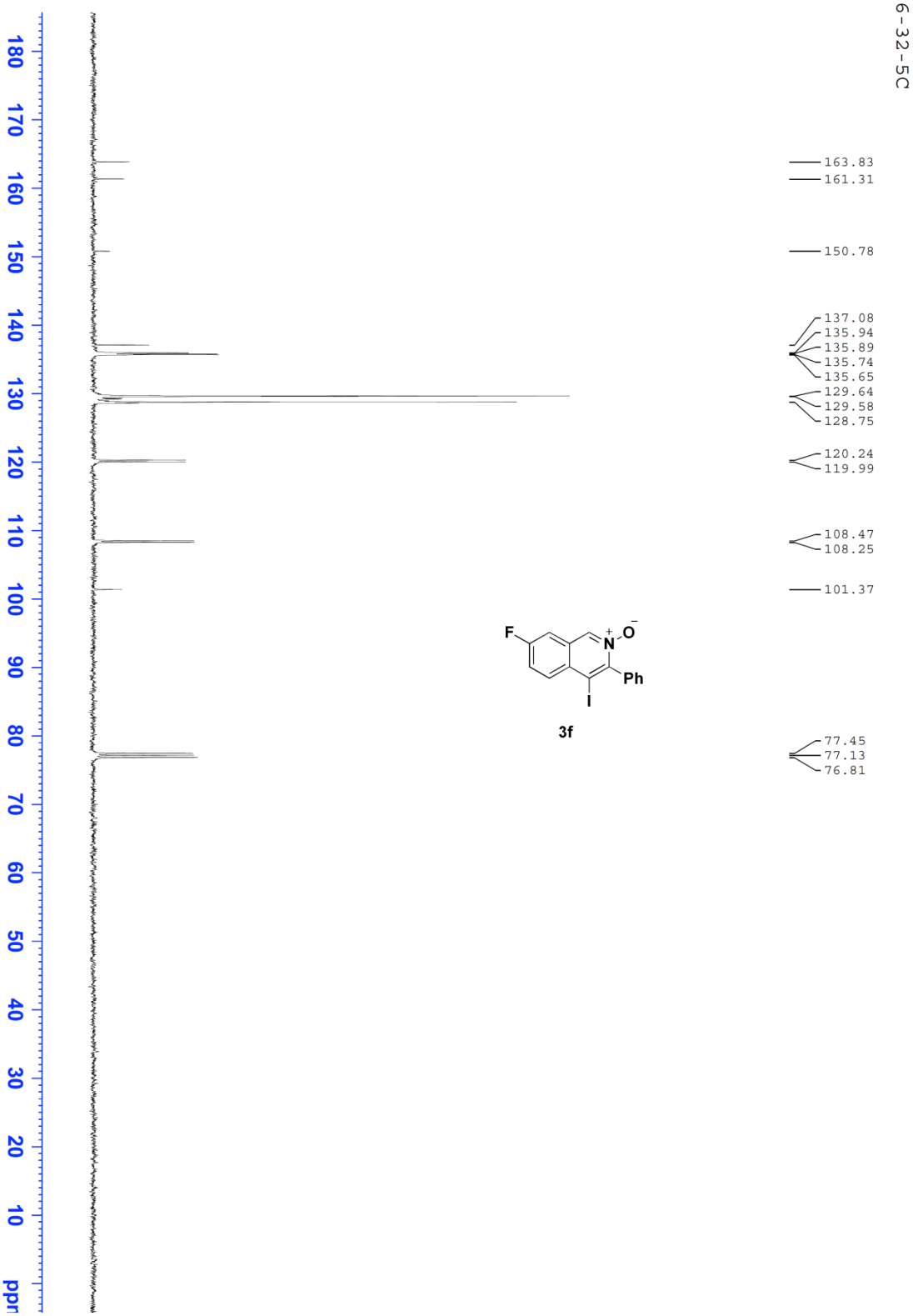
3d

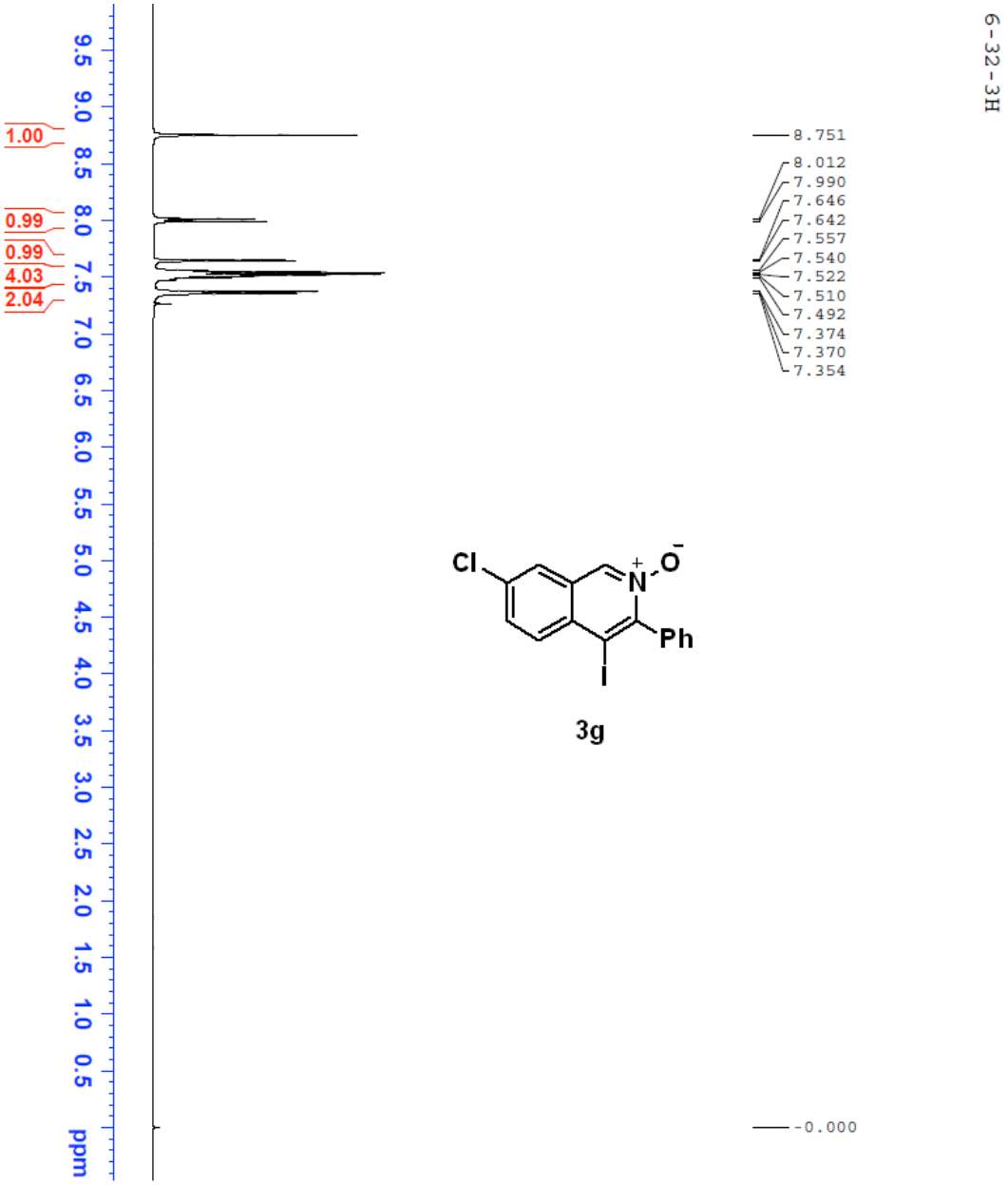

6-40-3H
8.844
7.787
7.782
7.762
7.757
7.727
7.713
7.705
7.691
7.559
7.542
7.523
7.511
7.493
7.474
7.400
7.395
7.378
7.361
1.00
0.93
1.06
3.06
3.03
F
N
O
Ph
I
3e
-0.005
ppm
Current Data Parameters
NAME wanghuanhuan
EXPNO 6400301
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130115
Time_ 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 38.64
DW 78.200 usec
DE 6.50 usec
TE 296.4 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00

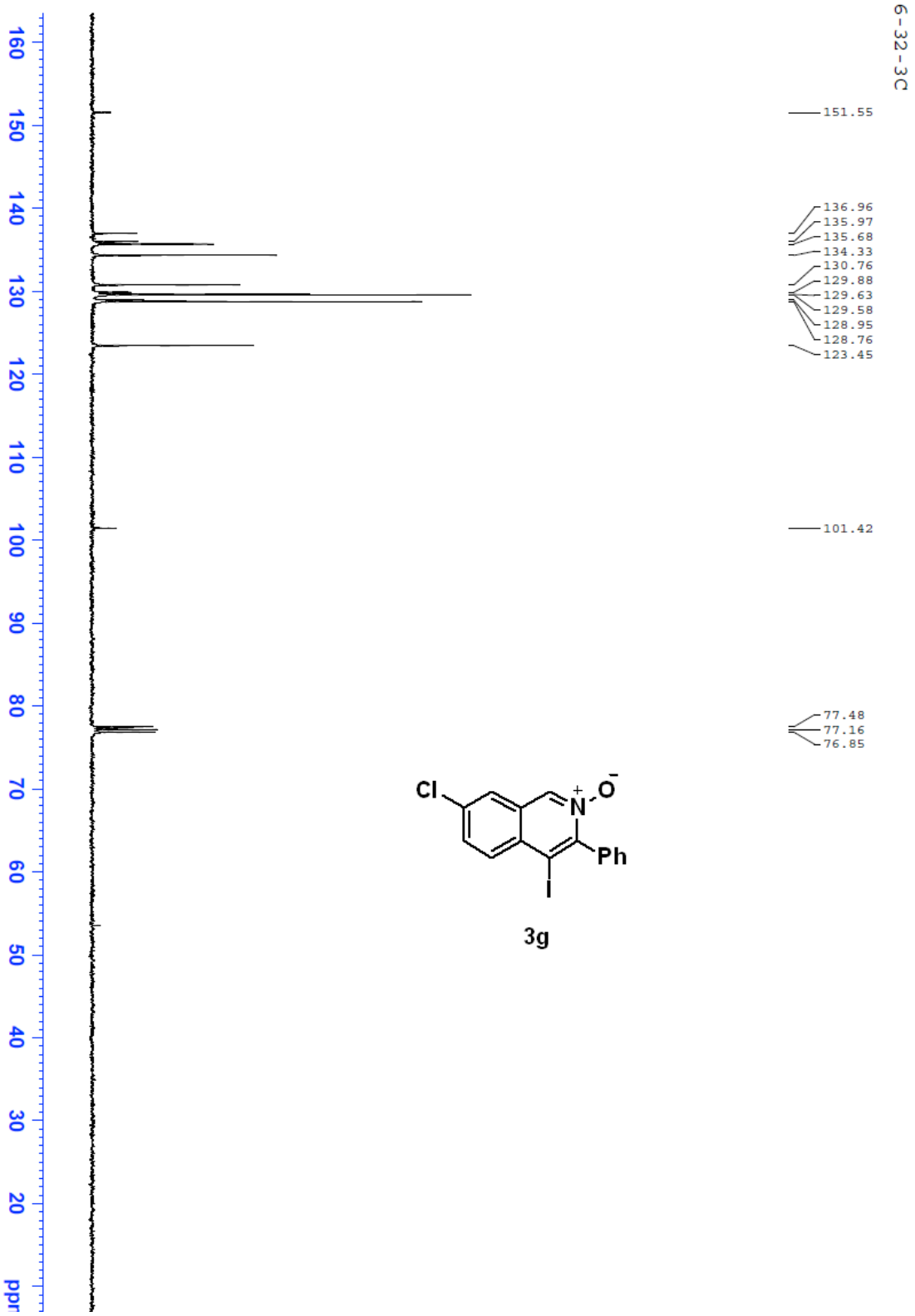


3e

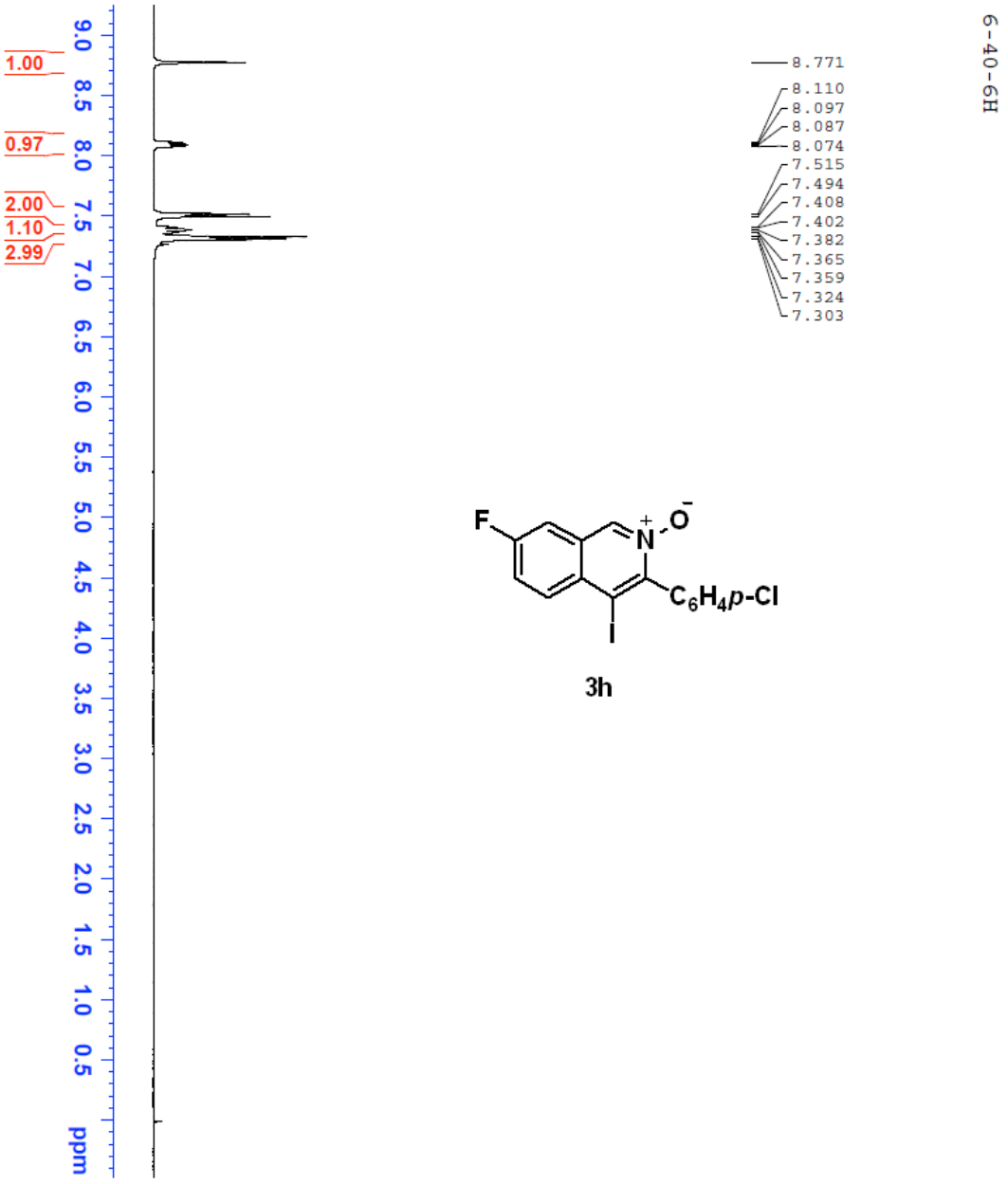
6-32-5H
8.788
8.117
8.104
8.093
8.081
7.560
7.543
7.525
7.512
7.501
7.494
7.476
7.399
7.393
7.357
7.330
7.324
7.309
7.303
F
N
O
Ph
I
3f
-0.001
1.00
0.95
2.98
3.97
9
8
7
6
5
4
3
2
1
0
ppm
Current Data Parameters
NAME wangbuanhuan
EXPNO 6320501
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130115
Time_ 15.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 38.64
DW 78.200 usec
DE 6.50 usec
TE 296.2 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00

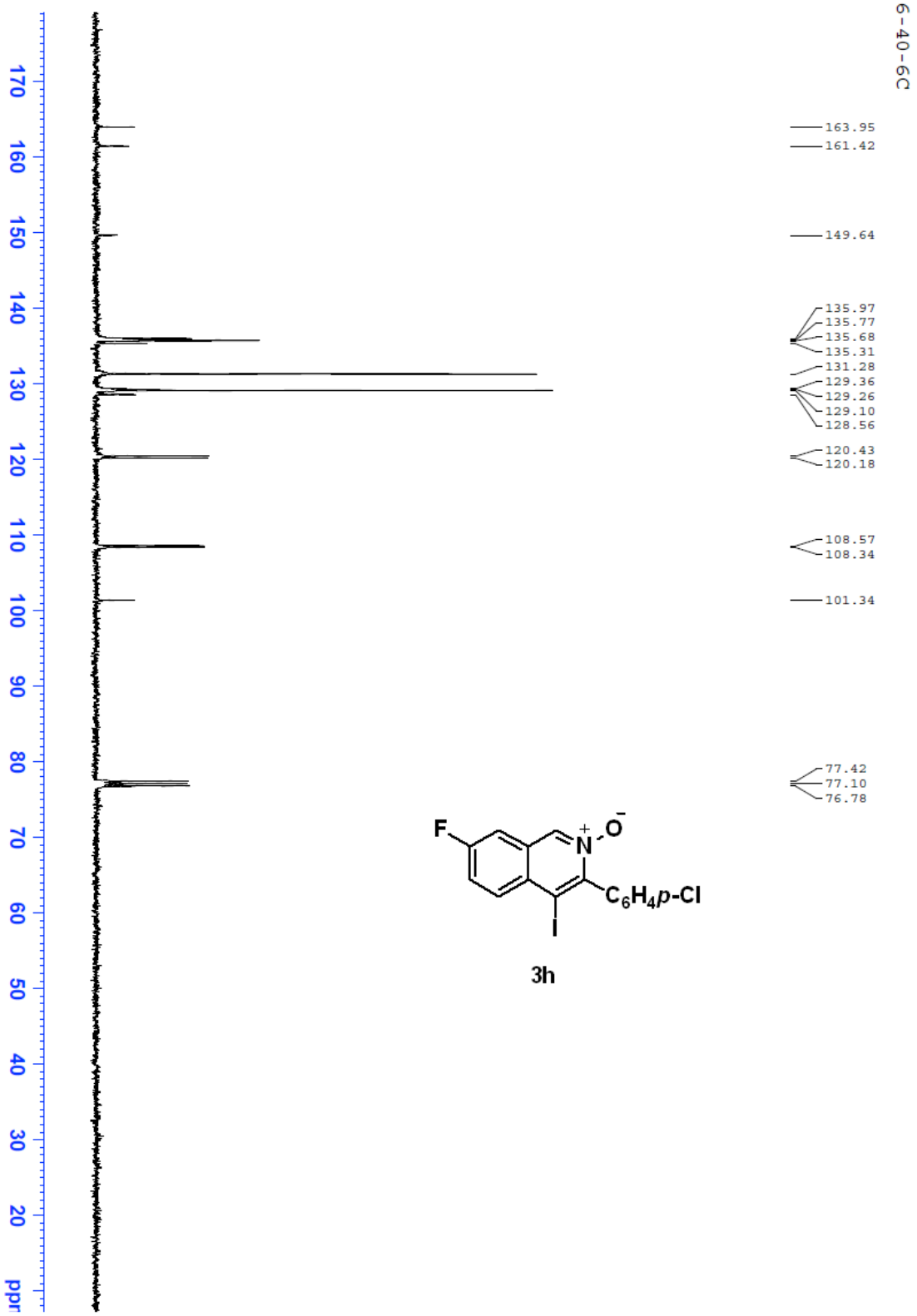



6-32-3H
8.751
8.012
7.990
7.646
7.642
7.557
7.540
7.522
7.510
7.492
7.374
7.370
7.354
-0.000
1.00
0.99
0.99
4.03
2.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
Cl
N
O
Ph
I
3g
BRUKER
Current Data Parameters
NAME wanghuanhuan
EXPNO 6320301
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130115
Time_ 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 36.02
DW 78.200 usec
DE 6.50 usec
TE 296.0 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00

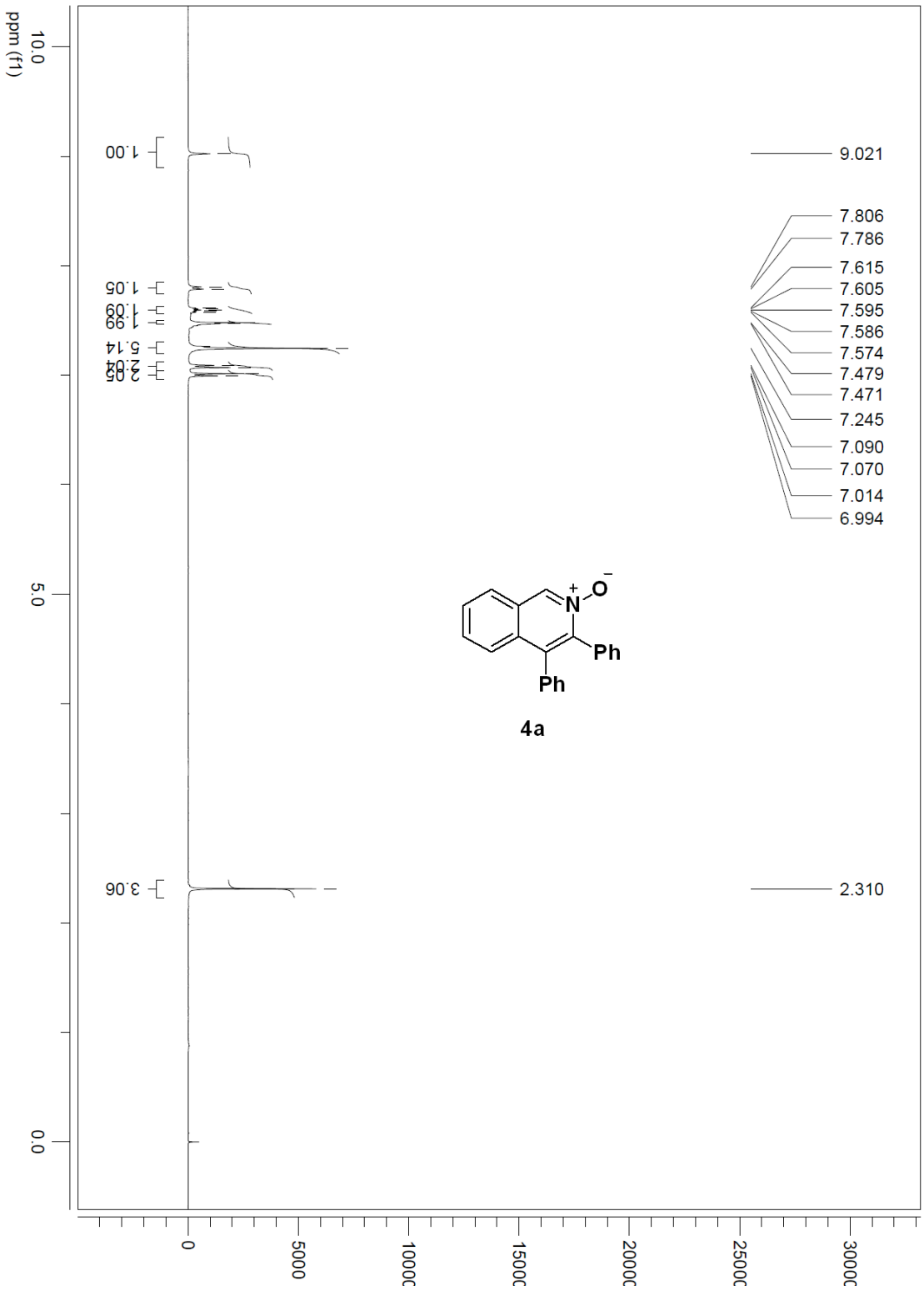

6-32-3C
151.55
136.96
135.97
135.68
134.33
130.76
129.88
129.63
129.58
128.95
128.76
123.45
101.42
77.48
77.16
76.85
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
Cl
N
O
Ph
I

3g

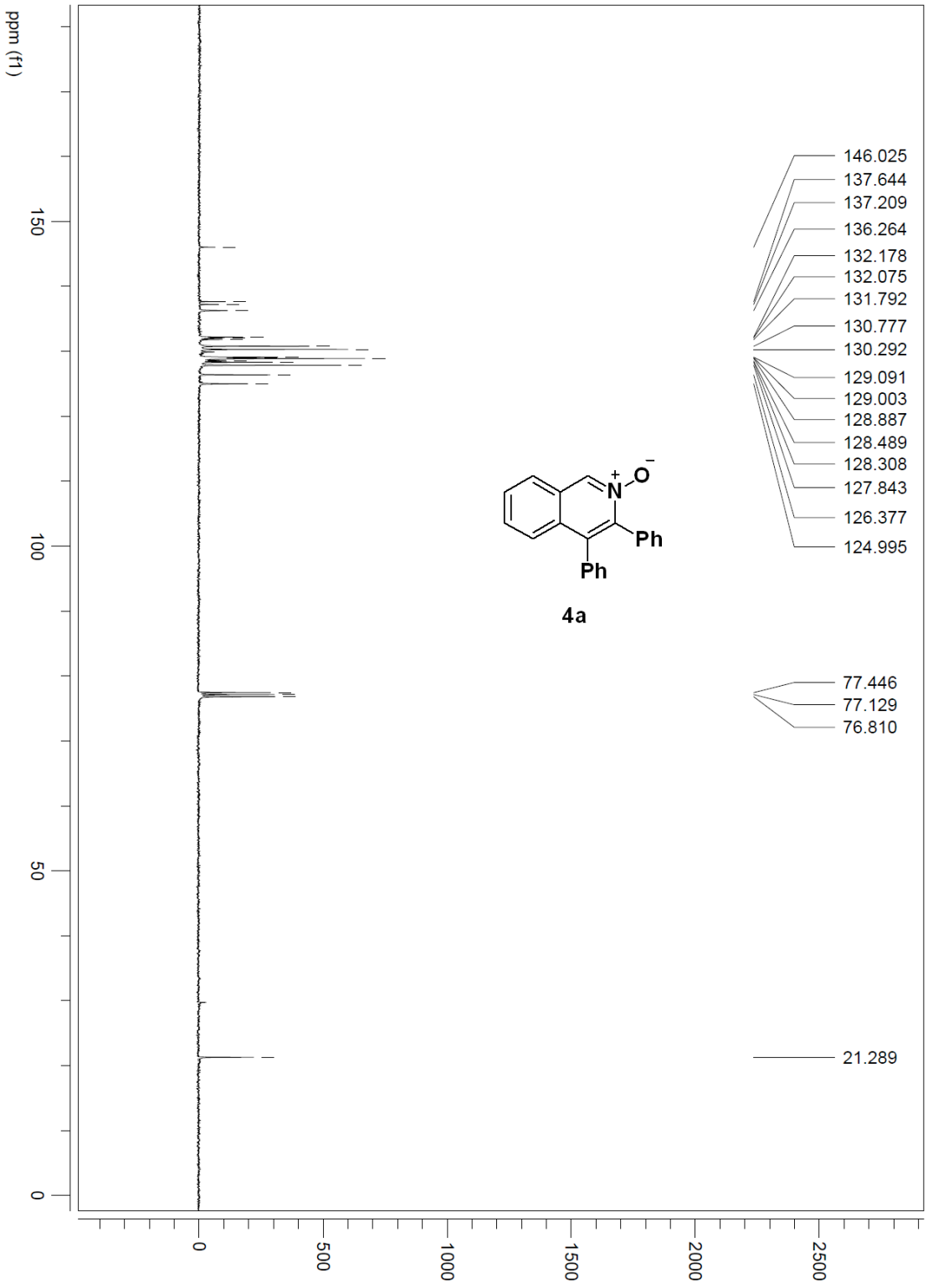

6-40-6H
8.771
8.110
8.097
8.087
8.074
7.515
7.494
7.408
7.402
7.382
7.365
7.359
7.324
7.303
F
N
O
C6H4p-Cl
3h
1.00
0.97
2.00
1.10
2.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
BRUKER
Current Data Parameters
NAME wanghuanhuan
EXPNO 6400601
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130121
Time_ 13.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 44.31
DW 78.200 usec
DE 6.50 usec
TE 302.0 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00



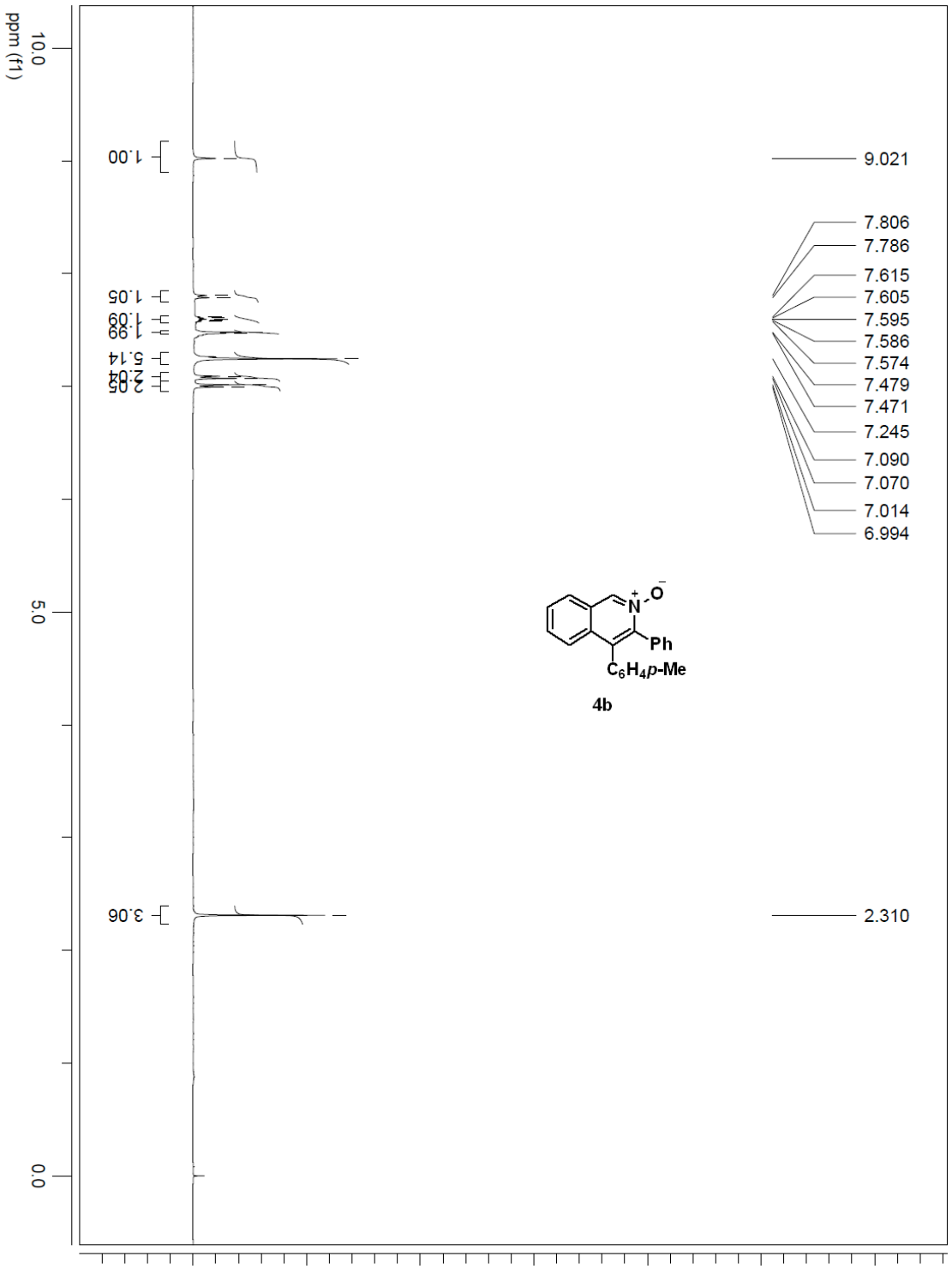
3h



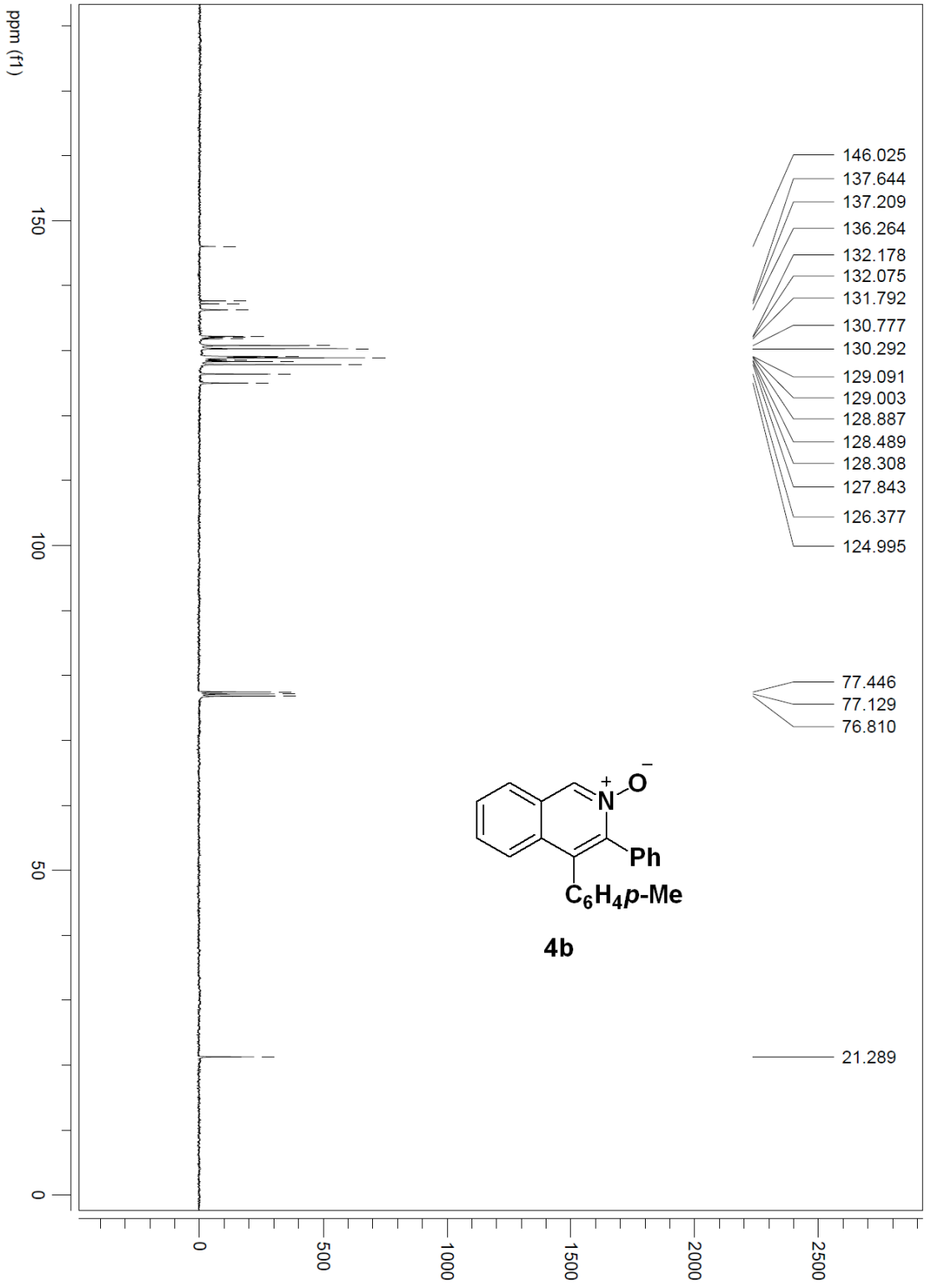
4a



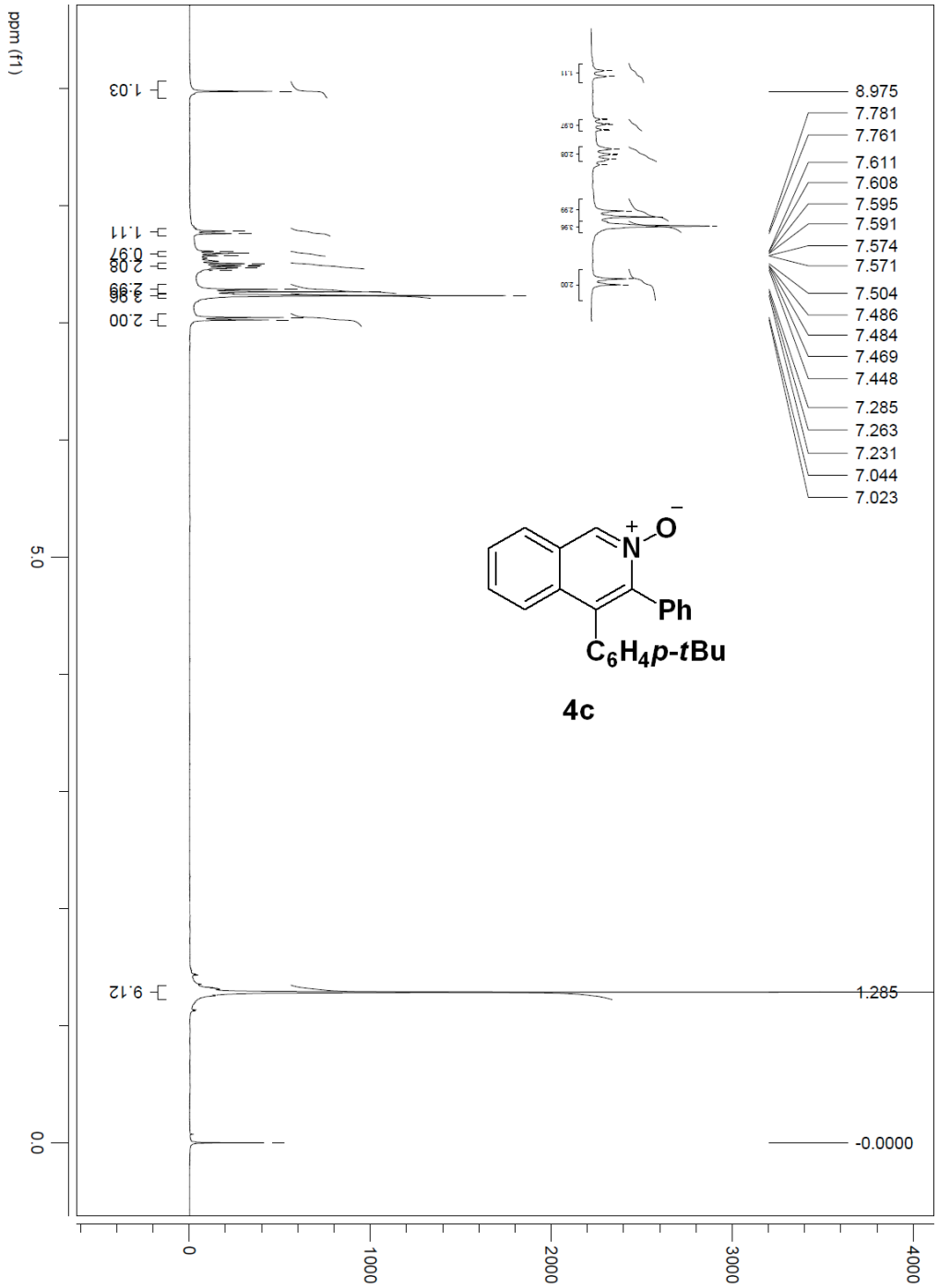
4a



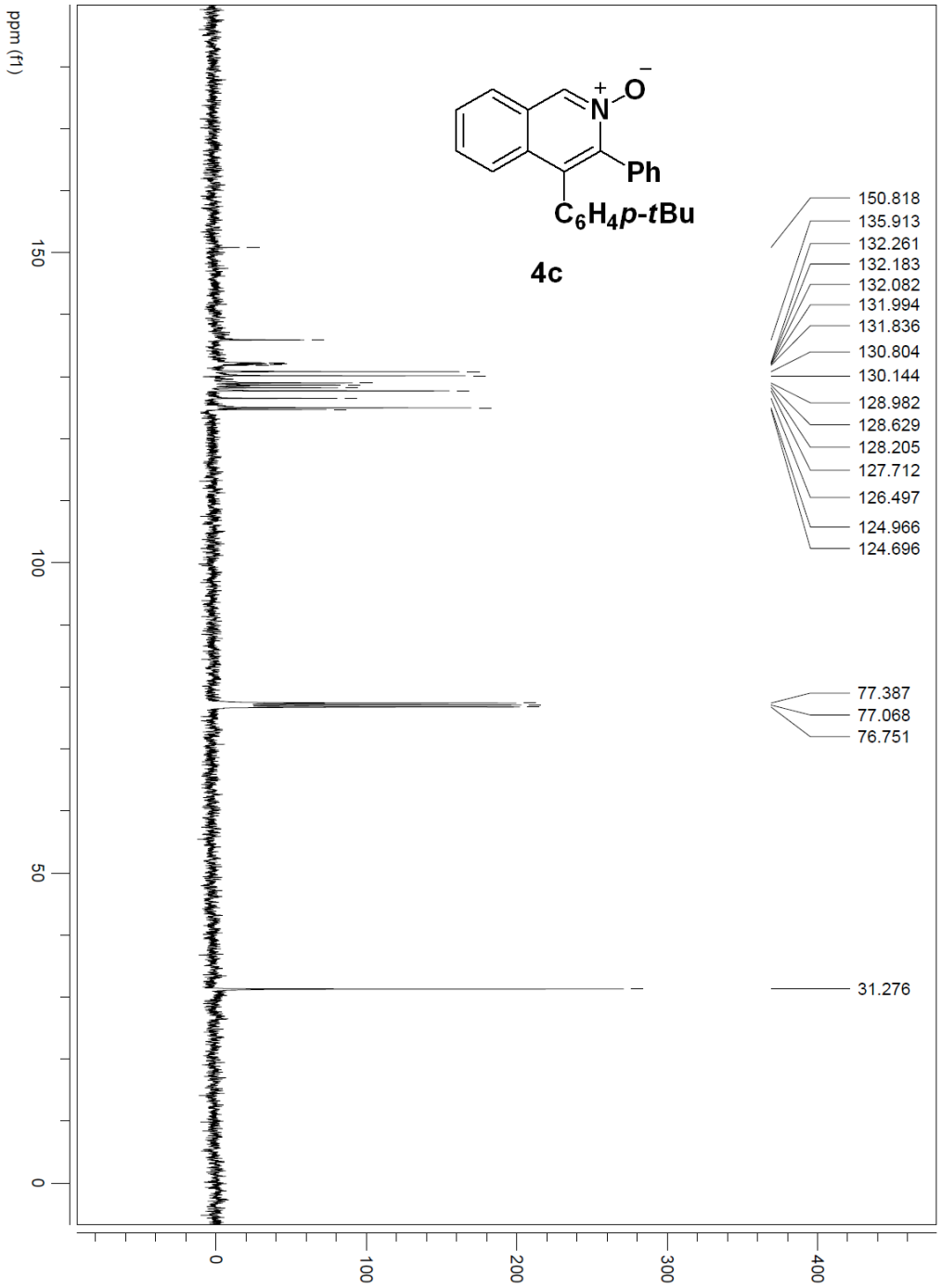
4b

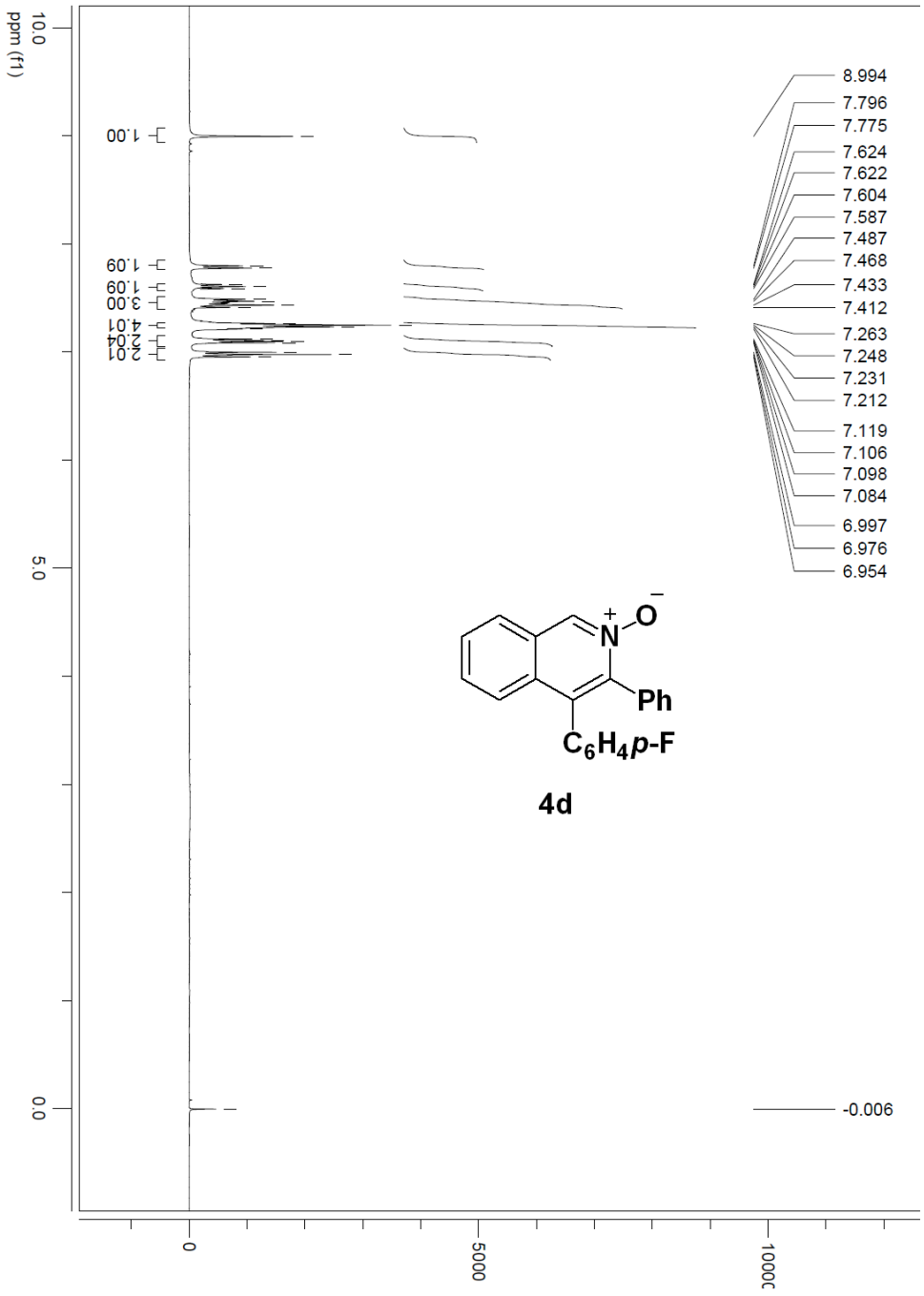


4b


ppm (f1)
5.0
0.0
1.03
1.11
0.97
2.08
2.99
3.96
2.00
9.12
8.975
7.781
7.761
7.611
7.608
7.595
7.591
7.574
7.571
7.504
7.486
7.484
7.469
7.448
7.285
7.263
7.231
7.044
7.023
1.285
-0.0000
0
1000
2000
3000
4000
N
O
Ph
C6H4p-tBu

4c

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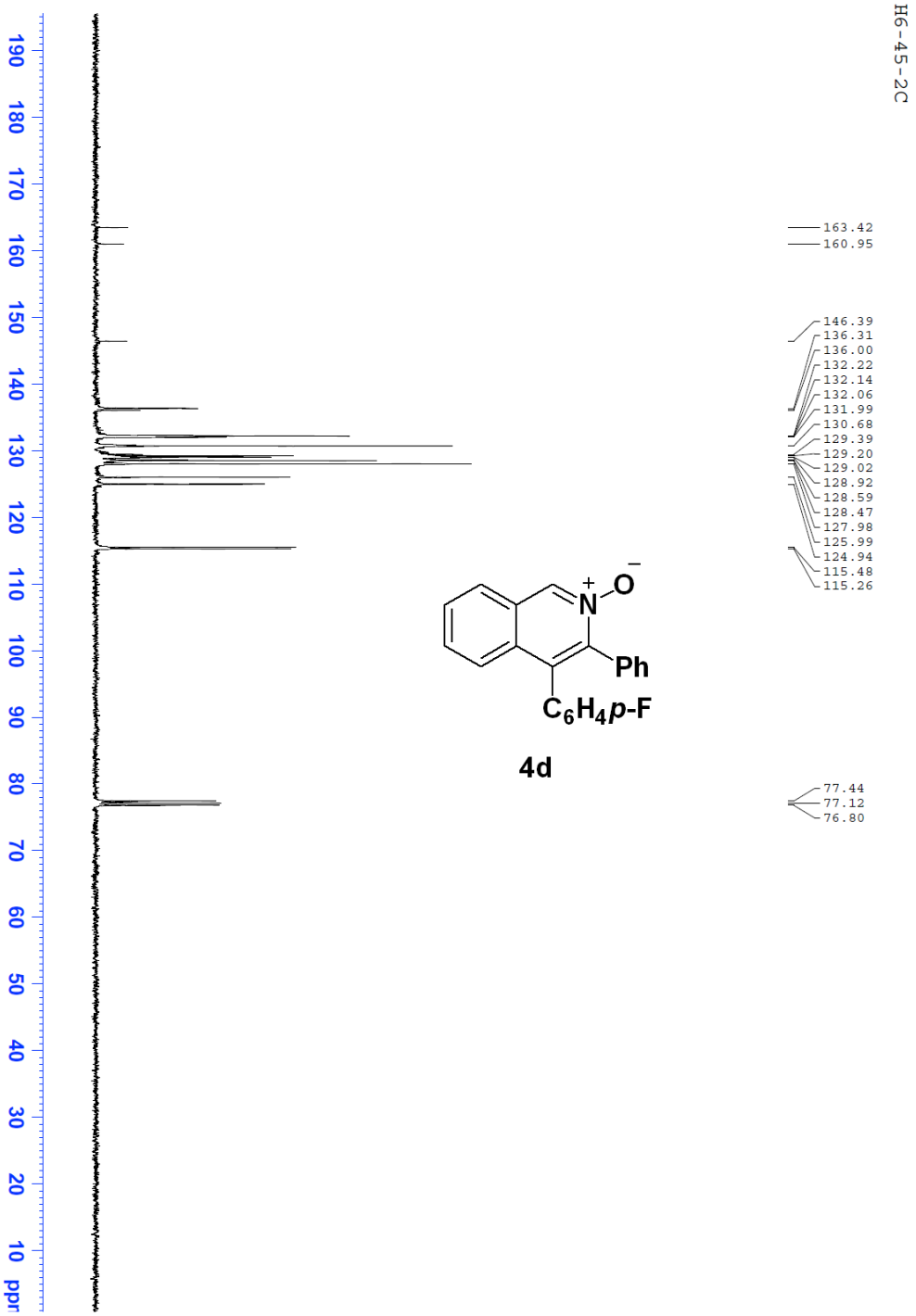
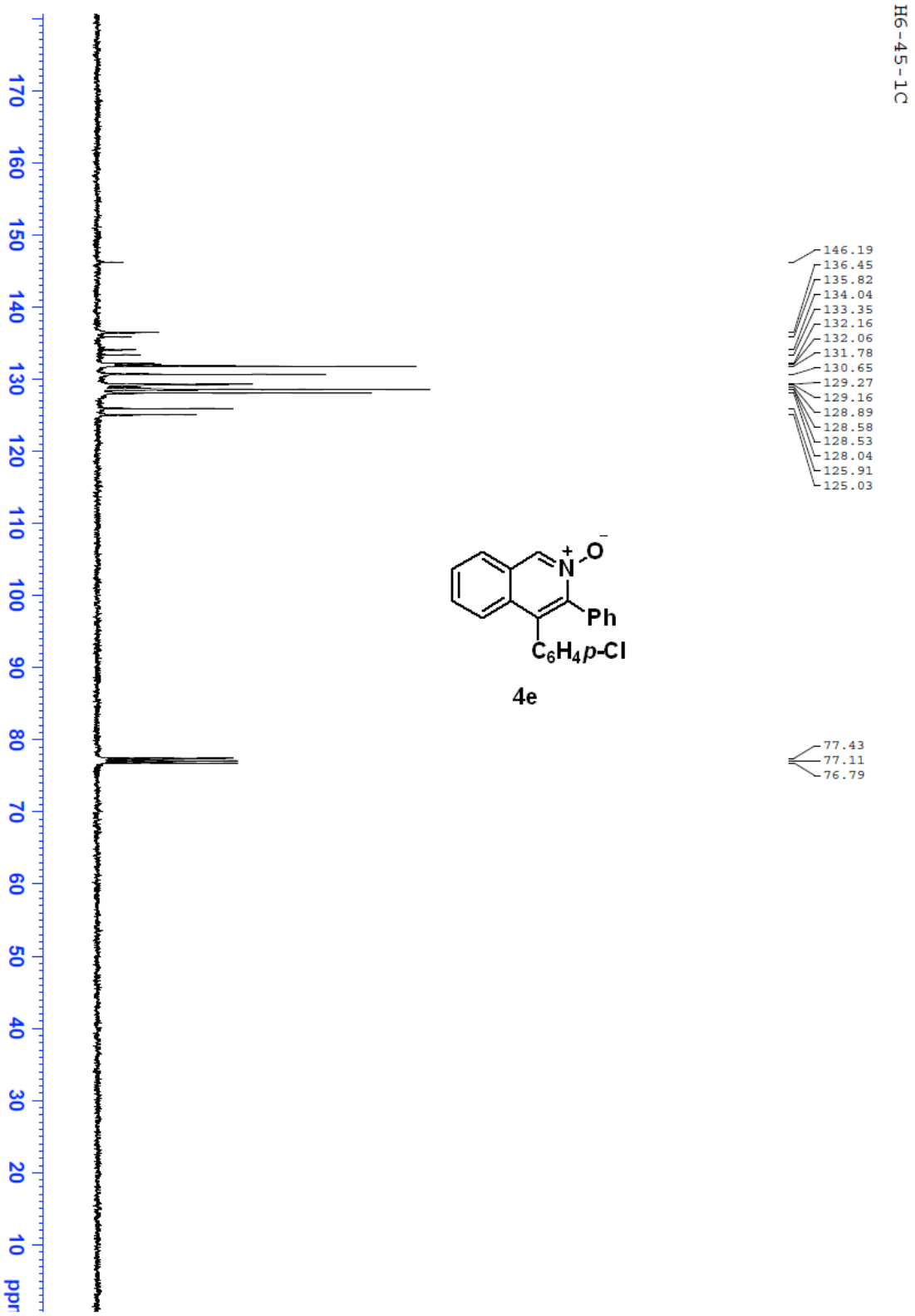
5.0
0.0
0
5000
10000
1.00
1.09
1.09
3.00
4.01
2.04
2.01
8.994
7.796
7.775
7.624
7.622
7.604
7.587
7.487
7.468
7.433
7.412
7.263
7.248
7.231
7.212
7.119
7.106
7.098
7.084
6.997
6.976
6.954
-0.006
N
O
Ph
C6H4p-F

4d

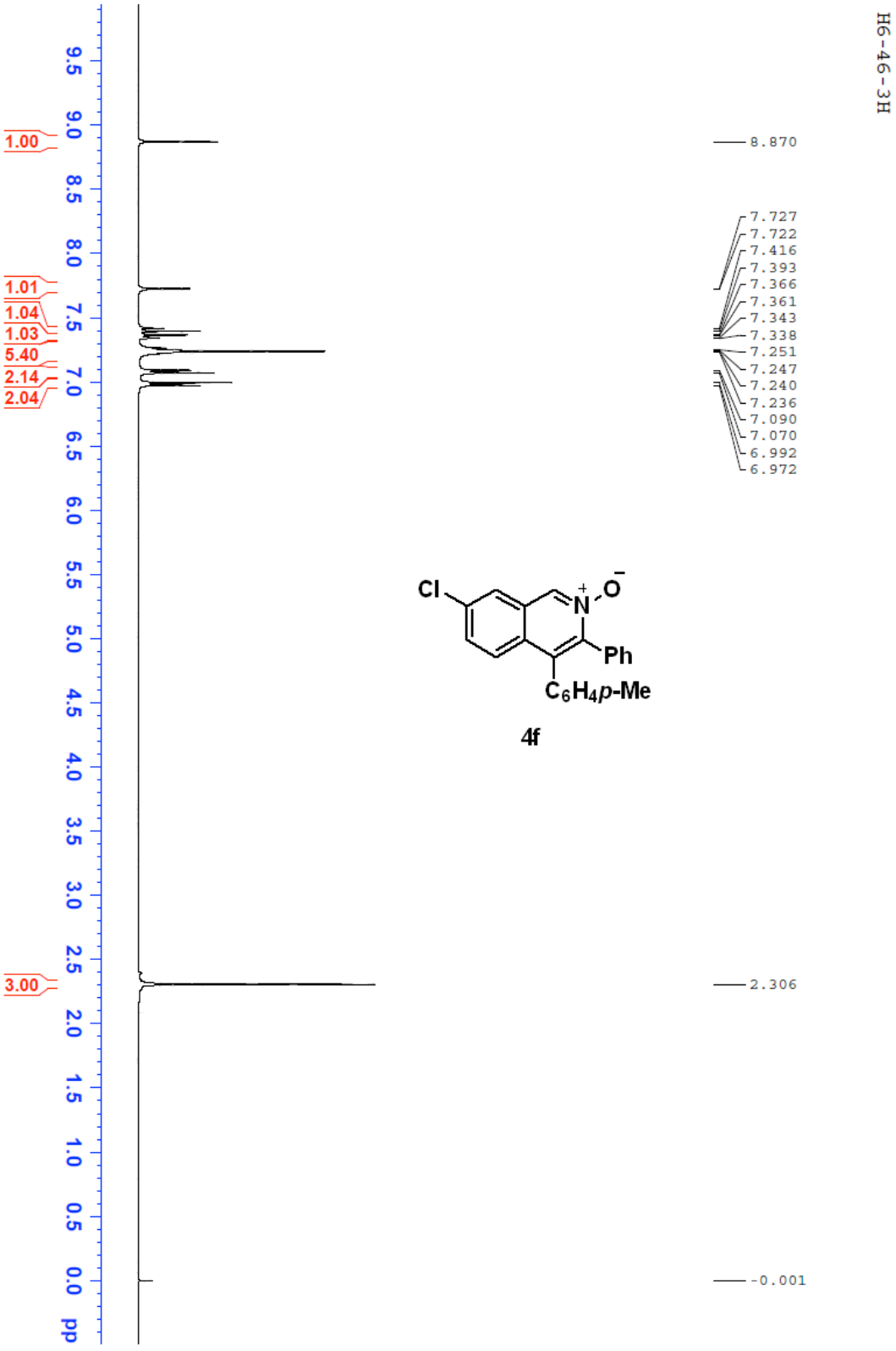

H6-45-2C
163.42
160.95
146.39
136.31
136.00
132.22
132.14
132.06
131.99
130.68
129.39
129.20
129.02
128.92
128.59
128.47
127.98
125.99
124.94
115.48
115.26
77.44
77.12
76.80
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
N
O
Ph
C6H4p-F

4d

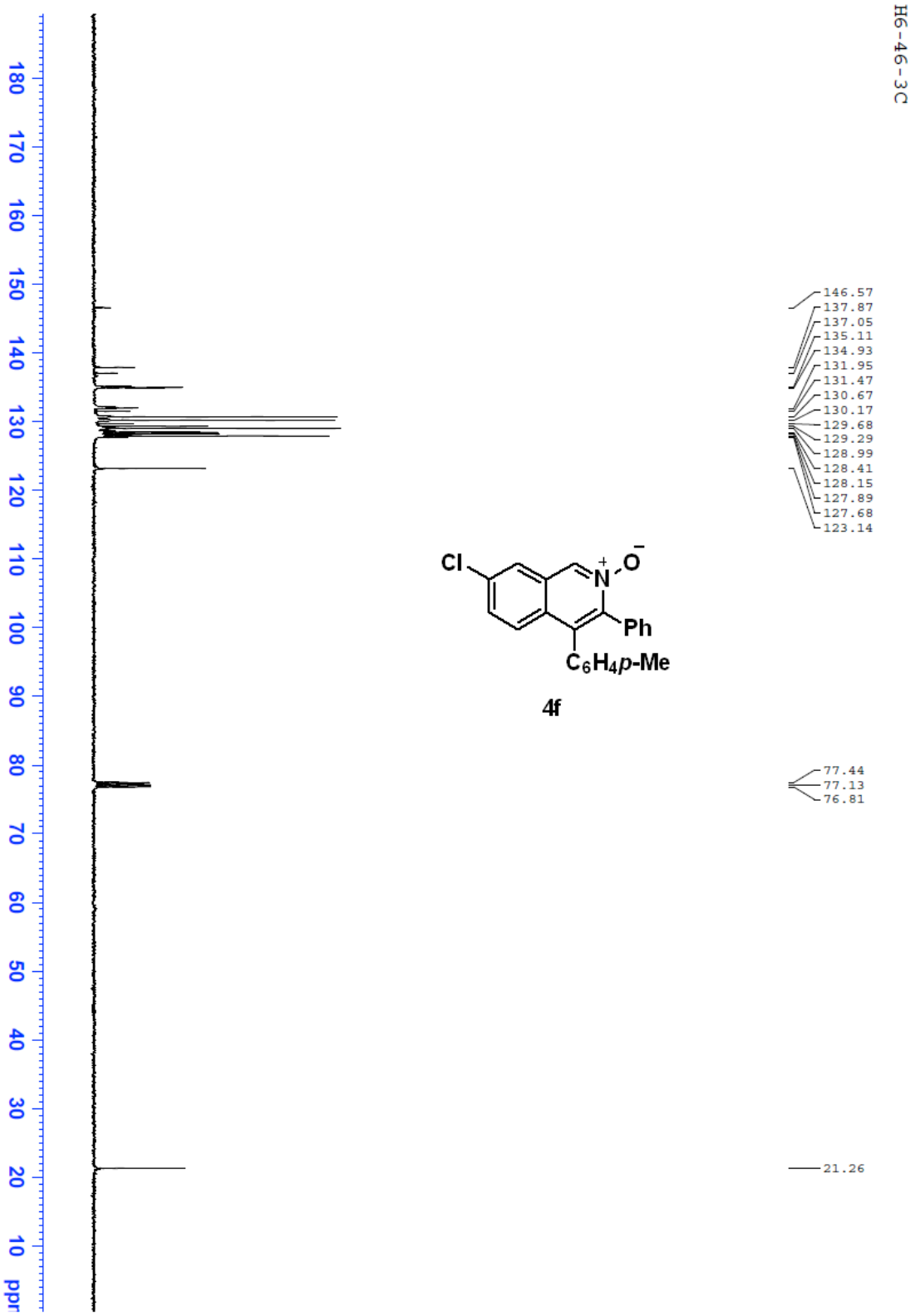
H6-45-1H
8.978
7.803
7.783
7.689
7.672
7.659
7.615
7.596
7.516
7.495
7.477
7.421
7.400
7.273
7.252
7.245
7.222
7.213
7.083
7.062
-0.005
Ph
C6H4p-Cl
4e
1.00
1.09
2.02
0.97
0.97
6.02
2.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
Current Data Parameters
NAME wanghuanhuan
EXPNO 6450101
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130319
Time_ 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5624576 sec
RG 51.14
DW 78.200 usec
DE 6.50 usec
TE 0 K
D1 6.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 399.7827985 MHz
NUC1 1H
P1 8.65 usec
PLW1 35.97499847 W
F2 - Processing parameters
SI 65536
SF 399.7800095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 10.00

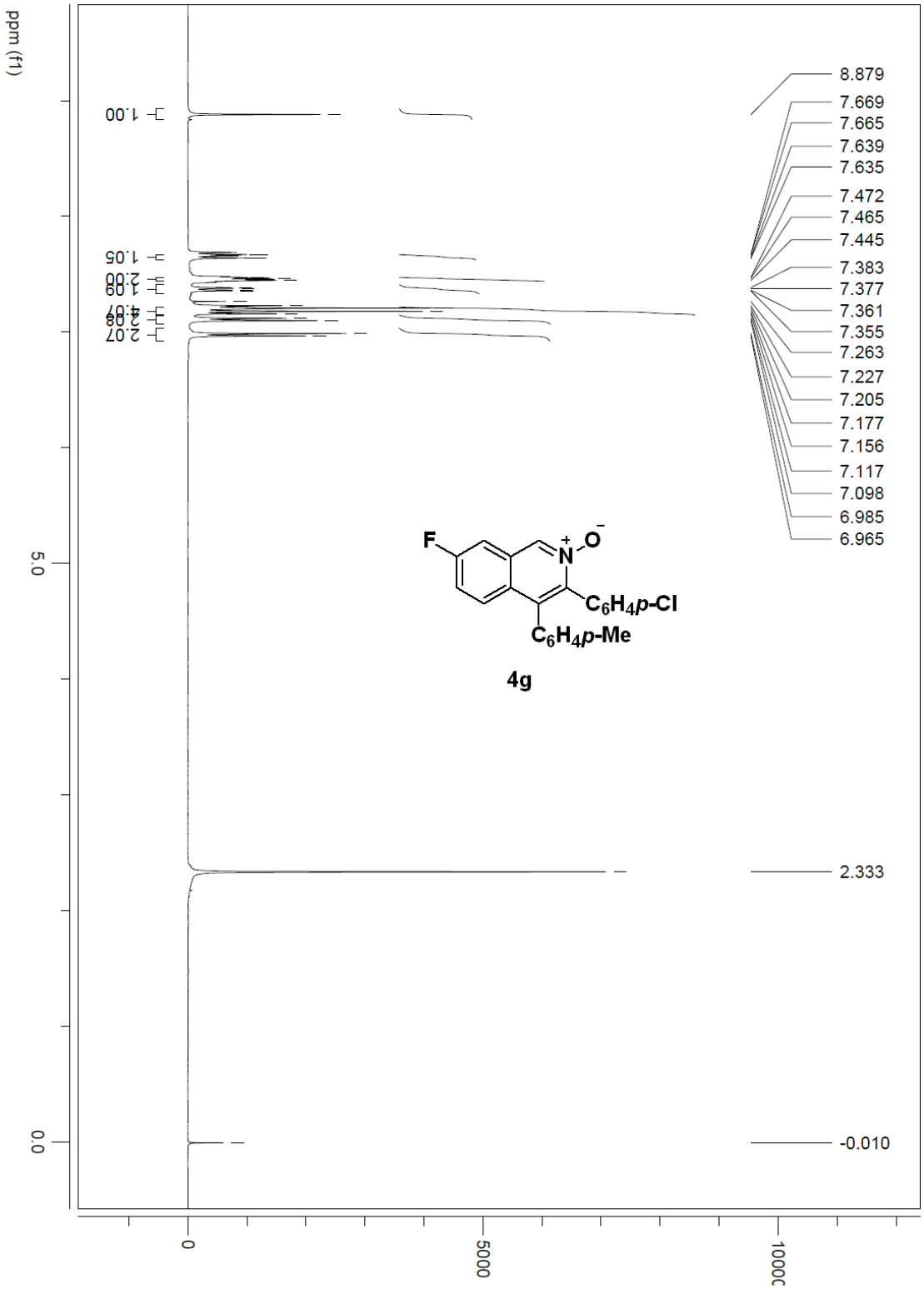


4e



4f


H6-46-3C
146.57
137.87
137.05
135.11
134.93
131.95
131.47
130.67
130.17
129.68
129.29
128.99
128.41
128.15
127.89
127.68
123.14
77.44
77.13
76.81
21.26
Cl
N
O
Ph
C6H4p-Me
4f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


ppm (f1)
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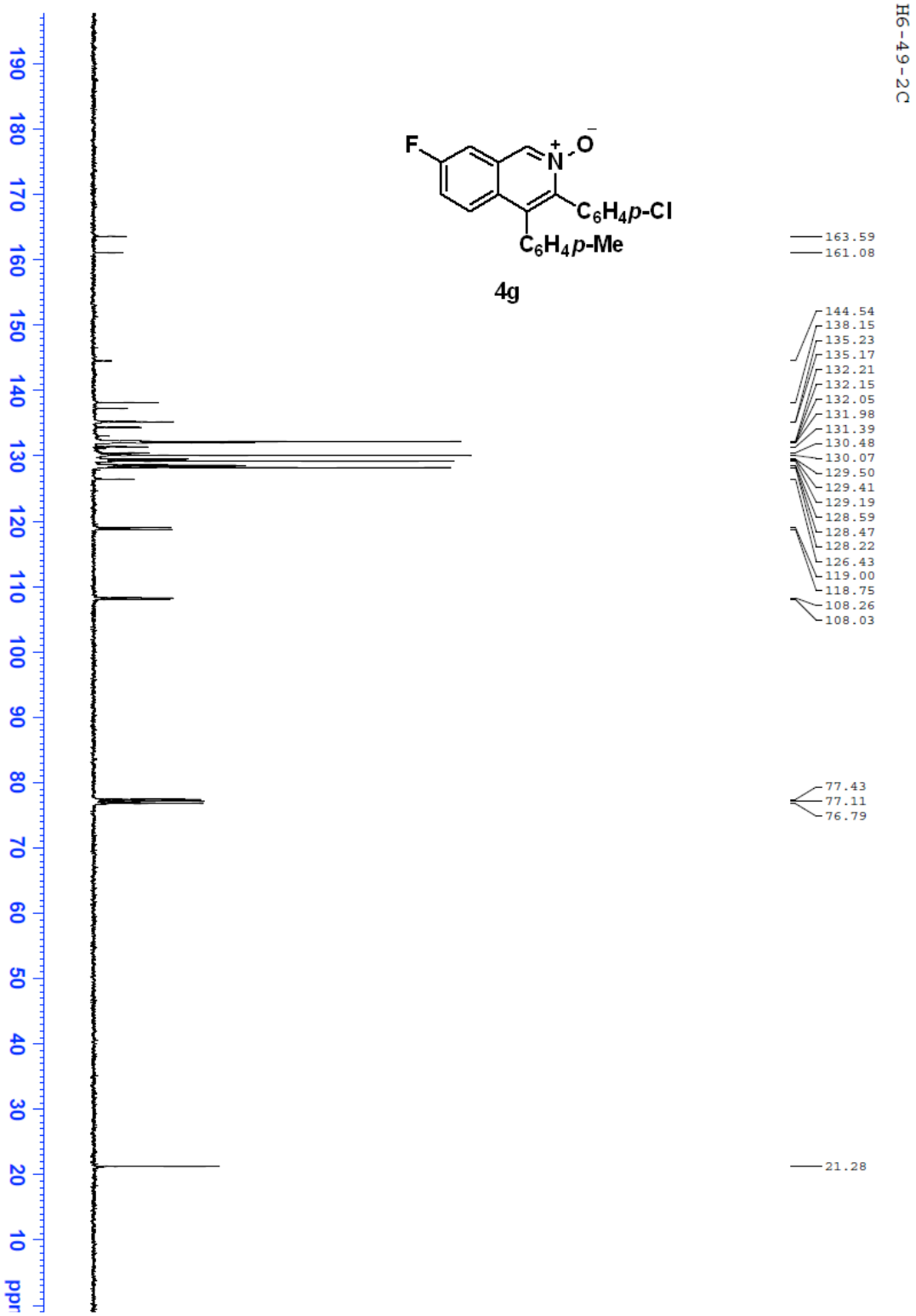
0.0
1.00
1.05
2.00
1.09
4.07
2.08
2.07
8.879
7.669
7.665
7.639
7.635
7.472
7.465
7.445
7.383
7.377
7.361
7.355
7.263
7.227
7.205
7.177
7.156
7.117
7.098
6.985
6.965
2.333
-0.010
F
N
O
C6H4p-Cl
C6H4p-Me
4g
0
5000
10000


H6-49-2C
F
N
O
C6H4p-Cl
C6H4p-Me
4g
163.59
161.08
144.54
138.15
135.23
135.17
132.21
132.15
132.05
131.98
131.39
130.48
130.07
129.50
129.41
129.19
128.59
128.47
128.22
126.43
119.00
118.75
108.26
108.03
77.43
77.11
76.79
21.28
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm