Supporting Information

Copper-Catalyzed Intermolecular Azidocyanation of Aryl Alkenes

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Contents:

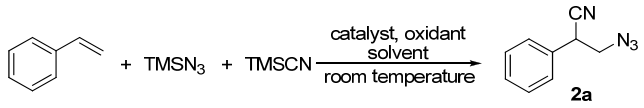
General Information:

All reactions under standard conditions were carried out under argon, dry atmosphere and monitored by thin-layer chromatography (TLC) on gel F254 plates. All reaction solvents were distilled according to the standard method before use. All products were purified through silica gel (200~300 mesh) column chromatography with light petroleum ether (bp. 60~90° C), ethyl acetate as eluent. ^{1}H and ^{13}C spectra were recorded in $CDCl_3$ on 400 MHz and 300 MHz instruments, and spectral data were reported in ppm. The MS data were obtained with SHIMADZU GCMS-QP2010 SE by means of EI (70 eV) technique and signals were given in m/z with relative intensity in brackets. High-resolution mass spectral analysis (HRMS) data were measured on the Bruker ApexII by means of the ESI technique. Melting point was measured with SGW-X4B instrument (uncorrected). The substrates 1a, 1b, 1c, 1d, 1e, 1f, 1g, 1h, 1i, 1j, 1k, 1l, 1m, 1n are known compounds purchased form Energy Chemical.

1. Experimental details for new compounds

1.1 Optimization of reaction conditions:

Table S1 Optimization of reaction conditions[a]

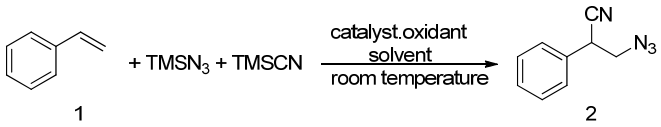


Entry	Catalyst（mol%）	Oxidant（equiv）	Solvent	Yield[b]
1	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	CH_2Cl_2	25%
2	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	DCE	23%
3	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	CH_3CN	45%
4	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	DMSO	35%
5	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	MeOH	52%
6	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	DMF	n.d.[c]
7	$Cu(OTf)_2$(5)	$PhI(OAc)_2$(1.1)	dioxane	n.d.[c]
8	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(1.1)	MeOH	65%
9	$Cu(OTf)_2$(20)	$PhI(OAc)_2$(1.1)	MeOH	63%
10	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	72%
11	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(2)	MeOH	67%
12	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(2.5)	MeOH	52%
13	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(3.0)	MeOH	41%
14[d]	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	72%
15[e]	$Cu(OTf)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	69%
16	$Cu(OTf)_2$(10)	PhIO(1.3)	MeOH	43%
17	$Cu(OTf)_2$(10)	$PhI(TFA)_2$(1.3)	MeOH	36%
18	$Cu(OTf)_2$(10)	TBHP(1.3)	MeOH	n.d.[c]
19	$Cu(OTf)_2$(10)	$K_2S_2O_8$(1.3)	MeOH	n.d.[c]
20	$Cu(OTf)_2$(10)	CAN(1.3)	MeOH	n.d.[c]
21	CuOTf(10)	$PhI(OAc)_2$(1.3)	MeOH	25%
22	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	84%
23[f]	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	74%
24[g]	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	55%
25[h]	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	65%
26[i]	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	46%
27	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(0.8)	MeOH	72%
28	$Cu(TFA)_2$(10)	$PhI(OAc)_2$(2)	MeOH	78%
29	$Cu(OAc)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	38%
30	CuBr(10)	$PhI(OAc)_2$(1.3)	MeOH	46%
31	CuCl(10)	$PhI(OAc)_2$(1.3)	MeOH	40%
32	$FeCl_3$(10)	$PhI(OAc)_2$(1.3)	MeOH	20%

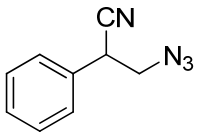
33	No catalyst	$PhI(OAc)_2$(1.3)	MeOH	25%
34	$Cu(MeCN)_4PF_6$(10)	$PhI(OAc)_2$(1.3)	MeOH	52%
35	$Pd(OAc)_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	n.d.
36	$PdCl_2$(10)	$PhI(OAc)_2$(1.3)	MeOH	n.d.
37	$Pd(PPh_3)_4$(10)	$PhI(OAc)_2$(1.3)	MeOH	45%
38	$Au(PPh_3)Cl$(10)	$PhI(OAc)_2$(1.3)	MeOH	n.d.
39	AgTFA(10)	$PhI(OAc)_2$(1.3)	MeOH	n.d.

[a] Reation condition: without other notification, all of the reactions were performed with styrene (0.3 mmol), $TMSN_3$ (1.1 equiv), TMSCN (2 equiv), catalyst and oxidant in solvent (1 mL) at room termperature under Ar for 10 min. [b] Isolated yield; [c] n.d. = not detected. [d] The reaction was carried out at 50 ºC; [e] The reaction was carried out at 100 ºC in seal tube; [f] $TMSN_3$ (1.5 equiv) and TMSCN (2 equiv) were used; [g] $TMSN_3$ (2 equiv) and TMSCN (2 equiv) were used; [h] $TMSN_3$ (1.1 equiv) and TMSCN (3 equiv) were used; [i] $TMSN_3$ (1.1 equiv) and TMSCN (4 equiv) were used.

1.2 General procedure 2a:

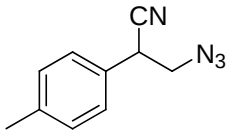


To a stirred solution of the styrene (35ul, 0.3mmol) in MeOH (1 mL) was successively added $TMSN_3$ (52ul, 0.33 mmol), TMSCN (82ul, 0.6 mmol), $Cu(TFA)_2$ (9mg, 0.03mmol) and $PhI(OAc)_2$ (147mg，0.46mmol) at room temperature. After stirred for 10 min, the mixture was concentrated under vacuum. The residue was purified by column chromatography (EtOAc: petroleum ether = 1:80) to give product **2a** (44mg, 84 %) as a yellow oil.



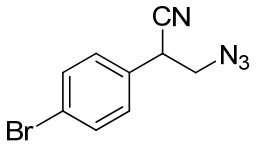
3-azido-2-phenylpropanenitrile (**2a**)

Pale yellow oil; 84% yield; **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.42-7.37 (m, 5H), 4.00 (t, *J* = 7.5 Hz, 1H), 3.71-3.67 (m, 7.5 Hz, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 131.8, 129.1, 128.8, 127.4, 118.3, 54.4, 37.2; MS m/z (%): 172 (M^+, 10), 144 (M^+-28, 60), 116 (100) ; **HRMS** (ESI) Calcd. for $C_9H_9N_2$ $[M-N_2+H]^+$: 145.0766, Found 145.0762.



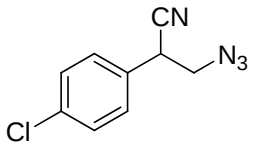
3-azido-2-(p-tolyl)propanenitrile (**2b**)

Pale yellow oil; 82% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.29 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 3.99 (t, *J* = 6.8 Hz, 1H), 3.74-3.65 (m, 2H), 2.40 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.0, 130.1, 129.2, 127.5, 118.8, 54.7, 37.8, 21.1; MS m/z (%): 186 (M^+, <1), 143 (M^+-43, 1), 130 (100), 116 (100) ; **HRMS** (ESI) Calcd. for $C_{10}H_{11}N_2$ $[M-N_2+H]^+$: 159.0922, Found 159.0917.



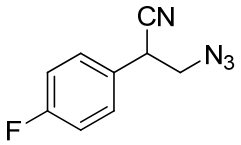
3-azido-2-(4-bromophenyl)propanenitrile (**2c**)

Pale yellow oil; 74% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 3.97 (t, *J* = 6.8 Hz, 1H), 3.70-3.67 (m, 2H); **^{13}C NMR**(100 MHz, $CDCl_3$): δ 132.6, 131.2, 129.4, 123.3, 118.1, 54.3, 37.6; MS m/z (%): 252 ($[M+2]^+$, <1), 250 (M^+, <1), 224 (1), 222 (1), 196 (100), 194 (98) ; **HRMS** (ESI) Calcd. for $C_9H_8BrN_2$ $[M-N_2+H]^+$: 222.9871, Found 222.9869.



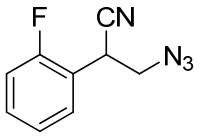
3-azido-2-(4-chlorophenyl)propanenitrile (**2d**)

Pale yellow oil; 78% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.44-7.41 (m, 2H), 7.35-7.33 (m, 2H), 4.01 (t, *J* = 6.6 Hz, 1H), 3.76-3.67 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 135.2, 130.7, 129.6, 129.1, 118.1, 54.4, 37.5; MS m/z (%): 163 ($[M-43]^+$, 3), 150 ($[M-56]^+$, 100), 124 (30), 117 (60) ; **HRMS** (ESI) Calcd. for $C_9H_8ClN_2$ $[M-N_2+H]^+$: 179.0376, Found 179.0372.



3-azido-2-(4-fluorophenyl)propanenitrile (**2e**)

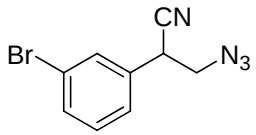
Pale yellow oil; 78% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.41-7.37 (m, 2H), 7.14 (t, *J* = 8.6 Hz, 2H), 4.02 (t, *J* = 6.6 Hz, 1H), 3.76-3.66 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 161.7 (d, *J* = 248 Hz), 129.5 (d, *J* = 9 Hz), 128.0 (d, *J* = 4 Hz), 118.4, 116.5 (d, *J* = 22 Hz), 54.6, 37.4; MS m/z (%): 147 ($[M-43]^+$, 5), 134 ($[M-56]^+$, 100), 108 (90) ; **HRMS** (ESI) Calcd. for $C_9H_8FN_2$ $[M-N_2+H]^+$: 163.0672, Found 163.0668.



3-azido-2-(2-fluorophenyl)propanenitrile (**2f**)

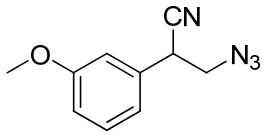
Pale yellow oil; 66% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48-7.44 (m, 1H), 7.34-7.30 (m, 1H), 7.19-7.15 (m, 1H), 7.08-7.04 (m, 1H), 4.26 (t, *J* = 6.4 Hz, 1H), 3.66-3.64 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 158.8 (d, *J* = 247 Hz), 130.1 (d, *J* = 8 Hz), 128.6 (d, *J* = 3 Hz), 124.1 (d, *J* = 3 Hz), 118.4 (d, *J* = 14 Hz), 116.7, 115.0 (d, *J* = 21 Hz), 51.9 (d, *J* = 1 Hz), 31.2 (d, *J* = 3 Hz); MS m/z

(%): 162 ([M-28]$^+$, 3), 134 ([M-56]$^+$, 100), 108 (90) ; **HRMS** (ESI) Calcd. for $C_9H_8FN_2$ [M-N_2+H]$^+$: 163.0672, Found 163.0668.



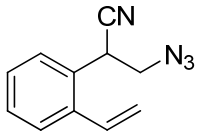
3-azido-2-(3-bromophenyl)propanenitrile (**2g**)

Pale yellow oil; 65% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.57-7.55 (m, 2H), 7.37-7.28 (m, 2H), 3.99 (t, *J* = 6.6 Hz, 1H), 3.76-3.69 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 134.3, 132.3, 130.9, 130.8, 126.4, 123.4 117.9, 54.4, 37.6; MS m/z (%):252 ([M+2]$^+$, <1), 250 (M$^+$, <1), 224 (1), 222 ([M-28]$^+$, 1), 209 ([M-43]$^+$, 3), 207 ([M-43]$^+$, 3), 196 (50), 194 (50), 116 (100) ; **HRMS** (ESI) Calcd. for $C_9H_8BrN_2$ [M-N_2+H]$^+$: 222.9871, Found 222.9867.



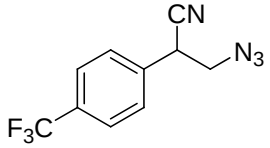
3-azido-2-(3-methoxyphenyl)propanenitrile (**2h**)

Pale yellow oil; 65% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.26-7.22 (m, 1H), 6.87-6.82 (m,3H), 3.88 (t, *J* = 6.8 Hz, 1H), 3.73 (s, 3H), 3.61-3.58 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 160.1, 133.4, 130.3, 119.6, 118.4, 114.2, 113.4, 55.2, 54.4, 37.9; MS m/z (%): 202 (M$^+$, 60), 174 (M$^+$-28, 20), 159 (M$^+$-43, 10), 146 (100) ; **HRMS** (ESI) Calcd. for $C_{10}H_{11}N_2O$ [M-N_2+H]$^+$: 175.0871, Found 175.0867.



3-azido-2-(3-vinylphenyl)propanenitrile (**2i**)

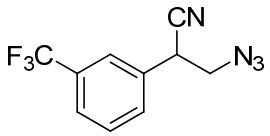
Pale yellow oil; 56% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.45-7.24 (m, 4H), 6.74-6.67 (m,1H), 5.82-5.76 (m, 1H), 5.34-5.30 (m, 1H), 4.00-3.96 (m, 1H), 3.73-3.64 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.7, 138.3, 135.7, 135.6, 132.4, 131.3, 129.5, 127.8, 127.0, 126.8, 126.6, 125.4, 118.4, 115.3, 115.2, 54.44, 54.41, 38.0, 37.7; MS m/z (%): 198 (M$^+$, 4), 170 (M$^+$-28, 4), 142 (100) ; **HRMS** (ESI) Calcd. for $C_{11}H_{11}N_2$ [M-N_2+H]$^+$: 171.0922, Found 171.0919.



3-azido-2-(4-(trifluoromethyl)phenyl)propanenitrile (**2j**)

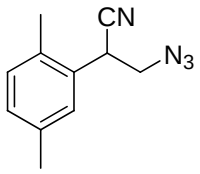
Pale yellow oil; 61% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 4.11 (t, *J* = 6.6 Hz, 1H), 3.78-3.76 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 136.1, 131.4

(q, *J* = 33 Hz), 128.3, 126.4 (q, *J* = 3 Hz), 123.7 (q, *J* = 271 Hz), 117.8, 54.2, 37.8; MS m/z (%): 240 (M^+, <1), 212 (M^+-28, 1), 197 (M^+-43, 3), 184 (100) ; **HRMS** (ESI) Calcd. for $C_{10}H_8F_3N_2$ $[M-N_2+H]^+$: 213.0640, Found 213.0634.



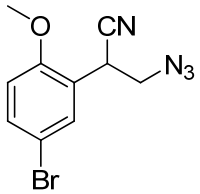
3-azido-2-(3-(trifluoromethyl)phenyl)propanenitrile (**2k**)

Pale yellow oil; 52% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.68-7.56 (m, 4H), 4.08 (t, *J* = 6.6 Hz, 1H), 3.76-3.74 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 133.3, 131.9 (q, *J* = 33 Hz), 130.1, 126.0 (q, *J* = 4 Hz), 124.6 (q, *J* = 4 Hz), 123.6 (q, *J* = 271 Hz), 117.8, 54.3, 37.8; MS m/z (%): 240 (M^+, <1), 197 (M^+-43, 2), 184 (25), 84 (100) ; **HRMS** (ESI) Calcd. for $C_{10}H_8F_3N_2$ $[M-N_2+H]^+$: 213.0640, Found 213.0636.



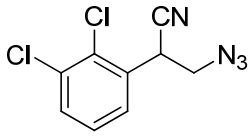
3-azido-2-(2,5-dimethylphenyl)propanenitrile (**2l**)

Pale yellow oil; 41% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.32 (s, 1H), 7.13 (s, 2H), 4.18 (q, *J* = 6.0 Hz, 1H), 3.73-3.62 (m, 2H), 2.38 (s, 3H), 2.34 (s, 3H); **^{13}C NMR**(100 MHz, $CDCl_3$): δ 136.9, 132.2, 131.2, 130.2, 129.8 , 128.5, 119.1, 53.6, 34.9, 20.9, 18.6; MS m/z (%): 200 (M^+, 4), 172 ($[M-28]^+$, 3), 157 ($[M-43]^+$, 2), 144 ($[M-56]^+$, 100), 117 (60) ; **HRMS** (ESI) Calcd. for $C_{11}H_{13}N_2$ $[M-N_2+H]^+$: 173.1079, Found 173.1075.



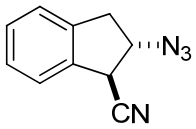
3-azido-2-(5-bromo-2-methoxyphenyl)propanenitrile (**2m**)

Pale yellow oil; 63% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50 (d, *J* = 2 Hz, 1H), 7.39 (dd, *J* = 2.4, 8.8 Hz, 1H), 6.73 (d, *J* = 8.8 Hz, 1H), 4.27 (q, *J* = 5.6 Hz, 1H), 3.79 (s, 3H), 3.64-3.54 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 155.2, 133.1, 131.8, 122.3, 118.2, 113.2, 112.6, 55.9, 52.3, 32.6; MS m/z (%): 282 ($[M+2]^+$, 23), 280 (M^+, 23), 226 (69), 224 ($[M-56]^+$, 69), 84 (100) ; **HRMS** (ESI) Calcd. for $C_{10}H_{10}BrN_2O$ $[M-N_2+H]^+$: 252.9977, Found 252.9974.



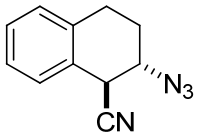
3-azido-2-(2,3-dichlorophenyl)propanenitrile (**2n**)

Pale yellow oil; 32% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56-7.53 (m, 2H), 7.34 (t, *J* = 7.8 Hz, 1H), 4.58 (dd, *J*= 4.8, 7.2 Hz, 1H), 3.81 (dd, *J* = 4.8, 12.4 Hz, 1H), 3.71 (dd, *J* = 7.2, 12.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 134.1, 132.0, 131.2, 131.2, 128.1, 127.9, 117.7, 52.3, 36.3; MS m/z (%): 212 ($[M-28]^+$, 2), 197 ($[M-43]^+$, 15), 184 (100); **HRMS** (ESI) Calcd. for $C_9H_7Cl_2N_2$ $[M-N_2+H]^+$: 212.9986, Found 212.9983.



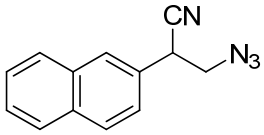
2-azido-2,3-dihydro-1H-indene-1-carbonitrile (**2o**)

Pale yellow oil; 67% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.33-7.17 (m, 4H), 4.45 (q, *J* = 7.6 Hz, 1H), 3.98 (d, *J* = 7.6 Hz, 1H), 3.32 (dd, *J* = 7.6, 16.0 Hz, 1H), 2.94 (q, *J* = 7.6, 16.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.8, 134.5, 129.4, 128.1, 125.1, 124.3, 118.5, 65.6, 41.3, 37.5; MS m/z (%): 184 (M^+, <1), 156 ($[M-28]^+$, 4), 141 ($[M-43]^+$, 4), 129 (100) ; **HRMS** (ESI) Calcd. for $C_{10}H_9N_2$ $[M-N_2+H]^+$: 157.0766, Found 157.0762.



2-azido-1,2,3,4-tetrahydronaphthalene-1-carbonitrile (**2p**)

White solid, mp 73-75 ºC; 37% yield; **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.40-7.37 (m, 1H), 7.25-7.20 (m, 2H), 7.13-7.10 (m, 1H), 4.07-4.00 (m, 1H), 3.86 (d, *J* = 9 Hz, 1H), 2.96-2.90 (m, 2H), 2.36-2.01 (m, 1H), 1.95-1.82 (m, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 134.4, 129.2, 128.6, 128.5, 127.3, 127.1, 119.4, 59.2, 37.6, 26.9, 26.4; MS m/z (%): 169 ($[M-29]^+$, 25), 155 ($[M-43]^+$, 6), 142 ($[M-56]^+$, 50), 116 (100) ; **HRMS** (ESI) Calcd. for $C_{11}H_{11}N_2$ $[M-N_2+H]^+$: 171.0922, Found 171.0918.

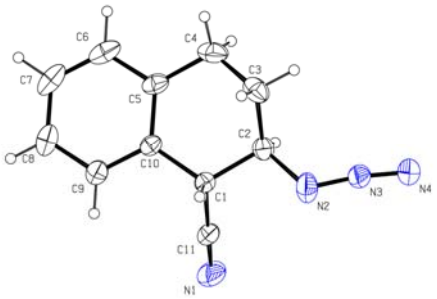


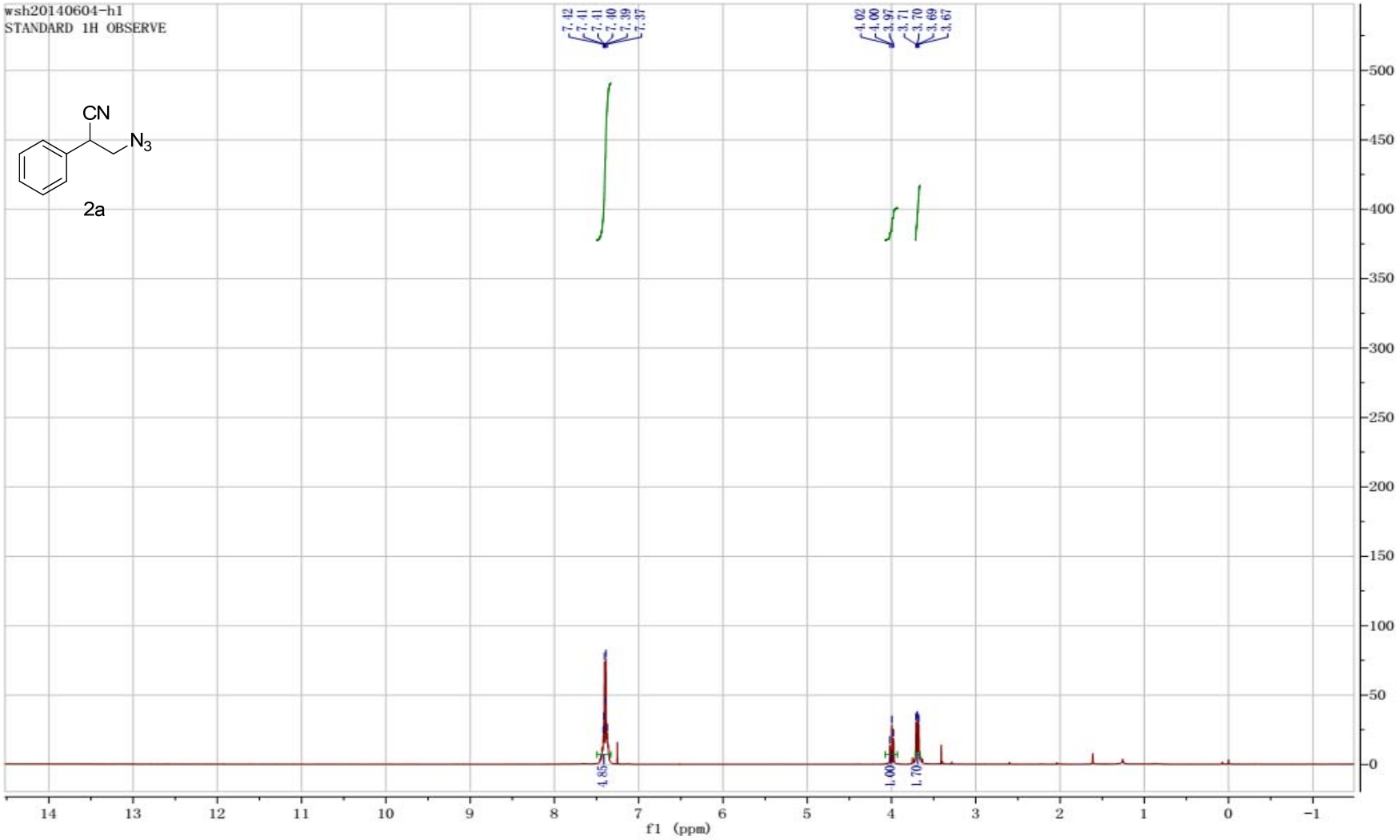
3-azido-2-(naphthalen-2-yl)propanenitrile (**2q**)

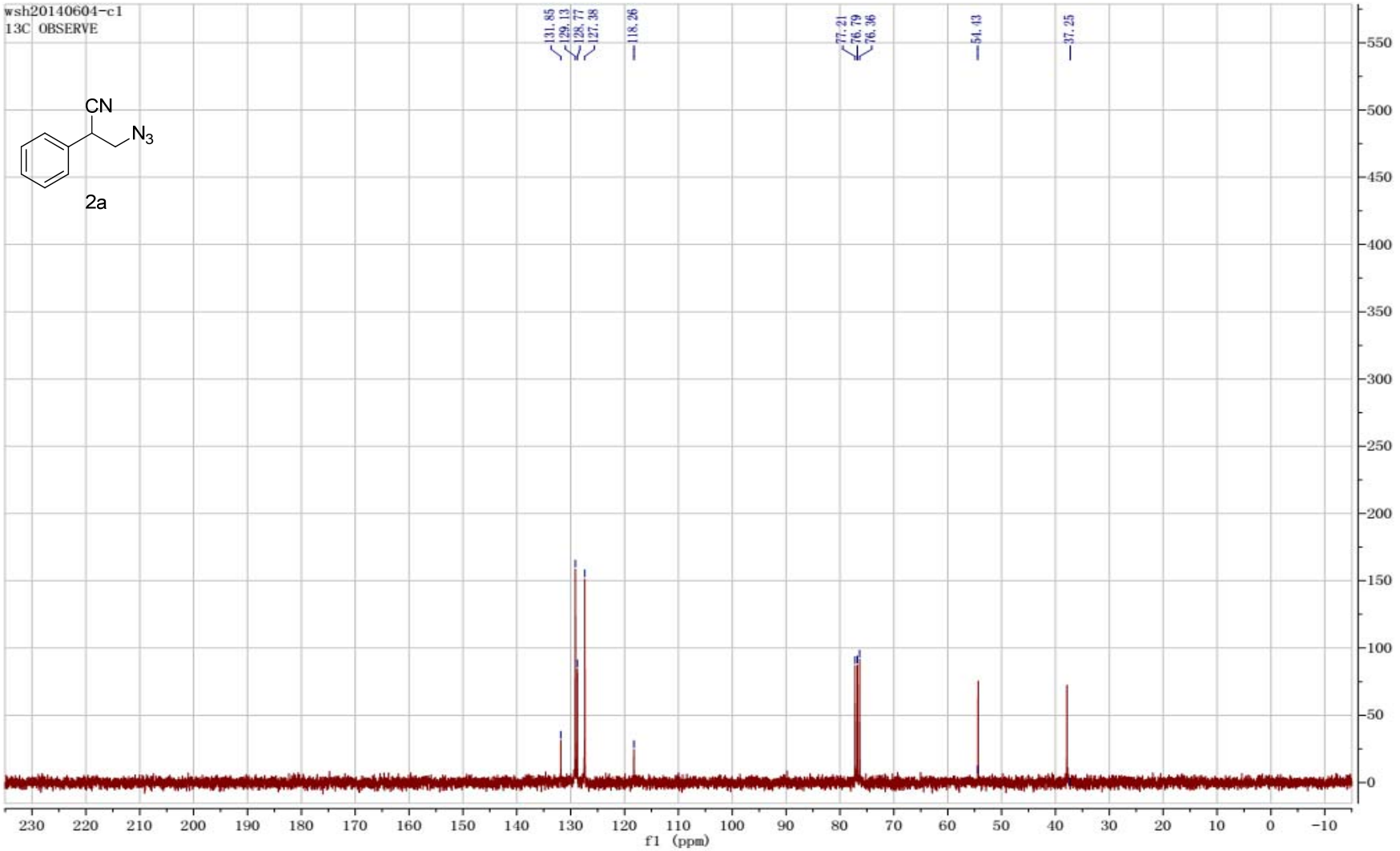
Pale yellow oil; 53% yield; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.93-7.88 (m, 4H), 7.58 (dd, *J* = 3.2, 8.4 Hz, 2H), 7.45 (dd, *J* = 2.0, 8.4 Hz, 1H), 4.16 (t, *J* = 6.8 Hz, 1H), 3.80-3.78 (m, 2H); **^{13}C NMR**

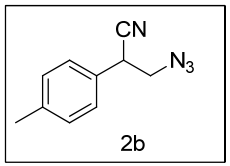
(100 MHz, $CDCl_3$): δ 133.3, 133.2, 129.5, 129.4, 128.0, 127.8, 127.3, 127.1, 127.0, 124.6, 118.7, 54.5, 38.3; MS m/z (%): 222 (M^+, 10), 194 ($[M-28]^+$, 4), 179($[M-43]^+$, 4), 166 ($[M-56]^+$, 100) ; **HRMS** (ESI) Calcd. for $C_{13}H_{11}N_2$ $[M-N_2+H]^+$: 195.0922, Found 195.0918.

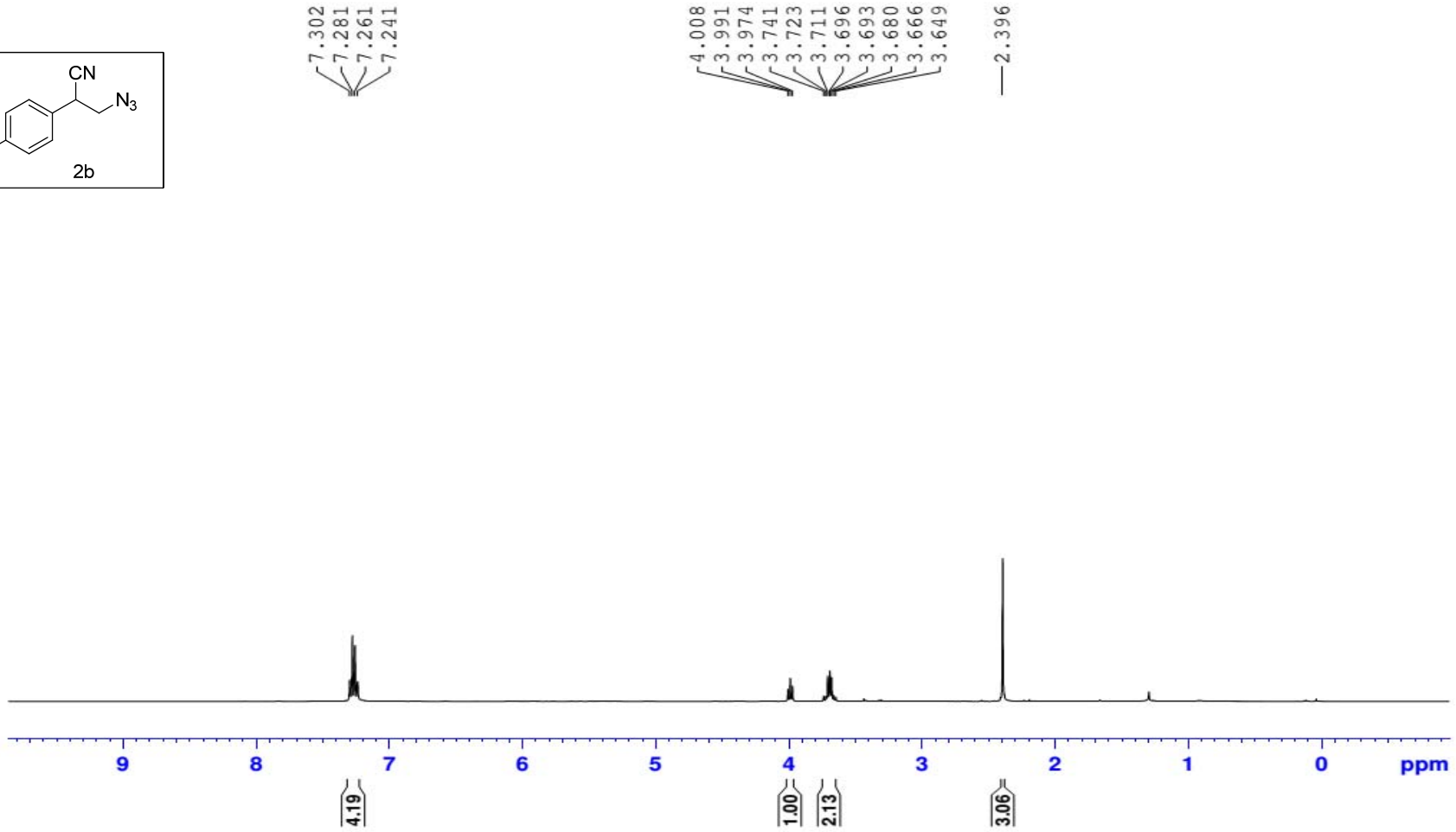
2. X-Ray ellipsoid plots of 2p (CCDC: 1008927)




wsh20140604-h1
STANDARD 1H OBSERVE
CN
N3
2a
7.42
7.41
7.41
7.40
7.39
7.37
4.02
4.00
3.97
3.71
3.70
3.69
3.67
4.85
1.00
1.70
f1 (ppm)


wsh20140604-c1
13C OBSERVE
131.85
129.13
128.77
127.38
118.26
77.21
76.79
76.36
54.43
37.25
CN
N3
2a
f1 (ppm)


CN
N3
2b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3.711
3.696
3.693
3.680
3.666
3.649
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8
7
6
5
4
3
2
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ppm
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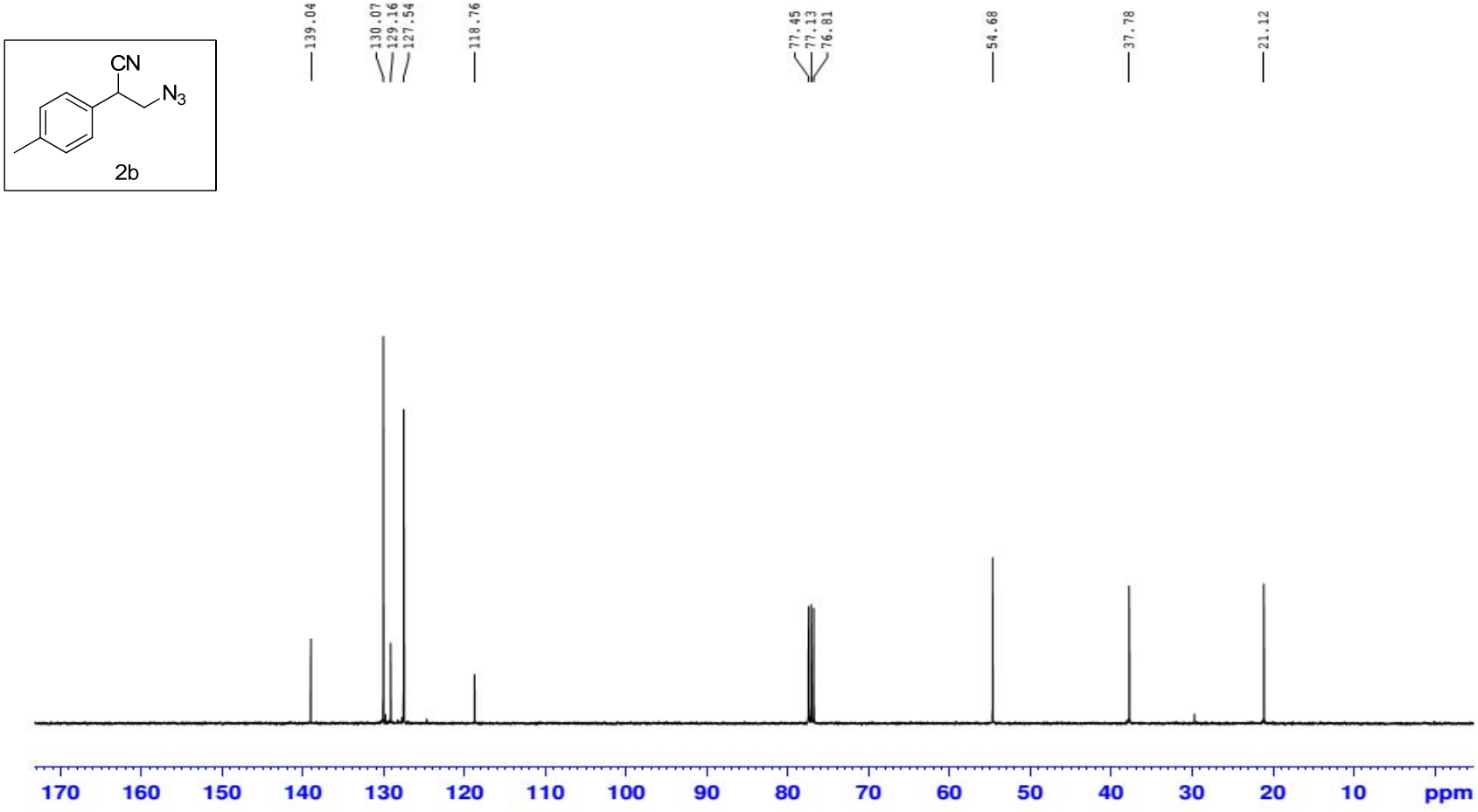
3.06


CN
N3
2b
139.04
130.07
129.16
127.54
118.76
77.45
77.13
76.81
54.68
37.78
21.12
170
160
150
140
130
120
110
100
90
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60
50
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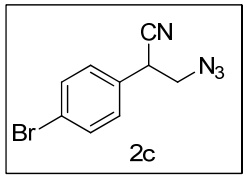
30
20
10
ppm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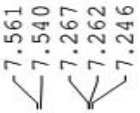
N3
Br
2c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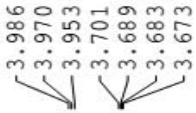
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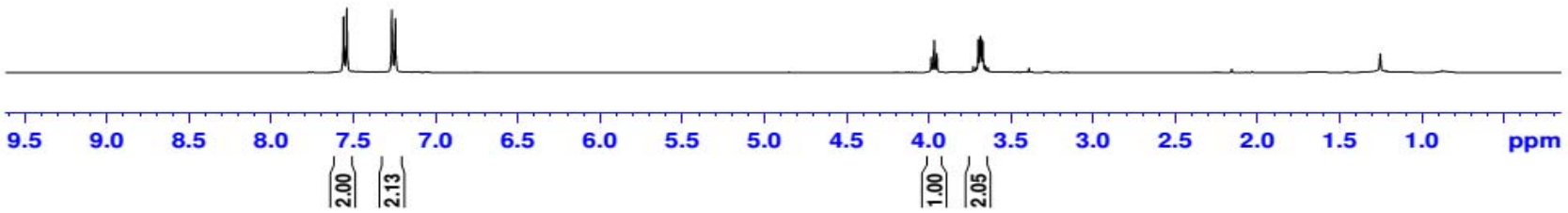
3.673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6.0
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2.0
1.5
1.0
ppm
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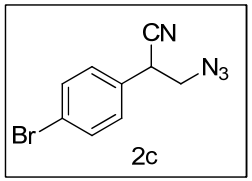
1.00
2.05


CN
N3
Br
2c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123.29
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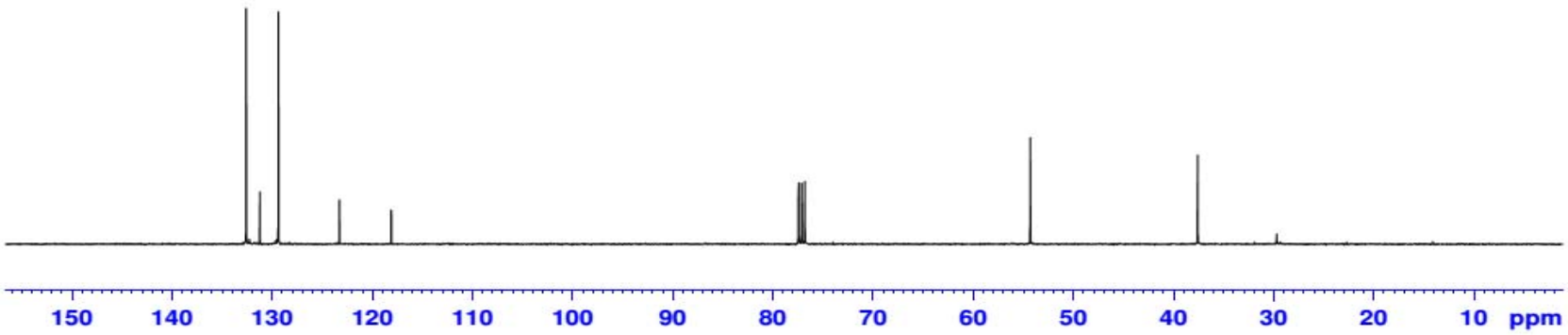
77.13
76.81
54.31
37.59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30
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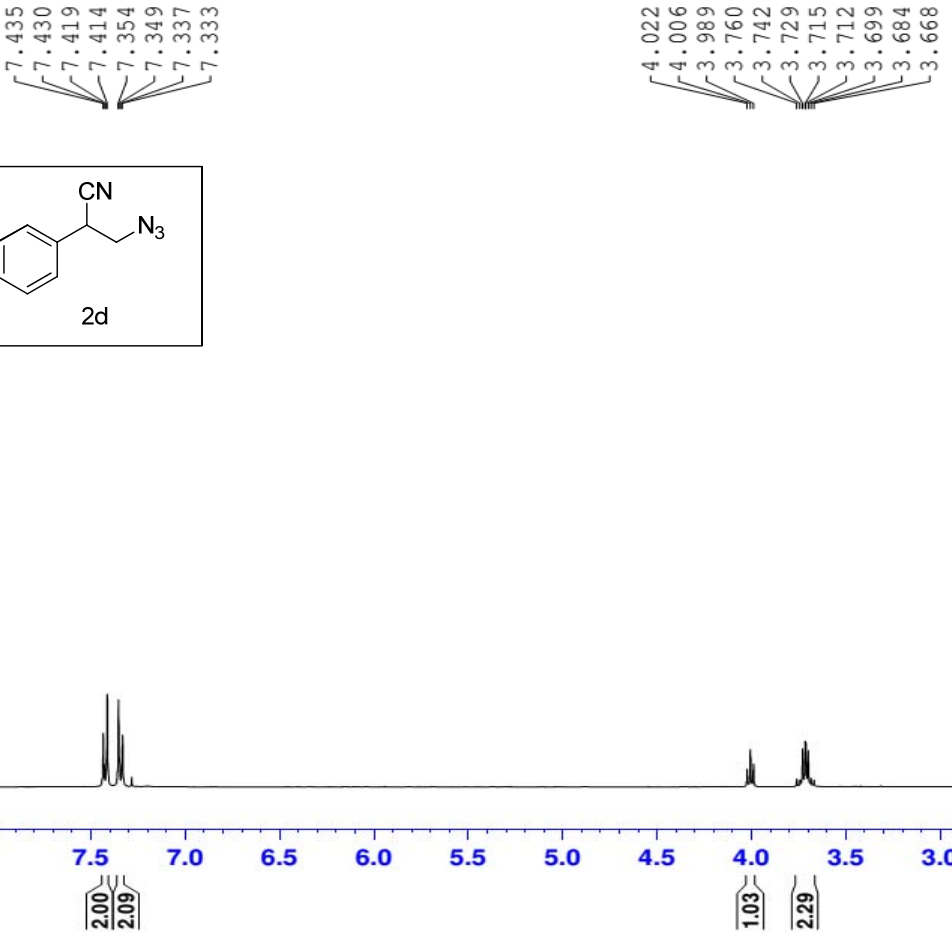
10
ppm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3.715
3.712
3.699
3.684
3.668
CN
N3
Cl
2d
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6.5
6.0
5.5
5.0
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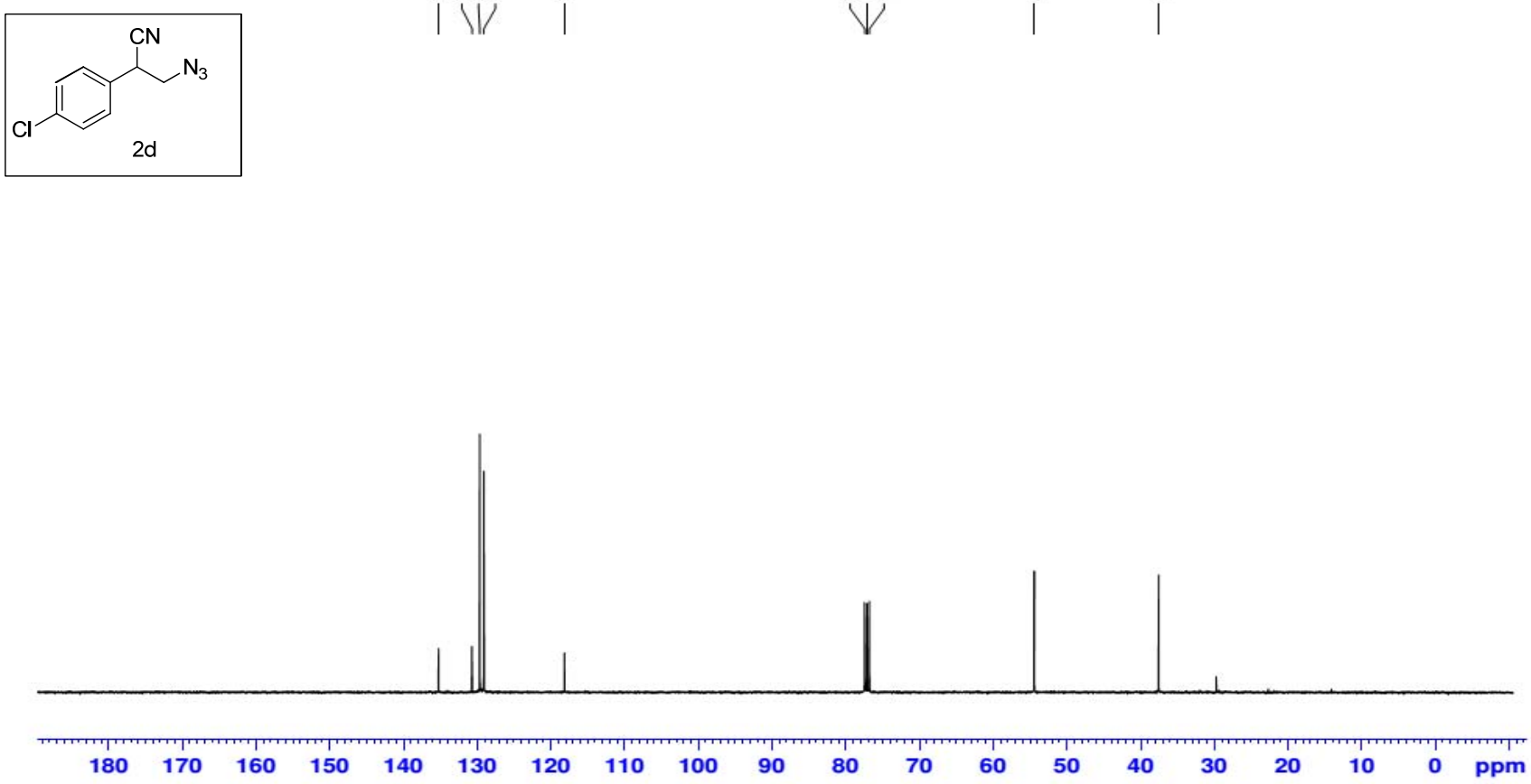
2.29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Cl
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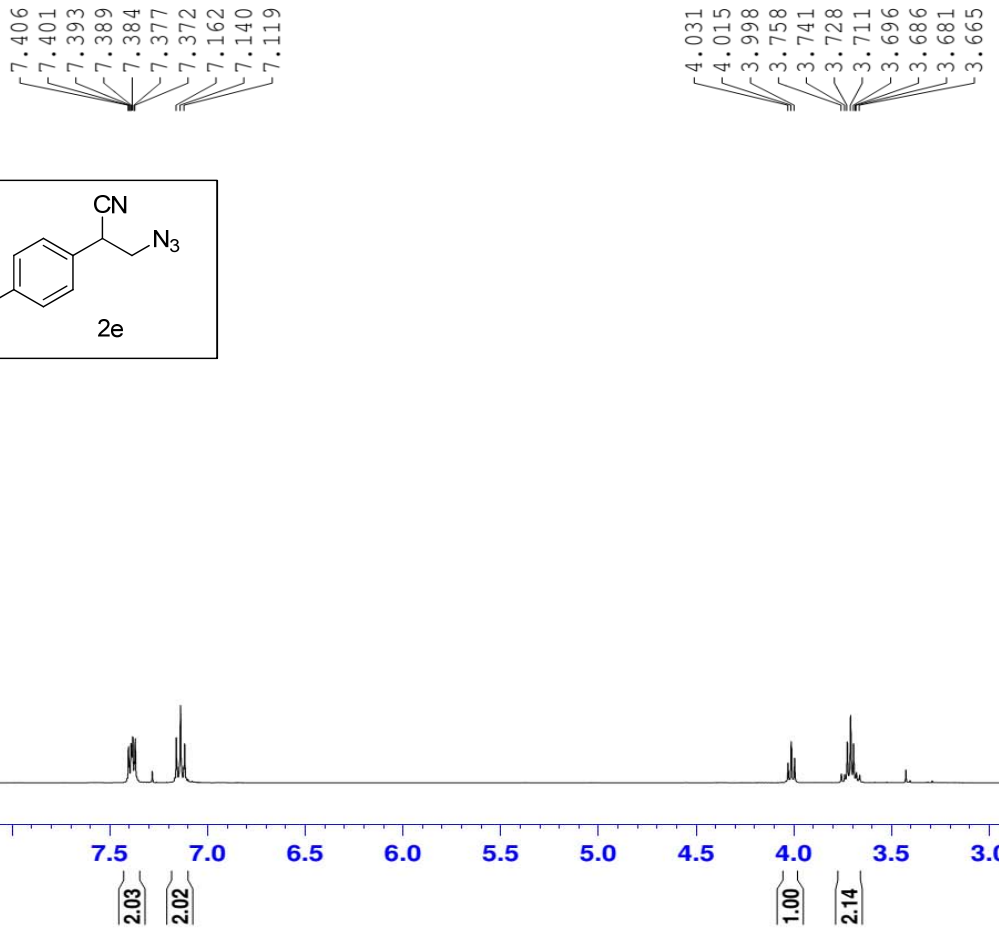
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3.711
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3.681
3.665
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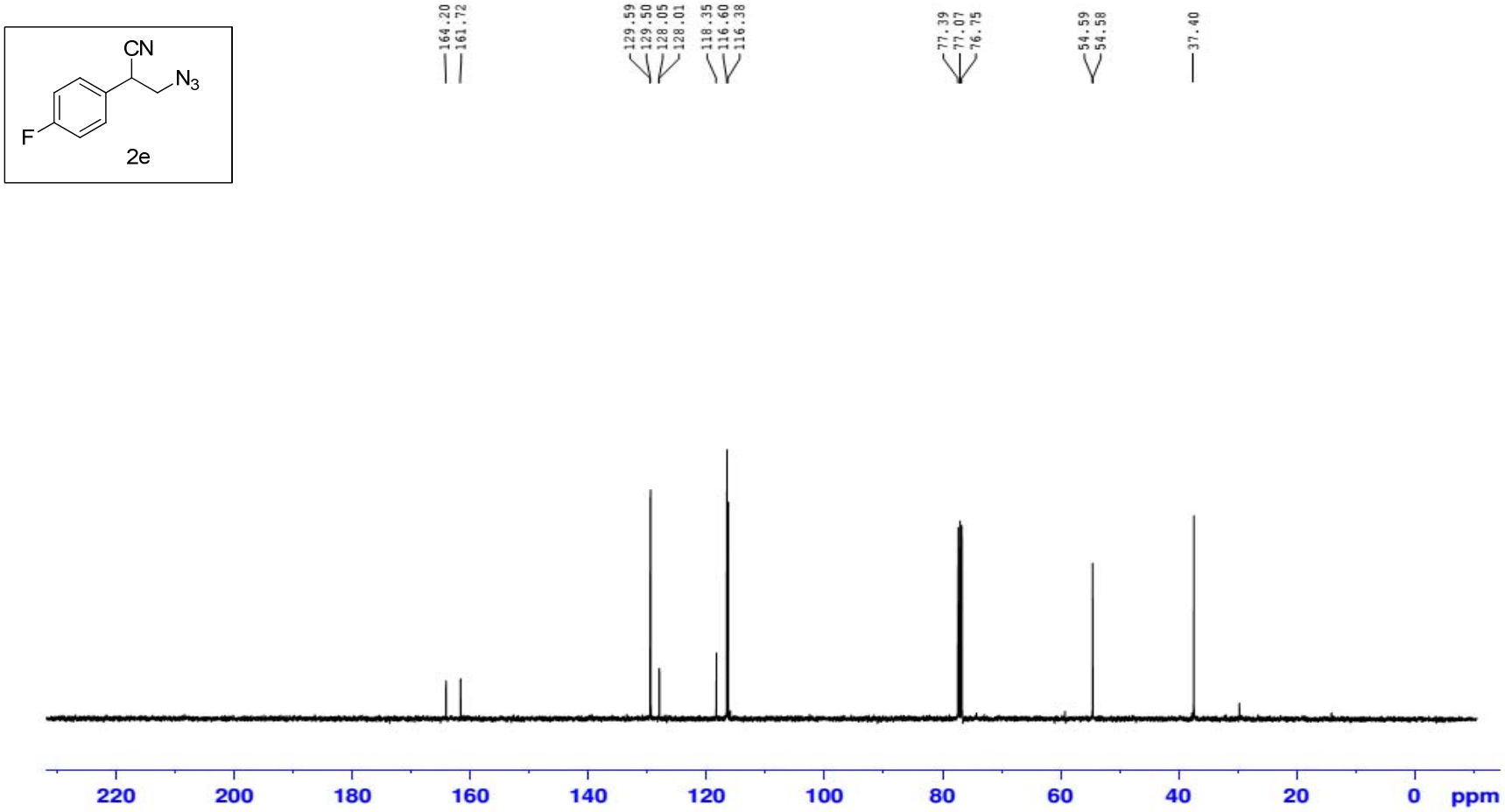
2.14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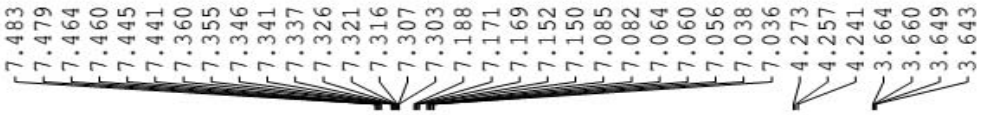
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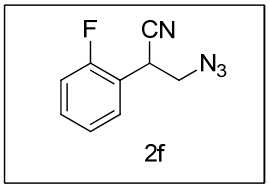
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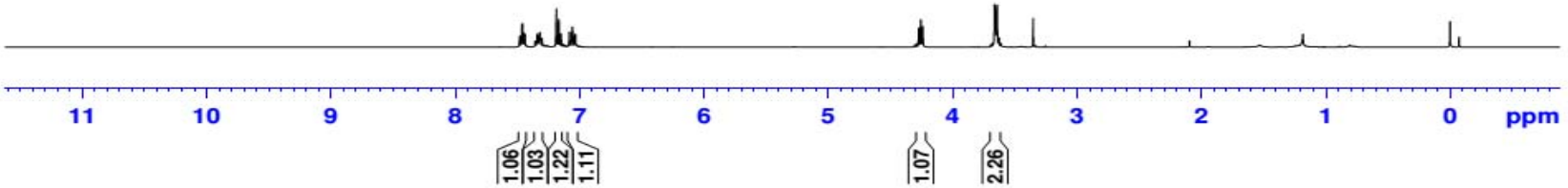
CN
N3
2f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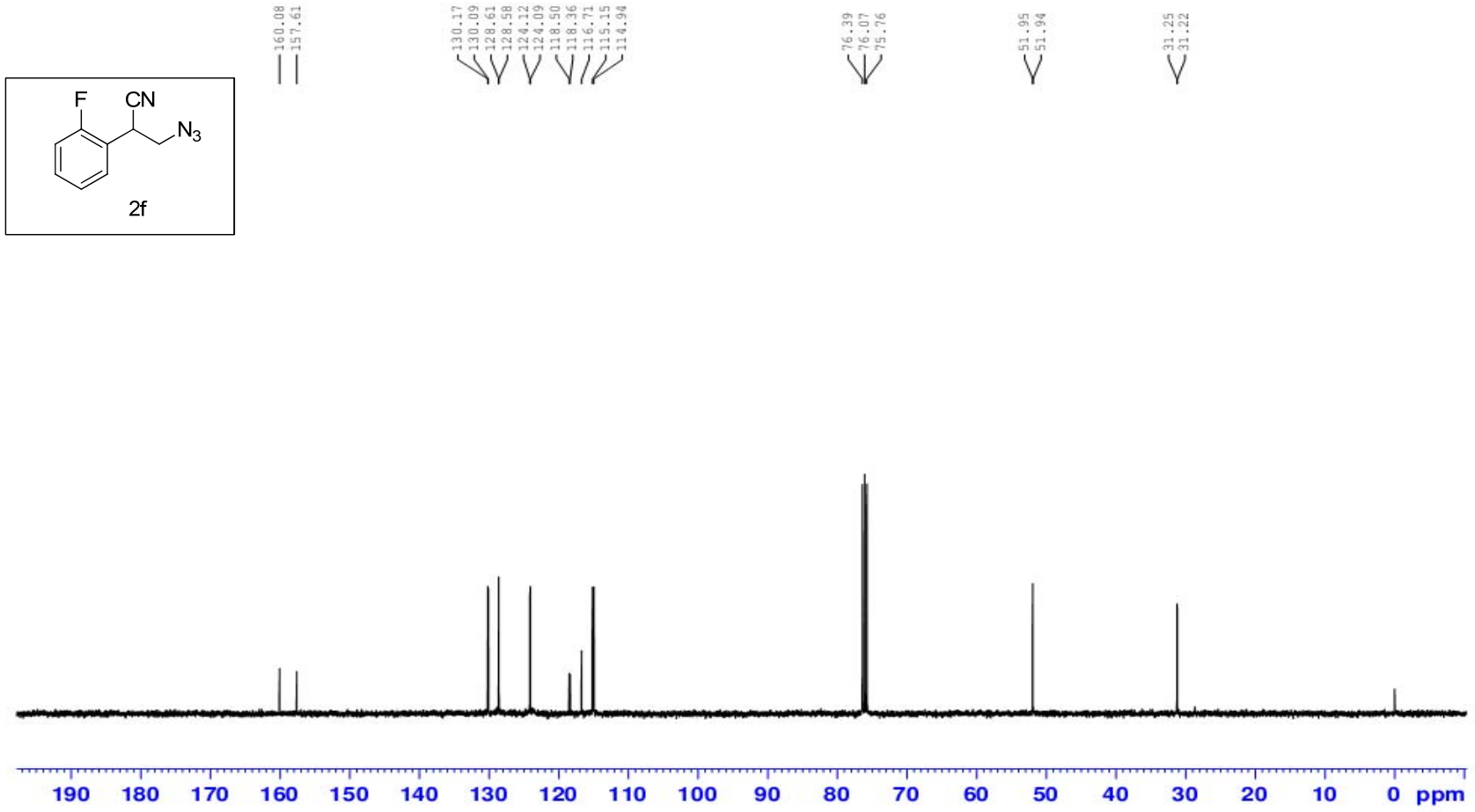
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114.94
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76.07
75.76
51.95
51.94
31.25
31.22
F
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N3
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80
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40
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0
ppm


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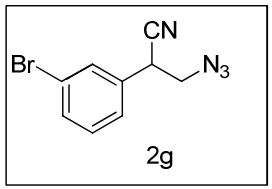
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Br
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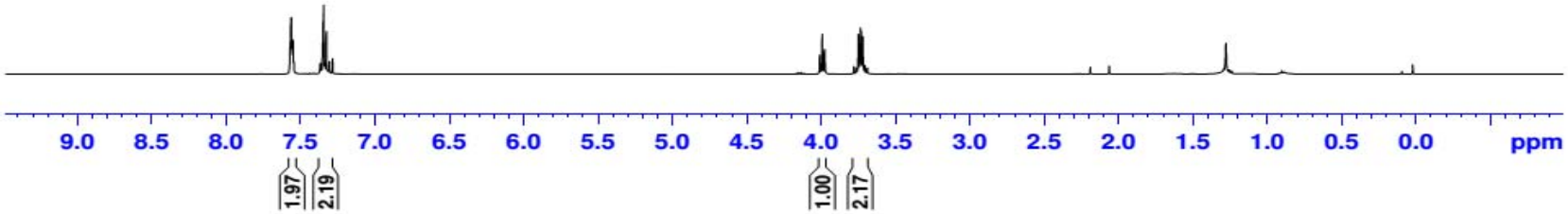
2g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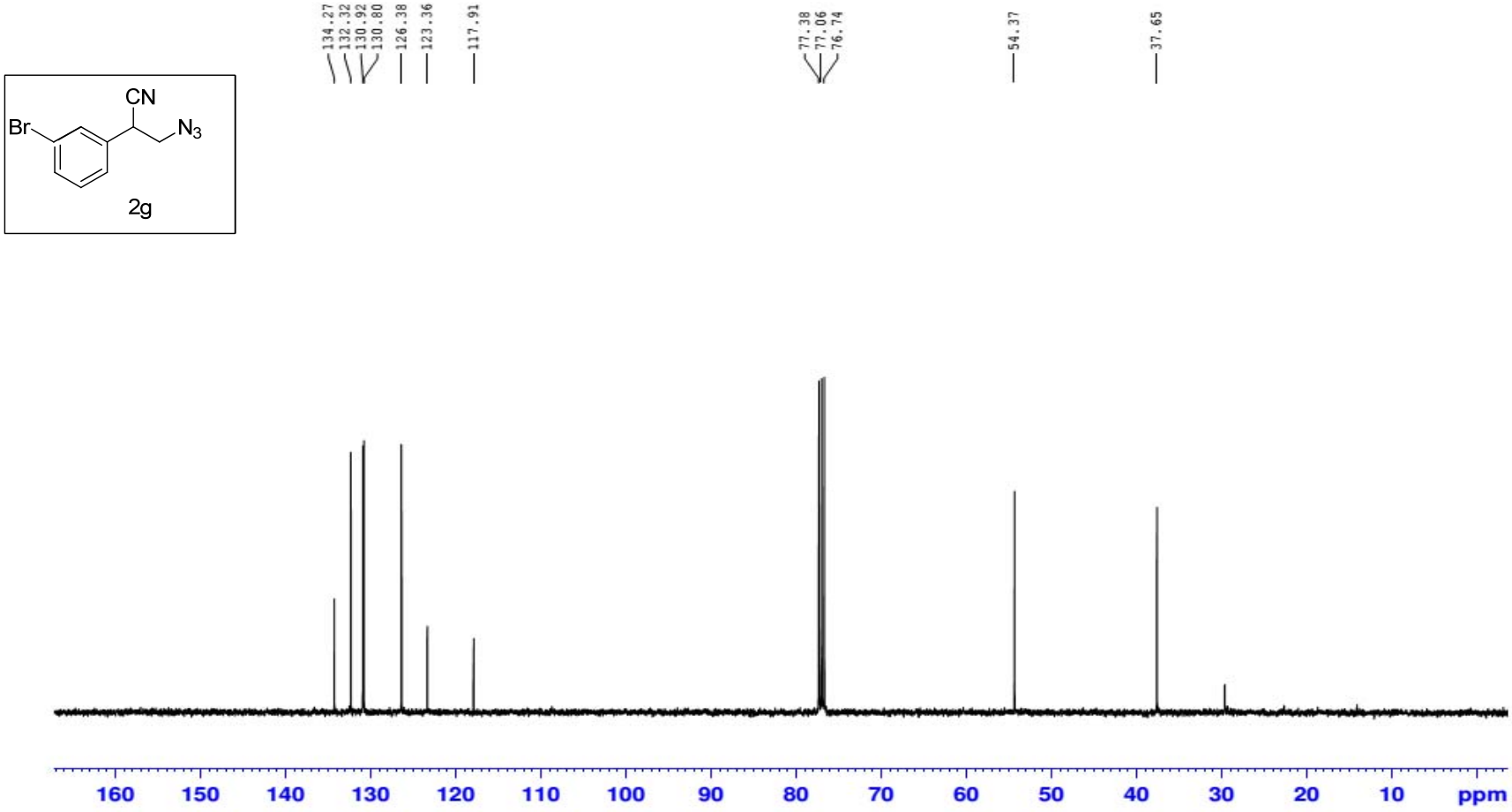
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Br
N3
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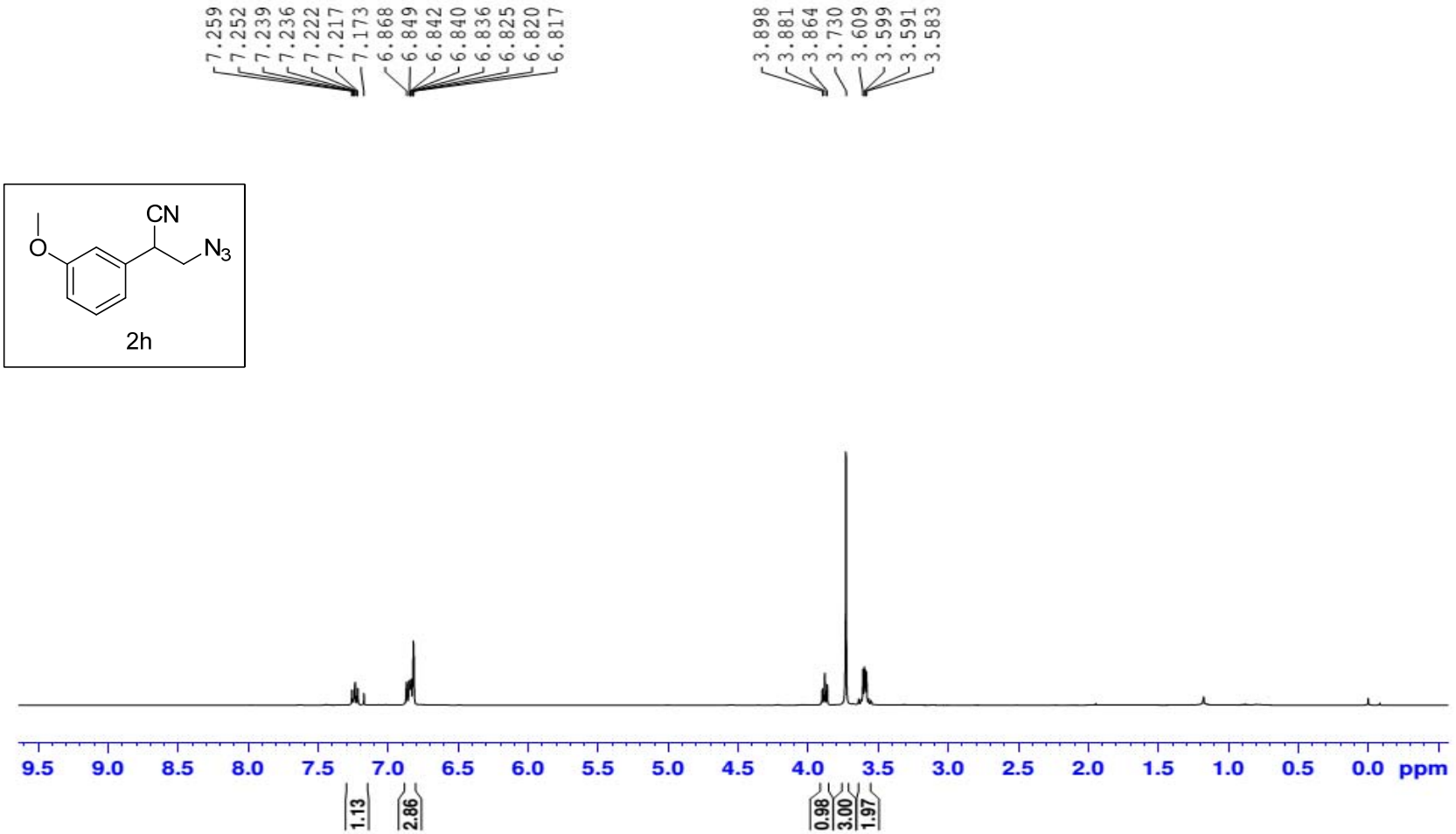
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6.820
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3.881
3.864
3.730
3.609
3.599
3.591
3.583
CN
O
N3
2h
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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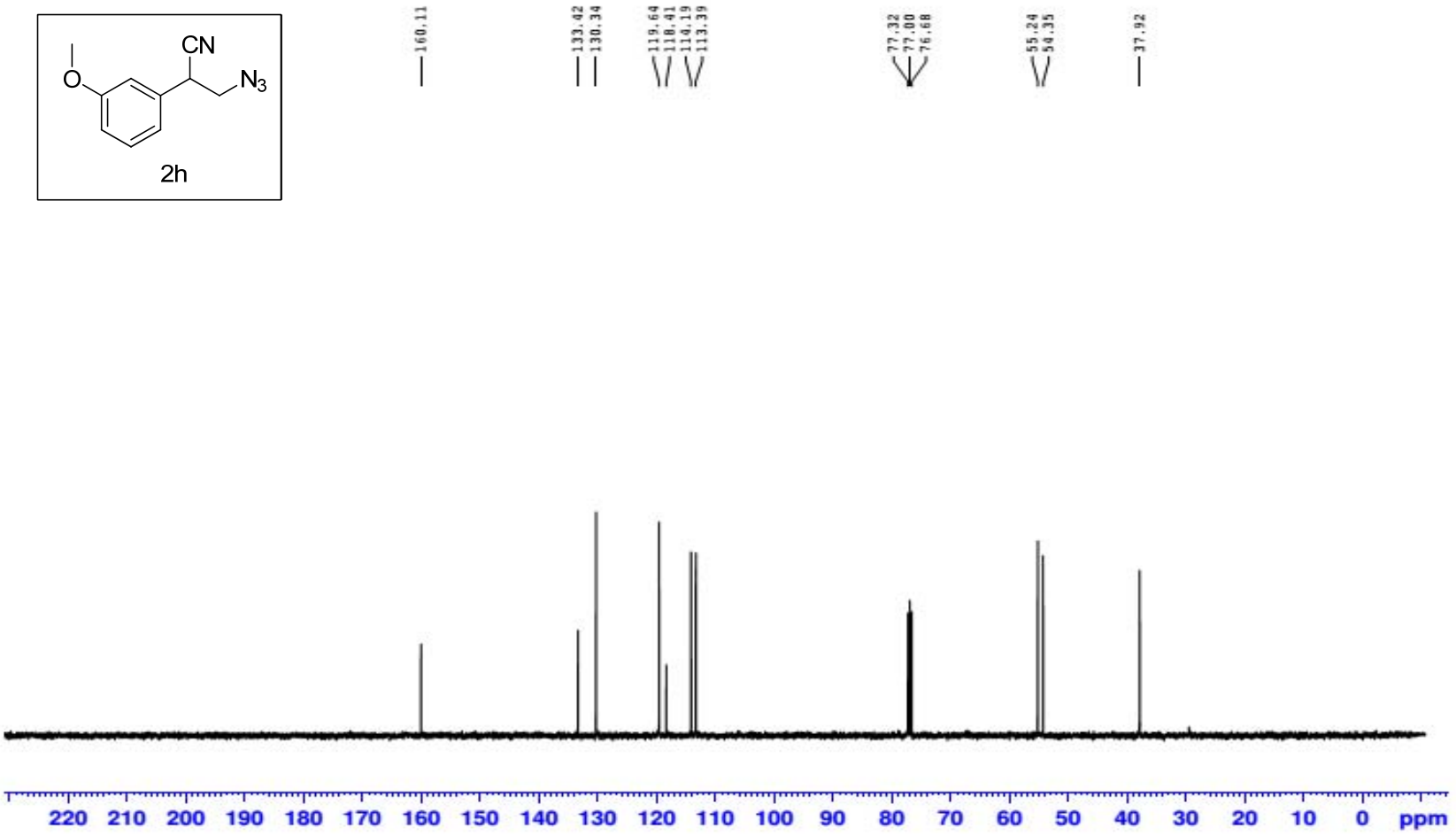
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O
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113.39
77.32
77.00
76.68
55.24
54.35
37.92
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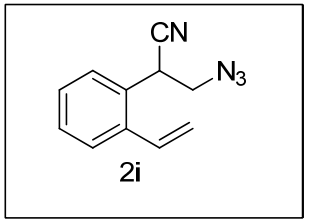
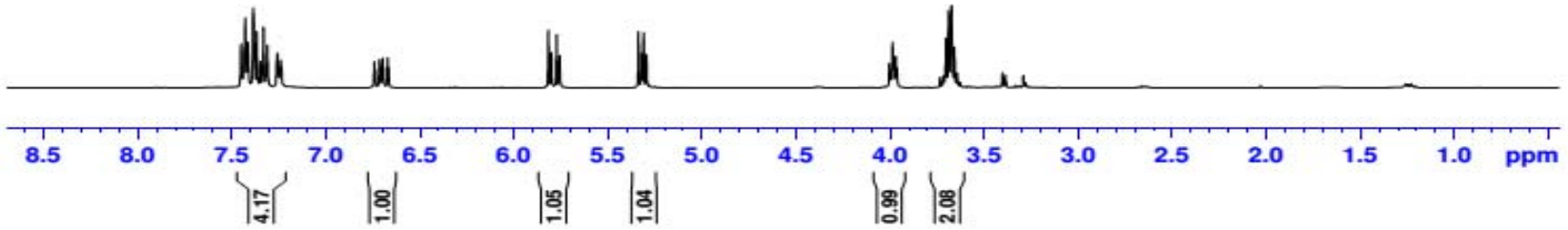

CN
N3
2i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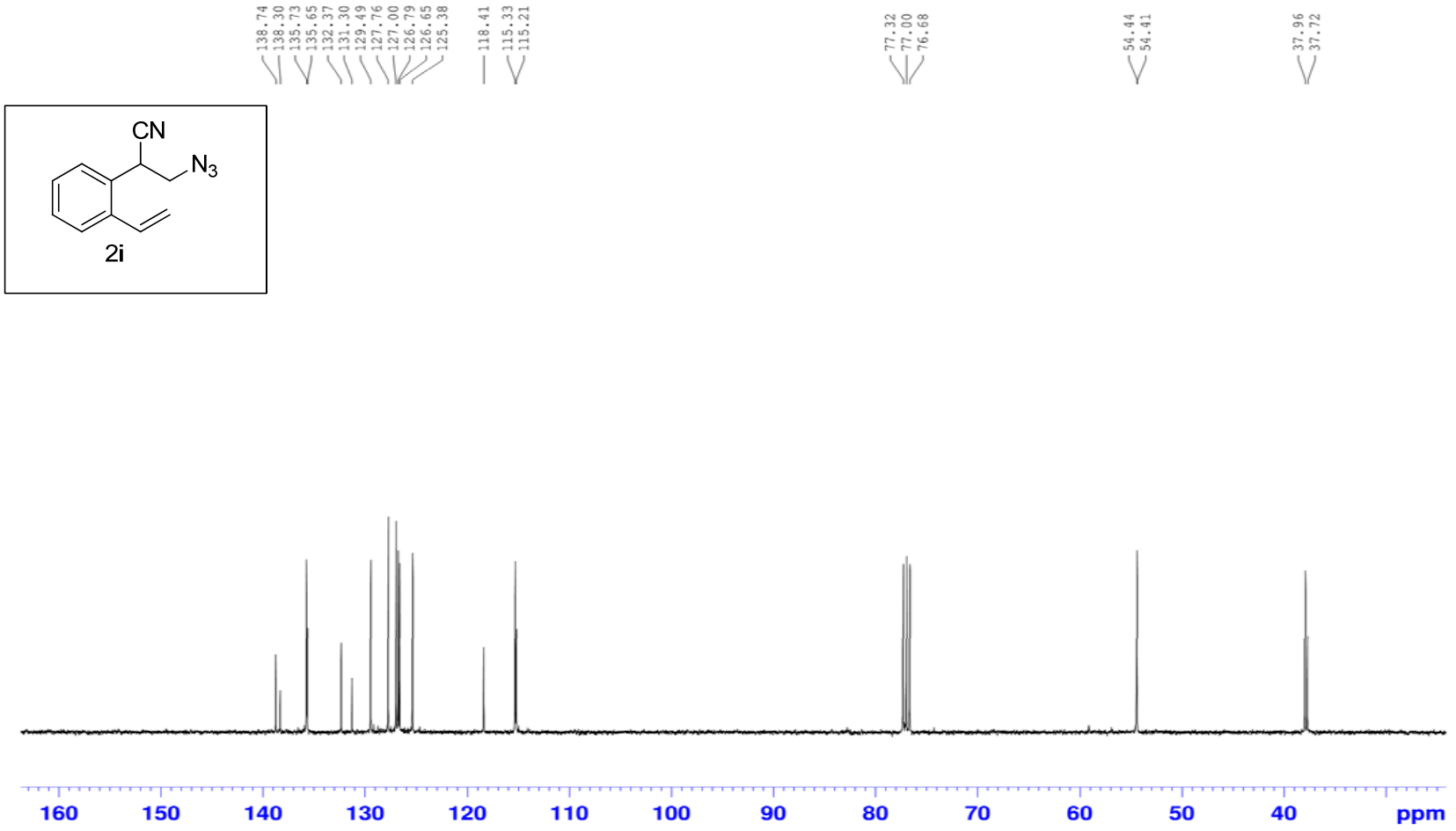
1.04
0.99
2.08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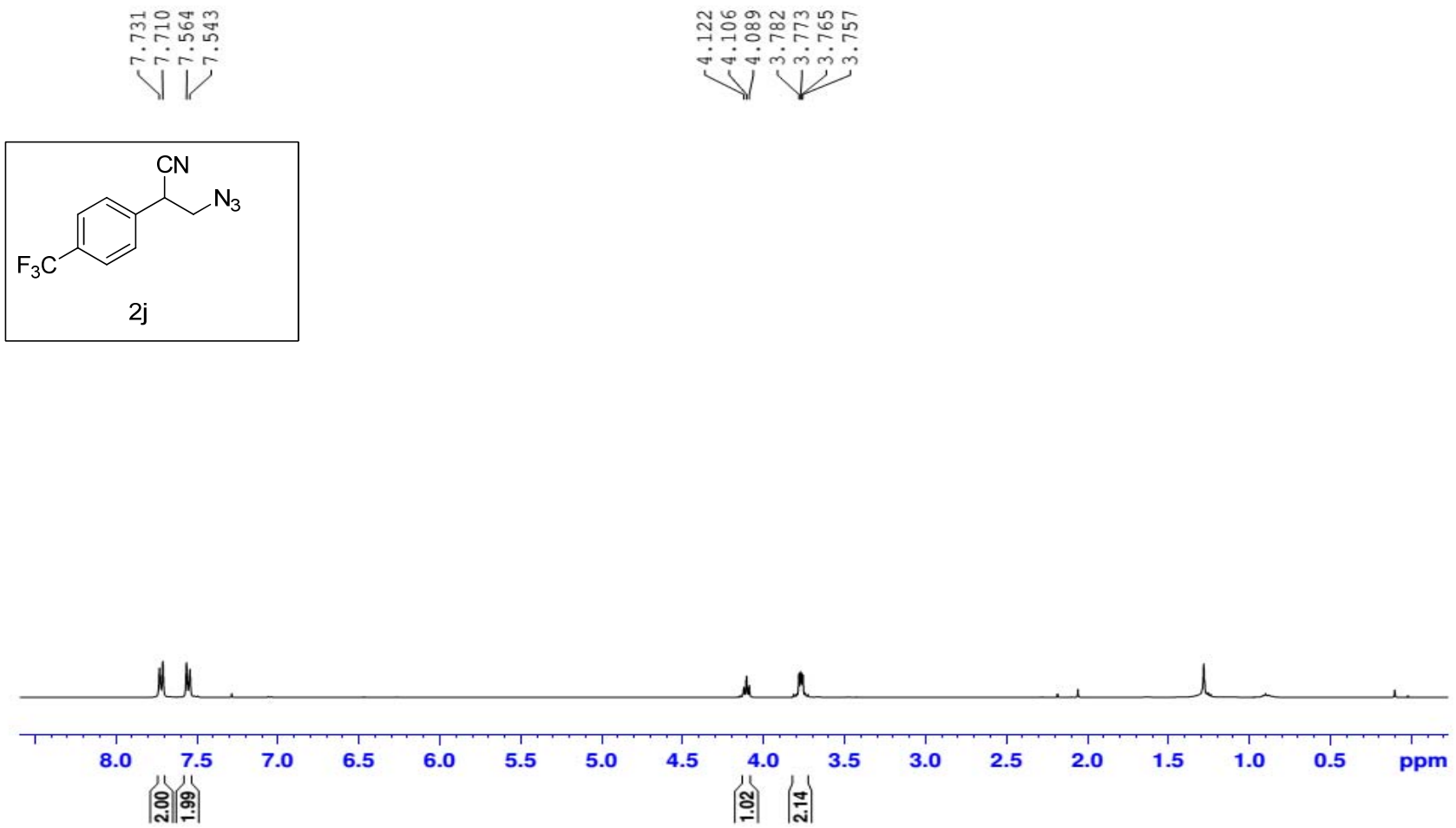
138.30
135.73
135.65
132.37
131.30
129.49
127.76
127.00
126.79
126.65
125.38
118.41
115.33
115.21
77.32
77.00
76.68
54.44
54.41
37.96
37.72
CN
N3
2i
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm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7.710
7.564
7.543
4.122
4.106
4.089
3.782
3.773
3.765
3.757
CN
N3
F3C
2j
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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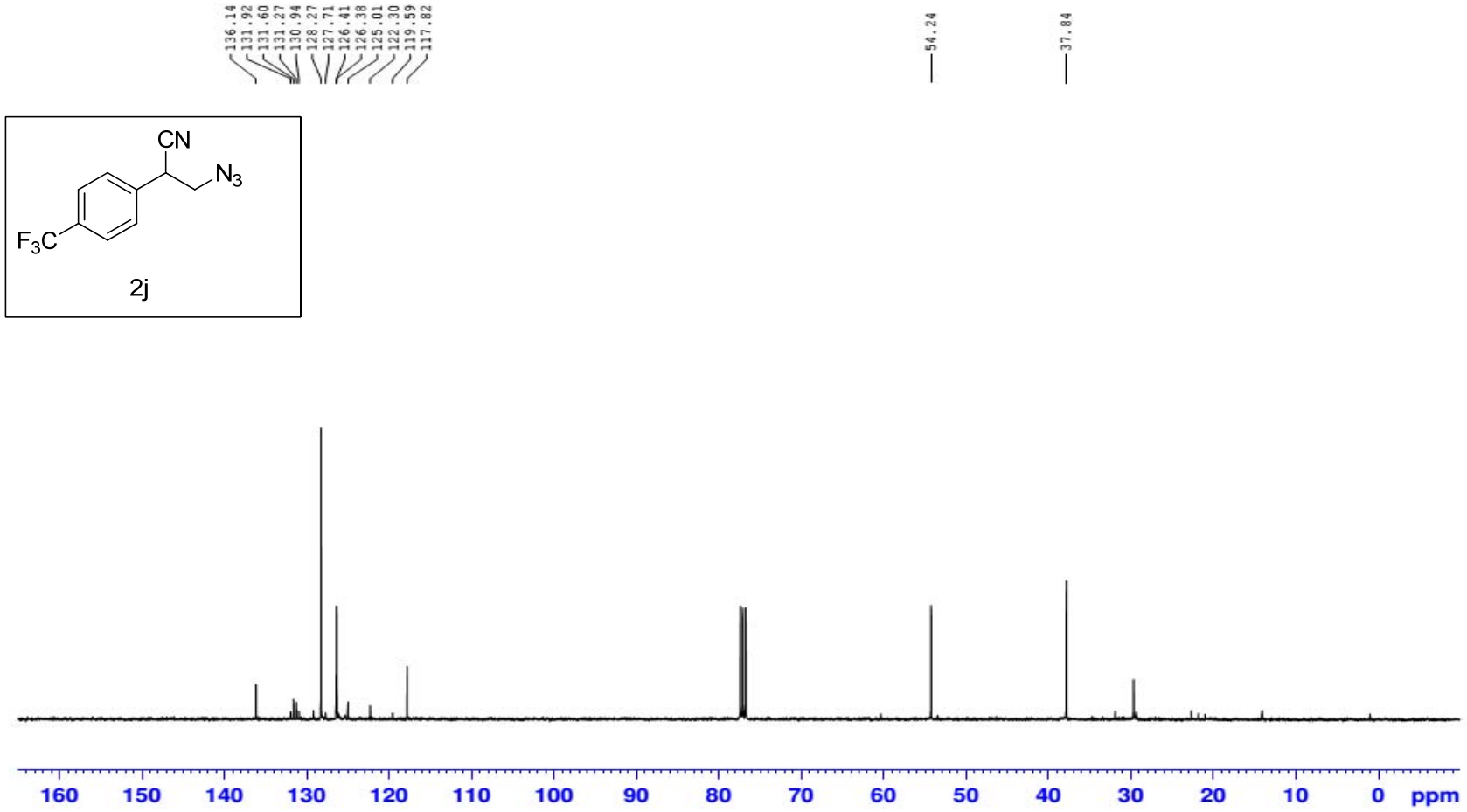
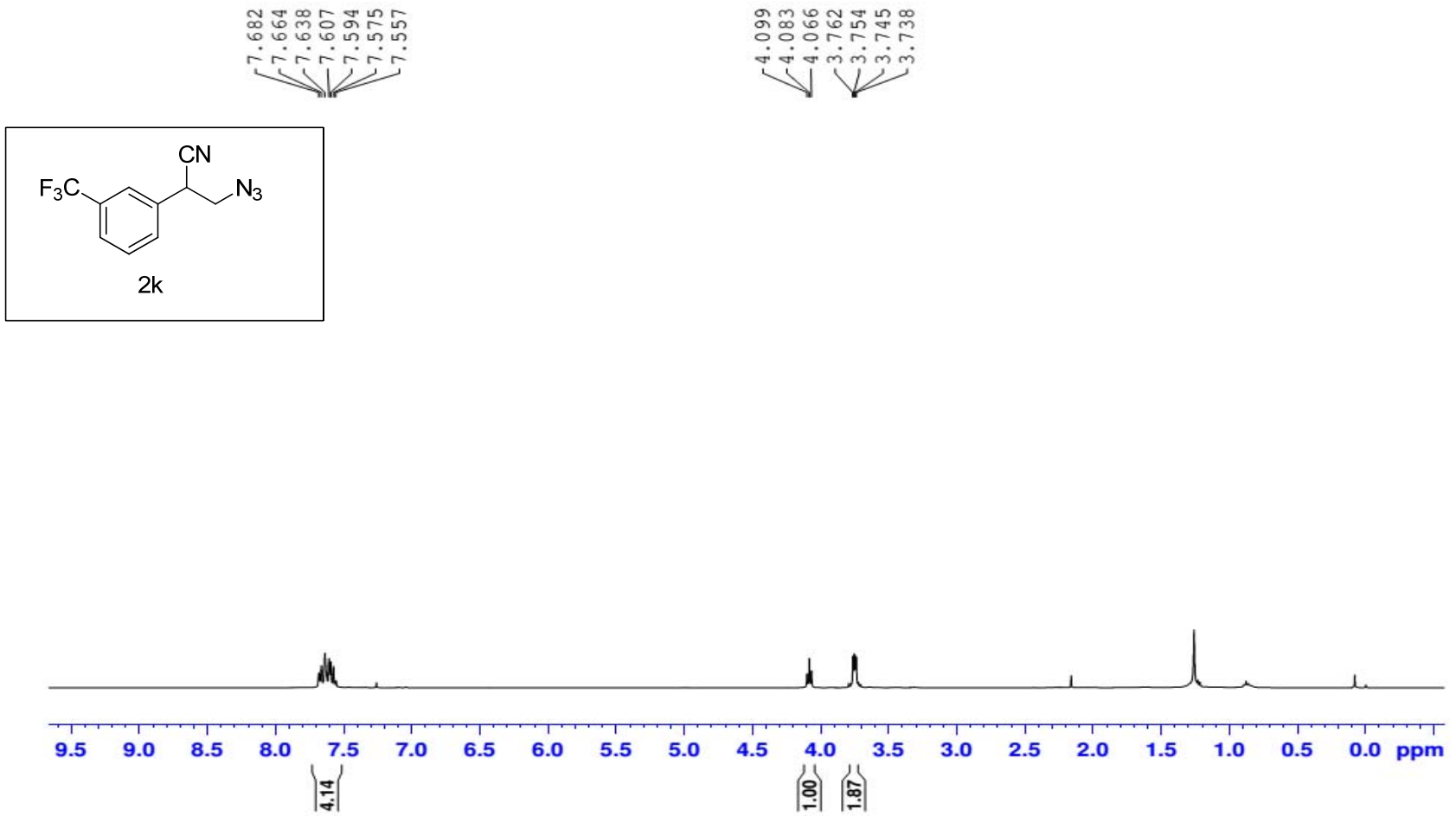
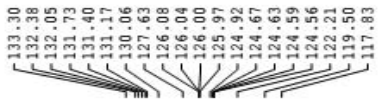
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
1.99
1.02
2.14


136.14
131.92
131.60
131.27
130.94
128.27
127.71
126.41
126.38
125.01
122.30
119.59
117.82
54.24
37.84
CN
N3
F3C
2j
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.682
7.664
7.638
7.607
7.594
7.575
7.557
4.099
4.083
4.066
3.762
3.754
3.745
3.738
CN
F3C
N3
2k
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
ppm
4.14
1.00
1.87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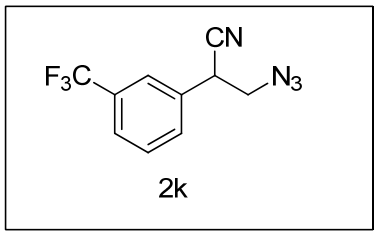
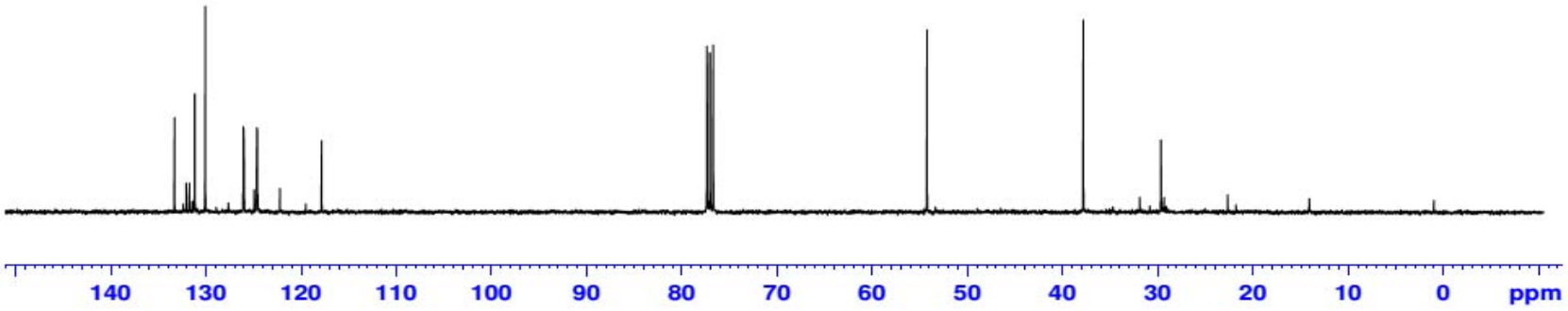
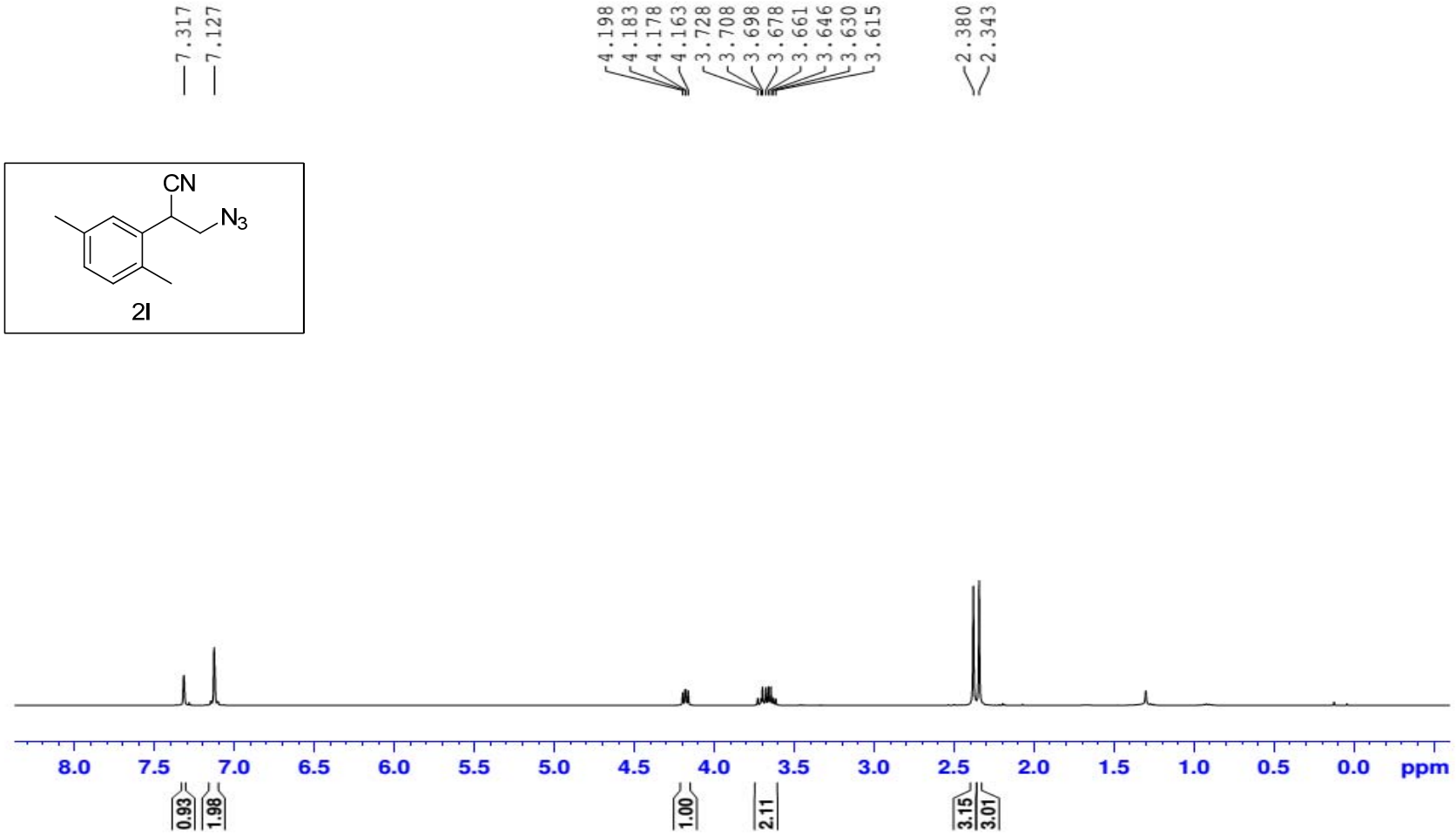
132.38
132.05
131.73
131.40
131.17
130.06
127.63
126.08
126.04
126.00
125.97
124.92
124.67
124.63
124.59
124.56
122.21
119.50
117.83


77.38
77.06
76.74
54.28
37.84


CN
F3C
N3
2k


140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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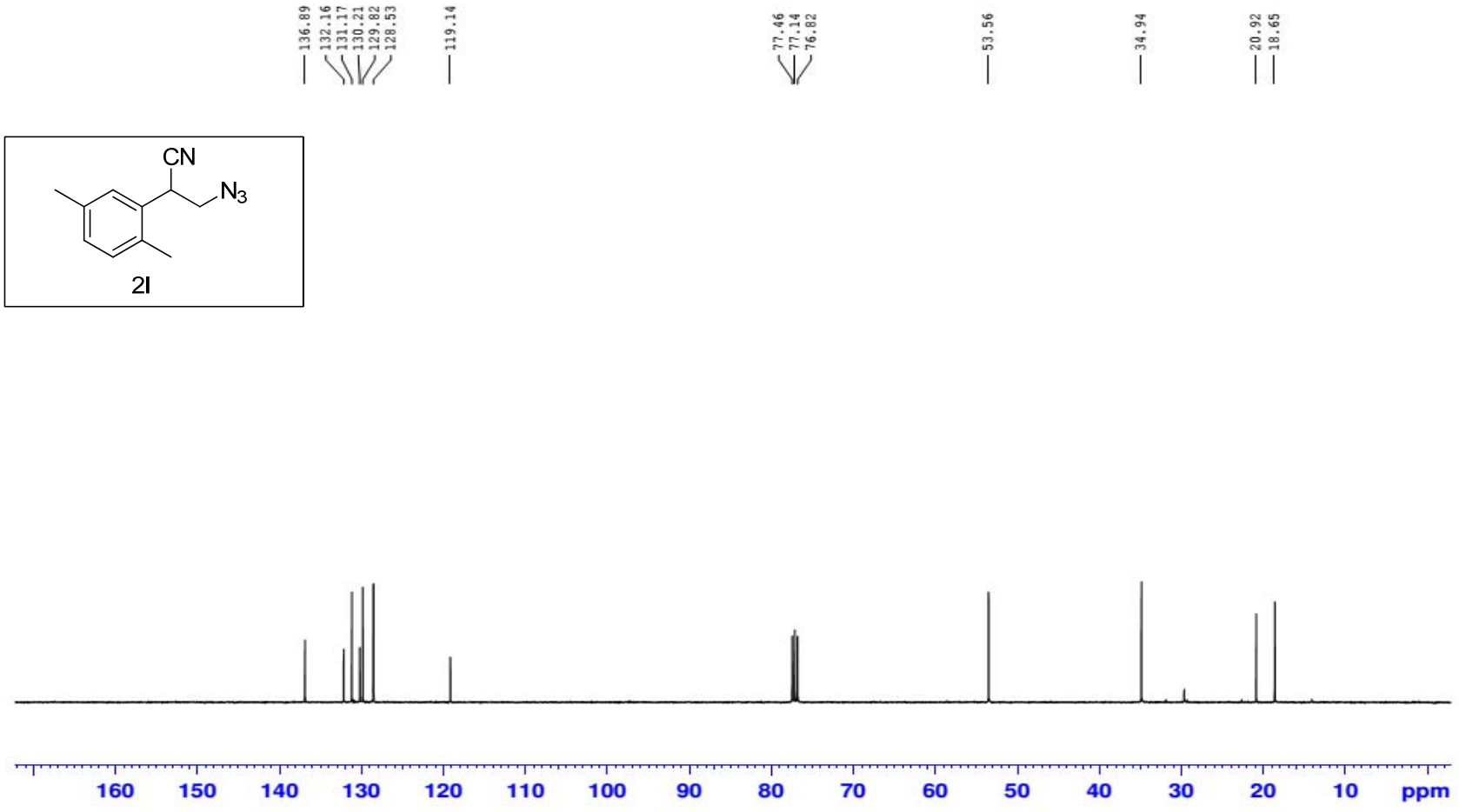
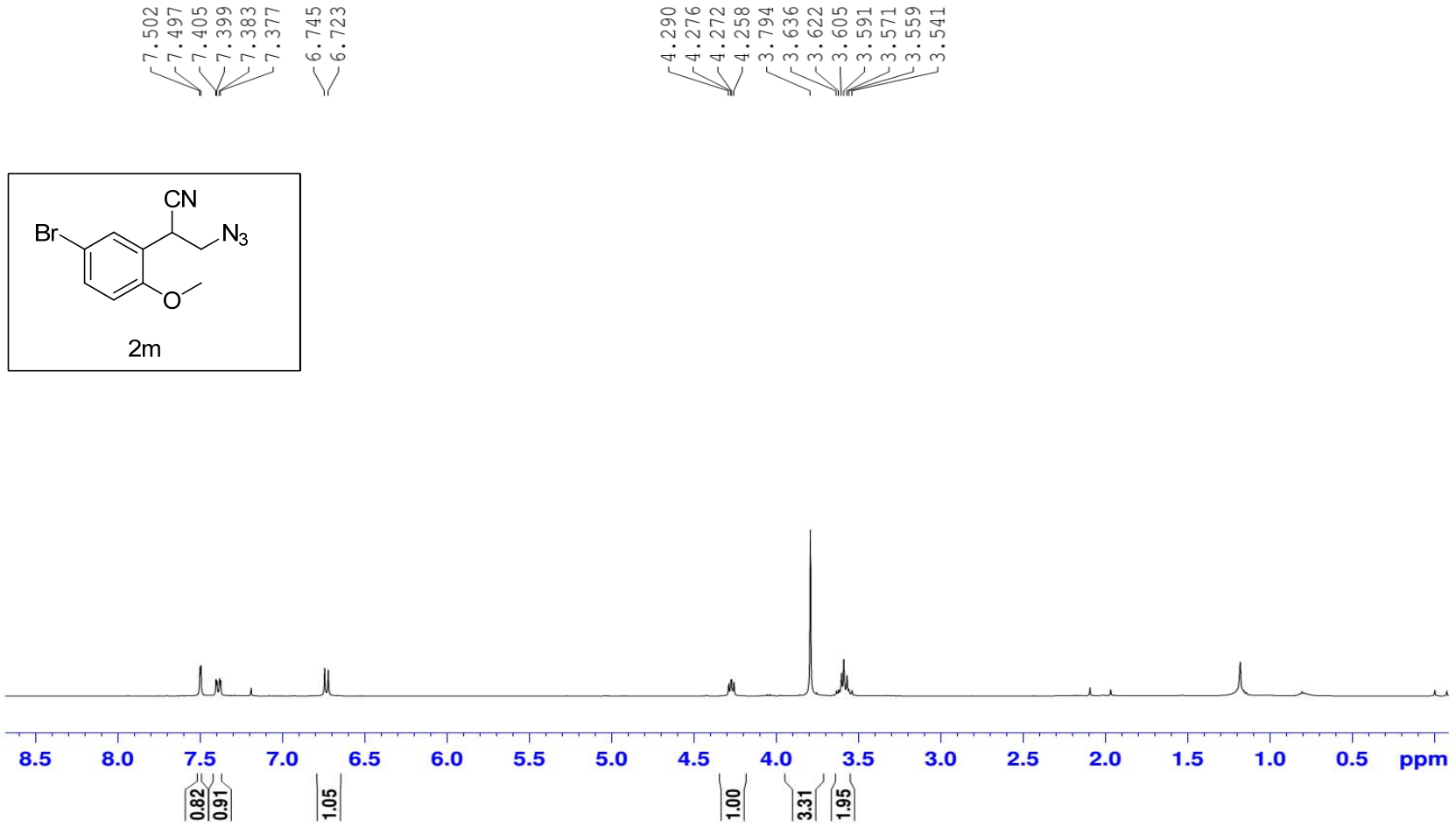
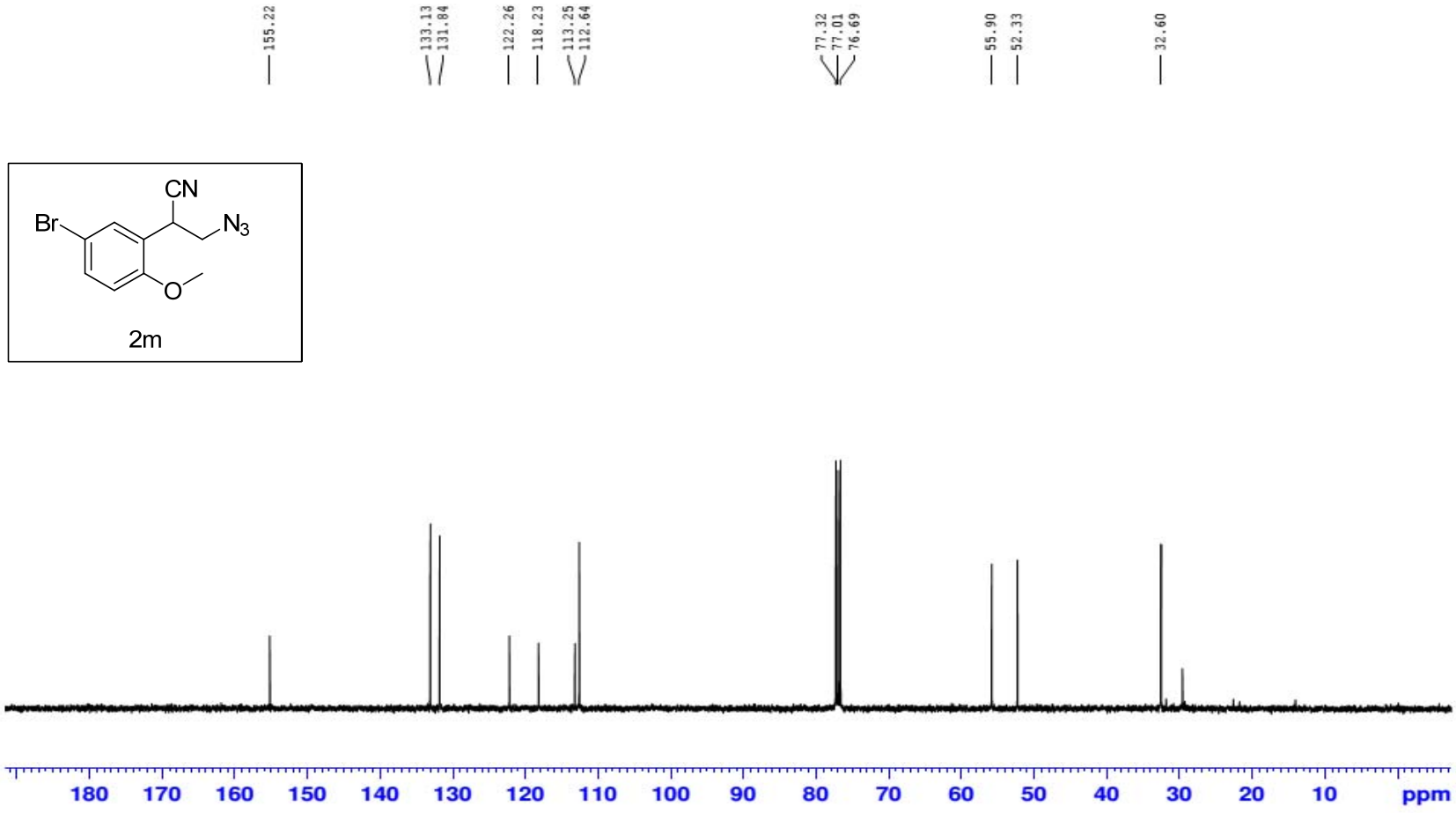
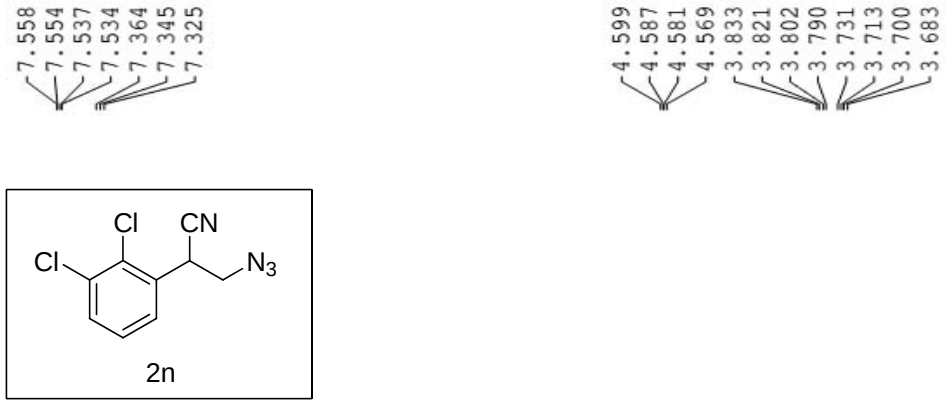
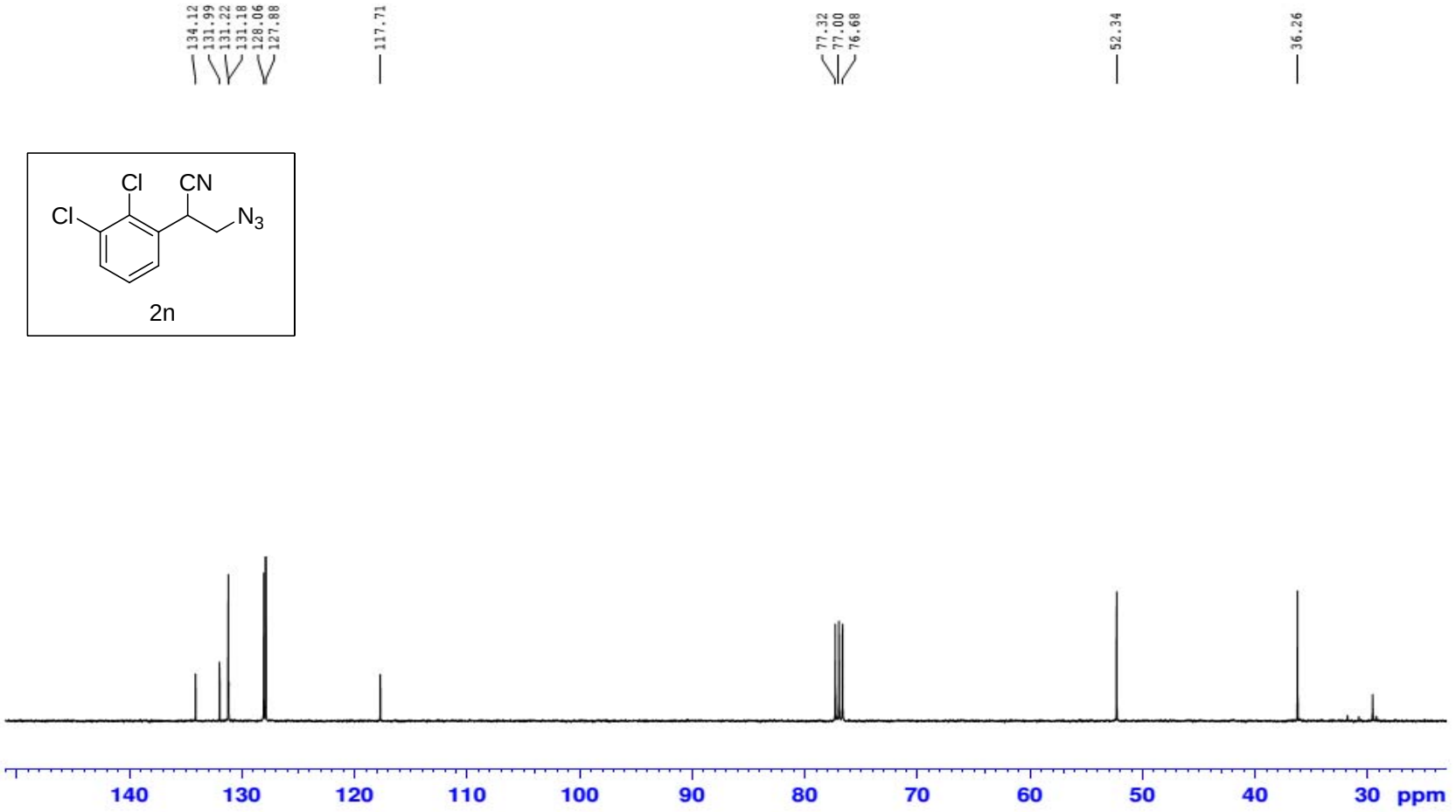
7.127
4.198
4.183
4.178
4.163
3.728
3.708
3.698
3.678
3.661
3.646
3.630
3.615
2.380
2.343
CN
N3
2l
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.93
1.98
1.00
2.11
3.15
3.01

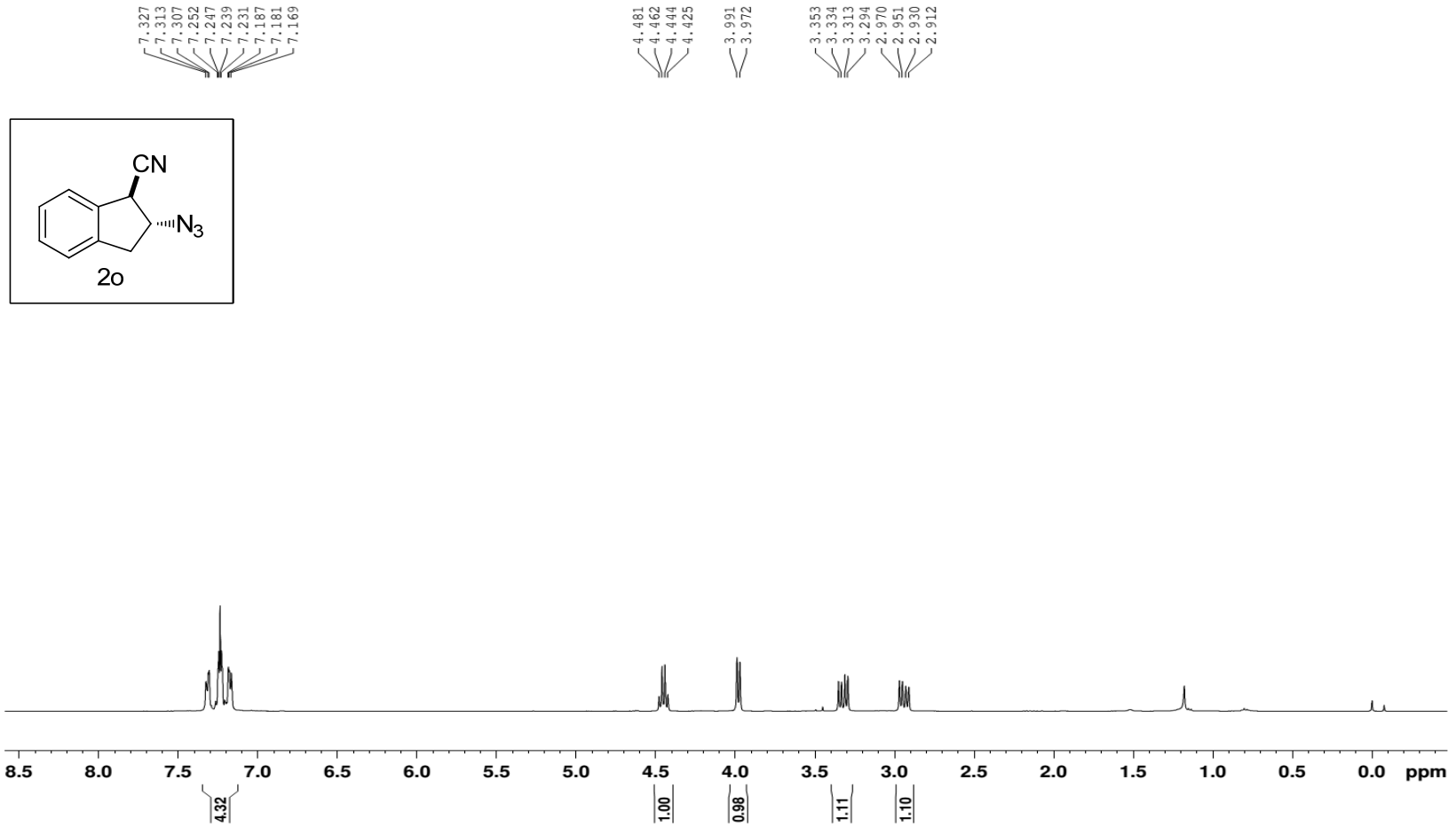

136.89
132.16
131.17
130.21
129.82
128.53
119.14
77.46
77.14
76.82
53.56
34.94
20.92
18.65
CN
N3
2l
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.502
7.497
7.405
7.399
7.383
7.377
6.745
6.723
4.290
4.276
4.272
4.258
3.794
3.636
3.622
3.605
3.591
3.571
3.559
3.541
CN
Br
N3
O
2m
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.82
0.91
1.05
1.00
3.31
1.95


155.22
133.13
131.84
122.26
118.23
113.25
112.64
77.32
77.01
76.69
55.90
52.33
32.60
CN
Br
N3
O
2m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.558
7.554
7.537
7.534
7.364
7.345
7.325
4.599
4.587
4.581
4.569
3.833
3.821
3.802
3.790
3.731
3.713
3.700
3.683
Cl
CN
Cl
N3
2n
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.03
1.10
1.01
1.08
1.12


134.12
131.99
131.22
131.18
128.06
127.88
117.71
77.32
77.00
76.68
52.34
36.26
Cl
CN
Cl
N3
2n
140
130
120
110
100
90
80
70
60
50
40
30
ppm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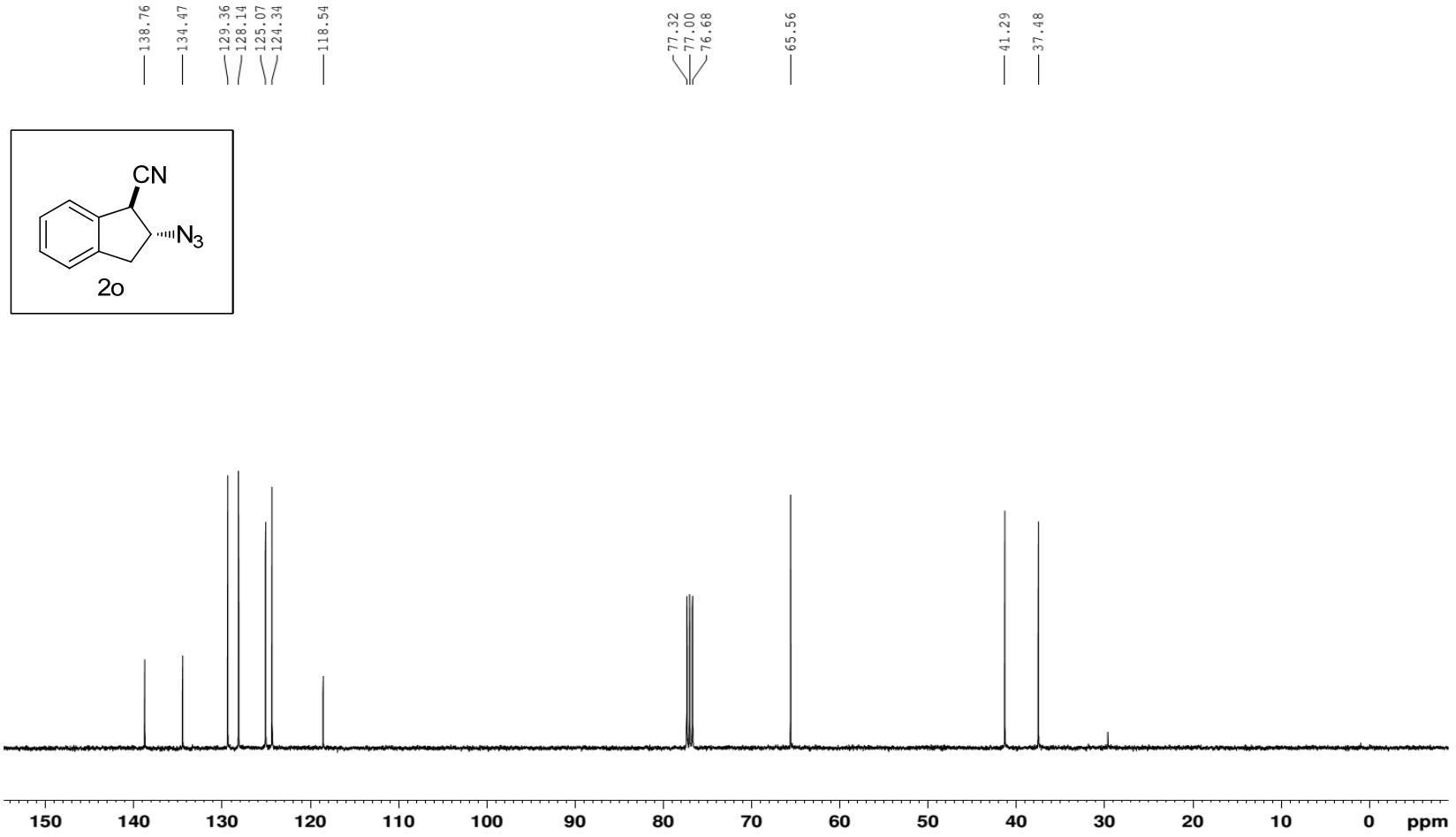
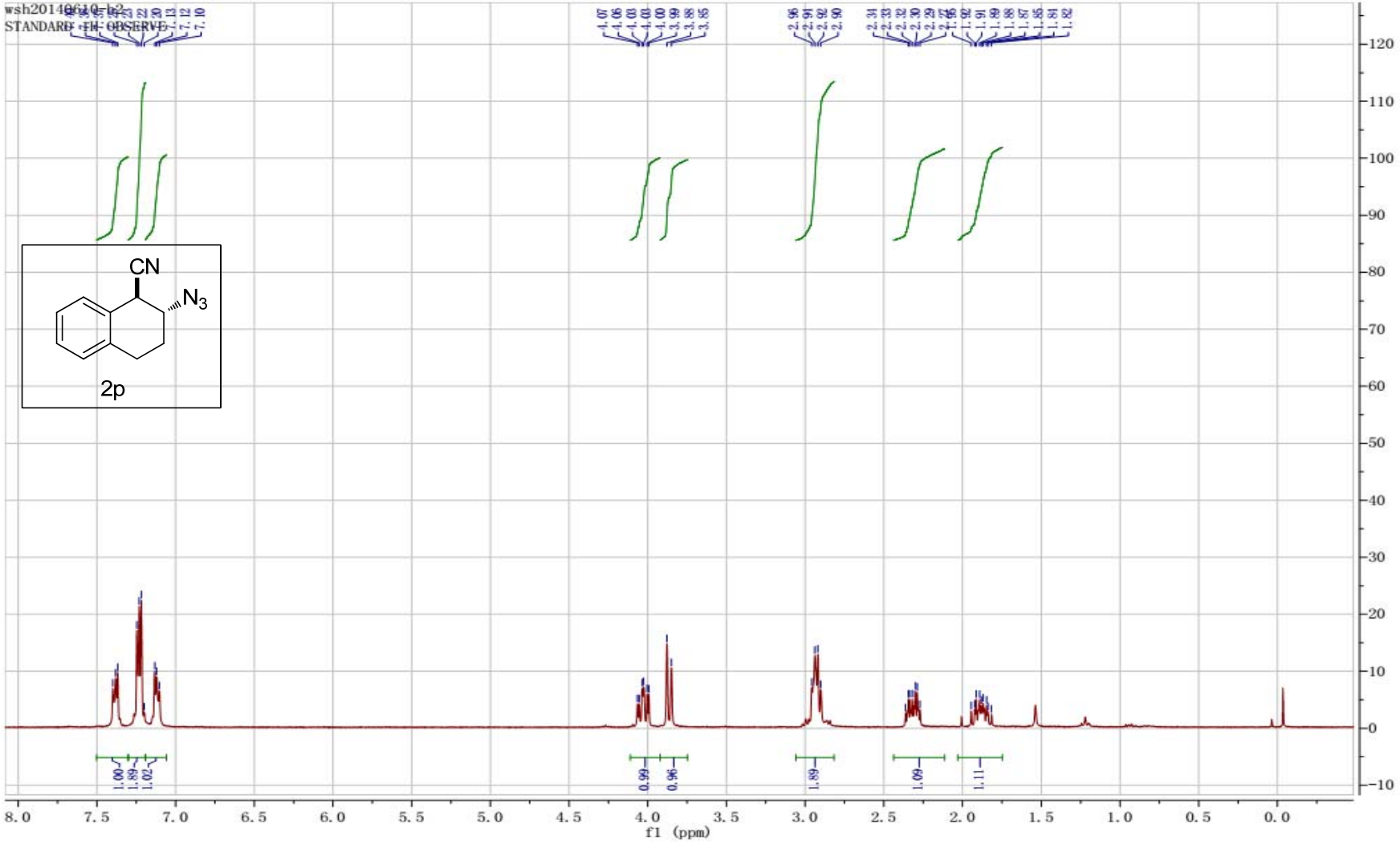
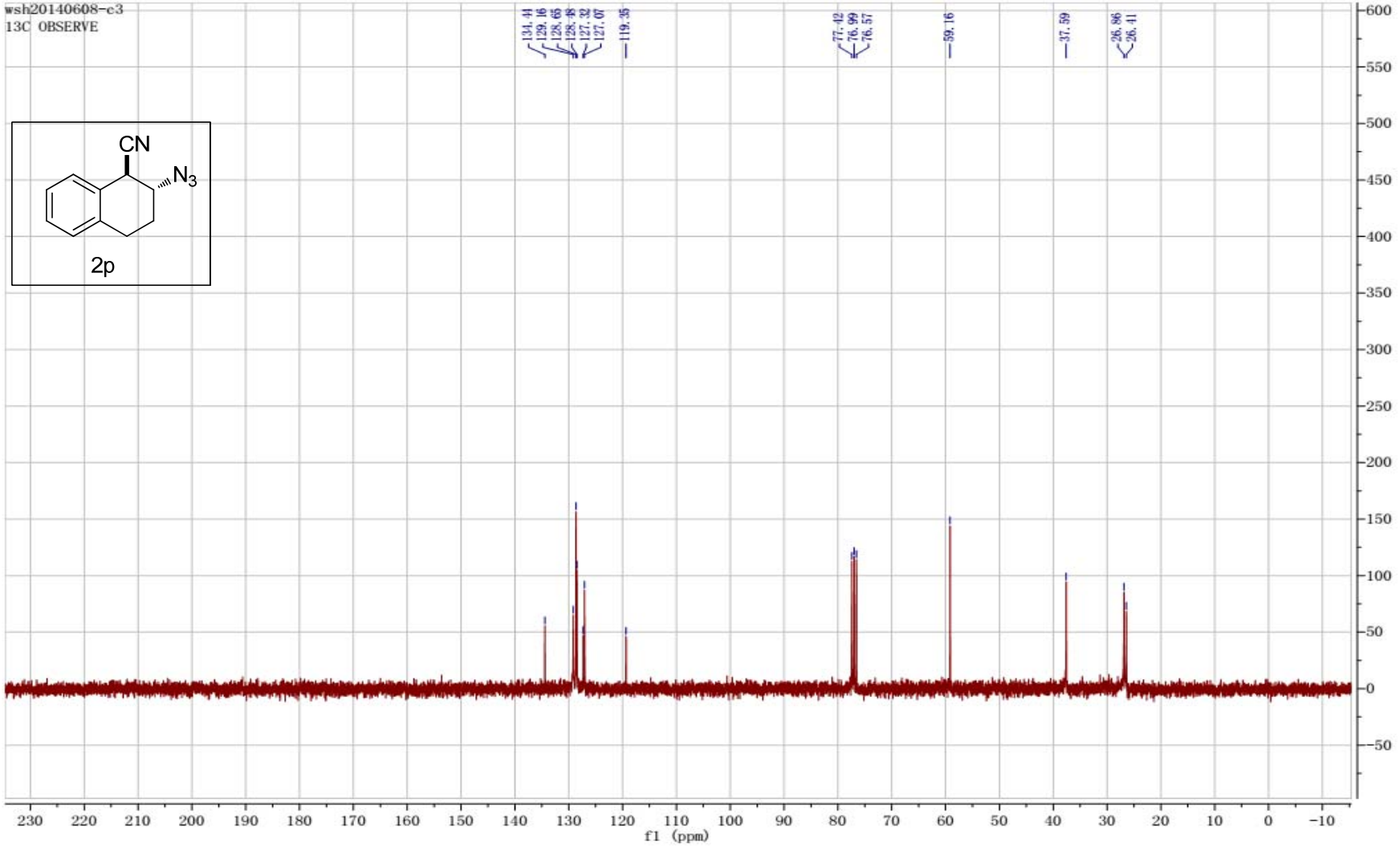
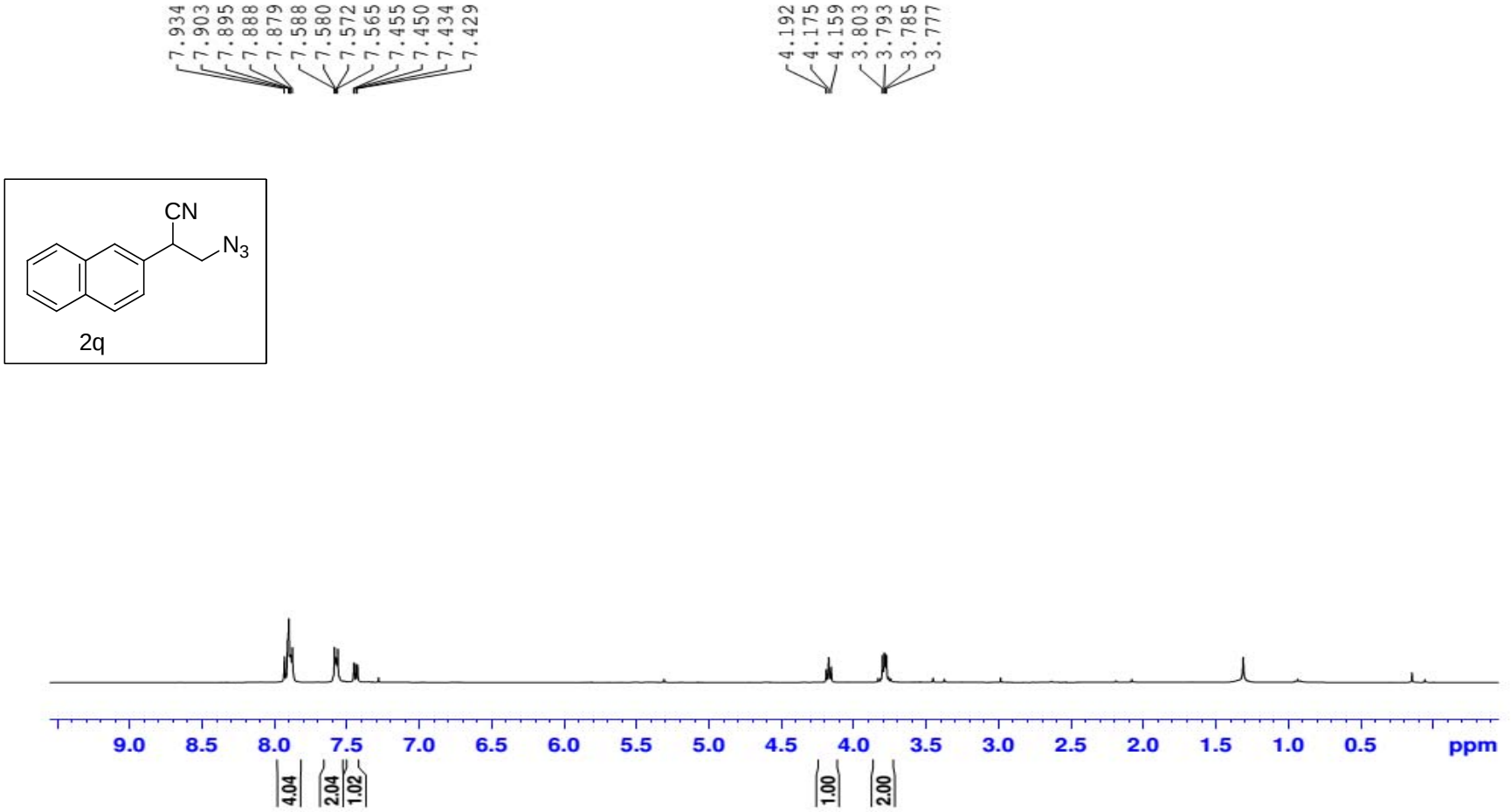
7.313
7.307
7.252
7.247
7.239
7.231
7.187
7.181
7.169
4.481
4.462
4.444
4.425
3.991
3.972
3.353
3.334
3.313
3.294
2.970
2.951
2.930
2.912
CN
N3
2o
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
4.32
1.00
0.98
1.11
1.10


138.76
134.47
129.36
128.14
125.07
124.34
118.54
77.32
77.00
76.68
65.56
41.29
37.48
CN
N3
2o
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


wsh20140610-h2
STANDARD 1H OBSERVE
CN
N3
2p
f1 (ppm)


wsh20140608-c3
13C OBSERVE
CN
N3
2p
134.41
129.16
128.65
128.48
127.32
127.07
119.35
77.42
76.99
76.57
59.16
37.59
26.86
26.41
f1 (ppm)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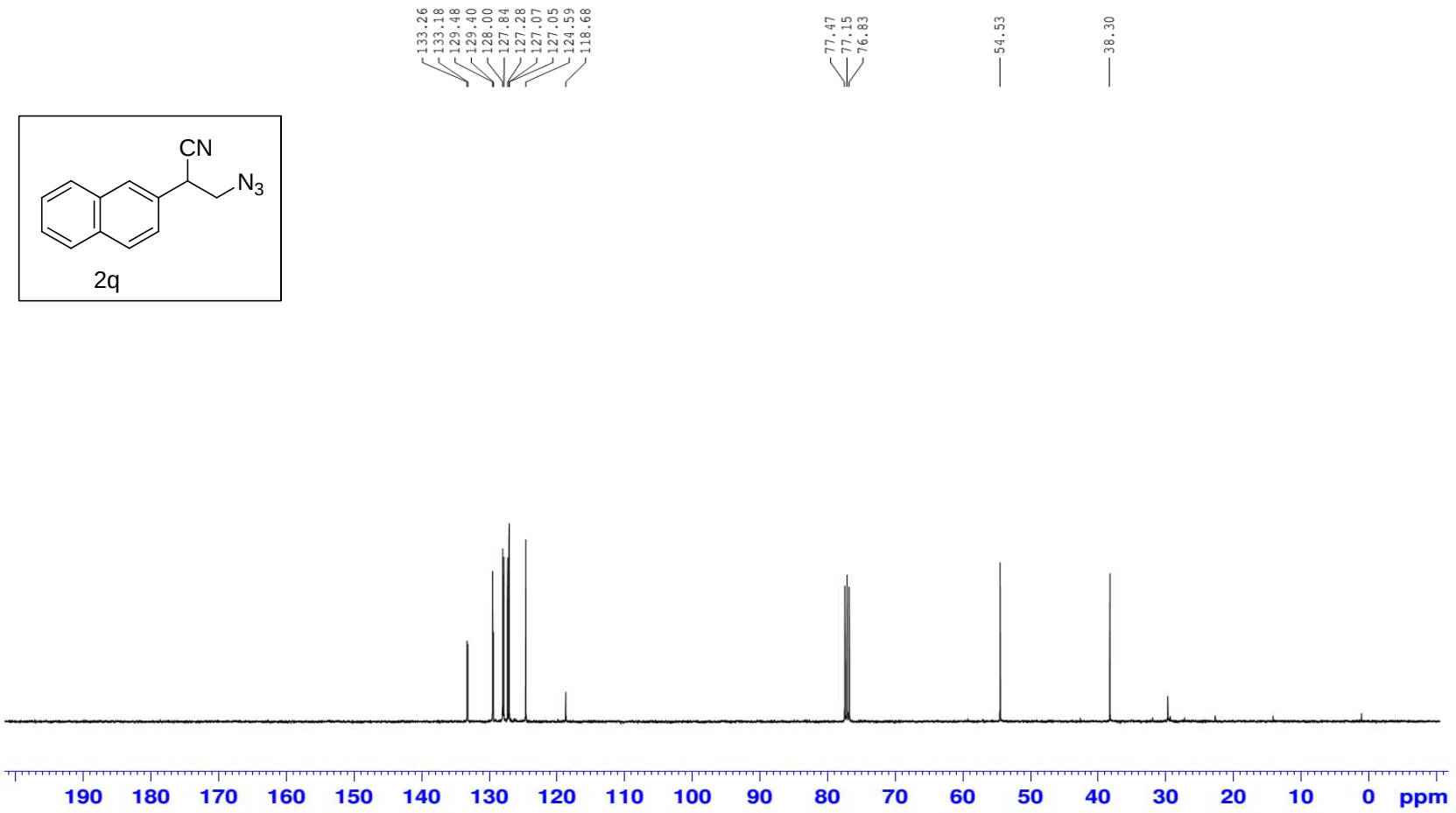
7.879
7.588
7.580
7.572
7.565
7.455
7.450
7.434
7.429
4.192
4.175
4.159
3.803
3.793
3.785
3.777
CN
N3
2q
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
4.04
2.04
1.02
1.00
2.00


133.26
133.18
129.48
129.40
128.00
127.84
127.28
127.07
127.05
124.59
118.68
77.47
77.15
76.83
54.53
38.30
CN
N3
2q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm