Supporting Information

Visible-light-promoted azidation/arylation of unactivated alkenes with Togni-N_3 via electrondonor–acceptor complexes

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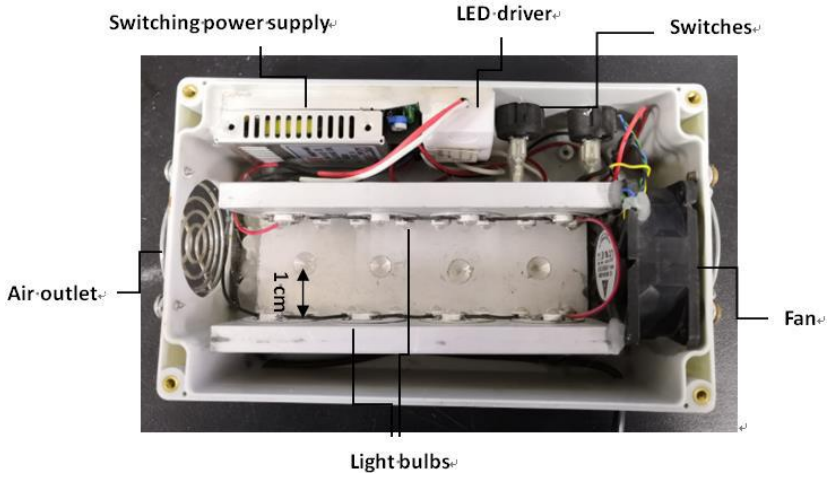
Contents

I. General Information

Chemicals were used as received without special purification unless stated otherwise. ^{1}H and ^{13}C NMR were recorded at ambient temperature on a 400 or 300 MHz NMR spectrometer (100 or 75 MHz for ^{13}C NMR). NMR experiments are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. NMR analysis was carried out at 298 K unless noted otherwise. HRMS was obtained on an ESI-LC-MS/MS spectrometer.

Figure S1 Photoreactor used in this research (6 W blue LEDs, λ_{max} = 450 nm)[1]



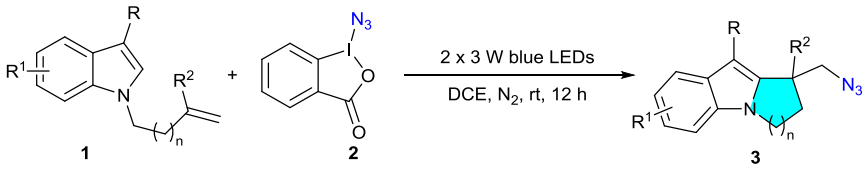
[1] Sun, S.; Zhou, C.; Yu, J.-T.; Cheng, J. Visible-Light-Driven Palladium-Catalyzed Oxy-Alkylation of 2-(1-Arylvinyl)anilines by Unactivated Alkyl Bromides and CO_2: Multicomponent Reactions toward 1,4-Dihydro-2*H*-3,1-benzoxazin-2-ones, *Org. Lett.* **2019**, *21*, 6579–6583.

Figure S2 The inside structure of photoreactor[2]

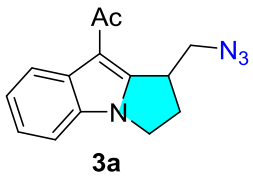
[2] Wei, Y.; Liu, S.; Li, M.-M.; Li, Y.; Lan, Y.; Lu, L.-Q.; Xiao, W.-J. Enantioselective Trapping of Pd-Containing 1,5-Dipoles by Photogenerated Ketenes: Access to 7-Membered Lactones Bearing Chiral Quaternary Stereocenters. *J. Am. Chem. Soc.* **2019**, *141*, 133-137.

II. Synthesis of azidated pyrrolo[1,2-*a*]indoles

General Procedure A



Under air, to an over-dried 20 mL Schlenk tube equipped with a Teflon cap was added *N*-alkene-linked indole **1** (0.2 mmol), Togni-N_3 **2** (0.3 mmol, 86.4 mg) and DCE (2.0 mL). The reaction vessel was evacuated and backfilled with N_2 in three times. Then, the Schlenk tube was stirred at room temperature under 2 × 3 W blue LEDs irradiation for 12 h. Then, the mixture was concentrated in vacuo. The residue was purified by silica gel flash chromatography (eluent: ethyl acetate-petroleum ether, 1:5 or 1:3) to give the pure desired product **3**.



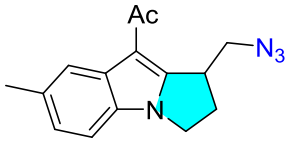
3a

1-(1-(Azidomethyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3a) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-1H-indol-3-yl)ethan-1-one **1a** (42.6 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 74% yield (37.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.92 (m, 1H), 7.33 – 7.23 (m, 3H + overlapped with $CDCl_3$), 4.23 – 4.12 (m, 2H), 3.93 – 3.82 (m, 3H), 2.89 – 2.79 (m, 1H), 2.68 (s, 3H), 2.63 –2.56 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 152.0, 132.7, 130.0, 122.2 (2C), 121.0, 110.6, 110.6, 53.1, 43.8, 39.5, 31.0, 30.5.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{14}H_{15}N_4O]^+$ 255.1240, found 255.1234.



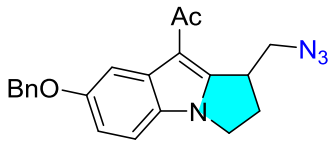
3b

1-(1-(Azidomethyl)-7-methyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3b) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-5-methyl-1H-indol-3-yl)ethan-1-one **1b** (45.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 65% yield (34.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.08 (dd, *J* = 8.2, 1.6 Hz, 1H), 4.21 – 4.10 (m, 2H), 3.92 – 3.81 (m, 3H), 2.88 – 2.79 (m, 1H), 2.67 (s, 3H), 2.62 – 2.55 (m, 1H), 2.51 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 151.9, 131.7, 131.0, 130.2, 123.6, 121.0, 110.3, 110.2, 53.1, 43.8, 39.6, 31.0, 30.5, 21.9.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O]^+$ 269.1397, found 269.1392.



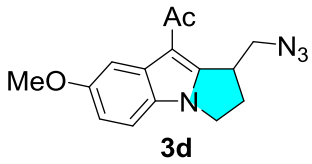
3c

1-(1-(Azidomethyl)-7-(benzyloxy)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3c) was prepared as a brown oil from 1-(5-(benzyloxy)-1-(but-3-en-1-yl)-1H-indol-3-yl)ethan-1-one **1c** (62.8 mg, 0.2 mmol) according to the General Procedure **A** (eluent: diethyl ether-petroleum ether, 1:2) in 51% yield (36.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.48 (m, 3H), 7.42 – 7.31 (m, 2H), 7.35 – 7.31 (m, 1H), 7.20 (d, *J* = 8.8 Hz, 1H), 6.97 (dd, *J* = 8.8, 2.4 Hz, 1H), 5.15 (s, 2H), 4.21 – 4.09 (m, 2H), 3.89 – 3.82 (m, 3H), 2.89 – 2.79 (m, 1H), 2.62 – 2.55 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 155.1, 152.1, 137.3, 130.8, 128.6, 128.0, 127.9, 127.6, 112.2, 111.1, 110.6, 105.8, 70.9, 53.2, 43.9, 39.7, 31.0, 30.3.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{21}H_{21}N_4O_2]^+$ 361.1659, found 361.1654.



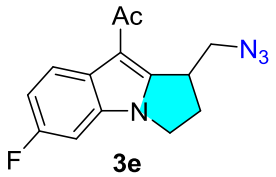
3d

1-(1-(Azidomethyl)-7-methoxy-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3d) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-5-methyl-1H-indol-3-yl)ethan-1-one **1d** (48.6 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 61% yield (34.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 2.4 Hz, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 6.90 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.21 – 4.08 (m, 2H), 3.89 – 3.81 (m, 6H), 2.89 – 2.79 (m, 1H), 2.65 – 2.55 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 193.0, 156.0, 152.0, 130.9, 127.8, 111.4, 111.1, 110.5, 104.2, 55.9, 53.2, 43.9, 39.8, 31.0, 30.2.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O_2]^+$ 285.1346, found 285.1337.



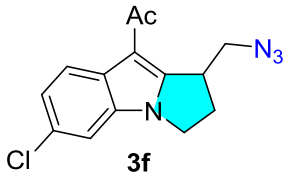
3e

1-(1-(Azidomethyl)-6-fluoro-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3e) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-6-fluoro-1H-indol-3-yl)ethan-1-one **1f** (46.2 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 60% yield (32.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.9, 5.0 Hz, 1H), 7.06 – 6.98 (m, 2H), 4.18 – 4.08 (m, 2H), 3.90 – 3.78 (m, 3H), 2.90 – 2.80 (m, 1H), 2.67 – 2.57 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.2, 159.5 (*J* = 241.2 Hz), 152.3, 132.7, 126.4, 121.9 (*J* = 9.7 Hz), 110.7, 110.5, 97.2 (*J* = 26.2 Hz), 53.2, 43.8, 39.5, 31.1, 30.4.

HRMS (ESI-TOF) *m/z* [M + H]$^+$: calcd. for $[C_{14}H_{14}FN_4O]^+$ 273.1146, found 273.1140.



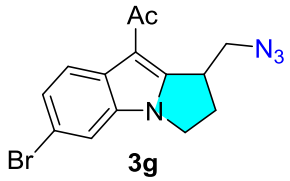
3f

1-(1-(Azidomethyl)-6-chloro-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)etha n-1-one (3f) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-6-chloro-1H-indol-3-yl)ethan-1-one **1g** (49.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 57% yield (32.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.7 Hz, 1H), 7.31 (d, *J* = 1.9 Hz, 1H), 7.24 (dd, *J* = 8.6, 1.9 Hz, 1H), 4.21 – 4.08 (m, 2H), 3.92 – 3.86 (m, 2H), 3.84 – 3.78 (m, 1H), 2.91 – 2.81 (m, 1H), 2.66 – 2.57 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 152.5, 133.0, 128.4, 128.2, 122.7, 121.9, 110.7, 110.6, 53.1, 43.9, 39.4, 31.1, 30.4.

HRMS (ESI-TOF) *m/z* [M + H]$^+$: calcd. for $[C_{14}H_{14}ClN_4O]^+$ 289.0851, found 289.0847.



3g

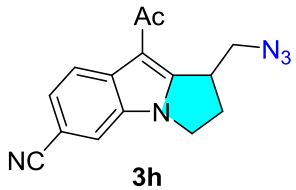
1-(1-(Azidomethyl)-6-bromo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3g) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-6-chloro-1H-indol-3-yl)ethan-1-one **1g** (49.4 mg, 0.2 mmol)

according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 70% yield (46.5 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.7 Hz, 1H), 7.47 (d, *J* = 1.8 Hz, 1H), 7.37 (dd, *J* = 8.7, 1.8 Hz, 1H), 4.21 – 4.09 (m, 2H), 3.92 – 3.78 (m, 2H), 3.84 – 3.77 (m, 1H), 2.90 – 2.80 (m, 1H), 2.68 – 2.57 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 152.4, 133.4, 128.8, 125.3, 122.3, 115.6, 113.6, 110.7, 53.1, 43.9, 39.4, 31.1, 30.4.

HRMS (ESI-TOF) *m*/*z* [M + Na]$^+$: calcd. for $[C_{14}H_{14}BrN_4O]^+$ 333.0346, found 333.0346.



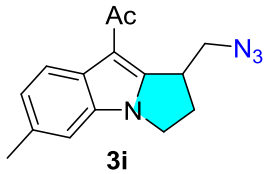
3h

9-Acetyl-1-(azidomethyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indole-6-carbonitrile (3h) was prepared as a brown oil from 3-acetyl-1-(but-3-en-1-yl)-1*H*-indole-6-carbonitrile **1h** (47.6 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:3) in 68% yield (38.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 1.7 Hz, 1H), 7.51 (dd, *J* = 8.4, 1.5 Hz, 1H), 4.30 – 4.17 (m, 2H), 4.00 – 3.91 (m, 2H), 3.82 (dd, *J* = 11.3, 2.9 Hz, 1H), 2.96 – 2.86 (m, 1H), 2.67 – 2.61 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 192.9, 155.2, 133.0, 131.6, 125.1, 121.7, 119.8, 115.1, 111.2, 104.9, 53.1, 44.3, 39.6, 31.1, 30.5.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{14}N_5O]^+$ 280.1193, found 280.1195.



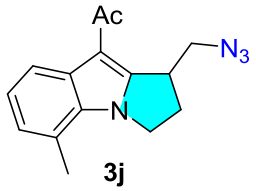
3i

1-(1-(azidomethyl)-6-methyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3i) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-6-methyl-1*H*-indol-3-yl)ethan-1-one **1i** (45.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 66% yield (35.3 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.6 Hz, 1H), 7.12 – 7.10 (m, 2H), 4.20 – 4.08 (m, 2H), 3.91 – 3.81 (m, 3H), 2.90 – 2.77 (m, 1H), 2.66 (s, 3H), 2.63 – 2.56 (m, 1H), 2.49 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 151.4, 133.0, 132.2, 127.8, 123.8, 120.7, 110.6, 110.5, 53.1, 43.6, 39.4, 31.0, 30.4, 21.5.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O]^+$ 269.1397, found 269.1394.



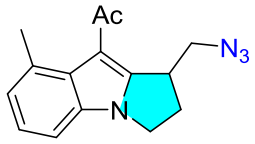
3j

1-(1-(azidomethyl)-5-methyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3j) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-7-methyl-1*H*-indol-3-yl)ethan-1-one **1j** (45.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 70% yield (37.5 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.2 Hz, 1H), 7.15 (t, *J* = 7.7 Hz, 1H), 6.98 (d, *J* = 7.2 Hz, 1H), 4.50 – 4.46 (m, 2H), 3.88 – 3.80 (m, 3H), 2.83 – 2.78 (m, 2H), 2.68 – 2.66 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 152.2, 132.2, 130.2, 124.0, 122.3, 121.6, 118.8, 110.5, 53.1, 47.0, 38.7, 31.1, 30.6, 18.1.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O]^+$ 269.1397, found 269.1393.



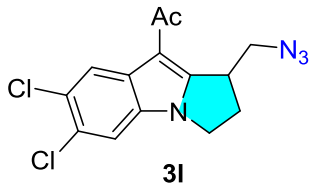
3k

1-(1-(Azidomethyl)-8-methyl-2,3-dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3k) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-4-methyl-1H-indol-3-yl)ethan-1-one **1k** (45.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 45% yield (24.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.14 (m, 1H), 7.10 (d, *J* = 7.9 Hz, 1H), 7.03 (d, *J* = 7.1 Hz, 1H), 4.17 – 4.13 (m, 2H), 3.83 – 3.74 (m, 2H), 3.63 – 3.58 (m, 1H), 2.89 – 2.79 (m, 1H), 2.70 (s, 3H), 2.62 – 2.56 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 194.2, 149.2, 133.2, 132.3, 128.9, 124.5, 122.9, 113.4, 107.6, 54.0, 43.4, 39.7, 31.2, 31.0, 22.9.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O]^+$ 269.1397, found 269.1392.



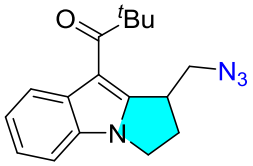
3l

1-(1-(Azidomethyl)-6,7-dichloro-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3l) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-5,6-dichloro-1*H*-indol-3-yl)ethan-1-one **1l** (56.2 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 73% yield (47.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.39 (s, 1H), 4.21 – 4.08 (m, 2H), 3.94 – 3.77 (m, 3H), 2.92 – 2.82 (m, 1H), 2.62 – 2.58 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 153.6, 131.4, 129.4, 126.5, 126.2, 122.2, 111.9, 110.2, 53.2, 44.1, 39.5, 31.2, 30.3.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{14}H_{13}Cl_2N_4O]^+$ 323.0461, found 323.0458.



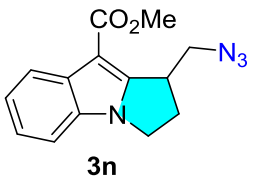
3m

1-(1-(Azidomethyl)-2,3-dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)-2,2-dimethylpropan-1-one (3m) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-1H-indol-3-yl)-2,2-dimethylpropan-1-one **1m** (51.0 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 83% yield (49.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.97 (m, 1H), 7.31 – 7.23 (m, 3H), 4.22 – 4.11 (m, 2H), 3.97 – 3.92 (m, 1H), 3.81 – 3.80 (m, 2H), 2.86 – 2.76 (m, 1H), 2.61 – 2.54 (m, 1H), 1.48 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 202.7, 154.4, 132.7, 128.0, 123.3, 121.7, 121.4, 110.5, 109.6, 53.2, 43.6, 43.0, 40.3, 30.9, 26.8.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{17}H_{21}N_4O]^+$ 297.1710, found 297.1707.



3n

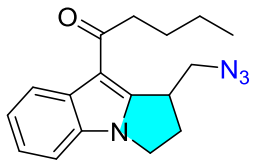
Methyl 1-(azidomethyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indole-9-carboxylate (3n) was prepared as a brown oil from methyl 1-(but-3-en-1-yl)-1H-indole-3-carboxylate **1n** (45.8 mg, 0.2 mmol) according to

the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 84% yield (45.4 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 8.09 (m, 1H), 7.28 – 7.22 (m, 3H + overlapped with $CDCl_3$), 4.23 – 4.10 (m, 2H), 3.93 (s, 3H), 3.89 – 3.77 (m, 2H), 2.89 – 2.80 (m, 1H), 2.63 – 2.56 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 151.4, 132.5, 130.6, 122.3, 121.9, 121.8, 110.0, 99.9, 53.4, 50.9, 43.8, 39.0, 31.1.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{14}H_{15}N_4O_2]^+$ 271.1190, found 271.1199.



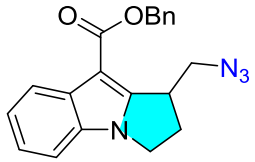
3o

1-(1-(Azidomethyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)pentan-1-one (3o) was prepared as a brown oil from methyl 1-(1-(but-3-en-1-yl)-1*H*-indol-3-yl)pentan-1-one **1o** (51.0 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 65% yield (38.5 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.90 (m, 1H), 7.36 – 7.23 (m, 3H + overlapped with $CDCl_3$), 4.22 – 4.11 (m, 2H), 3.93 – 3.85 (m, 3H), 3.01 (td, *J* = 7.2, 1.4 Hz, 2H), 2.89 – 2.79 (m, 1H), 2.63 – 2.56 (m, 1H), 1.82 – 1.75 (m, 2H), 1.53 – 1.43 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 152.0, 132.6, 129.6, 122.1, 122.1, 121.2, 110.5, 110.4, 53.0, 43.7, 42.0, 39.6, 31.0, 26.2, 22.6, 14.0.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{17}H_{21}N_4O]^+$ 297.1710, found 297.1705.



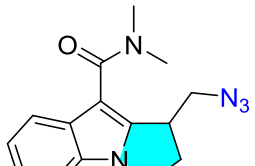
3p

Benzyl 1-(azidomethyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indole-9-carboxylate (3p) was prepared as a brown oil from methyl benzyl 1-(but-3-en-1-yl)-1H-indole-3-carboxylate **1p** (61.0 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 72% yield (49.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 6.4, 2.8 Hz, 1H), 7.49 – 7.47 (m, 2H), 7.42 – 7.32 (m, 3H), 7.27 – 7.21 (m, 3H + overlapped with $CDCl_3$), 5.45 – 5.33 (m, 2H), 4.20 – 4.08 (m, 2H), 3.85 – 3.79 (m, 2H), 3.72 – 3.67 (m, 1H), 2.87 – 2.77 (m, 1H), 2.60 – 2.53 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 151.5, 136.6, 132.5, 130.7, 128.6, 128.1 (2C), 122.3, 122.0, 121.8, 110.0, 99.8, 65.5, 53.2, 43.8, 39.0, 31.1.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{20}H_{19}N_4O_2]^+$ 347.1503, found 347.1502.



3q

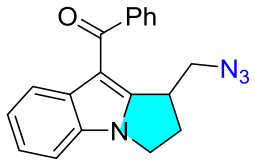
1-(Azidomethyl)-N,N-dimethyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole-9-carboxamide (3q) was prepared as a brown oil from 1-(but-3-en-1-yl)-N,N-dimethyl-1H-indole-3-carboxamide **1q** (48.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 42% yield (23.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.48 (m, 1H), 7.28 – 7.15 (m, 3H + overlapped with $CDCl_3$), 4.23 – 4.16 (m, 1H), 4.12 – 4.05 (m, 1H), 3.95 – 3.77 (m,

3H), 3.13 (s, 6H), 2.86 – 2.78 (m, 1H), 2.58 – 2.50 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 147.1, 131.9, 129.7, 121.4, 120.7, 120.6, 110.1, 103.8, 53.6 (2C), 43.4, 38.2, 31.6.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{18}N_5O]^+$ 284.1506, found 284.1503.



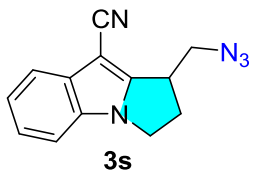
3r

(1-(Azidomethyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (3r) was prepared as a brown oil from (1-(but-3-en-1-yl)-1H-indol-3-yl)(phenyl)methanone **1r** (55.1 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 55% yield (34.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.76 (m, 2H), 7.60 – 7.55 (m, 1H), 7.52 – 7.47 (m, 3H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.13 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 4.27 – 4.16 (m, 2H), 3.85 – 3.79 (m, 1H), 3.58 – 3.56 (m, 2H), 2.93 – 2.83 (m, 1H), 2.62 – 2.54 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.6, 152.0, 141.2, 132.7, 131.4, 130.9, 128.4, 128.3, 122.5, 122.0, 121.9, 110.2, 109.6, 53.3, 43.8, 39.5, 31.1.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{19}H_{17}N_4O]^+$ 317.1397, found 317.1390.



3s

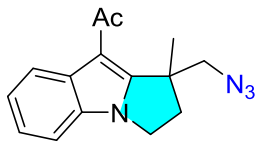
1-(Azidomethyl)-2,3-dihydro-1*H*-pyrrolo[1,2-a]indole-9-carbonitrile (3s) was prepared as a brown oil from 1-(but-3-en-1-yl)-1H-indole-3-carbonitrile **1s**

(39.2 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 71% yield (33.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.68 (m, 1H), 7.32 – 7.23 (m, 3H + overlapped with $CDCl_3$), 4.27 – 4.21 (m, 1H), 4.16 – 4.10 (m, 1H), 3.91 – 3.85 (m, 1H), 3.79 – 3.71 (m, 2H), 2.9 – 2.85 (m, 1H), 2.60 – 2.52 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 132.0, 131.9, 123.2, 122.1, 119.8, 115.8, 110.6, 78.2, 53.0, 44.2, 38.3, 31.4.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{13}H_{12}N_5]^+$ 238.1087, found 238.1084.



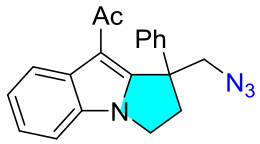
3t

1-(1-(azidomethyl)-1-methyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3t) was prepared as a brown oil from 1-(1-(3-methylbut-3-en-1-yl)-1H-indol-3-yl)ethan-1-one **1t** (45.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 81% yield (43.4 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.88 (m, 1H), 7.38 – 7.23 (m, 3H + overlapped with $CDCl_3$), 4.40 (d, *J* = 11.8 Hz, 1H), 4.24 – 4.11 (m, 2H), 3.59 (d, *J* = 11.8 Hz, 1H), 2.83 – 2.76 (m, 1H), 2.71 (s, 3H), 2.42 – 2.36 (m, 1H), 1.51 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 155.0, 132.2, 130.2, 122.1, 122.0, 120.9, 110.6, 110.4, 57.4, 46.1, 43.4, 39.0, 31.3, 21.9.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O]^+$ 269.1397, found 269.1395.



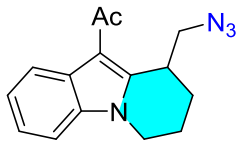
3u

1-(1-(azidomethyl)-1-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3u) was prepared as a brown oil from 1-(1-(3-methylbut-3-en-1-yl)-1H-indol-3-yl)ethan-1-one **1u** (57.8 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 35% yield (22.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.32 (m, 1H), 7.51 (s, 1H), 7.47 – 7.40 (m, 4H), 7.29 – 7.27 (m, 2H), 7.17 – 7.13 (m, 1H), 4.26 – 4.18 (m, 1H), 3.99 – 3.92 (m, 1H), 3.79 – 3.71 (m, 2H), 2.67 – 2.59 (m, 1H), 2.49 – 2.38 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 192.9, 137.7, 136.2, 134.5, 129.3, 128.8, 126.4, 125.6, 123.5, 122.8, 122.6, 117.4, 109.3, 59.8, 42.2, 36.8, 27.6.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{20}H_{19}N_4O]^+$ 331.1553, found 331.1564.



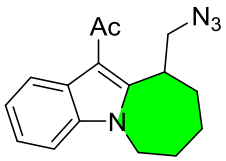
3v

1-(9-(azidomethyl)-6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)ethan-1-one (3v) was prepared as a brown oil from 1-(1-(pent-4-en-1-yl)-1H-indol-3-yl)ethan-1-one **1v** (45.4 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 71% yield (38.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.89 (m, 1H), 7.37 – 7.25 (m, 3H + overlapped with $CDCl_3$), 4.336 – 4.28 (m, 1H), 4.09 – 4.04 (m, 1H), 3.92 – 3.85 (m, 2H), 3.30 – 3.25 (m, 1H), 2.72 (s, 3H), 2.29 – 2.07 (m, 3H), 1.92 – 1.83 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.8, 145.3, 136.2, 126.1, 122.5, 122.2, 120.4, 113.0, 109.8, 52.6, 42.5, 33.7, 31.7, 21.8, 17.8.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{15}H_{17}N_4O]^+$ 269.1397, found 269.1390.



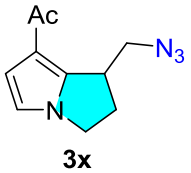
3w

1-(10-(azidomethyl)-7,8,9,10-tetrahydro-6H-azepino[1,2-a]indol-11-yl)ethan-1-one (3w) was prepared as a brown oil from 1-(1-(hex-5-en-1-yl)-1H-indol-3-yl)ethan-1-one **1w** (48.2 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 49% yield (27.6 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.89 (m, 1H), 7.39 – 7.37 (m, 1H), 7.31 – 7.25 (m, 2H), 4.91 – 4.86 (m, 1H), 4.57 (dt, *J* = 14.8, 3.7 Hz, 1H), 4.11 – 4.04 (m, 1H), 3.74 – 3.64 (m, 2H), 2.74 (s, 3H), 2.23 – 2.16 (m, 1H), 2.09 – 2.03 (m, 1H), 1.92 – 1.67 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 148.3, 136.3, 126.0, 122.3, 121.8, 120.8, 114.8, 109.7, 52.4, 44.3, 35.4, 32.2, 27.7, 27.1, 23.4.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{16}H_{19}N_4O]^+$ 283.1553, found 283.1556.



3x

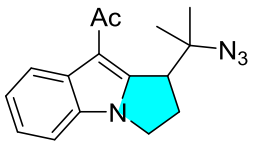
1-(1-(Azidomethyl)-2,3-dihydro-1H-pyrrolizin-7-yl)ethan-1-one (3x) was prepared as a brown oil from 1-(1-(but-3-en-1-yl)-1H-pyrrol-3-yl)ethan-1-one **1x** (32.6 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl

acetate-petroleum ether, 1:5) in 55% yield (22.5 mg).

^{1}H NMR (300 MHz, $CDCl_3$) δ 6.59 – 6.55 (m, 2H), 4.12 – 3.92 (m, 2H), 3.85 – 3.63 (m, 3H), 2.80 – 3.67 (m, 1H), 2.50 – 2.39 (m, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 194.1, 142.3, 117.8, 114.9, 114.6, 53.2, 46.2, 38.8, 31.5, 27.4.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{10}H_{13}N_4O]^+$ 205.1084, found 205.1090.



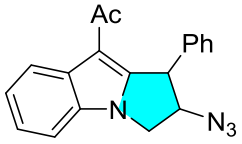
3y

1-(1-(2-Azidopropan-2-yl)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one (3y) was prepared as a brown oil from 1-(1-(4-methylpent-3-en-1-yl)-1H-indol-3-yl)ethan-1-one **1y** (48.2 mg, 0.2 mmol) according to the General Procedure **A** (eluent: ethyl acetate-petroleum ether, 1:5) in 80% yield (45.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.82 (m, 1H), 7.34 – 7.25 (m, 3H + overlapped with $CDCl_3$), 4.32 – 4.25 (m, 1H), 4.19 – 4.12 (m, 1H), 3.71 (dd, *J* = 7.7, 2.5 Hz, 1H), 2.73 (s, 3H), 2.50 – 2.32 (m, 2H), 1.65 (s, 3H), 1.63 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.8, 148.2, 135.0, 126.8, 122.1, 122.0, 120.4, 114.3, 109.7, 67.3, 39.7, 39.1, 32.6, 25.9, 23.4, 21.9.

HRMS (ESI-TOF) *m*/*z* [M + H]$^+$: calcd. for $[C_{16}H_{19}N_4O]^+$ 283.1553, found 283.1550.



3z

1-(2-Azido-1-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-9-yl)ethan-1-one

(3z) was prepared as a brown oil from 1-(1-cinnamyl-1H-indol-3-yl)ethan-1-one **1z** (55.0 mg, 0.2 mmol) according to the General Procedure **A** (eluent: dichloromethane-petroleum ether, 3:1) in 28% yield (17.7 mg).

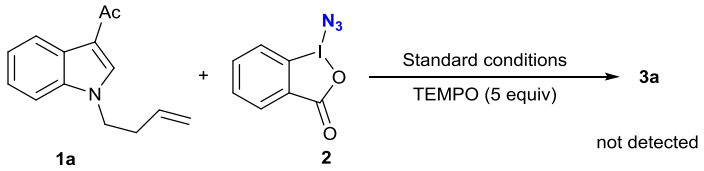
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.34 (m, 1H), 7.35 – 7.29 (m, 6H), 7.07 – 7.03 (m, 2H), 4.88 (d, *J* = 1.6 Hz, 1H), 4.65 (dt, *J* = 5.5, 1.6 Hz, 1H), 4.45 (dd, *J* = 11.7, 5.4 Hz, 1H), 4.18 (dd, *J* = 11.8, 1.7 Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 149.2, 137.8, 132.5, 130.6, 129.4, 128.1, 127.2, 123.1, 122.9, 122.8, 111.7, 109.9, 71.8, 53.1, 49.0, 29.6.

HRMS (ESI-TOF) *m*/*z* [M + Na]$^{+}$: calcd. for $[C_{19}H_{17}N_4O]^{+}$ 317.1397, found 317.1390.

VI. The Control Experiment

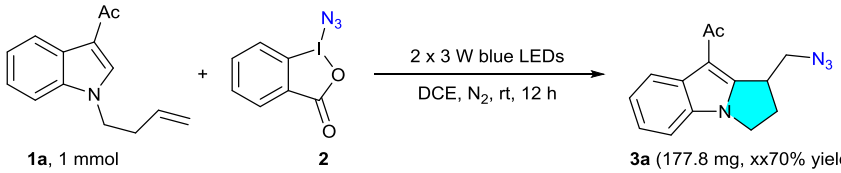
The radical trapping experiment with TEMPO



Under air, to an over-dried 20 mL Schlenk tube equipped with a Teflon cap was added *N*-alkene-linked indole **1a** (0.1 mmol, 42.6 mg), Togni-N_3 **2** (0.15 mmol, 43.2 mg), TEMPO (0.5 mmol, 78.1 mg) and DCE (1.0 mL). The reaction vessel was evacuated and backfilled with N_2 in three times. Then, the Schlenk tube was stirred at room temperature under 16 W blue LEDs irradiation for 12 h. Then, the mixture was analyzed by TLC or GC-MS, it was found that none of the desired product **3a** could be detected.

VII. 1-mmol Scale Reaction and Derivation

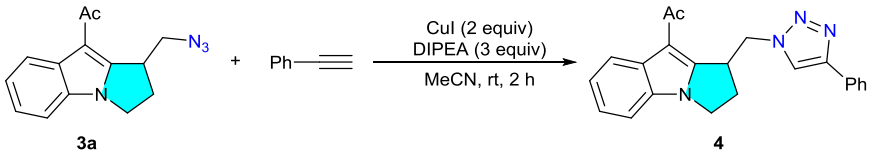
(a) 1-mmol scale reaction of 1a and Togni-N_3



Under air, to an over-dried 20 mL Schlenk tube equipped with a Teflon cap was added *N*-alkene-linked indole **1a** (1 mmol, 213.1 mg), Togni-N_3 **2** (1.5 mmol, 432.1 mg) and DCE (2.0 mL). The reaction vessel was evacuated and backfilled with N_2 in three times. Then, the Schlenk tube was stirred at room temperature under 16 W blue LEDs irradiation for 12 h. Then, the mixture was concentrated in vacuo. The residue was purified by silica gel flash chromatography (eluent: ethyl acetate-petroleum ether, 1:5) to give the pure desired product **3a** in 70% yield (177.8 mg).

Figure S2 Photoreactor used for 1-mmol scale reaction

(b) CuI-promoted click reaction of **3a** with phenylacetylene[3]



An oven-dried sealed tube (20 mL) containing **3a** (50.8 mg, 0.2 mmol), CuI

[3] M.-Z. Lu, C.-Q. Wang and T.-P. Loh, *Org. Lett*., **2015**, *17*, 6110−6113.

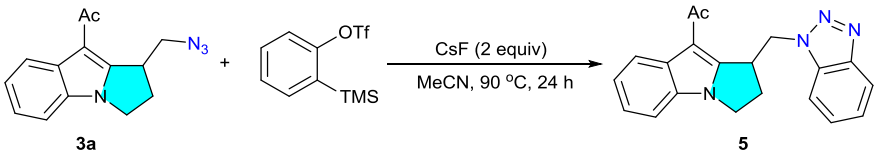
(76.0 mg, 0.40 mmol), was evacuated and purged with nitrogen gas three times. Then, phenylacetylene (22.4 mg, 0.22 mmol), *N*,*N*-diisopropylethylamine (77.6 mg, 0.6 mmol) and MeCN (2.0 mL) were added via syringe. The reaction mixture was stirred at room temperature for 2 h. The reaction was quenched with NH_4Cl (aq.), extracted with CH_2Cl_2 (10× 3 mL), washed with brine, dried over anhydrous sodium sulfate. The solvent was removed in vacuo and the residue was purified by flash chromatography on silica gel (EA/PE=1:2) to give the desired product **4** in 90% yield (64.1 mg).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (s, 1H), 8.05 (d, J = 6.8 Hz, 1H), 7.73 (d, J = 7.1 Hz, 2H), 7.41 – 7.37 (m, 3H), 7.31 – 7.27 (m, 1H), 7.21 – 7.18 (m, 2H), 4.92 – 4.89 (m, 1H), 4.76 – 4.70 (m, 1H), 4.23 – 4.13 (m, 2H), 3.84 – 3.77 (m, 1H), 2.76 – 2.71 (m, 1H), 2.50 (s, 3H), 1.19 – 1.16 (m, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 191.4, 150.1, 131.6, 129.0, 128.2, 127.2, 124.5, 121.4, 121.3, 120.5, 110.2, 109.4, 50.3, 42.3, 39.2, 39.0, 29.7, 29.0.

HRMS (ESI-TOF) m/z [M + H]$^+$: calcd. for $[C_{22}H_{21}N_4O]^+$ 357.1710, found 357.1706.

(c) Reaction of **3a** with 2-(trimethylsilyl)phenyl trifluoromethanesulfonate[3]



An oven-dried sealed tube (20 mL) containing **3a** (50.8 mg, 0.20 mmol), CsF (60.8 mg, 0.40 mmol), was evacuated and purged with nitrogen gas three times. Then, 2-(trimethylsilyl)phenyl trifluoromethanesulfonate (119.4 mg, 0.40 mmol) and MeCN (2.0 mL) were added via syringe. The reaction mixture was stirred at 90 °C for 24 h. After cooling to ambient temperature, the reaction was quenched with NH_4Cl (aq.), extracted with EA (3 × 10 mL), dried over anhydrous sodium sulfate. The solvent was removed in vacuo and the residue was purified by flash chromatography on silica gel (EA/PE=1:2) to

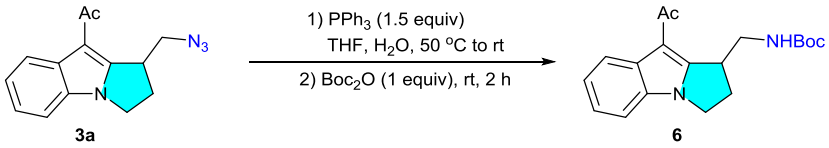
give the desired product **5** in 50% yield (33.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.97 (m, 2H), 7.90 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.48 (ddd, *J* = 8.2, 6.9, 1.0 Hz, 1H), 7.36 – 7.24 (m, 4H + overlapped with $CDCl_3$), 5.31 (dd, *J* = 14.0, 3.2 Hz, 1H), 4.81 (dd, *J* = 14.0, 9.6 Hz, 1H), 4.26 – 4.20 (m, 1H), 4.15 – 4.09 (m, 1H), 4.05 – 3.99 (m, 1H), 2.89 – 2.82 (m, 1H), 2.78 (s, 3H), 2.68 – 2.58 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 151.3, 145.9, 133.0, 132.6, 129.6, 127.6, 124.1, 122.3, 122.3, 120.7, 119.6, 110.8, 110.7, 110.1, 48.9, 43.2, 39.8, 30.6, 30.3.

HRMS (ESI-TOF) *m/z* [M + H]$^+$: calcd. for $[C_{20}H_{19}N_4O]^+$ 331.1553, found 331.1547.

(d) Reduction of **3a**[4]



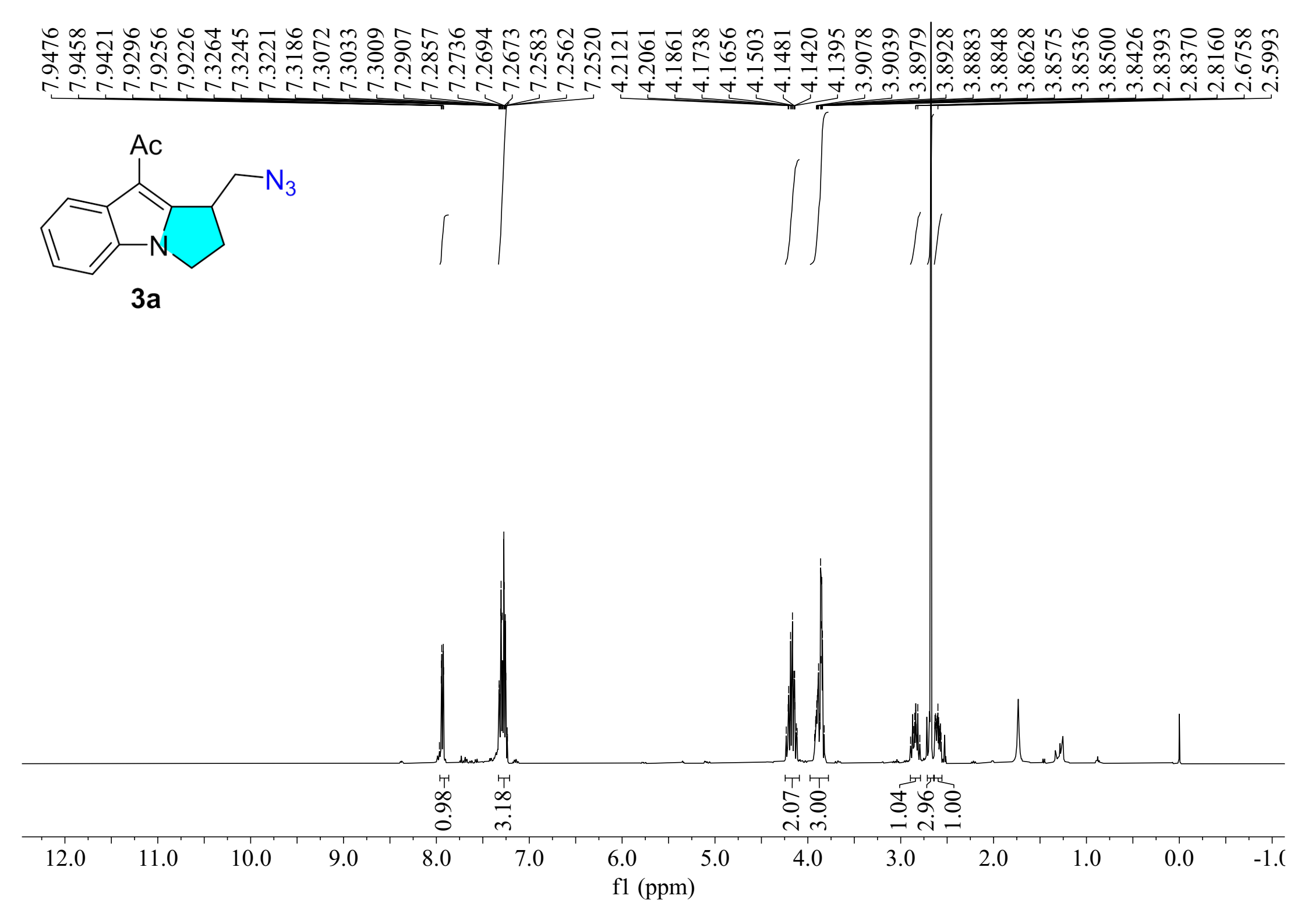
In an oven-dried sealed tube (20 mL) was added **3a** (50.8 mg, 0.2 mmol) and triphenylphosphine (78.7 mg, 0.3 mmol). Then, to this mixture dry THF (1 mL) was added and the resulting solution was heated at 50 °C for 4 h. The reaction mixture was cooled to room temperature and 2 mL of water was added. The resulting solution was stirred at room temperature for 16 hours. To the reaction mixture solution of di-tert-butyldicarbonate (43.6 mg, 0.2 mmol) in THF (1 mL) was added. Resulting mixture was stirred at room temperature for 2 h. The reaction mixture was diluted with EA and washed with H_2O. Aqueous was extracted with EA. The combined organic phase was dried over sodium sulfate and concentrated under reduced pressure. Then the residue was purified by silica gel flash chromatography (eluent: ethyl acetate-petroleum ether, 1:2) to give the pure desired product **6** in 72% yield (47.2 mg).

[4] L. Zhu, H. Yu, Z. Xu, X. Jiang, L. Lin and R. Wang, *Org. Lett.*, 2014, *16*, 562−1565.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.96 (m, 1H), 7.29 – 7.23 (m, 3H + overlapped with $CDCl_3$), 5.32 (brs, 1H), 4.15 – 4.08 (m, 2H), 3.83 – 3.77 (m, 1H), 3.61 – 3.48 (m, 2H), 2.78 – 2.72 (m, 1H), 2.64 – 2.57 (m, 4H), 1.40 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 156.4, 152.8, 132.6, 123.0, 122.1, 122.1, 121.1, 110.6, 110.3, 79.2, 43.3, 42.8, 40.4, 31.4, 30.1, 28.3.

HRMS (ESI-TOF) *m*/*z* [M + H]$^{+}$: calcd. for $[C_{19}H_{25}N_2O_3]^{+}$ 329.1860, found 329.1861.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7.3009
7.2907
7.2857
7.2736
7.2694
7.2673
7.2583
7.2562
7.2520
4.2121
4.2061
4.1861
4.1738
4.1656
4.1503
4.1481
4.1420
4.1395
3.9078
3.9039
3.8979
3.8928
3.8883
3.8848
3.8628
3.8575
3.8536
3.8500
3.8426
2.8393
2.8370
2.8160
2.6758
2.5993
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N3
N
3a
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3.18
2.07
3.00
1.04
2.96
1.00
12.0
11.0
10.0
9.0
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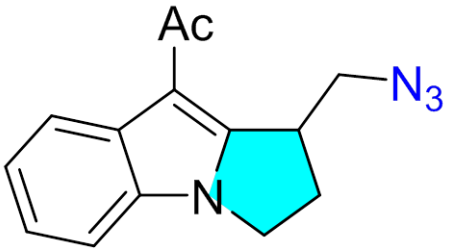

3a

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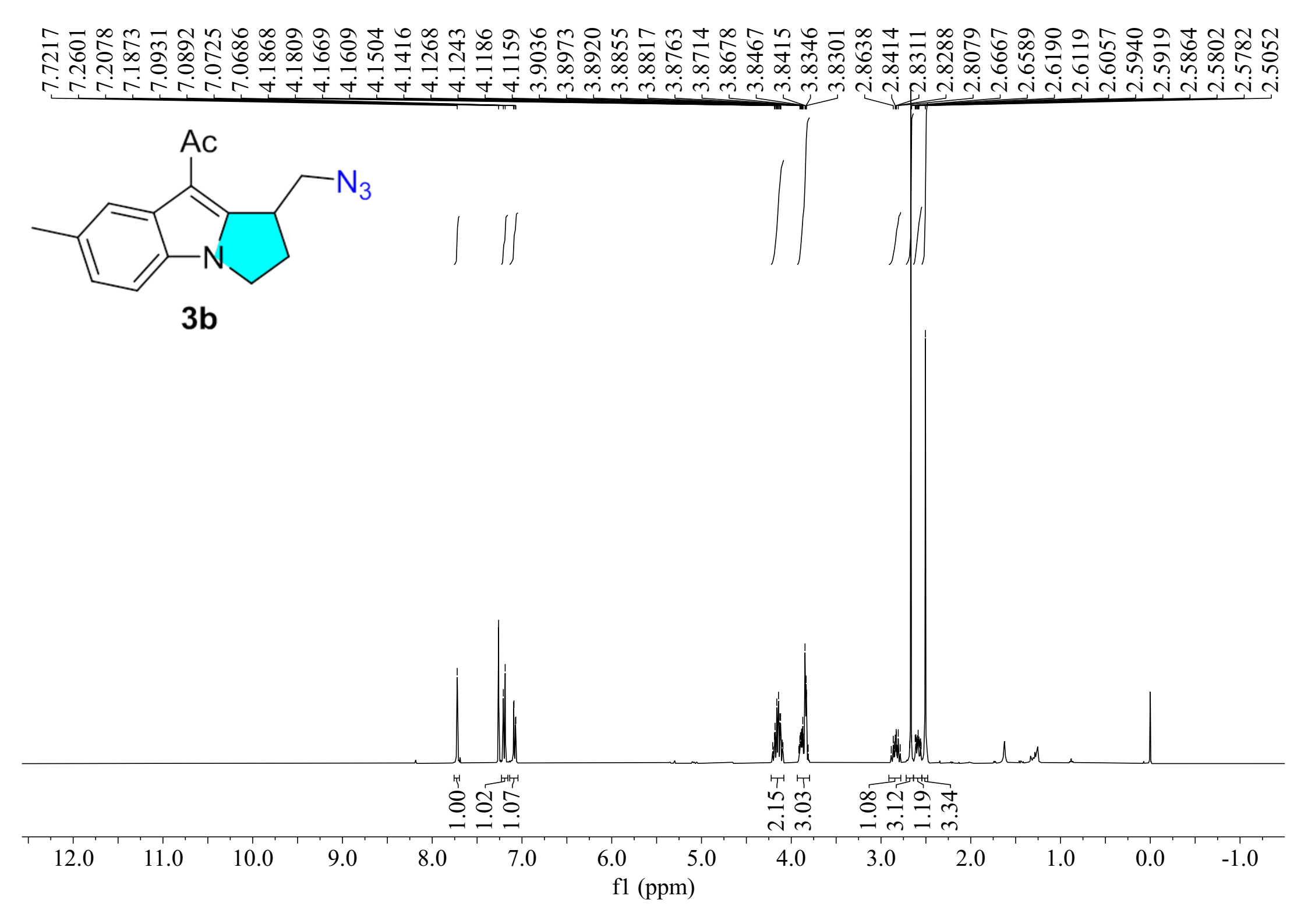
122.25
122.22
121.03
110.64
110.61
77.39
77.07
76.75
53.11
43.80
39.52
31.03
30.52

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)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4.1609
4.1504
4.1416
4.1268
4.1243
4.1186
4.1159
3.9036
3.8973
3.8920
3.8855
3.8817
3.8763
3.8714
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3.8415
3.8346
3.8301
2.8638
2.8414
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2.6589
2.6190
2.6119
2.6057
2.5940
2.5919
2.5864
2.5802
2.5782
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N
3b
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1.02
1.07
2.15
3.03
1.08
3.12
1.19
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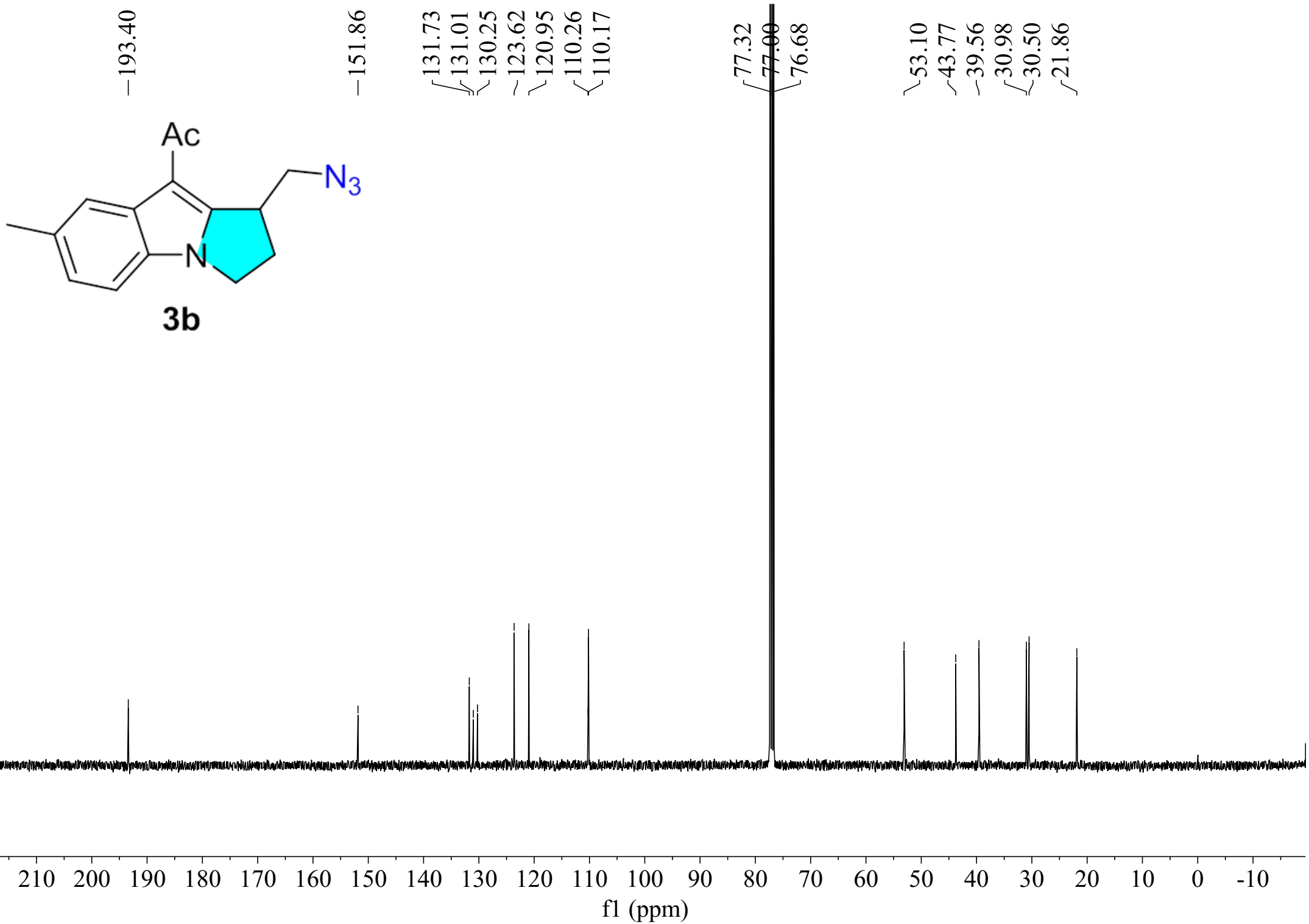
f1 (ppm)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123.62
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110.26
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77.32
77.00
76.68
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43.77
39.56
30.98
30.50
21.86
Ac
N3
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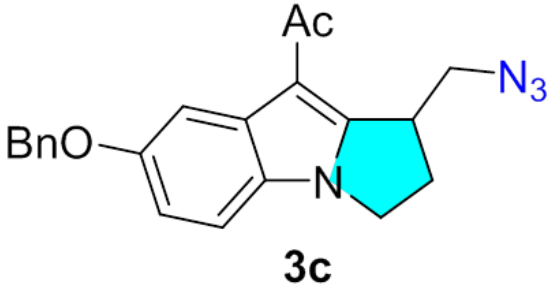
3b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



3c

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3.00 2.02 1.05 1.04 1.04 2.02 2.02 3.00 1.08 3.99

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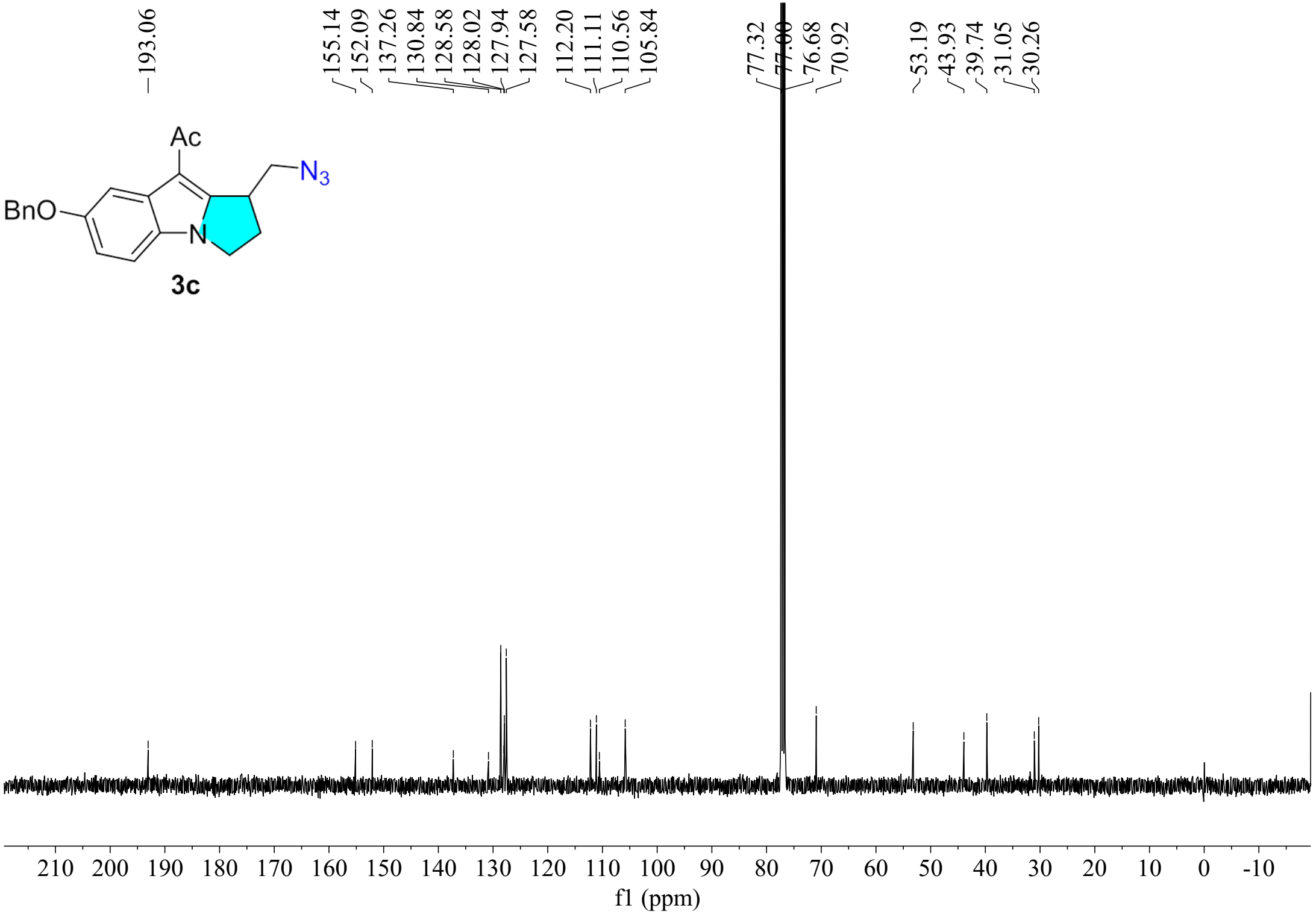
f1 (ppm)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70.92
53.19
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BnO
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3c
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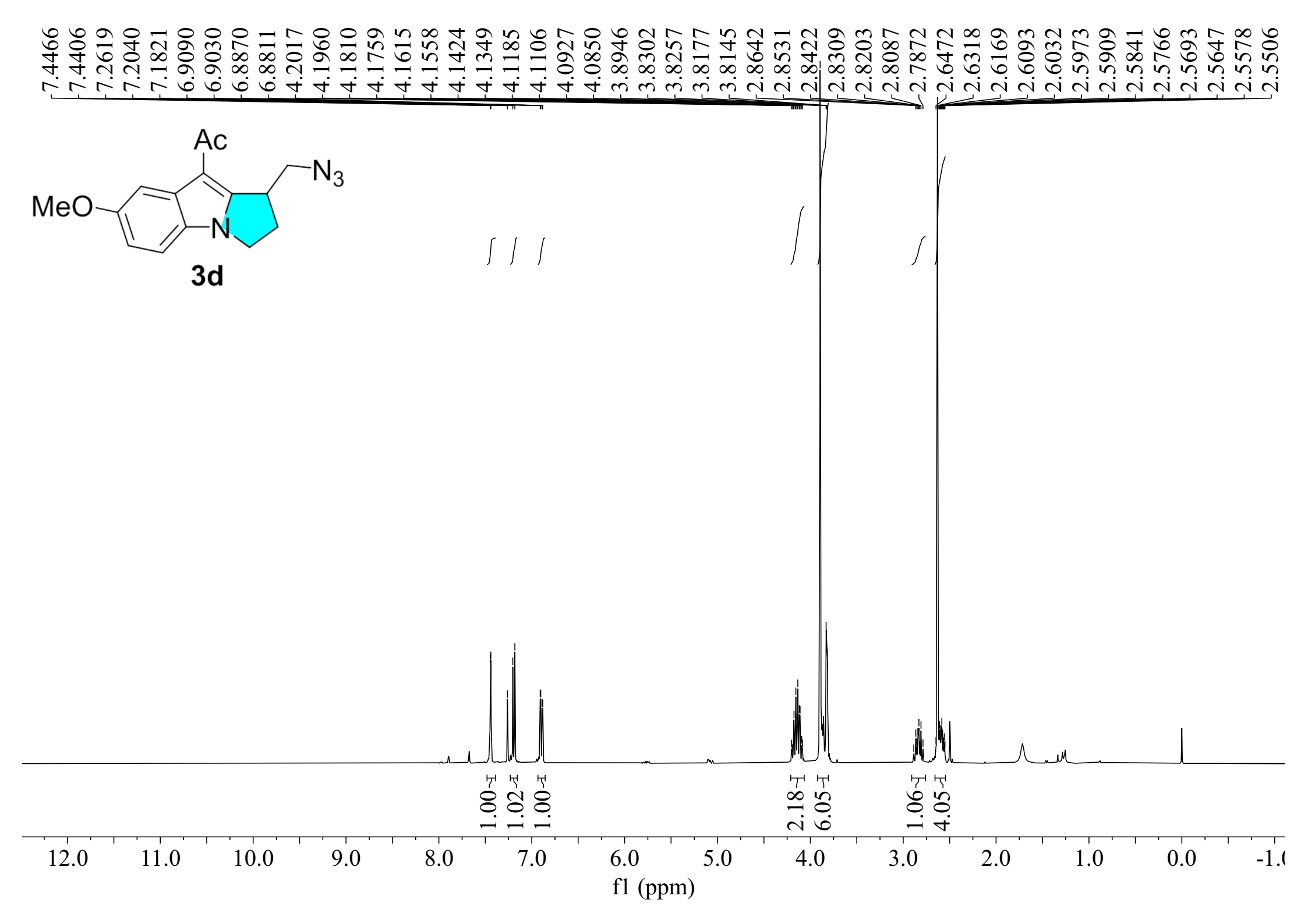
f1 (ppm)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4.1810
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4.1106
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3.8145
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2.8531
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2.8203
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2.6032
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2.5909
2.5841
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2.5578
2.5506
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MeO
N
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1.02
1.00
2.18
6.05
1.06
4.05
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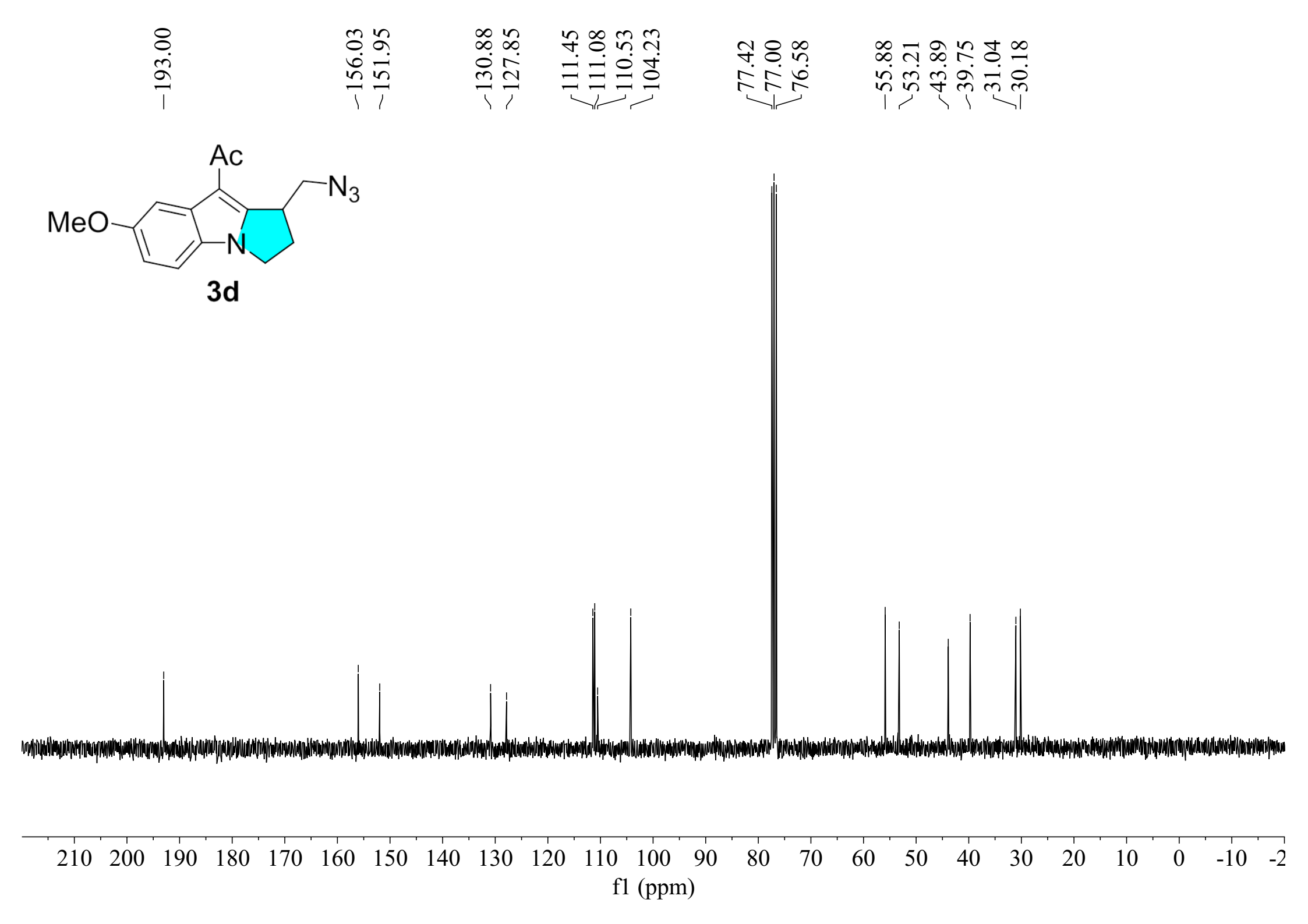
0.0
f1 (ppm)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55.88
53.21
43.89
39.75
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N3
MeO
N
3d
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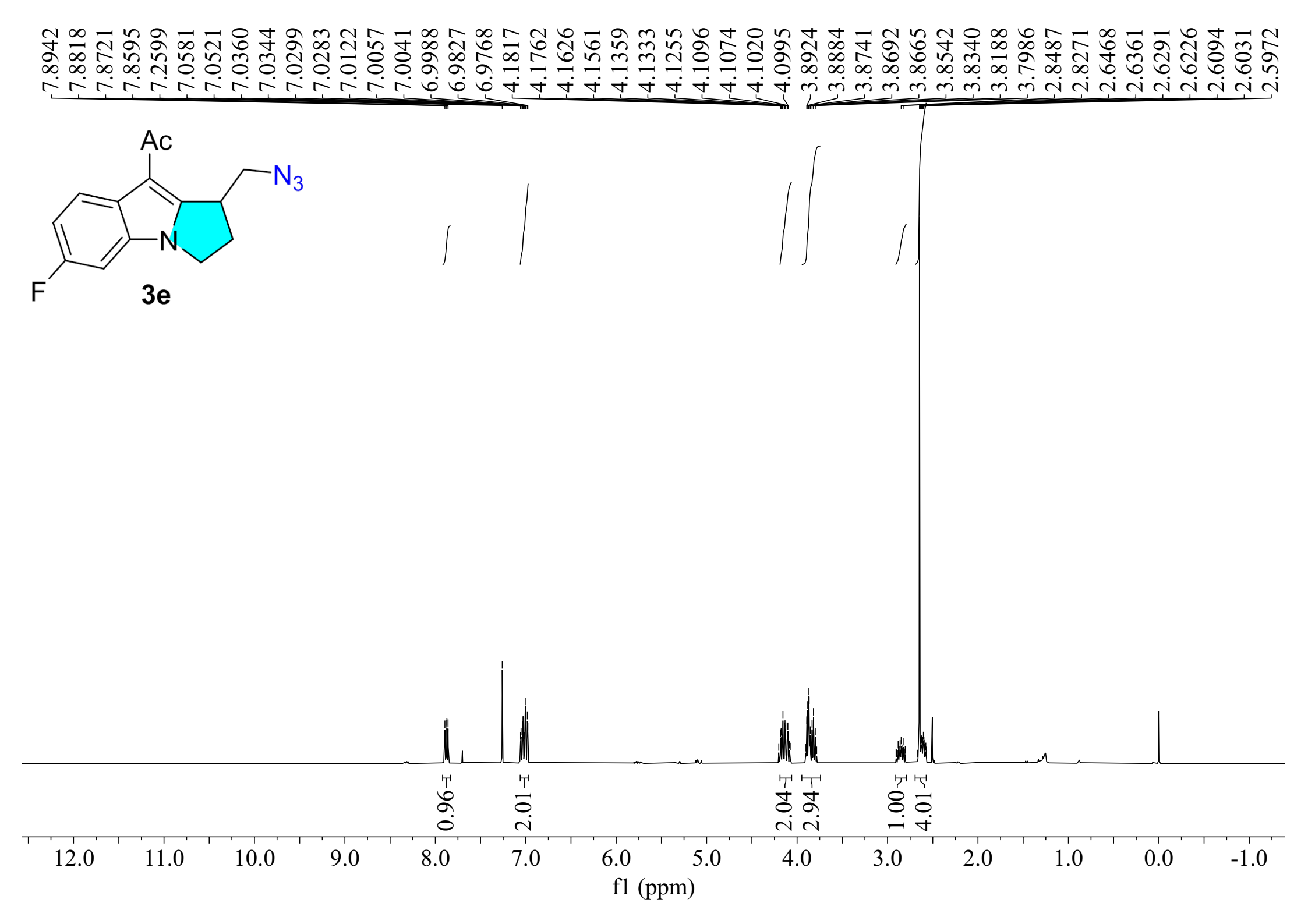
f1 (ppm)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7.0057
7.0041
6.9988
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6.9768
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4.1762
4.1626
4.1561
4.1359
4.1333
4.1255
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2.04
2.94
1.00
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11.0
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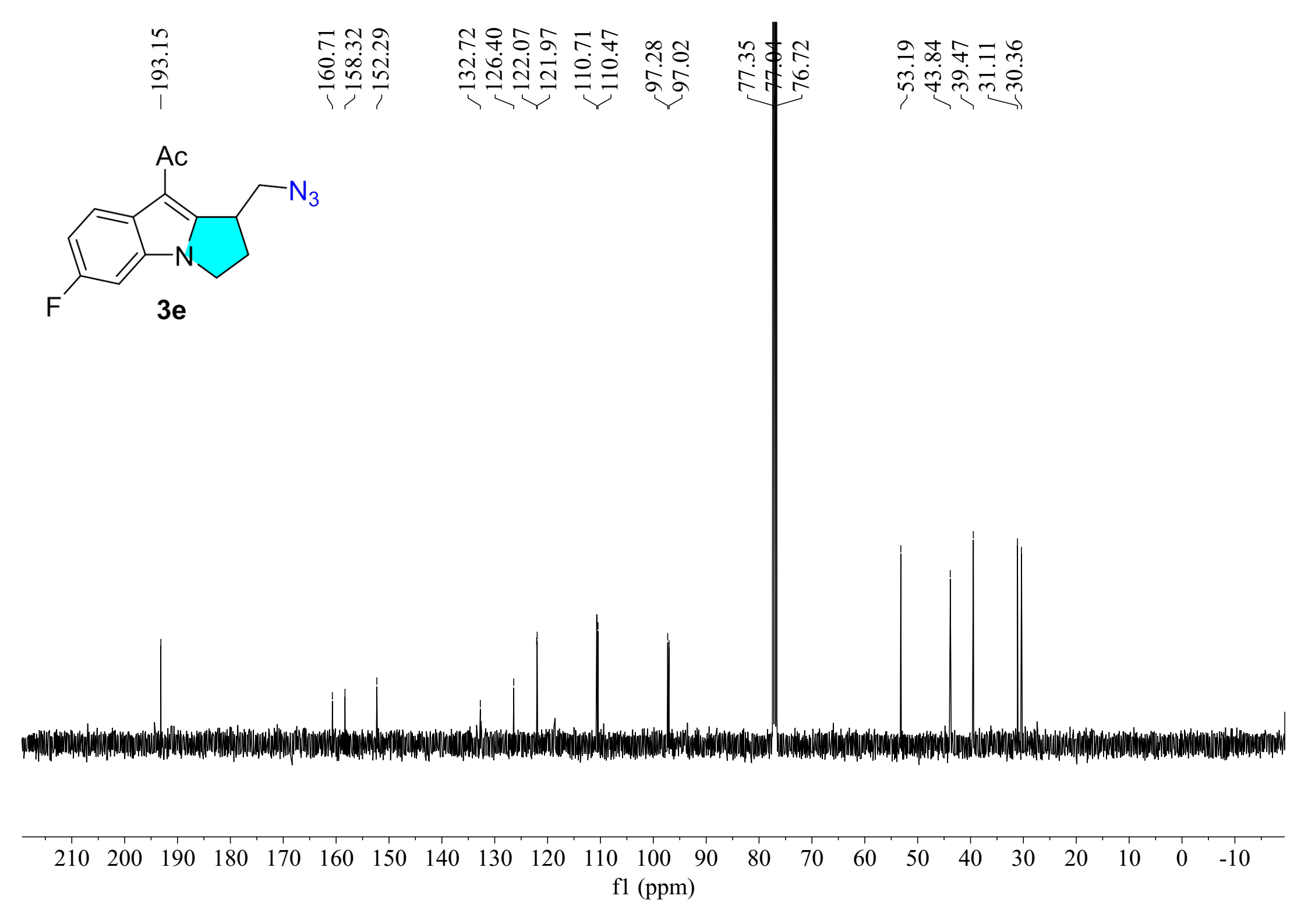
f1 (ppm)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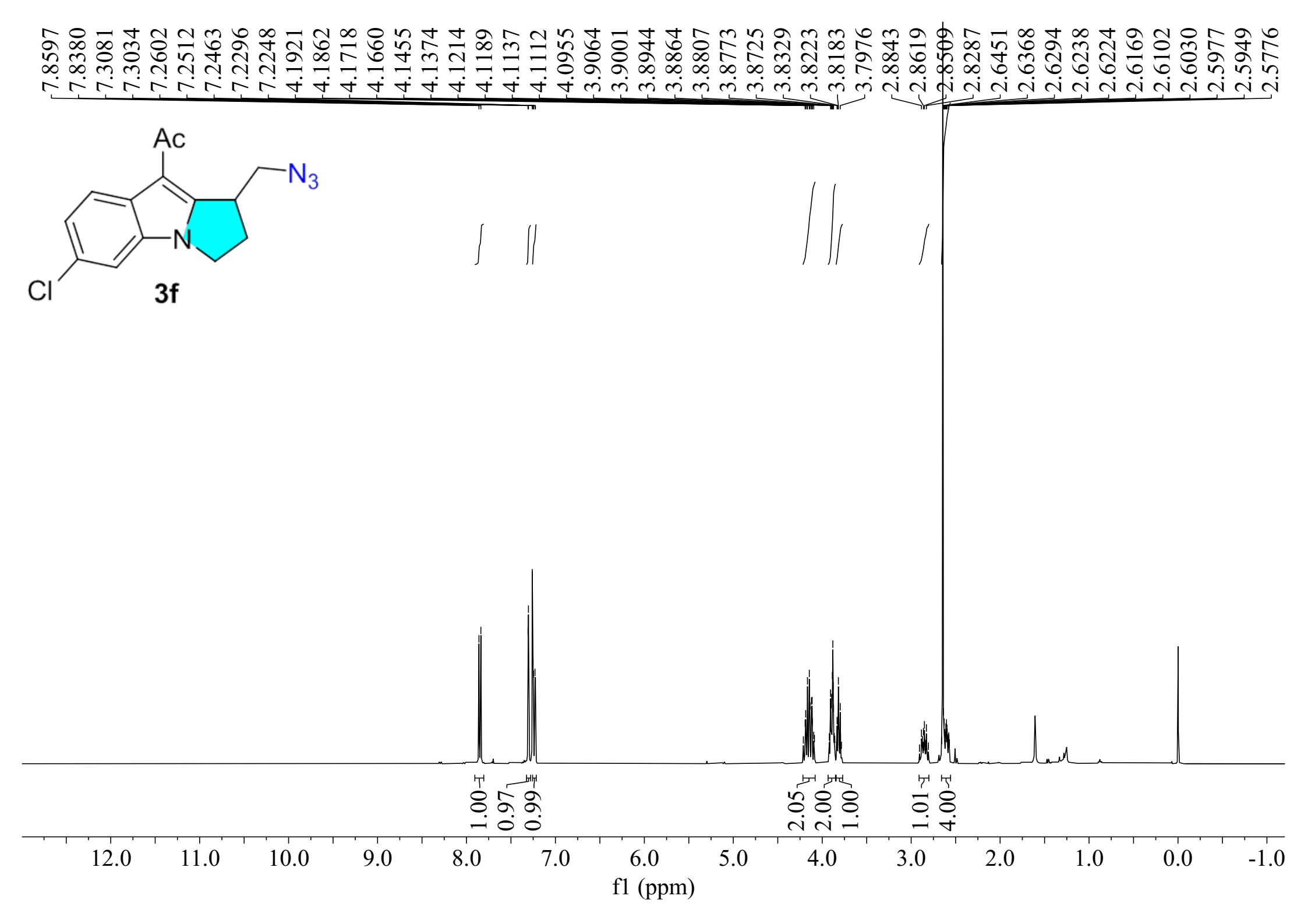
f1 (ppm)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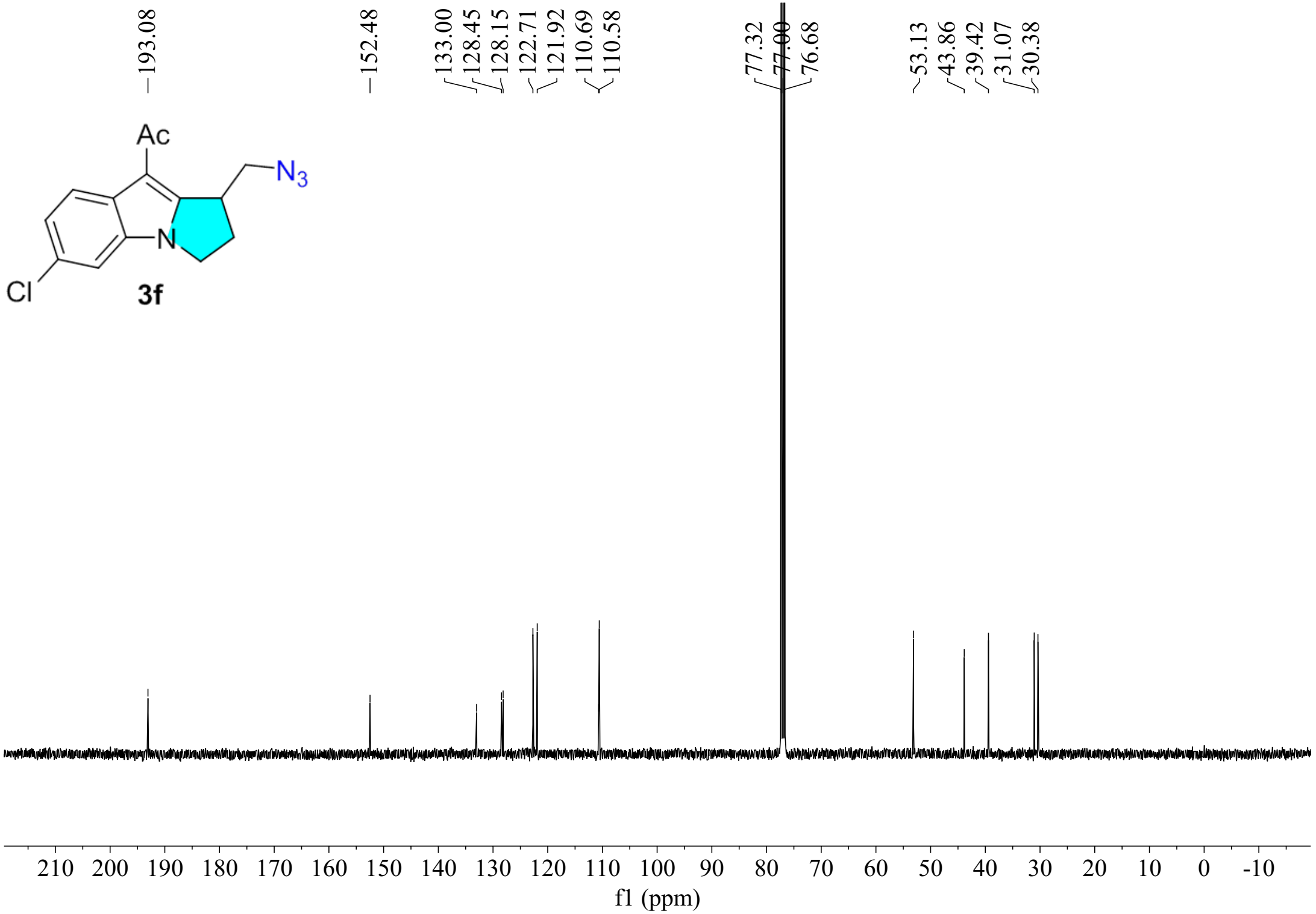
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43.86
39.42
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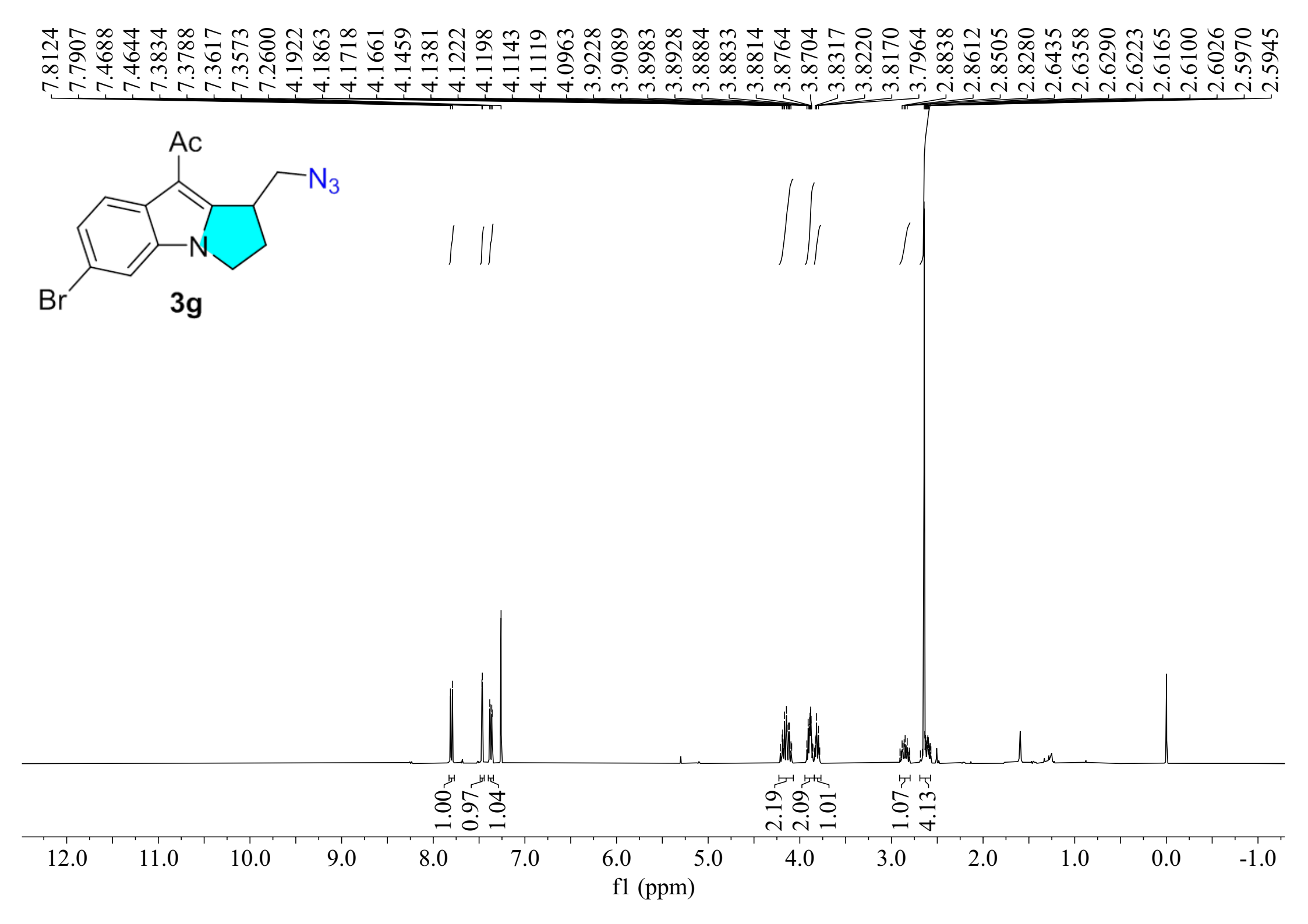
N
Cl
3f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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2.09
1.01
1.07
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10.0
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6.0
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4.0
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1.0
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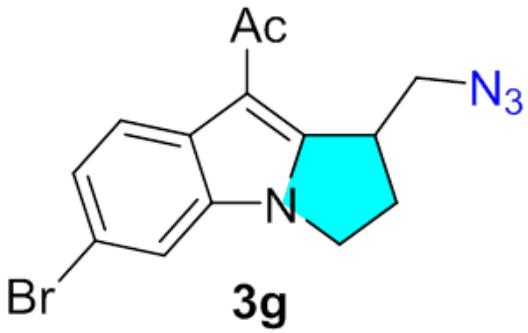
-1.0
f1 (ppm)



3g

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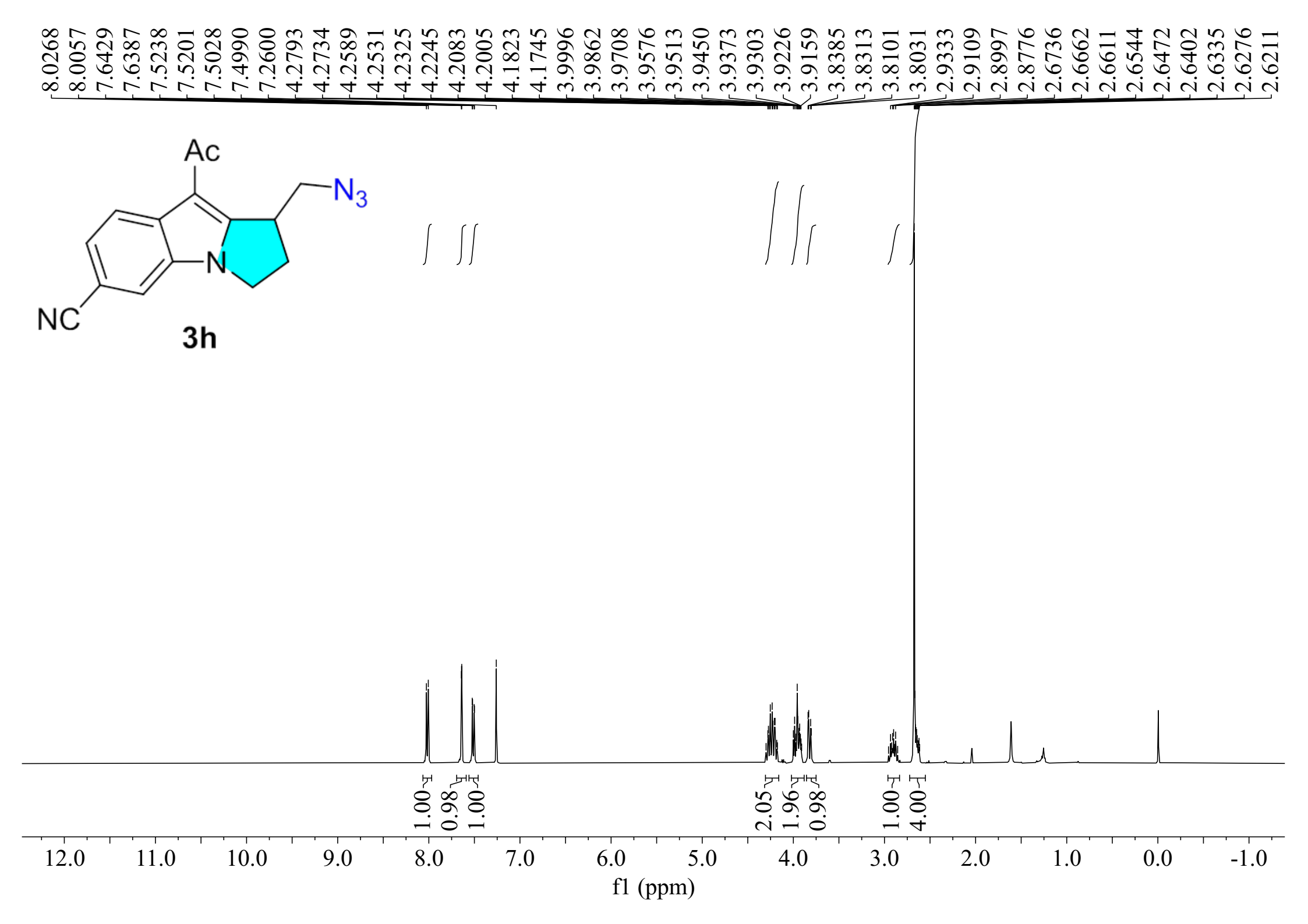
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)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3.9513
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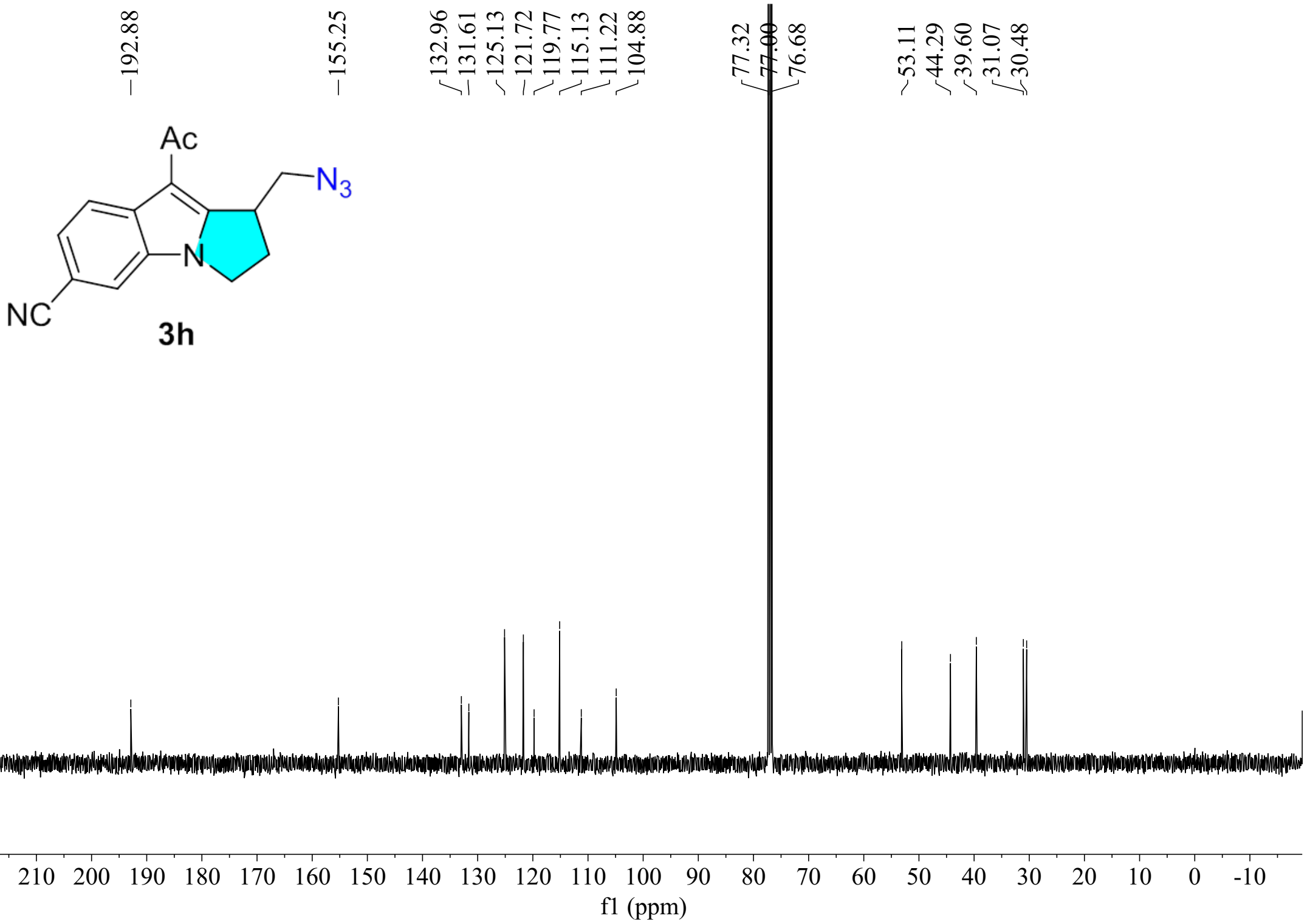
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121.72
119.77
115.13
111.22
104.88
77.32
77.00
76.68
53.11
44.29
39.60
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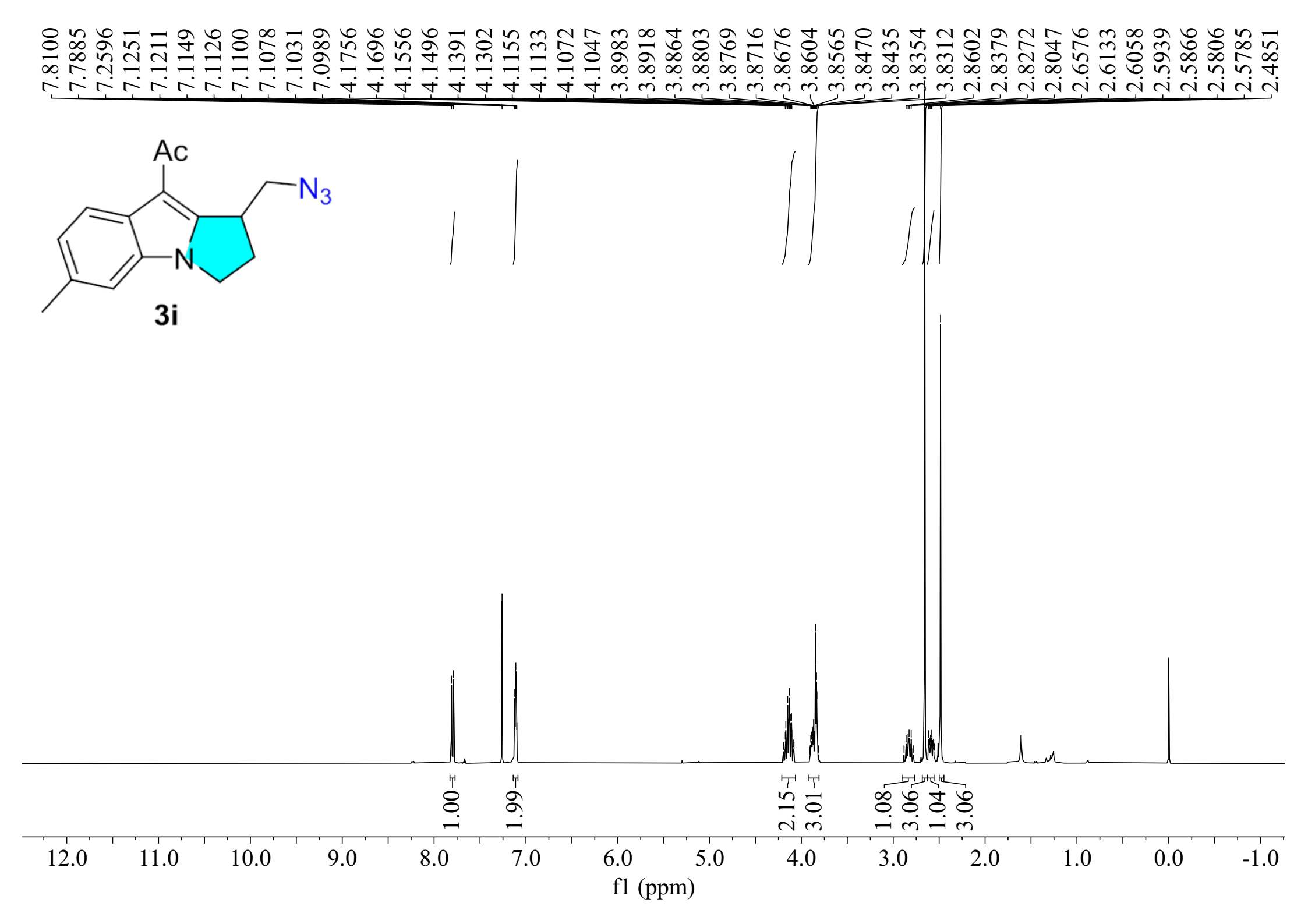
Ac
N3
N
NC
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.1031
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4.1756
4.1696
4.1556
4.1496
4.1391
4.1302
4.1155
4.1133
4.1072
4.1047
3.8983
3.8918
3.8864
3.8803
3.8769
3.8716
3.8676
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3.8565
3.8470
3.8435
3.8354
3.8312
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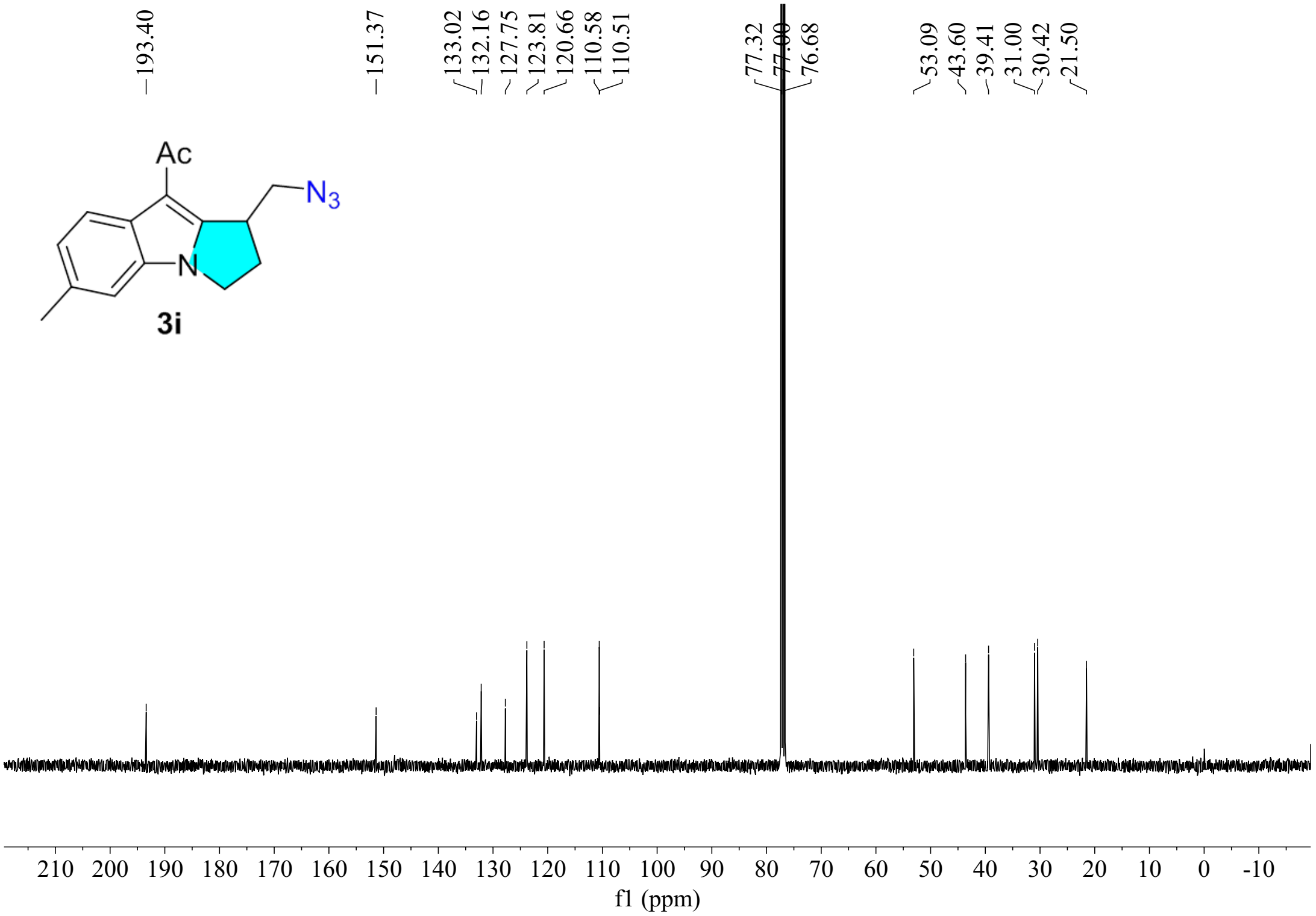
2.8379
2.8272
2.8047
2.6576
2.6133
2.6058
2.5939
2.5866
2.5806
2.5785
2.4851
Ac
N3
N
3i
1.00
1.99
2.15
3.01
1.08
3.06
1.04
3.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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77.00
76.68
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43.60
39.41
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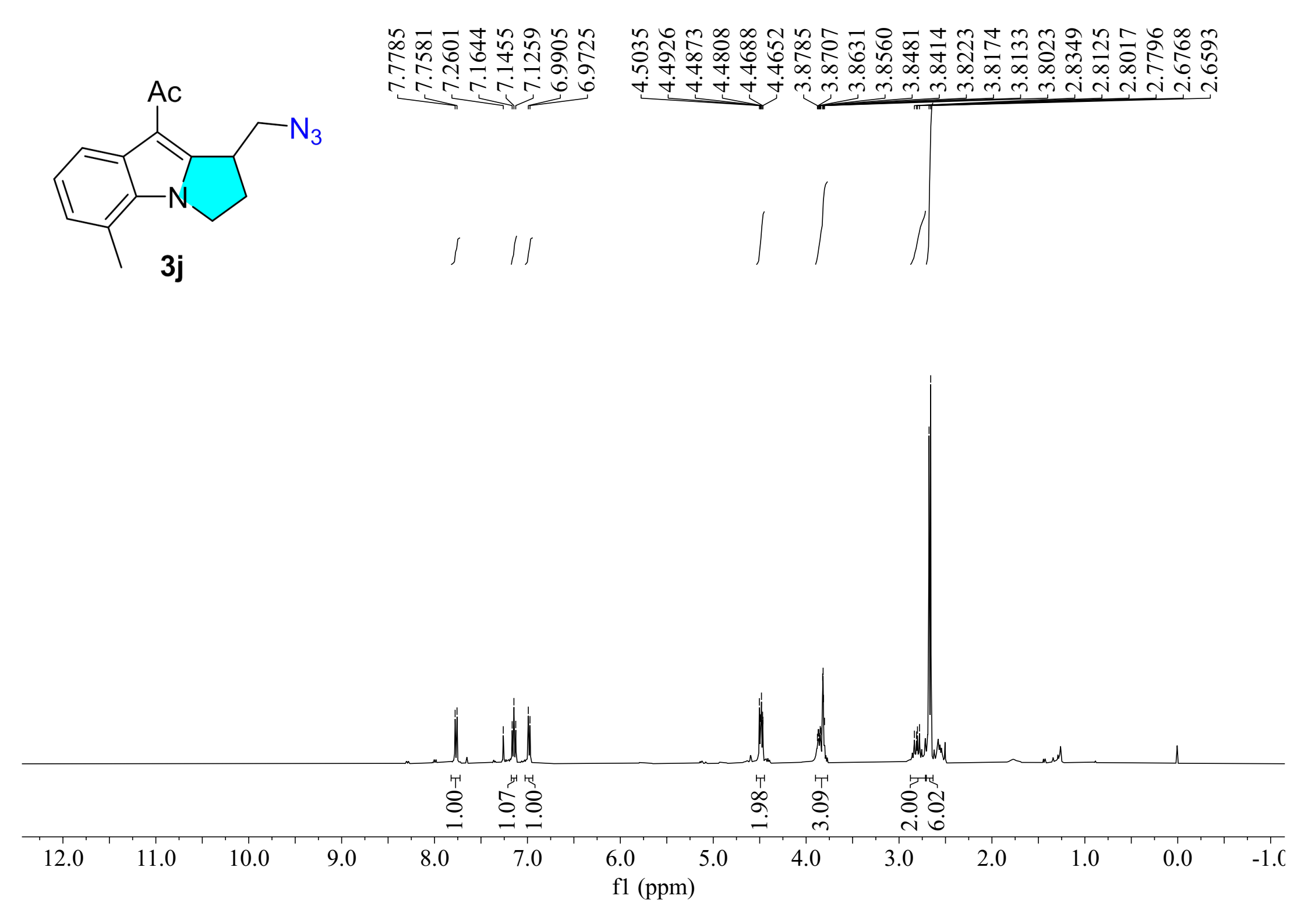
Ac
N3
N
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Ac
N3
N
3j
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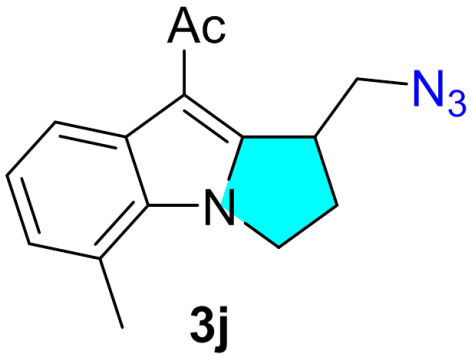
7.1455
7.1259
6.9905
6.9725
4.5035
4.4926
4.4873
4.4808
4.4688
4.4652
3.8785
3.8707
3.8631
3.8560
3.8481
3.8414
3.8223
3.8174
3.8133
3.8023
2.8349
2.8125
2.8017
2.7796
2.6768
2.6593
1.00
1.07
1.00
1.98
3.09
2.00
6.02
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)



3j

193.48
152.21
132.24
130.24
123.95
122.26
121.57
118.75
110.52
77.32
77.00
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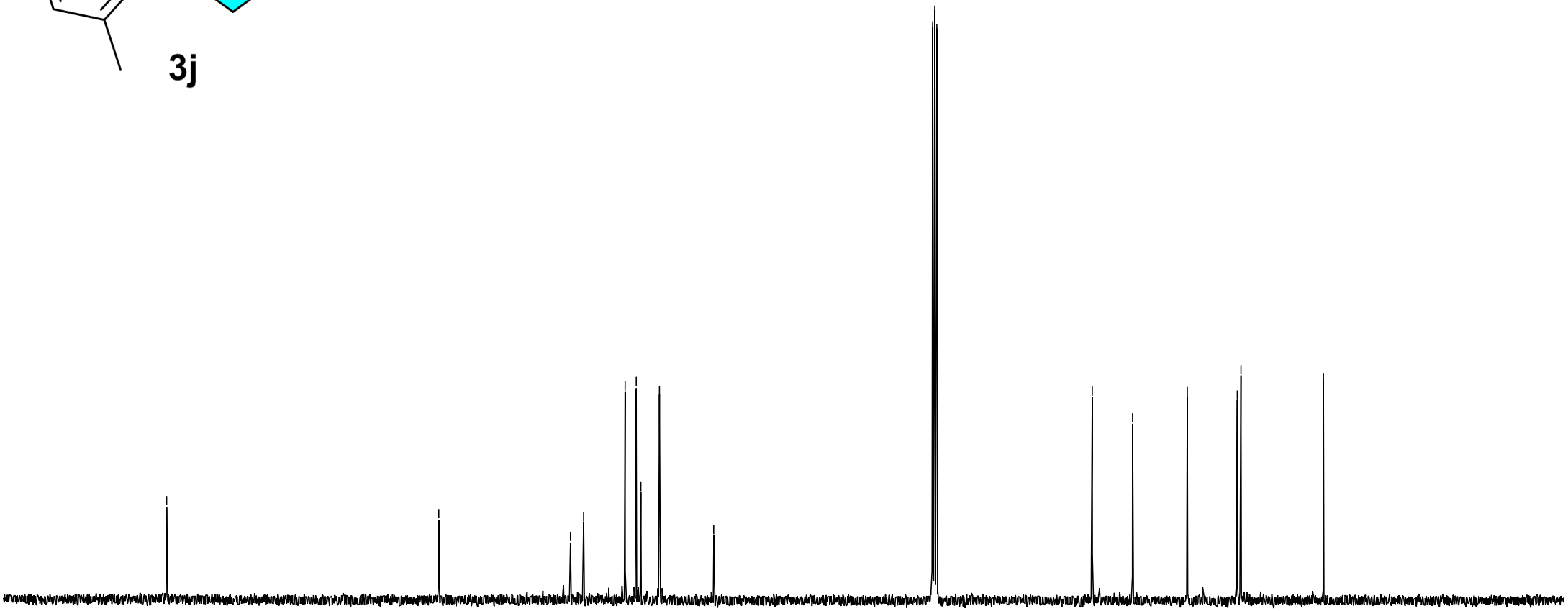
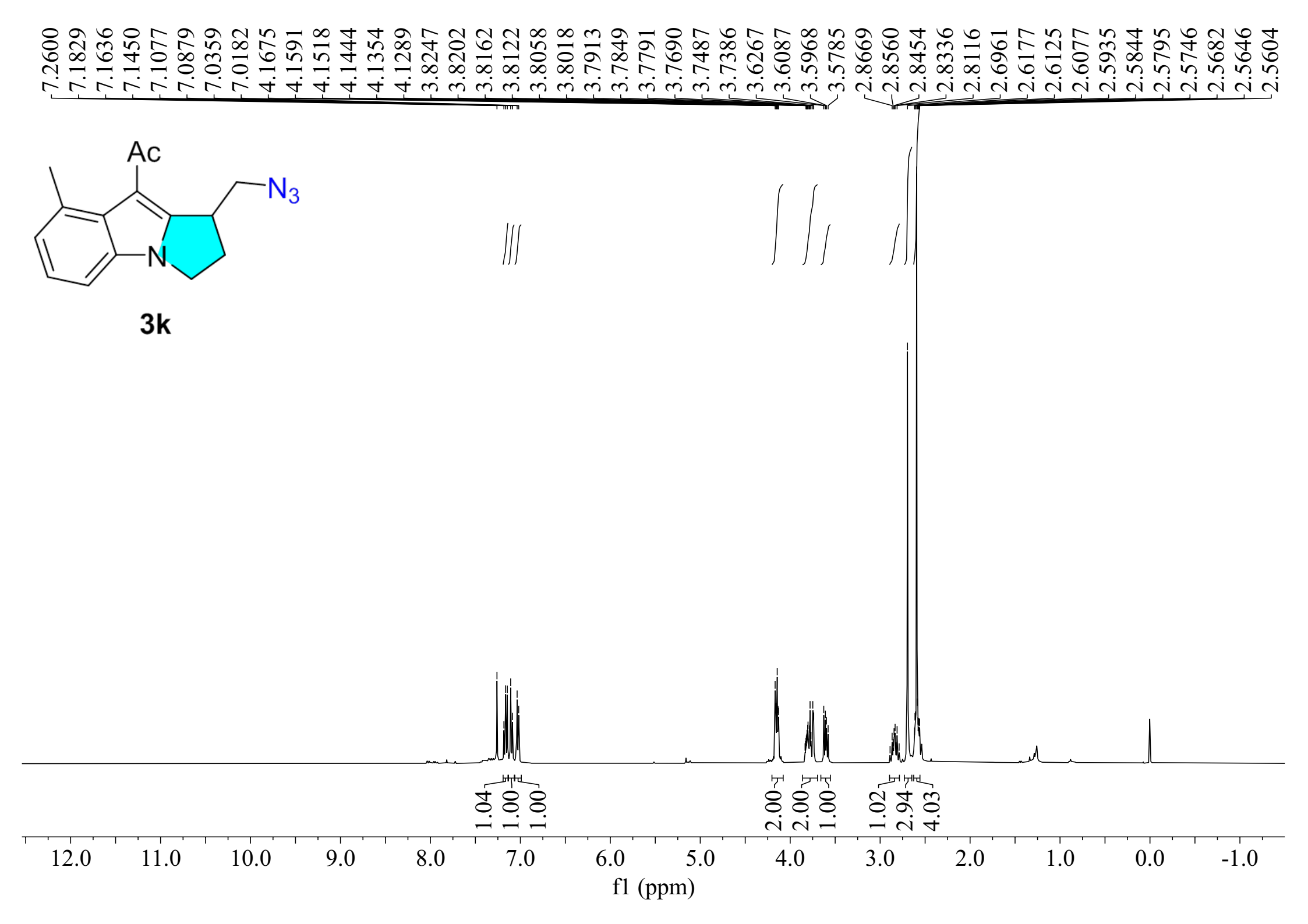
53.11
47.00
38.70
31.12
30.56
18.06



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)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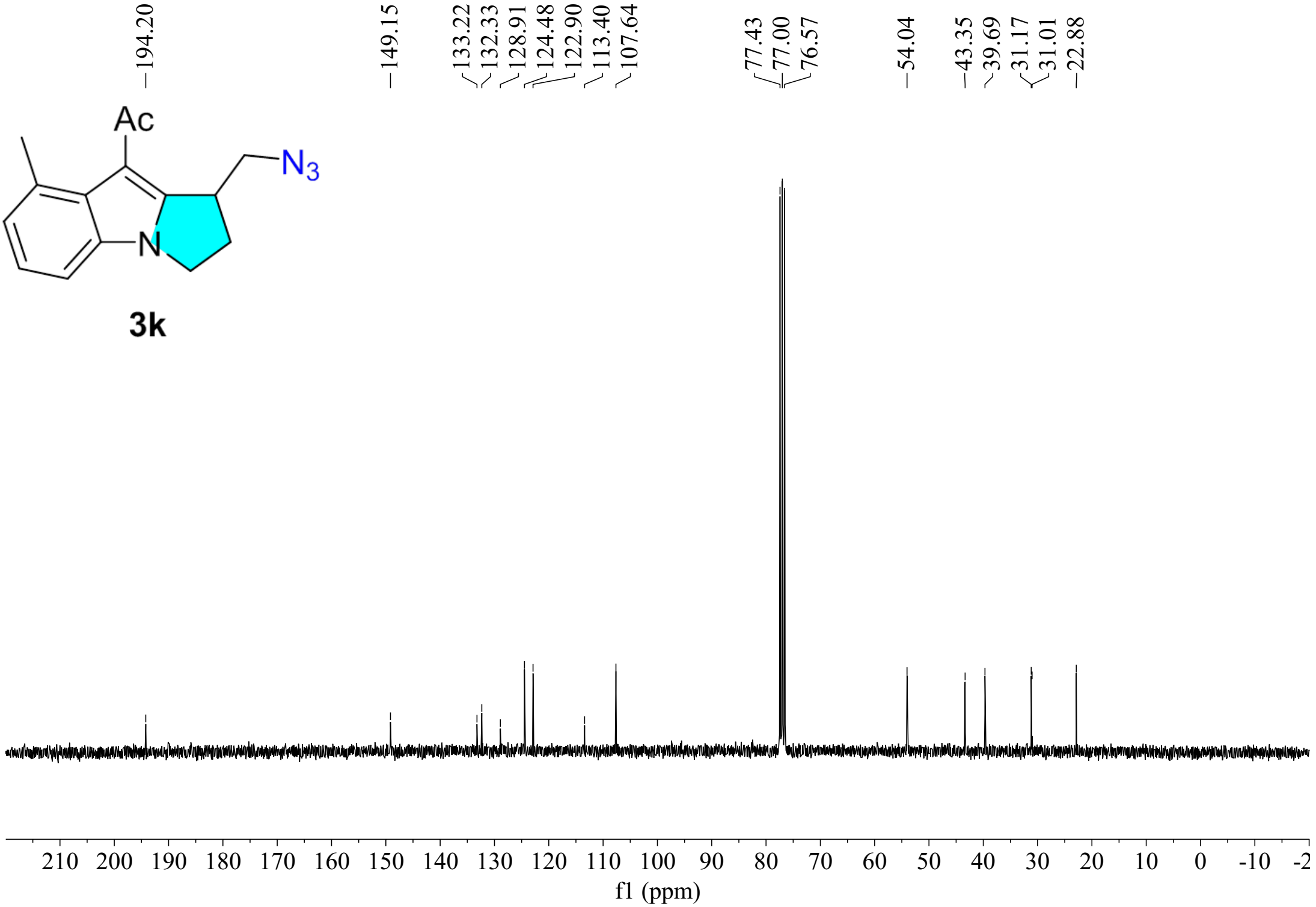
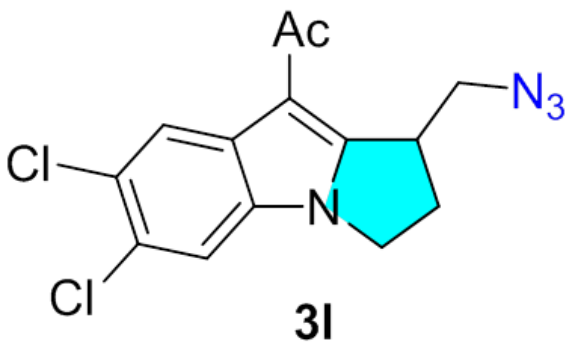
4.1518
4.1444
4.1354
4.1289
3.8247
3.8202
3.8162
3.8122
3.8058
3.8018
3.7913
3.7849
3.7791
3.7690
3.7487
3.7386
3.6267
3.6087
3.5968
3.5785
2.8669
2.8560
2.8454
2.8336
2.8116
2.6961
2.6177
2.6125
2.6077
2.5935
2.5844
2.5795
2.5746
2.5682
2.5646
2.5604
Ac
N3
N
3k
1.04
1.00
1.00
2.00
2.00
1.00
1.02
2.94
4.03
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


194.20
149.15
133.22
132.33
128.91
124.48
122.90
113.40
107.64
77.43
77.00
76.57
54.04
43.35
39.69
31.17
31.01
22.88
Ac
N3
N
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)



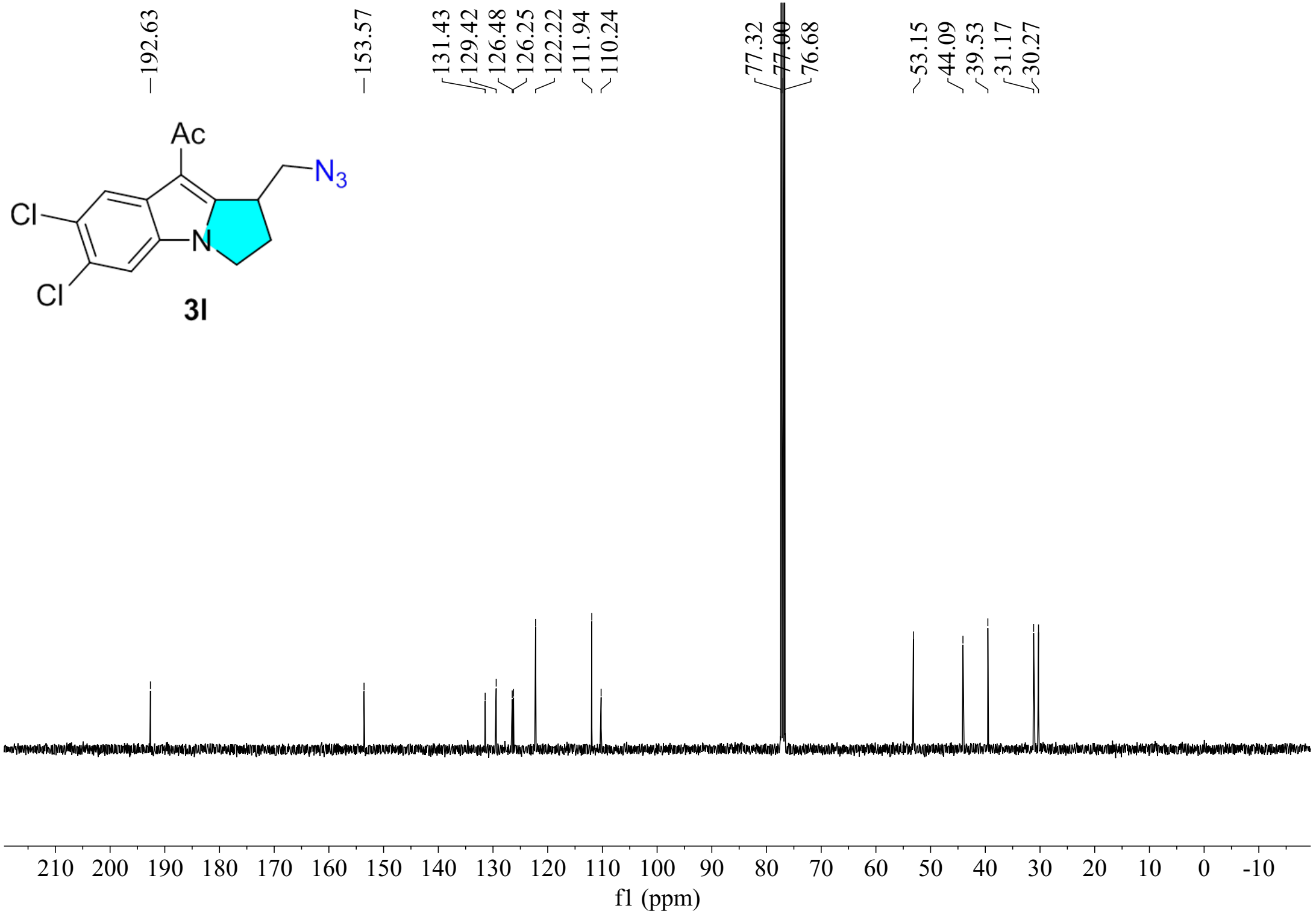
3l

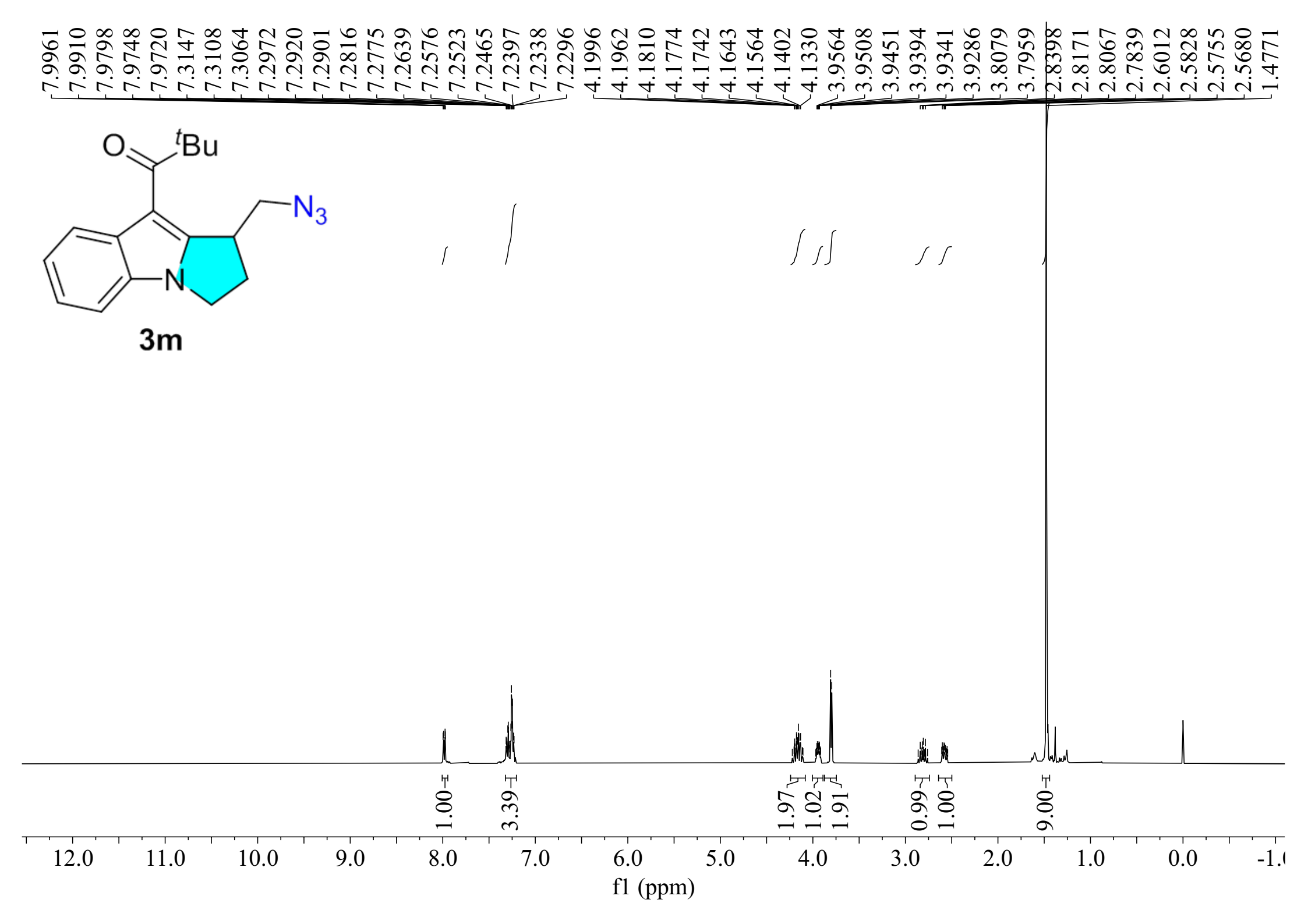
8.0126 7.3895 7.2599 4.2076 4.1872 4.1816 4.1671 4.1613 4.1409 4.1383 4.1306 4.1142 4.1067 4.0886 4.0809 3.9380 3.9242 3.9094 3.8988 3.8952 3.8891 3.8808 3.8744 3.8669 3.8596 3.8530 3.8183 3.8054 3.7988 3.7777 3.7733 3.7699 2.9226 2.9003 2.8896 2.8780 2.8668 2.8560 2.8447 2.8269 2.8222 2.6216 2.5763

1.00 1.02 2.03 3.00 1.00 4.06

12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.

f1 (ppm)


192.63
153.57
131.43
129.42
126.48
126.25
122.22
111.94
110.24
77.32
77.00
76.68
53.15
44.09
39.53
31.17
30.27
Ac
N3
Cl
Cl
N
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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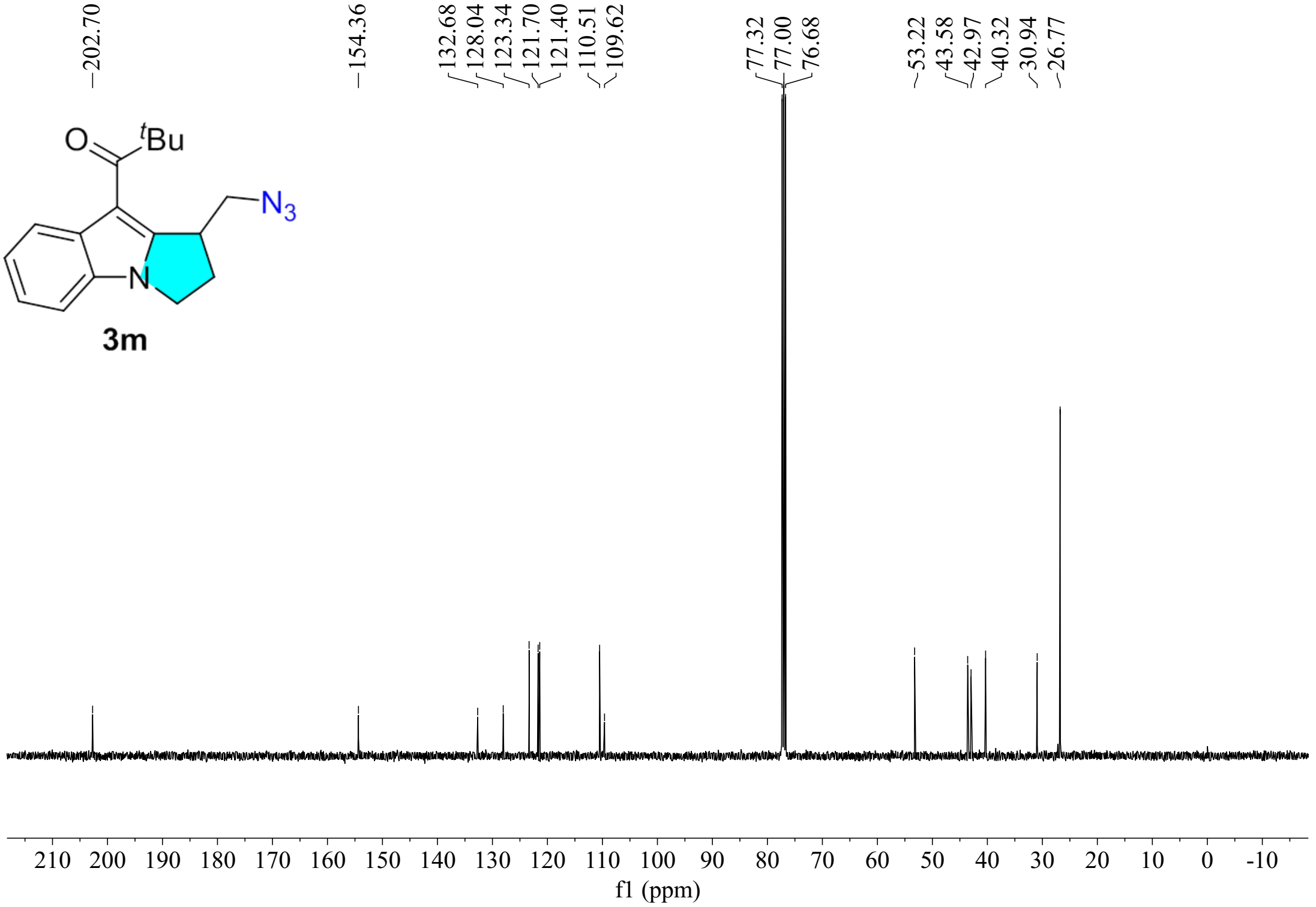
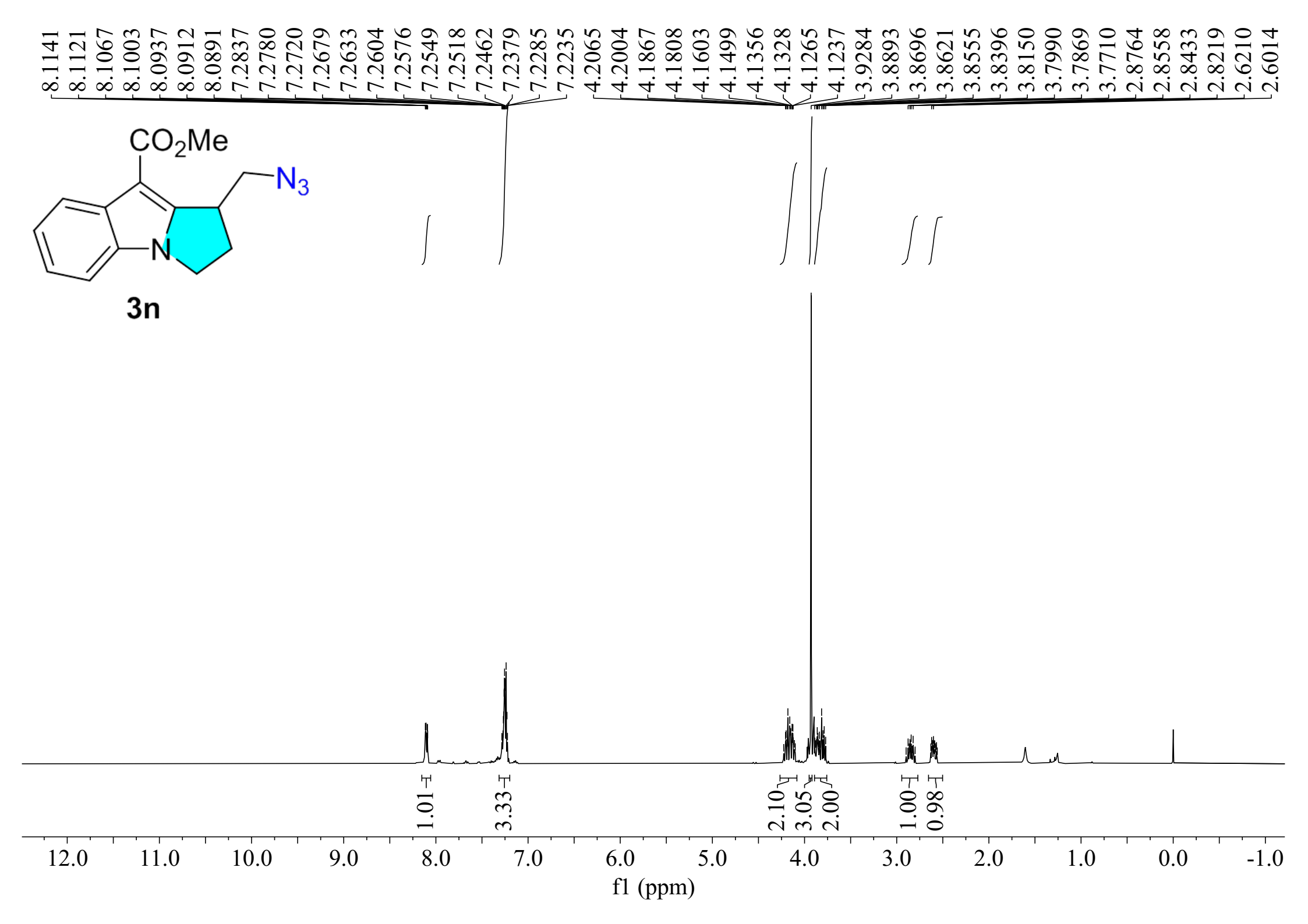
7.9910
7.9798
7.9748
7.9720
7.3147
7.3108
7.3064
7.2972
7.2920
7.2901
7.2816
7.2775
7.2639
7.2576
7.2523
7.2465
7.2397
7.2338
7.2296
4.1996
4.1962
4.1810
4.1774
4.1742
4.1643
4.1564
4.1402
4.1330
3.9564
3.9508
3.9451
3.9394
3.9341
3.9286
3.8079
3.7959
2.8398
2.8171
2.8067
2.7839
2.6012
2.5828
2.5755
2.5680
1.4771
O
tBu
N3
N
3m
1.00
3.39
1.97
1.02
1.91
0.99
1.00
9.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


202.70
154.36
132.68
128.04
123.34
121.70
121.40
110.51
109.62
77.32
77.00
76.68
53.22
43.58
42.97
40.32
30.94
26.77
O
tBu
N3
N
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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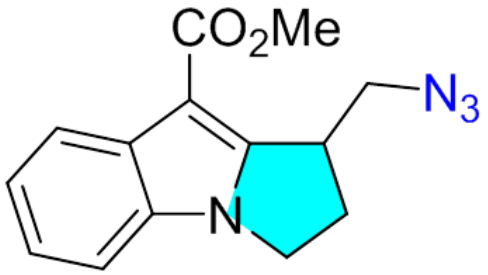
8.1121
8.1067
8.1003
8.0937
8.0912
8.0891
7.2837
7.2780
7.2720
7.2679
7.2633
7.2604
7.2576
7.2549
7.2518
7.2462
7.2379
7.2285
7.2235
4.2065
4.2004
4.1867
4.1808
4.1603
4.1499
4.1356
4.1328
4.1265
4.1237
3.9284
3.8893
3.8696
3.8621
3.8555
3.8396
3.8150
3.7990
3.7869
3.7710
2.8764
2.8558
2.8433
2.8219
2.6210
2.6014
CO2Me
N3
N
3n
1.01
3.33
2.10
3.05
2.00
1.00
0.98
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

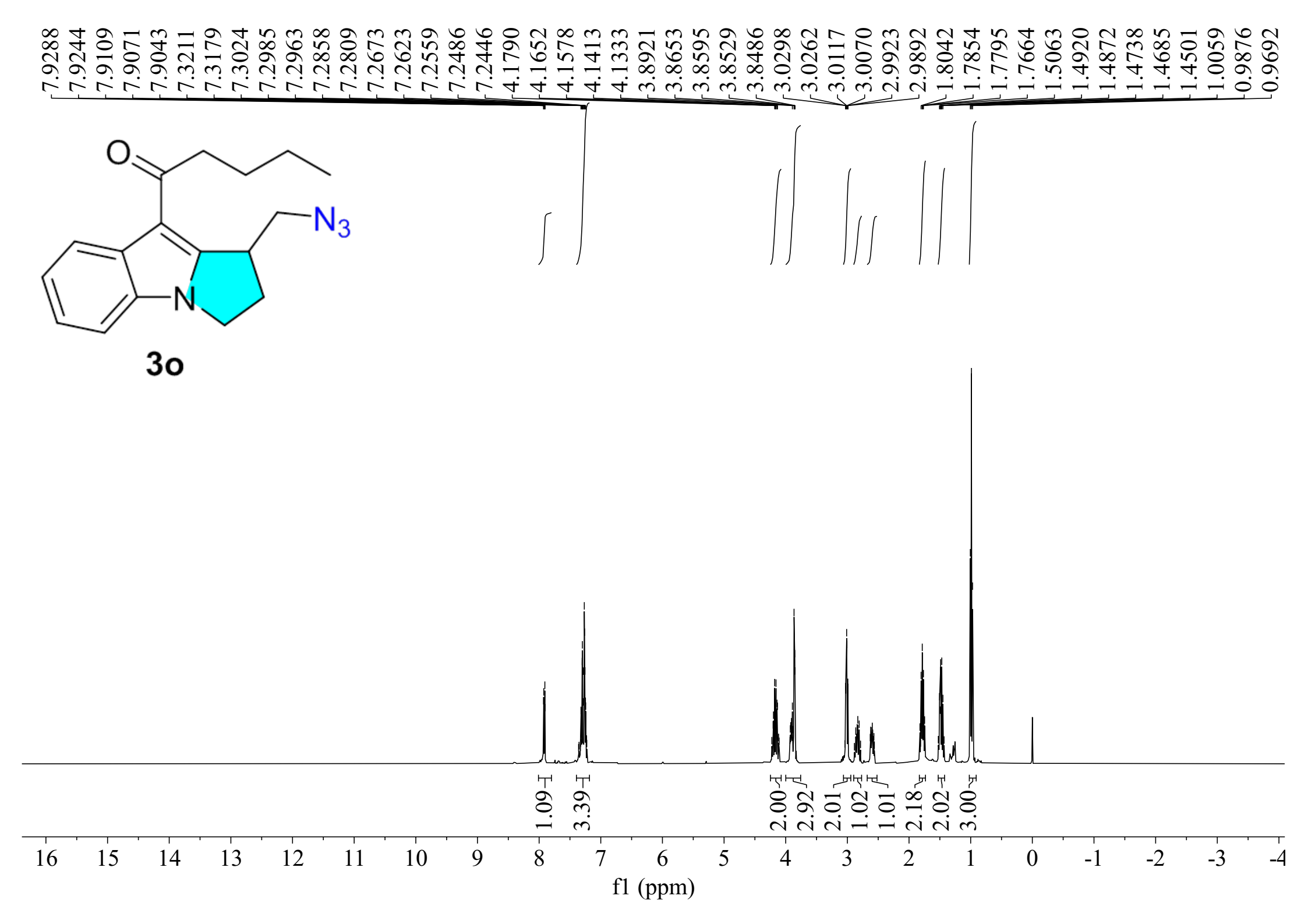


3n

165.60
151.35
132.51
130.59
122.29
121.92
121.80
110.05
99.92
77.32
77.00
76.68
53.39
50.89
43.79
38.96
31.13

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)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7.3179
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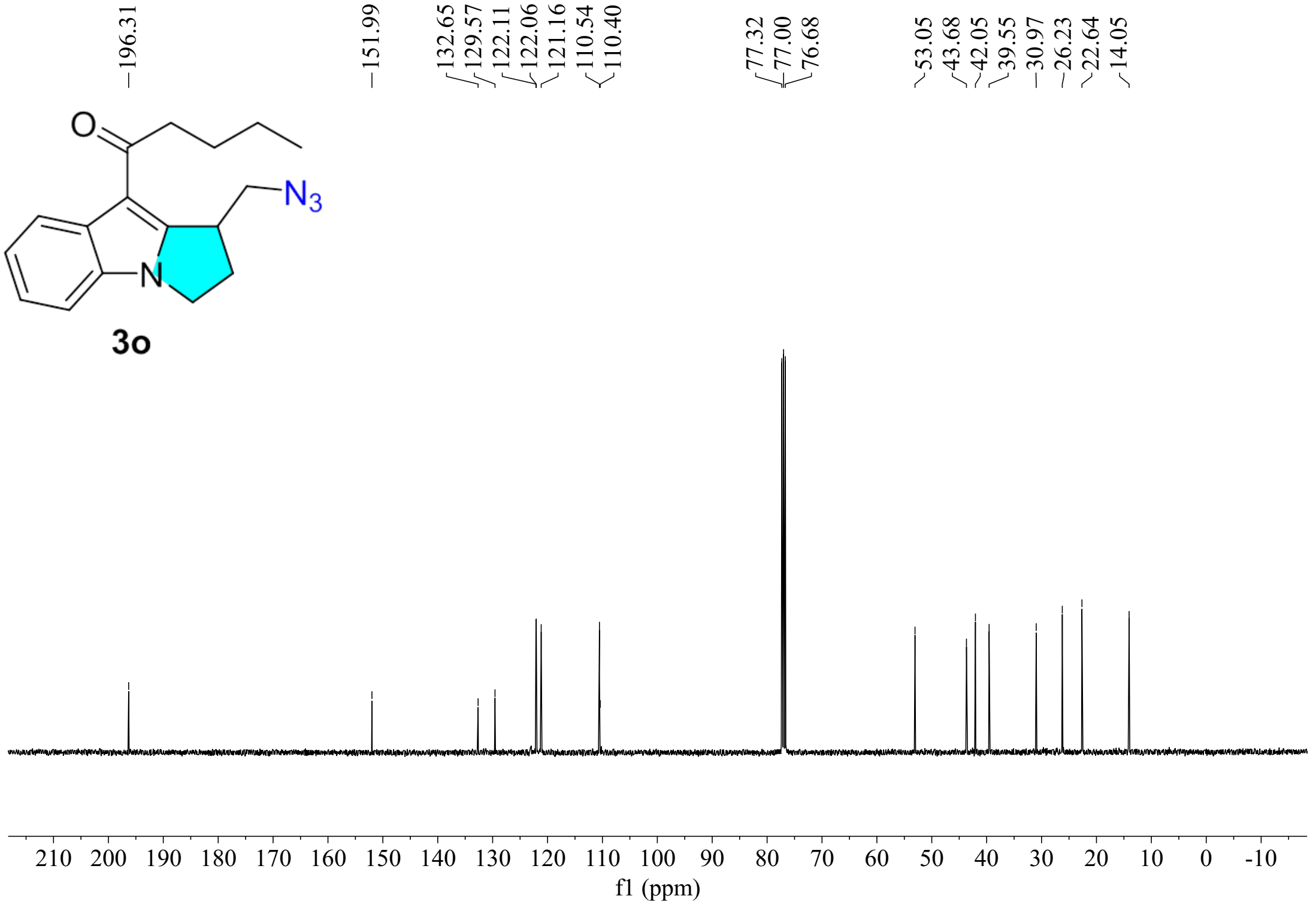
7.2985
7.2963
7.2858
7.2809
7.2673
7.2623
7.2559
7.2486
7.2446
4.1790
4.1652
4.1578
4.1413
4.1333
3.8921
3.8653
3.8595
3.8529
3.8486
3.0298
3.0262
3.0117
3.0070
2.9923
2.9892
1.8042
1.7854
1.7795
1.7664
1.5063
1.4920
1.4872
1.4738
1.4685
1.4501
1.0059
0.9876
0.9692
O
N3
N
3o
1.09
3.39
2.00
2.92
2.01
1.02
1.01
2.18
2.02
3.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)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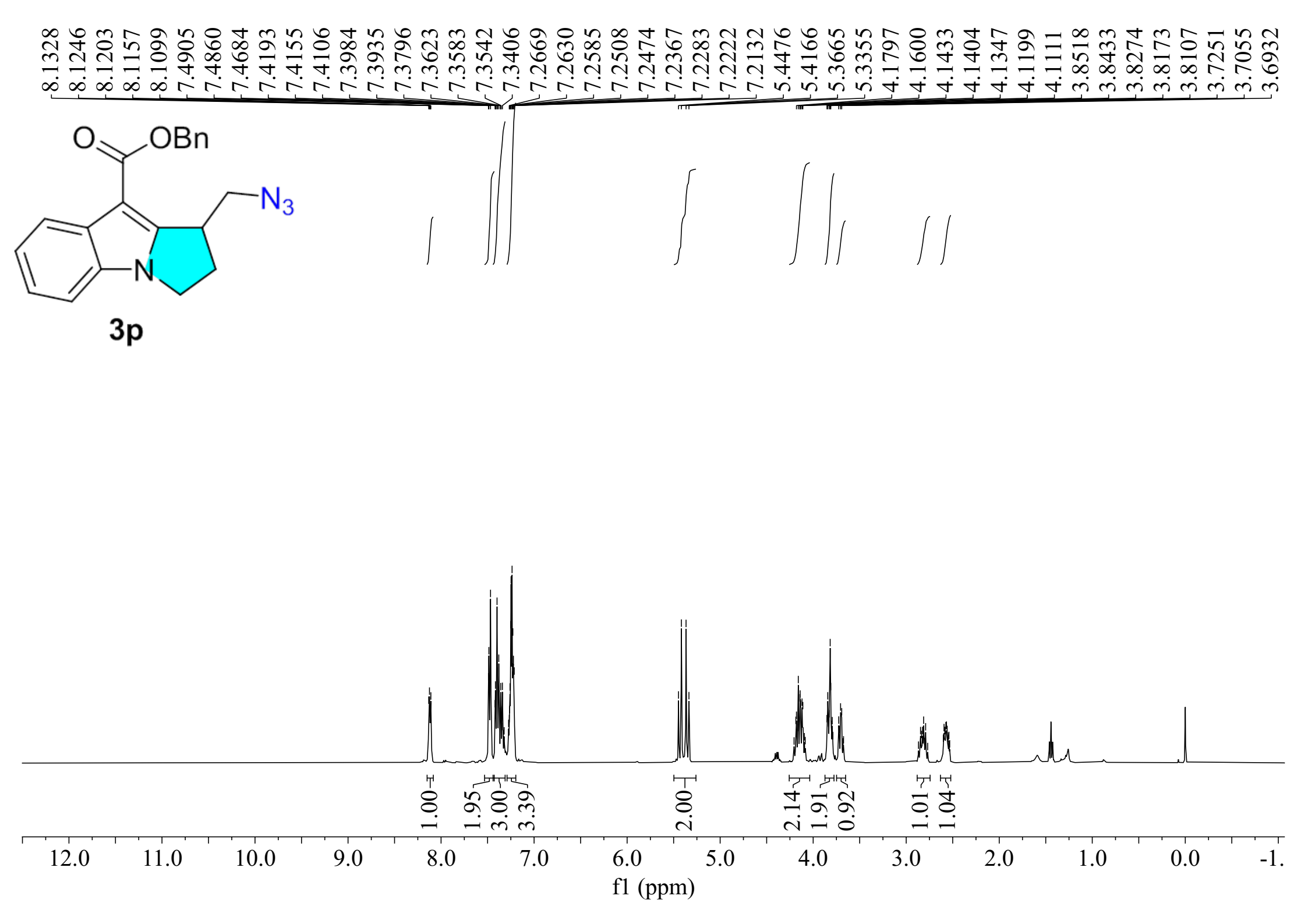
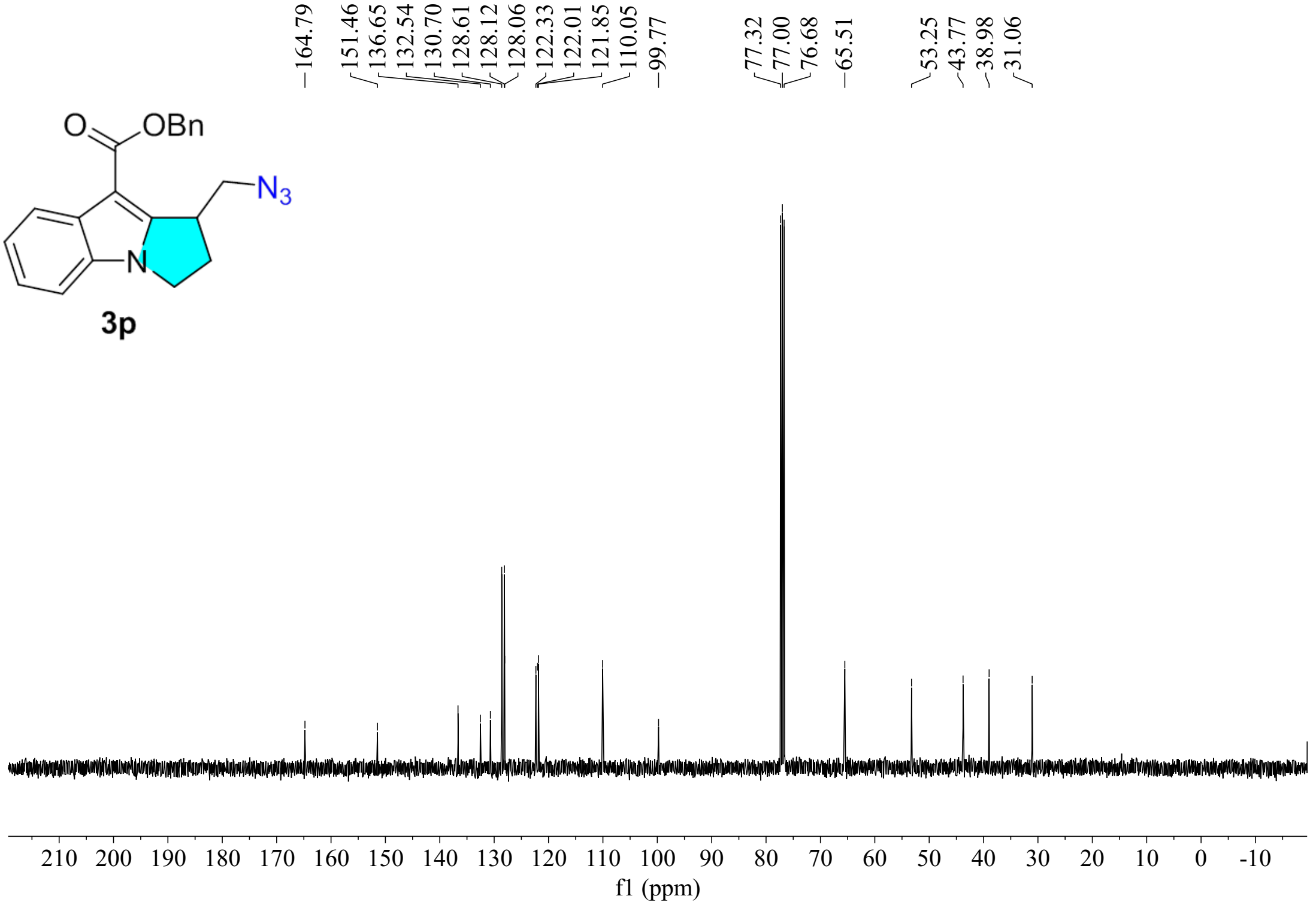
122.06
121.16
110.54
110.40
77.32
77.00
76.68
53.05
43.68
42.05
39.55
30.97
26.23
22.64
14.05
O
N3
N
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.1328
8.1246
8.1203
8.1157
8.1099
7.4905
7.4860
7.4684
7.4193
7.4155
7.4106
7.3984
7.3935
7.3796
7.3623
7.3583
7.3542
7.3406
7.2669
7.2630
7.2585
7.2508
7.2474
7.2367
7.2283
7.2222
7.2132
5.4476
5.4166
5.3665
5.3355
4.1797
4.1600
4.1433
4.1404
4.1347
4.1199
4.1111
3.8518
3.8433
3.8274
3.8173
3.8107
3.7251
3.7055
3.6932
O
OBn
N3
N
3p
1.00
1.95
3.00
3.39
2.00
2.14
1.91
0.92
1.01
1.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.
f1 (ppm)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130.70
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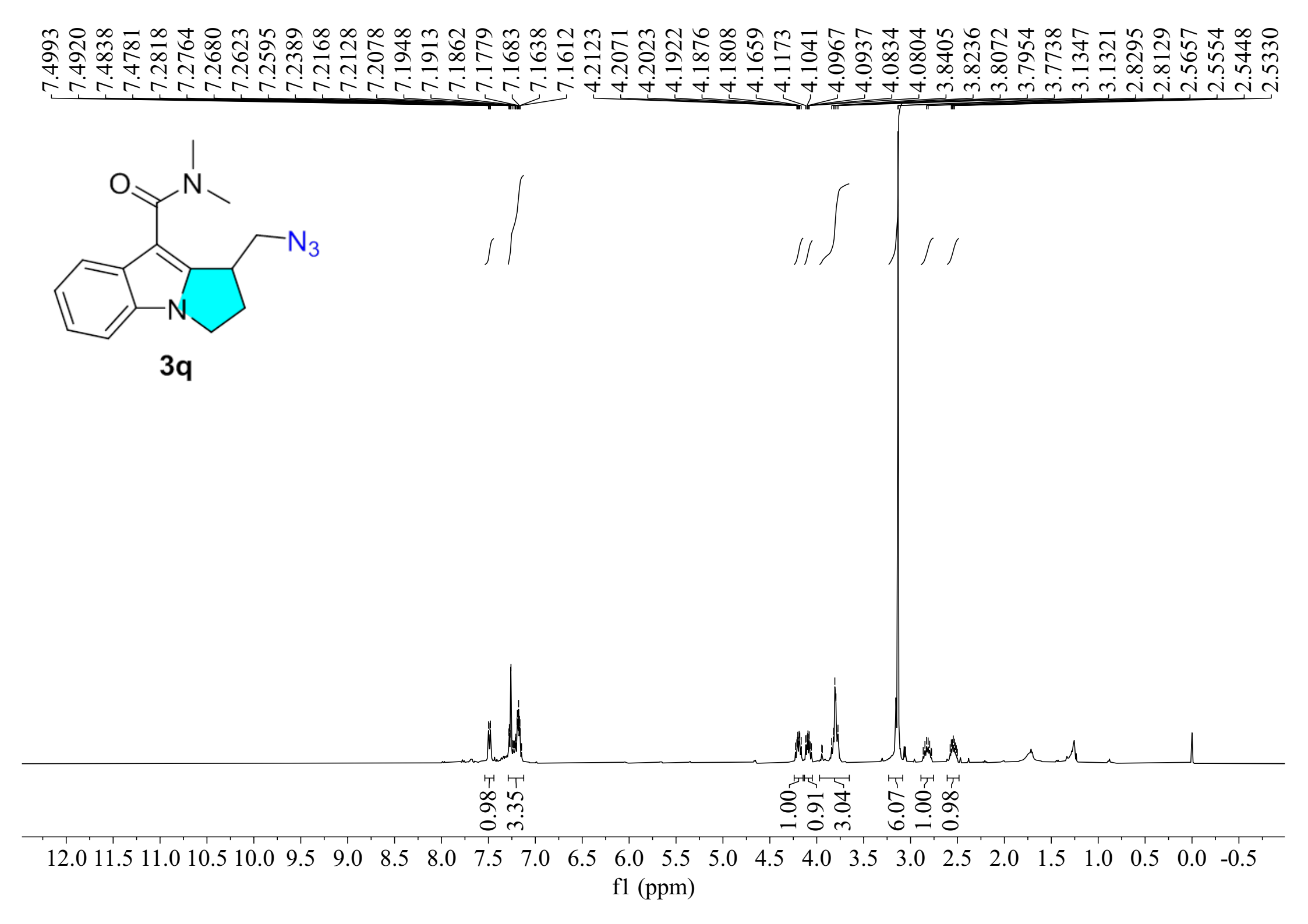
128.12
128.06
122.33
122.01
121.85
110.05
99.77
77.32
77.00
76.68
65.51
53.25
43.77
38.98
31.06
O
OBn
N3
N
3p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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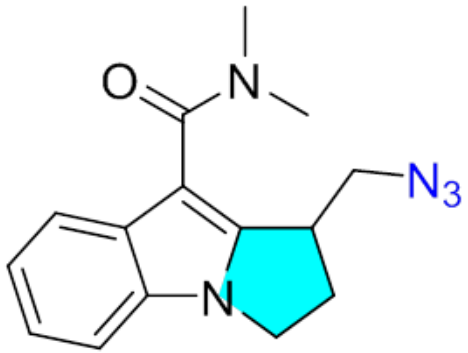
7.2168
7.2128
7.2078
7.1948
7.1913
7.1862
7.1779
7.1683
7.1638
7.1612
4.2123
4.2071
4.2023
4.1922
4.1876
4.1808
4.1659
4.1173
4.1041
4.0967
4.0937
4.0834
4.0804
3.8405
3.8236
3.8072
3.7954
3.7738
3.1347
3.1321
2.8295
2.8129
2.5657
2.5554
2.5448
2.5330
O
N
N3
N
3q
0.98
3.35
1.00
0.91
3.04
6.07
1.00
0.98
12.0 11.5 11.0 10.5 10.0 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 0.0 -0.5
f1 (ppm)

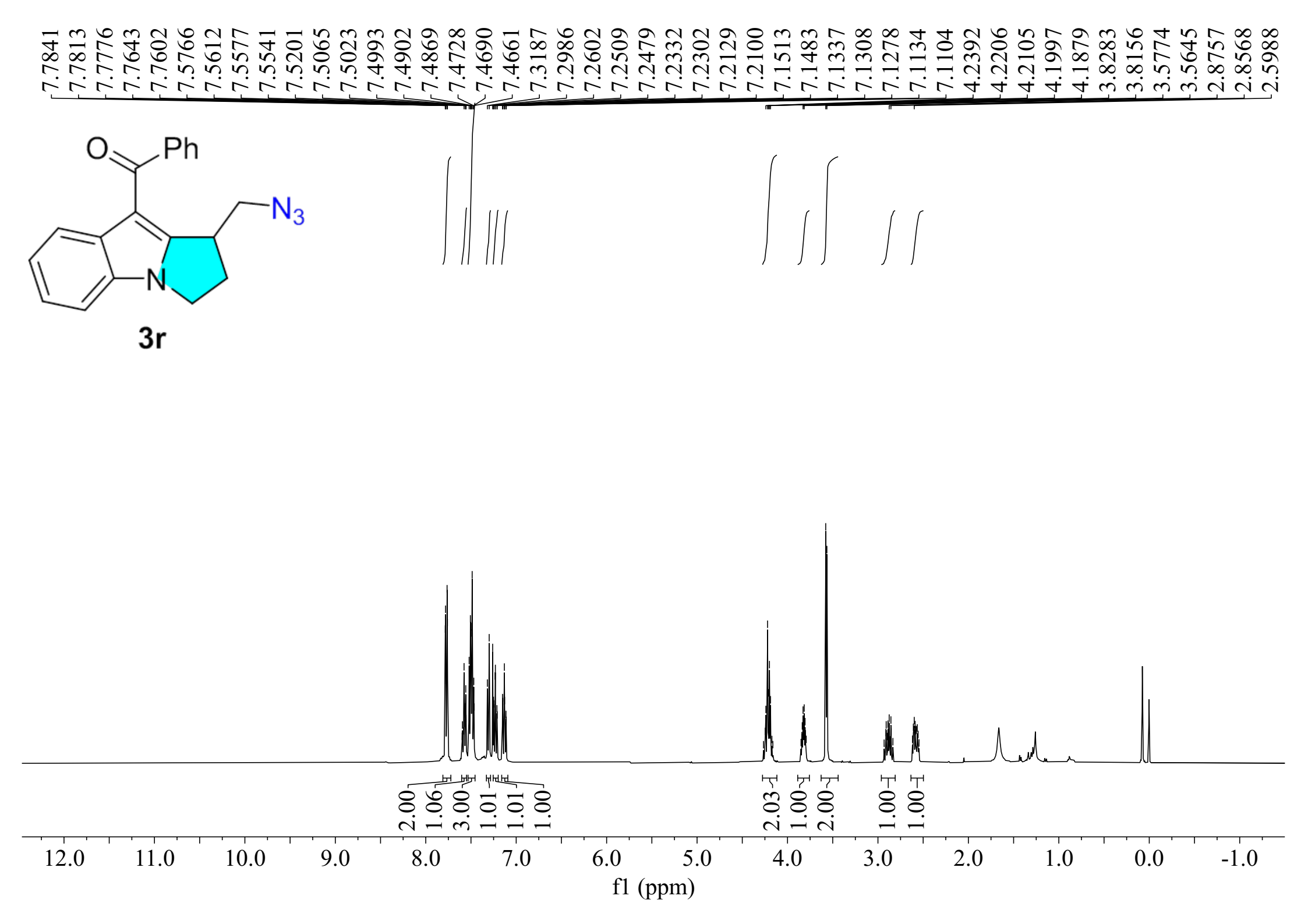


3q

168.04
147.09
131.86
129.72
121.45
120.67
120.65
110.09
103.85
77.32
77.00
76.68
53.61
43.39
38.24
31.59

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)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7.7602
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7.5612
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7.5541
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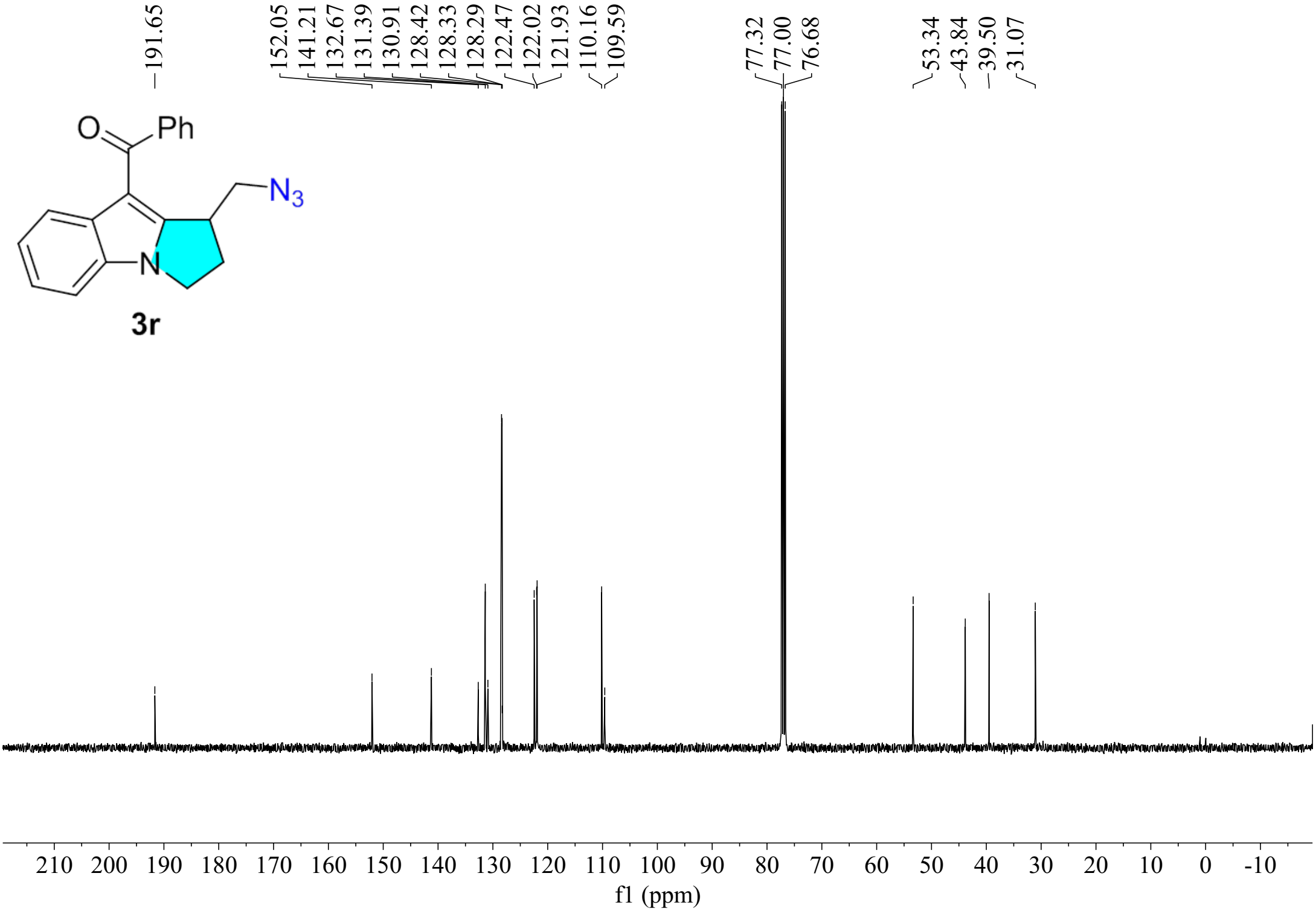
7.5065
7.5023
7.4993
7.4902
7.4869
7.4728
7.4690
7.4661
7.3187
7.2986
7.2602
7.2509
7.2479
7.2332
7.2302
7.2129
7.2100
7.1513
7.1483
7.1337
7.1308
7.1278
7.1134
7.1104
4.2392
4.2206
4.2105
4.1997
4.1879
3.8283
3.8156
3.5774
3.5645
2.8757
2.8568
2.5988
O
Ph
N3
N
3r
2.00
1.06
3.00
1.01
1.01
1.00
2.03
1.00
2.00
1.00
1.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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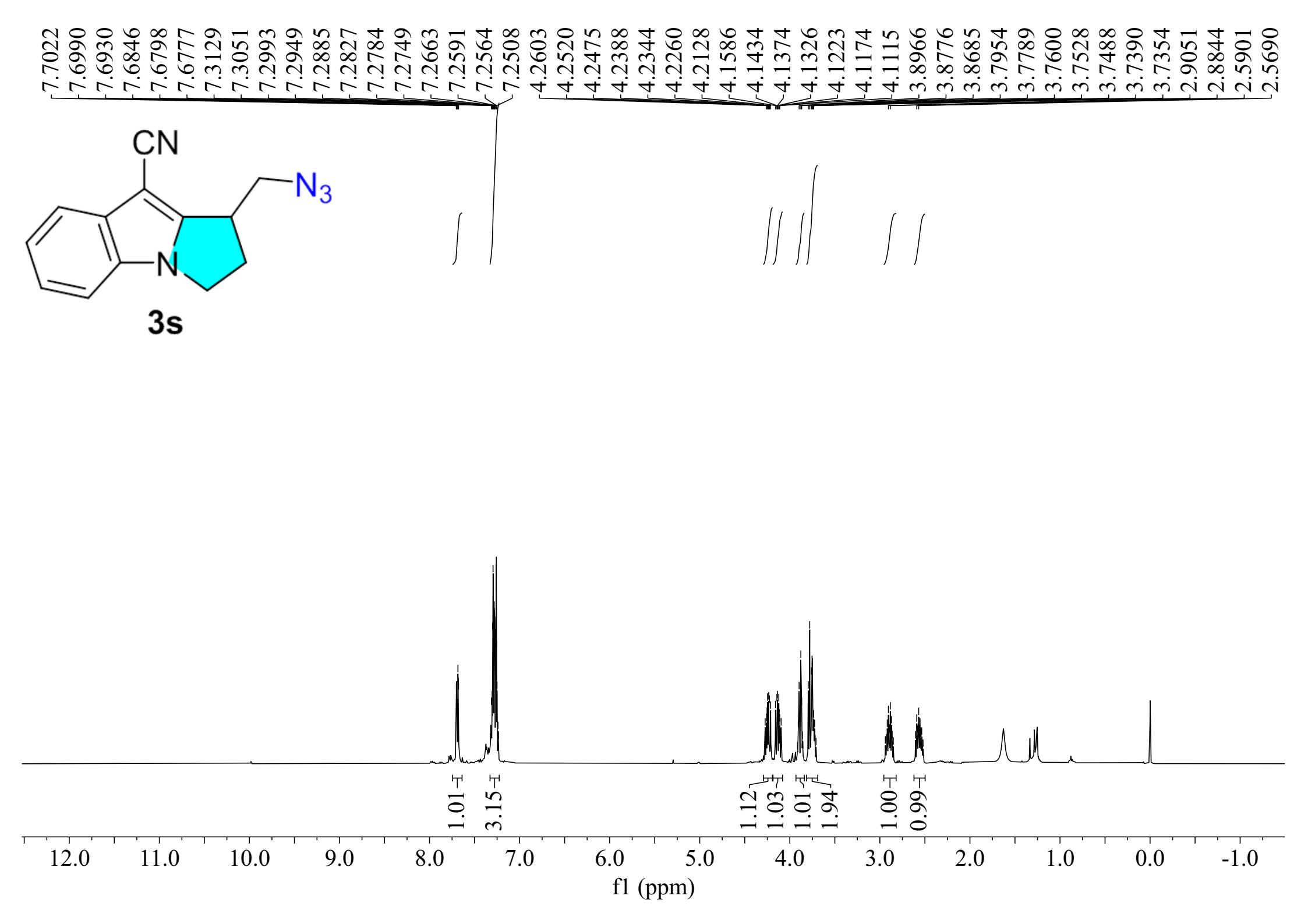
132.67
131.39
130.91
128.42
128.33
128.29
122.47
122.02
121.93
110.16
109.59
77.32
77.00
76.68
53.34
43.84
39.50
31.07
O
Ph
N3
N
3r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.2885
7.2827
7.2784
7.2749
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7.2591
7.2564
7.2508
4.2603
4.2520
4.2475
4.2388
4.2344
4.2260
4.2128
4.1586
4.1434
4.1374
4.1326
4.1223
4.1174
4.1115
3.8966
3.8776
3.8685
3.7954
3.7789
3.7600
3.7528
3.7488
3.7390
3.7354
2.9051
2.8844
2.5901
2.5690
CN
N3
N
3s
1.01
3.15
1.12
1.03
1.01
1.94
1.00
0.99
12.0
11.0
10.0
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5.0
4.0
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1.0
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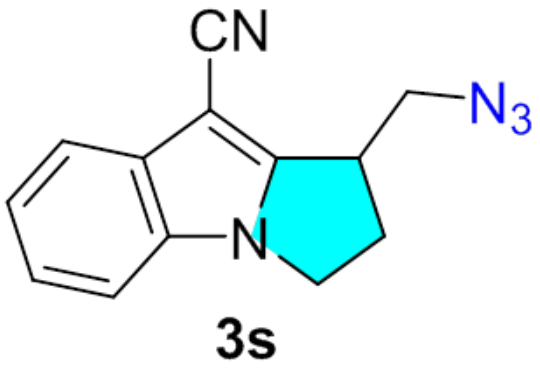
-1.0
f1 (ppm)



3s

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131.88
123.25
122.11
119.85
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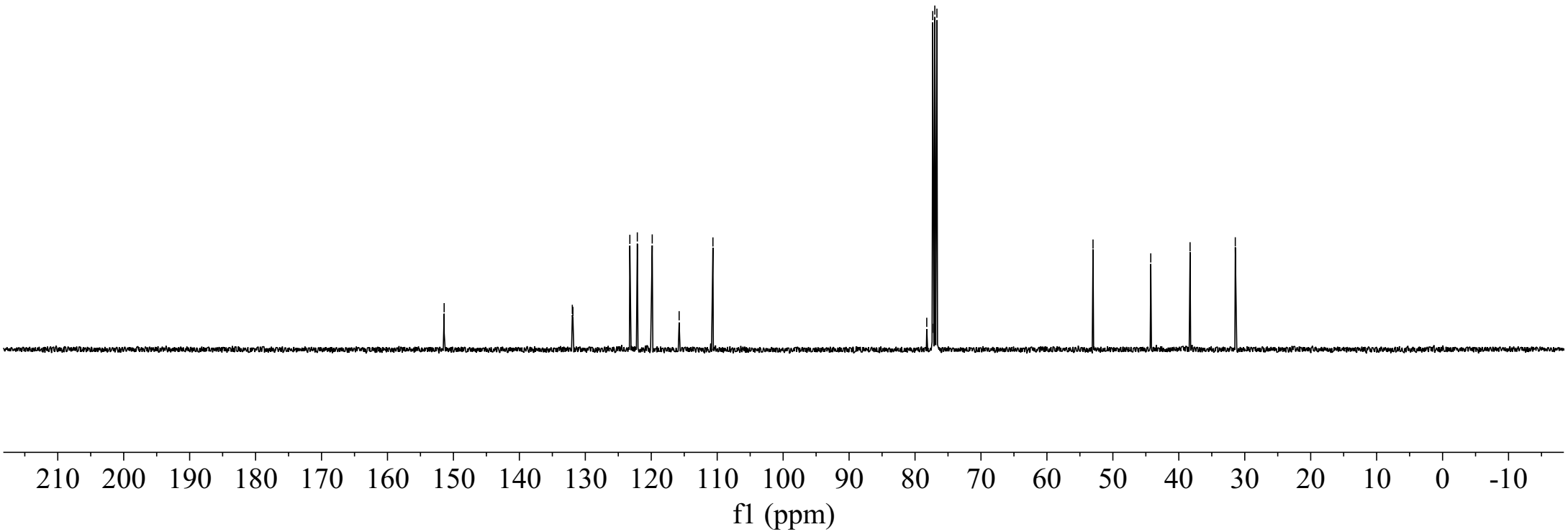
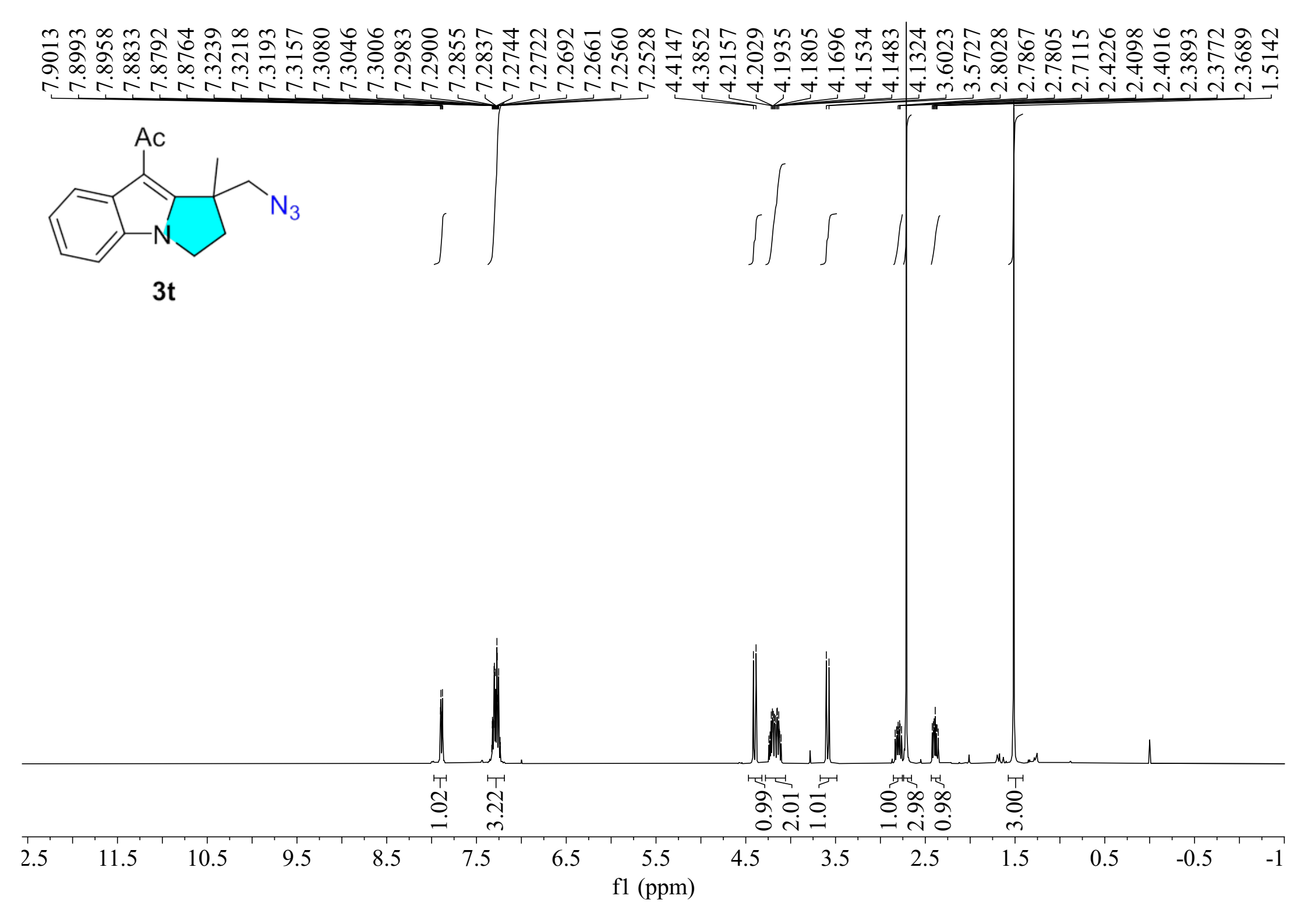
110.65
78.22
77.32
77.20
77.00
76.68
53.01
44.25
38.29
31.43

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7.3157
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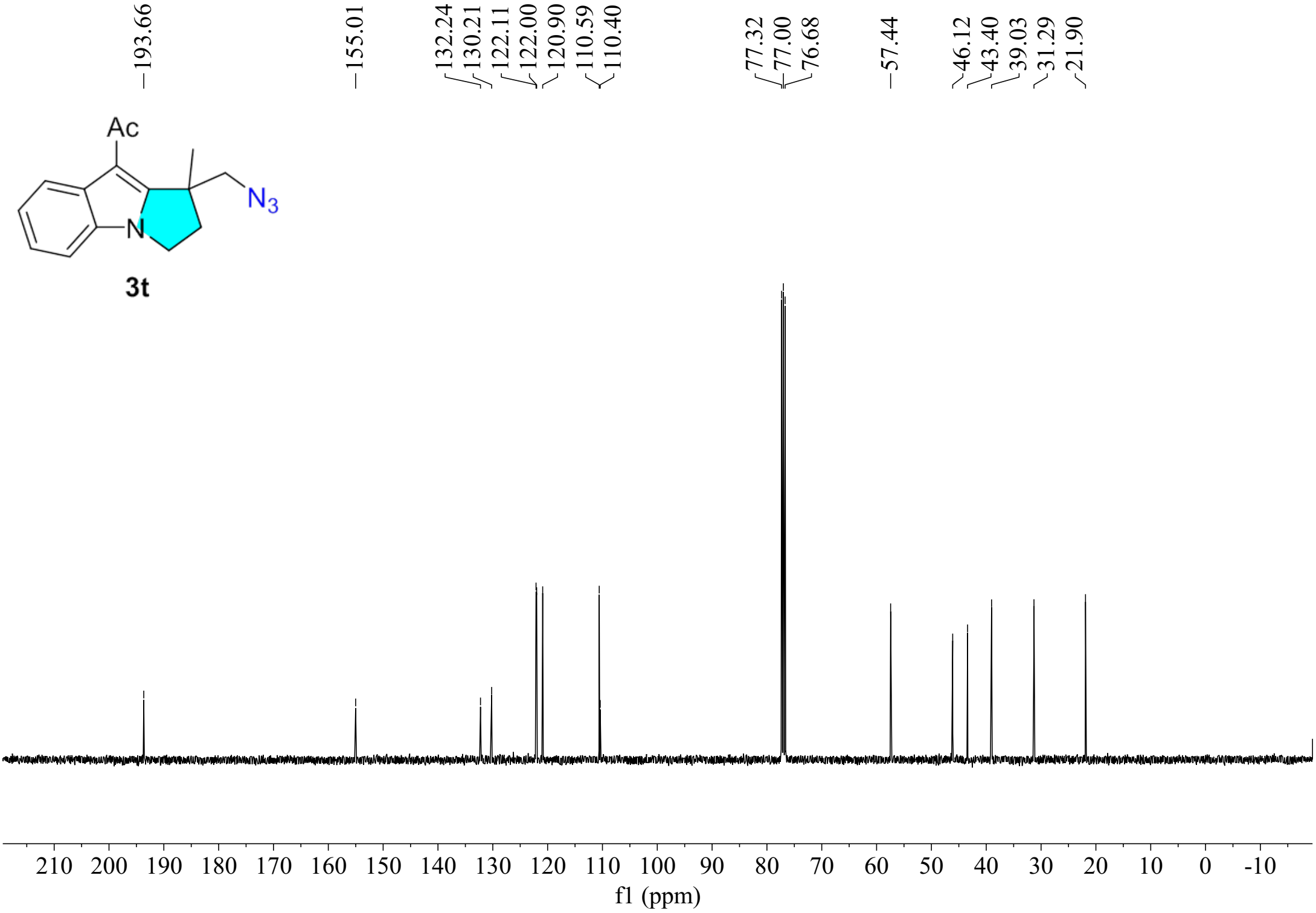
7.3046
7.3006
7.2983
7.2900
7.2855
7.2837
7.2744
7.2722
7.2692
7.2661
7.2560
7.2528
4.4147
4.3852
4.2157
4.2029
4.1935
4.1805
4.1696
4.1534
4.1483
4.1324
3.6023
3.5727
2.8028
2.7867
2.7805
2.7115
2.4226
2.4098
2.4016
2.3893
2.3772
2.3689
1.5142
Ac
N3
N
3t
1.02
3.22
0.99
2.01
1.01
1.00
2.98
0.98
3.00
2.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1
f1 (ppm)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155.01
132.24
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122.00
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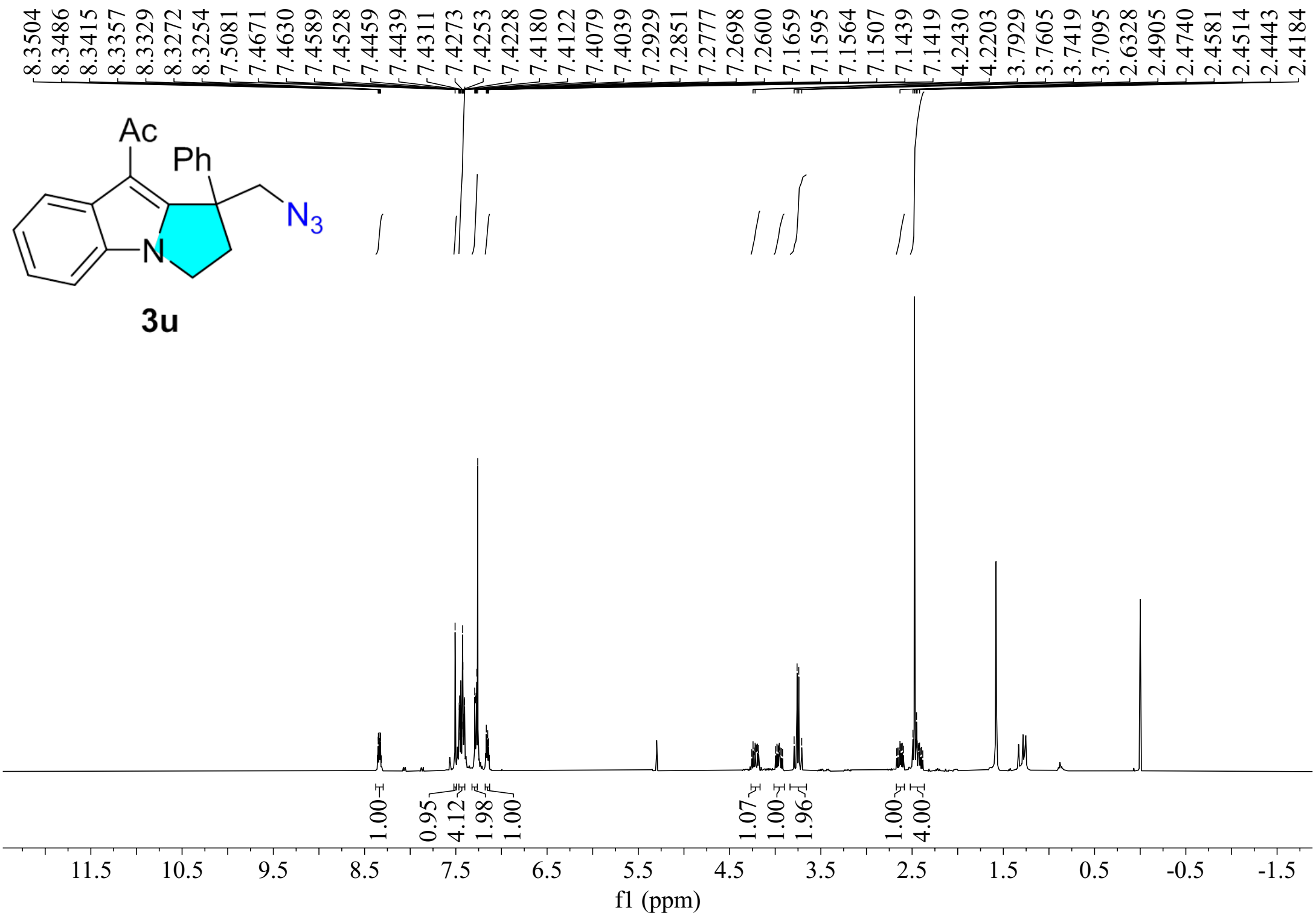
110.59
110.40
77.32
77.00
76.68
57.44
46.12
43.40
39.03
31.29
21.90
Ac
N3
N
3t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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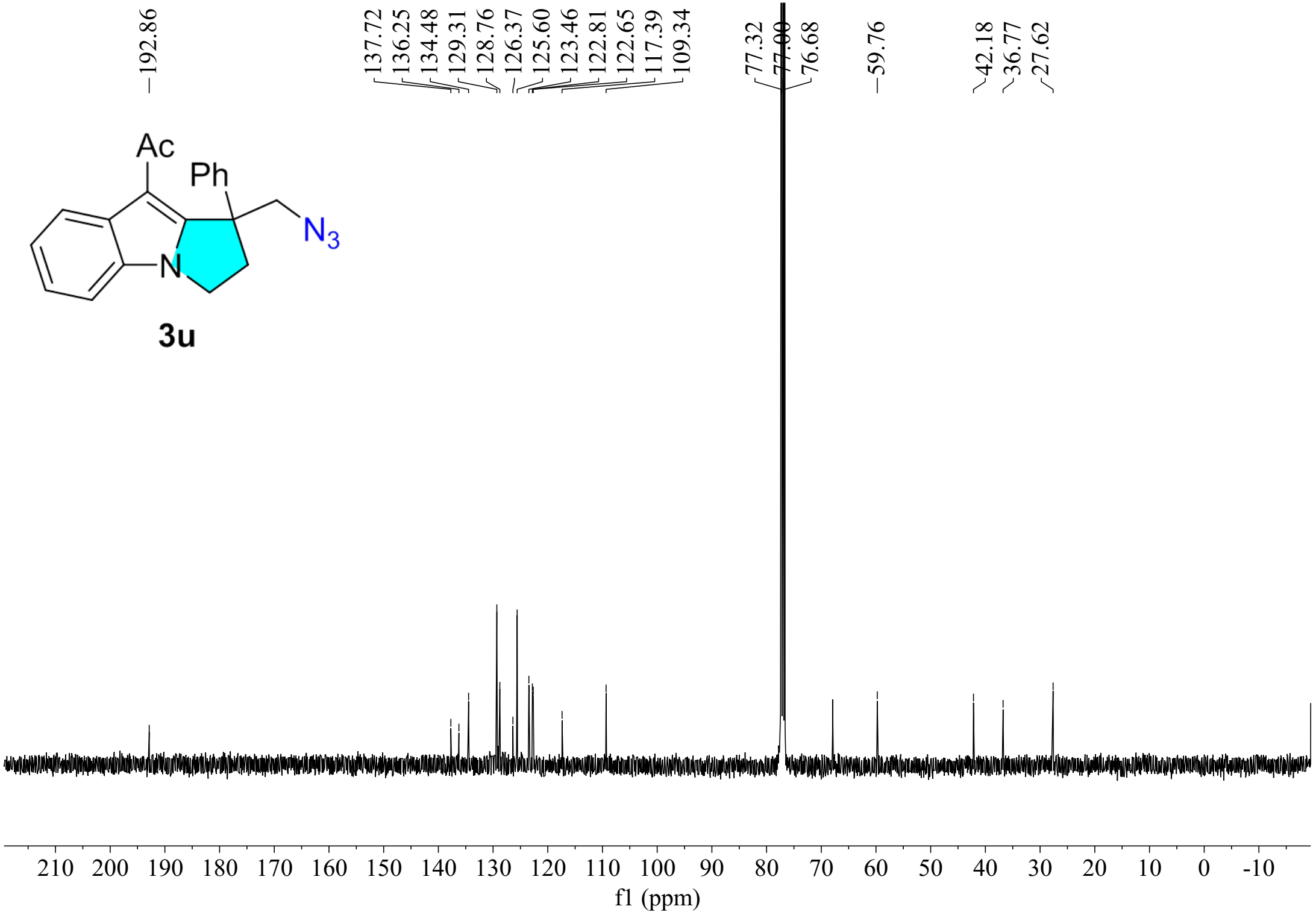
8.3272
8.3254
7.5081
7.4671
7.4630
7.4589
7.4528
7.4459
7.4439
7.4311
7.4273
7.4253
7.4228
7.4180
7.4122
7.4079
7.4039
7.2929
7.2851
7.2777
7.2698
7.2600
7.1659
7.1595
7.1564
7.1507
7.1439
7.1419
4.2430
4.2203
3.7929
3.7605
3.7419
3.7095
2.6328
2.4905
2.4740
2.4581
2.4514
2.4443
2.4184
Ac
Ph
N3
N
3u
1.00
0.95
4.12
1.98
1.00
1.07
1.00
1.96
1.00
4.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)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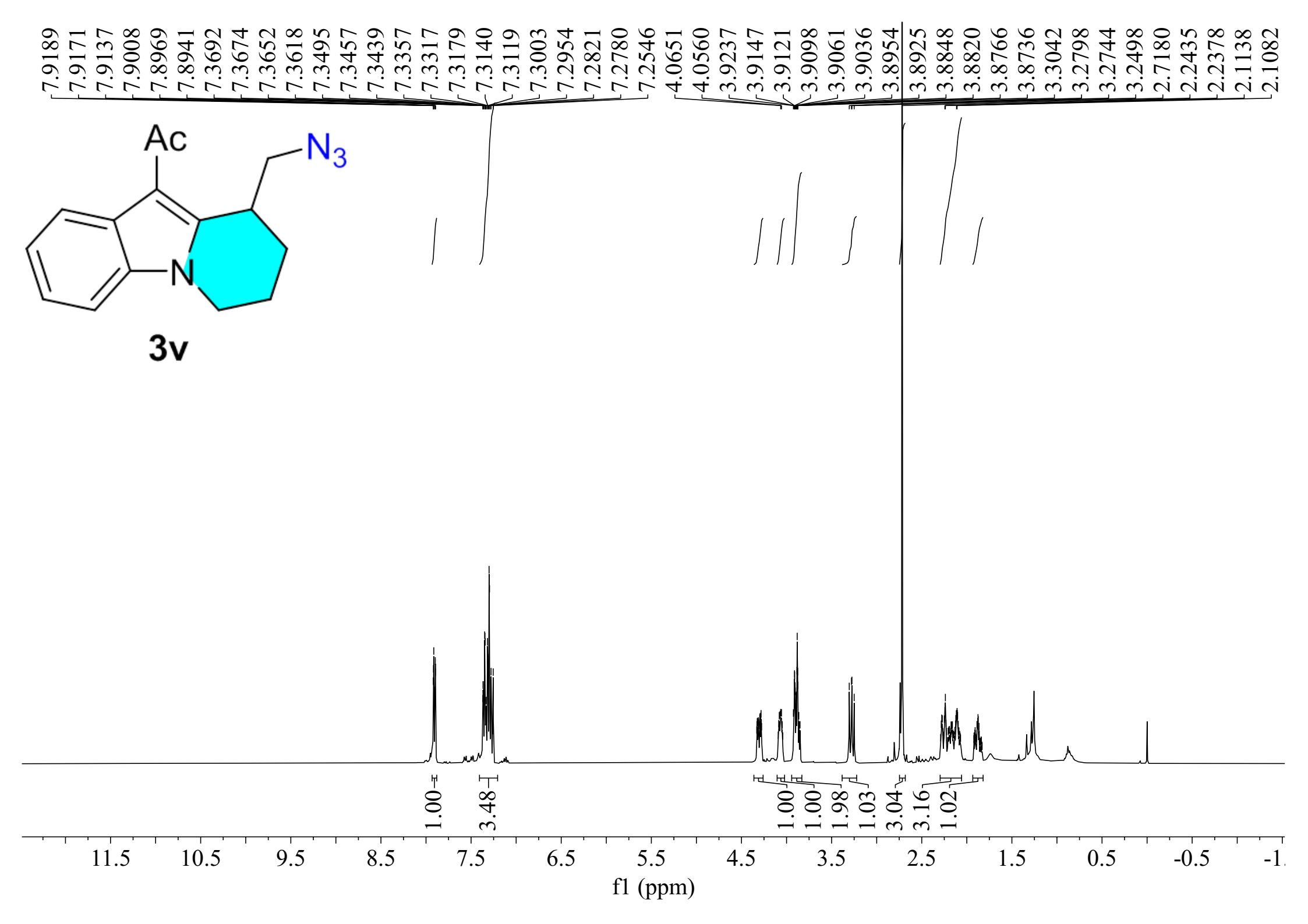
128.76
126.37
125.60
123.46
122.81
122.65
117.39
109.34
77.32
77.00
76.68
59.76
42.18
36.77
27.62
Ac
Ph
N3
N
3u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.3692
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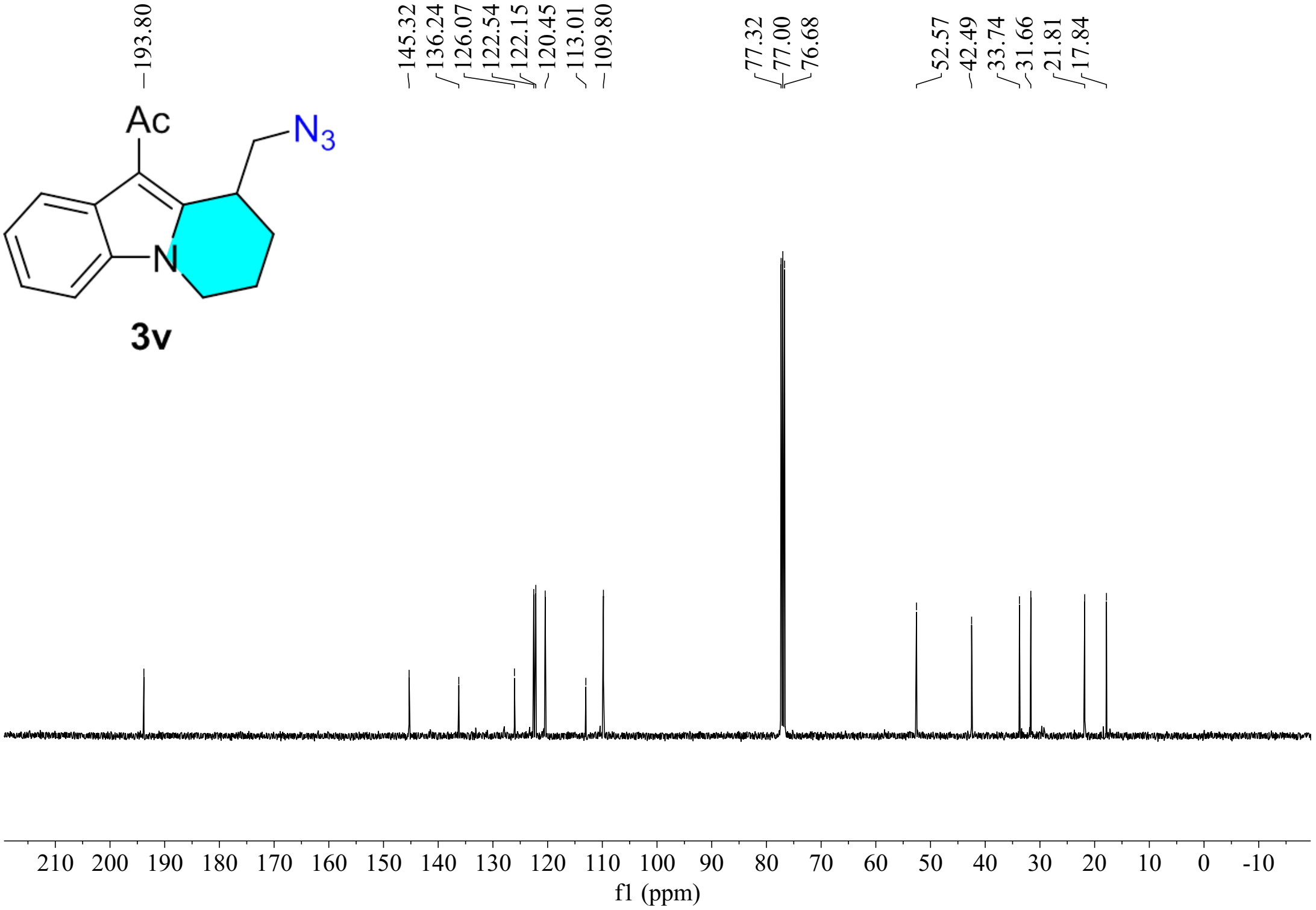
7.3652
7.3618
7.3495
7.3457
7.3439
7.3357
7.3317
7.3179
7.3140
7.3119
7.3003
7.2954
7.2821
7.2780
7.2546
4.0651
4.0560
3.9237
3.9147
3.9121
3.9098
3.9061
3.9036
3.8954
3.8925
3.8848
3.8820
3.8766
3.8736
3.3042
3.2798
3.2744
3.2498
2.7180
2.2435
2.2378
2.1138
2.1082
Ac
N3
N
3v
1.00
3.48
1.00
1.00
1.98
1.03
3.04
3.16
1.02
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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120.45
113.01
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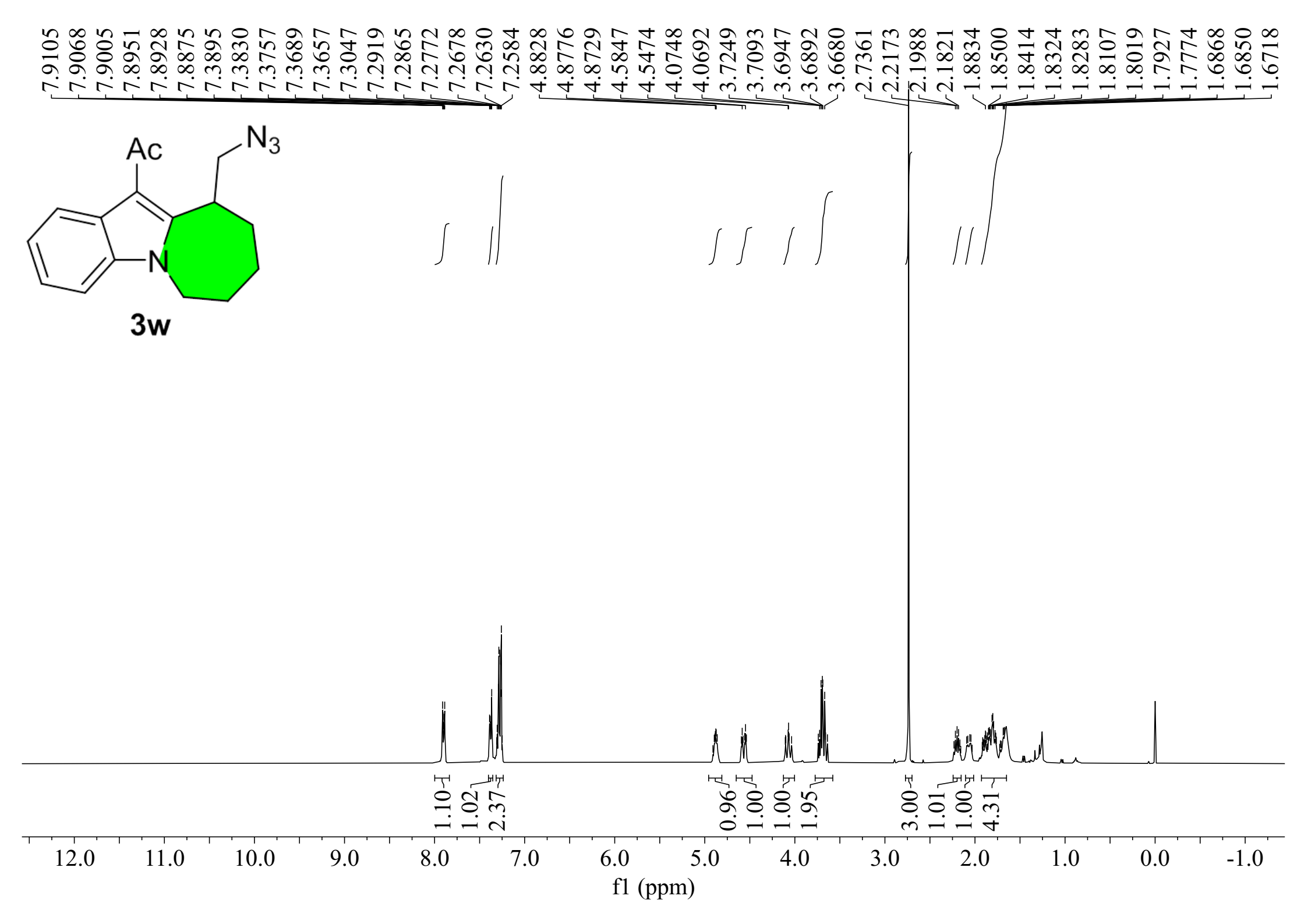
77.32
77.00
76.68
52.57
42.49
33.74
31.66
21.81
17.84
Ac
N3
N
3v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.3895
7.3830
7.3757
7.3689
7.3657
7.3047
7.2919
7.2865
7.2772
7.2678
7.2630
7.2584
4.8828
4.8776
4.8729
4.5847
4.5474
4.0748
4.0692
3.7249
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3.6947
3.6892
3.6680
2.7361
2.2173
2.1988
2.1821
1.8834
1.8500
1.8414
1.8324
1.8283
1.8107
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1.7927
1.7774
1.6868
1.6850
1.6718
Ac
N3
N
3w
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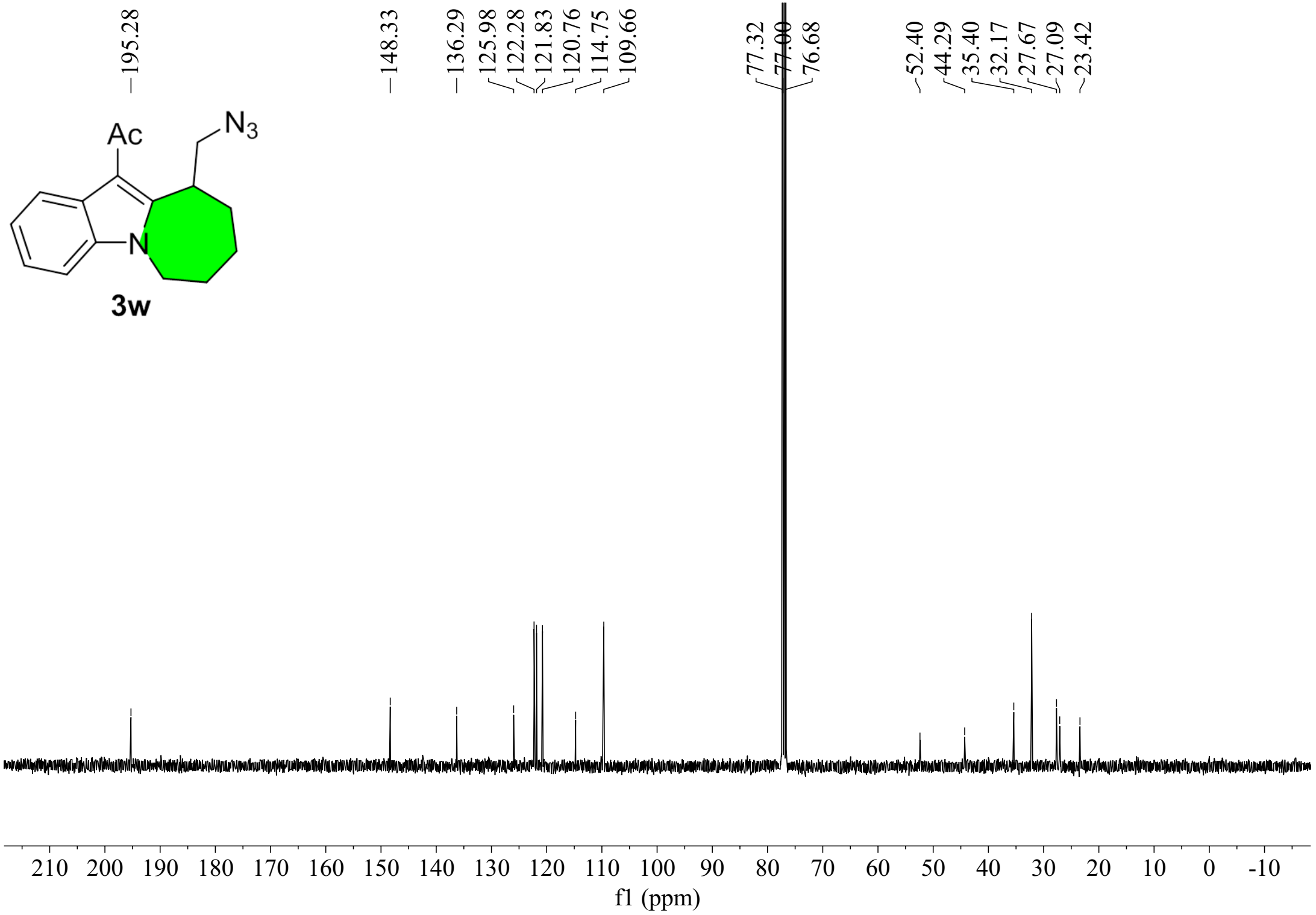
1.02
2.37
0.96
1.00
1.00
1.95
3.00
1.01
1.00
4.31
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)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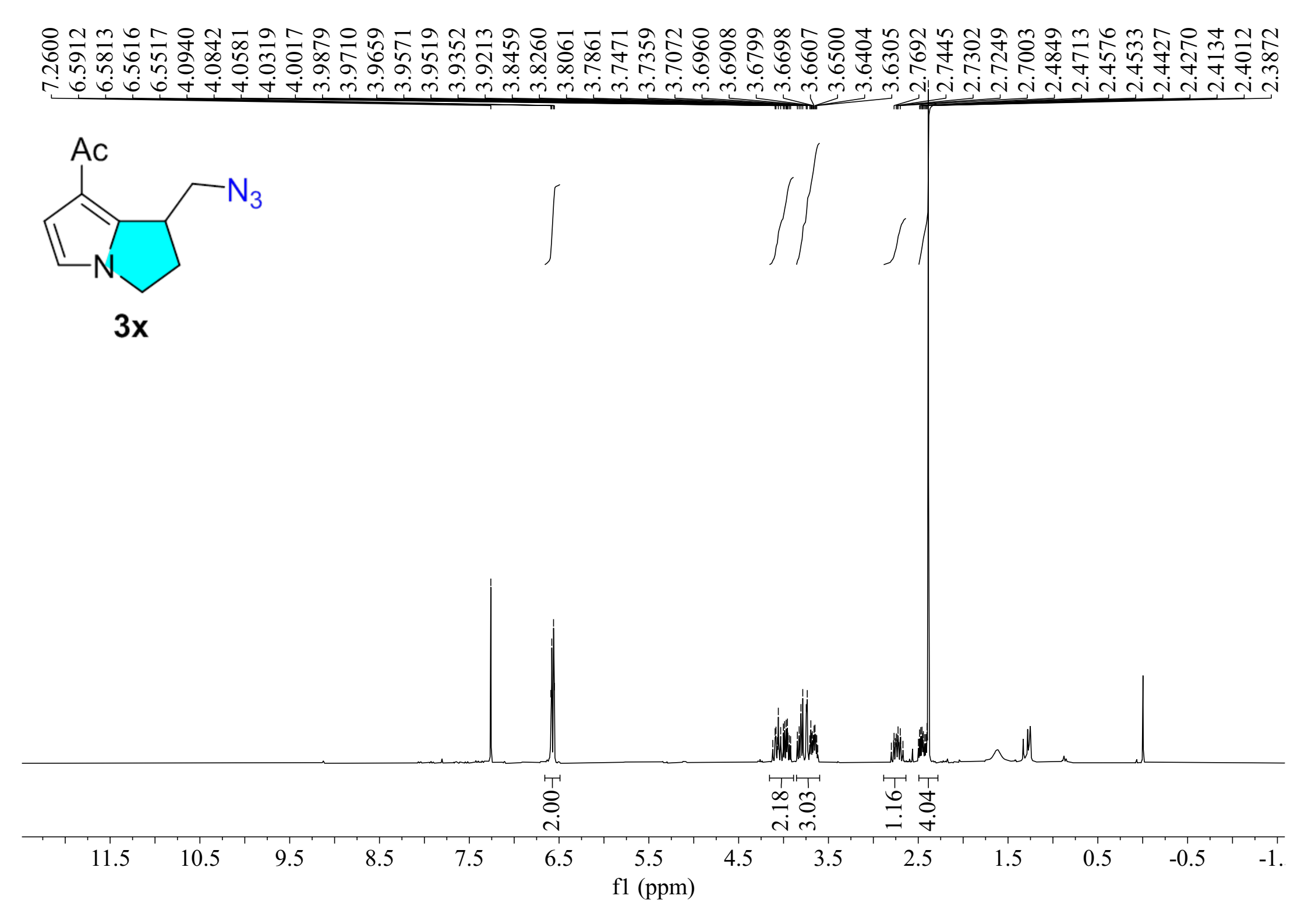
122.28
121.83
120.76
114.75
109.66
77.32
77.00
76.68
52.40
44.29
35.40
32.17
27.67
27.09
23.42
Ac
N3
N
3w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.0842
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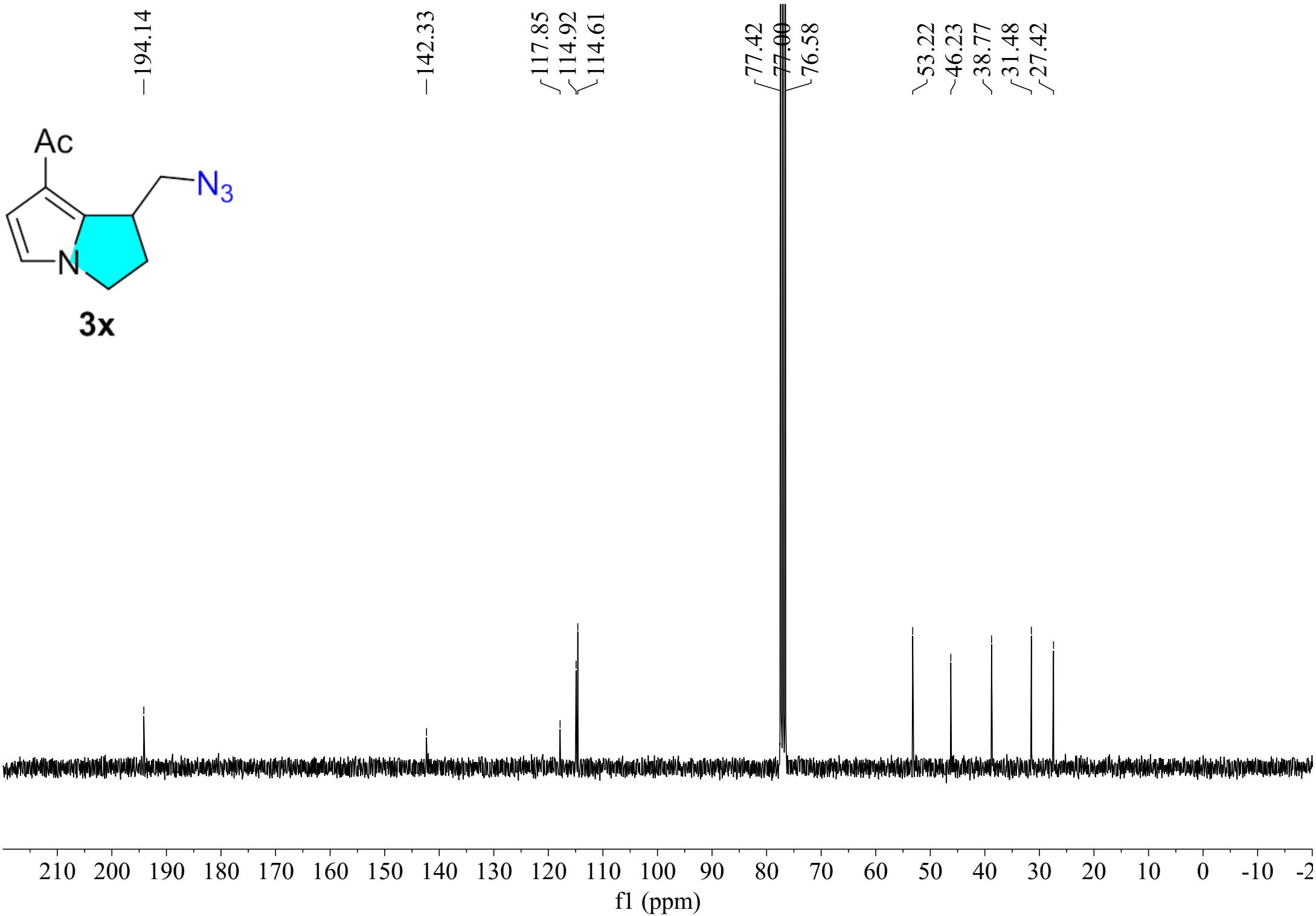
4.0319
4.0017
3.9879
3.9710
3.9659
3.9571
3.9519
3.9352
3.9213
3.8459
3.8260
3.8061
3.7861
3.7471
3.7359
3.7072
3.6960
3.6908
3.6799
3.6698
3.6607
3.6500
3.6404
3.6305
2.7692
2.7445
2.7302
2.7249
2.7003
2.4849
2.4713
2.4576
2.4533
2.4427
2.4270
2.4134
2.4012
2.3872
Ac
N3
N
3x
2.00
2.18
3.03
1.16
4.04
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.
f1 (ppm)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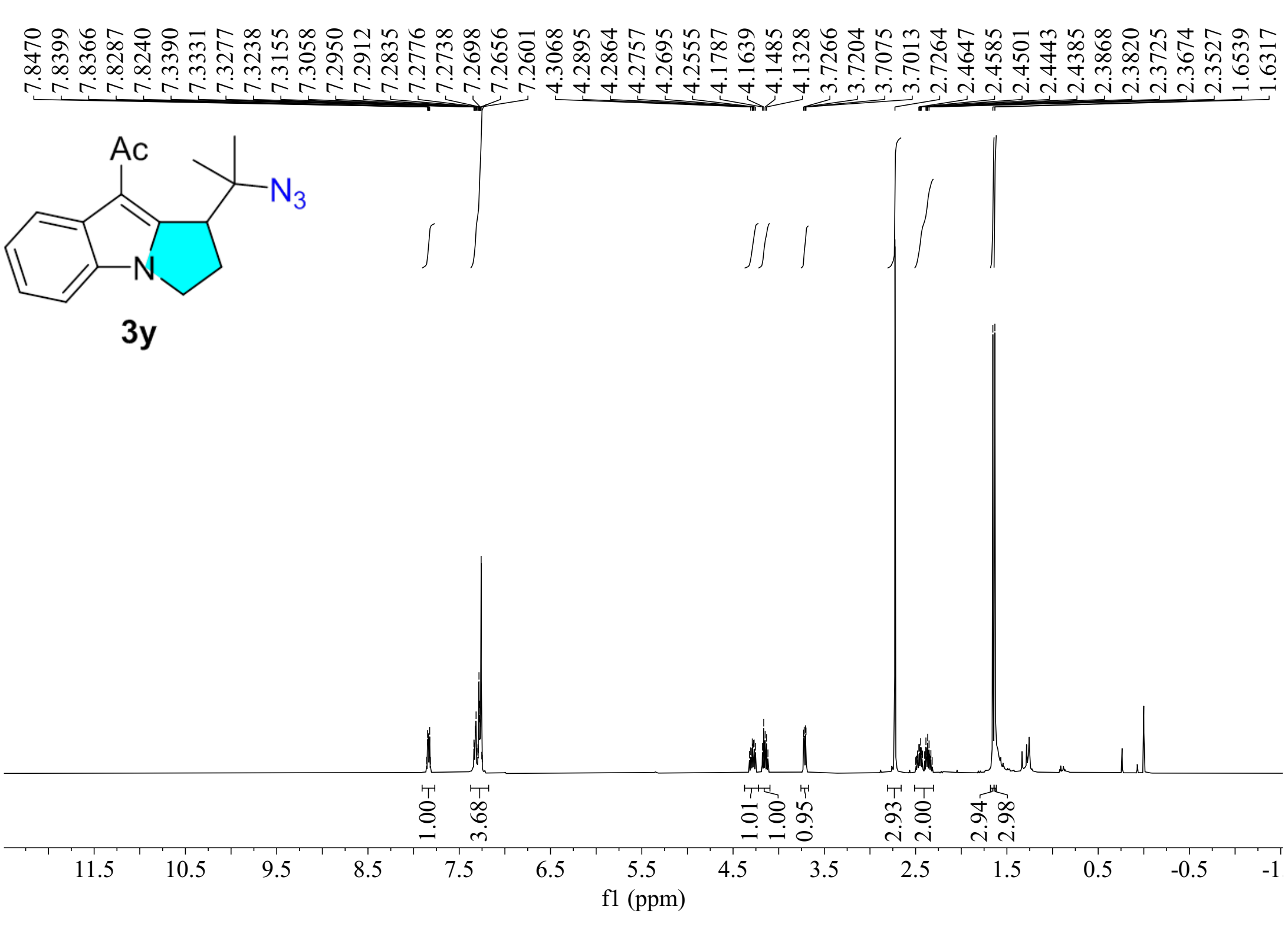
114.92
114.61
77.42
77.00
76.58
53.22
46.23
38.77
31.48
27.42
Ac
N3
N
3x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)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7.2912
7.2835
7.2776
7.2738
7.2698
7.2656
7.2601
4.3068
4.2895
4.2864
4.2757
4.2695
4.2555
4.1787
4.1639
4.1485
4.1328
3.7266
3.7204
3.7075
3.7013
2.7264
2.4647
2.4585
2.4501
2.4443
2.4385
2.3868
2.3820
2.3725
2.3674
2.3527
1.6539
1.6317
Ac
N3
N
3y
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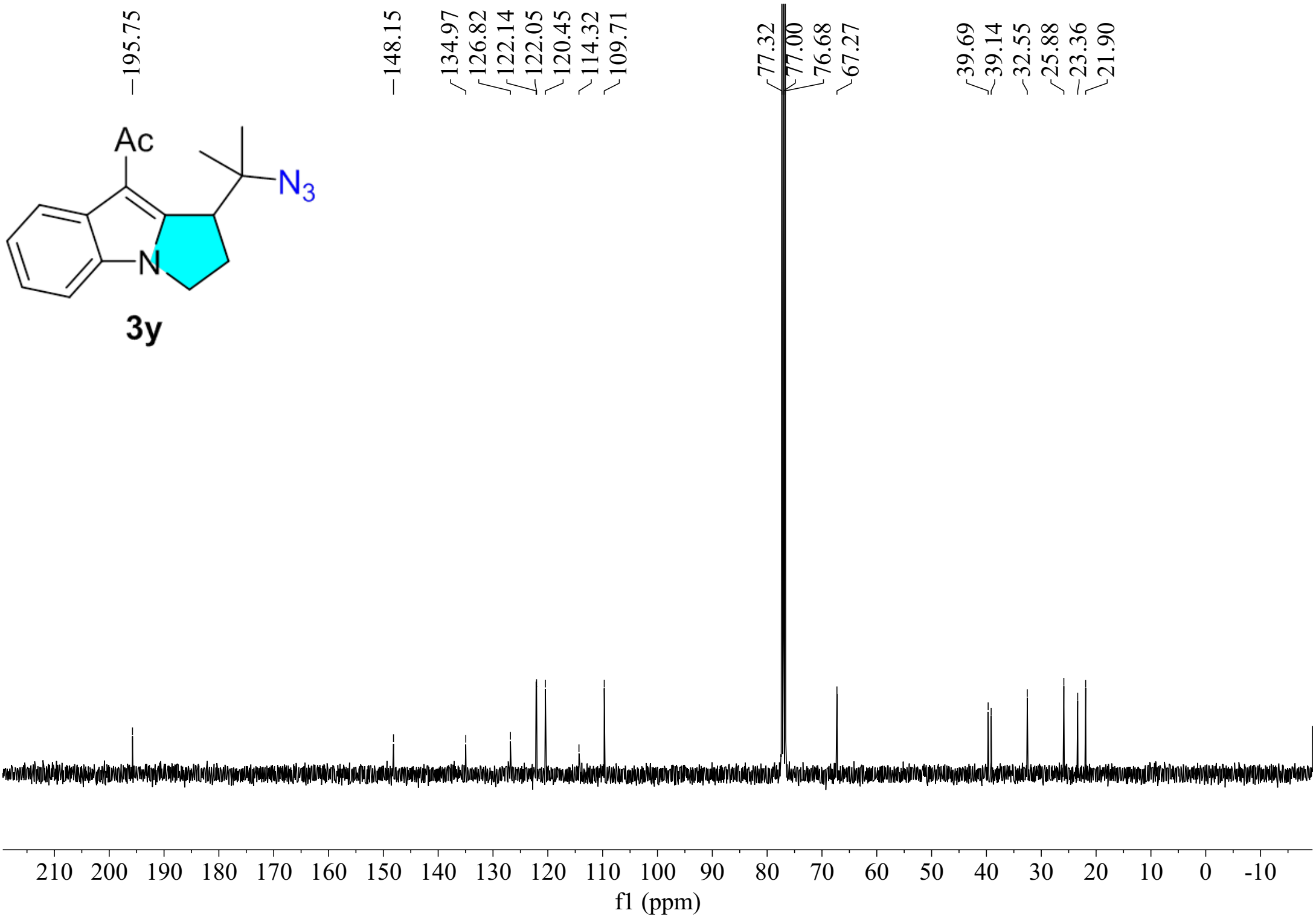
3.68
1.01
1.00
0.95
2.93
2.00
2.94
2.98
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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122.05
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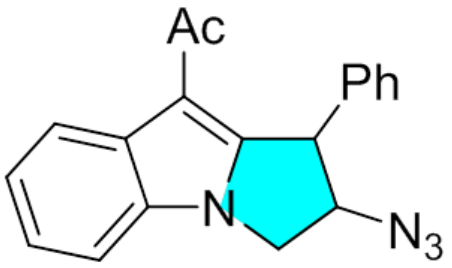
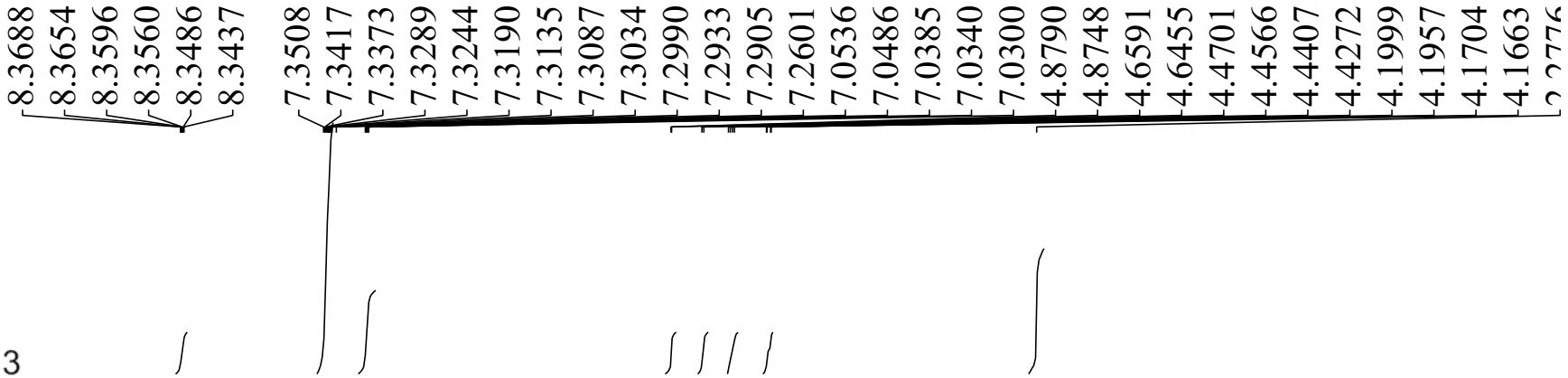
114.32
109.71
77.32
77.00
76.68
67.27
39.69
39.14
32.55
25.88
23.36
21.90
Ac
N3
N
3y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Ac
Ph
N
N_3

3z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8.3486
8.3437
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7.3373
7.3289
7.3244
7.3190
7.3135
7.3087
7.3034
7.2990
7.2933
7.2905
7.2601
7.0536
7.0486
7.0385
7.0340
7.0300
4.8790
4.8748
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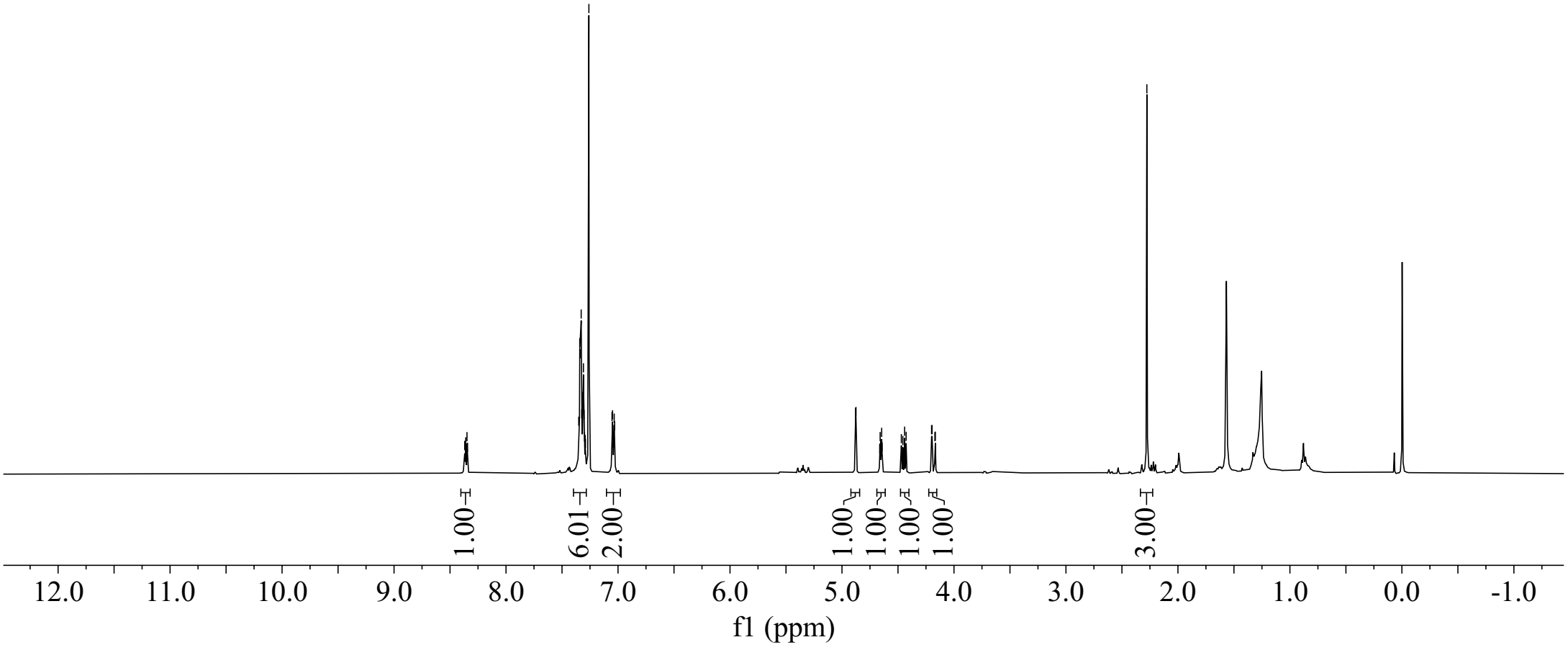
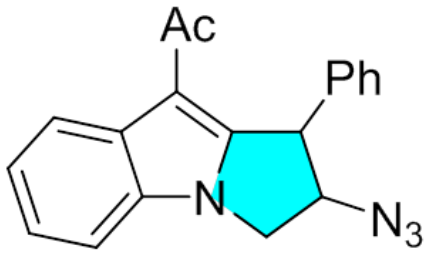
4.1957
4.1704
4.1663


1.00
6.01
2.00
1.00
1.00
1.00
1.00
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)



3z

192.61
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137.76
132.51
130.61
129.42
128.13
127.22
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122.85
111.69
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76.68
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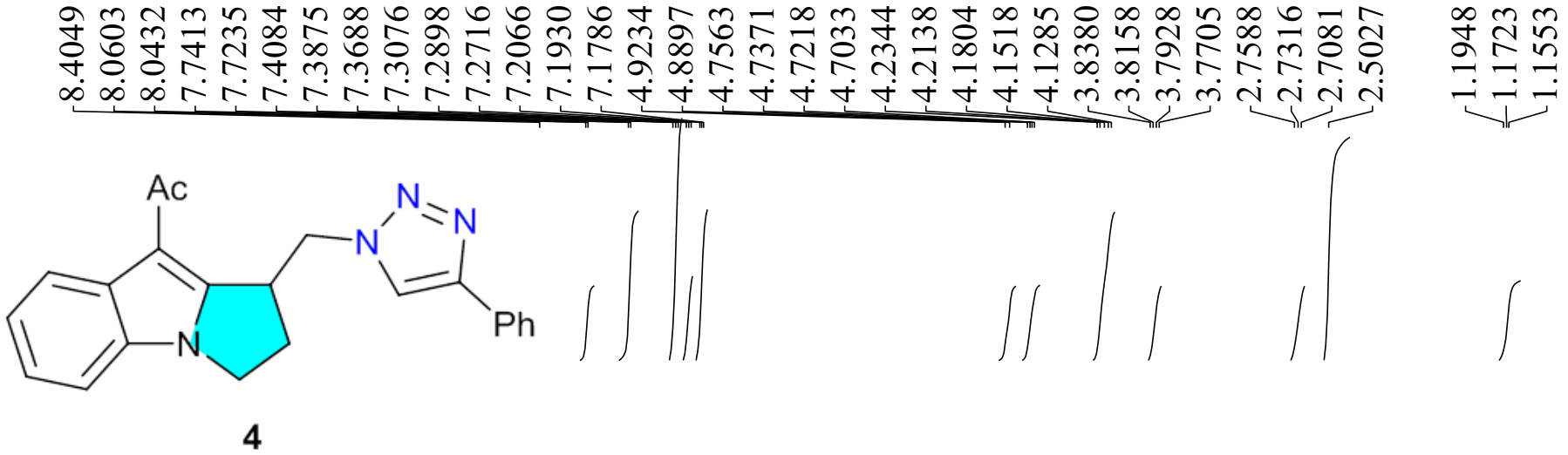
48.98
29.59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7.2716
7.2066
7.1930
7.1786
4.9234
4.8897
4.7563
4.7371
4.7218
4.7033
4.2344
4.2138
4.1804
4.1518
4.1285
3.8380
3.8158
3.7928
3.7705
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Ac
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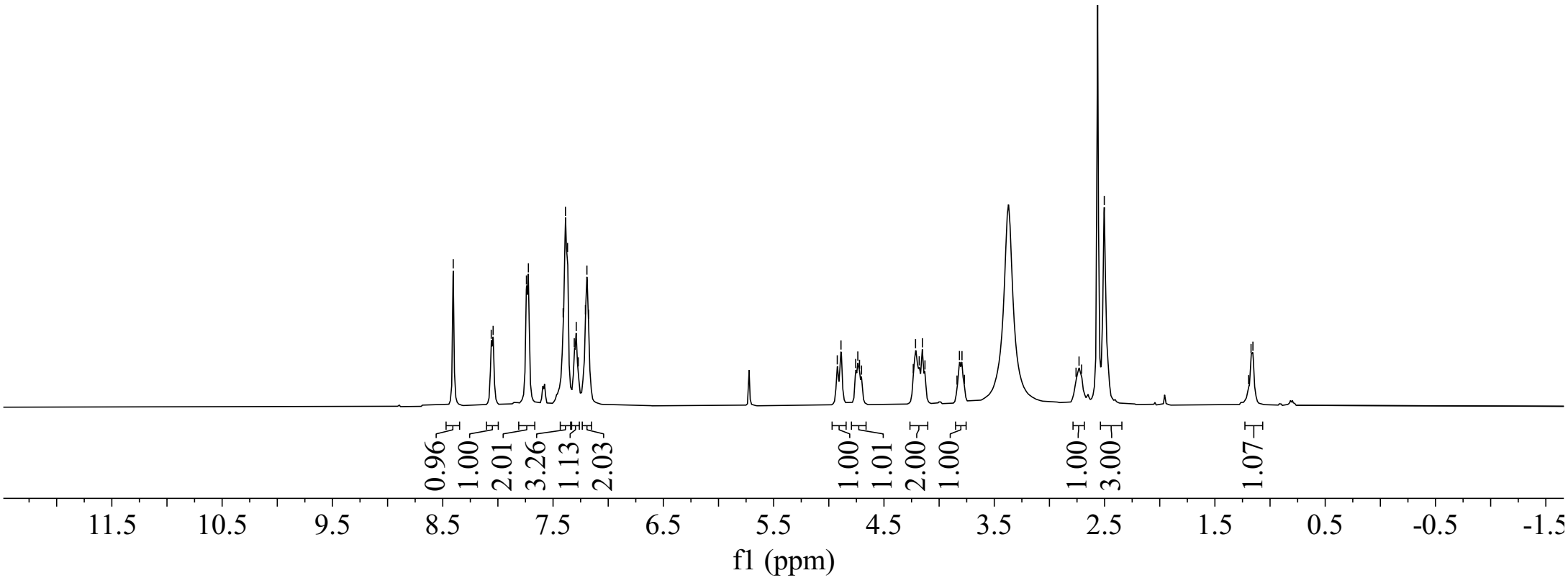
N
N
Ph
N

4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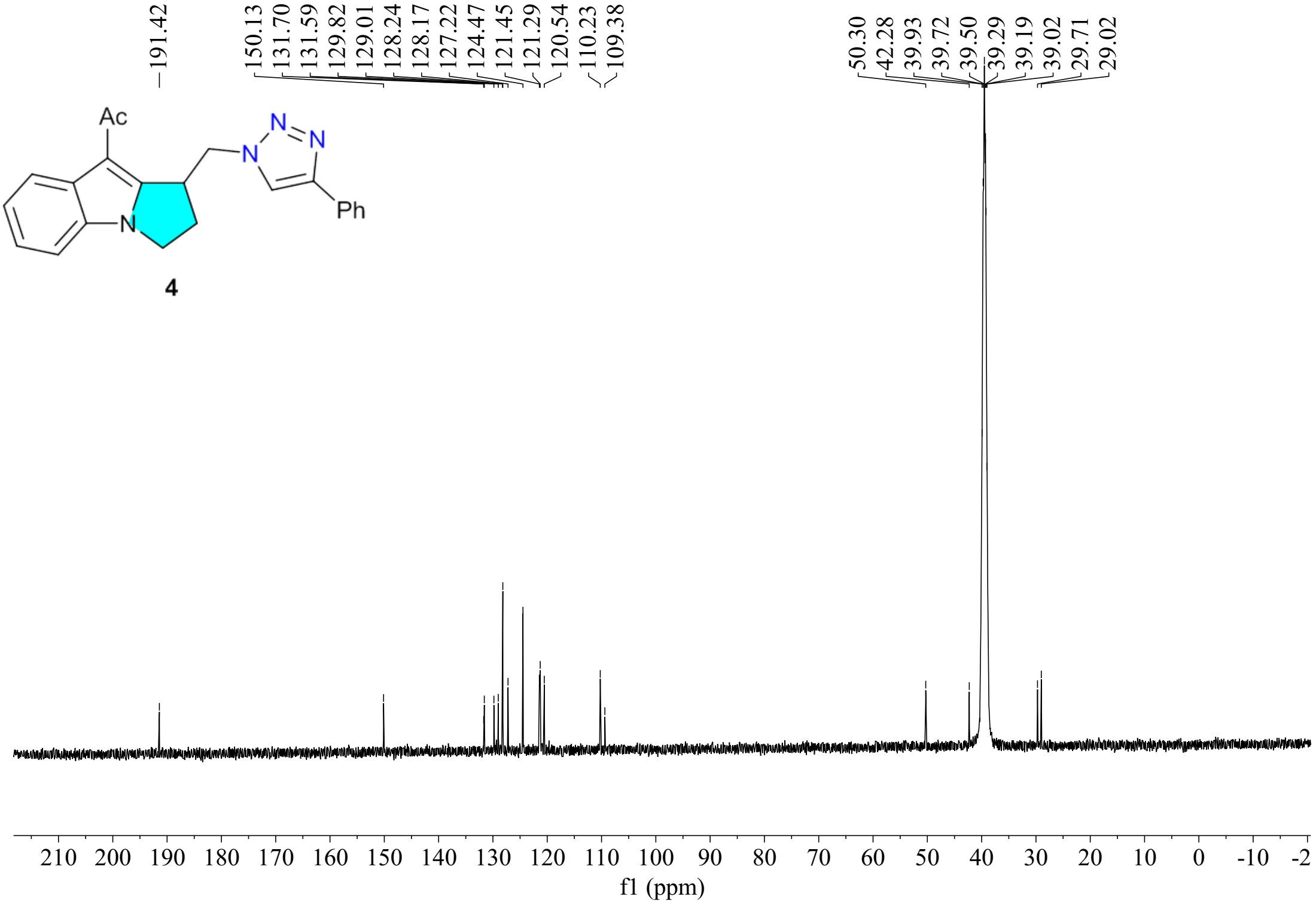
1.00
1.01
2.00
1.00
1.00
3.00
1.07
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)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128.17
127.22
124.47
121.45
121.29
120.54
110.23
109.38
50.30
42.28
39.93
39.72
39.50
39.29
39.19
39.02
29.71
29.02
Ac
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N
N
N
Ph
4
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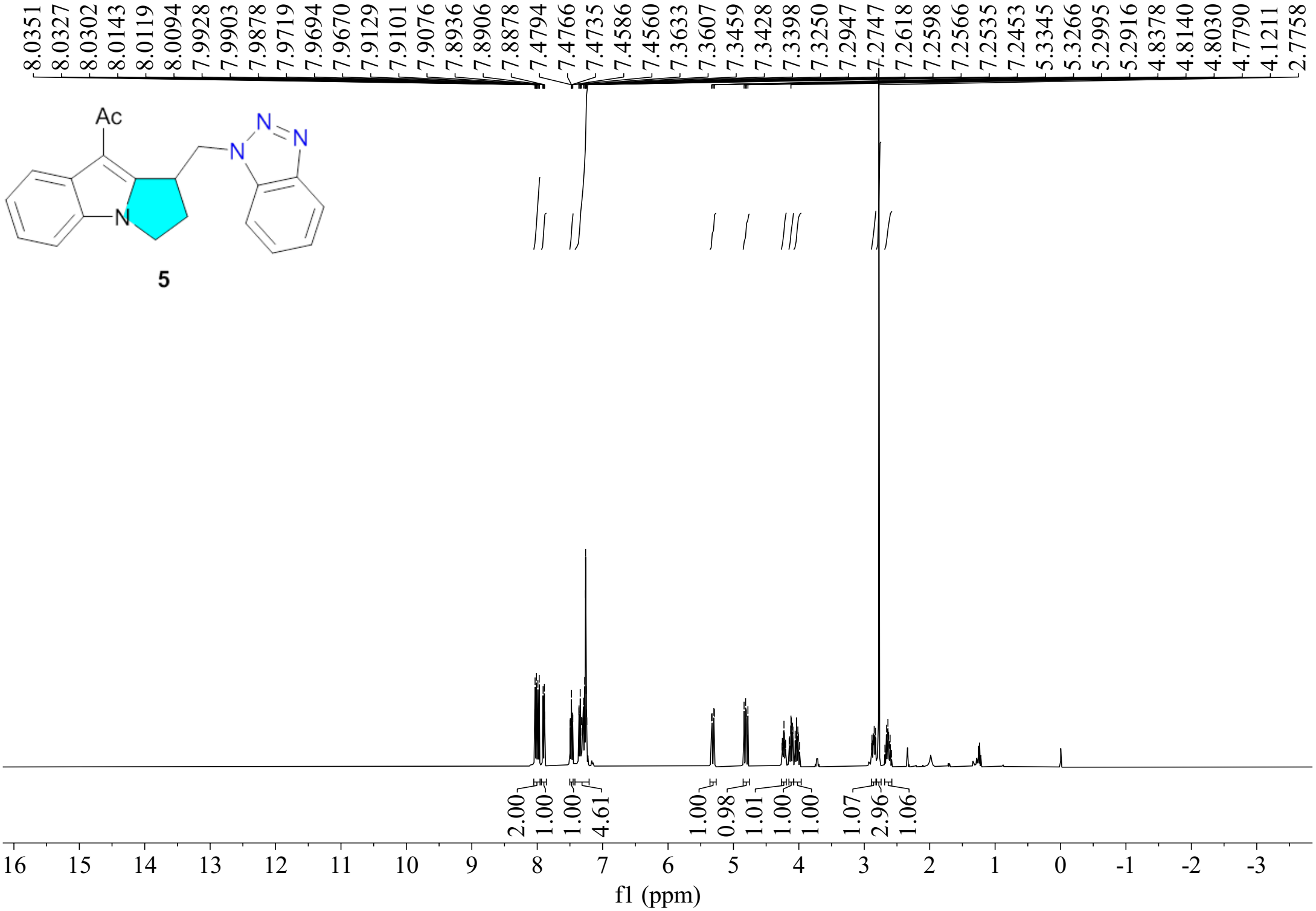
f1 (ppm)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7.2453
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5.2995
5.2916
4.8378
4.8140
4.8030
4.7790
4.1211
2.7758
Ac
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N
N
N
5
2.00
1.00
1.00
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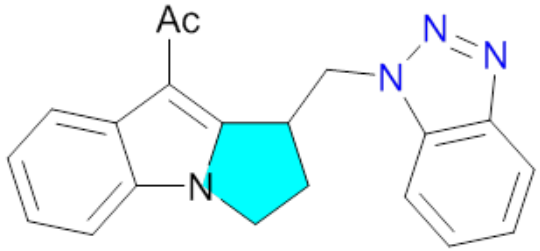
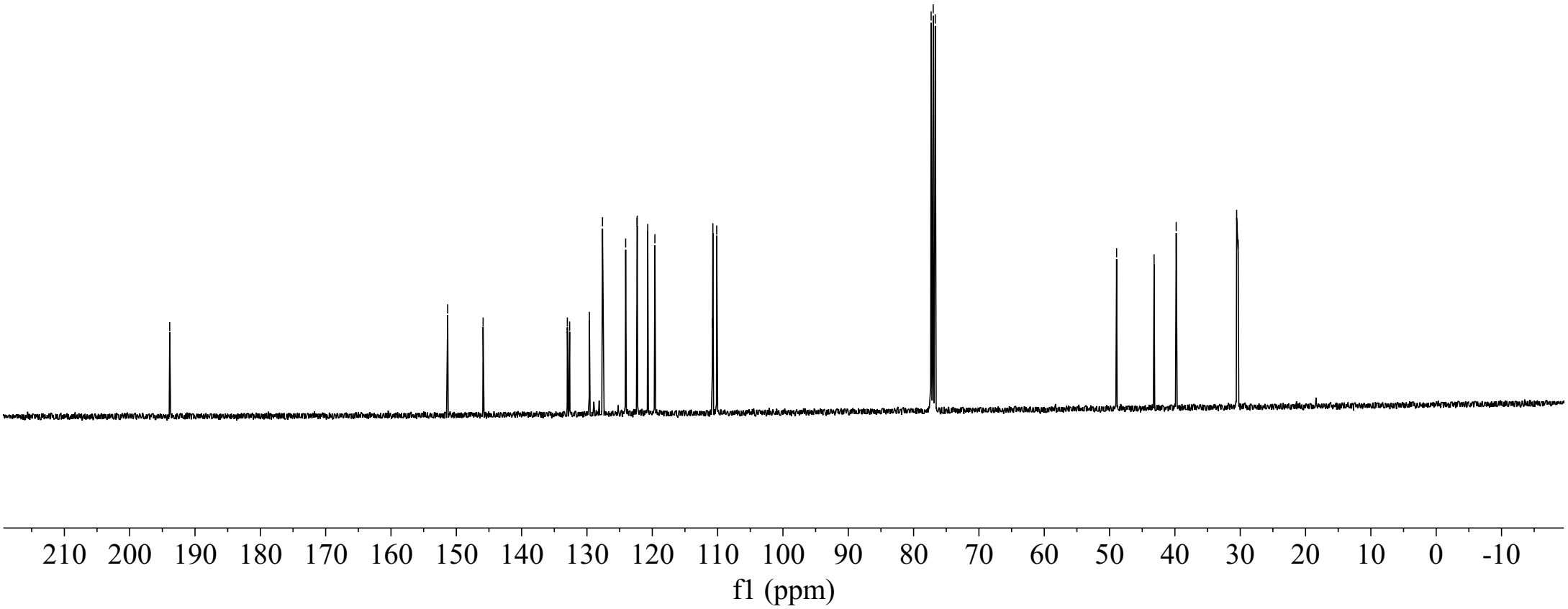
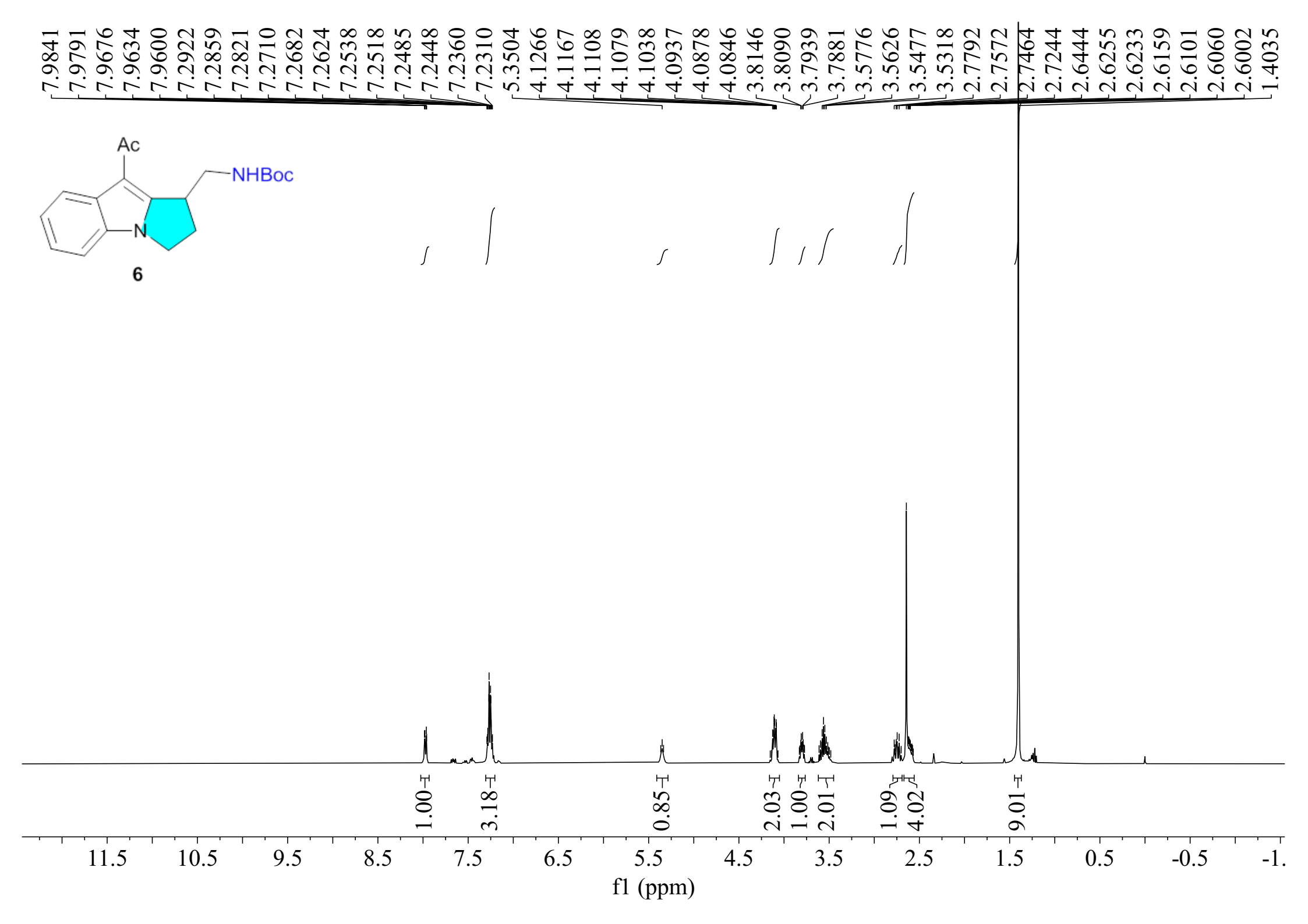
1.00
0.98
1.01
1.00
1.00
1.07
2.96
1.06
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)



5

193.87
151.32
145.90
133.00
132.65
129.63
127.62
124.08
122.34
122.31
120.70
119.60
110.81
110.73
110.14
77.32
77.00
76.68
48.93
43.19
39.80
30.55
30.31

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7.9791
7.9676
7.9634
7.9600
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7.2859
7.2821
7.2710
7.2682
7.2624
7.2538
7.2518
7.2485
7.2448
7.2360
7.2310
5.3504
4.1266
4.1167
4.1108
4.1079
4.1038
4.0937
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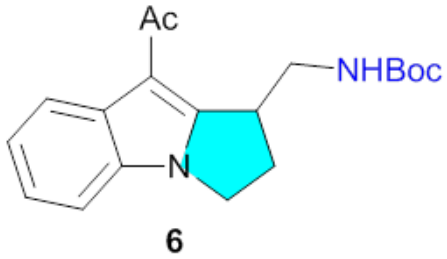
4.0846
3.8146
3.8090
3.7939
3.7881
3.5776
3.5626
3.5477
3.5318
2.7792
2.7572
2.7464
2.7244
2.6444
2.6255
2.6233
2.6159
2.6101
2.6060
2.6002
1.4035
Ac
NHBoc
N
6
1.00
3.18
0.85
2.03
1.00
2.01
1.09
4.02
9.01
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.
f1 (ppm)



6

193.58
156.43
152.82
132.63
129.97
122.11
122.08
121.09
110.61
110.33
79.15
77.32
77.00
76.68
43.32
42.84
40.37
31.37
30.13
28.26