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Supporting Information

Metal-Free Formal Carbon–Halogen Bond Insertion: Facile Syntheses of 3-Halo 3,3'-Disubstitutedoxindoles and Spirooxindole-γ-butyrolactones

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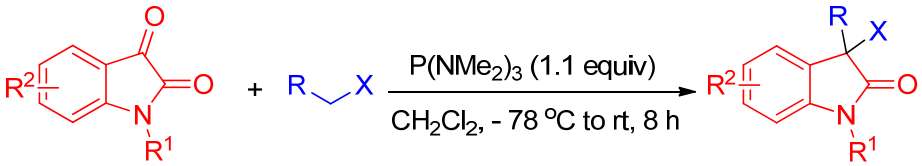
I. General Information

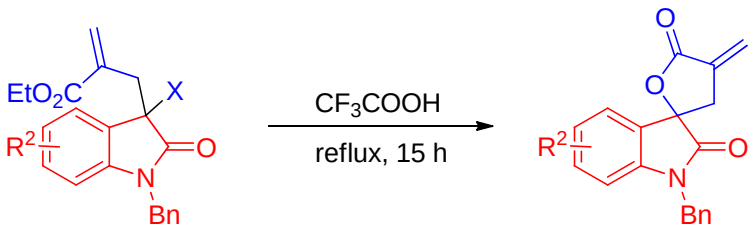
Unless otherwise noted, all reactions were carried out in nitrogen atmosphere under anhydrous conditions. Solvents were purified prior to use according to standard procedures. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ with tetramethylsilane (TMS) as the internal standard. Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether/ethyl acetate as eluant. Isatins[1] were prepared according to the literature procedures. The allylic bromides and chlorides were prepared from corresponding Morita-Baylis-Hillman adducts or commercially available.

II. Typical Procedure for the C–X Insertion Reactions



Under N_2 atmosphere and at - 78 °C, a solution of $P(NMe_2)_3$ (0.22 mmol, 40 μL) in CH_2Cl_2 (0.5 mL) was added dropwise by means of syringe to a solution of isatin (0.2 mmol), allylic/benzylic bromide/chloride (0.3 mmol), and 4Å molecular sieves (100 mg) in CH_2Cl_2 (1.5 mL). The resulting reaction mixture was then slowly warmed up to room temperature and stirred at rt until isatin was completely consumed, as monitored by TLC. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel by gradient elution with petroleum ether/ ethyl acetate (20:1-5:1) to give the C–X bond insertion product.

III. Typical Procedure for the Preparation of Spirooxindole-γ-butyrolactones

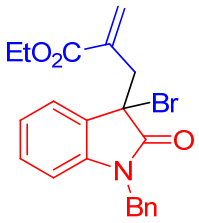


The corresponding insertion product (0.2 mmol) was dissolved in trifluoroacetic acid (3.0 mL),

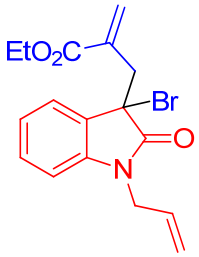
1 (*a*) S.-H. Cao, X.-C. Zhang, Y. Wei and M. Shi, *Eur. J. Org. Chem.*, 2011, 2668; (*b*) K. Aikawa, S. Mimura, Y. Numata and K. Mikami, *Eur. J. Org. Chem.*, 2011, 62.

and the resulting mixture was heated under reflux for 15 h. After the reaction was cooled to room temperature, DCM (30 mL) was added, and the mixture was washed with water (2 × 10 mL) and saturated brine (10 mL) sequentially. The organic phase was dried over anhydrous Na_2SO_4, and purified using column chromatography isolation on silica gel by gradient elution with petroleum ether / ethyl acetate (15:1～3:1) to give the spirooxindole product.

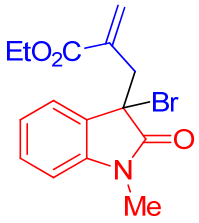
IV. Analytical Data for Compounds 6 to 39



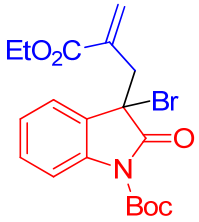
6. Yield 75%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.36 – 7.22 (m, 6H), 7.15 (td, *J* = 7.8, 1.3 Hz, 1H), 7.01 (td, *J* = 7.6, 0.9 Hz, 1H), 6.61 (d, *J* = 7.8 Hz, 1H), 6.09 (s, 1H), 5.63 (d, *J* = 0.8 Hz, 1H), 4.96 (d, *J* = 15.9 Hz, 1H), 4.86 (d, *J* = 15.8 Hz, 1H), 4.03 – 3.86 (m, 2H), 3.77 (d, *J* = 13.6 Hz, 1H), 3.42 (d, *J* = 13.6 Hz, 1H), 1.08 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 166.2, 141.5, 134.9, 134.9, 130.1, 129.9, 128.7, 128.1, 127.6, 126.9, 126.1, 122.8, 109.6, 60.8, 55.2, 43.9, 39.3, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{21}BrNO_3$ 414.0699, found 414.0691.



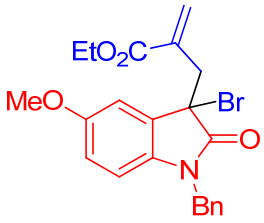
7. Yield 56%; yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.24 (td, *J* = 7.8, 1.2 Hz, 1H), 7.04 (td, *J* = 7.6, 0.9 Hz, 1H), 6.75 (d, *J* = 7.9 Hz, 1H), 6.10 (s, 1H), 5.87 – 5.73 (m, 1H), 5.63 (d, *J* = 0.8 Hz, 1H), 5.24 – 5.14 (m, 2H), 4.48 – 4.38 (m, 1H), 4.30 – 4.19 (m, 1H), 4.02 – 3.88 (m, 2H), 3.73 (d, *J* = 13.6 Hz, 1H), 3.37 (d, *J* = 13.6 Hz, 1H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.3, 166.2, 141.6, 134.9, 130.5, 130.1, 129.9, 128.1, 126.1, 122.8, 117.5, 109.4, 60.8, 55.1, 42.5, 39.3, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{17}H_{19}BrNO_3$ 364.0543, found 364.0536.



8. Yield 50%; yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.29 (td, *J* = 7.8, 1.2 Hz, 1H), 7.05 (td, *J* = 7.6, 0.9 Hz, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 6.11 (s, 1H), 5.62 (d, *J* = 0.7 Hz, 1H), 4.02 – 3.92 (m, 2H), 3.69 (d, *J* = 13.7 Hz, 1H), 3.34 (d, *J* = 13.7 Hz, 1H), 3.21 (s, 3H), 1.13 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 166.2, 142.4, 135.0, 130.2, 129.7, 128.2, 125.9, 122.8, 108.5, 60.9, 55.2, 39.3, 26.6, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{15}H_{17}BrNO_3$ 338.0386, found 338.0370.

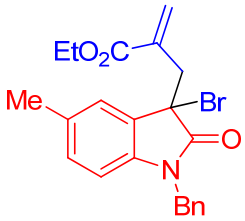


9. Yield 51%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.2 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.32 (ddd, *J* = 9.0, 8.0, 1.4 Hz, 1H), 7.15 (td, *J* = 7.6, 0.9 Hz, 1H), 6.16 (s, 1H), 5.65 (d, *J* = 0.6 Hz, 1H), 4.04 – 3.93 (m, 2H), 3.73 (d, *J* = 14.0 Hz, 1H), 3.44 (d, *J* = 13.9 Hz, 1H), 1.65 (s, 9H), 1.13 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 166.1, 148.7, 138.4, 134.7, 130.5, 130.3, 127.1, 125.9, 124.6, 115.2, 84.9, 60.9, 55.4, 39.6, 27.9, 13.9; HRMS–ESI $[M + Na]^+$ Calcd for $C_{19}H_{22}BrNO_5Na$ 446.0574, found 446.0579.

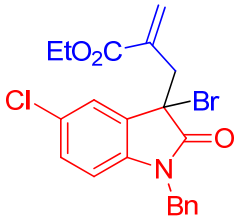


10. Yield 81%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.14 (m, 5H), 6.97 (d, *J* = 2.6 Hz, 1H), 6.61 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.43 (d, *J* = 8.6 Hz, 1H), 6.02 (s, 1H), 5.56 (d, *J* = 0.8 Hz, 1H), 4.85 (d, *J* = 15.9 Hz, 1H), 4.77 (d, *J* = 15.9 Hz, 1H), 3.97 – 3.82 (m, 2H), 3.67 (s, 3H), 3.66 (d, *J* = 13.6 Hz, 4H), 3.33 (d, *J* = 13.6 Hz, 1H), 1.02 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.4, 166.2, 155.9, 135.0, 134.9, 134.7, 129.9, 129.1, 128.7, 127.6, 126.9, 115.3, 112.5, 110.2, 60.9, 55.7, 55.5, 44.0, 39.2, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{22}H_{23}BrNO_4$

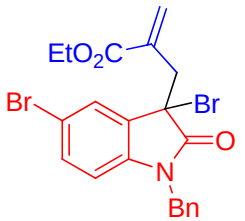
444.0805, found 444.0797.



11. Yield 51%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.20 (m, 6H), 6.95 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.50 (d, *J* = 8.0 Hz, 1H), 6.09 (s, 1H), 5.61 (d, *J* = 0.6 Hz, 1H), 4.94 (d, *J* = 15.9 Hz, 1H), 4.86 (d, *J* = 15.8 Hz, 1H), 4.04 – 3.87 (m, 2H), 3.74 (d, *J* = 13.7 Hz, 1H), 3.41 (d, *J* = 13.6 Hz, 1H), 2.28 (s, 3H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 166.3, 139.1, 135.0, 135.0, 132.4, 130.5, 129.8, 128.7, 128.1, 127.6, 126.9, 126.6, 109.4, 60.8, 55.5, 43.9, 39.2, 20.9, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{22}H_{23}BrNO_3$ 428.0856, found 428.0852.

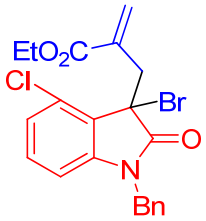


12. Yield 59%; pale yellow solid; mp 144-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 2.1 Hz, 1H), 7.35 – 7.27 (m, 3H), 7.24 – 7.19 (m, 2H), 7.12 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.54 (d, *J* = 8.4 Hz, 1H), 6.14 (s, 1H), 5.66 (d, *J* = 0.5 Hz, 1H), 4.93 (d, *J* = 15.9 Hz, 1H), 4.87 (d, *J* = 15.9 Hz, 1H), 4.12 – 3.91 (m, 2H), 3.73 (d, *J* = 13.7 Hz, 1H), 3.41 (d, *J* = 13.6 Hz, 1H), 1.17 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.3, 166.1, 140.0, 134.7, 134.4, 130.5, 130.0, 129.7, 128.8, 128.3, 127.8, 126.9, 126.5, 110.7, 61.1, 54.2, 44.1, 39.2, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}BrClNO_3$ 448.0310, found 448.0314.

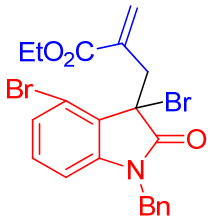


13. Yield 78%; pale yellow solid; 117-118 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 2.0 Hz, 1H), 7.35 – 7.25 (m, 4H), 7.24 – 7.19 (m, 2H), 6.49 (d, *J* = 8.4 Hz, 1H), 6.14 (s, 1H), 5.65 (s, 1H), 4.93 (d, *J* = 15.9 Hz, 1H), 4.87 (d, *J* = 15.9 Hz, 1H), 4.13 – 3.91 (m, 2H), 3.72 (d, *J* = 13.6 Hz,

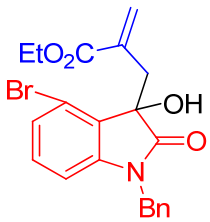
1H), 3.41 (d, J = 13.7 Hz, 1H), 1.18 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 166.1, 140.5, 134.7, 134.4, 132.9, 130.5, 130.0, 129.2, 128.8, 127.9, 126.9, 115.4, 111.1, 61.2, 54.1, 44.1, 39.2, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}Br_2NO_3$ 491.9804, found 491.9790.



14. Yield 63%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.22 (m, 5H), 7.11 (t, J = 8.0 Hz, 1H), 6.99 (dd, J = 8.2, 0.6 Hz, 1H), 6.58 – 6.50 (m, 1H), 6.08 (d, J = 0.6 Hz, 1H), 5.57 (d, J = 0.8 Hz, 1H), 4.97 (d, J = 15.9 Hz, 1H), 4.83 (d, J = 15.9 Hz, 1H), 4.07 – 3.96 (m, 2H), 3.96 – 3.88 (m, 1H), 3.52 (d, J = 13.9 Hz, 1H), 1.12 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 165.9, 143.4, 134.9, 134.5, 132.9, 131.1, 130.0, 128.8, 127.8, 127.0, 124.8, 124.3, 108.1, 60.9, 54.6, 44.3, 38.1, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}BrClNO_3$ 448.0310, found 448.0325.

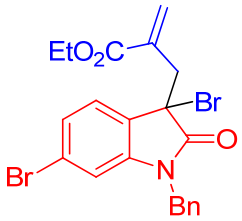


15. Yield 67%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.22 (m, 5H), 7.18 (dd, J = 8.2, 0.5 Hz, 1H), 7.03 (t, J = 8.0 Hz, 1H), 6.58 (d, J = 7.8 Hz, 1H), 6.07 (d, J = 0.6 Hz, 1H), 5.54 (d, J = 0.8 Hz, 1H), 4.97 (d, J = 15.9 Hz, 1H), 4.83 (d, J = 15.9 Hz, 1H), 4.08 (d, J = 14.0 Hz, 1H), 4.06 – 3.91 (m, 2H), 3.51 (d, J = 14.0 Hz, 1H), 1.12 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 165.9, 143.7, 134.9, 134.5, 131.2, 129.9, 128.8, 127.8, 127.5, 127.0, 126.3, 121.6, 108.6, 60.9, 55.7, 44.2, 37.7, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}Br_2NO_3$ 491.9804, found 491.9807.

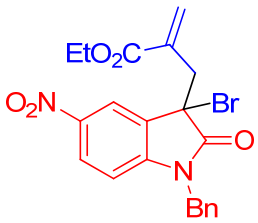


15'. Yield 7%; white solid; mp 133-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.20 (m, 5H),

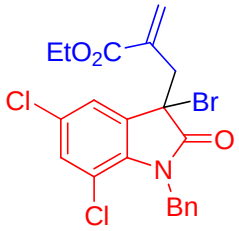
7.18 – 7.11 (m, 1H), 7.02 (t, J = 8.0 Hz, 1H), 6.59 (d, J = 7.8 Hz, 1H), 6.19 (d, J = 1.1 Hz, 1H), 5.63 (s, 1H), 4.94 (d, J = 15.8 Hz, 1H), 4.70 (d, J = 15.8 Hz, 1H), 4.24 (s, 1H), 4.18 – 3.99 (m, 2H), 3.35 (d, J = 13.5 Hz, 1H), 3.28 (d, J = 13.6 Hz, 1H), 1.21 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.1, 167.3, 144.1, 134.8, 134.3, 130.8, 129.9, 128.7, 127.9, 127.7, 127.1, 127.0, 119.7, 108.5, 77.5, 61.2, 43.8, 38.2, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{21}BrNO_4$ 430.0648, found 430.0657.



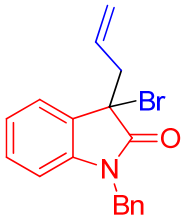
16. Yield 64%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 4H), 7.26 – 7.21 (m, 2H), 7.16 (dd, J = 8.0, 1.7 Hz, 1H), 6.78 (d, J = 1.6 Hz, 1H), 6.11 (s, 1H), 5.65 (d, J = 0.6 Hz, 1H), 4.93 (d, J = 15.9 Hz, 1H), 4.85 (d, J = 15.9 Hz, 1H), 4.06 – 3.90 (m, 2H), 3.75 (d, J = 13.6 Hz, 1H), 3.40 (d, J = 13.6 Hz, 1H), 1.11 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 166.1, 142.8, 134.7, 134.4, 130.3, 128.9, 127.9, 127.5, 127.0, 126.9, 125.8, 123.9, 112.9, 61.0, 54.2, 44.1, 39.1, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}Br_2NO_3$ 491.9804, found 491.9804.



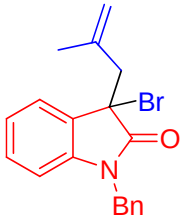
17. Yield 40%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, J = 2.3 Hz, 1H), 8.13 (dd, J = 8.7, 2.3 Hz, 1H), 7.37 – 7.31 (m, 3H), 7.26 – 7.20 (m, 2H), 6.74 (d, J = 8.7 Hz, 1H), 6.20 (s, 1H), 5.72 (s, 1H), 4.98 (d, J = 3.0 Hz, 2H), 4.07 – 3.87 (m, 2H), 3.78 (d, J = 13.8 Hz, 1H), 3.47 (d, J = 13.8 Hz, 1H), 1.16 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.8, 165.9, 146.9, 143.5, 134.3, 133.8, 131.1, 129.3, 129.1, 128.2, 126.9, 126.8, 122.0, 109.5, 61.3, 52.9, 44.5, 39.0, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}BrN_2O_5$ 459.0550, found 459.0540.



18. Yield 63%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 2.0 Hz, 1H), 7.36 – 7.22 (m, 3H), 7.22 – 7.13 (m, 3H), 6.14 (s, 1H), 5.62 (s, 1H), 5.36 (d, *J* = 16.3 Hz, 1H), 5.26 (d, *J* = 16.3 Hz, 1H), 4.14 – 3.95 (m, 2H), 3.71 (d, *J* = 13.7 Hz, 1H), 3.40 (d, *J* = 13.7 Hz, 1H), 1.21 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 166.0, 136.6, 136.4, 134.2, 132.1, 131.9, 131.1, 128.6, 128.5, 127.4, 126.2, 125.4, 116.2, 61.3, 53.3, 45.2, 39.1, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{19}BrCl_2NO_3$ 481.9920, found 481.9926.

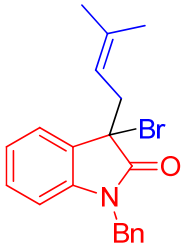


19. Yield 43%; pale yellow semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.34 – 7.26 (m, 5H), 7.19 (td, *J* = 7.8, 1.2 Hz, 1H), 7.06 (td, *J* = 7.6, 0.9 Hz, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 5.52 (dddd, *J* = 16.6, 10.1, 8.0, 6.3 Hz, 1H), 5.16 (dd, *J* = 17.1, 1.3 Hz, 1H), 5.11 – 5.05 (m, 1H), 4.97 (d, *J* = 15.8 Hz, 1H), 4.88 (d, *J* = 15.8 Hz, 1H), 3.25 – 3.08 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 141.4, 135.0, 130.9, 129.9, 129.4, 128.8, 127.7, 127.1, 124.8, 123.2, 120.9, 109.7, 54.9, 44.0, 43.3; HRMS–ESI $[M + H]^+$ Calcd for $C_{18}H_{17}BrNO$ 342.0488, found 342.0488.

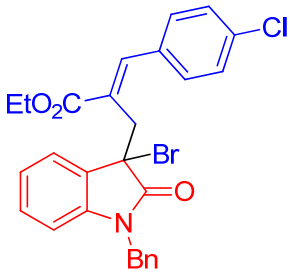


20. Yield 30%; pale yellow solid; mp 108-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (dd, *J* = 7.4, 0.8 Hz, 1H), 7.35 – 7.26 (m, 5H), 7.19 (td, *J* = 7.8, 1.2 Hz, 1H), 7.07 (td, *J* = 7.6, 0.8 Hz, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 4.99 (d, *J* = 15.8 Hz, 1H), 4.88 (d, *J* = 15.8 Hz, 1H), 4.75 – 4.70 (m, 1H), 4.66 (s, 1H), 3.40 (d, *J* = 13.6 Hz, 1H), 3.19 (d, *J* = 13.6 Hz, 1H), 1.41 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 141.7, 139.5, 135.1, 130.0, 129.6, 128.7, 127.7, 127.2, 125.0, 123.1, 116.9,

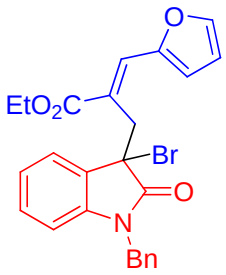
109.8, 55.5, 46.3, 44.1, 23.8; HRMS–ESI $[M + H]^+$ Calcd for $C_{19}H_{19}BrNO$ 356.0645, found 356.0644.



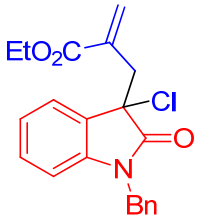
21. Yield 25%; pale yellow solid; mp 99-101 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.34 – 7.26 (m, 3H), 7.25 – 7.21 (m, 2H), 7.18 (td, *J* = 7.8, 1.3 Hz, 1H), 7.06 (td, *J* = 7.6, 1.0 Hz, 1H), 6.63 (d, *J* = 7.7 Hz, 1H), 5.13 (d, *J* = 15.9 Hz, 1H), 4.83 – 4.76 (m, 1H), 4.73 (d, *J* = 15.9 Hz, 1H), 3.25 (dd, *J* = 14.0, 8.6 Hz, 1H), 3.10 (dd, *J* = 14.0, 6.4 Hz, 1H), 1.59 (s, 3H), 1.57 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 141.6, 137.8, 135.2, 129.9, 129.8, 128.8, 127.6, 126.9, 124.6, 123.1, 116.7, 109.6, 55.6, 43.9, 38.2, 25.8, 18.3; HRMS–ESI $[M + H]^+$ Calcd for $C_{20}H_{21}BrNO$ 370.0801, found 370.0791.



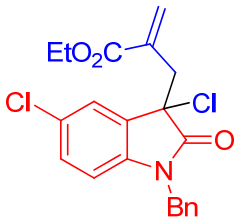
22. Yield 44%; pale yellow solid; mp 198-220 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.36 – 7.20 (m, 10H), 7.13 (td, *J* = 7.8, 1.2 Hz, 1H), 6.93 (td, *J* = 7.6, 0.9 Hz, 1H), 6.60 (d, *J* = 7.8 Hz, 1H), 4.89 (d, *J* = 15.9 Hz, 1H), 4.83 (d, *J* = 15.9 Hz, 1H), 3.96 (qd, *J* = 7.1, 0.7 Hz, 2H), 3.87 (d, *J* = 14.4 Hz, 1H), 3.81 (d, *J* = 14.6 Hz, 1H), 1.10 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 167.6, 141.4, 140.7, 135.1, 134.6, 133.2, 130.4, 129.9, 128.8, 128.7, 128.6, 127.6, 127.0, 125.9, 122.8, 109.4, 61.1, 55.1, 43.9, 35.8, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{27}H_{24}BrClNO_3$ 524.0623, found 524.0617.



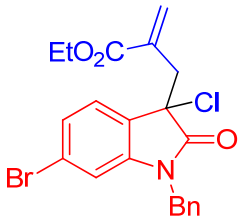
23. Yield 70%; pale yellow solid; mp 137-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 2H), 7.34 – 7.23 (m, 6H), 7.08 (td, *J* = 7.8, 1.2 Hz, 1H), 6.87 (td, *J* = 7.6, 0.9 Hz, 1H), 6.66 (d, *J* = 3.4 Hz, 1H), 6.59 (d, *J* = 7.8 Hz, 1H), 6.43 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.93 (d, *J* = 15.8 Hz, 1H), 4.85 (d, *J* = 15.8 Hz, 1H), 4.10 (d, *J* = 14.5 Hz, 1H), 4.08 – 4.00 (m, 2H), 3.94 (d, *J* = 14.5 Hz, 1H), 1.15 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 167.9, 150.6, 144.6, 141.1, 135.3, 129.7, 129.6, 128.7, 128.5, 127.6, 127.1, 125.8, 122.9, 122.5, 117.1, 111.9, 109.3, 60.9, 55.6, 43.9, 36.5, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{25}H_{23}BrNO_4$ 480.0805, found 480.0809.



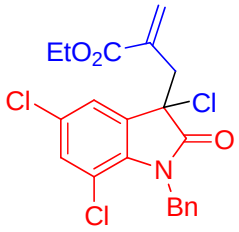
24. Yield 83%; colorless semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.35 – 7.22 (m, 5H), 7.17 (td, *J* = 7.8, 1.2 Hz, 1H), 7.03 (td, *J* = 7.6, 0.9 Hz, 1H), 6.64 (d, *J* = 7.8 Hz, 1H), 6.12 (d, *J* = 0.9 Hz, 1H), 5.66 (d, *J* = 0.8 Hz, 1H), 4.98 (d, *J* = 15.9 Hz, 1H), 4.83 (d, *J* = 15.9 Hz, 1H), 4.00 – 3.86 (m, 2H), 3.62 (d, *J* = 13.5 Hz, 1H), 3.29 (d, *J* = 13.5 Hz, 1H), 1.08 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.4, 166.2, 141.8, 134.9, 134.2, 130.2, 128.7, 127.7, 127.0, 125.7, 122.8, 109.5, 64.2, 60.8, 43.9, 39.2, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{21}ClNO_3$ 370.1204, found 370.1192.



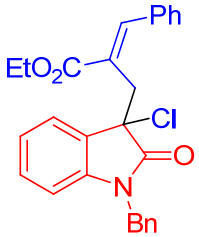
25. Yield 72%; white solid; mp 147-148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 1.5 Hz, 1H), 7.36 – 7.25 (m, 3H), 7.22 (d, *J* = 7.3 Hz, 2H), 7.14 (dd, *J* = 8.4, 1.7 Hz, 1H), 6.57 (d, *J* = 8.4 Hz, 1H), 6.16 (s, 1H), 5.68 (s, 1H), 4.95 (d, *J* = 15.9 Hz, 1H), 4.83 (d, *J* = 15.9 Hz, 1H), 4.10 – 3.90 (m, 2H), 3.58 (d, *J* = 13.5 Hz, 1H), 3.28 (d, *J* = 13.5 Hz, 1H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 166.1, 140.3, 134.4, 133.8, 130.7, 130.1, 129.2, 128.8, 128.3, 127.9, 126.9, 126.1, 110.6, 63.7, 61.1, 44.1, 39.1, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}Cl_2NO_3$ 404.0815, found 404.0803.



26. Yield 69%; colorless semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.22 (m, 6H), 7.17 (d, *J* = 8.0 Hz, 1H), 6.80 (s, 1H), 6.12 (s, 1H), 5.66 (s, 1H), 4.94 (d, *J* = 15.9 Hz, 1H), 4.81 (d, *J* = 15.9 Hz, 1H), 4.07 – 3.87 (m, 2H), 3.60 (d, *J* = 13.5 Hz, 1H), 3.26 (d, *J* = 13.5 Hz, 1H), 1.11 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 166.1, 143.1, 134.3, 133.9, 130.4, 128.8, 127.9, 127.1, 126.9, 126.6, 125.8, 123.9, 112.8, 63.6, 60.9, 44.1, 39.0, 13.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{20}BrClNO_3$ 448.0310, found 448.0306.

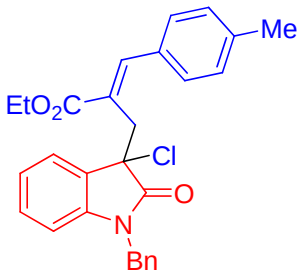


27. Yield 63%; white solid; mp 146-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 2.0 Hz, 1H), 7.34 – 7.22 (m, 3H), 7.22 – 7.14 (m, 3H), 6.16 (s, 1H), 5.64 (s, 1H), 5.35 (d, *J* = 16.3 Hz, 1H), 5.25 (d, *J* = 16.3 Hz, 1H), 4.14 – 3.94 (m, 2H), 3.56 (d, *J* = 13.6 Hz, 1H), 3.27 (d, *J* = 13.6 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 166.0, 136.9, 136.4, 133.4, 132.1, 131.8, 131.2, 128.6, 128.6, 127.4, 126.3, 125.0, 116.1, 62.9, 61.2, 45.2, 39.1, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{21}H_{19}Cl_3NO_3$ 438.0425, found 438.0438.

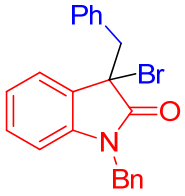


28. Yield 53%; white semi-solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.37 – 7.26 (m, 10H), 7.21 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.14 (td, *J* = 7.8, 1.2 Hz, 1H), 6.93 (td, *J* = 7.6, 0.8 Hz, 1H), 6.61 (d, *J* = 7.8 Hz, 1H), 4.90 (d, *J* = 15.8 Hz, 1H), 4.81 (d, *J* = 15.9 Hz, 1H), 4.07 – 3.93 (m, 2H), 3.80 (d, *J* = 14.4 Hz, 1H), 3.71 (d, *J* = 14.5 Hz, 1H), 1.13 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 168.0, 142.5, 141.7, 135.1, 134.8, 129.9, 129.1, 128.7, 128.6, 128.5, 128.4, 127.6, 127.5, 127.1, 125.5, 122.8, 109.4, 64.5, 61.0, 44.0, 35.6, 13.9; HRMS–ESI $[M + H]^+$ Calcd for

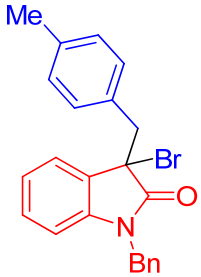
$C_{27}H_{25}ClNO_3$ 446.1517, found 446.1515.



29. Yield 49%; white solid; mp 158-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.35 – 7.27 (m, 5H), 7.26 – 7.21 (m, 3H), 7.19 – 7.11 (m, 3H), 6.94 (td, *J* = 7.6, 0.8 Hz, 1H), 6.62 (d, *J* = 7.8 Hz, 1H), 4.92 (d, *J* = 15.9 Hz, 1H), 4.82 (d, *J* = 15.9 Hz, 1H), 4.05 – 3.90 (m, 2H), 3.82 (d, *J* = 14.4 Hz, 1H), 3.71 (d, *J* = 14.4 Hz, 1H), 2.37 (s, 3H), 1.12 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 168.2, 142.6, 141.7, 138.9, 135.2, 131.9, 129.9, 129.3, 128.7, 128.6, 127.6, 127.1, 126.5, 125.6, 122.8, 109.4, 64.6, 60.9, 44.0, 35.7, 21.4, 14.0; HRMS–ESI $[M + H]^+$ Calcd for $C_{28}H_{27}ClNO_3$ 460.1674, found 460.1675.

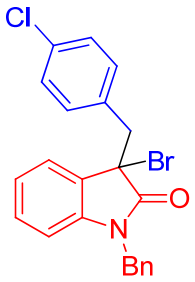


30. Yield 54%; pale yellow solid; mp 170-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.50 (m, 1H), 7.23 – 7.06 (m, 8H), 7.04 – 6.96 (m, 2H), 6.70 – 6.61 (m, 2H), 6.43 – 6.36 (m, 1H), 5.06 (d, *J* = 16.1 Hz, 1H), 4.50 (d, *J* = 16.1 Hz, 1H), 3.89 (d, *J* = 13.2 Hz, 1H), 3.79 (d, *J* = 13.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 141.5, 134.5, 134.2, 130.6, 130.0, 129.0, 128.6, 128.2, 127.3, 127.2, 126.4, 125.0, 123.0, 109.8, 56.1, 45.2, 43.8; HRMS–ESI $[M + H]^+$ Calcd for $C_{22}H_{19}BrNO$ 392.0645, found 392.0630.

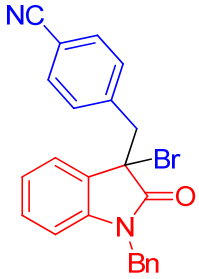


31. Yield 30%; pale yellow solid; mp 188-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 1H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.14 – 7.05 (m, 4H), 6.90 (d, *J* = 8.1 Hz, 2H), 6.86 (d, *J* = 8.1 Hz, 2H), 6.65 (d, *J* = 7.3 Hz, 2H), 6.42 – 6.35 (m, 1H), 5.09 (d, *J* = 16.1 Hz, 1H), 4.48 (d, *J* = 16.1 Hz,

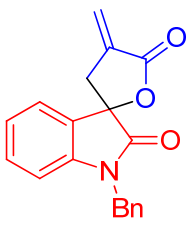
1H), 3.83 (d, *J* = 13.2 Hz, 1H), 3.74 (d, *J* = 13.2 Hz, 1H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 141.6, 136.8, 134.5, 131.1, 130.5, 129.9, 129.2, 128.9, 128.5, 127.3, 126.5, 125.1, 123.0, 109.8, 56.3, 44.8, 43.9, 21.1; HRMS–ESI $[M + H]^+$ Calcd for $C_{23}H_{21}BrNO$ 406.0801, found 406.0784.



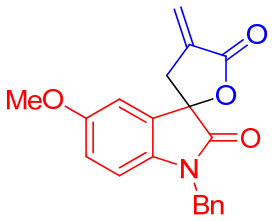
32. Yield 43%; pale yellow solid; mp 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.49 (m, 1H), 7.22 – 7.15 (m, 3H), 7.14 – 7.08 (m, 2H), 7.08 – 7.02 (m, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.69 – 6.58 (m, 2H), 6.48 – 6.38 (m, 1H), 5.08 (d, *J* = 16.0 Hz, 1H), 4.47 (d, *J* = 16.0 Hz, 1H), 3.84 (d, *J* = 13.2 Hz, 1H), 3.73 (d, *J* = 13.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.4, 141.6, 134.4, 133.4, 132.6, 131.9, 130.3, 128.7, 128.6, 128.4, 127.5, 126.4, 124.9, 123.2, 110.0, 55.6, 44.6, 43.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{22}H_{18}BrClNO$ 426.0255, found 426.0244.



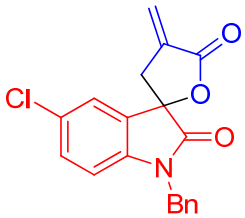
33. Yield 48%; pale yellow solid; mp 174-176 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.39 – 7.30 (m, 2H), 7.25 – 7.09 (m, 5H), 7.06 (d, *J* = 8.3 Hz, 2H), 6.73 (d, *J* = 7.1 Hz, 2H), 6.50 (d, *J* = 7.9 Hz, 1H), 4.99 (d, *J* = 15.9 Hz, 1H), 4.53 (d, *J* = 15.9 Hz, 1H), 3.90 (d, *J* = 13.1 Hz, 1H), 3.79 (d, *J* = 13.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.1, 141.5, 139.4, 134.4, 131.9, 131.3, 130.5, 128.6, 128.3, 127.8, 126.6, 124.9, 123.3, 118.4, 111.3, 110.0, 54.9, 45.1, 43.9; HRMS–ESI $[M + H]^+$ Calcd for $C_{23}H_{18}BrN_2O$ 417.0597, found 417.0580.



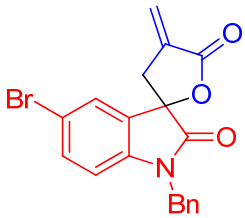
34. Yield 71%; pale yellow solid; mp 134-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.23 (m, 7H), 7.15 – 7.04 (m, 1H), 6.76 (d, *J* = 7.9 Hz, 1H), 6.50 – 6.39 (m, 1H), 5.83 (t, *J* = 2.4 Hz, 1H), 4.92 (d, *J* = 15.6 Hz, 1H), 4.86 (d, *J* = 15.7 Hz, 1H), 3.42 – 3.32 (m, 1H), 3.22 – 3.11 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 168.9, 143.0, 134.8, 132.7, 131.2, 128.9, 127.9, 127.3, 126.6, 124.2, 123.7, 123.2, 109.9, 79.3, 44.0, 36.4; HRMS–ESI $[M + H]^+$ Calcd for $C_{19}H_{16}NO_3$ 306.1125, found 306.1127.



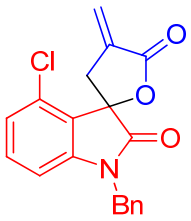
35. Yield 35%; pale yellow solid; mp 121-122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.24 (m, 5H), 6.92 (d, *J* = 2.5 Hz, 1H), 6.79 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.64 (d, *J* = 8.6 Hz, 1H), 6.43 (t, *J* = 2.8 Hz, 1H), 5.82 (t, *J* = 2.4 Hz, 1H), 4.89 (d, *J* = 15.7 Hz, 1H), 4.83 (d, *J* = 15.7 Hz, 1H), 3.75 (s, 3H), 3.37 (dt, *J* = 17.2, 2.3 Hz, 1H), 3.14 (dt, *J* = 17.2, 2.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.4, 168.9, 156.7, 136.1, 134.9, 132.6, 128.9, 127.9, 127.7, 127.2, 123.3, 115.7, 111.2, 110.6, 79.6, 55.8, 44.1, 36.5; HRMS–ESI $[M + H]^+$ Calcd for $C_{20}H_{18}NO_4$ 336.1230, found 336.1233.



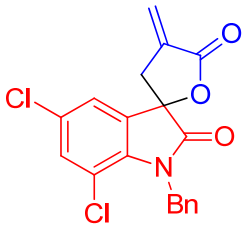
36. Yield 67%; pale yellow solid; mp 152-154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.21 (m, 7H), 6.67 (d, *J* = 8.4 Hz, 1H), 6.44 (t, *J* = 2.8 Hz, 1H), 5.85 (t, *J* = 2.4 Hz, 1H), 4.91 (d, *J* = 15.7 Hz, 1H), 4.83 (d, *J* = 15.7 Hz, 1H), 3.37 (dt, *J* = 17.2, 2.4 Hz, 1H), 3.14 (dt, *J* = 17.3, 2.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 168.5, 141.4, 134.3, 132.1, 131.0, 129.1, 129.0, 128.2, 128.1, 127.2, 124.7, 123.8, 111.1, 78.9, 44.1, 36.2; HRMS–ESI $[M + H]^+$ Calcd for $C_{19}H_{15}ClNO_3$ 340.0735, found 340.0739.



37. Yield 51%; pale yellow solid; mp 128-130 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 1.9 Hz, 1H), 7.39 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.37 – 7.23 (m, 5H), 6.63 (d, *J* = 8.3 Hz, 1H), 6.46 (t, *J* = 2.7 Hz, 1H), 5.85 (t, *J* = 2.4 Hz, 1H), 4.91 (d, *J* = 15.7 Hz, 1H), 4.83 (d, *J* = 15.7 Hz, 1H), 3.38 (dt, *J* = 17.2, 2.3 Hz, 1H), 3.15 (dt, *J* = 17.2, 2.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.1, 168.5, 141.9, 134.3, 133.9, 132.1, 129.0, 128.6, 128.1, 127.5, 127.2, 123.8, 116.3, 111.5, 78.9, 44.1, 36.2; HRMS–ESI $[M + H]^+$ Calcd for $C_{19}H_{14}BrNO_3$ 384.0230, found 384.0227.

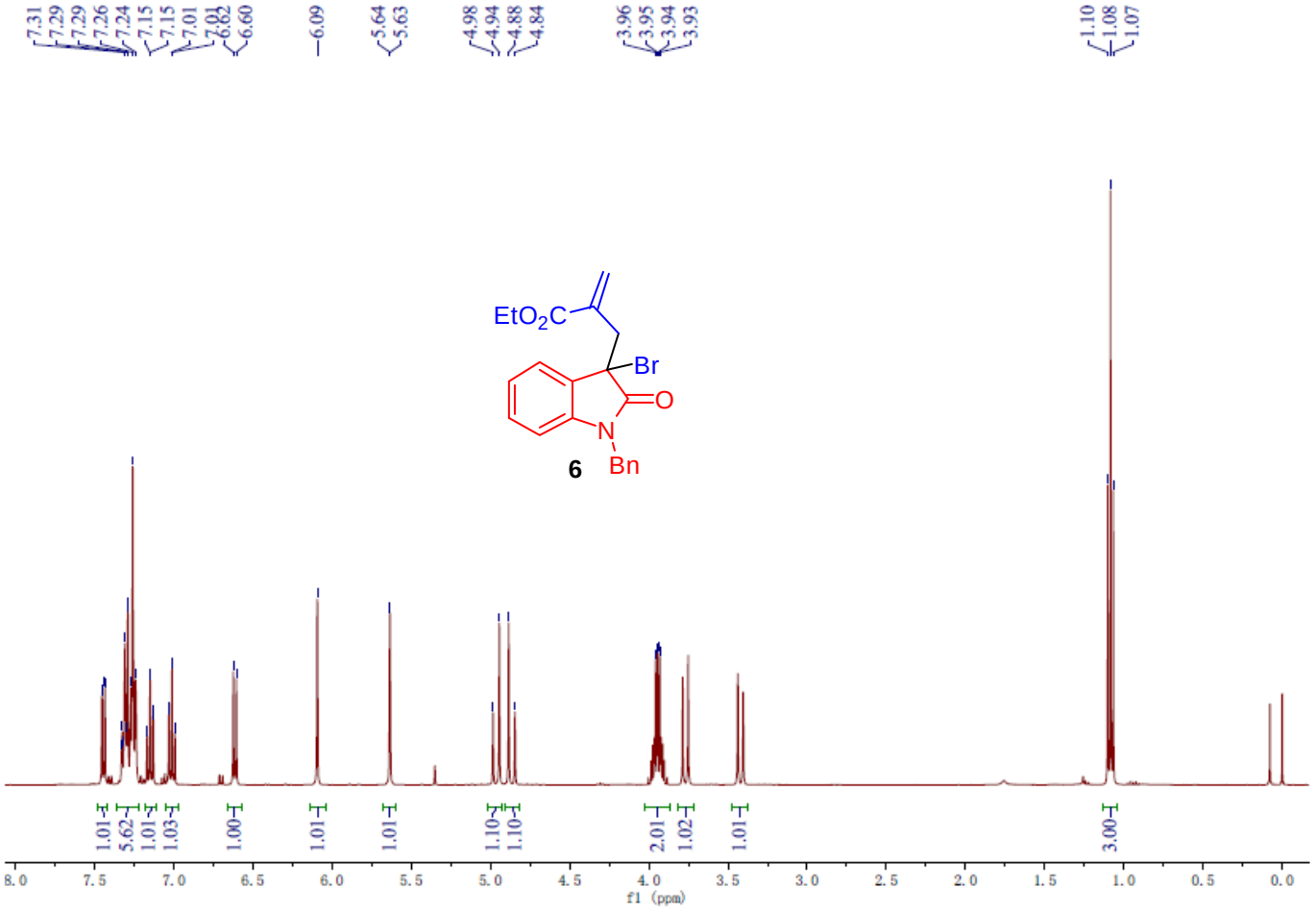


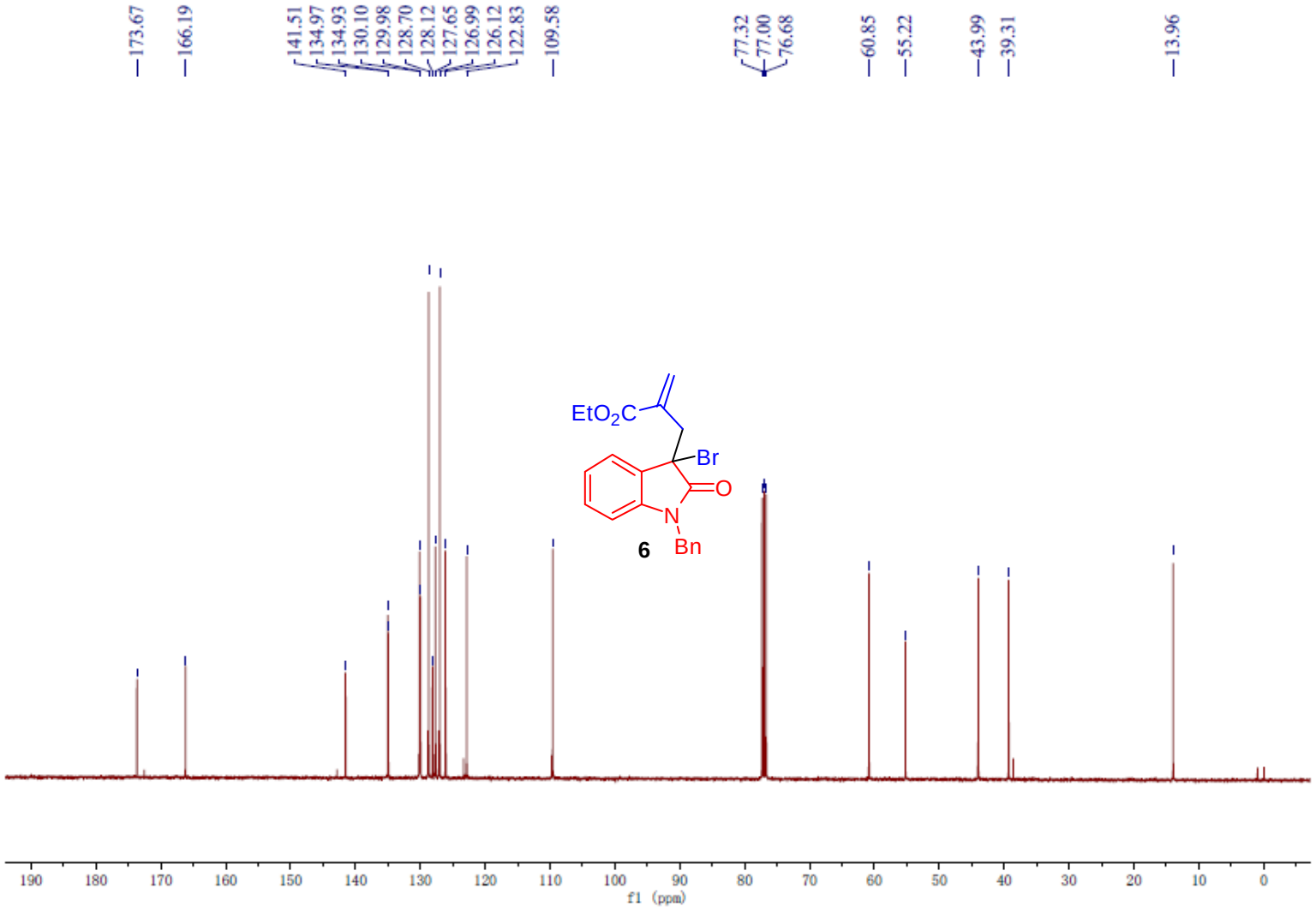
38. Yield 70%; pale yellow solid; mp 82-84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.24 (m, 5H), 7.21 (t, *J* = 8.1 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 7.9 Hz, 1H), 6.44 (t, *J* = 2.9 Hz, 1H), 5.83 (t, *J* = 2.6 Hz, 1H), 4.92 (d, *J* = 15.7 Hz, 1H), 4.84 (d, *J* = 15.7 Hz, 1H), 3.49 (dt, *J* = 17.6, 2.9 Hz, 1H), 3.32 (dt, *J* = 17.6, 2.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.3, 168.8, 144.7, 134.4, 132.6, 132.2, 132.1, 129.0, 128.1, 127.2, 124.3, 123.5, 123.3, 108.4, 79.2, 44.2, 33.2; HRMS–ESI $[M + H]^+$ Calcd for $C_{19}H_{15}ClNO_3$ 340.0735, found 340.0743.



39. Yield 71%; pale yellow solid; mp 154-156 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 4H), 7.25 – 7.22 (m, 1H), 7.22 – 7.16 (m, 2H), 6.46 (t, *J* = 2.8 Hz, 1H), 5.86 (t, *J* = 2.5 Hz, 1H), 5.34 (d, *J* = 16.2 Hz, 1H), 5.24 (d, *J* = 16.2 Hz, 1H), 3.38 (dt, *J* = 17.3, 2.5 Hz, 1H), 3.13 (dt, *J* = 17.3, 2.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 168.2, 137.8, 136.0, 132.9, 131.6, 130.8, 129.5, 128.8, 127.6, 126.3, 124.2, 123.5, 116.9, 78.2, 45.1, 36.5; HRMS–ESI $[M + H]^+$ Calcd for $C_{19}H_{14}Cl_2NO_3$ 374.0345, found 374.0338.

V. ^{1}H and ^{13}C NMR Spectra of Compounds 6 to 39

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Bn
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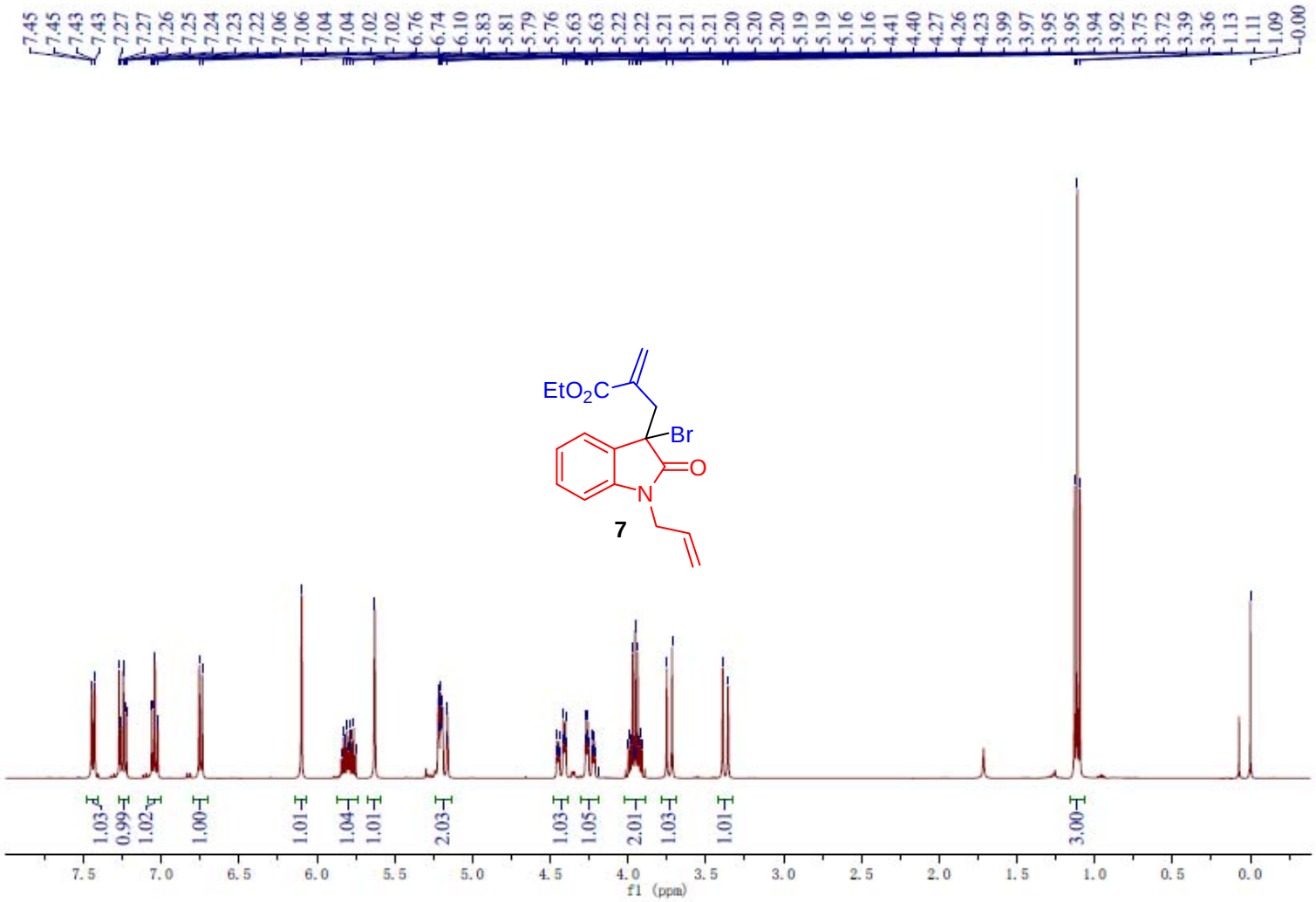
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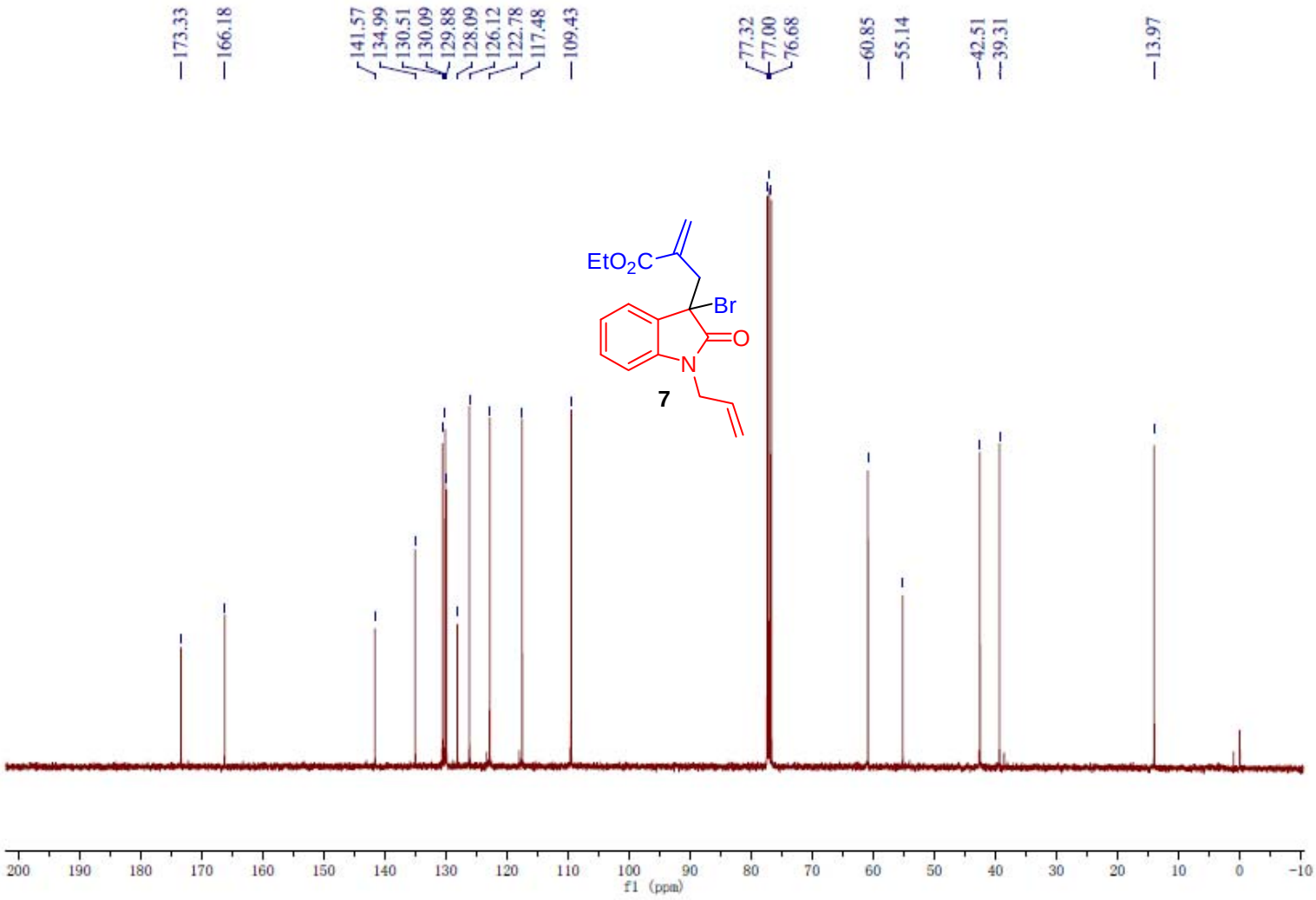
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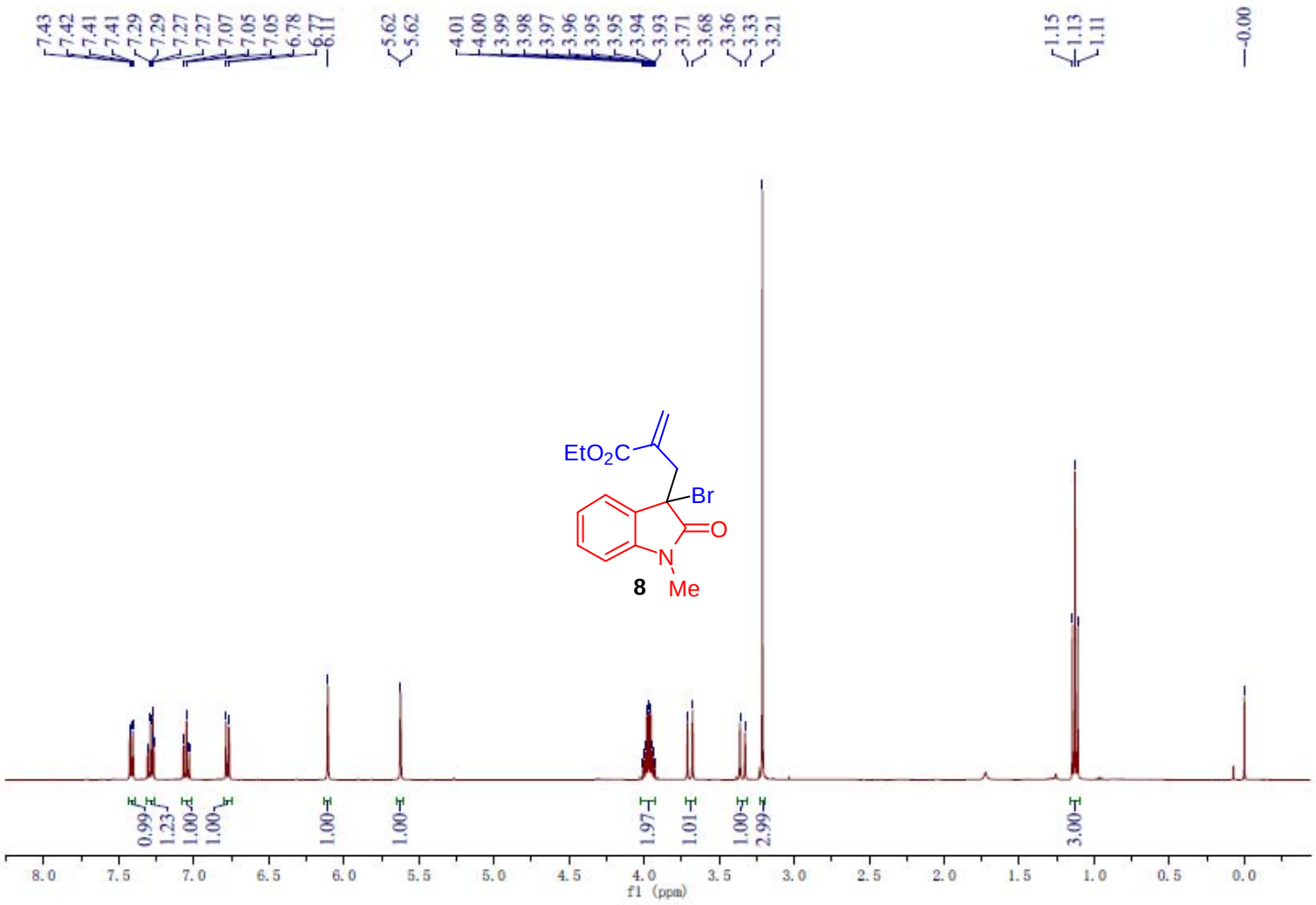
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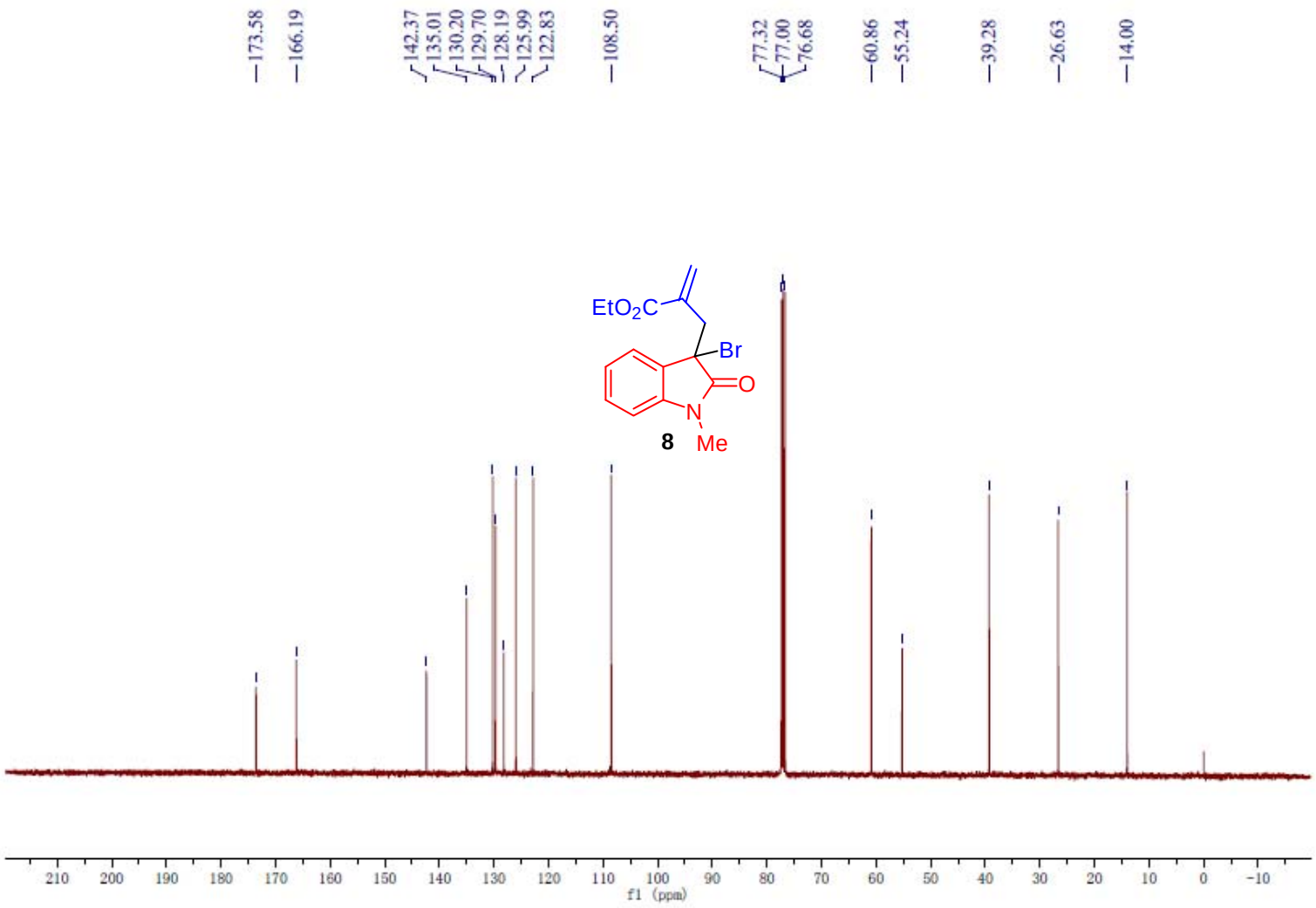
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26.63
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N
Me
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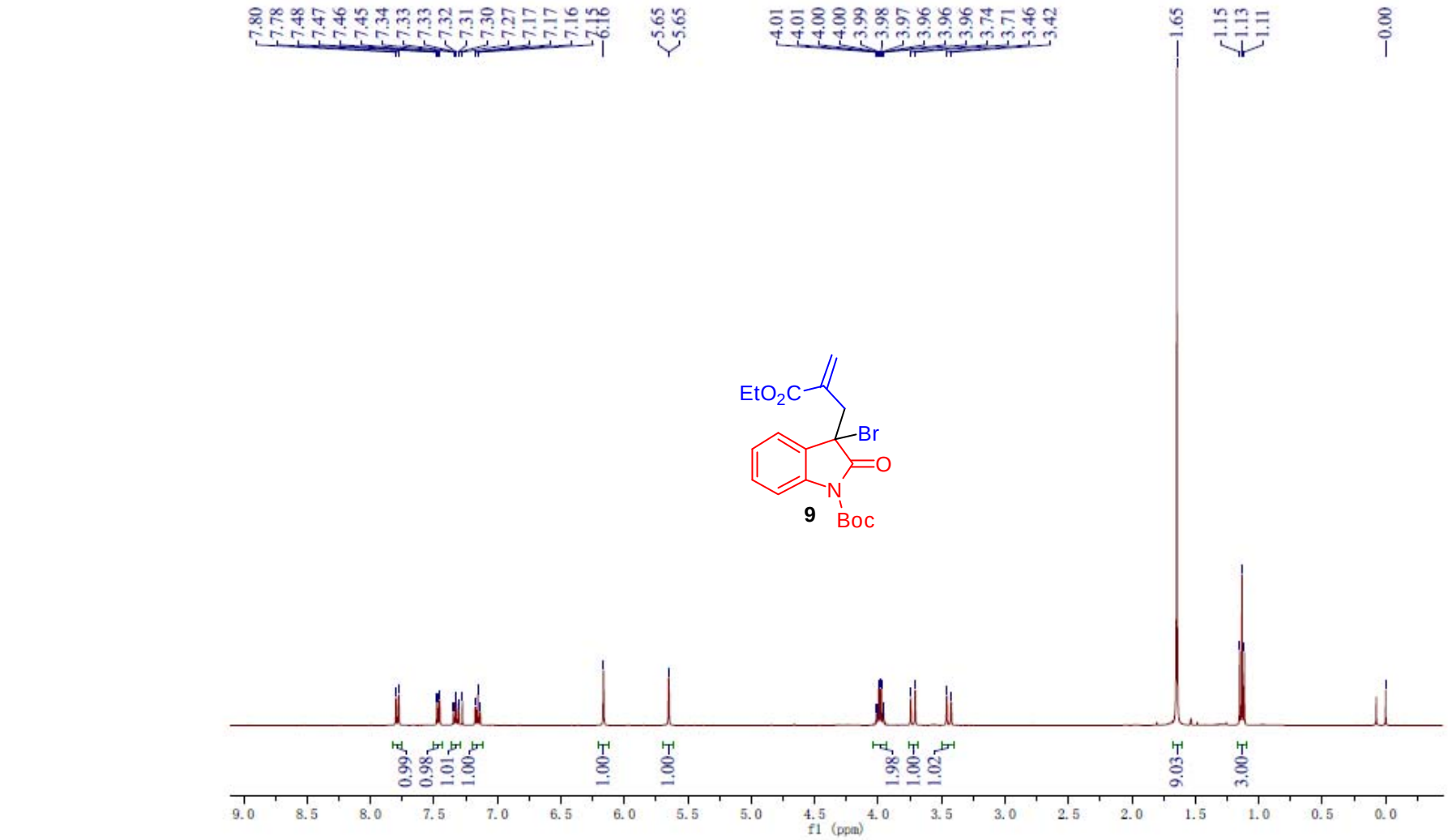
f1 (ppm)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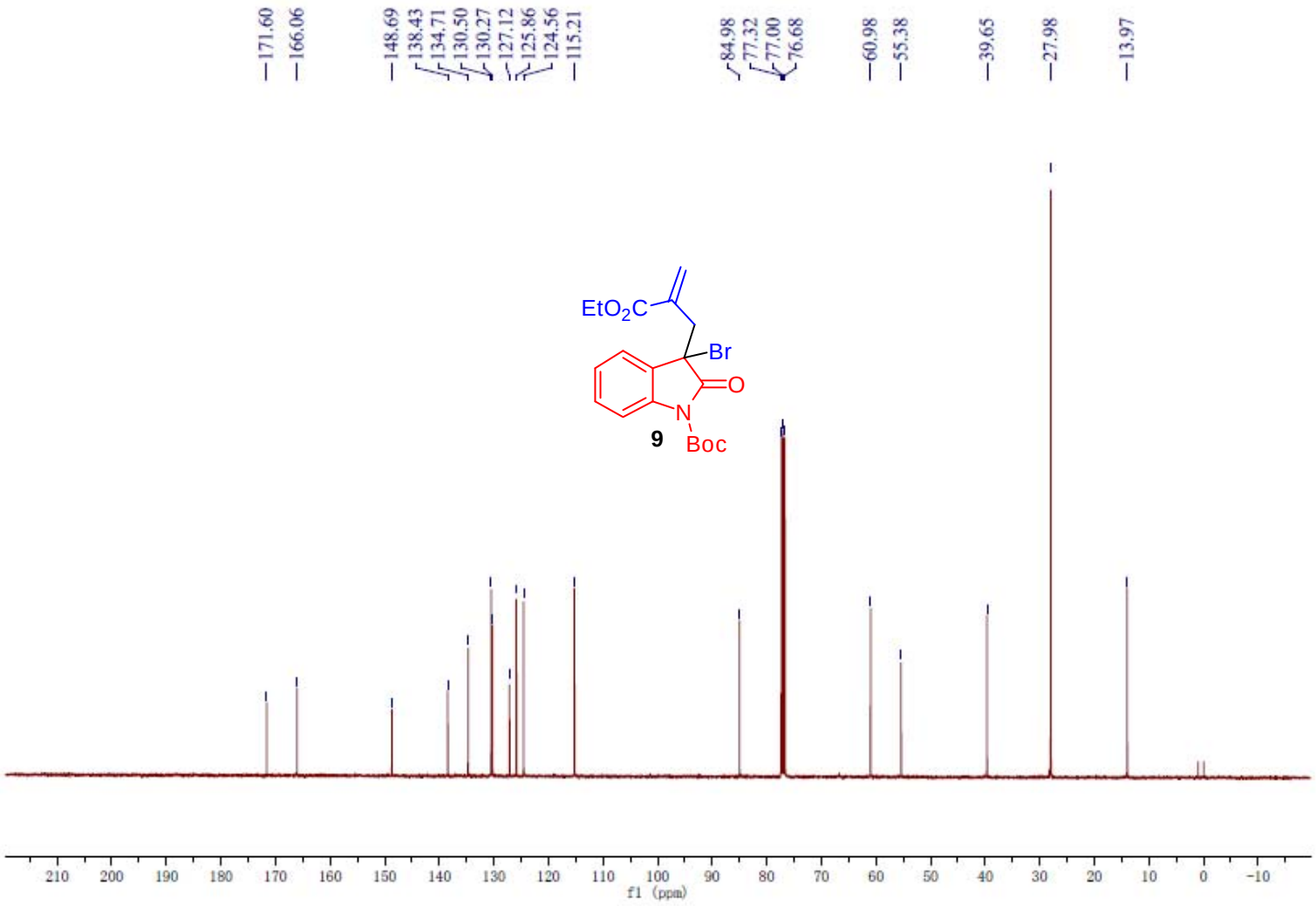
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Boc
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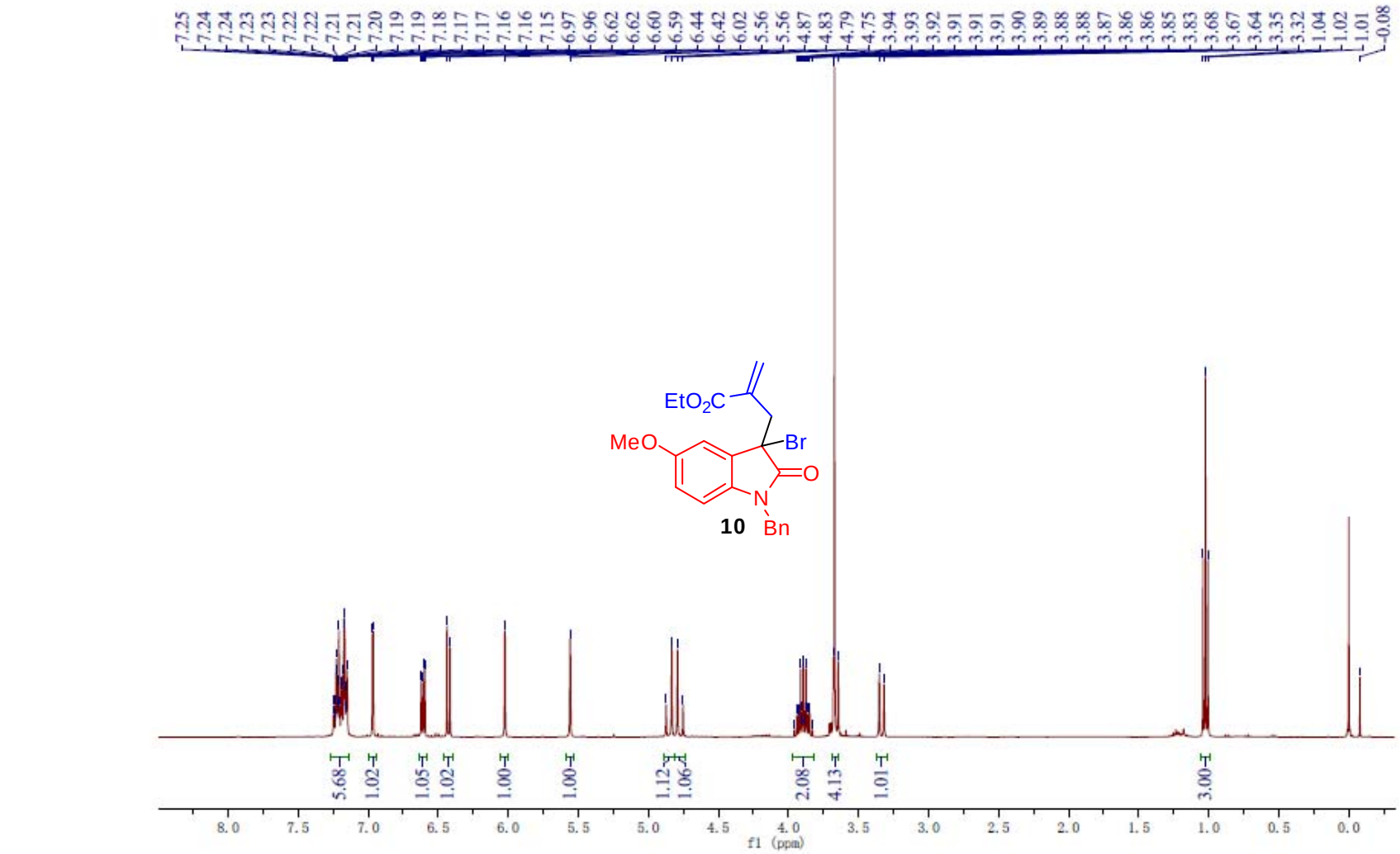
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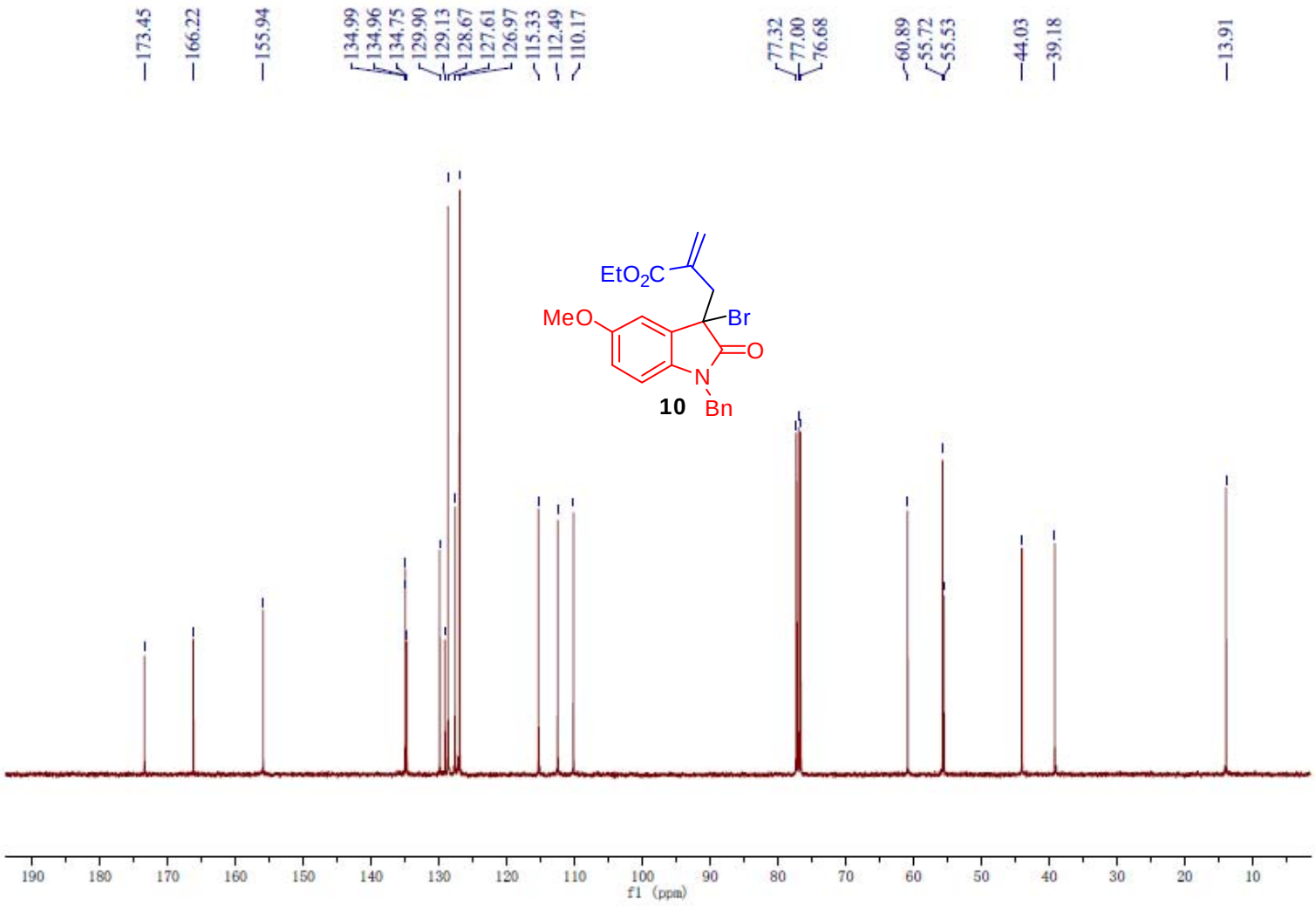
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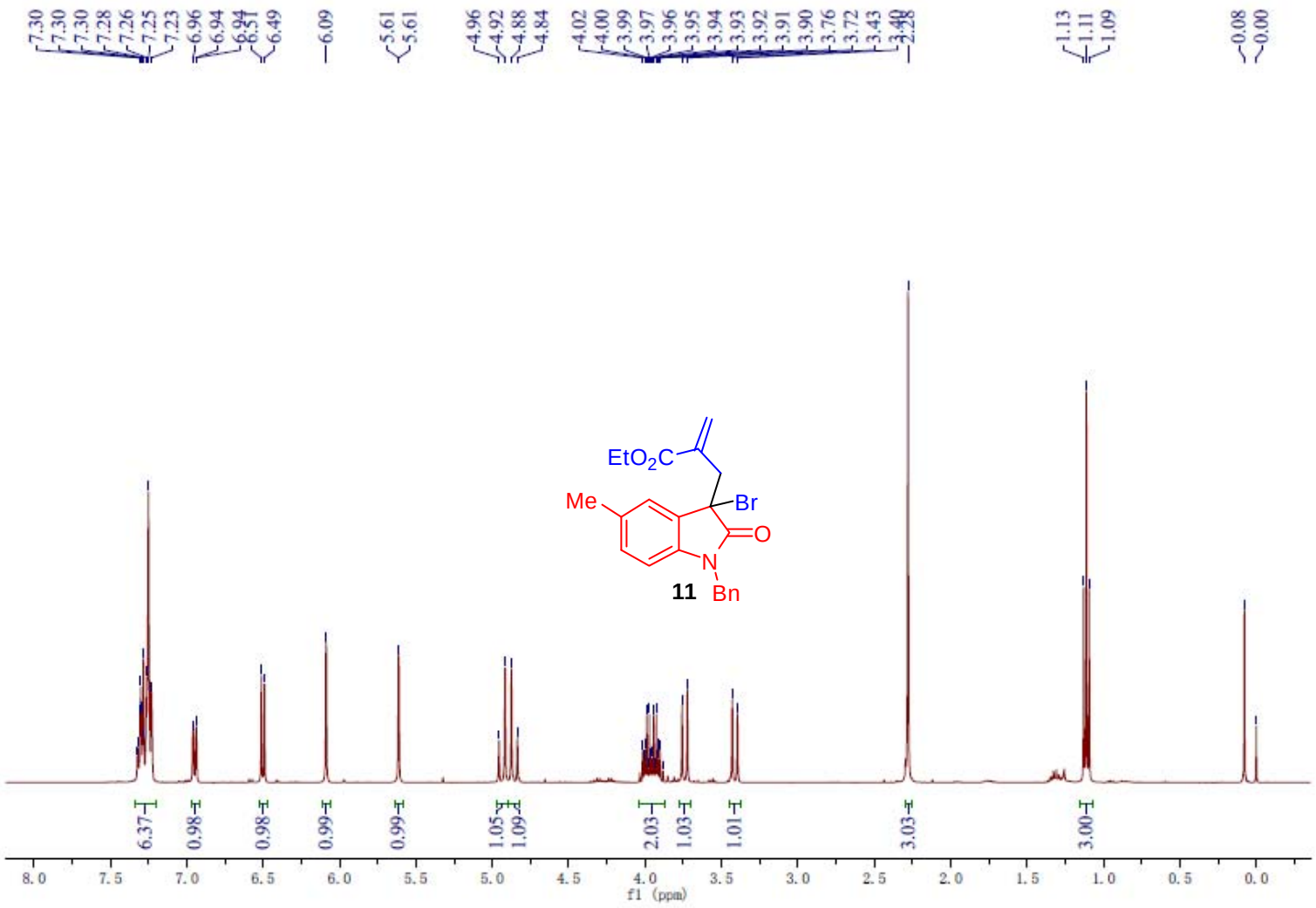
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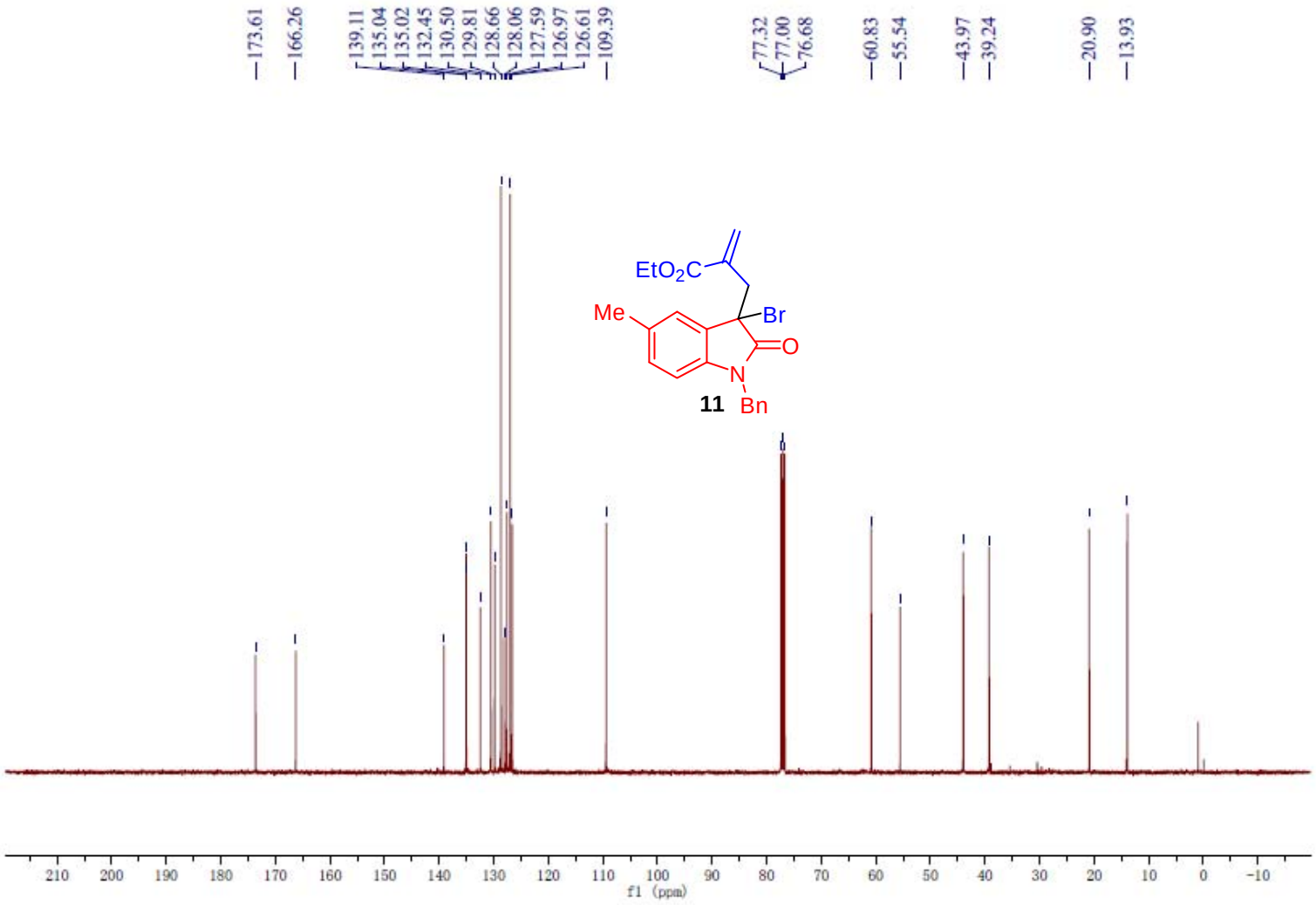
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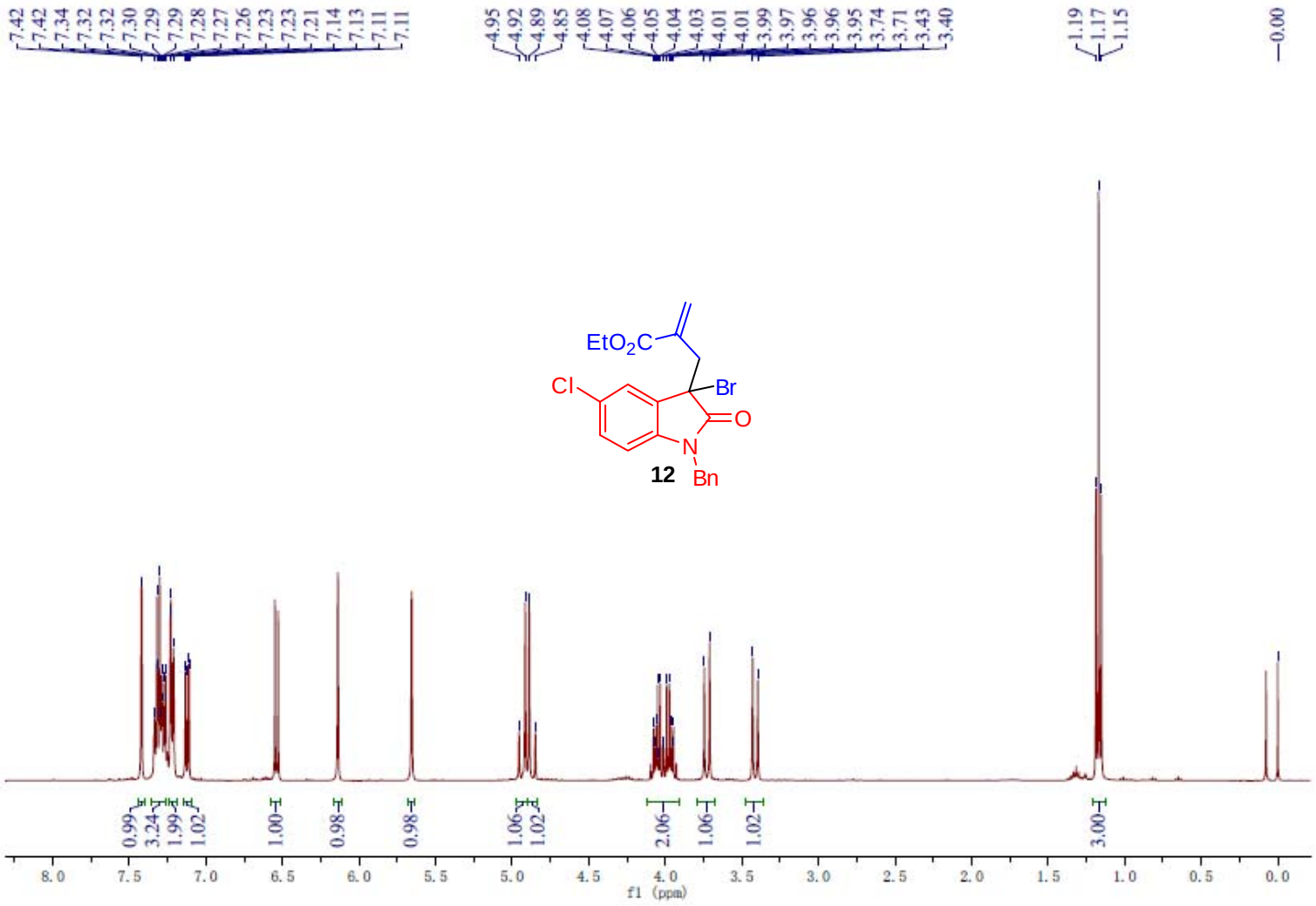
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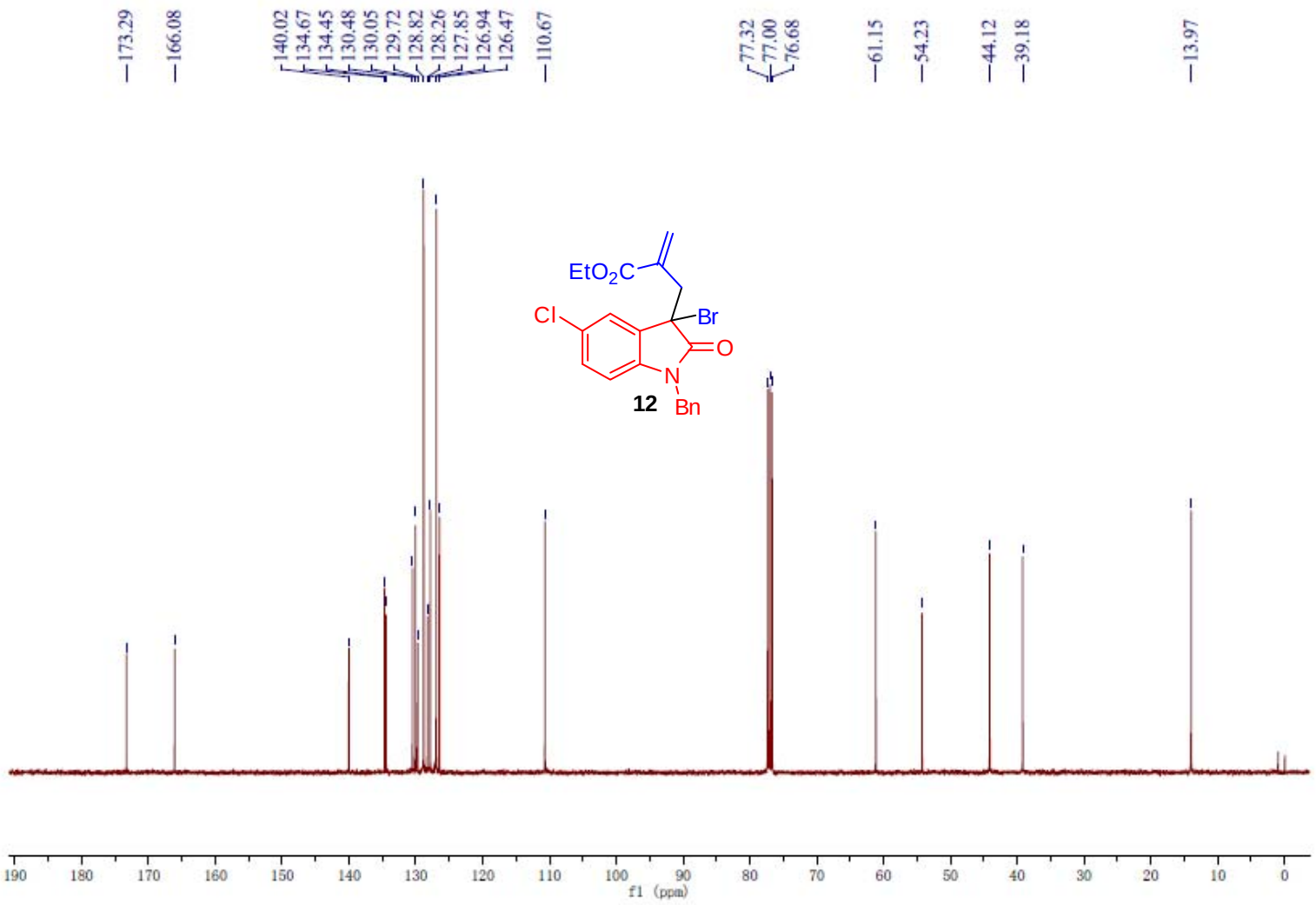
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Bn
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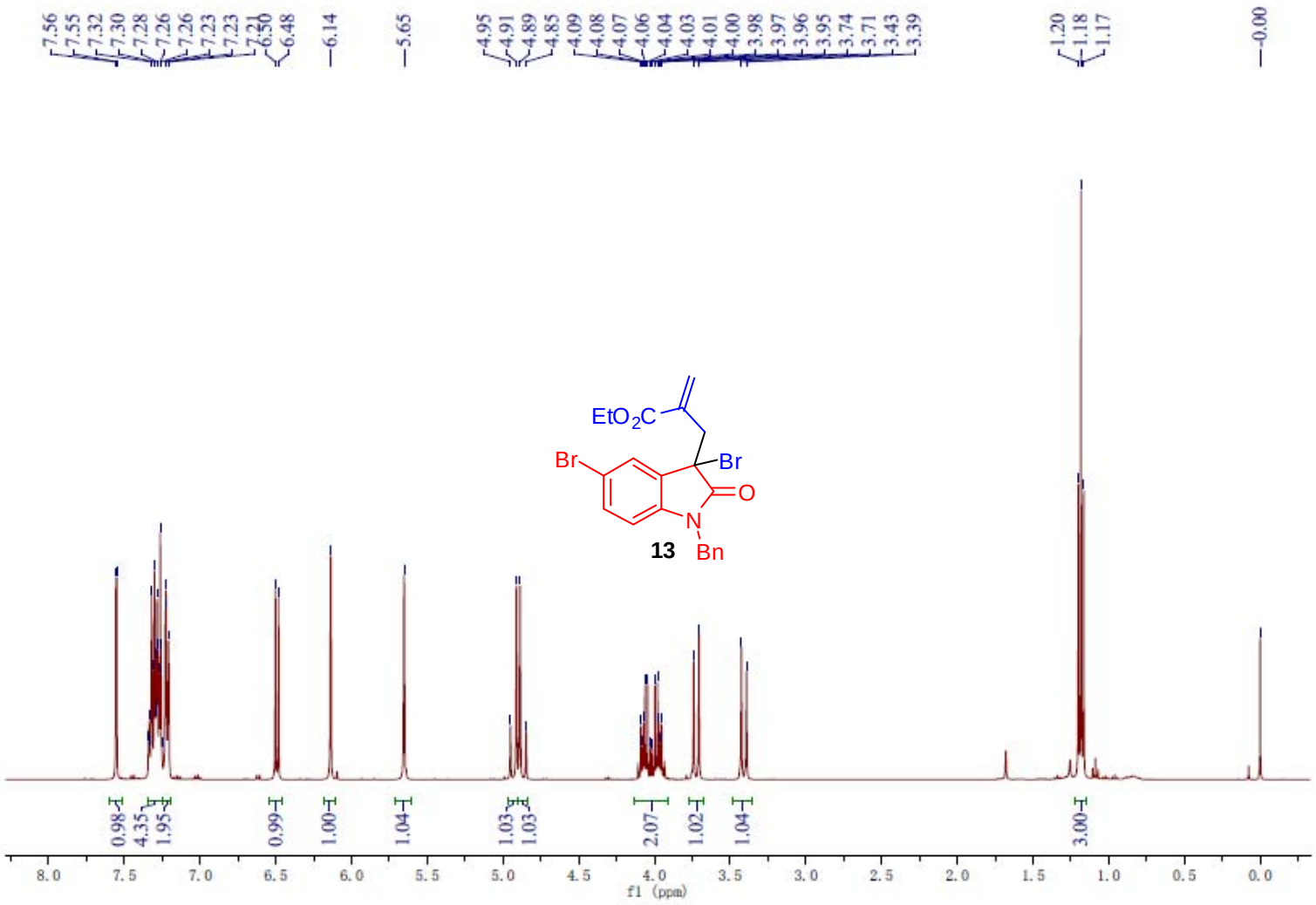
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Br
Br
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Bn
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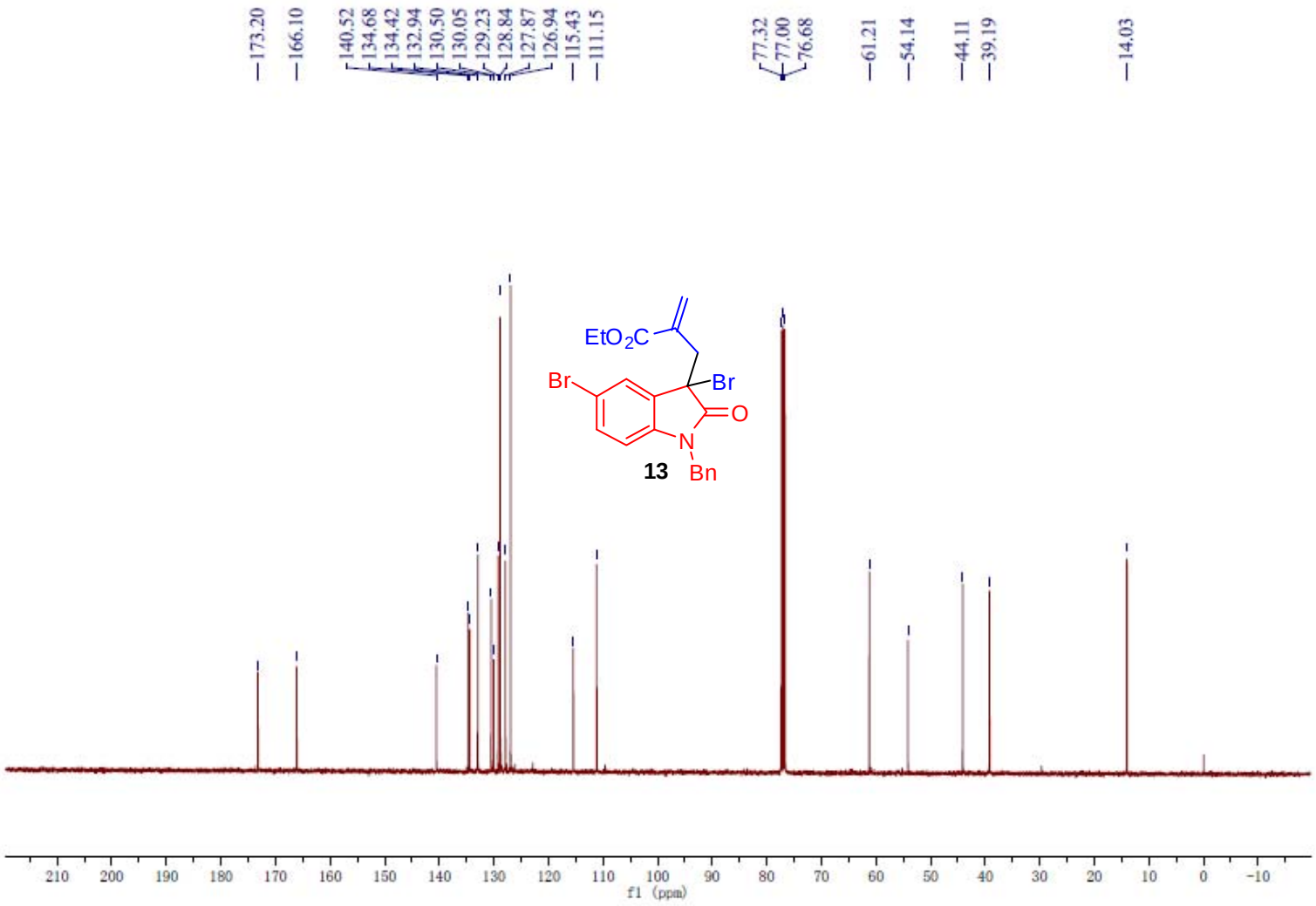
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Br
Br
O
N
Bn
13
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200
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180
170
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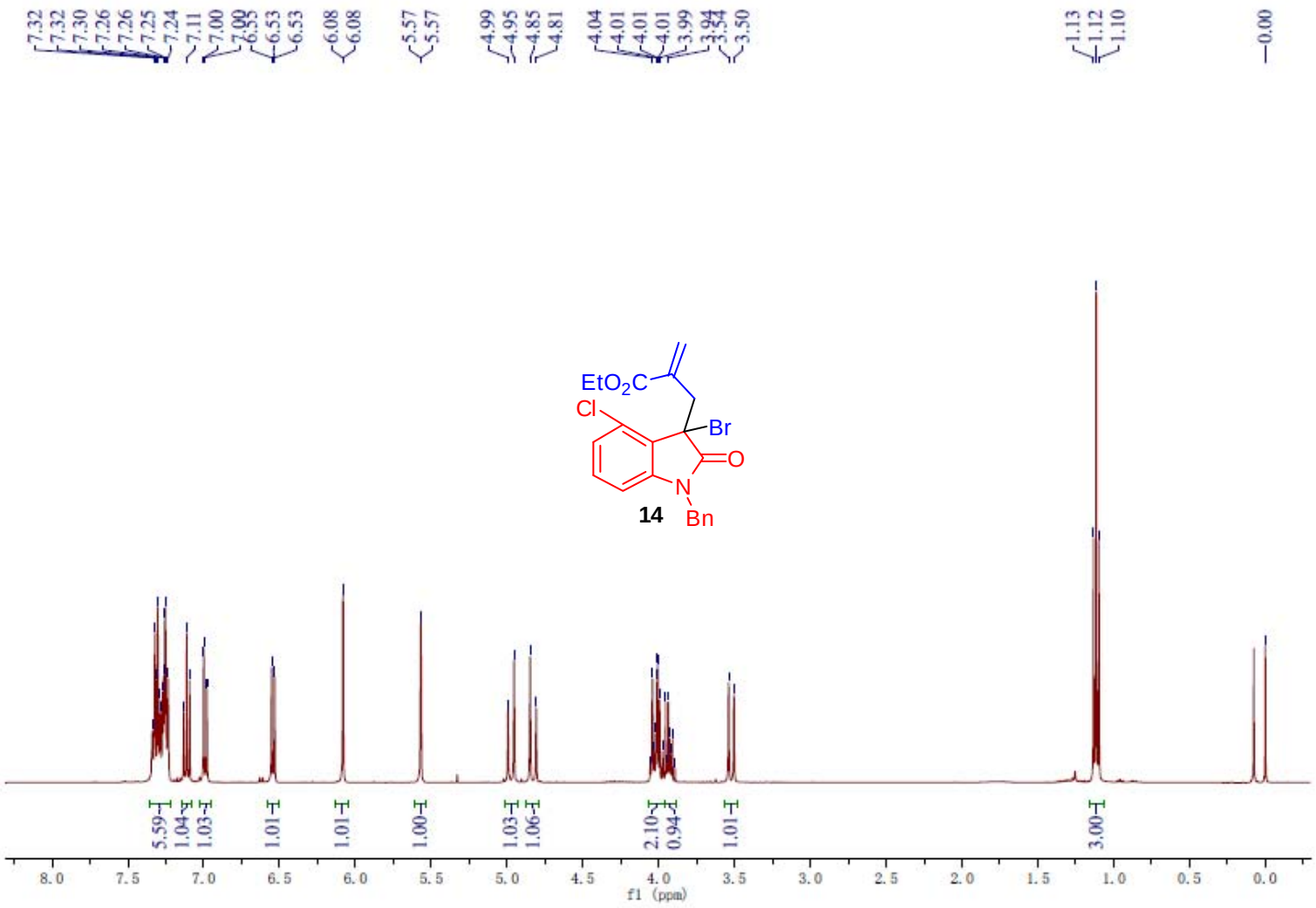
f1 (ppm)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4.01
4.01
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Br
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Bn
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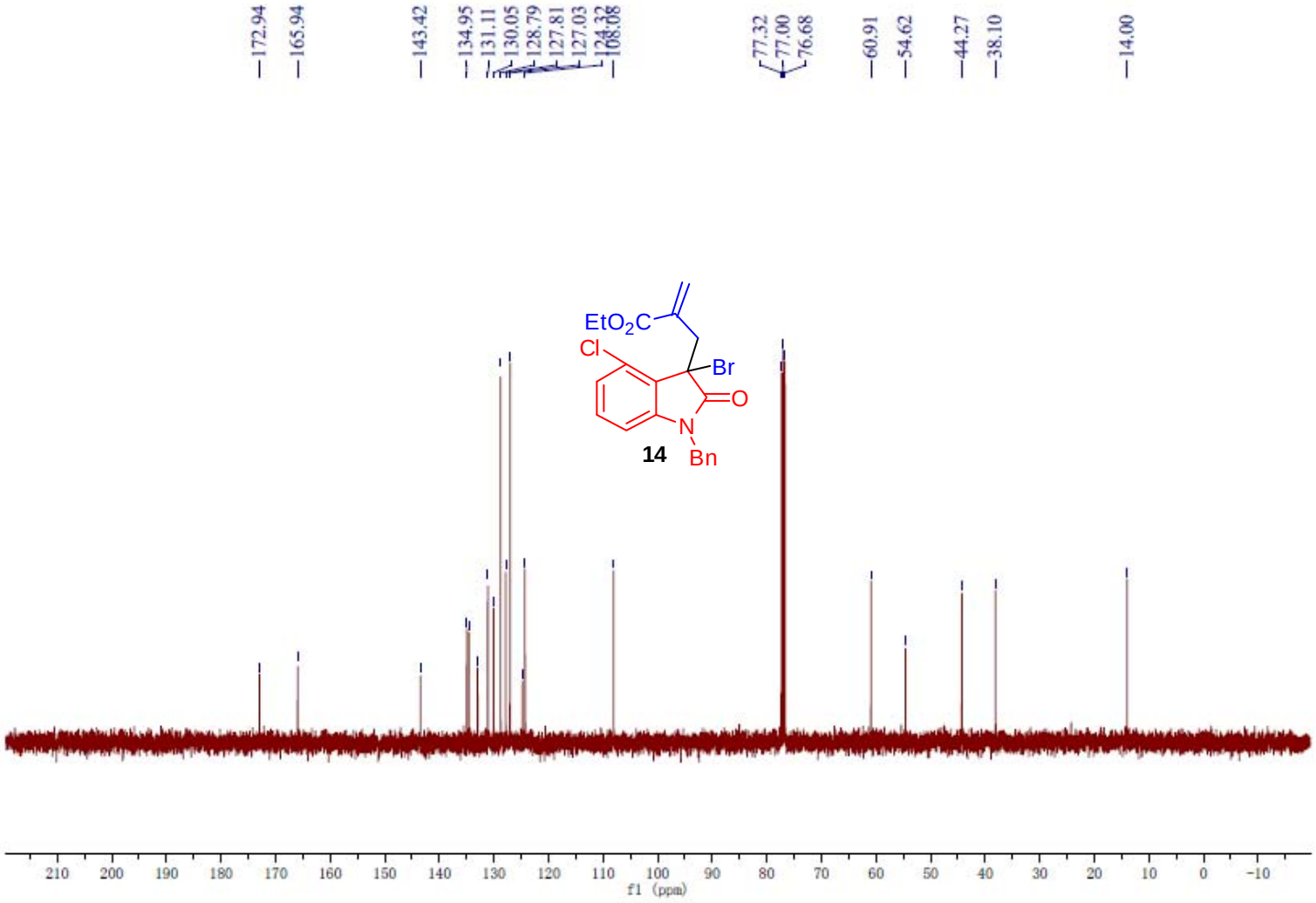
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38.10
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Br
O
N
Bn
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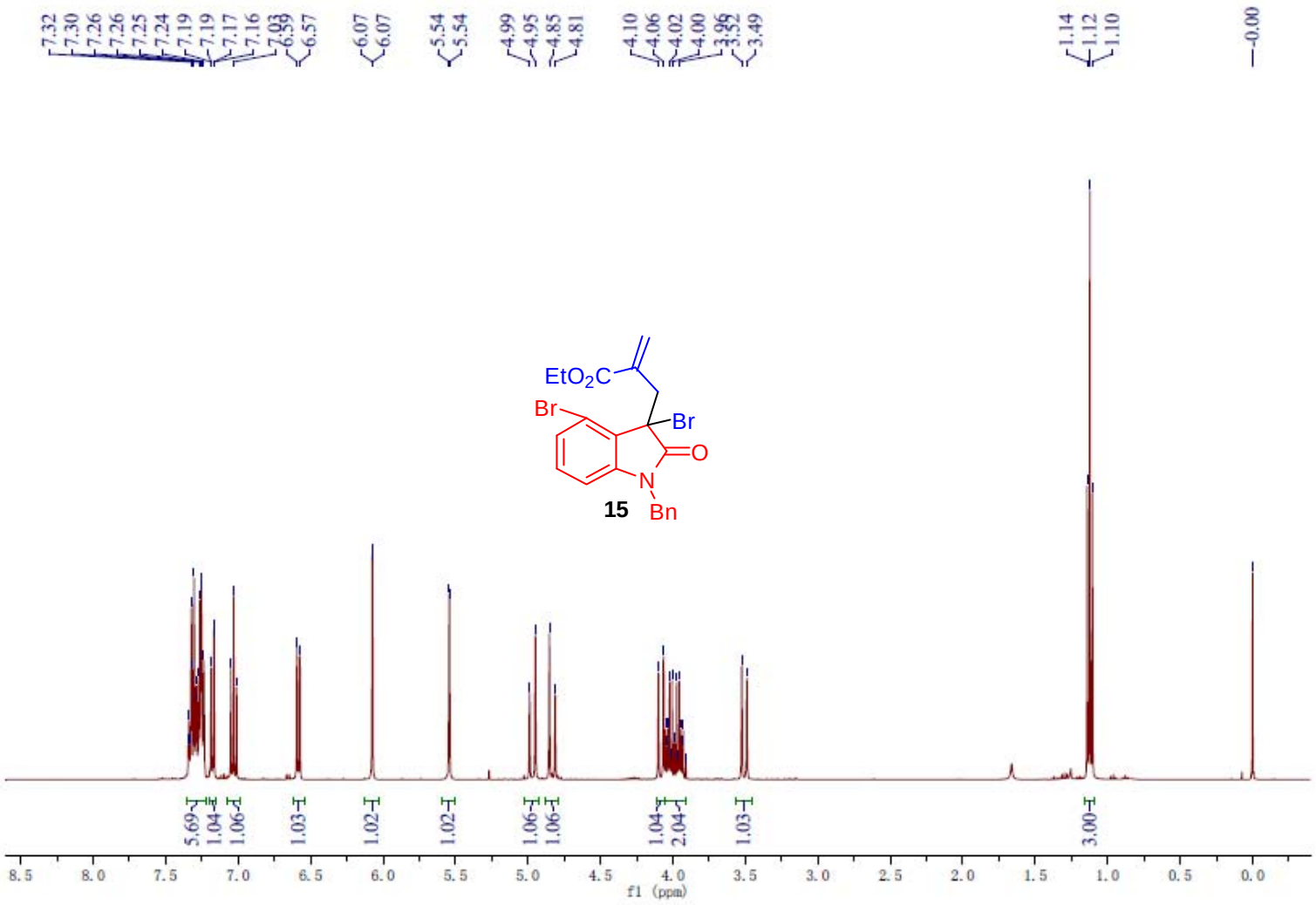
f1 (ppm)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Br
Br
O
N
Bn
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1.02
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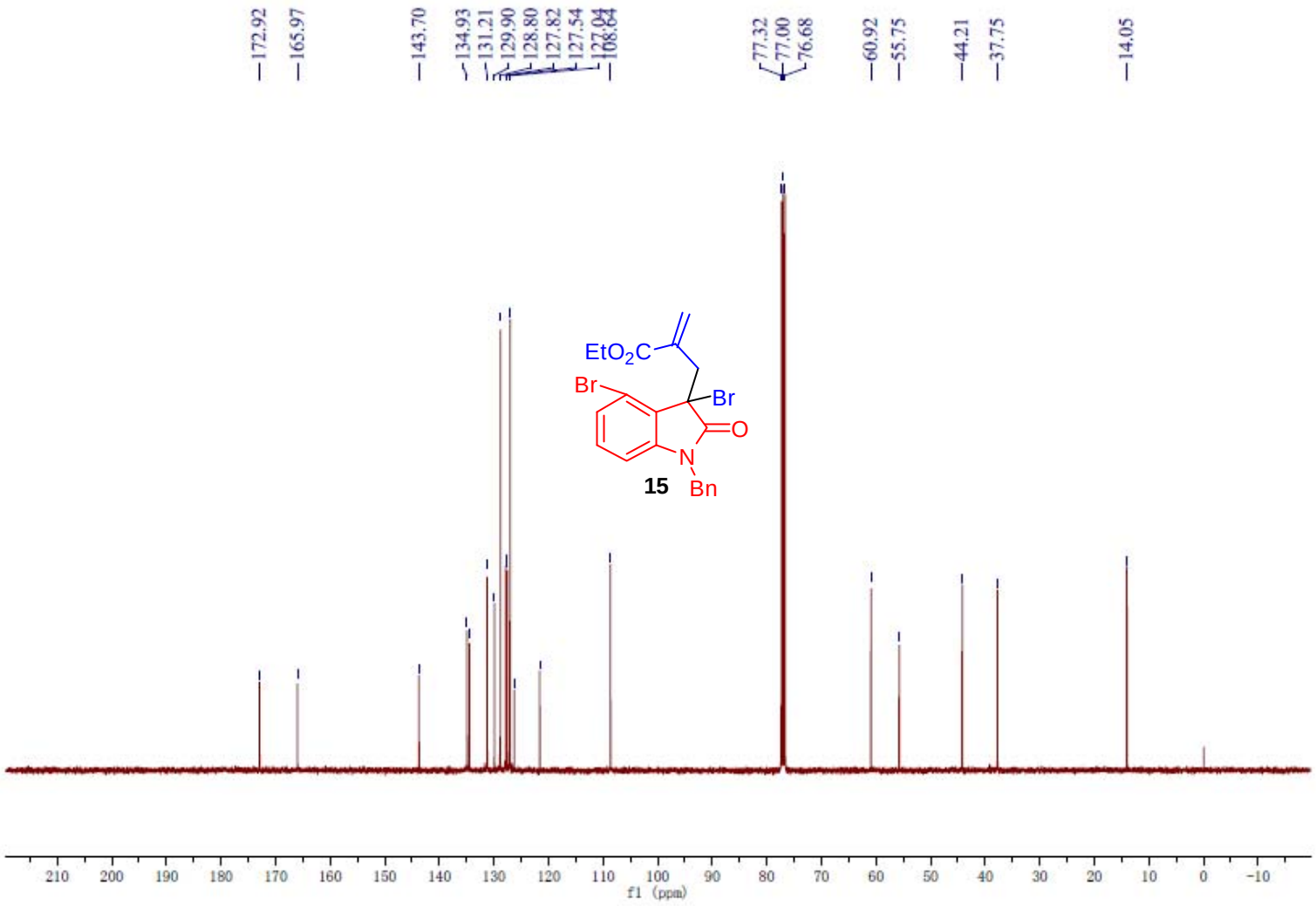
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14.05
EtO2C
Br
Br
O
N
Bn
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200
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180
170
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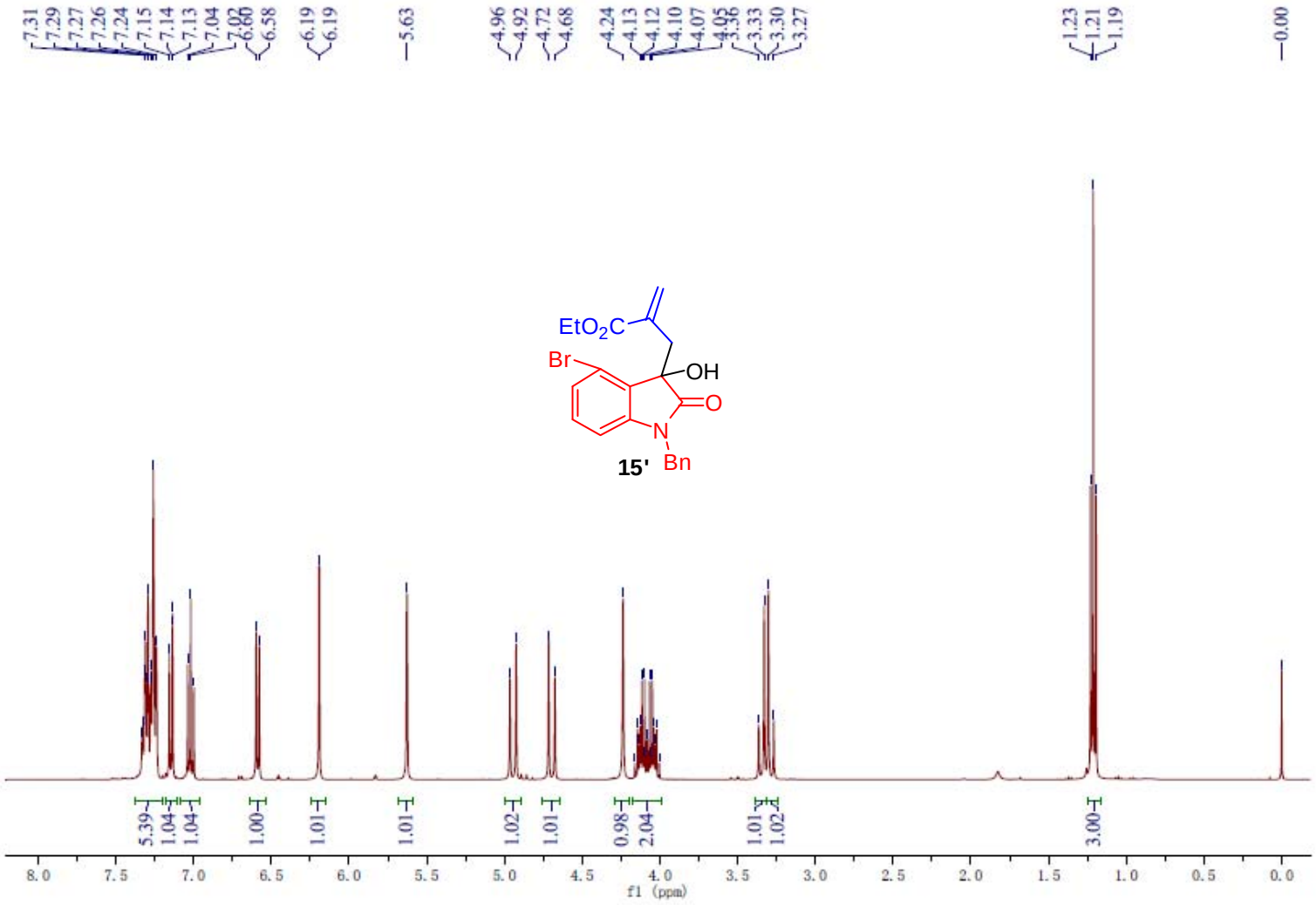
f1 (ppm)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5.63
4.96
4.92
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4.24
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4.12
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4.07
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3.33
3.30
3.27
1.23
1.21
1.19
0.00
EtO2C
Br
OH
O
N
Bn
15'
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1.04
1.04
1.00
1.01
1.01
1.02
1.01
0.98
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1.01
1.02
3.00
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6.0
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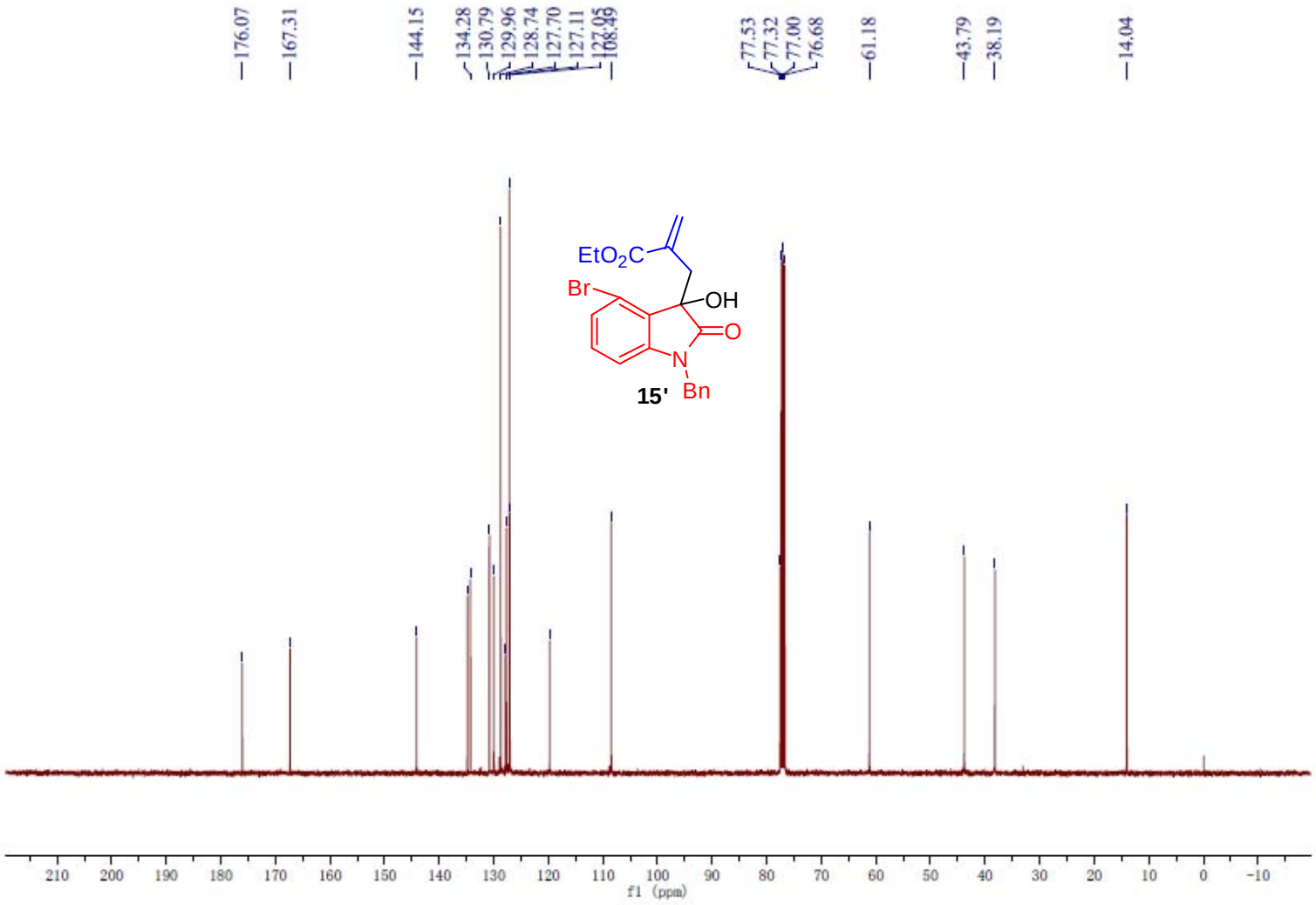
f1 (ppm)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61.18
43.79
38.19
14.04
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OH
O
N
Bn
15'
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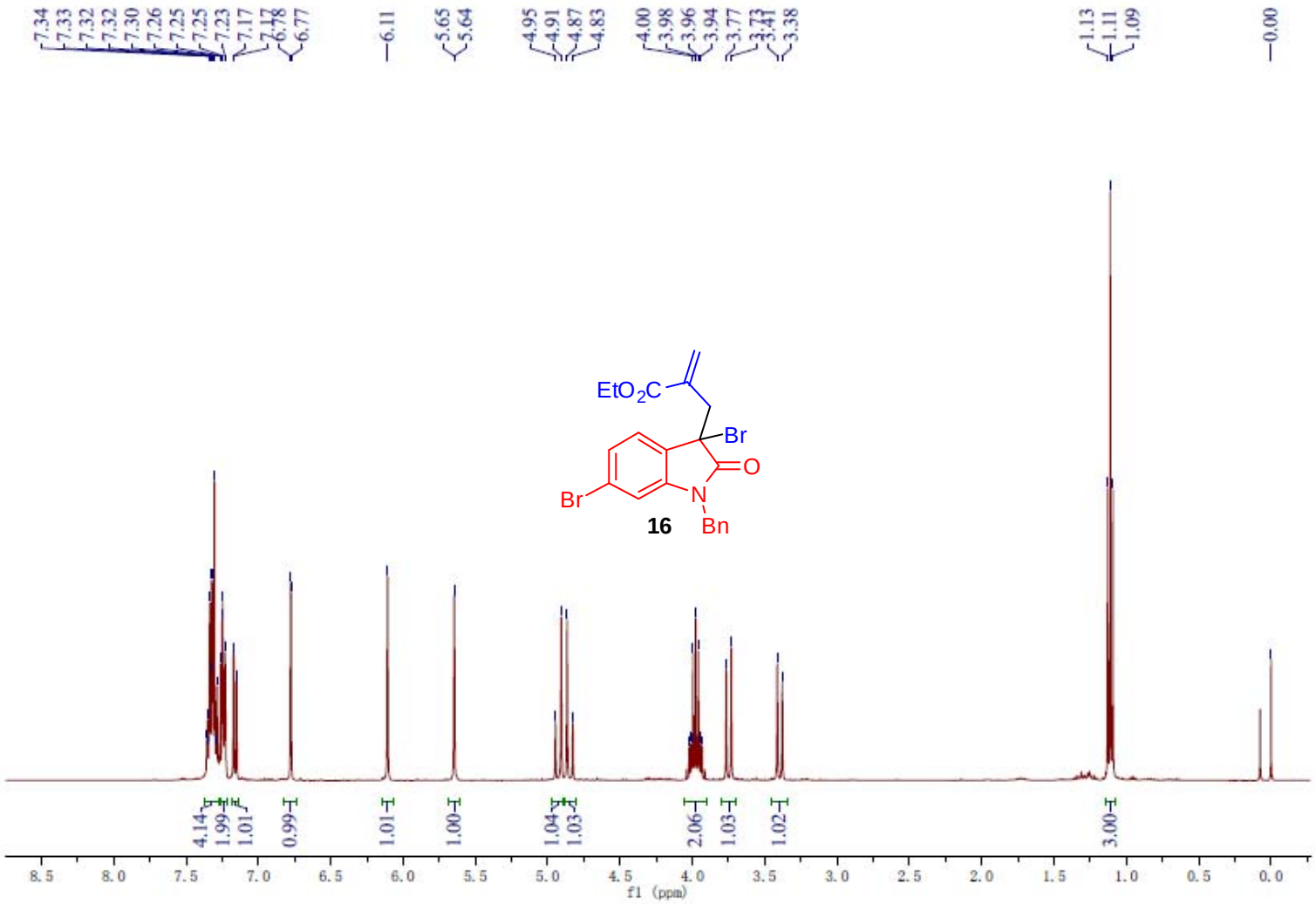
f1 (ppm)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Br
O
Br
N
Bn
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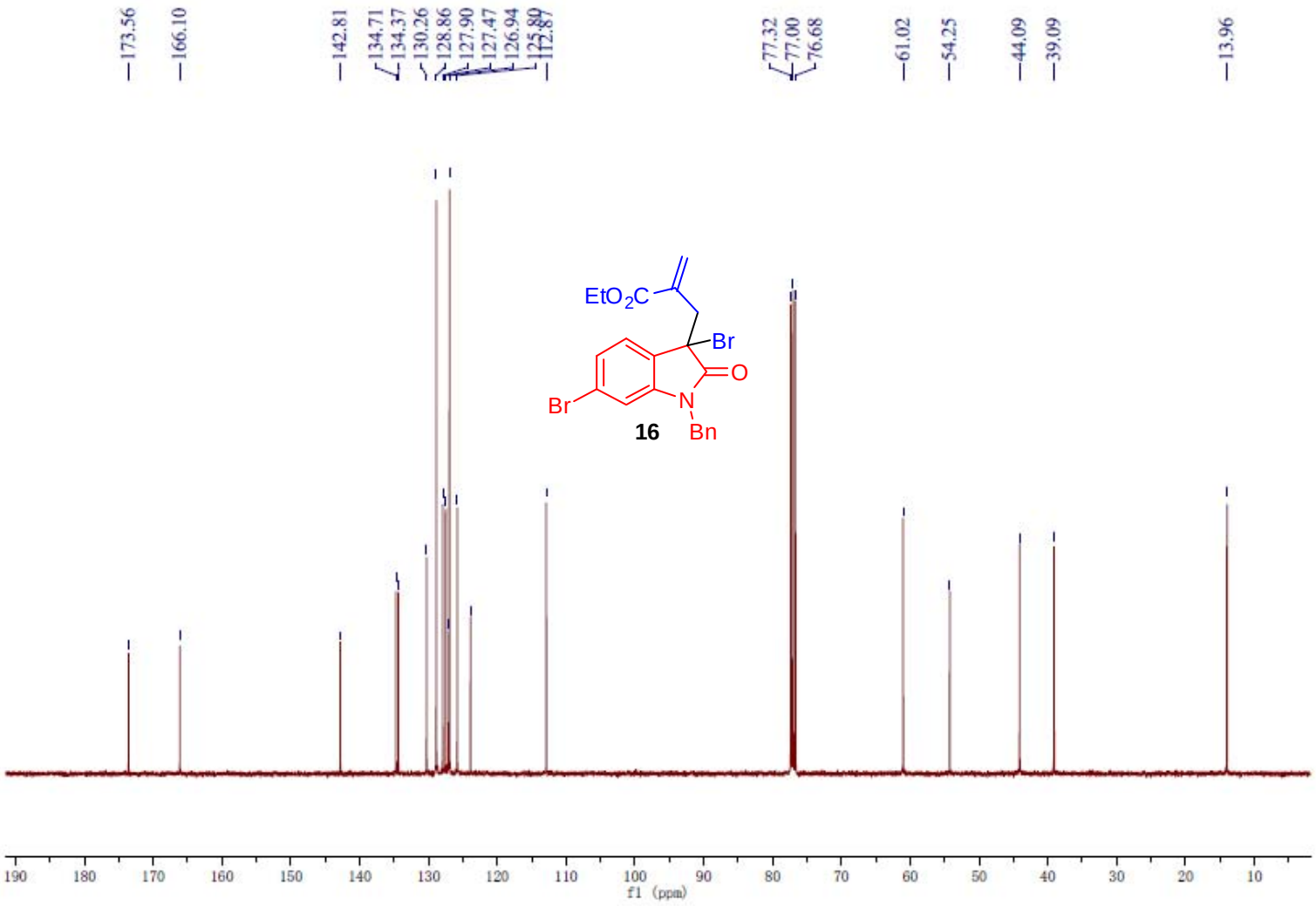
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61.02
54.25
44.09
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13.96
EtO2C
Br
O
Br
N
Bn
16
190
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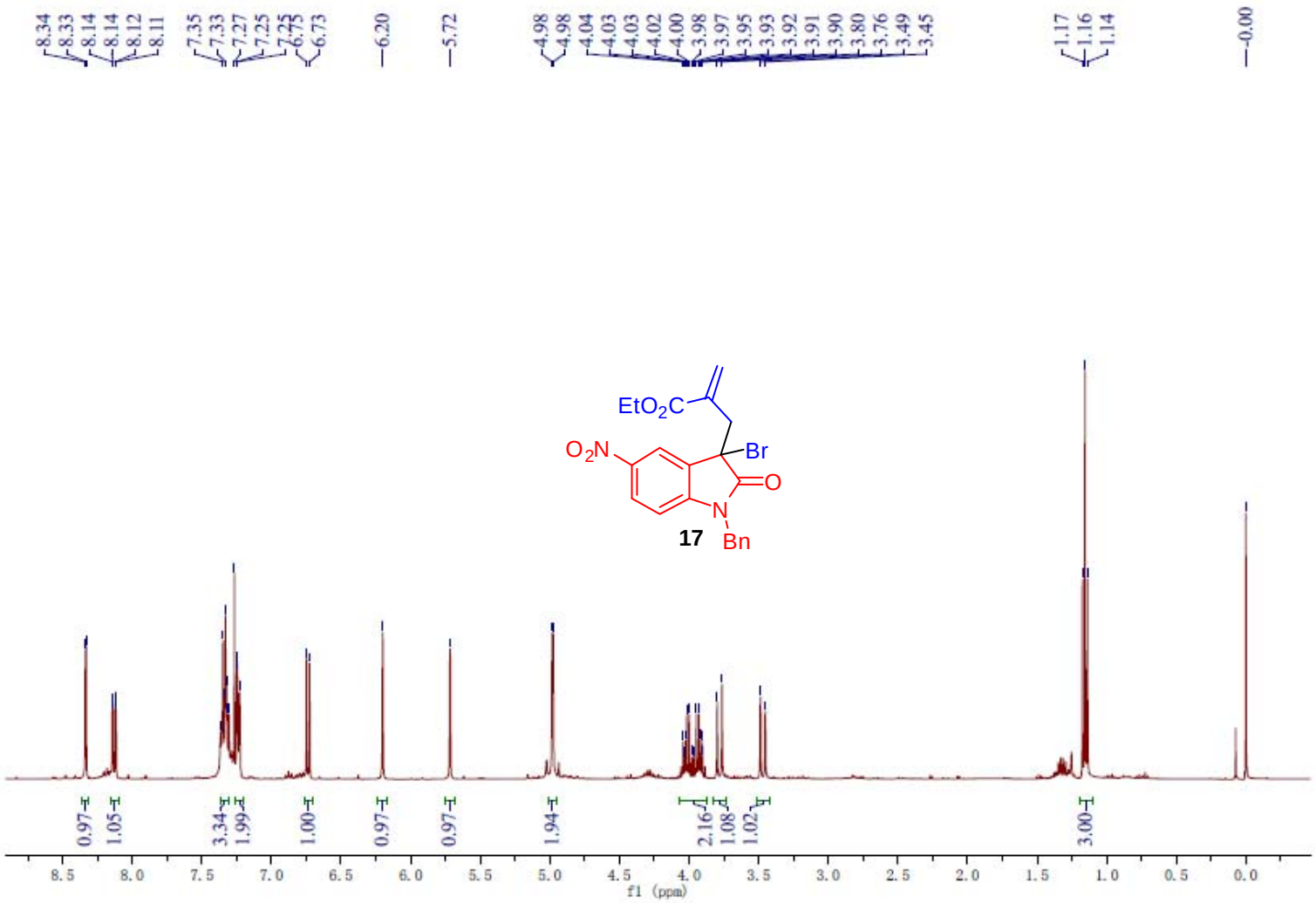
f1 (ppm)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4.04
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4.03
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EtO2C
O2N
Br
O
N
Bn
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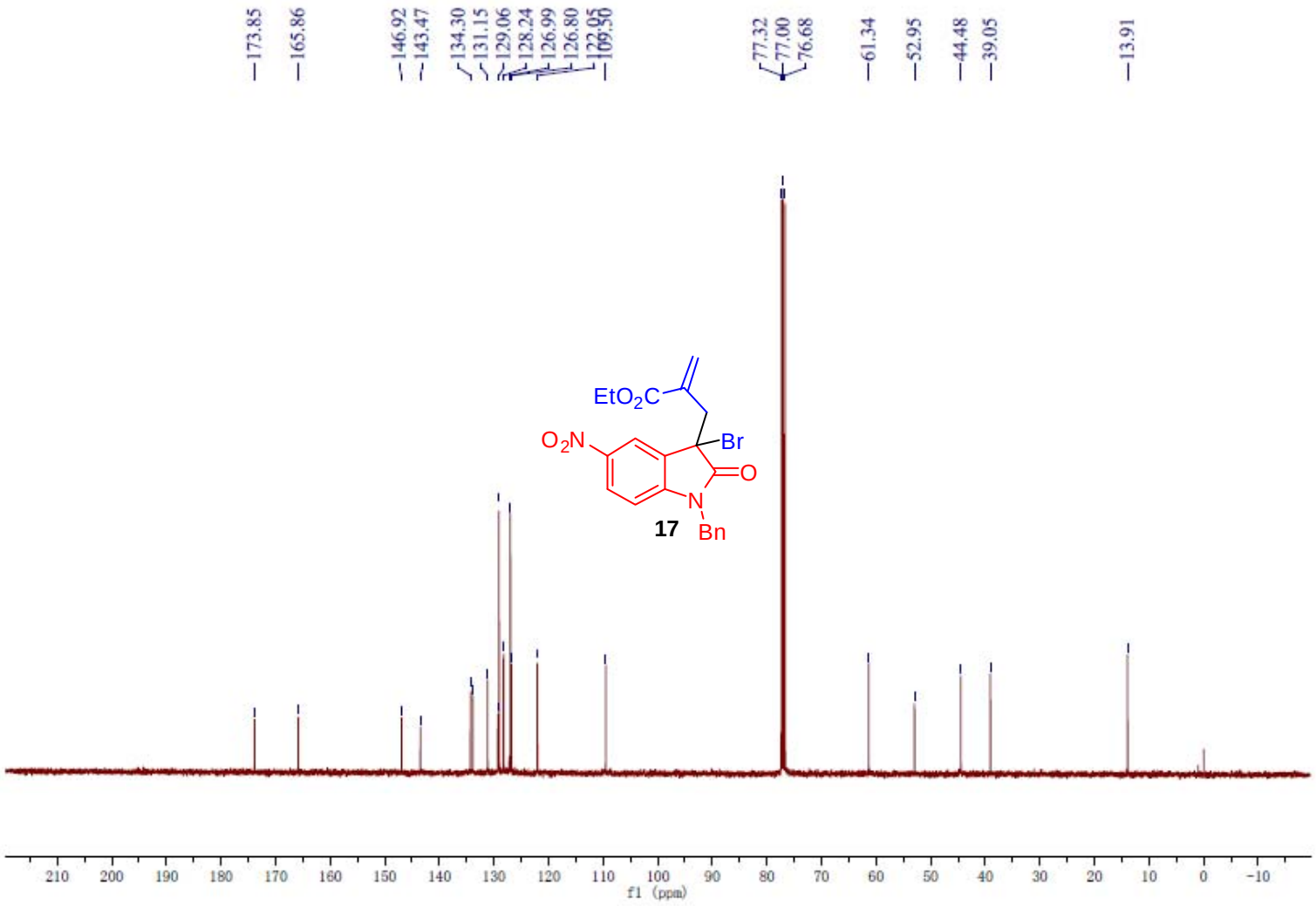
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N
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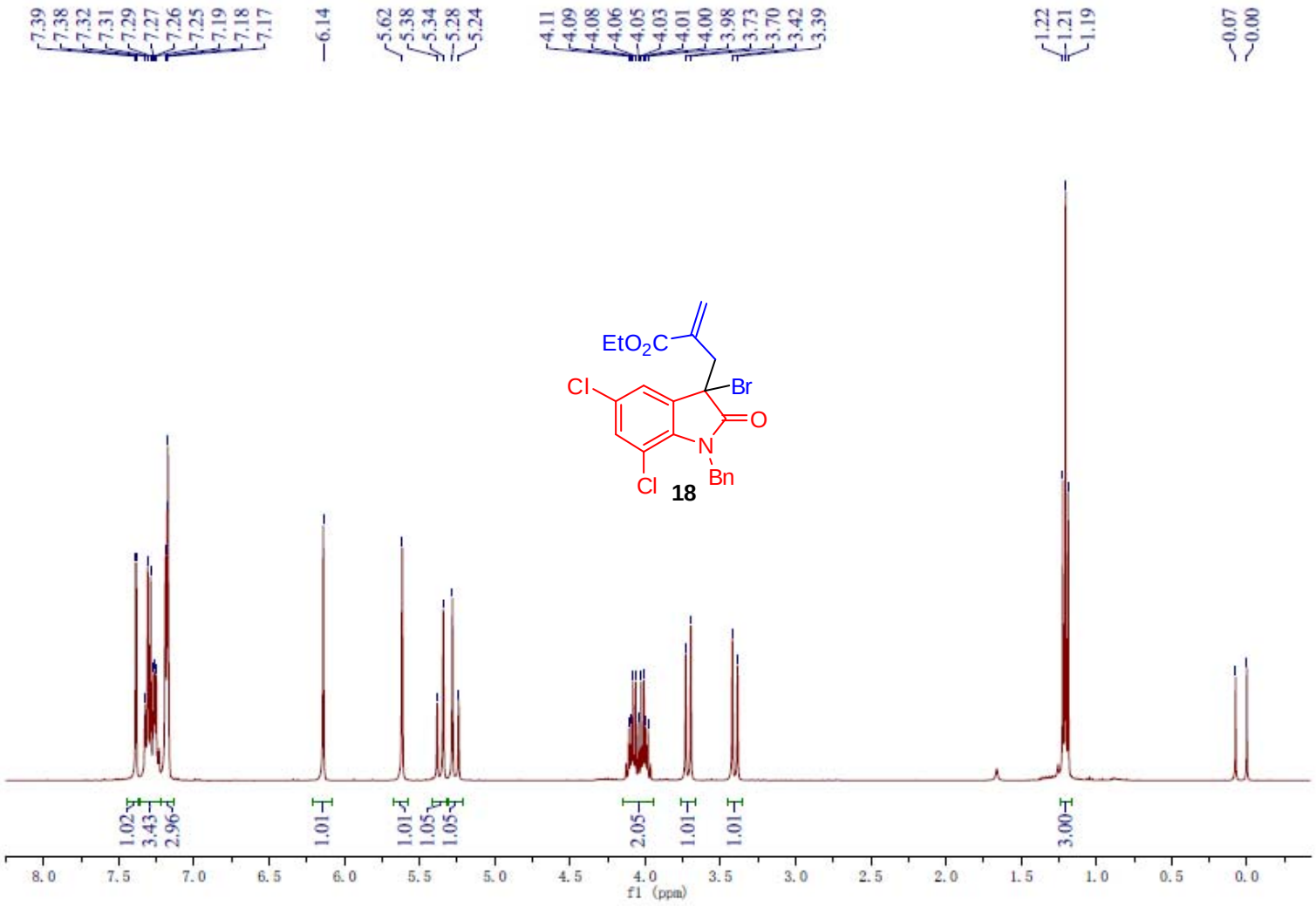
f1 (ppm)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Cl
Br
O
N
Bn
Cl
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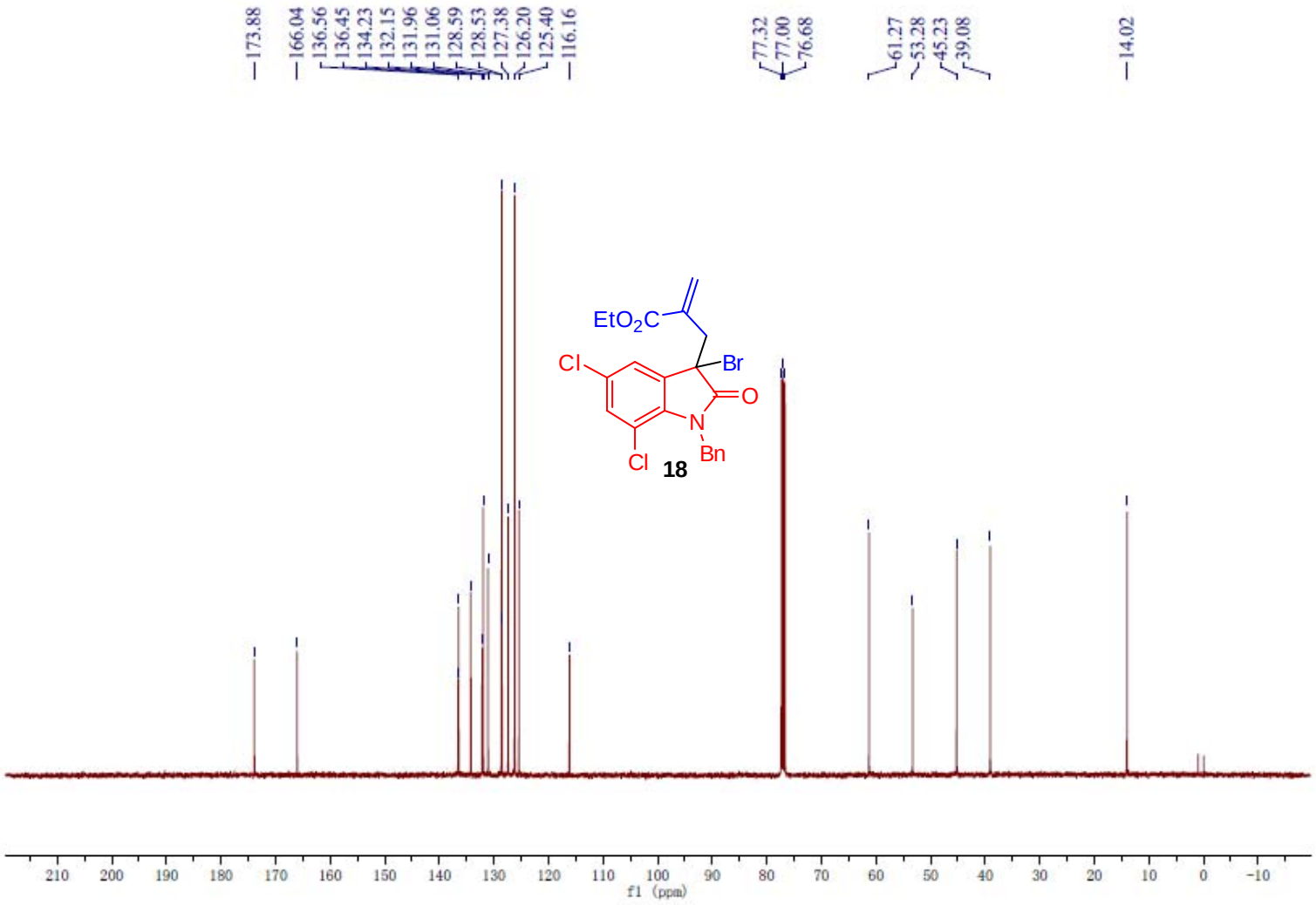
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14.02
EtO2C
Cl
Br
O
N
Bn
Cl
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210
200
190
180
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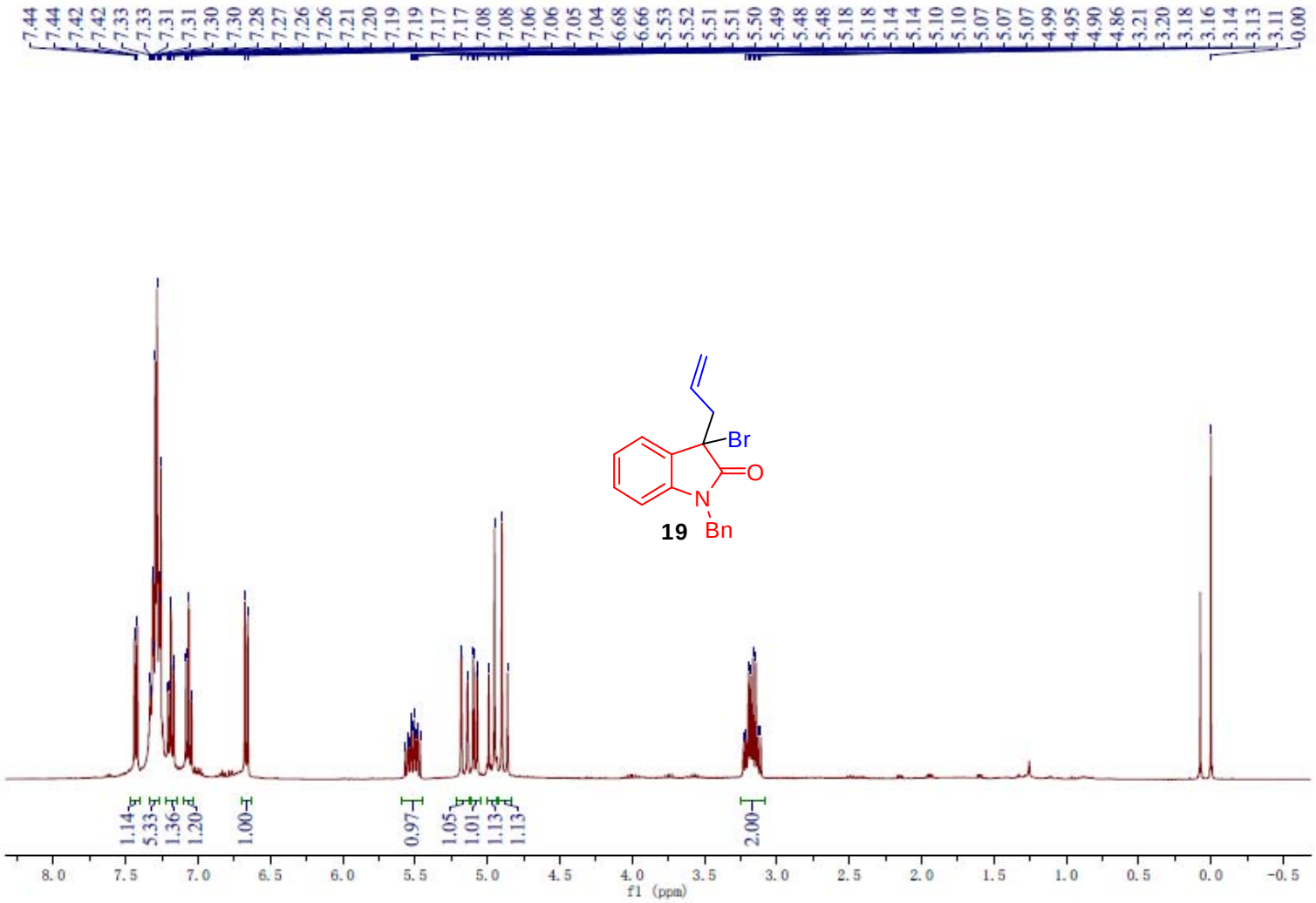
f1 (ppm)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Br
O
N
Bn
19
1.14 5.33 1.36 1.20 1.00 0.97 1.05 1.01 1.13 1.13 2.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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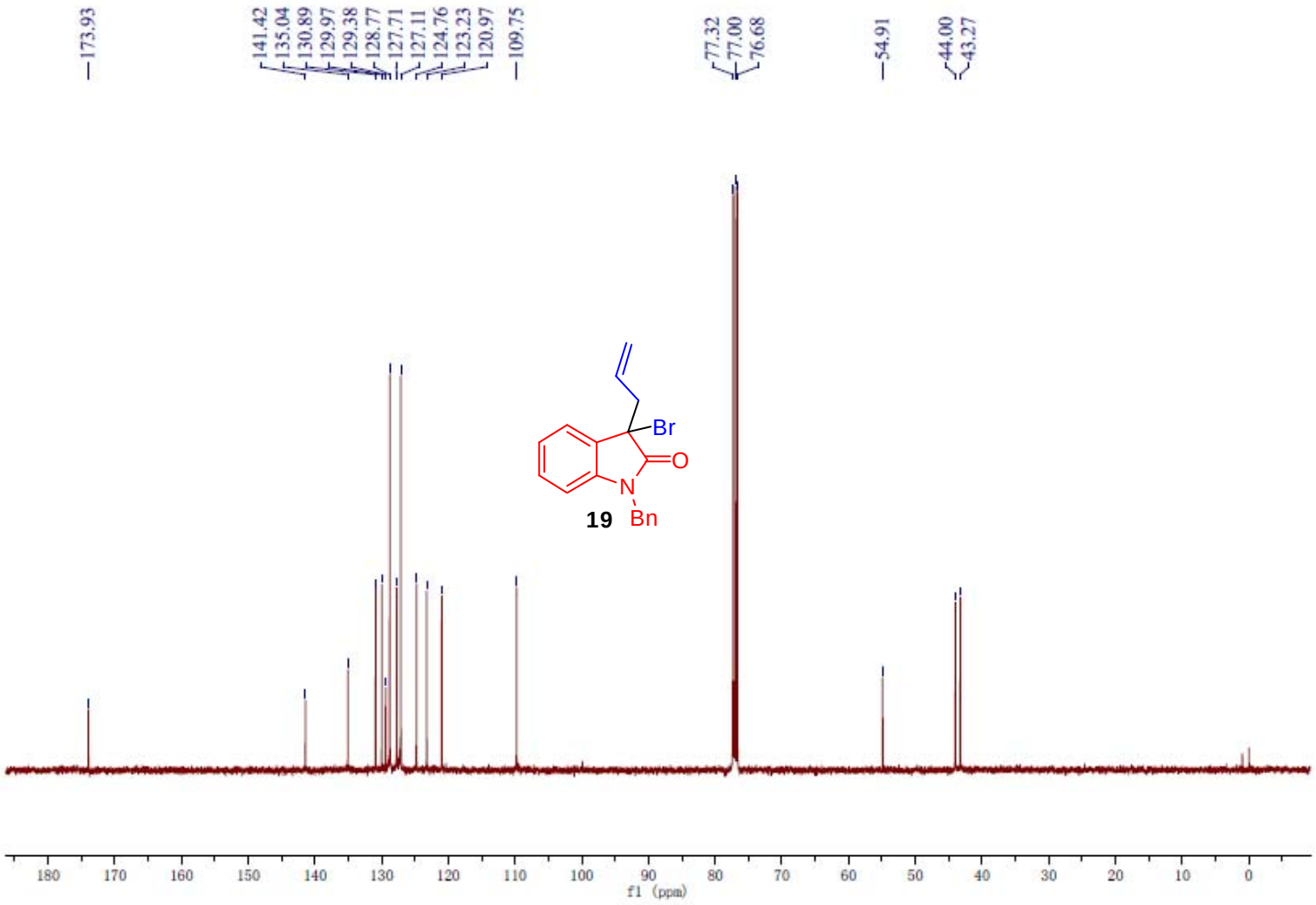
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44.00
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Br
O
N
Bn
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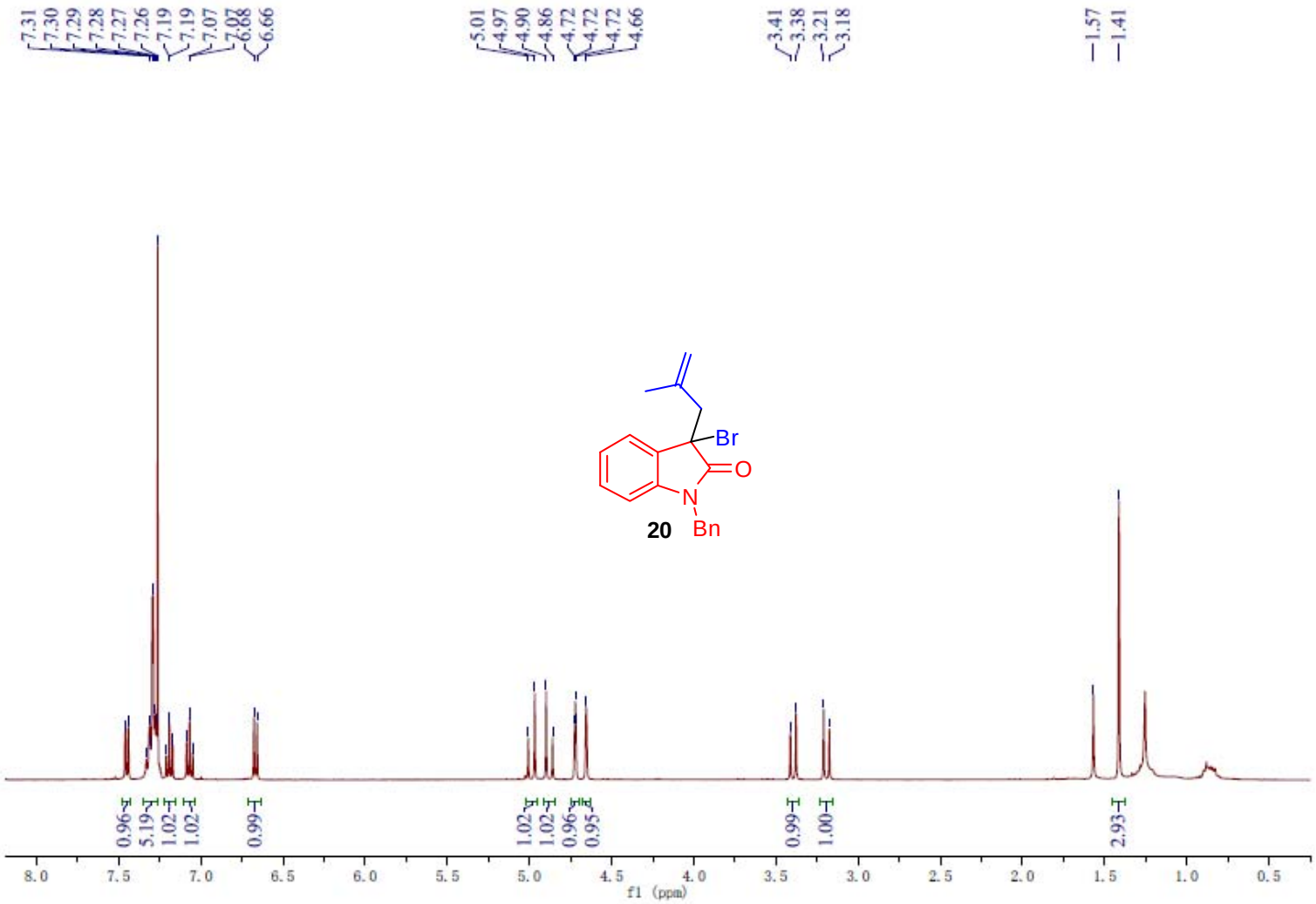
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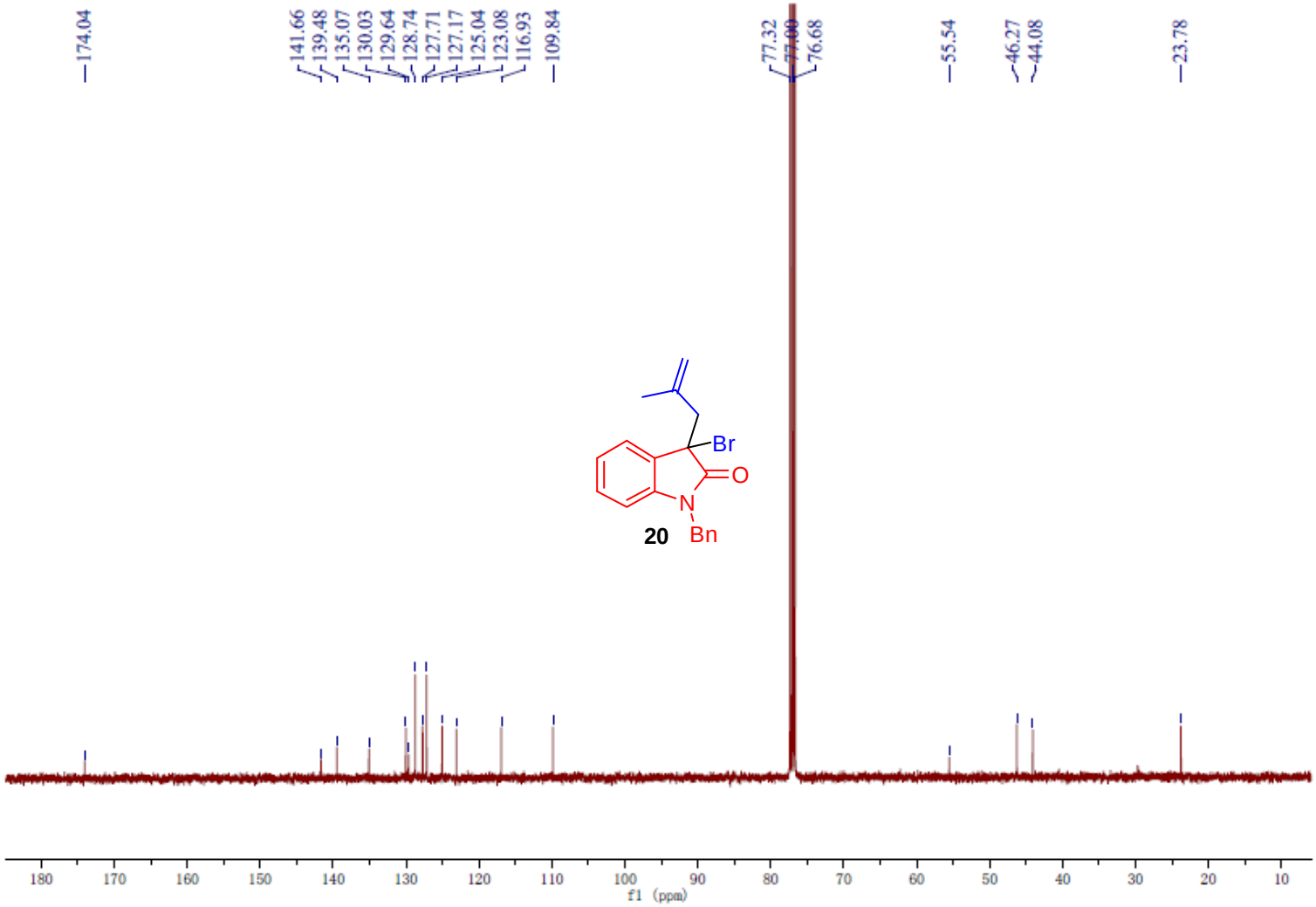
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Bn
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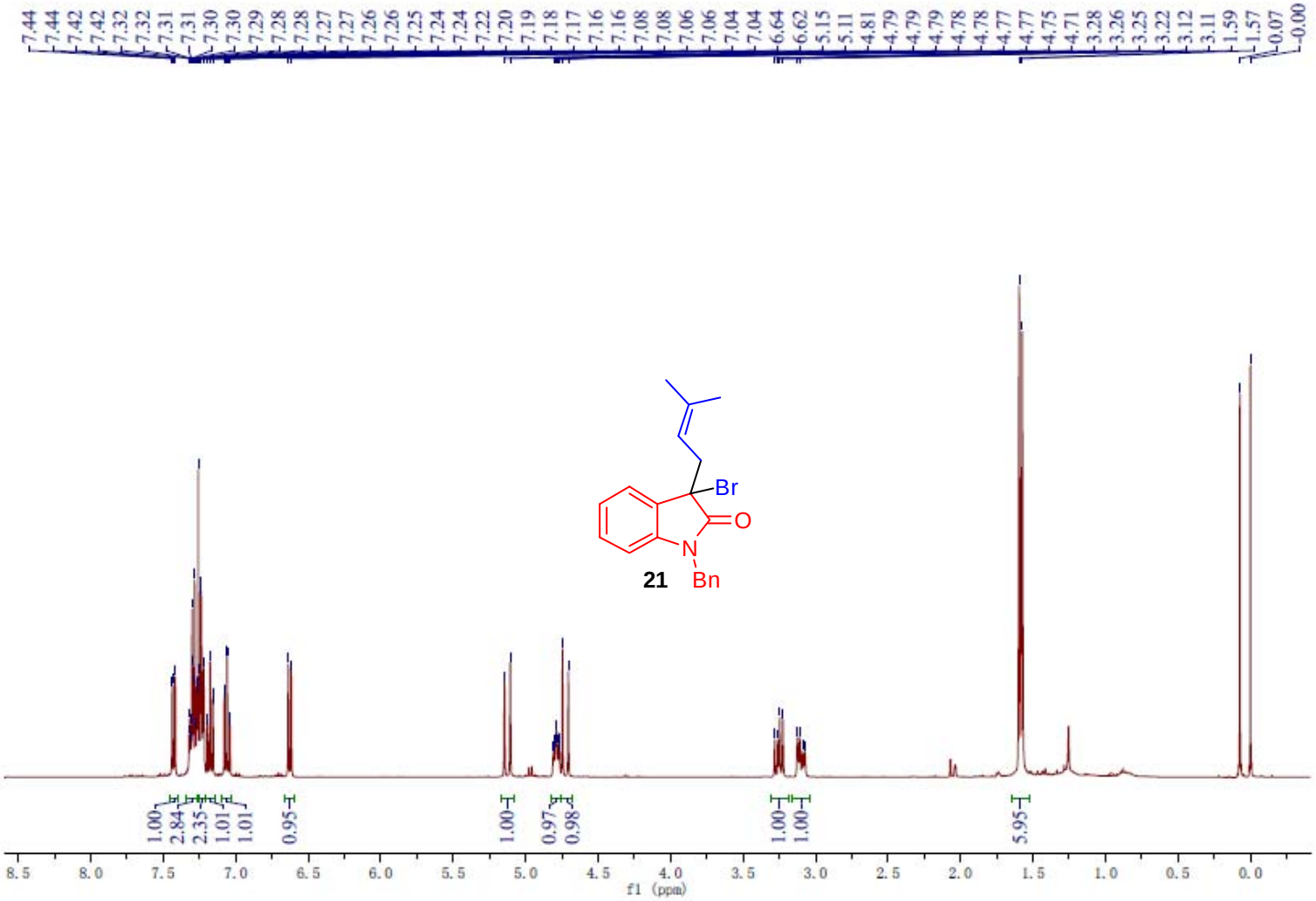
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Bn
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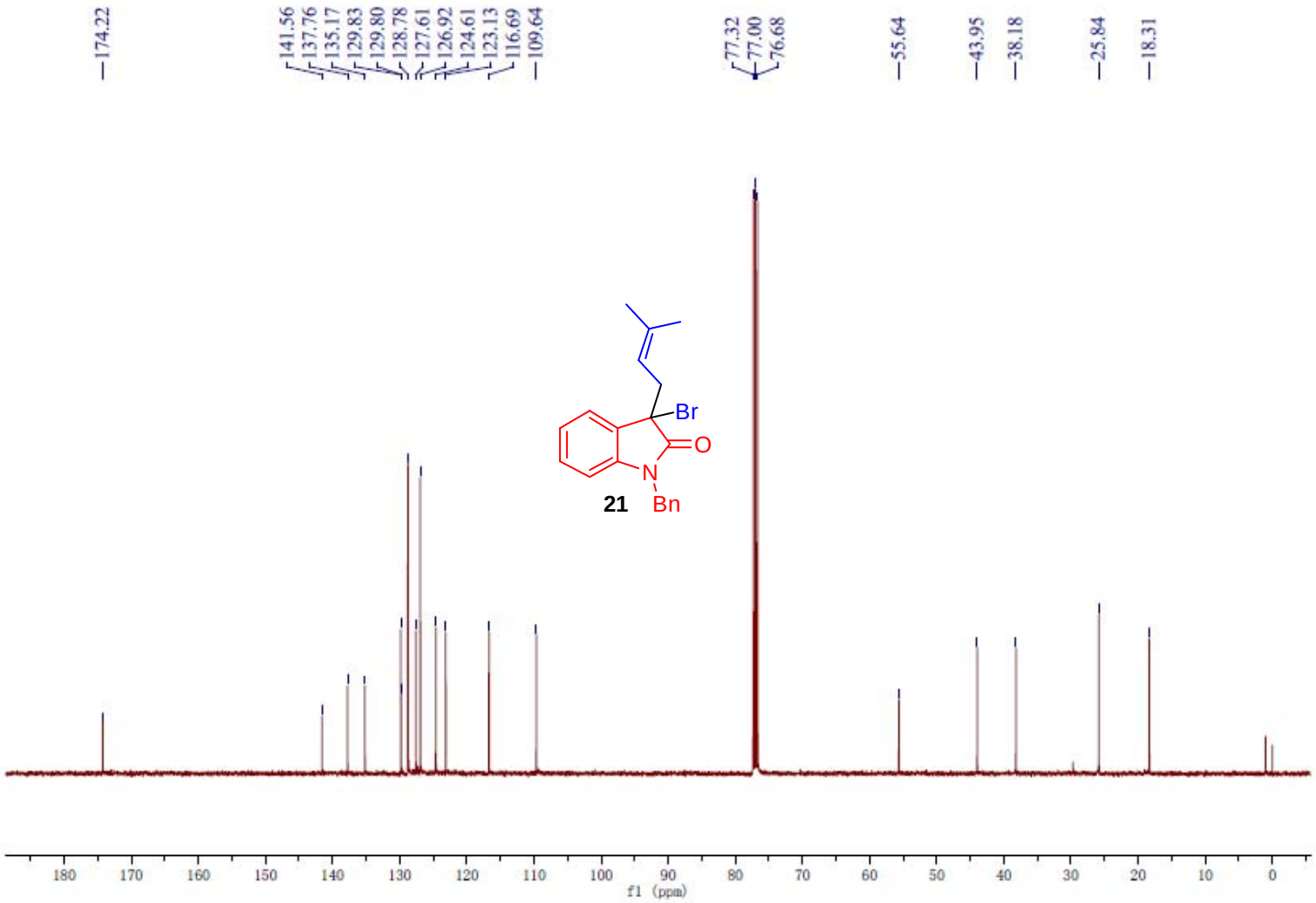
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Br
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N
Bn
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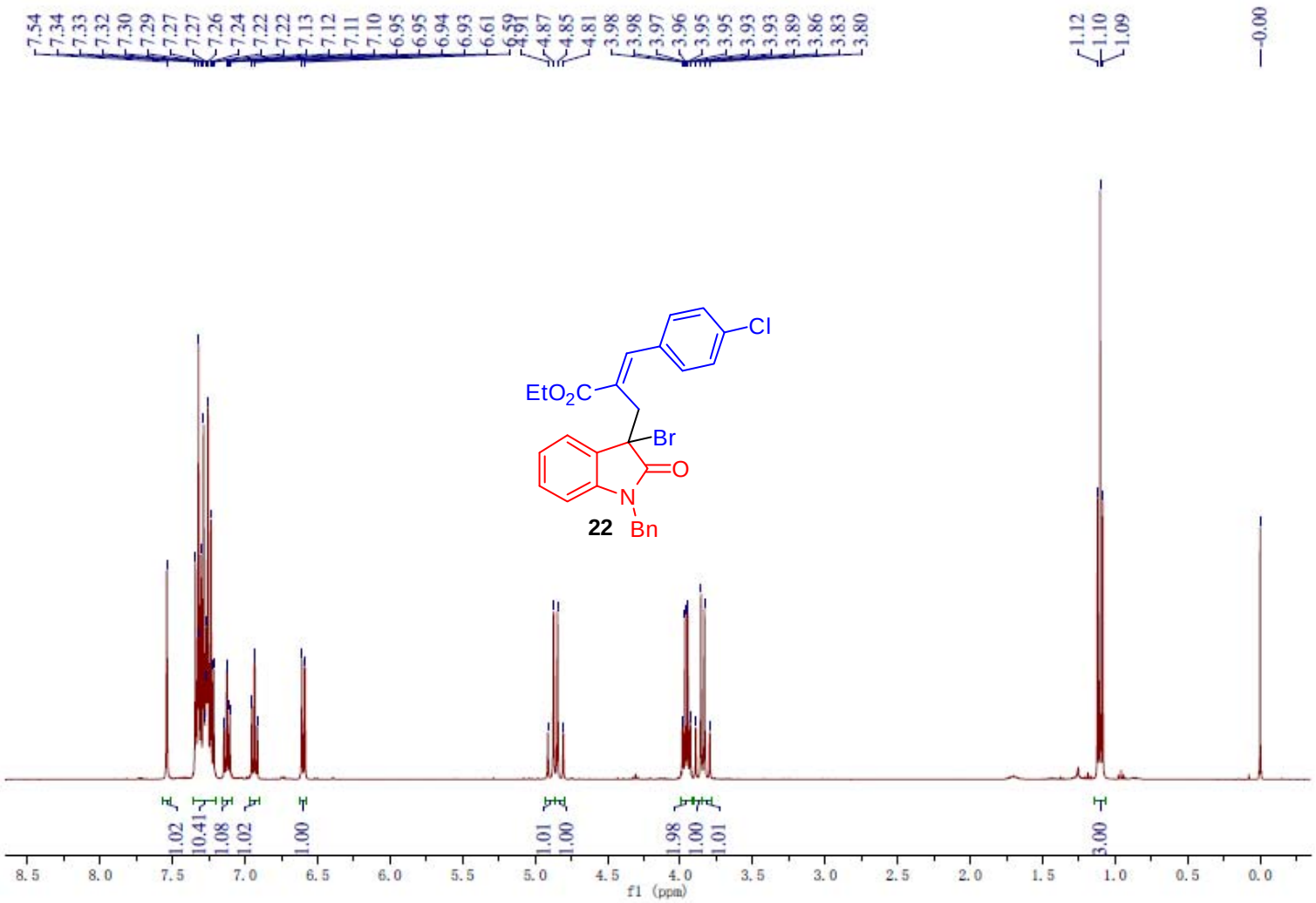
f1 (ppm)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Br
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N
Bn
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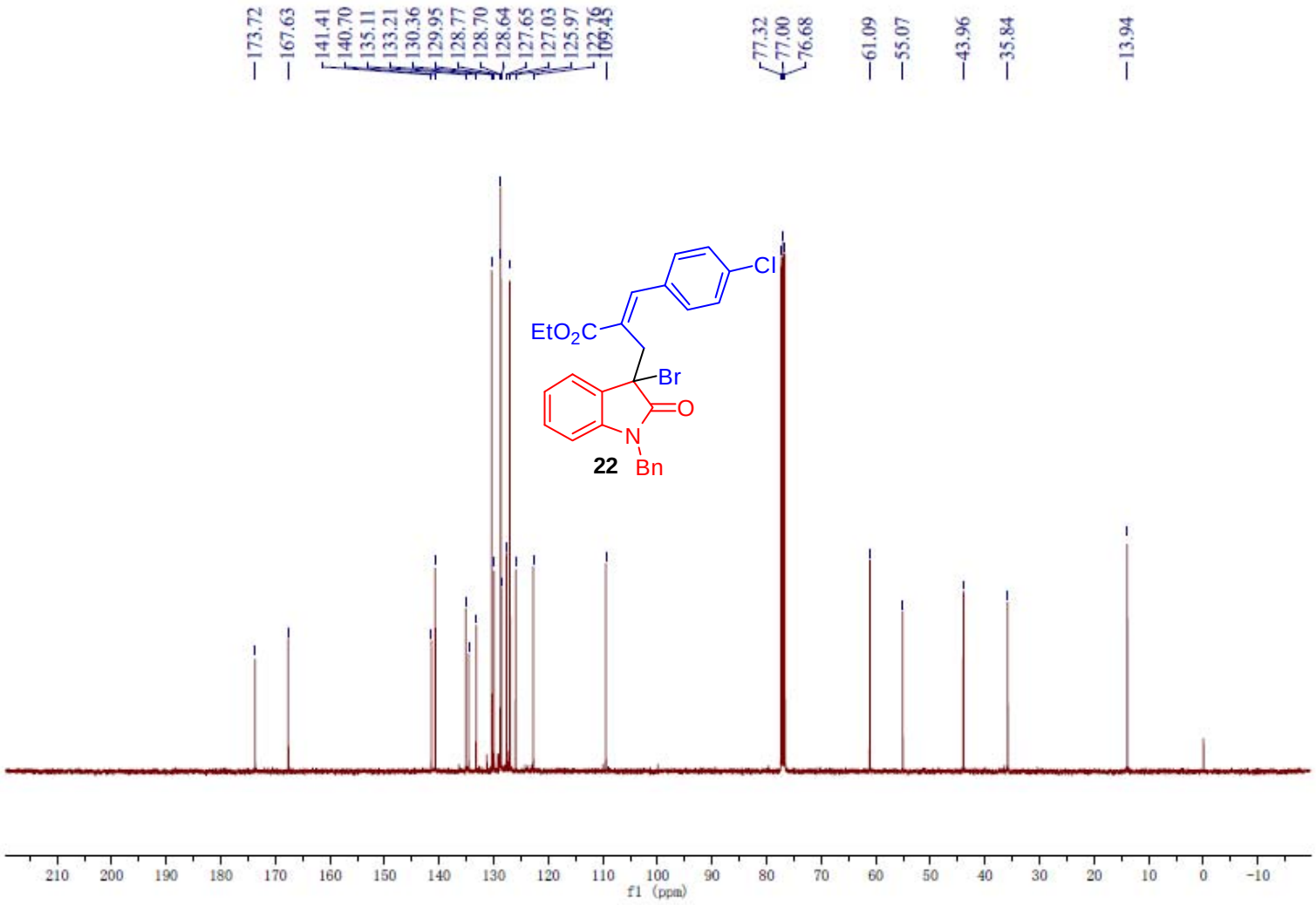
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35.84
13.94
Cl
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Br
O
N
Bn
22
210
200
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180
170
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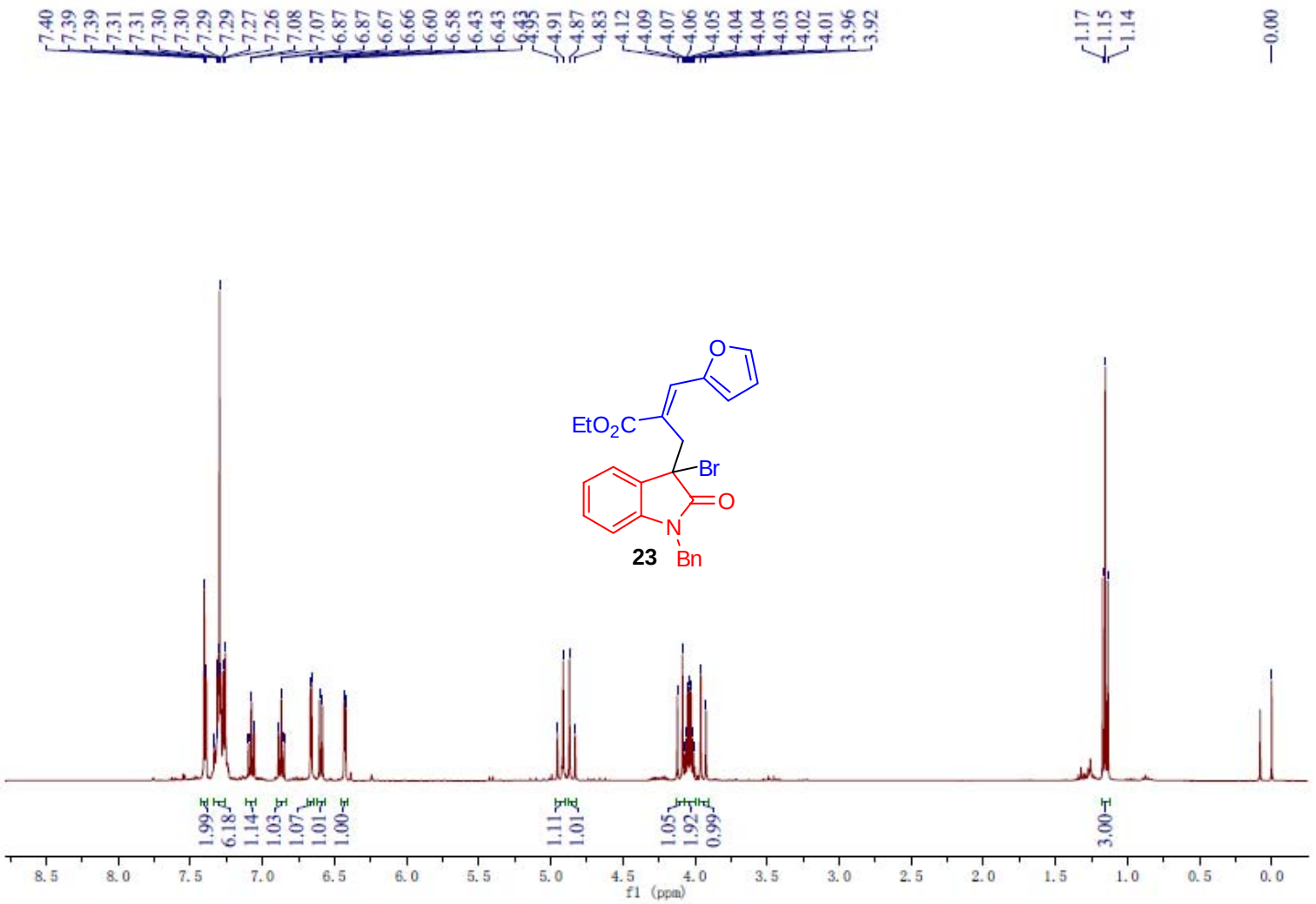
f1 (ppm)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Br
O
O
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Bn
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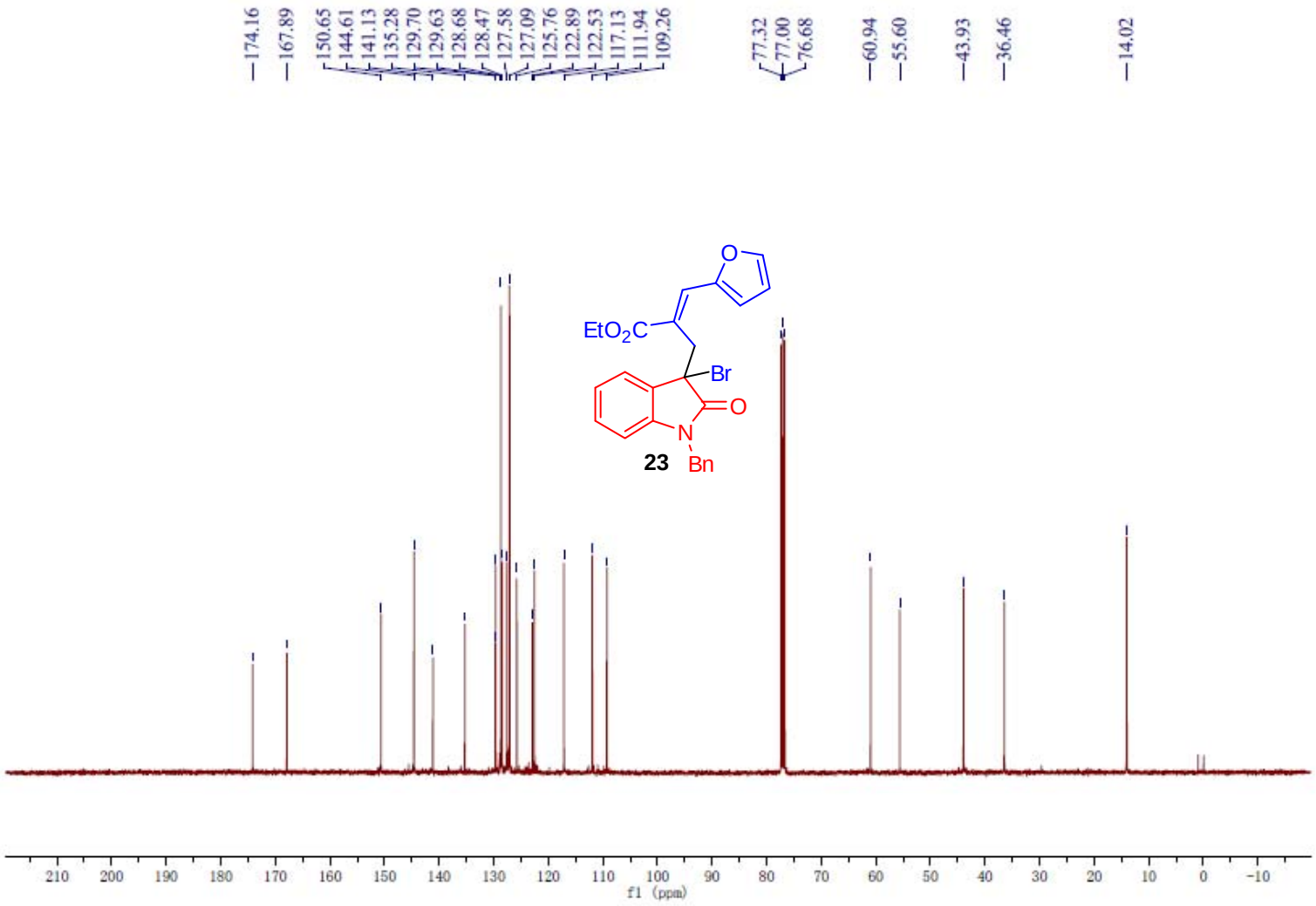
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55.60
43.93
36.46
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Br
O
N
Bn
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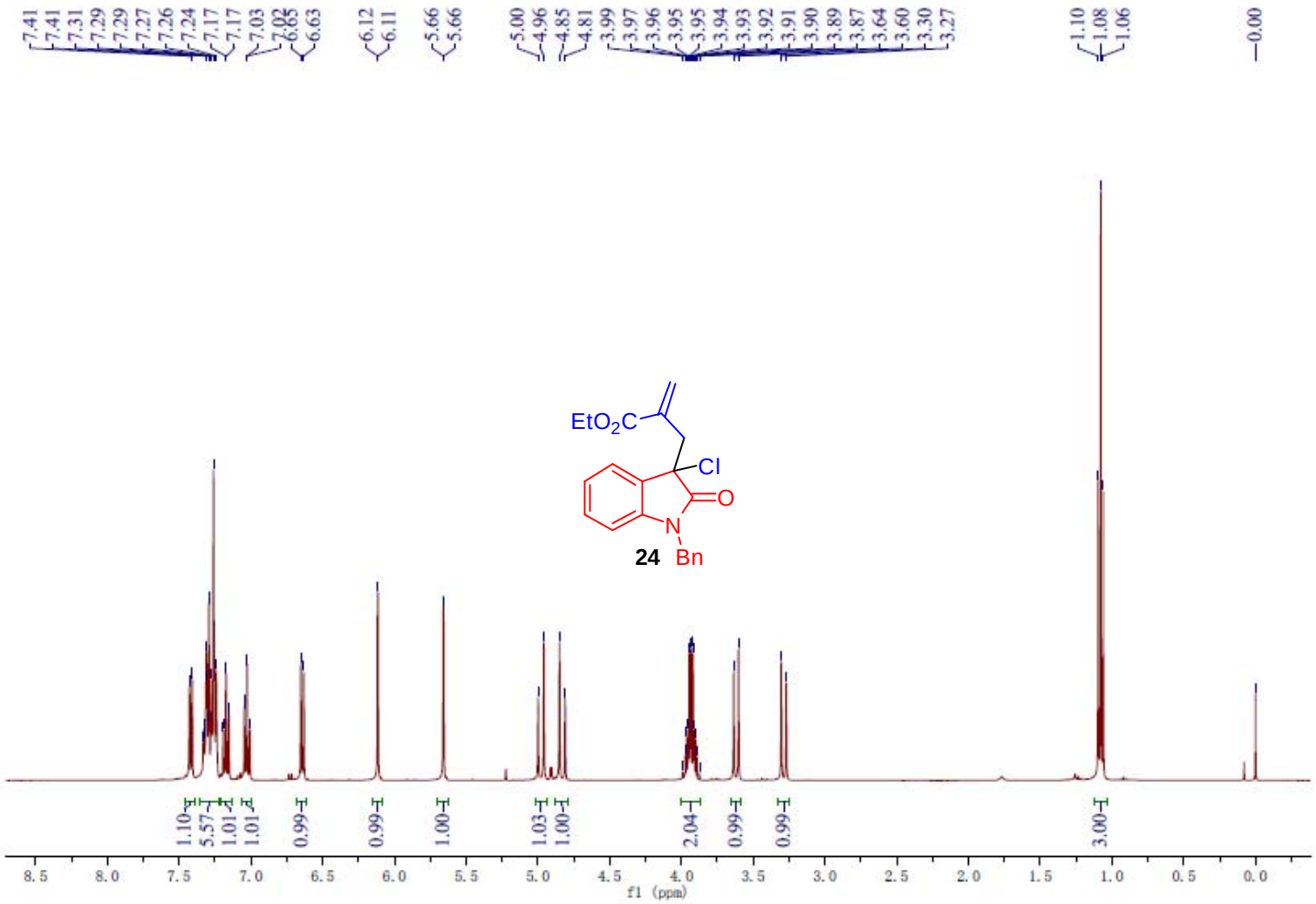
f1 (ppm)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3.96
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3.94
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3.92
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1.08
1.06
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EtO2C
Cl
O
N
Bn
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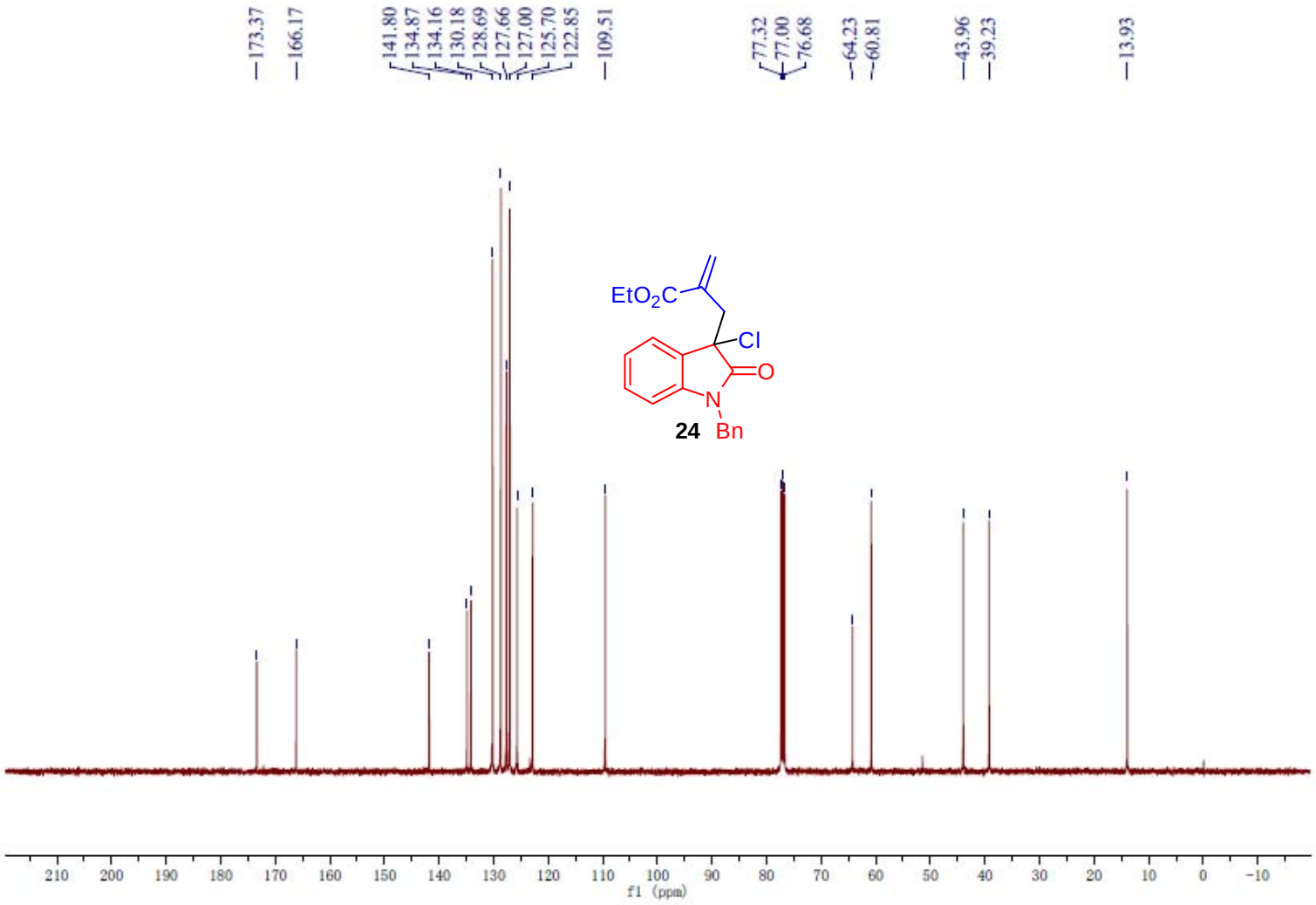
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64.23
60.81
43.96
39.23
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Cl
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N
Bn
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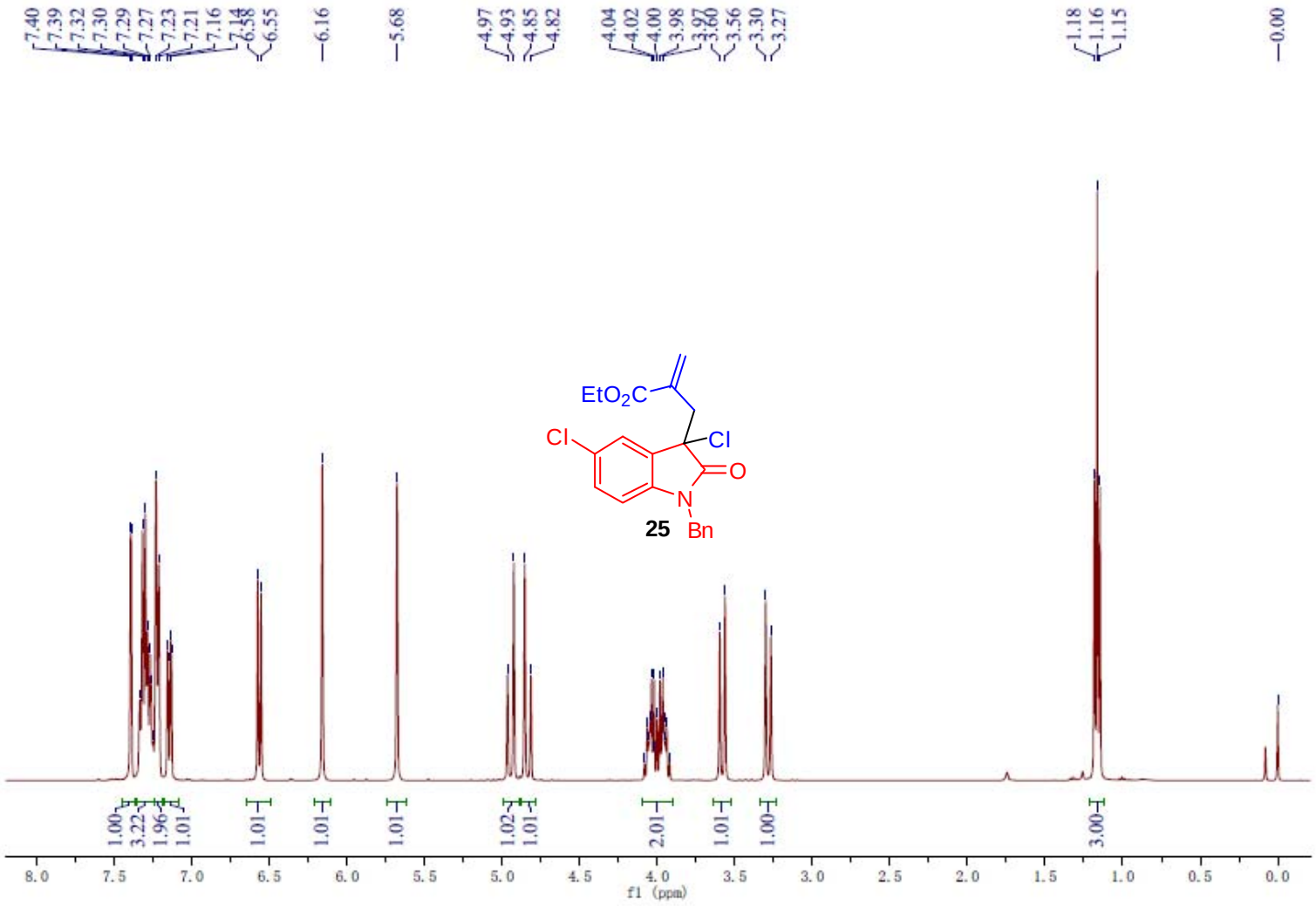
f1 (ppm)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5.68
4.97
4.93
4.85
4.82
4.04
4.02
4.00
3.98
3.97
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1.18
1.16
1.15
0.00
EtO2C
Cl
Cl
O
N
Bn
25
1.00
3.22
1.96
1.01
1.01
1.01
1.01
1.02
1.01
2.01
1.01
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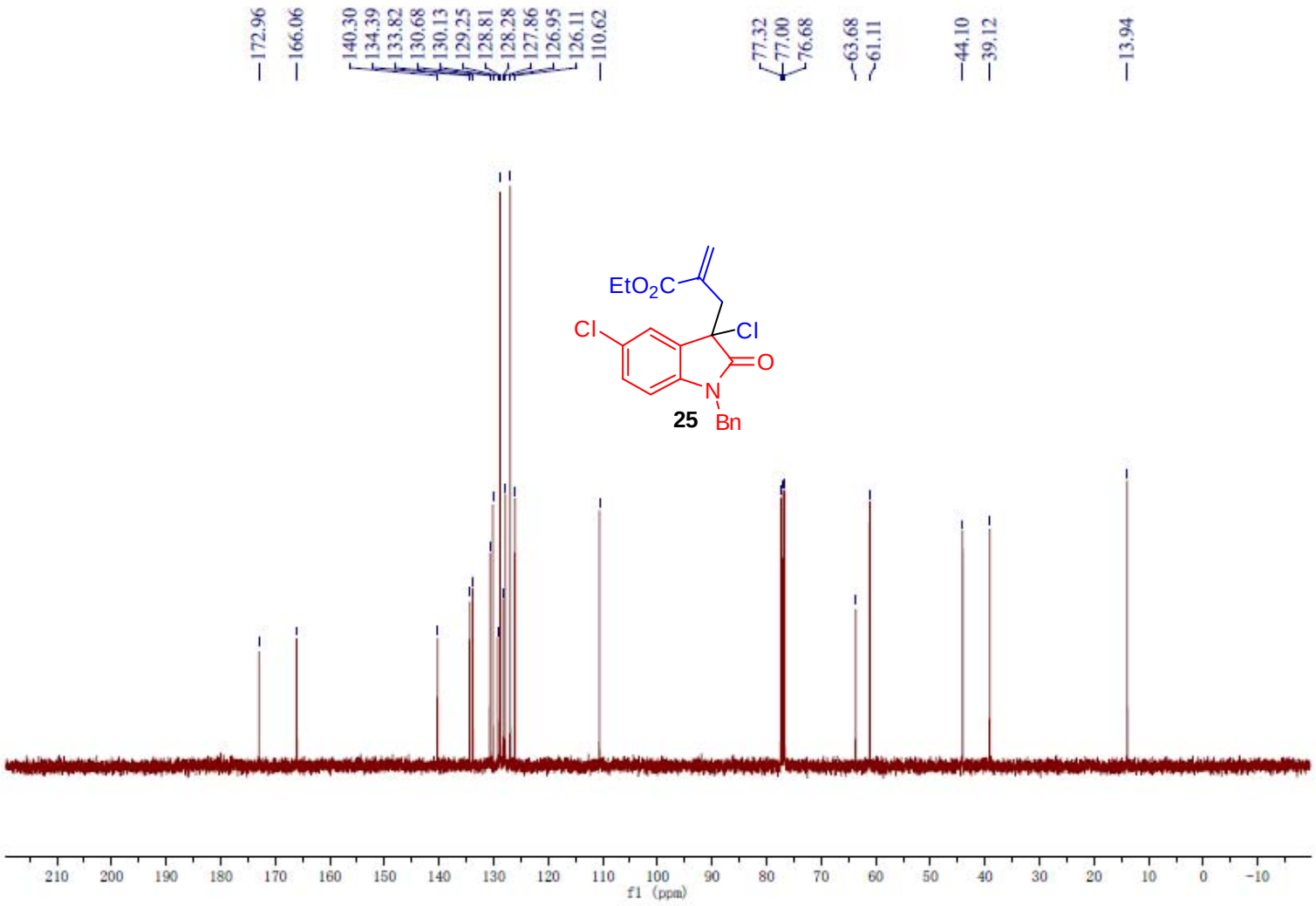
f1 (ppm)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63.68
61.11
44.10
39.12
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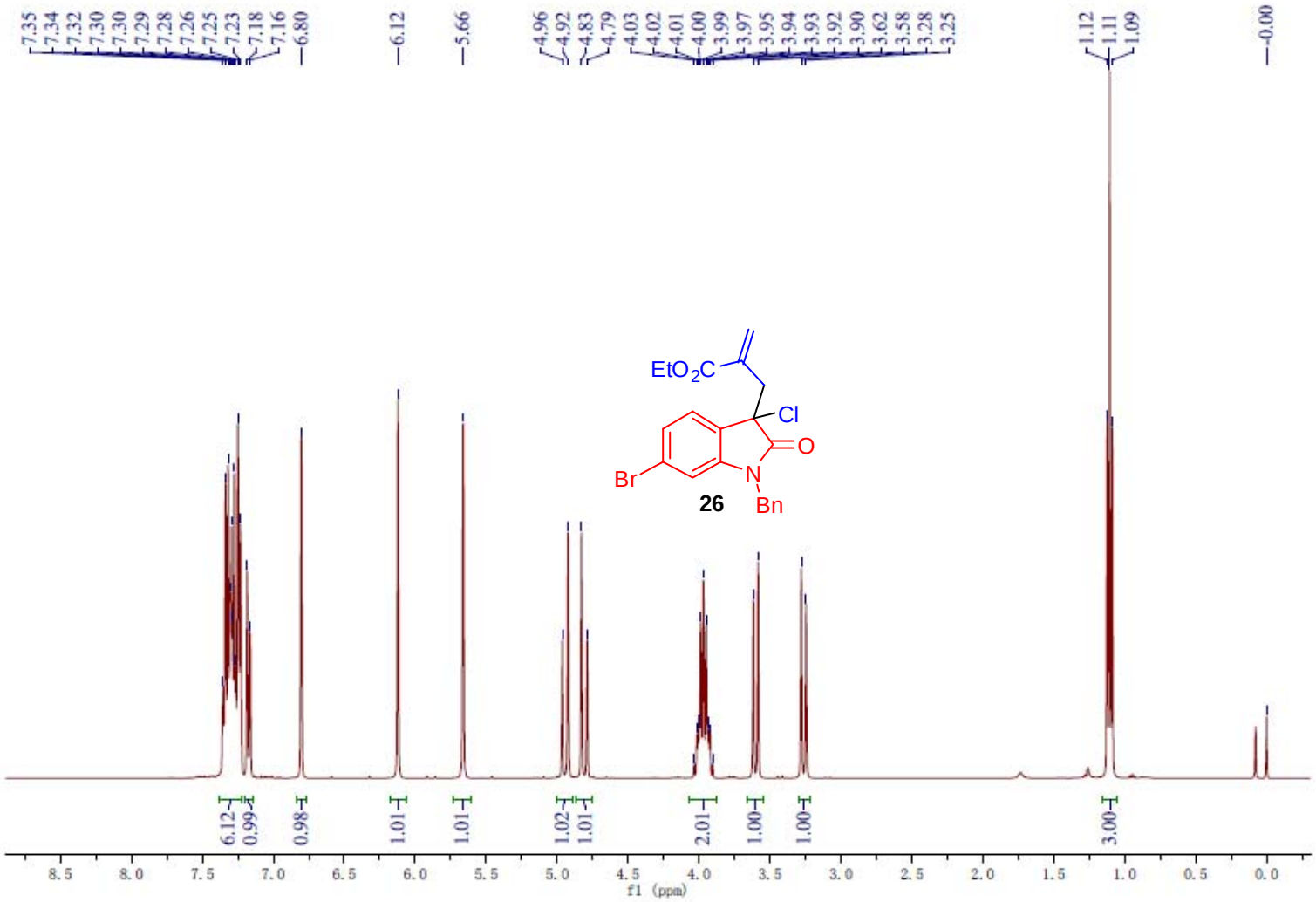
EtO2C
Cl
Cl
O
N
Bn
25
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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4.01
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3.97
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3.28
3.25
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1.11
1.09
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Cl
O
Br
N
Bn
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0.98
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1.01
1.02
1.01
2.01
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1.00
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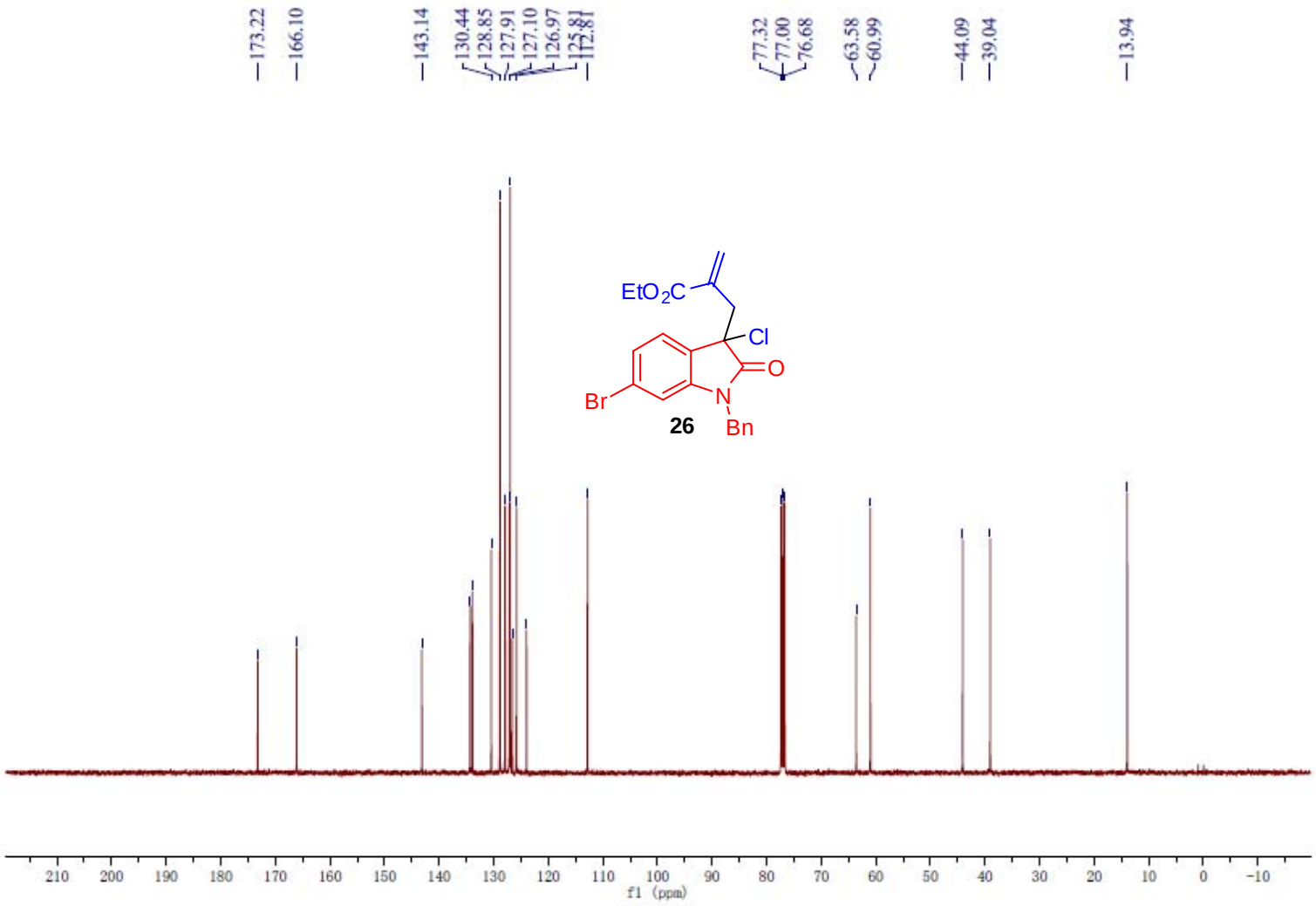
0.0
f1 (ppm)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39.04
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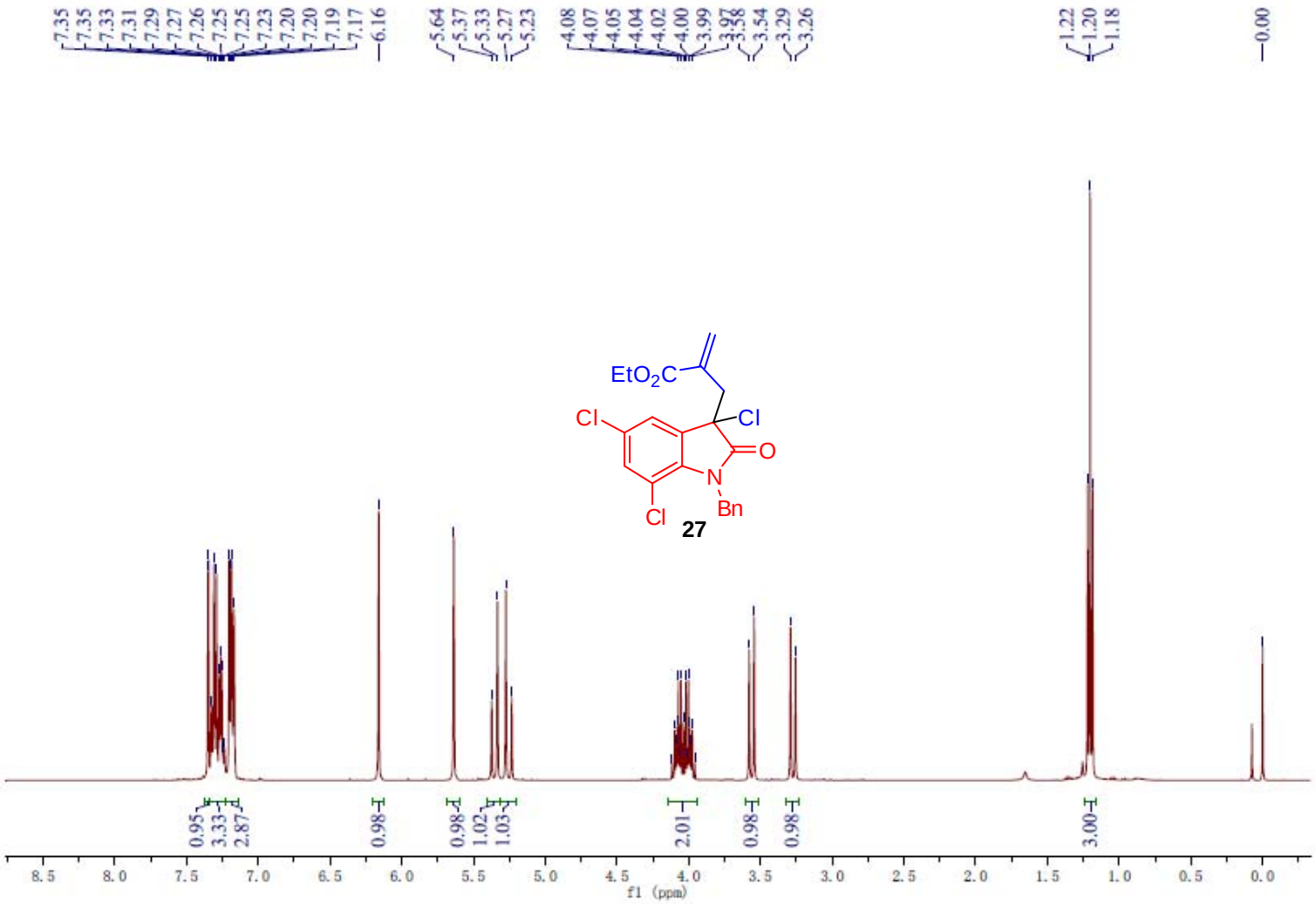
O
Br
N
Bn
26
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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5.27
5.23
4.08
4.07
4.05
4.04
4.02
4.00
3.99
3.97
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1.20
1.18
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EtO2C
Cl
Cl
O
N
Bn
Cl
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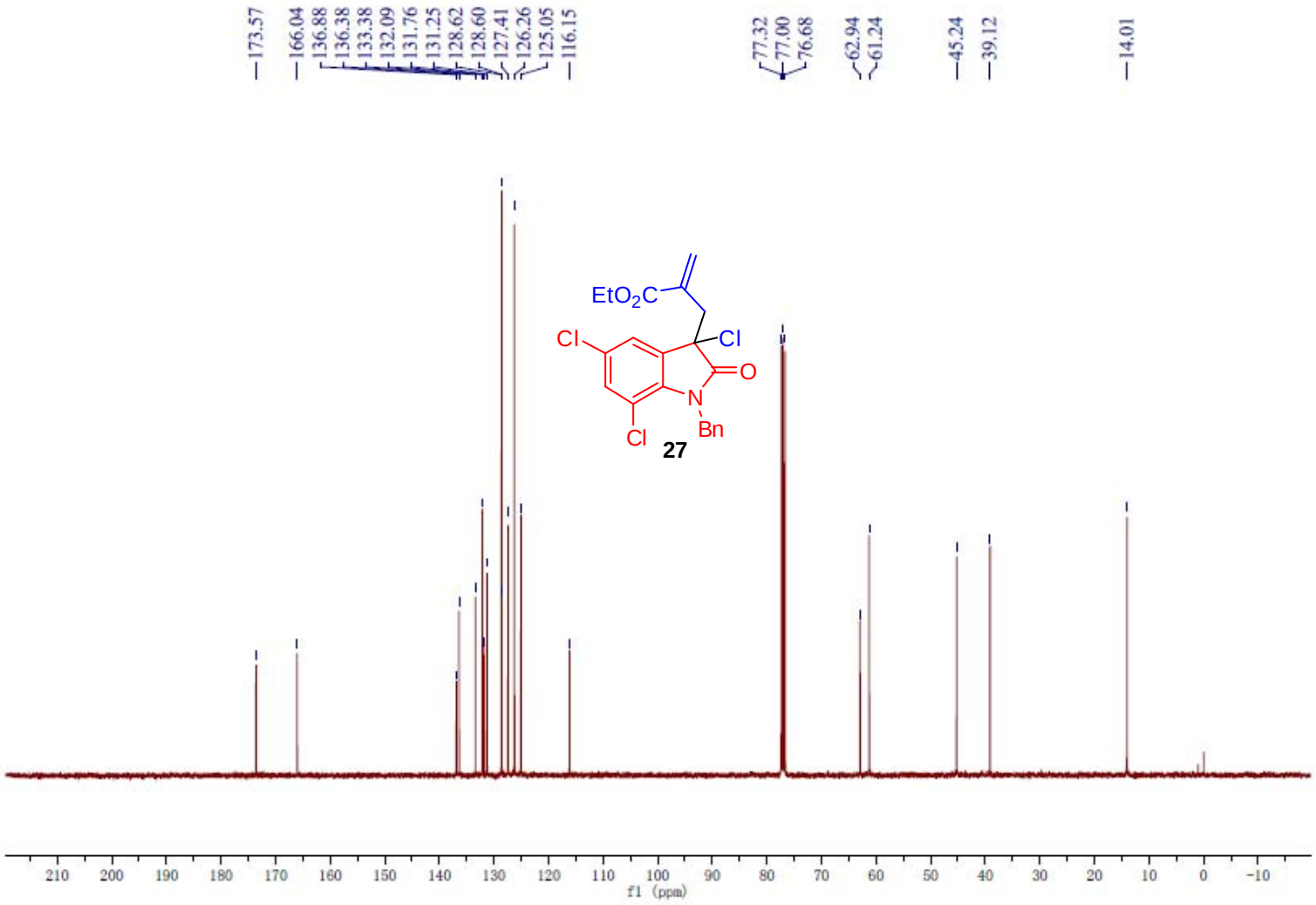
f1 (ppm)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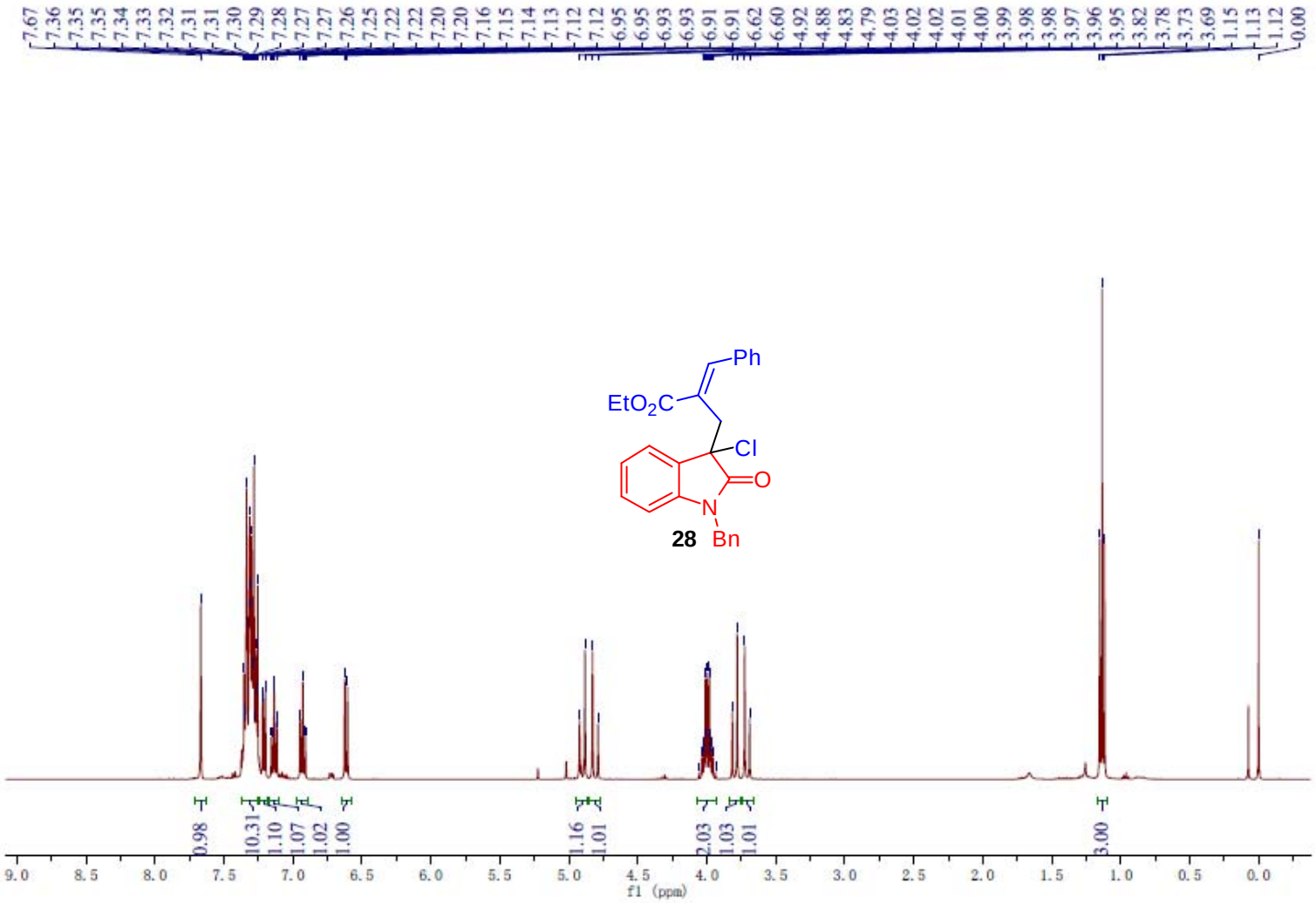
77.00
76.68
62.94
61.24
45.24
39.12
14.01
EtO2C
Cl
Cl
O
N
Bn
Cl
27
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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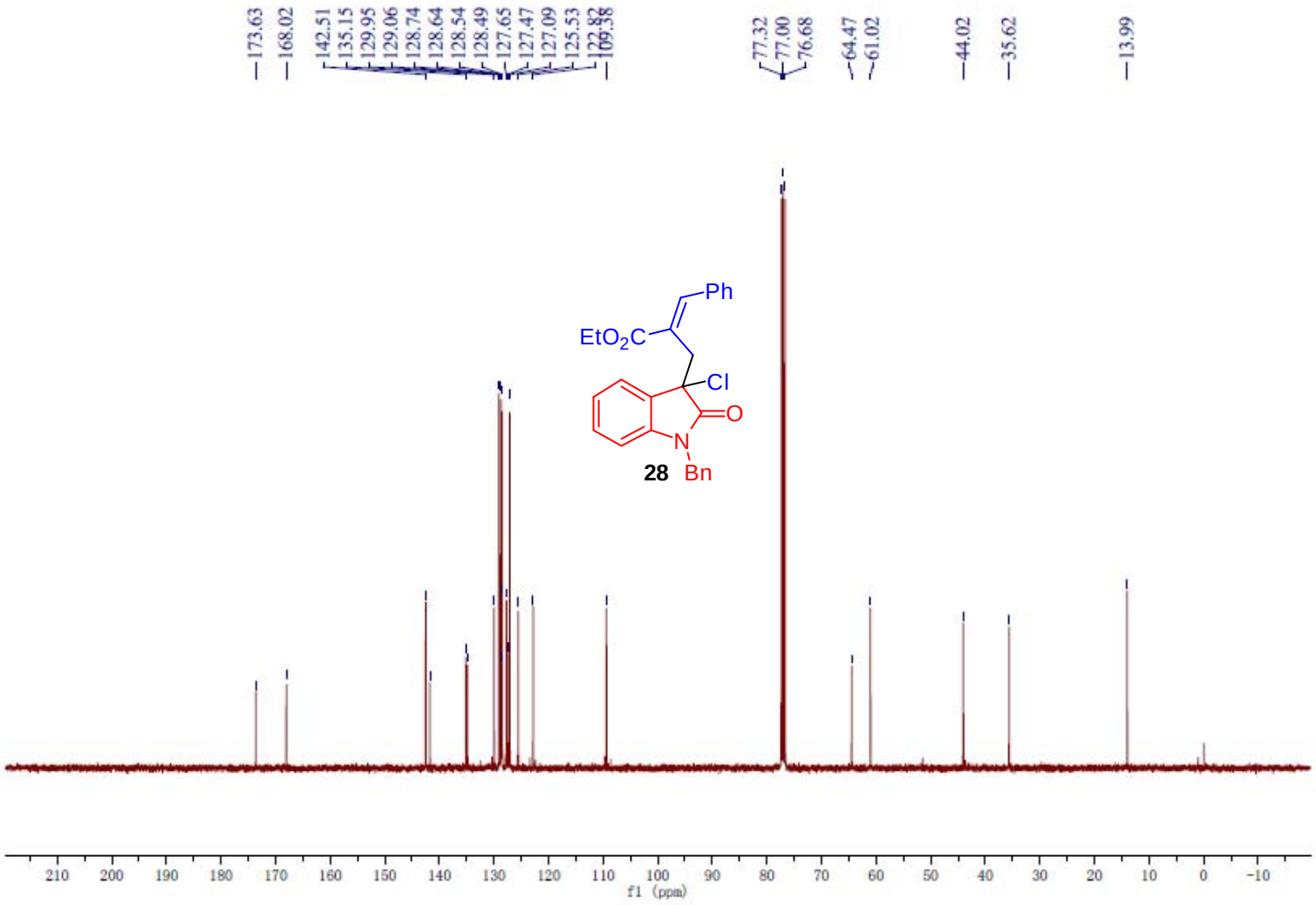
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13.99
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Cl
O
N
Bn
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30
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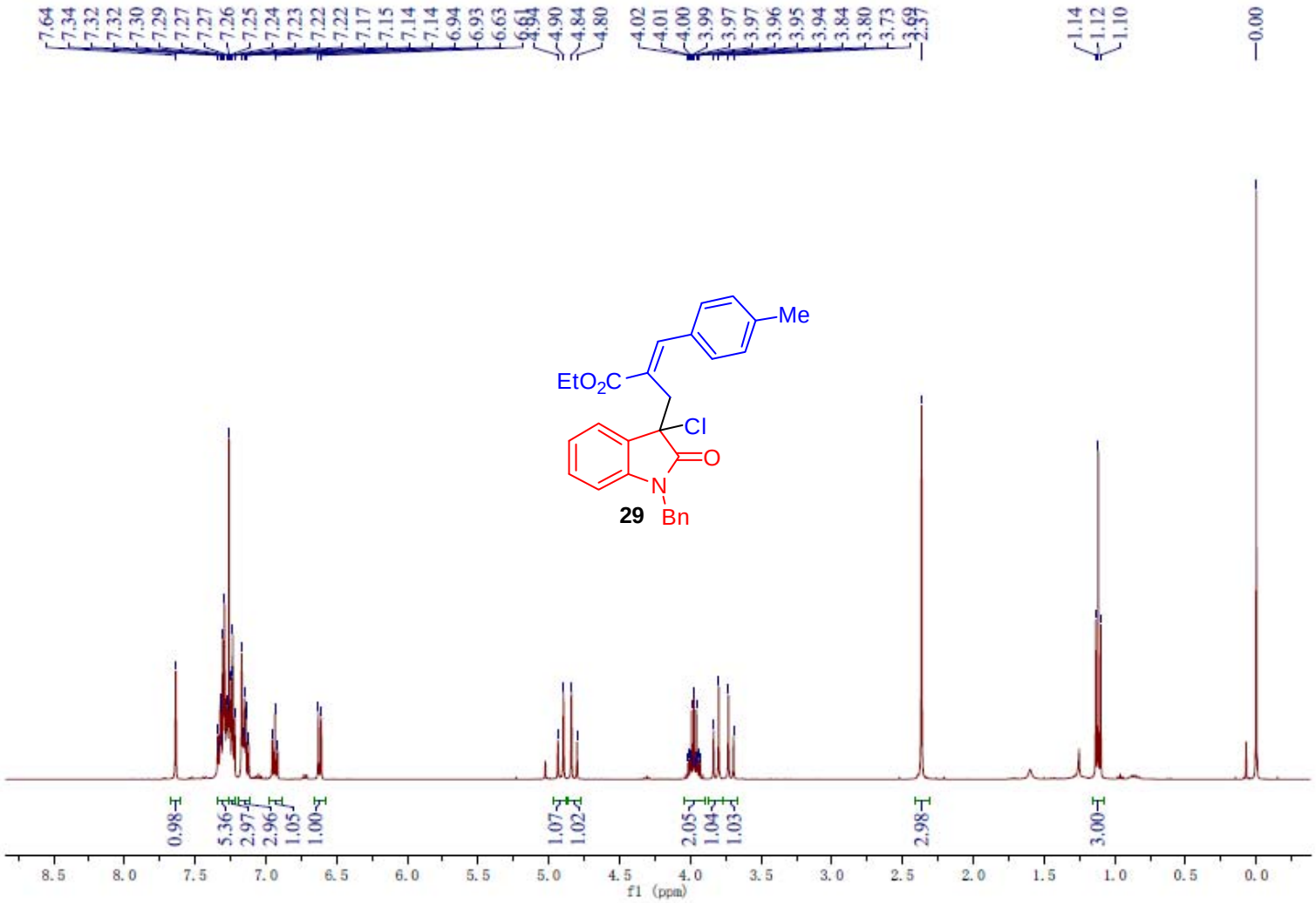
f1 (ppm)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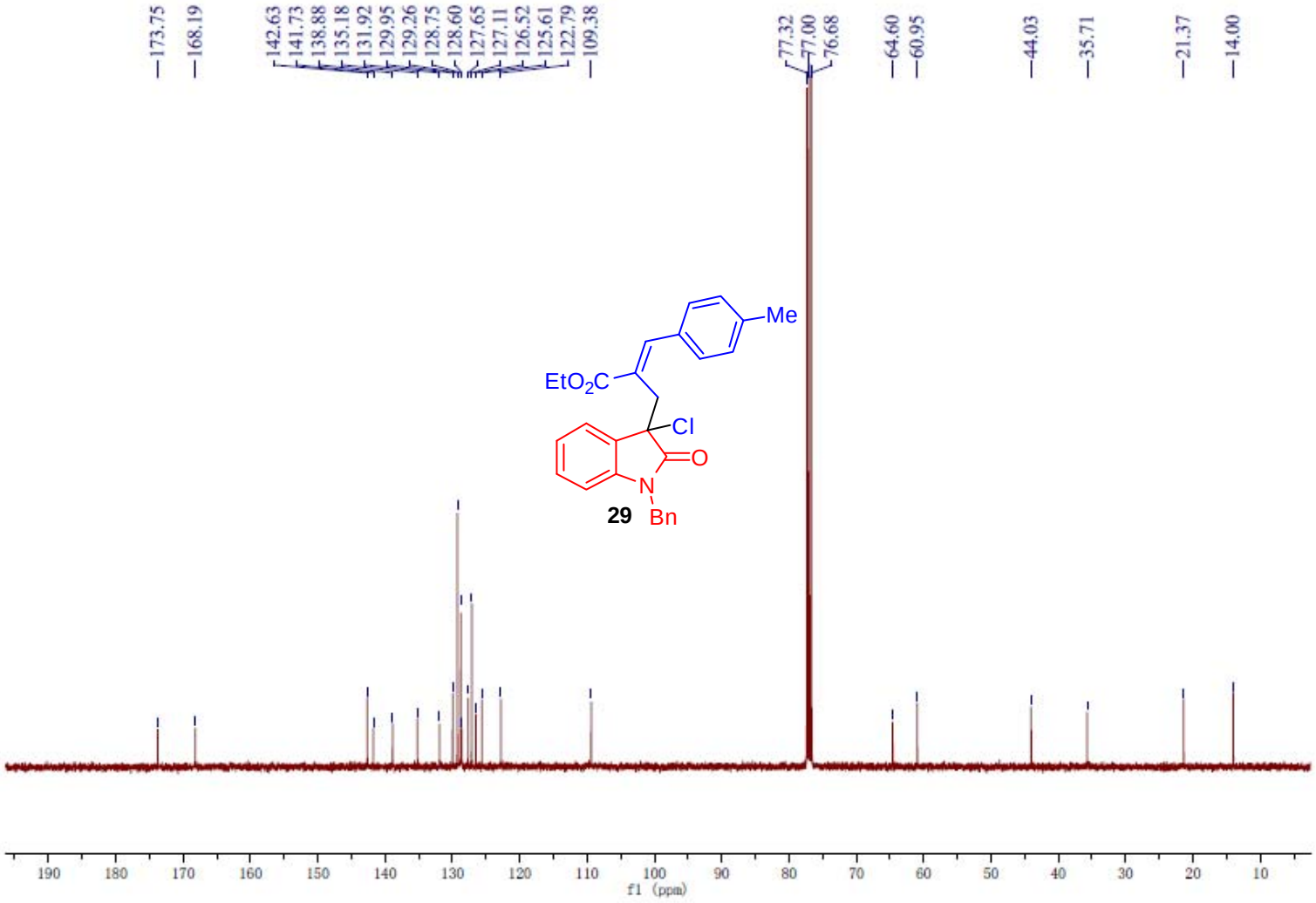
f1 (ppm)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77.00
76.68
64.60
60.95
44.03
35.71
21.37
14.00
Me
EtO2C
Cl
O
N
Bn
29
190
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140
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120
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100
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80
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60
50
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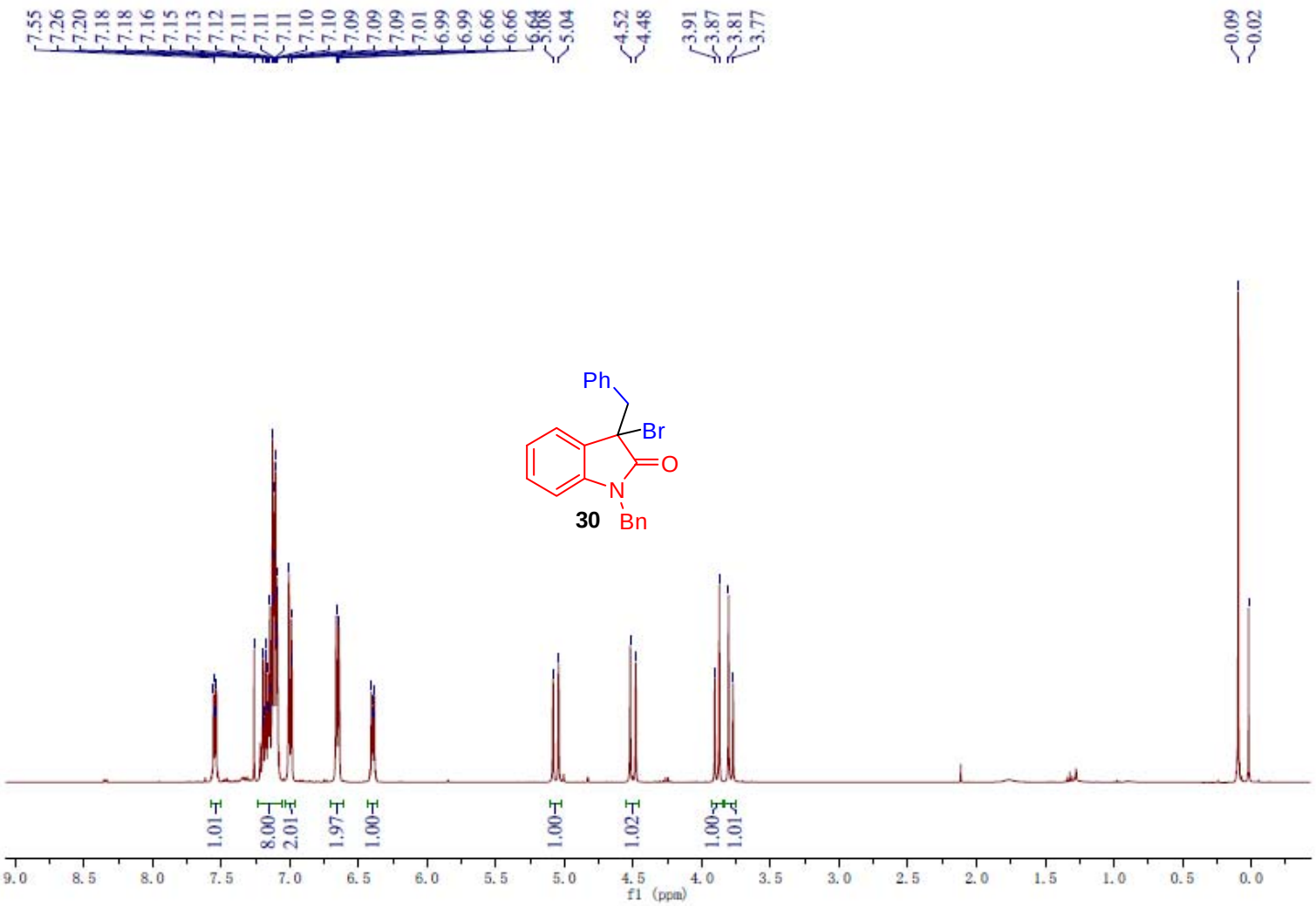
20
10
f1 (ppm)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7.10
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7.09
7.09
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Ph
Br
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Bn
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1.01
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2.0
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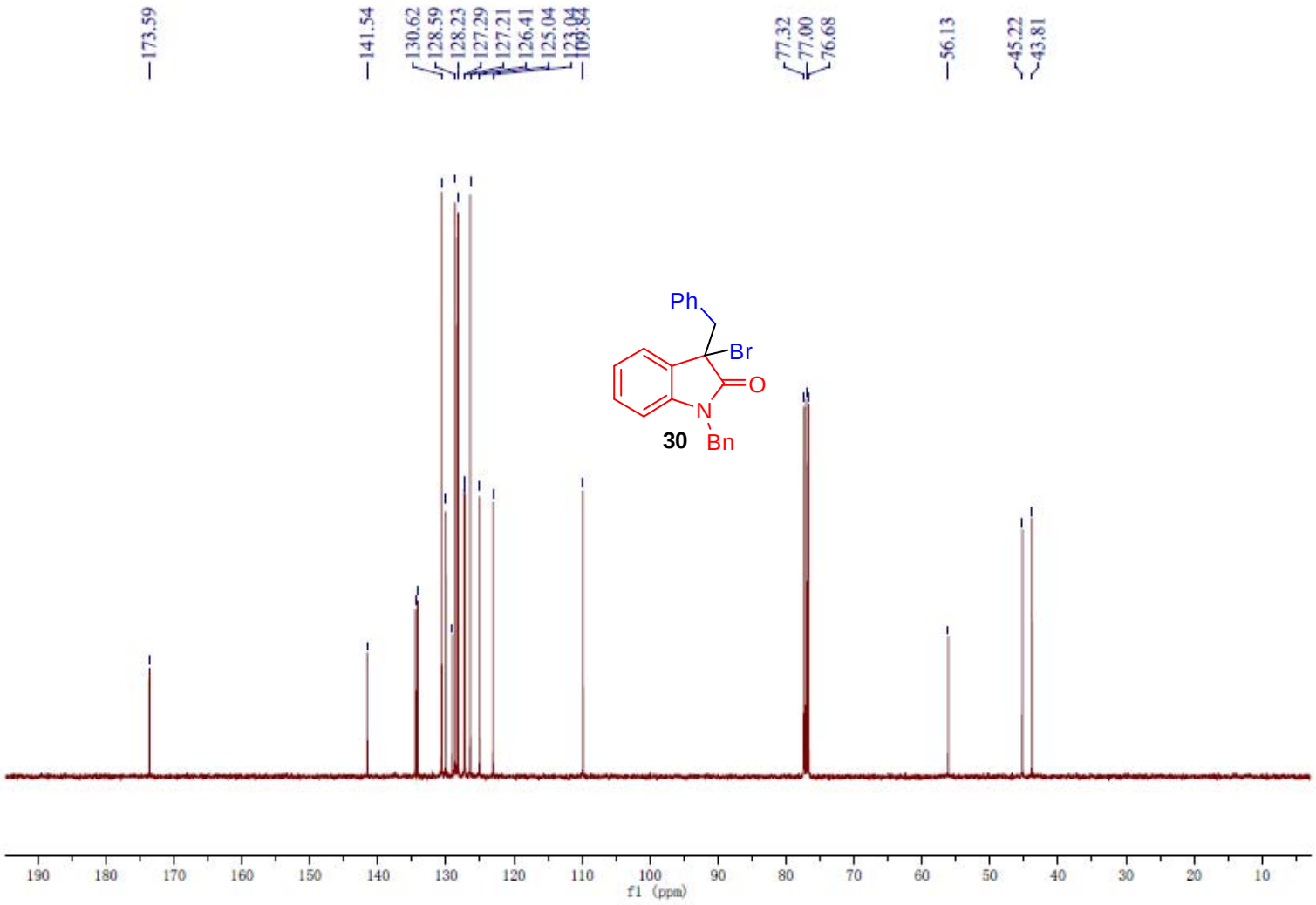
0.0
f1 (ppm)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76.68
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45.22
43.81
Ph
Br
O
N
Bn
30
190
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80
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60
50
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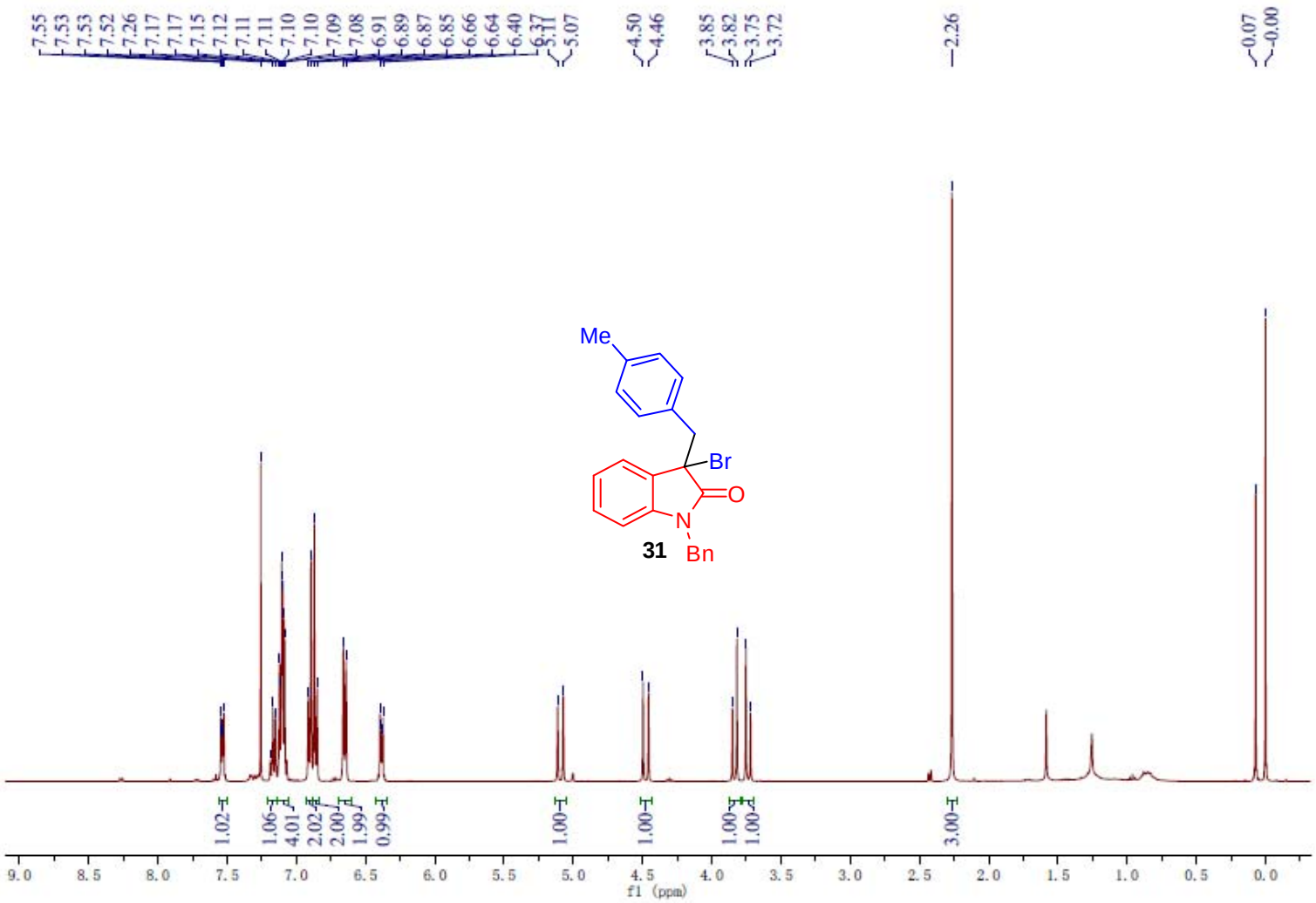
f1 (ppm)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7.08
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Bn
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2.0
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1.0
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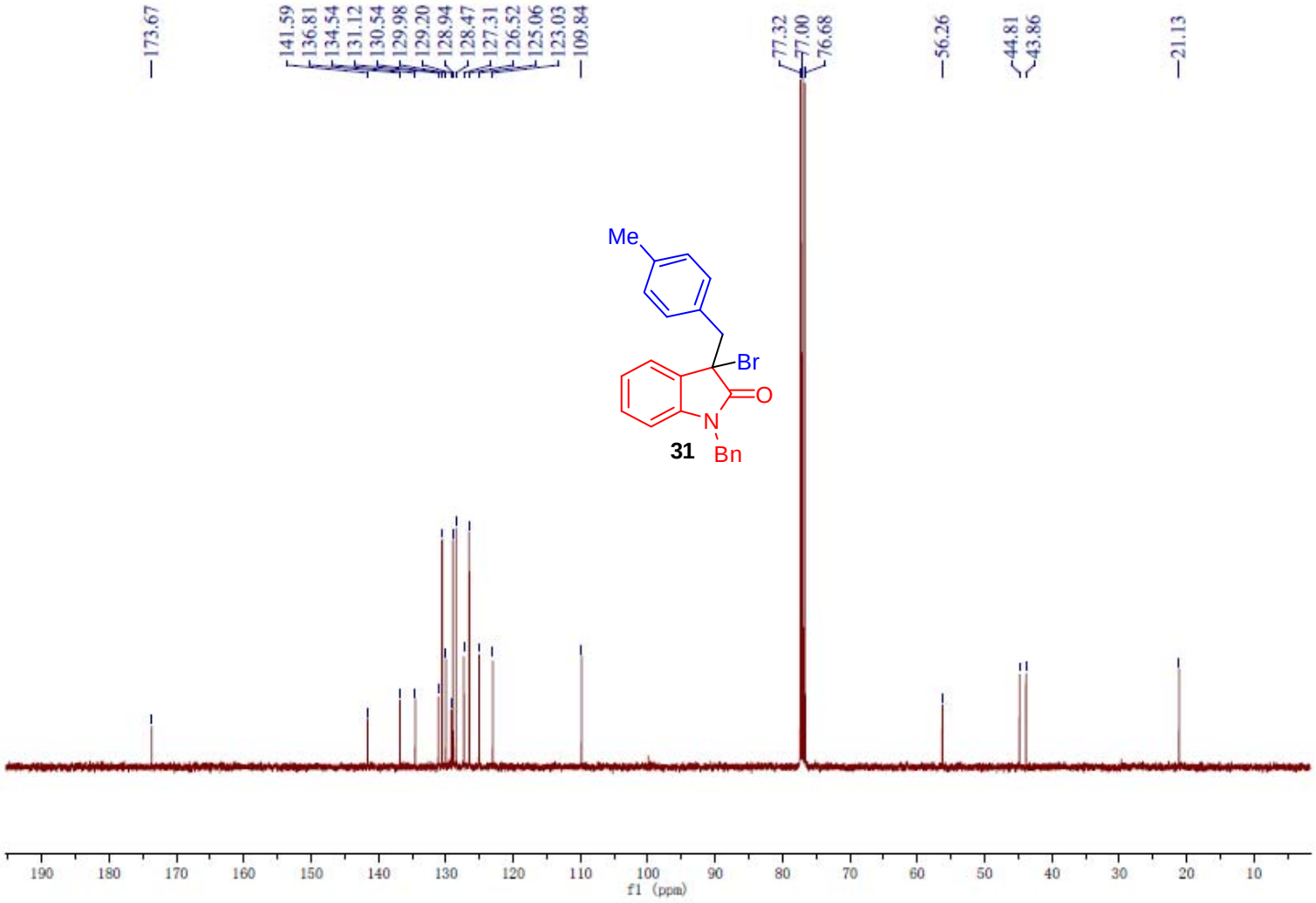
0.0
f1 (ppm)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109.84
77.32
77.00
76.68
56.26
44.81
43.86
21.13
Me
Br
O
N
Bn
31
190
180
170
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140
130
120
110
100
90
80
70
60
50
40
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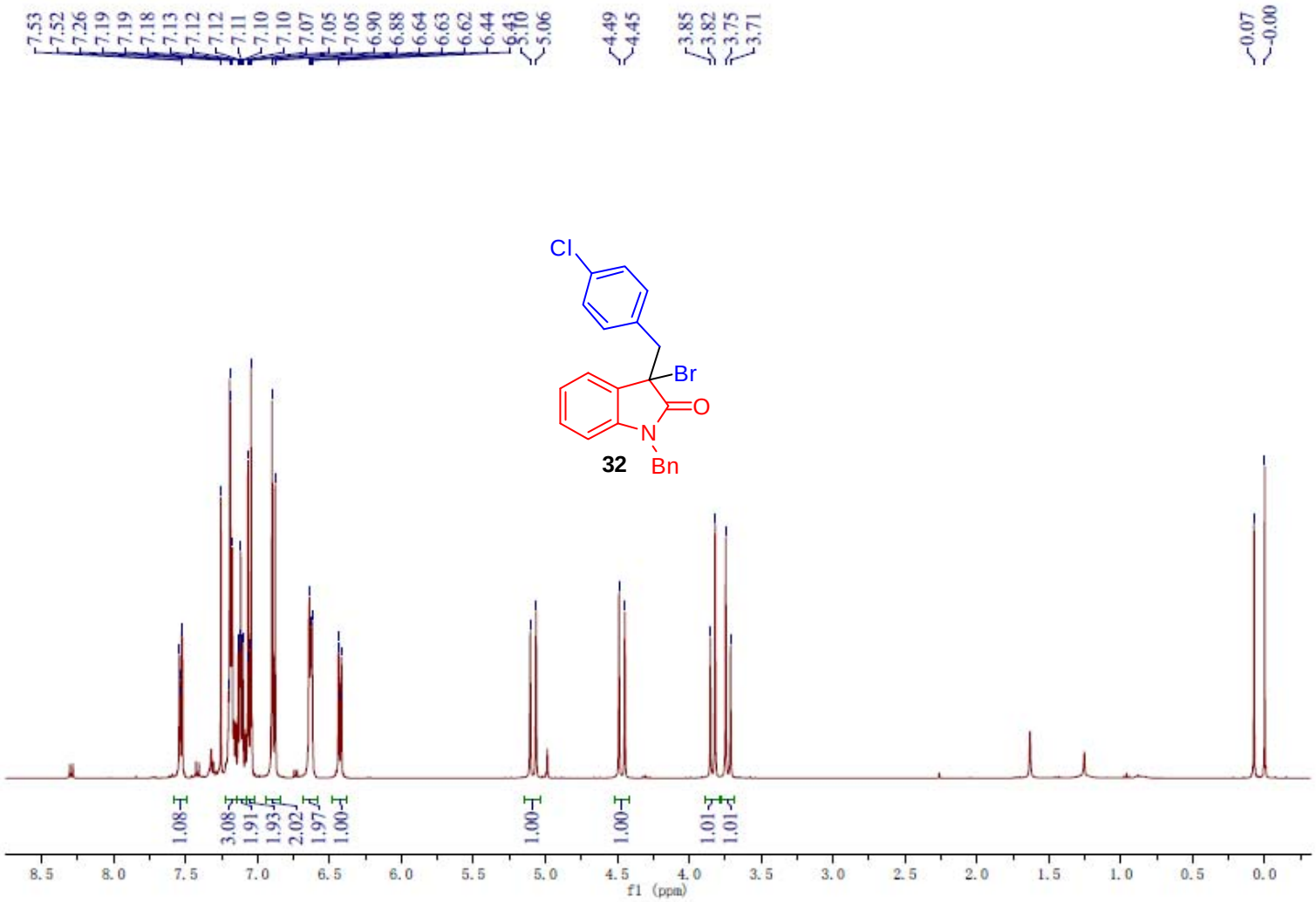
20
10
f1 (ppm)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7.05
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3.71
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-0.00
Cl
Br
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Bn
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1.01
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
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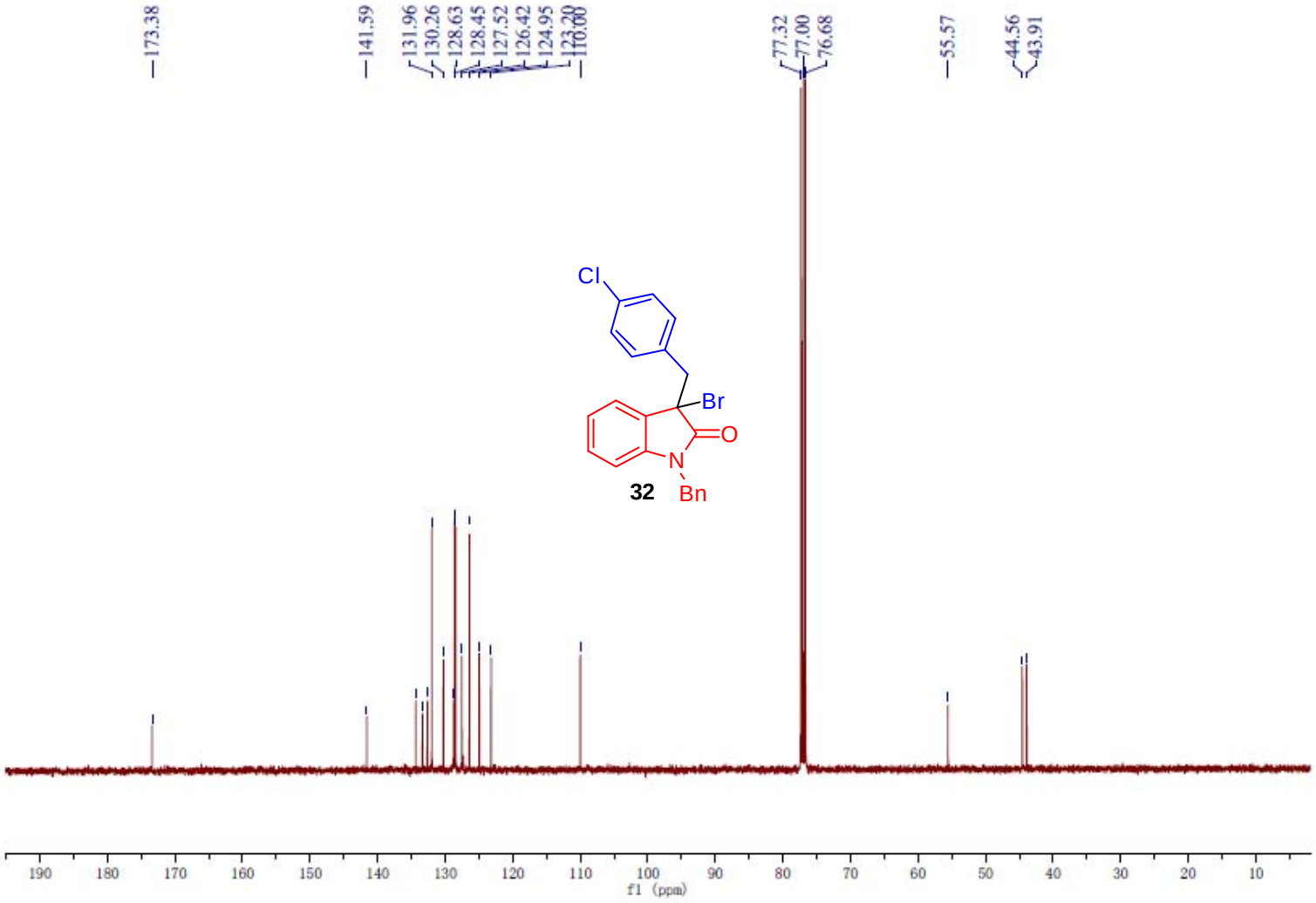
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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123.20
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77.32
77.00
76.68
55.57
44.56
43.91
Cl
Br
O
N
Bn
32
190
180
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140
130
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100
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60
50
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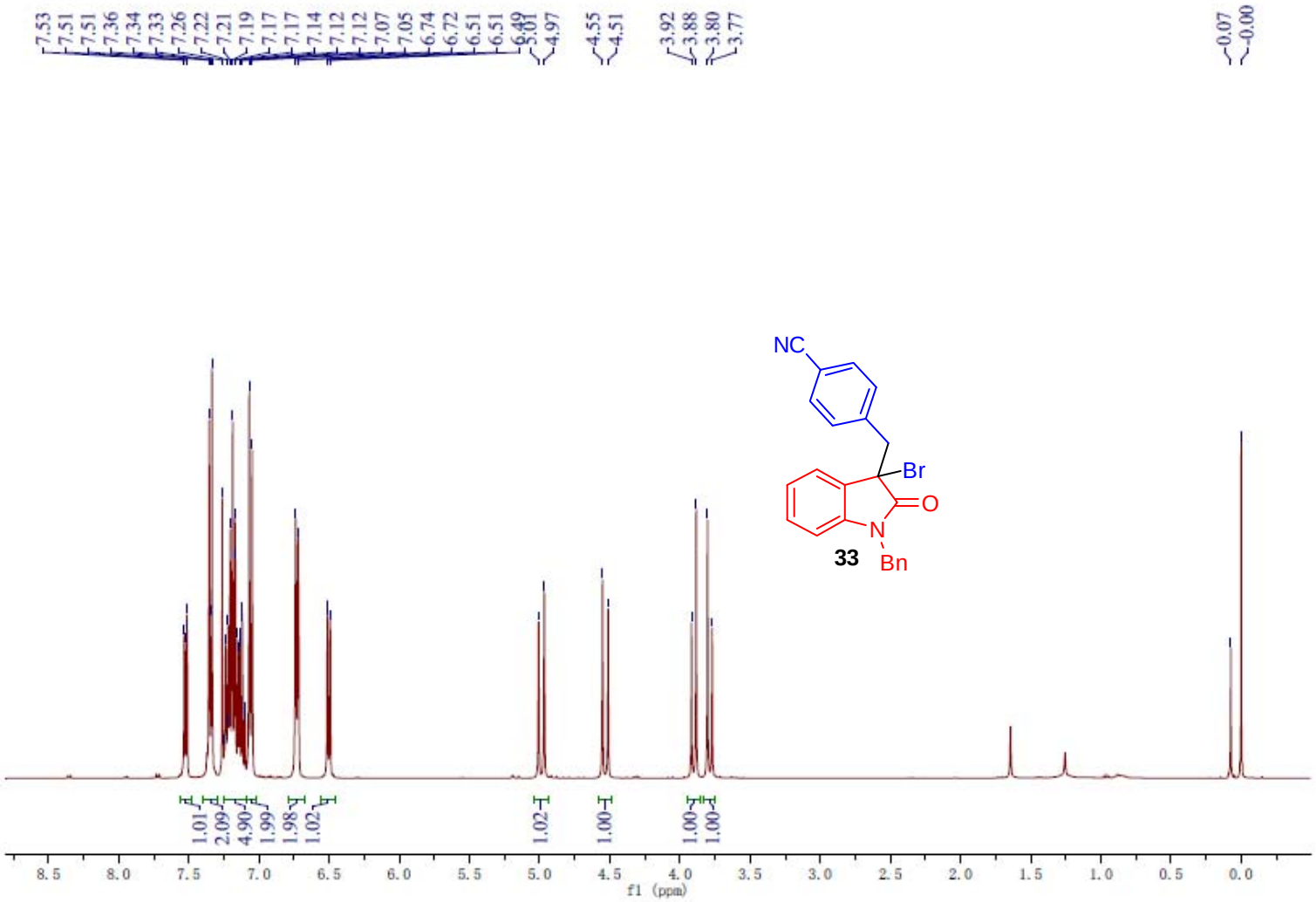
f1 (ppm)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7.14
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7.12
7.07
7.05
6.74
6.72
6.51
6.51
6.49
3.01
4.97
4.55
4.51
3.92
3.88
3.80
3.77
0.07
0.00
NC
Br
O
N
Bn
33
1.01
2.09
4.90
1.99
1.98
1.02
1.02
1.00
1.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
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1.5
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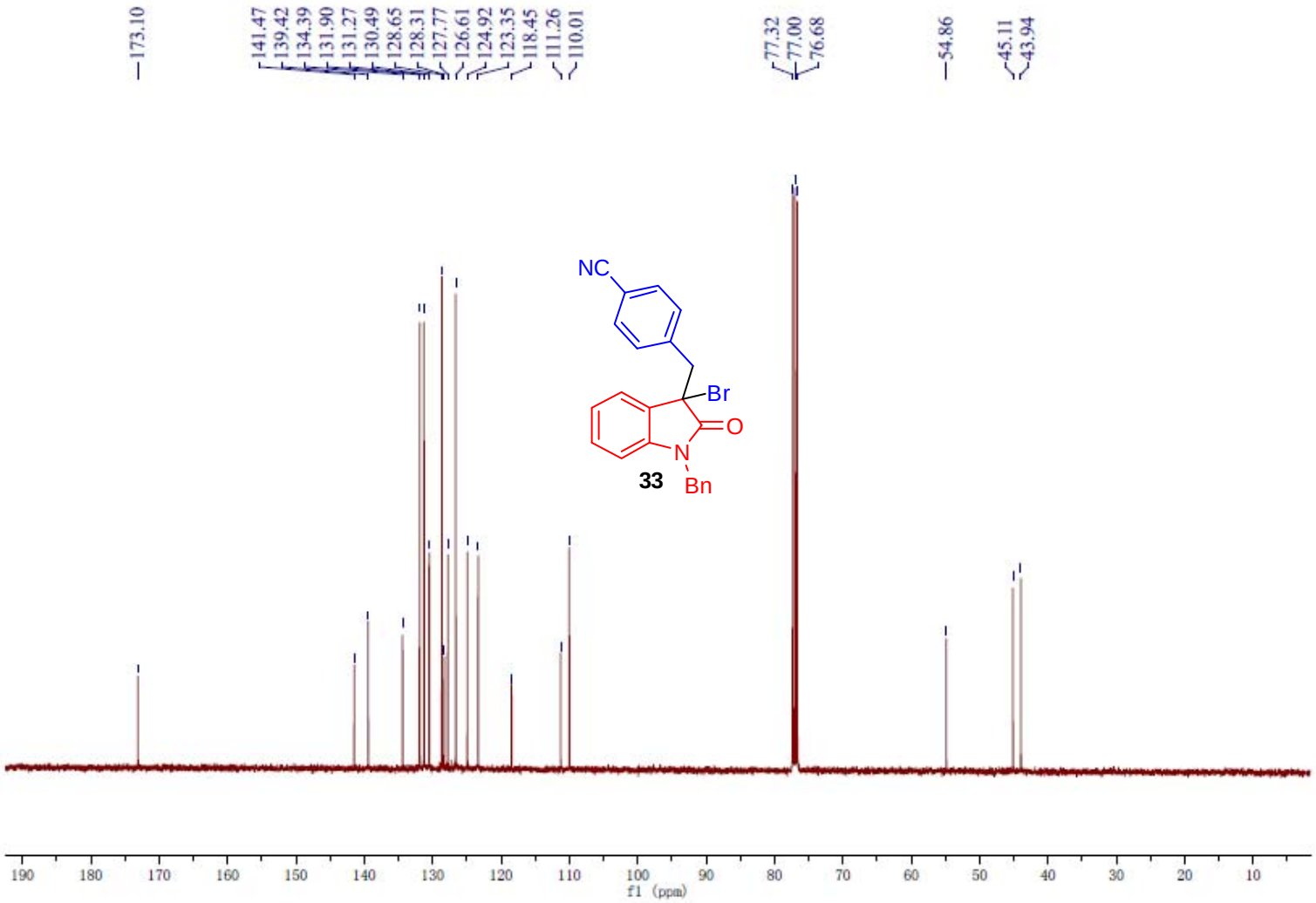
f1 (ppm)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124.92
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118.45
111.26
110.01
77.32
77.00
76.68
54.86
45.11
43.94
NC
Br
O
N
Bn
33
190
180
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140
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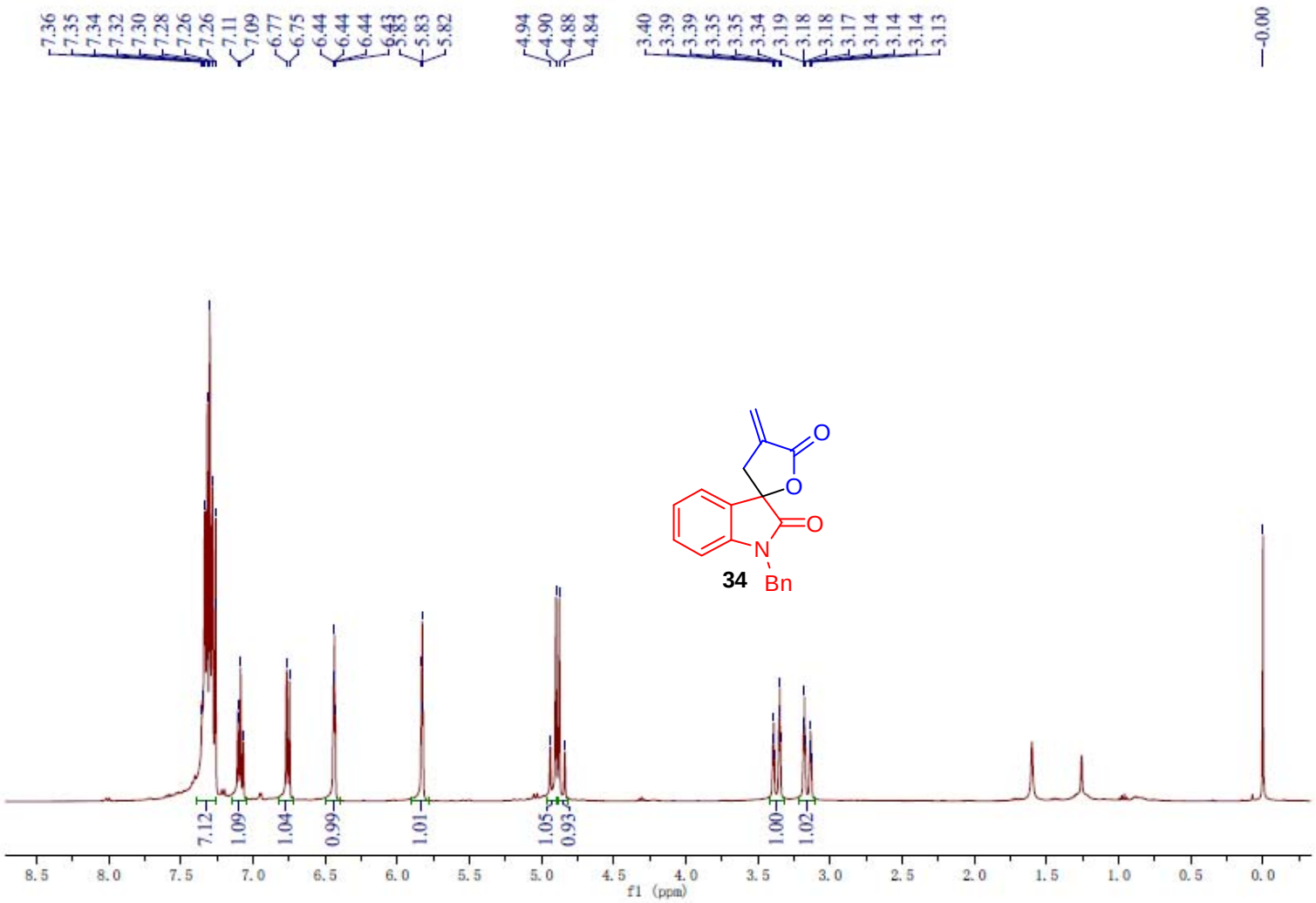
f1 (ppm)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7.26
7.11
7.09
6.77
6.75
6.44
6.44
6.44
6.43
5.83
5.83
5.82
4.94
4.90
4.88
4.84
3.40
3.39
3.39
3.35
3.35
3.34
3.19
3.18
3.18
3.17
3.14
3.14
3.14
3.13
-0.00
O
O
O
N
34 Bn
7.12
1.09
1.04
0.99
1.01
1.05
0.93
1.00
1.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
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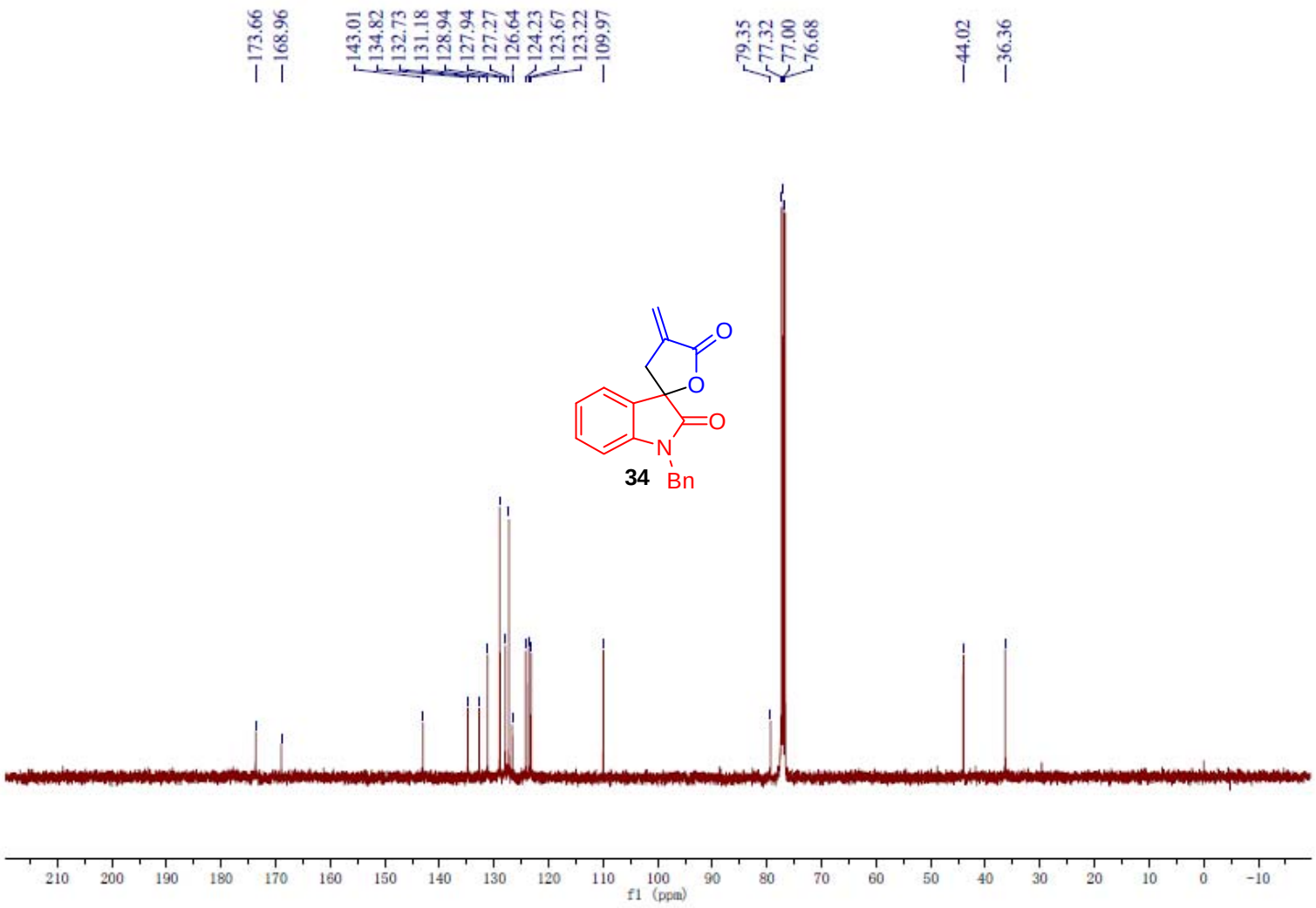
f1 (ppm)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123.67
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77.32
77.00
76.68
44.02
36.36
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O
O
N
Bn
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200
190
180
170
160
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80
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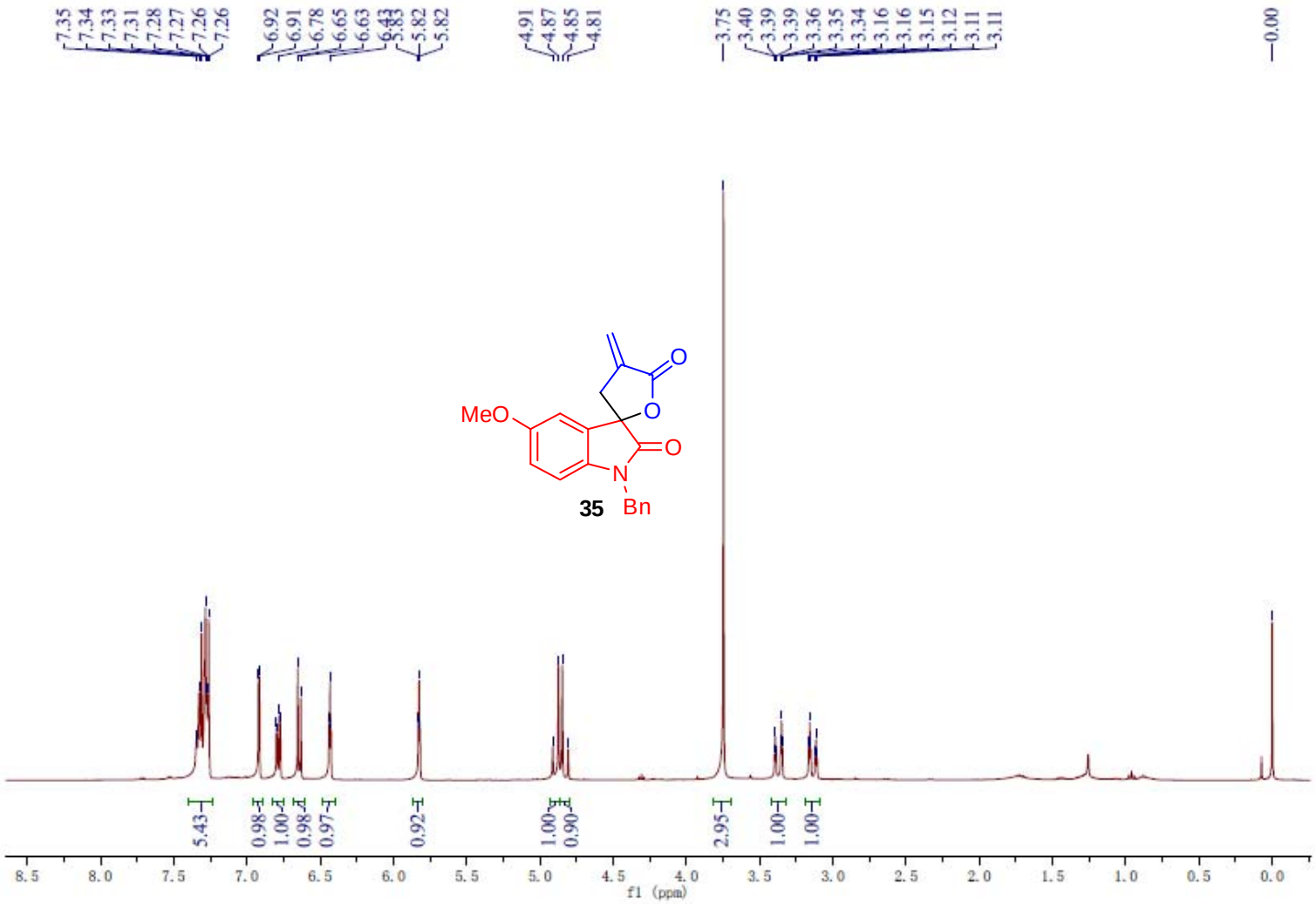
f1 (ppm)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6.63
6.43
5.83
5.82
5.82
4.91
4.87
4.85
4.81
3.75
3.40
3.39
3.39
3.36
3.35
3.34
3.16
3.16
3.15
3.12
3.11
3.11
0.00
MeO
O
O
O
N
Bn
35
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0.98
1.00
0.98
0.97
0.92
1.00
0.90
2.95
1.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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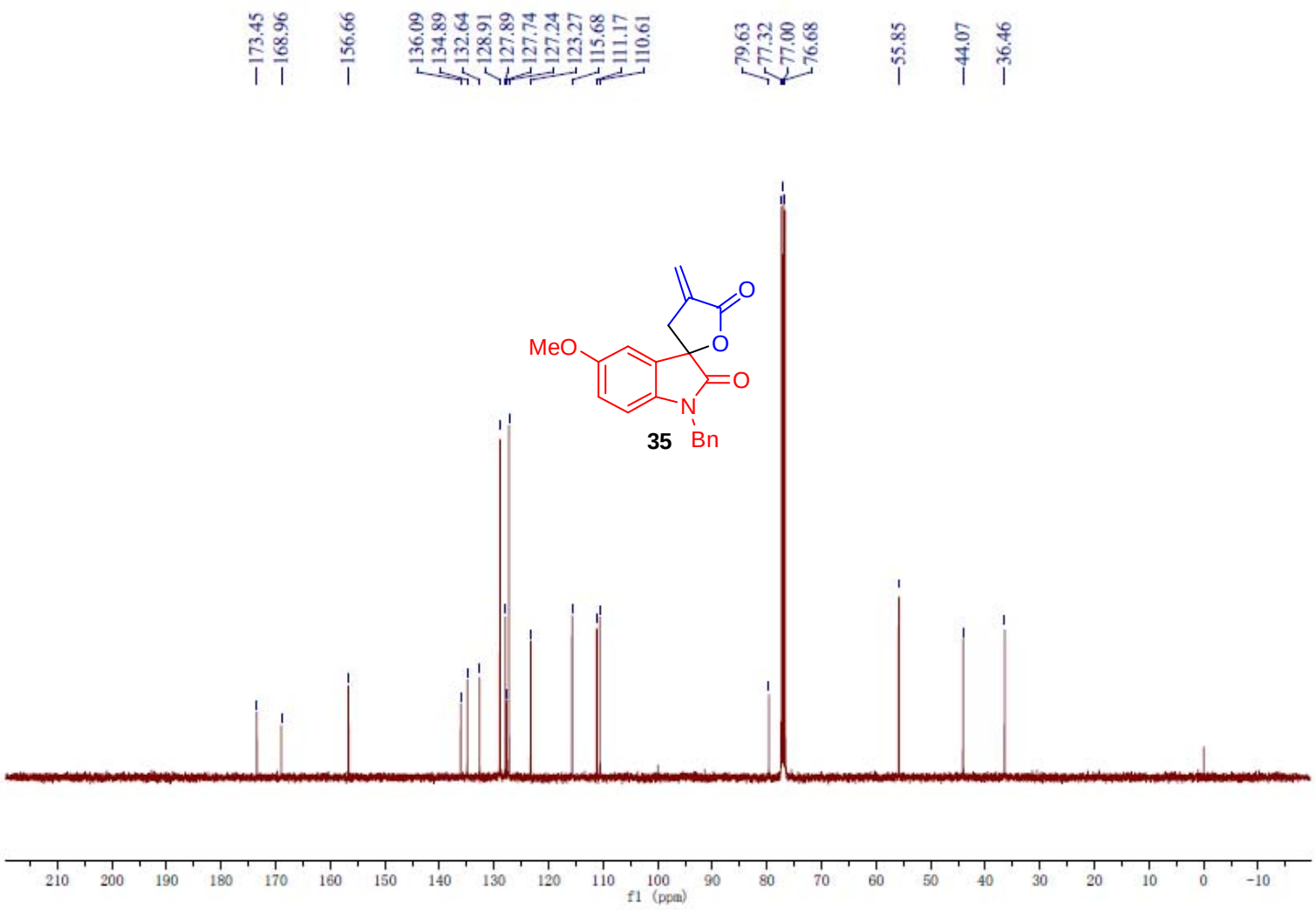
0.0
f1 (ppm)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127.89
127.74
127.24
123.27
115.68
111.17
110.61
79.63
77.32
77.00
76.68
55.85
44.07
36.46
MeO
O
O
O
N
Bn
35
210
200
190
180
170
160
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140
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120
110
100
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80
70
60
50
40
30
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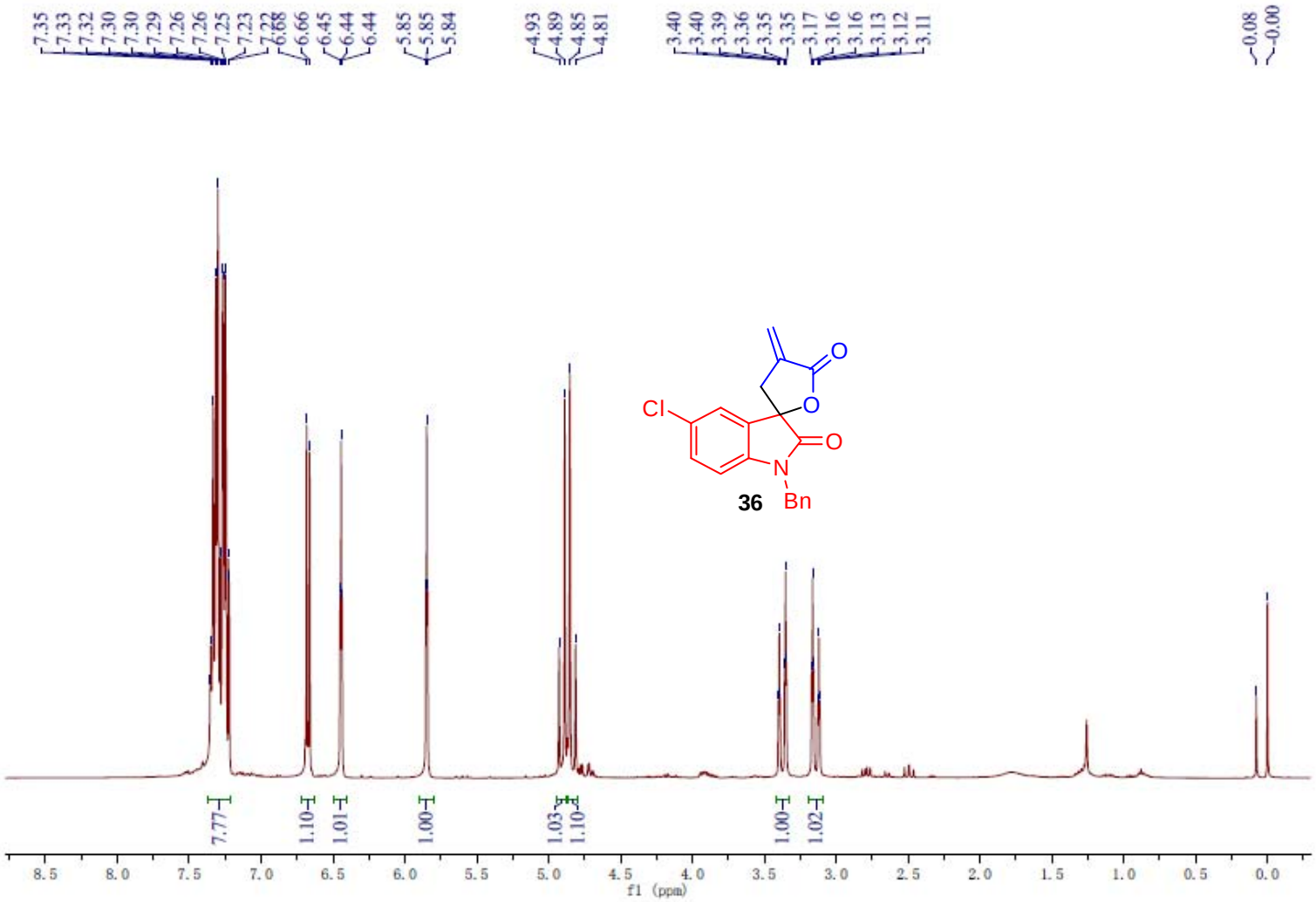
0
-10
f1 (ppm)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7.22
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6.44
6.44
5.85
5.85
5.84
4.93
4.89
4.85
4.81
3.40
3.40
3.39
3.36
3.35
3.35
3.17
3.16
3.16
3.13
3.12
3.11
0.08
-0.00
Cl
O
O
O
N
Bn
36
7.77
1.10
1.01
1.00
1.03
1.10
1.00
1.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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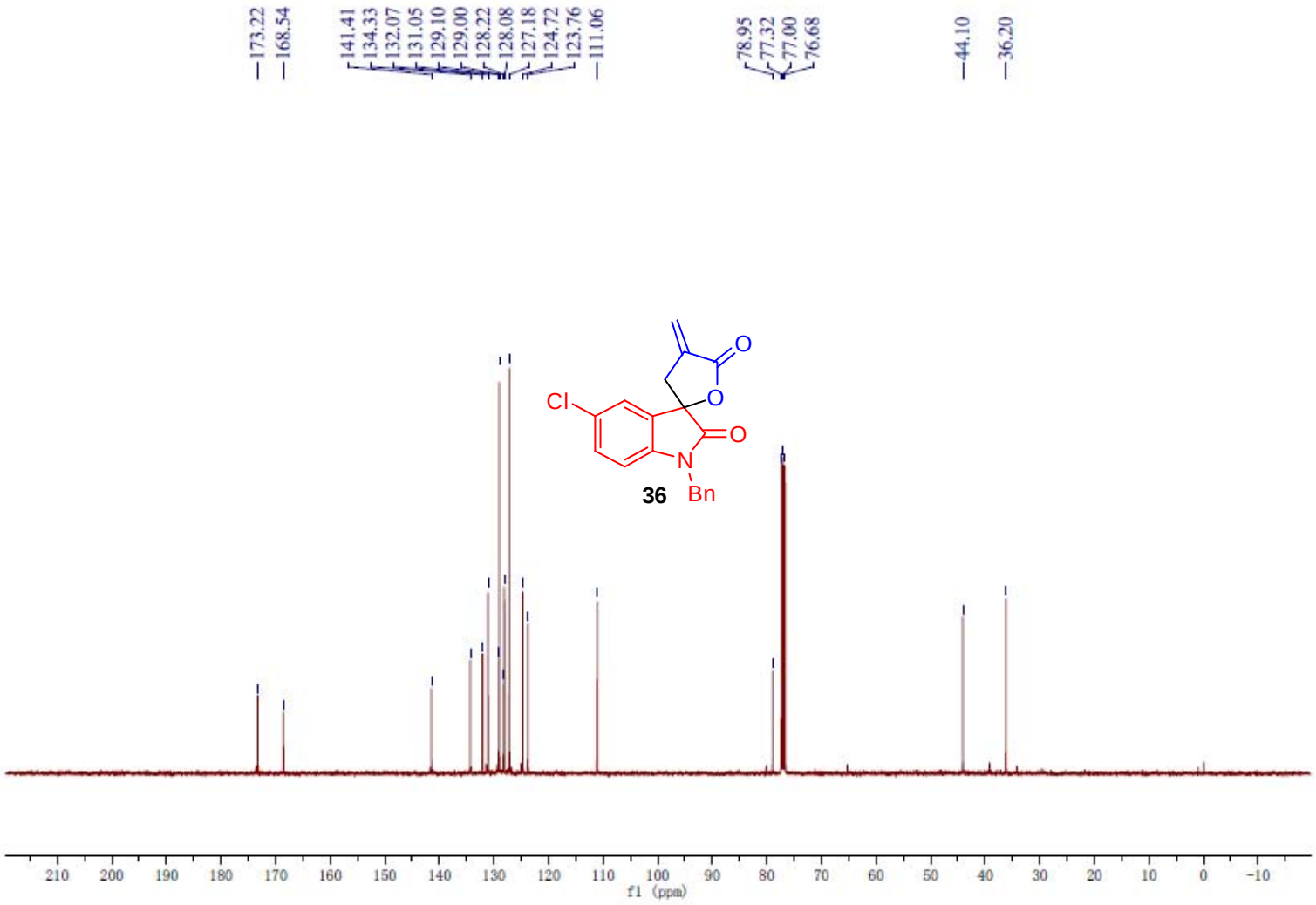
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.22
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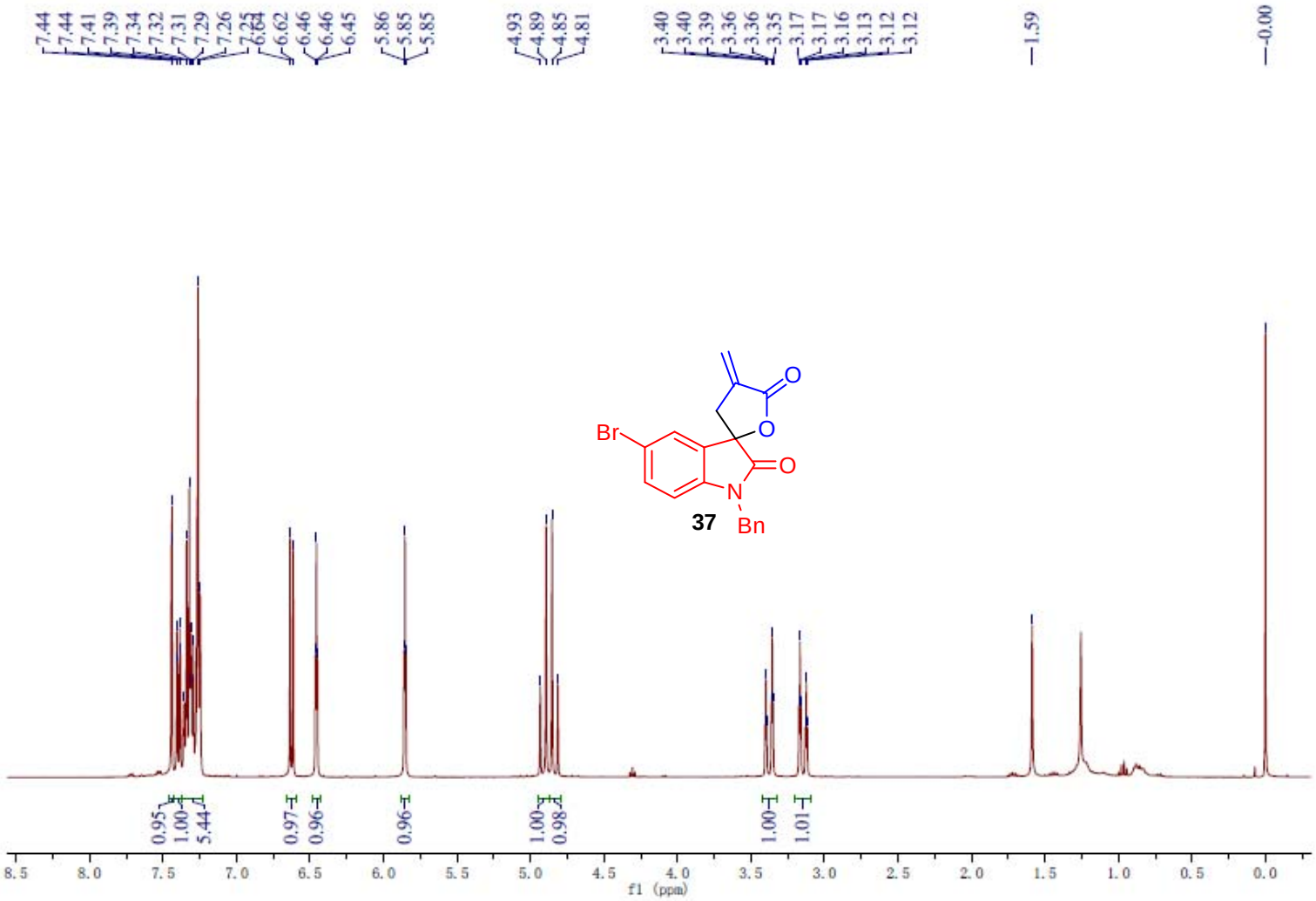
124.72
123.76
111.06
78.95
77.32
77.00
76.68
44.10
36.20
Cl
O
O
O
N
Bn
36
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.29
7.26
7.25
6.64
6.62
6.46
6.46
6.45
5.86
5.85
5.85
4.93
4.89
4.85
4.81
3.40
3.40
3.39
3.36
3.36
3.35
3.17
3.17
3.16
3.13
3.12
3.12
1.59
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O
O
N
Bn
37
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1.00
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0.97
0.96
0.96
1.00
0.98
1.00
1.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
2.0
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1.0
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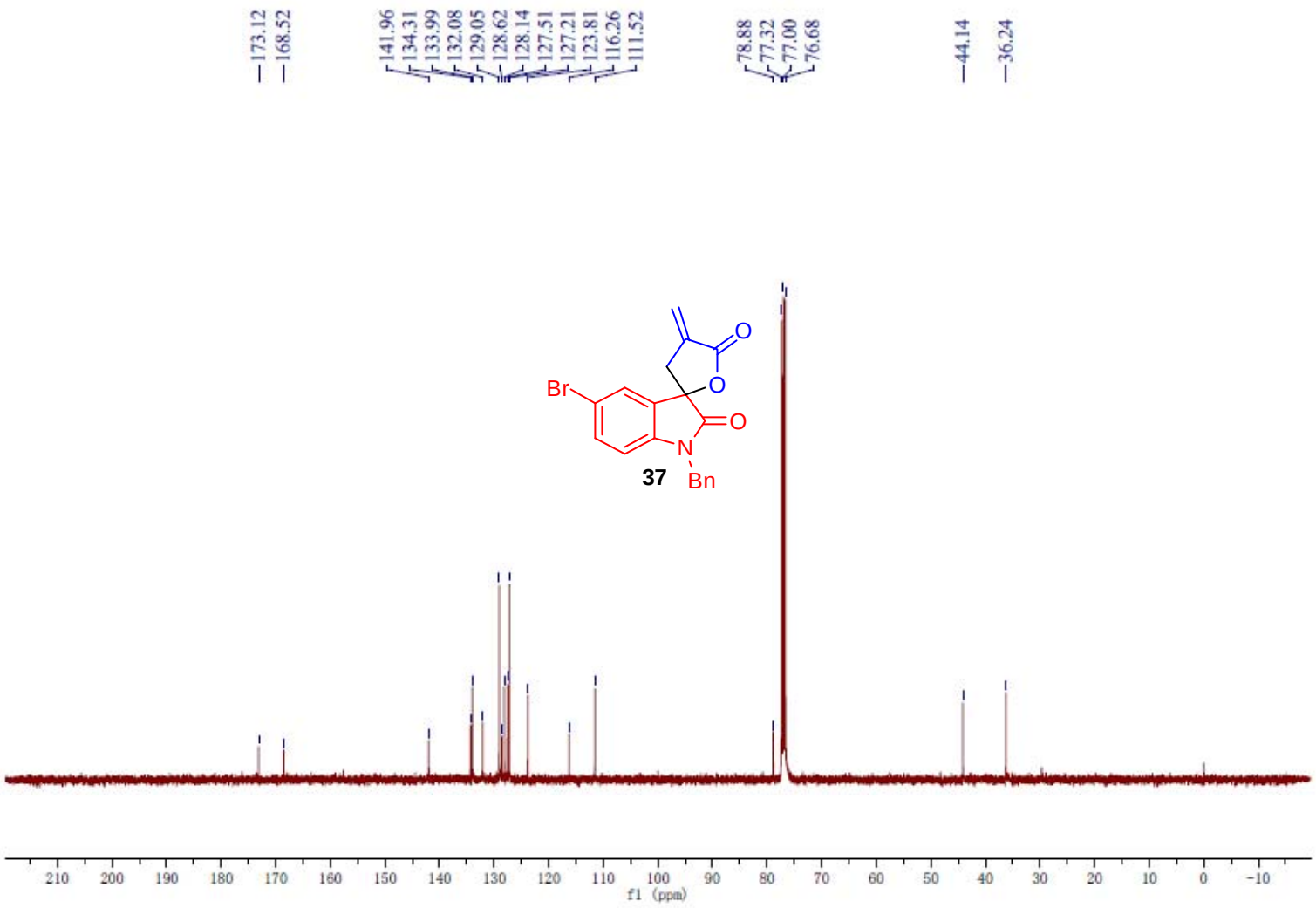
0.0
f1 (ppm)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78.88
77.32
77.00
76.68
44.14
36.24
Br
O
O
O
N
Bn
37
210
200
190
180
170
160
150
140
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120
110
100
90
80
70
60
50
40
30
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10
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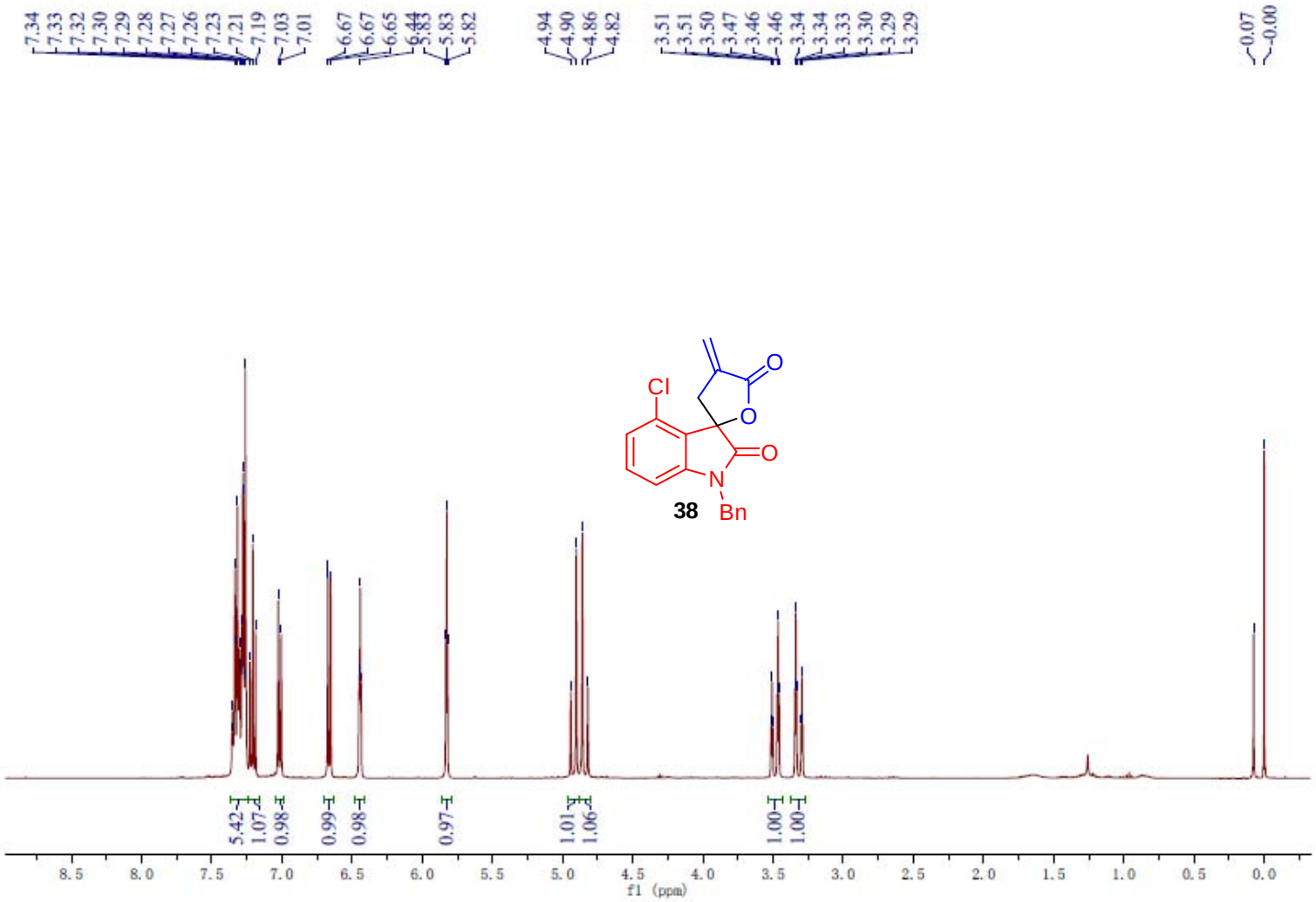
-10
f1 (ppm)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7.21
7.19
7.03
7.01
6.67
6.67
6.65
6.44
5.83
5.83
5.82
4.94
4.90
4.86
4.82
3.51
3.51
3.50
3.47
3.46
3.46
3.34
3.34
3.33
3.30
3.29
3.29
0.07
-0.00
Cl
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N
Bn
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0.99
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1.01
1.06
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6.0
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4.5
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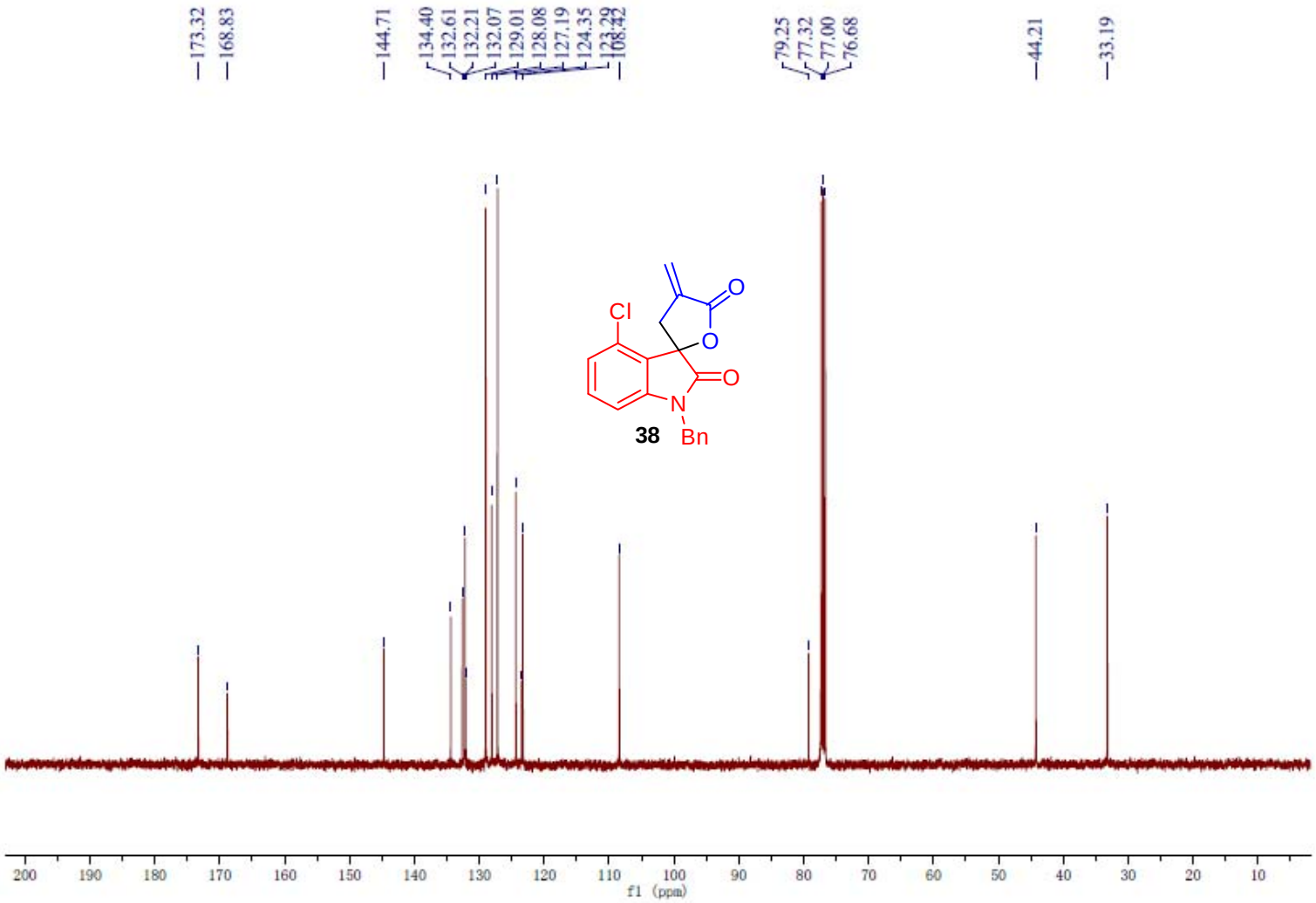
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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79.25
77.32
77.00
76.68
44.21
33.19
Cl
O
O
O
N
Bn
38
200
190
180
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140
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120
110
100
90
80
70
60
50
40
30
20
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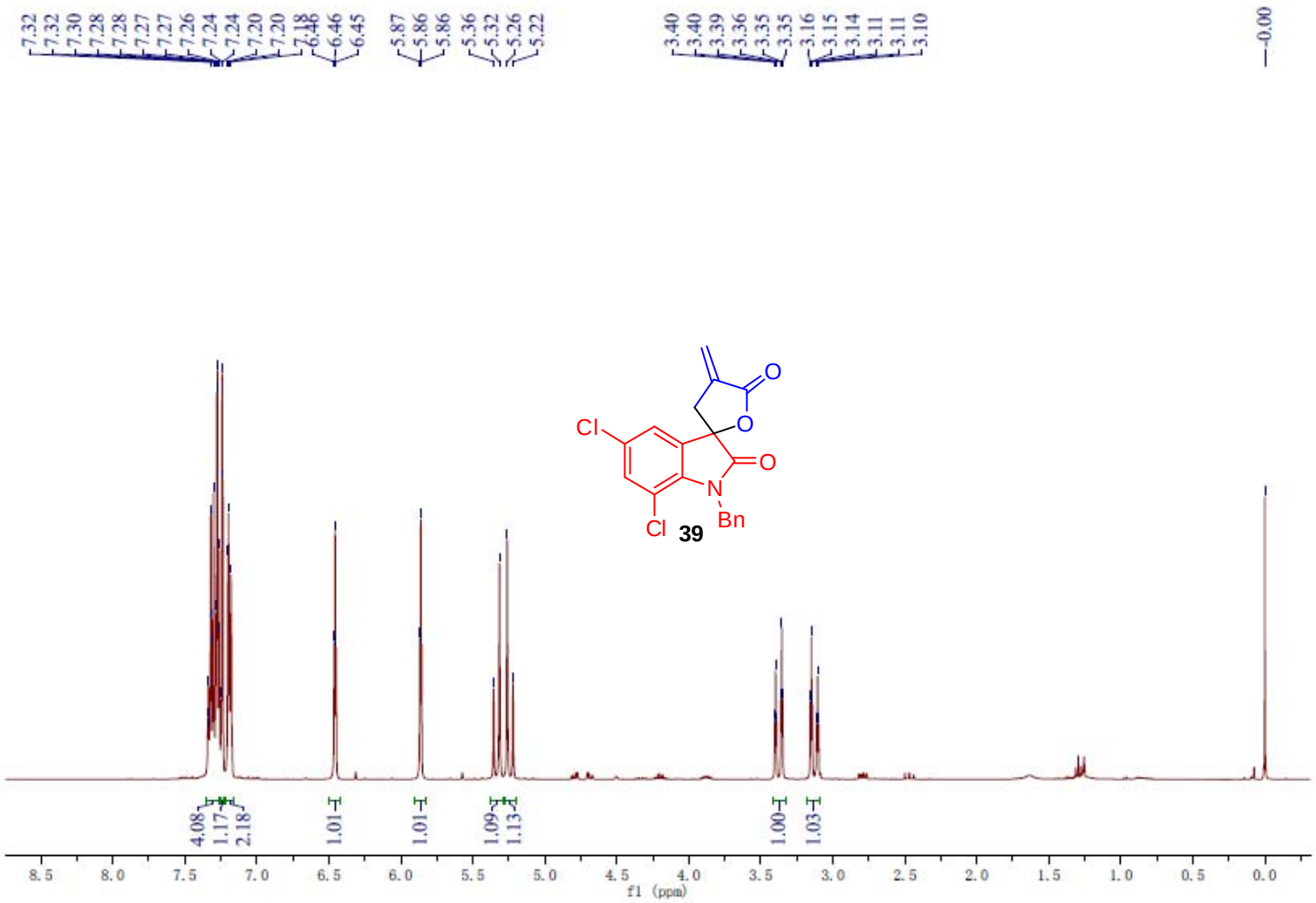
f1 (ppm)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6.46
6.45
5.87
5.86
5.86
5.36
5.32
5.26
5.22
3.40
3.40
3.39
3.36
3.35
3.35
3.16
3.15
3.14
3.11
3.11
3.10
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Cl
O
O
O
N
Bn
Cl
39
4.08
1.17
2.18
1.01
1.01
1.09
1.13
1.00
1.03
8.5
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7.5
7.0
6.5
6.0
5.5
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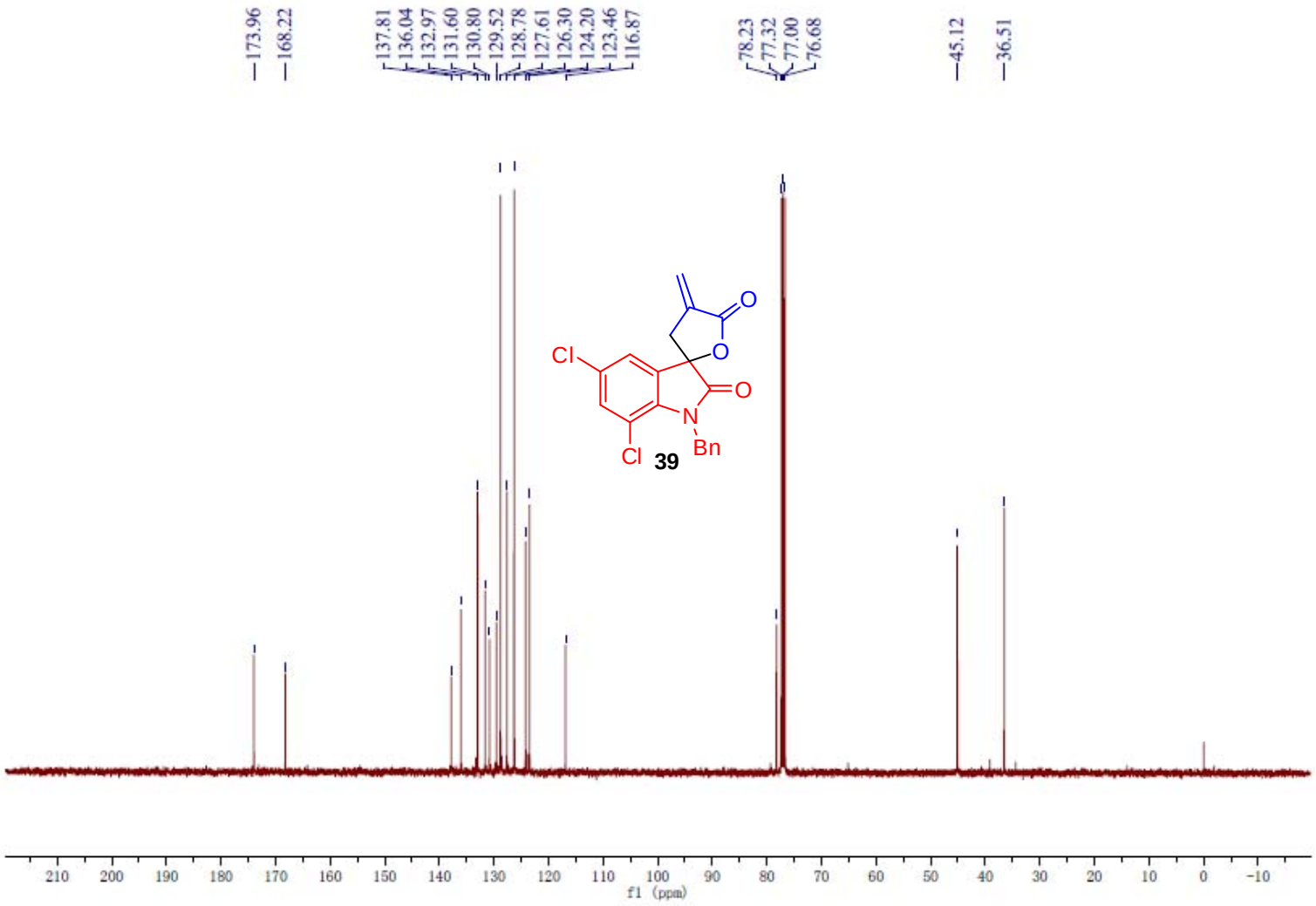
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.52
128.78
127.61
126.30
124.20
123.46
116.87
78.23
77.32
77.00
76.68
45.12
36.51
Cl
O
O
O
N
Bn
Cl
39
210
200
190
180
170
160
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140
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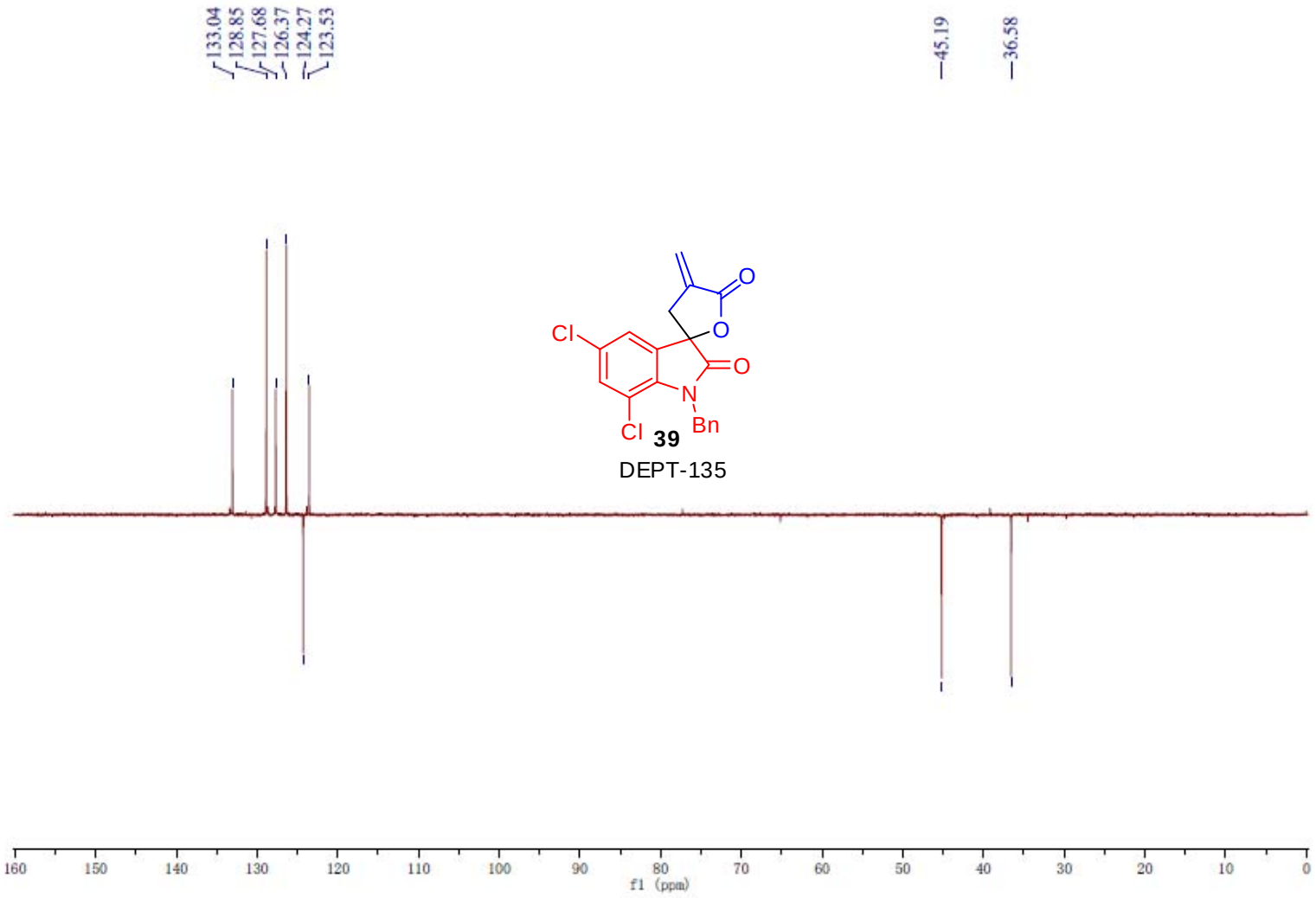
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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123.53
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36.58
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O
O
N
Bn
Cl
39
DEPT-135
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)