Supporting Information

$InCl_3$-catalyzed 5-*exo*-*dig* cyclization/1,6-conjugate addition of *N*-propargylamides with *p*-QMs to construct oxazole derivatives

Guang-Ming Nan,[a] Xue Li, [a] Tian-Yu Yao,[b] Ting-Xun Yan,[b] Li-Rong Wen,[b,*] and Ming Li[a,b,*]

[a]University and College Key Lab of Natural Product Chemistry and Application in Xinjiang, Yili Normal University, Yining 835000, China

[b]State Key Laboratory Base of Eco-Chemical Engineering, College of Chemistry and Molecular Engineering, Qingdao University of Science & Technology, Qingdao 266042, China

Table of the contents

1. General methods

Unless noted, all commercial reagents and solvents were used without further purification. Melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected. ^{1}H NMR spectra were recorded on 500 MHz and ^{13}C NMR spectra were recorded on 125 MHz by using a Bruker Avance 500 spectrometer. Chemical shifts were reported in parts per million (δ) relative to tetramethylsilane (TMS). High-resolution mass spectra were obtained on a Waters Xevo G2-XS QTof spectrometer with an ESI source. The X-ray single-crystal diffraction was performed on Saturn 724+ instrument. The IR spectra were recorded on an FT-IR spectrometer, and only major peaks are reported in cm^{-1}. Silica gel (200–300 mesh) for column chromatography and silica GF254 for TLC were produced by Qingdao Marine Chemical Company (China).

2. Molecular structure and crystallographic data of 3ad

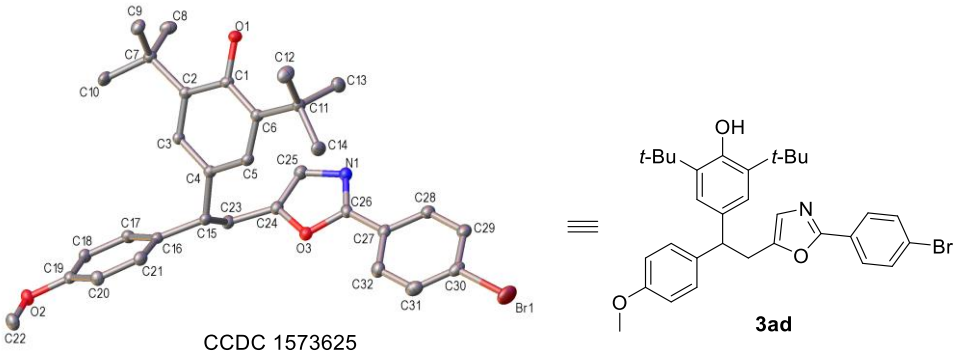


Figure S1. X-ray crystal structure of **3ad**

Table S1. Crystal data and structure refinement for **3ad**

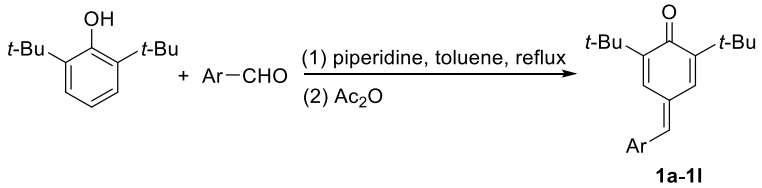
Empirical formula	C32 H36 Br N O3
Formula weight	562.53
Temperature	173.15 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.157(3) Å
	b = 11.335(4) Å
	c = 13.795(4) Å
Volume	1405.6(7) Å^3
Z	2
Density (calculated)	1.329 Mg/m^3
Absorption coefficient	1.495 mm^{-1}
F(000)	588
Crystal size	0.174 x 0.121 x 0.032 mm^3
Theta range for data collection	1.598 to 27.418°.

Index ranges	-14<=h<=14, -14<=k<=14, -17<=l<=17
Reflections collected	19581
Independent reflections	6349 [R(int) = 0.0507]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.88668
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6349 / 0 / 342
Goodness-of-fit on F^2	1.153
Final R indices [I>2sigma(I)]	R1 = 0.0640, wR2 = 0.1122
R indices (all data)	R1 = 0.0795, wR2 = 0.1198
Extinction coefficient	n/a
Largest diff. peak and hole	0.477 and -0.585 e.Å^{-3}

3. Preparation of starting materials

3.1 Preparation of *para*-quinone methides (*p*-QMs)

1a-1l were synthesized according to the following procedure[1]:

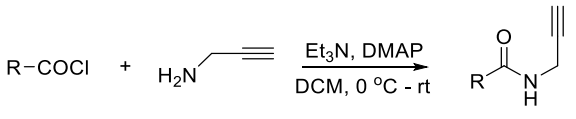


1a-1l

In a Dean-Stark apparatus, a solution of phenols (1 equiv) and the corresponding aldehydes (1 equiv) in toluene was heated to reflux. Piperidine (2 equiv) was added dropwise within 1 h. The reaction mixture was continued to reflux for 3 h. After cooling just below the boiling point of the reaction mixture, acetic anhydride (2 equiv) was added and stirring was continued for 15 min. Then the reaction mixture was poured into water and extracted with CH_2Cl_2. The combined organic phases were dried over anhydrous $MgSO_4$ and solvents were removed under reduced pressure. The crude products were purified by flash column chromatography and further recrystallized from *n*-hexane, affording the desired *p*-QMs **1a-1l**.

1m[2], **1n**[2] and **1o**[3] were prepared according to the reported procedures.

3.2 Preparation of *N*-propargylamides[4]

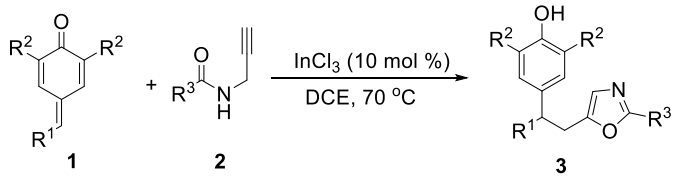


2

To a solution of propargyl amine (138 μL, 2 mmol), DMAP (4.8 mg, 0.04 mmol) and Et_3N (274 μL, 2 mmol) in CH_2Cl_2 (5 mL) at 0 °C was added acid chloride (2 mmol) in CH_2Cl_2 (1 mL). The reaction mixture was stirred at 0 °C for 30 min, then allowed to warm to rt for 3 h. The

reaction was quenched by the addition of H_2O (5 mL). The layers were separated and the aqueous fraction was extracted with CH_2Cl_2 (3 × 5 mL). The combined organic fractions were washed with 10% (w/w) aqueous citric acid, dried ($MgSO_4$) and concentrated in *vacuo* to afford *N*-propargylamides **2**.

4. Synthesis of products 3

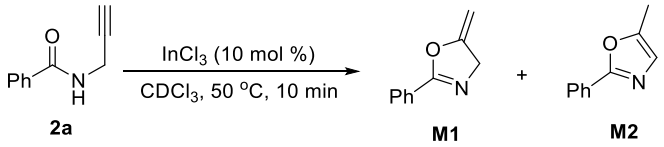


p-QMs **1** (0.5 mmol, 1.0 equiv), substituted *N*-propargylamides **2** (0.75 mmol, 1.5 equiv) and $InCl_3$ (0.05 mmol, 10 mol%) were dissolved in DCE (2.5 mL). The reaction mixture was stirred at 70 °C. After the reaction was completed (detected by TLC, PE/EA = 20:1), solvent was directly removed under reduced pressure and the crude mixture was purified by silica gel flash column chromatography (PE/EA = 20:1 to 10:1) to afford the pure products **3**.

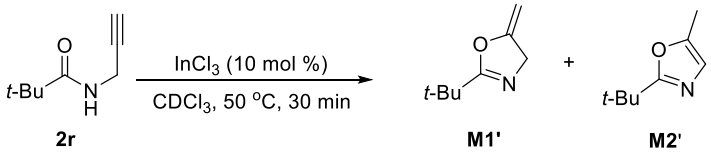
5. Synthesis of compound 4

To a solution of **3aa** (0.5 mmol, 1.0 equiv) in dry DCM (10 mL), DDQ (0.5 mmol, 1.0 equiv) was added. The reaction mixture was stirred at rt for 10 min and then filtered through a pad of celite. The solvent was removed under reduced pressure and the residue was purified by silica gel flash column chromatography (PE/EA = 15:1) to afford compound **4**.

6. Observation of cyclization intermediates M1 and M2 by *in situ* ^{1}H NMR



N-propargylamide **2a** (0.1 mmol, 1.0 equiv) and $InCl_3$ (0.01 mmol, 10 mol%) were dissolved in $CDCl_3$ (0.5 mL) in a NMR tube. After heated at 50 °C for 10 min, the reaction mixture was detected by ^{1}H NMR, and the result is as follows. According to their character peaks, **M1**[5] and **M2**[4] were both observed in a ratio of 1:2.5 (Figure S2).



N-propargylamide **2r** (0.1 mmol, 1.0 equiv) and $InCl_3$ (0.01 mmol, 10 mol%) were dissolved in $CDCl_3$ (0.5 mL) in a NMR tube. After heated at 50 °C for 30 min (**2r** is less active than **2a** to

cyclize), the reaction mixture was detected by ^{1}H NMR, and the result is as follows. According to the character peaks, **M1'**[6] and **M2'**[4] were observed in a ratio of 3:97 (Figure S3).

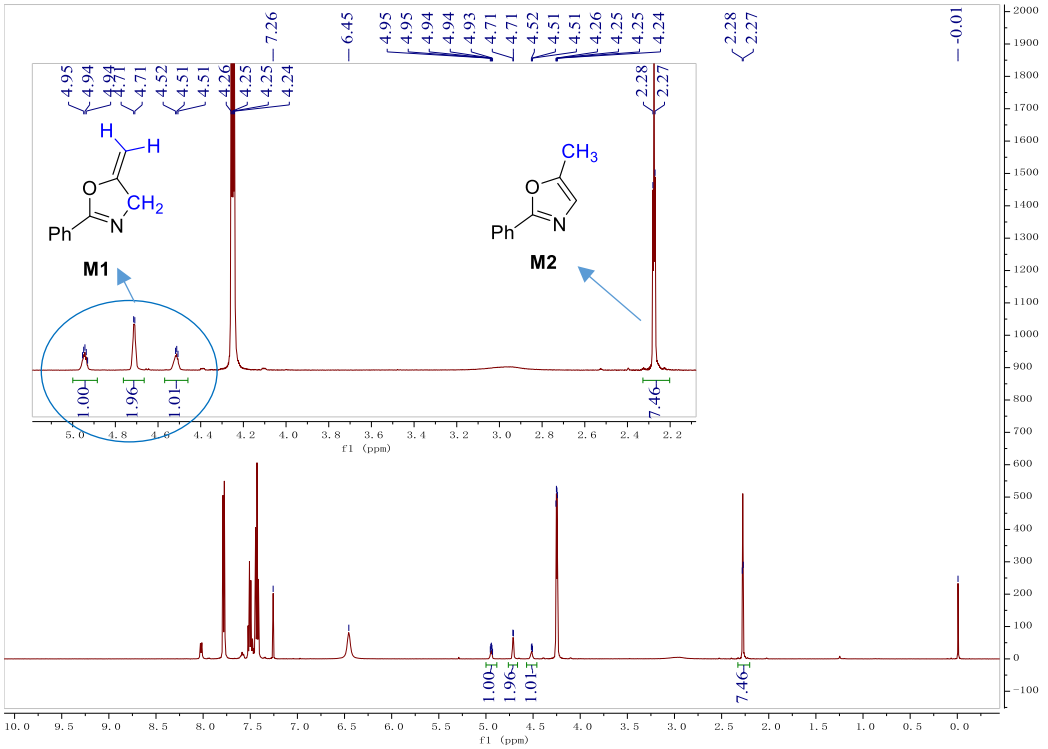


Figure S2. The *in situ* ^{1}H NMR spectrum of cyclization process of **2a**

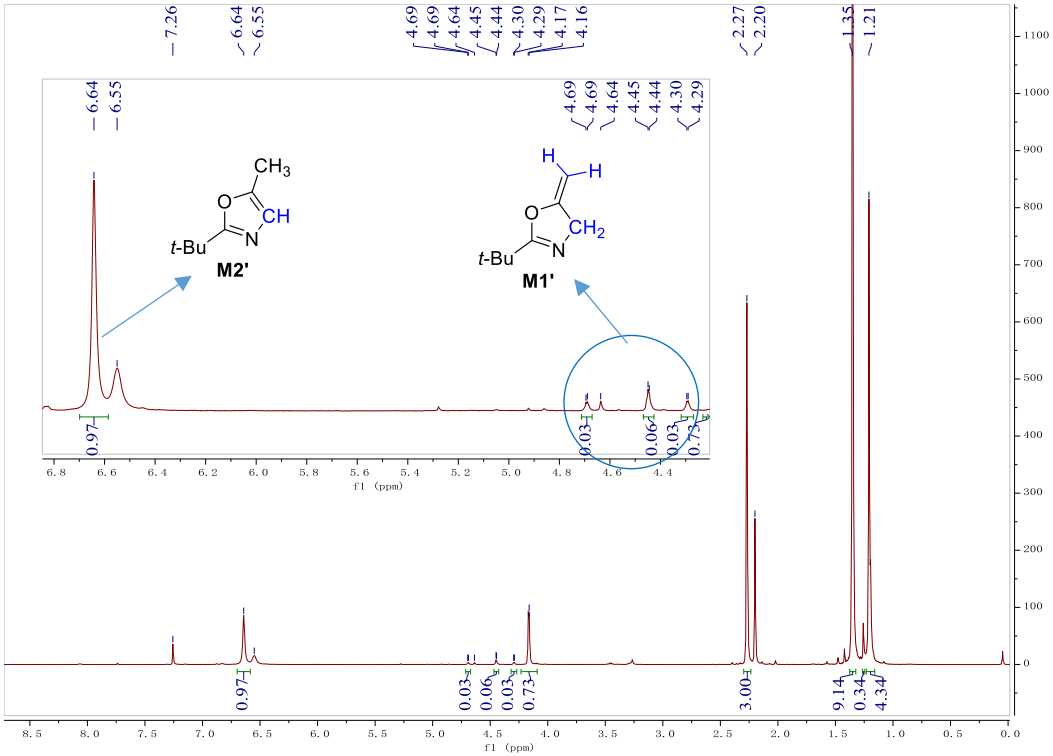
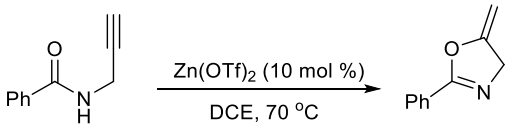


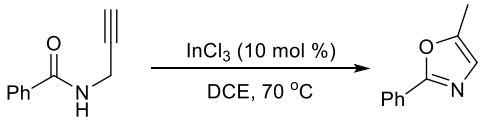
Figure S3. The *in situ* ^{1}H NMR spectrum of cyclization process of **2r**

7. Synthesis of M1[7] and M2



2a **M1**, 70%

N-propargylamide **2a** (0.5 mmol, 1.0 equiv) and $Zn(OTf)_2$ (0.05 mmol, 10 mol%) were dissolved in DCE (2.5 mL). The reaction mixture was stirred at 70 °C. After the reaction was completed (detected by TLC), solvent was directly removed under reduced pressure and the crude mixture was purified by silica gel flash column chromatography to afford **M1** (70%).



2a **M2**, 78%

N-propargylamide **2a** (0.5 mmol, 1.0 equiv) and $InCl_3$ (0.05 mmol, 10 mol%) were dissolved in DCE (2.5 mL). The reaction mixture was stirred at 70 °C. After the reaction was completed (detected by TLC), solvent was directly removed under reduced pressure and the crude mixture was purified by silica gel flash column chromatography to afford **M2** (78%).

8. References

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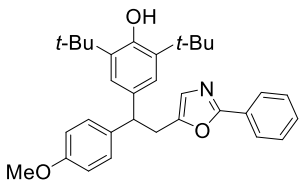
[7] B. Wang, Y. Chen, L. Zhou, J. Wang, C.-H. Tung and Z. Xu, *J. Org. Chem*., 2015, **80**, 12718–12724.

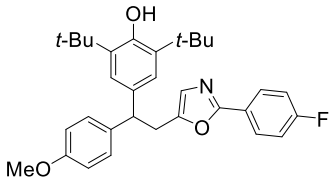
9. Characterization of compounds 3, 4, M1 and M2

2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-phenyloxazol-5-yl)ethyl)phenol (3aa)



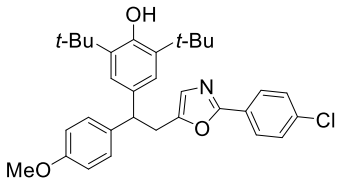
White solid, 227 mg, 94% yield, M.p. = 111-113 °C. **IR (KBr)** υ 3416, 3072, 3001, 2951, 2907, 2869, 2831, 1610, 1597, 1549, 1512, 1439, 1362, 1298, 1248, 1178, 1120, 1042, 840, 771, 745, 711, 690 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.95 – 7.89 (m, 2H), 7.48 – 7.37 (m, 3H), 7.20 (d, J = 8.6 Hz, 2H), 7.05 (s, 2H), 6.85 (d, J = 8.7 Hz, 2H), 6.63 (s, 1H), 5.08 (s, 1H, missing after deuteriation), 4.28 (t, J = 8.0 Hz, 1H), 3.79 (s, 3H), 3.41 (d, J = 8.0 Hz, 2H), 1.41 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.4, 158.0, 152.2, 151.4, 136.0, 135.7, 134.3, 129.8, 128.6, 128.6, 127.7, 125.9, 124.9, 124.1, 113.8, 55.2, 49.1, 34.3, 32.9, 30.2; **HRMS (ESI-TOF, [M+H]$^+$)** calcd for $C_{32}H_{38}NO_3$, 484.2852, found 484.2842.

2,6-Di-*tert*-butyl-4-(2-(2-(4-fluorophenyl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)phenol (3ab)



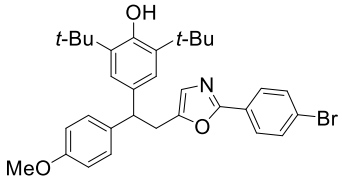
White solid, 241 mg, 96% yield, M.p. = 121-124 °C. **IR (KBr)** υ 3567, 3081, 2965, 2871, 2832, 1661, 1610, 1588, 1555, 1511, 1497, 1434, 1363, 1303, 1231, 1179, 1118, 1039, 995, 887, 846, 770, 740, 699, 642 cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.93 – 7.83 (m, 2H), 7.19 (d, J = 8.5 Hz, 2H), 7.10 (t, J = 8.6 Hz, 2H), 7.02 (s, 2H), 6.84 (d, J = 8.6 Hz, 2H), 6.60 (s, 1H), 5.07 (s, 1H), 4.25 (t, J = 7.9 Hz, 1H), 3.78 (s, 3H), 3.39 (d, J = 8.0 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 163.7 (d, $^1J_{FC}$ = 250.3 Hz), 159.6, 158.0, 152.2, 151.5, 136.0, 135.7, 134.3, 128.6, 128.0 (d, $^3J_{FC}$ = 8.5 Hz), 124.9, 124.1, 115.7 (d, $^2J_{FC}$ = 22.0 Hz), 113.8, 55.2, 49.1, 34.3, 32.9, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{37}NO_3F$, 502.2757, found 502.2759.

2,6-Di-*tert*-butyl-4-(2-(2-(4-chlorophenyl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)phenol (3ac)



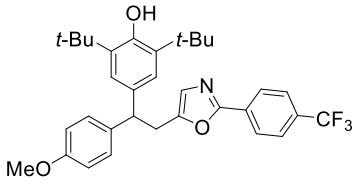
White solid, 251 mg, 97% yield, M.p. = 112-113 °C. **IR (KBr)** υ 3383, 3000, 2959, 2907, 2868, 2829, 1610, 1512, 1511, 1484, 1437, 1362, 1251, 1176, 1119, 1093, 1043, 840, 770, 745, 735, 696 cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.82 (d, J = 8.5 Hz, 2H), 7.38 (d, J = 8.6 Hz, 2H), 7.18 (d, J = 8.6 Hz, 2H), 7.01 (s, 2H), 6.83 (d, J = 8.6 Hz, 2H), 6.61 (s, 1H), 5.07 (s, 1H), 4.24 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.38 (d, J = 7.9 Hz, 2H), 1.38 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 159.5, 158.0, 152.2, 151.7, 135.9, 135.8, 135.7, 134.2, 128.9, 128.6, 127.2, 126.2, 125.1, 124.0, 113.8, 55.2, 49.1, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{37}NO_3Cl$, 518.2462, found 518.2456.

4-(2-(2-(4-Bromophenyl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)-2,6-di-*tert*-butylphenol (3ad)



White solid, 267 mg, 95% yield, M.p. = 107-109 °C. **IR (KBr)** υ 3442, 3125, 3000, 2959, 2917, 2868, 2829, 1652, 1610, 1541, 1512, 1480, 1437, 1361, 1305, 1251, 1177, 1119, 1076, 1043, 1011, 880, 838, 829, 771, 732 cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.75 (d, J = 8.5 Hz, 2H), 7.54 (d, J = 8.6 Hz, 2H), 7.17 (d, J = 8.6 Hz, 2H), 7.01 (s, 2H), 6.83 (d, J = 8.7 Hz, 2H), 6.61 (s, 1H), 5.06 (s, 1H), 4.24 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.38 (d, J = 7.9 Hz, 2H), 1.38 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 159.5, 158.1, 152.2, 151.8, 135.9, 135.8, 134.2, 131.8, 128.6, 127.4, 126.6, 125.1, 124.1, 124.0, 113.8, 55.2, 49.1, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{37}NO_3Br$, 562.1957, found 562.1956.

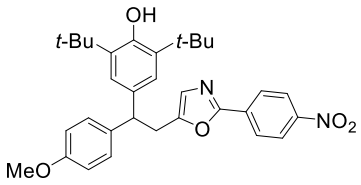
2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-(4-(trifluoromethyl)phenyl)oxazol-5-yl)ethyl) phenol (3ae)



White solid, 268 mg, 97% yield, M.p. = 116-118 °C. **IR (KBr)** υ 3594, 3441, 3065, 3032, 2959, 2915, 2836, 1622, 1612, 1600, 1583, 1554, 1512, 1435, 1323, 1254, 1183, 1157, 1121, 1073, 1030, 849, 823, 711 cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.00 (d, J = 8.1 Hz, 2H), 7.66 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 8.6 Hz, 2H), 7.02 (s, 2H), 6.83 (d, J = 8.7 Hz, 2H), 6.66 (s, 1H), 5.07 (s, 1H), 4.26 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.41 (d, J = 8.2 Hz, 2H), 1.38 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ.159.0, 158.1, 152.4, 152.3, 135.8, 135.7, 134.2, 131.4 (q, $^2J_{FC}$ = 33.5 Hz), 130.8, 128.6, 126.1, 125.6, 125.4, 124.0, 123.9

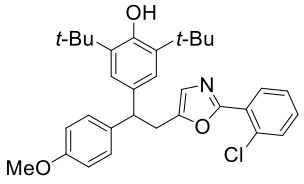
(q, $^1J_{FC}$ = 271.2 Hz), 113.8, 55.2, 49.1, 34.3, 32.9, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{33}H_{37}NO_3F_3$, 552.2726, found 552.2728.

2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-(4-nitrophenyl)oxazol-5-yl)ethyl)phenol (3af)



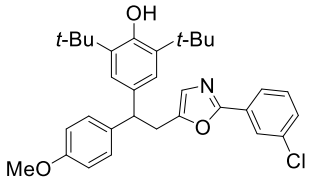
Pale yellow solid, 257 mg, 97% yield, M.p. = 140-142 °C. **IR (KBr)** υ 3623, 3440, 3111, 2960, 2838, 1611, 1584, 1547, 1515, 1438, 1338, 1311, 1250, 1237, 1179, 1109, 1035, 880, 853, 842, 713 cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.26 (d, J = 8.9 Hz, 2H), 8.03 (d, J = 8.9 Hz, 2H), 7.18 (d, J = 8.7 Hz, 2H), 7.01 (s, 2H), 6.83 (d, J = 8.6 Hz, 2H), 6.71 (s, 1H), 5.08 (s, 1H), 4.25 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.42 (d, J = 6.7 Hz, 2H), 1.38 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 158.3, 158.1, 153.3, 152.3, 148.2, 135.8, 135.7, 134.1, 133.0, 128.6, 126.5, 126.0, 124.0, 113.9, 55.2, 49.1, 34.3, 33.0, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{37}N_2O_5$, 529.2702, found 529.2698.

2,6-Di-*tert*-butyl-4-(2-(2-(2-chlorophenyl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)phenol (3ag)



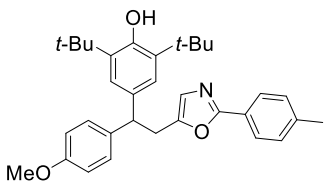
White solid, 244 mg, 94% yield, M.p. = 82-84 °C. **IR (KBr)** υ 3633, 3447, 3065, 3005, 2957, 2912, 2870, 2833, 1611, 1574, 1512, 1458, 1435, 1361, 1302, 1250, 1179, 1112, 1038, 994, 886, 831, 769, 734, 669cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.85 – 7.78 (m, 1H), 7.50 – 7.44 (m, 1H), 7.35 – 7.27 (m, 2H), 7.20 (d, J = 8.6 Hz, 2H), 7.03 (s, 2H), 6.84 (d, J = 8.6 Hz, 2H), 6.72 (s, 1H), 5.08 (s, 1H), 4.29 (t, J = 7.9 Hz, 1H), 3.78 (s, 3H), 3.42 (d, J = 7.9 Hz, 2H), 1.40 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 158.2, 158.0, 152.2, 151.8, 136.0, 135.7, 134.2, 132.1, 131.1, 130.5, 128.6, 126.7, 126.5, 125.0, 124.1, 113.8, 55.2, 49.1, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{37}NO_3Cl$, 518.2462, found 518.2454.

2,6-Di-*tert*-butyl-4-(2-(2-(3-chlorophenyl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)phenol (3ah)



White solid, 212 mg, 82% yield, M.p. = 118-120 °C. **IR (KBr)** υ 3625, 3447, 3092, 3006, 2964, 2912, 2872, 2833, 1612, 1593, 1543, 1511, 1478, 1435, 1359, 1304, 1254, 1181, 1103, 1033, 999, 885, 840, 797, 775, 727, 682cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.86 (s, 1H), 7.78 (dt, J = 7.0, 1.5 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.18 (d, J = 8.6 Hz, 2H), 7.02 (s, 2H), 6.83 (d, J = 8.7 Hz, 2H), 6.63 (s, 1H), 5.07 (s, 1H), 4.24 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.39 (d, J = 8.0 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 159.1, 158.1, 152.2, 152.0, 135.9, 135.7, 134.7, 134.2, 129.9, 129.8, 129.3, 128.6, 125.9, 125.2, 124.0, 124.0, 113.8, 55.2, 49.1, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{37}NO_3Cl$, 518.2462, found 518.2463.

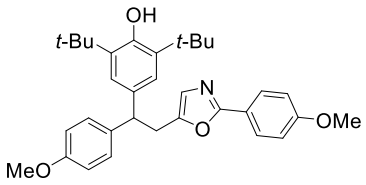
2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-(p-tolyl)oxazol-5-yl)ethyl)phenol (3ai)



White solid, 204 mg, 82% yield, M.p. = 117-118 °C. **IR (KBr)** υ 3421, 3002, 2959, 2920, 2869, 1612, 1555, 1512, 1498, 1464, 1437, 1362, 1304, 1250, 1179, 1115, 1038, 993, 881, 840, 825, 771, 732, cm^{-1}; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.80 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 7.9 Hz, 2H), 7.18 (d, J = 8.5 Hz, 2H), 7.03 (s, 2H), 6.83 (d, J = 8.5 Hz, 2H), 6.59 (s, 1H), 5.07 (s, 1H), 4.26 (t, J = 7.9 Hz, 1H), 3.77 (s, 3H), 3.38 (d, J = 7.9 Hz, 2H),

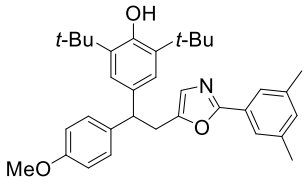
2.39 (s, 3H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.6, 158.0, 152.2, 151.0, 140.0, 136.1, 135.7, 134.4, 129.3, 128.7, 125.9, 125.0, 124.8, 124.1, 113.8, 55.2, 49.1, 34.3, 32.9, 30.3, 21.4; **HRMS (ESI-TOF, $[M+H]^+$)** calcd for $C_{33}H_{40}NO_3$, 498.3008, found 498.3001.

2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-(4-methoxyphenyl)oxazol-5-yl)ethyl)phenol (3aj)



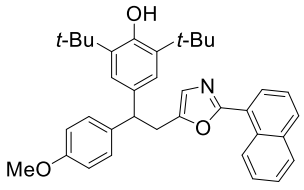
White solid, 187 mg, 73% yield, M.p. = 122-123 °C. **IR (KBr)** υ 3417, 3245, 3001, 2959, 2912, 2869, 2837, 1611, 1557, 1513, 1498, 1436, 1361, 1305, 1255, 1176, 1119, 1029, 955, 984, 894, 840, 800, 771, 742cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.84 (d, J = 8.8 Hz, 2H), 7.17 (d, J = 8.6 Hz, 2H), 7.02 (s, 2H), 6.92 (d, J = 8.8 Hz, 2H), 6.82 (d, J = 8.6 Hz, 2H), 6.56 (s, 1H), 5.06 (s, 1H), 4.25 (t, J = 7.9 Hz, 1H), 3.84 (s, 3H), 3.77 (s, 3H), 3.37 (d, J = 8.0 Hz, 2H), 1.38 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.9, 160.5, 158.0, 152.2, 150.7, 136.1, 135.7, 134.4, 128.7, 127.5, 124.6, 124.1, 120.6, 114.0, 113.8, 55.3, 55.2, 49.1, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, $[M + H]^+$)** calcd for $C_{33}H_{40}NO_4$, 514.2957, found 514.2960.

2,6-Di-*tert*-butyl-4-(2-(2-(3,5-dimethylphenyl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)phenol (3ak)



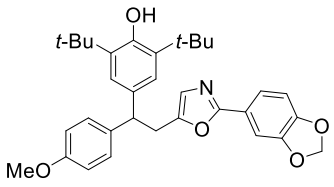
White solid, 200 mg, 78% yield, M.p. = 149-152 °C. **IR (KBr)** υ 3626, 3583, 3000, 2955, 2911, 2869, 2832, 1609, 1547, 1511, 1435, 1359, 1303, 1255, 1176, 1119, 1040, 995, 854, 827, 770, 736, 687 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.52 (s, 2H), 7.18 (d, J = 8.6 Hz, 2H), 7.04 (s, 3H), 6.83 (d, J = 8.6 Hz, 2H), 6.60 (s, 1H), 5.07 (s, 1H), 4.25 (t, J = 7.9 Hz, 1H), 3.77 (s, 3H), 3.38 (d, J = 7.9 Hz, 2H), 2.35 (s, 6H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.7, 158.0, 152.2, 151.1, 138.2, 136.1, 135.6, 134.3, 131.5, 128.7, 127.5, 124.8, 124.1, 123.7, 113.7, 55.2, 49.1, 34.3, 33.0, 30.3, 21.2; **HRMS (ESI-TOF, $[M + H]^+$)** calcd for $C_{34}H_{42}NO_3$, 512.3165, found 512.3165.

2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-(naphthalen-1-yl)oxazol-5-yl)ethyl)phenol (3al)



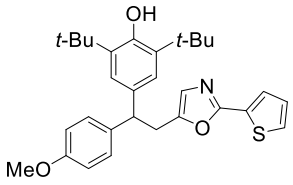
White solid, 187 mg, 70% yield, M.p. = 105-107 °C. **IR (KBr)** υ 3612, 3442, 3051, 3004, 2956, 2912, 2870, 2829, 1611, 1596, 1528, 1513, 1435, 1359, 1302, 1248, 1179, 1110, 1030, 986, 886, 840, 805, 775, 742 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.11 (d, J = 8.6 Hz, 1H), 7.99 (d, J = 7.1 Hz, 1H), 7.94 – 7.84 (m, 2H), 7.63 – 7.56 (m, 1H), 7.56 – 7.47 (m, 2H), 7.23 (d, J = 8.6 Hz, 2H), 7.07 (s, 2H), 6.85 (d, J = 8.6 Hz, 2H), 6.79 (s, 1H), 5.08 (s, 1H), 4.32 (t, J = 7.9 Hz, 1H), 3.78 (s, 3H), 3.47 (d, J = 7.9 Hz, 2H), 1.40 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.3, 158.0, 152.2, 151.1, 136.0, 135.7, 134.4, 133.8, 130.6, 130.0, 128.7, 128.4, 127.4, 127.3, 126.2, 126.1, 125.0, 124.9, 124.2, 124.1, 113.8, 55.2, 49.3, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, $[M + H]^+$)** calcd for $C_{36}H_{40}NO_3$, 534.3008, found 534.3007.

4-(2-(2-(Benzo[*d*][1,3]dioxol-5-yl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)-2,6-di-*tert*-butyl-phenol (3am)



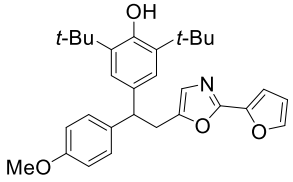
White solid, 142 mg, 54% yield, M.p. = 121-124 °C. **IR (KBr)** υ 3625, 3452, 3072, 3009, 2958, 2907, 2836, 1611, 1553, 1514, 1485, 1436, 1303, 1253, 1182, 1105, 1038, 938, 881, 833, 770, 733 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.48 – 7.39 (m, 1H), 7.38 – 7.31 (m, 1H), 7.18 (d, J = 8.5 Hz, 2H), 7.02 (s, 2H), 6.87 – 6.77 (m, 3H), 6.56 (s, 1H), 6.01 (s, 2H), 5.07 (s, 1H), 4.24 (t, J = 7.9 Hz, 1H), 3.77 (s, 3H), 3.36 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.2, 158.0, 152.2, 150.9, 149.0, 147.9, 136.0, 135.6, 134.3, 128.7, 124.7, 124.1, 122.0, 120.5, 113.7, 108.5, 106.3, 101.4, 55.2, 49.1, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{33}H_{38}NO_5$, 528.2750, found 528.2749.

2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-(thiophen-2-yl)oxazol-5-yl)ethyl)phenol (3an)



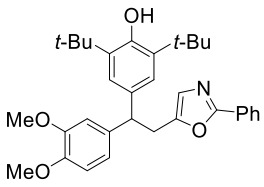
White solid, 159 mg, 65% yield, M.p. = 130-132 °C. **IR (KBr)** υ 3626, 3421, 3114, 3003, 2954, 2913, 2871, 2833, 1610, 1512, 1436, 1362, 1250, 1179, 1120, 1040, 841, 724, 708, 669 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.54 (d, J = 2.7 Hz, 1H), 7.36 (d, J = 4.8 Hz, 1H), 7.18 (d, J = 8.5 Hz, 2H), 7.10 – 7.04 (m, 1H), 7.02 (s, 2H), 6.83 (d, J = 8.6 Hz, 2H), 6.54 (s, 1H), 5.06 (s, 1H), 4.25 (t, J = 7.9 Hz, 1H), 3.77 (s, 3H), 3.37 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 158.0, 156.6, 152.2, 150.9, 135.9, 135.7, 134.2, 130.4, 128.6, 127.7, 127.5, 126.8, 124.8, 124.0, 113.8, 55.2, 48.9, 34.3, 32.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{30}H_{36}NO_3S$, 490.2416, found 490.2412.

2,6-Di-*tert*-butyl-4-(2-(2-(furan-2-yl)oxazol-5-yl)-1-(4-methoxyphenyl)ethyl)phenol (3ao)



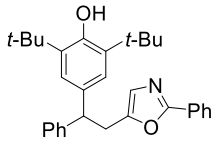
White solid, 142 mg, 60% yield, M.p. = 98-101 °C. **IR (KBr)** υ 3630, 3421, 3125, 3003, 2953, 2911, 2866, 2833, 1614, 1513, 1439, 1361, 1248, 1179, 1120, 1040, 840, 750 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.51 (s, 1H), 7.16 (d, J = 8.6 Hz, 2H), 7.01 (s, 2H), 6.89 (d, J = 3.4 Hz, 1H), 6.82 (d, J = 8.6 Hz, 2H), 6.56 (s, 1H), 6.50 (dd, J = 3.3, 1.7 Hz, 1H), 5.07 (s, 1H), 4.26 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 3.41 – 3.31 (m, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 158.0, 153.3, 152.2, 150.9, 143.8, 143.2, 135.8, 135.6, 134.2, 128.6, 124.8, 124.0, 113.8, 111.6, 110.4, 55.2, 48.8, 34.3, 32.8, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{30}H_{36}NO_4$, 474.2744, found 474.2640.

2,6-Di-*tert*-butyl-4-(1-(3,4-dimethoxyphenyl)-2-(2-phenyloxazol-5-yl)ethyl)phenol (3ba)



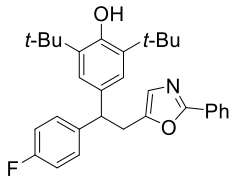
White solid, 239 mg, 93% yield, M.p. = 110-112 °C. **IR (KBr)** υ 3628, 3455, 3064, 3000, 2956, 2908, 2872, 2833, 1593, 1548, 1515, 1484, 1436, 1358, 1321, 1258, 1237, 1144, 1120, 1027, 994, 888, 855, 776, 711, 692 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.95 – 7.87 (m, 2H), 7.45 – 7.37 (m, 3H), 7.05 (s, 2H), 6.85 – 6.76 (m, 3H), 6.63 (s, 1H), 5.09 (s, 1H), 4.26 (t, J = 7.9 Hz, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 3.39 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.4, 152.3, 151.3, 148.7, 147.4, 136.4, 135.7, 134.0, 129.8, 128.6, 127.7, 125.9, 125.0, 124.1, 119.6, 111.2, 111.0, 55.8, 55.7, 49.5, 34.3, 33.1, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{33}H_{40}NO_4$, 514.2957, found 514.2957.

2,6-Di-*tert*-butyl-4-(1-phenyl-2-(2-phenyloxazol-5-yl)ethyl)phenol (3ca)



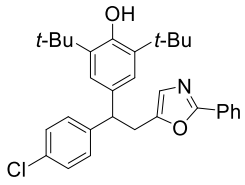
White solid, 206 mg, 91% yield, M.p. = 121-123 °C. **IR (KBr)** υ 3525, 3064, 3015, 2957, 2920, 2873, 1598, 1548, 1490, 1450, 1437, 1367, 1358, 1294, 1235, 1102, 1025, 996, 881, 824, 777, 741, 710, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.95 – 7.86 (m, 2H), 7.46 – 7.36 (m, 3H), 7.33 – 7.27 (m, 4H), 7.23 – 7.18 (m, 1H), 7.05 (s, 2H), 6.63 (s, 1H), 5.08 (s, 1H), 4.31 (t, J = 7.9 Hz, 1H), 3.52 – 3.36 (m, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.4, 152.3, 151.3, 143.9, 135.7, 134.0, 129.8, 128.6, 128.4, 127.7, 127.7, 126.3, 125.9, 124.9, 124.2, 49.9, 34.3, 32.7, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{31}H_{36}NO_2$, 454.2746, found 454.2737.

2,6-Di-*tert*-butyl-4-(1-(4-fluorophenyl)-2-(2-phenyloxazol-5-yl)ethyl)phenol (3da)



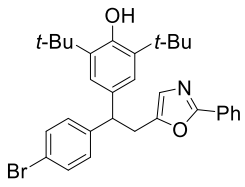
White solid, 177 mg, 75% yield, M.p. = 118-120 °C. **IR (KBr)** υ 3640, 3531, 3065, 3014, 2959, 2916, 2874, 1598, 1548, 1509, 1490, 1439, 1432, 1367, 1295, 1235, 1159, 1101, 1025, 996, 880, 846, 777, 744, 710, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.95 – 7.86 (m, 2H), 7.45 – 7.37 (m, 3H), 7.25 – 7.19 (m, 2H), 7.01 (s, 2H), 7.00 – 6.93 (m, 2H), 6.63 (s, 1H), 5.09 (s, 1H), 4.30 (t, J = 7.9 Hz, 1H), 3.40 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 161.4 (d, $^1J_{FC}$ = 243.6 Hz), 160.5, 152.3, 151.0, 139.5, 135.8, 133.8, 129.9, 129.2, 128.6, 127.6, 125.9, 125.0, 124.0, 115.2 (d, $^2J_{FC}$ = 21.2 Hz), 49.1, 34.3, 32.8, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{31}H_{35}NO_2F$, 472.2652, found 472.2648.

2,6-Di-*tert*-butyl-4-(1-(4-chlorophenyl)-2-(2-phenyloxazol-5-yl)ethyl)phenol (3ea)



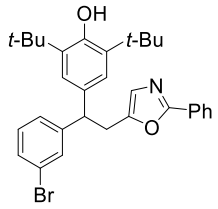
White solid, 164 mg, 67% yield, M.p. = 108-110 °C. **IR (KBr)** υ 3635, 3278, 3003, 2957, 2912, 2871, 1647, 1596, 1549, 1491, 1439, 1362, 1304, 1281, 1199, 1120, 1092, 1015, 997, 927, 883, 842, 771, 711, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.93 – 7.84 (m, 2H), 7.47 – 7.36 (m, 3H), 7.26 – 7.25 (m, 2H), 7.19 (d, J = 8.3 Hz, 2H), 7.01 (s, 2H), 6.63 (s, 1H), 5.10 (s, 1H), 4.29 (t, J = 7.9 Hz, 1H), 3.40 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.6, 152.4, 150.8, 142.4, 135.9, 133.4, 132.1, 129.9, 129.1, 128.6, 128.5, 127.6, 125.9, 125.1, 124.0, 49.3, 34.3, 32.6, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{31}H_{35}NO_2Cl$, 488.2356, found 488.2360.

4-(1-(4-Bromophenyl)-2-(2-phenyloxazol-5-yl)ethyl)-2,6-di-*tert*-butylphenol (3fa)



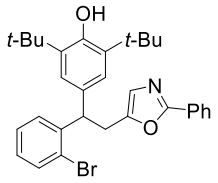
White solid, 186 mg, 70% yield, M.p. = 129-131 °C. **IR (KBr)** υ 3634, 3416, 3004, 2956, 2913, 2870, 1644, 1596, 1549, 1488, 1439, 1362, 1220, 1200, 1181, 1120, 1074, 1101, 997, 927, 883, 841, 777, 711, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.92 – 7.84 (m, 2H), 7.44 – 7.38 (m, 5H), 7.14 (d, J = 8.4 Hz, 2H), 7.01 (s, 2H), 6.64 (s, 1H), 5.10 (s, 1H), 4.27 (t, J = 7.9 Hz, 1H), 3.40 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.6, 152.4, 150.8, 142.9, 135.9, 133.3, 131.5, 129.9, 129.5, 128.6, 127.6, 125.9, 125.1, 124.0, 120.2, 49.4, 34.3, 32.5, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{31}H_{35}NO_2Br$, 532.1851, found 532.1851.

4-(1-(3-Bromophenyl)-2-(2-phenyloxazol-5-yl)ethyl)-2,6-di-*tert*-butylphenol (3ga)



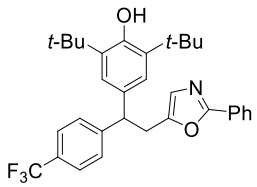
White solid, 221 mg, 83% yield, M.p. = 108-111 °C. **IR (KBr)** υ 3634, 3127, 3067, 3008, 2946, 2914, 2867, 1644, 1601, 1589, 1551, 1473, 1433, 1359, 1205, 1121, 1072, 993, 792, 772, 714, 710, 687 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 – 7.88 (m, 2H), 7.47 – 7.38 (m, 4H), 7.36 – 7.31 (m, 1H), 7.24 – 7.20 (m, 1H), 7.19 – 7.14 (m, 1H), 7.02 (s, 2H), 6.66 (s, 1H), 5.13 (s, 1H), 4.28 (t, J = 7.9 Hz, 1H), 3.42 (d, J = 7.9 Hz, 2H), 1.40 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.6, 152.5, 150.7, 146.2, 135.9, 133.1, 130.9, 130.0, 129.9, 129.5, 128.6, 127.6, 126.4, 125.9, 125.1, 124.1, 122.5, 49.7, 34.3, 32.5, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{31}H_{35}NO_2Br$, 532.1851, found 532.1852.

4-(1-(2-Bromophenyl)-2-(2-phenyloxazol-5-yl)ethyl)-2,6-di-*tert*-butylphenol (3ha)



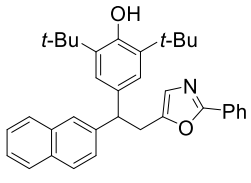
White solid, 35 mg, 13% yield, M.p. = 118-120 °C. **IR (KBr)** υ 3628, 3424, 3059, 2961, 2911, 2869, 1633, 1597, 1544, 1483, 1466, 1435, 1361, 1181, 1021, 995, 888, 818, 753, 742, 712, 691, 645 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.98 – 7.84 (m, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.46 – 7.38 (m, 3H), 7.38 – 7.32 (m, 1H), 7.30 – 7.24 (m, 2H), 7.13 (s, 2H), 7.07 – 7.00 (m, 1H), 6.67 (s, 1H), 5.09 (s, 1H), 4.91 (t, J = 7.9 Hz, 1H), 3.49 – 3.39 (m, 2H), 1.40 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.5, 152.4, 150.8, 143.0, 135.7, 133.1, 132.5, 129.8, 128.6, 128.4, 127.8, 127.7, 127.6, 125.9, 125.0, 124.9, 124.4, 47.6, 34.3, 31.9, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{31}H_{35}NO_2Br$, 532.1851, found 532.1851.

2,6-Di-*tert*-butyl-4-(2-(2-phenyloxazol-5-yl)-1-(4-(trifluoromethyl)phenyl)ethyl)phenol (3ia)



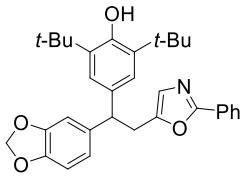
White solid, 47 mg, 18% yield, M.p. = 120-122 °C. **IR (KBr)** υ 3639, 3425, 3005, 2960, 2912, 2870, 1617, 1598, 1550, 1440, 1363, 1323, 1201, 1161, 1135, 1070, 1018, 884, 851, 727, 711, 692 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.89 – 7.84 (m, 2H), 7.55 (d, J = 8.2 Hz, 2H), 7.43 – 7.36 (m, 5H), 7.03 (s, 2H), 6.65 (s, 1H), 5.12 (s, 1H), 4.36 (t, J = 7.9 Hz, 1H), 3.45 (d, J = 7.9 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.7, 152.6, 150.6, 148.0, 136.0, 132.9, 129.9, 128.7 (q, $^2J_{FC}$ = 33.5 Hz), 128.6, 128.1, 127.5, 125.9, 125.4, 125.1, 124.2 (q, $^1J_{FC}$ = 270.0 Hz), 124.0, 49.9, 34.3, 32.4, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{35}NO_2F_3$, 522.2620, found 522.2627.

2,6-Di-*tert*-butyl-4-(1-(naphthalen-2-yl)-2-(2-phenyloxazol-5-yl)ethyl)phenol (3ja)



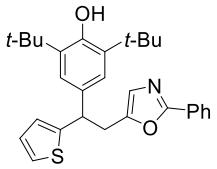
White solid, 219 mg, 87% yield, M.p. = 177-180 °C. **IR (KBr)** υ 3627, 3447, 3061, 3008, 2958, 2915, 2871, 1633, 1597, 1548, 1485, 1432, 1359, 1233, 1108, 1025, 814, 775, 749, 710, 692 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.90 – 7.85 (m, 2H), 7.81 – 7.76 (m, 3H), 7.74 (s, 1H), 7.47 – 7.38 (m, 6H), 7.10 (s, 2H), 6.65 (s, 1H), 5.09 (s, 1H), 4.49 (t, J = 7.9 Hz, 1H), 3.60 – 3.48 (m, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.5, 152.4, 151.2, 141.4, 135.8, 133.8, 133.5, 132.2, 129.8, 128.6, 128.1, 127.8, 127.7, 127.5, 126.4, 126.0, 125.9, 125.5, 125.0, 124.3, 50.0, 34.3, 32.6, 30.3; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{35}H_{38}NO_2$, 504.2903, found 504.2902.

4-(1-(Benzo[*d*][1,3]dioxol-5-yl)-2-(2-phenyloxazol-5-yl)ethyl)-2,6-di-*tert*-butylphenol (3ka)



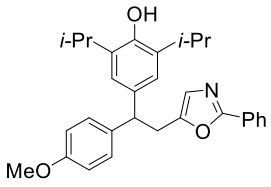
White solid, 209 mg, 84% yield, M.p. = 98-100 °C. **IR (KBr)** υ 3634, 3420, 3057, 3006, 2960, 2915, 2871, 2765, 1631, 1598, 1549, 1503, 1490, 1442, 1361, 1248, 1200, 1120, 1042, 939, 814, 772, 711, 690 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.95 – 7.87 (m, 2H), 7.46 – 7.36 (m, 3H), 7.03 (s, 2H), 6.79 – 6.67 (m, 3H), 6.64 (s, 1H), 5.91 (d, J = 2.2 Hz, 2H), 5.09 (s, 1H), 4.23 (t, J = 8.0 Hz, 1H), 3.37 (d, J = 8.0 Hz, 2H), 1.39 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.4, 152.3, 151.1, 147.6, 145.9, 137.9, 135.7, 134.0, 129.8, 128.6, 127.6, 125.9, 125.0, 124.0, 120.6, 108.1, 100.8, 49.5, 34.3, 32.8, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{32}H_{36}NO_4$, 498.2644, found 498.2644.

2,6-Di-*tert*-butyl-4-(2-(2-phenyloxazol-5-yl)-1-(thiophen-2-yl)ethyl)phenol (3la)



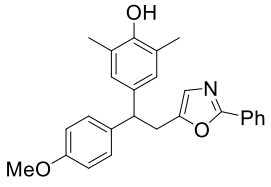
White solid, 191 mg, 83% yield, M.p. = 111-113 °C. **IR (KBr)** υ 3631, 3566, 3103, 3068, 3014, 2958, 2910, 2871, 1603, 1551, 1482, 1434, 1357, 1236, 1109, 1067, 992, 878, 818, 774, 713, 703, 690 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.94 – 7.86 (m, 2H), 7.44 – 7.37 (m, 3H), 7.15 (d, J = 5.1 Hz, 1H), 7.08 (s, 2H), 6.93 – 6.88 (m, 1H), 6.84 (d, J = 3.4 Hz, 1H), 6.67 (s, 1H), 5.11 (s, 1H), 4.53 (t, J = 7.8 Hz, 1H), 3.52 – 3.33 (m, 2H), 1.38 (s, 18H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.6, 152.6, 150.6, 148.0, 135.8, 133.5, 129.9, 128.6, 127.6, 126.5, 125.9, 125.2, 124.3, 124.1, 123.7, 45.8, 34.6, 34.3, 30.2; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{29}H_{34}NO_2S$, 460.2310, found 460.2305.

2,6-Diisopropyl-4-(1-(4-methoxyphenyl)-2-(2-phenyloxazol-5-yl)ethyl)phenol (3ma)



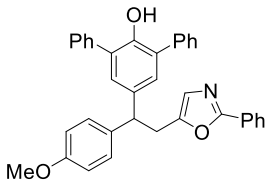
White solid, 182 mg, 80% yield, M.p. = 142-143 °C. **IR (KBr)** υ 3241, 3056, 3033, 2959, 2932, 2865, 2837, 1643, 1610, 1551, 1510, 1470, 1302, 1250, 1174, 1040, 993, 831, 779, 715, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.96 – 7.86 (m, 2H), 7.46 – 7.35 (m, 3H), 7.16 (d, J = 8.5 Hz, 2H), 6.90 (s, 2H), 6.81 (d, J = 8.5 Hz, 2H), 6.60 (s, 1H), 4.84 (s, 1H), 4.29 (t, J = 7.9 Hz, 1H), 3.76 (s, 3H), 3.39 (d, J = 7.9 Hz, 2H), 3.16 – 3.02 (m, 2H), 1.24 – 1.14 (m, 12H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.4, 158.0, 151.3, 148.5, 136.0, 135.5, 133.6, 129.8, 128.6, 127.7, 125.9, 124.9, 122.6, 113.8, 55.2, 48.8, 32.8, 27.2, 22.7; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{30}H_{34}NO_3$, 456.2539, found 456.2534.

4-(1-(4-Methoxyphenyl)-2-(2-phenyloxazol-5-yl)ethyl)-2,6-dimethylphenol (3na)



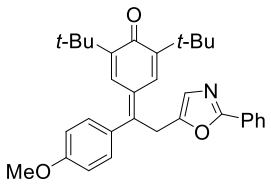
White solid, 154 mg, 77% yield, M.p. = 138-140 °C. **IR (KBr)** υ 3394, 3250, 3056, 3027, 2998, 2914, 2835, 1610, 1593, 1546, 1512, 1482, 1445, 1323, 1302, 1251, 1206, 1121, 1035, 990, 871, 858, 798, 781, 714, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.98 – 7.87 (m, 2H), 7.43 – 7.38 (m, 3H), 7.15 (d, J = 8.5 Hz, 2H), 6.85 (s, 2H), 6.81 (d, J = 8.5 Hz, 2H), 6.61 (s, 1H), 4.80 (s, 1H), 4.23 (t, J = 7.9 Hz, 1H), 3.75 (s, 3H), 3.37 (d, J = 7.9 Hz, 2H), 2.18 (s, 6H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.4, 158.0, 151.2, 150.8, 136.1, 135.3, 129.9, 128.6, 128.5, 127.7, 125.9, 124.9, 123.1, 113.8, 55.2, 48.1, 32.5, 16.1; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{26}H_{26}NO_3$, 400.1913, found 400.1909.

5'-(1-(4-Methoxyphenyl)-2-(2-phenyloxazol-5-yl)ethyl)-[1,1':3',1''-terphenyl]-2'-ol (3oa)



White solid, 189 mg, 72% yield, M.p. = 160-163 °C. **IR (KBr)** *υ* 3532, 3426, 3141, 3060, 2932, 2836, 1610, 1543, 1513, 1468, 1430, 1247, 1225, 1180, 1115, 1029, 909, 833, 777, 710, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** *δ* 7.98 – 7.89 (m, 2H), 7.51 – 7.48 (m, 3H), 7.48 – 7.30 (m, 10H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.16 (s, 2H), 6.84 (d, *J* = 8.5 Hz, 2H), 6.68 (s, 1H), 5.38 (s, 1H), 4.39 (t, *J* = 7.9 Hz, 1H), 3.77 (s, 3H), 3.54 – 3.39 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** *δ* 160.6, 158.2, 151.0, 147.9, 137.6, 135.9, 135.6, 129.9, 129.3, 129.1, 128.8, 128.7, 128.6, 127.6, 126.0, 125.1, 114.0, 55.2, 48.4, 32.5; **HRMS (ESI-TOF, [M + H]$^+$)** calcd for $C_{36}H_{30}NO_2$, 524.2226, found 524.2225.

2,6-Di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(2-phenyloxazol-5-yl)ethylidene)cyclohexa-2,5-dien-1-one (4)



Yellow solid, 217 mg, 90% yield, M.p. = 174-176 °C. **IR (KBr)** *υ* 3440, 3070, 3003, 2954, 2912, 2861, 1634, 1613, 1602, 1542, 1506, 1363, 1255, 1175, 1031, 843, 834, 776, 714, 691 cm^{-1}; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.96–7.88 (m, 2H), 7.59 (d, *J* = 2.6 Hz, 1H), 7.44–7.38 (m, 3H), 7.29–7.23 (m, 2H), 7.07 (d, *J* = 2.6 Hz, 1H), 6.95 (d, *J* = 8.7 Hz, 2H), 6.76 (s, 1H), 4.28 (s, 2H), 3.86 (s, 3H), 1.37 (s, 9H), 1.20 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$)** *δ* 186.2, 161.2, 160.1, 148.9, 148.7, 148.1, 147.0, 132.0, 131.3, 131.1, 130.2, 129.8, 128.7, 128.1, 127.3, 126.0, 125.3, 113.7, 55.3, 35.5, 35.2, 31.8, 29.6, 29.4; **HRMS (ESI-TOF, [M+H]$^+$)** calcd for $C_{32}H_{36}NO_3$, 482.2695, found 482.2693.

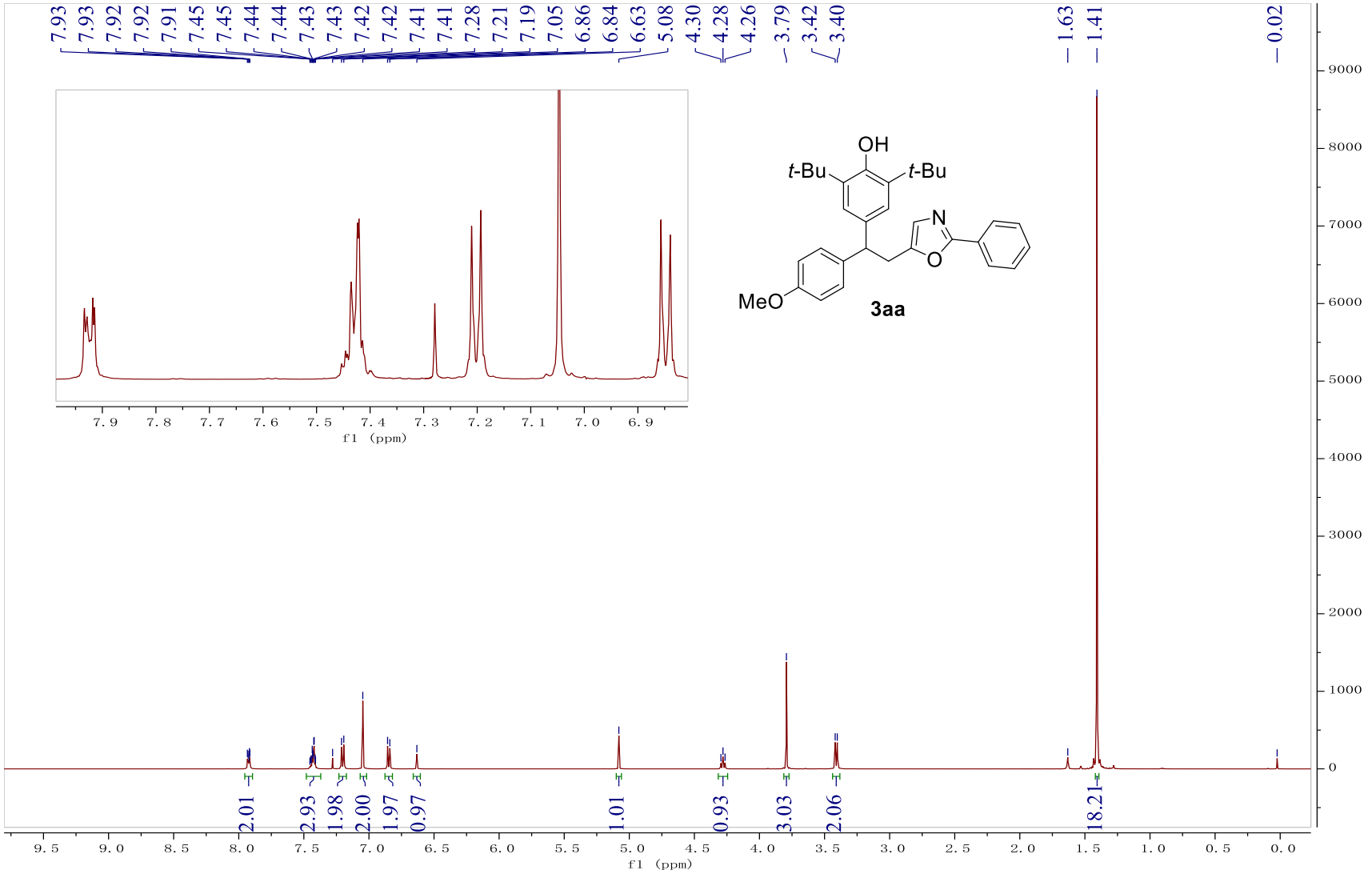
5-Methylene-2-phenyl-4,5-dihydrooxazole (M1)[4]

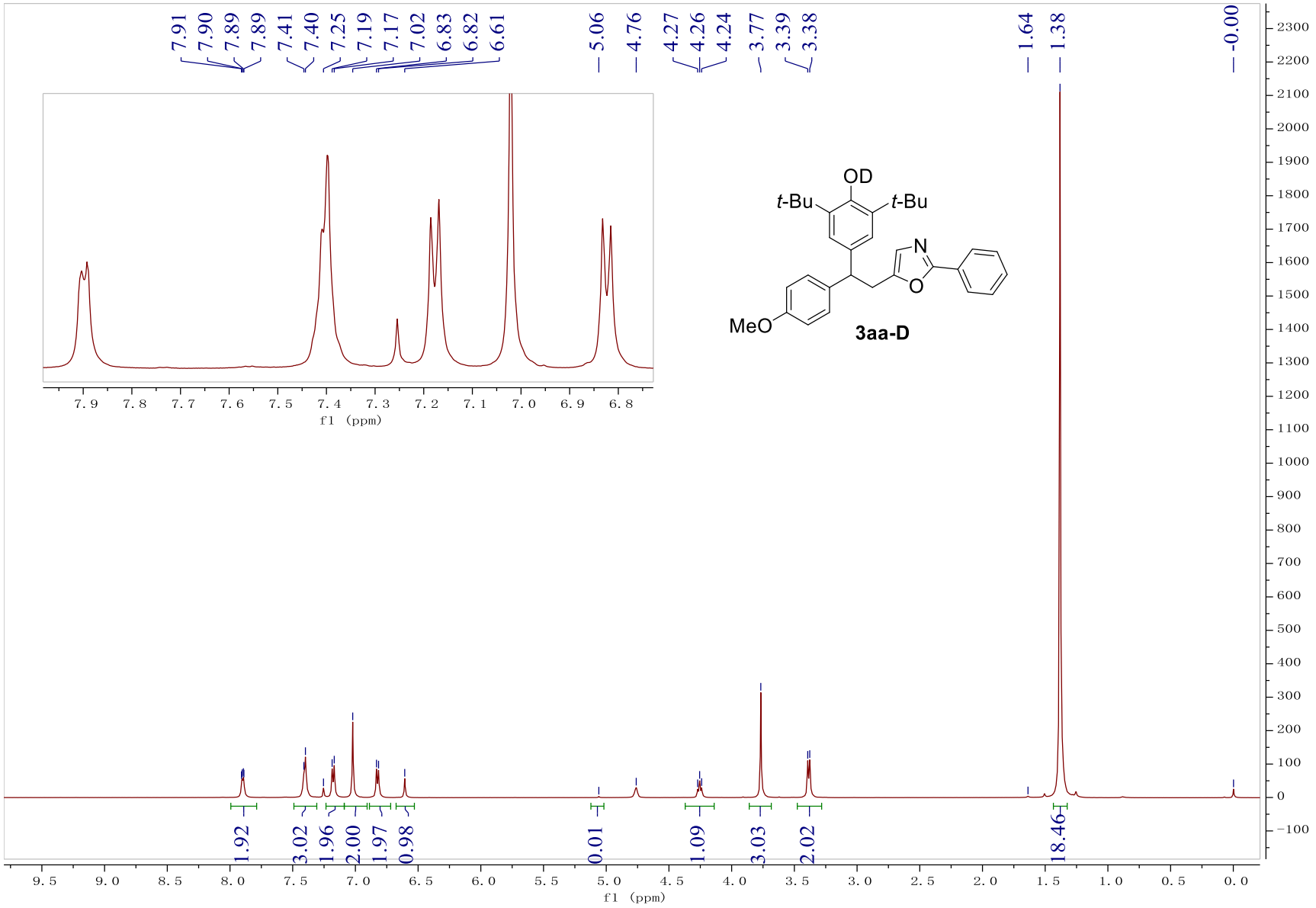
Pale yellow oil, **^{1}H NMR (500 MHz, $CDCl_3$)** *δ* 8.00–7.96 (m, 2H), 7.54–7.49 (m, 1H), 7.47–7.42 (m, 2H), 4.82 (q, *J* = 3.0 Hz, 1H), 4.66 (t, *J* = 2.8 Hz, 2H), 4.37 (q, *J* = 2.7 Hz, 1H).

5-Methyl-2-phenyloxazole (M2)[4]

Pale yellow oil, **^{1}H NMR (500 MHz, $CDCl_3$)** *δ* 8.04–7.95 (m, 2H), 7.50–7.36 (m, 3H), 6.83 (s, 1H), 2.39 (s, 3H).

10. ^{1}H NMR and ^{13}C NMR spectra of 3, 4, M1 and M2

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7.89
7.89
7.41
7.40
7.25
7.19
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7.02
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6.82
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5.06
4.76
4.27
4.26
4.24
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OD
t-Bu
t-Bu
N
O
MeO
3aa-D
f1 (ppm)
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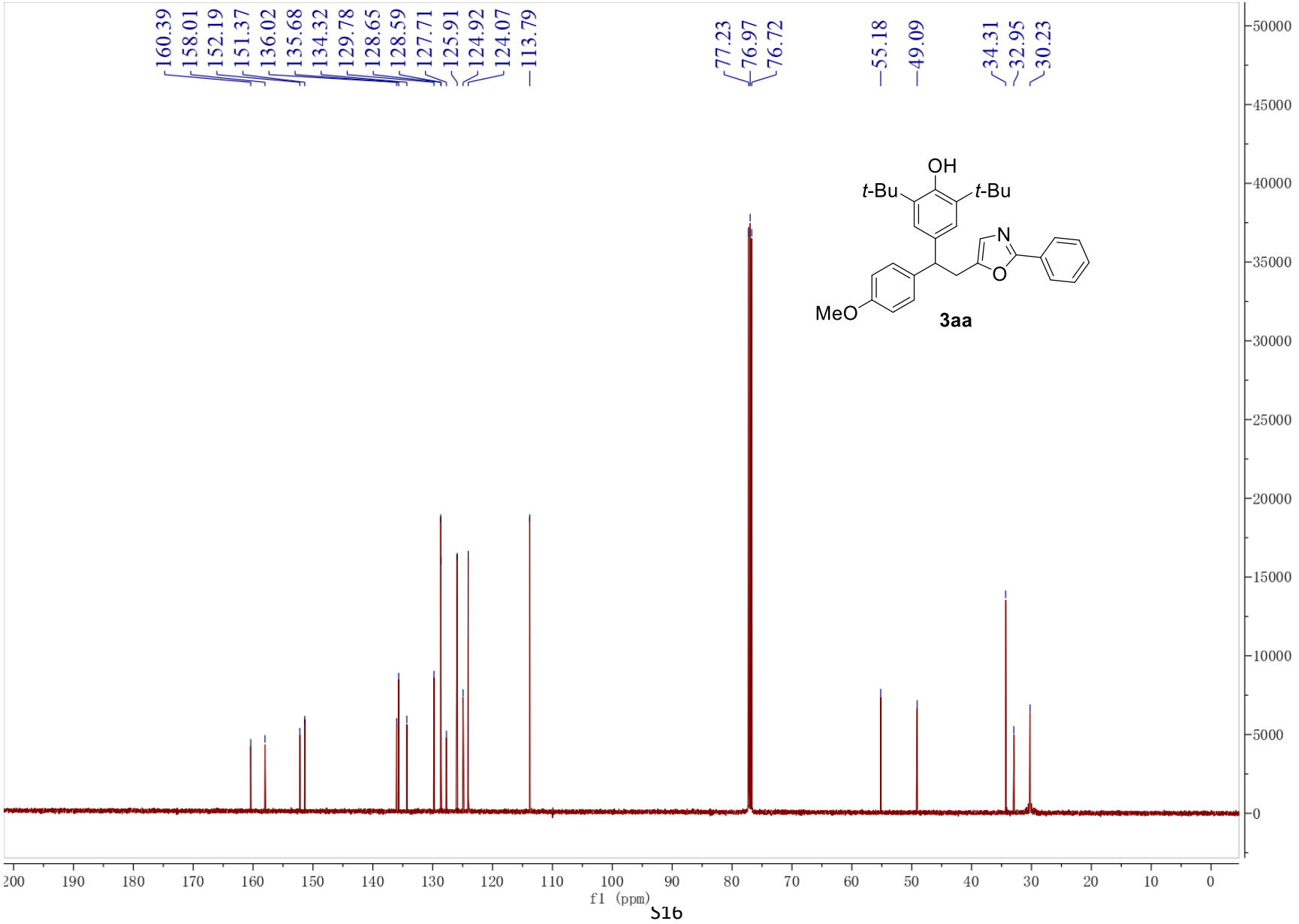
1.97
0.98
0.01
1.09
3.03
2.02
18.46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151.37
136.02
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134.32
129.78
128.65
128.59
127.71
125.91
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124.07
113.79
77.23
76.97
76.72
55.18
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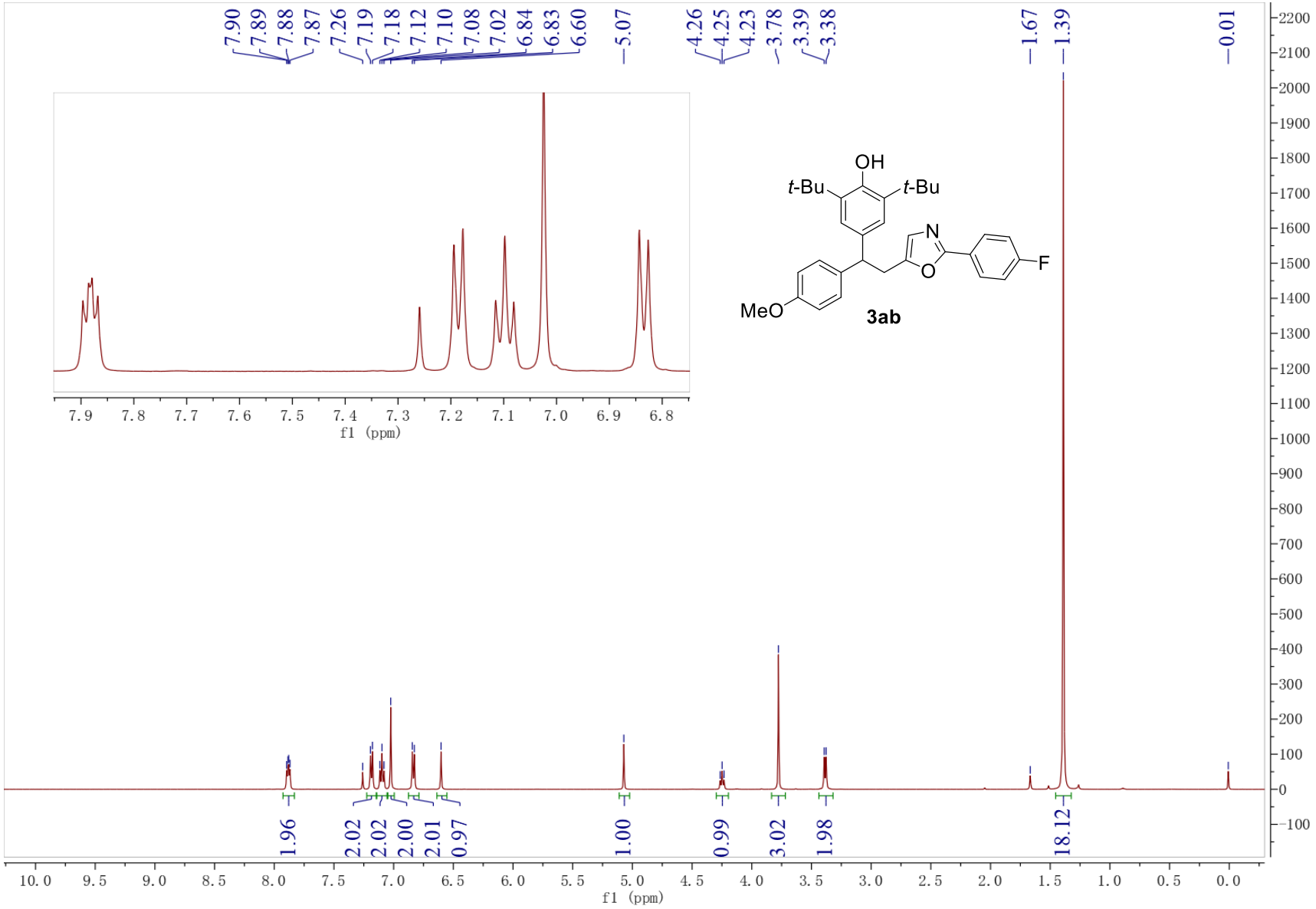
34.31
32.95
30.23
OH
t-Bu
t-Bu
N
O
MeO
3aa
f1 (ppm)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7.12
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7.08
7.02
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6.83
6.60
5.07
4.26
4.25
4.23
3.78
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3.38
1.67
1.39
0.01
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t-Bu
t-Bu
N
O
F
MeO
3ab
f1 (ppm)
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2.02
2.02
2.00
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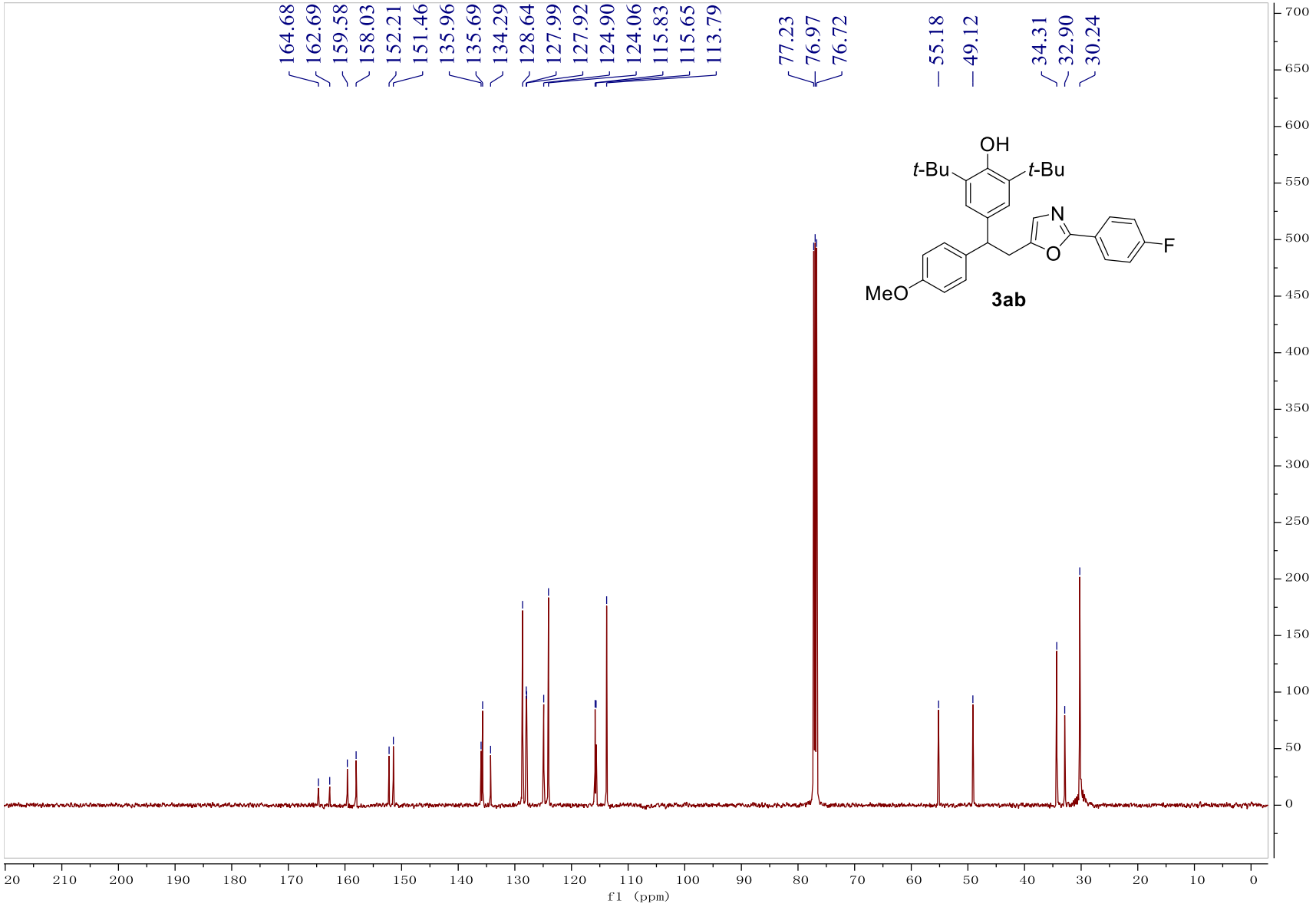
1.00
0.99
3.02
1.98
18.12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151.46
135.96
135.69
134.29
128.64
127.99
127.92
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77.23
76.97
76.72
55.18
49.12
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30.24
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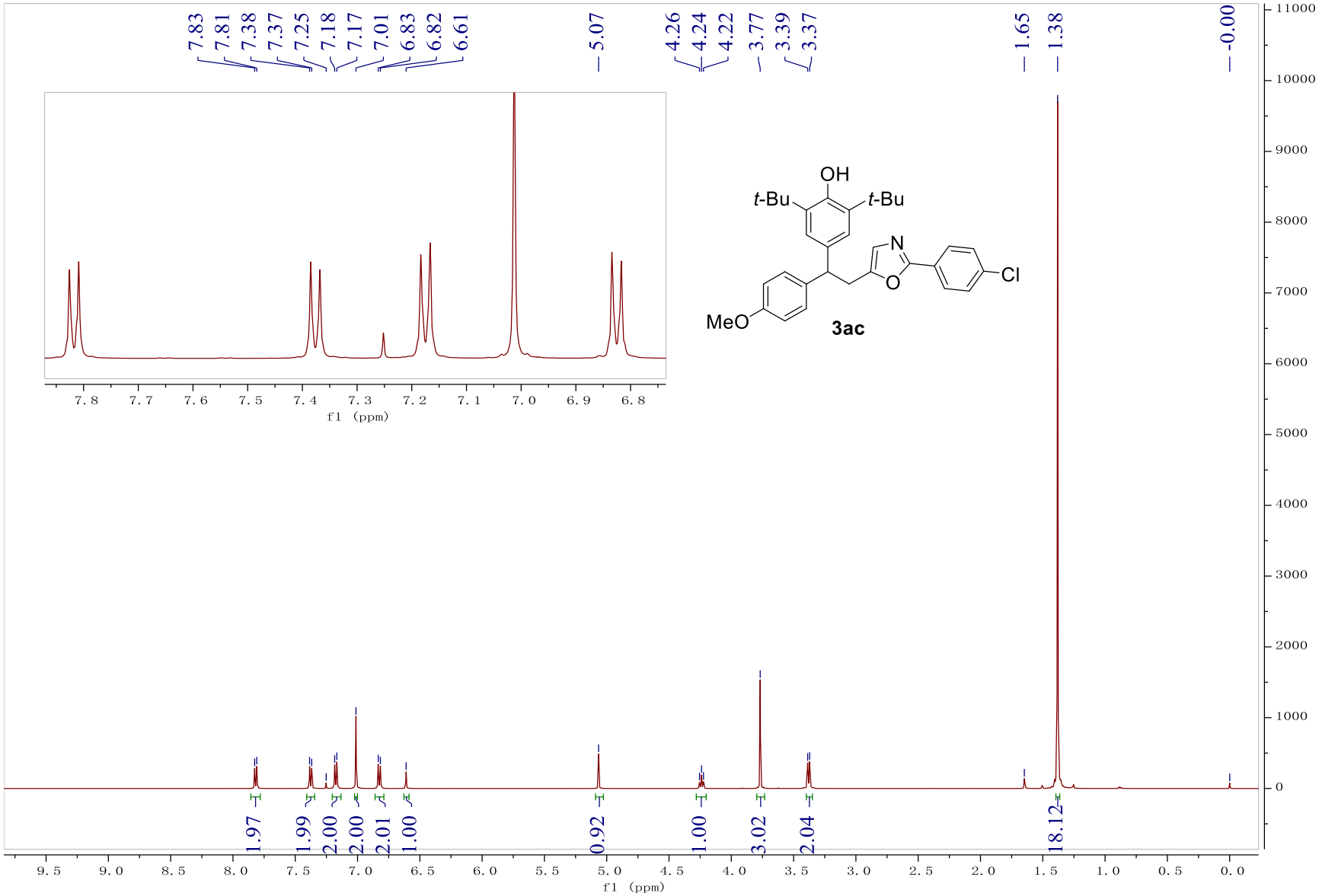
t-Bu
t-Bu
N
O
F
MeO
3ab
f1 (ppm)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t-Bu
N
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Cl
MeO
3ac
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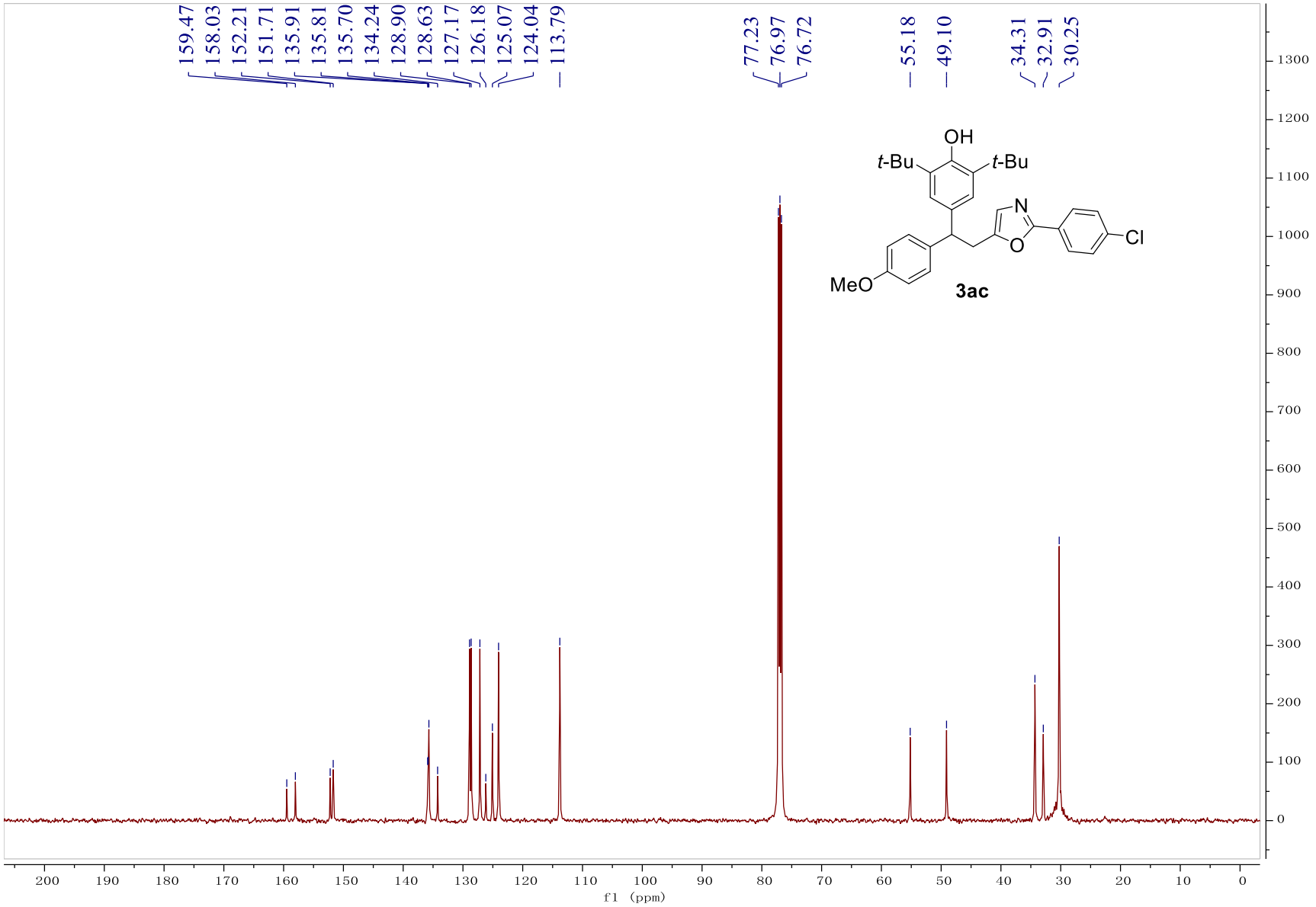
1.00
0.92
1.00
3.02
2.04
18.12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128.63
127.17
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124.04
113.79
77.23
76.97
76.72
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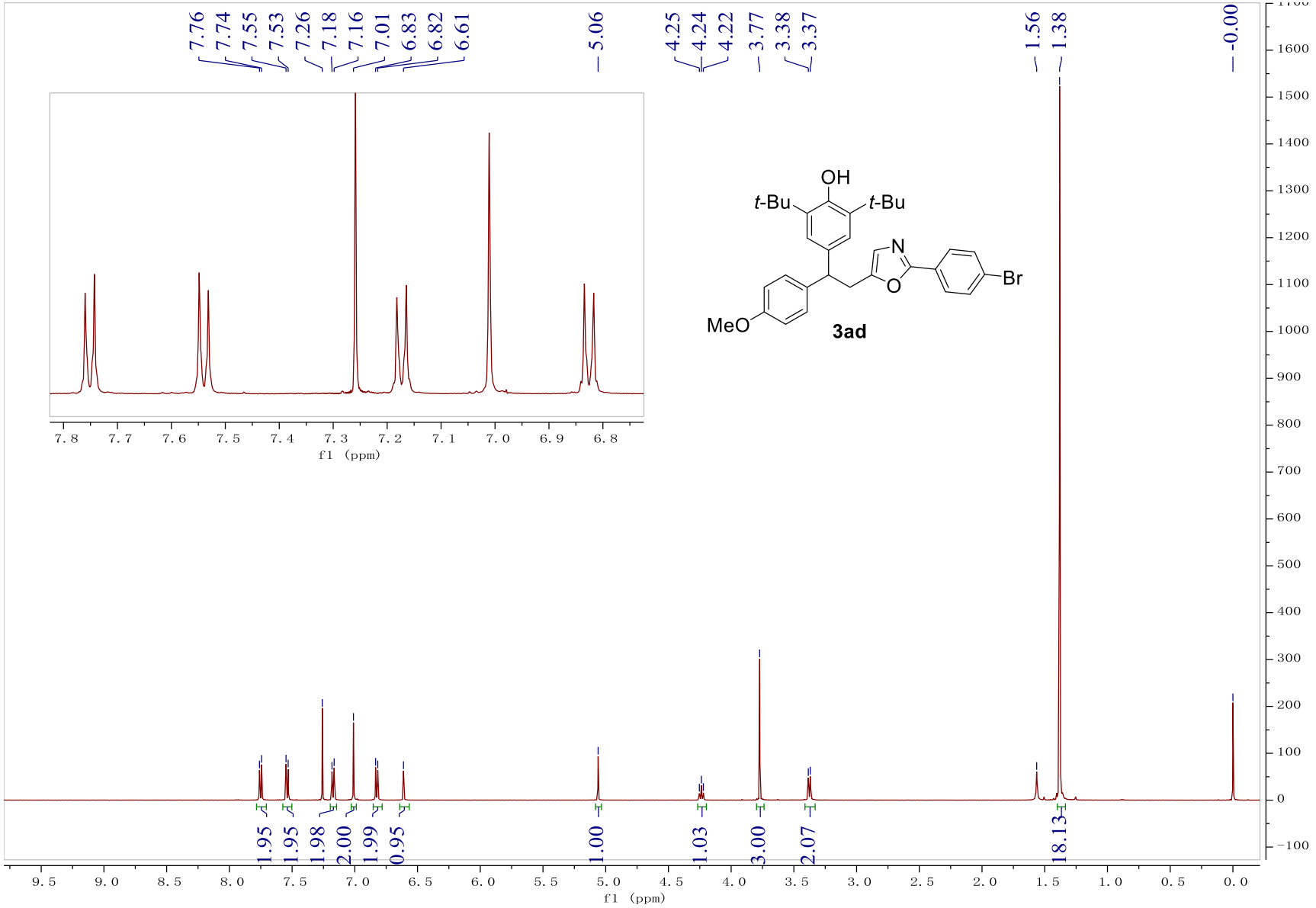
t-Bu
N
O
Cl
MeO
3ac
f1 (ppm)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6.82
6.61
5.06
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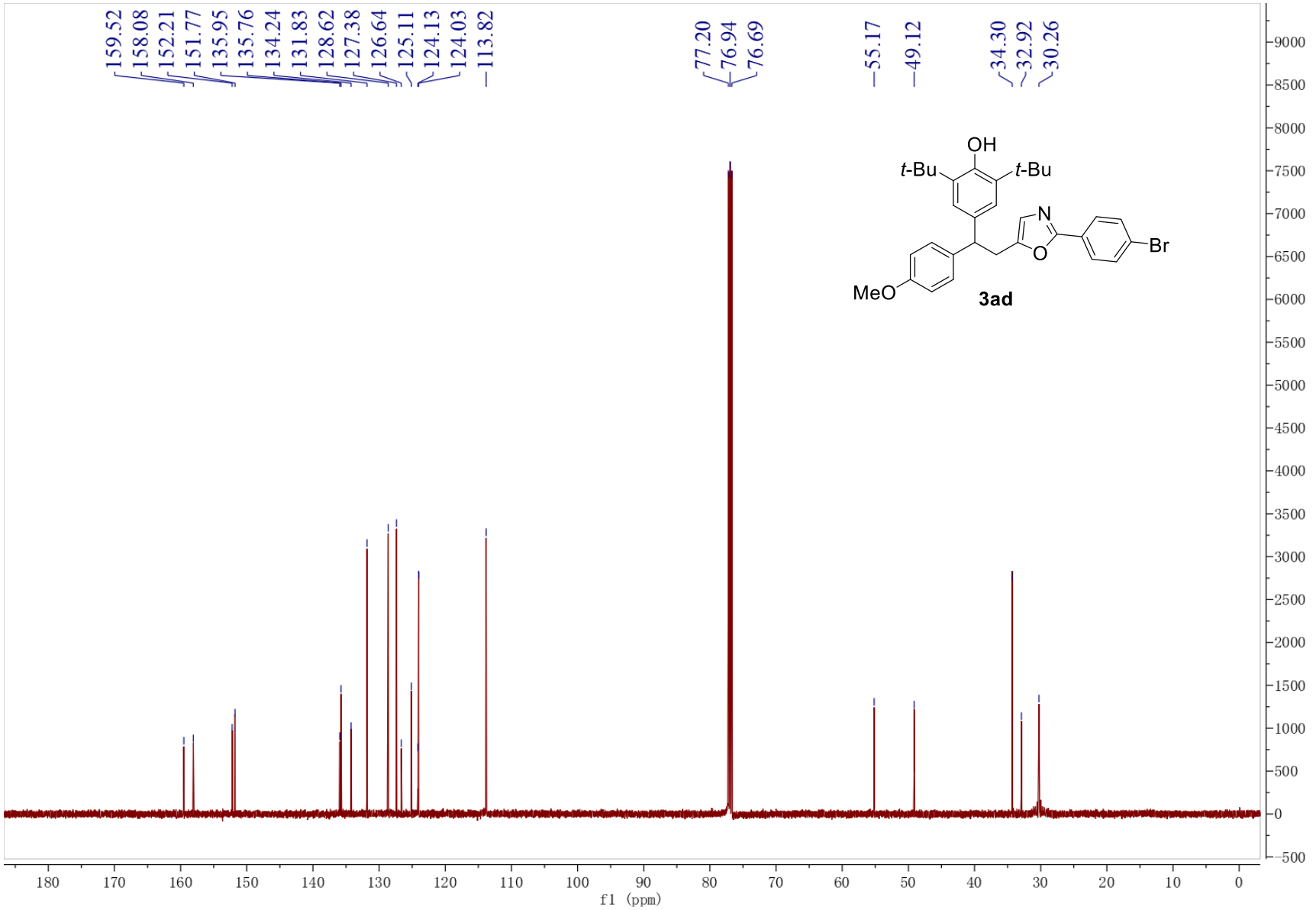
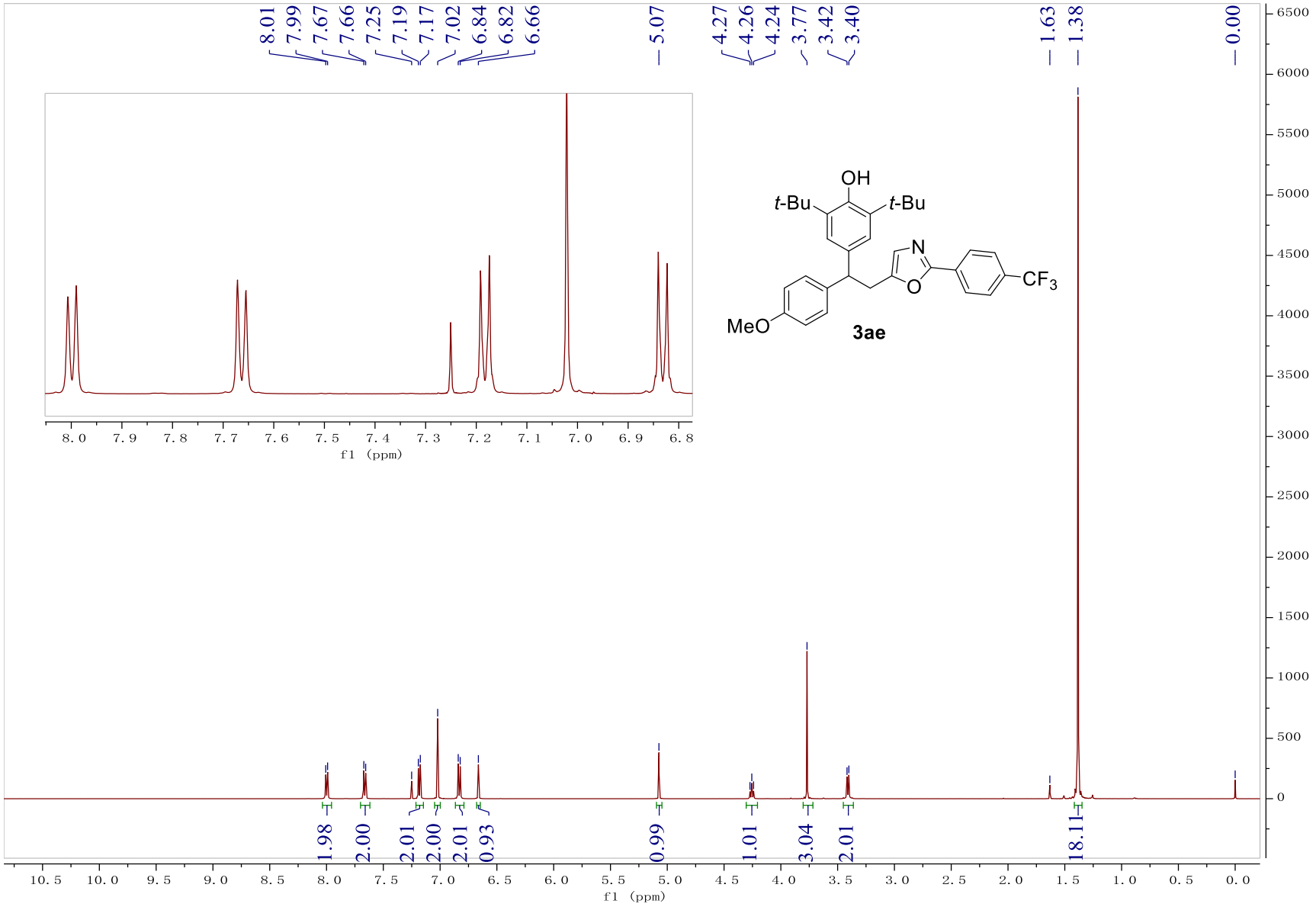
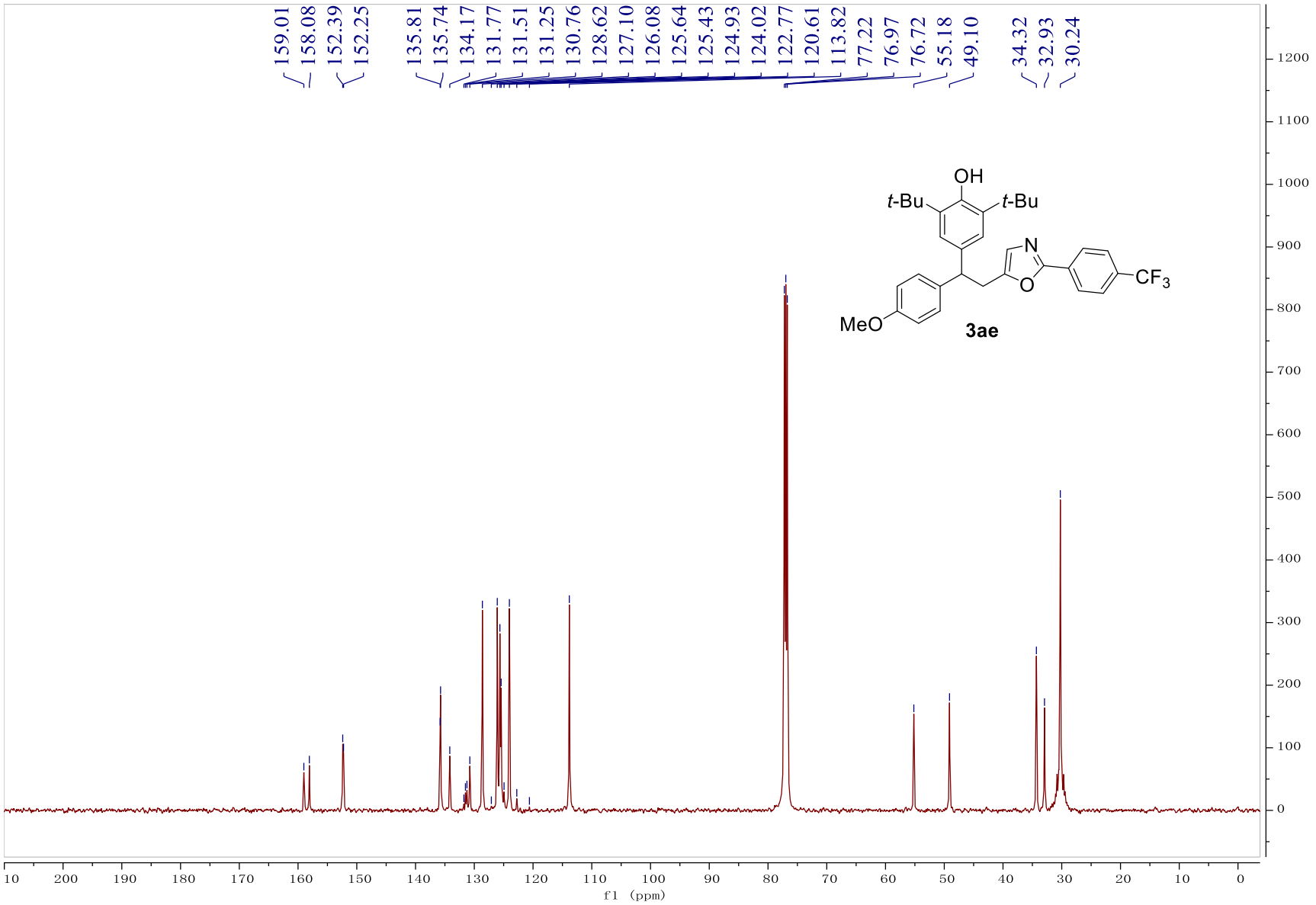
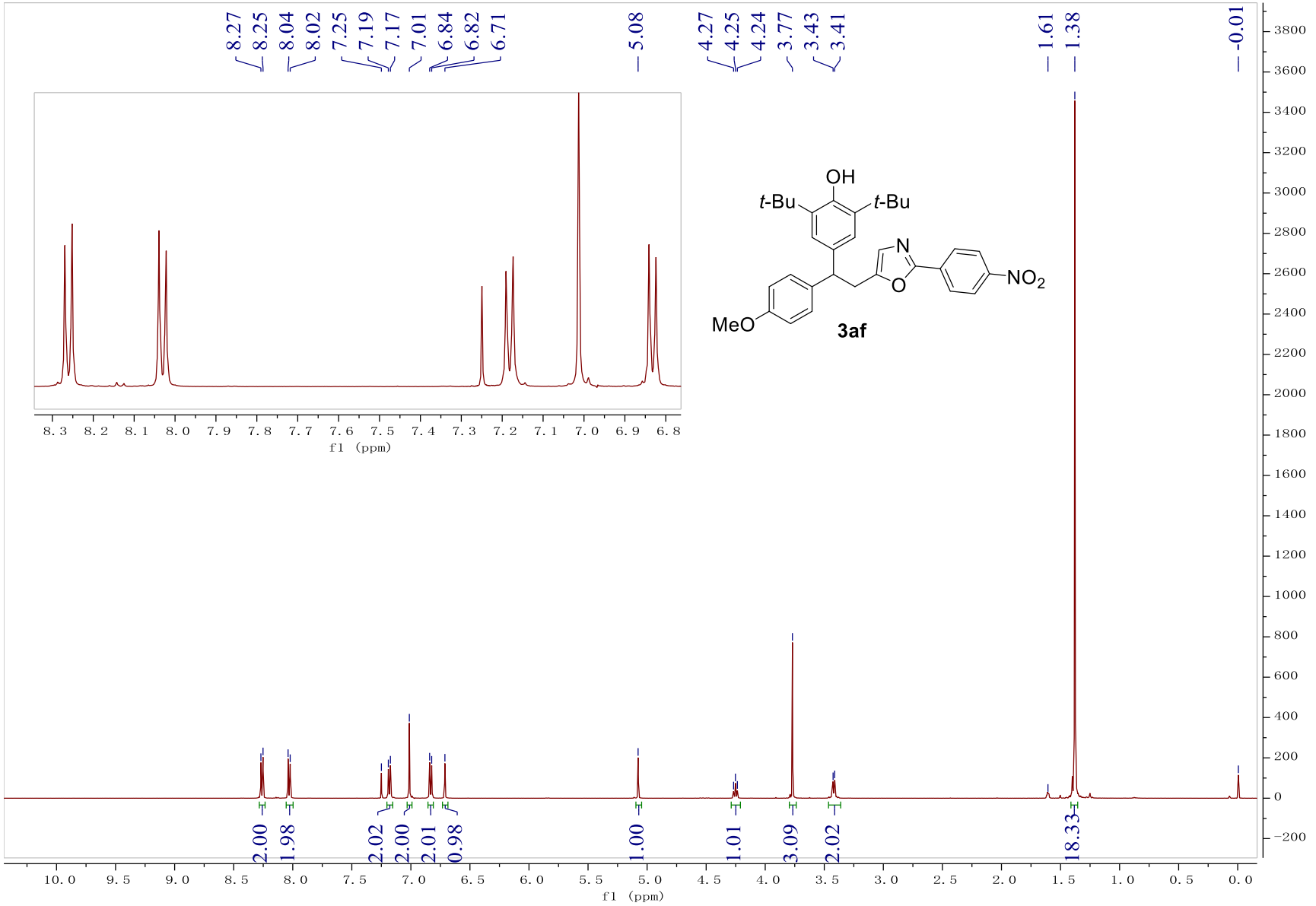
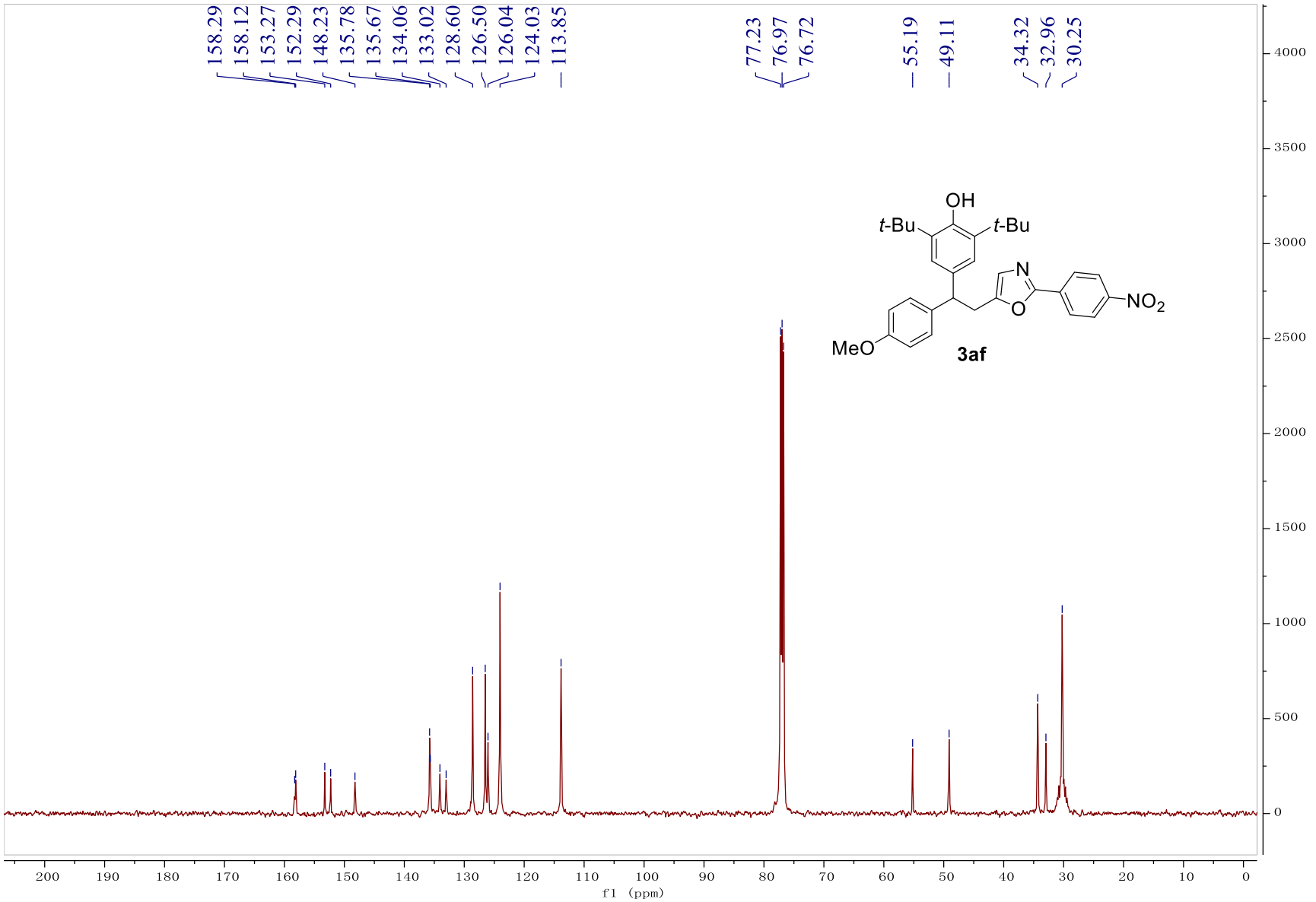
4.24
4.22
3.77
3.38
3.37
1.56
1.38
-0.00
OH
t-Bu
t-Bu
N
O
Br
MeO
3ad
f1 (ppm)
1.95
1.95
1.98
2.00
1.99
0.95
1.00
1.03
3.00
2.07
18.13

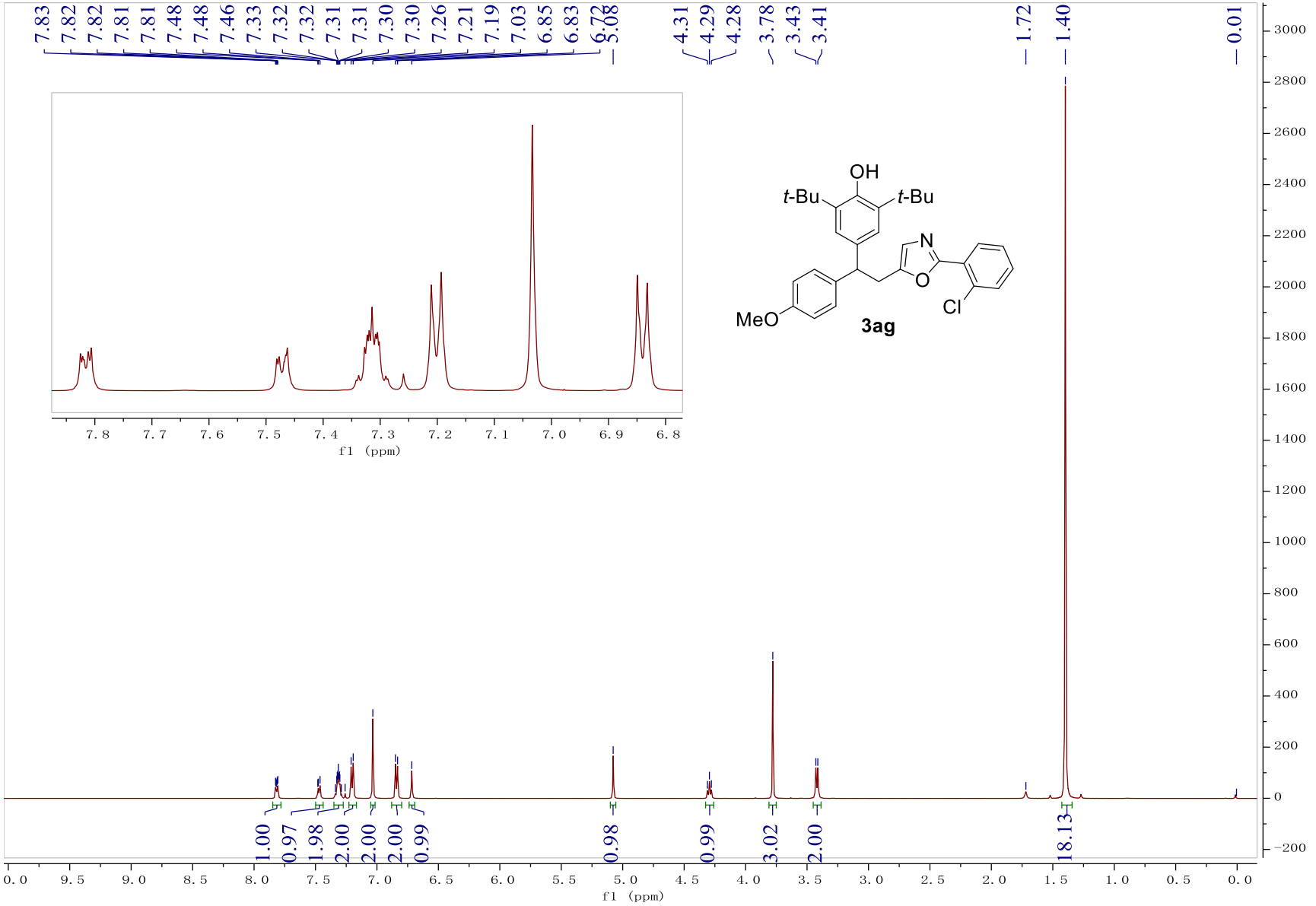

159.52
158.08
152.21
151.77
135.95
135.76
134.24
131.83
128.62
127.38
126.64
125.11
124.13
124.03
113.82
77.20
76.94
76.69
55.17
49.12
34.30
32.92
30.26
OH
t-Bu
t-Bu
N
O
Br
MeO
3ad
f1 (ppm)

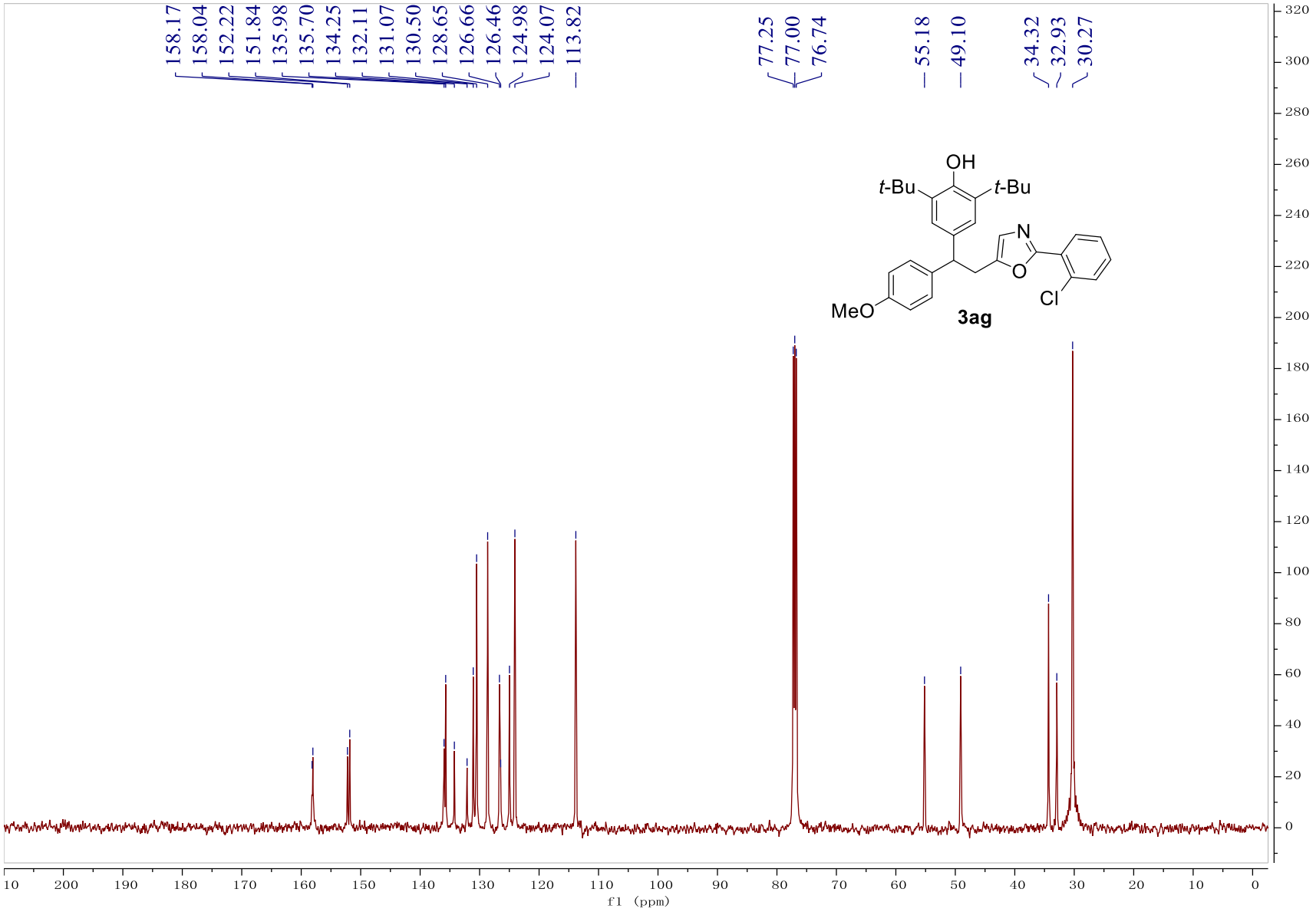

8.01
7.99
7.67
7.66
7.25
7.19
7.17
7.02
6.84
6.82
6.66
5.07
4.27
4.26
4.24
3.77
3.42
3.40
1.63
1.38
0.00
OH
t-Bu
t-Bu
N
O
CF3
MeO
3ae
1.98
2.00
2.01
2.00
2.01
0.93
0.99
1.01
3.04
2.01
18.11
f1 (ppm)

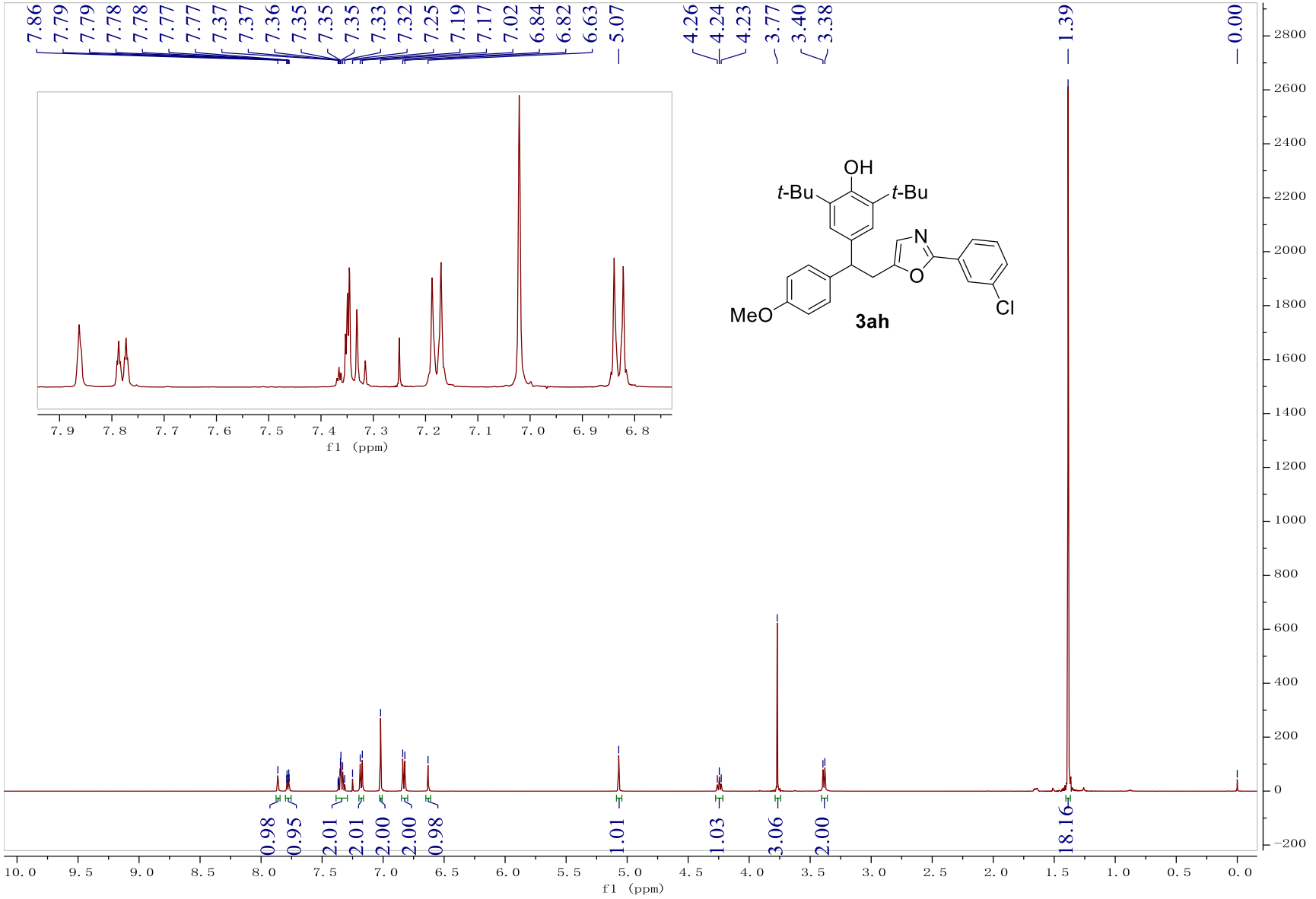

159.01
158.08
152.39
152.25
135.81
135.74
134.17
131.77
131.51
131.25
130.76
128.62
127.10
126.08
125.64
125.43
124.93
124.02
122.77
120.61
113.82
77.22
76.97
76.72
55.18
49.10
34.32
32.93
30.24
OH
t-Bu
t-Bu
N
O
CF3
MeO
3ae
f1 (ppm)

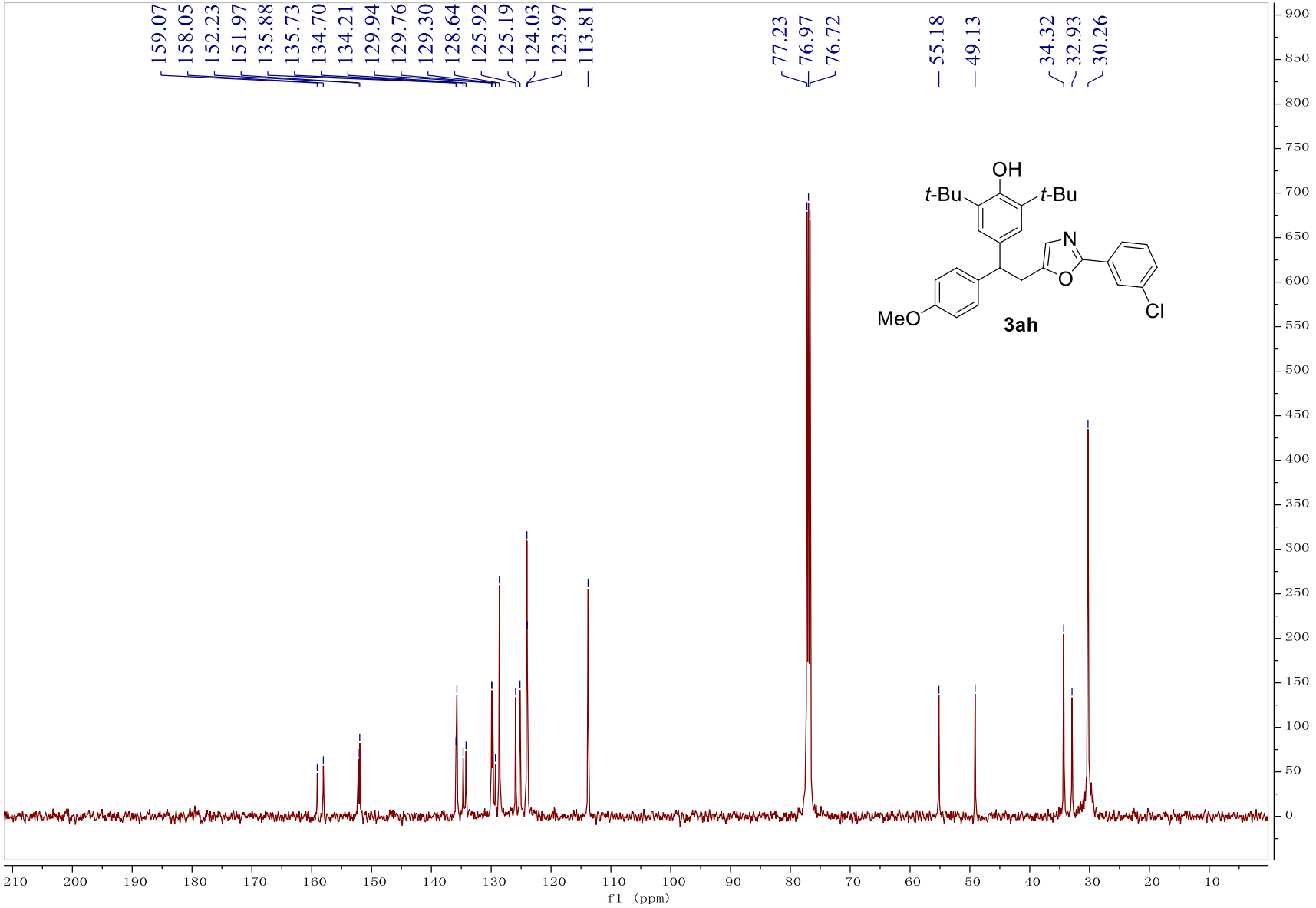

8.27
8.25
8.04
8.02
7.25
7.19
7.17
7.01
6.84
6.82
6.71
5.08
4.27
4.25
4.24
3.77
3.43
3.41
1.61
1.38
-0.01
OH
t-Bu
t-Bu
N
O
NO2
MeO
3af
f1 (ppm)
2.00
1.98
2.02
2.00
2.01
0.98
1.00
1.01
3.09
2.02
18.33

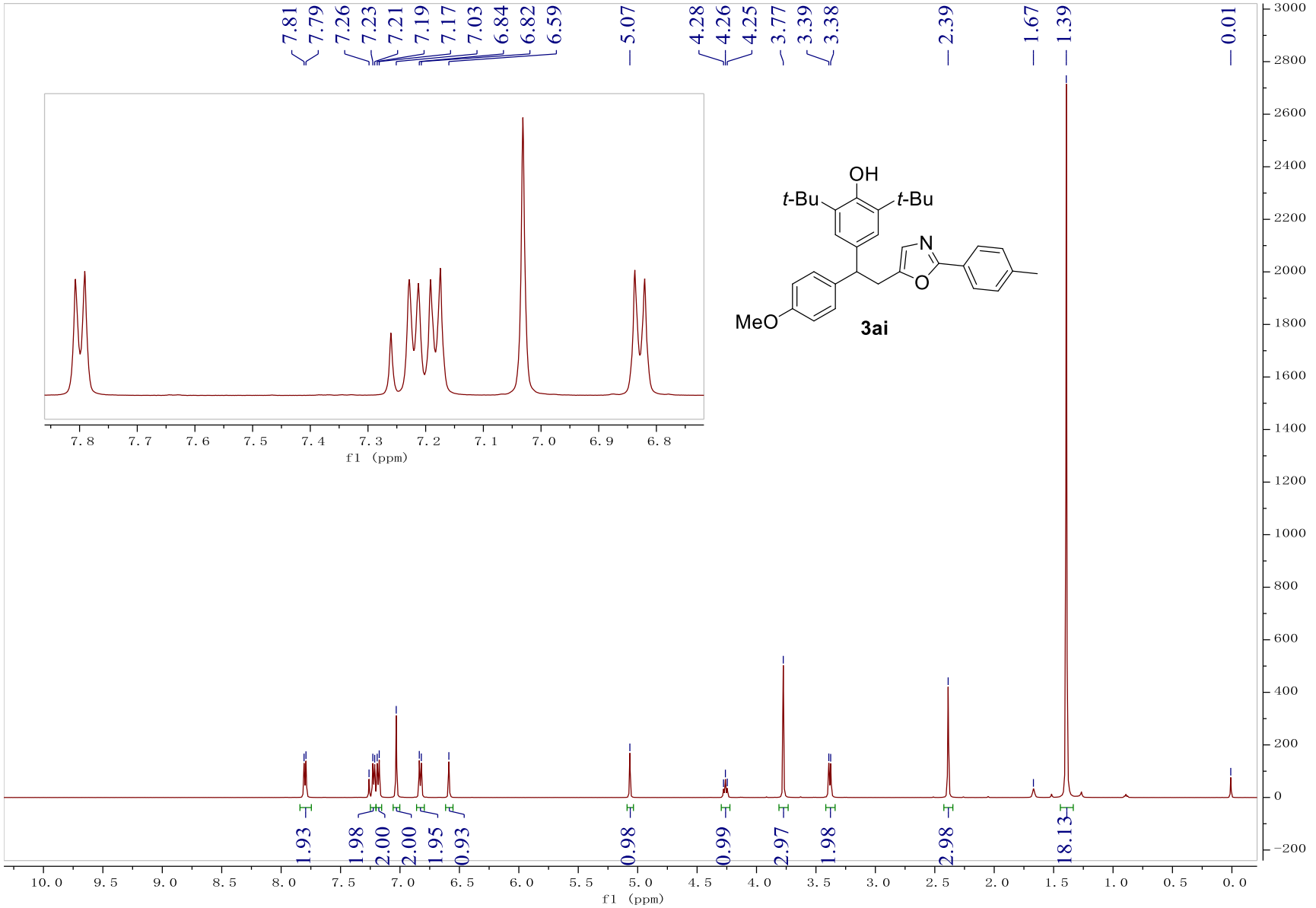

158.29
158.12
153.27
152.29
148.23
135.78
135.67
134.06
133.02
128.60
126.50
126.04
124.03
113.85
77.23
76.97
76.72
55.19
49.11
34.32
32.96
30.25
OH
t-Bu
t-Bu
N
O
NO2
MeO
3af
4000
3500
3000
2500
2000
1500
1000
500
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

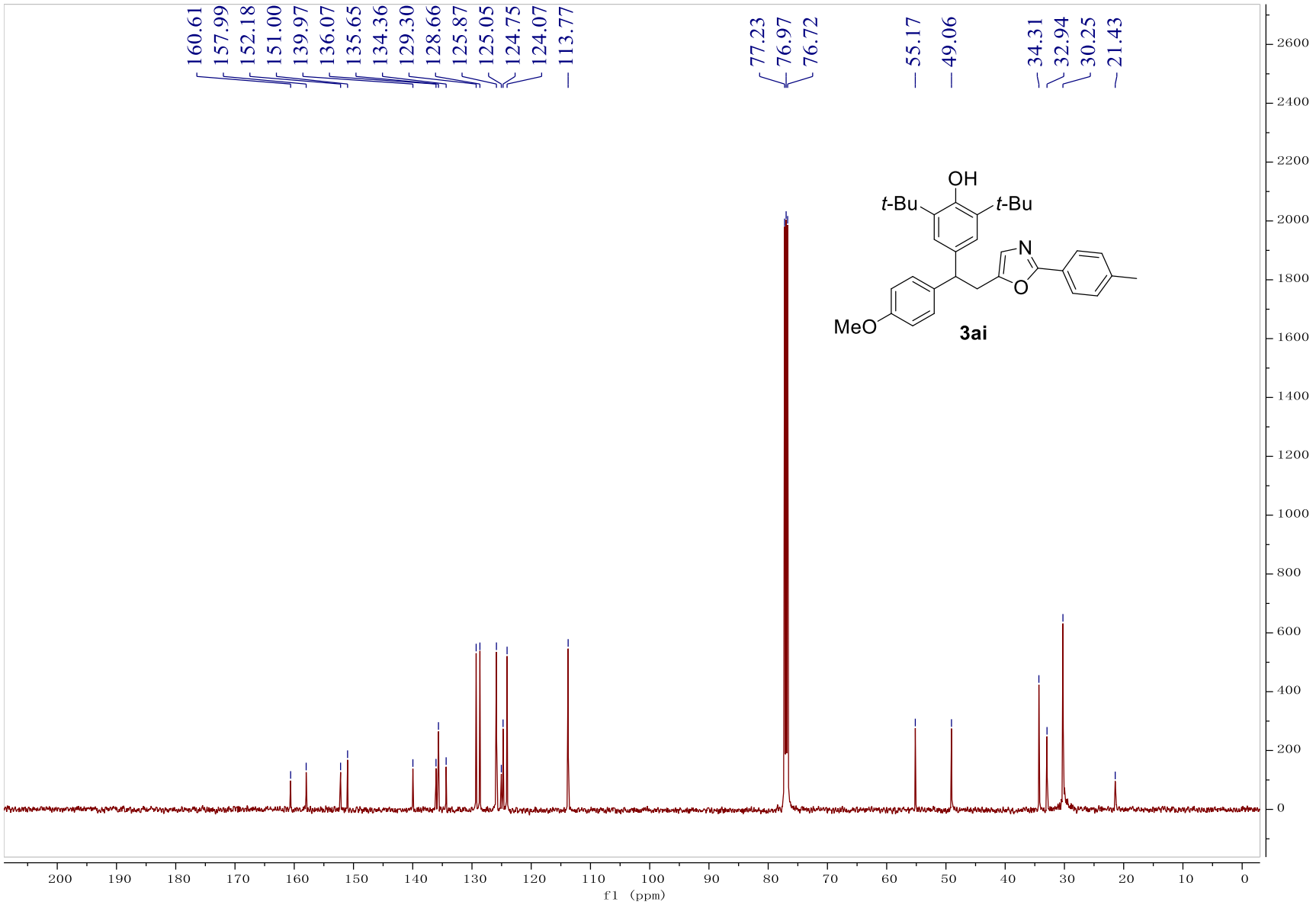

7.83
7.82
7.82
7.81
7.81
7.48
7.48
7.46
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.26
7.21
7.19
7.03
6.85
6.83
6.72
5.08
4.31
4.29
4.28
3.78
3.43
3.41
1.72
1.40
0.01
OH
t-Bu
t-Bu
N
O
Cl
MeO
3ag
f1 (ppm)
1.00
0.97
1.98
2.00
2.00
2.00
0.99
0.98
0.99
3.02
2.00
18.13
f1 (ppm)

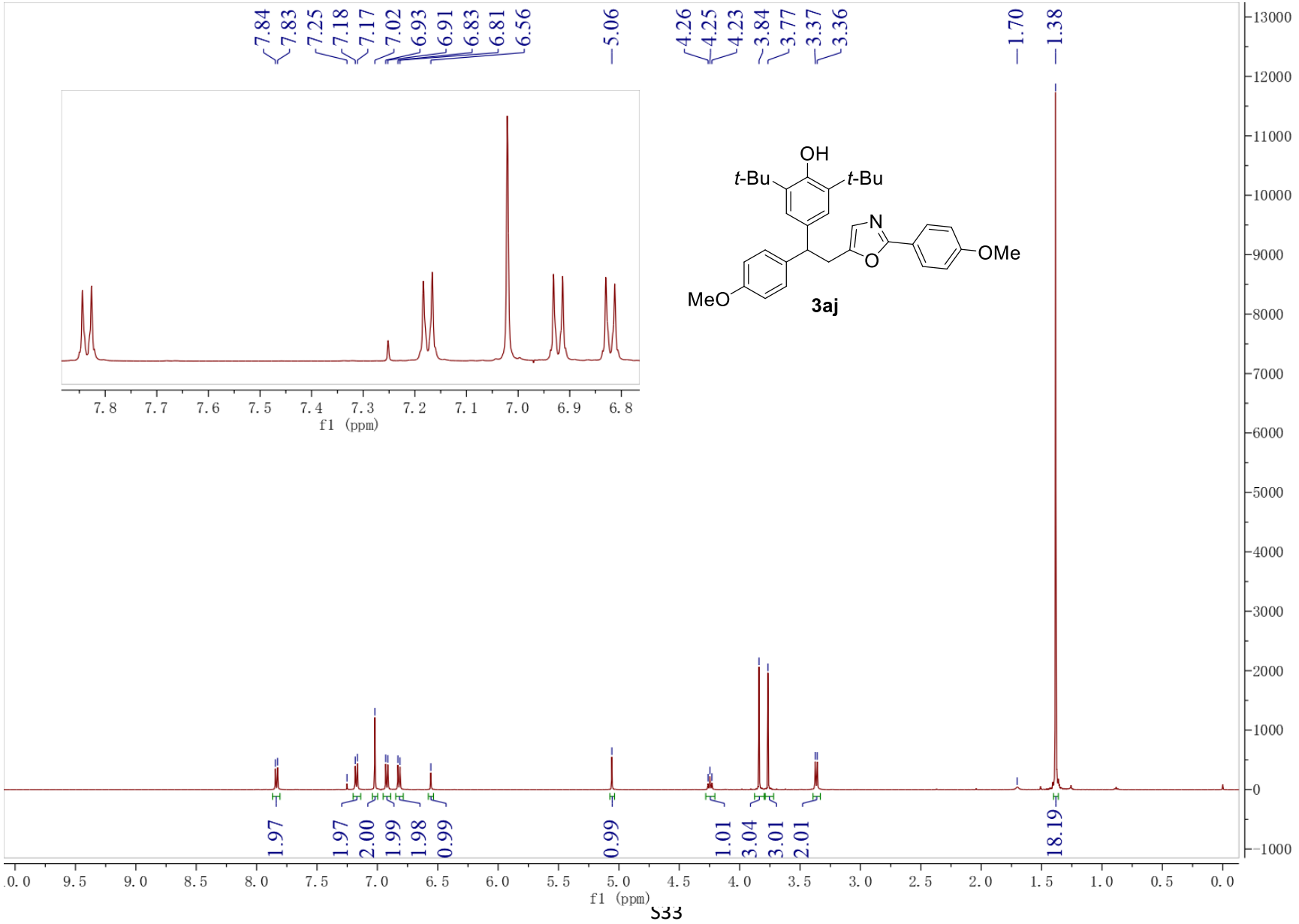

158.17
158.04
152.22
151.84
135.98
135.70
134.25
132.11
131.07
130.50
128.65
126.66
126.46
124.98
124.07
113.82
77.25
77.00
76.74
55.18
49.10
34.32
32.93
30.27
OH
t-Bu
t-Bu
N
O
Cl
MeO
3ag
f1 (ppm)

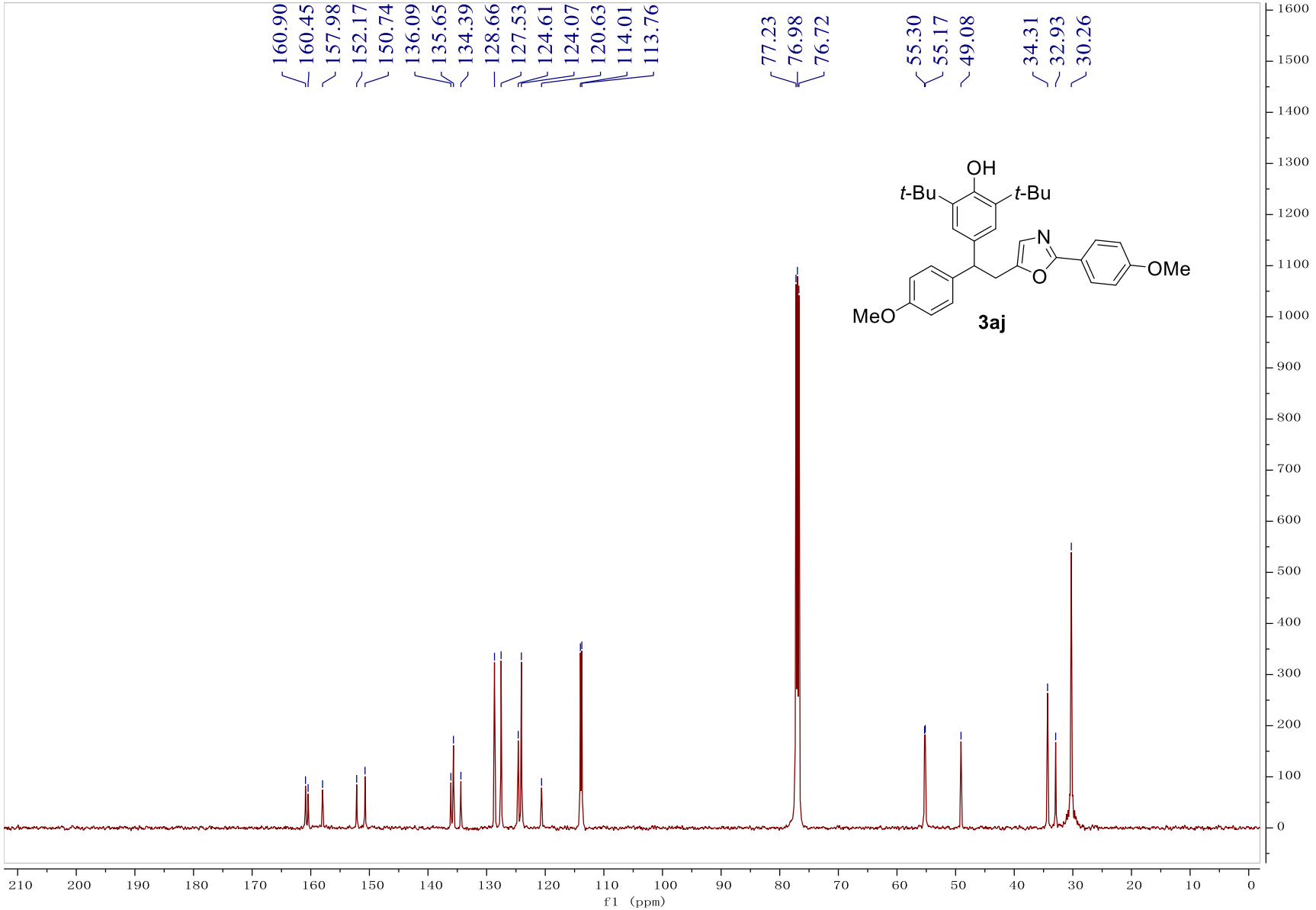

7.86
7.79
7.79
7.78
7.78
7.77
7.77
7.37
7.37
7.36
7.35
7.35
7.35
7.33
7.32
7.25
7.19
7.17
7.02
6.84
6.82
6.63
5.07
4.26
4.24
4.23
3.77
3.40
3.38
1.39
0.00
OH
t-Bu
t-Bu
N
O
MeO
Cl
3ah
f1 (ppm)
0.98
0.95
2.01
2.01
2.00
2.00
0.98
1.01
1.03
3.06
2.00
18.16

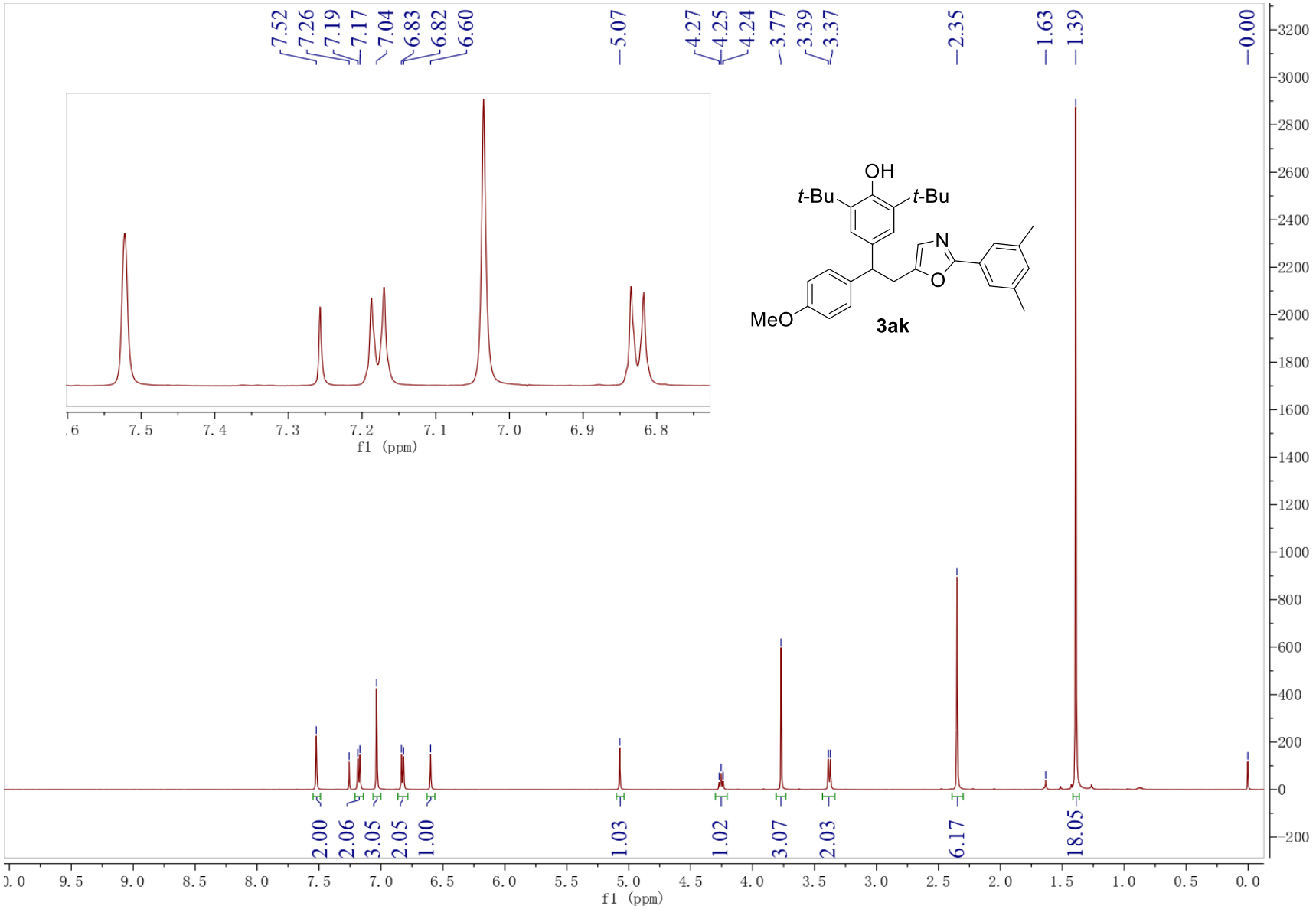

159.07
158.05
152.23
151.97
135.88
135.73
134.70
134.21
129.94
129.76
129.30
128.64
125.92
125.19
124.03
123.97
113.81
77.23
76.97
76.72
55.18
49.13
34.32
32.93
30.26
OH
t-Bu
t-Bu
N
O
MeO
Cl
3ah
f1 (ppm)

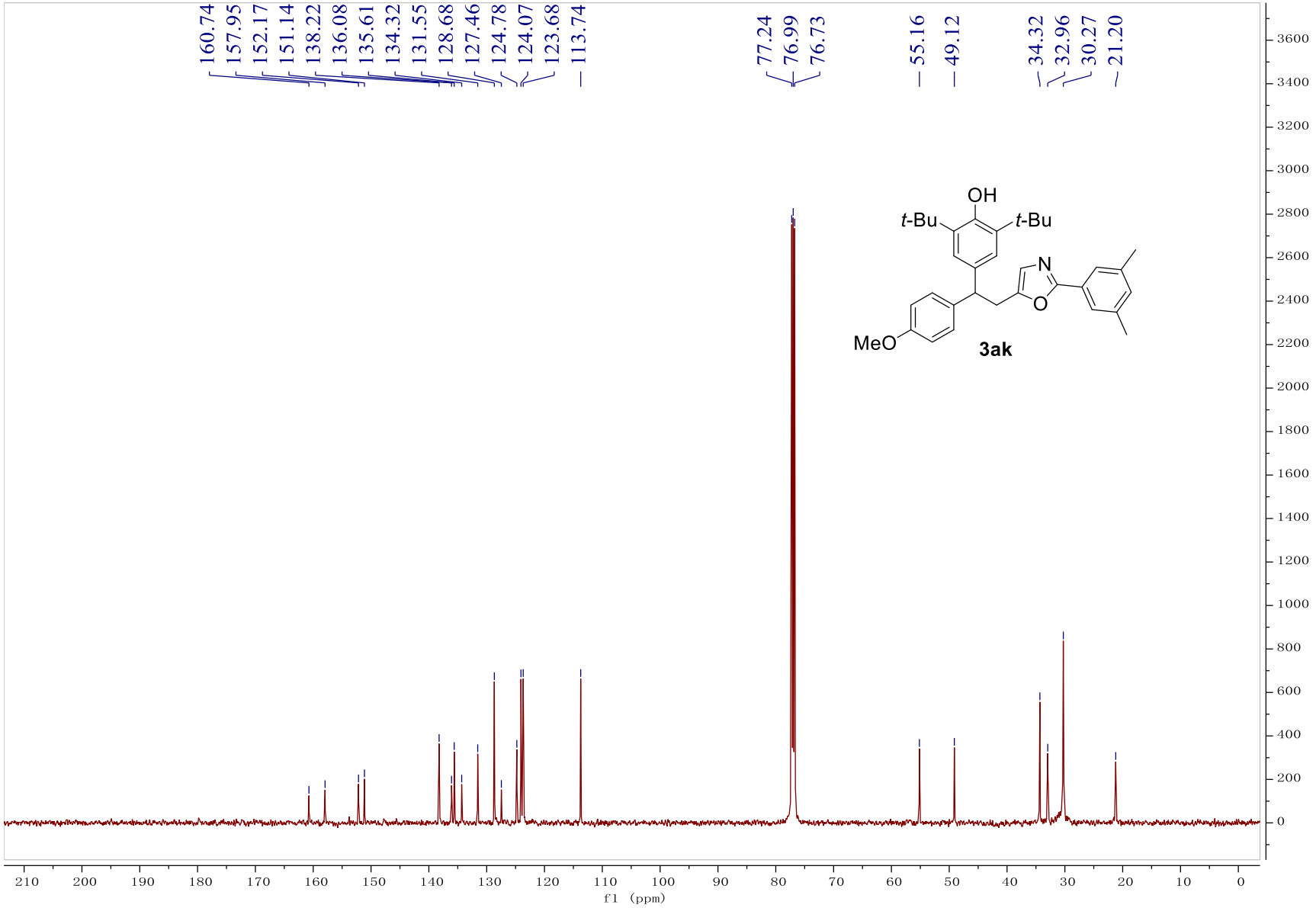

7.81
7.79
7.26
7.23
7.21
7.19
7.17
7.03
6.84
6.82
6.59
5.07
4.28
4.26
4.25
3.77
3.39
3.38
2.39
1.67
1.39
0.01
OH
t-Bu
t-Bu
N
O
MeO
3ai
f1 (ppm)
1.93
1.98
2.00
2.00
1.95
0.93
0.98
0.99
2.97
1.98
2.98
18.13


160.61
157.99
152.18
151.00
139.97
136.07
135.65
134.36
129.30
128.66
125.87
125.05
124.75
124.07
113.77
77.23
76.97
76.72
55.17
49.06
34.31
32.94
30.25
21.43
OH
t-Bu
t-Bu
N
O
MeO
3ai
f1 (ppm)


7.84
7.83
7.25
7.18
7.17
7.02
6.93
6.91
6.83
6.81
6.56
5.06
4.26
4.25
4.23
3.84
3.77
3.37
3.36
1.70
1.38
OH
t-Bu
t-Bu
N
O
OMe
MeO
3aj
f1 (ppm)
1.97
1.97
2.00
1.99
1.98
0.99
0.99
1.01
3.04
3.01
2.01
18.19


160.90
160.45
157.98
152.17
150.74
136.09
135.65
134.39
128.66
127.53
124.61
124.07
120.63
114.01
113.76
77.23
76.98
76.72
55.30
55.17
49.08
34.31
32.93
30.26
OH
t-Bu
t-Bu
N
O
OMe
MeO
3aj
f1 (ppm)


7.52
7.26
7.19
7.17
7.04
6.83
6.82
6.60
5.07
4.27
4.25
4.24
3.77
3.39
3.37
2.35
1.63
1.39
0.00
OH
t-Bu
t-Bu
N
O
MeO
3ak
f1 (ppm)
2.00
2.06
3.05
2.05
1.00
1.03
1.02
3.07
2.03
6.17
18.05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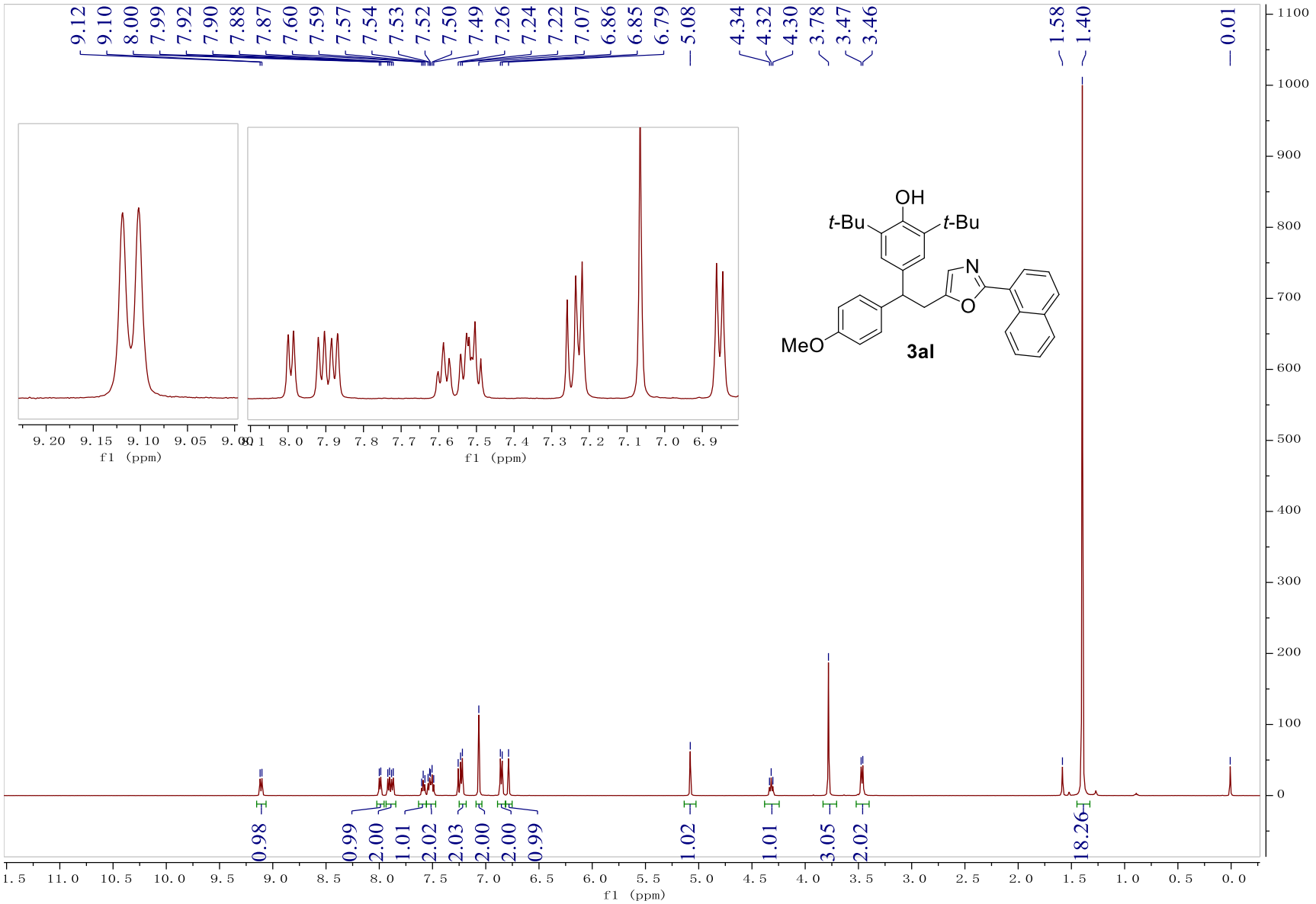
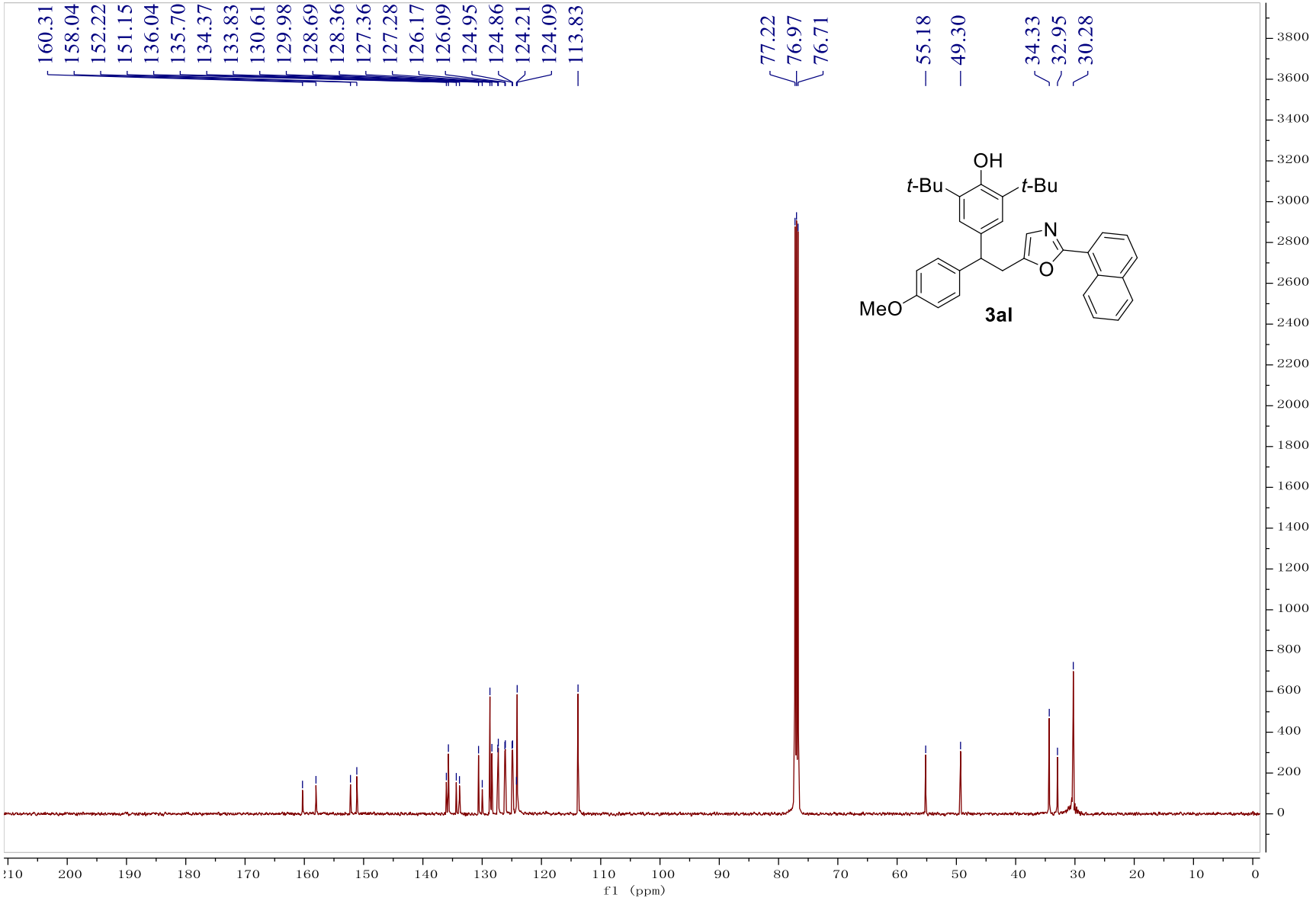
157.95
152.17
151.14
138.22
136.08
135.61
134.32
131.55
128.68
127.46
124.78
124.07
123.68
113.74
77.24
76.99
76.73
55.16
49.12
34.32
32.96
30.27
21.20
OH
t-Bu
t-Bu
N
O
MeO
3ak
f1 (ppm)


9.12
9.10
8.00
7.99
7.92
7.90
7.88
7.87
7.60
7.59
7.57
7.54
7.53
7.52
7.50
7.49
7.26
7.24
7.22
7.07
6.86
6.85
6.79
5.08
4.34
4.32
4.30
3.78
3.47
3.46
1.58
1.40
0.01
OH
t-Bu
t-Bu
N
O
MeO
3al
f1 (ppm)
0.98
0.99
2.00
1.01
2.02
2.03
2.00
2.00
0.99
1.02
1.01
3.05
2.02
18.26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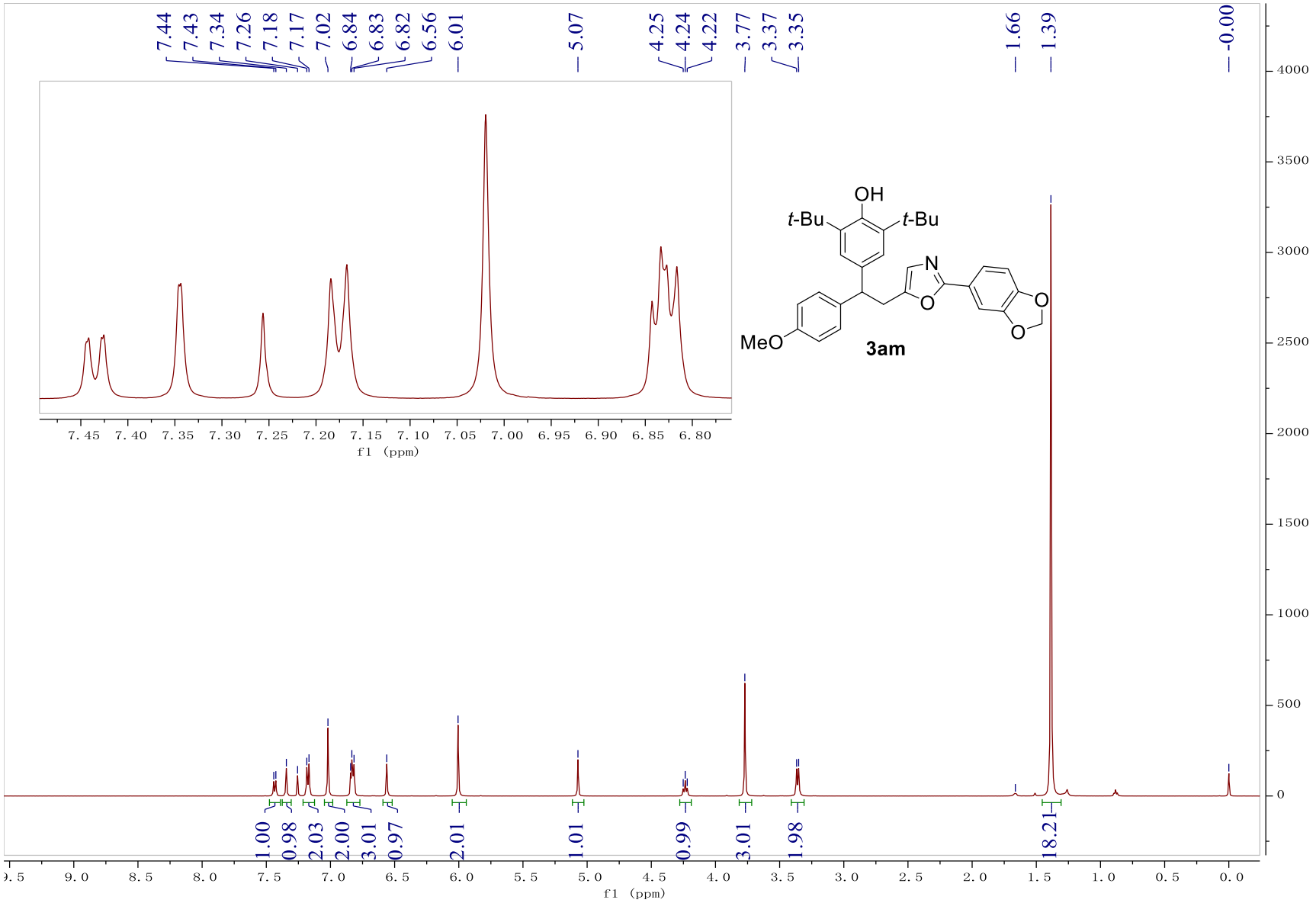
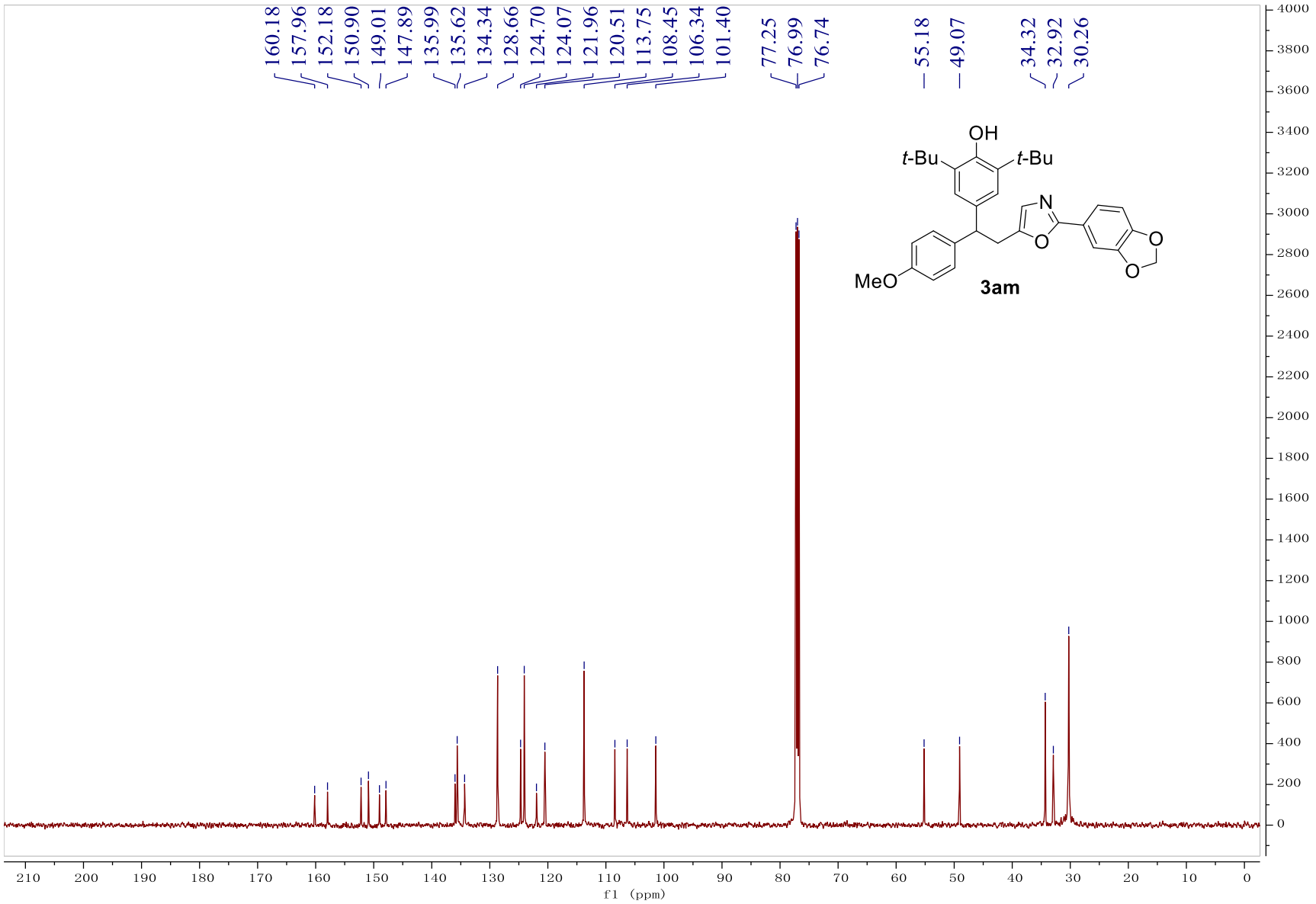
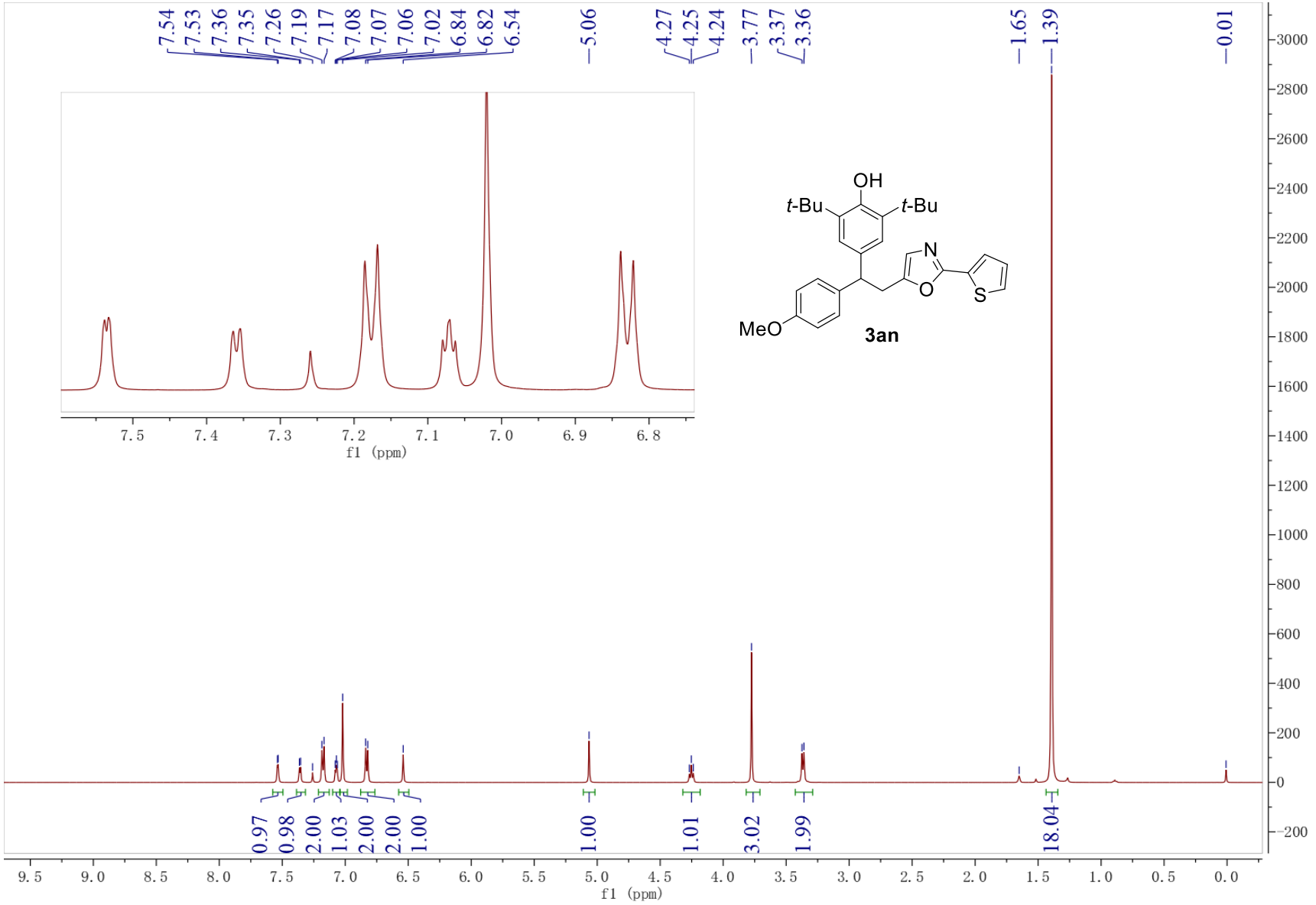
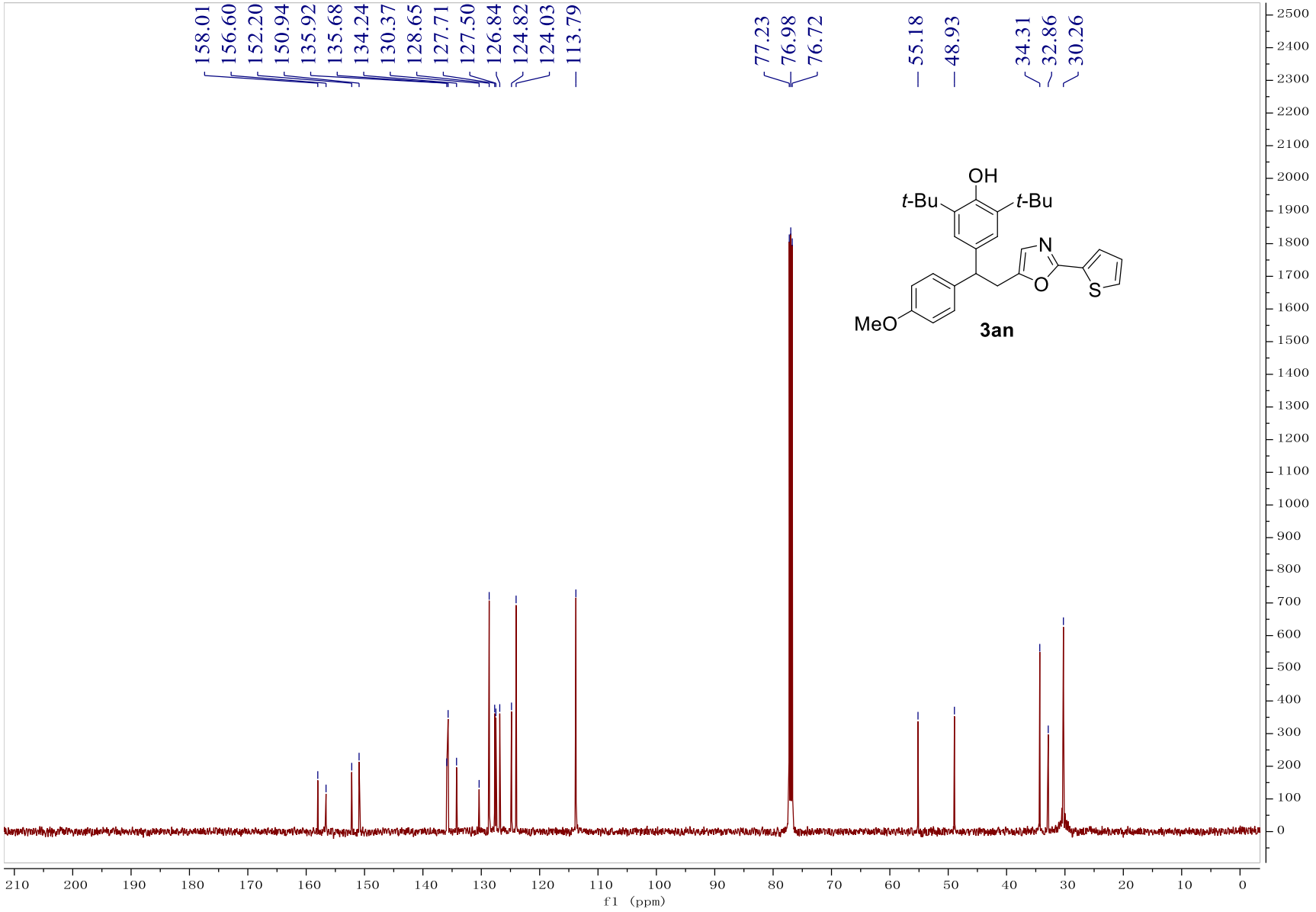
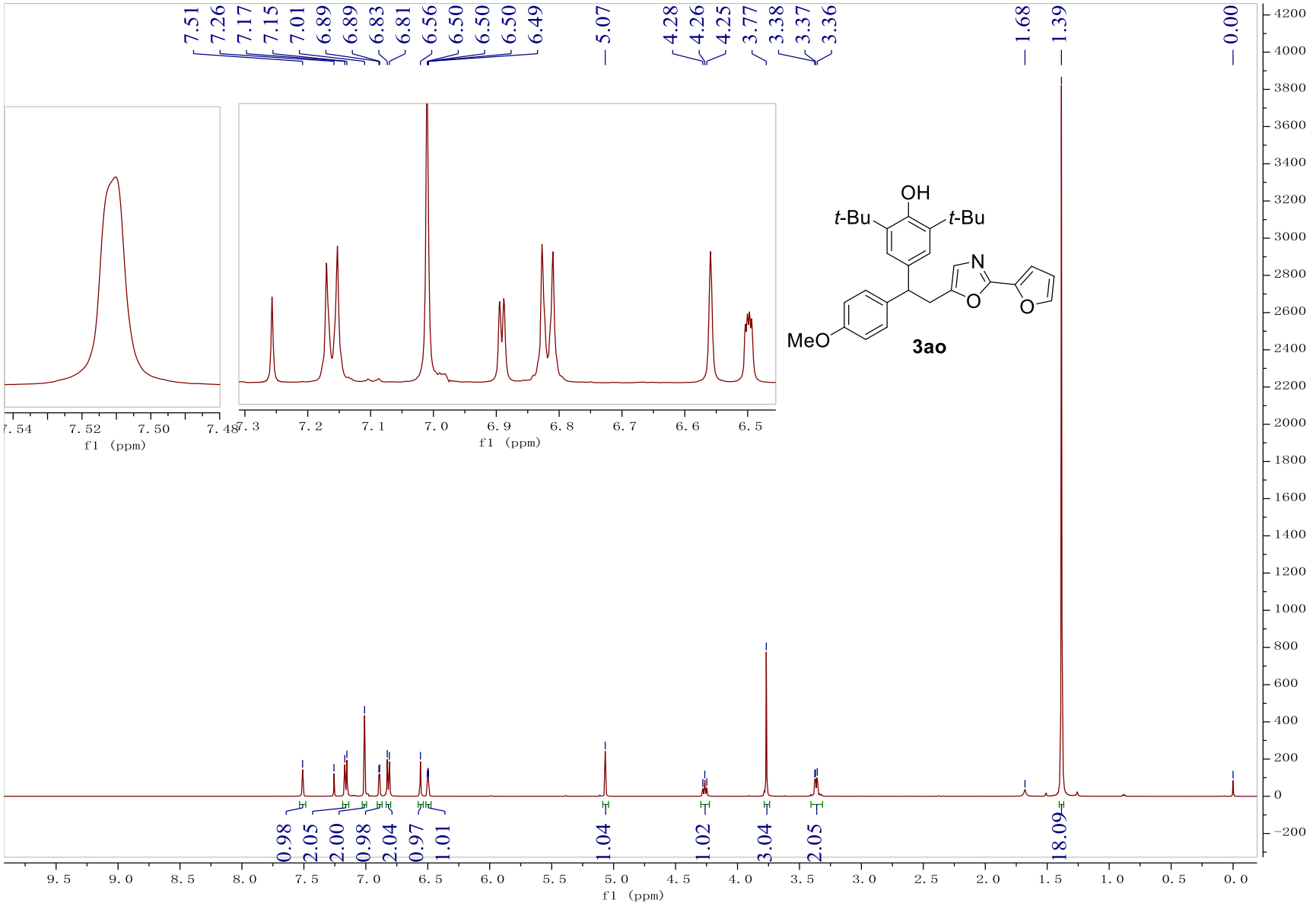
158.04
152.22
151.15
136.04
135.70
134.37
133.83
130.61
129.98
128.69
128.36
127.36
127.28
126.17
126.09
124.95
124.86
124.21
124.09
113.83
77.22
76.97
76.71
55.18
49.30
34.33
32.95
30.28
OH
t-Bu
t-Bu
N
O
MeO
3al
f1 (ppm)

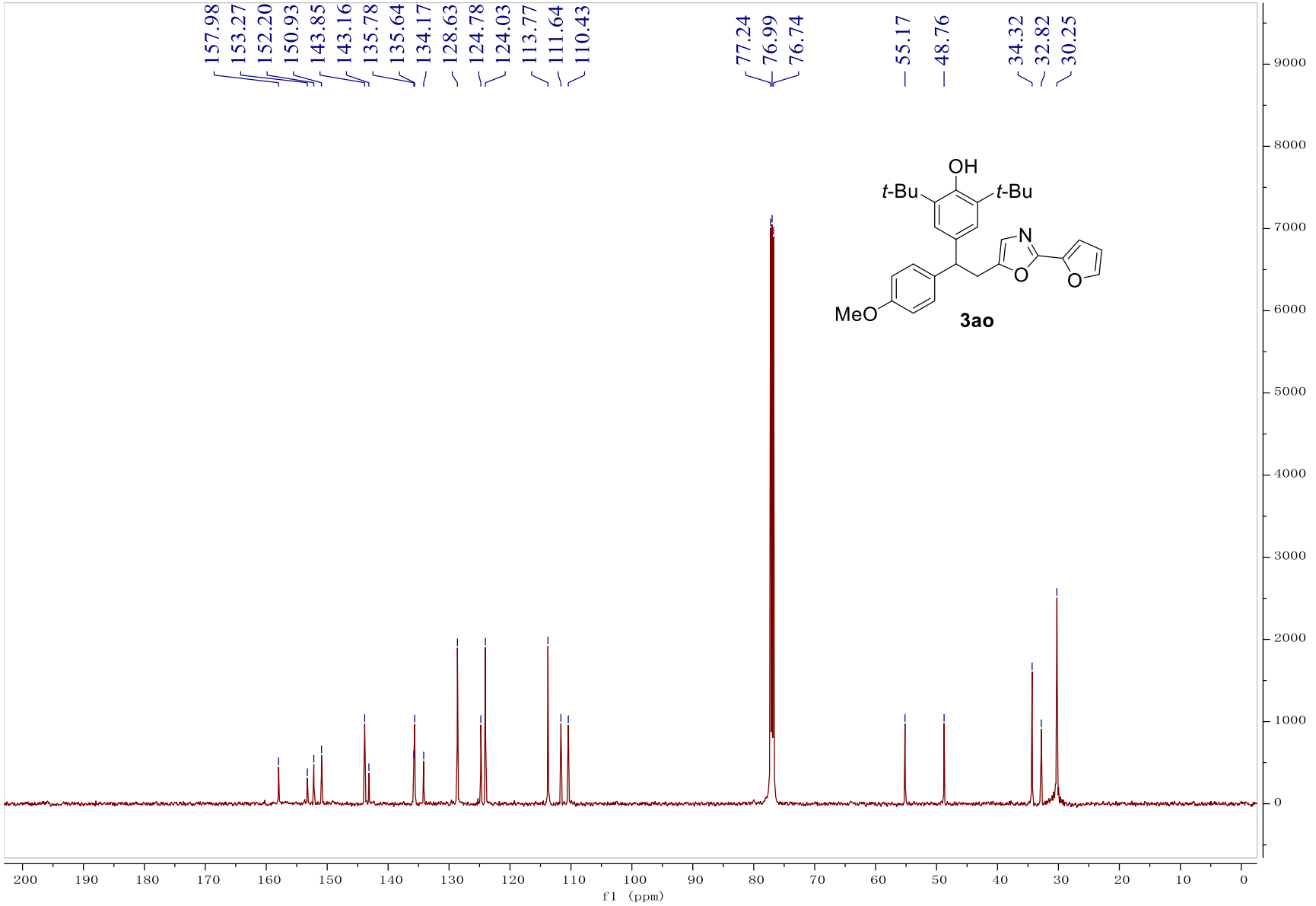

7.44
7.43
7.34
7.26
7.18
7.17
7.02
6.84
6.83
6.82
6.56
6.01
5.07
4.25
4.24
4.22
3.77
3.37
3.35
1.66
1.39
-0.00
OH
t-Bu
t-Bu
N
O
O
O
MeO
3am
f1 (ppm)
1.00
0.98
2.03
2.00
3.01
0.97
2.01
1.01
0.99
3.01
1.98
18.21

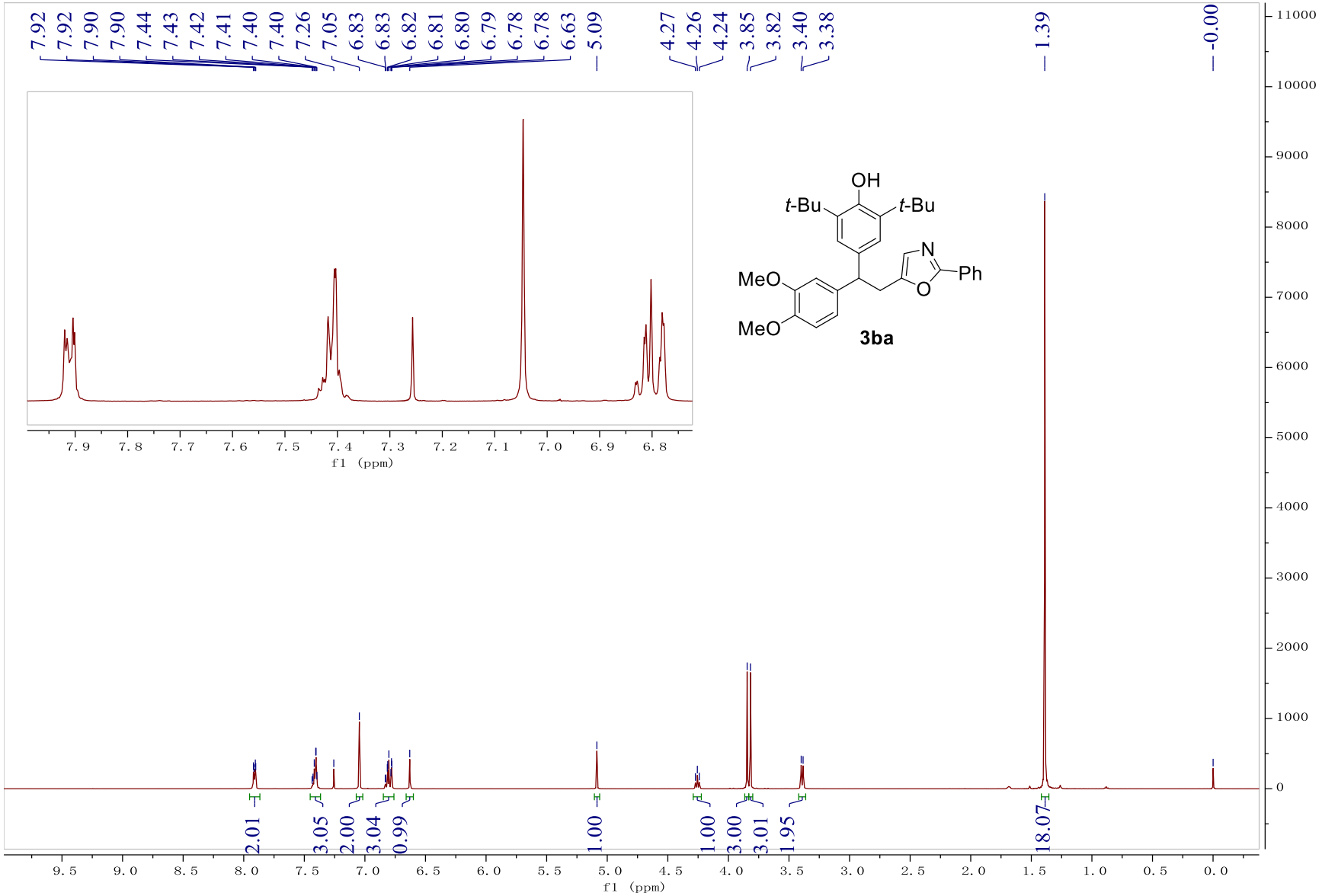

160.18
157.96
152.18
150.90
149.01
147.89
135.99
135.62
134.34
128.66
124.70
124.07
121.96
120.51
113.75
108.45
106.34
101.40
77.25
76.99
76.74
55.18
49.07
34.32
32.92
30.26
OH
t-Bu
t-Bu
N
O
O
O
MeO
3am
f1 (ppm)

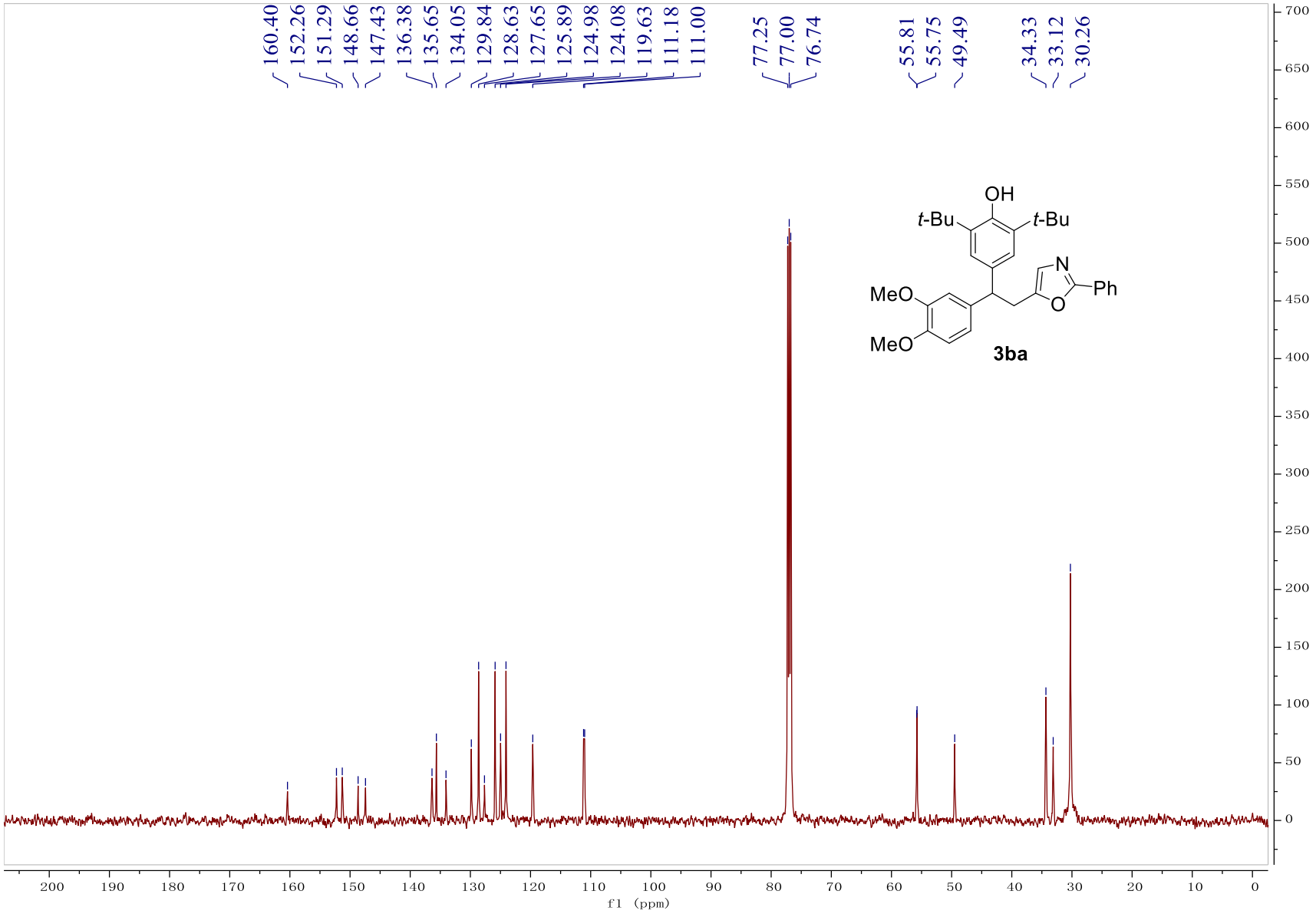

7.54
7.53
7.36
7.35
7.26
7.19
7.17
7.08
7.07
7.06
7.02
6.84
6.82
6.54
5.06
4.27
4.25
4.24
3.77
3.37
3.36
1.65
1.39
0.01
OH
t-Bu
t-Bu
N
O
S
MeO
3an
f1 (ppm)
0.97
0.98
2.00
1.03
2.00
2.00
1.00
1.00
1.01
3.02
1.99
18.04

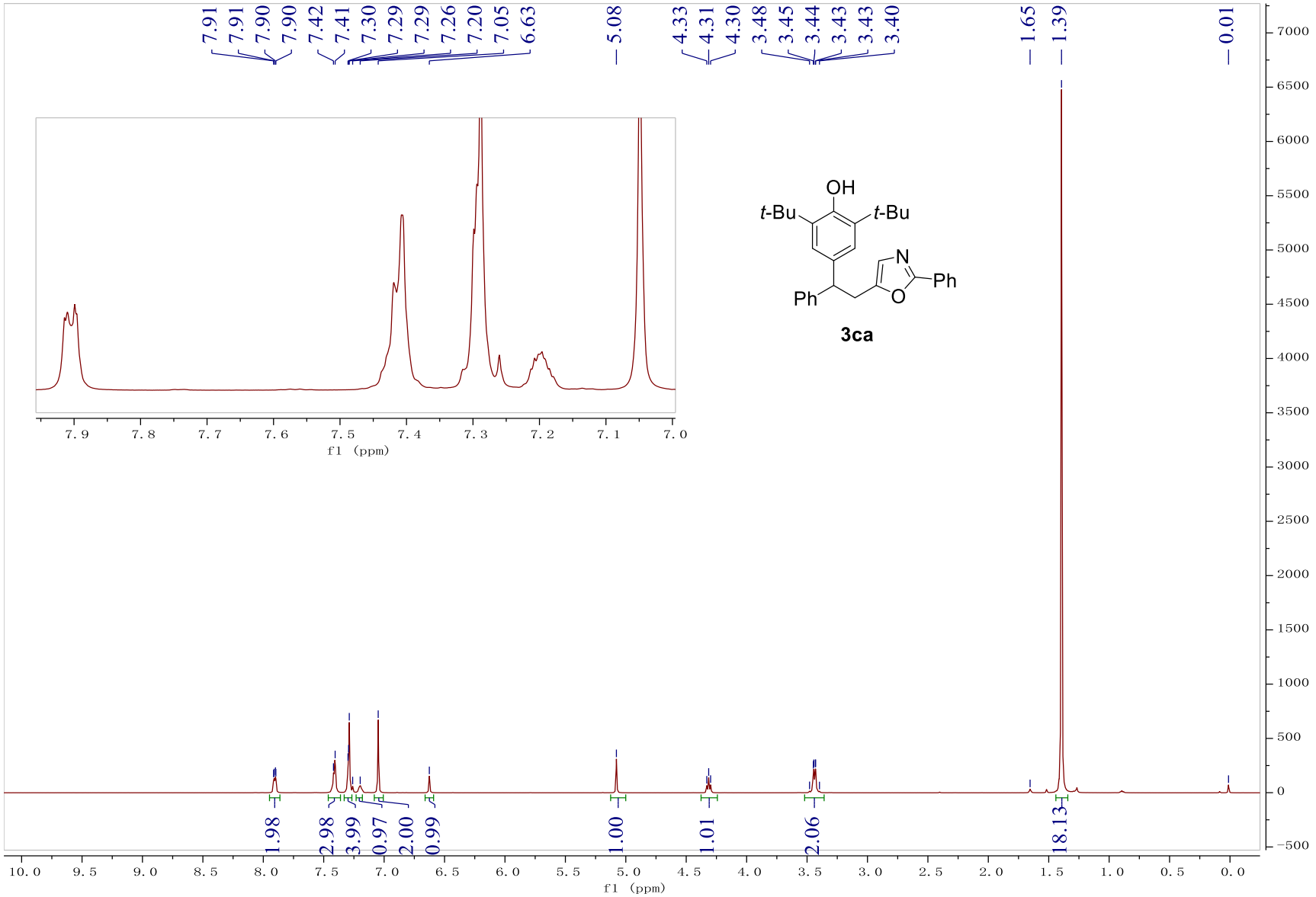

158.01
156.60
152.20
150.94
135.92
135.68
134.24
130.37
128.65
127.71
127.50
126.84
124.82
124.03
113.79
77.23
76.98
76.72
55.18
48.93
34.31
32.86
30.26
OH
t-Bu
t-Bu
N
O
S
MeO
3an
f1 (ppm)

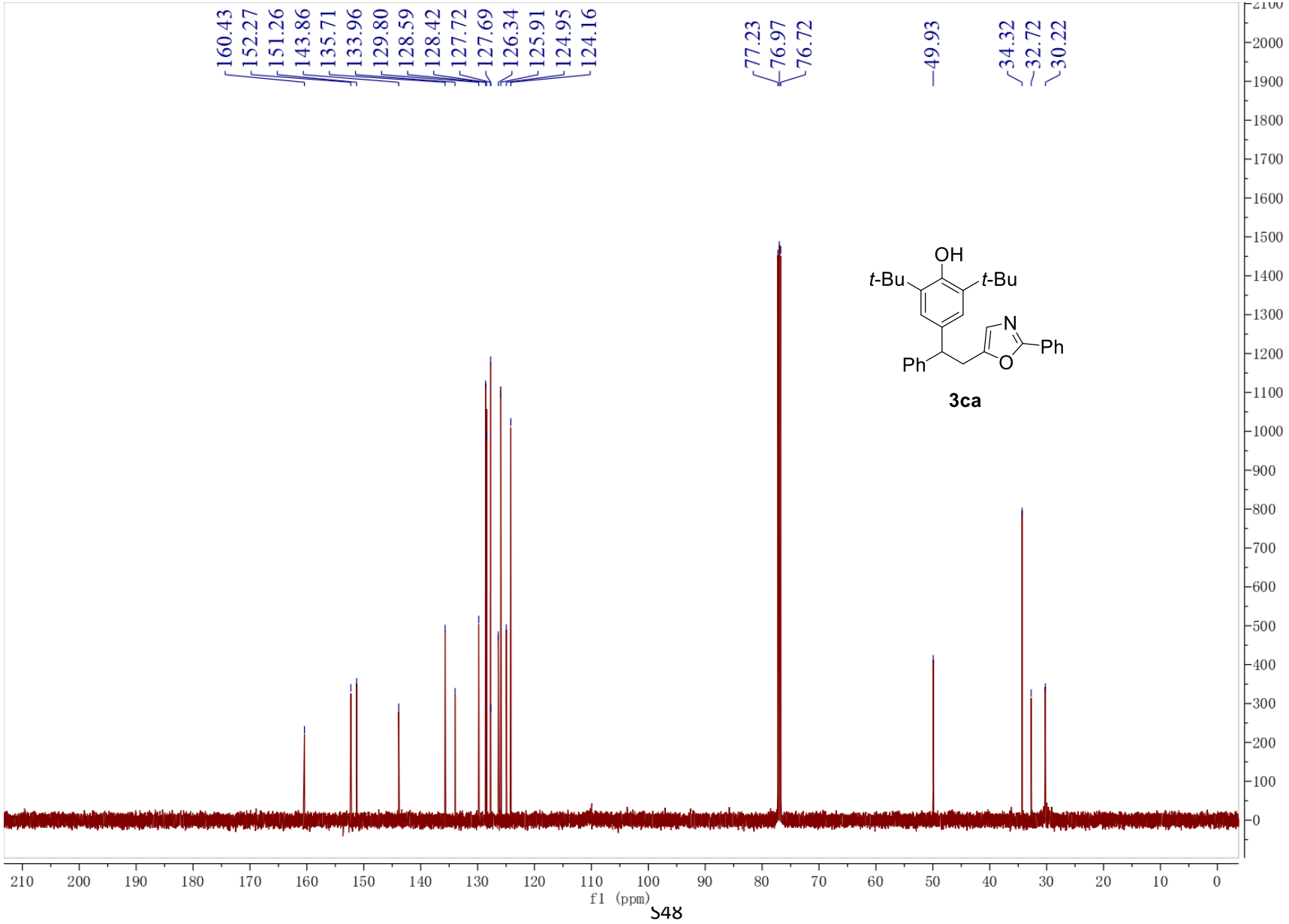

7.51
7.26
7.17
7.15
7.01
6.89
6.89
6.83
6.81
6.56
6.50
6.50
6.50
6.49
5.07
4.28
4.26
4.25
3.77
3.38
3.37
3.36
1.68
1.39
0.00
OH
t-Bu
t-Bu
N
O
O
MeO
3ao
f1 (ppm)
0.98
2.05
2.00
0.98
2.04
0.97
1.01
1.04
1.02
3.04
2.05
18.09


157.98
153.27
152.20
150.93
143.85
143.16
135.78
135.64
134.17
128.63
124.78
124.03
113.77
111.64
110.43
77.24
76.99
76.74
55.17
48.76
34.32
32.82
30.25
OH
t-Bu
t-Bu
N
O
O
MeO
3ao
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.92
7.92
7.90
7.90
7.44
7.43
7.42
7.41
7.40
7.40
7.26
7.05
6.83
6.83
6.82
6.81
6.80
6.79
6.78
6.78
6.63
5.09
4.27
4.26
4.24
3.85
3.82
3.40
3.38
1.39
-0.00
f1 (ppm)
OH
t-Bu
t-Bu
N
Ph
O
MeO
MeO
3ba
2.01
3.05
2.00
3.04
0.99
1.00
1.00
3.00
3.01
1.95
18.07
f1 (ppm)


160.40
152.26
151.29
148.66
147.43
136.38
135.65
134.05
129.84
128.63
127.65
125.89
124.98
124.08
119.63
111.18
111.00
77.25
77.00
76.74
55.81
55.75
49.49
34.33
33.12
30.26
OH
t-Bu
t-Bu
N
Ph
O
MeO
MeO
3ba
f1 (ppm)


7.91
7.91
7.90
7.90
7.42
7.41
7.30
7.29
7.29
7.26
7.20
7.05
6.63
5.08
4.33
4.31
4.30
3.48
3.45
3.44
3.43
3.43
3.40
1.65
1.39
0.01
OH
t-Bu
t-Bu
N
Ph
Ph
O
3ca
f1 (ppm)
1.98
2.98
3.99
0.97
2.00
0.99
1.00
1.01
2.06
18.13
f1 (ppm)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151.26
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133.96
129.80
128.59
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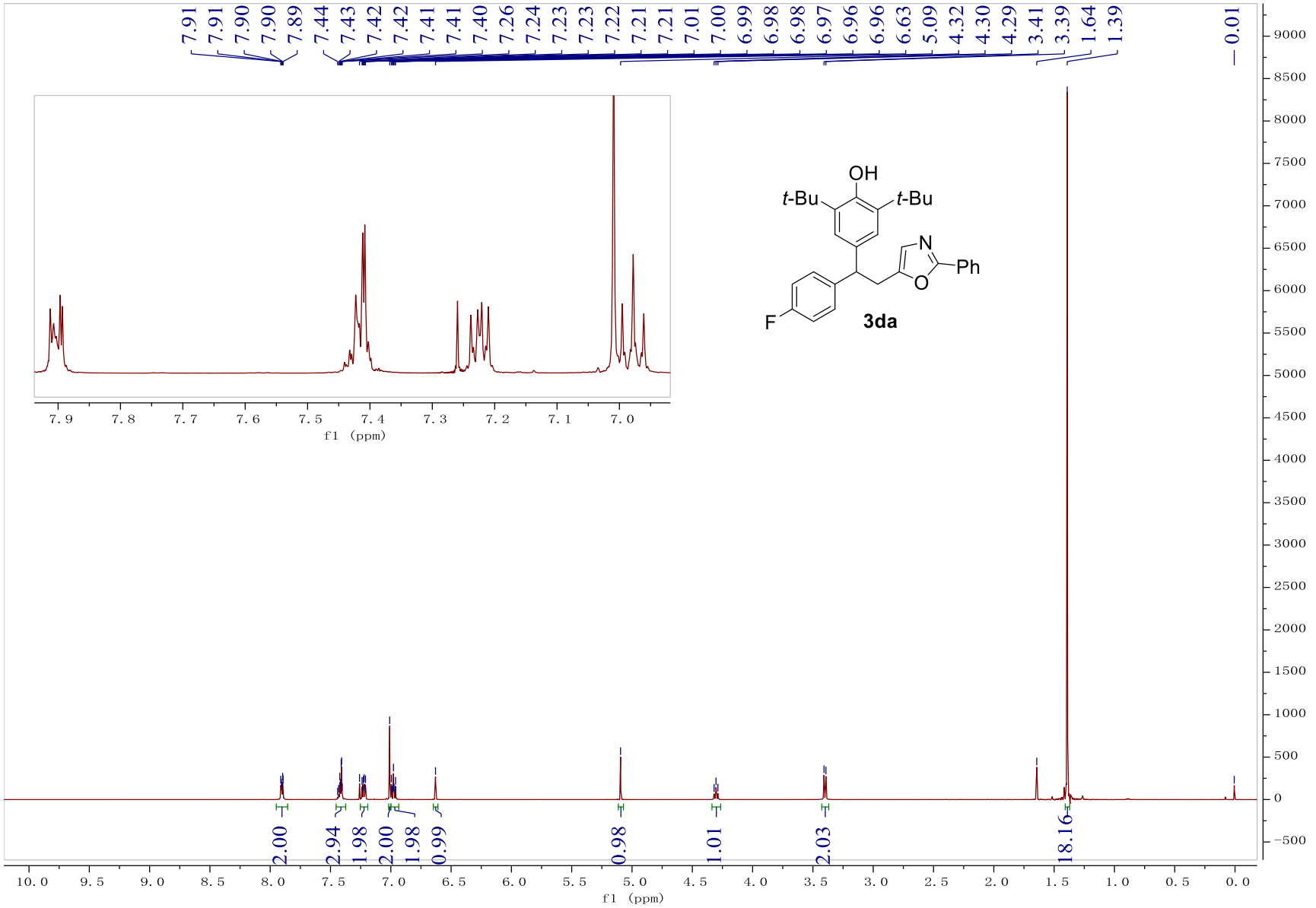
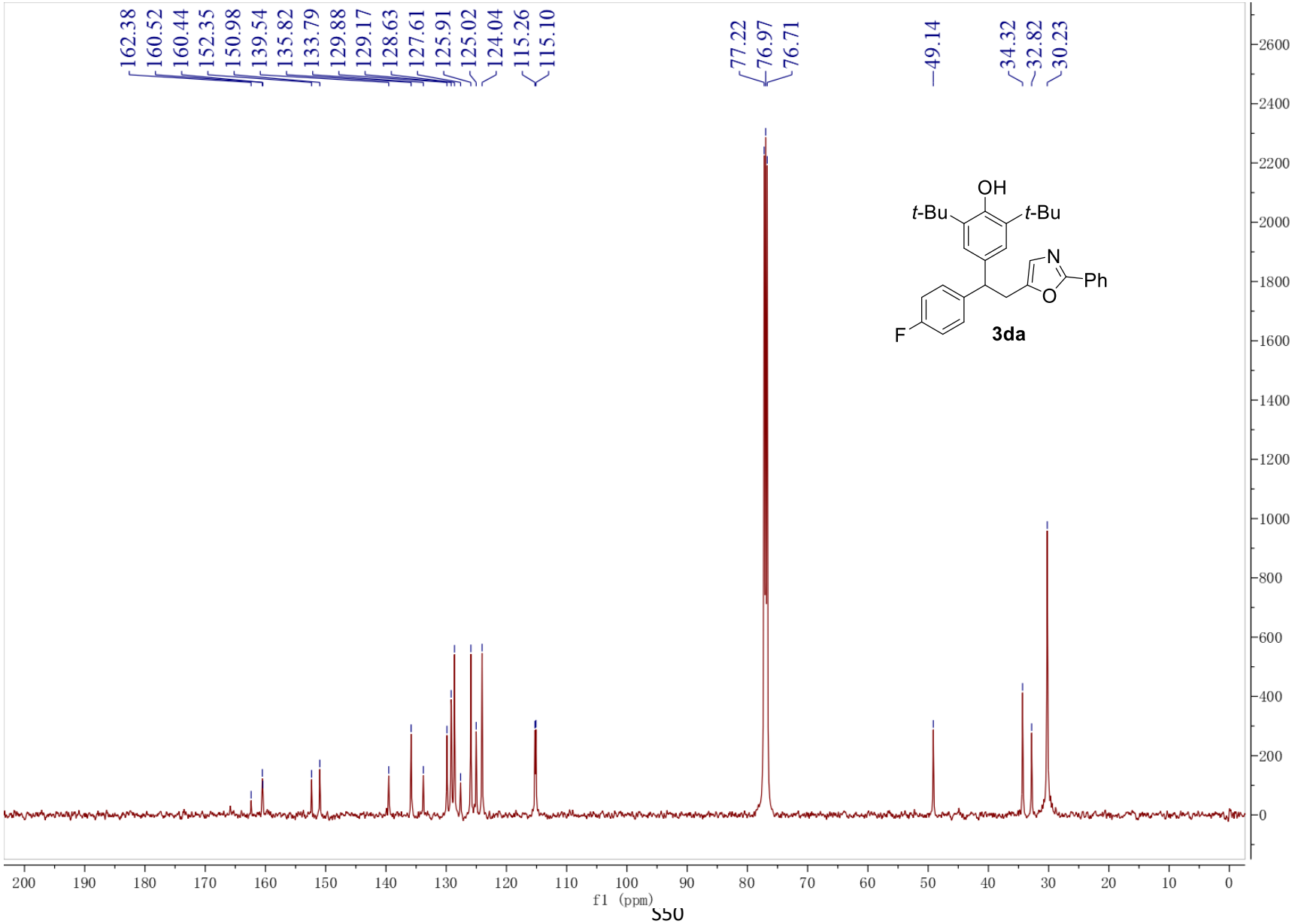
127.72
127.69
126.34
125.91
124.95
124.16
77.23
76.97
76.72
49.93
34.32
32.72
30.22
OH
t-Bu
t-Bu
N
Ph
Ph
O
3ca
f1 (ppm)


7.91 7.91 7.90 7.90 7.89 7.44 7.43 7.42 7.42 7.41 7.41 7.40 7.26 7.24 7.23 7.23 7.22 7.21 7.21 7.01 7.00 6.99 6.98 6.98 6.97 6.96 6.96 6.63 5.09 4.32 4.30 4.29 3.41 3.39 1.64 1.39 0.01
OH
t-Bu
t-Bu
N
Ph
O
F
3da
f1 (ppm)
2.00 2.94 1.98 2.00 1.98 0.99 0.98 1.01 2.03 18.16
f1 (ppm)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160.44
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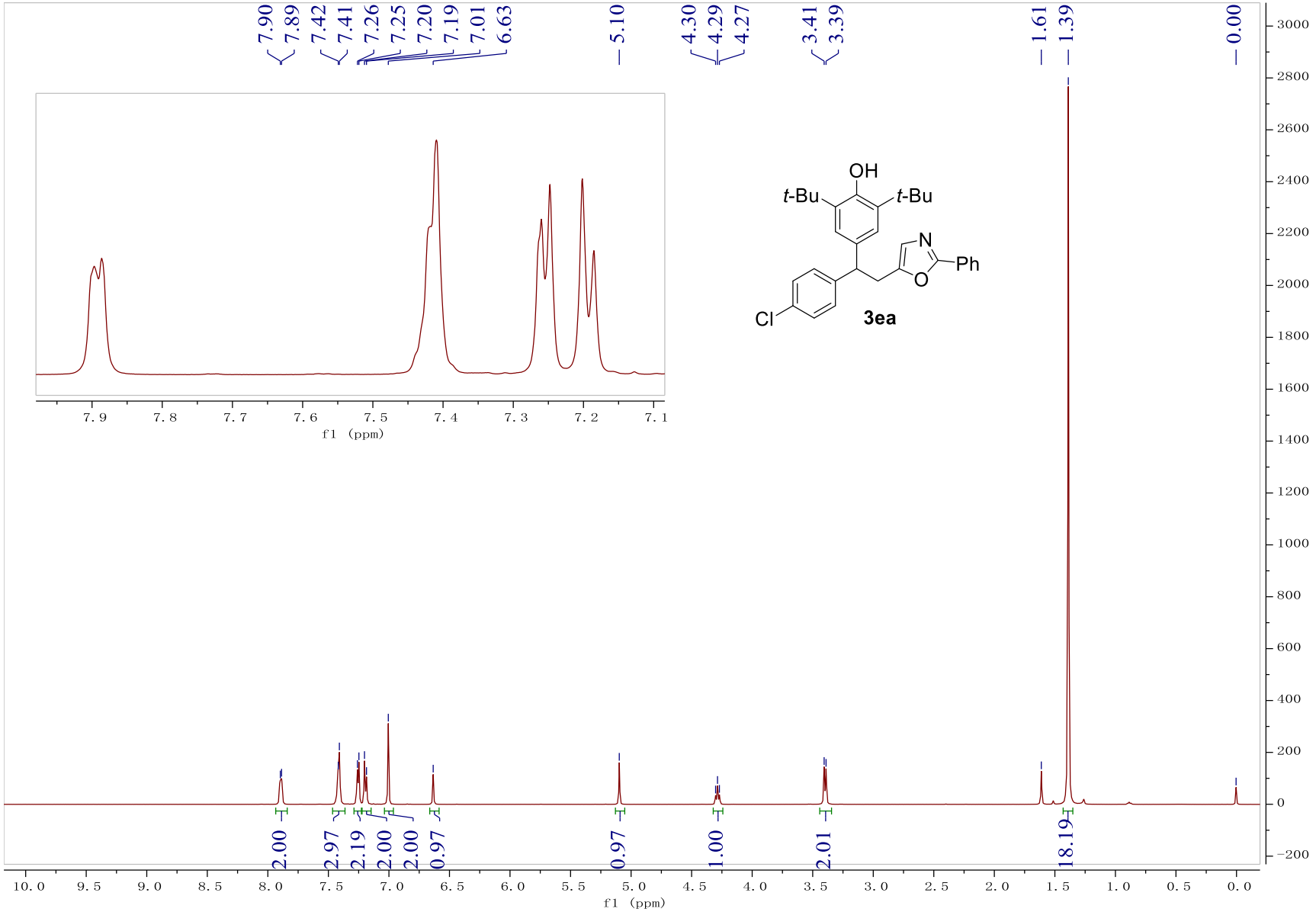
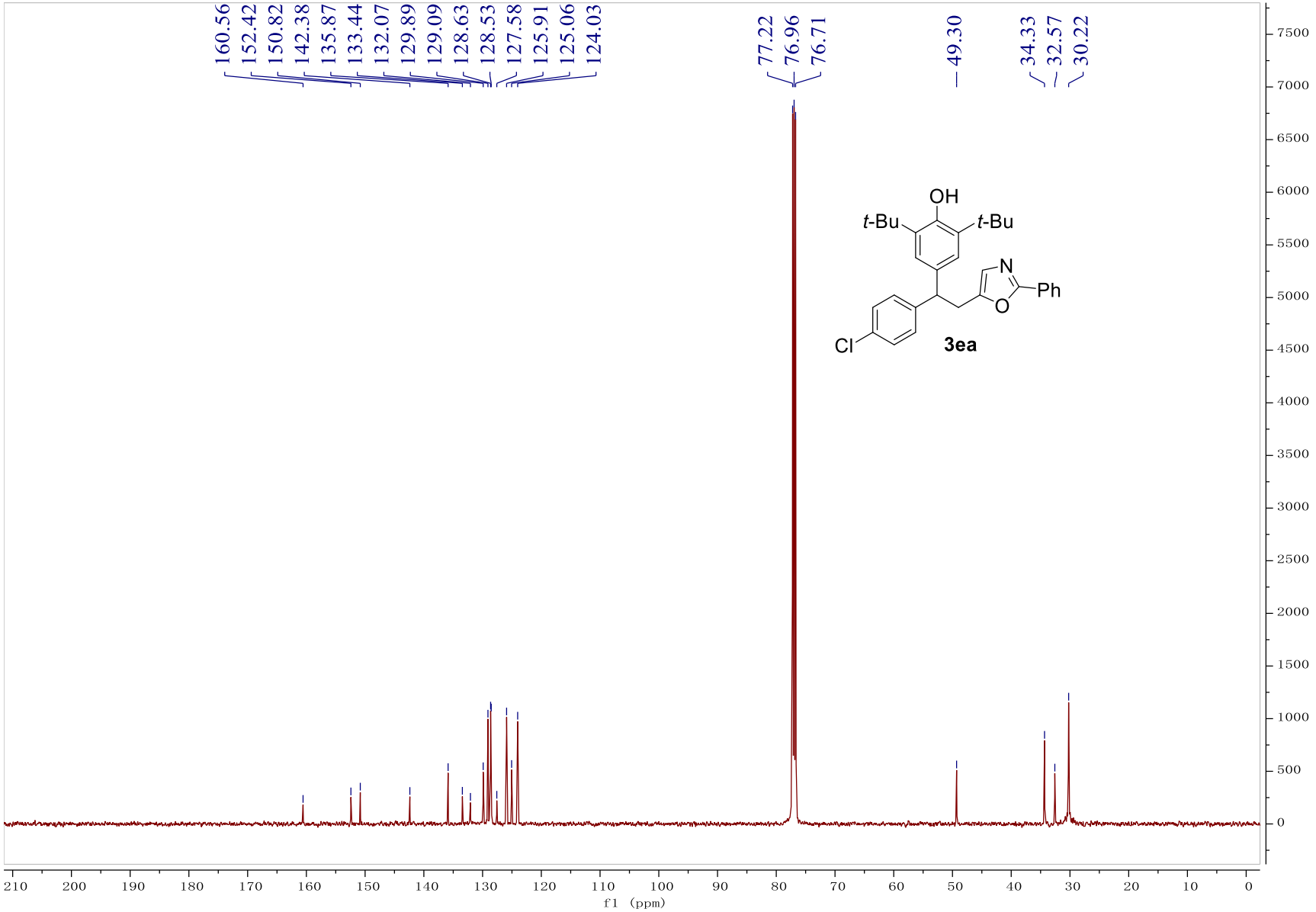
150.98
139.54
135.82
133.79
129.88
129.17
128.63
127.61
125.91
125.02
124.04
115.26
115.10
77.22
76.97
76.71
49.14
34.32
32.82
30.23
OH
t-Bu
t-Bu
N
Ph
O
F
3da
f1 (ppm)


7.90
7.89
7.42
7.41
7.26
7.25
7.20
7.19
7.01
6.63
5.10
4.30
4.29
4.27
3.41
3.39
1.61
1.39
0.00
OH
t-Bu
t-Bu
N
Ph
O
Cl
3ea
f1 (ppm)
2.00
2.97
2.19
2.00
2.00
0.97
0.97
1.00
2.01
18.19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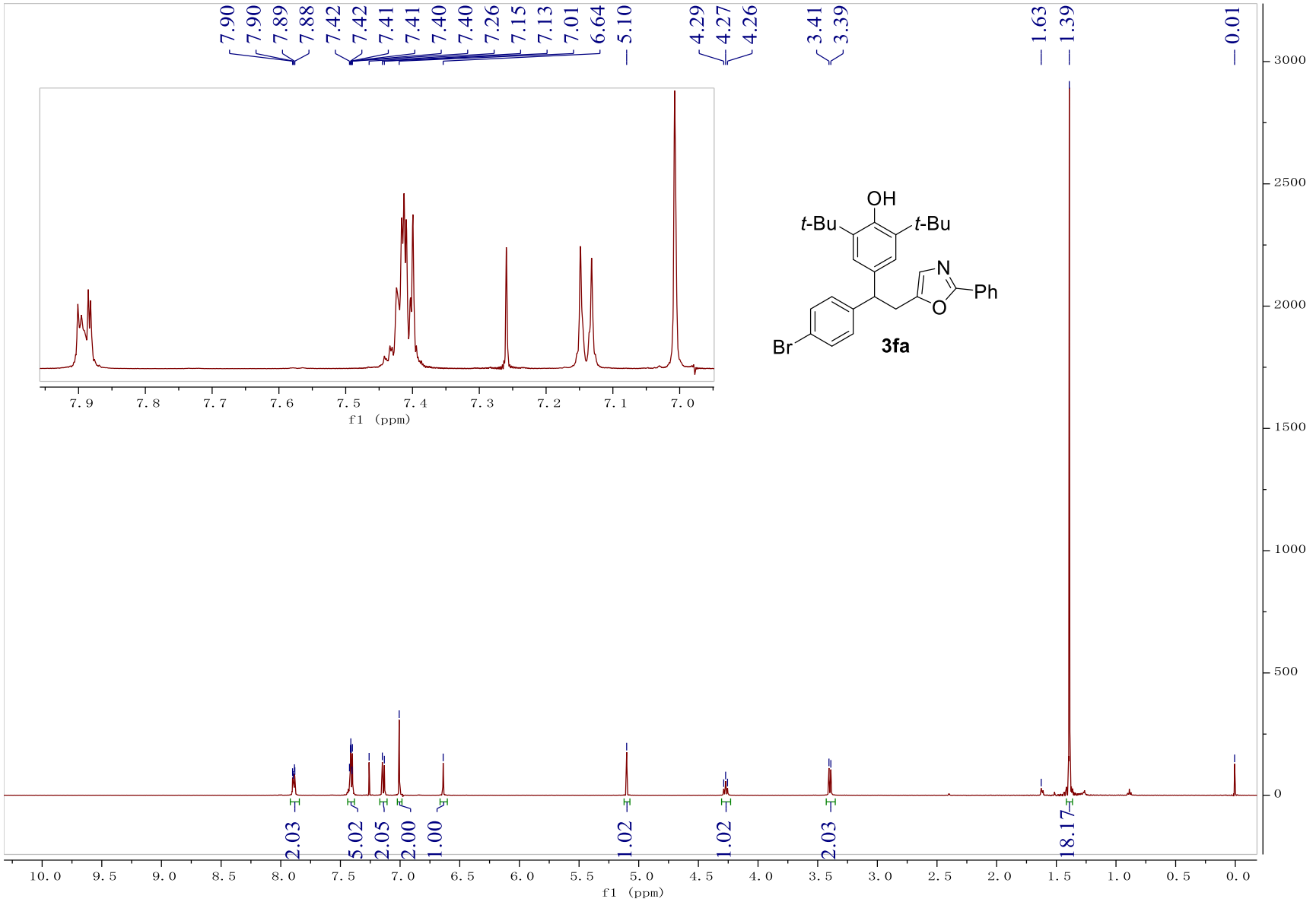
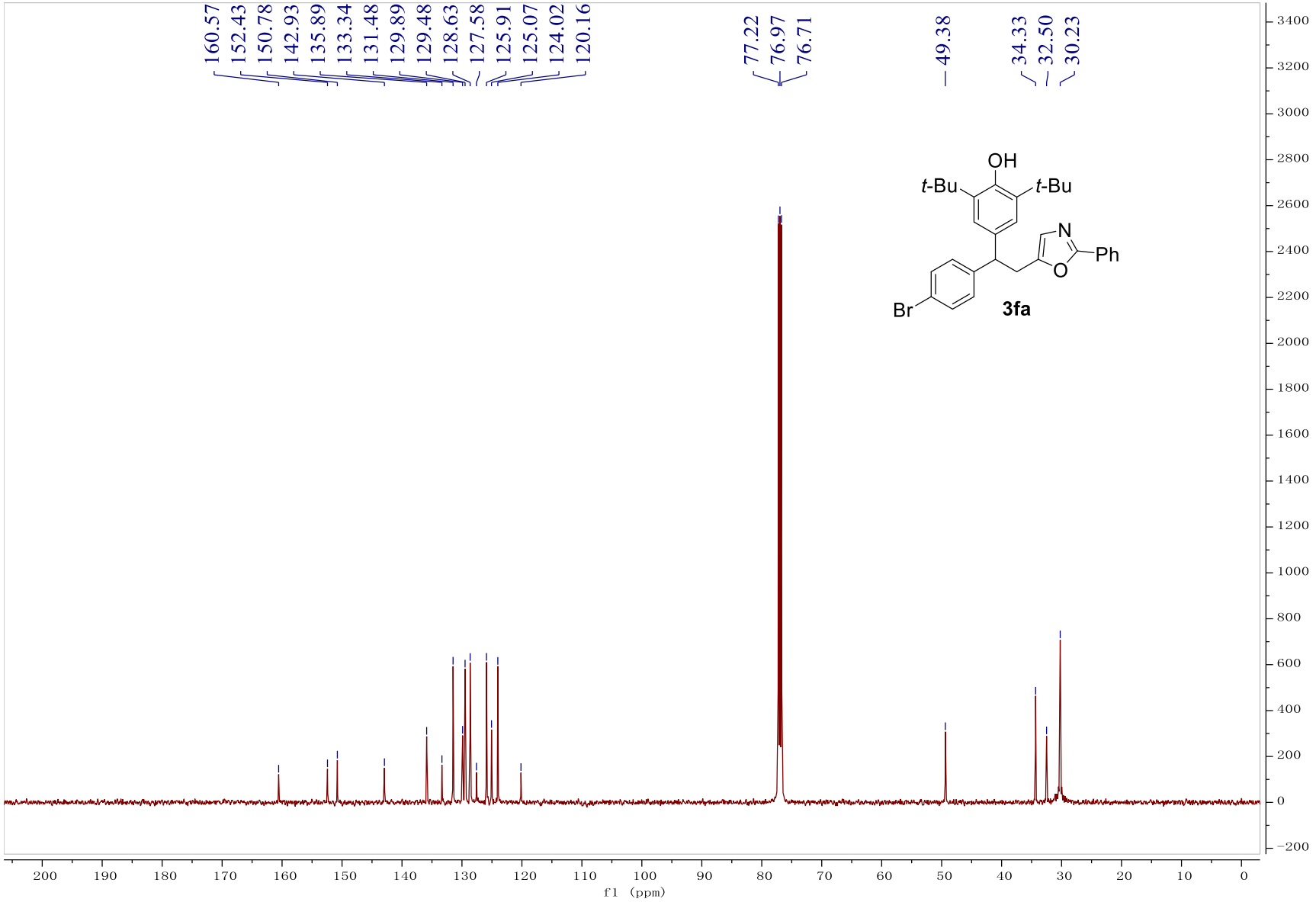
152.42
150.82
142.38
135.87
133.44
132.07
129.89
129.09
128.63
128.53
127.58
125.91
125.06
124.03
77.22
76.96
76.71
49.30
34.33
32.57
30.22
OH
t-Bu
t-Bu
N
Ph
O
Cl
3ea
f1 (ppm)


7.90
7.90
7.89
7.88
7.42
7.42
7.41
7.41
7.40
7.40
7.26
7.15
7.13
7.01
6.64
5.10
4.29
4.27
4.26
3.41
3.39
1.63
1.39
0.01
OH
t-Bu
t-Bu
N
Ph
O
Br
3fa
f1 (ppm)
2.03
5.02
2.05
2.00
1.00
1.02
1.02
2.03
18.17
f1 (ppm)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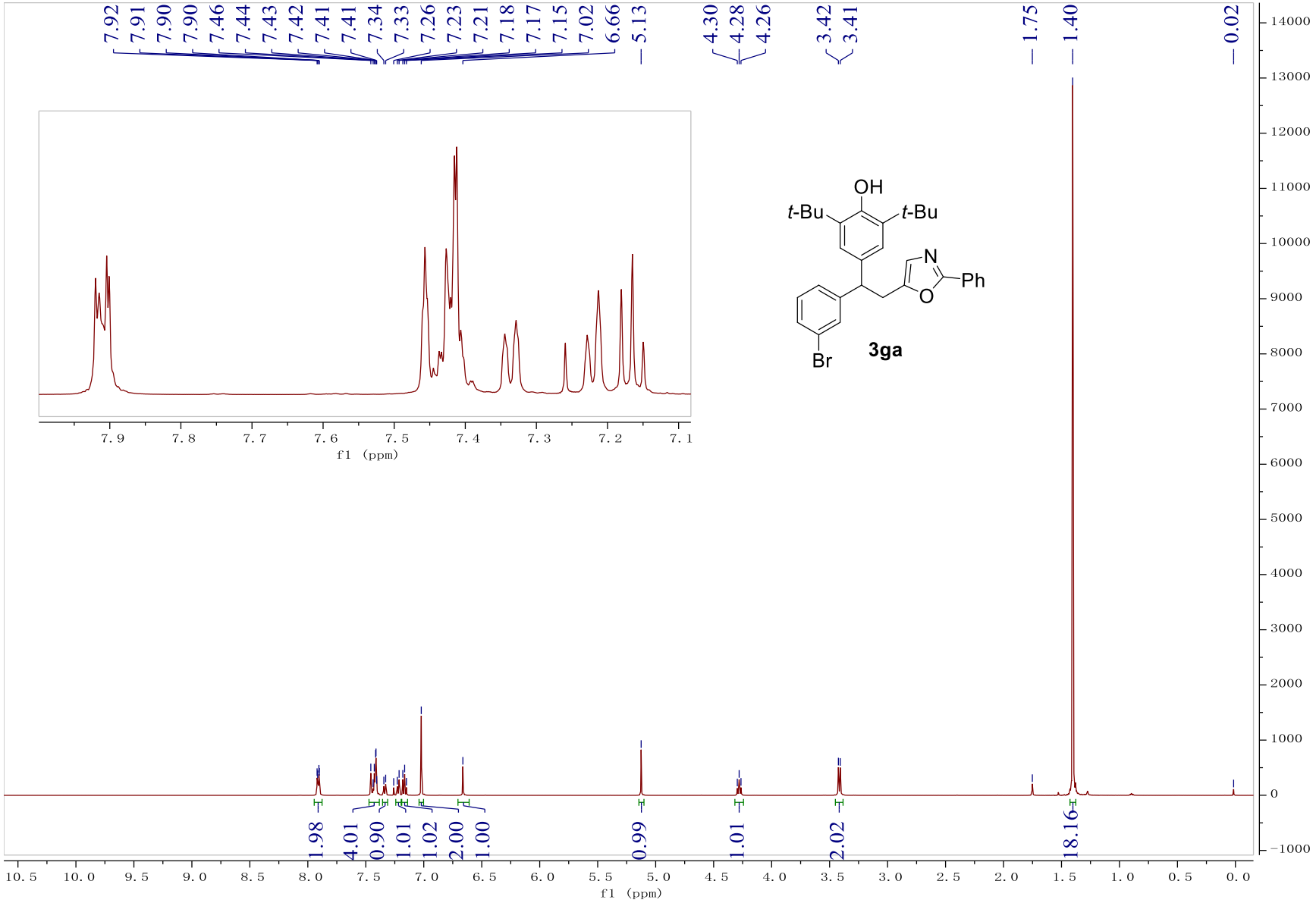
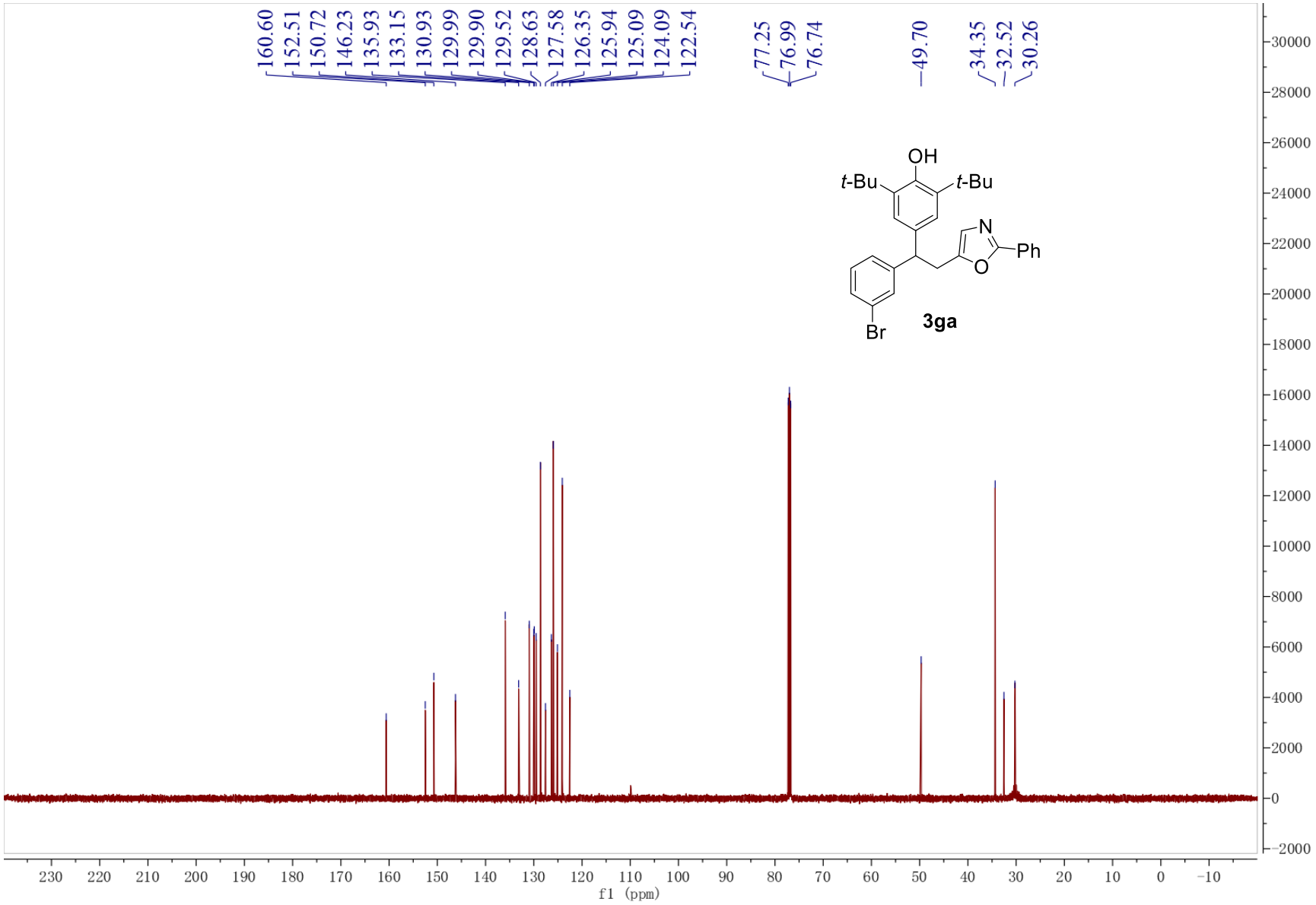
150.78
142.93
135.89
133.34
131.48
129.89
129.48
128.63
127.58
125.91
125.07
124.02
120.16
77.22
76.97
76.71
49.38
34.33
32.50
30.23
OH
t-Bu
t-Bu
N
Ph
O
Br
3fa
f1 (ppm)


7.92
7.91
7.90
7.90
7.46
7.44
7.43
7.42
7.41
7.41
7.34
7.33
7.26
7.23
7.21
7.18
7.17
7.15
7.02
6.66
5.13
4.30
4.28
4.26
3.42
3.41
1.75
1.40
0.02
OH
t-Bu
t-Bu
N
Ph
O
Br
3ga
f1 (ppm)
1.98
4.01
0.90
1.01
1.02
2.00
1.00
0.99
1.01
2.02
18.16
f1 (ppm)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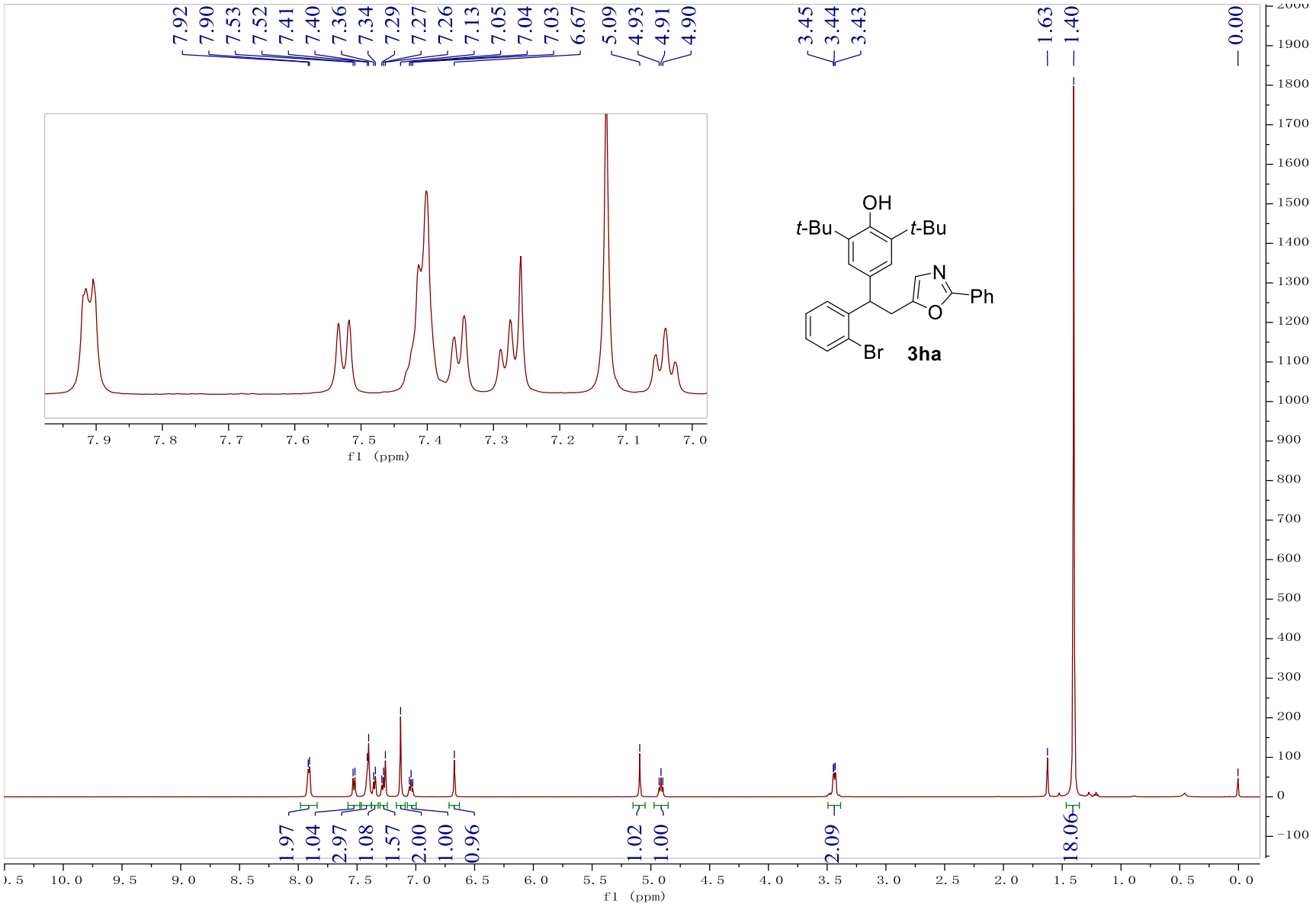
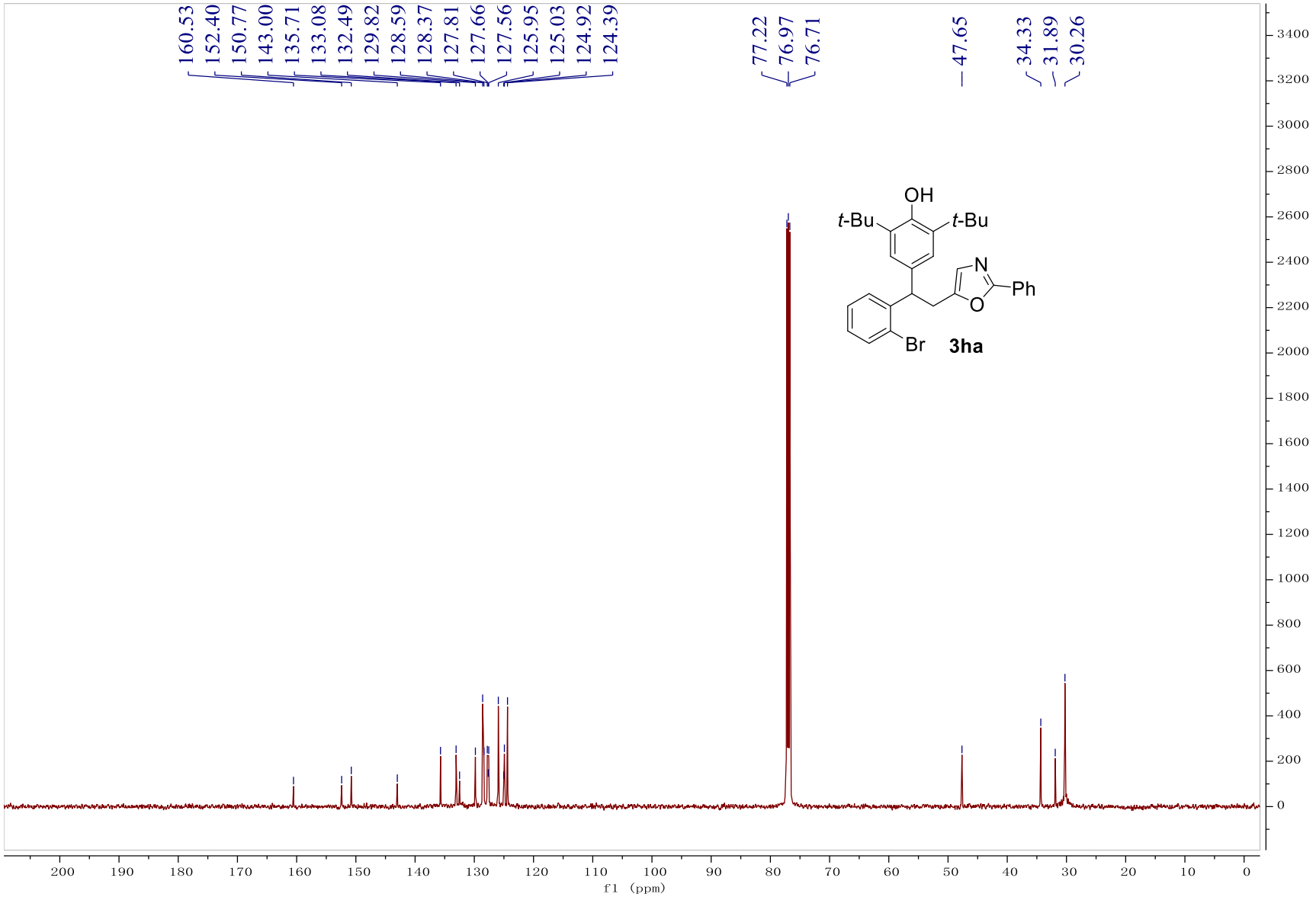
152.51
150.72
146.23
135.93
133.15
130.93
129.99
129.90
129.52
128.63
127.58
126.35
125.94
125.09
124.09
122.54
77.25
76.99
76.74
49.70
34.35
32.52
30.26
OH
t-Bu
t-Bu
N
Ph
O
Br
3ga
f1 (ppm)


7.92
7.90
7.53
7.52
7.41
7.40
7.36
7.34
7.29
7.27
7.26
7.13
7.05
7.04
7.03
6.67
5.09
4.93
4.91
4.90
3.45
3.44
3.43
1.63
1.40
0.00
OH
t-Bu
t-Bu
N
Ph
O
Br
3ha
f1 (ppm)
1.97
1.04
2.97
1.08
1.57
2.00
1.00
0.96
1.02
1.00
2.09
18.06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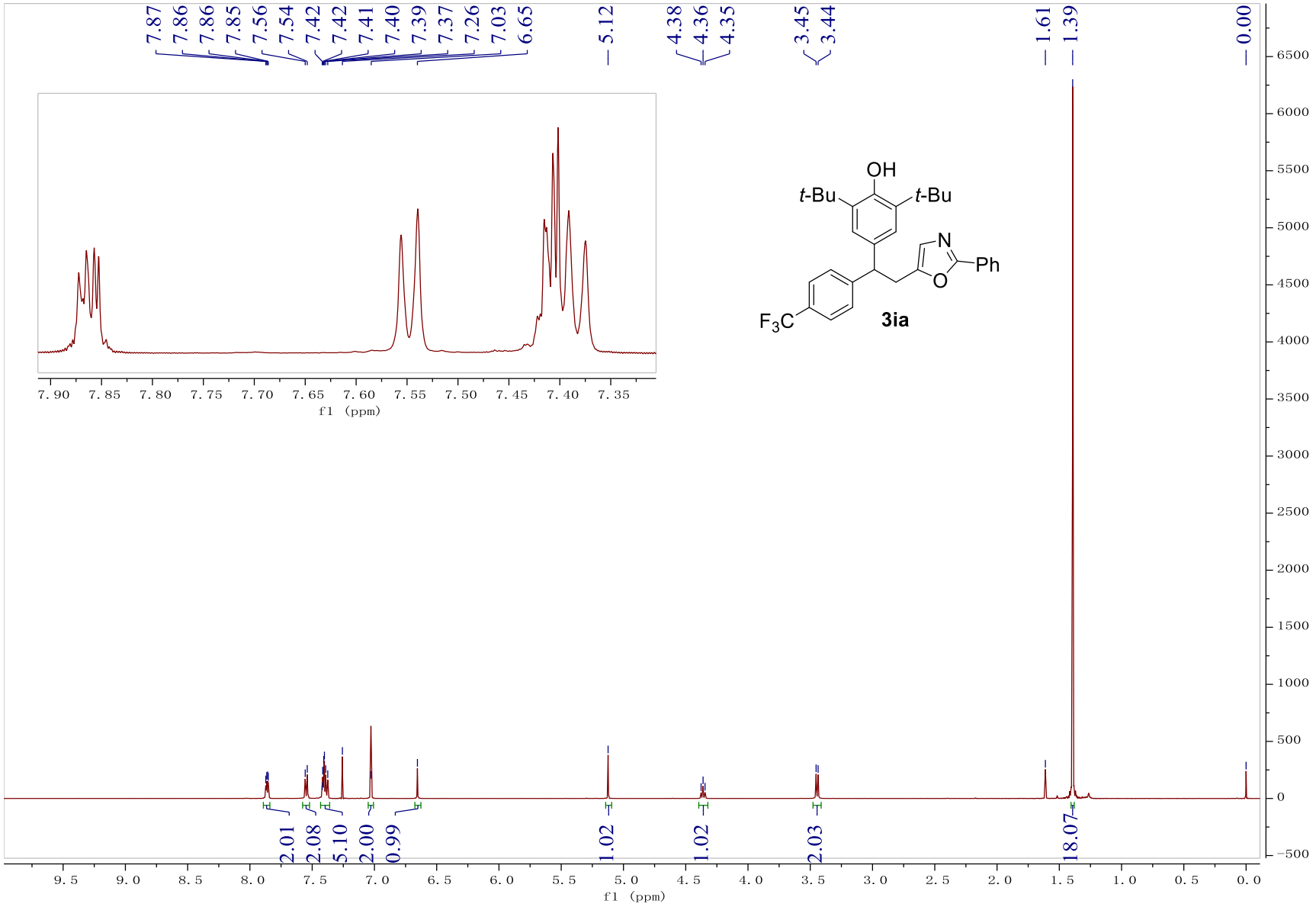
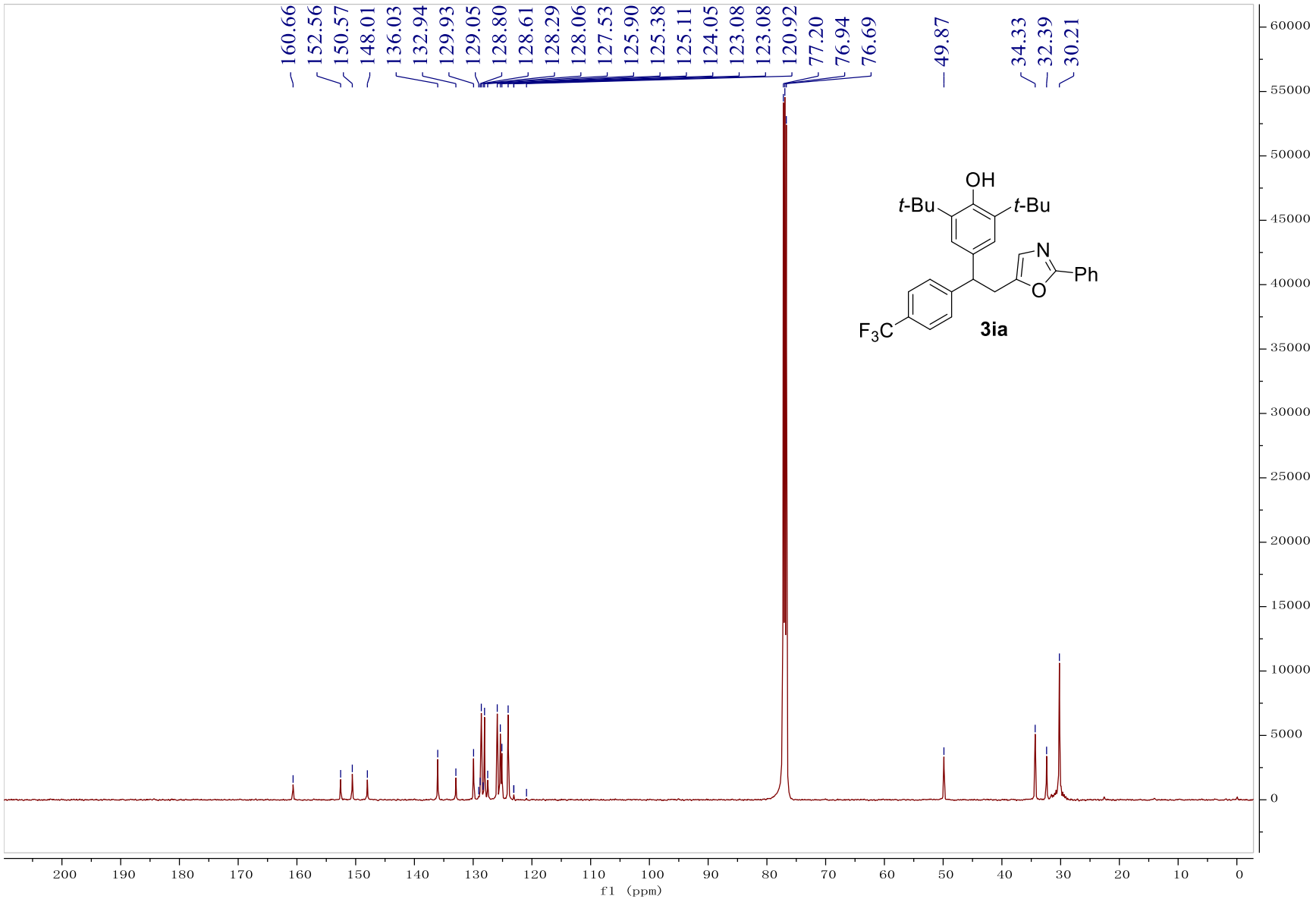
152.40
150.77
143.00
135.71
133.08
132.49
129.82
128.59
128.37
127.81
127.66
127.56
125.95
125.03
124.92
124.39
77.22
76.97
76.71
47.65
34.33
31.89
30.26
OH
t-Bu
t-Bu
N
Ph
O
Br
3ha
f1 (ppm)


7.87
7.86
7.86
7.85
7.56
7.54
7.42
7.42
7.41
7.40
7.39
7.37
7.26
7.03
6.65
5.12
4.38
4.36
4.35
3.45
3.44
1.61
1.39
0.00
OH
t-Bu
t-Bu
N
Ph
O
F3C
3ia
f1 (ppm)
2.01
2.08
5.10
2.00
0.99
1.02
1.02
2.03
18.07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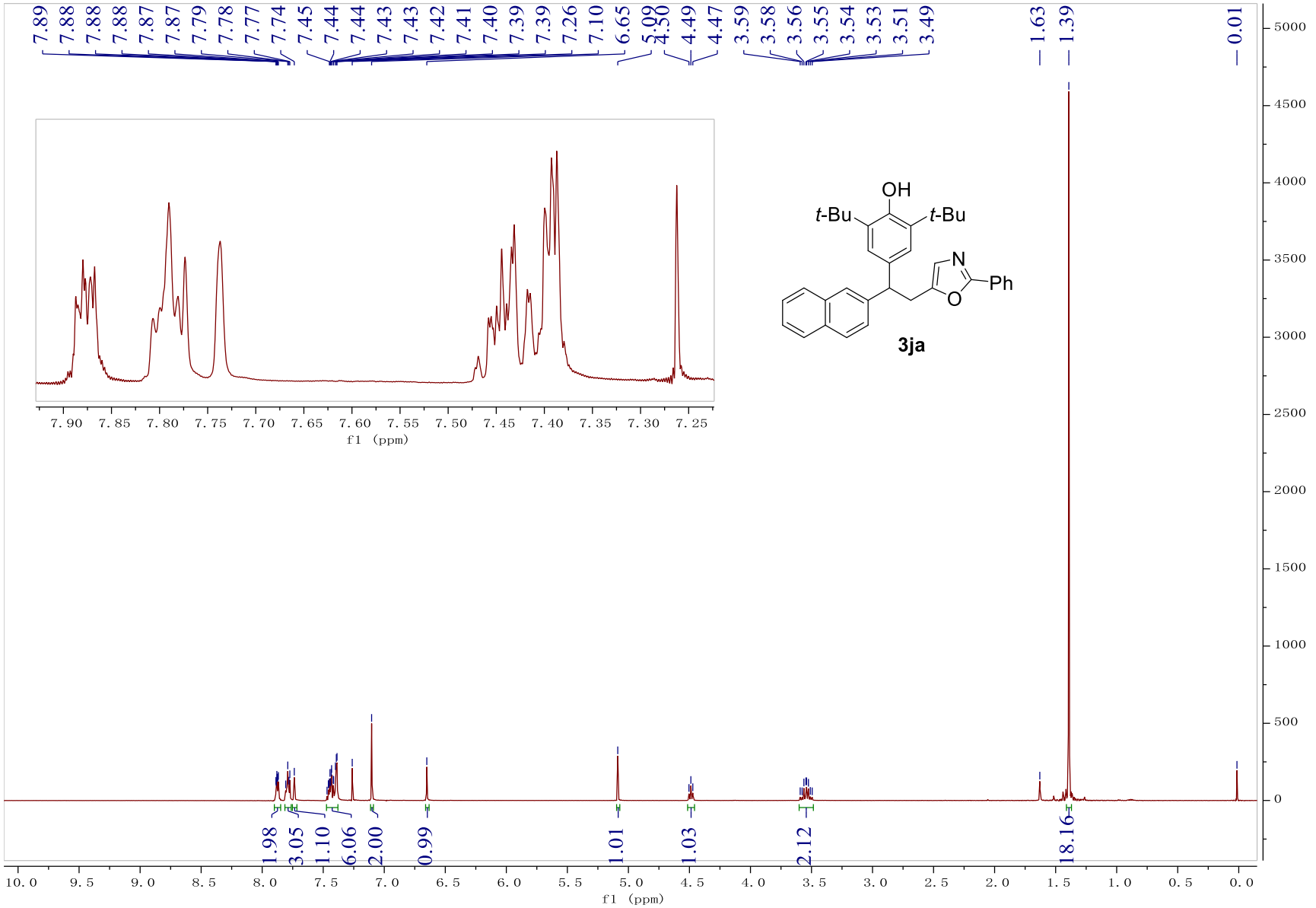
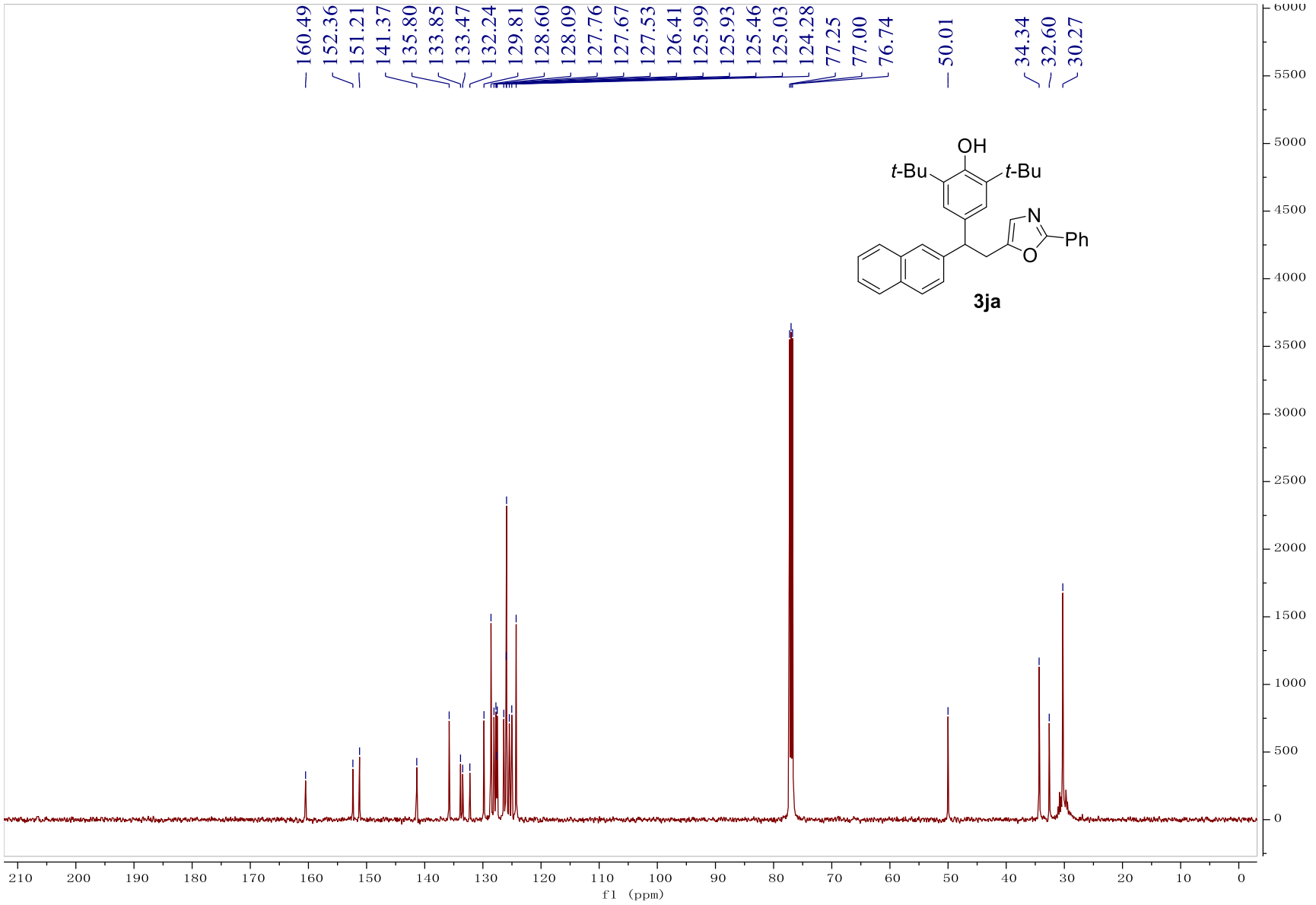
152.56
150.57
148.01
136.03
132.94
129.93
129.05
128.80
128.61
128.29
128.06
127.53
125.90
125.38
125.11
124.05
123.08
123.08
120.92
77.20
76.94
76.69
49.87
34.33
32.39
30.21
OH
t-Bu
t-Bu
N
Ph
O
F3C
3ia
f1 (ppm)


7.89 7.88 7.88 7.88 7.87 7.87 7.79 7.78 7.77 7.74 7.45 7.44 7.44 7.43 7.43 7.42 7.41 7.40 7.39 7.39 7.26 7.10 6.65 5.09 4.50 4.49 4.47 3.59 3.58 3.56 3.55 3.54 3.53 3.51 3.49 1.63 1.39 0.01
7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25
f1 (ppm)
OH
t-Bu
t-Bu
N
O
Ph
3ja
1.98 3.05 1.10 6.06 2.00 0.99 1.01 1.03 2.12 18.16
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)
5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0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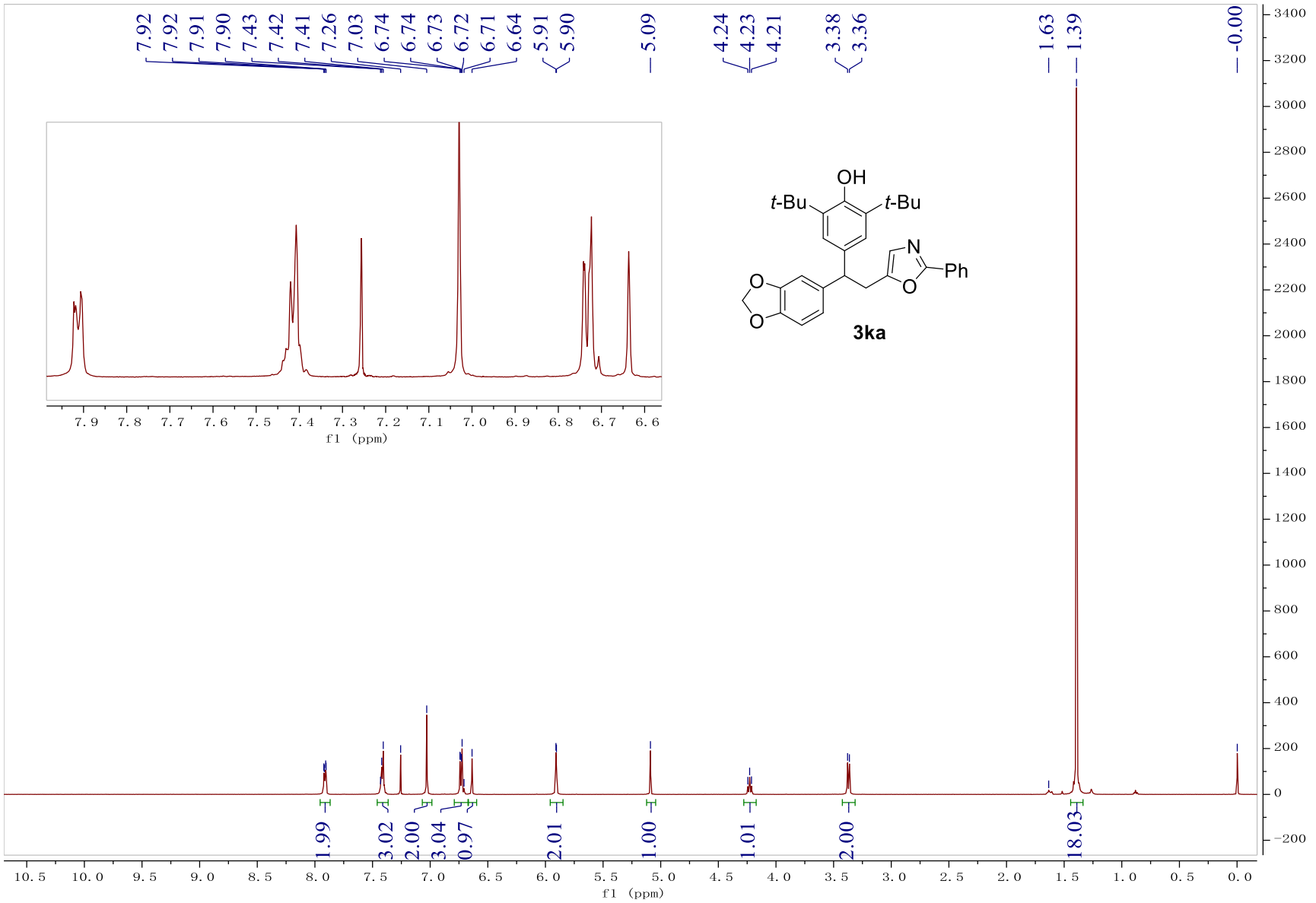
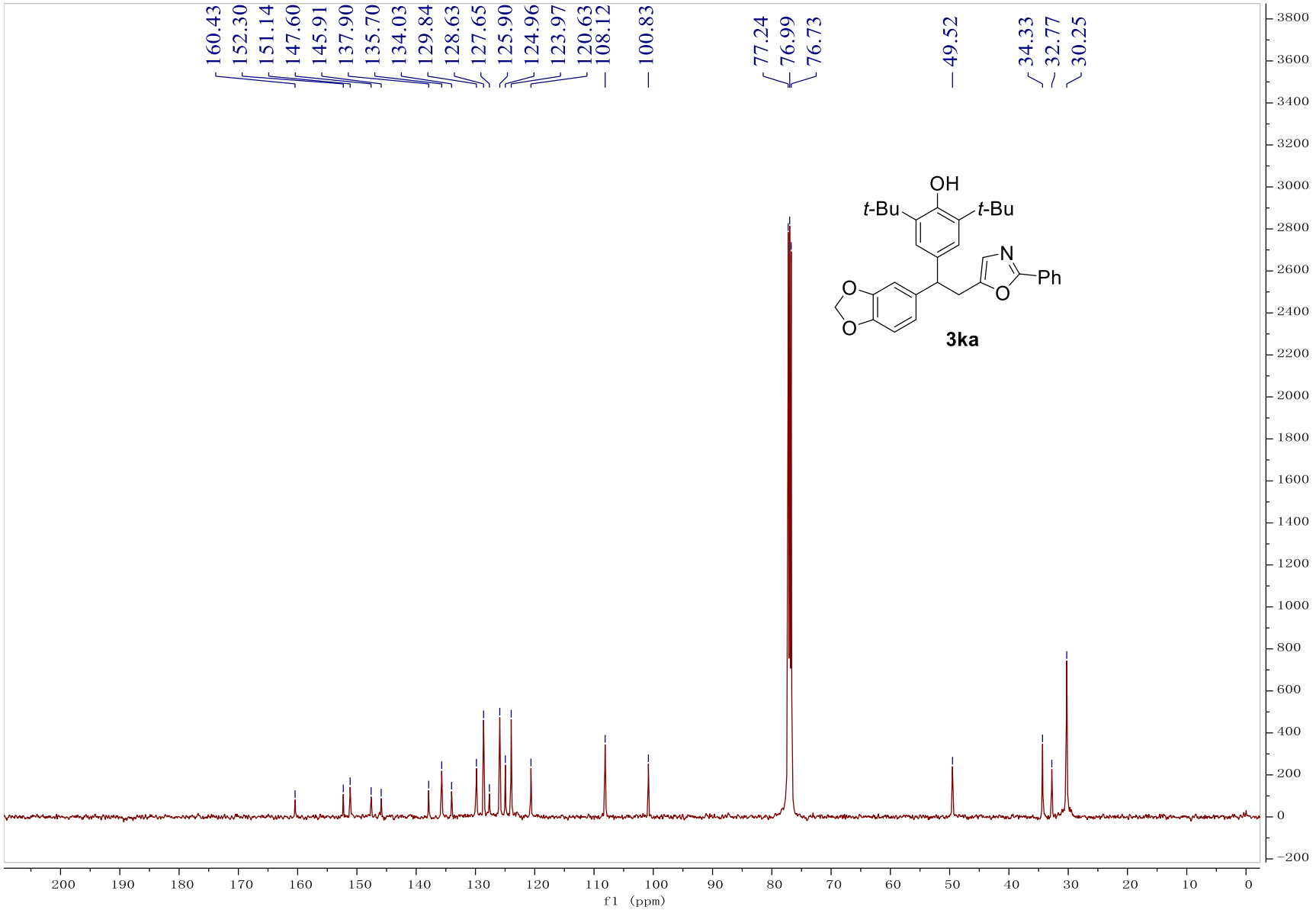
151.21
141.37
135.80
133.85
133.47
132.24
129.81
128.60
128.09
127.76
127.67
127.53
126.41
125.99
125.93
125.46
125.03
124.28
77.25
77.00
76.74
50.01
34.34
32.60
30.27
OH
t-Bu
t-Bu
N
Ph
O
3ja
f1 (ppm)


7.92
7.92
7.91
7.90
7.43
7.42
7.41
7.26
7.03
6.74
6.74
6.73
6.72
6.71
6.64
5.91
5.90
5.09
4.24
4.23
4.21
3.38
3.36
1.63
1.39
-0.00
OH
t-Bu
t-Bu
N
Ph
O
O
O
3ka
f1 (ppm)
1.99
3.02
2.00
3.04
0.97
2.01
1.00
1.01
2.00
18.03
f1 (ppm)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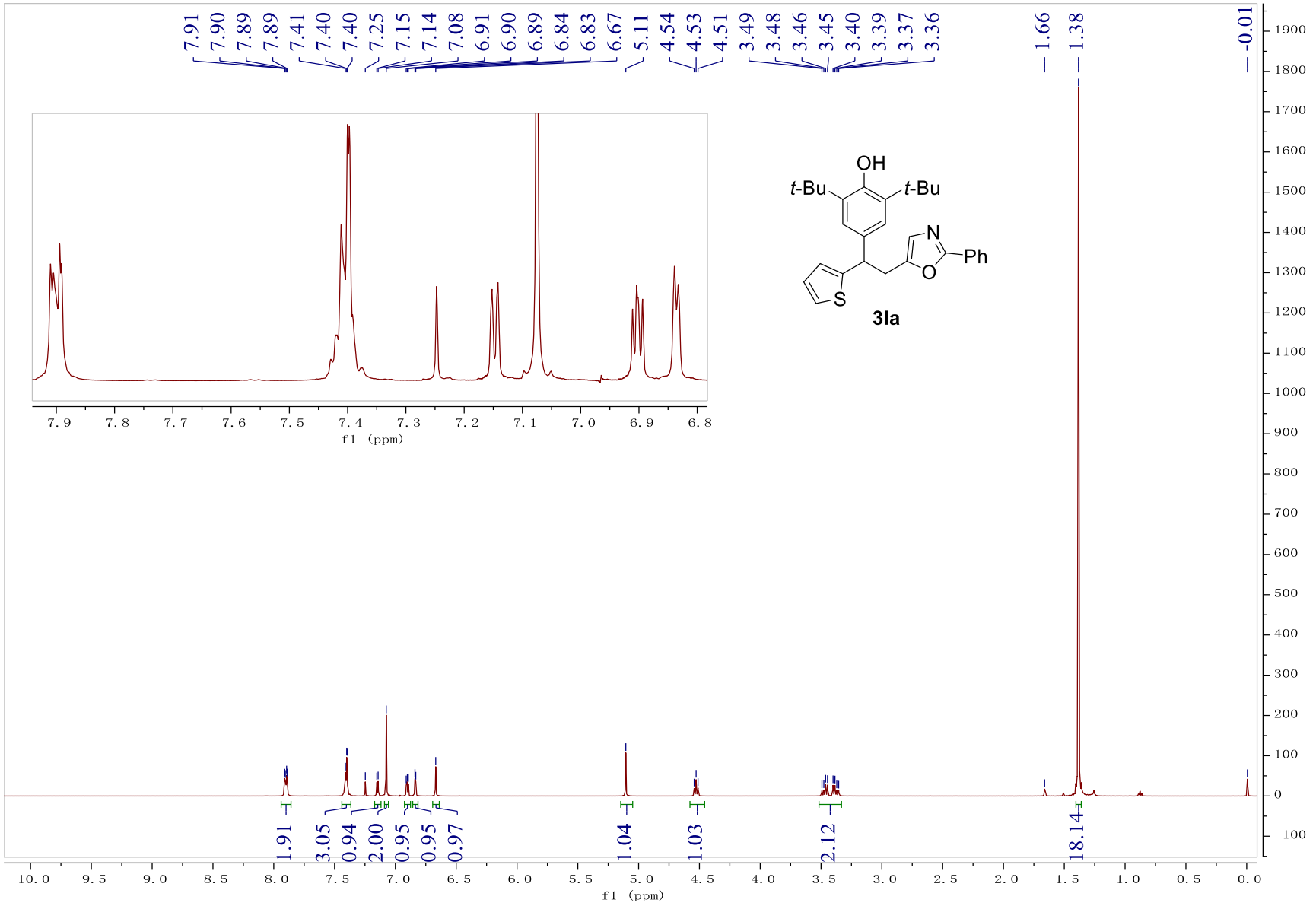
151.14
147.60
145.91
137.90
135.70
134.03
129.84
128.63
127.65
125.90
124.96
123.97
120.63
108.12
100.83
77.24
76.99
76.73
49.52
34.33
32.77
30.25
OH
t-Bu
t-Bu
N
Ph
O
O
O
3ka
f1 (ppm)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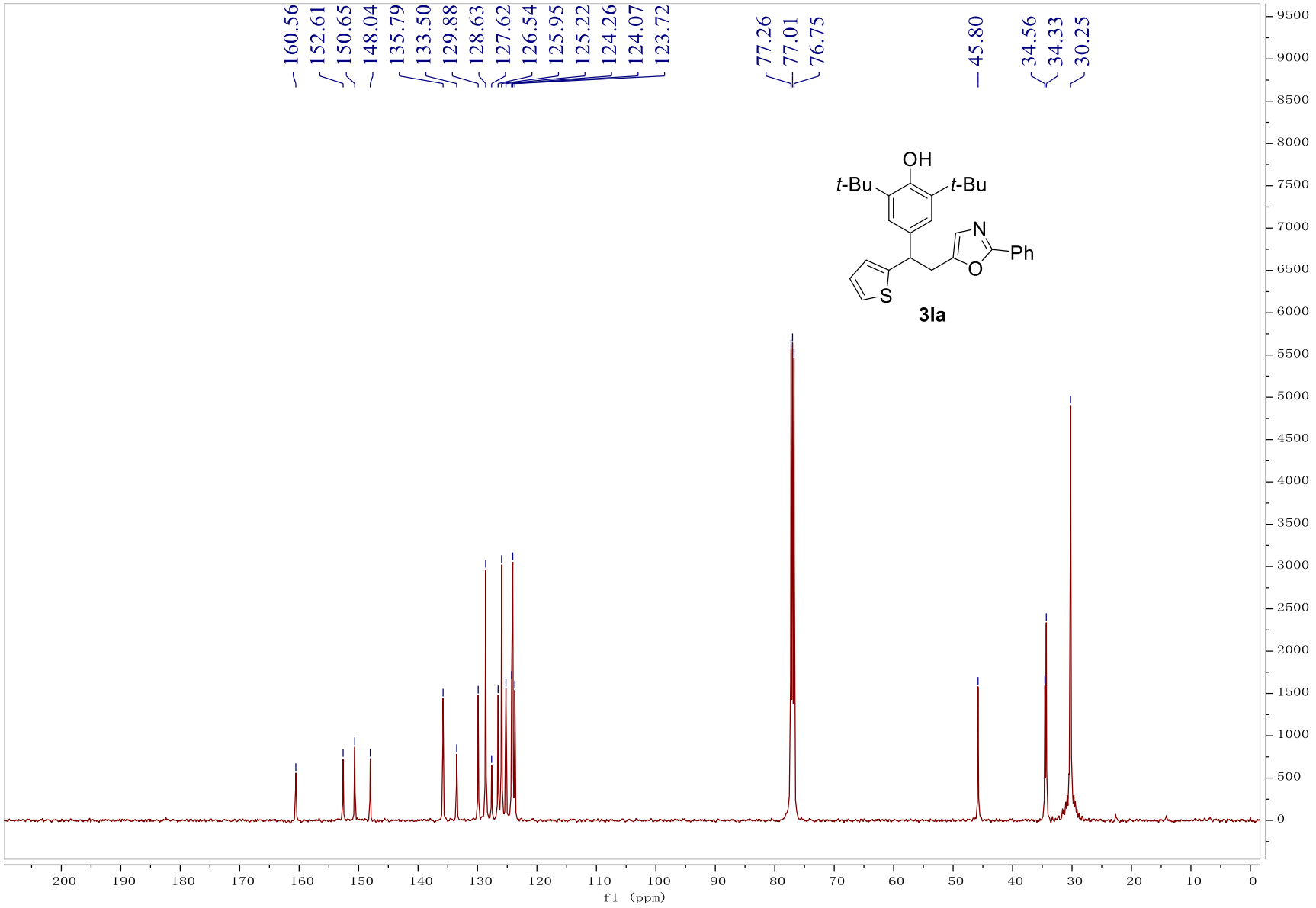
7.90
7.89
7.89
7.41
7.40
7.40
7.25
7.15
7.14
7.08
6.91
6.90
6.89
6.84
6.83
6.67
5.11
4.54
4.53
4.51
3.49
3.48
3.46
3.45
3.40
3.39
3.37
3.36
1.66
1.38
-0.01
OH
t-Bu
t-Bu
N
Ph
O
S
3Ia
f1 (ppm)
1.91
3.05
0.94
2.00
0.95
0.95
0.97
1.04
1.03
2.12
18.14
f1 (ppm)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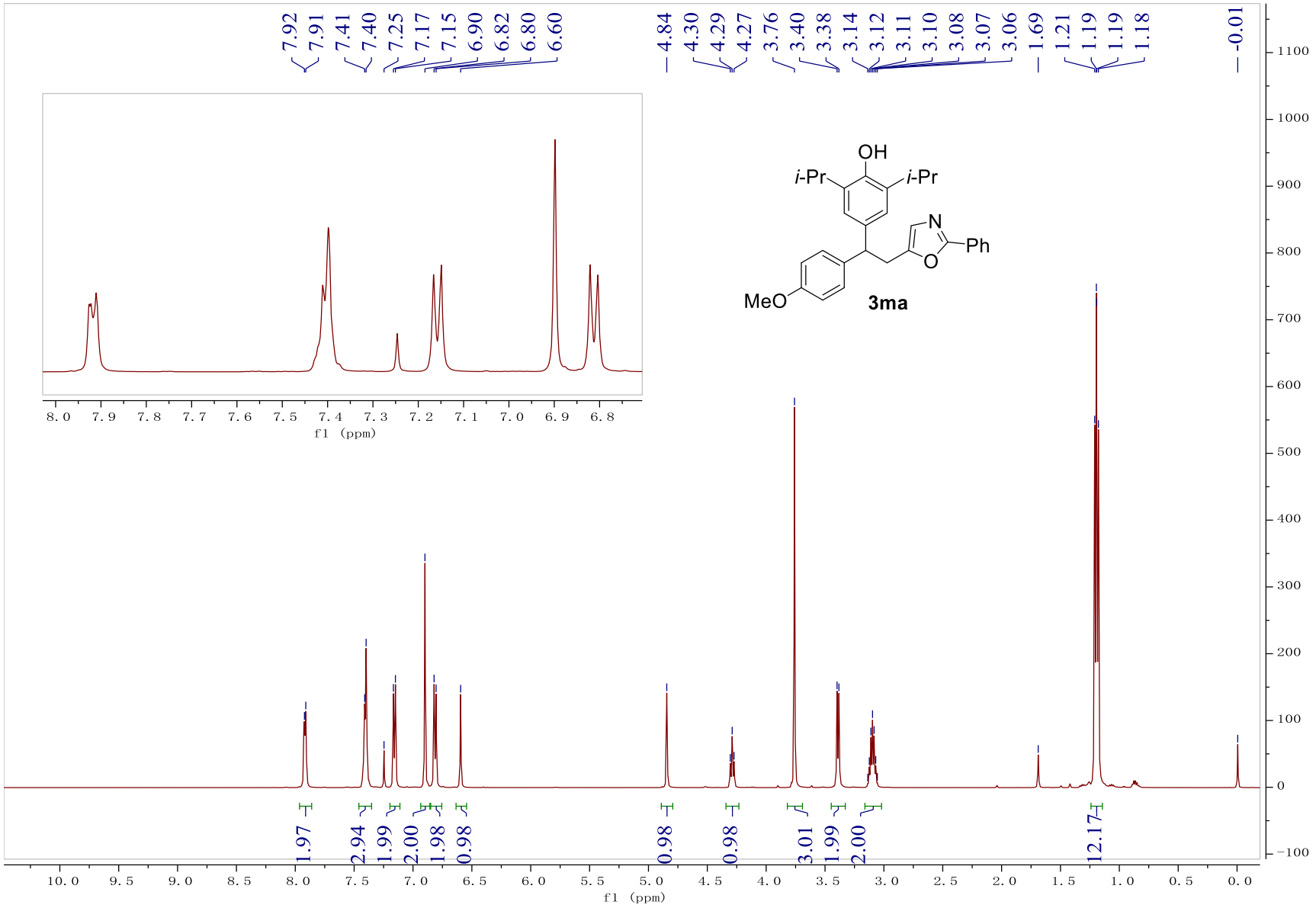
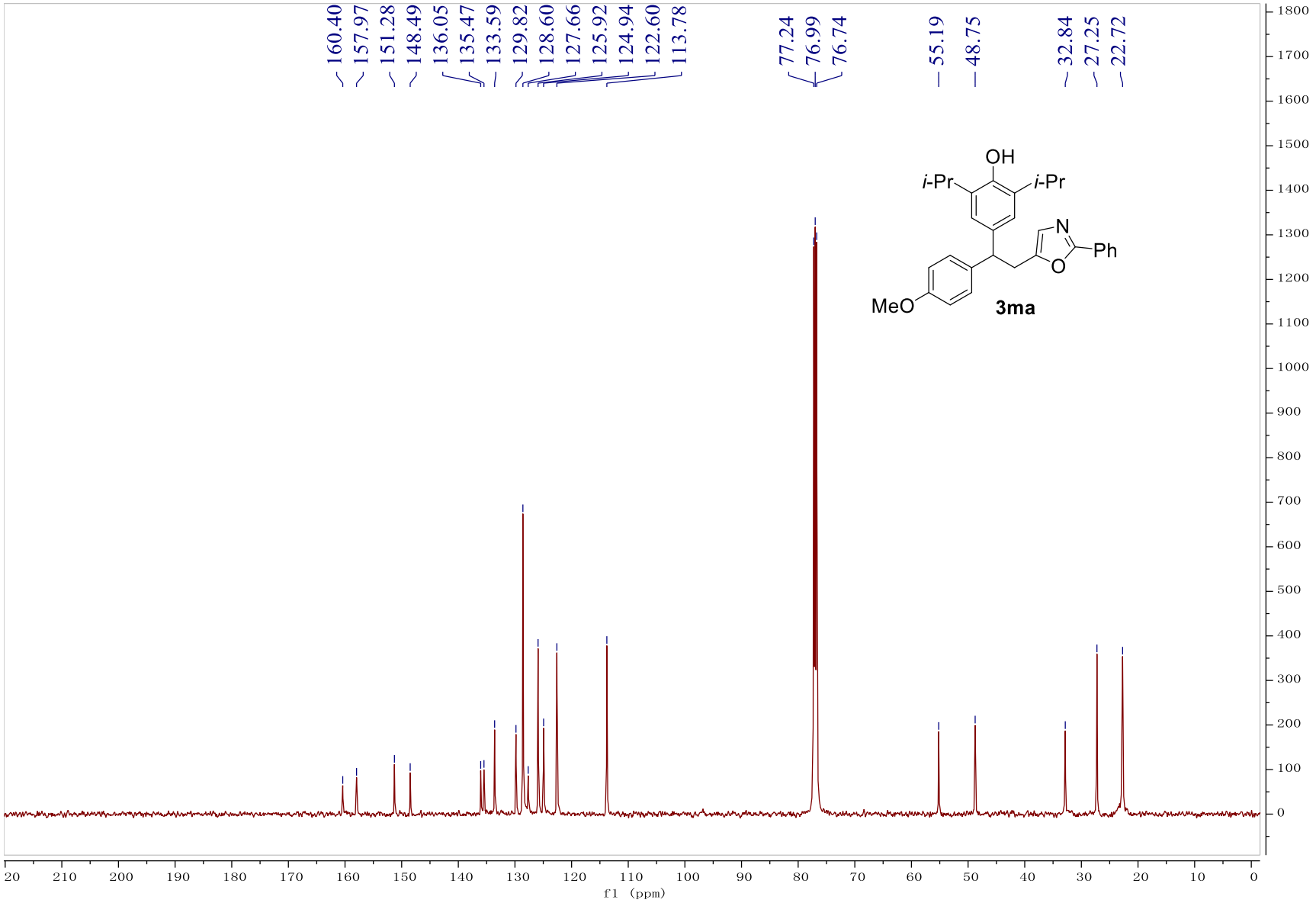
133.50
129.88
128.63
127.62
126.54
125.95
125.22
124.26
124.07
123.72
77.26
77.01
76.75
45.80
34.56
34.33
30.25
OH
t-Bu
t-Bu
N
Ph
O
S
3la
f1 (ppm)


7.92
7.91
7.41
7.40
7.25
7.17
7.15
6.90
6.82
6.80
6.60
4.84
4.30
4.29
4.27
3.76
3.40
3.38
3.14
3.12
3.11
3.10
3.08
3.07
3.06
1.69
1.21
1.19
1.19
1.18
-0.01
OH
i-Pr
i-Pr
N
Ph
O
MeO
3ma
f1 (ppm)
1.97
2.94
1.99
2.00
1.98
0.98
0.98
0.98
3.01
1.99
2.00
12.17
f1 (ppm)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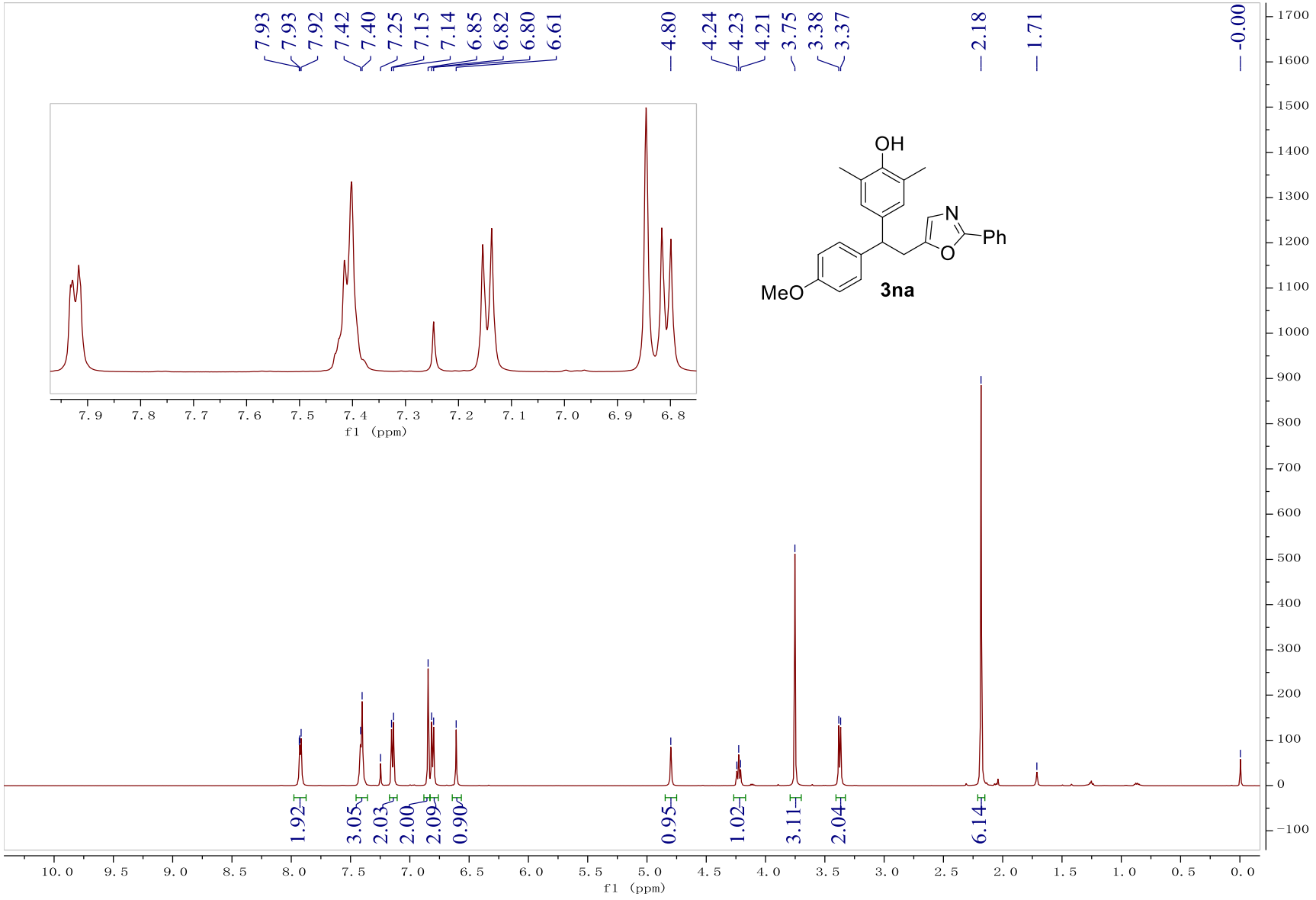
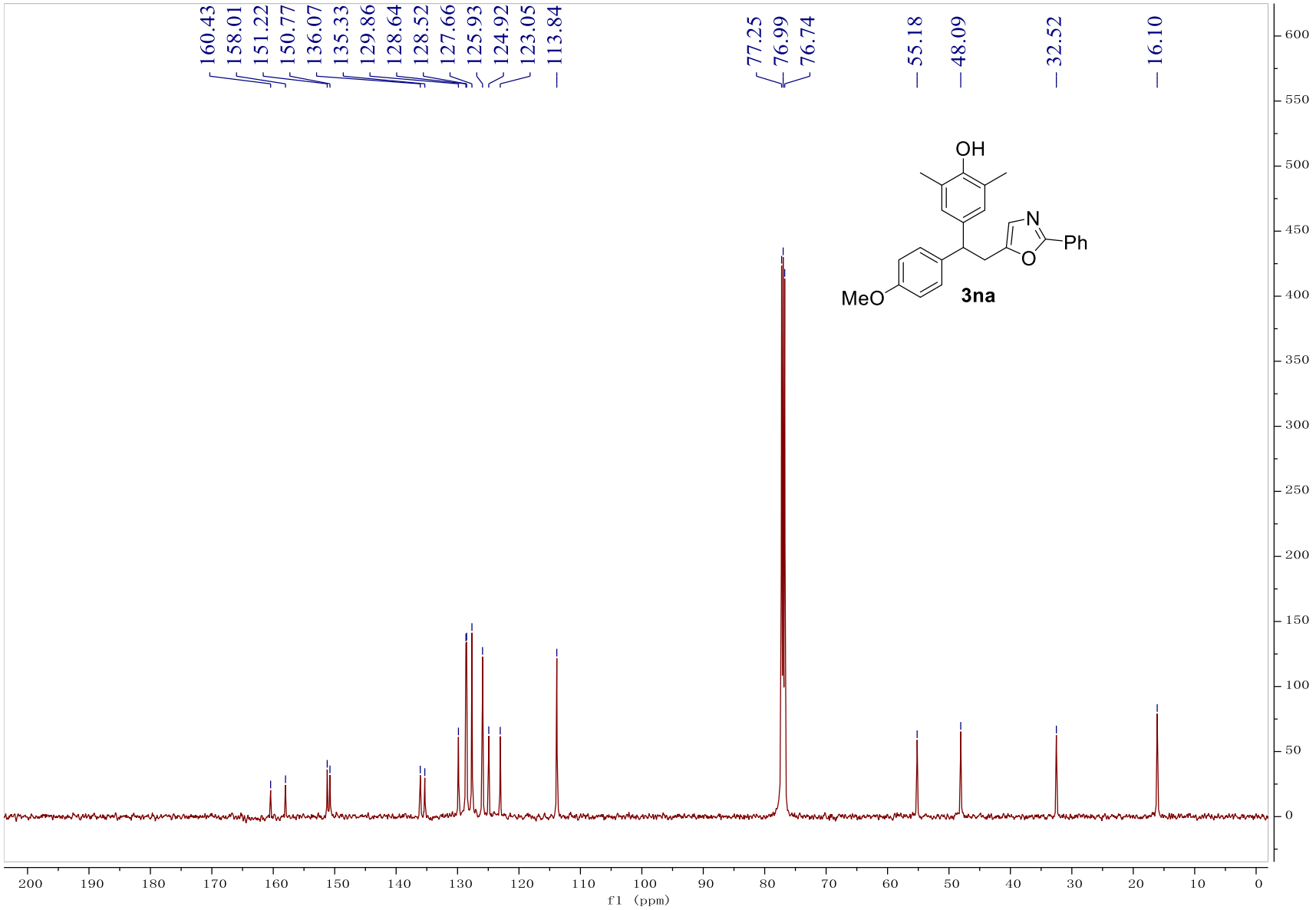
151.28
148.49
136.05
135.47
133.59
129.82
128.60
127.66
125.92
124.94
122.60
113.78
77.24
76.99
76.74
55.19
48.75
32.84
27.25
22.72
OH
i-Pr
i-Pr
N
Ph
O
MeO
3ma
f1 (ppm)


7.93
7.93
7.92
7.42
7.40
7.25
7.15
7.14
6.85
6.82
6.80
6.61
4.80
4.24
4.23
4.21
3.75
3.38
3.37
2.18
1.71
-0.00
OH
N
Ph
O
MeO
3na
f1 (ppm)
1.92
3.05
2.03
2.00
2.09
0.90
0.95
1.02
3.11
2.04
6.14
f1 (ppm)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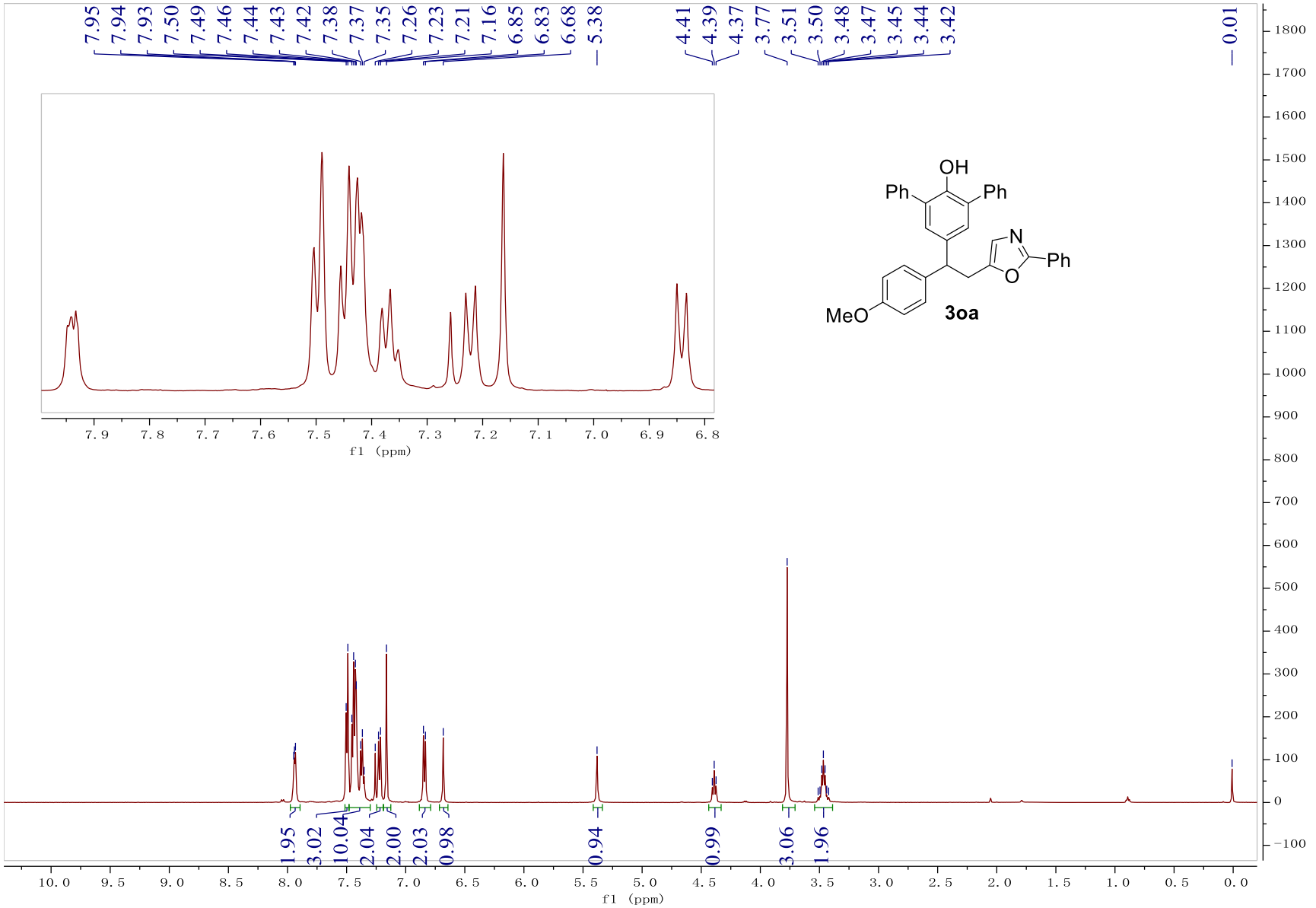
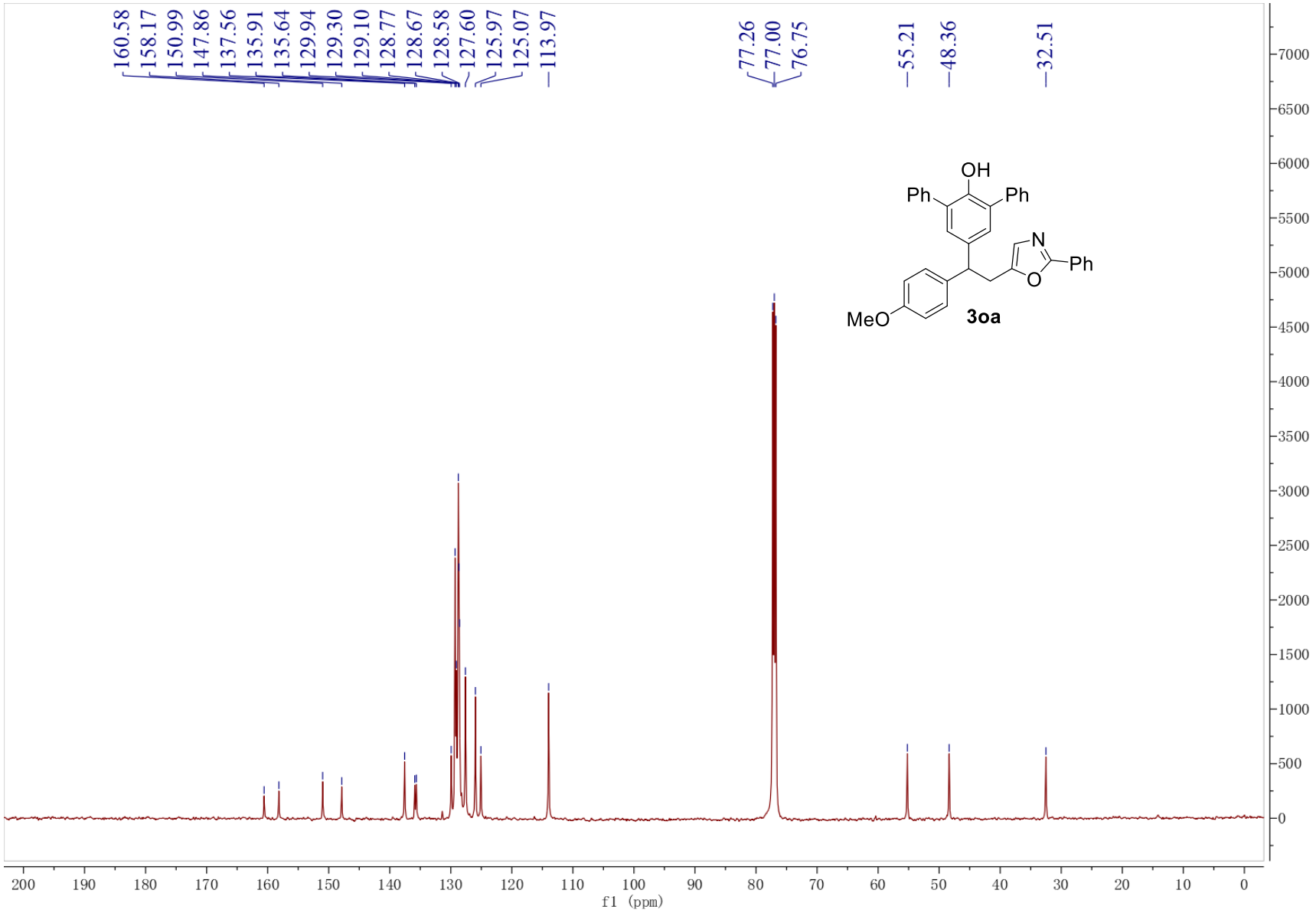
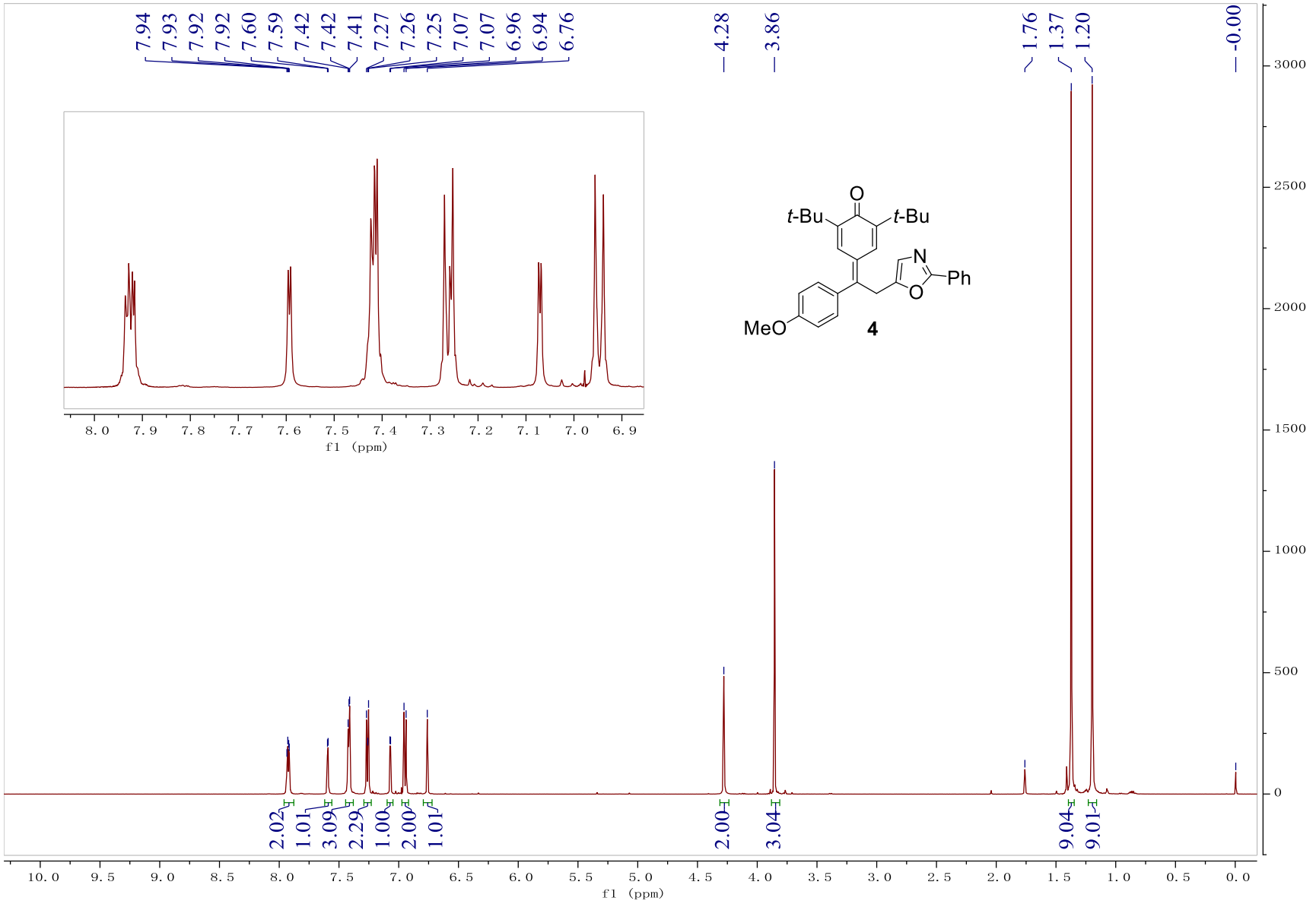
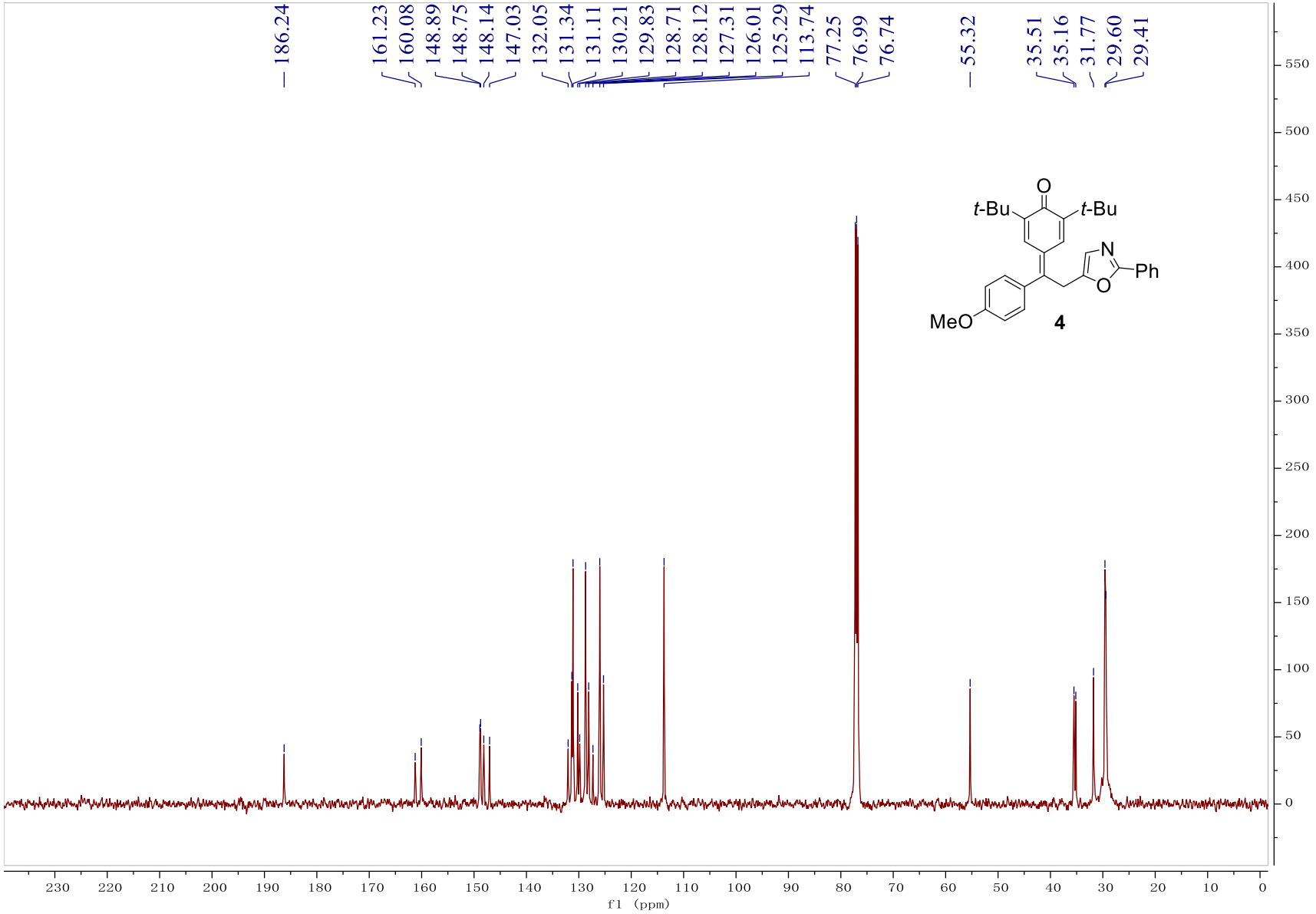
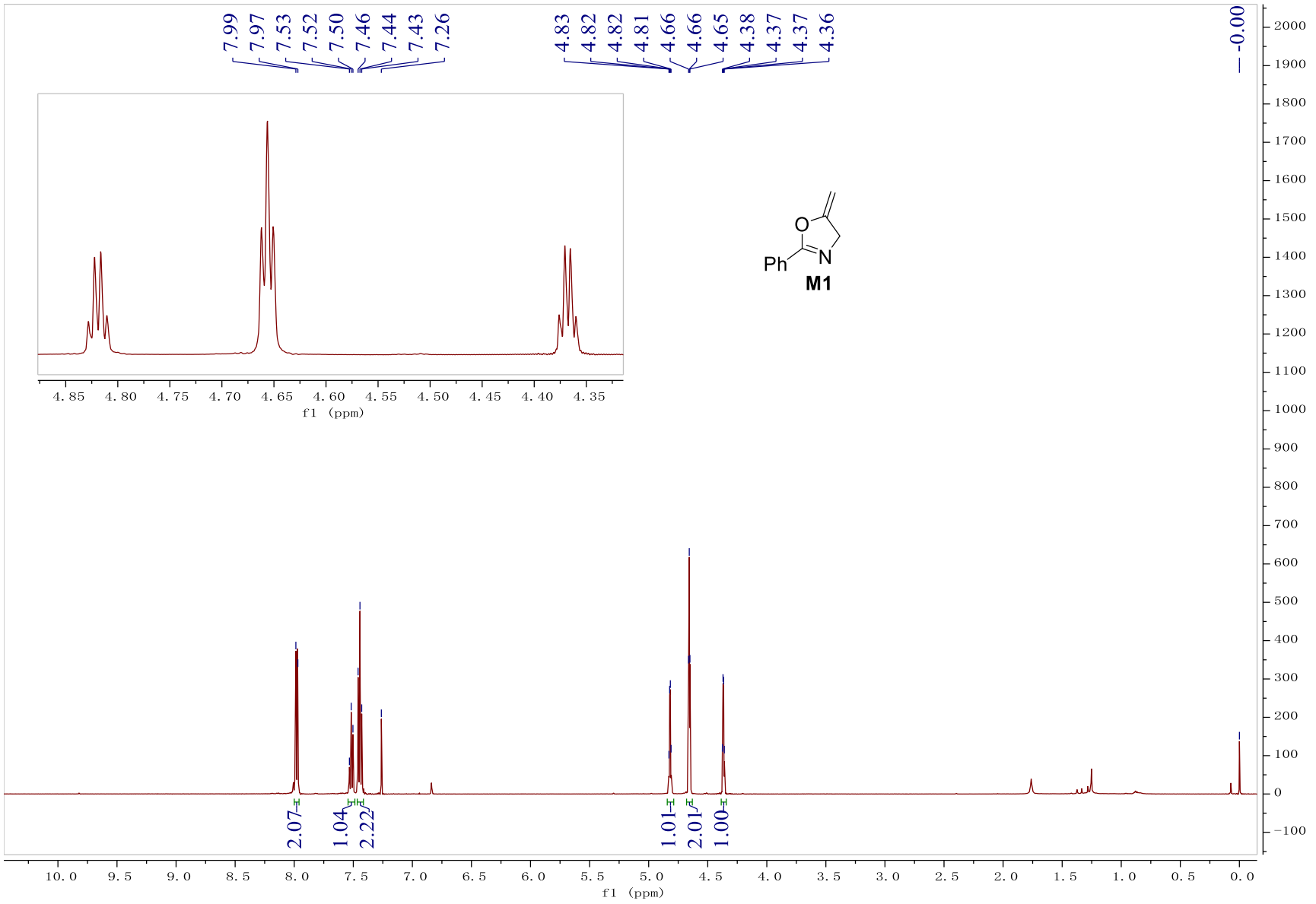
151.22
150.77
136.07
135.33
129.86
128.64
128.52
127.66
125.93
124.92
123.05
113.84
77.25
76.99
76.74
55.18
48.09
32.52
16.10
OH
N
O
Ph
MeO
3na
f1 (ppm)

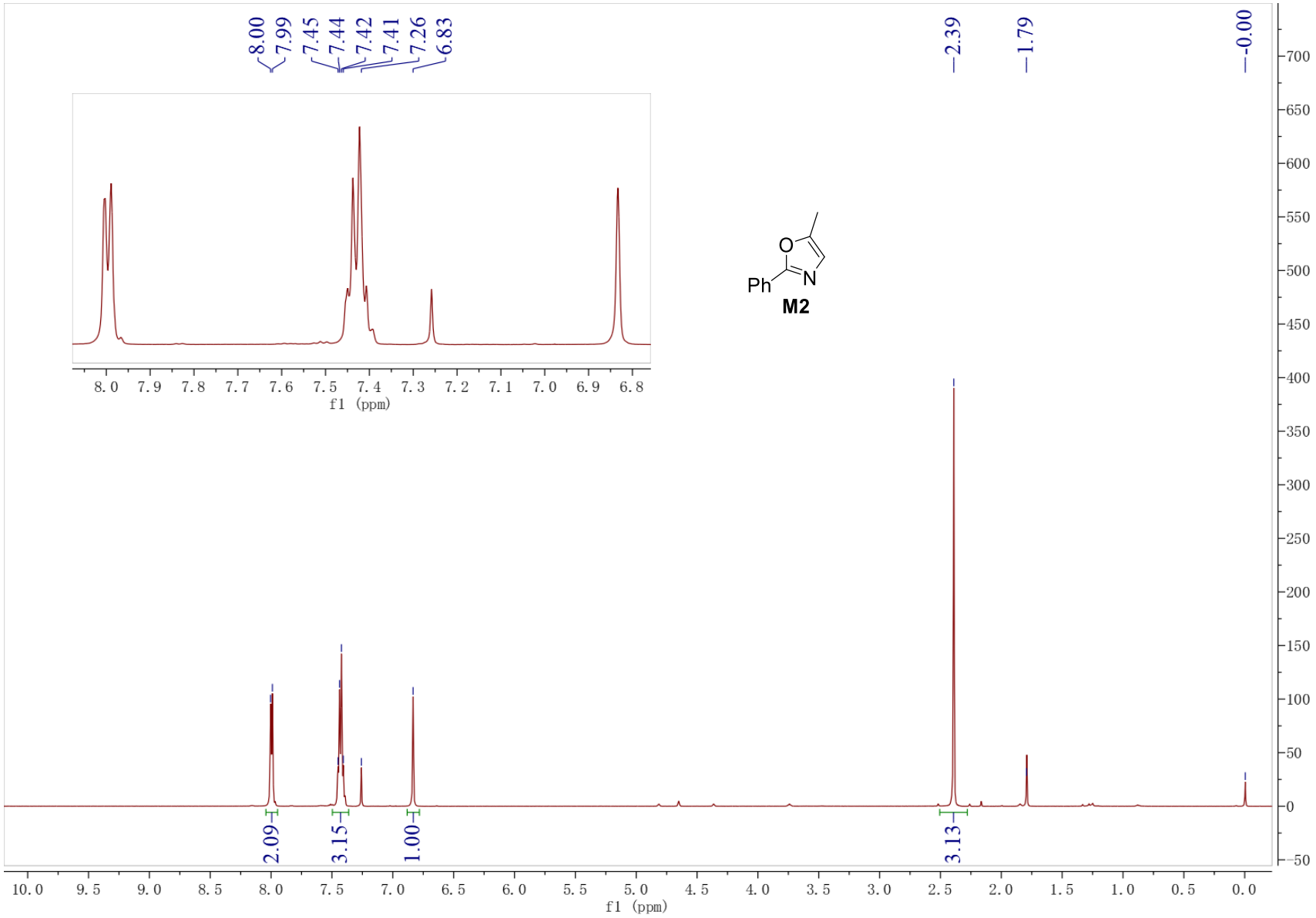

7.95
7.94
7.93
7.50
7.49
7.46
7.44
7.43
7.42
7.38
7.37
7.35
7.26
7.23
7.21
7.16
6.85
6.83
6.68
5.38
4.41
4.39
4.37
3.77
3.51
3.50
3.48
3.47
3.45
3.44
3.42
0.01
OH
Ph
Ph
N
Ph
O
MeO
3oa
f1 (ppm)
1.95
3.02
10.04
2.04
2.00
2.03
0.98
0.94
0.99
3.06
1.96


160.58
158.17
150.99
147.86
137.56
135.91
135.64
129.94
129.30
129.10
128.77
128.67
128.58
127.60
125.97
125.07
113.97
77.26
77.00
76.75
55.21
48.36
32.51
OH
Ph
Ph
N
Ph
O
MeO
3oa
f1 (ppm)


7.94
7.93
7.92
7.92
7.60
7.59
7.42
7.42
7.41
7.27
7.26
7.25
7.07
7.07
6.96
6.94
6.76
4.28
3.86
1.76
1.37
1.20
-0.00
t-Bu
t-Bu
O
N
Ph
O
MeO
4
f1 (ppm)
2.02
1.01
3.09
2.29
1.00
2.00
1.01
2.00
3.04
9.04
9.01


186.24
161.23
160.08
148.89
148.75
148.14
147.03
132.05
131.34
131.11
130.21
129.83
128.71
128.12
127.31
126.01
125.29
113.74
77.25
76.99
76.74
55.32
35.51
35.16
31.77
29.60
29.41
t-Bu
t-Bu
O
N
Ph
O
MeO
4
f1 (ppm)


7.99
7.97
7.53
7.52
7.50
7.46
7.44
7.43
7.26
4.83
4.82
4.82
4.81
4.66
4.66
4.65
4.38
4.37
4.37
4.36
-0.00
4.85 4.80 4.75 4.70 4.65 4.60 4.55 4.50 4.45 4.40 4.35
f1 (ppm)
O
Ph
N
M1
2.07
1.04
2.22
1.01
2.01
1.00
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)


8.00
7.99
7.45
7.44
7.42
7.41
7.26
6.83
2.39
1.79
0.00
Ph
O
N
M2
2.09
3.15
1.00
3.13
f1 (ppm)