Supporting Information

for

Au(I)/Au(III)-catalyzed Sonogashira-type reactions of functionalized terminal alkynes with arylboronic acids under mild conditions

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Experimental details and spectra of new compounds

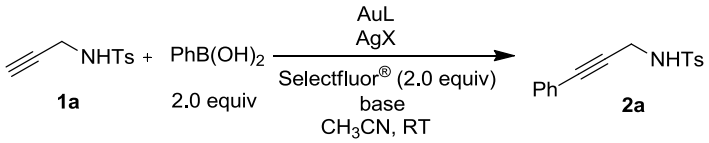
1. General information

Unless otherwise noted, commercial materials were directly used without further purification. Anhydrous acetonitrile (MeCN) and triethylamine (NEt_3) were distilled from CaH_2 under a nitrogen atmosphere prior to use. Reactions were monitored by thin layer chromatography (TLC) using Whatman® pre-coated silica gel plates. Flash column chromatography was performed on SiliCycle® silica gel (230–400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker 400 MHz spectrometer and chemical shifts are reported in ppm, relative to $CHCl_3$ (7.26 ppm for ^{1}H, and 77.00 ppm for ^{13}C) unless otherwise noted. Splitting patterns of an apparent multiplet associated with an averaged coupling constant were designed as s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet).

2. General procedure for conditions screening

Propargyl tosylamide **1a** (83.7 mg, 0.4 mmol) was dissolved in MeCN (2 mL) and $PhB(OH)_2$ (97.5 mg, 0.8 mmol), the gold catalyst (5 mol % or 2.5 mol %) and base (1.05 equiv) added followed by Selectfluor® (283.4 mg, 0.8 mmol). The reaction mixture was stirred at room temperature for 10–24 h and the reaction was monitored by TLC. After completion, the reaction mixture was diluted with EtOAc and filtered through a pad of celite. The filtrate was concentrated under reduced pressure and the crude product purified by chromatography on silica gel (using hexanes/EtOAc as eluent).

Table S1:

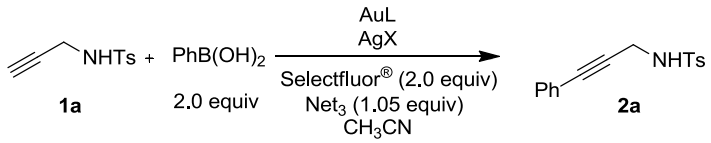


entry	AuL (mol %)	AgX (mol %)	base (equiv)	t (h)	Yield (%)
1	Ph_3PAuCl (5)	-	Et_3N (1.05)	22	trace
2	Ph_3PAuCl (5)	AgOTf (5)	Et_3N (1.05)	18	56
3	AuCl (5)	AgOTf (5)	Et_3N (1.05)	24	21
4	-	AgOTf (5)	Et_3N (1.05)	24	0
5[b]	Ph_3PAuCl (5)	AgOTf (5)	Et_3N (1.05)	22	0
6[c]	Ph_3PAuCl (5)	AgOTf (5)	Et_3N (1.05)	22	41
7	Ph_3PAuCl (5)	$AgBF_4$ (5)	Et_3N (1.05)	10	65

8	Ph_3PAuCl (5)	$AgSbF_4$(5)	Et_3N (1.05)	10	62
9	Ph_3PAuCl (5)	$AgNO_3$(5)	Et_3N (1.05)	10	45[a]
10	Ph_3PAuCl (5)	$AgPF_6$(5)	Et_3N (1.05)	10	40[a]
11	Ph_3PAuCl (5)	AgOAc(5)	Et_3N (1.05)	10	0
12	Ph_3PAuCl (5)	$AgBF_4$ (5)	Et_3N (1.2)	10	69[a]
13	dppf$(AuCl)_2$ (2.5)	AgOTf (5)	Et_3N (1.05)	14	39[a]
14	dppp$(AuCl)_2$ (2.5)	AgOTf (5)	Et_3N (1.05)	14	56 (65[a])
15	dppp$(AuCl)_2$ (2.5)	$AgBF_4$ (5)	Et_3N (1.05)	14	0
16	dppe$(AuCl)_2$ (2.5)	AgOTf (5)	Et_3N (1.05)	14	48[a]
17	dppb$(AuCl)_2$ (2.5)	AgOTf (5)	Et_3N (1.05)	14	65[a]
18	dppp$(AuCl)_2$ (5)	AgOTf (5)	Et_3N (1.05)	16	59[a]
19	dppp$(AuCl)_2$ (5)	AgOTf (5)	$K_3PO_4 \cdot 3H_2O$ (1.5)	22	59
20	dppp$(AuCl)_2$ (5)	AgOTf (5)	$K_3PO_4 \cdot 3H_2O$ (1.5)+ Et_3N (0.5)	22	47
21	dppp$(AuCl)_2$ (5)	AgOTf (5)	K_2CO_3 (1.5)	22	34
22	Ph_3PAuCl (5)	AgOTf (5)	Et_3N (1.5)	22	53
23	Ph_3PAuCl (5)	AgOTf (5)	iPr_2NH (1.05)	12	trace
24	Ph_3PAuCl (5)	AgOTf (5)	Bu_3N (1.05)	12	trace
25	Ph_3PAuCl (5)	AgOTf (5)	TMEDA (1.05)	12	trace
26	Ph_3PAuCl (5)	AgOTf (5)	$PhNMe_2$ (1.05)	12	ND

[a]Yield determined by ^1H NMR. [b]Selectfluor® (0 equiv). [c]$PhB(OH)_2$ (1.5 equiv).

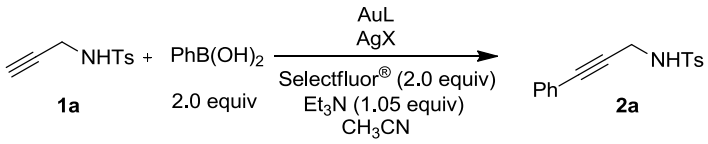
Table S2:



entry	1a (mmol)	AuL (mol %)	AgX (mol %)	T (°C)	t (h)	product (yield %)
1	0.4	(XPhos)AuCl (5)	AgOTf (5)	RT	24	trace
2[a]	0.4	(XPhos)AuCl (5)	AgOTf (5)	RT	24	trace
3	0.4	Ph_3PAuCl (5)	$AgBF_4$ (5)	55	3.5	63
4[b]	0.48	Ph_3PAuCl (5)	$AgBF_4$ (5)	RT	24	trace
5[c]	0.4	Ph_3PAuCl (5)	$AgBF_4$ (5)	RT	24	trace
6[d]	0.48	Ph_3PAuCl (5)	AgOTf (5)	RT	24	ND
7	0.4	Ph_3PAuCl (5)	AgOTf (5)	40	24	46

[a]base: $K_3PO_4 \cdot 3H_2O$ (1.5 equiv). [b]S: $PhB(OH)_2$ = 1.2: 1. [c]**1a**: $PhB(OH)_2$ = 1.5: 1. [d]**1a**: $PhB(OH)_2$ = 1.5: 1.

Table S3[a]:

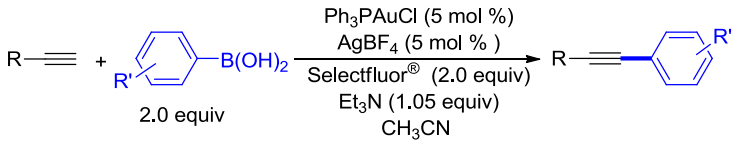


entry	1a (mmol)	AuL (mol %)	AgX (mol %)	T (°C)	t (h)	product (yield %)
1	0.4	Ph_3PAuCl (5)	AgOTf (5)	50	12	72 (73[b])
2	0.4	Ph_3PAuCl (5)	AgOTf (5)	rt	12	59[b]
3	0.2	Ph_3PAuCl (5)	$AgBF_4$ (5)	rt	12	80[b]

4	0.2	Ph_3PAuCl (5)	$AgPF_6$ (5)	rt	16	40[b]
5	0.2	Ph_3PAuCl (5)	AgOAc (5)	rt	16	0
6	0.4	Ph_3PAuCl (5)	$AgBF_4$ (5)	rt	12	75(80[b])
7	0.4	Ph_3PAuCl (5)	AgOTf (5)	rt	16	70[b]
8	0.2	dppm$(AuCl)_2$ (5)	AgOTf (5)	rt	16	83[b]
9	0.4	dppm$(AuBr)_2$ (5)	-	rt	16	trace

[a]The reaction was carried out under an atmosphere of nitrogen (N_2). [b]Yield determined by ^1H NMR.

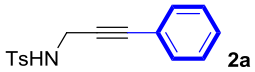
3. General procedure



All reactions were carried out under an atmosphere of nitrogen (N_2).

The alkyne (83.7 mg, 0.4 mmol) was dissolved in MeCN (2 mL), $PhB(OH)_2$ (97.5 mg, 0.8 mmol), Ph_3PAuCl (5 mol %), $AgBF_4$ (5 mol %) and Et_3N (1.05 equiv) were added followed by Selectfluor® (283.4 mg, 0.8 mmol). The reaction mixture was stirred at the noted temperature for 12–45 h and the reaction monitored by TLC. After completion, the reaction mixture was diluted with EtOAc and filtered through a pad of celite. The filtrate was concentrated under reduced pressure and the crude product was purified by chromatography on silica gel (using hexanes/EtOAc as eluents).

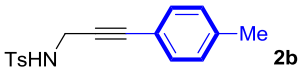
(1) *N*-(3-Phenylprop-2-ynyl)-*p*-toluenesulfonamide (2a)



2a

The reaction of propargyl tosylamide **1a** and phenylboronic acid was carried out at room temperature for 12 h to afford compound **2a** (hexanes/EtOAc = 3/1) in 75% yield as a pale orange solid. Its spectroscopic data were in accord with those reported in the literature [1]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.30–7.22 (m, 5H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.88 (t, *J* = 5.6 Hz, 1H), 4.06 (d, *J* = 6.4 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 136.8, 131.5, 129.7, 128.4, 128.1, 127.5, 122.0, 84.7, 83.2, 33.7, 21.4.

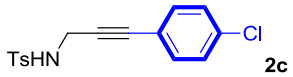
(2) 4-Methyl-*N*-(3-*p*-tolylprop-2-ynyl)benzenesulfonamide (2b)



2b

The reaction of propargyl tosylamide **1b** and phenylboronic acid was carried out at room temperature for 18 h to afford compound **2b** (hexanes/EtOAc = 5/1) in 70% yield as a white solid. Its spectroscopic data were in accord with those reported in the literature [2]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.6 Hz, 2H), δ 7.26 (d, *J* = 8.0 Hz, 2H), 7.05–7.00 (m, 4H), 4.88 (t, *J* = 6.0 Hz, 1H), 4.06 (d, *J* = 6.0 Hz, 2H), 2.36 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 138.6, 136.8, 131.4, 129.6, 128.9, 127.4, 118.9, 84.8, 82.5, 33.8, 21.42, 21.40. EI-MS (*m*/*z*, relative intensity): 299 (M^+, 2.99), 91 (100). HRMS (EI) calcd. for $[C_{17}H_{17}NO_2S]^+$: 299.0980, found 299.0984.

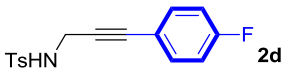
(3) *N*-[3-(4-Chlorophenyl)-prop-2-ynyl]-*p*-toluenesulfonamide (2c)



2c

The reaction of propargyl tosylamide **1c** and 4-chlorophenylboronic acid was carried out at 50 °C for 12 h to afford **2c** (hexanes/EtOAc = 5/1) in 89% yield as a white solid. Its spectroscopic data were in accord with those reported in the literature [3]. ^{1}H NMR (400 MHz, CDCl3) δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 7.6 Hz, 2H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 4.85 (t, *J* = 6.0 Hz, 1H), 4.06 (d, *J* = 6.0 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 136.8, 134.6, 132.7, 129.7, 128.5, 127.5, 120.5, 84.2, 83.6, 33.7, 21.5. EI-MS (*m*/*z*, relative intensity): 319 (M^+, 1.89), 164 (100). HRMS (EI) calcd. for $[C_{16}H_{14}NO_2SCl]^+$: 319.0434, found 319.0441.

(4) *N*-[3-(4-Fluorophenyl)-prop-2-ynyl]-*p*-toluenesulfonamide (2d)

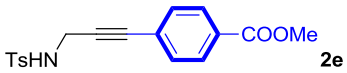


2d

The reaction of propargyl tosylamide **1d** and phenylboronic acid was carried out at 50 °C for 12 h to afford **2d** (hexanes/EtOAc = 5/1) in 58% yield as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.13–7.10 (m, 2H), 7.00–6.92 (m, 2H), 4.82 (s, 1H), 4.07 (d, *J* = 6.0 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5 (d, $^{1}J_{C,F}$ = 248 Hz), 143.7, 136.8, 133.5, 133.4, 129.6, 127.5, 118.1, 115.4 (d, $^{2}J_{C,F}$ = 22 Hz), 83.6, 83.0, 33.6, 21.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ 110.33. EI-MS (*m*/*z*, relative intensity): 303 (M^+, 0.78), 148 (100). HRMS (EI) calcd. for

$[C_{16}H_{14}NO_2SF]^+$: 303.0729, found 303.0732.

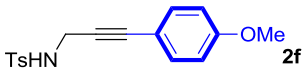
(5) Methyl 4-[3-(4-methylphenylsulfonamido)prop-1-ynyl]benzoate (2e)



2e

The reaction of propargyl tosylamide **1e** and 4-(methoxycarbonyl)-phenylboronic acid was carried out at 50 °C for 12 h to afford **2e** (hexanes/EtOAc = 5/1) in 66% yield as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.6 Hz, 2H), 7.81 (d, *J* = 7.2 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 7.6 Hz, 2H), 4.87 (t, *J* = 5.6 Hz, 1H), 4.10 (d, *J* = 5.6 Hz, 2H), 3.92 (s, 3 H), 2.36 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 143.7, 136.8, 131.4, 129.6, 129.2, 127.5, 126.7, 86.3, 83.8, 52.3, 33.6, 21.4. EI-MS (*m*/*z*, relative intensity): 343 (M^+, 1), 188 (100). HRMS (EI) calcd. for $[C_{18}H_{17}NO_4S]^+$: 343.0878, found 343.0879.

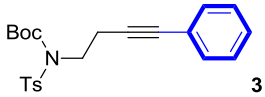
(6) *N*-[3-(4-Methoxyphenyl)-prop-2-ynyl]-*p*-toluenesulfonamide (2f)



2f

The product could not be separated from the unreacted starting material. Based on the ^{1}H NMR of the mixture, **2f** was produced in 31% yield.

(7) *tert*-Butyl 4-phenylbut-3-ynyl(tosyl)carbamate (3)

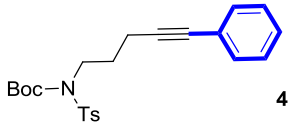


3

The reaction was carried out at 50 °C for 12 h to give **3** (hexanes/EtOAc = 5/1) in 48% yield as a viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz,

2H), 7.37 (s, 2H), 7.27 (s, 5H), 4.09 (t, *J* = 7.2 Hz, 1H), 2.88 (t, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 1.34 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.8, 144.2, 137.2, 131.6, 129.2, 128.1, 127.9, 127.8, 123.4, 86.0, 84.5, 82.5, 45.3, 27.8, 21.5, 20.8. EI-MS (*m*/*z*, relative intensity): 399 (M^+, 0.46), 128 (100). HRMS (EI) calcd. for $[C_{22}H_{25}NO_4S]^+$: 399.1504, found 399.1471.

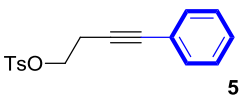
(8) *tert*-Butyl 5-phenylpent-4-ynyl(tosyl)carbamate (4)



4

The reaction was run at 50 °C for 12 h to give **4** (hexanes/EtOAc = 5/1) in 68% yield as a viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 2H), 7.41–7.40 (m, 2H), 7.31–7.27 (m, 5H), 3.98 (t, *J* = 7.2 Hz, 1H), 2.50 (t, *J* = 6.8 Hz, 2H), 2.43 (s, 3H), 2.07 (t, *J* = 6.8 Hz, 1H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 144.1, 137.3, 131.6, 129.2, 128.1, 127.8, 127.6, 123.7, 88.7, 84.2, 81.2, 46.4, 29.2, 27.8, 21.6, 17.0. EI-MS (*m*/*z*, relative intensity): 313 (M^+−100, 0.19), 57 (100). HRMS (EI) calcd. for $[C_{18}H_{19}NO_2S]^+$: 313.1137, found 313.1139.

(9) 4-Phenylbut-3-yn-1-yltosylate (5)

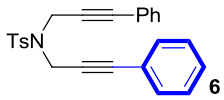


5

The reaction was run at room temperature for 12 h to give **6** (hexanes/EtOAc = 5/1) in 71% yield as a pale yellow oil. Its spectroscopic data were in accord

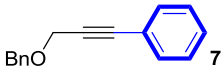
with those reported in the literature [4]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 2H), 7.32–7.26 (m, 7H), 4.19 (t, *J* = 6.8 Hz, 1H), 2.79 (t, *J* = 6.8 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 132.9, 131.7, 130.0, 128.3, 128.2, 128.0, 123.0, 83.9, 82.7, 67.8, 21.7, 20.4.

(10) 4-Methyl-*N*,*N*-bis(3-phenylprop-2-ynyl)benzenesulfonamide (6)



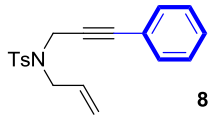
The reaction was run at room temperature for 12 h to give **6** (hexanes/EtOAc = 5/1) in 71% yield as a pale yellow oil. Its spectroscopic data were in accord with those reported in the literature [5]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.31–7.20 (m, 12H), 7.27 (s, 5H), 4.45 (s, 4H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 135.3, 131.7, 129.6, 128.5, 128.1, 128.0, 122.2, 85.8, 81.6, 37.5, 21.4.

(8) (3-Benzyloxyprop-1-ynyl)benzene (7)



The reaction was run at 50 °C for 12 h to give **7** (hexanes/EtOAc = 5/1) in 71% yield as a yellow oil. Its spectroscopic data were in accord with those reported in the literature [6]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48–7.46 (m, 2H), 7.41–7.30 (m, 8H), 4.69 (s, 2H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.4, 131.8, 128.4, 128.3, 128.1, 127.9, 122.6, 86.5, 85.0, 71.6, 57.9.

(11) *N*-Allyl-4-methyl-*N*-(3-phenylprop-2-ynyl)benzenesulfonamide (8)



8

The reaction was run at room temperature for 12 h to give **8** (hexanes/EtOAc = 5/1) in 82% yield as a white solid. Its spectroscopic data were in accord with those reported in the literature [7]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.6 Hz, 2H), 7.30–7.22 (m, 5H), 7.05 (d, *J* = 7.2 Hz, 2H), 5.87–5.73 (m, 1H), 5.35–5.27 (m, 2H), 4.31 (s, 2H), 3.88 (d, *J* = 6.4 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 135.8, 132.0, 131.4, 129.5, 128.4, 128.1, 127.8, 122.1, 120.0, 85.7, 81.6, 49.2, 36.7, 21.4.

4. References

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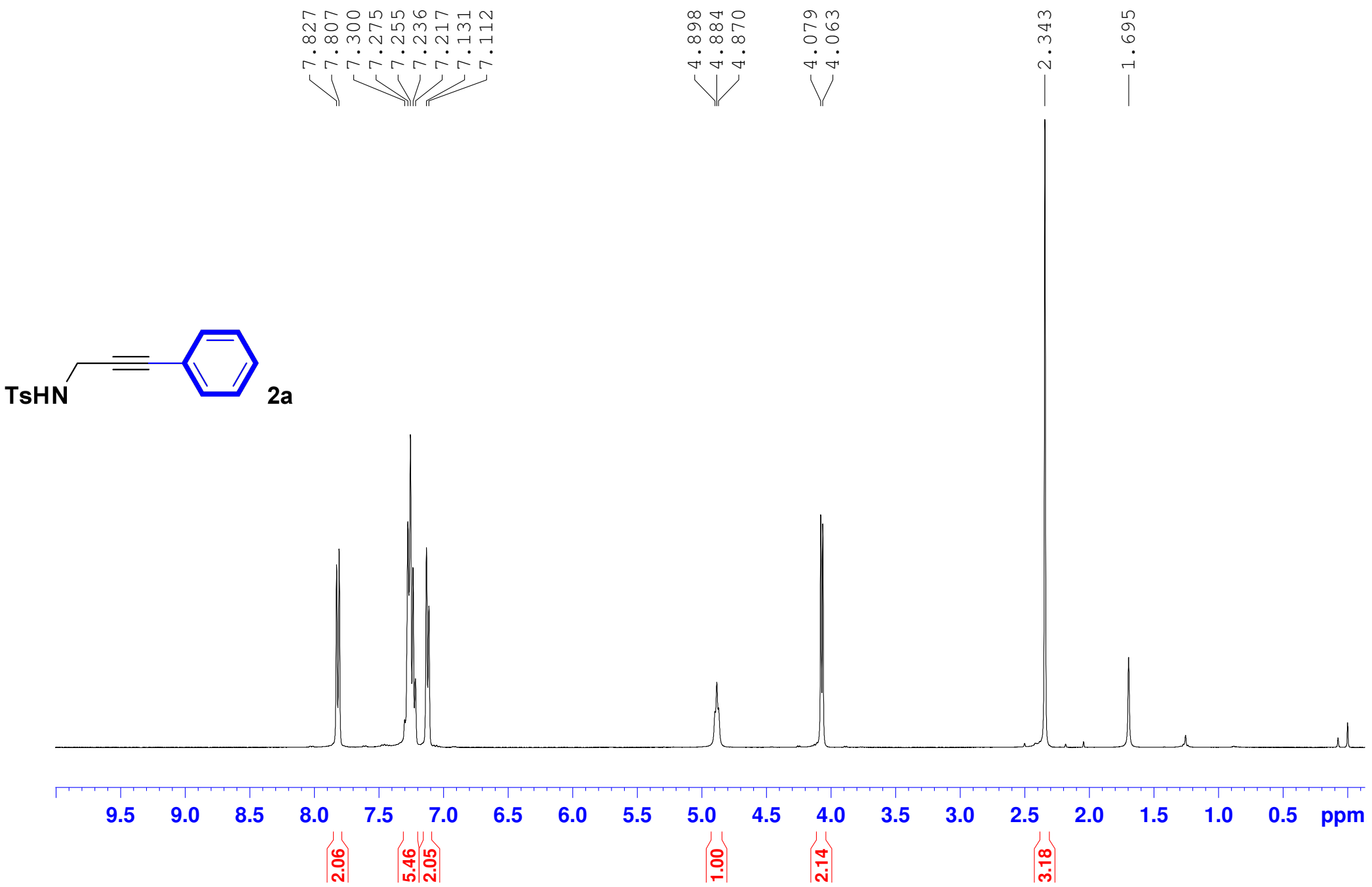
5. ^{1}H and ^{13}C NMR spectra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4.079
4.063
2.343
1.695
TsHN
2a
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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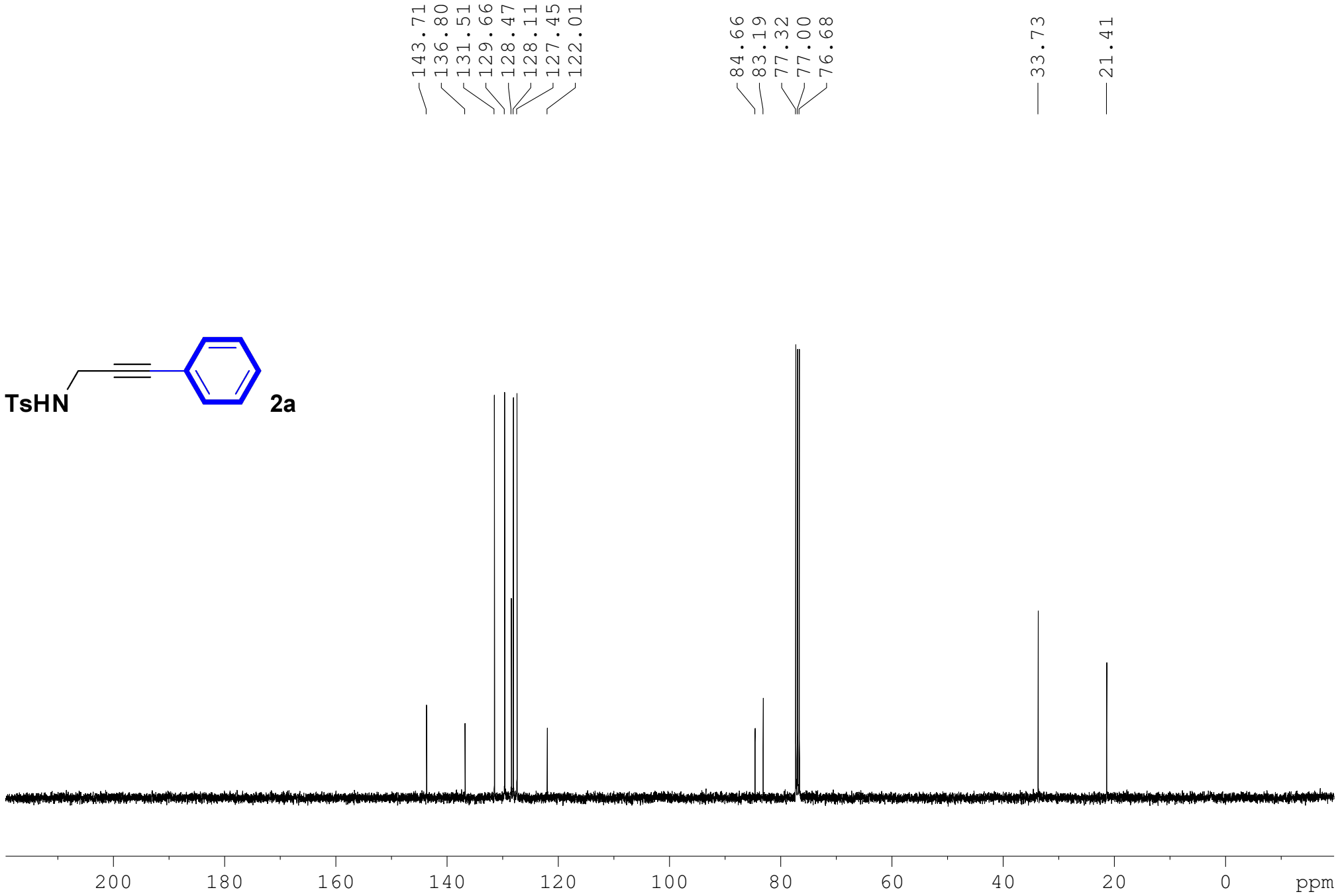
3.18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83.19
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120
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40
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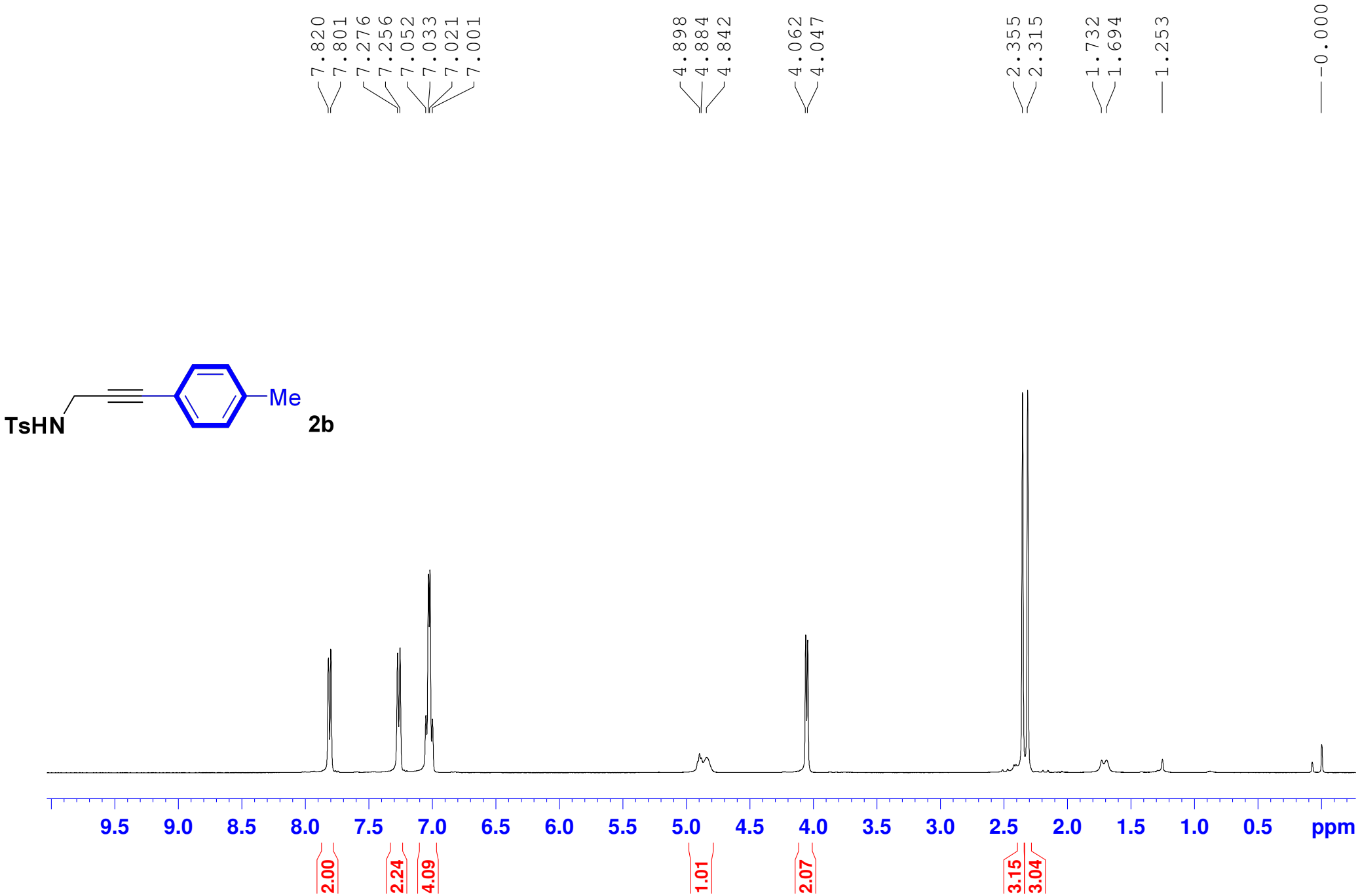
0
ppm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2.355
2.315
1.732
1.694
1.253
0.000
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Me
2b
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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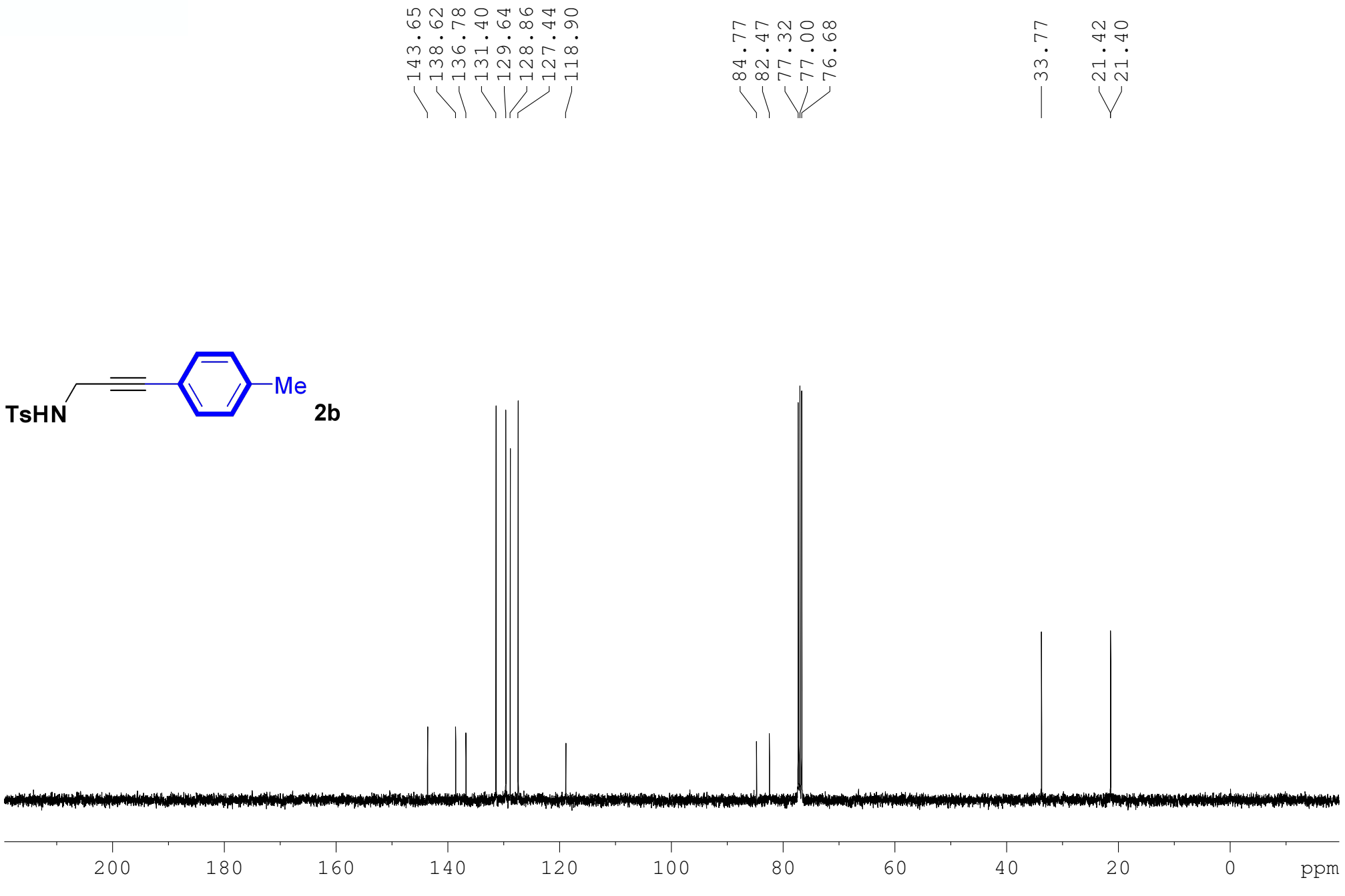
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127.44
118.90
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82.47
77.32
77.00
76.68
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TsHN
Me
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140
120
100
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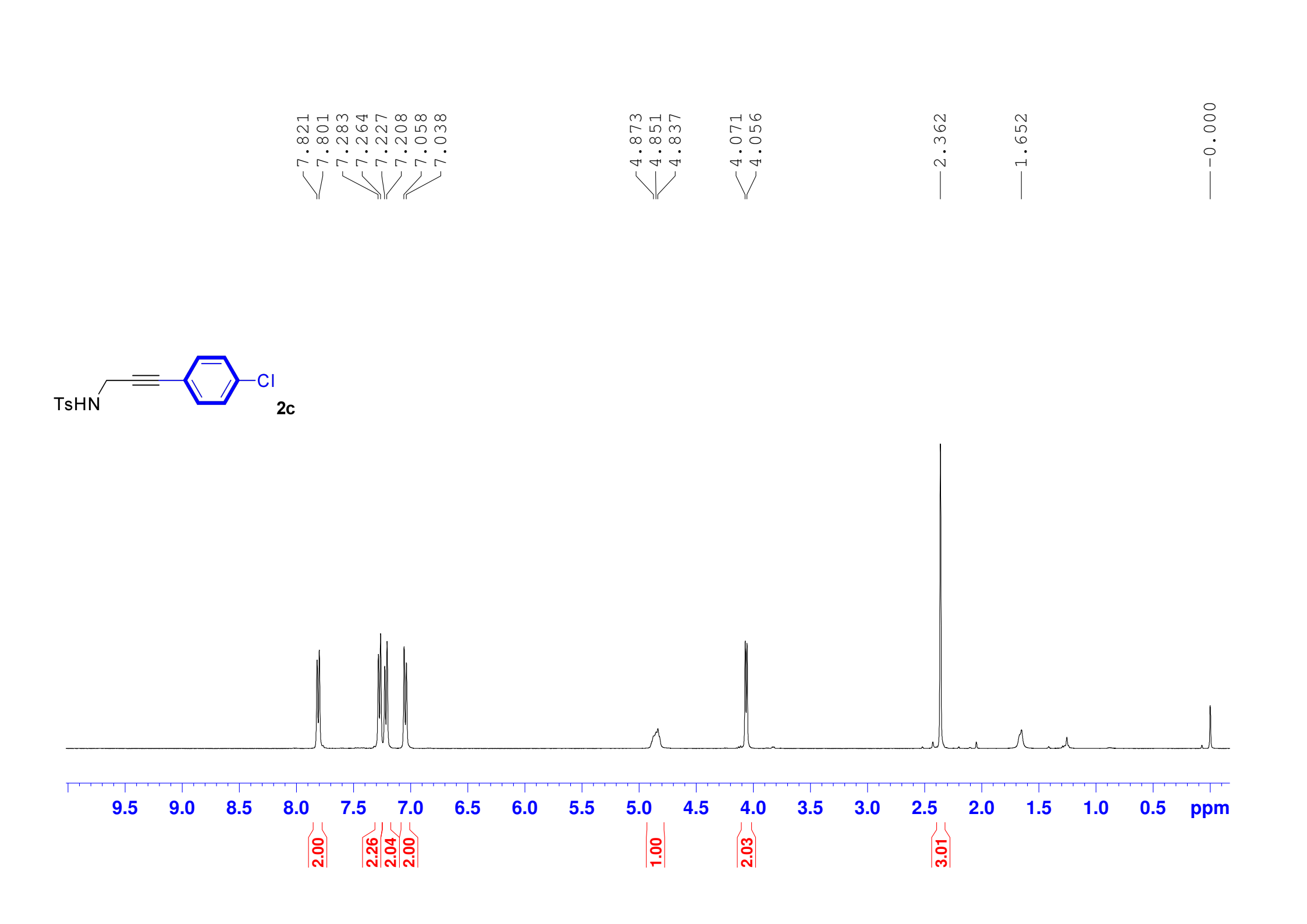
60
40
20
0
ppm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4.056
2.362
1.652
0.000
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Cl
2c
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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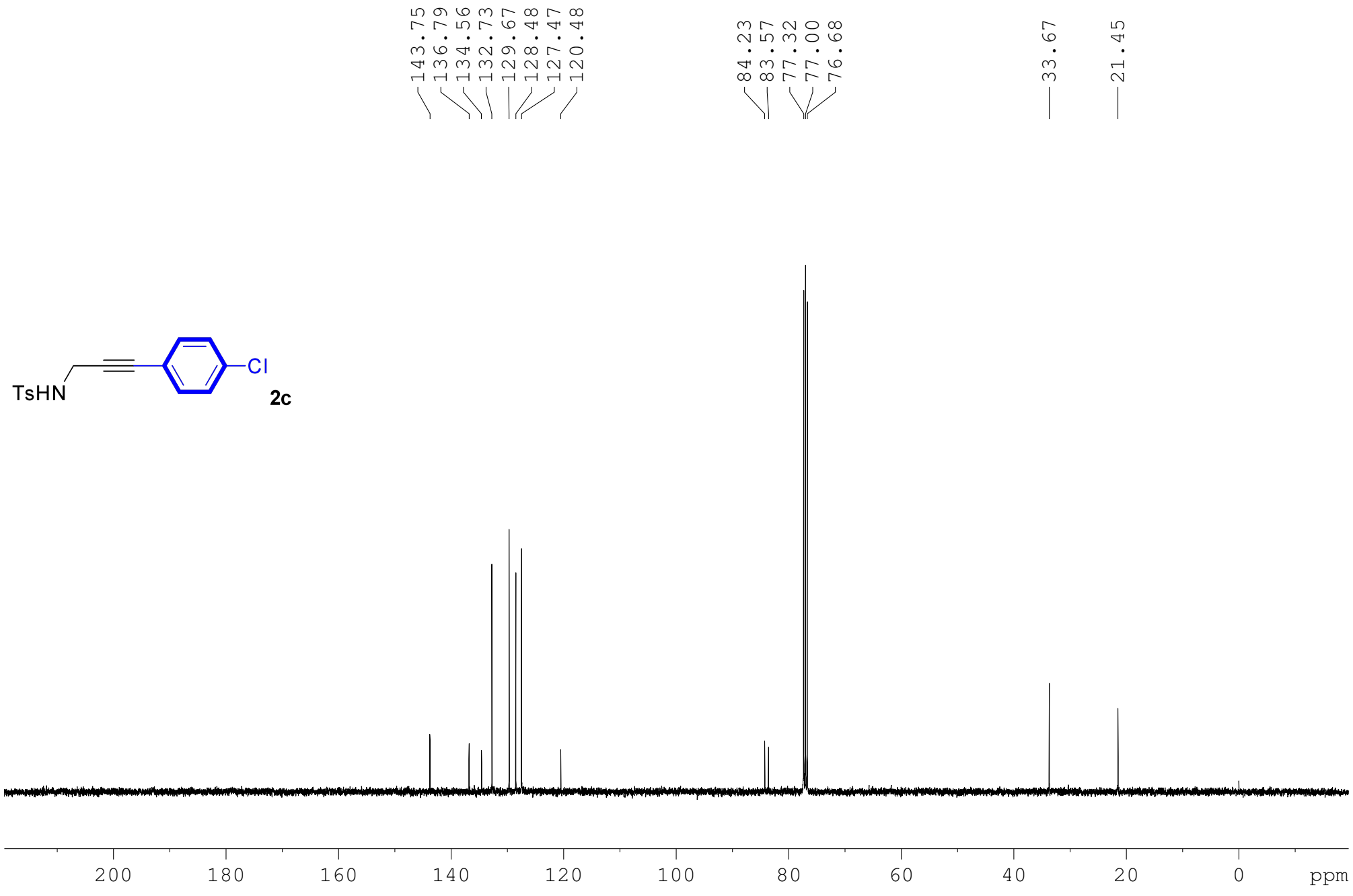
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Cl
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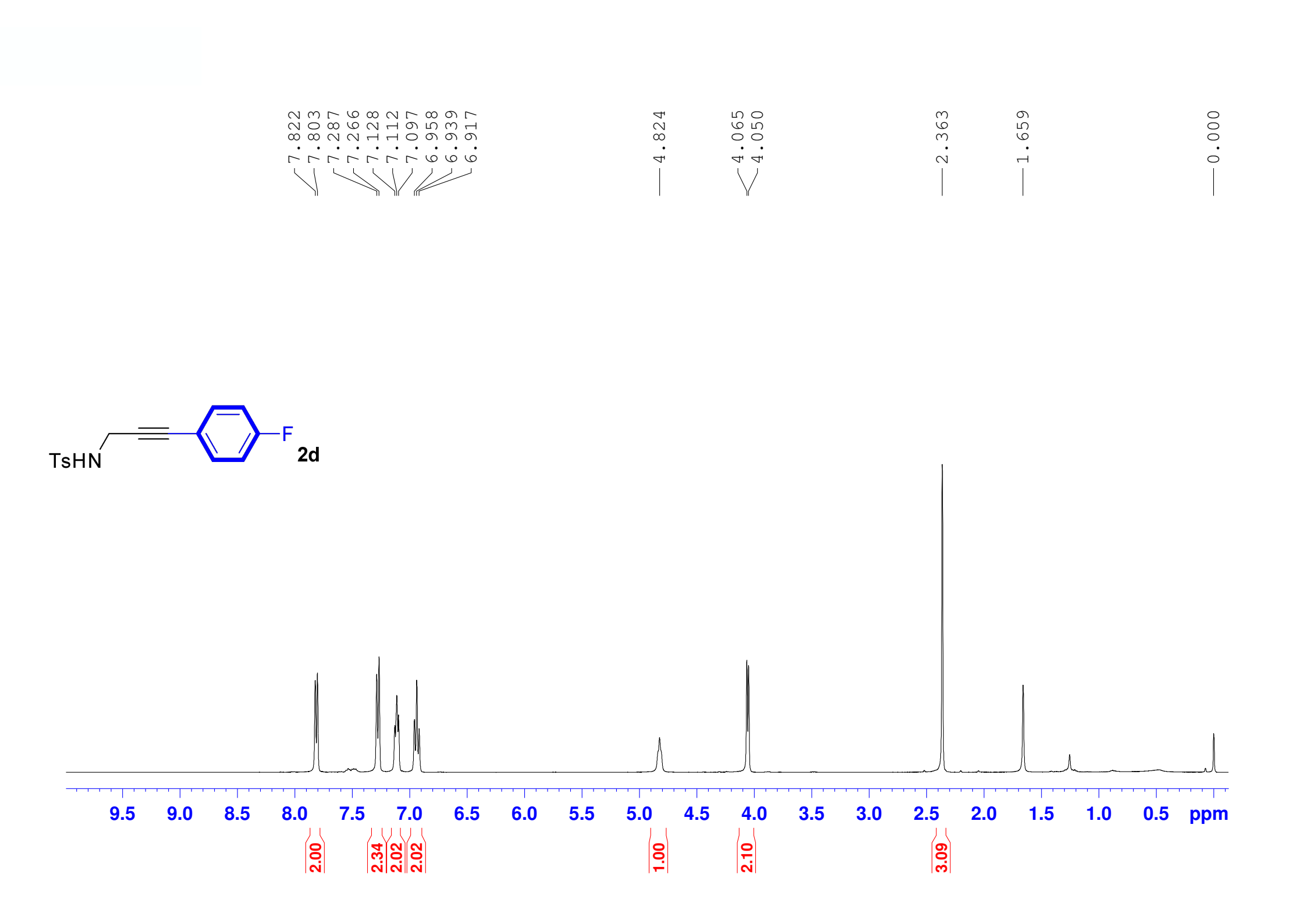
ppm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5.0
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3.0
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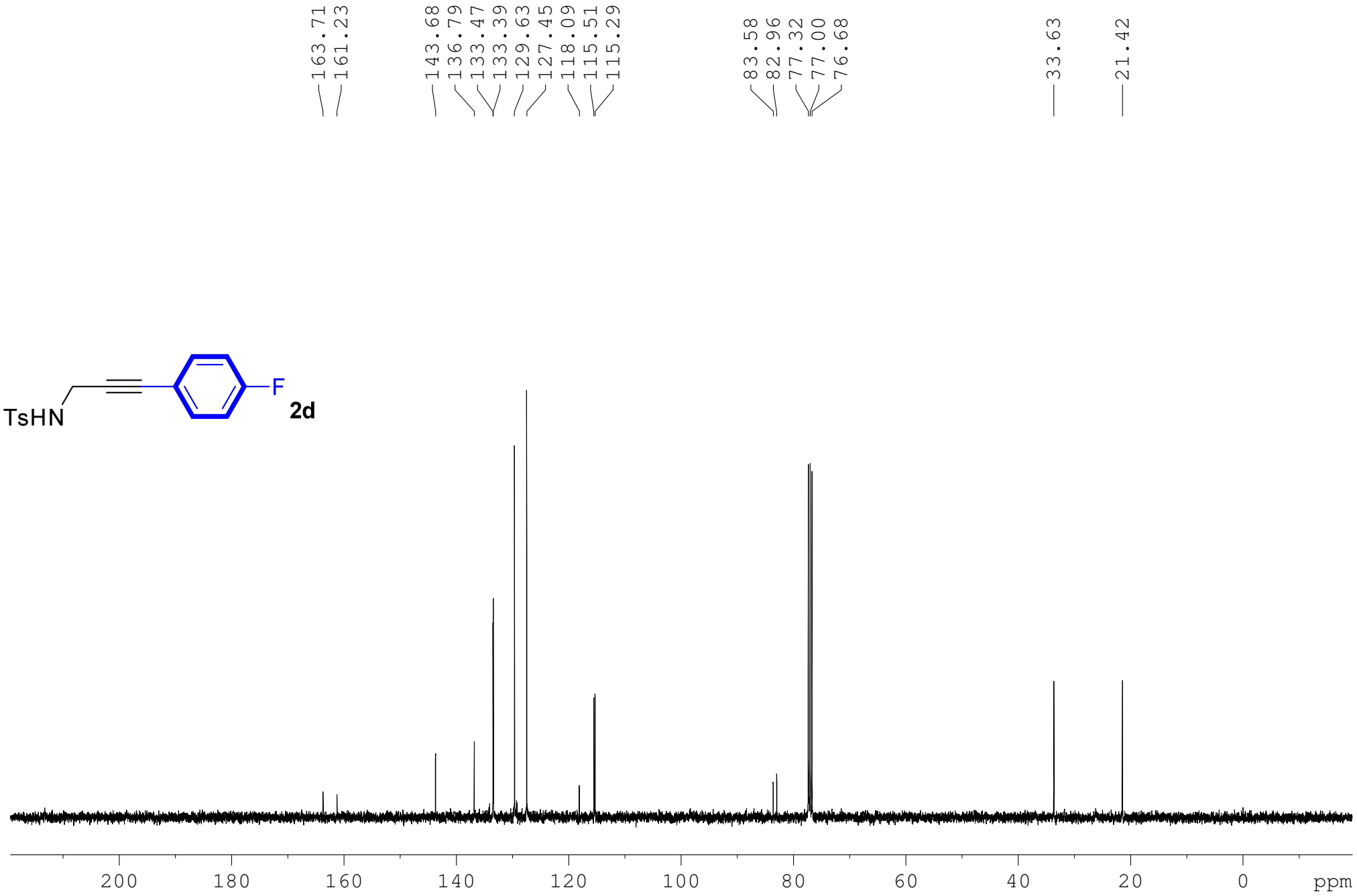
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77.32
77.00
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33.63
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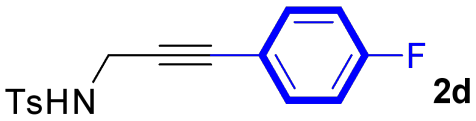

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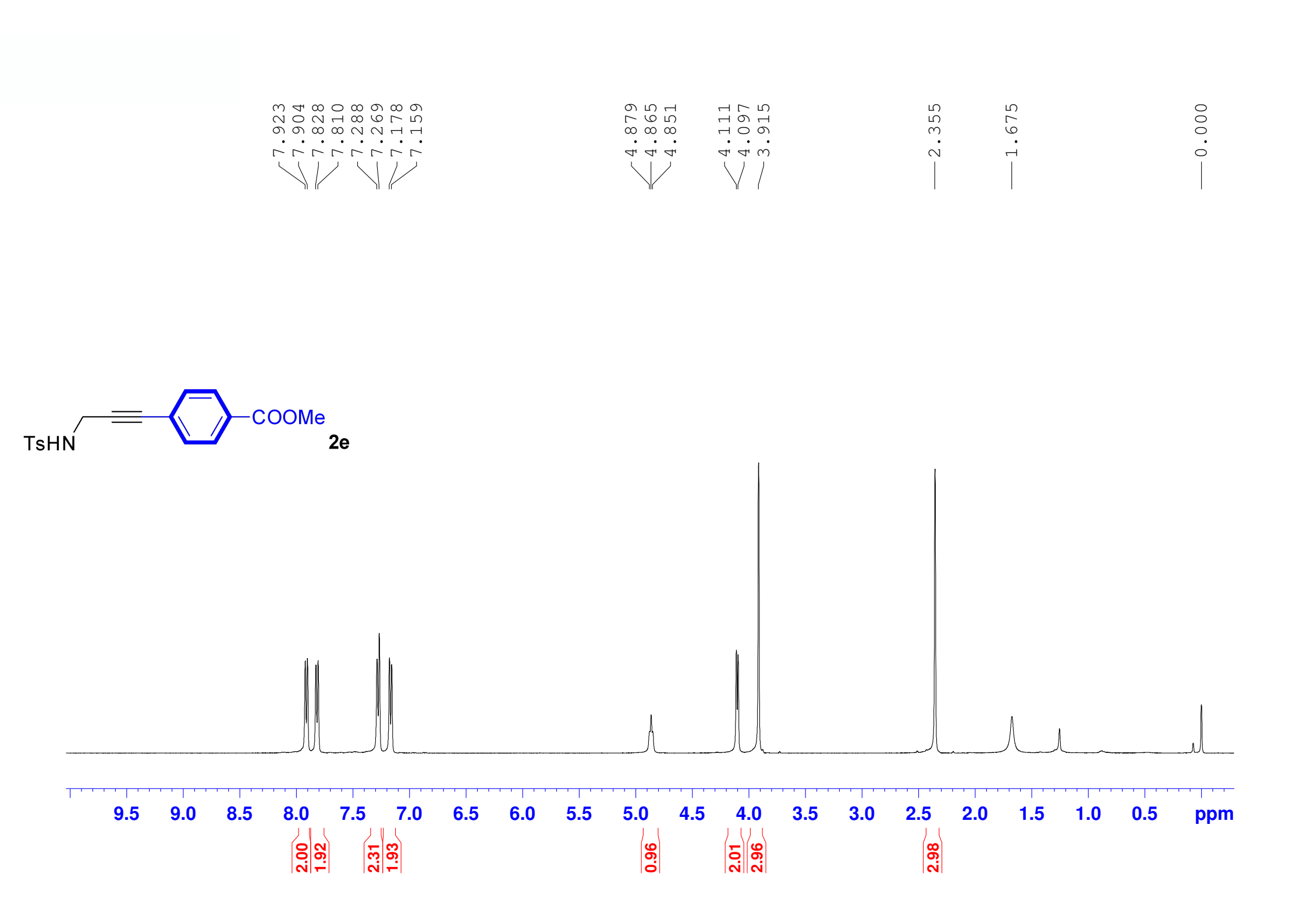
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COOMe
2e
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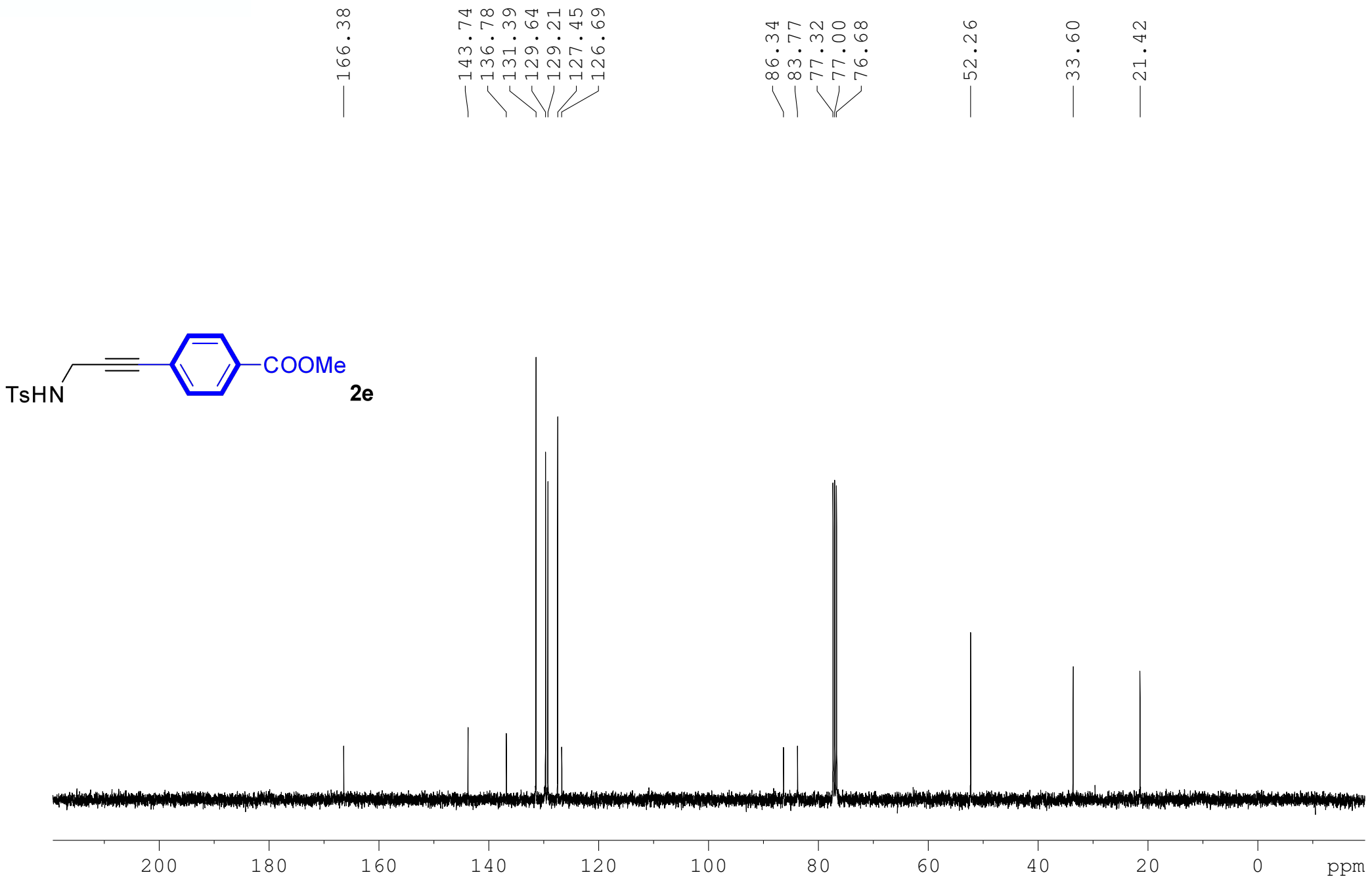
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52.26
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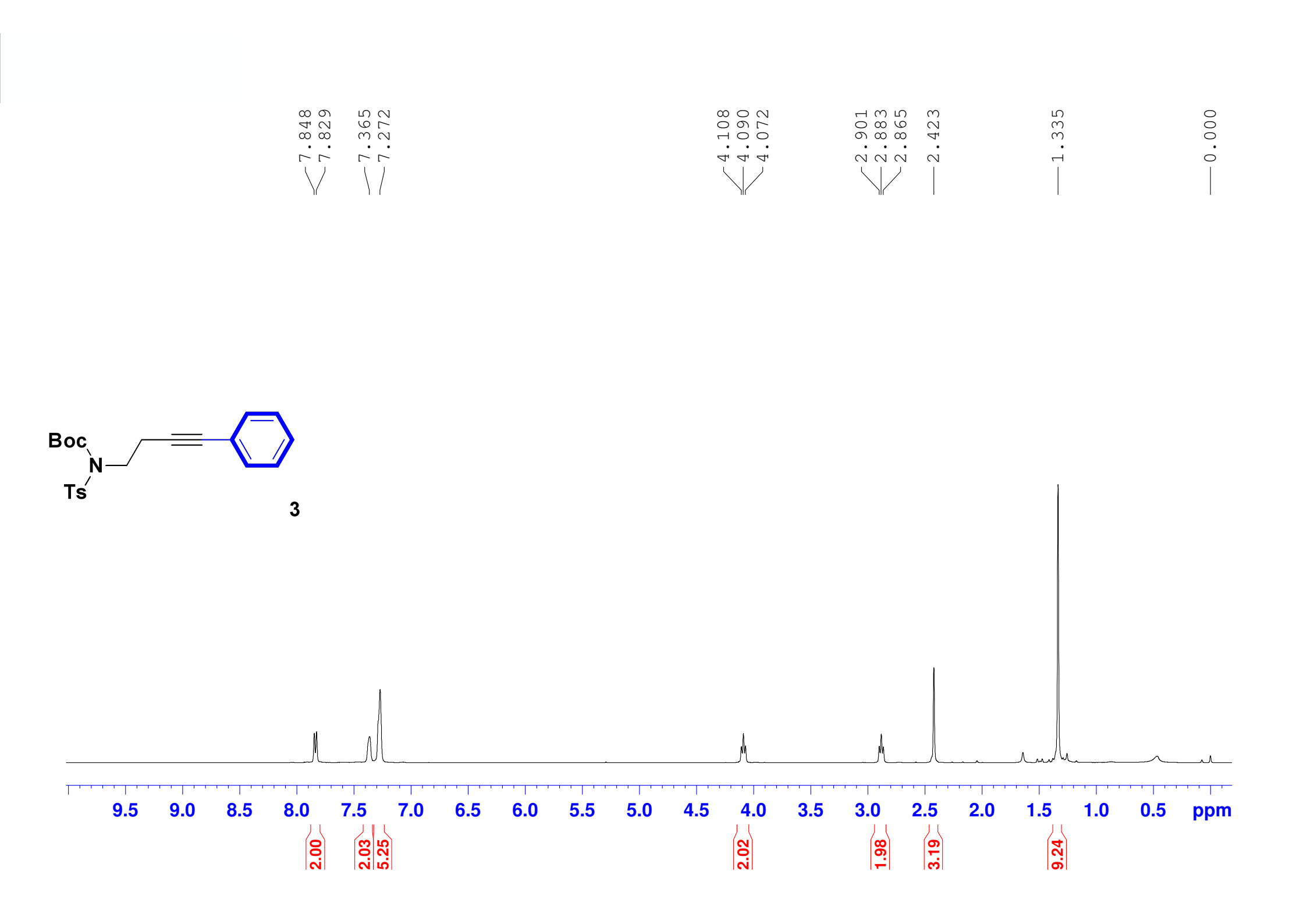
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0.000
Boc
N
Ts
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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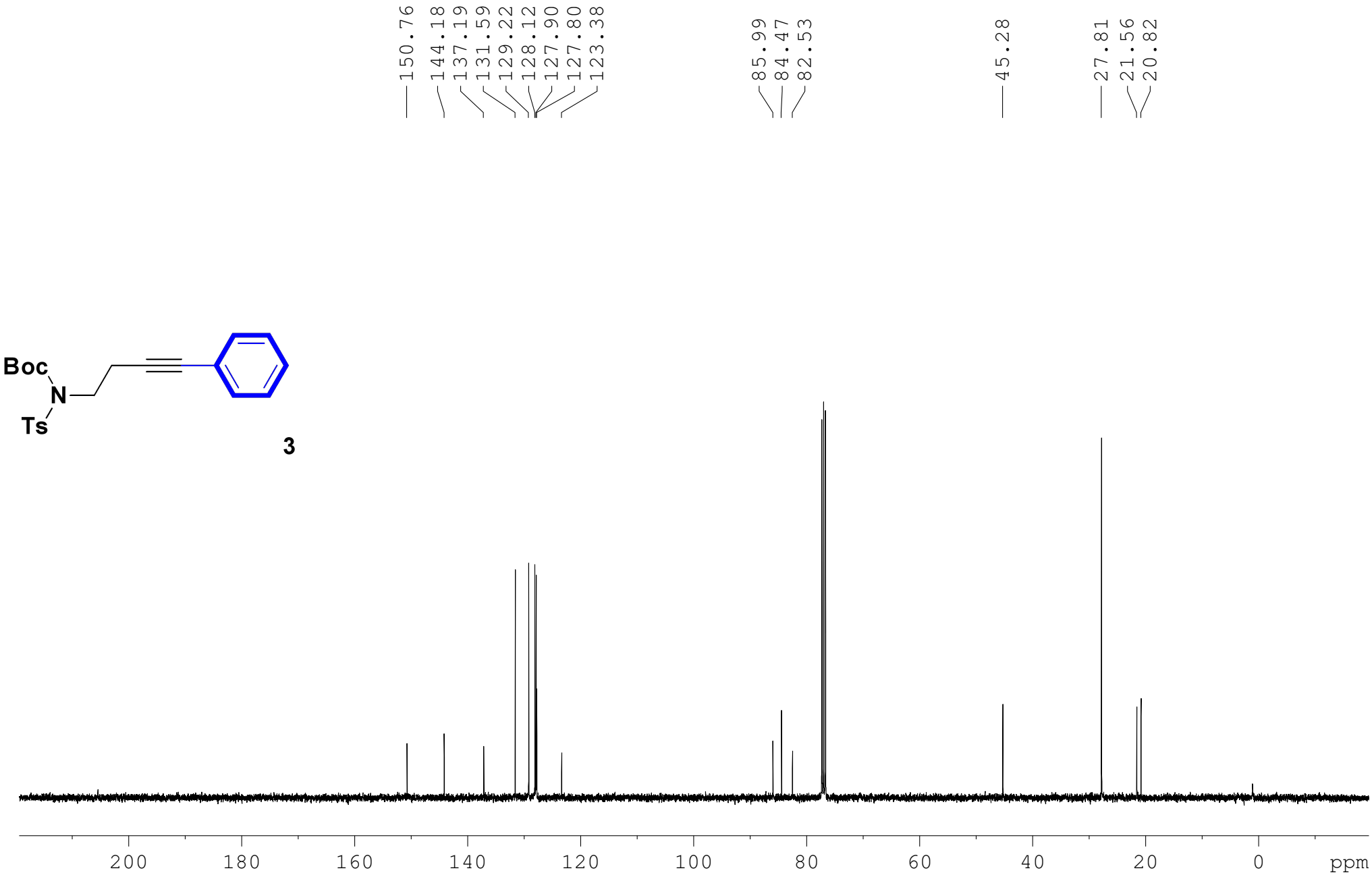
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27.81
21.56
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Boc
N
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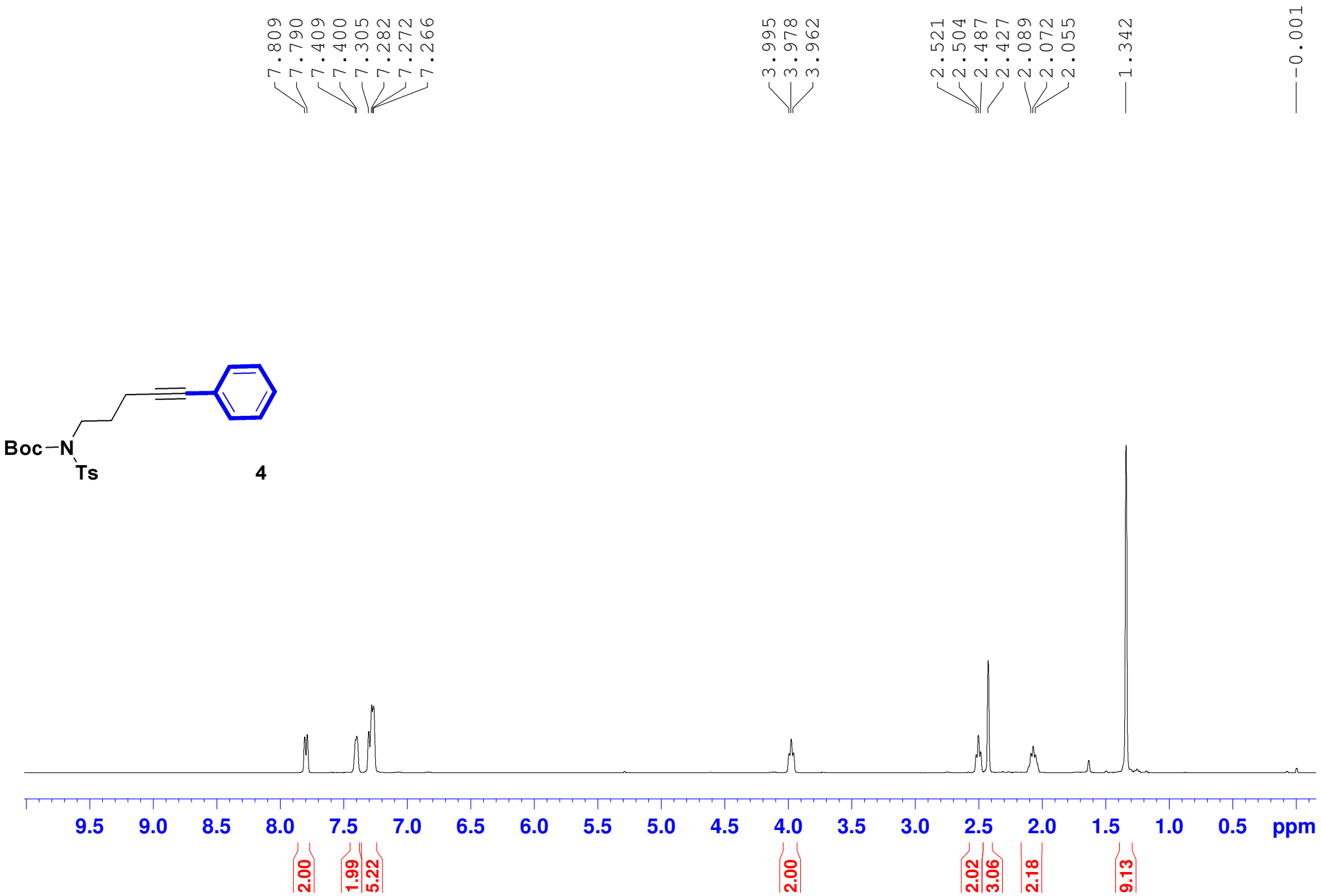
120
100
80
60
40
20
0
ppm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2.427
2.089
2.072
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Boc
N
Ts
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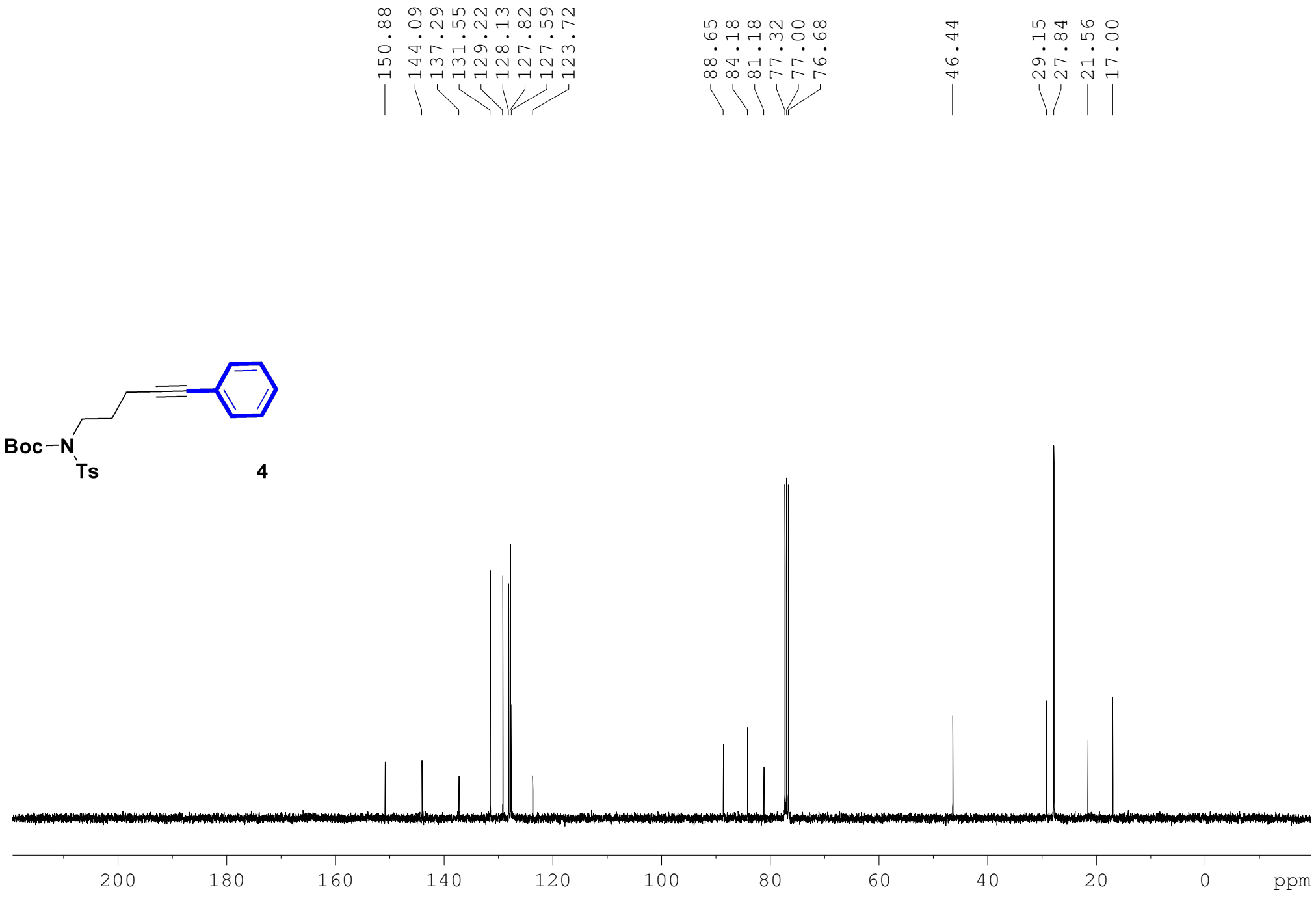
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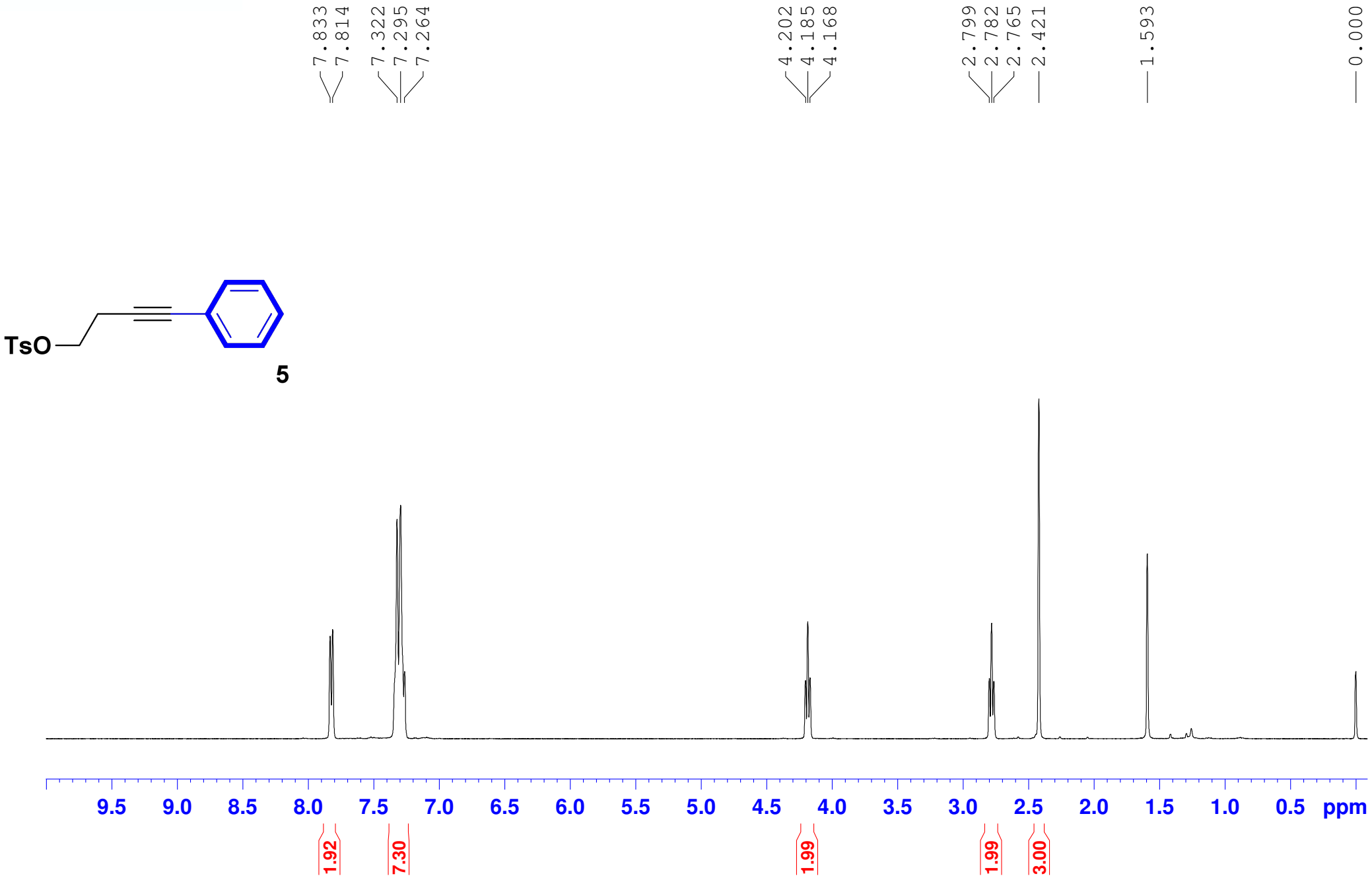
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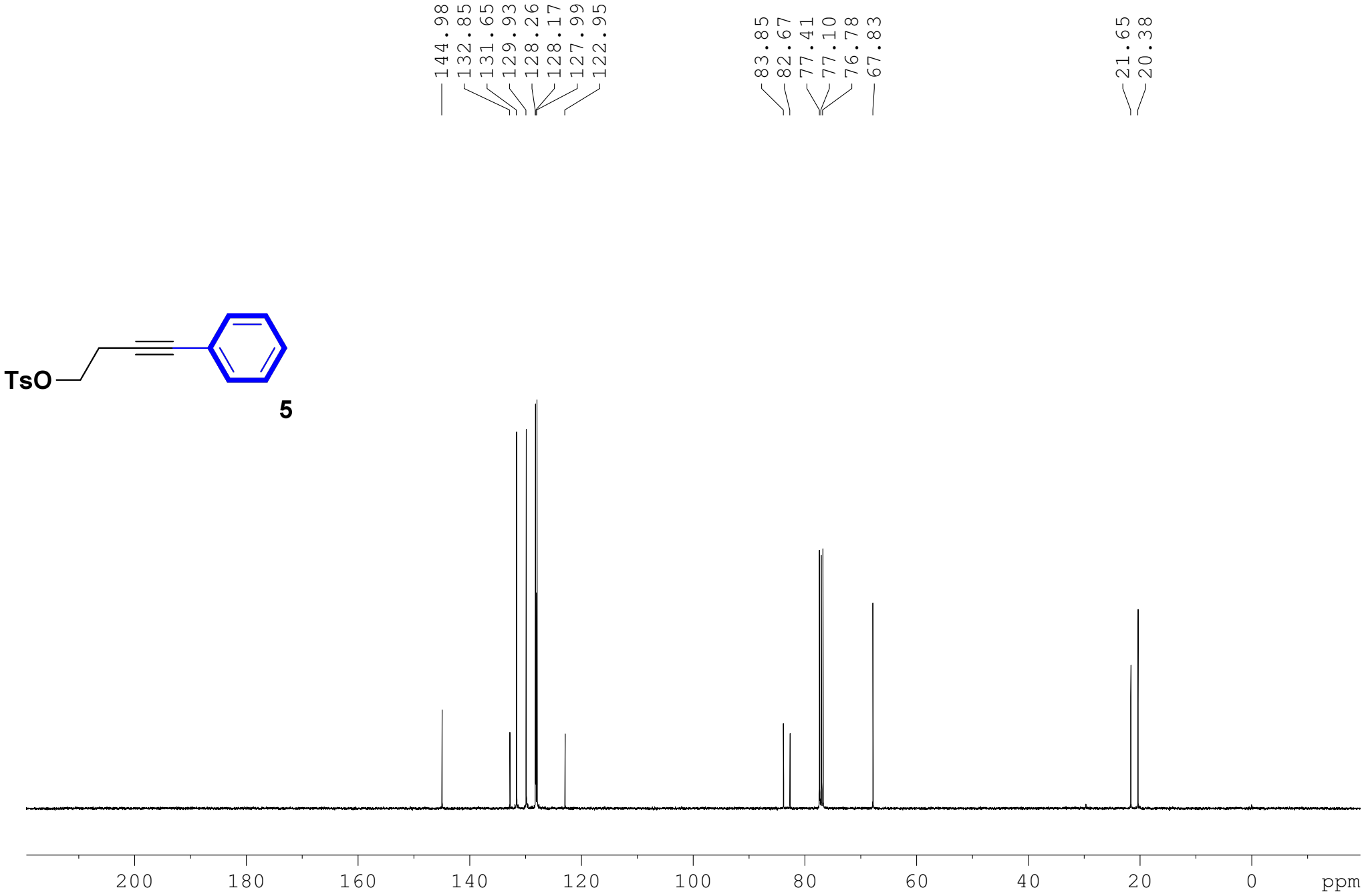
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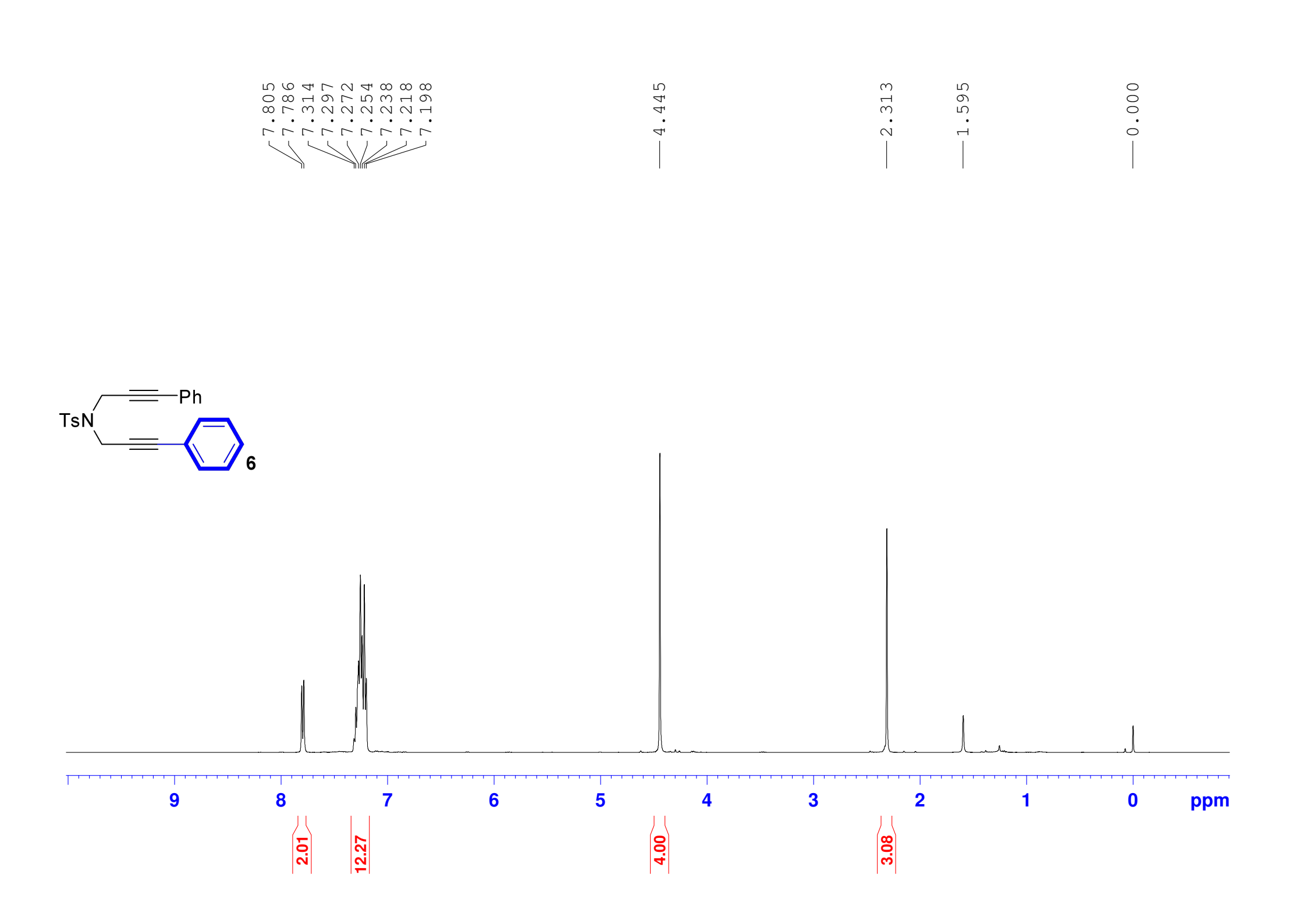
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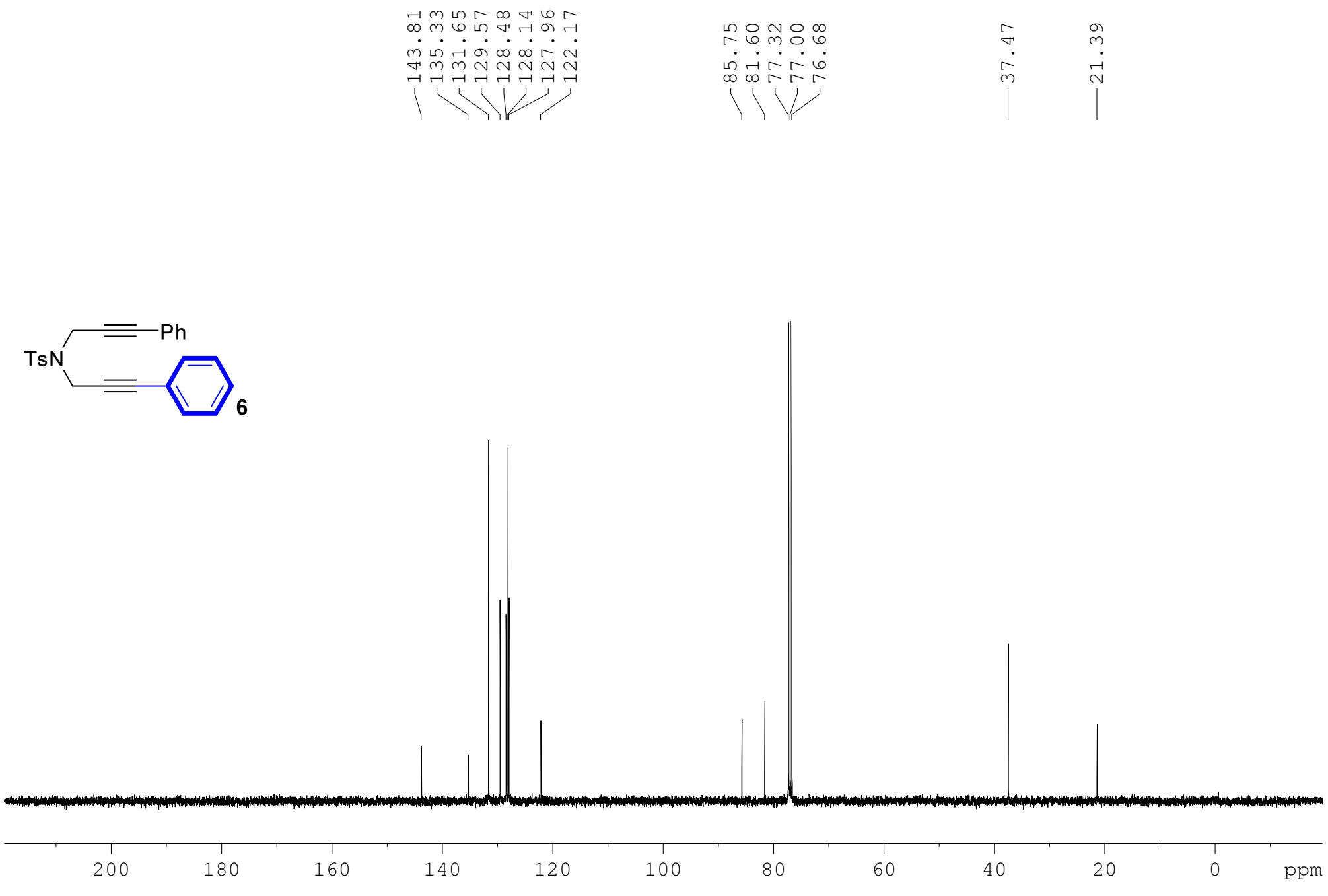
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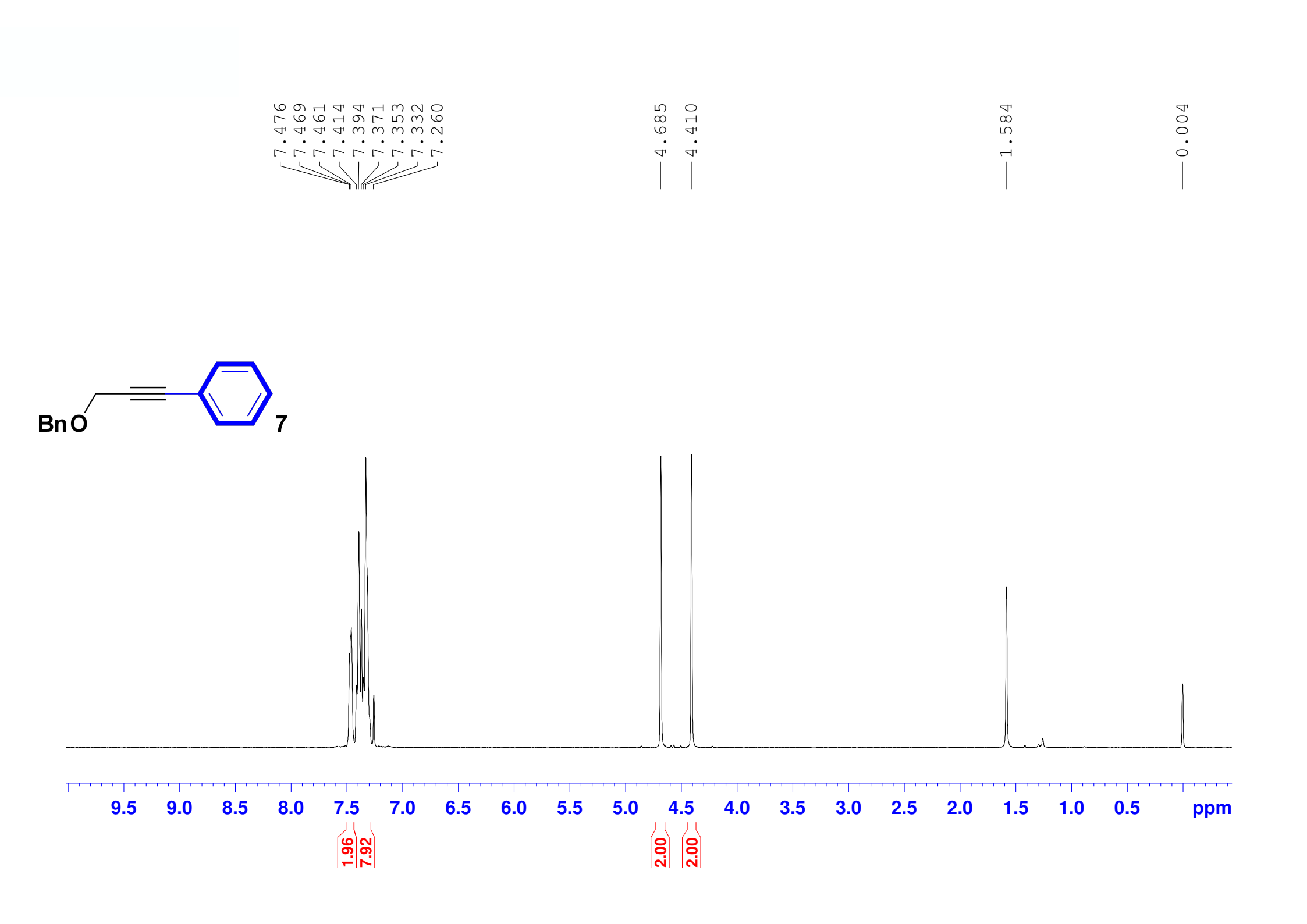
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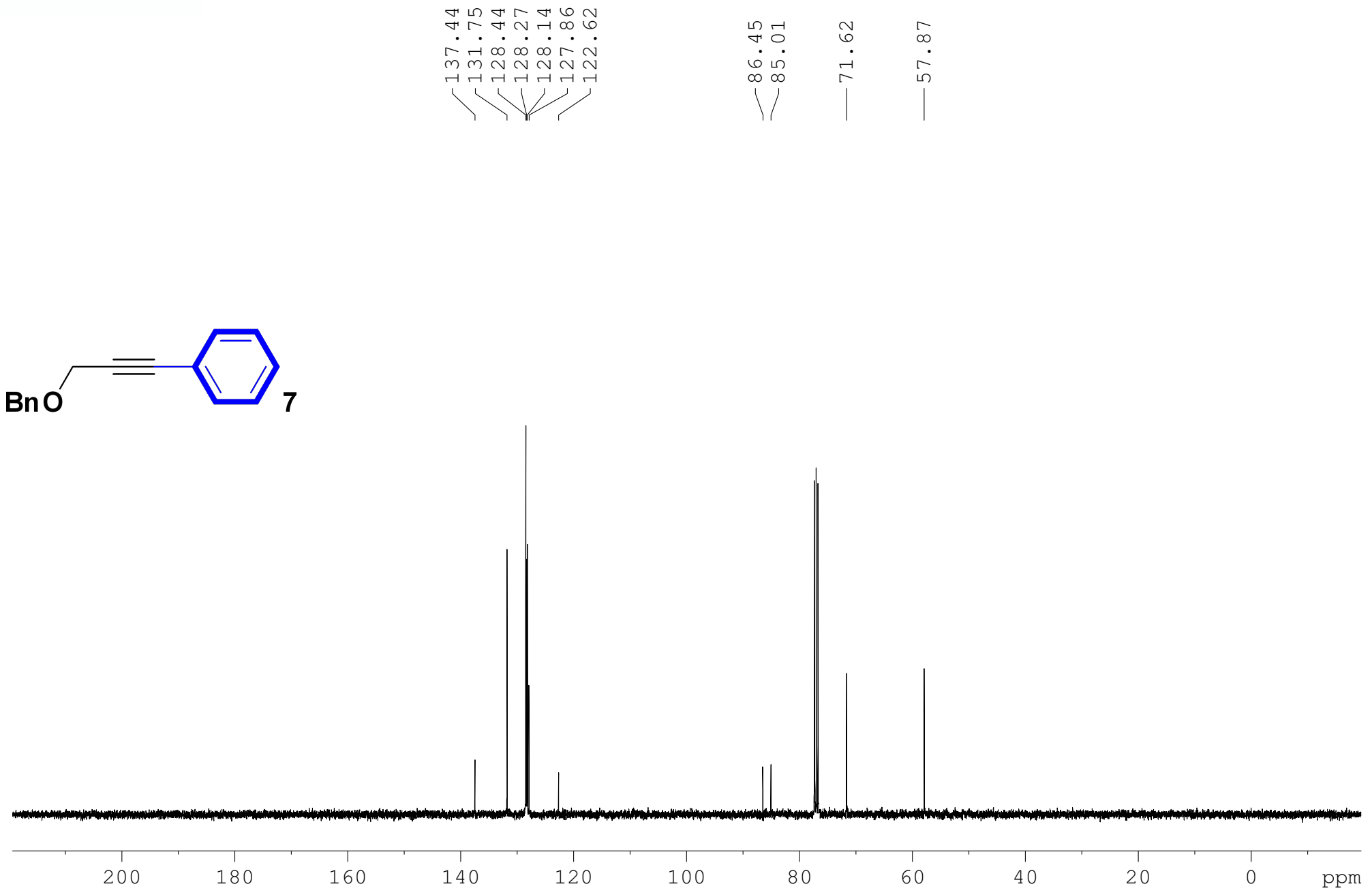
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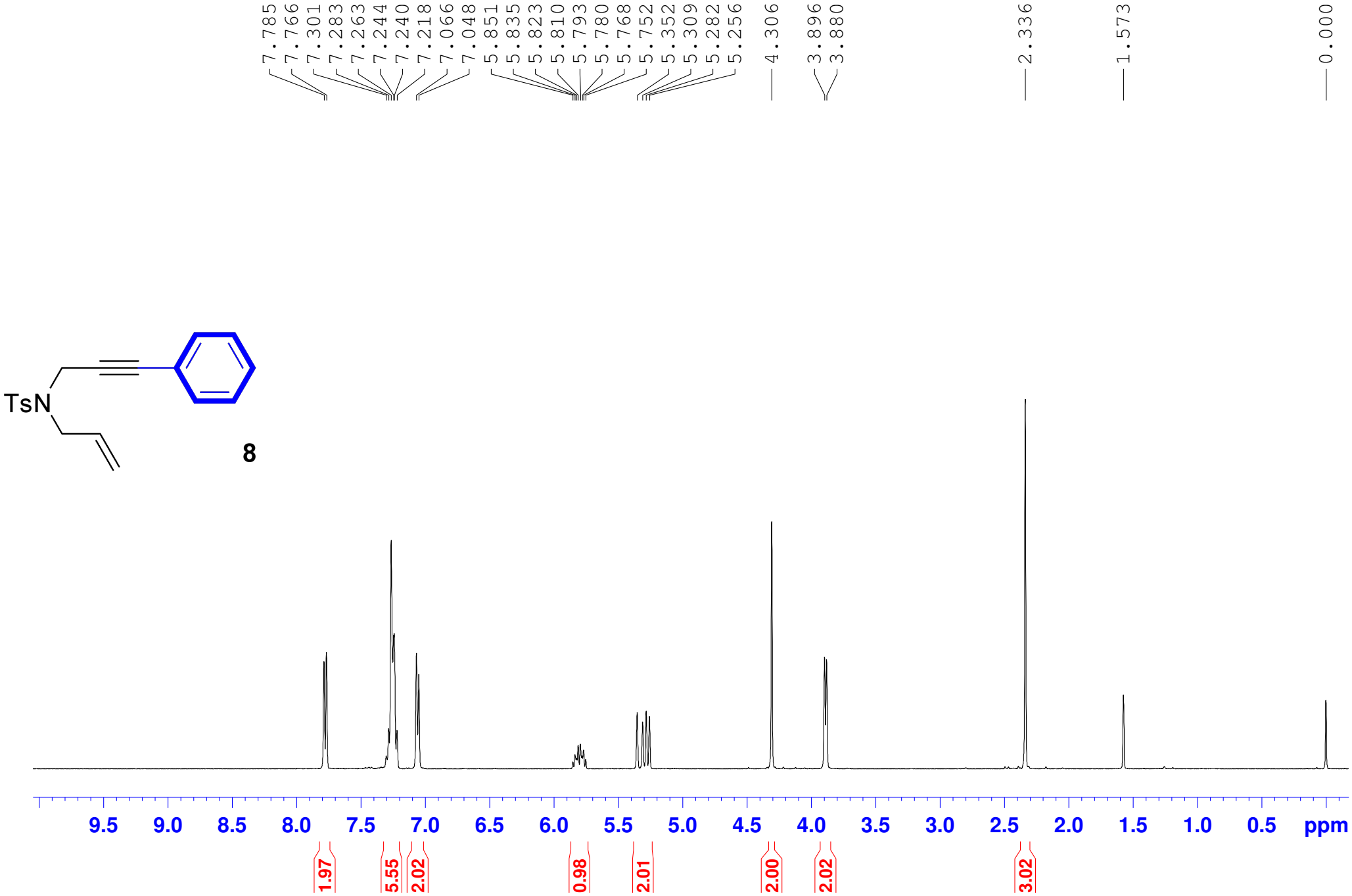
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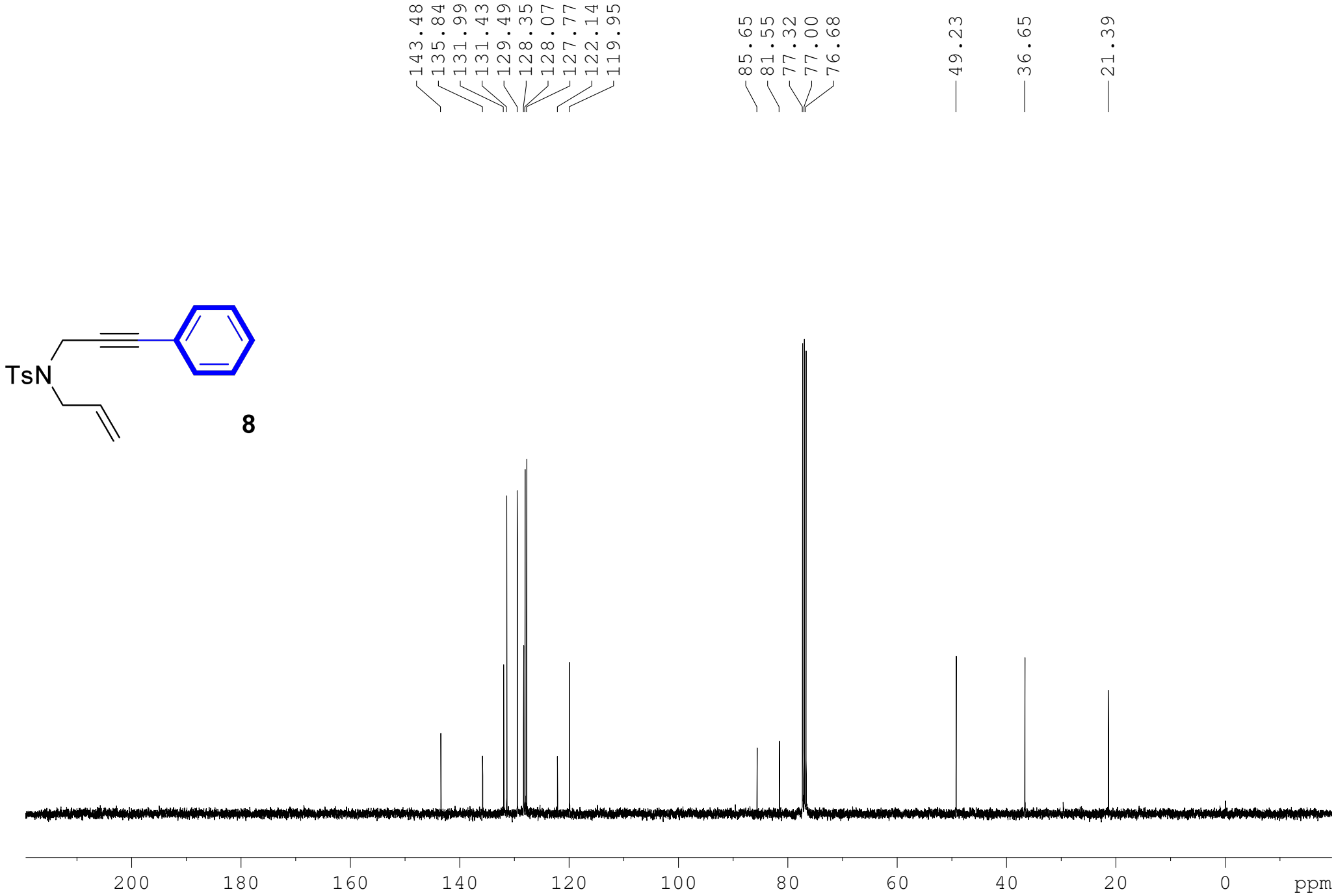
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49.23
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21.39
TsN
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200
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ppm