Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Visible-light Promoted Intermolecular Halofunctionalization of Alkenes with *N*-Halogen Saccharins

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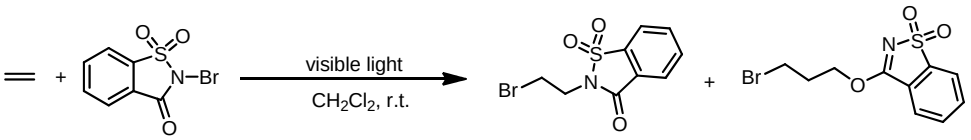
Supporting Information

General Information

Commercial reagents were used as received. ^{1}H, ^{13}C and ^{19}F NMR spectra were measured on a NMR instrument (300 MHz, 400 MHz and 500 MHz for ^{1}H NMR; 75 MHz, 101 MHz, and 126 MHz for ^{13}C NMR). Tetramethylsilane (TMS) served as the internal standard for ^{1}H NMR, and $CDCl_3$ served as the internal standard for ^{13}C NMR. TOCSY, HMBC and HSQC are used to determine the selectivity of products. The following abbreviations were used to express the multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; br = broad. Alkenes (**1-3a)-(1-3r)** are commercially available. A *In-situ* FT-IR spectroscopy was carried out on a ReactIR 15 (Si Comp probe) with a spectral range of 2000-650 cm^{-1} at 4 cm^{-1} resolution. All measurements were performed at room temperature, collecting data every 15 seconds.

General Procedure for halofuntionlization:



NBSA (0.20 mmol) were dissolved in dry CH_2Cl_2 (1.0 mL) in a 10 mL tube under nitrogen atmosphere. To the mixture, alkenes (1.1 eq) were added and stirred at room temperature under fluorescent lamp. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was directly separated by flash column chromatography on silica gel eluting with a mixture of petrol ether and EtOAc (10/1). Collected fractions were concentrated *in vacuo* and the product was dried under high vaccum. **3a-3f**, **3n** are commercially available.

Control experiments: Light responsive behaviors (I)

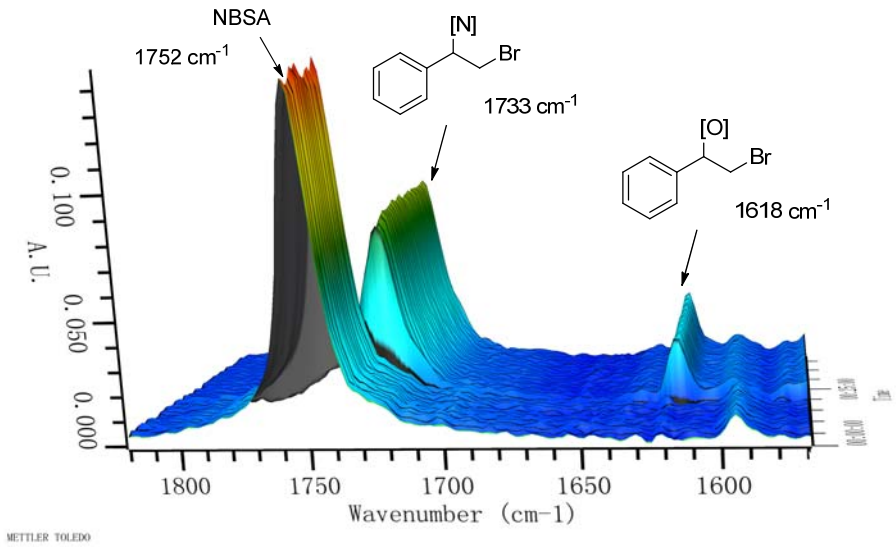
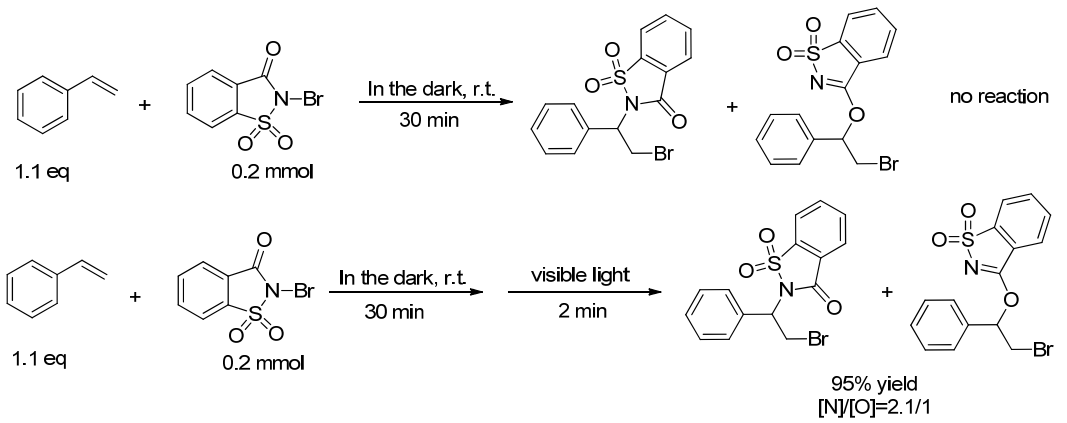


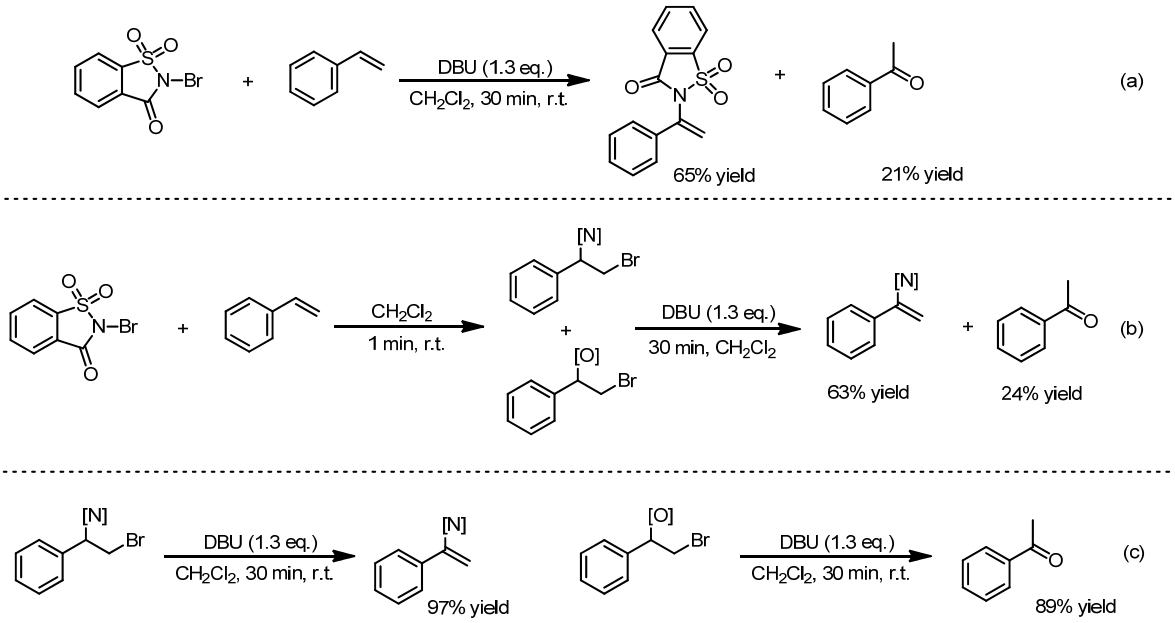
Figure 1: **NBSA** (0.2 mmol), styrene (0.22 mmol), CH_2Cl_2 (1.0 mL). The consumption of **NBSA**, bromoamine product and bromoether product were monitored by in-situ IR at 1752, 1733, 1618 cm^{-1}.

Control experiments: Light responsive behaviors (II)



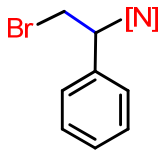
Scheme 1. The reactions were conducted in the dark room using **NBSA** (0.2 mmol), styrene (0.22 mmol), CH_2Cl_2 (1.0 mL) for 30 min. Then the second reaction was removed to the laboratory with ambient light. Yields are of isolated products.

Control experiments: Light responsive behaviors (III)



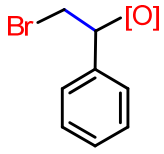
Scheme 2. The reactions were conducted with NBSA (0.2 mmol), styrene (0.22 mmol), CH_2Cl_2 (1.0 mL), DBU (1.3 eq.) for 30 min. The second reaction was first without DBU with ambient light for 1 min. Then DBU was added to this tube. The third reaction were conducted with the bromofunctionlization products and DBU (1.3 eq.). Isolated yields.

Spectra Data for Products:



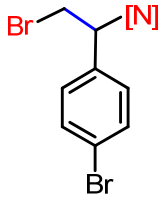
64% yield, 46.97 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.11-7.98 (m, 1 H), 7.93-7.78 (m, 3 H), 7.61 (dd, *J* = 7.7, 1.6 Hz, 2 H), 7.45-7.32 (m, 3 H), 5.45 (dd, *J* = 8.9, 7.1 Hz, 1 H), 4.54 (dd, *J* = 10.6, 9.1 Hz, 1 H), 4.13 (dd, *J* = 10.7, 7.0 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 137.4, 135.3, 135.1, 134.5, 129.3, 128.9, 128.6, 127.0, 125.4, 121.0, 58.5, 29.9 ppm; IR (KBr, cm^{-1}): 3089, 3034, 2923, 1728, 1496, 1455, 1337, 1294, 1255, 1185, 750, 582; HRMS (ESI^+) calcd for $[C_{15}H_{13}BrNO_3S]^+$: 365.9794, found 365.9797.



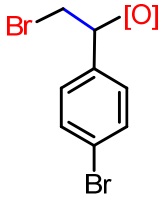
31% yield, 22.37 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93-7.83 (m, 2 H), 7.81-7.69 (m, 2 H), 7.70-7.78 (m, 5 H), 6.33 (dd, *J* = 7.9, 4.7 Hz, 1 H), 3.93 (dd, *J* = 11.2, 7.9 Hz, 1 H), 3.80 (dd, *J* = 11.3, 4.7 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.5, 143.8, 135.5, 134.4, 133.7, 129.9, 129.2, 127.0, 126.9, 123.6, 122.2, 82.5, 32.9 ppm; IR (KBr, cm^{-1}): 3070, 3034, 2923, 1614, 1554, 1396, 1334, 1174, 1150, 770, 618; HRMS (ESI^+) calcd for HRMS (ESI^+) calcd for $[C_{15}H_{13}BrNO_3S]^+$: 365.9794, found 365.9798.



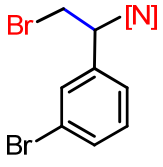
60% yield, 53.39 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.03 (d, J = 6.3 Hz, 1 H), 7.94-7.77 (m, 3 H), 7.58-7.43 (m, 4 H), 5.39 (t, *J* = 8.0 Hz, 1 H), 4.52-4.34 (m, 1 H), 4.13 (ddd, *J* = 10.6, 7.6, 1.1 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 137.3, 135.2, 134.6, 134.2, 132.1, 130.4, 126.9, 125.5, 123.6, 121.1, 57.7, 29.3 ppm; IR (KBr, cm^{-1}): 3092, 3039, 2925, 1728, 1339, 1293, 1254, 1184,750, 584; HRMS (ESI^+) calcd for $[C_{15}H_{12}Br_2NO_3S]^+$: 443.8899, found 443.8895.



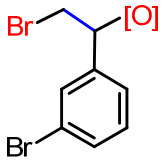
32% yield, 28.10 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.89-7.74 (m, 4 H), 7.65-7.48 (m, 2 H), 7.35 (d, *J* = 7.6 Hz, 2 H), 6.27 (t, *J* = 5.7 Hz, 1 H), 3.99-3.83 (m, 1 H), 3.83-3.65 (m, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.4, 143.7, 134.6, 134.5, 133.7, 132.4, 128.7, 126.6, 124.2, 123.5, 122.2, 81.6, 32.5 ppm; IR (KBr, cm^{-1}): 3040, 2923, 2856, 1614, 1554, 1392, 1335, 1174, 606; HRMS (ESI^+) calcd for $[C_{15}H_{12}Br_2NO_3S]^+$: 443.8899, found 443.8902.



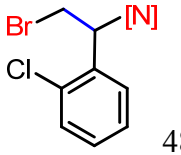
54% yield, 47.96 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.07-8.01 (m, 1 H), 7.94-7.79 (m, 3 H), 7.76 (t, *J* = 1.8 Hz, 1 H), 7.57-7.47 (m, 2 H), 7.28 (d, *J* = 7.9 Hz, 1 H), 7.24 (s, 1 H), 5.44-5.31 (m, 1 H), 4.46 (dd, *J* = 10.7, 8.7 Hz, 1 H), 4.11 (dd, *J* = 10.7, 7.4 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 137.4, 137.4, 135.2, 134.7, 132.5, 131.7, 130.4, 127.3, 126.9, 125.5, 122.9, 121.1, 57.7, 29.4 ppm; IR (KBr, cm^{-1}): 3067, 2956, 2928, 1728, 1571, 1339, 1293, 1185, 749, 602; HRMS (ESI^+) calcd for $[C_{15}H_{12}Br_2NO_3S]^+$: 443.8899, found 443.8899.



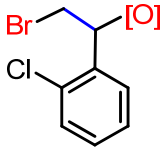
32% yield, 28.21 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.88 (t, *J* = 6.2 Hz, 2 H), 7.82-7.90 (m, 2 H), 7.61 (s, 1 H), 7.54 (d, *J* = 8.4 Hz, 1 H), 7.41 (d, *J* = 7.7 Hz, 1 H), 7.30 (t, *J* = 7.8 Hz, 1 H), 6.27 (dd, *J* = 7.4, 4.9 Hz, 1 H), 3.89 (dd, *J* = 11.3, 7.6 Hz, 1 H), 3.78 (dd, *J* = 11.3, 4.9 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.4, 143.7, 137.7, 134.6, 133.8, 133.0, 130.7, 129.8, 126.6, 126.0, 123.6, 123.2, 122.2, 81.4, 32.6 ppm; IR (KBr, cm^{-1}): 2925, 2955, 1614, 1552, 1392, 1174, 1146, 770; HRMS (ESI^+) calcd for $[C_{15}H_{12}Br_2NO_3S]^+$: 443.8899, found 443.8901.



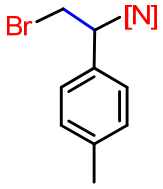
48% yield, 38.33 mg.

^{1}H NMR (400 MHz, CDCl3): δ 8.15-8.08 (m, 1 H), 7.88-7.81 (m, 3 H), 7.78-7.72 (m, 1 H), 7.48-7.41 (m, 1 H), 7.37-7.32 (m, 2 H), 6.06 (dd, *J* = 8.6, 7.5 Hz, 1 H), 4.42 (dd, *J* = 10.7, 8.7 Hz, 1 H), 4.10 (dd, *J* = 10.7, 7.4 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, CDCl3): δ 159.0 137.6, 135.2, 134.6, 134.4, 132.3, 130.7, 130.2, 129.2, 127.5, 126.8, 125.6, 121.0, 54.7, 29.2 ppm; IR (KBr, cm^{-1}): 3095, 3070, 2928, 1732, 1443, 1339, 1293, 1186, 750, 582; HRMS (ESI^{+}) calcd for $[C_{15}H_{12}BrClNO_3S]^{+}$: 399.9404, found 399.9399.



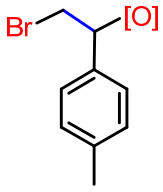
37% yield, 29.49 mg.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13-8.11(m, 2 H), 7.76-7.74 (m, 2 H), 7.52-7.48 (m, 1 H), 7.45-7.41 (m, 1 H), 7.36-7.29 (m, 2 H), 6.69 (dd, *J* = 7.1, 4.0 Hz, 1 H), 3.95 (dd, *J* = 11.5, 4.0 Hz, 1 H), 3.87 (dd, *J* = 11.5, 7.1 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.2, 143.8, 134.6, 133.8, 133.4, 132.5, 130.7, 130.4, 127.6, 127.4, 126.6, 123.5, 122.2, 32.0 ppm; IR (KBr, cm^{-1}): 3073, 30131, 2962, 1615, 1557, 1336, 1176, 970, 770; $[C_{15}H_{12}BrClNO_3S]^{+}$: 399.9404, found 399.9401.



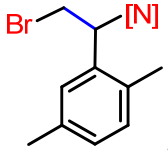
62% yield, 47.02 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.07-7.98 (m, 1 H), 7.90-7.77 (m, 3 H), 7.50 (d, *J* = 8.1 Hz, 2 H), 7.20 (d, *J* = 8.0 Hz, 2 H), 5.43 (dd, *J* = 8.7, 7.4 Hz, 1 H), 4.52 (dd, *J* = 10.4, 9.2 Hz, 1 H), 4.12 (dd, *J* = 10.6, 7.1 Hz, 1 H), 2.34 (s, 3 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 139.3, 137.4, 135.0, 134.5, 132.2, 129.6, 128.5, 127.1, 125.4, 121.0, 58.3, 30.0, 21.3 ppm; IR (KBr, cm^{-1}): 2923, 2853, 1727, 1337, 1184, 752, 585; HRMS (ESI^{+}) calcd for $[C_{16}H_{15}BrNO_3S]^{+}$: 379.9951, found 379.9949.



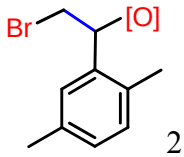
27% yield, 20.44 mg.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89-7.82 (m, 2 H), 7.76-7.69 (m, 2 H), 7.36 (d, *J* = 8.1 Hz, 2 H), 7.22 (d, *J* = 8.0 Hz, 2 H), 6.29 (dd, *J* = 8.0, 4.8 Hz, 1 H), 3.93 (dd, *J* = 11.2, 8.1 Hz, 1 H), 3.77 (dd, *J* = 11.2, 4.8 Hz, 1 H), 2.36 (s, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.4, 143.7, 140.0, 134.4, 133.6, 132.5, 129.8, 127.0, 126.9, 123.5, 122.1, 82.5, 32.9, 21.4 ppm; IR (KBr, cm^{-1}): 3034, 2925, 1613, 1553, 1394, 1174, 771, 617; HRMS (ESI^+) calcd for $[C_{16}H_{15}BrNO_3S]^+$: 379.9951, found 379.9954.



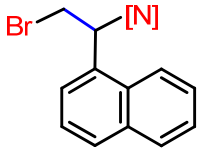
51% yield, 39.92 mg.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 6.0 Hz, 1 H), 7.88-7.78 (m, 3 H), 7.54 (s, 1 H), 7.16-7.06 (m, 2 H), 5.80 (t, *J* = 7.9 Hz, 1 H), 4.53 (t, *J* = 9.7 Hz, 1 H), 4.05 (dd, *J* = 10.5, 7.1 Hz, 1 H), 2.36 (s, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.1, 137.7, 136.2, 135.1, 134.5, 133.9, 132.9, 131.0, 130.2, 128.3, 126.9, 125.6, 120.9, 54.9, 30.7, 21.4, 19.2 ppm; IR (KBr, cm^{-1}): 2955, 2924, 2867, 1721, 1339, 1249, 1184, 750, 583; HRMS (ESI^+) calcd for $[C_{17}H_{17}BrNO_3S]^+$: 394.0107, found 394.0109.



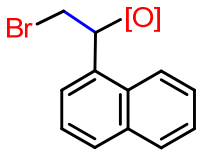
28% yield, 22.18 mg.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (dd, *J* = 14.6, 7.0 Hz, 2 H), 7.76 (p, *J* = 7.3 Hz, 2 H), 7.19 (s, 1 H), 7.13-7.04 (m, 2 H), 6.48 (dd, *J* = 8.8, 4.1 Hz, 1 H), 3.95-3.83 (m, 1 H), 3.68 (dd, *J* = 11.4, 4.2 Hz, 1 H), 2.47 (s, 3 H), 2.31 (s, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.5, 143.8, 136.3, 134.3, 133.9, 133.7, 133.0, 131.1, 130.5, 126.9, 126.2, 123.5, 122.1, 79.9, 32.5, 21.2, 19.0 ppm; IR (KBr, cm^{-1}): 2962, 2925, 2851, 1728, 1338, 1176, 749, 583; HRMS (ESI^+) calcd for $[C_{17}H_{17}BrNO_3S]^+$: 394.0107, found 394.0104.



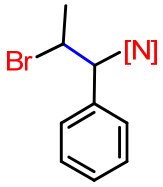
60% yield, 54.38 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1 H), 8.02 (d, *J* = 6.9 Hz, 1 H), 7.90-7.71 (m, 7-H), 7.53-7.47 (m, 2-H), 5.65 (t, J = 7.9 Hz, 1H), 4.64 (t, *J* = 9.8 Hz, 1H), 4.26 (dd, *J* = 10.4, 7.4 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.9, 137.3, 135.0, 134.5, 133.5, 133.1, 132.6, 128.8, 128.4, 128.2, 127.8, 127.0, 126.9, 126.6, 125.7, 125.4, 121.0, 58.6, 29.9 ppm; IR (KBr, cm^{-1}): 3059, 2979, 1728, 1338, 1250, 1184, 748, 677, 584; HRMS (ESI^+) calcd for $[C_{17}H_{17}BrNO_3S]^+$: 415.9951, found 415.9954.



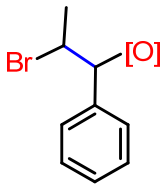
31% yield, 28.62 mg.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (s, 1 H), 7.88 (dd, *J* = 15.3, 7.5 Hz, 5 H), 7.79-7.70 (m, 2 H), 7.55 (d, *J* = 8.1 Hz, 3 H), 6.57-6.43 (m, 1 H), 4.09-3.98 (m, 1 H), 3.87 (dd, *J* = 11.2, 4.7 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.5, 143.8, 134.4, 133.9, 133.7, 133.1, 132.7, 129.2, 128.4, 127.9, 127.22, 127.20, 127.0, 126.9, 123.59, 123.58, 122.2, 82.7, 32.8 ppm; IR (KBr, cm^{-1}): 3059, 2965, 2929, 1614, 1555, 1334, 1180, 819, 608; HRMS (ESI^+) calcd for $[C_{17}H_{17}BrNO_3S+]^+$: 415.9951, found 415.9953.



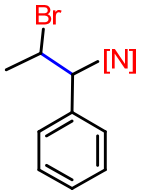
51% yield, 38.72 mg.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02-7.94 (m, 1 H), 7.88-7.74 (m, 3 H), 7.73-7.67 (m, 2H), 7.44-7.31 (m, 3 H), 5.45-5.35 (m, 1 H), 5.21 (d, *J* = 11.0 Hz, 1 H), 1.91 (d, *J* = 6.5 Hz, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 137.3, 136.0, 135.1, 134.5, 129.4, 129.1, 128.6, 126.8, 125.4, 121.0, 63.4, 45.3, 23.8 ppm; IR (KBr, cm^{-1}): 3034, 2979, 2931, 1728, 1339, 1186, 1168, 698, 583; HRMS (ESI^+) calcd for $[C_{16}H_{15}BrNO_3S]^+$: 379.9951, found 379.9959.



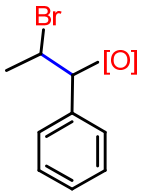
32% yield, 24.20 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.84 (m, 2H), 7.80-7.72 (m, 2H), 7.49-7.43 (m, 2H), 7.43-7.36 (m, 3H), 6.25 (d, *J* = 5.2 Hz, 1H), 4.65-4.57 (m, 1H), 1.76 (d, *J* = 6.8 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.3, 143.6, 134.6, 134.5, 133.7, 129.5, 128.6, 127.5, 126.7, 123.4, 122.1, 85.5, 48.7, 21.2 ppm; IR (KBr, cm^{-1}): 3037, 2981, 2934, 1616, 1557, 1396, 1175, 772, 703; HRMS (ESI^+) calcd for $[C_{16}H_{15}BrNO_3S]^+$: 379.9951, found 379.9947.



35% yield, 45.34 mg.

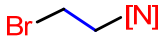
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.92 (m, 1H), 7.90-7.85 (m, 1H), 7.77-7.73 (m, 1H), 7.74-7.64 (m, 3H), 7.61-7.56 (m, 1H), 7.59-7.49 (m, 2H), 7.32-7.21 (m, 4H), 5.60-5.45 (m, 1H), 5.35-5.25 (m, 1H), 5.11 (d, *J* = 11.0 Hz, 1H), 4.97 (d, *J* = 11.0 Hz, 1H), 1.80 (d, *J* = 6.5 Hz, 1H), 1.54 (d, *J* = 6.7 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 158.5, 137.3, 137.1, 136.0, 135.8, 135.1, 134.9, 134.5, 134.4, 129.4, 129.1, 129.1, 129.0, 128.6, 127.1, 126.8, 125.4, 125.4, 121.0, 120.9, 65.3, 63.4, 46.3, 45.3, 24.3, 23.8 ppm; IR (KBr, cm^{-1}): 3039, 2976, 1727, 1339, 1252, 1186, 750, 584; HRMS (ESI^+) calcd for $[C_{16}H_{15}BrNO_3S]^+$: 379.9951, found 379.9952.

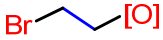


60% yield, 26.67 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.82 (m, 3H), 7.80-7.69 (m, 3H), 7.48-7.35 (m, 8H), 6.25 (d, *J* = 5.2 Hz, 1H), 6.12 (d, *J* = 8.3 Hz, 1H), 4.66-4.52 (m, 2H), 1.76 (d, *J* = 6.8 Hz, 2H), 1.59 (d, *J* = 6.9 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.3, 143.6, 134.9, 134.6, 134.5, 134.3, 133.7, 133.7, 129.8, 129.5, 129.1, 128.7, 127.5, 127.5, 126.9, 126.7, 123.5, 123.5, 122.1, 122.0, 87.0, 85.5, 49.0, 48.7, 22.3, 21.2 ppm; IR (KBr, cm^{-1}): 3031, 2981, 2934, 1615, 1396, 1336, 1174, 934, 772, 610; HRMS

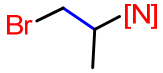
(ESI$^+$) calcd for $[C_{16}H_{15}BrNO_3S]^+$: 379.9951, found 379.9955.





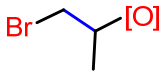
95% yield, 54.90 mg.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10-7.99 (m, 1 H), 7.96-7.84 (m, 4 H), 7.83-7.69 (m, 2 H), 4.91-4.84 (m, 1 H), 4.15 (t, *J* = 7.5 Hz, 2 H), 3.77-3.71 (m, 1 H), 3.65 (dd, *J* = 7.9, 7.2 Hz, 2 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ169.1, 158.7, 149.6, 143.6, 137.5, 135.23, 134.7, 134.5, 133.7, 127.1, 125.5, 123.6, 122.1, 121.2, 70.6, 40.0, 27.3, 27.0 ppm; IR (KBr, cm^{-1}): 3092, 3034, 2929, 1732, 1336, 1297, 1259, 1178, 750, 585; HRMS (ESI$^+$) calcd for $[C_9H_9BrNO_3S]^+$: 289.9481, found 289.9486.



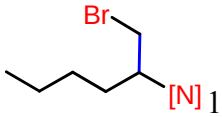
61.9% yield, 41.7 mg.

^{13}C NMR (75 MHz, $CDCl_3$): δ 167.2, 134.5, 131.7, 123.6, 88.3, 68.7, 46.5, 37.3 ppm; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12- 8.00 (m, 2H), 7.96-7.77 (m, 7H), 4.57 (dd, J = 14.4, 7.2 Hz, 1H), 4.53-4.45 (m, 1H), 4.16 (dd, J = 14.8, 6.8 Hz, 1H), 4.01 (dd, J = 14.8, 8.3 Hz, 1H), 3.94 (dd, J = 10.4, 7.4 Hz, 1H), 3.71 (dd, J = 10.4, 7.5 Hz, 1H), 1.75 (t, J = 6.6 Hz, 7H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 159.0, 158.8, 137.7, 137.5, 135.2, 135.0, 134.7, 134.5, 127.1, 127.1, 125.6, 125.3, 121.2, 120.9, 51.6, 46.5, 43.8, 32.6, 23.4, 17.1 ppm. IR (KBr, cm^{-1}): 3098, 2929, 1731, 1337, 1256, 1812, 751, 564; HRMS (ESI$^+$) calcd for $[C_{10}H_{11}NO_3BrS]^+$: 303.9638, found 303.9642.



28.1% yield, 18.9 mg.

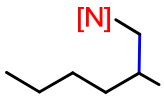
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.87 (m, 1H), 7.85-7.68 (m, 4H), 5.55-5.40 (m, 1H), 4.72 (s, 1H), 4.44 (dd, J = 13.1, 6.5 Hz, 1H), 4.21 (t, J = 6.0 Hz, 1H), 3.72 (dd, J = 11.2, 4.7 Hz, 1H), 3.64 (dd, J = 11.2, 5.1 Hz, 1H), 1.81 (d, J = 6.8 Hz, 1H), 1.62 (d, J = 6.3 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 143.9, 134.5, 134.4, 133.9, 133.7, 133.7, 126.9, 123.6, 123.6, 122.2, 122.1, 85.4, 75.4, 42.8, 34.0, 22.2, 18.5 ppm; IR (KBr, cm^{-1}): 3031, 2987, 2931, 1614, 1555, 1399, 1332, 1174, 771, 749, 616; HRMS (ESI$^+$) calcd for $[C_{10}H_{11}NO_3BrS]^+$: 303.9638, found 303.9635.



18.81 mg.

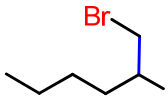
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.0 Hz, 1H), 7.93-7.80 (m, 3H), 4.54-4.42 (m, 1H), 3.97 (dd, *J* = 10.5, 8.4 Hz, 1H), 3.73 (dd, *J* = 10.6, 6.6 Hz, 1H), 2.30-2.10 (m,

1H), 2.10-1.95 (m, 1H), 1.46-1.31 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 137.6, 135.0, 134.5, 127.0, 125.5, 120.9, 56.6, 32.1, 30.7, 28.7, 22.3, 13.9 ppm; IR (KBr, cm^{-1}): 2959, 2834, 2870, 1731, 1338, 1293, 1184, 751, 583; HRMS (ESI^+) calcd for $[C_{13}H_{17}NO_3BrS]^+$: 346.0107, found 346.0103.



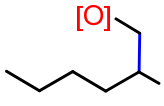
18.79 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.06 (m, 1H), 7.95-7.83 (m, 3H), 4.50-4.35 (m, 1H), 4.19 (dd, *J* = 14.9, 7.2 Hz, 1H), 4.07 (dd, *J* = 14.9, 7.9 Hz, 1H), 1.97-1.89 (m, 1H), 1.85-1.75 (m, 1H), 1.69-1.59 (m, 1H), 1.47-1.29 (m, 3H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 137.5, 135.2, 134.7, 127.1, 125.6, 121.2, 51.0, 45.5, 35.5, 29.5, 22.1, 14.0 ppm; IR (KBr, cm^{-1}): 3078, 2923, 2854, 1736, 1338, 1182, 761, 585; HRMS (ESI^+) calcd for $[C_{13}H_{17}NO_3BrS]^+$: 346.0107, found 346.0111.



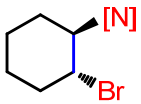
10.97 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 6.7, 1.6 Hz, 1H), 7.85-7.66 (m, 3H), 5.41-5.30 (m, 1H), 3.79 (dd, *J* = 11.5, 4.3 Hz, 1H), 3.65 (dd, *J* = 11.4, 4.7 Hz, 1H), 2.06-1.89 (m, 2H), 1.45-1.35 (m, 4H), 0.93 (t, J = 7.0 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 143.7, 134.4, 133.7, 127.0, 123.6, 122.1, 80.8, 32.7, 32.0, 27.1, 22.5, 14.0 ppm; IR (KBr, cm^{-1}): 2955, 2924, 2854, 1553, 1396, 1174, 788, 595; HRMS (ESI^+) calcd for $[C_{13}H_{17}NO_3BrS]^+$: 346.0107, found 346.0104.



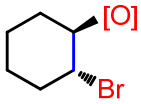
9.98 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.88 (m, 1H), 7.83-7.72 (m, 3H), 4.88-4.70 (m, 2H), 4.33 (m, 1H), 2.05-1.85 (m, *J* = 14.0, 9.3, 4.4 Hz, 2H), 1.53-1.30 (m, 4H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 143.7, 134.5, 133.7, 126.7, 123.6, 122.2, 74.6, 49.8, 34.9, 29.4, 22.2, 14.0 ppm; IR (KBr, cm^{-1}): 2956, 2923, 2854, 1732, 1558, 1339, 1175, 770; HRMS (ESI^+) calcd for $[C_{13}H_{17}NO_3BrS]^+$: 346.0107, found 346.0113.



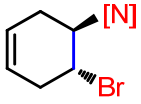
66% yield, 45.42 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.1 Hz, 1H), 7.91-7.79 (m, 3H), 4.86 (s, 1H), 4.25 (s, 1H), 2.60-2.45 (m, 1H), 2.28-2.16 (m, 2H), 2.01-1.85 (m, 2H), 1.82-1.73 (m, 1H), 1.54-1.36 (m, 2H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.8, 137.8, 134.9, 134.4, 127.4, 125.5, 120.9, 60.4, 50.6, 38.5, 31.6, 26.8, 25.6. ppm; IR (KBr, cm^{-1}): 2959, 2928, 1732, 1455, 1337, 1292, 1182, 1061, 753, 585; HRMS (ESI^+) calcd for $[C_{13}H_{15}NO_3BrS]^+$: 343.9951, found 343.9949.



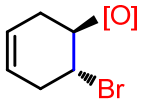
29% yield, 19.75 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.5 Hz, 1H), 7.82-7.67 (m, 3H), 5.21 (td, *J* = 9.3, 4.3 Hz, 1H), 4.20 (td, *J* = 10.1, 4.4 Hz, 1H), 2.56-2.36 (m, 2H), 2.02-1.74 (m, 3H), 1.65-1.39 (m, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.4, 143.6, 134.3, 133.6, 127.1, 123.6, 122.0, 84.2, 51.1, 35.6, 30.6, 25.4, 23.2 ppm; IR (KBr, cm^{-1}): 2943, 2865, 1614, 1557, 140, 1361, 1336, 1174, 936, 613; HRMS (ESI^+) calcd for $[C_{13}H_{15}NO_3BrS]^+$: 343.9951, found 343.9954.



52% yield, 35.57 mg.

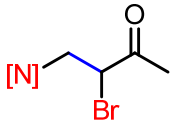
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10-8.04 (m, 1H), 7.96-7.76 (m, 3H), 5.76-5.67 (m, 1H), 5.65-5.53 (m, 1H), 5.10 (td, *J* = 10.9, 5.9 Hz, 1H), 4.48 (td, *J* = 11.2, 5.7 Hz, 1H), 3.14-2.88 (m, 2H), 2.86-2.72 (m, 1H), 2.70-2.68 (m, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 137.5, 135.0, 134.5, 127.2, 125.6, 125.5, 125.1, 121.0, 56.0, 47.3, 37.8, 30.5 ppm; IR (KBr, cm^{-1}): 3098, 3037, 2926, 2848, 1731, 1366, 1292, 1181, 752, 586; HRMS (ESI^+) calcd for $[C_{13}H_{13}NO_3BrS]^+$: 341.9794, found 341.9793.



25% yield, 16.94 mg.

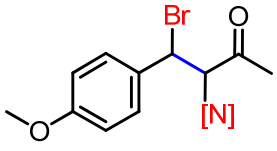
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.5 Hz, 1H), 7.81-7.67 (m, 3H), 5.75-5.59 (m, 2H), 5.54-5.45 (m, 1H), 4.46 (dd, *J* = 14.0, 7.3 Hz, 1H), 3.09-2.89 (m, 2H), 2.77-2.65 (m, 1H), 2.50-2.36 (m, 1H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 168.5, 143.7, 134.4, 133.7, 126.9, 124.3, 123.6, 123.1, 122.1, 79.8, 45.6, 34.0, 29.5 ppm; IR

(KBr, cm^{-1}): 3040, 2962, 293, 1614, 1557, 1399, 1174, 771, 674; HRMS (ESI^+) calcd for $[C_{13}H_{13}NO_3BrS]^+$: 341.9794, found 341.9797.



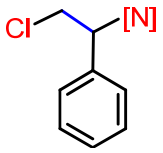
75% yield, 49.64 mg.

^1H NMR (300 MHz, $CDCl_3$) δ 8.11-8.05 (m, 1H), 7.99-7.80 (m, 3H), 4.86 (t, *J* = 7.4 Hz, 1H), 4.39 (dd, *J* = 15.2, 7.1 Hz, 1H), 4.25 (dd, *J* = 15.2, 7.7 Hz, 1H), 2.44 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.8, 158.7, 137.5, 135.3, 134.7, 127.1, 125.7, 121.2, 46.8, 40.7, 27.3 ppm; IR (KBr, cm^{-1}): 2987, 2857, 1764, 1719, 1651, 1395, 1378, 1086, 941, 714; HRMS (ESI^+) calcd for $[C_{11}H_{11}BrNO_4S]^+$: 331.9587, found 331.9583.



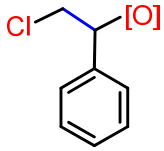
91% yield, 79.53 mg.

^1H NMR (300 MHz, CD_2Cl_2) δ 7.96-7.84 (m, 1H), 7.75-7.65 (m, 3H), 7.50-7.44 (m, 2H), 6.86-6.78 (m, 2H), 5.69 (d, *J* = 11.7 Hz, 1H), 5.55 (d, *J* = 11.7 Hz, 1H), 3.69 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (75 MHz, CD_2Cl_2) δ 199.3, 160.6, 158.8, 137.5, 135.6, 135.0, 131.0, 127.7, 127.0, 125.7, 121.0, 114.2, 57.4, 55.7, 49.8, 27.2 ppm; IR (KBr, cm^{-1}): 2953, 2925, 2854, 1729, 1515, 1243, 1182, 1029, 749, 584; HRMS (ESI^+) calcd for $[C_{23}H_{19}BrNO_4S]^+$: 500.0162, found 500.0160.



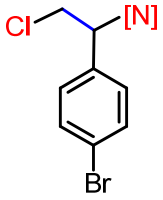
62% yield, 39.8 mg.

^1H NMR (300 MHz, $CDCl_3$): δ 8.04 (d, *J* = 7.6 Hz, 1 H), 7.84 (m, 3 H), 7.60 (d, *J* = 6.7 Hz, 2 H), 7.44-7.33 (m, 3 H), 5.41 (dd, *J* = 9.0, 6.8 Hz, 1 H), 4.69 (dd, *J* = 11.4, 9.3 Hz, 1 H), 4.25 (dd, *J* = 11.5, 6.7 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ158.9, 137.5, 135.1, 134.8, 134.5, 129.3, 129.0, 128.6, 127.1, 125.4, 121.1, 58.6, 42.3 ppm; IR (KBr, cm^{-1}): 3040, 2923, 1730, 1336 1293, 1186, 750, 699, 584; HRMS (ESI^+) calcd for $[C_{15}H_{13}ClNO_3S]^+$: 322.0299, found 322.0298.



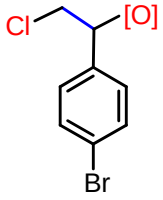
29% yield, 19.0 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93-7.83 (m, 2H), 7.81-7.69 (m, 2H), 7.70-7.78 (m, 5H), 6.33 (dd, *J* = 7.9, 4.7 Hz, 1H), 3.93 (dd, *J* = 11.2, 7.9 Hz, 1H), 3.80 (dd, *J* = 11.3, 4.7 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.6, 143.8, 135.0, 134.4, 133.7, 129.9, 129.2, 127.1, 126.9, 123.6, 122.2, 82.7, 45.7 ppm; IR (KBr, cm^{-1}): 2959, 2928, 2854, 1555, 1396, 1337, 1174, 771; HRMS (ESI^+) calcd for HRMS (ESI^+) calcd for $[C_{15}H_{13}ClNO_3S]^+$: 322.0299, found 322.0294.



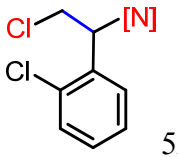
54% yield, 42.84 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.08-7.99 (m, 1 H), 7.95-7.77 (m, 3 H), 7.59-7.41 (m, 4 H), 5.35 (dd, *J* = 8.5, 7.3 Hz, 1 H), 4.59 (dd, *J* = 11.5, 8.7 Hz, 1 H), 4.25 (dd, *J* = 11.5, 7.2 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, CDCl3) δ 158.9, 137.4, 135.2, 134.7, 133.8, 132.2, 130.4, 127.0, 125.5, 123.6, 121.1, 57.8, 41.9 ppm; IR (KBr, cm^{-1}): 2920, 2854, 1731, 1339, 1185, 750, 584; HRMS (ESI^+) calcd for $[C_{15}H_{12}BrClNO_3S]^+$: 398.9332, found 398.9335.



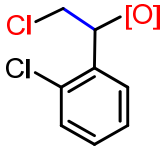
28% yield, 22.56 mg.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.91-7.71 (m, 4 H), 7.59 -7.54 (m, 2 H), 7.39-7.33 (m, 2 H), 6.26 (dd, *J* = 7.4, 4.6 Hz, 1 H), 4.04 (dd, *J* = 12.1, 7.4 Hz, 1 H), 3.93 (dd, *J* = 12.1, 4.6 Hz, 1 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ168.2, 143.6, 134.5, 134.4, 133.6, 132.3, 128.6, 126.5, 124.0, 123.4, 122.1, 81.5, 32.3 ppm; IR (KBr, cm^{-1}): 2923, 2853, 1614, 1555, 1393, 1174, 770, 608; HRMS (ESI^+) calcd for $[C_{15}H_{12}BrClNO_3S]^+$: 398.9332, found 398.9337.



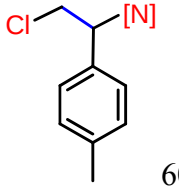
52%yield, 35.50 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.07 (m, 1 H), 7.90-7.81 (m, 3 H), 7.77-7.72 (m, 1 H), 7.44 (dt, *J* = 6.5, 3.0 Hz, 1 H), 7.37-7.32 (m, 2 H), 6.04 (dd, *J* = 8.8, 7.1 Hz, 1 H), 4.57 (dd, *J* = 11.4, 8.9 Hz, 1 H), 4.22 (dd, *J* = 11.4, 7.0 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 137.6, 135.2, 134.6, 134.4, 131.8, 130.7, 130.2, 129.2, 127.5, 126.7, 125.6, 120.9, 54.8, 41.7 ppm; IR (KBr, cm^{-1}): 3095, 3070, 1732, 1340, 1293, 1186, 750, 583; HRMS (ESI^+) calcd for $[C_{15}H_{12}Cl_2NO_3S]^+$: 342.9831, found 342.9833.



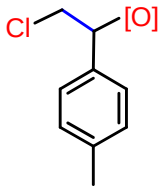
27% yield, 18.70 mg.

1H NMR (300 MHz, CDCl3) δ 7.91 (m, 2 H), 7.83-7.73 (m, 2 H), 7.55-7.48 (m, 1 H), 7.47-7.41 (m, 1 H), 7.37-7.30 (m, 2 H), 6.70 (dd, *J* = 6.8, 3.8 Hz, 1 H), 4.06 (m, 2 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.4, 143.9, 134.6, 133.8, 132.8, 132.5, 130.7, 130.4, 127.8, 127.4, 126.6, 123.5, 122.3, 79.4, 44.7 ppm; IR (KBr, cm^{-1}): 3070, 2959, 1615, 1556, 1394, 1338, 1176, 749; $[C_{15}H_{12}Cl_2NO_3S]^+$: 342.9831, found 342.9877.



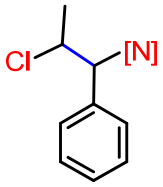
60% yield, 44.9 mg.

1H NMR (300 MHz, CDCl3): δ 8.07-7.98 (m, 1 H), 7.90-7.77 (m, 3 H), 7.50 (d, *J* = 8.1 Hz, 2 H), 7.20 (d, *J* = 8.0 Hz, 2 H), 5.43 (dd, *J* = 8.7, 7.4 Hz, 1 H), 4.52 (dd, *J* = 10.4, 9.2 Hz, 1 H), 4.12 (dd, *J* = 10.6, 7.1 Hz, 1 H), 2.34 (s, 3 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.8, 139.3, 137.4, 135.0, 134.5, 132.2, 129.6, 128.5, 127.1, 125.4, 121.0, 58.3, 30.0, 21.3 ppm; IR (KBr, cm^{-1}): 3037, 2923, 1731, 1339, 1252, 1186, 751, 587; HRMS (ESI^+) calcd for $[C_{16}H_{15}ClNO_3S]^+$: 336.0456, found 336.0459.



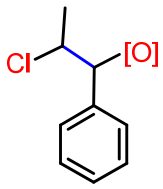
23% yield, 15.50 mg.

1H NMR (400 MHz, CDCl3): δ 7.89-7.82 (m, 2 H), 7.76-7.69 (m, 2 H), 7.36 (d, *J* = 8.1 Hz, 2 H), 7.22 (d, *J* = 8.0 Hz, 2 H), 6.29 (dd, *J* = 8.0, 4.8 Hz, 1 H), 3.93 (dd, *J* = 11.2, 8.1 Hz, 1 H), 3.77 (dd, *J* = 11.2, 4.8 Hz, 1 H), 2.36 (s, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.4, 143.7, 140.0, 134.4, 133.6, 132.5, 129.8, 127.0, 126.9, 123.5, 122.1, 82.5, 32.9, 21.4 ppm; IR (KBr, cm^{-1}): 3031, 2962, 2923, 1614, 1556, 1389, 1174, 781, 610; HRMS (ESI^+) calcd for $[C_{16}H_{15}ClNO_3S]^+$: 336.0456, found 336.0452.



51% yield, 34.22 mg.

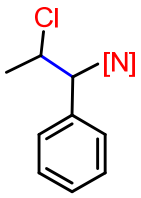
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 6.4, 2.0 Hz, 1 H), 7.99 (d, *J* = 7.0 Hz, 1 H), 7.89-7.74 (m, 5 H), 7.70 (d, *J* = 7.0 Hz, 2 H), 7.65 (dd, *J* = 7.7, 1.4 Hz, 1 H), 7.42 -7.32 (m, 5 H), 5.55 (m, 1 H), 5.39 (m, 1 H), 5.10 (d, *J* = 10.7 Hz, 1 H), 5.00 (d, *J* = 10.8 Hz, 1 H), 1.72 (d, *J* = 6.4 Hz, 3 H), 1.47 (d, *J* = 6.6 Hz, 2 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.96, 158.59, 137.36, 137.15, 135.74, 135.49, 135.09, 134.87, 134.54, 134.42, 129.45, 129.37, 129.13, 129.02, 128.58, 127.13, 126.77, 125.38, 125.36, 121.07, 120.95, 64.93, 63.15, 54.70, 54.14, 23.27, 22.84; IR (KBr, cm^{-1}): 3037, 2990, 2937, 1728, 1456, 1339, 1186, 983, 750; HRMS (ESI^+) calcd for $[C_{16}H_{15}ClNO_3S+]^+$: 336.0456, found 336.0451.



32% yield, 21.44 mg.

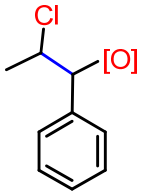
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.83 (m, 3 H), 7.76 (tt, *J* = 7.4, 5.8 Hz, 3 H), 7.50 -7.35 (m, 8 H), 6.24 (d, *J* = 4.9 Hz, 1 H), 6.09 (d, *J* = 8.1 Hz, 1 H), 4.63-4.55 (m, 1 H), 4.52 (m, 1 H), 1.57 (d, *J* = 6.7 Hz, 3 H), 1.42 (d, *J* = 6.8 Hz, 2 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 168.4, 143.7, 134.8, 134.5, 134.3, 134.1, 133.7, 133.6, 129.8, 129.5, 129.1, 128.7, 127.7, 127.6, 126.9, 126.8, 123.5, 123.5, 122.1, 122.0, 87.0, 85.4,

58.1, 57.5, 21.4, 20.4 ppm; IR (KBr, cm^{-1}): 3034, 2987, 2934, 1615, 1557, 1396, 1337, 1174, 994, 772, 703; HRMS (ESI^+) calcd for $[C_{16}H_{15}ClNO_3S+]^+$: 336.0456, found 336.0452.



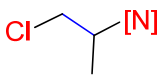
51% yield, 34 mg.

^1H NMR (400 MHz, $CDCl_3$) δ 8.07-7.96 (m, 1H), 7.89-7.75 (m, 4H), 7.73-7.62 (m, 3H), 7.43-7.31 (m, 4H), 5.55 (m, 1H), 5.38 (m, 1H), 5.10 (d, *J* = 10.7 Hz, 1H), 5.00 (d, *J* = 10.8 Hz, 1H), 1.72 (d, *J* = 6.4 Hz, 3H), 1.47 (d, J = 6.6 Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.0, 158.6, 137.4, 137.2, 135.7, 135.5, 135.1, 134.9, 134.6, 134.4, 129.5, 129.4, 129.1, 129.0, 128.6, 127.2, 126.8, 125.4, 125.4, 121.1, 121.0, 65.0, 63.2, 54.7, 54.2, 23.3, 22.9 ppm; IR (KBr, cm^{-1}): 3037, 2990, 2937, 1728, 1456, 1339, 1186, 983, 750; HRMS (ESI^+) calcd for $[C_{16}H_{15}ClNO_3S+]^+$: 336.0456, found 336.0451.



27% yield, 18.1 mg.

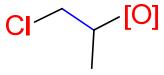
^1H NMR (400 MHz, $CDCl_3$) δ 7.91-.83 (m, 3H), 7.76 (m, *J* = 7.4, 5.8 Hz, 3H), 7.50-7.35 (m, 8H), 6.24 (d, *J* = 4.9 Hz, 1H), 6.09 (d, *J* = 8.1 Hz, 1H), 4.63 – 4.55 (m, 1H), 4.52 (dt, *J* = 13.7, 6.9 Hz, 1H), 1.57 (d, *J* = 6.7 Hz, 3H), 1.42 (d, *J* = 6.8 Hz, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 168.4, 143.7, 134.8, 134.5, 134.3, 134.1, 133.7, 133.6, 129.8, 129.5, 129.1, 128.7, 127.7, 127.6, 126.9, 126.8, 123.5, 123.5, 122.1, 122.0, 87.0, 85.4, 77.5, 77.2, 76.8, 58.1, 57.5, 21.4, 20.4 ppm; IR (KBr, cm^{-1}): 3034, 2987, 2934, 1615, 1557, 1396, 1337, 1174, 994, 772, 703; HRMS (ESI^+) calcd for $[C_{16}H_{15}ClNO_3S]^+$: 336.0456, found 336.0452.



56% yield, 39.1mg.

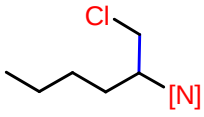
^1H NMR (300 MHz, $CDCl_3$): δ 8.12-8.01 (m, 1 H), 7.99-7.79 (m, 4 H), 4.63-4.41 (m, 1 H), 4.13-4.01 (m, 1 H), 3.92 (dd, *J* = 14.8, 7.3 Hz, 1 H), 3.83 (dd, *J* = 11.2, 7.2 Hz, 1 H), 1.72 (d, *J* = 7.0 Hz, 3H), 1.60 (d, *J* = 6.6 Hz, 2H) ppm; ^{13}C NMR (101 MHz,

$CDCl_3$) δ 159.1, 158.9, 137.7, 137.6, 135.2, 135.0, 134.7, 134.5, 127.2, 127.1, 125.6, 125.4, 121.2, 121.0, 53.3, 51.8, 46.2, 44.8, 22.6, 16.4 ppm; IR (KBr, cm^{-1}): 2998, 2932, 1732, 1462, 1333, 1188, 990, 754; HRMS (ESI^+) calcd for $[C_{10}H_{11}ClNO_3S]^+$: 260.0143, found 260.0143.



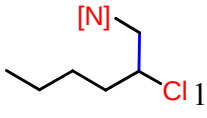
27% yield, 14.0 mg.

^1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.6 Hz, 1 H), 7.85-7.66 (m, 4 H), 5.57-5.43 (m, 1 H), 4.71 (dd, *J* = 11.1, 4.4 Hz, 1 H), 4.63 (dd, *J* = 11.4, 7.1 Hz, 1 H), 4.43 (dd, *J* = 12.0, 6.4 Hz, 1 H), 3.87 (dd, *J* = 12.1, 4.1 Hz, 1 H), 3.78 (dd, *J* = 12.1, 5.2 Hz, 1 H), 1.64 (d, *J* = 6.8 Hz, 1 H), 1.61 (d, *J* = 6.3 Hz, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 143.7, 143.6, 134.5, 134.4, 133.7, 133.7, 127.0, 123.6, 122.2, 122.1, 78.0, 75.2, 52.9, 46.1, 21.4, 17.4 ppm; IR (KBr, cm^{-1}): 3039, 2982, 2930, 1616, 1556, 1399, 1331, 1172, 770, 760, 616 ppm; HRMS (ESI^+) calcd for $[C_{10}H_{11}ClNO_3S]^+$: 260.0143, found 260.0140.



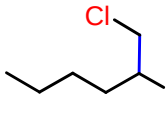
15.91 mg.

1H NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 6.2, 1.7 Hz, 1 H), 7.96-7.74 (m, 3 H), 4.51-4.37 (m, 1 H), 4.11 (dd, *J* = 11.3, 8.5 Hz, 1 H), 3.85 (dd, *J* = 11.3, 6.4 Hz, 1 H), 2.20 (m, 1 H), 1.97 (m, 1 H), 1.39 (m, 4 H), 0.90 (t, *J* = 7.0 Hz, 3 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 137.7, 135.0, 134.5, 127.1, 125.5, 120.9, 56.7, 44.2, 29.9, 28.6, 22.3, 13.9 ppm; IR (KBr, cm^{-1}): 2962, 2931, 2867, 1731, 1338, 1293, 1252, 1183, 751, 584; HRMS (ESI^+) calcd for $[C_{13}H_{17}ClNO_3S]^+$: 302.0612, found 302.0615.



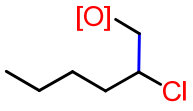
15.74 mg.

^1H NMR (300 MHz, $CDCl_3$) δ 8.13-8.03 (m, 1 H), 7.97-7.81 (m, 3 H), 4.43-4.31 (m, 1 H), 4.08 (dd, *J* = 14.8, 7.6 Hz, 1 H), 3.96 (dd, *J* = 14.8, 6.8 Hz, 1 H), 1.96-1.82 (m, 1 H), 1.79-1.58 (m, 2 H), 1.41 (m, 3H), 0.92 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 137.6, 135.2, 134.6, 127.2, 125.6, 121.2, 58.7, 45.3, 35.2, 28.3, 22.3, 14.0 ppm; IR (KBr, cm^{-1}): 2959, 2929, 2862, 1737, 1339, 1183, 751, 586; HRMS (ESI^+) calcd for $[C_{13}H_{17}ClNO_3S]^+$: 302.0612, found 302.0609.



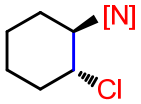
9.30 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.1 Hz, 1 H), 7.85-7.68 (m, 3 H), 5.41 (dd, *J* = 7.4, 2.8 Hz, 1 H), 3.94 (dd, *J* = 12.3, 3.9 Hz, 1 H), 3.79 (dd, *J* = 12.3, 4.7 Hz, 1 H), 2.11-1.86 (m, 2 H), 1.41 (m, 4 H), 0.93 (t, *J* = 6.7 Hz, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 143.7, 134.4, 133.7, 127.0, 123.6, 122.1, 81.4, 44.6, 30.9, 27.1, 22.51, 14.0 ppm; IR (KBr, cm^{-1}): 2973, 2817, 1613, 1564, 1359, 1157, 776, 593; HRMS (ESI^+) calcd for $[C_{13}H_{17}ClNO_3S]^+$: 302.0612, found 302.0615.

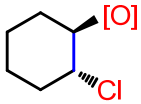


9.26 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.3 Hz, 1 H), 7.76 (m, 3 H), 4.77 (dd, *J* = 11.6, 4.3 Hz, 1 H), 4.65 (dd, *J* = 11.6, 7.3 Hz, 1 H), 4.29 (m, 1 H), 1.94-1.76 (m, 2 H), 1.61-1.54 (m, 1 H), 1.48-1.33 (m, 3 H), 0.95 (t, *J* = 7.2 Hz, 3 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1, 143.8, 134.5, 133.7, 126.7, 123.6, 122.2, 74.5, 58.2, 34.3, 28.3, 22.3, 14.0 ppm; IR (KBr, cm^{-1}): 2923, 2877, 1635, 1549, 1421, 1347, 1156, 772; HRMS (ESI^+) calcd for $[C_{13}H_{17}ClNO_3S]^+$: 302.0612, found 302.0607.

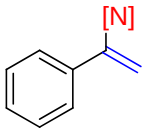


^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10-8.01 (m, 1 H), 7.93-7.77 (m, 3 H), 4.73 (m, 1 H), 4.18 (s, 1 H), 2.43 (m, 1 H), 2.29-2.15 (m, 2 H), 1.94-1.68 (m, 3 H), 1.45 (m, 2 H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9, 137.9, 134.8, 134.4, 127.4, 125.4, 120.9, 60.3, 58.6, 37.5, 31.1, 25.8, 25.5 ppm; IR (KBr, cm^{-1}): 2948, 2865, 1614, 1557, 1340, 1363, 1335, 1175, 771, 614; HRMS (ESI^+) calcd for $[C_{13}H_{15}ClNO_3S]^+$: 300.0456, found 300.0454.



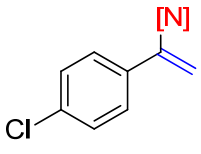
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 6.8, 1.7 Hz, 1 H), 7.82-7.66 (m, 3 H), 5.15 (m, 1 H), 4.10 (m, 1 H), 2.56-2.45 (m, 1 H), 2.39-2.28 (m, 1 H), 1.91-1.72 (m, 3 H), 1.46 (m, 3 H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.6, 143.7, 134.3, 133.6, 127.2, 123.6, 122.1, 84.4, 59.8, 34.9, 30.2, 24.6, 23.3 ppm; IR (KBr, cm^{-1}): 2956,

2874, 1599, 1370, 1332, 1153, 879, 773, 592; HRMS (ESI^+) calcd for $[C_{13}H_{15}ClNO_3S]^+$: 300.0456, found 300.0452.



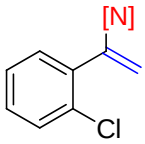
68% yield.

^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.6 Hz, 1 H), 8.01 (d, *J* = 7.6 Hz, 1 H), 7.96 -7.89 (m, 1 H), 7.86 (dd, *J* = 7.9, 7.1 Hz, 1 H), 7.55-7.47 (m, 2 H), 7.40-7.32 (m, 3 H), 6.02 (s, 1 H), 5.84 (s, 1 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 138.3, 136.1, 135.3, 135.0, 134.6, 129.5, 128.9, 126.9, 126.2, 125.8, 121.4, 118.4 ppm; IR (KBr, cm^{-1}): 2921, 2849, 1736, 1627, 1338, 1307, 1185, 1168, 583; HRMS (ESI^+) calcd for $[C_{15}H_{12}NO_3S]^+$: 286.0532, found 286.0534.



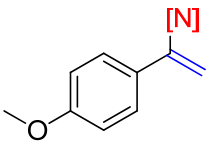
57% yield.

^1H NMR (400 MHz, $CDCl_3$) δ 8.11-8.05 (m, 1 H), 8.00 (d, *J* = 7.5 Hz, 1 H), 7.89 (m, 2 H), 7.49-7.41 (m, 2 H), 7.37-7.29 (m, 2 H), 6.00 (d, *J* = 1.2 Hz, 1 H), 5.84 (d, *J* = 1.2 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 158.0, 138.1, 135.4, 135.4, 135.0, 134.6, 133.6, 129.1, 127.5, 126.7, 125.8, 121.4, 118.9, ppm; IR (KBr, cm^{-1}): 2925, 2853, 1738, 1628, 1595, 1340, 1312, 1186, 1012, 751; HRMS (ESI^+) calcd for $[C_{15}H_{11}ClNO_3S]^+$: 320.0143, found 320.0140.



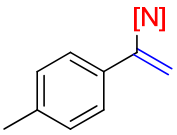
62% yield.

^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.6 Hz, 1 H), 8.01 (d, *J* = 7.6 Hz, 1 H), 7.96 7.89 (m, 1 H), 7.86 (dd, *J* = 7.9, 7.1 Hz, 1 H), 7.557.47 (m, 2 H), 7.407.32 (m, 3 H), 6.02 (s, 1 H), 5.84 (s, 1 H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 157.4, 137.8, 135.2, 134.58, 134.1, 133.2, 133.0, 130.6, 130.3, 130.3, 127.1, 126.7, 125.7, 121.2, 119.9 ppm; IR (KBr, cm^{-1}): 2919, 2849, 1737, 1342, 1306, 1184, 749, 581; HRMS (ESI^+) calcd for $[C_{15}H_{11}ClNO_3S]^+$: 320.0143, found 320.0144.



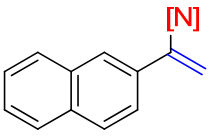
65% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.5 Hz, 1 H), 8.00 (d, *J* = 7.6 Hz, 1 H), 7.92 (td, *J* = 7.6, 1.0 Hz, 1 H), 7.85 (td, *J* = 7.5, 0.9 Hz, 1 H), 7.48-7.37 (m, 2 H), 6.95-6.80 (m, 2 H), 5.91 (d, *J* = 0.6 Hz, 1 H), 5.71 (d, *J* = 0.6 Hz, 1H), 3.80 (s, 3H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 160.6, 158.1, 138.3, 135.5, 135.2, 134.5, 127.6, 127.5, 126.9, 125.7, 121.4, 116.5, 114.2, 55.4 ppm; IR (KBr, cm^{-1}): 2931, 2840, 1737, 1608, 1513, 1339, 1307, 1254, 1185, 1029, 836, 752, 584; HRMS (ESI^+) calcd for $[C_{16}H_{14}NO_4S]^+$: 316.0638, found 316.0641.



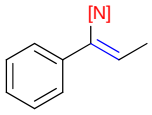
68% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.4 Hz, 1 H), 7.99 (d, *J* = 7.6 Hz, 1 H), 7.87 (m, 2 H), 7.40 (d, *J* = 8.2 Hz, 2 H), 7.17 (d, *J* = 8.0 Hz, 2 H), 5.98 (d, *J* = 0.7 Hz, 1 H), 5.78 (d, *J* = 0.7 Hz, 1 H), 2.35 (s, 3H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 158.0, 139.5, 138.2, 135.9, 135.2, 134.5, 132.1, 129.5, 126.8, 126.0, 125.7, 121.3, 117.3, 21.32 ppm; IR (KBr, cm^{-1}): 2922, 2861, 1739, 1628, 1463, 1340, 1308, 1185, 823, 751, 585; HRMS (ESI^+) calcd for $[C_{16}H_{14}NO_3S]^+$: 300.0689, found 300.0685.



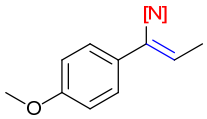
65% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.6 Hz, 1 H), 8.02 (d, *J* = 7.6 Hz, 1 H), 7.97-7.88 (m, 2 H), 7.84 (dd, *J* = 15.7, 7.2 Hz, 4 H), 7.64 (dd, *J* = 8.6, 1.7 Hz, 1 H), 7.54-7.42 (m, 2 H), 6.16 (s, 1 H), 5.93 (s, 1 H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 158.1, 138.3, 136.2, 136.1, 135.3, 134.6, 133.8, 133.2, 132.4, 128.8, 128.7, 127.8, 126.9, 126.6, 125.9, 125.8, 123.5, 121.4, 118.8 ppm; IR (KBr, cm^{-1}): 2925, 2854, 1736, 1339, 1308, 1185, 750, 584; HRMS (ESI^+) calcd for $[C_{19}H_{14}NO_3S]^+$: 336.0689, found 336.0693.



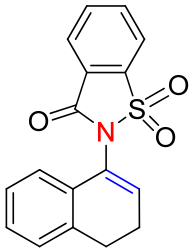
57% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.11 (m, 1 H), 7.99 (d, *J* = 7.2 Hz, 1 H), 7.91 (m, 2 H), 7.48 (dd, *J* = 8.1, 1.4 Hz, 2 H), 7.37-7.28 (m, 3 H), 6.74 (q, J = 7.1 Hz, 1 H), 1.92 (d, J = 7.1 Hz, 3 H). ppm; ^{13}C NMR (101 MHz, CDCl3) δ 158.3, 138.6, 135.8, 135.2, 134.6, 132.9, 128.7, 128.6, 128.5, 127.1, 125.9, 125.8, 121.3, 15.0 ppm; IR (KBr, cm^{-1}): 2921, 2849, 1731, 1340, 1187, 751, 583; HRMS (ESI^+) calcd for $[C_{17}H_{16}NO_3S]^+$: 300.0689, found 300.0693.



62% yield.

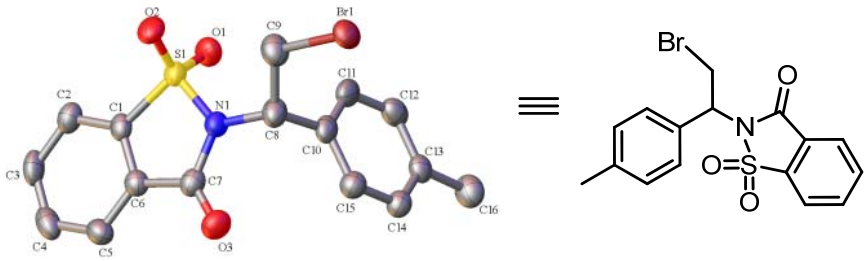
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.11 (m, 1 H), 7.99 (d, *J* = 7.2 Hz, 1 H), 7.91 (m, 2 H), 7.48 (dd, *J* = 8.1, 1.4 Hz, 2 H), 7.37-7.28 (m, 3 H), 6.74 (q, *J* = 7.1 Hz, 1 H), 1.92 (d, *J* = 7.1 Hz, 3 H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ 159.6, 158.2, 138.1, 135.0, 134.4, 130.7, 130.6, 128.4, 127.1, 126.7, 125.5, 121.3, 113.8, 55.3, 14.9 ppm; IR (KBr, cm^{-1}): 2936, 2839, 1737, 1608, 1513, 1336, 1185, 1040, 842, 751; HRMS (ESI^+) calcd for $[C_{17}H_{16}NO_4S]^+$: 330.0795, found 330.0792.



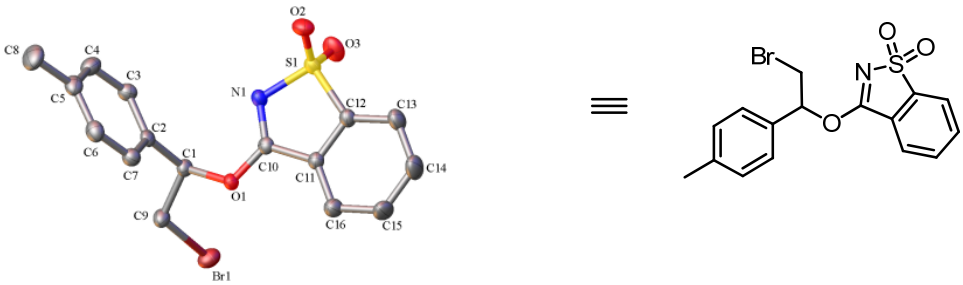
51% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.09 (m, 1 H), 7.98 (d, *J* = 7.4 Hz, 1 H), 7.94-7.81 (m, 2 H), 7.22-7.11 (m, 3 H), 7.06 (d, *J* = 7.5 Hz, 1 H), 6.51 (t, *J* = 4.7 Hz, 1 H), 2.96 (s, 2 H), 2.61 (td, *J* = 8.2, 4.7 Hz, 2 H) ppm; ^{13}C NMR (101 MHz, CDCl3) δ158.3, 138.2, 136.1, 135.2, 134.5, 134.3, 130.3, 128.6, 128.0, 127.0, 126.9, 126.8, 125.7, 122.6, 121.3, 27.0, 23.5 ppm; IR (KBr, cm^{-1}): 2941, 2887, 2832, 1739, 1340, 1305, 1185, 751, 584; HRMS (ESI^+) calcd for $[C_{17}H_{14}NO_3S]^+$: 312.0689, found 312.0686.

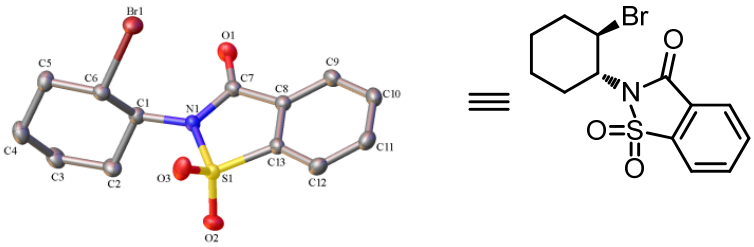
X-ray crystal structure:



Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1430133. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

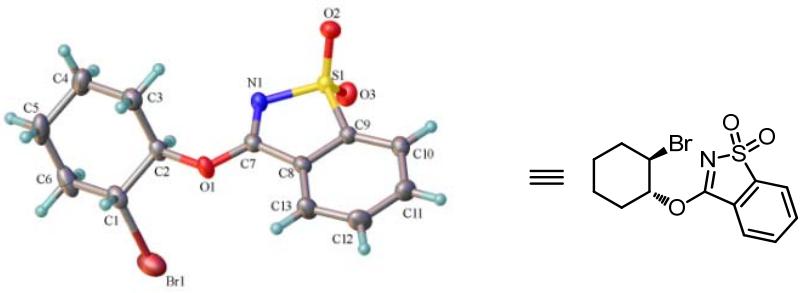


Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1442748. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

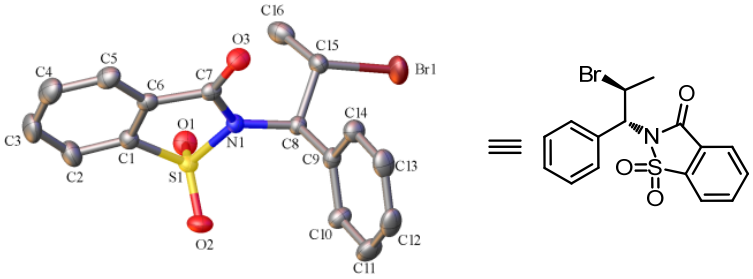


Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no.

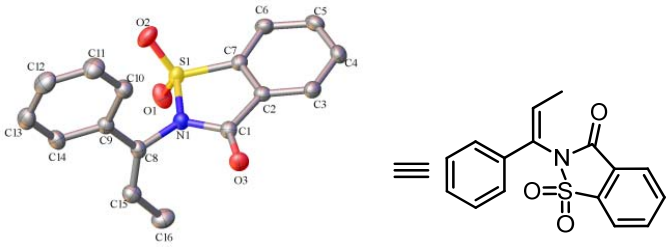
CCDC-1430132. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).



Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1430129. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

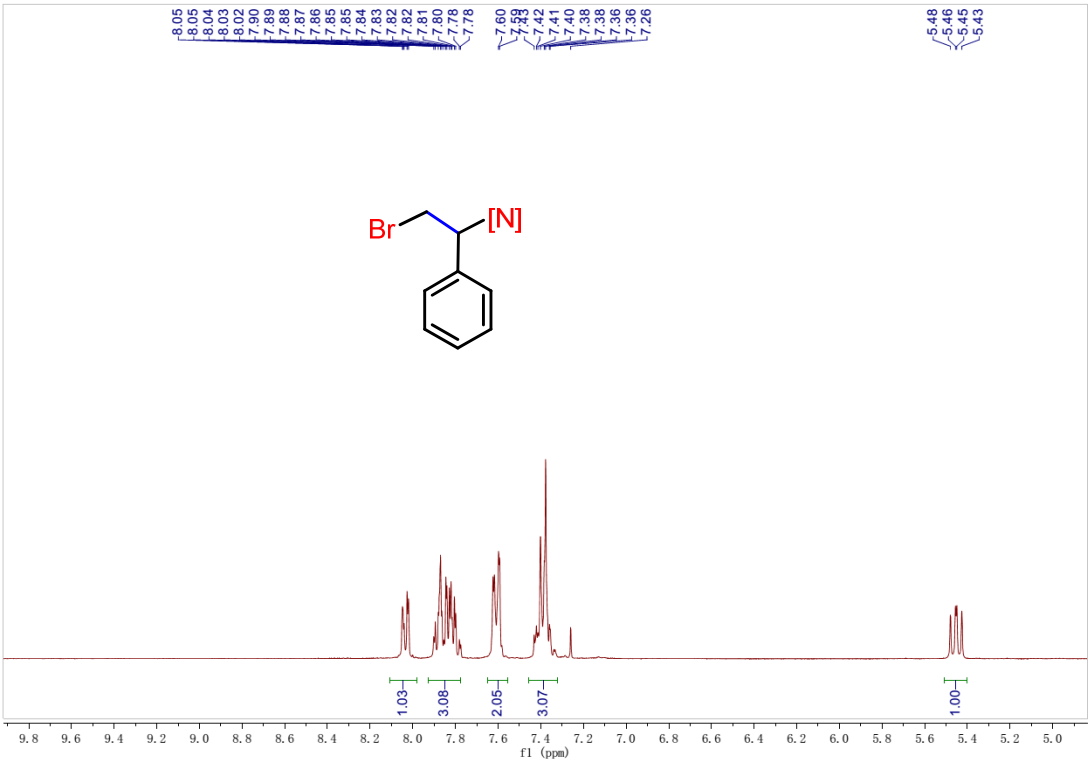


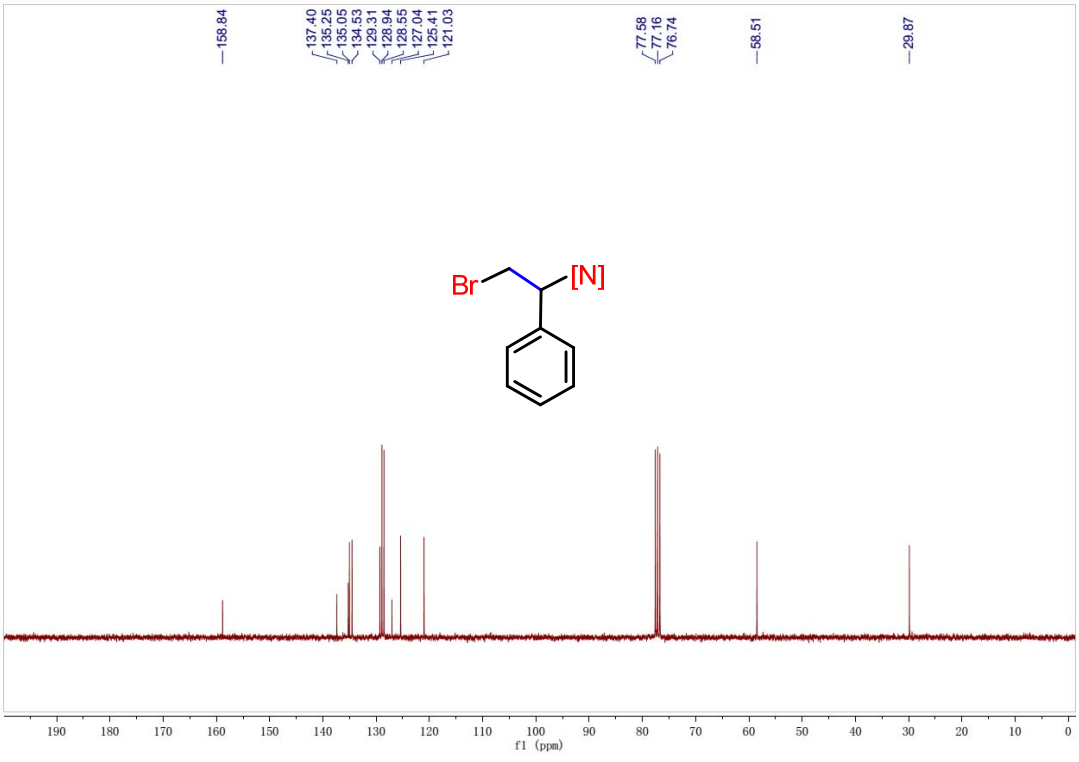
Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1430134. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).



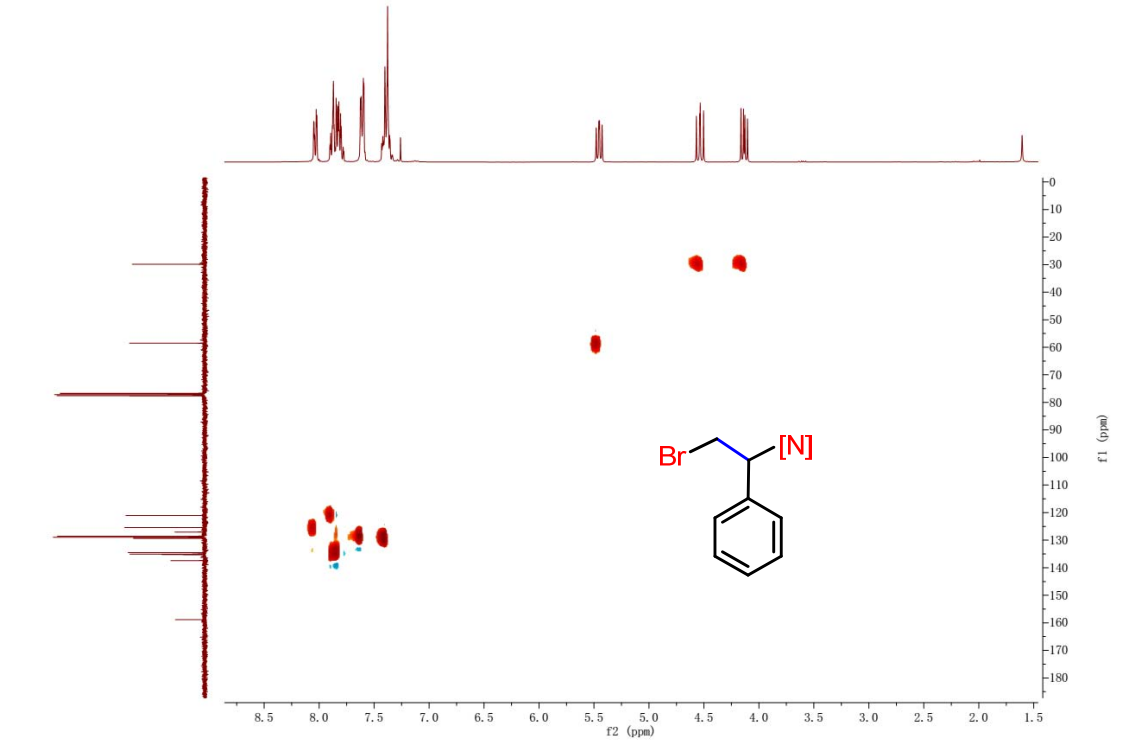
Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1442630. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

NMR Spectra:

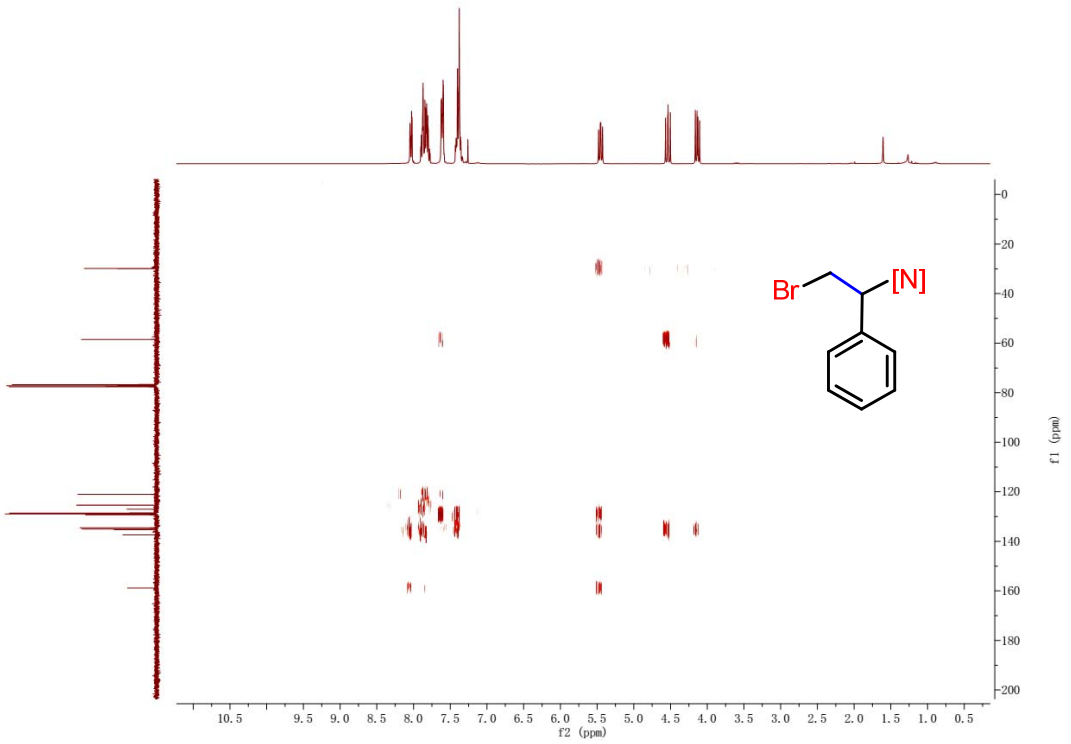

8.05
8.05
8.04
8.03
8.02
7.90
7.89
7.88
7.87
7.86
7.85
7.85
7.84
7.83
7.82
7.82
7.81
7.80
7.78
7.78
7.60
7.59
7.43
7.42
7.41
7.40
7.38
7.38
7.36
7.36
7.26
5.48
5.46
5.45
5.43
Br
[N]
1.03
3.08
2.05
3.07
1.00
9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0
f1 (ppm)

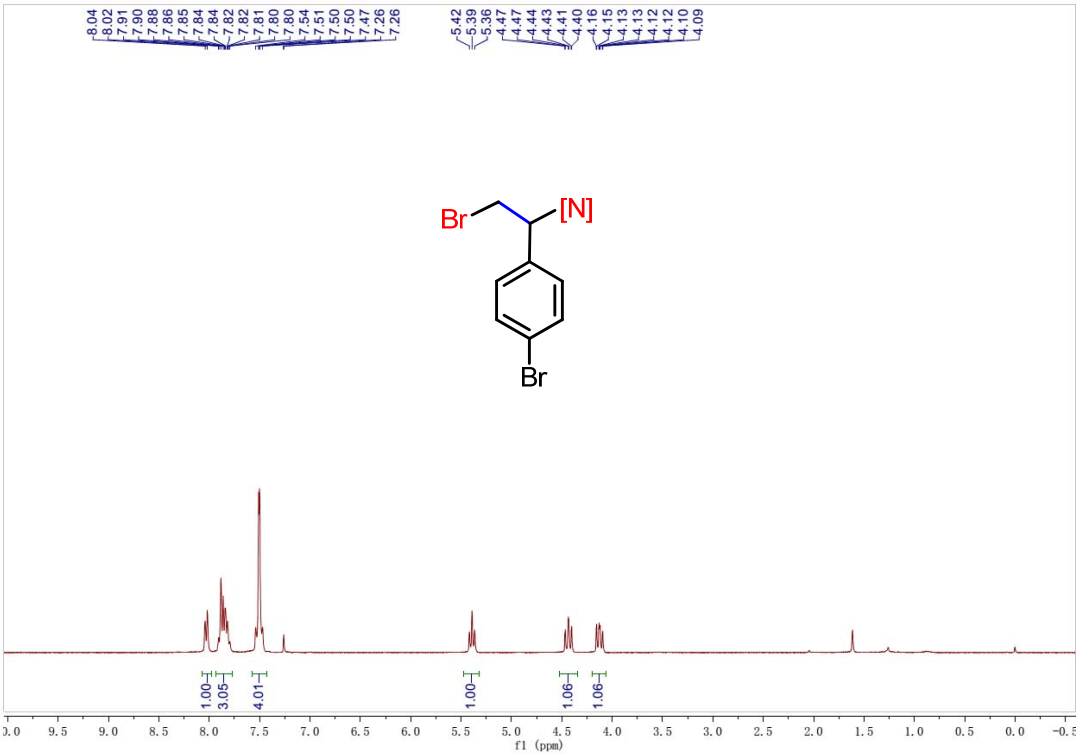

158.84
137.40
135.25
135.05
134.53
129.31
128.94
128.55
127.04
125.41
121.03
77.58
77.16
76.74
58.51
29.87
Br
[N]
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

HSQC:



HMBC:




8.04
8.02
7.91
7.90
7.88
7.86
7.85
7.84
7.84
7.82
7.82
7.81
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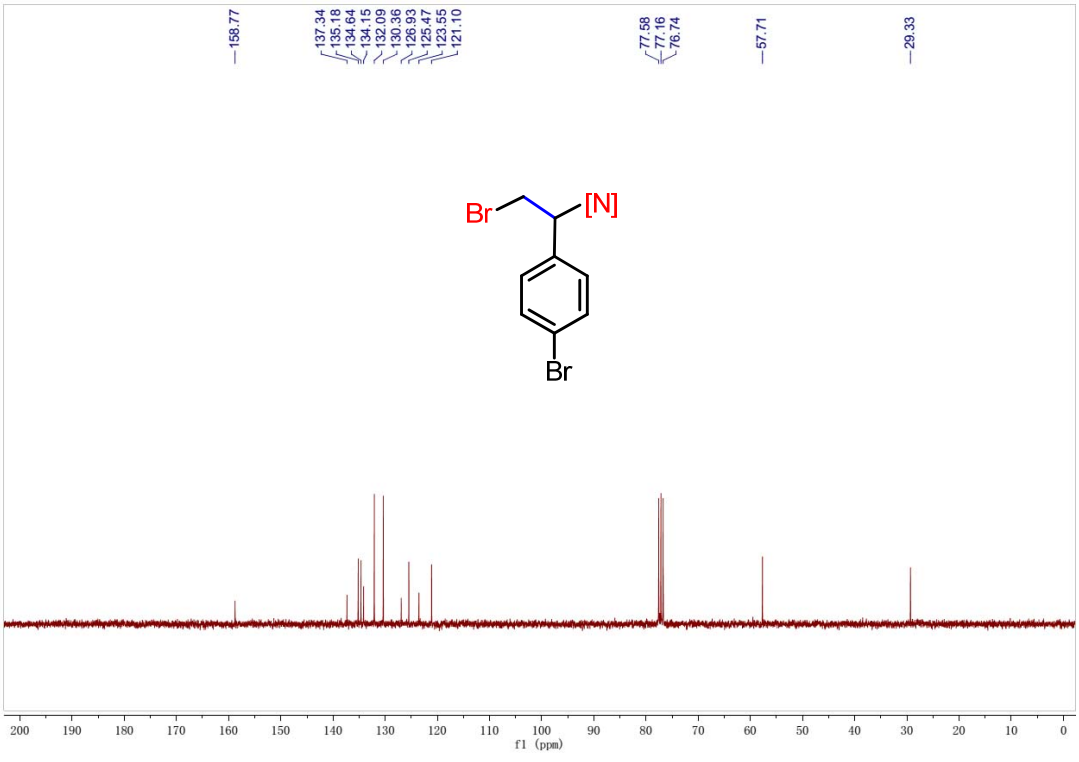
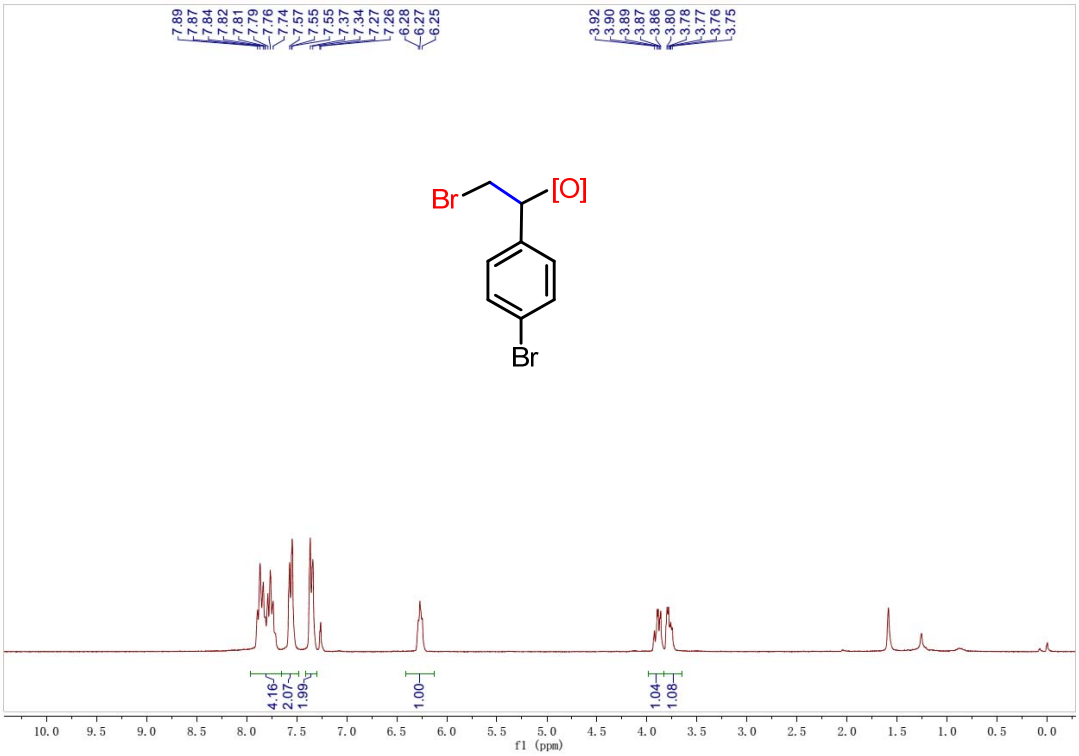
7.80
7.54
7.51
7.50
7.50
7.47
7.26
7.26
5.42
5.39
5.36
4.47
4.44
4.43
4.41
4.40
4.16
4.15
4.13
4.12
4.12
4.10
4.09
Br
[N]
Br
1.00
3.05
4.01
1.00
1.06
1.06
f1 (ppm)


158.77
137.34
135.18
134.64
134.15
132.09
130.36
126.93
125.47
123.55
121.10
77.58
77.16
76.74
57.71
29.33
Br
[N]
Br
f1 (ppm)


7.89
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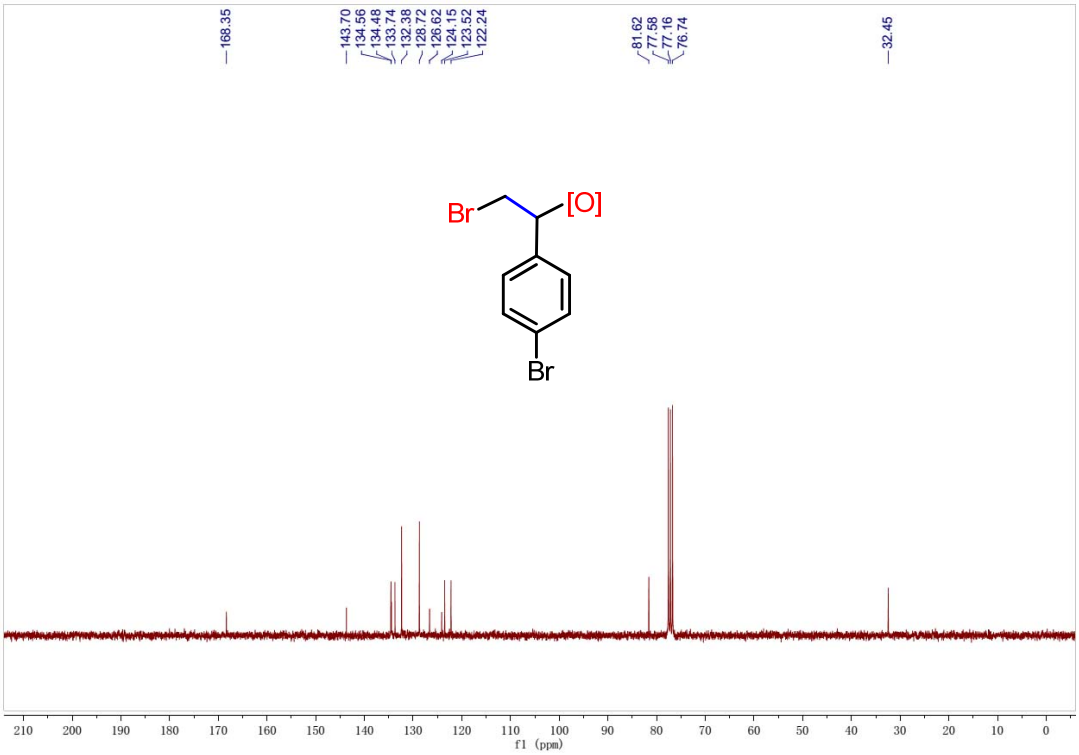
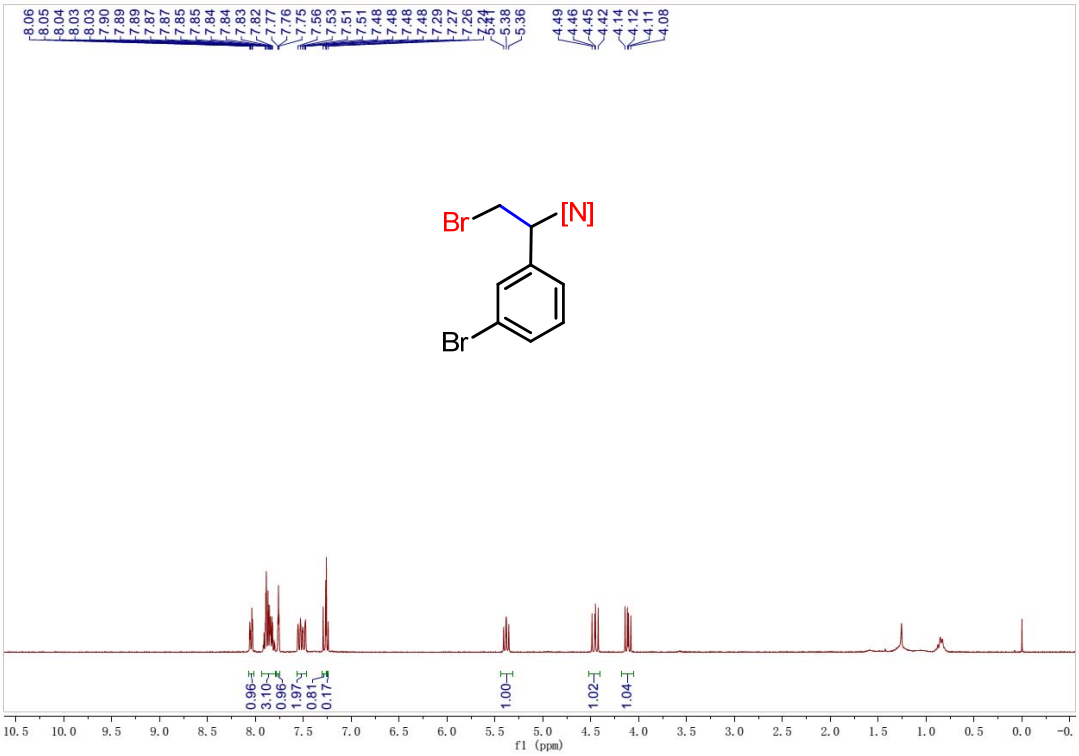
7.84
7.82
7.81
7.79
7.76
7.74
7.57
7.55
7.55
7.37
7.34
7.27
7.26
6.28
6.27
6.25
3.92
3.90
3.89
3.87
3.86
3.80
3.78
3.77
3.76
3.75
Br
[O]
Br
4.16
2.07
1.99
1.00
1.04
1.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.35
143.70
134.56
134.48
133.74
132.38
128.72
126.62
124.15
123.52
122.24
81.62
77.58
77.16
76.74
32.45
Br
[O]
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.06
8.05
8.04
8.03
8.03
7.90
7.89
7.89
7.87
7.87
7.85
7.85
7.84
7.84
7.83
7.82
7.77
7.76
7.75
7.56
7.53
7.51
7.51
7.48
7.48
7.48
7.48
7.29
7.27
7.26
5.41
5.38
5.36
4.49
4.46
4.45
4.42
4.14
4.12
4.11
4.08
Br
[N]
Br
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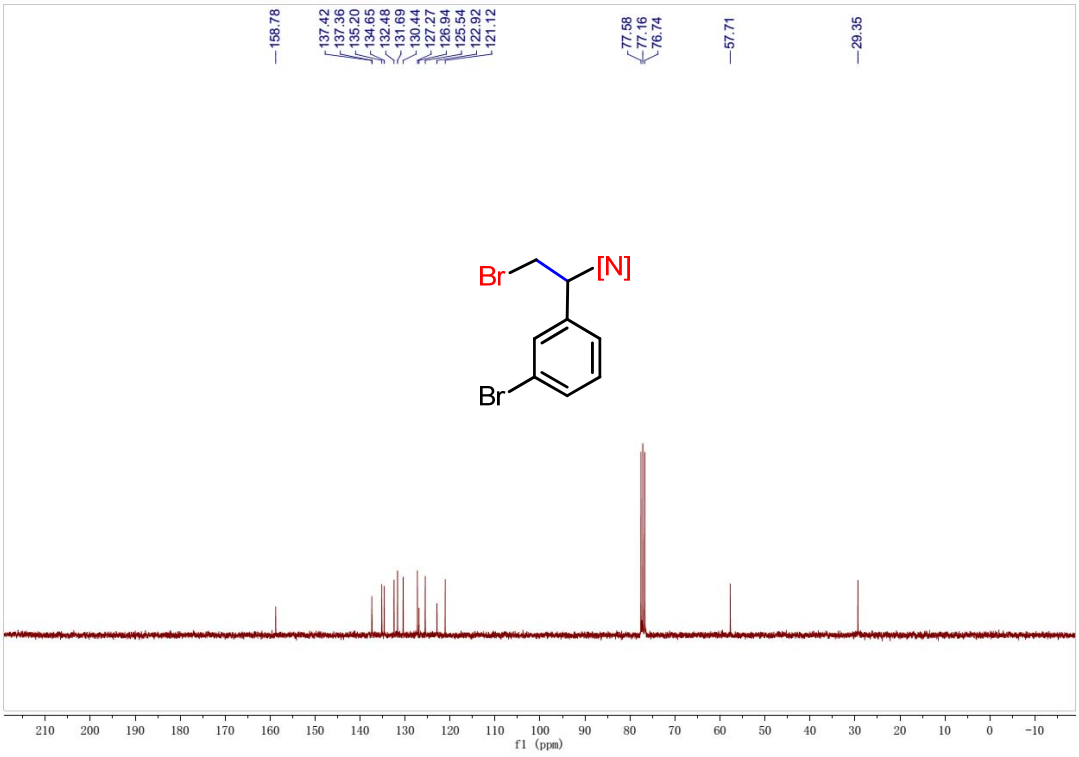
3.10
0.96
1.97
0.81
0.17
1.00
1.02
1.04
f1 (ppm)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131.69
130.44
127.27
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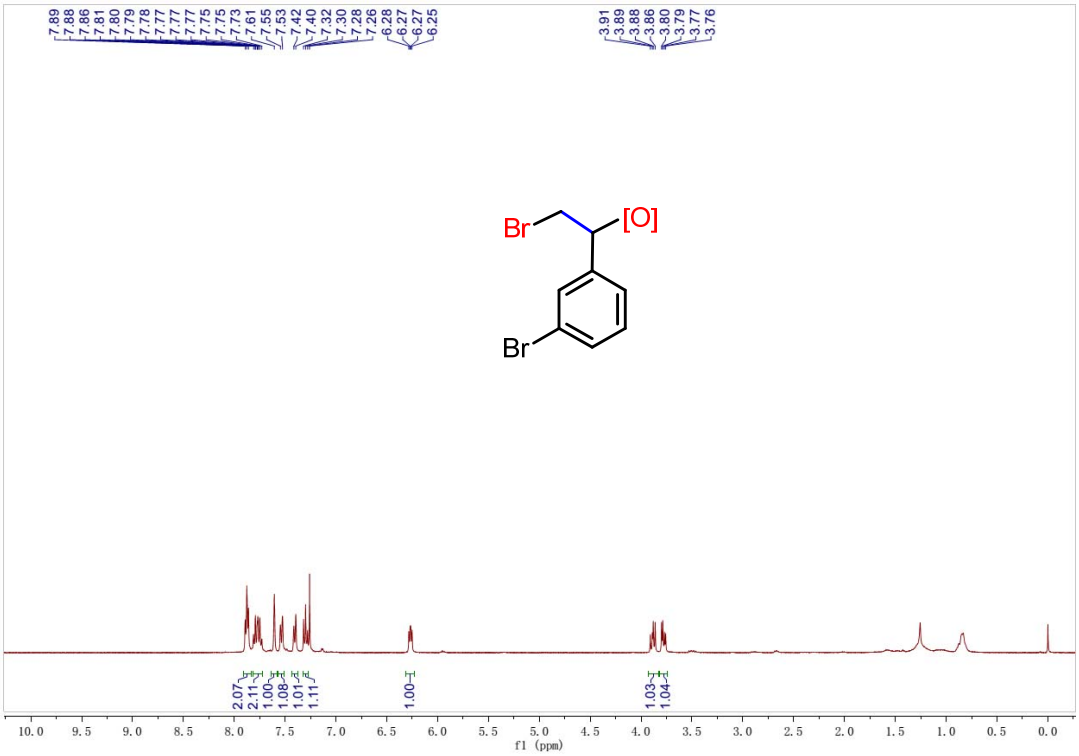
122.92
121.12
77.58
77.16
76.74
57.71
29.35
Br
[N]
Br
f1 (ppm)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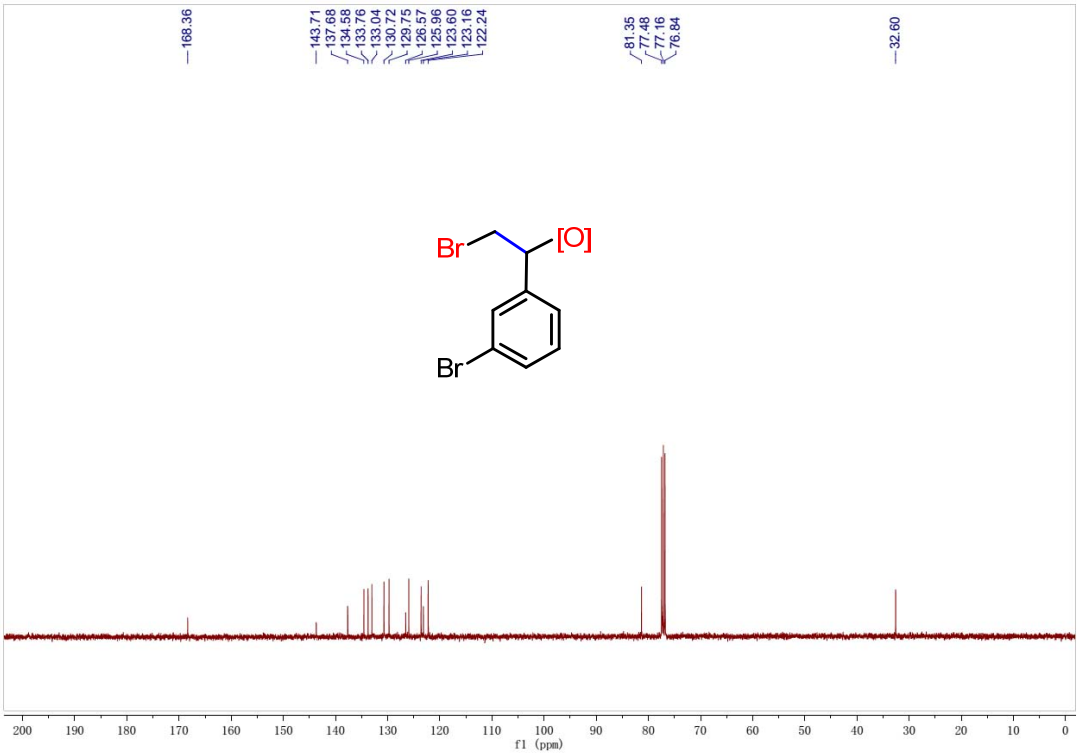
7.77
7.77
7.77
7.75
7.75
7.73
7.61
7.55
7.53
7.42
7.40
7.32
7.30
7.28
7.26
6.28
6.27
6.27
6.25
3.91
3.89
3.88
3.86
3.80
3.79
3.77
3.76
Br
[O]
Br
2.07
2.11
1.00
1.08
1.01
1.11
1.00
1.03
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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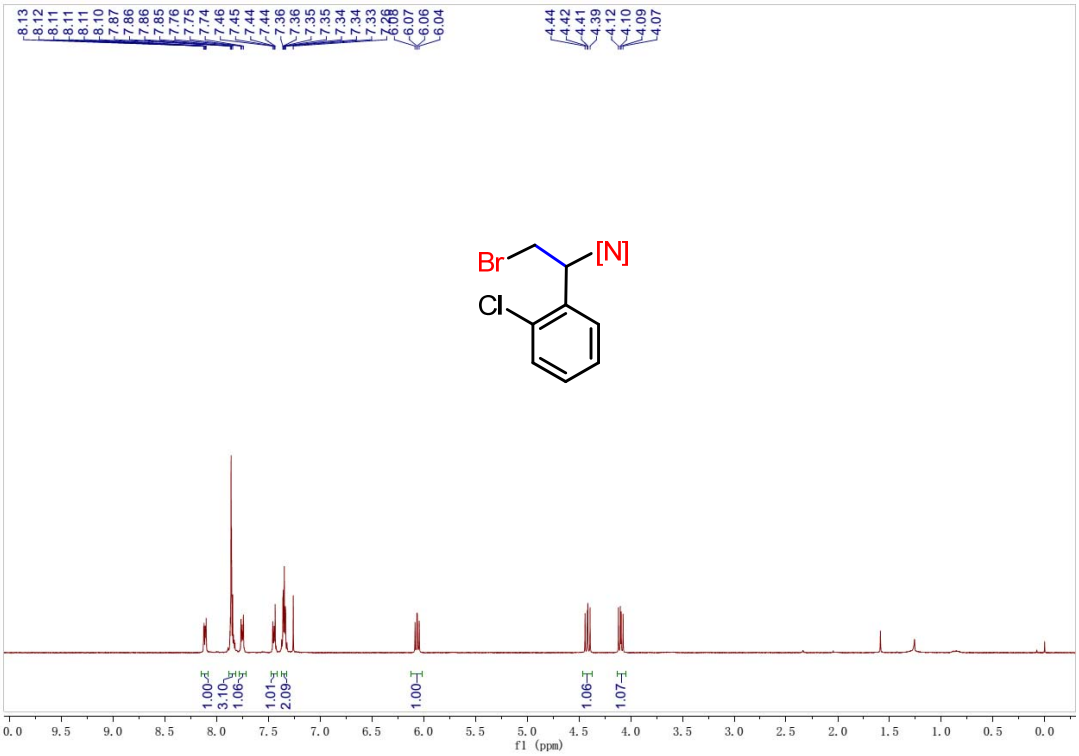
133.04
130.72
129.75
126.57
125.96
123.60
123.16
122.24
81.35
77.48
77.16
76.84
32.60
Br
[O]
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.11
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7.87
7.86
7.86
7.85
7.76
7.75
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7.46
7.45
7.44
7.44
7.36
7.36
7.35
7.35
7.34
7.34
7.33
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6.07
6.06
6.04
4.44
4.42
4.41
4.39
4.12
4.10
4.09
4.07
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Cl
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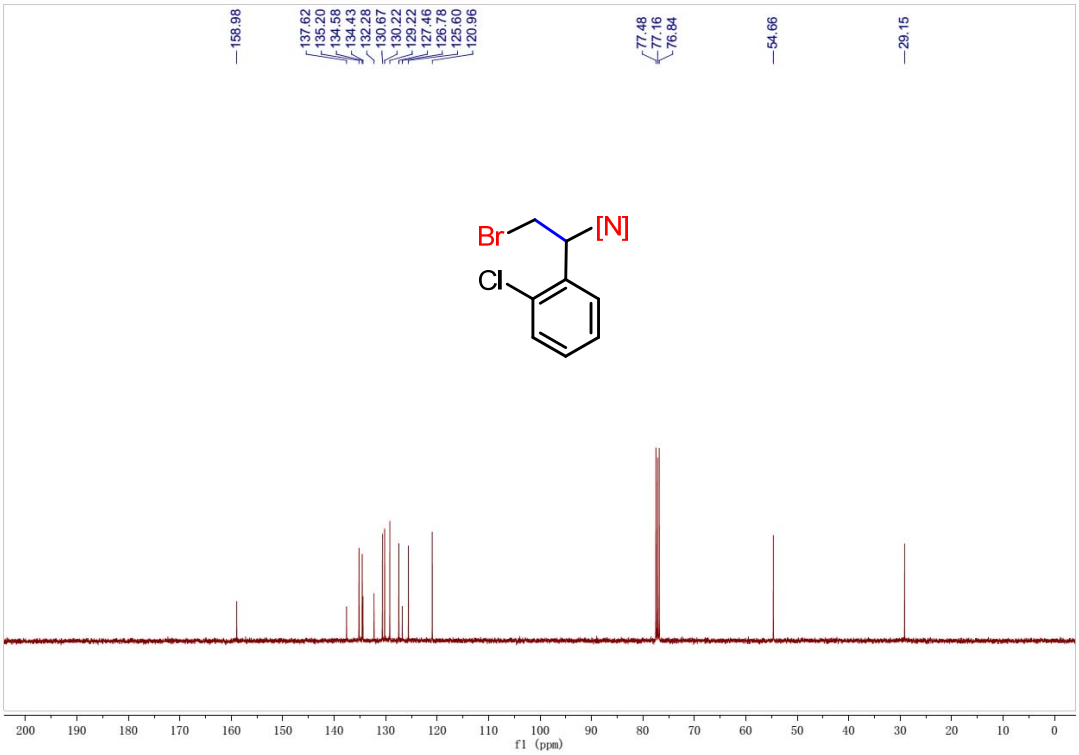
3.10
1.06
1.01
2.09
1.00
1.06
1.07
f1 (ppm)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130.22
129.22
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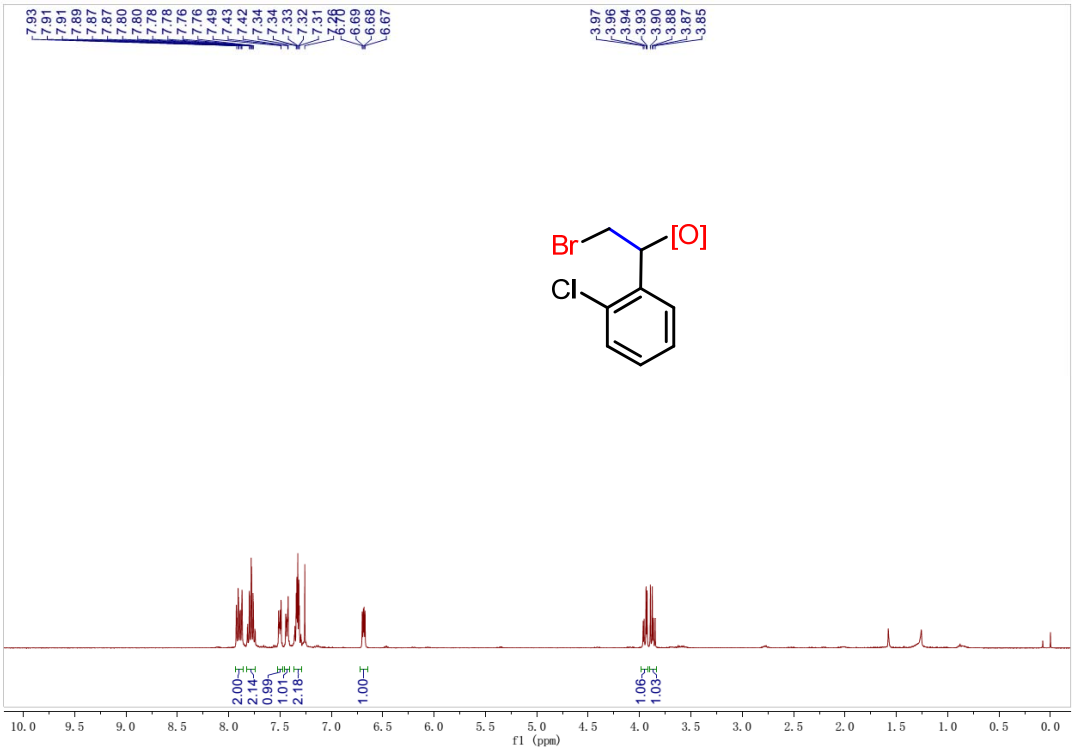
120.96
77.48
77.16
76.84
54.66
29.15
Br
[N]
Cl
f1 (ppm)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7.87
7.80
7.80
7.78
7.78
7.76
7.76
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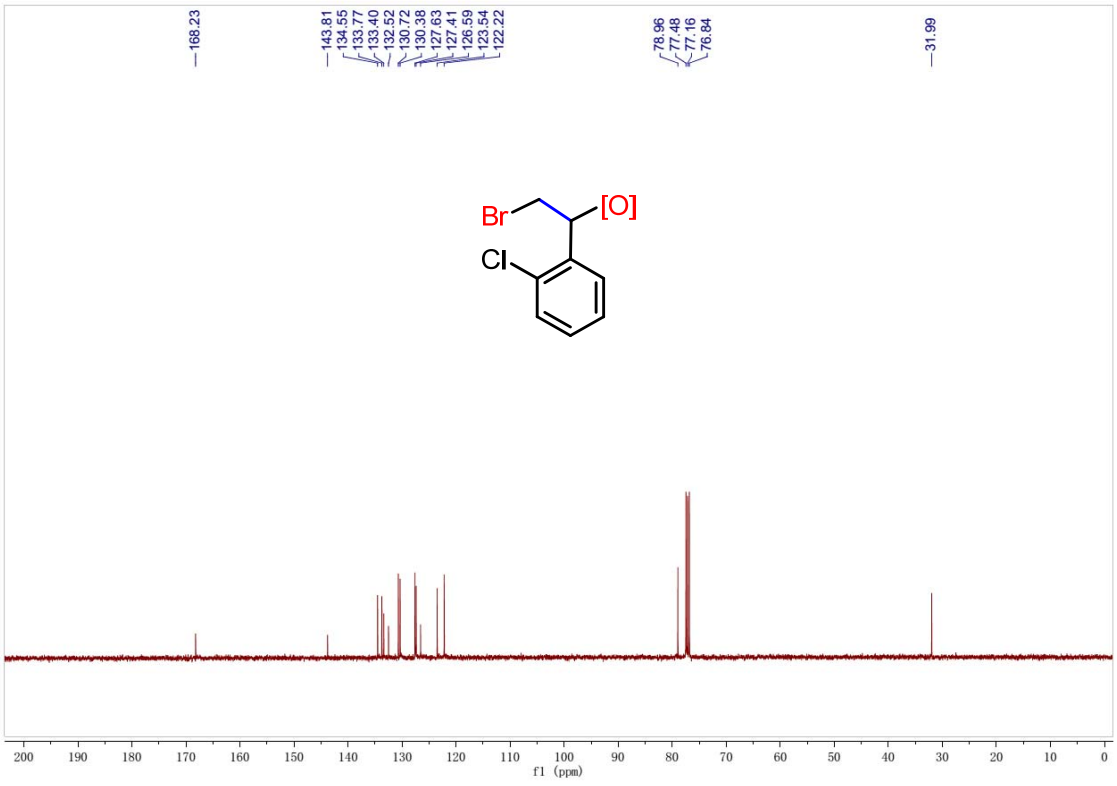
7.43
7.42
7.34
7.34
7.33
7.32
7.31
6.69
6.68
6.67
3.97
3.96
3.94
3.93
3.90
3.88
3.87
3.85
Br
[O]
Cl
2.00
2.14
0.99
1.01
2.18
1.00
1.06
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.52
130.72
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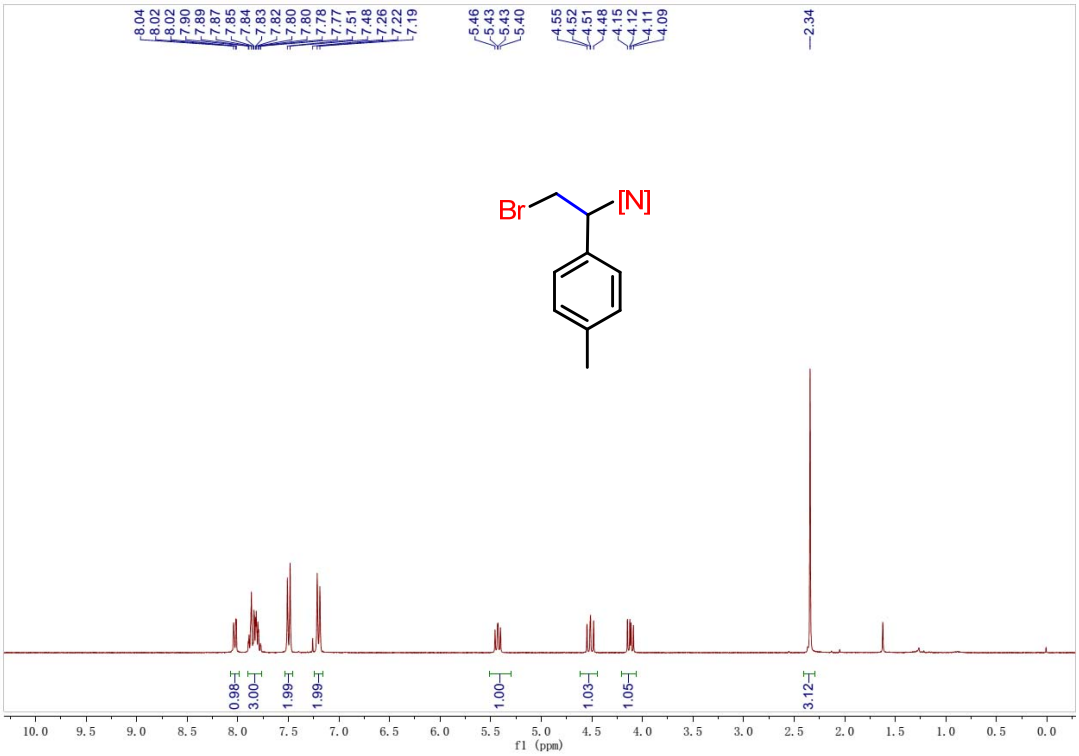
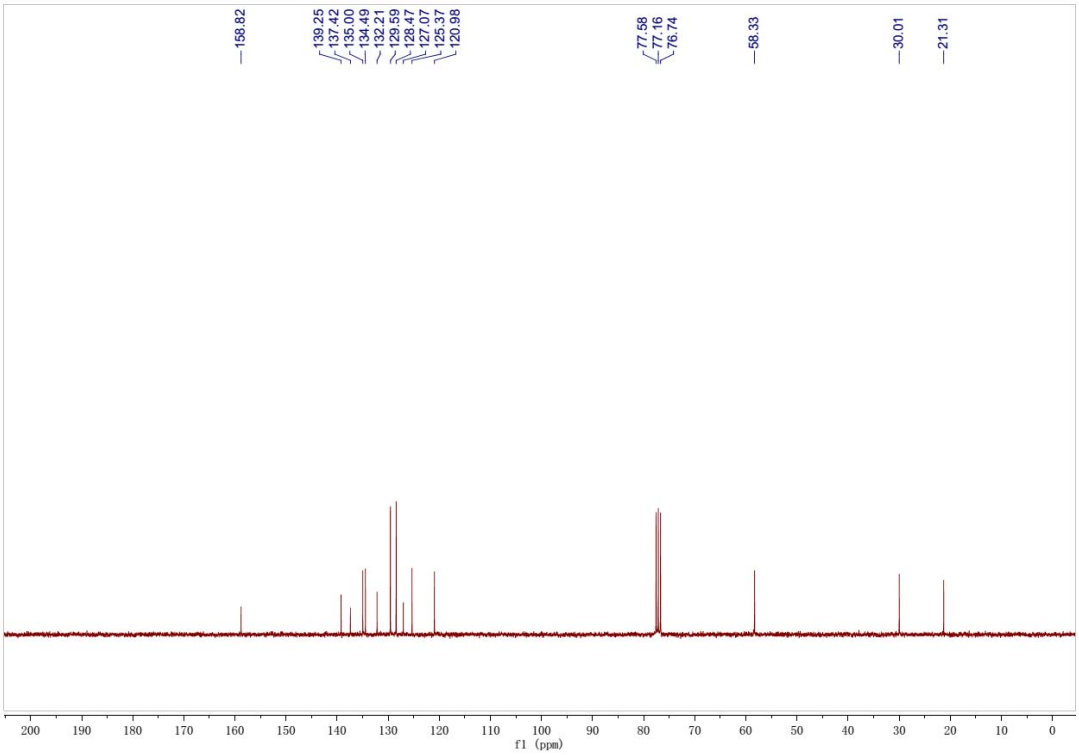
127.63
127.41
126.59
123.54
122.22
78.96
77.48
77.16
76.84
31.99
Br
[O]
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.04
8.02
8.02
7.90
7.89
7.87
7.85
7.84
7.83
7.82
7.80
7.80
7.78
7.77
7.51
7.48
7.26
7.22
7.19
5.46
5.43
5.43
5.40
4.55
4.52
4.51
4.48
4.15
4.12
4.11
4.09
2.34
Br
[N]
0.98
3.00
1.99
1.99
1.00
1.03
1.05
3.12
f1 (ppm)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134.49
132.21
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128.47
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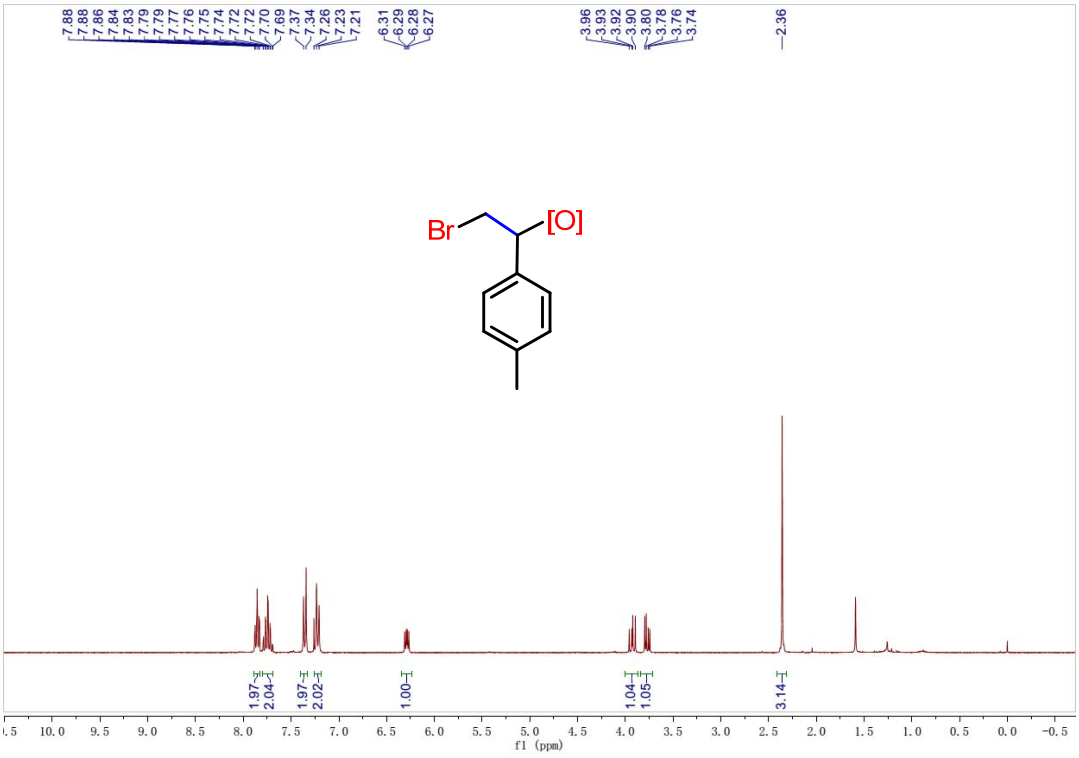
125.37
120.98
77.58
77.16
76.74
58.33
30.01
21.31
f1 (ppm)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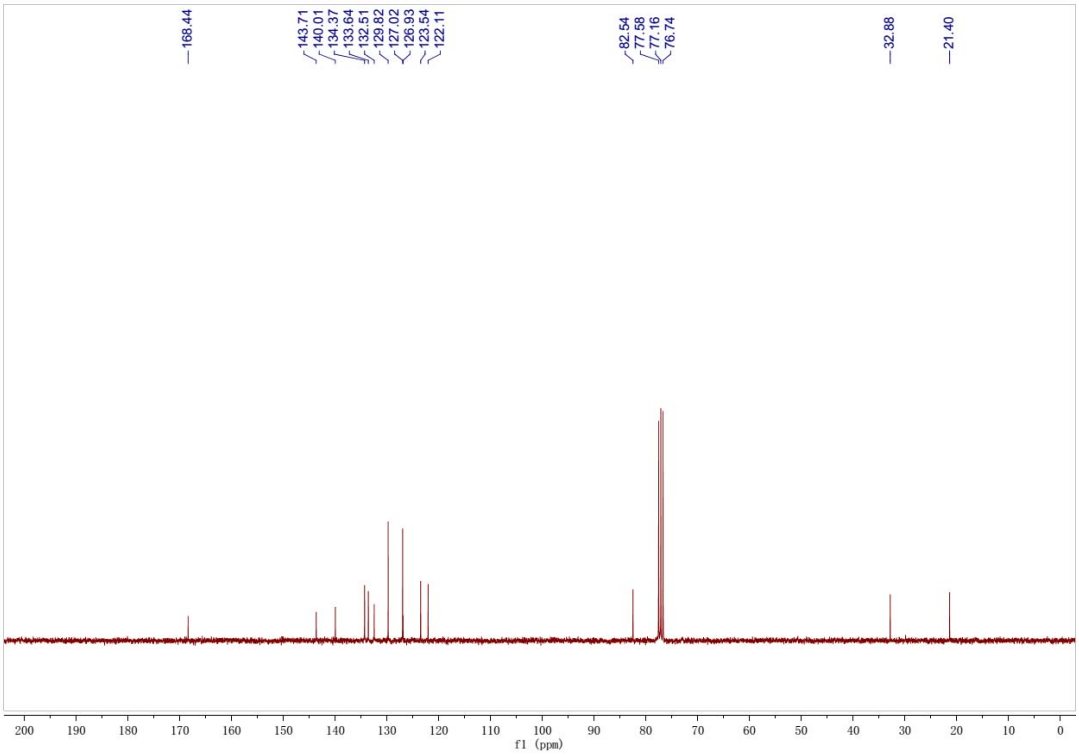
7.88
7.86
7.84
7.83
7.79
7.79
7.77
7.76
7.75
7.74
7.72
7.72
7.70
7.69
7.37
7.34
7.26
7.23
7.21
6.31
6.29
6.28
6.27
3.96
3.93
3.92
3.90
3.80
3.78
3.76
3.74
2.36
Br
[O]
1.97
2.04
1.97
2.02
1.00
1.04
1.05
3.14
f1 (ppm)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133.64
132.51
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127.02
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123.54
122.11
82.54
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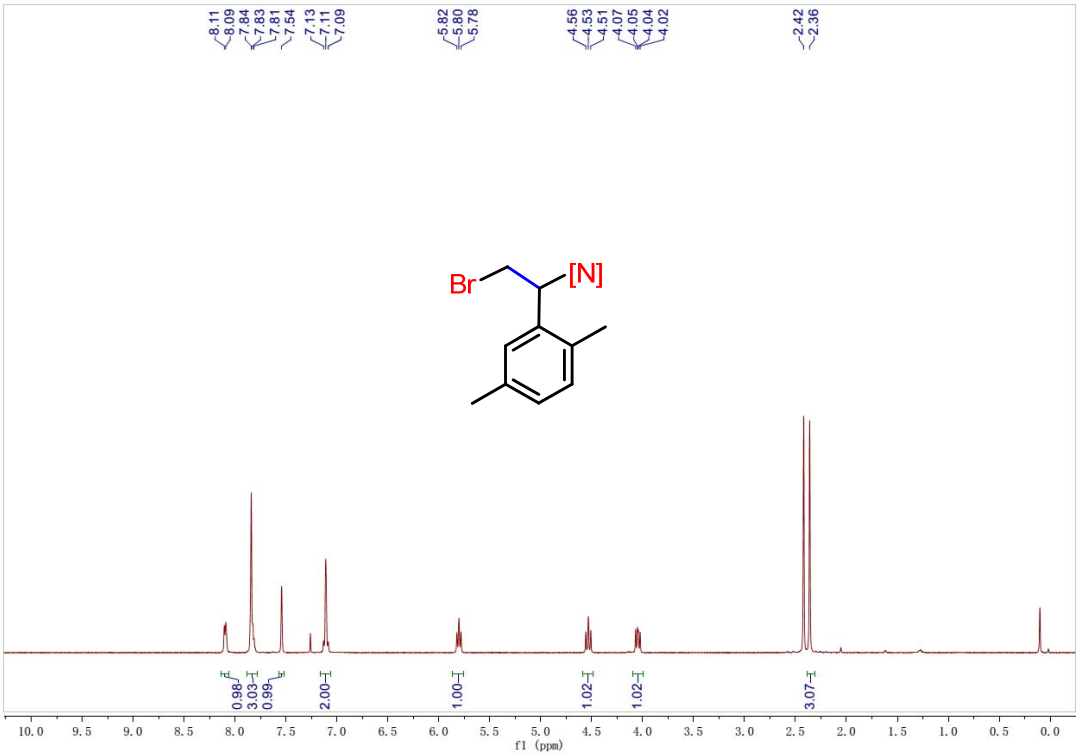
77.16
76.74
32.88
21.40
f1 (ppm)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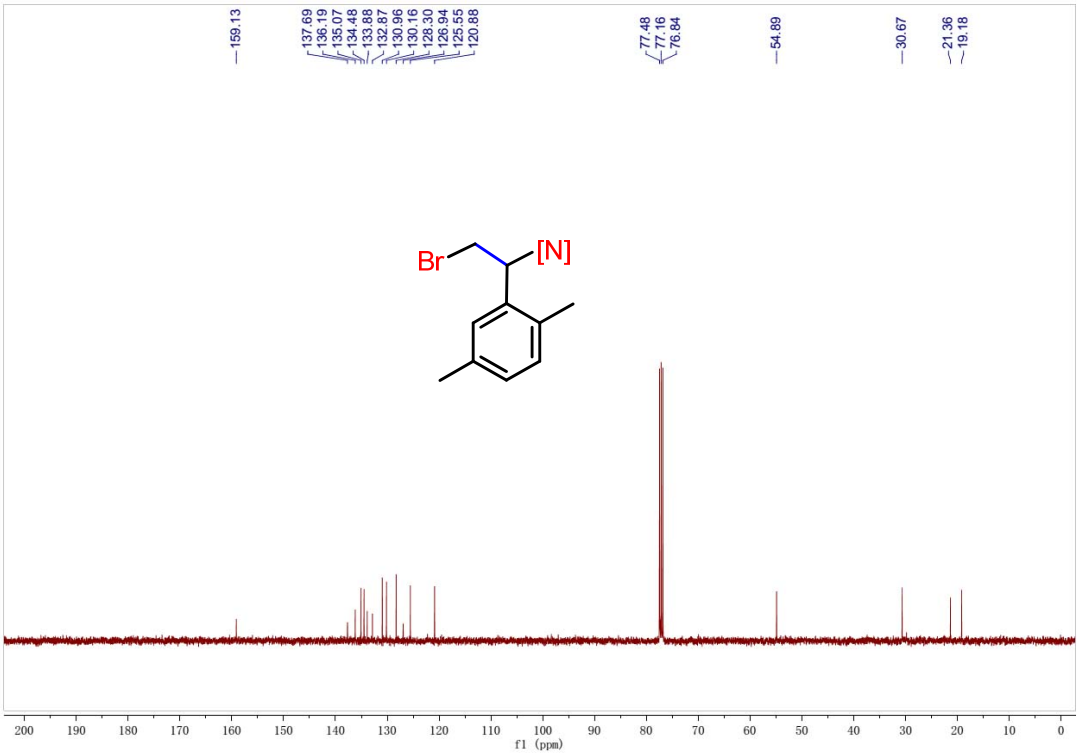
8.09
7.84
7.83
7.81
7.54
7.13
7.11
7.09
5.82
5.80
5.78
4.56
4.53
4.51
4.07
4.05
4.04
4.02
2.42
2.36
Br
[N]
0.98
3.03
0.99
2.00
1.00
1.02
1.02
3.07
f1 (ppm)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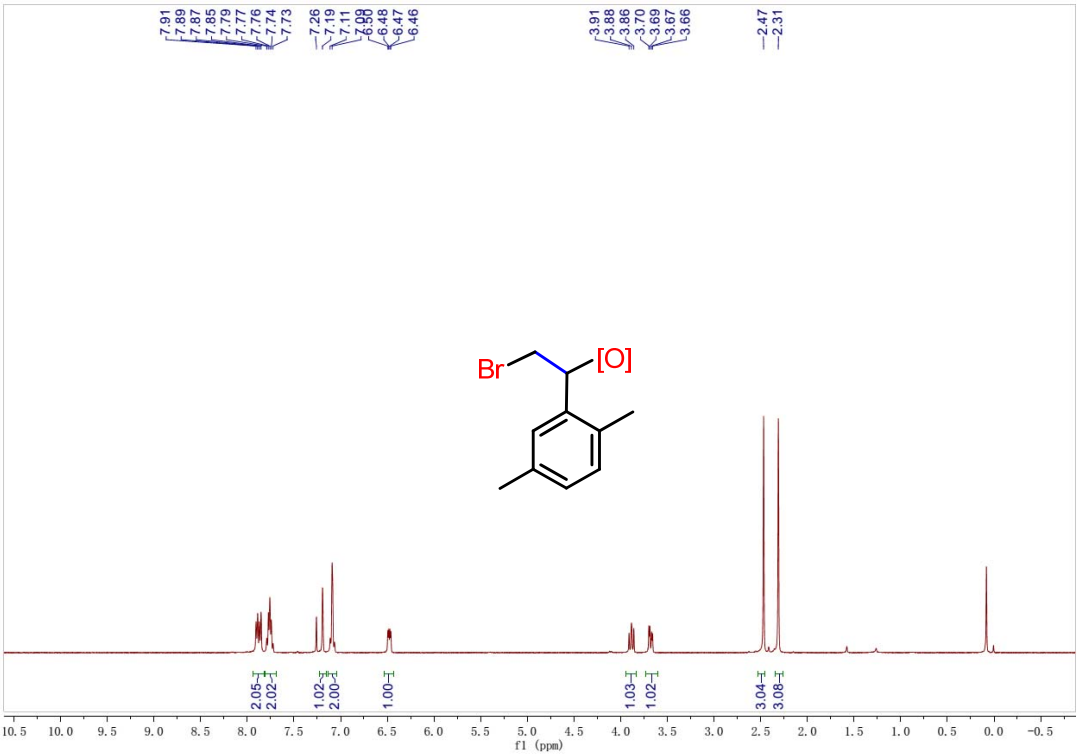
132.87
130.96
130.16
128.30
126.94
125.55
120.88
77.48
77.16
76.84
54.89
30.67
21.36
19.18
Br
[N]
f1 (ppm)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7.89
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7.85
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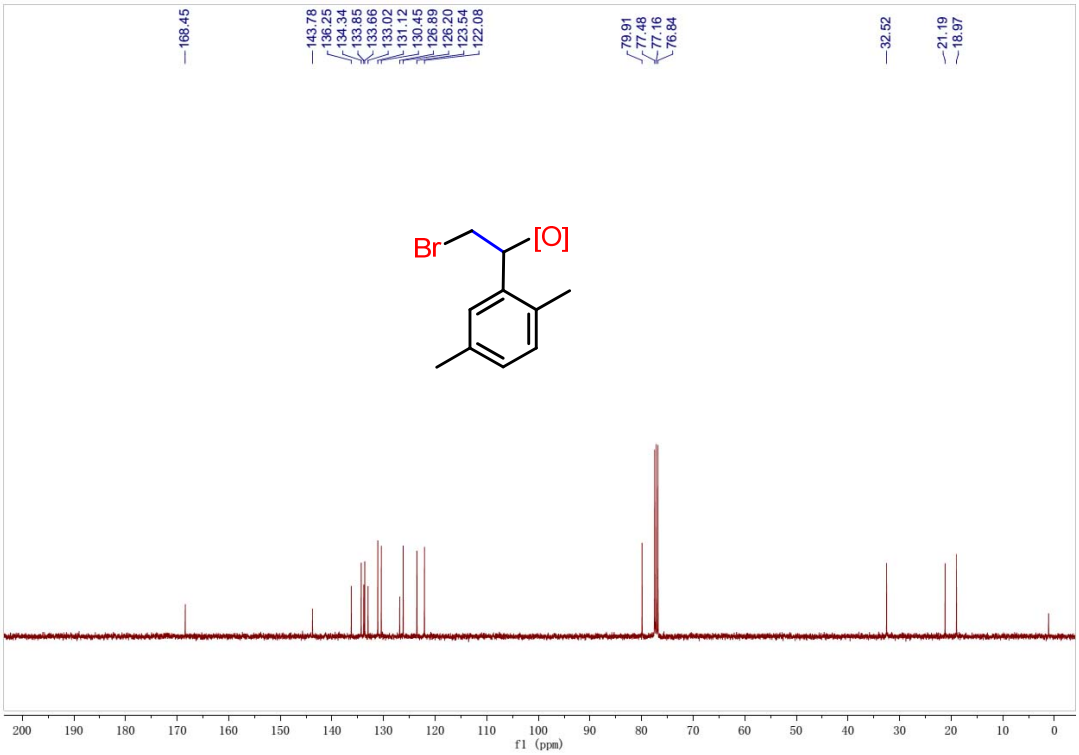
7.77
7.76
7.74
7.73
7.26
7.19
7.11
7.09
6.50
6.48
6.47
6.46
3.91
3.88
3.86
3.70
3.69
3.67
3.66
2.47
2.31
Br
[O]
2.05
2.02
1.02
2.00
1.00
1.03
1.02
3.04
3.08
f1 (ppm)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134.34
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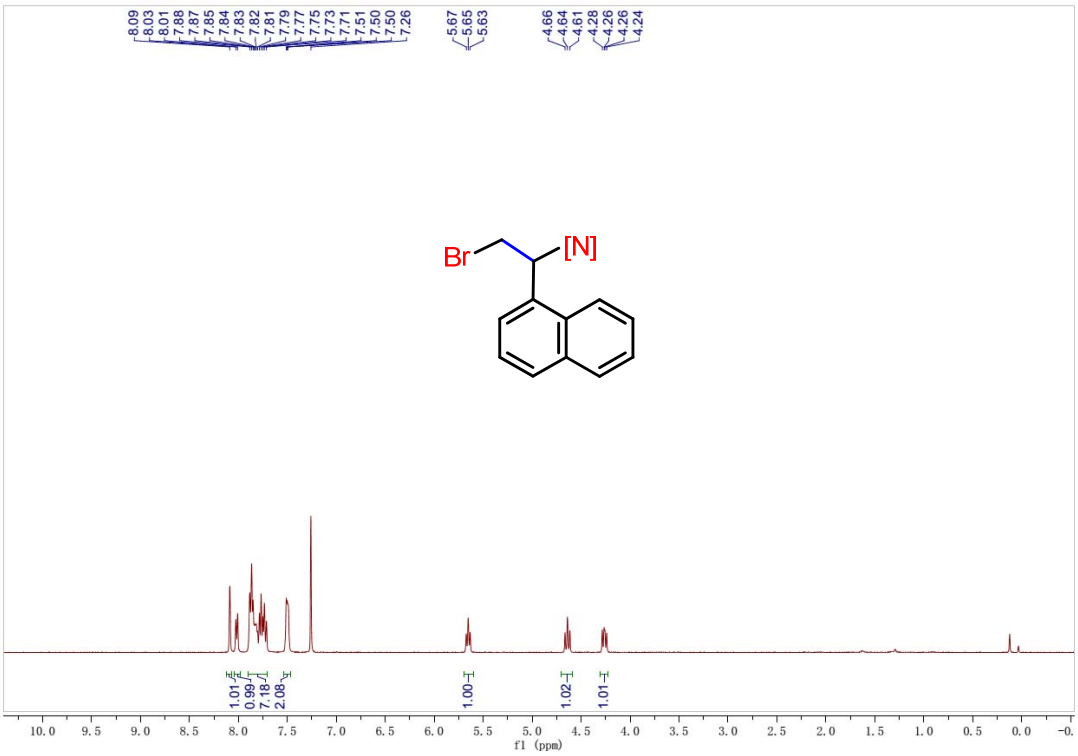
133.66
133.02
131.12
130.45
128.89
126.20
123.54
122.08
79.91
77.48
77.16
76.84
32.52
21.19
18.97
Br
[O]
f1 (ppm)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8.03
8.01
7.88
7.87
7.85
7.84
7.83
7.82
7.81
7.79
7.77
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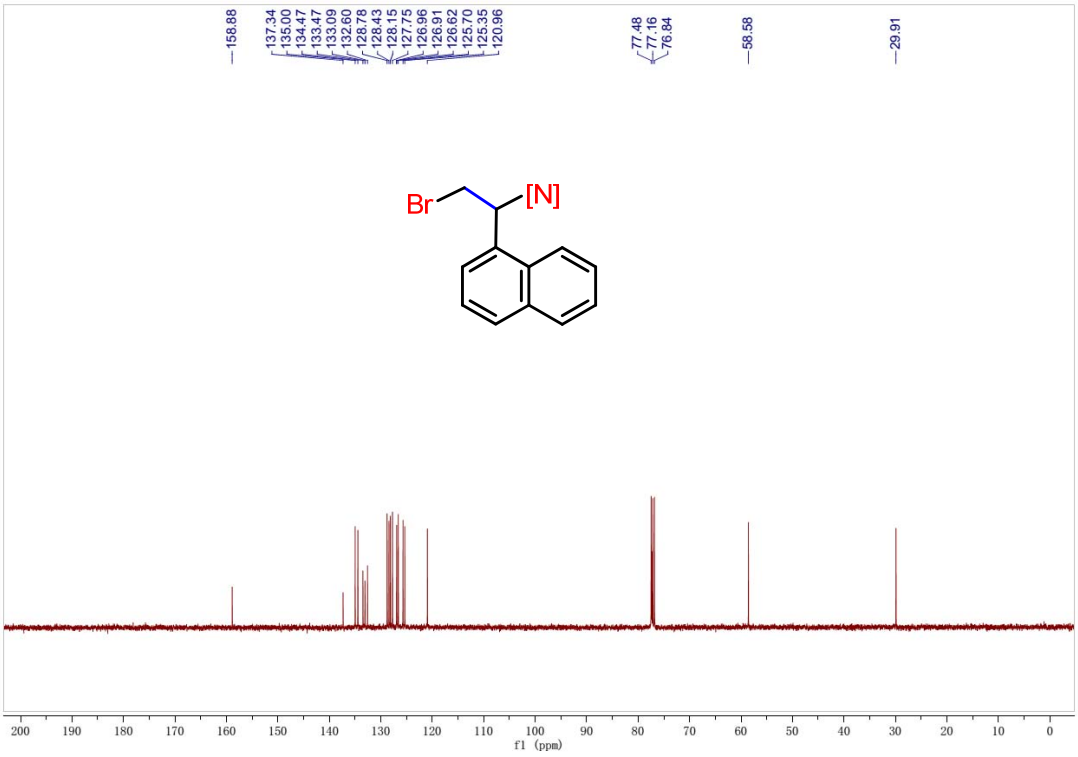
7.73
7.71
7.51
7.50
7.50
7.26
5.67
5.65
5.63
4.66
4.64
4.61
4.28
4.26
4.26
4.24
Br
[N]
1.01
0.99
7.18
2.08
1.00
1.02
1.01
f1 (ppm)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133.09
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127.75
126.96
126.91
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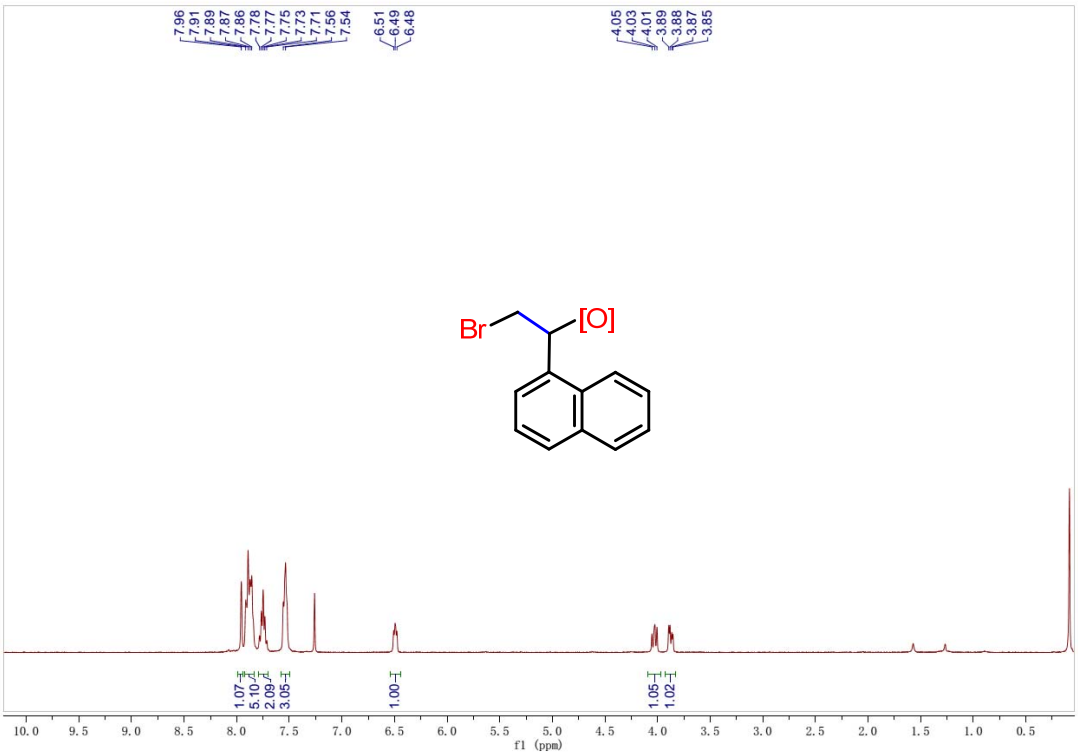
120.96
77.48
77.16
76.84
58.58
29.91
Br
[N]
f1 (ppm)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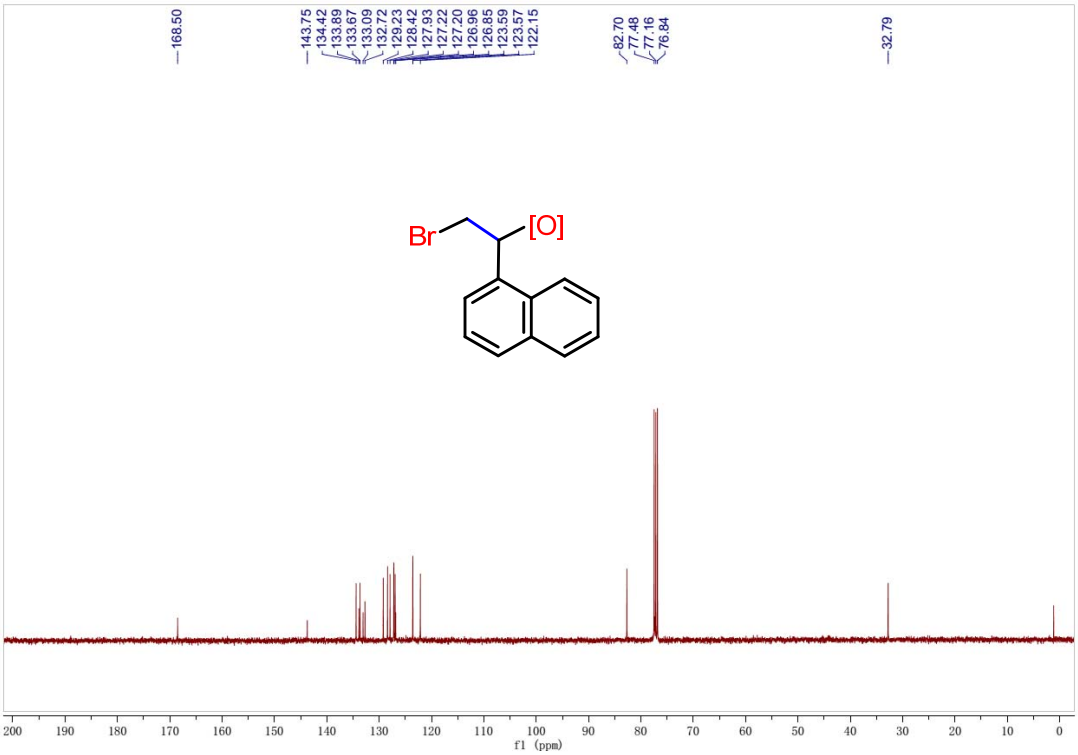
7.86
7.78
7.77
7.75
7.73
7.71
7.56
7.54
6.51
6.49
6.48
4.05
4.03
4.01
3.89
3.88
3.87
3.85
Br
[O]
1.07
5.10
2.09
3.05
1.00
1.05
1.02
f1 (ppm)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127.22
127.20
126.96
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123.59
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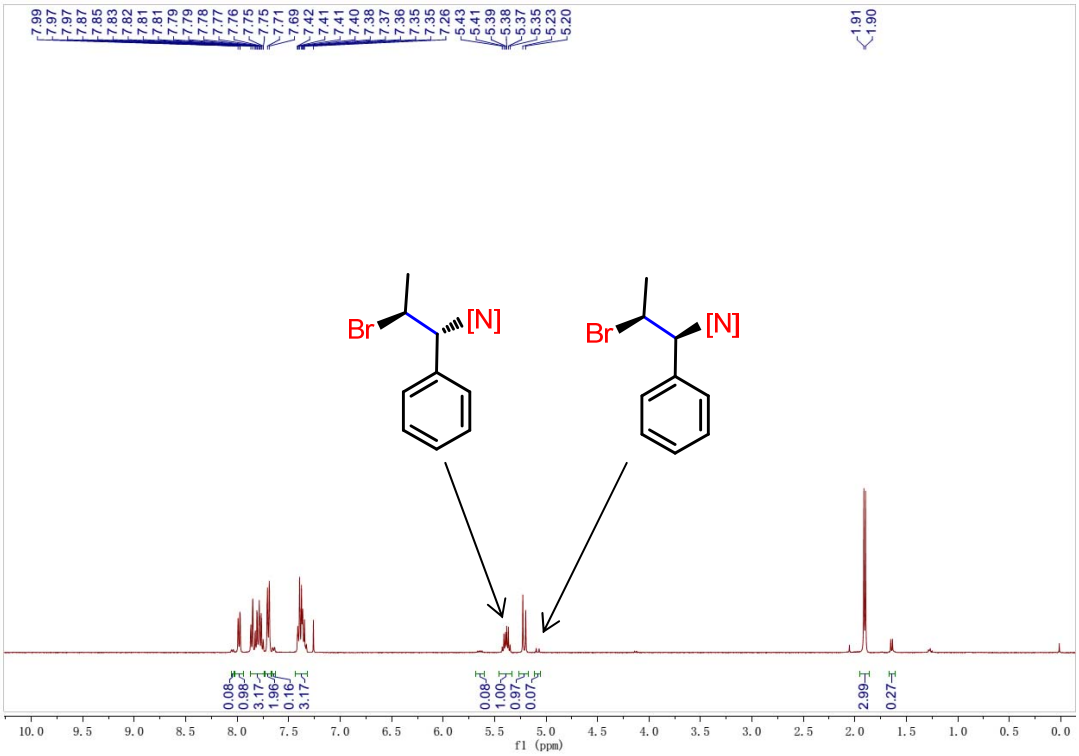
122.15
82.70
77.48
77.16
76.84
32.79
Br
[O]
f1 (ppm)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7.78
7.77
7.76
7.75
7.75
7.71
7.69
7.42
7.41
7.41
7.40
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7.36
7.35
7.35
7.26
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5.41
5.39
5.38
5.37
5.35
5.23
5.20
1.91
1.90
Br
[N]
Br
[N]
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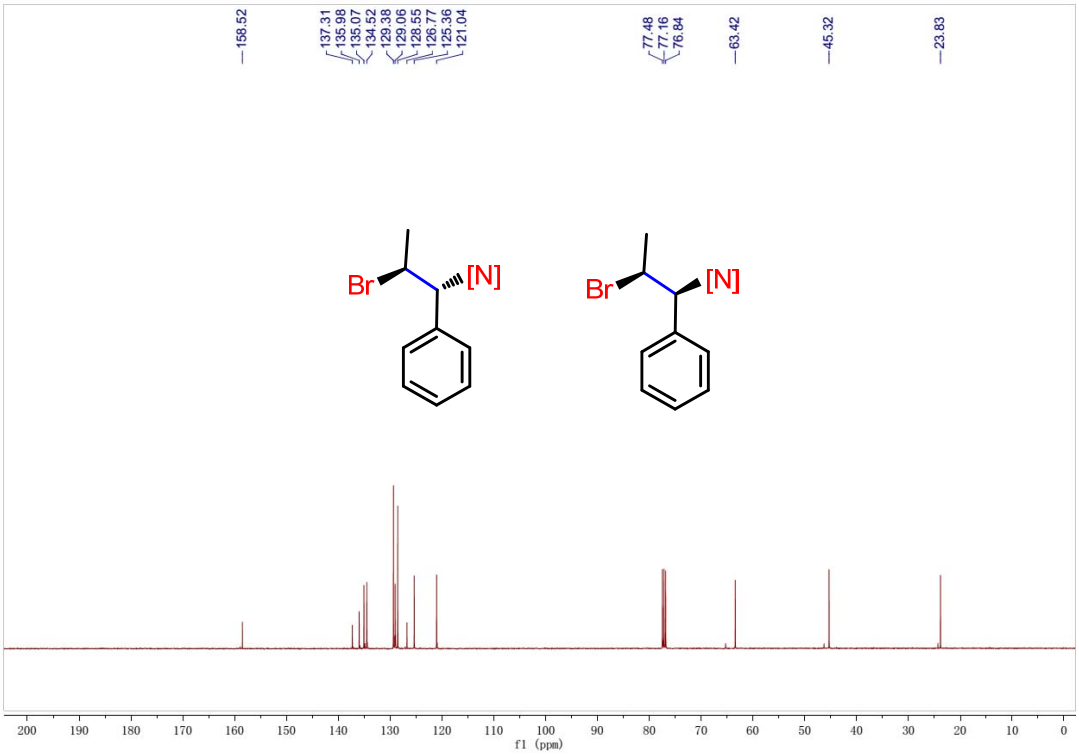
0.98
3.17
1.96
0.16
3.17
0.08
1.00
0.97
0.07
2.99
0.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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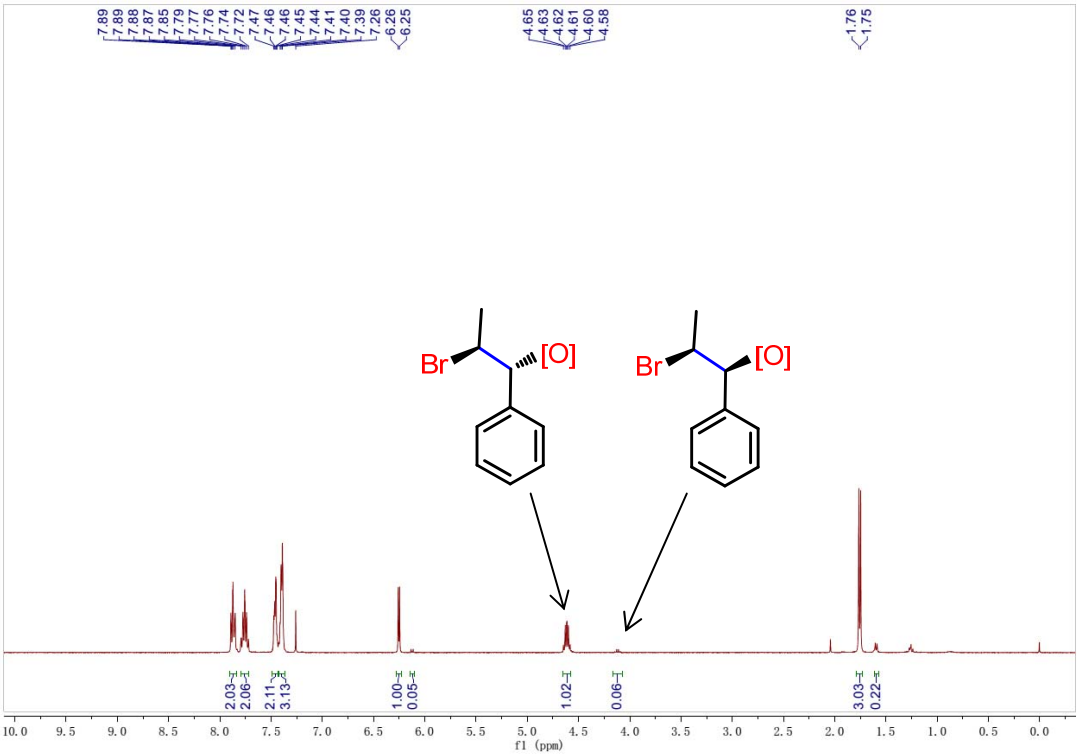
128.55
126.77
125.36
121.04
77.48
77.16
76.84
63.42
45.32
23.83
Br
[N]
Br
[N]
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.77
7.76
7.74
7.72
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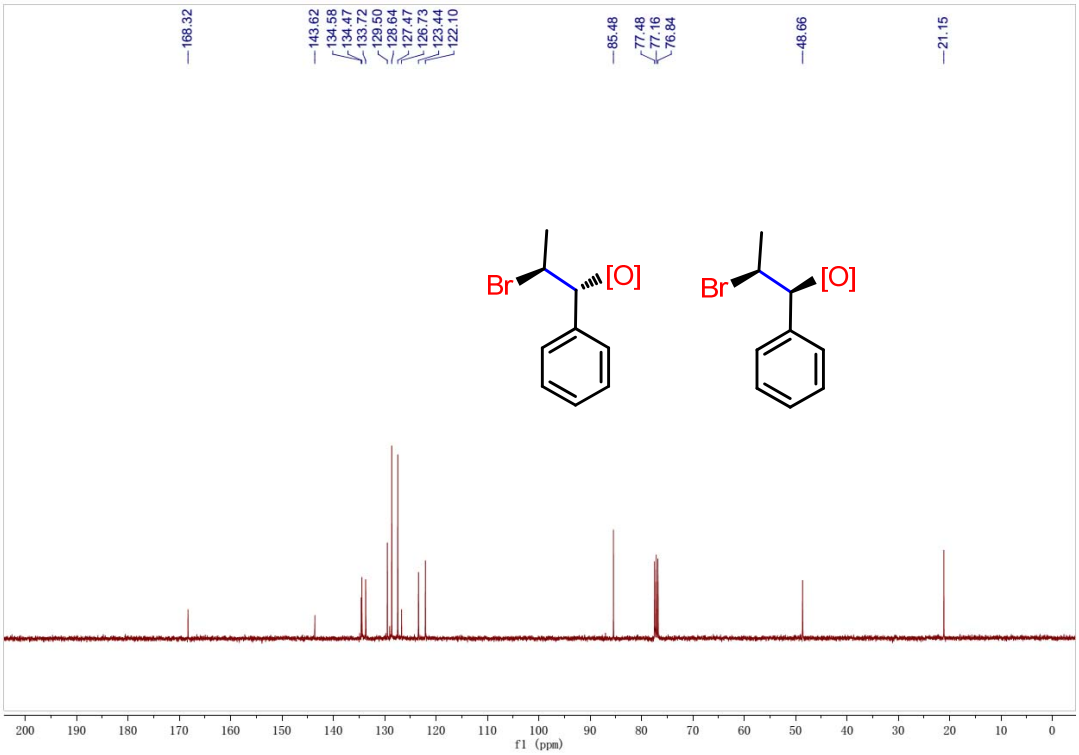
7.46
7.46
7.45
7.44
7.41
7.40
7.39
7.26
6.26
6.25
4.65
4.63
4.62
4.61
4.60
4.58
1.76
1.75
Br
[O]
Br
[O]
2.03
2.06
2.11
3.13
1.00
0.05
1.02
0.06
3.03
0.22
f1 (ppm)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129.50
128.64
127.47
126.73
123.44
122.10
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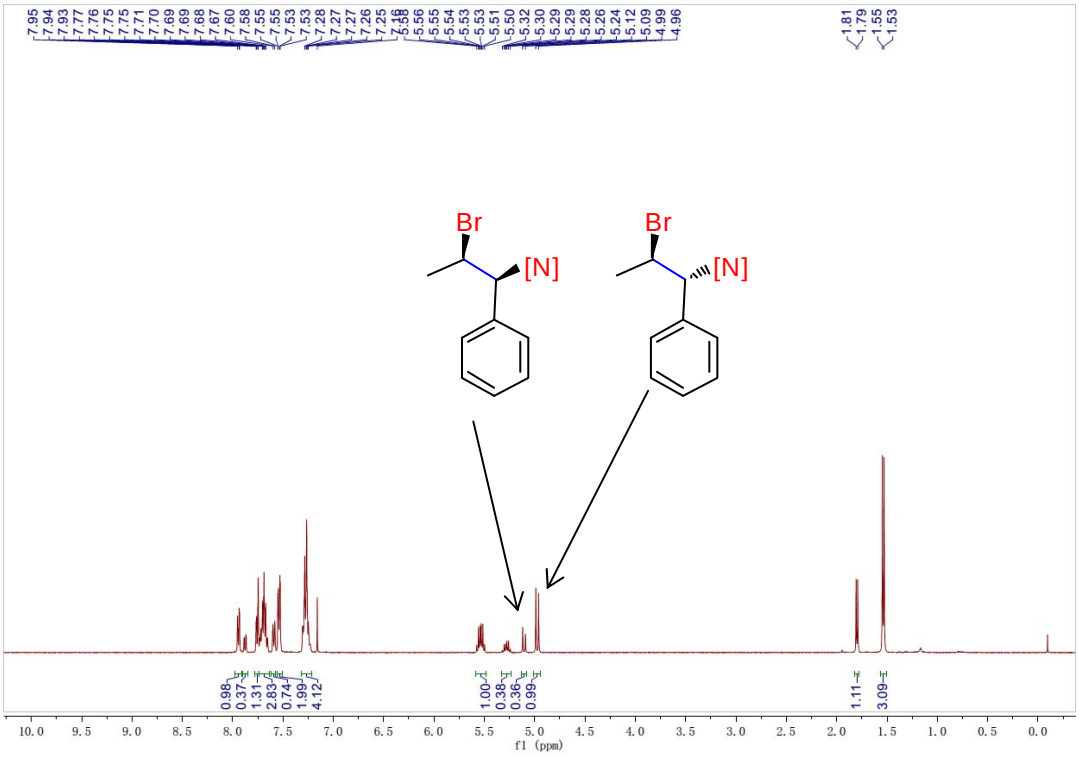
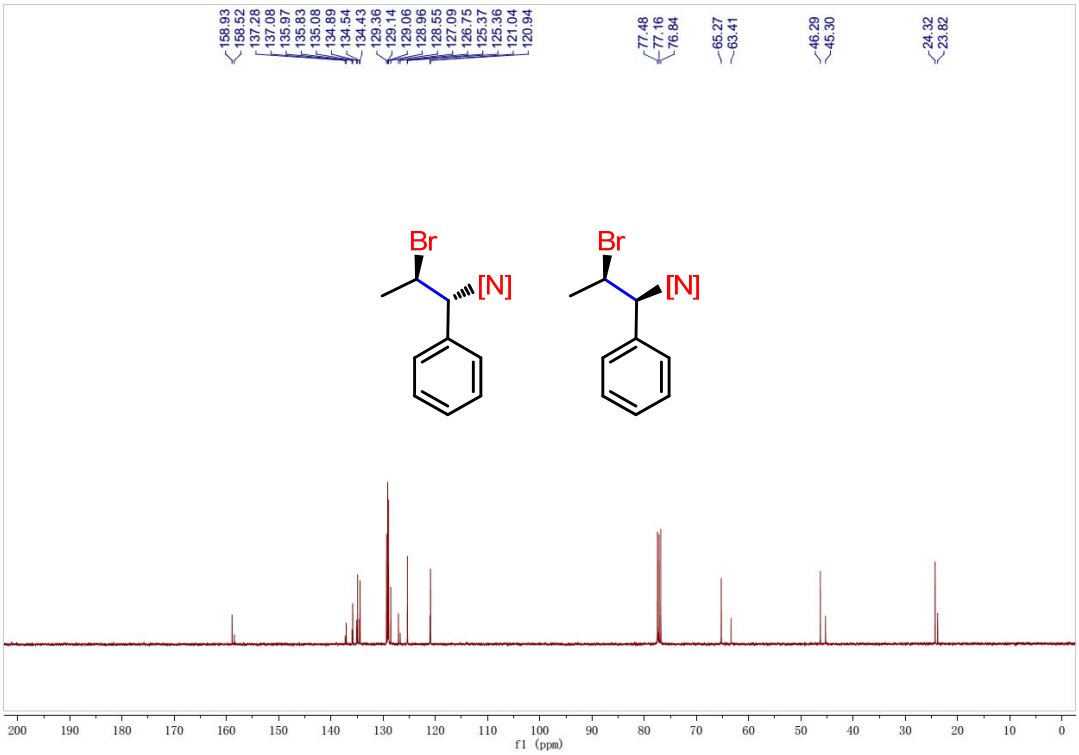
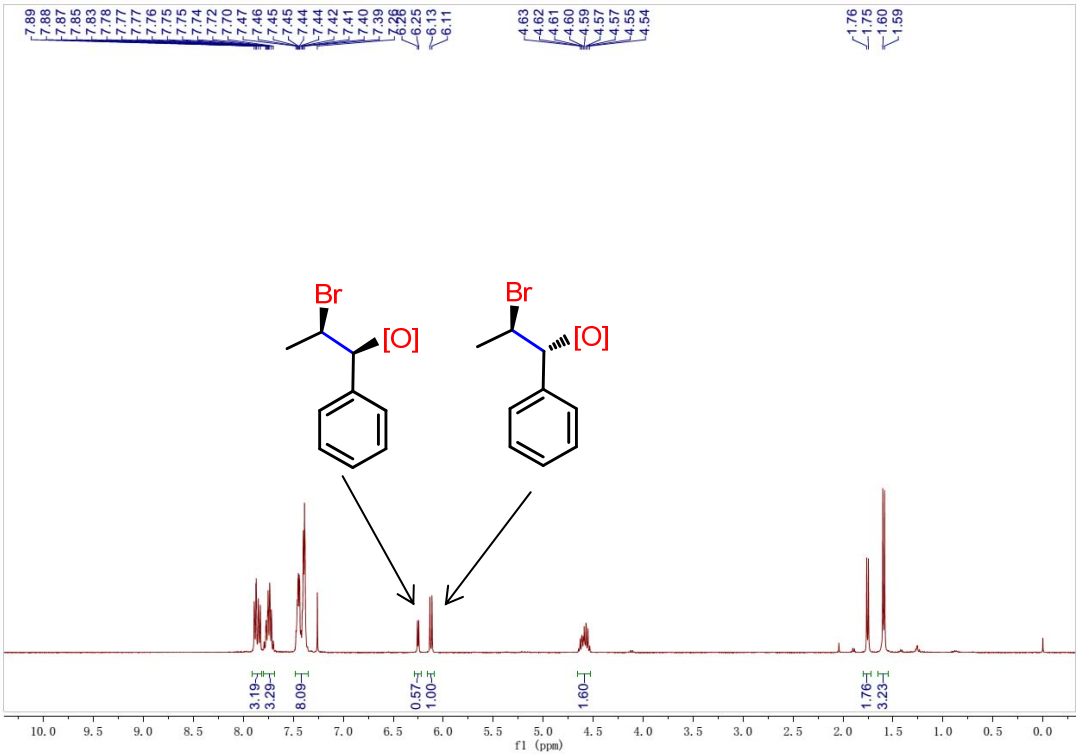
77.48
77.16
76.84
48.66
21.15
Br
[O]
Br
[O]
f1 (ppm)


Br
[N]
Br
[N]
f1 (ppm)


Br
[N]
Br
[N]
f1 (ppm)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7.78
7.77
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7.75
7.74
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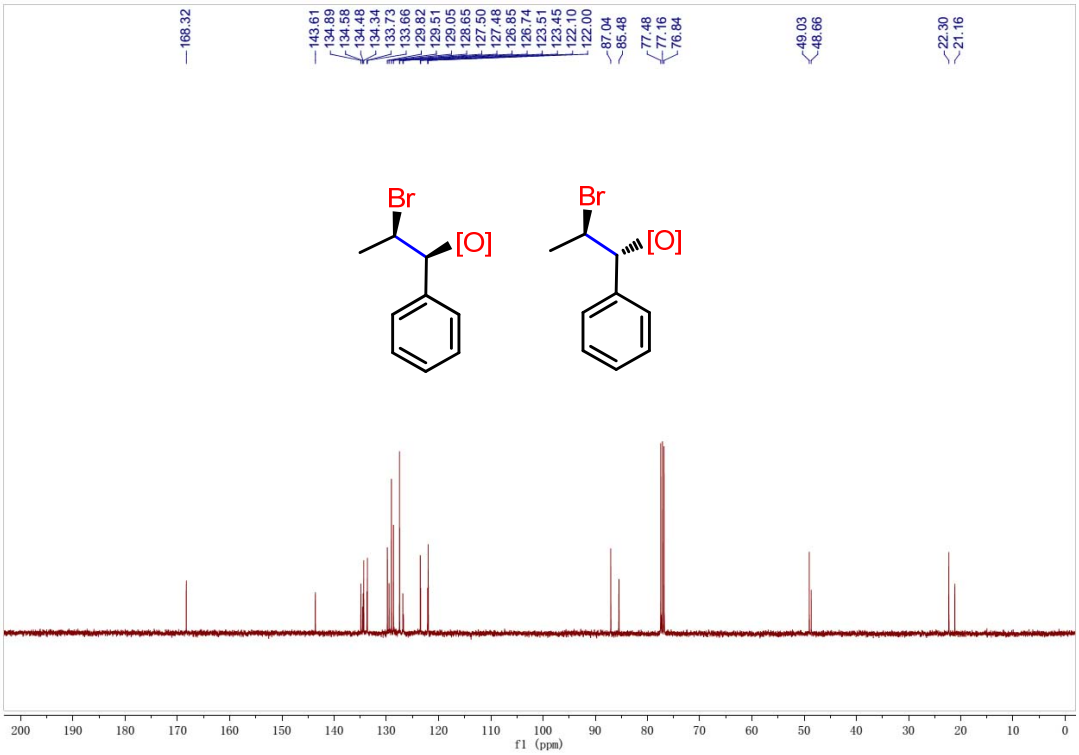
7.70
7.47
7.46
7.45
7.45
7.44
7.44
7.42
7.41
7.40
7.39
7.26
6.25
6.13
6.11
4.63
4.62
4.61
4.60
4.59
4.57
4.57
4.55
4.54
1.76
1.75
1.60
1.59
Br
[O]
Br
[O]
3.19
3.29
8.09
0.57
1.00
1.60
1.76
3.23
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.34
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133.66
129.82
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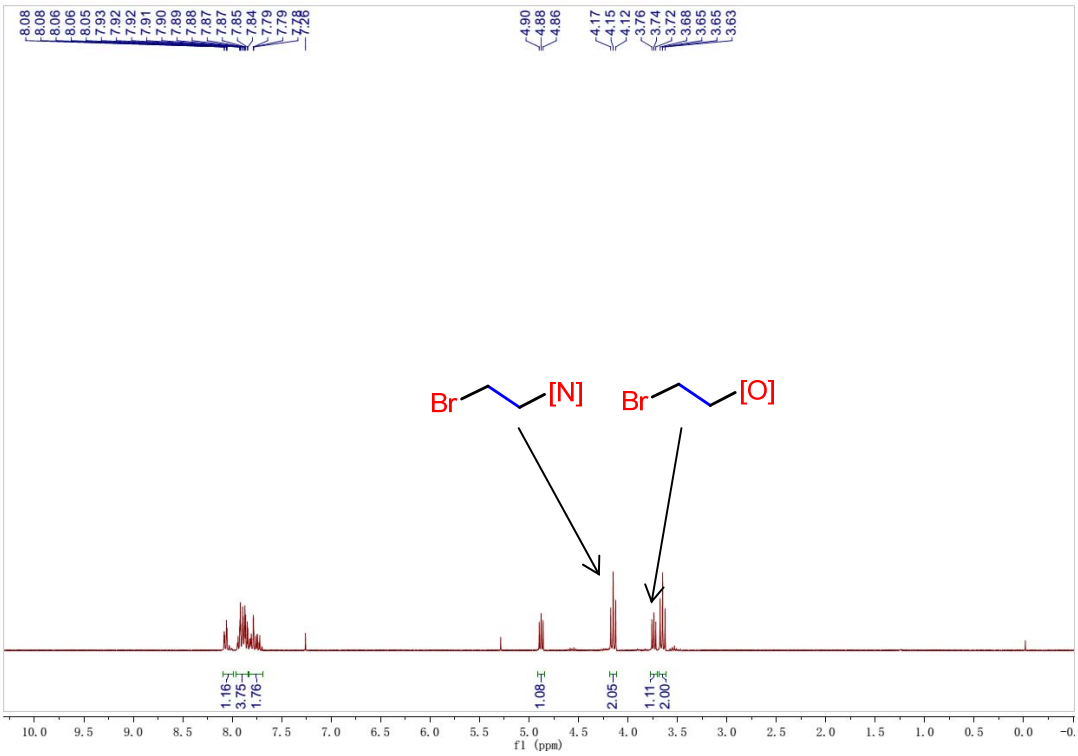
129.05
128.65
127.50
127.48
126.85
126.74
123.51
123.45
122.10
122.00
87.04
85.48
77.48
77.16
76.84
49.03
48.66
22.30
21.16
Br
[O]
Br
[O]
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.08
8.08
8.06
8.06
8.05
7.93
7.92
7.92
7.91
7.90
7.89
7.88
7.87
7.87
7.85
7.84
7.79
7.79
7.78
7.26
4.90
4.88
4.86
4.17
4.15
4.12
3.76
3.74
3.72
3.68
3.65
3.65
3.63
Br
[N]
Br
[O]
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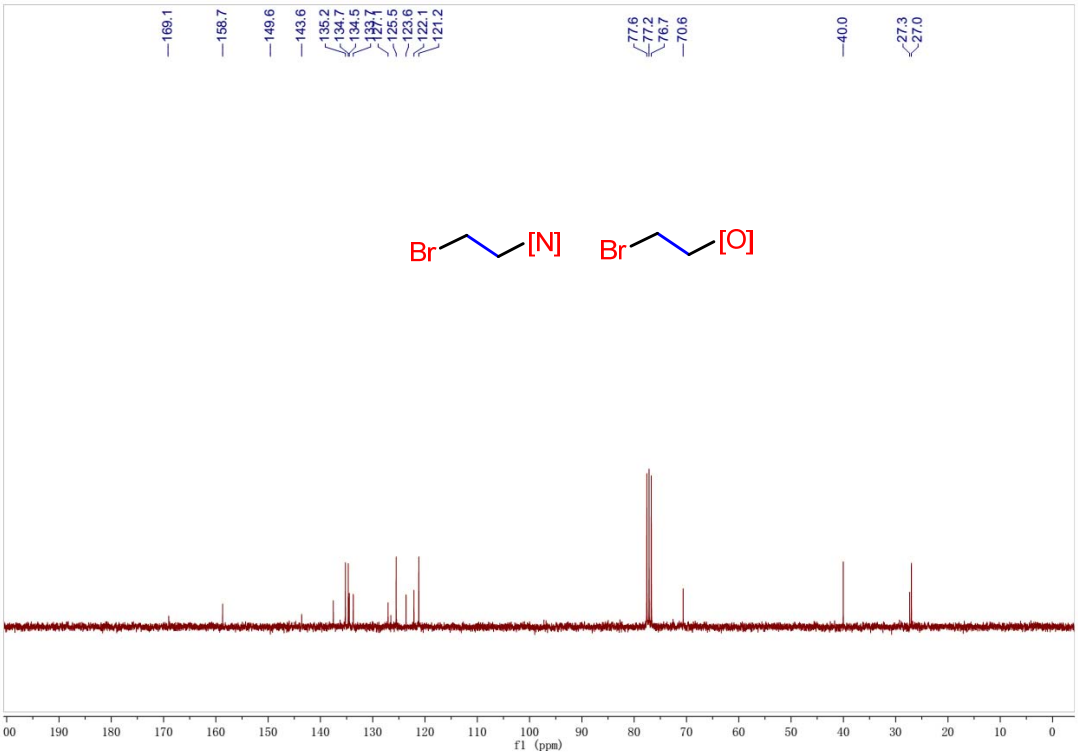
3.75
1.76
1.08
2.05
1.11
2.00
f1 (ppm)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158.7
149.6
143.6
135.2
134.7
134.5
127.1
125.5
123.6
122.1
121.2
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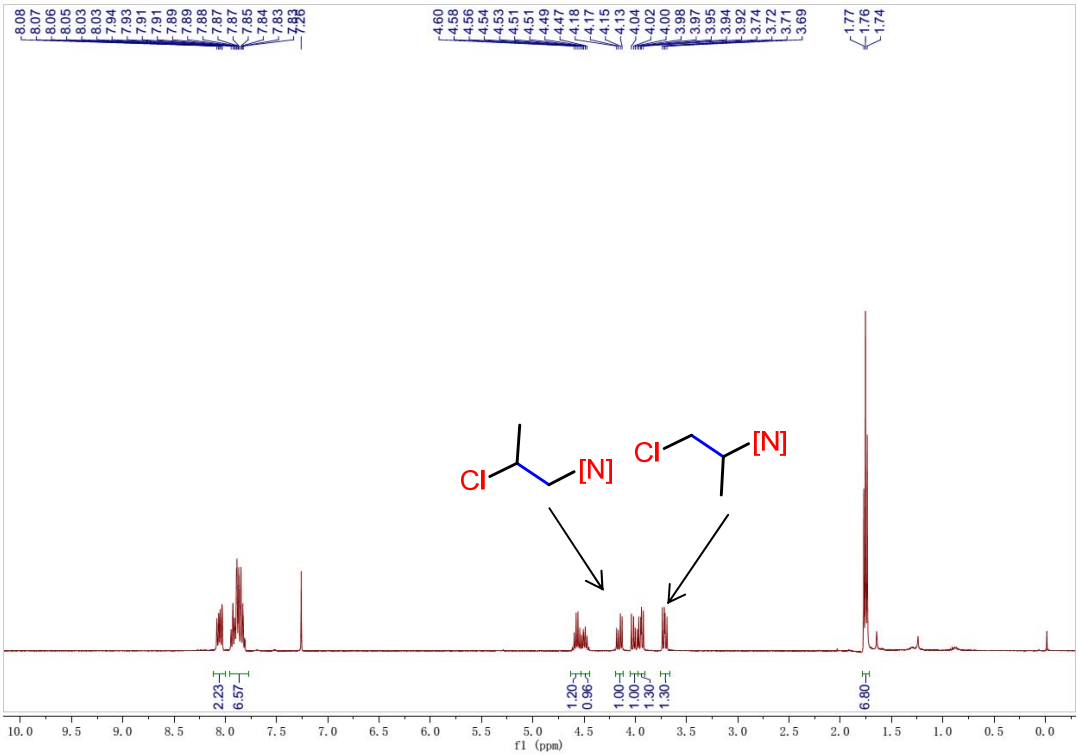
77.2
76.7
70.6
40.0
27.3
27.0
Br
[N]
Br
[O]
f1 (ppm)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7.87
7.87
7.85
7.84
7.83
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4.58
4.56
4.54
4.53
4.51
4.51
4.49
4.47
4.18
4.17
4.15
4.13
4.04
4.02
4.00
3.98
3.97
3.95
3.94
3.92
3.74
3.72
3.71
3.69
1.77
1.76
1.74
Cl
[N]
Cl
[N]
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1.20
0.96
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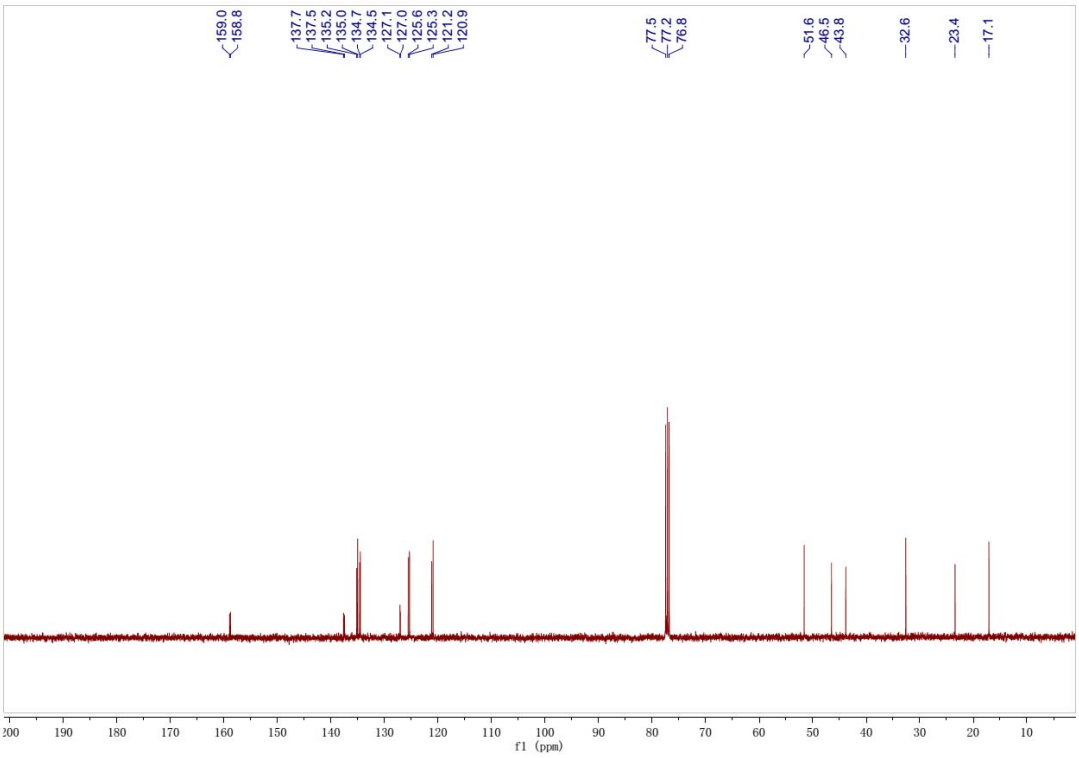
1.00
1.30
1.30
6.80
f1 (ppm)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158.8
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135.2
135.0
134.7
134.5
127.1
127.0
125.6
125.3
121.2
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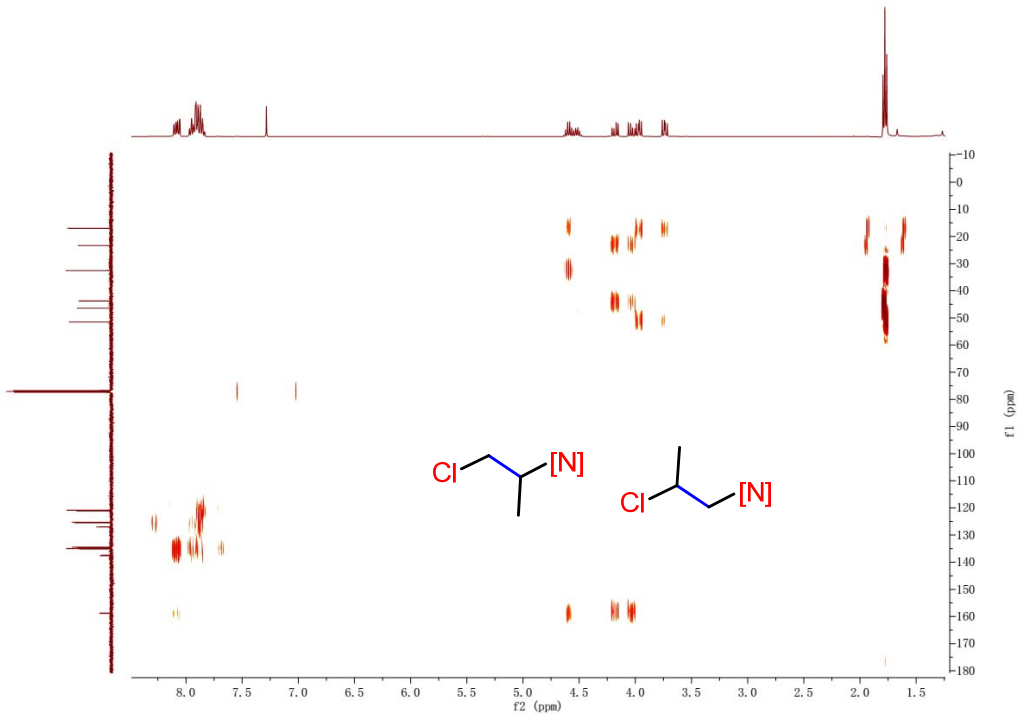
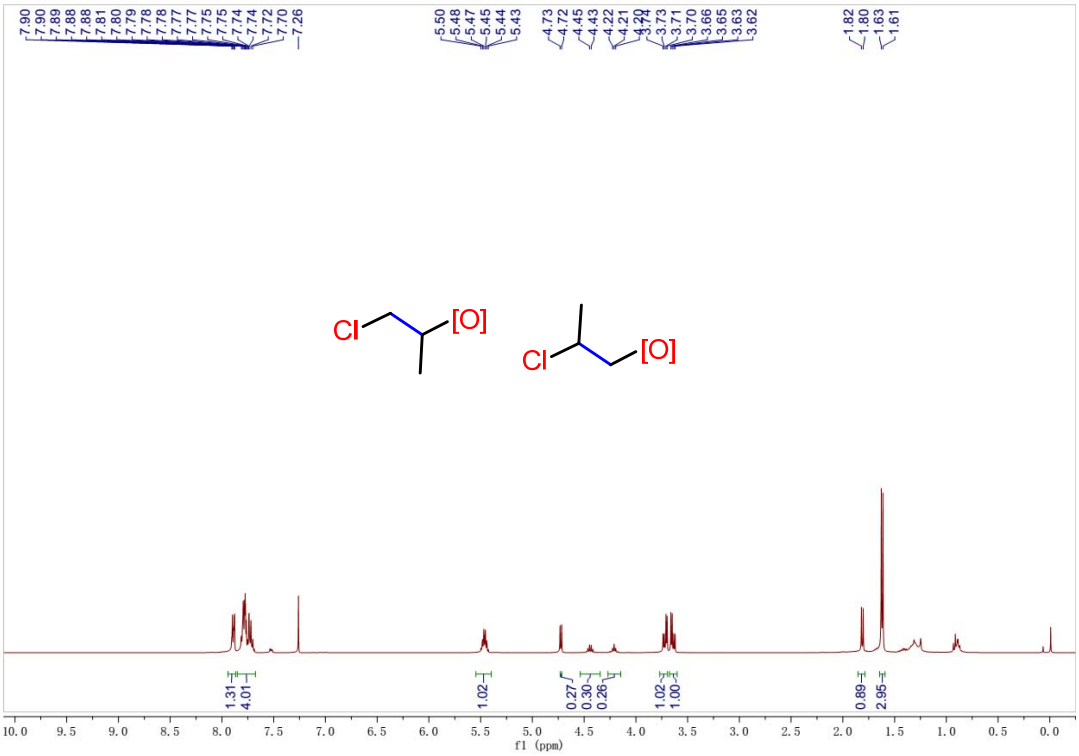
77.2
76.8
51.6
46.5
43.8
32.6
23.4
17.1
f1 (ppm)


Cl
[N]
Cl
[N]
f2 (ppm)
f1 (ppm)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7.80
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7.75
7.74
7.74
7.72
7.70
7.26
5.50
5.48
5.47
5.45
5.44
5.43
4.73
4.72
4.45
4.43
4.22
4.21
4.20
3.74
3.73
3.71
3.70
3.66
3.65
3.63
3.62
1.82
1.80
1.63
1.61
Cl
[O]
Cl
[O]
1.31
4.01
1.02
0.27
0.30
0.26
1.02
1.00
0.89
2.95
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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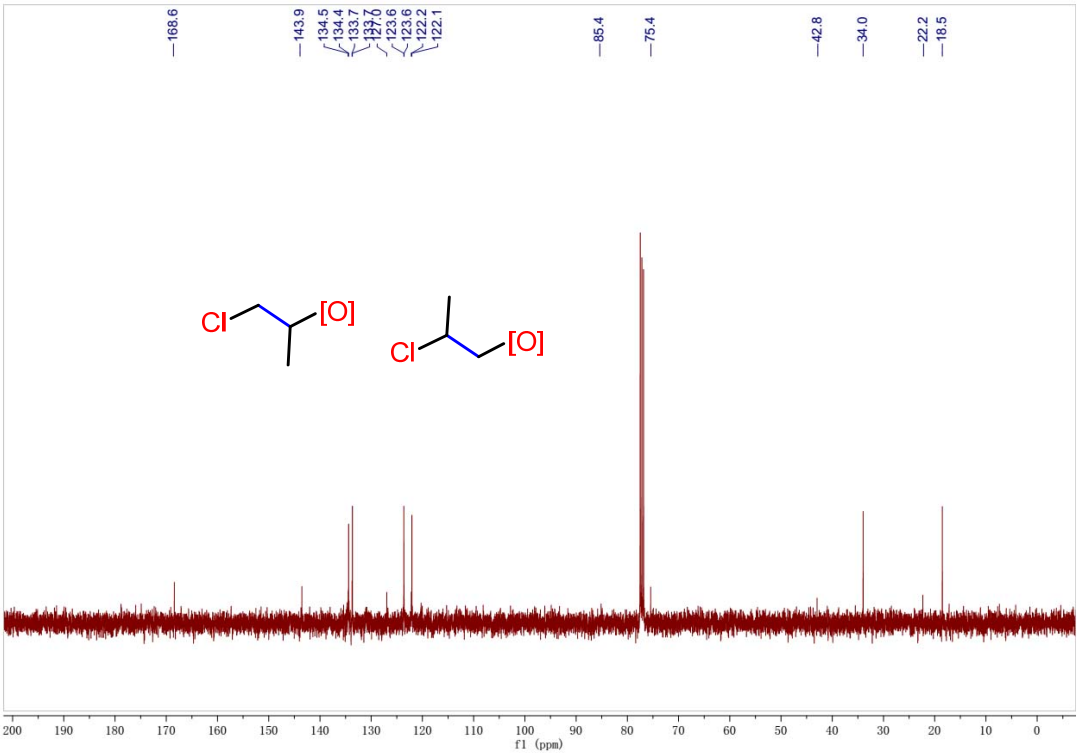
1.0
0.5
0.0
f1 (ppm)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133.7
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123.6
123.6
122.2
122.1
85.4
75.4
42.8
34.0
22.2
18.5
Cl
[O]
Cl
[O]
200
190
180
170
160
150
140
130
120
110
100
90
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70
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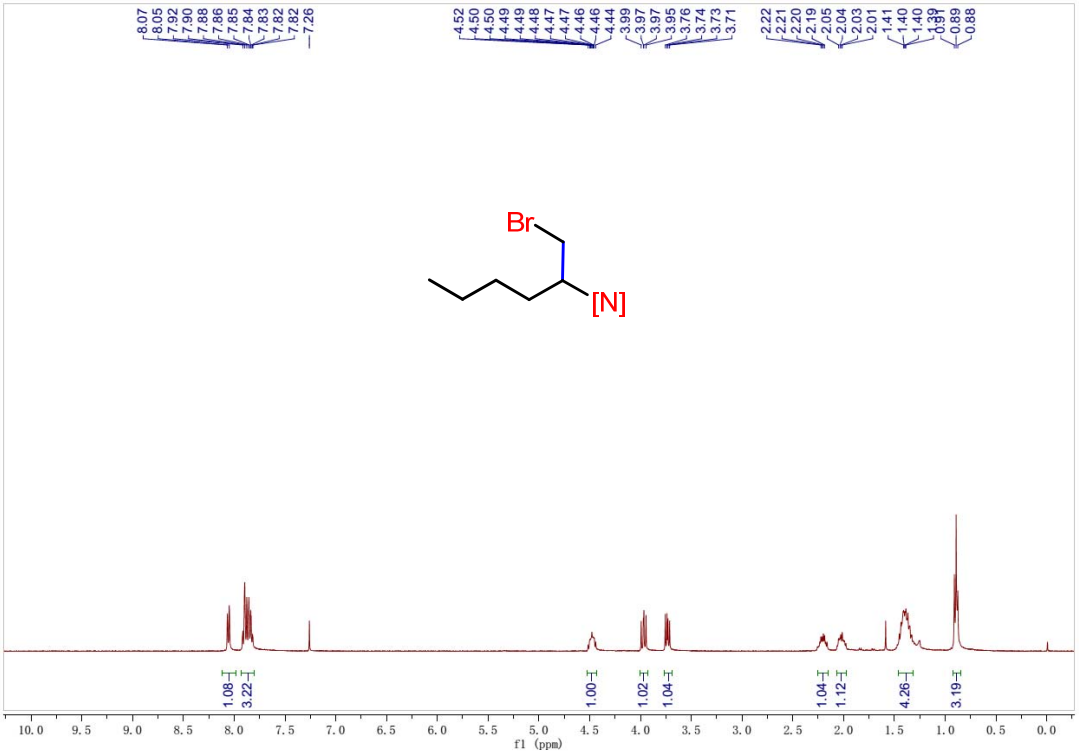
50
40
30
20
10
0
f1 (ppm)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7.90
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7.86
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7.84
7.83
7.82
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7.26
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4.50
4.49
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4.48
4.47
4.47
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4.46
4.44
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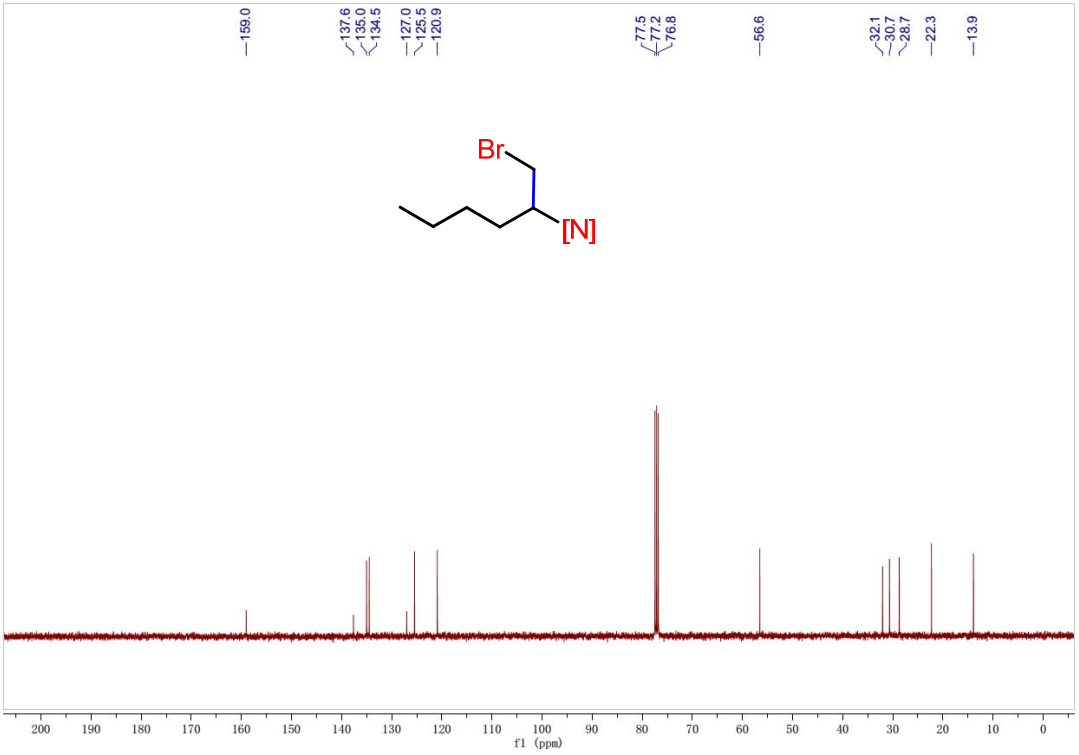
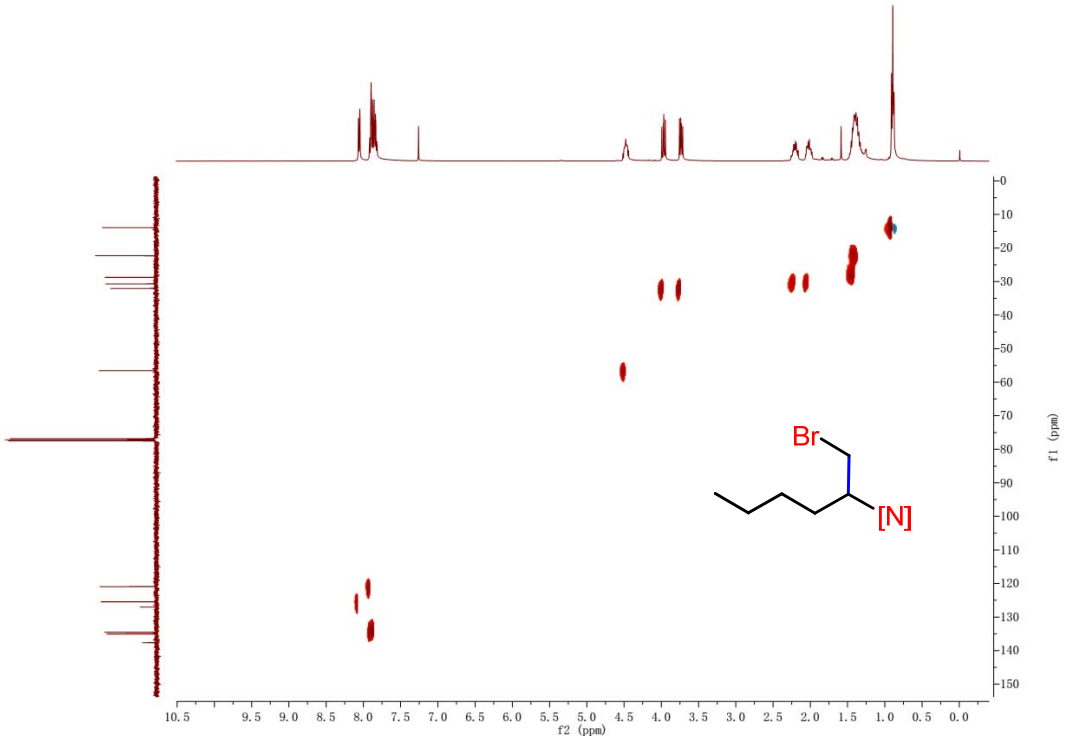
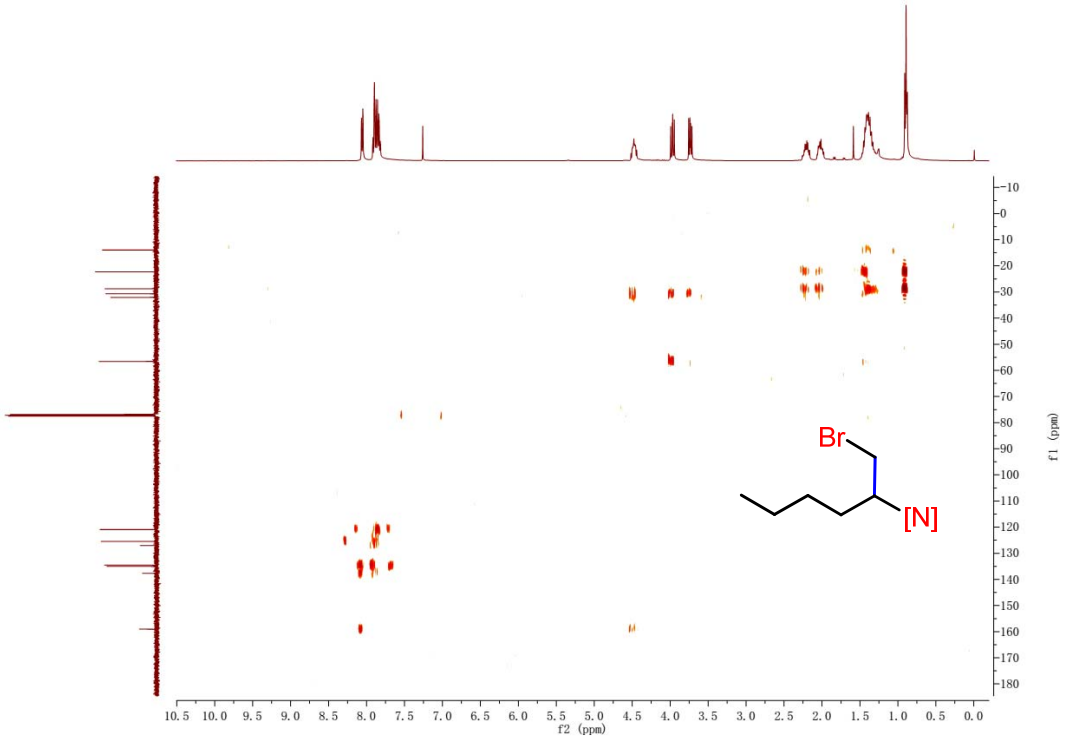
3.97
3.95
3.76
3.74
3.73
3.71
2.22
2.21
2.20
2.19
2.05
2.04
2.03
2.01
1.41
1.40
1.40
1.39
0.91
0.89
0.88
Br
[N]
1.08
3.22
1.00
1.02
1.04
1.04
1.12
4.26
3.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

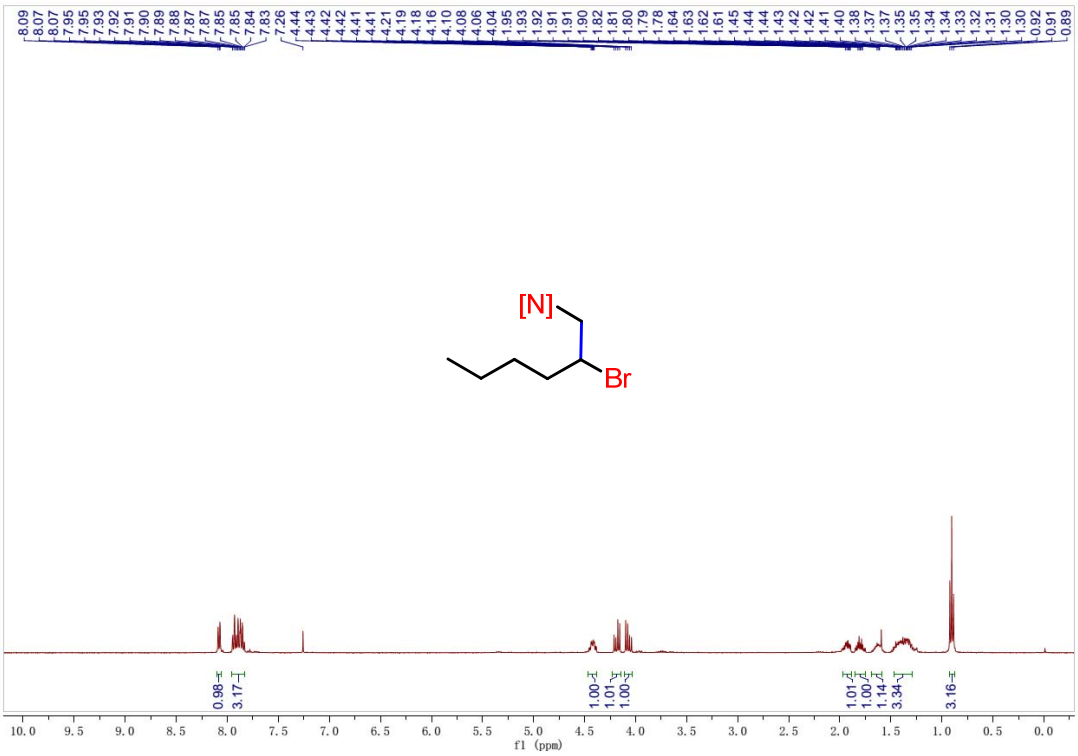

159.0
137.6
135.0
134.5
127.0
125.5
120.9
77.5
77.2
76.8
56.6
32.1
30.7
28.7
22.3
13.9
Br
[N]
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

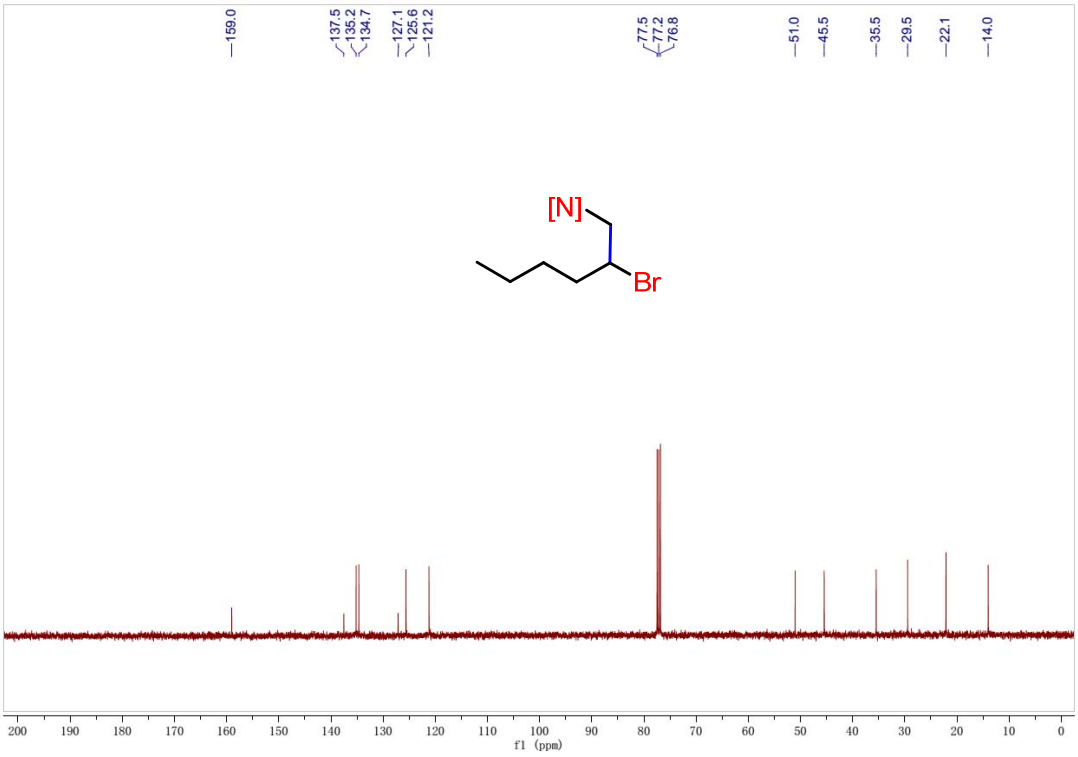
HSQC:



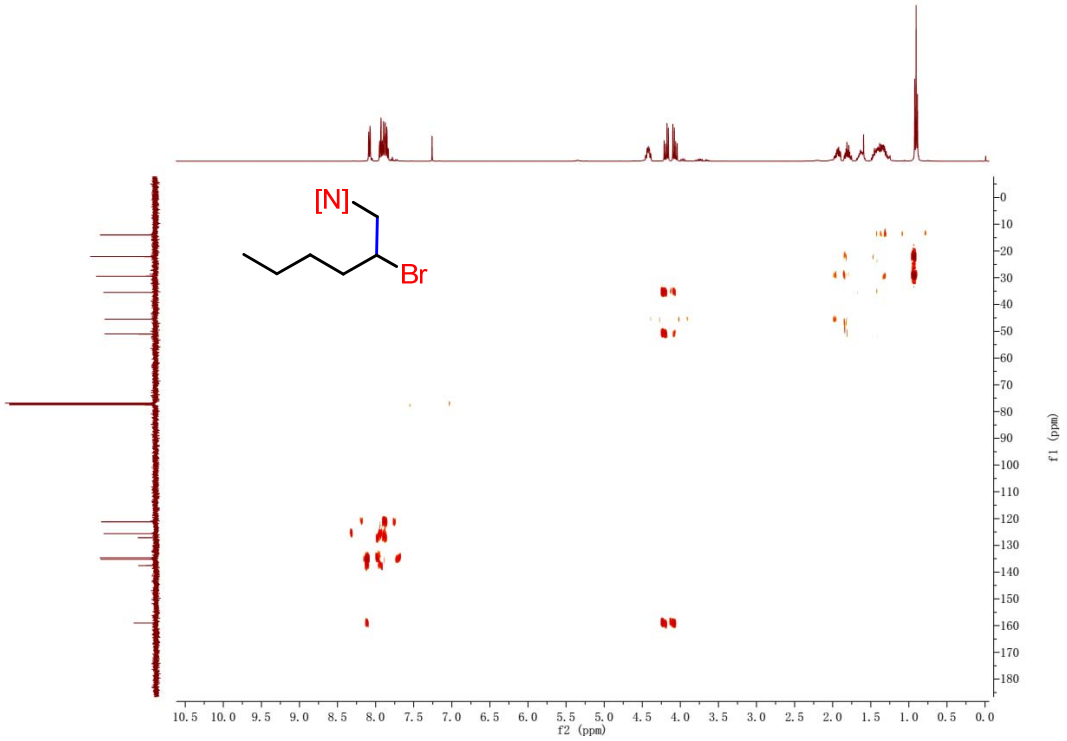
HMBC:

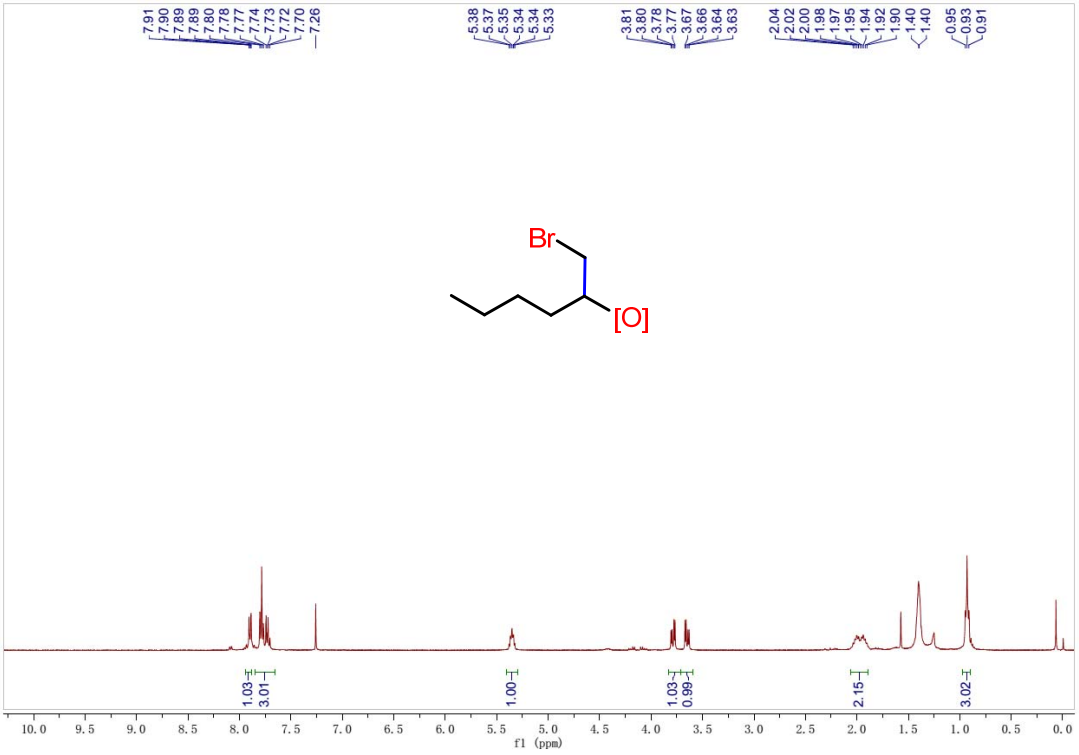



[N]
Br
f1 (ppm)


[N]
Br
f1 (ppm)

HMBC:


[N]
Br
f2 (ppm)
f1 (ppm)


7.91
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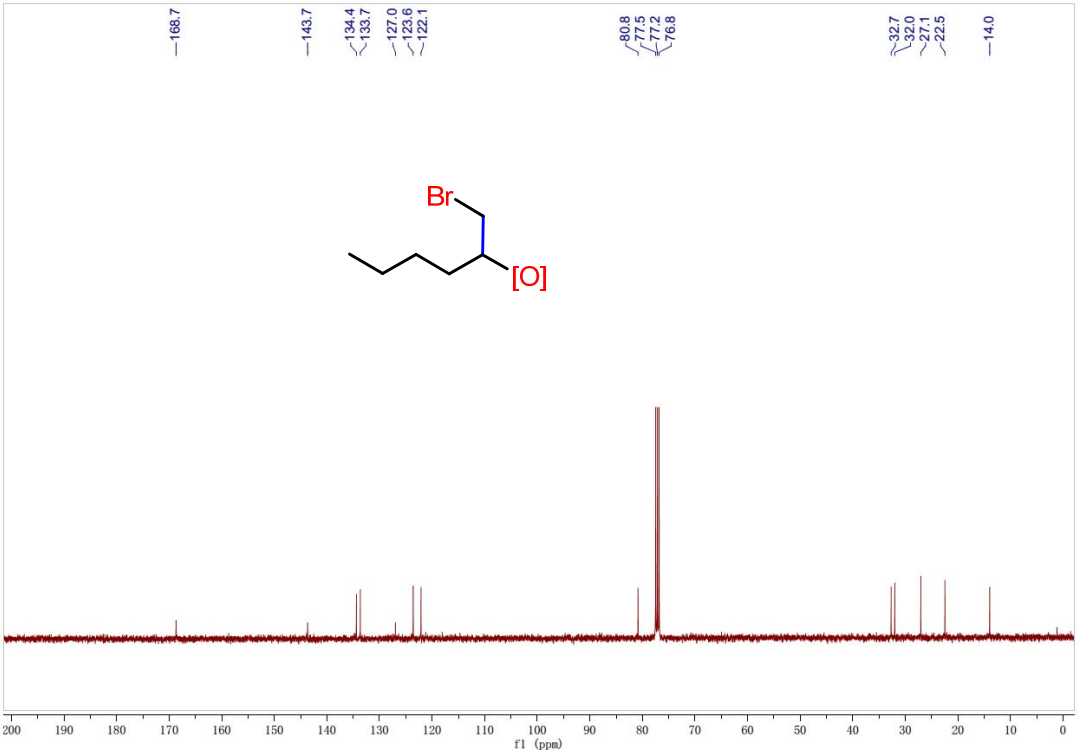
7.89
7.89
7.80
7.78
7.77
7.74
7.73
7.72
7.70
7.26
5.38
5.37
5.35
5.34
5.34
5.33
3.81
3.80
3.78
3.77
3.67
3.66
3.64
3.63
2.04
2.02
2.00
1.98
1.97
1.95
1.94
1.92
1.90
1.40
1.40
0.95
0.93
0.91
Br
[O]
1.03
3.01
1.00
1.03
0.99
2.15
3.02
f1 (ppm)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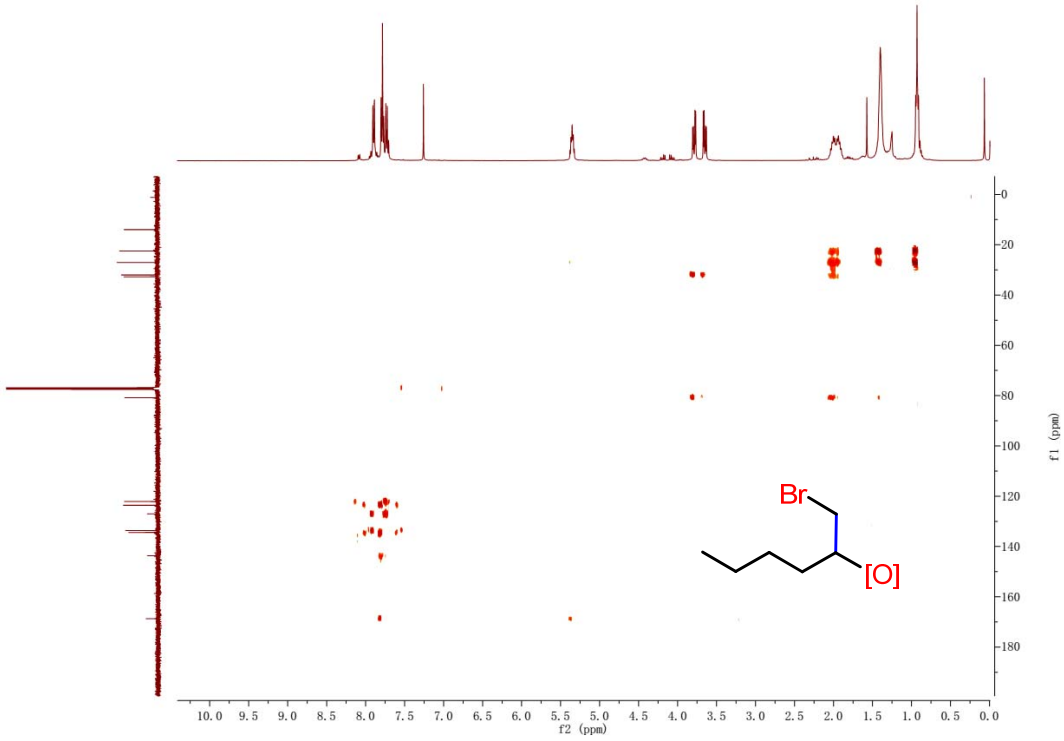
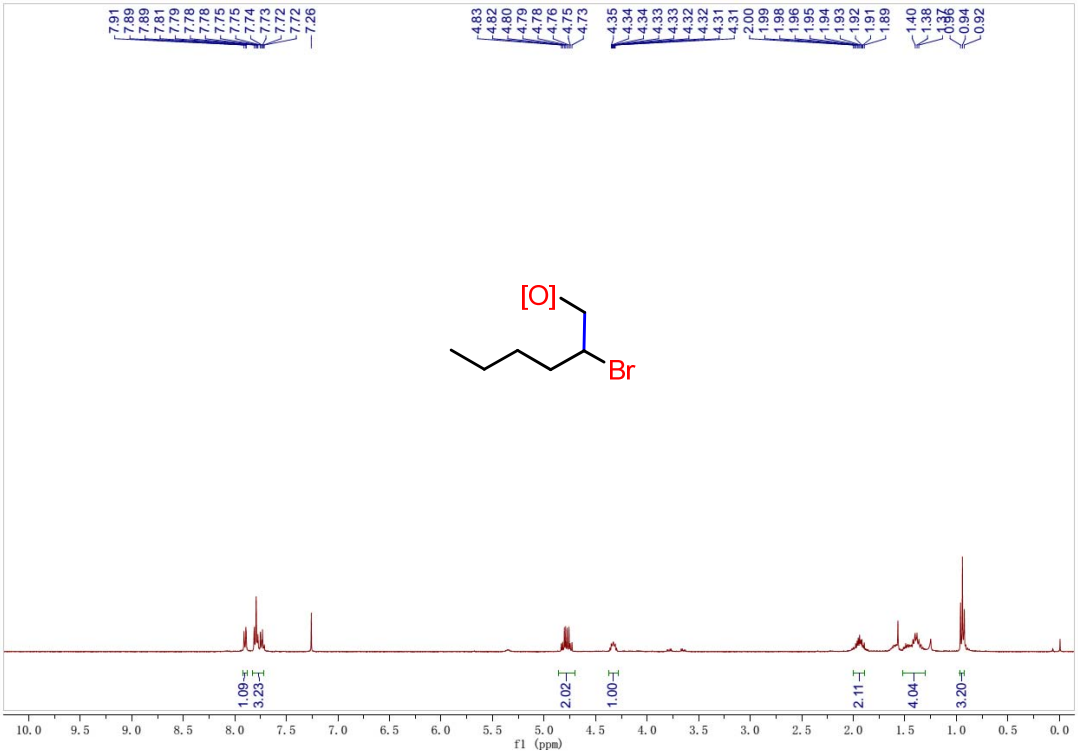
143.7
134.4
133.7
127.0
123.6
122.1
80.8
77.5
77.2
76.8
32.7
32.0
27.1
22.5
14.0
Br
[O]
f1 (ppm)

HMBC:


Br
[O]
f2 (ppm)
f1 (ppm)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7.89
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7.75
7.74
7.73
7.72
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7.26
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4.82
4.80
4.79
4.78
4.76
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4.73
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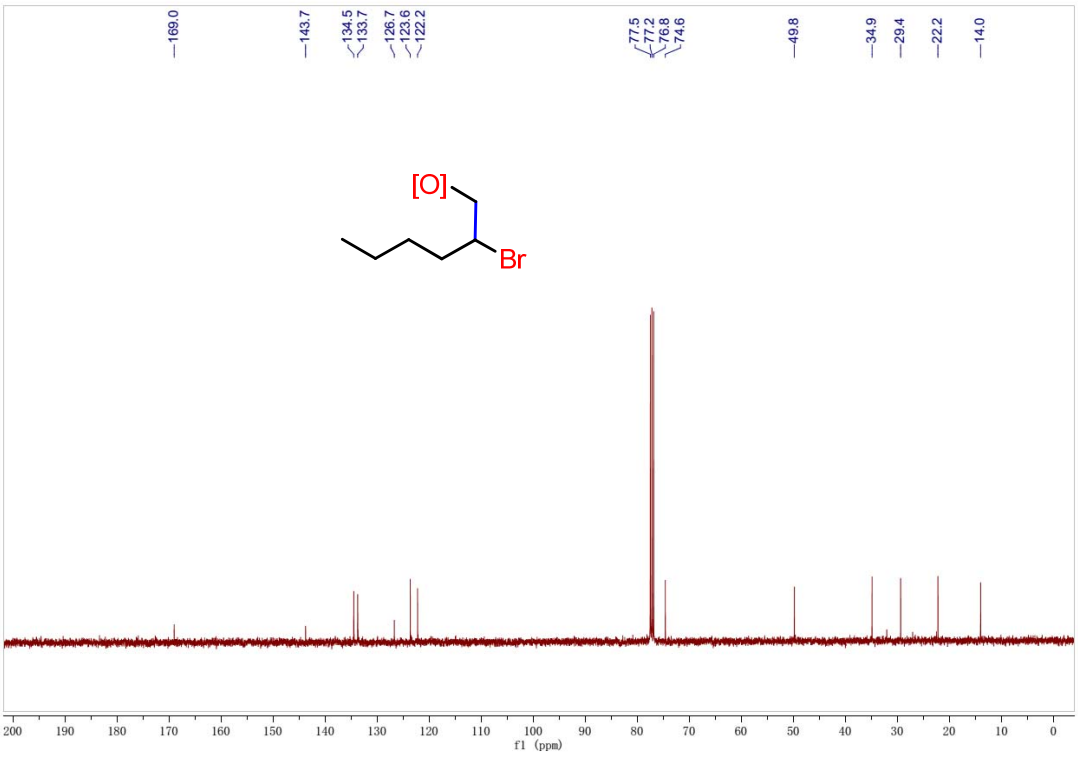
1.99
1.98
1.96
1.95
1.94
1.93
1.92
1.91
1.89
1.40
1.38
0.96
0.94
0.92
[O]
Br
1.09
3.23
2.02
1.00
2.11
4.04
3.20
f1 (ppm)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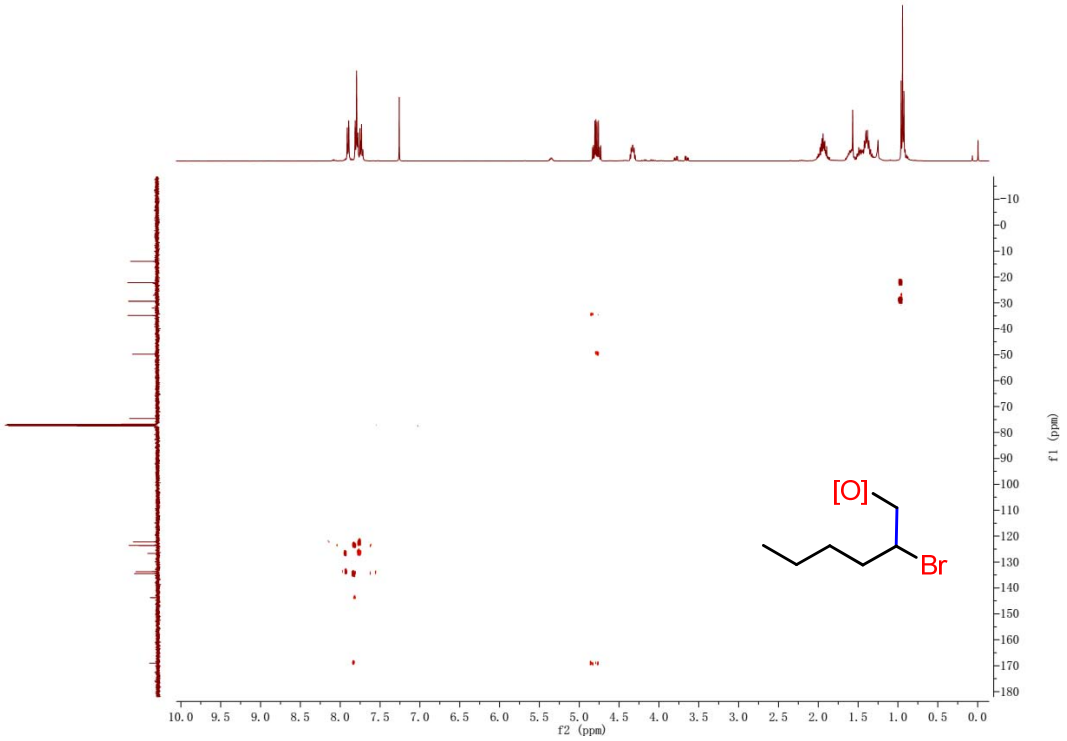
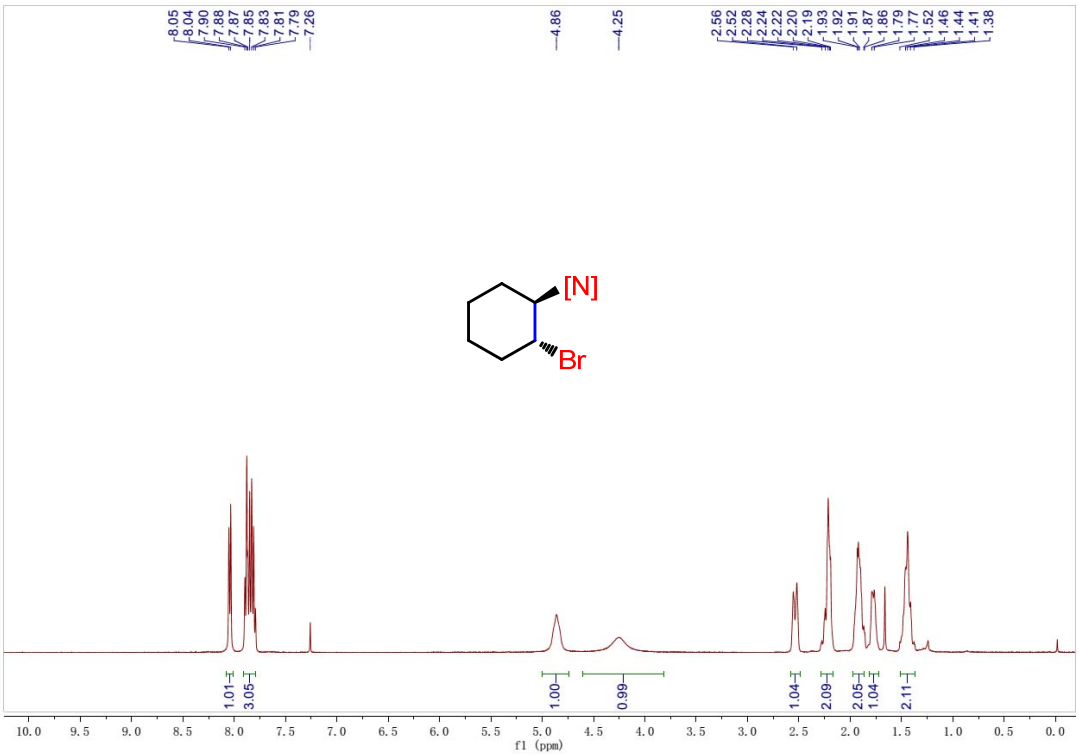
133.7
126.7
123.6
122.2
77.5
77.2
76.8
74.6
49.8
34.9
29.4
22.2
14.0
[O]
Br
f1 (ppm)

HMBC:

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8.04
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7.85
7.83
7.81
7.79
7.26
4.86
4.25
2.56
2.52
2.28
2.24
2.22
2.20
2.19
1.93
1.92
1.91
1.87
1.86
1.79
1.77
1.52
1.46
1.44
1.41
1.38
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Br
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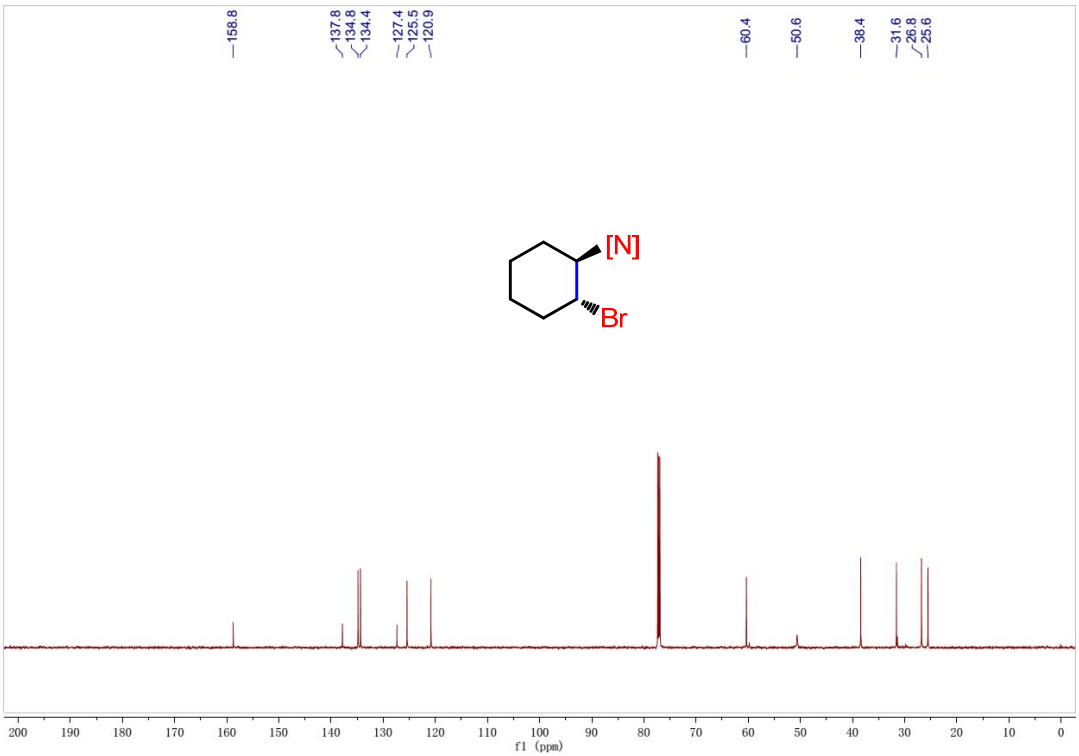
3.05
1.00
0.99
1.04
2.09
2.05
1.04
2.11
f1 (ppm)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137.8
134.8
134.4
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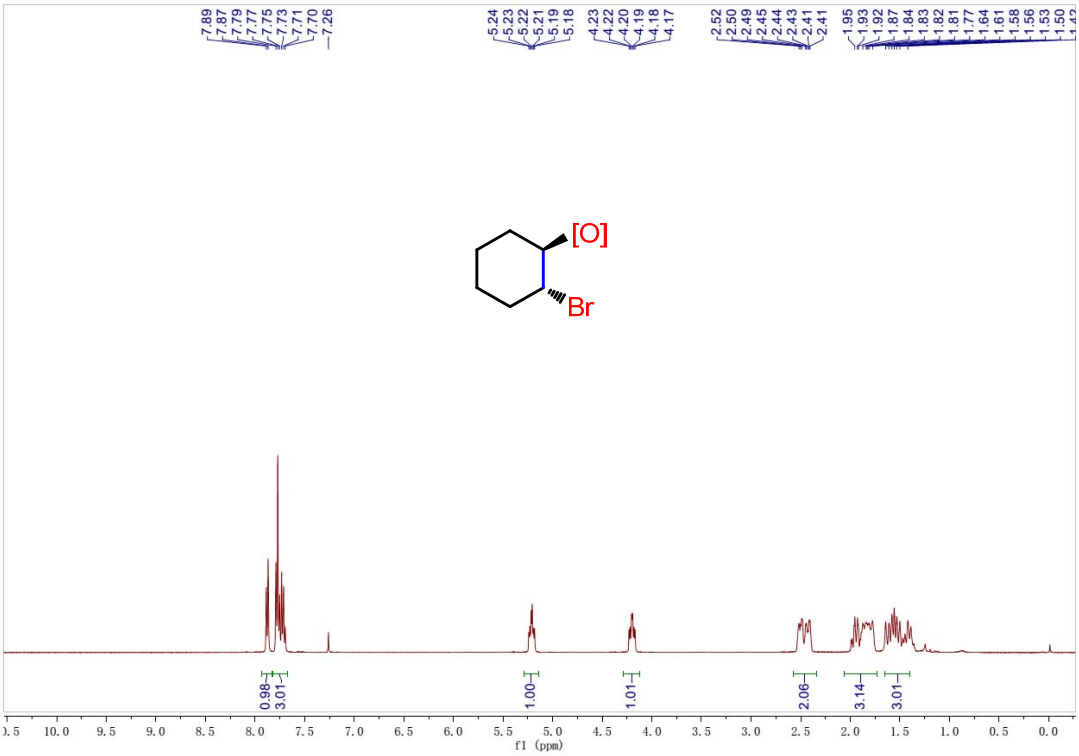
125.5
120.9
60.4
50.6
38.4
31.6
26.8
25.6
[N]
Br
f1 (ppm)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5.22
5.21
5.19
5.18
4.23
4.22
4.20
4.19
4.18
4.17
2.52
2.50
2.49
2.45
2.44
2.43
2.41
2.41
1.95
1.93
1.92
1.87
1.84
1.83
1.82
1.81
1.77
1.64
1.61
1.58
1.56
1.53
1.50
[O]
Br
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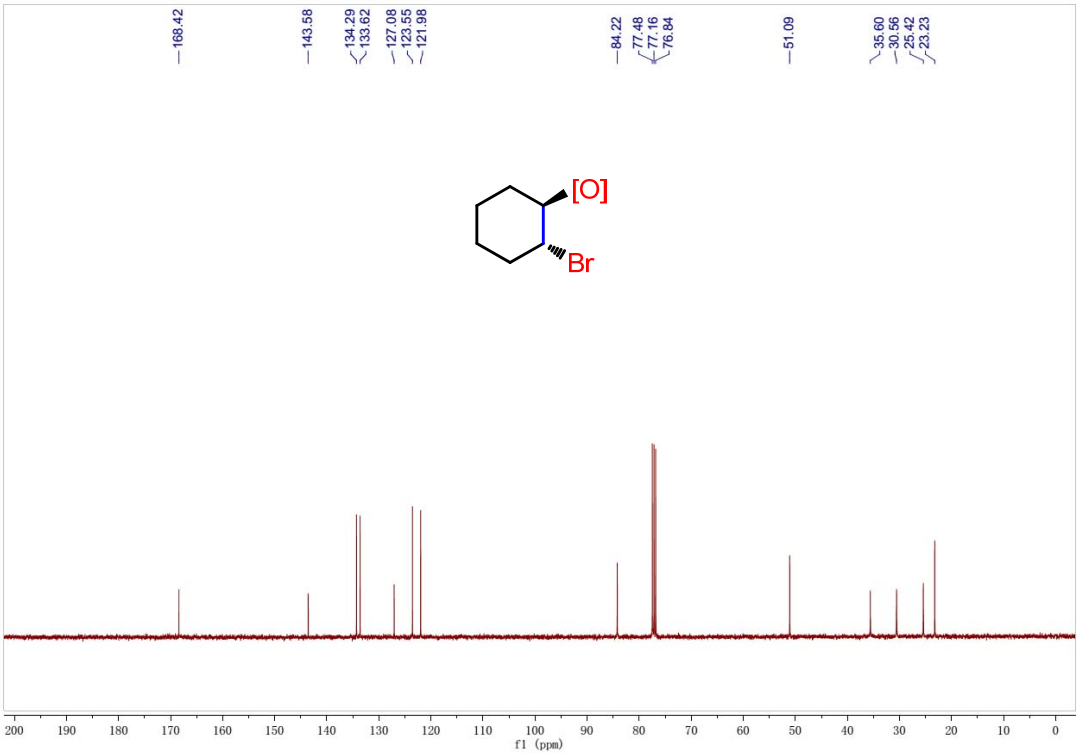
3.01
1.00
1.01
2.06
3.14
3.01
f1 (ppm)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123.55
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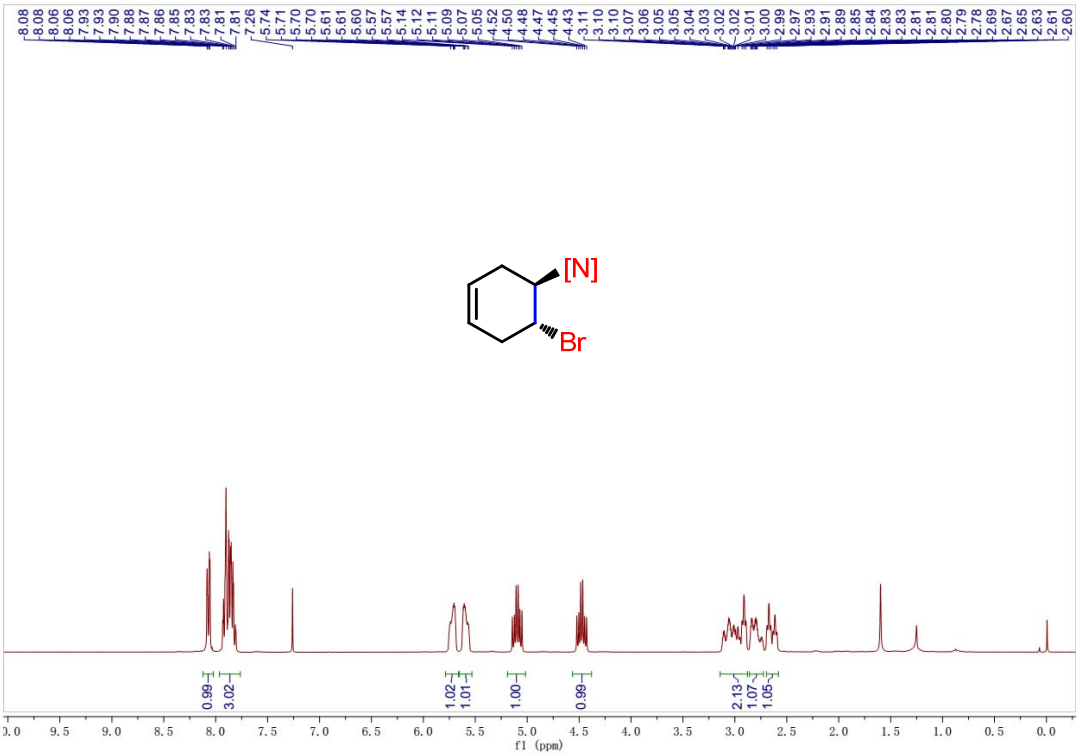
76.84
51.09
35.60
30.56
25.42
23.23
[O]
Br
f1 (ppm)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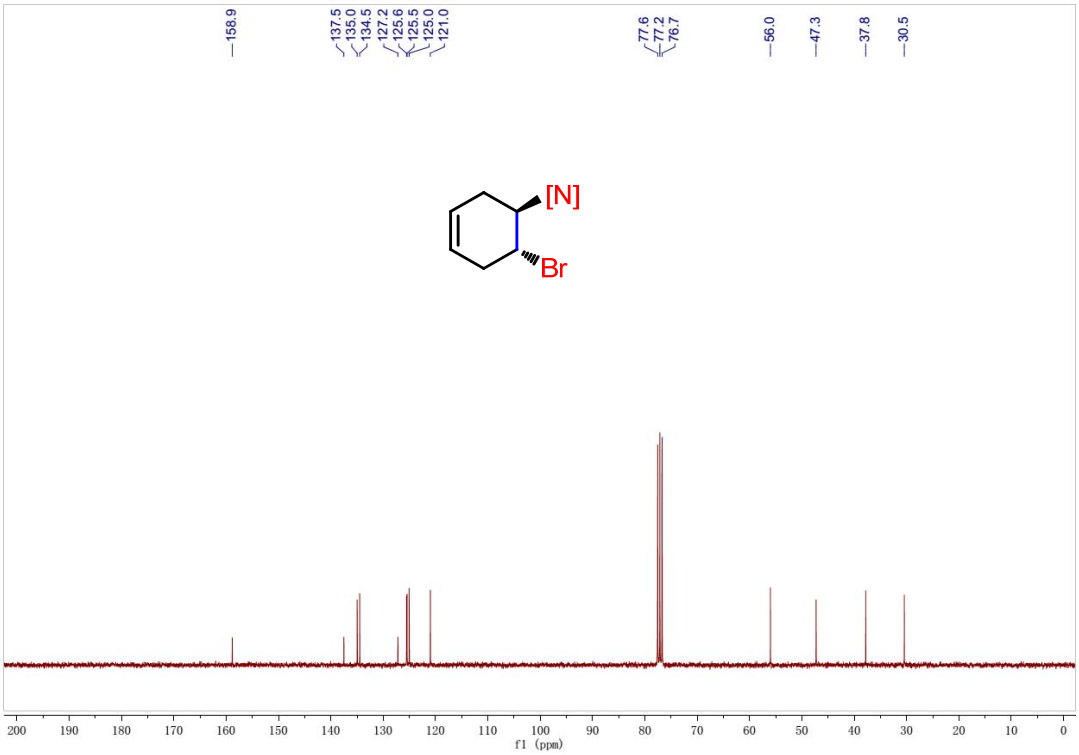
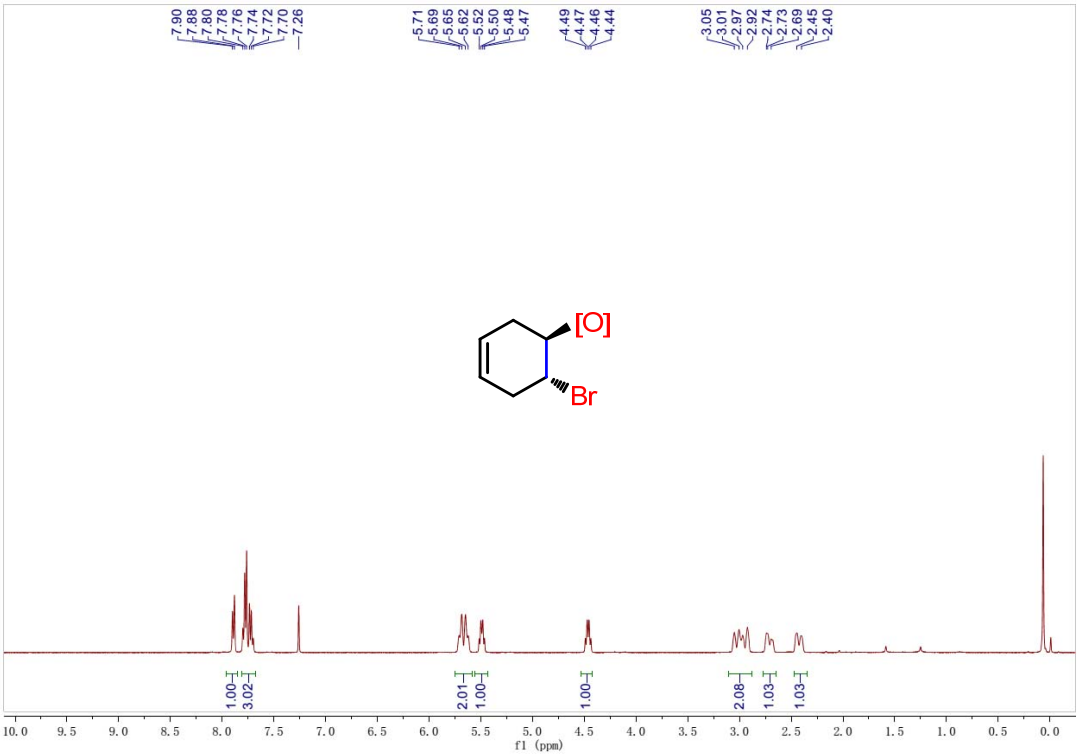
Br
f1 (ppm)


[N]
Br
f1 (ppm)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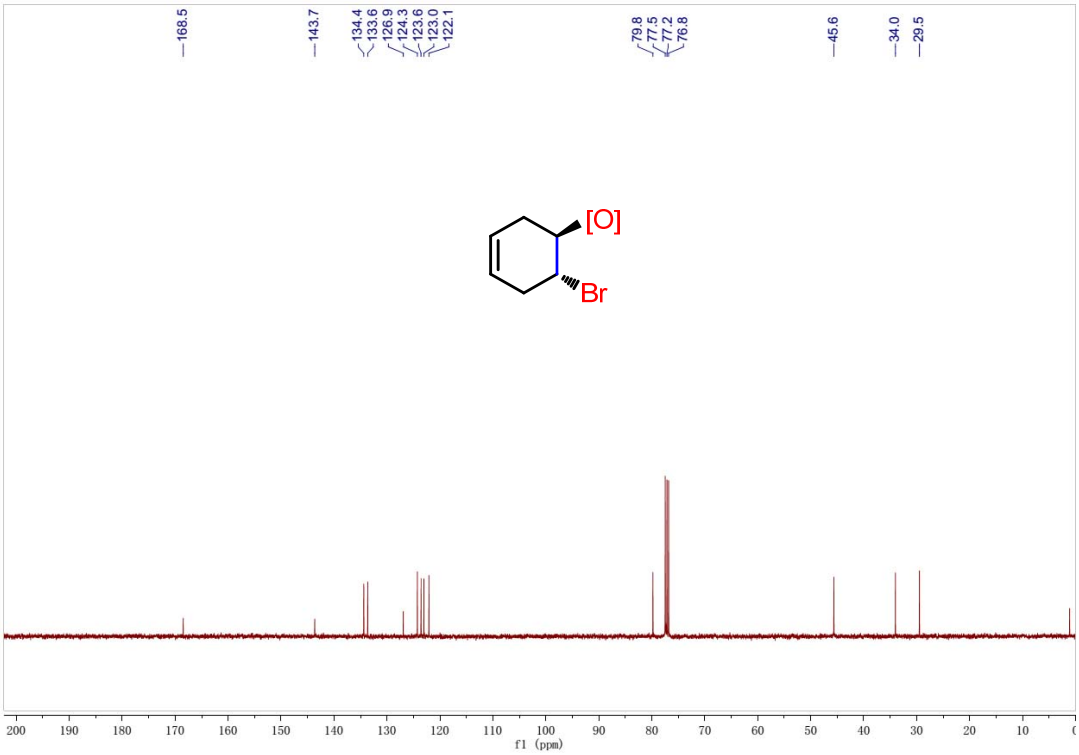
7.70
7.26
5.71
5.69
5.65
5.62
5.52
5.50
5.48
5.47
4.49
4.47
4.46
4.44
3.05
3.01
2.97
2.92
2.74
2.73
2.69
2.45
2.40
[O]
Br
1.00
3.02
2.01
1.00
1.00
2.08
1.03
1.03
f1 (ppm)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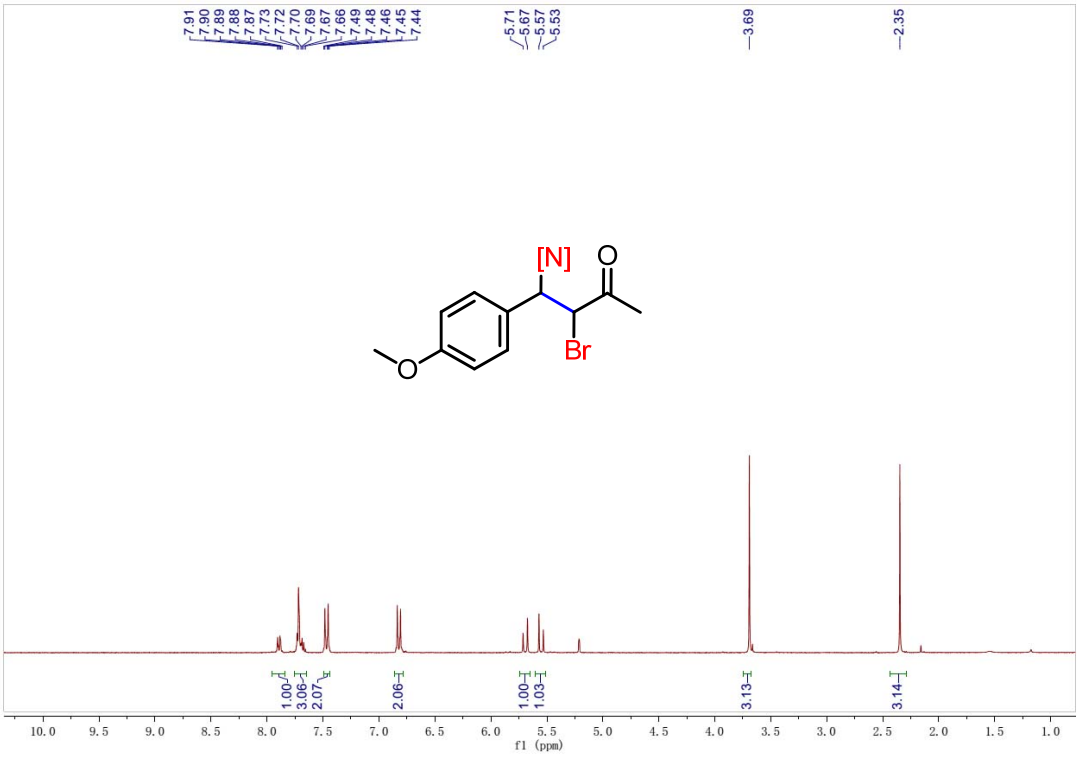
133.6
126.9
124.3
123.6
123.0
122.1
79.8
77.5
77.2
76.8
45.6
34.0
29.5
[O]
Br
f1 (ppm)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7.70
7.69
7.67
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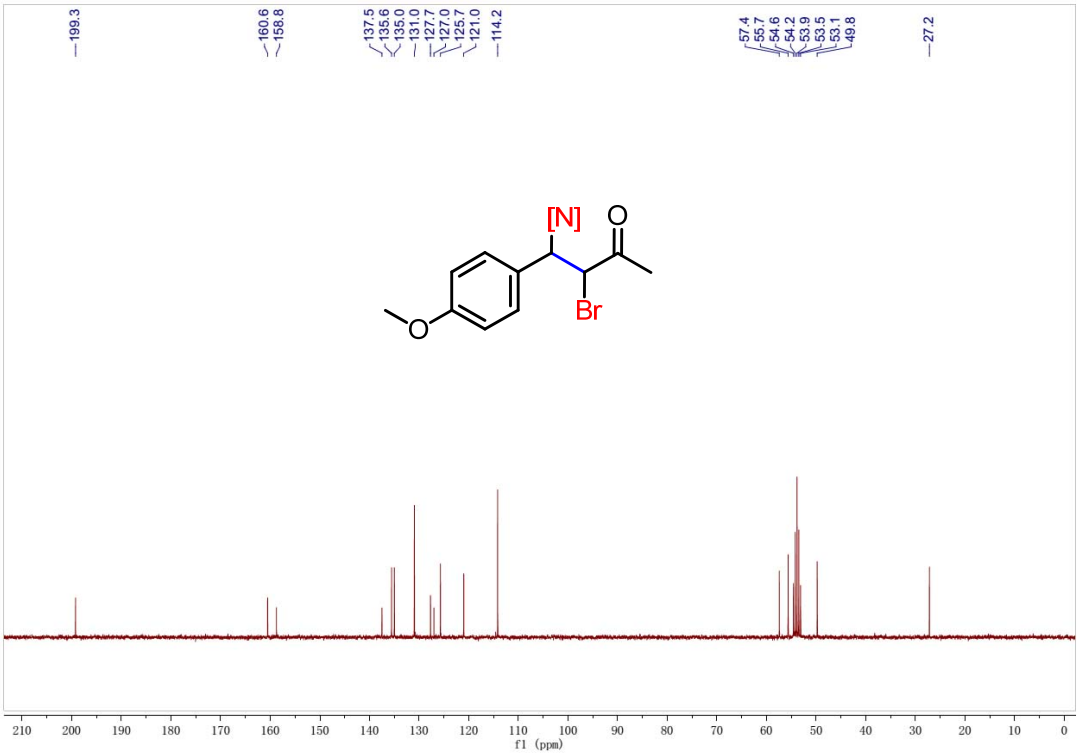
7.49
7.48
7.46
7.45
7.44
5.71
5.67
5.57
5.53
3.69
2.35
[N]
O
Br
O
1.00
3.06
2.07
2.06
1.00
1.03
3.13
3.14
f1 (ppm)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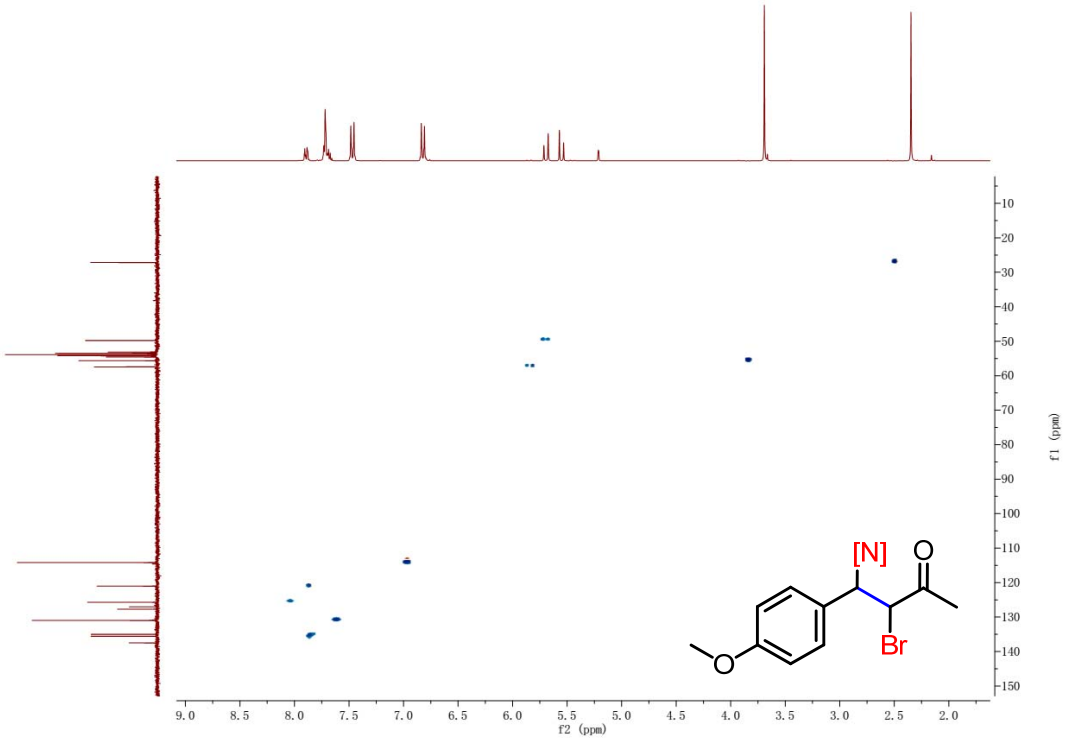
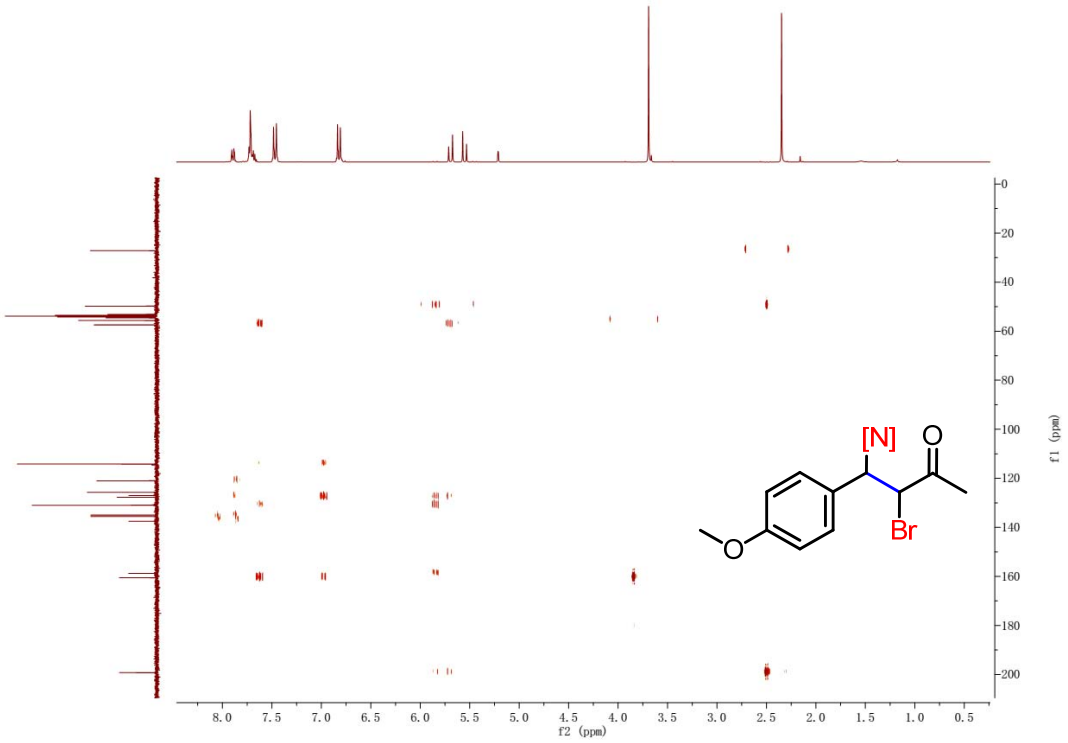
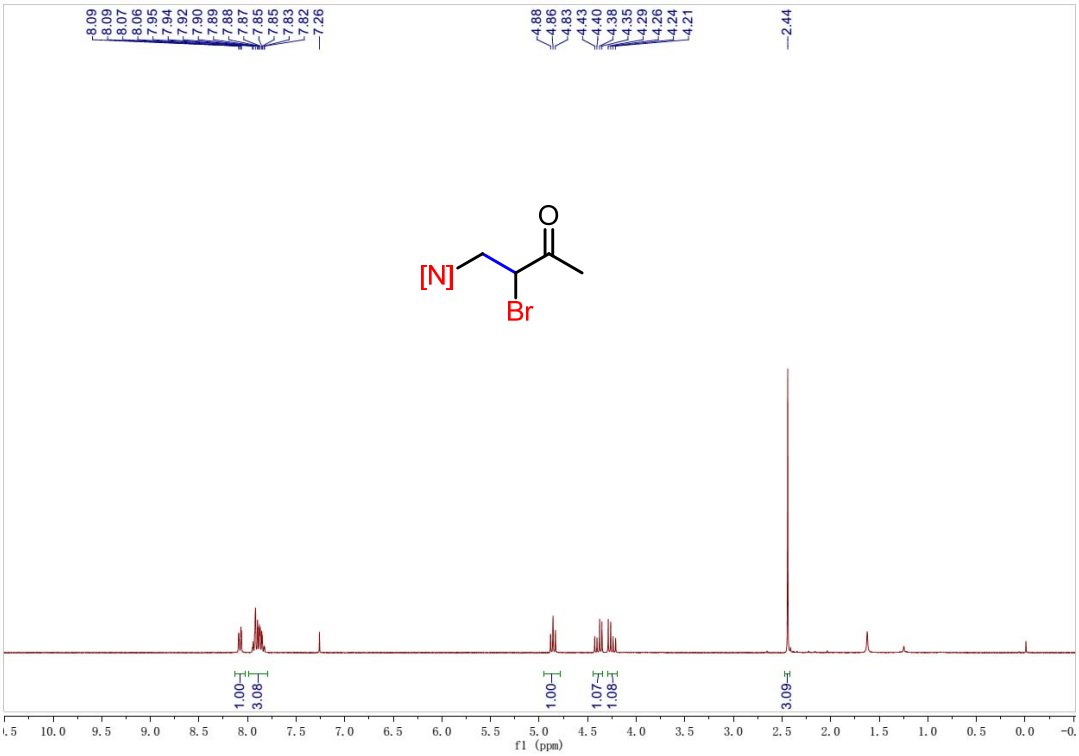
131.0
127.7
127.0
125.7
121.0
114.2
57.4
55.7
54.6
54.2
53.9
53.5
53.1
49.8
27.2
[N]
O
Br
O
f1 (ppm)

HSQC：



HMBC：

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8.09
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8.06
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7.94
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7.88
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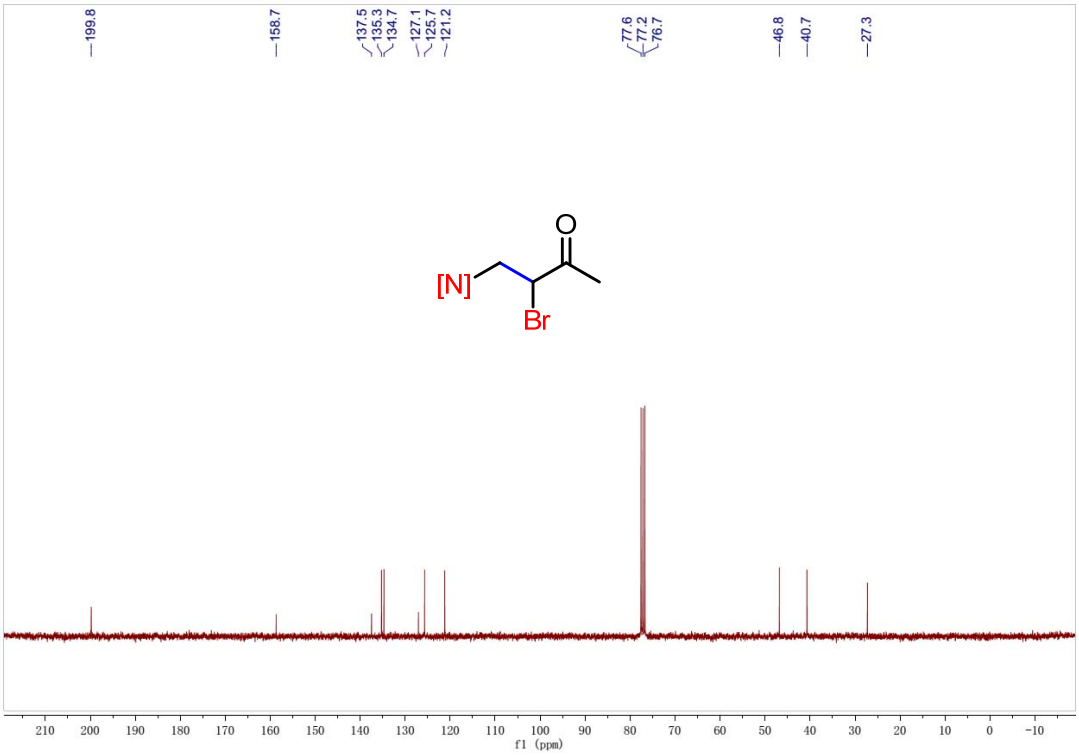
7.85
7.85
7.83
7.82
7.26
4.88
4.86
4.83
4.43
4.40
4.38
4.35
4.29
4.26
4.24
4.21
2.44
[N]
Br
1.00
3.08
1.00
1.07
1.08
3.09
f1 (ppm)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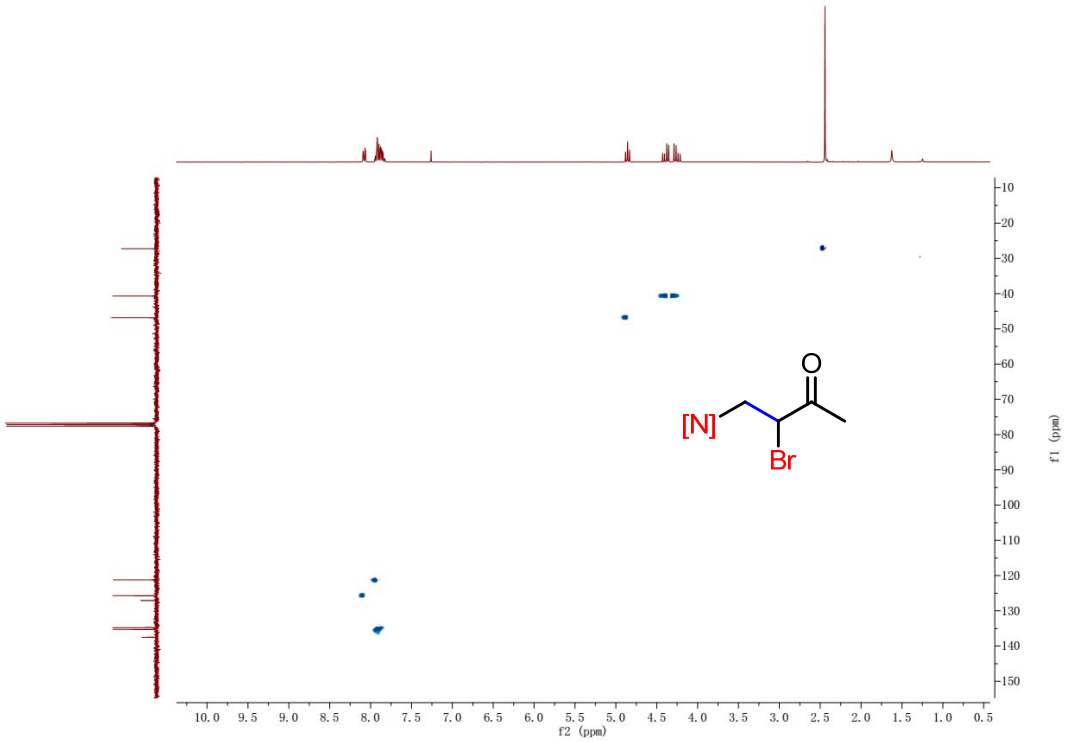
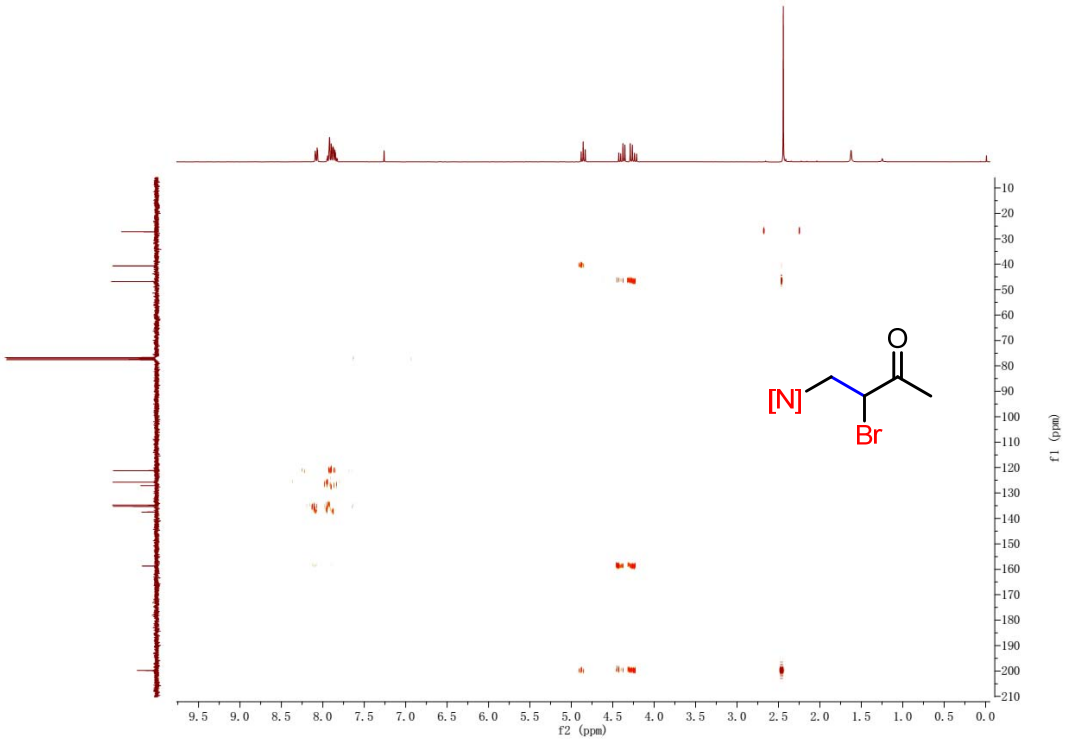
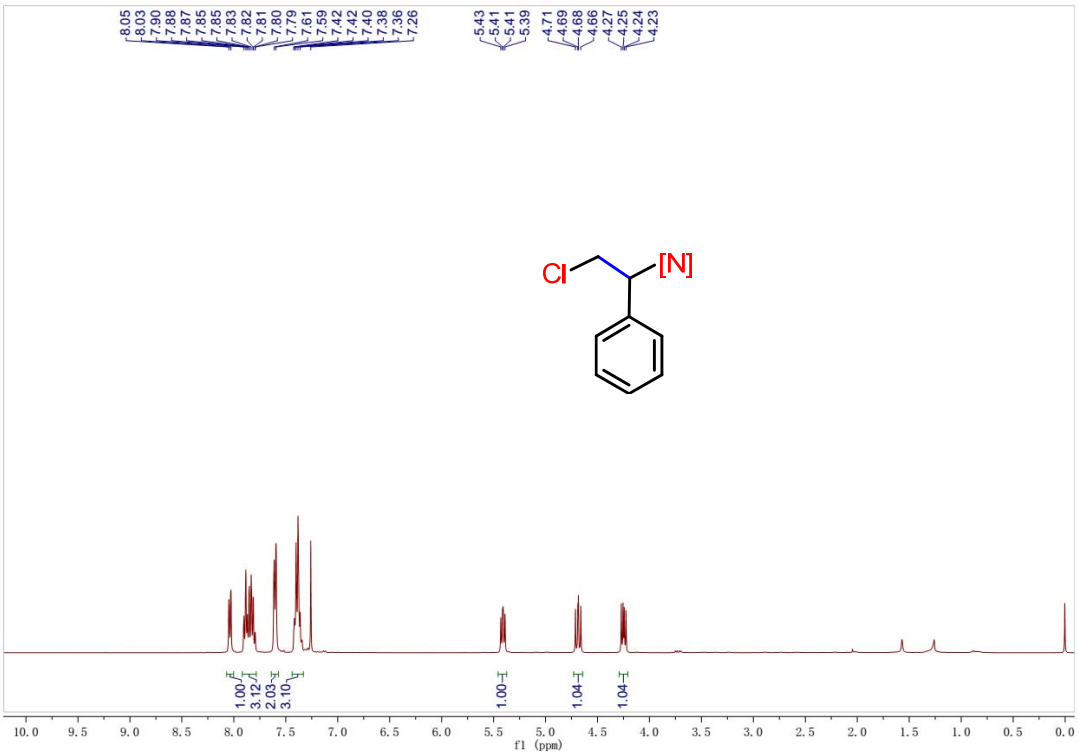
158.7
137.5
135.3
134.7
127.1
125.7
121.2
77.6
77.2
76.7
46.8
40.7
27.3
[N]
Br
f1 (ppm)

HSQC：



HMBC：

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8.03
7.90
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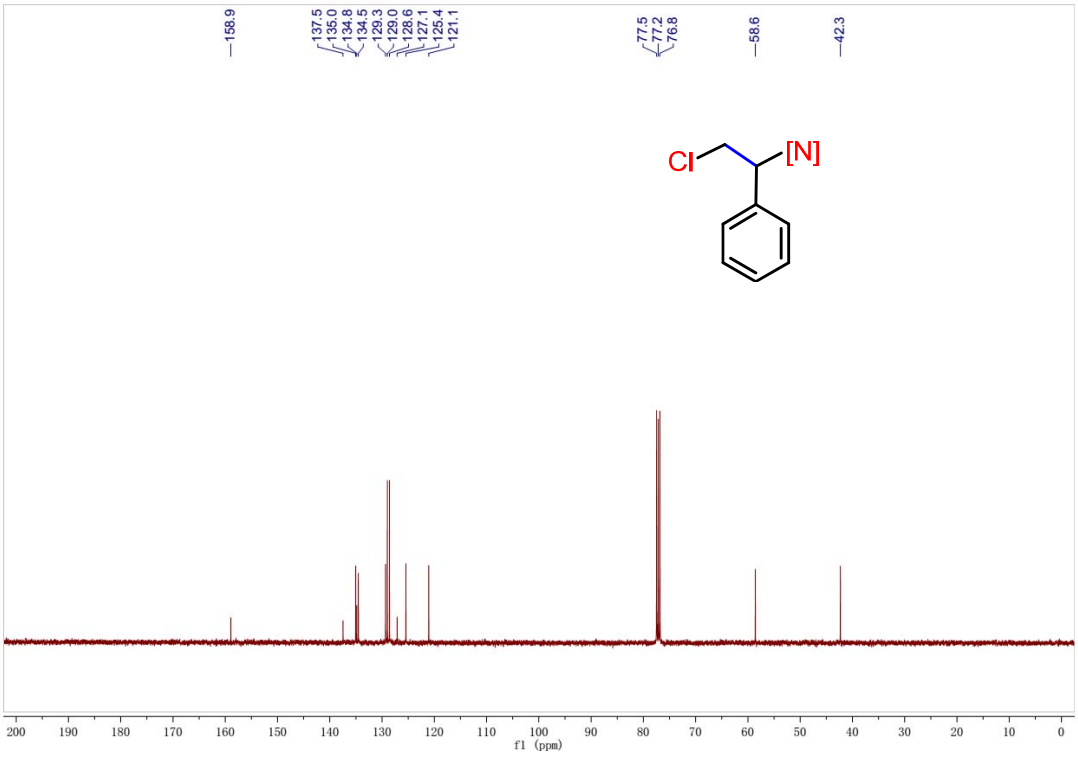
7.85
7.85
7.83
7.82
7.81
7.80
7.79
7.61
7.59
7.42
7.42
7.40
7.38
7.36
7.26
5.43
5.41
5.41
5.39
4.71
4.69
4.68
4.66
4.27
4.25
4.24
4.23
Cl
[N]
1.00
3.12
2.03
3.10
1.00
1.04
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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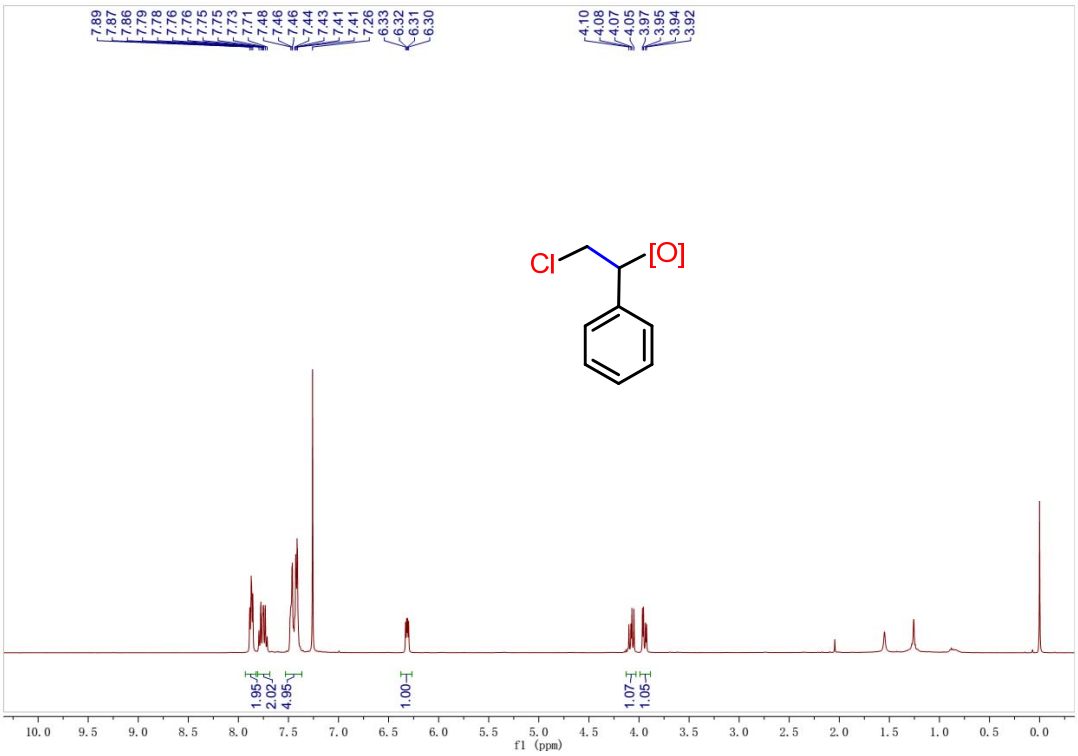
128.6
127.1
125.4
121.1
77.5
77.2
76.8
58.6
42.3
Cl
[N]
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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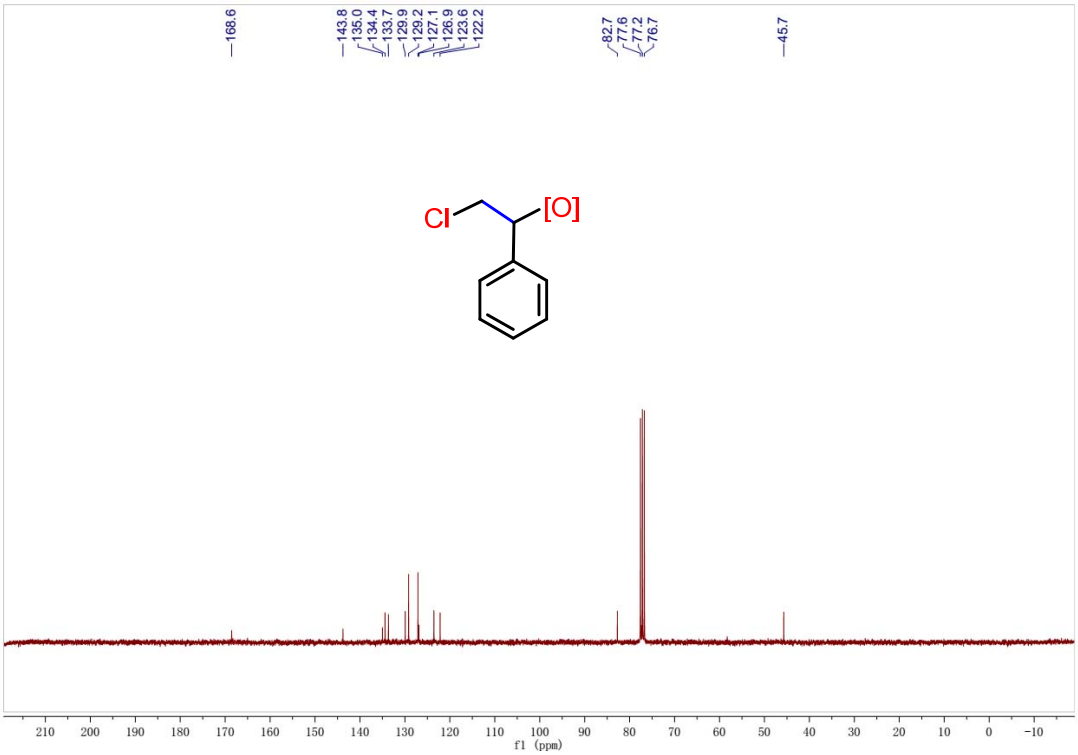
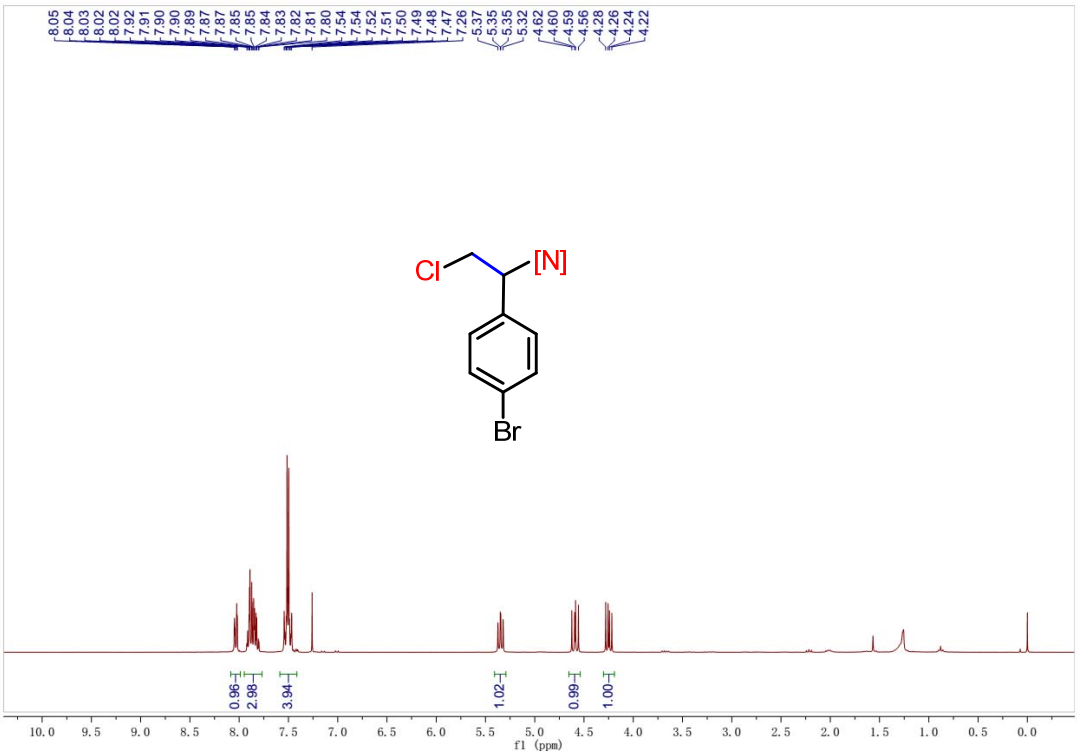
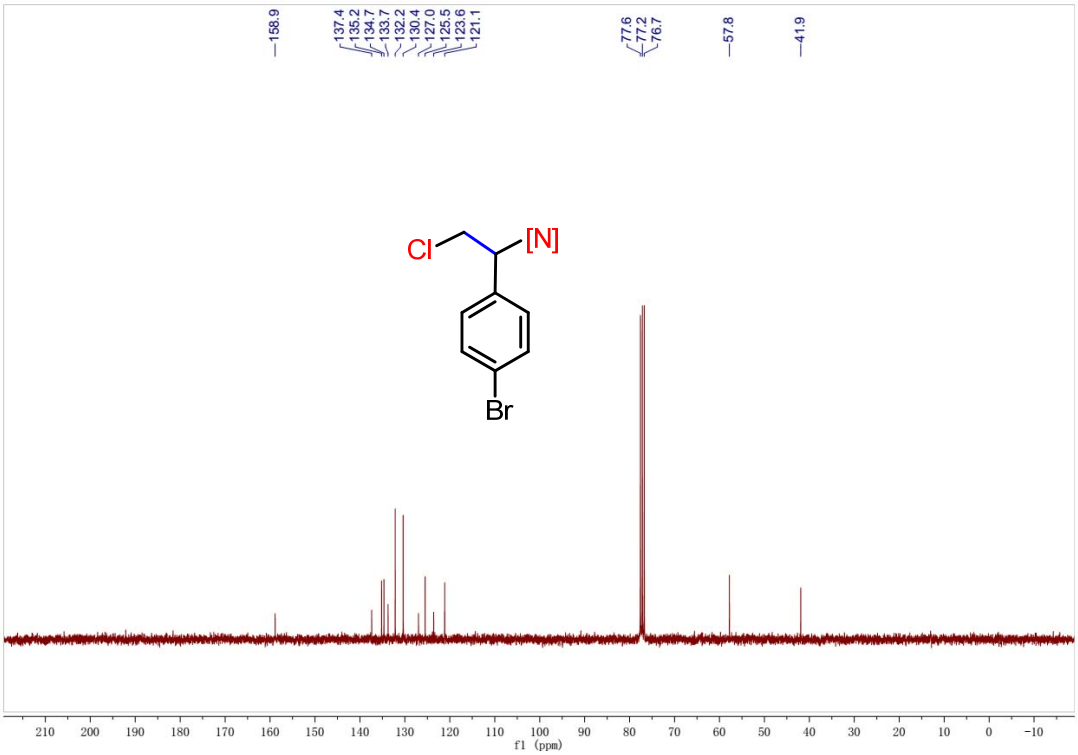
7.76
7.76
7.75
7.75
7.73
7.71
7.48
7.46
7.46
7.44
7.43
7.41
7.41
7.26
6.33
6.32
6.31
6.30
4.10
4.08
4.07
4.05
3.97
3.95
3.94
3.92
Cl
[O]
1.95
2.02
4.95
1.00
1.07
1.05
f1 (ppm)


168.6
143.8
135.0
134.4
133.7
129.9
129.2
127.1
126.9
123.6
122.2
82.7
77.6
77.2
76.7
45.7
Cl
[O]
f1 (ppm)


8.05
8.04
8.03
8.02
8.02
7.92
7.91
7.90
7.90
7.89
7.87
7.87
7.85
7.85
7.84
7.83
7.82
7.81
7.80
7.54
7.54
7.52
7.51
7.50
7.49
7.48
7.47
7.26
5.37
5.35
5.35
5.32
4.62
4.60
4.59
4.56
4.28
4.26
4.24
4.22
Cl
[N]
Br
0.96
2.98
3.94
1.02
0.99
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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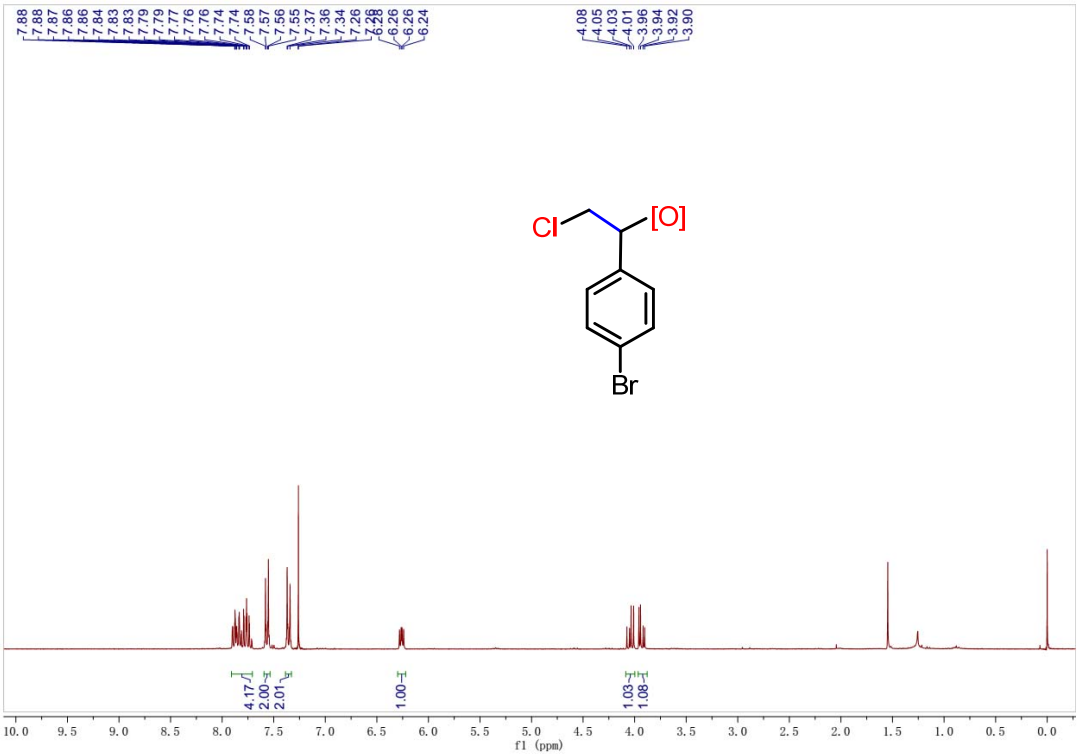
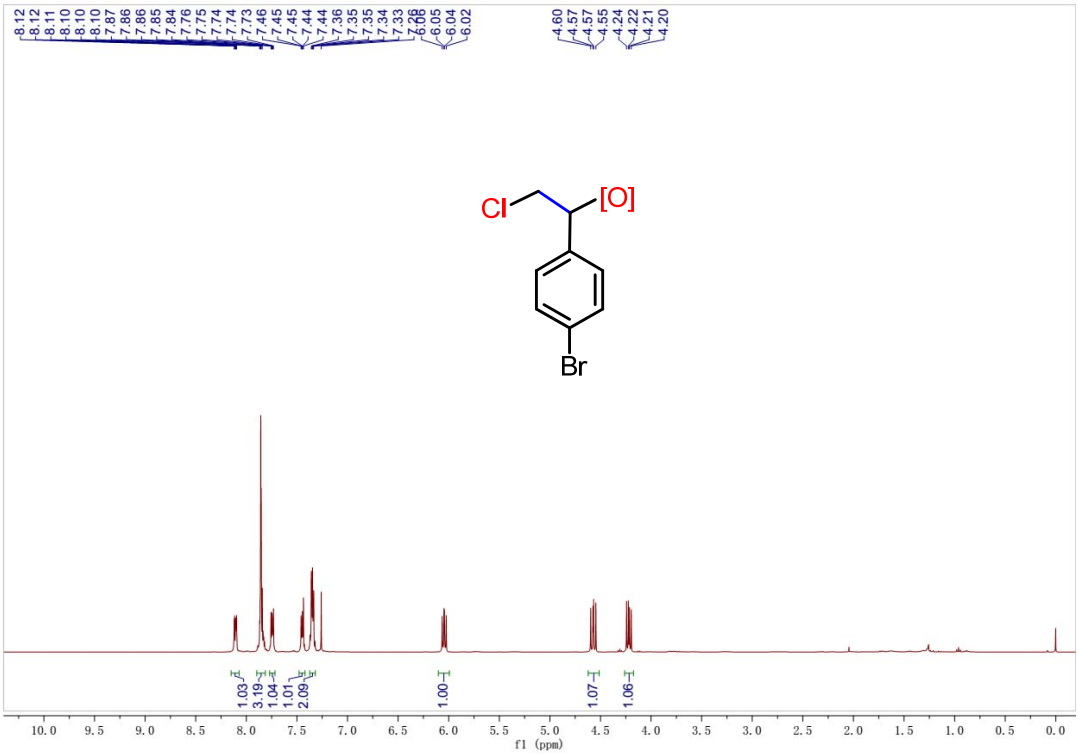
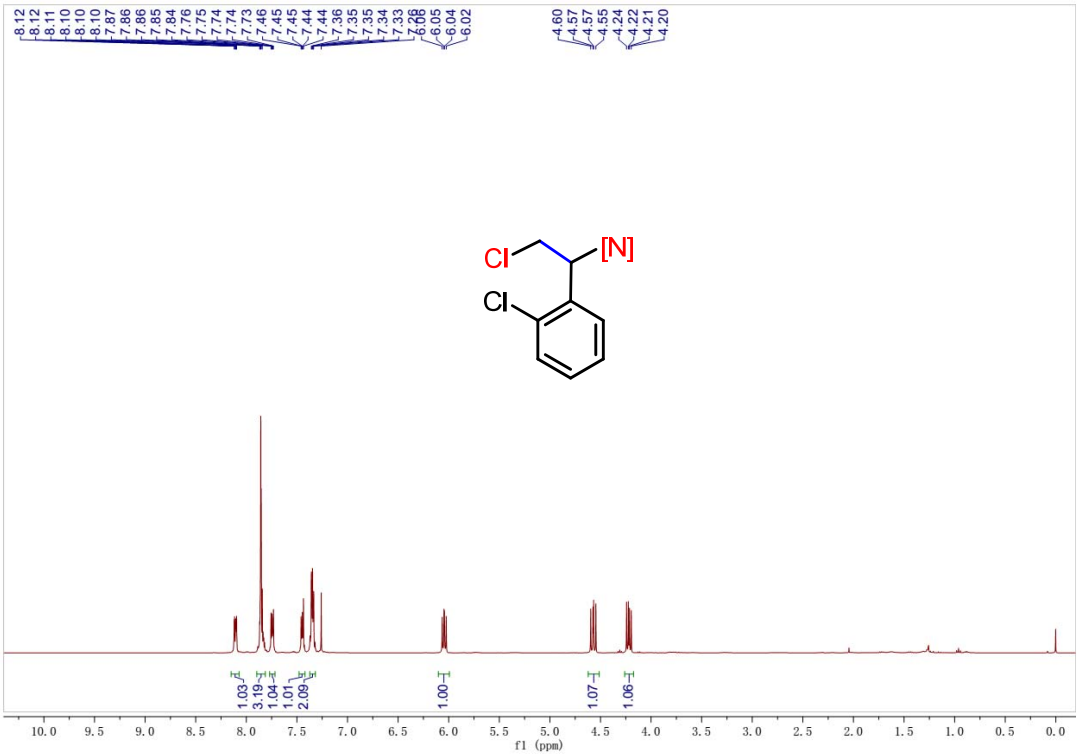
137.4
135.2
134.7
133.7
132.2
130.4
127.0
125.5
123.6
121.1
77.6
77.2
76.7
57.8
41.9
Cl
[N]
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


Cl
[O]
Br
f1 (ppm)


Cl
[O]
Br
f1 (ppm)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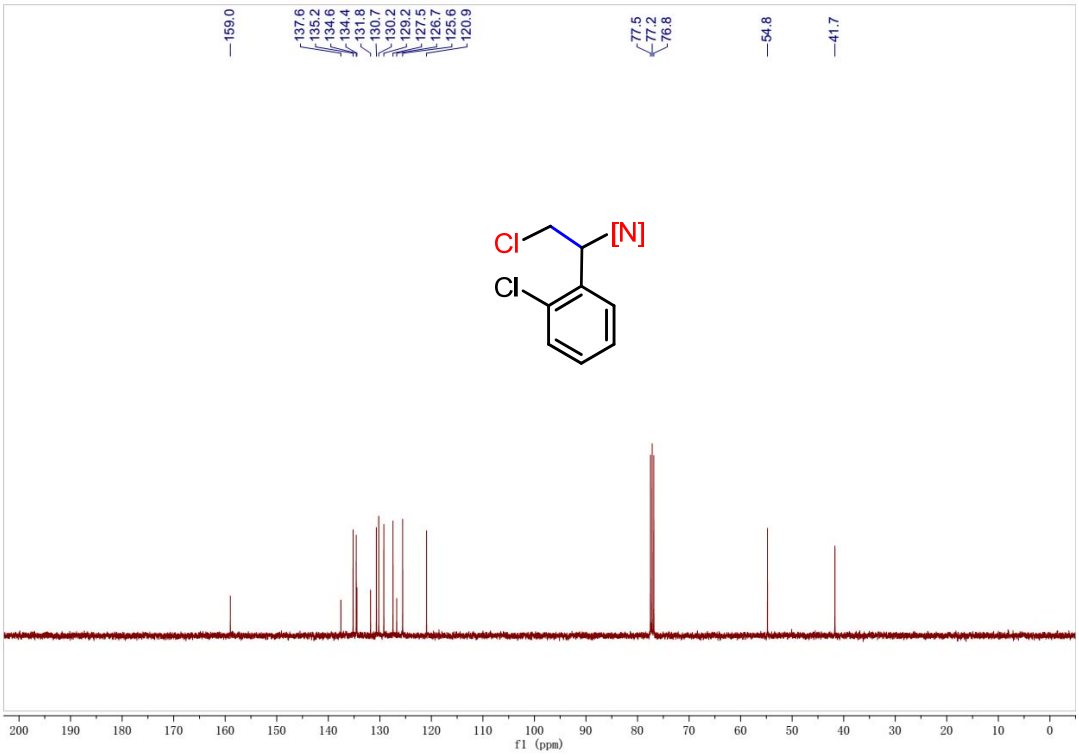
8.12
8.11
8.10
8.10
8.10
7.87
7.86
7.86
7.85
7.84
7.76
7.75
7.74
7.74
7.73
7.46
7.45
7.45
7.44
7.44
7.36
7.35
7.35
7.34
7.33
7.26
6.05
6.04
6.02
4.60
4.57
4.57
4.55
4.24
4.22
4.21
4.20
Cl
[N]
Cl
1.03
3.19
1.04
1.01
2.09
1.00
1.07
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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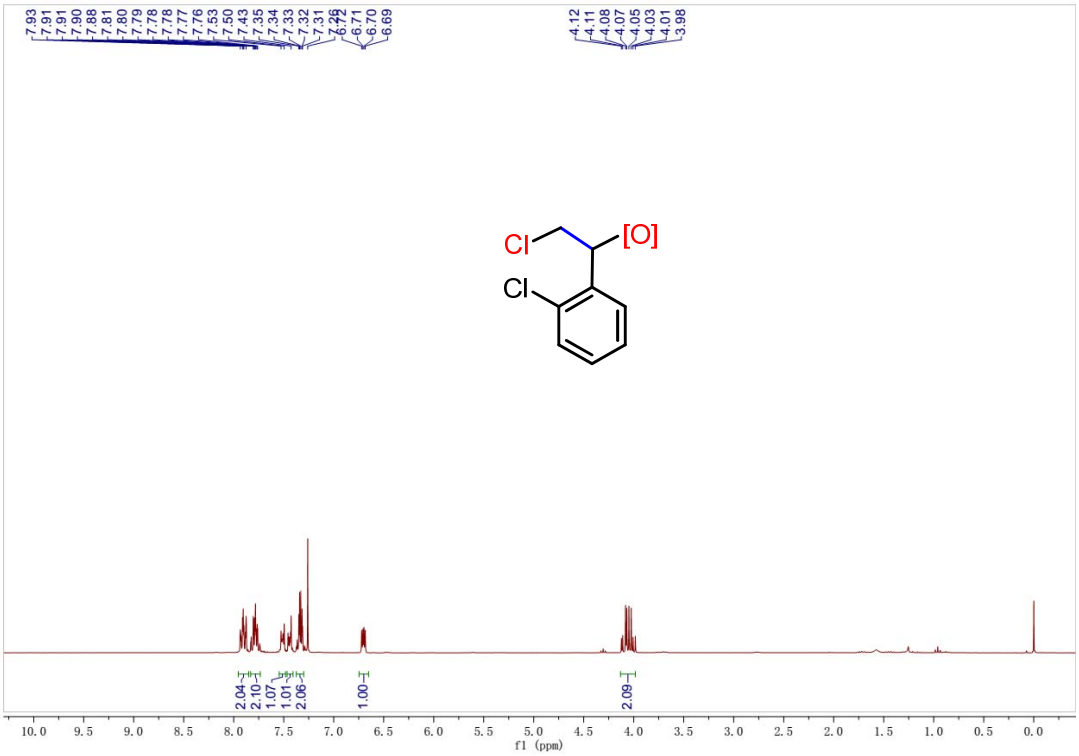
137.6
135.2
134.6
134.4
131.8
130.7
130.2
129.2
127.5
126.7
125.6
120.9
77.5
77.2
76.8
54.8
41.7
Cl
[N]
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.91
7.90
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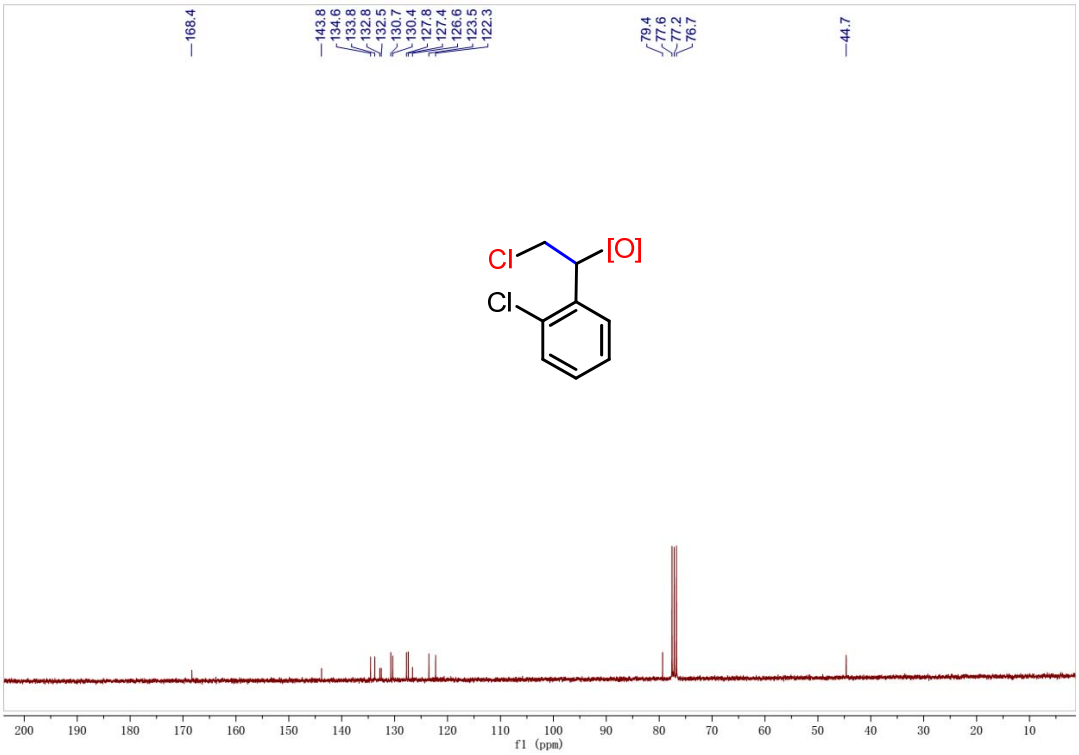
7.81
7.80
7.79
7.78
7.78
7.77
7.76
7.53
7.50
7.43
7.35
7.34
7.33
7.32
7.31
6.71
6.70
6.69
4.12
4.11
4.08
4.07
4.05
4.03
4.01
3.98
Cl
[O]
Cl
2.04
2.10
1.07
1.01
2.06
1.00
2.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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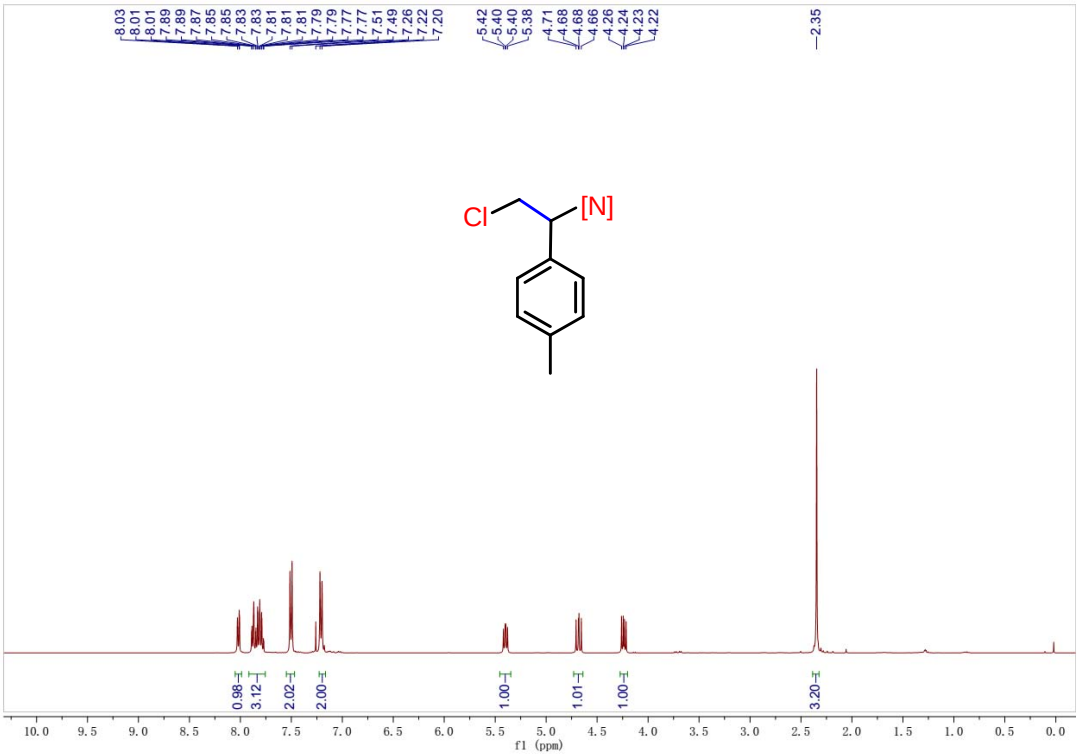
134.6
133.8
132.8
132.5
130.7
130.4
127.8
127.4
126.6
123.5
122.3
79.4
77.6
77.2
76.7
44.7
Cl
[O]
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.01
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7.85
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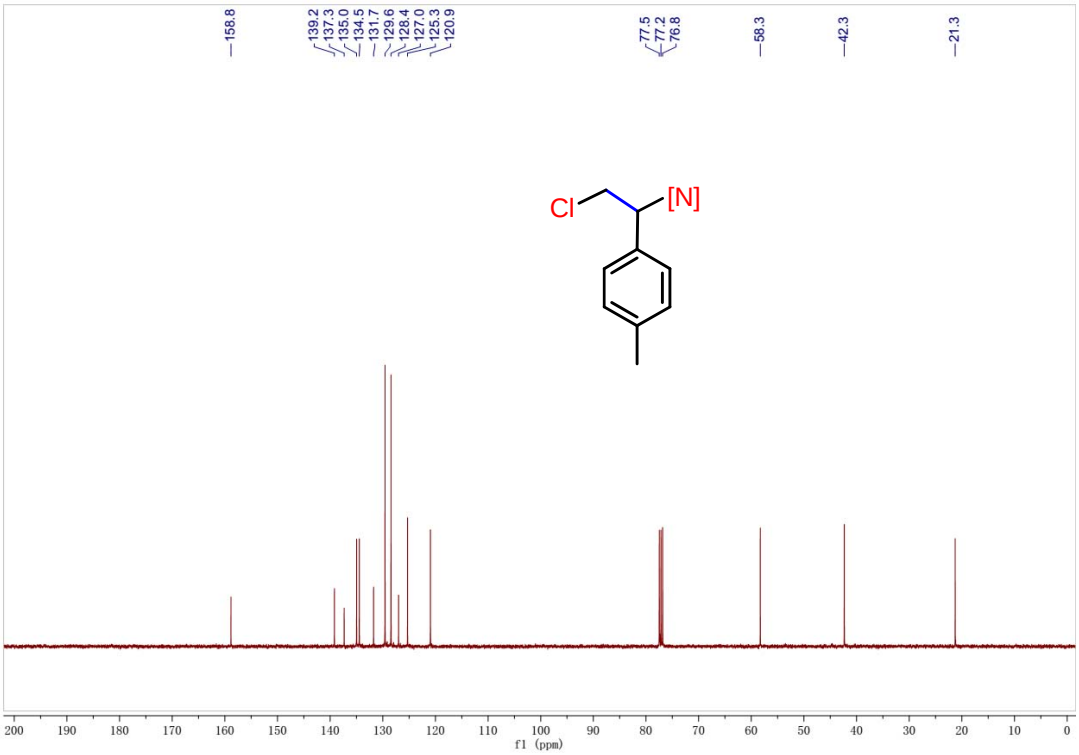
7.83
7.81
7.81
7.81
7.79
7.79
7.77
7.77
7.51
7.49
7.26
7.22
7.20
5.42
5.40
5.40
5.38
4.71
4.68
4.68
4.66
4.26
4.24
4.23
4.22
2.35
Cl
[N]
0.98
3.12
2.02
2.00
1.00
1.01
1.00
3.20
f1 (ppm)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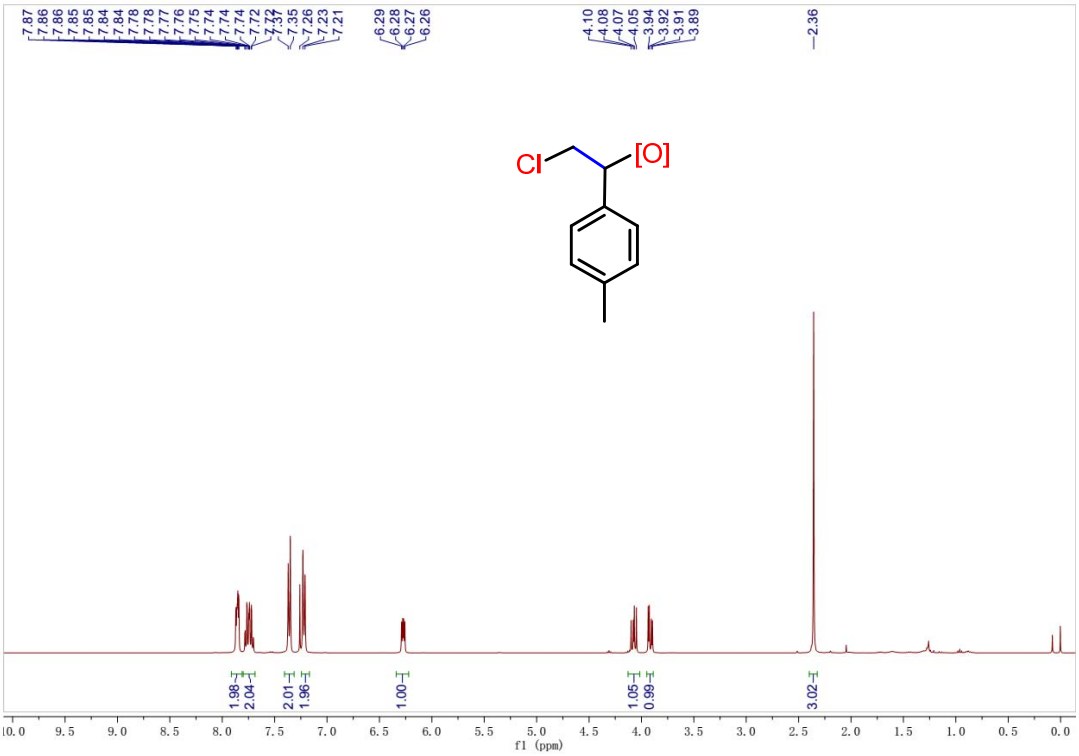
139.2
137.3
135.0
134.5
131.7
129.6
128.4
127.0
125.3
120.9
77.5
77.2
76.8
58.3
42.3
21.3
Cl
[N]
f1 (ppm)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7.84
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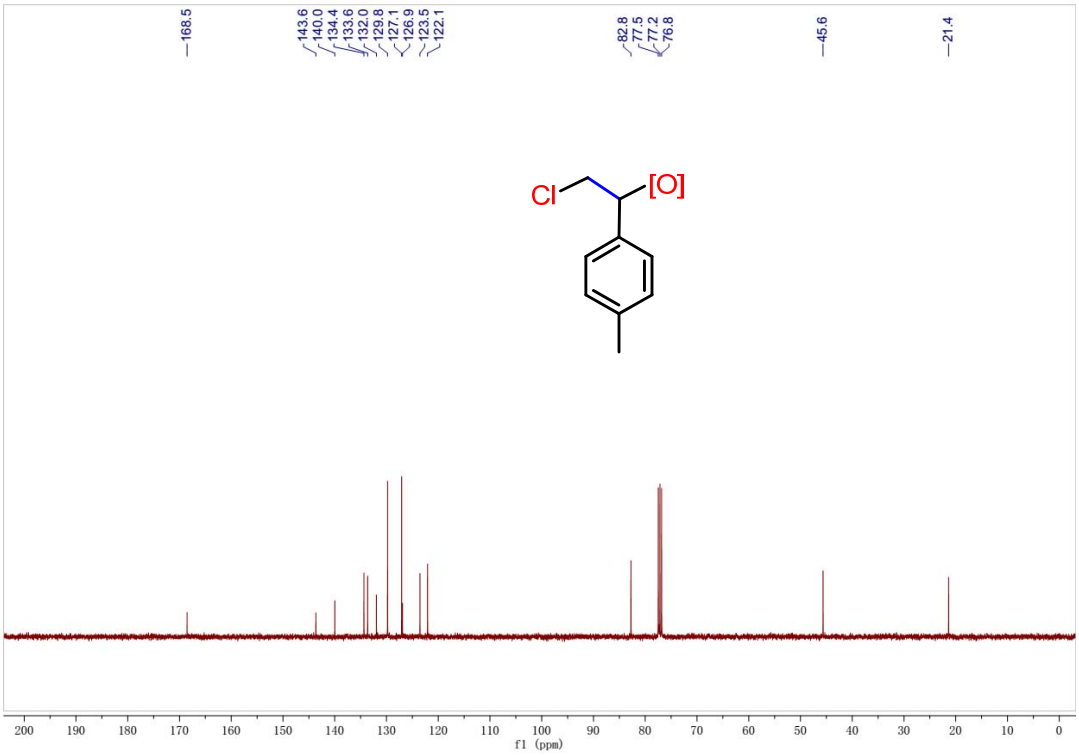
7.78
7.77
7.76
7.75
7.74
7.74
7.74
7.72
7.37
7.35
7.26
7.23
7.21
6.29
6.28
6.27
6.26
4.10
4.08
4.07
4.05
3.94
3.92
3.91
3.89
2.36
Cl
[O]
1.98
2.04
2.01
1.96
1.00
1.05
0.99
3.02
f1 (ppm)


168.5
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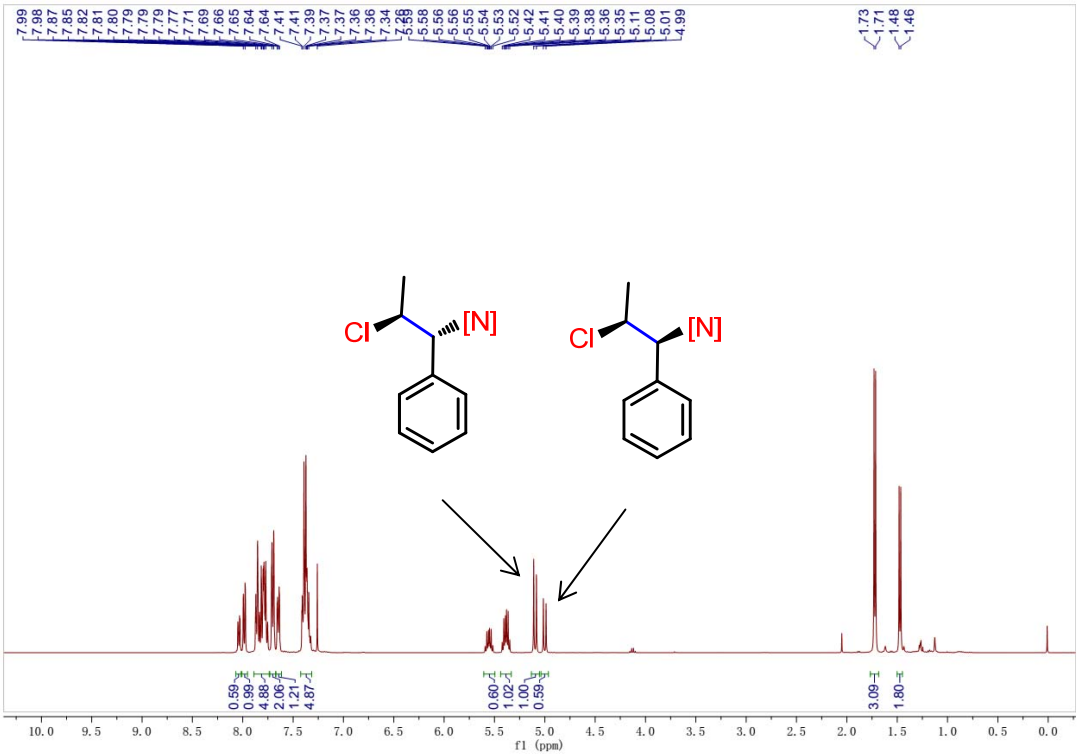
134.4
133.6
132.0
129.8
127.1
126.9
123.5
122.1
82.8
77.5
77.2
76.8
45.6
21.4
Cl
[O]
f1 (ppm)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7.80
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7.79
7.79
7.77
7.71
7.69
7.66
7.65
7.64
7.64
7.41
7.41
7.39
7.37
7.37
7.36
7.36
7.34
7.26
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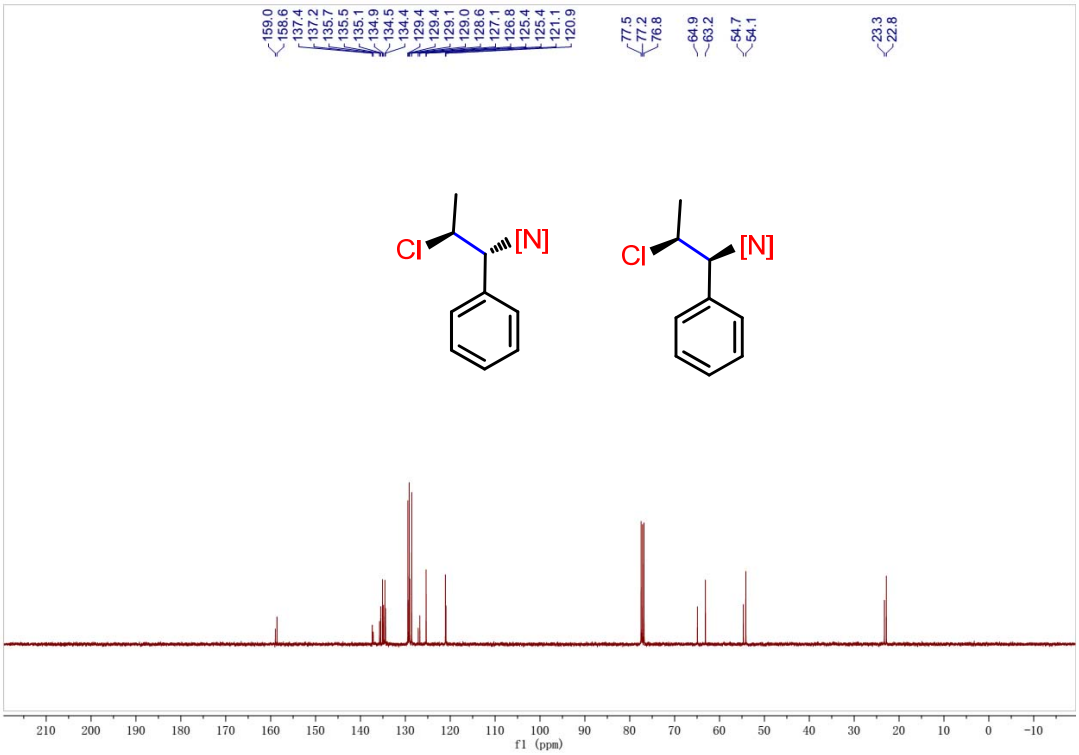
5.58
5.56
5.55
5.54
5.53
5.52
5.42
5.41
5.40
5.39
5.38
5.36
5.35
5.11
5.08
5.01
4.99
1.73
1.71
1.48
1.46
Cl
[N]
Cl
[N]
0.59
0.99
4.88
2.06
1.21
4.87
0.60
1.02
1.00
0.59
3.09
1.80
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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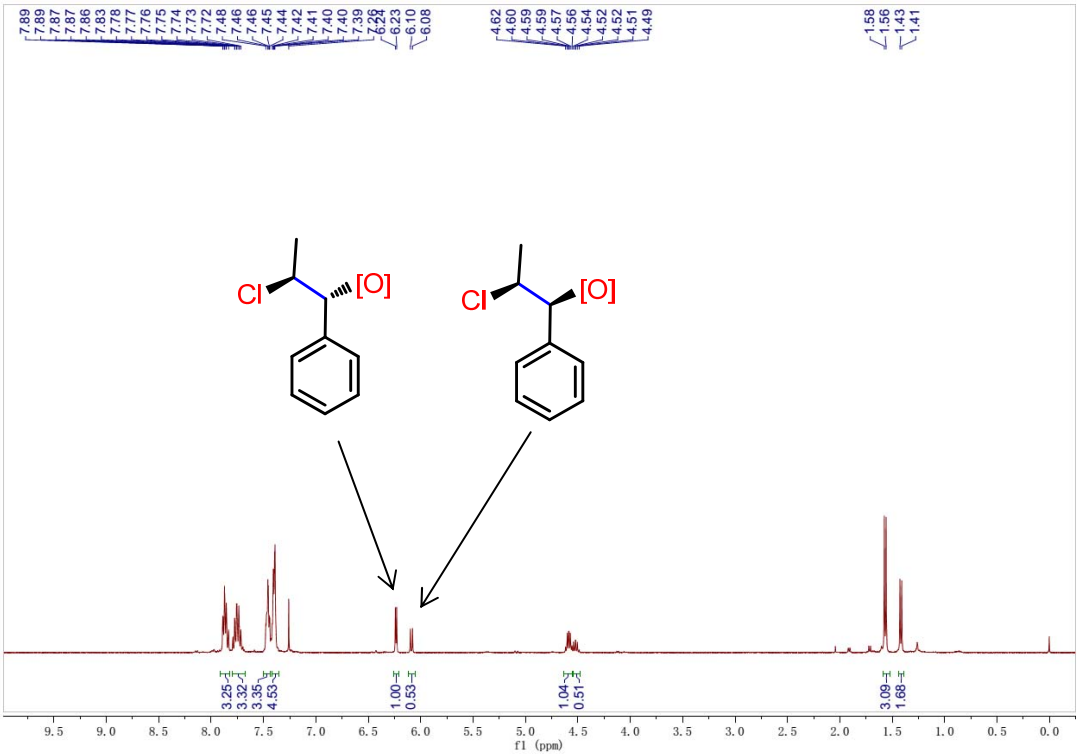
158.6
137.4
137.2
135.7
135.5
135.1
134.9
134.5
134.4
129.4
129.4
129.1
129.0
128.6
127.1
126.8
125.4
125.4
121.1
120.9
77.5
77.2
76.8
64.9
63.2
54.7
54.1
23.3
22.8
Cl
[N]
Cl
[N]
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.75
7.74
7.73
7.72
7.48
7.46
7.46
7.45
7.44
7.42
7.41
7.40
7.40
7.39
6.24
6.23
6.10
6.08
4.62
4.60
4.59
4.59
4.57
4.56
4.54
4.52
4.52
4.51
4.49
1.58
1.56
1.43
1.41
Cl
[O]
Cl
[O]
3.25
3.32
3.35
4.53
1.00
0.53
1.04
0.51
3.09
1.68
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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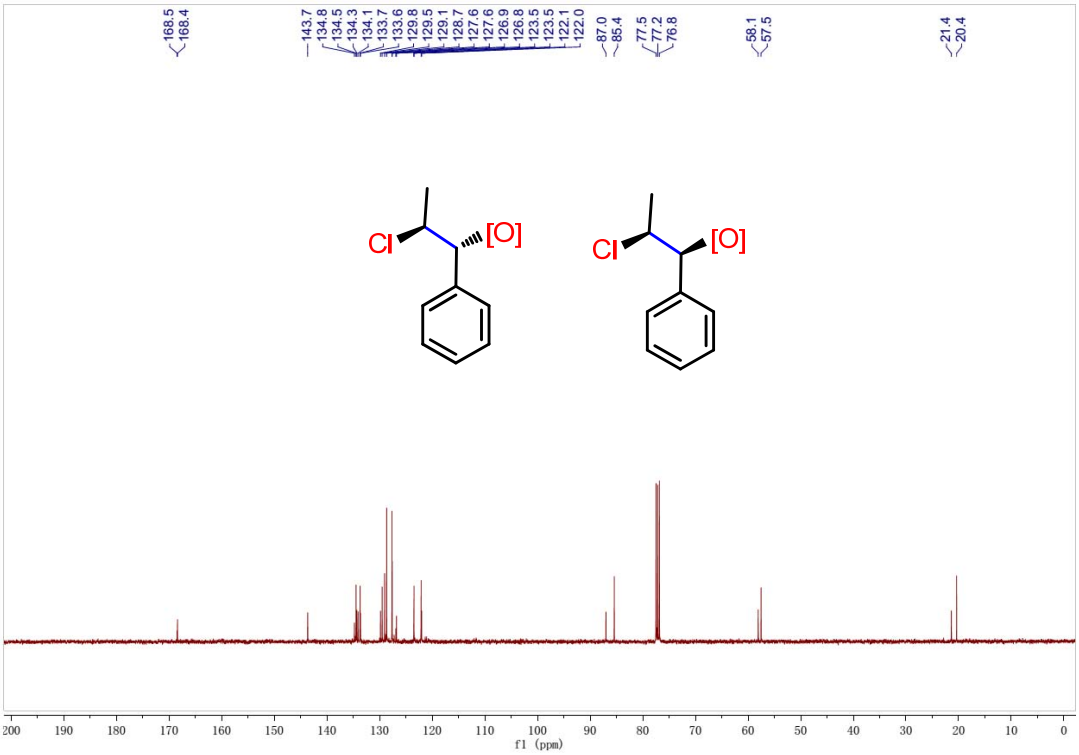
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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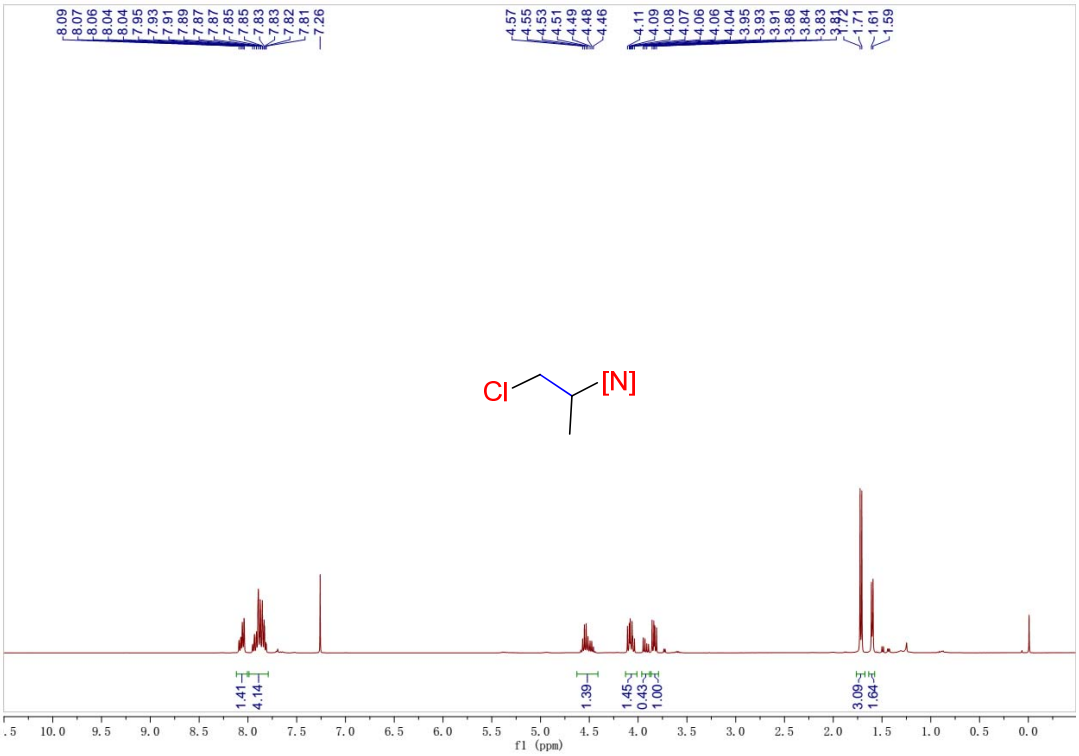
168.4
143.7
134.8
134.5
134.3
134.1
133.7
133.6
129.8
129.5
129.1
128.7
127.6
127.6
126.9
126.8
123.5
123.5
122.1
122.0
87.0
85.4
77.5
77.2
76.8
58.1
57.5
21.4
20.4
Cl
[O]
Cl
[O]
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.04
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7.85
7.83
7.83
7.82
7.81
7.26
4.57
4.55
4.53
4.51
4.49
4.48
4.46
4.11
4.09
4.08
4.07
4.06
4.06
4.04
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3.83
3.81
1.72
1.71
1.61
1.59
Cl
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4.14
1.39
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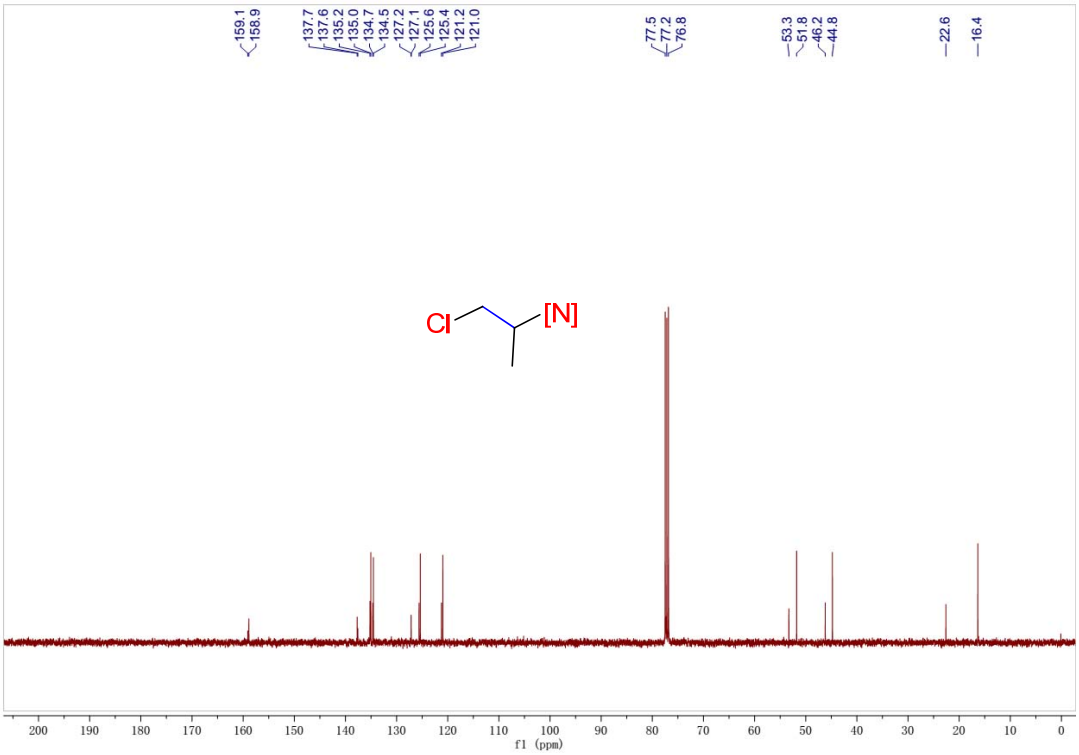
1.00
3.09
1.64
f1 (ppm)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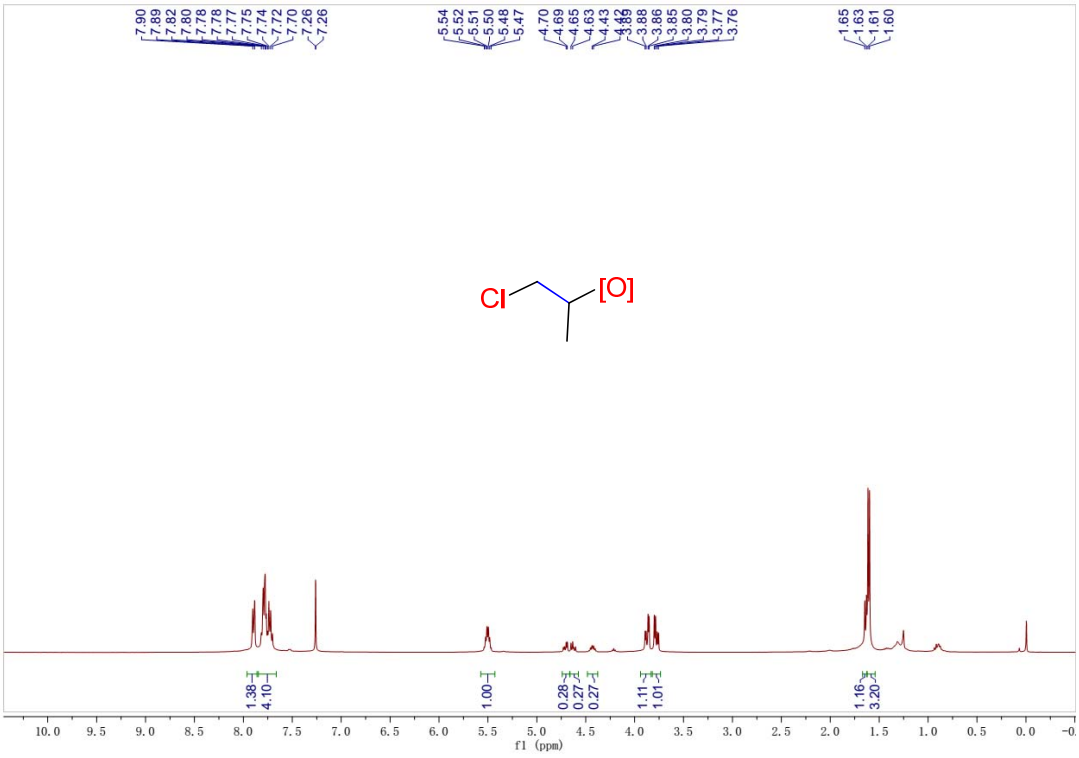
158.9
137.7
137.6
135.2
135.0
134.7
134.5
127.2
127.1
125.6
125.4
121.2
121.0
77.5
77.2
76.8
53.3
51.8
46.2
44.8
22.6
16.4
Cl
[N]
f1 (ppm)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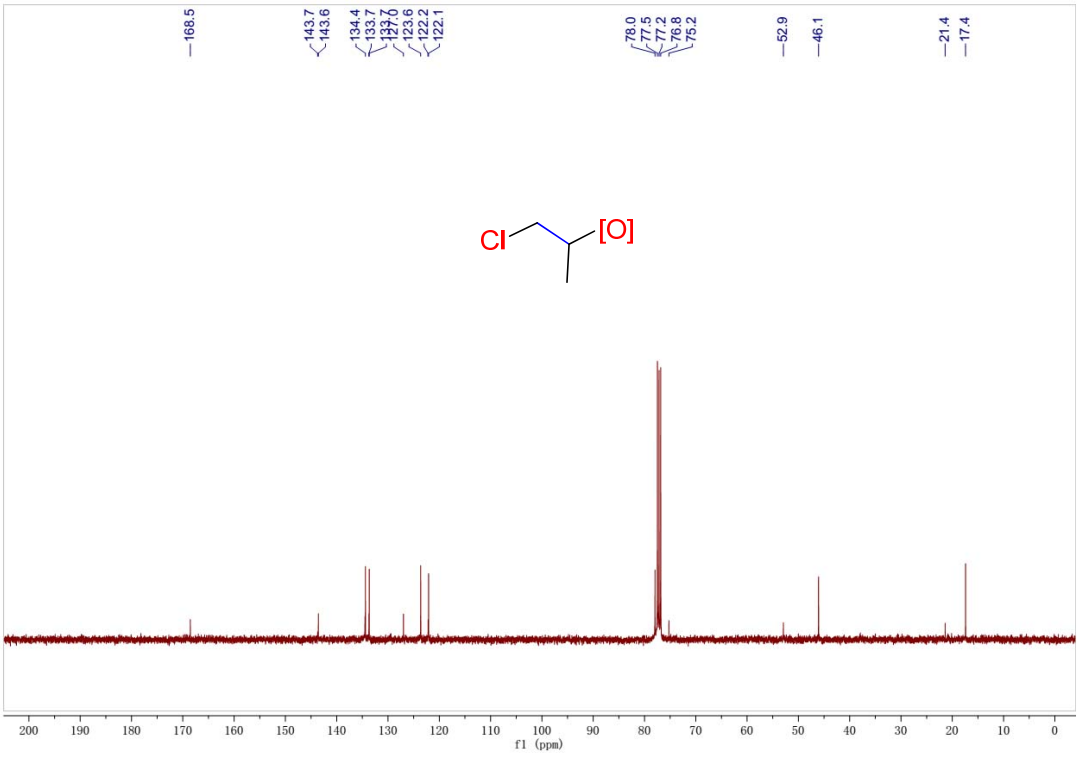
7.78
7.77
7.75
7.74
7.72
7.70
7.26
7.26
5.54
5.52
5.51
5.50
5.48
5.47
4.70
4.69
4.65
4.63
4.43
3.88
3.86
3.85
3.80
3.79
3.77
3.76
1.65
1.63
1.61
1.60
Cl
[O]
1.38
4.10
1.00
0.28
0.27
0.27
1.11
1.01
1.16
3.20
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.5
143.7
143.6
134.4
133.7
133.7
127.0
123.6
122.2
122.1
78.0
77.5
77.2
76.8
75.2
52.9
46.1
21.4
17.4
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[O]
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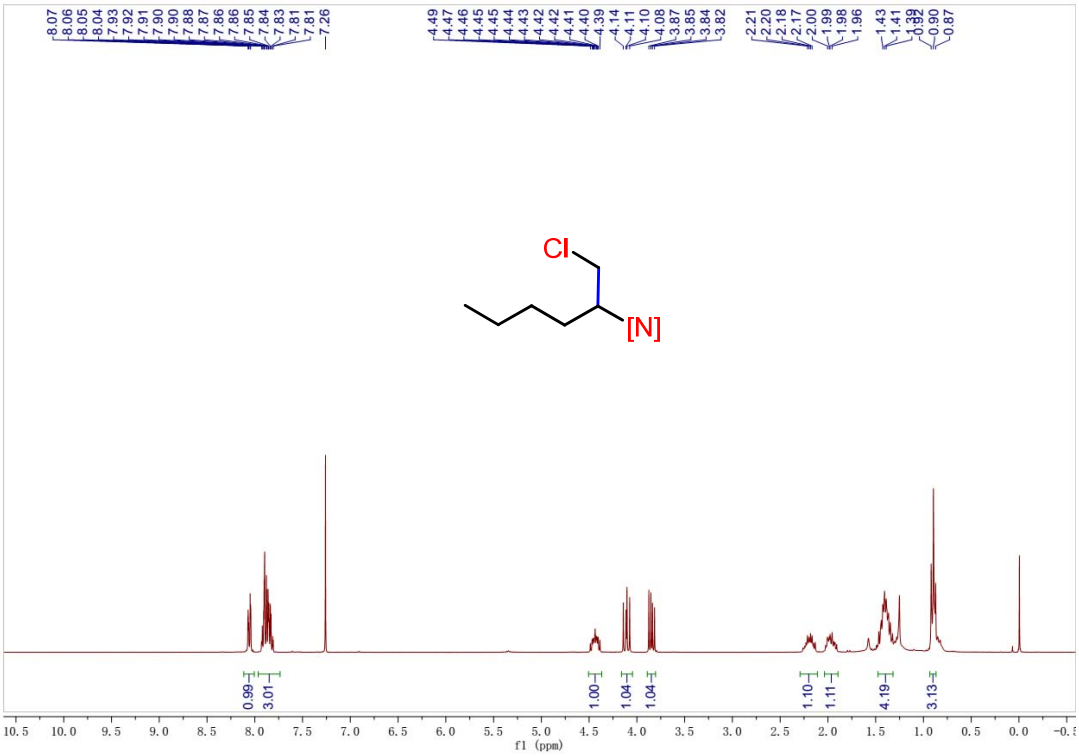
f1 (ppm)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8.04
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7.85
7.84
7.83
7.81
7.81
7.26
4.49
4.47
4.46
4.45
4.45
4.44
4.43
4.42
4.42
4.41
4.40
4.39
4.14
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4.08
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3.85
3.84
3.82
2.21
2.20
2.18
2.17
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1.98
1.96
1.43
1.41
0.90
0.87
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1.00
1.04
1.04
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1.11
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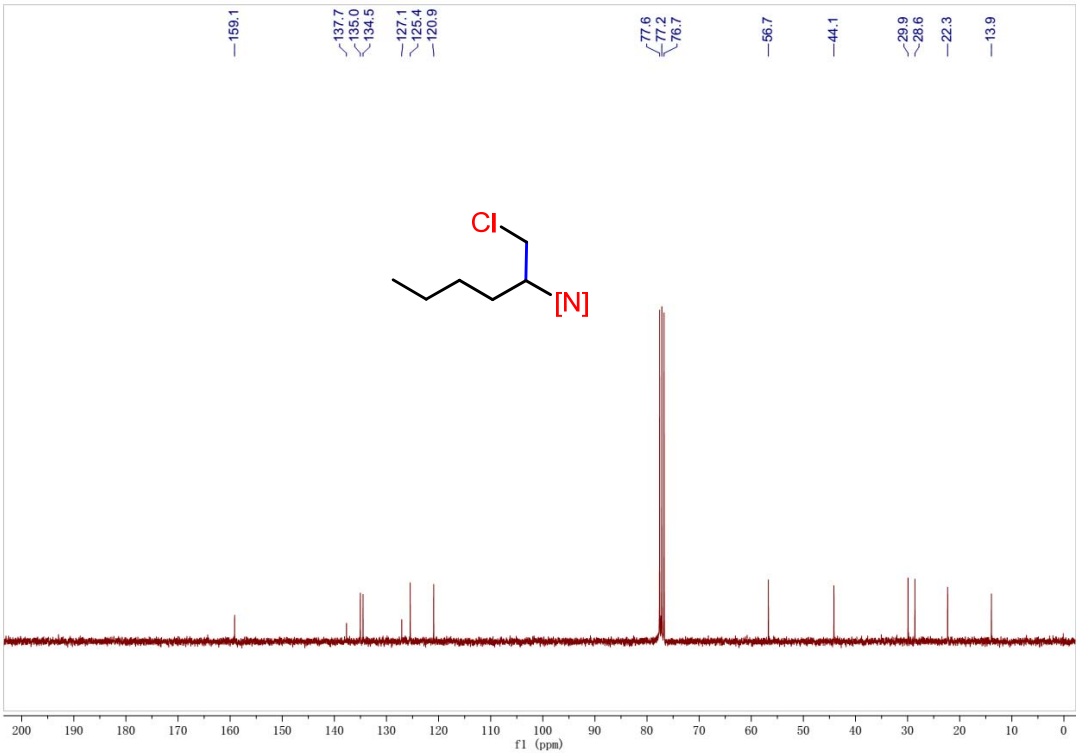
3.13
f1 (ppm)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125.4
120.9
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77.2
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56.7
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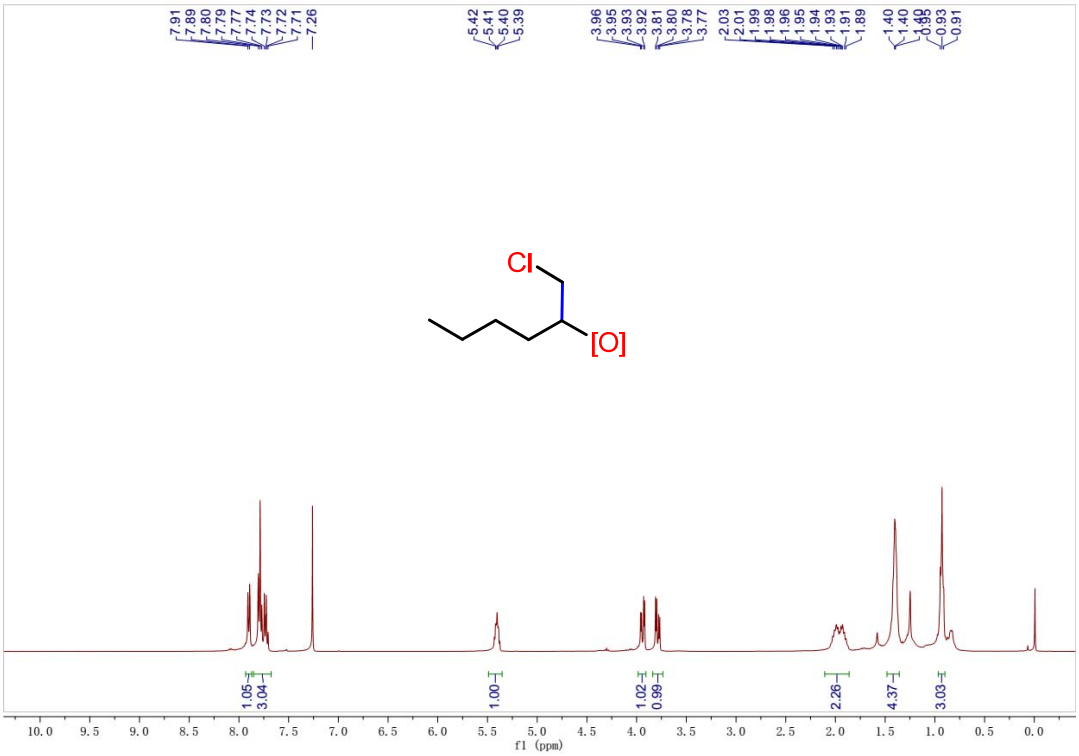
29.9
28.6
22.3
13.9
Cl
[N]
f1 (ppm)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7.72
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7.26
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5.41
5.40
5.39
3.96
3.95
3.93
3.92
3.81
3.80
3.78
3.77
2.03
2.01
1.99
1.98
1.96
1.95
1.94
1.93
1.91
1.89
1.40
1.40
0.95
0.93
0.91
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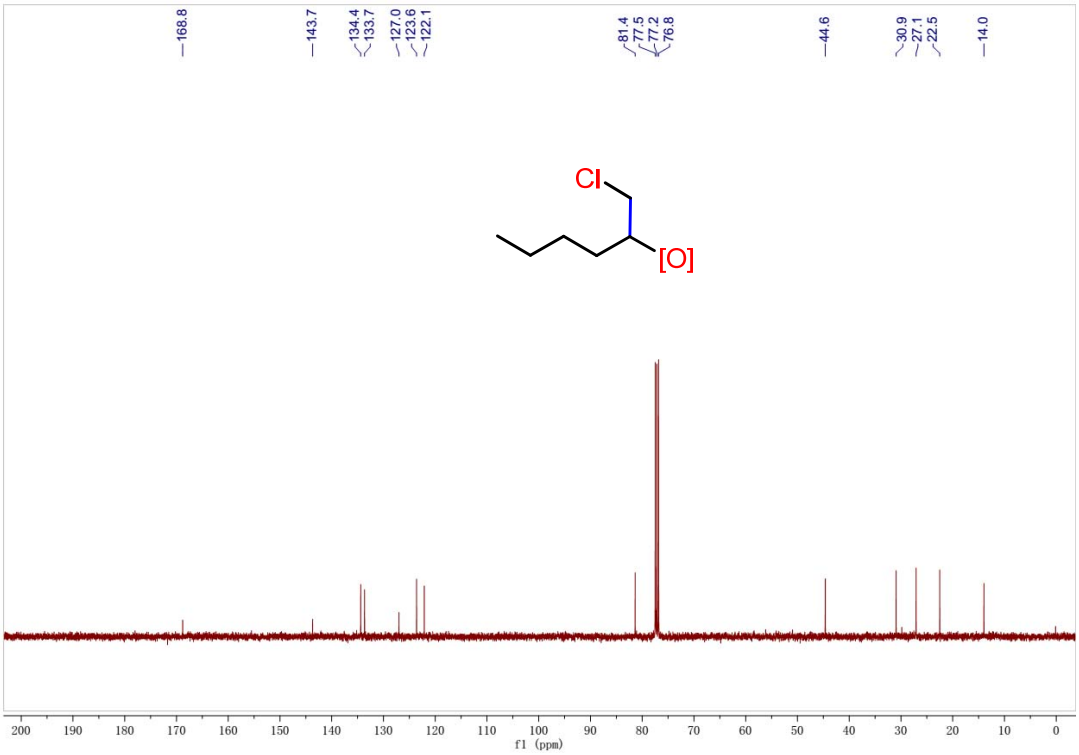
3.04
1.00
1.02
0.99
2.26
4.37
3.03
f1 (ppm)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122.1
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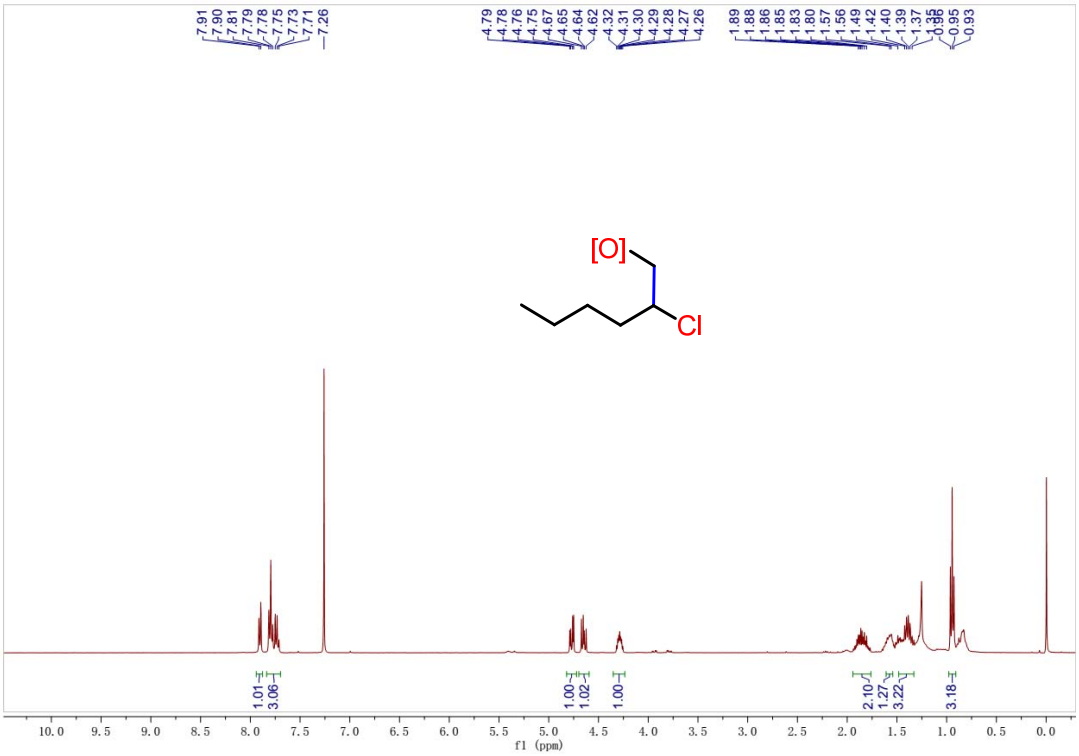
76.8
44.6
30.9
27.1
22.5
14.0
Cl
[O]
f1 (ppm)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7.71
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4.76
4.75
4.67
4.65
4.64
4.62
4.32
4.31
4.30
4.29
4.28
4.27
4.26
1.89
1.88
1.86
1.85
1.83
1.80
1.57
1.56
1.49
1.42
1.40
1.39
1.37
0.96
0.95
0.93
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Cl
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1.00
1.02
1.00
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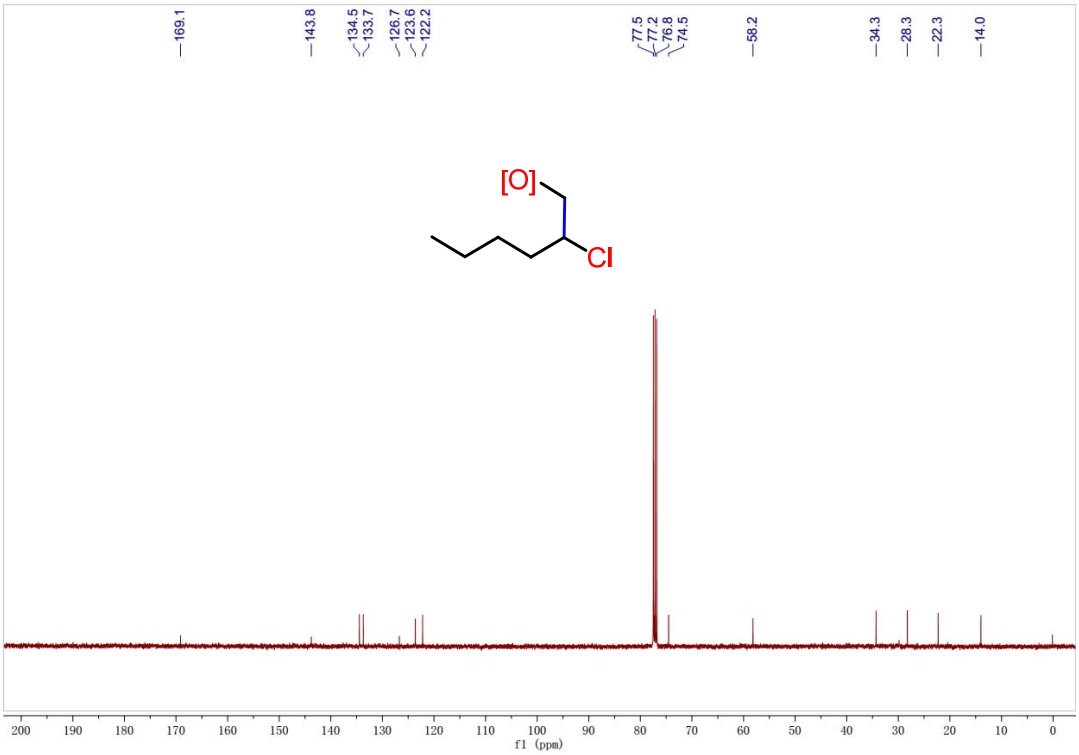
1.27
3.22
3.18
f1 (ppm)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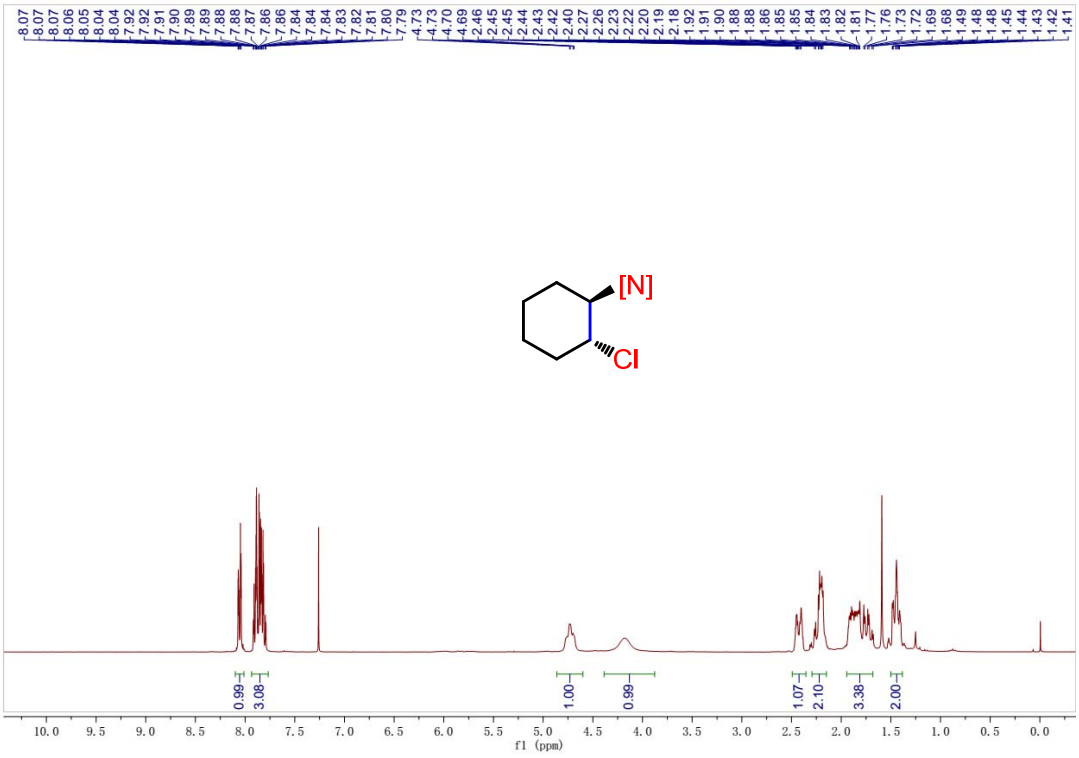
134.5
133.7
126.7
123.6
122.2
77.5
77.2
76.8
74.5
58.2
34.3
28.3
22.3
14.0
[O]
Cl
f1 (ppm)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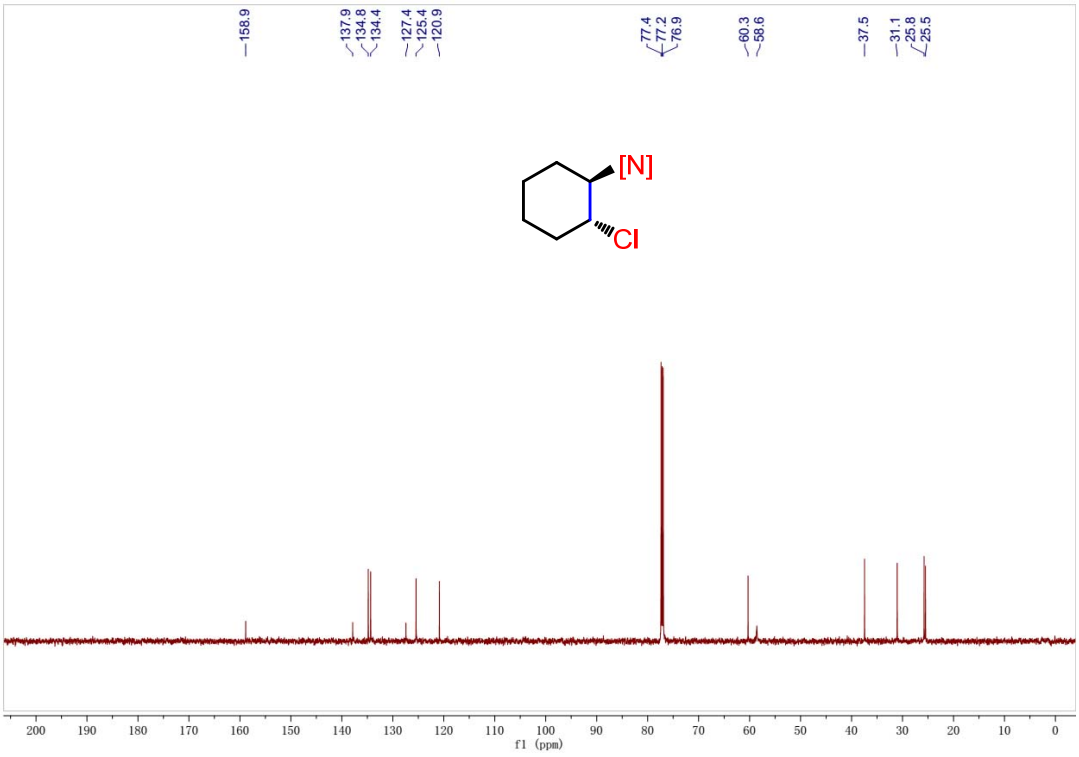
Cl
f1 (ppm)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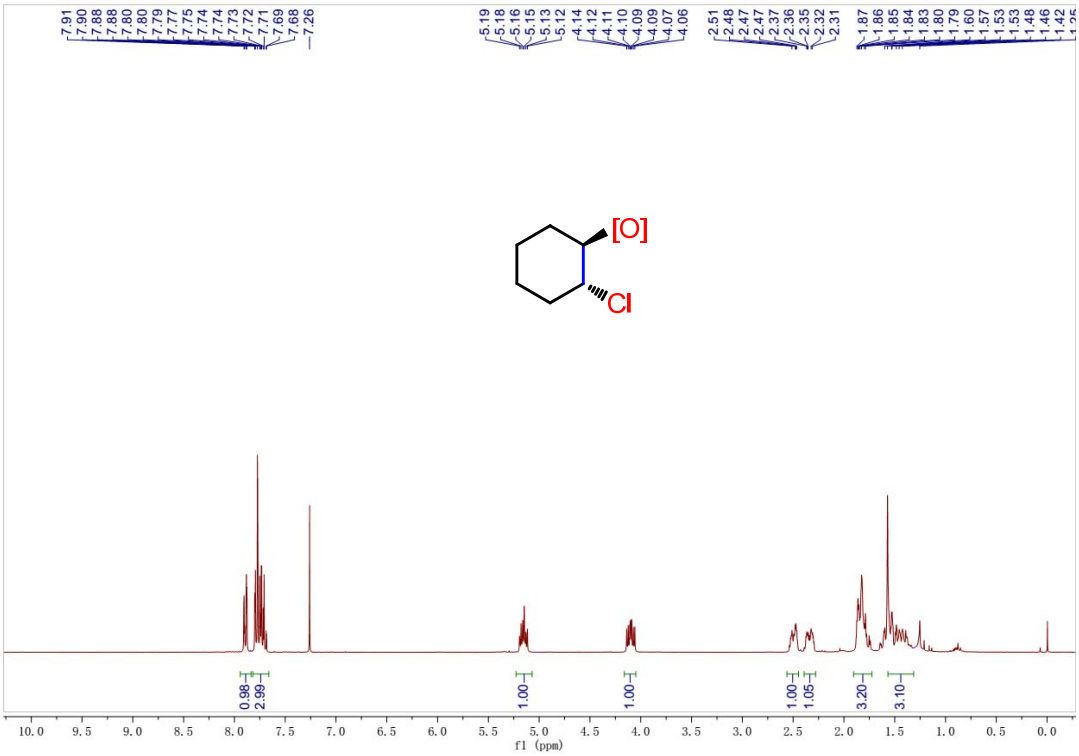
Cl
f1 (ppm)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7.88
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7.80
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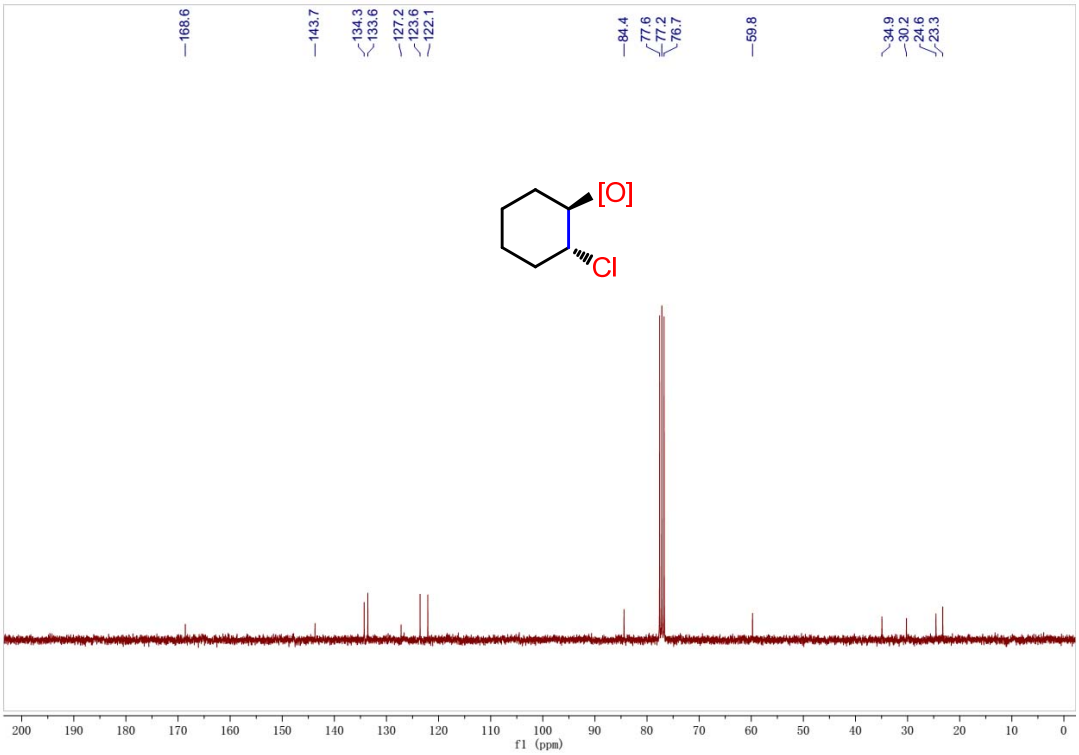
7.74
7.74
7.73
7.72
7.71
7.69
7.68
7.26
5.19
5.18
5.16
5.15
5.13
5.12
4.14
4.12
4.11
4.10
4.09
4.09
4.07
4.06
2.51
2.48
2.47
2.47
2.37
2.36
2.35
2.32
2.31
1.87
1.86
1.85
1.84
1.83
1.80
1.79
1.60
1.57
1.53
1.53
1.48
1.46
1.42
[O]
Cl
0.98
2.99
1.00
1.00
1.00
1.05
3.20
3.10
f1 (ppm)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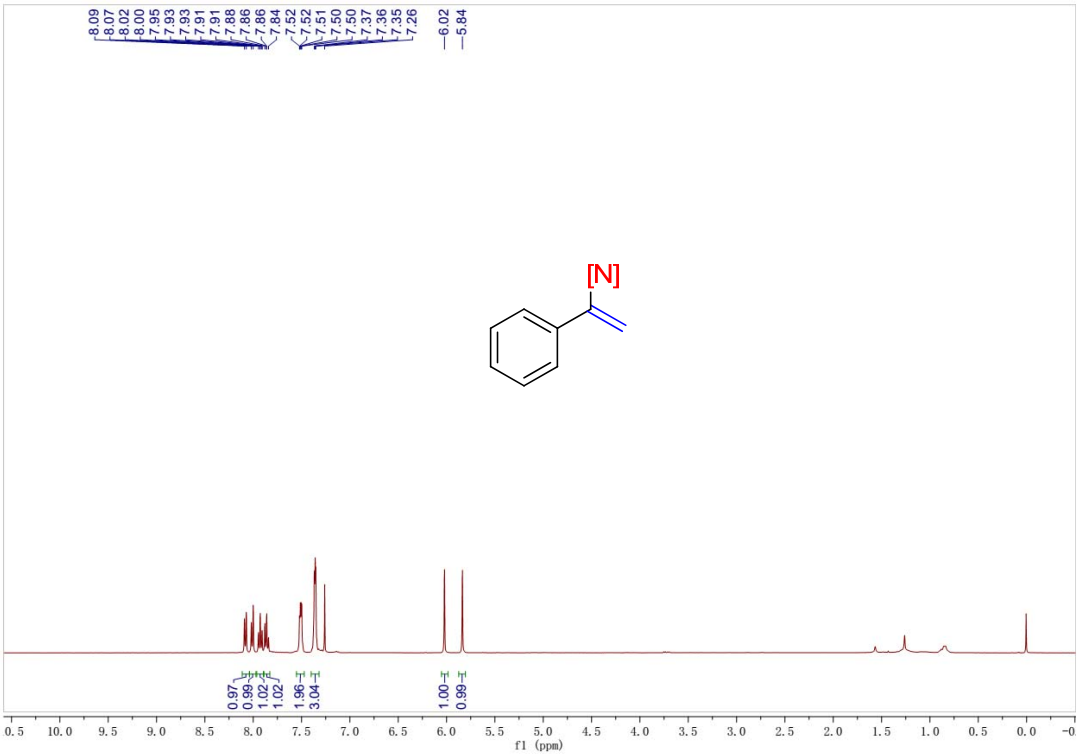
134.3
133.6
127.2
123.6
122.1
84.4
77.6
77.2
76.7
59.8
34.9
30.2
24.6
23.3
[O]
Cl
f1 (ppm)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8.02
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7.93
7.93
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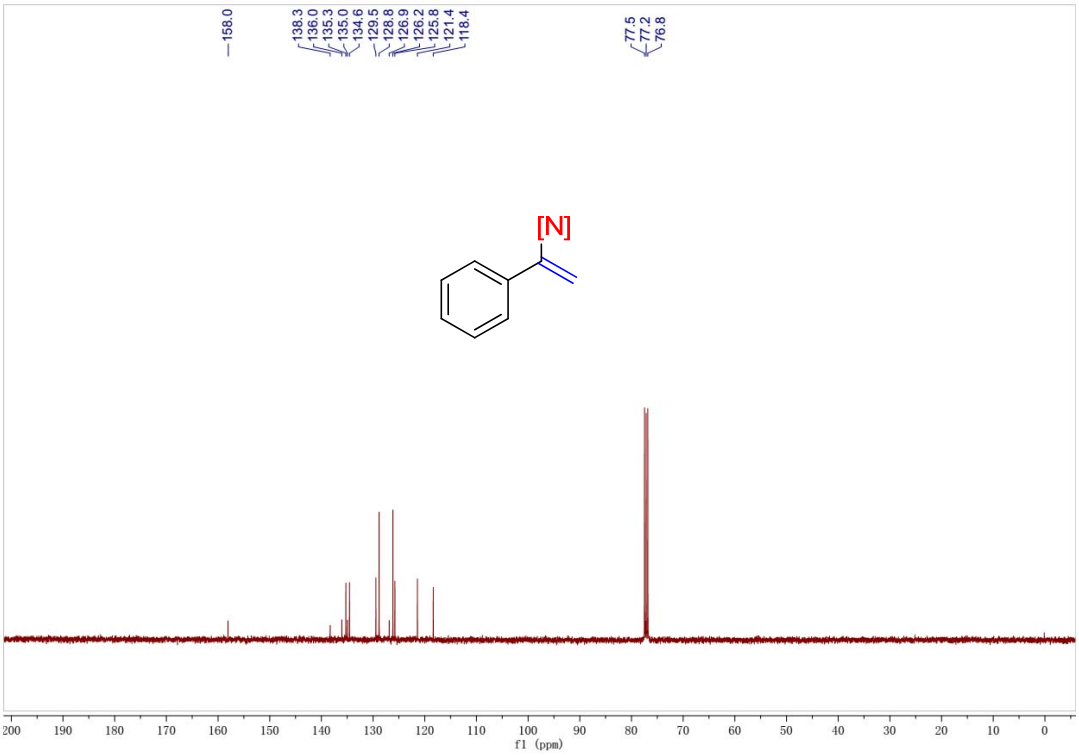
7.91
7.88
7.86
7.86
7.84
7.52
7.52
7.51
7.50
7.50
7.37
7.36
7.35
7.26
6.02
5.84
[N]
0.97
0.99
1.02
1.02
1.96
3.04
1.00
0.99
f1 (ppm)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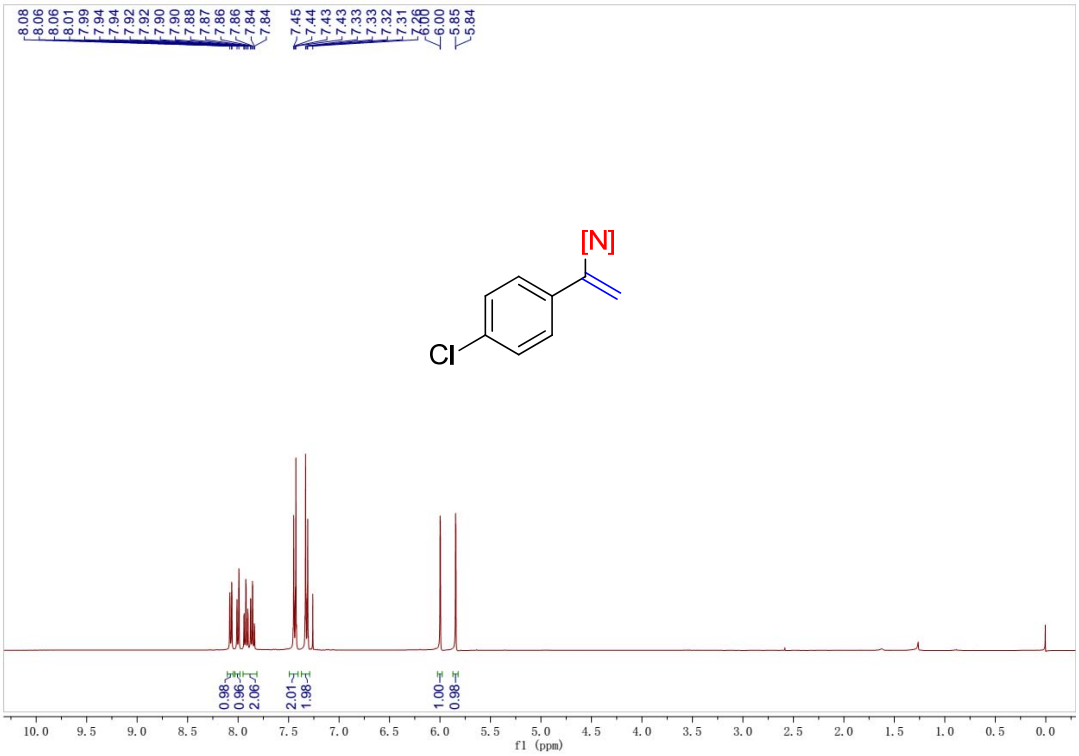
136.0
135.3
135.0
134.6
129.5
128.8
126.9
126.2
125.8
121.4
118.4
77.5
77.2
76.8
[N]
f1 (ppm)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8.06
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7.90
7.90
7.88
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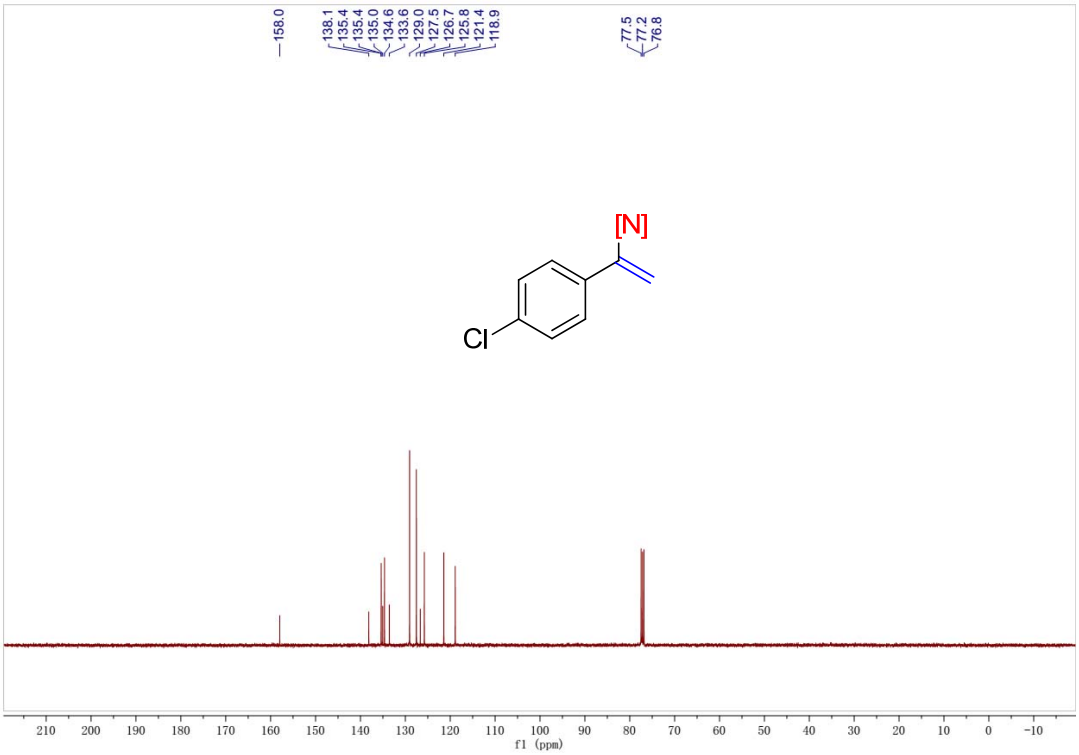
7.86
7.86
7.84
7.84
7.45
7.44
7.43
7.43
7.33
7.33
7.32
7.31
7.26
6.00
5.85
5.84
[N]
Cl
0.98
0.96
2.06
2.01
1.98
1.00
0.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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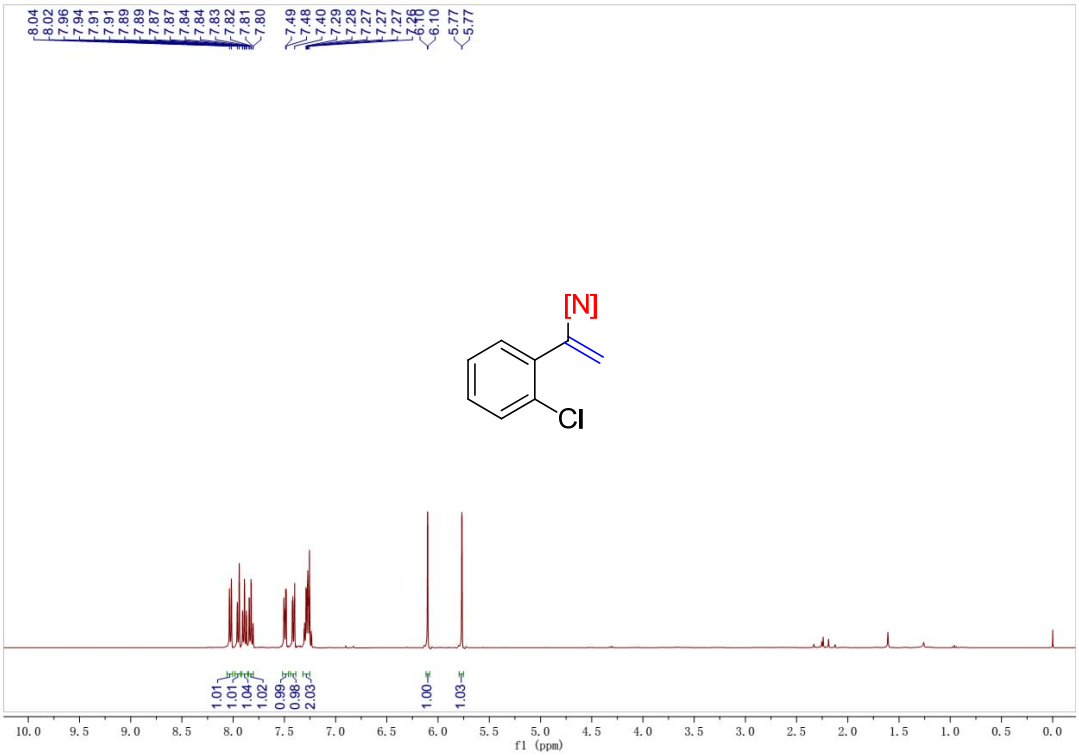
135.4
135.4
135.0
134.6
133.6
129.0
127.5
126.7
125.8
121.4
118.9
77.5
77.2
76.8
[N]
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.02
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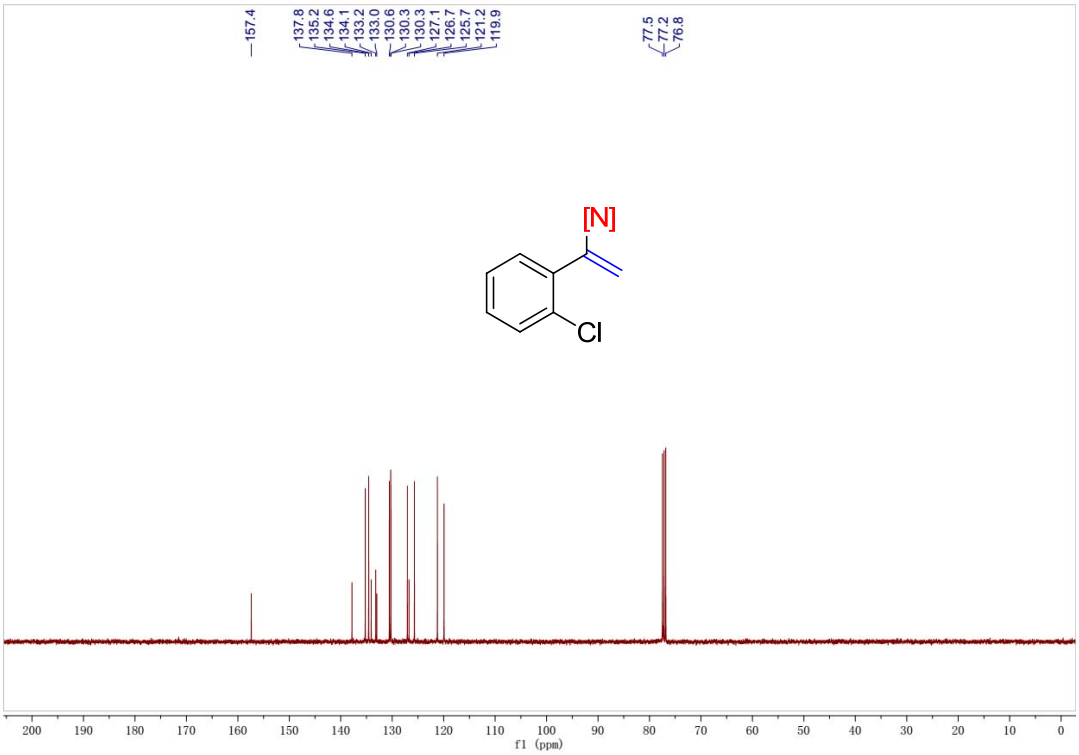
7.94
7.91
7.91
7.89
7.89
7.87
7.87
7.84
7.84
7.83
7.82
7.81
7.80
7.49
7.48
7.40
7.29
7.28
7.27
7.27
7.27
7.26
6.10
5.77
5.77
[N]
Cl
1.01
1.01
1.04
1.02
0.99
0.98
2.03
1.00
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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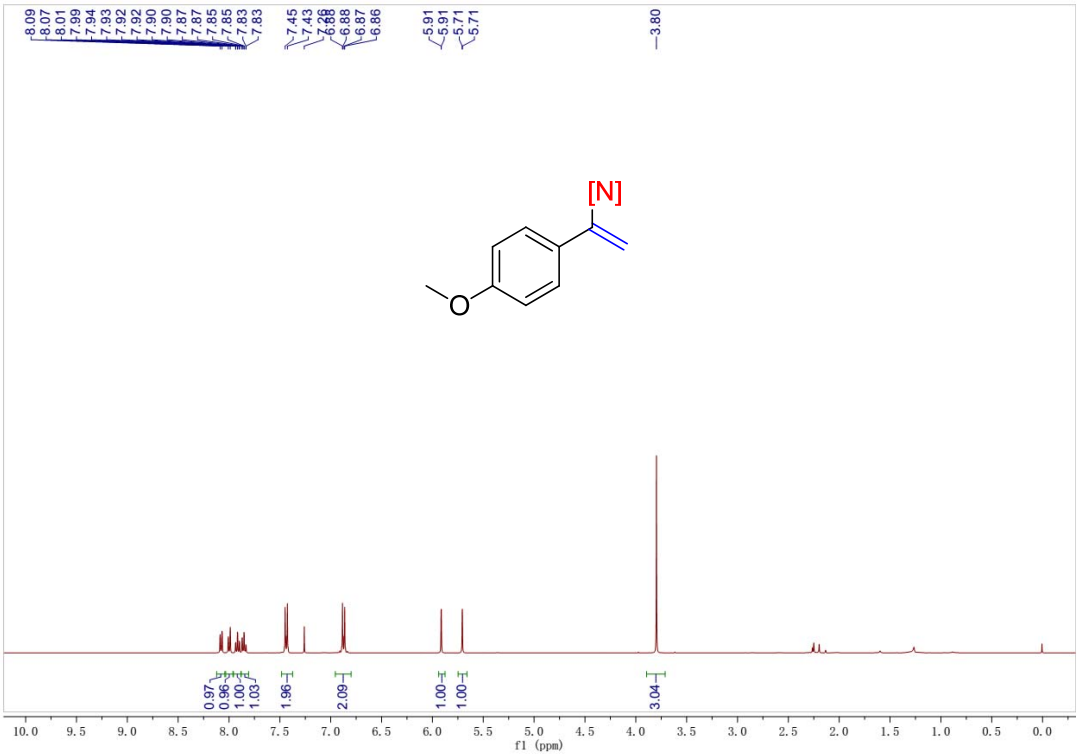
137.8
135.2
134.6
134.1
133.2
133.0
130.6
130.3
130.3
127.1
126.7
125.7
121.2
119.9
77.5
77.2
76.8
[N]
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.07
8.01
7.99
7.94
7.93
7.92
7.92
7.90
7.90
7.87
7.87
7.85
7.85
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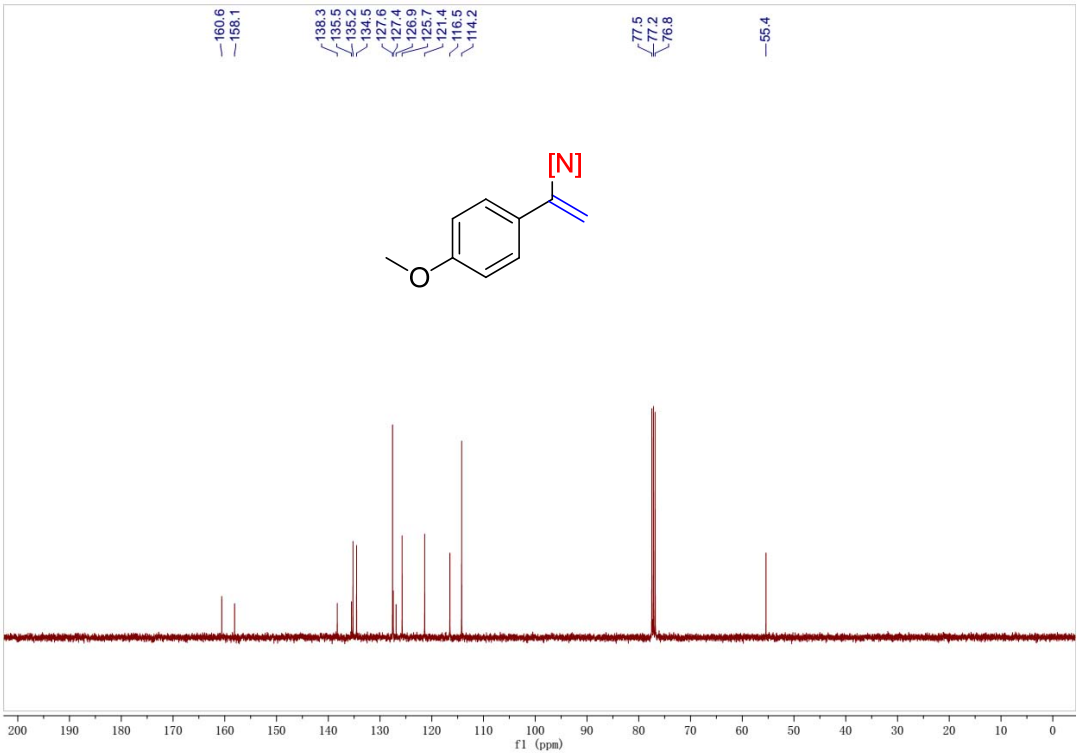
7.83
7.45
7.43
6.88
6.87
6.86
5.91
5.91
5.71
5.71
3.80
[N]
O
0.97
0.96
1.00
1.03
1.96
2.09
1.00
1.00
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.5
135.2
134.5
127.6
127.4
126.9
125.7
121.4
116.5
114.2
77.5
77.2
76.8
55.4
[N]
O
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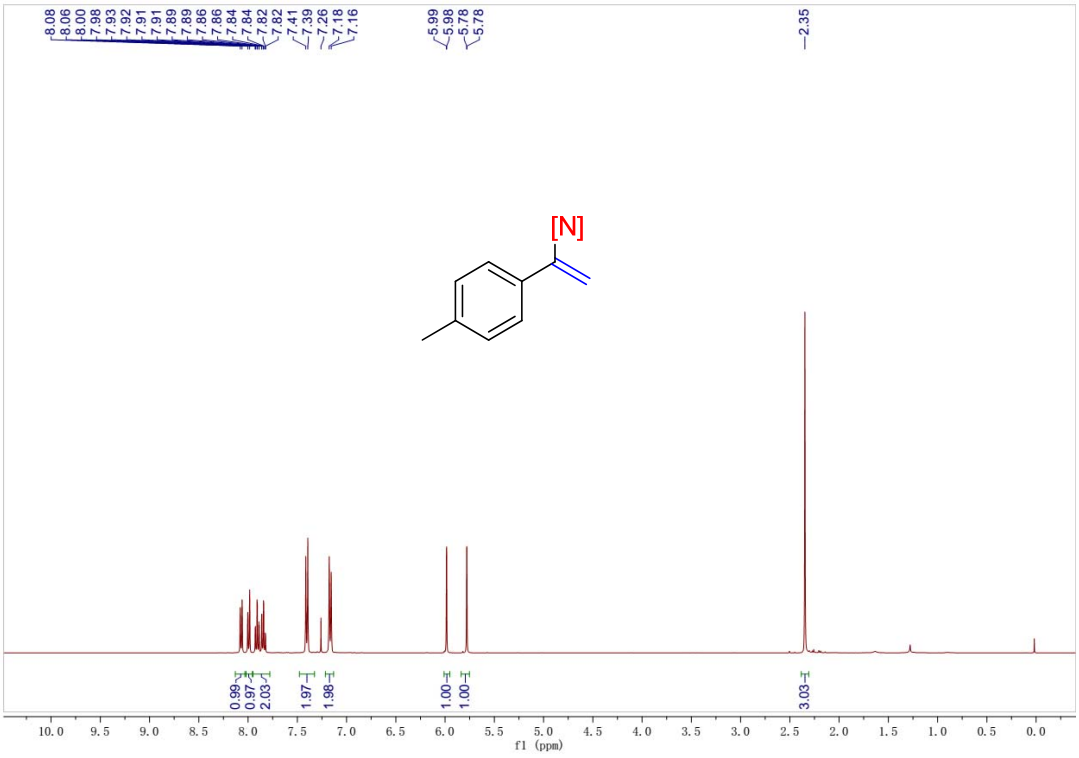
f1 (ppm)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7.91
7.91
7.89
7.89
7.86
7.86
7.84
7.84
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7.82
7.41
7.39
7.26
7.18
7.16
5.99
5.98
5.78
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2.35
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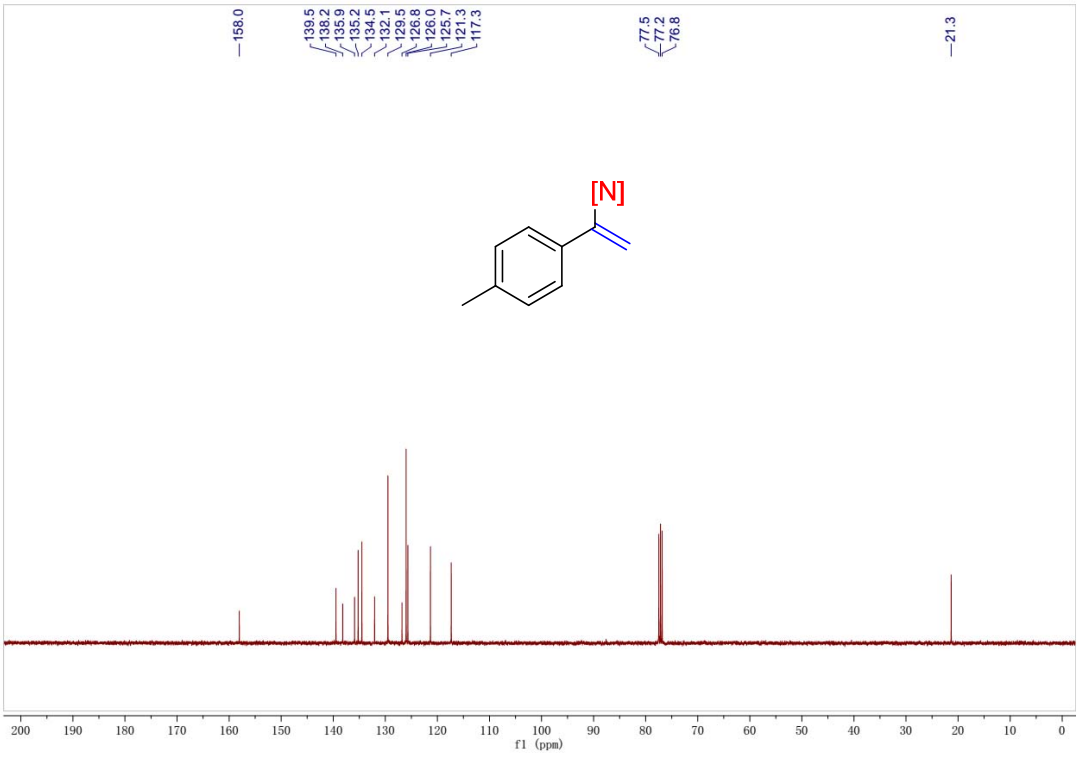
0.97
2.03
1.97
1.98
1.00
1.00
3.03
f1 (ppm)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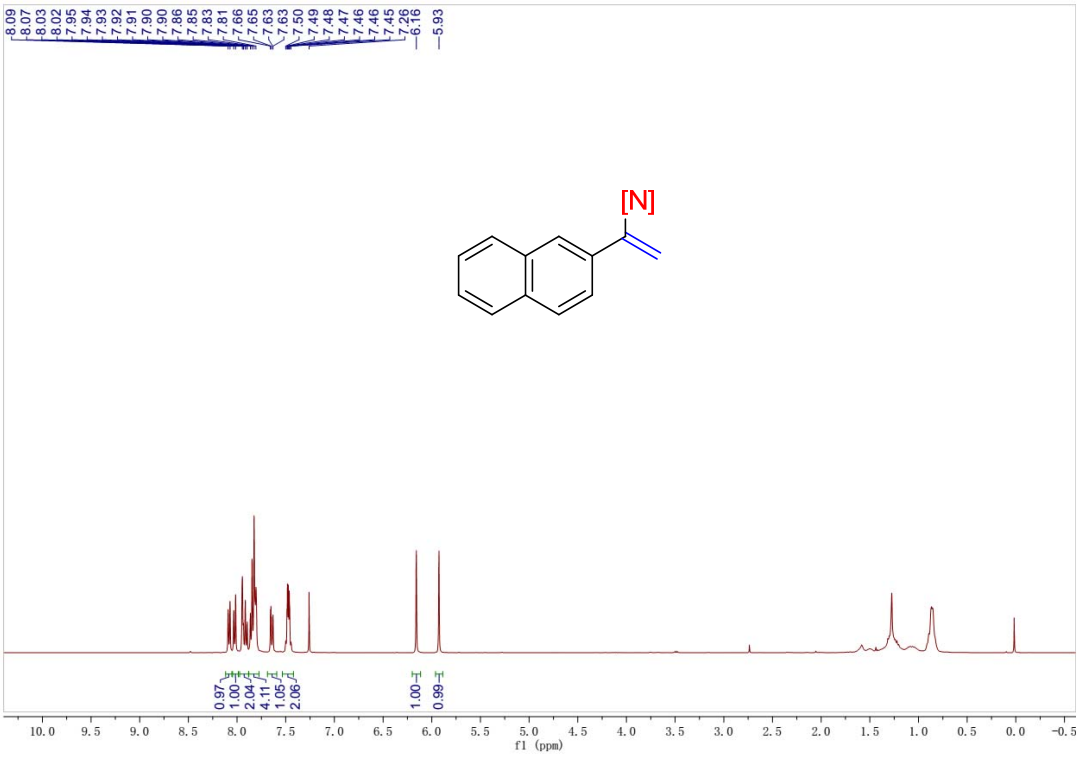
138.2
135.9
135.2
134.5
132.1
129.5
126.8
126.0
125.7
121.3
117.3
77.5
77.2
76.8
21.3
[N]
f1 (ppm)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7.90
7.90
7.86
7.85
7.83
7.81
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7.65
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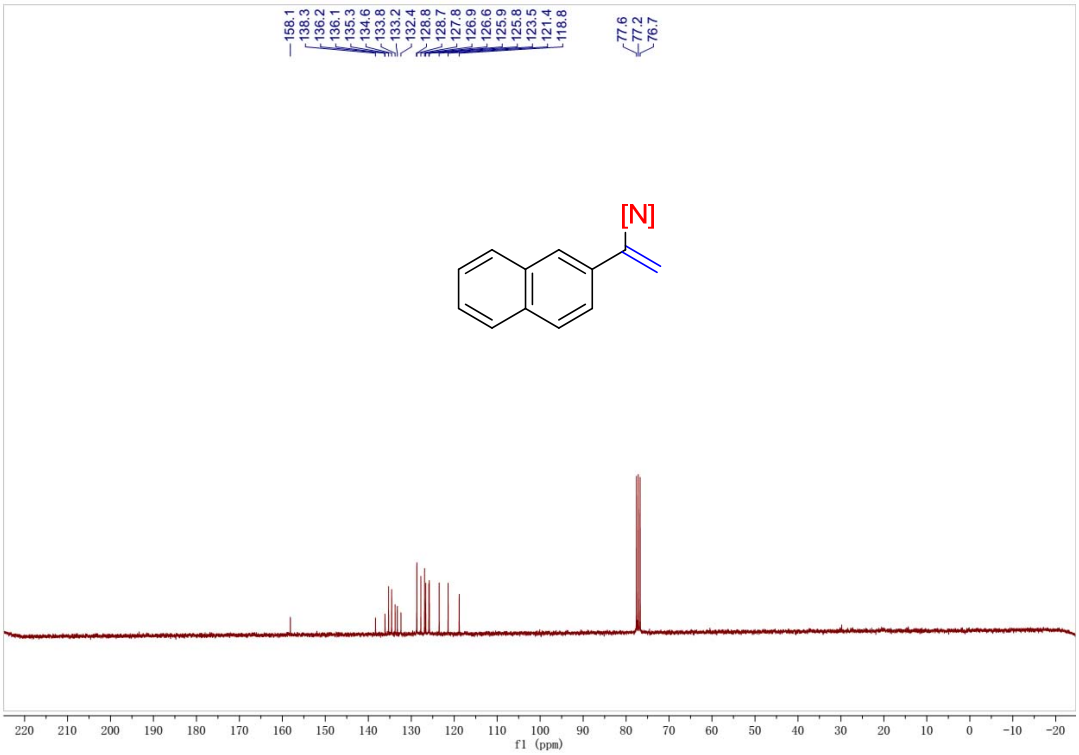
7.63
7.50
7.49
7.48
7.47
7.46
7.46
7.45
7.26
6.18
5.93
[N]
0.97
1.00
2.04
4.11
1.05
2.06
1.00
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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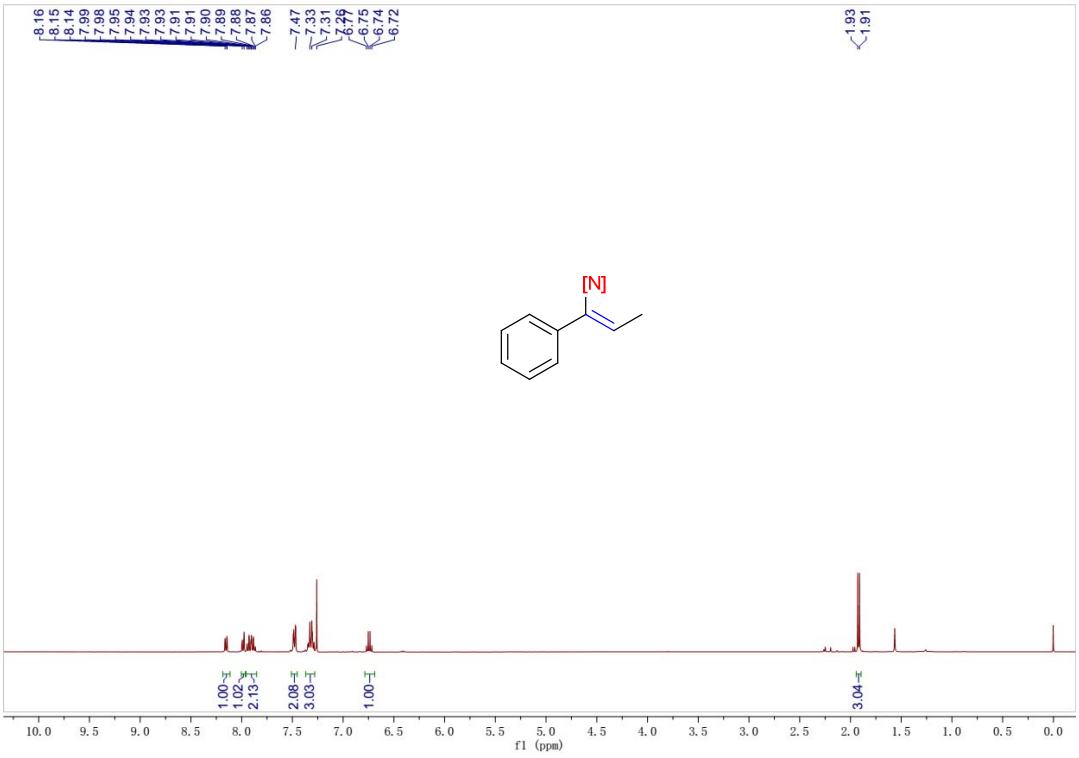
136.2
136.1
135.3
134.6
133.8
133.2
132.4
128.8
128.7
127.8
126.9
126.6
125.9
125.8
123.5
121.4
118.8
77.6
77.2
76.7
[N]
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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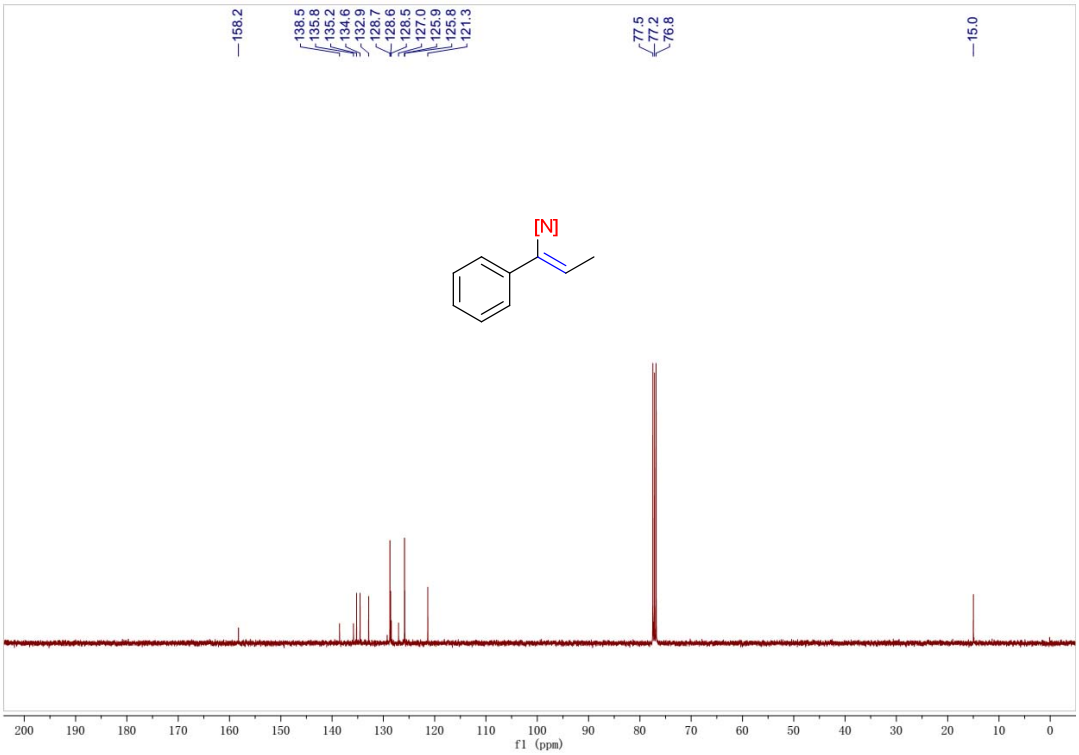
7.88
7.87
7.86
7.47
7.33
7.31
7.26
6.77
6.75
6.74
6.72
1.93
1.91
[N]
1.00
1.02
2.13
2.08
3.03
1.00
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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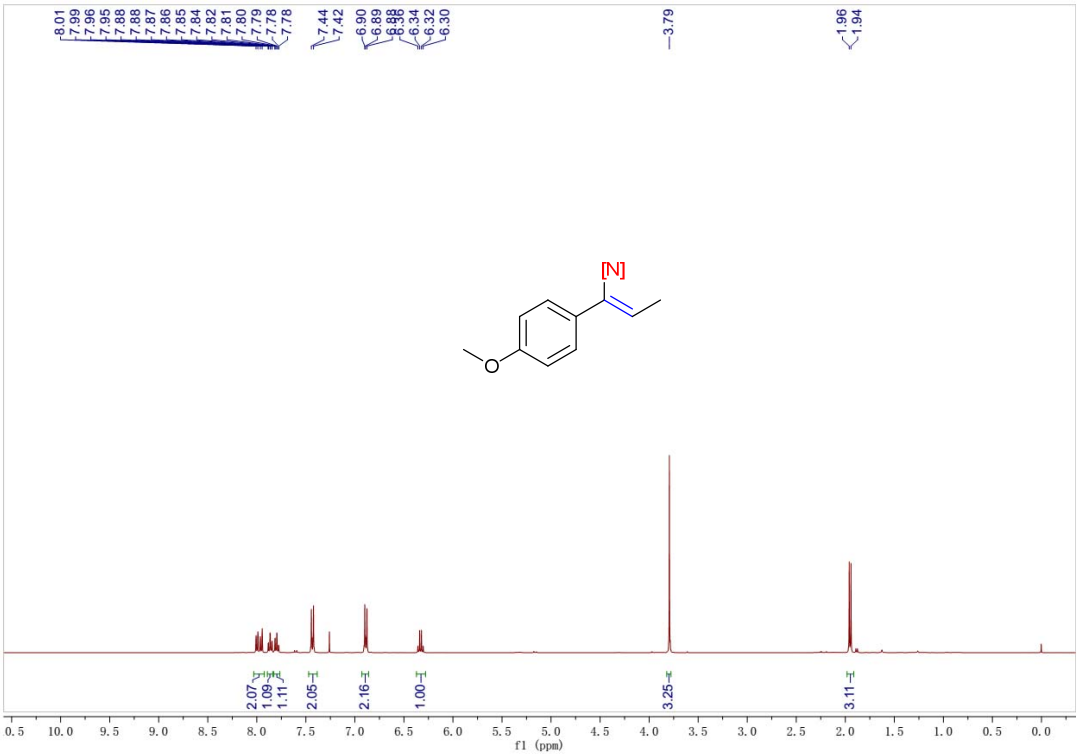
135.2
134.6
132.9
128.7
128.6
128.5
127.0
125.9
125.8
121.3
77.5
77.2
76.8
15.0
[N]
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.01
7.99
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7.95
7.88
7.88
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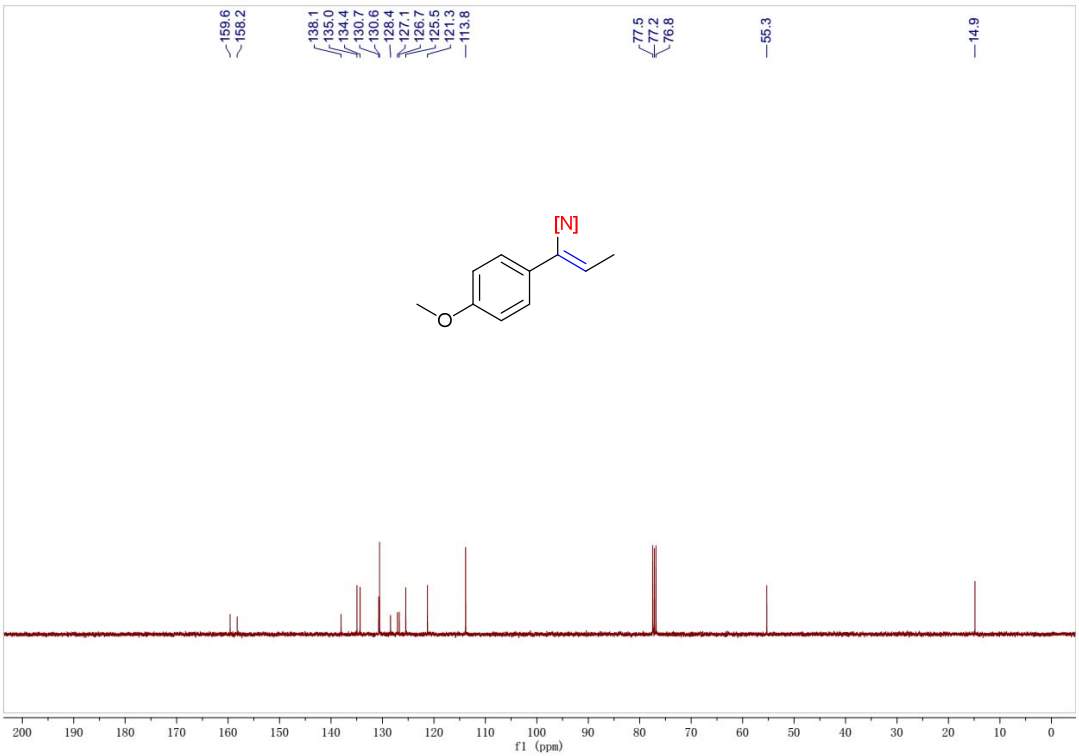
7.86
7.85
7.84
7.82
7.81
7.80
7.79
7.78
7.78
7.44
7.42
6.90
6.89
6.34
6.32
6.30
3.79
1.96
1.94
[N]
O
2.07
1.09
1.11
2.05
2.16
1.00
3.25
3.11
f1 (ppm)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158.2
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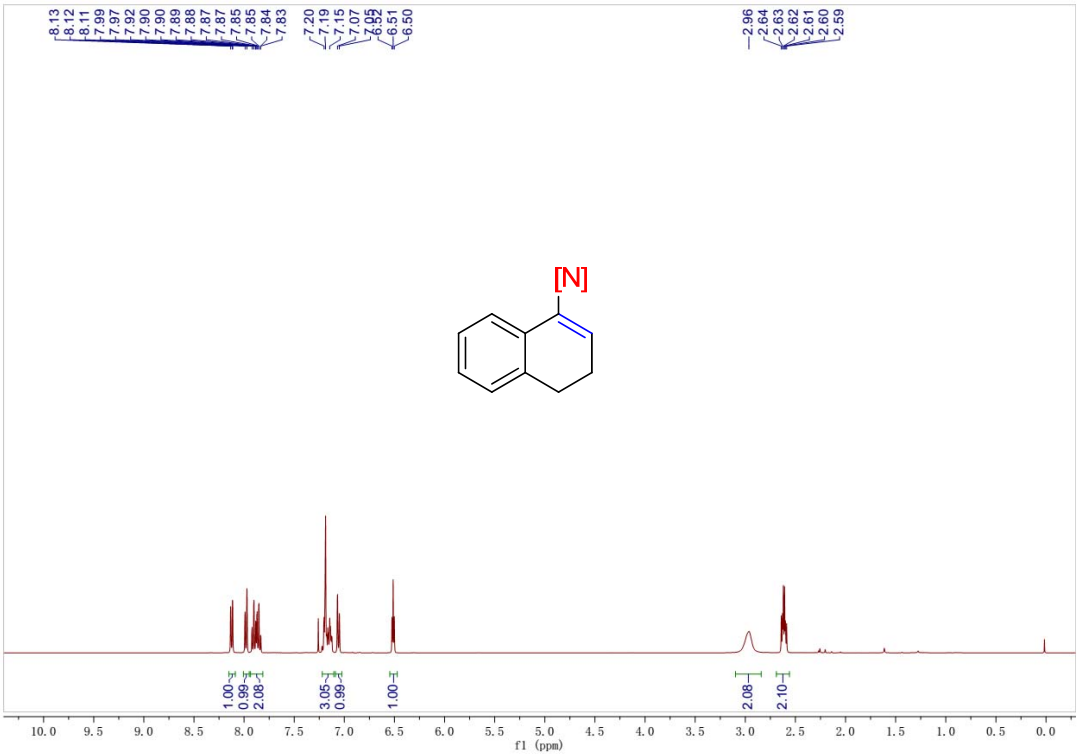
135.0
134.4
130.7
130.6
128.4
127.1
126.7
125.5
121.3
113.8
77.5
77.2
76.8
55.3
14.9
[N]
O
f1 (ppm)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8.12
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7.99
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7.88
7.87
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7.85
7.84
7.83
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7.19
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6.52
6.51
6.50
2.96
2.64
2.63
2.62
2.61
2.60
2.59
[N]
1.00
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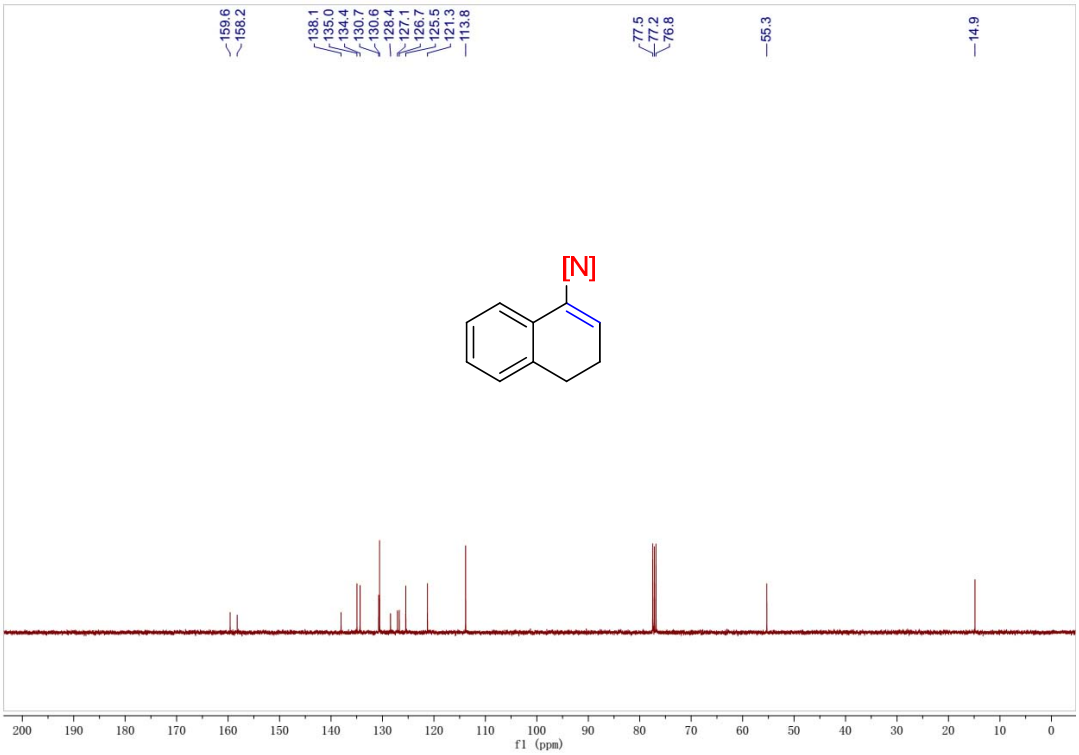
2.08
3.05
0.99
1.00
2.08
2.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


159.6
158.2
138.1
135.0
134.4
130.7
130.6
128.4
127.1
126.7
125.5
121.3
113.8
77.5
77.2
76.8
55.3
14.9
[N]
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)