Supporting Information

Iron-catalysed chemo- and ortho-selective C-H bond functionalization of phenols with α-aryl-α-diazoacetates

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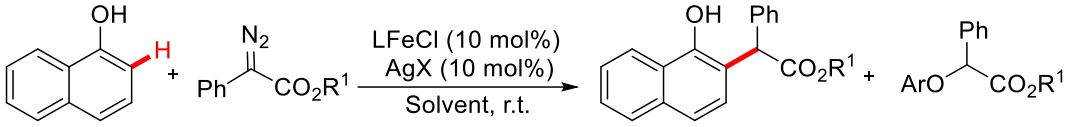
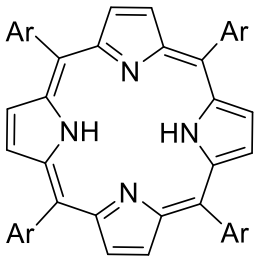
Content:

Table S1: Optimization of Reaction Conditions.



1a **2a-2d** **3aa-3ad** **4aa-4ad**

Entry	R^1	L	AgX	Solvent	**3aa-3ad** (%)[a]	**4aa-4ad** (%)[a]
1	Me	**L1**	$AgSbF_6$	CH_2Cl_2	39	19
2	Me	**L2**	$AgSbF_6$	CH_2Cl_2	33	15
3	Me	**L3**	$AgSbF_6$	CH_2Cl_2	39	23
4	Me	**L4**	$AgSbF_6$	CH_2Cl_2	71	16
5	Me	**L5**	$AgSbF_6$	CH_2Cl_2	60	19
6	Me	**L6**	$AgSbF_6$	CH_2Cl_2	60	15
7	Me	**L7**	$AgSbF_6$	CH_2Cl_2	-	-
8	Me	**L8**	$AgSbF_6$	CH_2Cl_2	52	15
9	Me	**L4**	AgOTf	CH_2Cl_2	trace	trace
10	Me	**L4**	$AgNTf_2$	CH_2Cl_2	trace	trace
11	Me	**L4**	$NaBAr_F$	CH_2Cl_2	58	15
12	**2a**/Me	**L4**	$AgBF_4$	CH_2Cl_2	32	N.D
13	**2a**/Me	**L4**	$AgPF_6$	CH_2Cl_2	Trace	Trace
14	**2a**/Me	**L4**	$AgClO_4$	CH_2Cl_2	Trace	Trace
15	**2a**/Me	**L4**	-	CH_2Cl_2	NR	NR
16	Me	**L4**	$AgSbF_6$	DCE	66	16
17	Me	**L4**	$AgSbF_6$	CH_3CN	NR	NR
18	Me	**L4**	$AgSbF_6$	Toluene	41	13
19	Me	**L4**	$AgSbF_6$	THF	52	10
20	Et	**L4**	$AgSbF_6$	CH_2Cl_2	75	12
21	^{i}Pr	**L4**	$AgSbF_6$	CH_2Cl_2	70	7
22	^{t}Bu	**L4**	$AgSbF_6$	CH_2Cl_2	81(69)	7.7
23	^{t}Bu	**L4**	-	CH_2Cl_2	NR	NR
24	^{t}Bu	-	$AgSbF_6$	CH_2Cl_2	-	trace
25[b]	^{t}Bu	**L1**	-	CH_2Cl_2	NR	NR
26	Me	**L1**	$AgSbF_6$	CH_2Cl_2	NR	NR
27[c]	^{t}Bu	**L1**	$AgSbF_6$	CH_2Cl_2	NR	NR



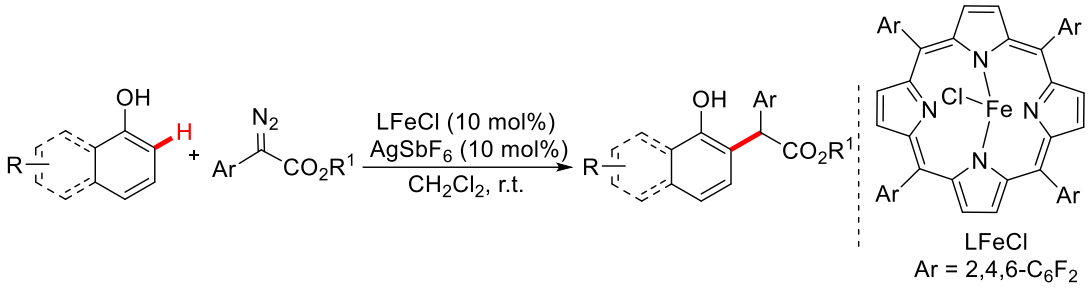
L1, Ar = Ph, L2, Ar = 4-$MeOC_6H_4$
L3, Ar = 4-$CF_3C_6H_4$, L4, Ar = 2,4,6-$F_3C_6H_2$
L5, Ar = C_6F_5 L6, Ar = 2,6-$F_2C_6H_3$
L7, Ar = 3,4,5-$F_3C_6H_2$ L8, Ar = 3,5-$(CF_3)_2C_6H_3$

Reaction Conditions: **1a** (0.4 mmol), **2a** (0.6 mmol), catalyst (10 mol%), solvent (5 mL), rt. [a]NMR yield, the number in parenthesis is isolated yield. [b]Cobalt porphyrin was used instead. [c]Manganese was used instead.

1. General Information:

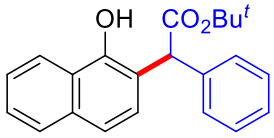
All air- and moisture-sensitive manipulations were carried out with standard Schlenk techniques under nitrogen or in a glove box under nitrogen. ^{1}H NMR, ^{13}C NMR spectra were measured at 400 MHz and 100 MHz in $CDCl_3$. Data for ^{1}H NMR spectra are reported as follows: chemical shift (ppm, referenced to TMS; s = singlet, d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm). THF, Toluene, 1,4-dioxne, Ether were distilled from sodium and benzophenone prior to be used. CH_2Cl_2, CH_3CN were distilled from CaH_2 prior to be used.

2. General procedure for the *ortho* C-H bond functionalization of naphthalenols[1]



In a dried glass tube, a mixture of LFeCl (0.04 mmol), AgX (0.04 mmol) in CH_2Cl_2 (4 mL) was stirred at room temperature for 15 mins. Subsequently, naphthalenol (0.4 mmol) was added to the reaction mixture at room temperature. Then a solution of diazo compounds (0.6 mmol) in CH_2Cl_2 (1 mL) was introduced into the reaction mixture by a syringe in a period of 15 mins. The resulting mixture was continually stirred at room temperature for 1 min. The mixture was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel (PE/EA = 10:1 to 5:1) to afford the desired product.

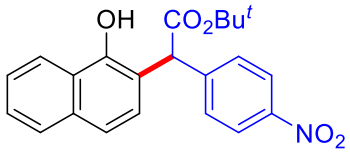
1) Synthesis of 3ad[2]



3ad

3ad，colorless oil, 69% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.40-7.45 (m, 1H), 8.34 (d, *J* = 6.4 Hz, 1H), 7.75-7.80 (m, 1H), 7.45-7.50 (m, 2H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.20-7.35 (m, 6H), 5.05 (s, 1H), 1.53 (s, 9H).

2) Synthesis of 3ae

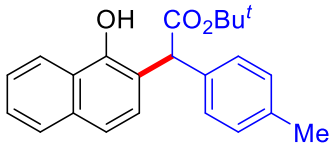


3ae

3ae，colorless oil, 61% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.28-8.32 (m, 1H), 8.14 (d, *J* = 8.0 Hz, 2H), 7.81 (dd, *J* = 8.0 Hz, 4 Hz, 1H), 7.40-7.50 (m, 5H), 7.23 (d, *J* = 8.0 Hz, 1H), 5.14 (s, 1H), 1.55 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.91, 56.97, 84.82, 115.46, 120.58, 122.56, 123.77, 125.60, 126.43, 126.90, 127.28,

128.43, 128.77, 134.57, 144.63, 147.09, 151.55, 174.67. MS(EI): m/z (%): 379 (M^+, 6.90), 57 (100); HRMS (EI) calcd. for $C_{22}H_{21}NO_5$: 379.1420, found: 379.1423.

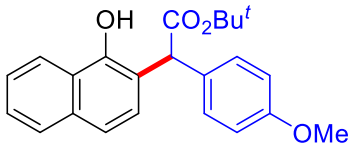
3) Synthesis of 3af



3af

3af，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.32-8.38 (m, 1H), 7.76-7.80 (m, 1H), 7.45-7.50 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.08-7.16 (m, 4H), 5.03 (s, 1H), 1,54 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 21.00, 27.96, 57.31, 83.85, 116.30, 119.86, 122.88, 125.16, 126.46, 126.53, 127.09, 127.15, 129.35, 129.51, 134.14, 134.37, 136.98, 151.76, 176.03. MS(EI): m/z (%): 348 (M^+, 6.98), 231 (100); HRMS (EI) calcd. for $C_{23}H_{24}O_3$: 348.1725, found: 348.1722.

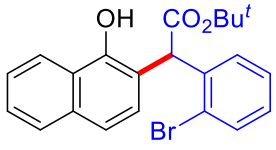
4) Synthesis of 3ag[2]



3ag

3ag，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.25 (m, 1H), 7.90-7.95 (m, 1H), 7.35-7.50 (m, 2H), 7.15-7.25 (m, 2H), 6.90-6.95 (m, 1H), 6.80-6.85 (m, 2H), 6.40-6.45 (m, 1H), 6.22 (bs, 1H), 5.52 (s, 1H), 3.78 (s, 3H), 1.45 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.95, 53.44, 55.20, 81.64, 107.98, 113.95, 122.62, 123.08, 124.71, 124.96, 126.28, 126.63, 127.34, 129.98, 130.51, 132.69, 151.20, 158.57, 173.29. MS(EI): m/z (%): 364 (M^+, 10.45), 263 (100); HRMS (EI) calcd. for $C_{23}H_{24}O_4$: 364.1675, found: 364.1680.

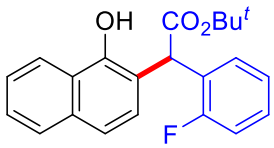
5) Synthesis of 3ah[2]



3ah

3ah，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.15-8.25 (m, 1H), 7.90-7.95 (m, 1H), 7.35-7.50 (m, 2H), 7.15-7.25 (m, 2H), 6.90-6.95 (m, 1H), 6.80-6.85 (m, 2H), 6.40-6.45 (m, 1H), 6.22 (bs, 1H), 5.52 (s, 1H), 3.78 (s, 3H), 1.45 (s, 9H).

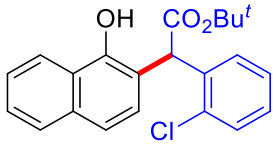
6) Synthesis of 3ai



3ai

3ai，colorless oil, 78% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.30-8.40 (m, 1H), 7.75-7.85 (m, 1H), 7.40-7.55 (m, 3H), 7.20-7.30 (m, 2H), 6.98-7.10 (m, 3H), 5.17 (s, 1H), 1.48 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.75, 51.84, 83.80, 113.95, [115.35, *J* = 21 Hz, 1C], 120.28, 122.72, [123.88, *J* = 21 Hz, 1C], [124.18, *J* = 3 Hz, 1C], 125.31, 126.24, 126.65, 127.22, 128.64, [129.34, *J* = 15 Hz, 1C], 129.35, 134.48, 151.94, [160.70, *J* = 45 Hz, 1C], 174.81**.** MS(EI): m/z (%): 352 (M^+, 7.82), 249 (100); HRMS (EI) calcd. for $C_{22}H_{21}O_3F$: 352.1475, found: 352.1478.

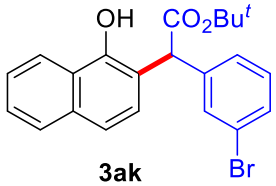
7) Synthesis of 3aj[2]



3aj

3aj，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.25-8.35 (m, 1H), 8.26 (s, 1H), 7.75-7.85 (m, 1H), 7.40-7.50 (m, 4H), 7.10-7.30 (m, 4H), 5.34 (s, 1H), 1.46 (s, 9H).

8) Synthesis of 3ak[2]

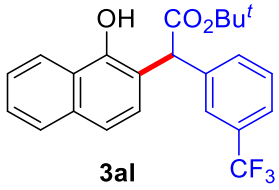


3ak

3ak，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.30-8.40 (m, 1H), 7.75-7.85 (m, 1H), 7.35-7.55 (m, 5H), 7.10-7.25 (m, 3H), 5.03 (s, 1H), 1.55

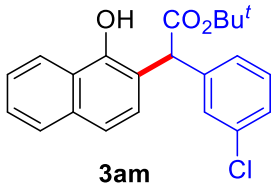
(s, 9H).

9) Synthesis of 3al[2]



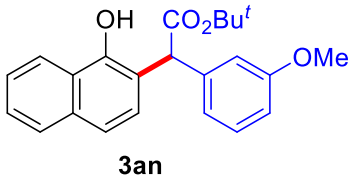
3al，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.35-8.40 (m, 1H), 7.80-7.85 (m, 1H), 7.40-7.65 (m, 7H), 7.20-7.30 (m, 1H), 5.14 (s, 1H), 1.57 (s, 9H).

10) Synthesis of 3am[2]



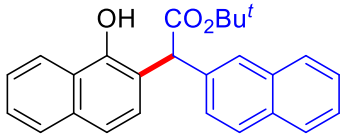
3am，colorless oil, 56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.26 (s, 1H), 8.25-8.35 (m, 1H), 7.70-7.80 (m, 1H), 7.35-7.50 (m, 3H), 7.10-7.25 (m, 5H), 5.01 (s, 1H), 1.52 (s, 9H).

11) Synthesis of 3an



3an，colorless oil, 61% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.30-8.40 (m, 1H), 7.75-7.80 (m, 1H), 7.40-7.50 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.15-7.25 (m, 2H), 6.75-6.85 (m, 3H), 5.02 (s, 1H), 3.70 (s, 3H), 1.52 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.93, 55.08, 57.52, 83.94, 112.31, 113.53, 116.05, 119.64, 119.89, 122.85, 125.17, 126.49, 127.09, 129.46, 129.59, 134.40, 138.71, 151.77, 159.72, 175.6. MS(EI): m/z (%): 364 (M^+, 8.39), 231 (100); HRMS (EI) calcd. for $C_{23}H_{24}O_4$: 364.1675, found: 364.1674.

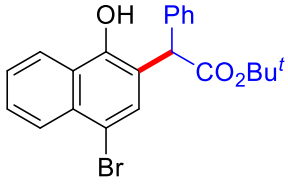
12) Synthesis of 3ao



3ao

3ao，white solid, 75% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.35-8.45 (m, 1H), 7.75-7.90 (m, 5H), 7.45-7.55 (m, 5H), 7.38-7.44 (s, 1H), 7.31-7.35 (m, 1H), 5.27 (s, 1H), 1.60 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.96, 57.65, 84.02, 116.12, 119.99, 122.86, 125.22, 125.58, 126.01, 126.17, 126.53, 126.54, 127.14, 127.48, 128.08, 128.41, 129.46, 132.50, 133.27, 134.43, 134.53, 151.84, 175.66. MS(EI): m/z (%): 384 (M^+, 6.71), 281 (100); HRMS (EI) calcd. for $C_{26}H_{24}O_3$: 384.1725, found: 384.1723.

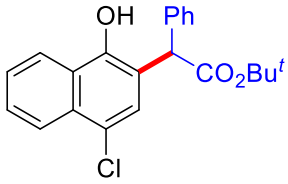
14) Synthesis of 3bd



3bd

3bd，light yellow oil, 53% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.37 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.55-7.62 (m, 1H), 7.48-7.55 (m, 2H), 7.20-7.32 (m, 5H), 4.98 (s, 1H), 1.54 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.91, 57.36, 84.48, 112.50, 116.90, 123.40, 125.94, 126.45, 127.15, 127.53, 127.76, 127.90, 128.75, 132.40, 132.61, 136.56, 151.87, 175.80. MS(EI): m/z (%): 412 (M^+, 2.41), 414 ($[M+2]^+$, 2.39), 311 (100); HRMS (EI) calcd. for $C_{22}H_{21}O_3Br$: 412.0674, found: 412.0677.

15) Synthesis of 3cd

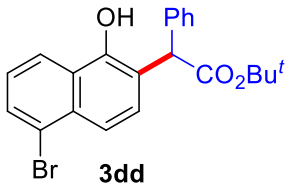


3cd

3cd，light yellow oil，75% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.57-7.63 (m, 1H), 7.50-7.55 (m, 1H), 7.34 (s, 1H), 7.21-7.31 (m, 5H), 4.98 (s, 1H), 1.54 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 27.91, 57.40, 84.43, 116.30, 122.52, 123.38, 123.85, 125.94, 127.18, 127.52, 127.59,

128.75, 129.05, 131.19, 136.58, 151.13, 175.74. MS(EI): m/z (%): 368 (M^+, 2.72), 370 ($[M+2]^+$, 0.97), 265 (100); HRMS (EI) calcd. for $C_{22}H_{21}O_3Cl$: 368.1179, found: 368.1177

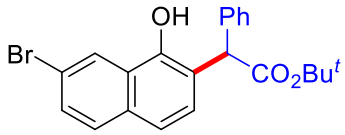
16) Synthesis of 3dd[2]



3dd

3dd，colorless oil，56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.71(s, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 7.70-7.80 (m, 2H), 7.20-7.35 (m, 7H), 5.06 (s, 1H), 1.52 (s, 9H).

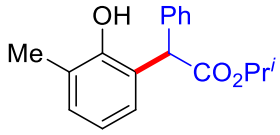
17) Synthesis of 3ed[2]



3ed

3ed，yellow solid，56% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.57 (s, 1H), 8.43 (s, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.44 (dd, *J* = 8.8 Hz, 1.6 Hz, 1H), 7.10-7.30 (m, 7H), 4.95 (s, 1H), 1.44 (s, 9H).

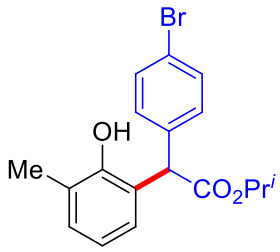
18) Synthesis of 6a



6a

6a，colorless oil，60% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.20-7.35 (m, 5H), 7.11 (d, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.78-6.85 (m, 1H), 5.14 (hept, *J* = 6.4 Hz, 1H), 5.03 (s, 1H), 2.24 (s, 3H), 1.32 (d, *J* = 6.4 Hz, 3H), 1.28 (d, *J* = 6.4 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 16.25, 21.61, 21.69, 55.69, 70.04, 120.07, 123.21, 126.77, 127.27, 127.55, 128.59, 129.08, 130.78, 137.05, 153.40, 175.13.

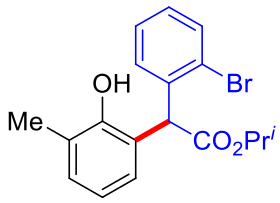
19) Synthesis of 6b



6b

6b，colorless oil，43% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.05-7.20 (m, 3H), 6.90-7.00 (m, 1H), 6.80-6.90 (m, 1H), 5.14 (hetp, *J* = 6.4 Hz, 1H), 4.99 (s, 1H), 1.33 (d, *J* = 6.4 Hz, 3H), 1.28 (d, *J* = 6.4 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 16.17, 21.57, 21.67, 54.77, 70.18, 77.32, 120.27, 121.31, 123.01, 126.61, 128.76, 129.46, 130.91, 131.65, 136.22, 153.11, 174.53. MS(EI): m/z (%): 362 (M^+, 8.00), 364 ($[M+2]^+$, 7.87), 195 (100); HRMS (EI) calcd. for $C_{18}H_{19}O_3Br$: 362.0518, found: 362.0524.

20) Synthesis of 6c



6c

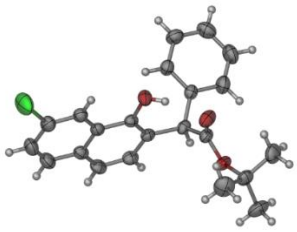
6c，white solid，45% yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.0 Hz, 1.2 Hz, 1H), 7.18-7.28 (m, 2H), 7.08-7.18 (m, 2H), 6.92-6.96 (m, 1H), 6.80-6.85 (m, 1H), 6.18 (s, 1H), 5.45 (s, 1H), 5.12 (hept, *J* = 6.4 Hz, 1H), 2.25 (s, 3H), 1.28 (d, *J* = 6.4 Hz, 3H), 1.22 (d, *J* = 6.4 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 16.08, 21.55, 53.93 69.58, 120.47, 122.66, 125.02, 125.10, 127.53, 128.36, 128.94, 130.25, 130.60, 133.04, 136.71, 152.70, 172.91. MS(EI): m/z (%): 362 (M^+, 6.15), 364 ($[M+2]^+$, 6.10), 195 (100); HRMS (EI) calcd. for $C_{18}H_{19}O_3Br$: 362.0518, found: 362.0516.

3. References

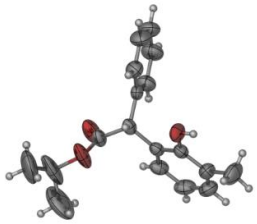
[1] The preparation of porphyrin iron catalysts, see: a) J. S. Lindsey, R. W. Wagner, *J. Org. Chem*. **1989**, *54*, 828; b) L.Wang, Y. She, R. Zhong, H. Ji, Y. Zhang, X. Song, *Org. Process Res. Dev*. **2006**, 10, 757.

[2] Z. Yu, Y. Li, P. Zhang, L. Liu, J. Zhang, *Chem. Sci*. **2019**, *10*, 6553.

4. X-ray crystal date for 3ed and 6a



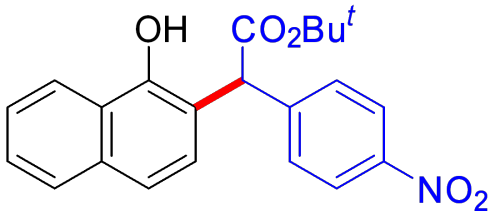
3ed



6a

5. NMR Spectra of new compounds

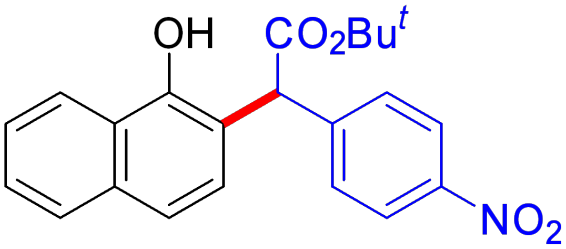
yzz-14-078-2



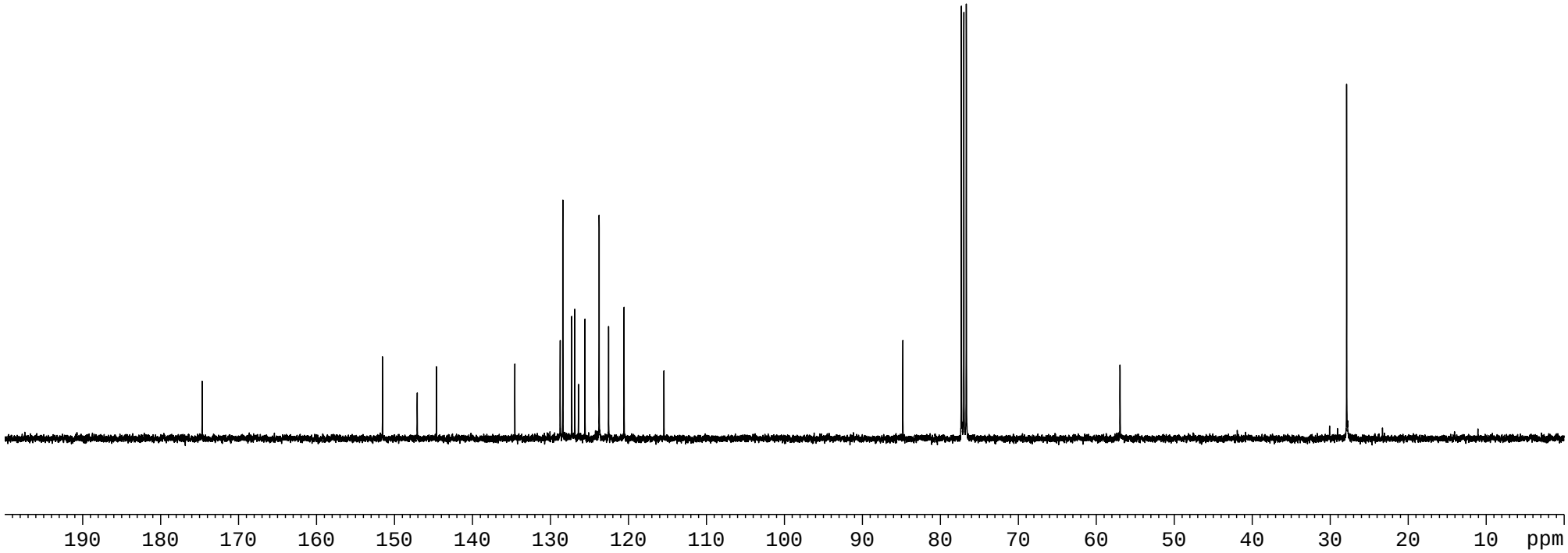
3ae

yzz-14-078-2-c

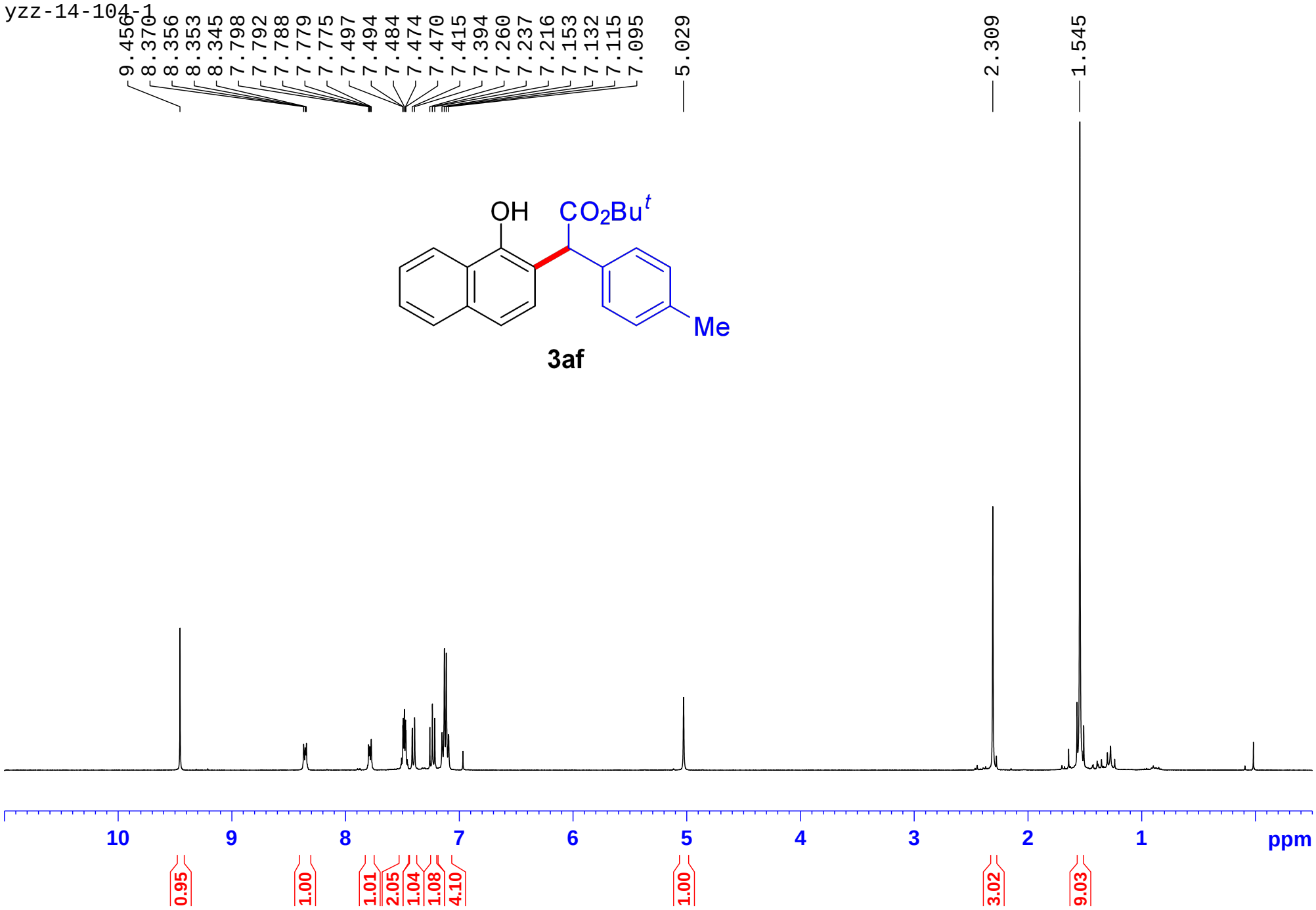
174.67
151.55
147.09
144.63
134.57
128.77
128.43
127.28
126.90
126.43
125.60
123.77
122.56
120.58
115.46
84.82
77.32
77.00
76.68
56.97
27.91



3ae



yzz-14-104-1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8.356
8.353
8.345
7.798
7.792
7.788
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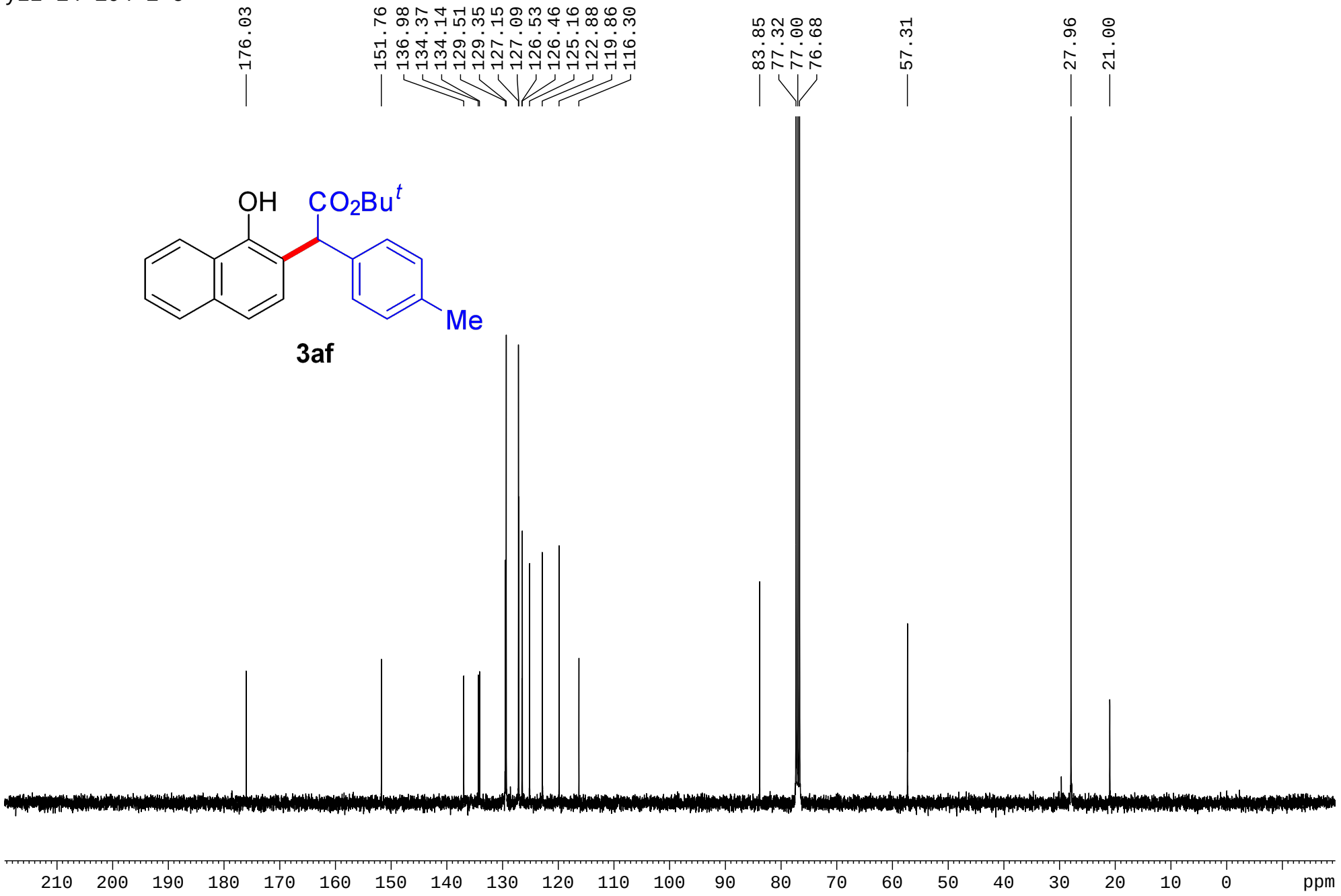
7.775
7.497
7.494
7.484
7.474
7.470
7.415
7.394
7.260
7.237
7.216
7.153
7.132
7.115
7.095
5.029
2.309
1.545
OH
CO2Bu^t
Me
3af
10
9
8
7
6
5
4
3
2
1
ppm
0.95
1.00
1.01
2.05
1.04
1.08
4.10
1.00
3.02
9.03

yzz-14-104-1-c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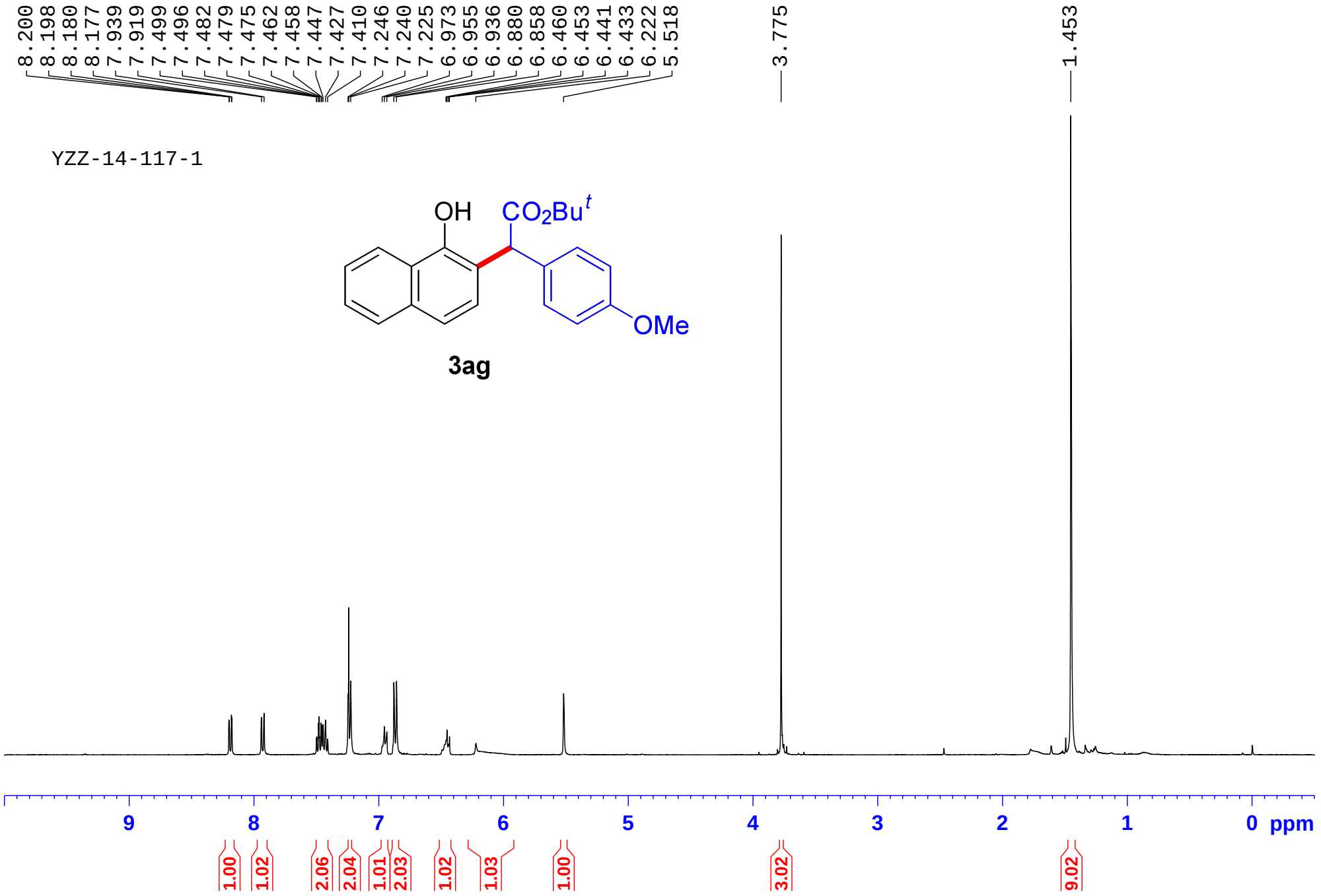
151.76
136.98
134.37
134.14
129.51
129.35
127.15
127.09
126.53
126.46
125.16
122.88
119.86
116.30
83.85
77.32
77.00
76.68
57.31
27.96
21.00
OH
CO2Bu^t
Me
3af
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.180
8.177
7.939
7.919
7.499
7.496
7.482
7.479
7.475
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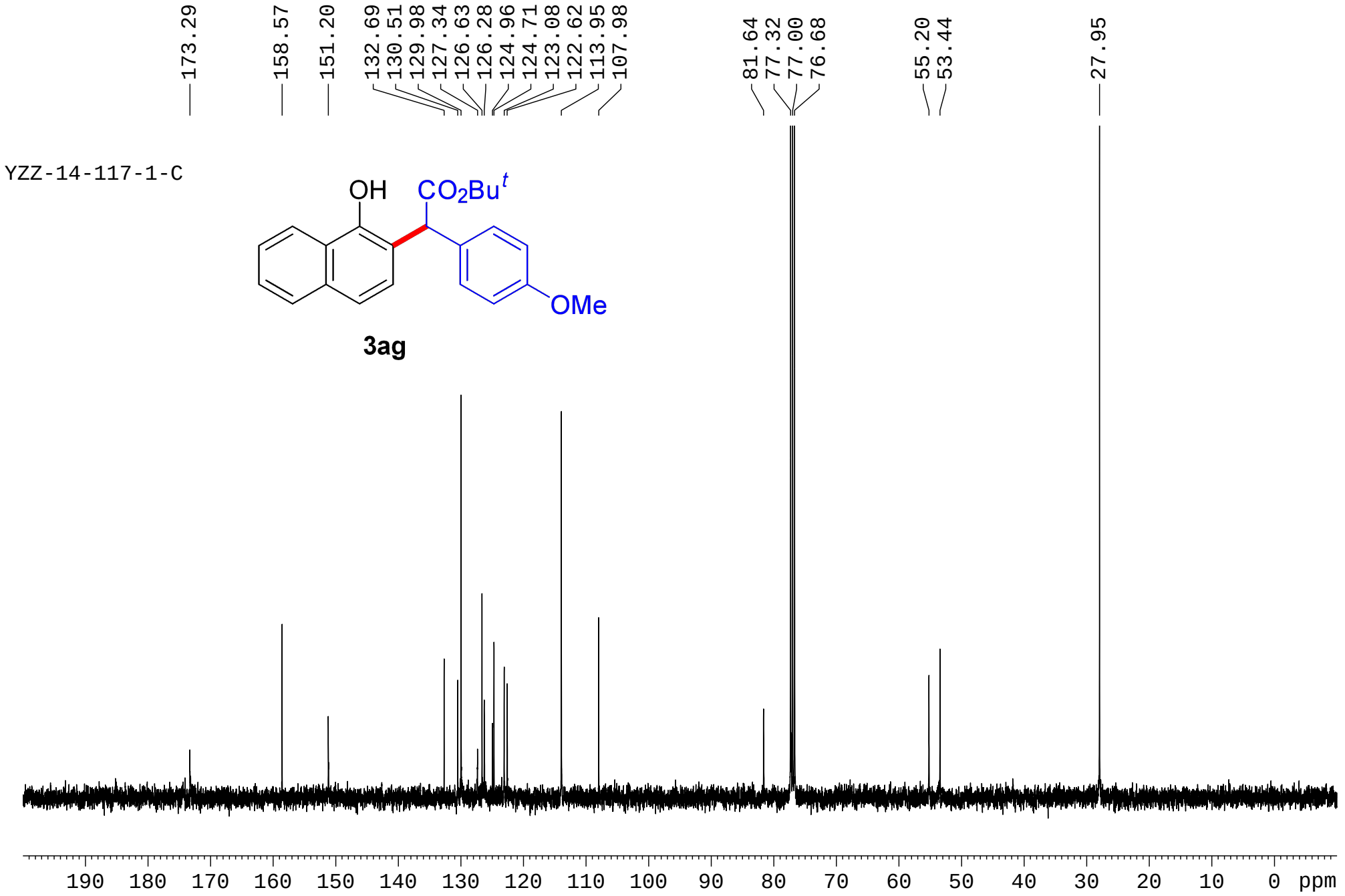
7.458
7.447
7.427
7.410
7.246
7.240
7.225
6.973
6.955
6.936
6.880
6.858
6.460
6.453
6.441
6.433
6.222
5.518
3.775
1.453
YZZ-14-117-1
OH
CO2Bu^t
OMe
3ag
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.02
2.06
2.04
1.01
2.03
1.02
1.03
1.00
3.02
9.02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158.57
151.20
132.69
130.51
129.98
127.34
126.63
126.28
124.96
124.71
123.08
122.62
113.95
107.98
81.64
77.32
77.00
76.68
55.20
53.44
27.95
YZZ-14-117-1-C
OH
CO2Bu^t
OMe
3ag
190
180
170
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150
140
130
120
110
100
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60
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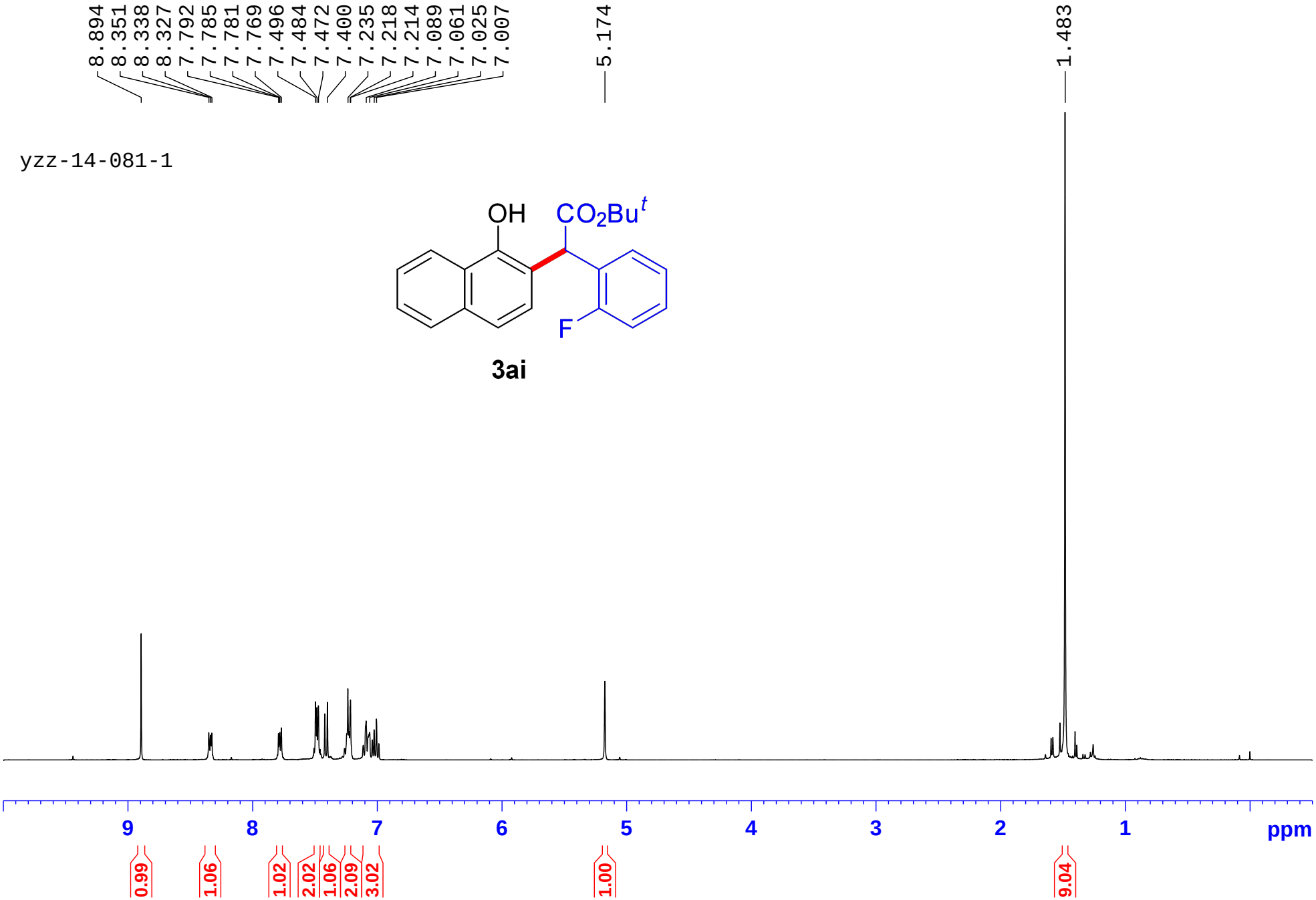
40
30
20
10
0
ppm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7.785
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7.769
7.496
7.484
7.472
7.400
7.235
7.218
7.214
7.089
7.061
7.025
7.007
5.174
1.483
yzz-14-081-1
OH
CO2Bu^t
F
3ai
9
8
7
6
5
4
3
2
1
ppm
0.99
1.06
1.02
2.02
1.06
2.09
3.02
1.00
9.04

yzz-14-081-1-c

174.81
161.92
159.47
151.94
134.48
129.41
129.35
129.26
127.22
126.65
126.24
125.31
124.19
124.16
123.95
123.81
122.72
120.28
115.46
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113.95
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77.32
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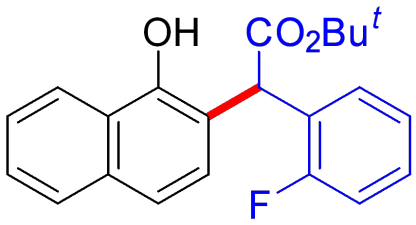
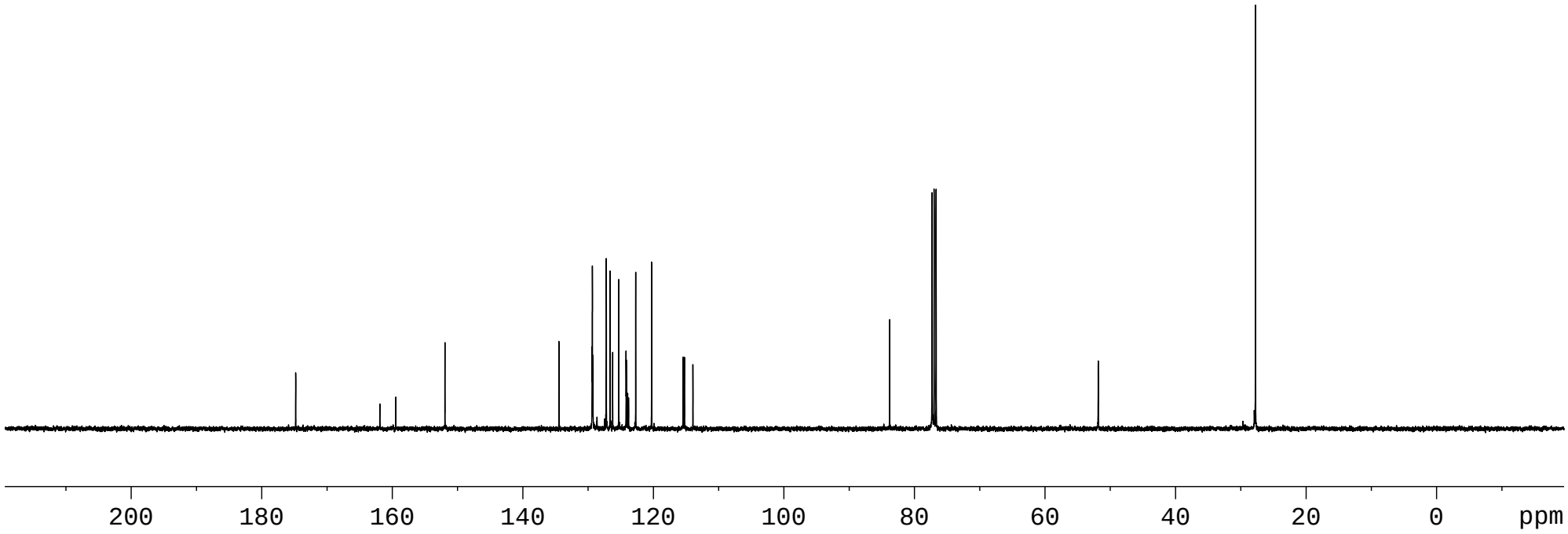
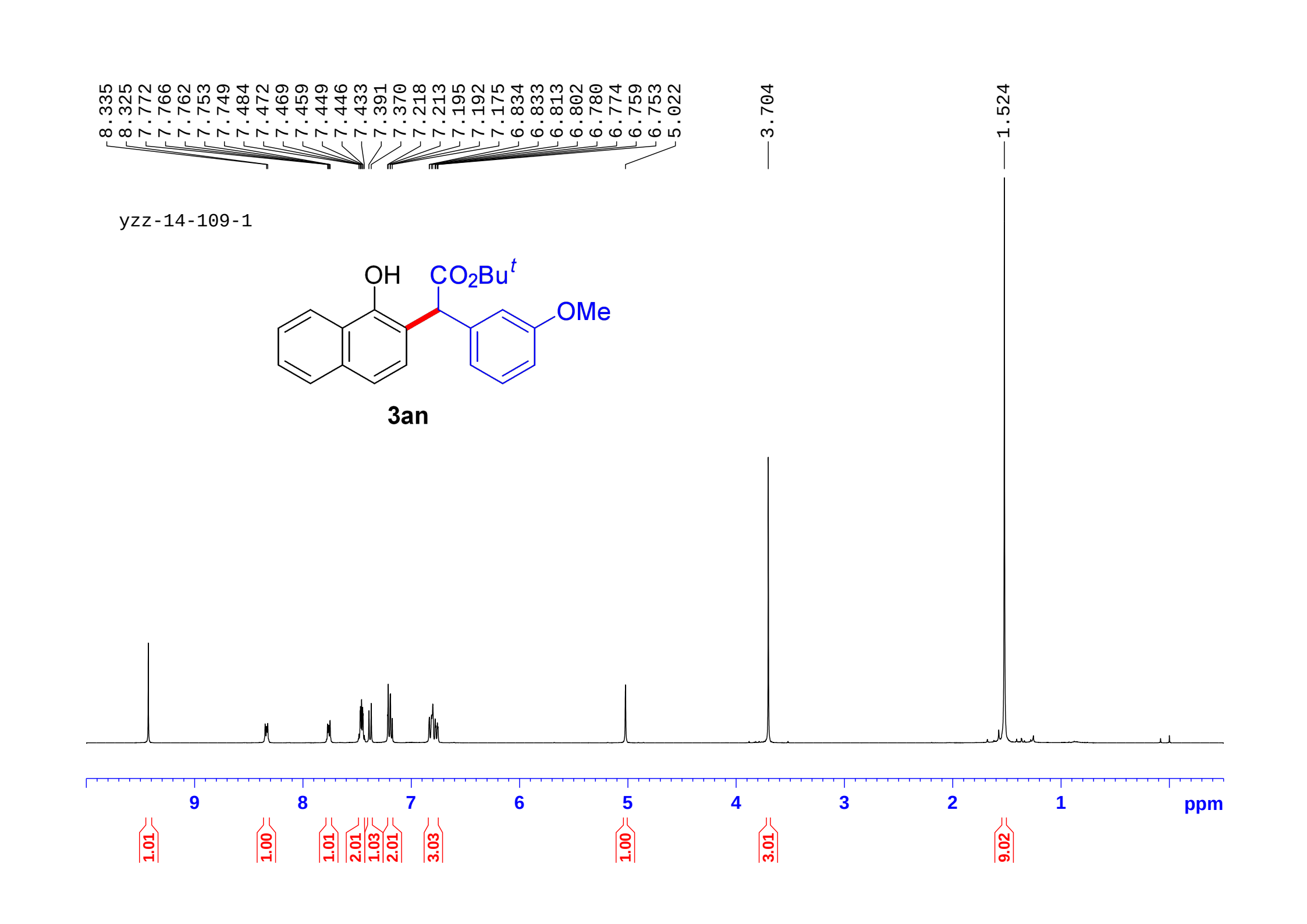
76.68
51.84
27.75



3ai

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7.472
7.469
7.459
7.449
7.446
7.433
7.391
7.370
7.218
7.213
7.195
7.192
7.175
6.834
6.833
6.813
6.802
6.780
6.774
6.759
6.753
5.022
3.704
1.524
yzz-14-109-1
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CO2Bu^t
OMe
3an
9
8
7
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5
4
3
2
1
ppm
1.01
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1.01
2.01
1.03
2.01
3.03
1.00
3.01
9.02

175.69
159.72
151.77
138.71
134.40
129.59
129.46
127.09
126.49
125.17
122.85
119.89
119.64
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113.53
112.31
83.94
77.32
77.00
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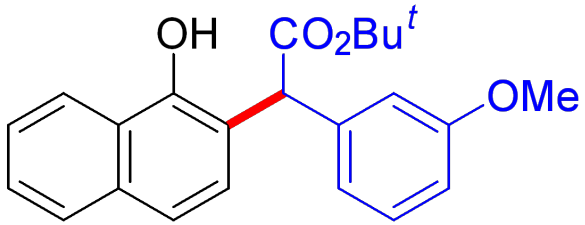
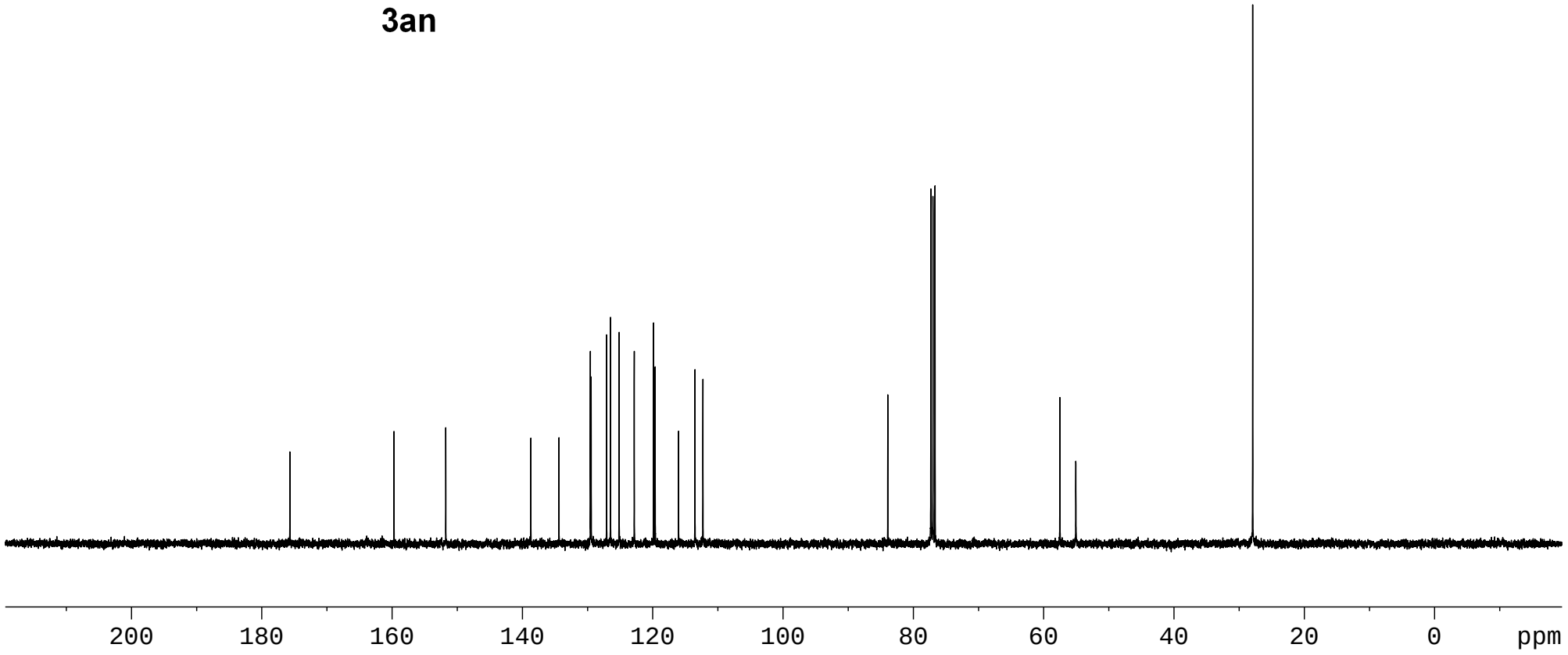
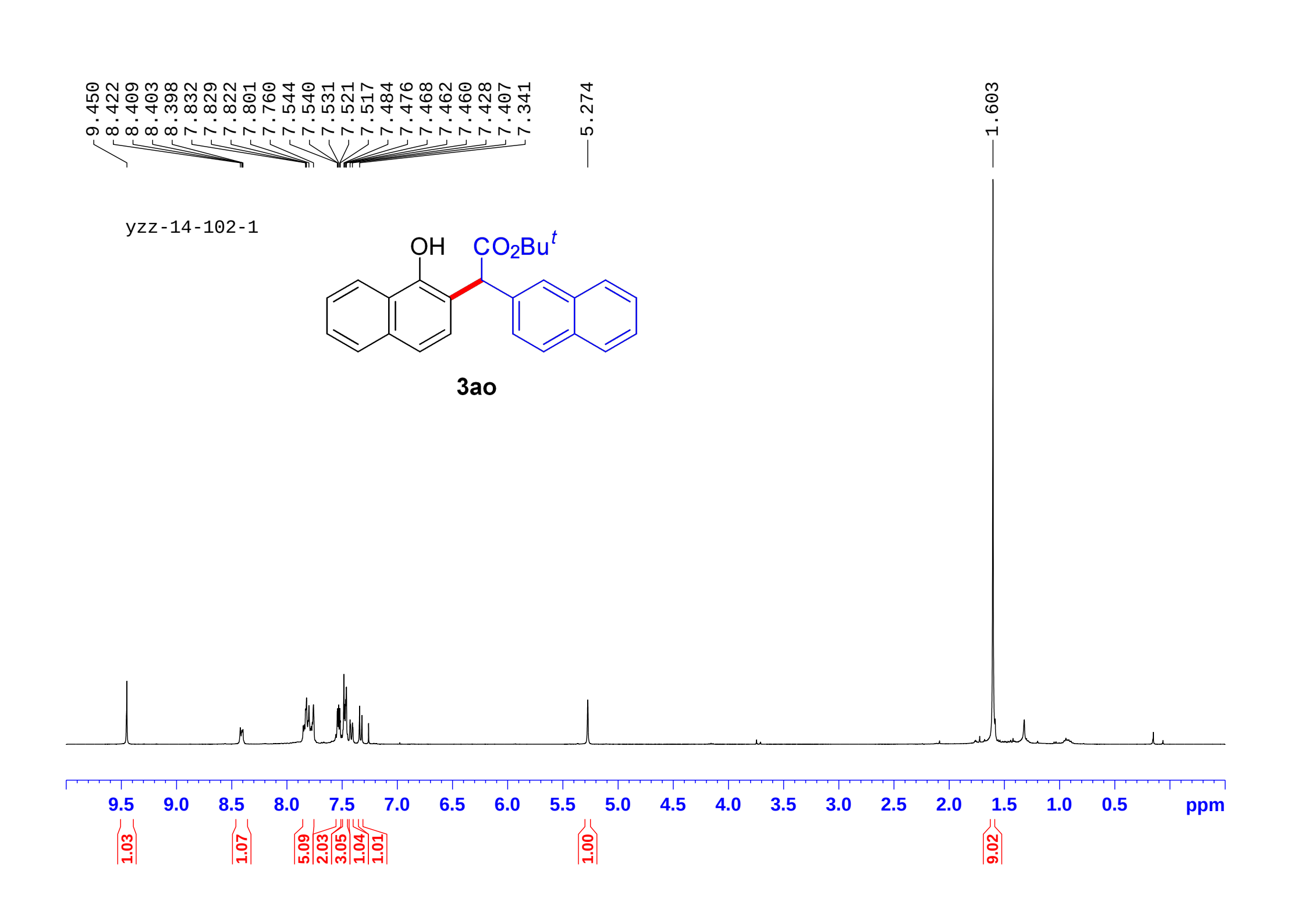
57.52
55.08
27.93

yzz-14-108-1



3an

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7.829
7.822
7.801
7.760
7.544
7.540
7.531
7.521
7.517
7.484
7.476
7.468
7.462
7.460
7.428
7.407
7.341
5.274
1.603
yzz-14-102-1
OH
CO2Bu^t
3ao
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
ppm
1.03
1.07
5.09
2.03
3.05
1.04
1.01
1.00
9.02

yzz-14-102-1-c

175.66
151.84
134.53
134.43
133.27
132.50
129.46
128.41
128.08
127.48
127.14
126.54
126.53
126.17
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125.58
125.22
122.86
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116.12
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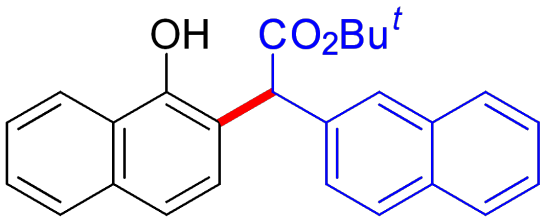
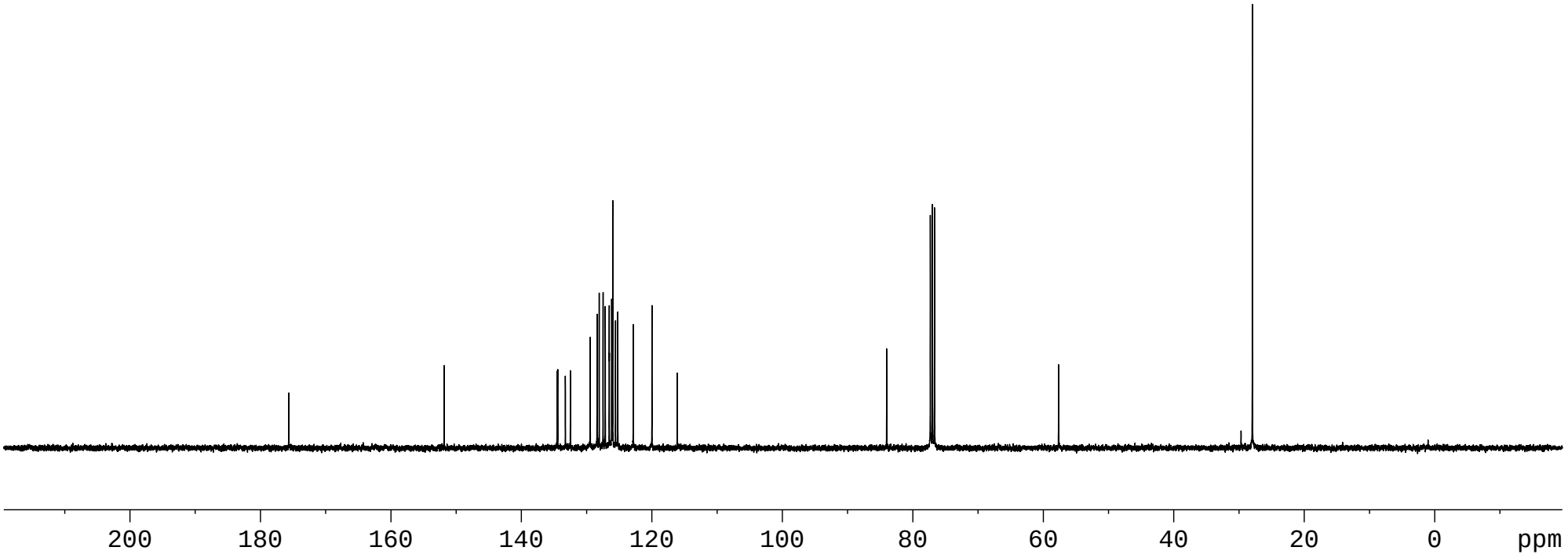
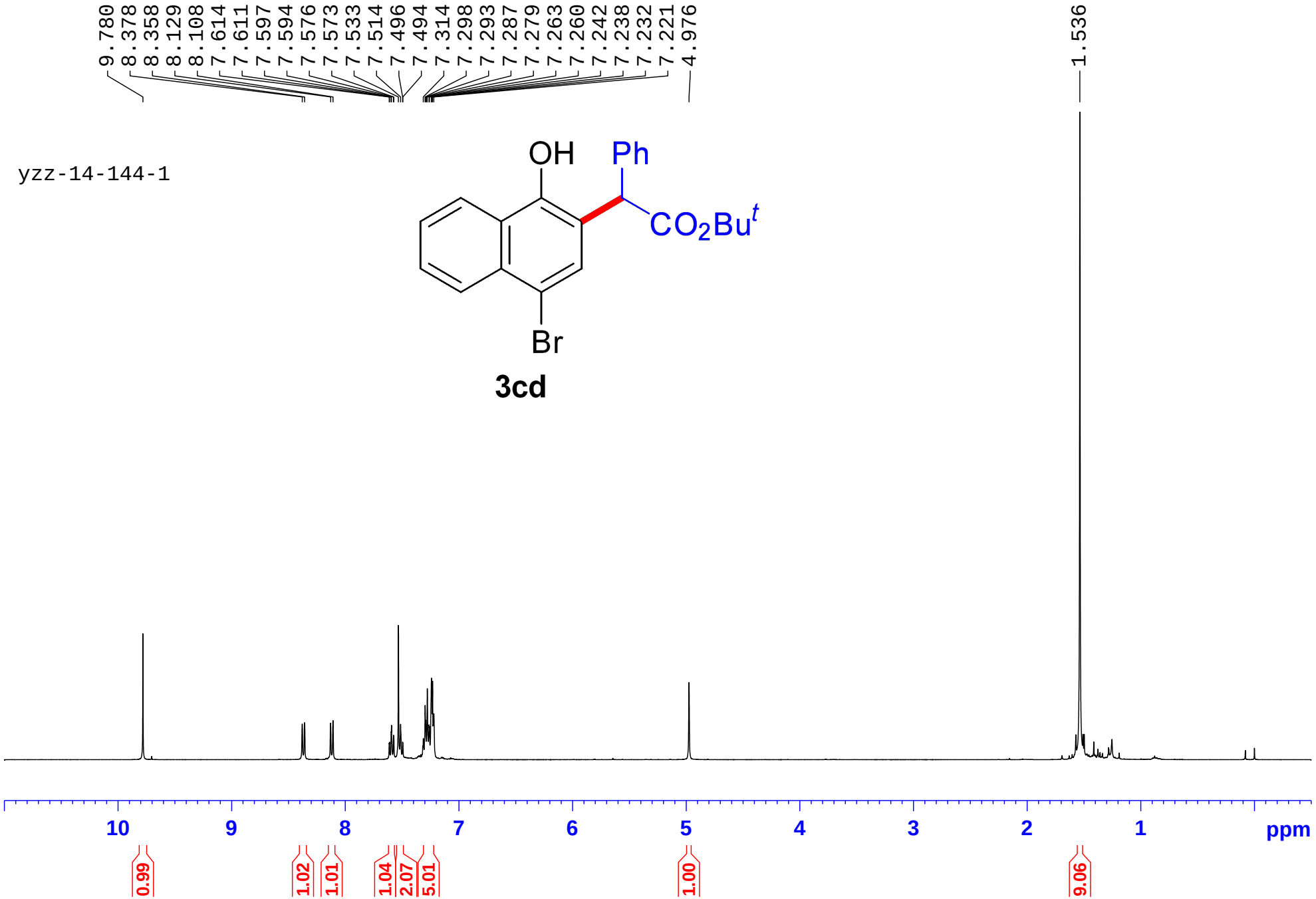
77.32
77.00
76.68
57.65
27.96



3ao

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7.597
7.594
7.576
7.573
7.533
7.514
7.496
7.494
7.314
7.298
7.293
7.287
7.279
7.263
7.260
7.242
7.238
7.232
7.221
4.976
1.536
yzz-14-144-1
OH
Ph
CO2But
Br
3cd
10
9
8
7
6
5
4
3
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1.04
2.07
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1.00
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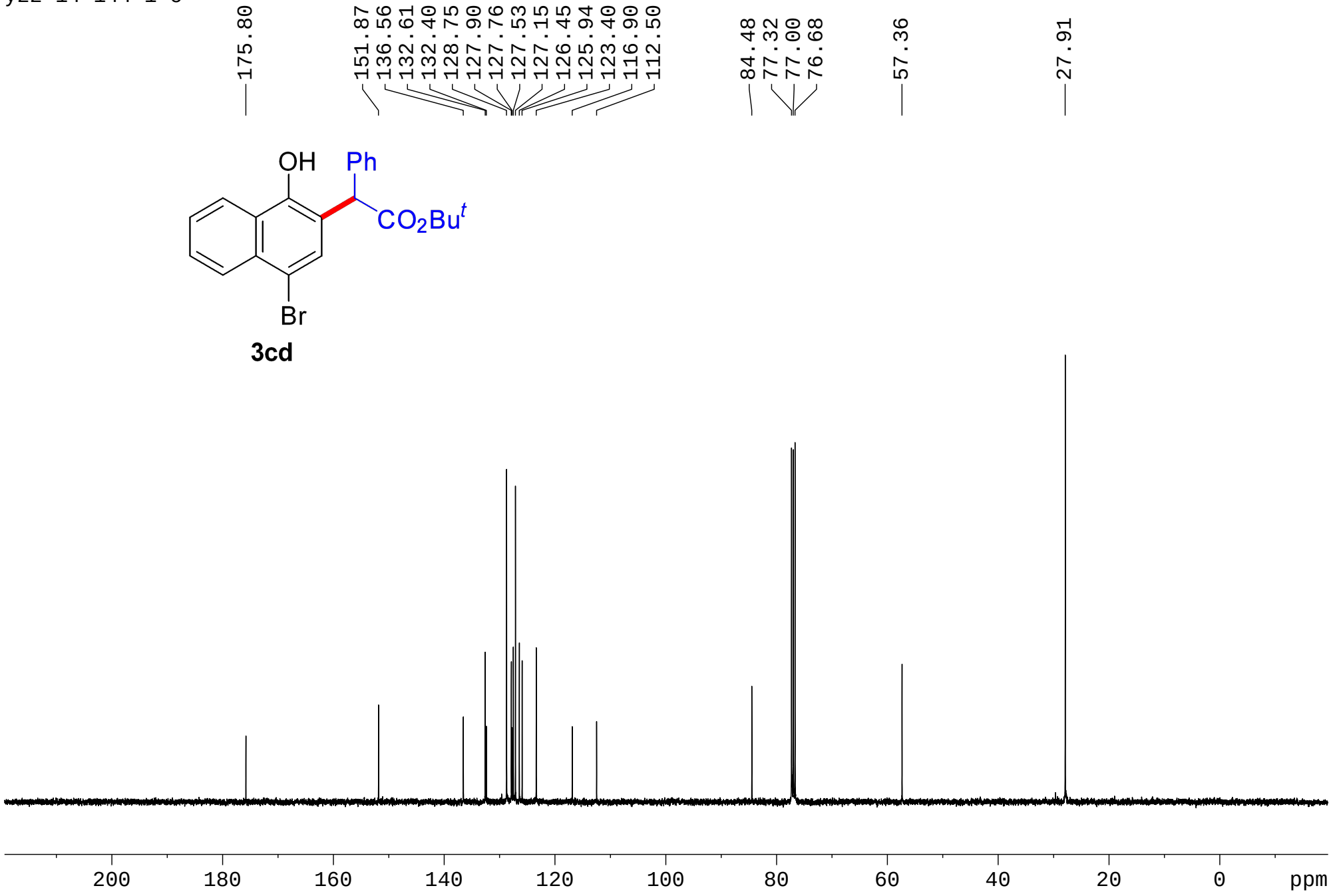
yzz-14-144-1-c



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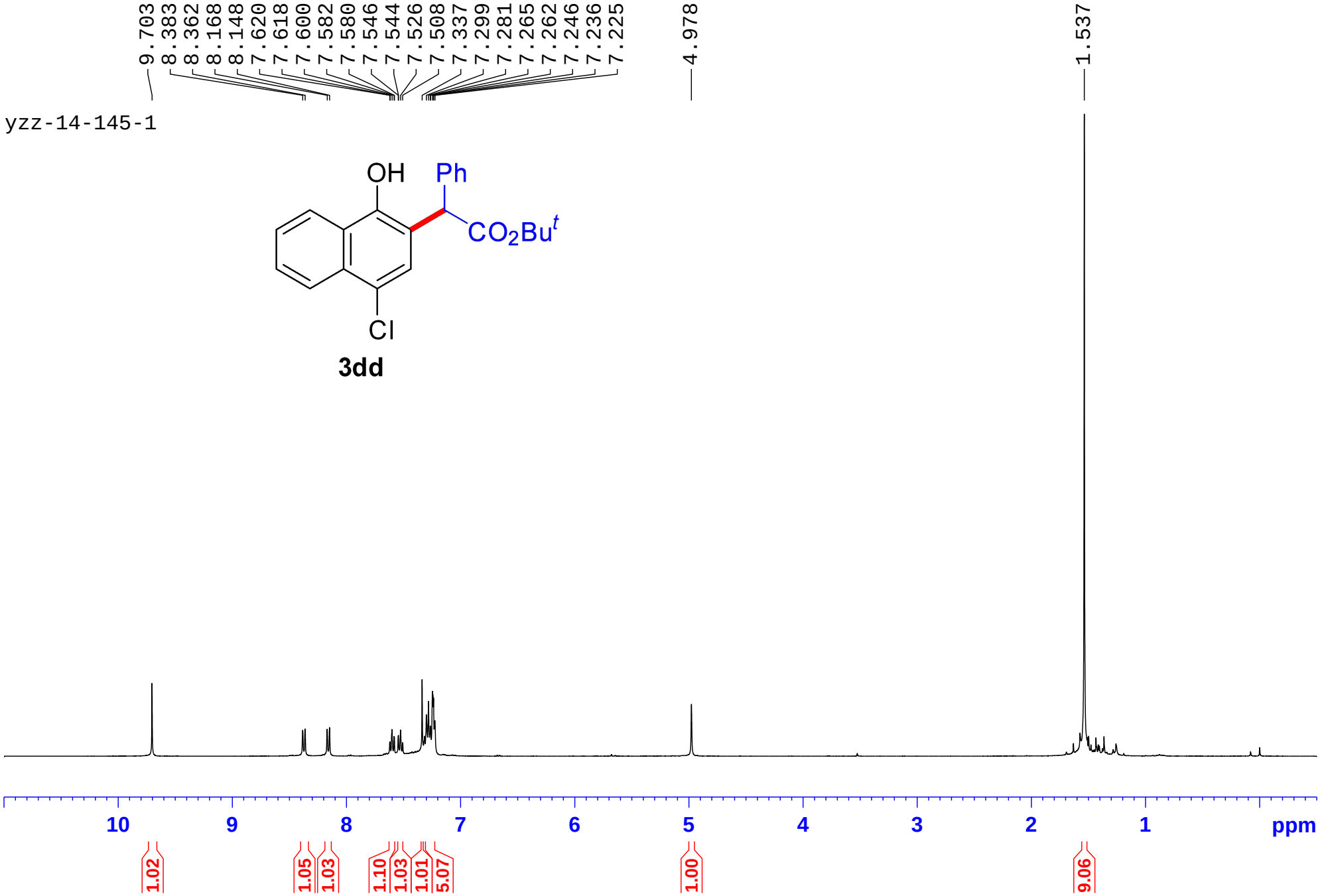
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8.148
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7.618
7.600
7.582
7.580
7.546
7.544
7.526
7.508
7.337
7.299
7.281
7.265
7.262
7.246
7.236
7.225
4.978
1.537
yzz-14-145-1
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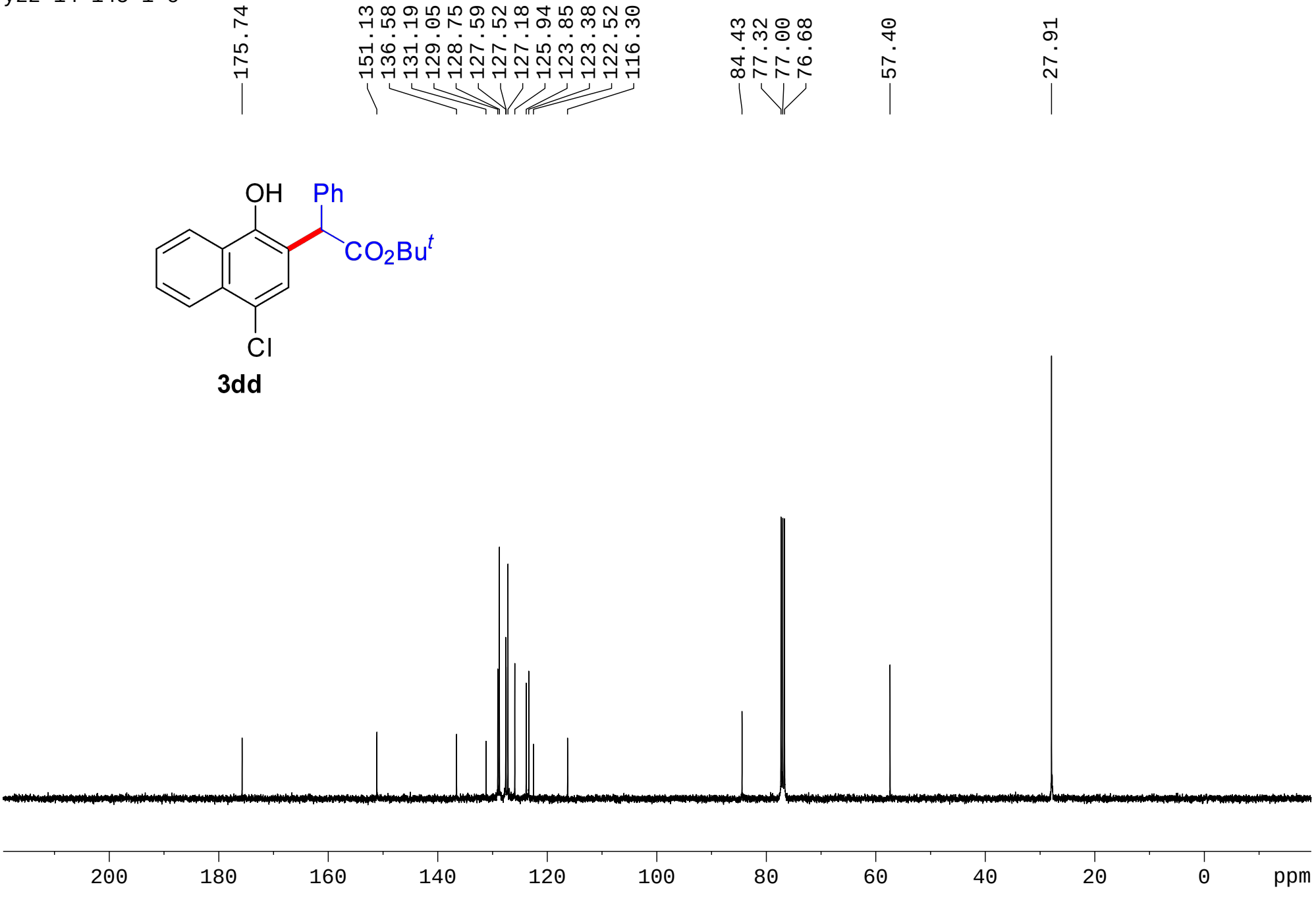
Ph
CO2Bu^t
Cl
3dd
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.05
1.03
1.10
1.03
1.01
5.07
1.00
9.06

yzz-14-145-1-c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136.58
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129.05
128.75
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127.52
127.18
125.94
123.85
123.38
122.52
116.30
84.43
77.32
77.00
76.68
57.40
27.91
OH
Ph
CO2But
Cl
3dd
200
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160
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120
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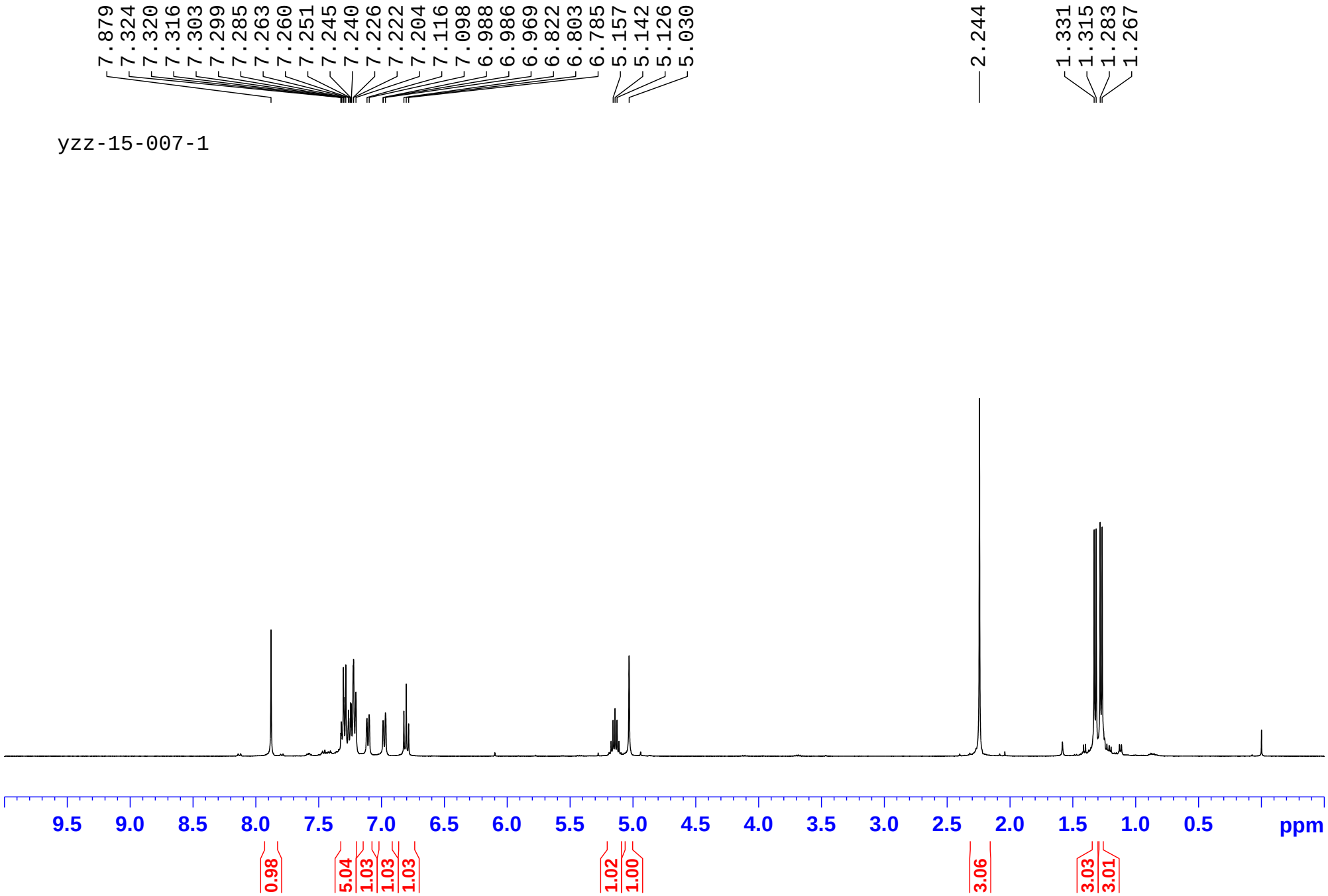
80
60
40
20
0
ppm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7.320
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7.303
7.299
7.285
7.263
7.260
7.251
7.245
7.240
7.226
7.222
7.204
7.116
7.098
6.988
6.986
6.969
6.822
6.803
6.785
5.157
5.142
5.126
5.030
2.244
1.331
1.315
1.283
1.267
yzz-15-007-1
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
ppm
0.98
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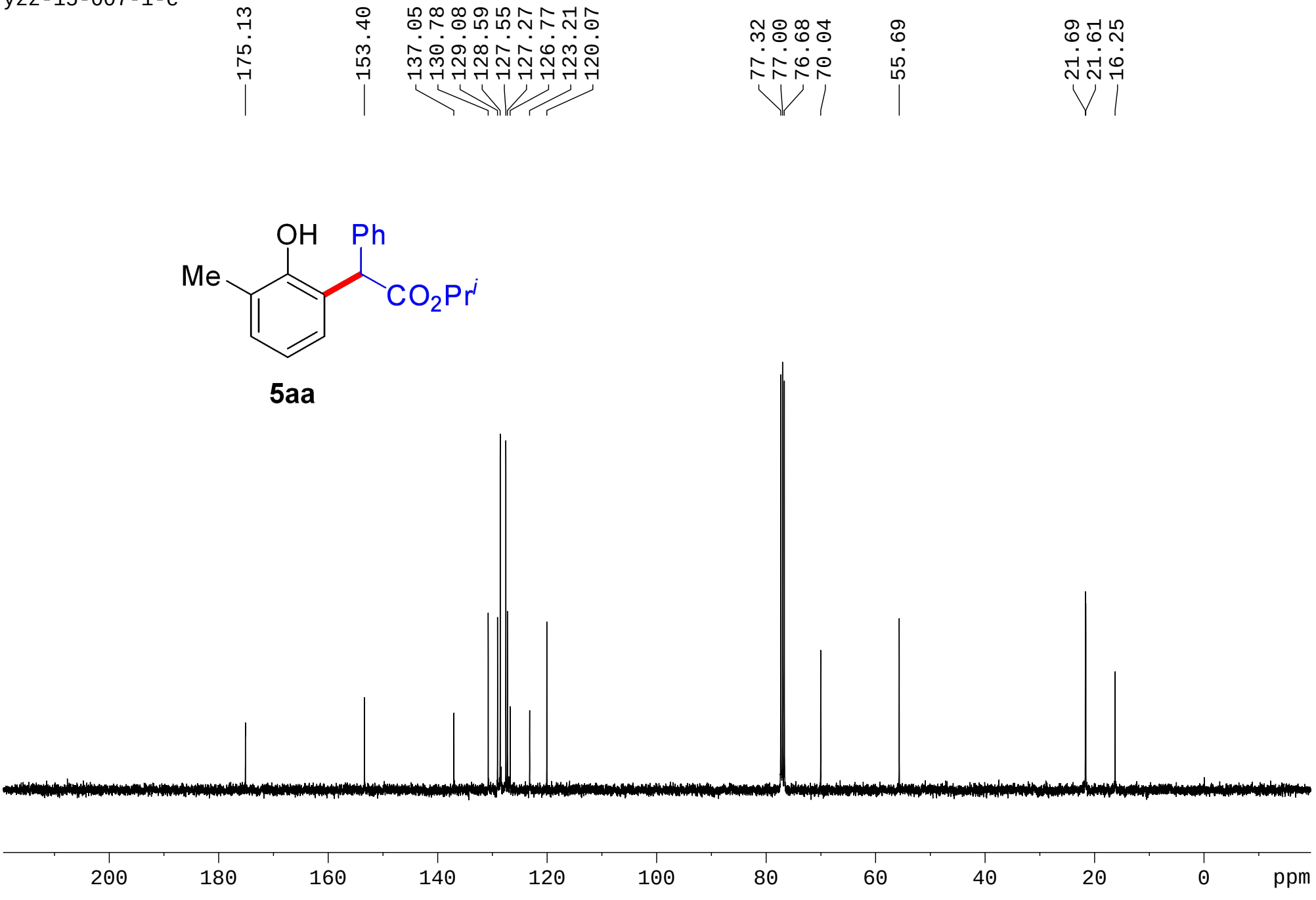
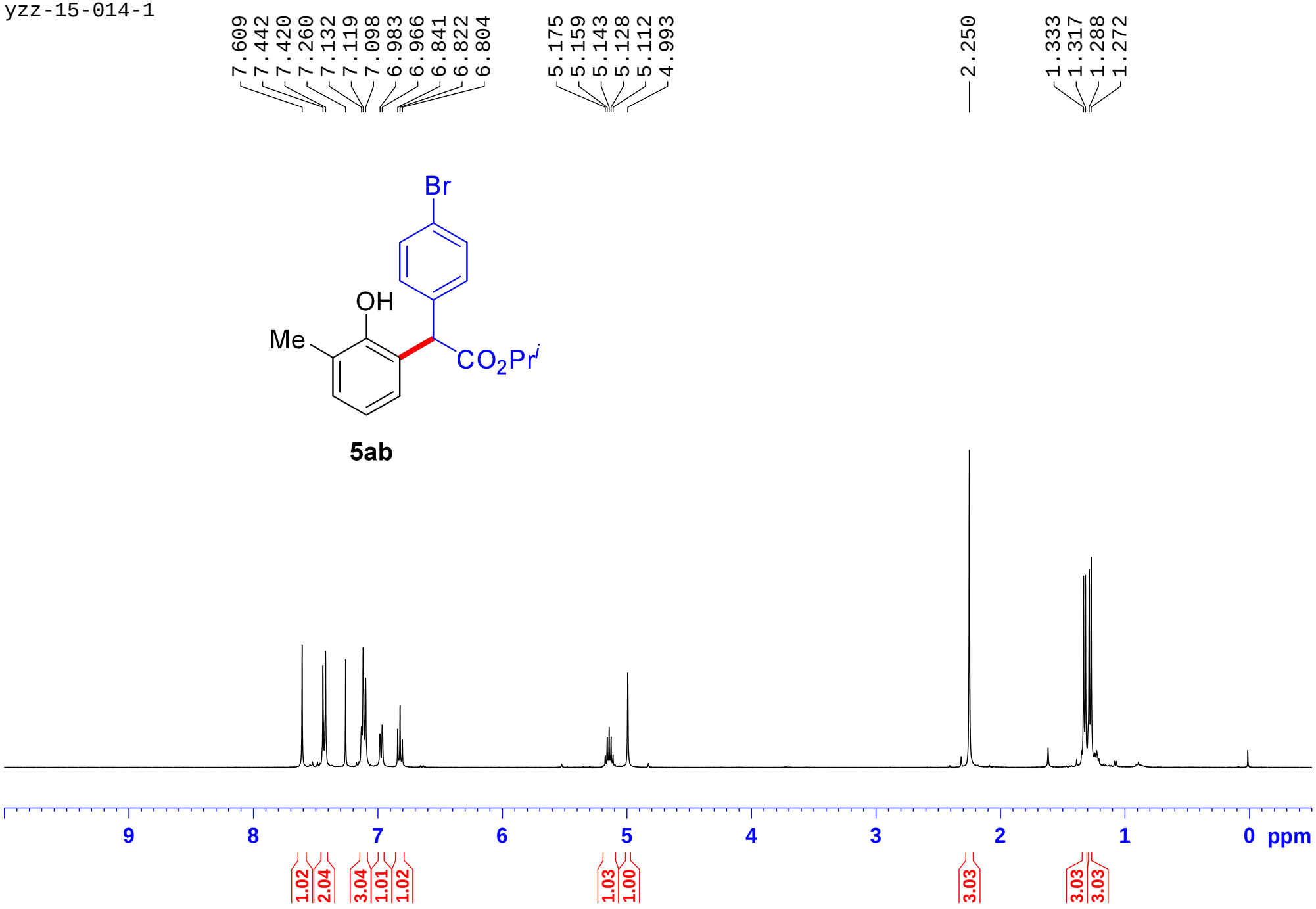
1.03
1.03
1.02
1.00
3.06
3.03
3.01

yzz-15-007-1-c



5aa

yzz-15-014-1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7.119
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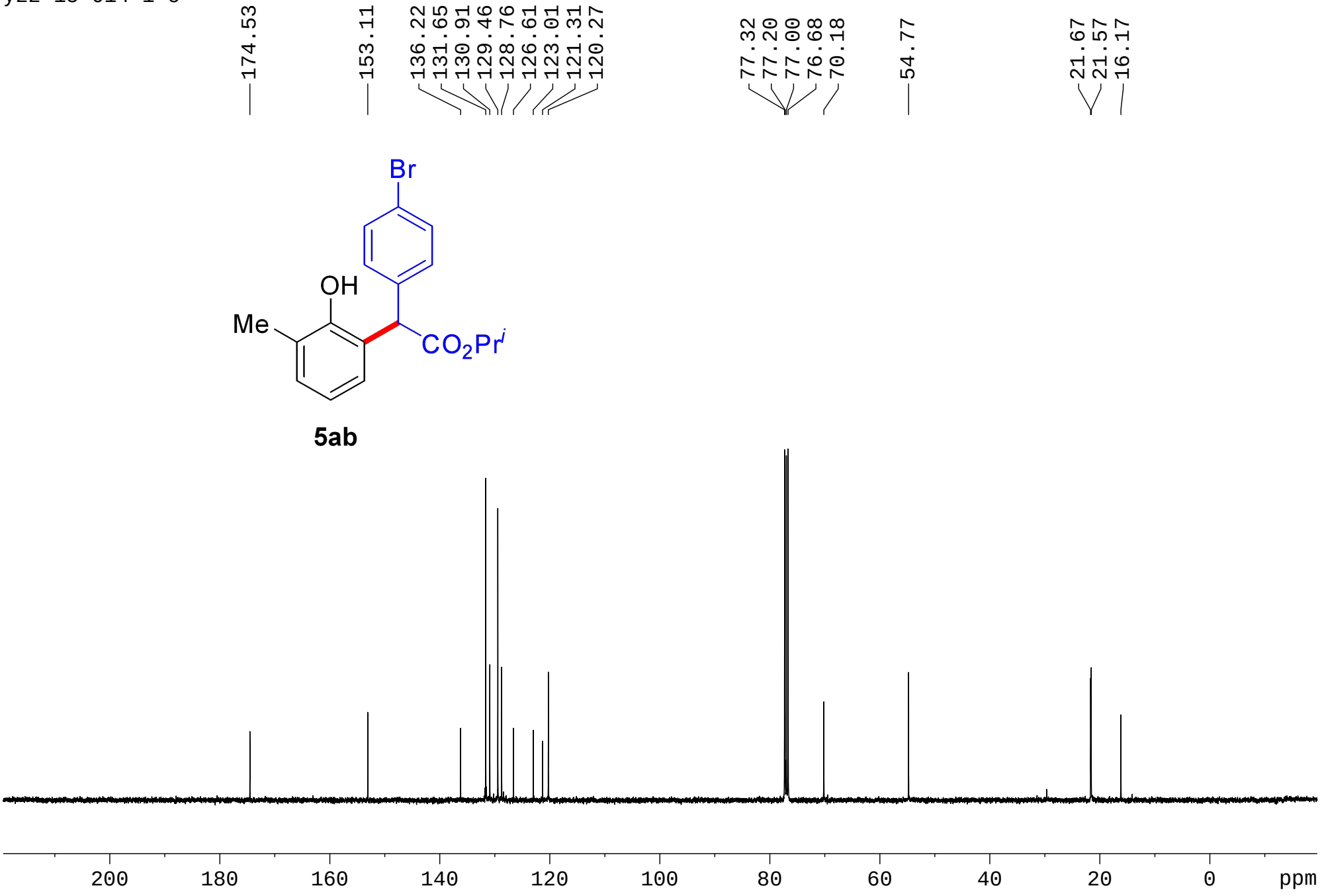
6.841
6.822
6.804
5.175
5.159
5.143
5.128
5.112
4.993
2.250
1.333
1.317
1.288
1.272
Br
OH
Me
CO2Pri
5ab
9
8
7
6
5
4
3
2
1
0 ppm
1.02
2.04
3.04
1.01
1.02
1.03
1.00
3.03
3.03
3.03

yzz-15-014-1-c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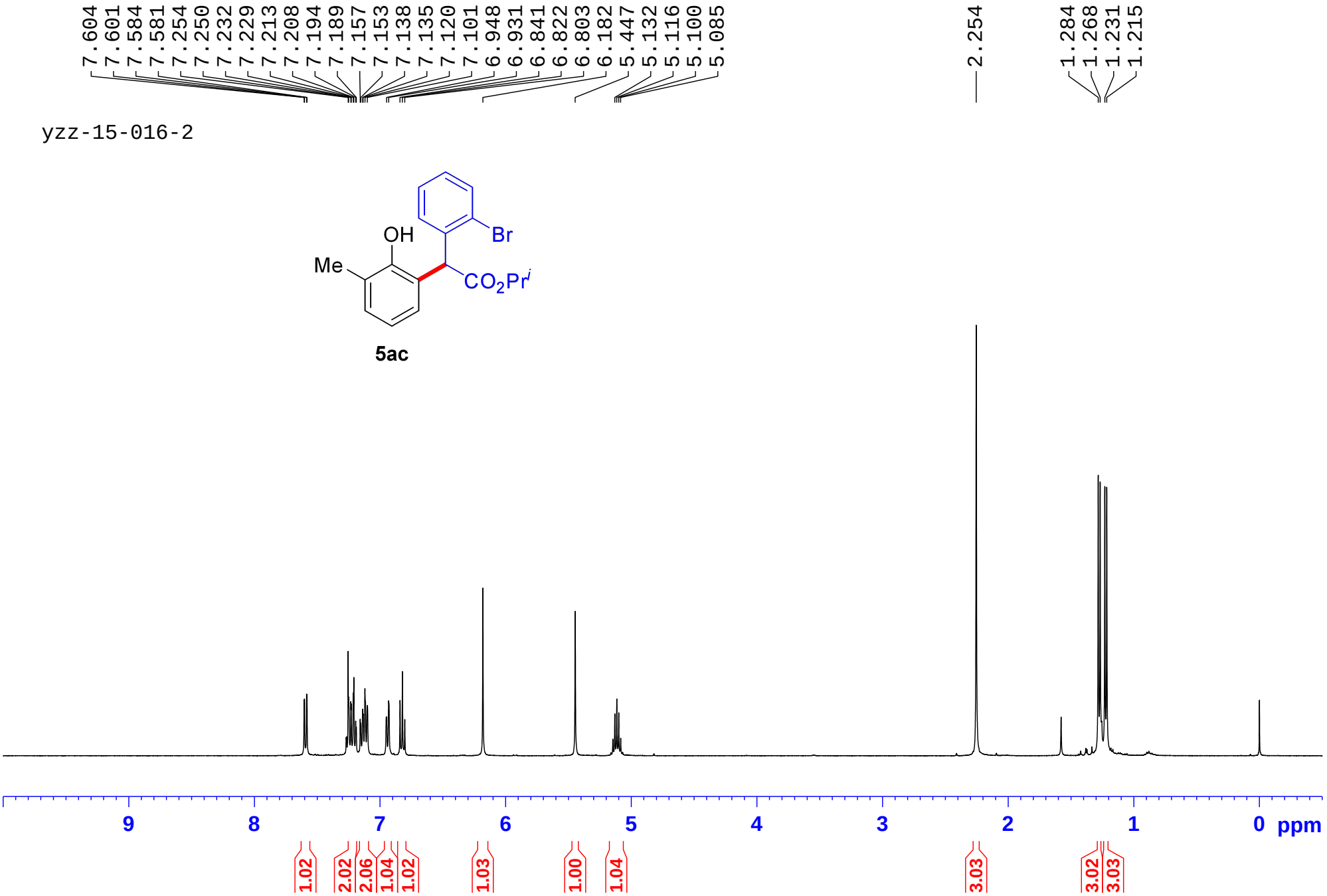
123.01
121.31
120.27
77.32
77.20
77.00
76.68
70.18
54.77
21.67
21.57
16.17
Br
OH
Me
CO2Pri
5ab
200
180
160
140
120
100
80
60
40
20
0
ppm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7.601
7.584
7.581
7.254
7.250
7.232
7.229
7.213
7.208
7.194
7.189
7.157
7.153
7.138
7.135
7.120
7.101
6.948
6.931
6.841
6.822
6.803
6.182
5.447
5.132
5.116
5.100
5.085
2.254
1.284
1.268
1.231
1.215
yzz-15-016-2
OH
Br
Me
CO2Pri
5ac
9
8
7
6
5
4
3
2
1
0
ppm
1.02
2.02
2.06
1.04
1.02
1.03
1.00
1.04
3.03
3.02
3.03

yzz-15-016-2-c

172.91
152.70
136.71
133.04
130.60
130.25
128.94
128.36
127.53
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125.02
122.66
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77.00
76.68
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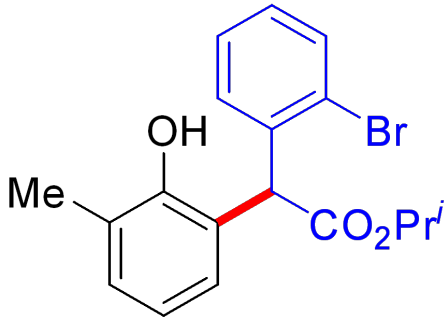
53.93
21.55
16.08



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