Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

for

Palladium-catalyzed aerobic oxidative cross-coupling of arylhydrazines with terminal alkynes

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CONTENTS

1. General experimental details and materials

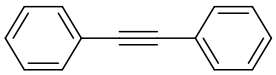
NMR spectra were recorded on BRUKER Avence III 500MHz spectrometers. Chemical shifts were reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. Coupling constants (*J*) were reported in Hz and referred to apparent peak multiplications.

All the reagents used were purchased from Alfa Aesar or J&K. The solvents were used directly without further purification. For liber some commercially obtained arylhydrazines from their hydrochloride salt forms, 10% NaOH aqueous solution was added with stirring for 10 min, then ethyl acetate was used to for extractions. The organic phase was dried by anhydrous $NaSO_4$ and concentrated under vacuum to afford pure arylhydrazines.

In a typical Sonogashira coupling reaction, arylhydrazine **1** (1.75 mmol), terminal alkyne **2** (0.5 mmol), $PdCl_2$ (0.025 mmol, 4.4 mg), PPh_3 (0.15 mmol, 39.3 mg), AcOH (1.5 mmol, 90 mg) and 1.5 mL of DMF were added to a 25 mL Schlenk tube under 1 atm of O_2 atmosphere. Then it was sealed and the resulting mixture was stirred at 50 °C for 12 h. After cooling to room temperature, water was added and the mixture was extracted with ethyl acetate for three times. The organic phases were combined, dried by anhydrous $NaSO_4$ and concentrated under vacuum. The residue was then purified by chromatography on silica gel with petroleum ether to give the corresponding product.

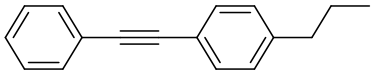
2. Synthesis of internal alkynes and the characterization data

1,2-Diphenylethyne (3aa) (CAS Registry Number 501-65-5)



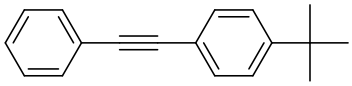
This product was obtained from the reaction of phenylhydrazine (**1a**) and phenylacetylene (**2a**) as a white solid (68 mg, 74% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.25-7.37 (m, 6H), 7.53-7.55 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 89.4, 123.3, 128.3, 128.4, 131.6.

1-(Phenylethynyl)-4-propylbenzene (3ab) (CAS Registry Number 1011301-57-7)



This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-ethynyl-4-propylbenzene (**2b**) as a white solid (87 mg, 79% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 0.94 (t, *J* = 7.0 Hz, 3H), 1.61-1.68 (m, 2H), 2.59 (t, *J* = 7.5 Hz, 2H), 7.15 (d, *J* = 5.0 Hz, 2H), 7.31-7.35 (m, 3H), 7.45 (d, *J* = 5.0 Hz, 2H), 7.51-7.53 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 13.8, 24.4, 38.0, 88.8, 89.6, 120.4, 123.5, 128.1, 128.3, 128.5, 131.5, 131.6, 143.2.

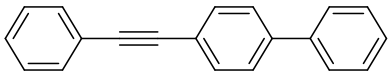
1-(*tert*-Butyl)-4-(phenylethynyl)benzene (3ac) (CAS Registry Number 29778-26-5)



This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-(*tert*-butyl)-4-ethynylbenzene (**2c**) as a white solid (90 mg, 77% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 1.33 (s,

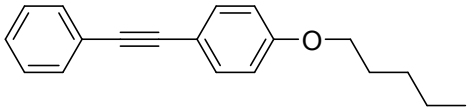
9H), 7.33-7.38 (m, 5H), 7.46-7.48 (m, 2H), 7.52-7.53 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 31.2, 34.8, 88.7, 89.5, 120.2, 123.5, 125.4, 128.1, 128.3, 131.3, 131.6, 151.5.

4-(Phenylethynyl)-1,1'-biphenyl (3ad) (CAS Registry Number 15784-39-1)



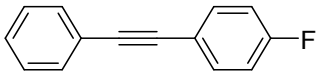
This product was obtained from the reaction of phenylhydrazine (**1a**) and 4-ethynyl-1,1'-biphenyl (**2d**) as a white solid (60 mg, 47% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.33-7.38 (m, 4H), 7.44-7.47 (m, 2H), 7.54-7.62 (m, 8H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 89.3, 90.1, 122.2, 123.3, 127.0, 127.6, 128.3, 128.4, 128.9, 131.6, 132.0, 140.3, 141.0.

1-(Pentyloxy)-4-(phenylethynyl)benzene (3ae) (CAS Registry Number 1380401-12-6)



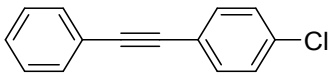
This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-ethynyl-4-(pentyloxy)benzene (**2e**) as a white solid (68 mg, 52% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 0.83-0.89 (m, 2H), 0.93 (t, J = 7.0 Hz, 3H), 1.26-1.29 (m, 3H), 1.35-1.45 (m, 4H), 1.77-1.82 (m, 2H), 3.97 (t, J = 6.5 Hz, 2H), 6.85-6.88 (m, 2H), 7.28-7.35 (m, 3H), 7.44-7.46 (m, 2H), 7.50-7.52 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 14.0, 22.5, 28.2, 28.9, 68.1, 88.0, 89.5, 114.5, 115.1, 123.7, 127.9, 128.3, 131.4, 133.0, 159.2.

1-Fluoro-4-(phenylethynyl)benzene (3af) (CAS Registry Number 405-29-8)



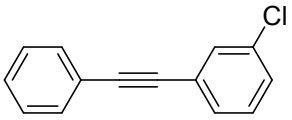
This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-ethynyl-4-fluorobenzene (**2f**) as a white solid (66 mg, 67% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.02-7.06 (m, 2H), 7.34-7.36 (m, 3H), 7.49-7.53 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 88.3, 89.1, 115.5 (J_{CF} = 17.5 Hz), 119.4, 123.1, 128.3, 128.4, 131.6, 133.5 (J_{CF} = 6.6 Hz), 163.5 (J_{CF} = 198.4 Hz); ^{19}F NMR (470 MHz, $CDCl_3$) δ = -111.0.

1-Chloro-4-(phenylethynyl)benzene (3ag) (CAS Registry Number 5172-02-1)



This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-chloro-4-ethynylbenzene (**2g**) as a white solid (81 mg, 76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.32-7.37 (m, 5H), 7.45-7.54 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 88.2, 90.3, 121.8, 122.9, 128.4, 128.5, 128.7, 131.6, 132.8, 134.3.

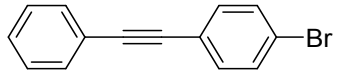
1-Chloro-3-(phenylethynyl)benzene (3ah) (CAS Registry Number 51624-34-1)



This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-chloro-3-

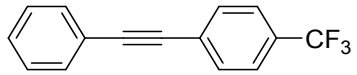
ethynylbenzene (**2h**) as a white solid (54 mg, 51% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.24-7.31 (m, 2H), 7.34-7.36 (m, 3H), 7.39-7.41 (m, 1H), 7.51-7.53 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 87.9, 90.6, 122.8, 125.0, 128.4, 128.5, 128.6, 129.6, 129.7, 131.5, 131.7, 134.2.

1-Bromo-4-(phenylethynyl)benzene (3ai) (CAS Registry Number 13667-12-4)



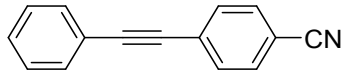
This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-bromo-4-ethynylbenzene (**2i**) as a white solid (80 mg, 62% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.33-7.40 (m, 5H), 7.47-7.53 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 88.3, 90.5, 122.2, 122.5, 122.9, 128.4, 128.5, 131.6, 131.6, 133.0.

1-(Phenylethynyl)-4-(trifluoromethyl)benzene (3aj) (CAS Registry Number 370-99-0)



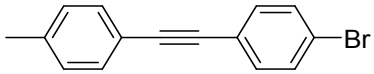
This product was obtained from the reaction of phenylhydrazine (**1a**) and 1-ethynyl-4-(trifluoromethyl)benzene (**2j**) as a white solid (85 mg, 69% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.37-7.38 (m, 3H), 7.54-7.56 (m, 2H), 7.59-7.64 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 88.0, 91.8, 122.6, 122.9, 125.0, 125.3 (q, J = 14.1 Hz), 127.1, 128.5, 128.8, 129.8 (t, J = 122.2 Hz), 131.8 (d, J = 27.7 Hz); ^{19}F NMR (470 MHz, $CDCl_3$) δ = -62.8.

4-(Phenylethynyl)benzonitrile (3ak) (CAS Registry Number 29822-79-5)



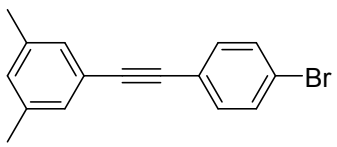
This product was obtained from the reaction of phenylhydrazine (**1a**) and 4-ethynylbenzonitrile (**2k**) as a white solid (64 mg, 63% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.35-7.36 (m, 3H), 7.51-7.52 (m, 2H), 7.56-7.61 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 87.7, 93.8, 111.5, 118.6, 122.2, 128.3, 128.5, 129.1, 131.8, 132.1, 132.1.

1-Bromo-4-(p-tolylethynyl)benzene (3bi) (CAS Registry Number 62856-42-2)



This product was obtained from the reaction of *p*-tolylhydrazine (**1b**) and 1-bromo-4-ethynylbenzene (**2i**) as a white solid (96 mg, 71% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 2.36 (s, 3H), 7.14-7.16 (m, 2H), 7.35-7.37 (m, 2H), 7.38-7.40 (m, 2H), 7.45-7.48 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 21.6, 87.7, 90.7, 119.8, 122.2, 122.5, 129.2, 131.5, 131.6, 133.0, 138.7.

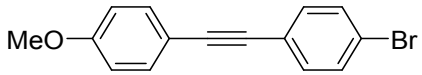
1-((4-Bromophenyl)ethynyl)-3,5-dimethylbenzene (3ci)



This product was obtained from the reaction of (3,5-dimethylphenyl)hydrazine (**1c**) and 1-bromo-4-ethynylbenzene (**2i**) as a white solid (75 mg, 53% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.98

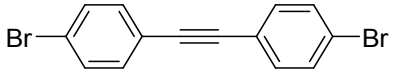
(s, 1H), 7.16 (s, 2H), 7.36-7.38 (m, 2H), 7.45-7.47 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 21.1, 87.6, 90.9, 122.3, 122.4, 122.5, 129.3, 130.5, 131.6, 133.0, 138.0. GC-MS (M^+) (*m/z* = 284, 286).

1-Bromo-4-((4-methoxyphenyl)ethynyl)benzene (3di) (CAS Registry Number 189099-57-8)



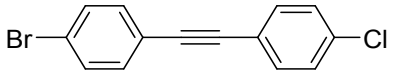
This product was obtained from the reaction of (4-methoxyphenyl)hydrazine (**1d**) and 1-bromo-4-ethynylbenzene (**2i**) as a white solid (71 mg, 50% yield).^{1}H NMR (500 MHz, $CDCl_3$) δ = 3.83 (s, 3H), 6.86-6.89 (m, 2H), 7.35-7.37 (m, 2H), 7.44-7.48 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 55.3, 87.1, 90.6, 114.1, 115.0, 122.1, 122.6, 131.6, 132.9, 133.1, 159.8.

1,2-Bis(4-bromophenyl)ethyne (3ei) (CAS Registry Number 2789-89-1)



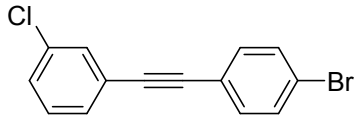
This product was obtained from the reaction of (4-bromophenyl)hydrazine (**1e**) and 1-bromo-4-ethynylbenzene (**2i**) as a white solid (105 mg, 63% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.37-7.38 (m, 4H), 7.48-7.49 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 89.4, 121.9, 122.8, 131.7, 133.0.

1-Bromo-4-((4-chlorophenyl)ethynyl)benzene (3eg) (CAS Registry Number 832744-28-2)



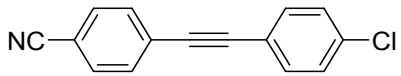
This product was obtained from the reaction of (4-bromophenyl)hydrazine (**1e**) and 1-chloro-4-ethynylbenzene (**2g**) as a white solid (97 mg, 67% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.31-7.39 (m, 2H), 7.36-7.39 (m, 2H), 7.43-7.46 (m, 2H), 7.47-7.50 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 89.2, 89.4, 100.0, 121.4, 121.9, 122.7, 128.8, 131.7, 132.8, 133.0, 134.6.

1-((4-Bromophenyl)ethynyl)-3-chlorobenzene (3fi) (CAS Registry Number 832744-27-1)



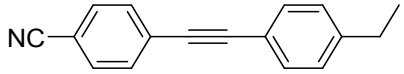
This product was obtained from the reaction of (3-chlorophenyl)hydrazine (**1f**) and 1-bromo-4-ethynylbenzene (**2i**) as a white solid (109 mg, 75% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.26-7.34 (m, 2H), 7.37-7.40 (m, 3H), 7.48-7.52 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 89.0, 89.4, 121.7, 122.9, 124.6, 128.8, 129.6, 129.7, 131.4, 131.7, 133.1, 134.3.

4-((4-Chlorophenyl)ethynyl)benzonitrile (3gg) (CAS Registry Number 54273-35-7)



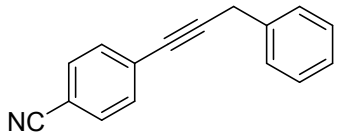
This product was obtained from the reaction of 4-hydrazinylbenzonitrile (**1g**) and 1-chloro-4-ethynylbenzene (**2g**) as a white solid (69 mg, 58% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.34-7.37 (m, 2H), 7.46-7.49 (m, 2H), 7.59-7.61 (m, 2H), 7.64-7.65 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 88.6, 92.6, 111.7, 118.4, 120.7, 127.9, 128.9, 132.1, 132.1, 133.0, 135.3.

4-((4-Ethylphenyl)ethynyl)benzonitrile (3gl) (CAS Registry Number 62856-07-9)



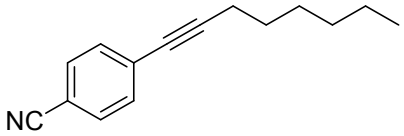
This product was obtained from the reaction of 4-hydrazinylbenzonitrile (**1g**) and 1-ethyl-4-ethynylbenzene (**2l**) as a white solid (83 mg, 72% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 1.25 (t, J = 7.5 Hz, 3H), 2.67 (q, J = 7.5 Hz, 2H), 7.21 (d, J = 8.0 Hz), 7.46 (d, J = 8.0 Hz), 7.58-7.64 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 15.3, 28.9, 87.2, 94.1, 111.2, 118.7, 119.4, 128.1, 128.5, 131.8, 132.0, 132.0, 145.7.

4-(3-Phenylprop-1-yn-1-yl)benzonitrile (3gm) (CAS Registry Number 851990-15-3)



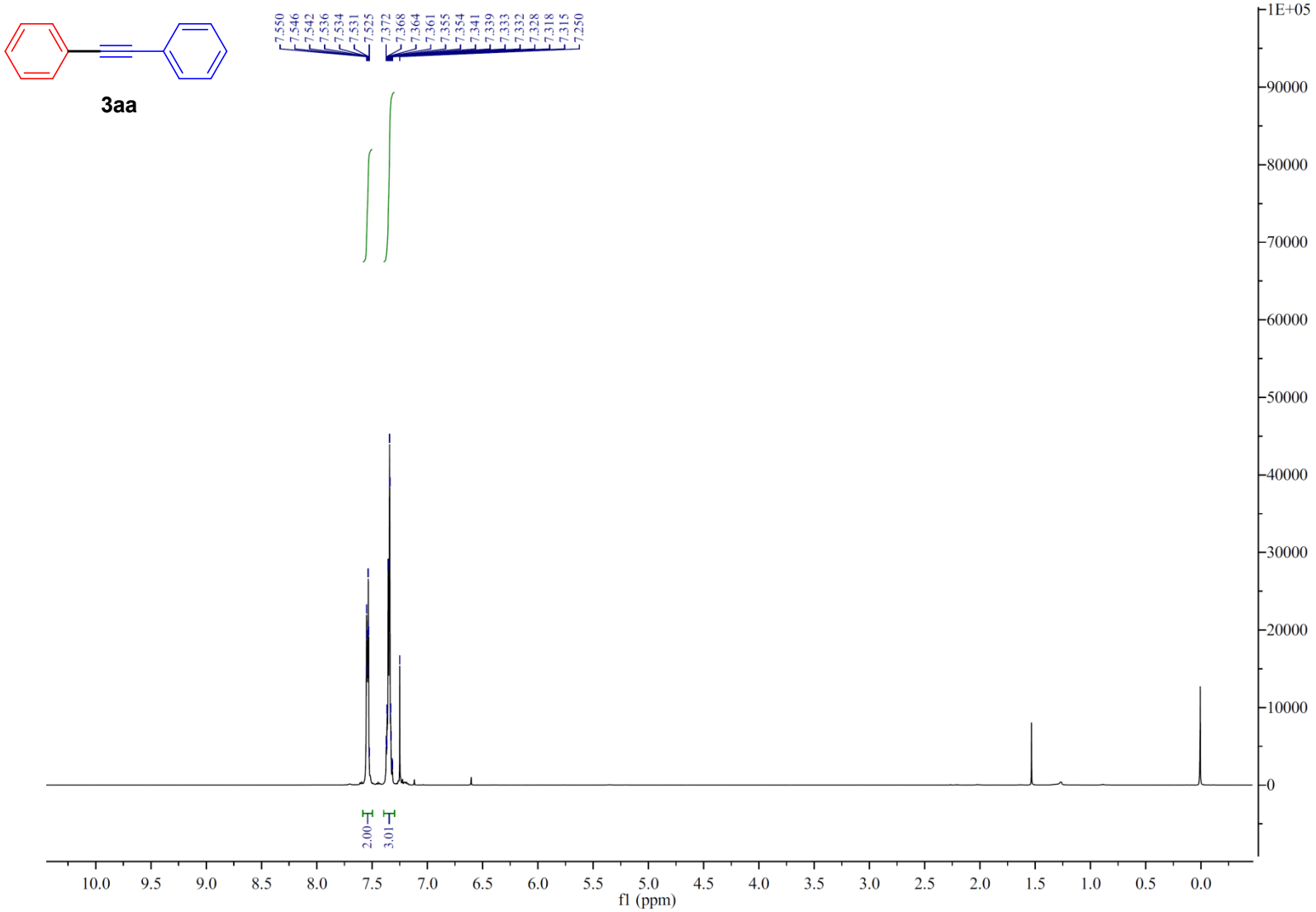
This product was obtained from the reaction of 4-hydrazinylbenzonitrile (**1g**) and prop-2-yn-1-ylbenzene (**2m**) as a white solid (109 mg, 75% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 3.86 (s, 2H), 7.26-7.29 (m, 1H), 7.34-7.40 (m, 4H), 7.51-7.52 (m, 2H), 7.58-7.59 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 25.8, 81.3, 92.7, 111.2, 118.6, 126.9, 127.9, 128.7, 128.7, 132.0, 132.2, 135.9.

4-(oct-1-yn-1-yl)benzonitrile (**3gn**) **(CAS Registry Number 312708-98-8)**



This product was obtained from the reaction of 4-hydrazinylbenzonitrile (**1g**) and 1-octyne (**2n**) as a light yellow liquid (30 mg, 28% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 0.91 (t, J = 7.0 Hz, 3H), 1.31-1.33(m, 4H), 1.42-1.48 (m, 2H), 1.58-1.64 (m, 2H), 2.43 (t, J = 7.0 Hz, 2H), 7.45-7.47 (m, 2H), 7.55-7.58 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 14.0, 19.5, 22.5, 28.4, 28.6, 31.3, 79.4, 95.7, 110.8, 118.7, 129.2, 131.9, 132.1.

3. Copies for ^{1}H NMR and ^{13}C NMR spectra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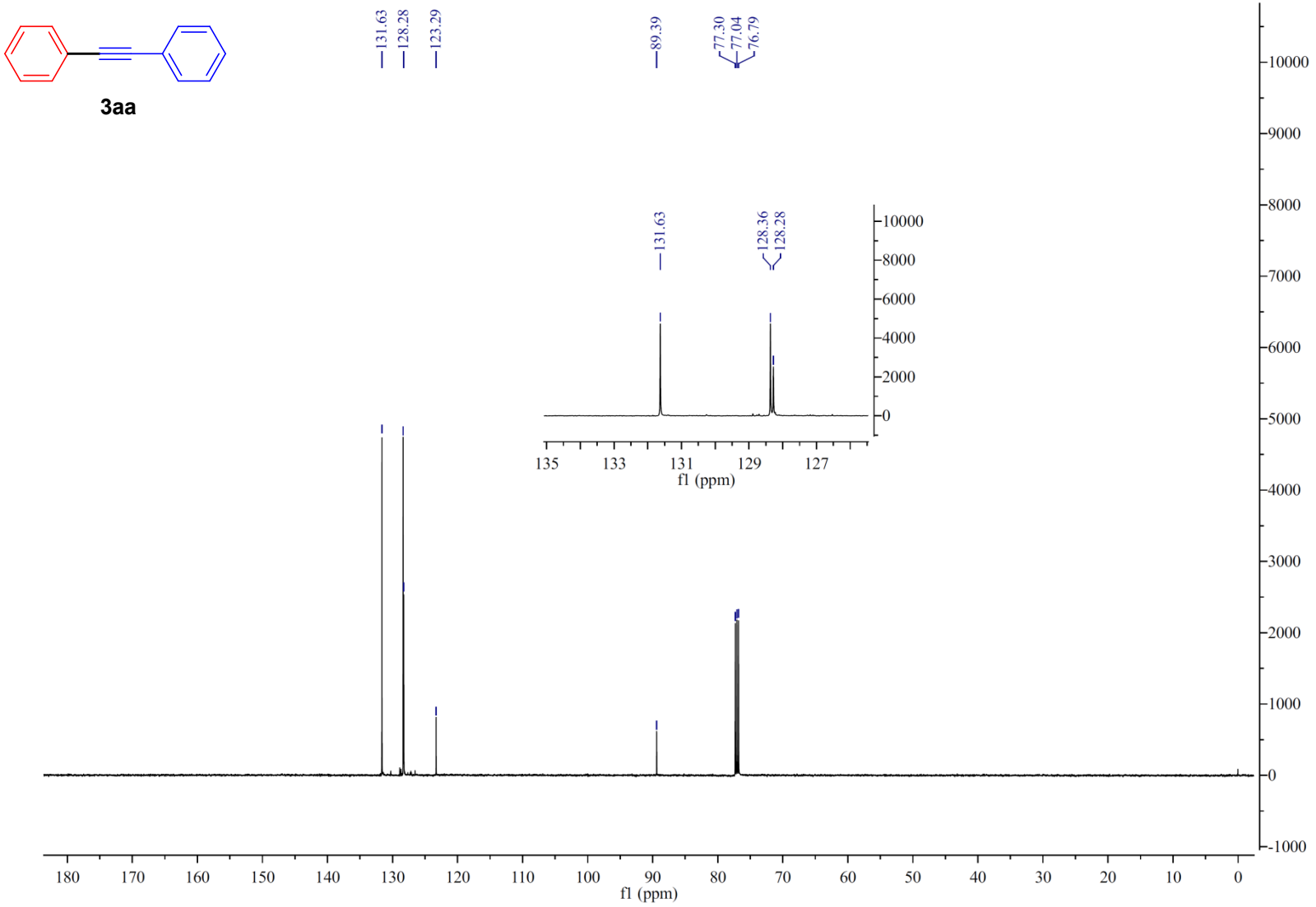
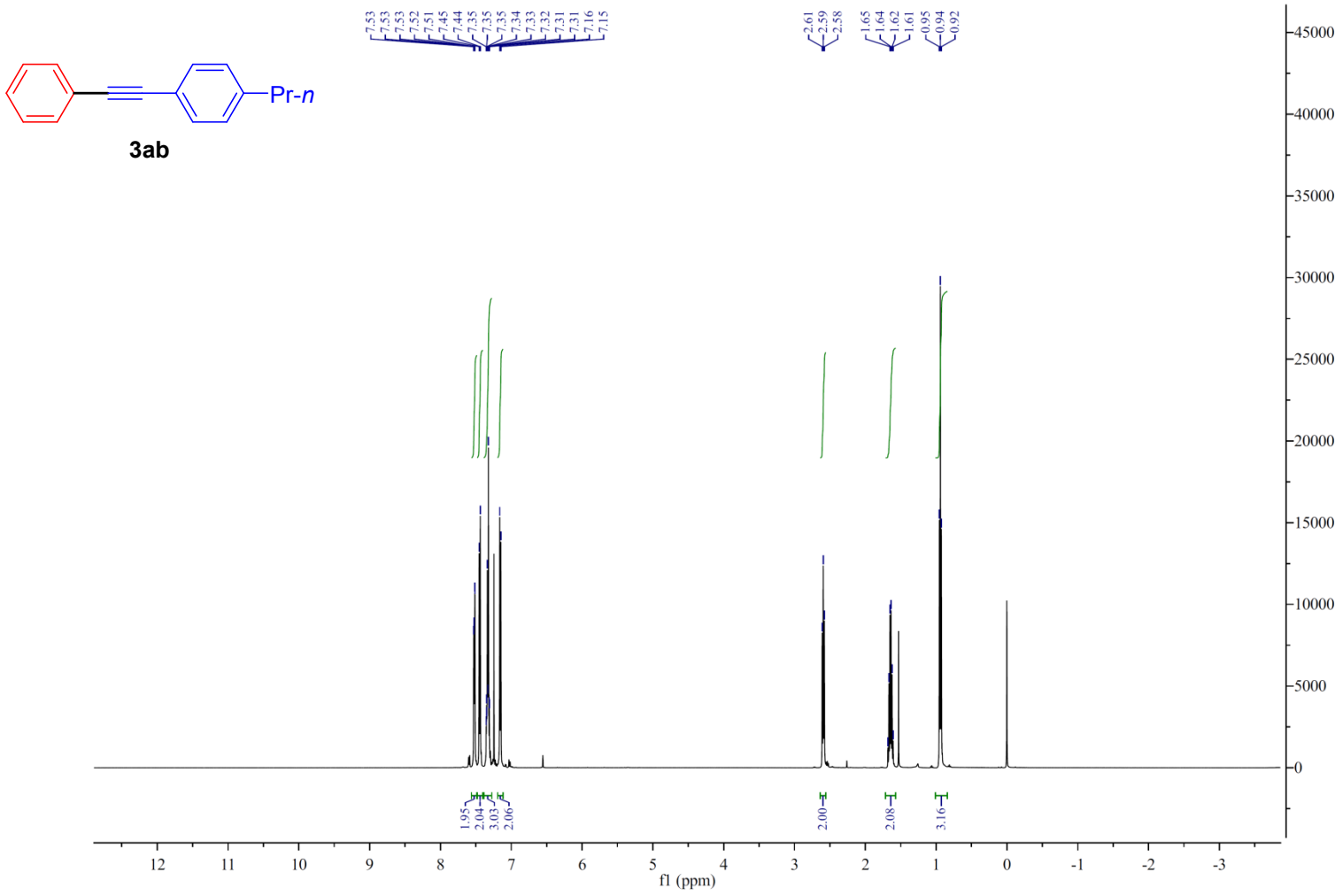
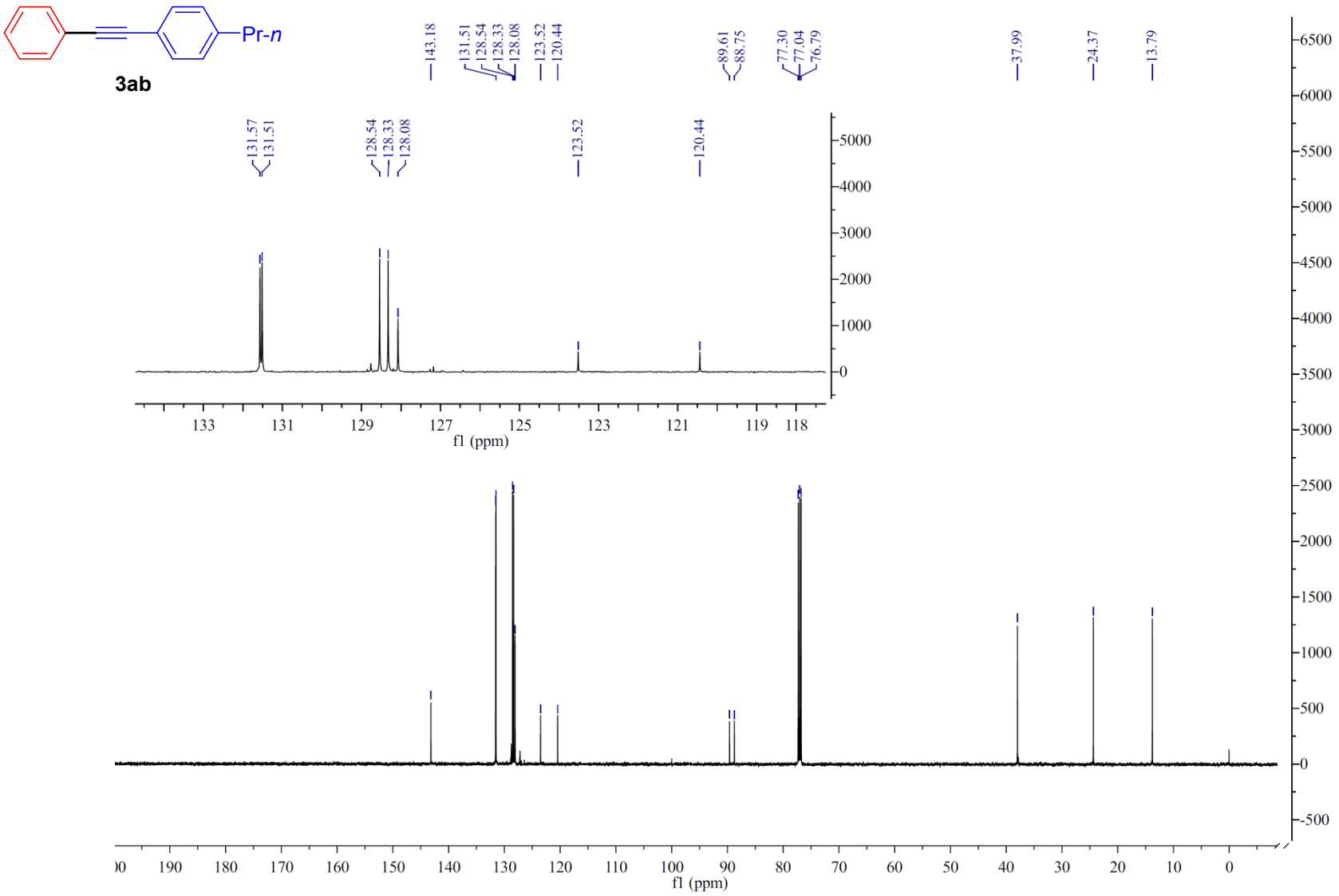
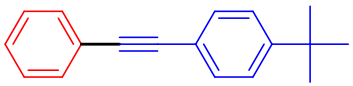
10000
0
2.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


3aa
131.63
128.28
123.29
89.39
77.30
77.04
76.79
131.63
128.36
128.28
f1 (ppm)
f1 (ppm)

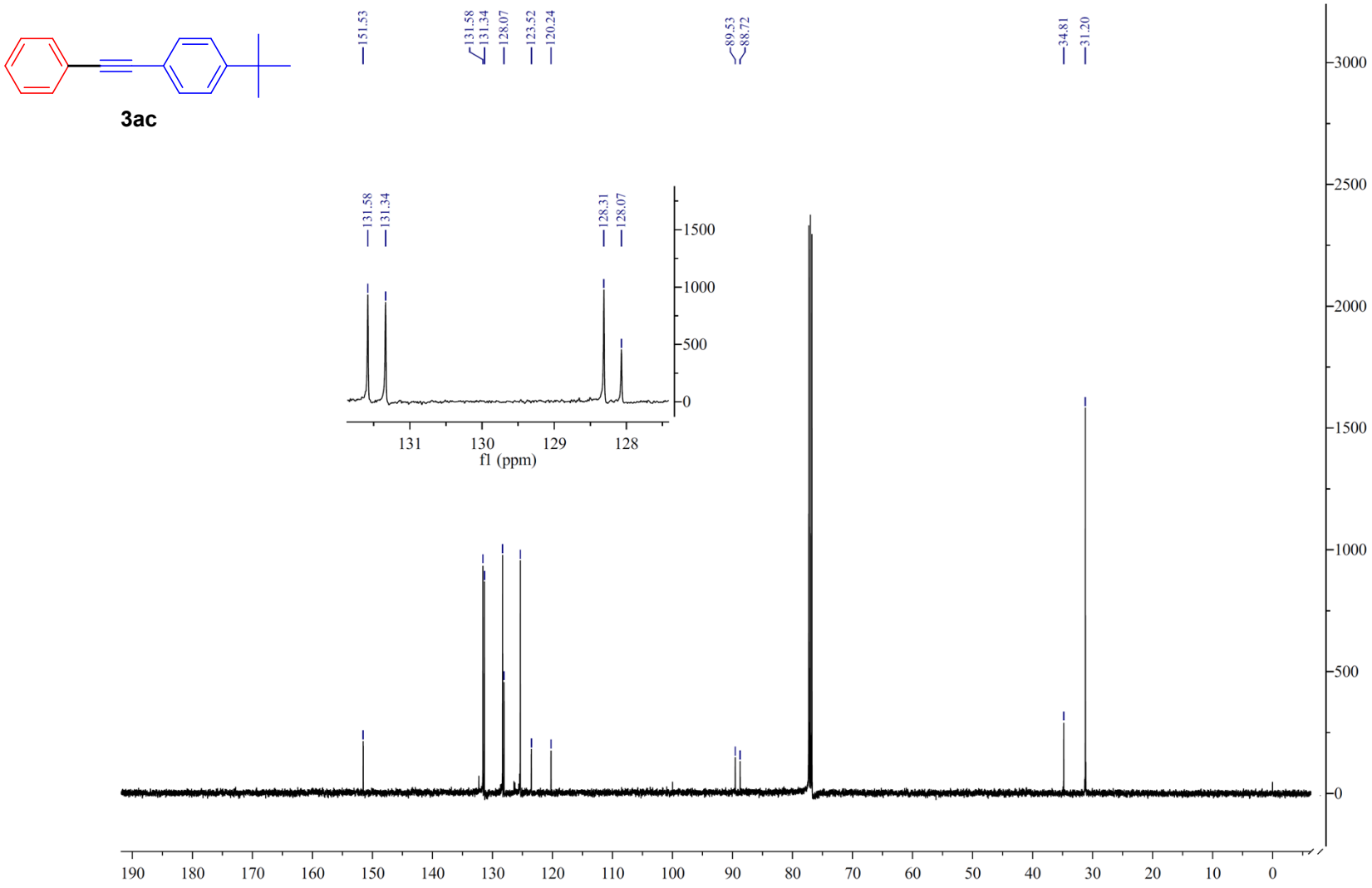

Pr-n
3ab
7.53
7.53
7.53
7.52
7.51
7.45
7.44
7.35
7.35
7.35
7.34
7.33
7.32
7.31
7.31
7.16
7.15
2.61
2.59
2.58
1.65
1.64
1.62
1.61
0.95
0.94
0.92
1.95
2.04
3.03
2.06
2.00
2.08
3.16
f1 (ppm)

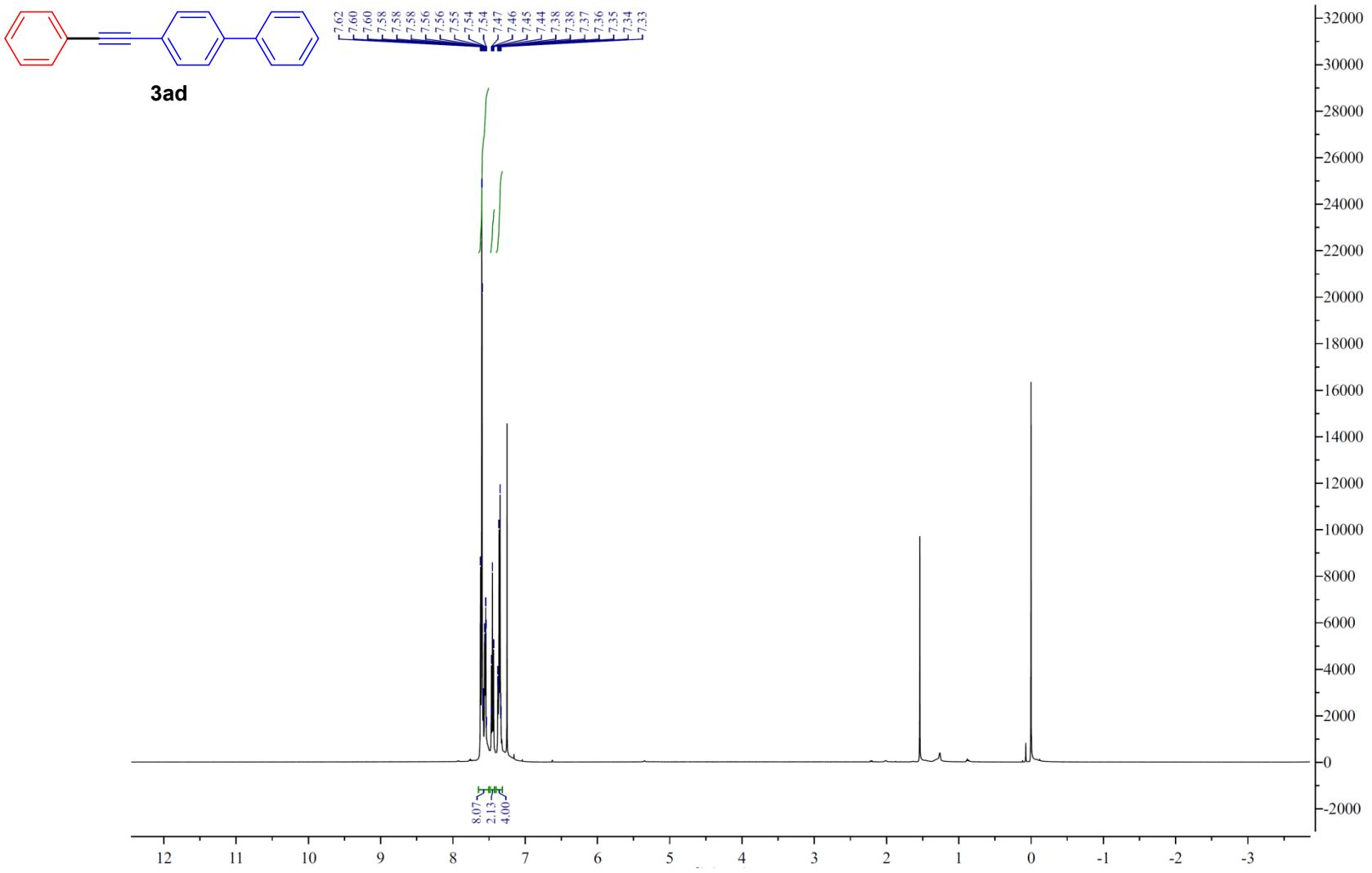

Pr-n
3ab
143.18
131.51
128.54
128.33
128.08
123.52
120.44
89.61
88.75
77.30
77.04
76.79
37.99
24.37
13.79
f1 (ppm)



3ac

7.53
7.53
7.52
7.52
7.48
7.46
7.46
7.38
7.36
7.34
7.33
7.33
7.25
1.33
2.00
2.11
5.07
9.11
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2


3ac
151.53
131.58
131.34
128.07
123.52
120.24
89.53
88.72
34.81
31.20
131.58
131.34
128.31
128.07
f1 (ppm)


3ad
7.62
7.60
7.60
7.58
7.58
7.58
7.56
7.56
7.55
7.54
7.54
7.47
7.46
7.45
7.44
7.38
7.38
7.37
7.36
7.35
7.34
7.33
8.07
2.13
4.00
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
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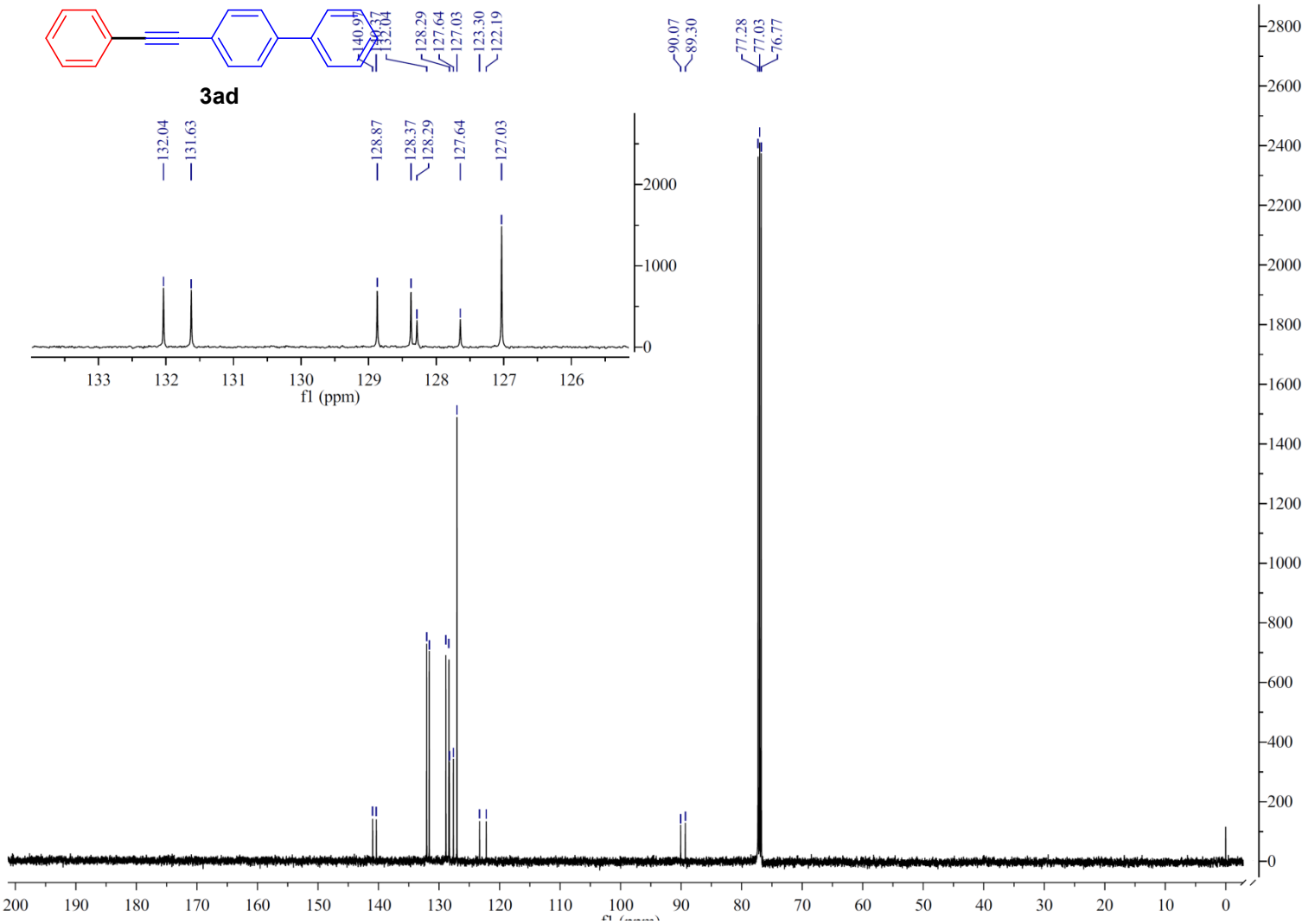
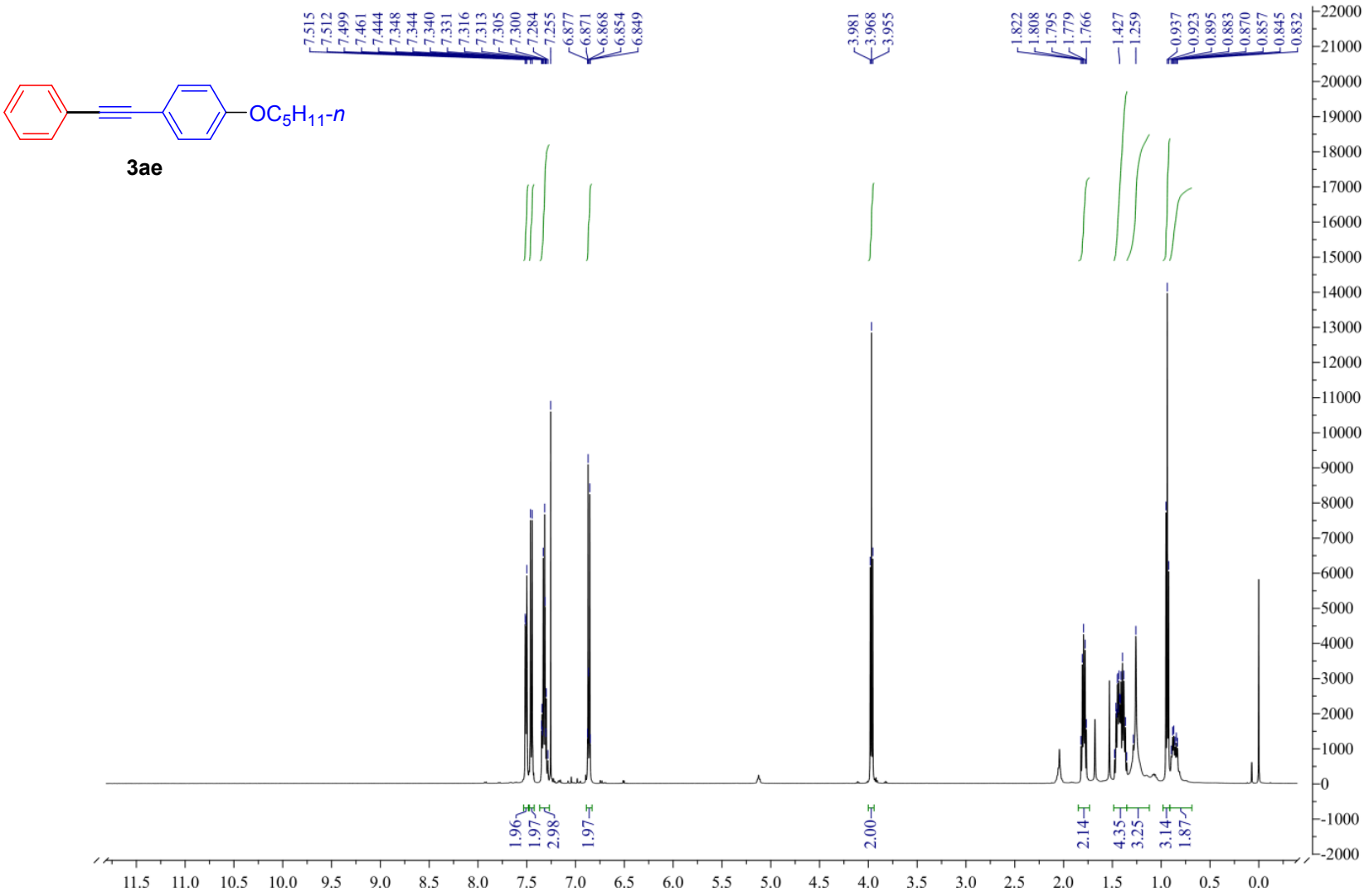
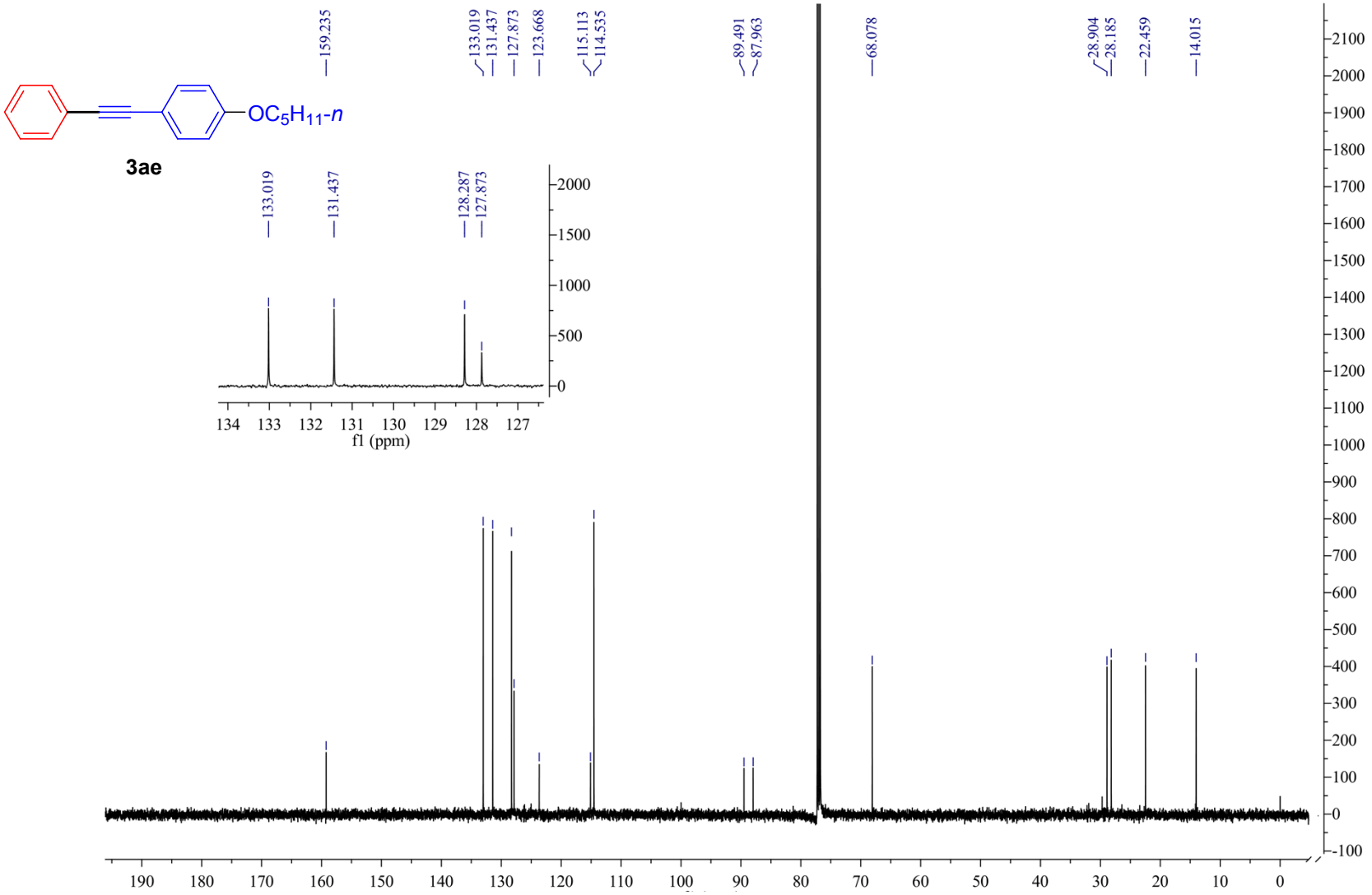
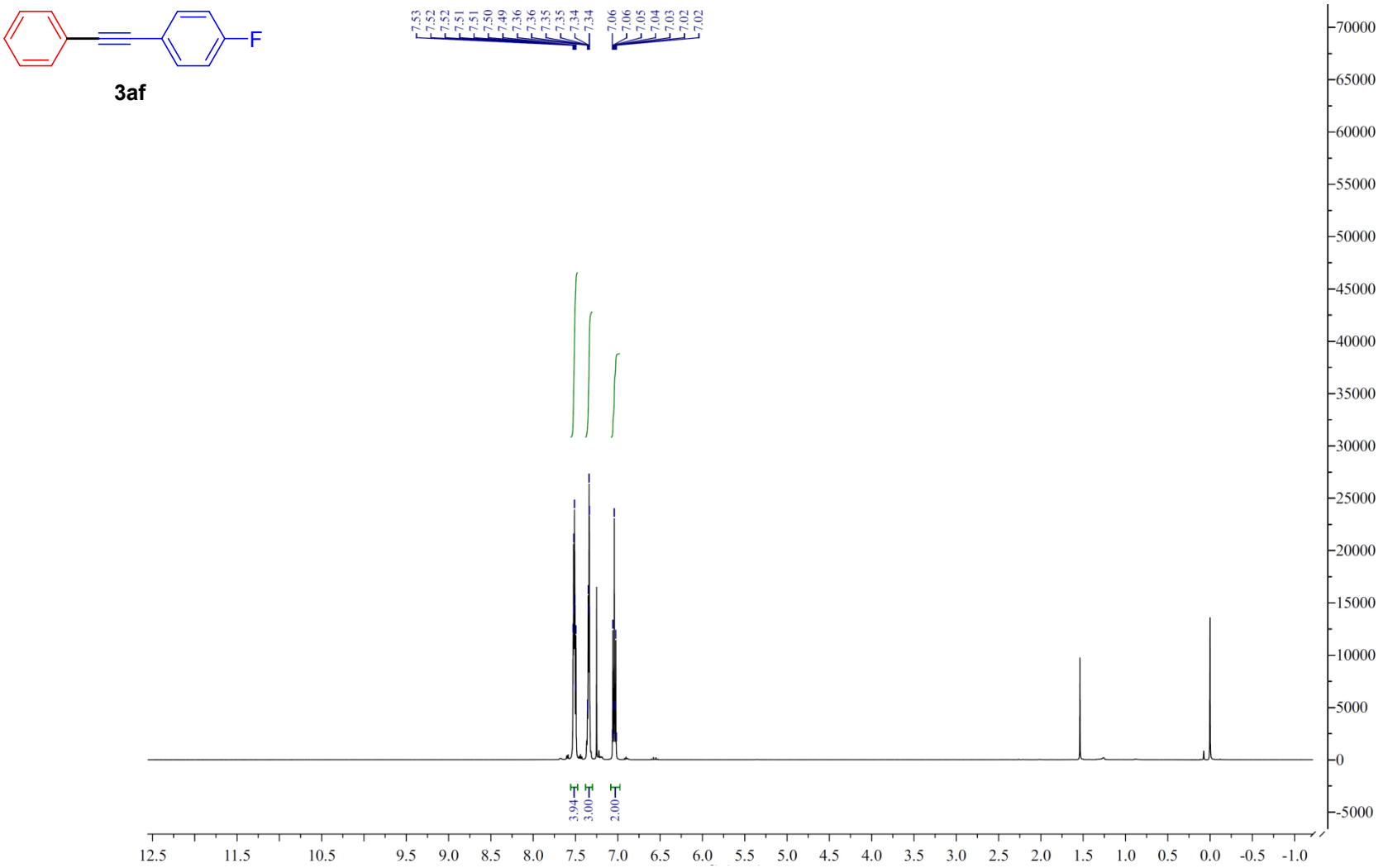
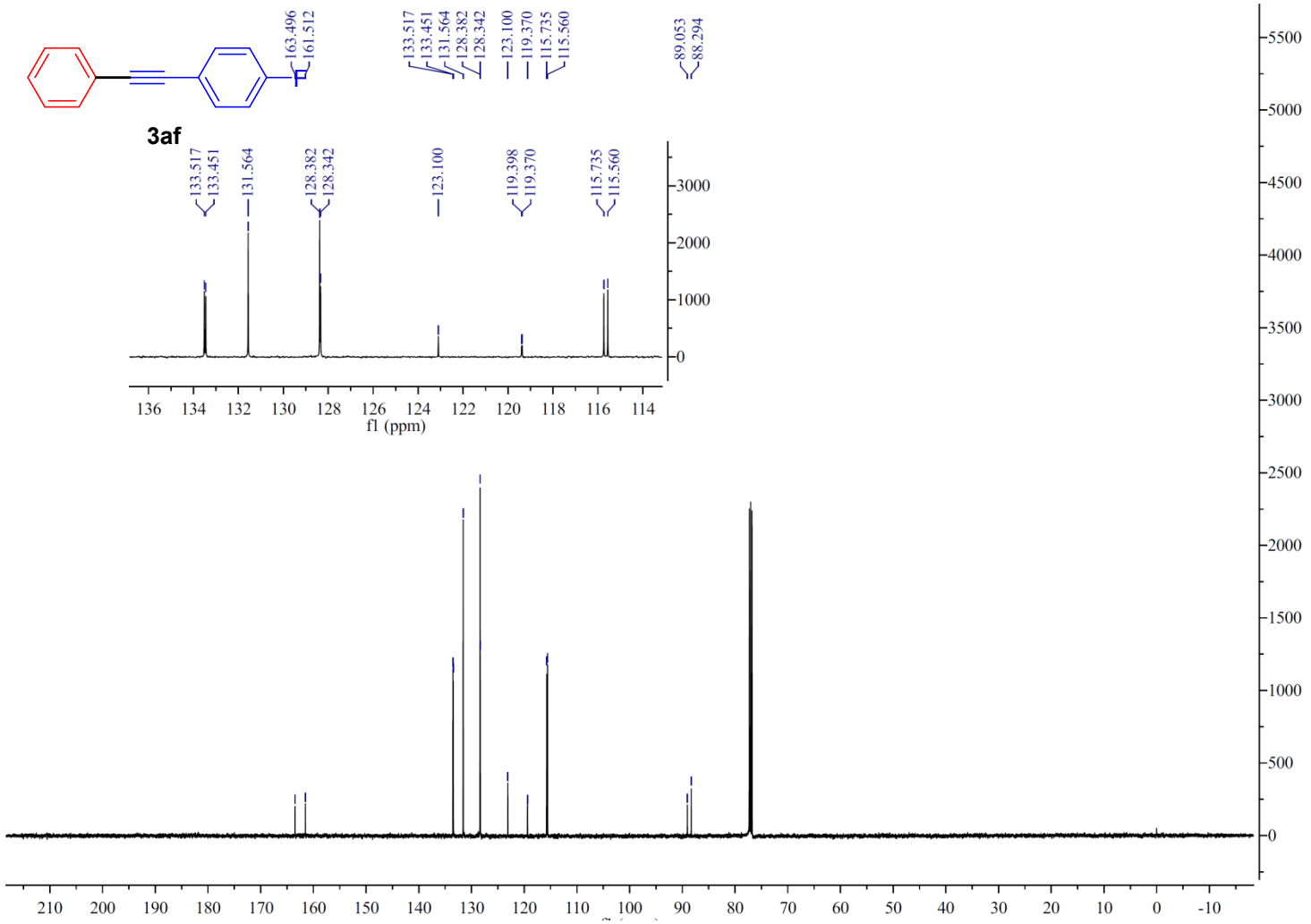
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3

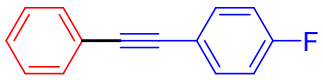

3ad
140.97
130.37
132.04
128.29
127.64
127.03
123.30
122.19
90.07
89.30
77.28
77.03
76.77
132.04
131.63
128.87
128.37
128.29
127.64
127.03
f1 (ppm)


OC5H11-n
3ae
7.515
7.512
7.499
7.461
7.444
7.348
7.344
7.340
7.331
7.316
7.313
7.305
7.300
7.284
7.255
6.877
6.871
6.868
6.854
6.849
3.981
3.968
3.955
1.822
1.808
1.795
1.779
1.766
1.427
1.259
0.937
0.923
0.895
0.883
0.870
0.857
0.845
0.832
1.96
1.97
2.98
1.97
2.00
2.14
4.35
3.25
3.14
1.87


159.235
133.019
131.437
127.873
123.668
115.113
114.535
89.491
87.963
68.078
28.904
28.185
22.459
14.015
OC5H11-n
3ae
133.019
131.437
128.287
127.873
f1 (ppm)

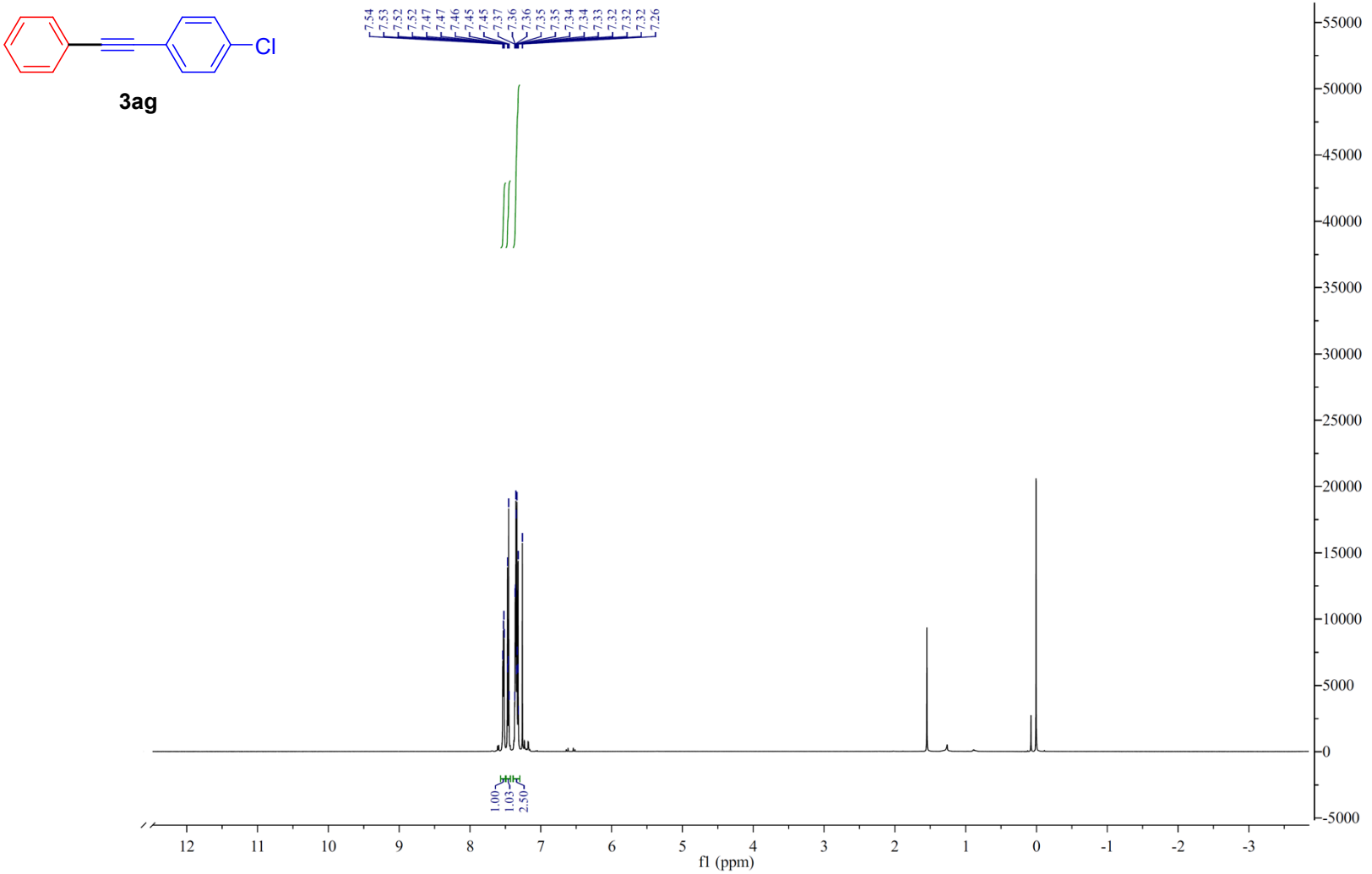

F
3af
7.53
7.52
7.52
7.51
7.51
7.50
7.49
7.36
7.36
7.35
7.35
7.34
7.34
7.06
7.06
7.05
7.04
7.03
7.02
7.02
3.94
3.00
2.00
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

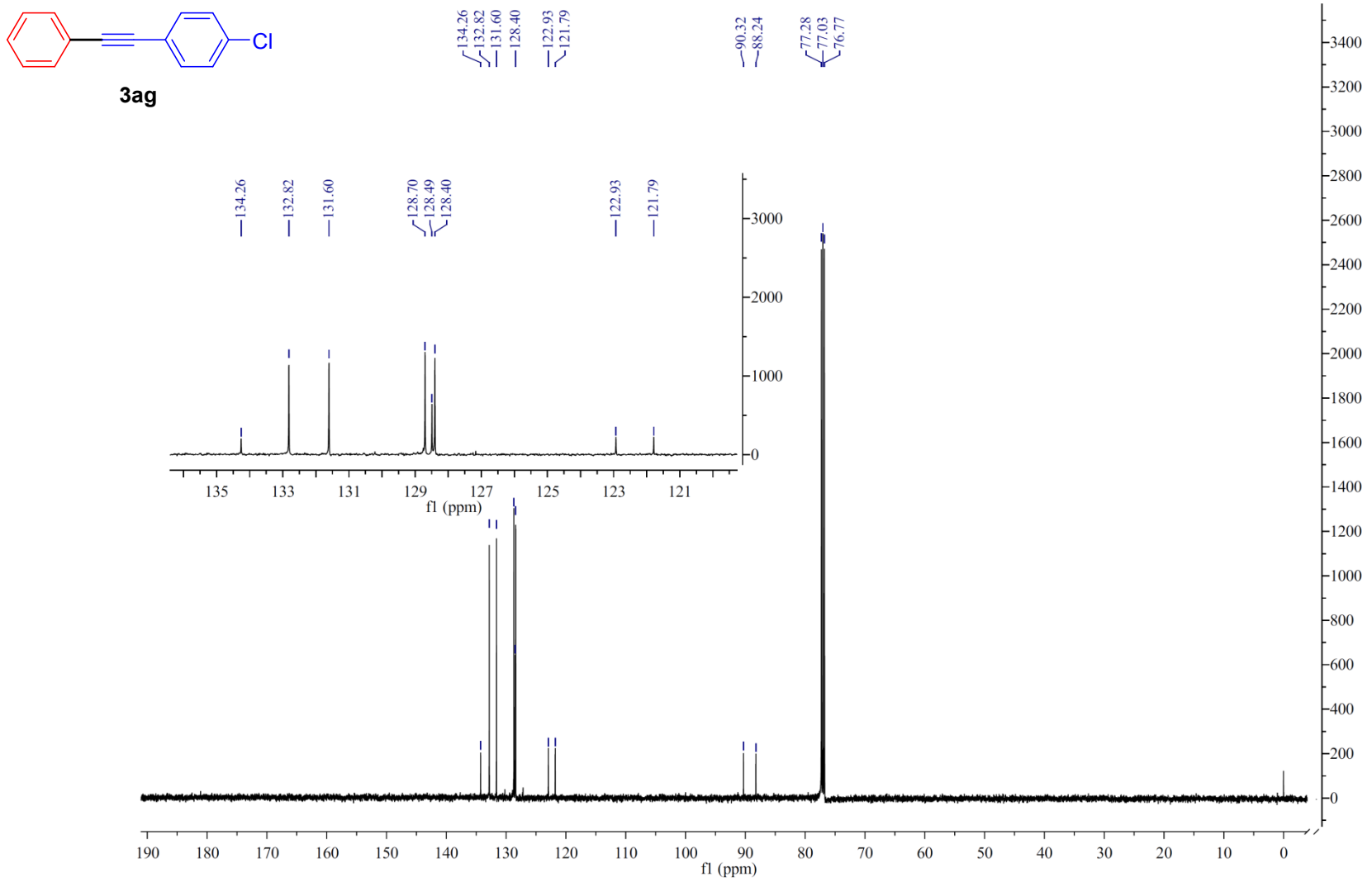

3af
163.496
161.512
133.517
133.451
131.564
128.382
128.342
123.100
119.370
115.735
115.560
89.053
88.294
f1 (ppm)

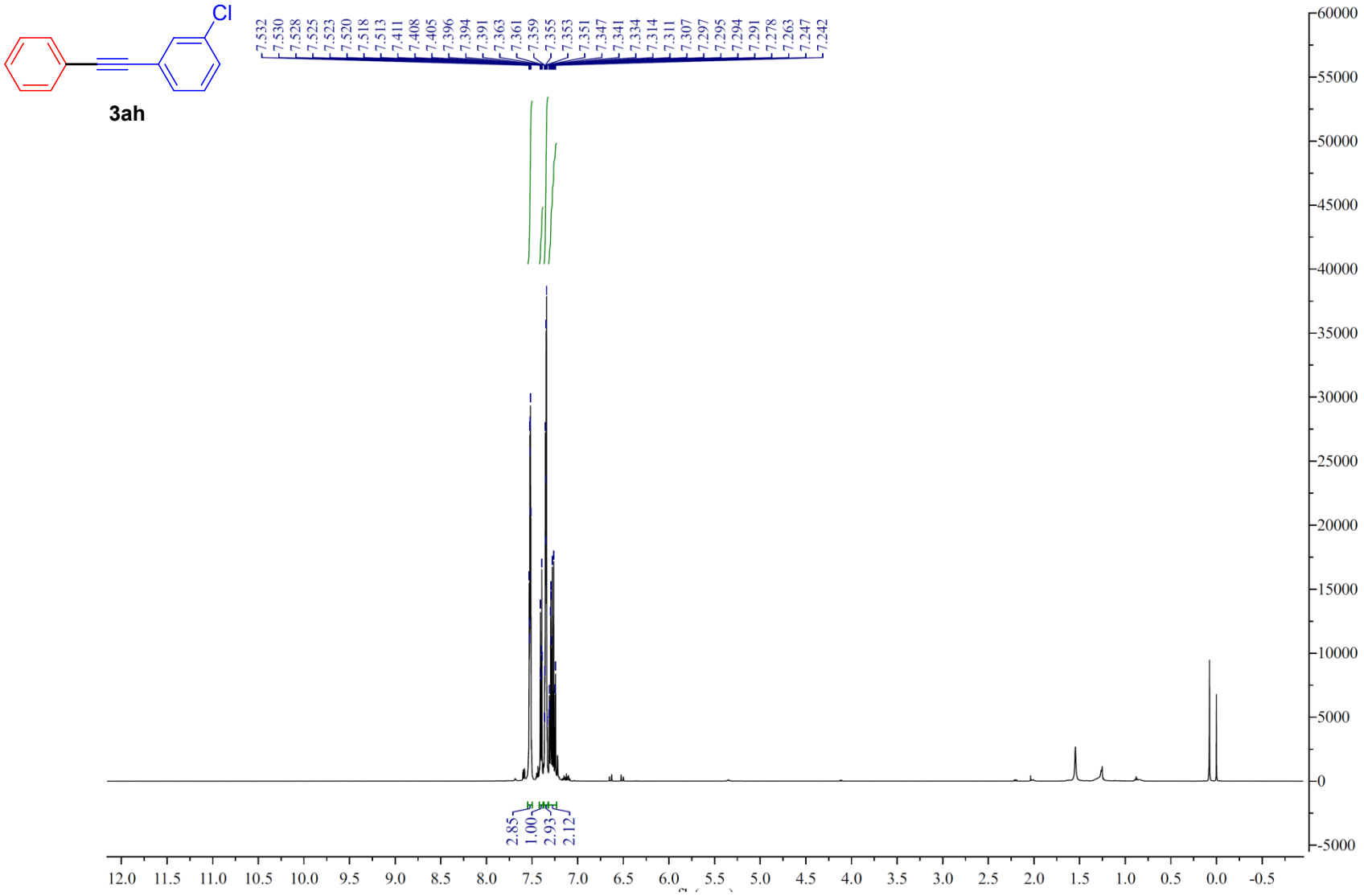

F

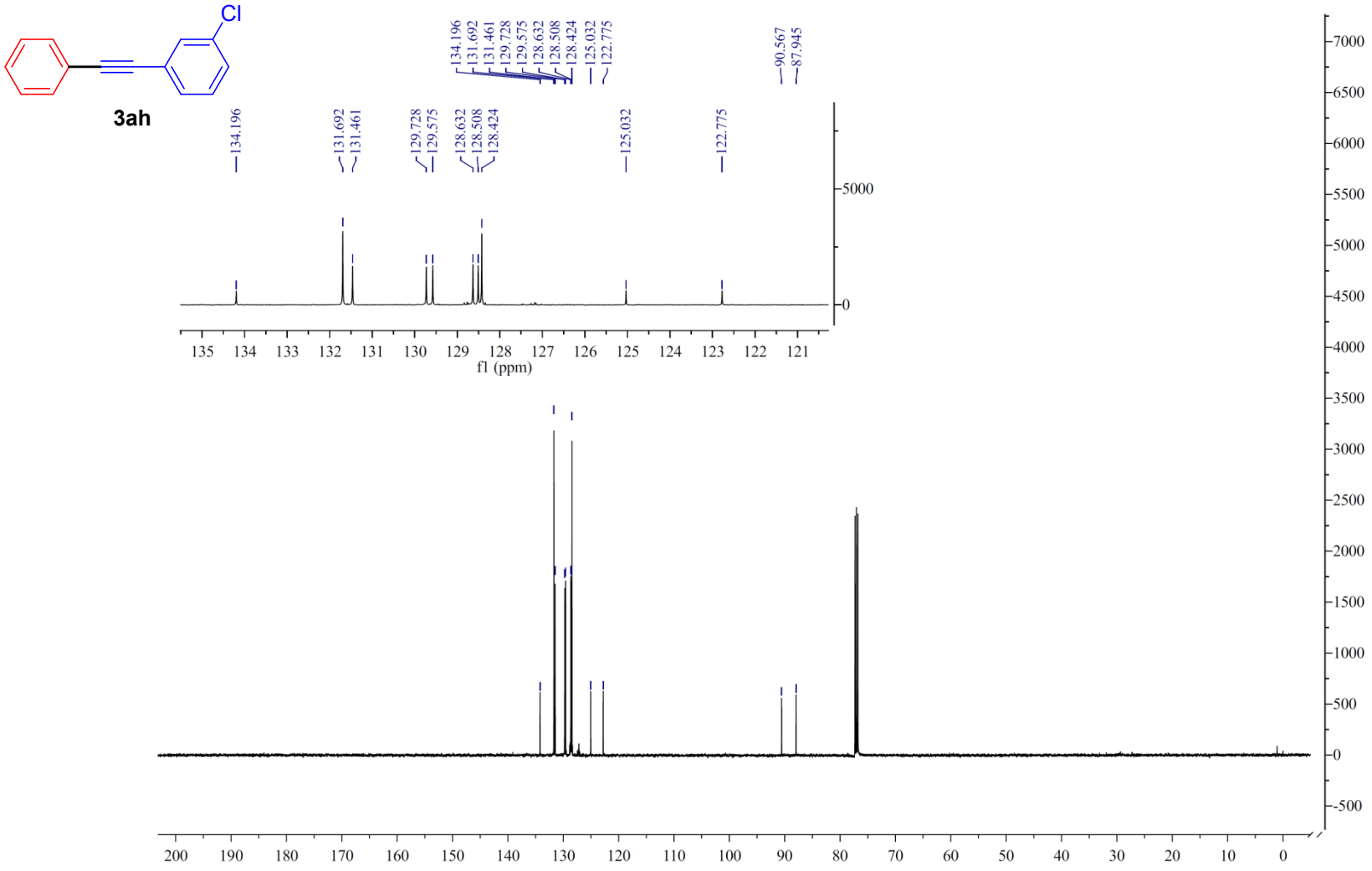
3af

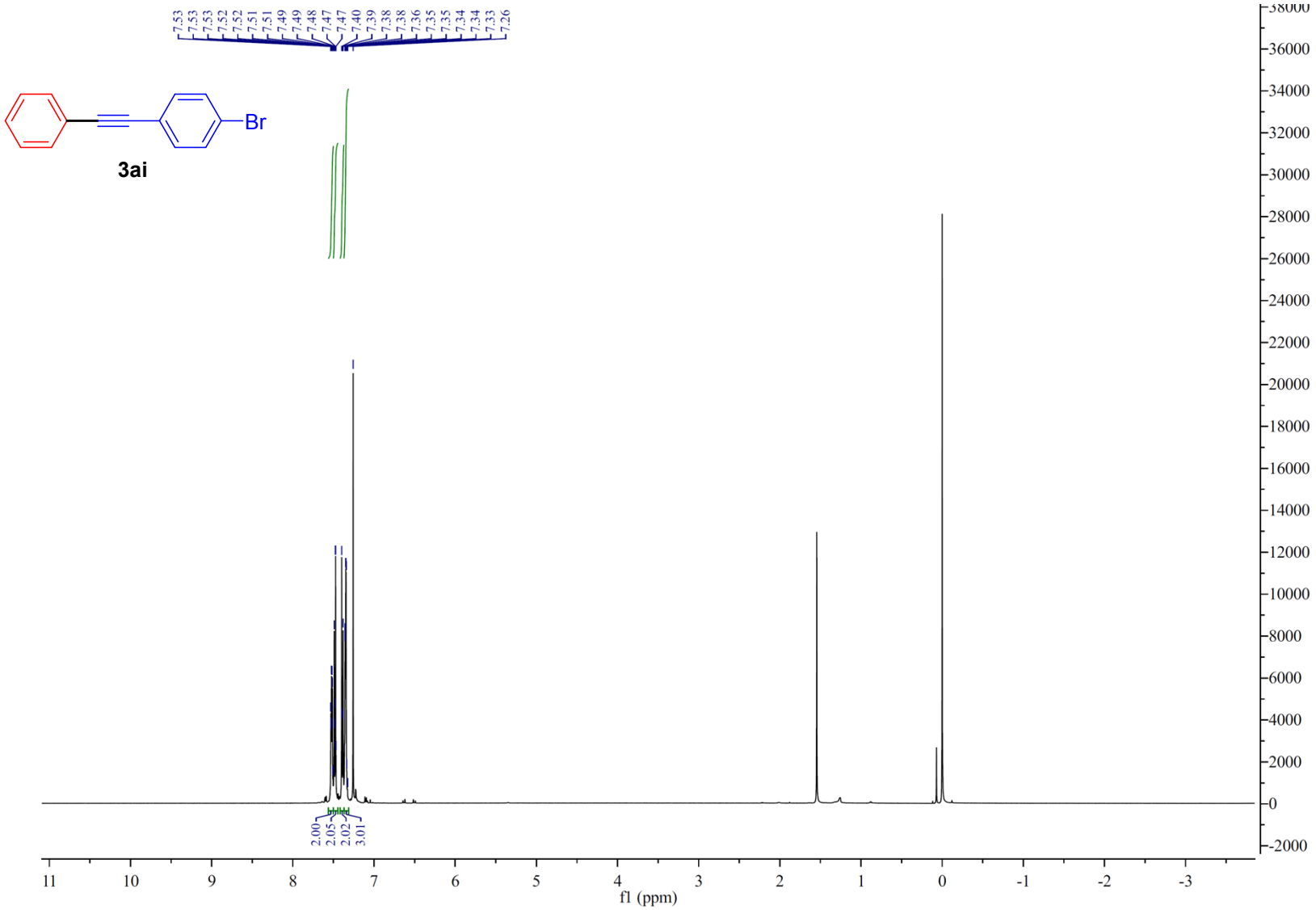
-110.992
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220

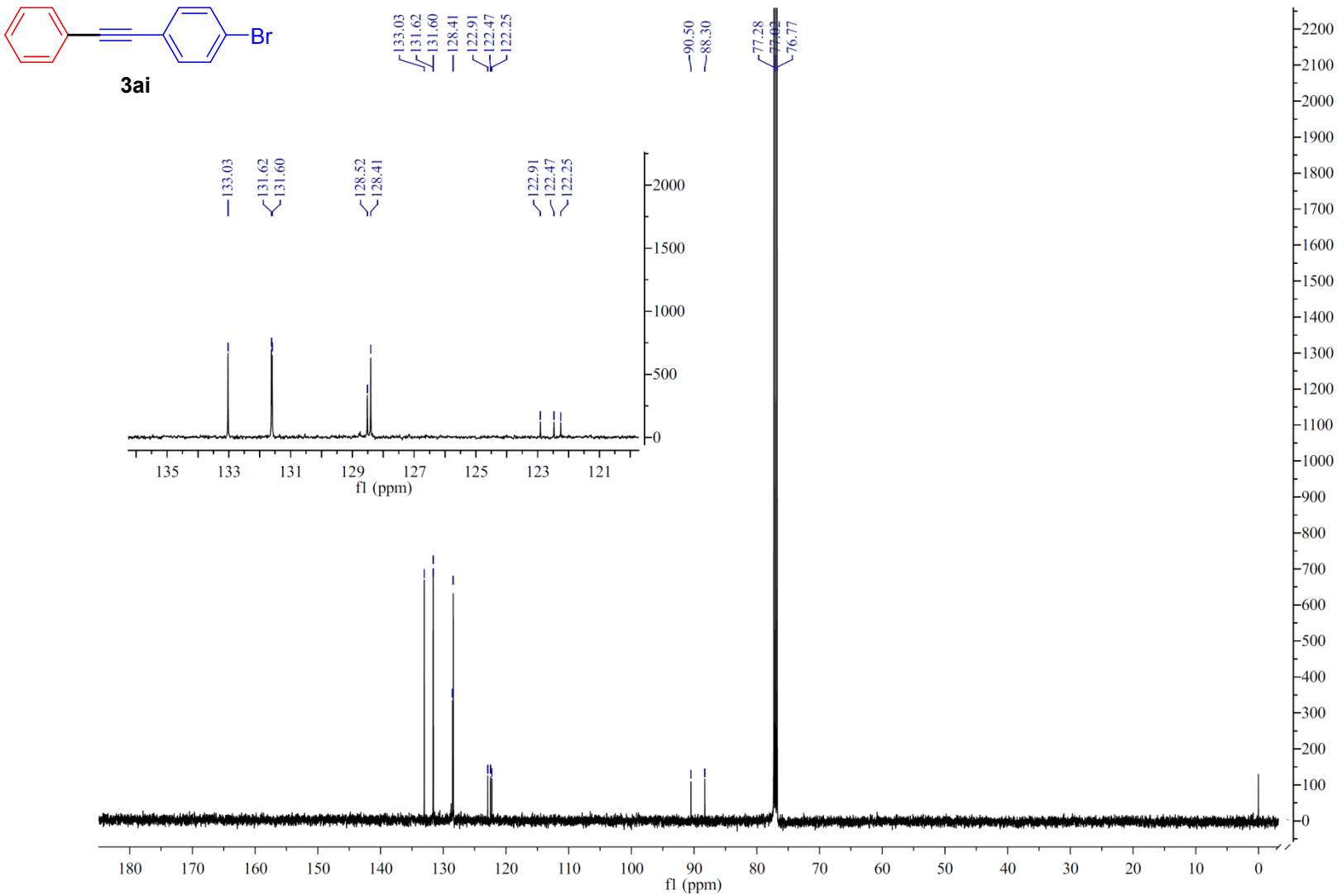

Cl
3ag
7.54
7.53
7.52
7.52
7.47
7.47
7.46
7.45
7.45
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.32
7.32
7.32
7.26
1.00
1.03
2.50
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

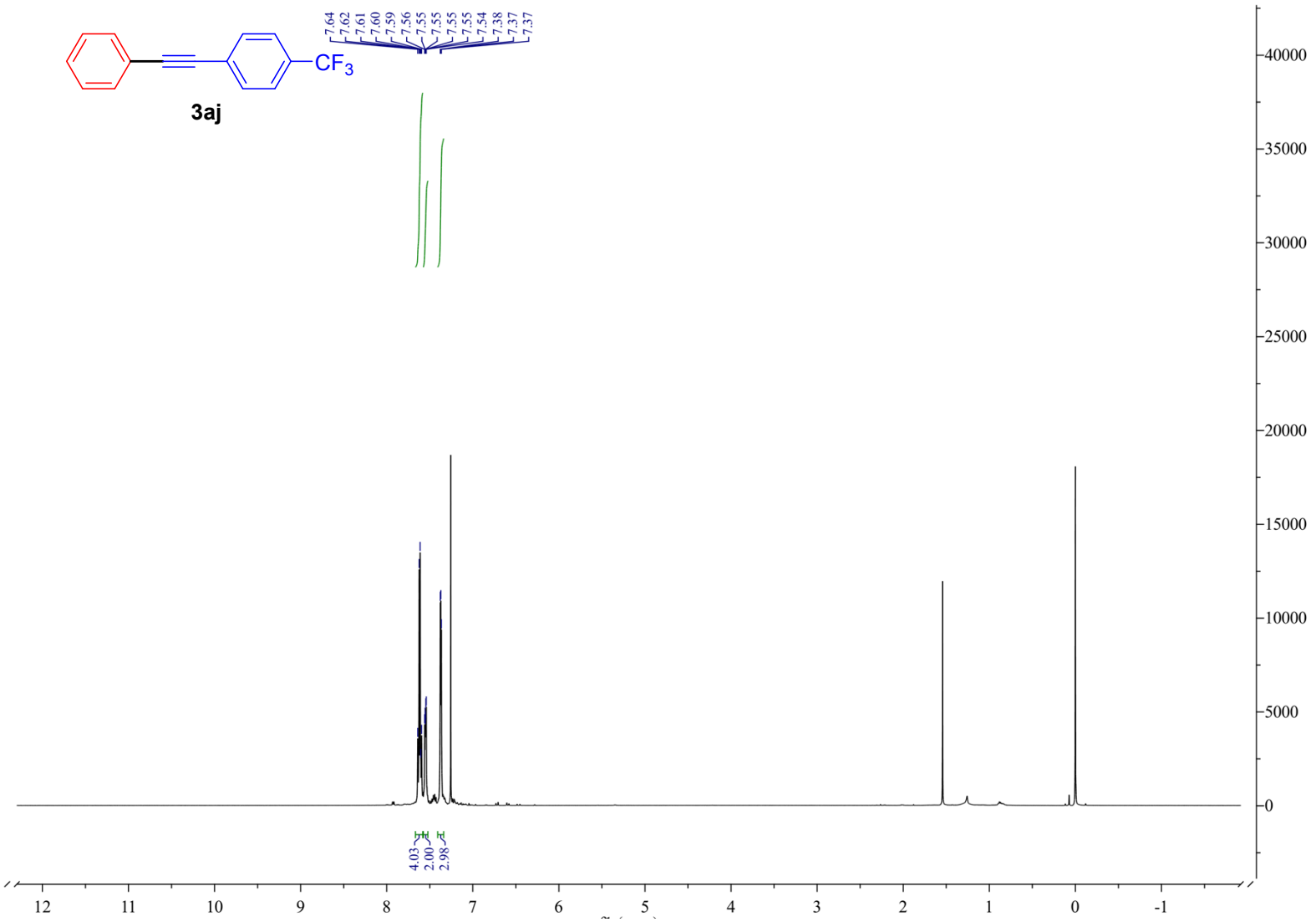

Cl
3ag
134.26
132.82
131.60
128.40
122.93
121.79
90.32
88.24
77.28
77.03
76.77
f1 (ppm)

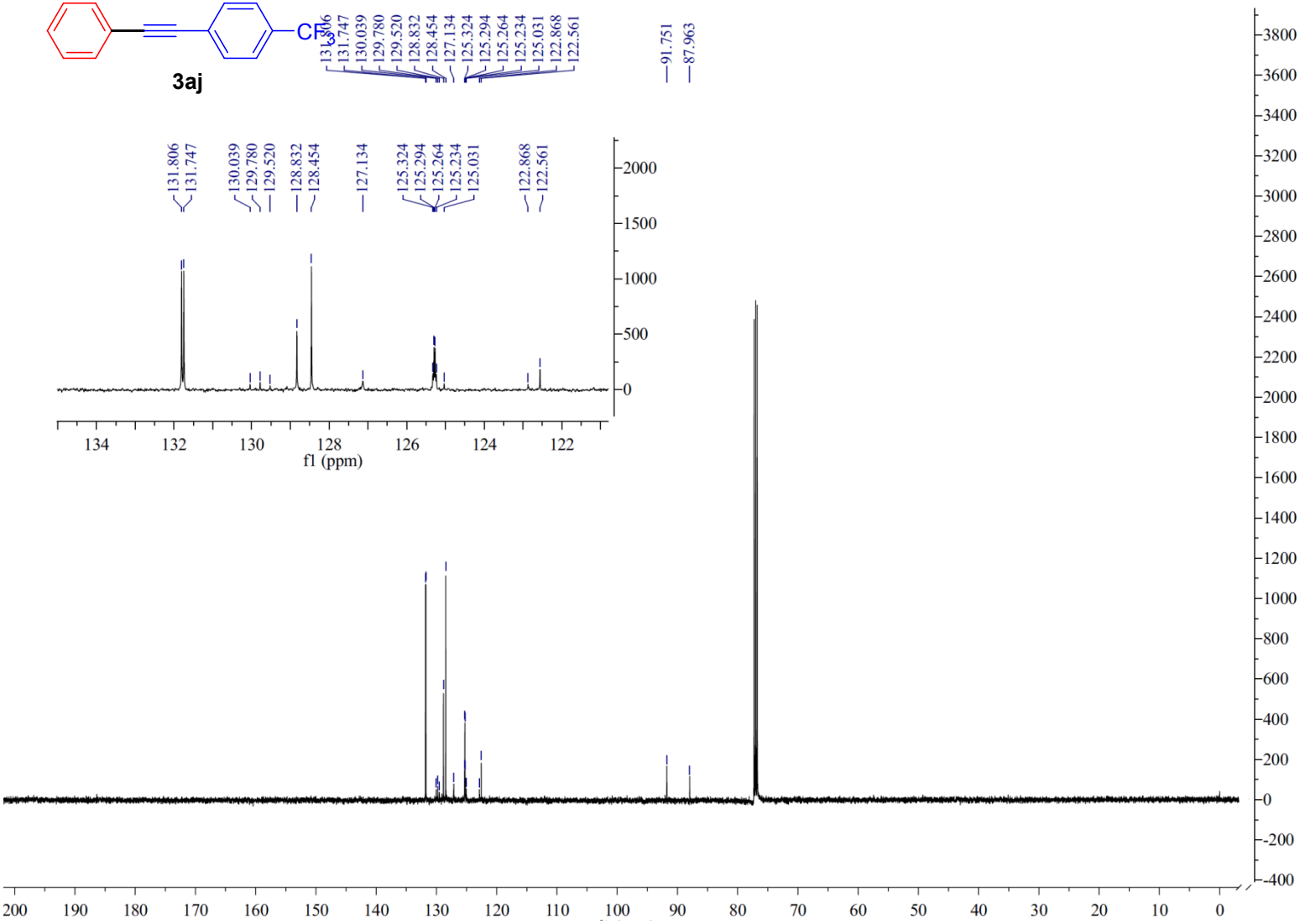

Cl
3ah
7.532
7.530
7.528
7.525
7.523
7.520
7.518
7.513
7.411
7.408
7.405
7.396
7.394
7.391
7.363
7.361
7.359
7.355
7.353
7.351
7.347
7.341
7.334
7.314
7.311
7.307
7.297
7.295
7.294
7.291
7.278
7.263
7.247
7.242
2.85
1.00
2.93
2.12
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

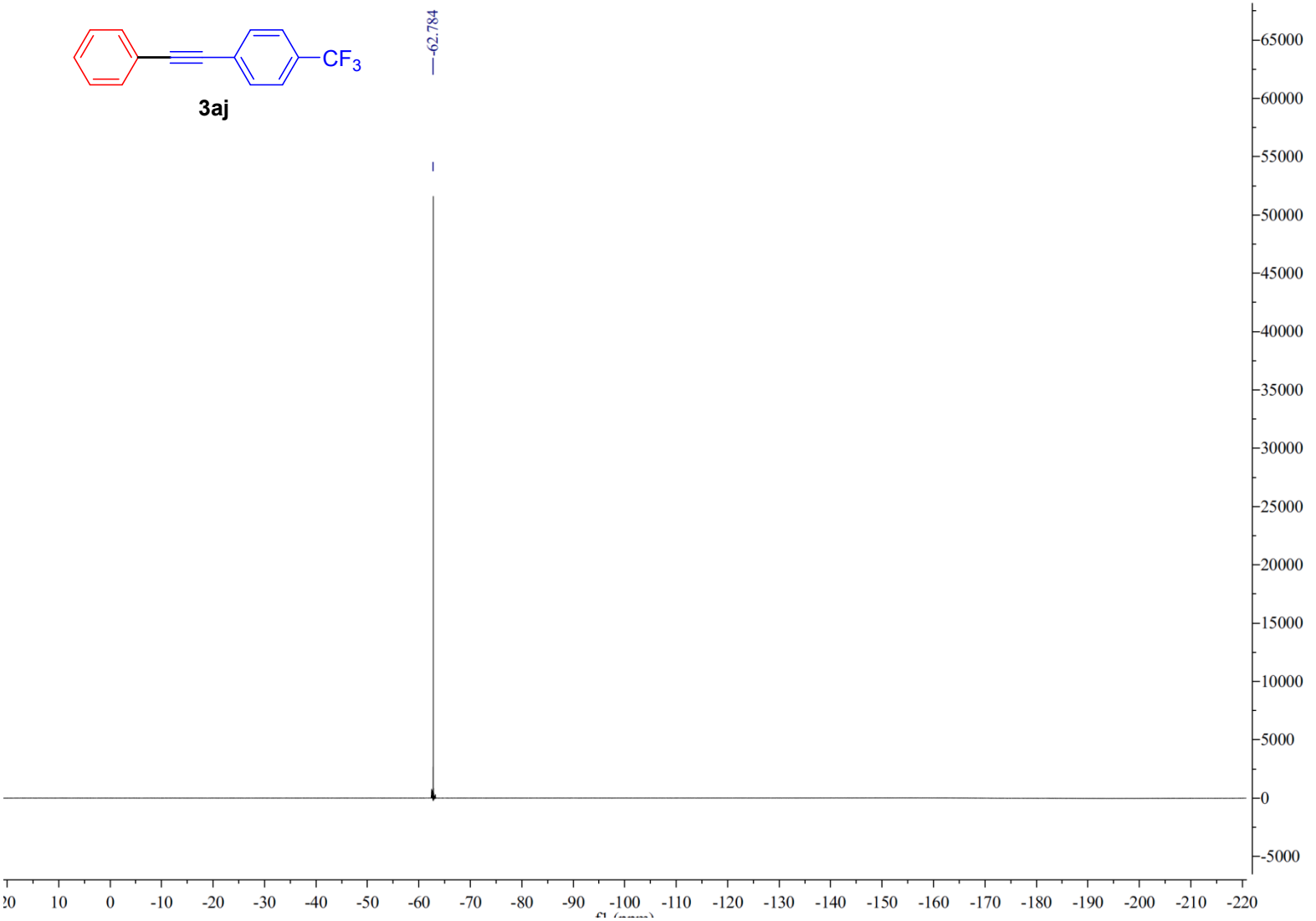

Cl
3ah
134.196
131.692
131.461
129.728
129.575
128.632
128.508
128.424
125.032
122.775
90.567
87.945
fl (ppm)

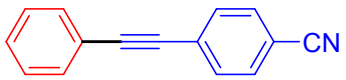

7.53
7.53
7.53
7.52
7.52
7.51
7.51
7.49
7.49
7.48
7.47
7.47
7.40
7.39
7.38
7.38
7.36
7.35
7.35
7.34
7.34
7.33
7.26
Br
3ai
2.00
2.05
2.02
3.01
f1 (ppm)


Br
3ai
133.03
131.62
131.60
128.41
122.91
122.47
122.25
90.50
88.30
77.28
77.03
76.77
f1 (ppm)


7.64
7.62
7.61
7.60
7.59
7.56
7.55
7.55
7.55
7.55
7.54
7.38
7.37
7.37
CF3
3aj
4.03
2.00
2.98
40000
35000
30000
25000
20000
15000
10000
5000
0
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

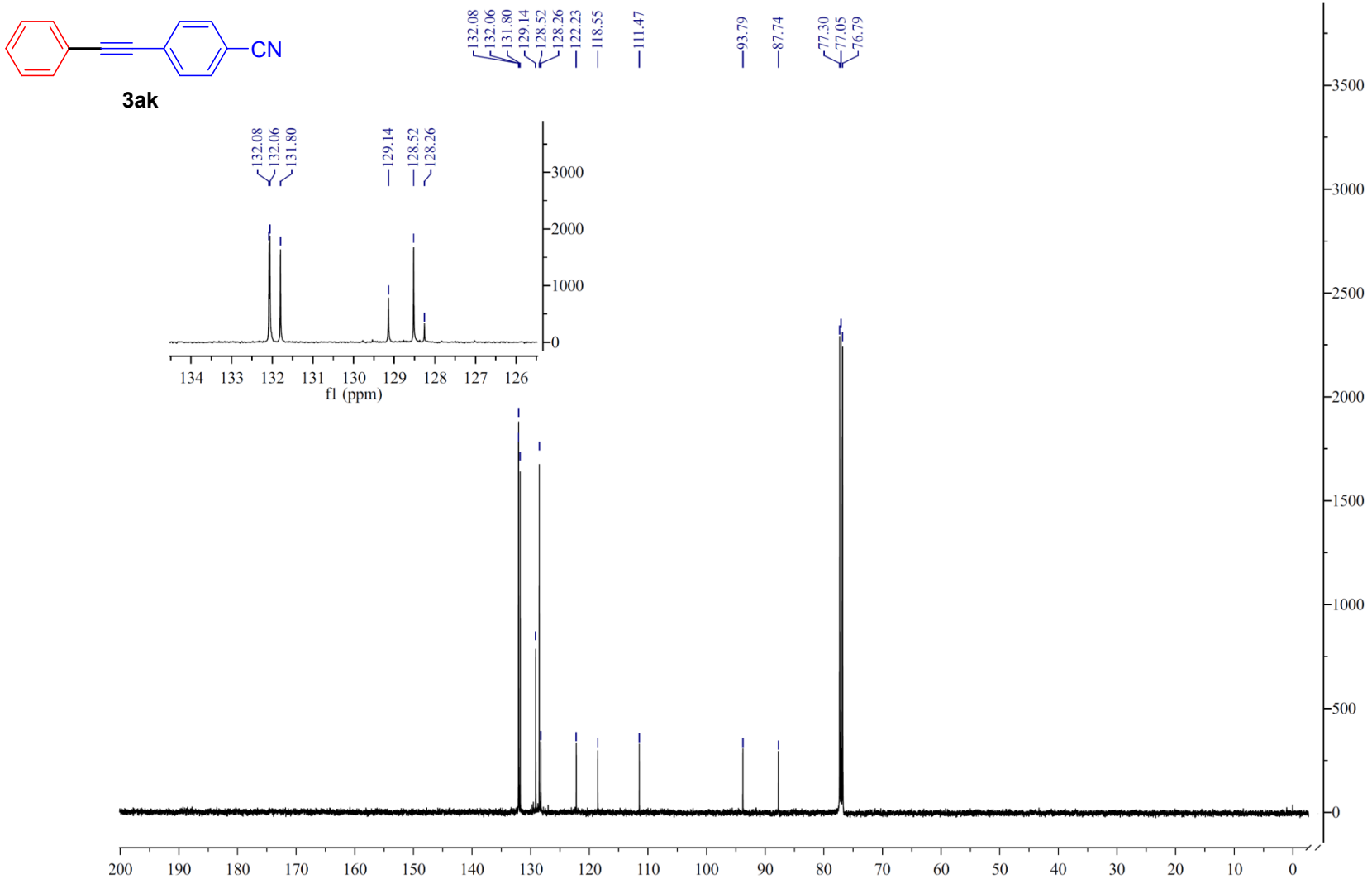

CF3
3aj
131.806
131.747
130.039
129.780
129.520
128.832
128.454
127.134
125.324
125.294
125.264
125.234
125.031
122.868
122.561
91.751
87.963
f1 (ppm)

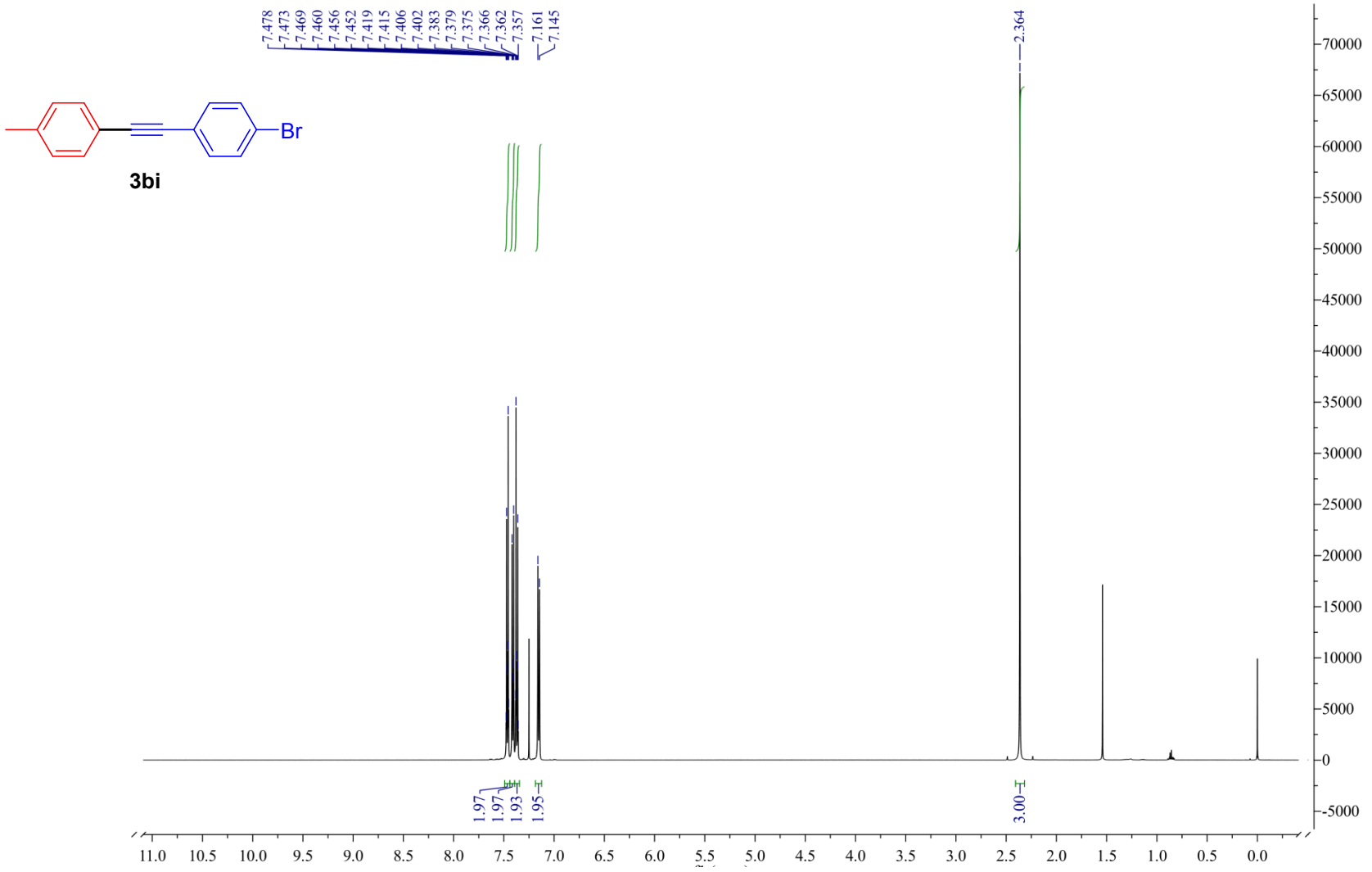

CF3
3aj
-62.784
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220

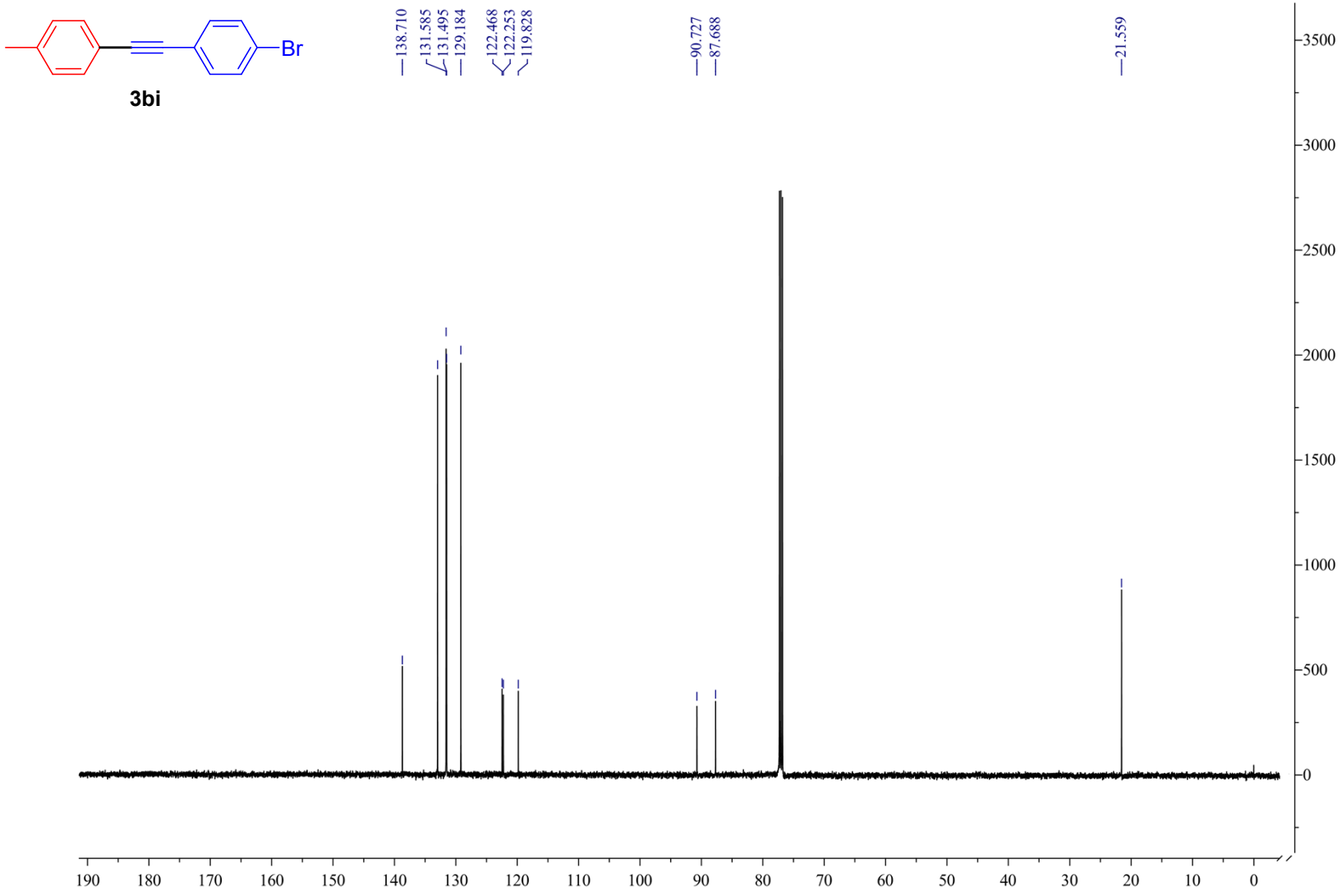

CN

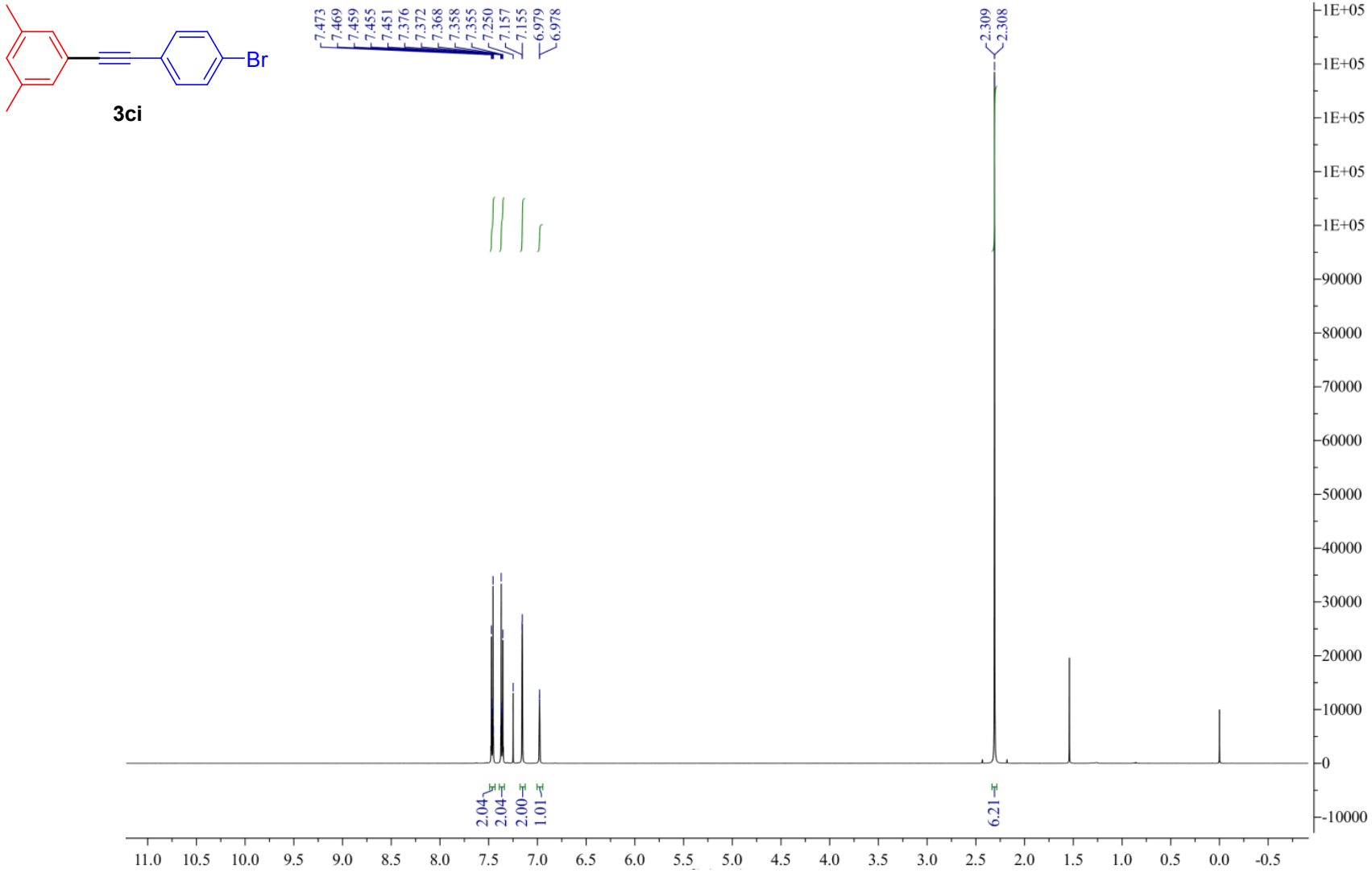
3ak

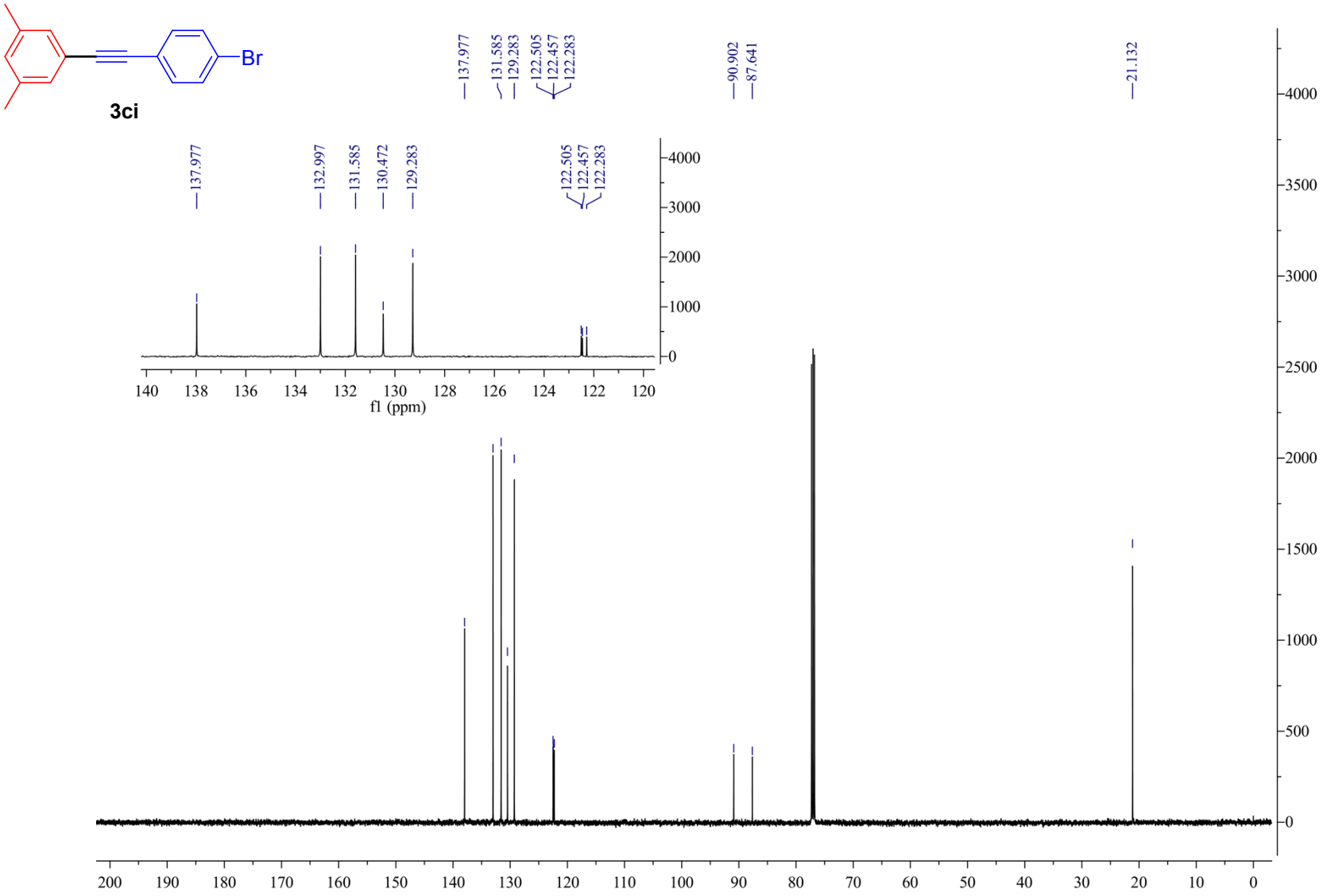
7.61
7.60
7.58
7.56
7.53
7.52
7.51
7.51
7.36
7.35
7.35
4.00
2.00
3.00
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

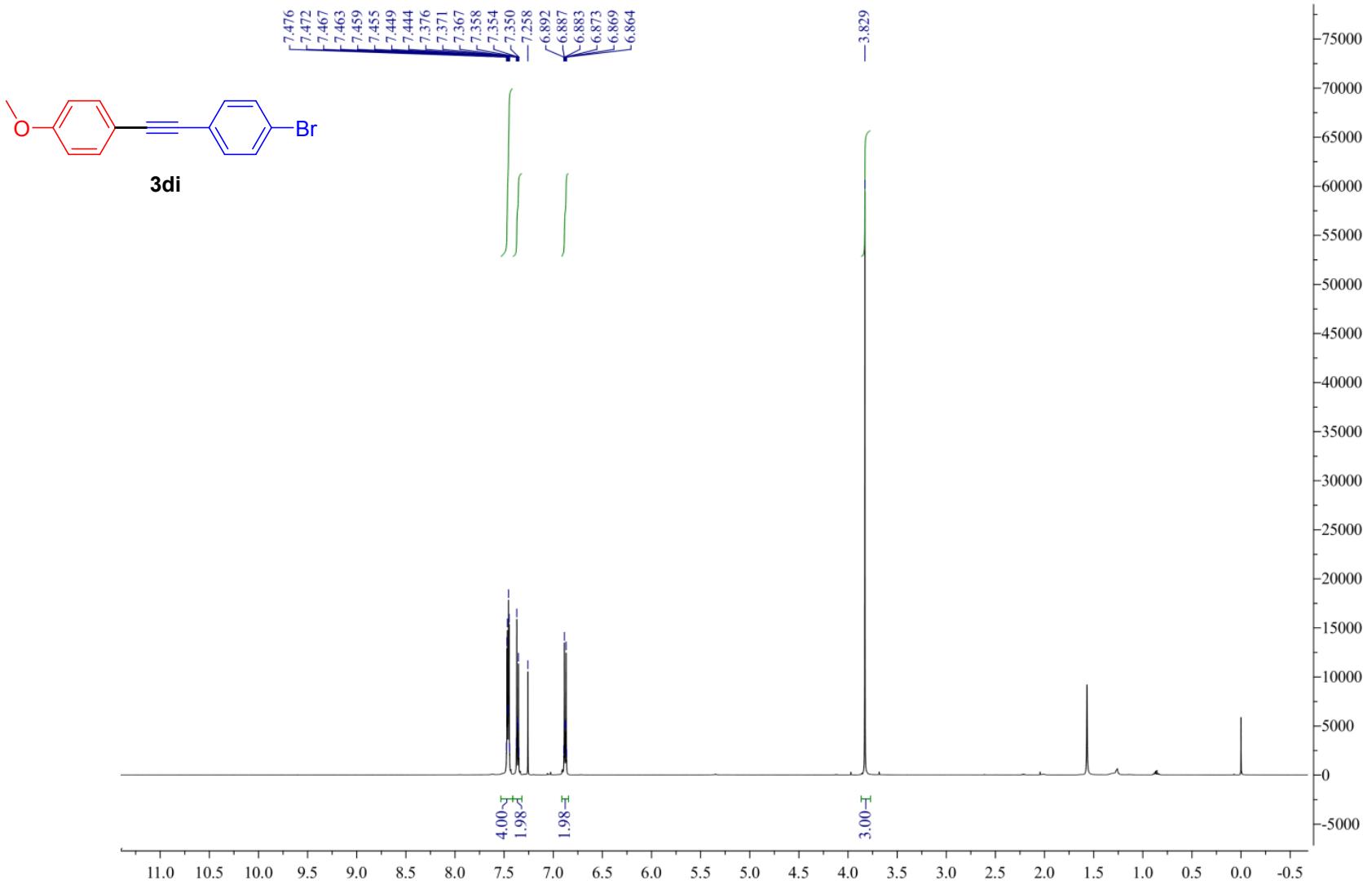

CN
3ak
132.08
132.06
131.80
129.14
128.52
128.26
122.23
118.55
111.47
93.79
87.74
77.30
77.05
76.79
f1 (ppm)

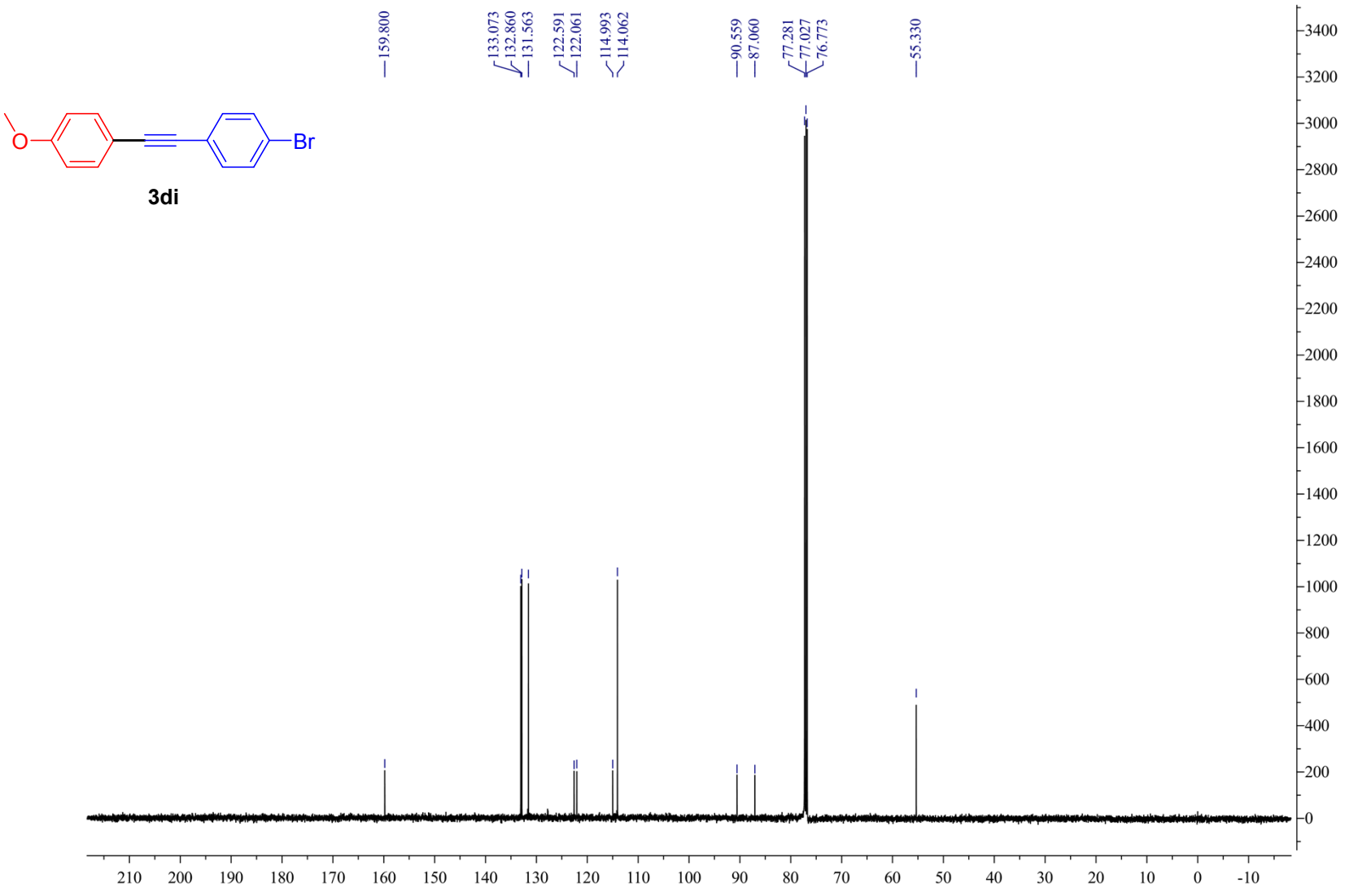

7.478
7.473
7.469
7.460
7.456
7.452
7.419
7.415
7.406
7.402
7.383
7.379
7.375
7.366
7.362
7.357
7.161
7.145
2.364
Br
3bi
1.97
1.97
1.93
1.95
3.00
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

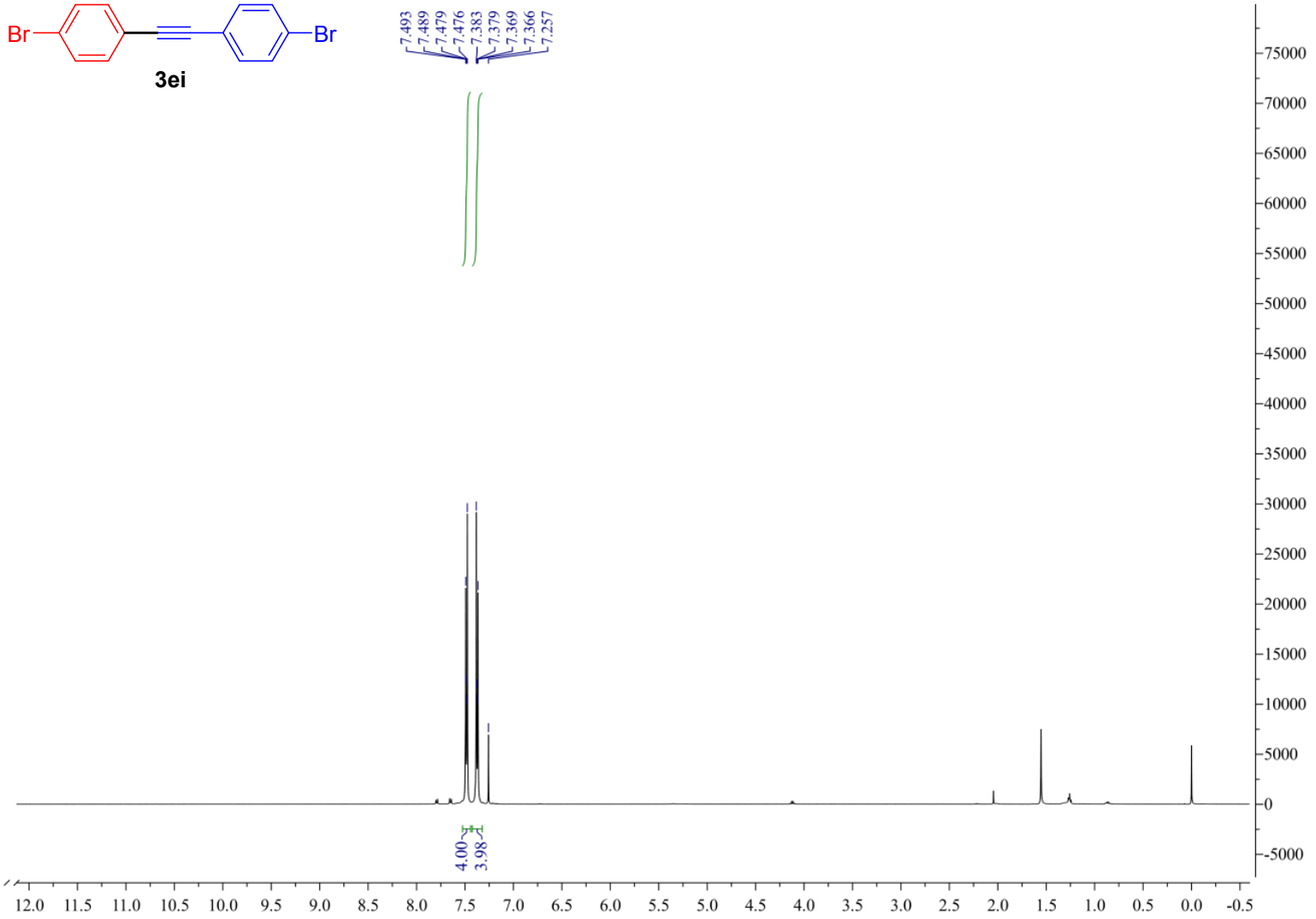

Br
3bi
138.710
131.585
131.495
129.184
122.468
122.253
119.828
90.727
87.688
21.559
3500
3000
2500
2000
1500
1000
500
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

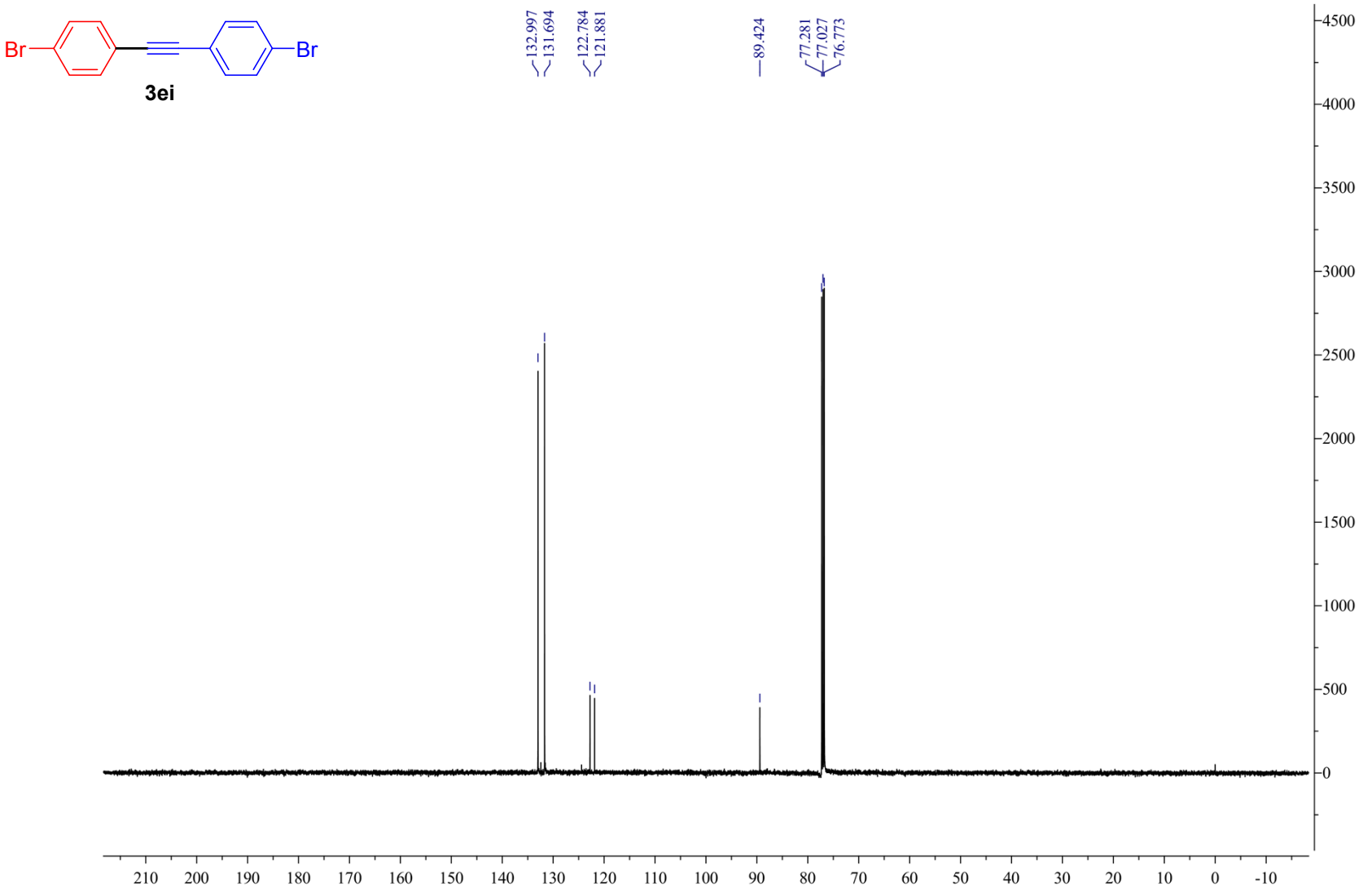

Br
3ci
7.473
7.469
7.459
7.455
7.451
7.376
7.372
7.368
7.358
7.355
7.250
7.157
7.155
6.979
6.978
2.309
2.308
2.04
2.04
2.00
1.01
6.21
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

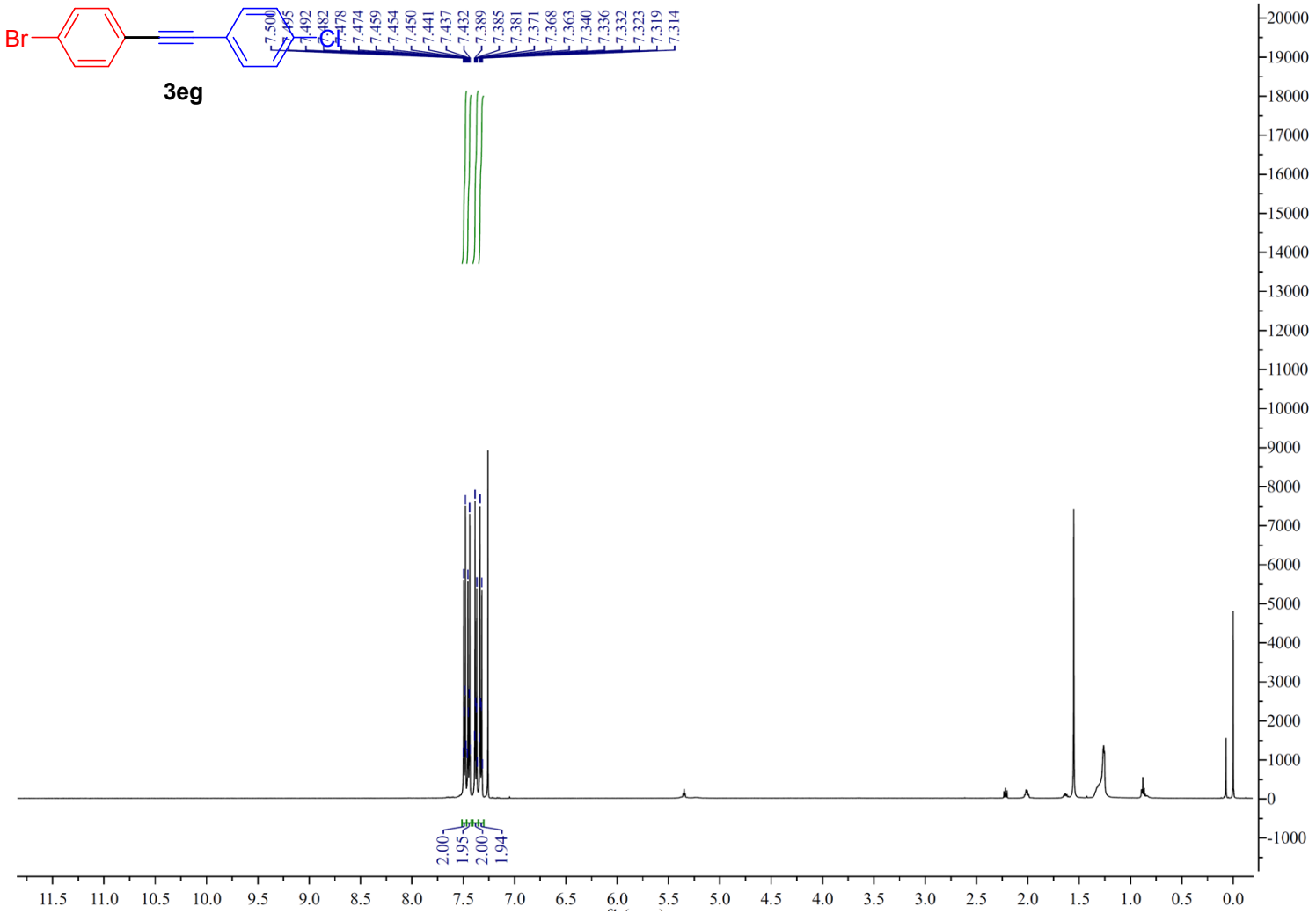

Br
3ci
137.977
131.585
129.283
122.505
122.457
122.283
90.902
87.641
21.132
137.977
132.997
131.585
130.472
129.283
122.505
122.457
122.283
f1 (ppm)

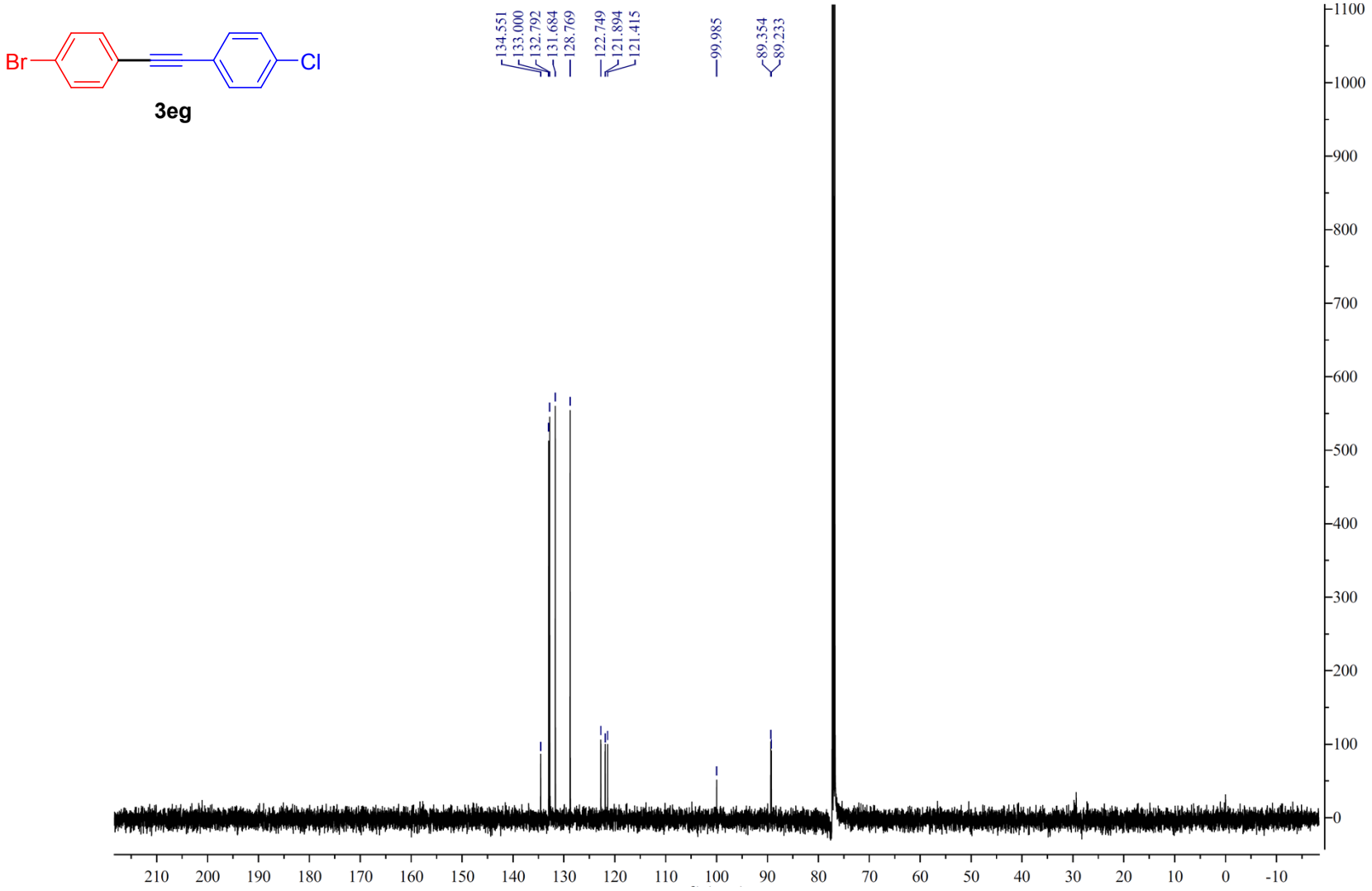

7.476
7.472
7.467
7.463
7.459
7.455
7.449
7.444
7.376
7.371
7.367
7.358
7.354
7.350
7.258
6.892
6.887
6.883
6.873
6.869
6.864
3.829
O
Br
3di
4.00
1.98
1.98
3.00

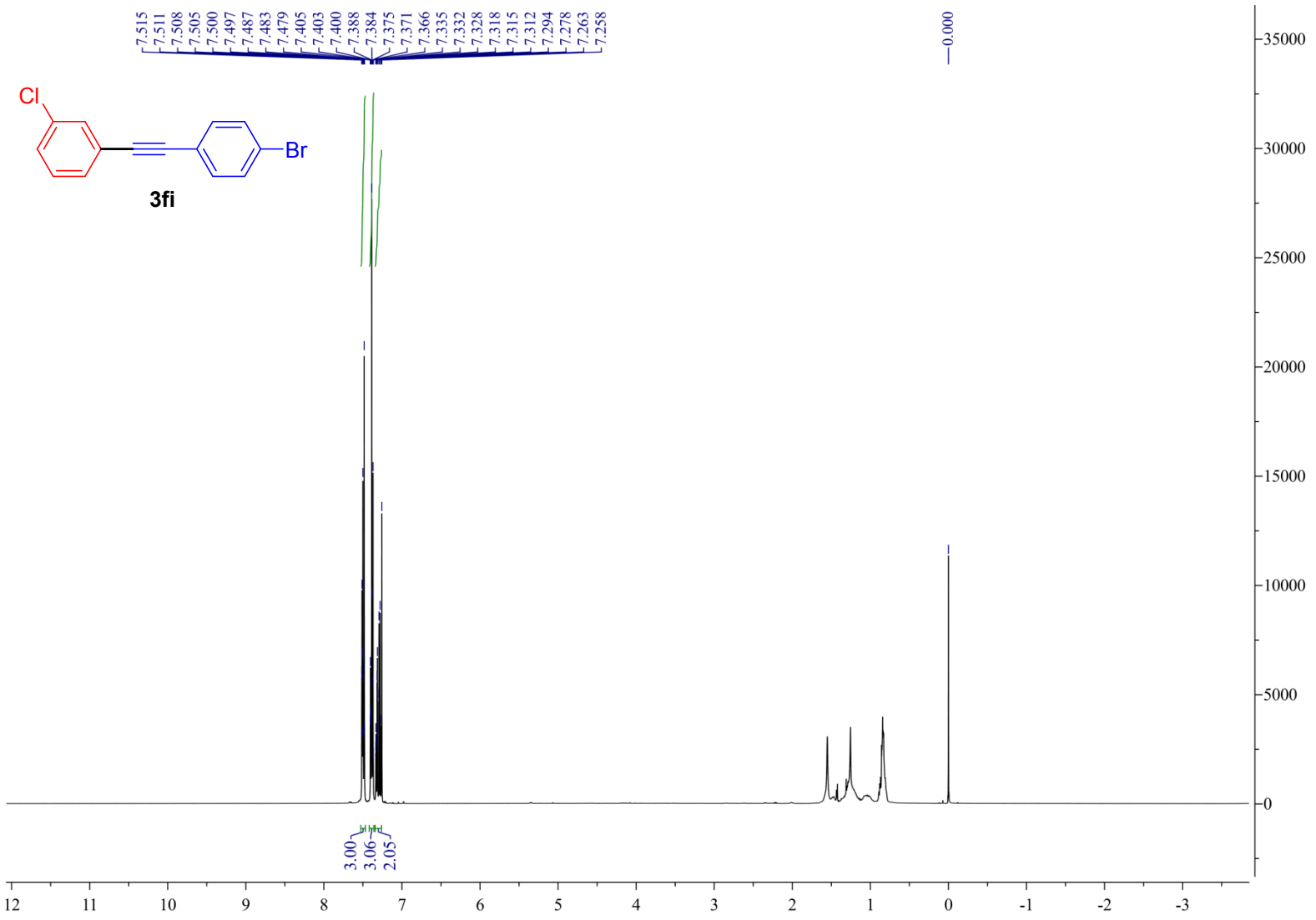

O
Br
3di
159.800
133.073
132.860
131.563
122.591
122.061
114.993
114.062
90.559
87.060
77.281
77.027
76.773
55.330

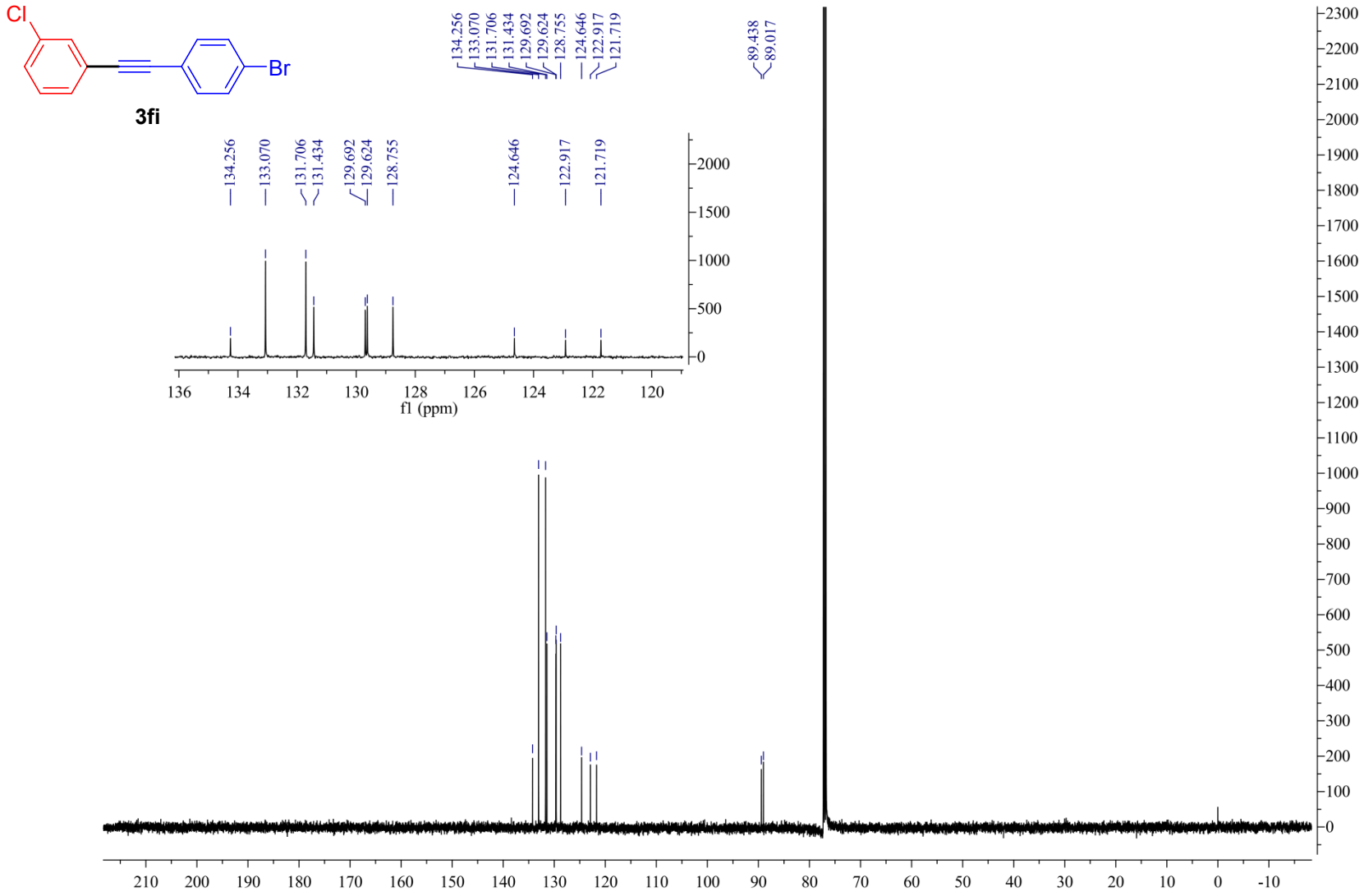

Br
Br
3ei
7.493
7.489
7.479
7.476
7.383
7.379
7.369
7.366
7.257
4.00
3.98
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

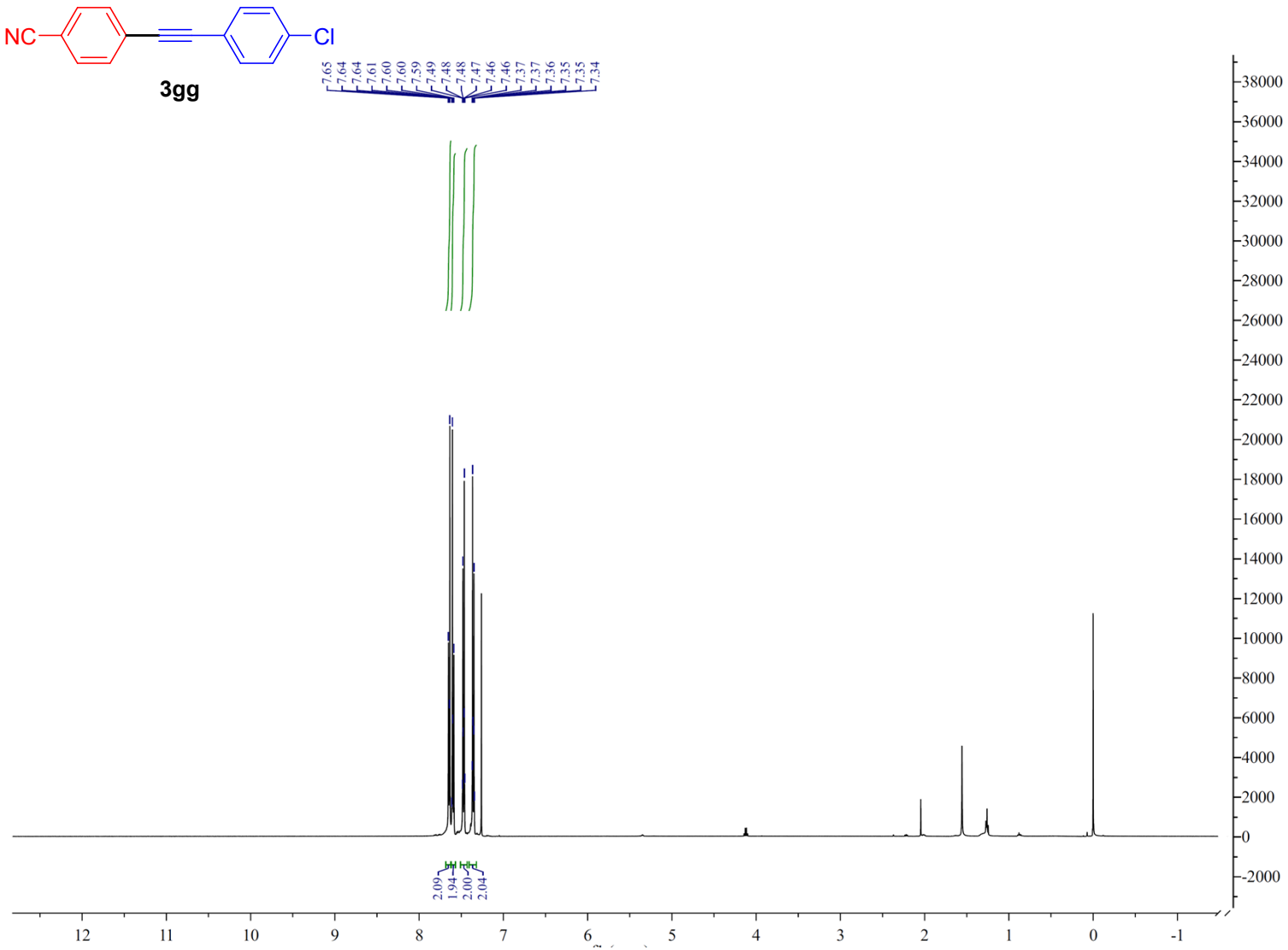

Br
Br
3ei
132.997
131.694
122.784
121.881
89.424
77.281
77.027
76.773
4500
4000
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

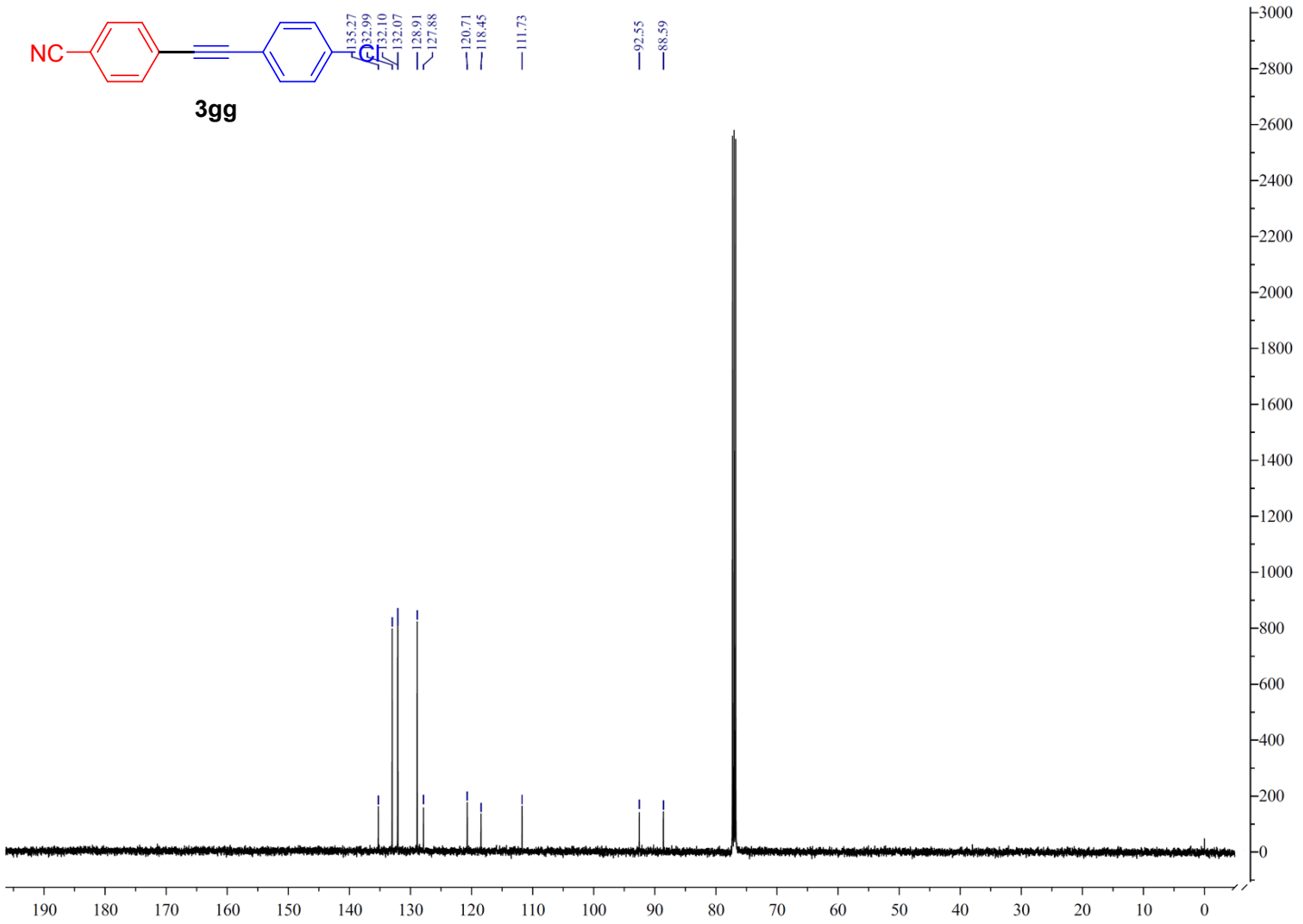

Br
Cl
3eg
7.500
7.495
7.492
7.482
7.478
7.474
7.459
7.454
7.450
7.441
7.437
7.432
7.389
7.385
7.381
7.371
7.368
7.363
7.340
7.336
7.332
7.323
7.319
7.314
2.00
1.95
2.00
1.94

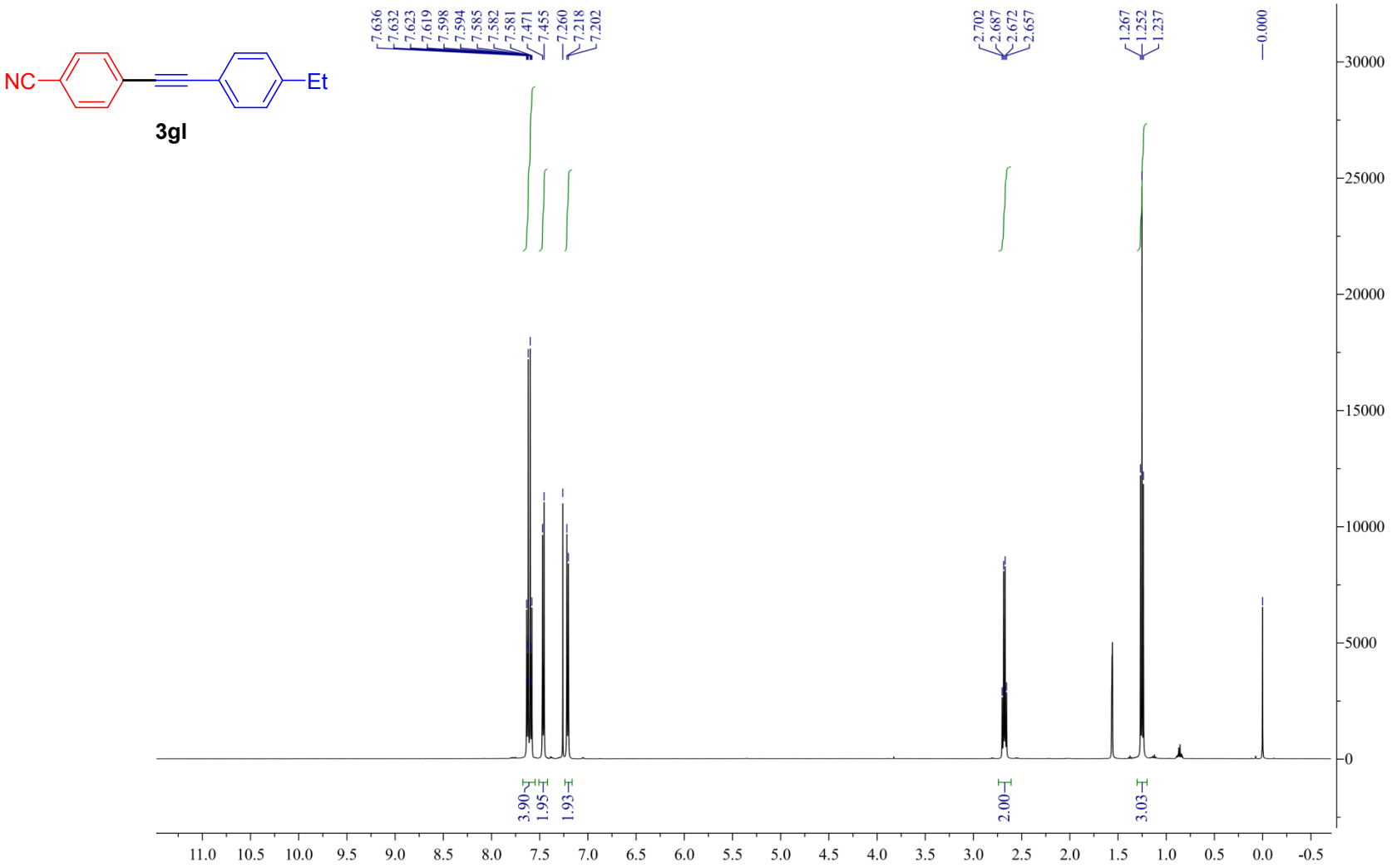

Br
Cl
3eg
134.551
133.000
132.792
131.684
128.769
122.749
121.894
121.415
99.985
89.354
89.233
1100
1000
900
800
700
600
500
400
300
200
100
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

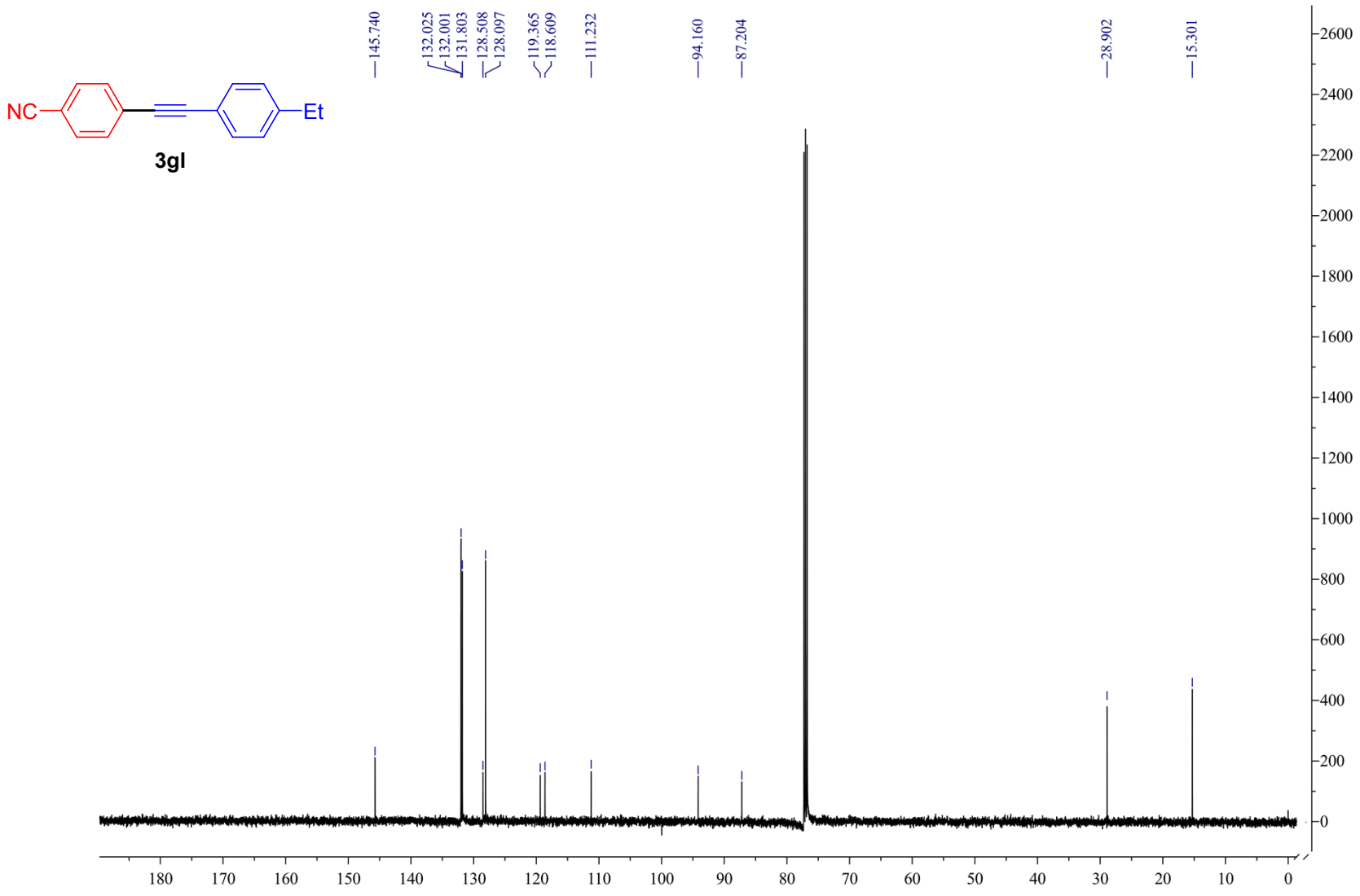

7.515
7.511
7.508
7.505
7.500
7.497
7.487
7.483
7.479
7.405
7.403
7.400
7.388
7.384
7.375
7.371
7.366
7.335
7.332
7.328
7.318
7.315
7.312
7.294
7.278
7.263
7.258
0.000
Cl
Br
3fi
3.00
3.06
2.05
35000
30000
25000
20000
15000
10000
5000
0
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3

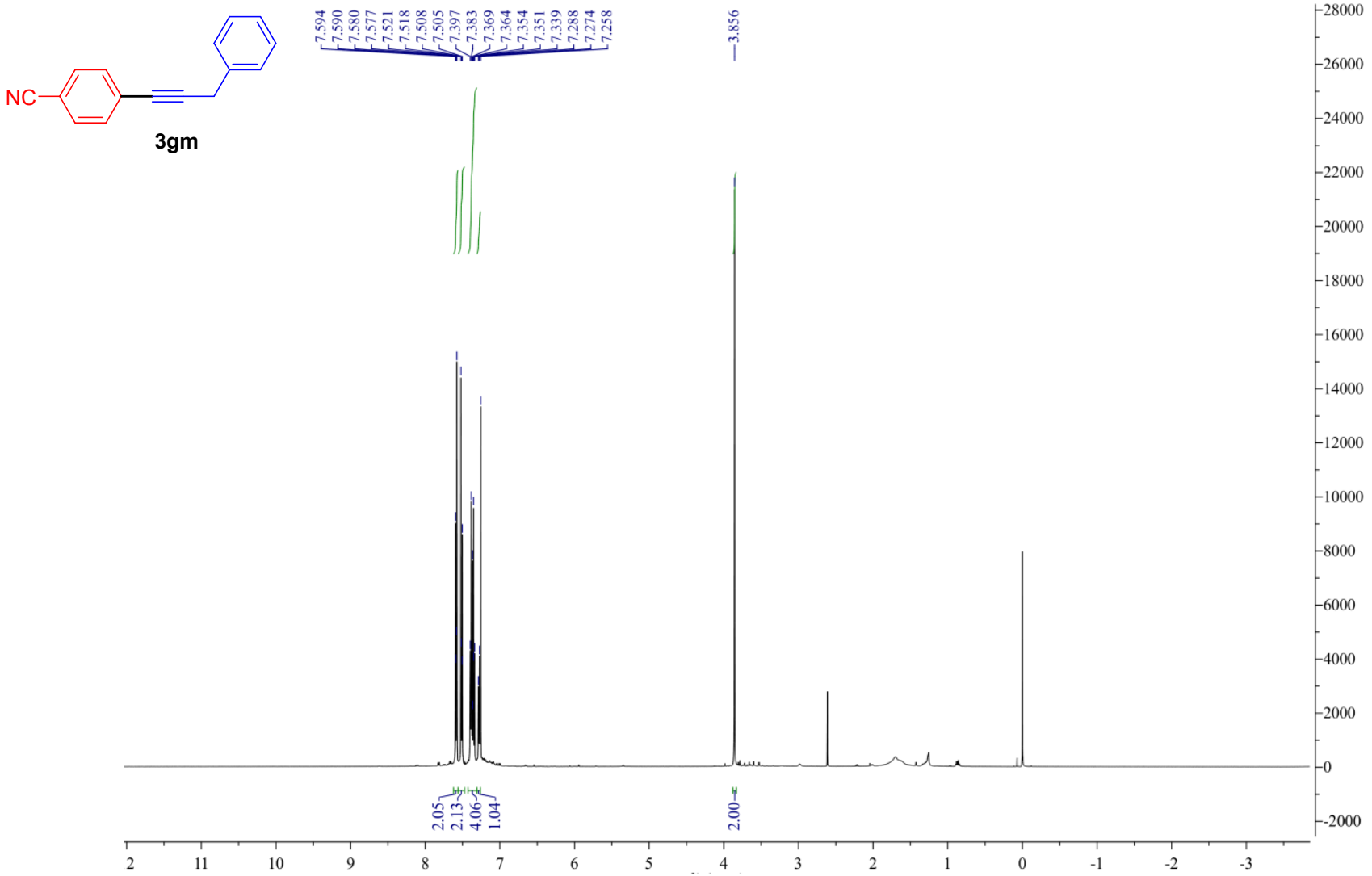

Cl
Br
3fi
134.256
133.070
131.706
131.434
129.692
129.624
128.755
124.646
122.917
121.719
89.438
89.017
fl (ppm)

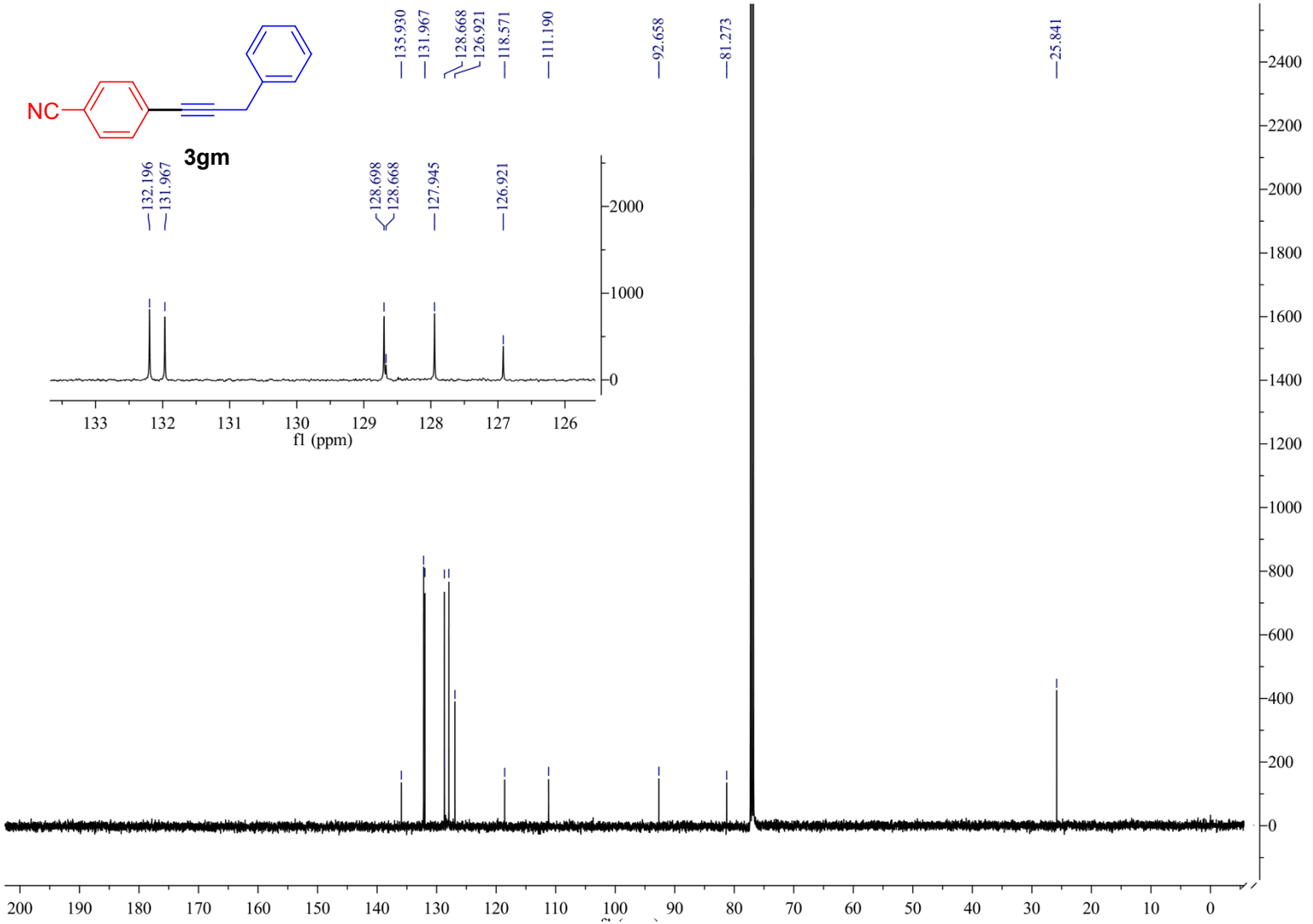

NC
Cl
3gg
7.65
7.64
7.64
7.61
7.60
7.60
7.59
7.49
7.48
7.48
7.47
7.46
7.46
7.37
7.37
7.36
7.35
7.35
7.34
2.09
1.94
2.00
2.04
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
12
11
10
9
8
7
6
5
4
3
2
1
0
-1


NC
Cl
135.27
132.99
132.10
132.07
128.91
127.88
120.71
118.45
111.73
92.55
88.59
3gg
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


NC
Et
3gl
7.636
7.632
7.623
7.619
7.598
7.594
7.585
7.582
7.581
7.471
7.455
7.260
7.218
7.202
2.702
2.687
2.672
2.657
1.267
1.252
1.237
0.000
3.90
1.95
1.93
2.00
3.03


NC
Et
3gl
145.740
132.025
132.001
131.803
128.508
128.097
119.365
118.609
111.232
94.160
87.204
28.902
15.301
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


NC
3gm
7.594
7.590
7.580
7.577
7.521
7.518
7.508
7.505
7.397
7.383
7.369
7.364
7.354
7.351
7.339
7.288
7.274
7.258
3.856
2.05
2.13
4.06
1.04
2.00


NC
3gm
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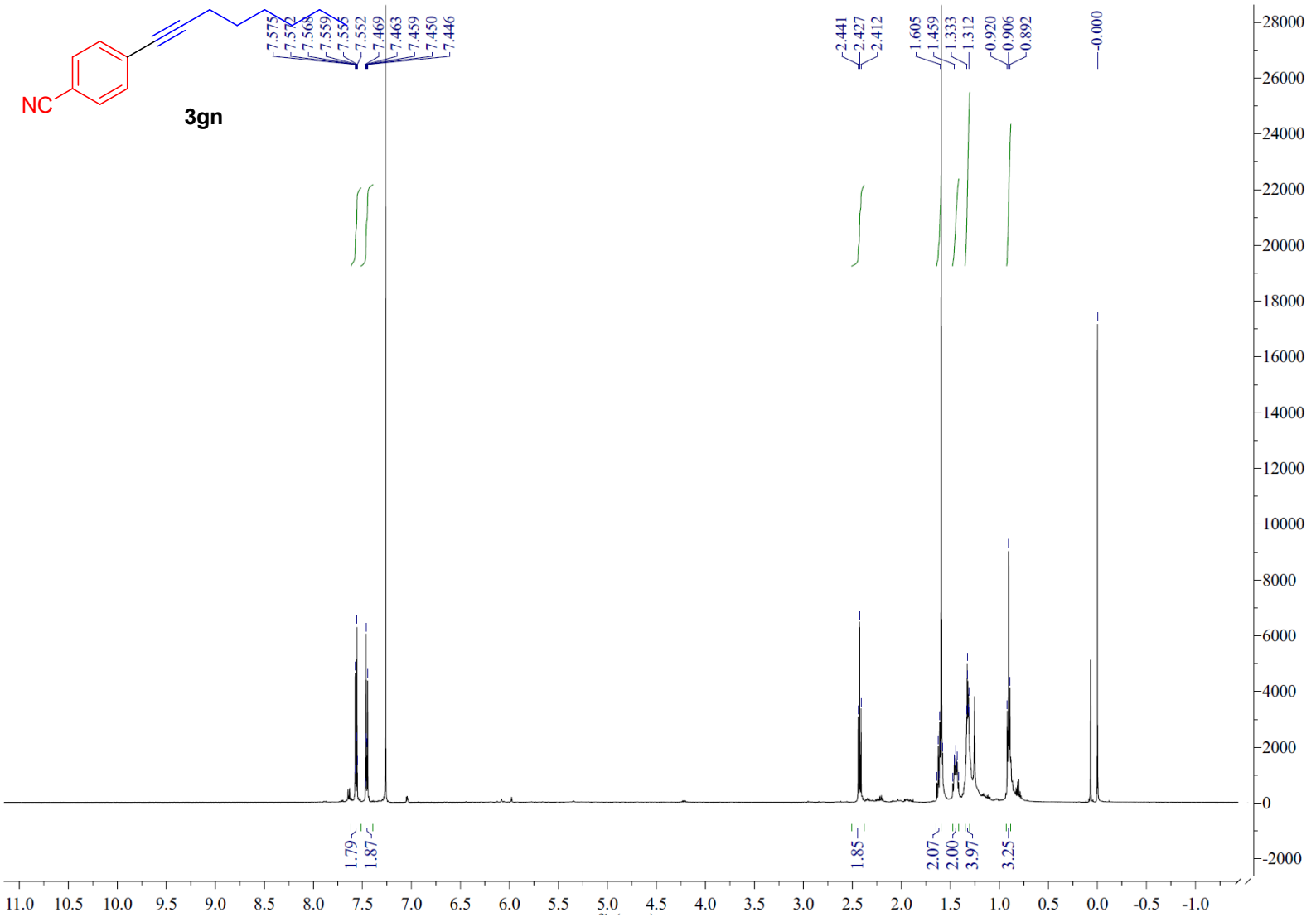
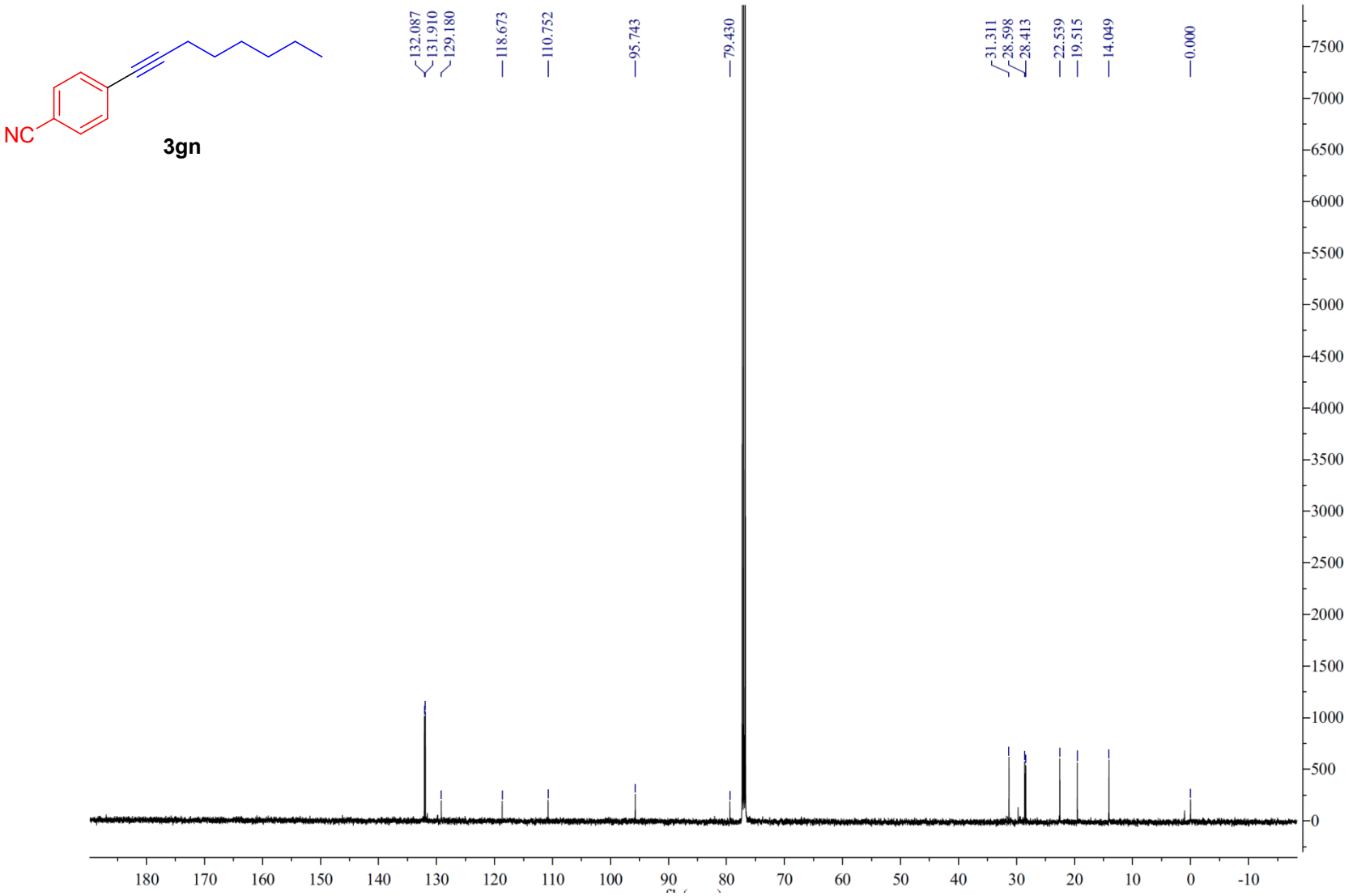
131.967
128.668
126.921
118.571
111.190
92.658
81.273
25.841
132.196
131.967
128.698
128.668
127.945
126.921
f1 (ppm)


NC
3gn
7.575
7.572
7.568
7.559
7.555
7.552
7.469
7.463
7.459
7.450
7.446
2.441
2.427
2.412
1.605
1.459
1.333
1.312
0.920
0.906
0.892
-0.000
1.79
1.87
1.85
2.07
2.00
3.97
3.25


NC
3gn
132.087
131.910
129.180
118.673
110.752
95.743
79.430
31.311
28.598
28.413
22.539
19.515
14.049
0.000