Supplementary information

Bu_4NI-catalyzed construction of *tert*-butyl peresters from alcohols

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1. Instrument

NMR spectra were recorded at 500 MHz for protons on JOEL JNM-ECA spectrometers. ^{1}H NMR chemical shifts (δ) are given in ppm relative to TMS (δ = 0.0). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard. Data Reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal), integration, coupling constant (Hz) and identification. All major chemicals and solvents were obtained from commercial sources and used without further purification.

2. Synthesis of *tert*-butyl peresters catalysed by Bu_4NI: Under air, alcohols (0.5 mmol), TBHP (2.5 mmol), Bu_4NI (20 mol%), water (2ml) were mixed in a screw cap vial. The mixture was stirred at RT in a closed reaction vessel. The reaction was monitored by TLC. After completion of the reaction, the solvent was evaporated under reduced pressure and the residue purified by column chromatography on silica gel to give the desired product.

3. Synthesis of allylic ester catalysed in two-step one-pot process: Under air, alcohols (0.5 mmol), TBHP (2.5 mmol), Bu_4NI (20 mol%), CH_2Cl_2 (2ml) were mixed in a screw cap vial. The mixture was stirred at RT for 16h. Then copper bromide (5 mol %), olefin (10.0 equiv) were added and stirred in an bath at 40 °C for 36 h. After completion of the reaction, the solvent was evaporated under reduced pressure and the residue purified by column chromatography on silica gel to give the desired product.

4. Characterization data of products:

tert-butyl benzoperoxoate (**3a**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.3 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 1.34 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.42 (s), 133.35 (s), 129.12 (s), 128.63 (s), 127.75 (s), 83.97 (s), 26.25 (s).

tert-butyl 2-methylbenzoperoxoate (**3b**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.85 (dd, *J* = 12.6, 4.3 Hz, 2H), 7.80 – 7.68 (m, 2H), 7.56 – 7.37 (m, 2H), 1.36 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.65 (s), 135.61 (s), 132.44 (s), 130.73 (s), 129.30 (s), 128.55 (d, *J* = 7.2 Hz), 127.84 (s), 126.95 (s), 124.89 (s), 124.49 (s), 84.08 (s), 26.34 (s).

tert-butyl 4-methylbenzoperoxoate (**3c**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 6.8 Hz, 2H), 2.42 (s, 3H), 1.41 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.55 (s), 144.14 (s), 129.25 (d, *J* = 19.9 Hz), 124.92 (s), 83.87 (s), 26.27 (s), 21.70 (s).

tert-butyl 3-fluorobenzoperoxoate (**3d**) IR(KBr) ν 1728, 1592, 1488, 1450, 1369 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.8 Hz, 1H), 7.64 (ddd, *J* = 9.1, 2.3, 1.6 Hz, 1H), 7.45 (td, *J* = 8.0, 5.5 Hz, 1H), 7.30 (tdd, *J* = 8.3, 2.6, 0.8 Hz, 1H), 1.42 (s, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.51 (s), 163.28 (d, *J* = 3.0 Hz), 161.54 (s), 130.39 (d, *J* = 7.9 Hz), 129.75 (d, *J* = 7.4 Hz), 124.90 (d, *J* = 3.2 Hz), 120.58 (s), 120.41 (s), 116.21 (s), 116.03 (s), 84.27 (s), 26.22 (s). HRMS (ESI) calculated for $C_{11}H_{13}FNaO_3$: 235.074050 $(M+Na)^+$, Found: 235.074093.

tert-butyl 2-fluorobenzoperoxoate (**3e**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.98 – 7.85 (m, 1H), 7.56 (ddd, *J* = 7.2, 5.0, 1.7 Hz, 1H), 7.26 (dd, *J* = 13.7, 6.2 Hz, 1H), 7.20 – 7.08 (m, 1H), 1.42 (s, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.86 (d, *J* = 3.5 Hz), 162.22 (s), 160.17 (s), 134.87 (d, *J* = 8.8 Hz), 132.03 (d, *J* = 1.2 Hz), 124.34 (d, *J* = 3.7 Hz), 116.99 (s), 116.81 (s), 116.33 (d, *J* = 12.8 Hz), 84.13 (s), 26.19 (s).

tert-butyl 4-fluorobenzoperoxoate (**3f**) ^1H NMR (500 MHz, $CDCl_3$) δ 8.11 – 7.82 (m, 2H), 7.14 (t, *J* = 8.7 Hz, 2H), 1.42 (s, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.92 (s), 164.89 (s), 163.47 (s), 131.71 (d, *J* = 9.3 Hz), 123.93 (d, *J* = 3.1 Hz), 115.98 (s), 115.81 (s), 84.09 (s), 77.30 (s), 77.04 (s), 76.79 (s), 26.22 (s).

tert-butyl 2-bromobenzoperoxoate (**3g**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.47 (m, 2H), 7.38 – 7.25 (m, 2H), 1.35 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.49 (s), 134.08 (s), 132.82 (s), 130.86 (s), 127.29 (s), 120.97 (s), 84.27 (s), 26.34 (s).

tert-butyl 3-bromobenzoperoxoate(**3h**) IR(KBr) ν 1728, 1573, 1475, 1368 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 8.08 (t, *J* = 1.7 Hz, 1H), 7.94 – 7.83 (m, 1H), 7.72 (ddd, *J* = 8.0, 2.0, 1.0 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H), 1.42 (s, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.10 (s), 136.35 (s), 132.05 (s), 130.22 (s), 129.64 (s), 127.69 (s), 122.71 (s), 84.32 (s), 77.29 (s), 77.04 (s), 76.79 (s), 26.24 (s). HRMS (ESI) calculated for $C_{11}H_{13}BrNaO_3$ 294.993810 $(M+Na)^+$, Found: 294.994027.

tert-butyl 4-bromobenzoperoxoate(**3i**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.6 Hz, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 1.33 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.66 (s), 130.99 (s), 129.57 (s), 127.49 (s), 125.56 (s), 83.16 (s), 25.21 (s).

tert-butyl 2-chlorobenzoperoxoate(**3j**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 7.3, 0.9 Hz, 1H), 7.43 – 7.33 (m, 2H), 7.26 (ddd, *J* = 7.8, 6.2, 2.4 Hz, 1H), 1.34 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.03 (s), 132.93 (d, *J* = 18.4 Hz), 131.03 (s), 130.84 (s), 128.54 (s), 126.78 (s), 84.22 (s), 77.32 (s), 77.07 (s), 76.81 (s), 26.30 (s).

tert-butyl 4-chlorobenzoperoxoate(**3k**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.7 Hz, 2H), 7.36 (d, *J* = 8.7 Hz, 2H), 1.34 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.56 (s), 138.88 (s), 129.49 (s), 128.02 (s), 125.12 (s), 83.17 (s), 76.28 (s), 76.03 (s), 75.78 (s), 25.22 (s).

tert-butyl 3-chlorobenzoperoxoate(**3l**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 1.42 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.23 (s), 134.84 (s), 133.43 (s), 129.99 (s), 129.44 (s), 129.15 (s), 127.26 (s), 84.31 (s).

methyl 4-((tert-butylperoxy)carbonyl)benzoate(**3m**) ^1H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.6 Hz, 2H), 8.02 (d, *J* = 8.6 Hz, 2H), 3.96 (s, 3H), 1.43 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.04 (s), 163.62 (s), 134.34 (s), 131.53 (s), 129.77 (s), 129.12 (s), 84.31 (s), 52.51 (s), 26.24 (s).

tert-butyl 4-(methylthio)benzoperoxoate (**3n**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.5 Hz, 2H), 7.26 (d, *J* = 6.4 Hz, 2H), 2.52 (s, 3H), 1.41 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.26 (s), 146.27 (s), 129.41 (s), 125.14 (s), 123.58 (s), 83.96 (s), 26.27 (s), 14.80 (s).

tert-butyl 3-phenoxybenzoperoxoate (**3o**) ^1H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.7 Hz, 1H), 7.61 – 7.56 (m, 1H), 7.45 – 7.28 (m, 3H), 7.23 – 7.17 (m, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J*

= 7.7 Hz, 2H), 1.39 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.87 (s), 157.74 (s), 156.39 (s), 130.03 (d, *J* = 8.0 Hz), 129.42 (s), 124.03 (s), 123.67 (s), 123.38 (s), 119.26 (s), 119.08 (s), 84.10 (s), 26.24 (s).

tert-butyl naphthalene-2-carboperoxoate (**3p**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.85 (dd, *J* = 12.6, 4.3 Hz, 2H), 7.80 – 7.68 (m, 2H), 7.56 – 7.37 (m, 2H), 1.36 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.65 (s), 135.61 (s), 132.44 (s), 130.73 (s), 129.30 (s), 128.55 (d, *J* = 7.2 Hz), 127.84 (s), 126.95 (s), 124.89 (s), 124.49 (s), 84.08 (s), 26.34 (s).

tert-butyl thiophene-2-carboxylate (**3q**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.62 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.14 (dd, *J* = 5.0, 3.8 Hz, 1H), 1.40 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.35 (s), 133.72 (s), 132.83 (s), 129.34 (s), 127.84 (s), 84.31 (s), 26.17 (s).

tert-butyl naphthalene-1-carboperoxoate (**3r**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, *J* = 8.6 Hz, 1H), 7.90 (dd, *J* = 21.3, 7.7 Hz, 2H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.41 (dt, *J* = 29.9, 7.7 Hz, 2H), 1.36 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.61 (s), 133.81 (s), 133.43 (s), 130.98 (s), 128.98 (s), 128.60 (s), 128.01 (s), 126.61 (s), 125.40 (s), 125.19 (s), 124.45 (s), 83.95 (s), 26.38 (s).

tert-butyl 4-methoxybenzoperoxoate (**3s**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 2H), 6.92 (d, *J* = 8.2 Hz, 2H), 3.88 (s, 3H), 1.61 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.63 (s), 162.97 (s), 131.38 (s), 124.54 (s), 113.39 (s), 80.52 (s), 55.40 (s), 28.27 (s).

cyclohex-2-en-1-yl 4-fluorobenzoate(**4a**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 2H), 7.13 (t, *J* = 7.8 Hz, 2H), 6.11 – 5.99 (m, 1H), 5.83 (t, *J* = 21.0 Hz, 1H), 5.53 (s, 1H), 2.07 (ddd, *J* = 35.7, 27.4, 13.6 Hz, 3H), 1.95 – 1.81 (m, 2H), 1.75 (d, *J* = 2.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.71 (s), 165.29 (s), 164.69 (s), 132.99 (s), 132.12 (d, *J* = 9.3 Hz), 127.07 (s), 125.62 (s), 115.48 (s), 115.30 (s), 68.81 (s), 28.42 (s), 24.95 (s), 18.94 (s).

cyclohex-2-en-1-yl 4-bromobenzoate(**4b**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.1 Hz, 2H), 7.62 (dd, *J* = 26.6, 8.9 Hz, 2H), 6.04 (d, *J* = 8.1 Hz, 1H), 5.85 (d, *J* = 9.7 Hz, 1H), 5.53 (s, 1H), 2.08 (dt, *J* = 35.4, 13.7 Hz, 3H), 1.95 – 1.82 (m, 2H), 1.72 (d, *J* = 20.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.49 (s), 132.08 (s), 130.59 (s), 130.13 (s), 128.72 (s), 126.81 (s), 124.48 (s), 67.97 (s), 27.36 (s), 23.92 (s), 17.89 (s), -0.00 (s).

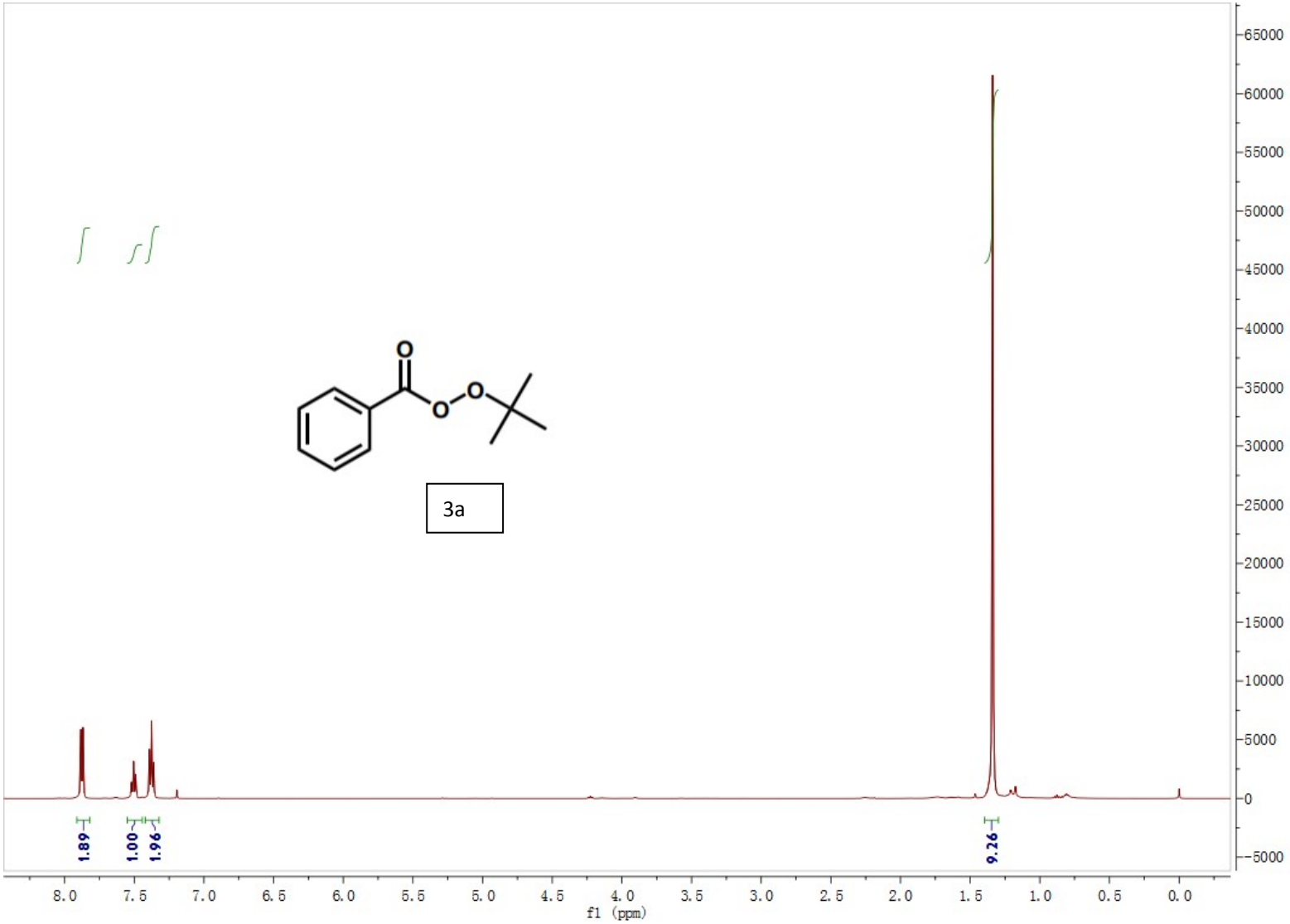
cyclohex-2-en-1-yl 3-phenoxybenzoate(**4c**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.6 Hz, 1H), 7.62 (s, 1H), 7.28 (dt, *J* = 16.7, 10.5 Hz, 3H), 7.12 – 6.99 (m, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 5.90 (d, *J* = 9.7 Hz, 1H), 5.73 (d, *J* = 9.8 Hz, 1H), 5.40 (s, 1H), 2.11 – 1.84 (m, 3H), 1.83 – 1.68 (m, 2H), 1.61 (d, *J* = 4.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.66 (s), 157.32 (s), 156.88 (s), 132.97 (s), 132.69 (s), 129.90 (s), 129.65 (s), 125.60 (s), 124.42 (s), 123.63 (s), 123.17 (s), 119.96 (s), 118.94 (s), 68.91 (s), 28.39 (s), 24.95 (s), 18.92 (s).

cyclohex-2-en-1-yl thiophene-2-carboxylate (**4d**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 22.1 Hz, 1H), 7.54 (t, *J* = 8.4 Hz, 1H), 7.05 (d, *J* = 36.3 Hz, 1H), 6.00 (d, *J* = 8.1 Hz, 1H), 5.82 (d, *J* = 9.9 Hz, 1H), 5.47 (s, 1H), 2.02 (ddd, *J* = 38.4, 28.0, 14.2 Hz, 3H), 1.91 – 1.75 (m, 2H), 1.68 (d, *J* = 5.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.94 (s), 133.51 (s), 132.17 (s), 131.98 (s), 131.10 (s), 126.61 (s), 124.54 (s), 67.97 (s), 27.38 (s), 23.91 (s), 17.88 (s).

cyclohex-2-en-1-yl 4-(methylthio)benzoate(**4e**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.9 Hz, 2H), 7.34 – 7.21 (m, 2H), 6.03 (d, *J* = 7.5 Hz, 1H), 5.85 (d, *J* = 9.8 Hz, 1H), 5.52 (s, 1H), 2.54 (s, 3H), 2.17 (d, *J* = 17.8 Hz, 1H), 2.11 – 1.93 (m, 2H), 1.88 (dd, *J* = 12.8, 7.2 Hz, 2H), 1.74 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.99 (s), 145.16 (s), 132.79 (s), 129.92 (s), 127.01 (s), 125.83 (s), 124.97 (s), 68.54 (s), 28.46 (s), 24.97 (s), 18.99 (s), 14.92 (s).

cyclohex-2-en-1-yl 2-naphthoate(**4f**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 22.5 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.87 (t, *J* = 12.0 Hz, 2H), 7.62 – 7.40 (m, 2H), 6.03 (d, *J* = 10.5 Hz, 1H), 5.89 (d, *J* = 9.8 Hz, 1H), 5.58 (s, 1H), 2.25 – 1.99 (m, 3H), 1.92 (dd, *J* = 19.8, 14.5 Hz, 2H), 1.74 (d, *J* = 2.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.42 (s), 135.51 (s), 132.91 (s), 132.54 (s), 130.97 (s), 129.35 (s), 128.30 – 127.97 (m), 127.76 (s), 126.57 (s), 125.86 (s), 125.38 (s), 68.83 (s), 28.52 (s), 25.02 (s), 19.06 (s).

cyclohex-2-en-1-yl 4-chlorobenzoate(**4g**) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.2 Hz, 2H), 7.45 (dd, *J* = 24.1, 8.3 Hz, 2H), 6.04 (d, *J* = 7.5 Hz, 1H), 5.85 (d, *J* = 9.7 Hz, 1H), 5.52 (s, 1H), 2.21 – 1.97 (m, 3H), 1.95 – 1.80 (m, 2H), 1.75 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.40 (s), 139.20 (s), 133.09 (s), 131.02 (s), 129.30 (s), 128.63 (s), 125.54 (s), 68.97 (s), 28.41 (s), 24.96 (s), 18.93 (s).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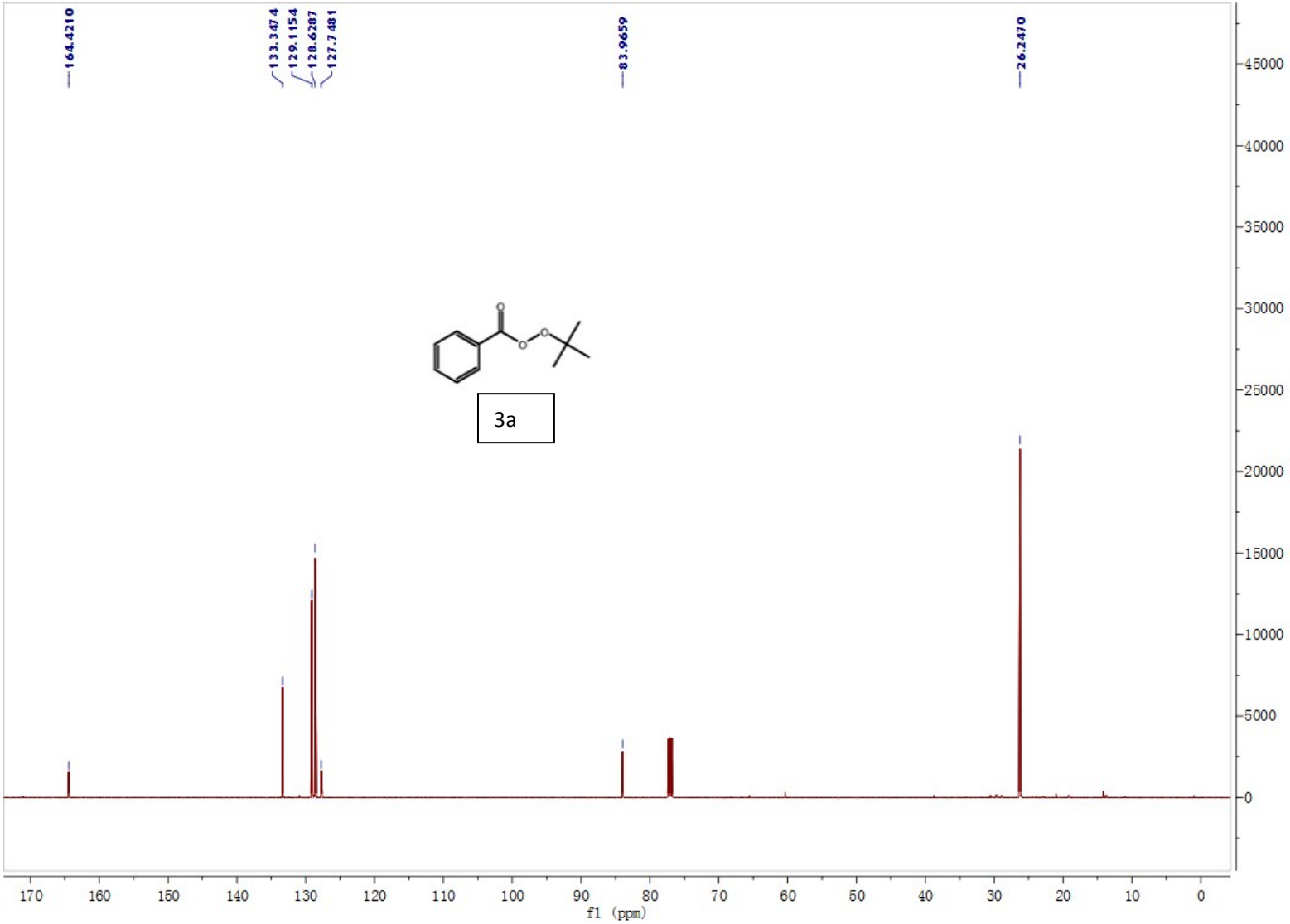
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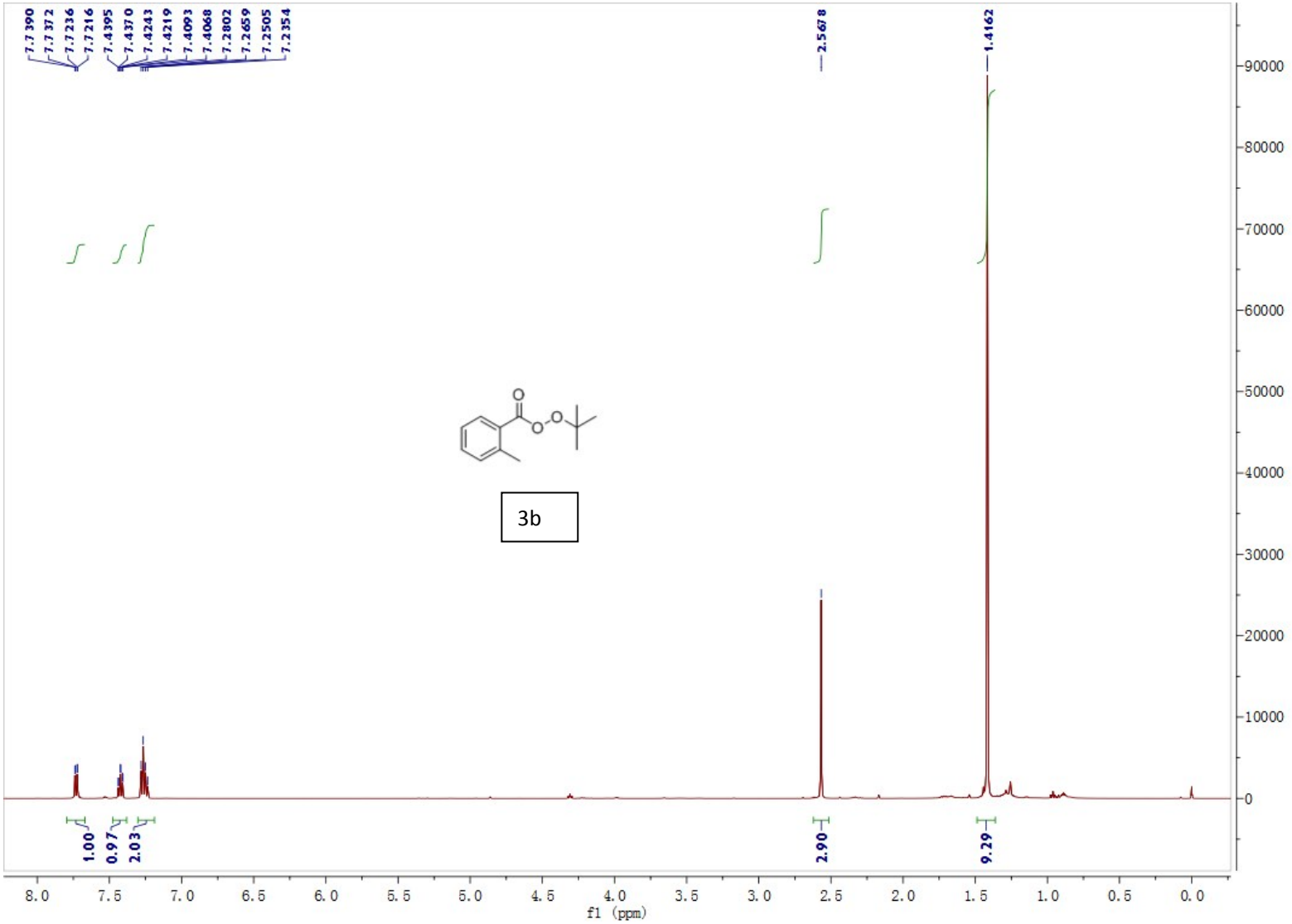
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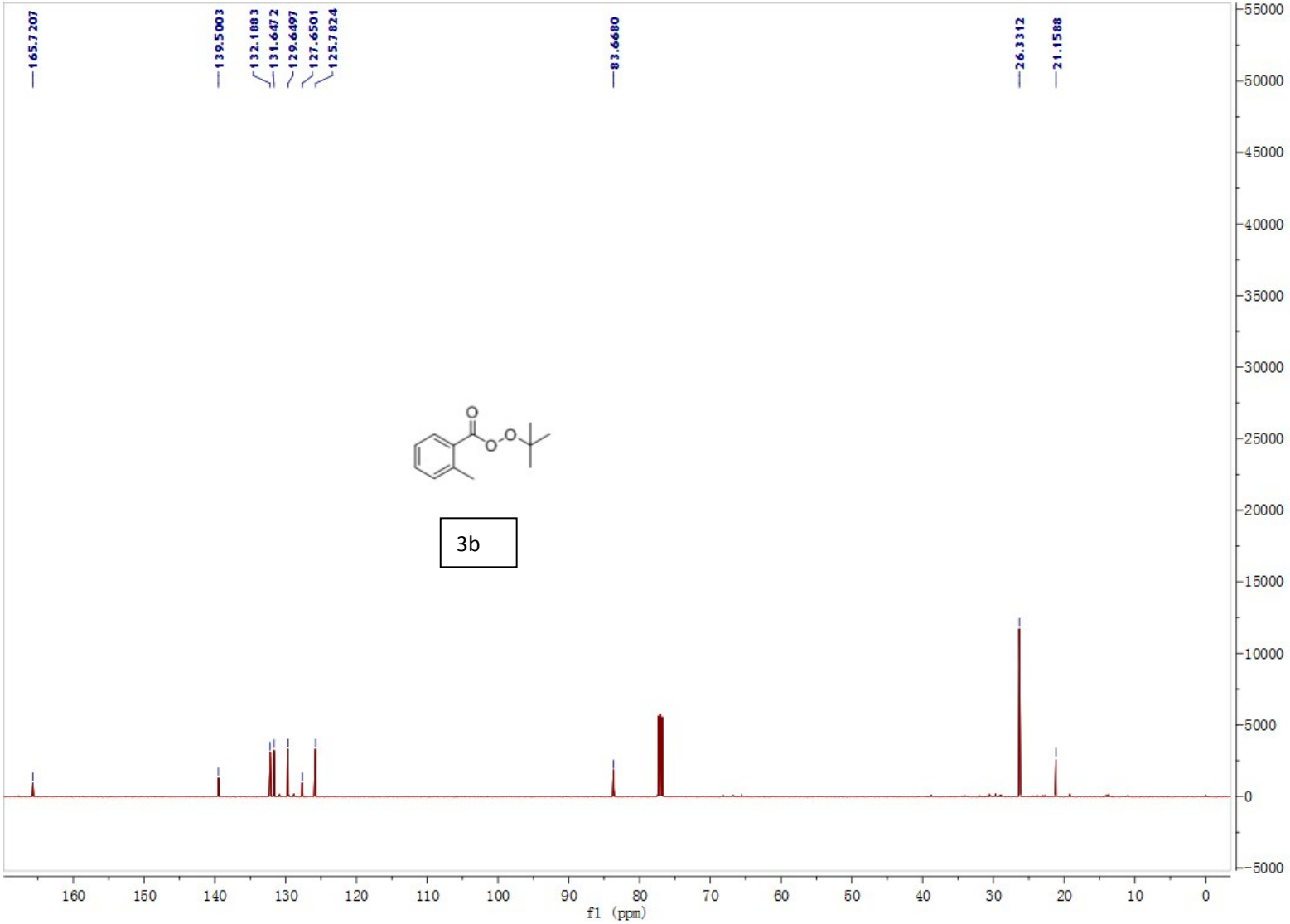
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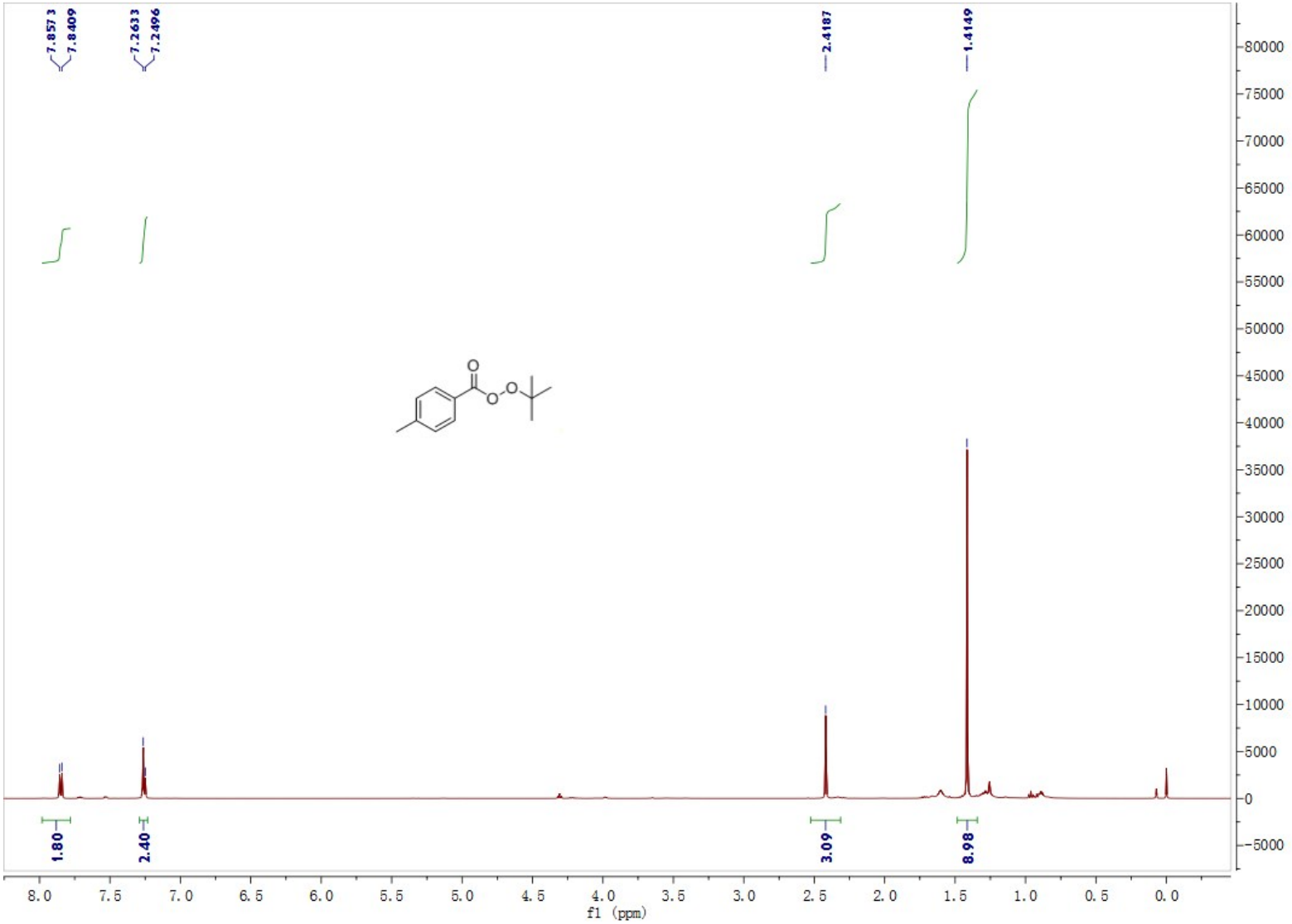
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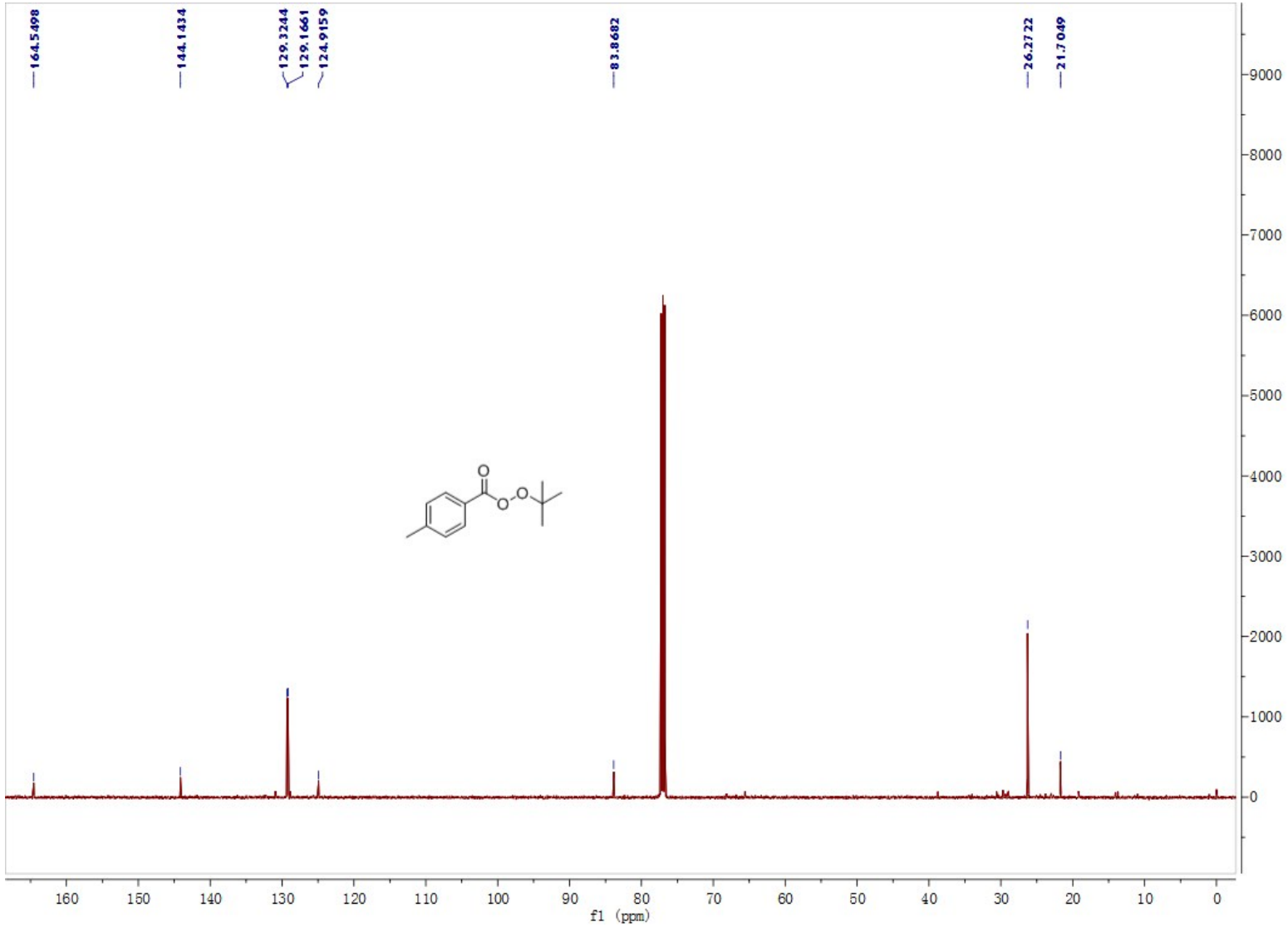
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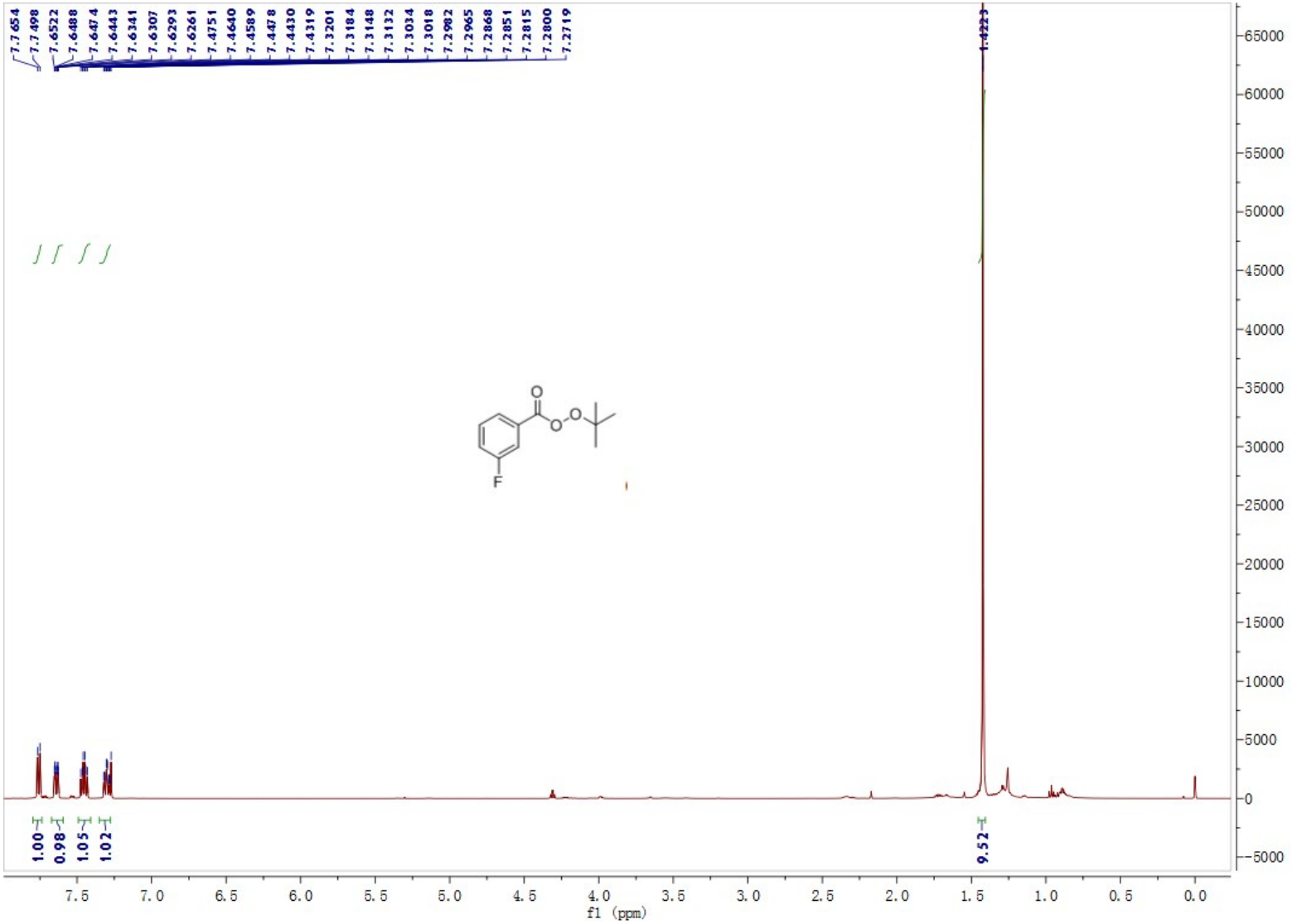
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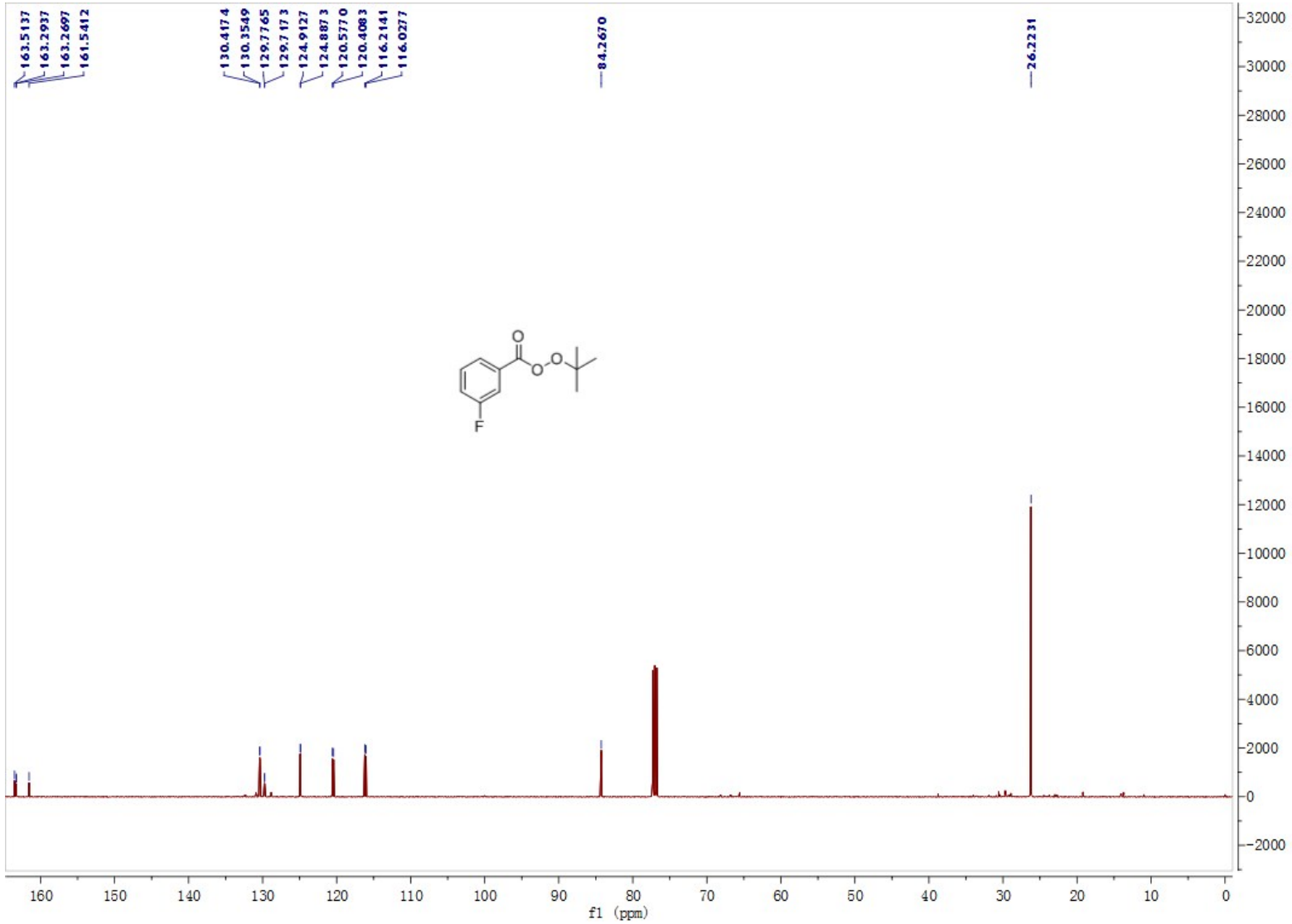
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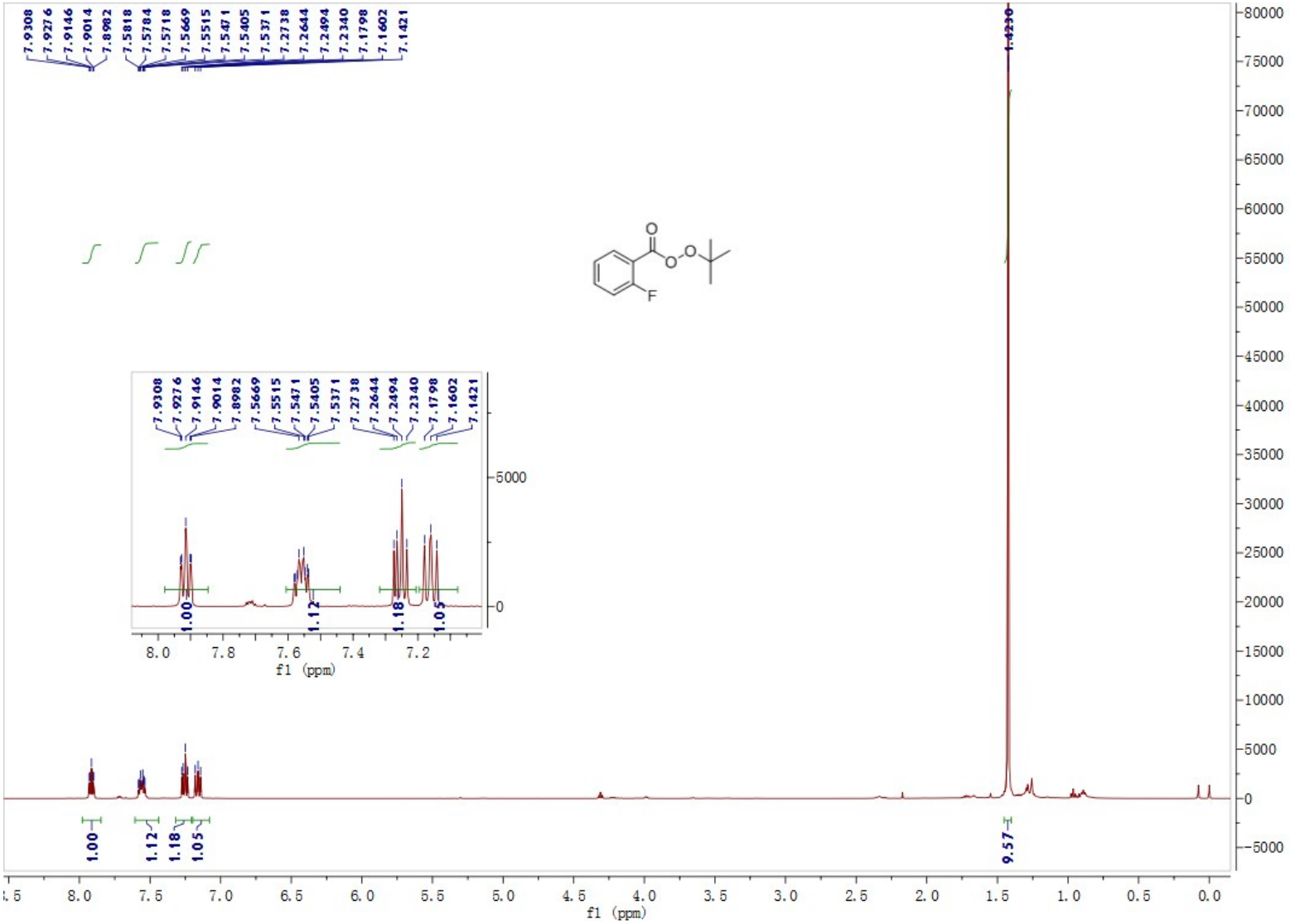
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7.8982
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7.5784
7.5718
7.5669
7.5515
7.5471
7.5405
7.5371
7.2738
7.2644
7.2494
7.2340
7.1798
7.1602
7.1421
1.4230
O
O
O
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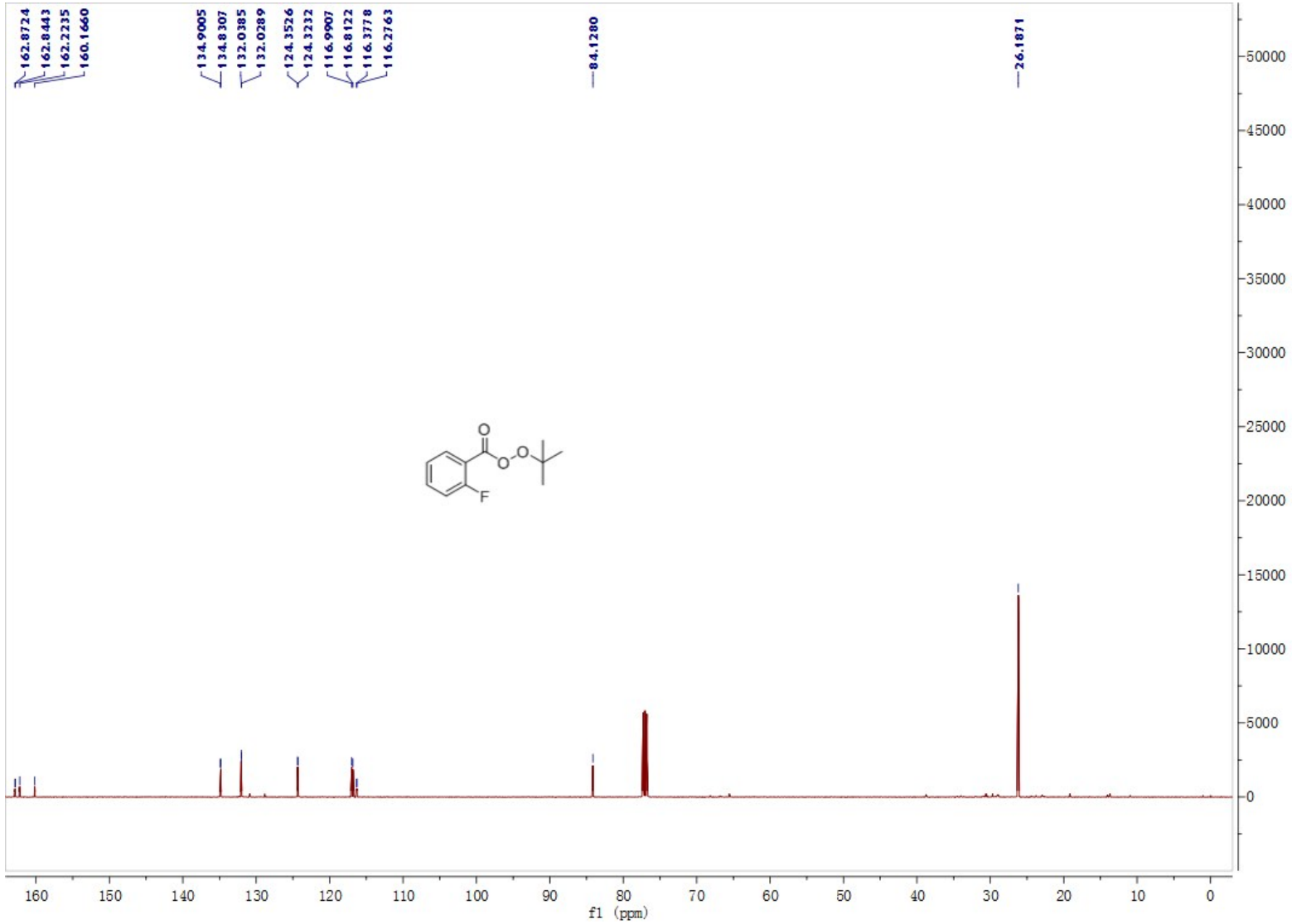
1.00
1.12
1.18
1.05
9.57
f1 (ppm)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162.2235
160.1660
134.9005
134.8307
132.0385
132.0289
124.3526
124.3232
116.9907
116.8122
116.3778
116.2763
84.1280
26.1871
O
O
O
F
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40000
35000
30000
25000
20000
15000
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5000
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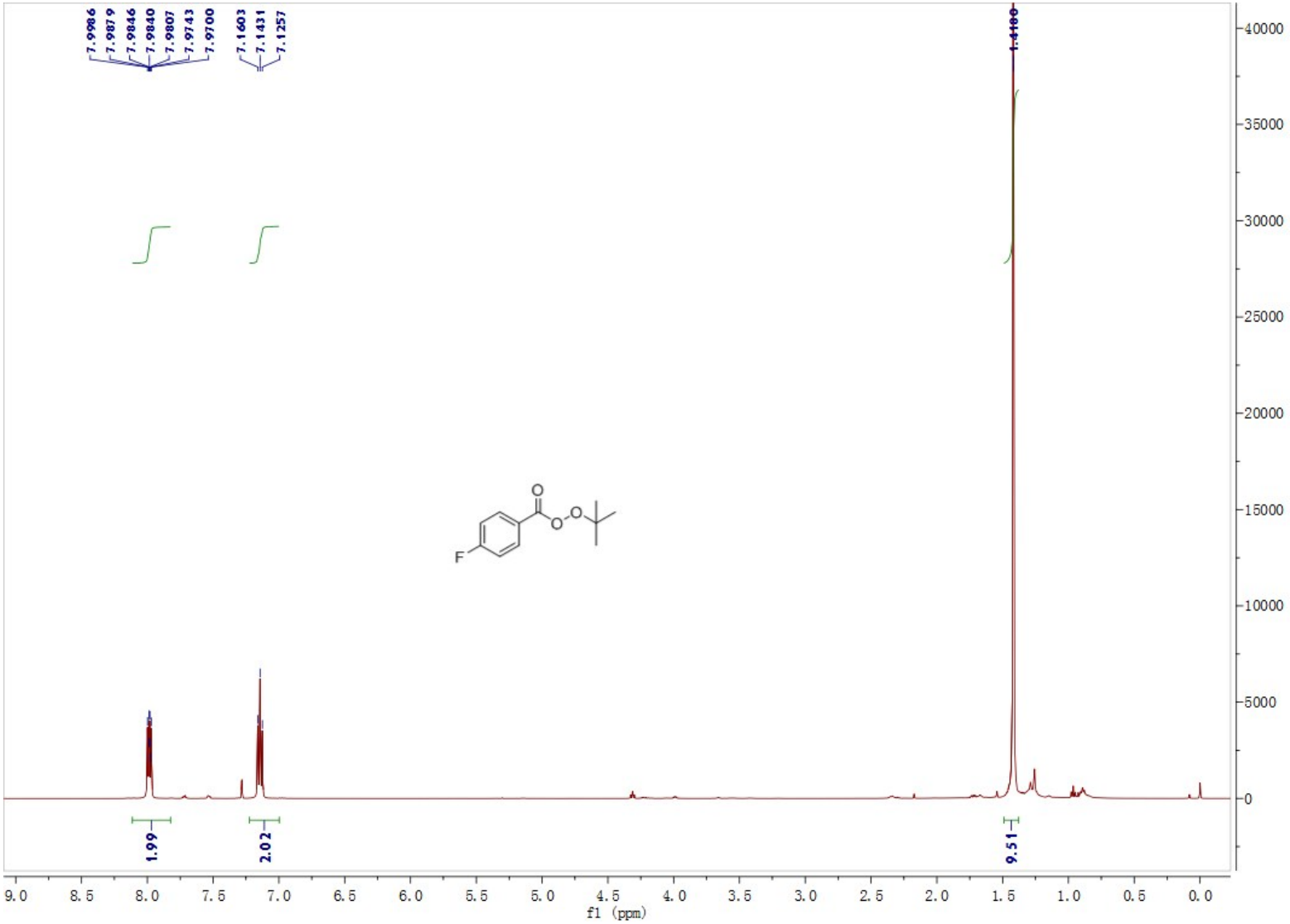
f1 (ppm)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7.1431
7.1257
1.4160
O
O
O
F
1.99
2.02
9.51
40000
35000
30000
25000
20000
15000
10000
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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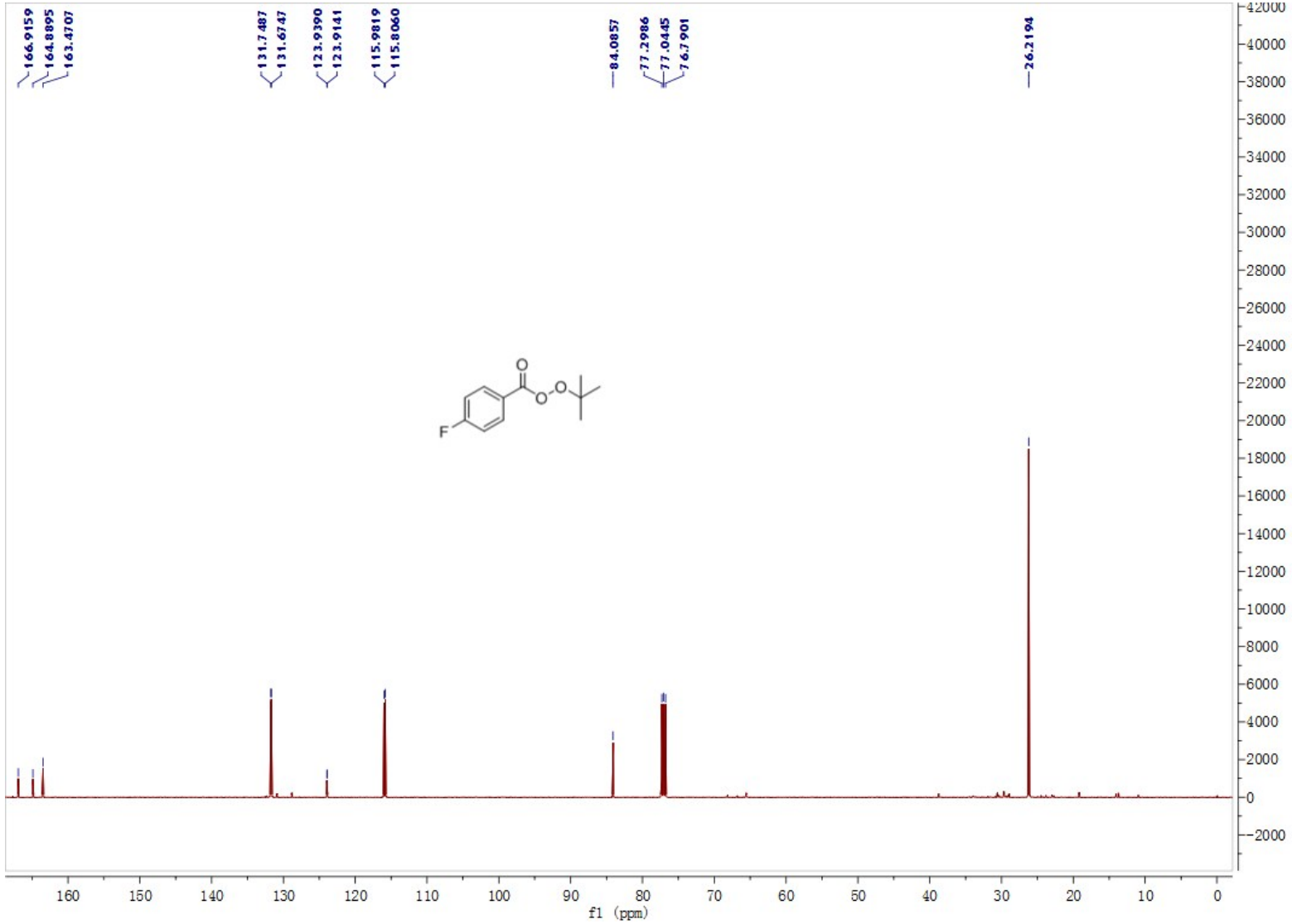
0.0
f1 (ppm)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115.8060
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77.2986
77.0445
76.7901
26.2194
F
O
O
O
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40000
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
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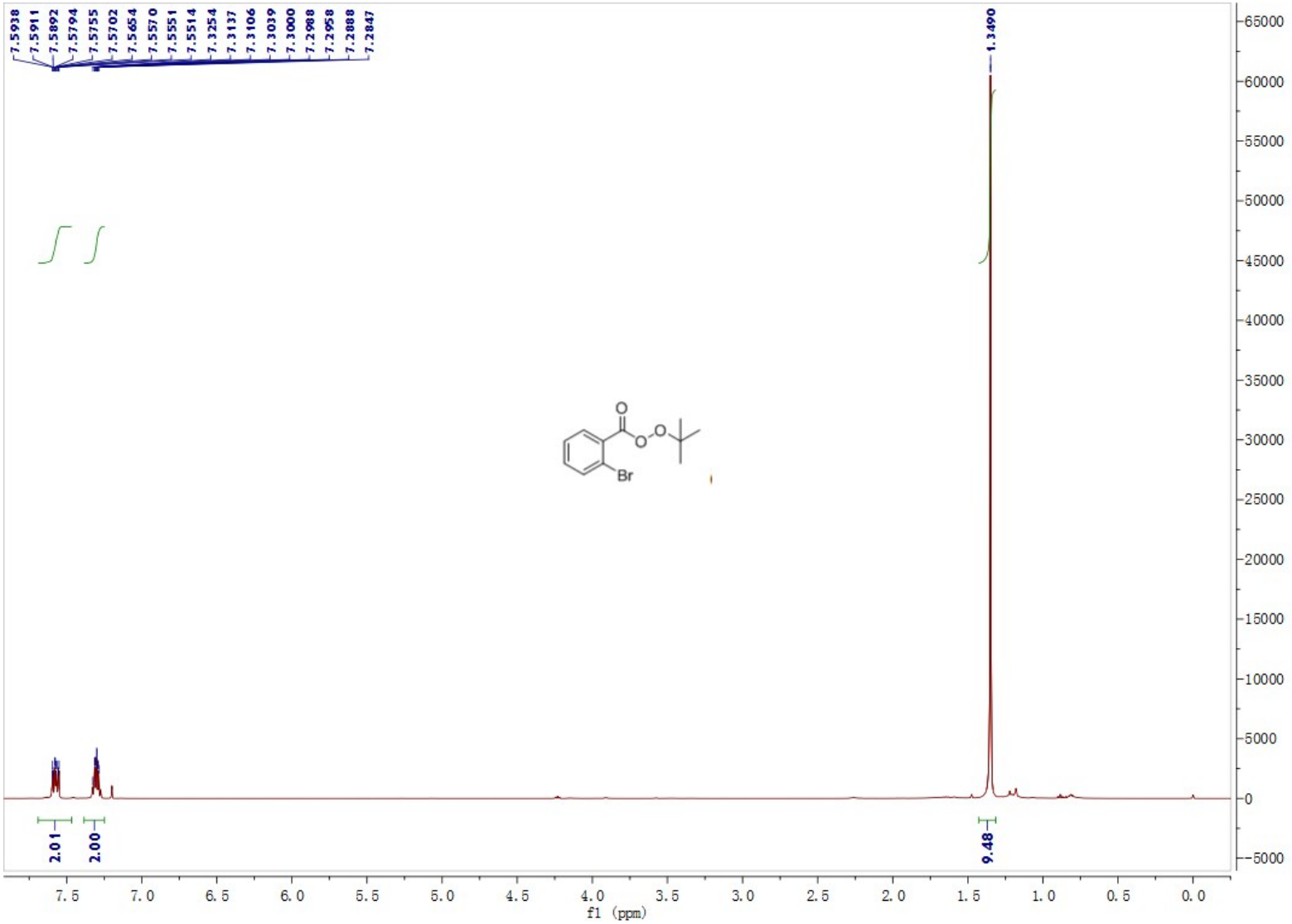
f1 (ppm)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7.5911
7.5892
7.5794
7.5755
7.5702
7.5654
7.5570
7.5551
7.5514
7.3254
7.3137
7.3106
7.3039
7.3000
7.2908
7.2958
7.2888
7.2847
1.3490
Br
O
O
O
2.01
2.00
9.48
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
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
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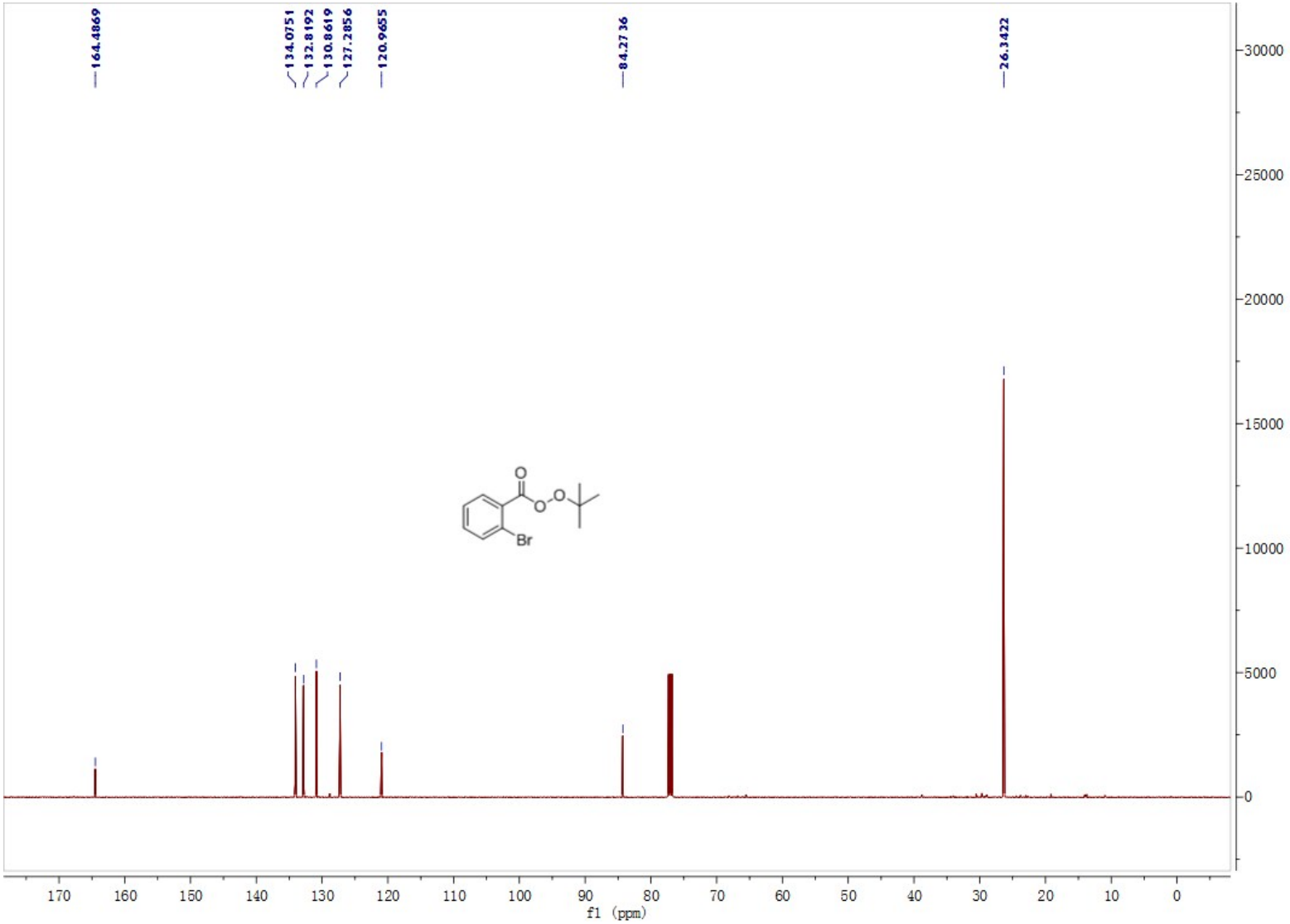
0.0
f1 (ppm)


164.4869
134.0751
132.8192
130.8619
127.2856
120.9655
84.2736
26.3422
O
O
O
Br
30000
25000
20000
15000
10000
5000
0
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130
120
110
100
90
80
70
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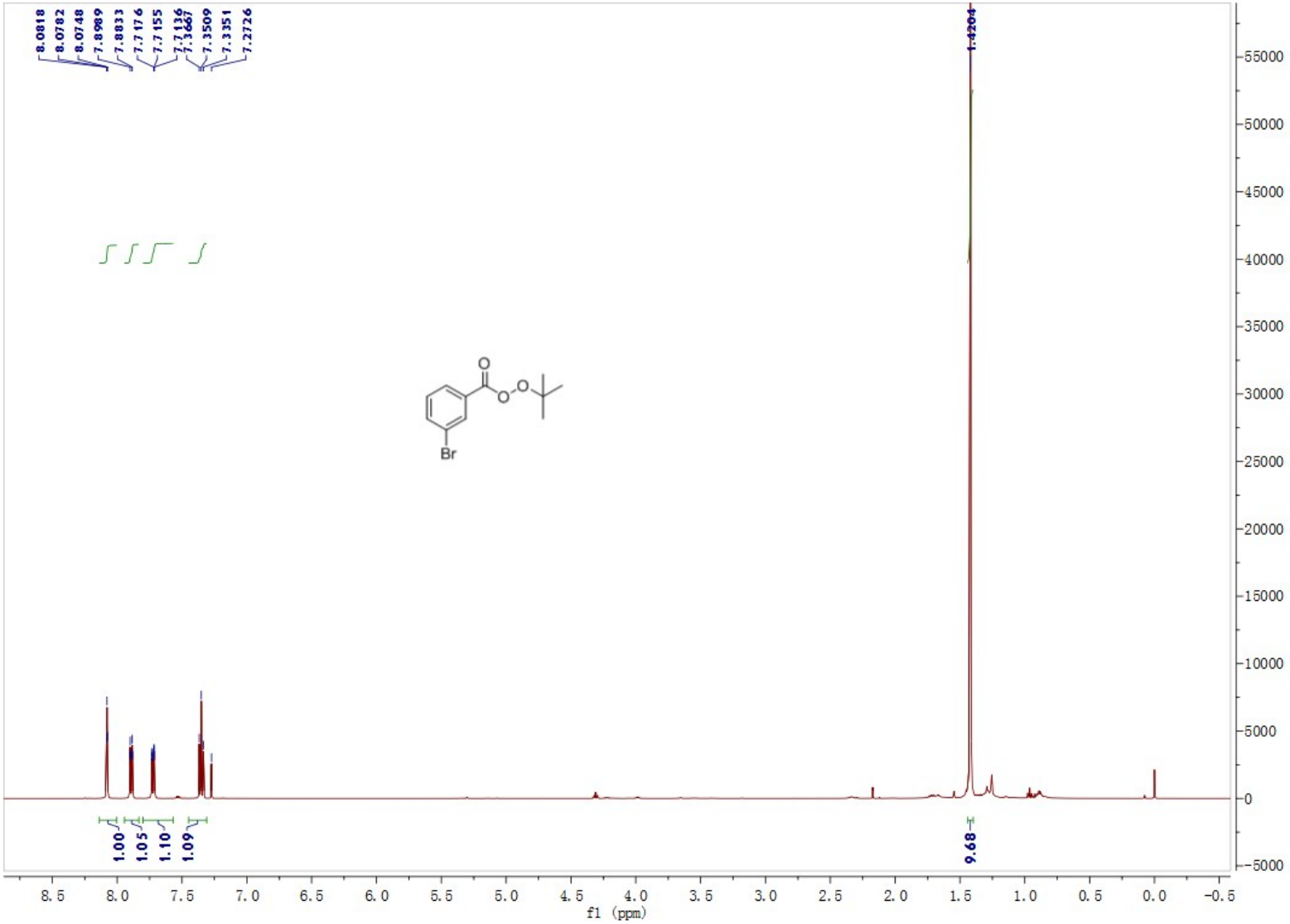
50
40
30
20
10
0
f1 (ppm)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8.0782
8.0748
7.8989
7.8833
7.7176
7.7155
7.7136
7.3667
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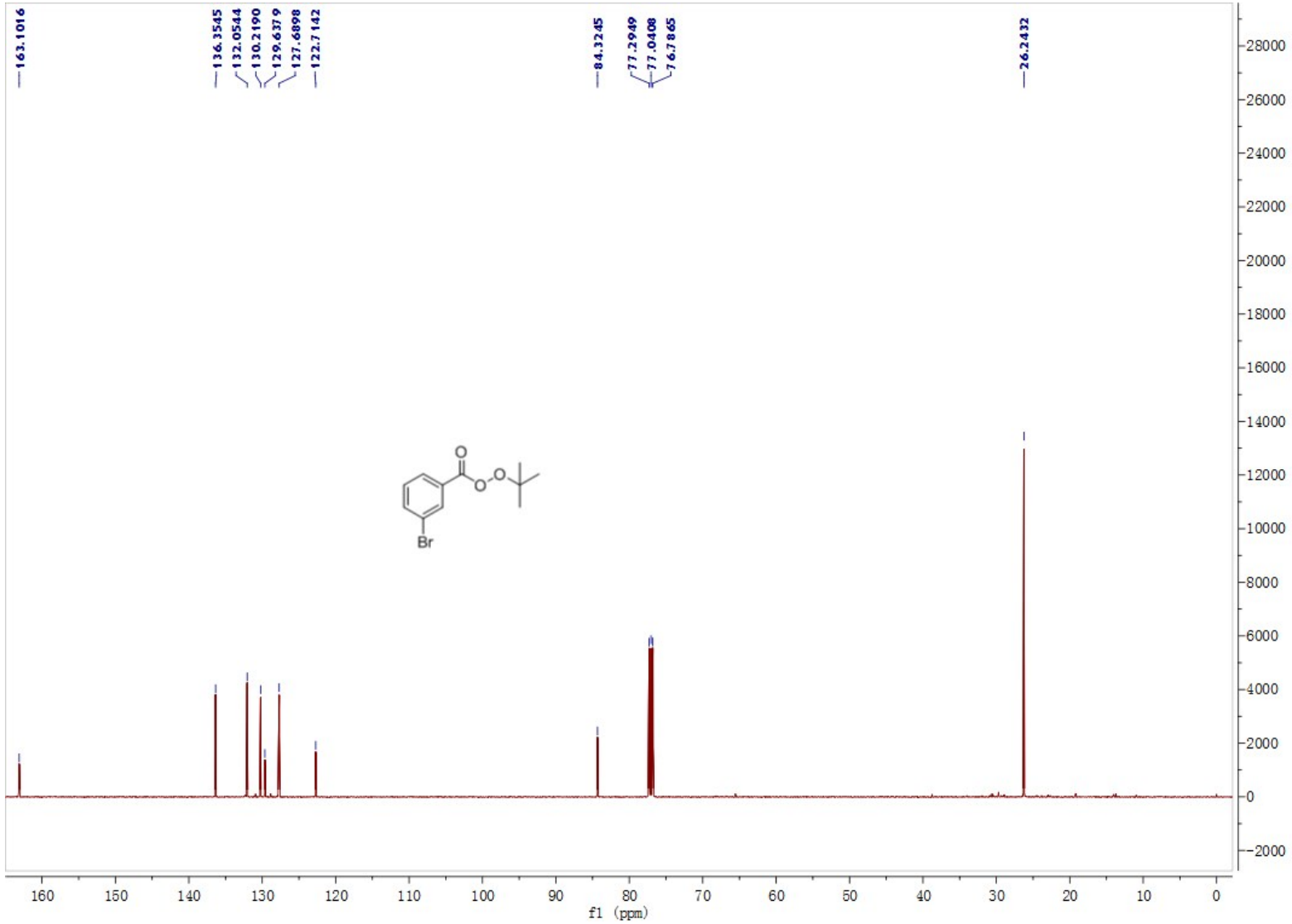
7.3351
7.2726
1.4204
Br
1.00
1.05
1.10
1.09
9.68
f1 (ppm)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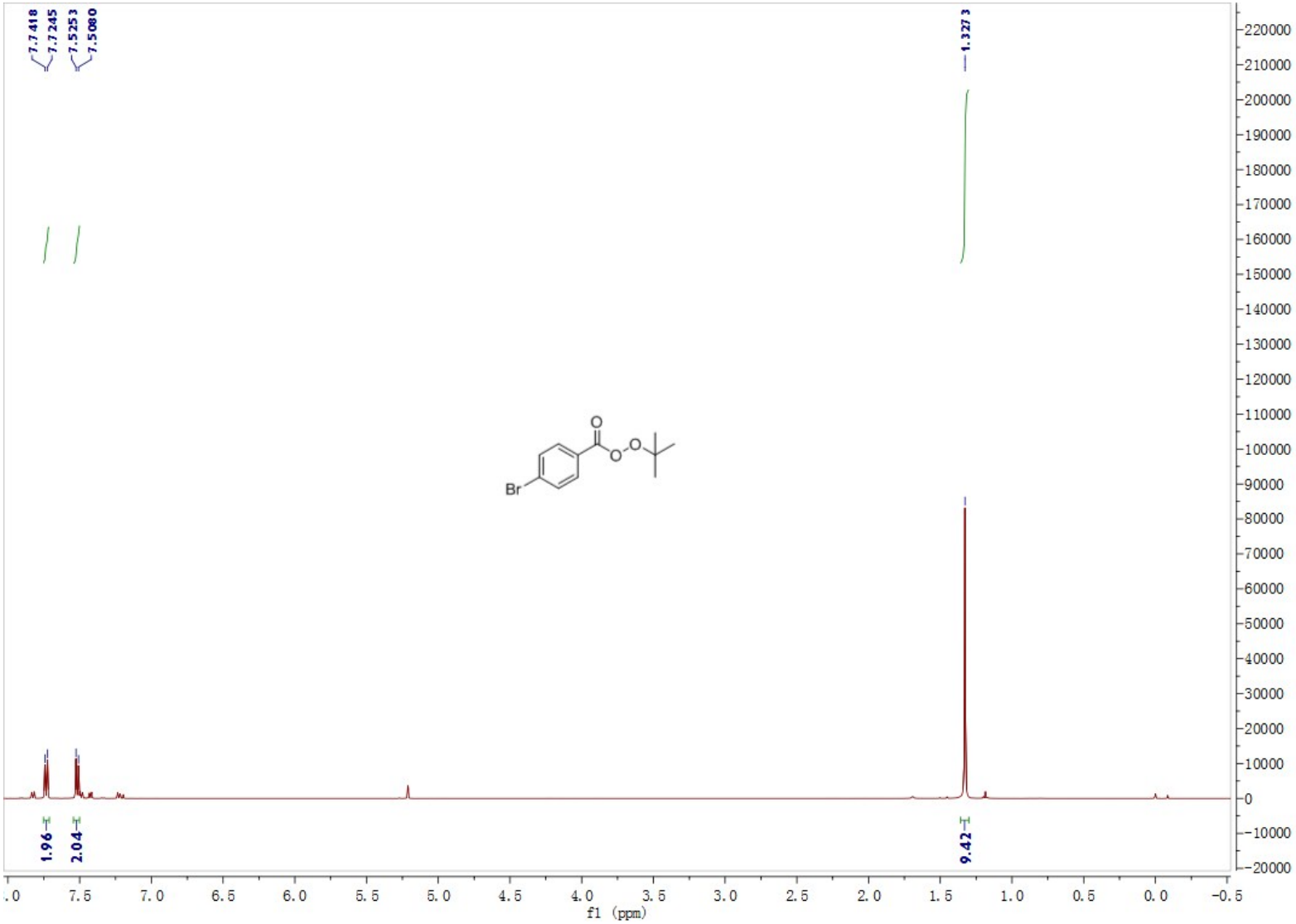
130.2190
129.6379
127.6898
122.7142
84.3245
77.2949
77.0408
76.7865
26.2432
O
O
O
Br
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.7418
7.7245
7.5253
7.5080
1.3273
Br
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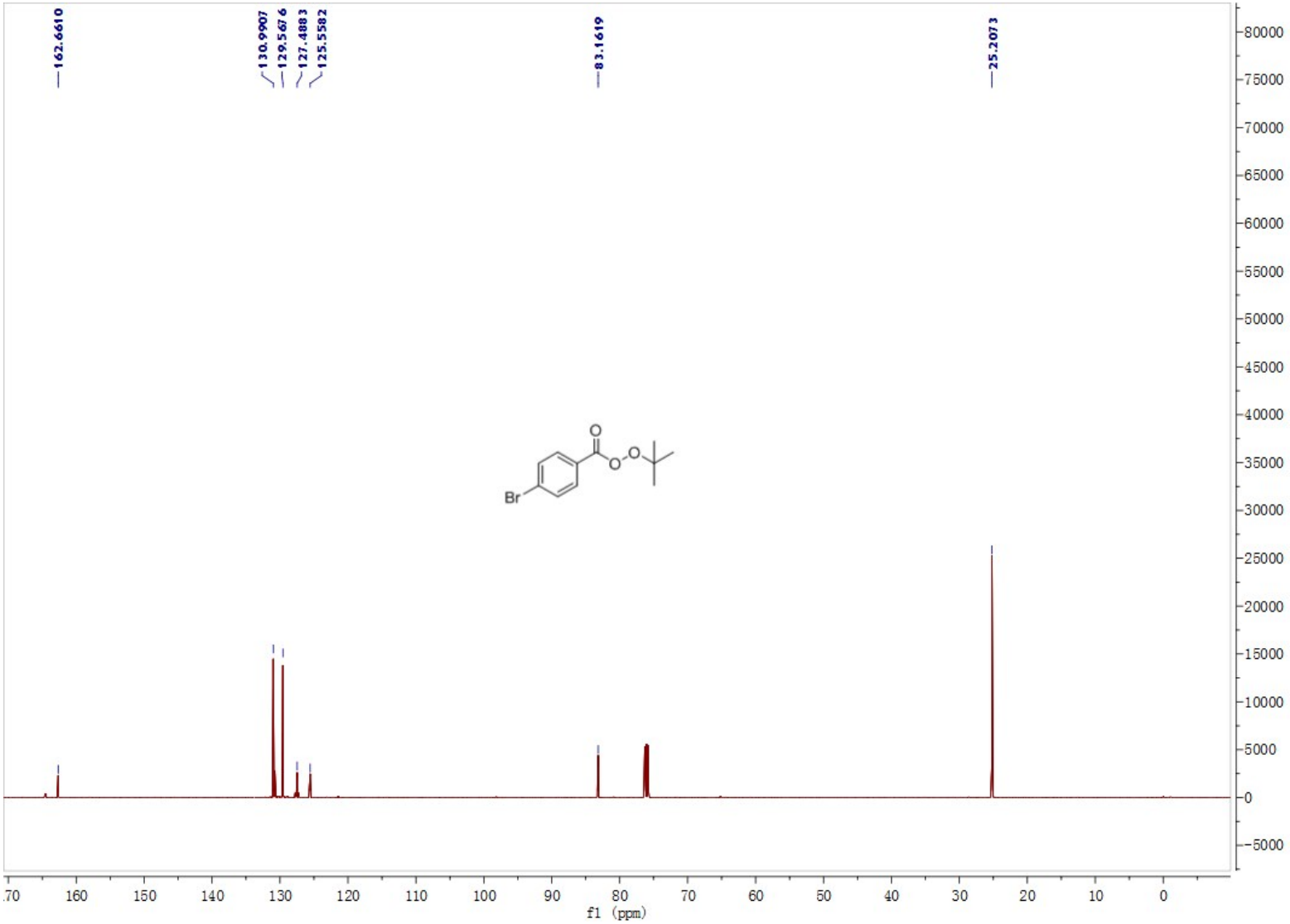
O
O
1.96
2.04
9.42
f1 (ppm)


162.6610
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129.5676
127.4883
125.5582
83.1619
25.2073
Br
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O
O
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70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
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150
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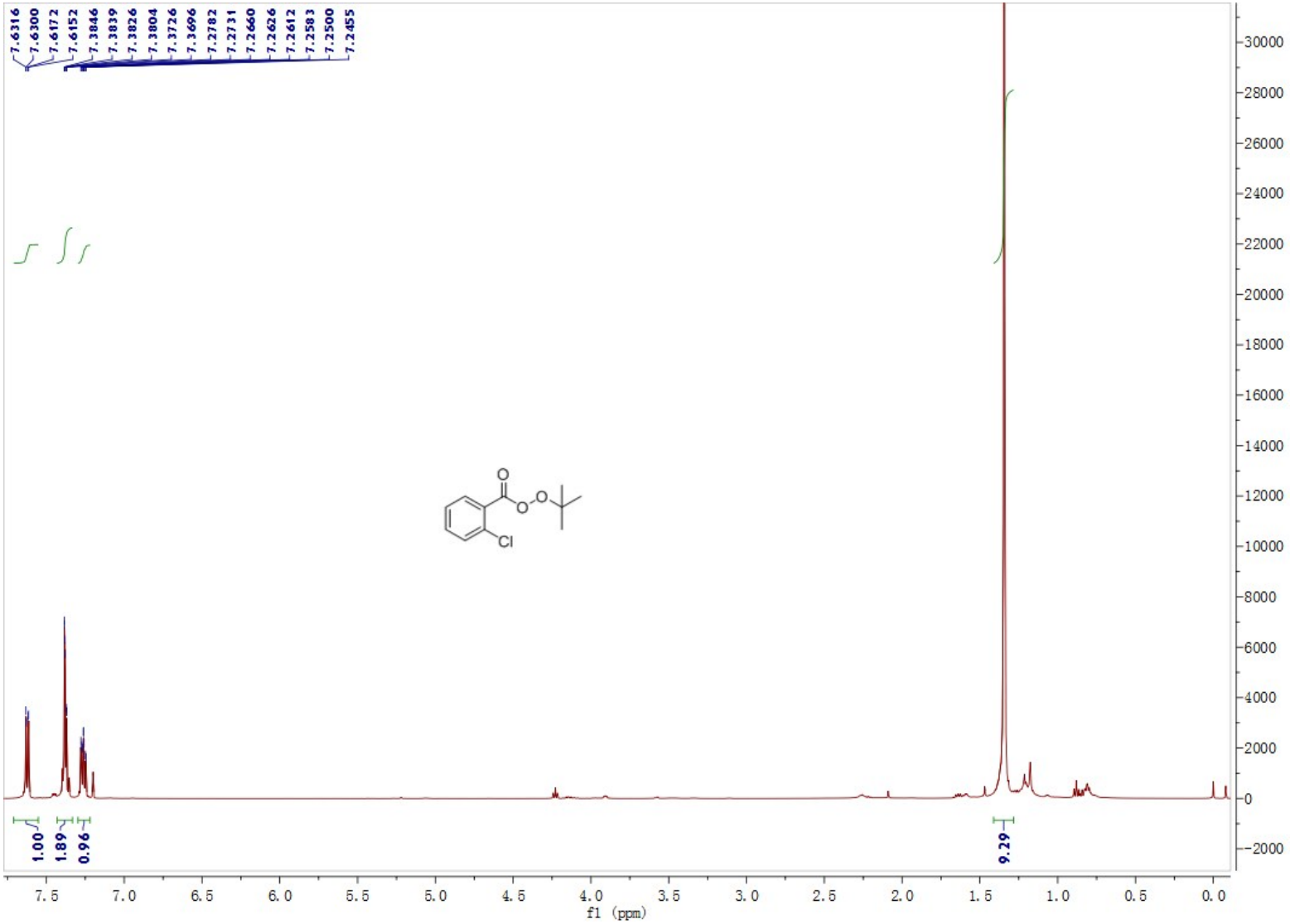
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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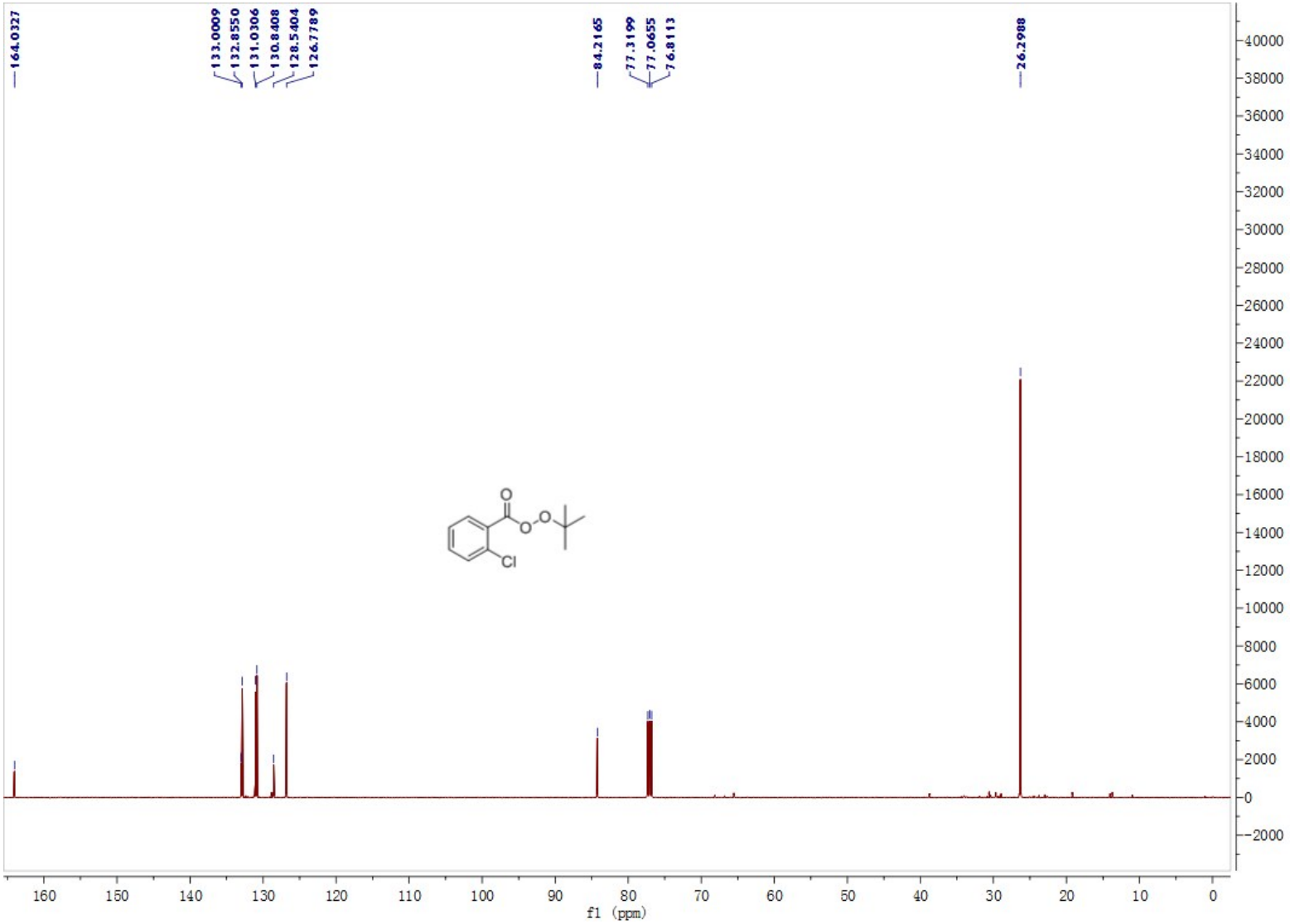
7.6172
7.6152
7.3846
7.3839
7.3826
7.3804
7.3726
7.3696
7.2782
7.2731
7.2660
7.2626
7.2612
7.2583
7.2500
7.2455
O
O
O
Cl
1.00
1.89
0.96
9.29
f1 (ppm)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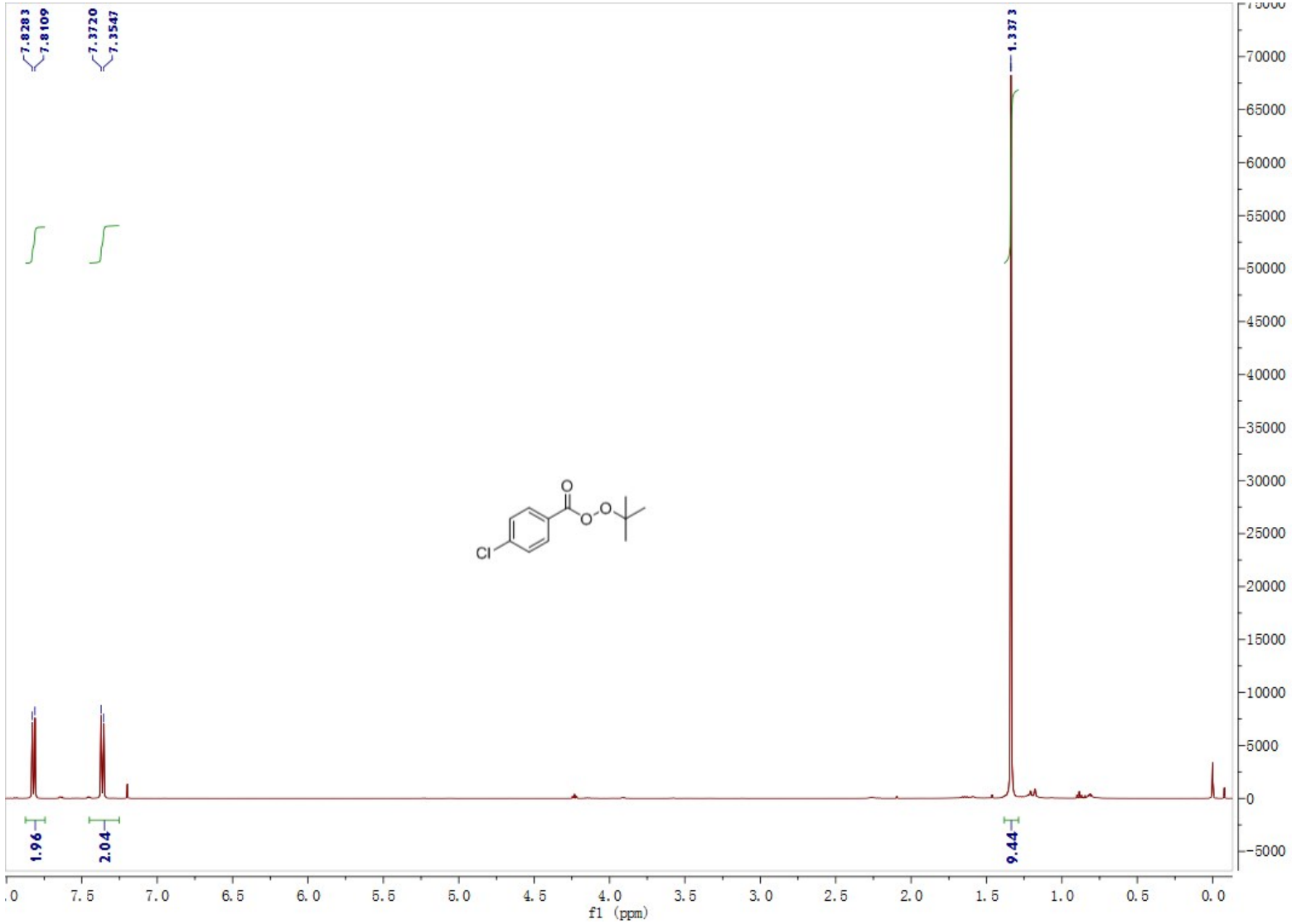
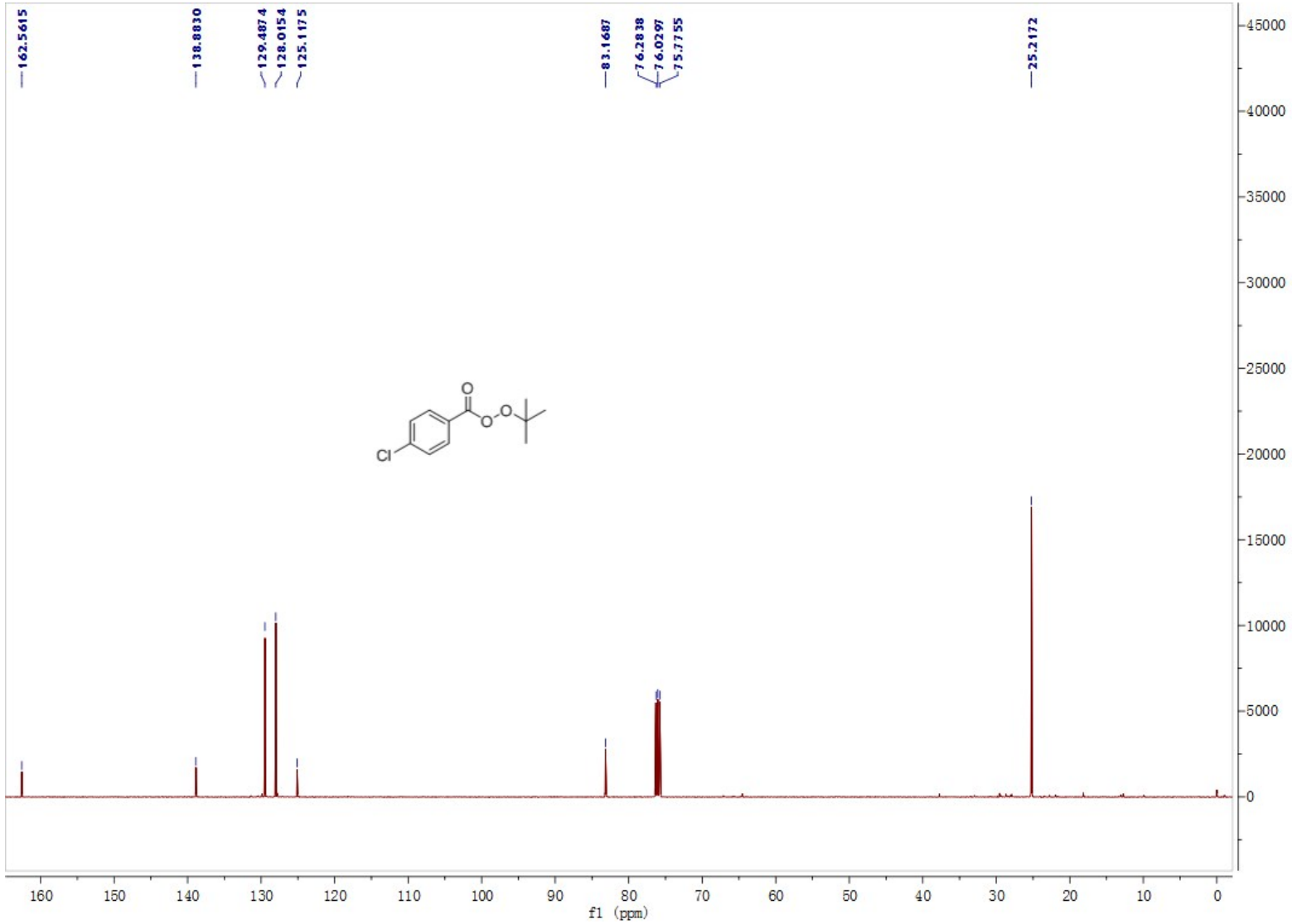
132.8550
131.0306
130.8408
128.5404
126.7789
84.2165
77.3199
77.0655
76.8113
26.2988
O
O
O
Cl
40000
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.8283
7.8109
7.3720
7.3547
1.3373
1.96
2.04
9.44
Cl
O
O
O
f1 (ppm)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129.4874
128.0154
125.1175
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76.2838
76.0297
75.7755
25.2172
Cl
O
O
O
45000
40000
35000
30000
25000
20000
15000
10000
5000
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150
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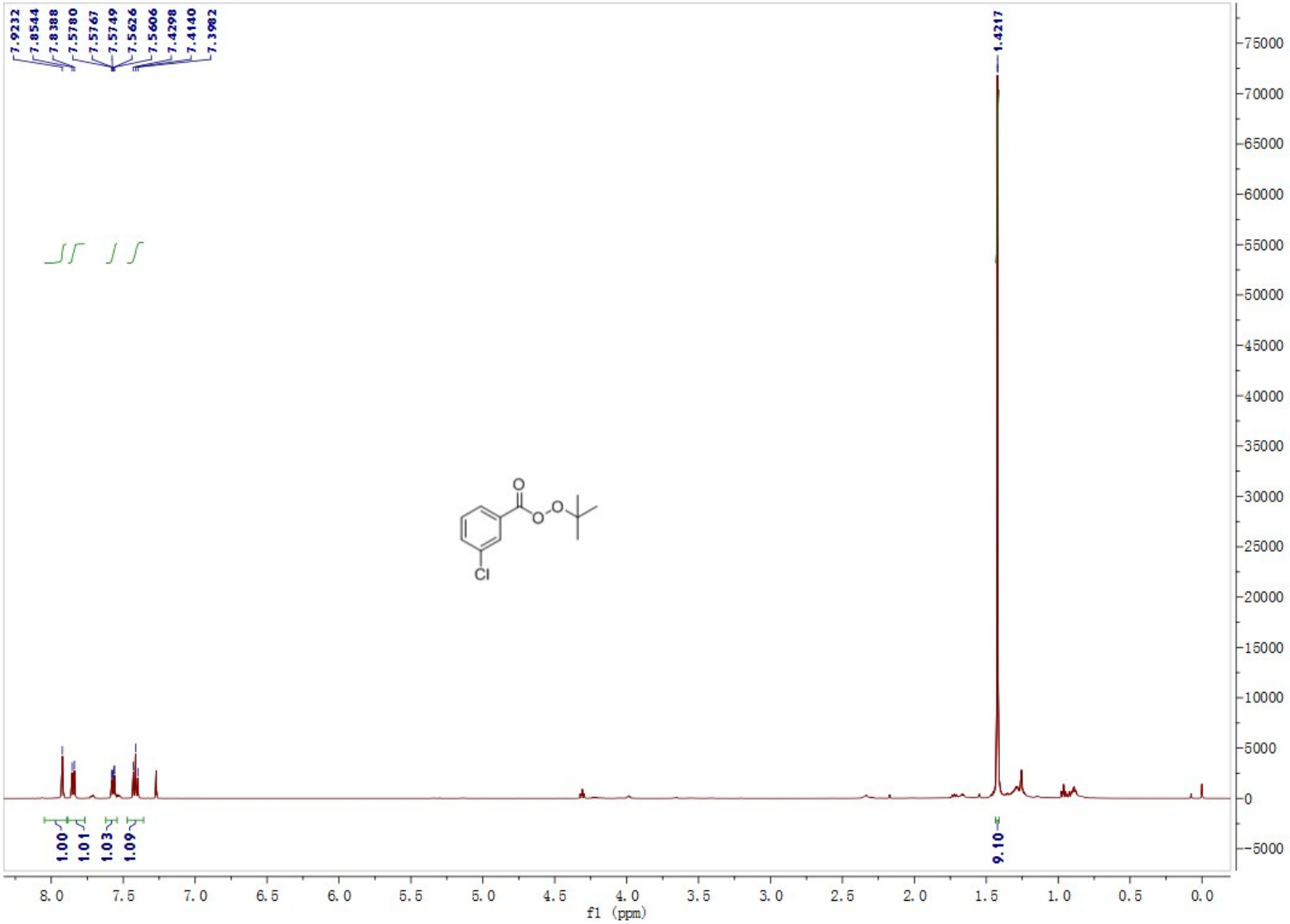
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.8388
7.5780
7.5767
7.5749
7.5626
7.5606
7.4298
7.4140
7.3982
1.4217
O
O
O
Cl
1.00
1.01
1.03
1.09
9.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
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10000
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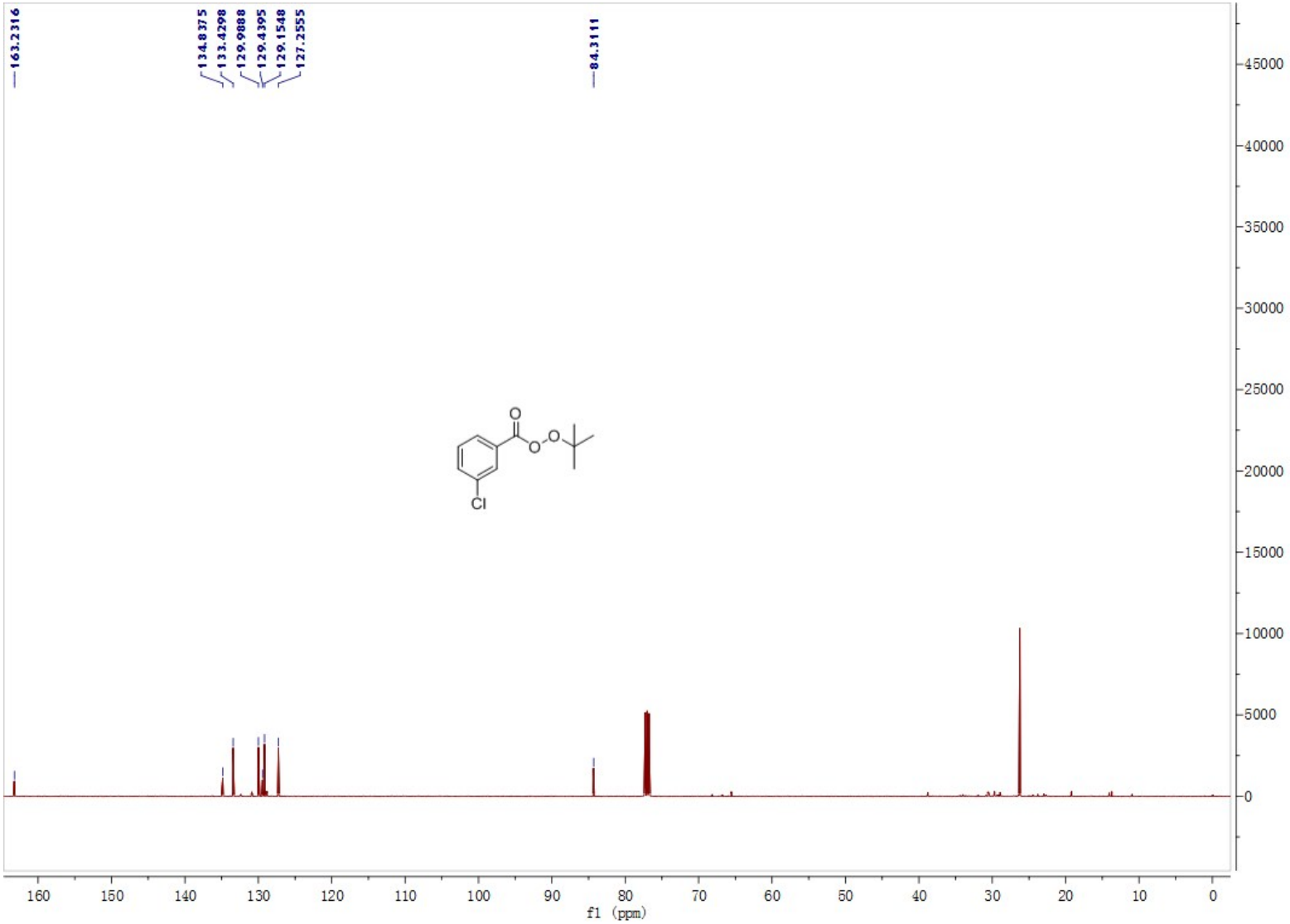
0
-5000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133.4298
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129.4395
129.1548
127.2555
84.3111
O
O
O
Cl
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
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150
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130
120
110
100
90
80
70
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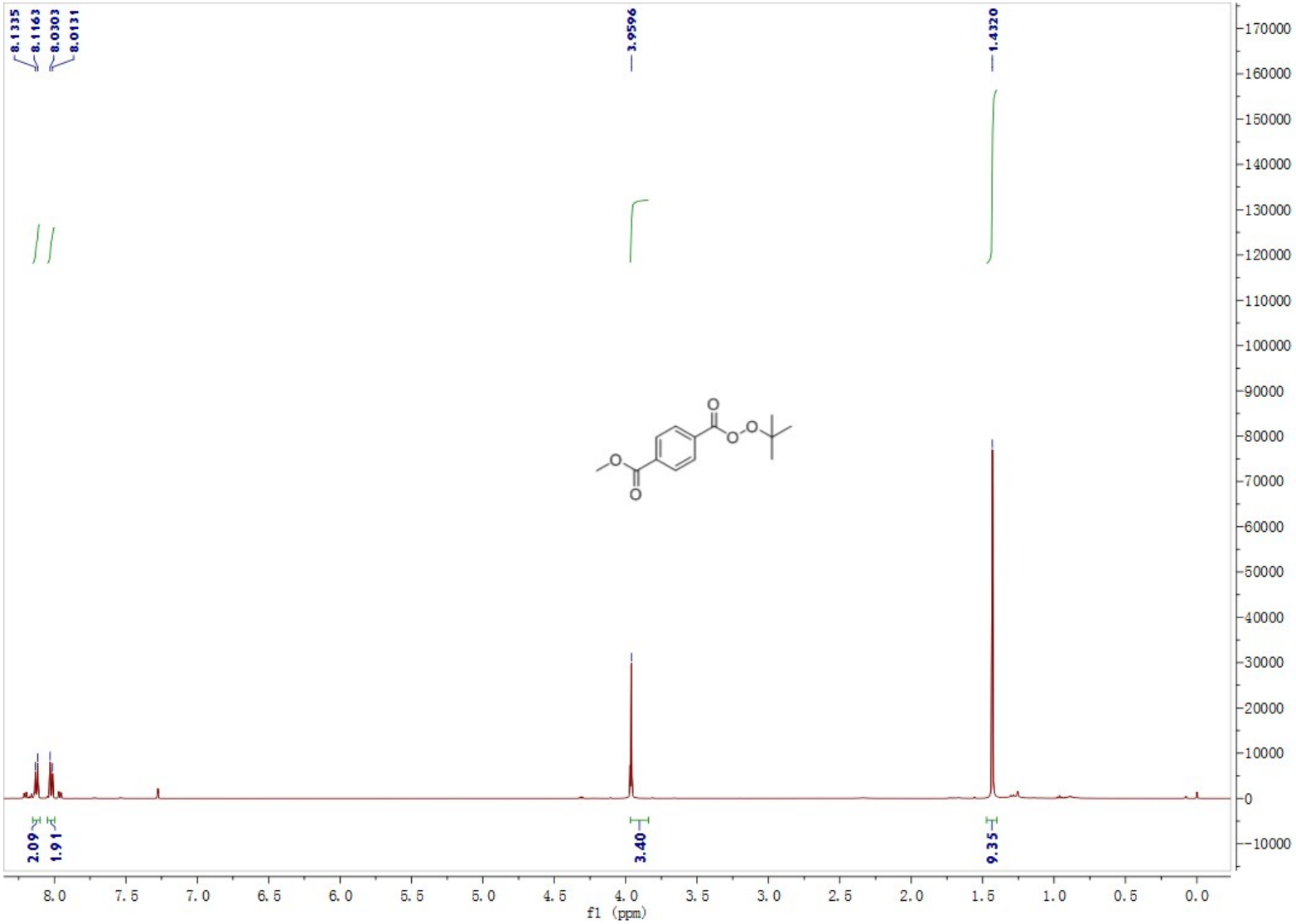
50
40
30
20
10
0
f1 (ppm)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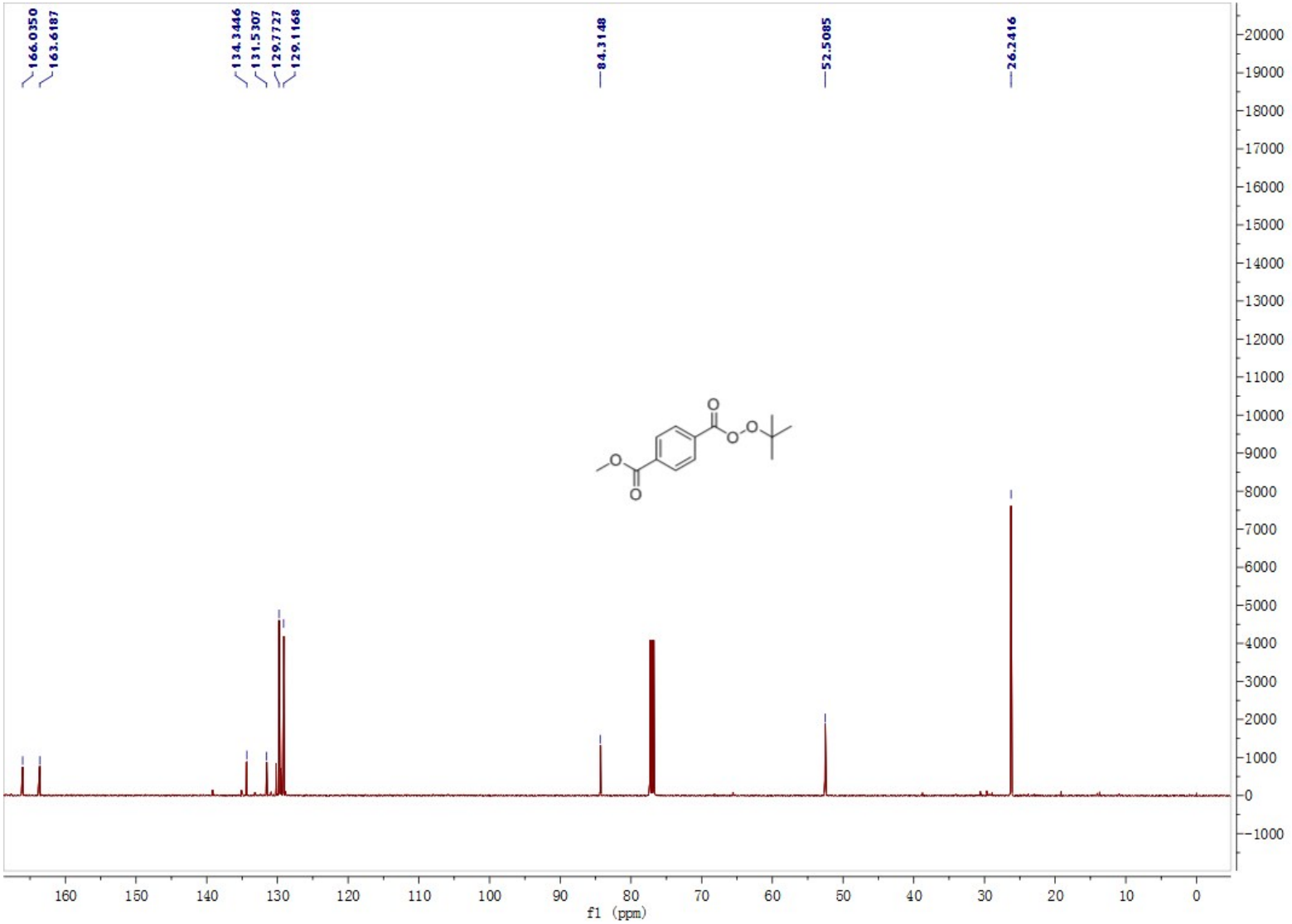
8.0303
8.0131
3.9596
1.4320
2.09
1.91
3.40
9.35
f1 (ppm)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131.5307
129.7727
129.1168
84.3148
52.5085
26.2416
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18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
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150
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130
120
110
100
90
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70
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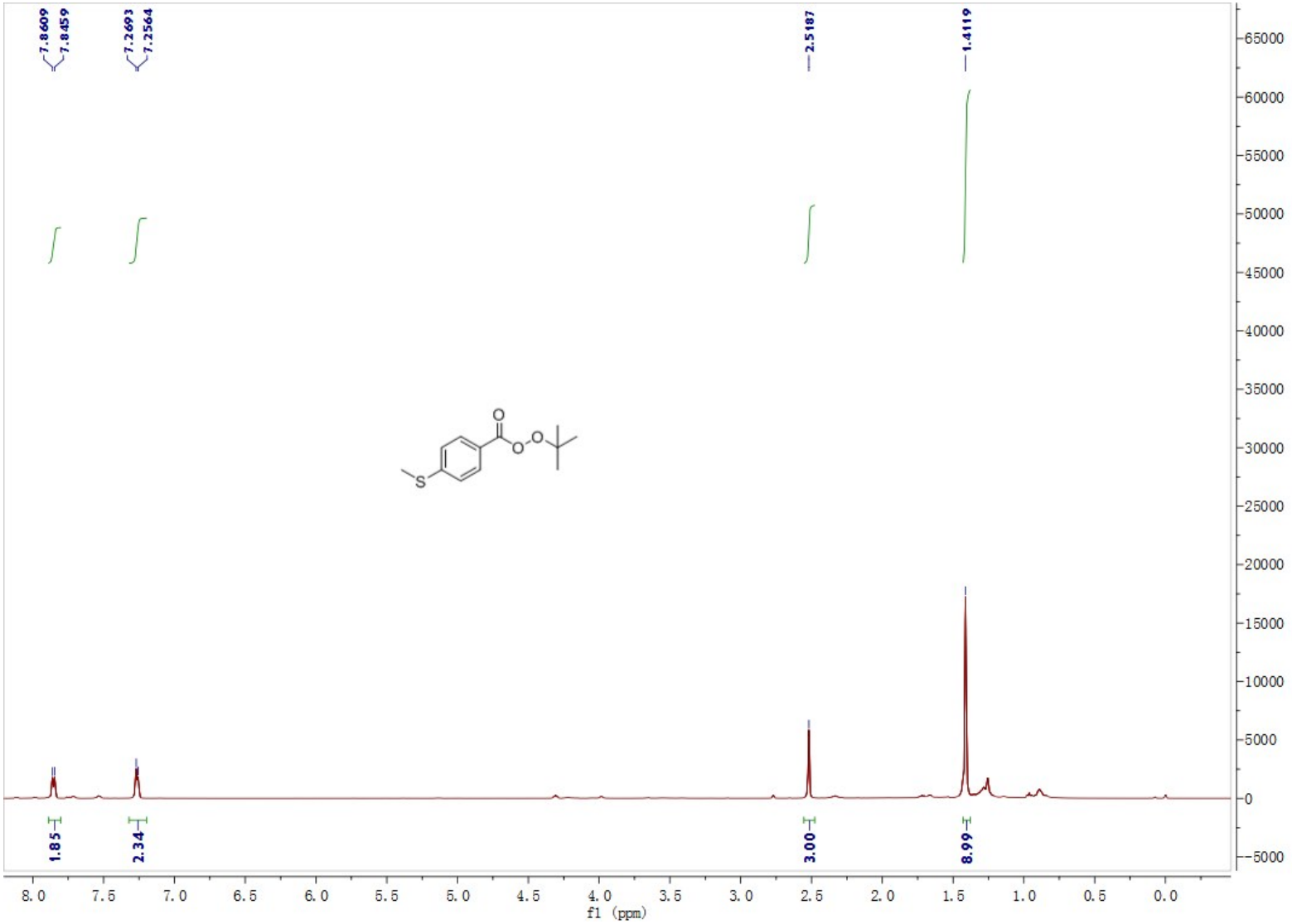
50
40
30
20
10
0
f1 (ppm)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7.8459
7.2693
7.2564
2.5187
1.4119
O
O
O
S
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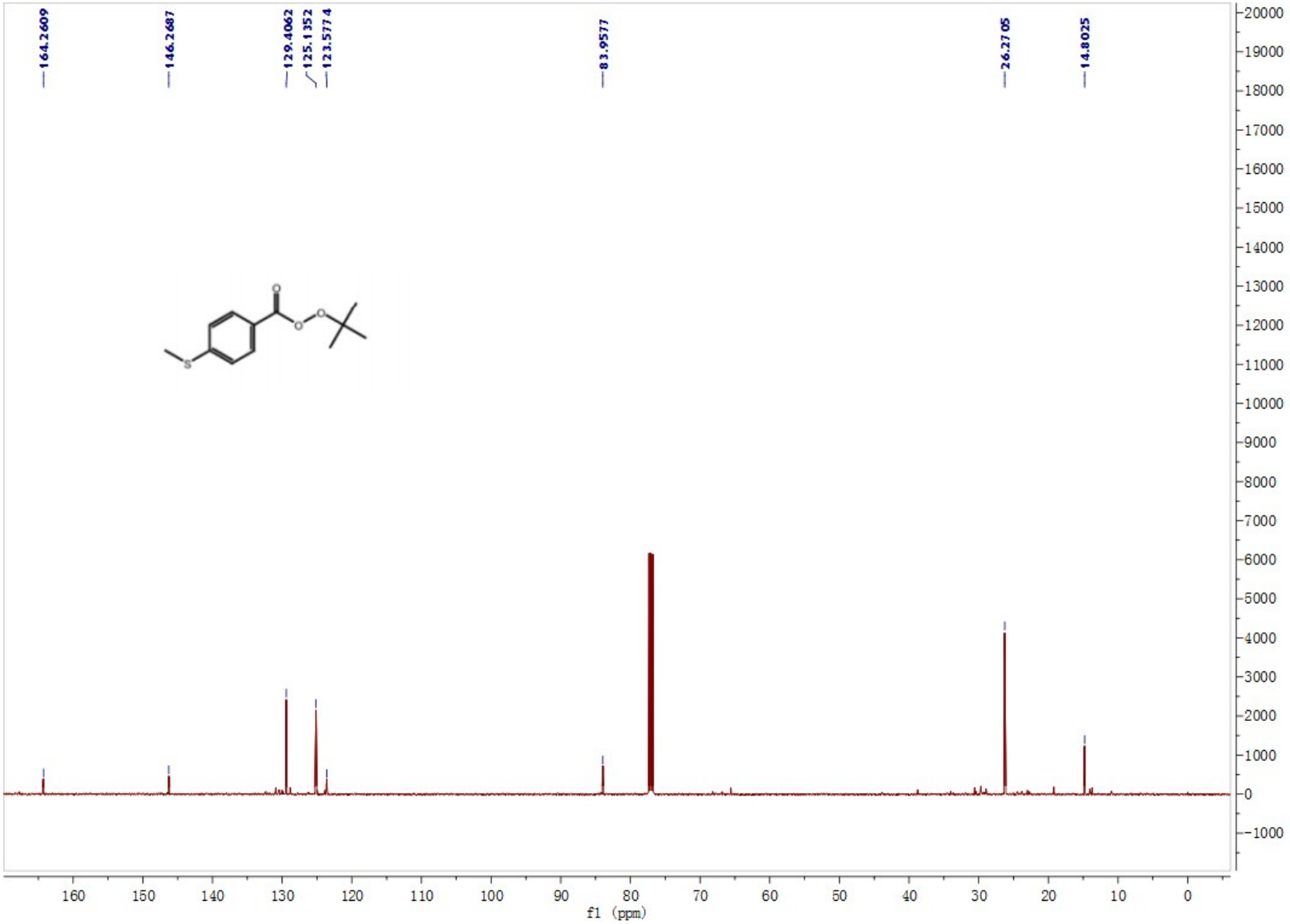
2.34
3.00
8.99
f1 (ppm)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14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
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130
120
110
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90
80
70
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50
40
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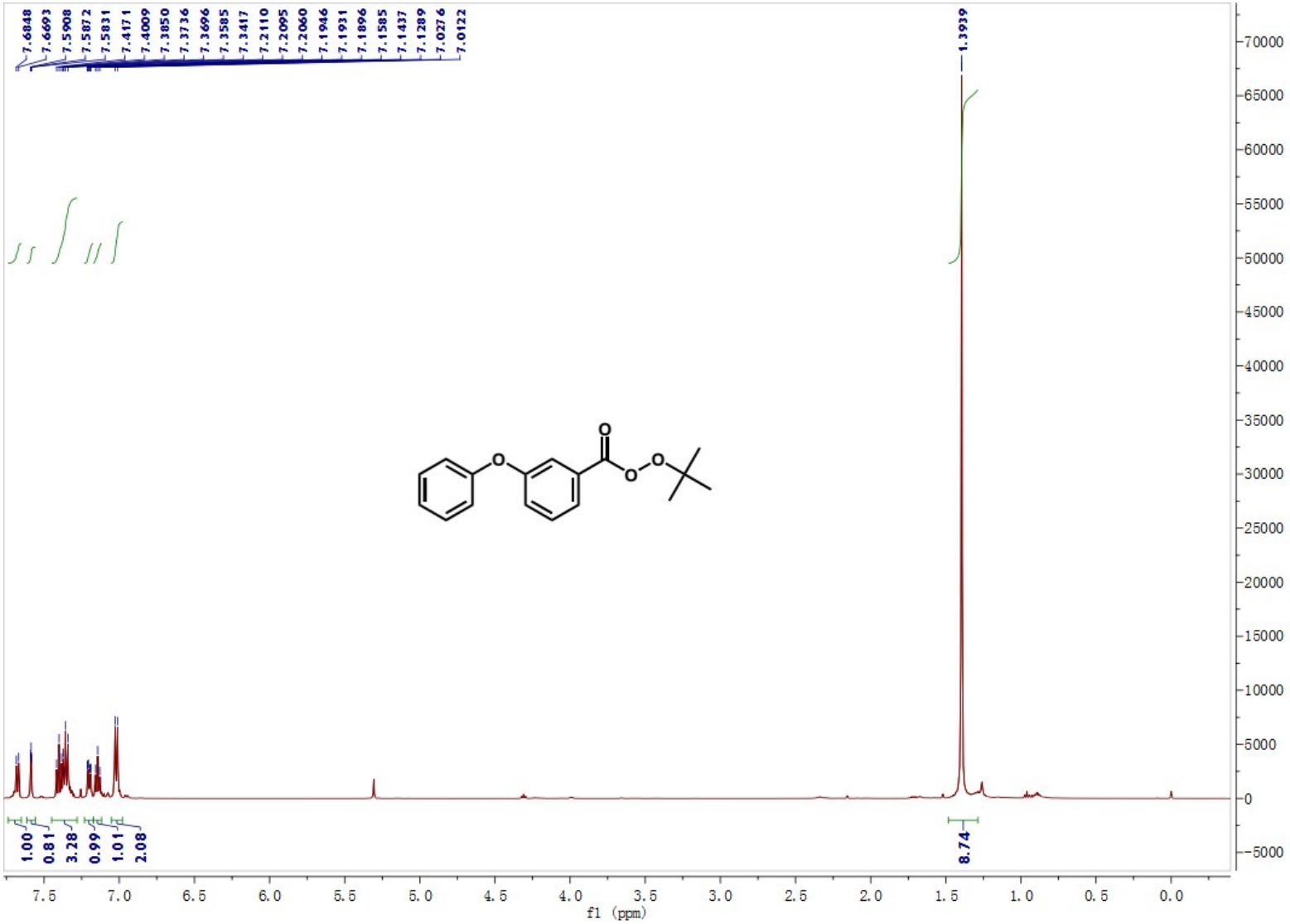
10
0
f1 (ppm)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7.5872
7.5831
7.4171
7.4009
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7.3736
7.3696
7.3585
7.3417
7.2110
7.2095
7.2060
7.1946
7.1931
7.1896
7.1585
7.1437
7.1289
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1.3939
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3.28
0.99
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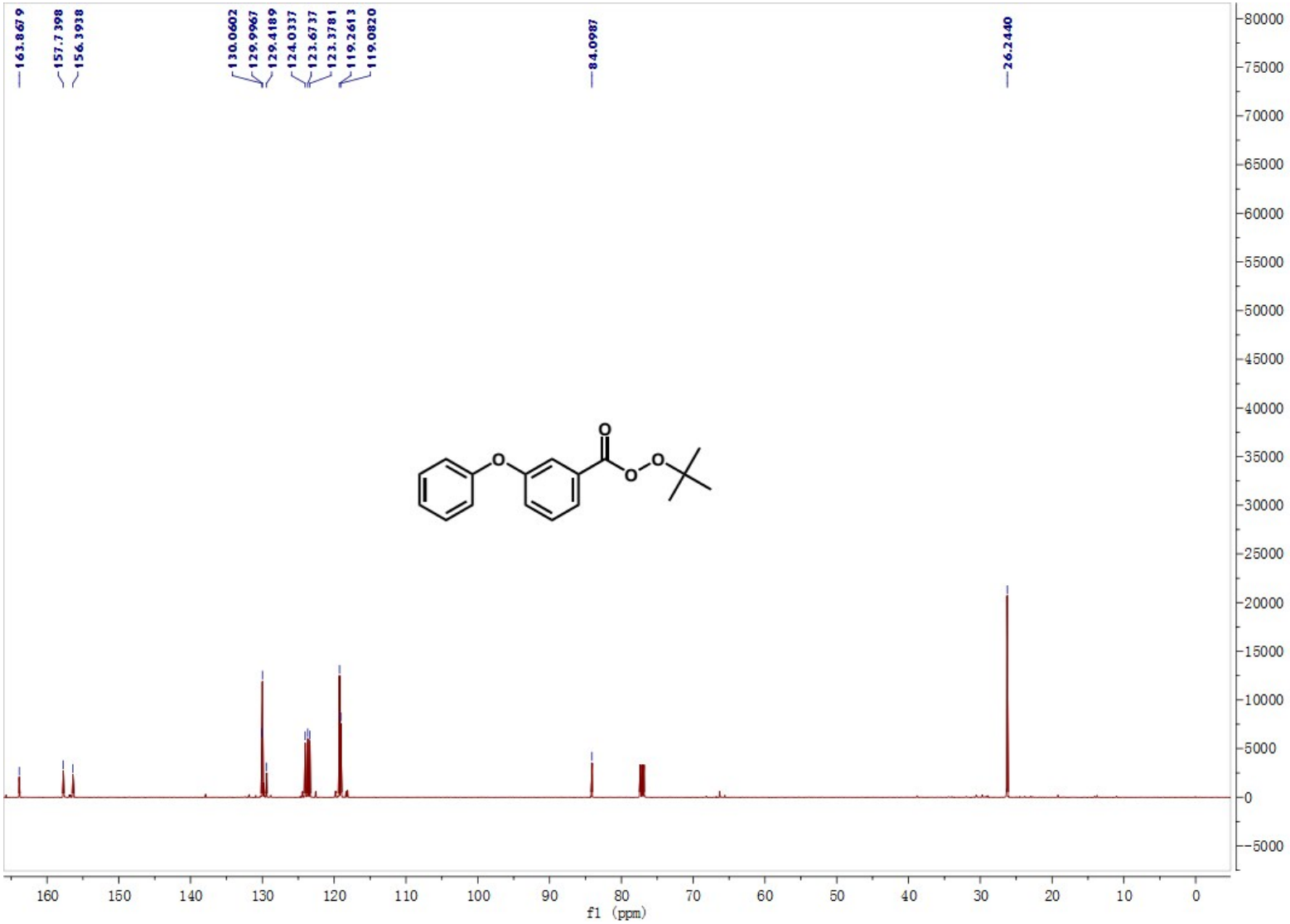
2.08
8.74
f1 (ppm)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80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
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120
110
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90
80
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50
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10
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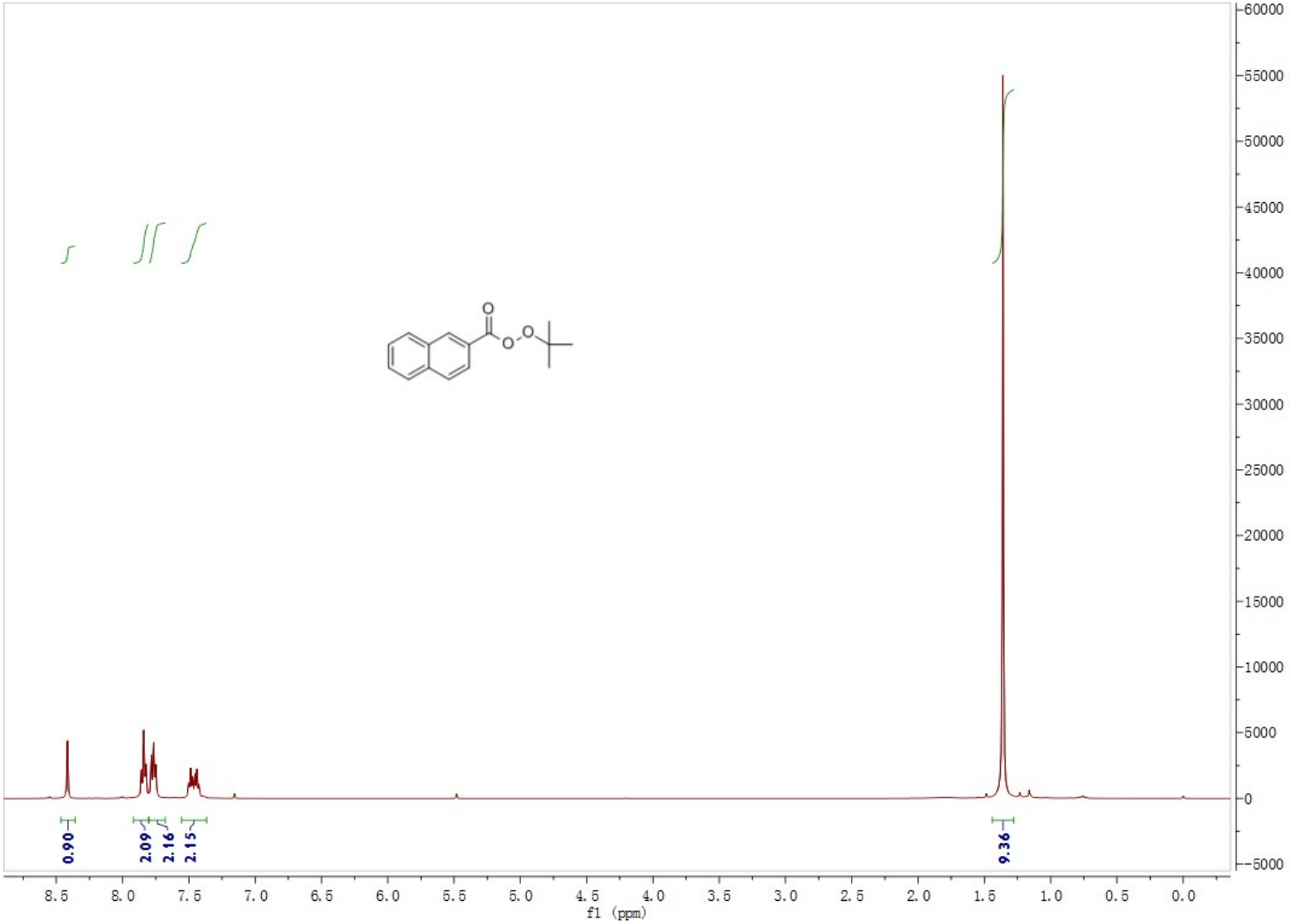
f1 (ppm)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30000
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15000
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5000
0
-5000
0.90
2.09
2.16
2.15
9.36
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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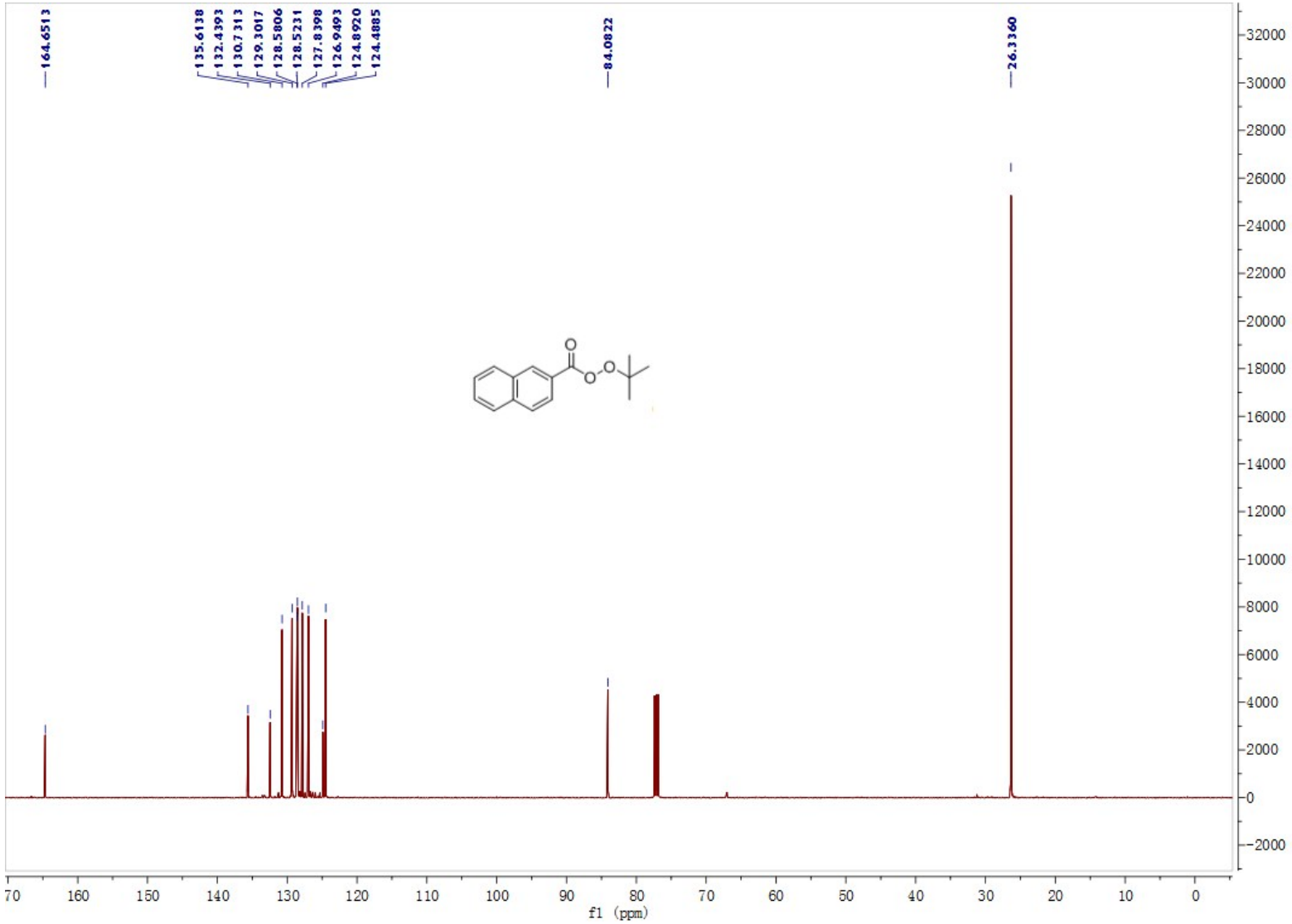
0.0
f1 (ppm)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128.5231
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126.9493
124.8920
124.4885
84.0822
26.3360
O
O
O
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
70
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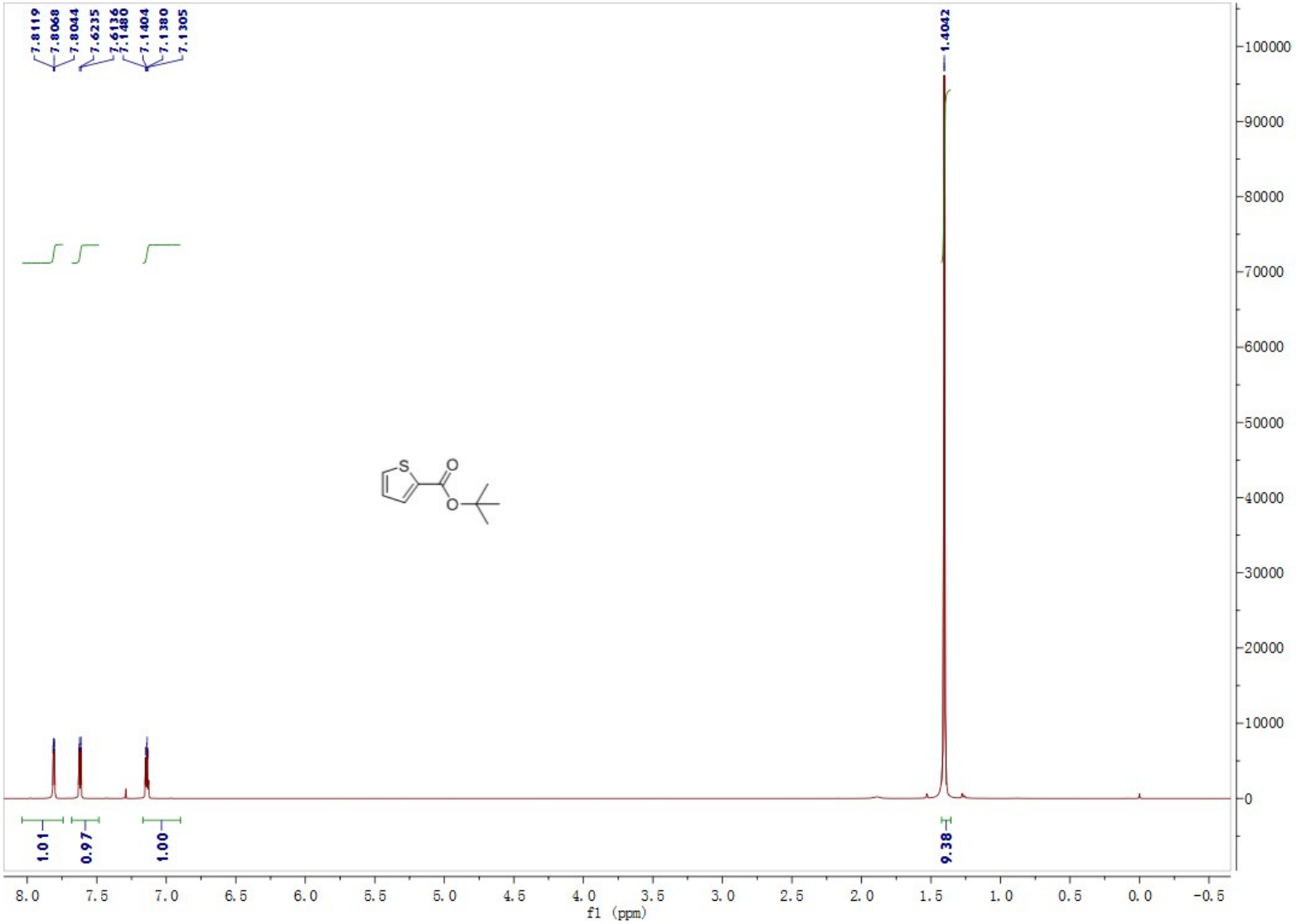
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6136
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7.1404
7.1380
7.1305
1.4042
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O
O
1.01
0.97
1.00
9.38
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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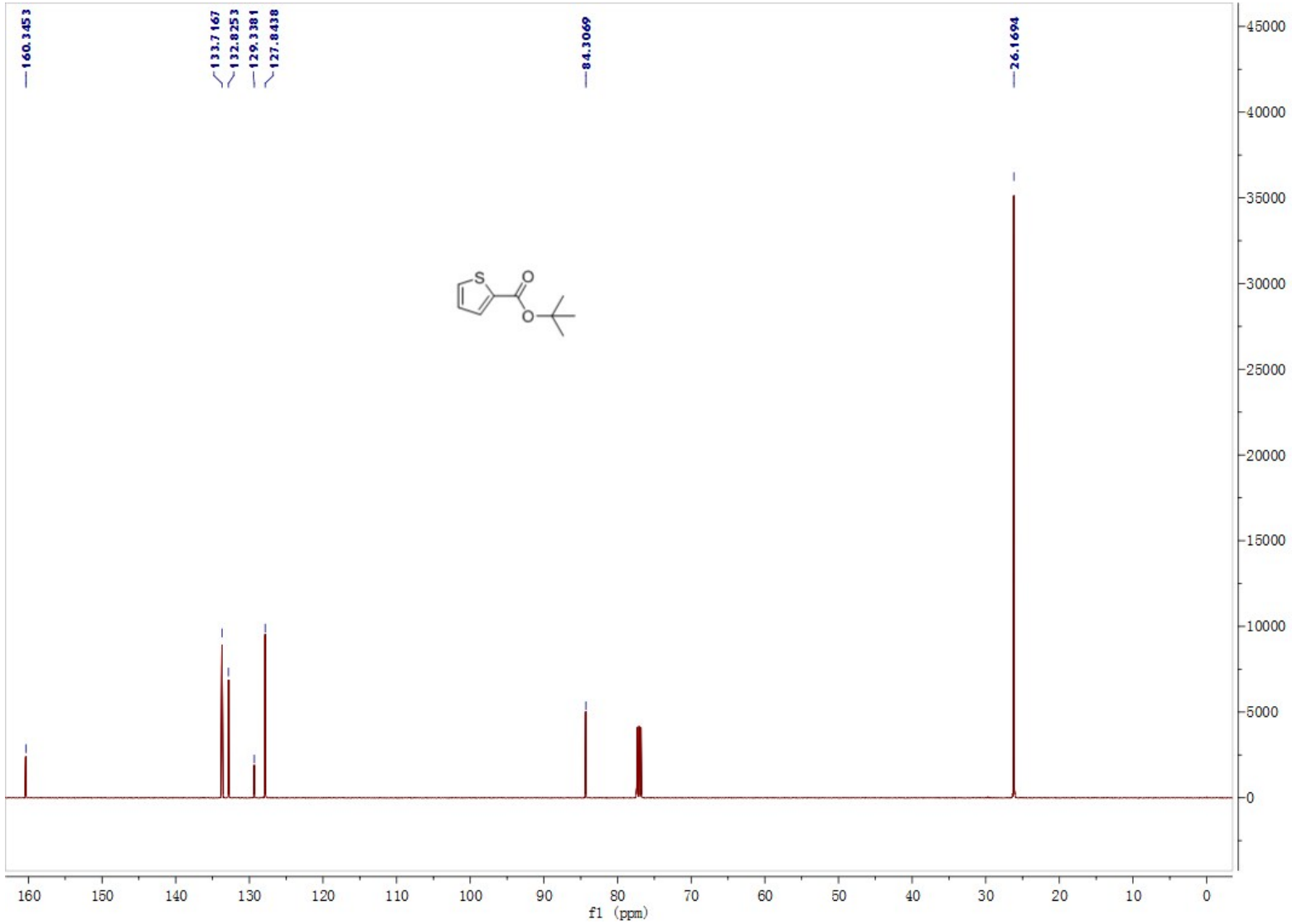
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


160.3453
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132.8253
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127.8438
84.3069
26.1694
S
O
O
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40000
35000
30000
25000
20000
15000
10000
5000
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110
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90
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70
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50
40
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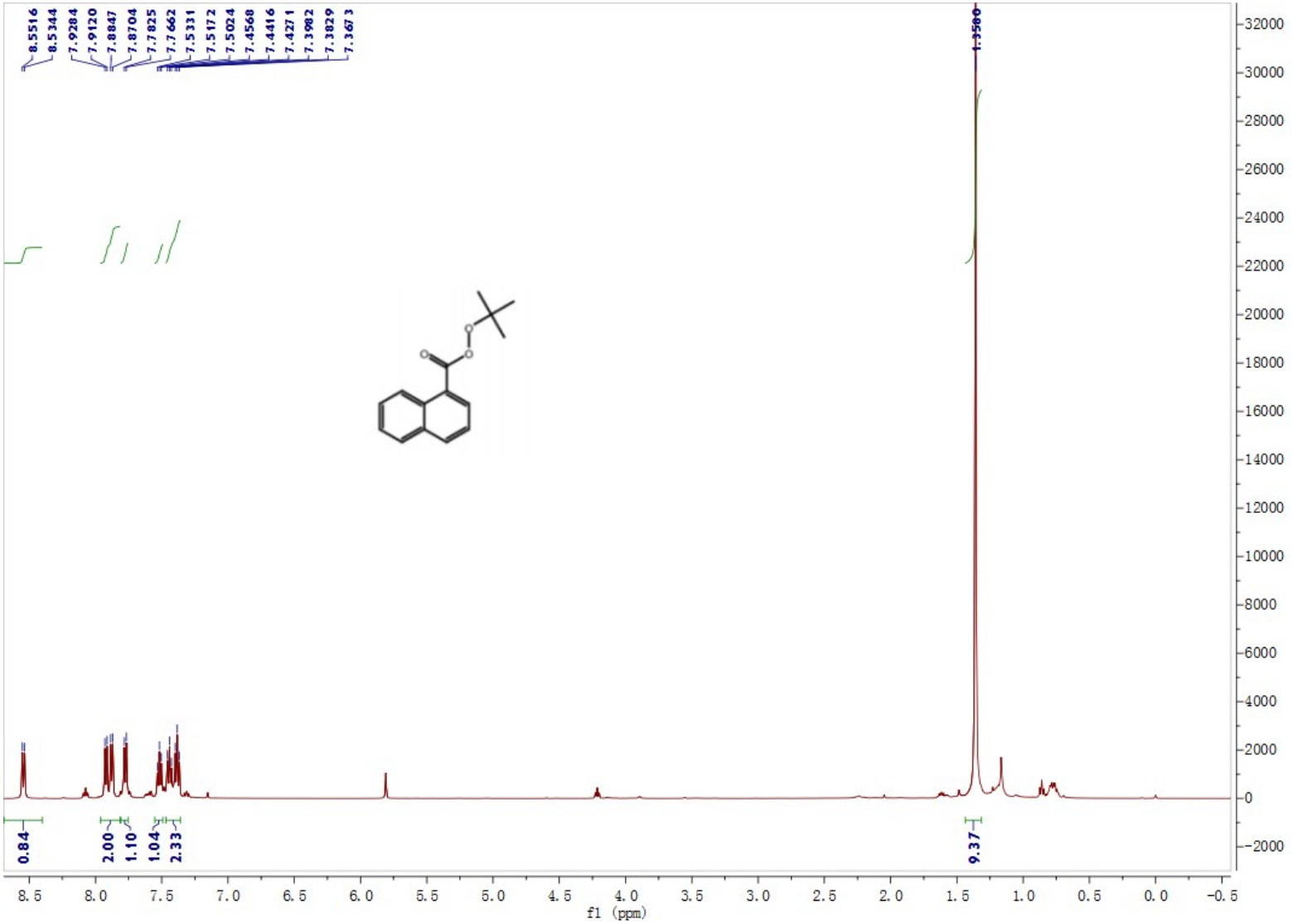
20
10
0
f1 (ppm)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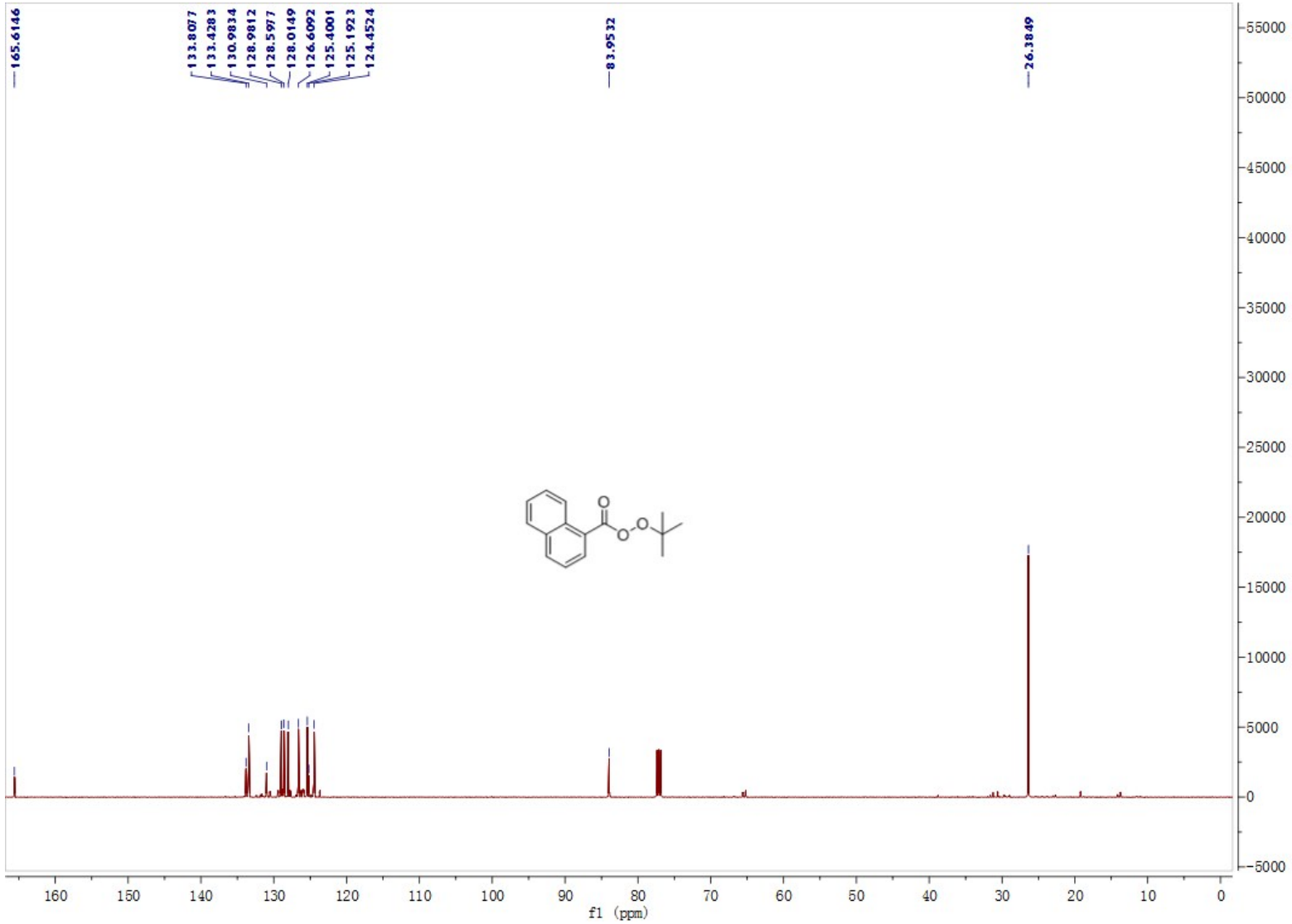
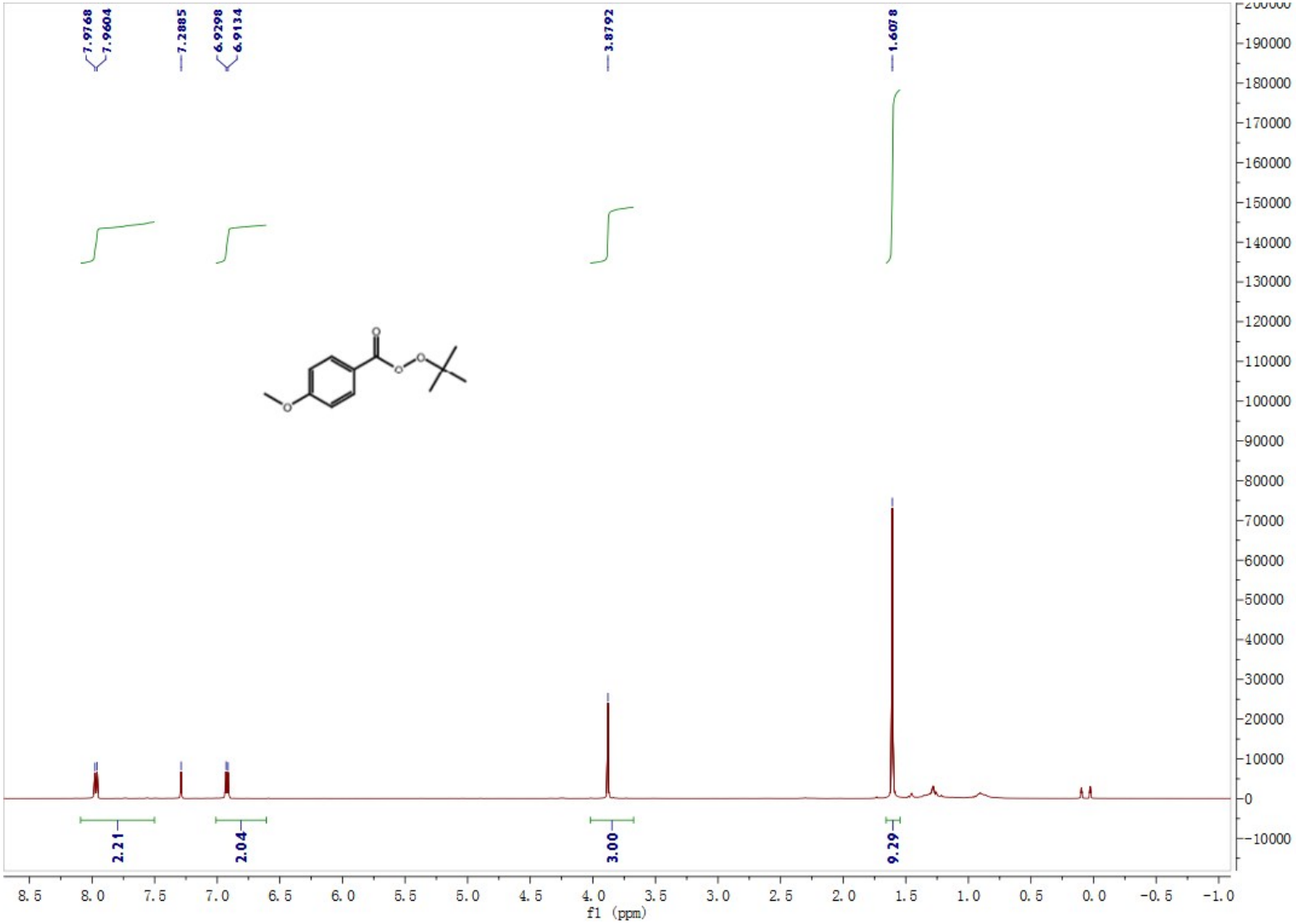
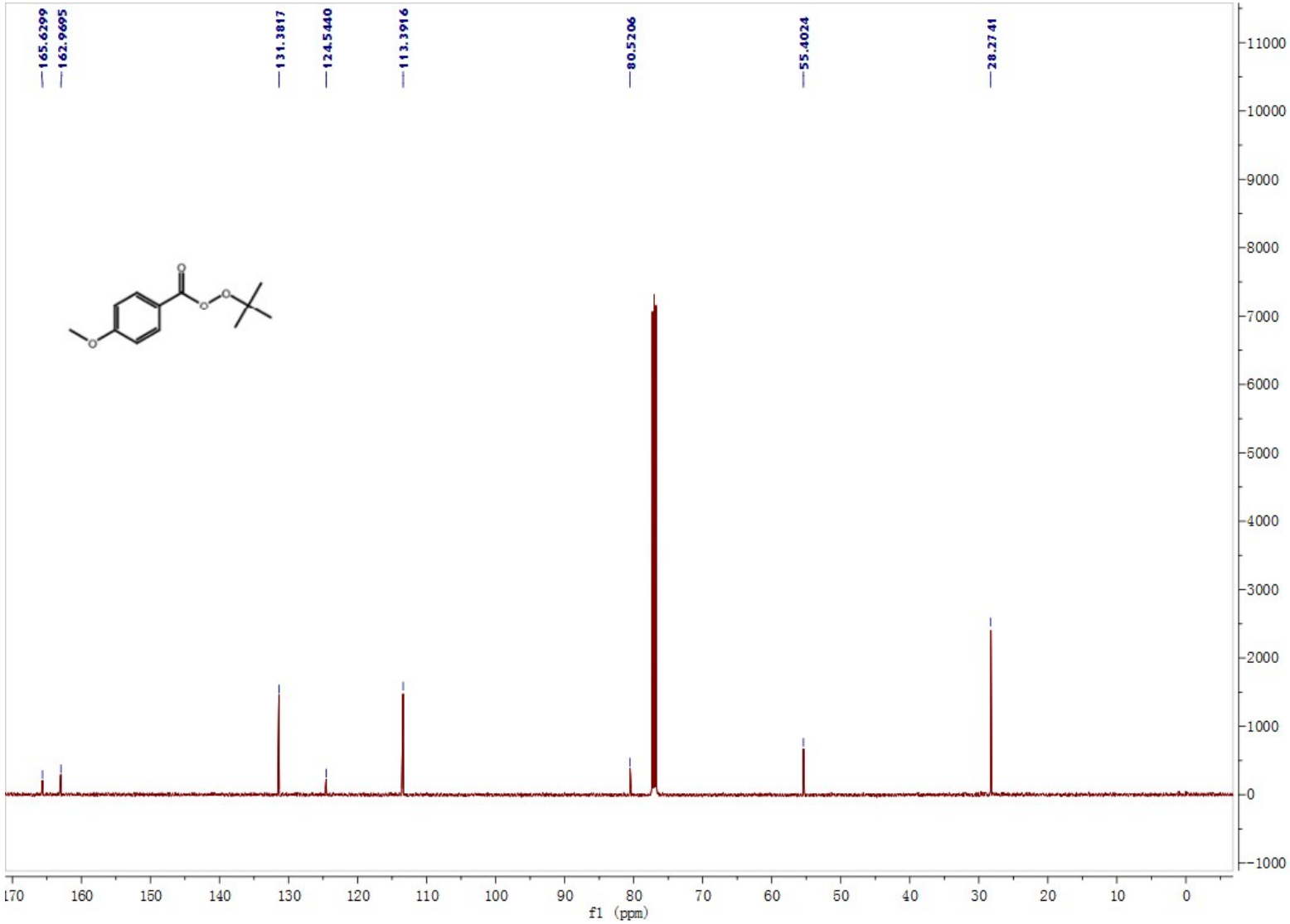
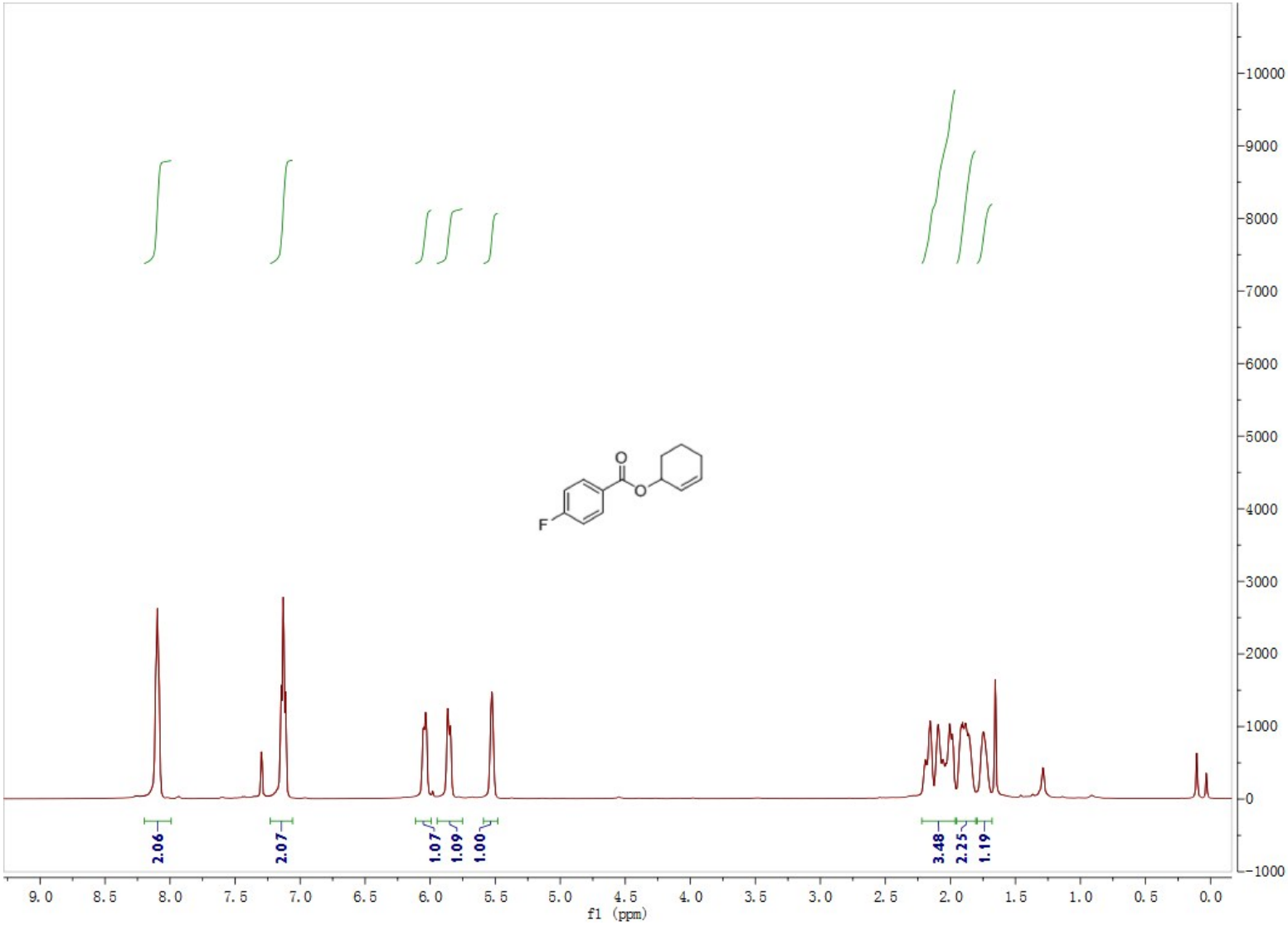
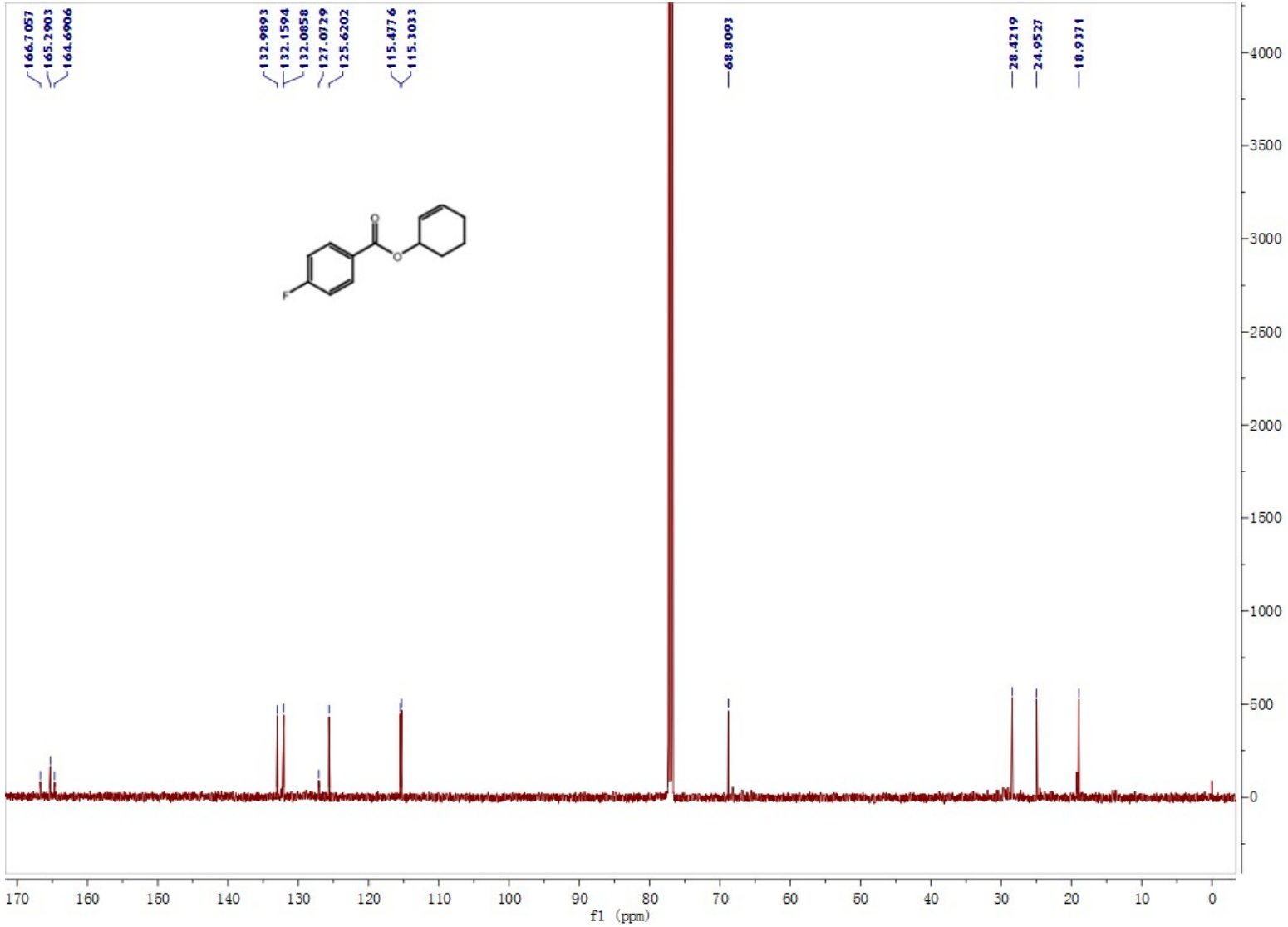
7.7825
7.7662
7.5331
7.5172
7.5024
7.4568
7.4416
7.4271
7.3982
7.3829
7.3673
1.3560
0.84
2.00
1.10
1.04
2.33
9.37
f1 (ppm)

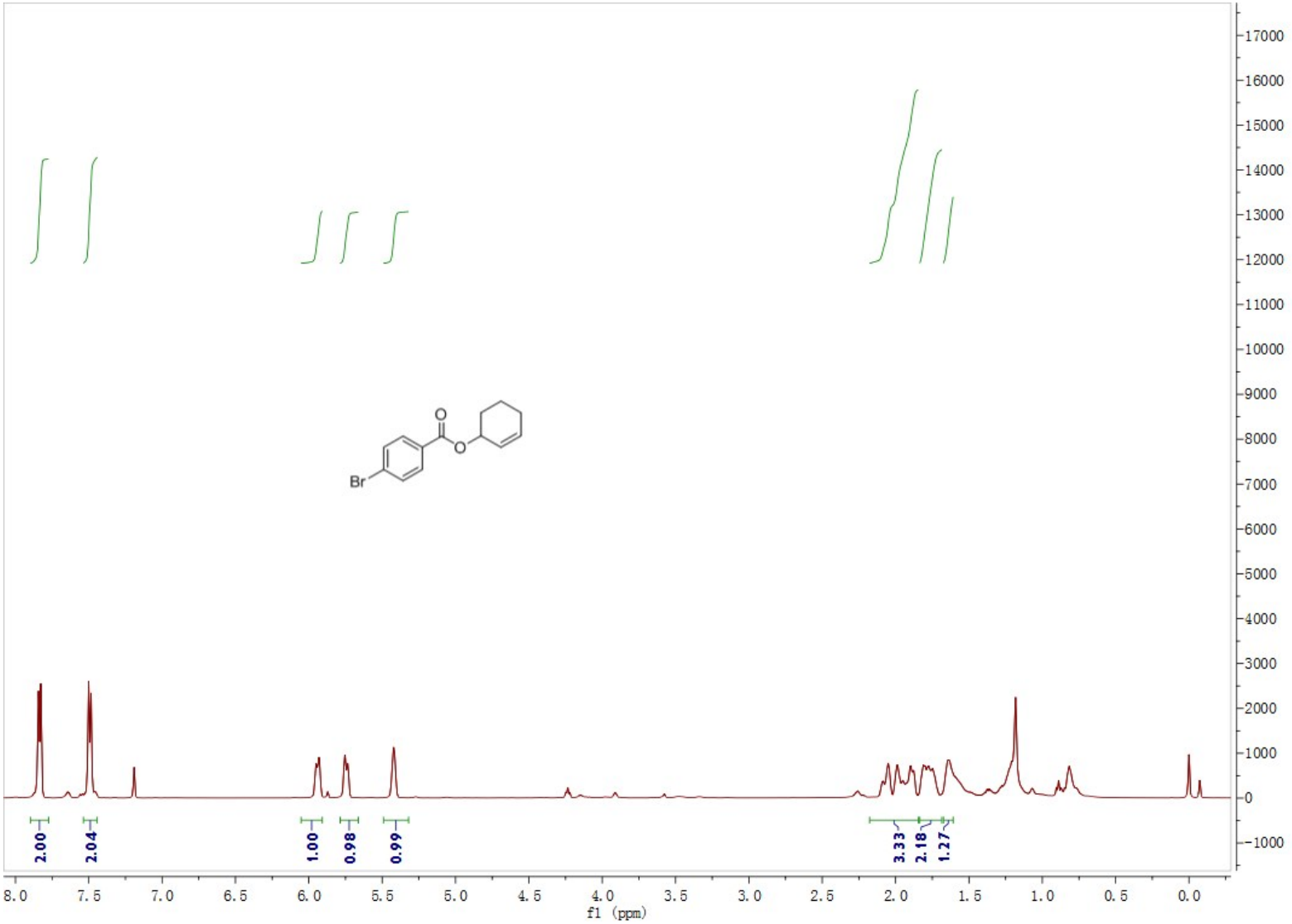

165.6146
133.8077
133.4283
130.9834
128.9812
128.5977
128.0149
126.6092
125.4001
125.1923
124.4524
83.9532
26.3849
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

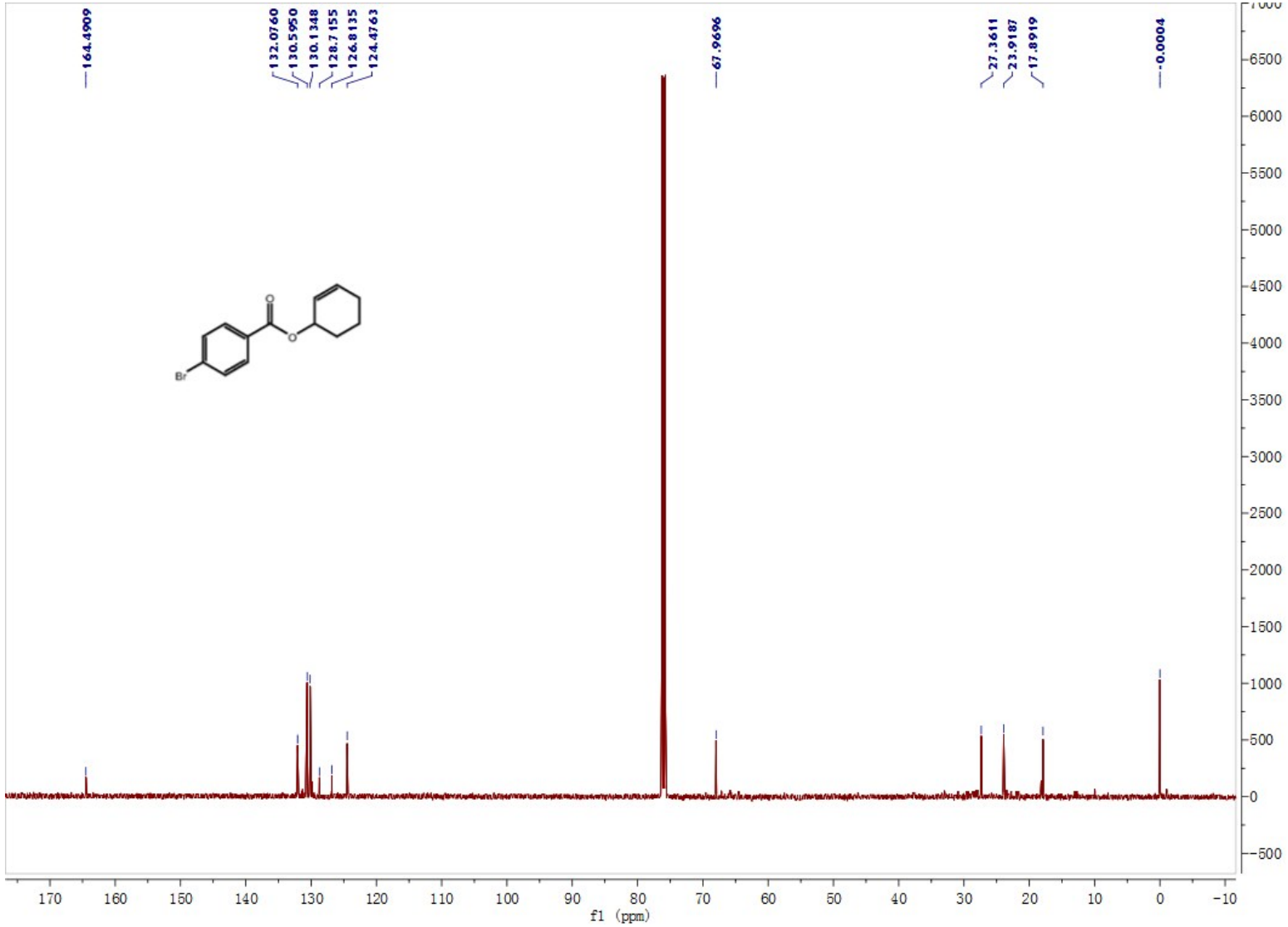

7.9768
7.9604
7.2885
6.9298
6.9134
3.8792
1.6078
2.21
2.04
3.00
9.29
f1 (ppm)

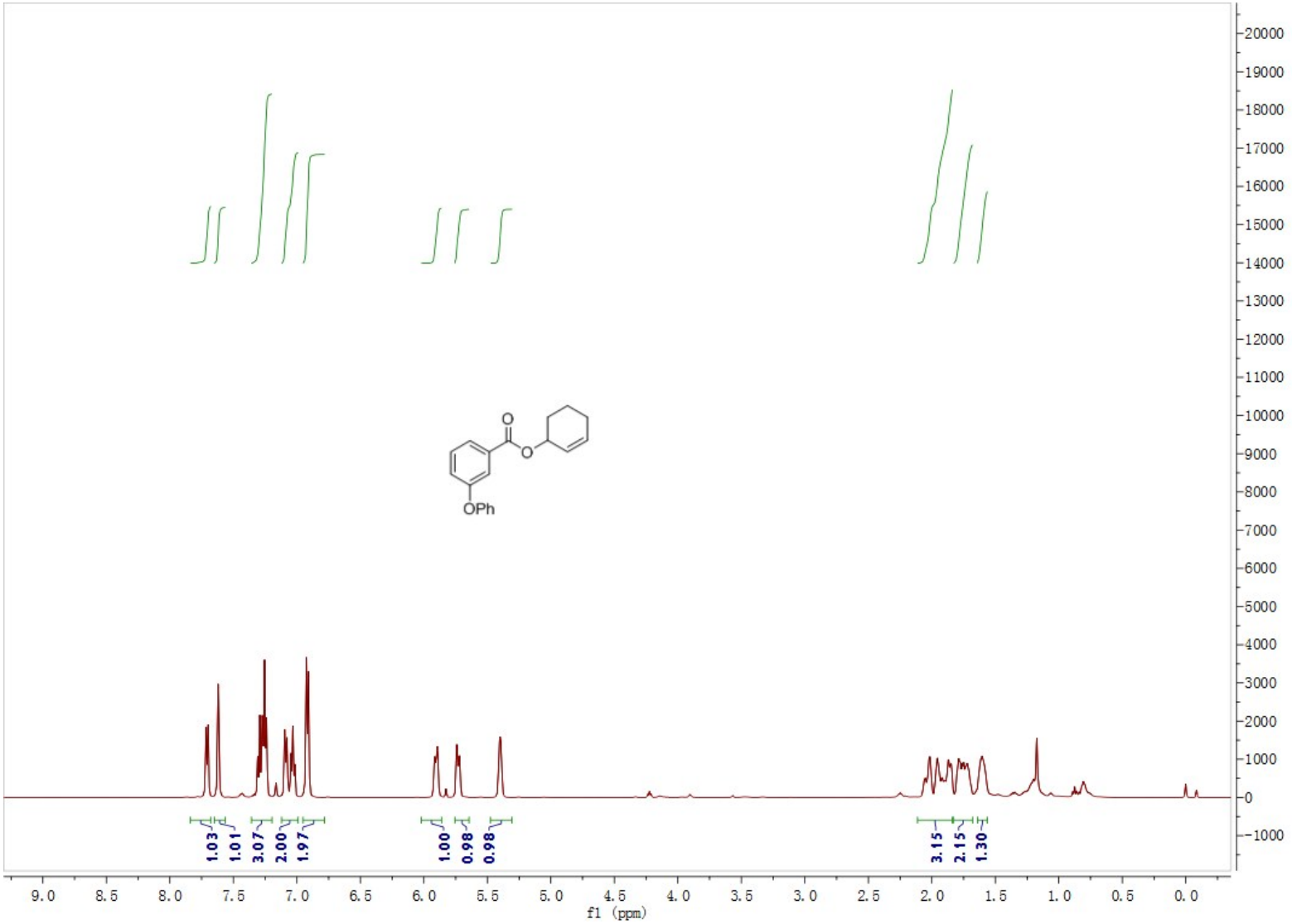

165.6299
162.9695
131.3817
124.5440
113.3916
80.5206
55.4024
28.2741
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

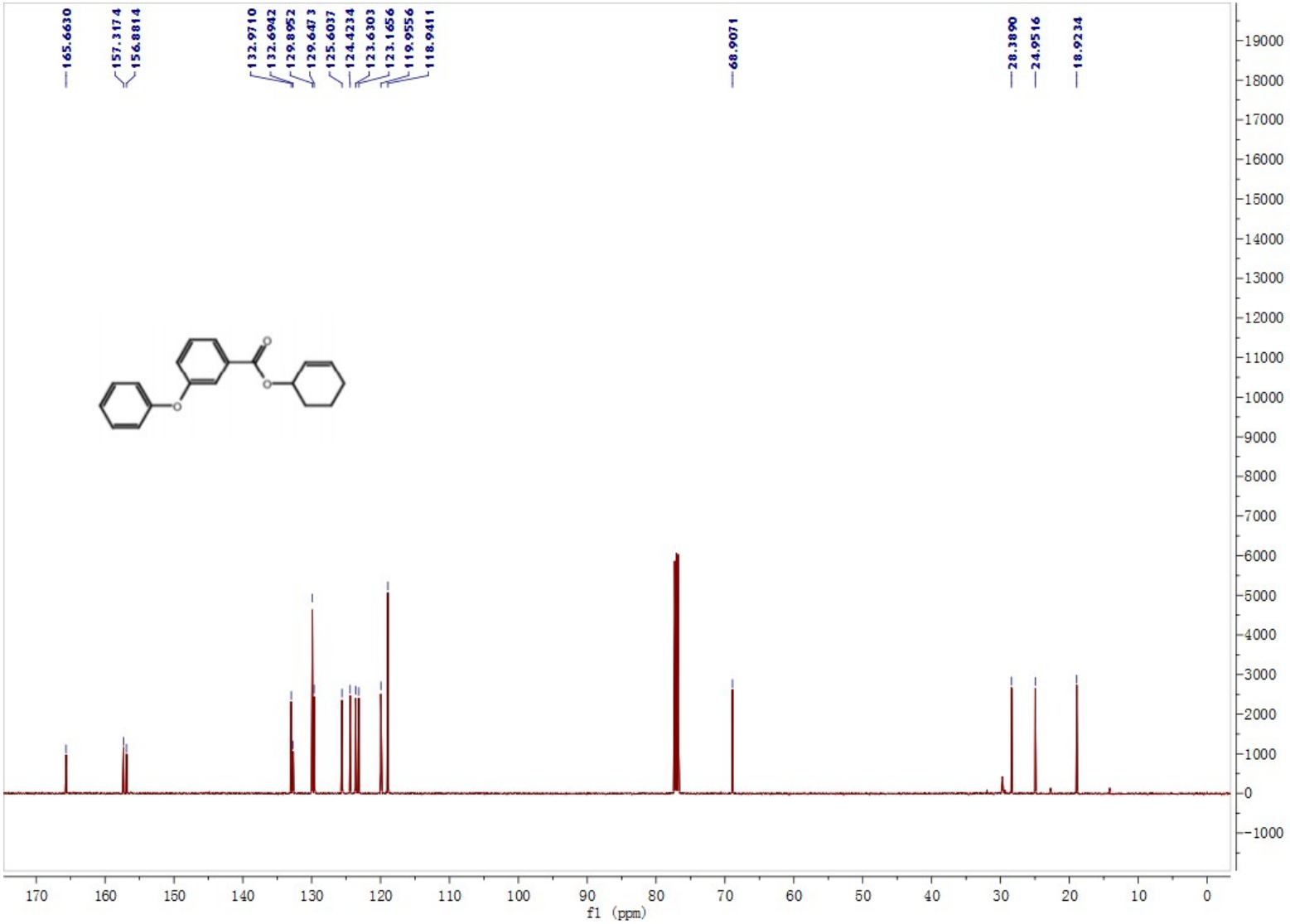

10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
O
O
F
2.06
2.07
1.07
1.09
1.00
3.48
2.25
1.19
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

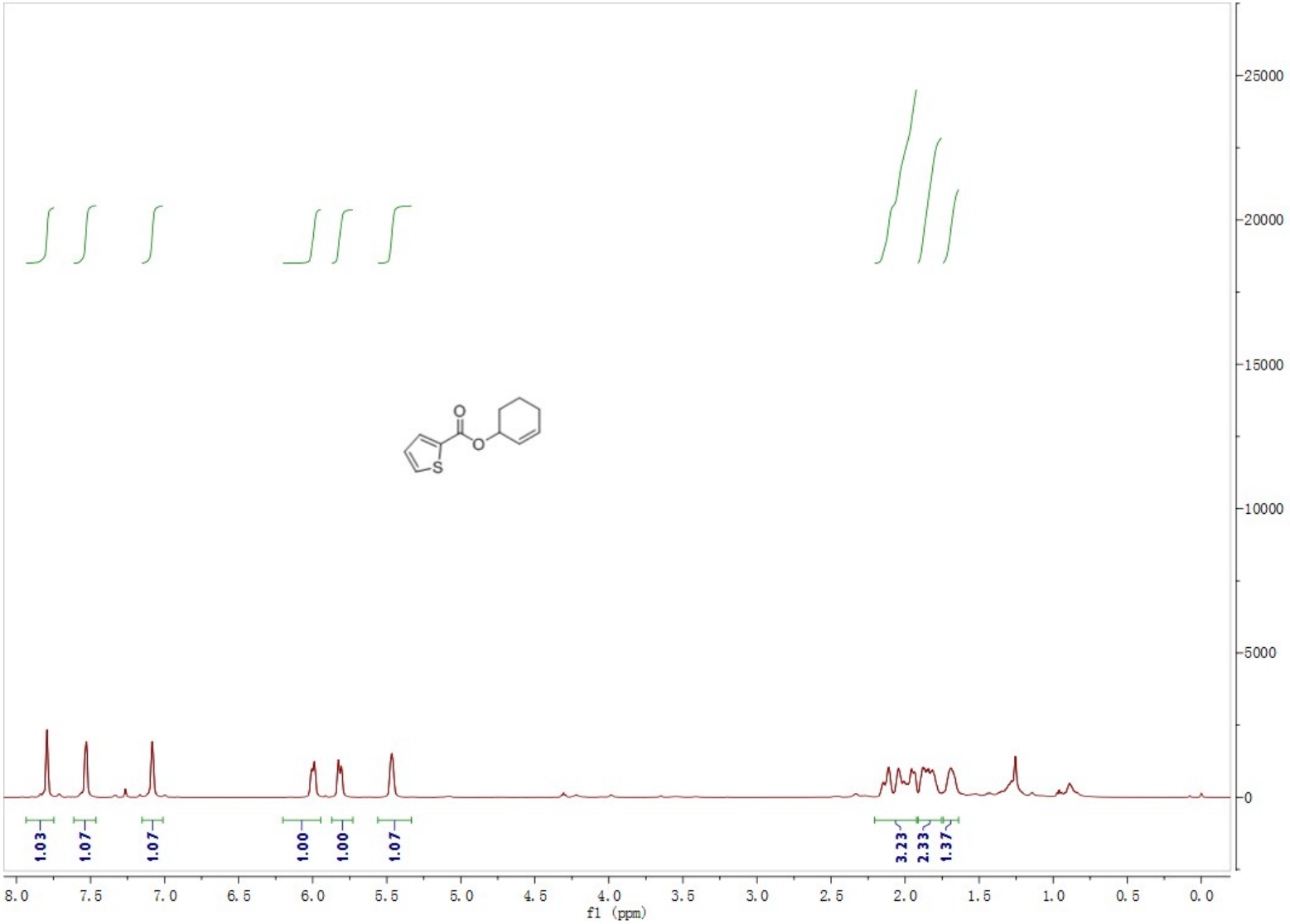

166.7057
165.2903
164.6906
132.9893
132.1594
132.0858
127.0729
125.6202
115.4776
115.3033
68.8093
28.4219
24.9527
18.9371
F
O
O
4000
3500
3000
2500
2000
1500
1000
500
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

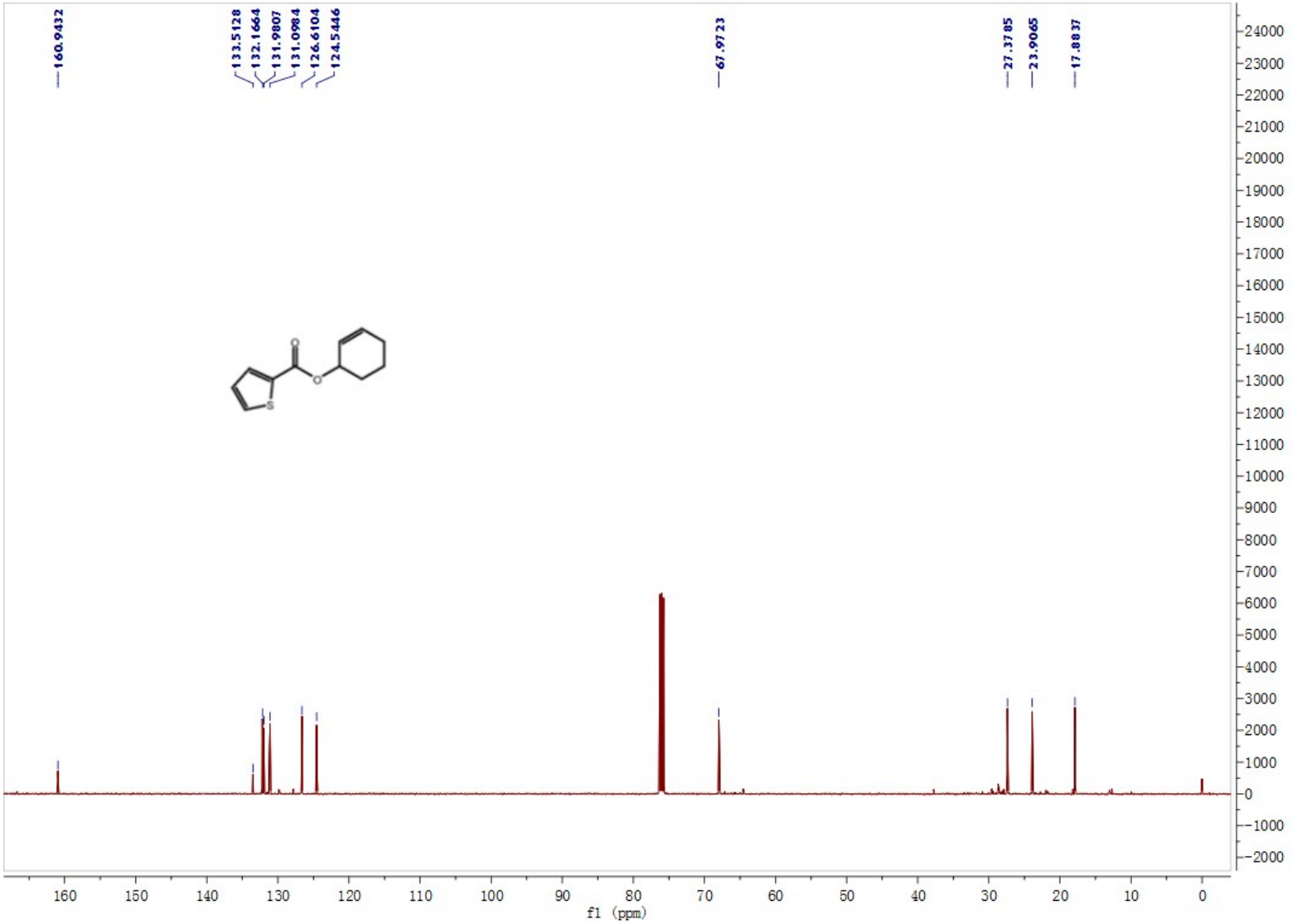

Br
O
O
2.00
2.04
1.00
0.98
0.99
3.33
2.18
1.27
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000

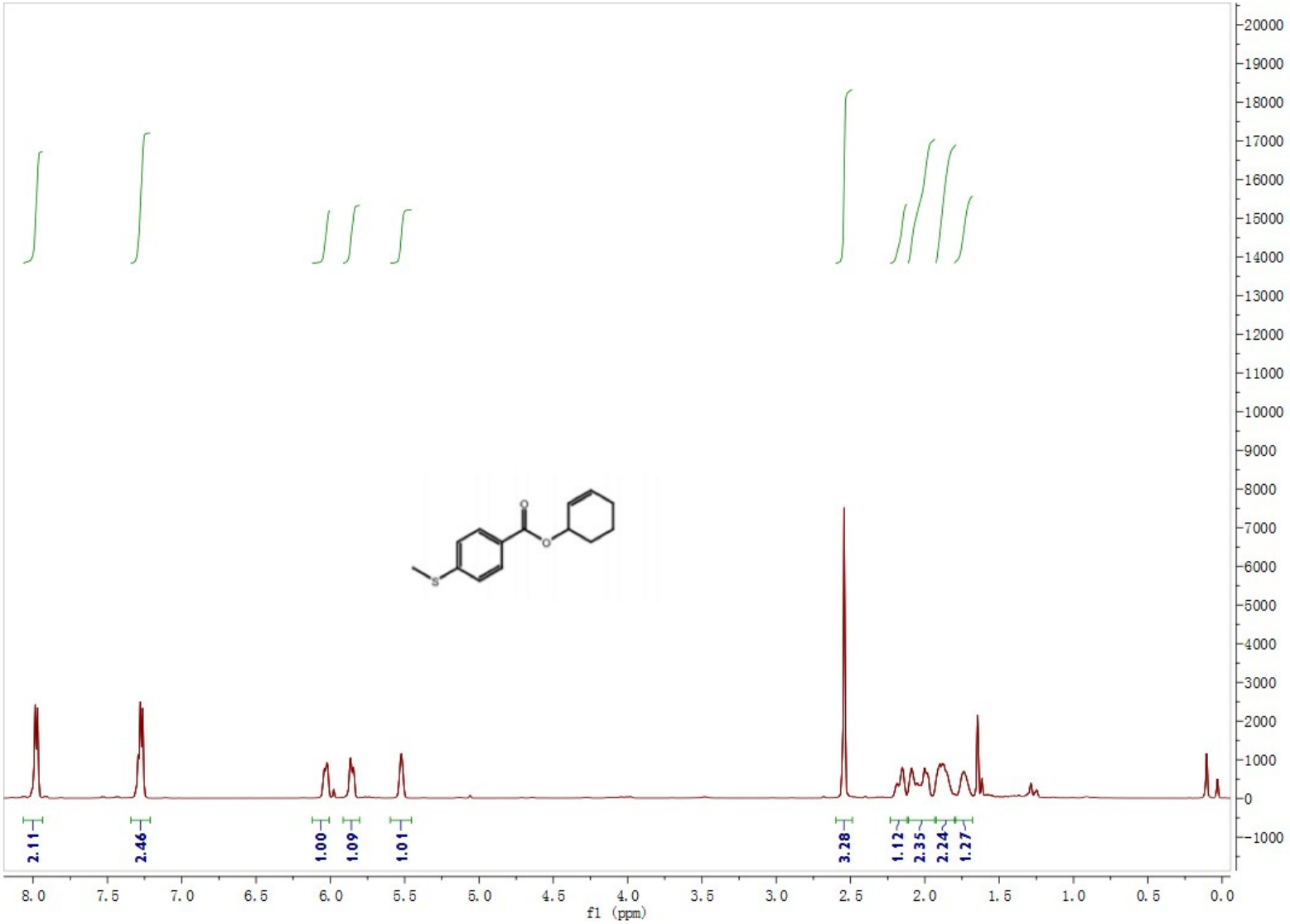

164.4909
132.0760
130.5950
130.1348
128.7155
126.8135
124.4763
67.9696
27.3611
23.9187
17.8919
-0.0004
Br
O
O
f1 (ppm)

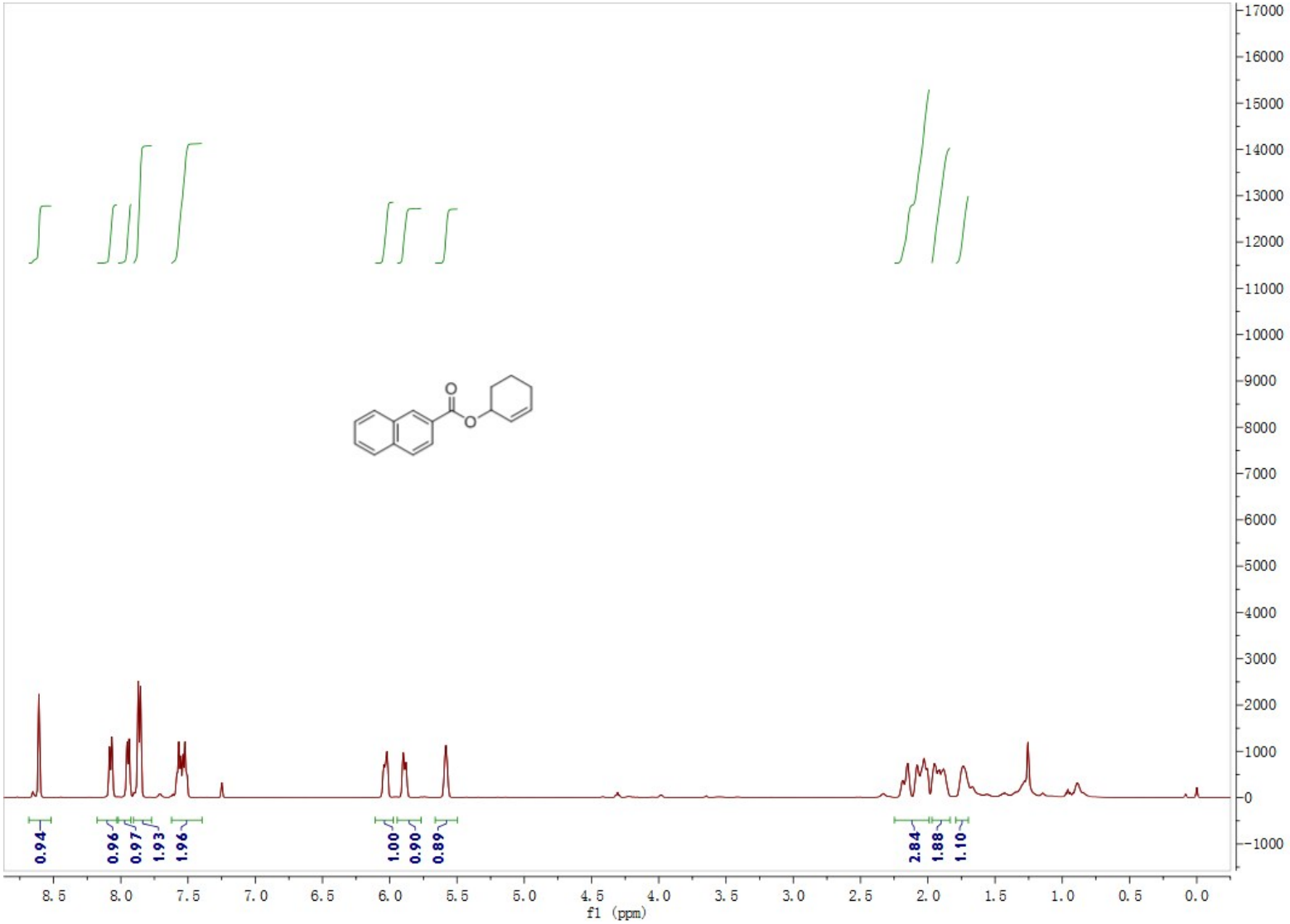

O
O
OPh
1.03
1.01
3.07
2.00
1.97
1.00
0.98
0.98
3.15
2.15
1.30
f1 (ppm)

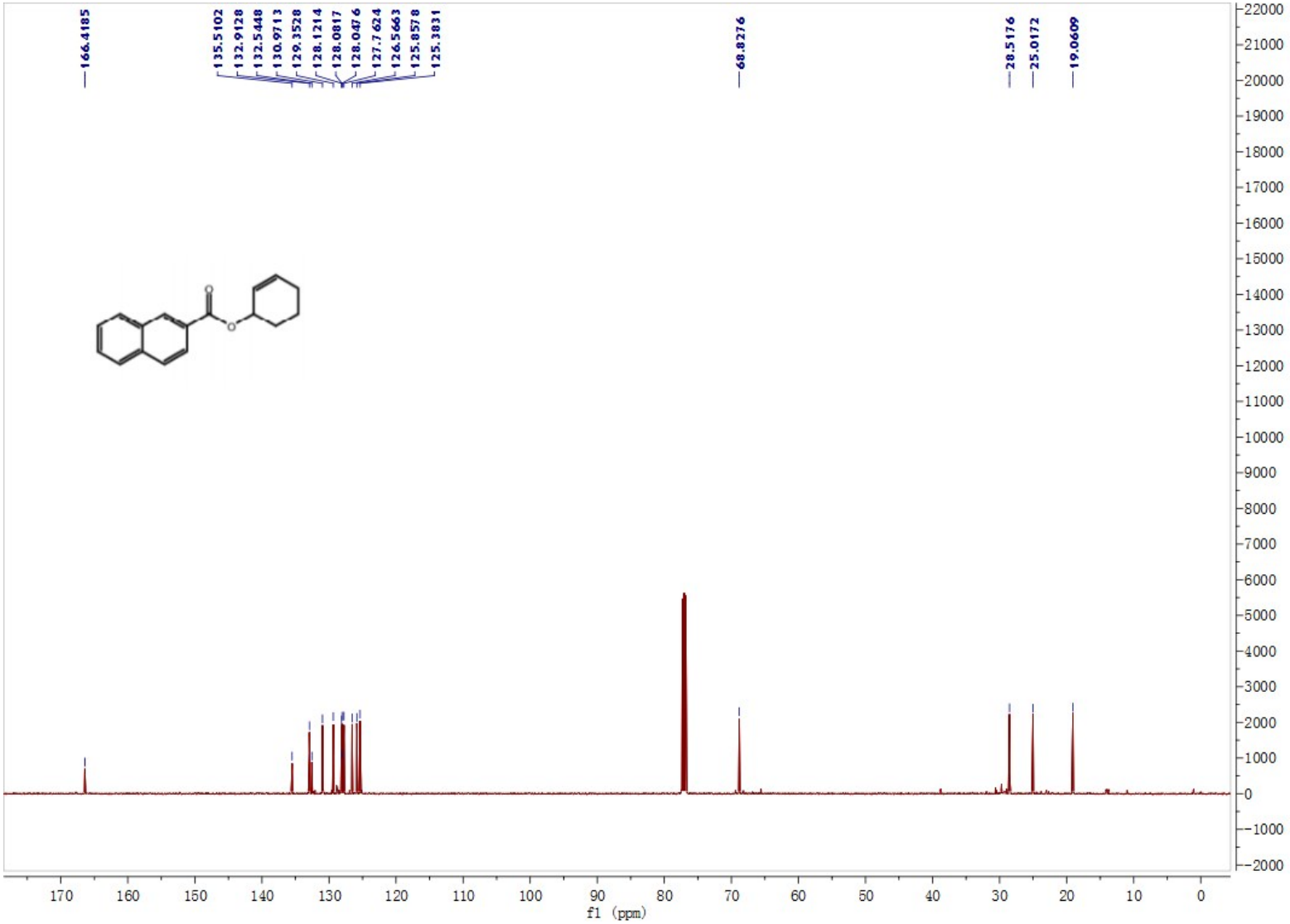

165.6630
157.3174
156.8814
132.9710
132.6942
129.8952
129.6473
125.6037
124.4234
123.6303
123.1656
119.9556
118.9411
68.9071
28.3890
24.9516
18.9234
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

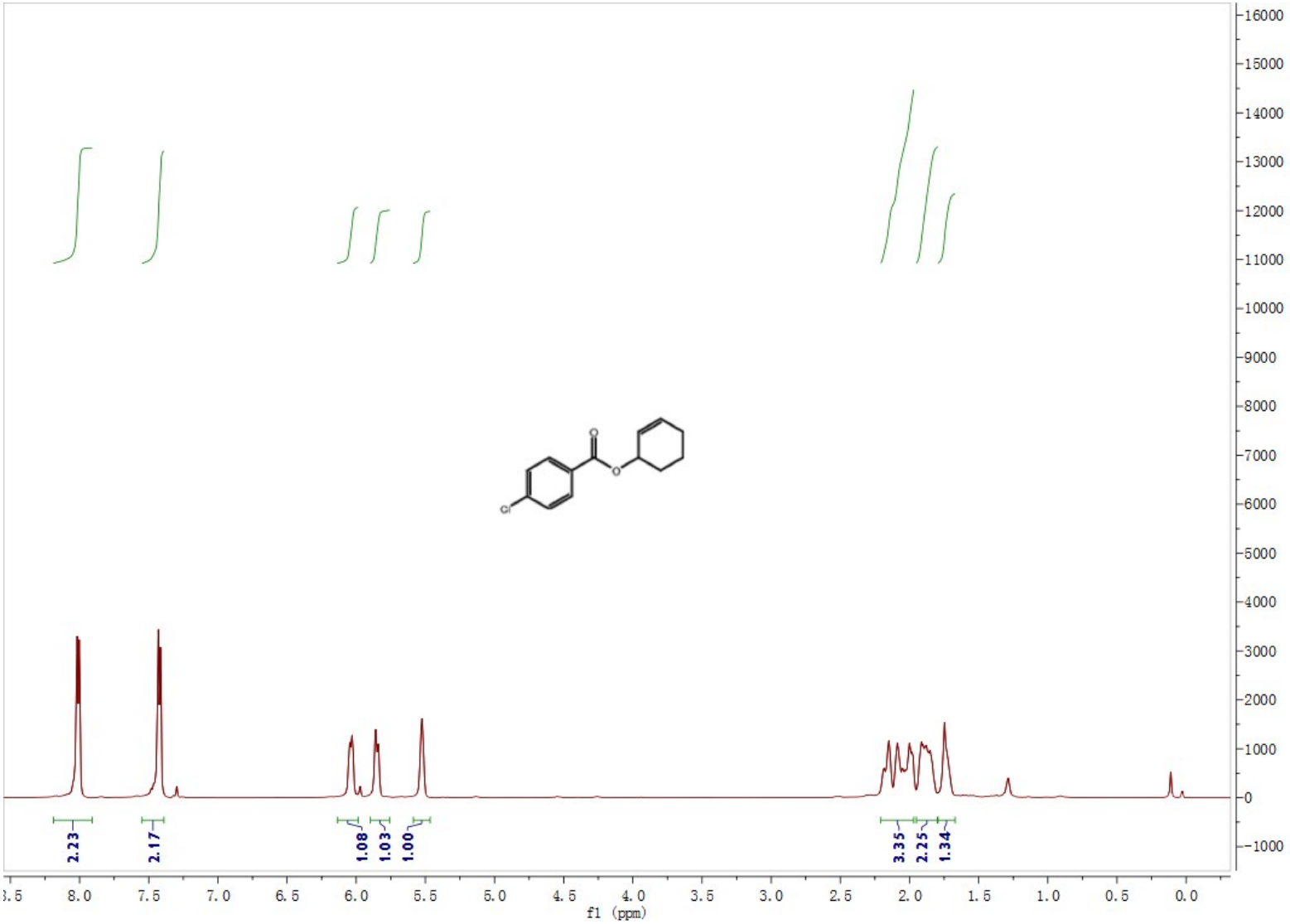

25000
20000
15000
10000
5000
0
1.03
1.07
1.07
1.00
1.00
1.07
3.23
2.33
1.37
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
O
S

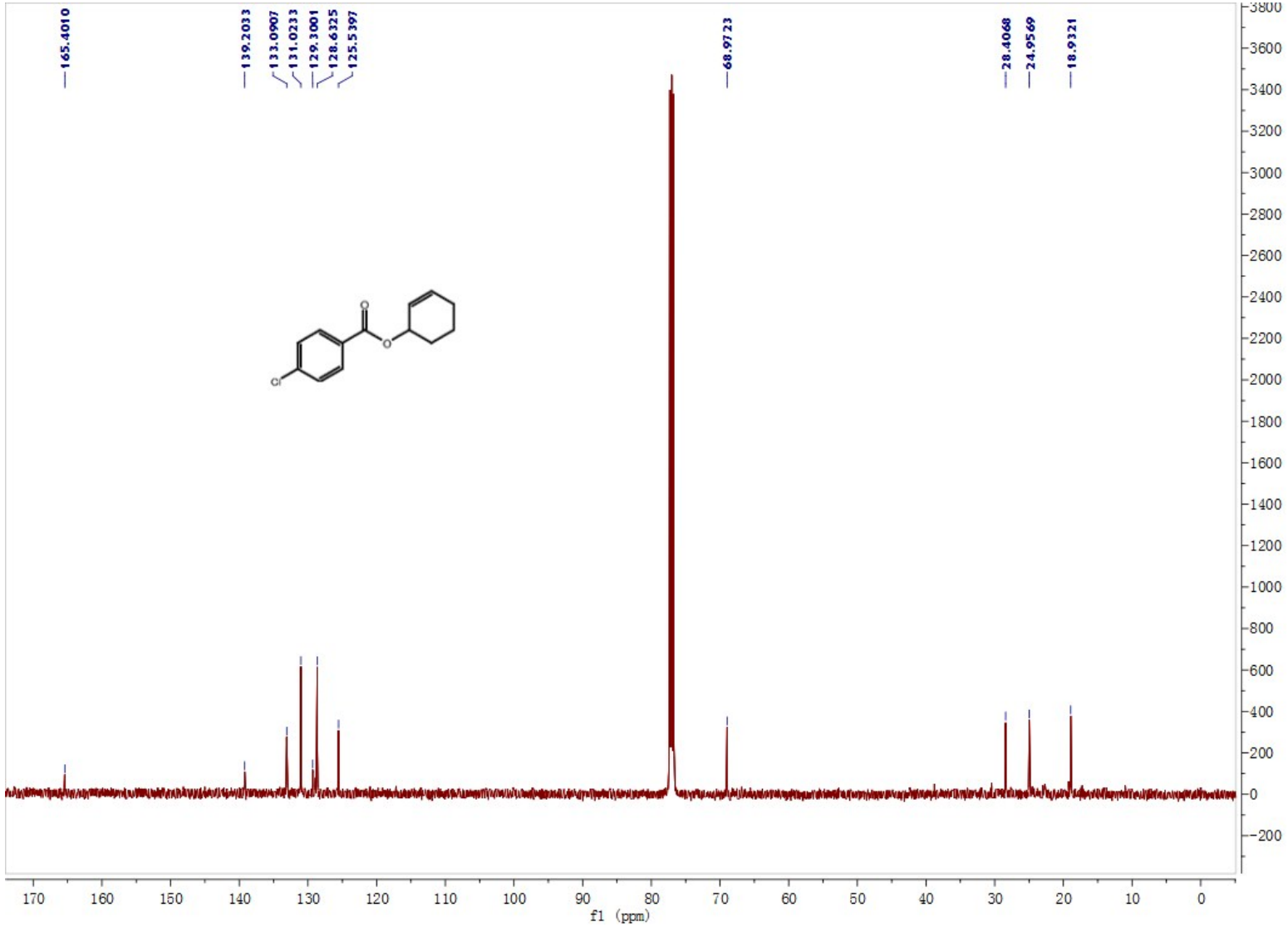

160.9432
133.5128
132.1664
131.9807
131.0984
126.6104
124.5446
67.9723
27.3785
23.9065
17.8837
O
O
S
24000
23000
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

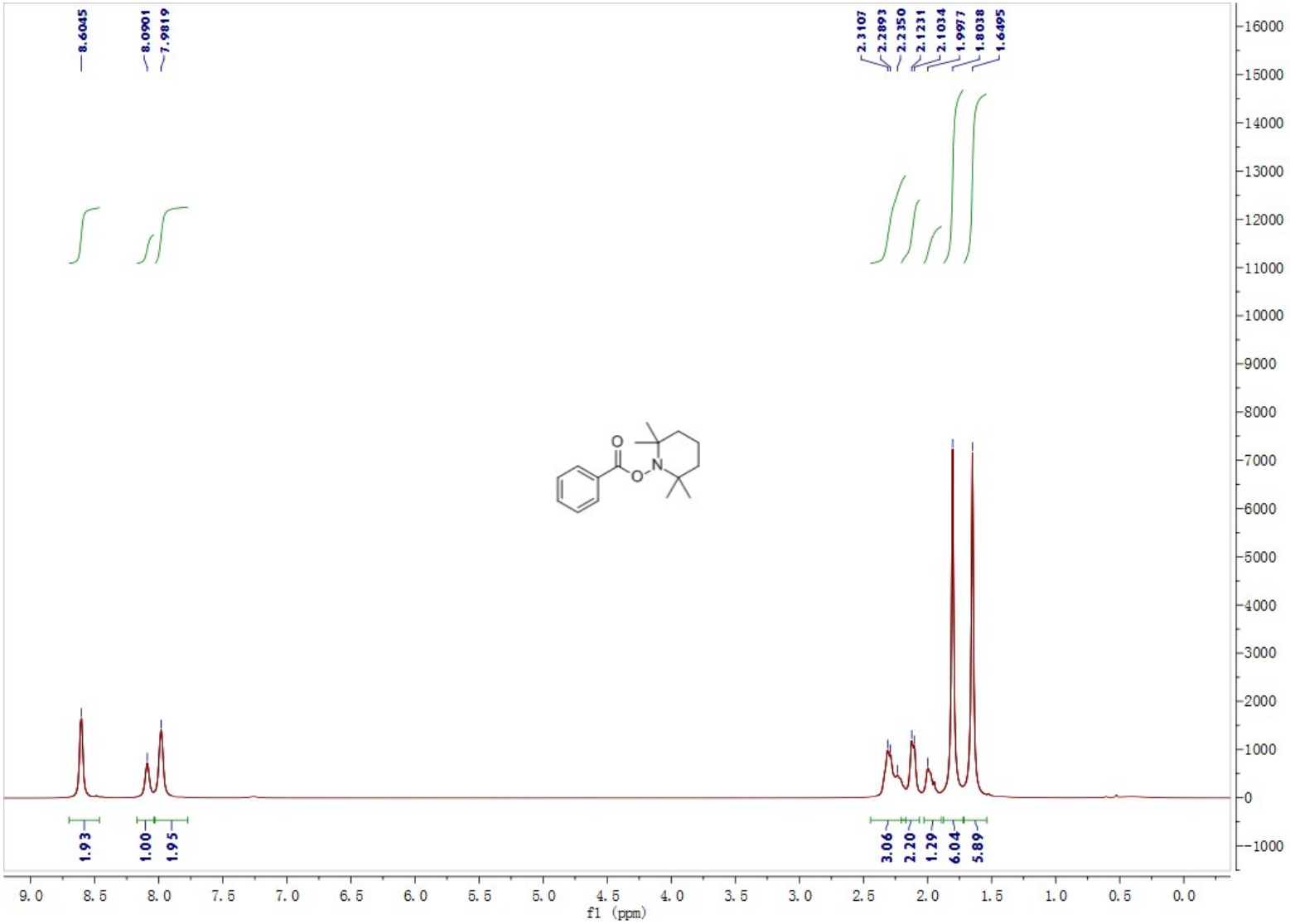

20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
2.11
2.46
1.00
1.09
1.01
3.28
1.12
2.35
2.24
1.27
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

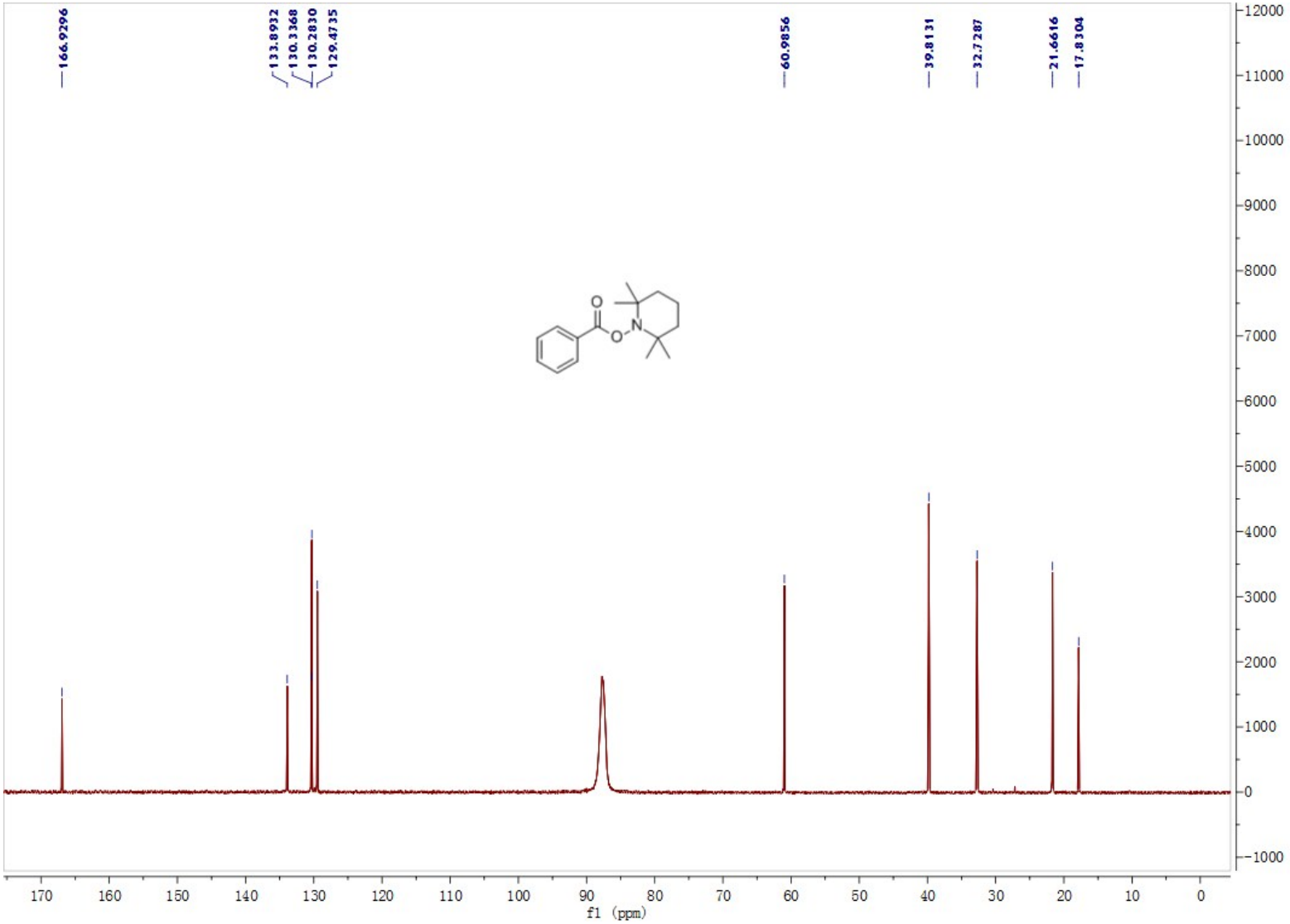

17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0.94
0.96
0.97
1.93
1.96
1.00
0.90
0.89
2.84
1.88
1.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.4185
135.5102
132.9128
132.5448
130.9713
129.3528
128.1214
128.0817
128.0476
127.7624
126.5663
125.8578
125.3831
68.8276
28.5176
25.0172
19.0609
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
2.23
2.17
1.08
1.03
1.00
3.35
2.25
1.34
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)


165.4010
139.2033
133.0907
131.0233
129.3001
128.6325
125.5397
68.9723
28.4068
24.9569
18.9321
Cl
O
O
f1 (ppm)


8.6045
8.0901
7.9819
2.3107
2.2893
2.2350
2.1231
2.1034
1.9977
1.8038
1.6495
O
O
N
1.93
1.00
1.95
3.06
2.20
1.29
6.04
5.89
f1 (ppm)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130.3368
130.2830
129.4735
60.9856
39.8131
32.7287
21.6616
17.8304
O
O
N
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)