Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for:

Fe-Catalyzed Denitrative Cyanoalkylation of Nitroalkenes with Cycloketone Oxime Esters via Reductive C-C Bond Formation

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CONTENTS

1. General experimental details and materials

All non-aqueous reactions and manipulations were using standard Schlenk techniques. All solvents before use were dried and degassed by standard methods and stored under argon atmosphere. All reactions were monitored by TLC with silica gel-coated plates. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. ^{1}H NMR, ^{13}C NMR spectra were measured in $CDCl_3$ and recorded on Bruker Avance III 500 MHz, and Bruker Avance III HD (600 MHz, Bruker BioSpin, Switzerland) spectrometer. Chemical shifts (δ) were given in ppm, referenced to the residual proton resonance of $CDCl_3$ (7.26), to the carbon resonance of $CDCl_3$ (77.16). Coupling constants (*J*) were given in Hertz (Hz). The term m, q, t, d, s referred to multiplet, quartet, triplet, doublet, singlet. High resolution mass spectra were recorded on a high-resolution mass spectrometer using electrospray ionization (ESI) techniques. Catalysts, reductants, ligands, additives and solvents were all purchased from Energy.

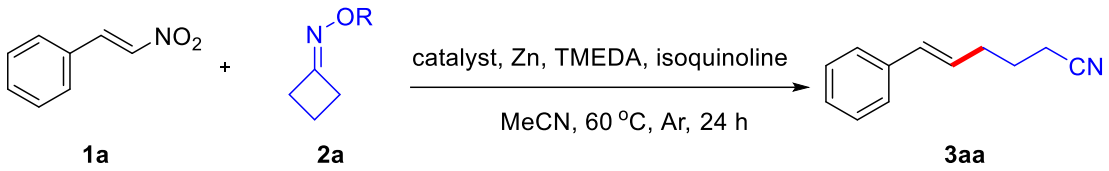
Synthesis of substrates (1a-1o): The substrates **1a-1o** were prepared according to known methods. [1]

Synthesis of substrates (2a-2j): The substrates **2a-2j** were prepared according to known methods. [2]

2. Optimization of the reaction conditions

(*E*)-(2-nitrovinyl)benzene **1a** (44.7 mg, 0.30 mmol) and cyclobutanone *O*-(4-(trifluoromethyl)benzoyl) oxime **2a** (115.7 mg, 0.45 mmol), catalyst (x mol%), ligand (x mol%), reductant (x equiv.), addition (x equiv.) and solvent (1.0 mL) were added to a flame-dried Young-type tube. The mixture was degassed by the freeze-thaw method, and then stirred under argon at designed temperature for designed hours. After cooling to room temperature, solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel and eluted with ethyl acetate/petroleum ether (1/20) to afford the desired product **3aa**. For solvent with high boiling point, the reaction mixture was treated with saturated NH_4Cl aqueous solution (10 mL) and extracted with ethyl acetate (4 × 10 mL). The solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel and eluted with ethyl acetate/petroleum ether (1/50-1/2) to afford the desired products **3aa**.

Table S1. Screening of the catalyst [a]



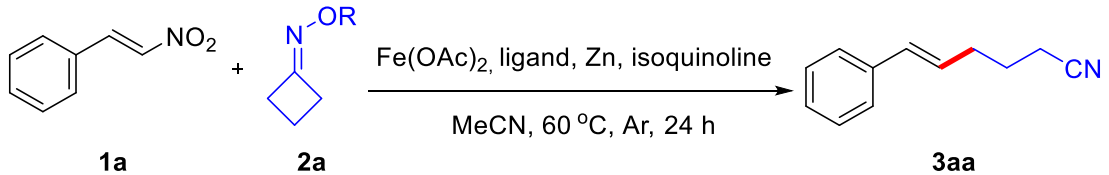
1a **2a** **3aa**

R = COC_6H_4-4-CF_3

entry	catalyst	yield (%)
1	$Ni(acac)_2$	ND
2	$NiBr_2$	10
3	$Cu(acac)_2$	ND
4	$CuBr_2$	34
5	$Fe(acac)_2$	49
6	Ferrocene	8
7	$FeCl_2$	44
8	$FeCl_3$	45
9	$Fe(OTf)_2$	43
10	$Fe(OTf)_3$	42
11	FeC_2O_4	49
12	**$Fe(OAc)_2$**	**51**

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), catalyst (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), TMEDA (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and MeCN (1.0 mL) under Ar at 60 °C for 24 h, isolated yield.

Table S2. Screening of the ligand [a]



1a **2a** **3aa**

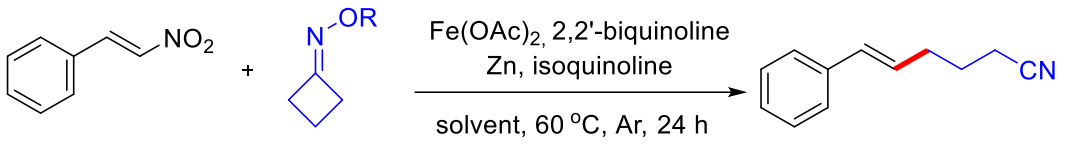
R = COC_6H_4-4-CF_3

entry	ligand	yield (%)
1	TMEDA	51
2	DPPM	49
3	DPPE	46
4	DPPP	44
5	DPPB	46
6	DPPF	53
7	Xantphos	53
8	**2,2'-biquinoline**	**57**
9	BINAP	51

10	S-phos	51
11	PCy_3	23
12	$P(OMe)_3$	44
13	PPh_3	50
14	dmbpy	51
15	1,10-phenanthroline	48
16	DMAP	52

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), ligand (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and MeCN (1.0 mL) under Ar at 60 °C for 24 h, isolated yield.

Table S3. Screening of mixed solvent [a]



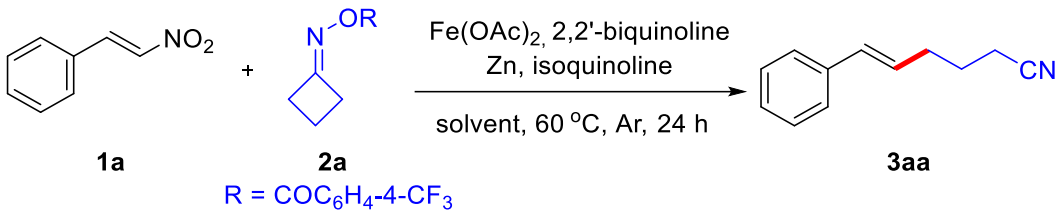
1a **2a** **3aa**

R = COC_6H_4-4-CF_3

entry	mixed solvent (1 : 1)	yield (%)
1	**DMA : PhMe**	**57**
2	DMA : THF	53
3	DMA : MeCN	55
4	DMA : DMF	54
5	DMA : DMSO	48
6	DMA : DCE	55
7	DMA : NMP	54
8	DMA : Dioxane	54
9	DMA : GDME	56

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and mixed solvent (1.0 mL) under Ar at 60 °C for 24 h, isolated yield.

Table S4. Screening of the ratio of DMA/PhMe [a]



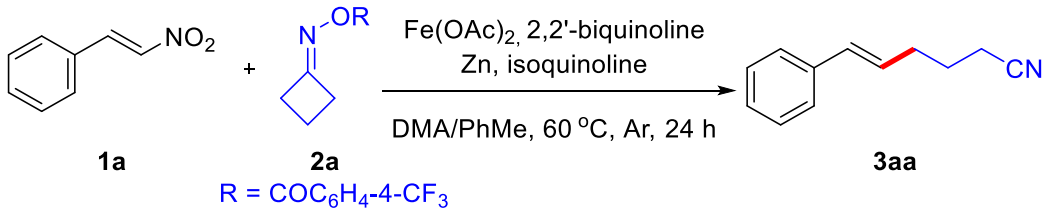
1a **2a** **3aa**

R = COC_6H_4-4-CF_3

entry	solvent (V_{DMA} : V_{PhMe})	yield (%)
1	1 : 4	54
2	2 : 3	57
3	1 : 1	57
3	3 : 2	55
4	**4 : 1**	**60**
5	10 : 1	57
6	20 : 1	56
7	50 : 1	55
8	100 : 1	51

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and DMA/PhMe (1.0 mL) under Ar at 60 °C for 24 h, isolated yield.

Table S5. Screening the ratio of 1a and 2a [a]



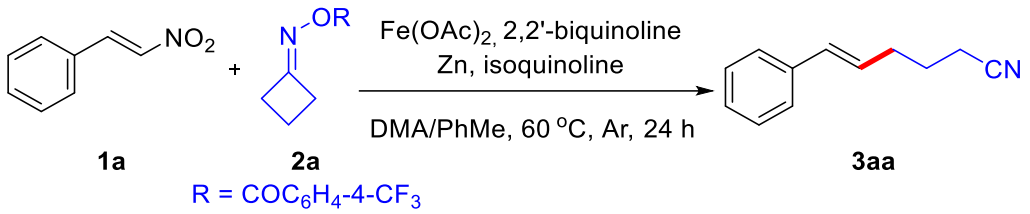
1a **2a** **3aa**

R = COC_6H_4-4-CF_3

entry	**1a** : **2a**	yield (%)
1	**1 : 1.5**	**60**
2	1 : 2.0	54
3	1 : 3.0	51
4	1.5 : 1	52
5	2.0 : 1	54
6	3.0 : 1	56

[a] Reaction conditions: 1.0 equiv. is 0.30 mmol, $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and DMA/PhMe (1.0 mL, DMA/PhMe = 0.8 mL DMA / 0.2 mL PhMe) under Ar at 60 °C for 24 h, isolated yield.

Table S6. Screening loading of the isoquinoline [a]



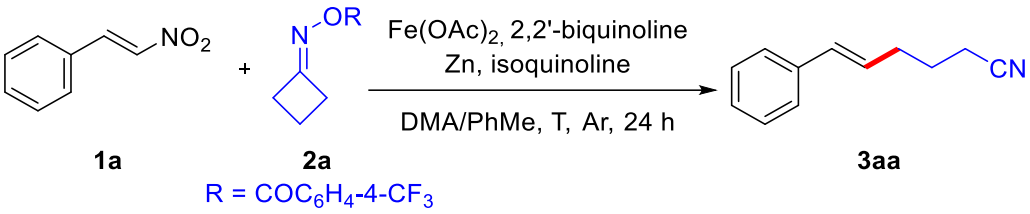
1a **2a** **3aa**

R = COC_6H_4-4-CF_3

entry	isoquinoline (equiv.)	yield (%)
1	0.2	53
2	0.5	53
3	1.0	56
4	**2.0**	**60**
5	3.0	59
6	4.0	56
7	5.0	53

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (x equiv.) and DMA/PhMe (1.0 mL, DMA/PhMe = 0.8 mL DMA / 0.2 mL PhMe) under Ar at 60 °C for 24 h, isolated yield.

Table S7. Screening of temperature [a]



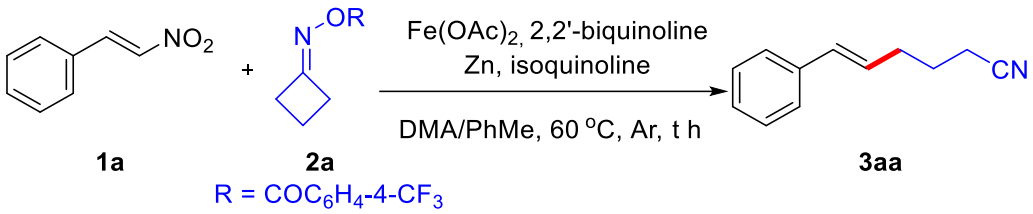
1a **2a** **3aa**

R = COC_6H_4-4-CF_3

entry	T (°C)	yield (%)
1	r.t.	51
2	40	52
3	**60**	**60**
4	80	51
5	100	49

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and DMA/PhMe (1.0 mL, DMA/PhMe = 0.8 mL DMA / 0.2 mL PhMe) under Ar at T °C for 24 h, isolated yield.

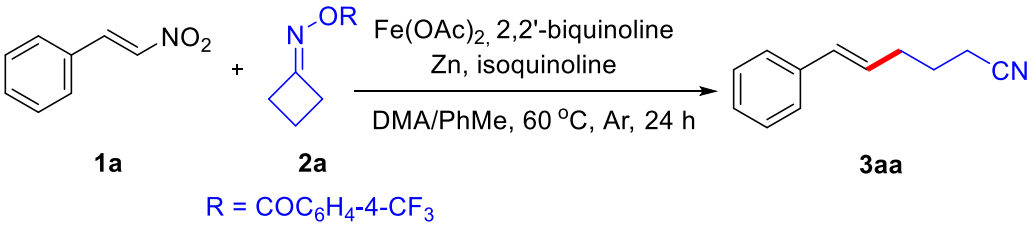
Table S8. Screening of time [a]



entry	t (h)	yield (%)
1	6	50
2	12	56
3	18	58
4	**24**	**60**

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.) and DMA/PhMe (1.0 mL, DMA/PhMe = 0.8 mL DMA / 0.2 mL PhMe) under Ar at 60 °C for t h, isolated yield.

Table S9. Control experiment [a]



entry	deviation from "standard" conditions	yield (%)
1	No $Fe(OAc)_2$	ND
2	No Zn	Trace
3	No 2,2'-biquinoline	50
4	No isoquinoline	51

[a] Reaction conditions: **1a** (44.7 mg, 0.30 mmol), **2a** (115.7 mg, 0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (2.0 equiv.), DMA/PhMe (1.0 mL, DMA/PhMe = 0.8 mL DMA / 0.2 mL PhMe) under Ar at 60 °C for 24 h, isolated yield.

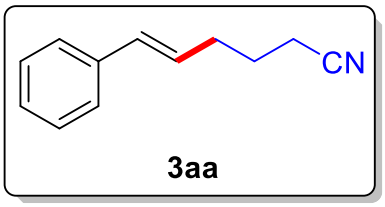
3. General procedure

Nitroalkenes **1** (0.3 mmol) and cycloketone oxime esters **2** (0.45 mmol), $Fe(OAc)_2$ (0.03 mmol, 10 mol%), Zn (0.3 mmol, 1.0 equiv.), 2,2'-biquinoline (0.0303 mmol, 10.1 mol%), isoquinoline (0.6 mmol, 2.0 equiv.), DMA/PhMe (1.0 mL, DMA/PhMe = 0.8

mL DMA / 0.2 mL PhMe) were added to a flame-dried Young-type tube. The mixture was degassed by the freeze-thaw method, and then stirred under Ar at 60 °C for 24 hours. After cooling to room temperature, the reaction mixture was treated with saturated NH_4Cl aqueous solution (10 mL) and extracted with ethyl acetate (4 × 10 mL). The solvent was removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel and eluted with ethyl acetate/petroleum ether (1/50-1/2) to afford the desired products **3**.

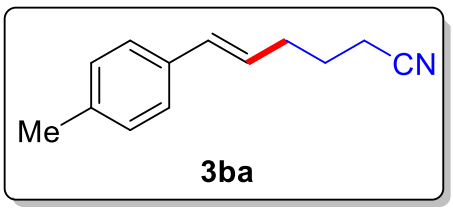
4. Experimental characterization data for products

(*E*)-6-phenylhex-5-enenitrile (3aa)[3]**:**



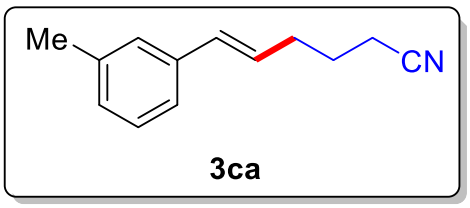
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (30.8 mg, 60% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 – 7.28 (m, 4H), 7.13 – 7.17 (m, 1H), 6.39 (d, *J* = 15.8 Hz, 1H), 6.03 – 6.08 (m, 1H), 2.28 – 2.32 (m, 4H), 1.74 – 1.79 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.1, 132.1, 128.7, 127.7, 127.4, 126.2, 119.7, 31.8, 25.0, 16.5.

(*E*)-6-(*p*-tolyl)hex-5-enenitrile (3ba)[4]**:**



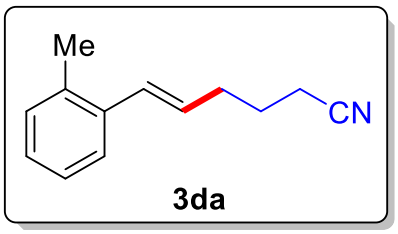
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (31.3 mg, 56% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 (d, *J* = 7.9 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 6.42 (d, *J* = 15.8 Hz, 1H), 6.04 – 6.09 (m, 1H), 2.34 – 2.38 (m, 4H), 2.33 (s, 3H), 1.80 – 1.85 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.2, 134.4, 131.9, 129.4, 126.6, 126.0, 119.8, 31.7, 25.1, 21.3, 16.5.

(*E*)-6-(*m*-tolyl)hex-5-enenitrile (3ca)[4]**:**



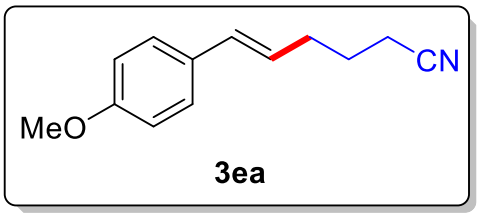
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (26.0 mg, 47% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 – 7.21 (m, 3H), 7.04 (d, *J* = 7.4 Hz, 1H), 6.43 (d, *J* = 15.8 Hz, 1H), 6.09 – 6.14 (m, 1H), 2.35 – 2.39 (m, 4H), 2.34 (s, 3H), 1.81 – 1.86 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.2, 137.1, 132.2, 128.6, 128.2, 127.5, 126.9, 123.3, 119.7, 31.8, 25.1, 21.5, 16.5.

(*E*)-6-(*o*-tolyl)hex-5-enenitrile (3da)[4]**:**



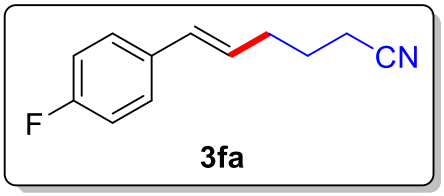
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (31.0 mg, 56% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 – 7.41 (m, 1H), 7.12 – 7.17 (m, 3H), 6.66 (d, *J* = 15.7 Hz, 1H), 5.97 – 6.02 (m, 1H), 2.38 – 2.42 (m, 4H), 2.33 (s, 3H), 1.82 – 1.87 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.3, 135.2, 130.4, 130.0, 129.1, 127.4, 126.2, 125.5, 119.7, 32.0, 25.1, 19.9, 16.5.

(*E*)-6-(4-methoxyphenyl)hex-5-enenitrile (3ea)[5]**:**



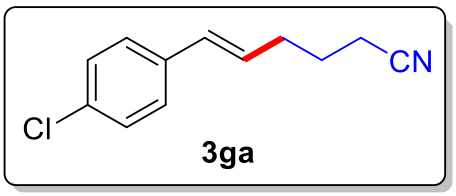
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (34.0 mg, 56% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.7 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 6.39 (d, *J* = 15.8 Hz, 1H), 5.95 – 6.00 (m, 1H), 3.79 (s, 3H), 2.32 – 2.38 (m, 4H), 1.79 – 1.84 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.0, 131.4, 129.9, 127.3, 125.4, 119.8, 114.0, 55.4, 31.7, 25.2, 16.5.

(*E*)-6-(4-fluorophenyl)hex-5-enenitrile (3fa)[4]**:**



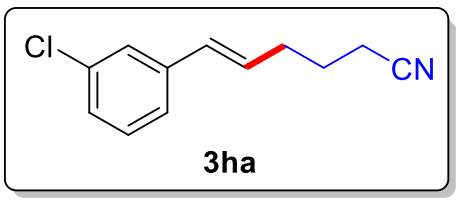
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (33.6 mg, 59% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 – 7.31 (m, 2H), 6.98 – 7.01 (m, 2H), 6.42 (d, *J* = 15.8 Hz, 1H), 6.02 – 6.07 (m, 1H), 2.35 – 2.40 (m, 4H), 1.81 – 1.86 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.2 (d, *J* = 246.3 Hz), 133.3 (d, *J* = 3.3 Hz), 130.9, 127.6 (d, *J* = 8.0 Hz), 127.4 (d, *J* = 2.2 Hz), 119.7, 115.5 (d, *J* = 21.5 Hz), 31.7, 25.0, 16.5.

(*E*)-6-(4-chlorophenyl)hex-5-enenitrile (3ga)[4]**:**



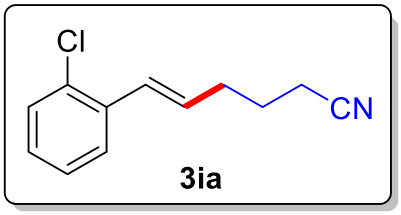
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (21.3 mg, 35% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 (s, 4H), 6.40 – 6.43 (m, 1H), 6.09 – 6.14 (m, 1H), 2.36 – 2.40 (m, 4H), 1.82 – 1.87 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.6, 133.0, 130.9, 128.8, 128.4, 127.4, 119.6, 31.8, 25.0, 16.6.

(*E*)-6-(3-chlorophenyl)hex-5-enenitrile (3ha)[6]**:**



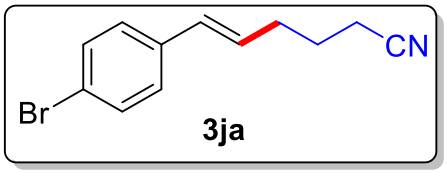
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (24.6 mg, 40% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (t, *J* = 1.6 Hz, 1H), 7.18 – 7.25 (m, 3H), 6.40 (d, *J* = 15.8 Hz, 1H), 6.12 – 6.17 (m, 1H), 2.37 – 2.41 (m, 4H), 1.82 – 1.87 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.0, 134.6, 130.8, 129.9, 129.4, 127.4, 126.0, 124.5, 119.6, 31.7, 24.9, 16.6.

(*E*)-6-(2-chlorophenyl)hex-5-enenitrile (3ia)[6]**:**



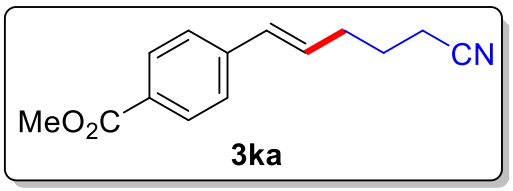
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (35.7 mg, 58% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.34 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.15 – 7.22 (m, 2H), 6.83 (d, *J* = 15.8 Hz, 1H), 6.09 – 6.14 (m, 1H), 2.40 – 2.44 (m, 4H), 1.84 – 1.89 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 135.3, 132.7, 130.7, 129.7, 128.5, 128.3, 126.9, 126.8, 119.6, 31.9, 24.9, 16.6.

(*E*)-6-(4-bromophenyl)hex-5-enenitrile (3ja)[3]**:**



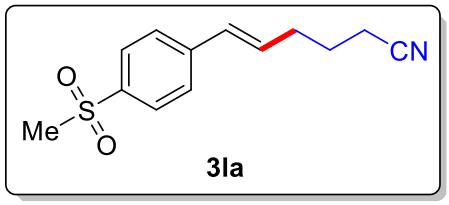
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid (46.1 mg, 61% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 6.39 (d, *J* = 15.8 Hz, 1H), 6.10 – 6.15 (m, 1H), 2.35 – 2.39 (m, 4H), 1.81 – 1.86 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.1, 131.7, 130.9, 128.6, 127.7, 121.1, 119.6, 31.7, 24.9, 16.6.

methyl (*E*)-4-(5-cyanopent-1-en-1-yl)benzoate (3ka)[7]**:**



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid (50.0 mg, 73% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 6.50 (d, *J* = 15.9 Hz, 1H), 6.24 – 6.30 (m, 1H), 3.91 (s, 3H), 2.39 – 2.44 (m, 4H), 1.84 – 1.89 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 141.7, 131.3, 130.6, 130.1, 129.0, 126.1, 119.5, 52.1, 31.8, 24.9, 16.6.

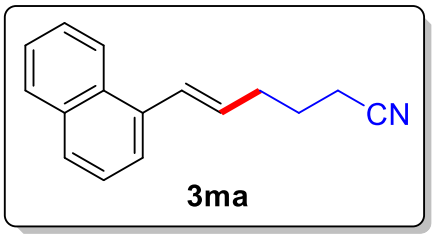
(*E*)-6-(4-(methylsulfonyl)phenyl)hex-5-enenitrile (3la):



3la

The title compound was prepared according to the general procedure and purified by column chromatography to give a yellow oil (43.2 mg, 58% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 6.53 (d, *J* = 15.9 Hz, 1H), 6.31 – 6.37 (m, 1H), 3.05 (s, 3H), 2.40 – 2.47 (m, 4H), 1.85 – 1.91 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.6, 138.9, 132.3, 130.4, 127.8, 126.8, 119.4, 44.6, 31.8, 24.7, 16.6. IR (KBr) ν_{max} 3022, 3009, 2852, 2336, 2328, 1680, 1658, 1613, 1555, 1537, 1441, 1406, 1186, 1089, 1014, 867, 829, 673, 536 cm^{-1}. HRMS(ESI): mass found: 250.0896, calculated mass for $C_{13}H_{16}NO_2S^+$ $[M+H]^+$: 250.0896.

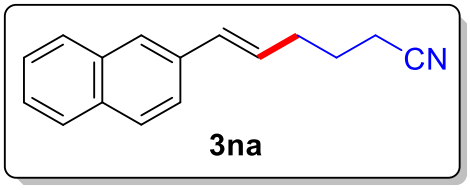
(*E*)-6-(naphthalen-1-yl)hex-5-enenitrile (3ma)[8]:



3ma

The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (32.3 mg, 49% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.3 Hz, 1H), 7.81 – 7.86 (m, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.40 – 7.56 (m, 4H), 7.20 (d, *J* = 15.5 Hz, 1H), 6.09 – 6.15 (m, 1H), 2.46 – 2.51 (m, 2H), 2.41 (t, *J* = 7.1 Hz, 2H), 1.86 – 1.91 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 135.0, 133.7, 131.2, 131.0, 129.4, 128.6, 127.8, 126.1, 125.9, 125.7, 123.8, 123.8, 119.6, 32.1, 25.1, 16.6.

(*E*)-6-(naphthalen-2-yl)hex-5-enenitrile (3na)[3]:

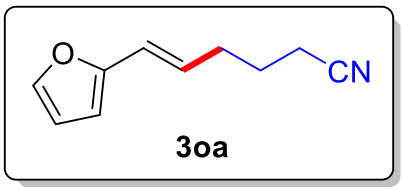


3na

The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (30.8 mg, 46% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (t, *J* = 9.4 Hz, 3H), 7.67 (s, 1H), 7.55 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.41 – 7.46 (m, 2H),

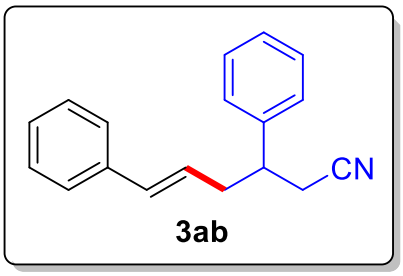
6.59 (d, *J* = 15.8 Hz, 1H), 6.20 – 6.25 (m, 1H), 2.35 – 2.41 (m, 4H), 1.80 – 1.85 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 134.6, 133.6, 132.9, 132.1, 128.3, 128.1, 128.0, 127.7, 126.4, 125.9, 125.8, 123.4, 119.7, 31.8, 25.0, 16.5.

(*E*)-6-(furan-2-yl)hex-5-enenitrile (3oa) [4]**:**



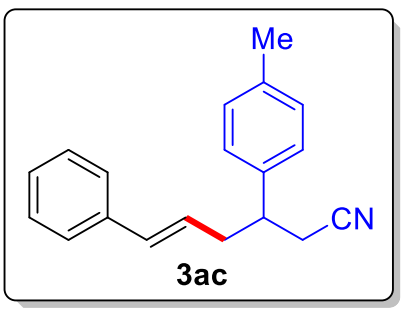
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (27.3 mg, 56% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (s, 1H), 6.36 (dd, *J* = 2.9, 1.9 Hz, 1H), 6.28 (d, *J* = 15.8 Hz, 1H), 6.18 (d, *J* = 3.1 Hz, 1H), 6.04 – 6.09 (m, 1H), 2.35 – 2.40 (m, 4H), 1.81 – 1.86 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.6, 141.8, 126.5, 120.7, 119.7, 111.4, 107.2, 31.5, 25.0, 16.5.

(*E*)-3,6-diphenylhex-5-enenitrile (3ab) [4]**:**



The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (43.3 mg, 58% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (t, *J* = 7.5 Hz, 2H), 7.28 – 7.29 (m, 4H), 7.20 – 7.25 (m, 4H), 6.47 (d, *J* = 15.8 Hz, 1H), 6.00 – 6.05 (m, 1H), 3.08 – 3.13 (m, 1H), 2.60 – 2.69 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.3, 137.0, 133.2, 129.0, 128.6, 127.6, 127.5, 127.2, 126.2, 126.2, 118.6, 42.1, 38.5, 24.0.

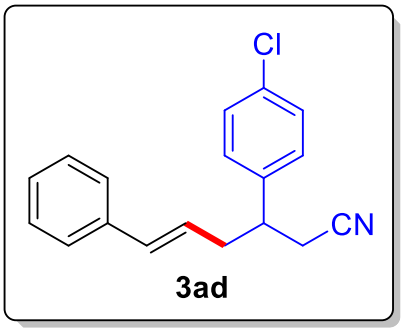
(*E*)-6-phenyl-3-(*p*-tolyl)hex-5-enenitrile (3ac):



The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (41.4 mg, 53% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 – 7.29 (m, 4H), 7.19 – 7.21 (m, 1H), 7.15 (dd, *J* = 16.8, 7.9 Hz, 4H), 6.46 (d, *J* = 15.8 Hz, 1H), 6.00 – 6.05 (m, 1H),

3.04 – 3.09 (m, 1H), 2.57 – 2.67 (m, 4H), 2.33 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.3, 137.2, 137.1, 133.1, 129.7, 128.6, 127.5, 127.1, 126.4, 126.2, 118.7, 41.8, 38.6, 24.1, 21.2. IR (KBr) ν_{max} 3054, 3025, 2854, 2350, 2336, 1694, 1660, 1594, 1555, 1494, 1423, 1373, 1244, 1116, 1090, 1045, 916, 814, 693, 535 cm^{-1}. HRMS(ESI): mass found: 262.1592, calculated mass for $C_{19}H_{20}N^+$ $[M+H]^+$: 262.1590.

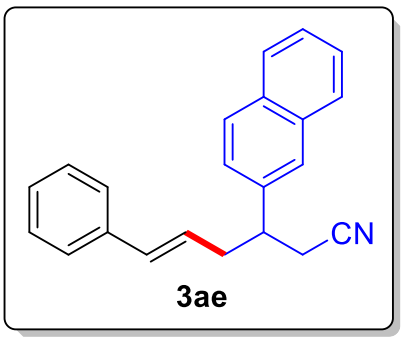
(*E*)-3-(4-chlorophenyl)-6-phenylhex-5-enenitrile (3ad)[4]:



3ad

The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (40.0 mg, 47% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.4 Hz, 2H), 7.29 – 7.31 (m, 4H), 7.19 – 7.24 (m, 3H), 6.47 (d, *J* = 15.8 Hz, 1H), 5.98 – 6.03 (m, 1H), 3.09 – 3.13 (m, 1H), 2.61 – 2.70 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.8, 136.9, 133.6, 133.5, 129.2, 128.7, 128.7, 127.7, 126.3, 125.7, 118.3, 41.7, 38.4, 24.0.

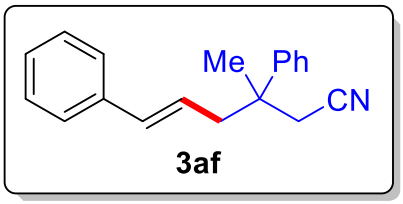
(*E*)-3-(naphthalen-2-yl)-6-phenylhex-5-enenitrile (3ae)[3]:



3ae

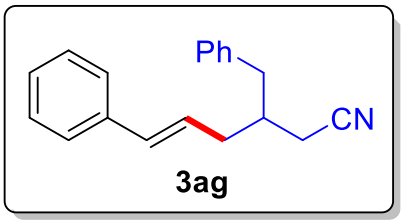
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (42.3 mg, 47% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 – 7.86 (m, 3H), 7.70 (s, 1H), 7.46 – 7.51 (m, 2H), 7.38 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.25 – 7.27 (m, 4H), 7.19 – 7.21 (m, 1H), 6.50 (d, *J* = 15.8 Hz, 1H), 6.03 – 6.08 (m, 1H), 3.26 – 3.30 (m, 1H), 2.70 – 2.79 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.7, 137.0, 133.6, 133.3, 132.9, 128.9, 128.7, 128.0, 127.8, 127.6, 126.5, 126.3, 126.2, 126.2, 126.1, 125.2, 118.6, 42.4, 38.6, 24.1. IR (KBr) ν_{max} 3054, 3024, 2849, 2340, 2320, 2176, 1696, 1661, 1614, 1505, 1445, 1434, 1417, 1373, 1270, 1244, 1124, 1017, 856, 818, 692, 460 cm^{-1}. HRMS(ESI): mass found: 298.1590, calculated mass for $C_{22}H_{20}N^+$ $[M+H]^+$: 298.1590.

(*E*)-3-methyl-3,6-diphenylhex-5-enenitrile (3af)[6]**:**



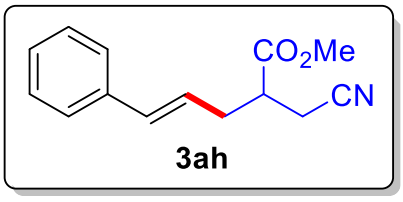
The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (26.7 mg, 34% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.40 (m, 4H), 7.28 – 7.30 (m, 1H), 7.24 - 7.25 (m, 4H), 7.19 – 7.21 (m, 1H), 6.45 – 6.48 (d, *J* = 15.8 Hz, 1H), 5.83 – 5.88 (m, 1H), 2.64 – 2.76 (m, 4H), 1.56 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.1, 137.1, 134.1, 128.9, 128.6, 127.6, 127.2, 126.3, 125.8, 124.8, 118.3, 45.2, 40.6, 30.3, 25.8.

(*E*)-3-benzyl-6-phenylhex-5-enenitrile (3ag)[4]**:**



The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (45.7 mg, 58% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.37 (m, 2H), 7.30 – 7.34 (m, 4H), 7.23 – 7.26 (m, 3H), 7.20 (d, *J* = 7.2 Hz, 2H), 6.51 (d, *J* = 15.8 Hz, 1H), 6.12 – 6.17 (m, 1H), 2.85 – 2.88 (dd, *J* = 13.8, 6.1 Hz, 1H), 2.67 – 2.70 (dd, *J* = 13.8, 8.7 Hz, 1H), 2.43 – 2.47 (m, 1H), 2.32 – 2.37 (m, 2H), 2.26 (dd, *J* = 16.8, 5.6 Hz, 1H), 2.13 – 2.18 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.9, 137.1, 133.4, 129.2, 128.8, 128.7, 127.6, 126.8, 126.4, 126.2, 118.6, 39.8, 37.7, 36.9, 20.8.

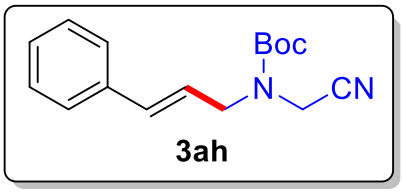
methyl (*E*)-2-(cyanomethyl)-5-phenylpent-4-enoate (3ah):



The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (37.1 mg, 54% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 – 7.35 (m, 4H), 7.23 – 7.24 (m, 1H), 6.52 (d, *J* = 15.7 Hz, 1H), 6.02 – 6.07 (m, 1H), 3.77 (s, 3H), 2.89 – 2.93 (m, 1H), 2.60 – 2.74 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.5, 136.6, 134.3, 128.7, 127.8, 126.3, 124.0, 117.9, 52.6, 41.4, 34.4, 18.6. IR (KBr) ν_{max} 3026,

2953, 2851, 2343, 2187, 1688, 1598, 1543, 1493, 1438, 1373, 1236, 1199, 1038, 968, 744, 694 cm^{-1} HRMS(ESI): mass found: 230.1174, calculated mass for $C_{14}H_{16}NO_2^+$ $[M+H]^+$: 230.1176.

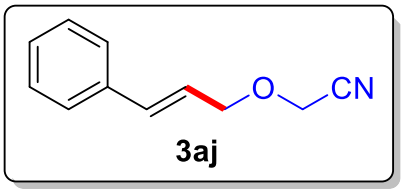
***tert*-butyl cinnamyl(cyanomethyl)carbamate (3ai)**[6]**:**



3ah

The title compound was prepared according to the general procedure and purified by column chromatography to give a yellow oil (17.3 mg, 21% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 – 7.40 (m, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.29 (m, 1H), 6.57 (s, 1H), 6.09 – 6.14 (m, 1H), 4.13 – 4.22 (m, 4H), 1.52 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.1, 128.8, 128.2, 126.6, 123.2, 116.1, 82.1, 49.3, 34.4, 28.3.

2-(cinnamyloxy)acetonitrile (3aj)[9]**:**



3aj

The title compound was prepared according to the general procedure and purified by column chromatography to give a colorless oil (13.0 mg, 25% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 – 7.42 (m, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.30 (m, 1H), 6.70 (d, *J* = 15.9 Hz, 1H), 6.21 – 6.25 (m, 1H), 4.29 - 4.31 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.0, 135.5, 128.8, 128.4, 126.8, 123.1, 116.1, 71.8, 54.8.

5. Radical test and gram-scale experiment

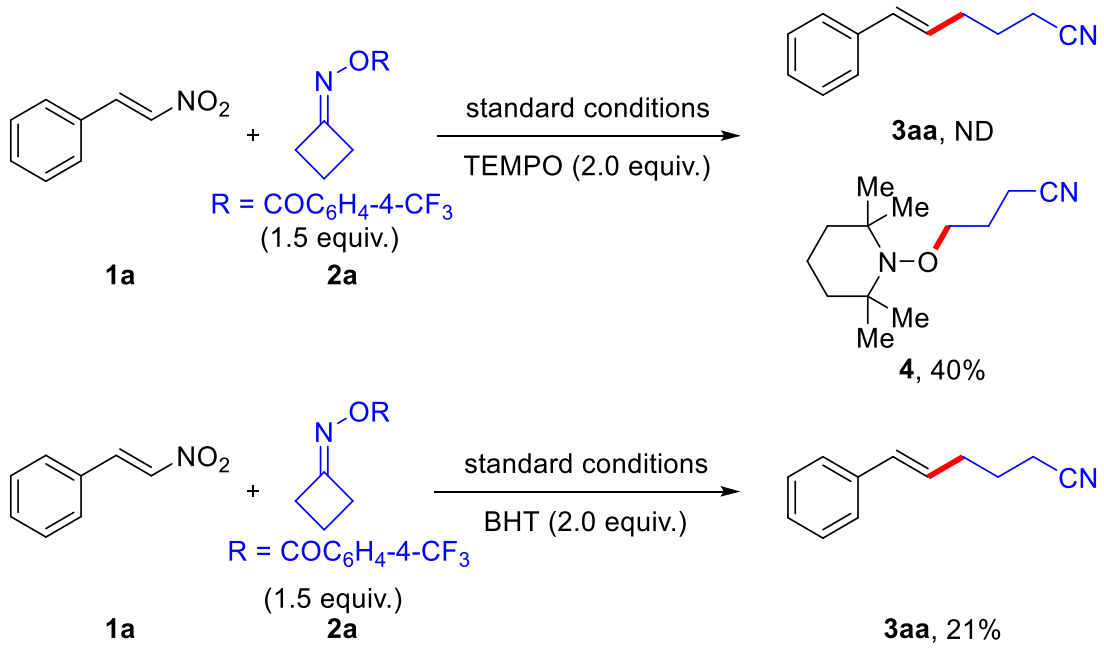
When TEMPO (2.0 equiv.) was introduced to the standard conditions, the TLC analysis and GC-MS analysis showed that it did not produce corresponding product at all. The residue was purified by flash column chromatography on silica gel and eluted with ethyl acetate/petroleum ether (1/100-1/50) to afford radical trapping product 4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)butanenitrile **4** (40.3 mg, 40% isolated yield, yield based on **2a**) as a yellowish oil. When BHT (2.0 equiv.) was introduced to the standard conditions, the desired product **3aa** was isolated in lower yield of 21% (10.8

mg). These results indicated that a radical path way might be involved in this novel reductive denitrative coupling reaction of nitroalkenes.

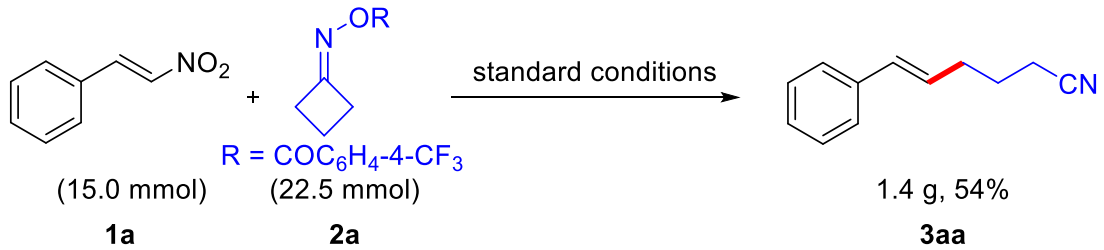
4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)butanenitrile (4)[10]**:** ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.84 (t, *J* = 5.8 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 1.87 – 1.91 (m, 2H), 1.52 – 1.57 (m, 1H), 1.44 – 1.48 (m, 4H), 1.31 – 1.33 (m, 1H), 1.15 (s, 6H), 1.09 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 119.8, 73.6, 59.9, 39.6, 33.2, 25.2, 20.1, 17.1, 14.5.

To demonstrate the synthetic versatility of the present catalytic system, the reaction of **1a** with **2a** on a 15 mmol scale was carried out under the standard reaction conditions, yielding 1.4 g of **3aa** in 54% yield.

a) Radical-trapping experiments



b) Gram-scale experiment



6. References

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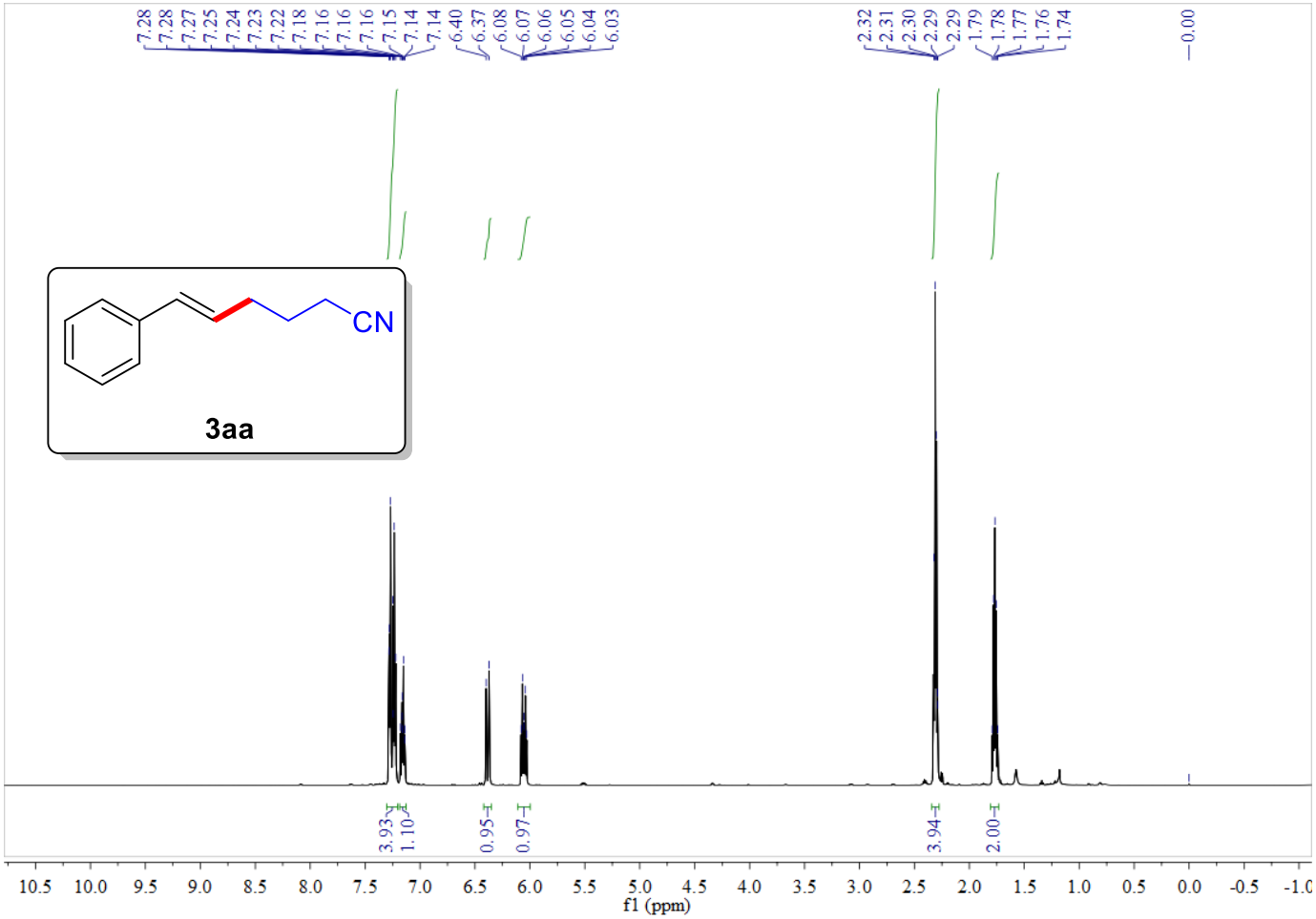
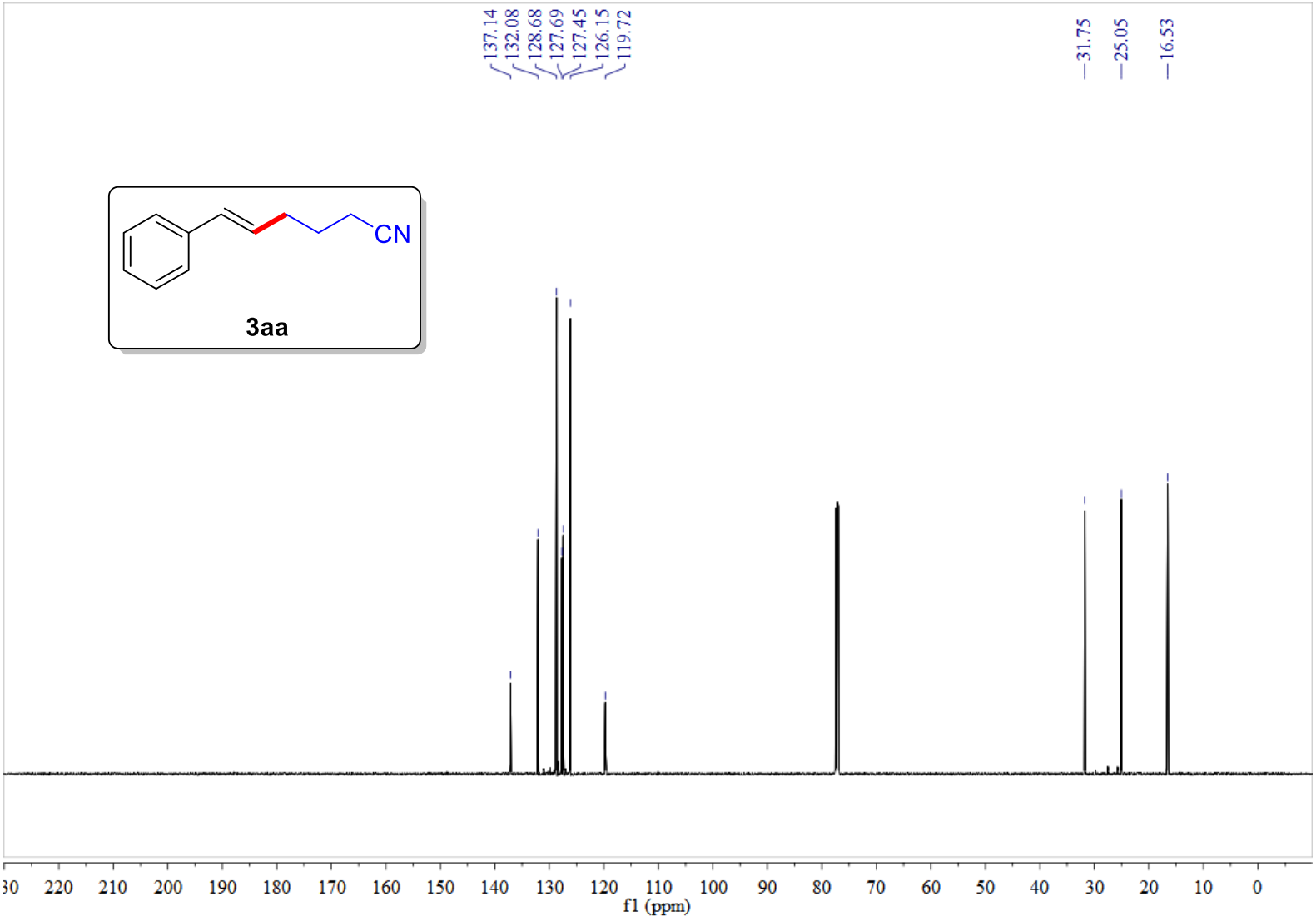
7. Copies for ^{1}H NMR ,^{13}C NMR spectra of the products




137.14
132.08
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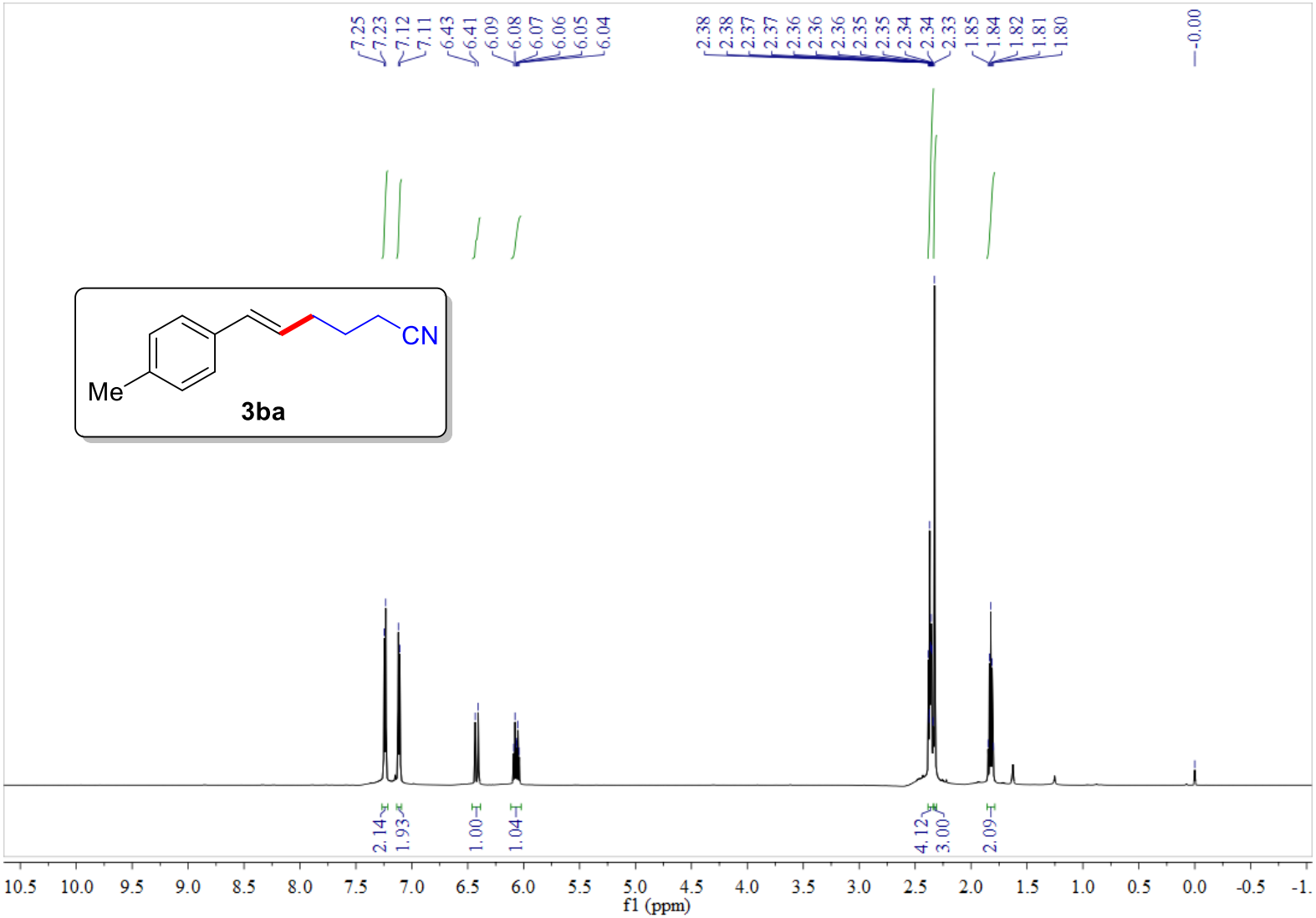
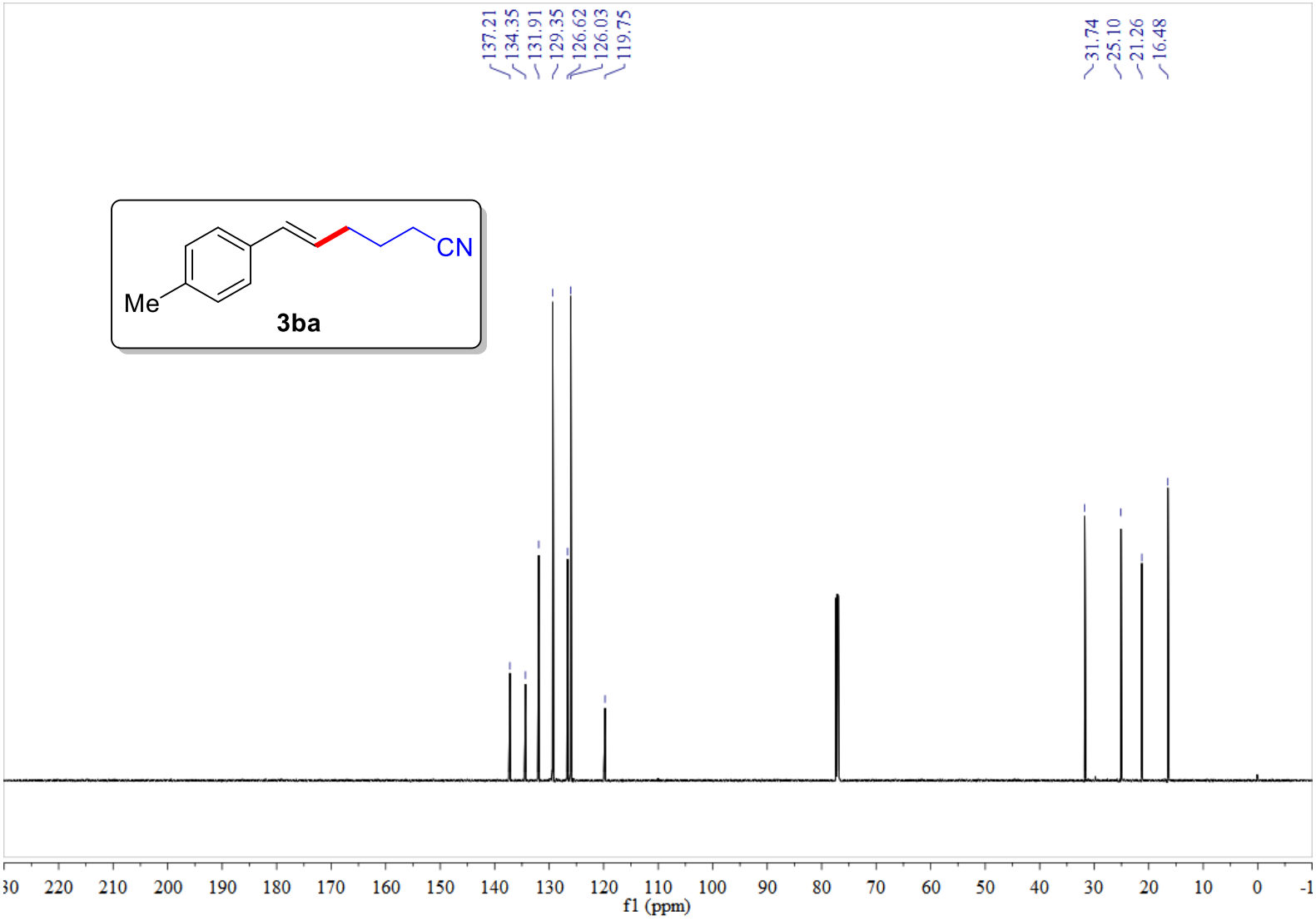
127.69
127.45
126.15
119.72
31.75
25.05
16.53
CN
3aa
f1 (ppm)


7.25
7.23
7.12
7.11
6.43
6.41
6.09
6.08
6.07
6.06
6.05
6.04
2.38
2.38
2.37
2.37
2.36
2.36
2.36
2.35
2.35
2.34
2.34
2.33
1.85
1.84
1.82
1.81
1.80
-0.00
CN
Me
3ba
2.14
1.93
1.00
1.04
4.12
3.00
2.09
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 -1.
f1 (ppm)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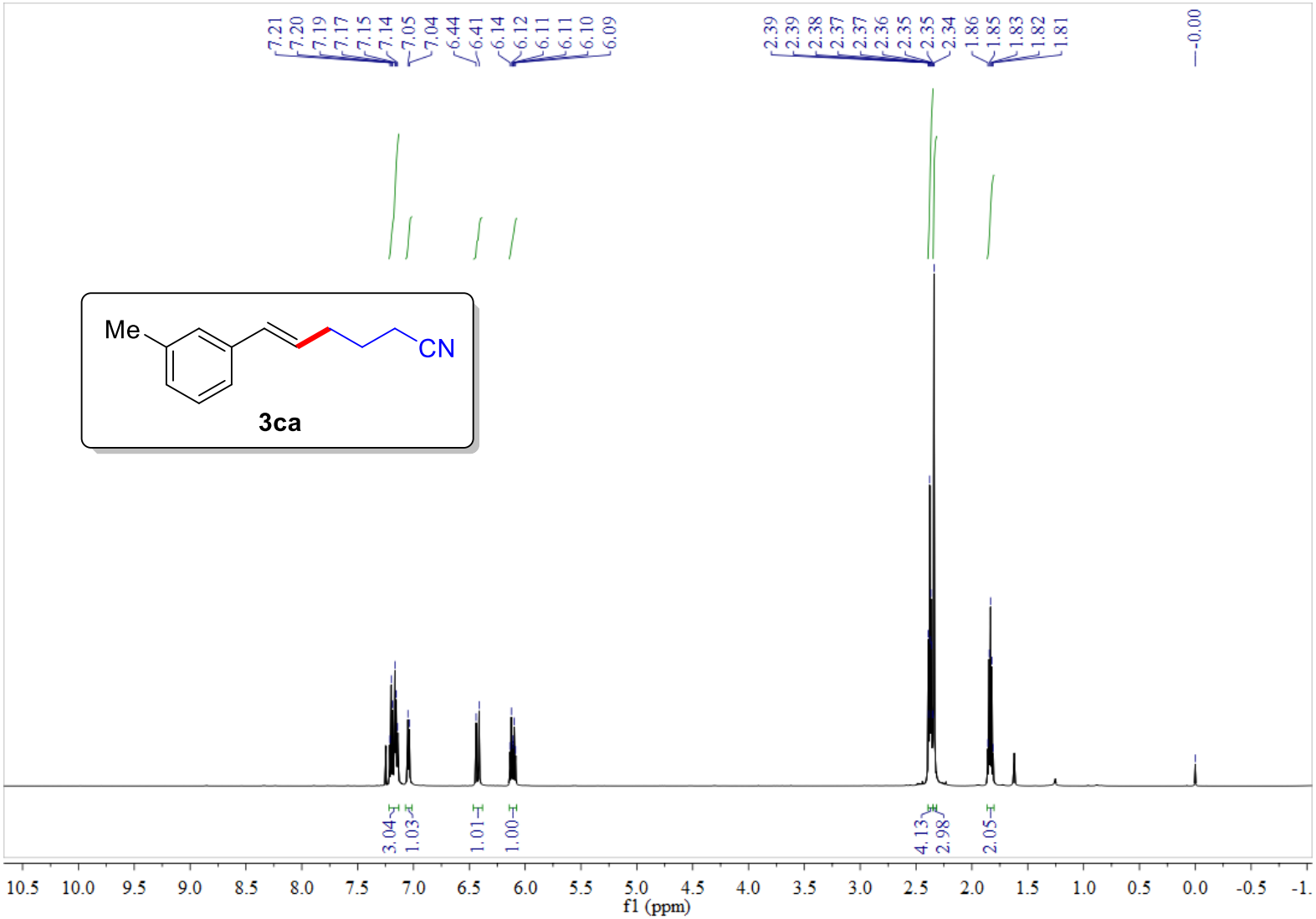
31.74
25.10
21.26
16.48
CN
Me
3ba
f1 (ppm)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6.14
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6.11
6.11
6.10
6.09
2.39
2.39
2.38
2.37
2.37
2.36
2.35
2.35
2.34
1.86
1.85
1.83
1.82
1.81
-0.00
Me
CN
3ca
3.04
1.03
1.01
1.00
4.13
2.98
2.05
10.5 10.0 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 -1.
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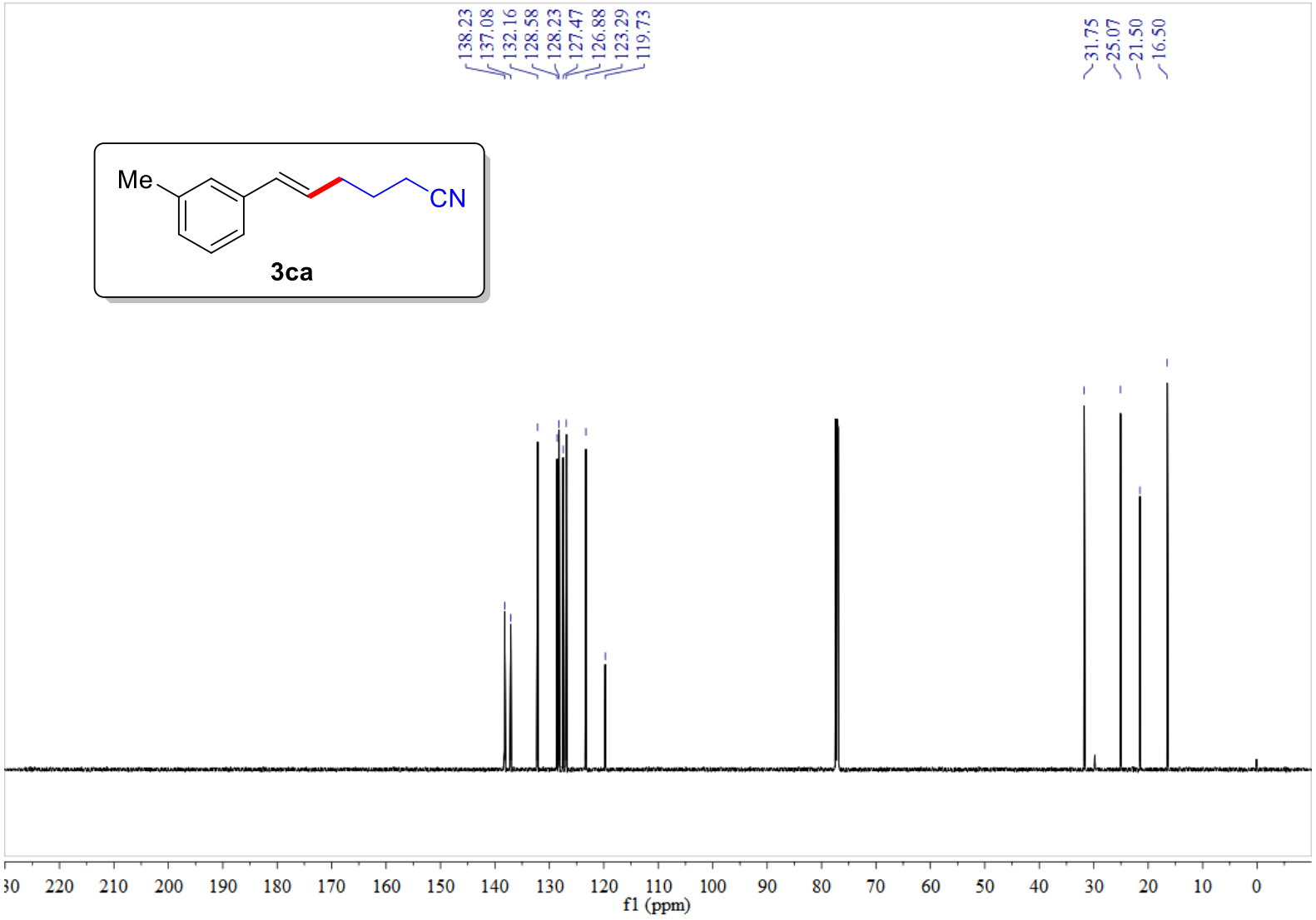
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16.50
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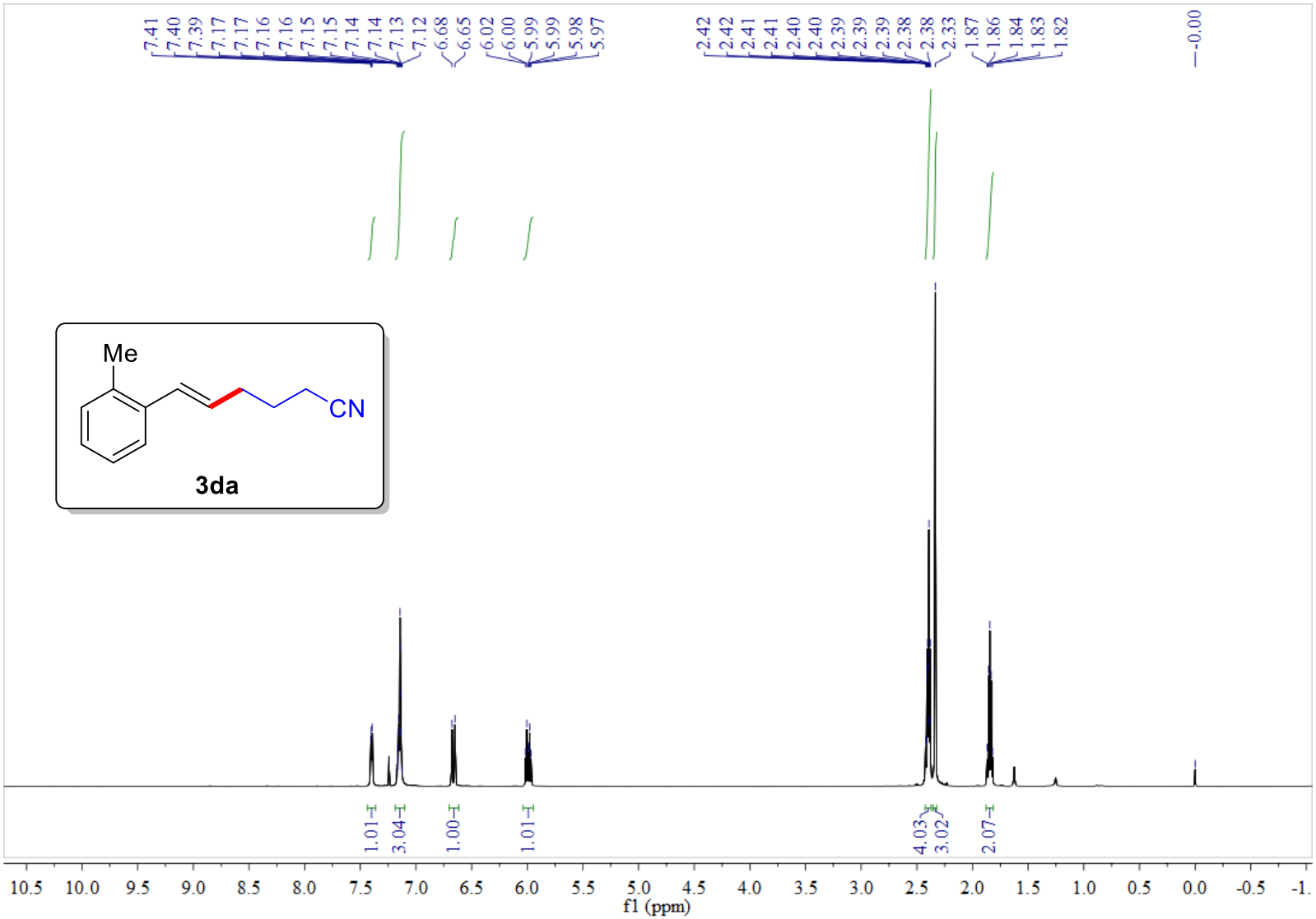
CN
3ca
f1 (ppm)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7.14
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7.13
7.12
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6.65
6.02
6.00
5.99
5.99
5.98
5.97
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2.42
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2.41
2.40
2.40
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2.39
2.38
2.38
2.33
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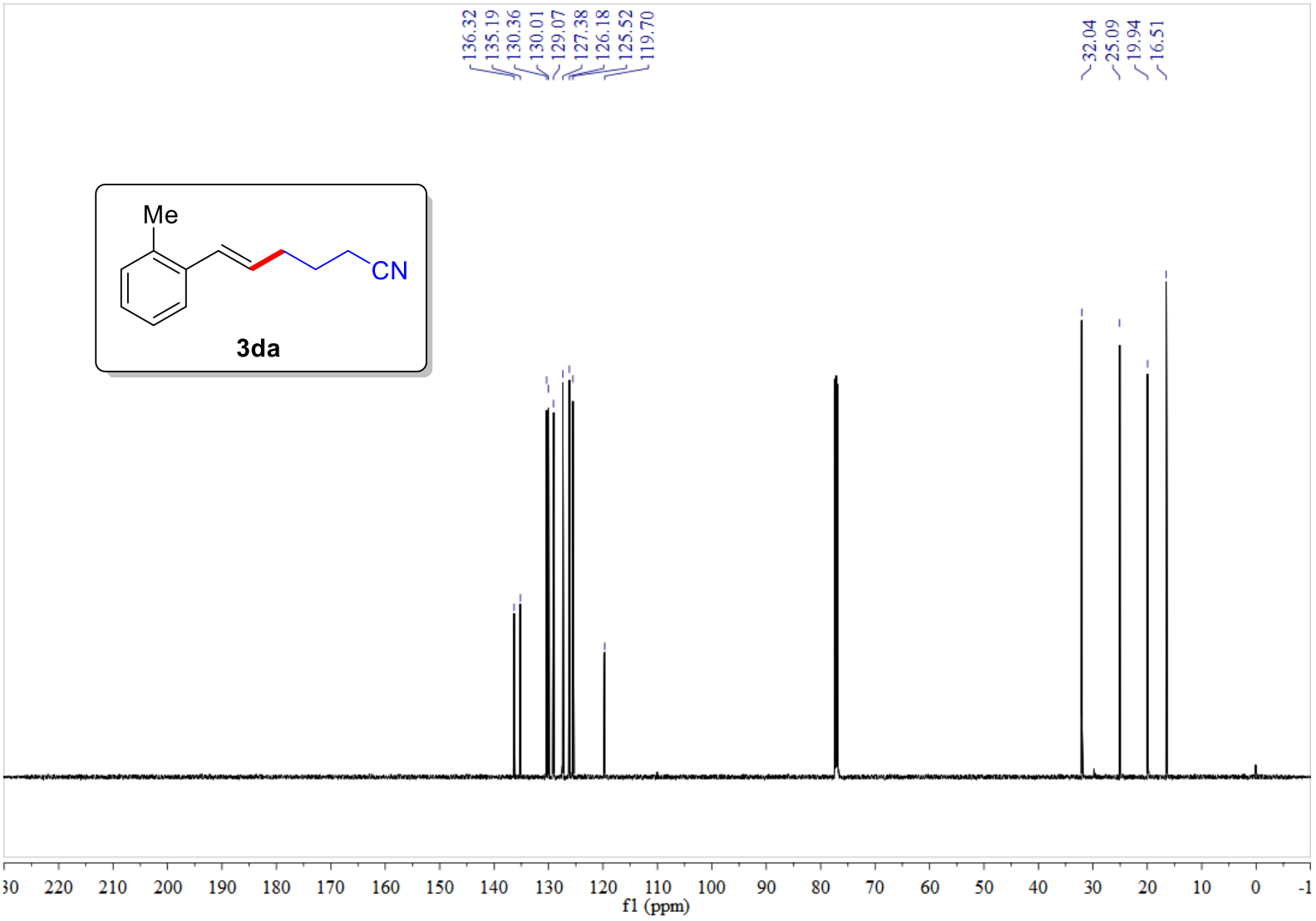
1.86
1.84
1.83
1.82
-0.00
Me
CN
3da
1.01
3.04
1.00
1.01
4.03
3.02
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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125.52
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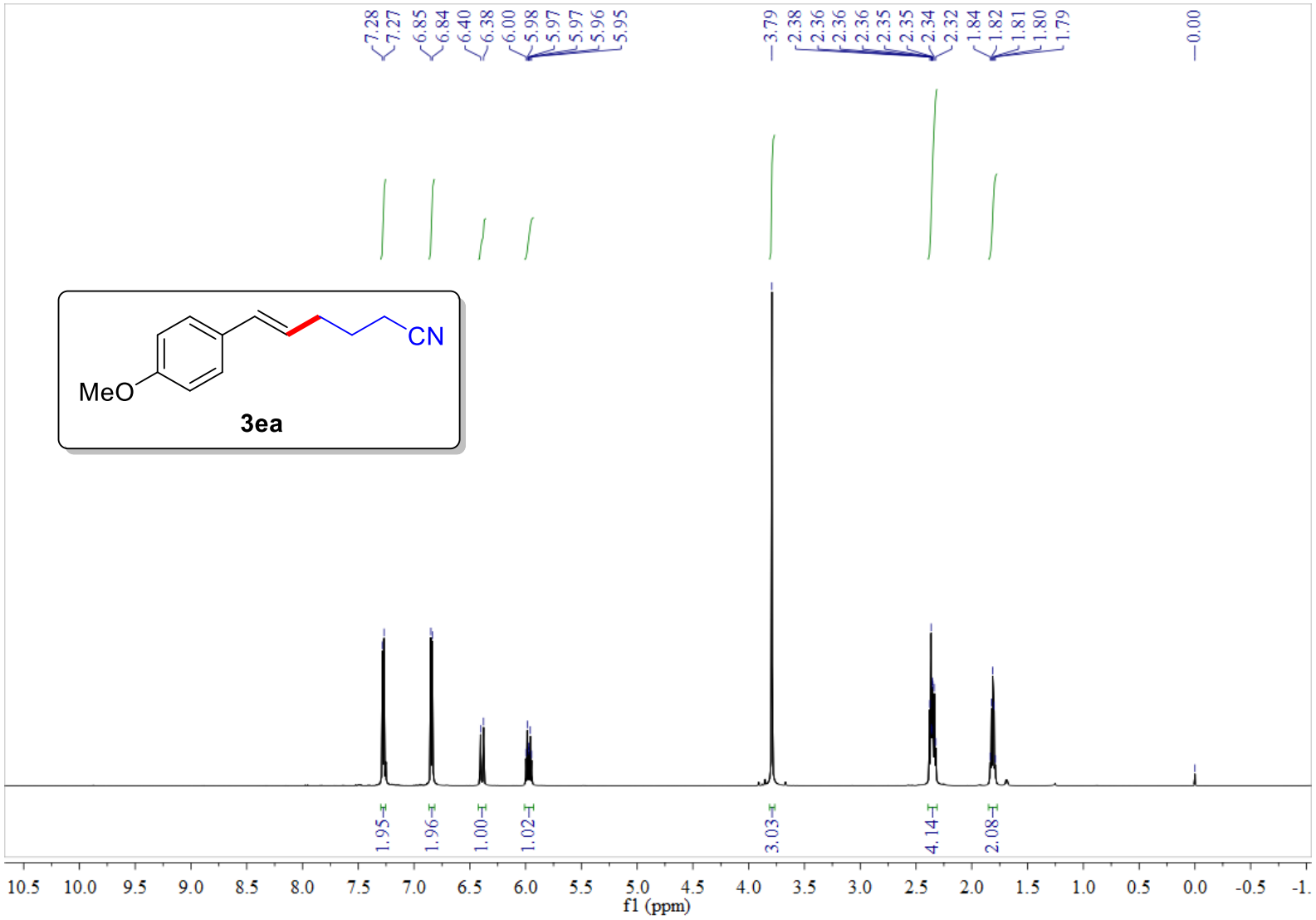
32.04
25.09
19.94
16.51
Me
CN
3da
f1 (ppm)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5.96
5.95
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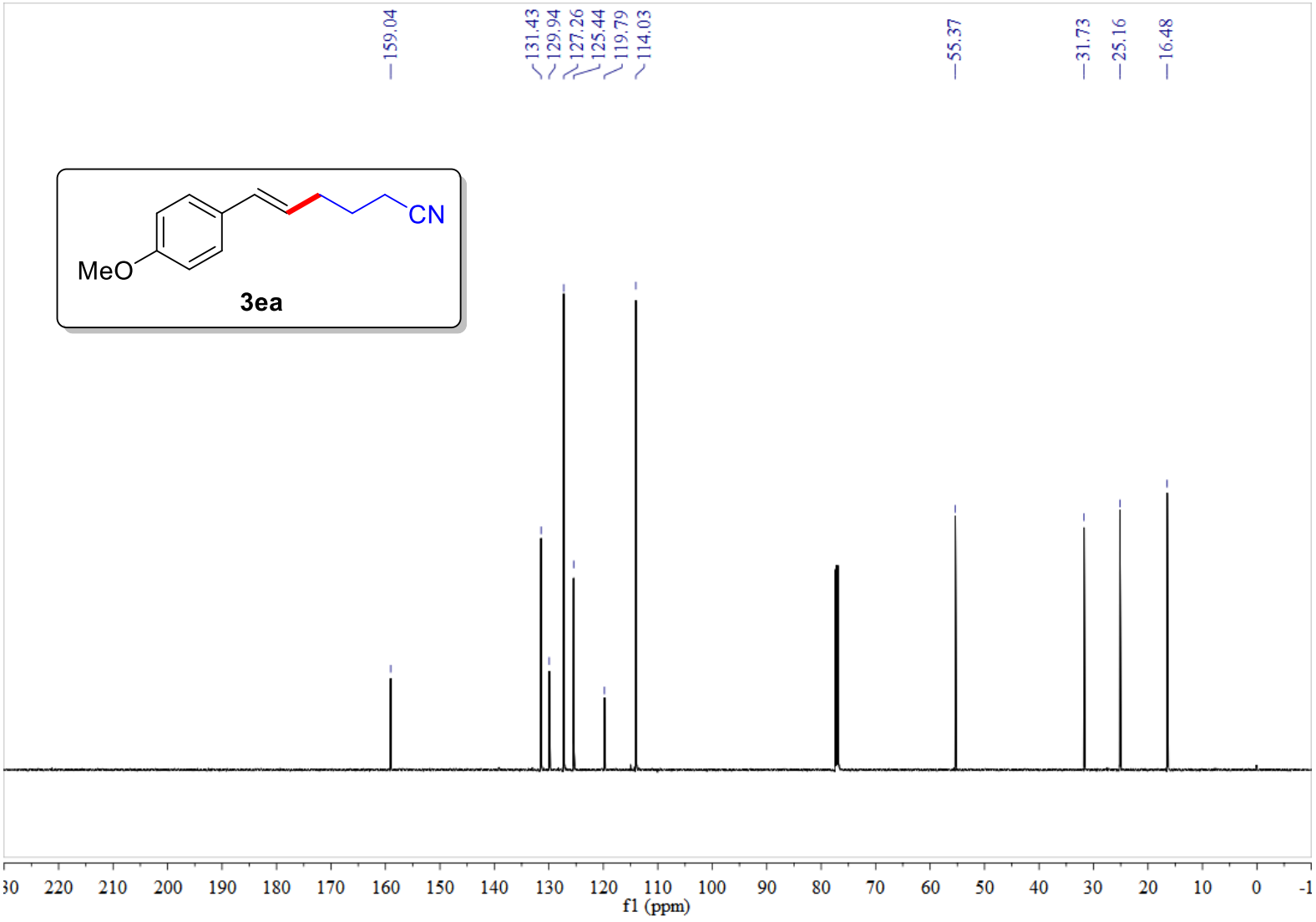
2.36
2.36
2.36
2.35
2.35
2.34
2.32
1.84
1.82
1.81
1.80
1.79
0.00
CN
MeO
3ea
1.95
1.96
1.00
1.02
3.03
4.14
2.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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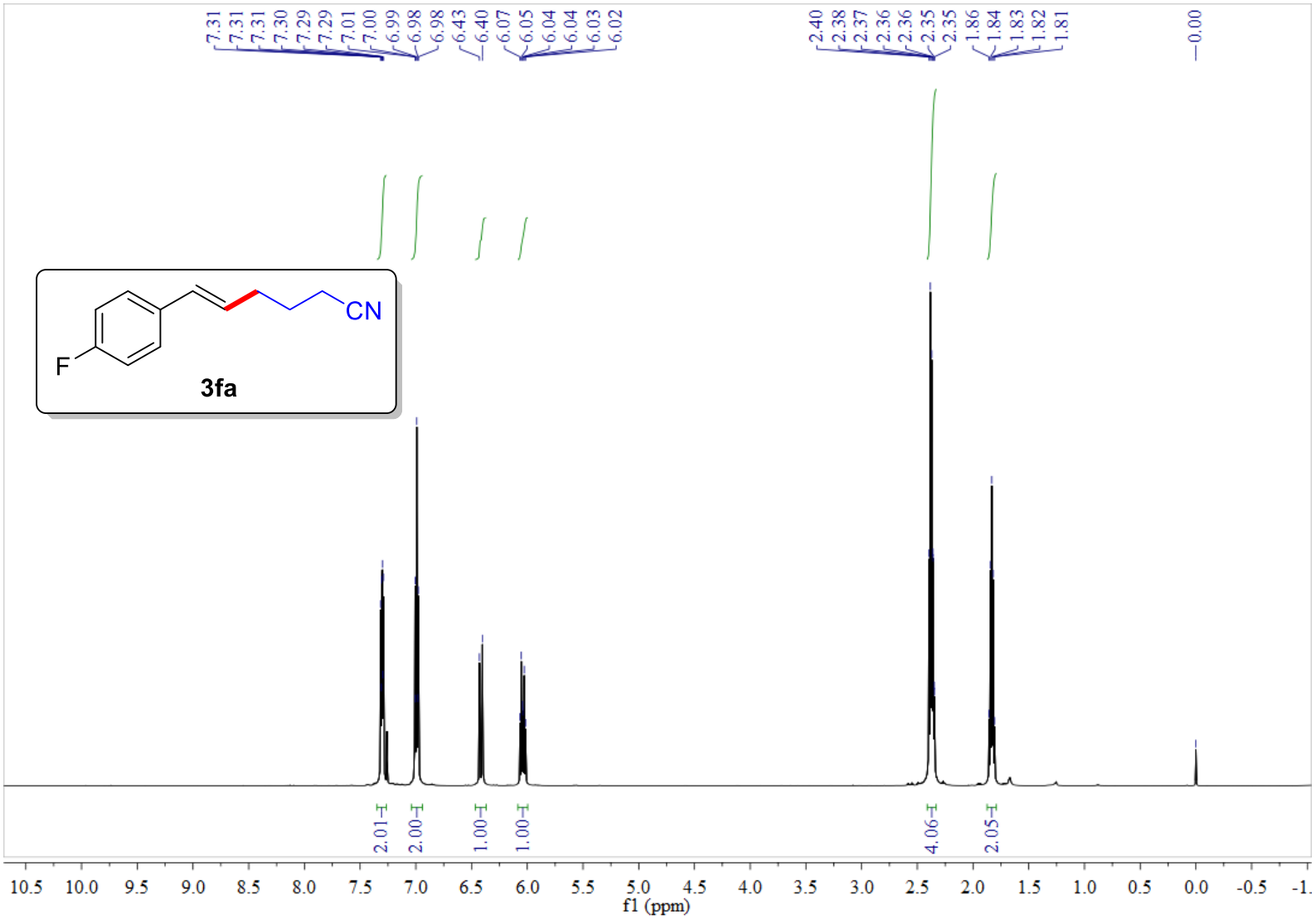
16.48
MeO
CN
3ea
f1 (ppm)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7.29
7.01
7.00
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6.98
6.98
6.43
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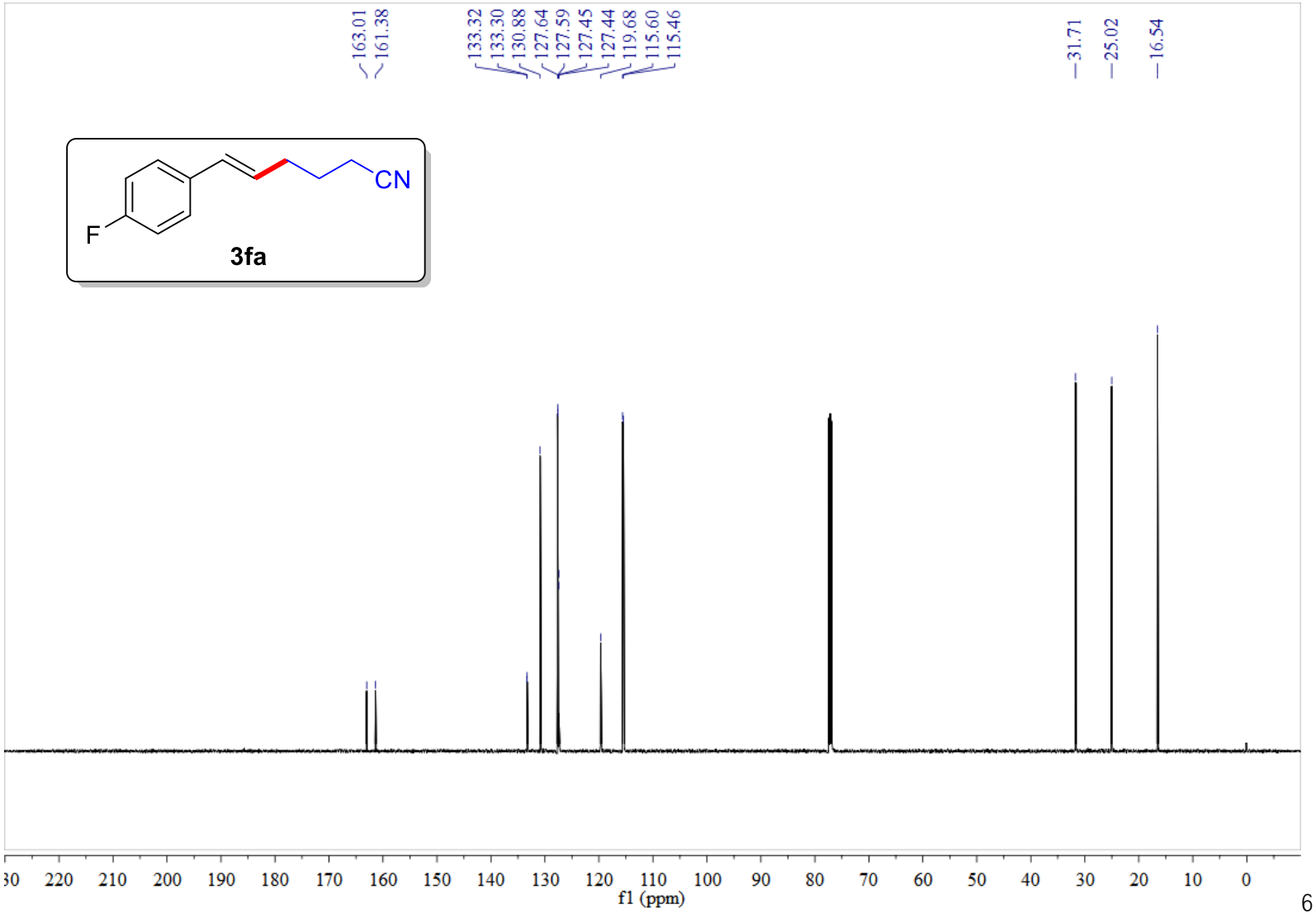
6.07
6.05
6.04
6.04
6.03
6.02
2.40
2.38
2.37
2.36
2.36
2.35
2.35
1.86
1.84
1.83
1.82
1.81
0.00
CN
F
3fa
2.01
2.00
1.00
1.00
4.06
2.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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161.38
133.32
133.30
130.88
127.64
127.59
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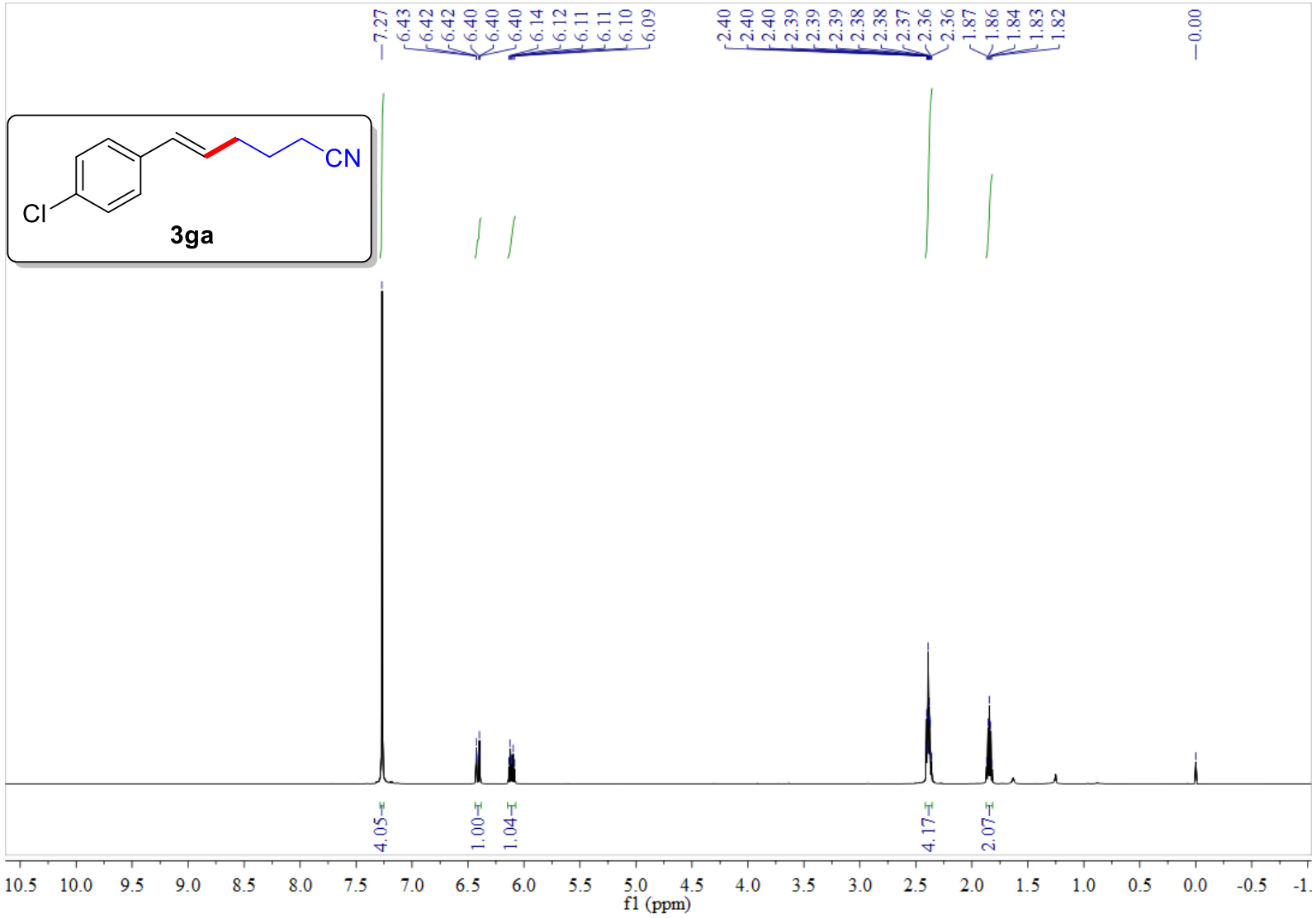
127.44
119.68
115.60
115.46
31.71
25.02
16.54
F
CN
3fa
f1 (ppm)

6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6.40
6.14
6.12
6.11
6.11
6.10
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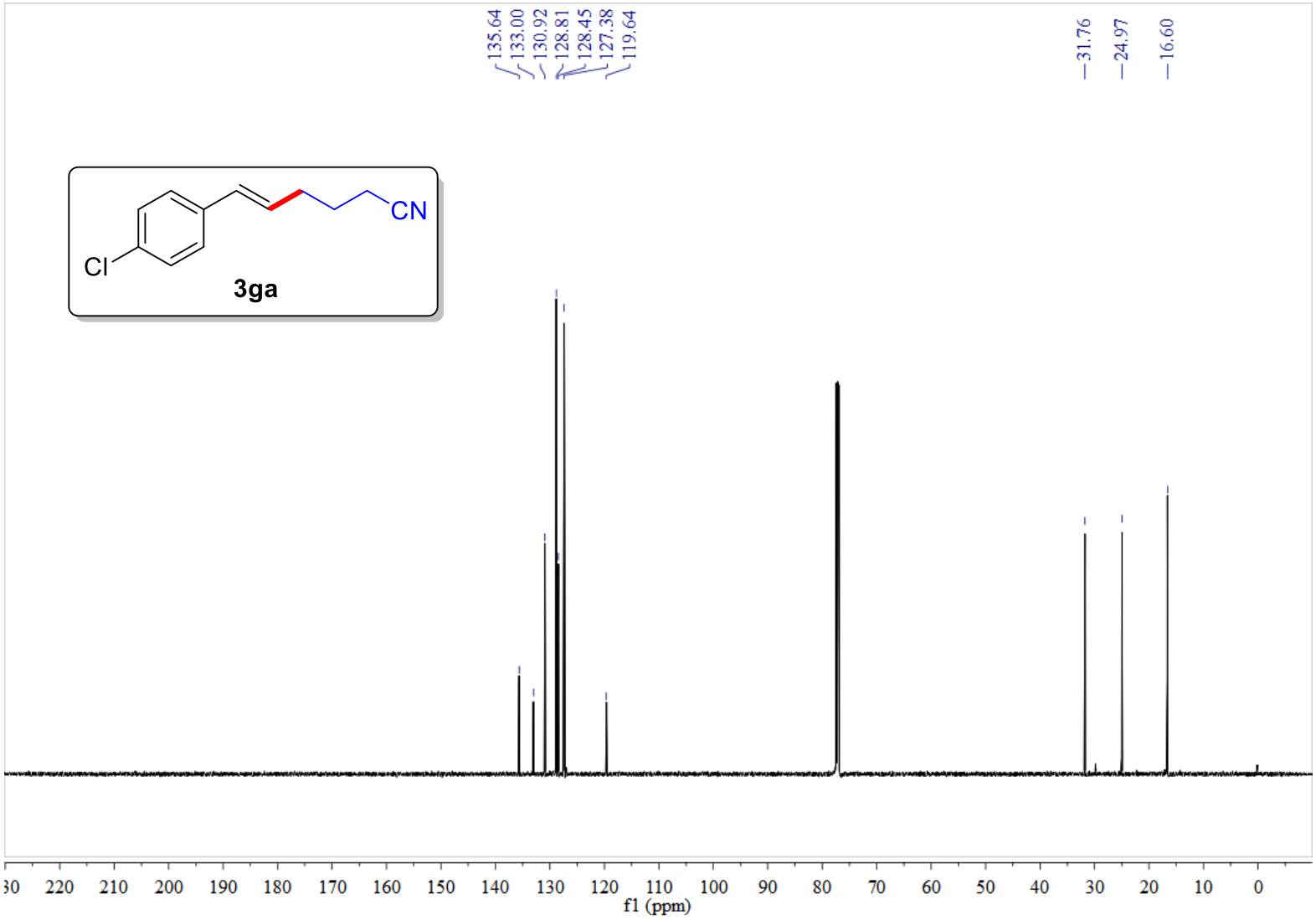
2.40
2.40
2.39
2.39
2.39
2.38
2.38
2.37
2.36
2.36
1.87
1.86
1.84
1.83
1.82
0.00
CN
Cl
3ga
4.05
1.00
1.04
4.17
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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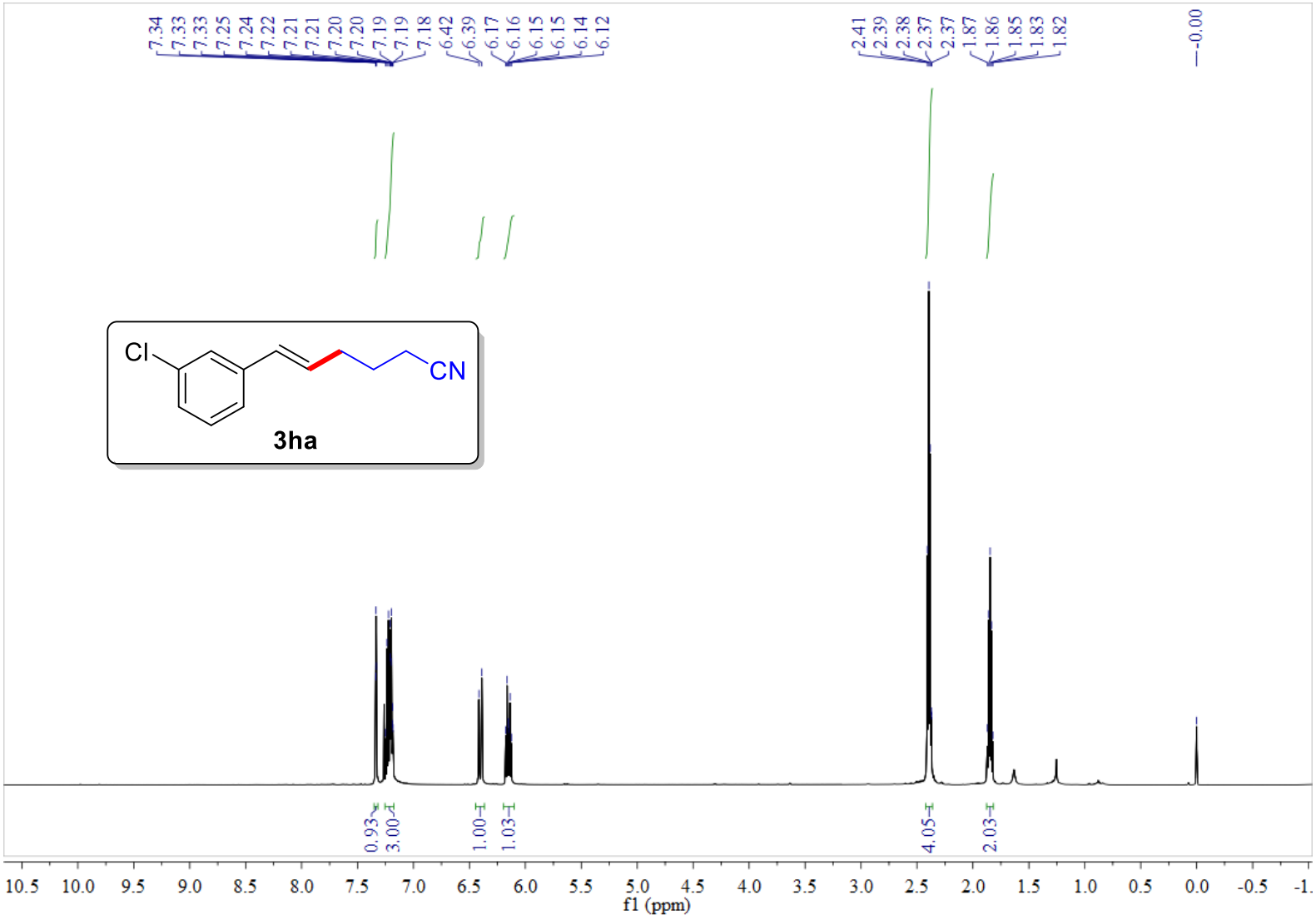
31.76
24.97
16.60
CN
Cl
3ga
f1 (ppm)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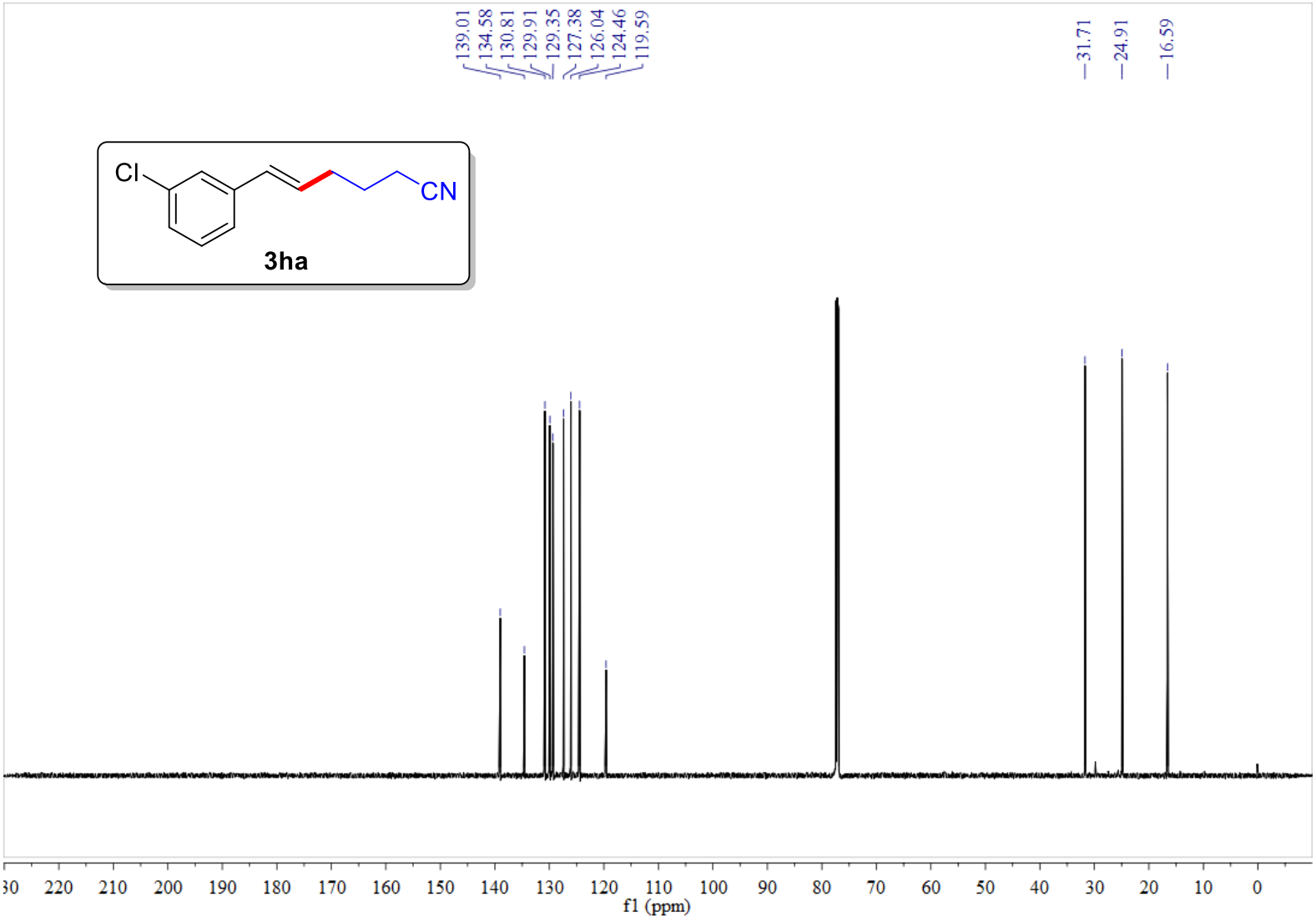
7.21
7.20
7.20
7.19
7.19
7.18
6.42
6.39
6.17
6.16
6.15
6.15
6.14
6.12
2.41
2.39
2.38
2.37
2.37
1.87
1.86
1.85
1.83
1.82
-0.00
Cl
CN
3ha
0.93
3.00
1.00
1.03
4.05
2.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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119.59
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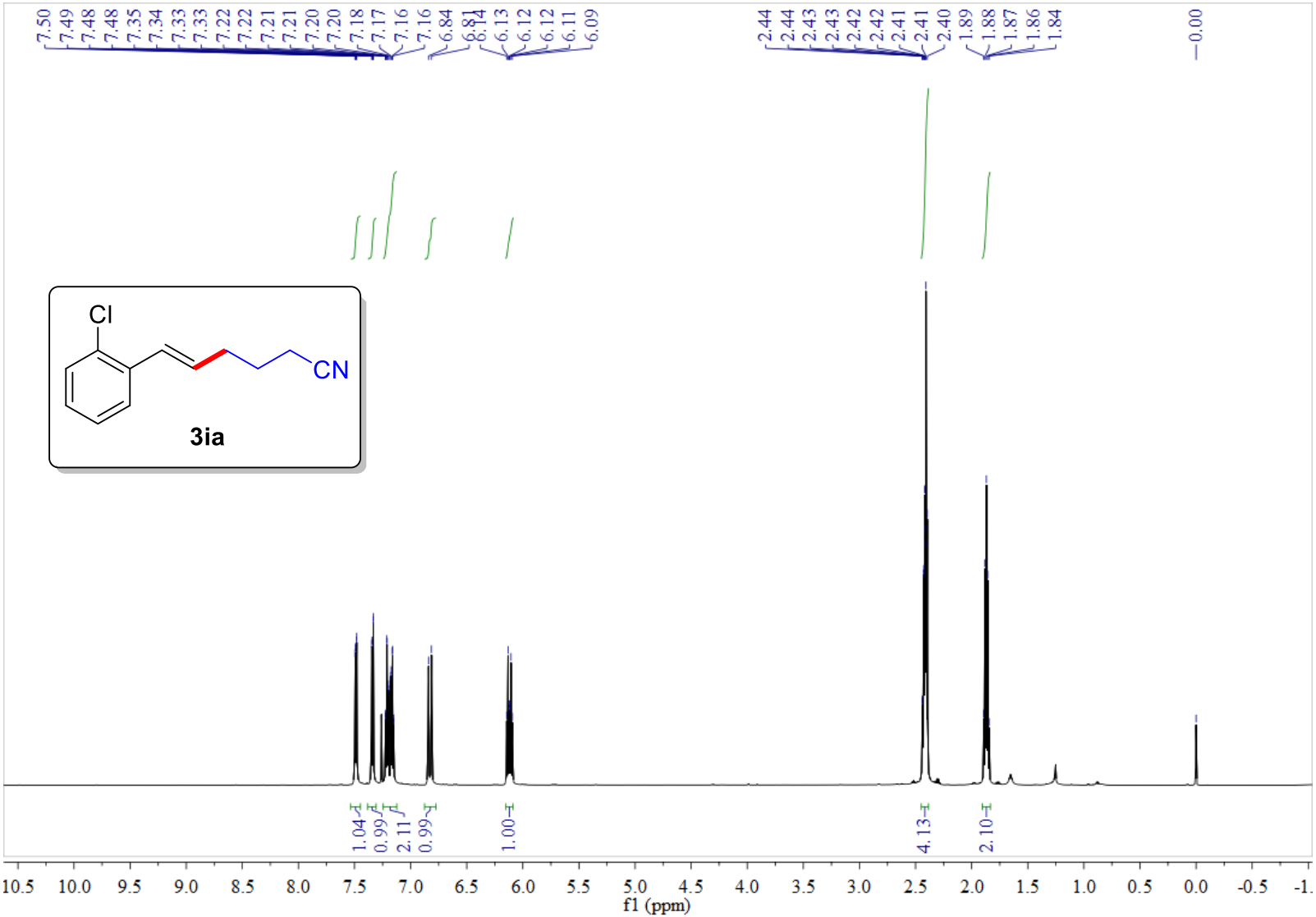
16.59
Cl
CN
3ha
f1 (ppm)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7.48
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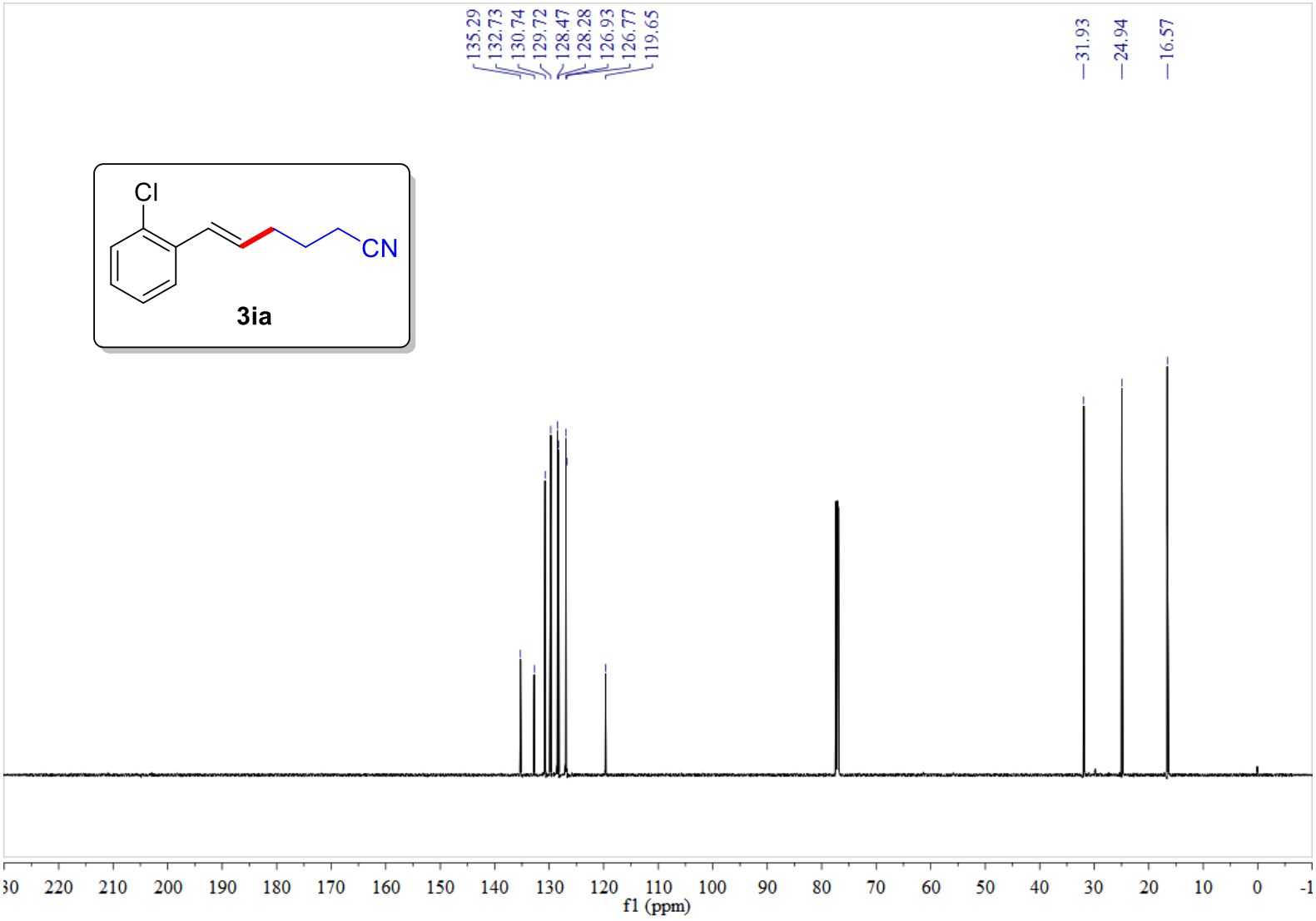
7.34
7.33
7.33
7.22
7.22
7.21
7.21
7.20
7.20
7.18
7.17
7.16
7.16
6.84
6.81
6.14
6.13
6.12
6.12
6.11
6.09
2.44
2.44
2.43
2.43
2.42
2.42
2.41
2.41
2.40
1.89
1.88
1.87
1.86
1.84
0.00
Cl
CN
3ia
1.04
0.99
2.11
0.99
1.00
4.13
2.10
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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126.77
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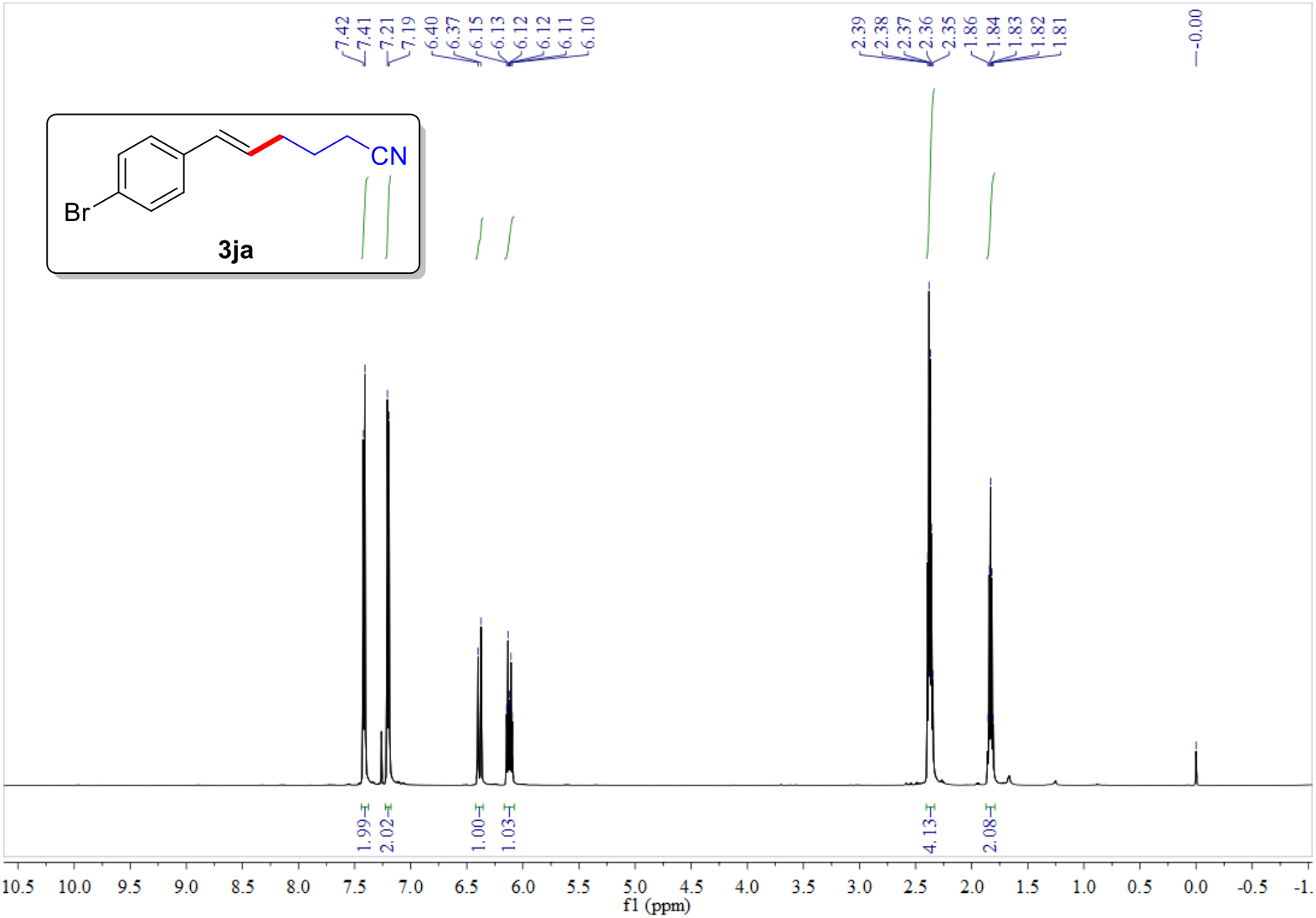
24.94
16.57
Cl
CN
3ia
f1 (ppm)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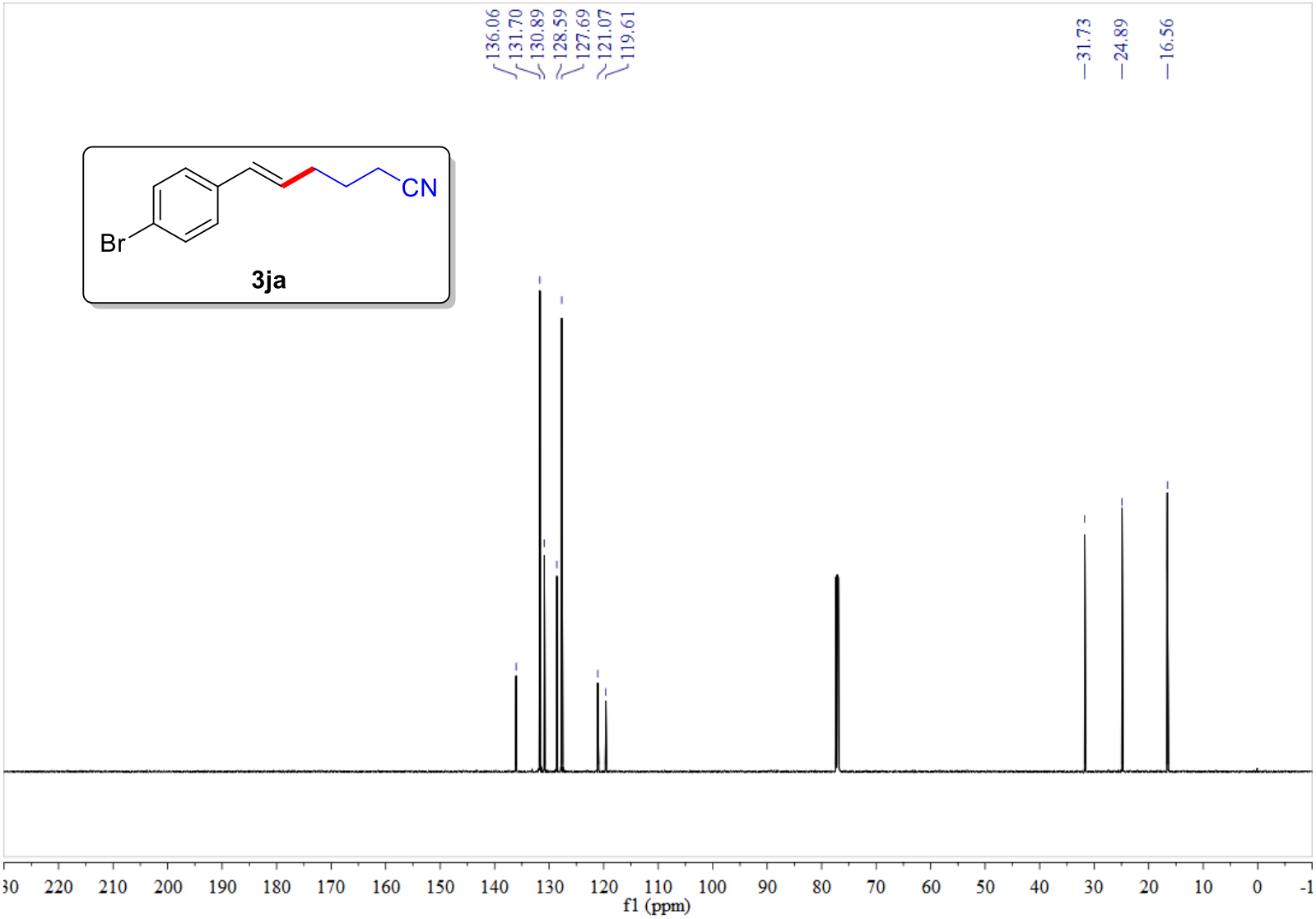
6.13
6.12
6.12
6.11
6.10
2.39
2.38
2.37
2.36
2.35
1.86
1.84
1.83
1.82
1.81
-0.00
Br
CN
3ja
1.99
2.02
1.00
1.03
4.13
2.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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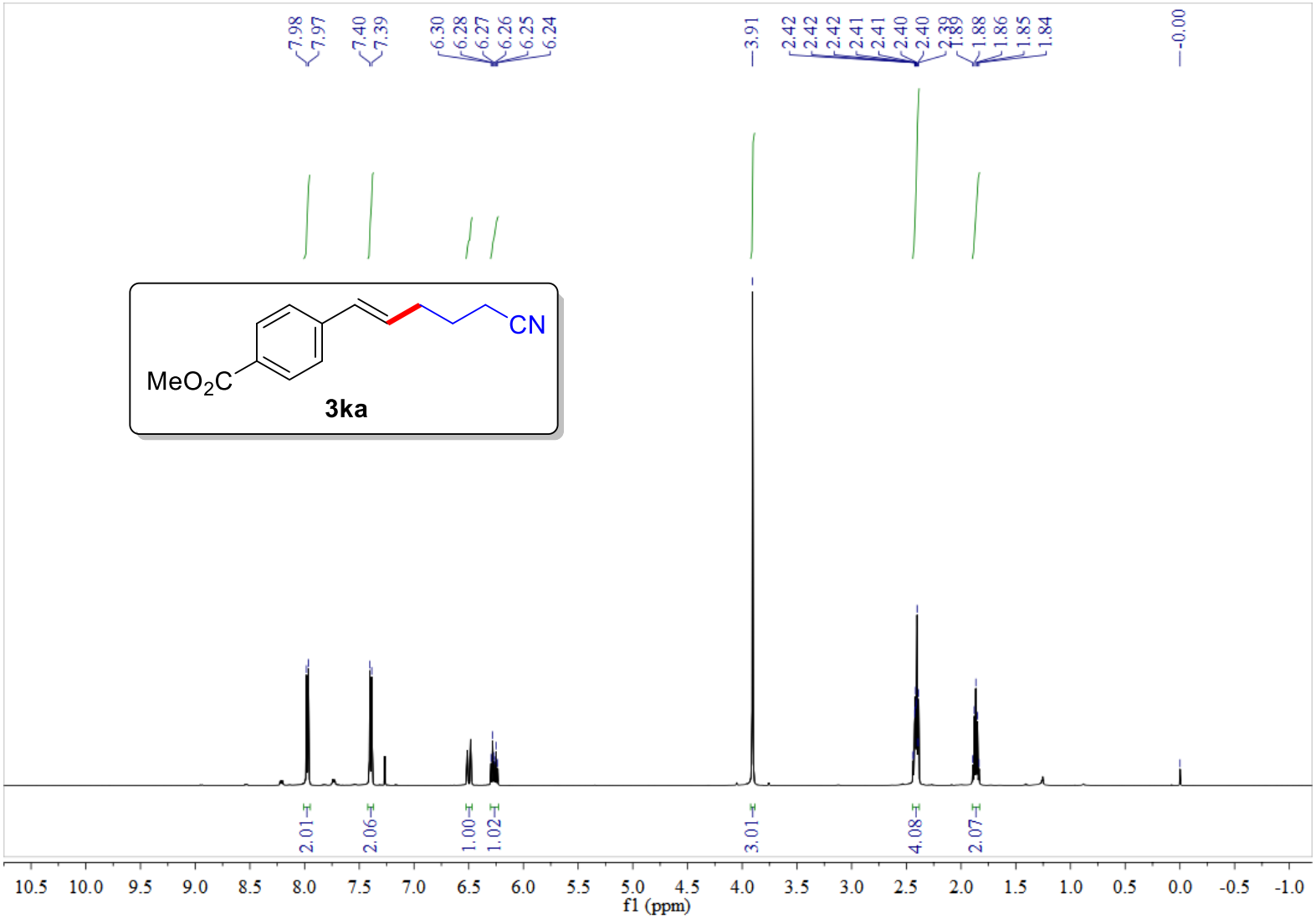
16.56
Br
CN
3ja
f1 (ppm)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6.26
6.25
6.24
3.91
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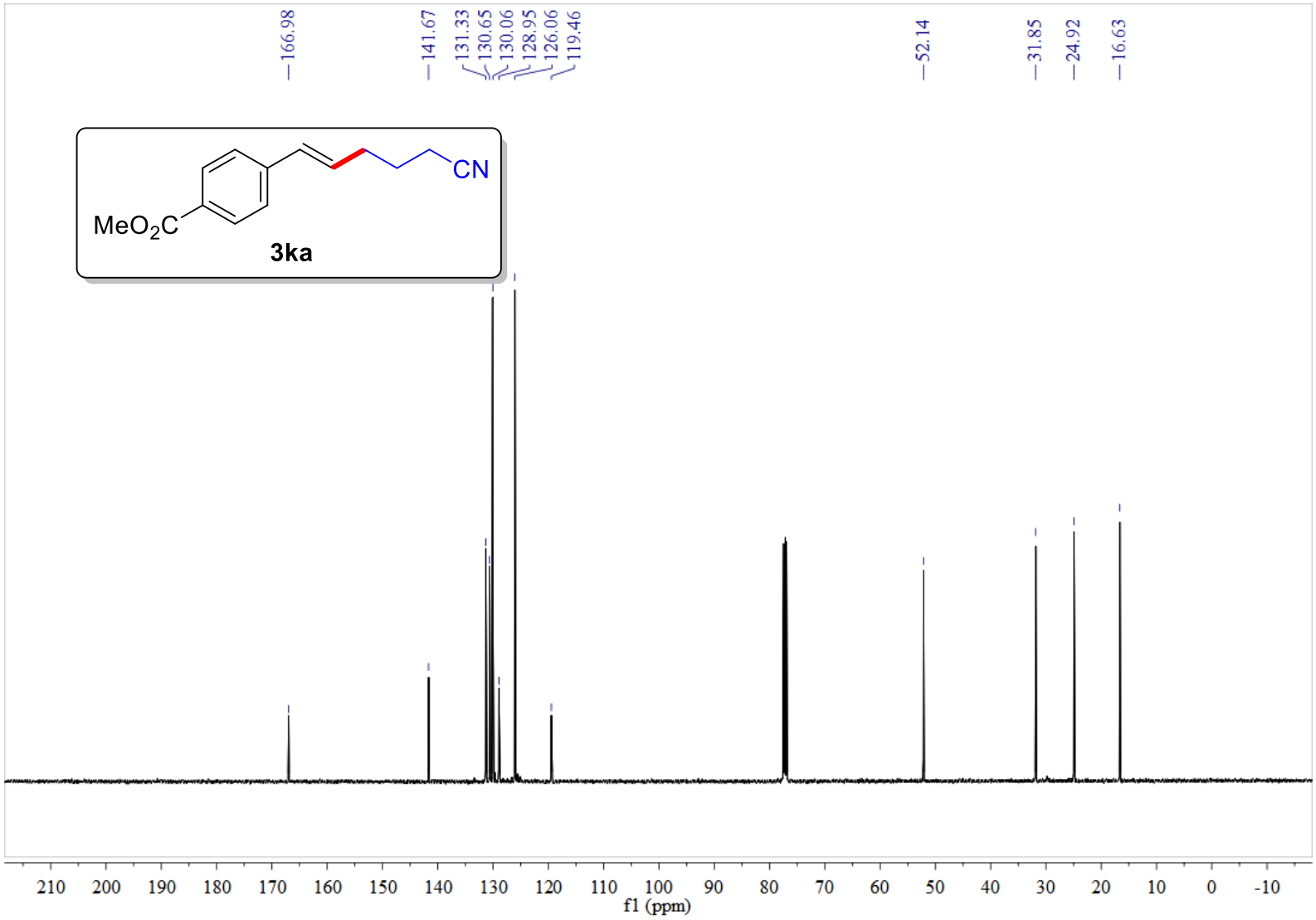
2.42
2.42
2.41
2.41
2.40
2.40
2.39
1.89
1.88
1.86
1.85
1.84
-0.00
CN
MeO2C
3ka
2.01
2.06
1.00
1.02
3.01
4.08
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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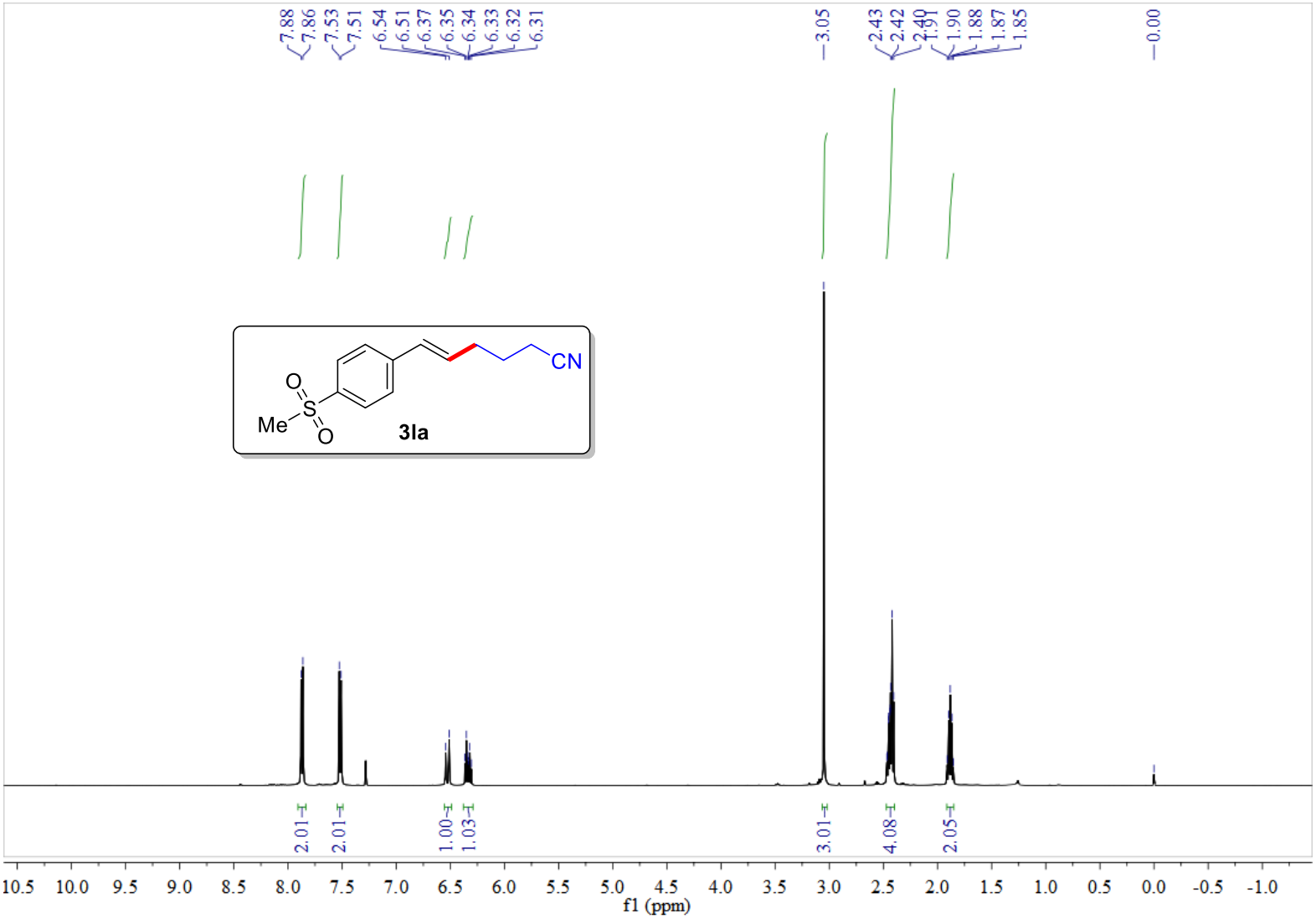
130.65
130.06
128.95
126.06
119.46
52.14
31.85
24.92
16.63
CN
MeO2C
3ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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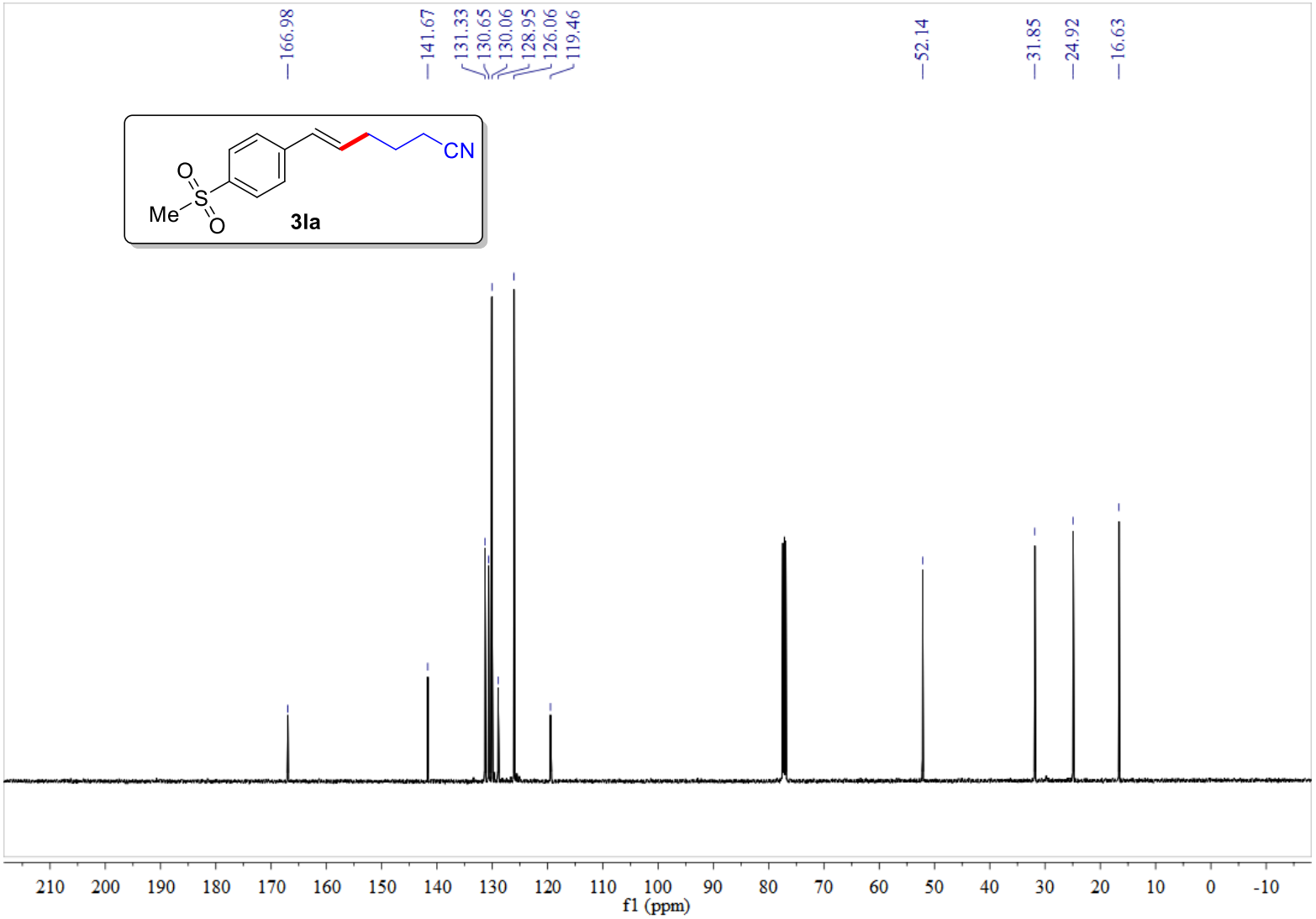
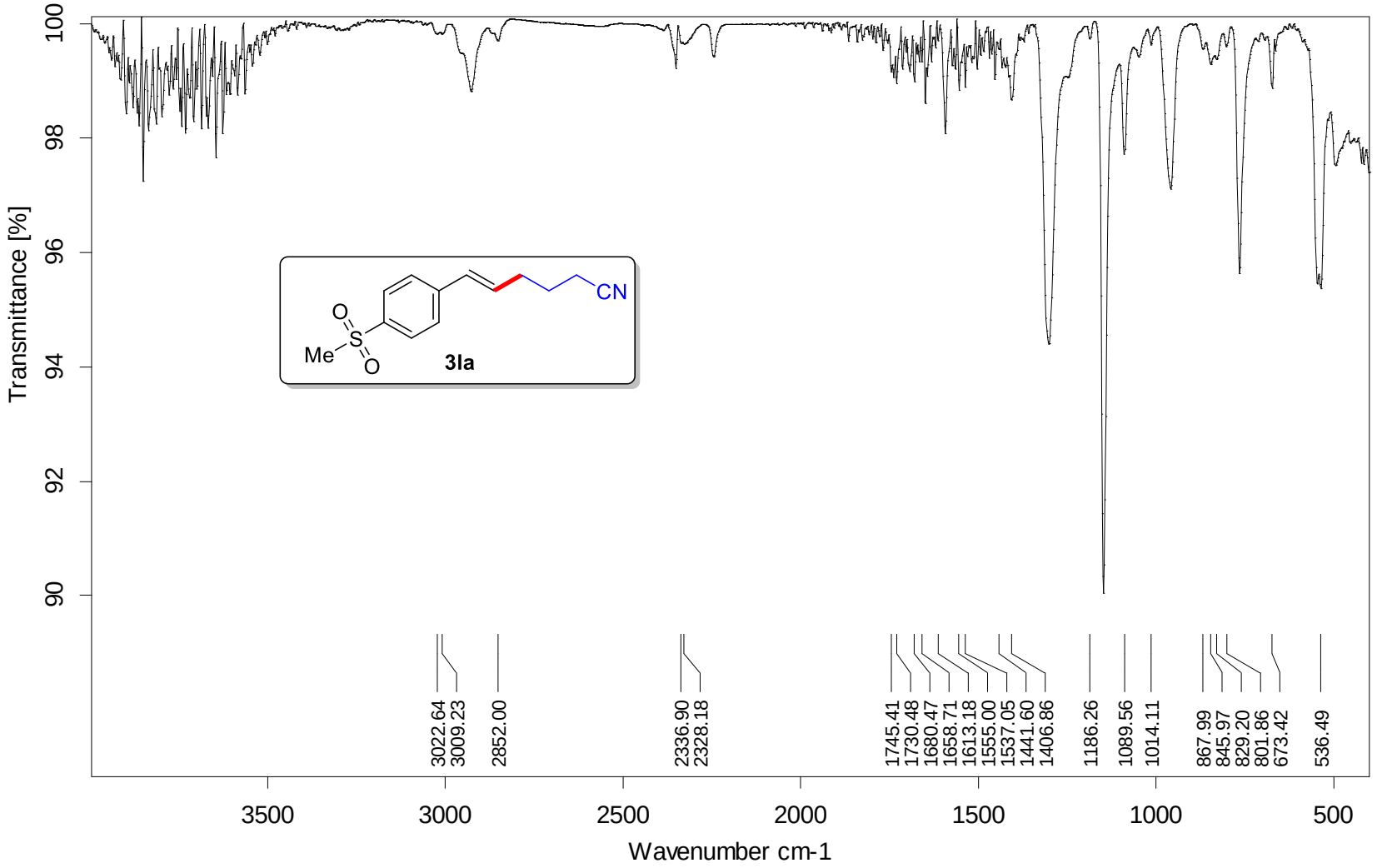
6.51
6.37
6.35
6.34
6.33
6.32
6.31
3.05
2.43
2.42
2.40
1.91
1.90
1.88
1.87
1.85
0.00
CN
O
S
O
Me
O
3Ia
2.01
2.01
1.00
1.03
3.01
4.08
2.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


166.98
141.67
131.33
130.65
130.06
128.95
126.06
119.46
52.14
31.85
24.92
16.63
CN
O
S
O
Me
3la
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)


Transmittance [%]
100
98
96
94
92
90
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
Me
S
O
O
CN
3la
3022.64
3009.23
2852.00
2336.90
2328.18
1745.41
1730.48
1680.47
1658.71
1613.18
1555.00
1537.05
1441.60
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1089.56
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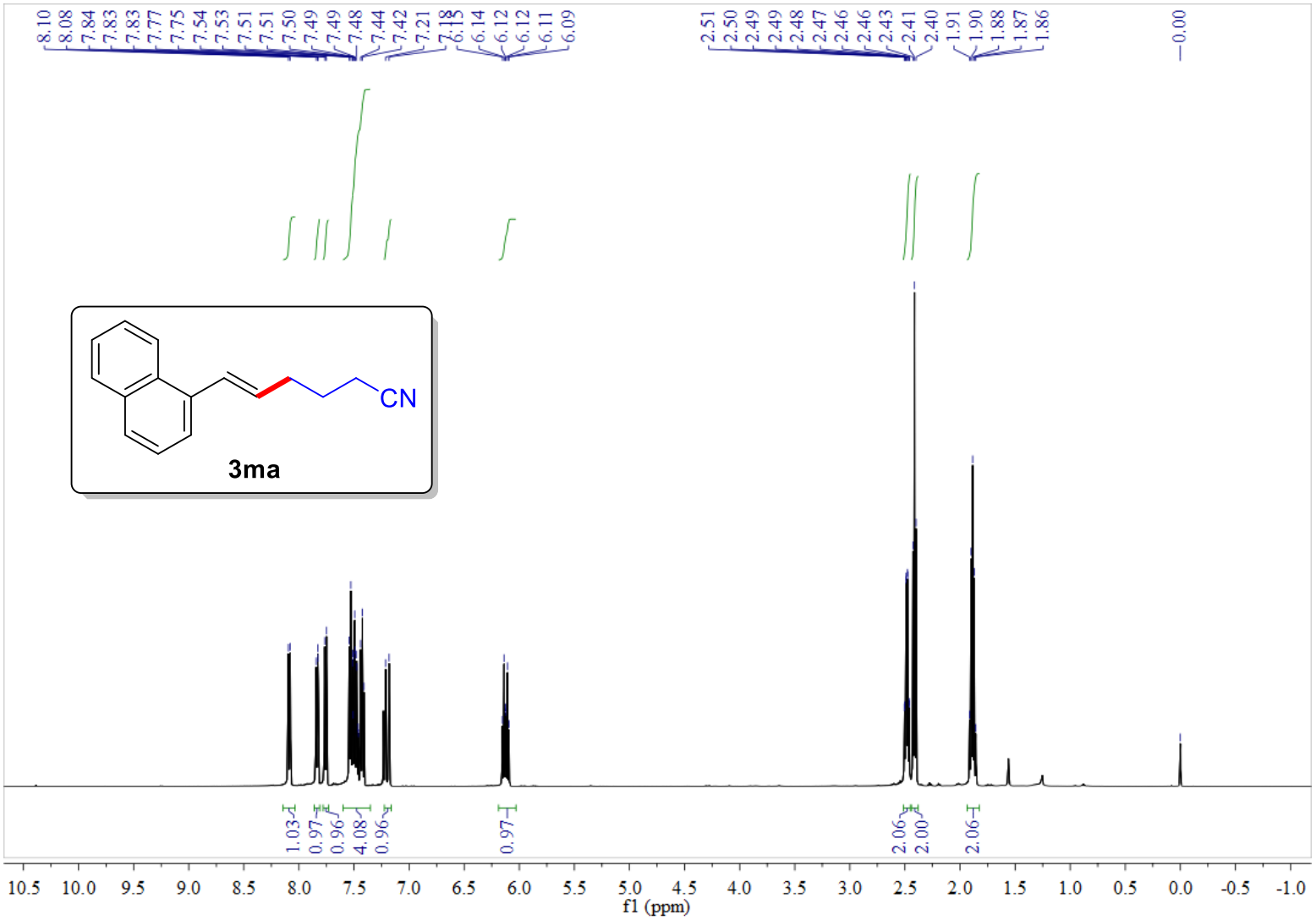
845.97
829.20
801.86
673.42
536.49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7.49
7.48
7.44
7.42
7.21
7.18
7.15
6.14
6.12
6.12
6.11
6.09
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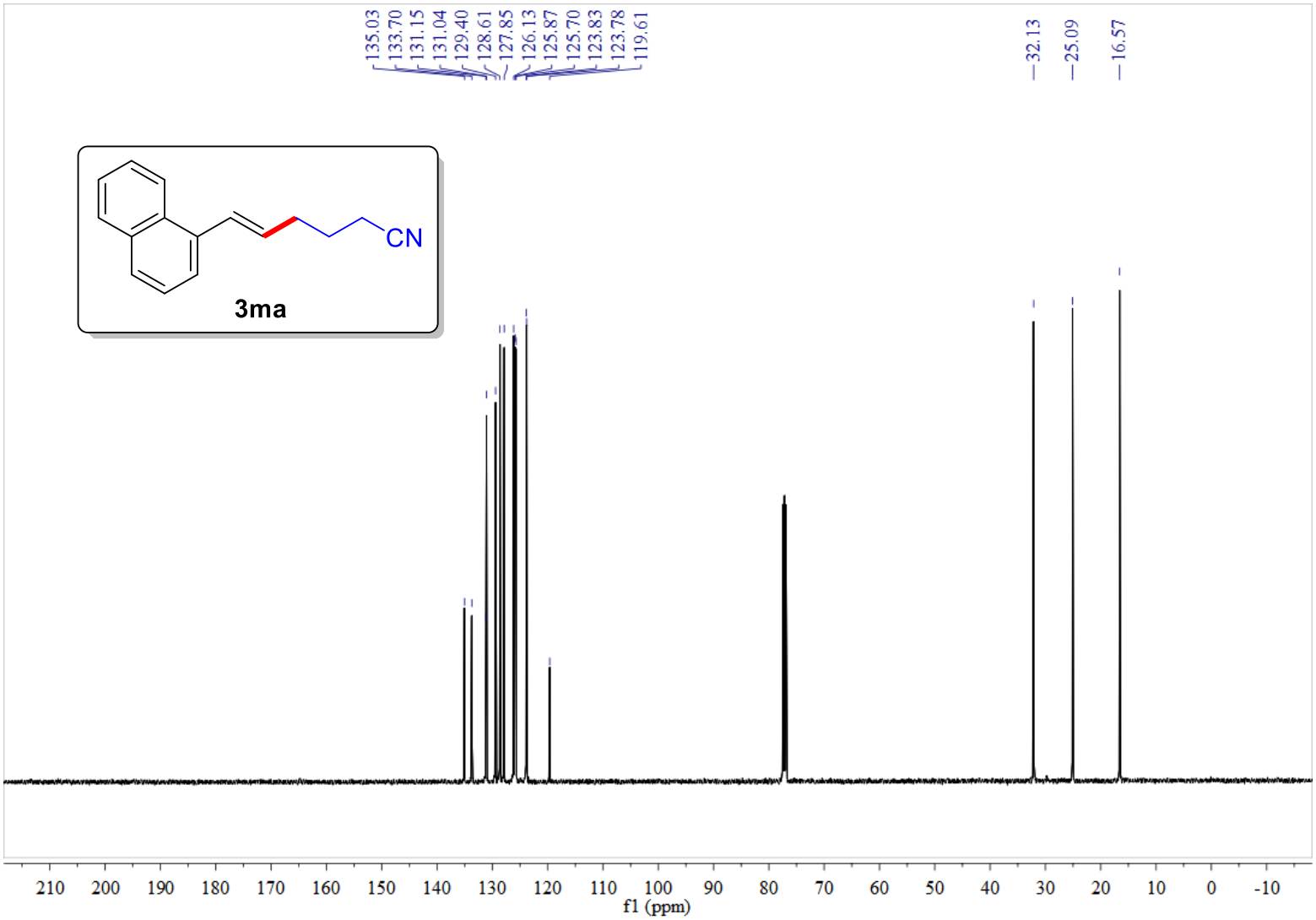
2.50
2.49
2.49
2.48
2.47
2.46
2.46
2.43
2.41
2.40
1.91
1.90
1.88
1.87
1.86
0.00
CN
3ma
1.03
0.97
0.96
4.08
0.96
0.97
2.06
2.00
2.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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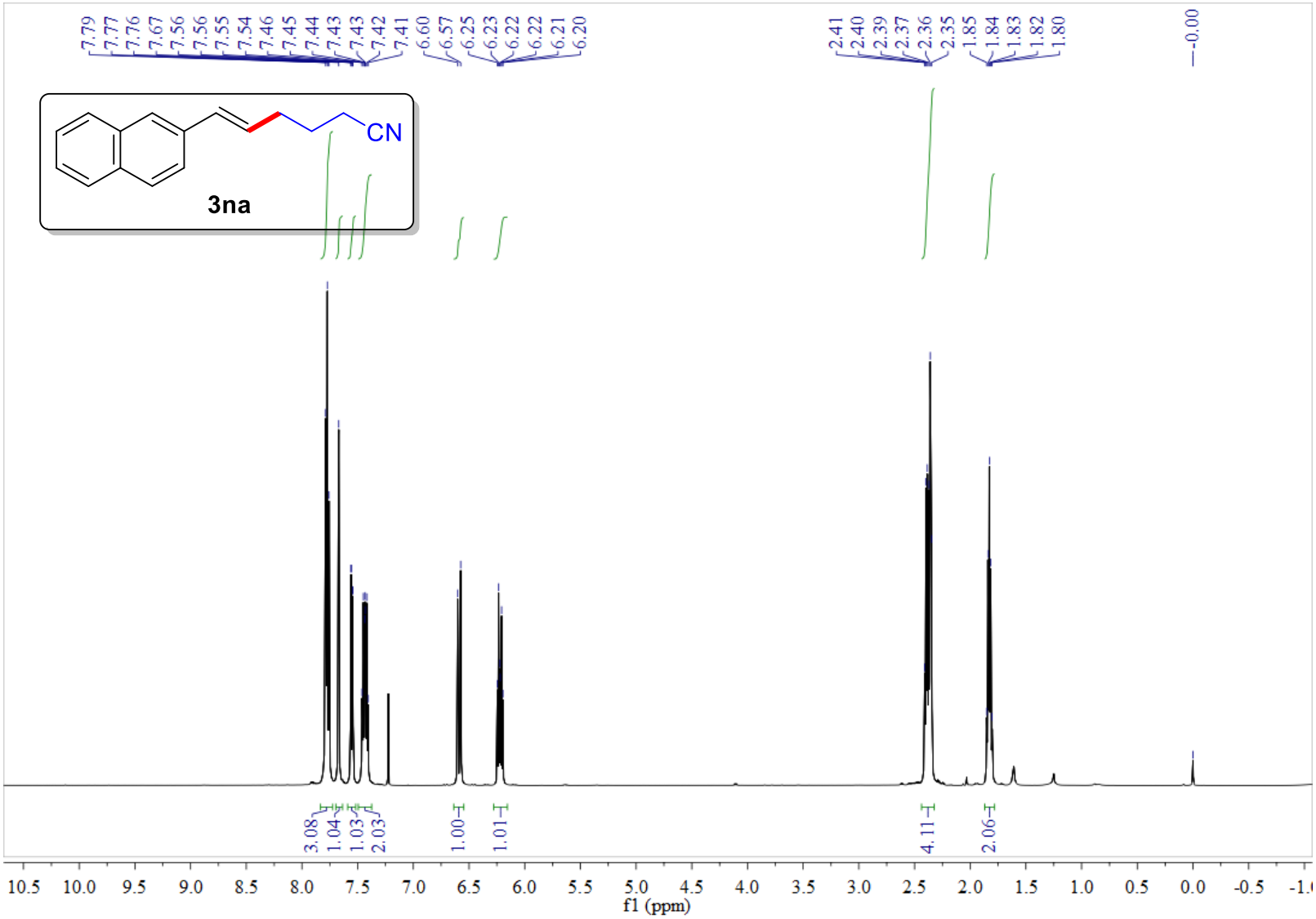
126.13
125.87
125.70
123.83
123.78
119.61
32.13
25.09
16.57
CN
3ma
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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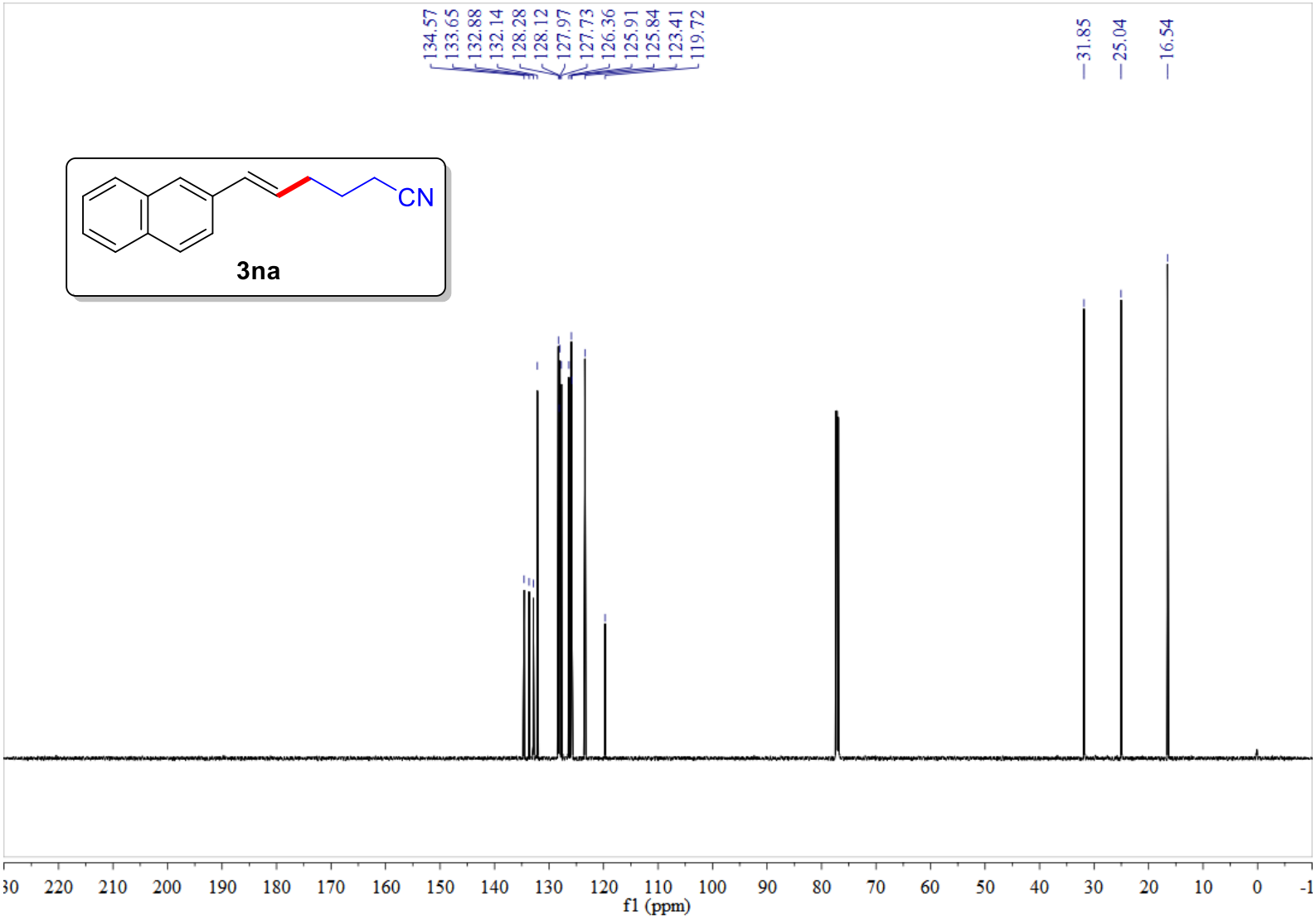
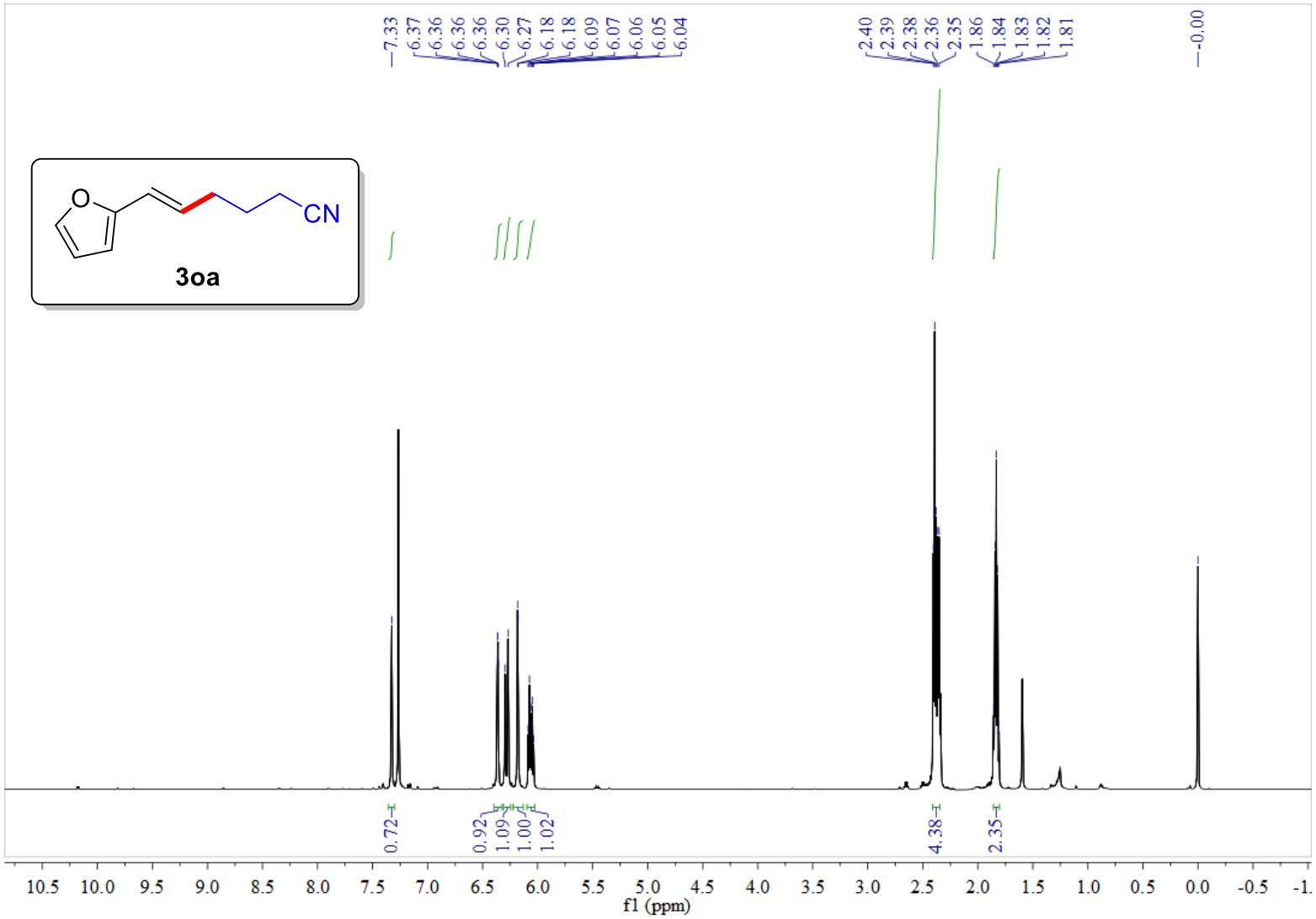
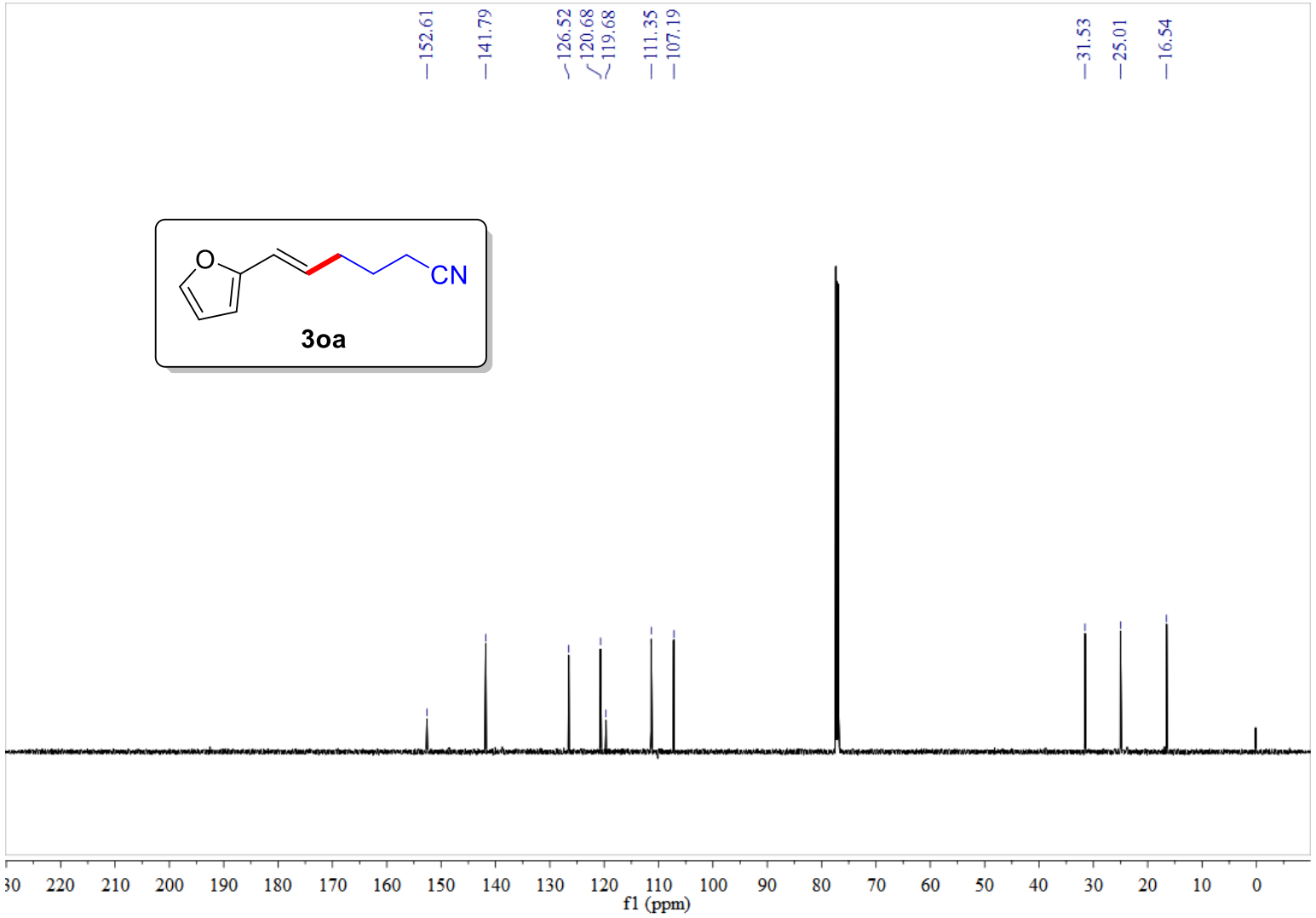
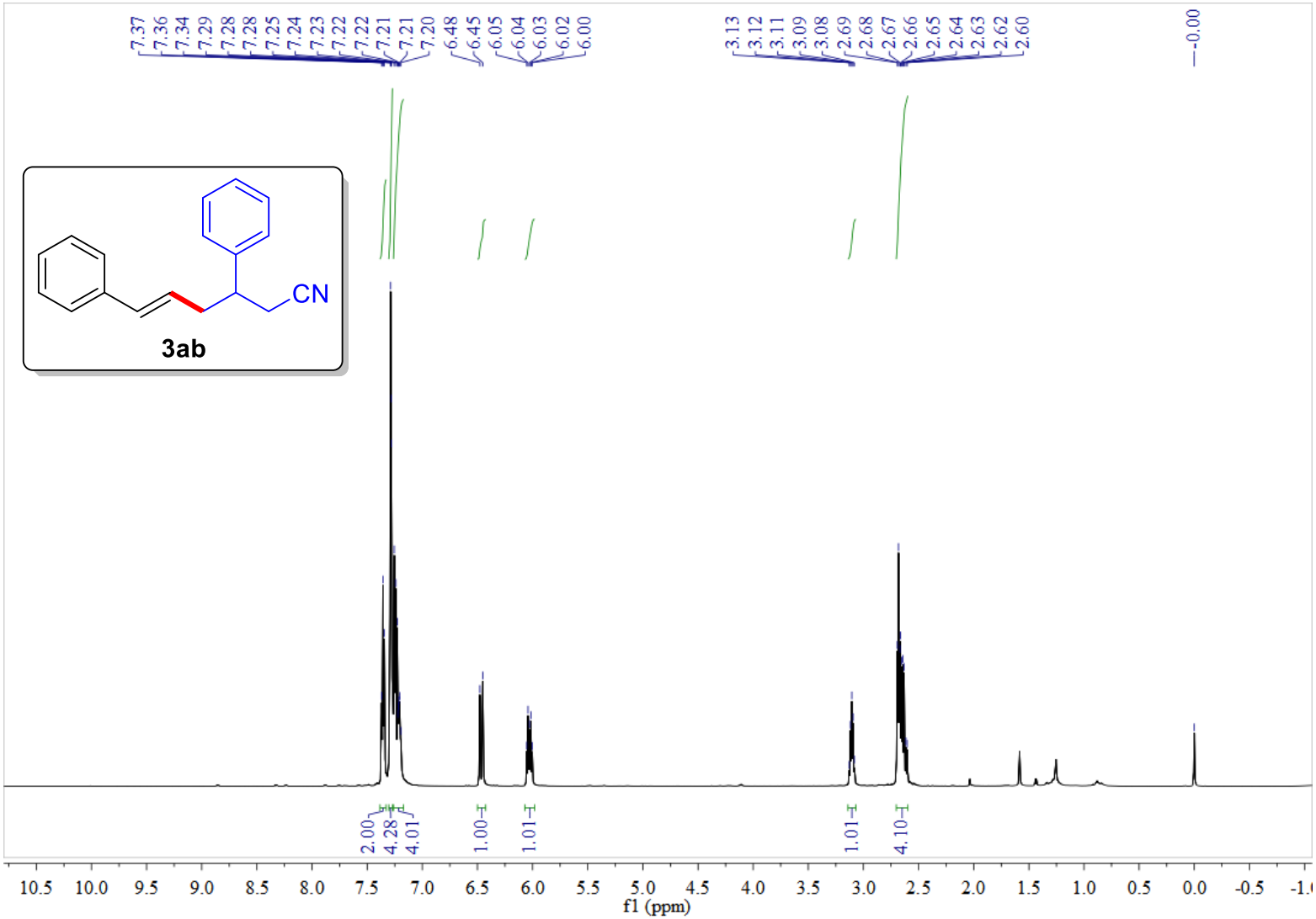
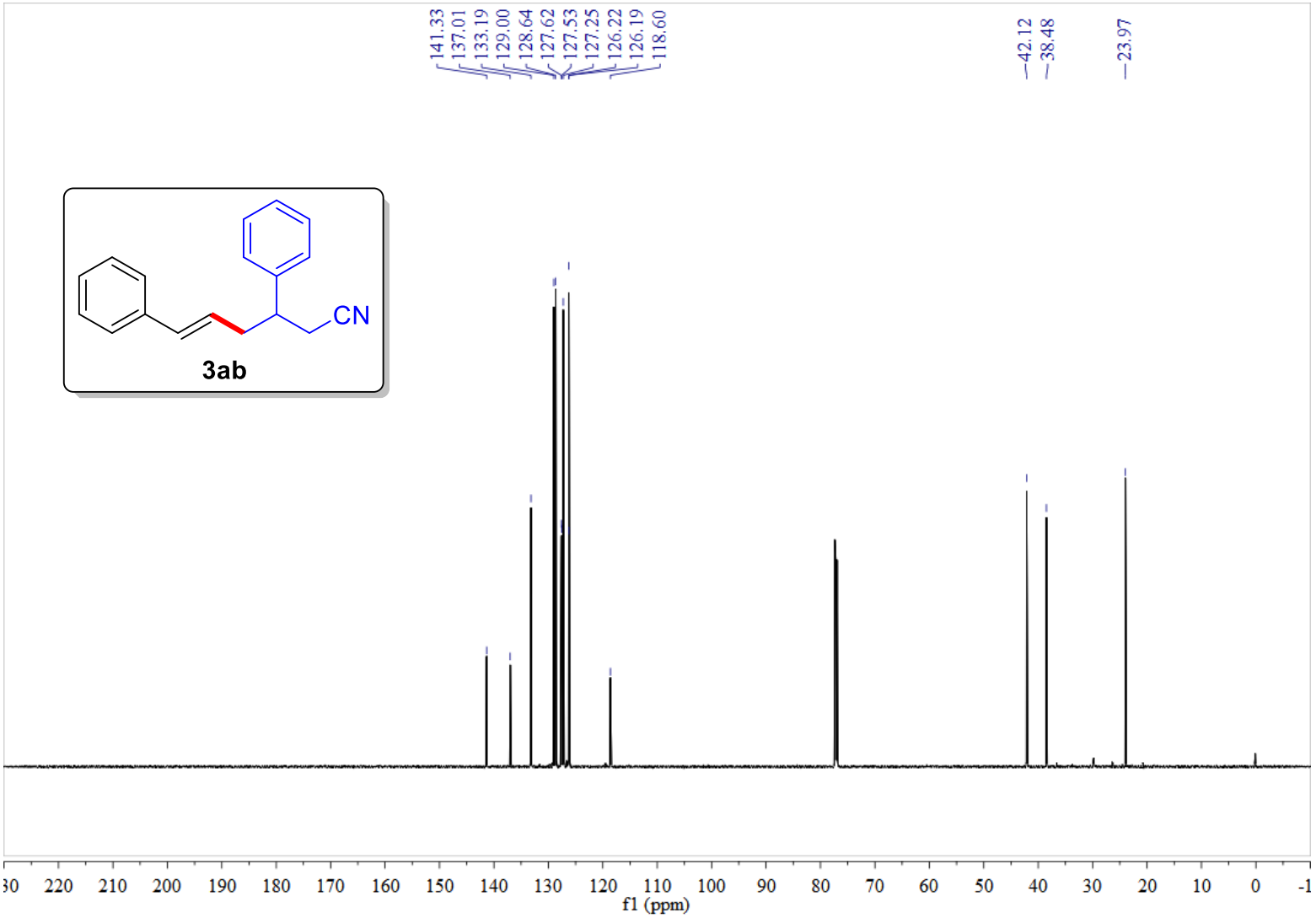
7.42
7.41
6.60
6.57
6.25
6.23
6.22
6.22
6.21
6.20
2.41
2.40
2.39
2.37
2.36
2.35
1.85
1.84
1.83
1.82
1.80
-0.00
CN
3na
3.08
1.04
1.03
2.03
1.00
1.01
4.11
2.06
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

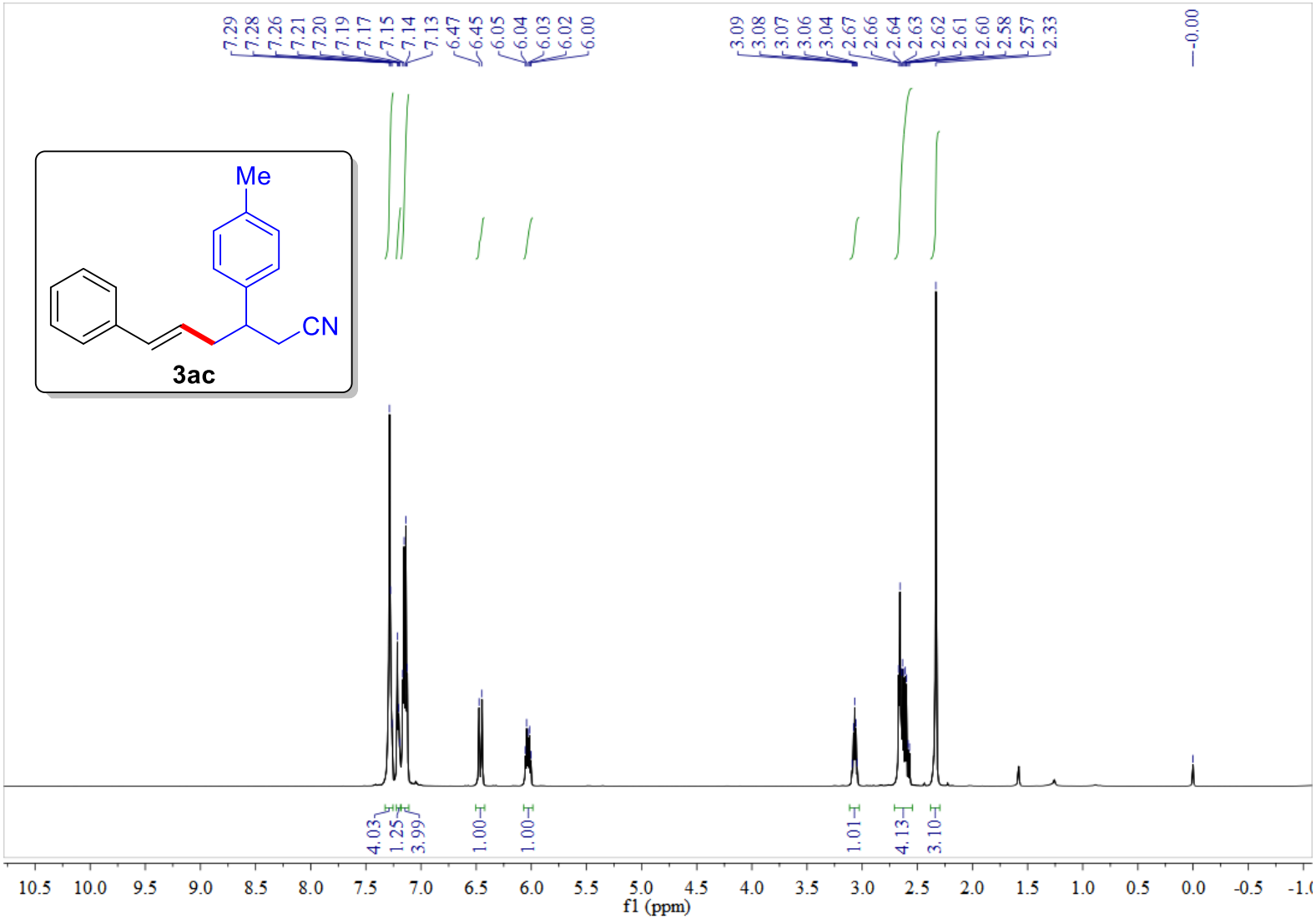

134.57
133.65
132.88
132.14
128.28
128.12
127.97
127.73
126.36
125.91
125.84
123.41
119.72
31.85
25.04
16.54
CN
3na
f1 (ppm)

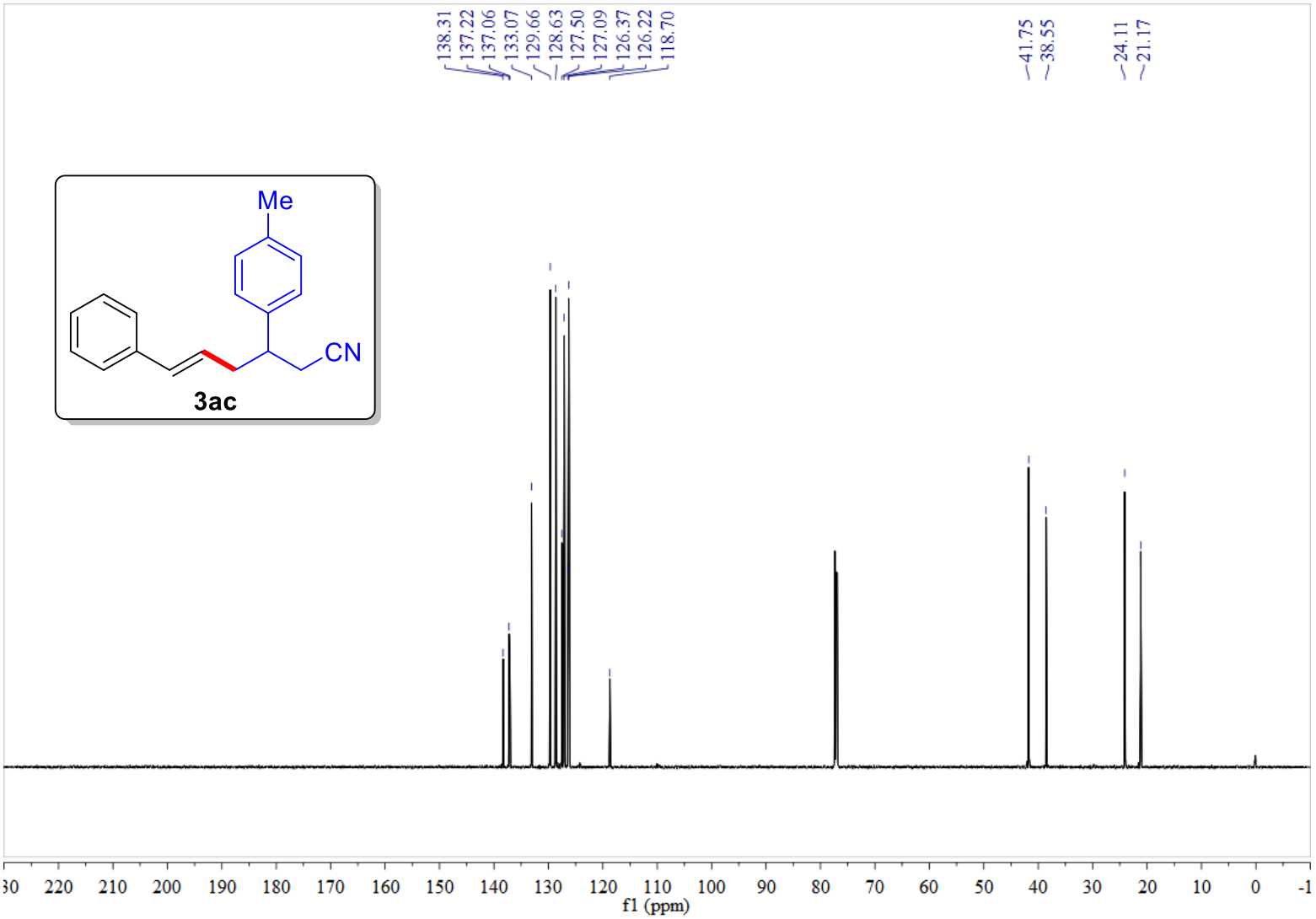

7.33
6.37
6.36
6.36
6.36
6.30
6.27
6.18
6.18
6.09
6.07
6.06
6.05
6.04
2.40
2.39
2.38
2.36
2.35
1.86
1.84
1.83
1.82
1.81
-0.00
O
CN
3oa
0.72
0.92
1.09
1.00
1.02
4.38
2.35
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

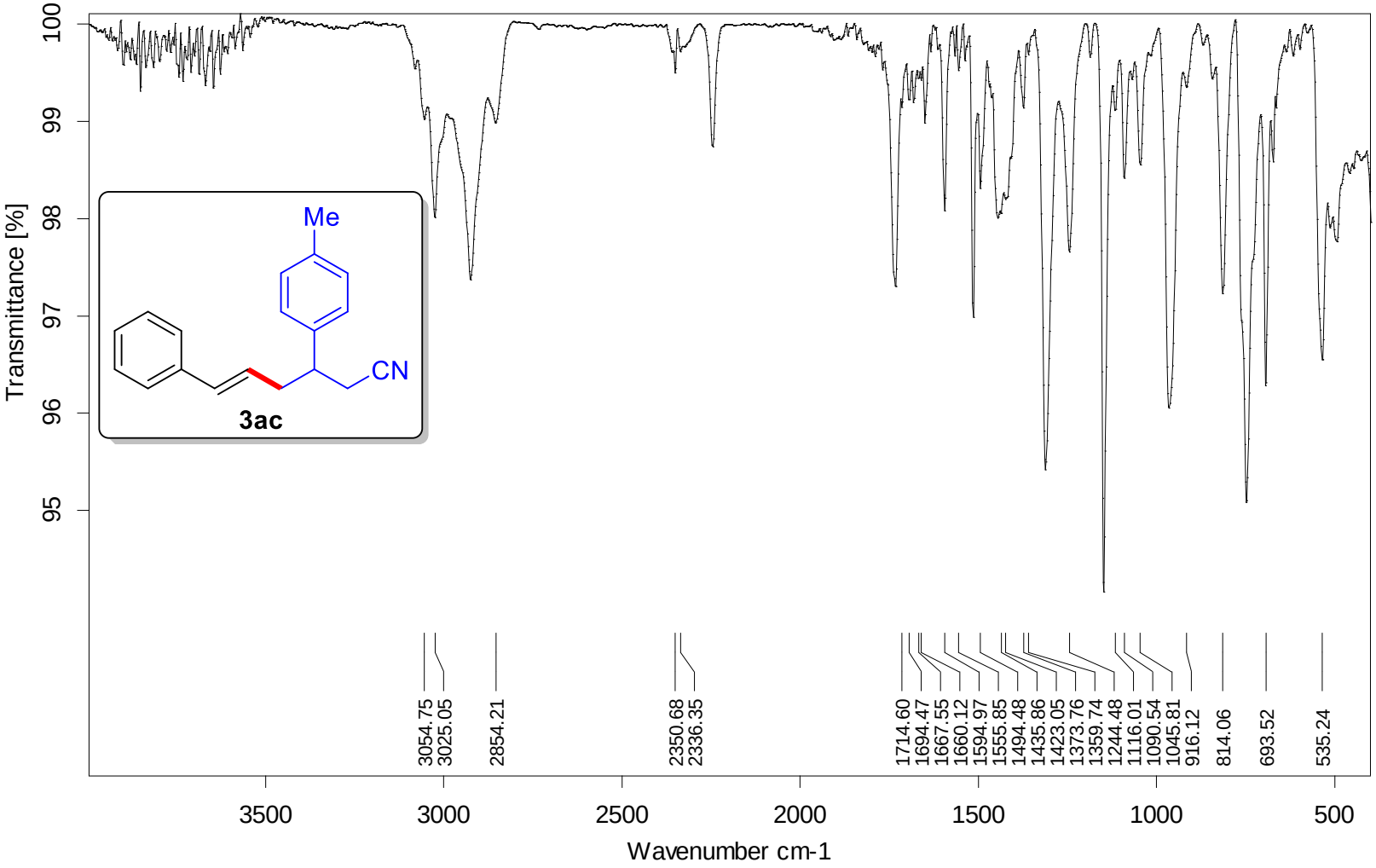

152.61
141.79
126.52
120.68
119.68
111.35
107.19
31.53
25.01
16.54
O
CN
3oa
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

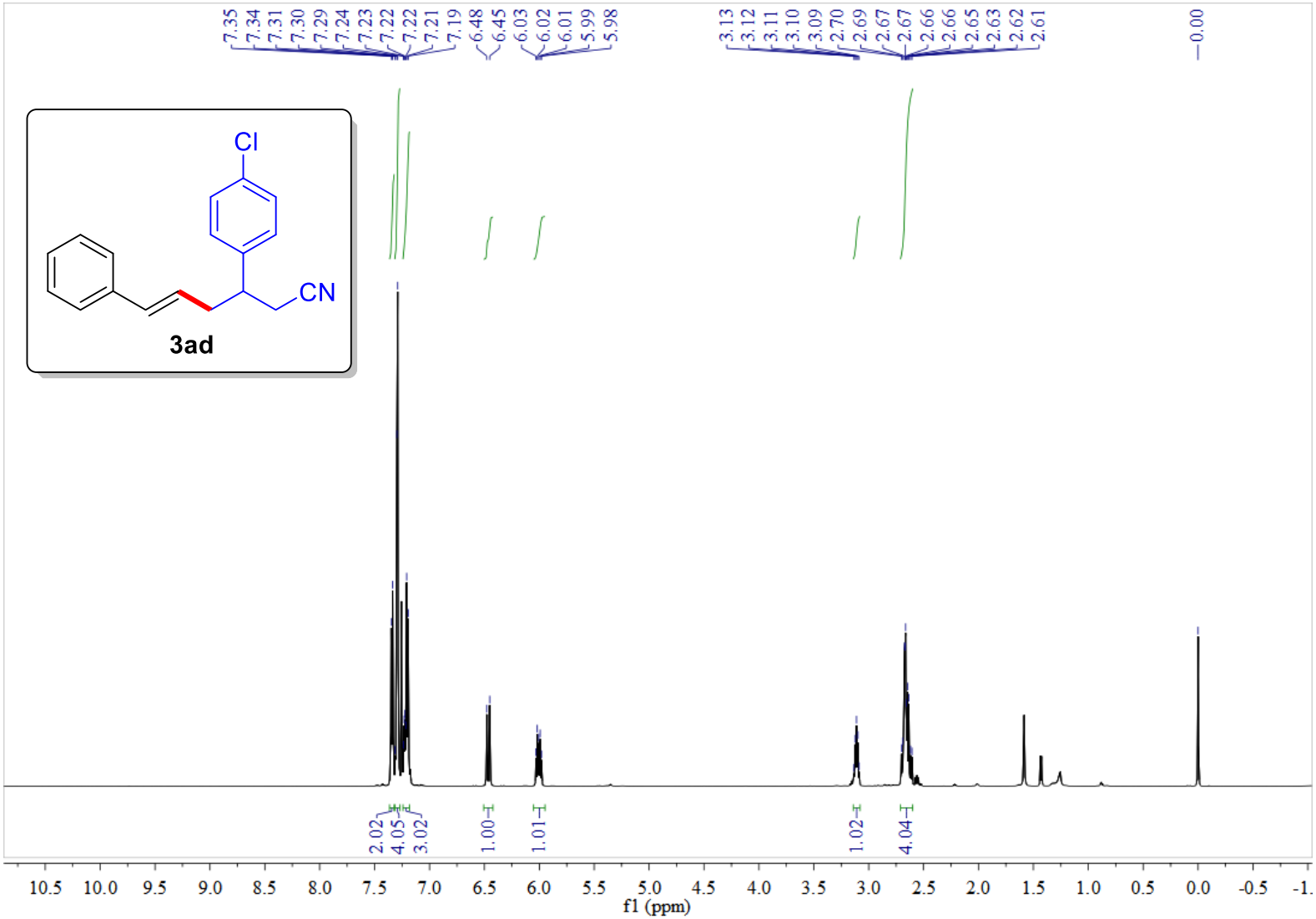

7.37
7.36
7.34
7.29
7.28
7.28
7.25
7.24
7.23
7.22
7.22
7.21
7.21
7.20
6.48
6.45
6.05
6.04
6.03
6.02
6.00
3.13
3.12
3.11
3.09
3.08
2.69
2.68
2.67
2.66
2.65
2.64
2.63
2.62
2.60
-0.00
CN
3ab
2.00
4.28
4.01
1.00
1.01
1.01
4.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

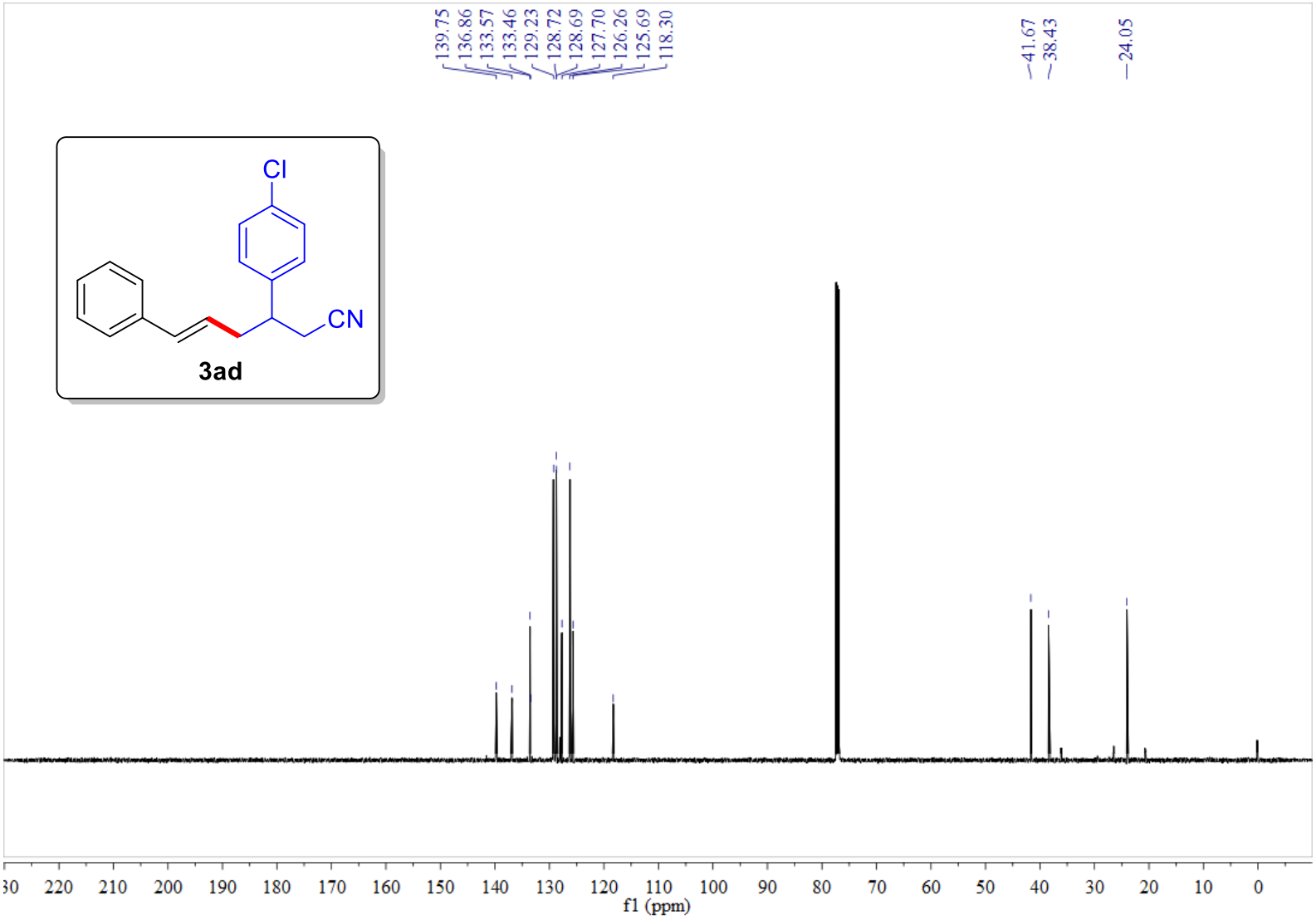

141.33
137.01
133.19
129.00
128.64
127.62
127.53
127.25
126.22
126.19
118.60
42.12
38.48
23.97
CN
3ab
f1 (ppm)

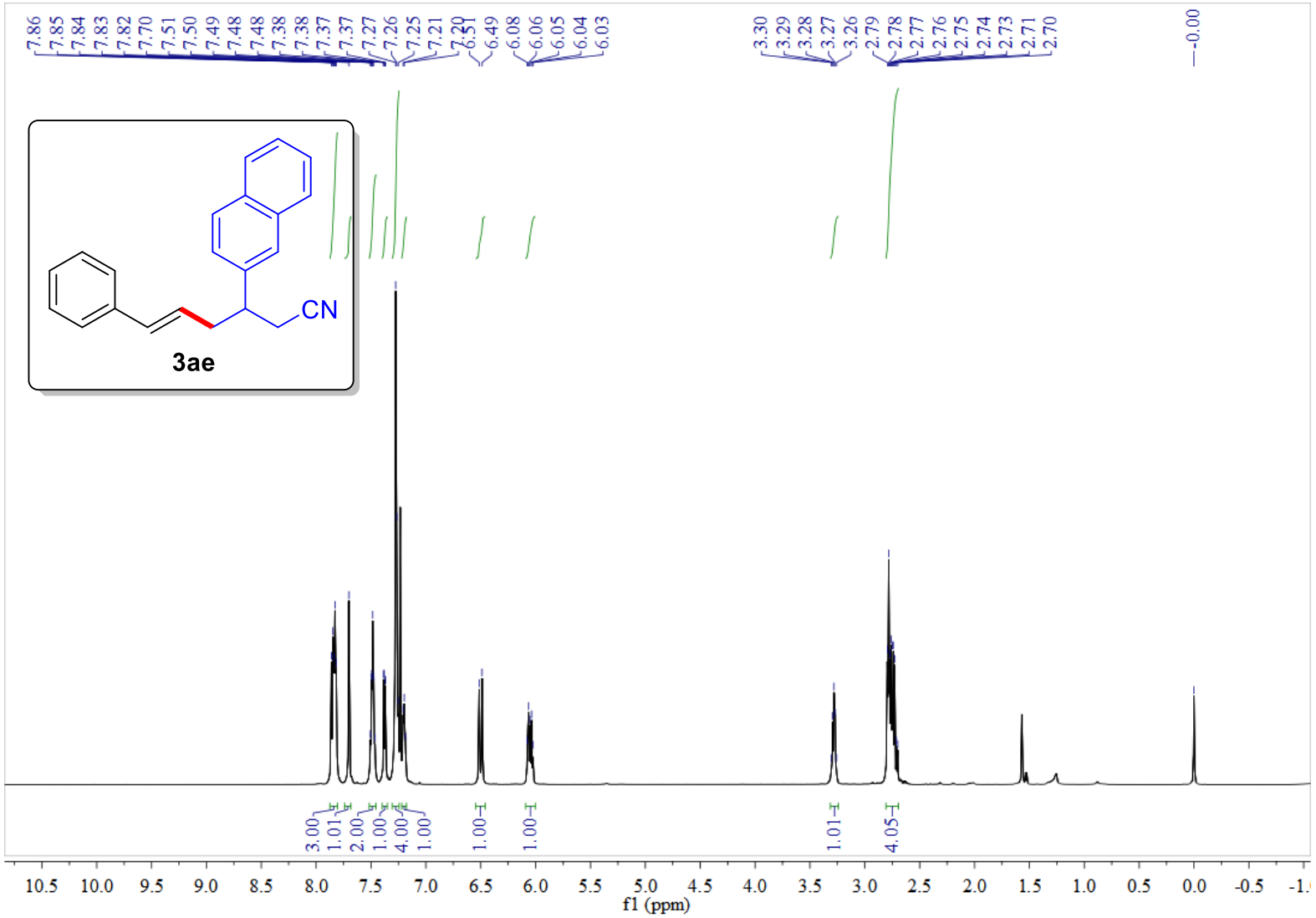

7.29
7.28
7.26
7.21
7.20
7.19
7.17
7.15
7.14
7.13
6.47
6.45
6.05
6.04
6.03
6.02
6.00
3.09
3.08
3.07
3.06
3.04
2.67
2.66
2.64
2.63
2.62
2.61
2.60
2.58
2.57
2.33
-0.00
Me
CN
3ac
4.03
1.25
3.99
1.00
1.00
1.01
4.13
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

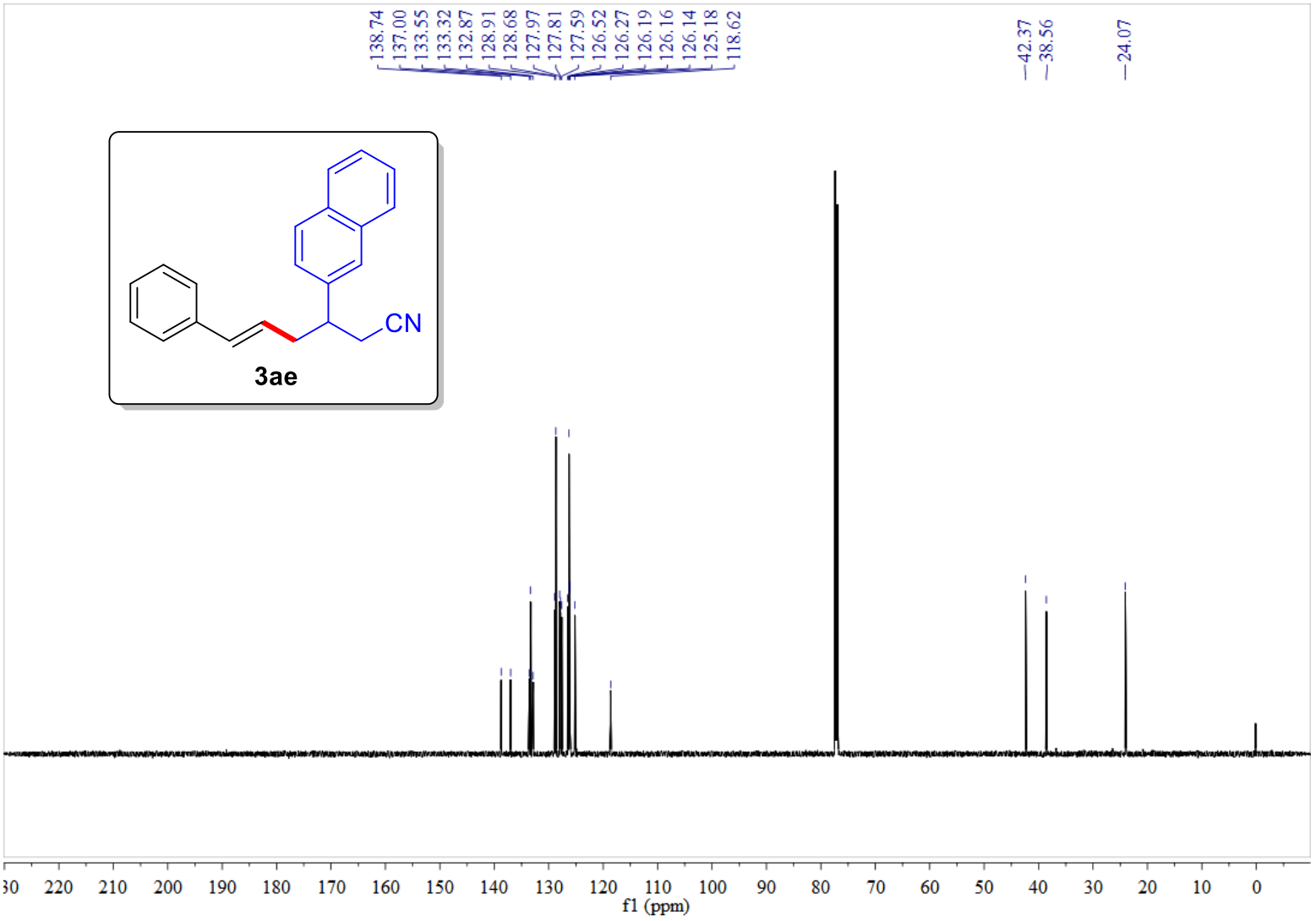

138.31
137.22
137.06
133.07
129.66
128.63
127.50
127.09
126.37
126.22
118.70
41.75
38.55
24.11
21.17
Me
CN
3ac
f1 (ppm)

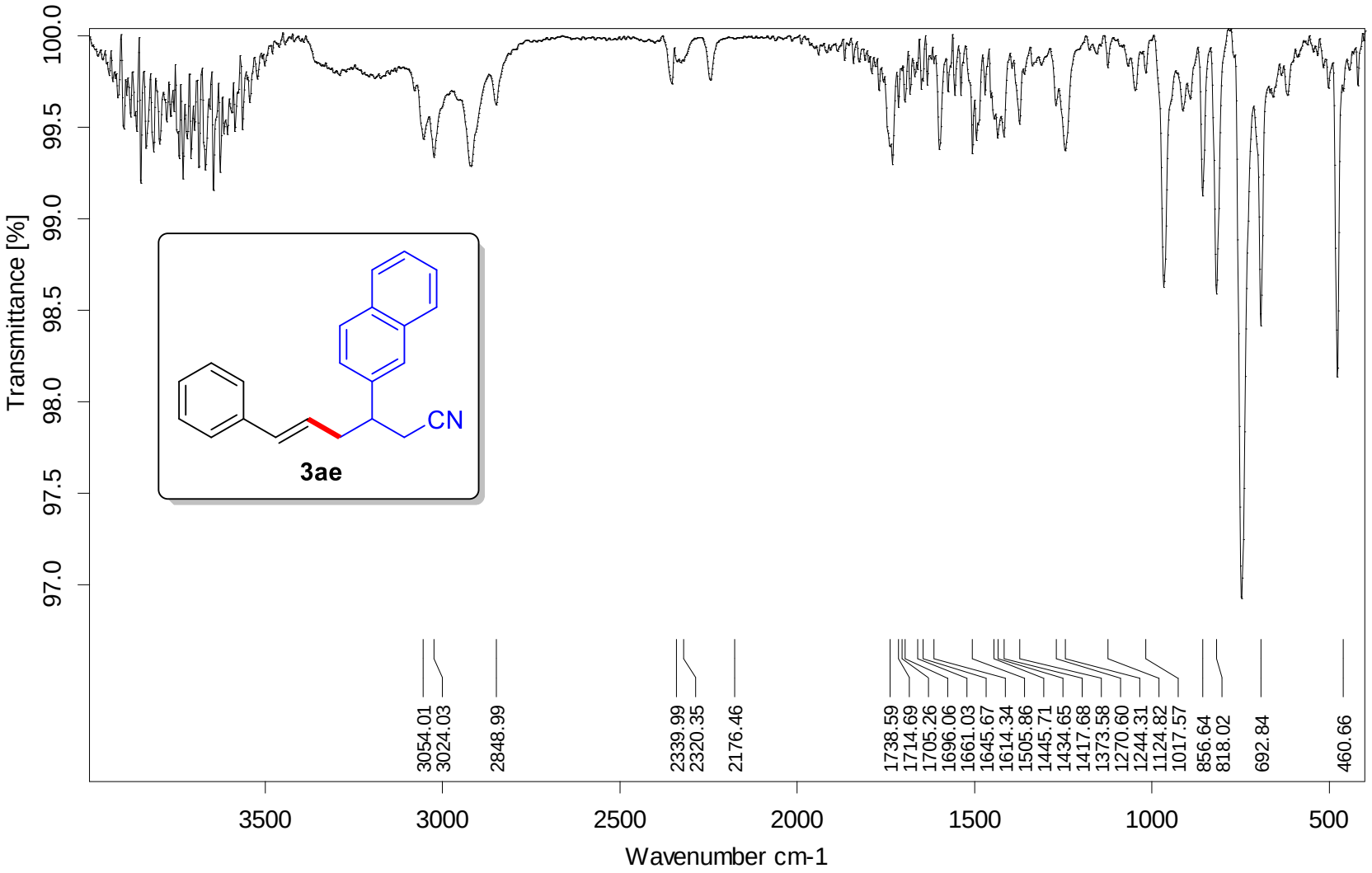

Transmittance [%]
100
99
98
97
96
95
Me
CN
3ac
3054.75
3025.05
2854.21
2350.68
2336.35
1714.60
1694.47
1667.55
1660.12
1594.97
1555.85
1494.48
1435.86
1423.05
1373.76
1359.74
1244.48
1116.01
1090.54
1045.81
916.12
814.06
693.52
535.24
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

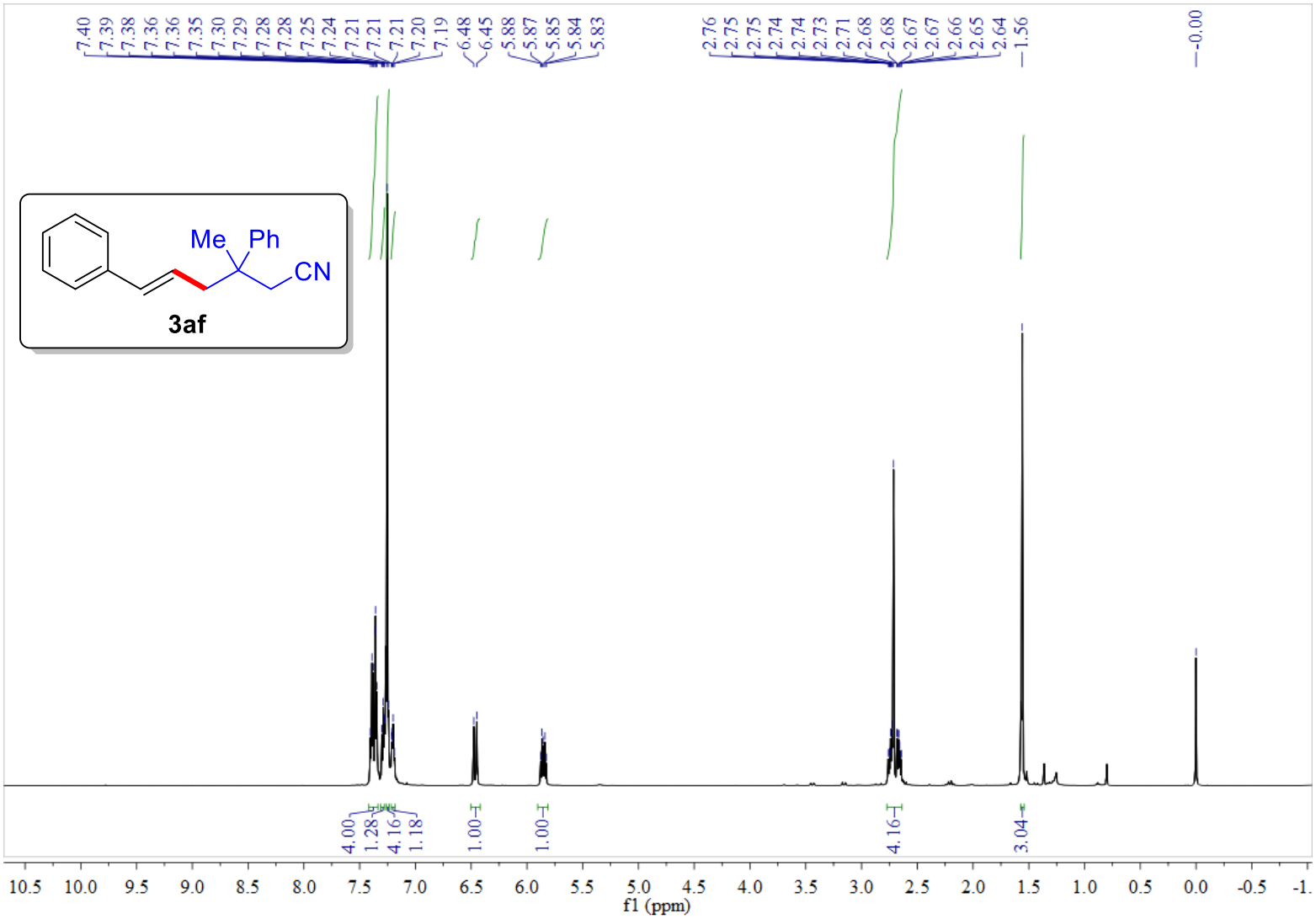

7.35
7.34
7.31
7.30
7.29
7.24
7.23
7.22
7.22
7.21
7.19
6.48
6.45
6.03
6.02
6.01
5.99
5.98
3.13
3.12
3.11
3.10
3.09
2.70
2.69
2.67
2.67
2.66
2.66
2.65
2.63
2.62
2.61
0.00
Cl
CN
3ad
2.02
4.05
3.02
1.00
1.01
1.02
4.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

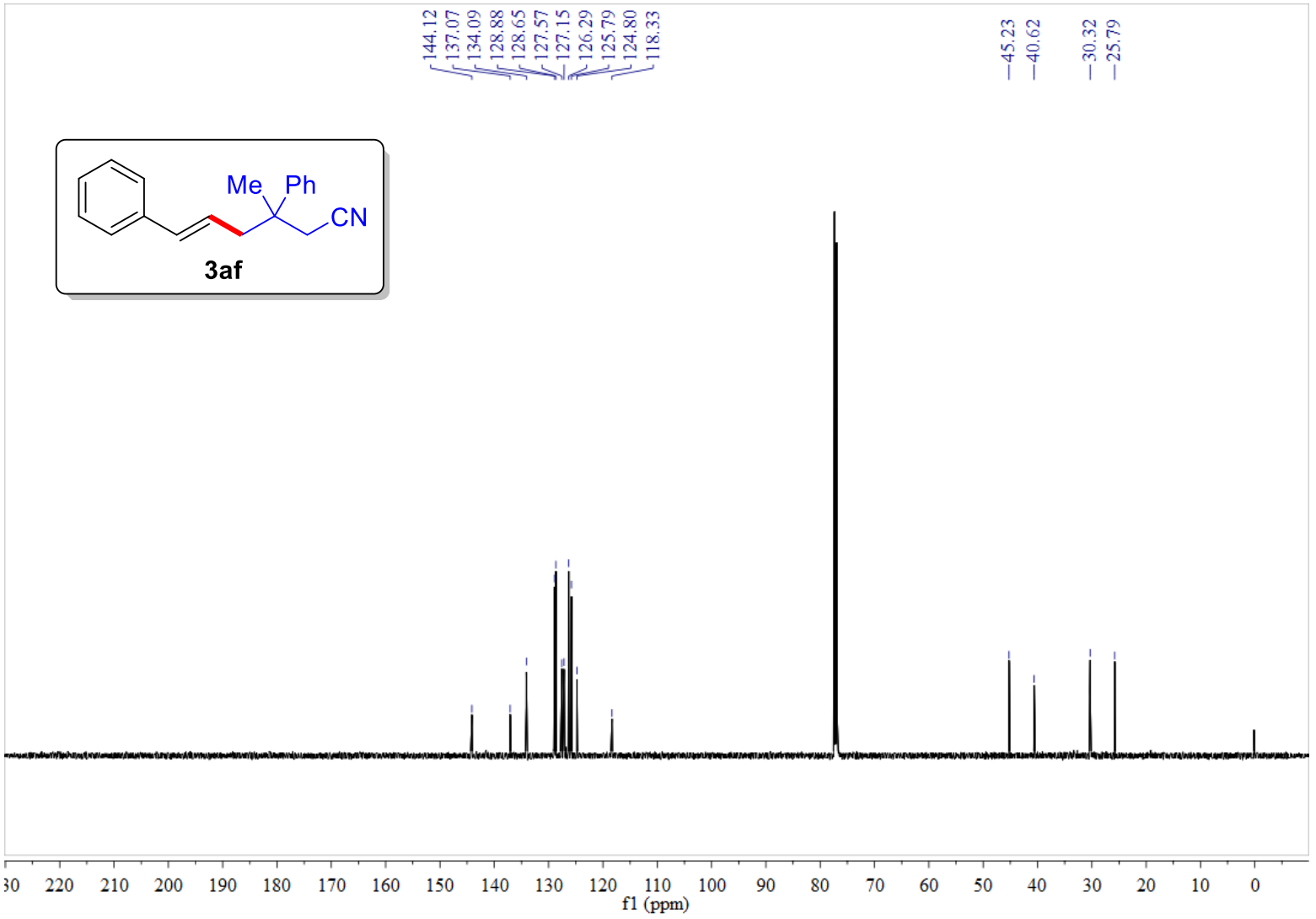

139.75
136.86
133.57
133.46
129.23
128.72
128.69
127.70
126.26
125.69
118.30
41.67
38.43
24.05
Cl
CN
3ad
f1 (ppm)

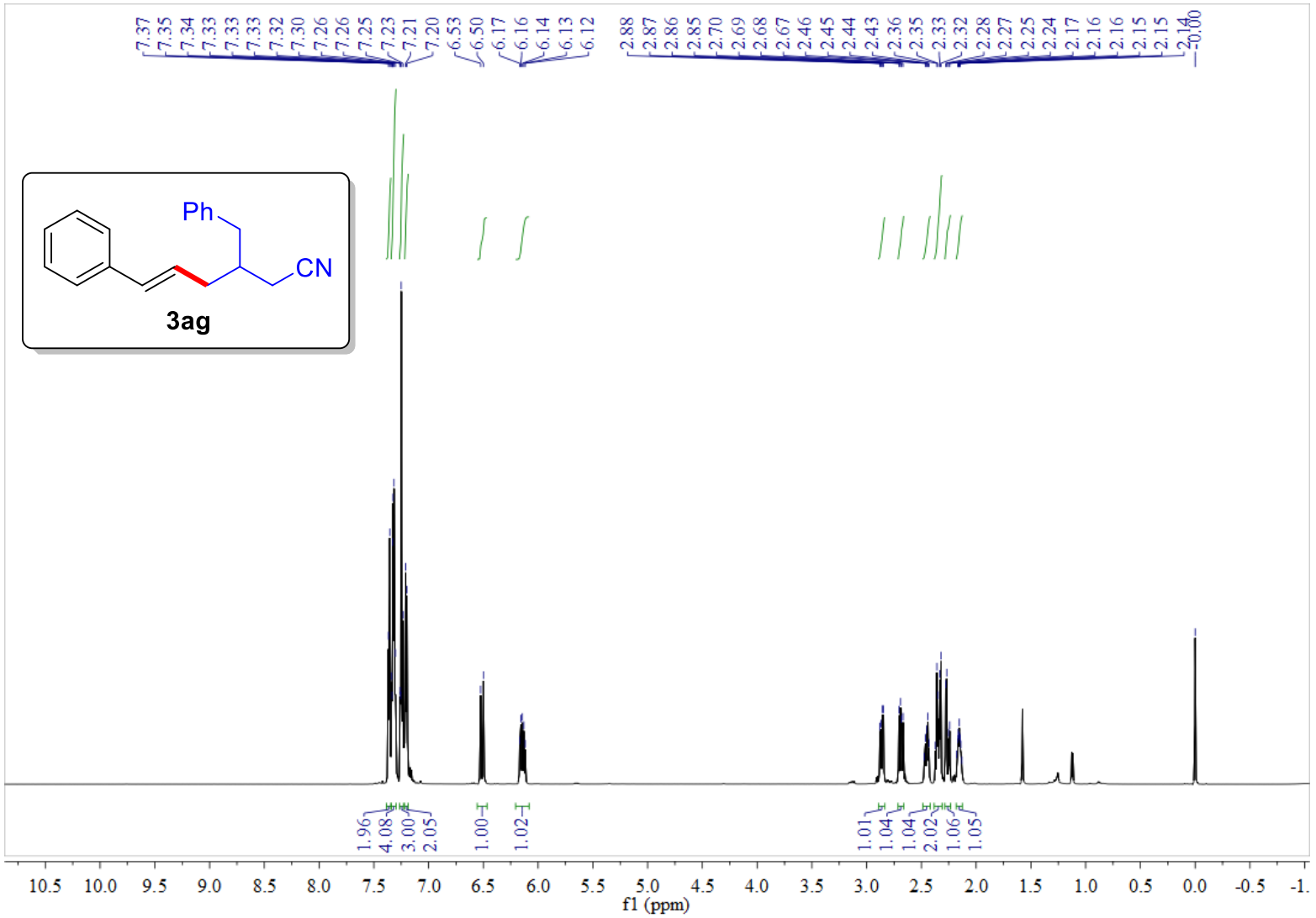

7.86
7.85
7.84
7.83
7.82
7.70
7.51
7.50
7.49
7.48
7.48
7.38
7.38
7.37
7.37
7.27
7.26
7.25
7.21
7.20
6.51
6.49
6.08
6.06
6.05
6.04
6.03
3.30
3.29
3.28
3.27
3.26
2.79
2.78
2.77
2.76
2.75
2.74
2.73
2.71
2.70
-0.00
CN
3ae
3.00
1.01
2.00
1.00
4.00
1.00
1.00
1.00
1.01
4.05
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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)

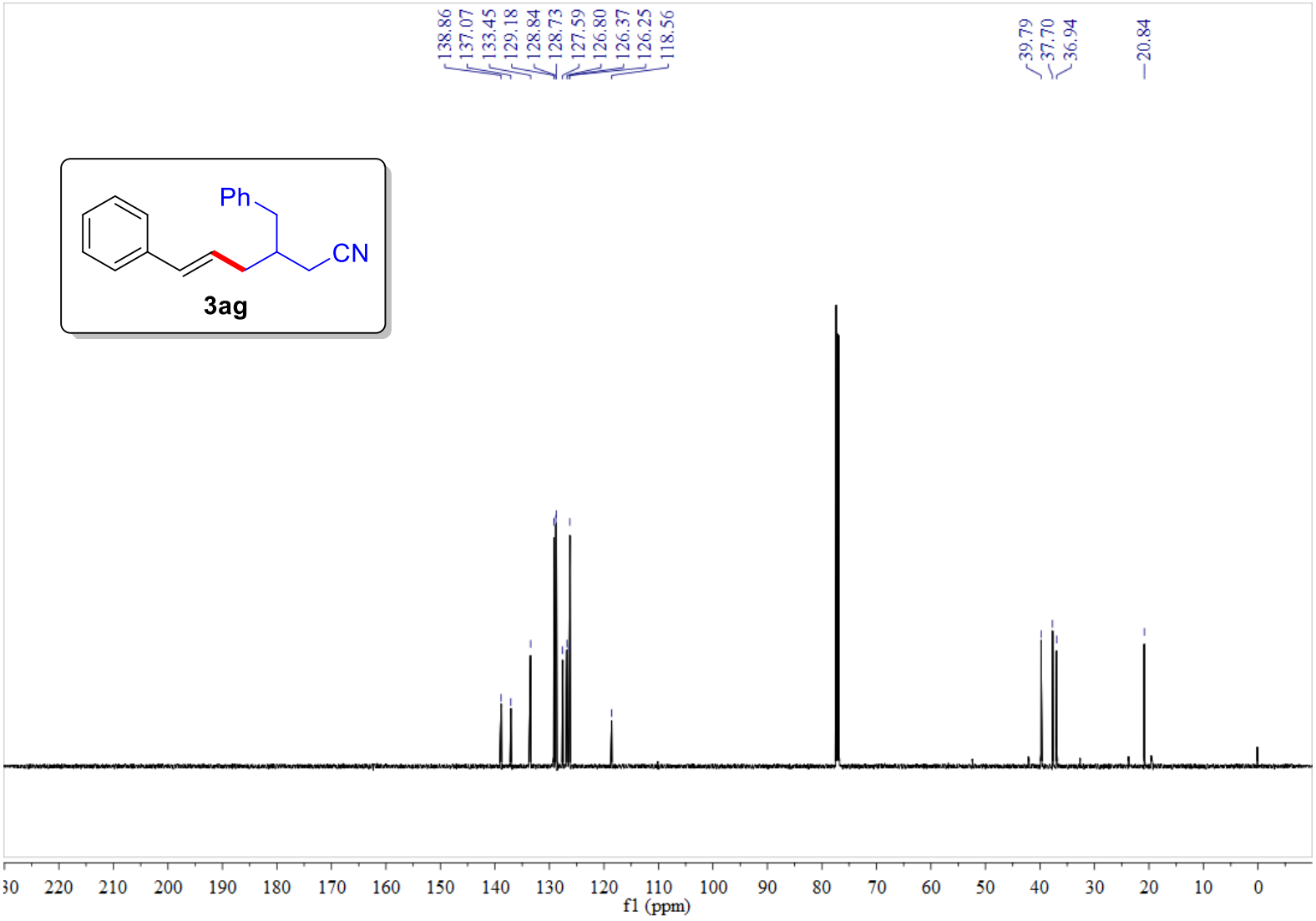

138.74
137.00
133.55
133.32
132.87
128.91
128.68
127.97
127.81
127.59
126.52
126.27
126.19
126.16
126.14
125.18
118.62
42.37
38.56
24.07
CN
3ae
f1 (ppm)

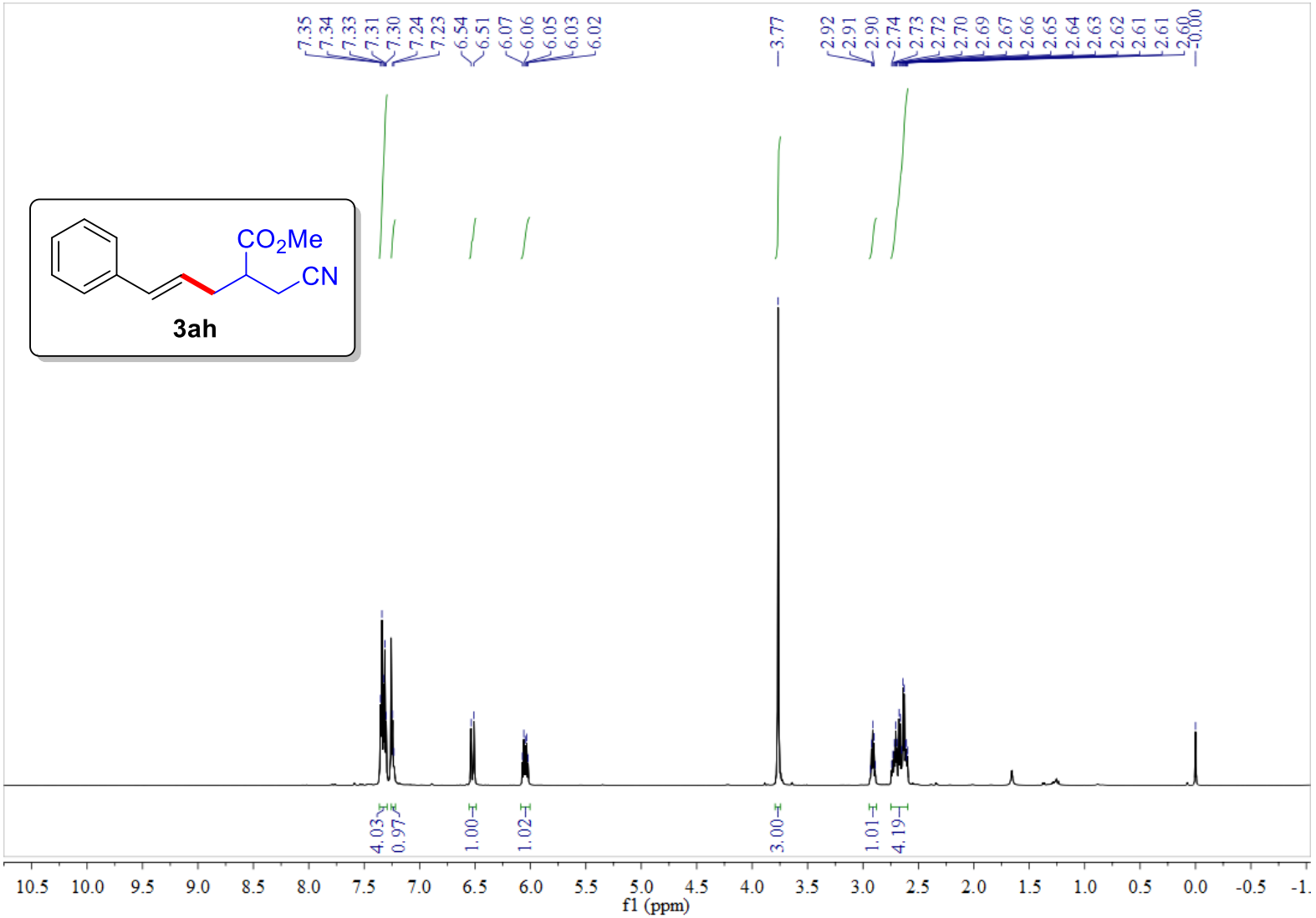

Transmittance [%]
100.0
99.5
99.0
98.5
98.0
97.5
97.0
CN
3ae
3054.01
3024.03
2848.99
2339.99
2320.35
2176.46
1738.59
1714.69
1705.26
1696.06
1661.03
1645.67
1614.34
1505.86
1445.71
1434.65
1417.68
1373.58
1270.60
1244.31
1124.82
1017.57
856.64
818.02
692.84
460.66
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

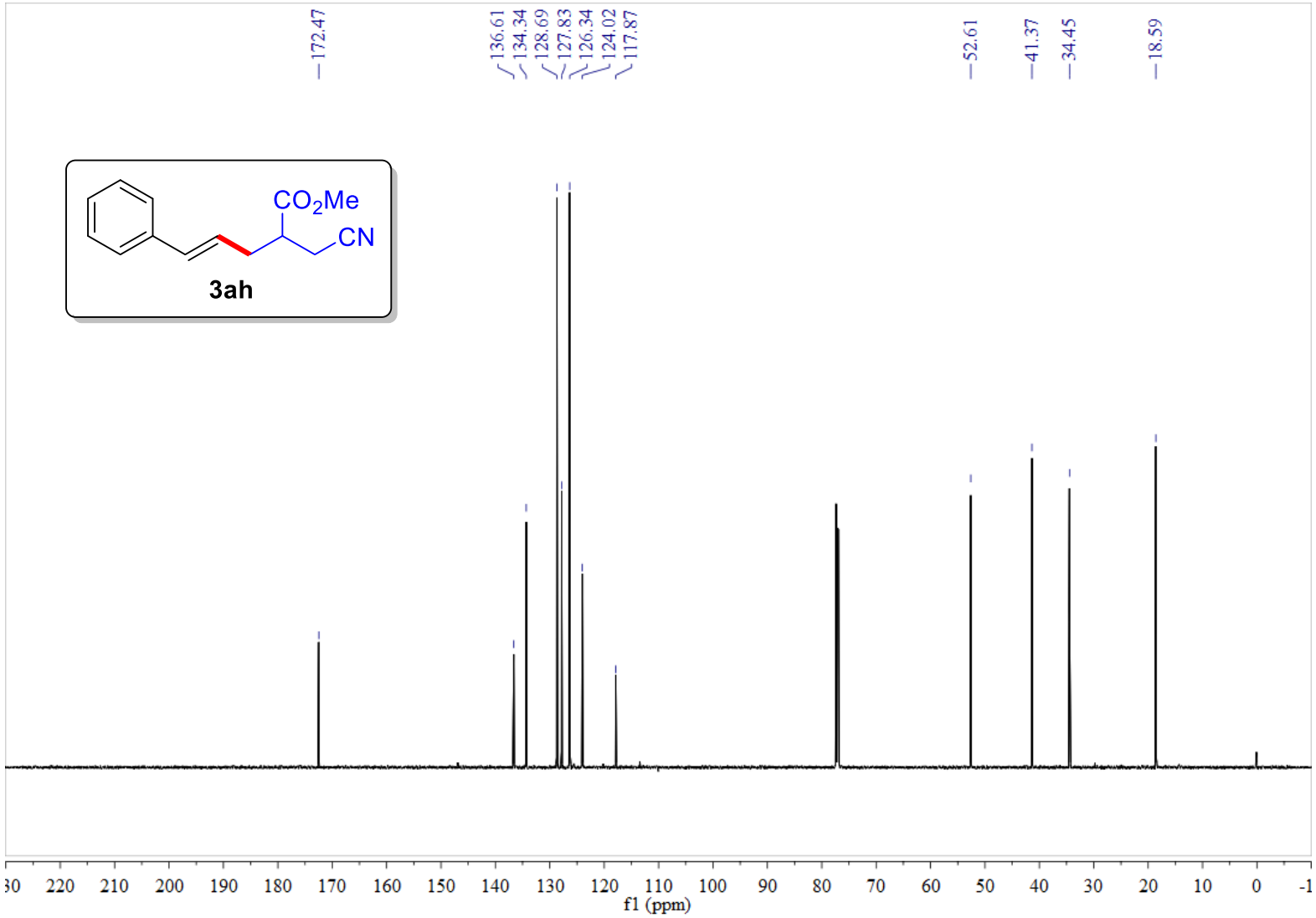

7.40
7.39
7.38
7.36
7.36
7.35
7.30
7.29
7.28
7.28
7.25
7.24
7.21
7.21
7.21
7.20
7.19
6.48
6.45
5.88
5.87
5.85
5.84
5.83
2.76
2.75
2.75
2.74
2.74
2.73
2.71
2.68
2.68
2.67
2.67
2.66
2.65
2.64
1.56
-0.00
Me
Ph
CN
3af
4.00
1.28
4.16
1.18
1.00
1.00
4.16
3.04
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

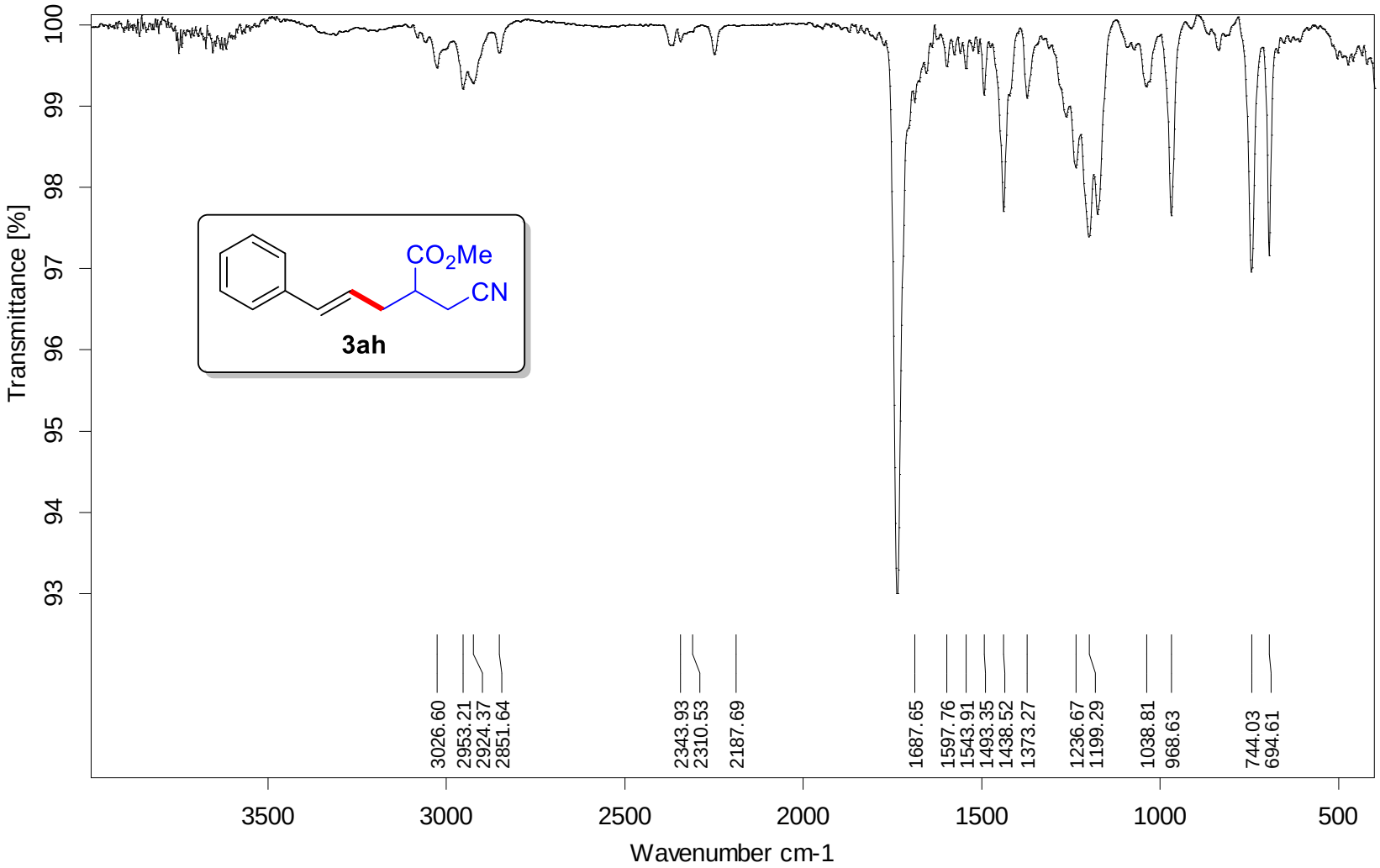

144.12
137.07
134.09
128.88
128.65
127.57
127.15
126.29
125.79
124.80
118.33
45.23
40.62
30.32
25.79
Me
Ph
CN
3af
f1 (ppm)

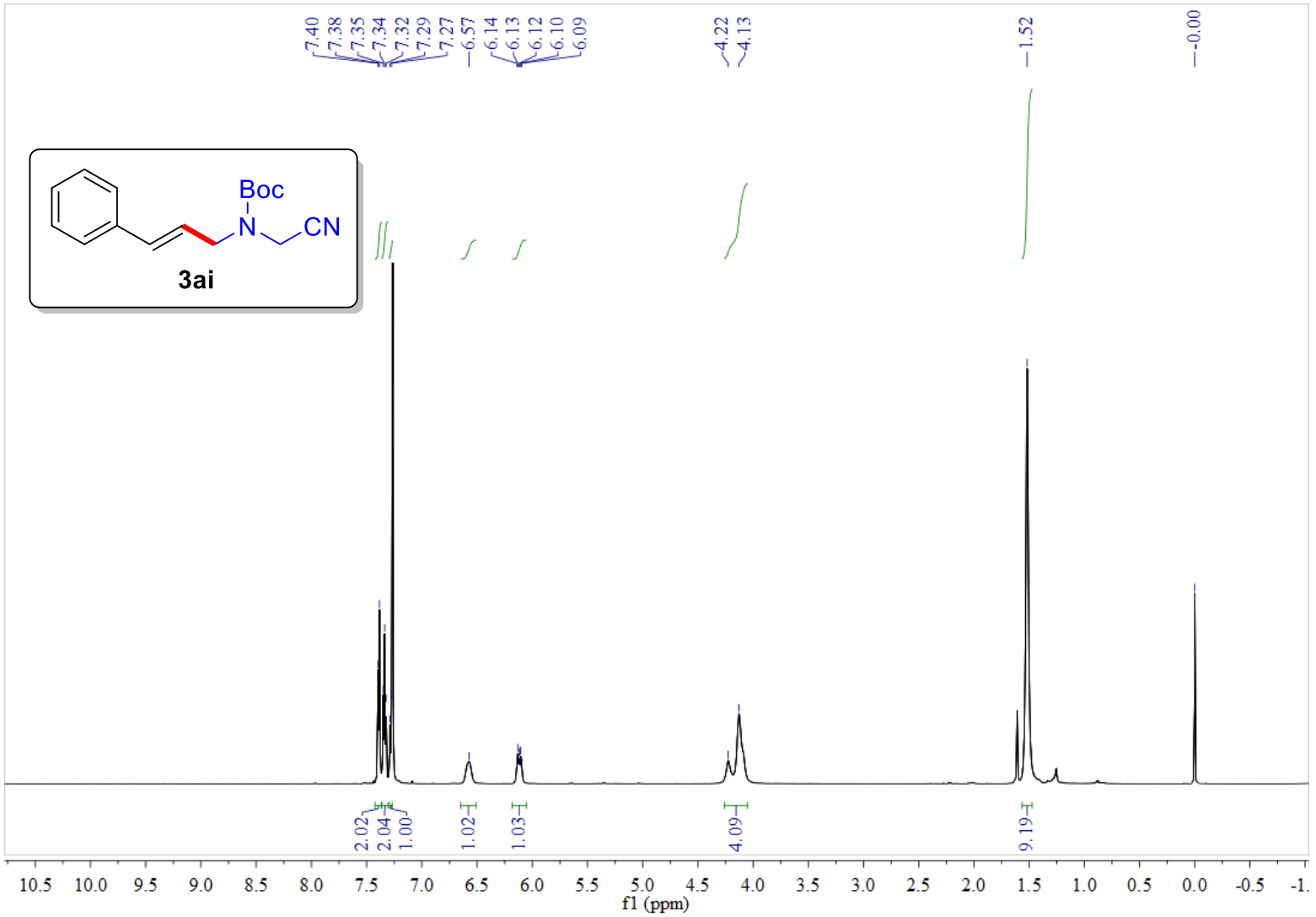

Ph
CN
3ag
f1 (ppm)

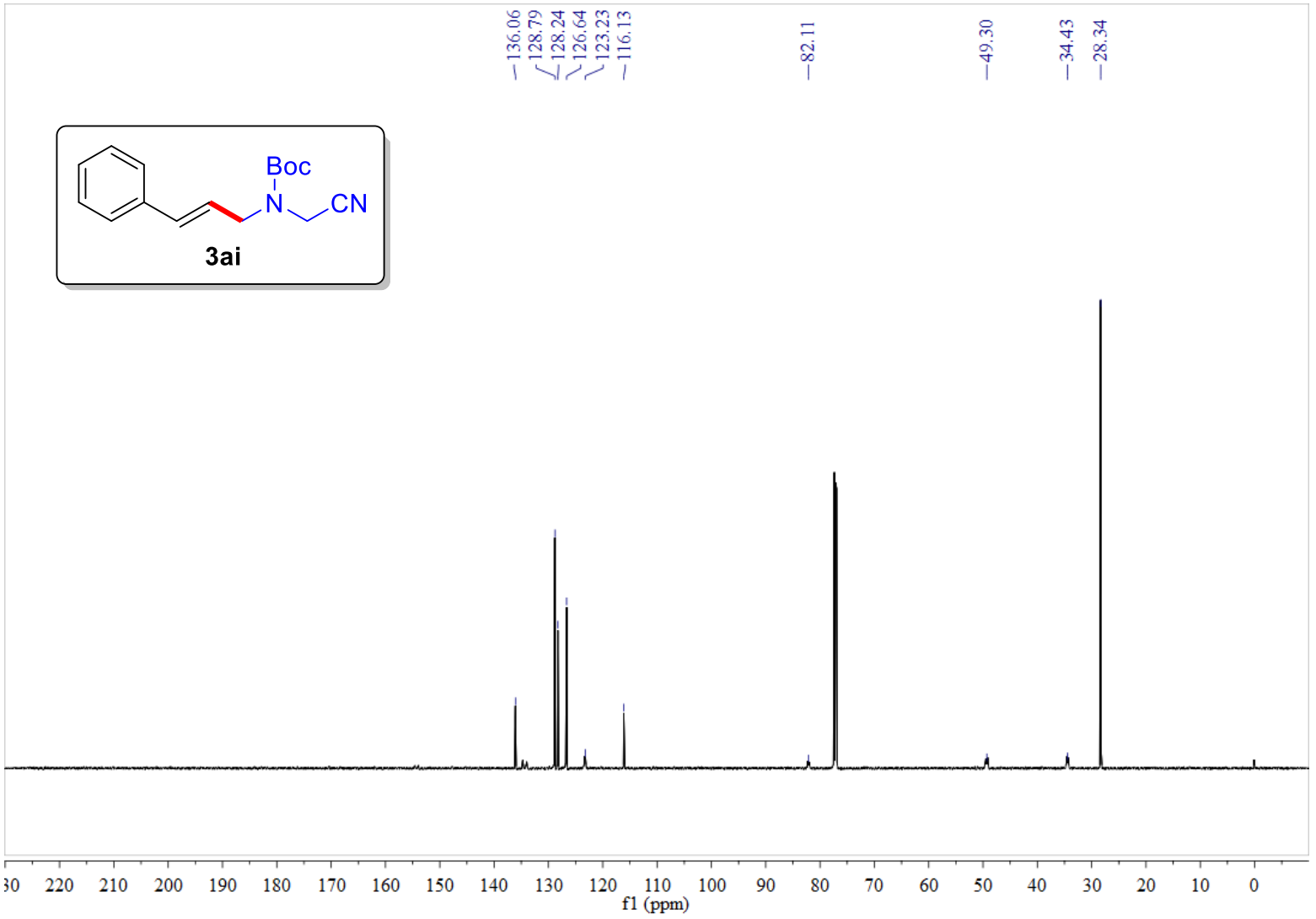

138.86
137.07
133.45
129.18
128.84
128.73
127.59
126.80
126.37
126.25
118.56
39.79
37.70
36.94
20.84
Ph
CN
3ag
f1 (ppm)

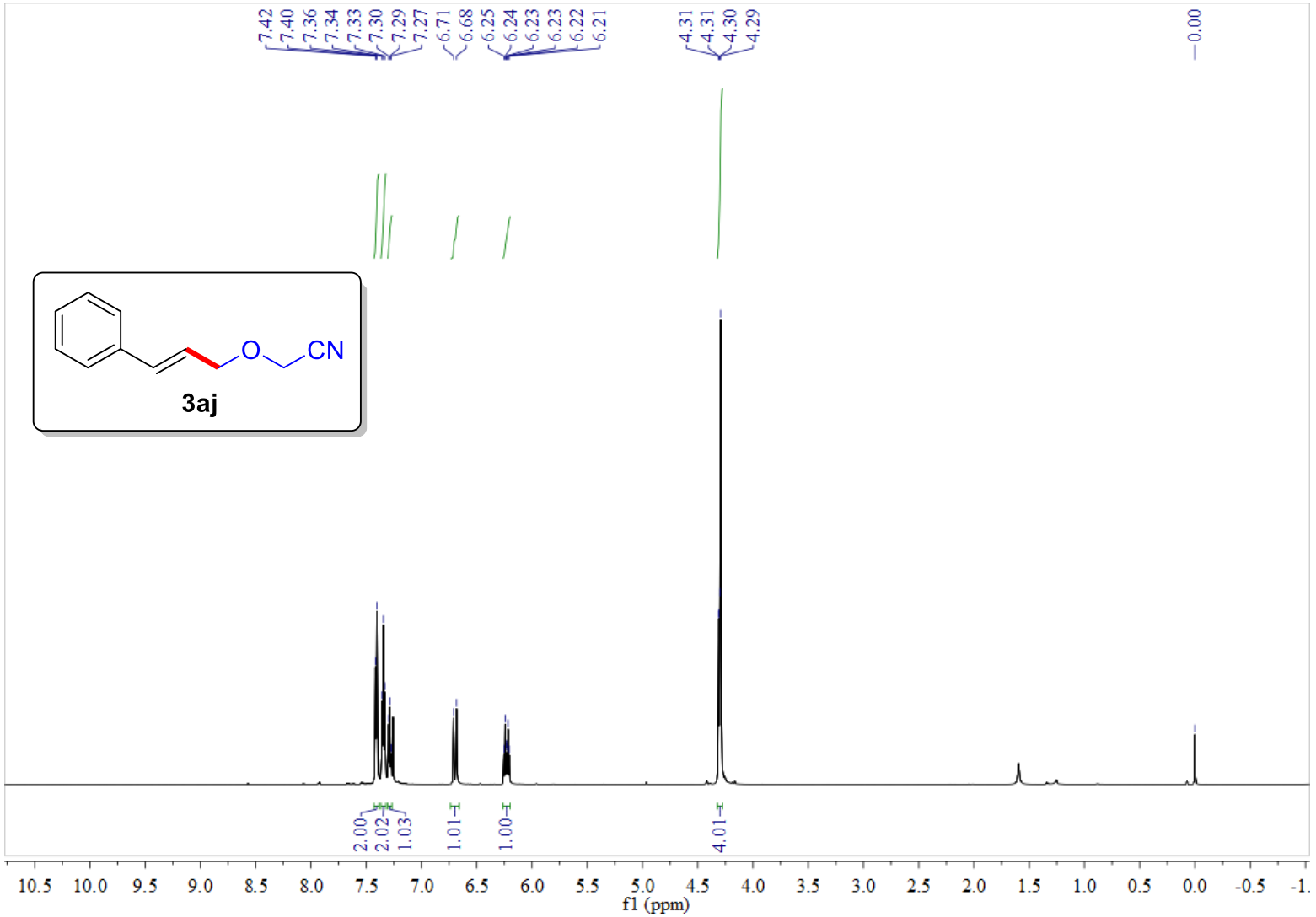

7.35
7.34
7.33
7.31
7.30
7.24
7.23
6.54
6.51
6.07
6.06
6.05
6.03
6.02
3.77
2.92
2.91
2.90
2.74
2.73
2.72
2.70
2.69
2.67
2.66
2.65
2.64
2.63
2.62
2.61
2.61
2.60
0.00
CO2Me
CN
3ah
4.03
0.97
1.00
1.02
3.00
1.01
4.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

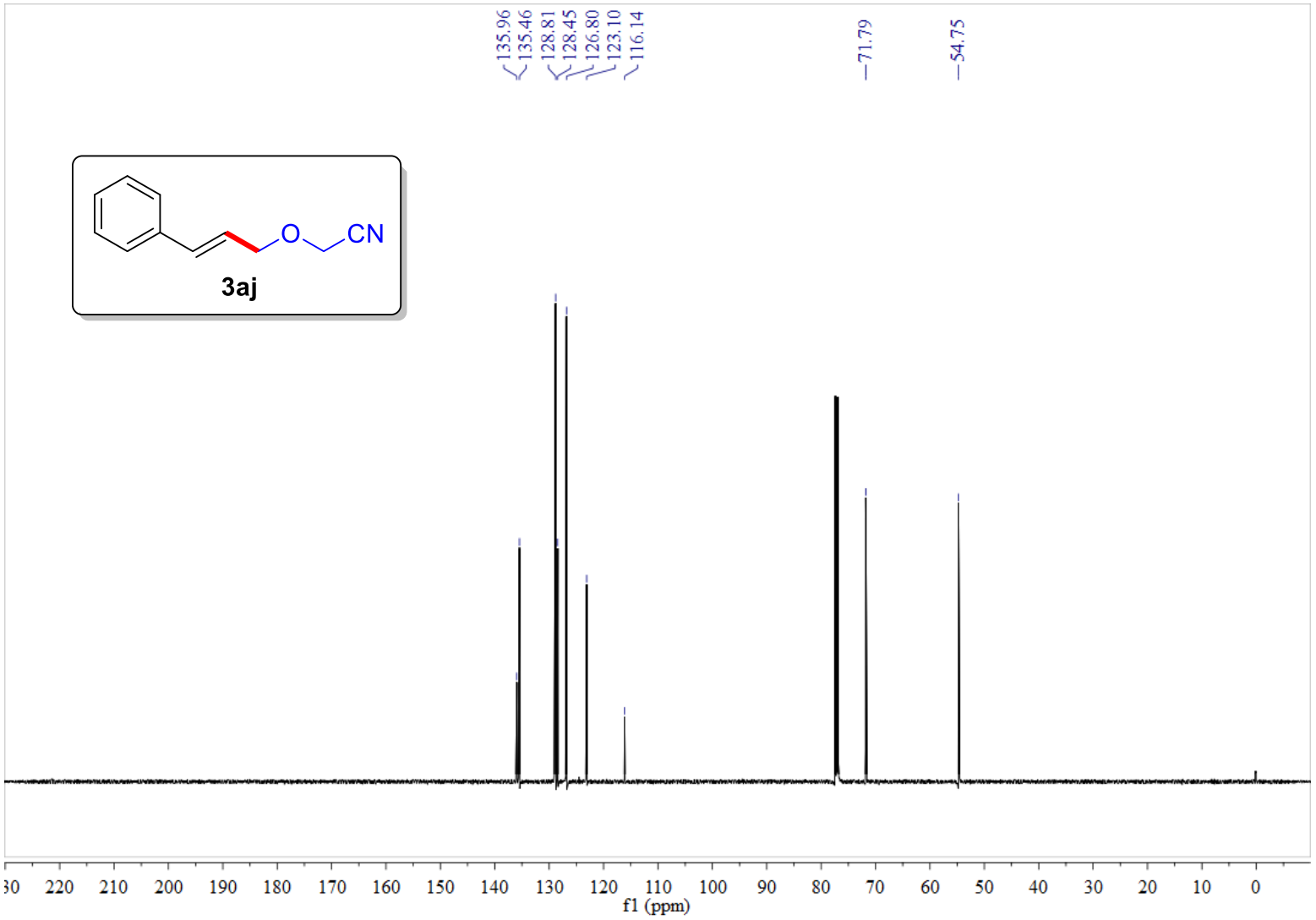

172.47
136.61
134.34
128.69
127.83
126.34
124.02
117.87
52.61
41.37
34.45
18.59
CO2Me
CN
3ah
f1 (ppm)

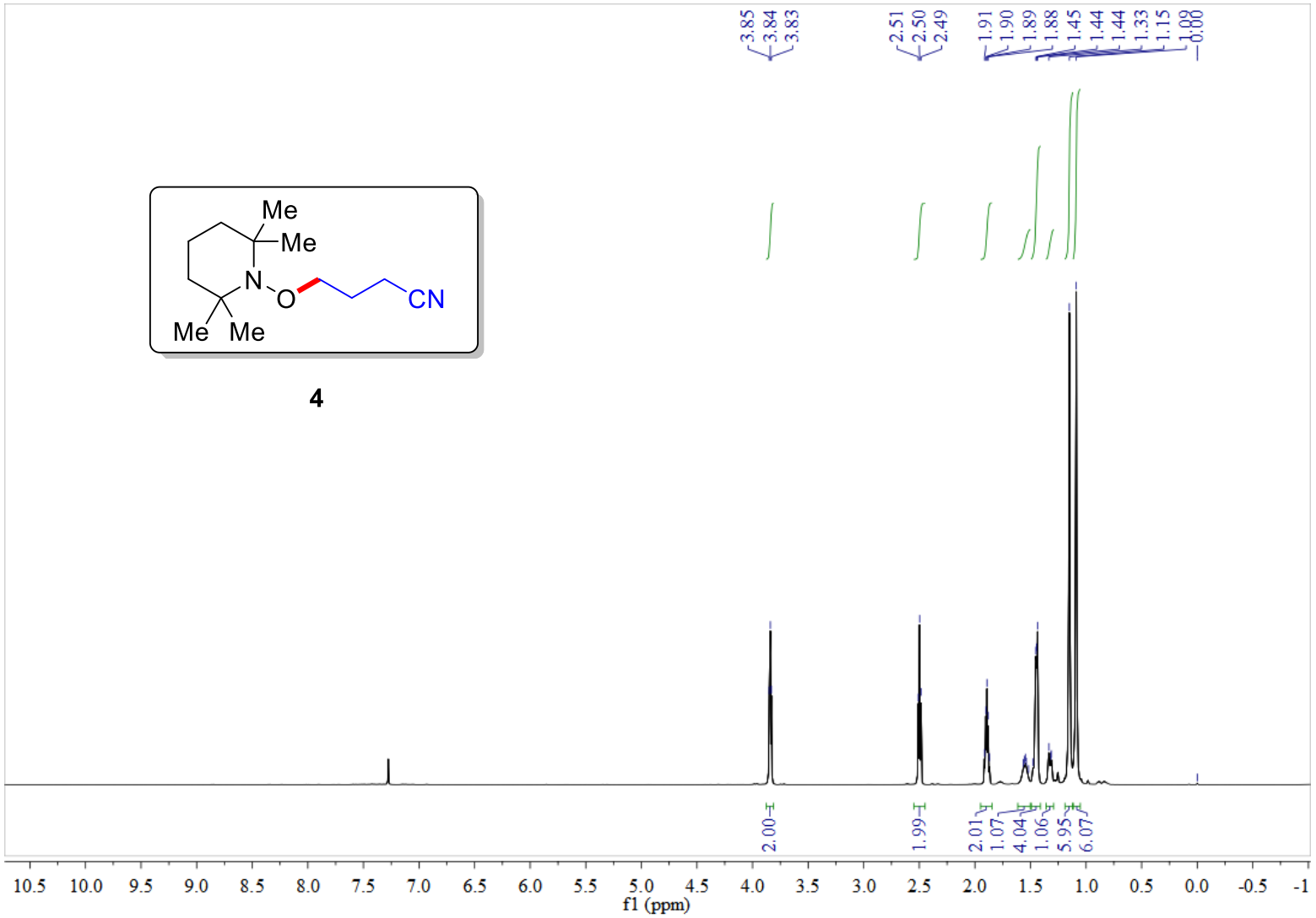

Transmittance [%]
100
99
98
97
96
95
94
93
CO2Me
CN
3ah
3026.60
2953.21
2924.37
2851.64
2343.93
2310.53
2187.69
1687.65
1597.76
1543.91
1493.35
1438.52
1373.27
1236.67
1199.29
1038.81
968.63
744.03
694.61
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


7.40
7.38
7.35
7.34
7.32
7.29
7.27
6.57
6.14
6.13
6.12
6.10
6.09
4.22
4.13
1.52
0.00
Boc
N
CN
3ai
2.02
2.04
1.00
1.02
1.03
4.09
9.19
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 -1.
f1 (ppm)

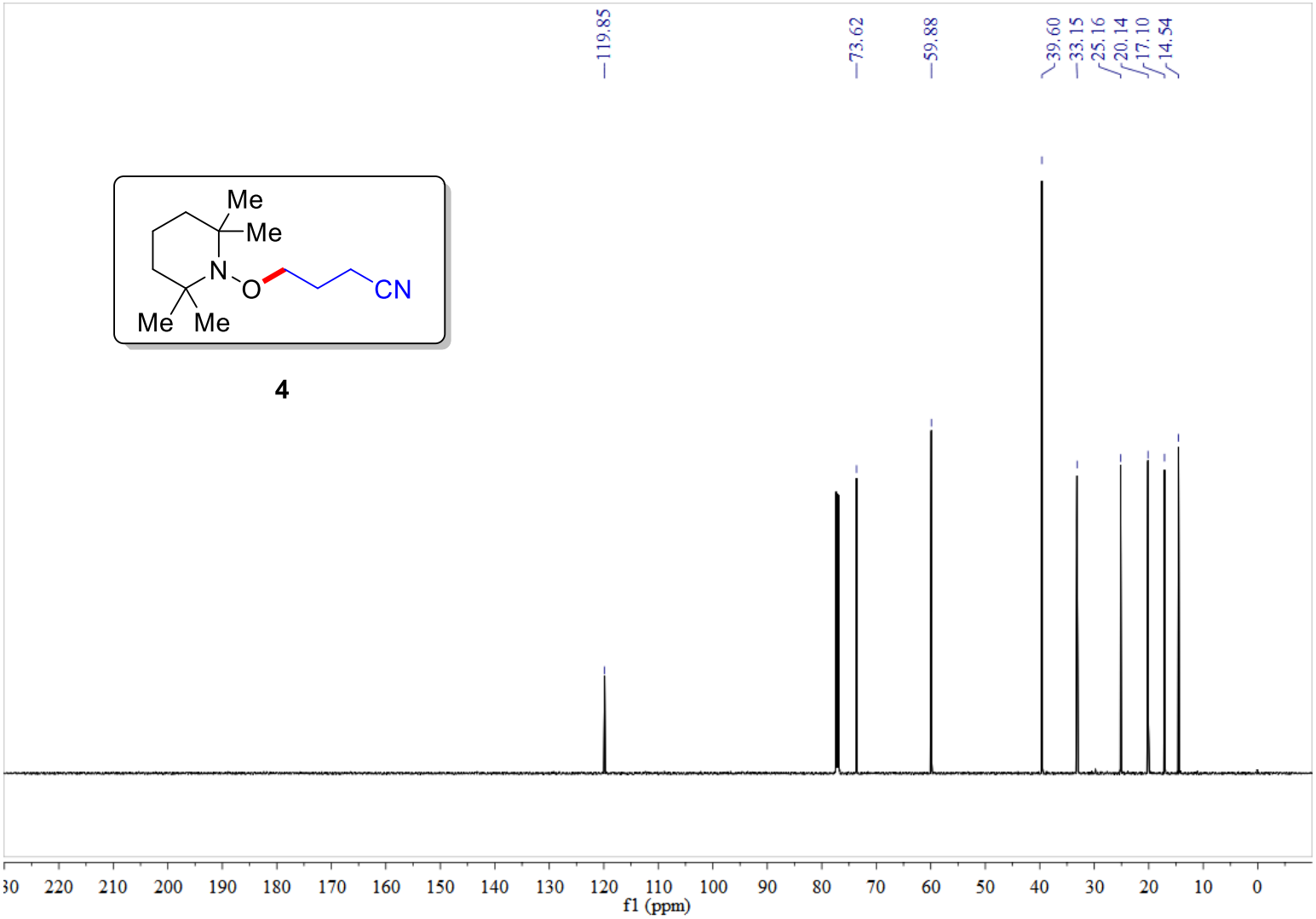

136.06
128.79
128.24
126.64
123.23
116.13
82.11
49.30
34.43
28.34
Boc
N
CN
3ai
f1 (ppm)


7.42
7.40
7.36
7.34
7.33
7.30
7.29
7.27
6.71
6.68
6.25
6.24
6.23
6.23
6.22
6.21
4.31
4.31
4.30
4.29
0.00
O
CN
3aj
2.00
2.02
1.03
1.01
1.00
4.01
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 -1.
f1 (ppm)


135.96
135.46
128.81
128.45
126.80
123.10
116.14
71.79
54.75
O
CN
3aj
f1 (ppm)


3.85
3.84
3.83
2.51
2.50
2.49
1.91
1.90
1.89
1.88
1.45
1.44
1.44
1.33
1.15
1.09
0.00
Me
Me
N
O
CN
Me
Me
2.00
1.99
2.01
1.07
4.04
1.06
5.95
6.07
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 -1
f1 (ppm)

4


119.85
73.62
59.88
39.60
33.15
25.16
20.14
17.10
14.54
Me
Me
N
O
CN
Me
Me
4
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)