Supporting Information

Peroxidation of 3,4-Dihydro-1,4-benzoxazin-2-ones

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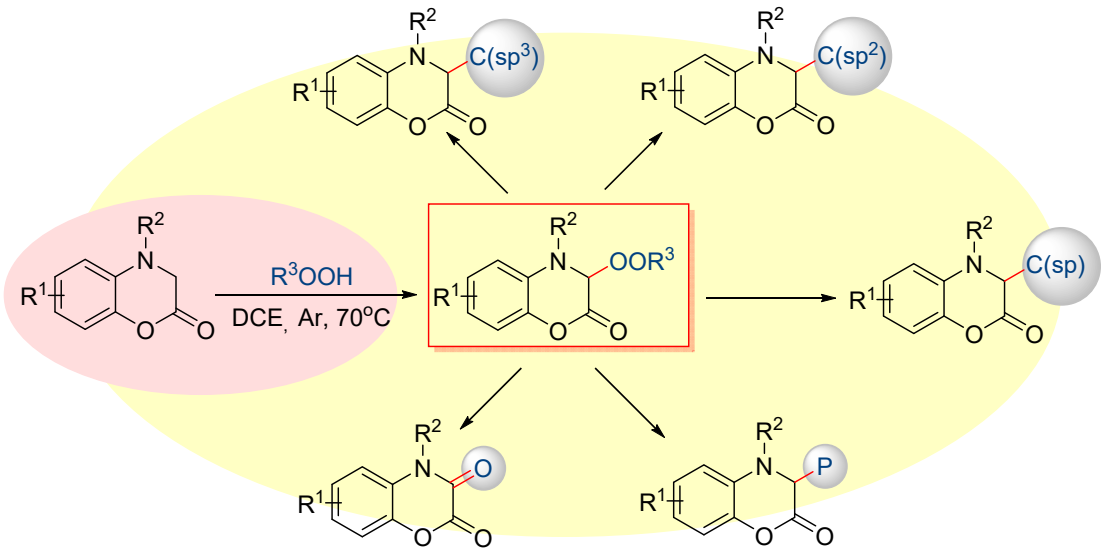

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General Information

The starting materials, reagents and solvents, were purchased from commercial suppliers and used without further purification. Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. Flash chromatography was carried out using silica gel (200−300 mesh). ^{1}H NMR (400 or 600 MHz) and ^{13}C NMR (150 MHz) spectra were measured with $CDCl_3$ as solvent. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. High resolution mass spectra (HR-MS) were recorded under electrospray ionization (ESI) conditions.

General procedure for peroxidation of 3,4-dihydro-1,4-benzoxazin-2-ones.

To a 10 mL reaction tube with a magnetic stirring bar, 3,4-dihydro-1,4-benzoxazin-2-one (**1**, 0.2 mmol) under argon atmosphere, TBHP (**2**, 0.4 mmol) and DCE (2 mL) were added successively. The resulting reaction mixture was performed at 70 ºC and completed within 3-8 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **3** (acetone/petroleum ether = 1:5 to 1:3).

Transformation from 3aa to 4

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), MeCN (2 mL), dimethyl malonate (0.6 mmol), $Fe(OTf)_2$ (10 mol %) were added successively. The resulting reaction mixture was performed at 60 ºC and completed within 4 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **5** (acetone/petroleum ether = 1:10).

Transformation from 3aa to 5

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), DCM (2 mL), cyclohexanone (0.4 mmol), $Fe(OTf)_2$ (10 mol %) were added successively. The resulting reaction mixture was performed at 70 ºC and completed within 3 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **5** (acetone/petroleum ether = 1:10).

Transformation from 3aa to 6

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol) and $Cu(OAc)_2$ (5 mol %) under argon atmosphere, DCE (1 mL) and 2-methyl-1,3-dioxolane (0.5 mL) were added successively. The resulting reaction mixture was performed at 60 ^oC and completed within 6 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **6** (acetone/petroleum ether = 1:10).

Transformation from 3aa to 7

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), MeCN (2 mL), N,N-dimethylaniline (0.4 mmol), HCl (10 mol %) were added successively. The resulting reaction mixture was performed at rt and completed within 6 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **7** (acetone/petroleum ether = 1:10).

Transformation from 3aa to 8

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), MeCN (2 mL), indole (0.4 mmol), $FeCl_2$ (10 mol %) were added successively. The resulting reaction mixture was performed at 60 ^oC and completed within 2 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **8** (acetone/petroleum ether = 1:10).

Transformation from 3aa to 9

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), DCM (2 mL), ethynylbenzene (0.4 mmol), CuBr (10 mol %) were added successively. The resulting reaction mixture was performed at 60 ^oC and completed within 8 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **9** (acetone/petroleum ether = 1:10).

Transformation from 3aa to 10

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), MeCN (2 mL), dimethyl phosphonate (0.4 mmol), $Cu(OAc)_2$ (10 mol %) were added successively. The resulting reaction mixture was performed at 70 °C and completed within 5 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **10** (acetone/petroleum ether = 1:10).

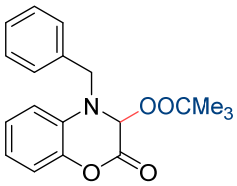
Transformation from 3aa to 11

To a 10 mL reaction tube with a magnetic stirring bar, **3aa** (0.2 mmol), $MeNO_2$ (1 mL), CuBr (10 mol %) were added successively. The resulting reaction mixture was performed at rt and completed within 9 hours as monitored by TLC. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **11** (acetone/petroleum ether = 1:10).

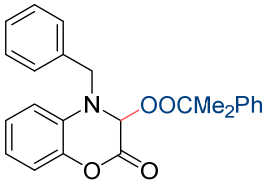
Gram-scale reaction

To a 50 mL reaction tube with a magnetic stirring bar, 3,4-dihydro-1,4-benzoxazin-2-one (**1a**, 5 mmol) under argon atmosphere, TBHP (**2**, 10 mmol) and DCE (30 mL) were added successively. The resulting reaction mixture was performed at 70 °C and completed overnight. After the reaction was completed, the reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography to afford the desired compounds **3aa** (acetone/petroleum ether = 1:5).

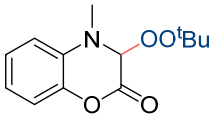
Characterization data for all compounds



4-benzyl-3-(tert-butylperoxy)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3aa) The desired pure product was obtained in 84% yield (55 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 5H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.04 – 7.01 (m, 1H), 6.91 – 6.88 (m, 1H), 6.84 (d, *J* = 8.1 Hz, 1H), 5.46 (s, 1H), 4.80 (d, *J* = 15.1 Hz, 1H), 4.59 (d, *J* = 15.1 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 141.2, 135.5, 131.3, 128.8, 127.9, 127.8, 124.9, 120.4, 116.3, 113.5, 86.8, 81.7, 52.3, 26.1. HRMS (ESI) exact mass calcd for $C_{19}H_{22}NO_4$ [M+H] m/z 328.1543, found 328.1548.

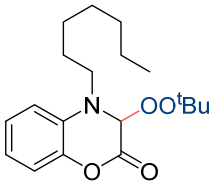


4-benzyl-3-((2-phenylpropan-2-yl)peroxy)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ab) The desired pure product was obtained in 81% yield (63 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 6H), 7.25 – 7.21 (m, 4H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.07 – 7.04 (m, 1H), 6.93 – 6.90 (m, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 5.42 (s, 1H), 4.67 (d, *J* = 15.2 Hz, 1H), 4.39 (d, *J* = 14.9 Hz, 1H), 1.46 (s, 3H), 1.44 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 144.1, 141.1, 135.3, 131.4, 128.9, 128.9, 128.0, 127.9, 127.8, 127.7, 127.3, 125.4, 124.9, 120.4, 116.5, 113.4, 86.5, 84.2, 51.9, 26.5, 26.1. HRMS (ESI) exact mass calcd for $C_{24}H_{24}NO_4$ [M+H] m/z 390.1700, found 390.1698.

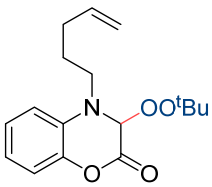


3-(tert-butylperoxy)-4-methyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ba) The desired pure product was obtained in 89% yield (45 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (t, *J* = 7.7 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.90 (t, *J* = 7.7 Hz, 1H), 6.83 (d, *J* =

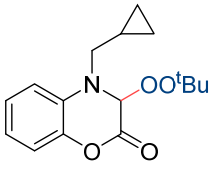
8.0 Hz, 1H), 5.46 (s, 1H), 3.14 (s, 3H), 1.07 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 141.0, 132.0, 125.0, 120.0, 116.0, 112.5, 88.7, 81.5, 36.0, 26.0. HRMS (ESI) exact mass calcd for $C_{13}H_{18}NO_4$ [M+H] m/z 252.1230, found 252.1235.



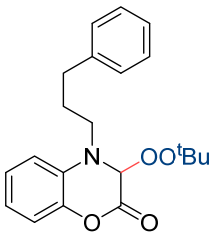
3-(tert-butylperoxy)-4-heptyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ca) The desired pure product was obtained in 75% yield (50 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.10 – 7.07 (m, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 6.88 – 6.85 (m, 2H), 5.49 (s, 1H), 3.59 – 3.54 (m, 1H), 3.39 – 3.34 (m, 1H), 1.76 – 1.68 (m, 3H), 1.35 – 1.27 (m, 7H), 1.07 (s, 9H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 141.1, 131.0, 124.8, 119.8, 116.4, 112.8, 87.4, 81.5, 48.8, 31.7, 29.0, 27.4, 26.9, 26.1, 22.5, 14.0. HRMS (ESI) exact mass calcd for $C_{19}H_{30}NO_4$ [M+H] m/z 336.2169, found 336.2167.



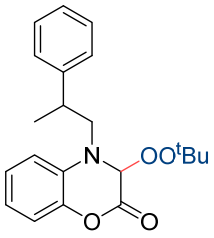
3-(tert-butylperoxy)-4-(pent-4-en-1-yl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3da) The desired pure product was obtained in 80% yield (49 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 – 7.05 (m, 2H), 6.90 – 6.85 (m, 2H), 5.86 – 5.74 (m, 1H), 5.48 (s, 1H), 5.10 – 5.01 (m, 2H), 3.66 – 3.58 (m, 1H), 3.43 – 3.35 (m, 1H), 2.13 (d, *J* = 6.8 Hz, 2H), 1.90 – 1.75 (m, 2H), 1.07 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 141.1, 137.3, 130.8, 124.8, 119.9, 116.4, 115.7, 112.8, 87.6, 81.5, 48.0, 30.9, 26.4, 26.1. HRMS (ESI) exact mass calcd for $C_{17}H_{24}NO_4$ [M+H] m/z 306.1700, found 306.1704.



3-(tert-butylperoxy)-4-(cyclopropylmethyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ea) The desired pure product was obtained in 87% yield (51 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 – 7.05 (m, 2H), 6.91 – 6.87 (m, 2H), 5.83 (s, 1H), 3.50 (dd, *J* = 13.4, 5.8 Hz, 1H), 3.17 (dd, *J* = 13.4, 7.6 Hz, 1H), 1.14 – 1.08 (m, 1H), 1.05 (s, 9H), 0.73 – 0.67 (m, 1H), 0.65 – 0.59 (m, 1H), 0.40 – 0.35 (m, 1H), 0.31 – 0.25 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.6, 141.1, 131.8, 124.8, 119.9, 116.2, 112.7, 85.5, 81.3, 52.4, 26.1, 8.5, 5.3, 3.3. HRMS (ESI) exact mass calcd for $C_{16}H_{22}NO_4$ [M+H] m/z 292.1543, found 292.1544.

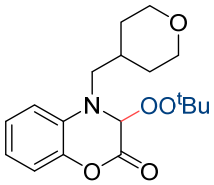


3-***(tert-butylperoxy)-4-(3-phenylpropyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3fa)*** The desired pure product was obtained in 84% yield (58 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 2H), 7.23 – 7.20 (m, 1H), 7.18 (d, *J* = 7.1 Hz, 2H), 7.08 – 7.04 (m, 2H), 6.89 – 6.86 (m, 1H), 6.77 (d, *J* = 8.2 Hz, 1H), 5.43 (s, 1H), 3.64 – 3.57 (m, 1H), 3.40 – 3.34 (m, 1H), 2.73 – 2.64 (m, 2H), 2.13 – 2.02 (m, 2H), 1.05 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.6, 138.5, 138.2, 128.2, 126.0, 125.8, 123.6, 122.3, 117.4, 113.9, 110.2, 85.0, 79.0, 45.4, 30.3, 26.0, 23.5. HRMS (ESI) exact mass calcd for $C_{21}H_{26}NO_4$ [M+H] m/z 356.1856, found 356.1860.

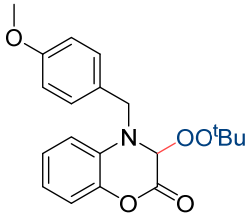


4-***(tert-butylperoxy)-4-(2-phenylpropyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ga, dr≈1.6)*** The desired pure product was obtained in 68% yield (48 mg) as a yellow liquid. Reaction time: 7 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.6 Hz, 1H), 7.30 – 7.20 (m, 5H), 7.11 (t, *J* = 7.7 Hz, 2H), 7.09 – 7.03 (m, 4H), 6.94 – 6.85 (m, 4H), 5.48 (s, 1H), 4.83 (s, 1H), 3.93 (d, *J* = 4.7 Hz, 1H), 3.91 (d, *J* = 4.7 Hz, 1H), 3.40 – 3.28 (m, 2H), 3.20 – 3.09 (m, 2H), 1.35 (d, *J* = 7.0 Hz, 3H), 1.30 (d, *J* = 6.8 Hz, 3H), 1.04 (s, 6H), 1.02 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 158.6, 143.6, 143.5, 141.2, 140.9,

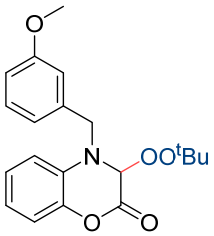
130.6, 130.4, 128.8, 128.7, 127.0, 126.9, 126.9, 126.8, 124.9, 124.9, 120.1, 119.8, 116.6, 116.6, 113.0, 112.6, 110.0, 88.3, 87.7, 81.6, 81.5, 56.1, 55.8, 37.6, 37.4, 26.0, 26.0, 19.1, 18.0. HRMS (ESI) exact mass calcd for $C_{21}H_{26}NO_4$ [M+H] m/z 356.1856, found 356.1859.



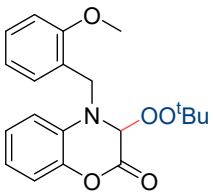
3-***(tert-butylperoxy)-4-((tetrahydro-2H-pyran-4-yl)methyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ha)*** The desired pure product was obtained in 82% yield (55 mg) as a yellow liquid. Reaction time: 7 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.11 – 7.04 (m, 2H), 6.90 – 6.84 (m, 2H), 5.42 (s, 1H), 3.99 – 3.93 (m, 2H), 3.63 (dd, *J* = 14.7, 5.1 Hz, 1H), 3.38 – 3.34 (m, 1H), 3.31 – 3.27 (m, 1H), 3.14 (dd, *J* = 14.7, 9.2 Hz, 1H), 1.99 – 1.93 (m, 1H), 1.68 – 1.62 (m, 2H), 1.37 – 1.27 (m, 2H), 1.05 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.0, 141.1, 130.8, 124.9, 120.1, 116.6, 112.8, 88.1, 81.6, 67.6, 67.4, 54.6, 33.4, 31.1, 30.6, 26.0. HRMS (ESI) exact mass calcd for $C_{18}H_{26}NO_5$ [M+H] m/z 336.1806, found 336.1803.



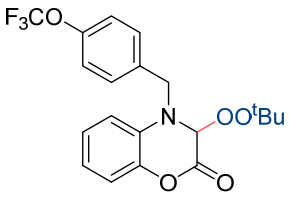
4-***(tert-butylperoxy)-4-(4-methoxybenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ia)*** The desired pure product was obtained in 85% yield (61 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 (d, *J* = 8.5 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 7.05 – 7.03 (m, 1H), 6.91 – 6.86 (m, 5H), 5.42 (s, 1H), 4.73 (d, *J* = 14.5 Hz, 1H), 4.50 (d, *J* = 14.5 Hz, 1H), 3.80 (s, 3H), 1.08 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4, 159.3, 141.2, 131.5, 129.3, 127.1, 124.9, 120.3, 116.3, 114.3, 113.5, 86.2, 81.6, 55.3, 51.6, 26.1. HRMS (ESI) exact mass calcd for $C_{20}H_{24}NO_5$ [M+H] m/z 358.1649, found 358.1648.



3-(tert-butylperoxy)-4-(3-methoxybenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ja) The desired pure product was obtained in 78% yield (56 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.04 – 7.01 (m, 1H), 6.92 – 6.88 (m, 2H), 6.86 (s, 1H), 6.84 – 6.81 (m, 2H), 5.47 (s, 1H), 4.76 (d, *J* = 15.1 Hz, 1H), 4.55 (d, *J* = 15.1 Hz, 1H), 3.77 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.1, 159.3, 141.2, 137.1, 131.3, 129.9, 124.9, 120.4, 120.0, 116.3, 113.5, 113.5, 113.1, 86.8, 81.7, 55.2, 52.3, 26.1. HRMS (ESI) exact mass calcd for $C_{20}H_{24}NO_5$ [M+H] m/z 358.1649, found 358.1651.



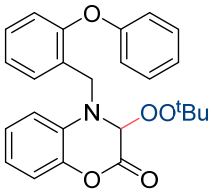
3-(tert-butylperoxy)-4-(2-methoxybenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ka) The desired pure product was obtained in 81% yield (58 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 (d, *J* = 6.3 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 7.03 – 7.00 (m, 1H), 6.90 – 6.83 (m, 5H), 5.60 (s, 1H), 4.81 (d, *J* = 15.8 Hz, 1H), 4.56 (d, *J* = 15.8 Hz, 1H), 3.84 (s, 3H), 1.10 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 157.5, 141.1, 131.1, 129.4, 129.0, 124.7, 123.8, 120.4, 119.8, 116.2, 113.4, 110.4, 87.6, 81.5, 55.3, 48.0, 26.1. HRMS (ESI) exact mass calcd for $C_{20}H_{24}NO_5$ [M+H] m/z 358.1649, found 358.1650.



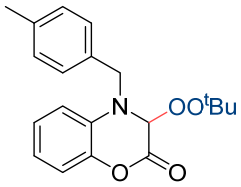
3-(tert-butylperoxy)-4-(4-(trifluoromethoxy)benzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one(3la)

The desired pure product was obtained in 68% yield (56 mg) as a yellow liquid. Reaction time: 7 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.0 Hz,

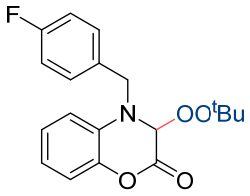
1H), 7.05 – 7.01 (m, 1H), 6.94 – 6.89 (m, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 5.46 (s, 1H), 4.79 (d, *J* = 15.5 Hz, 1H), 4.61 (d, *J* = 15.5 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 148.8, 141.2, 134.4, 131.0, 129.0, 125.0, 121.3, 120.7, 116.5, 113.5, 87.1, 81.8, 51.7, 26.1. HRMS (ESI) exact mass calcd for $C_{20}H_{21}N_3O5$ [M+H] m/z 412.1366, found 412.1362.



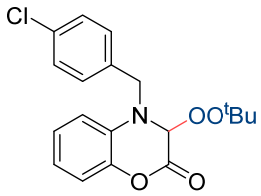
3-(tert-butylperoxy)-4-(2-phenoxybenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ma) The desired pure product was obtained in 67% yield (56 mg) as a yellow liquid. Reaction time: 7 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.4 Hz, 1H), 7.32 – 7.29 (m, 2H), 7.26 – 7.23 (m, 1H), 7.11 – 7.05 (m, 3H), 7.03 – 7.00 (m, 2H), 6.91 (d, *J* = 8.3 Hz, 3H), 6.88 – 6.84 (m, 2H), 5.55 (s, 1H), 4.87 (d, *J* = 15.8 Hz, 1H), 4.61 (d, *J* = 15.8 Hz, 1H), 1.06 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 157.0, 154.9, 141.0, 131.0, 130.0, 129.8, 129.2, 126.9, 124.8, 123.7, 123.3, 120.0, 119.3, 118.0, 116.3, 113.3, 87.3, 81.6, 47.6, 26.1. HRMS (ESI) exact mass calcd for $C_{25}H_{26}NO_5$ [M+H] m/z 420.1806, found 420.1805.



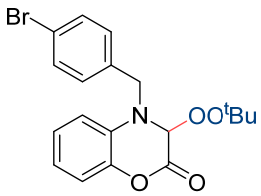
3-(tert-butylperoxy)-4-(4-methylbenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3na) The desired pure product was obtained in 88% yield (60 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.21 (d, *J* = 7.9 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.05 – 7.01 (m, 1H), 6.91 – 6.87 (m, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 5.44 (s, 1H), 4.75 (d, *J* = 14.8 Hz, 1H), 4.53 (d, *J* = 14.8 Hz, 1H), 2.34 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4, 141.2, 137.6, 132.3, 131.4, 129.5, 127.9, 124.9, 120.3, 116.3, 113.5, 86.5, 81.7, 52.0, 26.1, 21.1. HRMS (ESI) exact mass calcd for $C_{20}H_{24}NO_4$ [M+H] m/z 342.1700, found 342.1706.



3-(tert-butylperoxy)-4-(4-fluorobenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3oa) The desired pure product was obtained in 84% yield (58 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.05 – 7.01 (m, 3H), 6.92 – 6.89 (m, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 5.44 (s, 1H), 4.76 (d, *J* = 15.1 Hz, 1H), 4.56 (d, *J* = 15.1 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2, 161.5, 159.2, 141.2, 131.2, 131.2, 131.1, 129.4, 129.4, 124.9, 120.6, 116.4, 115.8, 115.7, 113.5, 86.8, 81.8, 51.7, 26.1. HRMS (ESI) exact mass calcd for $C_{19}H_{21}FNO_4$ [M+H] m/z 346.1449, found 346.1447.

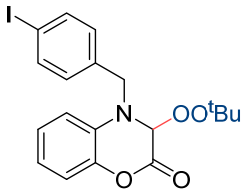


3-(tert-butylperoxy)-4-(4-chlorobenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3pa) The desired pure product was obtained in 88% yield (64 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.03 – 7.00 (m, 1H), 6.92 – 6.89 (m, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 5.45 (s, 1H), 4.75 (d, *J* = 15.5 Hz, 1H), 4.57 (d, *J* = 15.5 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 141.1, 134.2, 133.7, 131.0, 129.0, 129.0, 124.9, 120.6, 116.4, 113.6, 87.1, 81.8, 51.9, 26.1. HRMS (ESI) exact mass calcd for $C_{19}H_{21}ClNO_4$ [M+H] m/z 362.1154, found 362.1152.

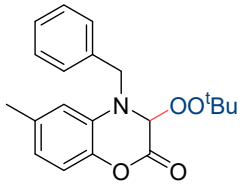


4-(4-bromobenzyl)-3-(tert-butylperoxy)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3qa) The desired pure product was obtained in 80% yield (65 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 8.3 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.03 – 7.00 (m, 1H), 6.92 – 6.89 (m, 1H), 6.75 (d, *J* = 8.0 Hz, 1H), 5.45 (s, 1H), 4.73 (d, *J* = 15.5 Hz, 1H),

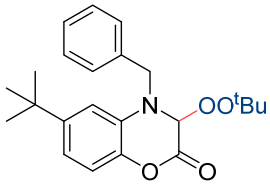
4.55 (d, J = 15.5 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 141.1, 134.7, 132.0, 129.3, 124.9, 121.7, 120.7, 116.4, 113.6, 87.1, 81.8, 52.0, 26.1. HRMS (ESI) exact mass calcd for $C_{19}H_{21}BrNO_4$ [M+H] m/z 406.0649, found 406.0641.



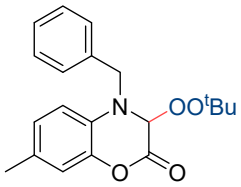
3-(tert-butylperoxy)-4-(4-iodobenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ra) The desired pure product was obtained in 75% yield (68 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, J = 8.2 Hz, 2H), 7.09 – 7.06 (m, 3H), 7.01 (t, J = 7.7 Hz, 1H), 6.90 (t, J = 7.7 Hz, 1H), 6.74 (d, J = 8.0 Hz, 1H), 5.45 (s, 1H), 4.72 (d, J = 15.6 Hz, 1H), 4.54 (d, J = 15.6 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 141.1, 137.9, 135.4, 130.9, 129.5, 124.9, 120.7, 116.4, 113.6, 93.2, 87.1, 81.8, 52.1, 26.1. HRMS (ESI) exact mass calcd for $C_{19}H_{21}INO_4$ [M+H] m/z 454.0510, found 454.0504.



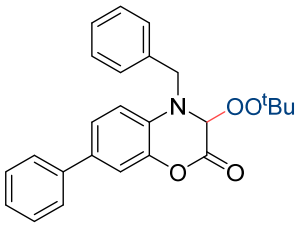
5-benzyl-3-(tert-butylperoxy)-6-methyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one(3sa) The desired pure product was obtained in 81% yield (55 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 5H), 6.96 (d, J = 8.1 Hz, 1H), 6.70 (d, J = 8.2 Hz, 1H), 6.67 (s, 1H), 5.42 (s, 1H), 4.79 (d, J = 14.9 Hz, 1H), 4.56 (d, J = 14.9 Hz, 1H), 2.26 (s, 3H), 1.10 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4, 139.1, 135.6, 134.7, 130.9, 128.8, 127.9, 127.9, 120.9, 116.0, 114.1, 86.7, 81.8, 52.1, 26.1, 21.3. HRMS (ESI) exact mass calcd for $C_{20}H_{24}NO_4$ [M+H] m/z 342.1700, found 342.1699.



5-***benzyl-6-(tert-butyl)-3-(tert-butylperoxy)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ta)*** The desired pure product was obtained in 80% yield (61 mg) as a yellow liquid. Reaction time: 7 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (d, *J* = 4.4 Hz, 4H), 7.30 – 7.26 (m, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.82 (s, 1H), 5.48 (s, 1H), 4.81 (d, *J* = 14.9 Hz, 1H), 4.59 (d, *J* = 14.9 Hz, 1H), 1.20 (s, 9H), 1.10 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4, 148.0, 139.0, 135.7, 130.3, 128.8, 127.9, 127.8, 117.2, 115.6, 111.3, 87.2, 81.8, 52.6, 34.6, 31.3, 26.1. HRMS (ESI) exact mass calcd for $C_{23}H_{30}NO_4$ [M+H] m/z 384.2169, found 384.2174.

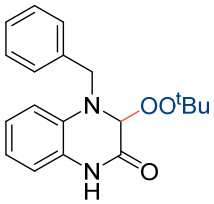


4-benzyl-3-(tert-butylperoxy)-7-methyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3ua) The desired pure product was obtained in 85% yield (58 mg) as a yellow liquid. Reaction time: 8 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 5H), 6.90 (s, 1H), 6.82 (d, *J* = 8.2 Hz, 1H), 6.71 (d, *J* = 8.2 Hz, 1H), 5.45 (s, 1H), 4.77 (d, *J* = 15.1 Hz, 1H), 4.57 (d, *J* = 15.1 Hz, 1H), 2.28 (s, 3H), 1.10 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4, 140.9, 135.7, 130.3, 128.8, 128.7, 127.8, 127.7, 125.3, 116.9, 113.4, 87.1, 81.7, 52.4, 26.1, 20.5. HRMS (ESI) exact mass calcd for $C_{20}H_{24}NO_4$ [M+H] m/z 342.1700, found 342.1696.

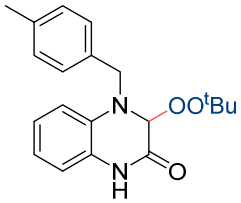


4-benzyl-3-(tert-butylperoxy)-7-phenyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (3va) The desired pure product was obtained in 69% yield (56 mg) as a yellow liquid. Reaction time: 7 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 – 7.35 (m, 8H), 7.33 – 7.30 (m, 2H), 7.15 – 7.10 (m, 2H), 7.05 (d, *J* = 1.8 Hz, 1H), 5.49 (s, 1H), 4.87 (d, *J* = 14.9 Hz, 1H), 4.63 (d, *J* = 14.9 Hz, 1H), 1.11 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 140.7, 140.6, 138.2, 135.4, 131.5, 128.9, 128.7, 128.0, 127.9, 127.3, 127.0, 119.2, 116.6, 112.5, 86.7, 81.8, 52.4, 26.1. HRMS (ESI) exact mass calcd for $C_{25}H_{26}NO_4$ [M+H] m/z

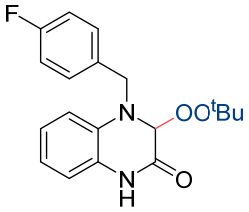
404.1856, found 404.1859.



4-benzyl-3-(tert-butylperoxy)-3,4-dihydroquinoxalin-2(1H)-one (3wa) The desired pure product was obtained in 78% yield (51 mg) as a yellow liquid. Reaction time: 3 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.80 (s, 1H), 7.32 (d, *J* = 4.3 Hz, 4H), 7.28 – 7.26 (m, 1H), 6.96 – 6.91 (m, 2H), 6.84 – 6.79 (m, 2H), 5.47 (s, 1H), 4.89 (d, *J* = 15.4 Hz, 1H), 4.70 (d, *J* = 15.4 Hz, 1H), 1.12 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.3, 136.4, 132.1, 128.7, 127.7, 127.5, 125.2, 123.9, 119.7, 115.6, 113.3, 89.9, 81.2, 52.9, 26.3. HRMS (ESI) exact mass calcd for $C_{19}H_{23}N_2O_3$ [M+H] m/z 327.1703, found 327.1704.

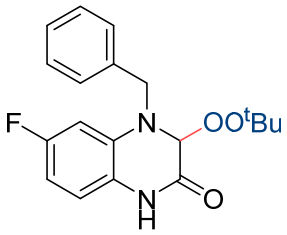


3-***(tert-butylperoxy)-4-(4-methylbenzyl)-3,4-dihydroquinoxalin-2(1H)-one (3xa)*** The desired pure product was obtained in 80% yield (58 mg) as a yellow liquid. Reaction time: 3 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.69 (s, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 2H), 6.96 – 6.93 (m, 1H), 6.90 (dd, *J* = 8.1, 1.4 Hz, 1H), 6.83 – 6.81 (m, 2H), 5.45 (s, 1H), 4.84 (d, *J* = 15.1 Hz, 1H), 4.64 (d, *J* = 15.1 Hz, 1H), 2.32 (s, 3H), 1.12 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.3, 137.2, 133.2, 132.2, 129.4, 127.7, 125.2, 123.9, 119.6, 115.6, 113.3, 89.6, 81.2, 52.6, 26.3, 21.1. HRMS (ESI) exact mass calcd for $C_{20}H_{25}N_2O_3$ [M+H] m/z 341.1860, found 341.1860.

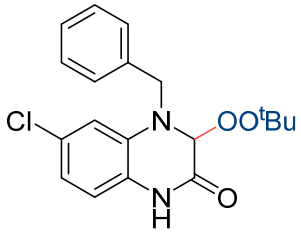


3-(tert-butylperoxy)-4-(4-fluorobenzyl)-3,4-dihydroquinoxalin-2(1H)-one (3ya) The desired pure product was obtained in 82% yield (57 mg) as a yellow liquid. Reaction time: 3 hours. ^{1}H NMR (600

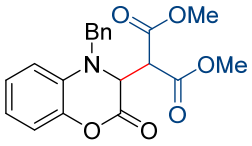
MHz, $CDCl_3$) δ 10.05 (s, 1H), 7.30 – 7.28 (m, 2H), 7.02 – 6.98 (m, 2H), 6.97 – 6.93 (m, 2H), 6.85 – 6.82 (m, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 5.44 (s, 1H), 4.85 (d, *J* = 15.4 Hz, 1H), 4.66 (d, *J* = 15.4 Hz, 1H), 1.12 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.0, 161.4, 161.4, 132.1, 132.1, 131.9, 129.3, 129.3 125.3, 123.9, 119.9, 115.8, 115.7, 115.5, 113.2, 89.8, 81.3, 52.3, 26.3. HRMS (ESI) exact mass calcd for $C_{19}H_{22}FN_2O_3$ [M+H] m/z 345.1609, found 345.1611.



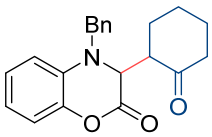
4-benzyl-3-(tert-butylperoxy)-6-fluoro-3,4-dihydroquinoxalin-2(1H)-one (3za) The desired pure product was obtained in 70% yield (48 mg) as a yellow liquid. Reaction time: 3 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.63 (s, 1H), 7.33 – 7.26 (m, 5H), 6.70 – 6.63 (m, 3H), 5.43 (s, 1H), 4.83 (d, *J* = 15.4 Hz, 1H), 4.67 (d, *J* = 15.4 Hz, 1H), 1.13 (s, 9H).^{13}C NMR (151 MHz, $CDCl_3$) δ 161.6, 136.1, 128.8, 127.7, 127.6, 113.9, 113.9,109.9,109.8, 103.2, 103.0, 89.8, 81.4, 53.3, 26.2. HRMS (ESI) exact mass calcd for $C_{19}H_{22}FN_2O_3$ [M+H] m/z 345.1609, found 345.1610.



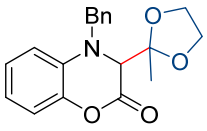
4-benzyl-3-(tert-butylperoxy)-6-chloro-3,4-dihydroquinoxalin-2(1H)-one (3z'a) The desired pure product was obtained in 76% yield (55 mg) as a yellow liquid. Reaction time: 3 hours. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.35 – 7.28 (m, 5H), 6.83 – 6.78 (m, 3H), 5.39 (s, 1H), 4.81 (d, *J* = 15.1 Hz, 1H), 4.65 (d, *J* = 15.1 Hz, 1H), 1.12 (s, 9H).^{13}C NMR (151 MHz, $CDCl_3$) δ 161.2, 135.5, 133.4, 129.1, 128.8, 127.9, 127.8, 124.0, 119.5, 116.3, 113.3, 88.9, 81.4, 52.7, 26.2. HRMS (ESI) exact mass calcd for $C_{19}H_{22}ClN_2O_3$ [M+H] m/z 361.1314, found 361.1308.



dimethyl 2-(4-benzyl-2-oxo-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)malonate (4) The desired pure product was obtained in 88% yield (65 mg) as a white solid, mp 95-96 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 3H), 7.19 (d, *J* = 7.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 1H), 7.02 – 6.99 (m, 1H), 6.90 – 6.86 (m, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 4.88 (d, *J* = 6.5 Hz, 1H), 4.59 (d, *J* = 15.6 Hz, 1H), 4.46 (d, *J* = 15.6 Hz, 1H), 3.70 (d, *J* = 6.5 Hz, 1H), 3.64 (s, 3H), 3.62 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.5, 166.4, 163.1, 142.0, 136.1, 131.2, 128.8, 127.9, 127.4, 125.3, 120.9, 116.7, 116.1, 59.8, 54.6, 53.0, 53.0, 52.9. HRMS (ESI) exact mass calcd for $C_{20}H_{20}NO_6$ [M+H] m/z 370.1285, found 370.1288.

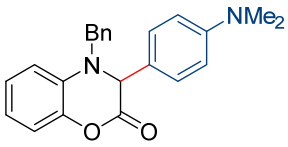


4-benzyl-3-(2-oxocyclohexyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (5) The desired pure product was obtained in 75% yield (50 mg) as a white solid, mp 129-131 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 2H), 7.25 – 7.20 (m, 3H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.02 – 6.99 (m, 1H), 6.89 – 6.85 (m, 1H), 6.79 (d, *J* = 8.1 Hz, 1H), 4.65 (d, *J* = 8.0 Hz, 1H), 4.55 (d, *J* = 15.4 Hz, 1H), 4.50 (d, *J* = 15.4 Hz, 1H), 2.51 – 2.45 (m, 1H), 2.43 – 2.39 (m, 1H), 2.27 – 2.21 (m, 1H), 2.03 – 1.99 (m, 1H), 1.89 – 1.82 (m, 2H), 1.65 – 1.60 (m, 1H), 1.57 – 1.52 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 209.3, 163.4, 142.5, 137.0, 132.1, 128.7, 127.6, 127.5, 125.1, 120.4, 116.7, 116.6, 59.0, 54.9, 50.1, 42.2, 31.2, 27.9, 24.6. HRMS (ESI) exact mass calcd for $C_{21}H_{22}NO_3$ [M+H] m/z 336.1594, found 336.1599.

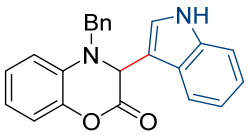


4-benzyl-3-(2-methyl-1,3-dioxolan-2-yl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (6) The desired pure product was obtained in 81% yield (53 mg) as a white liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 5H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.08 – 7.05 (m, 1H), 6.95 – 6.92 (m, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 4.91 (s, 1H), 4.76 (d, *J* = 14.6 Hz, 1H), 4.46 (d, *J* = 14.6 Hz, 1H), 4.17 – 4.13 (m, 1H), 4.10 – 4.06 (m, 1H), 3.76 – 3.71 (m, 1H), 3.69 – 3.65 (m, 1H), 2.02 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.7,

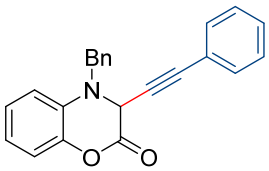
159.8, 140.8, 135.2, 130.7, 129.0, 128.1, 128.0, 125.2, 120.9, 116.6, 114.0, 84.2, 66.6, 63.0, 52.0, 20.8. HRMS (ESI) exact mass calcd for $C_{19}H_{20}NO_4$ [M+H] m/z 326.1387, found 326.1383.



4-benzyl-3-(4-(dimethylamino)phenyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (7) The desired pure product was obtained in 73% yield (52 mg) as a yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 5H), 7.07 (d, *J* = 7.9 Hz, 1H), 7.04 – 7.01 (m, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.86 – 6.82 (m, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 6.57 (d, *J* = 8.8 Hz, 2H), 4.98 (s, 1H), 4.61 (d, *J* = 15.0 Hz, 1H), 4.08 (d, *J* = 14.9 Hz, 1H), 2.90 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.2, 150.7, 141.2, 136.0, 133.7, 128.8, 128.3, 127.7, 127.7, 125.4, 121.7, 119.3, 116.6, 113.2, 112.4, 62.3, 51.3, 40.2. HRMS (ESI) exact mass calcd for $C_{23}H_{23}N_2O_2$ [M+H] m/z 359.1754, found 359.1753.

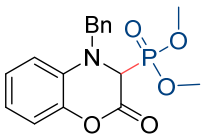


4-benzyl-3-(1H-indol-3-yl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (8) The desired pure product was obtained in 80% yield (57 mg) as a yellow solid, mp 64-66 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.27 (m, 6H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.14 – 7.09 (m, 2H), 7.08 – 7.04 (m, 1H), 6.92 – 6.88 (m, 1H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.73 (s, 1H), 5.40 (s, 1H), 4.61 (d, *J* = 14.8 Hz, 1H), 4.15 (d, *J* = 14.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.5, 141.9, 136.1, 135.8, 134.2, 128.8, 127.8, 127.8, 126.1, 125.4, 122.8, 120.5, 119.9, 119.2, 116.6, 113.9, 111.3, 108.8, 55.9, 51.6. HRMS (ESI) exact mass calcd for $C_{23}H_{19}N_2O_2$ [M+H] m/z 355.1441, found 355.1433.

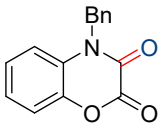


4-benzyl-3-(phenylethynyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (9) The desired pure product was obtained in 67% yield (49 mg) as a yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 – 7.33 (m,

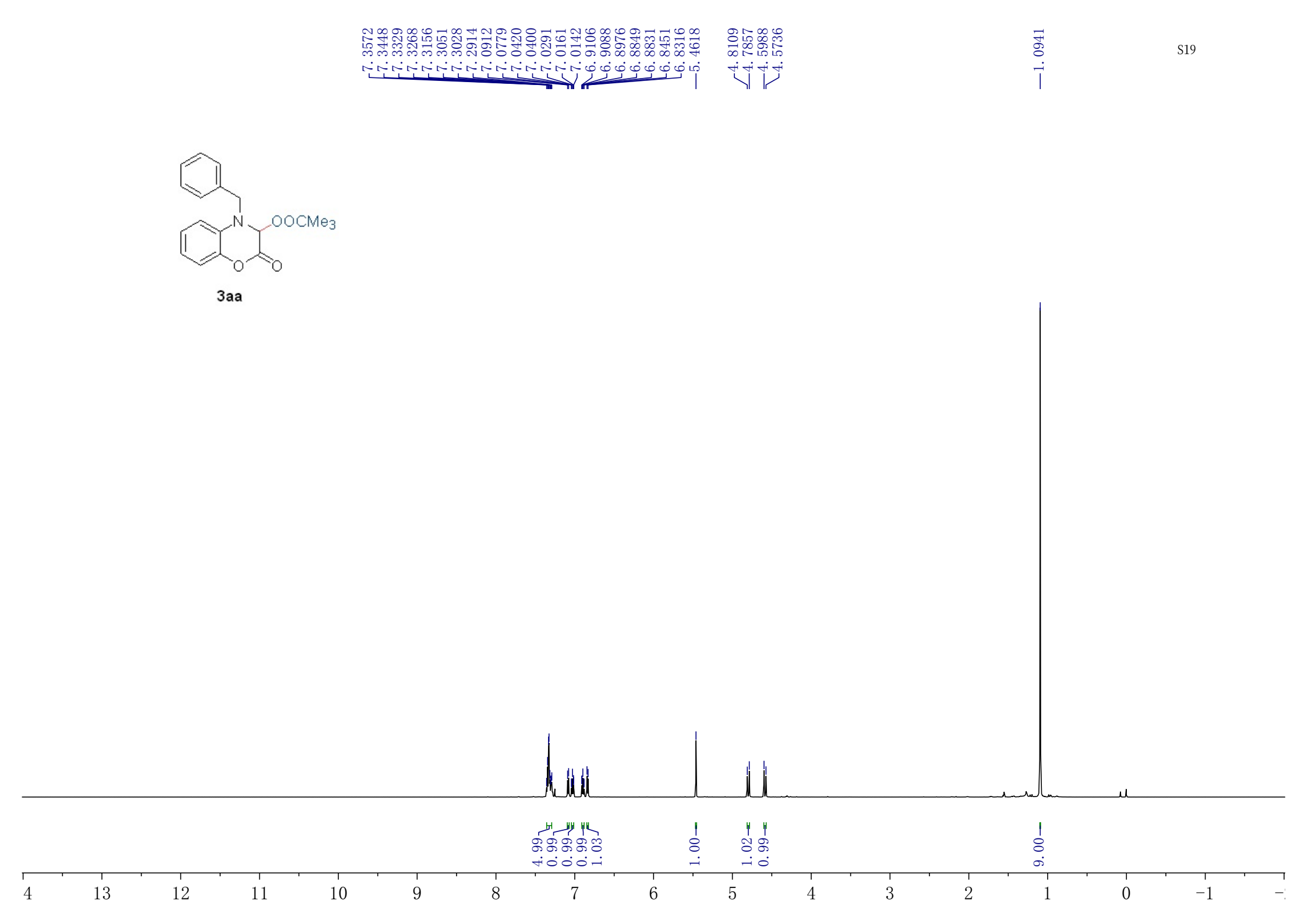
6H), 7.32 – 7.28 (m, 1H), 7.26 – 7.24 (m, 3H), 7.17 – 7.11 (m, 2H), 7.00 – 6.94 (m, 2H), 4.80 (s, 1H), 4.70 (d, *J* = 13.5 Hz, 1H), 4.14 (d, *J* = 13.5 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.4, 142.2, 135.0, 133.7, 132.0, 129.0, 129.0, 128.6, 128.2, 125.3, 121.3, 121.2, 116.7, 114.7, 87.3, 78.9, 51.7, 51.2. HRMS (ESI) exact mass calcd for $C_{23}H_{18}NO_2$ [M+H] m/z 340.1332, found 340.1329.



dimethyl (4-benzyl-2-oxo-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)phosphonate (10) The desired pure product was obtained in 81% yield (56 mg) as a white solid, mp 123-124 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 5H), 7.09 – 7.06 (m, 2H), 6.94 – 6.88 (m, 2H), 4.73 (d, *J* = 14.0 Hz, 1H), 4.48 (dd, *J* = 14.0, 4.2 Hz, 1H), 4.41 (d, *J* = 15.7 Hz, 1H), 3.67 (d, *J* = 11.0 Hz, 3H), 3.28 (d, *J* = 11.0 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.9, 161.8, 142.2, 135.0, 133.09, 129.0, 128.5, 128.2, 125.5, 120.6, 116.5, 114.2, 114.2, 57.9, 57.0, 53.3, 53.3, 53.1, 53.0, 52.5. HRMS (ESI) exact mass calcd for $C_{17}H_{19}NO_5P$ [M+H] m/z 348.0995, found 348.1001.



4-benzyl-2H-benzo[b][1,4]oxazine-2,3(4H)-dione (11) The desired pure product was obtained in 81% yield (42 mg) as a yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 – 7.28 (m, 5H), 7.22 – 7.18 (m, 1H), 7.11 – 7.05 (m, 2H), 6.85 – 6.80 (m, 1H), 5.00 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.7, 142.7, 134.7, 130.8, 129.0, 128.3, 127.6, 123.8, 122.5, 110.0, 110.0, 108.9, 46.1. HRMS (ESI) exact mass calcd for $C_{15}H_{12}NO_3$ [M+H] m/z 254.0812, found 254.0815.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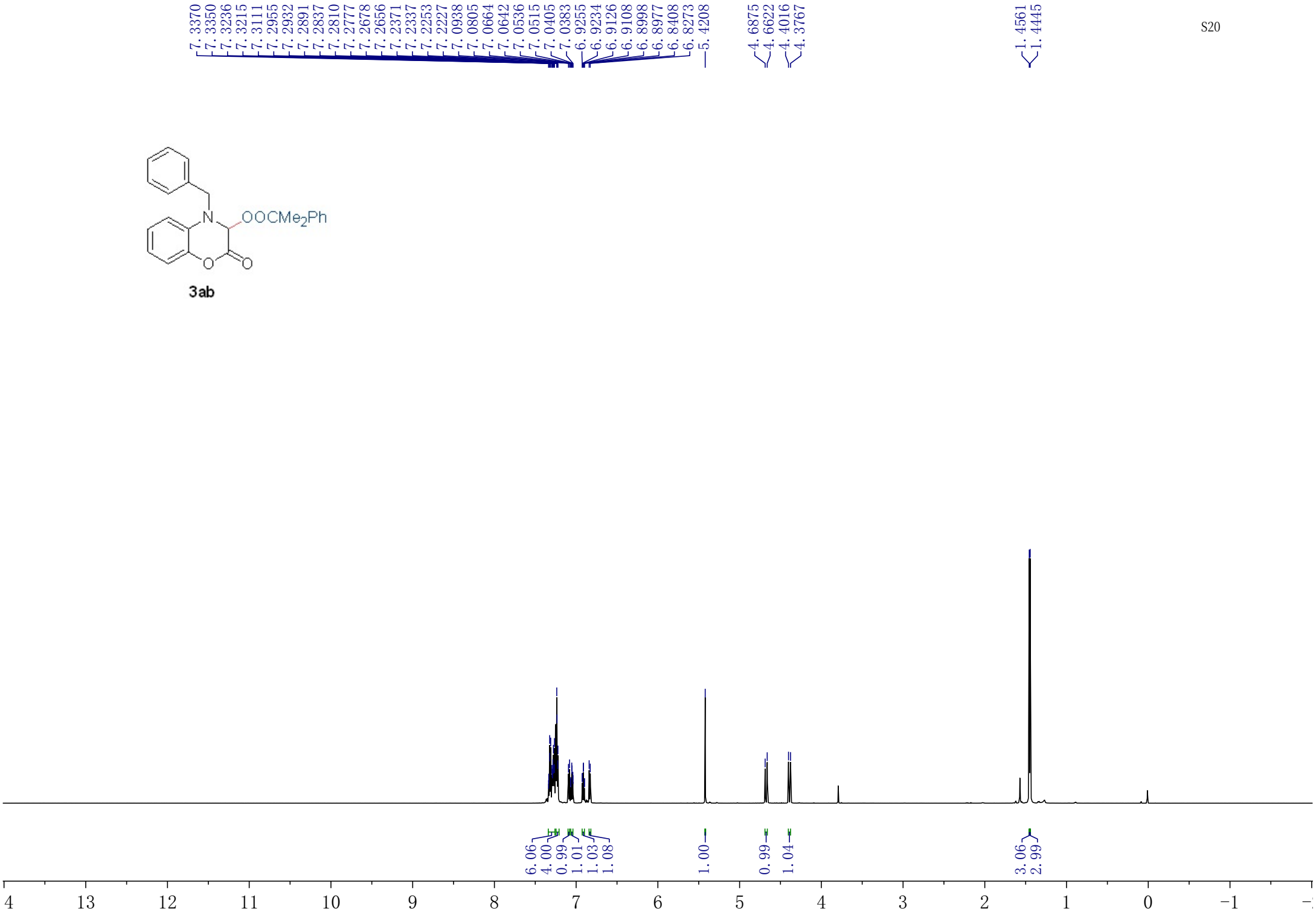
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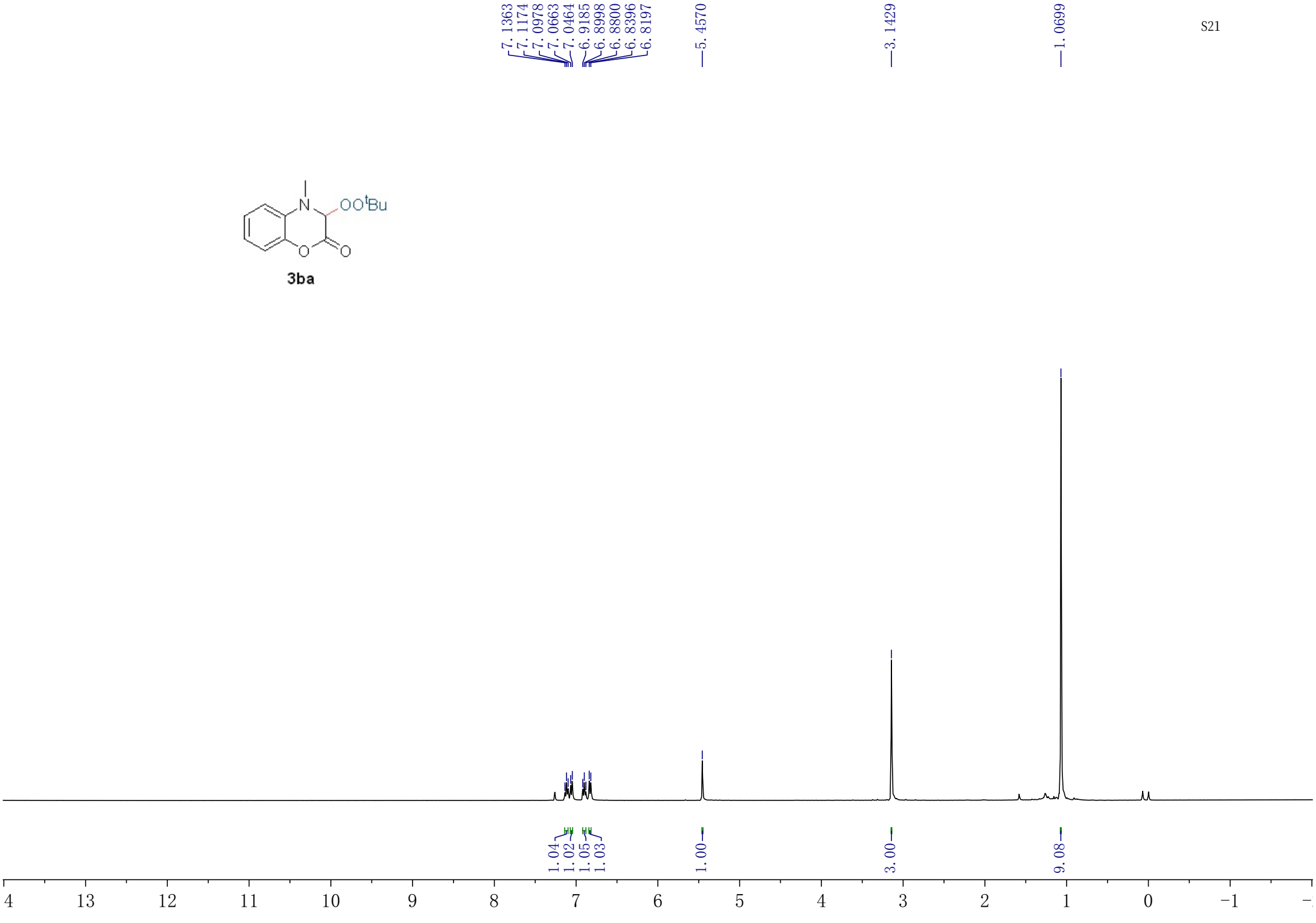
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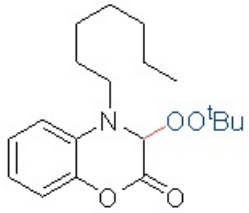
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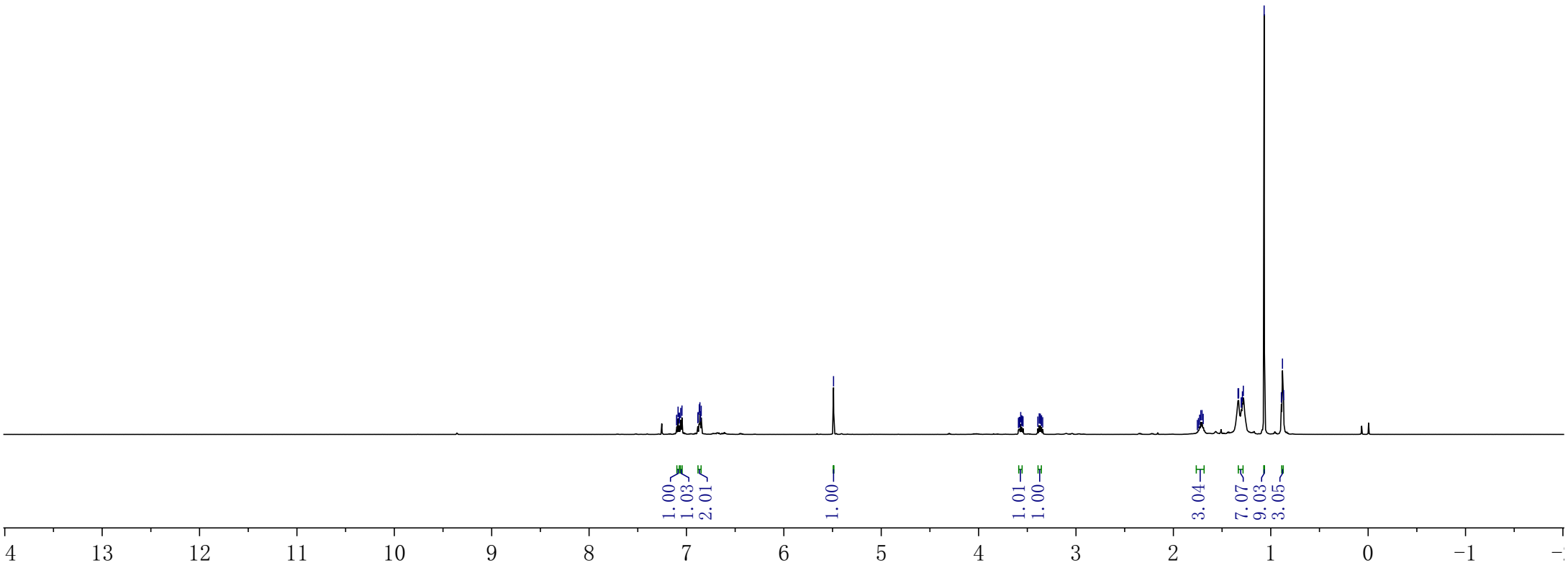
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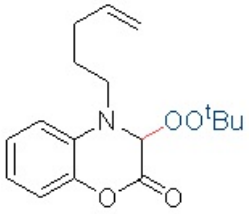
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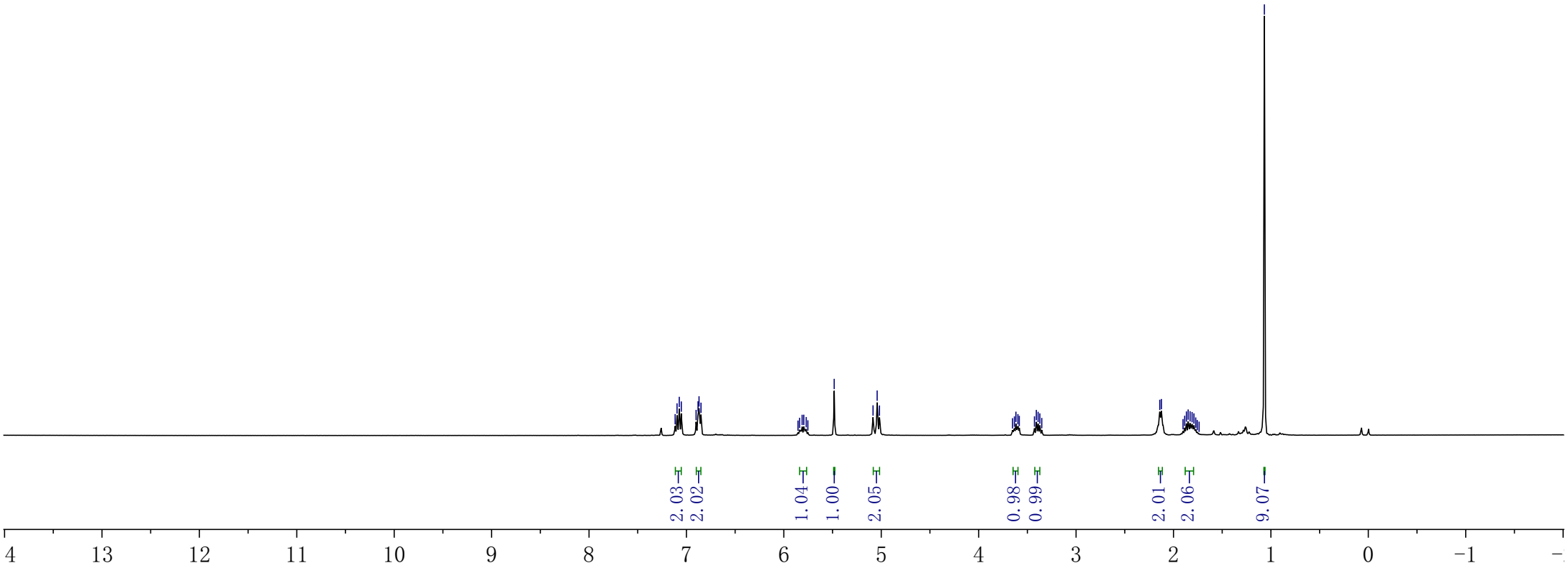
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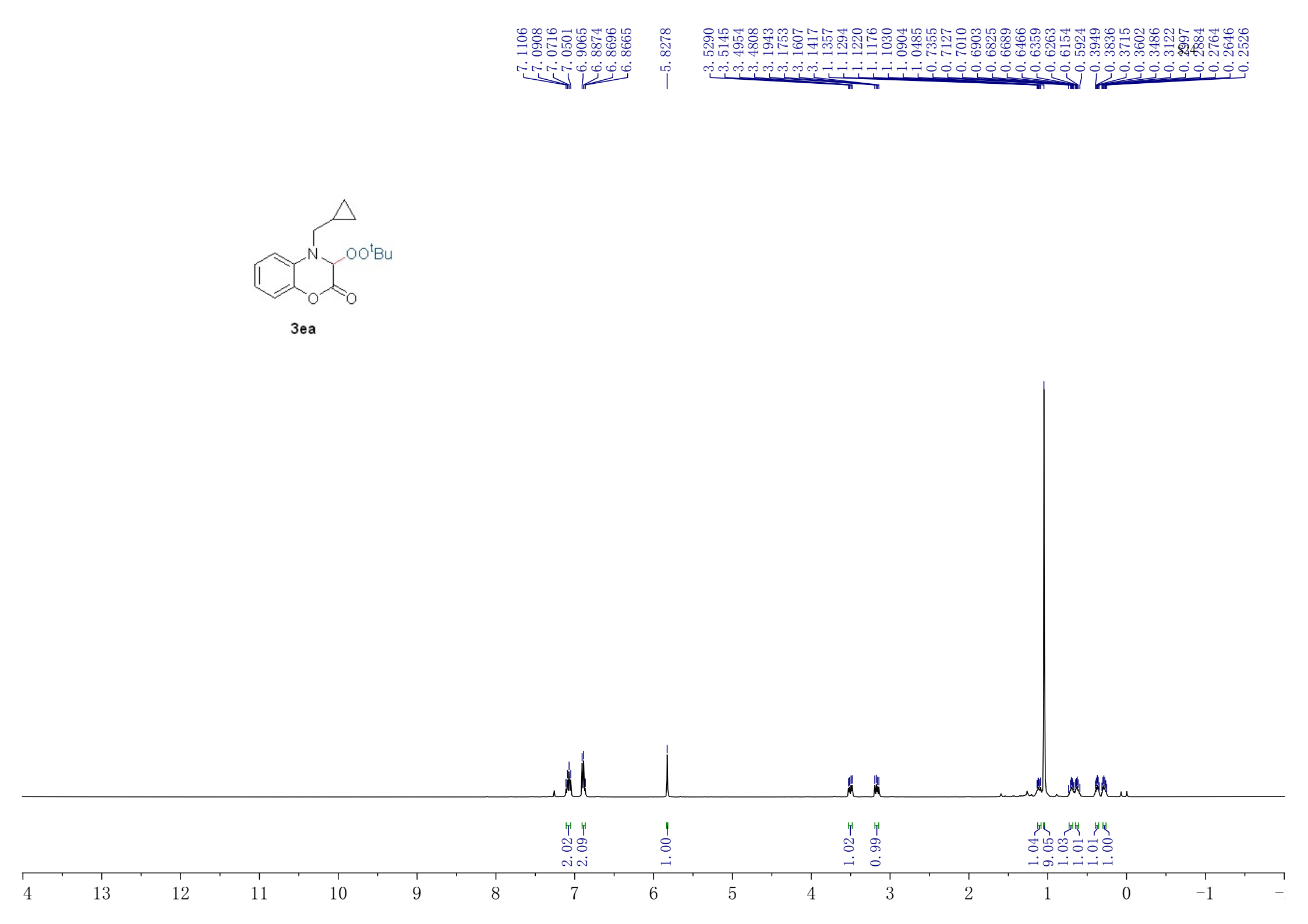
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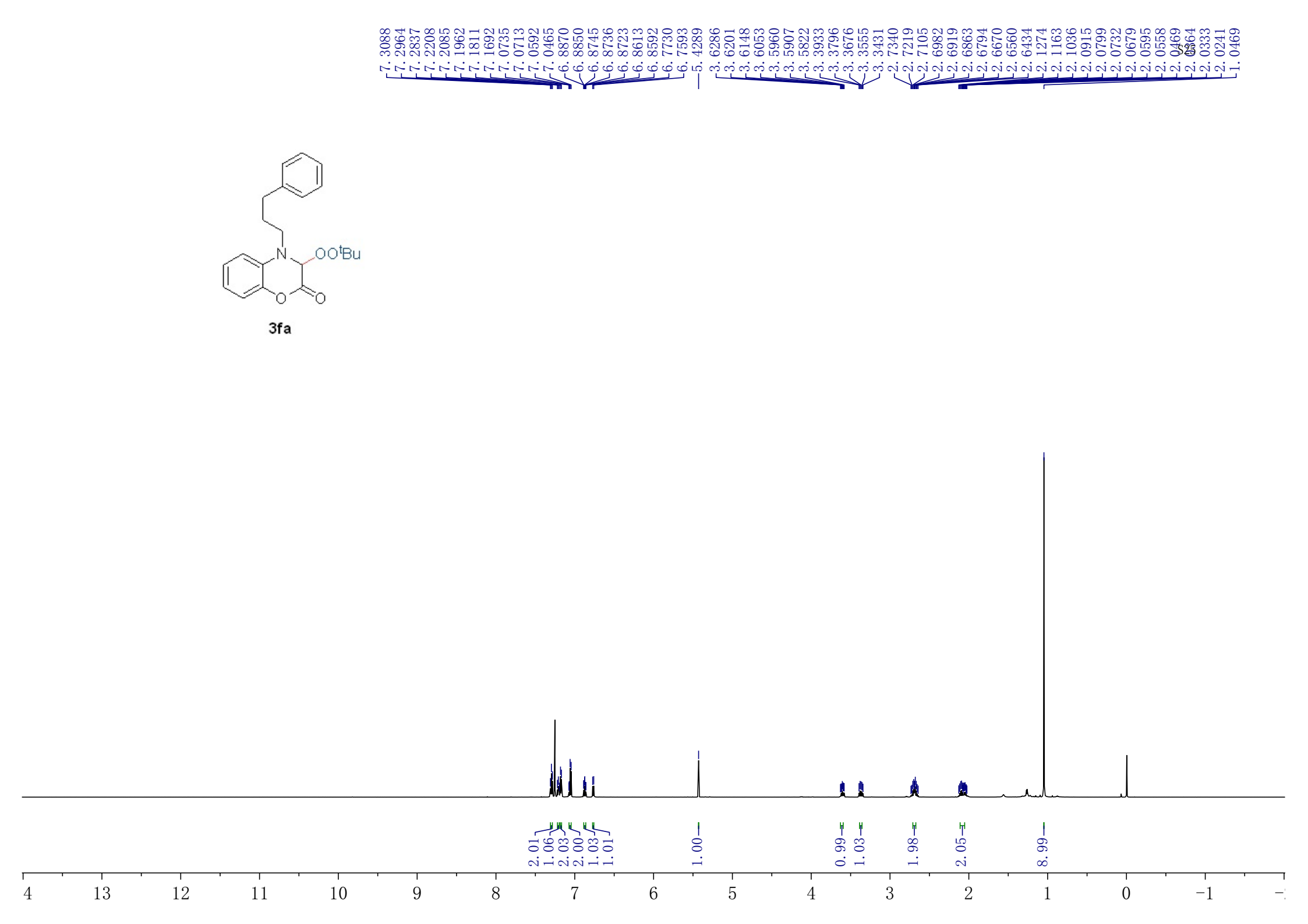
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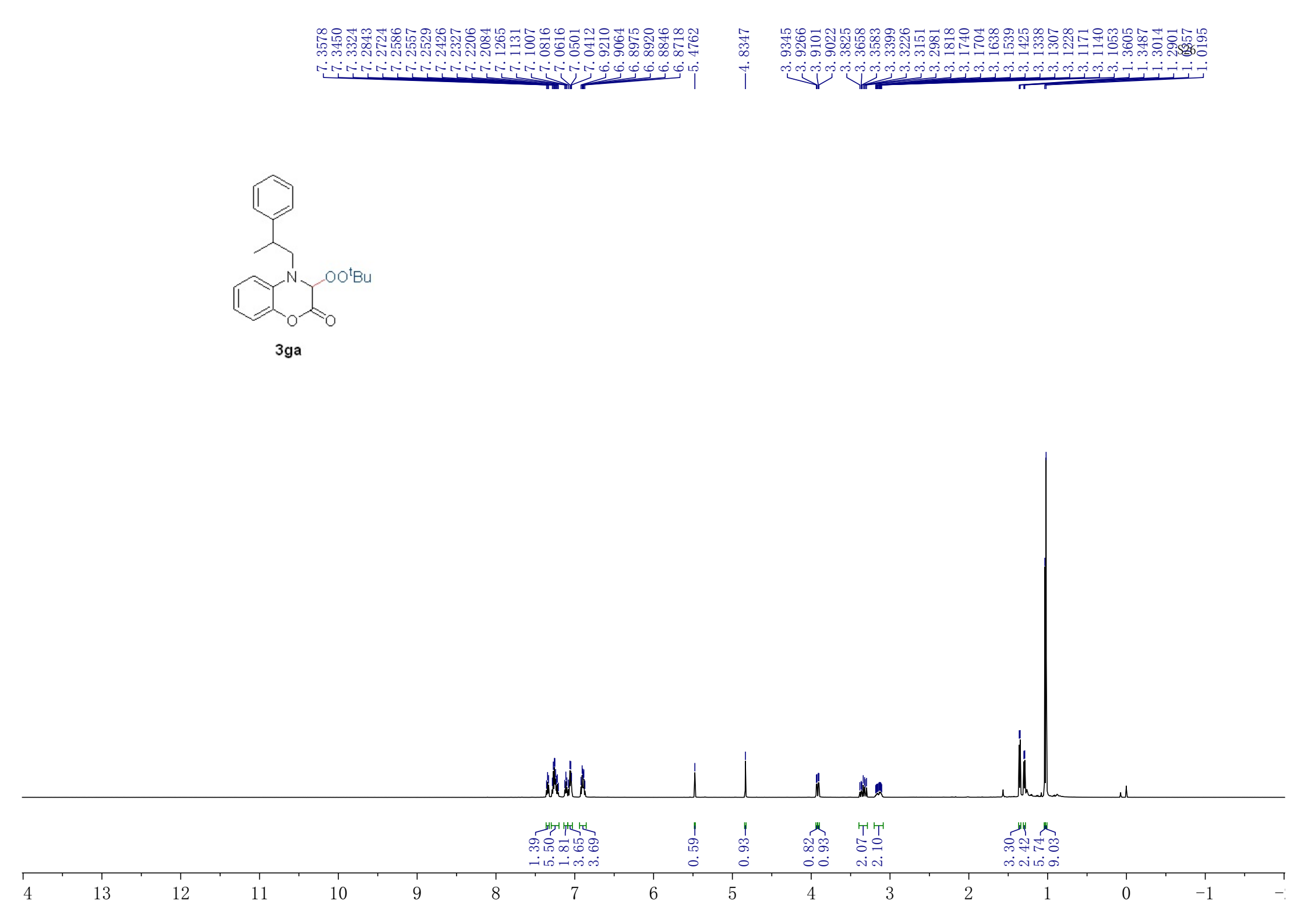
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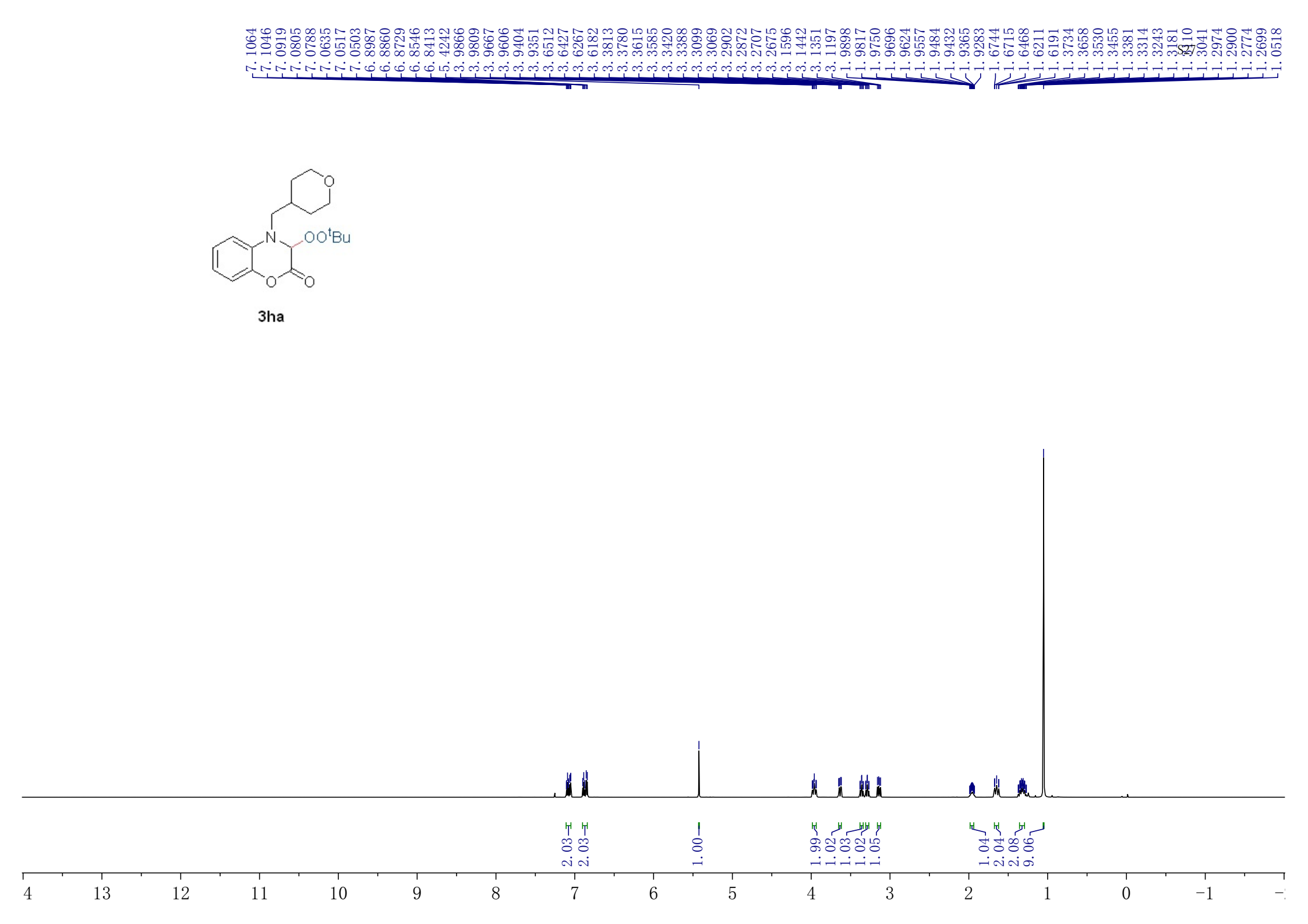
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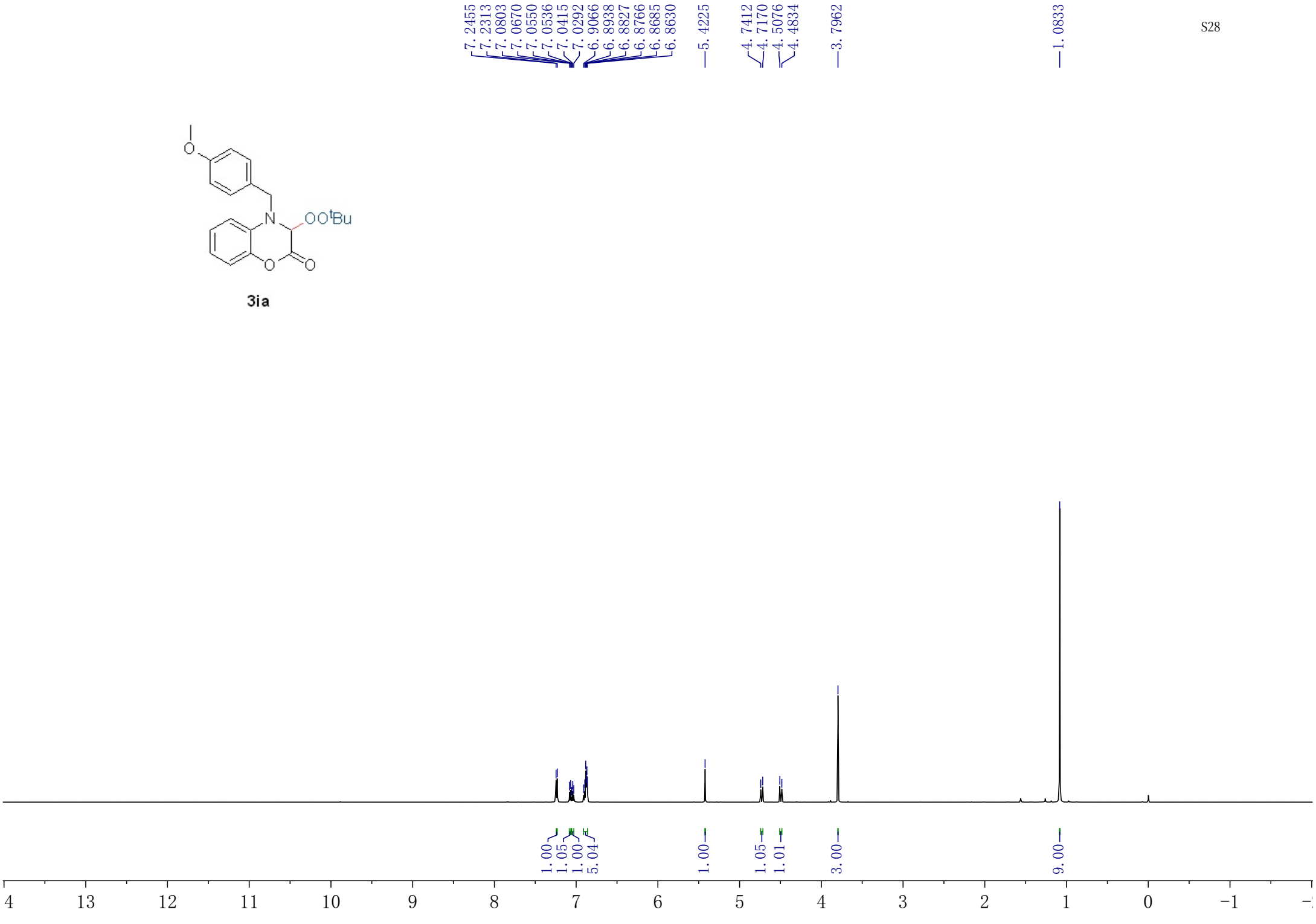
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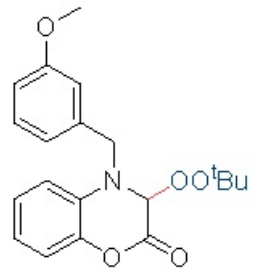

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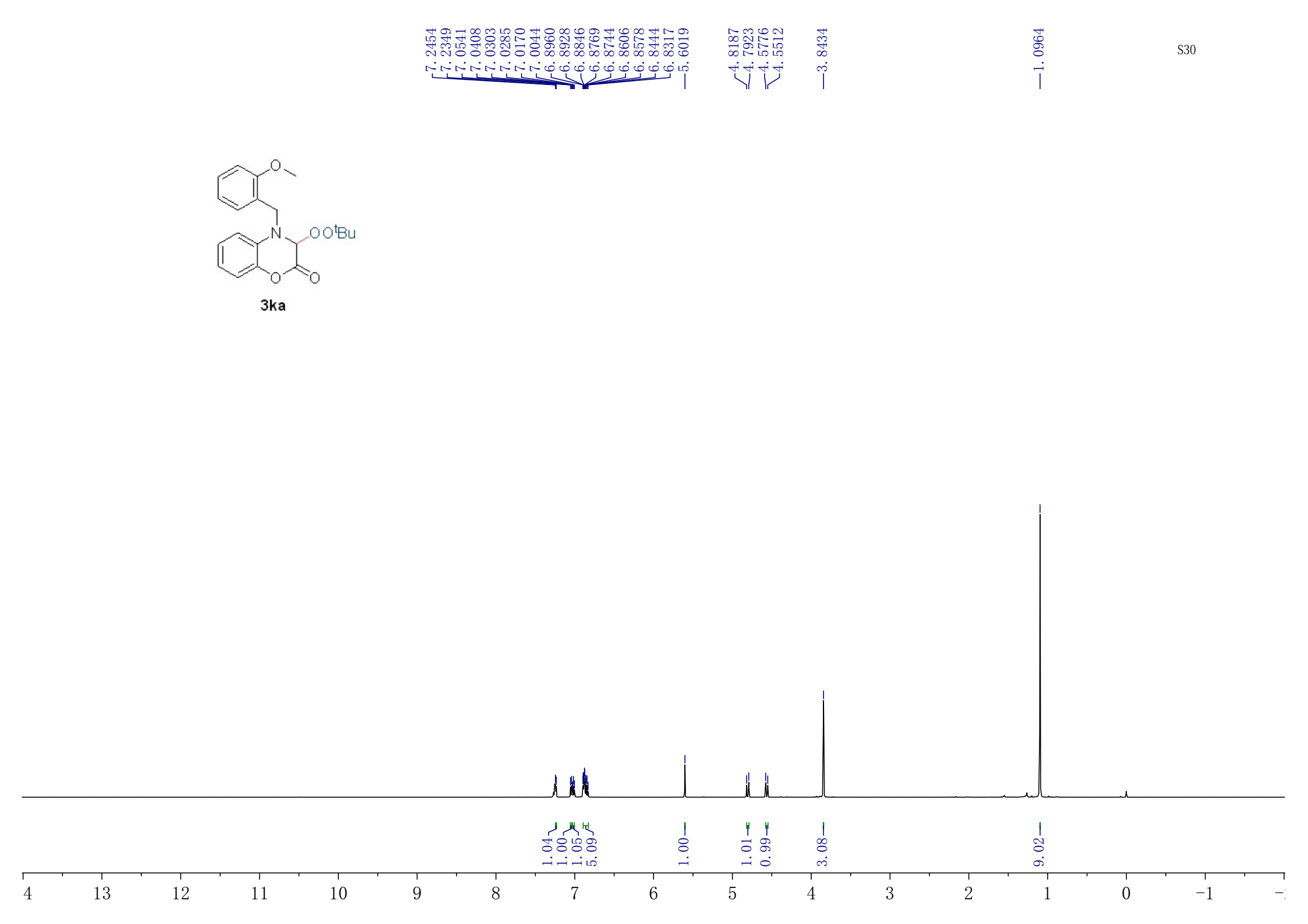
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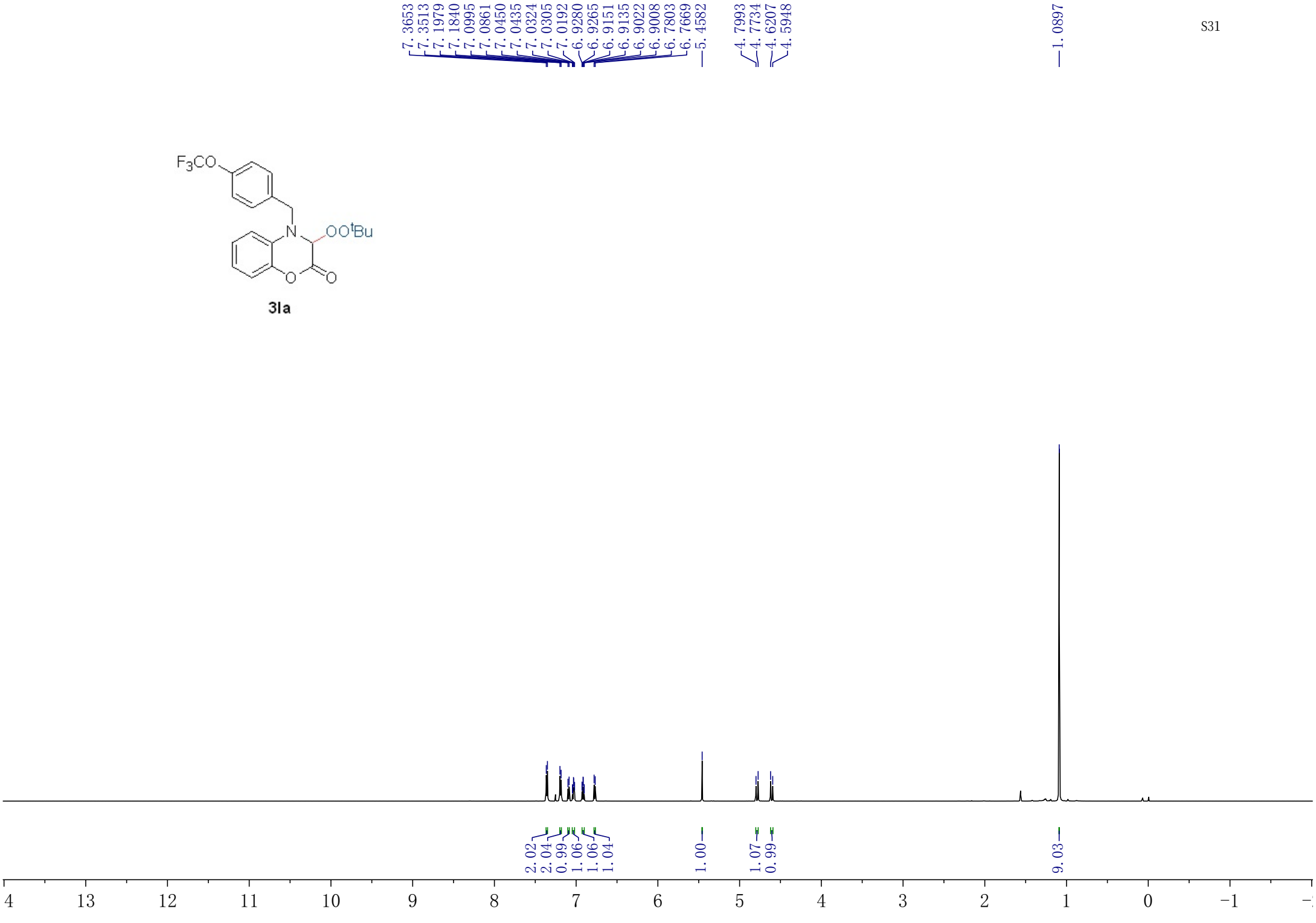
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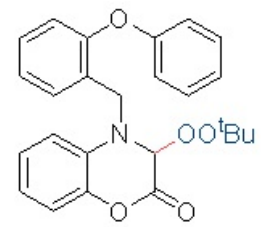

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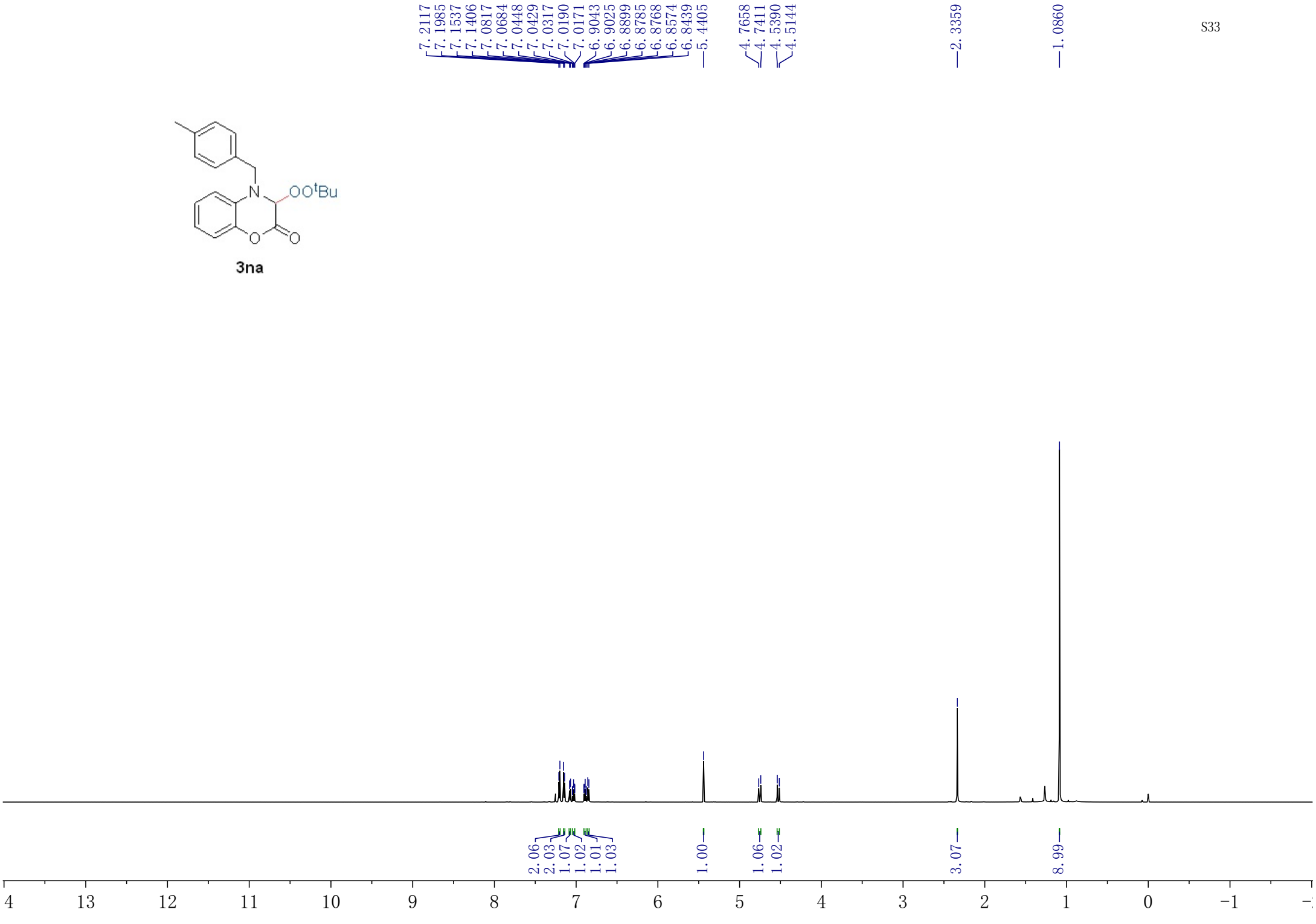
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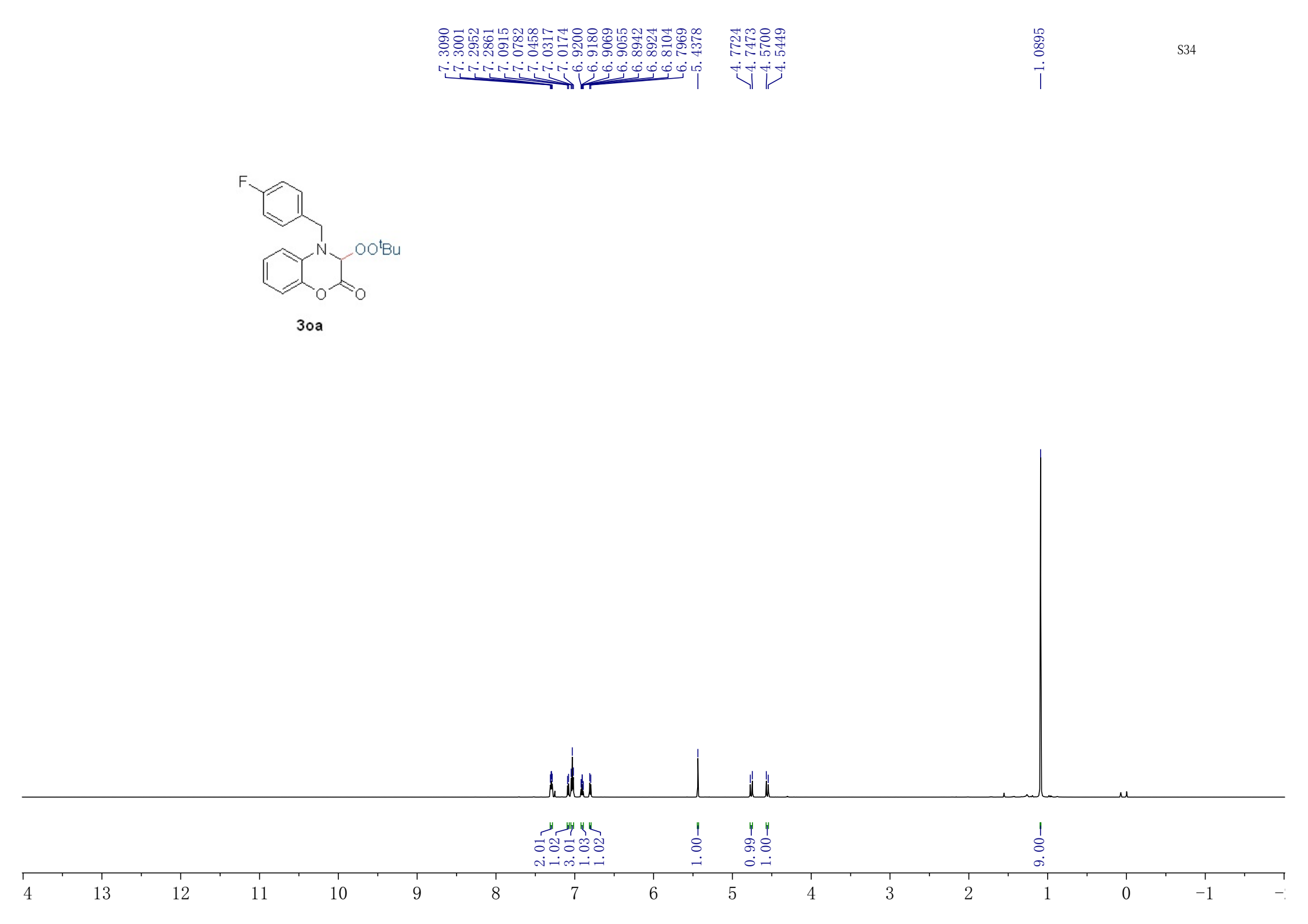
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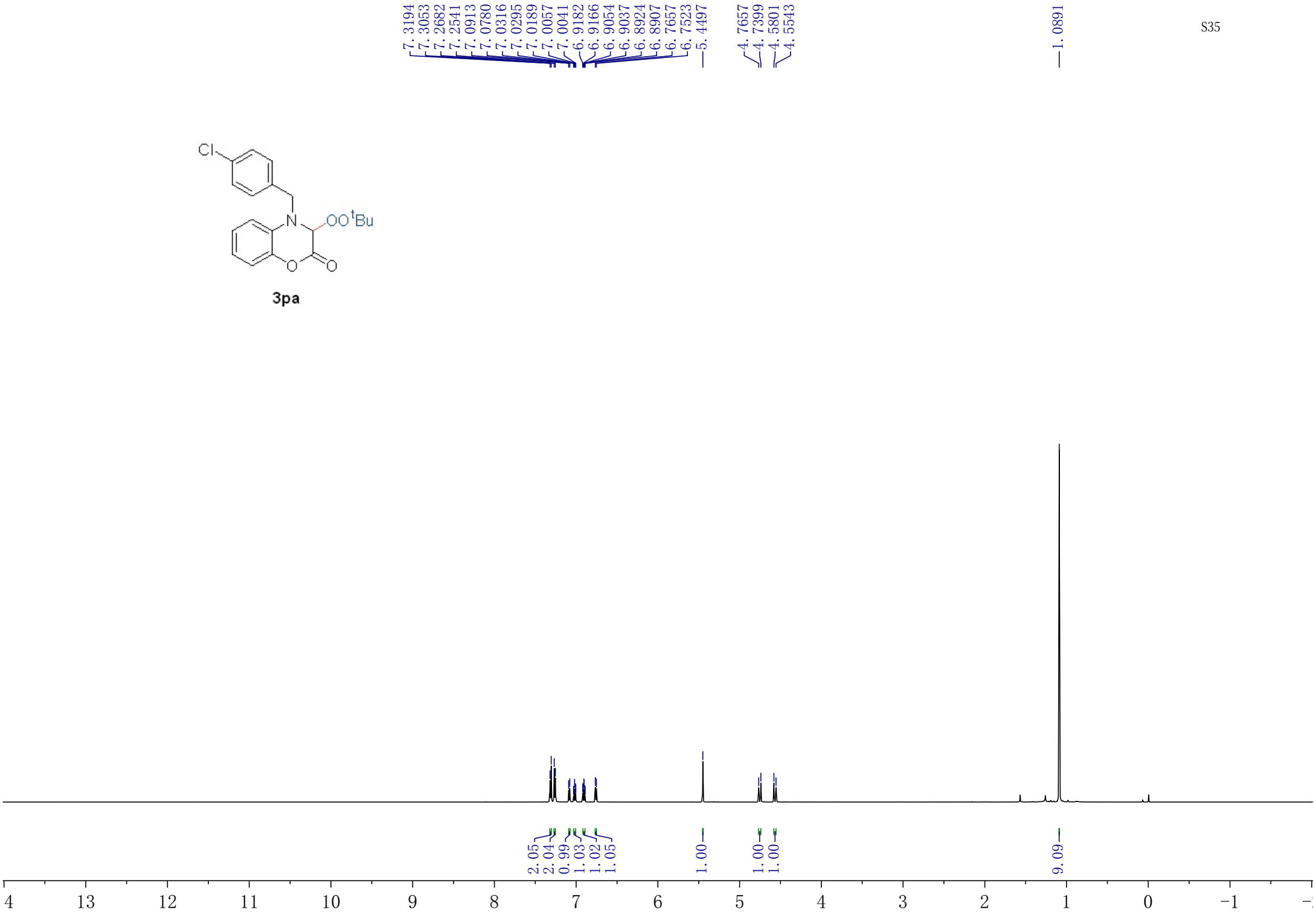
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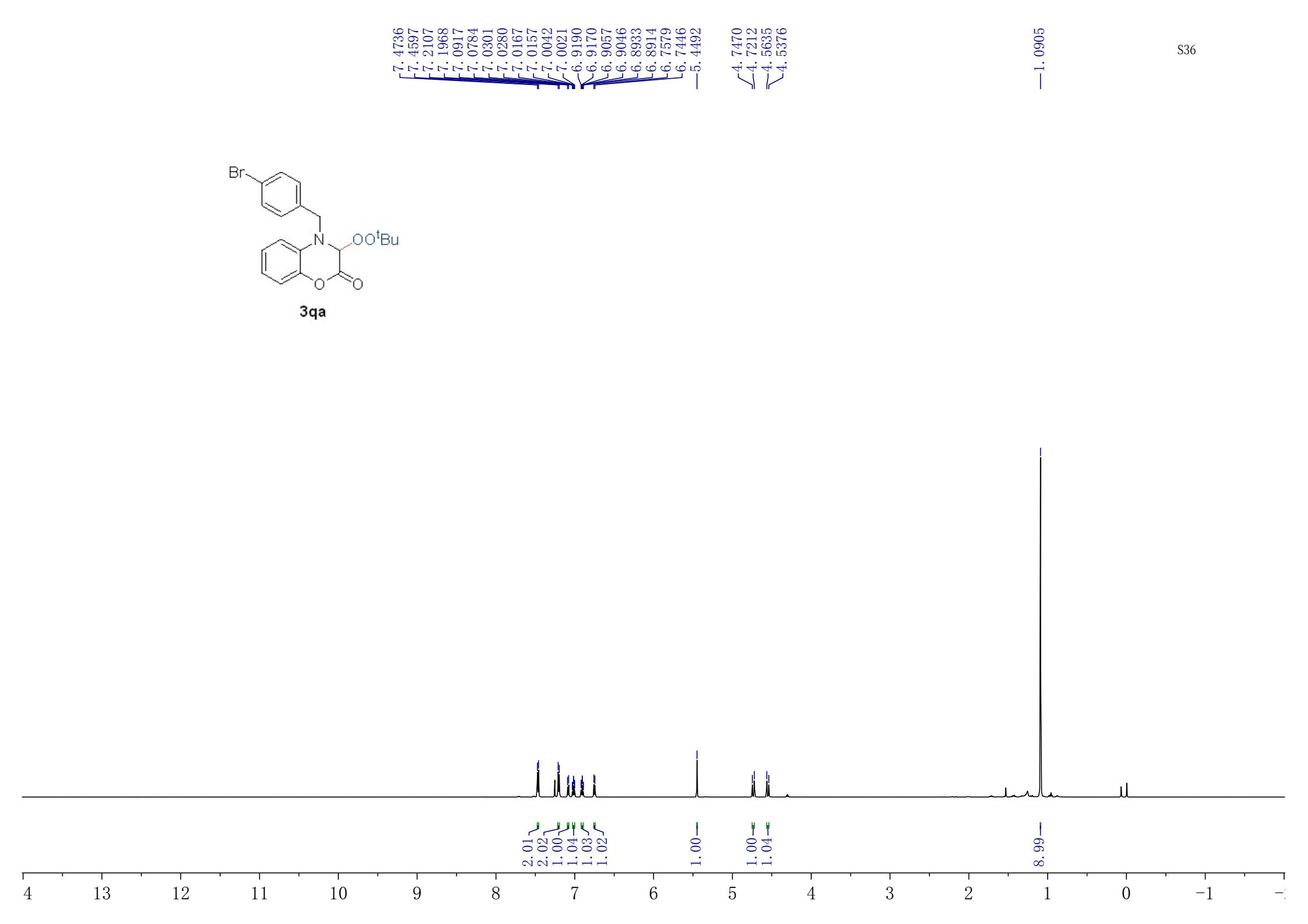
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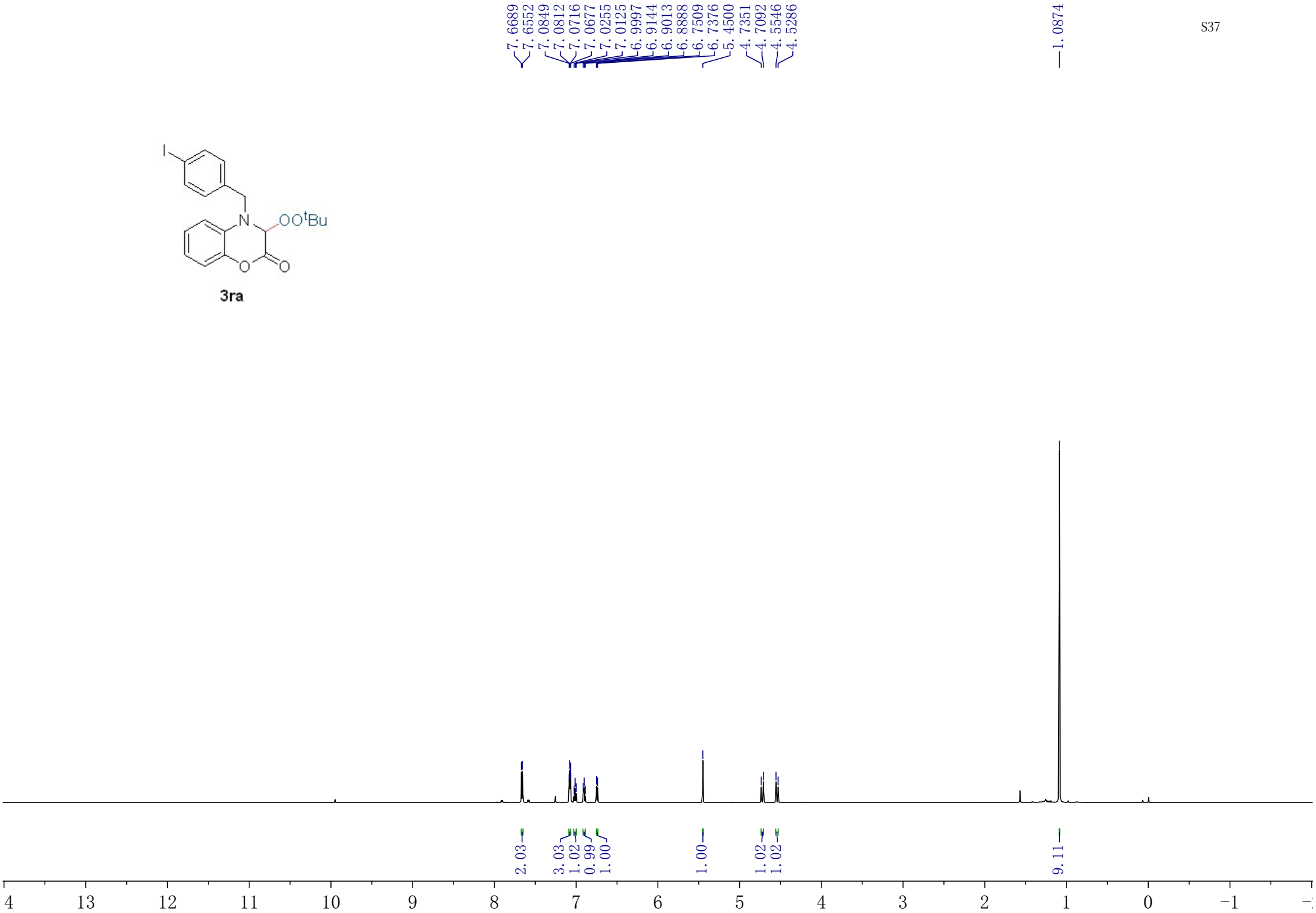
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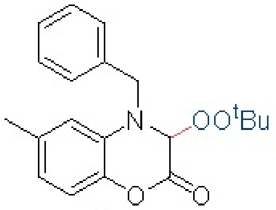
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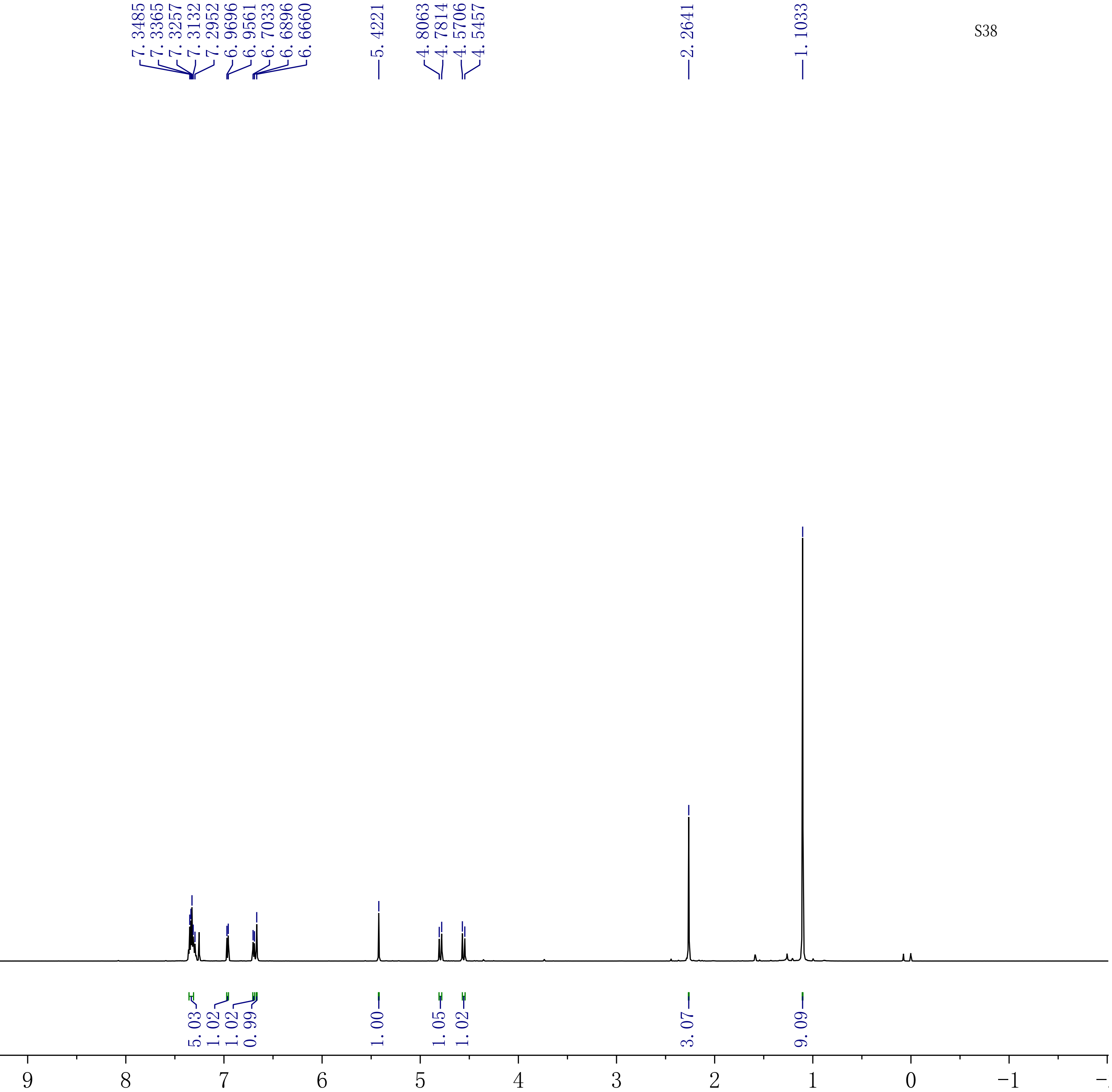
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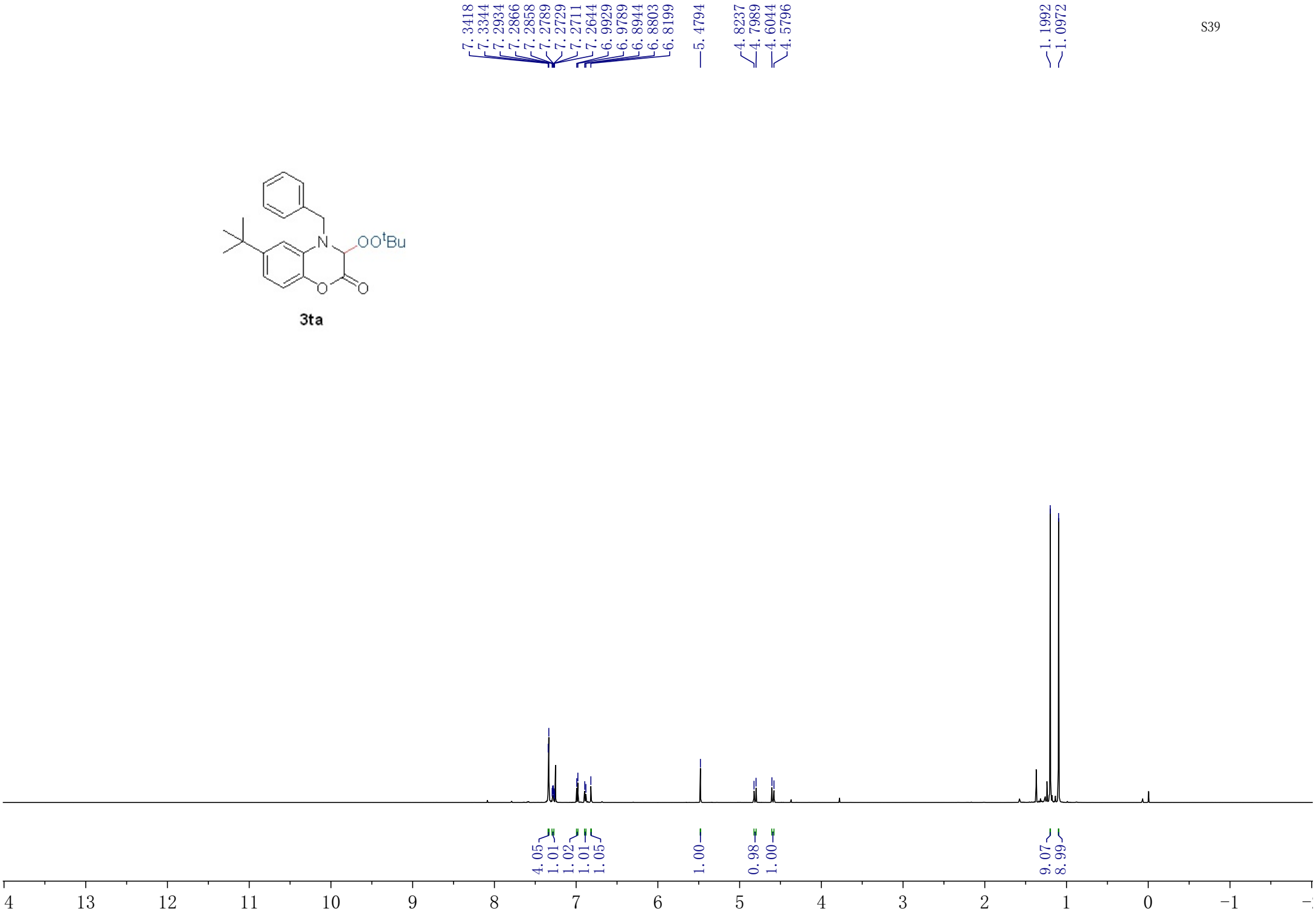
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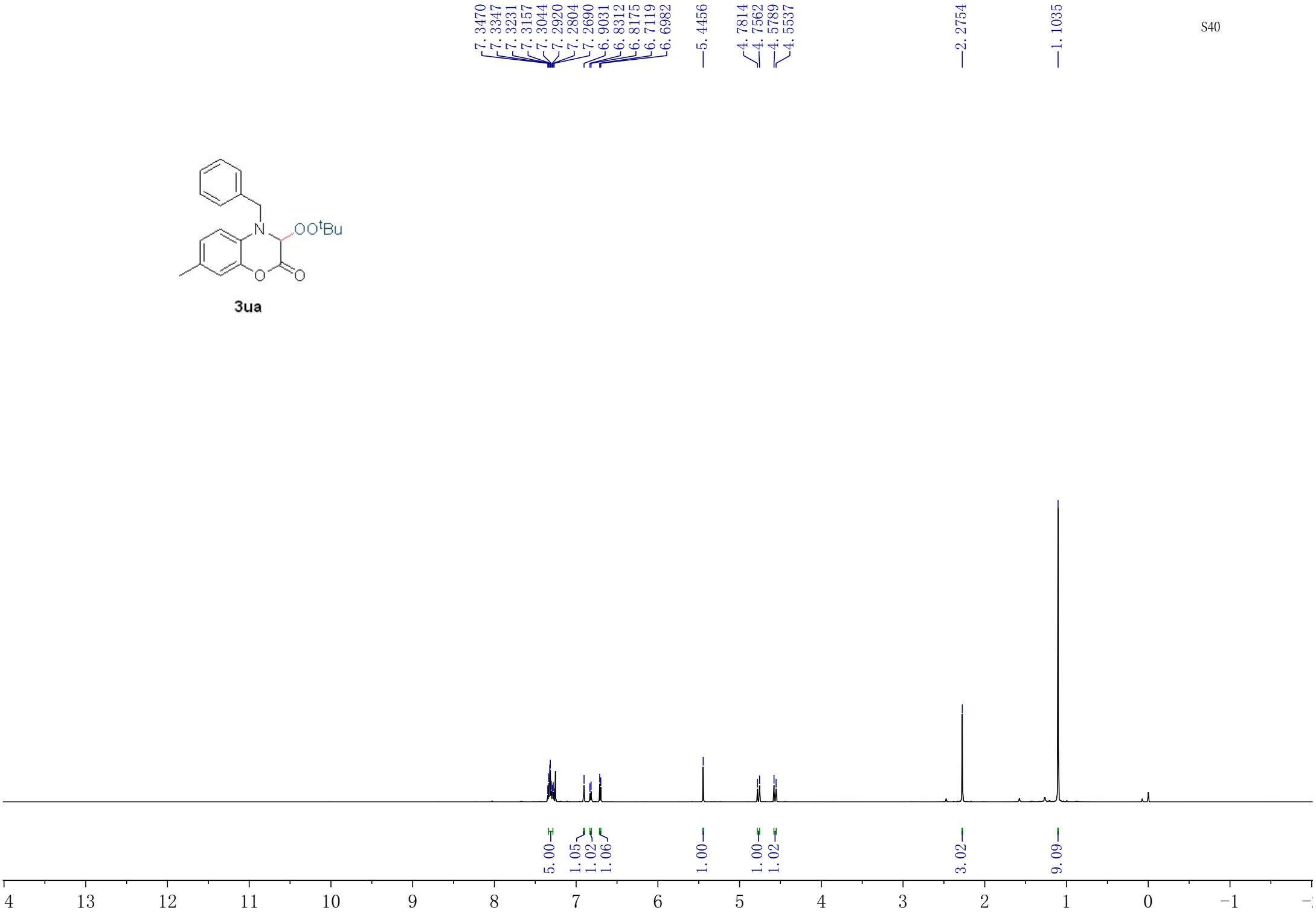
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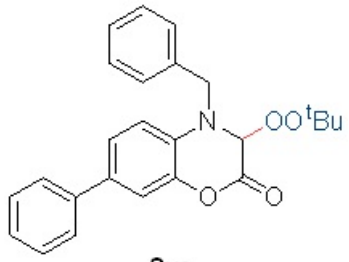
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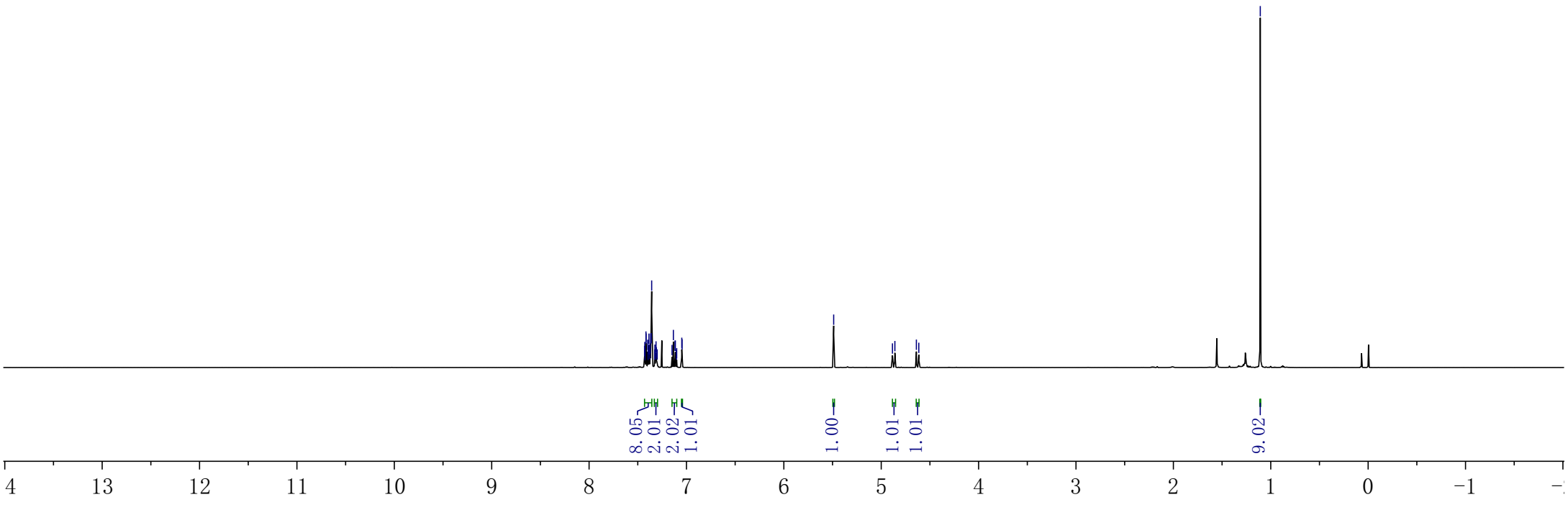
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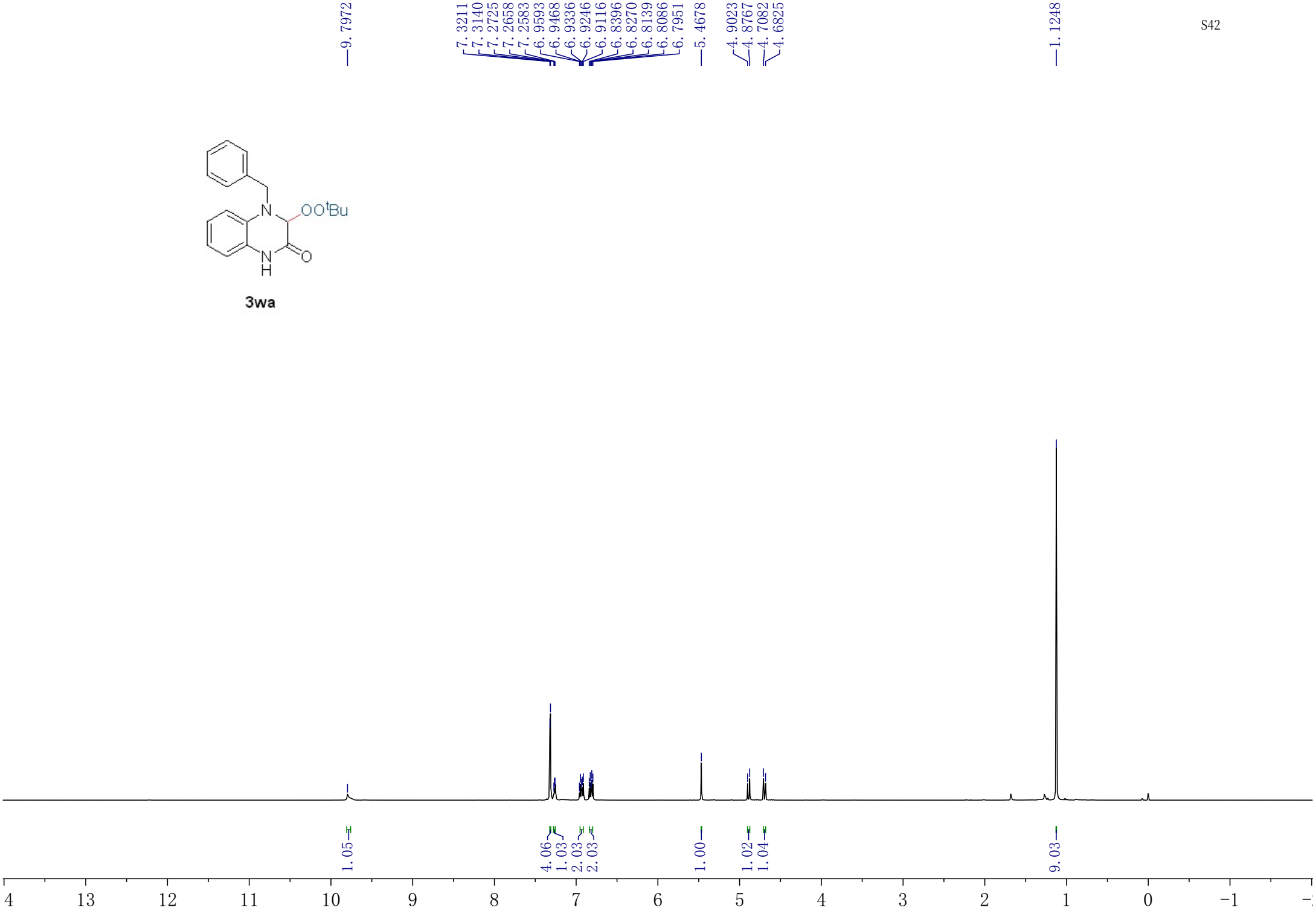
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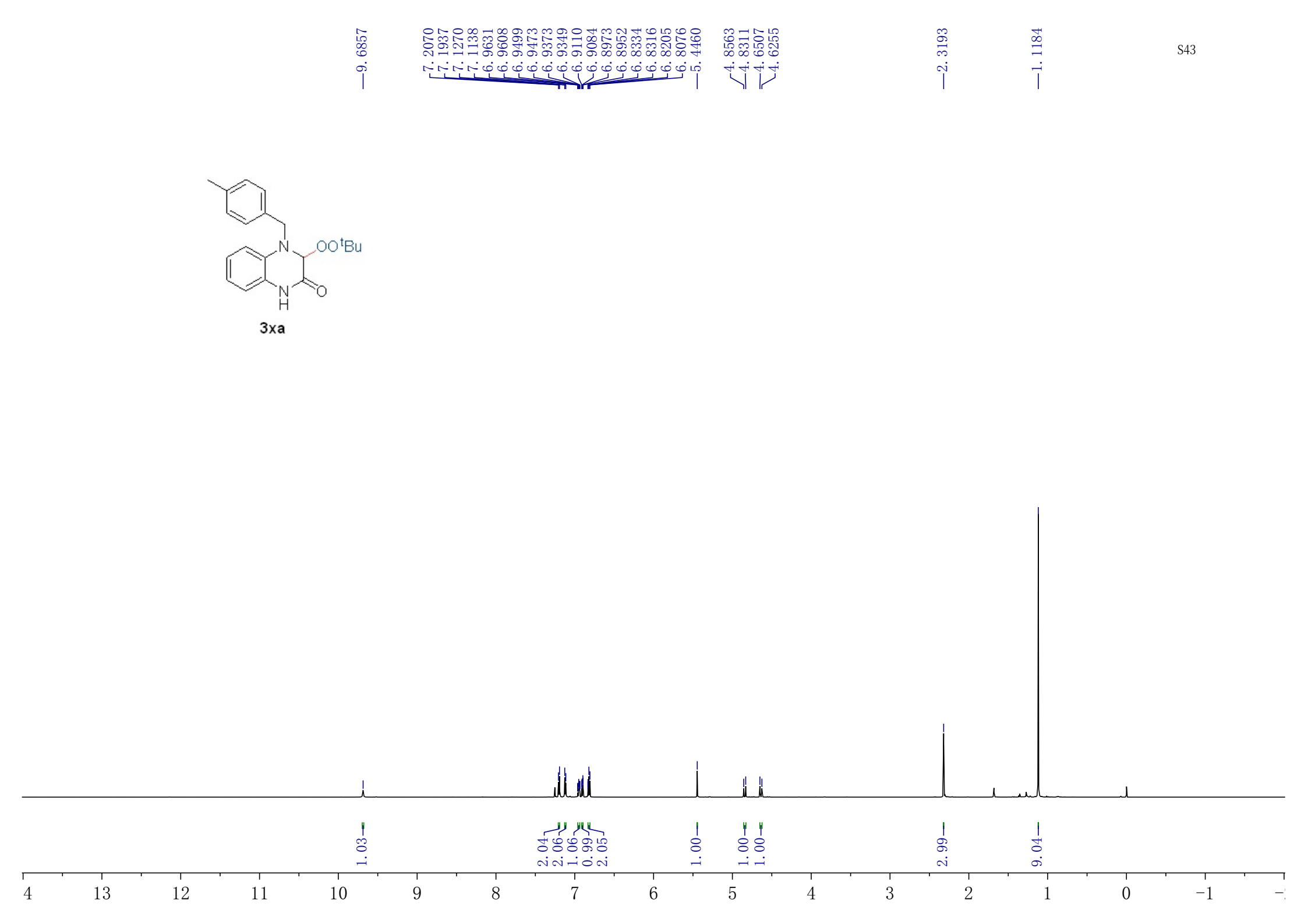
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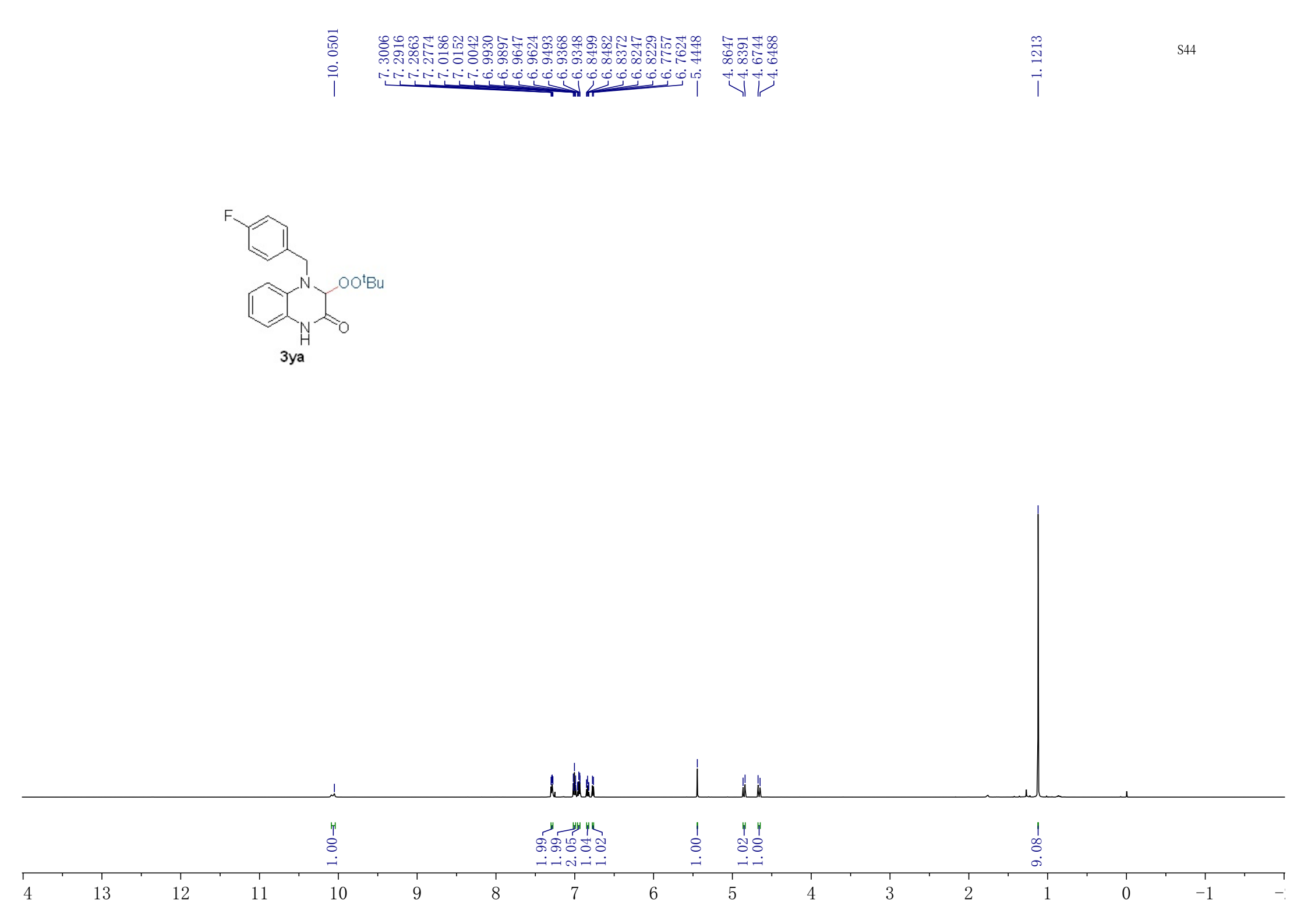
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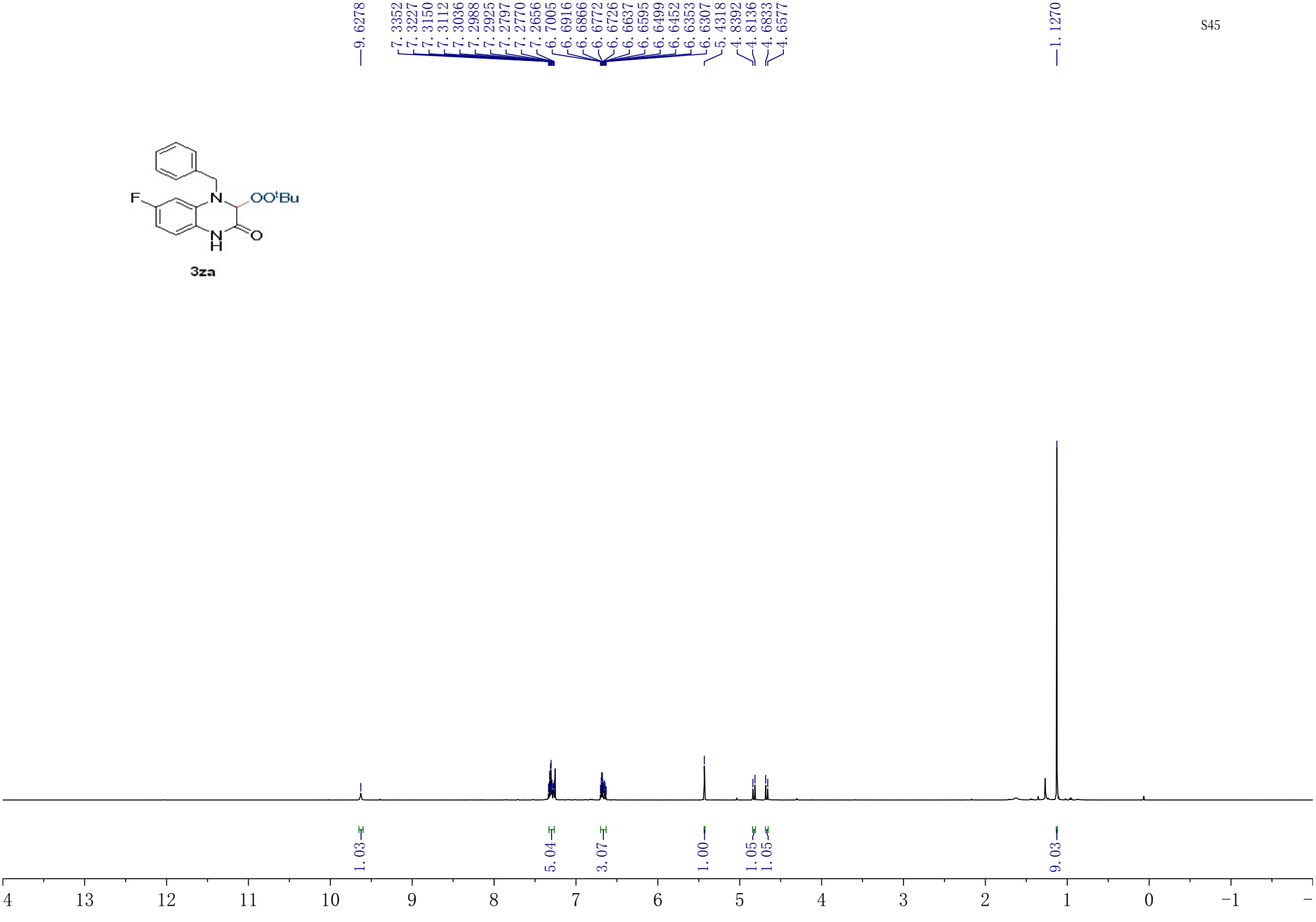
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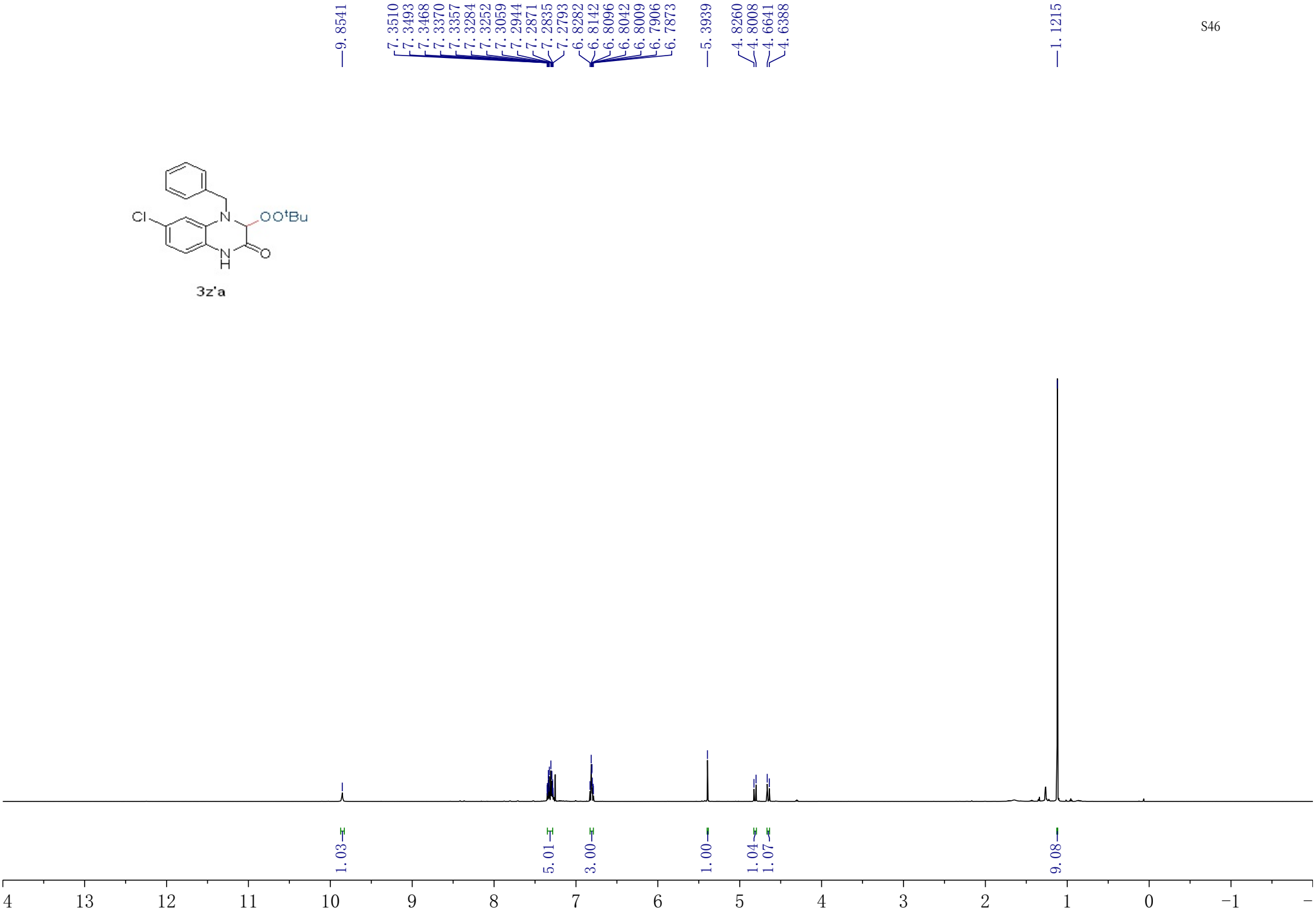
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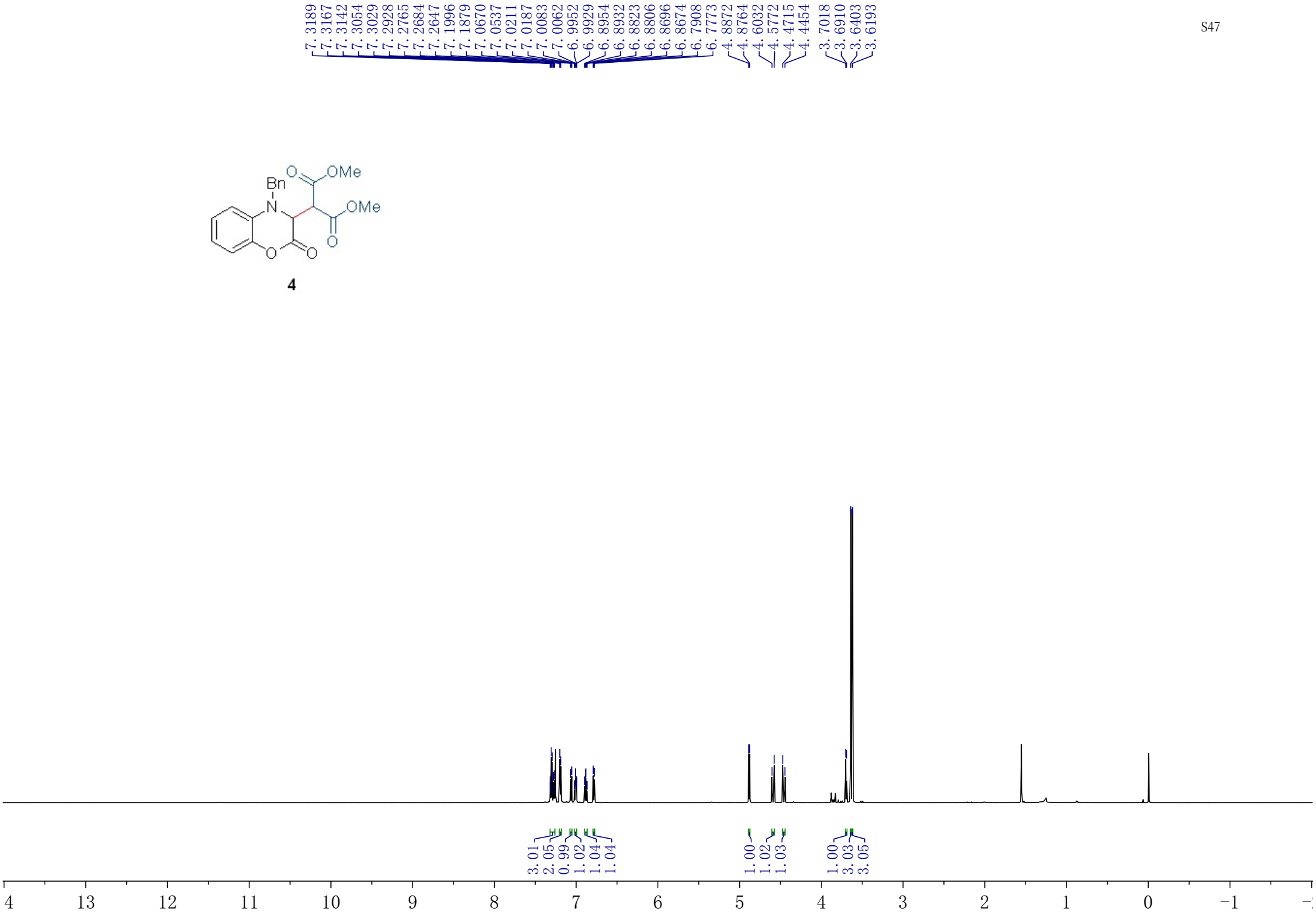
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1.00
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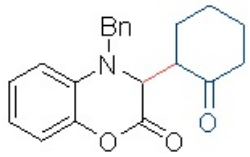

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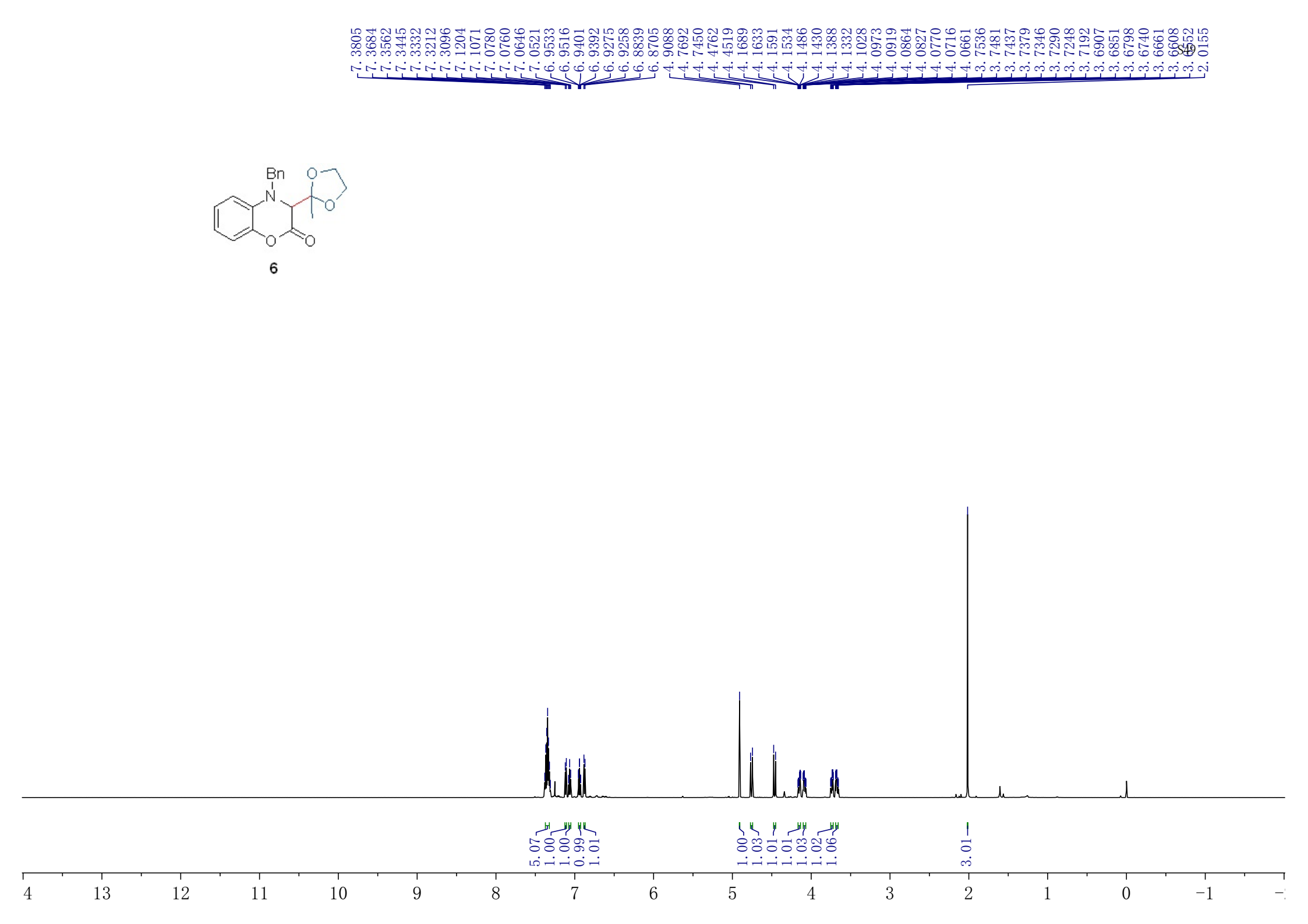
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1.00
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1.01
1.01
1.03
1.02
1.06
3.01
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NMe2
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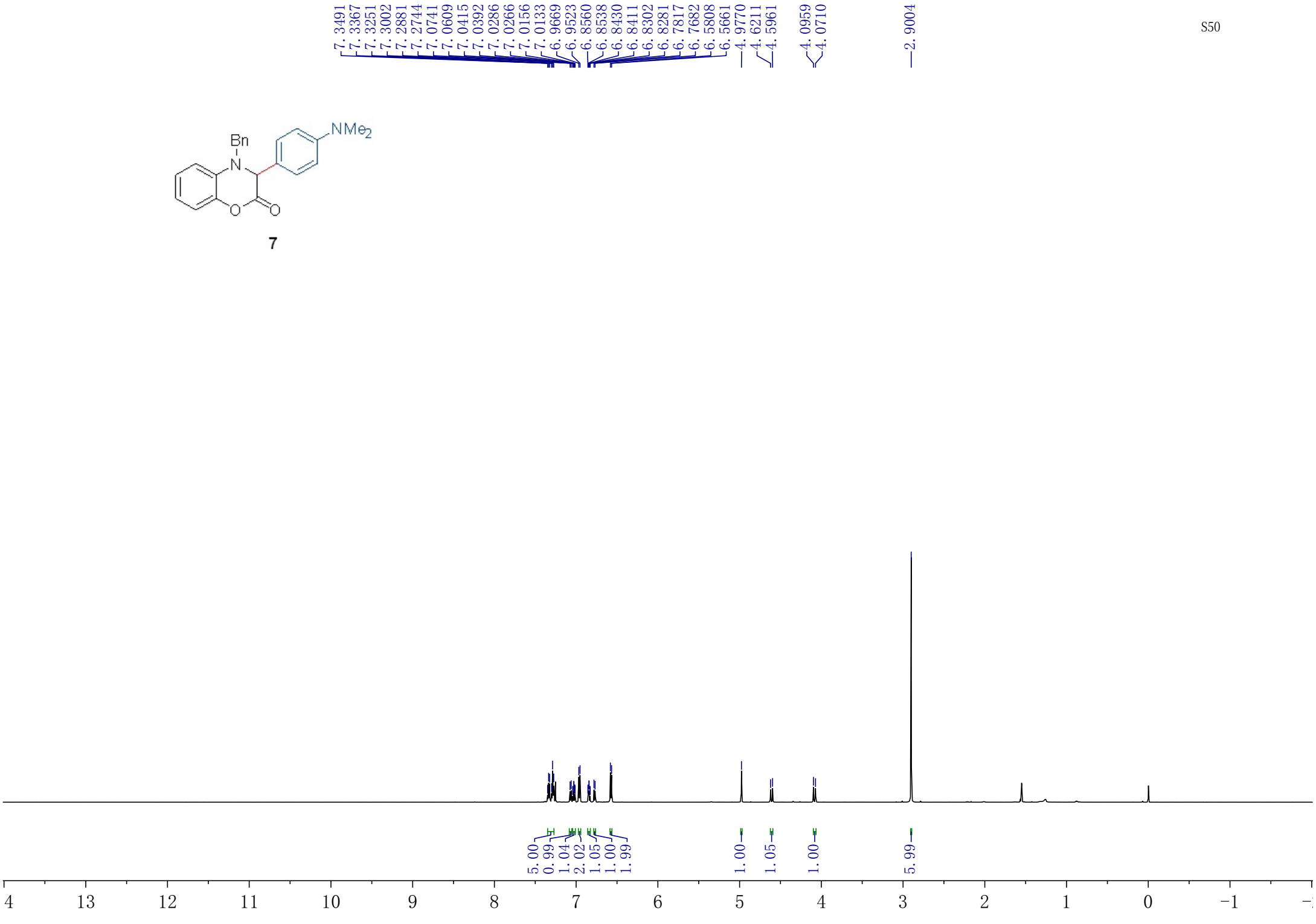
7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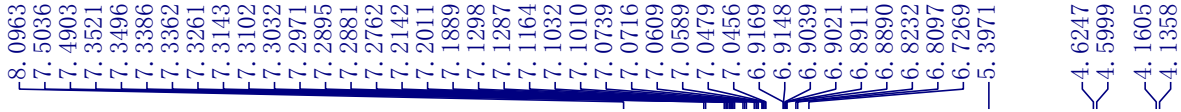
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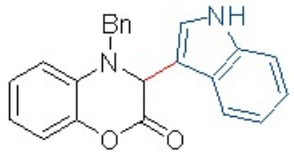
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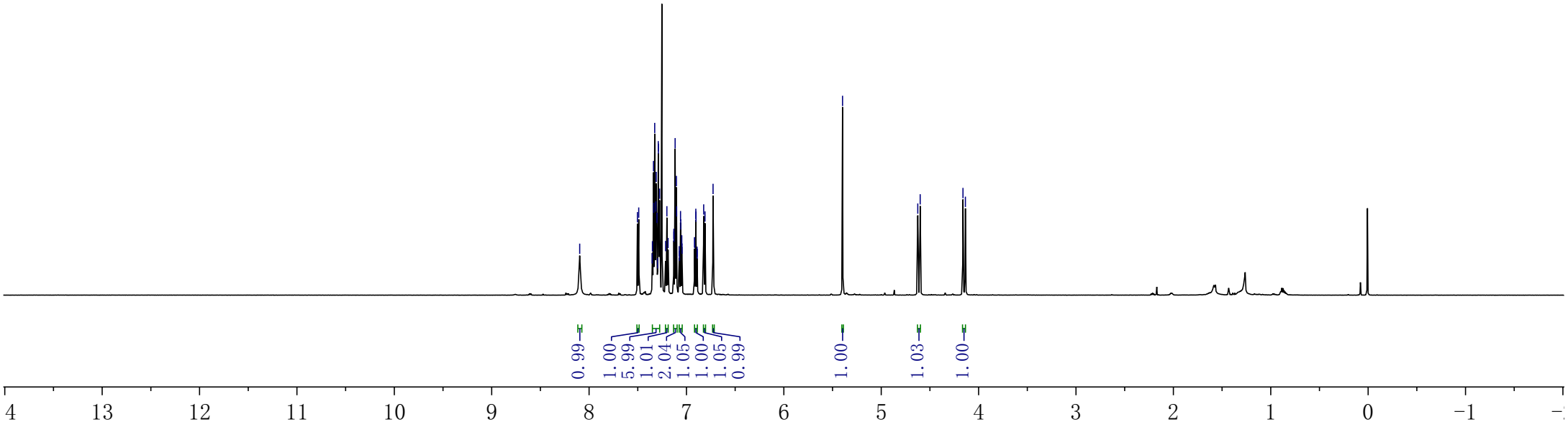
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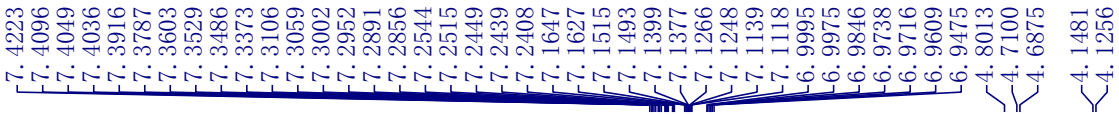
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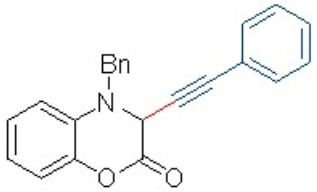
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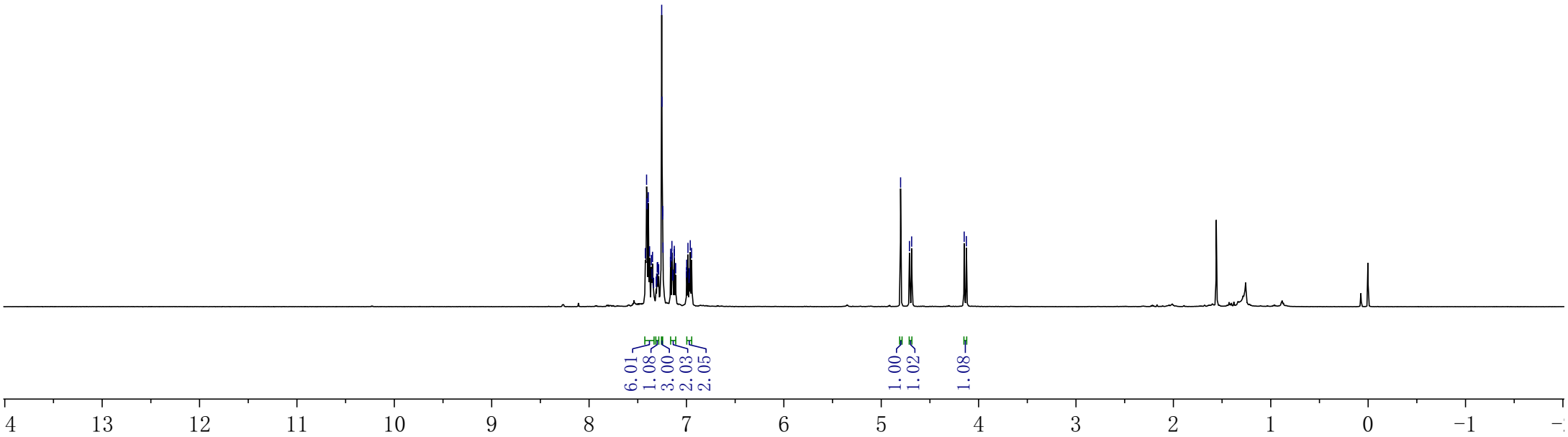
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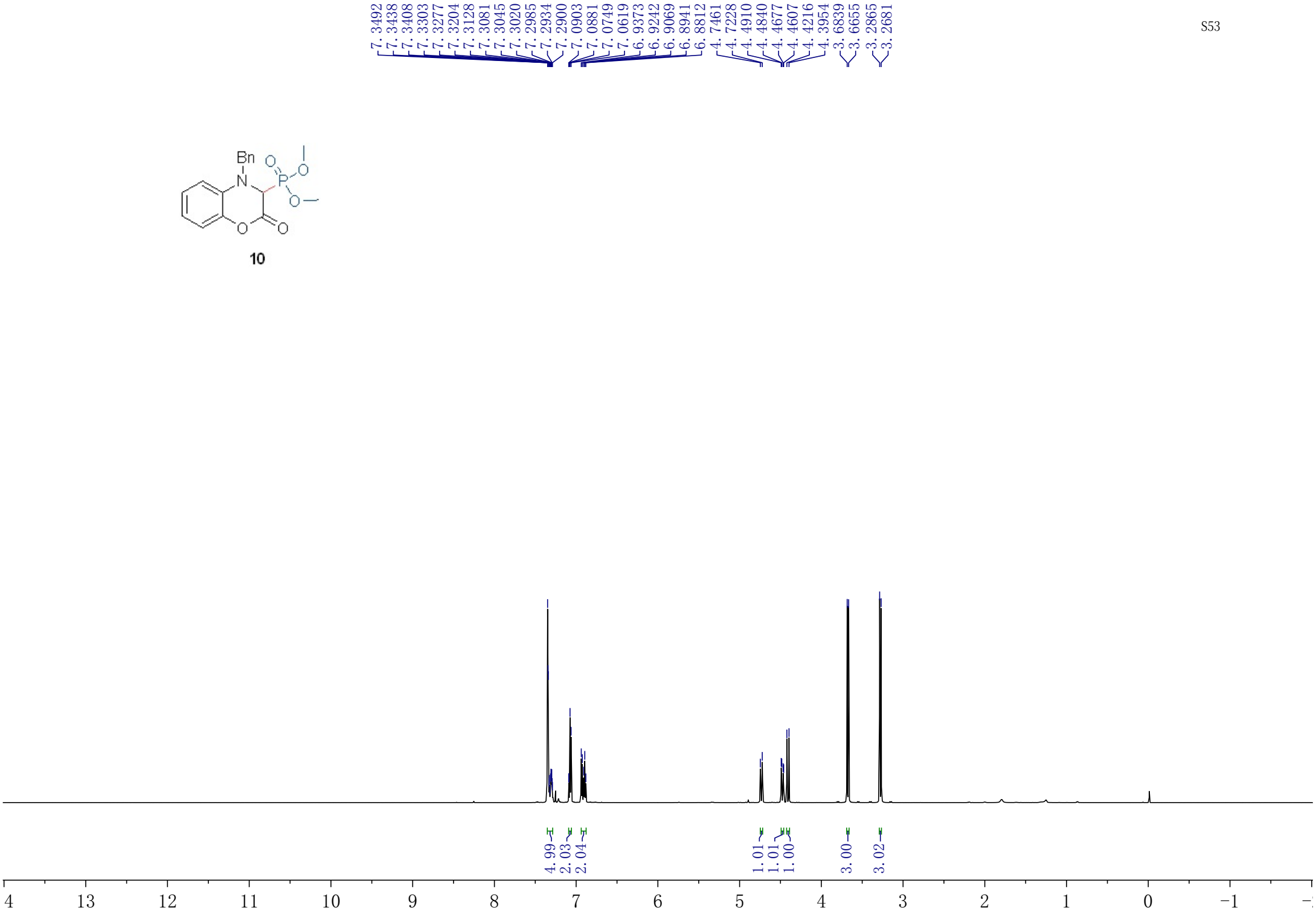
10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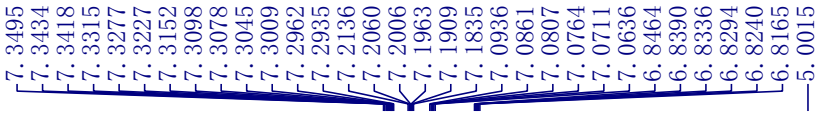
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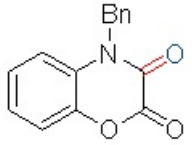
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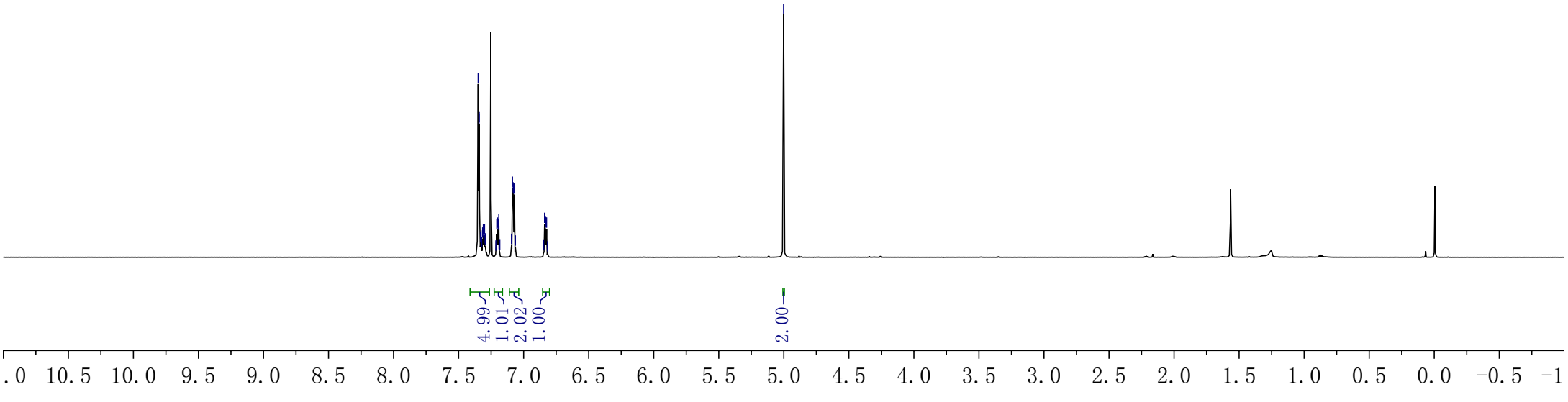
11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141.15
135.48
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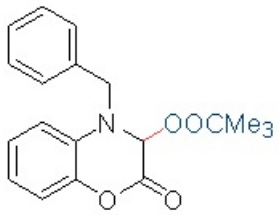
127.87
127.77
124.90
120.38
116.32
113.53
86.77
81.70
52.27
26.08



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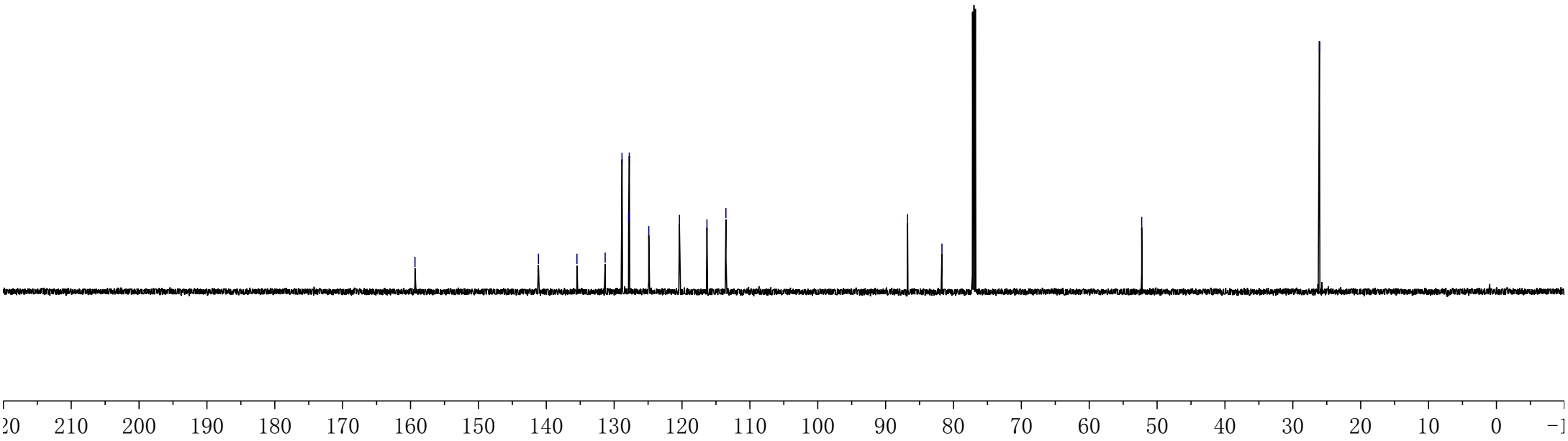

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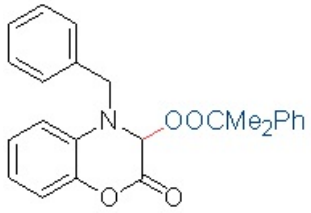

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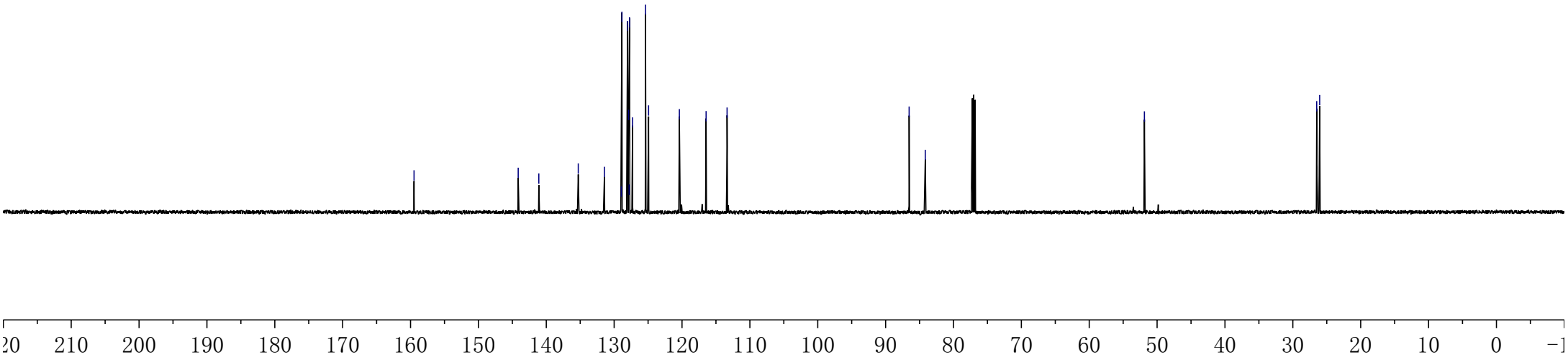

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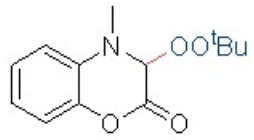

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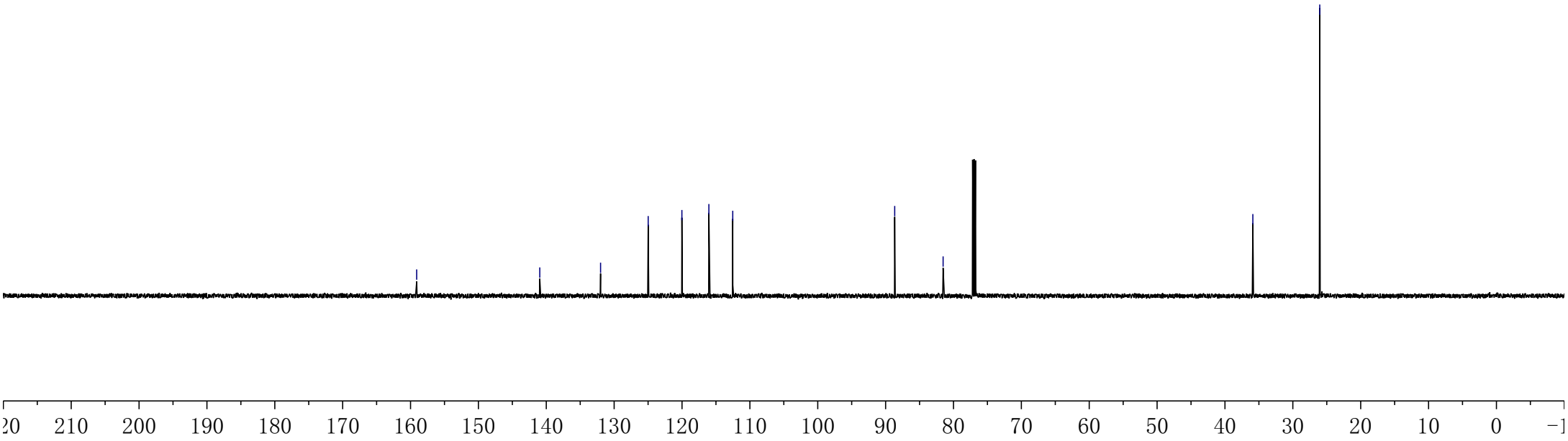

N
OO^{t}Bu
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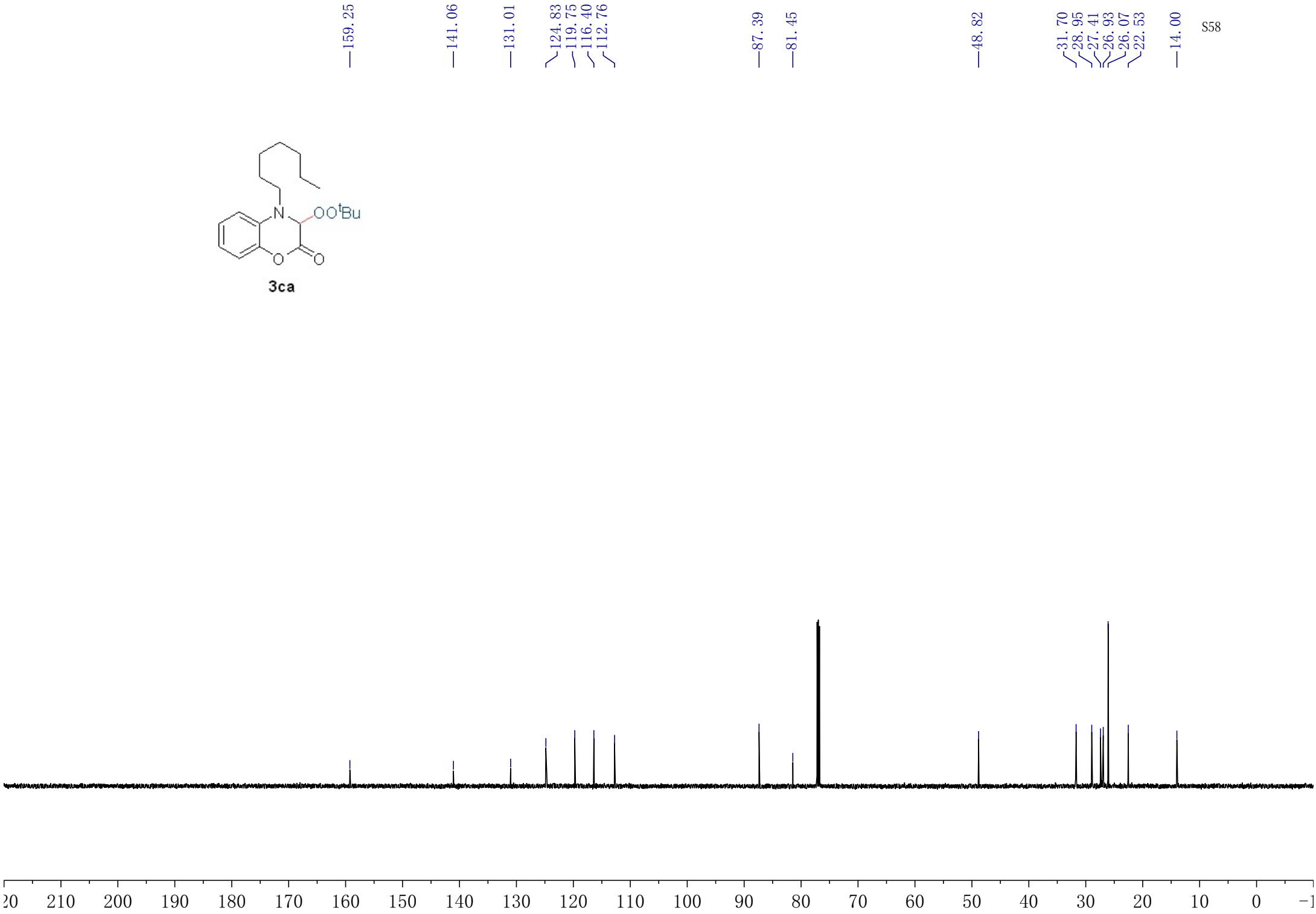
3ca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150
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-1

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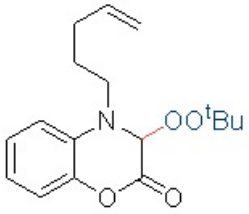

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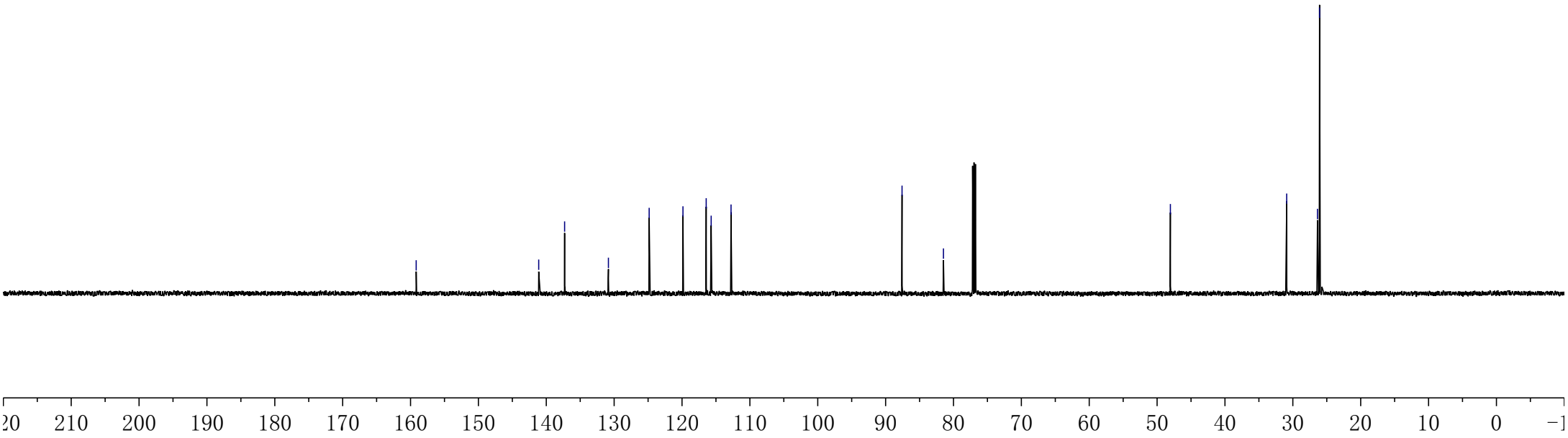

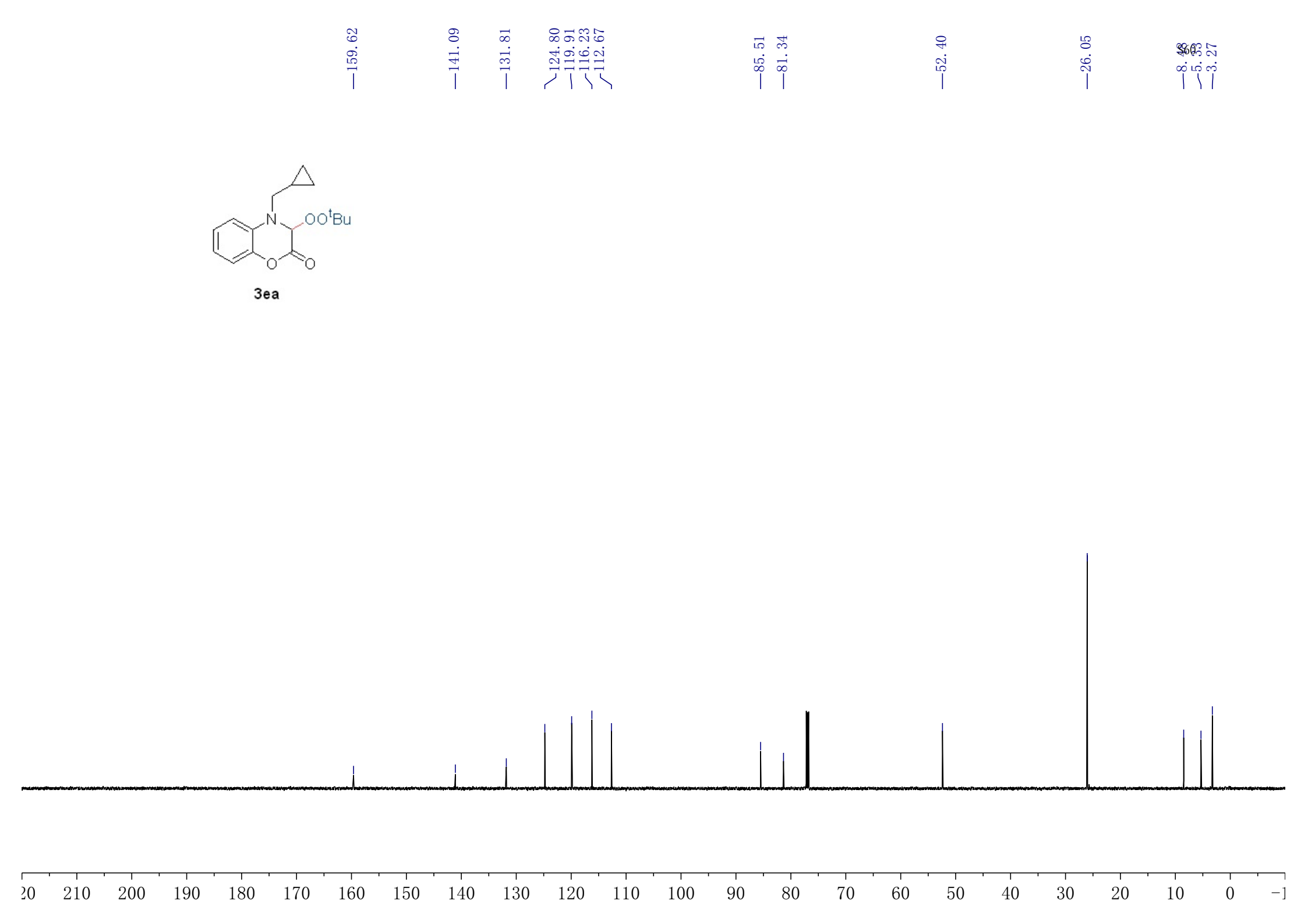
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5.33
3.27
OO^{t}Bu
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3ea
210
200
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180
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160
150
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60
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20
10
0

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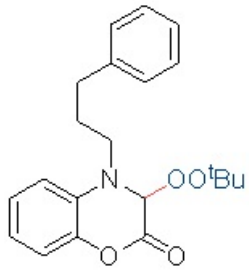

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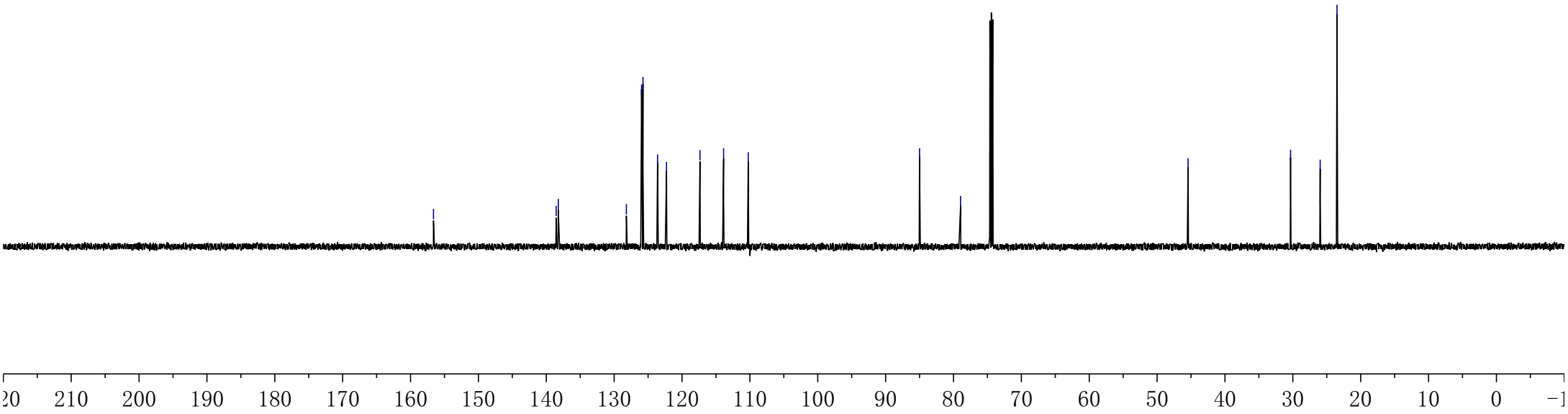

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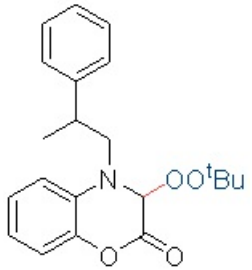

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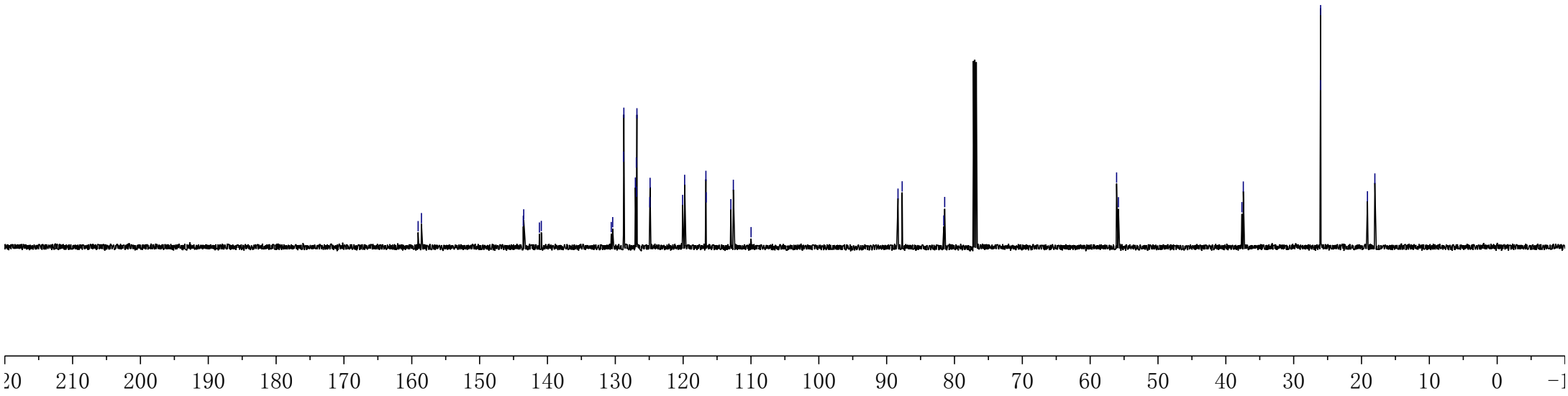

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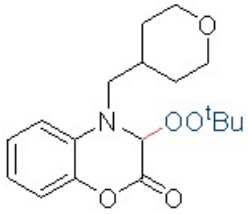

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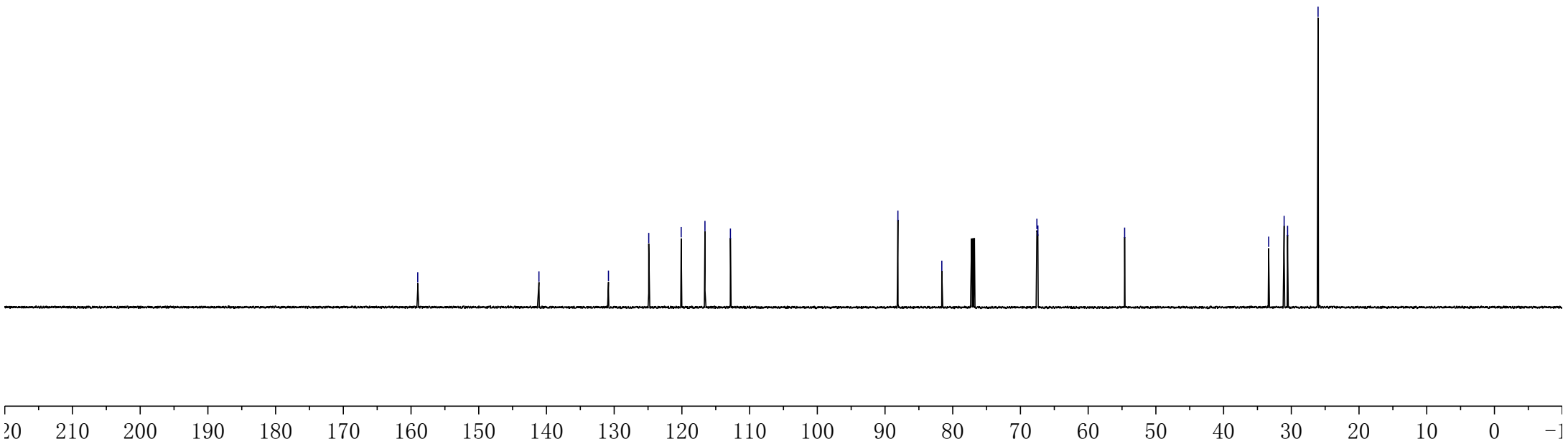

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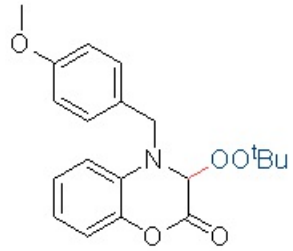

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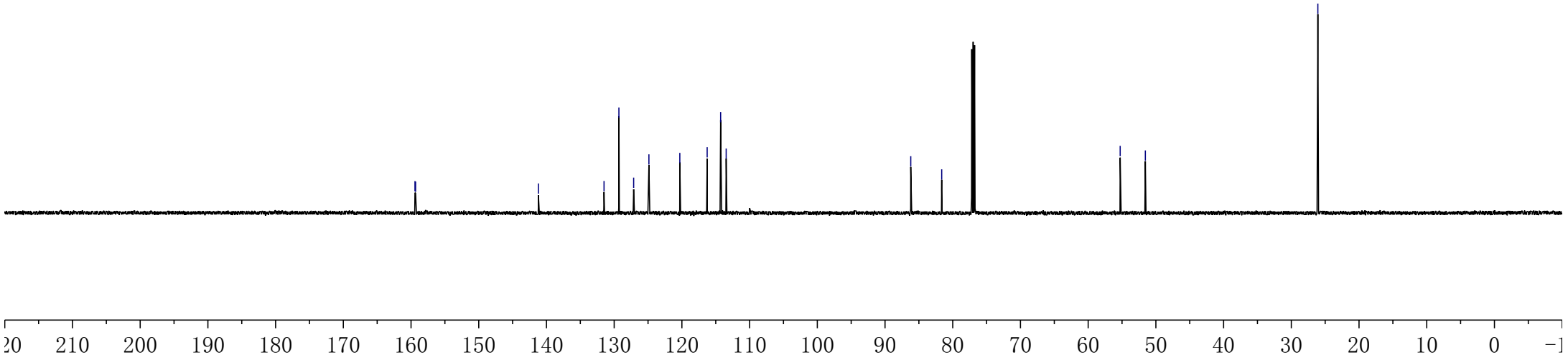

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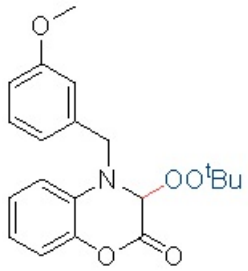

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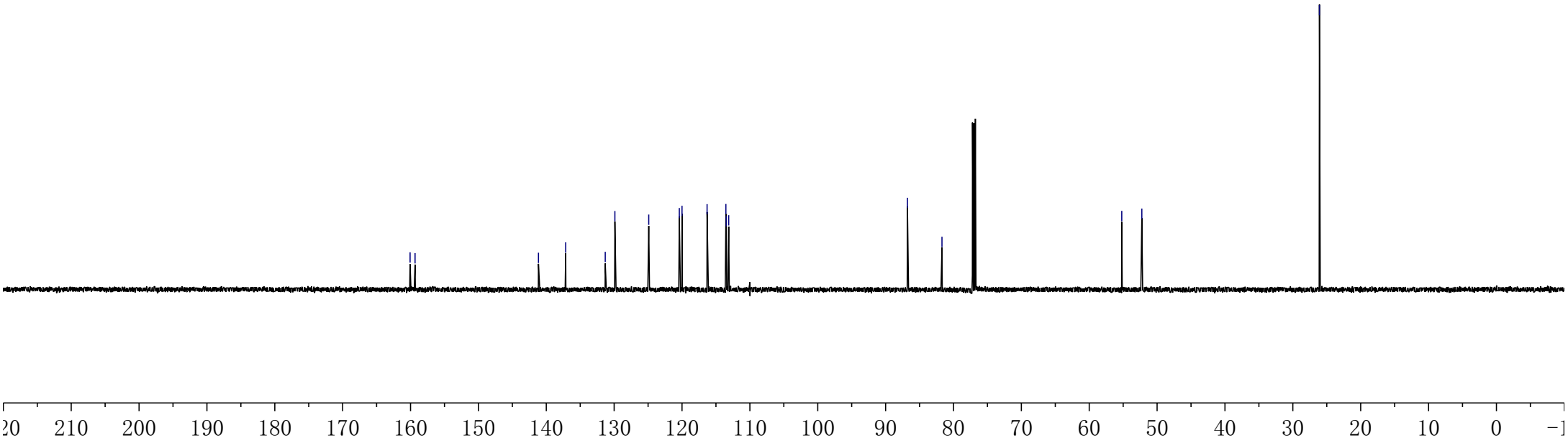

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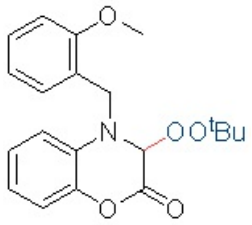

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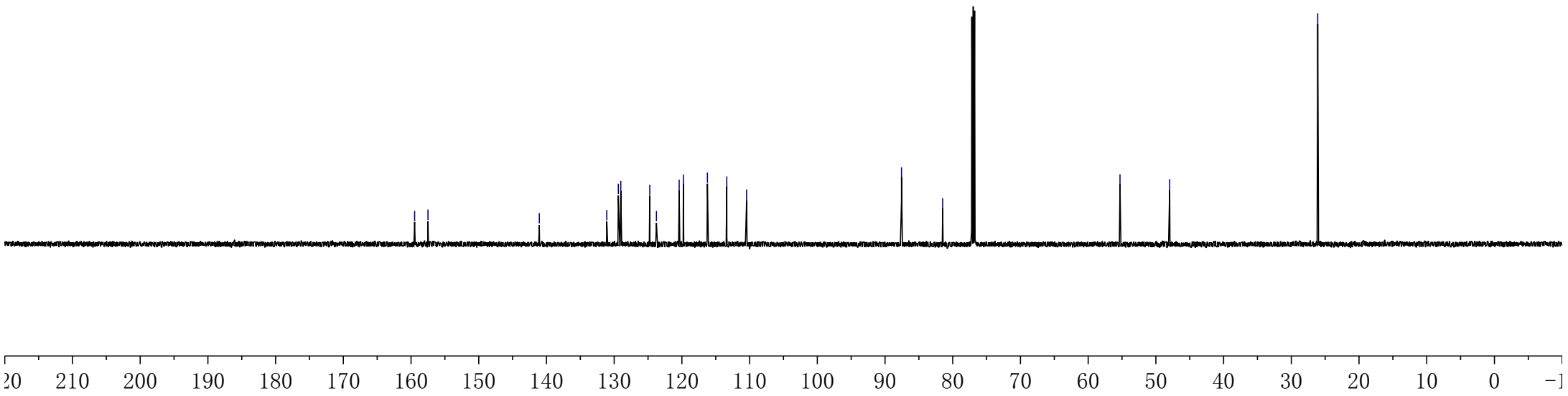

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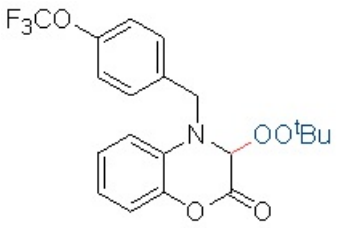

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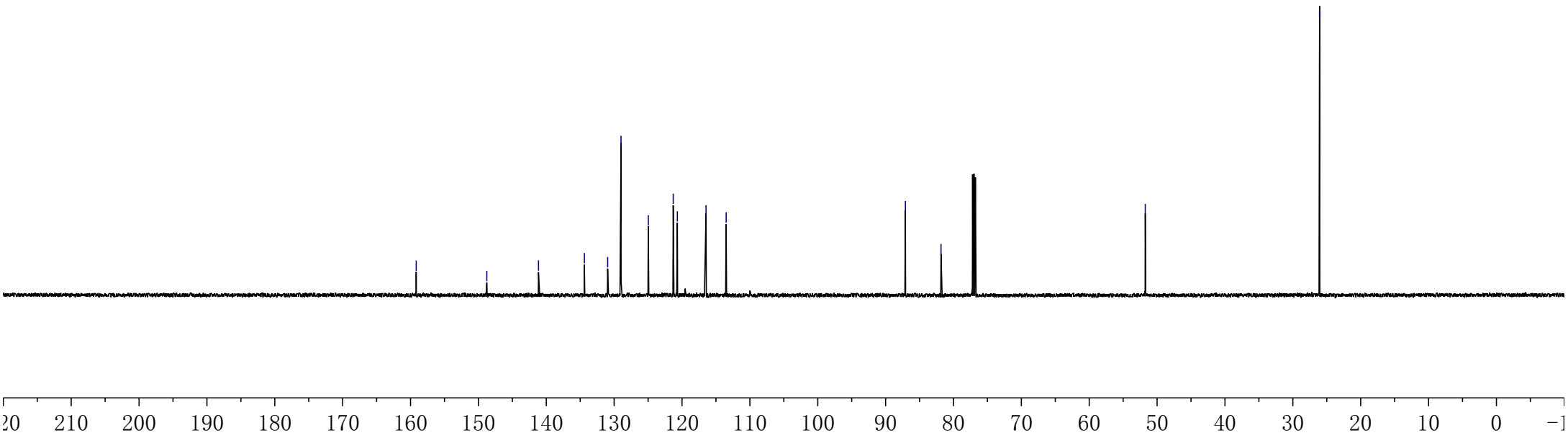

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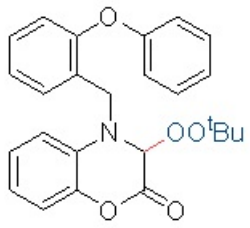

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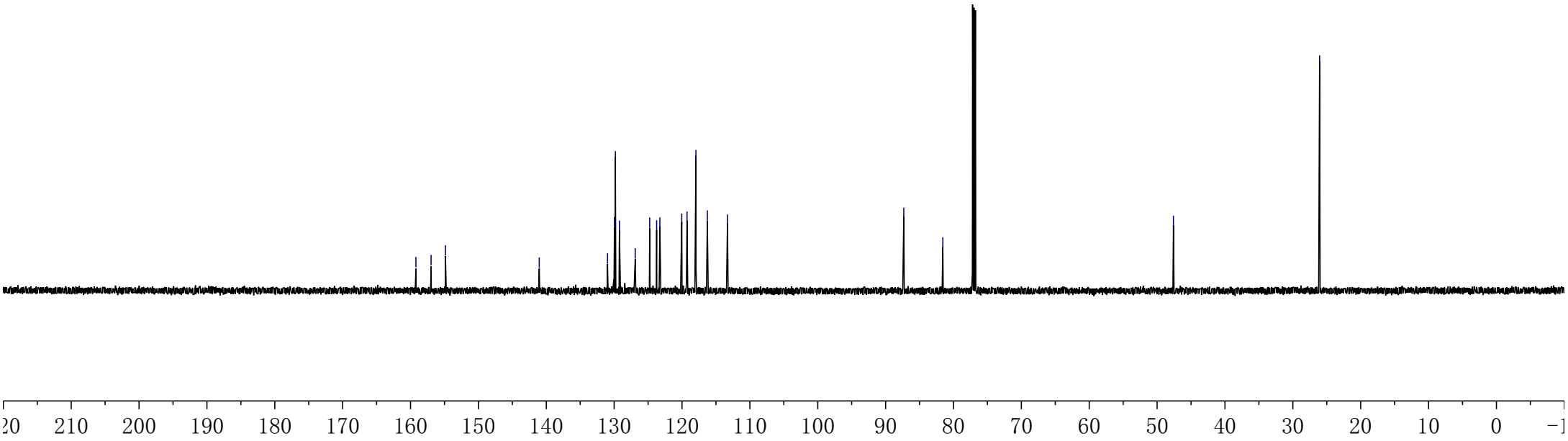

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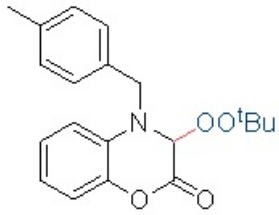

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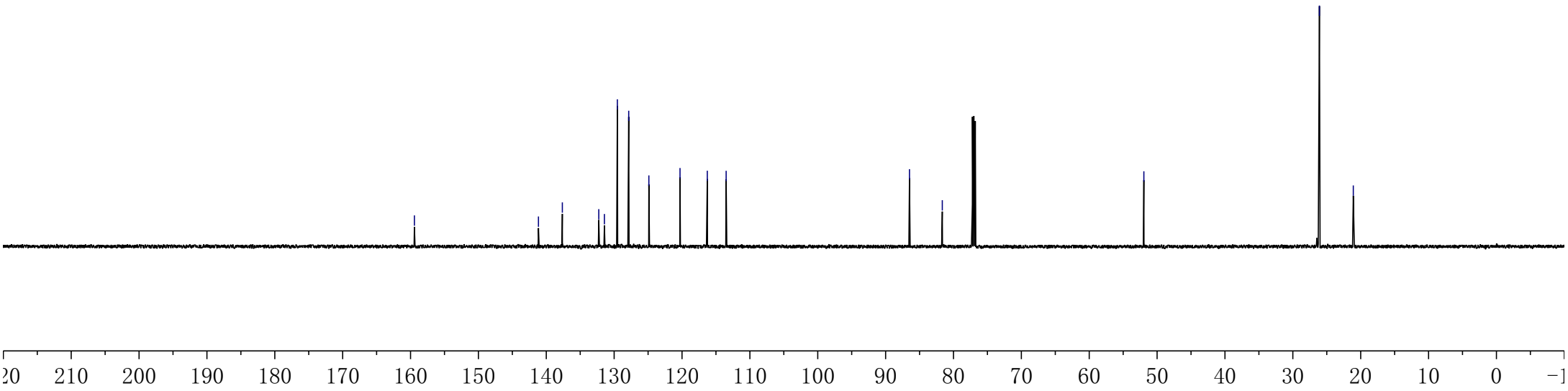

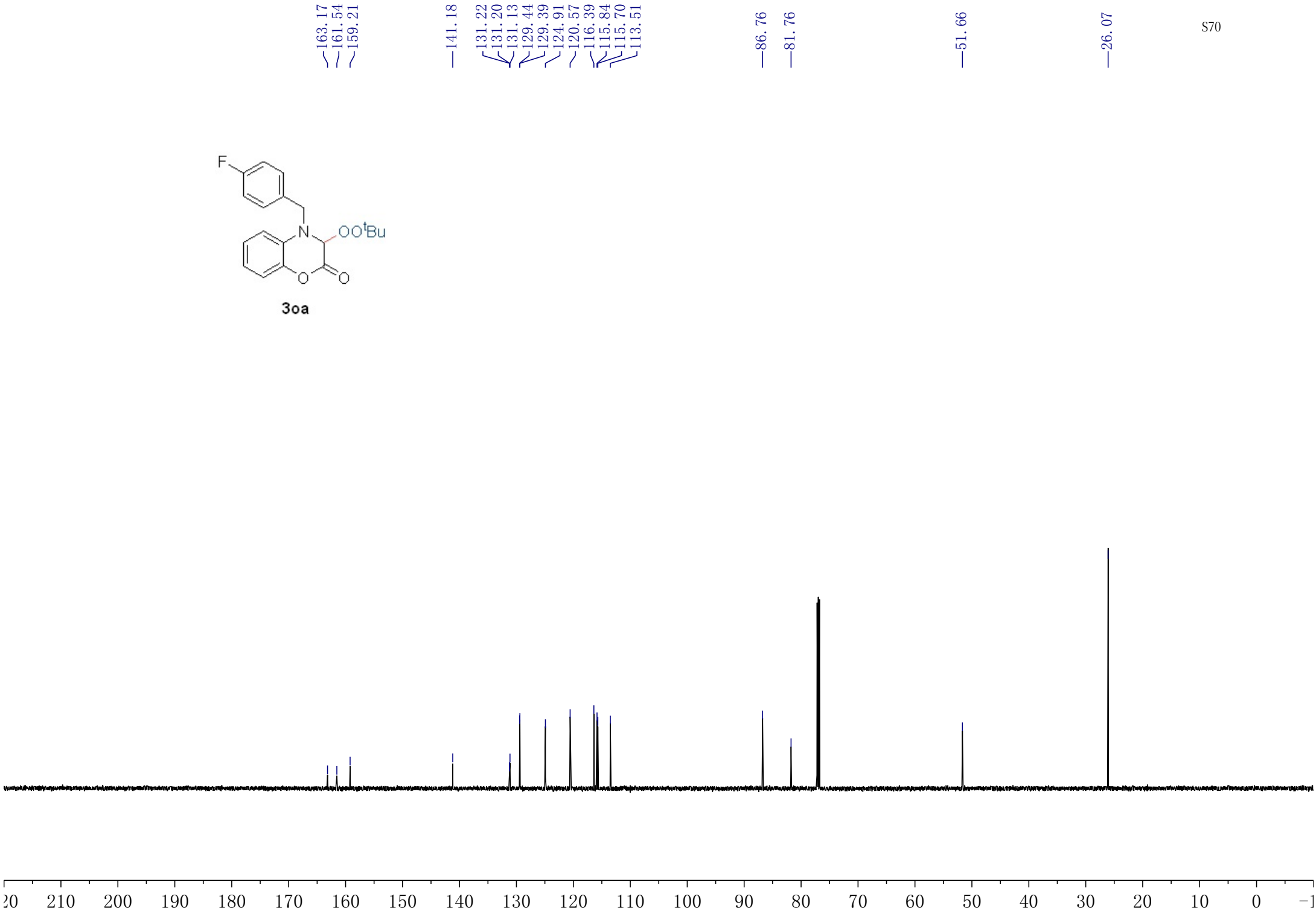
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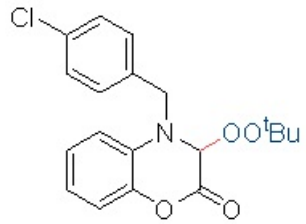

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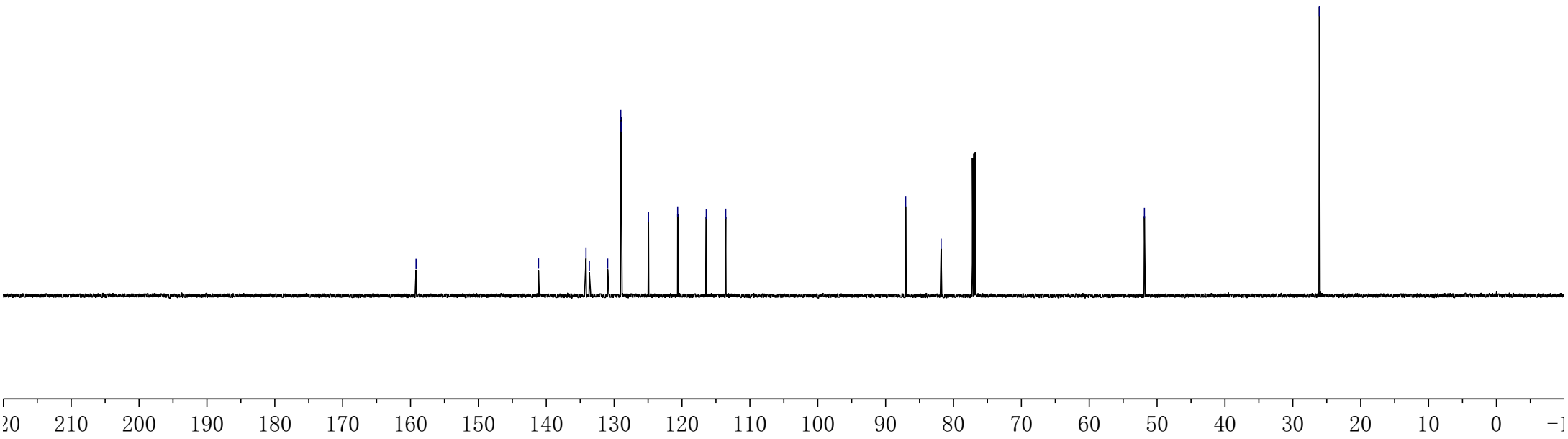

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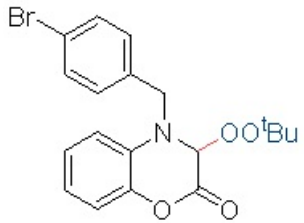

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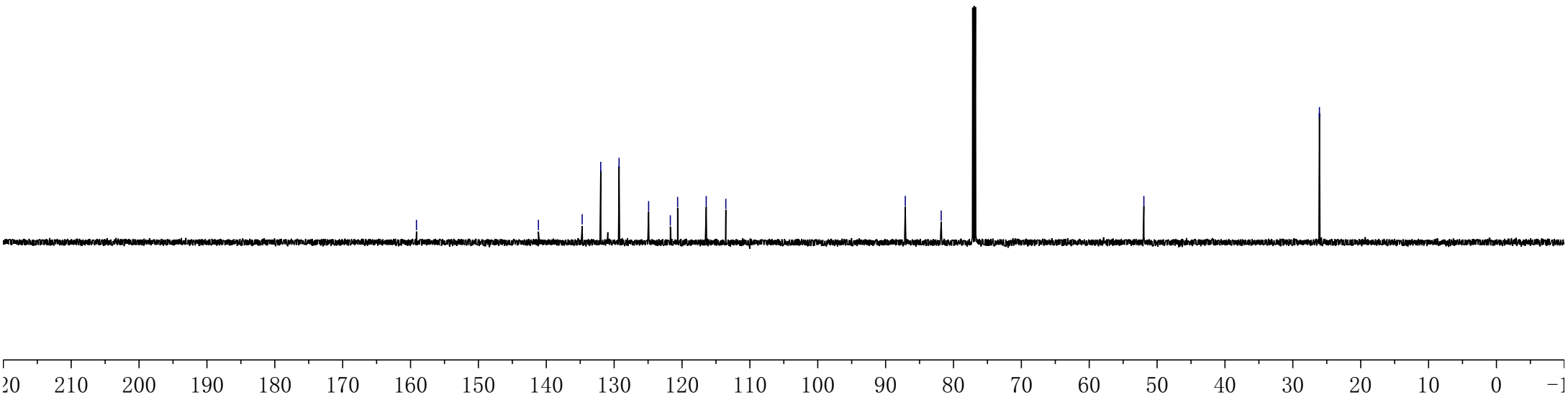

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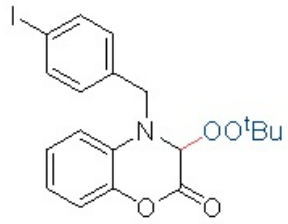

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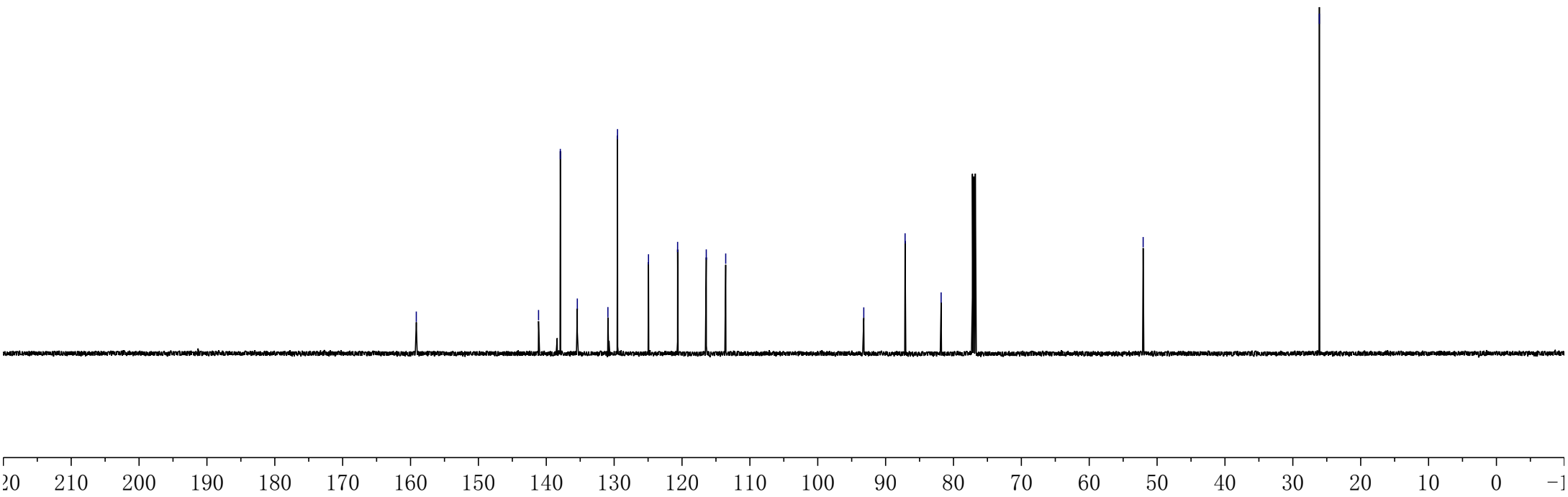

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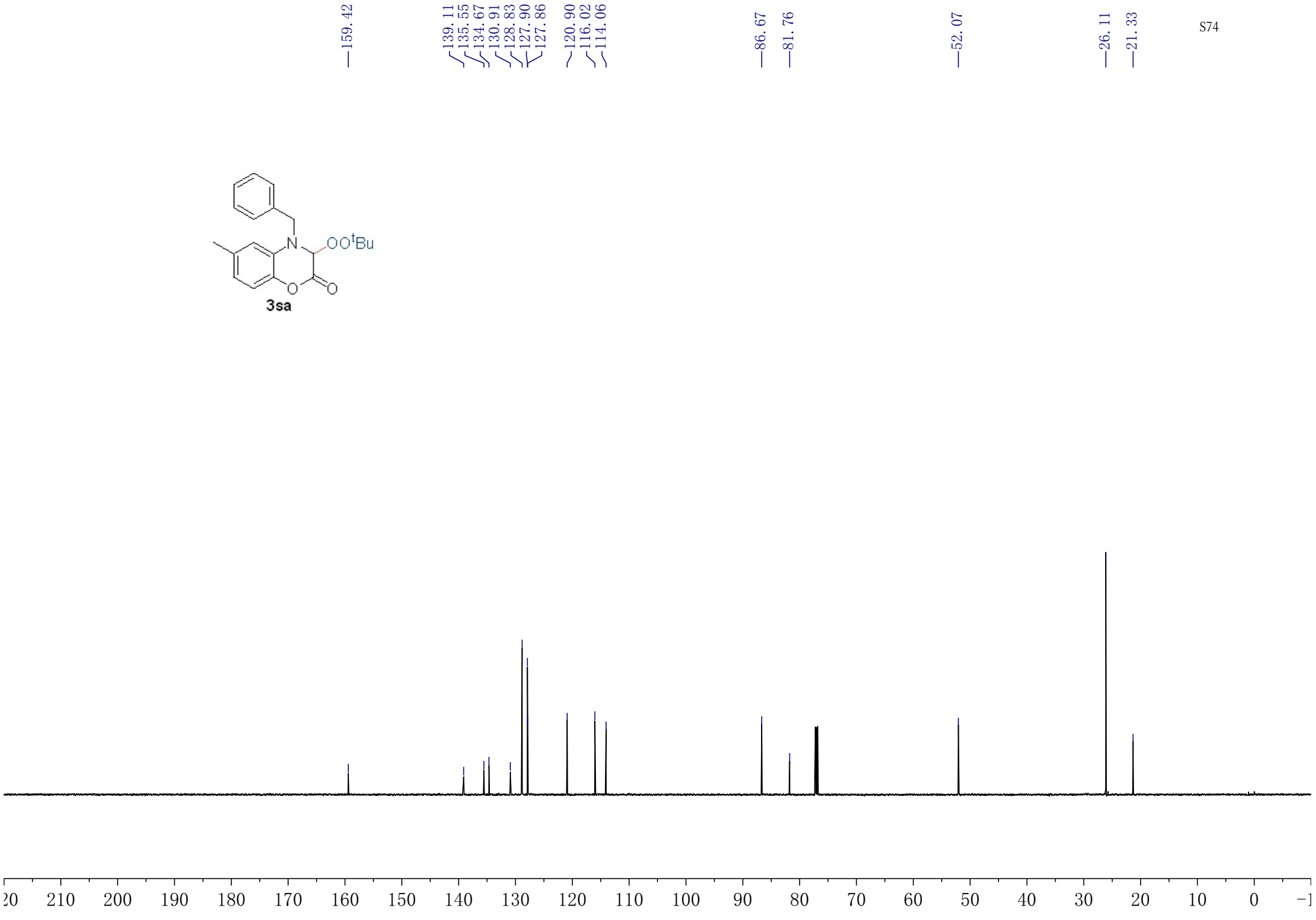
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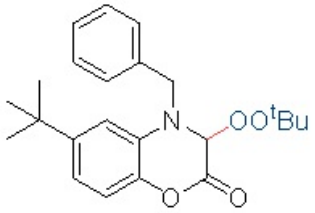

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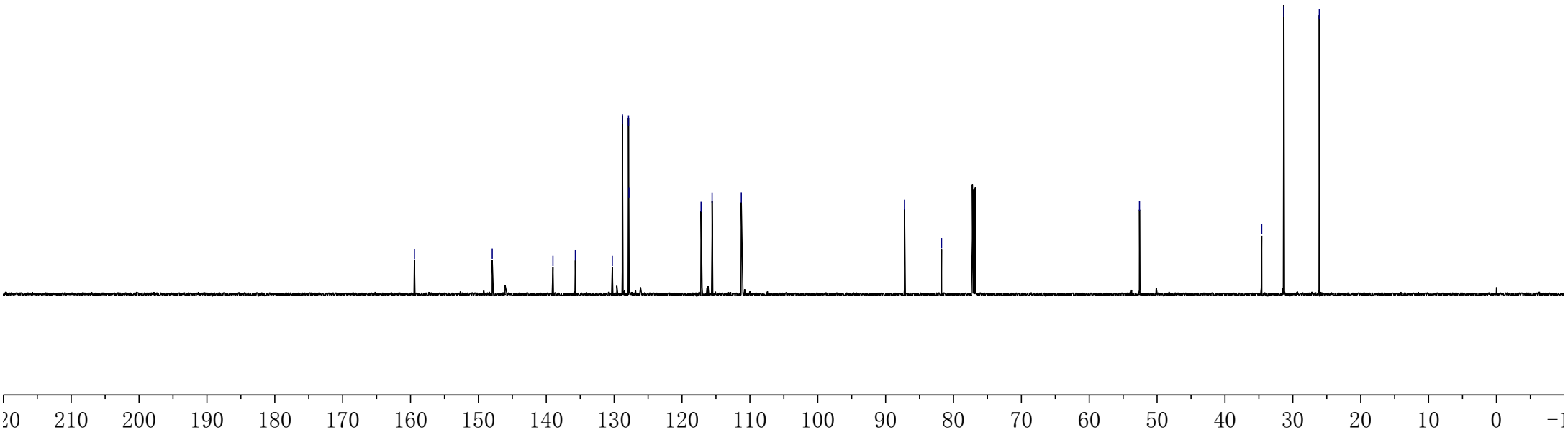

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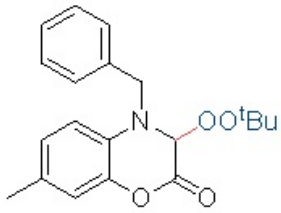

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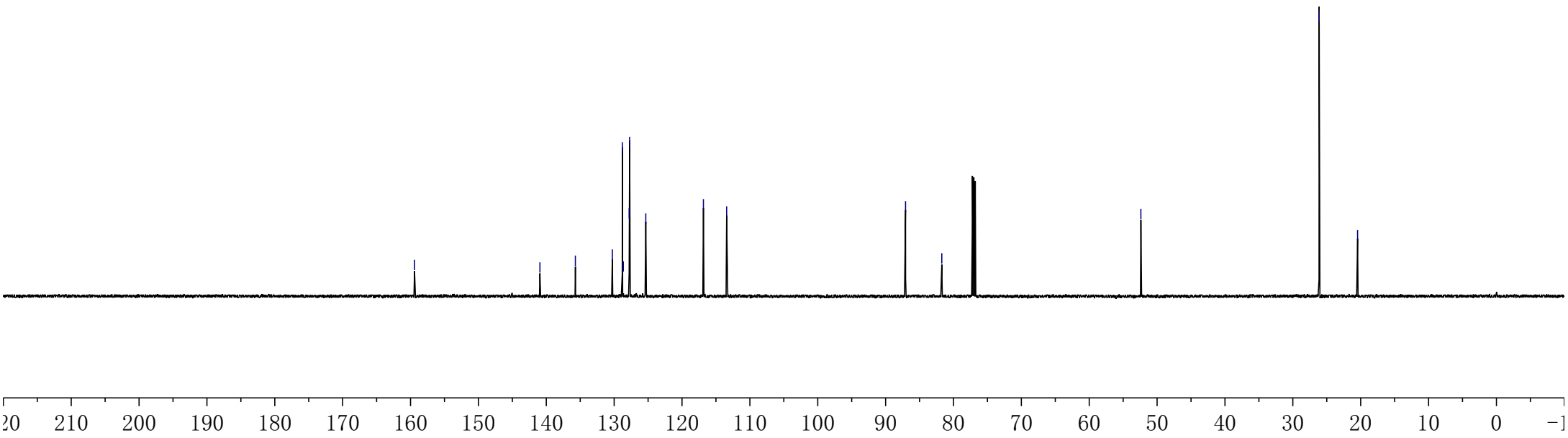

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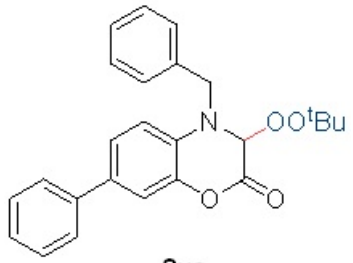

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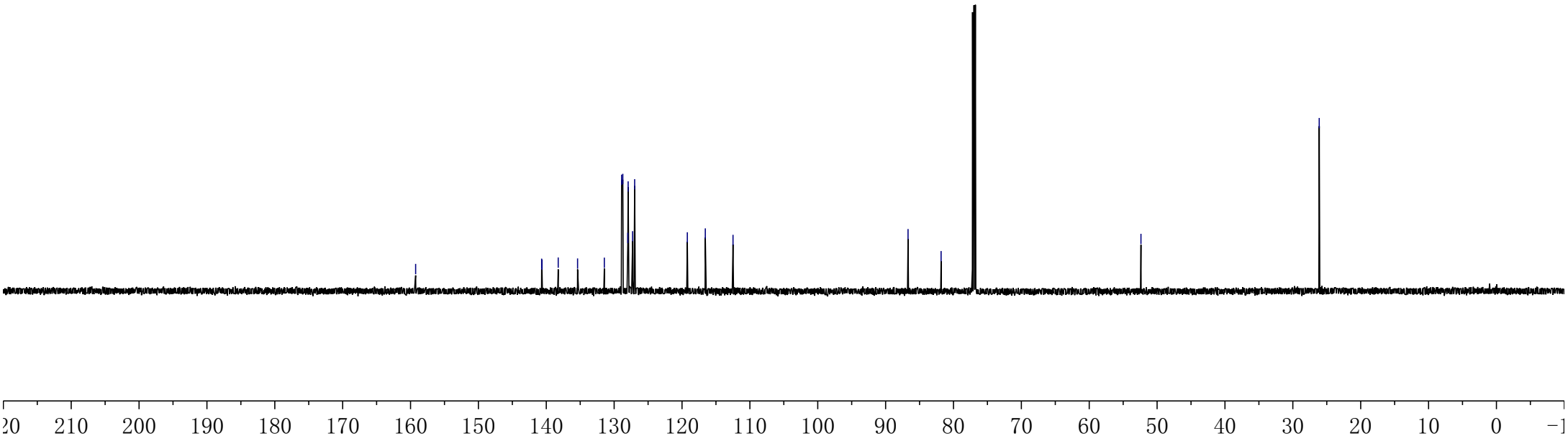

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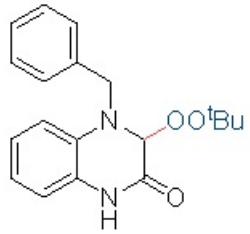

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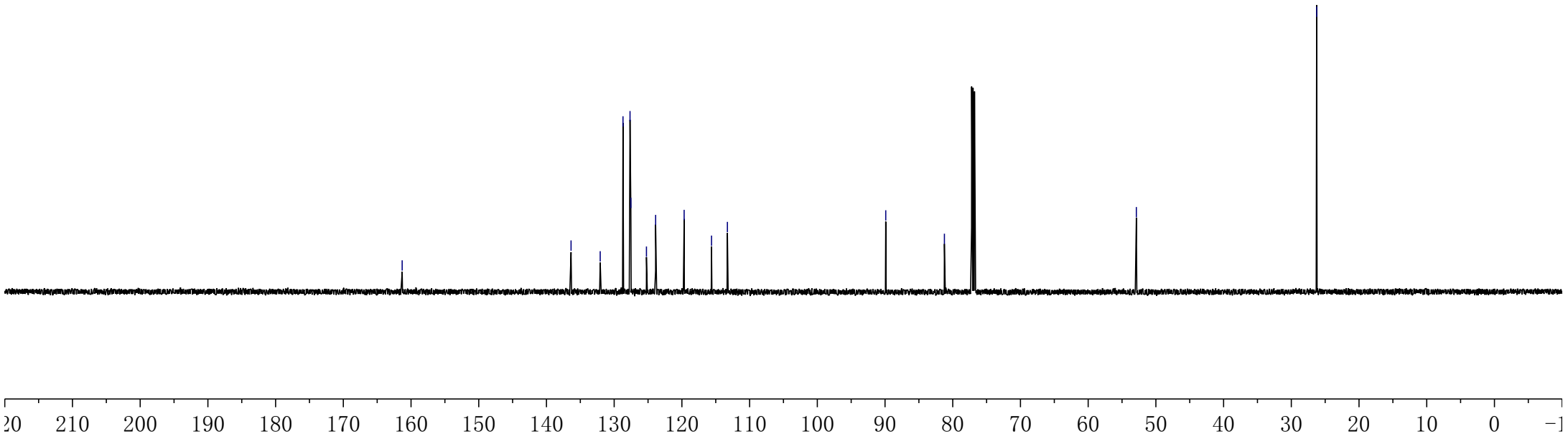

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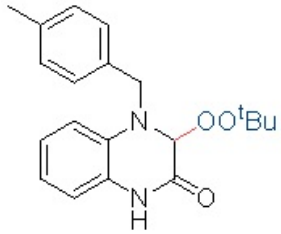

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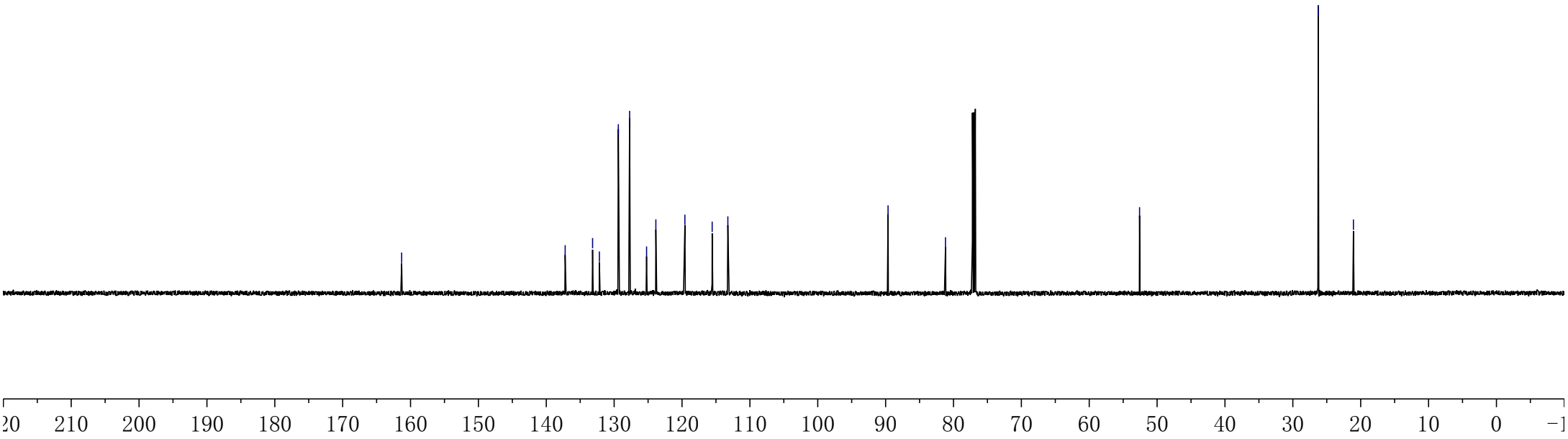

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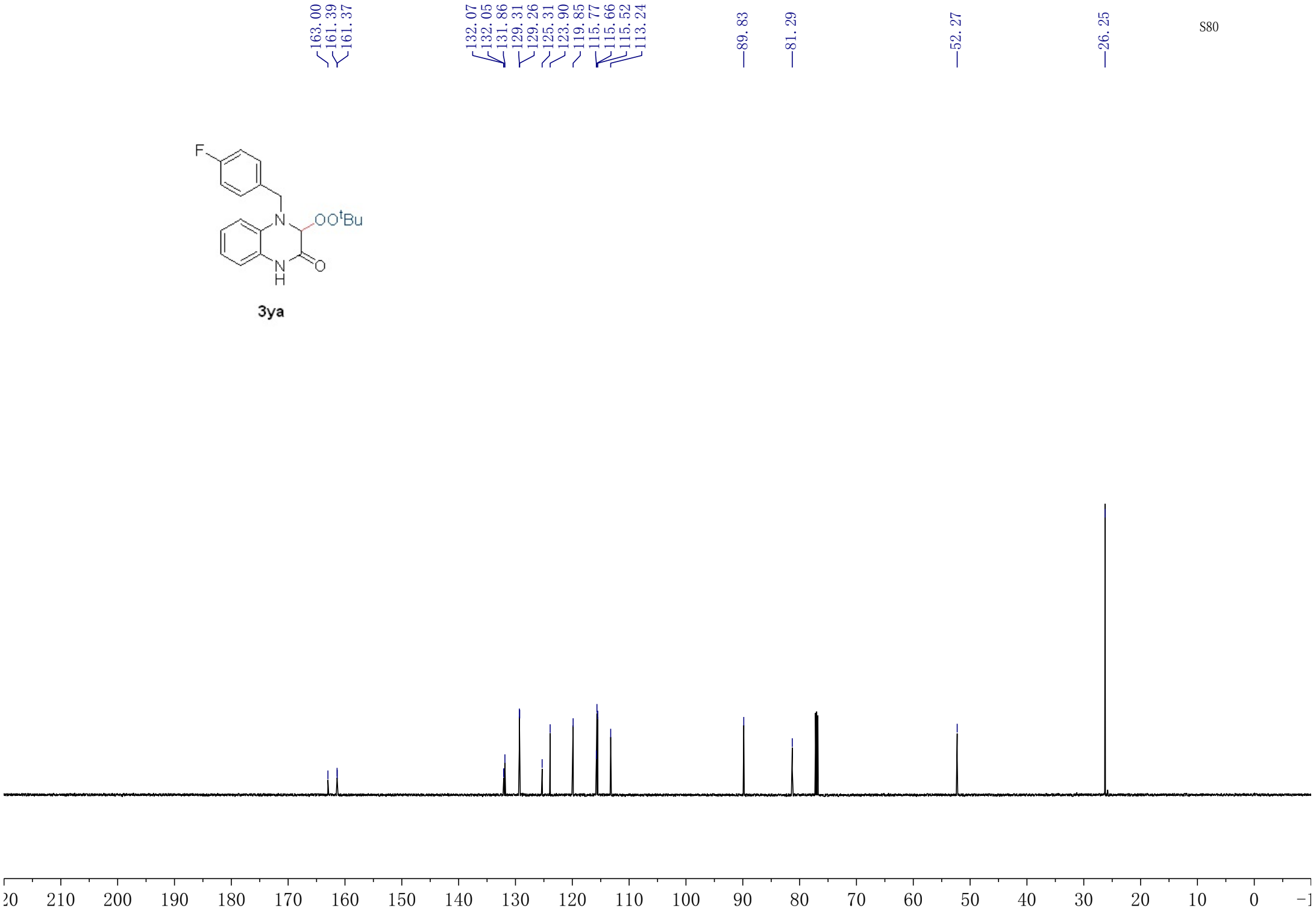
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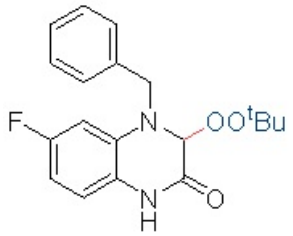

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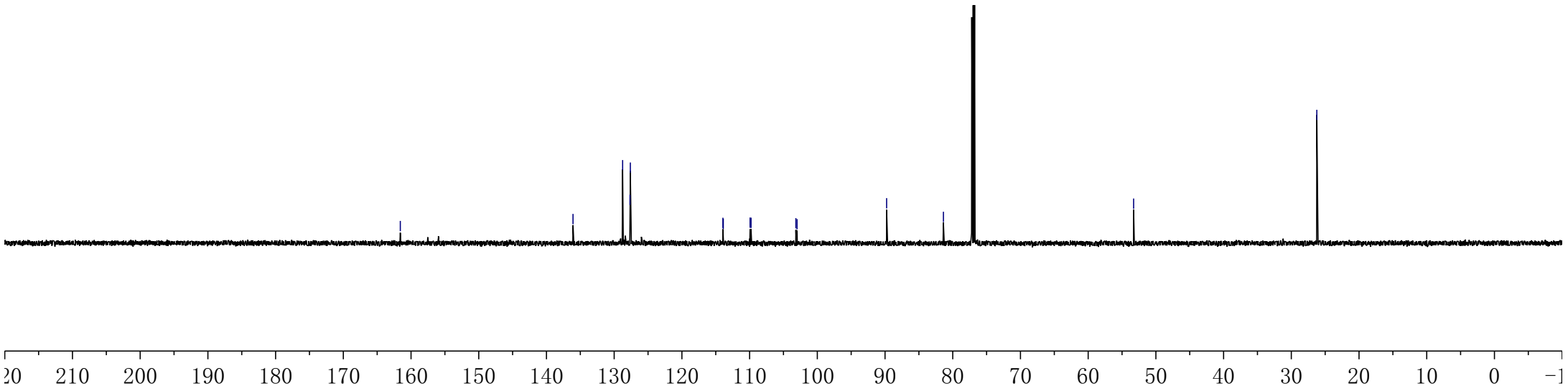

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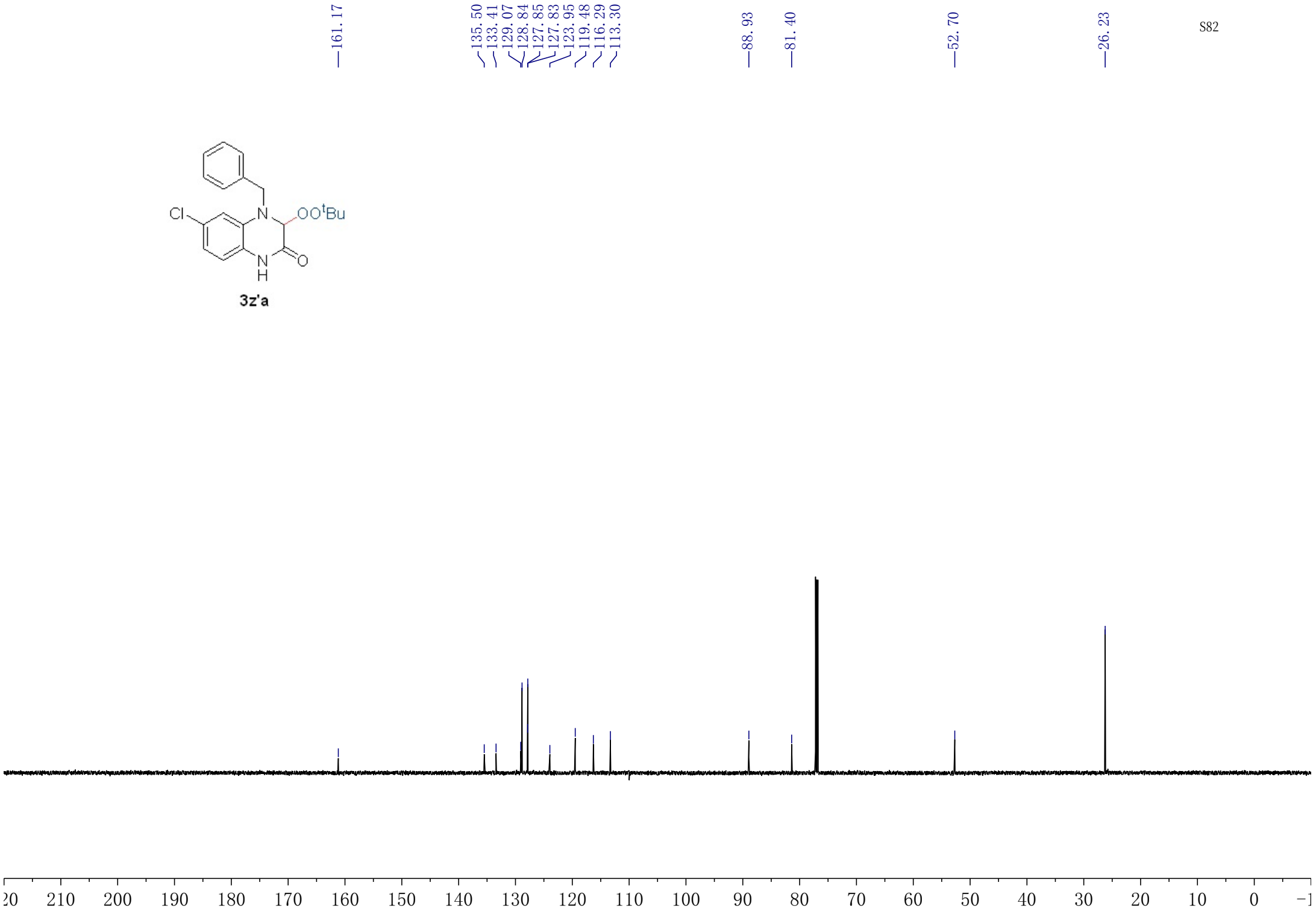
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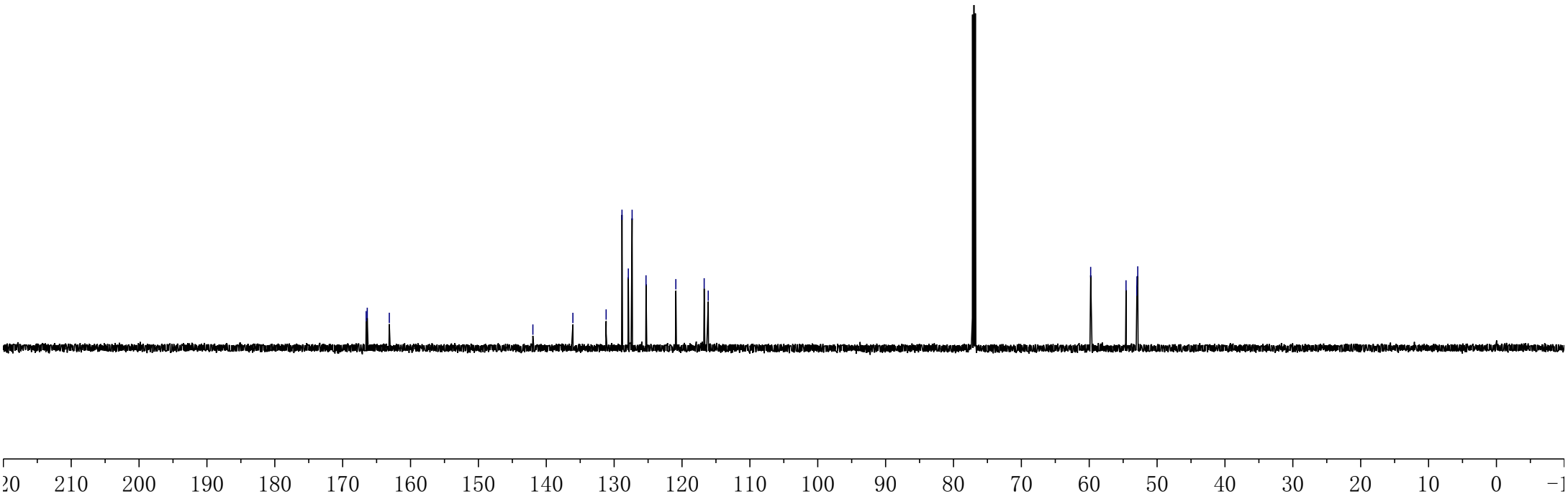

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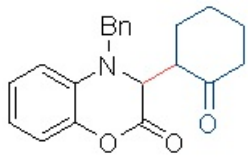

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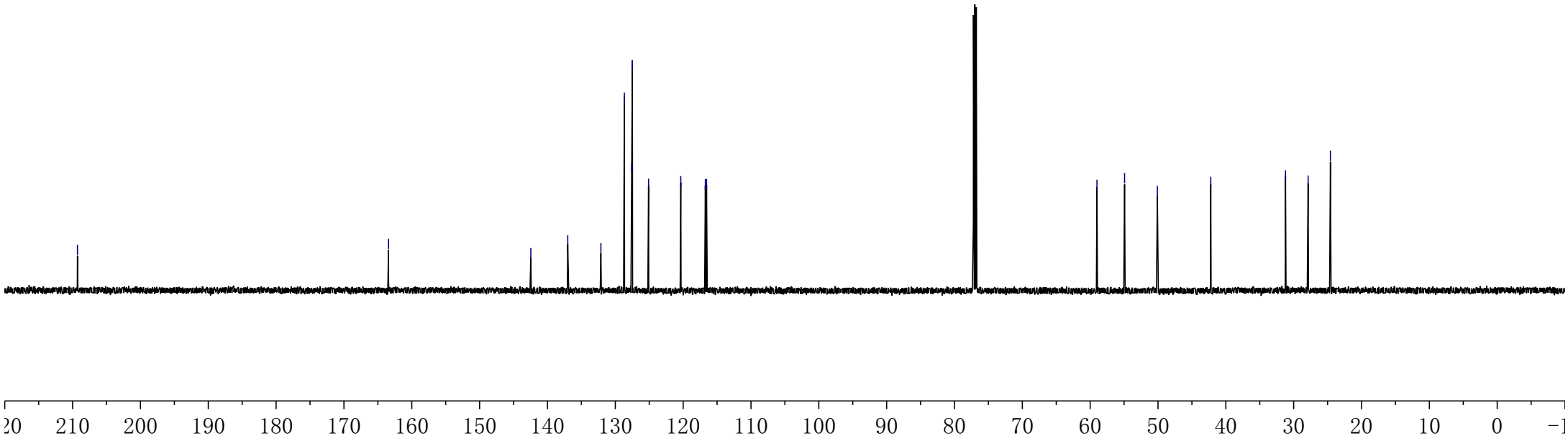

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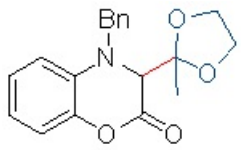

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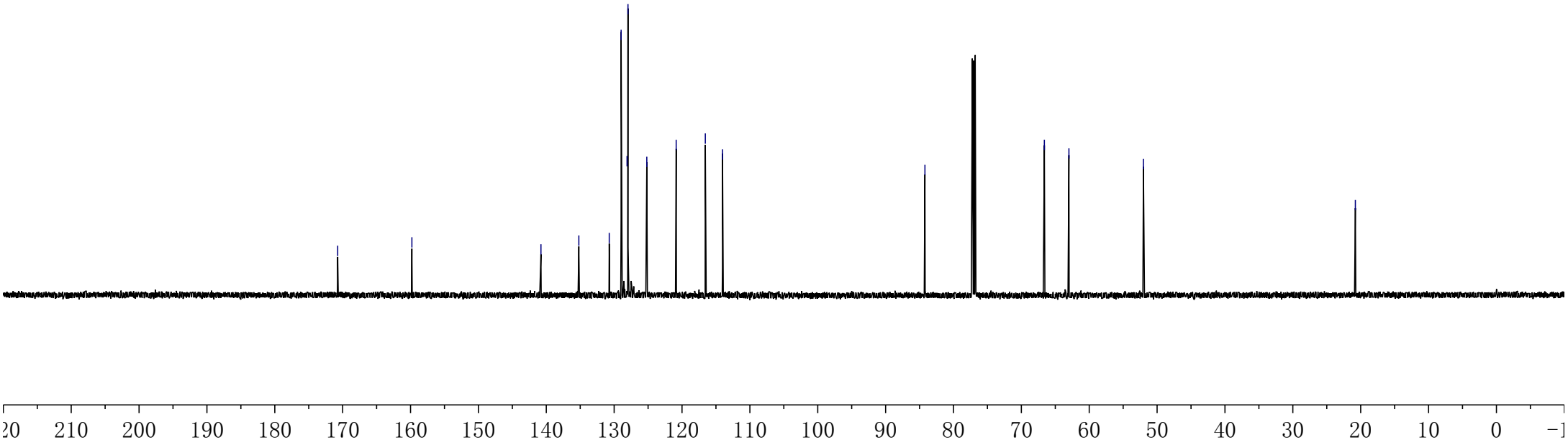

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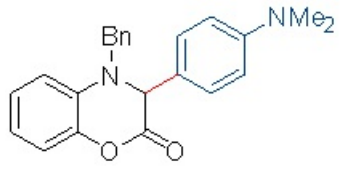

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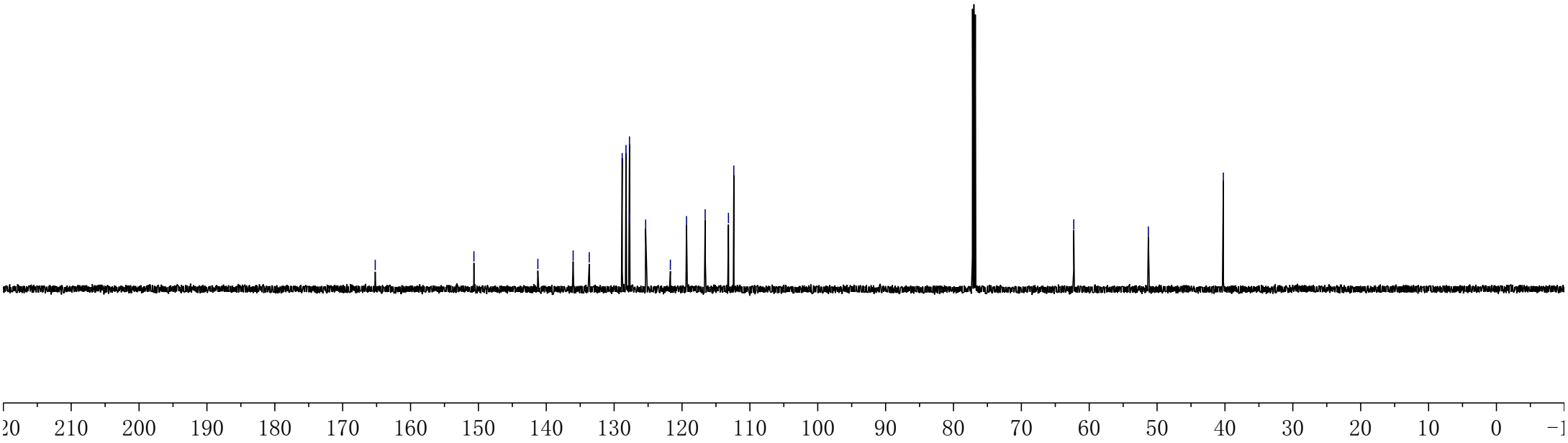

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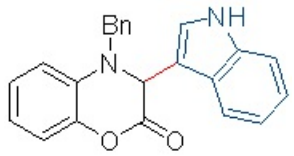

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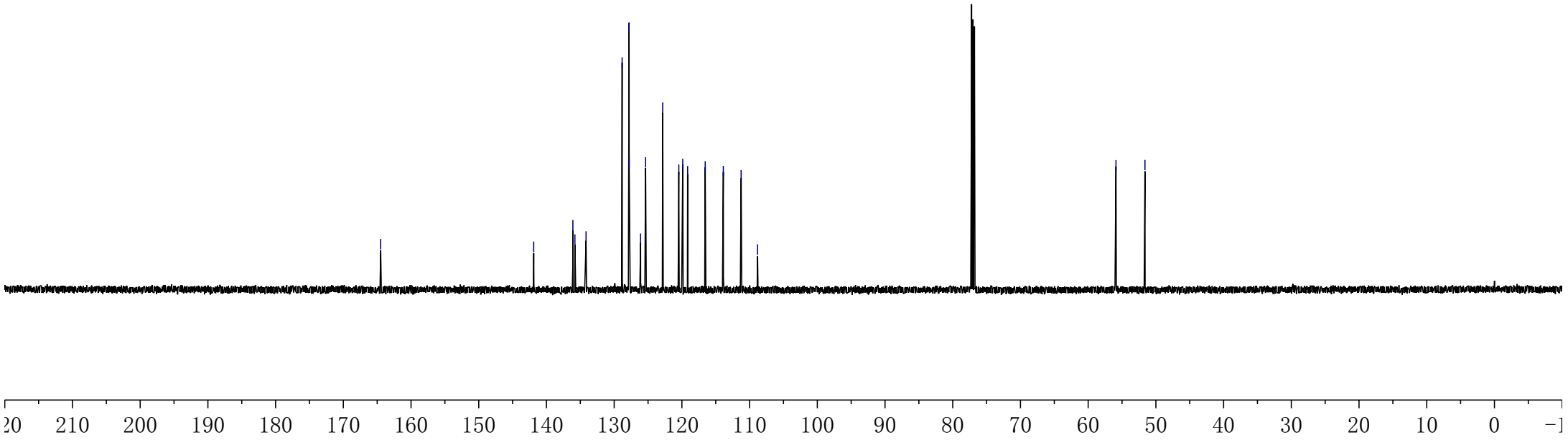

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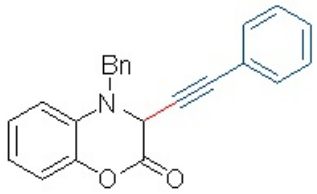

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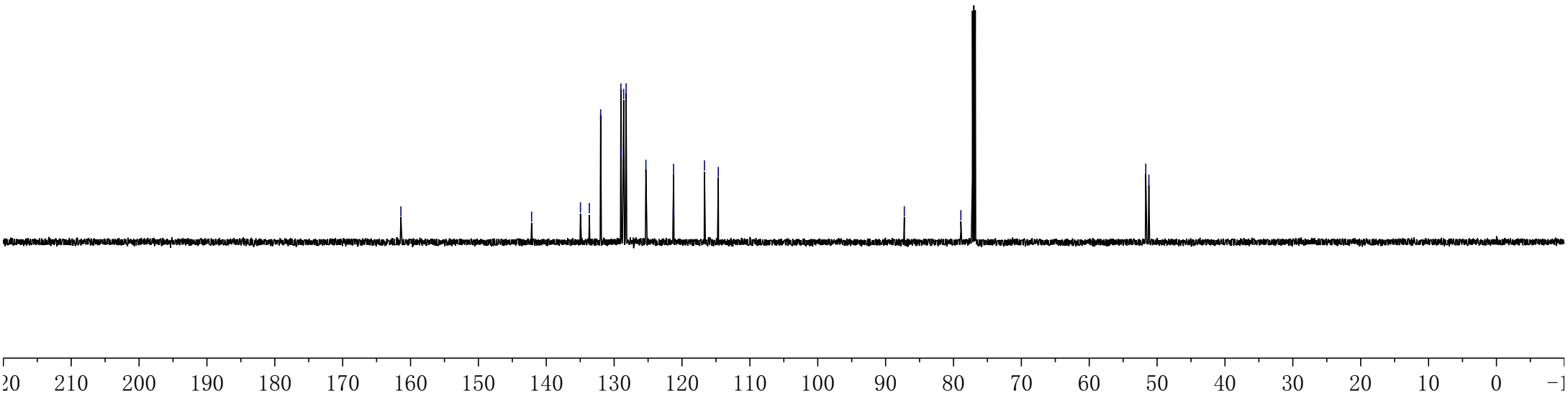

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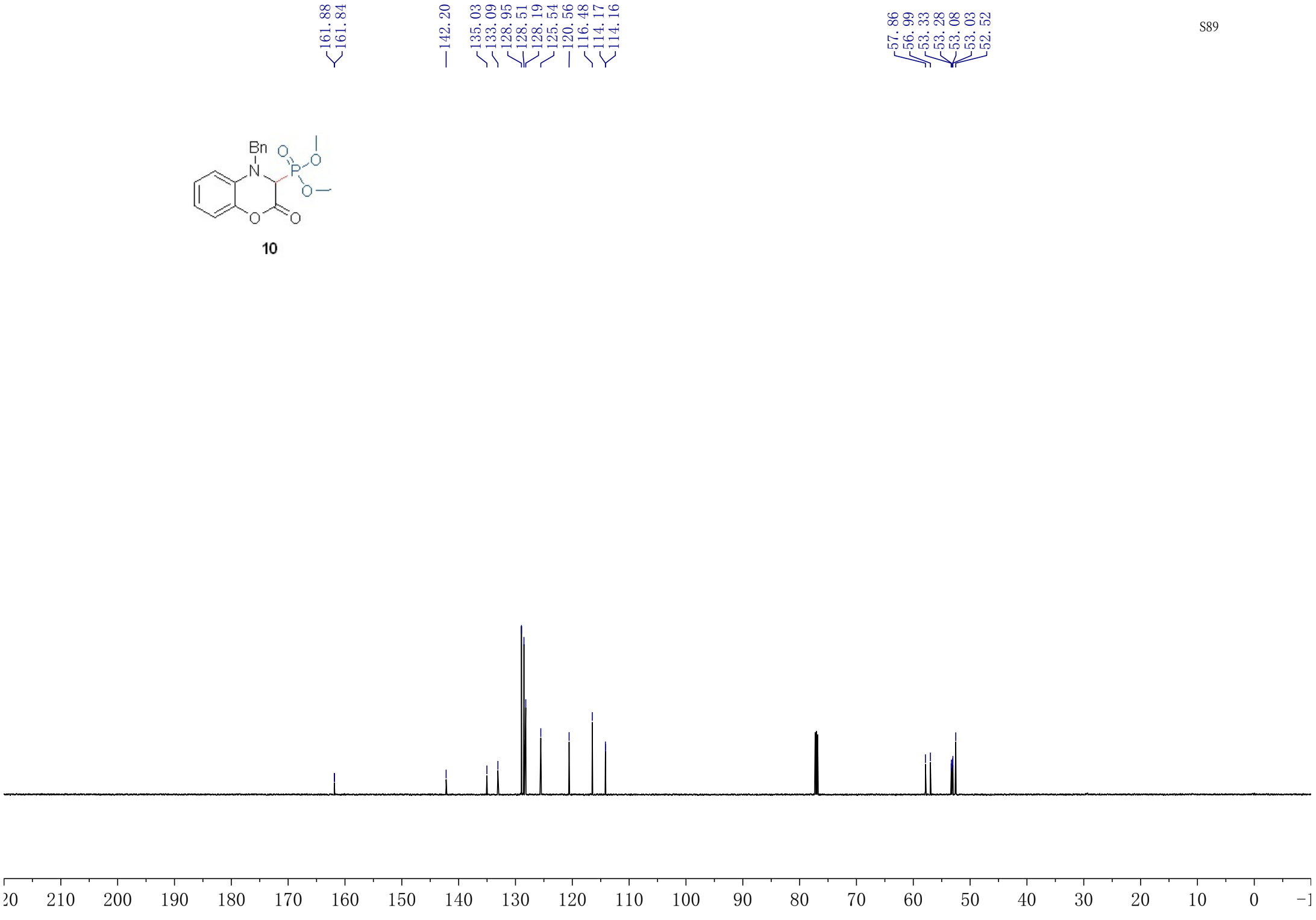
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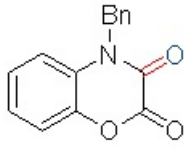
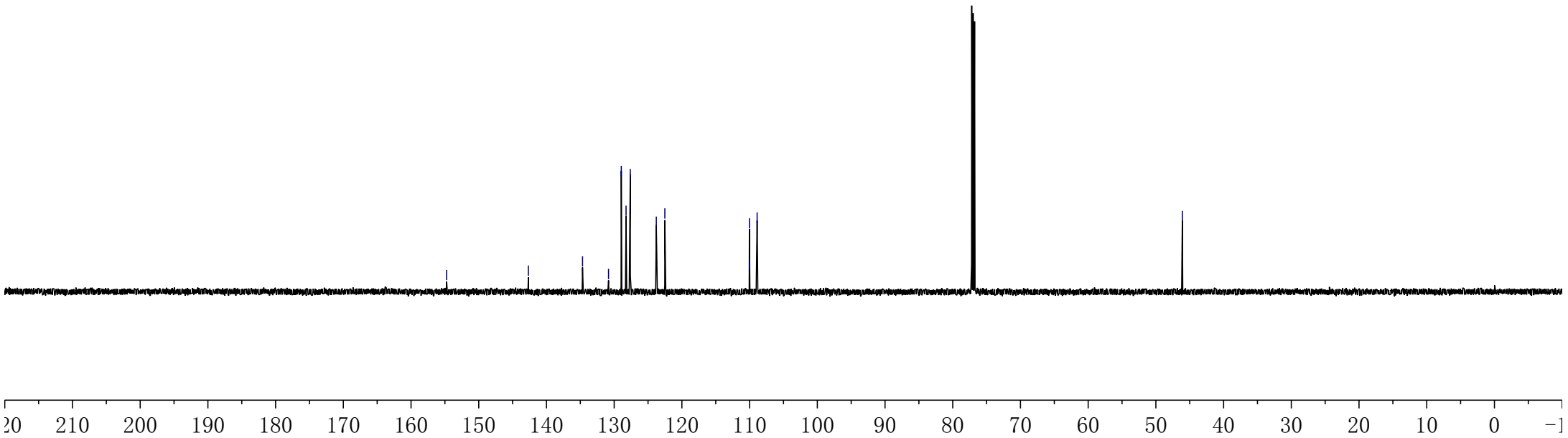
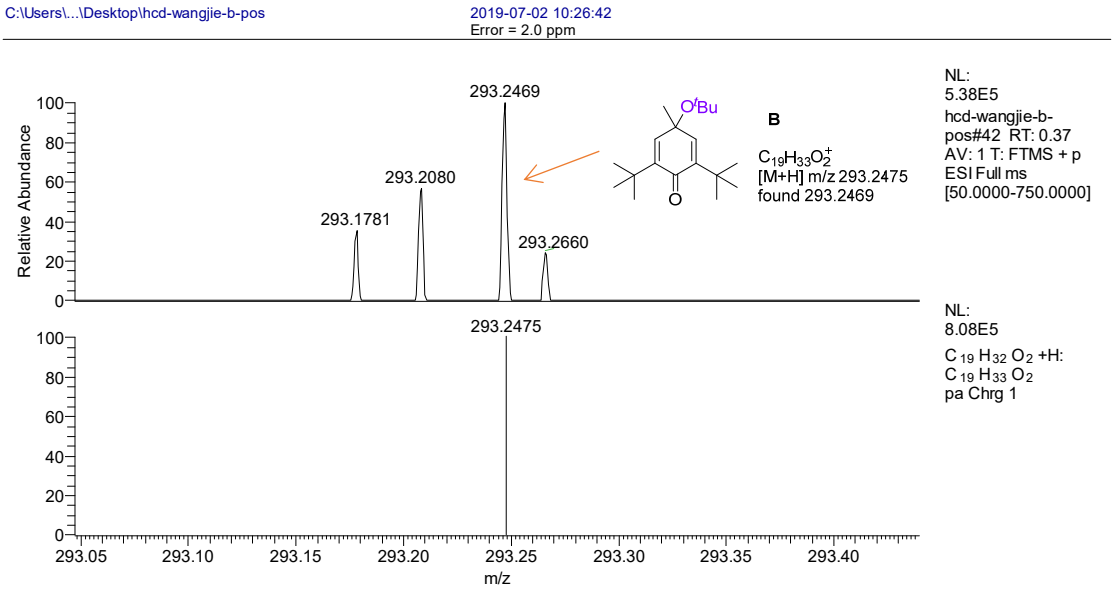
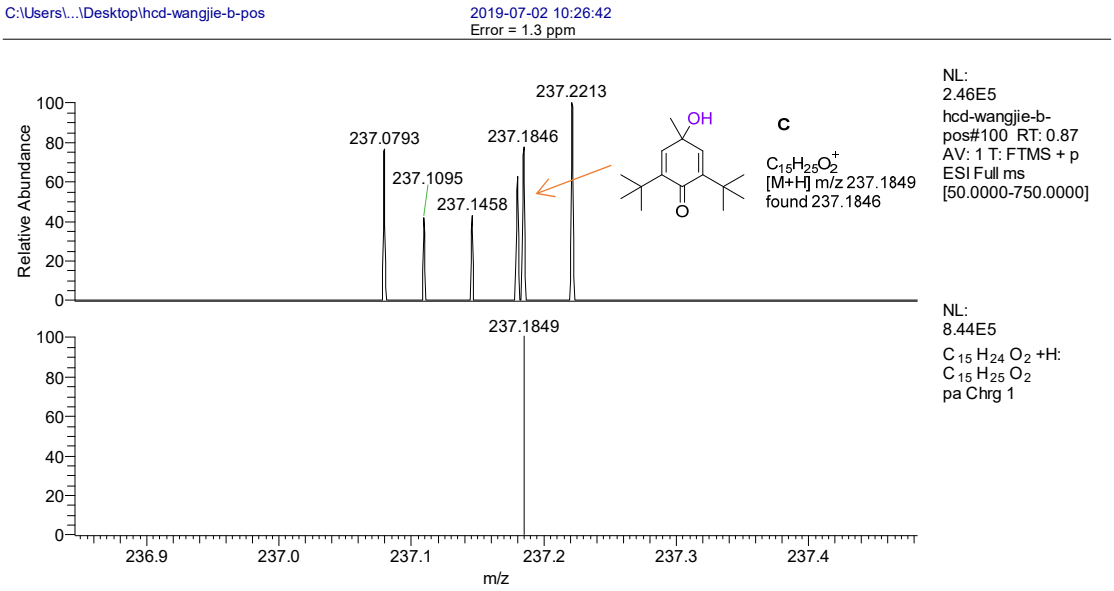
108.89
46.09

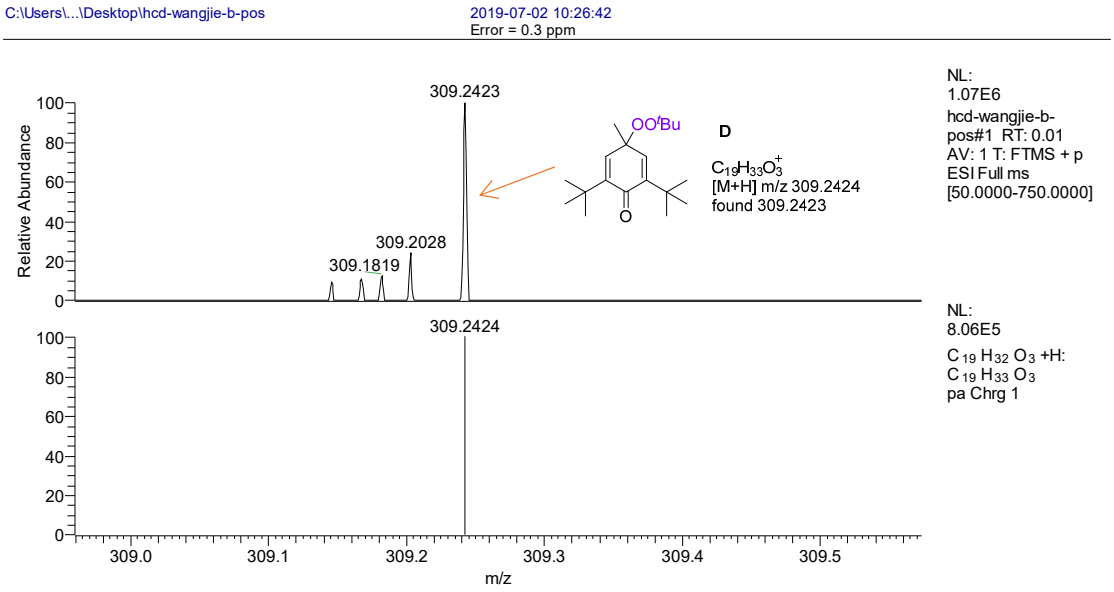


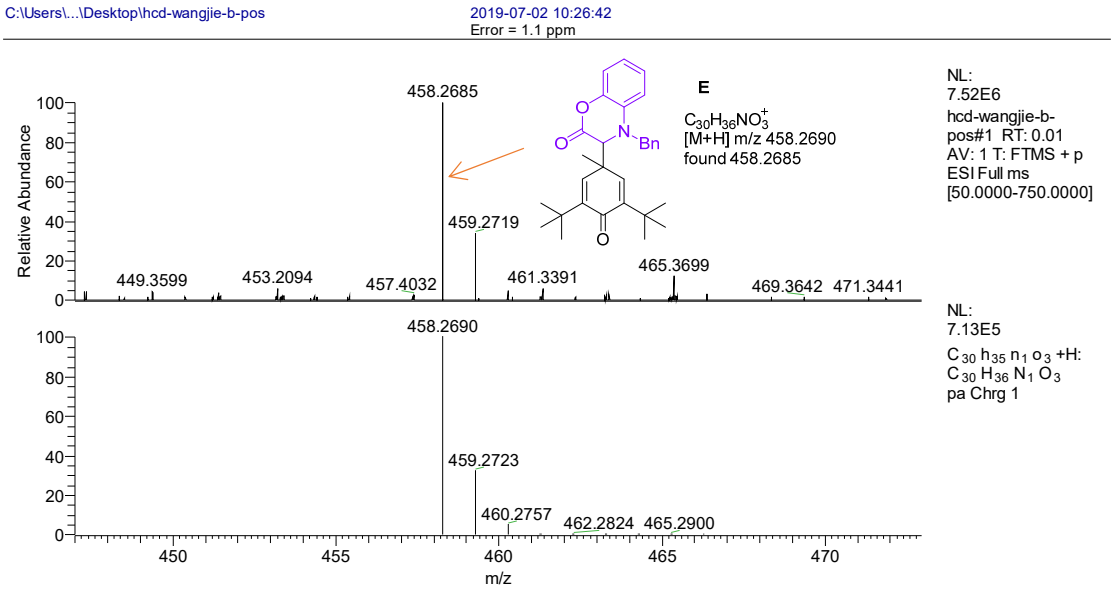
11




C:\Users\...\Desktop\hcd-wangjie-b-pos
2019-07-02 10:26:42
Error = 2.0 ppm
Relative Abundance
293.2469
293.2080
293.1781
293.2660
O'Bu
O
B
C19H33O2+
[M+H] m/z 293.2475
found 293.2469
NL:
5.38E5
hcd-wangjie-b-pos#42 RT: 0.37
AV: 1 T: FTMS + p
ESI Full ms
[50.0000-750.0000]
293.2475
NL:
8.08E5
C 19 H 32 O 2 +H:
C 19 H 33 O 2
pa Chrg 1
293.05
293.10
293.15
293.20
293.25
293.30
293.35
293.40
m/z


C:\Users\...\Desktop\hcd-wangjie-b-pos
2019-07-02 10:26:42
Error = 1.3 ppm
Relative Abundance
237.2213
237.0793
237.1846
237.1095
237.1458
OH
O
C
C15H25O2+
[M+H] m/z 237.1849
found 237.1846
NL:
2.46E5
hcd-wangjie-b-pos#100 RT: 0.87
AV: 1 T: FTMS + p
ESI Full ms
[50.0000-750.0000]
237.1849
NL:
8.44E5
C 15 H 24 O 2 +H:
C 15 H 25 O 2
pa Chrg 1
236.9
237.0
237.1
237.2
237.3
237.4
m/z


C:\Users\...\Desktop\hcd-wangjie-b-pos
2019-07-02 10:26:42
Error = 0.3 ppm
Relative Abundance
309.2423
309.2028
309.1819
OO^{t}Bu
O
D
$C_{19}H_{33}O_3^+$
[M+H] m/z 309.2424
found 309.2423
NL:
1.07E6
hcd-wangjie-b-pos#1 RT: 0.01 AV: 1 T: FTMS + p ESI Full ms [50.0000-750.0000]
309.2424
NL:
8.06E5
C 19 H 32 O 3 +H:
C 19 H 33 O 3
pa Chrg 1
309.0
309.1
309.2
309.3
309.4
309.5
m/z


C:\Users\...\Desktop\hcd-wangjie-b-pos
2019-07-02 10:26:42
Error = 1.1 ppm
Relative Abundance
458.2685
459.2719
449.3599
453.2094
457.4032
461.3391
465.3699
469.3642
471.3441
O
N
Bn
O
E
$C_{30}H_{36}NO_3^+$
[M+H] m/z 458.2690
found 458.2685
NL:
7.52E6
hcd-wangjie-b-pos#1 RT: 0.01 AV: 1 T: FTMS + p ESI Full ms [50.0000-750.0000]
458.2690
459.2723
460.2757
462.2824
465.2900
NL:
7.13E5
C 30 h 35 n 1 o 3 +H:
C 30 H 36 N 1 O 3
pa Chrg 1
450
455
460
465
470
m/z