Supporting Information

$Sc(OTf)_3$-Catalyzed [3+2]-Cycloaddition of Nitrones with Ynones

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I. The synthetic details data for the substrates 4, 7 and 10.

General Procedure for the Synthesis of 4. To a solution of benzaldehyde **1** (5.01 g, 47.1 mmol, 1.0 equiv) in 150 mL 50% EtOH was added powdered NaOH (2.07 g, 51.8 mmol, 1.1 equiv) followed by hydroxylamine hydrochloride (3.60 g, 51.8 mmol, 1.1 equiv) in small portions. The mixture was allowed to stir at rt for 1 h, ethanol was removed by vacuo and extracted with EtOAc (3 x 200 mL) and washed with water (3 x 200 mL). The combined organic layers were dried over $MgSO_4$ and concentrated in vacuo resulted the yellow oil **2**. The resulting oxime was dissolved 75 mL methanol and $NaBH_3CN$ (6.51g, 103.7 mmol, 2.2 equiv) was added in small portions by maintaining the pH ~ 2 using 2 N HCl at rt. The reaction mixture was allowed to stir for 3 h before adding 6 N NaOH until pH ~ 9. The reaction mixture was concentrated in vacuo and the product was extracted with EtOAc (3 x 100 mL), dried over anhydrous $MgSO_4$ and concentrated in vacuo. The dried crude N-benzyl-hydroxylamine **3** was added to flask containing corresponding aldehyde (4.01g, 37.7 mmol, 0.8 equiv), Na_2SO_4 (10.00g, 70.65 mmol, 1.5 equiv) in 190 mL dry DCM under argon atmosphere and the mixture was allowed to stir for 18 h. The mixture was filtered, the filtrate was concentrated in vacuo and purified by flash chromatography on silica gel (PE/EA) to give **4**.

(*Z*)-N-Benzyl-1-phenylmethanimine oxide 4a. Yellow solid (18.13 g, 90%, PE/EA = 100:1); mp 82–84 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24–8.17 (m, 2H), 7.50–7.44 (m, 2H), 7.43–7.35 (m, 7H), 5.05 (s, 2H) ppm.

(*Z*)-N-Benzyl-1-(2-chlorophenyl)methanimine oxide 4b. White solid (3.07 g, 45%, PE/EA = 8:1); mp 87–89 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.33–9.27 (m, 1H), 7.93 (s, 1H), 7.53–7.48 (m, 2H), 7.45–7.37 (m, 4H), 7.34–7.28 (m, 2H), 5.10 (s, 2H) ppm.

(*Z*)-N-Benzyl-1-(3-chlorophenyl)methanimine oxide 4c. Yellow oil (2.61 g, 38%, PE/EA = 8:1); IR (film) ν_{max}: 3066, 3031, 2946, 1576, 1457, 1152, 714, 697 cm^{-1};^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.98–7.94 (m, 1H), 7.50–7.45 (m, 2H), 7.44–7.38 (m, 3H), 7.38–7.28 (m, 3H), 5.05 (s, 2H) ppm; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 134.5, 132.9, 132.0, 130.4, 129.7, 129.3, 129.2, 129.1, 128.1, 126.7, 71.5 ppm; HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{14}H_{13}ClNO^+$: 246.0682, found: 246.0684.

(*Z*)-N-Benzyl-1-(3-bromophenyl)methanimine oxide 4d. Yellow solid (3.93 g, 48%, PE/EA = 5:1); mp 66–68 °C; IR (film) ν_{max}: 3065, 3031, 2945, 1575, 1457, 1426, 1192, 1150, 710, 683 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.05–8.01 (m, 1H), 7.53–7.44 (m, 3H), 7.44–7.37 (m, 3H), 7.35 (s, 1H), 7.26–7.22(m, 1H), 5.05 (s, 2H) ppm; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 133.3, 132.9, 132.8, 132.2, 131.0, 129.9, 129.3, 129.2, 129.1, 127.1, 122.6, 71.5 ppm; HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{14}H_{13}BrNO^+$: 290.0175, found: 290.0176.

(*Z*)-N-Benzyl-1-(4-chlorophenyl)methanimine oxide 4e. White solid (4.16 g, 61%, PE/EA = 10:1); mp 123–125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19–8.13 (m, 2H), 7.49–7.44 (m, 2H), 7.43–7.38 (m, 3H), 7.38–7.32 (m, 3H), 5.04 (s, 2H) ppm.

(*Z*)-N-Benzyl-1-(4-methoxyphenyl)methanimine oxide 4f. White solid (1.96 g, 28%, PE/EA = 5:1); mp 101–103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24–8.15 (m, 2H), 7.48–7.43 (m, 2H), 7.42–7.34 (m, 3H), 7.31 (s, 1H), 6.93–6.86 (m, 2H), 5.00 (s, 2H), 3.81 (s, 3H) ppm.

(*Z*)-N-Benzyl-1-(p-tolyl)methanimine oxide 4g. White solid (4.37 g, 67%, PE/EA = 10:1); mp 118–120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14–8.09 (m, 2H), 7.50–7.45 (m, 2H), 7.43–7.34 (m, 4H), 7.23–7.18 (m, 2H), 5.03 (s, 2H), 2.37 (s, 3H) ppm.

(*Z*)-N-Benzyl-1-(4-(methylthio)phenyl)methanimine oxide 4h. White solid (2.37 g, 33%, PE/EA = 10:1); mp 113–115 °C; IR (film) ν_{max}: 3065, 2981, 2916, 1574, 1543, 1457, 1423, 1147, 826, 711 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15–8.11 (m, 2H), 7.48–7.44(m, 2H), 7.43–7.37 (m, 3H), 7.33 (s, 1H), 7.24–7.19 (m, 2H), 5.03 (s, 2H), 2.49 (s, 3H) ppm; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 142.0, 133.9, 133.3, 129.3, 129.0, 128.9, 127.0, 125.4, 71.1, 15.0 ppm; HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{15}H_{16}NOS^+$: 258.0947, found: 258.0950.

(*Z*)-N-Benzyl-1-(4-cyanophenyl)methanimine oxide 4i. Yellow solid (2.93 g, 38%, PE/EA = 6:1); mp 156–158 °C; IR (film) ν_{max}: 2223, 1596, 1573, 1493, 1453, 1172, 1153, 861, 698, 564 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32–8.25 (m, 2H), 7.68–7.60 (m, 2H), 7.49–7.38 (m, 6H), 5.09 (s, 2H) ppm; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 134.3, 132.7, 132.5, 132.2, 129.3, 129.1, 128.5, 118.5, 113.0, 72.0 ppm; HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{15}H_{13}N_2O^+$: 237.1022, found: 237.1023.

(*Z*)-N-Benzyl-1-(4-nitrophenyl)methanimine oxide 4j. Yellow solid (1.05 g, 17%, PE/EA = 8:1); mp 117–119 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38–8.33 (m, 2H), 8.25–8.18 (m, 2H), 7.54 (s, 1H), 7.51–7.46 (m, 2H), 7.45–7.38 (m, 3H), 5.11 (s, 2H) ppm.

(*Z*)-N-Benzyl-1-(4-(trifluoromethyl)phenyl)methanimine oxide 4k. White solid (3.53 g, 45%, PE/EA = 6:1); mp 138–140 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34–8.28 (m, 2H), 7.66–7.60 (m, 2H), 7.51–7.39 (m, 6H), 5.09 (s, 2H) ppm.

(*Z*)-N-Benzyl-1-(thiophen-2-yl)methanimine oxide 4l. Yellow solid (2.85 g, 46%, PE/EA = 8:1); mp 116–118 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.49–7.35 (m, 7H), 7.15–7.09 (m, 1H), 5.07 (s, 2H) ppm.

General Procedure for the Synthesis of 7. $PdCl_2(PPh_3)_2$ (98 mg, 0.14 mmol, 0.001 equiv) and CuI (97 mg, 0.51 mmol, 0.005 equiv) were suspended in THF (196 mL). Then the respective benzoyl chloride derivate (13.76g, 97.9 mmol, 1 equiv) and arylacetylene (10.00g, 97.9 mmol, 1 equiv) were added to the suspension. After the addition of Et_3N (10 mL) the reaction mixture was stirred overnight. Subsequently saturated NH_4Cl solution (70 mL) was added to the reaction mixture. The aqueous phase was extracted with EtOAc (3 x 200 mL). The organic phases were combined and washed with brine (200 mL) and dried over $MgSO_4$. The mixture was filtered, the filtrate was concentrated in vacuo and purified by flash chromatography on silica gel (PE/EA) to give **7**.

1,3-Diphenylprop-2-yn-1-one 7a. Yellow solid (18.13 g, 90%, PE/EA = 100:1); mp 47–49 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28–8.23 (m, 2H), 7.75–7.68 (m, 2H), 7.67–7.61 (m, 1H), 7.58–7.48 (m, 3H), 7.47–7.41 (m, 2H) ppm.

3-(4-Chlorophenyl)-1-phenylprop-2-yn-1-one 7b. Yellow solid (1.94 g, 53%, PE/EA = 100:1); mp 108–110°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23–8.18 (m, 2H), 7.67–7.59 (m, 3H), 7.55–7.49 (m, 2H), 7.42–7.38 (m, 2H) ppm.

3-(4-Ethoxyphenyl)-1-phenylprop-2-yn-1-one 7c. Yellow solid (4.71 g, 92%, PE/EA = 20:1); mp 64–66 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25–8.19 (m, 2H), 7.66–7.58 (m, 3H), 7.55–7.48 (m, 2H), 6.94–6.89(m, 2H), 4.13–4.04 (m, 2H), 1.49–1.40 (m, 3H) ppm; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 178.2, 161.3, 137.2, 135.3, 134.0, 129.6, 128.7, 115.0, 111.8, 94.6, 87.0, 63.9, 14.8 ppm; HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{17}H_{15}O_2^+$: 251.1066, found: 251.1067.

1-Phenyl-3-p-tolylprop-2-yn-1-one 7d. Yellow solid (2.91 g, 77%, PE/EA = 30:1); mp 60–62 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25–8.20 (m, 2H), 7.64–7.56 (m, 3H), 7.55–7.49 (m, 2H), 7.25–7.20 (m, 2H), 2.41 (s, 3H) ppm.

4-(3-Oxo-3-phenylprop-1-ynyl)benzonitrile 7e. Brown solid (2.20 g, 67%, PE/EA = 30:1); mp 73–75 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.73–8.67 (m, 1H), 8.25–8.18 (m, 2H), 7.98–7.95 (m, 1H), 7.69–7.62 (m, 1H), 7.57–7.50 (m, 2H), 7.41–7.35 (m, 1H) ppm.

1-Phenyl-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one 7f. Yellow solid (0.93 g, 40%, PE/EA = 100:1); mp 84–86 °C; ^{1}H NMR (500MHz, $CDCl_3$) δ 8.24–8.19 (m, 2H), 7.81–7.76 (m, 2H), 7.71–7.63 (m, 3H), 7.57–7.51 (m, 2H) ppm.

Methyl 4-(3-oxo-3-phenylprop-1-ynyl)benzoate 7g. Yellow solid (2.89 g, 87%, PE/EA = 30:1); mp 97–99 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25–8.19 (m, 2H), 8.12–8.07 (m, 2H), 7.77–7.72 (m, 2H), 7.68–7.62 (m, 1H), 7.56–7.50 (m, 2H), 3.97–3.91 (m, 3H) ppm.

3-(4-Nitrophenyl)-1-phenylprop-2-yn-1-one 7h. Brown solid (636 mg, 19%, PE/EA = 40:1); mp 155–157 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35–8.25 (m, 2H), 8.24–8.16 (m, 2H), 7.89–7.79 (m, 2H), 7.72–7.63 (m, 1H), 7.59–7.51 (m, 2H) ppm.

3-Cyclopropyl-1-phenylprop-2-yn-1-one 7i. Yellow oil (3.49 g, 68%, PE/EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13–8.08 (m, 2H), 7.62–7.55 (m, 1H), 7.49–7.43 (m, 2H), 1.58–1.49 (m, 1H), 1.09–0.98 (m, 4H) ppm.

1-Phenyl-3-(thiophen-3-yl)prop-2-yn-1-one 7j. Yellow solid (2.93 g, 38%, PE/EA = 5:1); mp 68–70 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24–8.17 (m, 2H), 7.87–7.83 (m, 1H), 7.66–7.59 (m, 1H), 7.55–7.49 (m, 2H), 7.40–7.35 (m, 1H), 7.34–7.30 (m, 1H) ppm.

1-Phenyl-3-(thiophen-2-yl)prop-2-yn-1-one 7k. Brown solid (2.84 g, 72%, PE/EA = 80:1); mp 58–60 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22–8.16 (m, 2H), 7.66–7.60 (m, 1H), 7.59–7.56 (m, 1H), 7.55–7.49 (m, 3H), 7.13–7.08 (m, 1H) ppm.

1-Phenyl-3-(pyridin-3-yl)prop-2-yn-1-one 7l. Yellow solid (1.58 g, 40%, PE/EA = 40:1); mp 143–145 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23–8.17 (m, 2H), 7.80–7.75 (m, 2H), 7.74–7.70 (m, 2H), 7.69–7.63 (m, 1H), 7.57–7.50 (m, 2H) ppm.

4-Oxo-4-phenylbut-2-ynyl acetate 7m. Yellow oil (1.92 g, 47%, PE/EA = 60:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13–8.09 (m, 2H), 7.64–7.59 (m, 1H), 7.51–7.46 (m, 2H), 4.94 (s, 2H), 2.15 (s, 3H) ppm.

4,4-Dimethyl-1-phenylpent-2-yn-1-one 7n. Colorless oil (2.71 g, 45%, PE/EA = 90:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16–8.11 (m, 2H), 7.62–7.57 (m, 1H), 7.51–7.45 (m, 2H), 4.94 (s, 2H), 2.15 (s, 3H) ppm.

1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-one 7o. Yellow solid (1.62 g, 58%, PE/EA = 80:1); mp 107–109 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19–8.11 (m, 2H), 7.71–7.65 (m, 2H), 7.53–7.47 (m, 3H), 7.46–7.40 (m, 2H) ppm.

1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-one 7p. White solid (1.46 g, 52%, PE/EA = 50:1); mp 101–103 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24–8.17 (m, 2H), 7.71–7.64 (m, 2H), 7.50–7.44 (m, 1H), 7.43–7.38 (m,

2H), 7.02–6.96 (m, 2H), 3.90 (s, 3H) ppm.

3-Phenyl-1-p-tolylprop-2-yn-1-one 7q. Yellow solid (1.53 g, 54%, PE/EA = 80:1); mp 71–73 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14–8.09 (m, 2H), 7.70–7.65 (m, 2H), 7.50–7.44 (m, 1H), 7.43–7.38 (m, 2H), 7.33–7.28 (m, 2H), 2.44 (s, 3H) ppm.

1-(4-Nitrophenyl)-3-phenylprop-2-yn-1-one 7r. Yellow solid (411 mg, 15%, PE/EA = 80:1); mp 161–163 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41–8.32 (m, 4H), 7.74–7.68 (m, 2H), 7.57–7.50 (m, 1H), 7.49–7.42 (m, 2H) ppm.

4-(3-Phenylpropioloyl)benzonitrile 7s. Yellow solid (1.29 g, 28%, PE/EA = 60:1); mp 50–52 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34–8.28 (m, 2H), 7.86–7.80 (m, 2H), 7.74–7.66 (m, 2H), 7.57–7.49 (m, 1H), 7.48–7.42 (m, 2H) ppm.

1-(Naphthalen-2-yl)-3-phenylprop-2-yn-1-one 7t. White solid (1.95 g, 72%, PE/EA = 80:1); mp 92–94 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.24–8.18 (m, 1H), 8.06–7.99 (m, 1H), 7.95–7.87(m, 2H), 7.76–7.70 (m, 2H), 7.65–7.54 (m, 2H), 7.52–7.41 (m, 3H) ppm.

3-Phenyl-1-(tetrahydro-2H-pyran-4-yl)prop-2-yn-1-one 7u. Yellow solid (2.93 g, 70%, PE/EA = 30:1); mp 40–42 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62–7.55 (m, 2H), 7.49–7.44 (m, 1H), 7.43–7.36 (m, 2H), 4.08–3.96 (m, 2H), 3.55–3.49 (m, 2H), 2.78–2.66 (m, 1H), 2.05–1.92 (m, 2H), 1.91–1.78 (m, 2H) ppm.

1-(3-Methylthiophen-2-yl)-3-phenylprop-2-yn-1-one 7v. Yellow solid (3.03 g, 69%, PE/EA = 100:1); mp 38–40 °C; IR (film) ν_{max}: 3100, 2924, 2197, 1618, 1522, 1400, 1307, 1282, 777, 755 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68–7.62 (m, 2H), 7.57–7.53 (m, 1H), 7.50–7.44 (m, 1H), 7.43–7.37 (m, 2H), 7.01–6.96 (m, 1H), 2.68 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 169.9, 146.2, 138.0, 133.1, 132.9, 130.7, 128.7, 120.2, 91.5, 88.2, 16.7 ppm. HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}OS^+$: 227.0525, found: 227.0526.

1-(3,5-Dimethylisoxazol-4-yl)-3-phenylprop-2-yn-1-one 7w. Yellow solid (3.55 g, 76%, PE/EA = 100:1); mp 107–109 °C; IR (film) ν_{max}: 2198, 1626, 1583, 1445, 1420, 1378, 1318, 1067, 758, 688 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65–7.60 (m, 2H), 7.54–7.49 (m, 1H), 7.47–7.41 (m, 2H), 2.85 (s, 3H), 2.58 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 175.6, 170.5, 159.3, 132.8, 131.1, 128.9, 119.6, 117.0, 92.4, 88.1, 13.8, 12.0 ppm; HRMS (ESI-Orbitrap) m/z: $[M+H]^+$ calcd for $C_{14}H_{12}NO_2^+$: 226.0862, found: 226.0863.

General Procedure for the Synthesis of 10. To a solution of trimethylsilyl acetylene (1.3 equiv.) in THF at 0 °C under Ar atmosphere, n-BuLi (1.2 equiv., 2.5 M in hexane) was added dropwise. The mixture was stirred for 15 min at 0 °C . The corresponding aldehyde (1.0 equiv.) was then added and the reaction was stirred for additional 30 min at 0 °C and warmed up to room temperature for 30 min. Then, the mixture was quenched with saturated NH_4Cl solution and extracted with diethyl ether. The organic layers were combined, washed with brine, dried over $MgSO_4$ and the solvent was evaporated under reduced pressure. K_2CO_3 (3.0 equiv.) was added to the crude mixture in MeOH and stirring was continued at room temperature for 2 h. The crude was filtered under a pad of celite and washed with dichloromethane. The residue was washed with ammonium chloride and brine and dried over $MgSO_4$. After evaporation of the solvent, the residue was purified by column chromatography on silica gel to afford the corresponding propargylic alcohol in 80-90% yield. The crude alcohol was dissolved in dichloromethane and treated with MnO_2 (15.0 equiv.). After stirring at room temperature for 2 h, the reaction was complete as determined by TLC. Excess MnO_2 was removed by filtration of the reaction mixture through a pad of celite. The filtrate was washed sequentially with water and brine and dried over $MgSO_4$. The mixture was filtered, the filtrate was concentrated in vacuo and purified by flash chromatography on silica gel (PE/EA) to give **10**.

1-(4-Bromophenyl)prop-2-yn-1-one 10a. Yellow solid (2.92 g, 45%, PE/EA = 40:1); mp 108–110 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05–7.97 (m, 2H), 7.68–7.61 (m, 2H), 3.46 (s, 1H) ppm.

1-P-tolylprop-2-yn-1-one 10b. White solid (2.82 g, 57%, PE/EA = 60:1); mp 44–46 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08–8.04 (m, 2H), 7.32–7.27 (m, 2H), 3.40 (s, 1H), 2.44 (s, 3H) ppm.

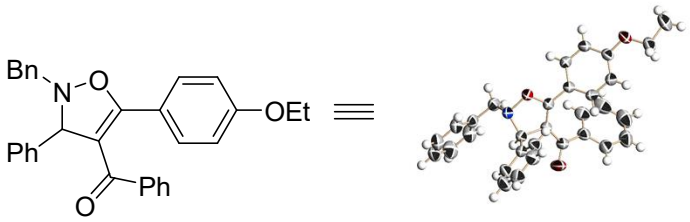
1-(3-Chlorophenyl)prop-2-yn-1-one 10c. Yellow solid (1.92 g, 37%, PE/EA = 60:1); mp 53–55 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 8.07–8.01 (m, 1H), 7.63–7.57 (m, 1H), 7.49–7.41 (m, 1H), 3.51 (s, 1H) ppm.

5-Phenylpent-1-yn-3-one 10d. Yellow oil (2.31 g, 42%, PE/EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32–7.27 (m, 2H), 7.23–7.18 (m, 3H), 3.23 (s, 1H), 3.02–2.97 (m, 2H), 2.95–2.90 (m, 2H) ppm.

1-Cyclohexylprop-2-yn-1-one 10e. Yellow oil (3.03 g, 67%, PE/EA = 70:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.22 (s, 1H), 2.47–2.39 (m, 1H), 2.03–1.97 (m, 2H), 1.82–1.77 (m, 2H), 1.69–1.63 (m, 1H), 1.47–1.40 (m, 2H), 1.34–1.23 (m, 3H) ppm.

II. X-Ray Structure for compound 11ac

ORTEP drawing of the X-ray crystallographic structure of **11ac (20191226hct1611** is the original test number for **11ac**):



CCDC 2032670. For detailed crystallographic data, please refer to the Cambridge Crystallographic Data Centre at www.ccdc.cam.ac.uk/data_request/cif.

Crystal Structure Report for 20191226hct1611

A clear light colourless block-like specimen of $C_{31}H_{27}NO_3$, approximate dimensions 0.100 mm x 0.200 mm x 0.300 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a d8 venture system (mo k_α, λ = 0.71073 Å).

Table 1: Data collection details for 20191226hct1611.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Phi	40.034	1.26	265.17	-116.00	24.00	1.00	184	10.00	0.71073	50	1.4	300
Omega	40.034	1.04	-42.82	86.28	64.87	1.00	51	10.00	0.71073	50	1.4	300

A total of 235 frames were collected. The total exposure time was 0.65 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 19036 reflections to a maximum θ angle of 25.75° (0.82 Å resolution), of which 4831 were independent (average redundancy 3.940, completeness = 99.4%, R_{int} = 3.55%, R_{sig} = 3.02%) and 3472 (71.87%) were greater than 2σ(F^2). The final cell constants of a = 12.3306(6) Å, b = 9.6662(6) Å, c = 21.3703(12) Å, β = 91.206(2)°, volume = 2546.6(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 6474 reflections above 20 σ(I) with 4.625° < 2θ < 51.31°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.887. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9770 and 0.9920.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{31}H_{27}NO_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 317 variables converged at R1 = 4.26%, for the observed data and wR2 = 11.38% for all data. The goodness-of-fit was 1.053. The largest peak in the final difference electron density synthesis was 0.117 $e^-/Å^3$ and the largest hole was -0.162 $e^-/Å^3$ with an RMS deviation of 0.035 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.204 g/cm^3 and F(000), 976 e^-.

Table 2. Sample and crystal data for 20191226hct1611.

Identification code	20191226hct1611	
Chemical formula	$C_{31}H_{27}NO_3$	
Formula weight	461.53 g/mol	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal size	0.100 x 0.200 x 0.300 mm	
Crystal habit	clear light colourless block	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 12.3306(6) Å	α = 90°
	b = 9.6662(6) Å	β = 91.206(2)°
	c = 21.3703(12) Å	γ = 90°
Volume	2546.6(2) $Å^3$	
Z	4	
Density (calculated)	1.204 g/cm^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	976	

Table 3. Data collection and structure refinement for 20191226hct1611.

Diffractometer	d8 venture
Theta range for data collection	2.31 to 25.75°
Index ranges	-14<=h<=15, -11<=k<=10, -26<=l<=26
Reflections collected	19036
Independent reflections	4831 [R(int) = 0.0355]
Coverage of independent reflections	99.4%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9920 and 0.9770
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4831 / 0 / 317
Goodness-of-fit on F^2	1.053
Final R indices	3472 data; I>2σ(I) R1 = 0.0426, wR2 = 0.0996
	all data R1 = 0.0641, wR2 = 0.1138
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0474P)^2+0.4169P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.117 and -0.162 $eÅ^{-3}$
R.M.S. deviation from mean	0.035 $eÅ^{-3}$

Table 4. Atomic coordinates and equivalent isotropic atomic

displacement parameters (Å^2) for 20191226hct1611.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.35313(9)	0.00980(12)	0.46596(6)	0.0635(3)
O2	0.72601(9)	0.32279(11)	0.33660(5)	0.0572(3)
O3	0.57981(10)	0.75366(13)	0.34904(8)	0.0892(5)
N1	0.79639(10)	0.42658(13)	0.30671(6)	0.0511(3)
C1	0.21721(19)	0.9251(3)	0.53138(12)	0.0993(8)
C2	0.28746(15)	0.0476(2)	0.51785(9)	0.0685(5)
C3	0.41783(12)	0.10792(17)	0.44085(8)	0.0500(4)
C4	0.42906(13)	0.24175(17)	0.46320(8)	0.0547(4)
C5	0.49741(13)	0.33203(17)	0.43348(8)	0.0540(4)
C6	0.55528(12)	0.29275(16)	0.38153(7)	0.0483(4)
C7	0.63193(12)	0.38721(16)	0.35260(7)	0.0485(4)
C8	0.78396(14)	0.40202(19)	0.23901(8)	0.0600(4)
C9	0.86027(13)	0.49785(18)	0.20599(7)	0.0519(4)
C10	0.96978(14)	0.4995(2)	0.22135(8)	0.0629(5)
C11	0.03849(15)	0.5913(2)	0.19323(9)	0.0729(5)
C12	0.99995(17)	0.6829(2)	0.14969(9)	0.0740(6)
C13	0.82260(15)	0.5894(2)	0.16194(9)	0.0735(5)
C14	0.89209(18)	0.6814(2)	0.13380(10)	0.0852(6)
C15	0.74983(12)	0.56234(16)	0.32637(7)	0.0480(4)
C16	0.63503(12)	0.52529(16)	0.34322(7)	0.0482(4)
C17	0.47605(13)	0.06638(17)	0.38905(8)	0.0569(4)
C18	0.54398(13)	0.15709(17)	0.36014(8)	0.0556(4)
C19	0.55253(13)	0.63171(17)	0.34754(8)	0.0562(4)
C20	0.43433(13)	0.59616(17)	0.34714(8)	0.0548(4)
C21	0.36643(14)	0.66800(19)	0.38658(9)	0.0644(5)
C22	0.25667(16)	0.6401(2)	0.38658(11)	0.0814(6)
C23	0.21368(17)	0.5443(3)	0.34683(12)	0.0897(7)
C24	0.27903(18)	0.4738(2)	0.30657(11)	0.0844(6)
C25	0.39010(15)	0.4985(2)	0.30659(9)	0.0658(5)
C26	0.81931(12)	0.62058(16)	0.37923(7)	0.0483(4)
C27	0.89065(14)	0.72699(19)	0.36794(8)	0.0623(5)
C28	0.96061(15)	0.7748(2)	0.41439(9)	0.0729(5)
C29	0.96050(15)	0.7159(2)	0.47225(9)	0.0732(5)
C30	0.89008(16)	0.6097(2)	0.48455(9)	0.0707(5)
C31	0.81949(15)	0.56289(19)	0.43845(8)	0.0625(5)

Table 5. Bond lengths (Å) for 20191226hct1611.

O1-C3	1.3572(18)	O1-C2	1.434(2)
O2-C7	1.3665(17)	O2-N1	1.4802(15)
O3-C19	1.226(2)	N1-C8	1.471(2)
N1-C15	1.4960(19)	C1-C2	1.499(3)
C1-H10	0.96	C1-H1	0.96
C1-H11	0.96	C2-H12	0.97
C2-H13	0.97	C3-C4	1.385(2)
C3-C17	1.391(2)	C4-C5	1.378(2)
C4-H14	0.93	C5-C6	1.385(2)
C5-H15	0.93	C6-C18	1.395(2)
C6-C7	1.461(2)	C7-C16	1.350(2)

C8-C9	1.506(2)	C8-H6	0.97
C8-H7	0.97	C9-C13	1.367(3)
C9-C10	1.383(2)	C10-C11	1.374(2)
C10-H3	0.93	C11-C12	1.362(3)
C11-H27	0.93	C12-C14	1.366(3)
C12-H2	0.93	C13-C14	1.381(3)
C13-H4	0.93	C14-H5	0.93
C15-C16	1.511(2)	C15-C26	1.512(2)
C15-H26	0.98	C16-C19	1.451(2)
C17-C18	1.369(2)	C17-H8	0.93
C18-H9	0.93	C19-C20	1.497(2)
C20-C25	1.385(2)	C20-C21	1.387(2)
C21-C22	1.380(3)	C21-H16	0.93
C22-C23	1.357(3)	C22-H20	0.93
C23-C24	1.372(3)	C23-H17	0.93
C24-C25	1.390(3)	C24-H18	0.93
C25-H19	0.93	C26-C27	1.378(2)
C26-C31	1.383(2)	C27-C28	1.381(3)
C27-H21	0.93	C28-C29	1.361(3)
C28-H22	0.93	C29-C30	1.374(3)
C29-H25	0.93	C30-C31	1.377(3)
C30-H23	0.93	C31-H24	0.93

Table 6. Bond angles (°) for 20191226hct1611.

C3-O1-C2	118.29(13)	C7-O2-N1	107.92(11)
C8-N1-O2	105.37(11)	C8-N1-C15	112.65(13)
O2-N1-C15	103.97(10)	C2-C1-H10	109.5
C2-C1-H1	109.5	H10-C1-H1	109.5
C2-C1-H11	109.5	H10-C1-H11	109.5
H1-C1-H11	109.5	O1-C2-C1	106.62(17)
O1-C2-H12	110.4	C1-C2-H12	110.4
O1-C2-H13	110.4	C1-C2-H13	110.4
H12-C2-H13	108.6	O1-C3-C4	124.87(15)
O1-C3-C17	115.49(15)	C4-C3-C17	119.64(14)
C5-C4-C3	119.36(15)	C5-C4-H14	120.3
C3-C4-H14	120.3	C4-C5-C6	121.76(15)
C4-C5-H15	119.1	C6-C5-H15	119.1
C5-C6-C18	118.08(14)	C5-C6-C7	121.10(14)
C18-C6-C7	120.68(14)	C16-C7-O2	112.73(13)
C16-C7-C6	134.53(14)	O2-C7-C6	112.42(13)
N1-C8-C9	107.96(13)	N1-C8-H6	110.1
C9-C8-H6	110.1	N1-C8-H7	110.1
C9-C8-H7	110.1	H6-C8-H7	108.4
C13-C9-C10	118.18(16)	C13-C9-C8	120.96(16)
C10-C9-C8	120.80(16)	C11-C10-C9	120.75(18)
C11-C10-H3	119.6	C9-C10-H3	119.6
C12-C11-C10	120.60(18)	C12-C11-H27	119.7
C10-C11-H27	119.7	C11-C12-C14	119.14(19)
C11-C12-H2	120.4	C14-C12-H2	120.4
C9-C13-C14	120.79(18)	C9-C13-H4	119.6
C14-C13-H4	119.6	C12-C14-C13	120.5(2)
C12-C14-H5	119.7	C13-C14-H5	119.7
N1-C15-C16	103.06(12)	N1-C15-C26	108.76(12)
C16-C15-C26	115.41(12)	N1-C15-H26	109.8
C16-C15-H26	109.8	C26-C15-H26	109.8

C7-C16-C19	132.01(14)	C7-C16-C15	107.41(13)
C19-C16-C15	120.58(14)	C18-C17-C3	120.34(15)
C18-C17-H8	119.8	C3-C17-H8	119.8
C17-C18-C6	120.82(15)	C17-C18-H9	119.6
C6-C18-H9	119.6	O3-C19-C16	119.41(15)
O3-C19-C20	119.16(15)	C16-C19-C20	121.37(14)
C25-C20-C21	119.11(16)	C25-C20-C19	122.02(16)
C21-C20-C19	118.80(16)	C22-C21-C20	120.5(2)
C22-C21-H16	119.8	C20-C21-H16	119.8
C23-C22-C21	120.2(2)	C23-C22-H20	119.9
C21-C22-H20	119.9	C22-C23-C24	120.3(2)
C22-C23-H17	119.8	C24-C23-H17	119.8
C23-C24-C25	120.4(2)	C23-C24-H18	119.8
C25-C24-H18	119.8	C20-C25-C24	119.49(19)
C20-C25-H19	120.3	C24-C25-H19	120.3
C27-C26-C31	118.20(15)	C27-C26-C15	120.06(14)
C31-C26-C15	121.56(14)	C26-C27-C28	121.03(17)
C26-C27-H21	119.5	C28-C27-H21	119.5
C29-C28-C27	120.03(18)	C29-C28-H22	120.0
C27-C28-H22	120.0	C28-C29-C30	119.94(18)
C28-C29-H25	120.0	C30-C29-H25	120.0
C29-C30-C31	120.09(18)	C29-C30-H23	120.0
C31-C30-H23	120.0	C30-C31-C26	120.72(17)
C30-C31-H24	119.6	C26-C31-H24	119.6

Table 7. Torsion angles (°) for 20191226hct1611.

C7-O2-N1-C8	-100.47(14)	C7-O2-N1-C15	18.22(15)
C3-O1-C2-C1	174.37(16)	C2-O1-C3-C4	2.8(2)
C2-O1-C3-C17	-177.44(15)	O1-C3-C4-C5	-179.92(15)
C17-C3-C4-C5	0.4(2)	C3-C4-C5-C6	0.2(3)
C4-C5-C6-C18	-1.0(3)	C4-C5-C6-C7	-176.60(15)
N1-O2-C7-C16	-6.70(17)	N1-O2-C7-C6	178.85(12)
C5-C6-C7-C16	-35.4(3)	C18-C6-C7-C16	149.07(19)
C5-C6-C7-O2	137.41(16)	C18-C6-C7-O2	-38.1(2)
O2-N1-C8-C9	-175.84(12)	C15-N1-C8-C9	71.45(16)
N1-C8-C9-C13	-122.75(18)	N1-C8-C9-C10	54.5(2)
C13-C9-C10-C11	0.3(3)	C8-C9-C10-C11	-176.99(16)
C9-C10-C11-C12	0.1(3)	C10-C11-C12-C14	-0.6(3)
C10-C9-C13-C14	-0.3(3)	C8-C9-C13-C14	177.05(18)
C11-C12-C14-C13	0.7(3)	C9-C13-C14-C12	-0.2(3)
C8-N1-C15-C16	91.94(14)	O2-N1-C15-C16	-21.63(14)
C8-N1-C15-C26	-145.10(13)	O2-N1-C15-C26	101.33(13)
O2-C7-C16-C19	173.09(16)	C6-C7-C16-C19	-14.1(3)
O2-C7-C16-C15	-7.84(18)	C6-C7-C16-C15	164.95(17)
N1-C15-C16-C7	18.64(16)	C26-C15-C16-C7	-99.77(16)
N1-C15-C16-C19	-162.17(14)	C26-C15-C16-C19	79.43(19)
O1-C3-C17-C18	-179.86(15)	C4-C3-C17-C18	-0.1(3)
C3-C17-C18-C6	-0.7(3)	C5-C6-C18-C17	1.2(3)
C7-C6-C18-C17	176.87(16)	C7-C16-C19-O3	165.42(19)
C15-C16-C19-O3	-13.5(3)	C7-C16-C19-C20	-17.5(3)
C15-C16-C19-C20	163.52(15)	O3-C19-C20-C25	134.3(2)
C16-C19-C20-C25	-42.8(2)	O3-C19-C20-C21	-42.6(3)
C16-C19-C20-C21	140.32(17)	C25-C20-C21-C22	1.7(3)
C19-C20-C21-C22	178.66(17)	C20-C21-C22-C23	-1.6(3)
C21-C22-C23-C24	0.4(3)	C22-C23-C24-C25	0.8(3)

C21-C20-C25-C24	-0.5(3)	C19-C20-C25-C24	-177.41(17)
C23-C24-C25-C20	-0.7(3)	N1-C15-C26-C27	103.72(17)
C16-C15-C26-C27	-141.09(16)	N1-C15-C26-C31	-71.33(18)
C16-C15-C26-C31	43.9(2)	C31-C26-C27-C28	0.1(3)
C15-C26-C27-C28	-175.12(16)	C26-C27-C28-C29	0.6(3)
C27-C28-C29-C30	-0.6(3)	C28-C29-C30-C31	-0.1(3)
C29-C30-C31-C26	0.8(3)	C27-C26-C31-C30	-0.8(3)
C15-C26-C31-C30	174.37(16)		

Table 8. Anisotropic atomic displacement parameters (Å^2) for 20191226hct1611.

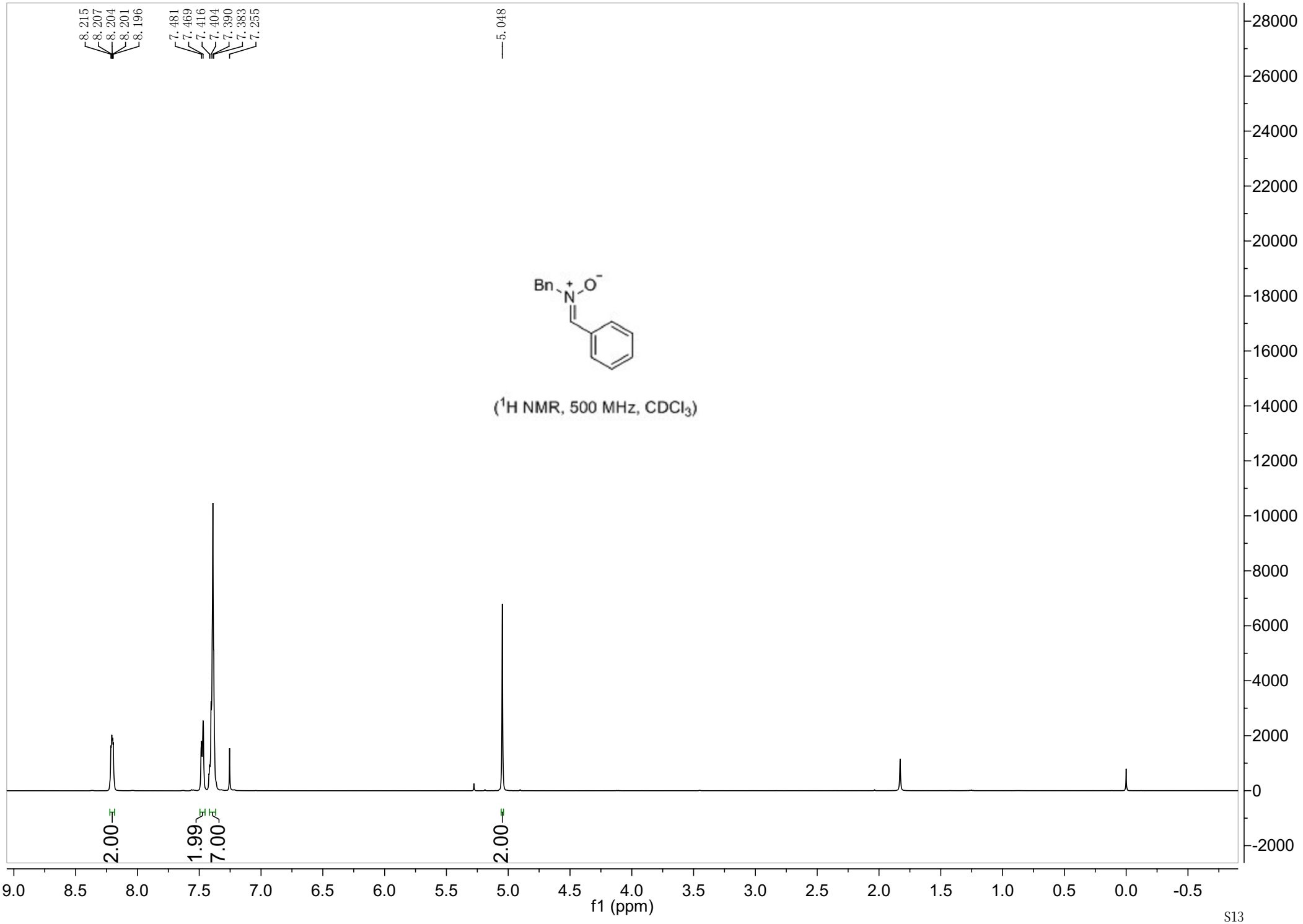
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

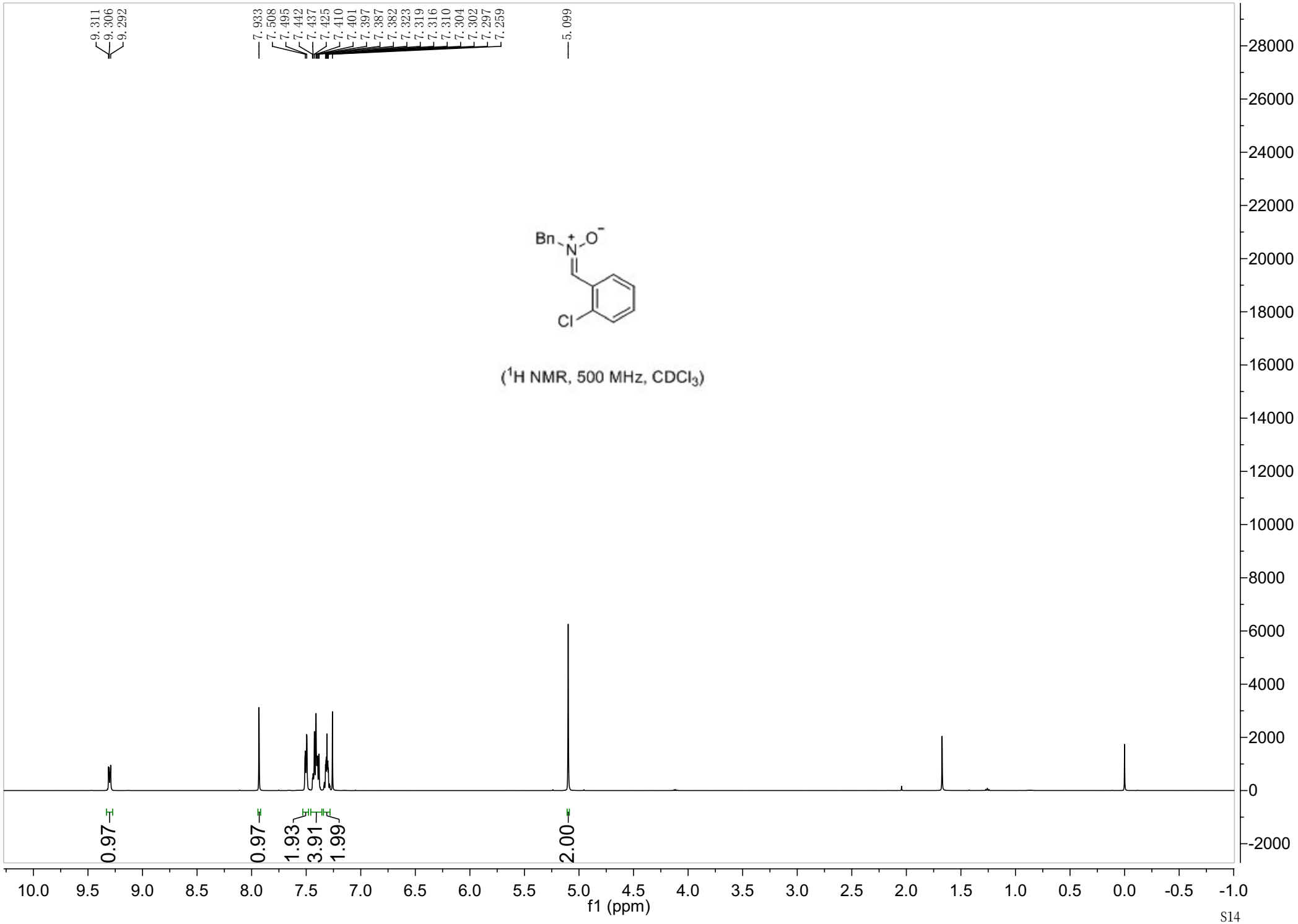
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0595(7)	0.0524(7)	0.0790(8)	0.0089(6)	0.0132(6)	-0.0096(6)
O2	0.0598(7)	0.0428(6)	0.0698(7)	0.0031(5)	0.0219(5)	0.0017(5)
O3	0.0649(8)	0.0413(7)	0.1622(15)	-0.0142(8)	0.0200(8)	-0.0043(6)
N1	0.0564(8)	0.0446(8)	0.0529(8)	-0.0023(6)	0.0160(6)	-0.0031(6)
C1	0.0921(16)	0.0933(18)	0.1139(19)	0.0204(14)	0.0334(14)	-0.0255(13)
C2	0.0599(10)	0.0715(13)	0.0746(12)	0.0153(10)	0.0148(9)	-0.0022(9)
C3	0.0445(8)	0.0447(9)	0.0610(10)	0.0079(8)	0.0022(7)	-0.0016(7)
C4	0.0596(10)	0.0499(10)	0.0549(10)	-0.0004(8)	0.0127(7)	-0.0012(8)
C5	0.0636(10)	0.0410(9)	0.0578(10)	-0.0045(7)	0.0105(8)	-0.0026(7)
C6	0.0500(8)	0.0395(8)	0.0557(9)	-0.0016(7)	0.0071(7)	-0.0013(7)
C7	0.0488(8)	0.0448(9)	0.0522(9)	-0.0033(7)	0.0085(7)	0.0014(7)
C8	0.0656(10)	0.0613(11)	0.0534(10)	-0.0118(8)	0.0112(8)	-0.0086(8)
C9	0.0557(9)	0.0601(10)	0.0403(8)	-0.0107(7)	0.0079(7)	-0.0006(8)
C10	0.0568(10)	0.0745(12)	0.0577(10)	0.0031(9)	0.0068(8)	0.0039(9)
C11	0.0569(10)	0.0969(16)	0.0654(12)	-0.0039(11)	0.0101(9)	-0.0084(10)
C12	0.0817(14)	0.0776(14)	0.0637(12)	-0.0028(10)	0.0230(10)	-0.0155(11)
C13	0.0608(11)	0.1013(16)	0.0583(11)	0.0111(11)	0.0005(8)	0.0016(11)
C14	0.0929(16)	0.0978(17)	0.0652(12)	0.0269(12)	0.0102(11)	0.0066(13)
C15	0.0533(9)	0.0414(8)	0.0496(9)	0.0000(7)	0.0100(7)	-0.0010(7)
C16	0.0477(8)	0.0430(9)	0.0541(9)	-0.0035(7)	0.0084(7)	-0.0027(6)
C17	0.0568(9)	0.0396(9)	0.0746(11)	-0.0061(8)	0.0078(8)	-0.0033(7)
C18	0.0570(9)	0.0469(9)	0.0634(10)	-0.0085(8)	0.0141(8)	-0.0003(7)
C19	0.0545(9)	0.0424(9)	0.0719(11)	-0.0032(8)	0.0091(8)	-0.0021(7)
C20	0.0522(9)	0.0467(9)	0.0654(10)	0.0080(8)	0.0016(8)	0.0014(7)
C21	0.0589(10)	0.0575(11)	0.0771(12)	0.0073(9)	0.0079(9)	0.0059(8)
C22	0.0574(11)	0.0879(16)	0.0995(16)	0.0196(13)	0.0144(11)	0.0084(11)
C23	0.0554(12)	0.1040(19)	0.1095(18)	0.0273(15)	-0.0058(12)	-0.0064(12)
C24	0.0778(14)	0.0834(15)	0.0907(15)	0.0125(12)	-0.0261(12)	-0.0199(12)
C25	0.0687(11)	0.0611(11)	0.0672(11)	0.0067(9)	-0.0065(9)	-0.0040(9)
C26	0.0473(8)	0.0461(9)	0.0521(9)	-0.0028(7)	0.0112(7)	-0.0003(7)
C27	0.0620(10)	0.0654(12)	0.0599(11)	0.0028(9)	0.0100(8)	-0.0147(9)
C28	0.0617(11)	0.0823(14)	0.0749(13)	-0.0045(11)	0.0078(9)	-0.0245(10)
C29	0.0618(11)	0.0912(15)	0.0665(12)	-0.0129(11)	-0.0015(9)	-0.0076(10)
C30	0.0825(13)	0.0774(14)	0.0521(10)	-0.0013(9)	0.0022(9)	-0.0037(11)
C31	0.0735(11)	0.0576(11)	0.0566(10)	0.0013(8)	0.0097(8)	-0.0123(9)

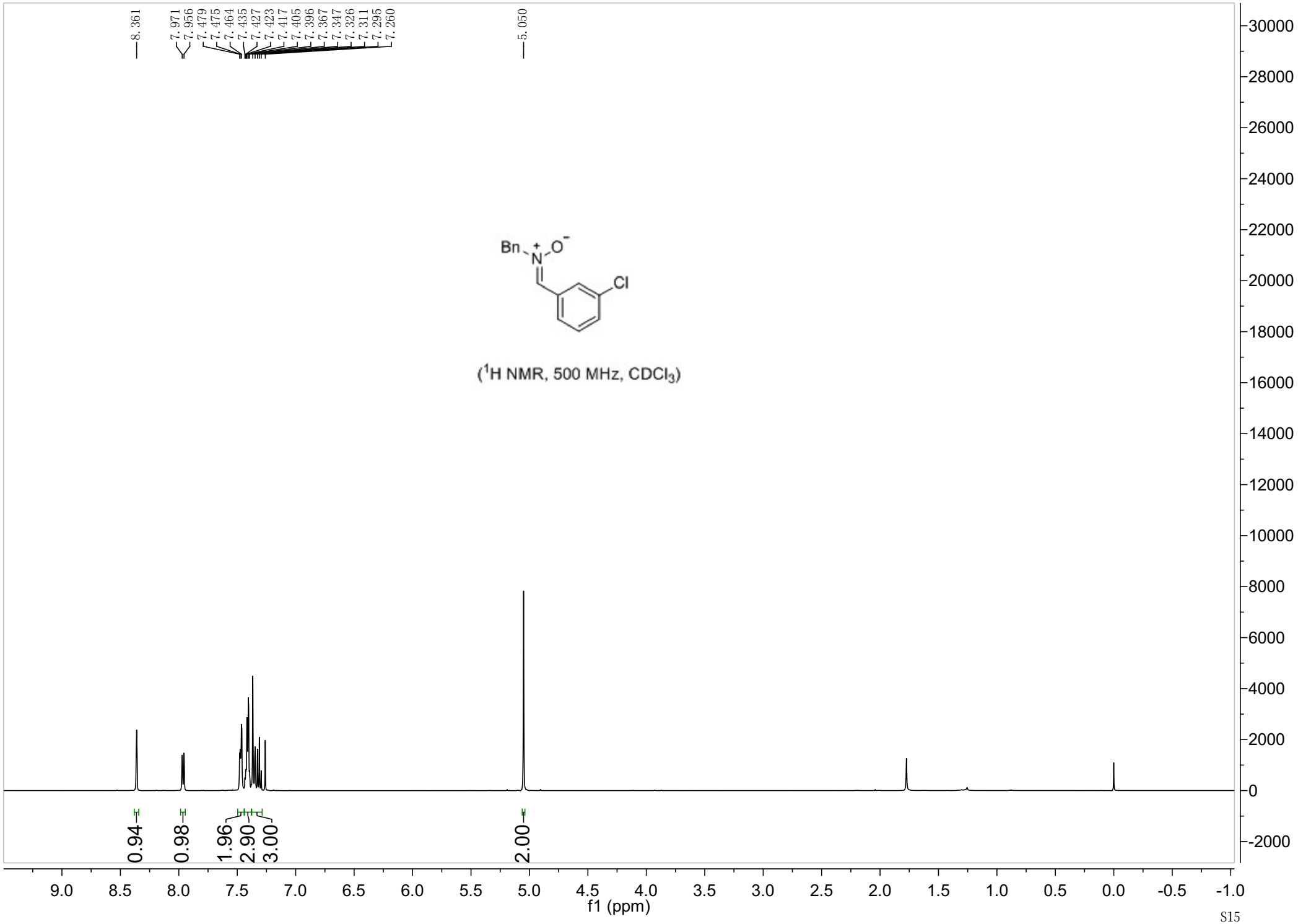
Table 9. Hydrogen atomic coordinates and isotropic atomic

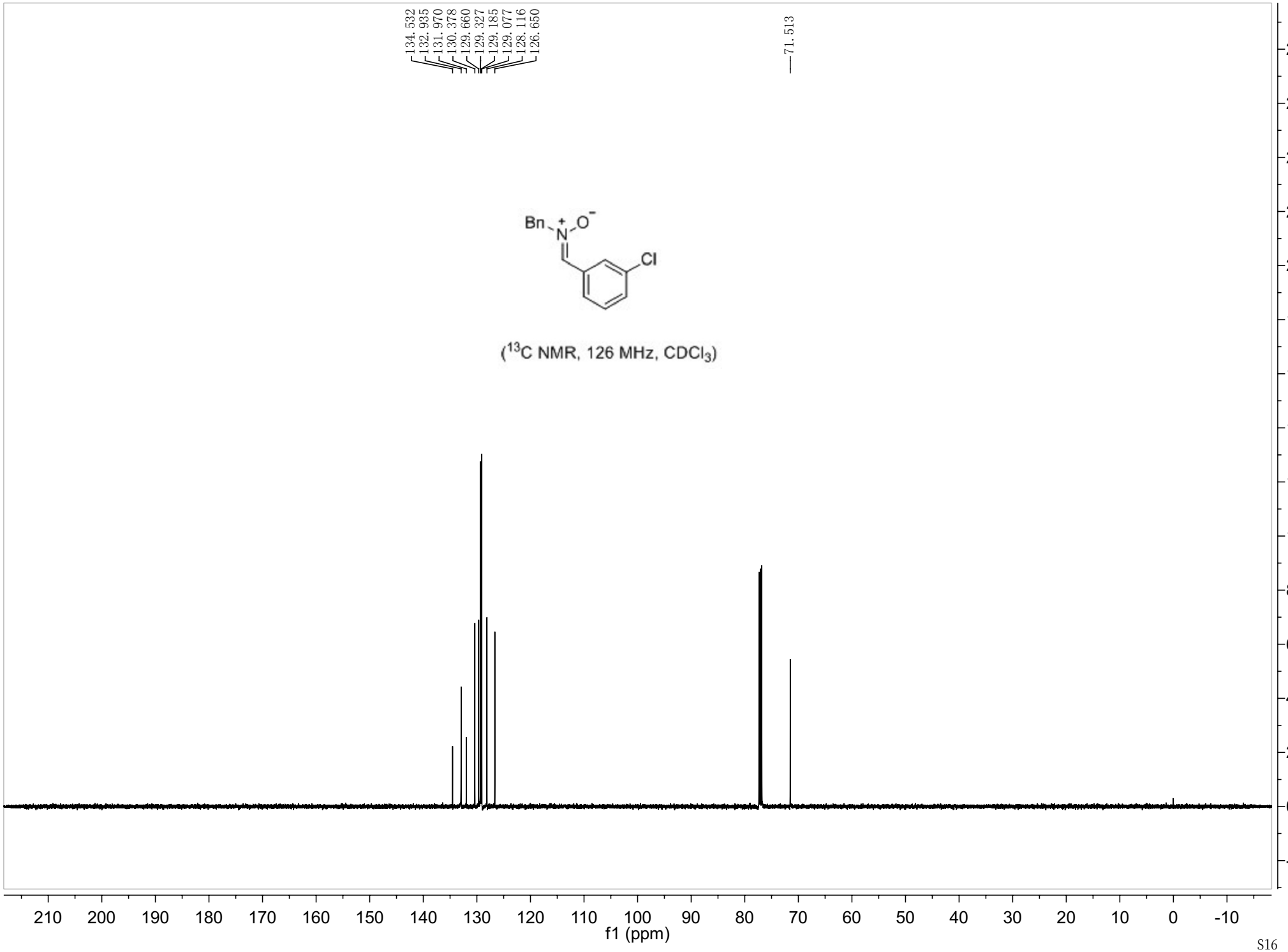
displacement parameters ($Å^2$) for 20191226hct1611.

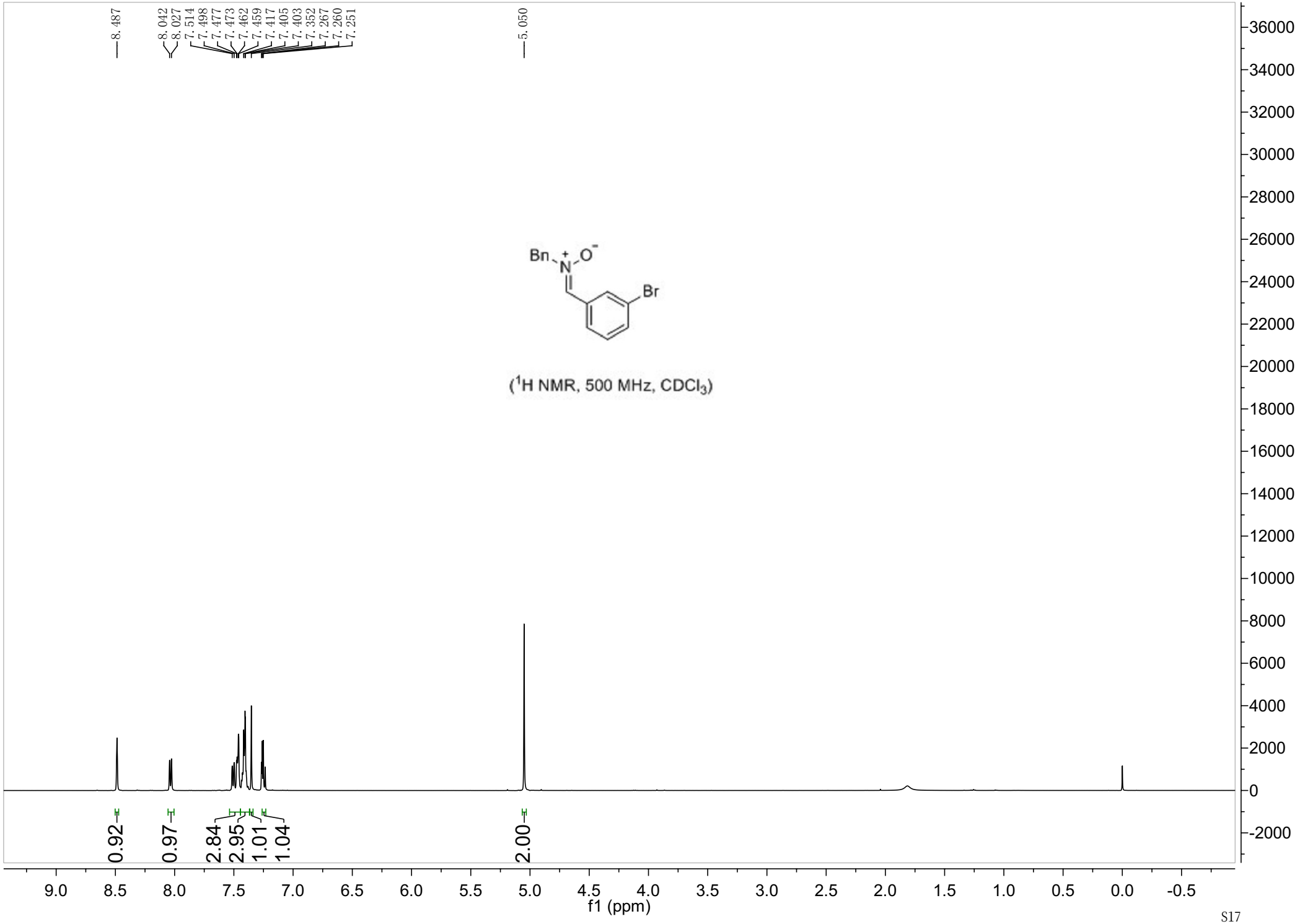
	x/a	y/b	z/c	U(eq)
H10	0.1697	-0.0923	0.4961	0.149
H1	0.1749	-0.0562	0.5676	0.149
H11	0.2620	-0.1545	0.5391	0.149
H12	0.2431	0.1275	0.5073	0.082
H13	0.3328	0.0700	0.5541	0.082
H14	0.3908	0.2704	0.4979	0.066
H15	0.5049	0.4217	0.4487	0.065
H6	0.7097	0.4200	0.2254	0.072
H7	0.8012	0.3066	0.2294	0.072
H3	0.9972	0.4377	0.2510	0.076
H27	1.1119	0.5910	0.2040	0.088
H2	1.0465	0.7456	0.1310	0.089
H4	0.7493	0.5898	0.1508	0.088
H5	0.8652	0.7429	0.1038	0.102
H26	0.7489	0.6267	0.2909	0.058
H8	0.4688	-0.0235	0.3740	0.068
H9	0.5831	0.1279	0.3258	0.067
H16	0.3951	0.7354	0.4132	0.077
H20	0.2120	0.6871	0.4139	0.098
H17	0.1396	0.5263	0.3469	0.108
H18	0.2488	0.4091	0.2791	0.101
H19	0.4344	0.4499	0.2796	0.079
H21	0.8917	0.7672	0.3284	0.075
H22	1.0078	0.8473	0.4061	0.087
H25	1.0081	0.7476	0.5034	0.088
H23	0.8901	0.5694	0.5241	0.085
H24	0.7714	0.4917	0.4472	0.075

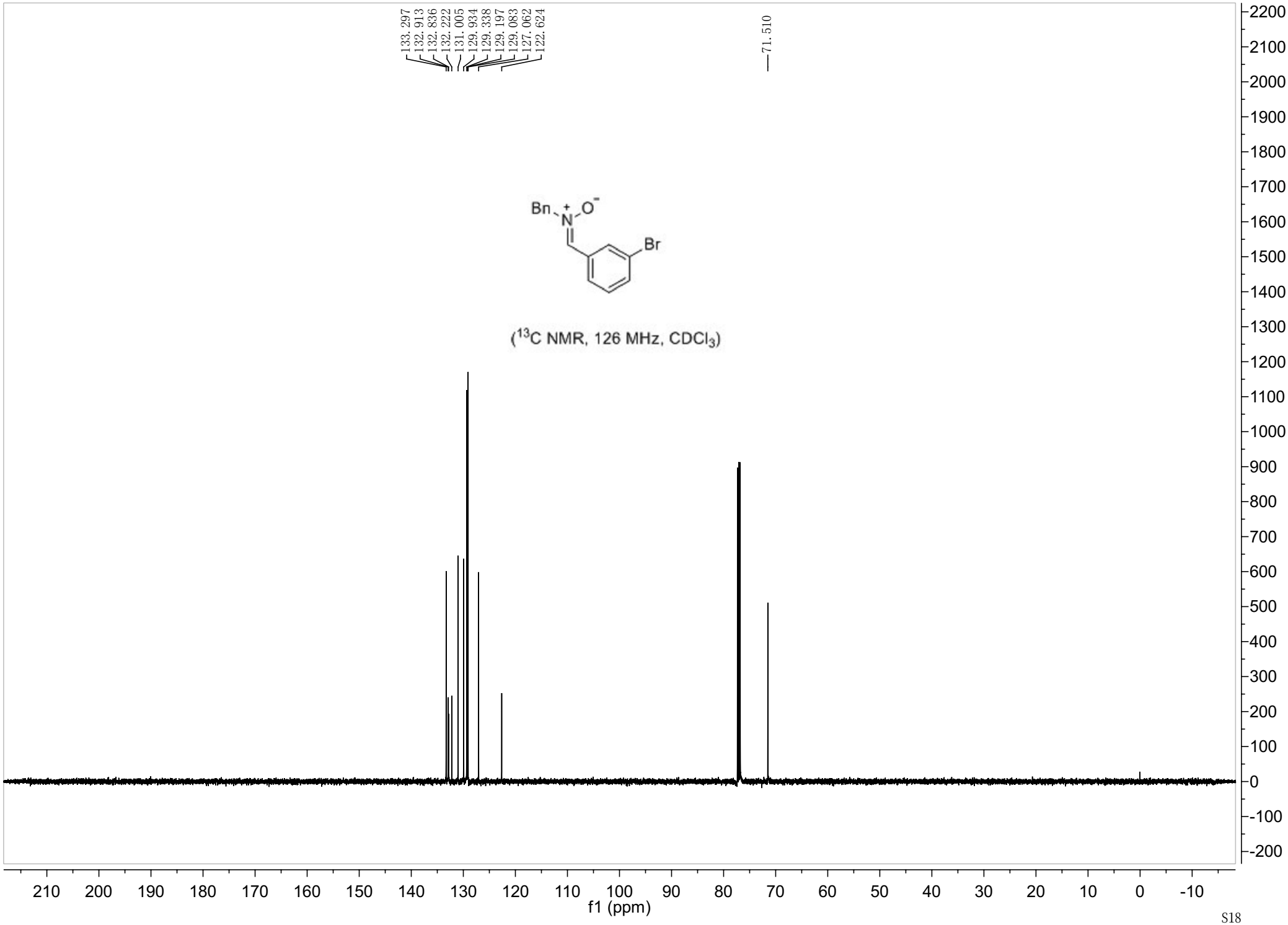

8.215
8.207
8.204
8.201
8.196
7.481
7.469
7.416
7.404
7.390
7.383
7.255
5.048
Bn
N
O
(^{1}H NMR, 500 MHz, $CDCl_3$)
2.00
1.99
7.00
2.00
f1 (ppm)

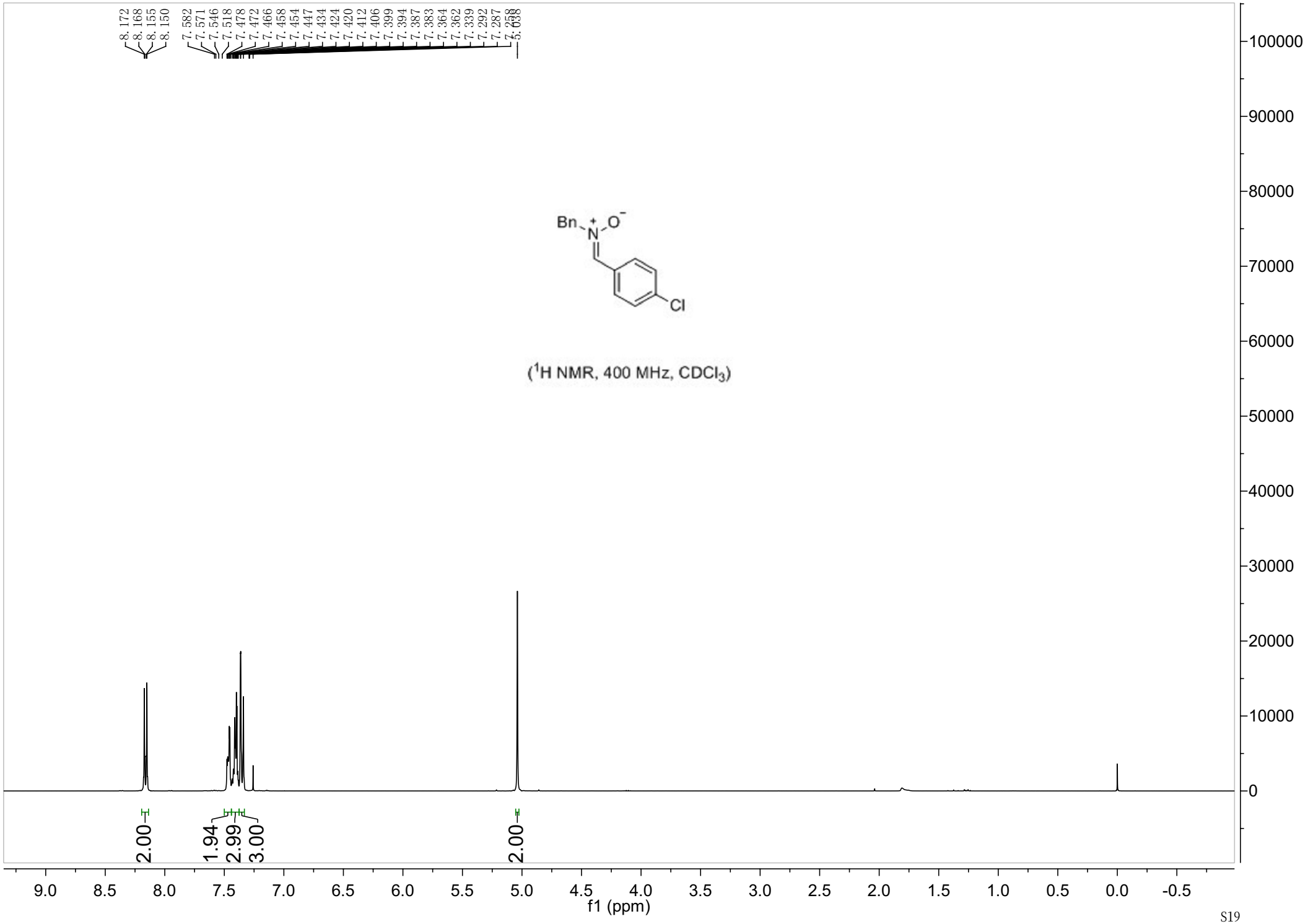

9.311
9.306
9.292
7.933
7.508
7.495
7.442
7.437
7.425
7.410
7.401
7.397
7.387
7.382
7.323
7.319
7.316
7.310
7.304
7.302
7.297
7.259
5.099
Bn
N
O
Cl
(1H NMR, 500 MHz, CDCl3)
0.97
0.97
1.93
3.91
1.99
2.00
f1 (ppm)

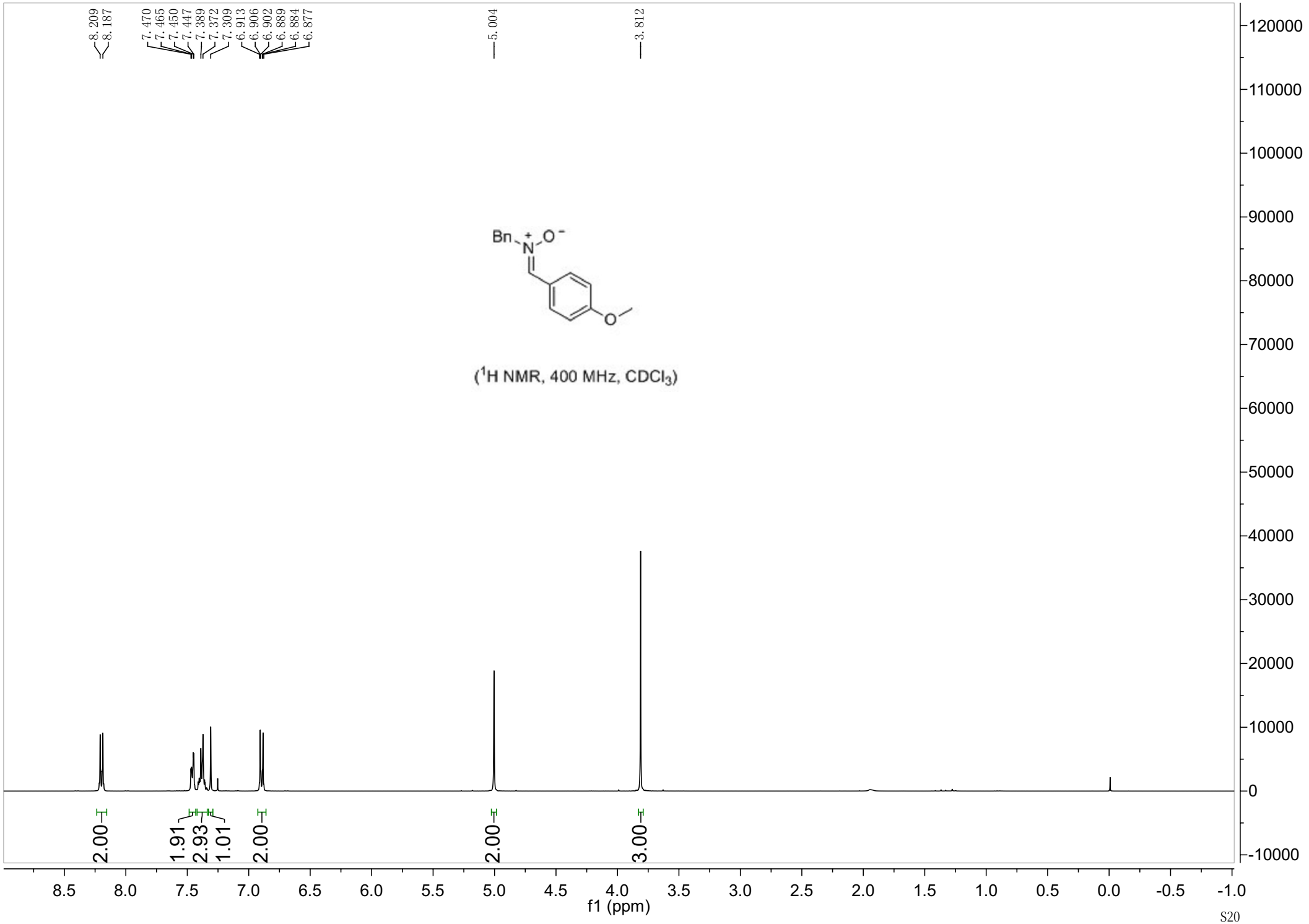

8.361
7.971
7.956
7.479
7.475
7.464
7.435
7.427
7.423
7.417
7.405
7.396
7.367
7.347
7.326
7.311
7.295
7.260
5.050
Bn
N
O
Cl
(1H NMR, 500 MHz, CDCl3)
0.94
0.98
1.96
2.90
3.00
2.00
f1 (ppm)

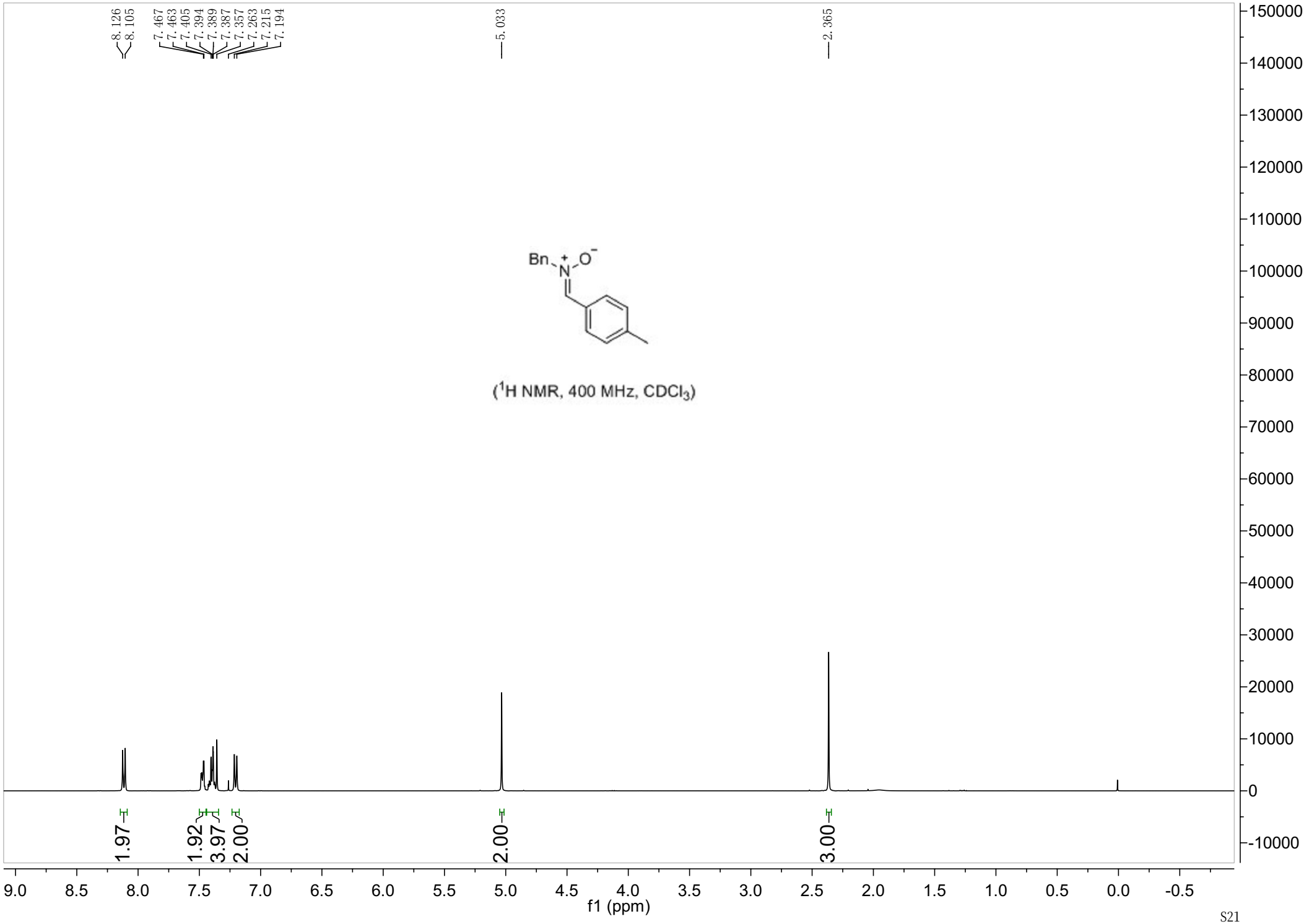

134.532
132.935
131.970
130.378
129.660
129.327
129.185
129.077
128.116
126.650
71.513
Bn
N
O
Cl
(13C NMR, 126 MHz, CDCl3)
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.487
8.042
8.027
7.514
7.498
7.477
7.473
7.462
7.459
7.417
7.405
7.403
7.352
7.267
7.260
7.251
5.050
Bn
N
O
Br
(1H NMR, 500 MHz, CDCl3)
0.92
0.97
2.84
2.95
1.01
1.04
2.00
f1 (ppm)

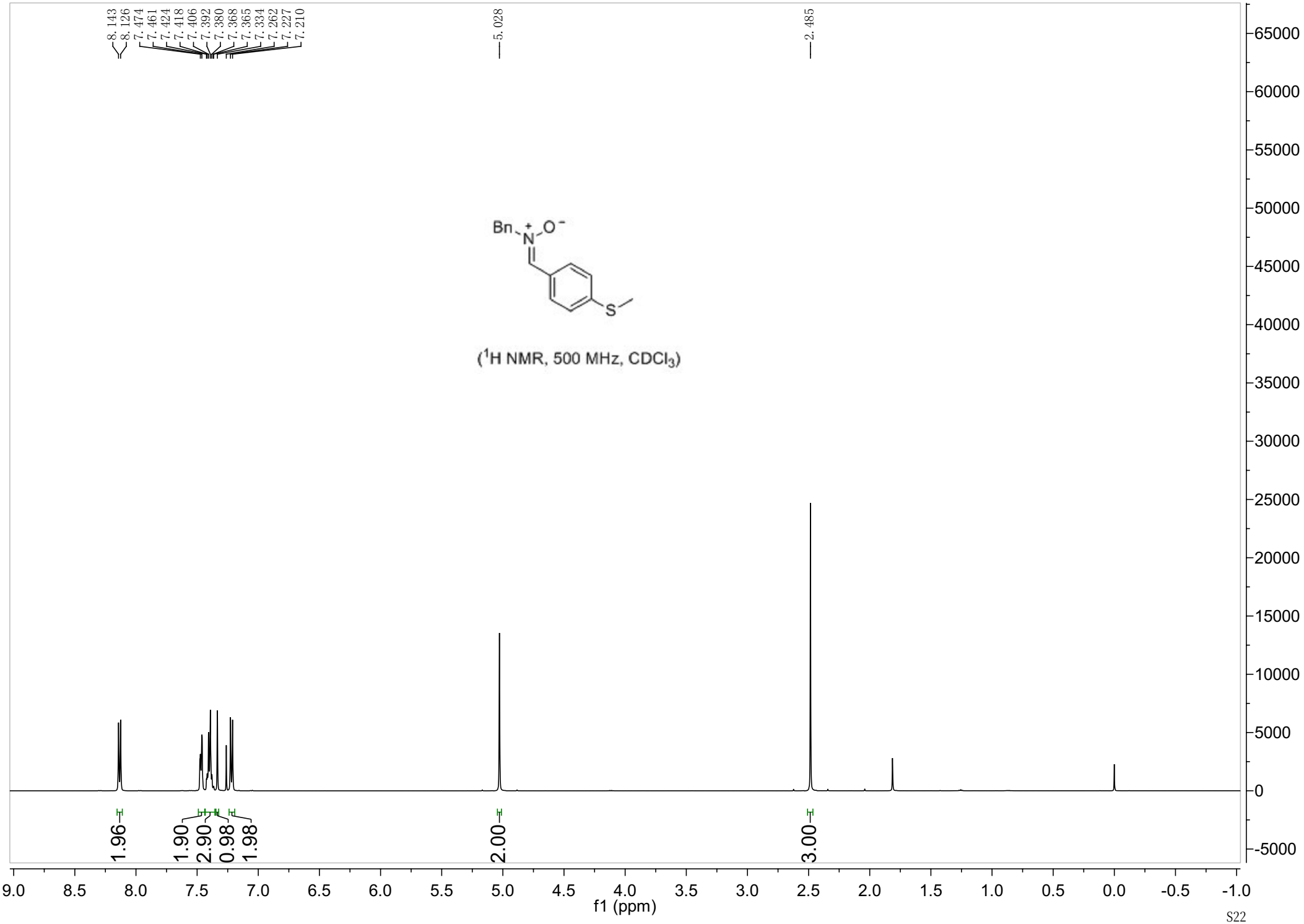

133.297
132.913
132.836
132.222
131.005
129.934
129.338
129.197
129.083
127.062
122.624
71.510
Bn
N
O
Br
(13C NMR, 126 MHz, CDCl3)
f1 (ppm)

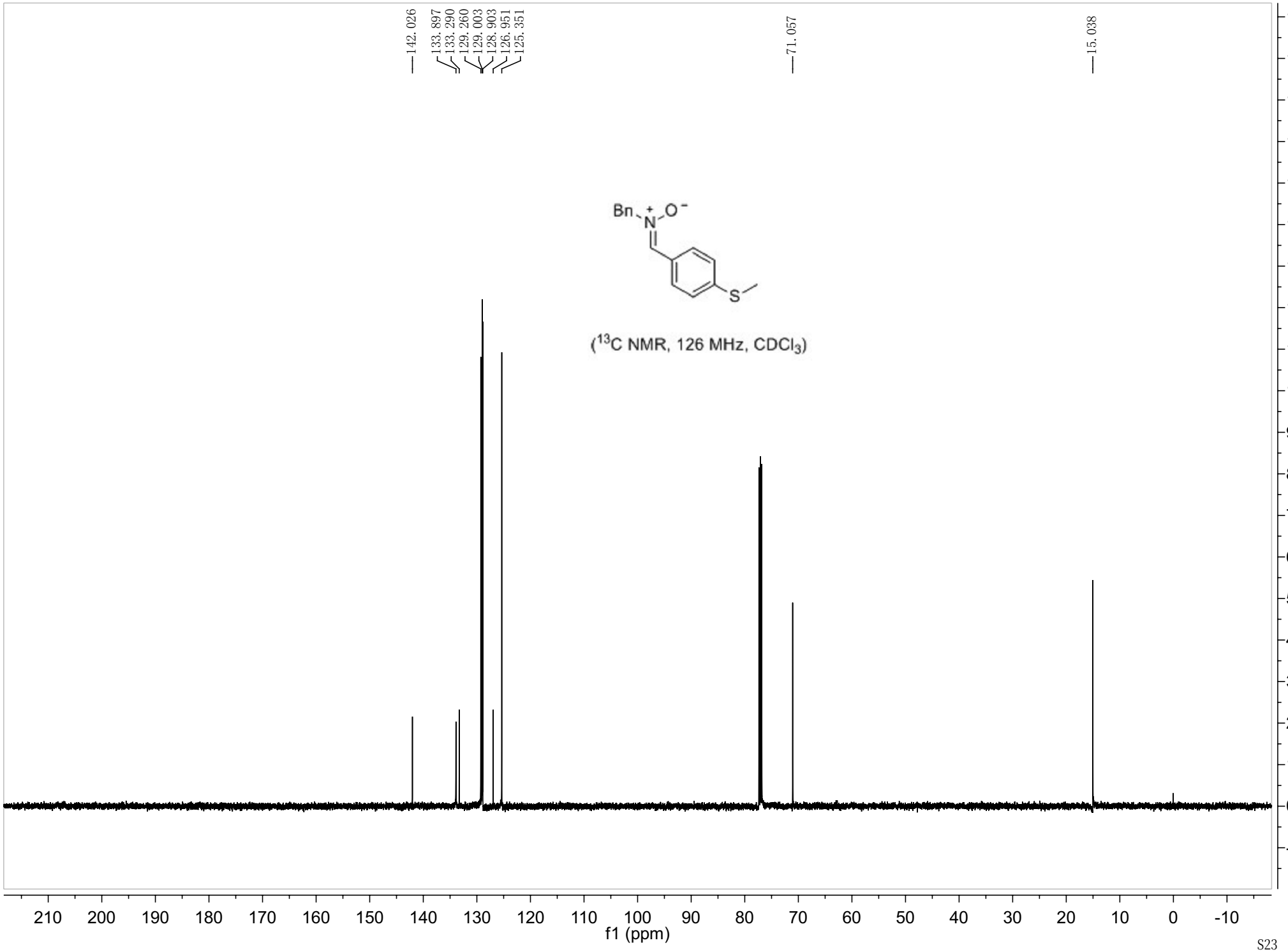

8.172
8.168
8.155
8.150
7.582
7.571
7.546
7.518
7.478
7.472
7.466
7.458
7.454
7.447
7.434
7.424
7.420
7.412
7.406
7.399
7.394
7.387
7.383
7.364
7.362
7.339
7.292
7.287
5.038
Bn
N
O
Cl
(1H NMR, 400 MHz, CDCl3)
2.00
1.94
2.99
3.00
2.00
f1 (ppm)

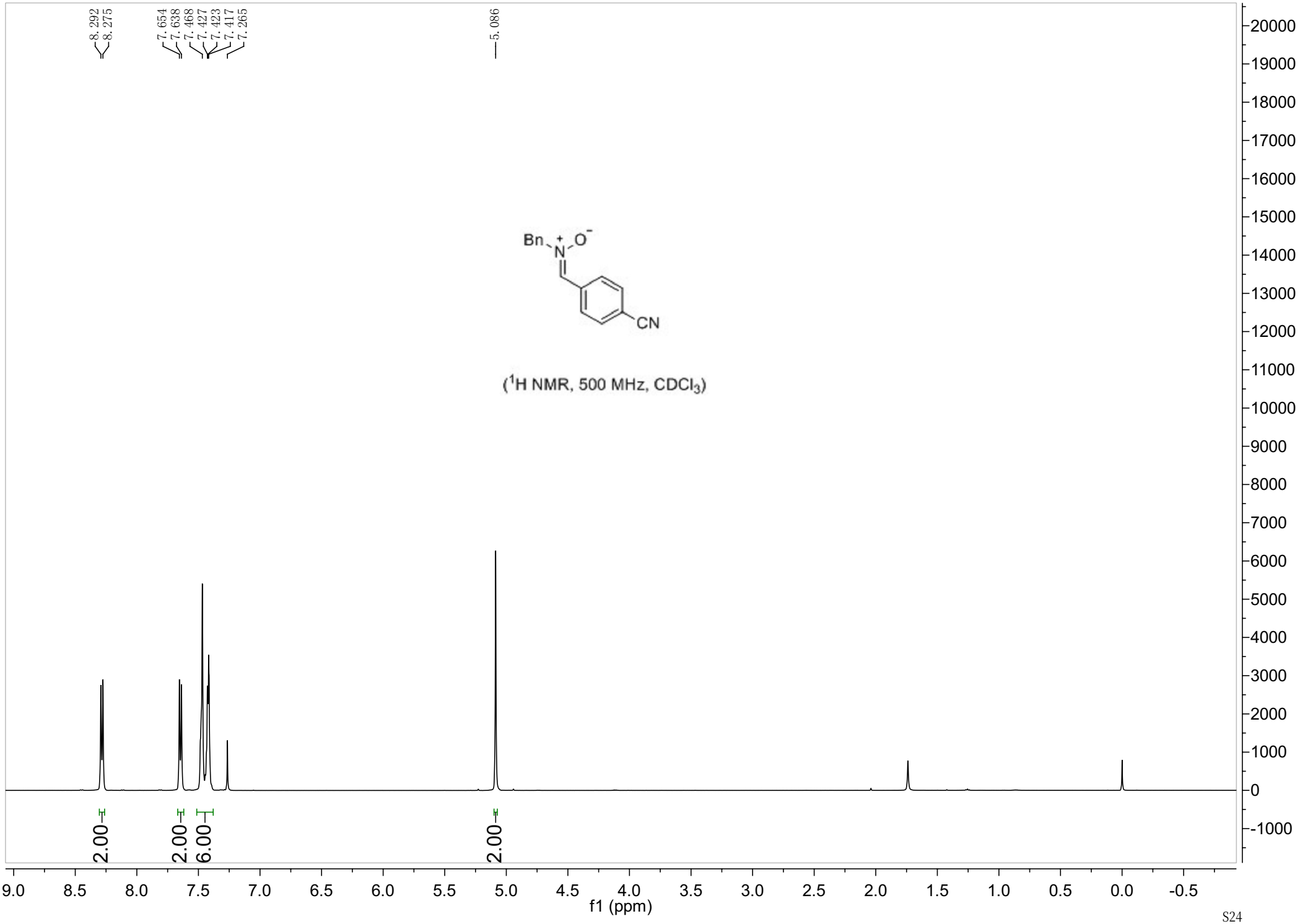

8.209
8.187
7.470
7.465
7.450
7.447
7.389
7.372
7.309
6.913
6.906
6.902
6.889
6.884
6.877
5.004
3.812
Bn
N
O
O
(1H NMR, 400 MHz, CDCl3)
2.00
1.91
2.93
1.01
2.00
2.00
3.00
f1 (ppm)

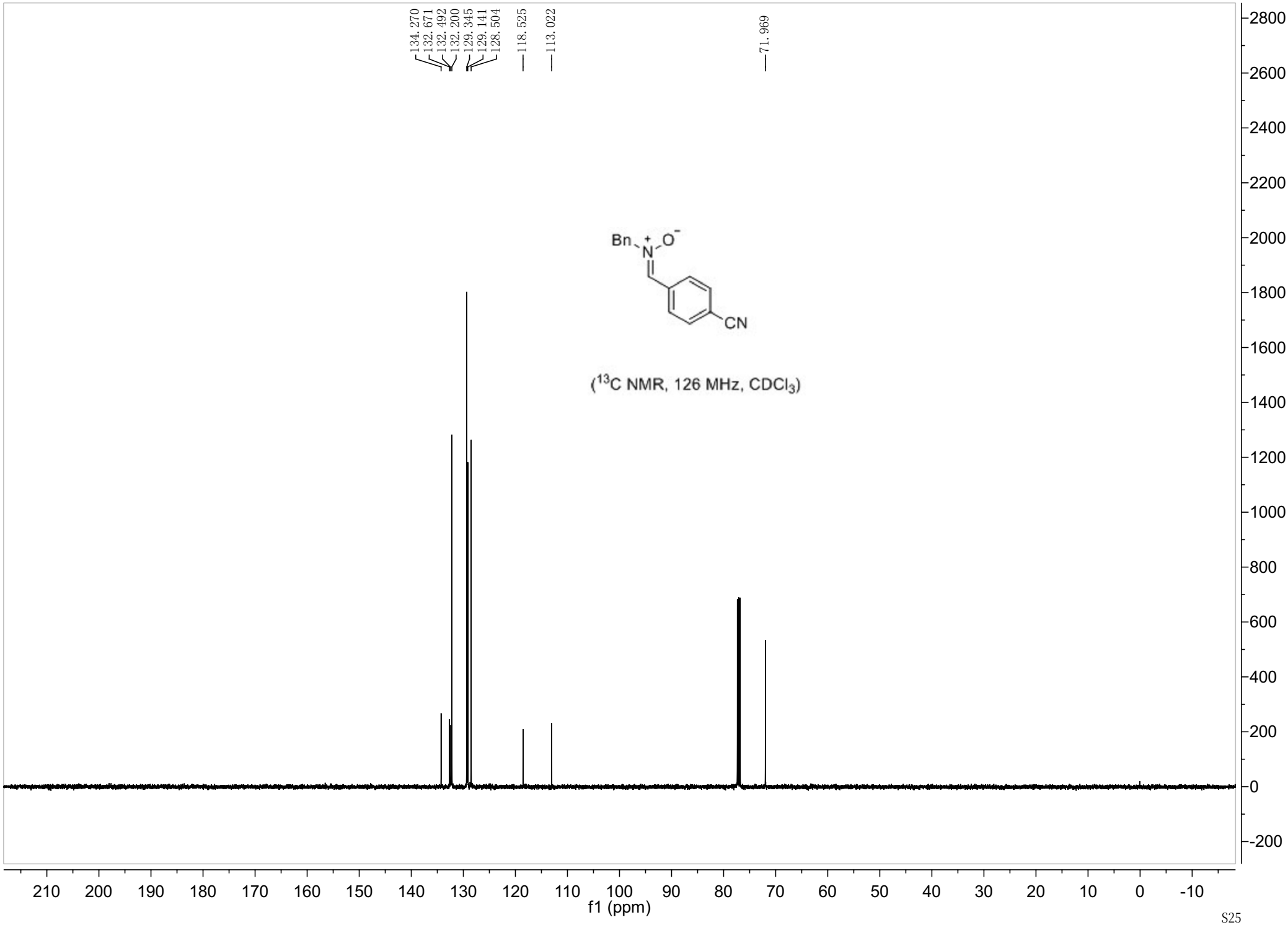


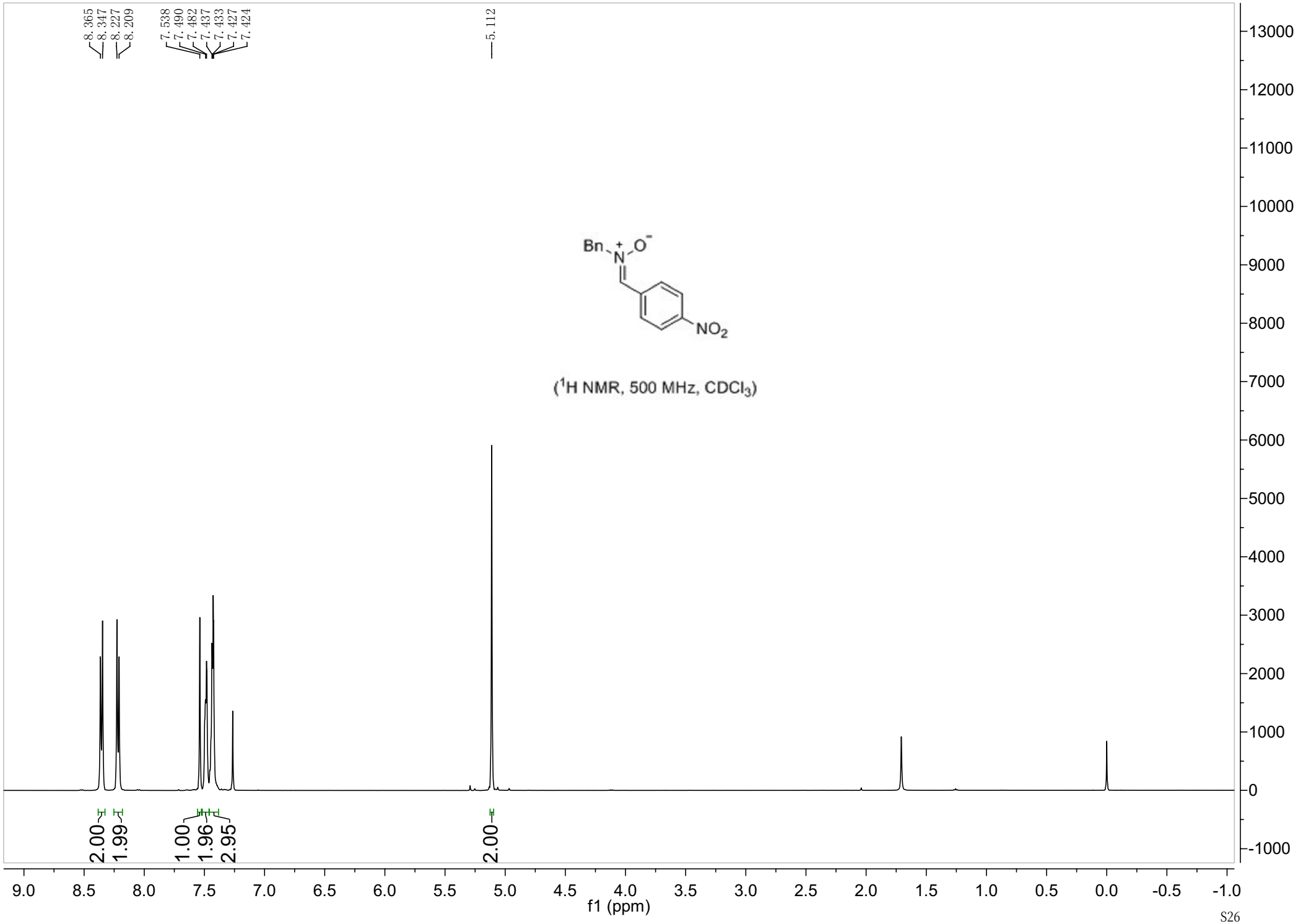
(^{1}H NMR, 400 MHz, $CDCl_3$)

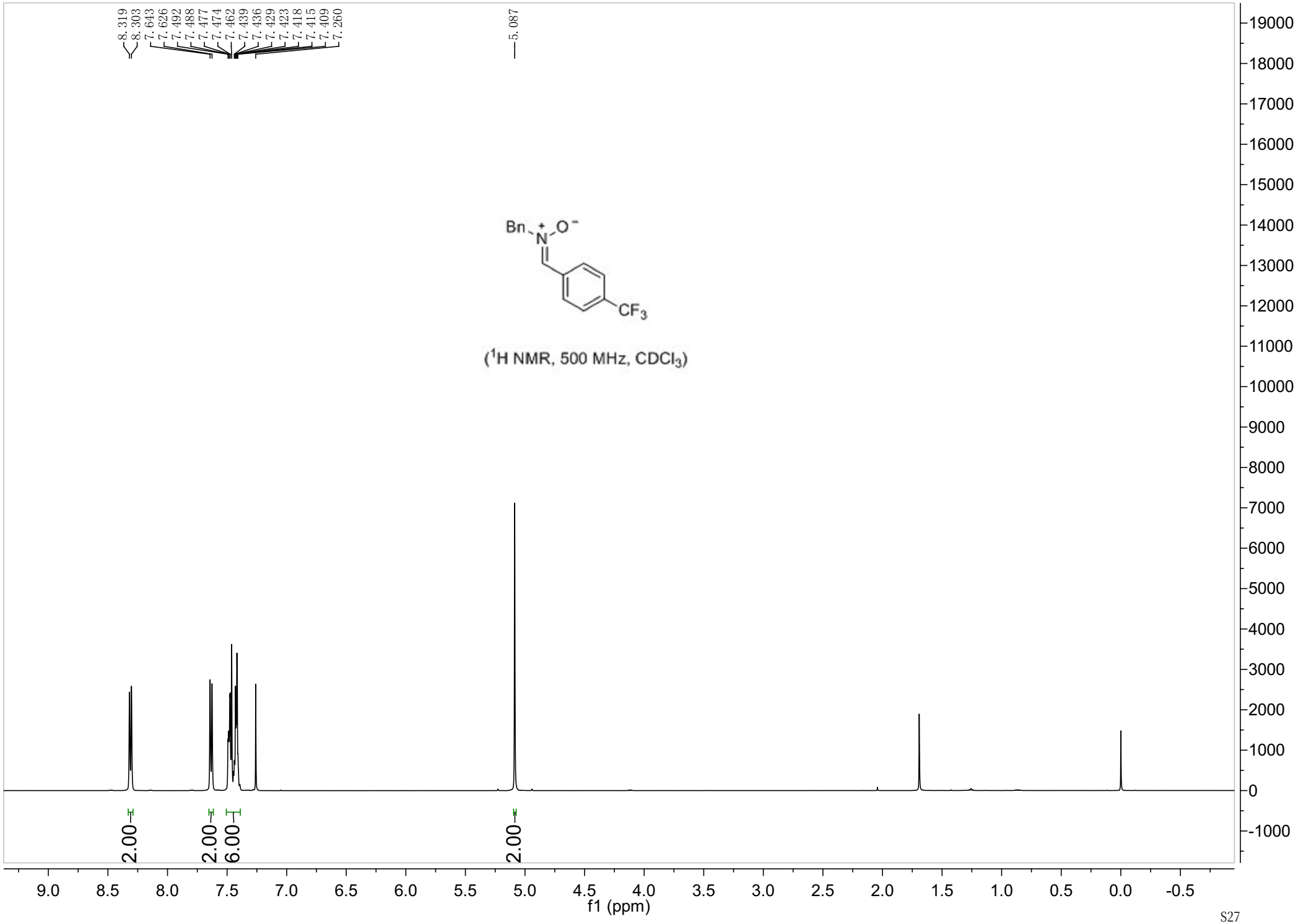

8.143
8.126
7.474
7.461
7.424
7.418
7.406
7.392
7.380
7.368
7.365
7.334
7.262
7.227
7.210
5.028
2.485
Bn
N
O
S
(1H NMR, 500 MHz, CDCl3)
1.96
1.90
2.90
0.98
1.98
2.00
3.00
f1 (ppm)

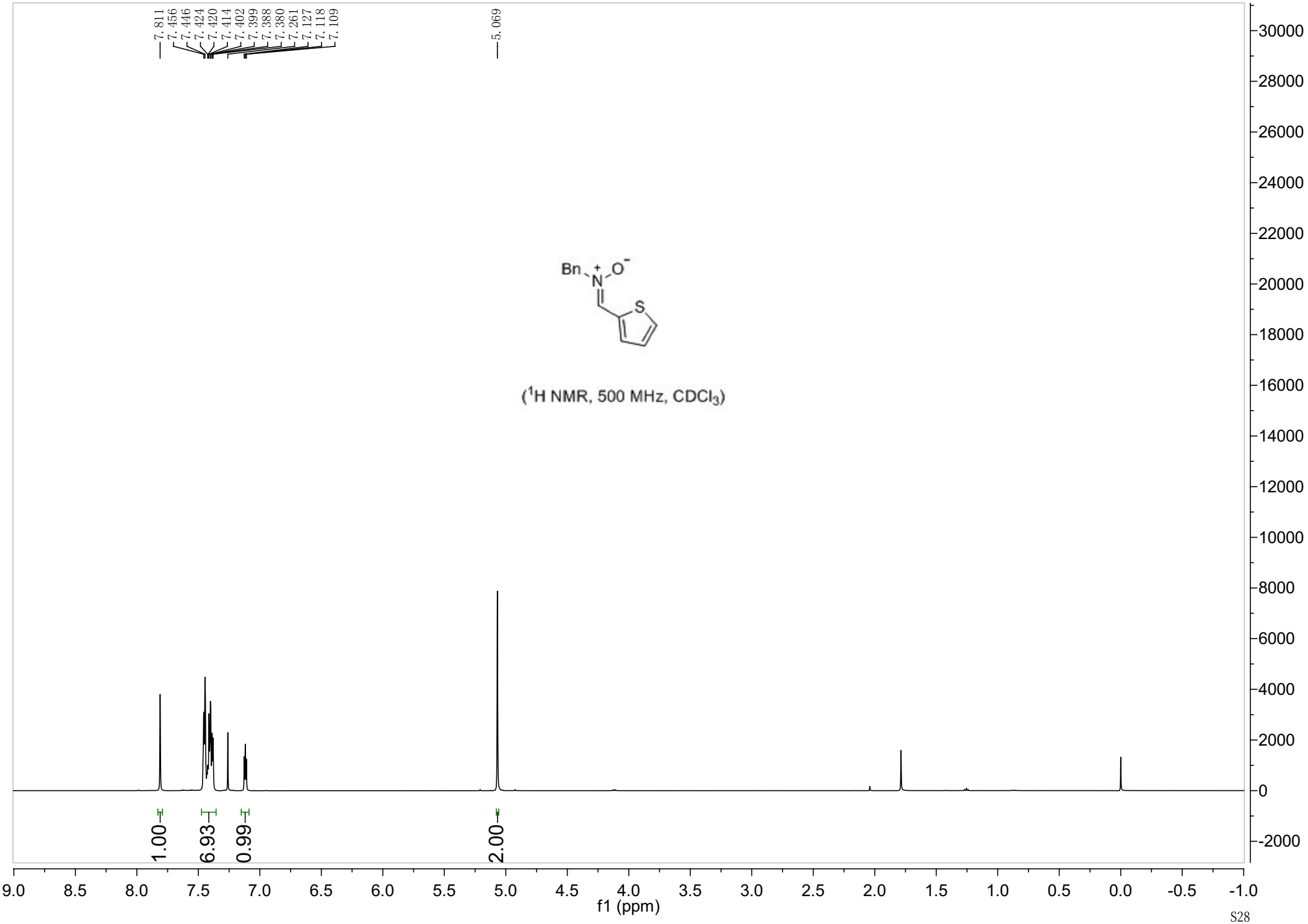

142.026
133.897
133.290
129.260
129.003
128.903
126.951
125.351
71.057
15.038
Bn
N
O
S
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

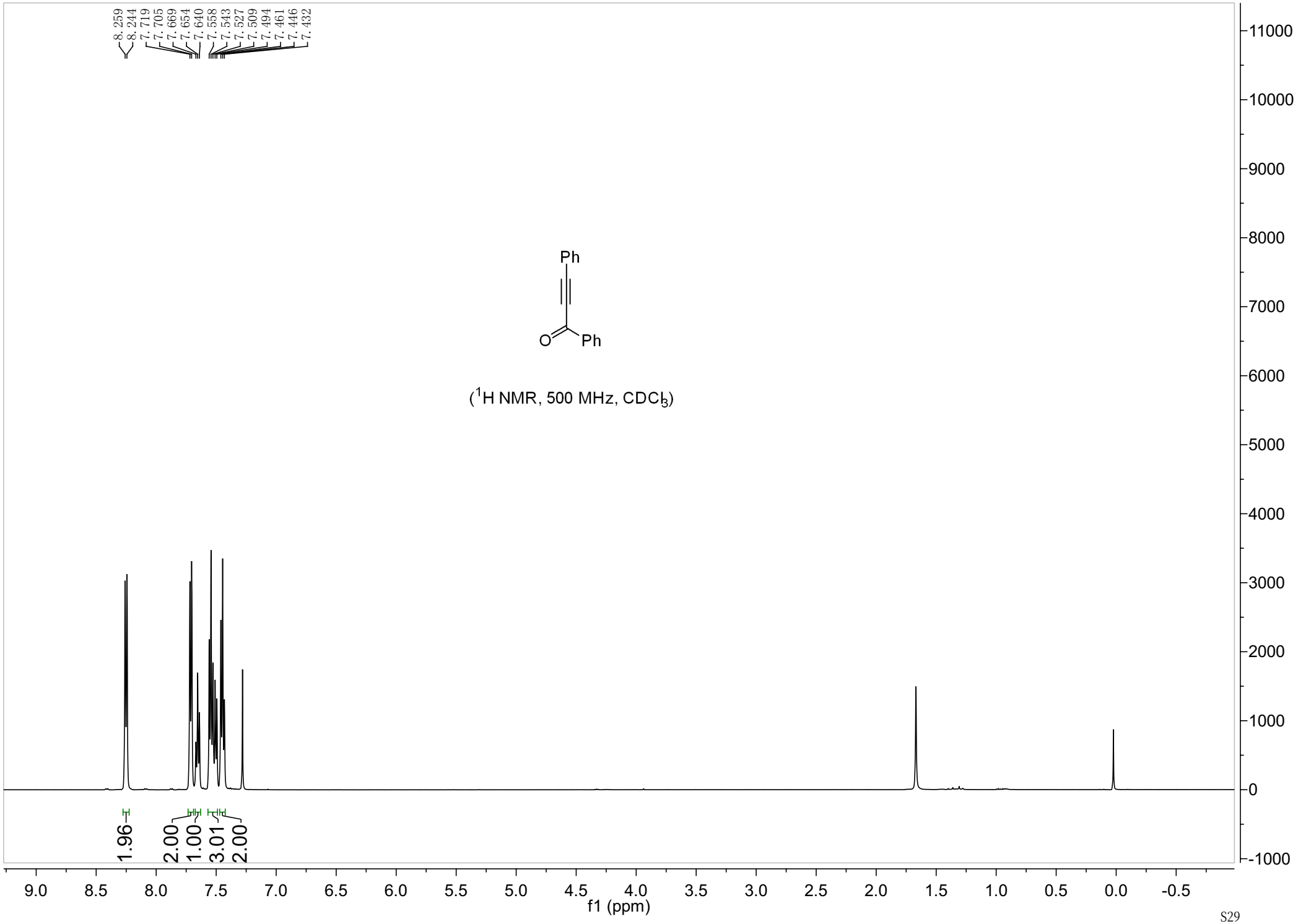

8.292
8.275
7.654
7.638
7.468
7.427
7.423
7.417
7.265
5.086
Bn
N
O
CN
(1H NMR, 500 MHz, CDCl3)
2.00
2.00
6.00
2.00
f1 (ppm)

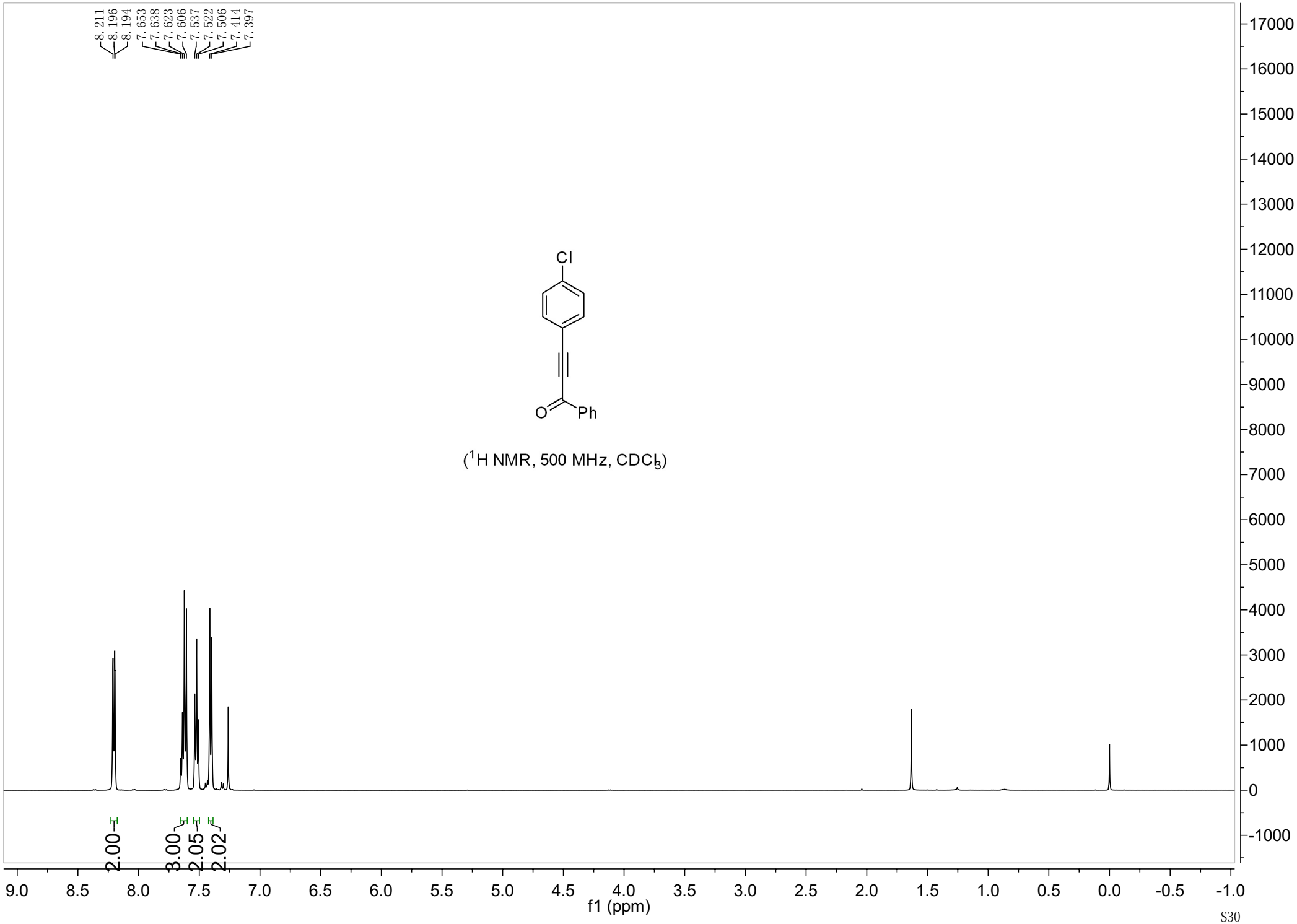

134.270
132.671
132.492
132.200
129.345
129.141
128.504
118.525
113.022
71.969
Bn
N
O
CN
(13C NMR, 126 MHz, CDCl3)
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

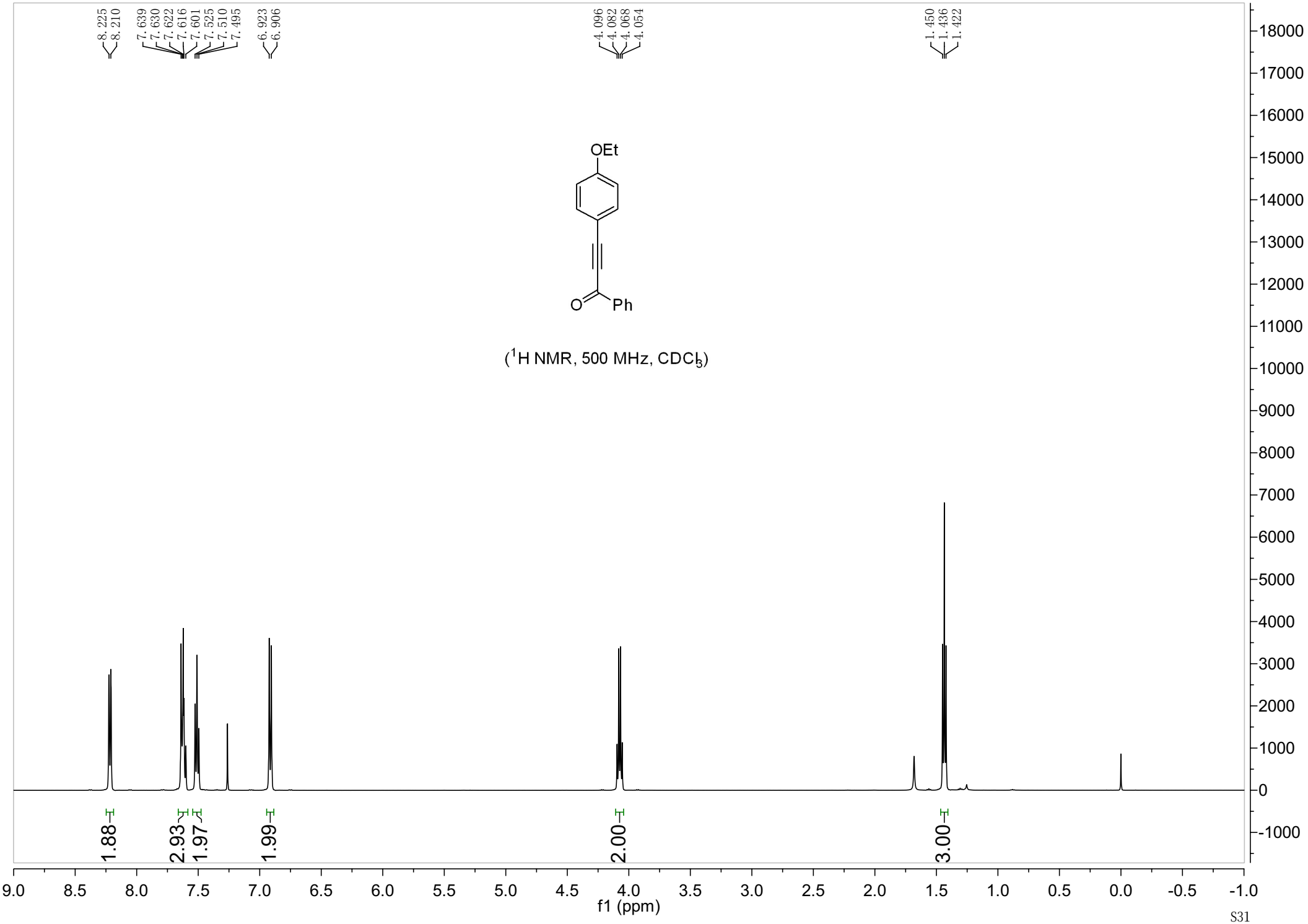

8.365
8.347
8.227
8.209
7.538
7.490
7.482
7.437
7.433
7.427
7.424
5.112
Bn
N
O
NO2
(1H NMR, 500 MHz, CDCl3)
2.00
1.99
1.00
1.96
2.95
2.00
f1 (ppm)

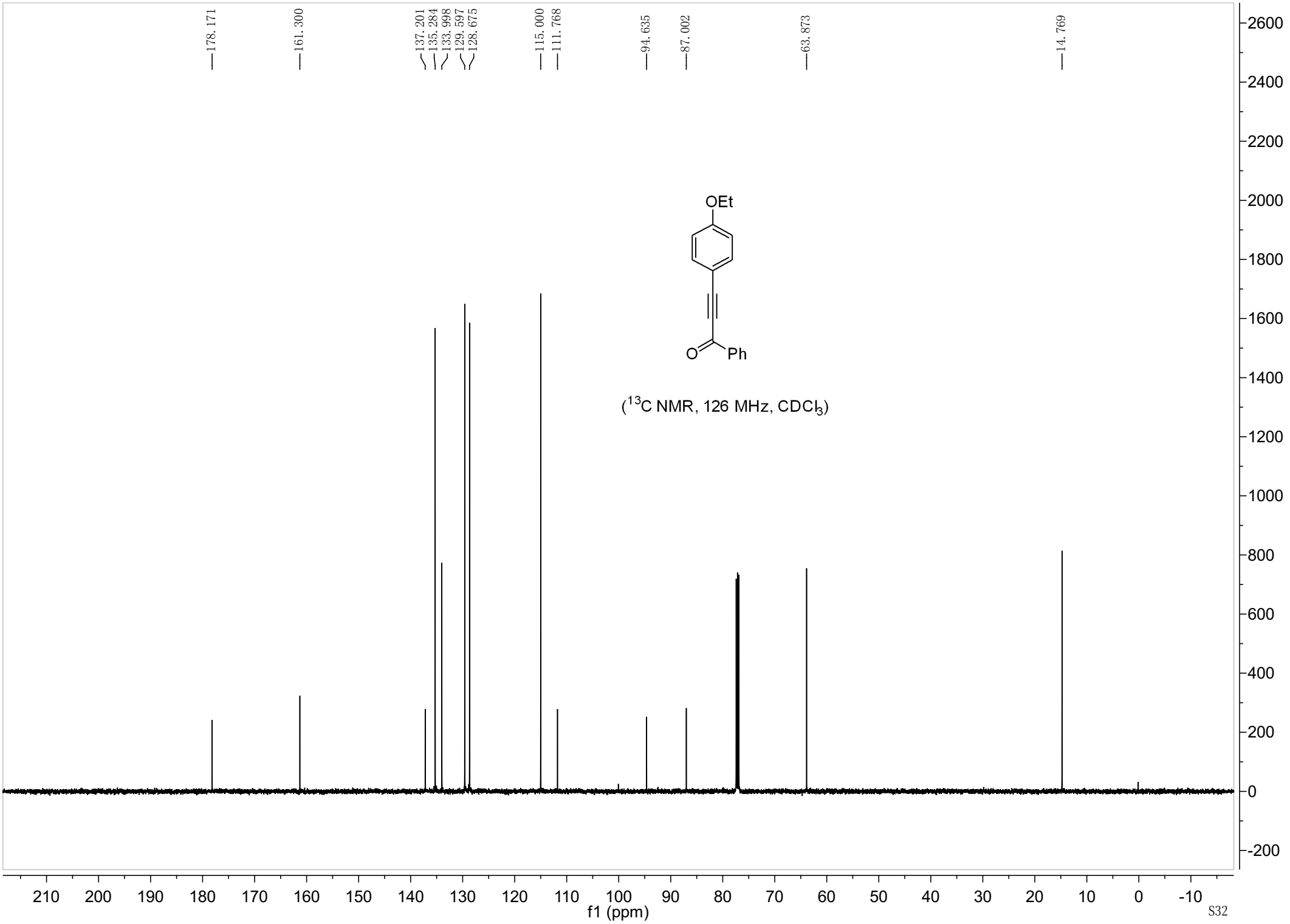

8.319
8.303
7.643
7.626
7.492
7.488
7.477
7.474
7.462
7.439
7.436
7.429
7.423
7.418
7.415
7.409
7.260
5.087
Bn
N
O
CF3
(1H NMR, 500 MHz, CDCl3)
2.00
2.00
6.00
2.00
f1 (ppm)

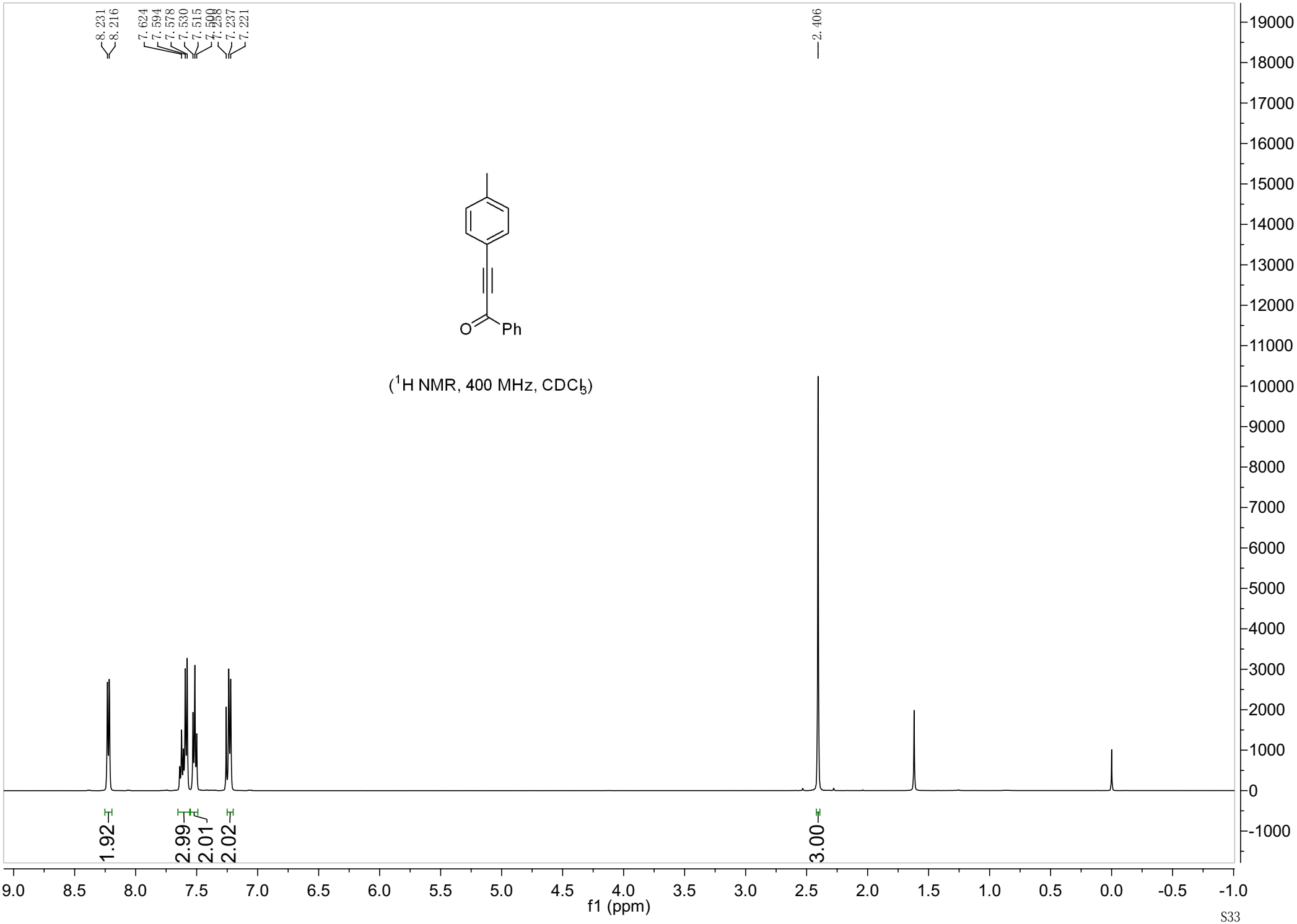

7.811
7.456
7.446
7.424
7.420
7.414
7.402
7.399
7.388
7.380
7.261
7.127
7.118
7.109
5.069
Bn
N
O
S
(1H NMR, 500 MHz, CDCl3)
1.00
6.93
0.99
2.00
f1 (ppm)

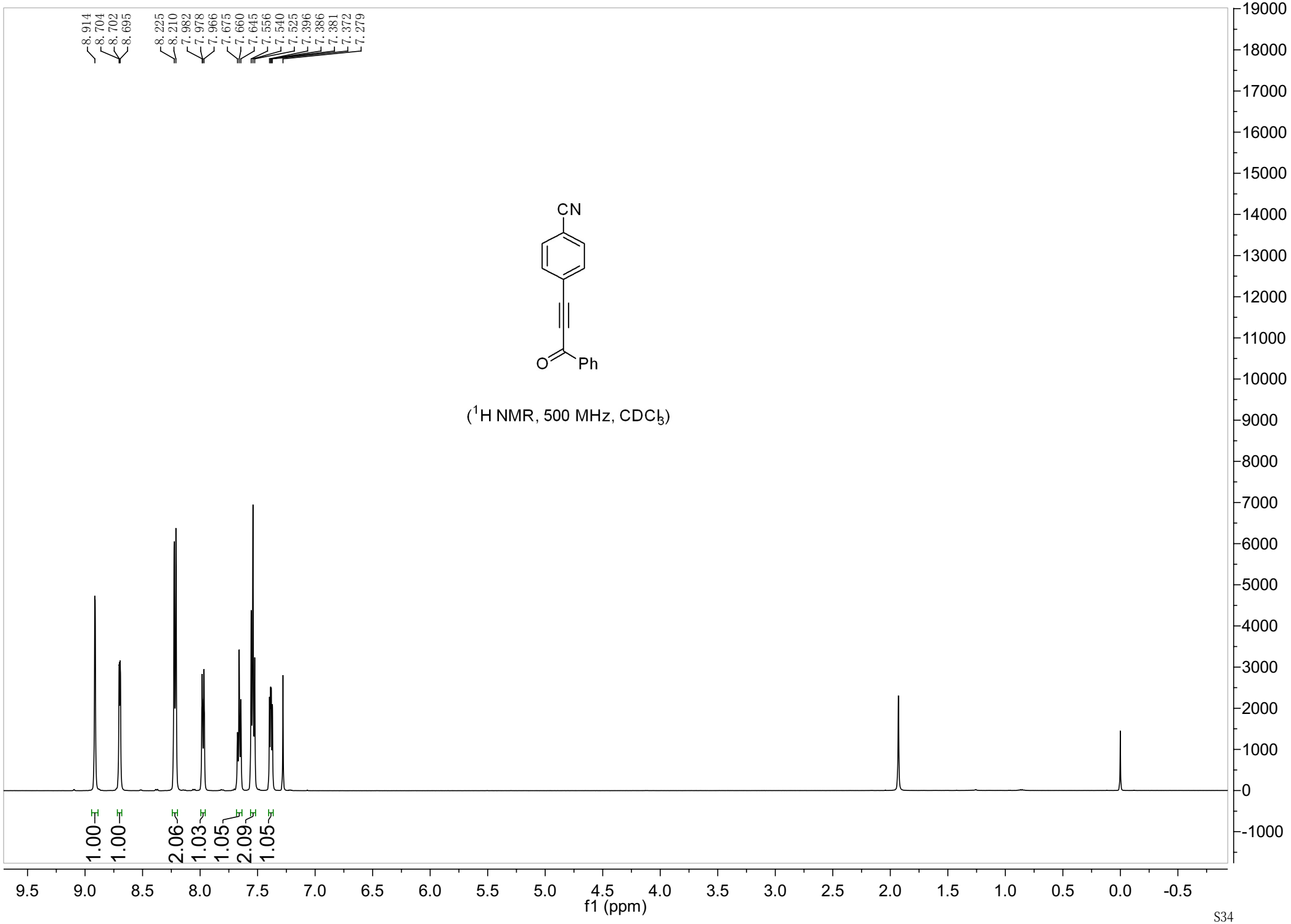

8.259
8.244
7.719
7.705
7.669
7.654
7.640
7.558
7.543
7.527
7.509
7.494
7.461
7.446
7.432
Ph
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.96
2.00
1.00
3.01
2.00
f1 (ppm)

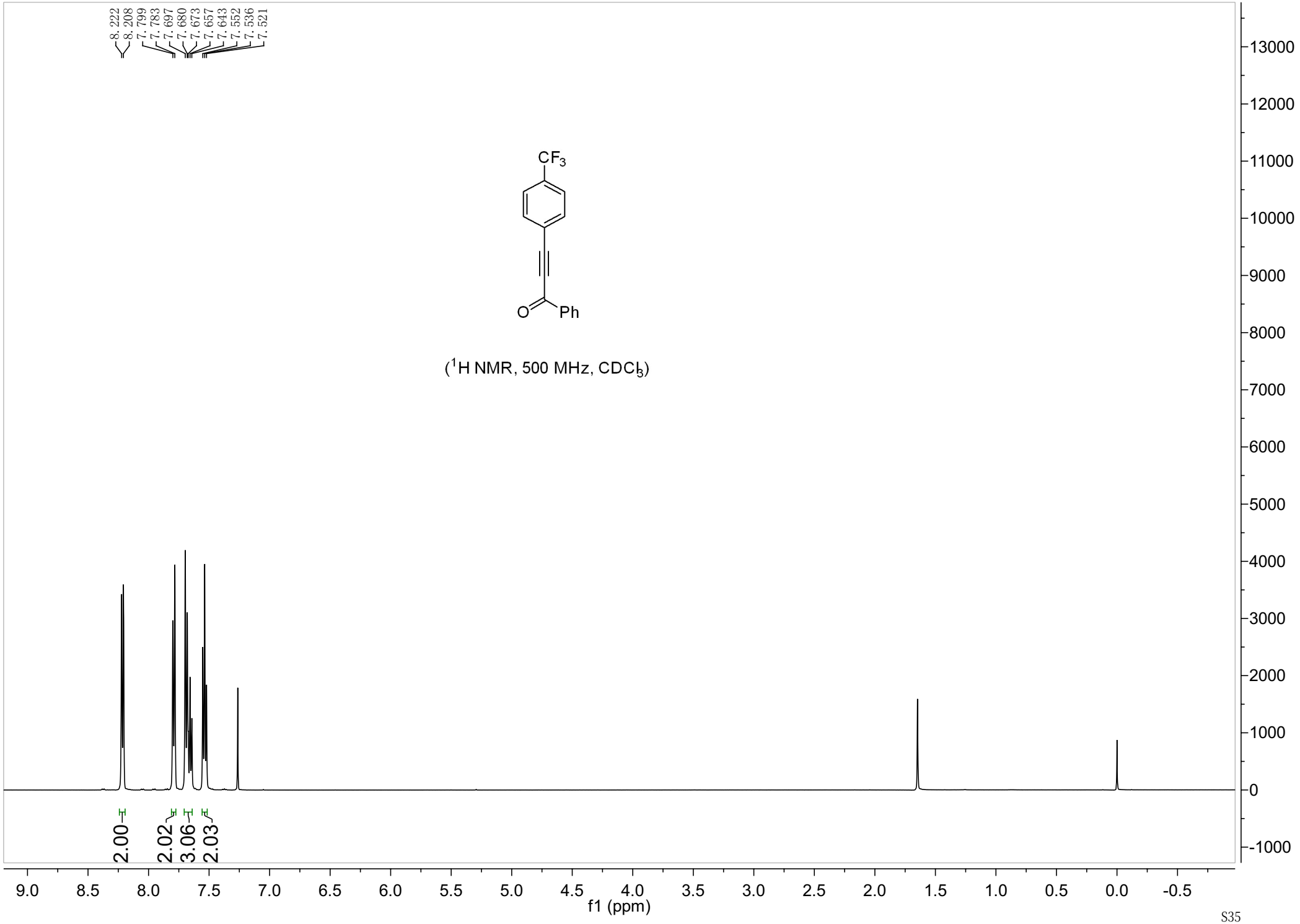

8.211
8.196
8.194
7.653
7.638
7.623
7.606
7.537
7.522
7.506
7.414
7.397
Cl
O
Ph
(1H NMR, 500 MHz, CDCl3)
2.00
3.00
2.05
2.02
f1 (ppm)

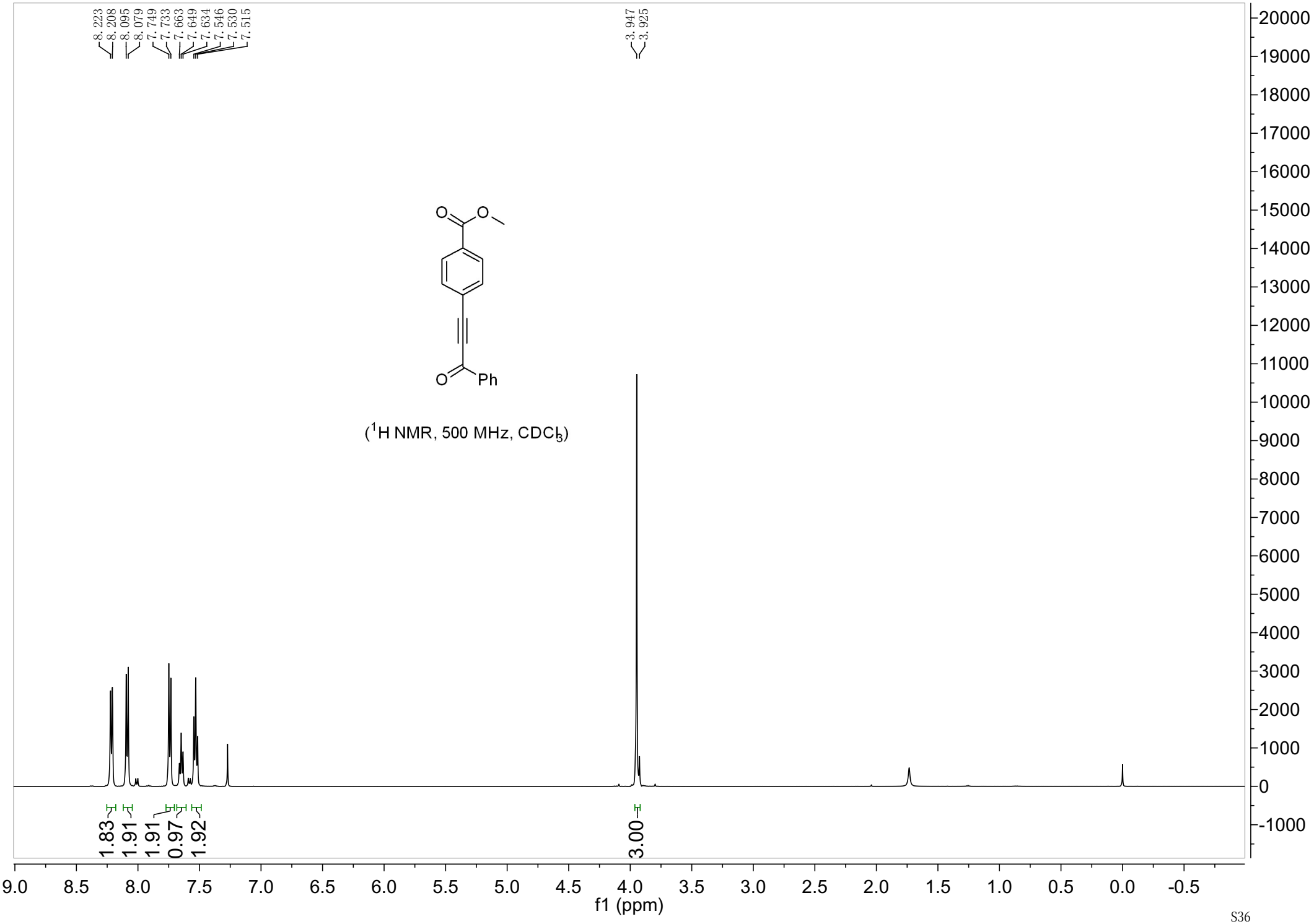

8.225
8.210
7.639
7.630
7.622
7.616
7.601
7.525
7.510
7.495
6.923
6.906
4.096
4.082
4.068
4.054
1.450
1.436
1.422
OEt
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.88
2.93
1.97
1.99
2.00
3.00
f1 (ppm)

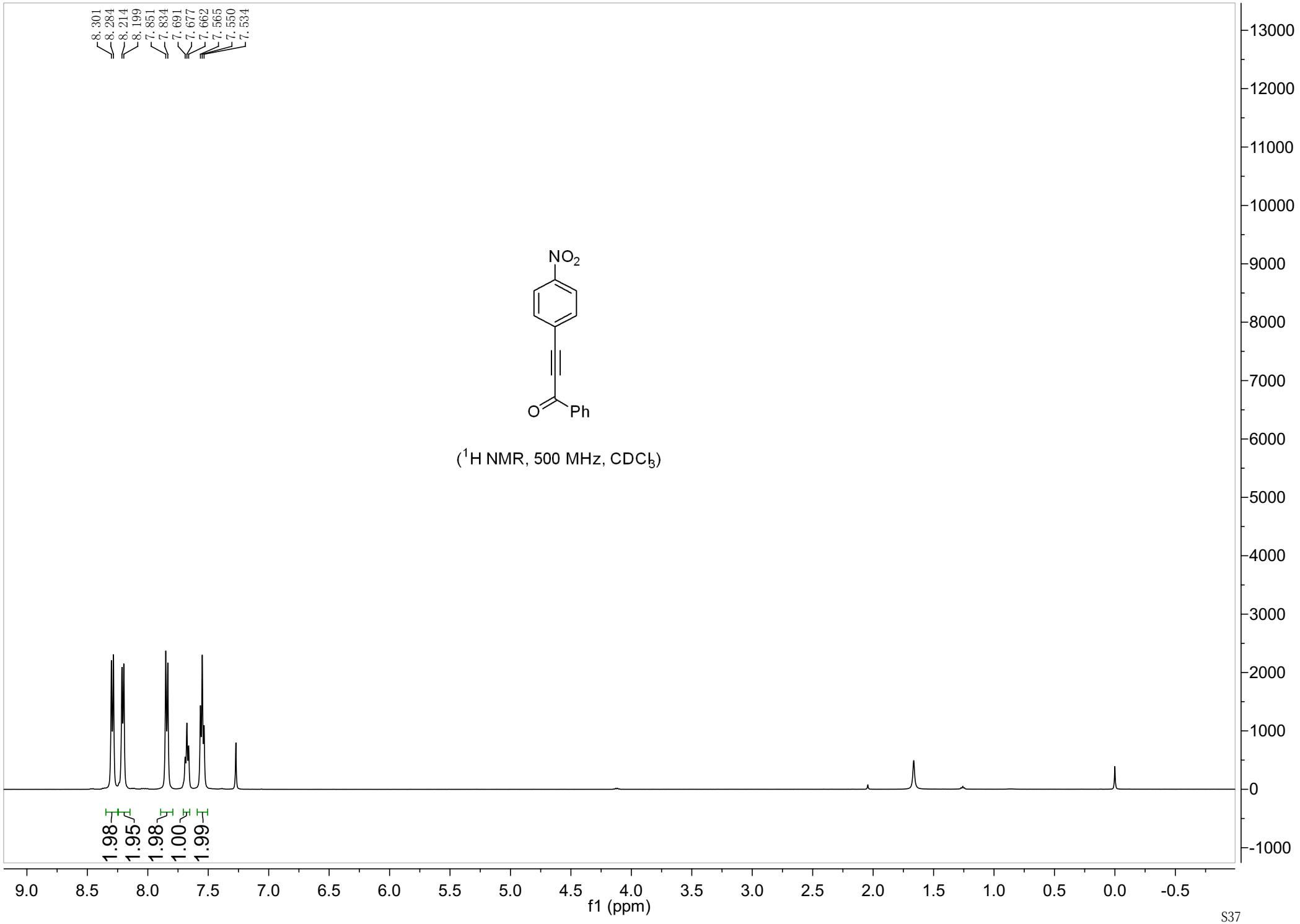

178.171
161.300
137.201
135.284
133.998
129.597
128.675
115.000
111.768
94.635
87.002
63.873
14.769
OEt
O
Ph
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

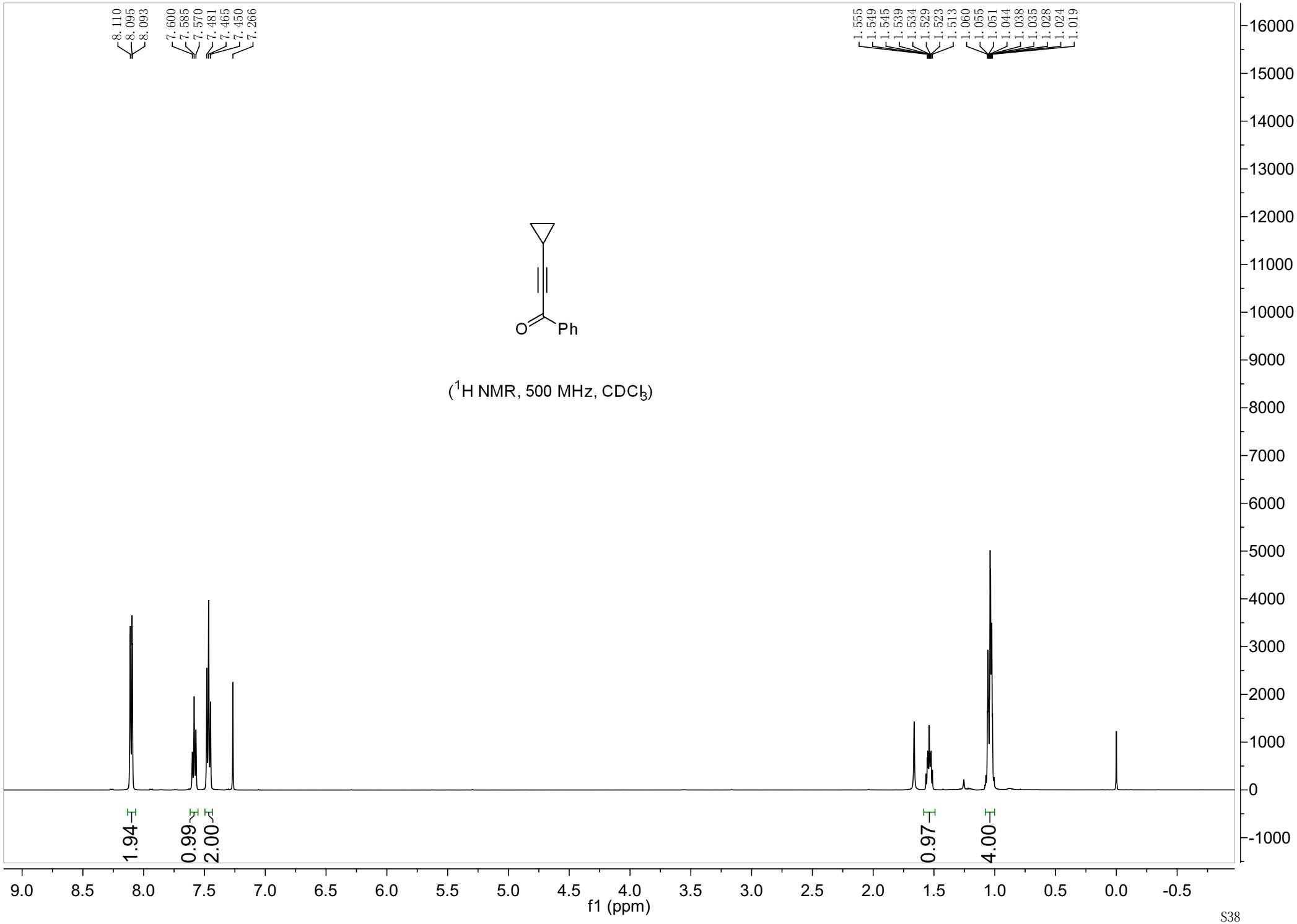

8.231
8.216
7.624
7.594
7.578
7.530
7.515
7.500
7.237
7.221
2.406
O
Ph
(1H NMR, 400 MHz, CDCl3)
1.92
2.99
2.01
2.02
3.00
f1 (ppm)

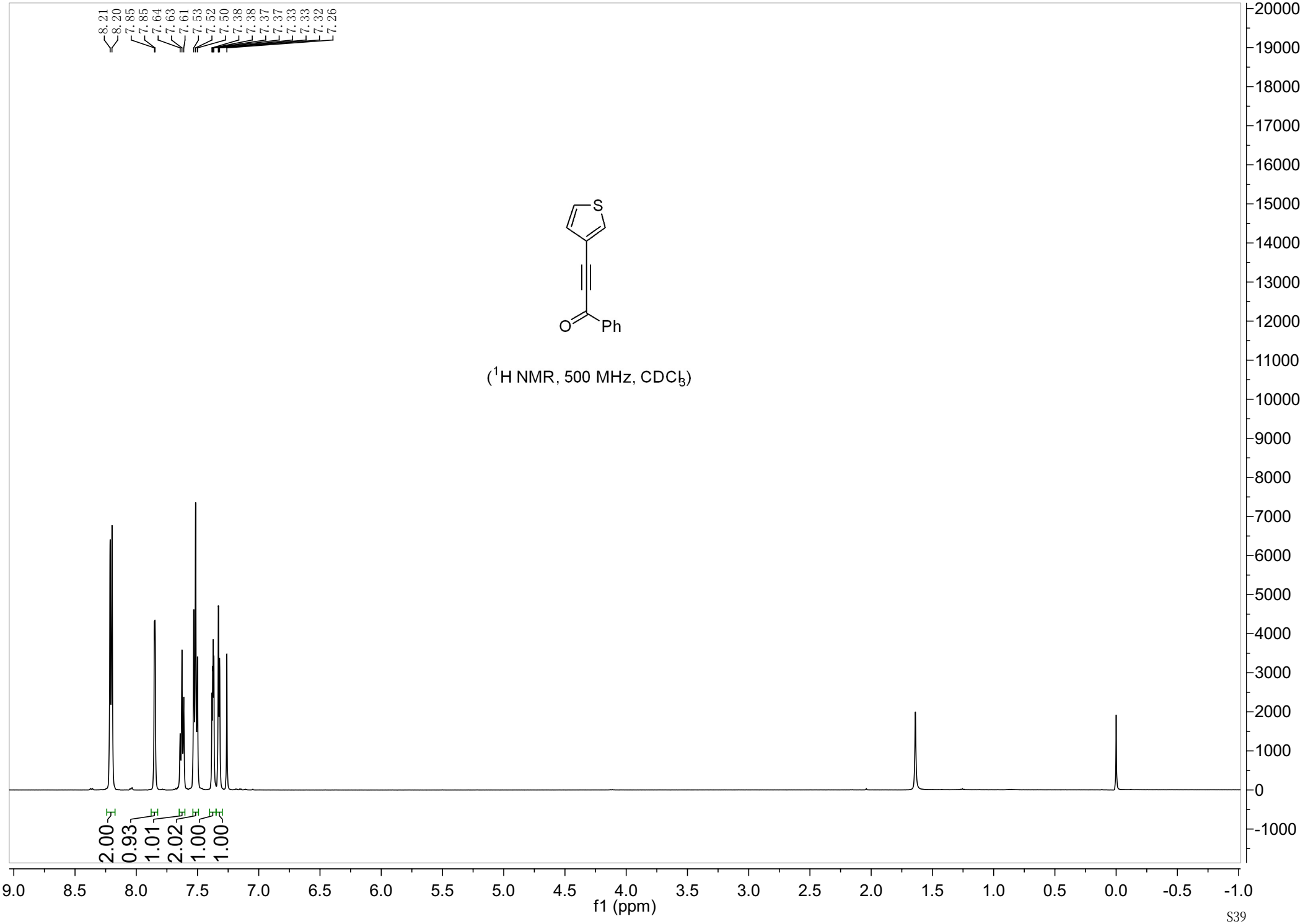

8.914
8.704
8.702
8.695
8.225
8.210
7.982
7.978
7.966
7.675
7.660
7.645
7.556
7.540
7.525
7.396
7.386
7.381
7.372
7.279
CN
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.00
1.00
2.06
1.03
1.05
2.09
1.05
f1 (ppm)

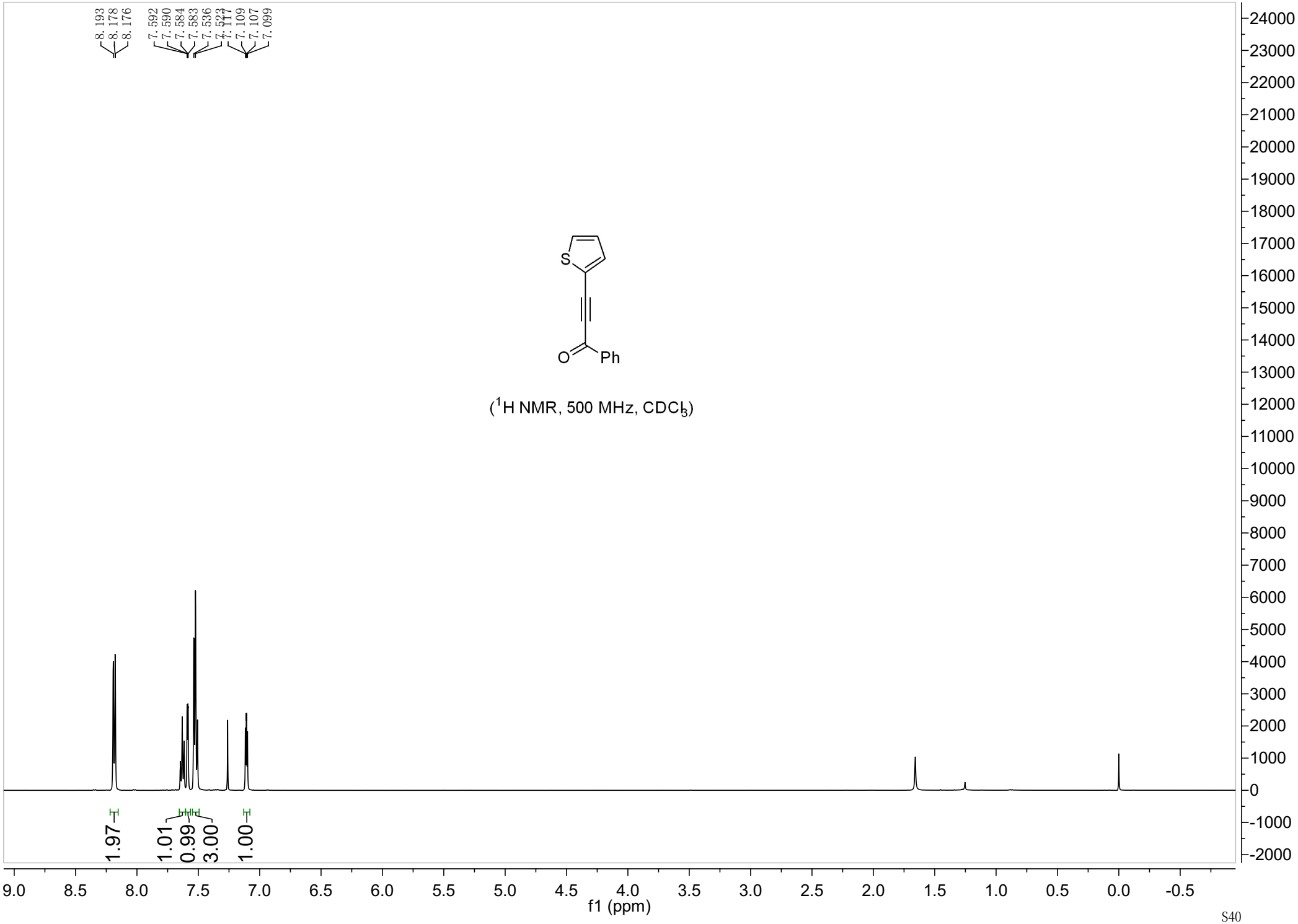

8.222
8.208
7.799
7.783
7.697
7.680
7.673
7.657
7.643
7.552
7.536
7.521
CF3
O
Ph
(1H NMR, 500 MHz, CDCl3)
2.00
2.02
3.06
2.03
f1 (ppm)

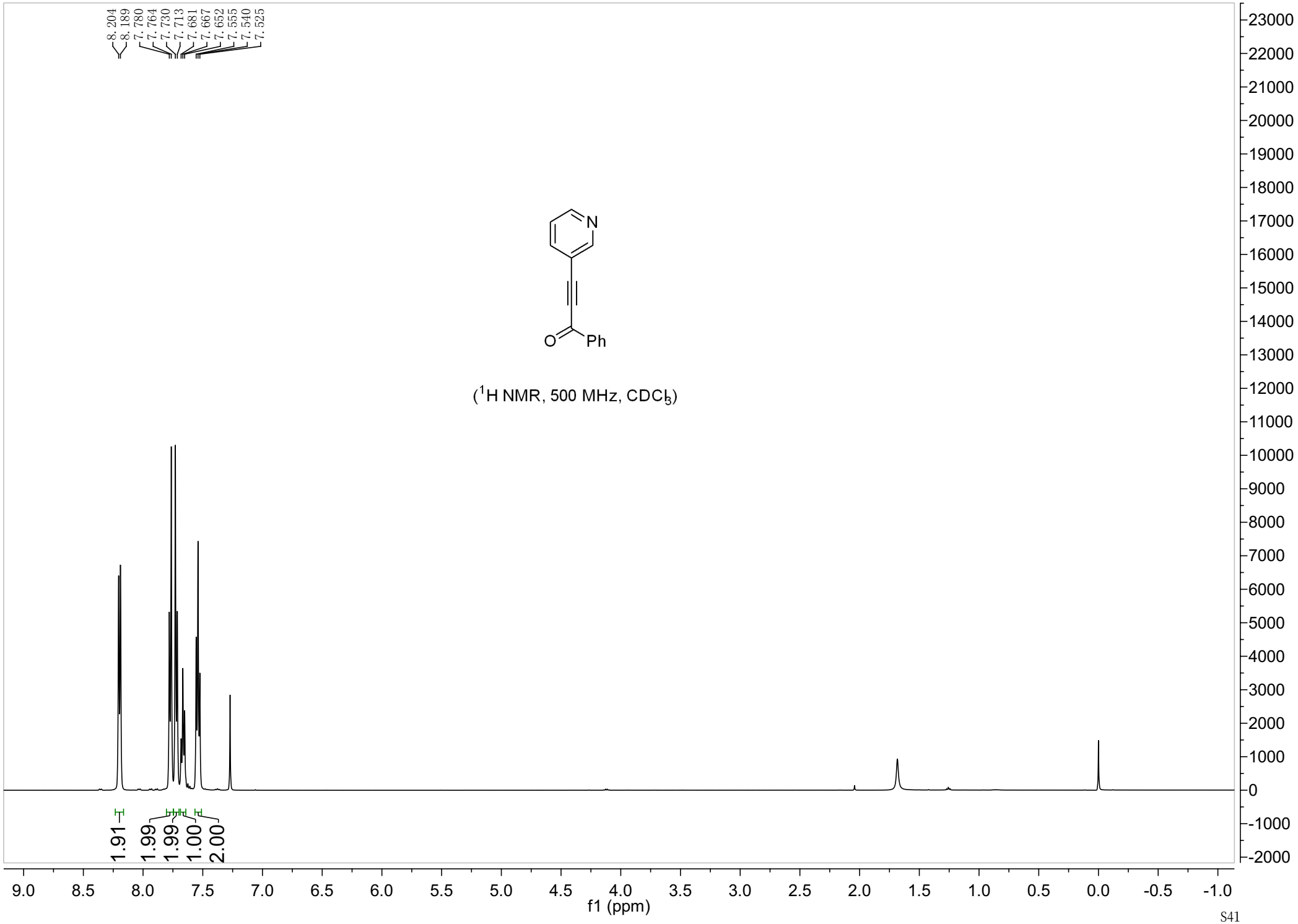

8.223
8.208
8.095
8.079
7.749
7.733
7.663
7.649
7.634
7.546
7.530
7.515
3.947
3.925
O
O
O
Ph
(^{1}H NMR, 500 MHz, CDCl$_3$)
1.83
1.91
1.91
0.97
1.92
3.00
f1 (ppm)

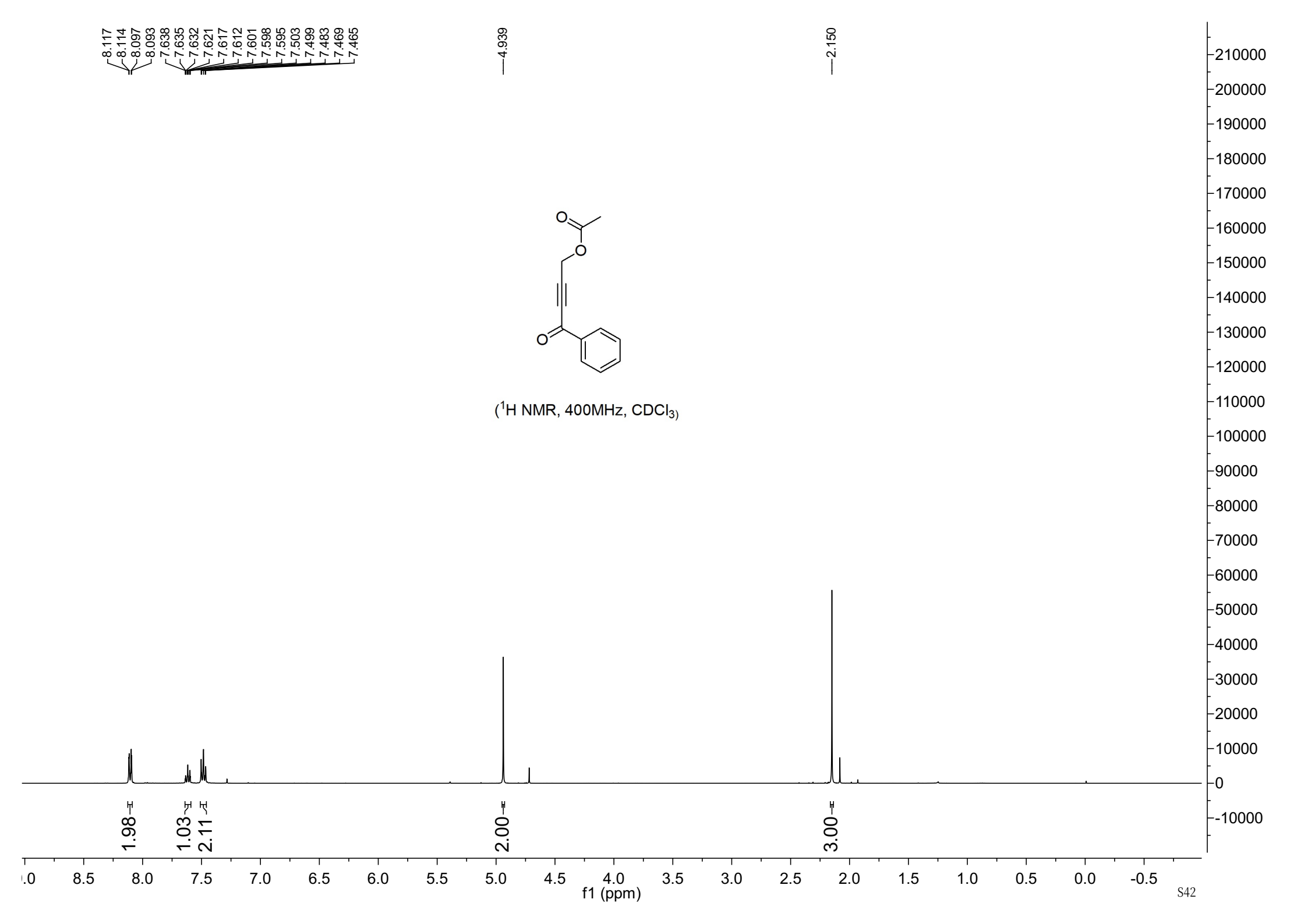

8.301
8.284
8.214
8.199
7.851
7.834
7.691
7.677
7.662
7.565
7.550
7.534
NO2
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.98
1.95
1.98
1.00
1.99
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

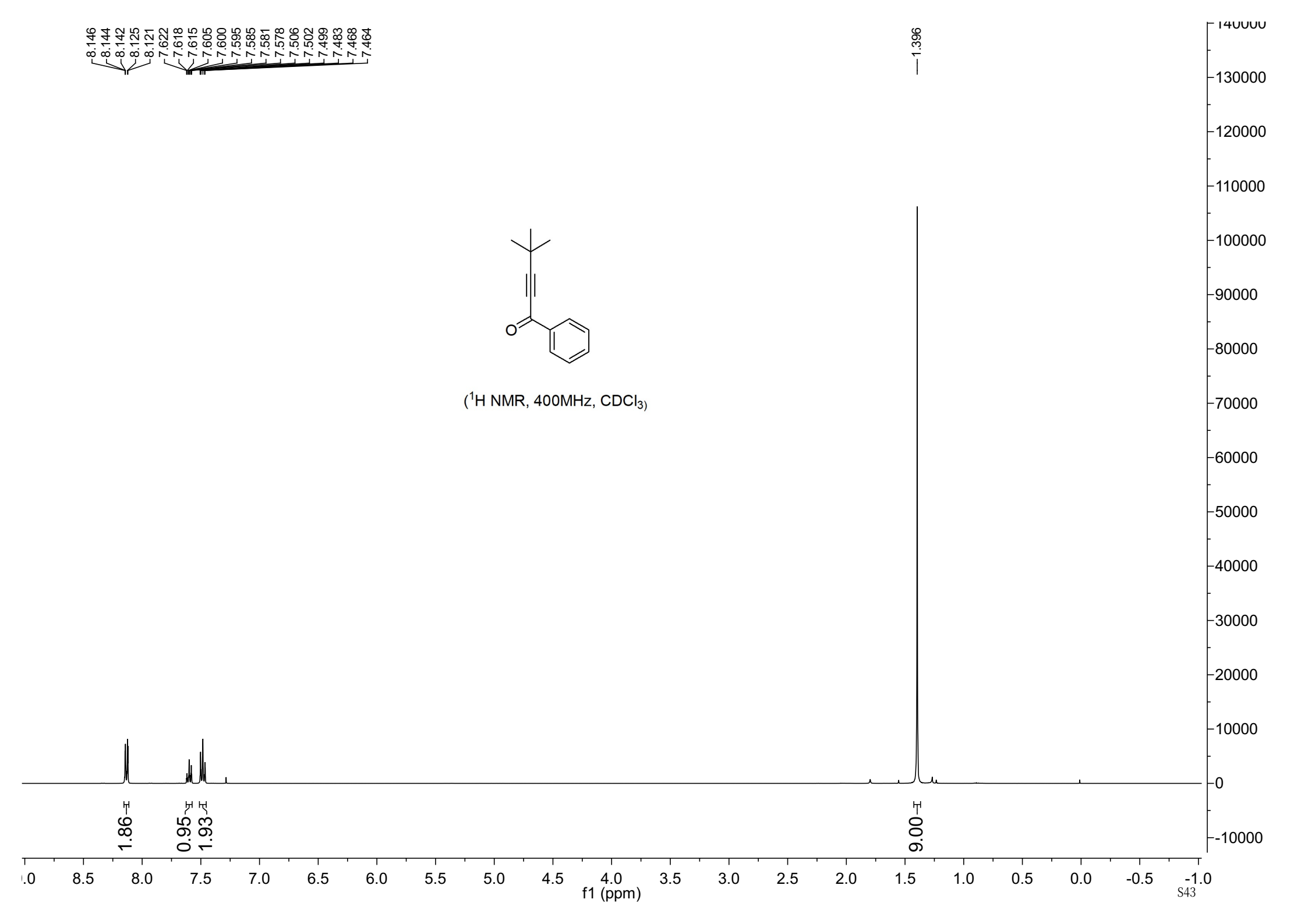

8.110
8.095
8.093
7.600
7.585
7.570
7.481
7.465
7.450
7.266
1.555
1.549
1.545
1.539
1.534
1.529
1.523
1.513
1.060
1.055
1.051
1.044
1.038
1.035
1.028
1.024
1.019
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.94
0.99
2.00
0.97
4.00
f1 (ppm)

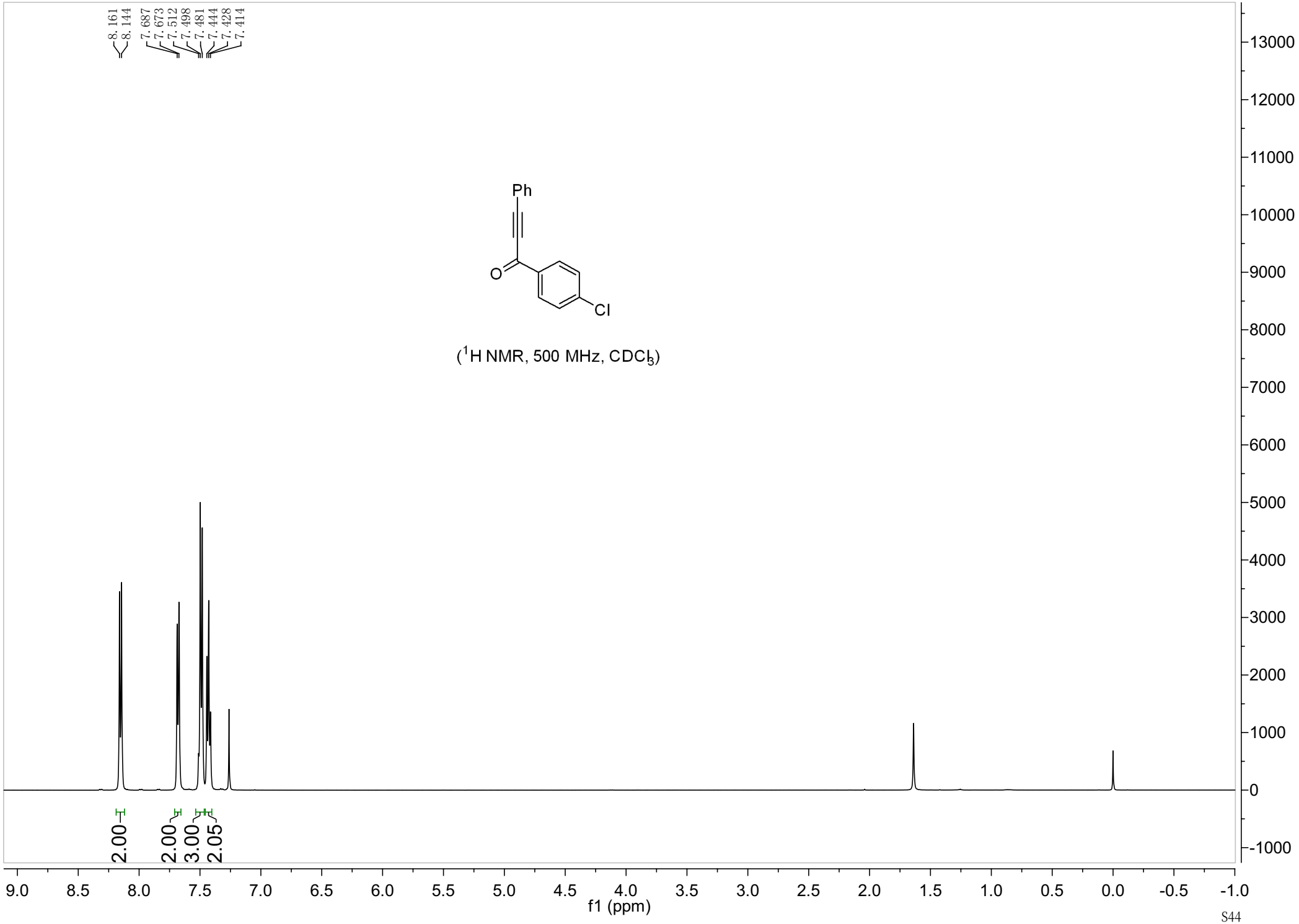

8.21
8.20
7.85
7.85
7.64
7.63
7.61
7.53
7.52
7.50
7.38
7.38
7.37
7.37
7.33
7.33
7.32
7.26
S
O
Ph
(1H NMR, 500 MHz, CDCl3)
2.00
0.93
1.01
2.02
1.00
1.00
f1 (ppm)

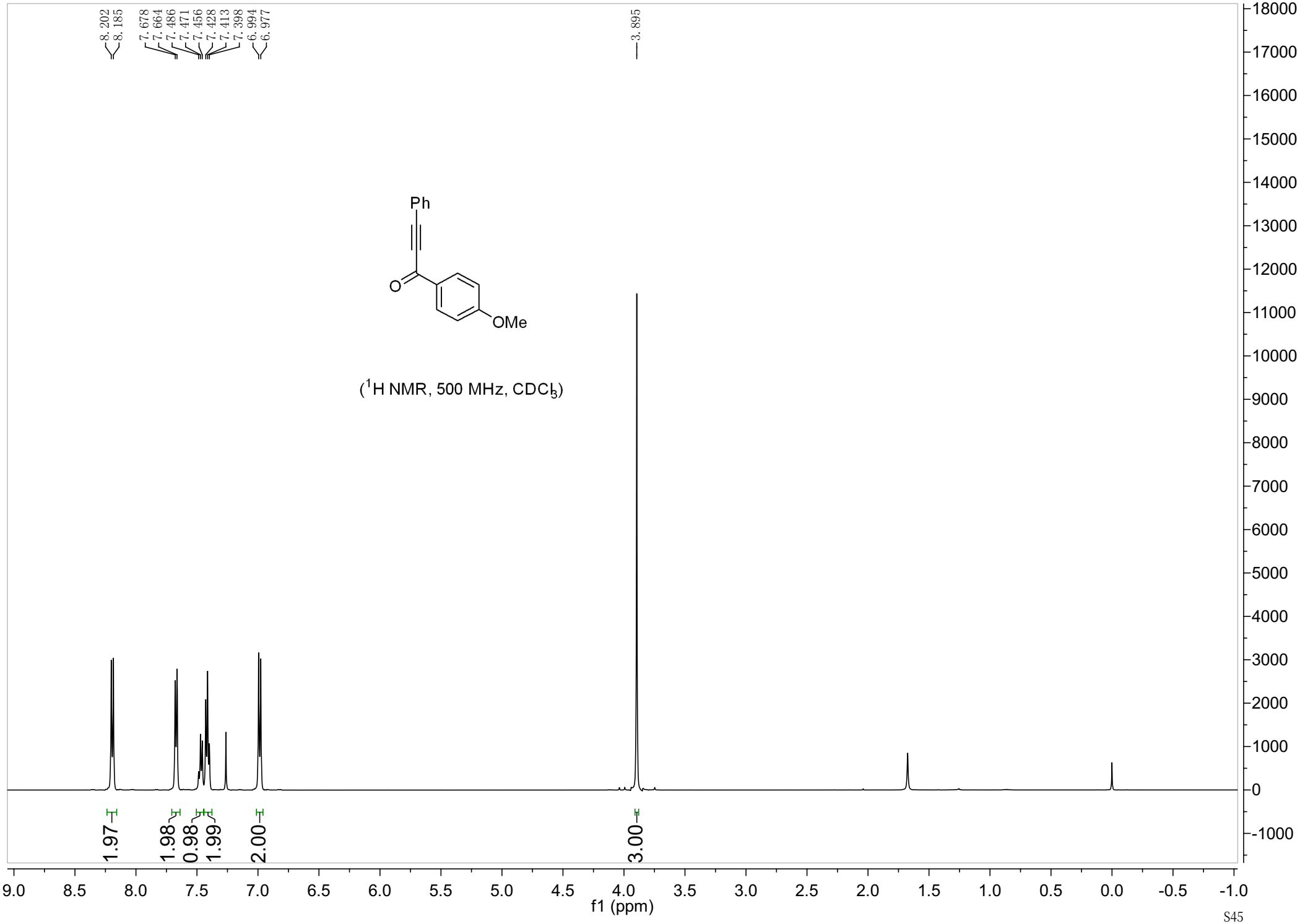

8.193
8.178
8.176
7.592
7.590
7.584
7.583
7.536
7.523
7.117
7.109
7.107
7.099
S
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.97
1.01
0.99
3.00
1.00
f1 (ppm)

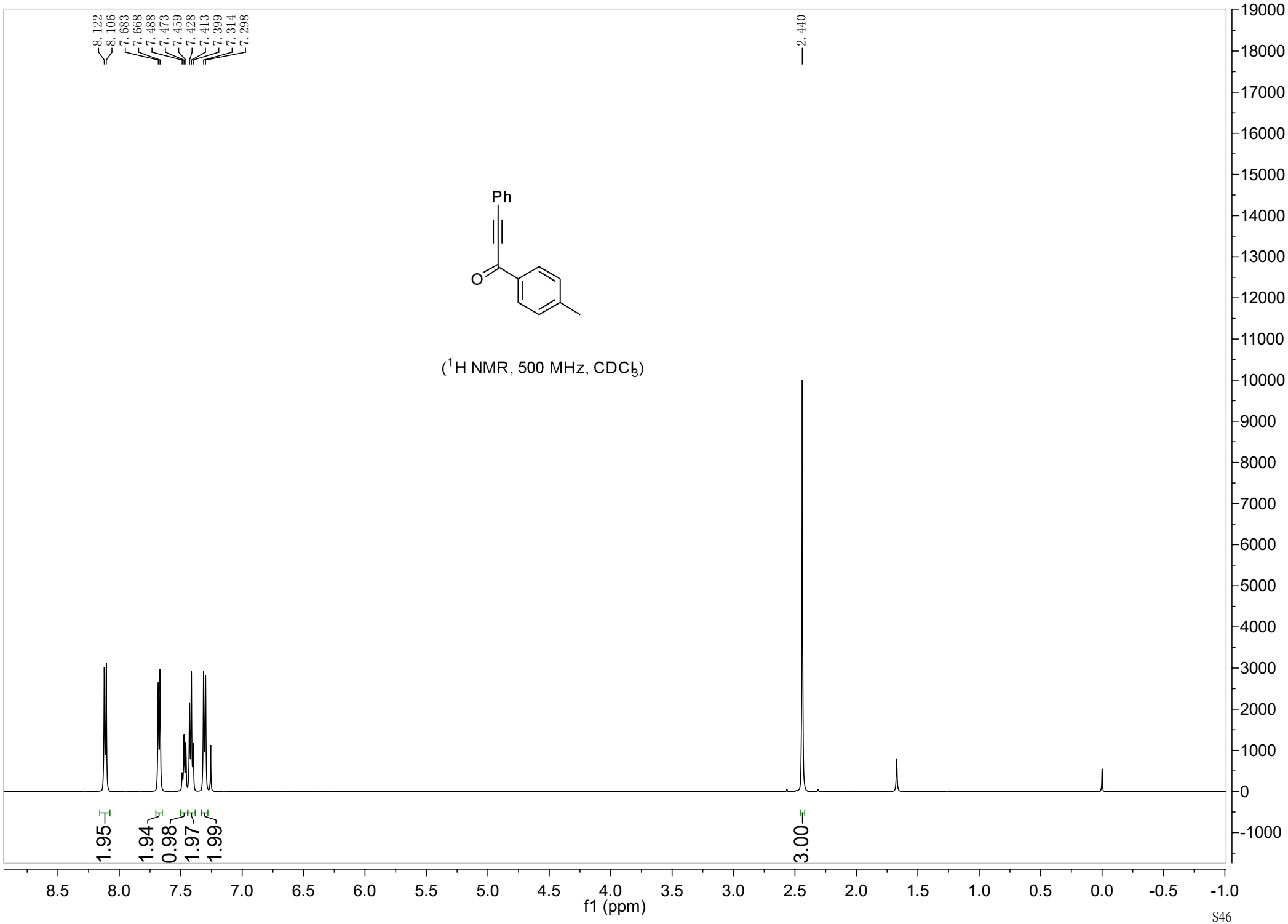

8.204
8.189
7.780
7.764
7.730
7.713
7.681
7.667
7.652
7.555
7.540
7.525
N
O
Ph
(1H NMR, 500 MHz, CDCl3)
1.91
1.99
1.99
1.00
2.00
f1 (ppm)

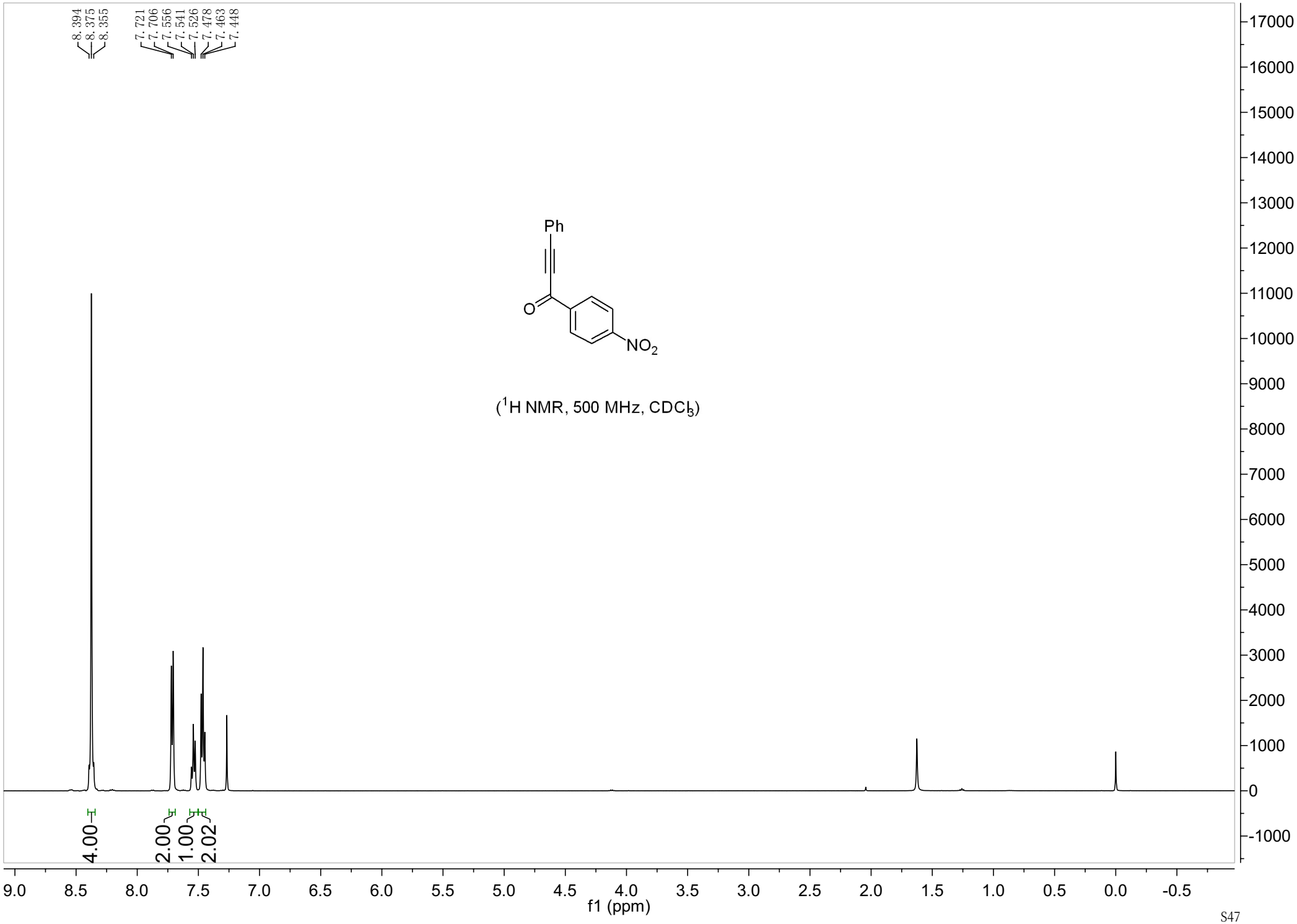

8.117
8.114
8.097
8.093
7.638
7.635
7.632
7.621
7.617
7.612
7.601
7.598
7.595
7.503
7.499
7.483
7.469
7.465
4.939
2.150
O
O
O
(1H NMR, 400MHz, CDCl3)
1.98
1.03
2.11
2.00
3.00
f1 (ppm)

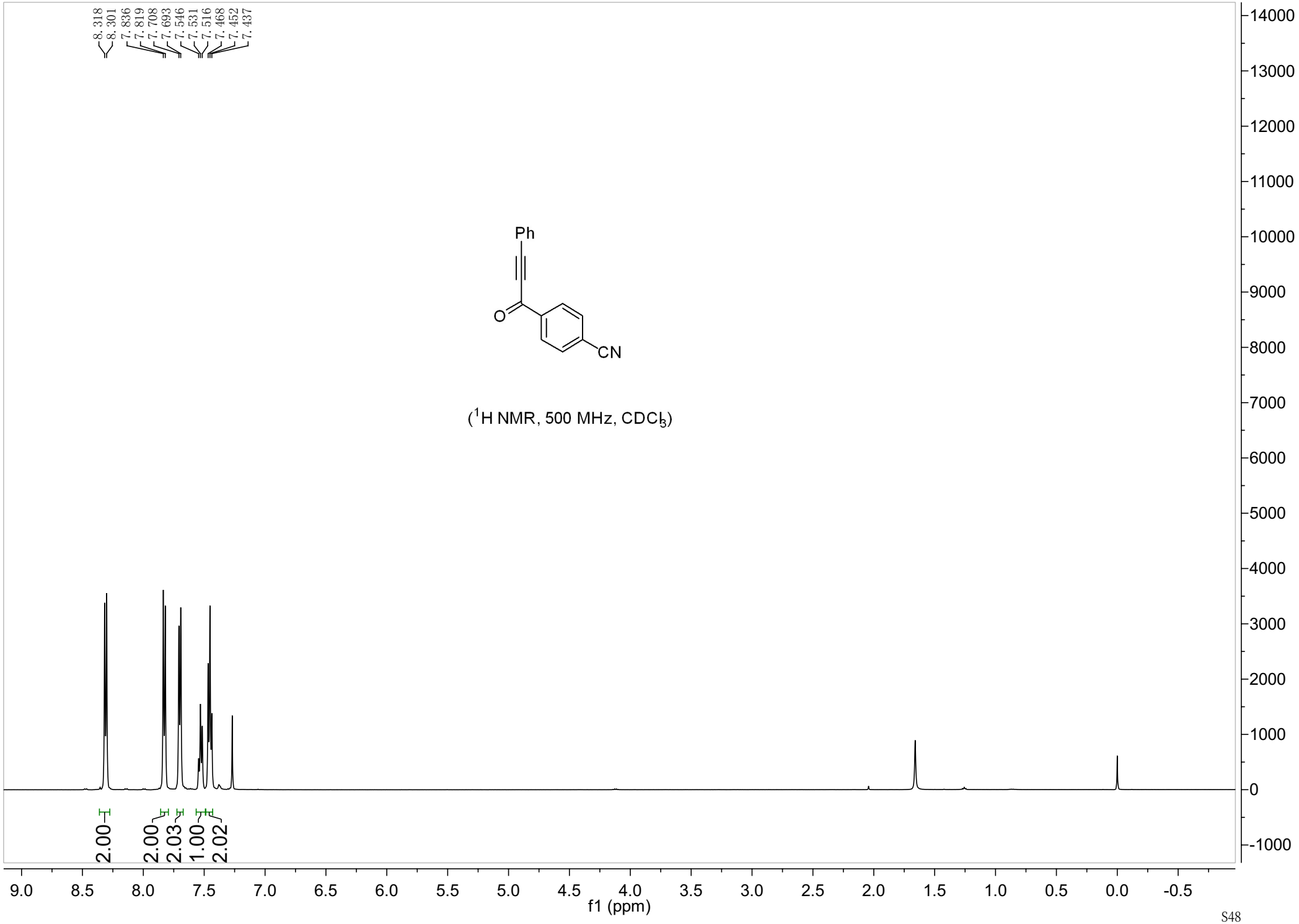

8.146
8.144
8.142
8.125
8.121
7.622
7.618
7.615
7.605
7.600
7.595
7.585
7.581
7.578
7.506
7.502
7.499
7.483
7.468
7.464
1.396
O
(1H NMR, 400MHz, CDCl3)
1.86
0.95
1.93
9.00
f1 (ppm)

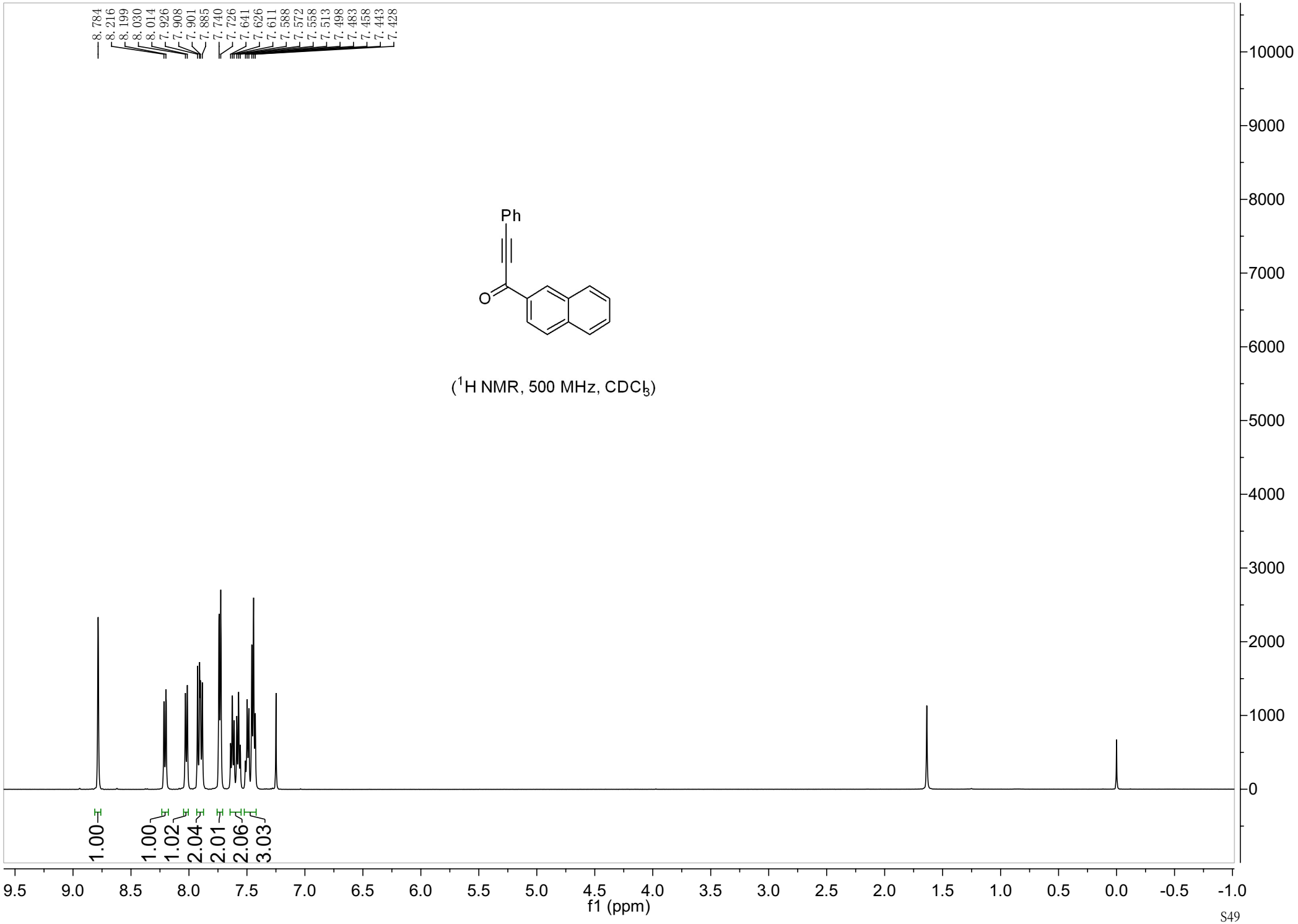

8.161
8.144
7.687
7.673
7.512
7.498
7.481
7.444
7.428
7.414
Ph
O
Cl
(1H NMR, 500 MHz, CDCl3)
2.00
2.00
3.00
2.05
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

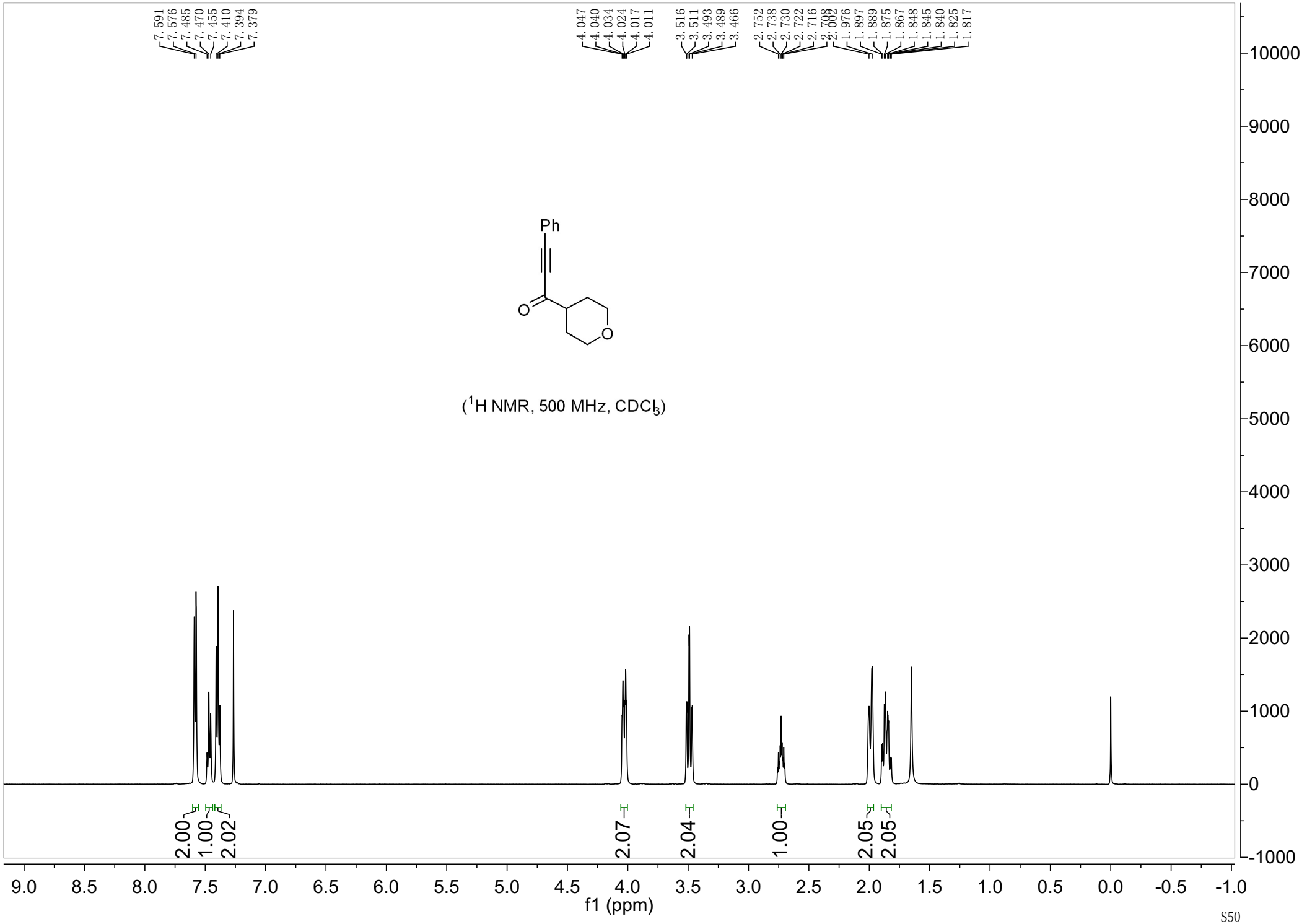

8.202
8.185
7.678
7.664
7.486
7.471
7.456
7.428
7.413
7.398
6.994
6.977
3.895
Ph
O
OMe
(1H NMR, 500 MHz, CDCl3)
1.97
1.98
0.98
1.99
2.00
3.00
f1 (ppm)

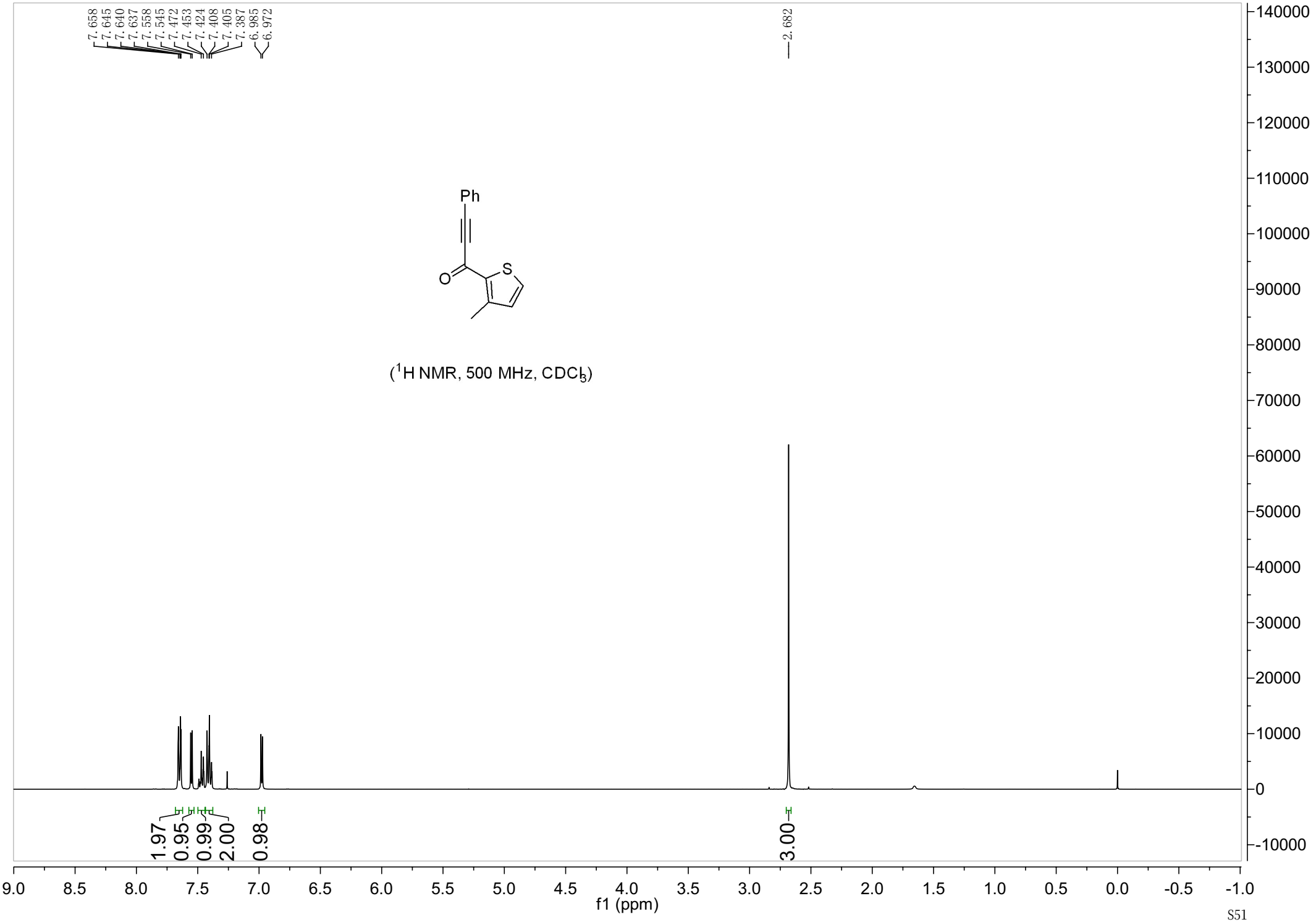

8.122
8.106
7.683
7.668
7.488
7.473
7.459
7.428
7.413
7.399
7.314
7.298
2.440
Ph
O
(1H NMR, 500 MHz, CDCl3)
1.95
1.94
0.98
1.97
1.99
3.00
f1 (ppm)

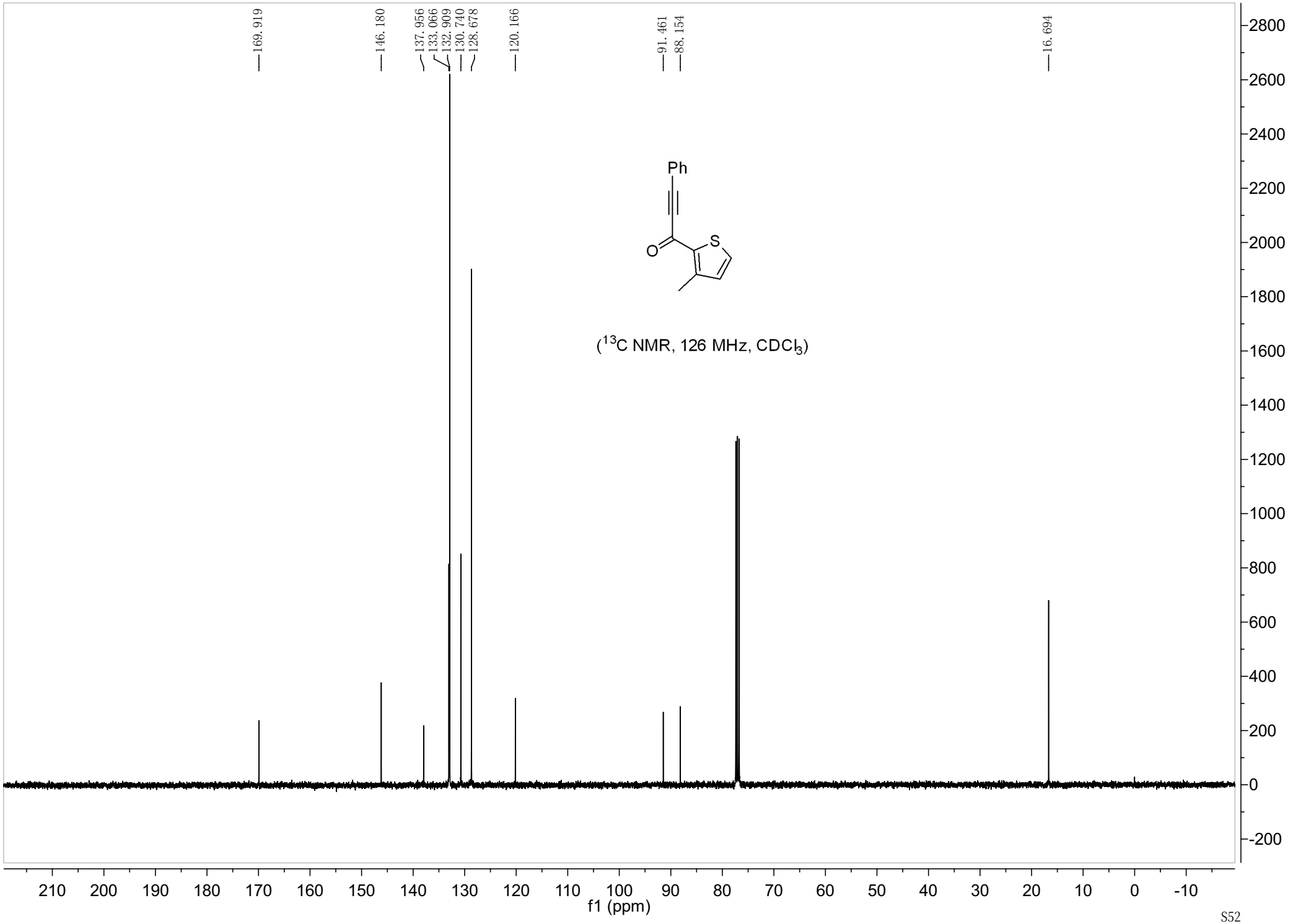

8.394
8.375
8.355
7.721
7.706
7.556
7.541
7.526
7.478
7.463
7.448
Ph
O
NO2
(1H NMR, 500 MHz, CDCl3)
4.00
2.00
1.00
2.02
f1 (ppm)

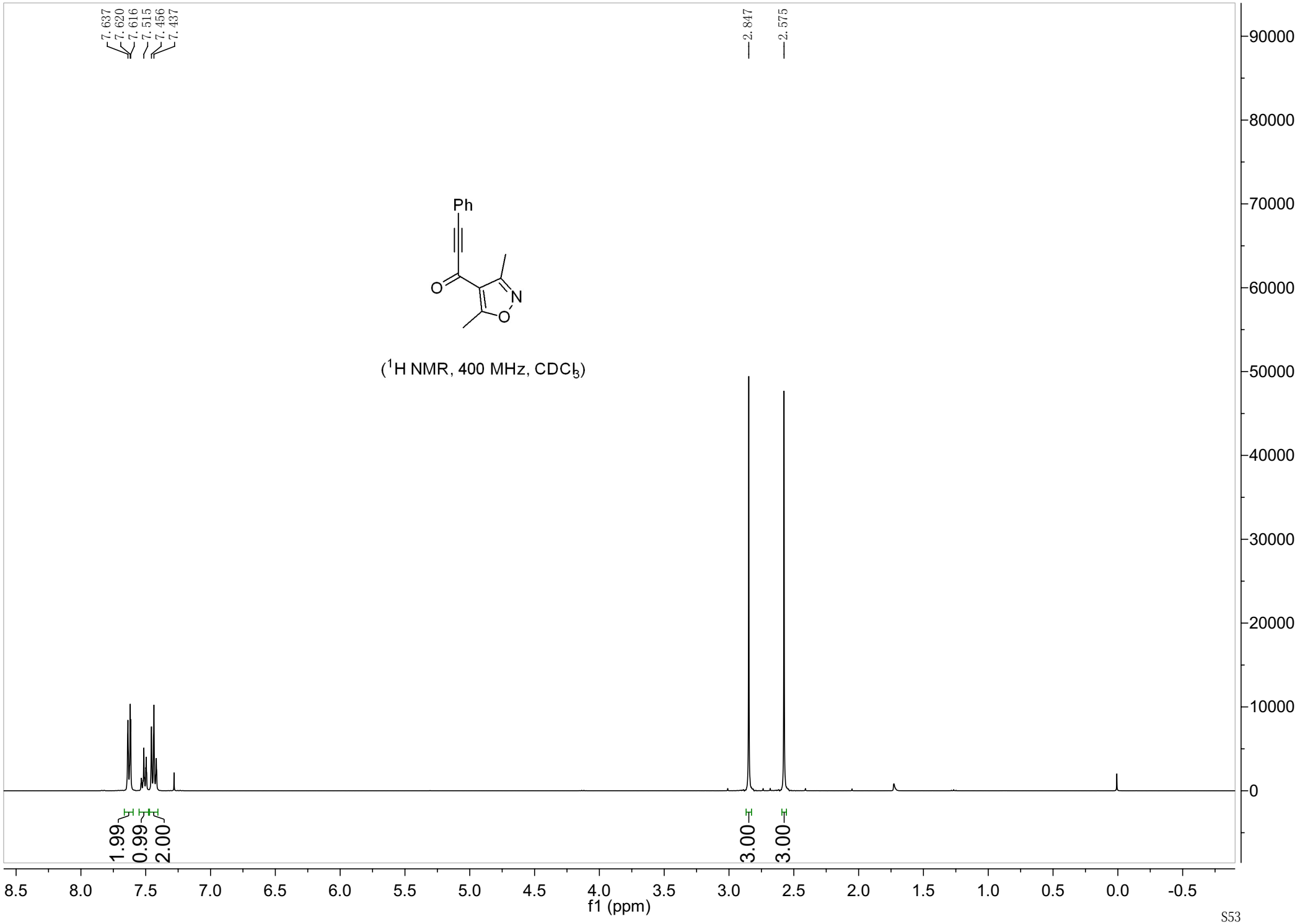

8.318
8.301
7.836
7.819
7.708
7.693
7.546
7.531
7.516
7.468
7.452
7.437
Ph
O
CN
(1H NMR, 500 MHz, CDCl3)
2.00
2.00
2.03
1.00
2.02
f1 (ppm)

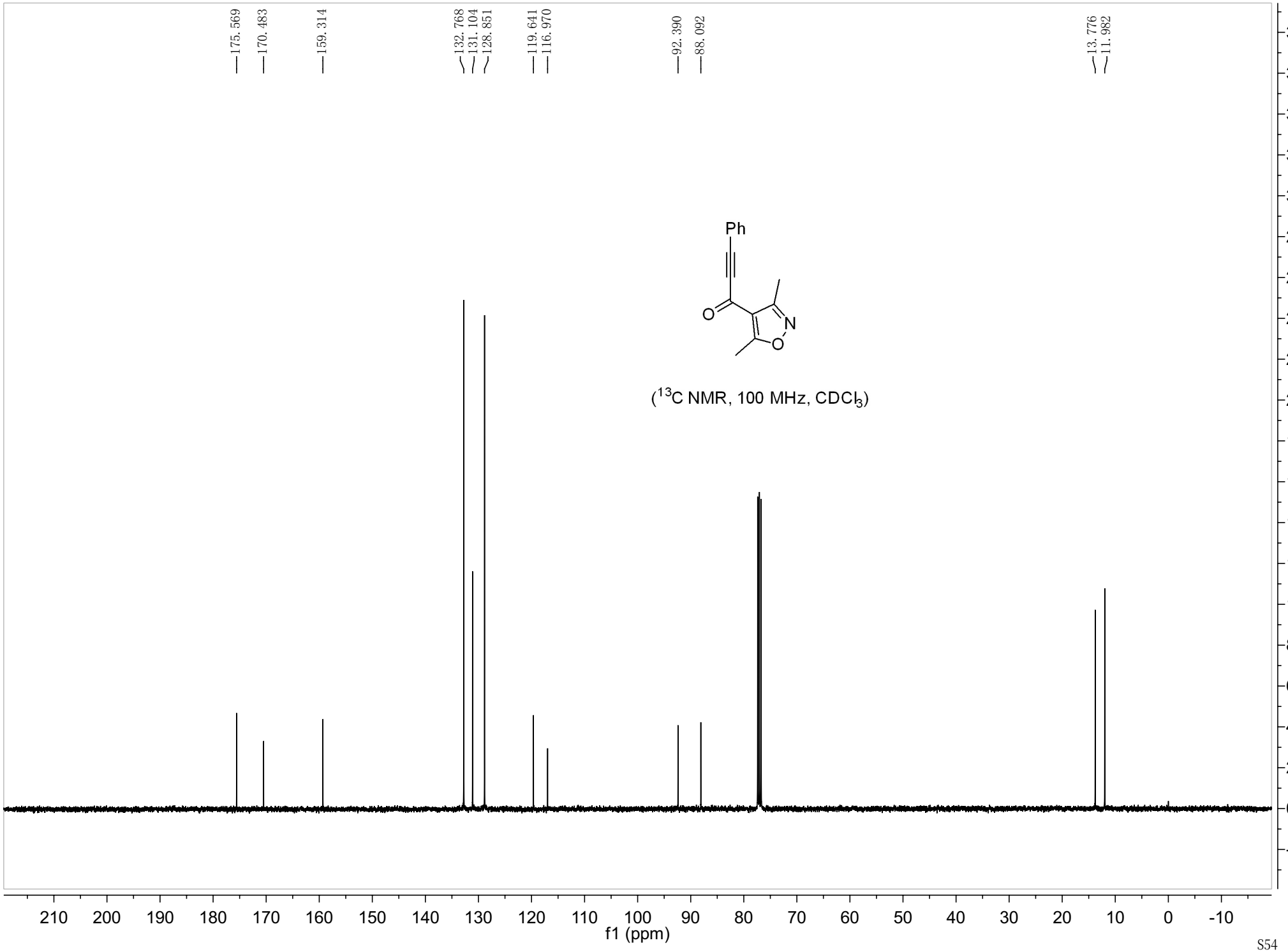

8.784
8.216
8.199
8.030
8.014
7.926
7.908
7.901
7.885
7.740
7.726
7.641
7.626
7.611
7.588
7.572
7.558
7.513
7.498
7.483
7.458
7.443
7.428
Ph
O
(1H NMR, 500 MHz, CDCl3)
1.00
1.00
1.02
2.04
2.01
2.06
3.03
f1 (ppm)

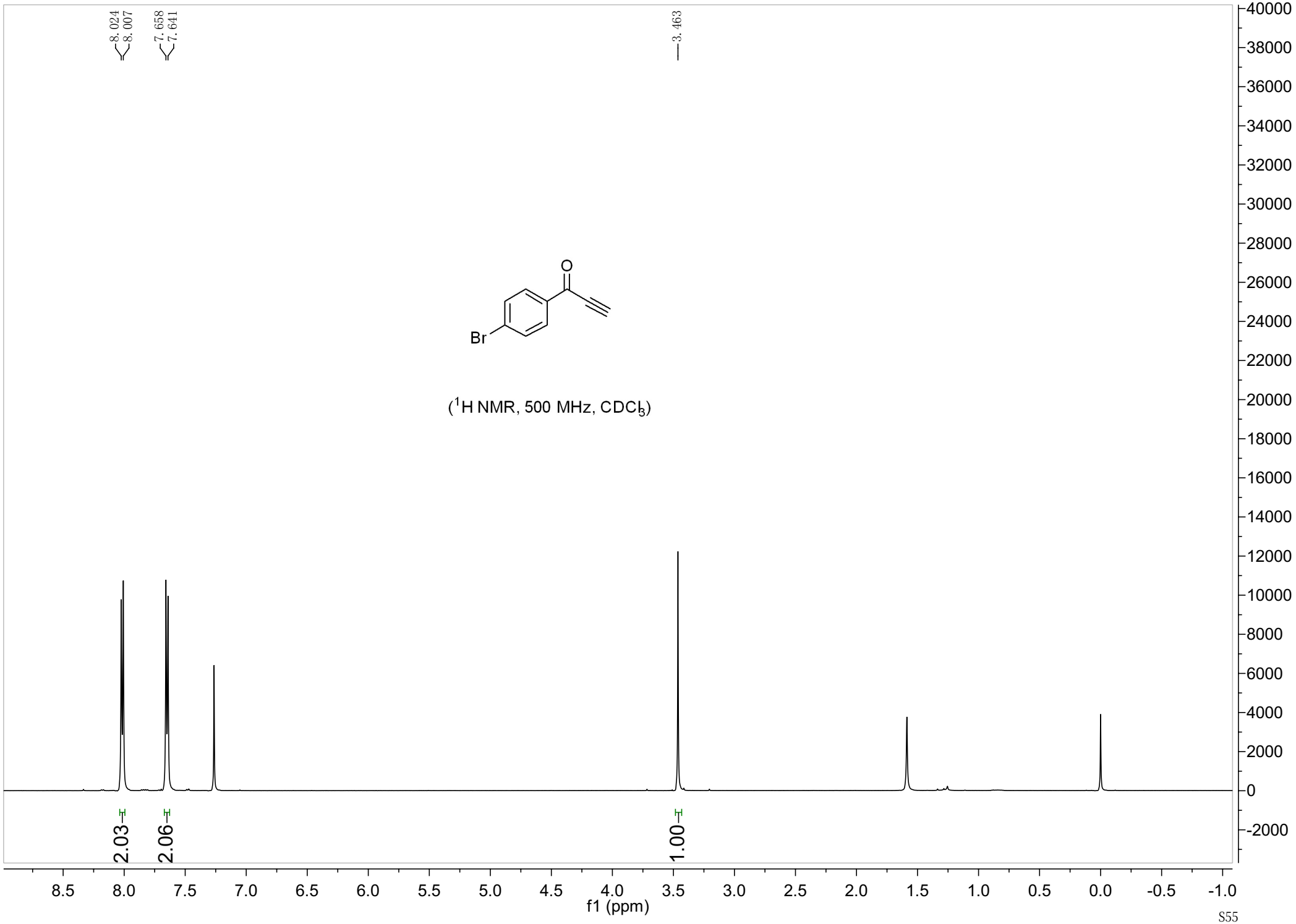

7.591
7.576
7.485
7.470
7.455
7.410
7.394
7.379
4.047
4.040
4.034
4.024
4.017
4.011
3.516
3.511
3.493
3.489
3.466
2.752
2.738
2.730
2.722
2.716
2.708
2.002
1.976
1.897
1.889
1.875
1.867
1.848
1.845
1.840
1.825
1.817
Ph
O
O
(^{1}H NMR, 500 MHz, CDCl$_3$)
2.00
1.00
2.02
2.07
2.04
1.00
2.05
2.05
f1 (ppm)

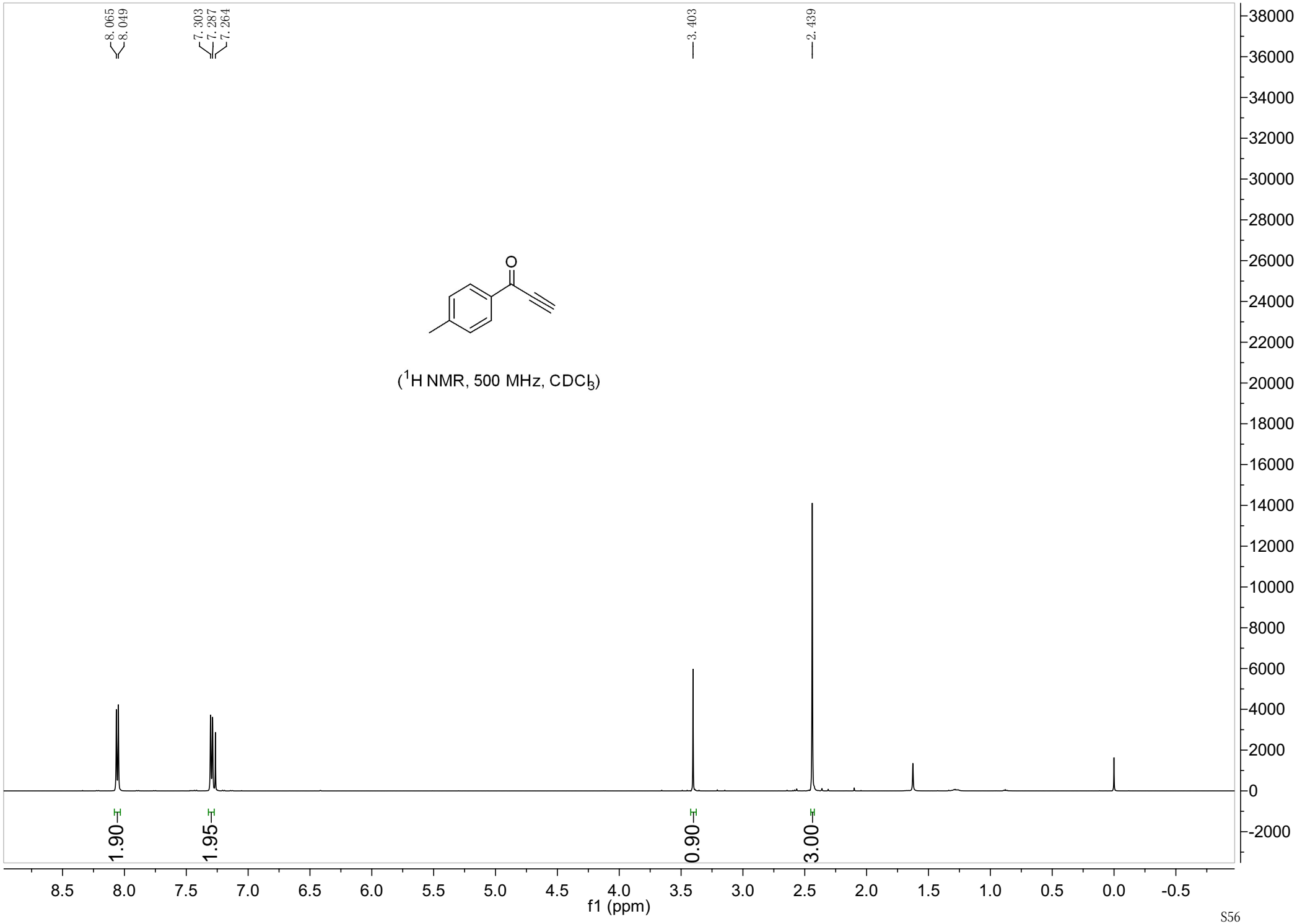

7.658
7.645
7.640
7.637
7.558
7.545
7.472
7.453
7.424
7.408
7.405
7.387
6.985
6.972
2.682
Ph
O
S
(1H NMR, 500 MHz, CDCl3)
1.97
0.95
0.99
2.00
0.98
3.00
f1 (ppm)

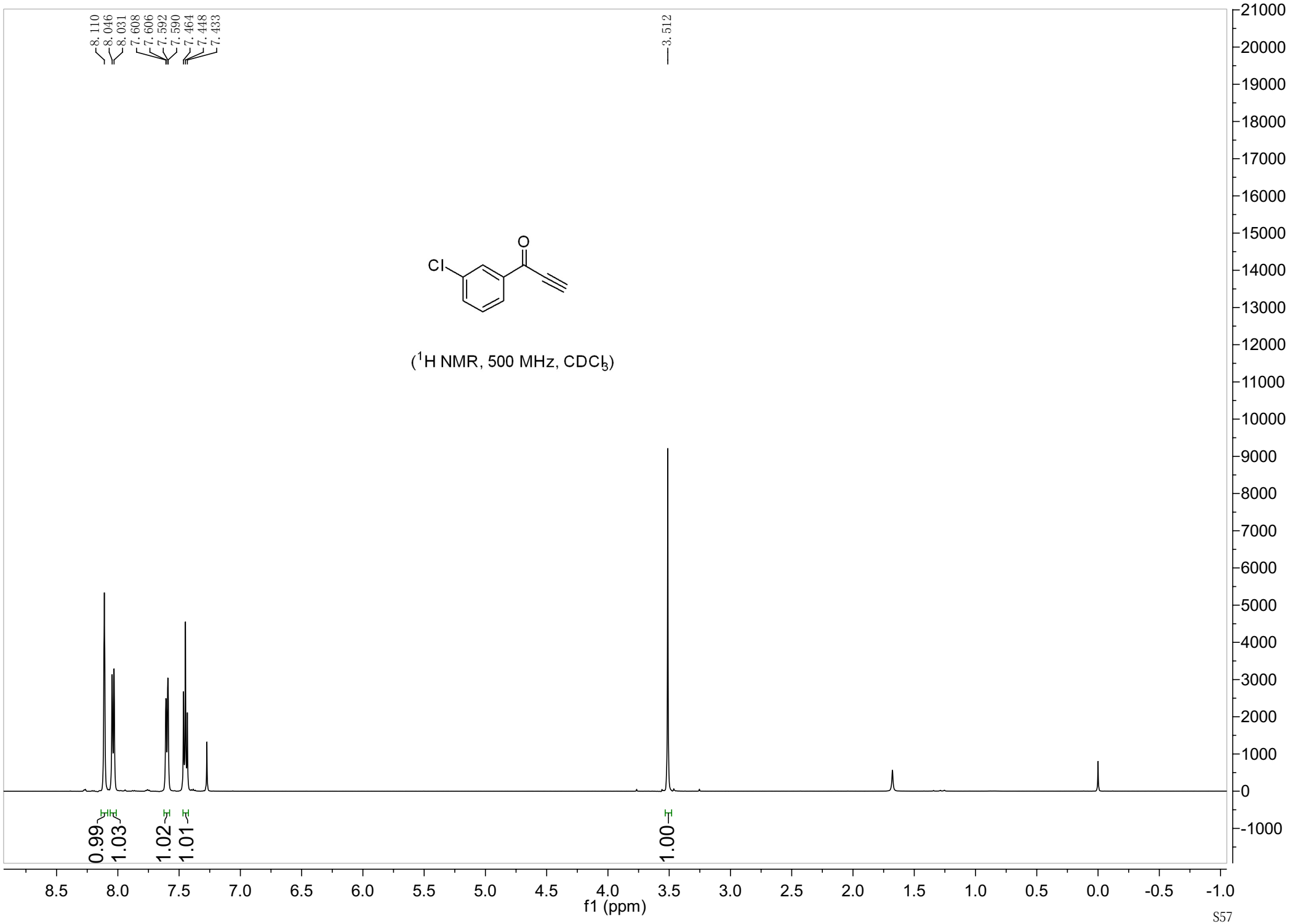

169.919
146.180
137.956
133.066
132.909
130.740
128.678
120.166
91.461
88.154
16.694
Ph
O
S
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

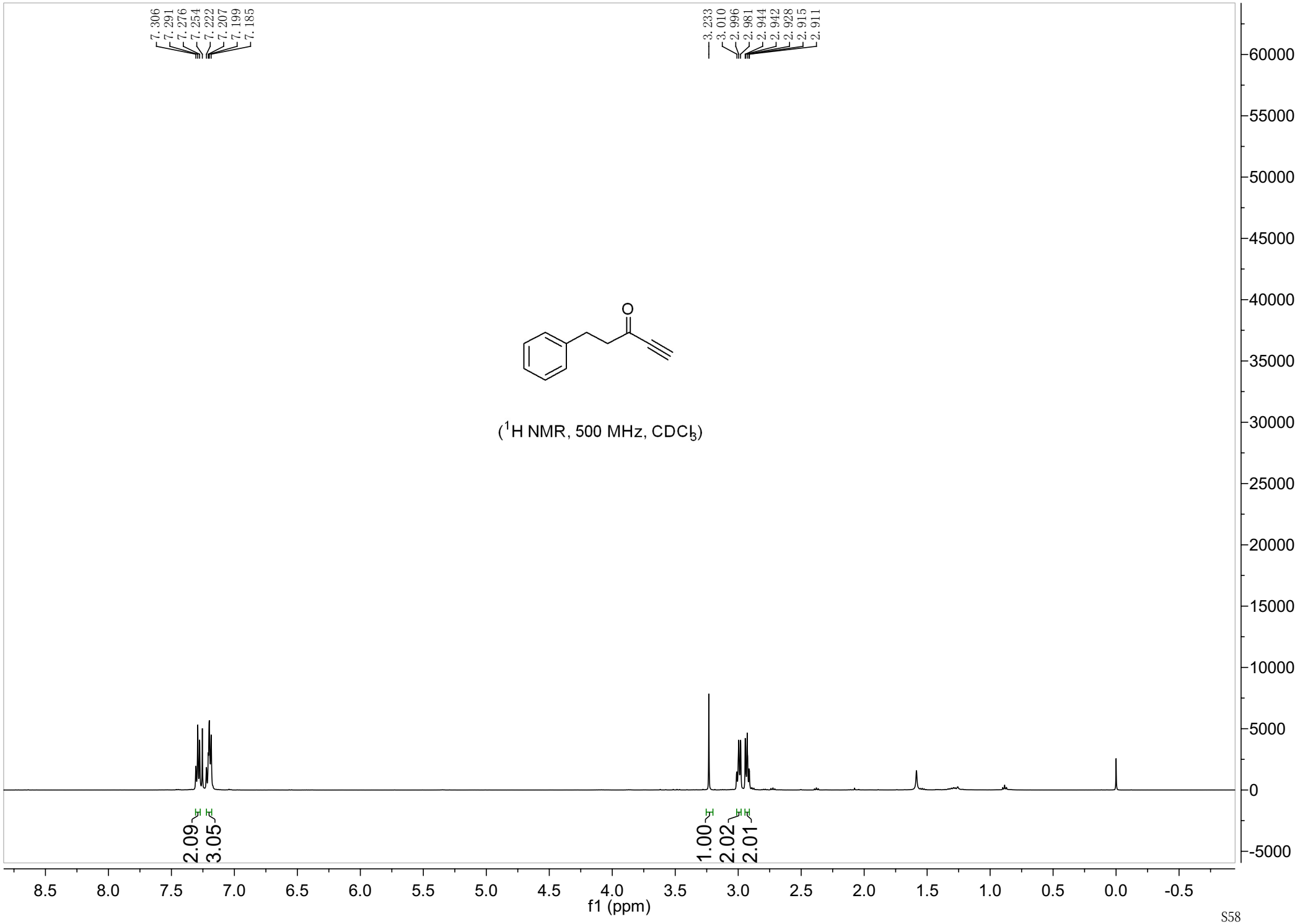

7.637
7.620
7.616
7.515
7.456
7.437
2.847
2.575
Ph
O
N
O
(1H NMR, 400 MHz, CDCl3)
1.99
0.99
2.00
3.00
3.00
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

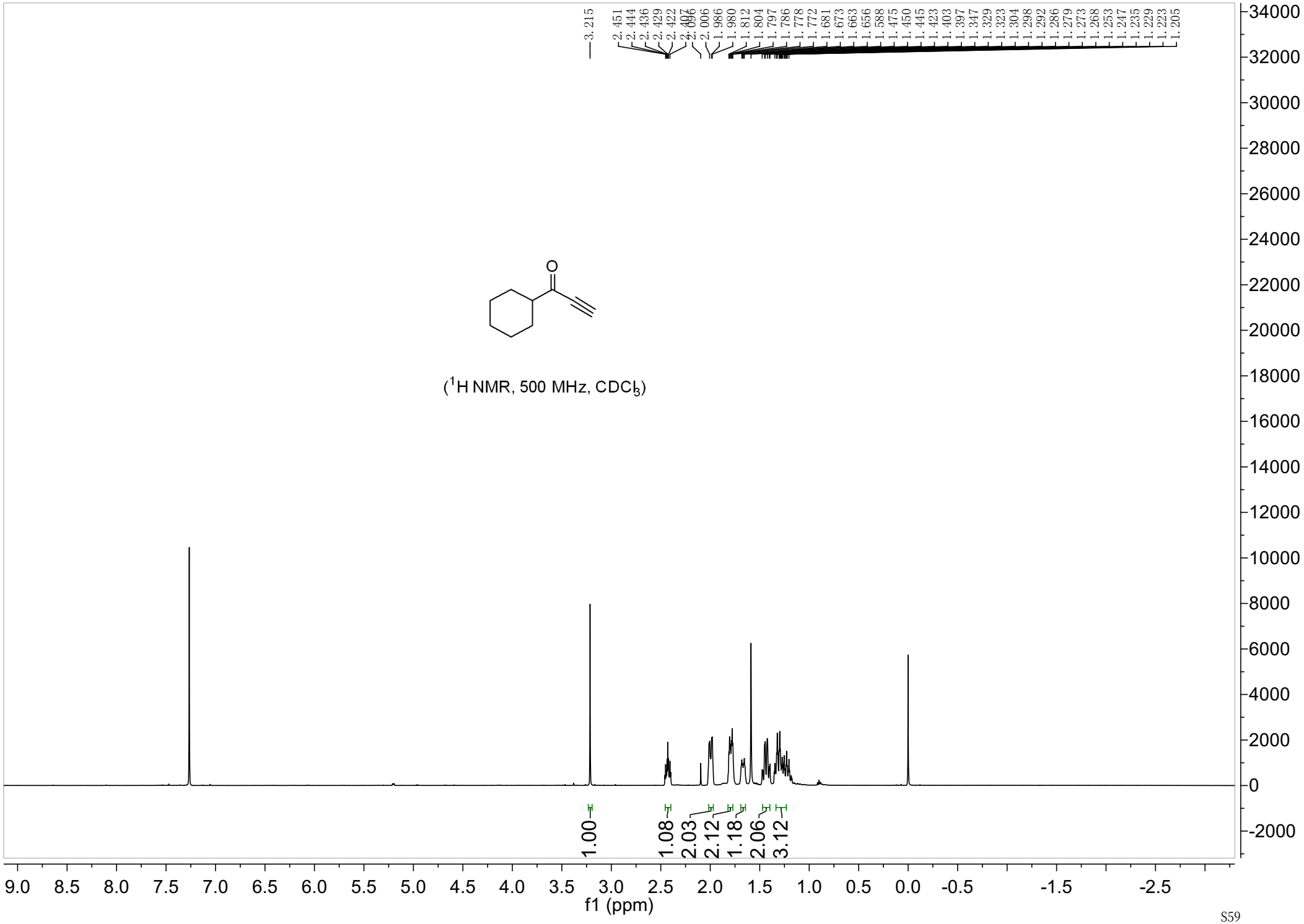

175.569
170.483
159.314
132.768
131.104
128.851
119.641
116.970
92.390
88.092
13.776
11.982
Ph
O
N
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

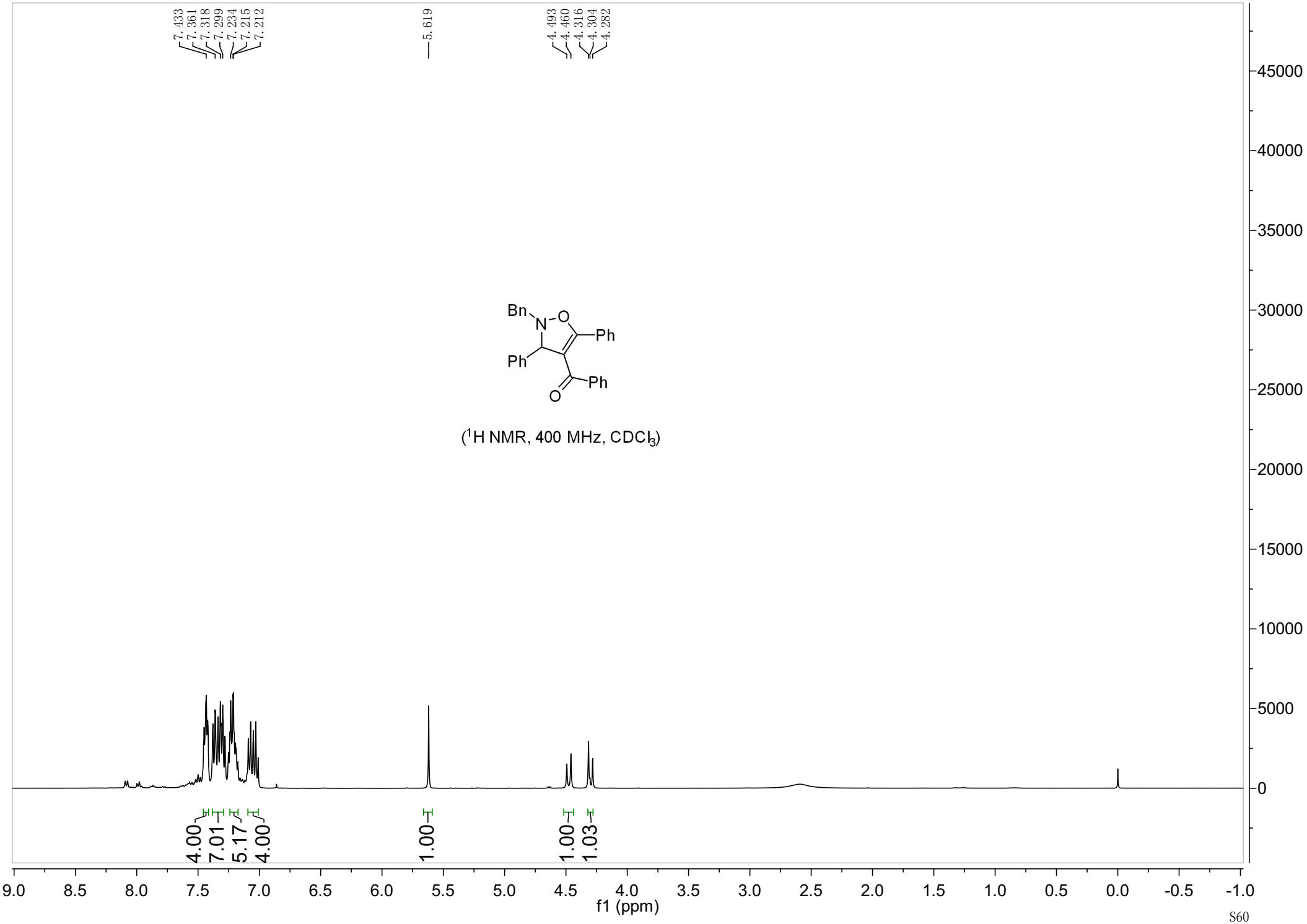

8.024
8.007
7.658
7.641
3.463
O
Br
(^{1}H NMR, 500 MHz, $CDCl_3$)
2.03
2.06
1.00
f1 (ppm)

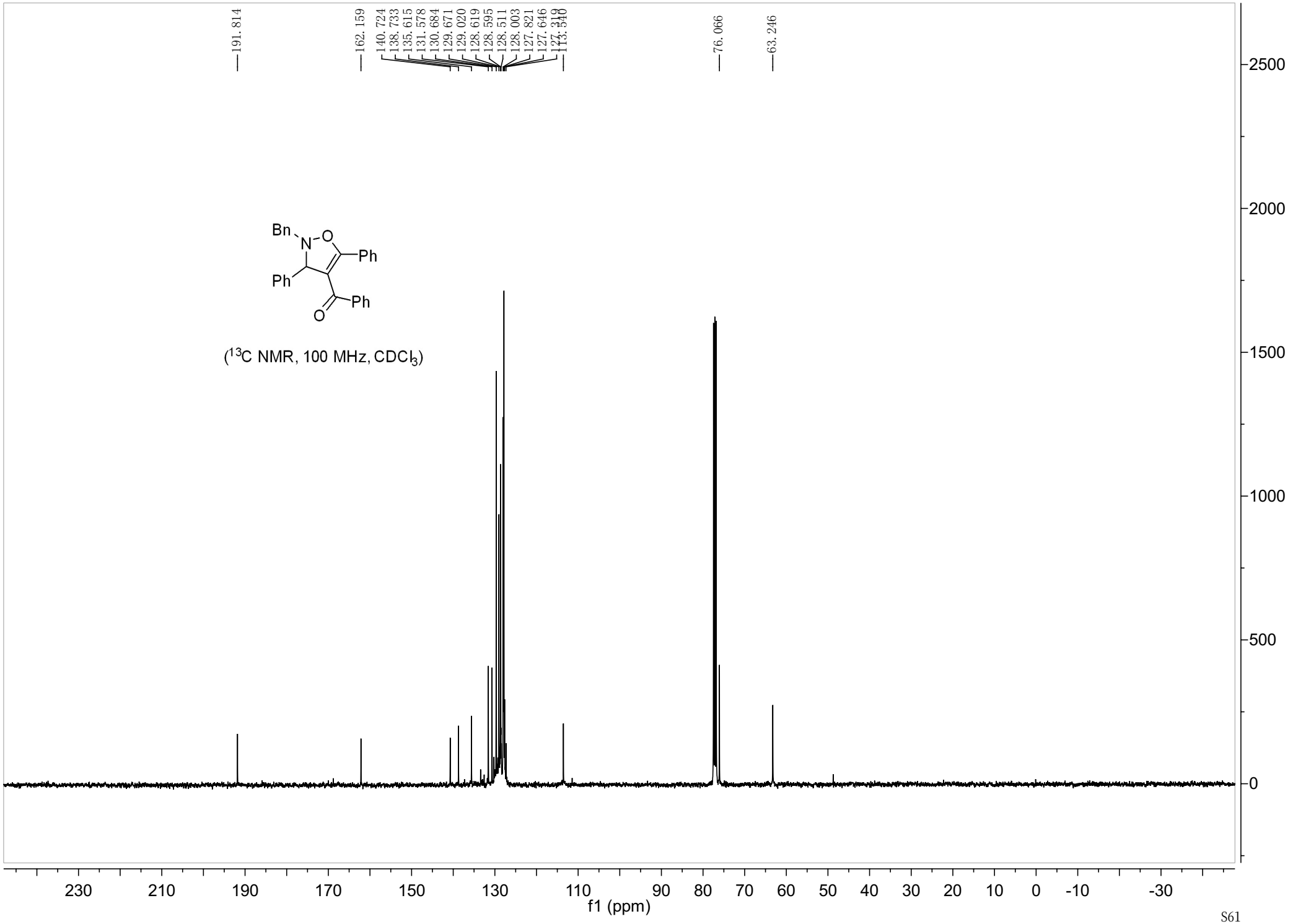

8.065
8.049
7.303
7.287
7.264
3.403
2.439
O
(^{1}H NMR, 500 MHz, $CDCl_3$)
1.90
1.95
0.90
3.00
f1 (ppm)

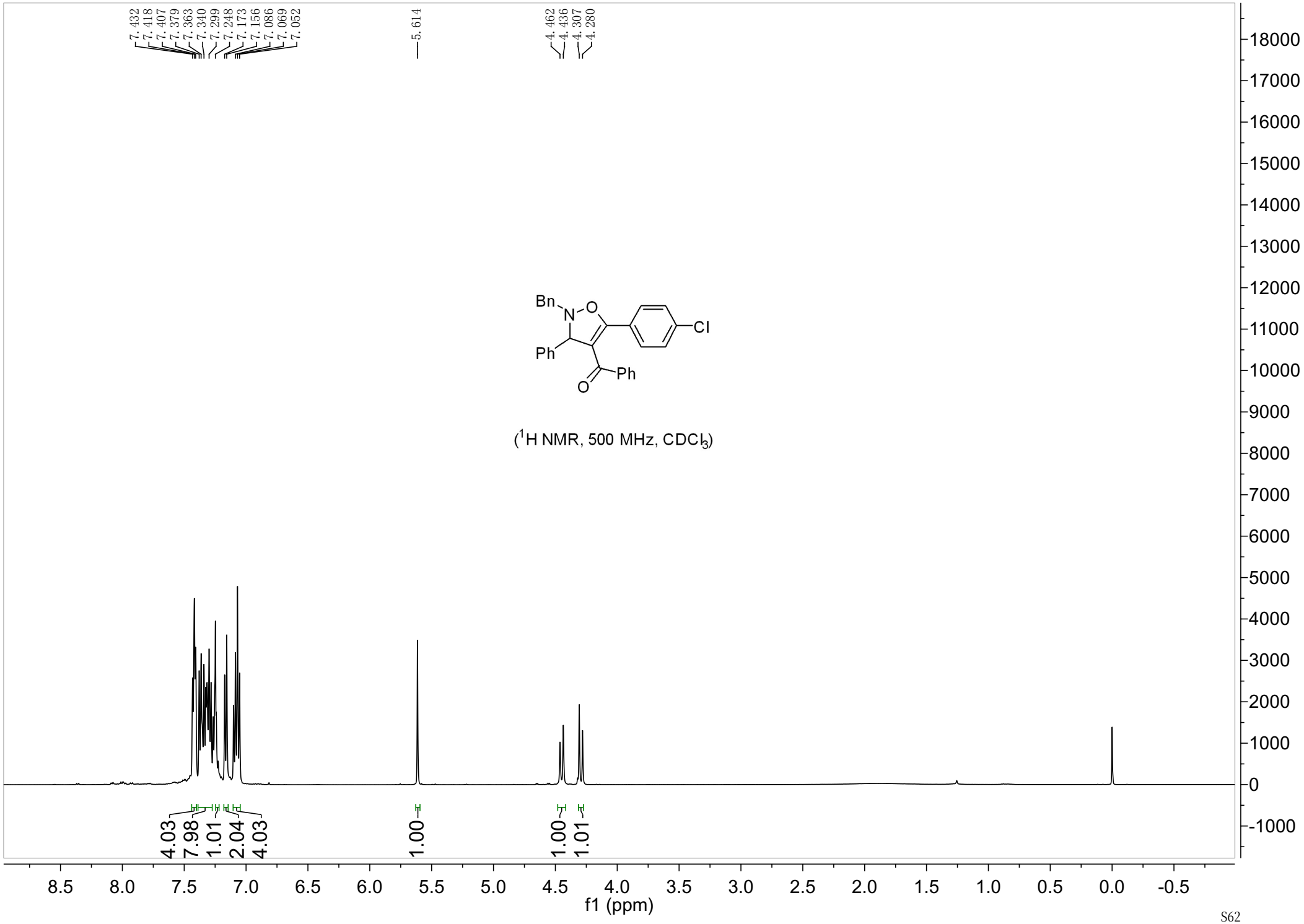

8.110
8.046
8.031
7.608
7.606
7.592
7.590
7.464
7.448
7.433
3.512
Cl
O
(1H NMR, 500 MHz, CDCl3)
0.99
1.03
1.02
1.01
1.00
f1 (ppm)

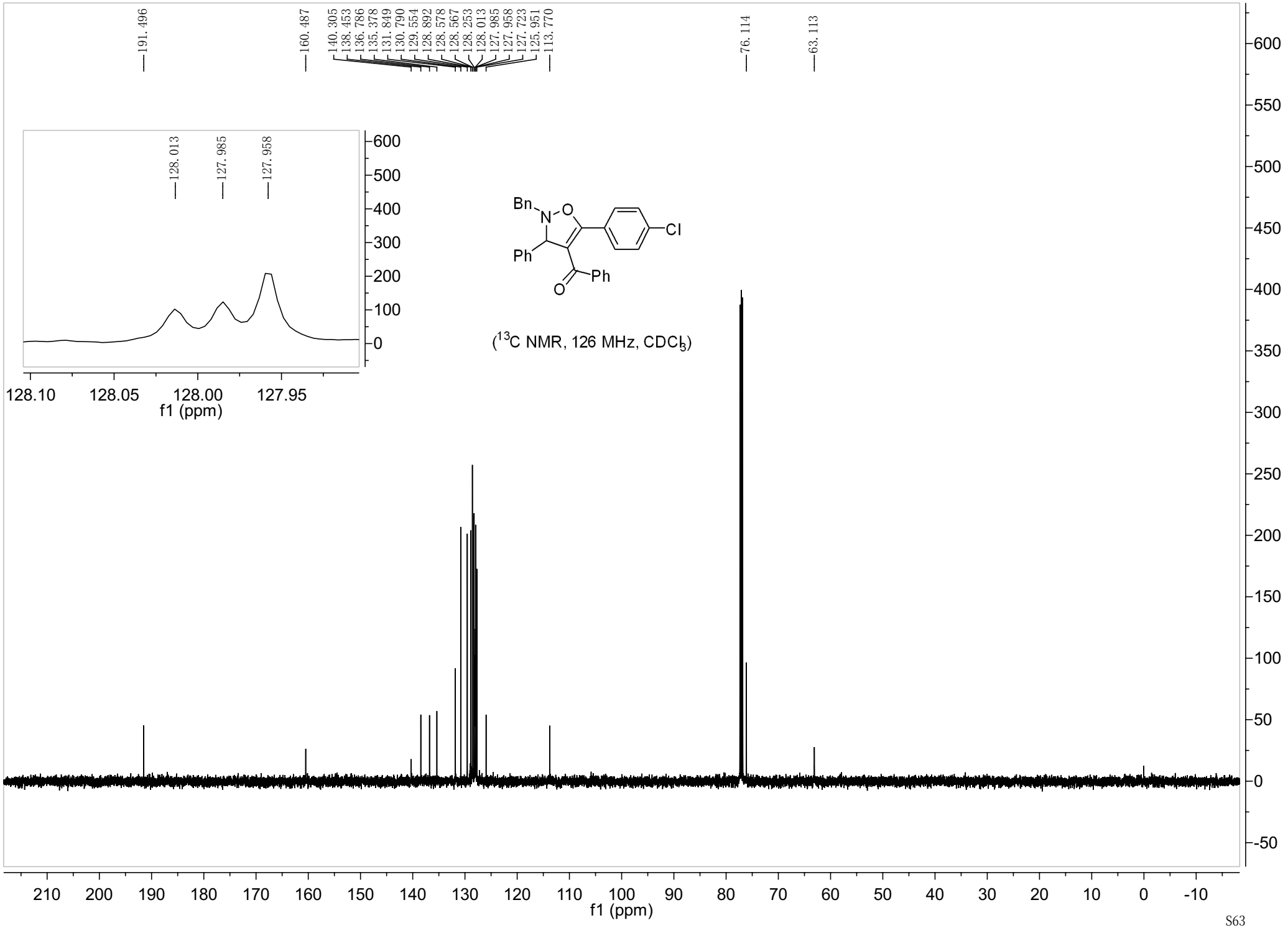

7.306
7.291
7.276
7.254
7.222
7.207
7.199
7.185
3.233
3.010
2.996
2.981
2.944
2.942
2.928
2.915
2.911
O
(^{1}H NMR, 500 MHz, CDCl$_3$)
2.09
3.05
1.00
2.02
2.01
f1 (ppm)

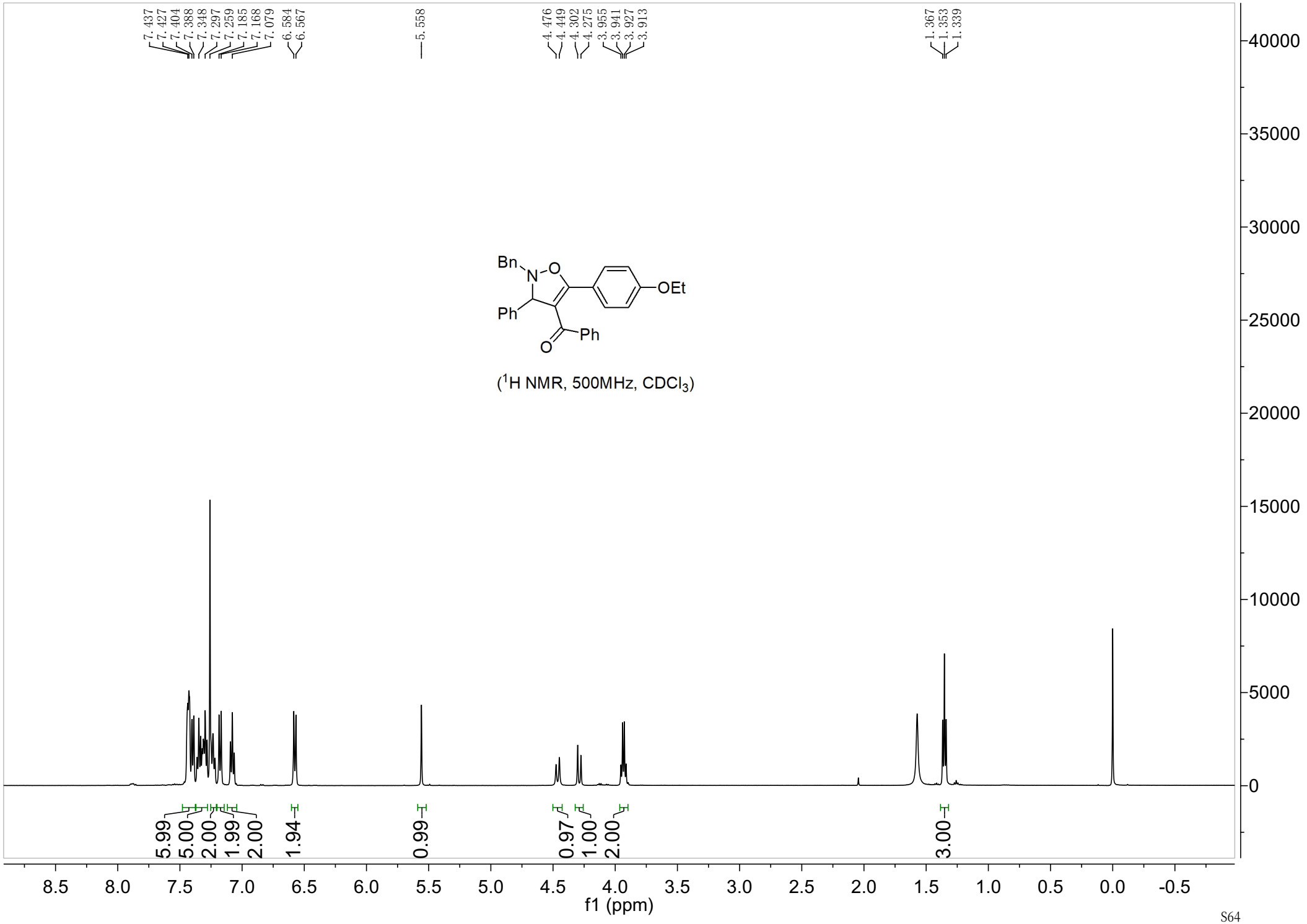

3.215
2.451
2.444
2.436
2.429
2.422
2.407
2.396
2.006
1.986
1.980
1.812
1.804
1.797
1.786
1.778
1.772
1.681
1.673
1.663
1.656
1.588
1.475
1.450
1.445
1.423
1.403
1.397
1.347
1.329
1.323
1.304
1.298
1.292
1.286
1.279
1.273
1.268
1.253
1.247
1.235
1.229
1.223
1.205
O
(^{1}H NMR, 500 MHz, CDCl$_3$)
1.00
1.08
2.03
2.12
1.18
2.06
3.12
f1 (ppm)

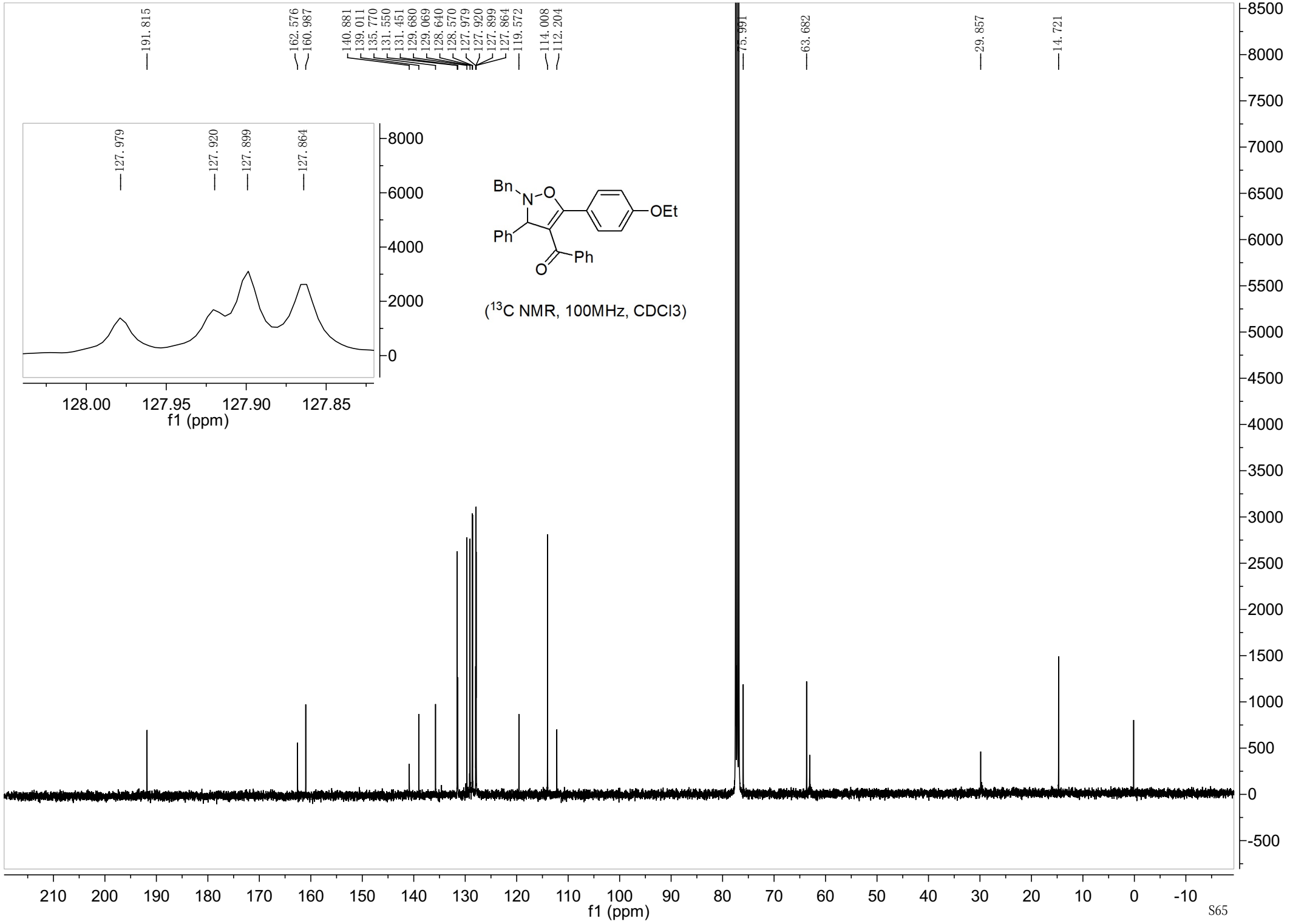

7.433
7.361
7.318
7.299
7.234
7.215
7.212
5.619
4.493
4.460
4.316
4.304
4.282
Bn
N
O
Ph
Ph
Ph
O
(1H NMR, 400 MHz, CDCl3)
4.00
7.01
5.17
4.00
1.00
1.00
1.03
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

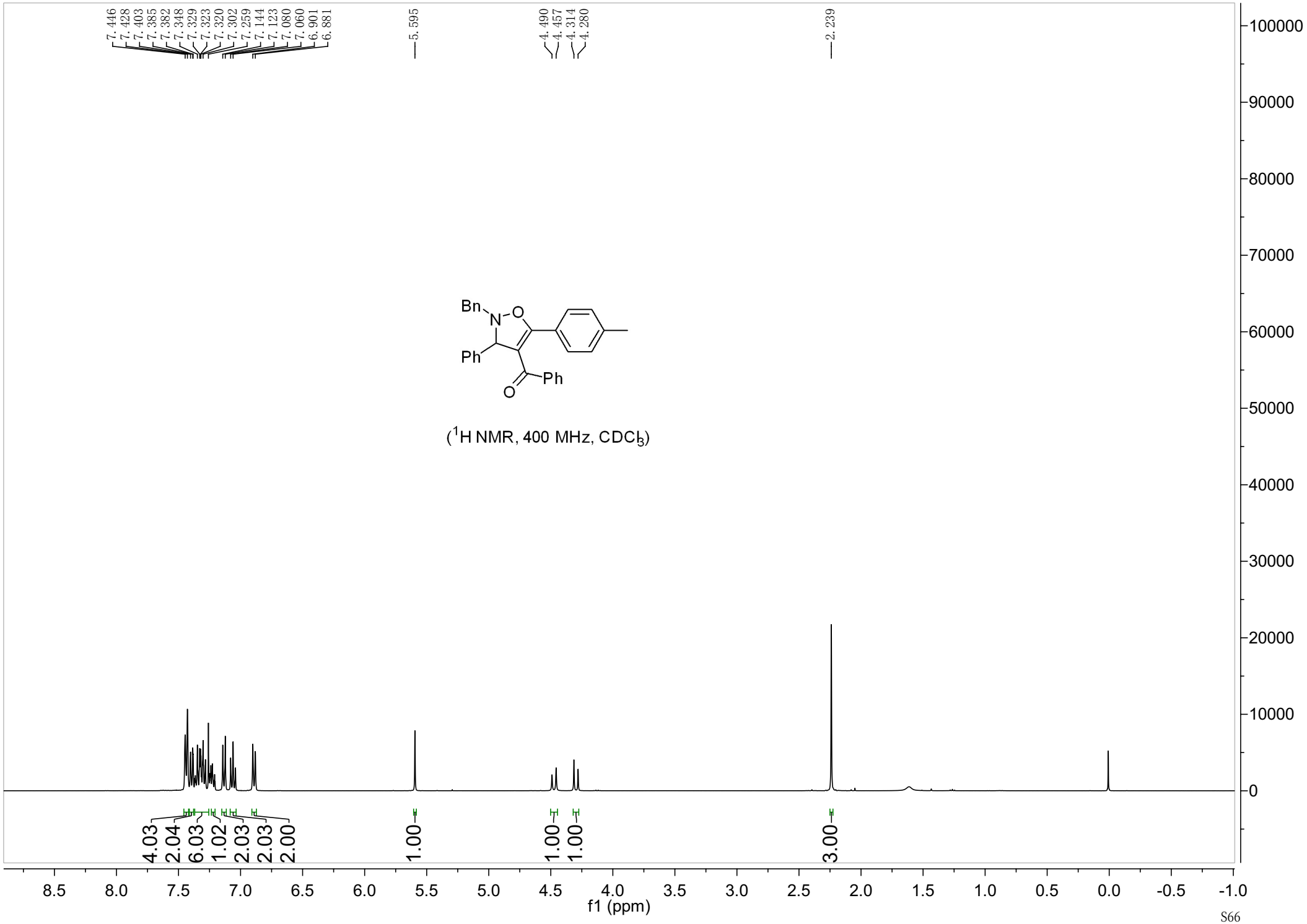

191.814
162.159
140.724
138.733
135.615
131.578
130.684
129.671
129.020
128.619
128.595
128.511
128.003
127.821
127.646
127.319
113.540
76.066
63.246
Bn
N
O
Ph
Ph
Ph
O
(13C NMR, 100 MHz, CDCl3)
2500
2000
1500
1000
500
0
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
f1 (ppm)

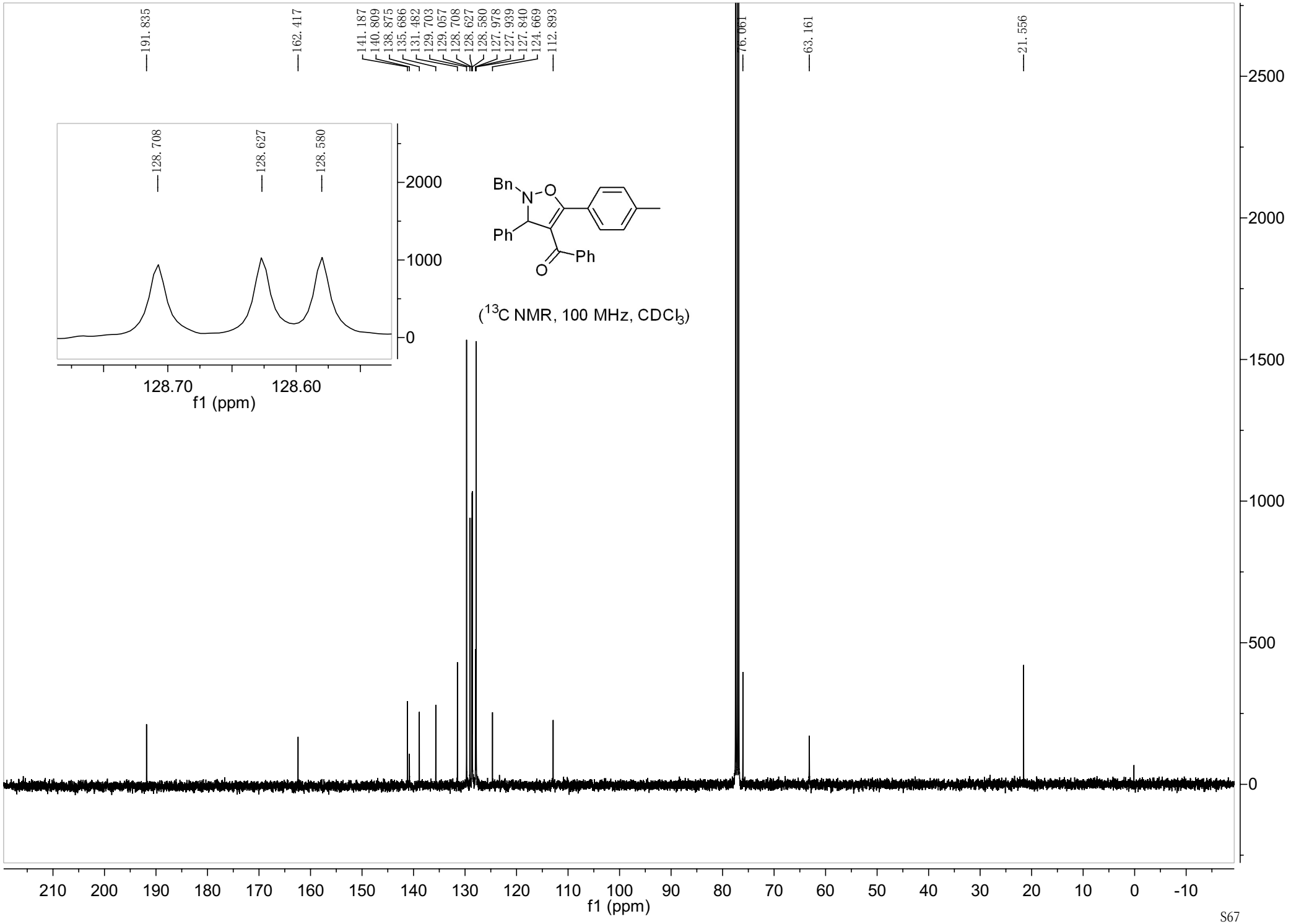

7.432
7.418
7.407
7.379
7.363
7.340
7.299
7.248
7.173
7.156
7.086
7.069
7.052
5.614
4.462
4.436
4.307
4.280
Bn
N
O
Cl
Ph
Ph
O
(1H NMR, 500 MHz, CDCl3)
4.03
7.98
1.01
2.04
4.03
1.00
1.00
1.01
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

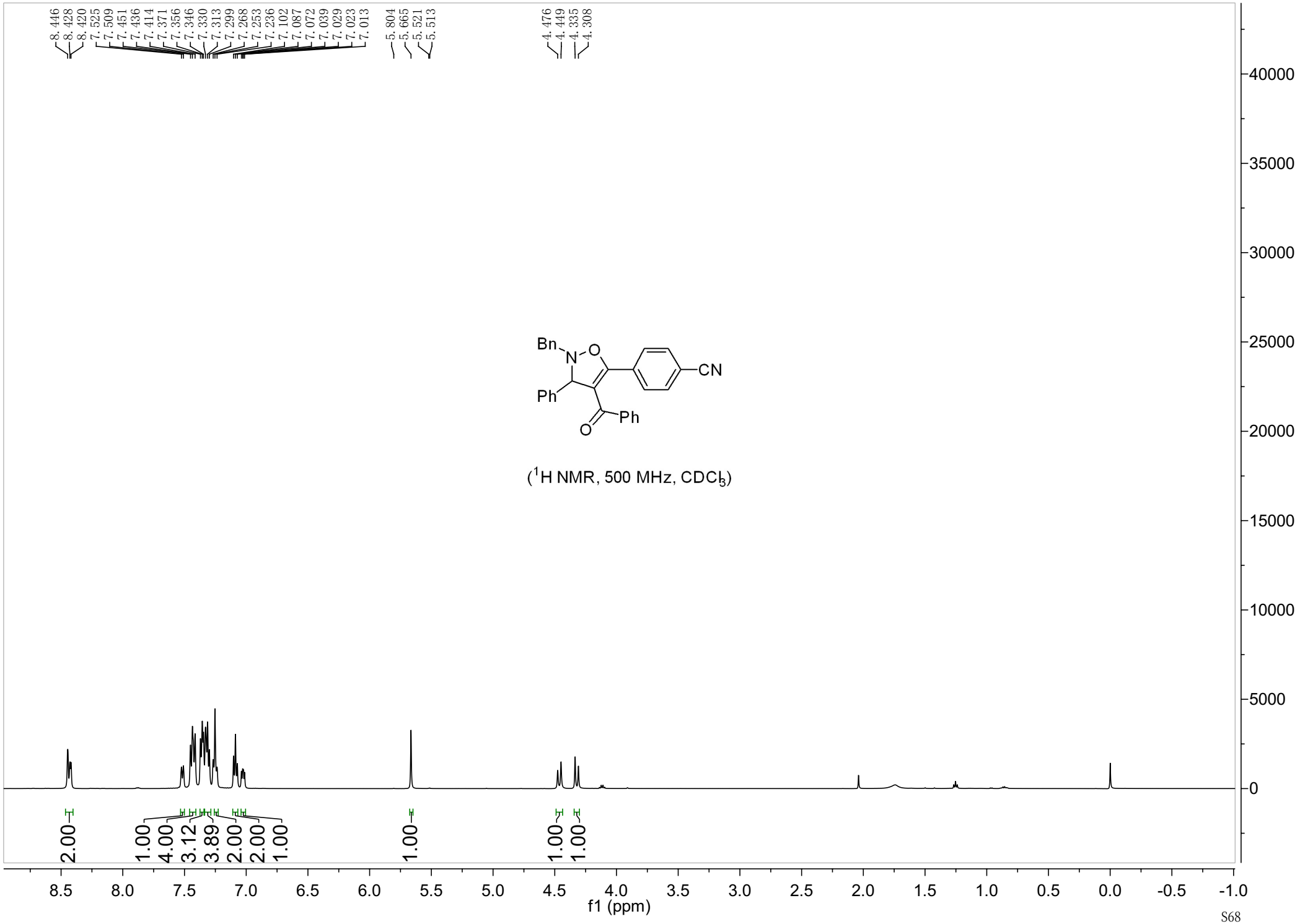

191.496
160.487
140.305
138.453
136.786
135.378
131.849
130.790
129.554
128.892
128.578
128.567
128.253
128.013
127.985
127.958
127.723
125.951
113.770
76.114
63.113
128.013
127.985
127.958
128.10
128.05
128.00
127.95
f1 (ppm)
Bn
N
O
Cl
Ph
Ph
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

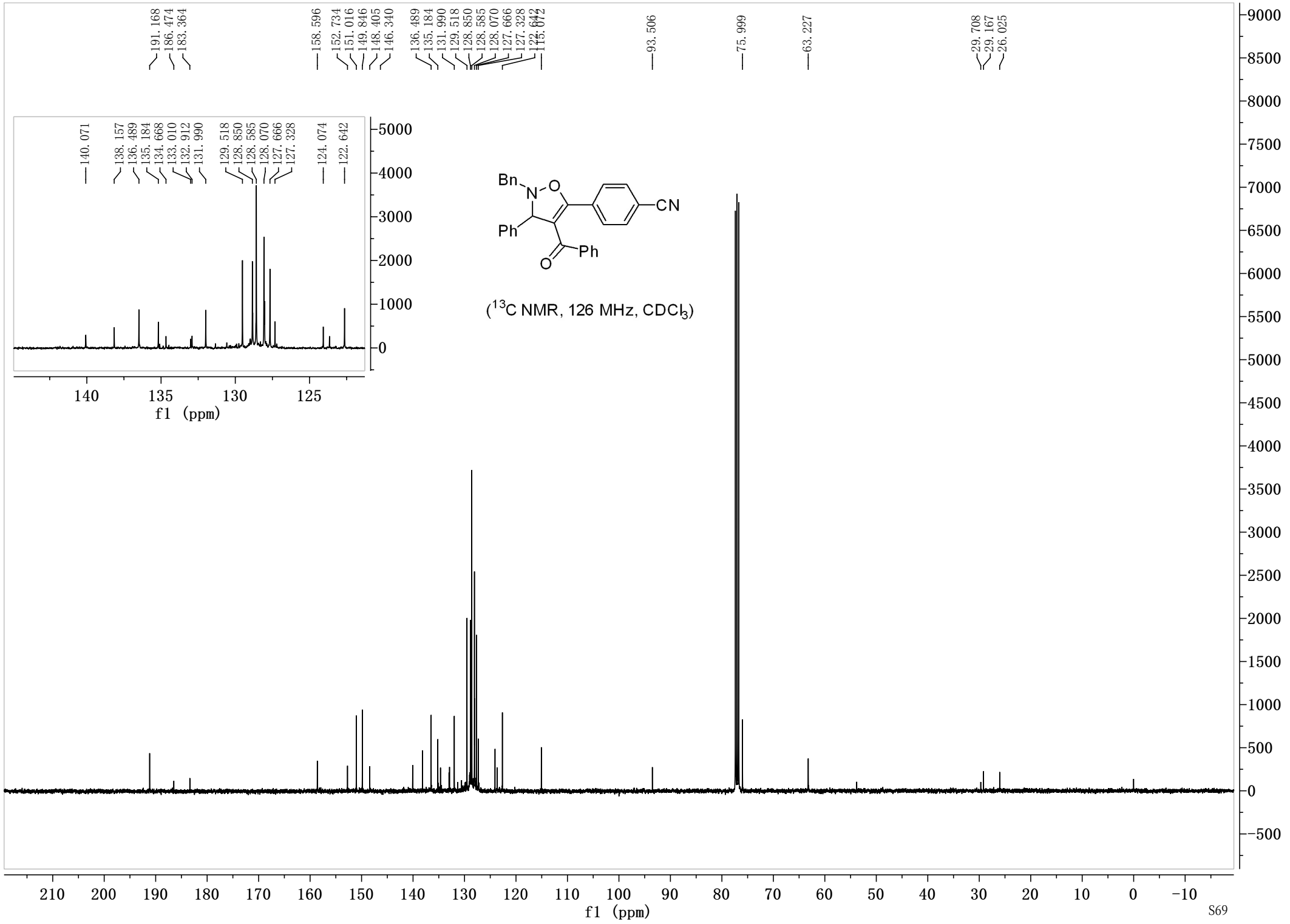

7.437
7.427
7.404
7.388
7.348
7.297
7.259
7.185
7.168
7.079
6.584
6.567
5.558
4.476
4.449
4.302
4.275
3.955
3.941
3.927
3.913
1.367
1.353
1.339
Bn
N
O
OEt
Ph
Ph
O
(1H NMR, 500MHz, CDCl3)
40000
35000
30000
25000
20000
15000
10000
5000
0
5.99
5.00
2.00
1.99
2.00
1.94
0.99
0.97
1.00
2.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

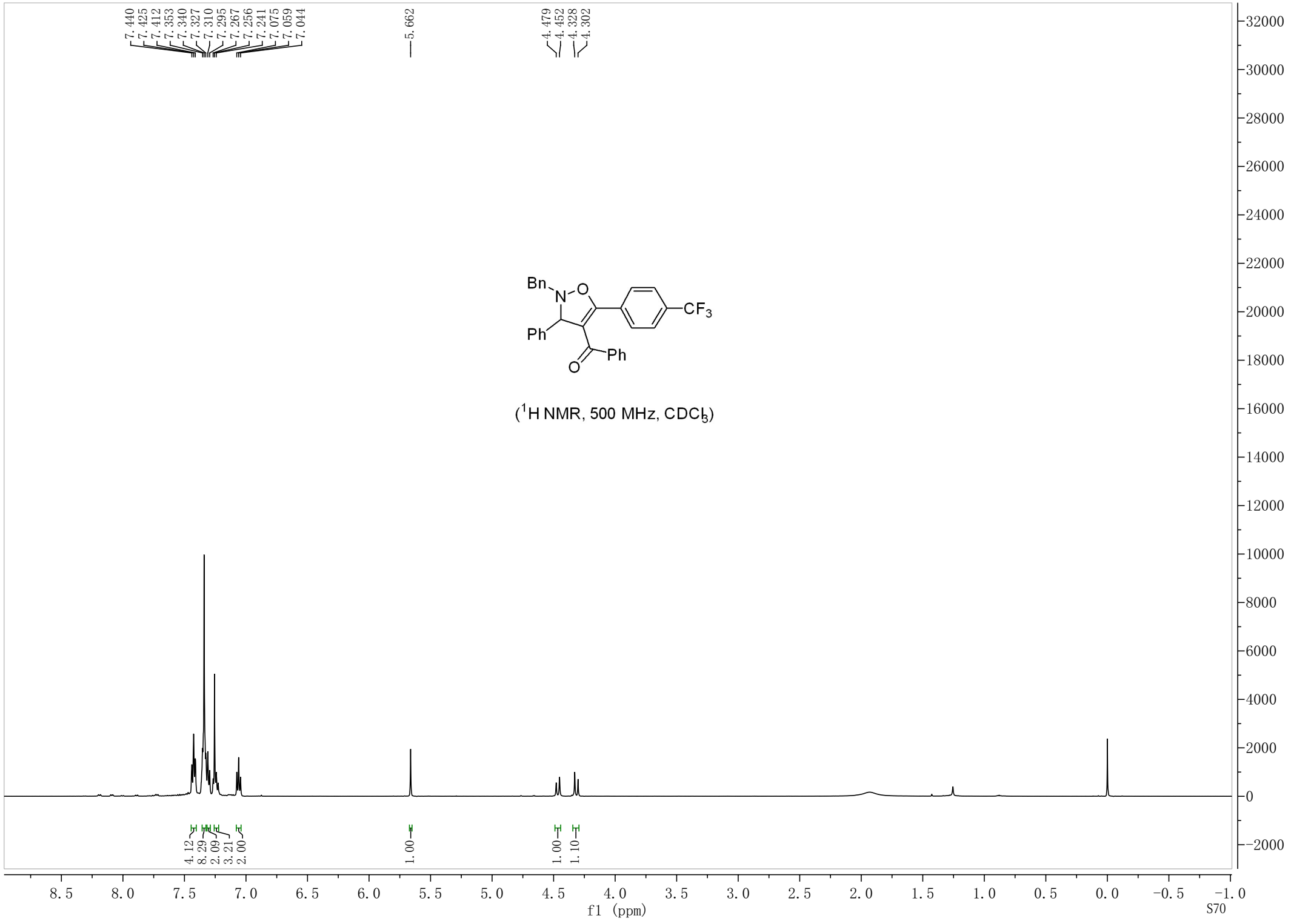

191.815
162.576
160.987
140.881
139.011
135.770
131.550
131.451
129.680
129.069
128.640
128.570
127.979
127.920
127.899
127.864
119.572
114.008
112.204
76.991
63.682
29.857
14.721
127.979
127.920
127.899
127.864
Bn
N
O
OEt
Ph
Ph
O
(^{13}C NMR, 100MHz, CDCl3)
f1 (ppm)
f1 (ppm)

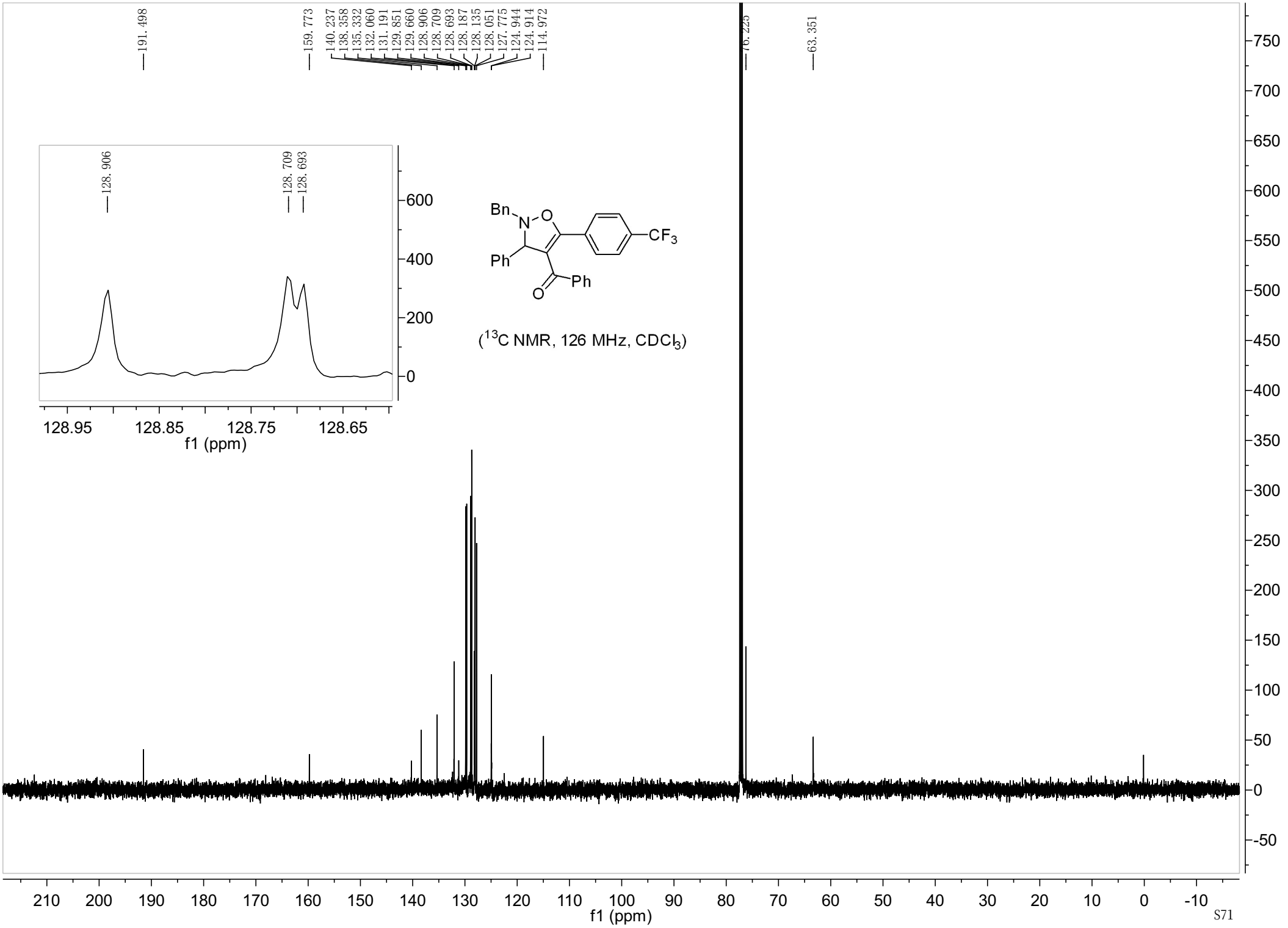

7.446
7.428
7.403
7.385
7.382
7.348
7.329
7.323
7.320
7.302
7.259
7.144
7.123
7.080
7.060
6.901
6.881
5.595
4.490
4.457
4.314
4.280
2.239
Bn
N
O
Ph
Ph
O
(1H NMR, 400 MHz, CDCl3)
4.03
2.04
6.03
1.02
2.03
2.03
2.00
1.00
1.00
1.00
3.00
f1 (ppm)

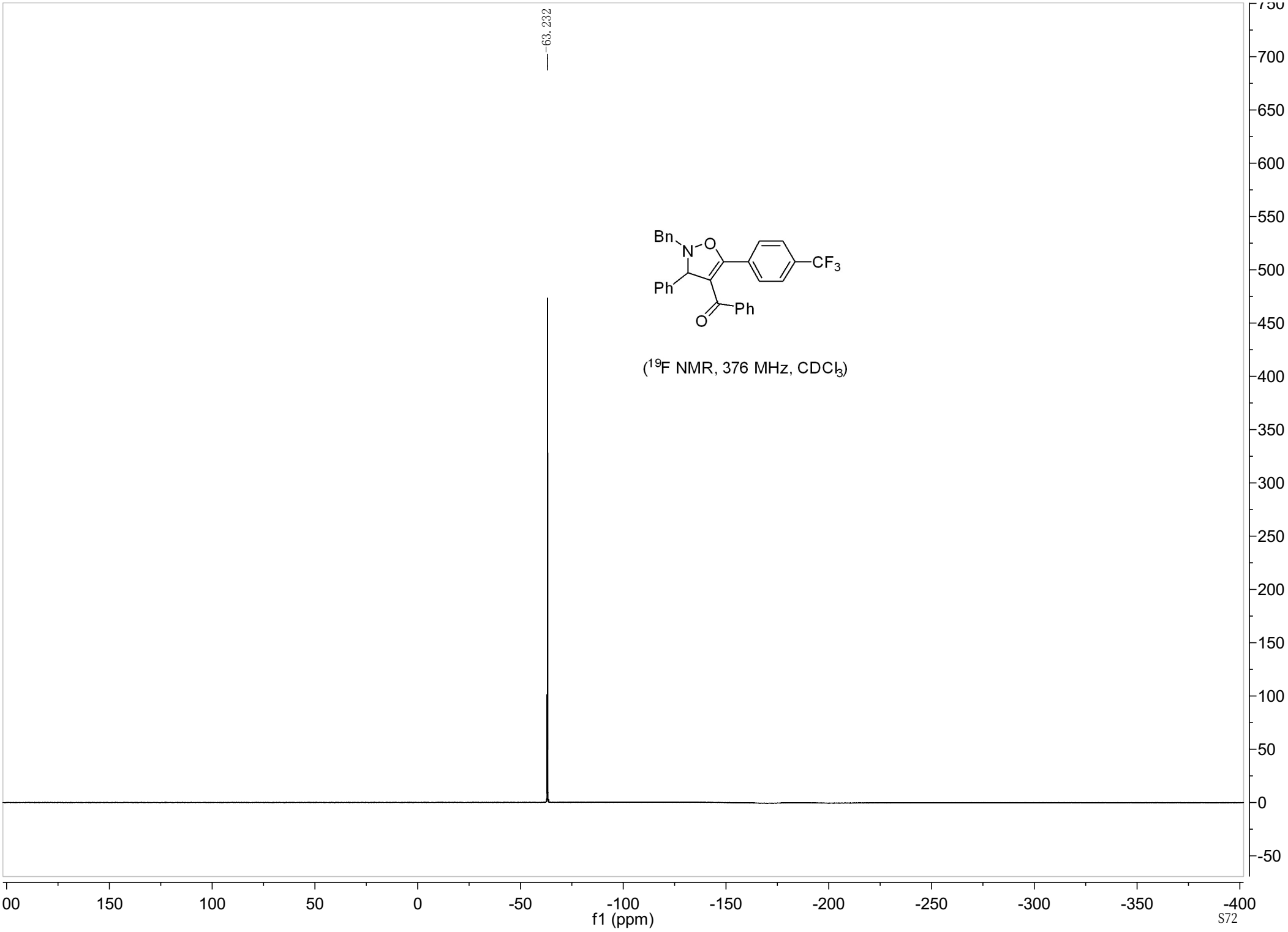

191.835
162.417
141.187
140.809
138.875
135.686
131.482
129.703
129.057
128.708
128.627
128.580
127.978
127.939
127.840
124.669
112.893
76.061
63.161
21.556
128.708
128.627
128.580
2000
1000
0
128.70
128.60
f1 (ppm)
Bn
N
O
Ph
Ph
O
(^{13}C NMR, 100 MHz, CDCl$_3$)
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

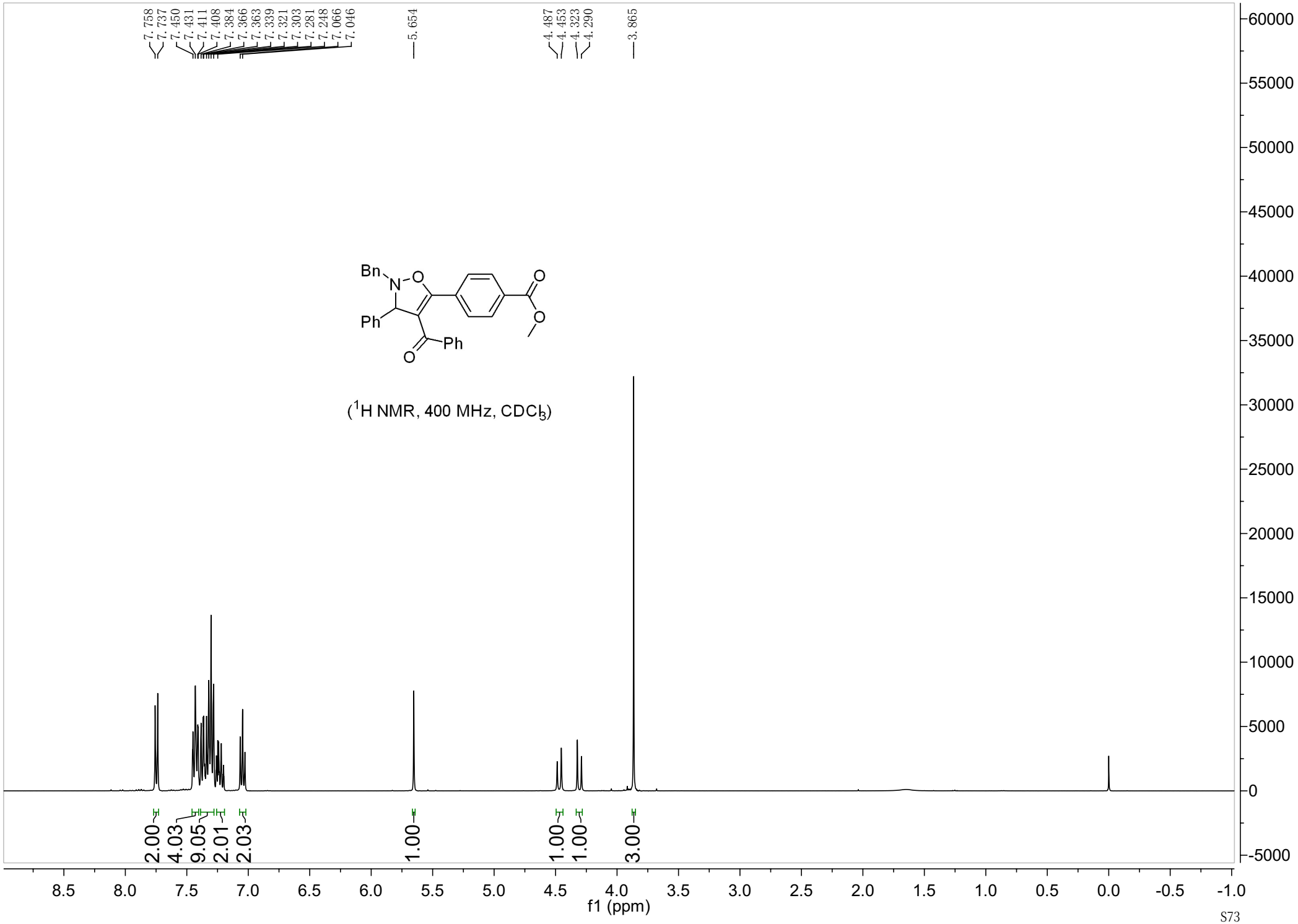

8.446
8.428
8.420
7.525
7.509
7.451
7.436
7.414
7.371
7.356
7.346
7.330
7.313
7.299
7.268
7.253
7.236
7.102
7.087
7.072
7.039
7.029
7.023
7.013
5.804
5.665
5.521
5.513
4.476
4.449
4.335
4.308
Bn
N
O
CN
Ph
Ph
O
(1H NMR, 500 MHz, CDCl3)
40000
35000
30000
25000
20000
15000
10000
5000
0
2.00
1.00
4.00
3.12
3.89
2.00
2.00
1.00
1.00
1.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

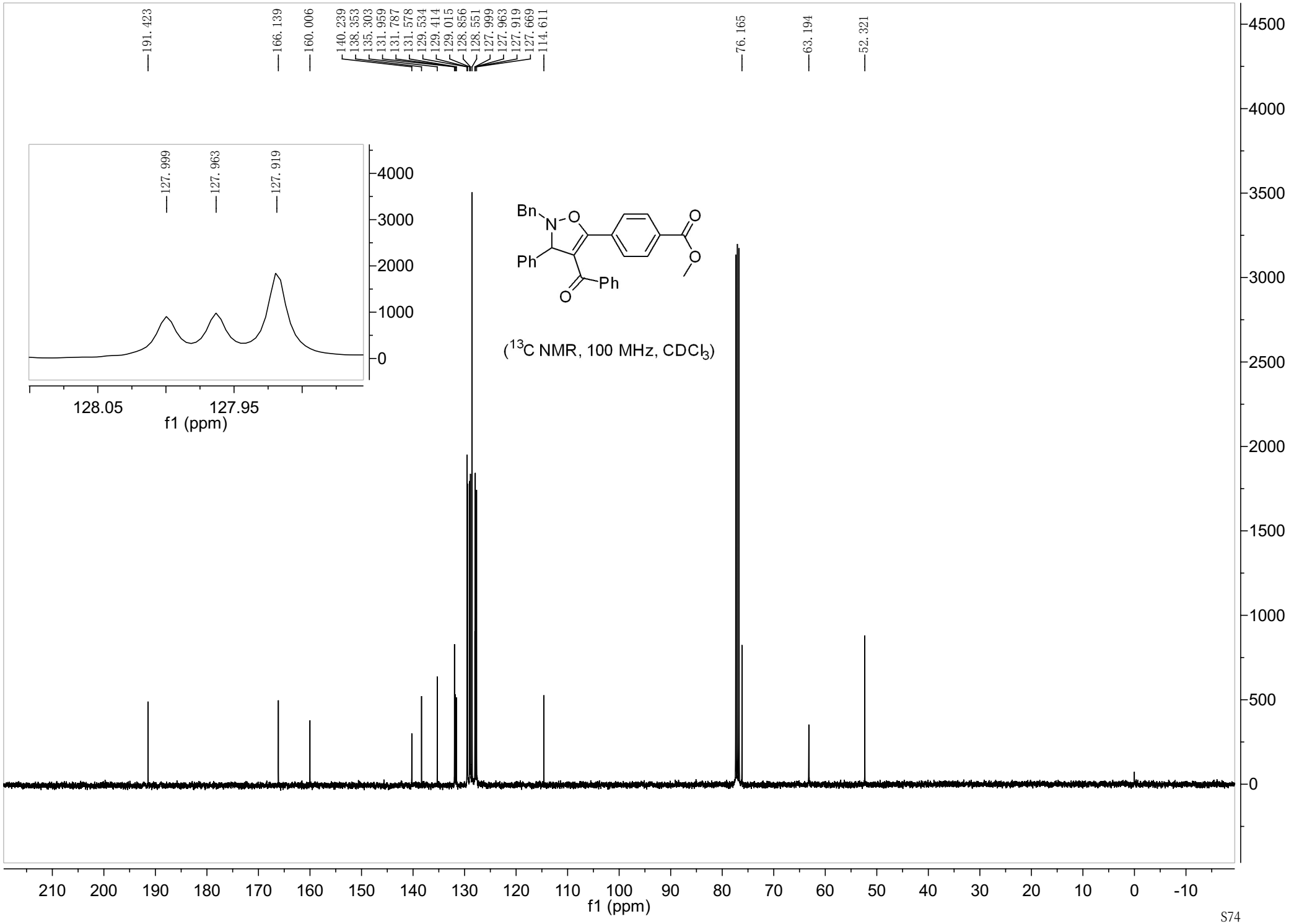

191.168
186.474
183.364
158.596
152.734
151.016
149.846
148.405
146.340
136.489
135.184
131.990
129.518
128.850
128.585
128.070
127.666
127.328
122.642
115.072
93.506
75.999
63.227
29.708
29.167
26.025
140.071
138.157
136.489
135.184
134.668
133.010
132.912
131.990
129.518
128.850
128.585
128.070
127.666
127.328
124.074
122.642
Bn
N
O
CN
Ph
Ph
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

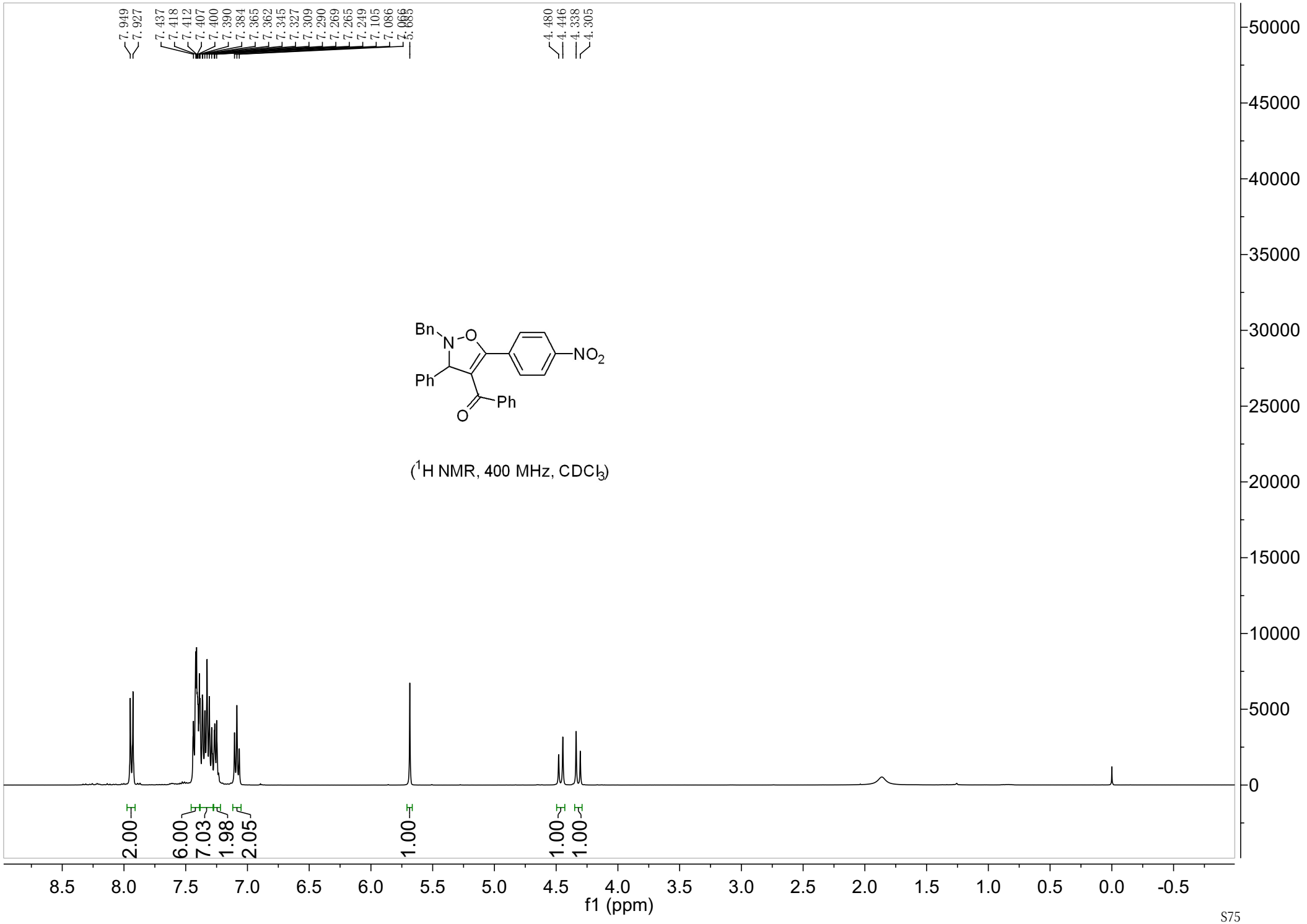

7.440
7.425
7.412
7.353
7.340
7.327
7.310
7.295
7.267
7.256
7.241
7.075
7.059
7.044
5.662
4.479
4.452
4.328
4.302
Bn
N
O
Ph
CF3
Ph
O
(1H NMR, 500 MHz, CDCl3)
4.12
8.29
2.09
3.21
2.00
1.00
1.00
1.10
f1 (ppm)

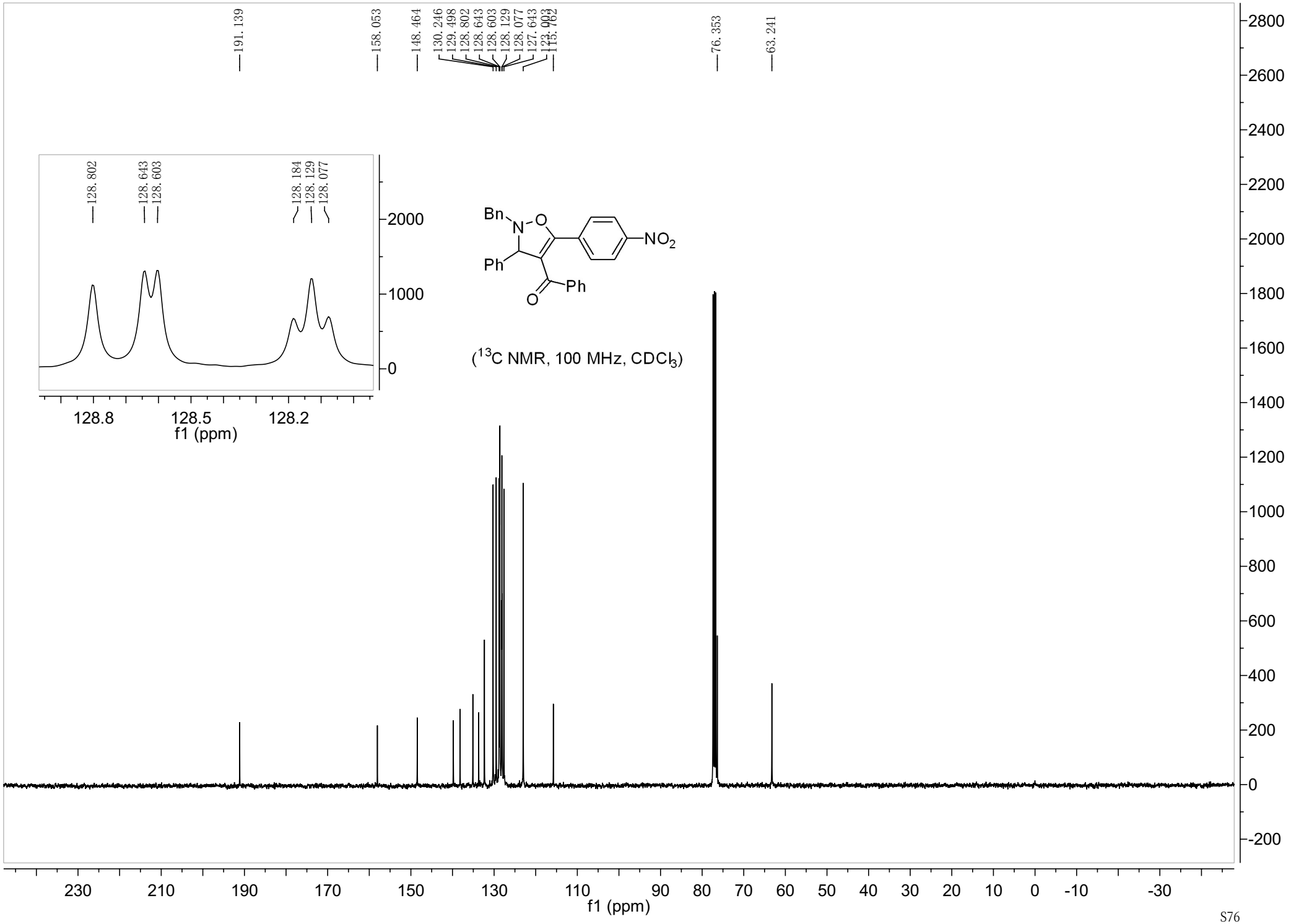

191.498
159.773
140.237
138.358
135.332
132.060
131.191
129.851
129.660
128.906
128.709
128.693
128.187
128.135
128.051
127.775
124.944
124.914
114.972
76.225
63.351
128.906
128.709
128.693
Bn
N
O
Ph
CF3
Ph
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

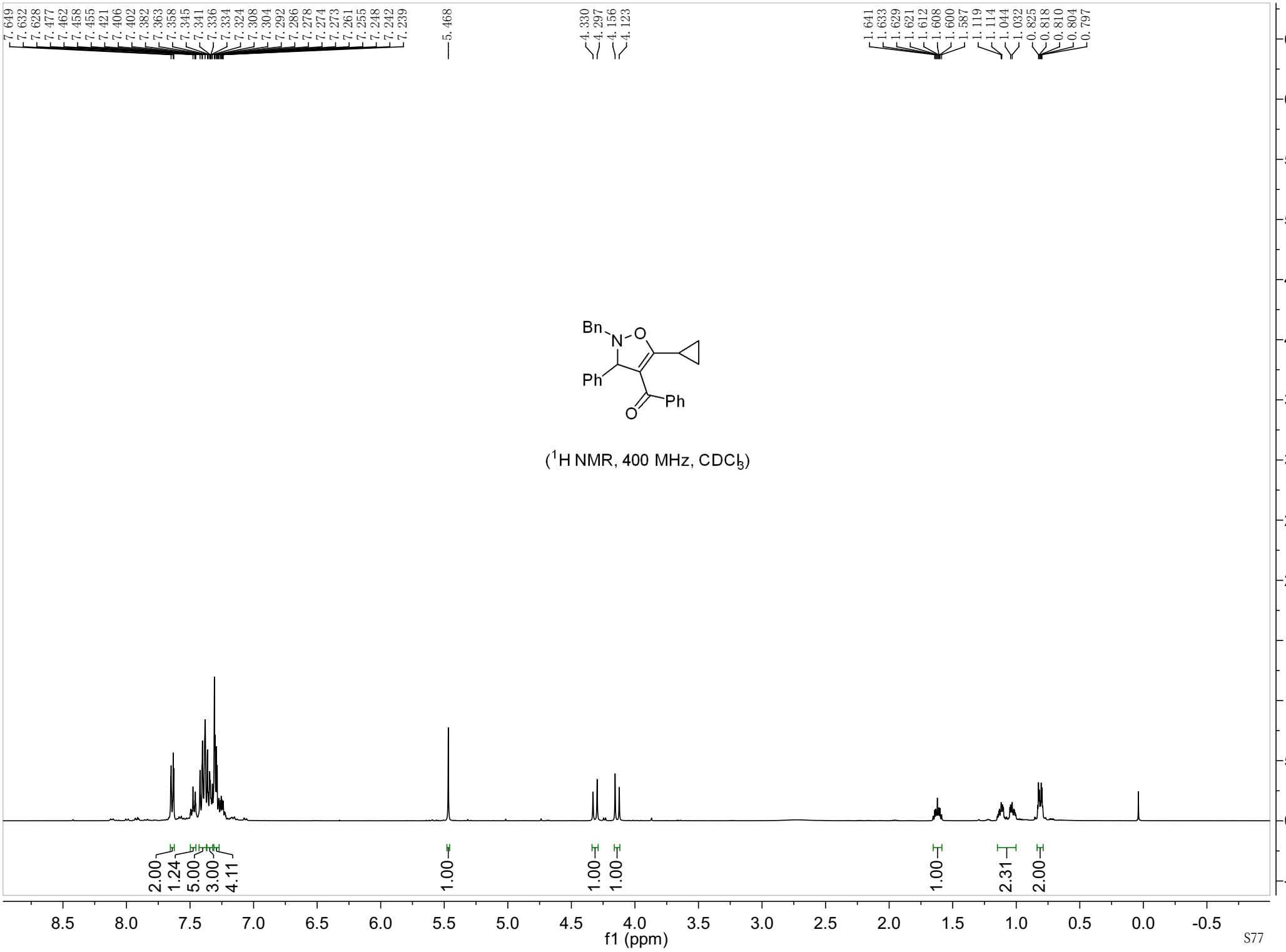

-63.232
Bn
N
O
CF3
Ph
Ph
O
(19F NMR, 376 MHz, CDCl3)
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-400
f1 (ppm)

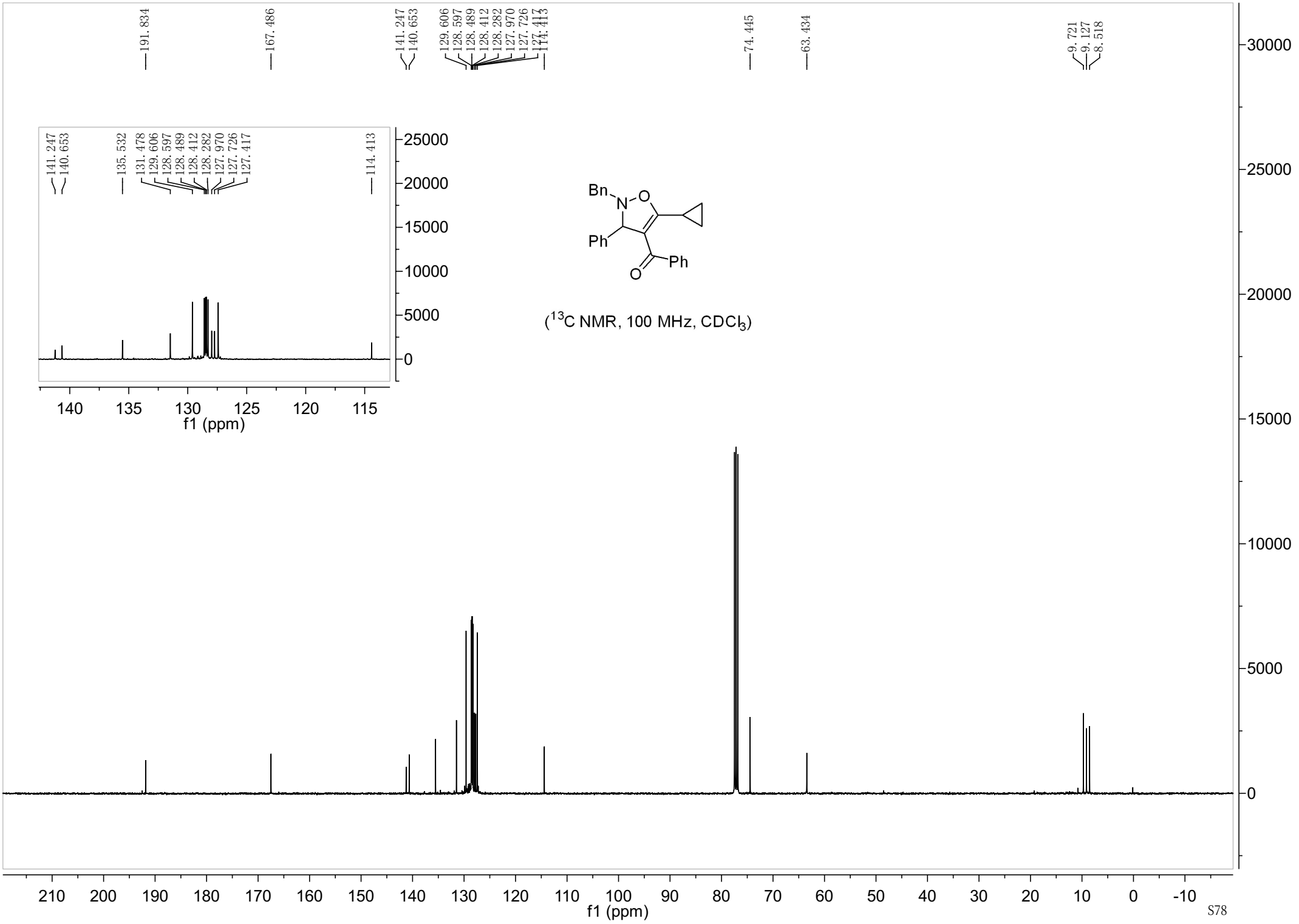

7.758
7.737
7.450
7.431
7.411
7.408
7.384
7.366
7.363
7.339
7.321
7.303
7.281
7.248
7.066
7.046
5.654
4.487
4.453
4.323
4.290
3.865
Bn
N
O
Ph
O
O
Ph
O
(1H NMR, 400 MHz, CDCl3)
2.00
4.03
9.05
2.01
2.03
1.00
1.00
1.00
3.00
f1 (ppm)

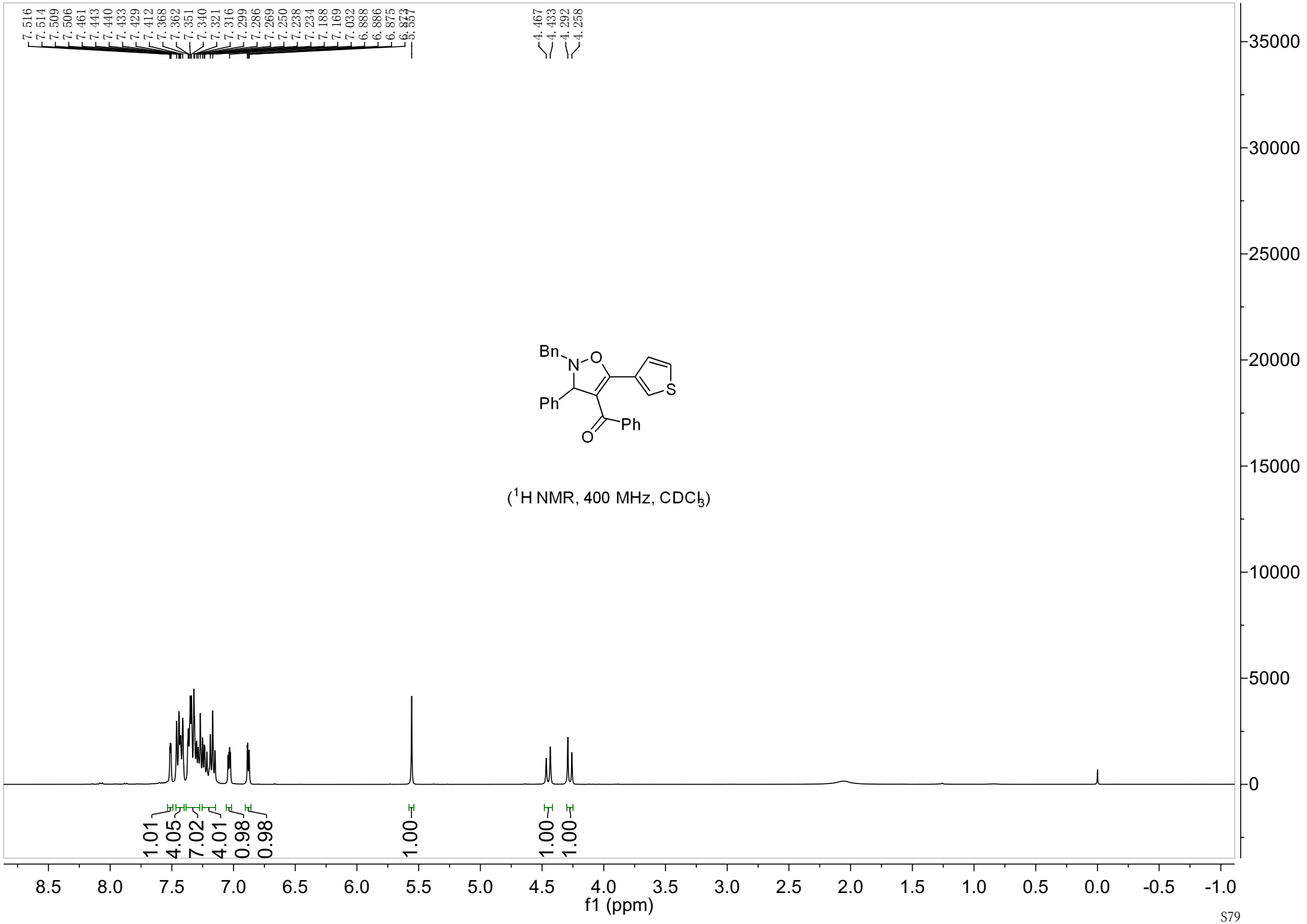

191.423
166.139
160.006
140.239
138.353
135.303
131.959
131.787
131.578
129.534
129.414
129.015
128.856
128.551
127.999
127.963
127.919
127.669
114.611
76.165
63.194
52.321
127.999
127.963
127.919
128.05
127.95
f1 (ppm)
Bn
N
O
Ph
O
O
O
Ph
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

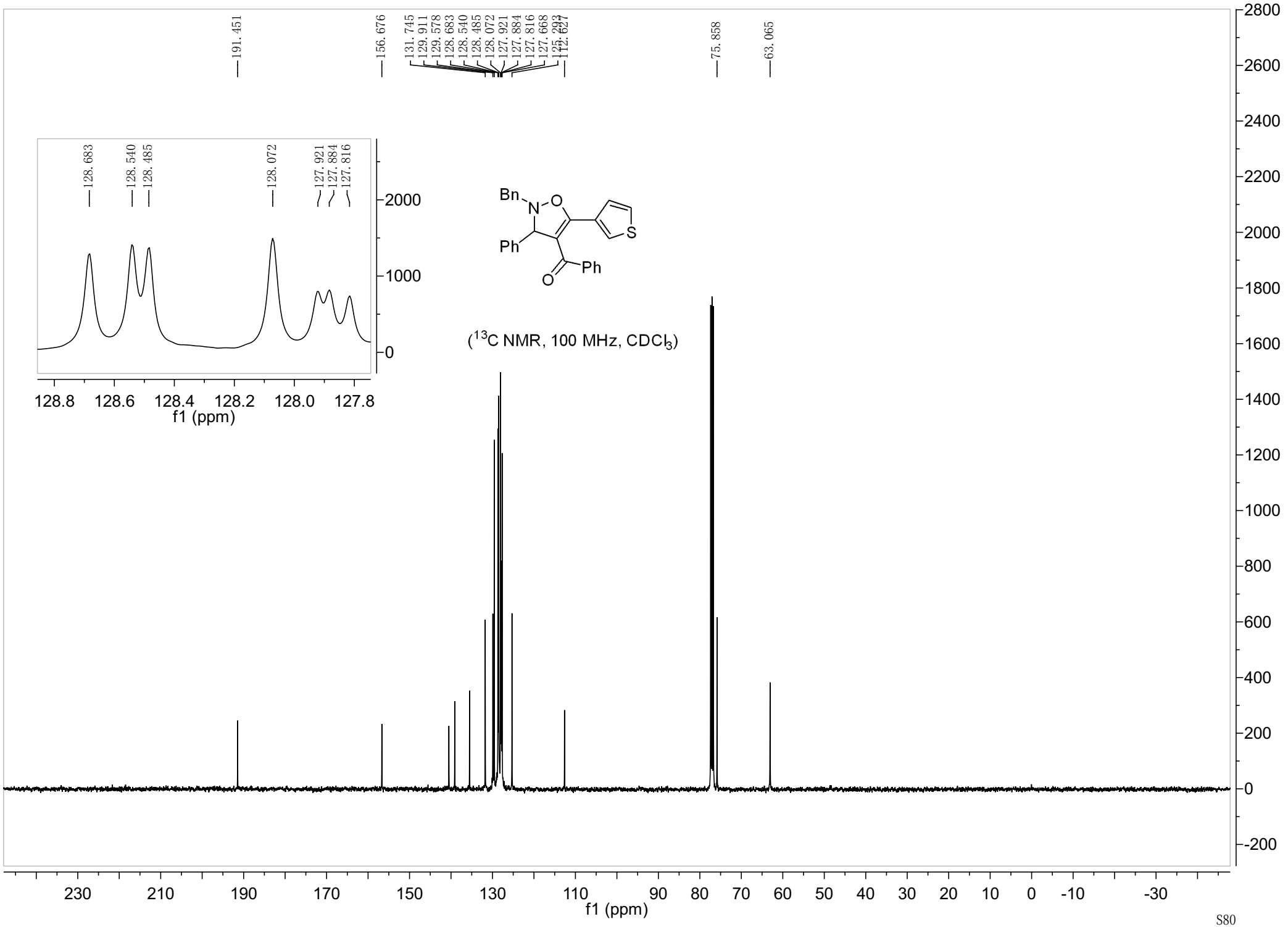

7.949
7.927
7.437
7.418
7.412
7.407
7.400
7.390
7.384
7.365
7.362
7.345
7.327
7.309
7.290
7.269
7.265
7.249
7.105
7.086
4.480
4.446
4.338
4.305
Bn
N
O
NO2
Ph
Ph
O
(1H NMR, 400 MHz, CDCl3)
2.00
6.00
7.03
1.98
2.05
1.00
1.00
1.00
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

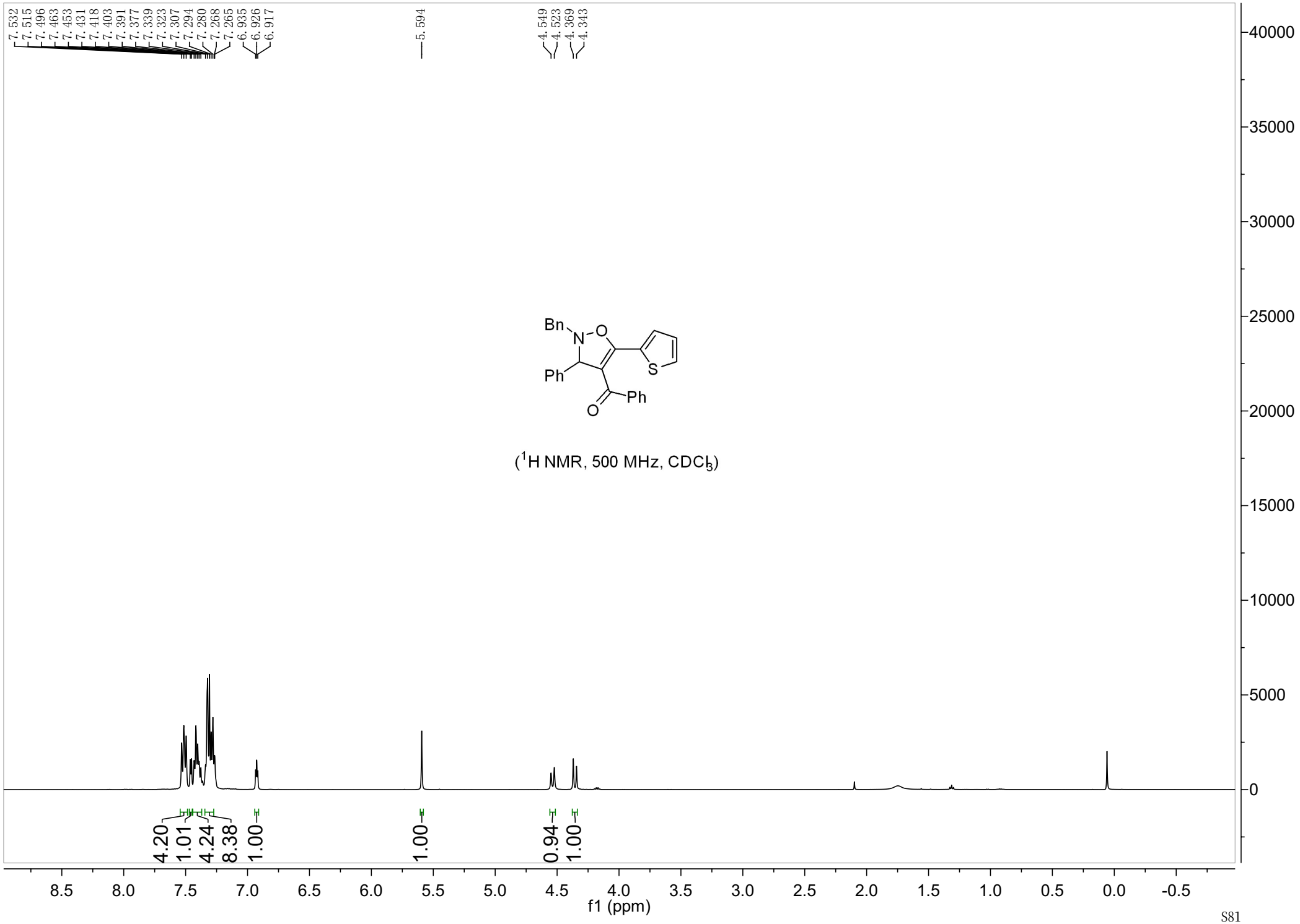

191. 139
158. 053
148. 464
130. 246
129. 498
128. 802
128. 643
128. 603
128. 129
128. 077
127. 643
123. 903
115. 762
76. 353
63. 241
128. 802
128. 643
128. 603
128. 184
128. 129
128. 077
Bn
N
O
NO2
Ph
Ph
O
(^{13}C NMR, 100 MHz, CDCl$_3$)
f1 (ppm)
f1 (ppm)

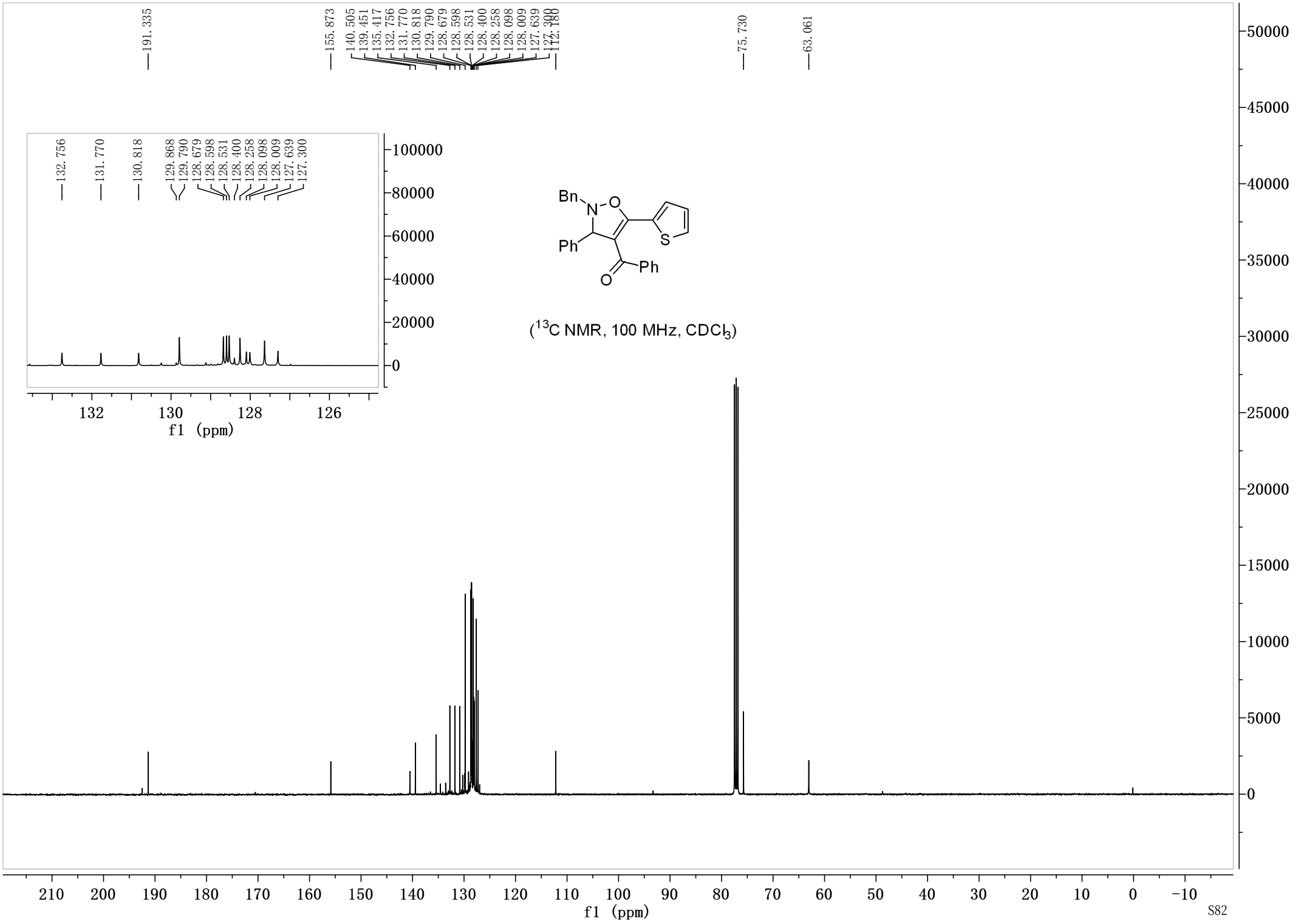

7.649
7.632
7.628
7.477
7.462
7.458
7.455
7.421
7.406
7.402
7.382
7.363
7.358
7.345
7.341
7.336
7.334
7.324
7.308
7.304
7.292
7.286
7.278
7.274
7.273
7.261
7.255
7.248
7.242
7.239
5.468
4.330
4.297
4.156
4.123
1.641
1.633
1.629
1.621
1.612
1.608
1.600
1.587
1.119
1.114
1.044
1.032
0.825
0.818
0.810
0.804
0.797
Bn
N
O
Ph
Ph
O
(1H NMR, 400 MHz, CDCl3)
2.00
1.24
5.00
3.00
4.11
1.00
1.00
1.00
1.00
2.31
2.00
f1 (ppm)

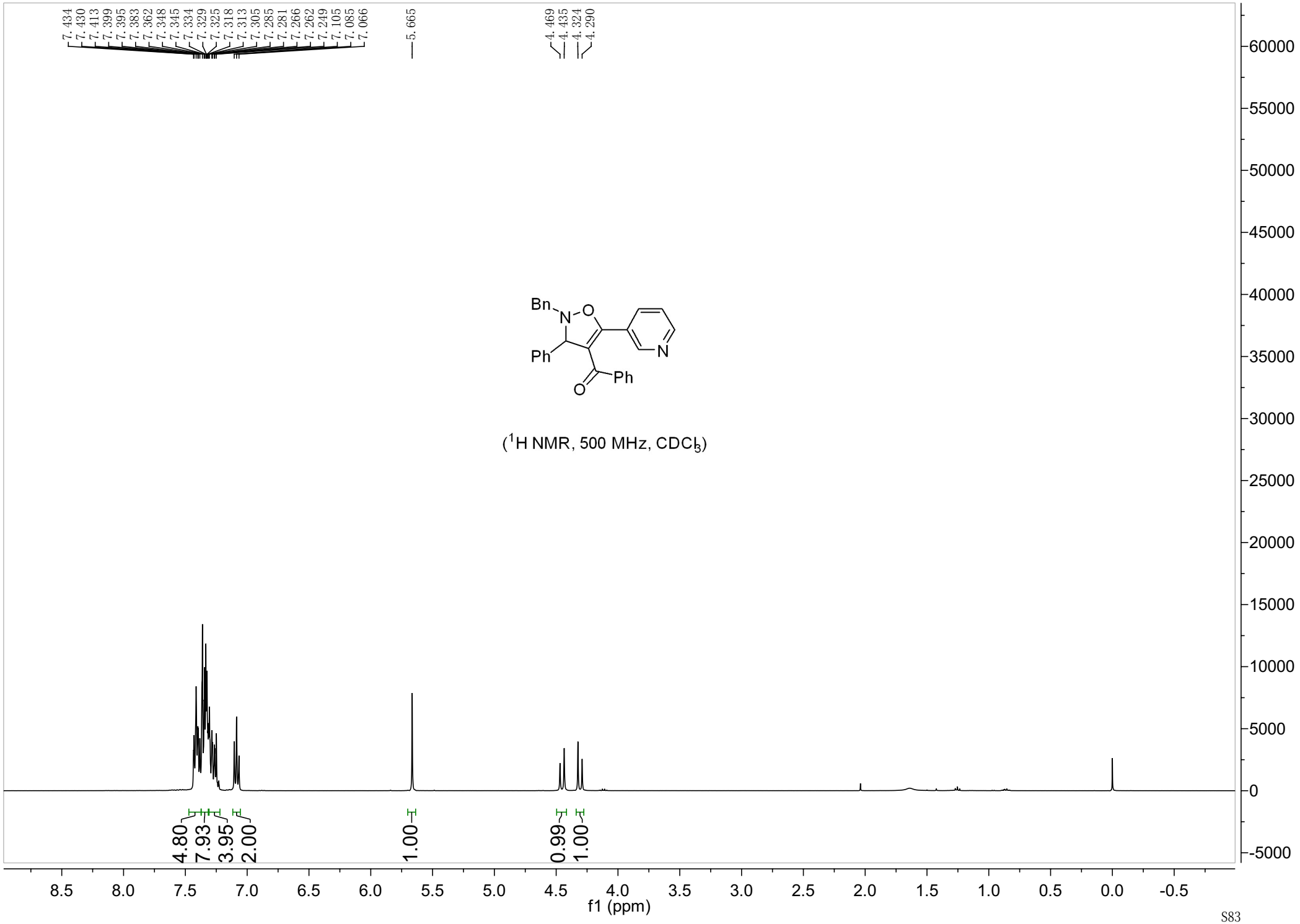

191.834
167.486
141.247
140.653
129.606
128.597
128.489
128.412
128.282
127.970
127.726
127.417
114.413
74.445
63.434
9.721
9.127
8.518
Bn
N
O
Ph
Ph
O
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)

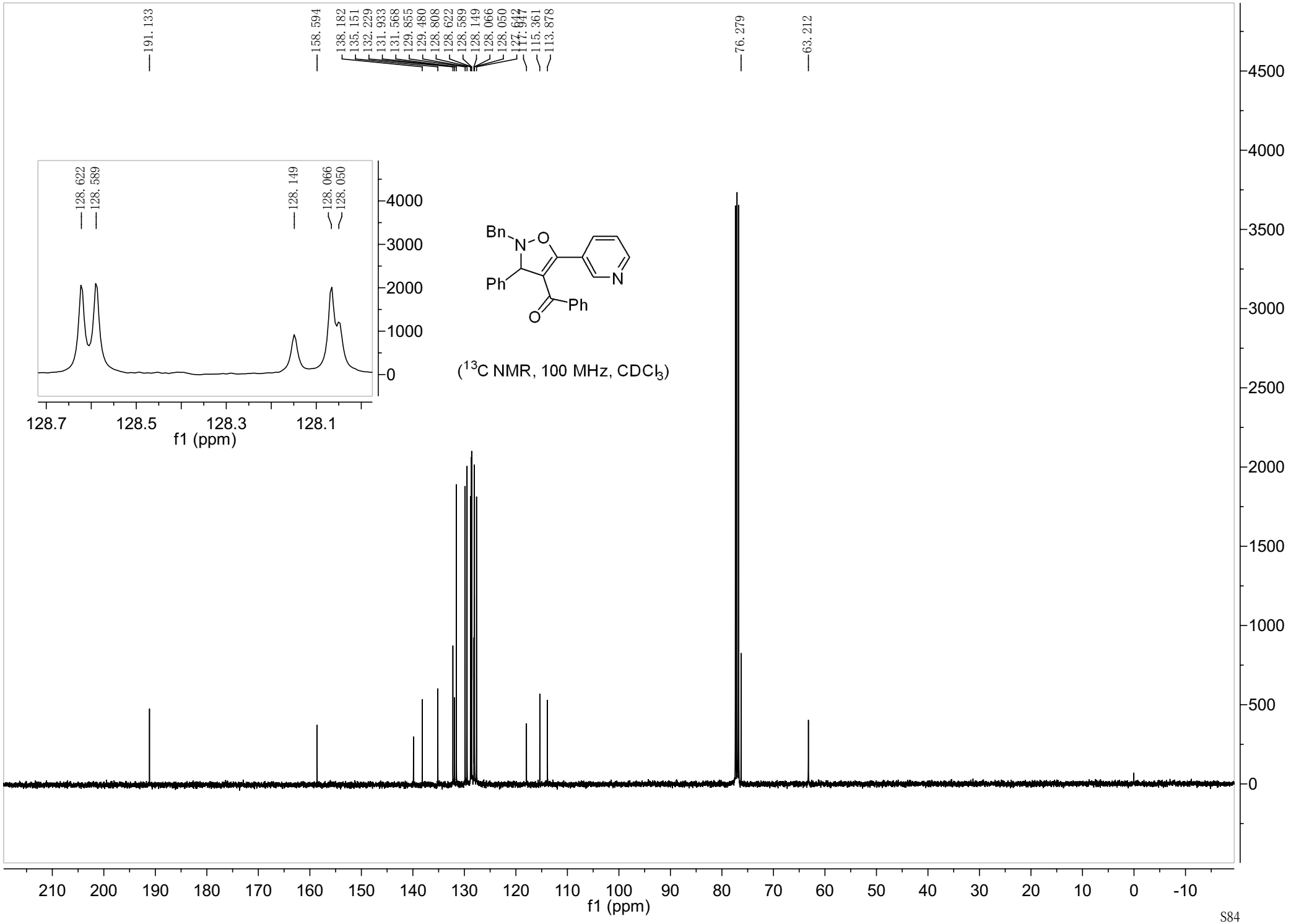

7.516
7.514
7.509
7.506
7.461
7.443
7.440
7.433
7.429
7.412
7.368
7.362
7.351
7.340
7.321
7.316
7.299
7.286
7.269
7.250
7.238
7.234
7.188
7.169
7.032
6.888
6.886
6.875
6.873
6.857
4.467
4.433
4.292
4.258
Bn
N
O
Ph
S
Ph
O
(1H NMR, 400 MHz, CDCl3)
35000
30000
25000
20000
15000
10000
5000
0
1.01
4.05
7.02
4.01
0.98
0.98
1.00
1.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

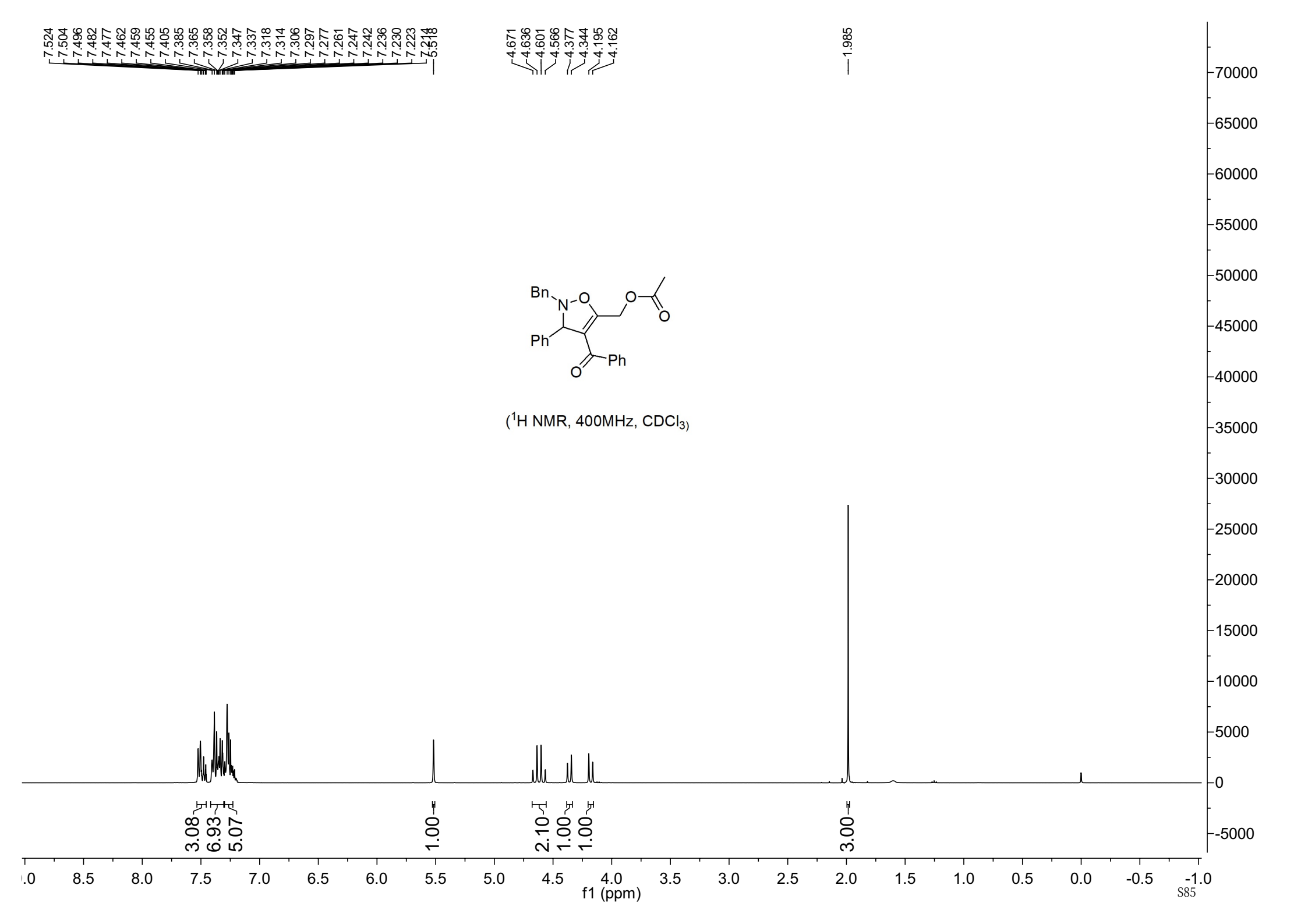

191.451
156.676
131.745
129.911
129.578
128.683
128.540
128.485
128.072
127.921
127.884
127.816
127.668
75.858
63.065
128.683
128.540
128.485
128.072
127.921
127.884
127.816
Bn
N
O
S
Ph
Ph
O
(^{13}C NMR, 100 MHz, CDCl$_3$)
f1 (ppm)
f1 (ppm)


7.532
7.515
7.496
7.463
7.453
7.431
7.418
7.403
7.391
7.377
7.339
7.323
7.307
7.294
7.280
7.268
7.265
6.935
6.926
6.917
5.594
4.549
4.523
4.369
4.343
Bn
N
O
Ph
S
Ph
O
(1H NMR, 500 MHz, CDCl3)
4.20
1.01
4.24
8.38
1.00
1.00
0.94
1.00
40000
35000
30000
25000
20000
15000
10000
5000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

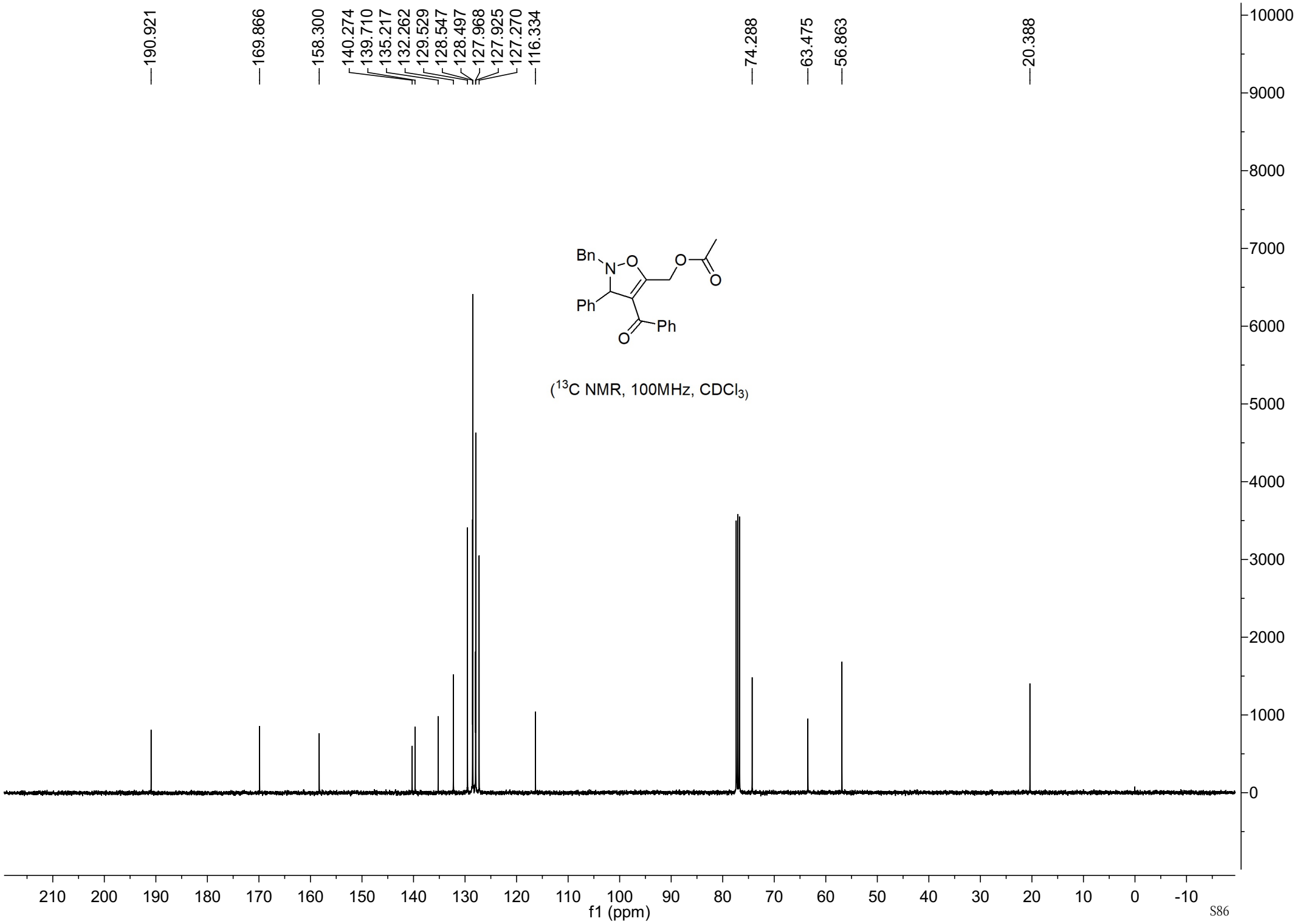

191.335
155.873
140.505
139.451
135.417
132.756
131.770
130.818
129.790
128.679
128.598
128.531
128.400
128.258
128.098
128.009
127.639
127.300
112.180
75.730
63.061
Bn
N
O
Ph
S
Ph
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

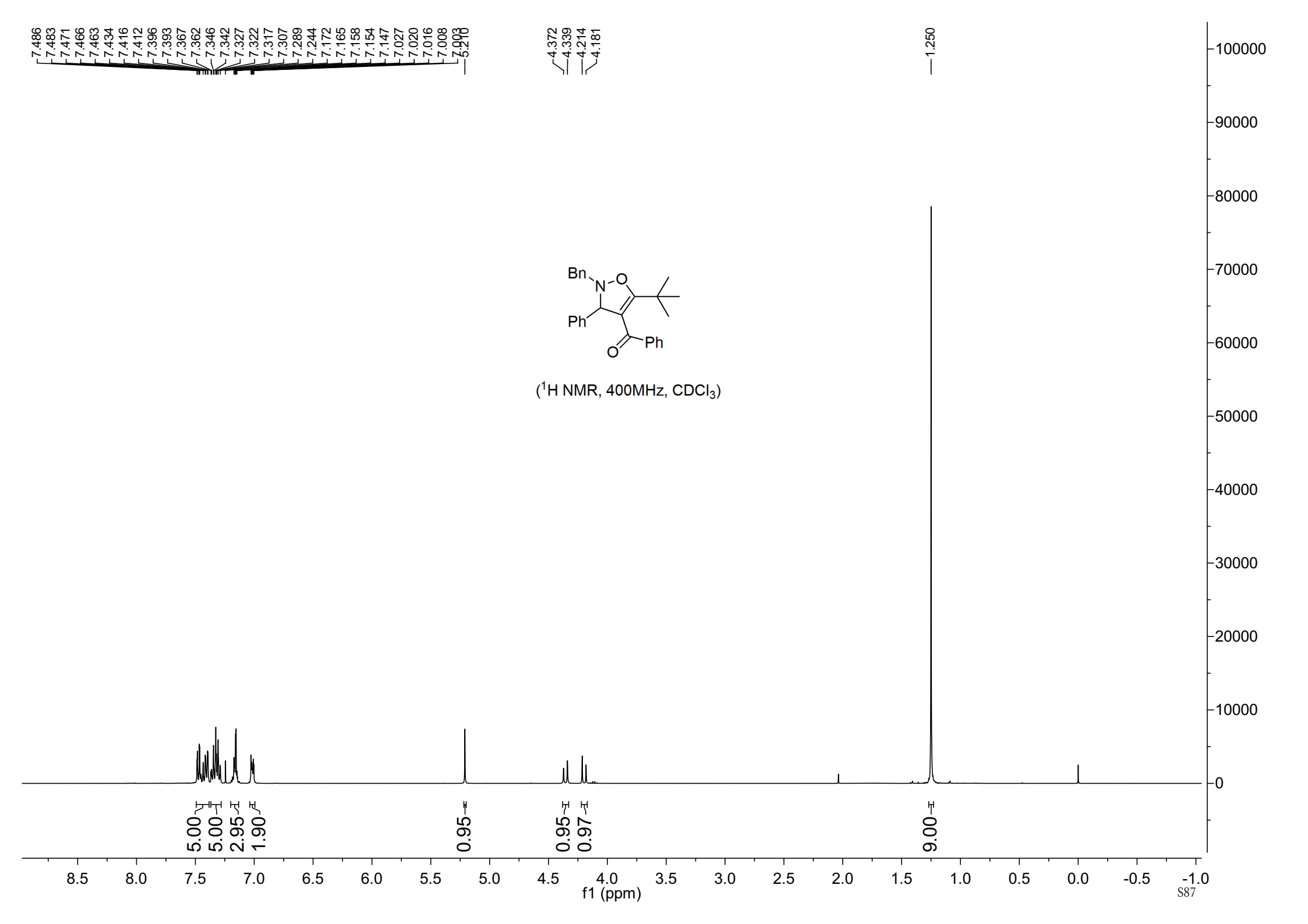

7.434
7.430
7.413
7.399
7.395
7.383
7.362
7.348
7.345
7.334
7.329
7.325
7.318
7.313
7.305
7.285
7.281
7.266
7.262
7.249
7.105
7.085
7.066
5.665
4.469
4.435
4.324
4.290
Bn
N
O
Ph
N
Ph
O
(1H NMR, 500 MHz, CDCl3)
4.80
7.93
3.95
2.00
1.00
0.99
1.00
f1 (ppm)

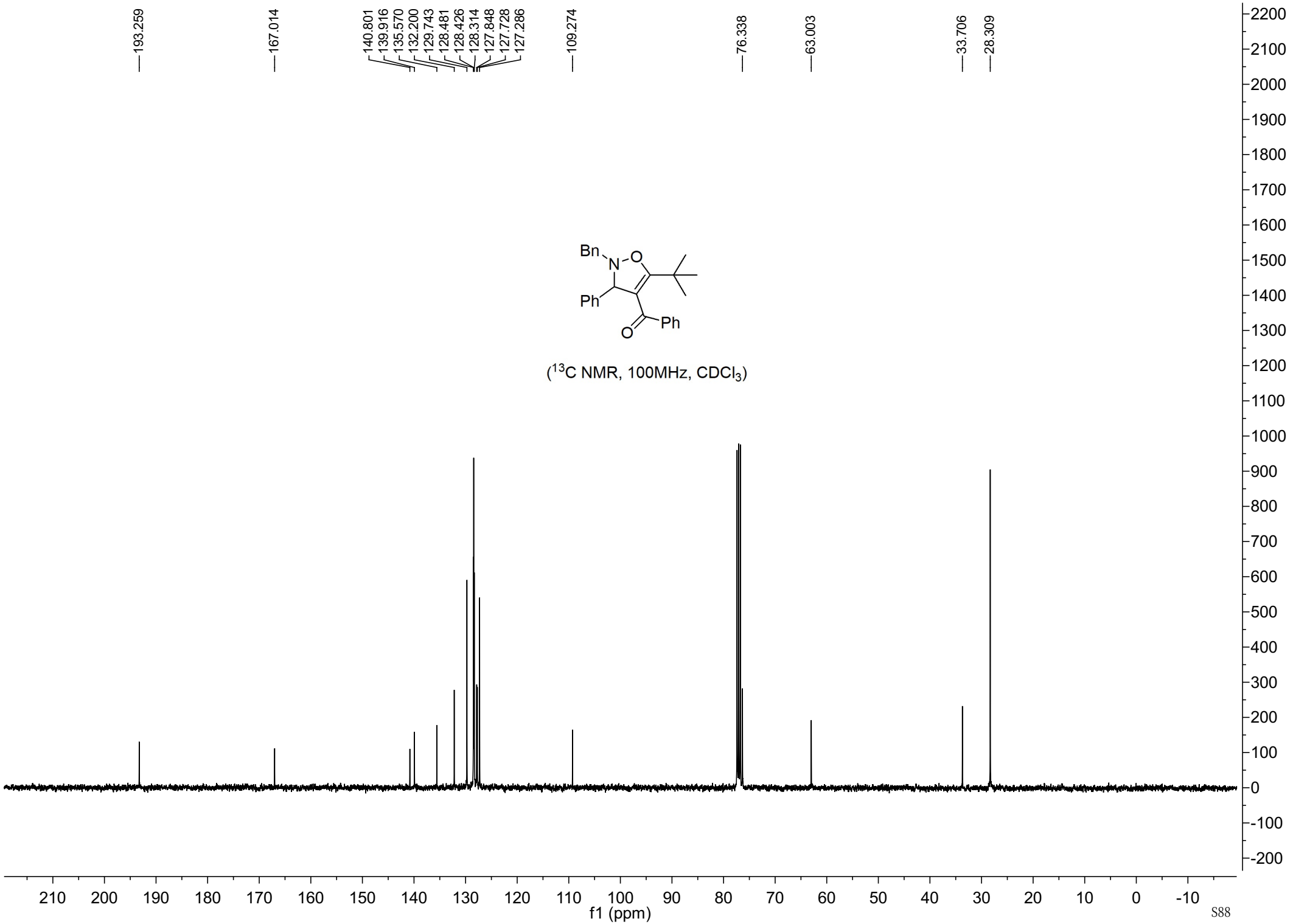

191.133
158.594
138.182
135.151
132.229
131.933
131.568
129.855
129.480
128.808
128.622
128.589
128.149
128.066
128.050
127.641
127.344
115.361
113.878
76.279
63.212
128.622
128.589
128.149
128.066
128.050
Bn
N
O
Ph
N
Ph
O
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)
f1 (ppm)

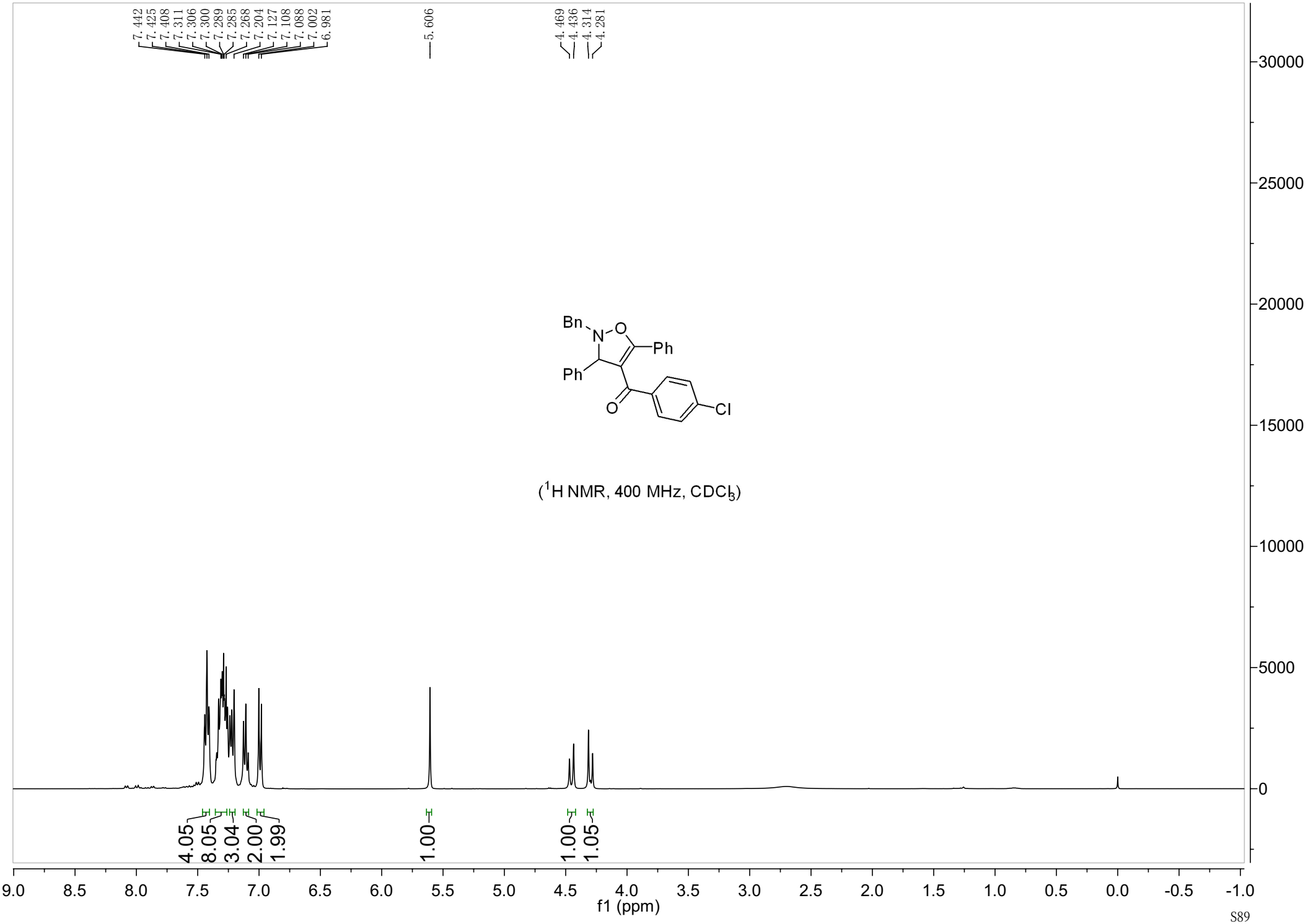


(^{1}H NMR, 400MHz, $CDCl_3$)


190.921
169.866
158.300
140.274
139.710
135.217
132.262
129.529
128.547
128.497
127.968
127.925
127.270
116.334
74.288
63.475
56.863
20.388
Bn
N
O
O
O
Ph
Ph
O
(^{13}C NMR, 100MHz, $CDCl_3$)
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.486
7.483
7.471
7.466
7.463
7.434
7.416
7.412
7.396
7.393
7.367
7.362
7.346
7.342
7.327
7.322
7.317
7.307
7.289
7.244
7.172
7.165
7.158
7.154
7.147
7.027
7.020
7.016
7.008
7.003
5.210
4.372
4.339
4.214
4.181
1.250
Bn
N
O
Ph
Ph
O
(^{1}H NMR, 400MHz, $CDCl_3$)
5.00
5.00
2.95
1.90
0.95
0.95
0.97
9.00
f1 (ppm)


193.259
167.014
140.801
139.916
135.570
132.200
129.743
128.481
128.426
128.314
127.848
127.728
127.286
109.274
76.338
63.003
33.706
28.309
Bn
N
O
Ph
O
Ph
(13C NMR, 100MHz, CDCl3)
f1 (ppm)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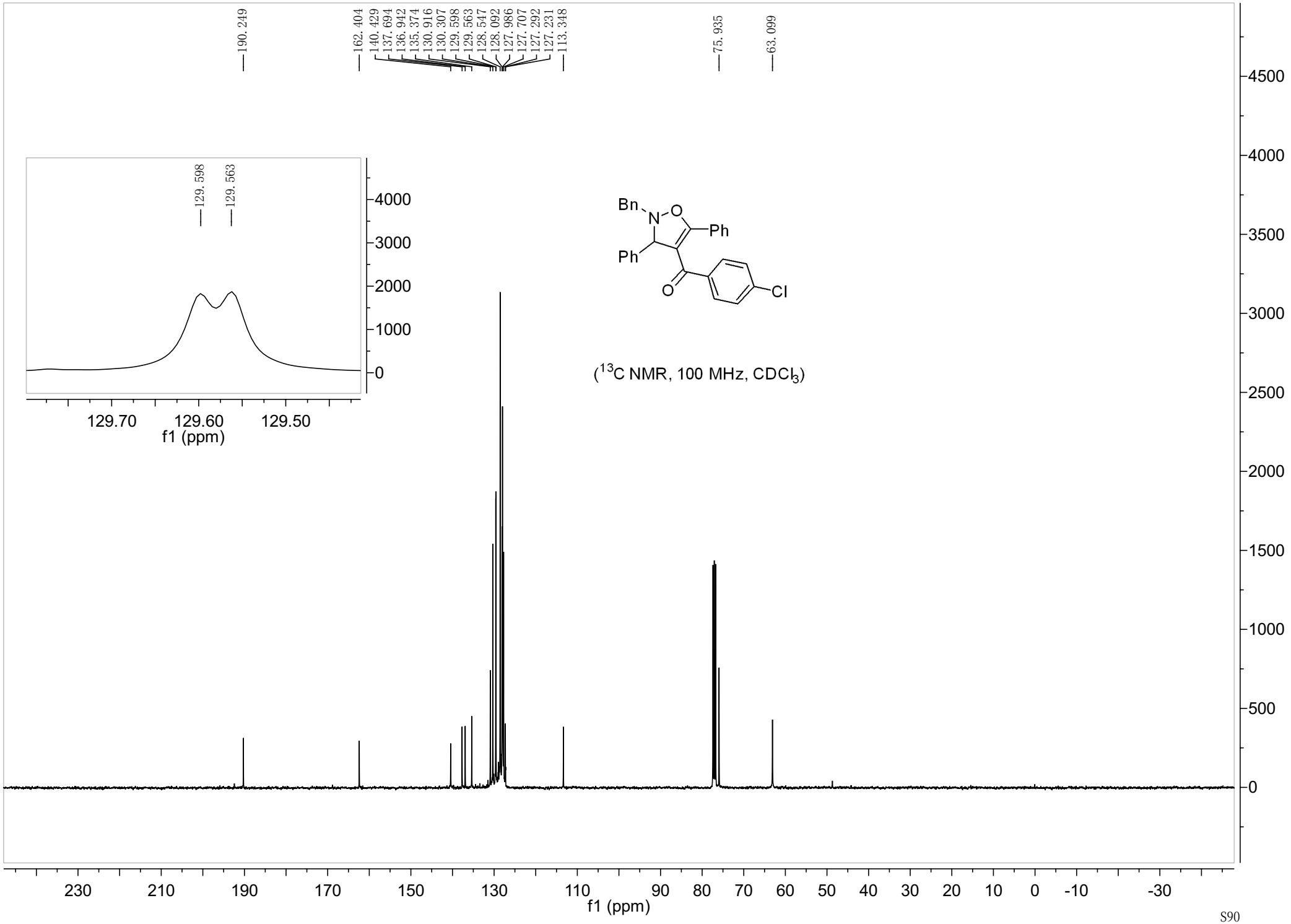
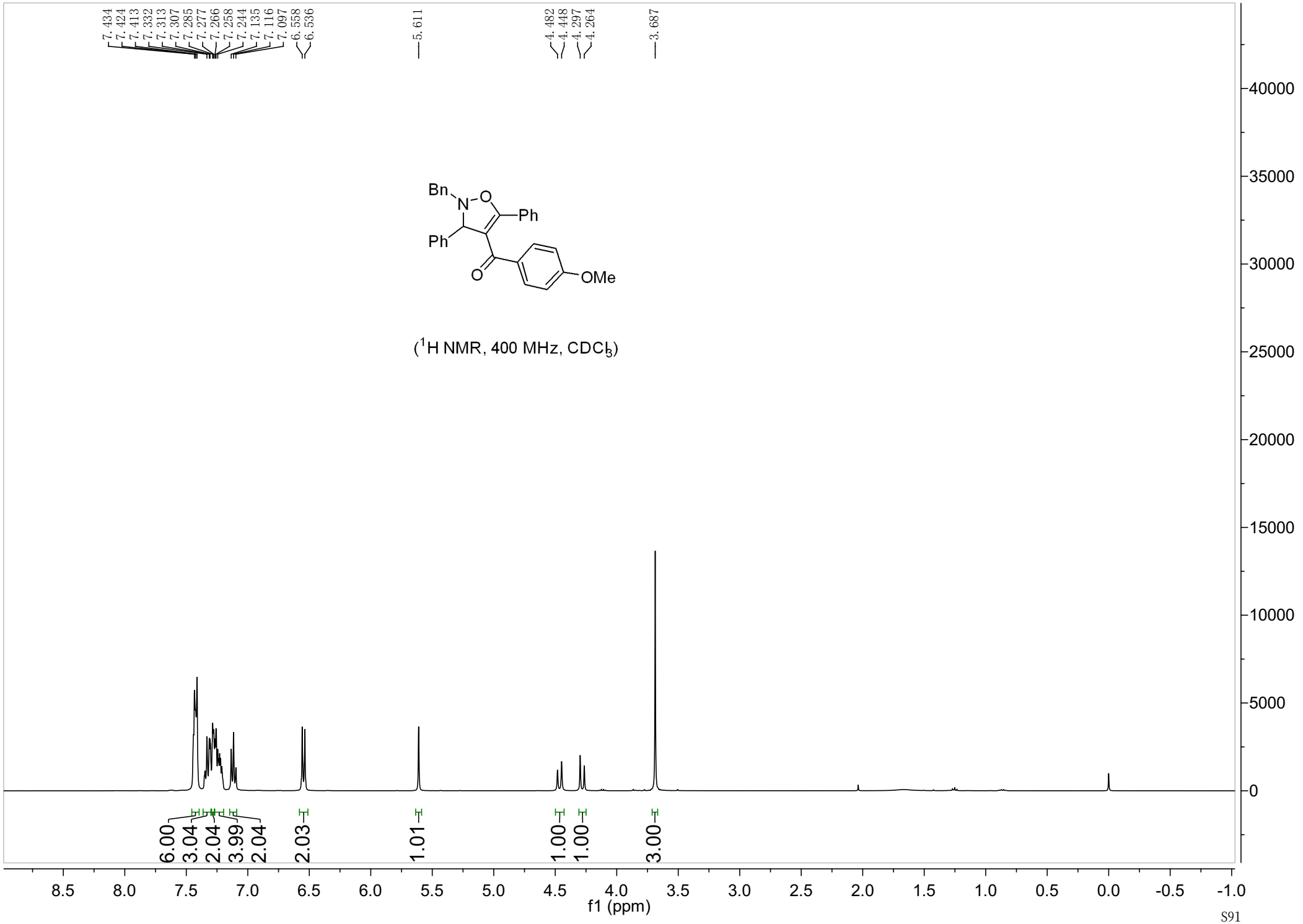
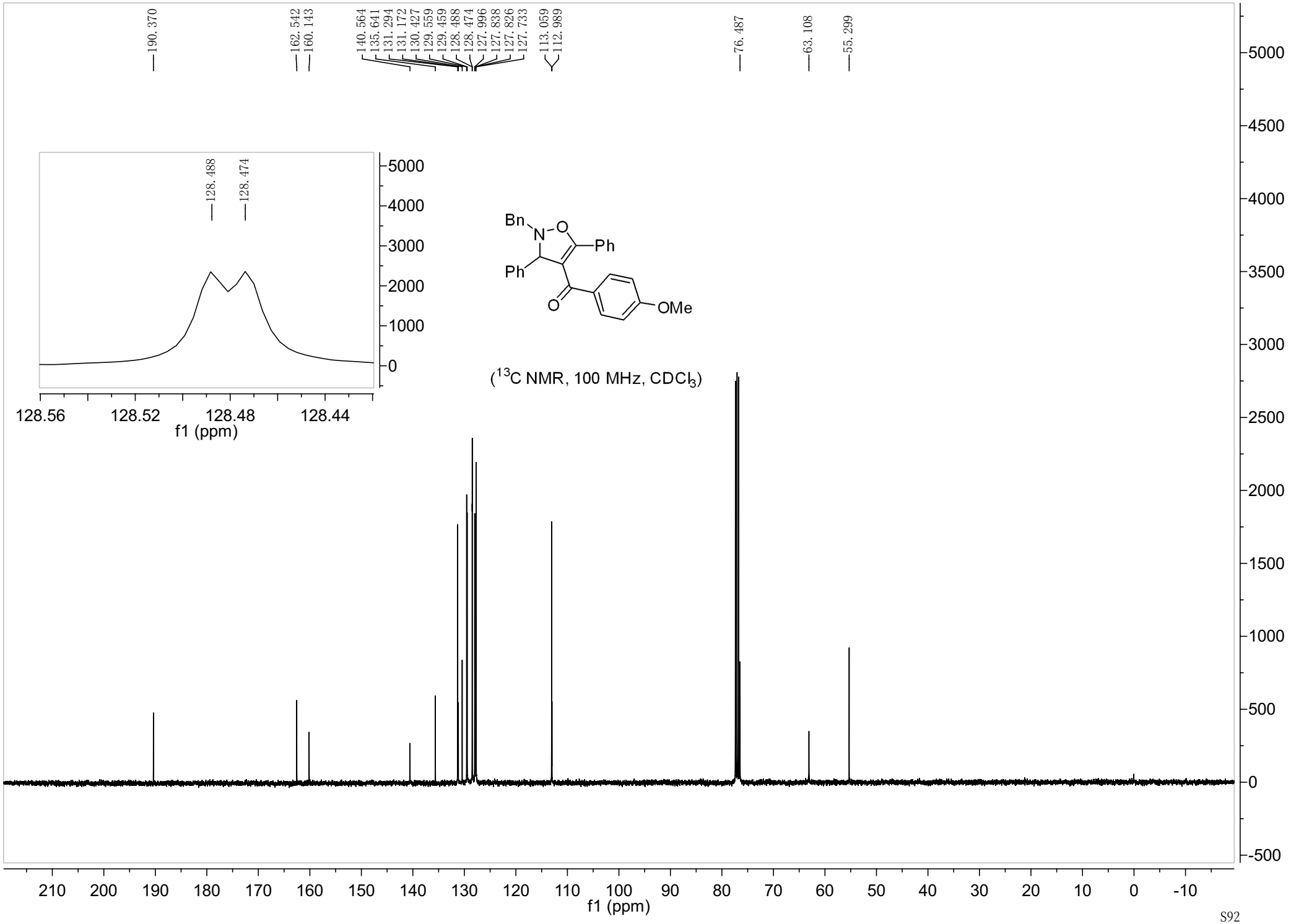
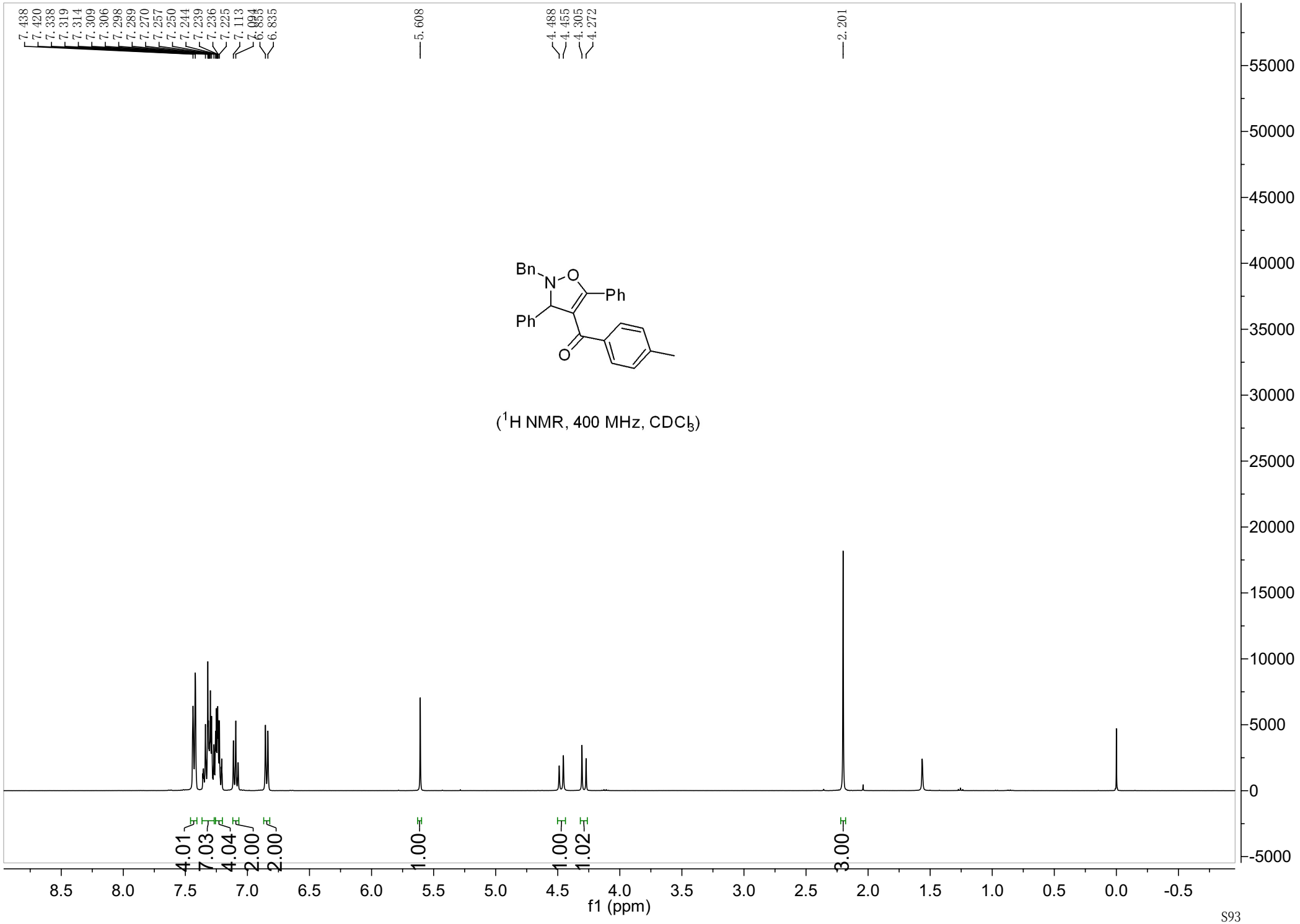
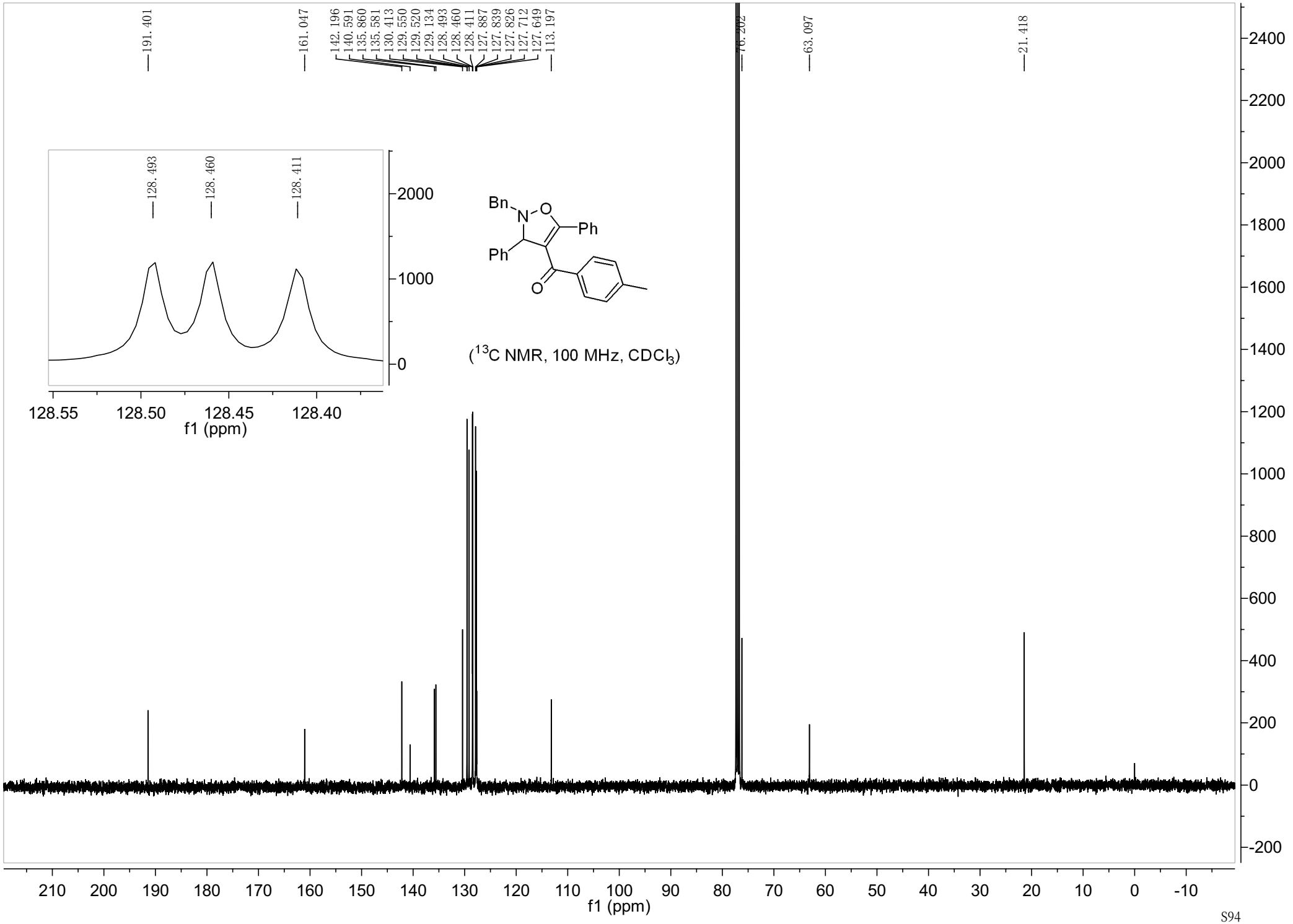
7.425
7.408
7.311
7.306
7.300
7.289
7.285
7.268
7.204
7.127
7.108
7.088
7.002
6.981
5.606
4.469
4.436
4.314
4.281
Bn
N
O
Ph
Ph
O
Cl
(1H NMR, 400 MHz, CDCl3)
4.05
8.05
3.04
2.00
1.99
1.00
1.00
1.05
30000
25000
20000
15000
10000
5000
0
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

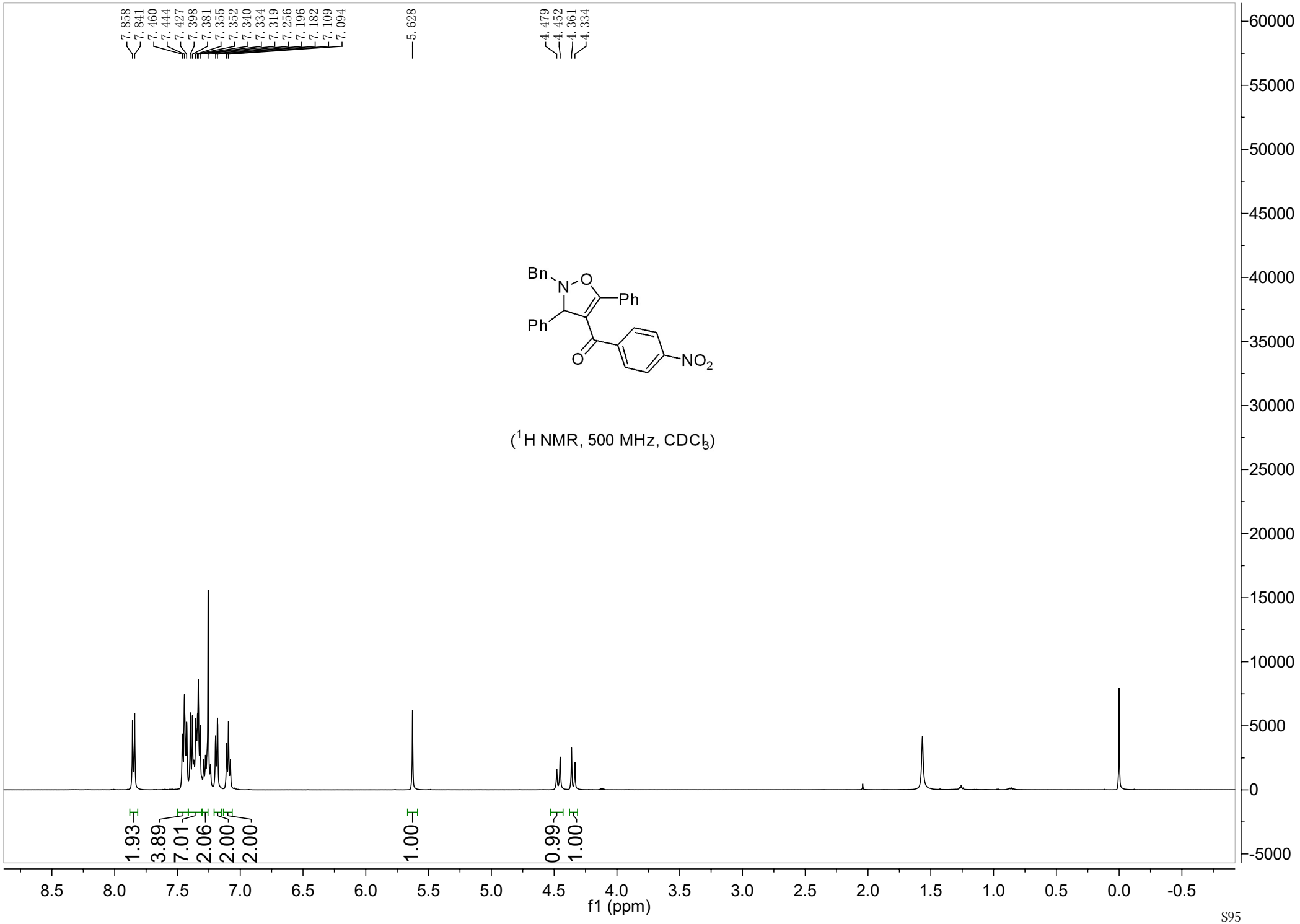

190.249
162.404
140.429
137.694
136.942
135.374
130.916
130.307
129.598
129.563
128.547
128.092
127.986
127.707
127.292
127.231
113.348
75.935
63.099
129.598
129.563
129.70
129.60
129.50
f1 (ppm)
Bn
N
O
Ph
Ph
O
Cl
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

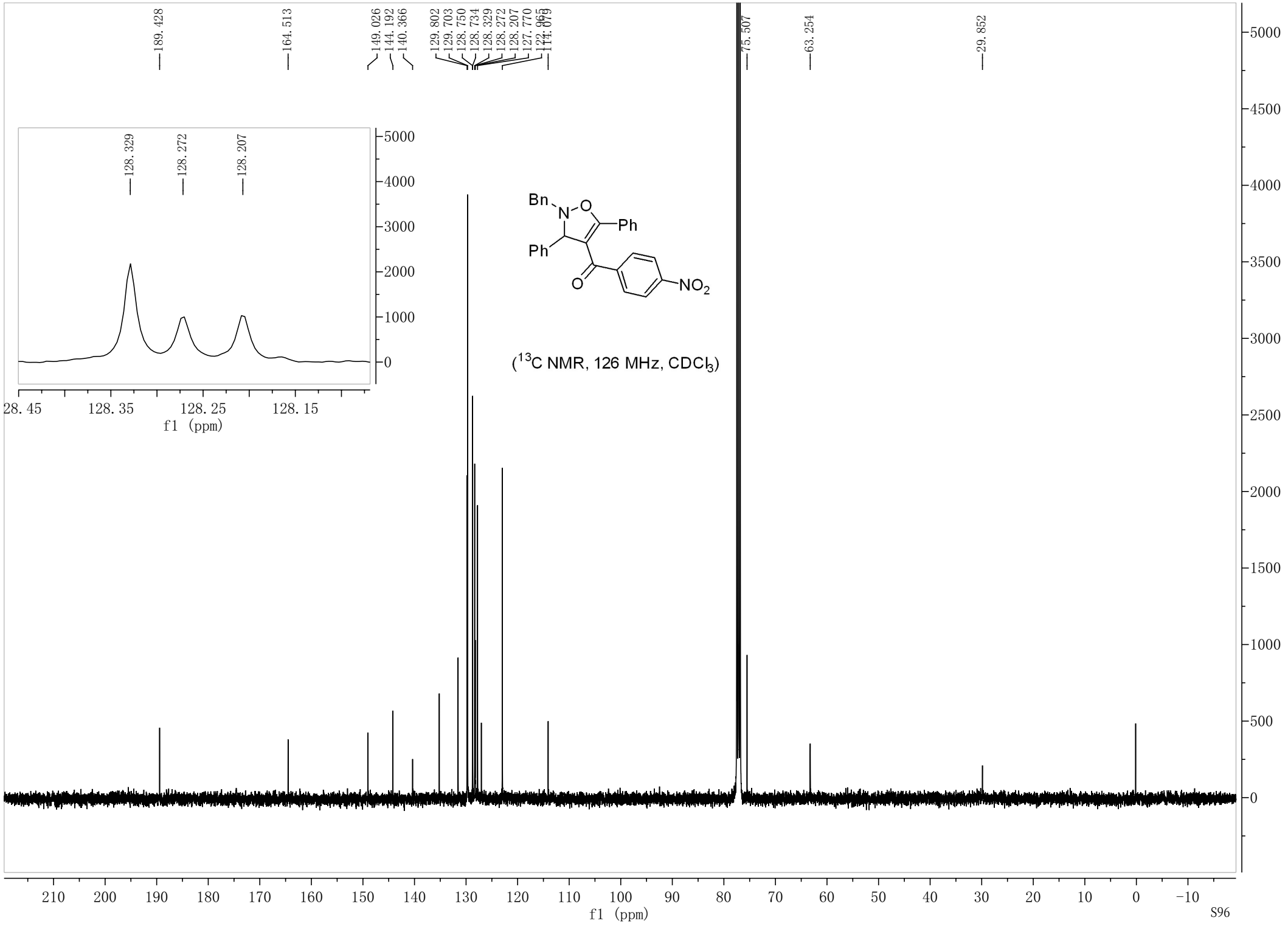

7.434
7.424
7.413
7.332
7.313
7.307
7.285
7.277
7.266
7.258
7.244
7.135
7.116
7.097
6.558
6.536
5.611
4.482
4.448
4.297
4.264
3.687
Bn
N
O
Ph
Ph
O
OMe
(1H NMR, 400 MHz, CDCl3)
40000
35000
30000
25000
20000
15000
10000
5000
0
6.00
3.04
2.04
3.99
2.04
2.03
1.01
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

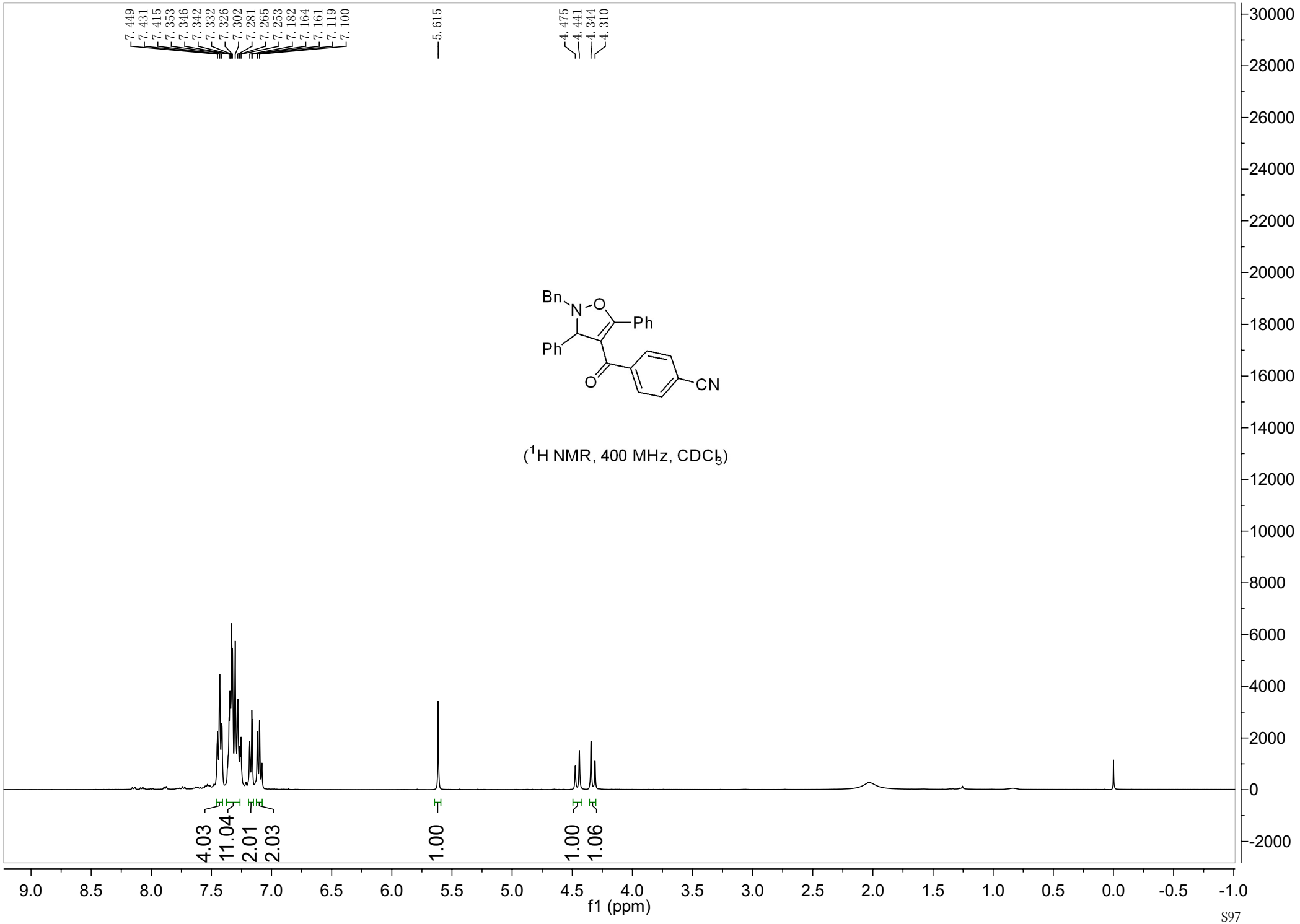

190.370
162.542
160.143
140.564
135.641
131.294
131.172
130.427
129.559
129.459
128.488
128.474
127.996
127.838
127.826
127.733
113.059
112.989
76.487
63.108
55.299
128.488
128.474
Bn
N
O
Ph
Ph
O
OMe
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

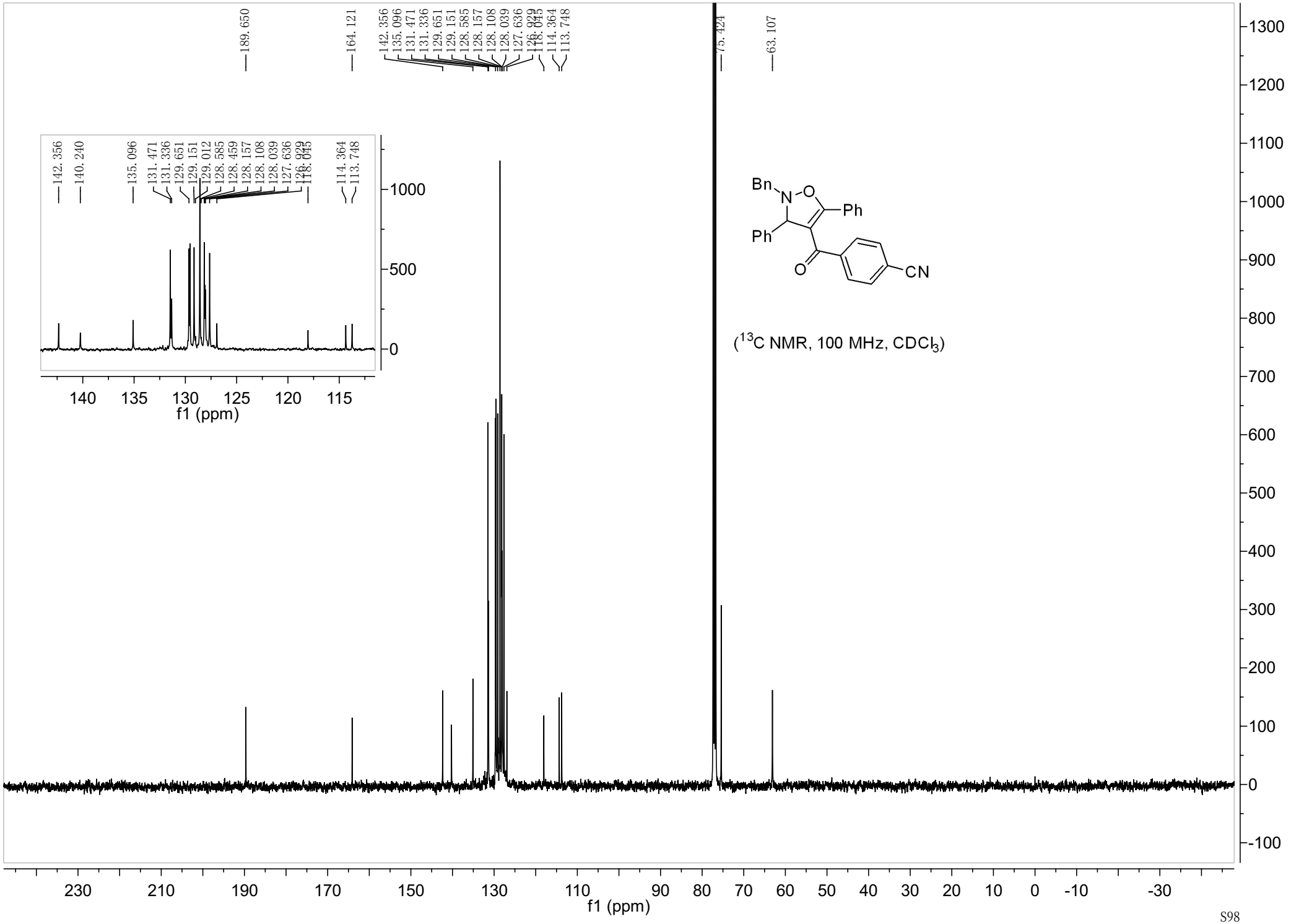

7.438
7.420
7.338
7.319
7.314
7.309
7.306
7.298
7.289
7.270
7.257
7.250
7.244
7.239
7.236
7.225
7.113
7.094
6.855
6.835
5.608
4.488
4.455
4.305
4.272
2.201
Bn
N
O
Ph
Ph
O
(1H NMR, 400 MHz, CDCl3)
4.01
7.03
4.04
2.00
2.00
1.00
1.00
1.02
3.00
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

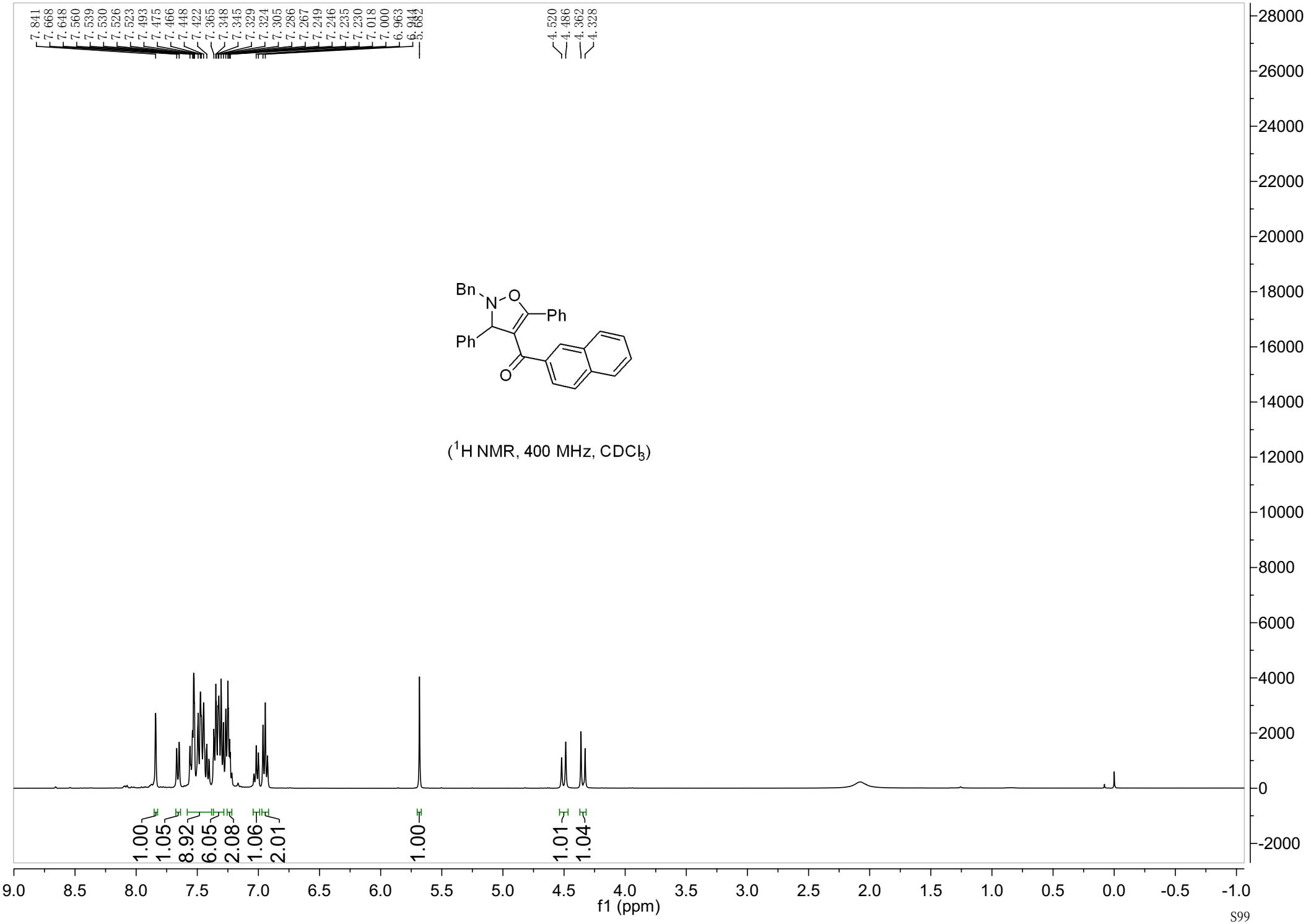

191.401
161.047
142.196
140.591
135.860
135.581
130.413
129.550
129.520
129.134
128.493
128.460
128.411
127.887
127.839
127.826
127.712
127.649
113.197
76.202
63.097
21.418
128.493
128.460
128.411
Bn
N
O
Ph
Ph
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

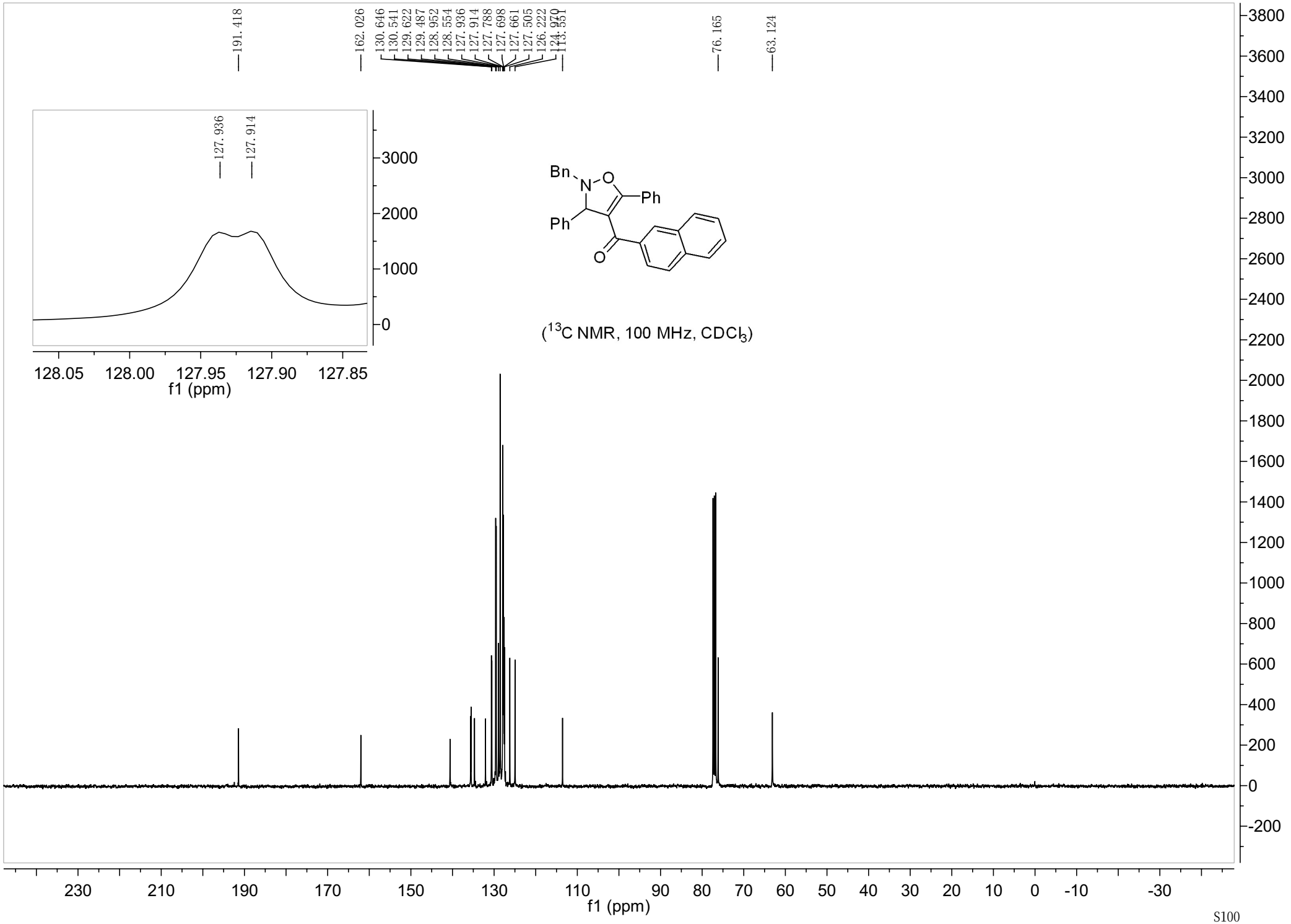

7.858
7.841
7.460
7.444
7.427
7.398
7.381
7.355
7.352
7.340
7.334
7.319
7.256
7.196
7.182
7.109
7.094
5.628
4.479
4.452
4.361
4.334
Bn
N
O
Ph
Ph
O
NO2
(1H NMR, 500 MHz, CDCl3)
1.93
3.89
7.01
2.06
2.00
2.00
1.00
0.99
1.00
f1 (ppm)

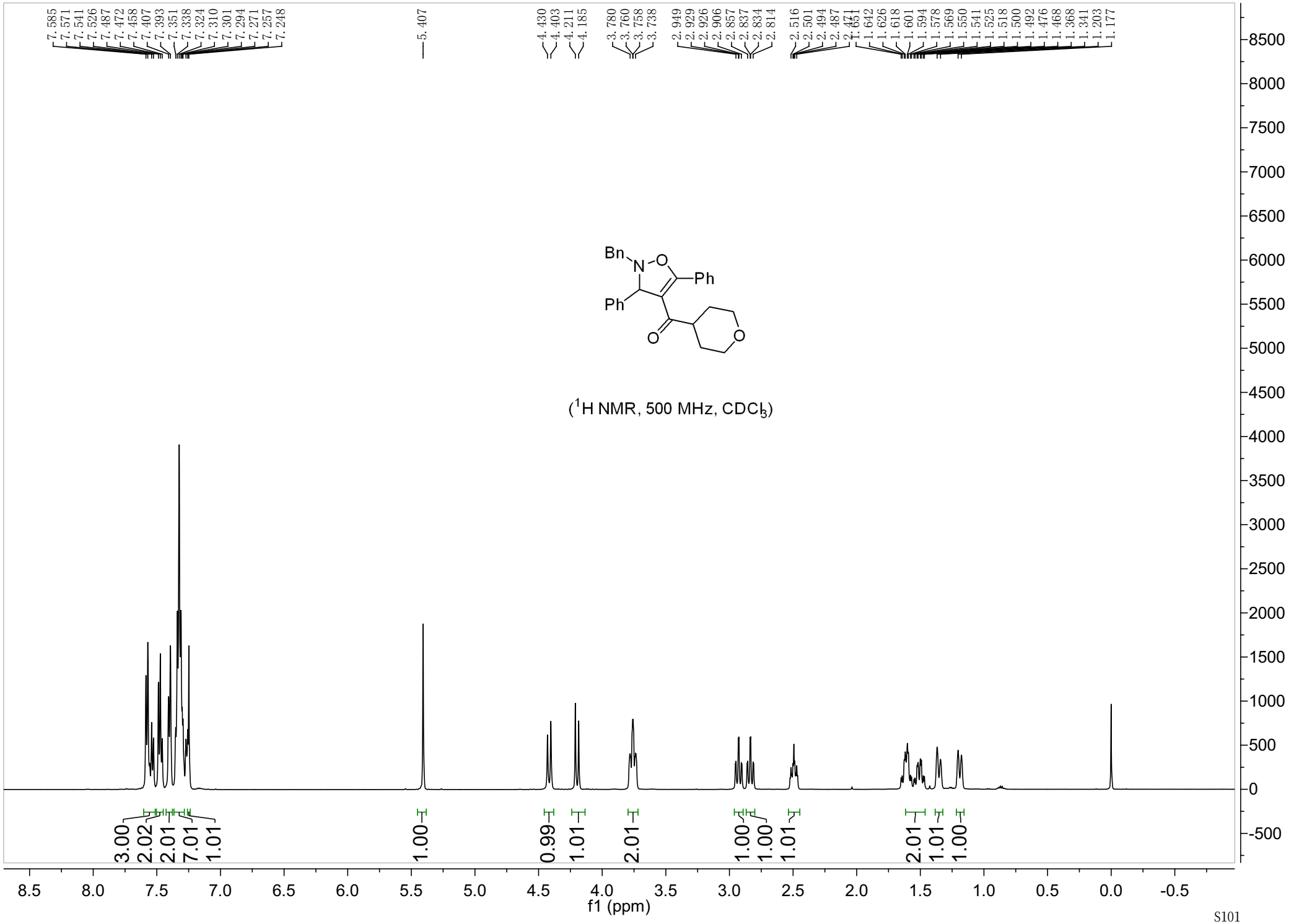

189.428
164.513
149.026
144.192
140.366
129.802
129.703
128.750
128.734
128.329
128.272
128.207
127.770
122.965
114.079
75.507
63.254
29.852
128.329
128.272
128.207
Bn
N
O
Ph
Ph
O
NO2
(^{13}C NMR, 126 MHz, CDCl$_3$)
f1 (ppm)
f1 (ppm)

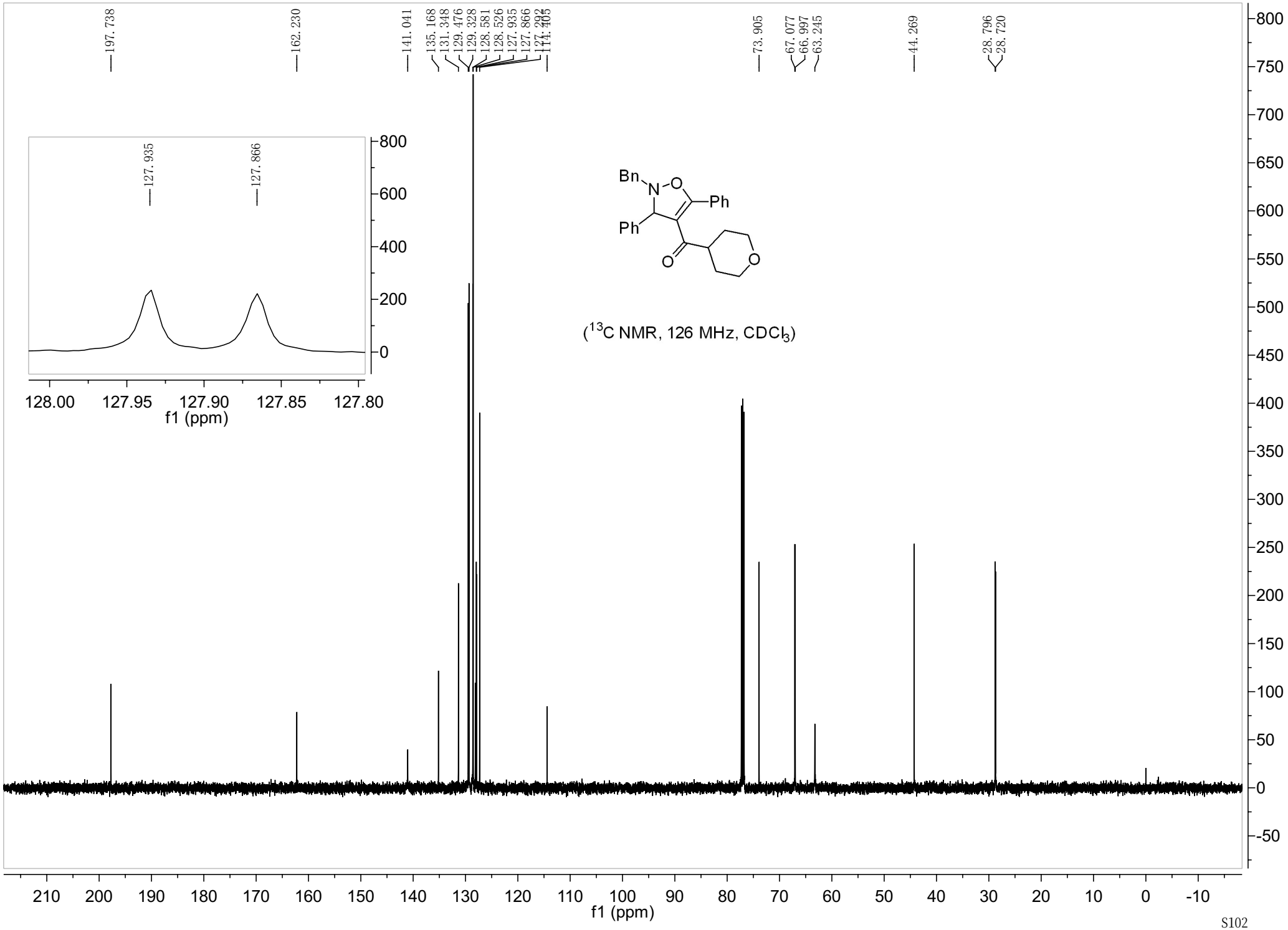

7.449
7.431
7.415
7.353
7.346
7.342
7.332
7.326
7.302
7.281
7.265
7.253
7.182
7.164
7.161
7.119
7.100
5.615
4.475
4.441
4.344
4.310
Bn
N
O
Ph
Ph
O
CN
(1H NMR, 400 MHz, CDCl3)
4.03
11.04
2.01
2.03
1.00
1.00
1.06
f1 (ppm)

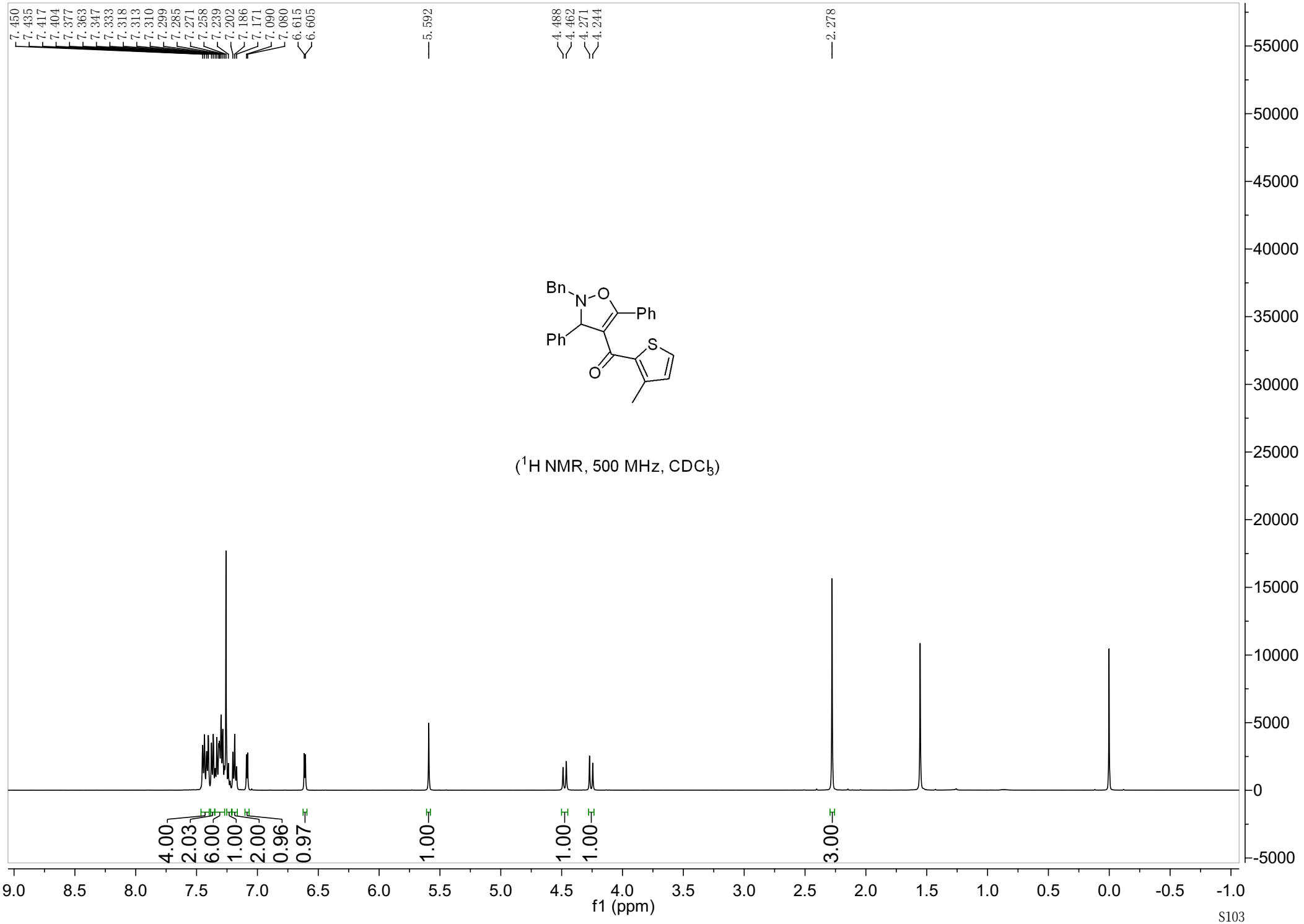

189.650
164.121
142.356
135.096
131.471
131.336
129.651
129.151
128.585
128.157
128.108
128.039
127.636
126.929
118.045
114.364
113.748
75.424
63.107
142.356
140.240
135.096
131.471
131.336
129.651
129.151
129.012
128.585
128.459
128.157
128.108
128.039
127.636
114.364
113.748
1000
500
0
140
135
130
125
120
115
f1 (ppm)
Bn
N
O
Ph
Ph
O
CN
(^{13}C NMR, 100 MHz, $CDCl_3$)
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
f1 (ppm)

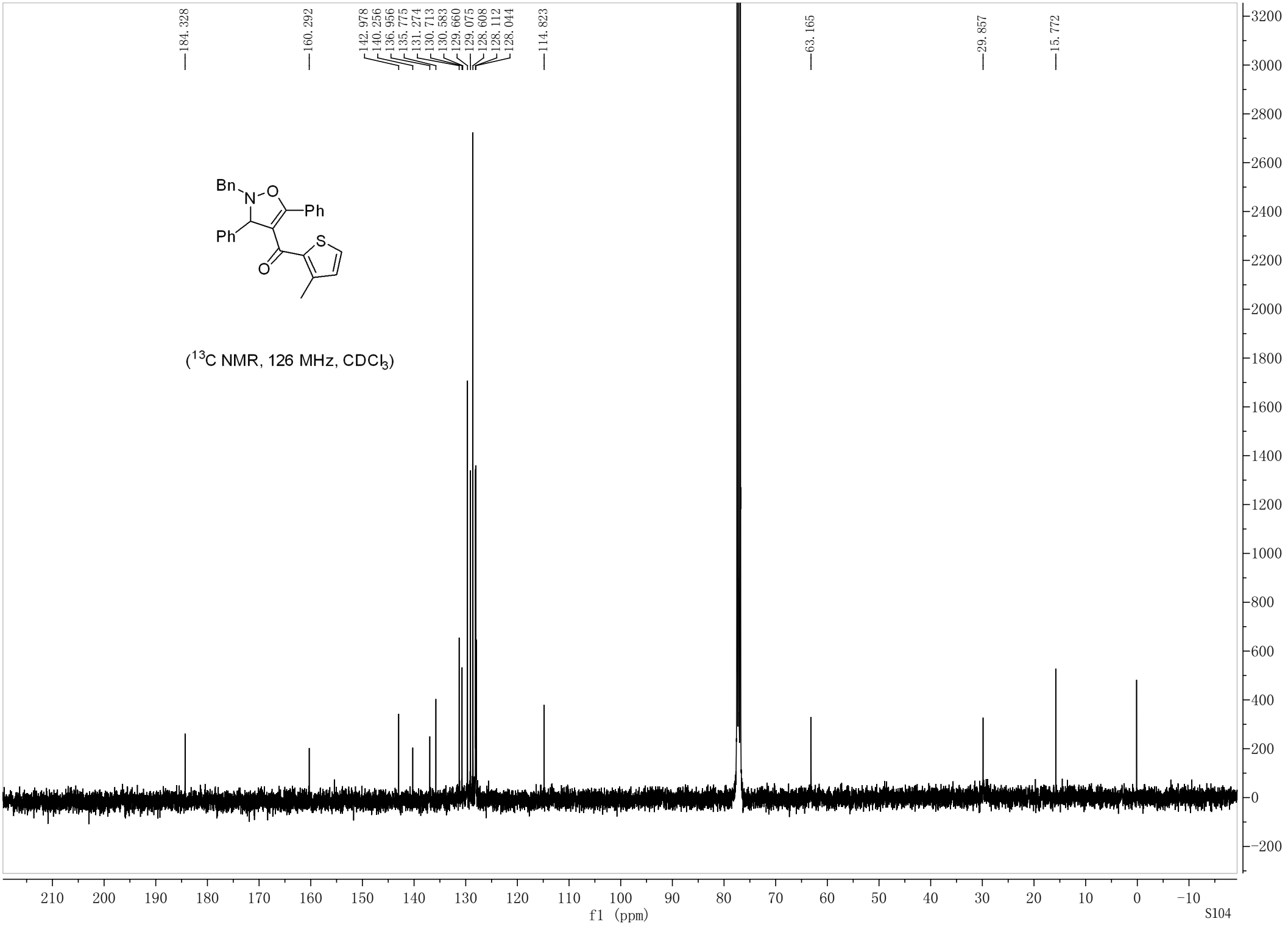

7.841
7.668
7.648
7.560
7.539
7.530
7.526
7.523
7.493
7.475
7.466
7.448
7.422
7.365
7.348
7.345
7.329
7.324
7.305
7.286
7.267
7.249
7.246
7.235
7.230
7.018
7.000
6.963
6.944
6.682
4.520
4.486
4.362
4.328
Bn
N
O
Ph
Ph
O
(1H NMR, 400 MHz, CDCl3)
1.00
1.05
8.92
6.05
2.08
1.06
2.01
1.00
1.01
1.04
f1 (ppm)

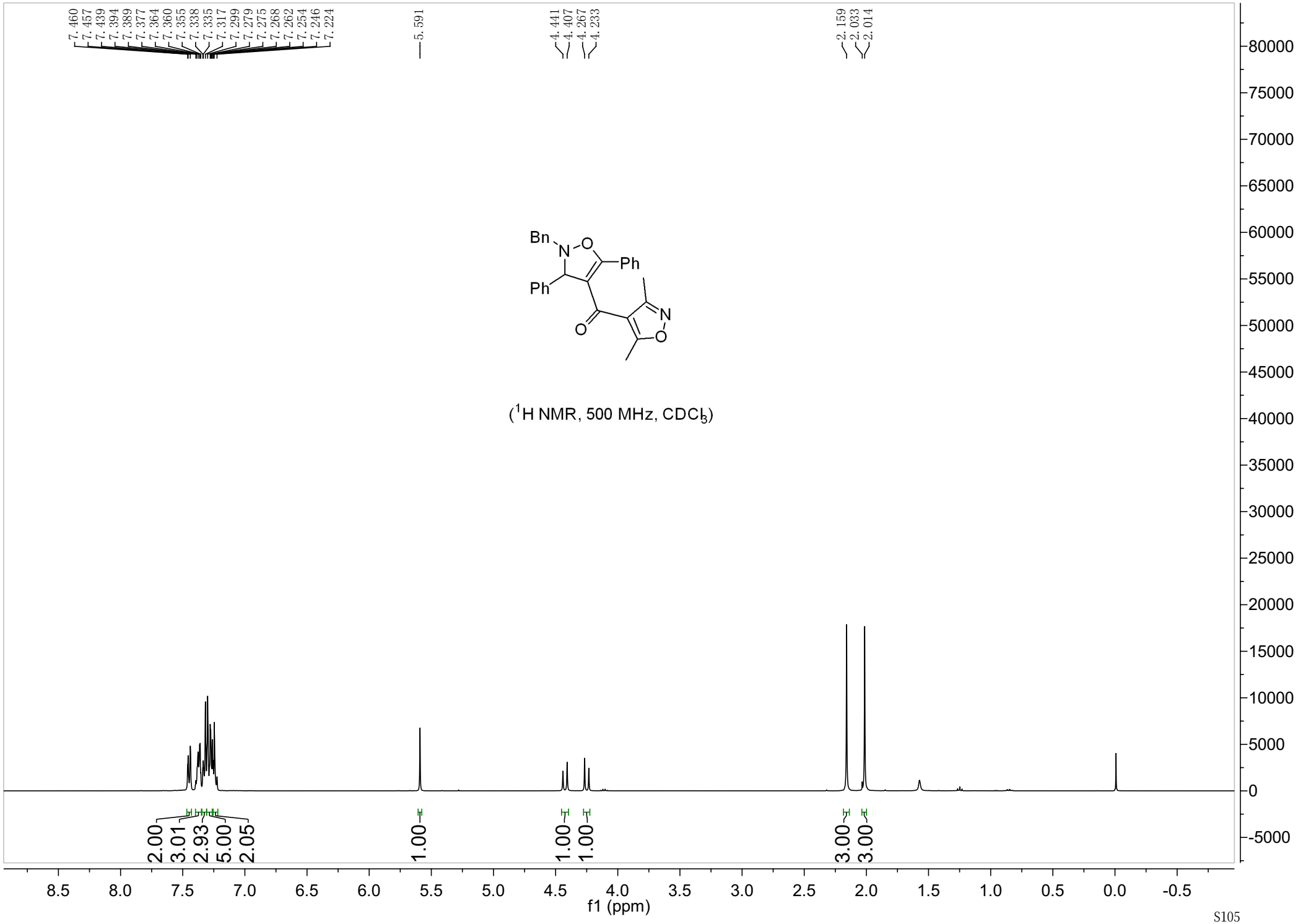

191.418
162.026
130.646
130.541
129.622
129.487
128.952
128.554
127.936
127.914
127.788
127.698
127.661
127.505
126.222
124.970
113.551
76.165
63.124
127.936
127.914
Bn
N
O
Ph
Ph
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

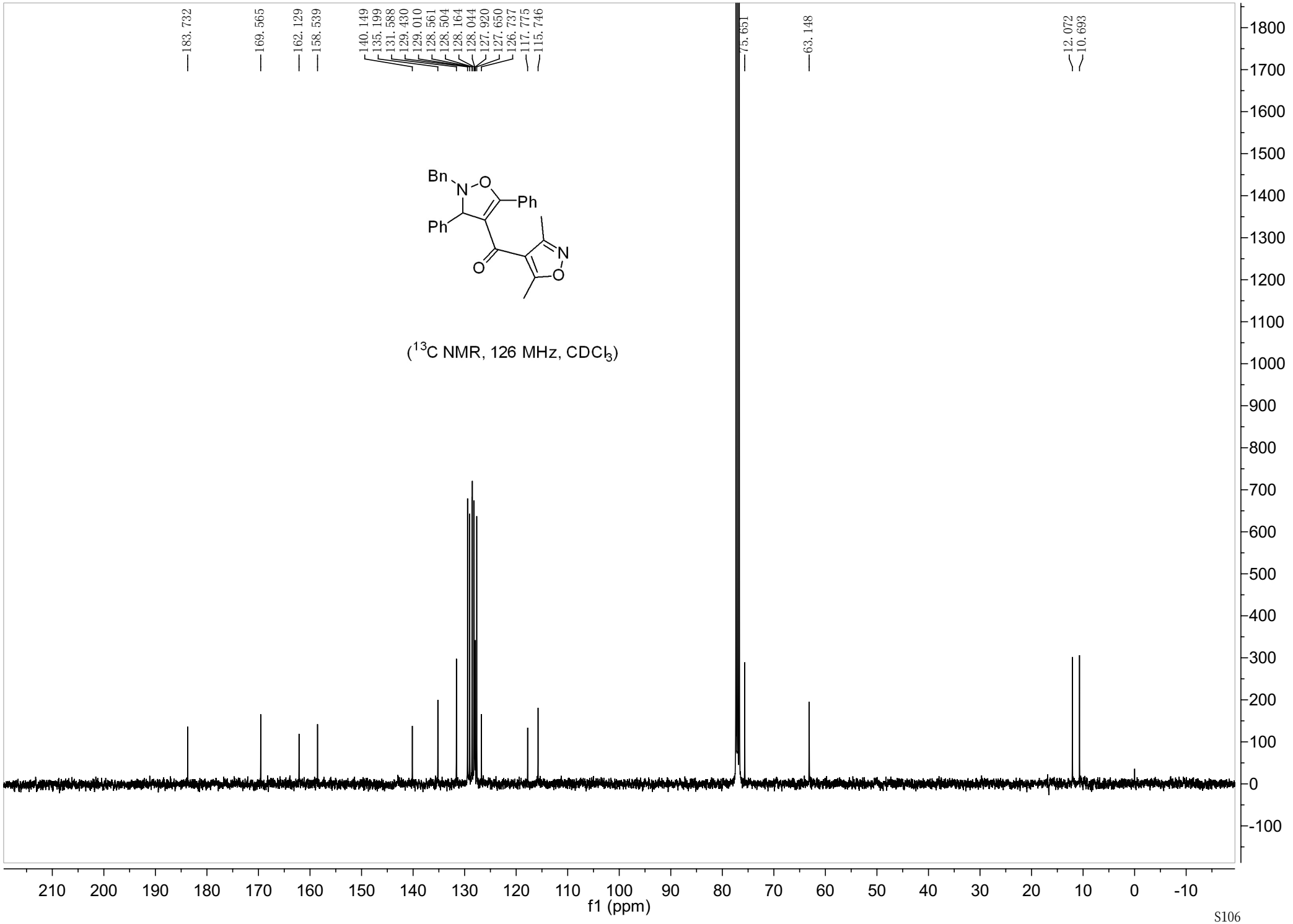

7.585
7.571
7.541
7.526
7.487
7.472
7.458
7.407
7.393
7.351
7.338
7.324
7.310
7.301
7.294
7.271
7.257
7.248
5.407
4.430
4.403
4.211
4.185
3.780
3.760
3.758
3.738
2.949
2.929
2.926
2.906
2.857
2.837
2.834
2.814
2.516
2.501
2.494
2.487
2.471
1.651
1.642
1.626
1.618
1.601
1.594
1.578
1.569
1.550
1.541
1.525
1.518
1.500
1.492
1.476
1.468
1.368
1.341
1.203
1.177
Bn
N
O
Ph
Ph
O
O
(1H NMR, 500 MHz, CDCl3)
3.00
2.02
2.01
7.01
1.01
1.00
0.99
1.01
2.01
1.00
1.00
1.01
2.01
1.01
1.00
f1 (ppm)


197.738
162.230
141.041
135.168
131.348
129.476
129.328
128.581
128.526
127.935
127.866
114.405
73.905
67.077
66.997
63.245
44.269
28.796
28.720
127.935
127.866
128.00
127.95
127.90
127.85
127.80
f1 (ppm)
Bn
N
O
Ph
Ph
O
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

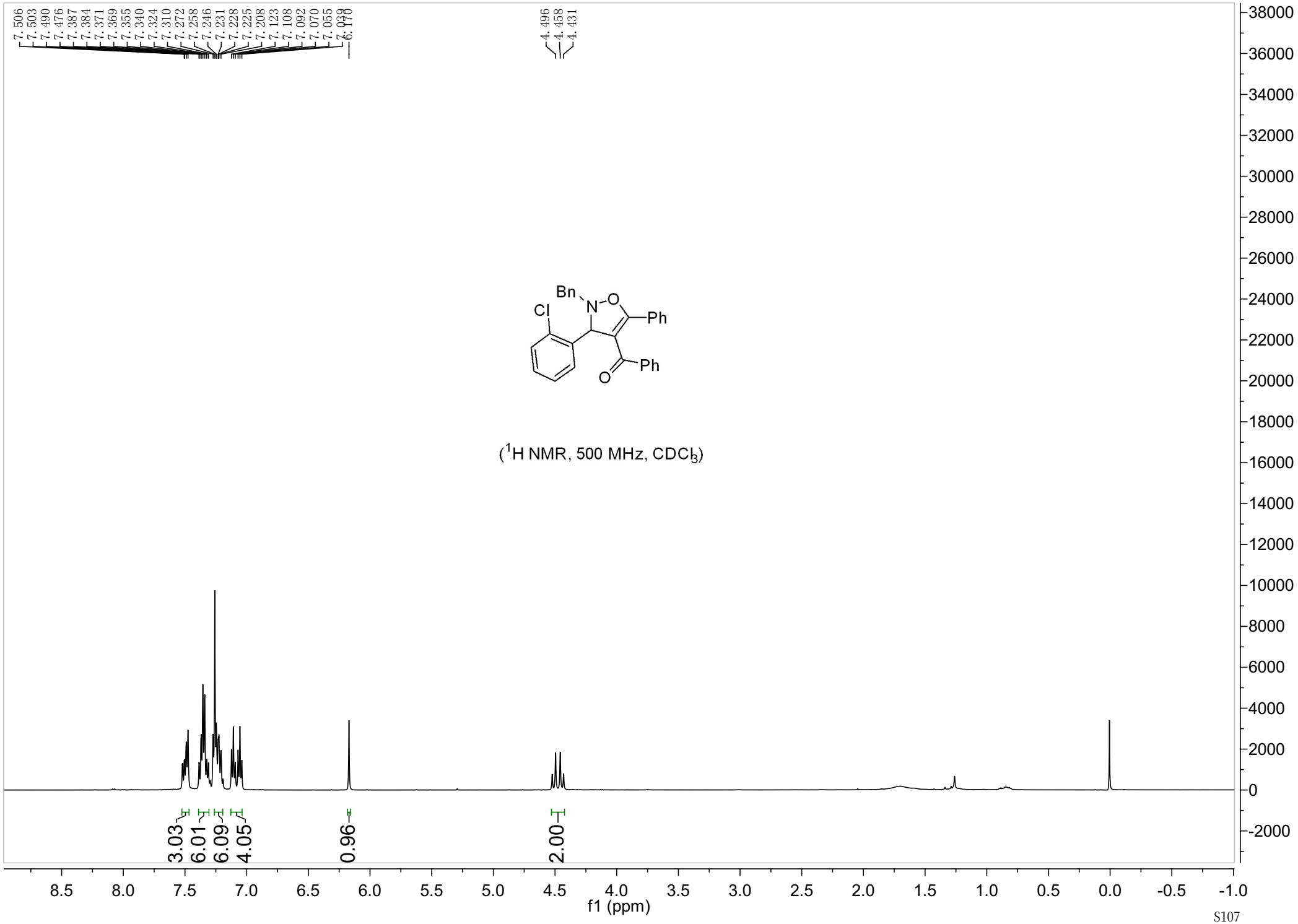

7.450
7.435
7.417
7.404
7.377
7.363
7.347
7.333
7.318
7.313
7.310
7.299
7.285
7.271
7.258
7.239
7.202
7.186
7.171
7.090
7.080
6.615
6.605
5.592
4.488
4.462
4.271
4.244
2.278
Bn
N
O
Ph
Ph
S
O
(1H NMR, 500 MHz, CDCl3)
4.00
2.03
6.00
1.00
2.00
0.96
0.97
1.00
1.00
1.00
3.00
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

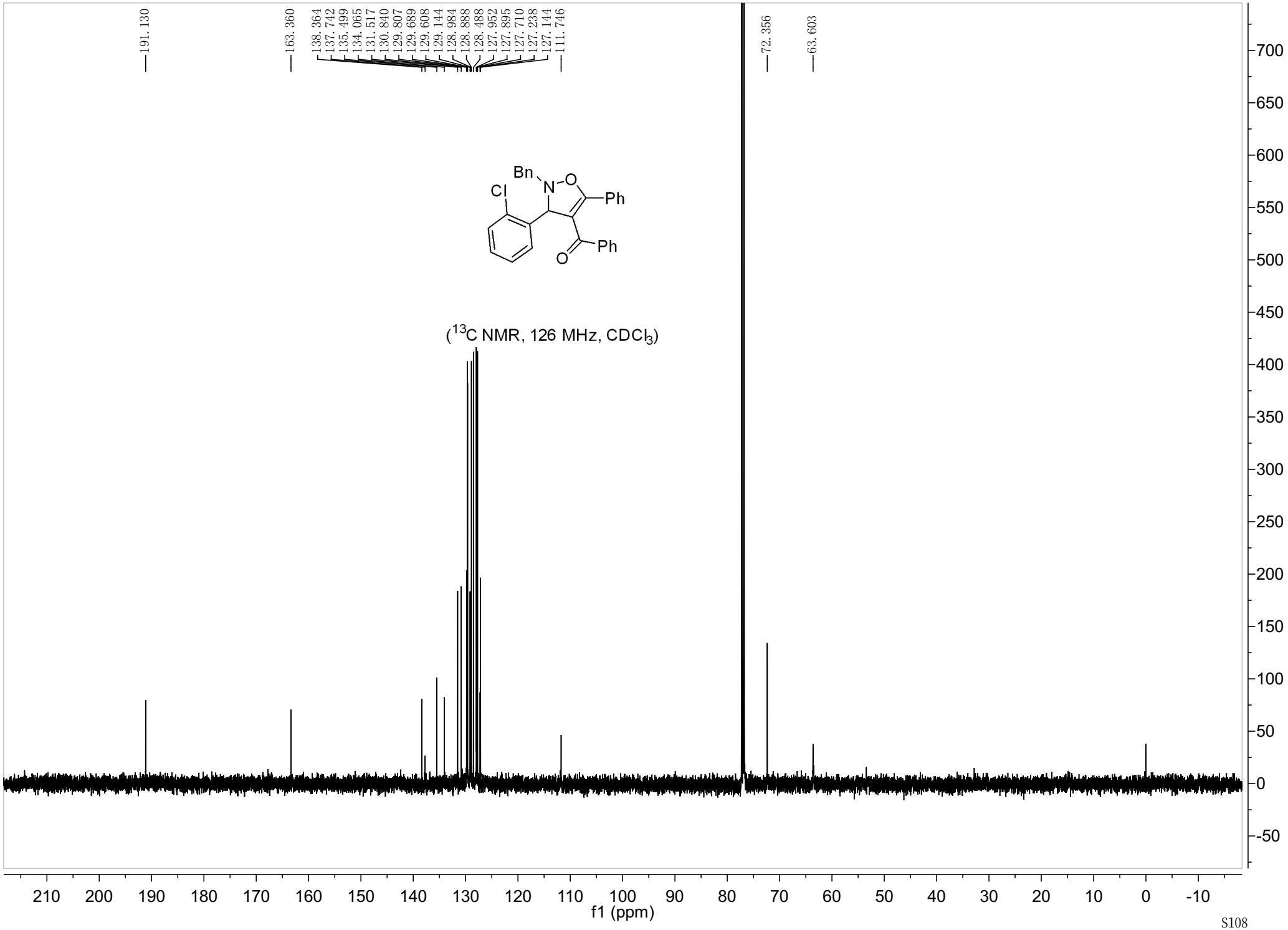

184.328
160.292
142.978
140.256
136.956
135.775
131.274
130.713
130.583
129.660
129.075
128.608
128.112
128.044
114.823
63.165
29.857
15.772
Bn
N
O
Ph
Ph
S
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

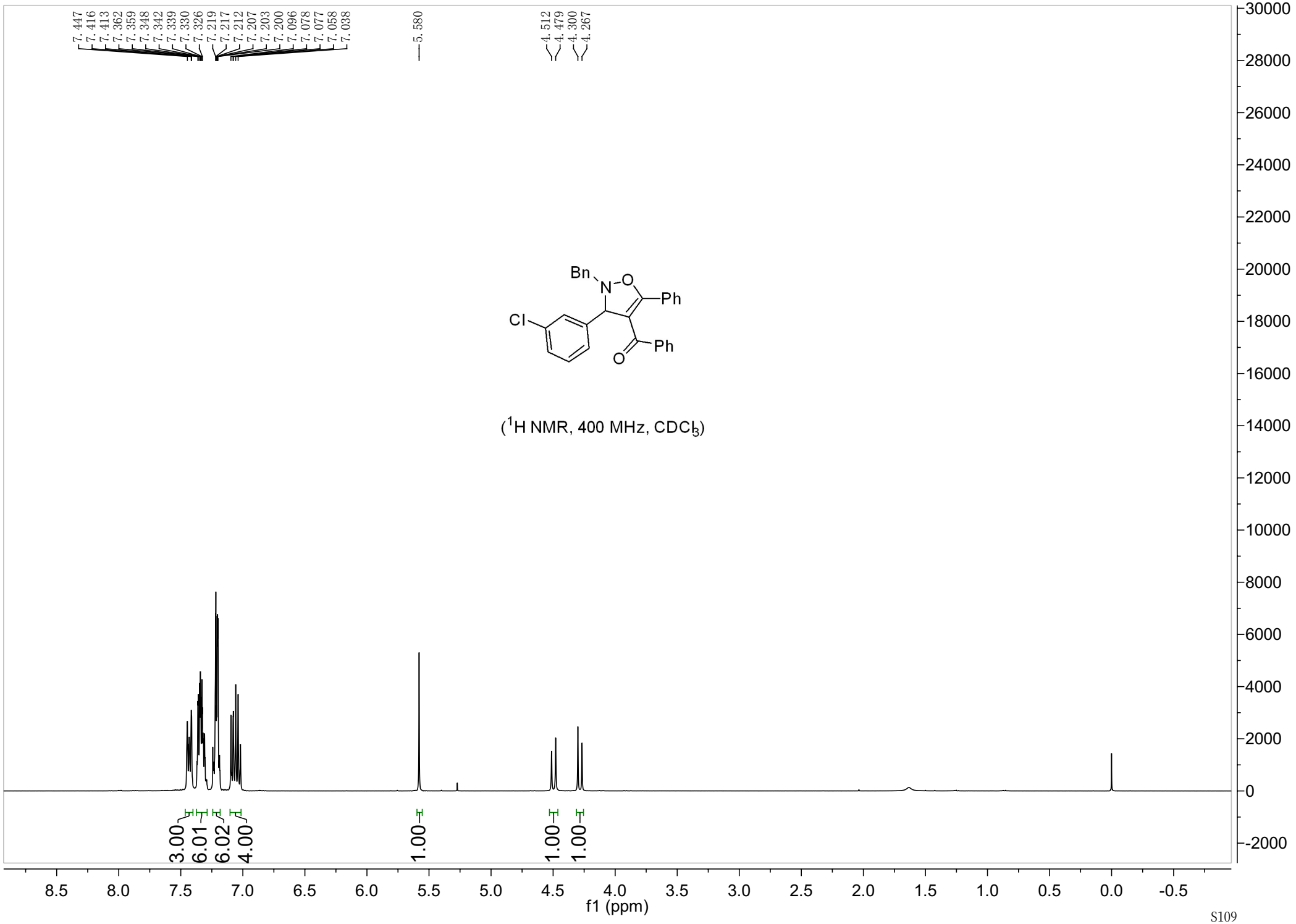

7.460
7.457
7.439
7.394
7.389
7.377
7.364
7.360
7.355
7.338
7.335
7.317
7.299
7.279
7.275
7.268
7.262
7.254
7.246
7.224
5.591
4.441
4.407
4.267
4.233
2.159
2.033
2.014
Bn
N
O
Ph
Ph
O
N
O
(1H NMR, 500 MHz, CDCl3)
2.00
3.01
2.93
5.00
2.05
1.00
1.00
1.00
3.00
3.00
f1 (ppm)

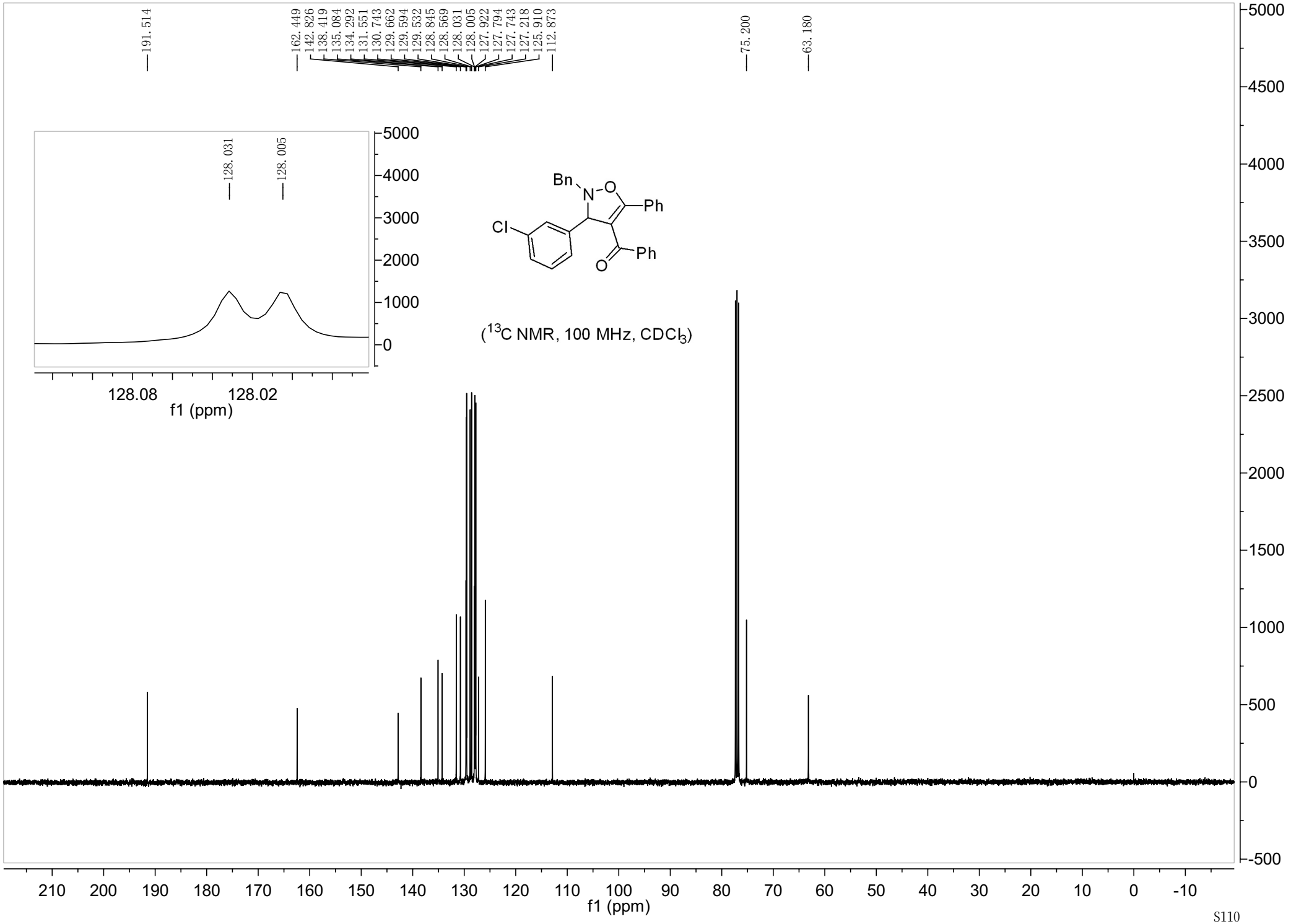


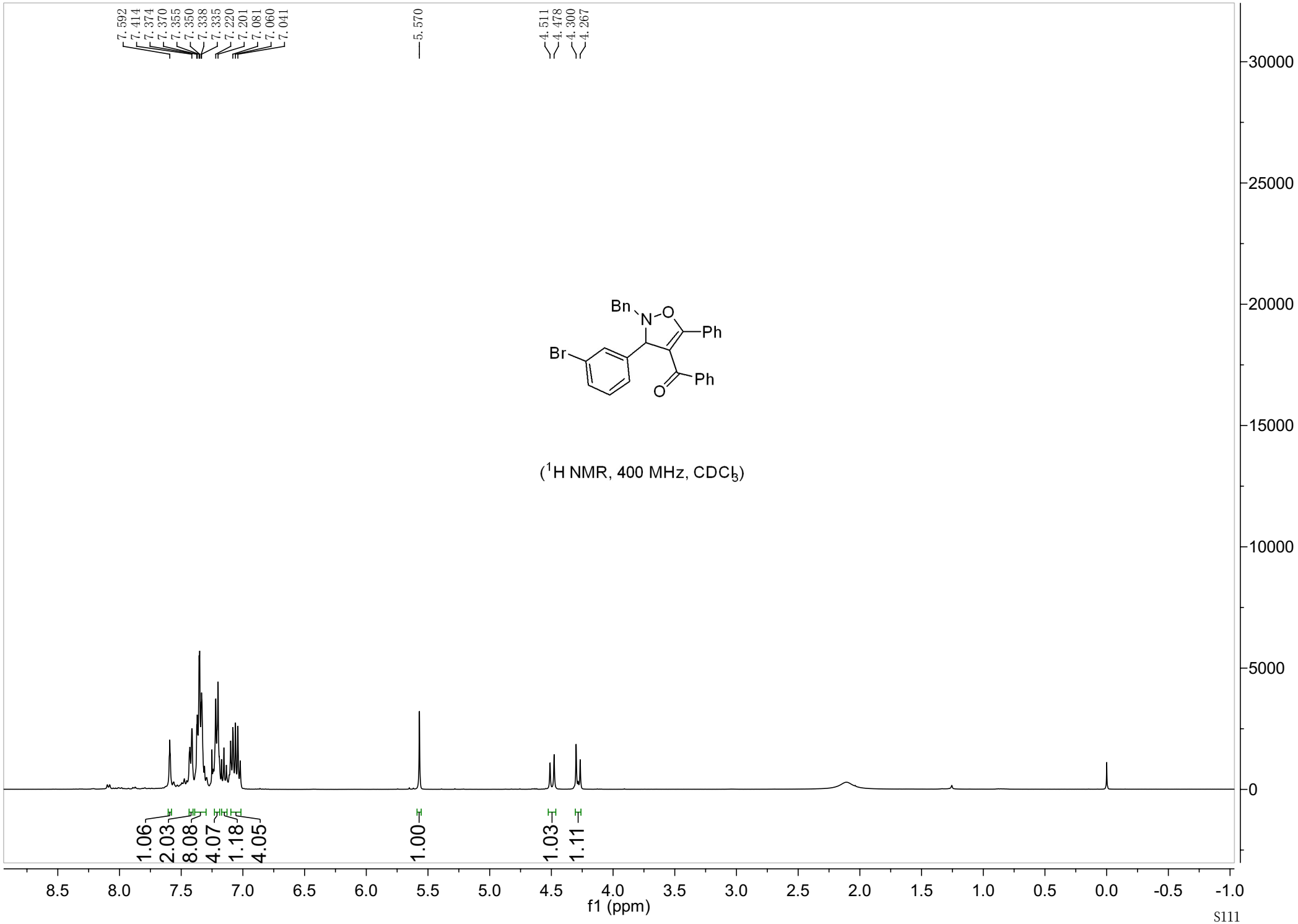
(^{13}C NMR, 126 MHz, $CDCl_3$)

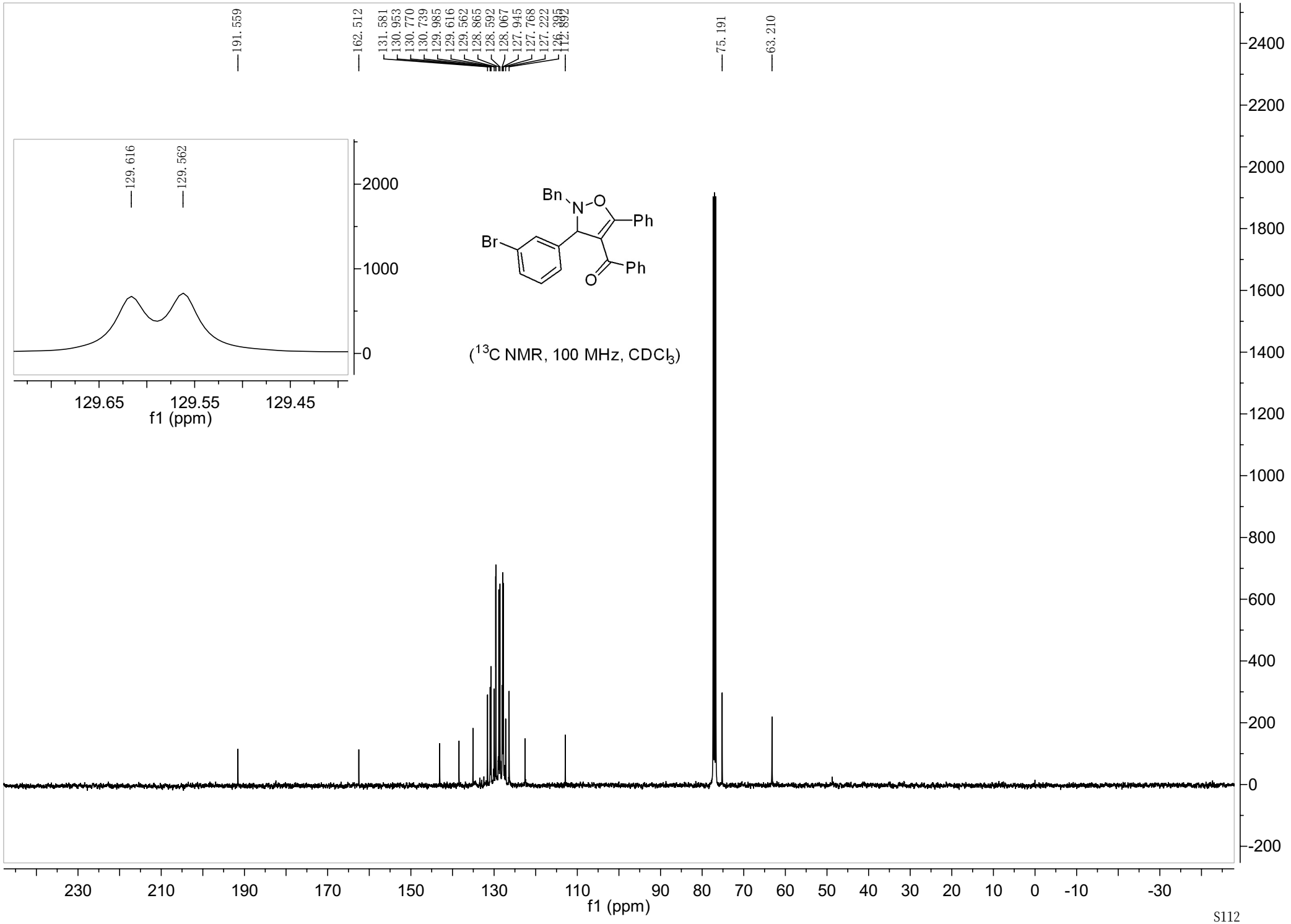

7.506
7.503
7.490
7.476
7.387
7.384
7.371
7.369
7.355
7.340
7.324
7.310
7.272
7.258
7.246
7.231
7.228
7.225
7.208
7.123
7.108
7.092
7.070
7.055
7.039
7.038
6.110
4.496
4.458
4.431
Bn
N
O
Cl
Ph
Ph
O
(1H NMR, 500 MHz, CDCl3)
3.03
6.01
6.09
4.05
0.96
2.00
f1 (ppm)

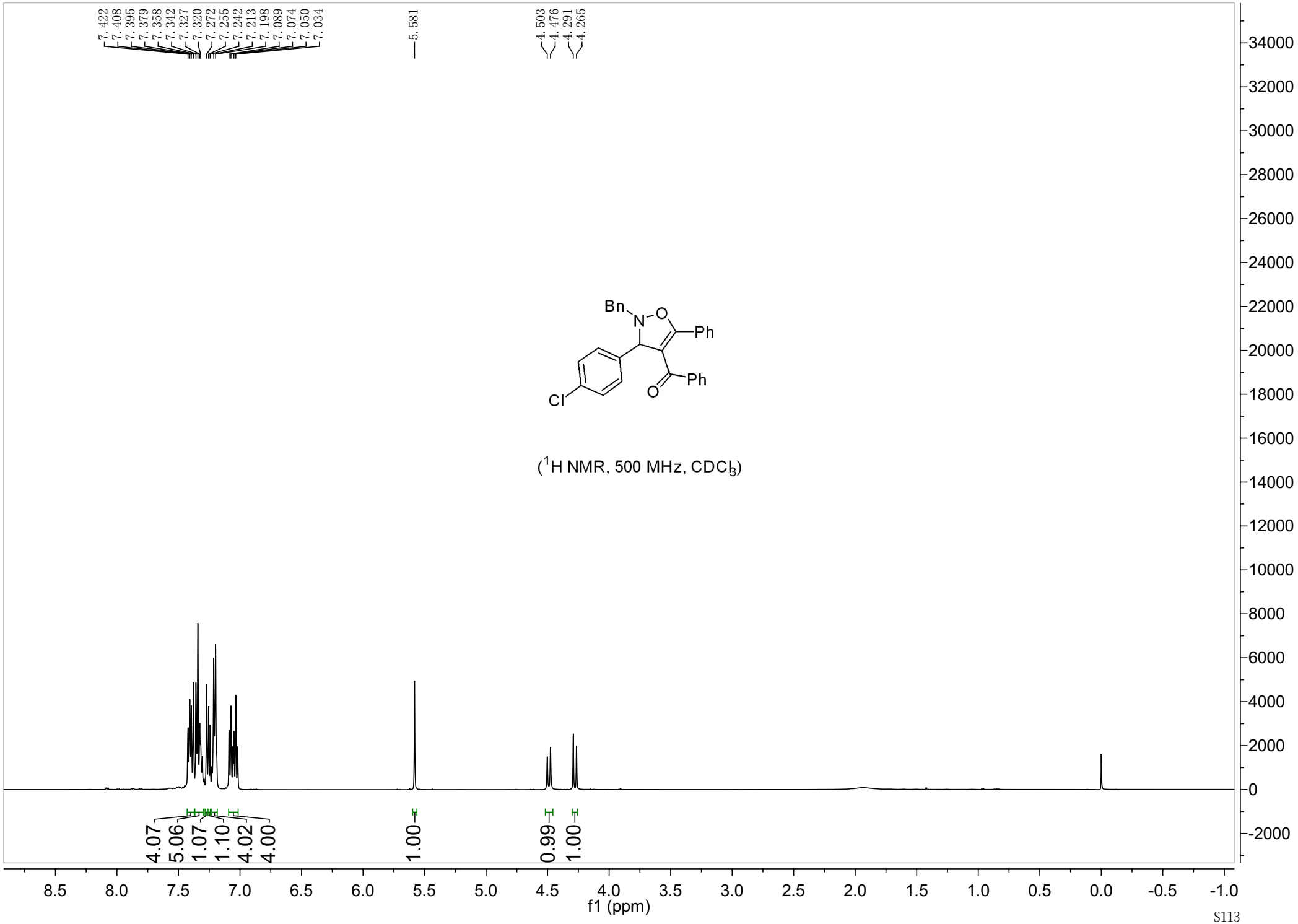

191. 130
163. 360
138. 364
137. 742
135. 499
134. 065
131. 517
130. 840
129. 807
129. 689
129. 608
129. 144
128. 984
128. 888
128. 488
127. 952
127. 895
127. 710
127. 238
127. 144
111. 746
72. 356
63. 603
Bn
N
O
Cl
Ph
Ph
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

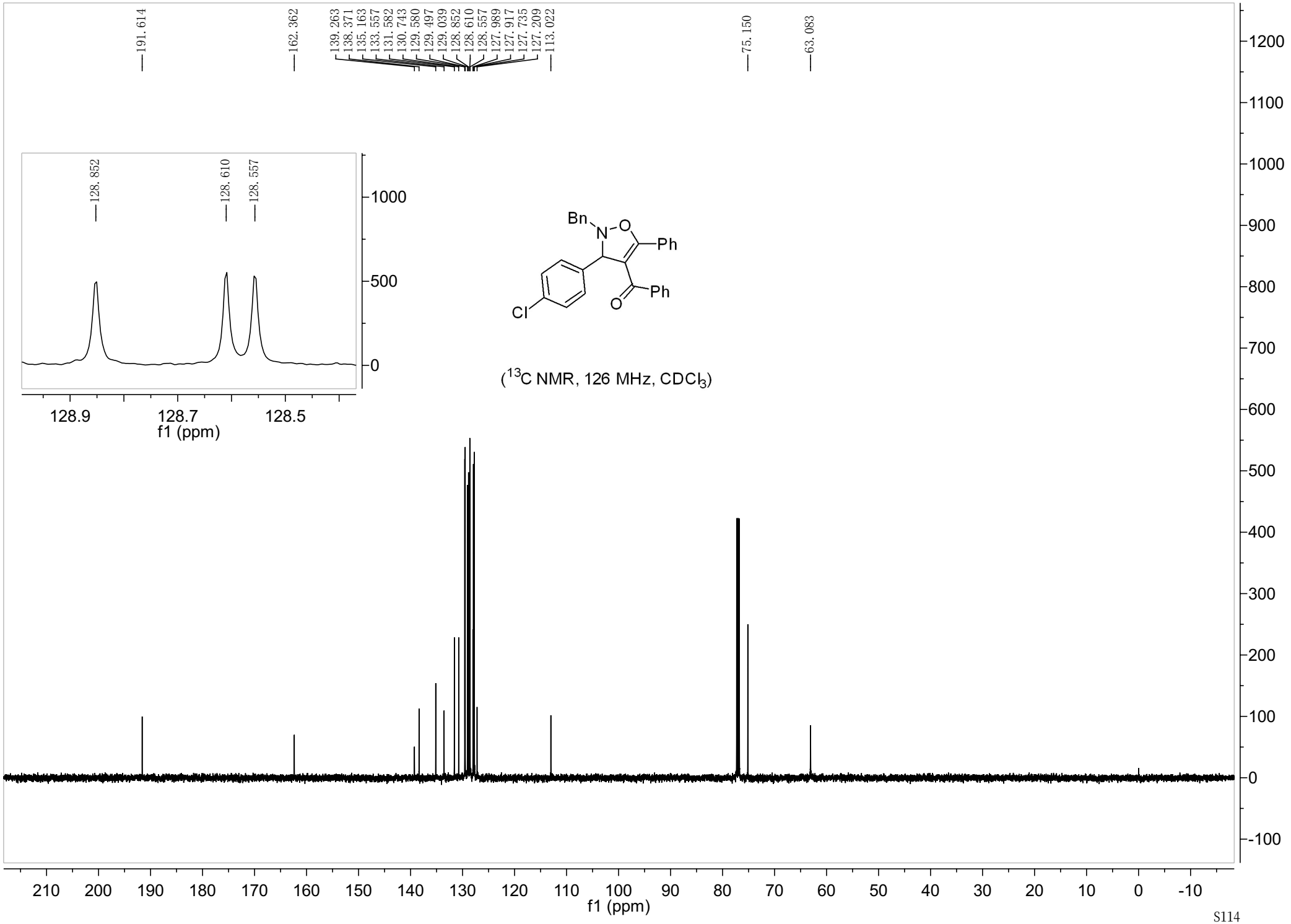

7.447
7.416
7.413
7.362
7.359
7.348
7.342
7.339
7.330
7.326
7.219
7.217
7.212
7.207
7.203
7.200
7.096
7.078
7.077
7.058
7.038
5.580
4.512
4.479
4.300
4.267
Bn
N
O
Ph
Cl
Ph
O
(1H NMR, 400 MHz, CDCl3)
3.00
6.01
6.02
4.00
1.00
1.00
1.00
f1 (ppm)

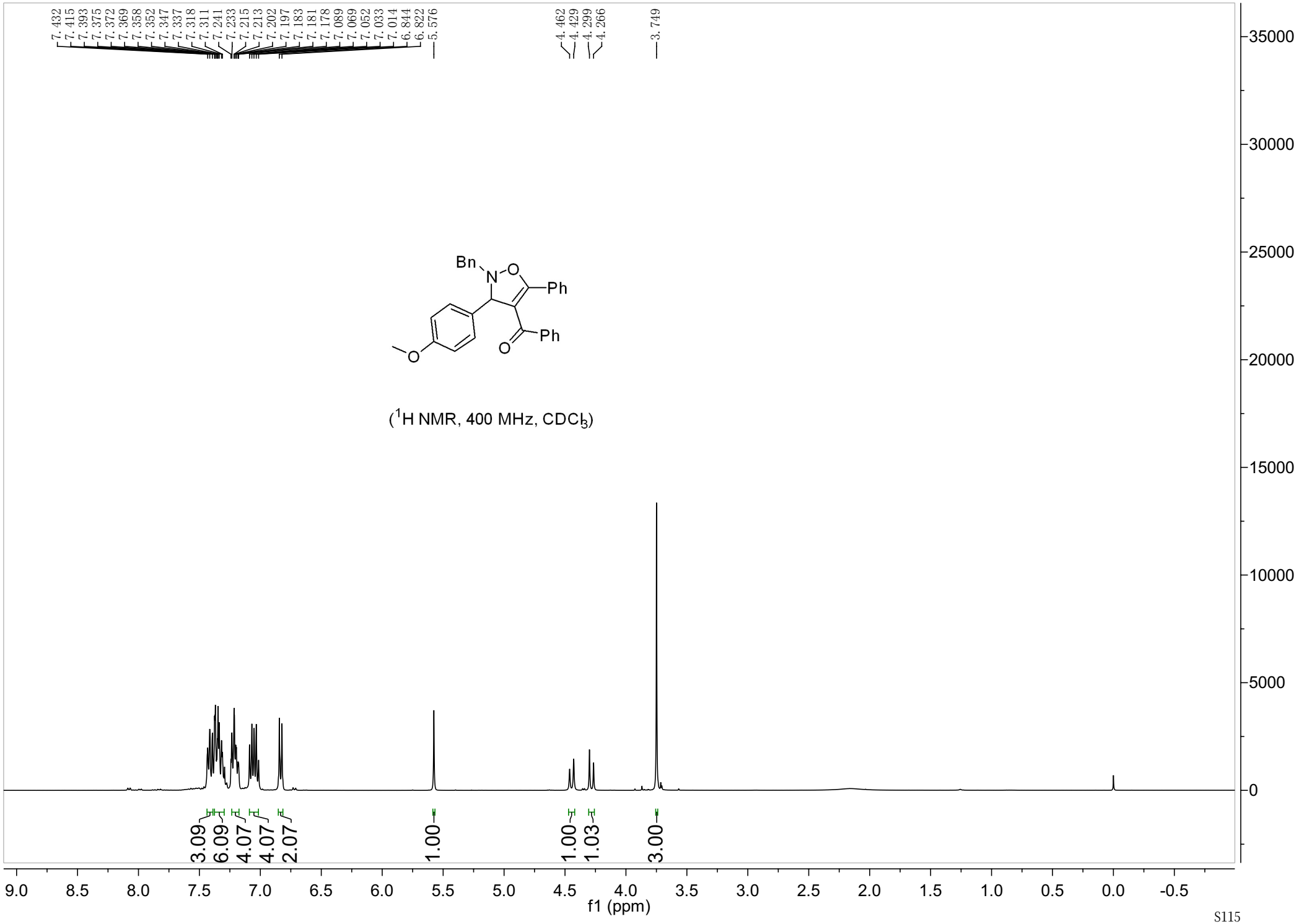

191.514
162.449
142.826
138.419
135.084
134.292
131.551
130.743
129.662
129.594
129.532
128.845
128.569
128.031
128.005
127.922
127.794
127.743
127.218
125.910
112.873
75.200
63.180
128.031
128.005
128.08
128.02
f1 (ppm)
Bn
N
O
Ph
Cl
Ph
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)


7.592
7.414
7.374
7.370
7.355
7.350
7.338
7.335
7.220
7.201
7.081
7.060
7.041
5.570
4.511
4.478
4.300
4.267
Bn
N
O
Ph
Br
Ph
O
(^{1}H NMR, 400 MHz, CDCl$_3$)
30000
25000
20000
15000
10000
5000
0
1.06
2.03
8.08
4.07
1.18
4.05
1.00
1.03
1.11
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

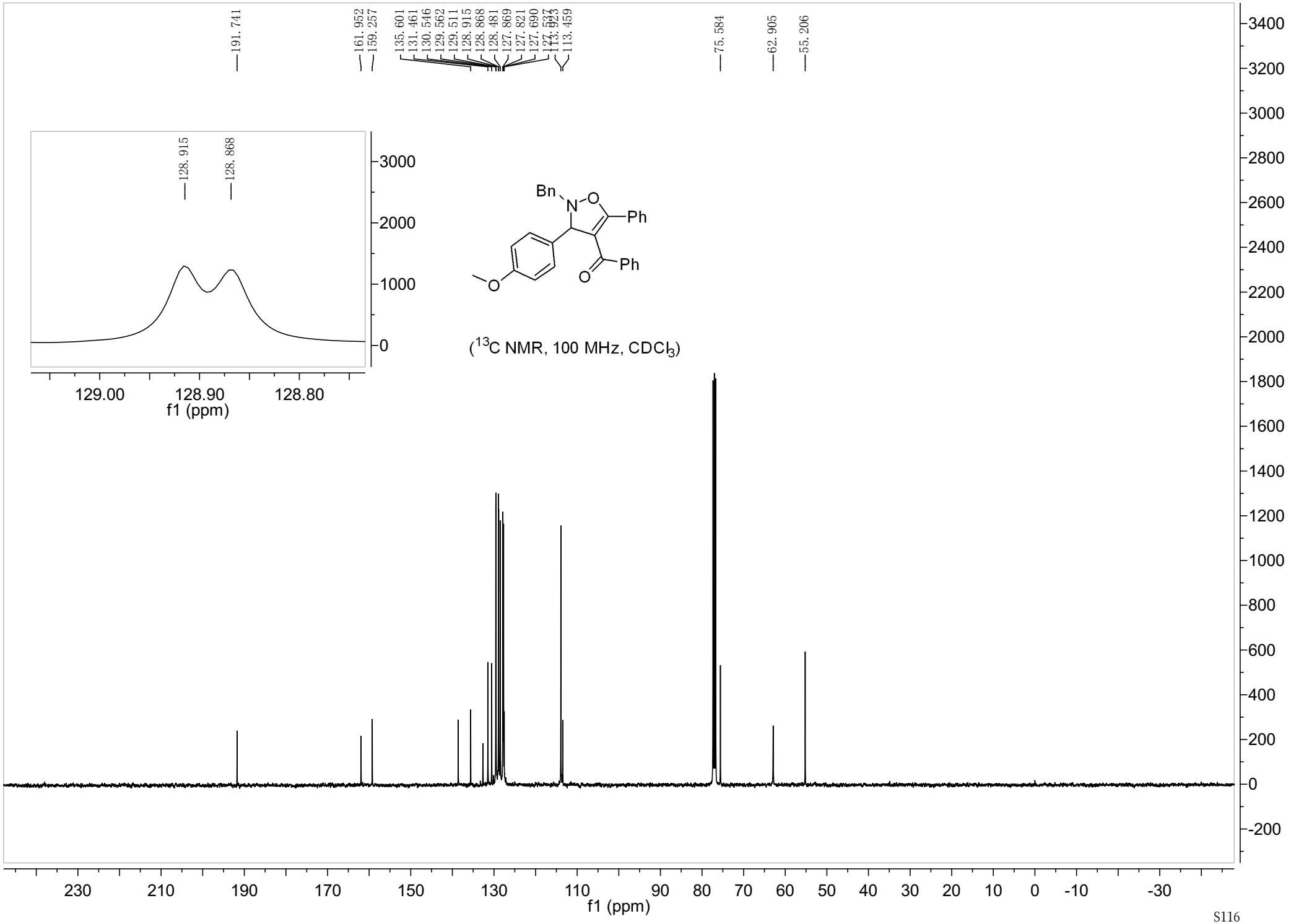

191.559
162.512
131.581
130.953
130.770
130.739
129.985
129.616
129.562
128.865
128.592
128.067
127.945
127.768
127.222
75.191
63.210
129.616
129.562
2000
1000
0
129.65
129.55
129.45
f1 (ppm)
Bn
N
O
Ph
Br
Ph
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-30
f1 (ppm)

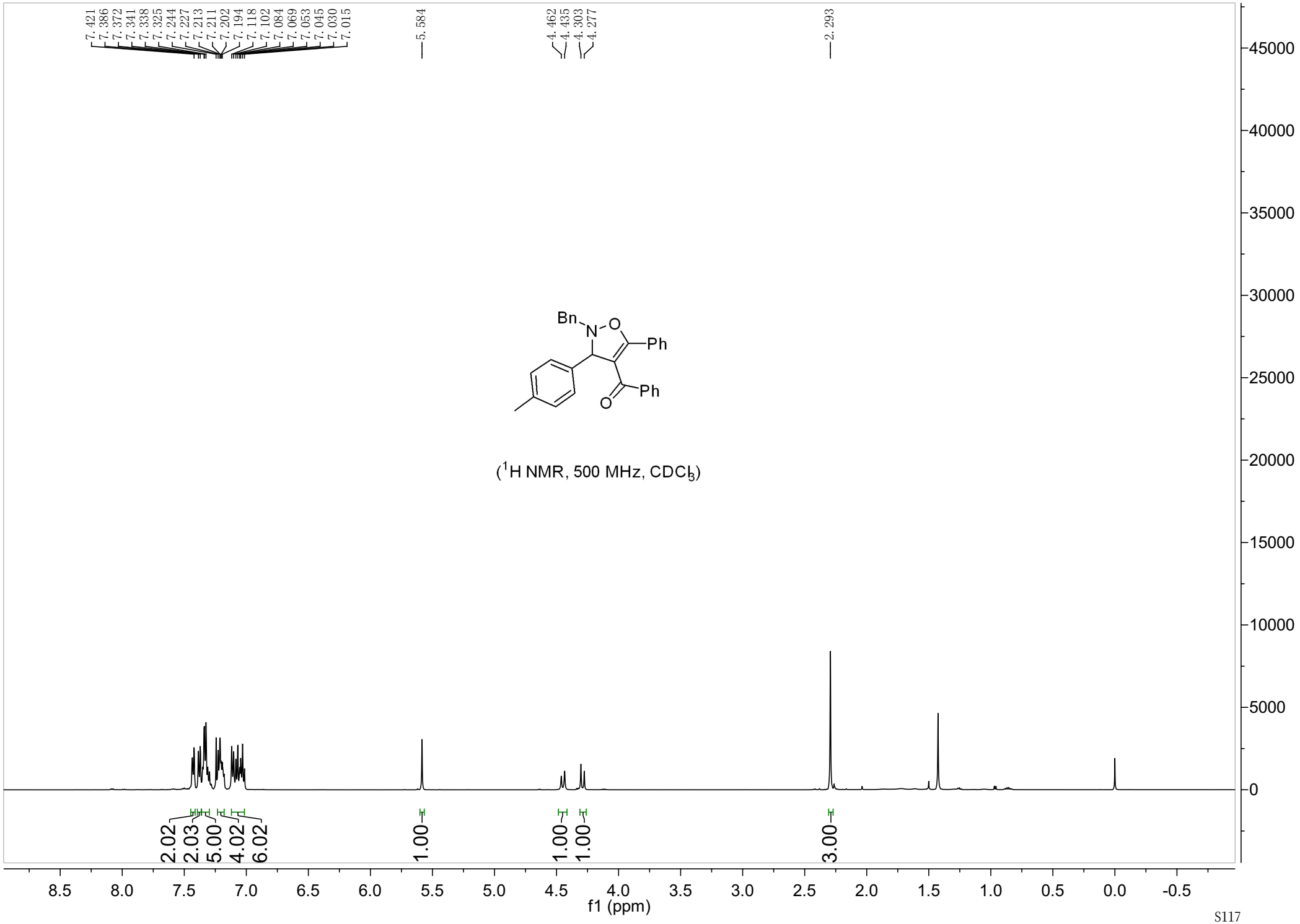

7.422
7.408
7.395
7.379
7.358
7.342
7.327
7.320
7.272
7.255
7.242
7.213
7.198
7.089
7.074
7.050
7.034
5.581
4.503
4.476
4.291
4.265
Bn
N
O
Ph
Ph
O
Cl
(1H NMR, 500 MHz, CDCl3)
4.07
5.06
1.07
1.10
4.02
4.00
1.00
0.99
1.00
f1 (ppm)

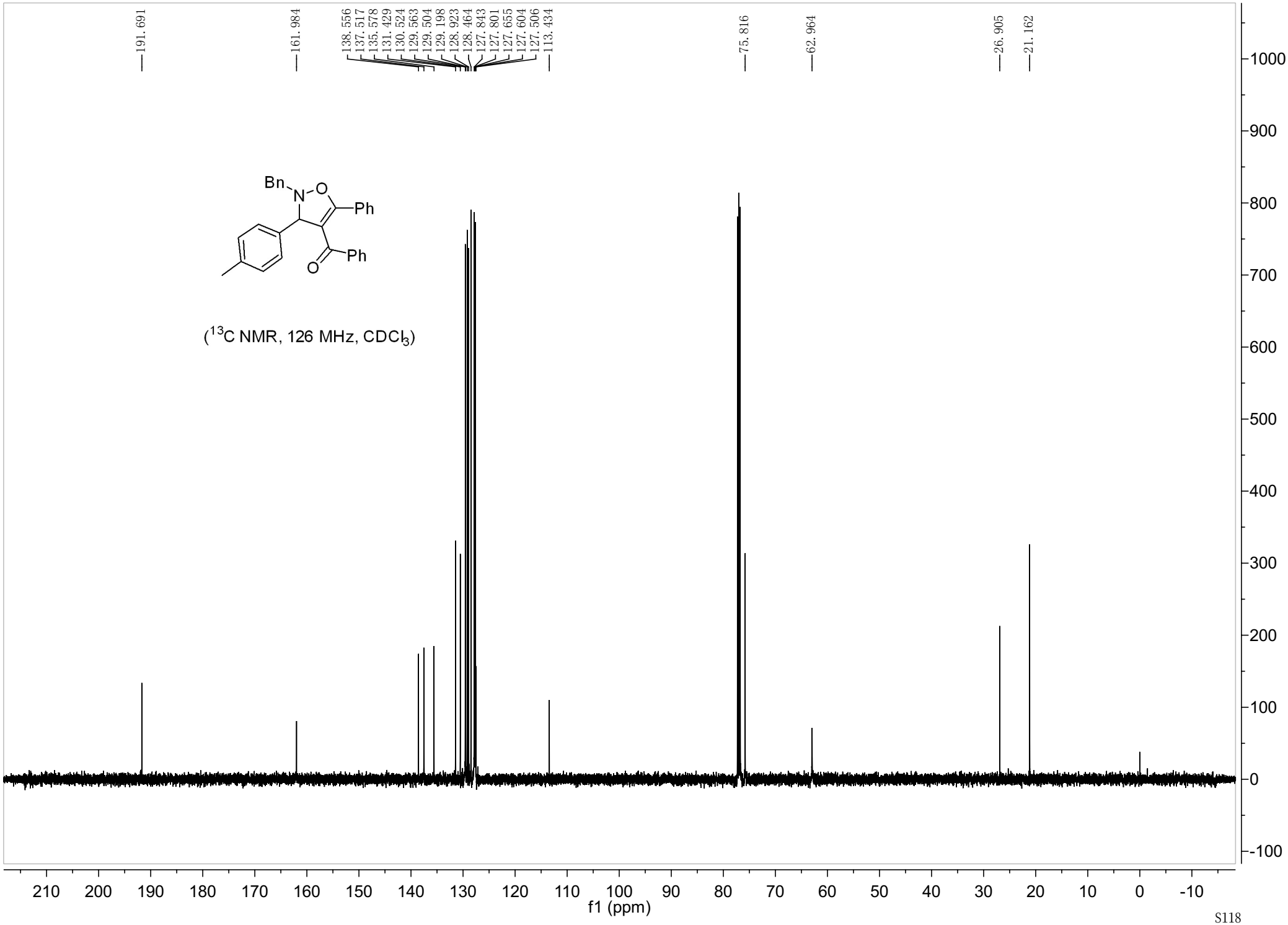

191.614
162.362
139.263
138.371
135.163
133.557
131.582
130.743
129.580
129.497
129.039
128.852
128.610
128.557
127.989
127.917
127.735
127.209
113.022
75.150
63.083
128.852
128.610
128.557
Bn
N
O
Ph
Ph
O
Cl
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

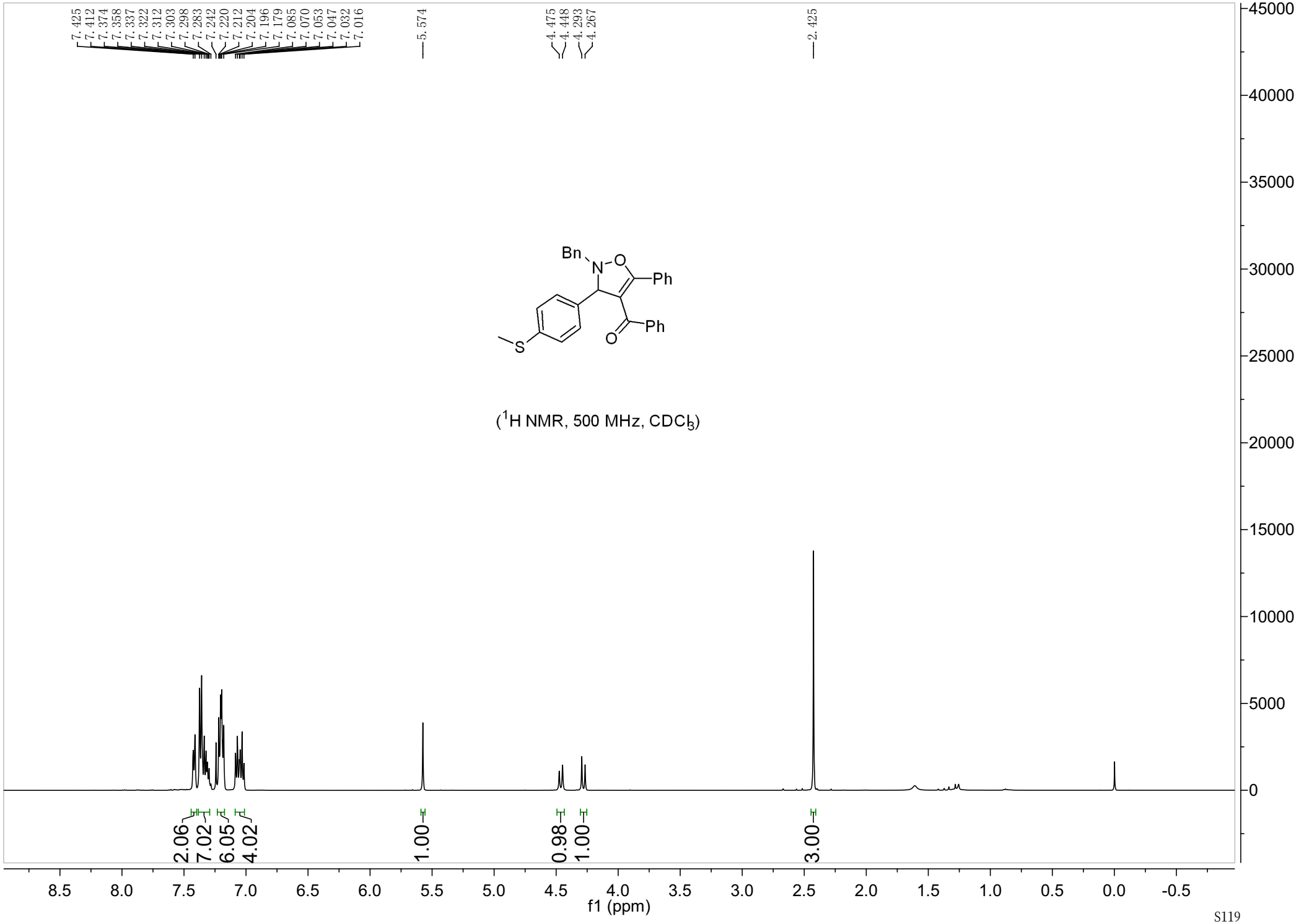


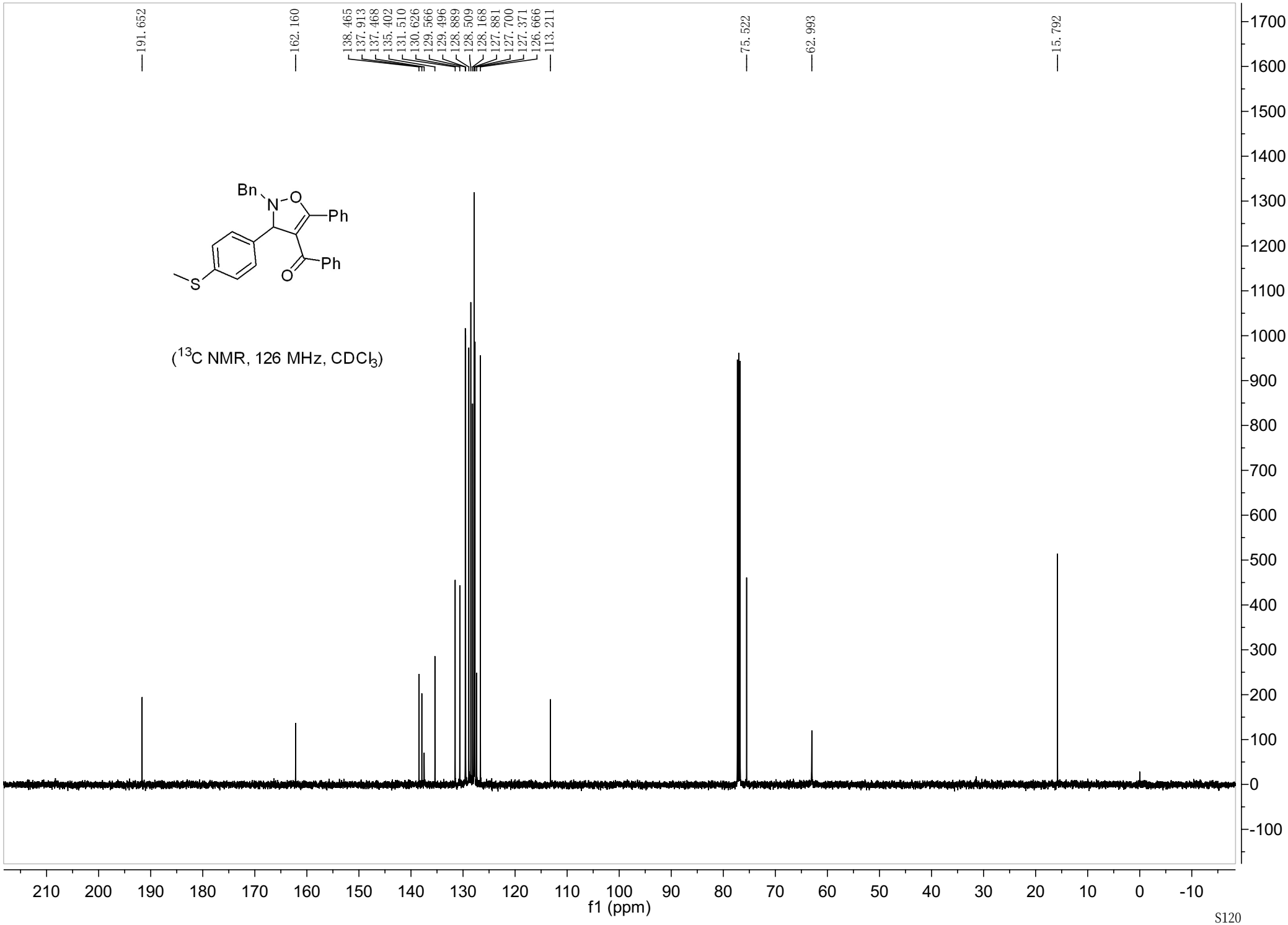
(^{1}H NMR, 400 MHz, $CDCl_3$)

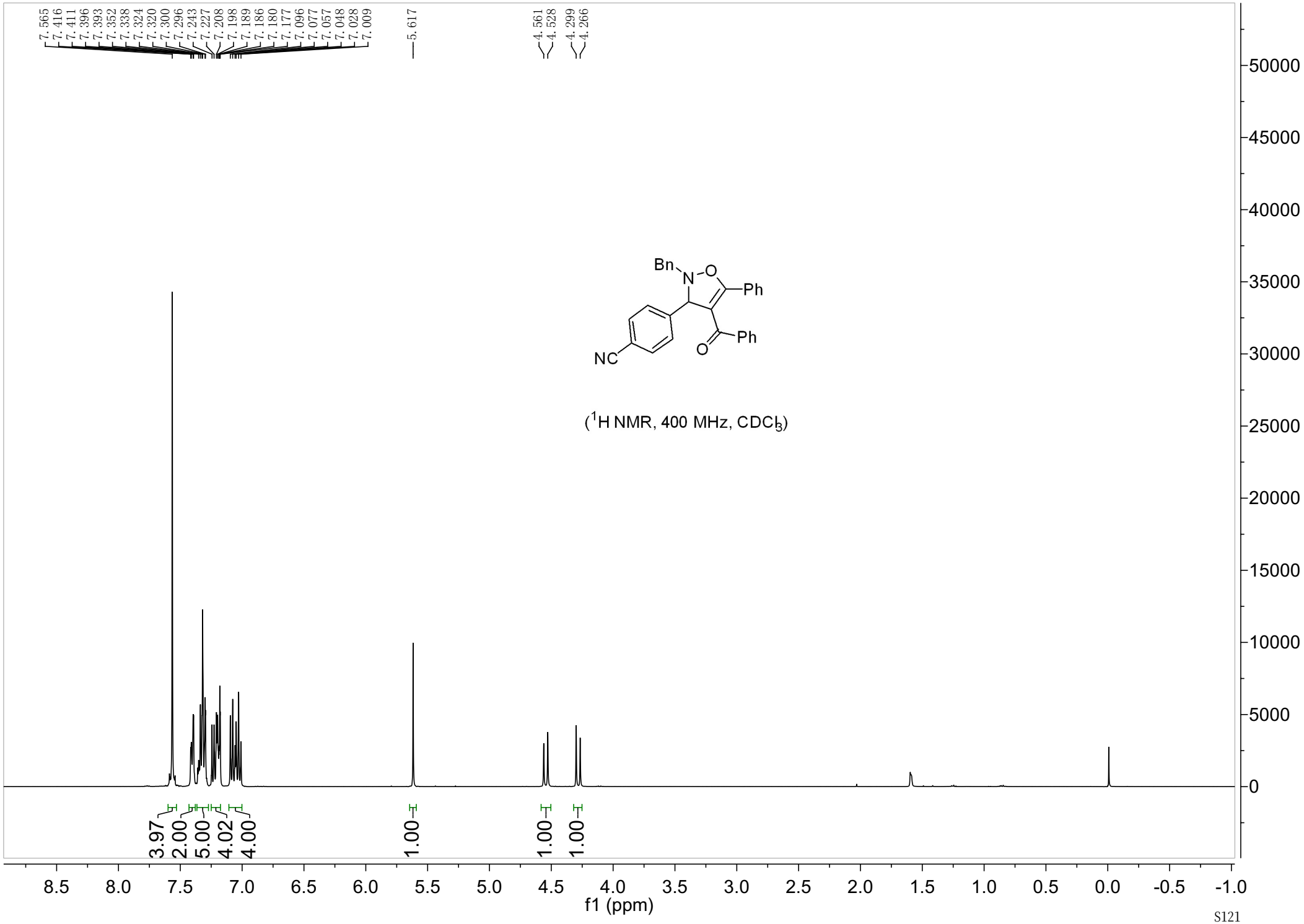

191.741
161.952
159.257
135.601
131.461
130.546
129.562
129.511
128.915
128.868
128.481
127.869
127.821
127.690
113.459
75.584
62.905
55.206
128.915
128.868
129.00
128.90
128.80
f1 (ppm)
Bn
N
O
Ph
Ph
O
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

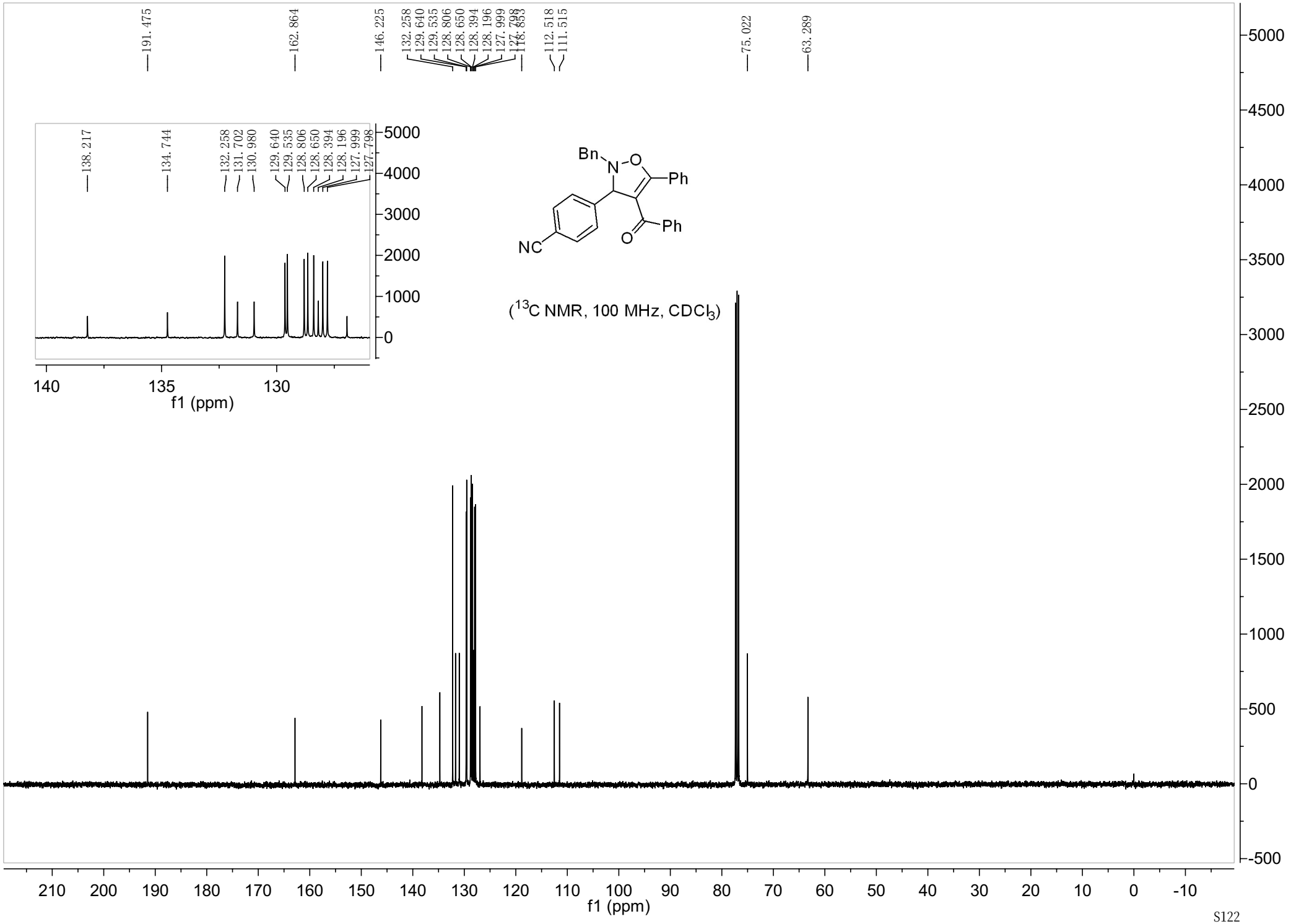

7.421
7.386
7.372
7.341
7.338
7.325
7.244
7.227
7.213
7.211
7.202
7.194
7.118
7.102
7.084
7.069
7.053
7.045
7.030
7.015
5.584
4.462
4.435
4.303
4.277
2.293
Bn
N
O
Ph
Ph
O
(1H NMR, 500 MHz, CDCl3)
2.02
2.03
5.00
4.02
6.02
1.00
1.00
1.00
3.00
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

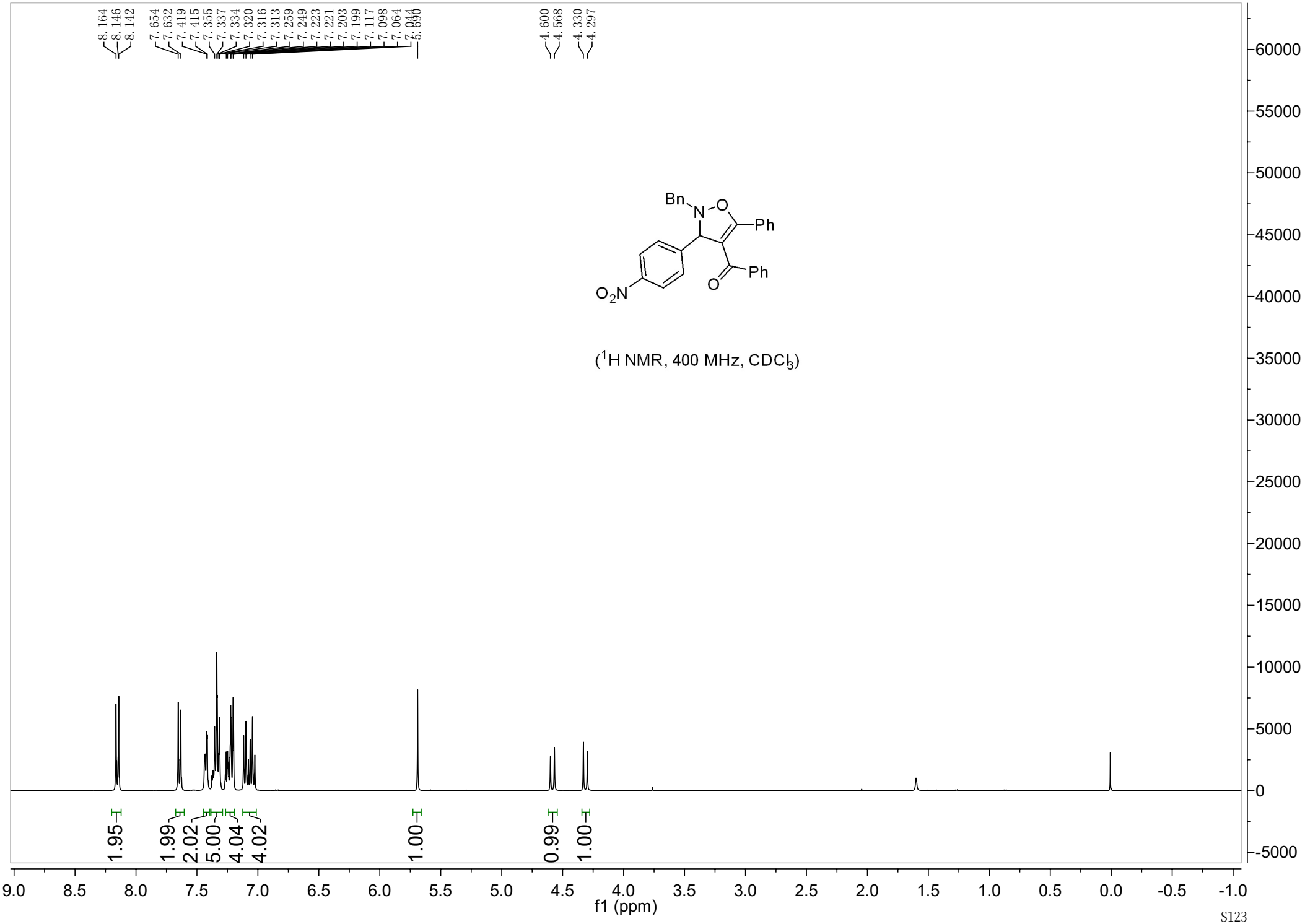

191.691
161.984
138.556
137.517
135.578
131.429
130.524
129.563
129.504
129.198
128.923
128.464
127.843
127.801
127.655
127.604
127.506
113.434
75.816
62.964
26.905
21.162
Bn
N
O
Ph
Ph
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
1000
900
800
700
600
500
400
300
200
100
0
-100
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

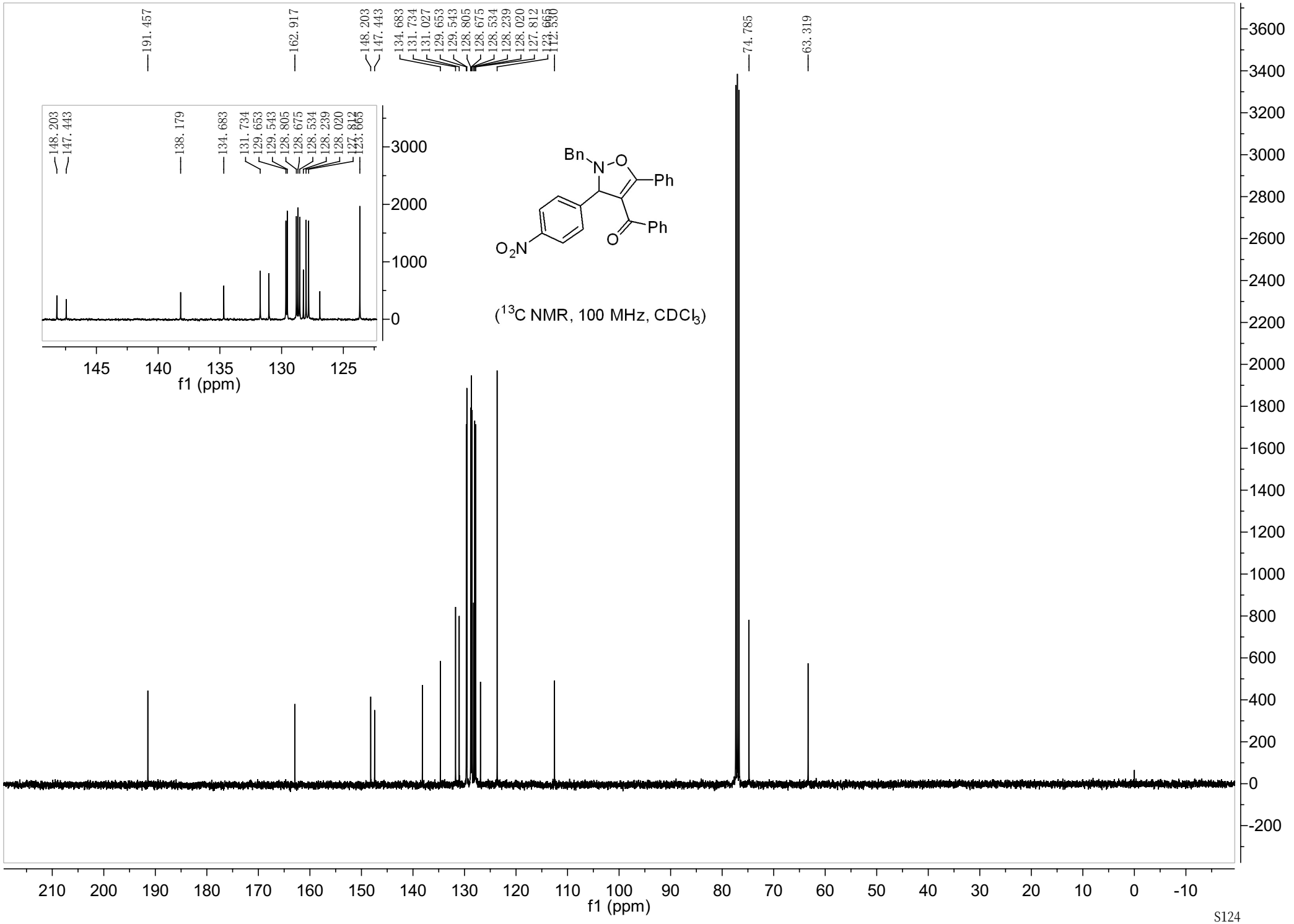

7.425
7.412
7.374
7.358
7.337
7.322
7.312
7.303
7.298
7.283
7.242
7.220
7.212
7.204
7.196
7.179
7.085
7.070
7.053
7.047
7.032
7.016
5.574
4.475
4.448
4.293
4.267
2.425
Bn
N
O
Ph
Ph
O
S
(1H NMR, 500 MHz, CDCl3)
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
2.06
7.02
6.05
4.02
1.00
0.98
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

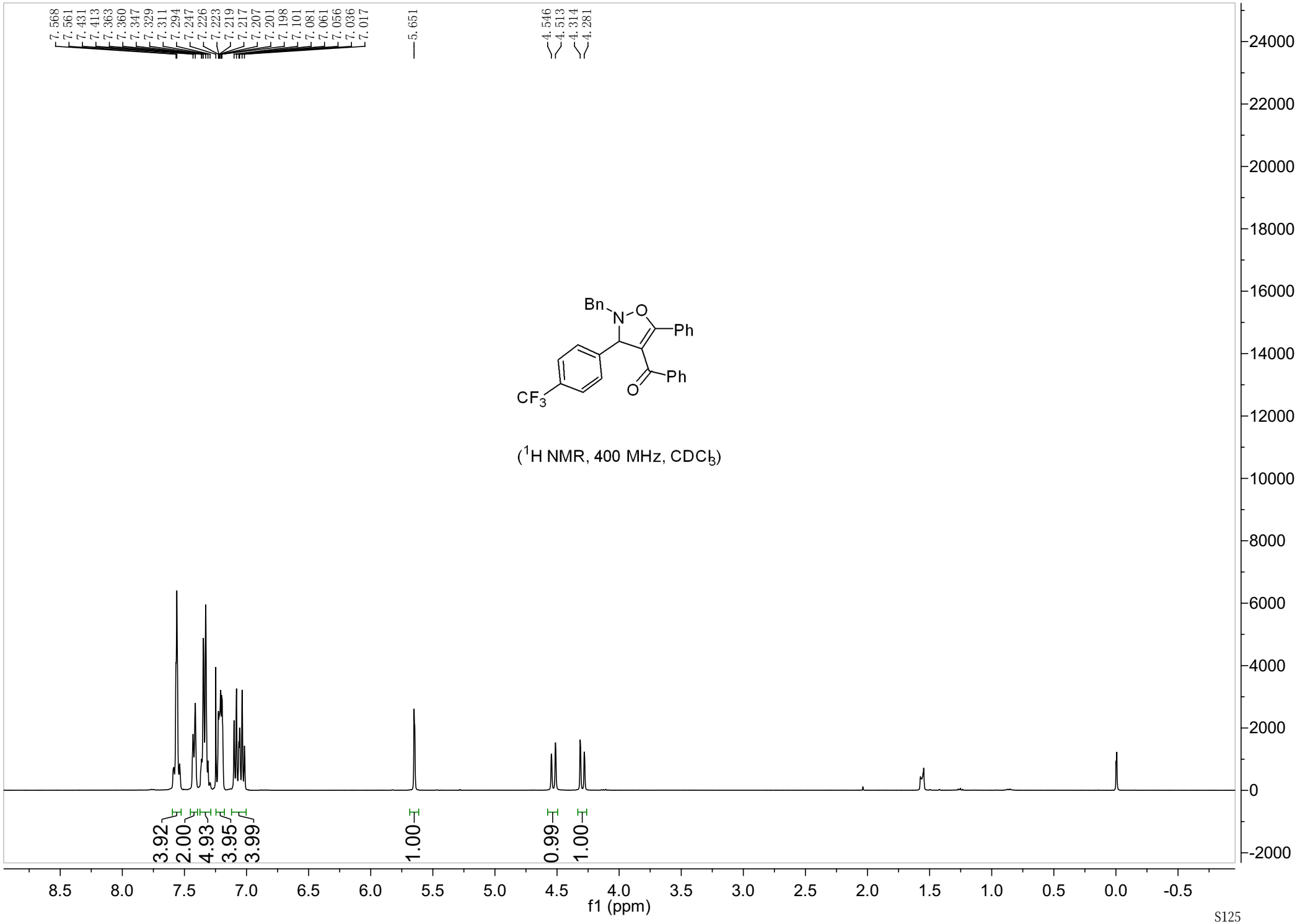

191.652
162.160
138.465
137.913
137.468
135.402
131.510
130.626
129.566
129.496
128.889
128.509
128.168
127.881
127.700
127.371
126.666
113.211
75.522
62.993
15.792
Bn
N
O
Ph
Ph
O
S
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)

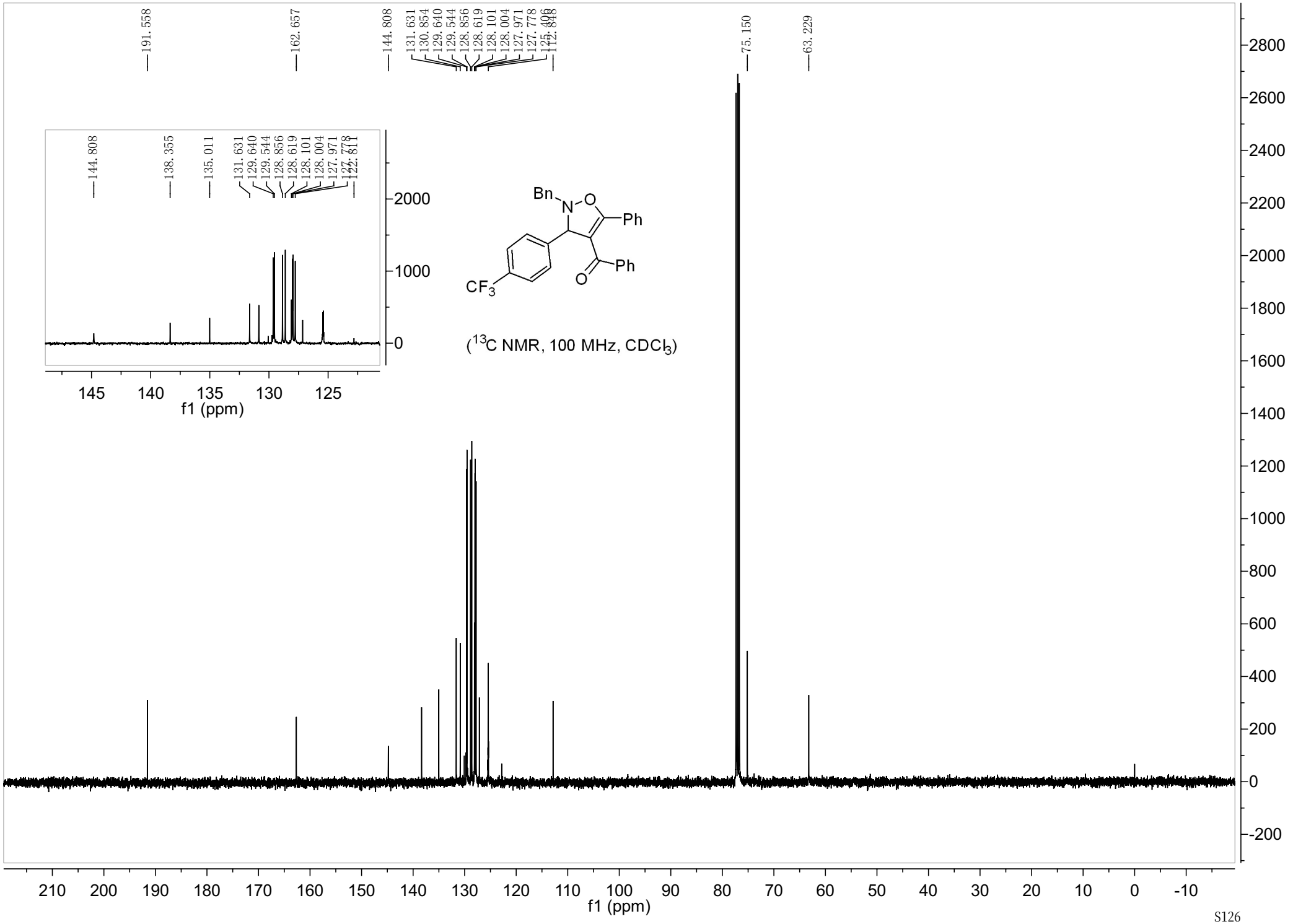

7.565
7.416
7.411
7.396
7.393
7.352
7.338
7.324
7.320
7.300
7.296
7.243
7.227
7.208
7.198
7.189
7.186
7.180
7.177
7.096
7.077
7.057
7.048
7.028
7.009
5.617
4.561
4.528
4.299
4.266
Bn
N
O
Ph
Ph
O
NC
(1H NMR, 400 MHz, CDCl3)
3.97
2.00
5.00
4.02
4.00
1.00
1.00
1.00
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

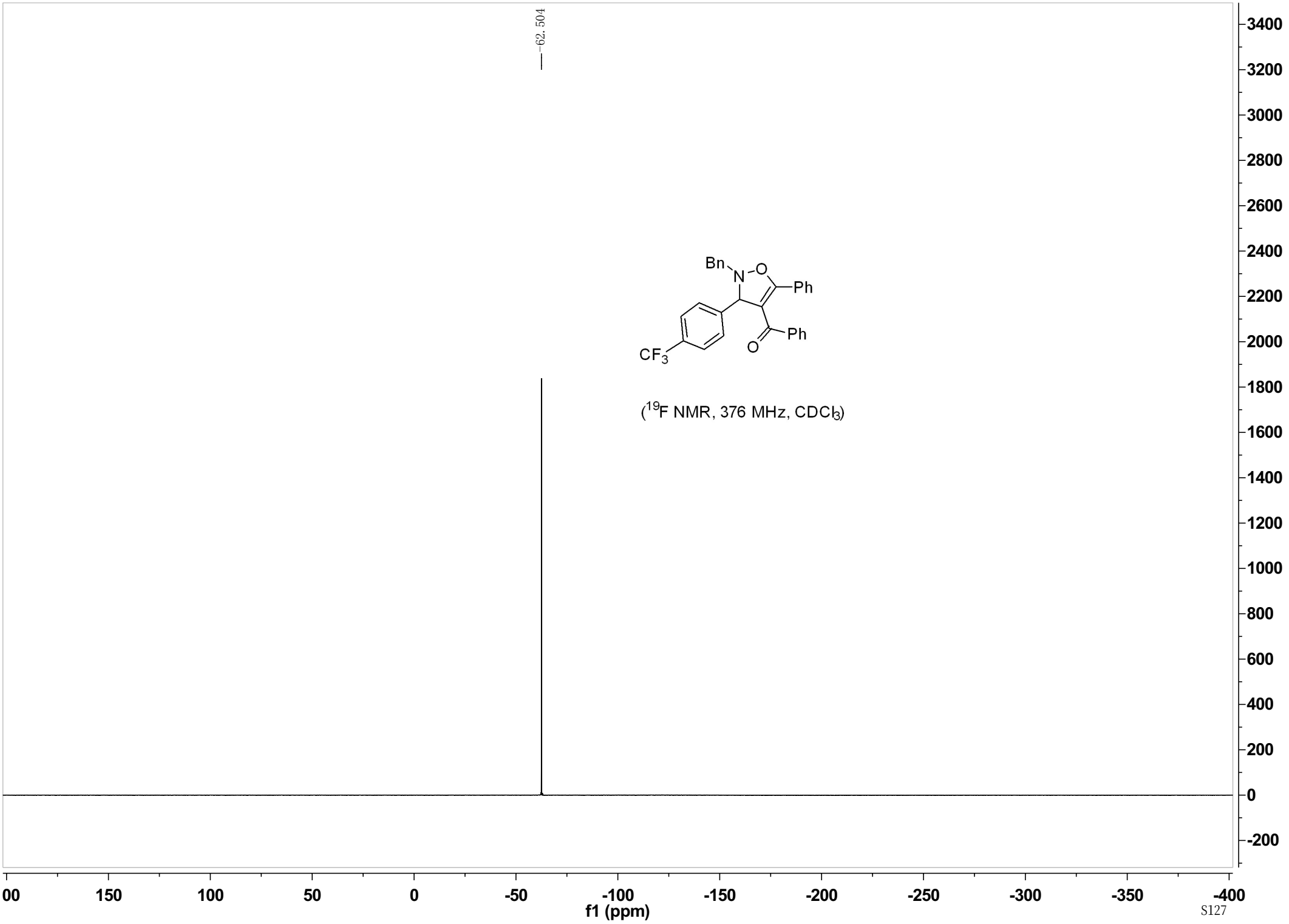

191.475
162.864
146.225
132.258
129.640
129.535
128.806
128.650
128.394
128.196
127.999
127.798
118.853
112.518
111.515
75.022
63.289
138.217
134.744
132.258
131.702
130.980
129.640
129.535
128.806
128.650
128.394
128.196
127.999
127.798
Bn
N
O
Ph
Ph
O
NC
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

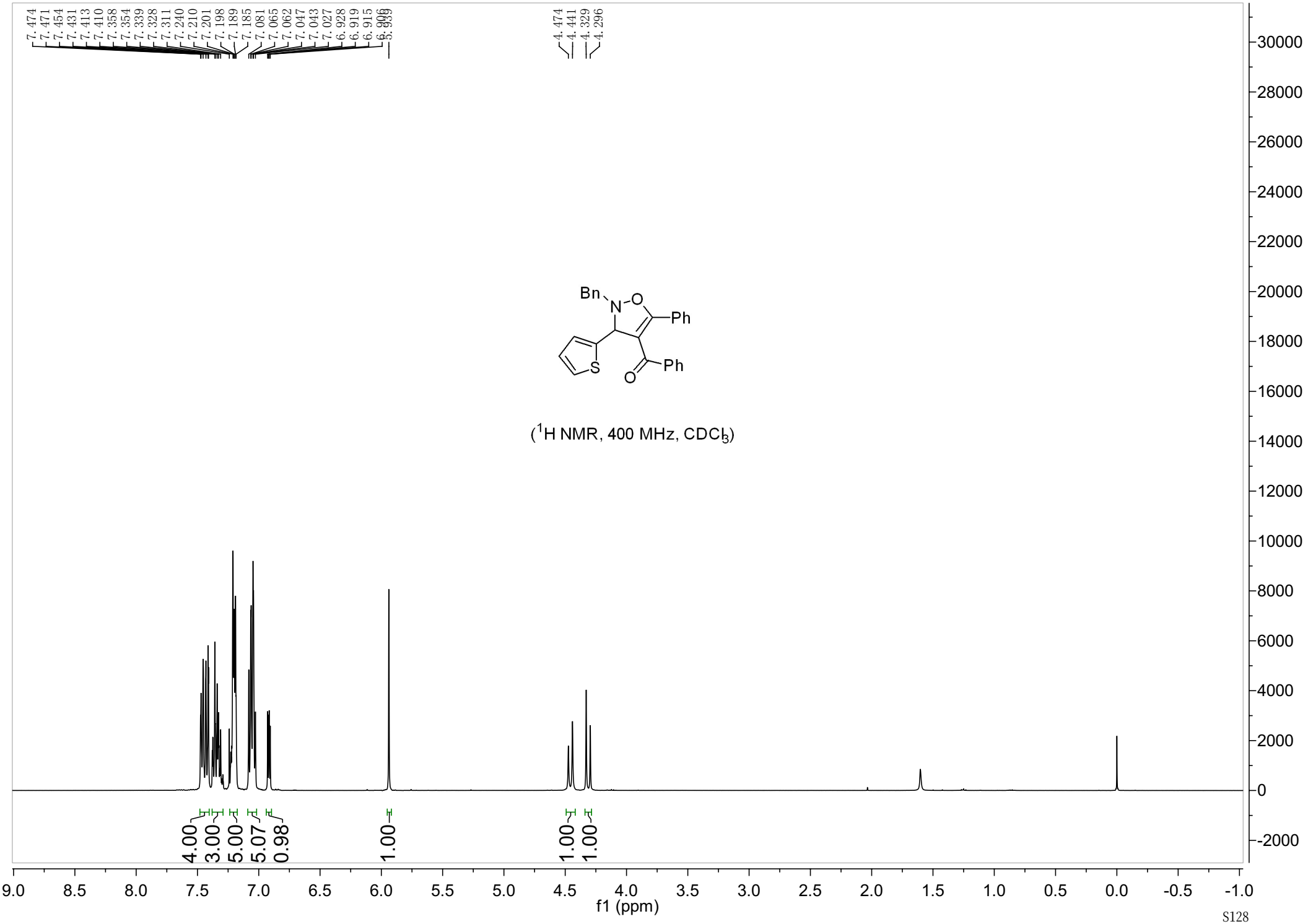

8.164
8.146
8.142
7.654
7.632
7.419
7.415
7.355
7.337
7.334
7.320
7.316
7.313
7.259
7.249
7.223
7.221
7.203
7.199
7.117
7.098
7.064
7.044
5.690
4.600
4.568
4.330
4.297
Bn
N
O
Ph
Ph
O
O_2N
(^{1}H NMR, 400 MHz, $CDCl_3$)
1.95
1.99
2.02
5.00
4.04
4.02
1.00
0.99
1.00
f1 (ppm)

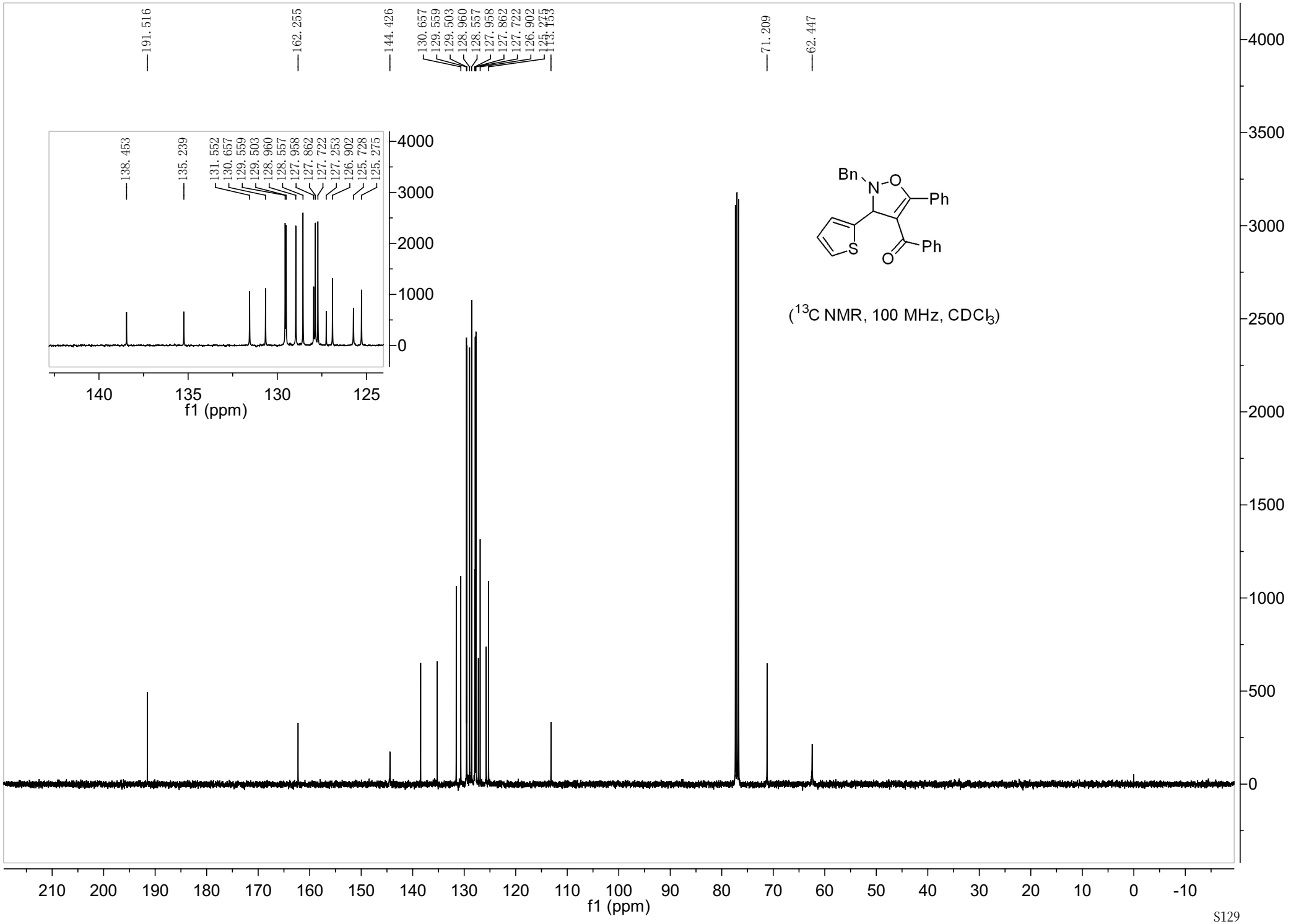

191.457
162.917
148.203
147.443
134.683
131.734
131.027
129.653
129.543
128.805
128.675
128.534
128.239
128.020
127.812
74.785
63.319
Bn
N
O
Ph
Ph
O
O_2N
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

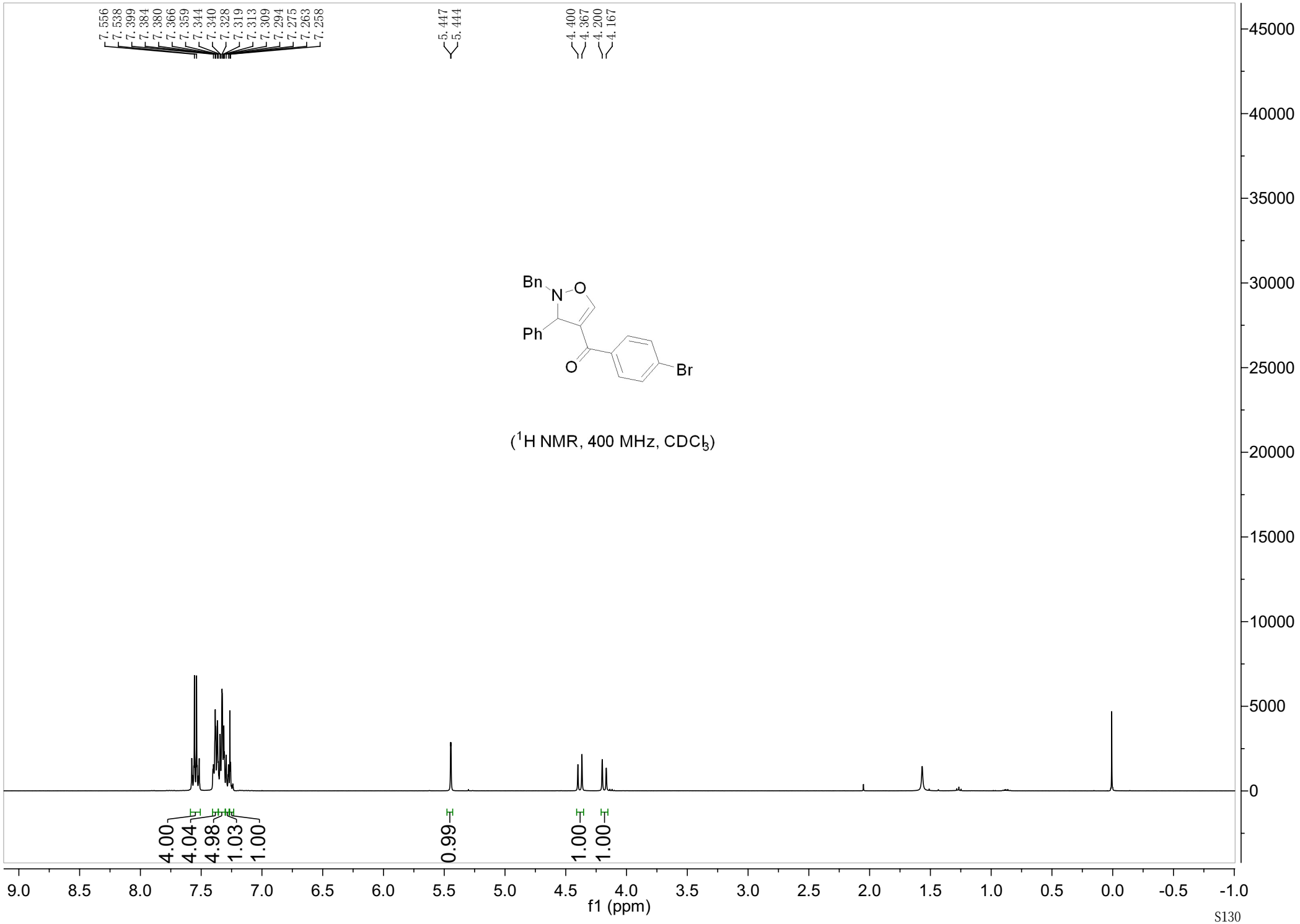

7.568
7.561
7.431
7.413
7.363
7.360
7.347
7.329
7.311
7.294
7.247
7.226
7.223
7.219
7.217
7.207
7.201
7.198
7.101
7.081
7.061
7.056
7.036
7.017
5.651
4.546
4.513
4.314
4.281
Bn
N
O
Ph
Ph
O
CF3
(1H NMR, 400 MHz, CDCl3)
3.92
2.00
4.93
3.95
3.99
1.00
0.99
1.00
f1 (ppm)

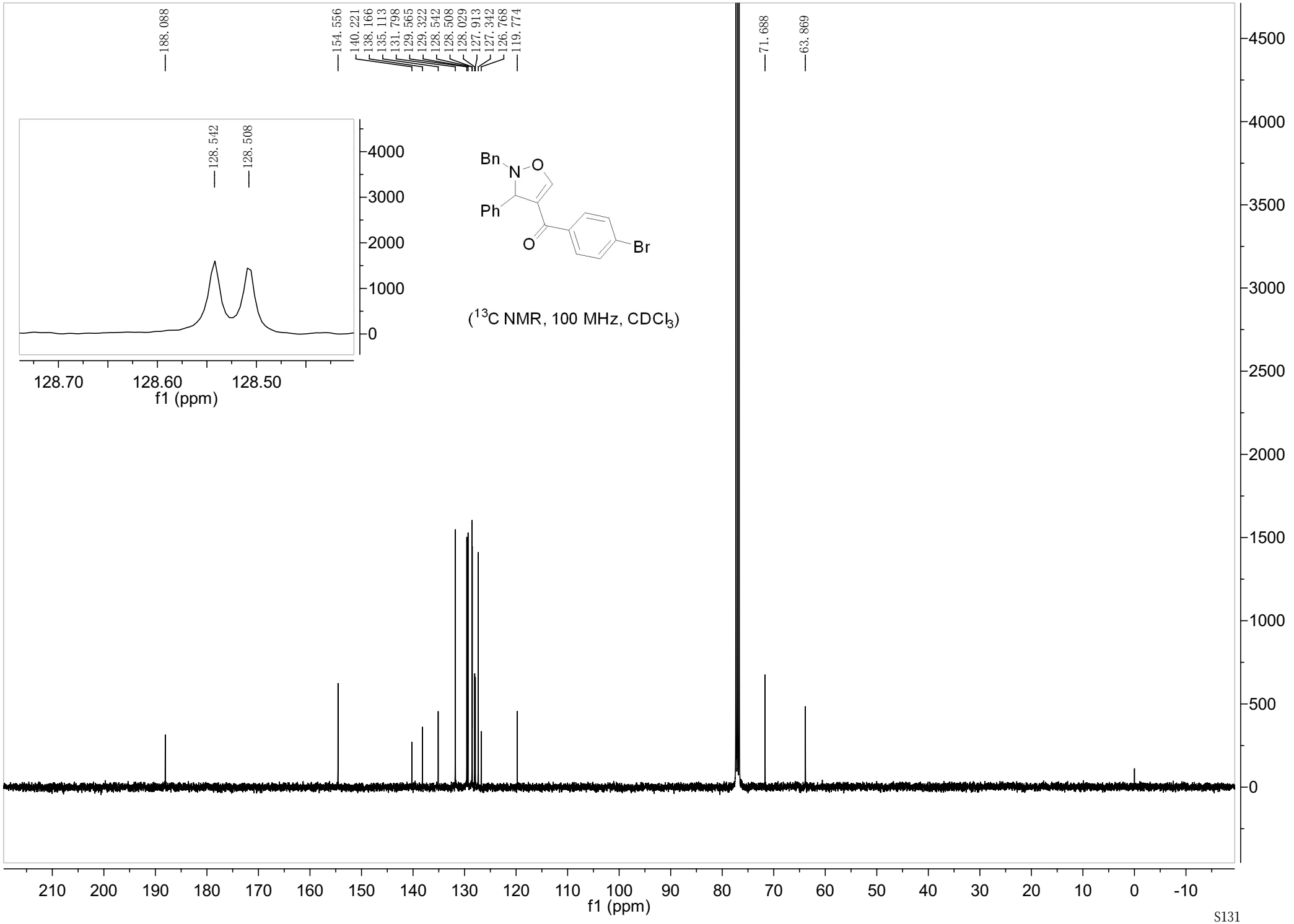

191.558
162.657
144.808
131.631
130.854
129.640
129.544
128.856
128.619
128.101
128.004
127.971
127.778
125.406
122.811
75.150
63.229
Bn
N
O
Ph
Ph
O
CF3
(^{13}C NMR, 100 MHz, CDCl$_3$)
f1 (ppm)

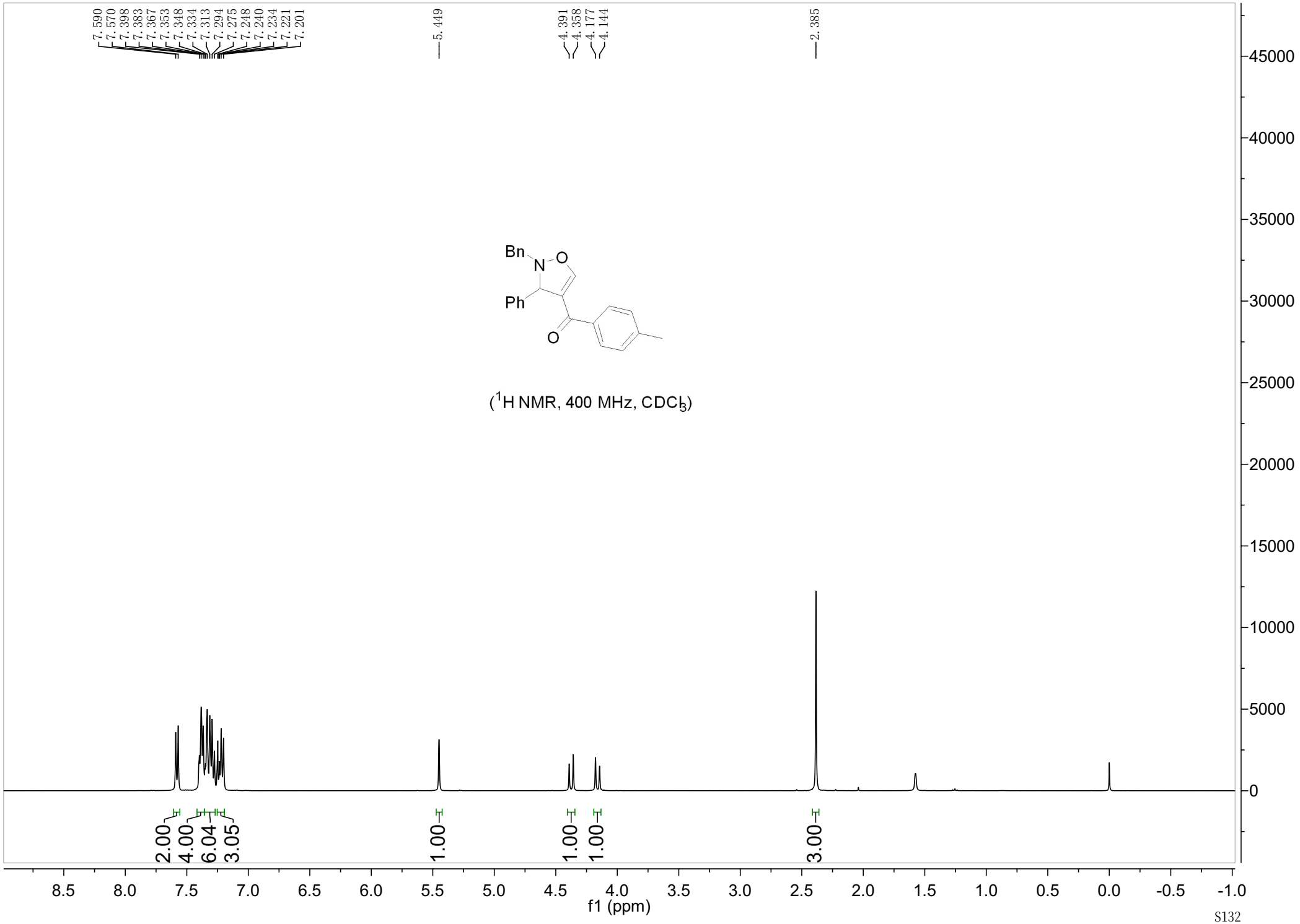

−62.504
Bn
N
O
Ph
Ph
O
CF3
(19F NMR, 376 MHz, CDCl3)
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-400
f1 (ppm)

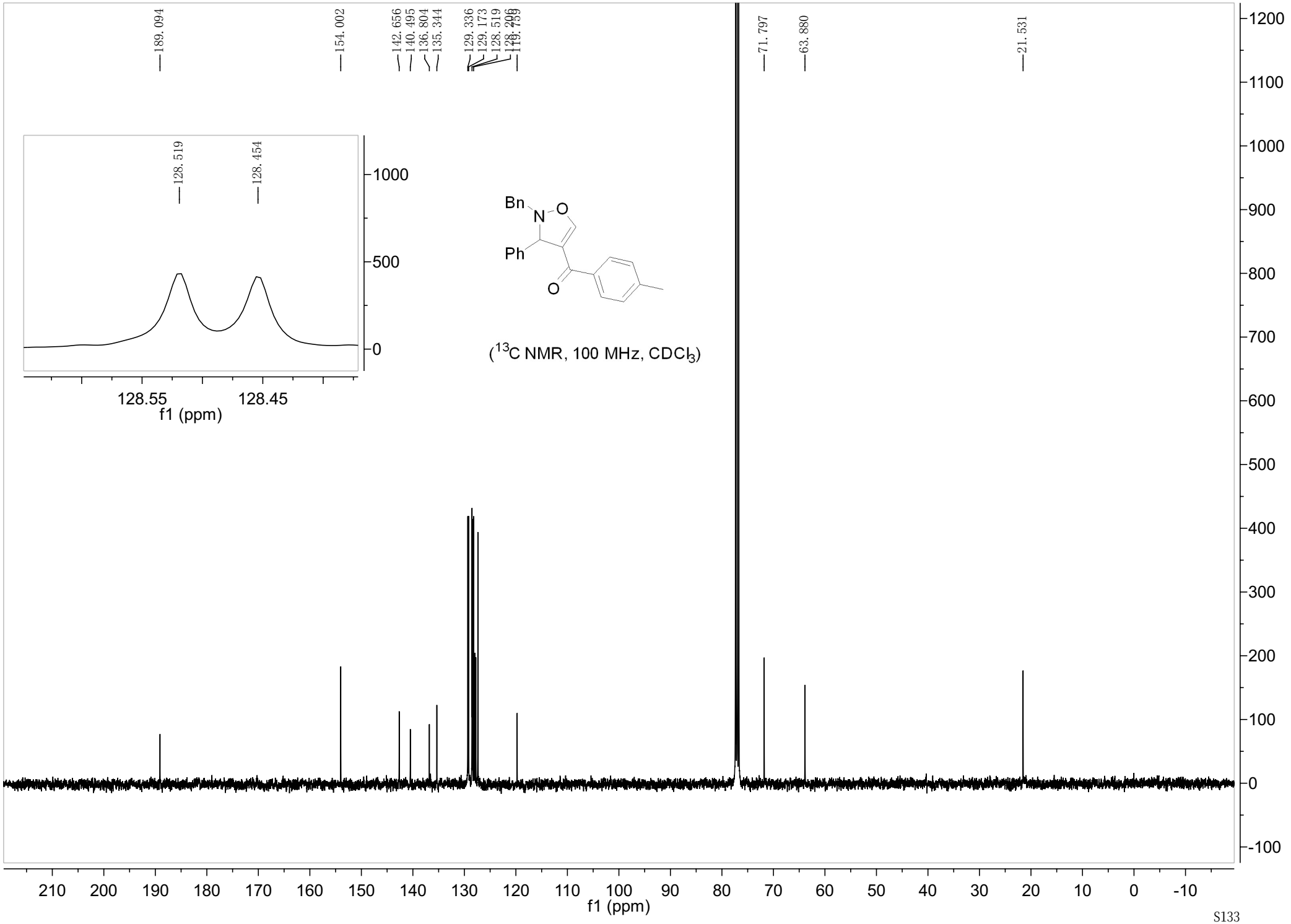

7.474
7.471
7.454
7.431
7.413
7.410
7.358
7.354
7.339
7.328
7.311
7.240
7.210
7.201
7.198
7.189
7.185
7.081
7.065
7.062
7.047
7.043
7.027
6.928
6.919
6.915
4.474
4.441
4.329
4.296
Bn
N
O
Ph
S
O
Ph
(^{1}H NMR, 400 MHz, CDCl$_3$)
4.00
3.00
5.00
5.07
0.98
1.00
1.00
1.00
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

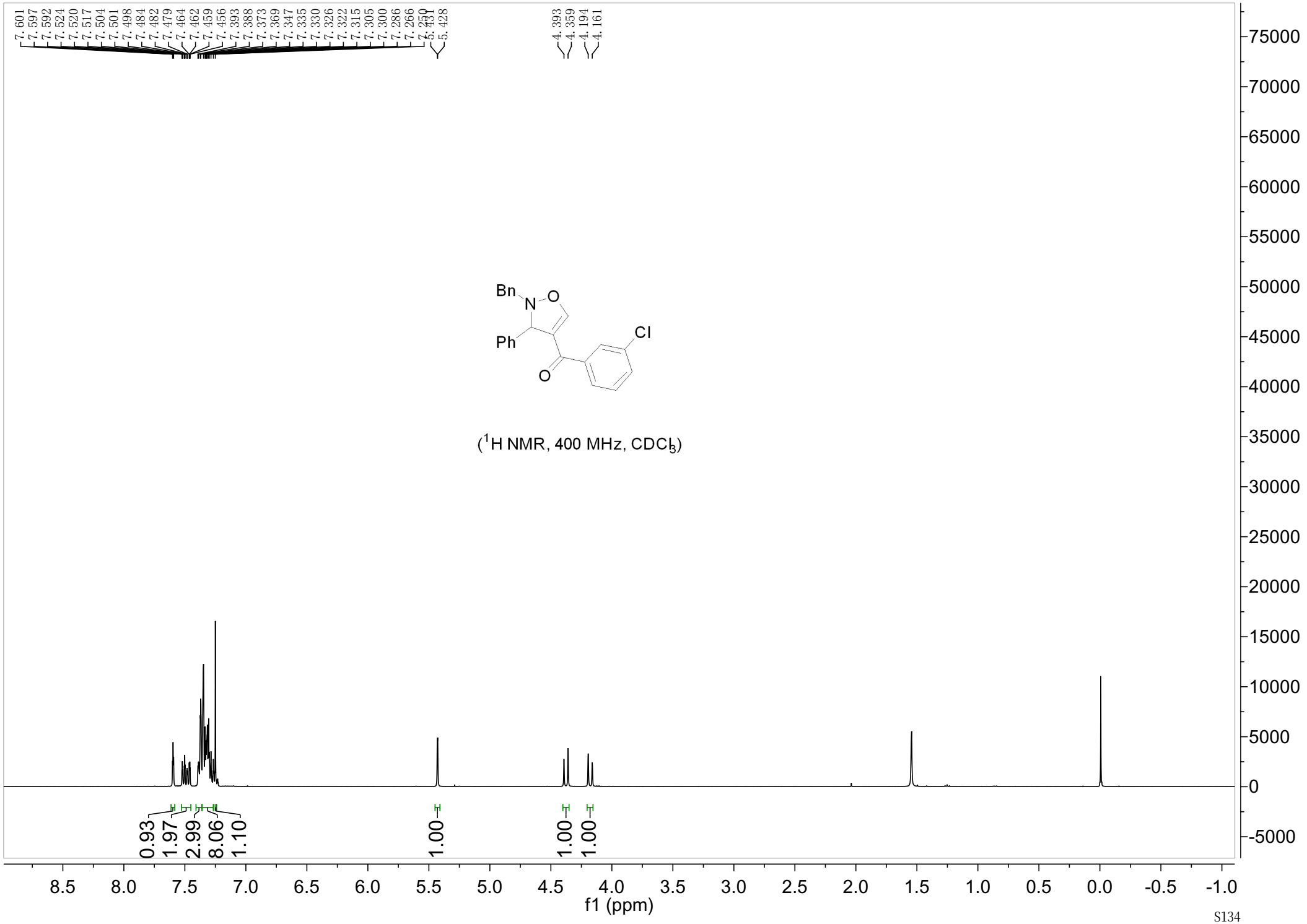

191.516
162.255
144.426
130.657
129.559
129.503
128.960
128.557
127.958
127.862
127.722
126.902
71.209
62.447
138.453
135.239
131.552
130.657
129.559
129.503
128.960
128.557
127.958
127.862
127.722
127.253
126.902
125.728
125.275
f1 (ppm)
Bn
N
O
Ph
Ph
S
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

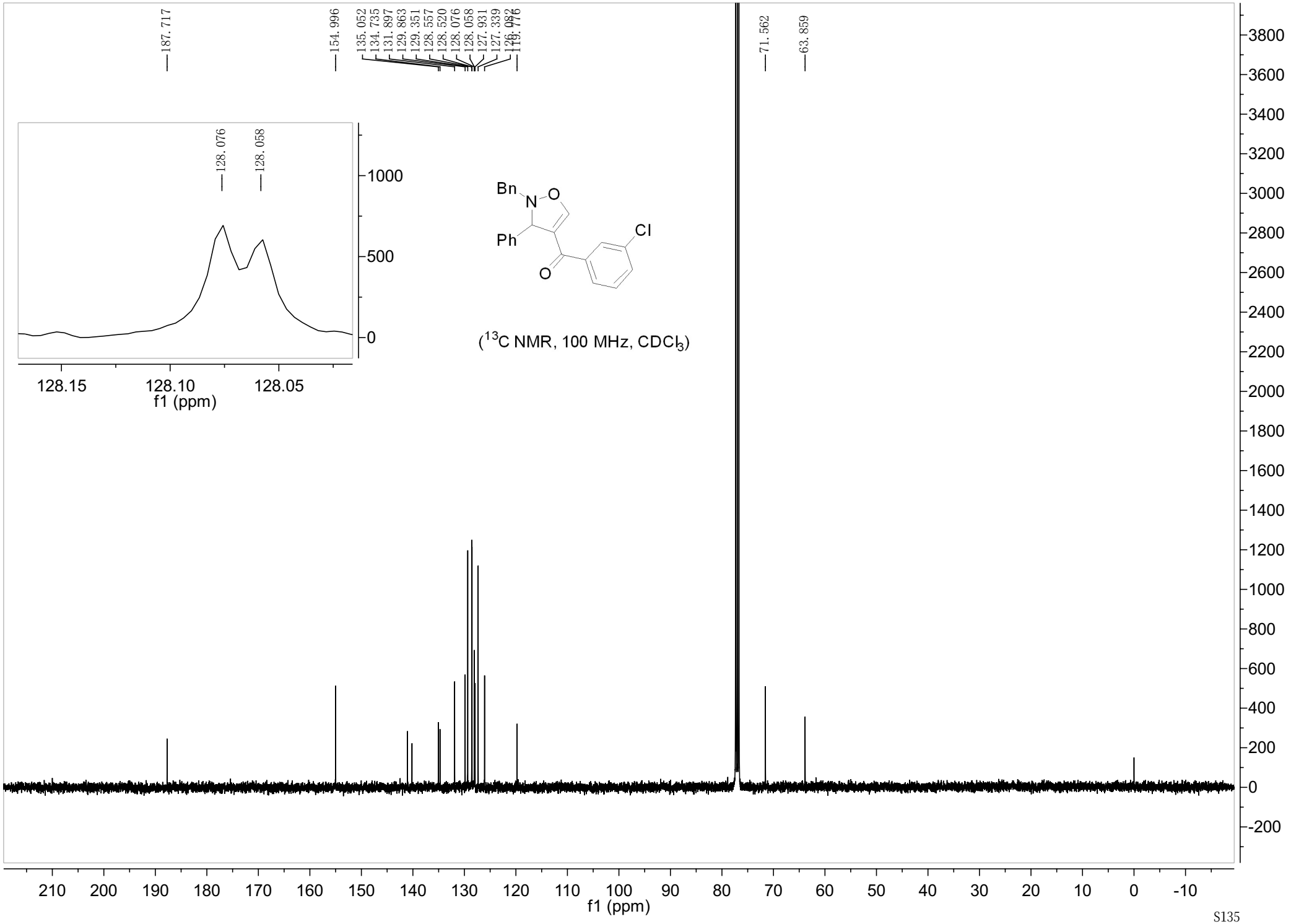

7.556
7.538
7.399
7.384
7.380
7.366
7.359
7.344
7.340
7.328
7.319
7.313
7.309
7.294
7.275
7.263
7.258
5.447
5.444
4.400
4.367
4.200
4.167
Bn
N
O
Ph
O
Br
(1H NMR, 400 MHz, CDCl3)
4.00
4.04
4.98
1.03
1.00
0.99
1.00
1.00
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

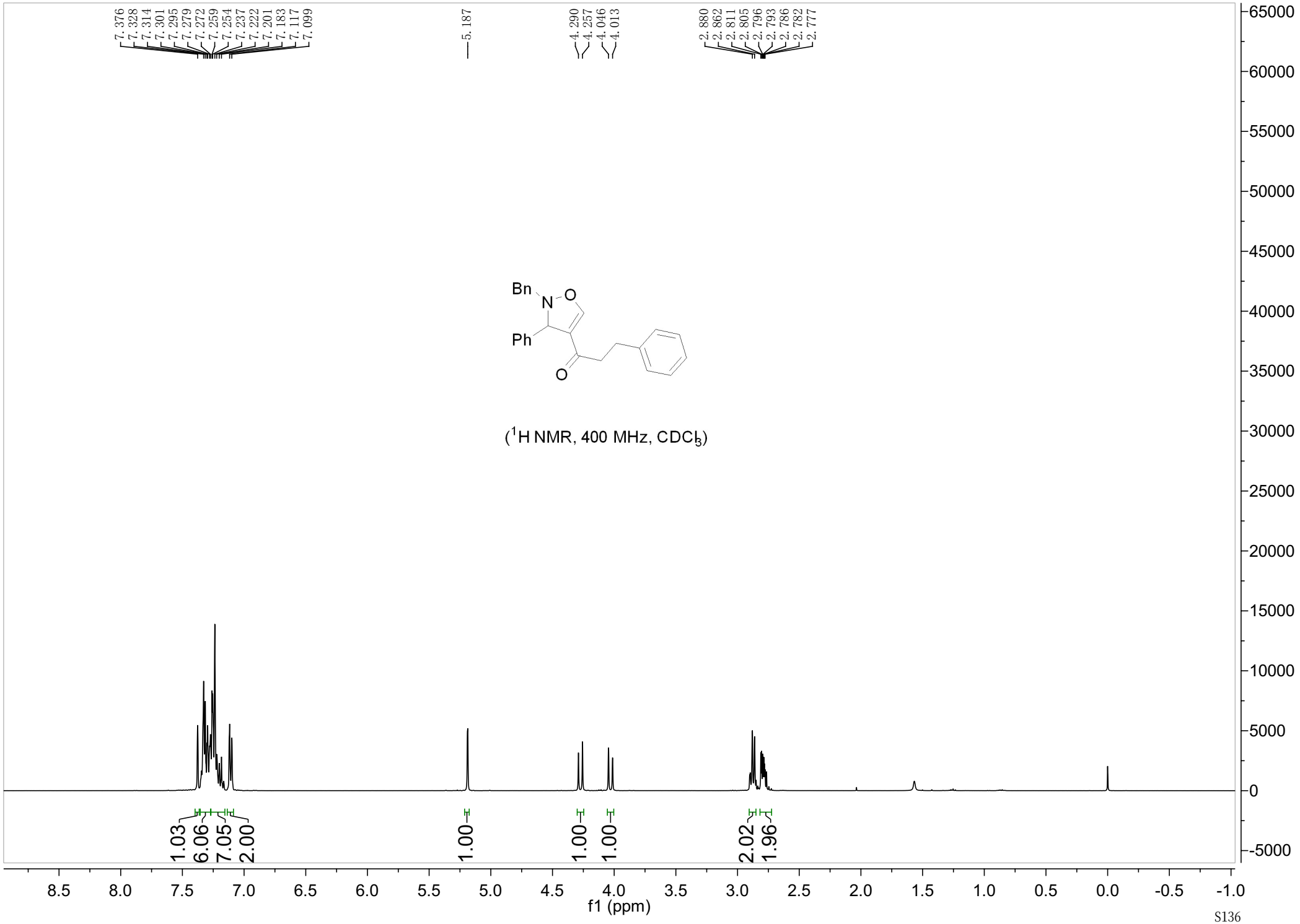

188.088
154.556
140.221
138.166
135.113
131.798
129.565
129.322
128.542
128.508
128.029
127.913
127.342
126.768
119.774
71.688
63.869
128.542
128.508
Bn
N
O
Ph
O
Br
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

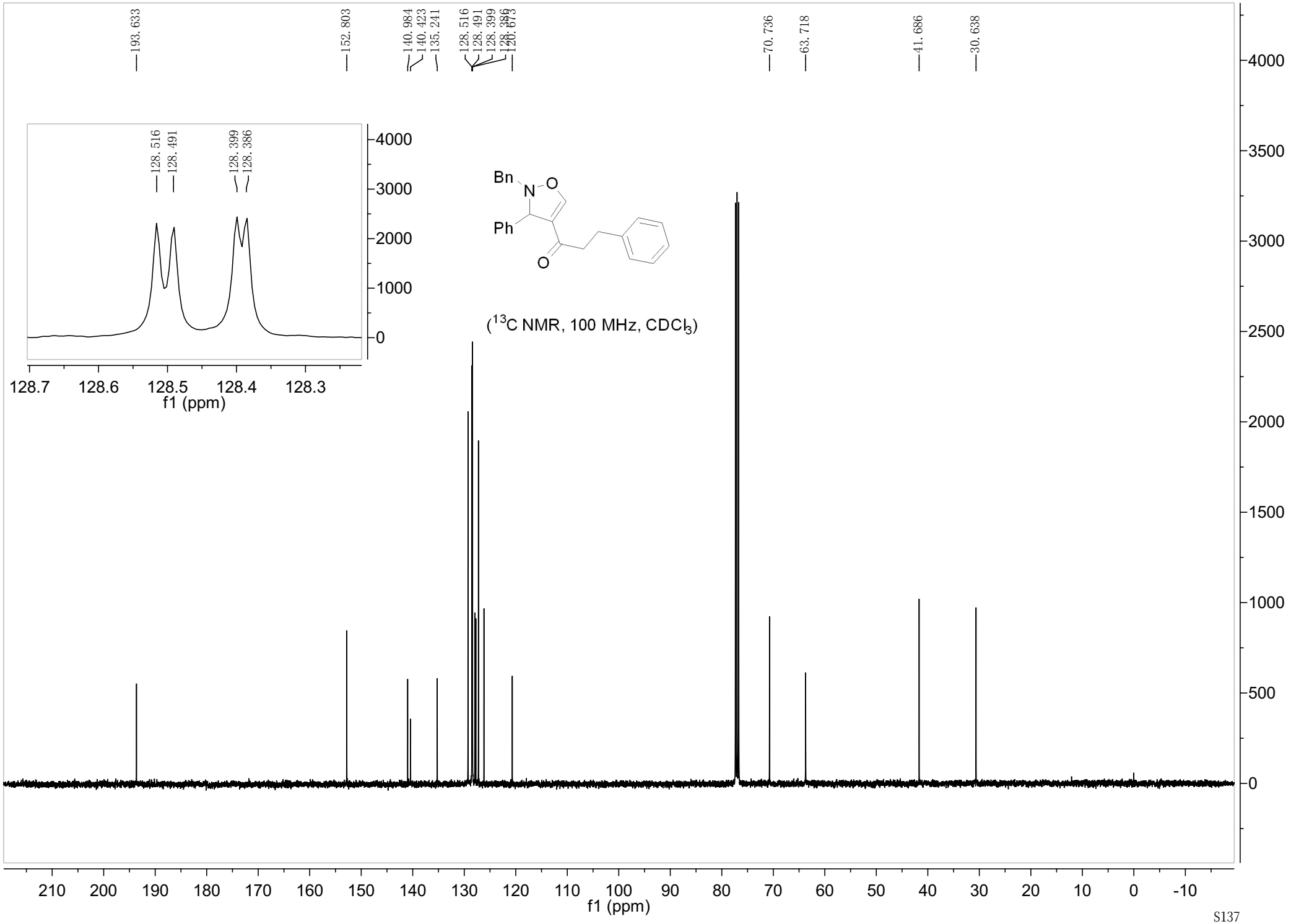

7.590
7.570
7.398
7.383
7.367
7.353
7.348
7.334
7.313
7.294
7.275
7.248
7.240
7.234
7.221
7.201
5.449
4.391
4.358
4.177
4.144
2.385
Bn
N
O
Ph
O
(1H NMR, 400 MHz, CDCl3)
2.00
4.00
6.04
3.05
1.00
1.00
1.00
3.00
f1 (ppm)

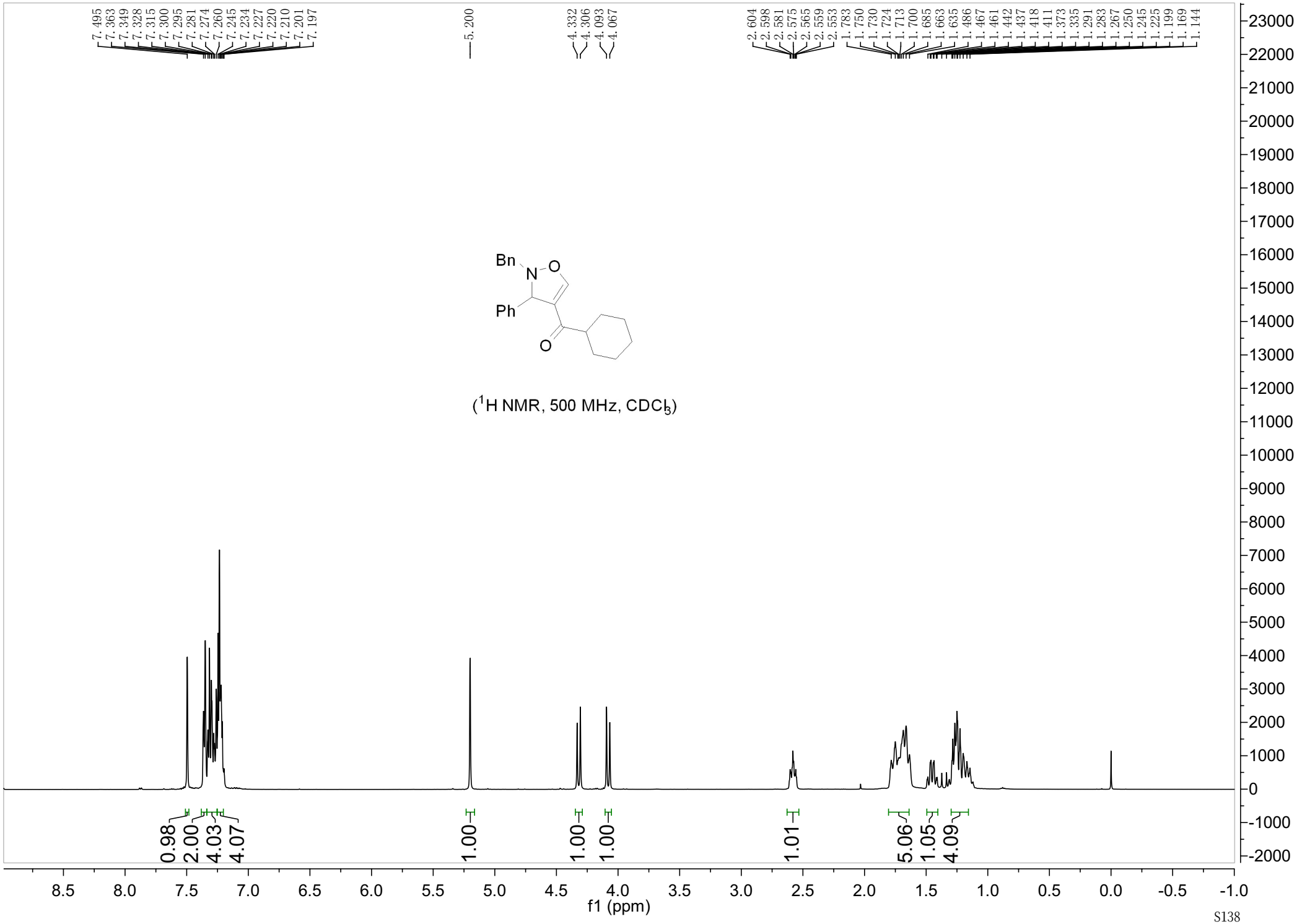

189.094
154.002
142.656
140.495
136.804
135.344
129.336
129.173
128.519
128.296
119.759
71.797
63.880
21.531
128.519
128.454
128.55
128.45
f1 (ppm)
Bn
N
O
Ph
O
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)

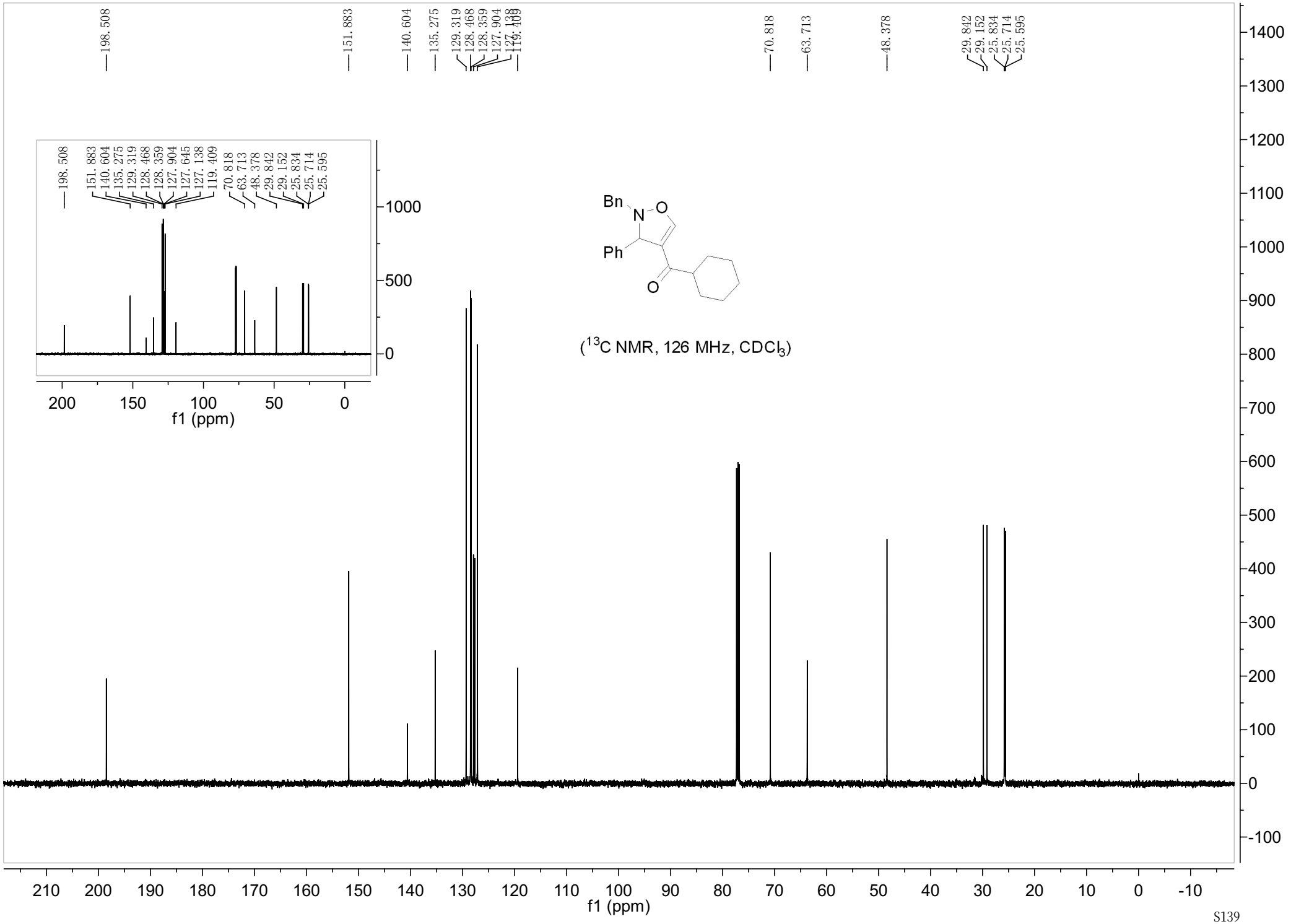

7.601
7.597
7.592
7.524
7.520
7.517
7.504
7.501
7.498
7.484
7.482
7.479
7.464
7.462
7.459
7.456
7.393
7.388
7.373
7.369
7.347
7.335
7.330
7.326
7.322
7.315
7.305
7.300
7.286
7.266
7.250
5.431
5.428
4.393
4.359
4.194
4.161
Bn
N
O
Ph
O
Cl
(1H NMR, 400 MHz, CDCl3)
0.93
1.97
2.99
8.06
1.10
1.00
1.00
1.00
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

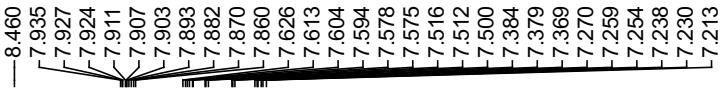

187.717
154.996
135.052
134.735
131.897
129.863
129.351
128.557
128.520
128.076
128.058
127.931
127.339
71.562
63.859
128.076
128.058
Bn
N
O
Ph
O
Cl
(^{13}C NMR, 100 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)

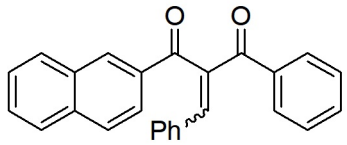

7.376
7.328
7.314
7.301
7.295
7.279
7.272
7.259
7.254
7.237
7.222
7.201
7.183
7.117
7.099
5.187
4.290
4.257
4.046
4.013
2.880
2.862
2.811
2.805
2.796
2.793
2.786
2.782
2.777
Bn
N
O
Ph
O
(1H NMR, 400 MHz, CDCl3)
1.03
6.06
7.05
2.00
1.00
1.00
1.00
2.02
1.96
f1 (ppm)


193.633
152.803
140.984
140.423
135.241
128.516
128.491
128.399
128.386
70.736
63.718
41.686
30.638
Bn
N
O
Ph
O
(^{13}C NMR, 100 MHz, CDCl$_3$)
f1 (ppm)

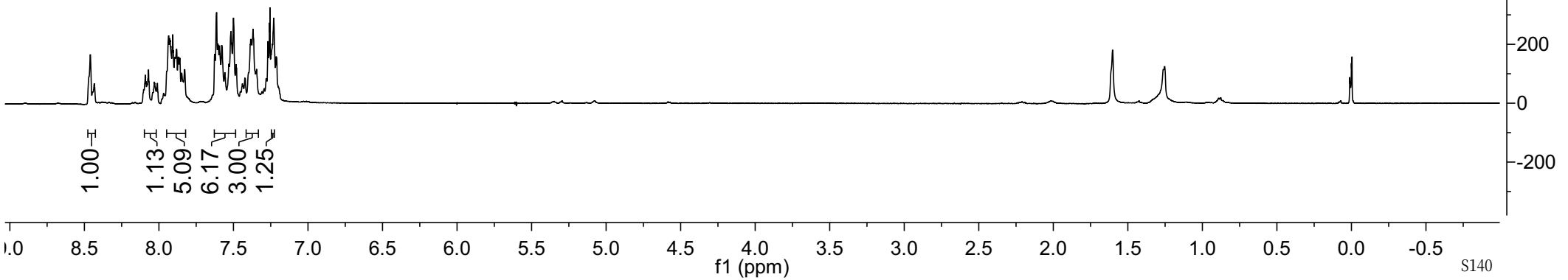

7.495
7.363
7.349
7.328
7.315
7.300
7.295
7.281
7.274
7.260
7.245
7.234
7.227
7.220
7.210
7.201
7.197
5.200
4.332
4.306
4.093
4.067
2.604
2.598
2.581
2.575
2.565
2.559
2.553
1.783
1.750
1.730
1.724
1.713
1.700
1.685
1.663
1.635
1.486
1.467
1.461
1.442
1.437
1.418
1.411
1.373
1.335
1.291
1.283
1.267
1.250
1.245
1.225
1.199
1.169
1.144
Bn
N
O
Ph
O
(1H NMR, 500 MHz, CDCl3)
0.98
2.00
4.03
4.07
1.00
1.00
1.00
1.01
5.06
1.05
4.09
f1 (ppm)

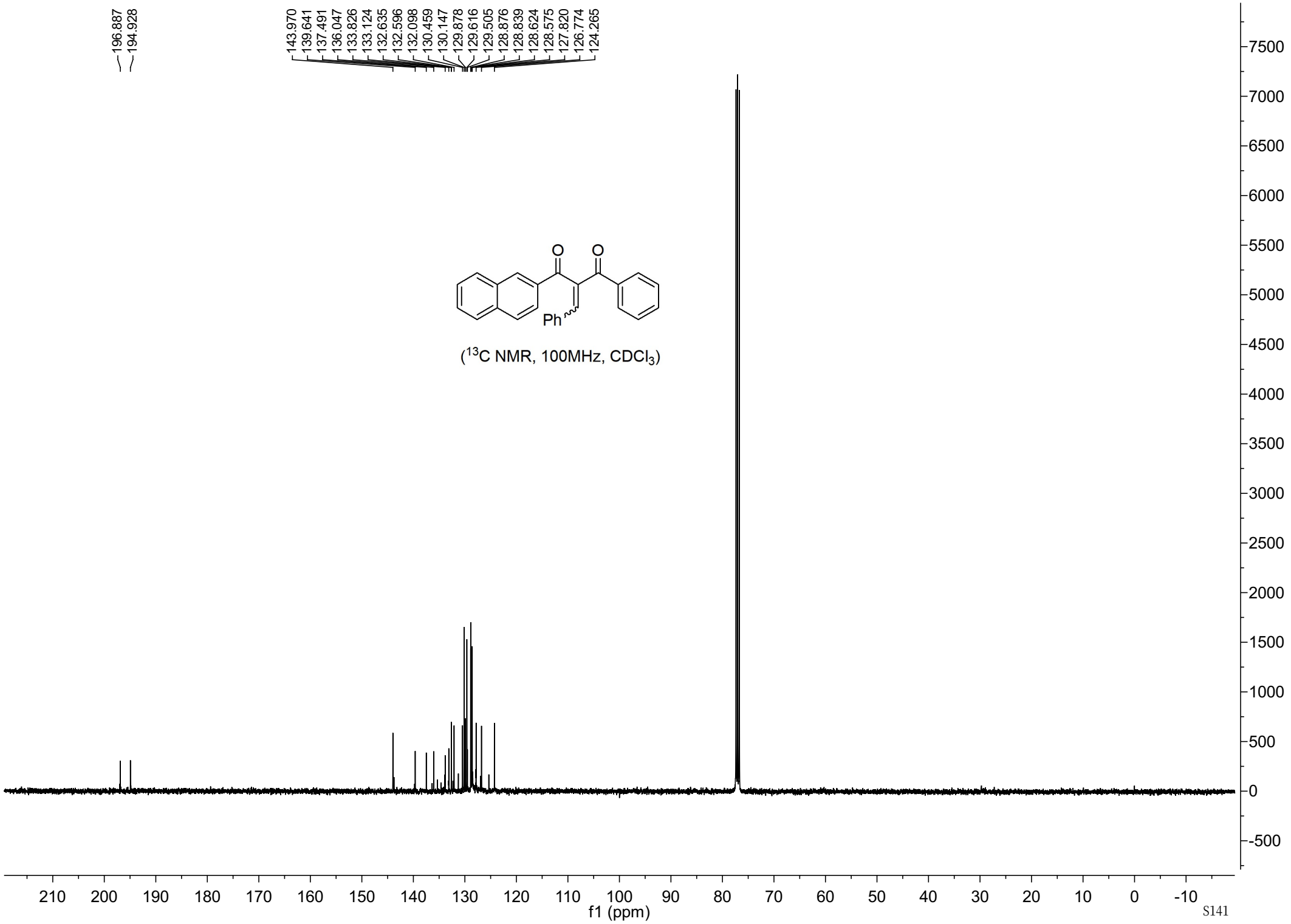

198.508
151.883
140.604
135.275
129.319
128.468
128.359
127.904
70.818
63.713
48.378
29.842
29.152
25.834
25.714
25.595
Bn
N
O
Ph
O
(^{13}C NMR, 126 MHz, $CDCl_3$)
f1 (ppm)





(^{1}H NMR, 400MHz, $CDCl_3$)




196.887
194.928
143.970
139.641
137.491
136.047
133.826
133.124
132.635
132.596
132.098
130.459
130.147
129.878
129.616
129.505
128.876
128.839
128.624
128.575
127.820
126.774
124.265
O
O
Ph
(13C NMR, 100MHz, CDCl3)
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)