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

Synthesis of pyrazolo[5,1-*a*]isoquinolines via a silver(I)-catalyzed reaction of (1-arylethylidene)hydrazides with *N*'-(2-alkynylbenzylidene)hydrazides

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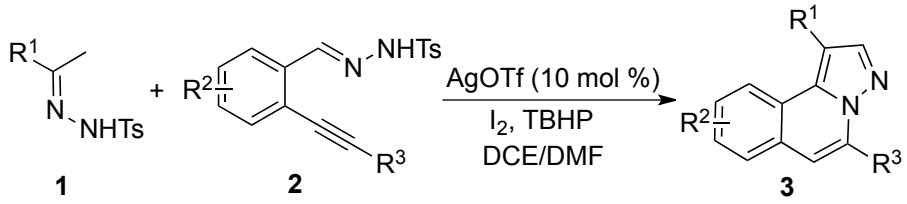
Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S2-S11).
3. ^{1}H and ^{13}C NMR spectra of compounds **3** (S12 –S53).

General experimental methods:

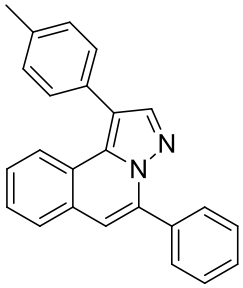
Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using 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 silver(I)-catalyzed reaction of (1-arylethylidene)hydrazides **1** with N'-(2-alkynylbenzylidene)hydrazides **2***

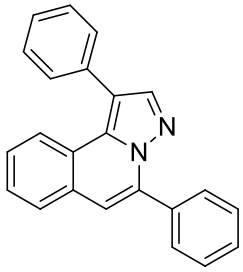


1 **2** **3**

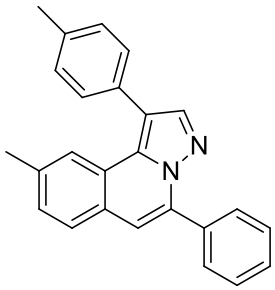
Silver triflate (10 mol %) was added to a solution of *N*'-(2-alkynylbenzylidene)hydrazide **2** (0.2 mmol) in DCE (1.0 mL) at 60 ^{o}C. After 1 hour, (1-arylethylidene)hydrazide **1** (2.0 equiv), iodine (0.2 equiv), TBHP (2.0 equiv), and DMF (2.0 mL) were added to the above suspension and the mixture was stirred at 60 ^{o}C. After completion of the reaction as indicated by TLC, the mixture was washed with saturated Na_2SO_3 and extracted by EtOAc. The organic solvent was evaporated and the residue was purified by flash column chromatograph (*n*-hexane/ethyl acetate = 2:1) to give the corresponding product **3**.



5-Phenyl-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3a**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.2 Hz, 1H), 7.91-7.85 (m, 3H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.53-7.48 (m, 3H), 7.46-7.40 (m, 3H), 7.29 (d, *J* = 7.8 Hz, 3H), 6.99 (s, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.7, 138.6, 137.2, 134.6, 134.0, 131.2, 129.9, 129.7, 129.5, 129.5, 129.3, 128.4, 127.7, 127.2, 126.9, 124.8, 123.3, 117.1, 112.9, 21.3. HRMS (ESI) calcd for $C_{24}H_{19}N_2^+$: 335.1543 ($M + H^+$), found: 335.1540.

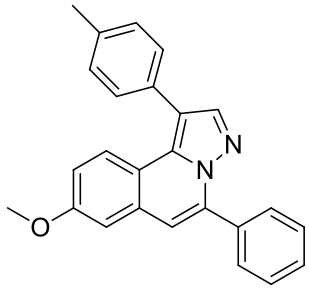


1,5-Diphenylpyrazolo[5,1-*a*]isoquinoline (**3b**).[1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.2 Hz, 1H), 7.93 (s, 1H), 7.86 (d, *J* = 6.8 Hz, 2H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.58-7.39 (m, 9H), 7.29-7.25 (m, 1H), 7.00 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.5, 134.6, 134.3, 134.0, 133.1, 130.1, 129.7, 129.5, 129.3, 128.8, 128.4, 127.8, 127.5, 127.3, 126.9, 124.6, 123.2, 117.1, 113.0.

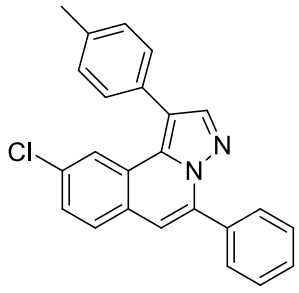


9-Methyl-5-phenyl-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3c**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90-7.85 (m, 4H), 7.58-7.48 (m, 7H), 7.29 (d, *J* = 7.8 Hz, 2H), 6.97 (s, 1H),

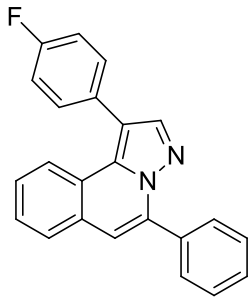
2.45 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.6, 137.7, 137.1, 136.8, 134.4, 134.2, 129.9, 129.5, 129.3, 129.1, 128.4, 127.5, 127.1, 124.8, 123.1, 116.9, 112.9, 21.8, 21.3. HRMS (ESI) calcd for $C_{25}H_{21}N_2^+$: 349.1699 (M + H^+), found: 349.1682.



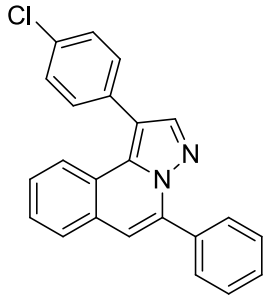
8-Methoxy-5-phenyl-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3d**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00-7.87 (m, 4H), 7.55-7.44 (m, 5H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.10 (d, *J* = 2.5 Hz, 1H), 6.96-6.93 (m, 2H), 3.88 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.0, 141.8, 137.0, 131.4, 131.3, 129.9, 129.4, 129.3, 128.4, 124.9, 116.4, 112.6, 108.3, 55.4, 21.3. HRMS (ESI) calcd for $C_{25}H_{21}N_2O^+$: 365.1648 (M + H^+), found: 365.1638.



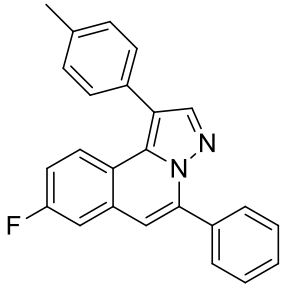
9-Chloro-5-phenyl-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3e**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 1.8 Hz, 1H), 7.92 (s, 1H), 7.87-7.84 (m, 3H), 7.60-7.59 (m, 1H), 7.54-7.49 (m, 3H), 7.45-7.43 (m, 2H), 7.39 (dd, *J* = 2.0, 8.44 Hz, 1H), 7.33-7.31 (m, 2H), 6.97 (s, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.8, 138.8, 137.6, 133.7, 132.6, 130.4, 129.7, 129.6, 129.4, 128.5, 128.4, 128.1, 128.0, 125.7, 122.6, 117.6, 112.1, 21.3. HRMS (ESI) calcd for $C_{24}H_{18}ClN_2^+$: 369.1153 (M + H^+), found: 369.1144.



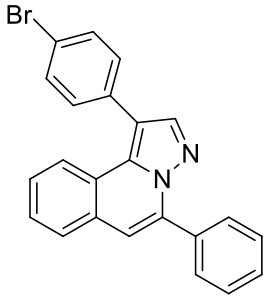
1-(4-Fluorophenyl)-5-phenylpyrazolo[5,1-*a*]isoquinoline (**3f**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.2 Hz, 2H), 7.90-7.87 (m, 2H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.55-7.47 (m, 6H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.24-7.18 (m, 2H), 7.05 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4 (d, J_{CF} = 245.4 Hz), 141.5, 138.5, 134.7, 133.7, 131.7, 130.1, 129.7, 129.5, 129.3, 128.4, 127.7, 127.3, 126.9, 124.5, 123.0, 115.9, 115.7 (d, $^{2}J_{CF}$ = 21.1 Hz), 113.0. HRMS (ESI) calcd for $C_{23}H_{16}FN_2^+$: 339.1292 (M + H^+), found: 339.1280.



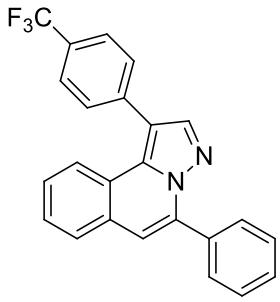
1-(4-Chlorophenyl)-5-phenylpyrazolo[5,1-*a*]isoquinoline (**3g**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.2 Hz, 1H), 7.90-7.87 (m, 3H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.55-7.49 9(m, 8H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.06 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.5, 138.5, 134.6, 133.8, 133.4, 132.7, 131.3, 129.8, 129.5, 129.4, 129.0, 128.4, 128.0, 127.4, 127.0, 124.4, 123.1, 115.8, 113.1. HRMS (ESI) calcd for $C_{23}H_{16}ClN_2^+$: 355.0997 (M + H^+), found: 355.0987.



8-Fluoro-5-phenyl-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3h**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (dd, *J* = 5.44, 8.96 Hz, 1H), 7.90 (s, 1H), 7.85 (d, *J* = 6.44 Hz, 2H), 7.51 (m, 3H), 7.43 (d, *J* = 7.88 Hz, 2H), 7.30 (d, *J* = 7.6 Hz, 3H), 7.01 (m, 1H), 6.93 (s, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.9, 138.4 (d, J_{CF} = 225.6 Hz), 134.3, 133.6, 131.5 (d, $^{3}J_{CF}$ = 9.0 Hz), 130.9, 129.9, 129.6, 129.5, 129.5, 128.4, 125.5 (d, $^{3}J_{CF}$ = 8.6 Hz), 121.3, 116.6, 115.4 (d, $^{2}J_{CF}$ = 23.2 Hz), 112.0, 111.8. HRMS (ESI) calcd for $C_{24}H_{18}FN_2^+$: 353.1443 (M + H^+), found: 353.1457.

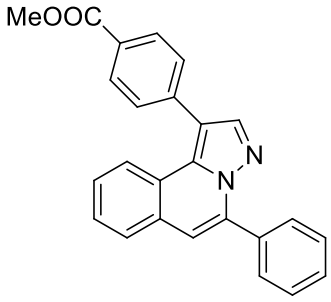


1-(4-Bromophenyl)-5-phenylpyrazolo[5,1-*a*]isoquinoline (**3i**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.88-7.84 (m, 3H), 7.67-7.58 (m, 3H), 7.51-7.41 (m, 6H), 7.32-7.30 (m, 1H), 7.01 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.4, 138.5, 134.6, 133.8, 133.2, 131.9, 131.7, 129.8, 129.5, 129.4, 128.4, 128.0, 127.4, 127.0, 124.4, 123.0, 121.5. HRMS (ESI) calcd for $C_{23}H_{16}BrN_2^+$: 399.0491 (M + H^+), found: 399.0480.

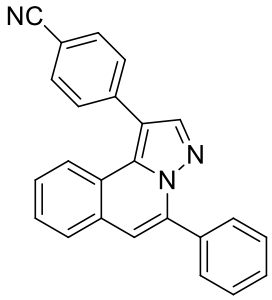


5-Phenyl-1-(4-(trifluoromethyl)phenyl)pyrazolo[5,1-*a*]isoquinoline (**3j**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.94 (s, 1H), 7.90-7.88 (m, 2H), 7.78-7.71 (m, 5H), 7.58-7.52 (m, 4H), 7.39-7.35 (m, 1H), 7.10 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.5, 138.6, 138.2, 134.7, 133.7, 130.2, 129.9, 129.5, 129.4, 128.4, 128.1, 127.5, 127.1, 124.4(q, J_{CF} = 267.7 Hz), 125.7, 124.2, 115.6, 113.3. HRMS (ESI) calcd for

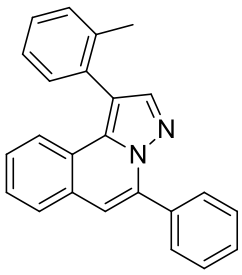
$C_{24}H_{16}F_3N_2^+$: 389.1260 (M + H^+), found: 389.1251.



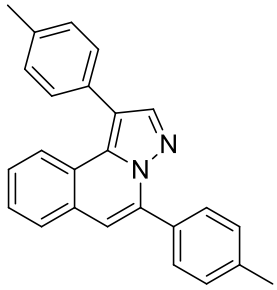
Methyl 4-(5-phenylpyrazolo[5,1-*a*]isoquinolin-1-yl)benzoate (**3k**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J* = 7.6 Hz, 2H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.95 (s, 1H), 7.88 (d, *J* = 6.6 Hz, 2H), 7.73-7.66 (m, 3H), 7.55-7.50 (m, 4H), 7.34-7.31 (m, 1H), 7.07 (s, 1H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.5, 138.6, 138.2, 134.7, 133.7, 130.2, 129.9, 129.5, 129.4, 129.0, 128.4, 128.2, 128.1, 127.4, 127.0, 124.3, 123.1, 116.1, 113.3, 52.2. HRMS (ESI) calcd for $C_{25}H_{19}N_2O_2^+$: 379.1441 (M + H^+), found: 379.1439.



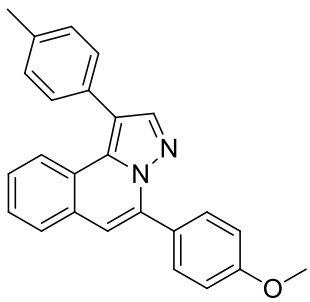
4-(5-Phenylpyrazolo[5,1-*a*]isoquinolin-1-yl)benzonitrile (**3l**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.2 Hz, 1H), 7.91 (s, 1H), 7.86 (d, *J* = 6.5 Hz, 2H), 7.78-7.68 (m, 5H), 7.55-7.50 (m, 4H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.09 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.4, 139.4, 138.5, 134.7, 133.6, 132.5, 130.5, 130.0, 129.5, 129.3, 128.4, 128.4, 127.6, 127.2, 124.0, 122.9, 118.9, 115.3, 113.5, 111.0. HRMS (ESI) calcd for $C_{24}H_{16}N_3^+$: 346.1339 (M + H^+), found: 346.1322.



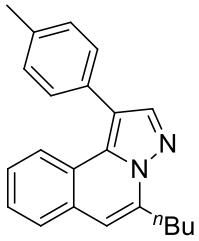
5-Phenyl-1-(*o*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3m**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92-7.89 (m, 3H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.56-7.49 (m, 4H), 7.45-7.37 (m, 4H), 7.33-7.24 (m, 2H), 7.04 (s, 1H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 138.6, 138.0, 134.9, 134.0, 133.6, 131.2, 130.3, 129.6, 129.3, 128.4, 128.1, 127.7, 127.2, 127.1, 126.1, 124.8, 123.0, 115.6, 112.8, 20.3. HRMS (ESI) calcd for $C_{24}H_{19}N_2^+$: 335.1543 ($M + H^+$), found: 335.1530.



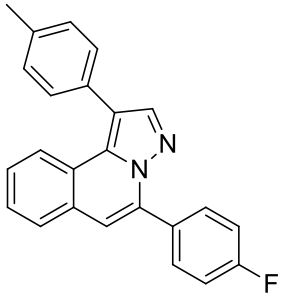
1,5-Di-*p*-tolylpyrazolo[5,1-*a*]isoquinoline (**3n**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 2.1 Hz, 1H), 7.76 (d, *J* = 6.9 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.47-7.41 (m, 3H), 7.34-7.26 (m, 5H), 6.99 (s, 1H), 2.45 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 138.7, 137.1, 134.5, 131.3, 131.1, 129.9, 129.8 129.5, 129.4, 129.1, 127.7, 127.1, 126.7, 124.7, 123.2, 117.0, 112.5, 21.5, 21.4. HRMS (ESI) calcd for $C_{25}H_{21}N_2^+$: 349.1699 ($M + H^+$), found: 349.1698.



5-(4-Methoxyphenyl)-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3o**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 8.2 Hz, 1H), 7.91 (s, 1H), 7.86-7.83 (m, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.48-7.46 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 3H), 7.07 (d, *J* = 8.8 Hz, 2H), 7.01 (s, 1H), 3.89 (s, 3H), 2,46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 141.6, 138.3, 137.1, 134.5, 131.2, 130.8, 129.9, 129.8, 129.4, 127.6, 127.0, 126.6, 126.3, 124.5, 123.2, 117.0, 113.8, 112.2, 55.4, 21.3. HRMS (ESI) calcd for $C_{25}H_{21}N_2O^+$: 365.1648 ($M + H^+$), found: 365.1640.

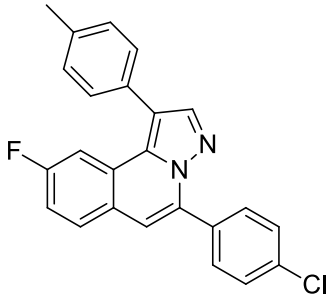


5-Butyl-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3p**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.92 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.45-7.39 (m, 3H), 7.29-7.21 (m, 3H), 6.81 (s, 1H), 3.19 (t, *J* = 7.7 Hz, 2H), 2.44 (s, 3H), 1.92-1.86 (m, 2H), 1.56-1.49 (m, 2H), 1.01 (t, *J* = 7.12 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 139.5, 137.0, 134.1, 131.4, 129.9, 129.7, 129.4, 127.5, 126.5, 126.0, 124.2, 123.1, 116.9, 109.8, 30.9, 29.7, 22.6, 21.3, 14.0. HRMS (ESI) calcd for $C_{22}H_{23}N_2^+$: 315.1856 ($M + H^+$), found: 315.1842.

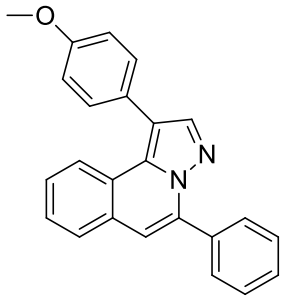


5-(4-Fluorophenyl)-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3q**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (s, 1H), 7.89-7.82 (m, 2H), 7.60 (s, 1H), 7.42 (s, 3H), 7.26-7.17 (m, 6H), 6.93 (s, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.3 (d, J_{CF} = 247.9 Hz), 141.7, 137.4 (d, $^{2}J_{CF}$ = 23.9 Hz), 134.6, 131.5 (d, $^{3}J_{CF}$ = 8.37 Hz), 131.1, 130.0, 129.9, 129.6,

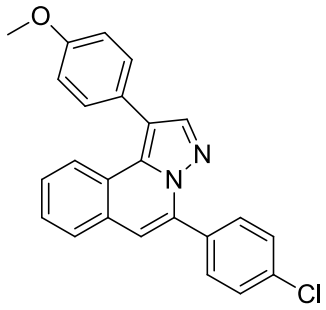
129.5, 127.8, 127.1(d, $^{2}J_{CF}$ = 23.0 Hz), 124.7, 123.3, 117.2, 115.5(d, $^{2}J_{CF}$ = 21.6 Hz), 112.9. HRMS (ESI) calcd for $C_{24}H_{18}FN_2^+$: 353.1449 (M + H^+), found: 353.1441.



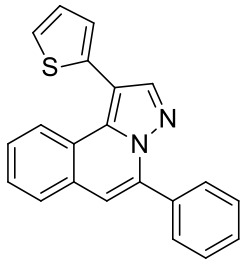
5-(4-Chlorophenyl)-9-fluoro-1-(*p*-tolyl)pyrazolo[5,1-*a*]isoquinoline (**3r**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (s, 1H), 7.82 (d, *J* = 8.6 Hz, 2H), 7.72-7.65 (m, 2H), 7.51-7.42 (m, 4H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.24-7.20 (m, 1H), 6.98 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2 (d, J_{CF} = 246.7 Hz), 141.7, 137.6, 136.6 (d, $^{2}J_{CF}$ = 24.5 Hz), 135.3, 133.6, 132.1, 130.8, 130.3, 130.1, 129.7 ,129.6, 129.3 (d, $^{3}J_{CF}$ = 8.8 Hz), 128.6, 127.6, 126.1, 126.0, 117.7, 116.5(d, $^{2}J_{CF}$ = 23.8 Hz), 112.2, 108.8 (d, $^{2}J_{CF}$ = 24.2 Hz). HRMS (ESI) calcd for $C_{24}H_{17}ClFN_2^+$: 387.1059 (M + H^+), found: 387.1053.



1-(4-Methoxyphenyl)-5-phenylpyrazolo[5,1-*a*]isoquinoline (**3s**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.1 Hz, 1H), 7.87 (m, 3H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.53-7.41 (m, 6H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.03 -6.98 (m, 3H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 141.7, 138.5, 134.6, 134.0, 131.2, 129.7, 129.5, 129.3, 128.4, 127.7, 127.2, 126.9, 126.4, 124.8, 123.2, 116.7, 114.2, 112.9, 55.4. HRMS (ESI) calcd for $C_{24}H_{19}N_2O^+$: 351.1492 (M + H^+), found: 351.1490.

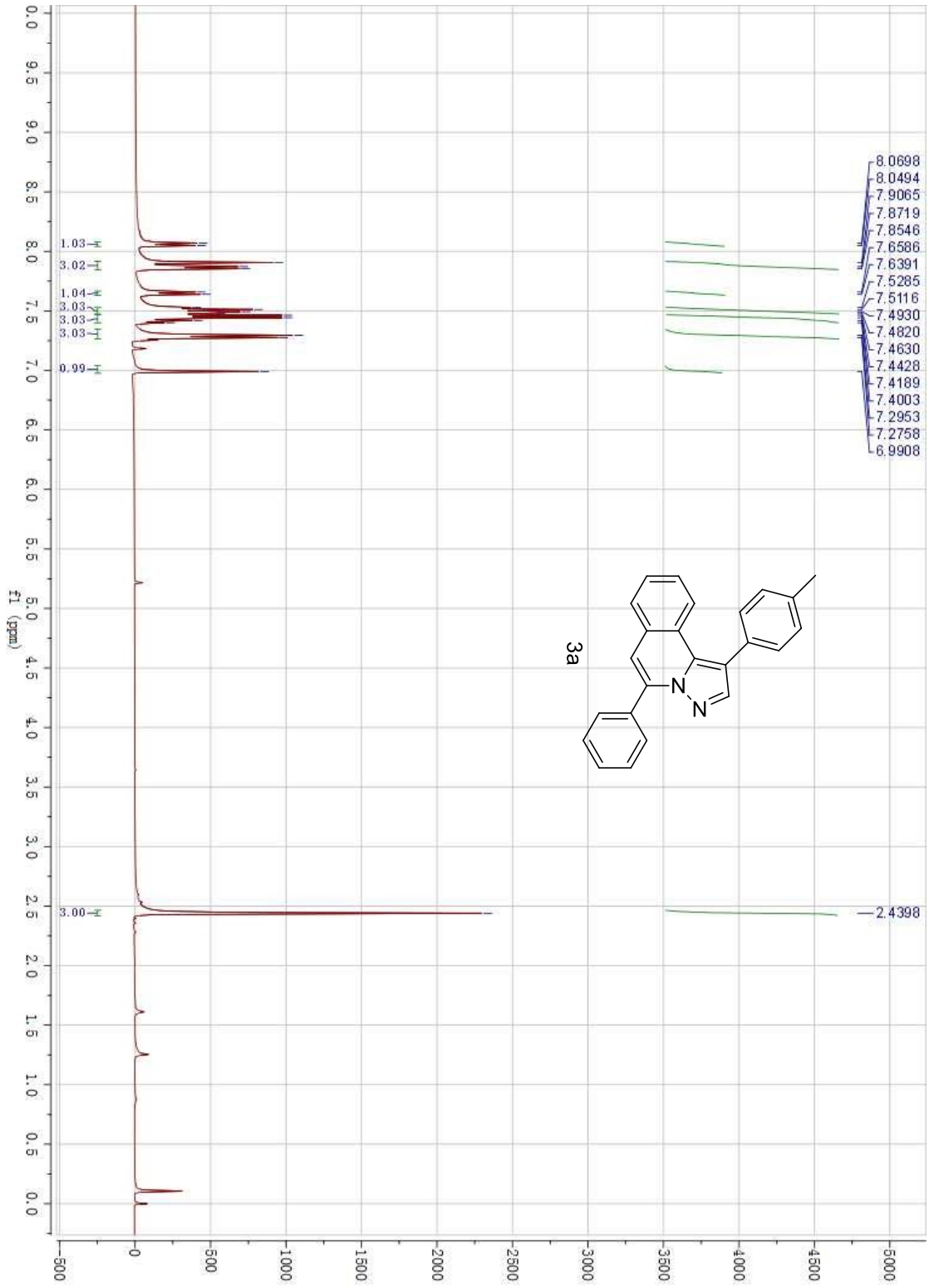


5-(4-Chlorophenyl)-1-(4-methoxyphenyl)pyrazolo[5,1-*a*]isoquinoline (**3t**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (s, 1H), 7.88-7.80 (m, 3H), 7.65 (s, 1H), 7.47 (s, 5H), 7.30 (s, 1H), 7.03-6.97 (m, 3H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 141.7, 137.3, 135.2, 134.6, 132.4, 131.2, 130.8, 129.5, 128.6, 127.8, 127.3, 127.2, 126.2, 124.8, 123.2, 116.9, 114.2, 112.9, 55.6. HRMS (ESI) calcd for $C_{24}H_{18}ClN_2O^+$: 385.1102 (M + H^+), found: 385.1100.



5-Phenyl-1-(thiophen-2-yl)pyrazolo[5,1-*a*]isoquinoline (**3u**). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14-8.12 (m, 1H), 7.98-7.97 (m, 1H), 7.86-7.84 (m, 2H), 7.68-7.66 (m, 1H), 7.52-7.42 (m, 5H), 7.36-7.32 (m, 1H), 7.22-7.17 (m, 2H), 7.04-7.03 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.6, 138.5, 135.7, 134.9, 133.8, 129.8, 129.5, 129.4, 128.4, 128.1, 127.9, 127.6, 127.2, 127.2, 126.3, 124.4, 123.3, 113.3, 108.7. HRMS (ESI) calcd for $C_{21}H_{15}N_2S^+$: 327.0950 (M + H^+), found: 327.0941.

1. W. Hao , T. Zhang, M. Cai, *Tetrahedron* **2013**, *69*, 9219.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7.4428
7.4189
7.4003
7.2953
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1.04
3.03
3.03
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3.00
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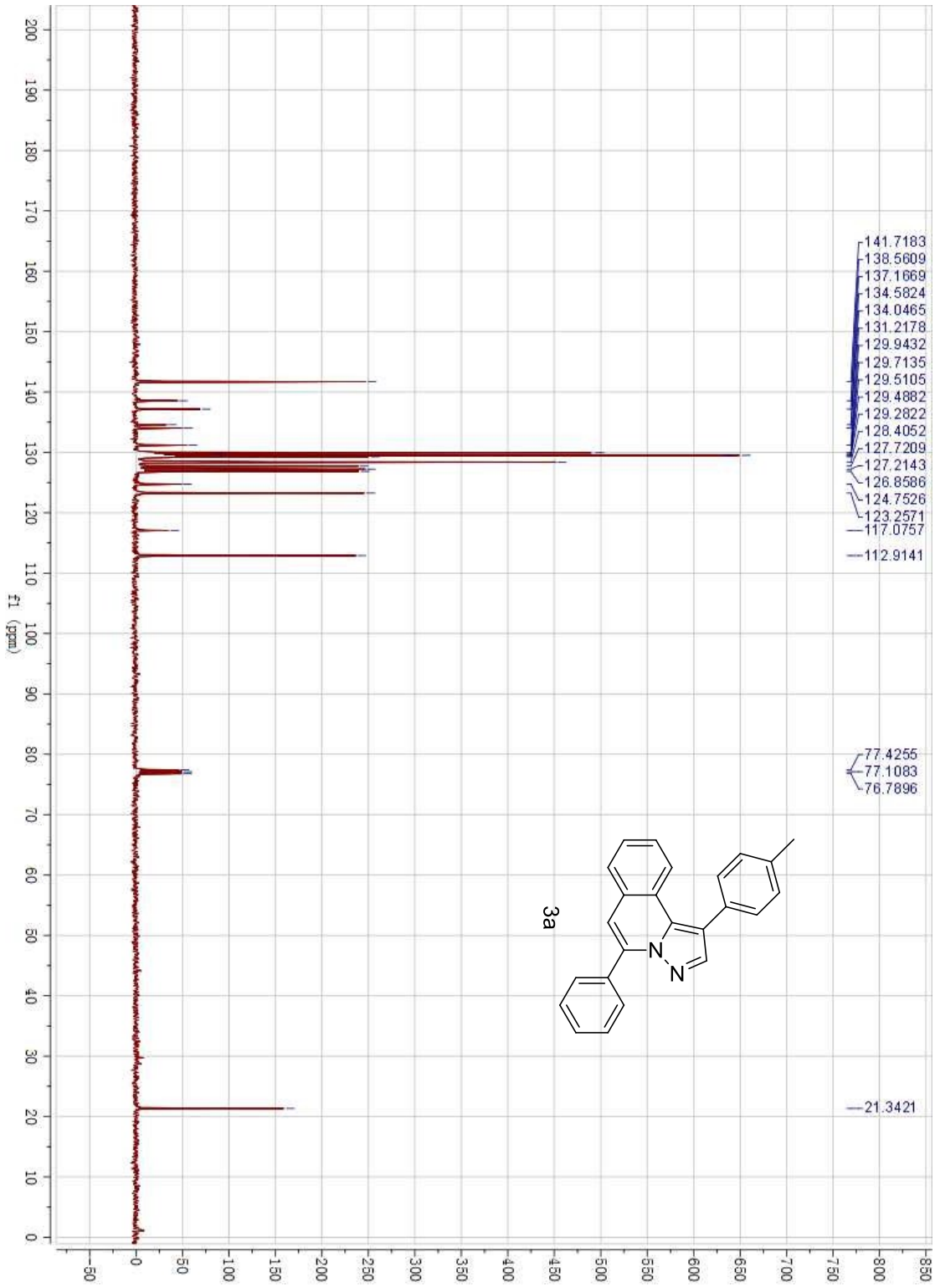
N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128.4052
127.7209
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124.7526
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f1 (ppm)
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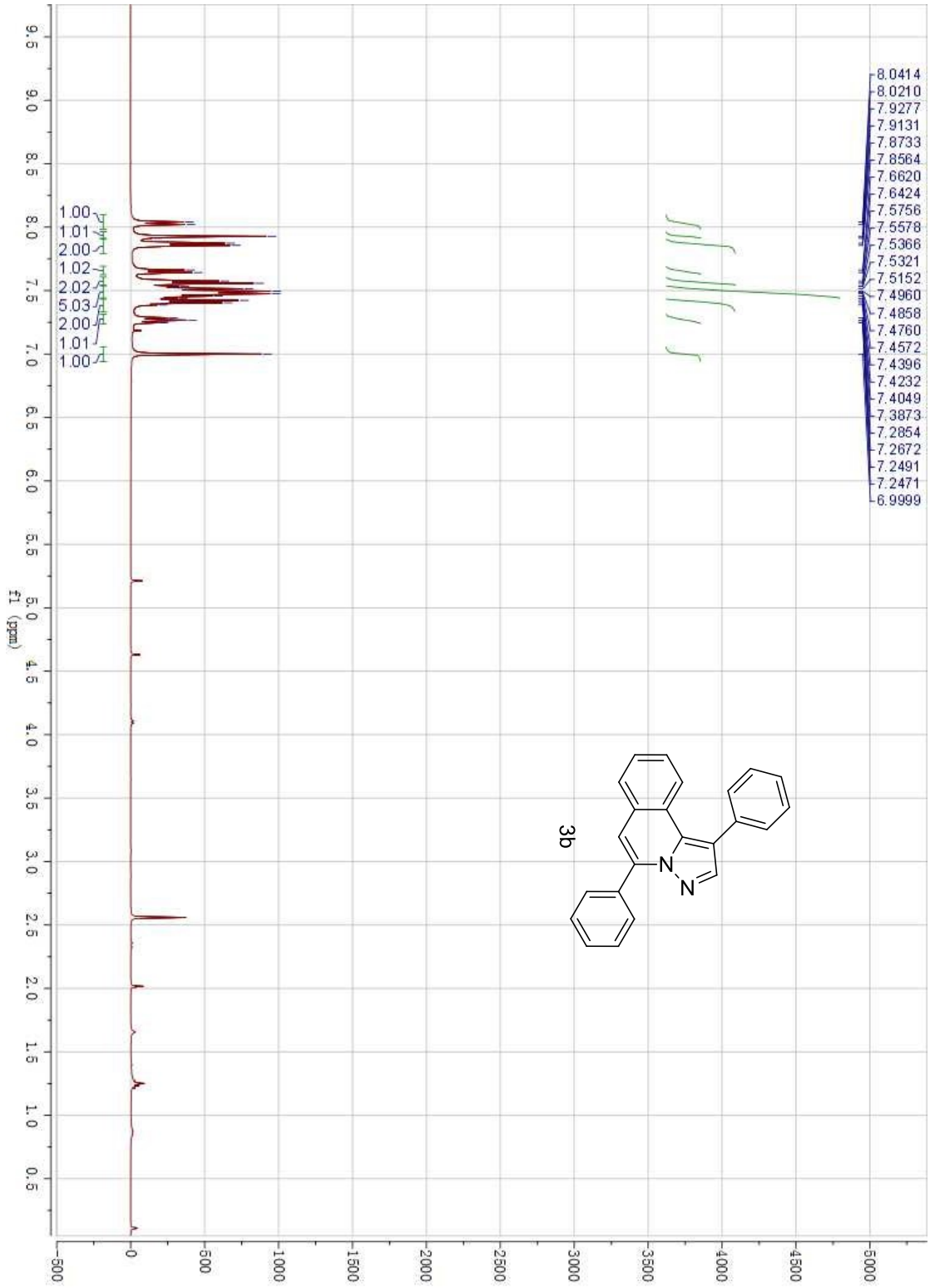
N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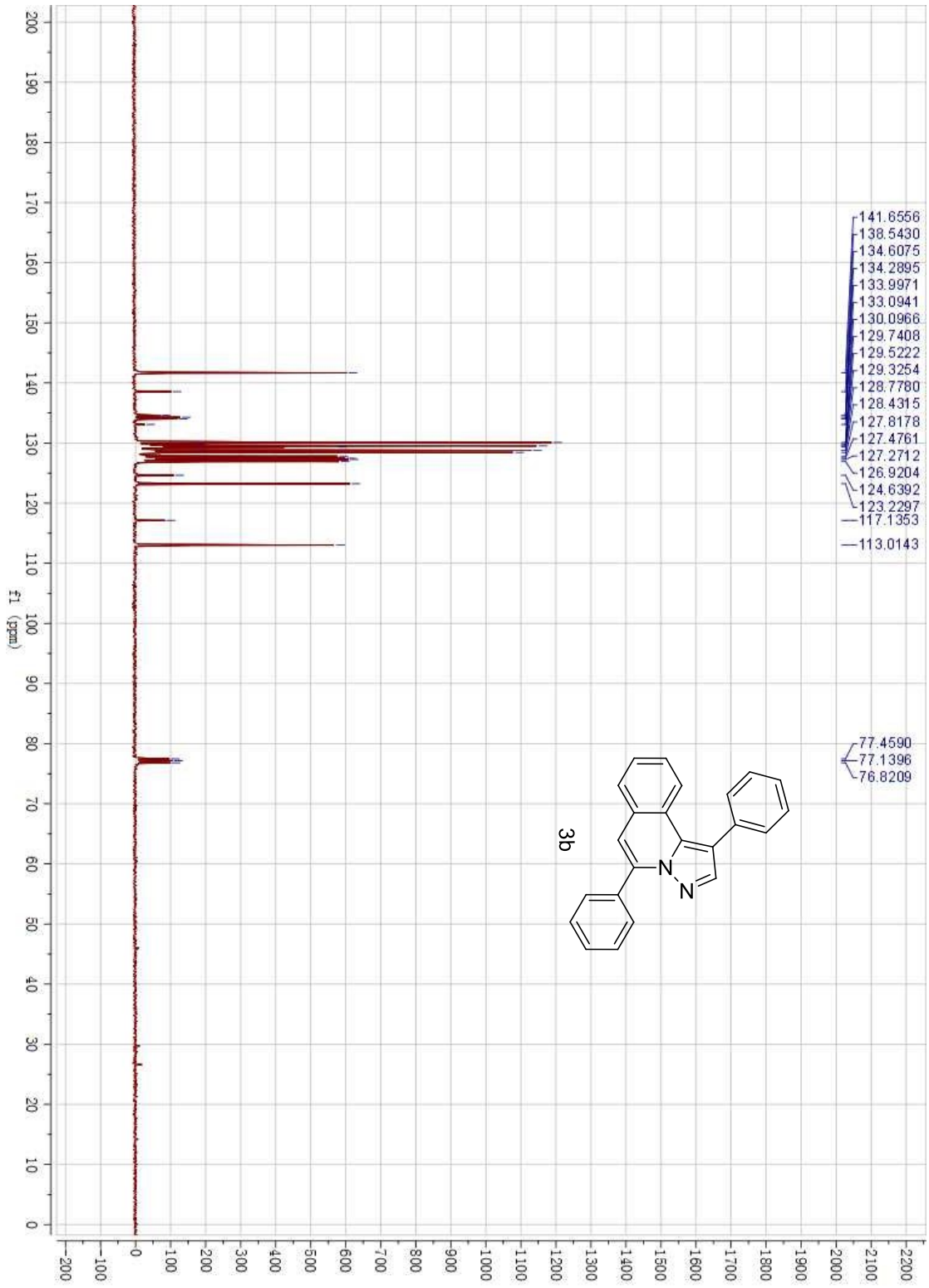
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f1 (ppm)
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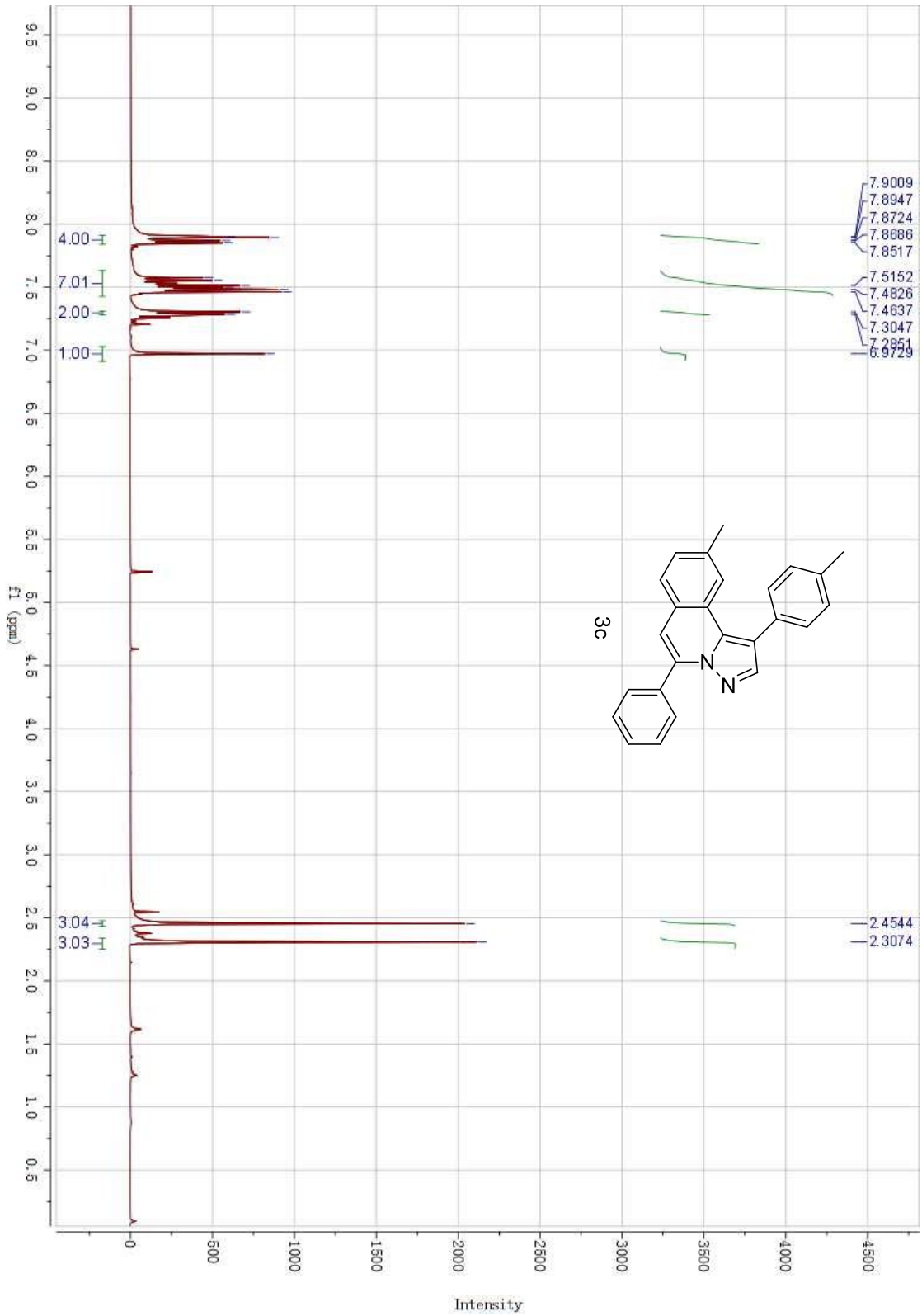
N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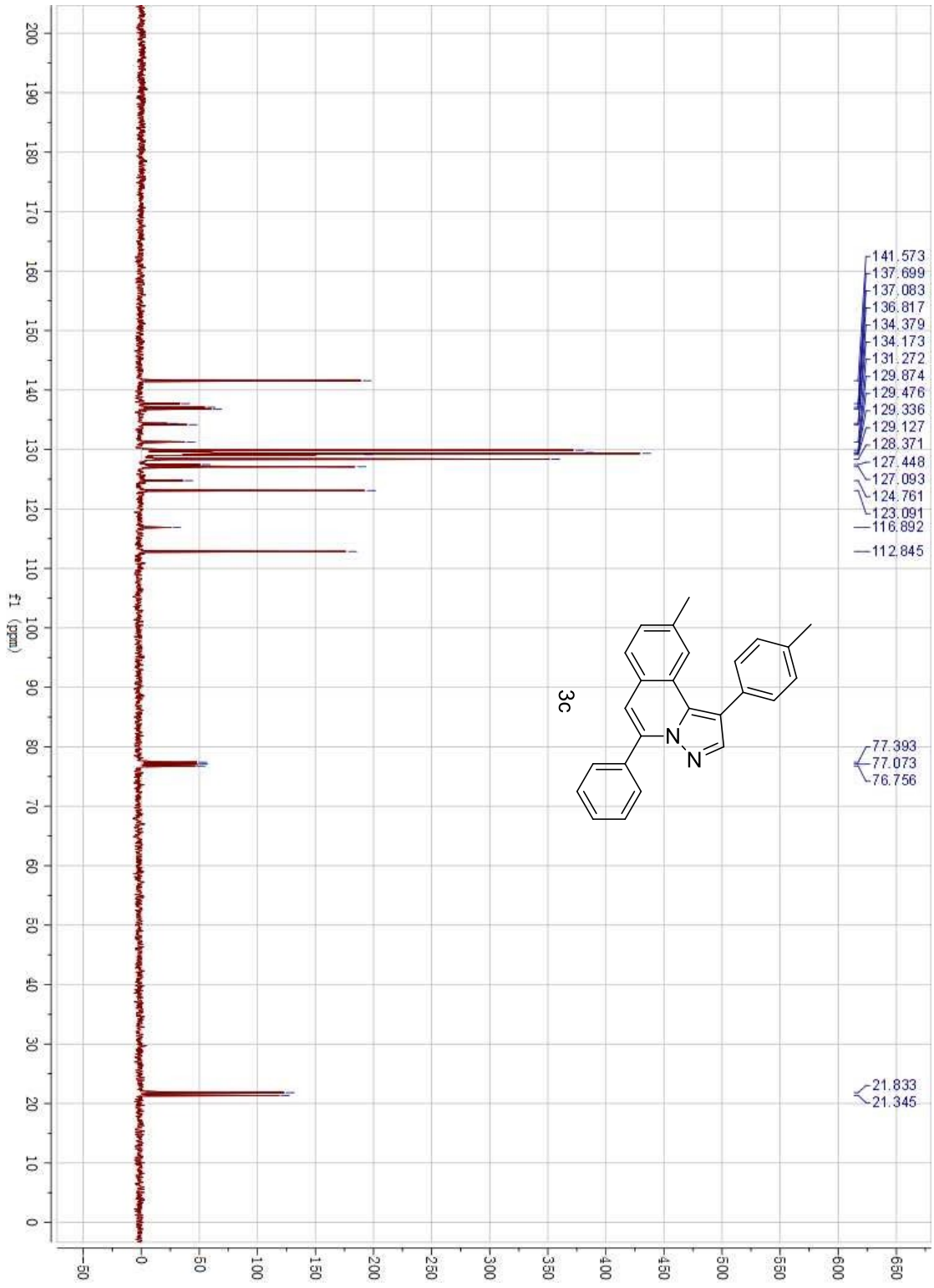
f1 (ppm)
Intensity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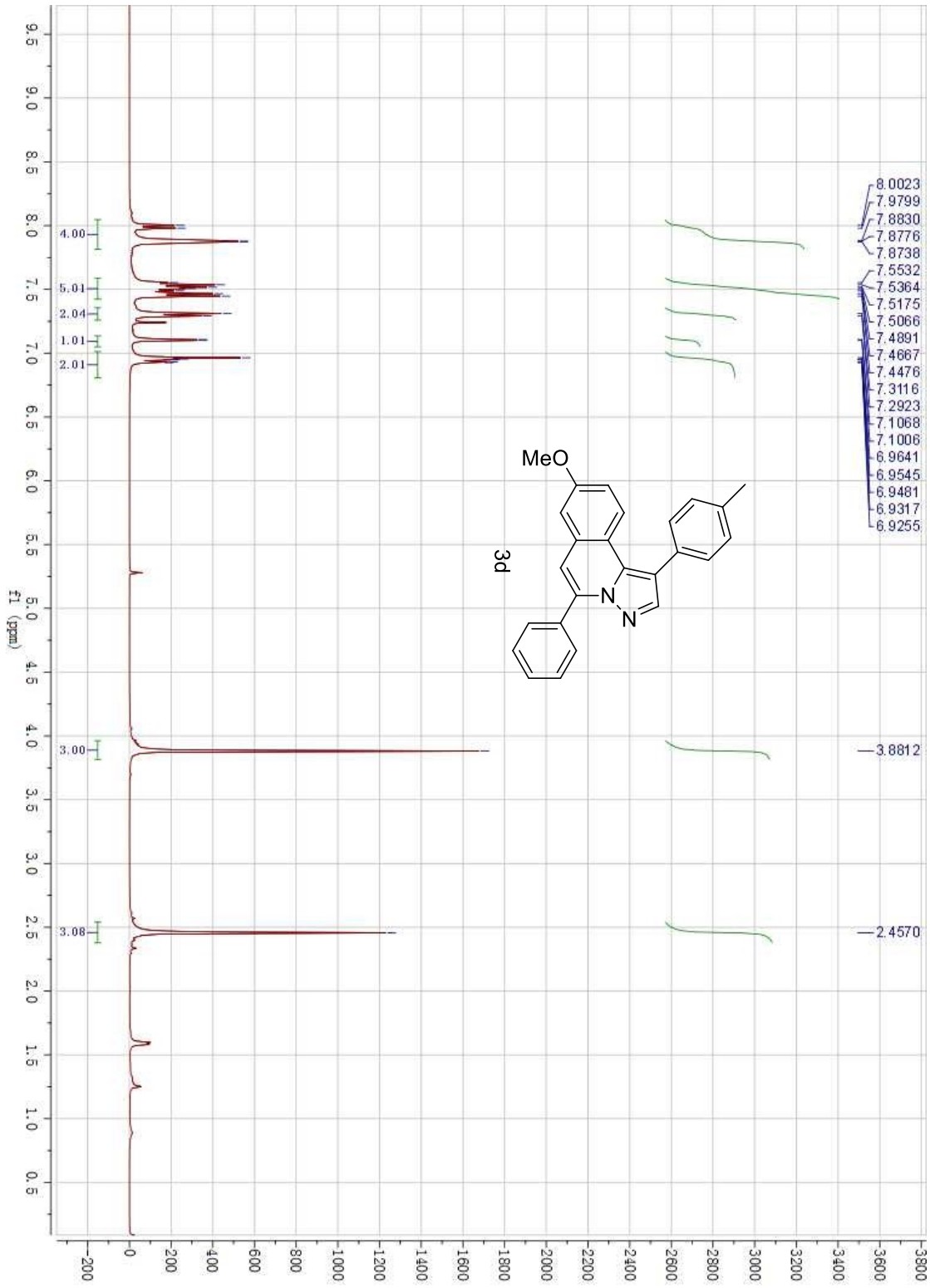
f1 (ppm)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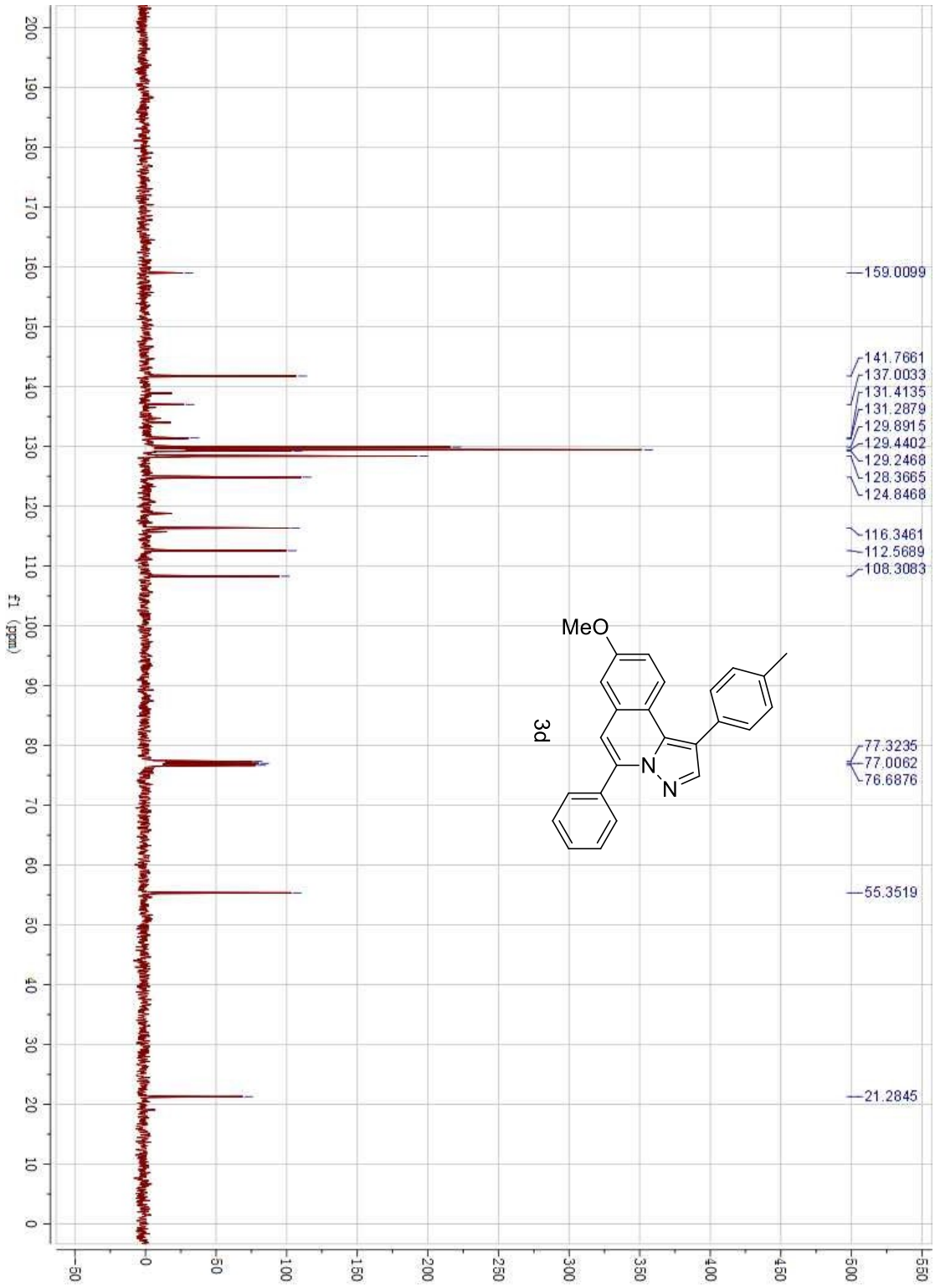
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MeO
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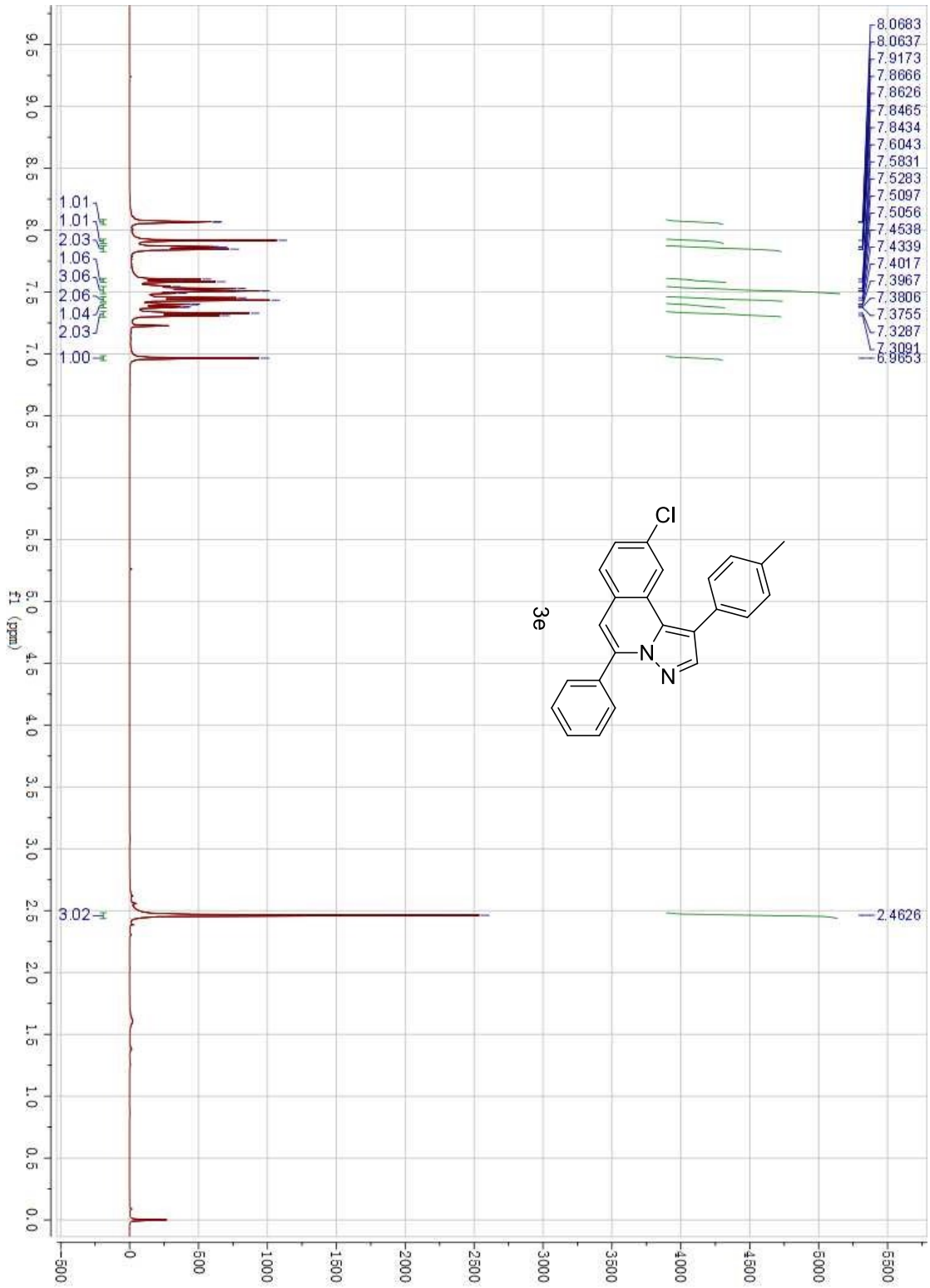
N
3d
f1 (ppm)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7.5056
7.4538
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7.4017
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7.3755
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3.06
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1.04
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Cl
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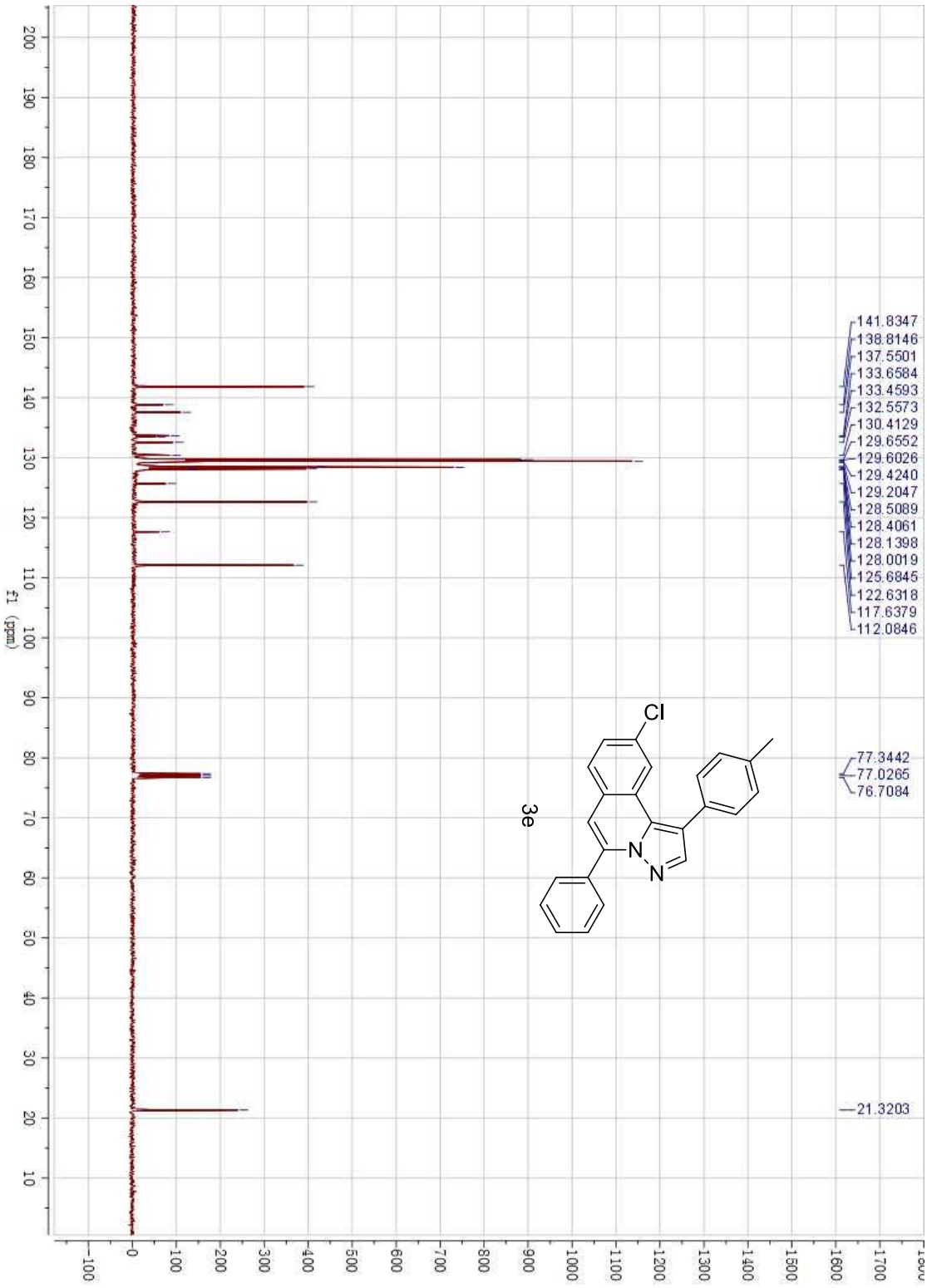
N
3e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Cl
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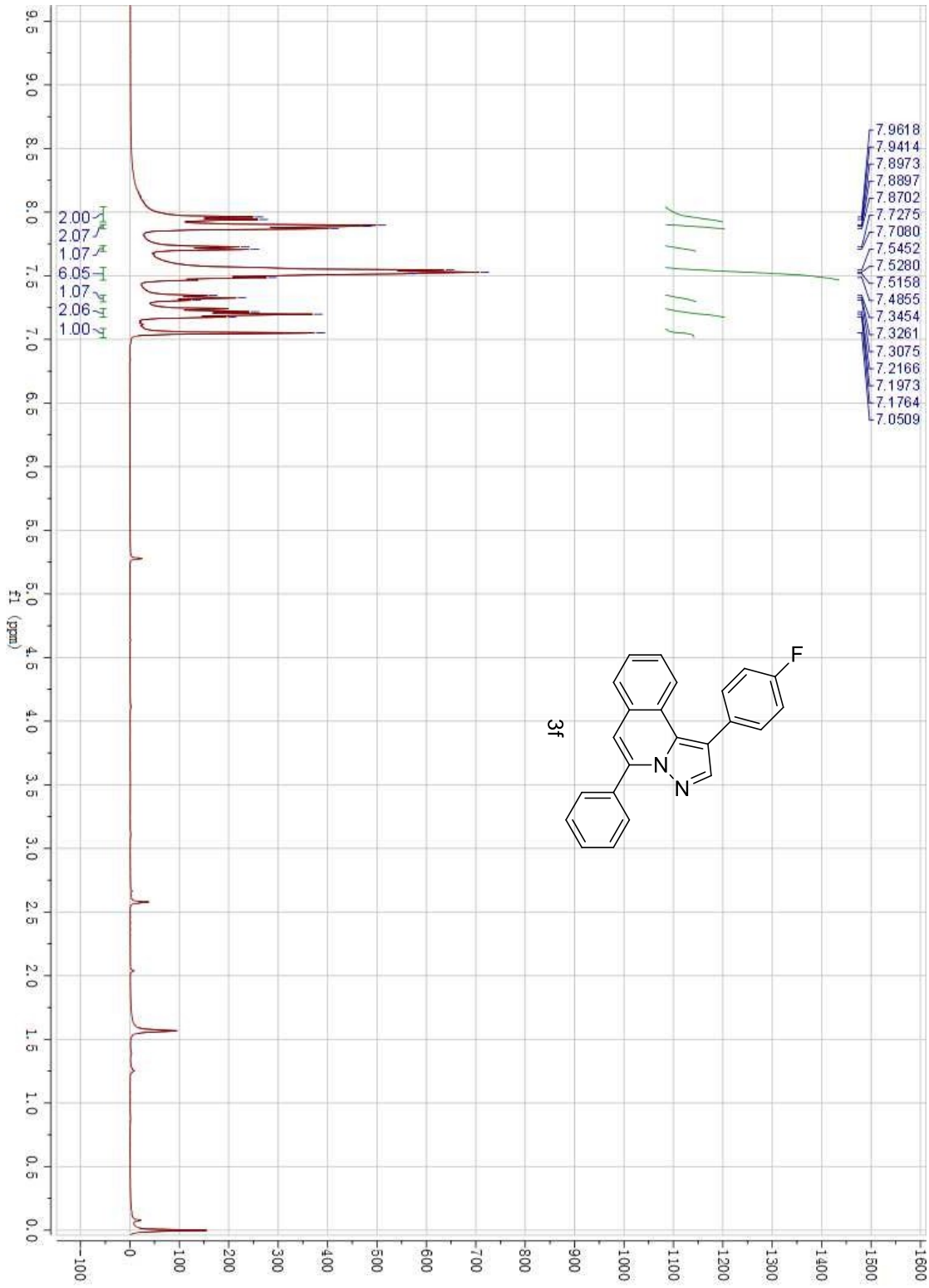
3e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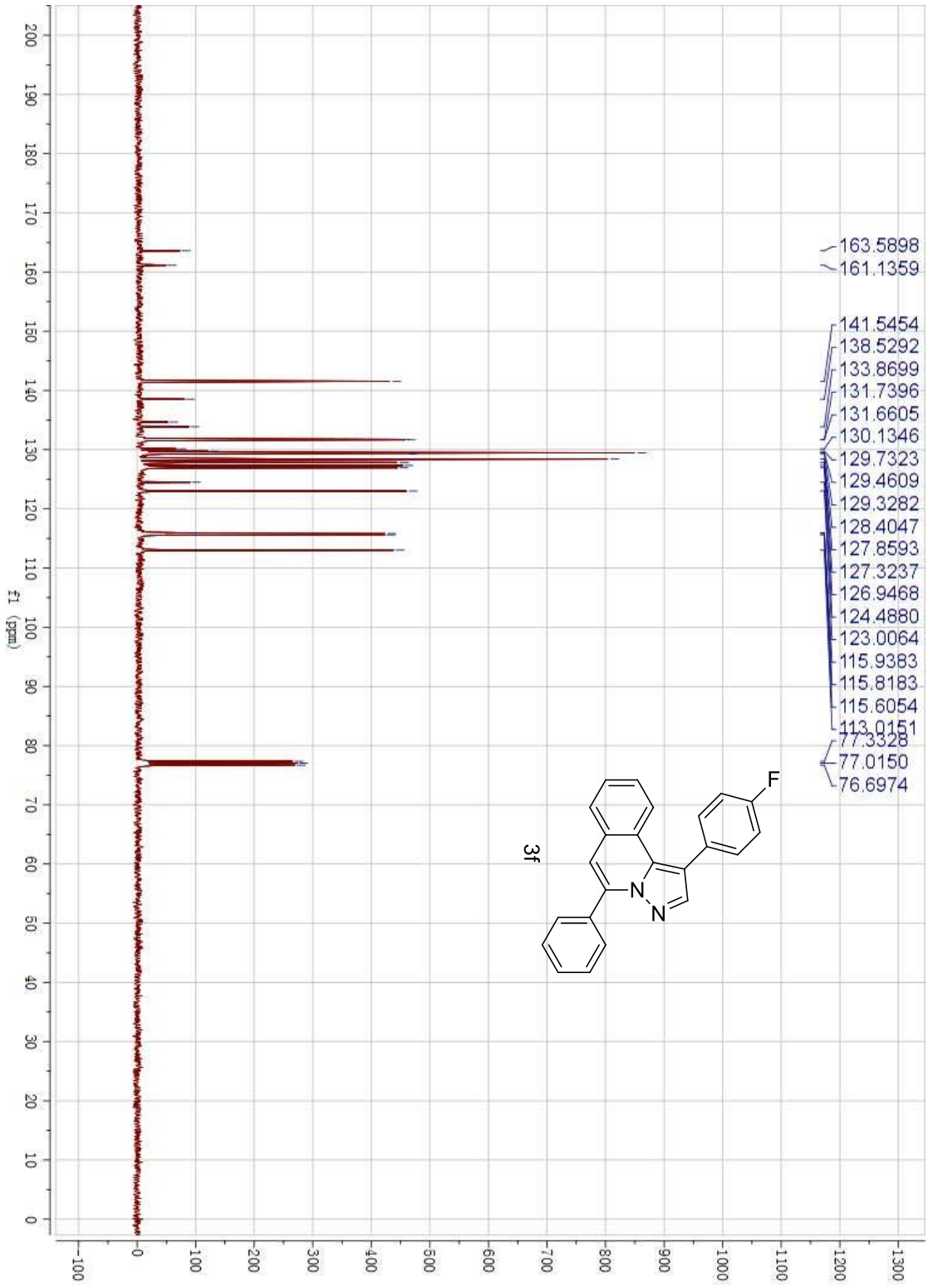
N
N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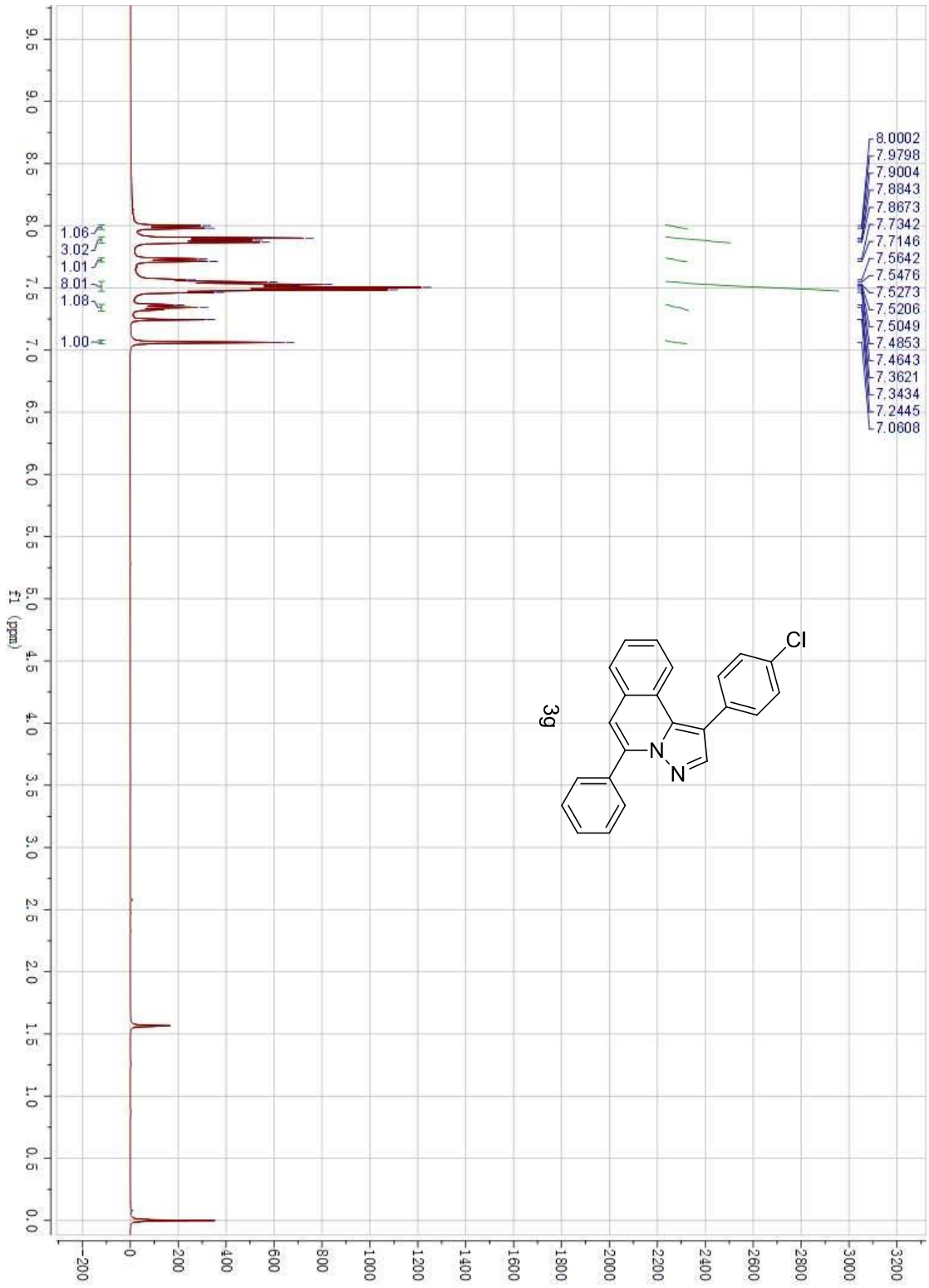
N
N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1.01
8.01
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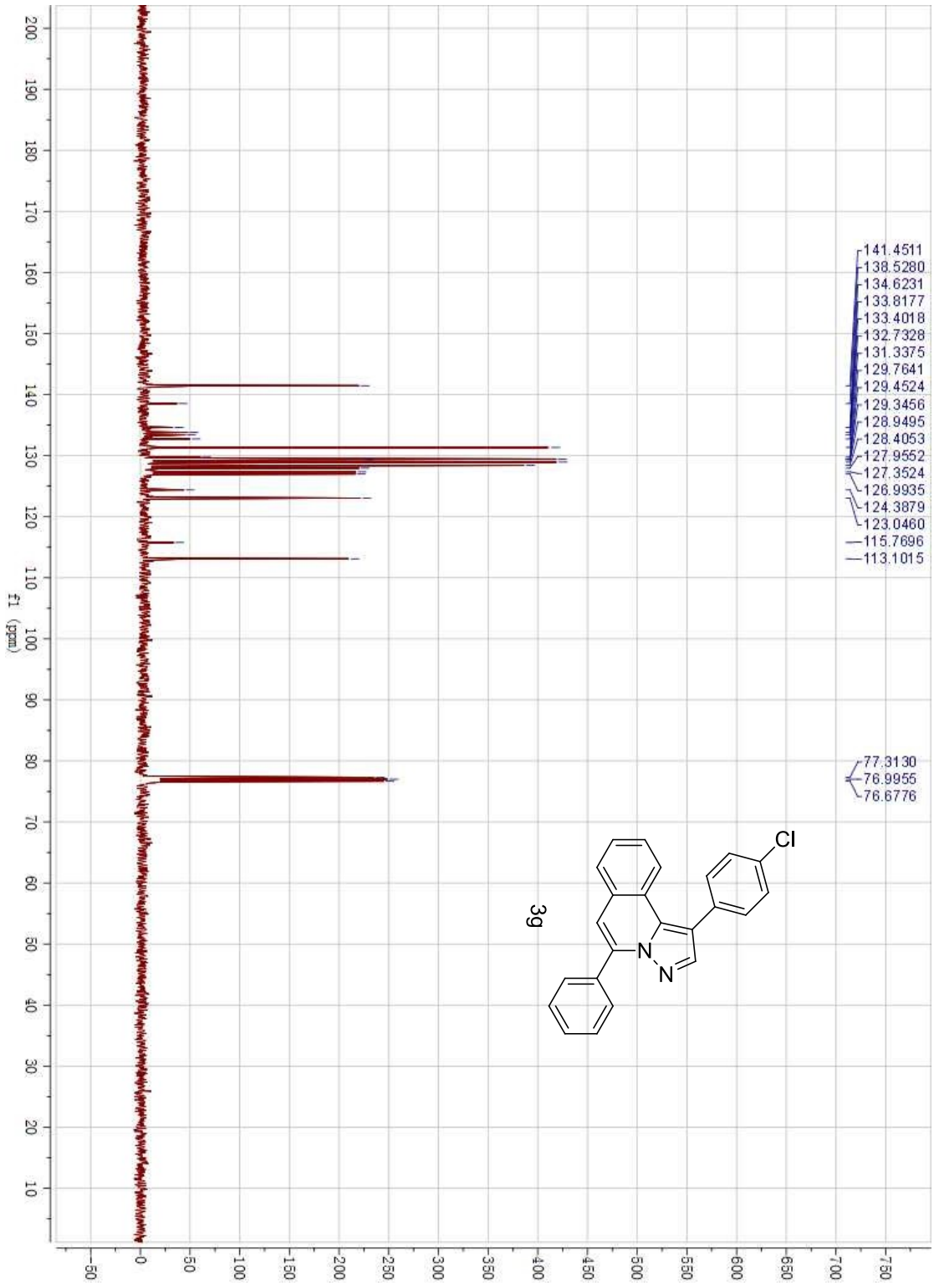
1.00
f1 (ppm)
Cl
N
N
3g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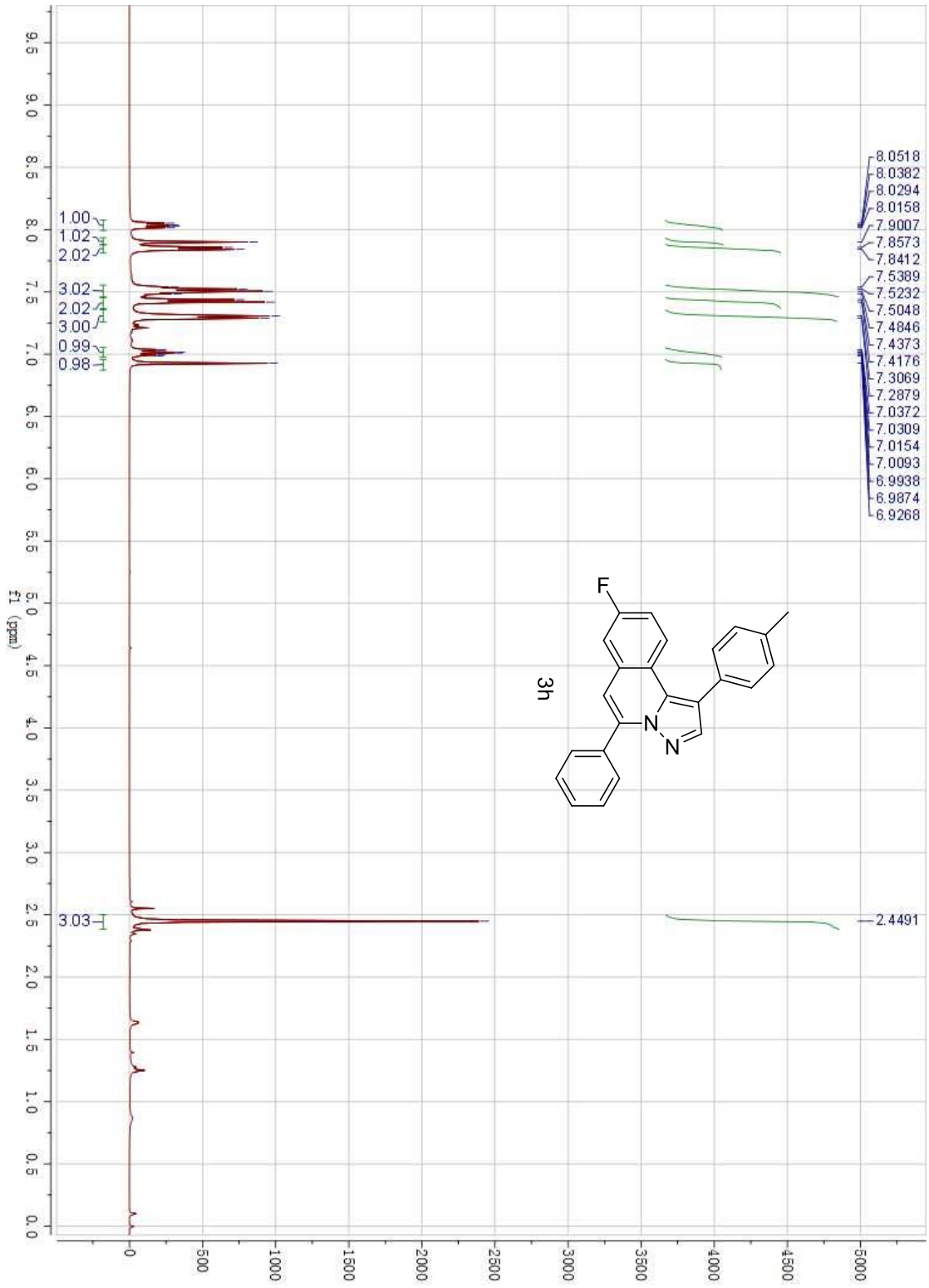
f1 (ppm)
Cl
N
N
3g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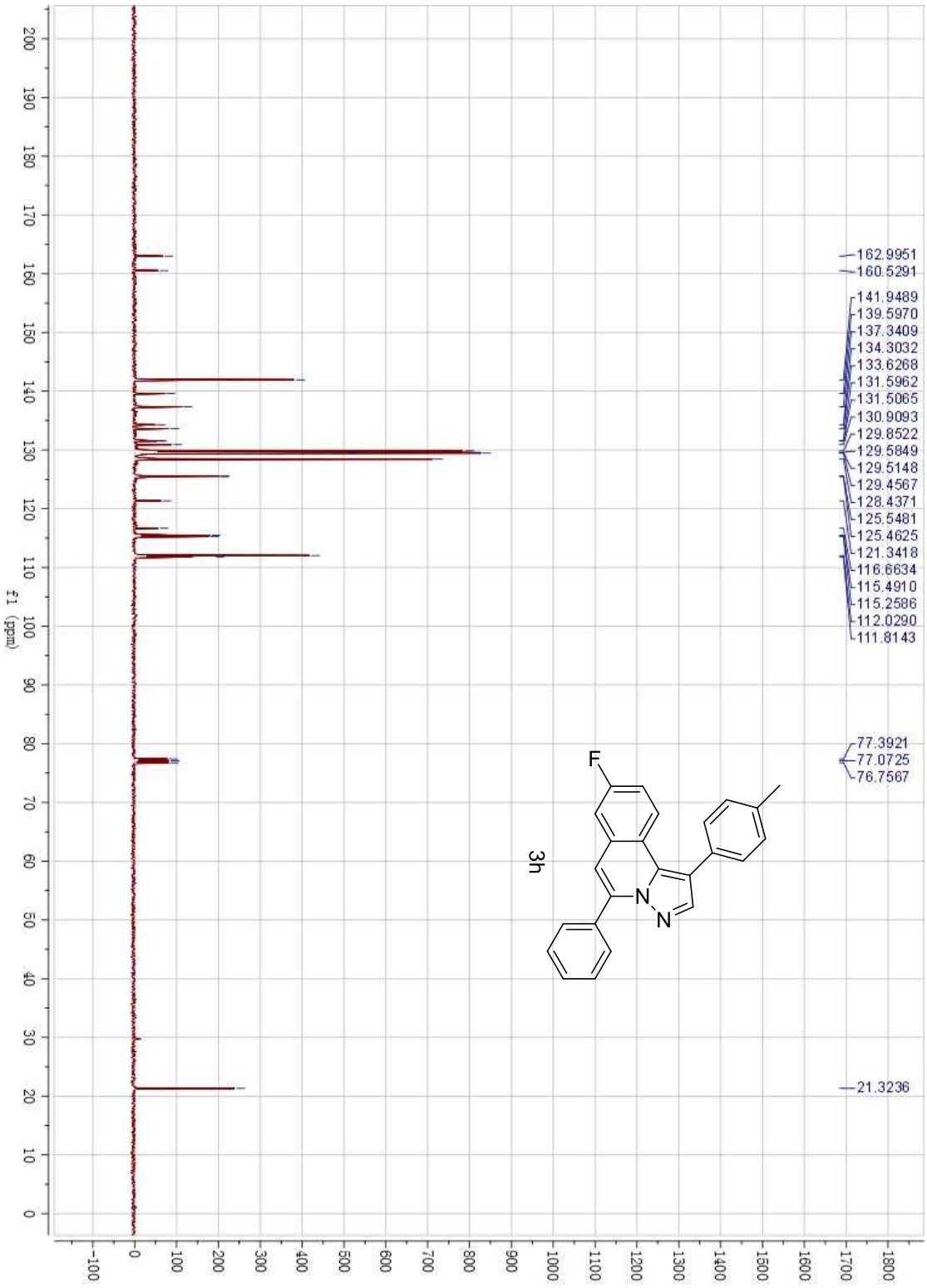
N
3h
f1 (ppm)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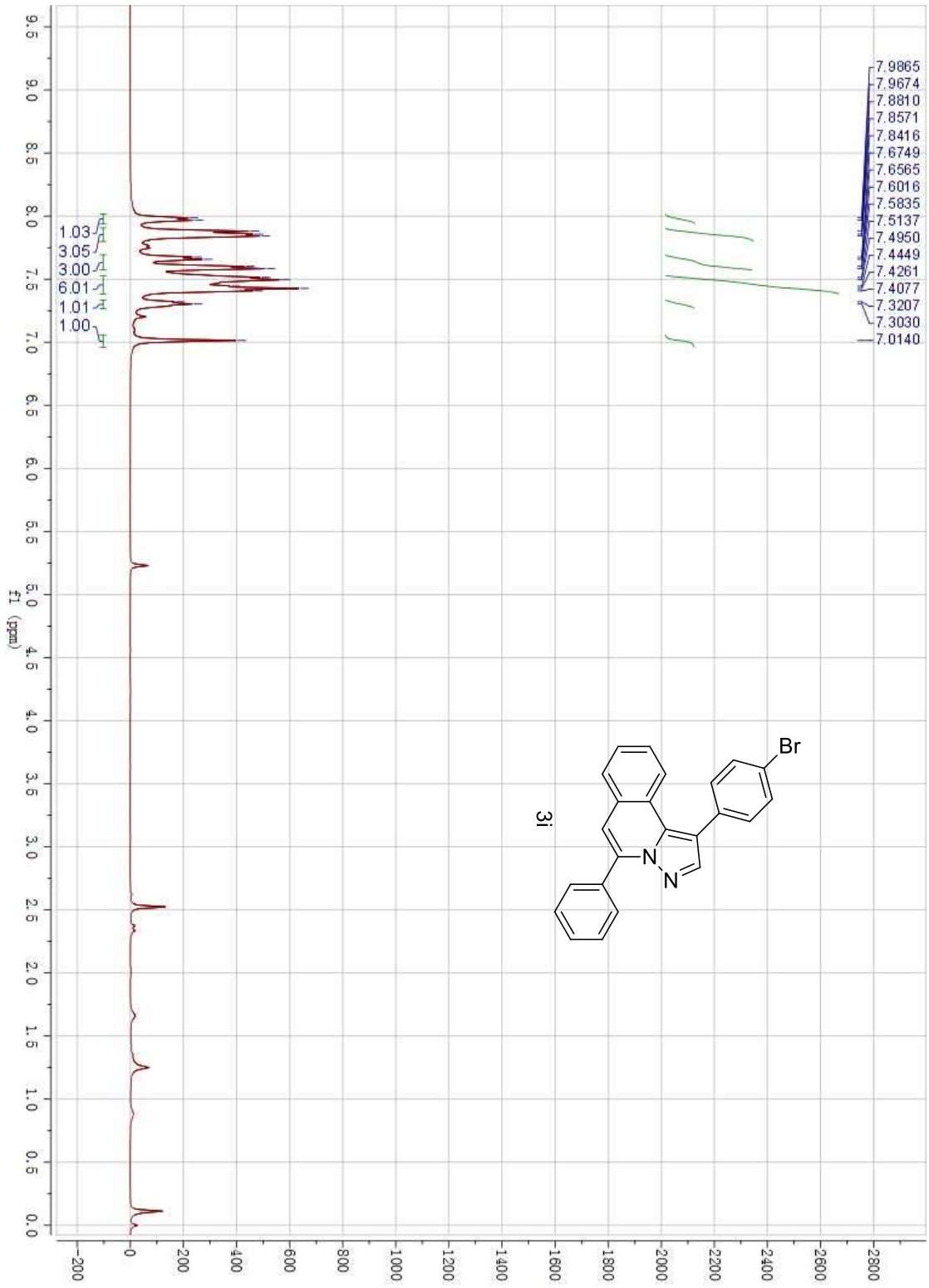
f1 (ppm)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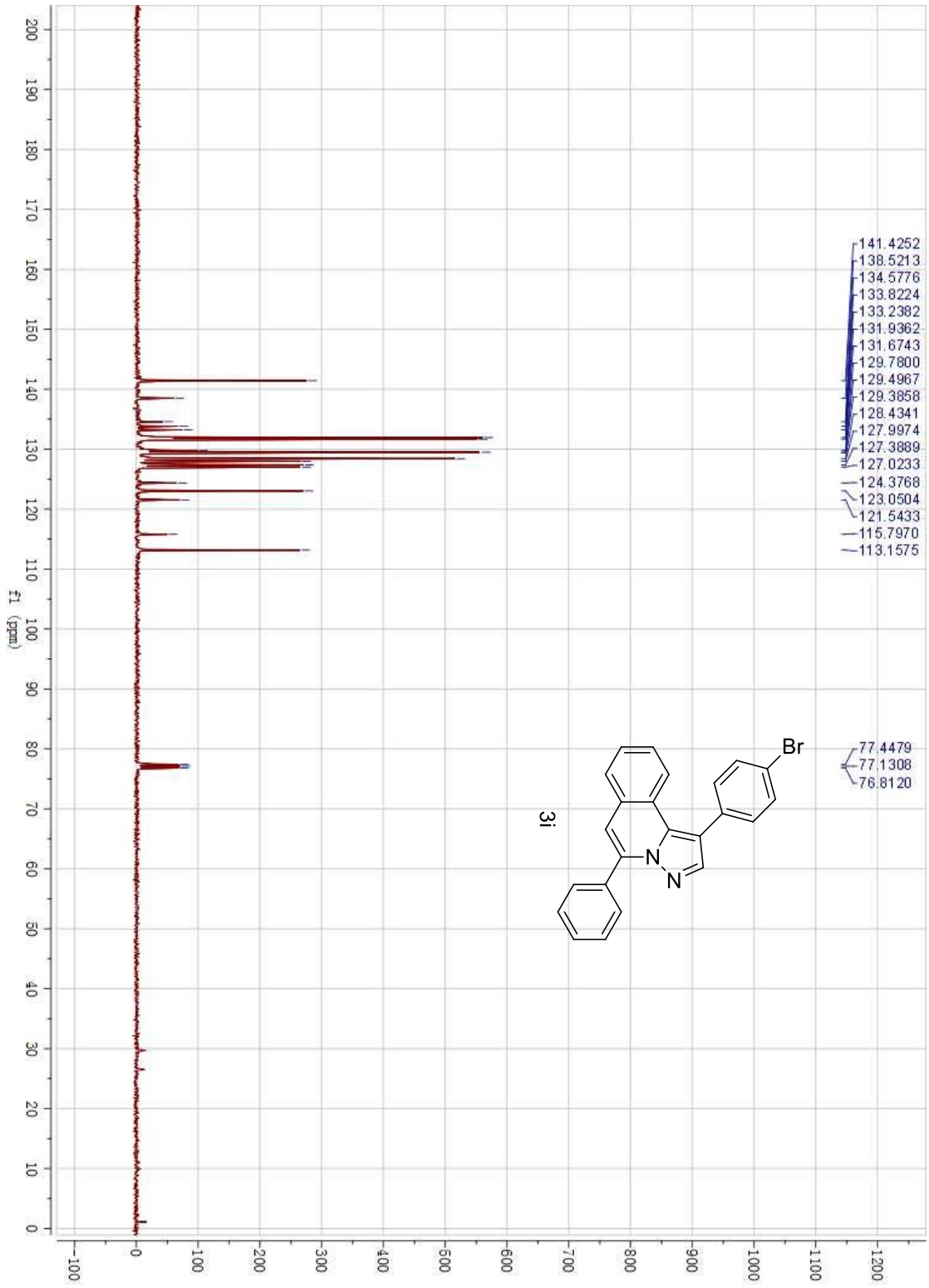
N
3i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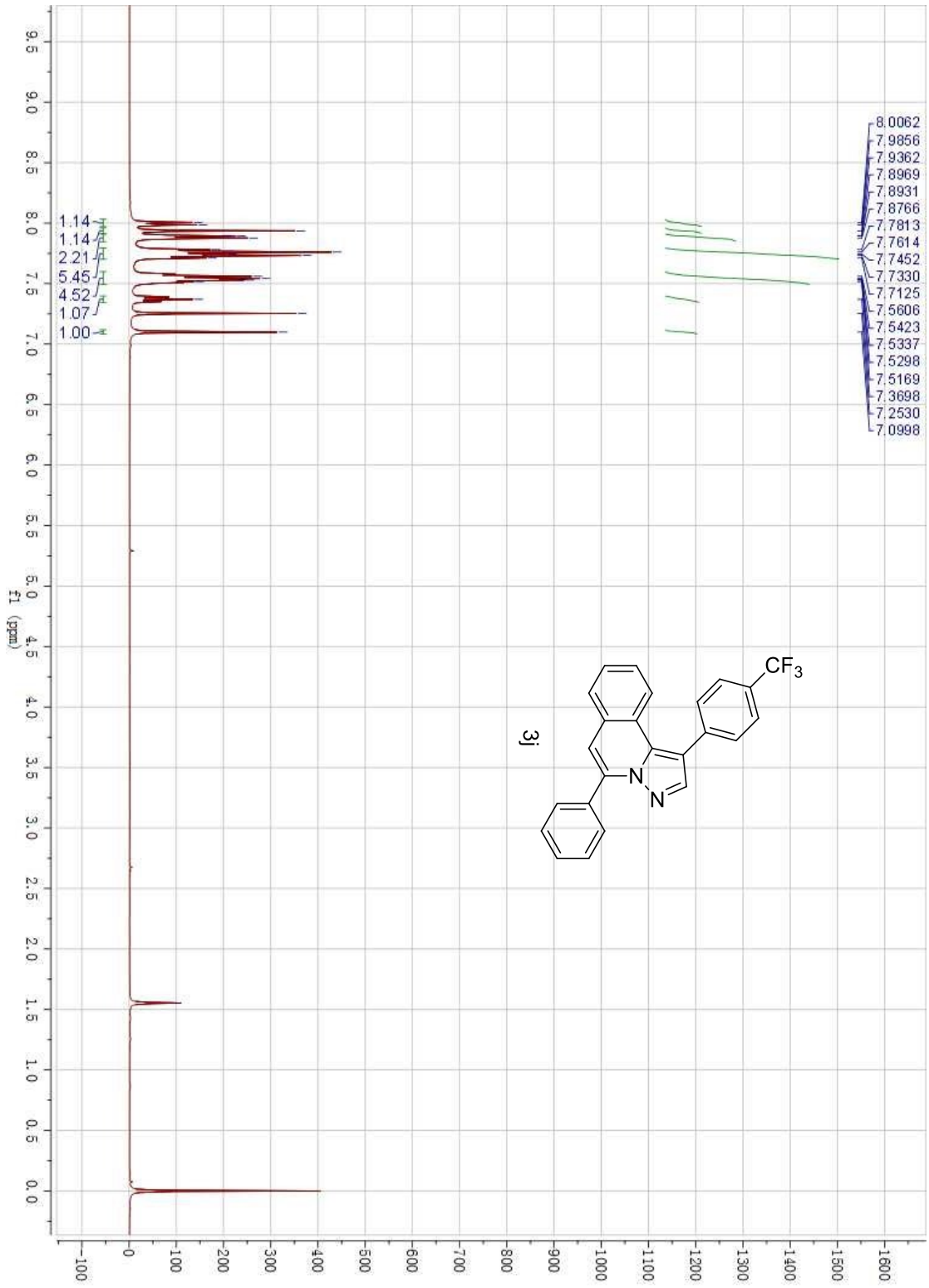
76.8120
f1 (ppm)
Br
N
N
3i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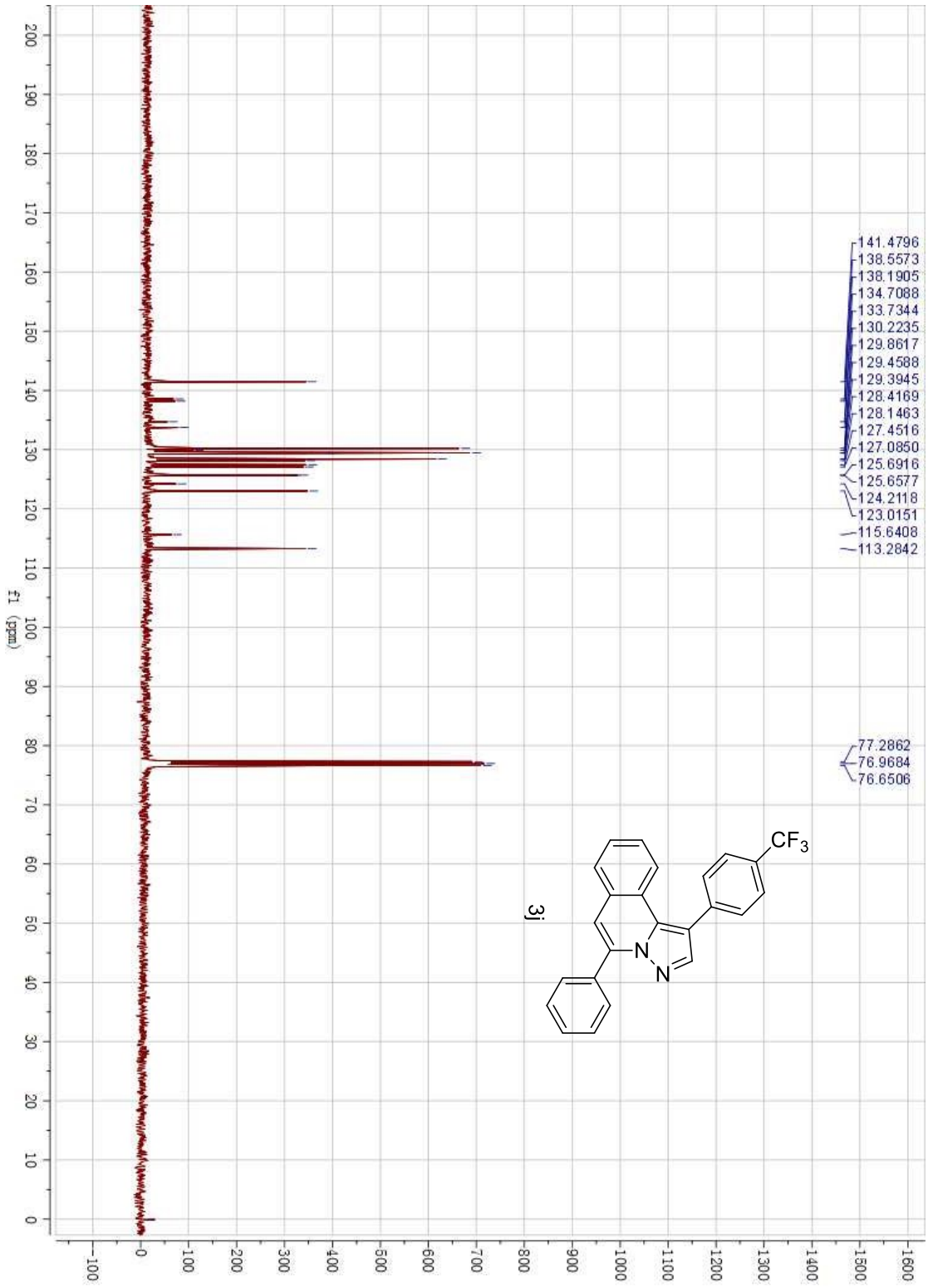
CF3
N
N
3j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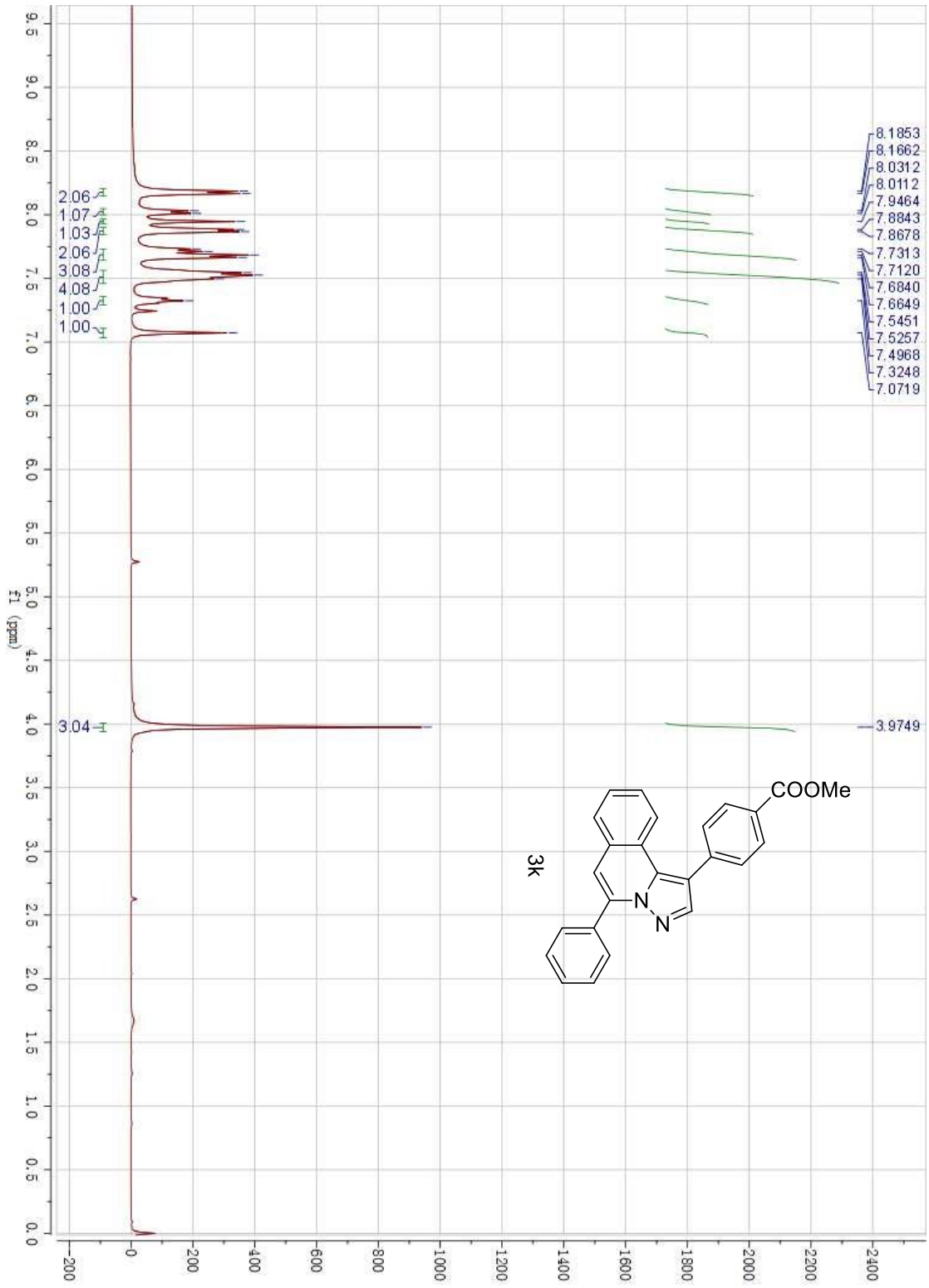
CF3
N
N
3j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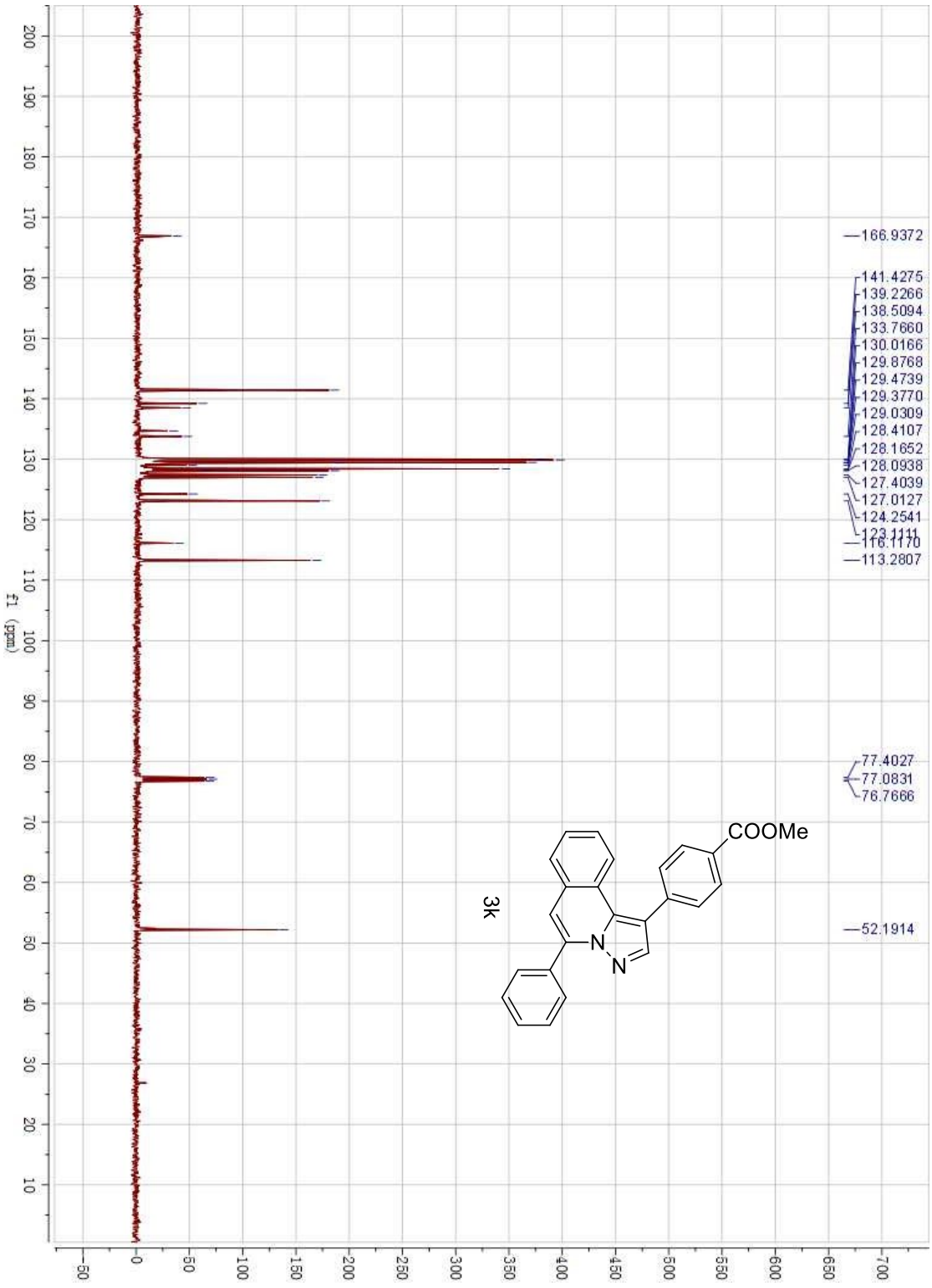
3k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128.1652
128.0938
127.4039
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124.2541
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77.0831
76.7666
52.1914
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COOMe
3k
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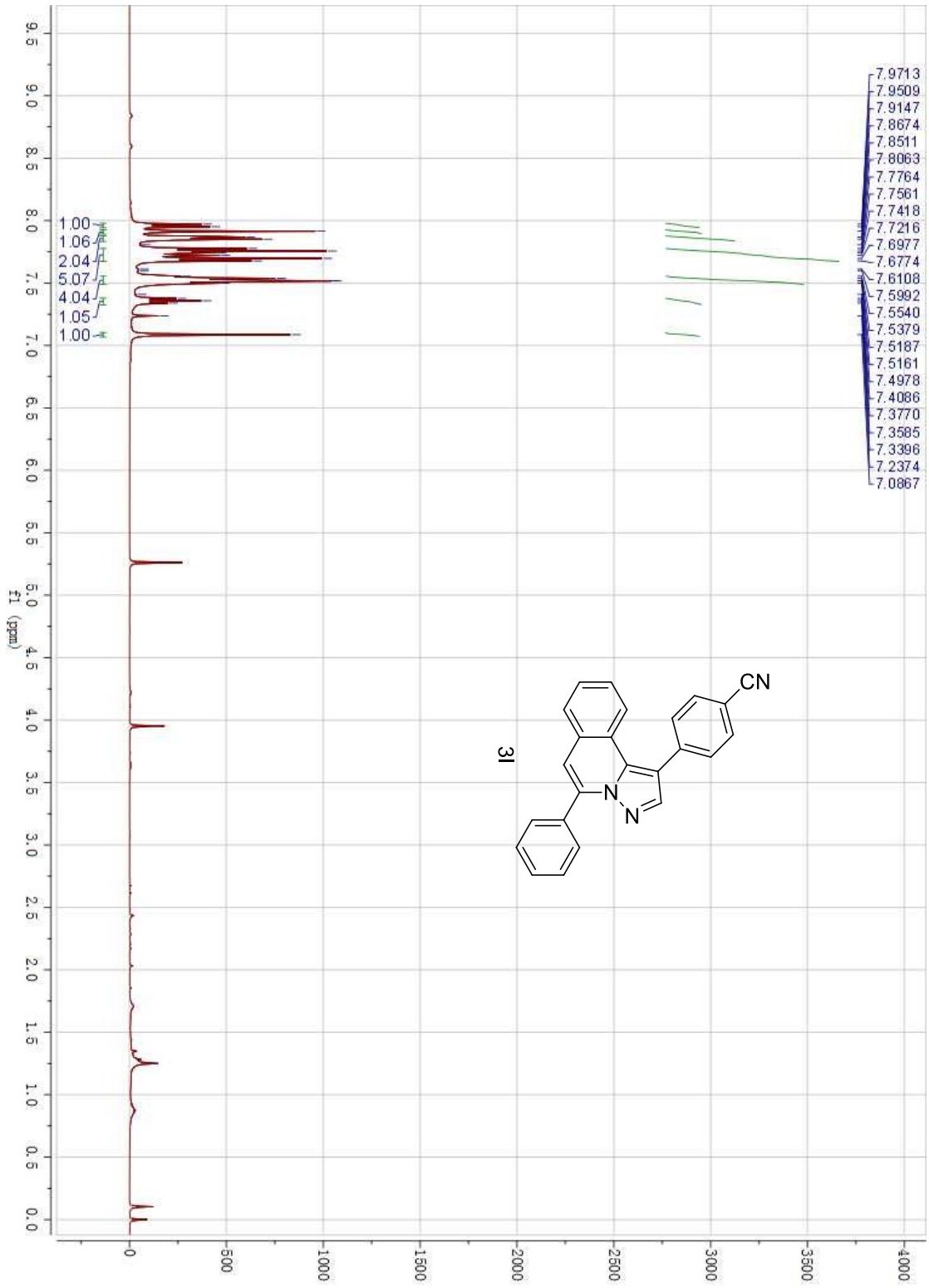
N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7.8511
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7.7764
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7.7216
7.6977
7.6774
7.6108
7.5992
7.5540
7.5379
7.5187
7.5161
7.4978
7.4086
7.3770
7.3585
7.3396
7.2374
7.0867
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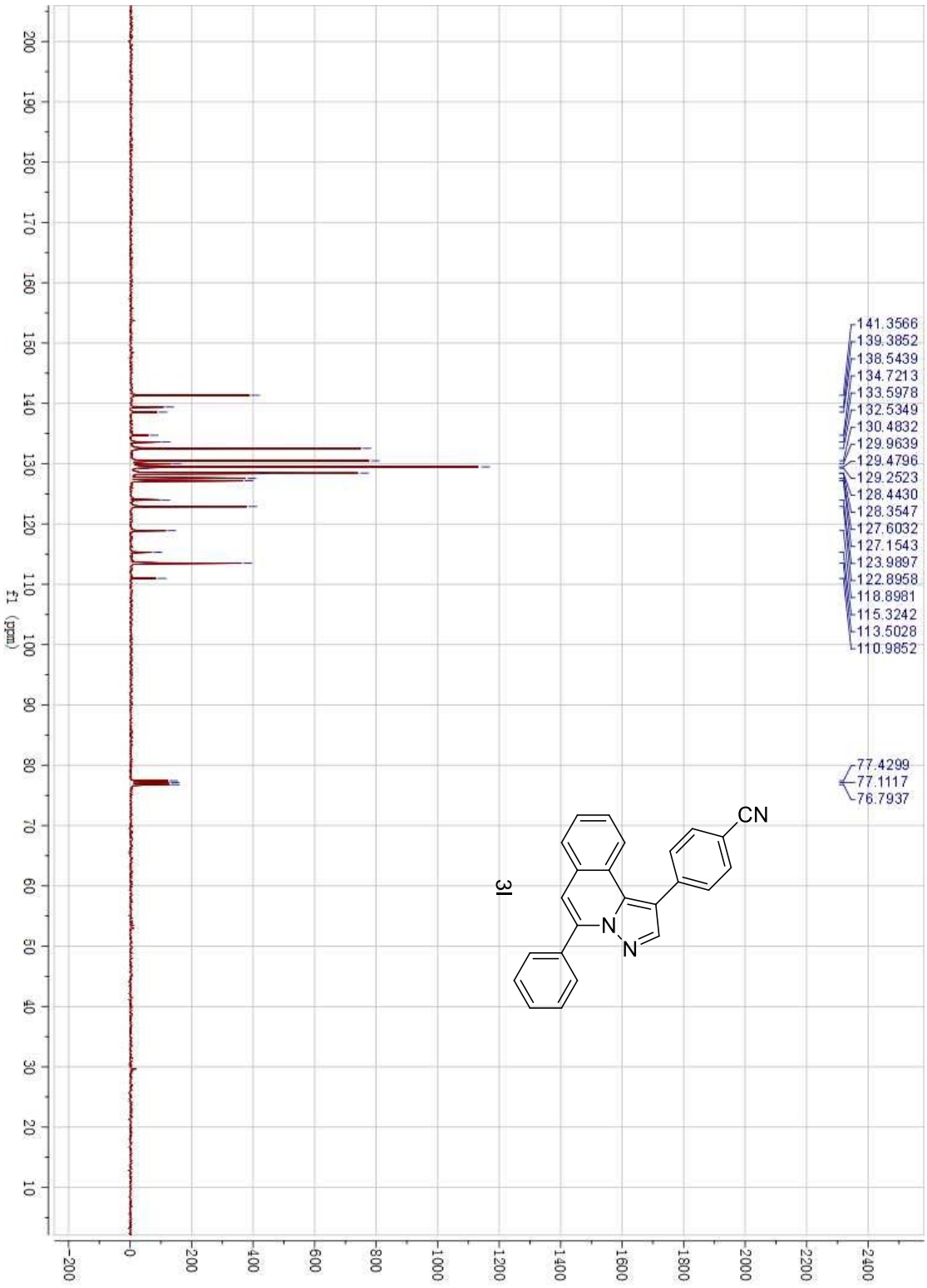
1.06
2.04
5.07
4.04
1.05
1.00
f1 (ppm)
CN
N
N
3l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130.4832
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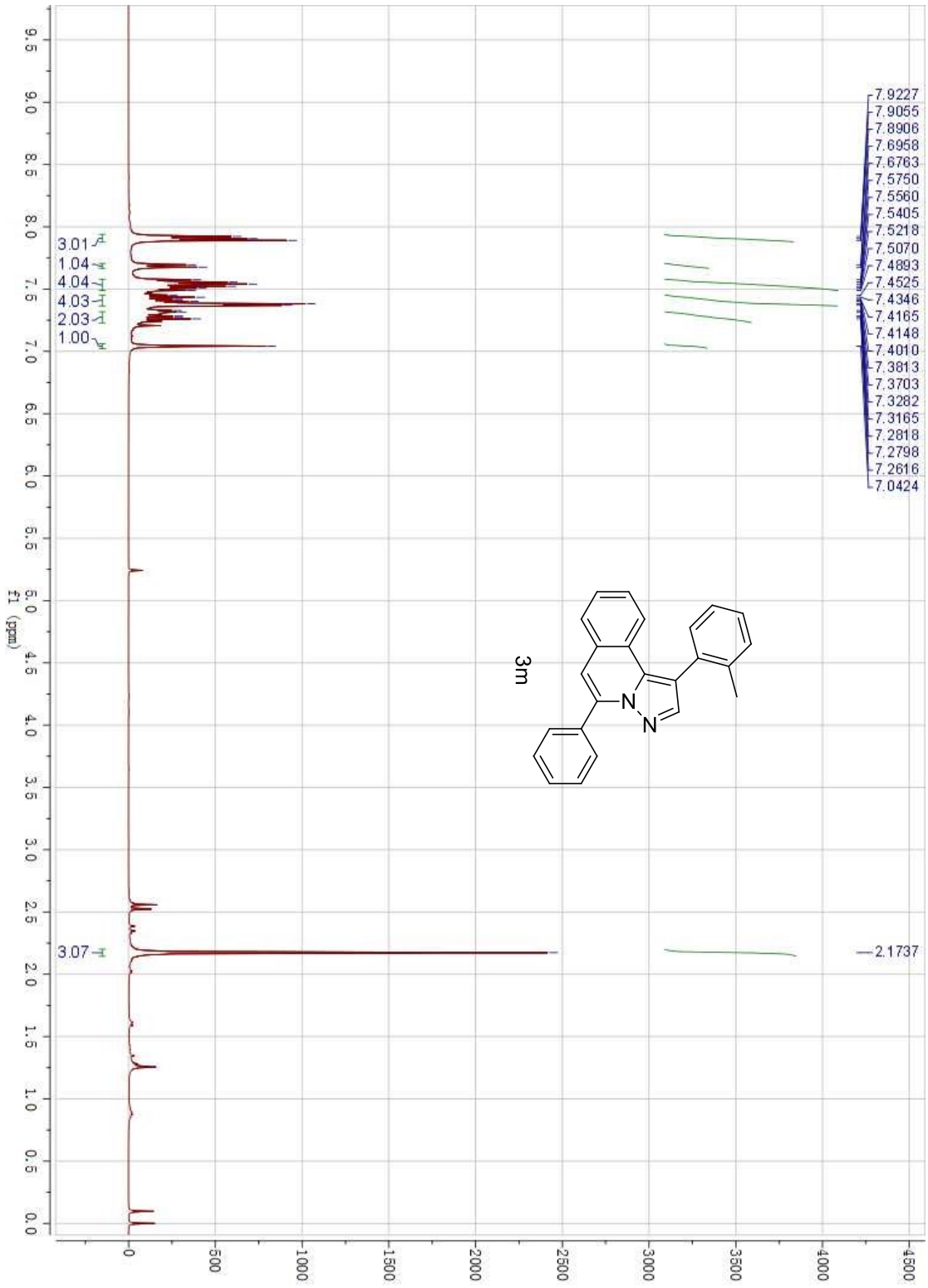
129.4796
129.2523
128.4430
128.3547
127.6032
127.1543
123.9897
122.8958
118.8981
115.3242
113.5028
110.9852
77.4299
77.1117
76.7937
f1 (ppm)
CN
N
N
3l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7.8906
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7.6763
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7.5560
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7.4893
7.4525
7.4346
7.4165
7.4148
7.4010
7.3813
7.3703
7.3282
7.3165
7.2818
7.2798
7.2616
7.0424
3.01
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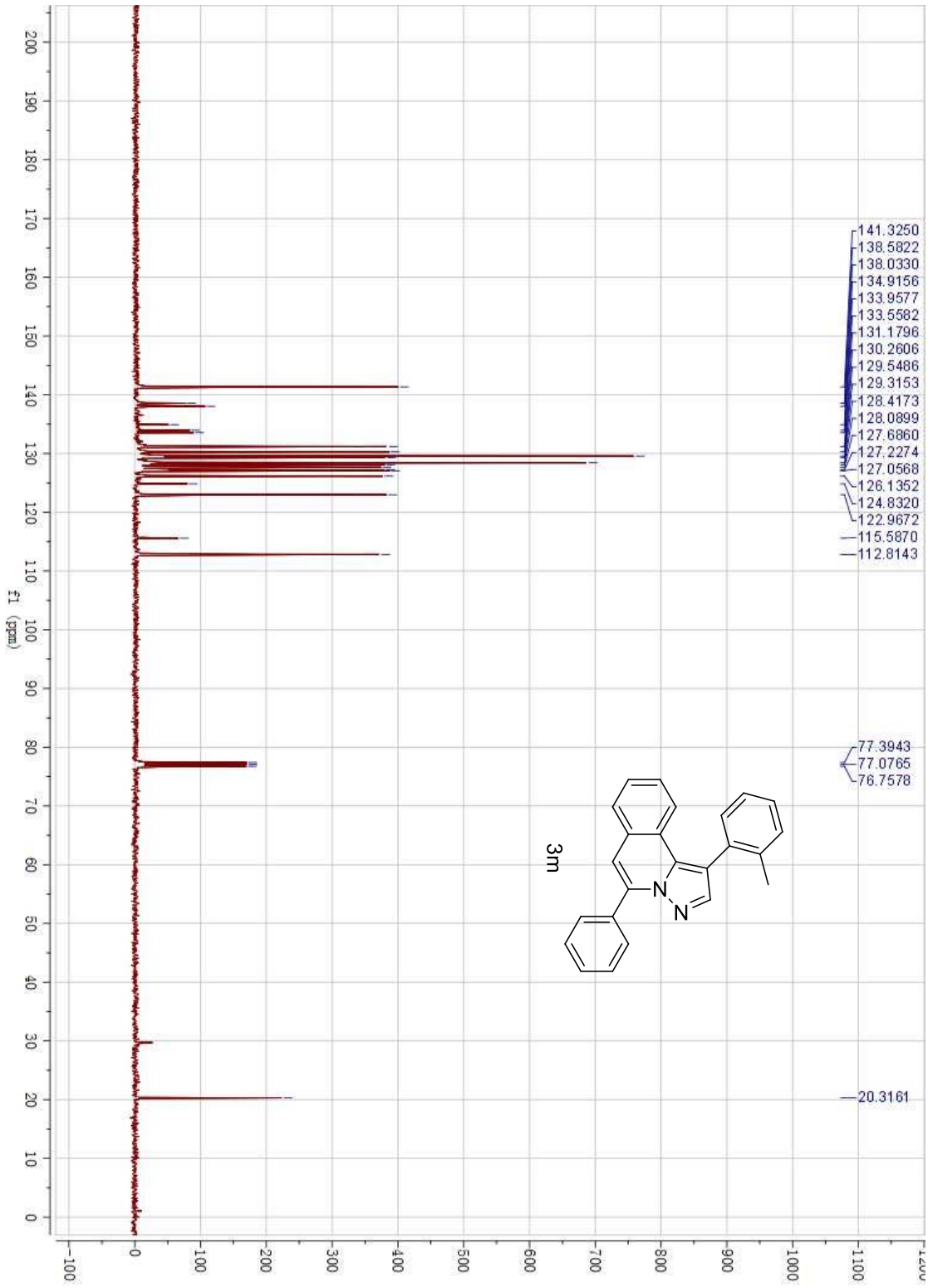
4.04
4.03
2.03
1.00
3.07
2.1737
3m
N
N
f1 (ppm)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128.0899
127.6860
127.2274
127.0568
126.1352
124.8320
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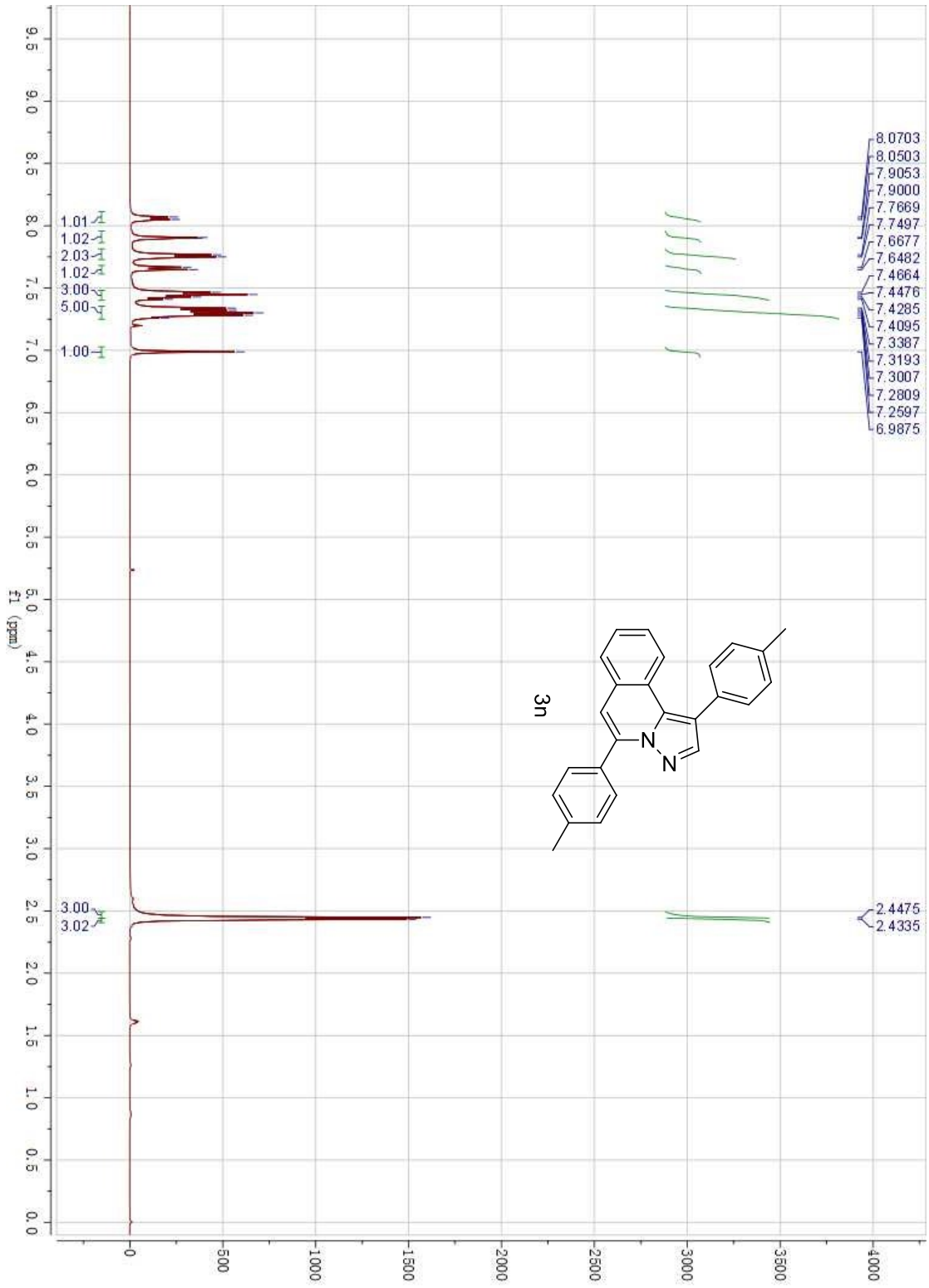
76.7578
20.3161
3m
N
N
f1 (ppm)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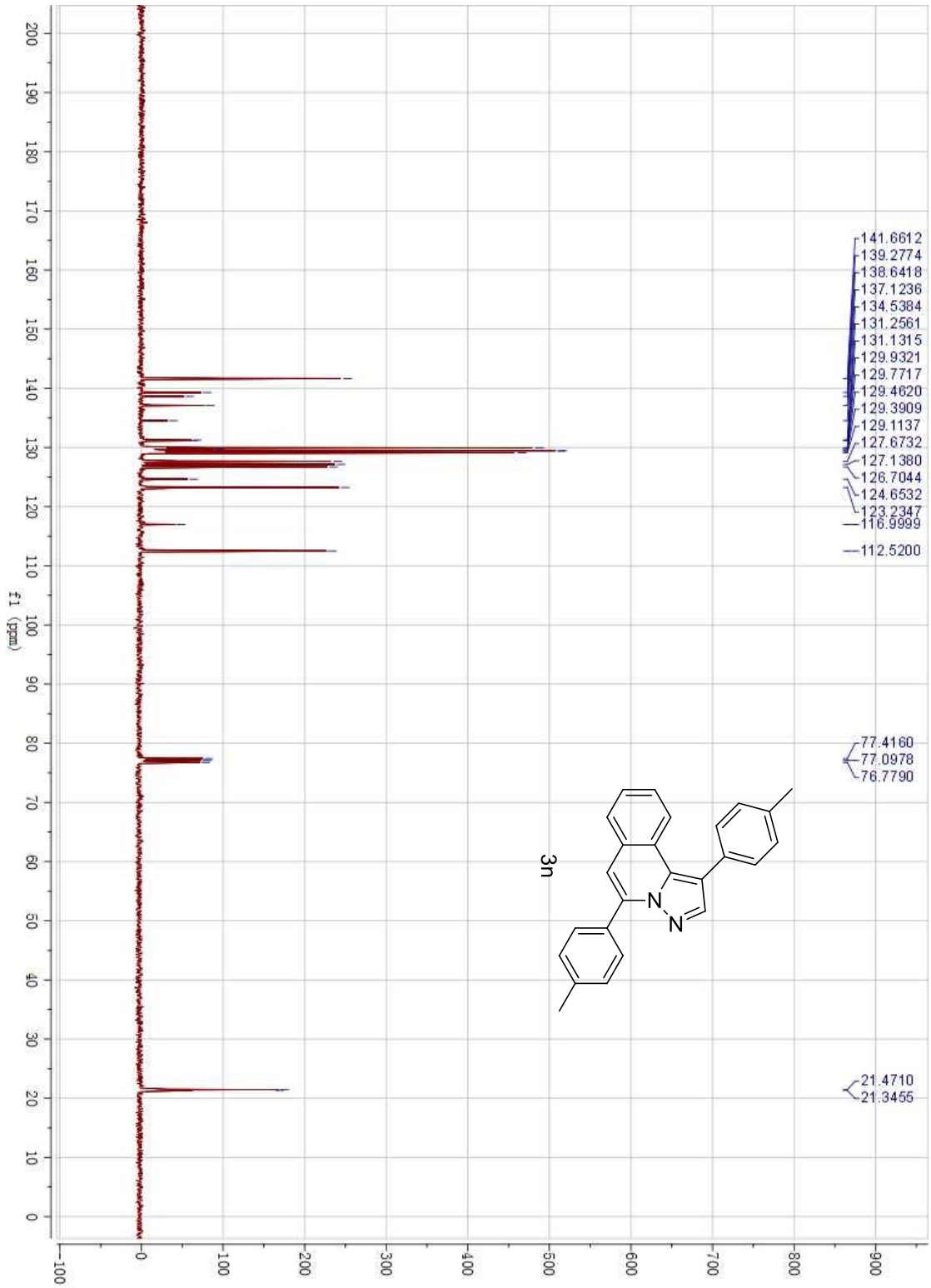
7.7669
7.7497
7.6677
7.6482
7.4664
7.4476
7.4285
7.4095
7.3387
7.3193
7.3007
7.2809
7.2597
6.9875
2.4475
2.4335
1.01
1.02
2.03
1.02
3.00
5.00
1.00
3.00
3.02
3n
N
N
f1 (ppm)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138.6418
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134.5384
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129.7717
129.4620
129.3909
129.1137
127.6732
127.1380
126.7044
124.6532
123.2347
116.9999
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77.4160
77.0978
76.7790
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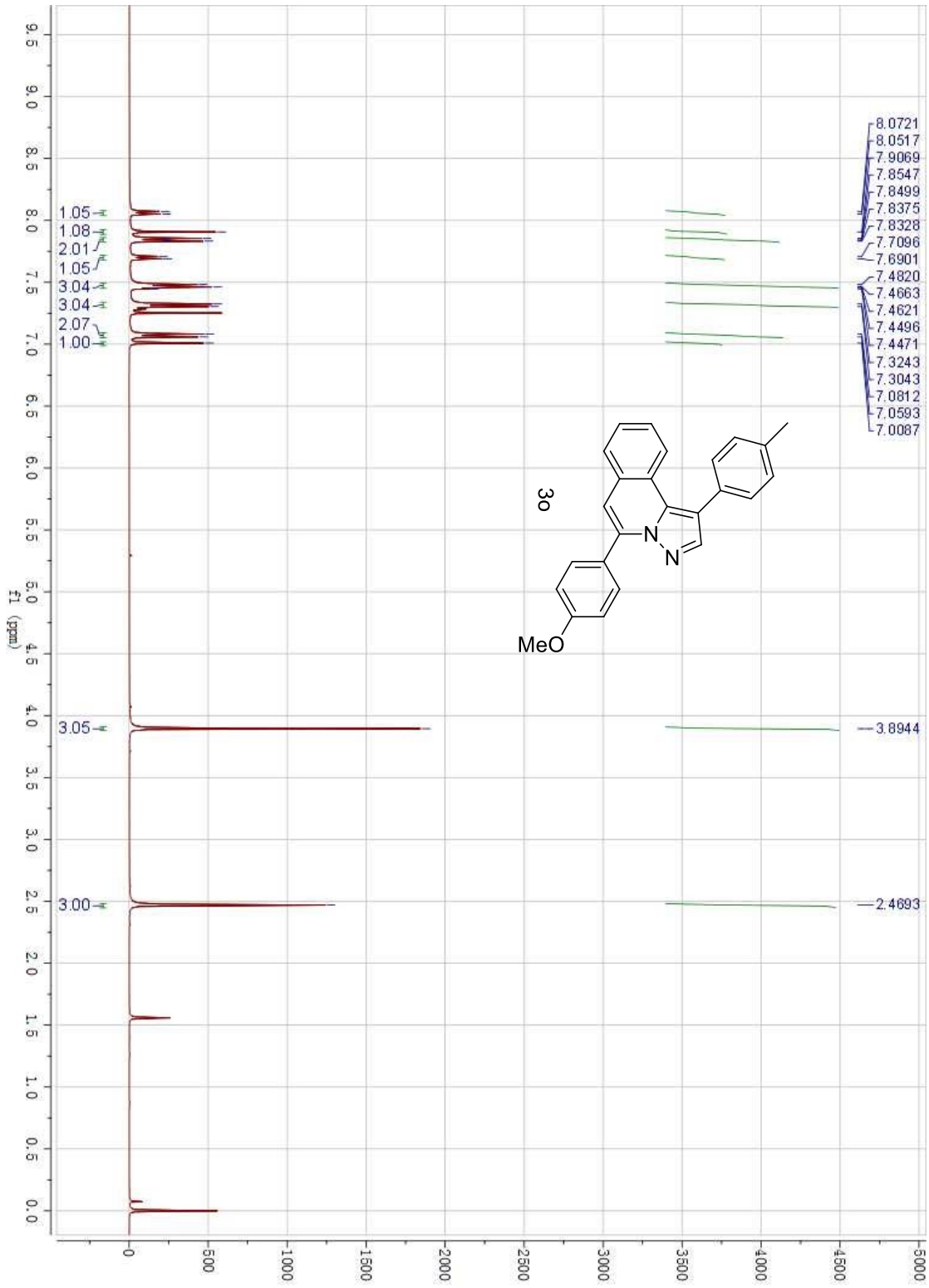
21.3455
3n
N
N
f1 (ppm)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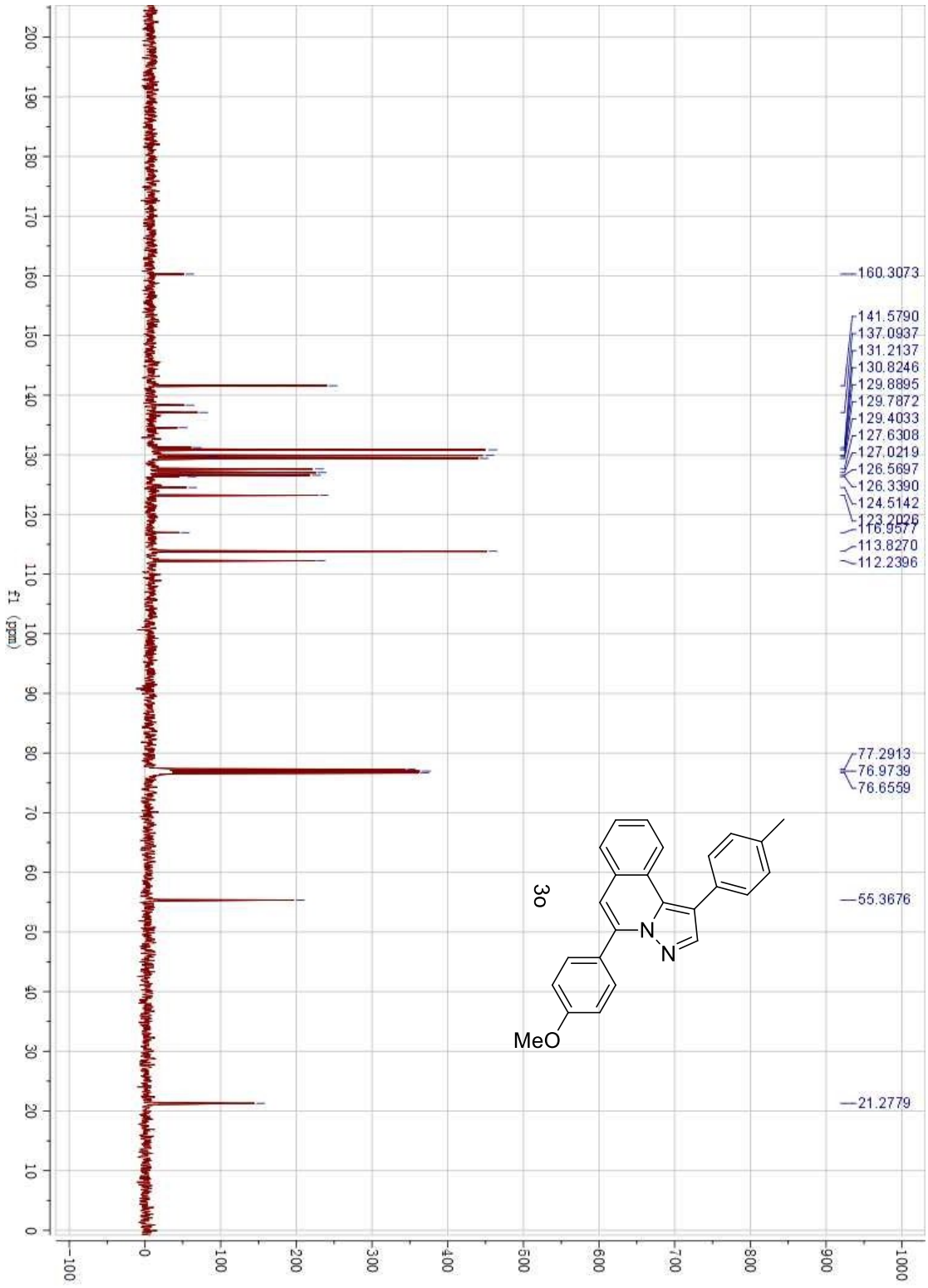
8.0517
7.9069
7.8547
7.8499
7.8375
7.8328
7.7096
7.6901
7.4820
7.4663
7.4621
7.4496
7.4471
7.3243
7.3043
7.0812
7.0593
7.0087
1.05
1.08
2.01
1.05
3.04
3.04
2.07
1.00
3.05
3.00
3.8944
2.4693
3o
MeO
N
N
f1 (ppm)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137.0937
131.2137
130.8246
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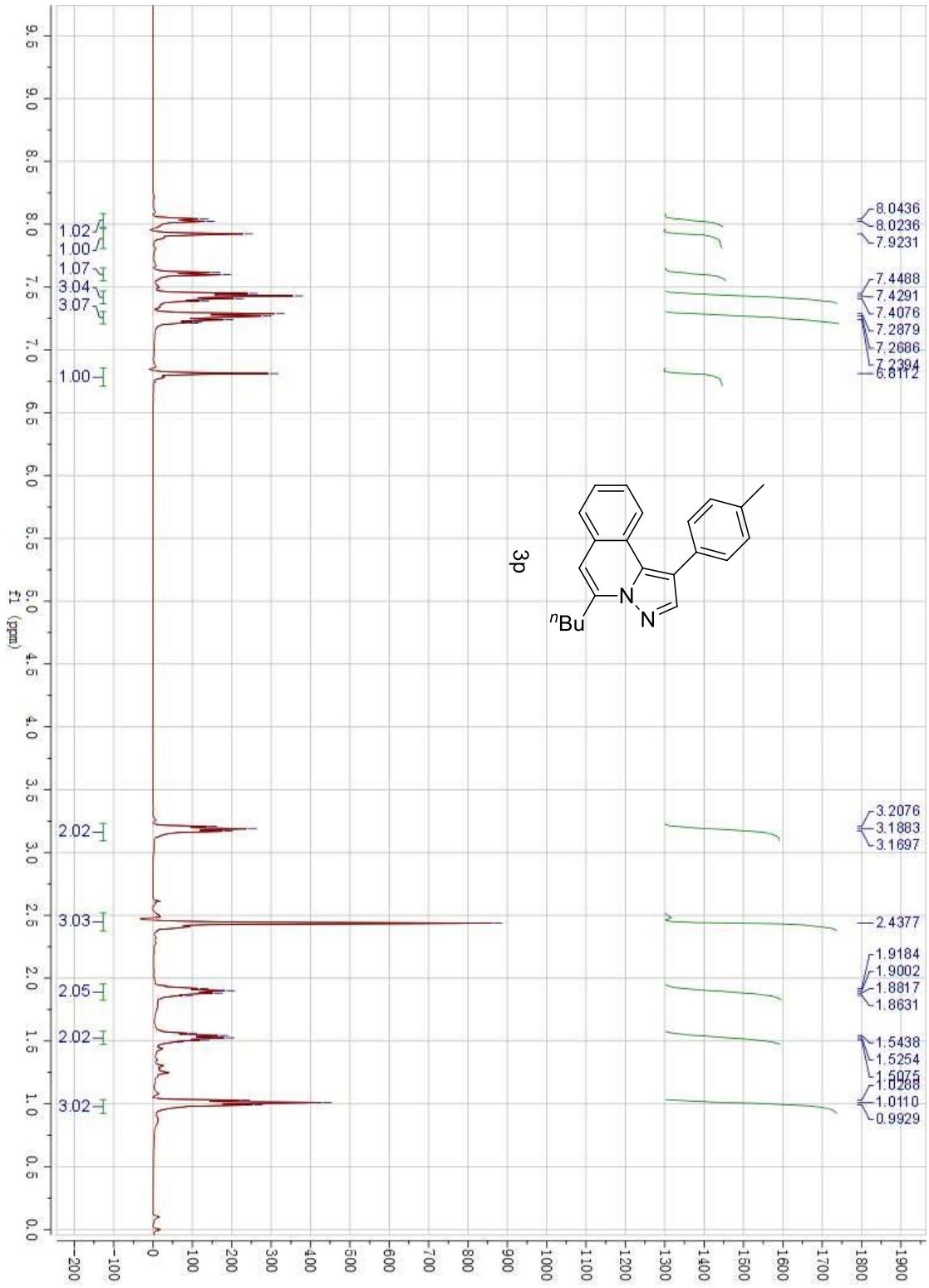
129.4033
127.6308
127.0219
126.5697
126.3390
124.5142
123.2026
116.9577
113.8270
112.2396
77.2913
76.9739
76.6559
55.3676
21.2779
f1 (ppm)
3o
MeO
N
N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7.9231
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7.4291
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7.2879
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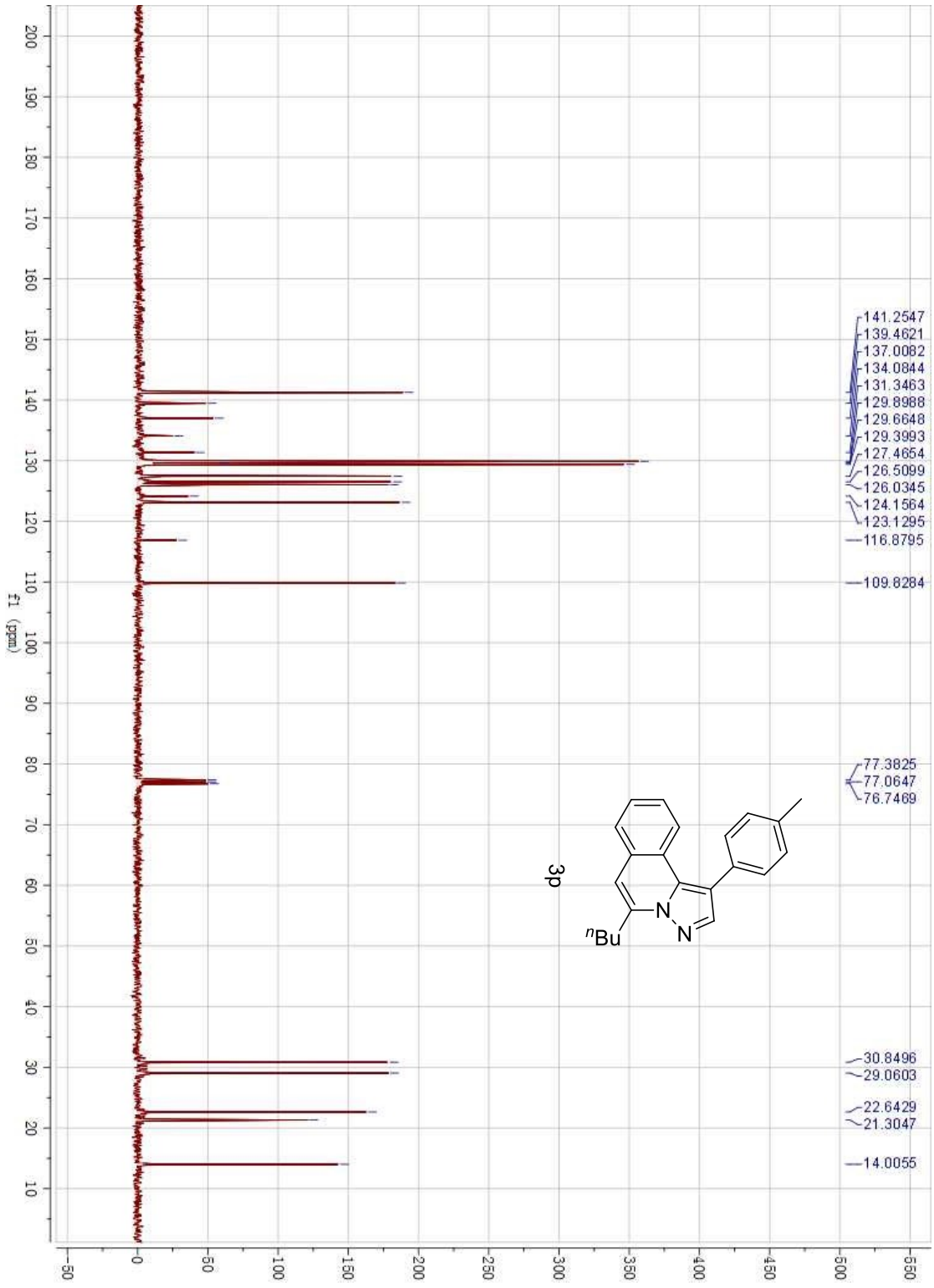
7.2394
6.8112
3.2076
3.1883
3.1697
2.4377
1.9184
1.9002
1.8817
1.8631
1.5438
1.5254
1.0288
1.0110
0.9929
1.02
1.00
1.07
3.04
3.07
1.00
2.02
3.03
2.05
2.02
3.02
3p
^{n}Bu
N
N
f1 (ppm)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126.0345
124.1564
123.1295
116.8795
109.8284
77.3825
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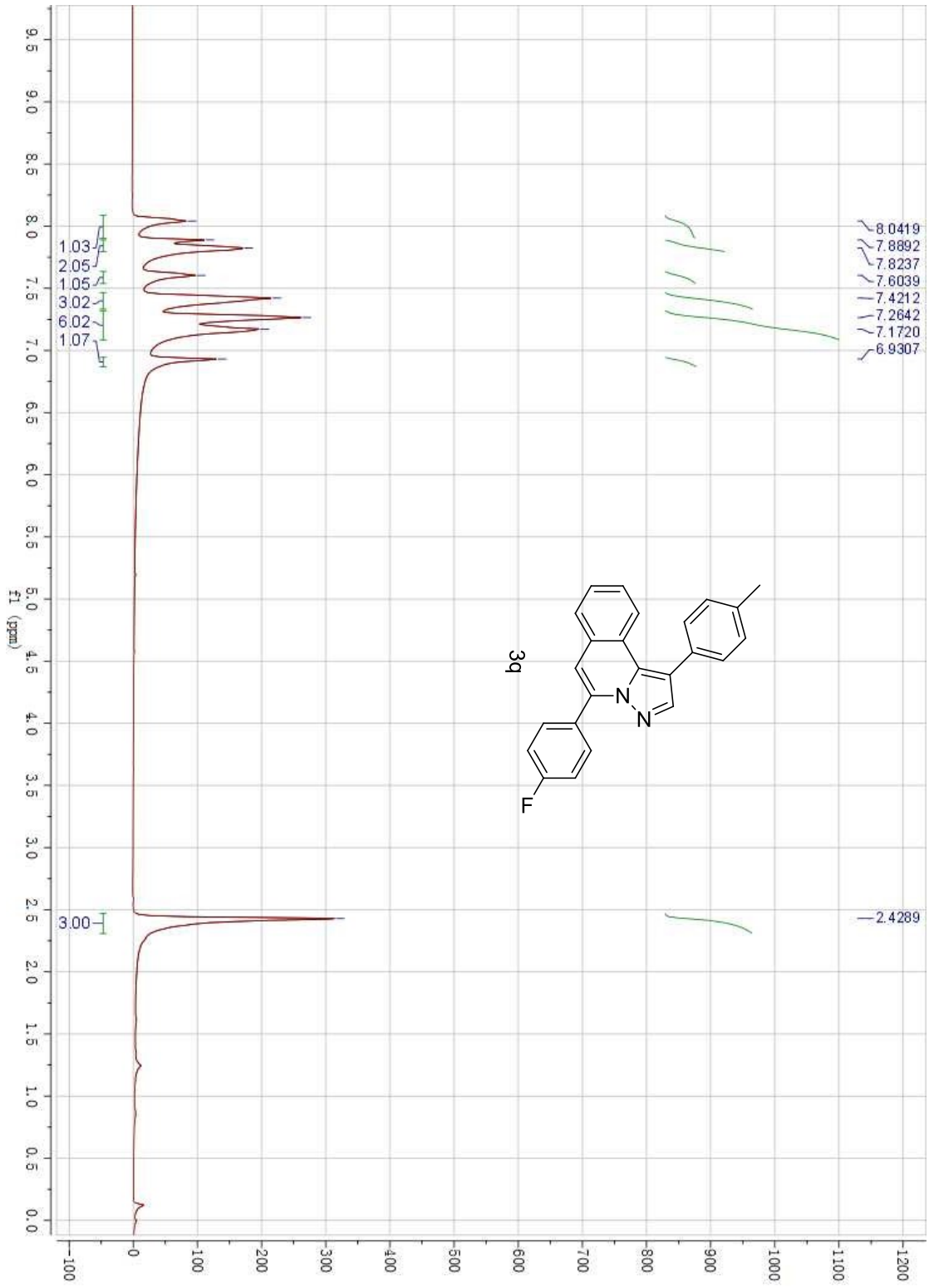
29.0603
22.6429
21.3047
14.0055
f1 (ppm)
3p
nBu
N
N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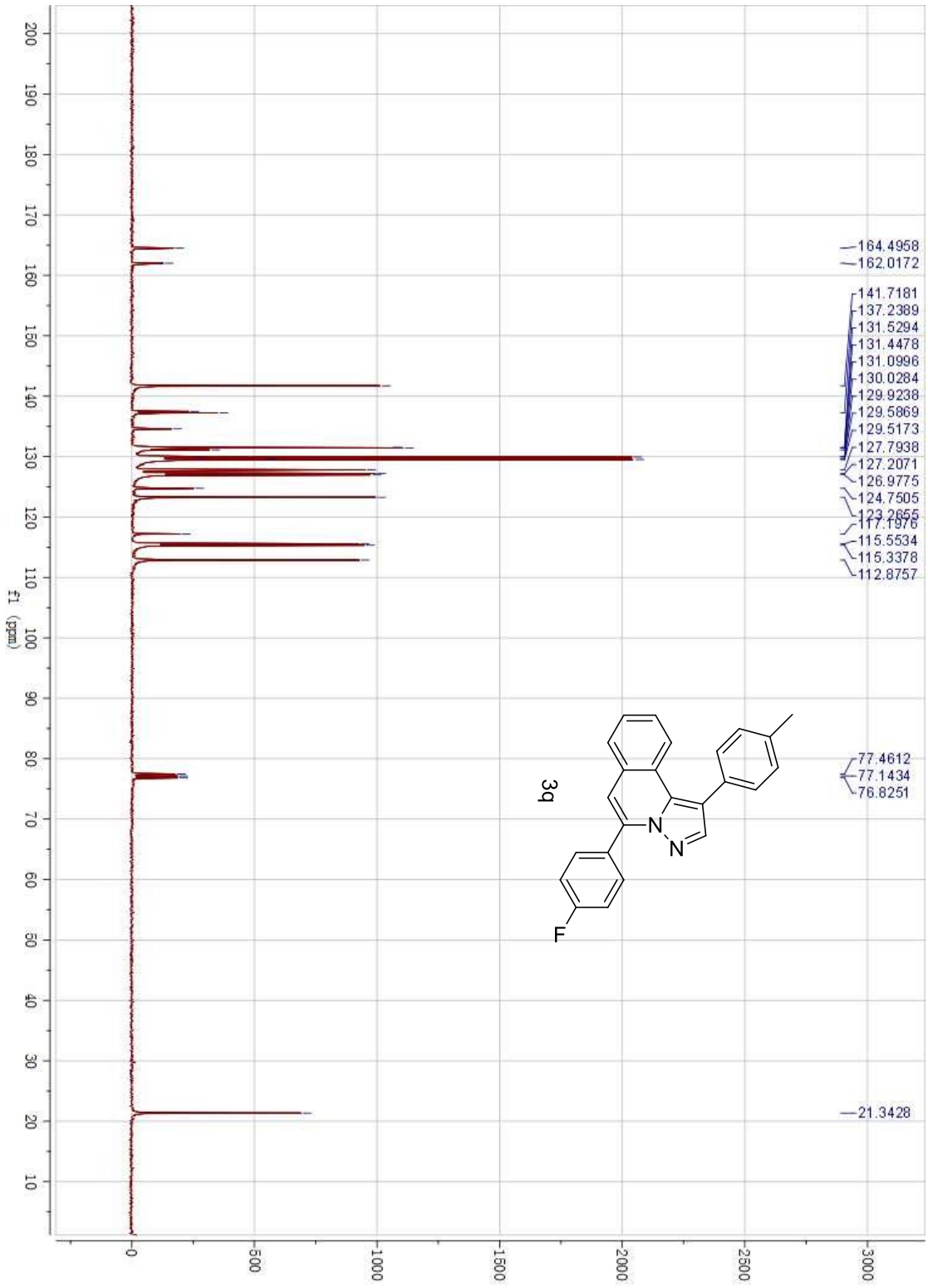
2.05
1.05
3.02
6.02
1.07
3.00
8.0419
7.8892
7.8237
7.6039
7.4212
7.2642
7.1720
6.9307
2.4289
3q
N
N
F
f1 (ppm)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129.5173
127.7938
127.2071
126.9775
124.7505
123.2655
117.1976
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112.8757
77.4612
77.1434
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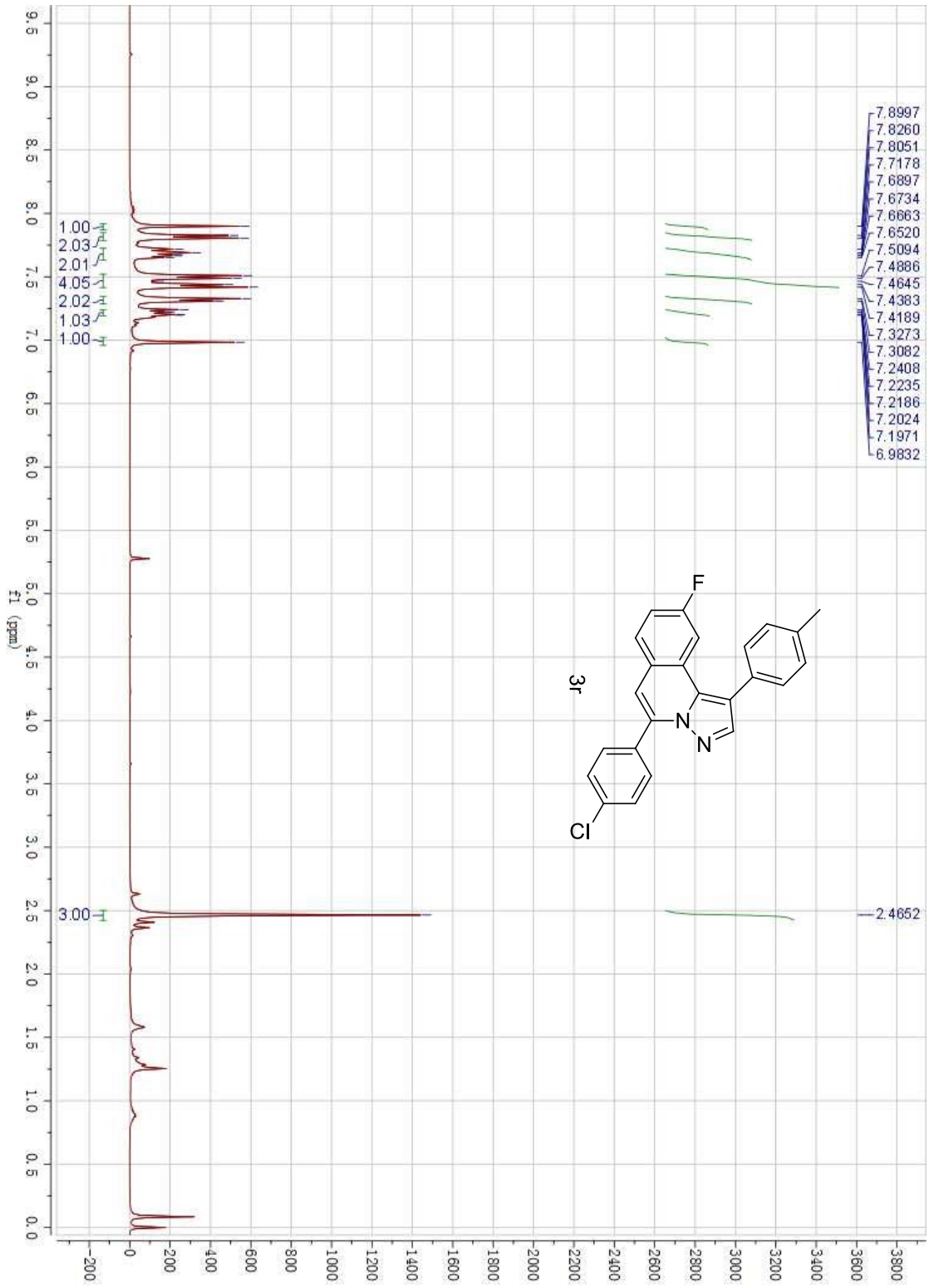
21.3428
3q
N
N
F
f1 (ppm)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7.8051
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7.6897
7.6734
7.6663
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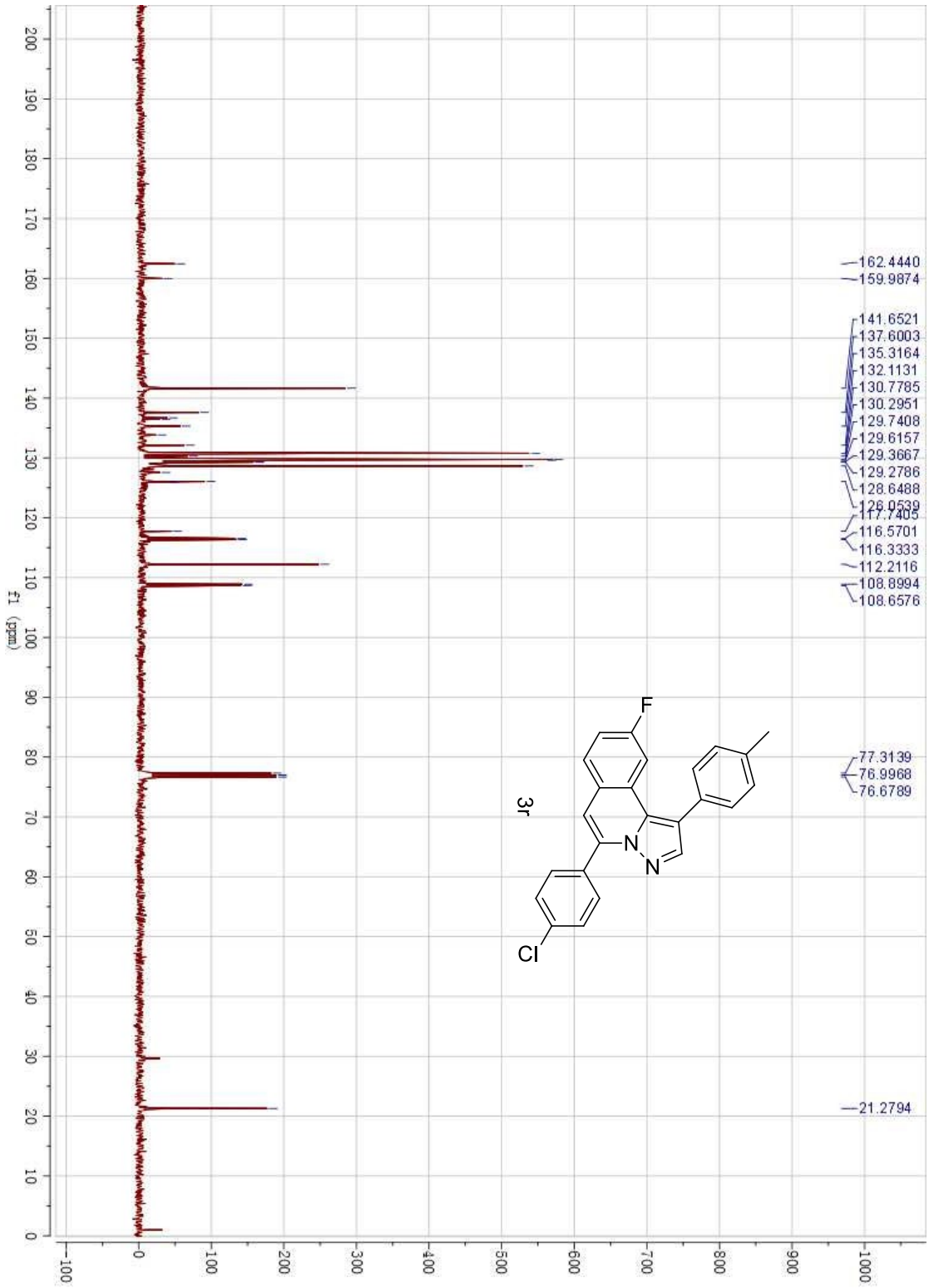
7.5094
7.4886
7.4645
7.4383
7.4189
7.3273
7.3082
7.2408
7.2235
7.2186
7.2024
7.1971
6.9832
1.00
2.03
2.01
4.05
2.02
1.03
1.00
3.00
2.4652
f1 (ppm)
F
Cl
N
N
3r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141.6521
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129.7408
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129.3667
129.2786
128.6488
126.0539
117.7405
116.5701
116.3333
112.2116
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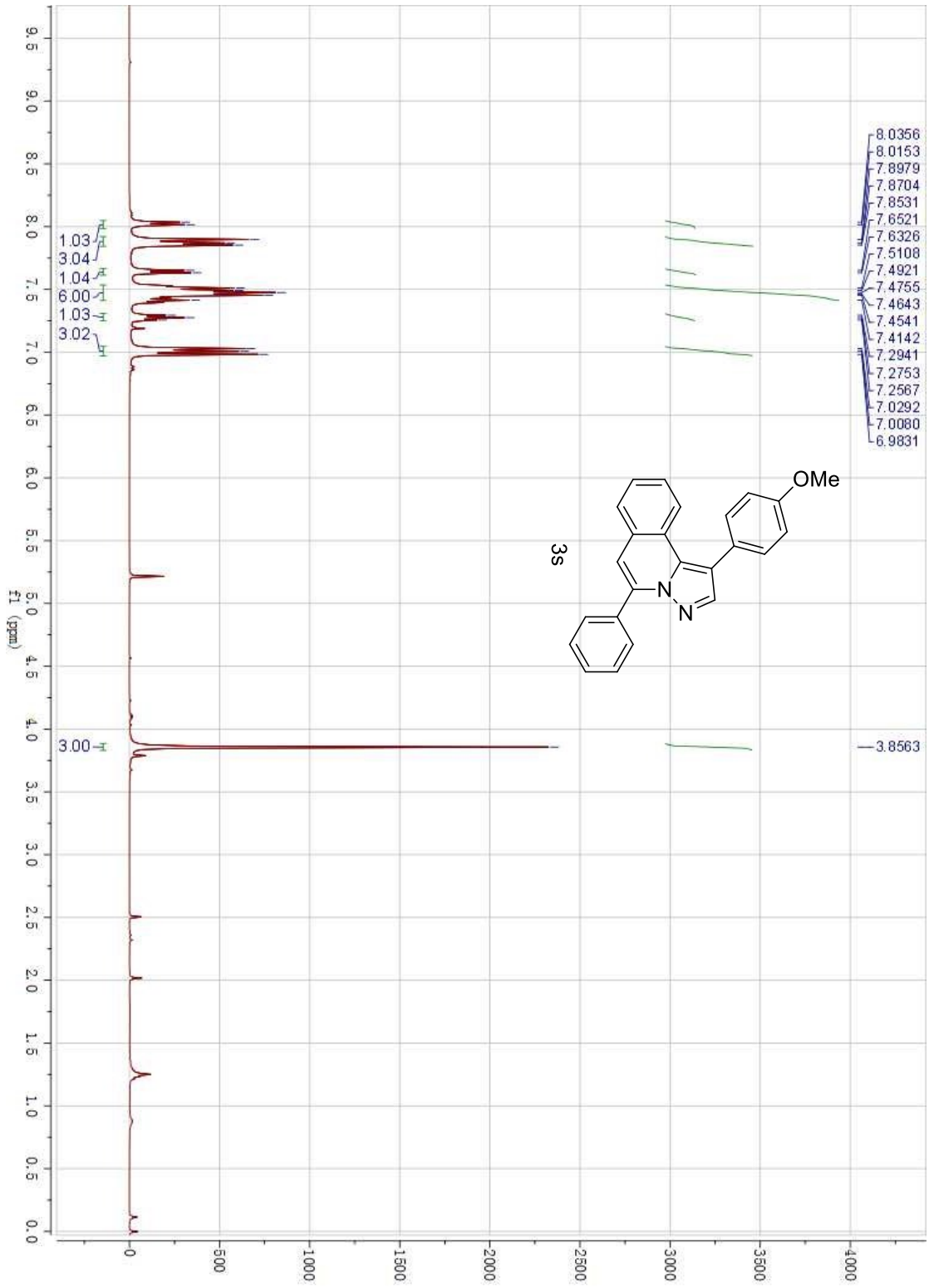
76.9968
76.6789
21.2794
f1 (ppm)
3r
F
N
N
Cl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7.4142
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7.2753
7.2567
7.0292
7.0080
6.9831
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1.04
6.00
1.03
3.02
3.00
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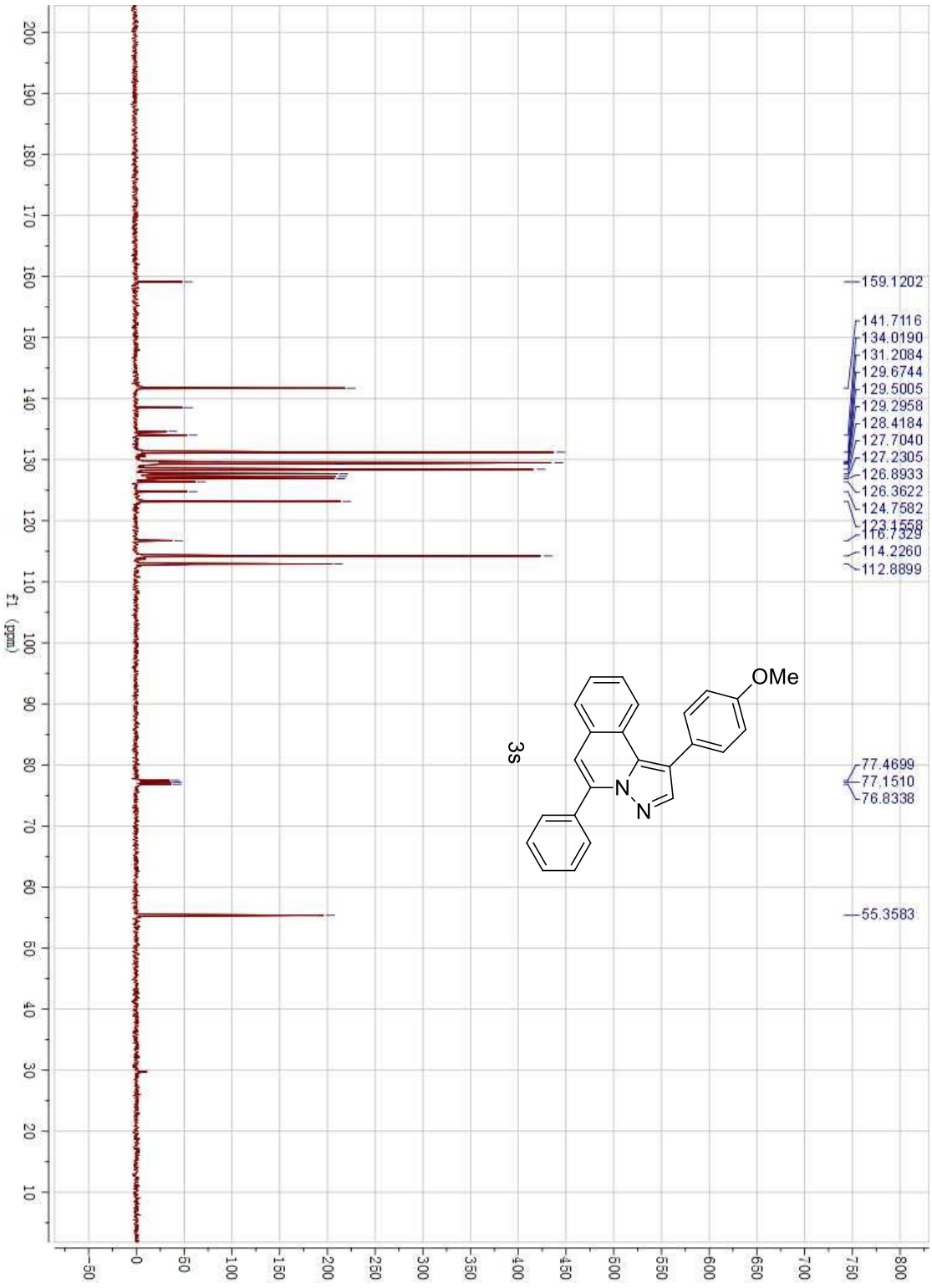
OMe
N
N
3s
f1 (ppm)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126.8933
126.3622
124.7582
123.1558
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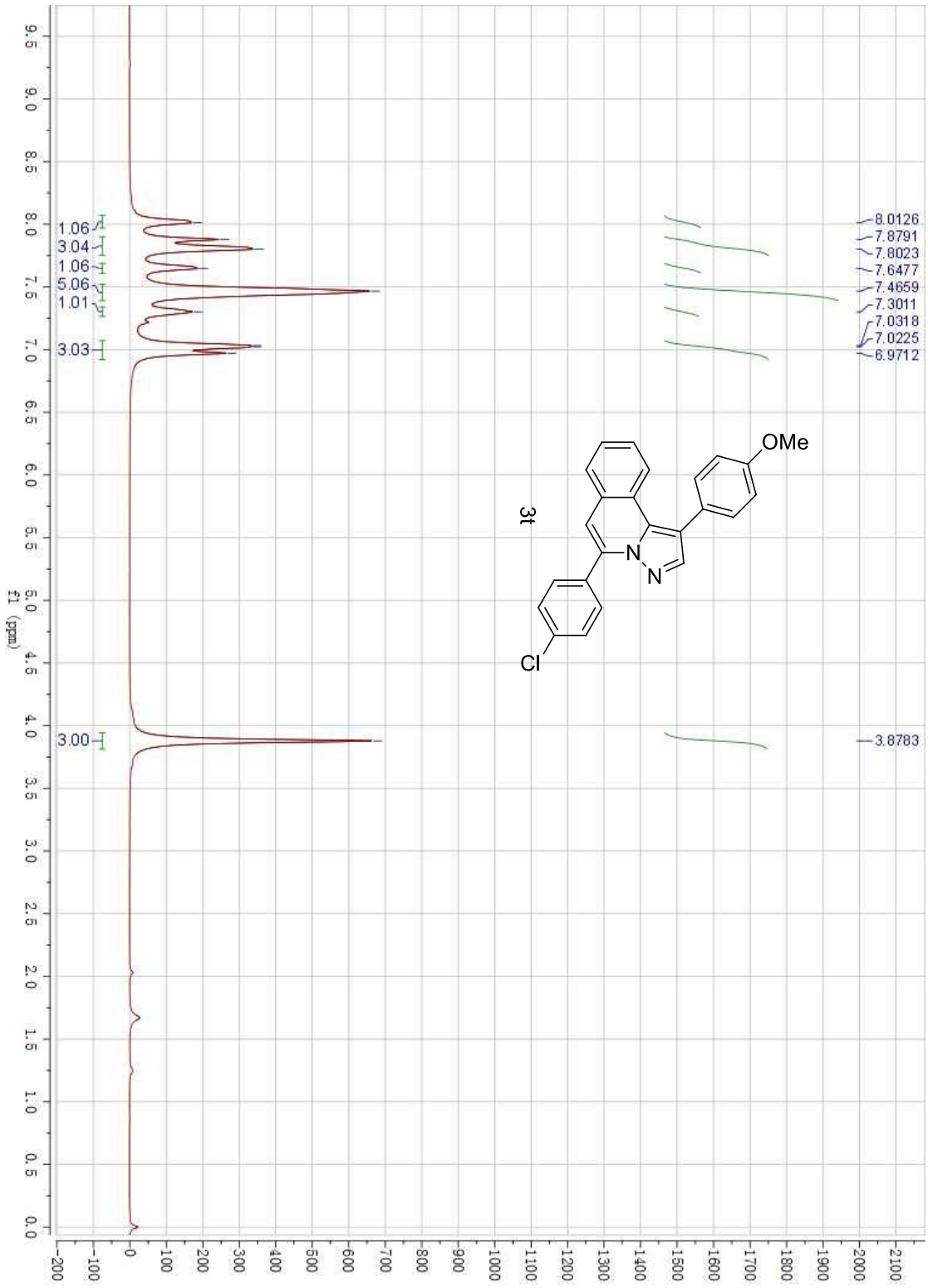
77.1510
76.8338
55.3583
OMe
N
N
3s
f1 (ppm)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3.04
1.06
5.06
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3.03
3.00
8.0126
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7.8023
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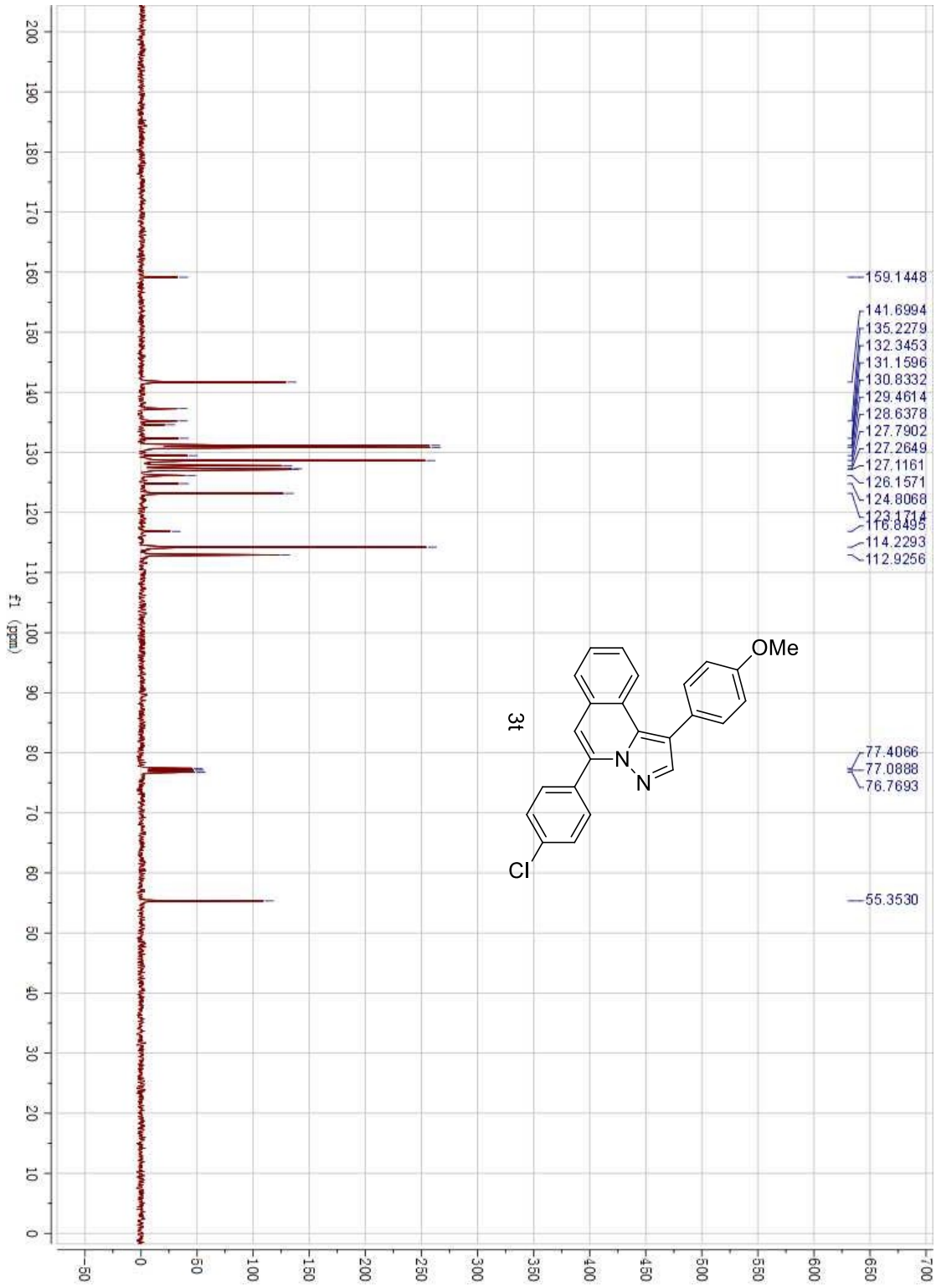
7.0318
7.0225
6.9712
3.8783
OMe
Cl
N
N
3t
f1 (ppm)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126.1571
124.8068
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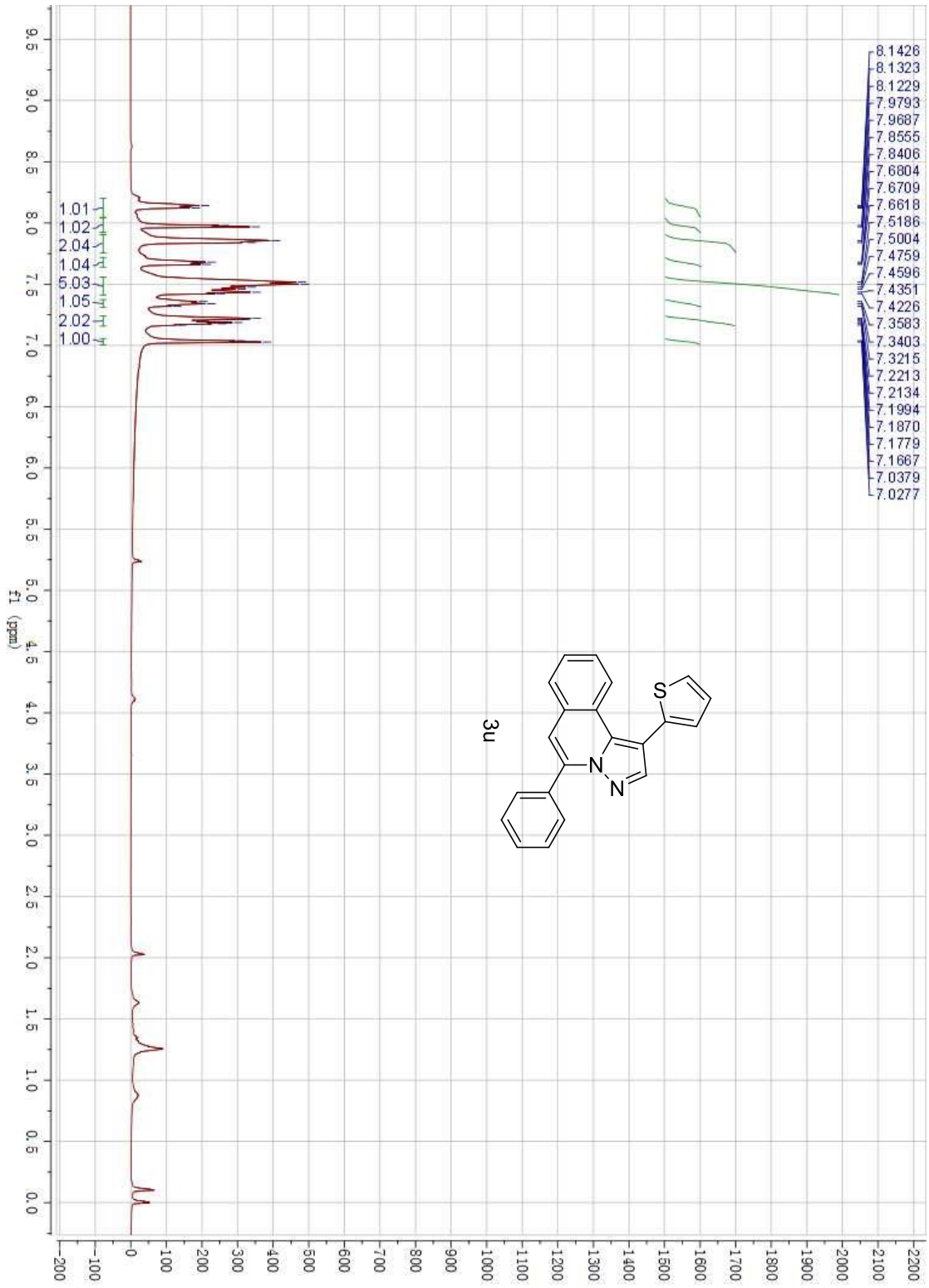
55.3530
OMe
Cl
N
N
3t
f1 (ppm)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1.02
2.04
1.04
5.03
1.05
2.02
1.00
8.1426
8.1323
8.1229
7.9793
7.9687
7.8555
7.8406
7.6804
7.6709
7.6618
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7.5004
7.4759
7.4596
7.4351
7.4226
7.3583
7.3403
7.3215
7.2213
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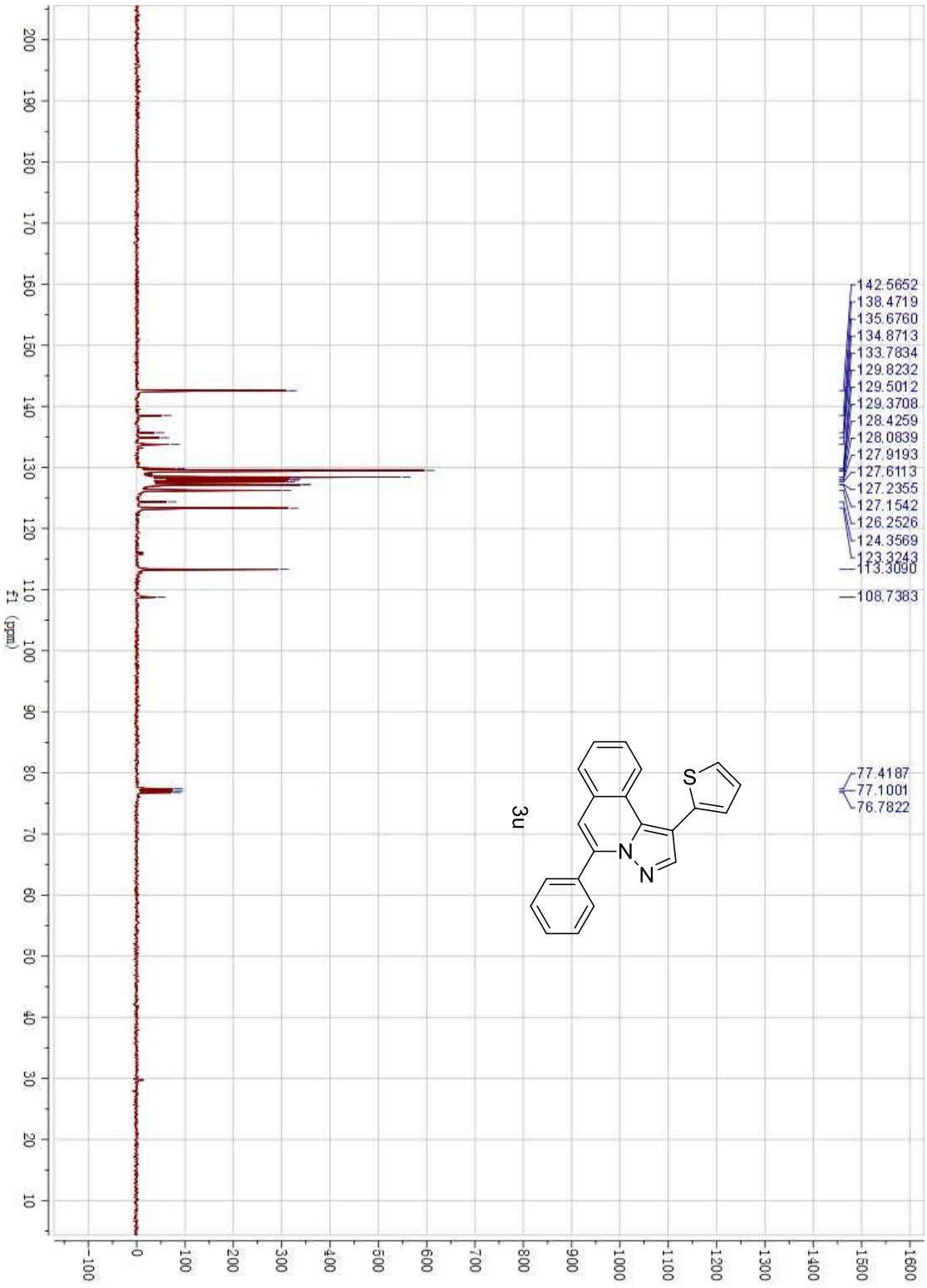
7.1870
7.1779
7.1667
7.0379
7.0277
f1 (ppm)
3u
S
N
N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127.6113
127.2355
127.1542
126.2526
124.3569
123.3243
113.3090
108.7383
77.4187
77.1001
76.7822
f1 (ppm)
3u
S
N
N