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Supporting Information

Divergent Synthesis of Oxa-Cyclic Nitrones through Gold(I)-Catalyzed 1,3-Azaprotio Transfer of Propargylic α-Ketocarboxylate Oximes: Experimental and DFT Studies

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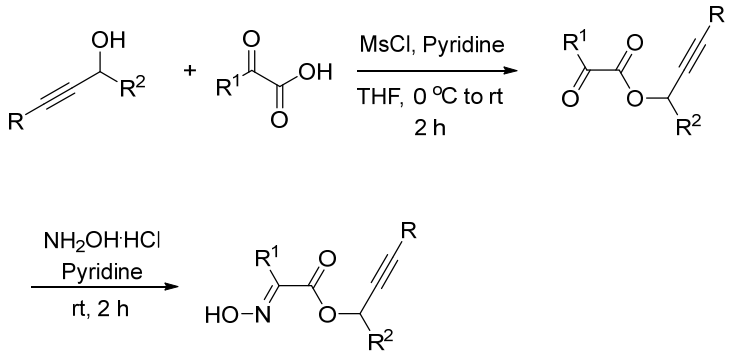
1. General information

^{1}H NMR spectra were obtained at 300 MHz or 400 MHz, and ^{13}C NMR spectra were obtained at 75 MHz or 100 MHz. Spectra were recorded in $CDCl_3$ or DMSO-d_6 solution using the residual protonated solvent as the internal standards, *J* values are given in Hz.

2. Experimental Details and Characterization Data

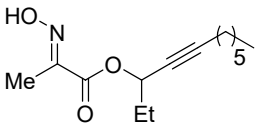
General procedure for the preparation of oxime 1a-1ab.



1

To a stirred solution of propargylic alcohol (1.0 equiv) and α-keto acid (2.0 equiv) and pyridine (5.0 equiv) in dry THF was added MsCl (2.4 equiv) dropwise at 0 ºC and stirred for 2 h at room temperature. Then the mixture was quenched by 10% citric acid aqueous solution, extracted with Et_2O. The combined organic layers were washed with brine and dried by anhydrous Na_2SO_4. The organic phase was concentrated under reduced pressure and the residue was purified by flash column chromatography to get the desired propargylic α-ketocarboxylate.

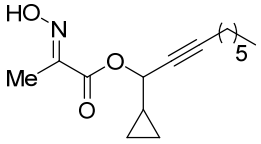
To a stirred solution of propargylic α-ketocarboxylate in pyridine was added hydroxylamine hydrochloride (2.0 equiv). After 1.5 h, the pyridine was concentrated mostly under reduced pressure. The residue was dissolved in dichloromethane, the formed solution was washed by 10% citric acid aqueous solution and brine successively. The organic phase was dried by anhydrous Na_2SO_4. After filtration, the solution was concentrated under reduced pressure. The residue was purified by flash column chromatography to get the desired product **1**.



1a

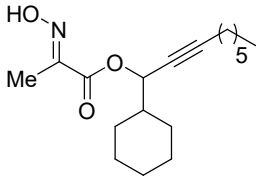
(*E*)-Undec-4-yn-3-yl 2-(Hydroxyimino)propanoate (1a). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.40 (tt, J_1 = 6.4 Hz, J_2 = 1.9 Hz, 1H), 2.18 (t, *J* = 7.1 Hz, 2H), 2.10 (s, 3H), 1.83 (p, *J* = 7.0 Hz, 2H), 1.48 (p, *J* = 7.2 Hz, 2H), 1.39-1.21 (m, 6H), 1.01 (t, *J* = 7.3 Hz, 3H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 149.0, 87.1, 67.3, 58.3, 31.2, 28.4, 28.35, 28.2, 22.5, 18.6, 14.0, 10.5, 9.3; IR (KBr) υ_{max} 2935, 1729, 1401, 1151, 1034 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{23}NNaO_3$ 276.1571 $[M+Na]^+$,

found 276.1582.



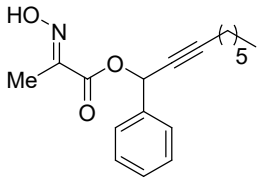
1b

(*E*)-1-Cyclopropylnon-2-ynyl 2-(Hydroxyimino)propanoate (1b). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.41 (s, 1H), 5.37 (dt, J_1 = 6.7 Hz, J_2 = 1.8 Hz, 1H), 2.17 (td, J_1 = 7.1 Hz, J_2 = 1.8 Hz, 2H), 2.10 (s, 3H), 1.47 (p, J = 7.7 Hz, 2H), 1.37-1.21 (m, 7H), 0.86 (t, J = 6.7 Hz, 3H), 0.57 (t, J = 6.0 Hz, 3H), 0.51-0.45 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 148.9, 87.3, 74.6, 69.7, 31.2, 28.4, 28.3, 22.4, 18.6, 14.3, 13.9, 10.4, 3.5, 2.0; IR (KBr) υ_{max} 2931, 1727, 1401, 1149, 1030 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{23}NNaO_3$ 276.1571 $[M+Na]^+$, found 276.1573.



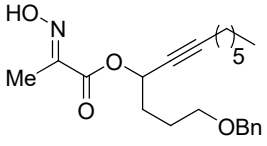
1c

(*E*)-1-Cyclohexylnon-2-ynyl 2-(Hydroxyimino)propanoate (1c). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.52 (s, 1H), 5.28 (dt, J_1 = 6.0 Hz, J_2 = 1.7 Hz, 1H), 2.19 (td, J_1 = 7.1 Hz, J_2 = 1.9 Hz, 2H), 2.10 (s, 3H), 1.86-1.64 (m, 6H), 1.48 (p, J = 6.6 Hz, 2H), 1.39-1.08 (m, 11H), 0.86 (t, J = 6.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 148.9, 87.5, 75.8, 70.4, 42.0, 31.2, 28.5, 28.4, 28.35, 28.1, 26.1, 25.7, 25.65, 22.46, 18.6, 13.9, 10.4; IR (KBr) υ_{max} 2930, 2857, 1729, 1452, 1402, 1151, 1032 cm^{-1}; HRMS (ESI) calcd for $C_{18}H_{29}NNaO_3$ 330.2040 $[M+Na]^+$, found 330.2040.



1d

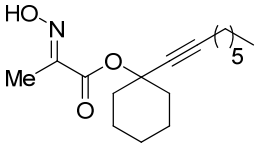
(*E*)-1-Phenylnon-2-ynyl 2-(Hydroxyimino)propanoate (1d). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.15 (s, 1H), 7.56-7.54 (m, 2H), 7.40-7.34 (m, 3H), 6.56 (d, J = 1.7 Hz, 1H), 2.26 (tt, J_1 = 7.1 Hz, J_2 = 1.8 Hz, 2H), 2.09 (d, J = 1.0 Hz, 3H), 1.57-1.50 (m, 1H), 1.41-1.25 (m, 7H), 0.88 (td, J_1 = 7.1 Hz, J_2 = 2.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 148.8, 137.1, 128.9, 128.6, 127.8, 89.2, 76.1, 67.6, 31.2, 28.5, 28.3, 22.5, 18.8, 14.0, 10.5; IR (KBr) υ_{max} 3133, 1729, 1400, 1154 cm^{-1}; HRMS (ESI) calcd for $C_{18}H_{23}NNaO_3$ 324.1571 $[M+Na]^+$, found 324.1570.



1e

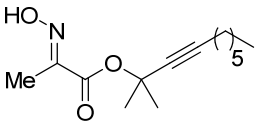
(*E*)-1-(Benzyloxy)dodec-5-yn-4-yl 2-(Hydroxyimino)propanoate (1e). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.35 (s, 1H), 7.36-7.30 (m, 4H), 7.30-7.27 (m, 1H), 5.50 (tt, J_1 = 6.4 Hz, J_2 =1.8 Hz, 1H), 4.51 (s, 2H), 3.51 (t, J = 6.2 Hz, 2H), 2.19 (td, J_1 = 7.2 Hz, J_2 = 1.8 Hz, 2H), 2.09 (s, 3H), 1.97-1.91 (m,

1H), 1.83-1.76 (m, 2H), 1.49 (p, J = 7.2 Hz, 2H), 1.39-1.25 (m, 7H), 0.88 (t, J = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 149.1, 138.3, 128.3, 127.6, 127.5, 87.2, 72.9, 69.5, 65.9, 31.9, 31.2, 28.4, 28.3, 25.3, 22.5, 18.7, 14.0, 10.5; IR (KBr) υ_{max} 3131, 2932, 1728, 1401, 1122, 1031 cm^{-1}; HRMS (ESI) calcd for $C_{22}H_{31}NNaO_4$ 396.2146 $[M+Na]^+$, found 396.2149.



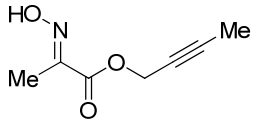
1f

(*E*)-1-(Oct-1-ynyl)cyclohexyl 2-(Hydroxyimino)propanoate (1f). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 2.22-2.13 (m, 4H), 2.05 (s, 3H), 1.87-1.81 (m, 2H), 1.62-1.57 (m, 4H), 1.54-1.44 (m, 3H), 1.39-1.21 (m, 7H), 0.85 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 149.3, 87.6, 79.2, 78.0, 37.1, 31.1, 28.3, 28.2, 25.0, 22.7, 22.4, 18.6, 13.8, 10.1; IR (KBr) υ_{max} 2934, 1731, 1401, 1155, 1016 cm^{-1}; HRMS (ESI) calcd for $C_{17}H_{27}NNaO_3$ 316.1884 $[M+Na]^+$, found 316.1881.



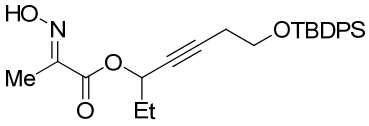
1g

(*E*)-2-Methyldec-3-yn-2-yl 2-(Hydroxyimino)propanoate (1g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.40 (s, 1H), 2.18 (t, J = 7.1 Hz, 2H), 2.06 (s, 3H), 1.70 (s, 6H), 1.47 (p, J = 7.5 Hz, 2H), 1.38-1.23 (m, 6H), 0.87 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7, 149.5, 85.7, 80.6, 74.5, 31.2, 29.2, 28.4, 22.5, 18.6, 14.0, 10.2; IR (KBr) υ_{max} 2931, 2860, 1731, 1402, 1127, 1032 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{23}NNaO_3$ 276.1571 $[M+Na]^+$, found 276.1569.



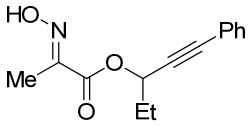
1h

(*E*)-But-2-ynyl 2-(Hydroxyimino)propanoate (1h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 4.80 (q, J = 2.4 Hz, 2H), 2.12 (s, 3H), 1.85 (t, J = 2.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 3129, 1739, 1401, 1142; IR (KBr) υ_{max} 3129, 1739, 1401, 1142 cm^{-1}; HRMS (ESI) calcd for $C_7H_9NNaO_3$ 178.0475 $[M+Na]^+$, found 178.0468.



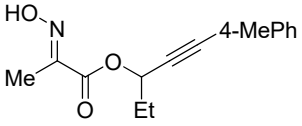
1i

(*E*)-7-(*tert*-Butyldiphenylsilyloxy)hept-4-yn-3-yl 2-(Hydroxyimino)propanoate (1i). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 7.69-7.67 (m, 4H), 7.45-7.36 (m, 6H), 5.42 (tt, J_1 = 6.4 Hz, J_2 = 1.8 Hz, 1H), 3.76 (t, J = 6.9 Hz, 2H), 2.49 (td, J_1 = 7.0 Hz, J_2 = 1.8 Hz, 2H), 2.09 (s, 3H), 1.84 (p, J = 6.9 Hz, 2H), 1.05 (s, 9H), 1.02 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 149.2, 135.5, 133.5, 129.7, 127.7, 83.9, 77.8, 67.1, 62.1, 28.2, 26.7, 22.9, 19.1, 10.5, 9.4; IR (KBr) υ_{max} 3131, 1728, 1401, 1151, 704 cm^{-1}; HRMS (ESI) calcd for $C_{26}H_{33}NNaO_4Si$ 474.2072 $[M+Na]^+$, found 474.2071.



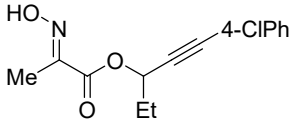
1j

(*E*)-1-Phenylpent-1-yn-3-yl 2-(Hydroxyimino)propanoate (1j). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 7.46-7.43 (m, 2H), 7.33-7.28 (m, 3H), 5.67 (t, *J* = 6.5 Hz, 1H), 2.14 (s, 3H), 1.98 (p, *J* = 6.8 Hz, 2H), 1.11 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 148.9, 131.8, 128.6, 128.2, 122.1, 85.9, 85.5, 67.2, 28.0, 10.5, 9.4; IR (KBr) υ_{max} 2931, 1782, 1697, 1576, 1453, 1171 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{15}NNaO_3$ 268.0945 $[M+Na]^+$, found 268.0943.



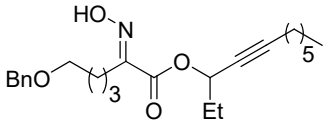
1k

(*E*)-1-p-Tolypent-1-yn-3-yl 2-(Hydroxyimino)propanoate (1k). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 5.66 (t, *J* = 6.4 Hz, 1H), 2.34 (s, 3H), 2.13 (s, 3H), 1.97 (p, *J* = 6.8 Hz, 2H), 1.10 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 149.3, 138.8, 131.8, 129.0, 119.1, 86.1, 84.9, 67.4, 28.2, 21.5, 10.5, 9.4; IR (KBr) υ_{max} 2976, 1736, 1401, 1156 cm^{-1}; HRMS (ESI) calcd for $C_{15}H_{17}NNaO_3$ 282.1101 $[M+Na]^+$, found 282.1098.



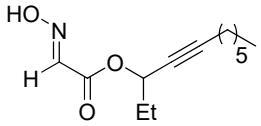
1l

(*E*)-1-(4-Chlorophenyl)pent-1-yn-3-yl 2-(Hydroxyimino)propanoate (1l). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.5 (s, 1H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 7.4 Hz, 2H), 5.64 (t, *J* = 6.4 Hz, 1H), 2.13 (s, 3H), 1.97 (p, *J* = 7.1 Hz, 2H), 1.10 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 148.9, 134.7, 133.1, 128.6, 120.6, 86.6, 84.9, 67.1, 28.0, 10.5, 9.4; IR (KBr) υ_{max} 3128, 1783, 1401, 1156 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{14}ClNNaO_3$ 302.0555 $[M+Na]^+$, found 302.0554.



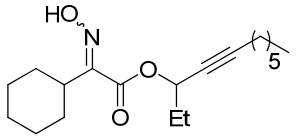
1m

(*E*)-Undec-4-yn-3-yl 6-(Benzyloxy)-2-(hydroxyimino)hexanoate (1m). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.3 (s, 1H), 7.33-7.29 (m, 4H), 7.28-7.25 (m, 1H), 5.40 (tt, J_1 = 6.4 Hz, J_2 = 1.8 Hz, 1H), 4.50 (s, 2H), 3.49 (t, J_1 = 5.9 Hz, 2H), 2.65 (t, *J* = 7.0 Hz, 2H), 2.18 (td, J_1 = 7.1 Hz, J_2 = 1.9 Hz, 2H), 1.82 (p, *J* = 6.8 Hz, 2H), 1.67-1.64 (m, 4H), 1.48 (p, *J* = 7.5 Hz, 2H), 1.39-1.22 (m, 6H), 1.01 (t, *J* = 7.4 Hz, 3H), 0.87 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 152.4, 138.5, 128.3, 127.6, 127.4, 87.0, 76.7, 72.8, 69.9, 67.2, 31.2, 29.5, 28.4, 28.3, 28.2, 24.4, 22.6, 22.5, 18.6, 14.0, 9.3; IR (KBr) υ_{max} 3309, 1733, 1558, 1473 cm^{-1}; HRMS (ESI) calcd for $C_{24}H_{35}NNaO_4$ 424.2459 $[M+Na]^+$, found 424.2459.



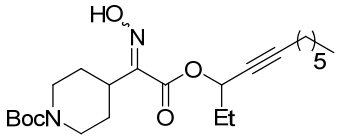
1n

(*E*)-Undec-4-yn-3-yl 2-(Hydroxyimino)acetate (1n). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.62 (s, 1H), 7.57 (s, 1H), 5.45 (tt, J_1 = 6.4 Hz, J_2 = 1.9 Hz, 1H), 2.20 (td, J_1 = 7.2 Hz, J_2 = 2.0 Hz, 2H), 1.83 (p, J = 7.0 Hz, 2H), 1.49 (p, J = 7.6 Hz, 2H), 1.40-1.23 (m, 6H), 1.02 (t, J = 7.4 Hz, 3H), 0.88 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 141.8, 87.4, 76.4, 67.3, 31.2, 28.4, 28.3, 28.27, 22.5, 18.7, 14.0, 9.3; IR (KBr) υ_{max} 3133, 1683, 1384, 1000 cm^{-1}; HRMS (ESI) calcd for $C_{13}H_{21}NNaO_3$ 262.1414 $[M+Na]^+$, found 262.1409.



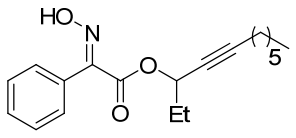
1o (*E* and *Z*)

(*E*) and (*Z*)-Undec-4-yn-3-yl 2-Cyclohexyl-2-(hydroxyimino)acetate (1o). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 5.47 (tt, J_1 = 4.2 Hz, J_2 =1.2 Hz, 0.2 H), 5.40 (tt, J_1 = 4.3 Hz, J_2 = 1.2 Hz, 0.8 Hz), 2.20 (td, J_1 = 4.7 Hz, J_2 = 1.3 Hz, 2H), 1.86-1.77 (m, 6H), 1.71-1.66 (m, 3H), 1.49 (p, J = 5.1 Hz, 2H), 1.39-1.23 (m, 10H), 1.05-1.01 (m, 3H), 0.90-0.87 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 156.6, 87.0, 67.0, 36.0, 31.3, 28.4, 28.39, 28.3, 27.9, 27.86, 26.2, 25.8, 22.5, 18.7, 14.0, 9.5; IR (KBr) υ_{max} 2932, 1732, 1401, 1128 cm^{-1}; HRMS (ESI) calcd for $C_{19}H_{31}NNaO_3$ 344.2197 $[M+Na]^+$, found 344.2198.



1p (E and Z)

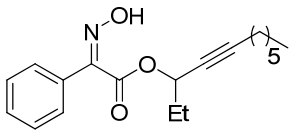
(*E*) and (*Z*)-*tert*-Butyl 4-[1-(hydroxyimino)-2-oxo-2-(undec-4-yn-3-yloxy)ethyl]piperidine -1-carboxylate (1p). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 5.46 (t, J = 6.3 Hz, 0.6H), 5.33 (t, J = 6.3 Hz, 0.4 H), 2.79-2.83 (m, 3H), 2.20-2.16 (m, 2H), 2.07-1.98 (m, 1H), 1.84-1.76 (m, 3H), 1.60-1.21 (m, 21H), 1.03-0.97 (m, 3H), 0.92-0.84 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 162.2, 154.74, 154.71, 153.7, 152.7, 87.5, 87.1, 79.7, 79.5, 77.2, 76.6, 76.4, 67.3, 67.2, 38.3, 34.4, 31.2, 28.4, 28.37, 28.35, 28.29, 28.25, 26.8, 22.5, 18.6, 18.58, 14.0, 9.4, 9.3; IR (KBr) υ_{max} 3130, 1736, 1695, 1401, 1167 cm^{-1}; HRMS (ESI) calcd for $C_{23}H_{38}N_2NaO_5$ 445.2673 $[M+Na]^+$, found 445.2680.



***E*-1q**

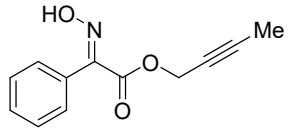
(*E*)-Undec-4-yn-3-yl 2-(Hydroxyimino)-2-phenylacetate (*E*-1q). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 7.58-7.54 (m, 2H), 7.45-7.42 (m, 3H), 5.46 (tt, J_1 = 6.4 Hz, J_2 = 1.9 Hz, 1H), 1.83 (p, J = 7.2 Hz, 2H), 1.48 (p, J = 7.5 Hz, 2H), 1.38-1.22 (m, 6H), 1.00 (t, J = 7.4 Hz, 3H), 0.88 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 148.8, 129.8, 129.5, 128.3, 127.8, 87.3, 76.6, 67.7, 31.2,

28.4, 28.3, 28.2, 22.5, 18.6, 14.0, 9.3; IR (KBr) υ_{max} 2933, 1732, 1196, 999 cm^{-1}; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3$ 338.1727 $[M+Na]^+$, found 338.1729.



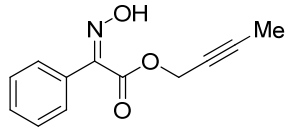
***Z*-1q**

(*Z*)-Undec-4-yn-3-yl 2-(Hydroxyimino)-2-phenylacetate (*Z*-1q). ^1H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 7.62-7.59 (m, 2H), 7.42-7.37 (m, 3H), 5.62 (tt, J_1 = 6.4 Hz, J_2 = 1.9 Hz, 1H), 2.24 (td, J_1 = 7.1 Hz, J_2 = 2.0 Hz, 2H), 1.89 (p, J = 7.0 Hz, 2H), 1.52 (p, J = 7.4 Hz, 2H), 1.43-1.23 (m, 6H), 1.05 (t, J = 7.4 Hz, 3H), 0.88 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 151.4, 130.4, 130.2, 128.7, 126.4, 87.5, 76.5, 67.7, 31.3, 28.4, 28.38, 28.3, 22.5, 18.7, 14.0, 9.4; IR (KBr) υ_{max} 2934, 1745, 1209, 947 cm^{-1}; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3$ 338.1727 $[M+Na]^+$, found 338.1729.



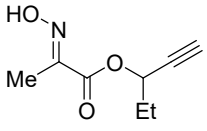
***E*-1r**

(*E*)-But-2-ynyl 2-(Hydroxyimino)-2-phenylacetate (*E*-1r). ^1H NMR (400 MHz, $CDCl_3$) δ 9.83 (s, 1H), 7.56-7.52 (m, 2H), 7.48-7.41 (m, 3H), 4.83 (q, J = 2.3 Hz, 2H), 1.83 (t, J = 2.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 149.0, 129.9, 129.3, 128.2, 128.0, 84.1, 72.3, 54.3, 3.6; IR (KBr) υ_{max} 3133, 1734, 1384, 1198 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{11}NNaO_3$ 240.0632 $[M+Na]^+$, found 240.0628.



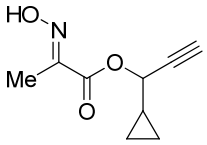
***Z*-1r**

(*Z*)-But-2-ynyl 2-(Hydroxyimino)-2-phenylacetate (*E*-1r). ^1H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.59-7.57 (m, 2H), 7.43-7.38 (m, 3H), 4.95 (d, J = 2.4 Hz, 2H), 1.88 (t, J = 2.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 151.2, 130.6, 129.9, 128.8, 126.4, 84.5, 72.1, 54.1, 3.7; IR (KBr) υ_{max} 3198, 1730, 1402, 1192, 1025 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{11}NNaO_3$ 240.0632 $[M+Na]^+$, found 240.0630.



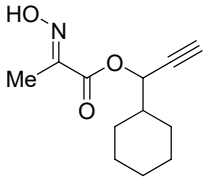
1s

(*E*)-Pent-1-yn-3-yl 2-(Hydroxyimino)propanoate (1s). ^1H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 5.41 (dt, J_1 = 6.5 Hz, J_2 = 2.1 Hz, 1H), 2.49 (d, J = 3.8 Hz, 1H), 2.12 (s, 3H), 1.93-1.86 (m, 2H), 1.06 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 149.0, 80.2, 74.3, 66.4, 27.8, 10.5, 9.2; IR (KBr) υ_{max} 3161, 2125, 1730, 1400, 1158 cm^{-1}; HRMS (ESI) calcd for $C_8H_{11}NNaO_3$ 192.0632 $[M+Na]^+$, found 192.0627.



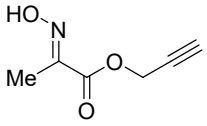
1t

(*E*)-Cyclopropylprop-2-ynyl 2-(Hydroxyimino)propanoate (1t). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.73 (s, 1H), 5.30 (dd, J_1 = 7.2 Hz, J_2 = 2.2 Hz, 1H), 2.47 (d, J = 2.2 Hz, 1H), 2.12 (s, 3H), 1.40-1.33 (m, 1H), 0.65-0.51 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 149.1, 78.5, 74.3, 68.9, 14.1, 10.5, 3.8, 2.2; IR (KBr) υ_{max} 3188, 1729, 1401, 1151 cm^{-1}; HRMS (ESI) calcd for $C_9H_{11}NNaO_3$ 204.0632 $[M+Na]^+$, found 204.0628.



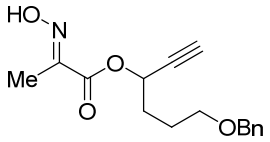
1u

(*E*)-Cyclohexylprop-2-ynyl 2-(Hydroxyimino)propanoate (1u). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.65 (s, 1H), 5.30 (dd, J_1 = 6.2 Hz, J_2 = 2.2 Hz, 1H), 2.48 (d, J = 2.2 Hz, 1H), 2.12 (s, 3H), 1.95-1.67 (m, 7H), 1.33-1.08 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 148.8, 79.4, 74.8, 69.5, 41.6, 28.3, 28.0, 26.0, 25.6, 25.57, 10.5; IR (KBr) υ_{max} 2929, 1731, 1401, 1163 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{17}NNaO_3$ 246.1101 $[M+Na]^+$, found 246.1099.



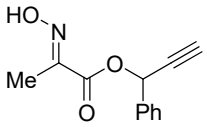
1v

(*E*)-Prop-2-ynyl 2-(Hydroxyimino)propanoate (1v). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.2 (s, 1H), 4.83 (d, J = 2.4 Hz, 2H), 2.51 (t, J = 2.4 Hz, 1H), 2.11 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 148.8, 76.8, 75.6, 53.1, 10.5; IR (KBr) υ_{max} 3132, 1741, 1401, 1144 cm^{-1}; HRMS (ESI) calcd for $C_6H_7NNaO_3$ 164.0319 $[M+Na]^+$, found 164.0318.



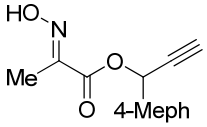
1w

(*E*)-6-(Benzyloxy)hex-1-yn-3-yl 2-(Hydroxyimino)propanoate (1w). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.6 (s, 1H), 7.36-7.25 (m, 5H), 5.49 (dt, J_1 = 6.5 Hz, J_2 = 2.1 Hz, 1H), 4.50 (s, 2H), 3.51 (t, J = 6.1 Hz, 2H), 2.50-2.49 (m, 1H), 2.08 (s, 3H), 2.01-1.96 (m, 2H), 1.84-1.75 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 148.7, 138.1, 128.3, 127.6, 127.5, 80.2, 74.4, 72.8, 69.2, 64.9, 31.3, 25.0, 10.5; IR (KBr) υ_{max} 3204, 1728, 1401, 1151 cm^{-1}; HRMS (ESI) calcd for $C_{16}H_{19}NNaO_4$ 312.1207 $[M+Na]^+$, found 312.1209.



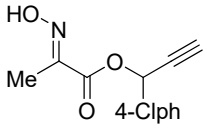
1x

(*E*)-1-(4-Phenyl)prop-2-ynyl 2-(Hydroxyimino)propanoate (1x). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 7.58-7.55 (m, 2H), 7.42-7.37 (m, 3H), 6.56 (d, *J* = 2.2 Hz, 1H), 2.70 (d, *J* = 2.3 Hz, 1H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 149.2, 135.8, 129.3, 128.8, 127.8, 79.5, 76.2, 66.7, 10.6; IR (KBr) υ_{max} 3131, 1725, 1400, 1157 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{11}NNaO_3$ 240.0632 $[M+Na]^+$, found 240.0627.



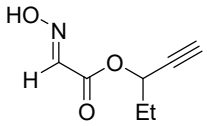
1y

(*E*)-1-(4-Methylphenyl)prop-2-ynyl 2-(Hydroxyimino)propanoate (1y). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (s, 1H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 6.8 Hz, 2H), 6.52 (d, *J* = 2.2 Hz, 1H), 2.68 (d, *J* = 2.3 Hz, 1H), 2.36 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 149.0, 139.3, 133.0, 129.4, 127.8, 79.7, 76.0, 66.7, 21.2, 10.5; IR (KBr) υ_{max} 3133, 2126, 1728, 1400, 1159 cm^{-1}; HRMS (ESI) calcd for $C_{13}H_{13}NNaO_3$ 254.0788 $[M+Na]^+$, found 254.0785.



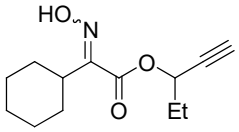
1z

(*E*)-1-(4-Chlorophenyl)prop-2-ynyl 2-(Hydroxyimino)propanoate (1z). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (s, 1H), 7.52-7.49 (m, 2H), 7.38-7.36 (m, 2H), 6.52 (d, *J* = 2.2 Hz, 1H), 2.71 (d, *J* = 2.3 Hz, 1H), 2.10 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 149.0, 135.4, 134.3, 129.3, 129.0, 79.1, 76.5, 66.0, 10.5; IR (KBr) υ_{max} 3128, 2349, 1736, 1401 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{10}ClNNaO_3$ 274.0242 $[M+Na]^+$, found 274.0238.



1aa

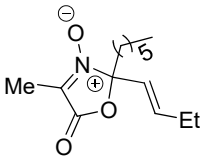
(*E*)-Pent-1-yn-3-yl 2-(Hydroxyimino)acetate (1aa). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.2 (s, 1H), 7.57 (s, 1H), 5.43 (dt, J_1 = 6.5 Hz, J_2 = 2.1 Hz, 1H), 2.51 (d, *J* = 2.2 Hz, 1H), 1.86 (p, *J* = 6.3 Hz, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 141.3, 79.9, 74.6, 66.4, 27.7, 9.1; IR (KBr) υ_{max} 3014, 2125, 1733, 1459, 1015 cm^{-1}; HRMS (ESI) calcd for $C_7H_9NNaO_3$ 178.0475 $[M+Na]^+$, found 178.0470.



1ab (*E* and *Z*)

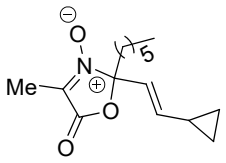
(*E* and Z)-Pent-1-yn-3-yl 2-Cyclohexyl-2-(hydroxyimino)acetate (1ab). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.74 (s, 1H), 9.21 (s, 0.5 H), 5.48 (dt, J_1 = 6.4 Hz, J_2 = 2.1 Hz, 0.5H), 5.38 (dt, J_1 = 6.5 Hz, J_2 = 2.0 Hz, 1H), 3.22-3.16 (m, 1.5H), 2.51 (d, J = 2.2 Hz, 0.5H), 2.49 (d, J = 2.1 Hz, 1H), 1.89-1.77 (m, 12H), 1.38-1.21 (m, 6H), 1.08-1.04 (m, 4.5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 162.3, 155.5, 155.1, 80.3, 80.0, 74.4, 74.2, 66.1, 66.0, 61.4, 40.2, 36.1, 36.0, 29.7, 29.6, 27.9, 27.8, 27.76, 27.73, 26.2, 25.8, 14.0, 9.22, 9.20; IR (KBr) υ_{max} 2933, 2361, 1736, 1155 cm^{-1}; HRMS (ESI) calcd for $C_{13}H_{19}NNaO_3$ 260.1258 $[M+Na]^+$, found 260.1258.

General procedure for the preparation of five-membered oxa-cyclic nitrones 2a-2r. To a stirred dichloromethane solution (2.0 mL) containing Ph_3PAuCl (0.0025 mmol, 1.2 mg) and $AgSbF_6$ (0.0025 mmol, 0.9 mg) was added oxime (0.1 mmol). The reaction mixture was stirred at at room temperature for 15 minutes. After removing the solvent under reduced pressure, the concentrated crude mixture was purified by flash column chromatography (petroleum ether /acetone as eluent) to give pure nitrone.



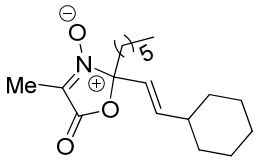
2a

(*E*)-2-(But-1-enyl)-2-hexyl-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2a). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.12 (td, J_1 = 15.6 Hz, J_2 = 6.3 Hz, 1H), 5.67 (td, J_1 = 15.7 Hz, J_2 = 1.6 Hz, 1H), 2.14-2.04 (m, 7H), 1.26-1.24 (m, 8H), 1.0 (t, J = 7.4 Hz, 3H), 0.85 (t, J = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 138.2, 126.9, 123.1, 105.7, 36.1, 31.4, 28.4, 25.0, 22.4, 21.7, 13.9, 12.5, 7.4; IR (KBr) υ_{max} 3129, 1789, 1596, 1403 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{23}NNaO_3$ 276.1571 $[M+Na]^+$, found 276.1582.



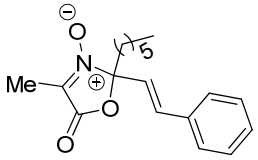
2b

(*E*)-2-(2-Cyclopropylvinyl)-2-hexyl-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2b). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.75 (d, J = 15.4 Hz, 1H), 5.52 (dd, J_1 = 15.5 Hz, J_2 = 9.4 Hz, 1H), 2.09 (s, 3H), 2.08-2.01 (m, 2H), 1.46-1.38 (m, 1H), 1.27-1.21 (m, 7H), 1.11-1.05 (m, 1H), 0.86 (t, J = 7.0 Hz, 3H), 0.81-0.79 (m, 2H), 0.51-0.43 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 140.6, 126.7, 121.1, 105.6, 36.2, 31.4, 28.4, 22.4, 21.7, 13.9, 13.7, 7.4, 7.39, 7.37; IR (KBr) υ_{max} 3162, 2931, 1727, 1401, 1149 cm^{-1}; HRMS (ESI) calcd for $C_{15}H_{23}NNaO_3$ 288.1571 $[M+Na]^+$, found 288.1571.



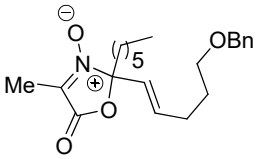
2c

(*E*)-2-(2-Cyclohexylvinyl)-2-hexyl-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2c). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.01 (dd, J_1 = 15.8 Hz, J_2 = 6.6 Hz, 1H), 5.62 (dd, J_1 = 15.8 Hz, J_2 = 1.4 Hz, 1H), 2.09 (s, 3H), 2.07-1.96 (m, 3H), 1.71-1.62 (m, 5H), 1.29-0.99 (m, 13H), 0.85 (t, J = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 142.0, 126.8, 121.7, 105.9, 40.1, 36.3, 32.1, 32.0, 31.4, 28.4, 25.9, 25.7, 22.4, 21.8, 13.9, 7.4; IR (KBr) υ_{max} 2928, 2854, 1788, 1595, 1405 cm^{-1}; HRMS (ESI) calcd for $C_{18}H_{29}NNaO_3$ 330.2040 $[M+Na]^+$, found 330.2046.



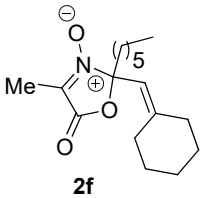
2d

(*E*)-2-hexyl-4-methyl-5-oxo-2-styryl-2,5-dihydrooxazole 3-oxide (2d). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.39 (m, 2H), 7.36-7.31 (m, 3H), 6.92 (d, J = 16.1 Hz, 1H), 6.39 (d, J = 16.0 Hz, 1H), 2.24-2.16 (m, 2H), 2.13 (s, 3H), 1.38-1.15 (m, 8H), 0.87 (t, J = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 134.5, 134.0, 129.1, 128.8, 127.1, 122.5, 105.9, 36.5, 31.4, 28.5, 22.4, 21.9, 13.9, 7.5; IR (KBr) υ_{max} 2931, 1788, 1595, 1404 cm^{-1}; HRMS (ESI) calcd for $C_{18}H_{23}NNaO_3$ 324.1571 $[M+Na]^+$, found 324.1569.



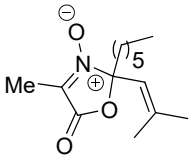
2e

(*E*)-2-(5-(Benzyloxy)pent-1-enyl)-2-hexyl-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2e). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 5H), 6.08 (dt, J_1 = 15.6 Hz, J_2 = 6.8 Hz, 1H), 5.70 (dt, J_1 = 15.6 Hz, J_2 = 1.5 Hz, 1H), 4.48 (s, 2H), 3.45 (t, J = 6.2 Hz, 2H), 2.23-2.16 (m, 2H), 2.09 (s, 3H), 2.07-2.03 (m, 2H), 1.71 (p, J = 6.6 Hz, 2H), 1.27-1.25 (m, 8H), 0.86 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 138.4, 136.2, 128.3, 127.6, 127.5, 126.8, 124.4, 105.6, 72.9, 69.1, 36.1, 31.4, 28.7, 28.5, 28.4, 22.4, 21.8, 13.9, 7.4; IR (KBr) υ_{max} 2930, 1786, 1594, 1403 cm^{-1}; HRMS (ESI) calcd for $C_{22}H_{31}NNaO_4$ 396.2146 $[M+Na]^+$, found 396.2141.



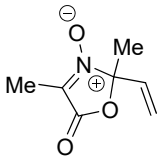
2f

2-(Cyclohexylidenemethyl)-2-hexyl-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2f). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.45 (s, 1H), 2.35-2.33 (m, 2H), 2.11 (s, 3H), 2.10-2.06 (m, 3H), 1.58-1.56 (m, 7H), 1.26-1.24 (m, 8H), 0.86 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 149.6, 127.8, 115.8, 106.6, 37.7, 37.6, 31.4, 30.3, 28.4, 28.38, 27.7, 26.1, 22.4, 21.7, 14.0, 7.5; IR (KBr) υ_{max} 2932, 1787, 1725, 1597, 1405 cm^{-1}; HRMS (ESI) calcd for $C_{17}H_{27}NNaO_3$ 316.1884 $[M+Na]^+$, found 318.1880.



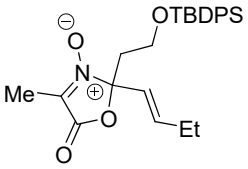
2g

2-Hexyl-4-methyl-2-(2-methylprop-1-enyl)-5-oxo-2,5-dihydrooxazole 3-oxide (2g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.48 (s, 1H), 2.10 (s, 3H), 2.09-2.07 (m, 2H), 1.82 (d, J = 0.6 Hz, 3H), 1.77 (d, J = 1.0 Hz, 3H), 1.26-1.22 (m, 8H), 0.85 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 141.8, 127.7, 118.8, 106.4, 37.4, 31.4, 28.4, 26.9, 22.4, 21.5, 19.4, 13.9, 7.4; IR (KBr) υ_{max} 2931, 1787, 1597, 1406 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{23}NNaO_3$ 276.1571 $[M+Na]^+$, found 276.1580.



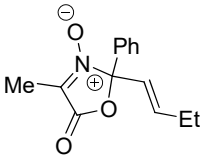
2h

2,4-Dimethyl-5-oxo-2-vinyl-2,5-dihydrooxazole 3-oxide (2h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.03 (dd, J_1 = 17.2 Hz, J_2 = 10.8 Hz, 1H), 5.66 (d, J = 17.2 Hz, 1H), 5.46 (d, J = 10.8 Hz, 1H), 2.09 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 132.4, 126.4, 120.3, 103.4, 23.5, 7.6; IR (KBr) υ_{max} 3125, 1789, 1596, 1402, 1164 cm^{-1}; HRMS (ESI) calcd for $C_7H_{10}NO_3$ 156.0656 $[M+H]^+$, found 156.0655.



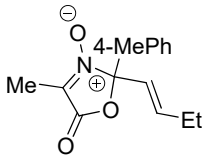
2i

(*E*)-2-(But-1-enyl)-2-(2-(tert-butyldiphenylsilyoxy)ethyl)-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2i). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.61 (m, 4H), 7.45-7.36 (m, 6H), 6.08 (dt, J_1 = 15.6 Hz, J_2 = 6.3 Hz, 1H), 5.67 (dt, J_1 = 15.6 Hz, J_2 = 1.6 Hz, 1H), 3.80-3.65 (m, 2H), 2.37 (td, J_1 = 6.0 Hz, J_2 = 2.4 Hz, 2H), 2.11-2.07 (m, 2H), 2.05 (s, 3H), 1.02 (s, 9H), 0.97 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 138.1, 135.5, 135.47, 133.1, 129.8, 129.76, 127.7, 126.4, 123.2, 104.3, 58.3, 38.6, 26.7, 25.0, 19.0, 12.5, 7.6; IR (KBr) υ_{max} 2963, 1788, 1595, 1403, 1111, 704 cm^{-1}; HRMS (ESI) calcd for $C_{26}H_{33}NNaO_4Si$ 474.2072 $[M+Na]^+$, found 474.2071.



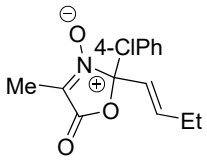
2j

(*E*)-2-(But-1-enyl)-4-methyl-5-oxo-2-phenyl-2,5-dihydrooxazole 3-oxide (2j). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.57 (m, 2H), 7.46-7.39 (m, 3H), 6.19 (dt, J_1 = 15.5 Hz, J_2 = 6.1 Hz, 1H), 6.04 (dt, J_1 = 15.6 Hz, J_2 = 1.6 Hz, 1H), 2.22-2.14 (m, 2H), 2.14 (s, 3H), 1.04 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 140.0, 134.2, 130.3, 128.6, 126.2, 123.4, 104.4, 25.1, 12.5, 7.7; IR (KBr) υ_{max} 2931, 1787, 1593, 1404 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{15}NNaO_3$ 268.0945 $[M+Na]^+$, found 268.0940.



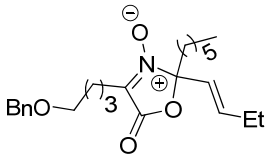
2k

(*E*)-2-(But-1-enyl)-4-methyl-2-(4-methylphenyl)-5-oxo-2,5-dihydrooxazole 3-oxide (2k). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 6.18 (dt, J_1 = 15.6 Hz, J_2 = 6.1 Hz, 1H), 6.03 (dt, J_1 = 15.6 Hz, J_2 = 1.6 Hz, 1H), 2.36 (s, 3H), 2.21-2.14 (m, 2H), 2.13 (s, 3H), 1.04 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 140.5, 139.9, 131.3, 129.3, 126.1, 123.4, 104.5, 25.1, 21.2, 12.5, 7.7; IR (KBr) υ_{max} 2930, 1788, 1594, 1402 cm^{-1}; HRMS (ESI) calcd for $C_{15}H_{17}NNaO_3$ 282.1101 $[M+Na]^+$, found 282.1099.



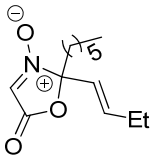
2l

(*E*)-2-(But-1-enyl)-2-(4-chlorophenyl)-4-methyl-5-oxo-2,5-dihydrooxazole 3-oxide (2l). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.53 (m, 2H), 7.40-7.38 (m, 2H), 6.16 (dt, J_1 = 15.6 Hz, J_2 = 6.1 Hz, 1H), 5.98 (dt, J_1 = 15.6 Hz, J_2 = 1.5 Hz, 1H), 2.19-2.15 (m, 2H), 2.13 (s, 3H), 1.03 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 140.6, 136.6, 132.7, 128.9, 127.7, 126.3, 123.2, 103.8, 25.1, 12.4, 7.7; IR (KBr) υ_{max} 2931, 1788, 1593, 1401, 1095 cm^{-1}; HRMS (ESI) calcd for $C_{14}H_{14}ClNNaO_3$ 302.0555 $[M+Na]^+$, found 302.0555.



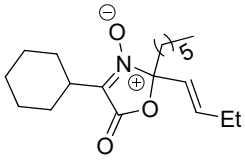
2m

(*E*)-4-((4-Benzyloxy)butyl)-2-(but-1-enyl)-2-hexyl-5-oxo-2,5-dihydrooxazole 3-oxide (2m). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.31 (m, 4H), 7.29-7.26 (m, 1H), 6.12 (dt, J_1 = 15.6 Hz, J_2 = 6.3 Hz, 1H), 5.67 (dt, J_1 = 15.6 Hz, J_2 = 1.6 Hz, 1H), 4.49 (s, 2H), 3.48 (t, J = 6.0 Hz, 2H), 2.59-2.54 (m, 2H), 2.14-2.04 (m, 4H), 1.76-1.63 (m, 4H), 1.29-1.25 (m, 8H), 1.00 (t, J = 7.4 Hz, 3H), 0.86 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 138.4, 138.1, 130.0, 128.3, 127.6, 127.5, 123.4, 105.3, 72.9, 69.4, 36.1, 31.4, 29.3, 28.4, 25.0, 22.4, 21.7, 21.69, 21.6, 13.9, 12.6; IR (KBr) υ_{max} 2931, 1784, 1585, 913, 744 cm^{-1}; HRMS (ESI) calcd for $C_{24}H_{36}NO_4$ 402.2639 $[M+H]^+$, found 402.2634.



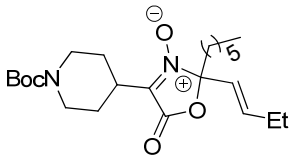
2n

(*E*)-2-(But-1-enyl)-2-hexyl-5-oxo-2,5-dihydrooxazole 3-oxide (2n). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 1H), 6.16 (dt, J_1 = 15.6 Hz, J_2 = 6.3 Hz, 1H), 5.66 (dt, J_1 = 15.6 Hz, J_2 = 1.7 Hz, 1H), 2.16-2.05 (m, 4H), 1.37-1.21 (m, 8H), 1.01 (t, J = 7.4 Hz, 3H), 0.87 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 138.7, 122.9, 117.2, 107.7, 36.1, 31.4, 28.4, 25.0, 22.4, 21.7, 13.9, 12.5; IR (KBr) υ_{max} 2931, 1790, 1565, 744 cm^{-1}; HRMS (ESI) calcd for $C_{13}H_{22}NO_3$ 240.1595 $[M+H]^+$, found 240.1604.



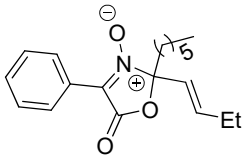
2o

(*E*)-2-(But-1-enyl)-4-cyclohexyl-2-hexyl-5-oxo-2,5-dihydrooxazole 3-oxide (2o). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.10 (dt, J_1 = 15.6 Hz, J_2 = 6.3 Hz, 1H), 5.66 (dt, J_1 = 15.6 Hz, J_2 = 1.7 Hz, 1H), 2.86 (tt, J_1 = 12.1 Hz, J_2 = 3.6 Hz, 1H), 2.14-2.01 (m, 4H), 1.88-1.77 (m, 4H), 1.74-1.65 (m, 3H), 1.34-1.20 (m, 10H), 1.08-1.04 (m, 1H), 1.00 (t, J = 7.4 Hz, 3H), 0.86 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.2, 138.0, 132.9, 123.5, 104.4, 36.1, 33.2, 31.4, 28.4, 27.1, 26.8, 25.7, 25.68, 25.3, 25.1, 22.4, 21.5, 13.9, 12.6; IR (KBr) υ_{max} 2931, 2857, 1782, 1574, 1400, 985 cm^{-1}; HRMS (ESI) calcd for $C_{19}H_{31}NNaO_3$ 344.2197 $[M+Na]^+$, found 344.2209.



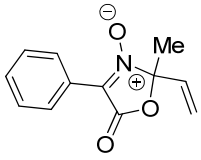
2p

(*E*)-2-(But-1-enyl)-4-(1-(tert-butoxycarbonyl)piperidin-4-yl)-2-hexyl-5-oxo-2,5-dihydrooxazole 3-oxide (2p). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.11 (dt, J_1 = 15.6 Hz, J_2 = 6.3 Hz, 1H), 5.65 (dt, J_1 = 15.6 Hz, J_2 = 1.6 Hz, 1H), 4.21 (s, br, 2H), 2.99 (tt, J_1 = 12.3 Hz, J_2 = 3.7 Hz, 1H), 2.74 (s, br, 2H), 2.14-1.95 (m, 6H), 1.65 (s, 1H), 1.46 (s, 9H), 1.28-1.24 (m, 9H), 1.00 (t, J = 7.4 Hz, 3H), 0.86 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9, 154.5, 138.3, 131.1, 123.3, 104.9, 79.7, 36.1, 31.7, 31.4, 28.4, 28.36, 26.1, 25.9, 25.0, 22.4, 21.5, 13.9, 12.5; IR (KBr) υ_{max} 2931, 1782, 1576, 1171 cm^{-1}; HRMS (ESI) calcd for $C_{23}H_{38}N_2NaO_5$ 445.2672 $[M+Na]^+$, found 445.2680.



2q

(*E*)-2-(But-1-enyl)-2-hexyl-5-oxo-4-phenyl-2,5-dihydrooxazole 3-oxide (2q). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67-8.63 (m, 2H), 7.52-7.48 (m, 3H), 6.20 (dt, J_1 = 15.6 Hz, J_2 = 6.2 Hz, 1H), 5.77 (dt, J_1 = 15.6 Hz, J_2 = 1.6 Hz, 1H), 2.22-2.10 (m, 4H), 1.38-1.19 (m, 8H), 1.02 (t, J = 7.4 Hz, 3H), 0.85 (t, J = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9, 138.3, 131.4, 128.5, 126.8, 124.5, 124.2, 123.5, 104.3, 36.5, 31.4, 28.5, 25.1, 22.4, 21.7, 13.9, 12.6; IR (KBr) υ_{max} 2930, 1781, 1565, 1398 cm^{-1}; HRMS (ESI) calcd for $C_{19}H_{25}NNaO_3$ 338.1727 $[M+Na]^+$, found 338.1727.

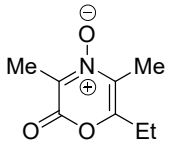


2r

(*E*)-2-(But-1-enyl)-2-hexyl-5-oxo-4-phenyl-2,5-dihydrooxazole 3-oxide (2r). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65-8.62 (m, 2H), 7.51-7.48 (m, 3H), 6.15 (dd, J_1 = 17.2 Hz, J_2 = 10.7 Hz, 1H), 5.75 (d, J = 17.2 Hz, 1H), 5.51 (d, J = 10.7 Hz, 1H), 1.93 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.4, 132.8, 131.6, 128.5, 126.8, 124.4, 120.4, 102.1, 23.8; IR (KBr) υ_{max} 3133, 1782, 1560, 1392 cm^{-1}; HRMS

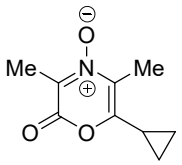
(ESI) calcd for $C_{12}H_{11}NNaO_3$ 240.0632 $[M+Na]^+$, found 240.0640.

General procedure for the preparation of six-membered nitrones 3s-3ab. To a stirred toluene solution (2.0 mL) containing JohnPhosAuCl (0.0025 mmol, 1.3 mg) and $AgNTf_2$ (0.0025 mmol, 1.0 mg) and MsOH (0.01 mmol) was added oxime (0.1 mmol). The reaction mixture was stirred at 110 ºC for 10 minutes. After cooling to room temperature, the crude mixture was purified by flash column chromatography (petroleum ether /acetone as eluent) to give the six-membered cyclic nitrone.



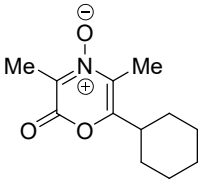
3s

6-Ethyl-3,5-dimethyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3s). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (q, *J* = 7.6 Hz, 2H), 2.29 (s, 3H), 2.17 (s, 3H), 1.23 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.2, 152.1, 133.1, 125.8, 24.2, 11.4, 11.3, 10.6; IR (KBr) υ_{max} 3309, 1719, 1491, 745 cm^{-1}; HRMS (ESI) calcd for $C_8H_{11}NNaO_3$ 192.0632 $[M+Na]^+$, found 192.0632.



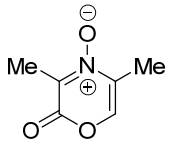
3t

6-Cyclopropyl-3,5-dimethyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3t). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.30 (s, 3H), 2.29 (s, 3H), 1.89-1.85 (m, 1H), 1.18-1.14 (m, 2H), 1.06-1.01 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 151.3, 132.2, 125.7, 11.4, 10.9, 10.4, 7.8; IR (KBr) υ_{max} 3127, 1719, 1665, 1487, 1401, 726 cm^{-1}; HRMS (ESI) calcd for $C_9H_{11}NNaO_3$ 204.0632 $[M+Na]^+$, found 204.0632.



3u

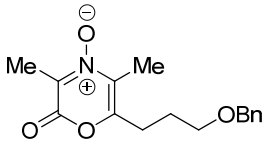
6-Cyclohexyl-3,5-dimethyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3u). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64-2.58 (m, 1H), 2.31 (s, 3H), 2.20 (s, 3H), 1.88-1.84 (m, 2H), 1.74-1.64 (m, 5H), 1.36-1.22 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.2, 154.3, 132.9, 125.3, 39.6, 29.4, 25.8, 25.3, 11.4, 10.4; IR (KBr) υ_{max} 2932, 2856, 1719, 1662, 1489, 728 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{17}NNaO_3$ 246.1101 $[M+Na]^+$, found 246.1113.



3v

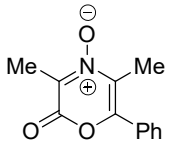
3,5-Dimethyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3v). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 1H), 2.34 (s, 3H), 2.14 (d, *J* = 1.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 137.2, 135.7, 129.9, 11.52, 11.5;

IR (KBr) υ_{max} 3129, 1720, 1487, 778 cm^{-1}; HRMS (ESI) calcd for $C_6H_7NNaO_3$ 164.0319 $[M+Na]^+$, found 164.0314.



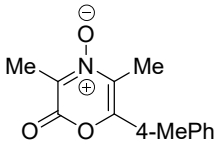
3w

6-(3-(Benzyloxy)propyl)-3,5-dimethyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3w). ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 5H), 4.48 (s, 2H), 3.50 (t, *J* = 5.8 Hz, 2H), 2.69 (t, *J* = 7.4 Hz, 2H), 2.31 (s, 3H), 2.19 (s, 3H), 2.02-1.96 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 150.7, 138.0, 133.1, 128.4, 127.7, 127.6, 126.61, 73.0, 68.3, 27.6, 26.9, 11.4, 10.7; IR (KBr) υ_{max} 2859, 1719, 1492, 1077, 728 cm^{-1}; HRMS (ESI) calcd for $C_{16}H_{20}NO_4$ 290.1387 $[M+H]^+$, found 290.1384.



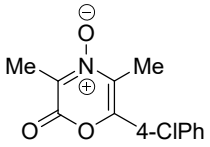
3x

3,5-Dimethyl-2-oxo-6-phenyl-2*H*-1,4-oxazine 4-oxide (3x). ^1H NMR (400 MHz, $CDCl_3$) δ 7.57-7.55 (m, 2H), 7.51-7.49 (m, 3H), 2.41 (d, *J* = 0.9 Hz, 3H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 148.6, 133.7, 130.9, 130.1, 128.8, 128.7, 127.4, 12.4, 11.7; IR (KBr) υ_{max} 3128, 1722, 1442, 1083, 724 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{11}NNaO_3$ 240.0632 $[M+Na]^+$, found 240.0627.



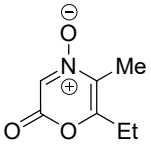
3y

3,5-Dimethyl-6-(4-methylphenyl)-2-oxo-2*H*-1,4-oxazine 4-oxide (3y). ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H), 2.41 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.9, 148.8, 141.5, 133.4, 129.4, 128.8, 127.2, 127.1, 21.5, 12.5, 11.7; IR (KBr) υ_{max} 3128, 1713, 1401, 849 cm^{-1}; HRMS (ESI) calcd for $C_{13}H_{14}NO_3$ 232.0969 $[M+H]^+$, found 232.0970.



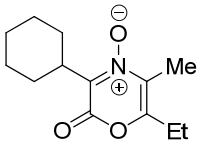
3z

6-(4-Chlorophenyl)-3,5-dimethyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3z). ^1H NMR (400 MHz, $CDCl_3$) δ 7.52-7.46 (m, 4H), 2.40 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 147.4, 137.2, 133.9, 130.1, 129.1, 128.5, 127.6, 12.4, 11.7; IR (KBr) υ_{max} 3094, 1711, 1448, 845 cm^{-1}; HRMS (ESI) calcd for $C_{12}H_{10}ClNNaO_3$ 274.0242 $[M+Na]^+$, found 274.0240.



3aa

6-Ethyl-5-methyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3aa). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (s, 1H), 2.59 (q, *J* = 7.6 Hz, 2H), 2.16 (s, 3H), 1.26 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 155.5, 126.4, 121.4, 24.4, 11.1, 9.9; IR (KBr) υ_{max} 3079, 1734, 1491, 745 cm^{-1}; HRMS (ESI) calcd for $C_7H_{10}NO_3$ 156.0655 $[M+Na]^+$, found 156.0655.



3ab

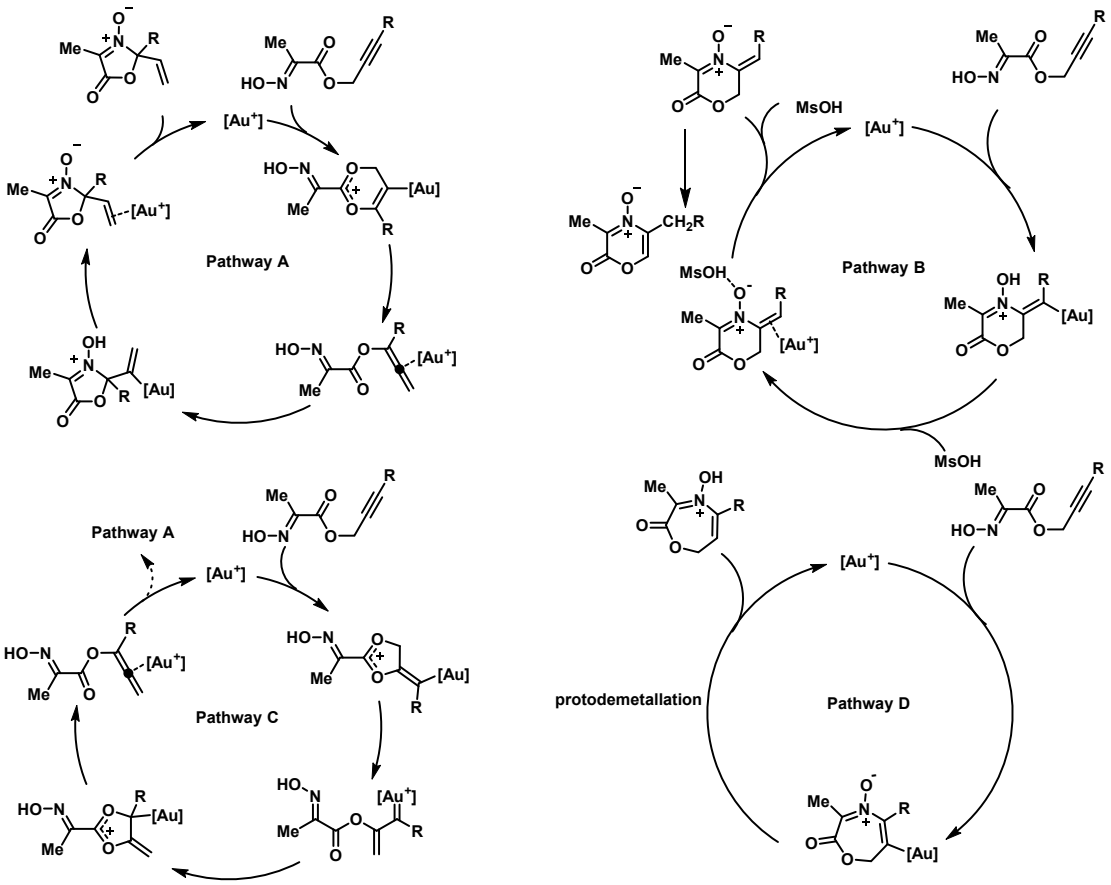
3-Cyclohexyl-6-ethyl-5-methyl-2-oxo-2*H*-1,4-oxazine 4-oxide (3ab). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.44 (tt, J_1 = 12.2 Hz, J_2 = 3.3 Hz, 1H), 2.55 (q, *J* = 7.6 Hz, 2H), 2.16 (s, 3H), 2.08-1.99 (m, 2H), 1.81-1.78 (m, 2H), 1.70-1.68 (m, 1H), 1.57-1.56 (m, 1H), 1.36-1.24 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 152.2, 139.4, 126.1, 36.1, 29.7, 26.4, 26.2, 25.6, 24.3, 11.3, 10.8; IR (KBr) υ_{max} 2933, 1719, 913, 745 cm^{-1}; HRMS (ESI) calcd for $C_{13}H_{19}NNaO_3$ 260.1258 $[M+Na]^+$, found 260.1254.

3. Mechanism study and quantum chemical calculations

3.1 Computational methodologies

All calculations were performed with the Gaussian 09 program[1]. Geometry optimizations of all minima and transition states involved were carried out using the B3LYP functional[2] and SMD[3] solvation model. In order to understand the selectivity, all calculations were performed in dichloromethane solvent. For geometry optimizations, the SDD[4] basis set and pseudopotential (Stuttgart/Dresden ECP) were used for gold and the 6-31G(d)[5] basis set for the other atoms. We labelled this basis set as SDD-6-31G(d). Frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. For single point energy calculations, the M06 functional[6] and def2-TZVP[7] basis set with the D3 version of Grimme's dispersion[8] were used (M06-D3), based on on the optimized structures from the SMD/B3LYP/SDD-6-31G(d) method. The keyword "5D" was used to specify that five d type orbitals were used for all elements in the calculations. Standard states for solutes in solution are the hypothetical states at 1 mol/L.

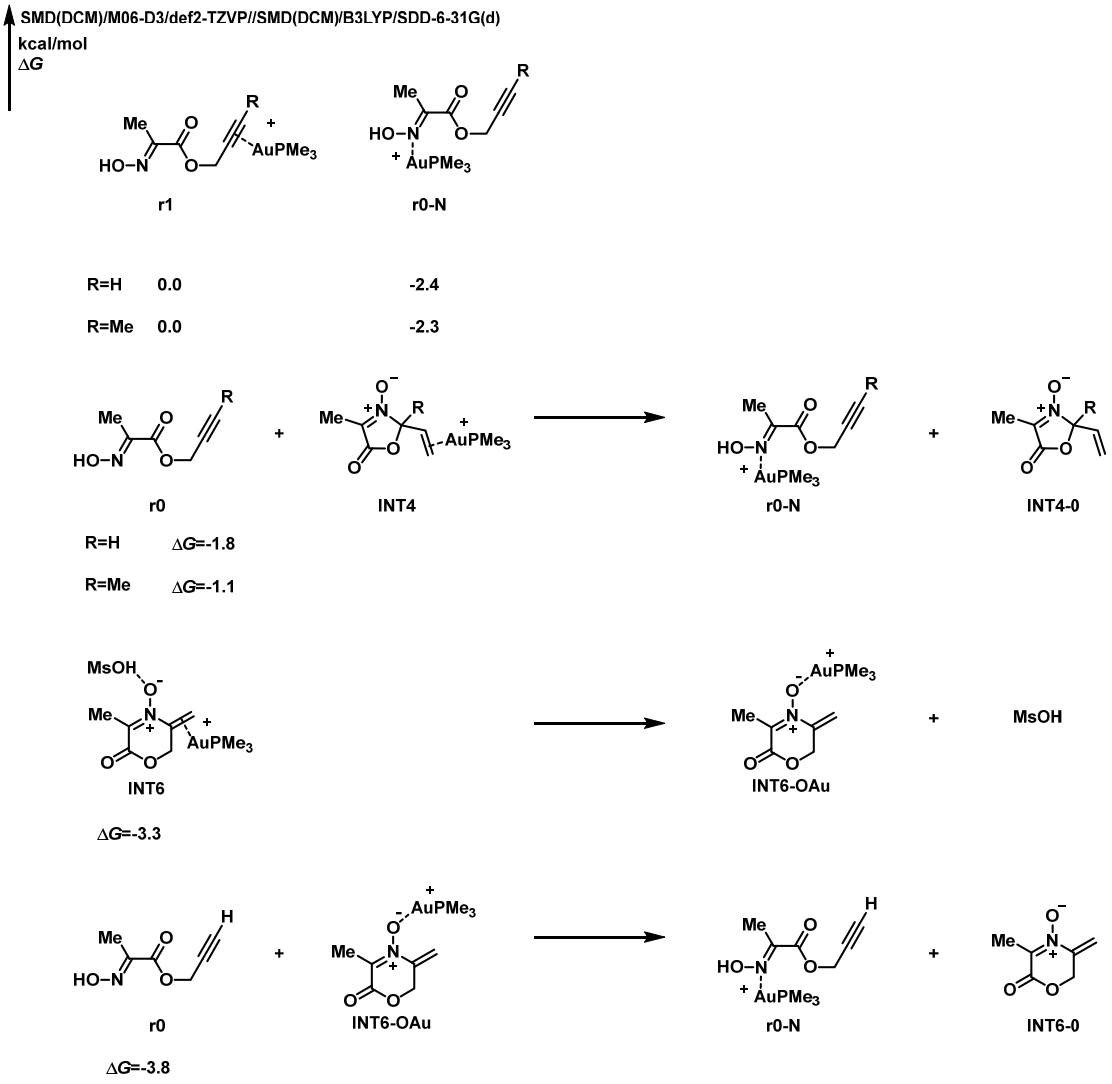
3.2 Proposed catalytic cycles for Au (I) catalyzed cyclization



Scheme S1: Proposed catalytic cycles A-D

3.3 Thermodynamic results of pathways A & B

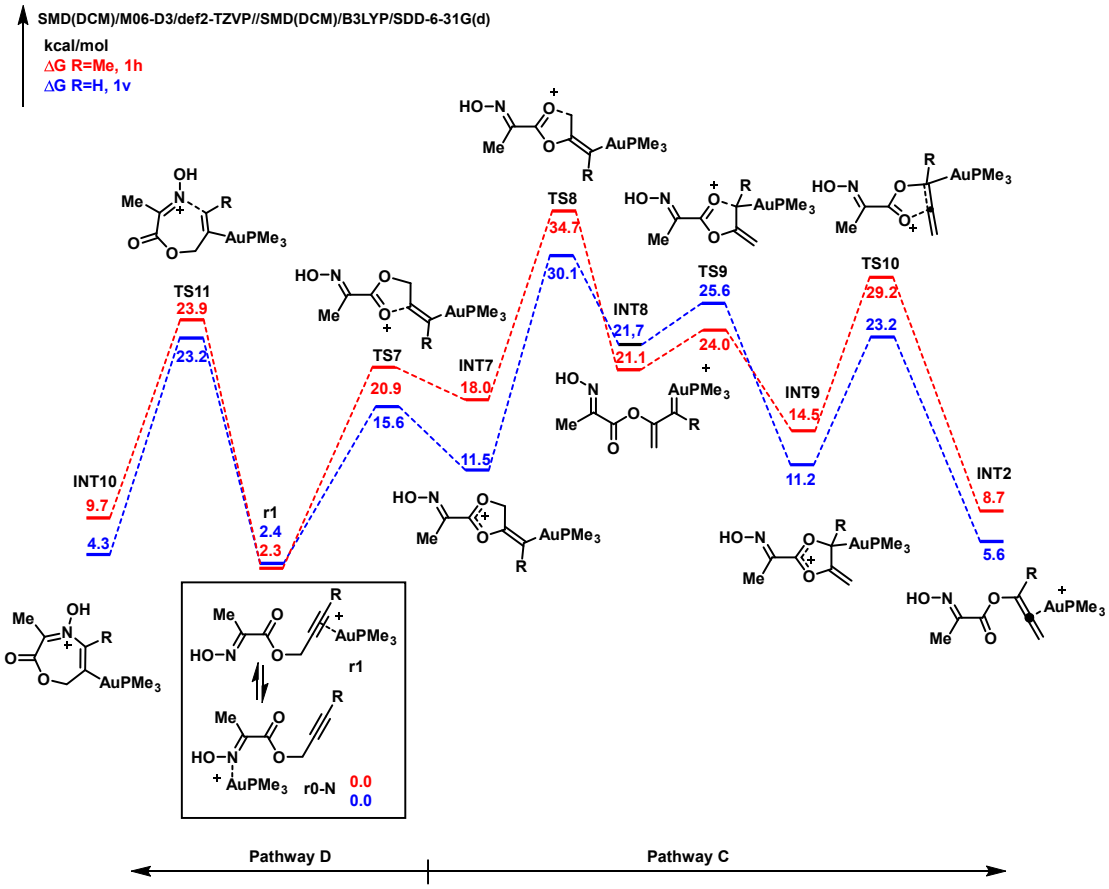
We first discuss the different coordination modes of Au-coordinated substrate complexes, finding that nitrogen atom is better than alkynyl group as the coordinating site by about 2 kcal/mol (Scheme S2). For the exchange reaction of catalyst-product complex and substrate, all these are exothermic in terms of Gibbs free energy. All these suggest that, the catalytic cycle can restart via ligand exchange reaction between substrate and product-Au complex.



Scheme S2: Thermodynamic results of pathways A & B

3.4 Gibbs free energy surfaces for pathways C & D

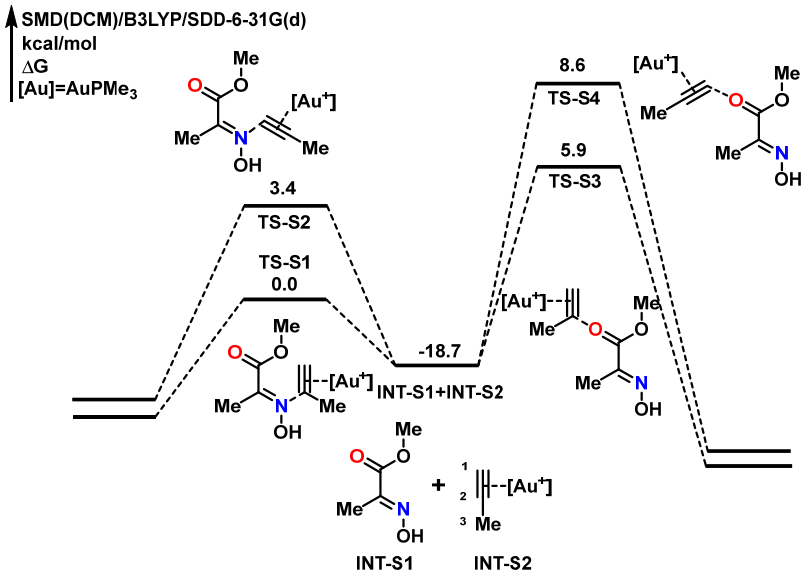
Pathway C shows a 1,2-acyloxy migration process via a 5-*exo* type attacking by oxygen atom in carbonyl moiety, which may lead to the formation of an alkenyl gold(I) carbenoid **INT8**. This intermediate may form the same allene intermediate **INT2** in Pathway A via the subsequent acyloxy migration. Similarly, a 7-*endo* type cyclization process attacked by nitrogen atom is named as pathway D. But compared with pathways A & B, these two pathways have higher energy barriers and should be ruled out.



Scheme S3: Gibbs free energy surfaces for pathways C & D

3.5 Study on intermolecular nucleophilic attack

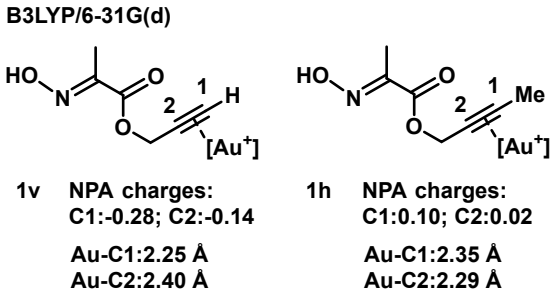
To further understand the relative nucleophilicities of oxygen and nitrogen atoms in the propargylic α-ketocarboxylate oximes, we studied a model system of the intermolecular reaction between methyl *(E)*-2-(hydroxyimino)propanoate and propyne (Scheme S4). Calculations indicated that nitrogen in the oxime moiety has stronger nucleophilicity than oxygen atom in carbonyl group because the former process is kinetically favored by about 5 kcal/mol than the latter process (**TS-S3** vs. **TS-S1**; **TS-S4** vs. **TS-S2**). Meanwhile, the effect of methyl group in the alkyne can be estimated, showing that the nucleophilic reaction favors to attack C2 over C1 by about 3 kcal/mol (**TS-S1** vs. **TS-S2**; **TS-S3** vs. **TS-S4**). All calculations in Scheme S4 were performed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level, and a standard state of 298 K and 1 mol/L was used for drawing the Gibbs free energy surfaces.



Scheme S4: Model reactions to understand the relative nucleophilicities and substitution effects in alkyne.

3.6 NPA charge analysis for Au-coordinated substrates

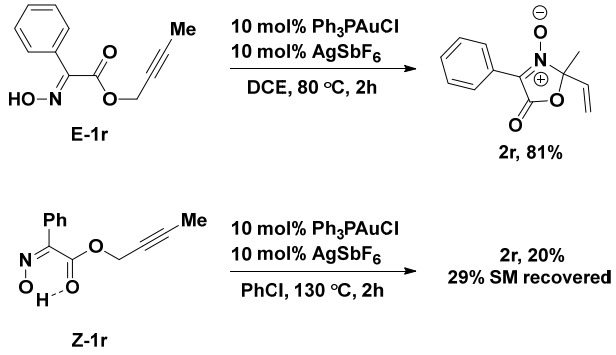
In order to understand the position of nucleophilic attack, a natural population analysis[9] (NPA) was conducted for substrates **1h** and **1v** at the B3LYP/6-31G (d) level (Scheme S5). For **1v**: the proximal C (sp) has a less negative positive NPA charge, however, for internal alkynyl oxime **1h**, because of the absence of alkyl group, the distal C (sp) gets more positive NPA charge. For the nucleophilic attack, carbon with more positive charge is more reactive than carbon with less positive charge. Therefore, C2 is more reactive than C1 in **1v** and this is just the opposite for **1h**.



Scheme S5: NPA charges and Au-C analysis for substrates **1h** & **1v**

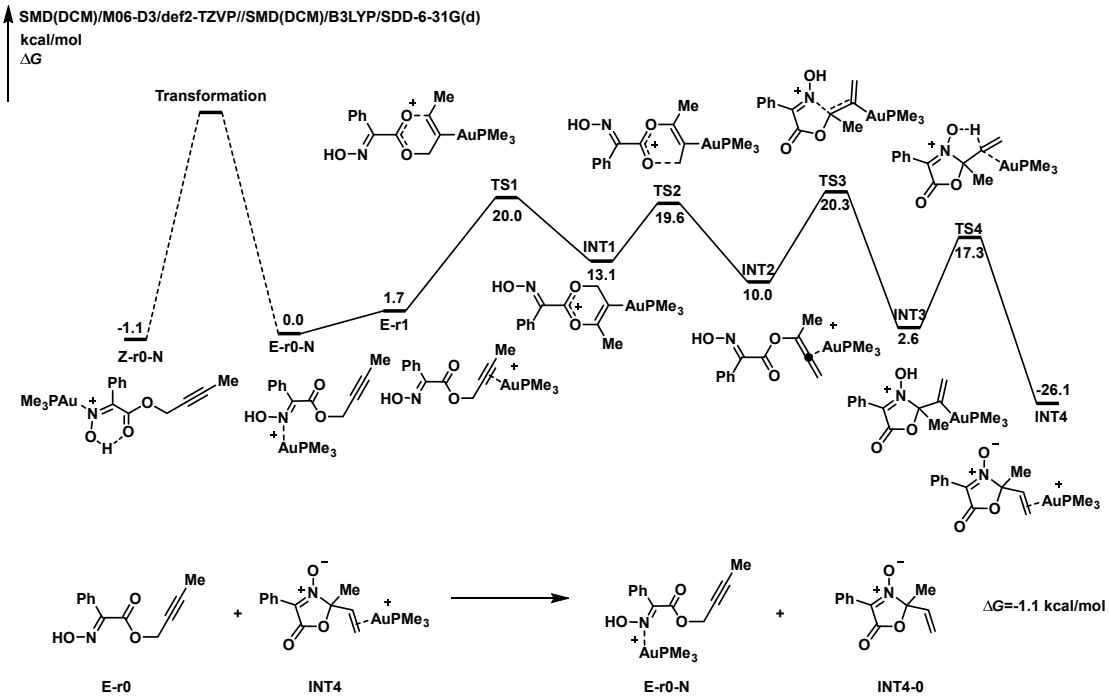
3.7 Experimental and calculational results for substrate *Z*/*E*-1r

Experimentally we observed that ***E*-1r** undergoes Au(I) catalyzed cyclization reaction to give nitrone **2r** at 80 ℃ (higher than standard reaction conditions). But ***Z*-1r** cannot give the reactivity at this temperature (Scheme 2, S6). Under relative more harsh conditions, ***Z*-1r** was converted to **2r** in 20% yield. Meanwhile, 29% of starting material was recovered.



Scheme S6: Reactions for ***E*-1r** and ***Z*-1r**.

We computed the Gibbs free energy surface of substrate ***E*-1r** (Scheme S7) and found the overall Gibbs free energy barrier is similar with the case of **1h** (from ***E*-r0-N** to **TS3**: 20.3 kcal/mol for **1r** and 20.2 kcal/mol for **1h)**. In the case of ***Z*-1r**, only if ***Z*-1r** can be converted to ***E*-1r**, can then this substrate give product **2r**, considering that the product **2r** has a cis-configuration of its N-O group and phenyl group, whereas in ***Z*-1r**, these two groups are in a trans-configuration. It is known that *E/Z*-oxime is hard to interconvert in gas phase, but relative easier in protonic solvent under acidic conditions.[10] We postulate that only part of ***Z*-1r** can be converted to ***E*-1r** so that only 20% product **2r** was obtained when the reaction was conducted at 130 ℃. Under these harsh conditions, 29% of reactant ***Z*-1r** was recovered and the rest could decompose in the reaction system.



Scheme S7: The PES for ***E*-1r** and ***Z*-1r**.

3.8 The comparisons of selectivity influenced by using different ligands on Au(I) center for calculations

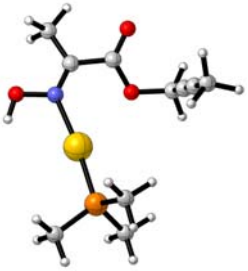
In the main text of our calculations, we used PMe_3 to replace PPh_3 and JohnPhos as the ligand. To assure that this simplification would not affect our conclusions, we computed two key transition states that determine regiochemistry in both pathways A and B for **1h** and **1v** using PPh_3 as the ligand, finding that calculations using PMe_3 and PPh_3 can both give correct regiochemistry consistent with those from experimental observations (see **Table S1** below).

Table S1

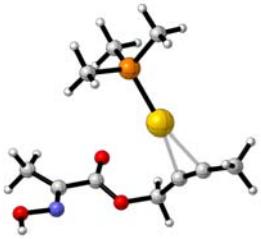
	$\Delta\Delta G$ (L = PMe_3)	$\Delta\Delta G$ (L = PPh_3)	Experimental result
TS 5 (1h) - TS 1 (1h)	2.2	2.7	Pathway A
TS 5 (1v) - TS 1 (1v)	-4.1	-2.6	Pathway B

3.9 3D structures [11]

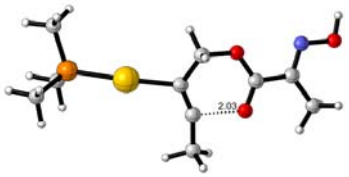
For **1h** system



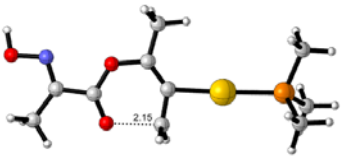
r0-N



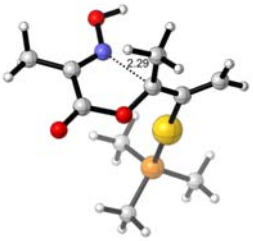
r1



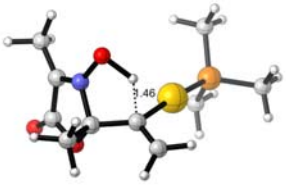
TS1



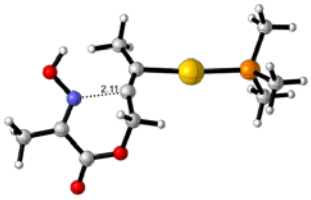
TS2



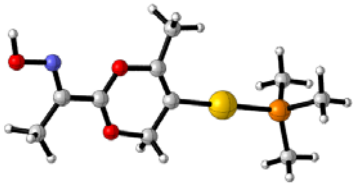
TS3



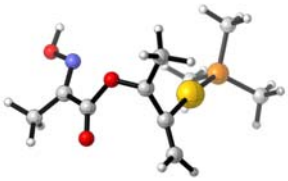
TS4



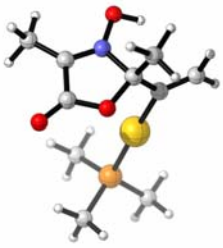
TS5



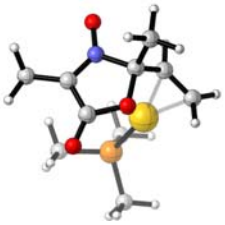
INT1



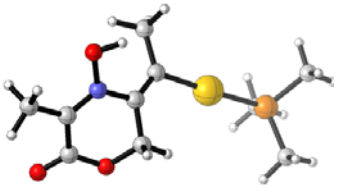
INT2



INT2

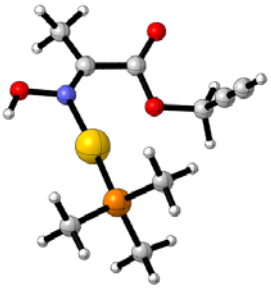


INT4

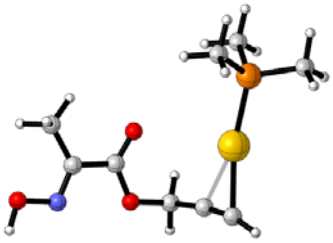


INT5

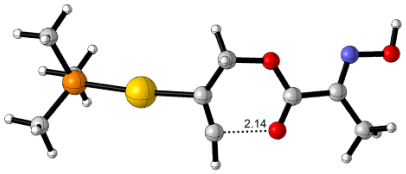
For **1v** system



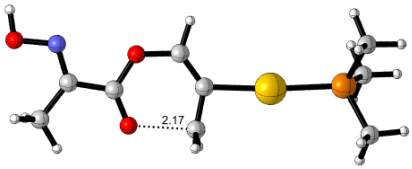
r0-N



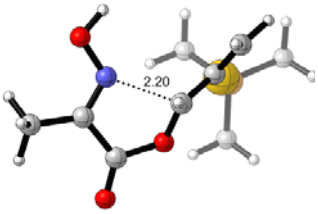
r1



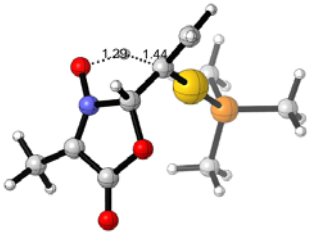
TS1



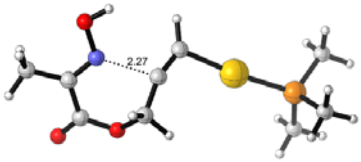
TS2



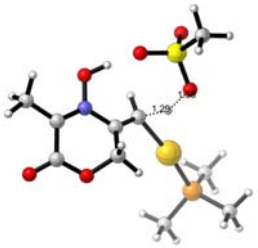
TS3



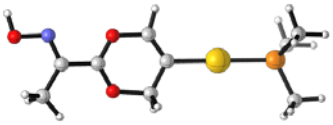
TS4



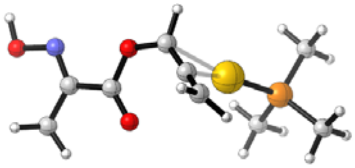
TS5



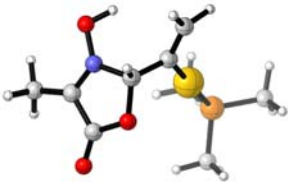
TS6



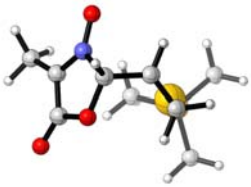
INT1



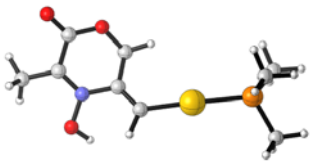
INT2



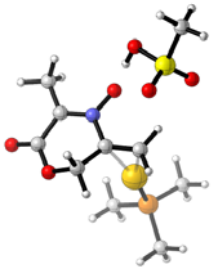
INT3



INT4

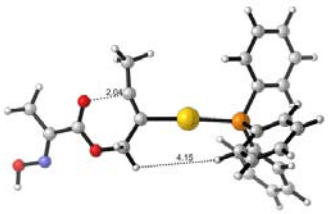


INT5

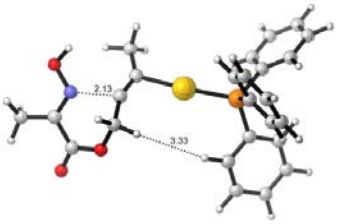


INT6

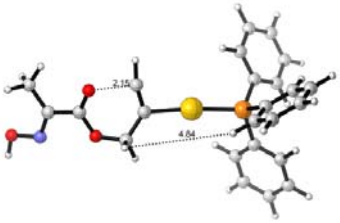
For L = PPh_3



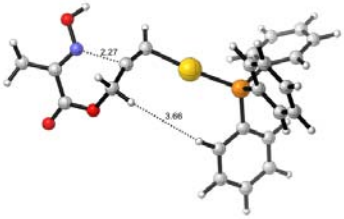
TS 1 (1h)



TS 5 (1h)



TS 1 (1v)



TS 5 (1v)

3.10 Energy data sheet

Thermal correction to Enthalpy ***CH***, Thermal correction to Gibbs Free Energy ***CG***, Single point energy in DCM by M06/def2-TZVP-D3 ***E*(M06)**, Sum of the Electronic and thermal Enthalpies ***H***, Sum of Electroinc and Thermal Free Energies ***G,*** Single point energy in DCM by B3LYP/6-31G(d) for intermolecular cases ***E*(B3LYP)**.

For **1h** system

	CH	***CG***	***E*(M06-D3)**	***H***	***G***
r1	0.294831	0.217296	-1149.093962	-1148.799131	-1148.876666
TS1	0.293488	0.218737	-1149.067342	-1148.773854	-1148.848605
INT1	0.295608	0.21957	-1149.079434	-1148.783826	-1148.859864
TS2	0.292407	0.215254	-1149.065763	-1148.773356	-1148.850509
INT2	0.293022	0.214908	-1149.08137	-1148.788348	-1148.866462
TS3	0.29191	0.218258	-1149.066328	-1148.774418	-1148.84807
INT3	0.294127	0.221618	-1149.095018	-1148.800891	-1148.8734
TS4	0.28909	0.217833	-1149.070823	-1148.781733	-1148.85299
INT4	0.294717	0.222052	-1149.13934	-1148.844623	-1148.917288
TS5	0.293286	0.218744	-1149.063868	-1148.770582	-1148.845124
INT5	0.295319	0.221023	-1149.089785	-1148.794466	-1148.868762
TS7	0.293427	0.217488	-1149.064483	-1148.771056	-1148.846995
INT7	0.295635	0.220885	-1149.072456	-1148.776821	-1148.851571
TS8	0.292685	0.218809	-1149.043899	-1148.751214	-1148.82509
INT8	0.293052	0.217184	-1149.063878	-1148.770826	-1148.846694
TS9	0.291743	0.21855	-1149.060692	-1148.768949	-1148.842142
INT9	0.293676	0.218609	-1149.075773	-1148.782097	-1148.857164
TS10	0.291351	0.216994	-1149.050822	-1148.759471	-1148.833828
INT10	0.295729	0.223222	-1149.088156	-1148.792427	-1148.864934
TS11	0.293197	0.218959	-1149.061172	-1148.767975	-1148.842213
r0-N	0.295149	0.217218	-1149.097553	-1148.802404	-1148.880335
r0	0.167878	0.113576	-552.3646253	-552.1967473	-552.2510493
INT4-0	0.167916	0.119655	-552.4094111	-552.2414951	-552.2897561

For **1v** system

	CH	***CG***	***E*(M06-D3)**	***H***	***G***
r1	0.263893	0.1892	-1109.782802	-1109.518909	-1109.593602
TS1	0.263209	0.190547	-1109.754266	-1109.491057	-1109.563719
INT1	0.266467	0.195417	-1109.772682	-1109.506215	-1109.577265
TS2	0.263107	0.190379	-1109.758432	-1109.495325	-1109.568053
INT2	0.263453	0.189702	-1109.778183	-1109.51473	-1109.588481
TS3	0.263108	0.192485	-1109.759478	-1109.49637	-1109.566993
INT3	0.265334	0.195957	-1109.792081	-1109.526747	-1109.596124
TS4	0.259775	0.190792	-1109.765495	-1109.50572	-1109.574703
INT4	0.266108	0.196766	-1109.833797	-1109.567689	-1109.637031
TS5	0.262772	0.191463	-1109.761709	-1109.498937	-1109.570246
INT5	0.26603	0.196393	-1109.794583	-1109.528553	-1109.59819
TS6	0.330622	0.246559	-1774.142435	-1773.811813	-1773.895876
INT6	0.336825	0.249562	-1774.191018	-1773.854193	-1773.941456
TS7	0.263076	0.190337	-1109.762939	-1109.499863	-1109.572602
INT7	0.265793	0.194396	-1109.773511	-1109.507718	-1109.579115
TS8	0.262507	0.190889	-1109.740295	-1109.477788	-1109.549406
INT8	0.263824	0.191252	-1109.754007	-1109.490183	-1109.562755
TS9	0.262387	0.191554	-1109.748193	-1109.485806	-1109.556639
INT9	0.264895	0.194304	-1109.773923	-1109.509028	-1109.579619
TS10	0.261976	0.19085	-1109.751225	-1109.489249	-1109.560375
INT10	0.266184	0.196205	-1109.786693	-1109.520509	-1109.590488
TS11	0.262815	0.189421	-1109.749895	-1109.48708	-1109.560474
r0-N	0.264399	0.190596	-1109.788013	-1109.523614	-1109.597417
r0	0.137283	0.087526	-513.0558874	-512.9186044	-512.9683614
INT4-0	0.138922	0.093449	-513.104274	-512.965352	-513.010825
INT6-OAu	0.266452	0.197406	-1109.822238	-1109.555786	-1109.624832
MsOH	0.068361	0.032202	-664.3570448	-664.2886838	-664.3248428

For **1r**

	CH	*CG*	*E*(M06-D3)	*H*	*G*
Z-r0-N	0.350782	0.265652	-1340.752448	-1340.401666	-1340.486796
E-r0-N	0.351325	0.264619	-1340.74967	-1340.398345	-1340.485051
E-r1	0.350758	0.265533	-1340.747869	-1340.397111	-1340.482336
TS1	0.34958	0.266838	-1340.720074	-1340.370494	-1340.453236
INT1	0.351637	0.26776	-1340.731929	-1340.380292	-1340.464169
TS2	0.348528	0.264406	-1340.718271	-1340.369743	-1340.453865
INT2	0.349366	0.265025	-1340.734176	-1340.38481	-1340.469151
TS3	0.348424	0.267266	-1340.71989	-1340.371466	-1340.452624
INT3	0.351077	0.271841	-1340.752741	-1340.401664	-1340.4809
TS4	0.34475	0.265176	-1340.722682	-1340.377932	-1340.457506
INT4	0.351537	0.271263	-1340.797943	-1340.446406	-1340.52668
E-r0	0.223882	0.16198	-744.0173369	-743.7934549	-743.8553569
INT4-0	0.224361	0.168385	-744.0670767	-743.8427157	-743.8986917

Intermolecular cases

	CH	*CG*	*E(B3LYP)*	*H*	*G*
TS-S1	0.315043	0.235518	-1150.460041	-1150.144998	-1150.224522
TS-S2	0.315384	0.236283	-1150.455437	-1150.140053	-1150.219154
TS-S3	0.315327	0.236972	-1150.452054	-1150.136727	-1150.215082
TS-S4	0.315564	0.23573	-1150.446533	-1150.130969	-1150.210802
INT-S1	0.126448	0.082174	-437.007848	-436.8814	-436.925674
INT-S2	0.18747	0.131736	-713.463378	-713.275908	-713.331642

For ligand = PPh_3

	CH	*CG*	*E(M06-D3)*	*H*	*G*
TS 1 (1h)	0.463317	0.362029	-1724.03298	-1723.569663	-1723.670951
TS 5 (1h)	0.463482	0.362657	-1724.029312	-1723.56583	-1723.666655
TS 1 (1v)	0.43321	0.335297	-1684.719458	-1684.286248	-1684.384161
TS 5 (1v)	0.431851	0.338235	-1684.726539	-1684.294688	-1684.388304

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4. Cartesian coordinates of all computed structures

For 1h system:

r1

O	4.60912700	-0.91630200	1.84405500
N	3.75259700	-0.06650800	1.17022000
C	3.50965600	-0.48740000	-0.02275700
C	4.07159700	-1.73849000	-0.62904000
C	2.56309000	0.34339300	-0.83007900
O	2.09403300	-0.03343500	-1.88763400
O	2.29573400	1.54350800	-0.26578600
C	1.34782600	2.38806800	-0.94456100
C	0.03583400	2.37235800	-0.26654900
C	-1.00638400	2.71375700	0.29793000
H	4.70933200	-0.48734600	2.71477500
H	3.76976900	-2.61664400	-0.04569400
H	3.72765600	-1.85633700	-1.65691000
H	5.16700700	-1.70524000	-0.61418400
H	1.75327700	3.40195300	-0.89162800
H	1.25522600	2.08541800	-1.98910700
Au	-1.05225200	0.38121800	0.00879300
P	-1.72042600	-1.84436000	0.02696200
C	-3.51336400	-2.03870300	0.34849900
H	-3.77885800	-3.10168600	0.35117200
H	-3.76522800	-1.60108100	1.31932900
H	-4.08552300	-1.52450900	-0.42986300
C	-1.40767100	-2.69107700	-1.56669600
H	-0.33656600	-2.67566000	-1.79037400
H	-1.75276200	-3.72959500	-1.51325900
H	-1.94127200	-2.17262700	-2.36918000
C	-0.87534600	-2.85191800	1.30216100
H	-1.07191400	-2.43341000	2.29411800
H	-1.23847600	-3.88488200	1.26500900
H	0.20435900	-2.84137100	1.12371400
C	-2.15720100	3.31610200	0.97261200
H	-3.08438400	3.12905500	0.42206300
H	-2.26471500	2.92230400	1.98848400
H	-2.00022000	4.39964300	1.03670100

INT1

C	-3.51556400	-0.26577900	-0.00069700
O	-2.87811100	-1.37825600	-0.00182800
C	-1.36543500	-1.42029500	-0.00537100
C	-0.72350100	-0.07747200	-0.00384300
C	-1.48214200	1.01472700	-0.00220300
O	-2.94736300	0.88842300	-0.00161500
C	-4.98330200	-0.33896900	0.00190600
N	-5.54788700	0.82616200	0.00364200
O	-6.90378700	0.72921000	0.00615000
C	-5.69907400	-1.65595300	0.00265900
Au	1.35876500	-0.05639400	-0.00301000
H	-1.13204600	-2.01090700	0.88315200
H	-1.13587200	-2.00710200	-0.89745900
H	-7.20618400	1.65972700	0.00726100
H	-6.34664700	-1.72861700	-0.87829200
H	-5.00154800	-2.49322000	-0.00031000
H	-6.34127400	-1.73048700	0.88740400
P	3.71059300	-0.04754500	0.00245500
C	4.44479200	0.69997800	1.51070400
H	4.11609100	0.14380100	2.39457600
H	5.53904700	0.67839500	1.45848500
H	4.10912200	1.73724600	1.60901700
C	4.45593600	0.89262900	-1.38890200
H	5.54972300	0.86818800	-1.32910000
H	4.13748200	0.45712400	-2.34132200
H	4.11723200	1.93303800	-1.35169100
C	4.46973800	-1.71657000	-0.10085200
H	5.56293700	-1.64256800	-0.09813300
H	4.14835800	-2.32057900	0.75376900
H	4.14443300	-2.21361000	-1.02037500
C	-1.16182700	2.46903600	-0.00053500
H	-1.57624800	2.96546300	0.88599700
H	-0.07713800	2.59860600	-0.00097900
H	-1.57725500	2.96768900	-0.88534900

TS1

C	3.56992000	0.06426200	-0.31215700
O	2.83380500	-1.02281500	-0.46560300
C	1.50970100	-0.90366900	-1.05893700
C	0.70118600	0.23173600	-0.49272800
C	1.17310200	1.38124200	-0.19912200
O	3.16109000	1.21116400	-0.55455500
C	4.94823800	-0.16442800	0.19676100
N	5.31074800	-1.40166600	0.24037300
O	6.59185100	-1.53635100	0.71781100
C	5.79649400	1.00557600	0.59380500
Au	-1.37385800	0.03260000	-0.12456500
H	1.63854600	-0.76723400	-2.13829900
H	1.05584500	-1.87354000	-0.87106900
H	6.74595900	-2.50035000	0.68968700
H	6.72905000	1.01154600	0.01839600
H	5.26849500	1.94505800	0.42886000
H	6.07059400	0.92840500	1.65249800
P	-3.64791600	-0.31085700	0.28180800
C	-4.76300400	0.70056800	-0.76674700
H	-4.57737100	0.47888100	-1.82247000
H	-5.81015500	0.48121100	-0.52996300
H	-4.56806000	1.76349100	-0.59264900
C	-4.13823500	0.07017500	2.00788000
H	-5.20663500	-0.12397300	2.15388300
H	-3.56053100	-0.55115800	2.69946300
H	-3.92947900	1.12241600	2.22571600
C	-4.17424800	-2.04641800	0.00604800
H	-5.24215500	-2.16091900	0.22222000
H	-3.98541800	-2.32737000	-1.03495500
H	-3.60012300	-2.71262600	0.65781000
C	1.18571300	2.76227400	0.26459500
H	1.77092600	2.87574400	1.18287300
H	1.58297500	3.43408800	-0.50329000
H	0.14864100	3.05159600	0.47460900

TS2

C	3.60150300	-0.42120800	-0.00956700
O	3.05291800	-1.52330700	-0.01067500
C	0.90324300	-1.46380200	0.00387800
C	0.73421600	-0.09044700	-0.00049500
C	1.57379400	0.93973700	-0.00809600
O	2.97667100	0.76471800	-0.01080300
C	5.08796500	-0.31109100	-0.00483000
N	5.55308200	0.89142300	0.00669100
O	6.92875500	0.90187900	0.02070100
C	5.91515400	-1.56091900	-0.00454000
Au	-1.38943600	-0.08335400	0.00295500
H	0.82731600	-2.04045500	-0.91662600
H	0.83576700	-2.03391500	0.92921900
H	7.14780300	1.85347500	0.02068500
H	6.48720500	-1.63579300	0.92811600
H	5.28663700	-2.44583800	-0.10621200
H	6.64022400	-1.53353700	-0.82528700
P	-3.73877700	0.01862600	0.00057500
C	-4.39206200	1.68504400	-0.39958300
H	-4.04711100	1.98904500	-1.39301900
H	-5.48763900	1.67657000	-0.38547700
H	-4.02738400	2.41023300	0.33470900
C	-4.49504400	-0.41694000	1.61340400
H	-5.58691500	-0.35021800	1.55264700
H	-4.21191300	-1.43723700	1.89105700
H	-4.13340900	0.26935200	2.38553600
C	-4.51654200	-1.10983300	-1.21864000
H	-5.60713000	-1.01140500	-1.18392200
H	-4.16346400	-0.86520800	-2.22528900
H	-4.24109400	-2.14445000	-0.99115100
C	1.26094600	2.39873500	-0.01359700
H	0.17800500	2.54658800	-0.01117400
H	1.68905600	2.89219100	0.86763500
H	1.68379700	2.88424100	-0.90175500

INT2

C	-3.00748600	-0.27250400	-0.20933600
O	-3.32738800	-1.05180600	-1.06752600
C	-0.65997400	-2.89592400	-1.31423100
C	-0.67595600	-2.01047400	-0.32746700
C	-1.31337200	-1.62915600	0.83523600
O	-2.25570800	-0.66178200	0.91045300
C	-3.38424000	1.16080000	-0.16717900
N	-2.80687800	1.86039100	0.75162300
O	-3.17853200	3.18080700	0.69305900
C	-4.34711900	1.68649400	-1.18801000
Au	0.89143200	-0.51923400	-0.08830500
H	-1.43908200	-3.65380800	-1.39193400
H	0.11056500	-2.89829100	-2.07941800
H	-2.69925300	3.58712600	1.44083700
H	-3.84509900	2.39848900	-1.85418200
H	-4.75860500	0.87302700	-1.78661200
H	-5.16358700	2.22389400	-0.69382700
P	2.63590800	1.03936000	-0.07085500
C	3.17124400	1.48557200	1.62497200
H	3.53136000	0.59149100	2.14343400
H	3.97425500	2.23010700	1.58446800
H	2.32453900	1.89761200	2.18279900
C	2.19313800	2.62203000	-0.88221100
H	3.03834200	3.31818300	-0.84119600
H	1.92849700	2.43652400	-1.92787100
H	1.33245100	3.06945500	-0.37531100
C	4.15002200	0.45823500	-0.92405500
H	4.92873700	1.22754700	-0.87542900
H	4.51427000	-0.45611100	-0.44525500
H	3.92316900	0.23999100	-1.97222300
C	-0.98325700	-2.17996100	2.18573200
H	-0.13104000	-2.85863600	2.13620500
H	-0.78310000	-1.37755400	2.90323500
H	-1.86501800	-2.73111800	2.54128600

TS3

C	-2.94615900	1.40307000	0.24528700
N	-2.57613600	0.48785500	1.06135200
C	-2.11870500	-1.20900500	-0.40025800
O	-2.06001000	-0.21810100	-1.30955700
C	-2.72514900	1.00611700	-1.17598200
O	-2.97067900	1.66105000	-2.14693300
O	-2.75540900	0.75216900	2.38025700
C	-3.52593900	2.73511700	0.58795700
C	-0.84467800	-1.74514900	0.00609700
C	-0.82906400	-3.06473700	0.33328300
Au	0.86862700	-0.55242300	-0.00433100
P	2.82678100	0.75165900	0.00409700
H	-2.38916900	-0.03120700	2.84091200
H	-4.36066800	2.61235400	1.28626100
H	-2.76775300	3.35645000	1.07992500
H	-3.87238100	3.24404400	-0.31254400
H	0.09027800	-3.55420600	0.64488500
H	-1.70167900	-3.71512700	0.26572400
C	2.88182100	2.02696800	1.32593500
H	2.79431900	1.54611700	2.30552600
H	3.82290100	2.58636000	1.28192800
H	2.04470500	2.72190600	1.20417200
C	4.36491000	-0.22447500	0.24006700
H	4.45961800	-0.96123100	-0.56410700
H	5.24287200	0.43103500	0.23390400
H	4.31959600	-0.75731000	1.19531200
C	3.10522700	1.68730100	-1.55197300
H	4.03414700	2.26523700	-1.49286700
H	3.16815300	0.99011100	-2.39356800
H	2.26689100	2.36884100	-1.72828800
C	-3.44908100	-1.87102700	-0.23283700
H	-3.49866900	-2.67954300	-0.97719300
H	-3.55872700	-2.31136400	0.75889300
H	-4.27504700	-1.18694000	-0.43323200

INT3

C	-2.59279600	1.46080200	0.48140200
N	-2.66735700	0.19998000	0.71122100
C	-2.35591200	-0.68521600	-0.48238900
O	-2.04723600	0.32672600	-1.46051500
C	-2.17801600	1.57836400	-0.96156500
O	-1.96883400	2.59087400	-1.57154900
O	-2.99992800	-0.34355800	1.89799700
C	-2.84115700	2.57993400	1.40451800
C	-1.12273000	-1.49419500	-0.11103400
C	-1.30311700	-2.79071300	0.20708100
Au	0.72416400	-0.53654600	-0.02434900
P	2.85551500	0.47284100	0.07464400
H	-2.51375500	-1.20783100	1.93059300
H	-3.79064900	3.05861400	1.12819100
H	-2.89390000	2.24439700	2.44142900
H	-2.05317200	3.33015700	1.28031600
H	-0.46382900	-3.40540800	0.52421500
H	-2.26156400	-3.30801000	0.15396000
C	3.12987800	1.52561000	1.55571900
H	3.00437200	0.92658300	2.46346800
H	4.13884700	1.95247200	1.54380700
H	2.39559200	2.33763500	1.57030600
C	4.24194200	-0.73238600	0.10360000
H	4.21339300	-1.34760300	-0.80150100
H	5.20406200	-0.21059000	0.15412400
H	4.14298800	-1.38963500	0.97337400
C	3.23505900	1.57342500	-1.34579000
H	4.23539900	2.00804400	-1.24143300
H	3.18699500	1.00022700	-2.27739000
H	2.49596300	2.37939600	-1.39661600
C	-3.62699300	-1.40331200	-0.92305600
H	-3.40252000	-1.98357600	-1.82133200
H	-3.98809800	-2.08188700	-0.14731800
H	-4.40931200	-0.67450000	-1.15120300

TS4

C	-2.60511300	1.45846100	0.48224000
N	-2.38914500	0.24732600	0.86950200
C	-2.44671100	-0.76374800	-0.24199400
O	-2.50033300	0.08741300	-1.39269400
C	-2.71300400	1.38447100	-1.01185400
O	-2.87914500	2.29125900	-1.78233100
O	-1.92692100	-0.24958700	1.99488000
C	-2.61930700	2.68663500	1.30120500
C	-1.16055900	-1.54411400	0.00711400
C	-1.05095500	-2.83483800	-0.37121400
Au	0.75342300	-0.51734000	0.05191600
P	2.81551600	0.56240100	-0.09053000
H	-1.15602400	-1.05077200	1.38229500
H	-3.60031600	3.17038300	1.21918900
H	-2.40984700	2.46177000	2.34862700
H	-1.87677200	3.39506100	0.91617300
H	-0.16847900	-3.41670100	-0.11639700
H	-1.80946200	-3.35872600	-0.95435200
C	3.15725100	1.70368000	1.30389100
H	3.14711500	1.14661600	2.24599800
H	4.13574600	2.17945300	1.17471100
H	2.38351300	2.47690900	1.34466300
C	4.23490100	-0.59862000	-0.11679100
H	4.14190400	-1.27824500	-0.96955300
H	5.17686400	-0.04462400	-0.19710400
H	4.24239100	-1.19082700	0.80376900
C	2.99679500	1.58342000	-1.60325400
H	3.98593900	2.05364300	-1.62798300
H	2.87339300	0.95483100	-2.49062900
H	2.22648300	2.36114300	-1.61594700
C	-3.74334400	-1.56148600	-0.15379400
H	-3.78296100	-2.26397200	-0.99092100
H	-3.78423800	-2.12091700	0.78368700
H	-4.60292400	-0.88830100	-0.21832800

INT4

C	2.27540700	1.62751500	-0.19602200
N	2.44611500	0.53187900	-0.90352600
C	2.52827400	-0.67763800	0.00460400
O	2.33998000	-0.12756000	1.30016600
C	2.17996200	1.24556100	1.21105700
O	1.98692000	1.93035000	2.18565900
O	2.55234300	0.39189600	-2.14816300
C	2.20169500	2.98936700	-0.77758400
C	1.43112500	-1.65240300	-0.36173400
C	0.74858700	-2.40273100	0.55572500
Au	-0.72137000	-0.69999300	-0.00414300
P	-2.65296500	0.60986300	-0.06749000
H	1.38793500	-1.89752500	-1.42089900
H	3.07126200	3.17916400	-1.41760900
H	1.30460400	3.10684100	-1.39845400
H	2.17590200	3.73216100	0.02296100
H	0.15879700	-3.25614500	0.22941100
H	0.91511800	-2.28909500	1.62384600
C	-3.82071700	0.09982300	-1.38213200
H	-4.10394200	-0.94730700	-1.23754400
H	-4.71902900	0.72601900	-1.34661500
H	-3.34485400	0.20512500	-2.36199800
C	-3.59593400	0.51800700	1.50039200
H	-2.98183900	0.89764800	2.32272900
H	-4.50873600	1.11870600	1.42153600
H	-3.86389000	-0.52181200	1.71132900
C	-2.32660200	2.39005500	-0.34772100
H	-3.27208600	2.94369700	-0.35424000
H	-1.68607900	2.77877300	0.44984200
H	-1.82130200	2.52755000	-1.30855300
C	3.90987800	-1.31132500	-0.12506000
H	3.98077600	-2.16397300	0.55531000
H	4.06798700	-1.65293200	-1.15097100
H	4.67528300	-0.57346000	0.13383200

TS5

C	-3.86051300	1.56036600	0.25912700
C	-4.42153100	0.18637800	-0.00165500
N	-3.58284600	-0.71612300	-0.36822800
C	-1.52416800	-0.24757500	-0.42927200
C	-1.84945400	1.04142300	-1.05011400
O	-2.61969400	1.88849100	-0.16223500
O	-4.50603800	2.37864800	0.87575700
C	-0.77799600	-1.11688700	0.12020400
Au	1.19966200	-0.27340100	0.00616000
P	3.42544900	0.42013800	0.02497300
C	3.86577600	1.58090000	-1.32505300
C	4.60375900	-0.97531300	-0.13918900
O	-4.11503600	-1.97254200	-0.51016300
C	-5.87445000	-0.06481900	0.24539300
H	-0.93112100	1.59980100	-1.24221400
H	-2.38843000	0.91090300	-1.99270100
H	3.25958600	2.48866400	-1.24529700
H	4.92619500	1.84933800	-1.26069300
H	3.67090600	1.11213300	-2.29465200
H	4.45213800	-1.68443100	0.68061000
H	4.43352600	-1.49416500	-1.08786300
H	5.63456600	-0.60525700	-0.10966900
H	-3.39315100	-2.49770100	-0.91061000
H	-6.30072900	-0.65071700	-0.57471100
H	-6.00082200	-0.64703700	1.16702400
H	-6.40987900	0.87837500	0.35195300
C	3.90611600	1.27930100	1.57262300
H	4.96299600	1.56561600	1.53475600
H	3.29278200	2.17691700	1.69966200
H	3.74032300	0.61815000	2.42885300
C	-0.93551600	-2.45415700	0.76971400
H	-0.41156800	-2.47663100	1.72985600
H	-1.98951900	-2.69582800	0.94298800
H	-0.48888600	-3.23317500	0.14153300

INT5

C	-4.12847200	1.38241900	0.15546300
C	-4.31920800	-0.10706700	-0.04037600
N	-3.24452600	-0.83997800	-0.11882900
C	-1.90987500	-0.30262200	-0.23327900
C	-1.98148000	1.06262600	-0.83825400
O	-2.92940300	1.90340600	-0.11326300
O	-5.03668000	2.04808200	0.59506800
C	-0.82016300	-0.98976400	0.15427200
Au	1.12953700	-0.34025700	0.06060800
P	3.38512700	0.35099000	0.00024500
C	4.06810100	0.79339000	1.64704000
C	3.68991900	1.83488400	-1.03906500
O	-3.41579900	-2.19392300	-0.01820900
C	-5.68235000	-0.68658000	0.01712500
H	-1.01915600	1.56229400	-0.75962000
H	-2.30302500	1.03235100	-1.88613700
H	-0.99999200	-1.98669900	0.56298800
H	4.01712400	-0.07318600	2.31390400
H	5.11071200	1.11763200	1.55598300
H	3.47654900	1.60379400	2.08505400
H	3.38891500	1.63025900	-2.07147400
H	3.09892900	2.67630000	-0.66329600
H	4.75156600	2.10519800	-1.02116200
H	-2.70083600	-2.59155600	-0.56720700
H	-5.75137800	-1.58431200	-0.60151300
H	-5.91953900	-0.97034100	1.05217900
H	-6.40966100	0.06201000	-0.30055600
C	4.53650300	-0.92046200	-0.65561200
H	5.56741500	-0.54981000	-0.64141800
H	4.47136000	-1.82733100	-0.04592400
H	4.25959700	-1.17277800	-1.68436900

TS7

C	-3.74428300	-0.10508000	0.21386400
O	-3.07814500	-1.24905700	0.25836100
C	-1.71990700	-1.03074500	0.72961800
C	-0.43453000	1.23282100	0.08755900
C	-1.30264700	0.34330600	0.37558900
O	-3.13840800	0.95974000	0.42695600
C	-5.18420700	-0.15492300	-0.10193100
N	-5.66018400	-1.35168100	-0.19666300
O	-6.99804200	-1.34099700	-0.48133400
C	-5.96091700	1.11577200	-0.26522700
Au	1.47125100	0.27783900	-0.00132800
H	-1.72449500	-1.19528900	1.81268100
H	-1.09513400	-1.77915800	0.24162100
H	-7.23418400	-2.28866200	-0.51831000
H	-6.78410400	1.14839800	0.45751800
H	-5.32269000	1.98785100	-0.11931400
H	-6.40434700	1.15893600	-1.26663500
P	3.63880500	-0.59016800	-0.11097500
C	3.77162500	-2.16861500	-1.03537100
H	3.41355900	-2.02970100	-2.06022700
H	4.81320700	-2.50765900	-1.05971000
H	3.15546200	-2.93260900	-0.55062500
C	4.36909000	-0.94337100	1.53501600
H	5.38132200	-1.34815700	1.42492000
H	4.41095700	-0.02234400	2.12488700
H	3.74612500	-1.67051700	2.06534900
C	4.82737500	0.54407100	-0.92806200
H	5.82843700	0.09930600	-0.94644800
H	4.50187800	0.74241600	-1.95414600
H	4.86518800	1.49240600	-0.38273500
C	-0.52475600	2.71204200	-0.13889900
H	-0.11316000	2.97555700	-1.11870800
H	-1.56080500	3.06062500	-0.08126600
H	0.06889300	3.24447700	0.61249900

INT7

C	-3.68594800	-0.27953100	0.00831300
O	-3.11031200	-1.44205100	-0.00293100
C	-1.64553200	-1.24235900	0.06217600
C	-0.47504900	1.09488000	0.01039800
C	-1.50378900	0.25893200	0.03543500

O	-2.90038100	0.73781300	0.03830100
C	-5.12963400	-0.11290100	-0.01172900
N	-5.75642600	-1.24861300	-0.01767500
O	-7.10043600	-1.08064900	-0.03237800
C	-5.75922800	1.24704800	-0.01778600
Au	1.44945400	0.29927900	0.00152400
H	-1.30976400	-1.71464800	0.98818500
H	-1.21927900	-1.75425300	-0.80201700
H	-7.45495400	-1.99333700	-0.03447600
H	-6.39993400	1.36401400	0.86335600
H	-5.00863700	2.03822000	-0.01732400
H	-6.39357800	1.35866500	-0.90408700
P	3.65399500	-0.54083000	-0.00947300
C	3.87592800	-2.08162100	-0.98463300
H	3.59139300	-1.90215500	-2.02638700
H	4.91985200	-2.41261900	-0.94965300
H	3.23497000	-2.87167800	-0.58006500
C	4.31266600	-0.95416900	1.65590800
H	5.33401200	-1.34384200	1.58053000
H	4.31503800	-0.05740700	2.28392200
H	3.67416200	-1.70730600	2.12888700
C	4.88417300	0.62678700	-0.71509600
H	5.89118400	0.19650200	-0.68003900
H	4.62448200	0.85023600	-1.75495100
H	4.87405200	1.56196200	-0.14595000
C	-0.66352200	2.59301400	-0.00778200
H	-0.18740900	3.02260400	-0.89795300
H	-1.71431300	2.90553400	0.00141900
H	-0.16441600	3.04785400	0.85683900

TS8

C	-3.19082300	-0.06186700	0.02942100
O	-3.89600100	-0.96899900	-0.44457600
C	-2.86271200	-2.51693400	0.42396800
C	-0.42714900	-2.00674500	0.00240900
C	-1.70686400	-1.72099200	0.38990100
O	-2.05381800	-0.36207800	0.67367400
C	-3.54971300	1.36398900	-0.08442500
N	-2.65928400	2.17546000	0.38268700
O	-3.04888300	3.47948900	0.25519100
C	-4.85559400	1.76239600	-0.70241700
Au	1.04625700	-0.55841400	-0.00648800
H	-3.59798000	-2.41207400	1.21493200
H	-2.91873700	-3.43343300	-0.15741300
H	-2.30787500	3.98283000	0.64588700
H	-4.67958300	2.34924200	-1.61149800
H	-5.45346300	0.88636600	-0.95586100
H	-5.41968100	2.39654000	-0.00961300
P	2.77197100	1.05576000	-0.04738400
C	3.08468900	1.84229700	1.58262500
H	3.36691400	1.07646900	2.31204700
H	3.89011800	2.58147900	1.50690000
H	2.17325800	2.33730500	1.93288500
C	2.45751500	2.45860500	-1.19027300
H	3.29100100	3.16959900	-1.16897100
H	2.33261400	2.08115300	-2.21026800
H	1.53771800	2.97321200	-0.89448500
C	4.40163800	0.38598300	-0.56547900
H	5.16549800	1.17128400	-0.54919900
H	4.70020100	-0.42116700	0.11108500
H	4.32550400	-0.02092100	-1.57903900
C	-0.06090600	-3.42138400	-0.33295200
H	0.61265700	-3.80905700	0.44464600
H	-0.90522800	-4.11642300	-0.41452300
H	0.51732300	-3.44172500	-1.26400400

INT8

C	2.48463600	-0.04893100	0.49837300
O	2.27626500	0.43596200	1.59249200
C	2.51033700	2.93598400	-1.12406500
C	0.49833900	2.11477400	0.02006000
C	1.81803500	1.94713300	-0.51482300
O	2.31492800	0.64842900	-0.66149600
C	2.95915000	-1.44543700	0.28753700
N	2.95613100	-1.85788000	-0.93376000
O	3.38772400	-3.16345500	-1.02926100
C	3.37765300	-2.25586000	1.47736300
Au	-0.85937200	0.58284600	-0.00319900
H	3.40382500	2.71026400	-1.69951300
H	2.15829200	3.96037500	-1.11668300
H	3.34426200	-3.34660400	-1.98712200
H	4.41351100	-2.59314400	1.35667300
H	3.29431300	-1.66947900	2.39286400
H	2.75517600	-3.15362600	1.56814000
P	-2.47721900	-1.14785100	-0.04829000
C	-1.93700000	-2.68339500	0.79885900
H	-2.72015500	-3.44756400	0.74243200
H	-1.02641700	-3.06426300	0.32555600
H	-1.72046100	-2.46655300	1.84975500
C	-2.92798200	-1.67063200	-1.74860800
H	-2.03720400	-2.03838200	-2.26773900
H	-3.68320200	-2.46380800	-1.71727800
H	-3.32650600	-0.81504100	-2.30301300
C	-4.06407500	-0.69420000	0.75364000
H	-4.77392000	-1.52699300	0.69943800
H	-3.88451700	-0.44219200	1.80371500
H	-4.49493100	0.17889700	0.25314400
C	0.10193900	3.42833300	0.56753700
H	0.82800800	4.23909500	0.45489000
H	-0.88729800	3.72590400	0.19959300
H	-0.04452500	3.25712100	1.64941900

TS9

C	-2.49583100	0.04469700	-0.32351700
O	-1.99725200	0.53253200	-1.33692300
C	-2.06466400	2.91299200	1.49254900
C	-0.57815100	1.87820600	-0.21558200
C	-1.68887900	1.88624600	0.72005900
O	-2.33463600	0.64997800	0.87250200
C	-3.28223700	-1.20756600	-0.31554900
N	-3.65352800	-1.59945000	0.85709500
O	-4.36012200	-2.77231600	0.79976600
C	-3.57262700	-1.91136600	-1.60651100
Au	0.91240800	0.46103000	-0.05356500
H	-2.80520000	2.78323400	2.27572300
H	-1.57769600	3.87696600	1.39580700
H	-4.57142800	-2.95698600	1.73566100
H	-4.65542600	-1.96601300	-1.76868400
H	-3.11321800	-1.39140800	-2.44782700
H	-3.19709000	-2.94020100	-1.56946000
P	2.67179900	-1.10175000	0.13917700
C	2.45413600	-2.57035300	-0.94038100
H	3.29327600	-3.26346500	-0.81454500
H	1.52200000	-3.08330000	-0.68323600
H	2.40222200	-2.25340800	-1.98680400
C	2.88574700	-1.77822400	1.83137700
H	1.96387200	-2.27558400	2.14933100
H	3.71033800	-2.49930800	1.85261200
H	3.10117900	-0.96240800	2.52871600
C	4.31366400	-0.41860400	-0.31244600
H	5.08689300	-1.18954700	-0.22194900
H	4.28933700	-0.05305100	-1.34393800
H	4.55959300	0.41847500	0.34871500
C	-0.35698300	3.09213600	-1.03929200
H	-1.22799700	3.74890200	-1.12552300
H	0.47640000	3.64464100	-0.57443600
H	0.01141900	2.81294700	-2.03282800

INT9

C	2.73569700	0.05734200	-0.06489100
O	1.86007900	0.20997800	-0.98255400
C	1.34147100	2.77269000	1.53565000
C	0.84230800	1.26767500	-0.53314000
C	1.53150400	1.75305600	0.70697600
O	2.62085700	0.85735200	0.95994900
C	3.77967400	-0.95051500	-0.15647900

N	4.59362600	-0.91569800	0.85209900
O	5.56442400	-1.85629400	0.74979200
C	3.84829500	-1.89176000	-1.32033400
Au	-0.98598400	0.25123900	-0.14497100
H	1.98691900	2.93145000	2.39242000
H	0.51807600	3.45741200	1.36668600
H	6.10217900	-1.73113100	1.55812100
H	3.81297300	-2.92648300	-0.96207100
H	3.02494100	-1.72880300	-2.01685500
H	4.79594800	-1.75980300	-1.85442700
P	-3.03555900	-0.83409200	0.24938700
C	-4.50491500	0.21923400	-0.06832900
H	-4.49657900	0.56019600	-1.10850000
H	-5.42674800	-0.34244500	0.11946700
H	-4.47905000	1.09662300	0.58571900
C	-3.25382600	-1.43425600	1.97052200
H	-4.22292500	-1.93275800	2.08425300
H	-2.45484100	-2.14048000	2.21796500
H	-3.19965900	-0.58996800	2.66527000
C	-3.28888100	-2.31755300	-0.80290100
H	-4.25639000	-2.78335600	-0.58522700
H	-3.25899000	-2.02820700	-1.85828100
H	-2.48972300	-3.04232900	-0.61792300
C	0.76335600	2.29830000	-1.64933700
H	1.73982900	2.75844300	-1.85369700
H	0.37316200	1.85350300	-2.56917100
H	0.07062400	3.08798300	-1.34044500

TS10

C	3.02679200	-0.28883800	-0.14417500
O	1.89642900	0.19980500	0.36551500
C	0.86264900	-2.87297800	-1.11641700
C	0.94886200	-0.88381600	0.65000400
C	1.16406200	-1.89316100	-0.30690500
O	3.07679900	-1.47615200	-0.50818700
C	4.17495800	0.63006800	-0.26910800
N	3.97020500	1.80037800	0.23704800
O	5.05842900	2.61553500	0.08427000
C	5.43532500	0.17421500	-0.93978600
Au	-1.05015200	-0.18824800	0.16568100
H	1.63292100	-3.51545800	-1.53309600
H	-0.17367100	-3.06505100	-1.38214100
H	4.78658800	3.44604400	0.52147600
H	6.29518800	0.35322600	-0.28545900
H	5.38655600	-0.88633500	-1.18873900
H	5.60113200	0.74804400	-1.85941700
P	-3.16890600	0.68905600	-0.28276500
C	-4.23031200	0.85870800	1.20352000
H	-3.74410000	1.51831600	1.92913300
H	-5.20397900	1.27920900	0.92858500
H	-4.37858200	-0.12228100	1.66598800
C	-4.14907100	-0.31506700	-1.46467700
H	-5.12581100	0.14974400	-1.63912200
H	-3.61116900	-0.39276400	-2.41486500
H	-4.29542600	-1.32175700	-1.06057300
C	-3.10480700	2.36827000	-1.01742600
H	-4.11841700	2.73414600	-1.21552900
H	-2.60242900	3.05341700	-0.32733700
H	-2.54143800	2.34138100	-1.95536700
C	1.07719800	-1.27489300	2.12274200
H	2.10024000	-1.59402500	2.36182300
H	0.81856200	-0.42505900	2.76058000
H	0.39083600	-2.09621000	2.34801600

INT10

C	3.50625600	-1.44234600	0.45183100
C	4.01937100	-0.10696100	-0.05739500
N	3.23524400	0.93449700	-0.07673200
C	1.00814400	0.03194900	-0.36730800
C	1.67055800	-1.13864400	-1.05174300
O	2.38948000	-1.94436600	-0.05958800
O	4.16225700	-2.01940100	1.28878700
C	1.79984000	1.01462700	0.12463900
Au	-1.05494000	0.01325000	-0.13641800
P	-3.39539900	-0.08657800	0.12419300
C	-3.93255200	-0.30740800	1.86706800
C	-4.19309100	-1.46753200	-0.78759100
O	3.89159600	2.14340700	-0.23894400
C	5.47781600	0.00800500	-0.33492100
H	0.95578800	-1.83801900	-1.47745800
H	2.37535500	-0.83965100	-1.84125000
H	-3.56804300	0.52871400	2.47258600
H	-5.02562100	-0.34817800	1.93053000
H	-3.51352400	-1.23583100	2.26810700
H	-3.99389000	-1.36593000	-1.85930600
H	-3.77977000	-2.42198600	-0.44615900
H	-5.27591300	-1.46388400	-0.62034700
H	3.32048700	2.67867100	-0.83384300
H	5.66219900	0.69548100	-1.16385900
H	5.99040800	0.40729100	0.55082500
H	5.89281200	-0.97696300	-0.55322200
C	-4.28387400	1.41753100	-0.44481600
H	-5.36284500	1.30986500	-0.28769300
H	-3.92520700	2.29042400	0.11022700
H	-4.09005100	1.57974100	-1.51010100
C	1.37282800	2.25324500	0.86789700
H	1.97574100	2.40666500	1.77008500
H	1.44098400	3.16227500	0.25710300
H	0.32716000	2.12987900	1.15699500

TS11

C	-3.63490300	-1.44110700	-0.40006700
C	-4.30566600	-0.17083400	0.06697400
N	-3.59484800	0.89578500	0.16786000
C	-0.95206500	0.08831500	0.34410200
C	-1.66567900	-1.05046900	1.01950800
O	-2.42291600	-1.81314300	0.04979600
O	-4.21899000	-2.15368000	-1.18667000
C	-1.46818500	1.12090200	-0.19728600
Au	1.16047600	0.05959100	0.09207700
P	3.47988600	-0.13477200	-0.08273100
C	4.04352900	-0.99663700	-1.60027900
C	4.22305000	-1.07916400	1.30304700
O	-4.34014000	2.02315000	0.43938900
C	-5.79422200	-0.19585600	0.24320100
H	-0.97609000	-1.77524900	1.44605200
H	-2.32323300	-0.67676700	1.81047600
H	3.69185800	-0.45711900	-2.48518900
H	5.13778400	-1.04934500	-1.62043200
H	3.63309200	-2.01111000	-1.62233400
H	3.99664700	-0.58410400	2.25255700
H	3.80533200	-2.09061400	1.32648700
H	5.30974000	-1.14132300	1.17835300
H	-3.68031700	2.72310300	0.61168400
H	-6.07357700	0.35884800	1.14400100
H	-6.28164500	0.29421700	-0.60890700
H	-6.15688100	-1.22205500	0.30888000
C	4.36104800	1.47449700	-0.09393000
H	5.44352400	1.31233500	-0.14417000
H	4.04396800	2.06196000	-0.96142300
H	4.12177200	2.03434000	0.81569200
C	-1.49441400	2.37117100	-0.95285300
H	-2.16209900	2.30165700	-1.81761000
H	-1.78143200	3.23047300	-0.33519100
H	-0.47902400	2.55860100	-1.32169600

r0-N

O	1.12418800	-3.05636900	-0.75595400
N	1.27452800	-1.77181100	-0.25746300
C	2.51146200	-1.44181500	-0.09992200
C	3.64300100	-2.35749000	-0.43714800
C	2.83332500	-0.04686700	0.37254900
O	3.88921300	0.48164700	0.10149600
O	1.85851000	0.50297800	1.10857500
C	2.05956800	1.89670800	1.51968600

C	1.74937400	2.82710200	0.44227700
C	1.49919800	3.61880600	-0.43988800
H	0.15678700	-3.18303600	-0.82096700
H	3.61931400	-2.60886900	-1.50436300
H	4.59529900	-1.88327000	-0.20147000
H	3.54652700	-3.29590100	0.11991100
H	1.38117200	2.01444300	2.36723200
H	3.08992900	2.00769000	1.86742100
Au	-0.58884000	-0.68750000	-0.02132800
P	-2.65855300	0.29576100	0.08369000
C	-3.17019200	0.73604600	1.78500500
H	-2.44422200	1.42805700	2.22266000
H	-4.15690600	1.21168300	1.76425700
H	-3.21560100	-0.16584700	2.40304000
C	-2.75375700	1.84825600	-0.88047400
H	-3.76123500	2.27190400	-0.80453200
H	-2.02676500	2.56908500	-0.49455800
H	-2.52557200	1.64418000	-1.93110200
C	-3.99032700	-0.77511700	-0.57504200
H	-4.03597500	-1.70596900	-0.00130000
H	-4.95372800	-0.25842000	-0.50336200
H	-3.78558400	-1.01527800	-1.62293500
C	1.21712800	4.57838700	-1.50335900
H	0.28361300	4.33276000	-2.02333600
H	1.11561200	5.59095600	-1.09452700
H	2.02433900	4.59449200	-2.24533800

r0

O	3.50804900	-1.23773100	-0.61224900
N	2.24367800	-1.04119700	-0.07696900
C	1.89269900	0.19565900	-0.14009100
C	2.72835800	1.30088400	-0.71341300
C	0.53919900	0.53180300	0.41155600
O	0.09006000	1.66276100	0.39987500
O	-0.10833500	-0.53232300	0.92065900
C	-1.42456200	-0.27144500	1.48176100
C	-2.46883800	-0.23832500	0.46161500
C	-3.35384100	-0.22011400	-0.36438000
H	3.64534700	-2.19722000	-0.50455400
H	2.98150200	1.08449300	-1.75776800
H	2.19507700	2.25033100	-0.66028100
H	3.67407900	1.38598100	-0.16493800
H	-1.58250800	-1.09798100	2.17932300
H	-1.39271800	0.66537000	2.04512400
C	-4.41758700	-0.19416600	-1.36406600
H	-5.36671100	-0.53926500	-0.93616200
H	-4.57320600	0.81830400	-1.75564400
H	-4.17736200	-0.84906800	-2.21048700

INT4-0

C	1.34491600	-0.23567800	-0.16679100
N	0.25618200	-0.96737000	-0.07309500
C	-0.92381000	-0.11292000	0.36793800
O	-0.33582100	1.17375900	0.53264000
C	1.00376000	1.13340700	0.20772000
O	1.70694500	2.11552400	0.25920000
O	0.10246800	-2.19480100	-0.29462700
C	2.66654900	-0.76637200	-0.58117200
C	-1.95630900	-0.12482500	-0.73035200
C	-2.41511700	0.96496700	-1.34200400
H	-2.31872900	-1.11860300	-0.98218400
H	2.99111900	-1.57111500	0.08980800
H	2.61930000	-1.18253300	-1.59515400
H	3.40907000	0.03473800	-0.56101400
H	-3.17477900	0.88780900	-2.11530400
H	-2.06077300	1.96082000	-1.09237900
C	-1.44218600	-0.64045300	1.69940200
H	-2.27693800	-0.01900400	2.03439700
H	-1.79009800	-1.66932700	1.57612700
H	-0.64700500	-0.61579500	2.45120700

INT6-0

C	-1.52630600	-0.94873400	-0.12877600
C	-1.26439000	0.48773500	0.06610600
N	-0.01836800	0.95841100	0.08664300
C	1.09595800	0.02490200	0.10824700
C	0.70537500	-1.32305400	0.61844100
O	-0.49169000	-1.81690800	-0.02280200
O	-2.62955200	-1.37259300	-0.42193400
C	2.30971200	0.47346300	-0.23161900
O	0.22479500	2.20504000	0.06443100
C	-2.38152700	1.47349800	0.06680100
H	1.47516500	-2.06720900	0.42136100
H	0.51943400	-1.28839600	1.70005800
H	-2.26380400	2.18448200	0.89249300
H	-2.38417500	2.06306100	-0.86009800
H	-3.33651200	0.95451700	0.15620600
H	2.37371600	1.52520300	-0.49883900
C	3.58098700	-0.30907200	-0.25955600
H	3.44654500	-1.37477200	-0.05804300
H	4.06672400	-0.19647800	-1.23741400
H	4.28421000	0.09398200	0.48235000

For 1v system:

r1

O	5.72694700	0.89075400	-1.06205200
N	4.70532100	0.14132100	-0.51391500
C	3.81549900	0.88802800	0.04326900
C	3.85833600	2.38516200	0.11082300
C	2.65540200	0.17269300	0.65536800
O	1.72643000	0.74809100	1.19061900
O	2.74561500	-1.17542500	0.55401700
C	1.68257900	-1.94133100	1.14382600
C	0.62319700	-2.23955300	0.16896600
C	-0.18115500	-2.63184700	-0.67373100
H	6.32779300	0.21476900	-1.42892000
H	3.78048000	2.81484900	-0.89548400
H	3.04110900	2.76678700	0.72348200
H	4.81416000	2.71803900	0.52993900
H	2.13630300	-2.88827600	1.45040200
H	1.27929100	-1.43416900	2.02255500
H	-0.70521600	-3.19674500	-1.42375900
Au	-1.15124600	-0.65856000	-0.17836200
P	-2.53828300	1.19601000	0.01453800
C	-4.29097800	0.81182000	-0.35241400
H	-4.89961700	1.71649300	-0.24496300
H	-4.38169900	0.43314900	-1.37511000
H	-4.65462900	0.04710500	0.34079700
C	-2.52800100	1.90290700	1.70420300
H	-1.51213600	2.21054200	1.97026700
H	-3.19417100	2.77169100	1.74953900
H	-2.86744400	1.14881100	2.42090400
C	-2.08476600	2.57218100	-1.10552800
H	-2.13958100	2.23481900	-2.14511900
H	-2.77037000	3.41440300	-0.96021100
H	-1.06144000	2.89684000	-0.89375000

TS1

C	-3.63220900	-0.30324700	-0.29840400
O	-2.93074500	0.78070600	-0.62822300
C	-1.61324700	0.64773100	-1.21082000
C	-0.75831300	-0.34076200	-0.47183100
C	-1.10692100	-1.44220700	0.02803900
O	-3.20577700	-1.45888300	-0.38474000
C	-5.00216400	-0.01803300	0.21371900
N	-5.35685700	1.22104300	0.17524300
O	-6.63059500	1.39803600	0.66465100
C	-5.85187800	-1.14971000	0.70843800
Au	1.32591700	-0.13849800	-0.07542900
H	-1.71984500	0.32036700	-2.25056000
H	-1.20643700	1.65601000	-1.18861100
H	-1.11813400	-2.38344500	0.54457600
H	-6.77648900	2.35932800	0.57534900
H	-6.78228800	-1.20431500	0.13157100
H	-5.32306600	-2.09935200	0.62475300
H	-6.13129400	-0.98334500	1.75519500

P	3.60234900	0.26016700	0.25420700
C	4.64145600	-1.24059300	0.08666100
H	4.52335800	-1.66154300	-0.91673400
H	5.69540100	-0.99121400	0.25249800
H	4.32809500	-1.99019500	0.81991100
C	3.99775900	0.93975200	1.91036800
H	5.07548100	1.11673800	1.99824900
H	3.46327600	1.88319100	2.05913700
H	3.68322500	0.23266700	2.68421700
C	4.29768600	1.46506800	-0.93891300
H	5.36252000	1.62410600	-0.73573400
H	4.17757000	1.08690700	-1.95893300
H	3.76788000	2.41878200	-0.85282700

INT1

C	-3.56330200	0.11456700	-0.01498900
O	-2.95380800	1.24349900	0.01005300
C	-1.44212600	1.33892800	-0.01388300
C	-0.76443500	0.01384600	-0.01823200
C	-1.51419600	-1.08091000	-0.03517000
O	-2.96203600	-1.02526200	-0.04829700
C	-5.03055300	0.14771400	-0.00092400
N	-5.56209600	-1.03301400	0.02273400
O	-6.91899000	-0.97533100	0.04761700
C	-5.78035000	1.44539400	-0.00235600
Au	1.31287600	-0.01858700	-0.00415900
H	-1.24002600	1.92880100	-0.91048600
H	-1.21649700	1.93608100	0.87164900
H	-1.23144200	-2.12310400	-0.04281900
H	-7.19477300	-1.91418100	0.05695400
H	-6.31107300	1.57322900	0.94848100
H	-5.11355100	2.29477900	-0.14999800
H	-6.53277900	1.43650900	-0.79793000
P	3.66423300	-0.04629400	0.01059800
C	4.40572100	-1.00484600	-1.36983100
H	4.09236900	-0.57602000	-2.32696900
H	5.49947400	-0.98708500	-1.30752600
H	4.05972300	-2.04245100	-1.32355800
C	4.38789900	-0.78360000	1.52868000
H	5.48242200	-0.76846000	1.48032100
H	4.05911800	-0.21712600	2.40595400
H	4.04582900	-1.81792200	1.63526100
C	4.43216900	1.61747400	-0.10795800
H	5.52491000	1.53745500	-0.10317400
H	4.11076200	2.10693600	-1.03289600
H	4.11318200	2.23181100	0.74017000

TS2

C	3.66715000	-0.27004400	-0.01921400
O	3.15754100	-1.39080000	-0.02921100
C	0.99096600	-1.43078000	-0.05888800
C	0.77551900	-0.06414500	-0.06319100
C	1.59698300	0.97739500	-0.06675000
O	2.99337600	0.89074800	-0.04808400
C	5.14554000	-0.09829300	0.03162600
N	5.55956100	1.12286500	0.00508000
O	6.93177900	1.19320900	0.06019000
C	6.02313500	-1.31012100	0.11421900
Au	-1.34355300	-0.04211300	-0.03615800
H	0.95387800	-2.00379700	-0.98380000
H	0.92677500	-2.00364700	0.86457300
H	1.30914900	2.01989300	-0.07557800
H	7.11126000	2.15256200	0.02640000
H	6.58588300	-1.30354100	1.05529800
H	5.43308900	-2.22529600	0.05959500
H	6.75621600	-1.30205100	-0.70001900
P	-3.68578000	0.14388700	0.05273400
C	-4.35122900	1.49181200	-0.99630700
H	-4.08345100	1.31178200	-2.04223400
H	-5.44215600	1.53752700	-0.90640400
H	-3.92312600	2.44973900	-0.68476000
C	-4.31940900	0.48919100	1.73875500
H	-5.41229100	0.56595700	1.72470900
H	-4.02397600	-0.31754200	2.41689200
H	-3.89611500	1.42910500	2.10678400
C	-4.56572500	-1.37015800	-0.49340100
H	-5.64913400	-1.21700500	-0.43735500
H	-4.28865500	-1.60691800	-1.52546500
H	-4.28601400	-2.21260600	0.14701200

INT2

C	2.61299000	0.12625800	-0.39019800
O	2.00985500	0.30922100	-1.42319900
C	0.17525400	3.18981100	-0.80076000
C	0.50314700	2.18057300	-0.02713700
C	1.09600100	1.44007700	0.93259500
O	2.18733100	0.61088600	0.82433200
C	3.87103100	-0.66150200	-0.28165000
N	4.38280500	-0.74397600	0.89889600
O	5.54266800	-1.48453100	0.89689100
C	4.44086800	-1.28287700	-1.52128100
Au	-0.93710200	0.41758600	0.16546900
H	0.78895800	4.09076500	-0.80098700
H	-0.68539200	3.16958400	-1.46324200
H	0.83778000	1.56436000	1.98137700
H	5.82402400	-1.46821200	1.83175900
H	4.50566900	-2.37075900	-1.40342300
H	3.82367300	-1.05264100	-2.39019500
H	5.45889000	-0.91581800	-1.69459300
P	-2.74626500	-1.03836100	-0.07308500
C	-3.54822200	-1.45877100	1.51963800
H	-3.90361700	-0.54574400	2.00714200
H	-4.39591700	-2.13063200	1.34504700
H	-2.82495500	-1.95043600	2.17738400
C	-2.28822800	-2.63723000	-0.84017900
H	-3.17451100	-3.27394500	-0.93793800
H	-1.85567700	-2.46194400	-1.83006500
H	-1.54564200	-3.14413300	-0.21612900
C	-4.06749400	-0.33472600	-1.12916000
H	-4.89688700	-1.04571600	-1.21348000
H	-4.43334900	0.59854700	-0.69007400
H	-3.66858800	-0.12361100	-2.12606700

TS3

C	3.75509600	-0.78232600	0.34555100
N	3.19726900	0.23036800	0.90138000
C	2.03807700	1.00820400	-0.80016200
O	2.05412100	-0.24341900	-1.26656900
C	3.13522600	-1.09153800	-0.97485100
O	3.40831000	-1.99512900	-1.70827100
O	3.72416600	0.64992700	2.07513300
C	4.88554100	-1.59682700	0.87622100
C	0.79239800	1.60366900	-0.44335100
C	0.88224200	2.96396000	-0.38602500
Au	-0.92798600	0.48259500	-0.11056700
P	-2.88232600	-0.77827700	0.26059300
H	2.92631300	1.60392200	-1.01212500
H	3.11475200	1.35323700	2.38459900
H	5.82779600	-1.04835100	0.75003700
H	4.74622100	-1.78421600	1.94503800
H	4.95767800	-2.54370800	0.33858000
H	0.02085800	3.58639500	-0.15642900
H	1.81482100	3.50038100	-0.57689600
C	-2.97588900	-1.55644700	1.92211500
H	-2.95517100	-0.78089500	2.69460100
H	-3.89912100	-2.13805900	2.02174800
H	-2.11596600	-2.21780300	2.06904900
C	-4.44071400	0.18335600	0.11643200
H	-4.51453600	0.62035700	-0.88453400
H	-5.30769800	-0.46340600	0.29151300
H	-4.44257400	0.99402900	0.85215800
C	-3.09131500	-2.17532500	-0.91255000
H	-4.01880400	-2.71956100	-0.70214400
H	-3.12255900	-1.79455100	-1.93840000
H	-2.24386200	-2.86254600	-0.82319000

INT3

C	-3.03972200	1.06573200	0.45481800
N	-2.87938900	-0.20477500	0.55265800
C	-2.35544700	-0.86589100	-0.69147100
O	-2.21408100	0.26022700	-1.55504300
C	-2.60506800	1.41122500	-0.94640600
O	-2.57705300	2.49834200	-1.45082500
O	-3.14379000	-0.93678600	1.64765900
C	-3.53670500	2.00534000	1.47365100
C	-1.08097500	-1.59653800	-0.36476700
C	-1.22907400	-2.93015400	-0.22566700
Au	0.67843700	-0.52733800	-0.08494100
P	2.70989000	0.64158500	0.18884200
H	-3.16293700	-1.50136900	-1.07232000
H	-2.57063400	-1.74410100	1.56061400
H	-4.59378700	2.22397200	1.26774900
H	-3.45069300	1.58683100	2.47860100
H	-2.98572600	2.94747700	1.39812200
H	-0.39943900	-3.56624400	0.07331800
H	-2.17189700	-3.44649600	-0.42669200
C	2.98671000	1.31157100	1.87738700
H	2.98826600	0.49165300	2.60303100
H	3.94433600	1.84138000	1.93093300
H	2.17902300	2.00370300	2.13664500
C	4.19759200	-0.38091500	-0.14814700
H	4.15887200	-0.75971300	-1.17457900
H	5.11019700	0.21107000	-0.01709700
H	4.22203800	-1.23459700	0.53672300
C	2.88978300	2.09307500	-0.92296100
H	3.85623800	2.58450600	-0.76491700
H	2.81844500	1.76654800	-1.96547300
H	2.08541400	2.80981100	-0.72849000

TS4

C	-3.02851800	1.05577600	0.48408800
N	-2.58839600	-0.10720000	0.83100300
C	-2.44567100	-1.04921200	-0.31778400
O	-2.63320300	-0.19424300	-1.43901800
C	-3.10340900	1.02359000	-1.01294900
O	-3.43646500	1.90800700	-1.75277600
O	-2.06203300	-0.55948400	1.94417300
C	-3.28703300	2.22764700	1.34368300
C	-1.11251600	-1.70540700	-0.05201400
C	-0.94382300	-3.00083400	-0.39646900
Au	0.68754400	-0.51117600	0.03842200
P	2.64264700	0.75476100	-0.06411300
H	-3.27937600	-1.75857100	-0.28108600
H	-1.17176800	-1.24905900	1.31024600
H	-4.32303100	2.55963700	1.20516800
H	-3.11525600	1.98935700	2.39483800
H	-2.63732300	3.05735900	1.04034800
H	-0.03555400	-3.54043100	-0.14009600
H	-1.69584600	-3.56243200	-0.95377600
C	3.57955600	0.80150100	1.51245600
H	3.85079600	-0.21635100	1.80965900
H	4.49089700	1.39764900	1.39229700
H	2.95911300	1.24284500	2.29865000
C	3.83778400	0.13930500	-1.31066000
H	3.38277700	0.16641200	-2.30566100
H	4.74067400	0.76003500	-1.30951000
H	4.11126100	-0.89489000	-1.07869700
C	2.35027700	2.51132600	-0.50287700
H	3.30201700	3.05002400	-0.56919400
H	1.83547000	2.57095500	-1.46696800
H	1.72193600	2.98295200	0.25920800

INT4

C	2.60915500	1.31909200	-0.20886600
N	2.53309800	0.26973500	-0.99908200
C	2.55184500	-0.99308100	-0.18156100
O	2.61327000	-0.54536500	1.15449600
C	2.64557000	0.84395600	1.17297800
O	2.68669300	1.46607200	2.20424400
O	2.45608900	0.21090400	-2.25183700
C	2.63448200	2.72112800	-0.68946400
C	1.36060900	-1.86299300	-0.48361300
C	0.66548200	-2.55349300	0.47112200
Au	-0.65402700	-0.71260500	0.00129400
P	-2.40461300	0.83940700	0.00305200
H	3.47226700	-1.52793000	-0.44447700
H	1.23774700	-2.09615900	-1.53917600
H	3.38065100	2.83983000	-1.48306200
H	1.66090400	3.01254100	-1.10436600
H	2.87605100	3.39092200	0.13886800
H	-0.01788600	-3.34659800	0.17741400
H	0.90480200	-2.46376000	1.52750100
C	-3.62488000	0.53466100	-1.32811500
H	-4.05298200	-0.46601200	-1.21384700
H	-4.42634900	1.28019000	-1.27872100
H	-3.13174000	0.59906800	-2.30281600
C	-3.35358800	0.81540800	1.56946000
H	-2.68845600	1.04270100	2.40817100
H	-4.15575800	1.56076100	1.53132300
H	-3.78815200	-0.17729100	1.72257300
C	-1.84312100	2.56865700	-0.21615100
H	-2.70376100	3.24616100	-0.18487300
H	-1.14470100	2.83562000	0.58266000
H	-1.33869400	2.67356600	-1.18158200

TS5

C	4.09370900	1.39249600	-0.13607900
C	4.59864000	-0.02103900	-0.06544900
N	3.70704600	-0.92586300	0.12825700
C	1.53225500	-0.33302600	0.38053600
C	2.04180900	0.83490400	1.10008300
O	2.83496500	1.70259000	0.26739900
O	4.77925100	2.27177400	-0.60730900
C	0.74738000	-1.15877000	-0.15018700
Au	-1.22679400	-0.33981600	-0.03899700
P	-3.45230700	0.34898700	-0.04762500
C	-4.19899200	0.44468000	1.62370200
C	-4.53671500	-0.77867900	-1.00301800
O	4.17297100	-2.21149700	0.05968500
C	6.04862700	-0.28727200	-0.32120400
H	1.19418200	1.44621100	1.42287100
H	2.60593900	0.53094100	1.98645000
H	-3.65708200	1.17886300	2.22807500
H	-5.25086700	0.74272400	1.55157700
H	-4.13185800	-0.53135800	2.11439900
H	-4.20247200	-0.81474500	-2.04454900
H	-4.48564100	-1.78788100	-0.58281600
H	-5.57256700	-0.42359200	-0.96773700
H	3.39418700	-2.76048100	0.28247300
H	6.41923800	-1.05166400	0.36838900
H	6.18733900	-0.66589800	-1.34187500
H	6.62877500	0.62926000	-0.21072700
C	-3.70325100	2.00529100	-0.79306600
H	-4.76737000	2.26621700	-0.78324400
H	-3.14197800	2.75496600	-0.22663600
H	-3.34086100	2.00143600	-1.82579700
H	0.83480200	-2.11774900	-0.64360100

INT5

C	4.13876800	1.37633400	-0.15509400
C	4.32309300	-0.11353000	0.03441300
N	3.24522800	-0.84122300	0.11707300
C	1.91336500	-0.29784900	0.23547400
C	1.99224600	1.06705300	0.84031200
O	2.94548000	1.90324700	0.11700500
O	5.04149000	2.03331800	-0.58937400
C	0.81936600	-0.98110700	-0.14699800
Au	-1.12939100	-0.32940200	-0.05298900
P	-3.39093400	0.34342600	-0.00726000
C	-3.90523700	1.29348600	-1.49294500
C	-3.84214900	1.41936200	1.41052000
O	3.41070400	-2.19539500	0.01450800

C	5.68250400	-0.70062600	-0.03462300
H	1.03273600	1.57193700	0.76014500
H	2.31174900	1.03508800	1.88876300
H	0.99314000	-1.97938000	-0.55525800
H	-3.73607400	0.69260800	-2.39209600
H	-4.96622100	1.55998800	-1.43130700
H	-3.30820400	2.20809500	-1.56819800
H	-3.64927100	0.89079400	2.34972900
H	-3.23630800	2.33095600	1.39314400
H	-4.90243800	1.69175800	1.36381700
H	2.69064300	-2.59122100	0.55807400
H	5.75144100	-1.59987100	0.58182600
H	5.90904700	-0.98414100	-1.07215700
H	6.41696100	0.04291000	0.27809000
C	-4.57177600	-1.06096500	0.08647500
H	-5.60485000	-0.69675000	0.06890200
H	-4.41230300	-1.73375900	-0.76205900
H	-4.40318500	-1.62137900	1.01176400

TS6

C	-2.65764600	-3.25647400	0.51139900
C	-3.36207800	-2.21709100	-0.33487500
N	-2.73216900	-1.09352700	-0.54666300
C	-1.50954600	-0.74633300	0.12172900
C	-1.43790000	-1.42142500	1.45313500
O	-1.64579100	-2.85329800	1.29078000
O	-2.98844900	-4.41509400	0.44261300
C	-0.67257700	0.16431800	-0.41956500
Au	1.47238600	0.03535400	-0.08892900
P	3.76241800	-0.35705800	-0.07295400
C	4.63750900	0.50465800	-1.43171100
C	4.17236500	-2.13160900	-0.26862300
O	-3.24176000	-0.21394100	-1.44326500
C	-4.65747400	-2.52471200	-0.97677400
H	-0.45360000	-1.30890100	1.90110000
H	-2.20742500	-1.03691900	2.13368500
H	-0.93826800	0.52142900	-1.41381800
H	4.48677000	1.58481100	-1.34137100
H	5.70956500	0.28247400	-1.38807000
H	4.23871100	0.17432800	-2.39582400
H	3.72796900	-2.70596700	0.55018600
H	3.76920400	-2.50140100	-1.21656700
H	5.25904000	-2.27087100	-0.25947600
H	-3.17462200	0.71192400	-0.98715100
H	-5.29254400	-1.63466600	-1.00078200
H	-4.48725600	-2.83673200	-2.01747900
H	-5.14800200	-3.34424800	-0.45076900
C	4.59608300	0.17498300	1.46921900
H	5.67002500	-0.03340400	1.40548000
H	4.44345100	1.24814200	1.61980500
H	4.17341200	-0.36373000	2.32293200
O	-0.88031200	2.40199600	0.84964700
H	-0.45727800	1.19445800	0.32535200
S	-2.09155700	3.00862300	0.10520000
C	-2.74366100	4.18356700	1.28629600
H	-1.97168500	4.92794200	1.49383600
H	-3.61834600	4.66034300	0.83726400
H	-3.02324600	3.65323900	2.19858100
O	-1.70334200	3.70599400	-1.13029900
O	-3.17296900	1.97160600	-0.07387000

INT6

C	0.01151400	3.39384300	-0.24104700
C	-0.88212800	2.61214900	0.66605100
N	-1.13026800	1.33794600	0.42425800
C	-0.68897900	0.74283900	-0.82499700
C	-0.45204100	1.75438300	-1.90614800
O	0.33026400	2.86922700	-1.44223700
O	0.49223300	4.44680500	0.11315200
C	-0.82871900	-0.60052600	-1.02958400
Au	1.35628700	-0.45635900	-0.27131500
P	3.49405100	-1.06806300	0.42025000
C	3.46914800	-2.38757800	1.68788400
C	4.42827600	0.32426300	1.15602000
O	-1.71586900	0.58101600	1.29216300
C	-1.37200000	3.20512500	1.93410000
H	0.09152700	1.31716500	-2.74147900
H	-1.42158100	2.12723500	-2.26125600
H	-1.29847100	-1.23849700	-0.28787300
H	2.98156700	-3.27905900	1.28163100
H	4.49529000	-2.63582500	1.98144900
H	2.91145200	-2.04632700	2.56542800
H	4.53279000	1.12767100	0.42048800
H	3.89192500	0.70805400	2.02926200
H	5.42236800	-0.02064700	1.46175100
H	-3.32008500	0.18960600	1.11050400
H	-2.44220700	3.00379000	2.05586700
H	-0.86222000	2.73888900	2.78876000
H	-1.18354700	4.27818000	1.94634700
C	4.52801300	-1.70243400	-0.95036700
H	5.51810700	-1.97702500	-0.56977700
H	4.05270900	-2.58302300	-1.39337200
H	4.63497400	-0.93088500	-1.71898600
O	-4.26459900	-0.79297100	-1.38596600
H	-0.67531400	-0.99691100	-2.02962000
S	-4.37086700	-1.32313900	-0.02005300
C	-6.04731000	-1.83898400	0.31146800
H	-6.26362400	-2.67275500	-0.36149500
H	-6.11883300	-2.15933000	1.35265900
H	-6.72179500	-1.00402000	0.11077400
O	-3.42780000	-2.38202700	0.37125300
O	-4.28064600	-0.10790500	1.04161200

TS7

C	3.84554300	-0.09651600	0.27345000
O	3.21216800	1.04876600	0.52196400
C	1.90193100	0.79973600	1.08400800
C	0.44477100	-1.23412900	0.11552500
C	1.34489500	-0.44548000	0.52981700
O	3.24420100	-1.16925700	0.41498900
C	5.24756700	-0.00838000	-0.18391700
N	5.72575800	1.19057600	-0.19886100
O	7.02446700	1.21085700	-0.63282900
C	5.98361300	-1.25324700	-0.57601500
Au	-1.47824800	-0.35174900	0.00409500
H	2.00703500	0.74017700	2.17250400
H	1.27731800	1.65423100	0.81753500
H	7.26514700	2.15714300	-0.59431500
H	6.88974700	-1.36236500	0.03047000
H	5.35714300	-2.13636300	-0.44595500
H	6.29941200	-1.18912800	-1.62367900
P	-3.65965500	0.46090400	-0.17573200
C	-3.75467000	2.25881900	-0.52696700
H	-3.24009300	2.48029700	-1.46724200
H	-4.80074800	2.57544400	-0.60423100
H	-3.26772200	2.81730500	0.27877400
C	-4.65407100	0.21890700	1.34585800
H	-5.66571500	0.61609600	1.20738500
H	-4.71392800	-0.84836500	1.58138800
H	-4.17511300	0.73546100	2.18357300
C	-4.62045800	-0.34313600	-1.51447900
H	-5.63821300	0.06104300	-1.54814600
H	-4.12953700	-0.16710500	-2.47695000
H	-4.66594400	-1.42223400	-1.33743300
H	0.51589000	-2.27338400	-0.18584100

INT7

C	3.79240100	0.15914900	0.00003500
O	3.30201500	1.35968000	-0.00162900
C	1.82700300	1.26499300	-0.00380700
C	0.50740900	-0.99491900	-0.00154800
C	1.57956000	-0.22215200	-0.00181700
O	2.93198200	-0.79904300	-0.00001000
C	5.21816000	-0.11610200	0.00174900
N	5.92857400	0.96964200	0.00007100
O	7.25456700	0.70103900	0.00134700

C	5.74361000	-1.51918400	0.00452400
Au	-1.44455100	-0.32928500	-0.00181000
H	1.47648200	1.78177000	0.89167000
H	1.47932800	1.77883500	-0.90209600
H	7.67839200	1.58380400	-0.00029500
H	6.37002200	-1.67873600	0.88923200
H	4.93523100	-2.25127300	0.00500800
H	6.37155100	-1.68161400	-0.87857400
P	-3.70376100	0.34187200	0.00198500
C	-4.16065700	1.50023700	-1.34909600
H	-3.94789600	1.03806600	-2.31840000
H	-5.22595300	1.75143500	-1.29691200
H	-3.57070200	2.41852500	-1.26477200
C	-4.23552100	1.19657400	1.53935800
H	-5.29746700	1.46109500	1.48647500
H	-4.06952300	0.54239100	2.40119500
H	-3.64424000	2.10790100	1.67576800
C	-4.87982600	-1.05797200	-0.17772700
H	-5.91406200	-0.69653700	-0.16514700
H	-4.69252900	-1.57914700	-1.12219700
H	-4.73676700	-1.76676500	0.64418200
H	0.70276100	-2.06895600	-0.00013100

TS8

C	-3.75229600	0.57550100	-0.10275700
O	-3.31380000	1.71538100	0.09789900
C	-1.49435000	1.42004000	-0.98836900
C	-0.61064300	-0.76638300	-0.25110300
C	-1.61578900	0.06769500	-0.63868300
O	-2.96498100	-0.37069600	-0.65526600
C	-5.13033800	0.17409400	0.23766200
N	-5.38932700	-1.07197900	0.01642600
O	-6.68090100	-1.38409900	0.33918200
C	-6.08799800	1.18641200	0.78868300
Au	1.36916600	-0.30118500	-0.05782400
H	-2.08320100	1.86221900	-1.78447200
H	-0.63586600	1.98522400	-0.63502800
H	-6.74717000	-2.33668100	0.13041000
H	-6.45155000	0.86520000	1.77120400
H	-5.61305600	2.16320500	0.88595900
H	-6.96112500	1.27611600	0.13234100
P	3.66876400	0.17456600	0.21489100
C	4.03392900	1.25153200	1.65643500
H	3.68672800	0.76858000	2.57535700
H	5.11099400	1.43801500	1.73201800
H	3.51085800	2.20660800	1.54487500
C	4.42359700	1.03911800	-1.21816600
H	5.48767300	1.22584300	-1.03575800
H	4.31519200	0.42623700	-2.11866100
H	3.91439000	1.99408800	-1.38290300
C	4.70959900	-1.31617200	0.46766500
H	5.76185700	-1.03410600	0.58366900
H	4.37790700	-1.84690700	1.36583000
H	4.60887500	-1.98764000	-0.39081200
H	-0.92959700	-1.80275200	-0.10702300

INT8

C	-2.54198400	0.05696700	-0.57972700
O	-2.23246800	0.39526400	-1.70263800
C	-2.56989200	3.24458600	0.52294000
C	-0.45203600	2.19645500	0.00491800
C	-1.83499600	2.12434500	0.27725400
O	-2.44311800	0.89012200	0.50012800
C	-3.07999200	-1.28889000	-0.23391200
N	-3.17804600	-1.54510000	1.02557500
O	-3.66151800	-2.81693500	1.24706600
C	-3.43998500	-2.23206300	-1.34179200
Au	0.90627900	0.71098100	0.00798400
H	-3.59977900	3.18457000	0.86532800
H	-2.11956900	4.22571400	0.41487400
H	-3.69189000	-2.88204300	2.22043600
H	-4.49363000	-2.52277500	-1.25932500
H	-3.26910000	-1.76959600	-2.31438600
H	-2.84632400	-3.15073600	-1.27033700
P	2.53915300	-1.01699600	0.02719000
H	-0.12942000	3.22390500	-0.18213600
C	1.99923600	-2.54769500	-0.82849200
H	2.78449400	-3.31020700	-0.78026900
H	1.09132700	-2.93404500	-0.35449600
H	1.77825800	-2.32401700	-1.87703200
C	2.99676300	-1.54910000	1.72287300
H	2.10860600	-1.92254100	2.24236300
H	3.75355700	-2.34038400	1.68346900
H	3.39538500	-0.69625600	2.28132500
C	4.11984400	-0.55041000	-0.77894200
H	4.83324700	-1.38069800	-0.73437900
H	3.93368900	-0.29143500	-1.82614400
H	4.54919400	0.32087100	-0.27408800

TS9

C	-2.56337700	0.13968100	-0.40109300
O	-1.99114000	0.43129000	-1.44990700
C	-2.09839200	3.26481000	0.89915500
C	-0.55834200	1.88843800	-0.43692300
C	-1.72257100	2.08717500	0.37110100
O	-2.43357600	0.92608500	0.69430700
C	-3.41384000	-1.05817500	-0.23717100
N	-3.91064000	-1.20704700	0.94532800
O	-4.67111100	-2.34267100	1.03477900
C	-3.62401800	-1.98330300	-1.39712400
Au	0.92551700	0.52371700	-0.15835000
H	-2.86682300	3.31964000	1.66470400
H	-1.57493700	4.17345400	0.62095400
H	-4.98158000	-2.33907500	1.96129400
H	-4.69130100	-2.04871700	-1.63781500
H	-3.08114400	-1.63700400	-2.27724400
H	-3.28643900	-2.99363400	-1.13934200
P	2.74770500	-0.93540500	0.22374400
H	-0.35968100	2.73332400	-1.10333300
C	2.62729100	-2.52465000	-0.68580400
H	3.49852800	-3.15181200	-0.46663300
H	1.71739000	-3.05491000	-0.38761600
H	2.58382600	-2.33134300	-1.76227900
C	2.95501400	-1.40992100	1.98386500
H	2.05056500	-1.91403700	2.33897300
H	3.81163700	-2.08336100	2.09768800
H	3.11788000	-0.51414900	2.59127700
C	4.36458600	-0.22650900	-0.27391600
H	5.17117600	-0.94124300	-0.07684100
H	4.34865700	0.01330100	-1.34178300
H	4.55381800	0.69340800	0.28824300

INT9

C	2.85075000	0.12914600	-0.18909300
O	1.89554700	-0.08354000	-1.01485300
C	1.32405000	3.12286000	0.59649000
C	0.87129100	1.01766100	-0.87661500
C	1.56878600	1.92208800	0.08922900
O	2.75730300	1.22917800	0.50324500
C	3.95431700	-0.80362800	-0.03803300
N	4.81681700	-0.41357200	0.84850700
O	5.83817600	-1.29458800	0.97554700
C	4.02455600	-2.06232400	-0.84736600
Au	-0.99414600	0.22614600	-0.27649200
H	2.00811900	3.58920800	1.29631700
H	0.42410200	3.65463900	0.30815100
H	6.41356100	-0.89806800	1.66130600
H	3.95087400	-2.93449700	-0.18758800
H	3.22427400	-2.10988900	-1.58680900
H	4.98961900	-2.11809500	-1.36185800
P	-3.08469900	-0.63106700	0.37237100
C	-4.51116300	0.15303000	-0.47605300
H	-4.42661100	0.00200800	-1.55695000
H	-5.45212400	-0.28406400	-0.12416500
H	-4.51533700	1.22880200	-0.27341600
C	-3.44219500	-0.43779800	2.16266300

H	-4.42191700	-0.86343400	2.40610200
H	-2.67158600	-0.94783700	2.74944900
H	-3.43516500	0.62451100	2.42693100
C	-3.27492000	-2.42758300	0.04552700
H	-4.26328500	-2.77436900	0.36726900
H	-3.15606500	-2.62064400	-1.02550000
H	-2.50329700	-2.98453900	0.58664800
H	0.80408300	1.44264000	-1.88014800

TS10

C	3.11734900	0.35984100	-0.05694600
O	1.94563300	-0.20364500	-0.36284600
C	1.01319200	3.10720900	0.61251800
C	0.97651300	0.81485900	-0.73151400
C	1.24559800	1.99289100	-0.02293800
O	3.19643300	1.59175300	0.06696200
C	4.27217600	-0.53896400	0.13620800
N	4.01555600	-1.78430400	-0.08939100
O	5.11775100	-2.57160500	0.10420200
C	5.59695000	0.01977900	0.55902700
Au	-1.02343100	0.19658900	-0.22182300
H	1.80550400	3.82093600	0.81750900
H	0.00329200	3.34009400	0.94227200
H	4.79057500	-3.47435000	-0.07726100
H	6.34935300	-0.16195800	-0.21724400
H	5.53015400	1.09247000	0.74341400
H	5.94114200	-0.48230700	1.47006000
P	-3.16441600	-0.61193900	0.25160700
C	-4.22833500	-0.78550800	-1.23240700
H	-3.75894500	-1.47274200	-1.94325200
H	-5.21259900	-1.17501400	-0.94940300
H	-4.35155000	0.18885100	-1.71565100
C	-4.11665700	0.44624200	1.40868400
H	-5.10495400	0.01109300	1.59412000
H	-3.57629800	0.53250700	2.35671900
H	-4.23717500	1.44629600	0.98047000
C	-3.14828900	-2.27490900	1.02454800
H	-4.17215800	-2.60599700	1.23068800
H	-2.66648400	-2.99055800	0.35100300
H	-2.58442400	-2.24253300	1.96198600
H	1.00349500	0.93120300	-1.81942200

INT10

C	-3.68683800	-1.29896600	-0.31235100
C	-4.09761600	0.12929200	-0.00355600
N	-3.23426600	1.09680800	-0.13841300
C	-1.04582400	0.10467900	0.29931100
C	-1.76109700	-0.96185200	1.09402100
O	-2.56771700	-1.79606600	0.20318600
O	-4.41794800	-1.95071500	-1.02289100
C	-1.81053500	1.04297400	-0.29644400
Au	1.01134400	0.06711500	0.08943600
P	3.35546400	-0.03614900	-0.13623500
C	3.92344400	-0.84026600	-1.68628100
C	4.18536500	-0.97831900	1.20425500
O	-3.77481400	2.36739700	-0.17983900
C	-5.54129500	0.40649000	0.23098400
H	-1.08242400	-1.67095700	1.56080600
H	-2.40998700	-0.53562900	1.87327900
H	3.53664800	-0.29121100	-2.55065800
H	5.01812900	-0.85642100	-1.73016600
H	3.54609300	-1.86699700	-1.72871200
H	3.96536700	-0.51653700	2.17212300
H	3.81210600	-2.00738900	1.21562700
H	5.26993800	-0.99057900	1.04946700
H	-3.09376400	2.95759000	0.21515100
H	-5.66491000	1.23168100	0.93678700
H	-6.02282400	0.69803500	-0.71237400
H	-6.03594100	-0.49205100	0.60240700
C	4.18104000	1.60445200	-0.13685200
H	5.26554000	1.48899400	-0.24137000
H	3.80122200	2.20577000	-0.96903100
H	3.96369700	2.12852400	0.79945200
H	-1.45316900	1.86387000	-0.90796300

TS11

C	-3.90114500	-1.25202000	-0.30195800
C	-4.37634800	0.14555600	0.02173700
N	-3.57908700	1.12121200	-0.23393900
C	-1.01957200	0.03039200	0.26115100
C	-1.81171000	-1.01265800	0.98257500
O	-2.68399800	-1.70791700	0.06681500
O	-4.63668900	-1.99129300	-0.91618700
C	-1.33162300	1.03540400	-0.42465700
Au	1.11361800	0.09798500	0.04547900
P	3.44054800	-0.05931400	-0.07153000
C	4.31551500	1.38888400	0.63485400
C	4.07677800	-0.22482100	-1.78269100
O	-4.16510700	2.35950800	-0.06004400
C	-5.80908500	0.31695900	0.43476900
H	-1.18370900	-1.79337700	1.40729200
H	-2.38571700	-0.54027100	1.78692400
H	-1.27068200	1.89736000	-1.06219300
H	4.03793100	1.51083200	1.68649900
H	5.39954500	1.24789500	0.56117100
H	4.03062800	2.29409800	0.08944500
H	3.65275900	-1.11897400	-2.25003400
H	3.78550600	0.65094600	-2.37111900
H	5.16939300	-0.30585200	-1.77226300
H	-3.46244100	2.99382800	-0.30225700
H	-5.87522400	1.01089900	1.27878400
H	-6.39072600	0.74785800	-0.38941100
H	-6.25044700	-0.64142400	0.71046100
C	4.09494400	-1.51273200	0.83451300
H	5.18697200	-1.54763600	0.75381300
H	3.81333700	-1.44751400	1.89018500
H	3.67225700	-2.43043100	0.41400000

r0-N

O	1.54768500	-2.83309100	-0.20275200
N	1.51859500	-1.45808800	-0.03682800
C	2.69759800	-0.93563300	-0.02343300
C	3.94387900	-1.74279500	-0.19374200
C	2.82481000	0.56017400	0.10582500
O	3.74594400	1.16226800	-0.39906400
O	1.84976800	1.11205200	0.84470000
C	1.88567300	2.56533800	0.98528100
C	1.29162100	3.23353400	-0.16717800
C	0.79580900	3.80929600	-1.10690100
H	0.60655800	-3.09882500	-0.21534700
H	3.91256600	-2.29254000	-1.14159800
H	4.81958700	-1.09447700	-0.18081100
H	4.02129600	-2.48432500	0.60978300
H	1.31419200	2.75818000	1.89537000
H	2.92142200	2.87955200	1.13679600
H	0.37456300	4.32594200	-1.94402500
Au	-0.46917100	-0.59269900	0.00195500
P	-2.62281400	0.19647300	0.00643000
C	-3.11895200	0.87067400	1.63519000
H	-2.44459200	1.68517000	1.91683500
H	-4.14489100	1.25147100	1.58400700
H	-3.06209300	0.08549300	2.39539400
C	-2.87522500	1.55732800	-1.19112700
H	-3.90755000	1.91962500	-1.13390200
H	-2.18838100	2.37886900	-0.96546900
H	-2.67334200	1.19841500	-2.20505100
C	-3.87090000	-1.07674700	-0.41096400
H	-3.81664100	-1.89700600	0.31158000
H	-4.87440100	-0.63792500	-0.38491800
H	-3.67479800	-1.47170500	-1.41246600

r0

O	-3.13603900	-1.13878800	0.35155100
N	-1.79196700	-1.01690900	0.03568000
C	-1.42129800	0.21595100	0.02476000
C	-2.31073700	1.38759800	0.31388200

C	0.01656700	0.47318000	-0.30925700
O	0.49494900	1.59099800	-0.34114200
O	0.71217100	-0.65048900	-0.57514000
C	2.10906500	-0.46557400	-0.91542400
C	2.94874700	-0.29836600	0.26916200
C	3.66134800	-0.17627800	1.23695900
H	-3.28099200	-2.10307900	0.33208400
H	-2.77913900	1.27655200	1.29843900
H	-1.74092300	2.31678100	0.28616500
H	-3.12155000	1.44043700	-0.42261400
H	2.37943900	-1.37602900	-1.45628000
H	2.21070000	0.39067600	-1.58788700
H	4.28543100	-0.05981500	2.09769500

INT4-0

C	1.20953700	-0.22571700	-0.09754800
N	0.19962600	-0.99980000	0.23659900
C	-0.96548900	-0.16088800	0.70570300
O	-0.48055000	1.16595400	0.62193500
C	0.81225800	1.16102300	0.13072300
O	1.43424900	2.18165400	-0.04299300
O	0.10886500	-2.25198000	0.20596600
C	2.50494700	-0.73341100	-0.61106300
C	-2.17568200	-0.41813300	-0.14225800
C	-2.81649000	0.52399600	-0.83101300
H	-1.13085800	-0.42913300	1.75472300
H	-2.50304400	-1.45485800	-0.13970100
H	2.95964300	-1.43084800	0.10278900
H	2.36480300	-1.27429300	-1.55521900
H	3.18893500	0.10151800	-0.77924600
H	-3.69570700	0.27817400	-1.42024000
H	-2.49615700	1.56178500	-0.82583000

INT6-OAu

C	3.66038800	1.25565200	0.47196400
C	2.53976800	0.84637300	-0.44255200
N	2.14444800	-0.40578000	-0.45041200
C	2.91451800	-1.42937100	0.20738100
C	4.33741100	-1.02647000	0.42550700
O	4.43347200	0.29892400	1.00382400
O	3.81576000	2.41997900	0.76652000
C	2.38206000	-2.62037100	0.47777700
Au	-0.88517500	-0.22611900	-0.32089600
P	-2.97831300	0.24296200	0.44988400
C	-4.28969000	-0.24773700	-0.73007900
C	-3.24223500	2.02494200	0.77661700
O	1.05551500	-0.78574100	-1.09631200
C	1.78284500	1.87669800	-1.19098000
H	4.82964300	-1.69870400	1.12619100
H	4.89011800	-1.02122700	-0.52136600
H	-4.23075800	-1.32348100	-0.92144800
H	-5.27435900	-0.00684300	-0.31429600
H	-4.15423200	0.28617500	-1.67559500
H	-2.53734100	2.36858600	1.53989000
H	-3.07653700	2.59773500	-0.14094400
H	-4.26633300	2.19207000	1.12800600
H	1.63999900	1.56093600	-2.23035300
H	0.77909200	2.00278400	-0.75577800
H	2.30949100	2.82983600	-1.15048900
C	-3.37507900	-0.61157900	2.01922700
H	-4.39043300	-0.35040800	2.33786300
H	-3.30822000	-1.69474200	1.87876600
H	-2.66436900	-0.31120300	2.79522400
H	1.36362000	-2.87132100	0.20652300
H	2.98508900	-3.37484200	0.97174400

MsOH

H	1.50905900	1.48576400	-0.11757800
O	0.37355000	-1.10351100	-1.04436800
S	0.09723000	-0.14034400	0.02196100
C	-1.65371800	0.19698500	0.09127000
H	-2.14722100	-0.74130500	0.35780000
H	-1.84076500	0.95700200	0.85194800
H	-1.99094400	0.53291500	-0.89164500
O	0.63374700	-0.39088200	1.36285000
O	0.59726600	1.34804500	-0.45592300

For 1r system:

Z-r0-N

O	-0.10506100	-2.71807400	-0.14361900
N	-0.18907700	-1.36169700	-0.08631400
C	-1.33434800	-0.74573200	-0.01553000
C	-2.61583400	-1.53026300	0.03814300
O	-2.63940300	-2.76114900	0.06038100
O	-3.69021900	-0.76693700	0.04054100
C	-4.98495200	-1.47092800	0.08236700
C	-6.04255300	-0.48024600	0.01186500
C	-6.95501600	0.31238000	-0.04667200
H	-1.04212200	-3.07225800	-0.08183700
H	-5.01413900	-2.16899700	-0.75960600
H	-5.02080900	-2.04887400	1.01102700
C	-8.05451200	1.26895500	-0.11604500
H	-7.80212100	2.19493100	0.41447900
H	-8.29367400	1.52658300	-1.15449900
H	-8.95854900	0.85515900	0.34673300
C	-1.33741300	0.73732800	-0.02325700
C	-1.89537700	1.45420200	1.04767500
C	-0.77374400	1.42949200	-1.10844300
C	-1.86705600	2.84810900	1.03926000
H	-2.33990400	0.92473500	1.88489900
C	-0.76117600	2.82559400	-1.11485800
H	-0.37093700	0.87489300	-1.95105600
C	-1.30184600	3.53510600	-0.04007800
H	-2.29131800	3.39798900	1.87427600
H	-0.33631800	3.35507900	-1.96283300
H	-1.29220700	4.62147000	-0.04629400
Au	1.77834800	-0.47102300	-0.02728600
P	3.89617700	0.40663500	0.09257300
C	4.17247600	1.38278700	1.61763200
H	5.19016100	1.78830700	1.62357200
H	3.45307600	2.20610800	1.66397000
H	4.03267800	0.74346500	2.49470100
C	5.21721700	-0.86083000	0.07181100
H	5.16913900	-1.42823800	-0.86269300
H	6.19782500	-0.37904500	0.15343900
H	5.08202800	-1.55114500	0.90989800
C	4.27662300	1.53903300	-1.29568800
H	5.28907000	1.94260900	-1.18468500
H	4.20511800	0.99648600	-2.24343700
H	3.55689400	2.36323900	-1.30633800

E-1r-0

O	-1.46509500	-2.00354000	-1.34646300
N	-1.03117700	-0.96672100	-0.53082800
C	-1.96615000	-0.28819900	0.05143000
C	-1.44781600	0.80801700	0.97110200
O	-1.53400100	0.73656100	2.17707900
O	-0.92366200	1.82203300	0.27974700
C	-0.40469300	2.93769300	1.08287000
C	0.16428300	3.92166700	0.17847000
C	0.64448300	4.76189800	-0.54876200
H	-0.65490000	-2.30131700	-1.80518900
H	-1.23419100	3.34780800	1.66747200
H	0.34066400	2.53971400	1.77813900
C	1.21850500	5.77845000	-1.42462200
H	1.48621000	5.34907600	-2.39746900
H	0.51075700	6.59696400	-1.60084700
H	2.12831300	6.20590000	-0.98625700
Au	1.09119300	-0.86108100	-0.18205800
P	3.35177100	-0.81869700	0.22158800
C	4.15008100	0.73677800	-0.32098400
H	3.70144800	1.58472600	0.20551800
H	5.22349700	0.70206900	-0.10419700
H	4.00169200	0.87297400	-1.39662800
C	3.74733800	-0.98842500	2.00109500
H	3.35998100	-1.94050100	2.37666900

H	4.83237200	-0.95531700	2.14894000
H	3.28081300	-0.17315400	2.56266300
C	4.25634700	-2.16765400	-0.62290500
H	5.32613800	-2.09796500	-0.39684900
H	3.87729900	-3.13631300	-0.28278400
H	4.10900700	-2.09144400	-1.70461300
C	-3.42302200	-0.47943200	-0.02357800
C	-4.24582700	0.65498000	0.13271300
C	-4.02320700	-1.74204400	-0.20588200
C	-5.63140500	0.53433200	0.08374200
H	-3.80463400	1.63787000	0.27021200
C	-5.41107000	-1.85466200	-0.23216800
H	-3.41202600	-2.62898600	-0.30548900
C	-6.21754800	-0.72138500	-0.09634100
H	-6.25164500	1.41901200	0.19167500
H	-5.86390800	-2.83345500	-0.36023800
H	-7.29916500	-0.81728600	-0.12618300

E-1r

O	3.34507000	-1.36249700	-2.56904900
N	2.38208100	-1.64083500	-1.62326200
C	2.60362500	-1.08929100	-0.47645800
C	1.54177500	-1.36416400	0.55264700
O	1.36995800	-0.66566800	1.53235100
O	0.80671300	-2.46180400	0.26457600
C	-0.31774600	-2.73857000	1.12187400
C	-1.57981900	-2.30618800	0.49110800
C	-2.69809500	-2.27027500	-0.02761400
H	3.04112600	-1.86803000	-3.34669900
H	-0.34336600	-3.82463300	1.24340500
H	-0.17474200	-2.26561900	2.09479500
Au	-1.90946600	-0.07127600	0.07545500
P	-1.73182200	2.24118400	-0.08307900
C	-3.12115100	2.99409700	-1.00965200
H	-2.99853100	4.08222700	-1.04460600
H	-3.14123000	2.60002500	-2.03035800
H	-4.06886300	2.75272300	-0.51870800
C	-1.71804500	3.06018300	1.55518900
H	-0.85806100	2.70728000	2.13285900
H	-1.65120400	4.14668300	1.43172400
H	-2.63415400	2.81260400	2.10028900
C	-0.21039100	2.80612200	-0.93100700
H	-0.19466200	2.42123500	-1.95538500
H	-0.18265800	3.90122900	-0.95473600
H	0.67097200	2.43402900	-0.39976200
C	3.73034000	-0.20074100	-0.09350700
C	4.38589000	-0.40141900	1.13339900
C	4.15472000	0.84466000	-0.93170500
C	5.45276600	0.41512900	1.50625400
H	4.06586600	-1.20300100	1.79207500
C	5.21145300	1.66959400	-0.54649200
H	3.65740300	1.01299300	-1.88006200
C	5.86643200	1.45456700	0.66897700
H	5.95827100	0.24118900	2.45213100
H	5.52544800	2.47928800	-1.19955800
H	6.69454800	2.09396700	0.96255400
C	-4.01956400	-2.46269600	-0.62908100
H	-4.79310000	-1.92883400	-0.06835100
H	-4.03101200	-2.10988100	-1.66542800
H	-4.25851300	-3.53288300	-0.62468000

TS1

C	-2.53599700	0.68715200	-0.54543700
O	-1.64700400	1.65964300	-0.62376600
C	-0.31744700	1.36761300	-1.14346100
C	0.27499300	0.09918200	-0.59272900
C	-0.38821300	-0.97384900	-0.38844200
O	-2.28826600	-0.49319700	-0.83962200
C	-3.88314500	1.09348100	-0.04478800
N	-3.97959800	2.35392100	0.22591500
O	-5.21609100	2.72254200	0.68326900
Au	2.33213200	-0.04239100	-0.12204200
H	-0.39475500	1.30022300	-2.23414000
H	0.26030500	2.24986900	-0.87802100
H	-5.12427000	3.68481600	0.82562200
P	4.60917800	-0.07625900	0.39778700
C	5.70602300	0.08391100	-1.06376400
H	5.49863900	1.02570100	-1.58158300
H	6.75668900	0.06706400	-0.75387400
H	5.52005000	-0.74375000	-1.75541100
C	5.15295500	-1.61487800	1.23682600
H	6.22515700	-1.56861800	1.45780400
H	4.59738700	-1.73906400	2.17180500
H	4.95350100	-2.47750900	0.59332300
C	5.11270300	1.28218000	1.52299200
H	6.18619400	1.22314000	1.73455000
H	4.89000300	2.24784500	1.05828500
H	4.55508000	1.20936700	2.46193400
C	-0.63548600	-2.35427600	0.00792200
H	-1.30396900	-2.41198700	0.87304900
H	-1.06318500	-2.93295300	-0.81721000
H	0.32848400	-2.80011700	0.28180000
C	-4.93607400	0.05616400	0.11200800
C	-5.28269000	-0.77353600	-0.96650500
C	-5.59778800	-0.09922200	1.34087800
C	-6.27959200	-1.73794600	-0.81775200
H	-4.77892300	-0.65985900	-1.92118600
C	-6.58434000	-1.07389300	1.48810400
H	-5.33537800	0.53804900	2.17882500
C	-6.92998400	-1.89225100	0.40915400
H	-6.54629500	-2.36931600	-1.66071800
H	-7.08533500	-1.19118600	2.44499200
H	-7.70289200	-2.64730800	0.52415500

INT1

C	-2.54469100	0.67238300	0.04485000
O	-2.12557000	-0.52639000	-0.12123700
C	-0.65005700	-0.85749200	-0.06599300
C	0.23337600	0.33671800	0.03222100
C	-0.30808000	1.54369200	0.16658000
O	-1.77304900	1.68616700	0.21696800
C	-4.00544000	0.88268500	0.02428700
N	-4.31449700	2.14274300	0.00269000
O	-5.65080500	2.37323800	-0.00001100
Au	2.28073700	-0.03821200	-0.01778300
H	-0.57113600	-1.52437400	0.79624600
H	-0.49781600	-1.43378200	-0.97996700
H	-5.71721000	3.34964400	-0.00961000
P	4.58680400	-0.49703500	-0.06320000
C	5.47010100	-0.07516200	1.49119500
H	5.04097900	-0.64025700	2.32490200
H	6.53585500	-0.31396000	1.40528300
H	5.35682800	0.99330400	1.70128500
C	5.50101100	0.40544500	-1.37578000
H	6.56853400	0.16064300	-1.34214600
H	5.09998700	0.13242200	-2.35731700
H	5.37538300	1.48431200	-1.23856700
C	4.98592500	-2.26540500	-0.35756300
H	6.07067900	-2.42002400	-0.36506900
H	4.54130900	-2.88098300	0.43100800
H	4.57181500	-2.58150100	-1.32040700
C	0.27408400	2.90810300	0.29625000
H	-0.02918500	3.38013200	1.23918600
H	1.36405400	2.83824400	0.27355000
H	-0.05534900	3.55986100	-0.52275600
C	-4.92923100	-0.28033100	0.00919000
C	-4.82293500	-1.28308900	0.98676600
C	-5.92342200	-0.37807800	-0.97816500
C	-5.70319400	-2.36464800	0.97854100
H	-4.06204700	-1.21271700	1.75865000
C	-6.79341500	-1.46745800	-0.98674700
H	-6.01009600	0.39090000	-1.73853200
C	-6.68766100	-2.45979700	-0.00836000
H	-5.61925100	-3.13180200	1.74286800
H	-7.55484700	-1.53944500	-1.75808000
H	-7.37015100	-3.30507600	-0.01586500

TS2			
C	-2.61835600	0.44731300	0.00602600
O	-2.27543500	-0.71124300	0.23889200
C	-0.15892900	-1.02643900	0.27951600
C	0.26026000	0.25721600	-0.02888900
C	-0.38516700	1.38727200	-0.29853200
O	-1.79852200	1.46272300	-0.29043400
C	-4.06199200	0.84638400	0.03862400
N	-4.24478900	2.12203700	0.13722400
O	-5.56633300	2.48921400	0.18050500
Au	2.34936600	-0.09797500	0.03288200
H	-0.16724000	-1.38053600	1.30917600
H	-0.20890200	-1.79730100	-0.48779700
H	-5.52280100	3.46294500	0.24221400
P	4.68454000	-0.37585400	0.05976800
C	5.59584100	1.10908600	-0.51206000
H	5.36319000	1.95876900	0.13765500
H	6.67528600	0.92305500	-0.48968200
H	5.29425800	1.35742100	-1.53450600
C	5.26904200	-1.74329000	-1.01478100
H	6.36129100	-1.81866800	-0.97275600
H	4.82870800	-2.68796000	-0.68044000
H	4.95913000	-1.55854200	-2.04802700
C	5.36388600	-0.74309800	1.72360600
H	6.45036200	-0.87433200	1.66996200
H	5.13232600	0.08157100	2.40507100
H	4.90929400	-1.65896500	2.11426700
C	0.17308500	2.72899900	-0.63782500
H	1.26546700	2.68732800	-0.64180300
H	-0.17362600	3.05558000	-1.62612300
H	-0.15185700	3.48125300	0.09131500
C	-5.09418500	-0.22073300	0.00002100
C	-5.03025800	-1.22101000	-0.98435900
C	-6.14497900	-0.24117100	0.93184400
C	-6.00522500	-2.21645700	-1.04139800
H	-4.22406600	-1.21388900	-1.71181400
C	-7.10971800	-1.24682700	0.87921500
H	-6.20296500	0.52491700	1.69710700
C	-7.04553900	-2.23316700	-0.10874200
H	-5.95038400	-2.97941900	-1.81288300
H	-7.91419500	-1.25765400	1.60931700
H	-7.80203800	-3.01207600	-0.15033000
INT2			
C	-1.93952300	-1.16636400	0.26283100
O	-2.20482700	-1.76444100	-0.74537700
C	0.72008600	-2.79054200	-1.78502600
C	0.65036000	-2.17365900	-0.61469400
C	0.18634100	-2.22208900	0.67965900
O	-0.91961100	-1.57915800	1.12980900
C	-2.64672400	0.04646100	0.76749900
N	-2.02445100	0.65909900	1.72329700
O	-2.67013800	1.78045400	2.17307900
Au	1.80582900	-0.36320100	-0.21420200
H	0.15573100	-3.70578700	-1.96232200
H	1.31740100	-2.41106200	-2.60862400
H	-2.09482900	2.09476000	2.89730900
P	3.07963900	1.59531800	-0.12640800
C	3.87097300	1.86851300	1.50415200
H	4.54392400	1.03542000	1.72976900
H	4.44148100	2.80405600	1.49468600
H	3.10363600	1.92092000	2.28275800
C	2.09603900	3.10499000	-0.46107200
H	2.73649500	3.99272500	-0.41198900
H	1.64857600	3.03703400	-1.45756600
H	1.29506200	3.19655700	0.27914700
C	4.44675600	1.62072900	-1.34620800
H	5.00968100	2.55699100	-1.26171300
H	5.11902500	0.77651000	-1.16391900
H	4.04001200	1.53427100	-2.35855600
C	0.88804600	-2.93949000	1.78992900
H	1.85082100	-3.33058900	1.45897600
H	1.02576000	-2.28776100	2.65874100
H	0.24585300	-3.77600100	2.09945400
C	-3.92009000	0.43669600	0.11150400
C	-4.91619800	-0.52888900	-0.11269400
C	-4.14324400	1.76196400	-0.29951900
C	-6.11768900	-0.17151100	-0.72336700
H	-4.75588400	-1.55592100	0.19985000
C	-5.34049300	2.10998400	-0.92353100
H	-3.38073000	2.51523900	-0.13629900
C	-6.33133300	1.14699300	-1.13315000
H	-6.88458600	-0.92434500	-0.88246900
H	-5.49931500	3.13548000	-1.24539200
H	-7.26530900	1.42333400	-1.61478700
TS3			
C	-2.55558900	0.30078600	0.00185900
N	-1.81224900	0.71823100	-0.96522100
C	-0.49904200	2.27409200	0.21467000
O	-0.81498800	1.46703500	1.23450300
C	-2.01332700	0.73985500	1.33134000
O	-2.42409700	0.44260600	2.41420900
O	-2.21807800	0.43568600	-2.22870300
C	0.84754200	2.14311700	-0.27209300
C	1.41288100	3.26744200	-0.78816900
Au	1.87953100	0.33734700	-0.07447200
P	3.09722300	-1.66201200	0.15479100
H	-1.50919300	0.80458500	-2.79518600
H	2.42504100	3.25503300	-1.18461400
H	0.92180100	4.24095500	-0.79670300
C	2.09773800	-3.19024400	-0.04051900
H	1.63678600	-3.20618800	-1.03340100
H	2.72651400	-4.07979900	0.07676500
H	1.30415700	-3.21038200	0.71347300
C	4.46736200	-1.84730900	-1.05466000
H	5.16136400	-1.00636100	-0.95637800
H	5.00983500	-2.78345500	-0.88122400
H	4.06329700	-1.84803200	-2.07216900
C	3.90208400	-1.84851800	1.79479400
H	4.46880000	-2.78518300	1.84062300
H	4.58039100	-1.00776900	1.97197800
H	3.13947300	-1.85088100	2.58034400
C	-1.43123700	3.40677900	-0.07438300
H	-1.04817400	4.27971800	0.47504200
H	-1.44373700	3.65662300	-1.13632400
H	-2.44564100	3.21332800	0.27696900
C	-3.77955300	-0.52215000	-0.05777400
C	-4.85354800	-0.25376600	0.81067900
C	-3.88527200	-1.57822200	-0.98229000
C	-6.01506600	-1.02053900	0.74337700
H	-4.78696200	0.55688500	1.52692800
C	-5.04409900	-2.35002800	-1.02986500
H	-3.06188300	-1.80078500	-1.65069800
C	-6.11213300	-2.07124500	-0.17233000
H	-6.84272500	-0.79784300	1.41037700
H	-5.11317200	-3.16997500	-1.73874200
H	-7.01667000	-2.67126000	-0.21699700
INT3			
C	-2.25930300	0.39268300	0.40524900
N	-1.80038800	1.38972000	-0.29225600
C	-0.82919800	2.28994200	0.42340700
O	-0.77973300	1.63369800	1.70180600
C	-1.57617400	0.54434100	1.75407300
O	-1.68059700	-0.15606900	2.72488000
O	-2.08782000	1.64088400	-1.58899000
C	0.50200100	2.16164800	-0.30830200
C	0.91450100	3.20632500	-1.05157200
Au	1.53597000	0.35782400	-0.17621100
P	2.77620700	-1.64517900	-0.03826700
H	-1.25499000	2.03422200	-1.95958600
H	1.83581600	3.14874800	-1.62676800
H	0.38922800	4.16022300	-1.11095500
C	2.07832800	-3.04729500	-0.99993200

H	2.01096400	-2.77384800	-2.05787000
H	2.70936300	-3.93706200	-0.89778600
H	1.07180400	-3.27659000	-0.63483800
C	4.50232200	-1.48263600	-0.64612900
H	5.02777300	-0.72106200	-0.06082700
H	5.03451100	-2.43630600	-0.55618100
H	4.49693500	-1.17130600	-1.69568100
C	2.94982800	-2.30498900	1.66791300
H	3.54068900	-3.22765500	1.66705300
H	3.44311700	-1.56118400	2.30198500
H	1.95858400	-2.51281100	2.08392000
C	-1.45718500	3.66712300	0.61519800
H	-0.76112900	4.29801600	1.17302200
H	-1.67110200	4.13875500	-0.34679800
H	-2.38973600	3.57475800	1.17839300
C	-3.18323900	-0.64450200	0.01397300
C	-3.98636600	-0.52520100	-1.14707600
C	-3.28692800	-1.80772000	0.81488500
C	-4.85667900	-1.55008200	-1.49329600
H	-3.94653300	0.36757900	-1.75647500
C	-4.15393600	-2.82849300	0.44533200
H	-2.68775000	-1.90412400	1.71063300
C	-4.93904900	-2.70355500	-0.70490600
H	-5.47718900	-1.44855700	-2.37814500
H	-4.22131200	-3.72153400	1.05870400
H	-5.61939800	-3.50231200	-0.98576400

TS4

C	-1.36678300	2.20296800	0.67424800
N	-1.45233500	0.95275400	0.97496300
C	-1.77643300	0.06170700	-0.21108600
O	-1.57933800	0.97410500	-1.29074600
C	-1.48429700	2.25953000	-0.81907500
O	-1.41902100	3.22651100	-1.52693600
O	-1.10788400	0.28051600	2.04881800
C	-1.08097800	3.34043200	1.57089900
C	-0.73139700	-1.03760400	-0.03355300
C	-0.97530000	-2.28220700	-0.49639800
Au	1.38418400	-0.55689000	0.01132700
P	3.65362600	-0.03535900	-0.12838300
H	-0.58061700	-0.64244300	1.36775500
H	-0.89012100	2.99771400	2.58961200
H	-0.21686700	3.89954600	1.19487100
H	-1.93675600	4.02734800	1.57175200
H	-0.27171200	-3.09188800	-0.31878800
H	-1.86215300	-2.53909500	-1.07645500
C	4.33033800	0.74974400	1.38465700
H	4.20922800	0.07222900	2.23570400
H	5.39369000	0.97823400	1.25194800
H	3.78620900	1.67629400	1.59341400
C	4.71848900	-1.49874800	-0.42454300
H	4.42199300	-1.99029700	-1.35630900
H	5.76909500	-1.19545800	-0.49423500
H	4.60271300	-2.21036600	0.39909000
C	4.04217500	1.12983100	-1.49066000
H	5.11850100	1.33145000	-1.52301300
H	3.72652700	0.69950900	-2.44616800
H	3.50267400	2.06961200	-1.33537500
C	-3.23712000	-0.38229600	-0.15442000
C	-3.69300400	-1.17075500	0.91426400
C	-4.12684900	-0.01958800	-1.17419900
C	-5.02558100	-1.57813400	0.96320500
H	-3.01993100	-1.45996700	1.71391300
C	-5.45751500	-0.44197300	-1.12328400
H	-3.78705000	0.58029200	-2.01040200
C	-5.91103400	-1.21809700	-0.05618200
H	-5.36896300	-2.18160300	1.79858100
H	-6.13617100	-0.16126500	-1.92368400
H	-6.94719300	-1.54234500	-0.01839100

INt4

C	-2.07381300	0.72022400	0.23476500
N	-1.54740000	1.50957500	-0.69413500
C	-0.64777900	2.55214100	-0.07246400
O	-0.70354000	2.25203100	1.31000200
C	-1.52370500	1.16702700	1.53047100
O	-1.68281500	0.72902300	2.64375400
O	-1.68252300	1.51354400	-1.94722900
C	0.75281200	2.39669300	-0.62594000
C	1.88643500	2.55174600	0.12313900
Au	1.65907400	0.25757100	-0.10424200
P	2.04596800	-2.04328500	0.01643600
H	0.80290900	2.39104500	-1.71249600
H	2.84873000	2.67926500	-0.36739200
H	1.84299800	2.73526100	1.19372600
C	3.10807200	-2.66672600	-1.33896900
H	4.07504900	-2.15467900	-1.31521800
H	3.26443200	-3.74463200	-1.21938300
H	2.62811200	-2.47449700	-2.30349000
C	2.88911600	-2.52673000	1.56896400
H	2.26837200	-2.25148100	2.42719600
H	3.06097600	-3.60874400	1.57646300
H	3.84912900	-2.00666100	1.64427300
C	0.51239200	-3.04170900	-0.05033600
H	0.76219200	-4.10631000	0.01956700
H	-0.14434600	-2.76821700	0.78088400
H	-0.01122700	-2.85289900	-0.99246400
C	-1.20995300	3.94263000	-0.35203000
H	-0.57400700	4.68999000	0.12987400
H	-1.23202800	4.12585900	-1.42890300
H	-2.22509000	4.01251000	0.05026400
C	-3.00297900	-0.38286500	0.01091500
C	-3.49991300	-1.11396900	1.11325100
C	-3.42711800	-0.74045700	-1.28870800
C	-4.38811600	-2.16739800	0.91620900
H	-3.19065300	-0.84908800	2.11635700
C	-4.31611700	-1.79814500	-1.46949500
H	-3.06484200	-0.18421400	-2.14237800
C	-4.80005500	-2.51595800	-0.37325800
H	-4.76188700	-2.71638200	1.77595900
H	-4.63375500	-2.05932500	-2.47512800
H	-5.49428000	-3.33847700	-0.52146700

E-r0

O	-1.04710200	2.65142400	0.40435300
N	-0.08995300	1.68259200	0.17032300
C	-0.57820500	0.49807200	0.01616800
C	0.44723100	-0.57827000	-0.22998800
O	0.15226300	-1.71543900	-0.54774500
O	1.71012500	-0.15304700	-0.06788200
C	2.73187100	-1.15672300	-0.32757800
C	4.03817000	-0.54874200	-0.11511100
C	5.13972800	-0.07645900	0.05298600
H	-0.51385800	3.46278800	0.49872000
H	2.56975000	-2.00693400	0.34364400
H	2.61865600	-1.51933500	-1.35499000
C	6.46574000	0.50025300	0.25566500
H	6.41977700	1.59603100	0.24319300
H	6.89210500	0.19323300	1.21818900
H	7.15736200	0.18692100	-0.53563500
C	-2.01229000	0.10684700	0.03186400
C	-2.43494100	-0.99031400	0.80081300
C	-2.96113800	0.81904000	-0.72063000
C	-3.78052600	-1.35666300	0.82825400
H	-1.71082500	-1.55225600	1.38164500
C	-4.30342400	0.44038700	-0.70184000
H	-2.64652100	1.66455600	-1.32243500
C	-4.71769800	-0.64497300	0.07489700
H	-4.09501700	-2.20197900	1.43439900
H	-5.02606700	0.99511400	-1.29425500
H	-5.76509100	-0.93451500	0.09244600

INT4-0

C	-0.07849000	0.16306300	-0.13914900
N	0.82553600	-0.80859800	-0.16995300
C	2.23051100	-0.24403200	-0.29133500

O	2.00124700	1.15576000	-0.36226500
C	0.66176100	1.43361000	-0.26223400
O	0.25999900	2.57369400	-0.29022100
O	0.68928900	-2.05872600	-0.11052900
C	3.00647600	-0.62387700	0.94545800
C	3.54930600	0.25109200	1.78939700
H	3.10449700	-1.69650600	1.09252400
H	4.11179800	-0.09160900	2.65376100
H	3.46097300	1.32449800	1.64929500
C	2.85674400	-0.74771700	-1.58538800
H	3.85505700	-0.31513400	-1.69275000
H	2.94015200	-1.83694500	-1.55532000
H	2.24093100	-0.45542500	-2.44173900
C	-1.52446100	-0.00308100	-0.01318300
C	-2.36077700	1.13429500	0.02283000
C	-2.11637400	-1.28209200	0.07900000
C	-3.74011800	0.99174200	0.14741200
H	-1.92272800	2.12180100	-0.04639400
C	-3.49859300	-1.40936200	0.20254100
H	-1.48907000	-2.16239800	0.05313100
C	-4.31713800	-0.27812200	0.23806600
H	-4.36701400	1.87887000	0.17430200
H	-3.93650400	-2.40147600	0.27162100
H	-5.39420000	-0.38442800	0.33488300

For intermolecular nucleophilic attack:

TS-S1

C	4.66728600	0.83848500	0.15133800
O	3.52448500	1.52999200	0.14694700
C	3.65845000	2.97085100	0.15146700
H	2.63804000	3.35289900	0.14859500
H	4.18757000	3.29657200	1.05004300
H	4.19724100	3.30437600	-0.73854200
O	5.77566900	1.33480600	0.17513300
C	4.46728200	-0.65494900	0.14570000
C	5.64989700	-1.53291400	0.41443400
H	5.79673700	-2.23417000	-0.41466300
H	6.54616000	-0.92646800	0.54274900
H	5.47936200	-2.13017800	1.31778400
N	3.29068300	-1.11406100	-0.09964100
O	3.22250900	-2.48841300	-0.06492700
H	2.27834700	-2.68444500	-0.23161700
C	1.35350300	-0.37654400	-0.58511000
C	0.60688800	-0.57771600	0.43060700
H	0.90145800	-0.92306500	1.41542400
C	1.61786000	0.01920500	-1.96996700
H	2.33600200	0.84231900	-2.01590500
H	1.98968300	-0.81941100	-2.56765900
H	0.66984900	0.36182200	-2.40219100
Au	-1.44733300	-0.17211000	0.15644600
P	-3.74323800	0.22133700	-0.01853400
C	-4.17672800	1.58583400	-1.16612200
H	-5.26188200	1.73583500	-1.18619900
H	-3.69114200	2.51046900	-0.83859900
H	-3.82717900	1.34465600	-2.17493900
C	-4.69485400	-1.22746000	-0.62067900
H	-4.54472700	-2.07318100	0.05784300
H	-5.76329200	-0.98952100	-0.66846300
H	-4.34367900	-1.51345000	-1.61724100
C	-4.52770800	0.67392300	1.57721100
H	-5.59869500	0.85685200	1.43518400
H	-4.39235500	-0.13833000	2.29830200
H	-4.05698400	1.57815800	1.97581400

TS-S2

C	-4.40689900	1.11943700	0.10957200
O	-3.27279500	1.75309100	-0.20169800
C	-3.21794900	3.15588300	0.15028500
H	-2.23720700	3.49694800	-0.18071800
H	-4.00943300	3.70492400	-0.36515800
H	-3.32298600	3.27928100	1.23069700
O	-5.37204700	1.64279500	0.62854500
C	-4.40119800	-0.34126200	-0.25947800
C	-5.69321100	-1.09548400	-0.21129200
H	-5.63431400	-1.90080100	0.53066300
H	-6.51042500	-0.42401900	0.05130800
H	-5.89488400	-1.56311100	-1.18142600
N	-3.27994500	-0.88235000	-0.58344400
O	-3.37954600	-2.22222200	-0.87835200
H	-2.46915800	-2.47635700	-1.13233700
C	-0.63065500	-1.04224500	0.38706300
C	-1.28432500	-0.34212200	-0.44991900
H	-1.35662200	0.43954700	-1.17900800
C	-0.88743700	-2.10994700	1.39817500
H	-0.57980500	-1.76800100	2.39208600
H	-1.94844800	-2.38091900	1.43308400
H	-0.30005600	-3.00575700	1.17022200
Au	1.35283600	-0.27581400	0.07037700
P	3.56490200	0.44125900	-0.13596500
C	4.53785500	0.22919600	1.40400900
H	5.56293300	0.58820700	1.26061700
H	4.06803400	0.79396800	2.21538900
H	4.56179900	-0.82878500	1.68359500
C	4.51615300	-0.44066800	-1.43288300
H	4.03696300	-0.29158100	-2.40578100
H	5.54360100	-0.06259800	-1.47445800
H	4.53416400	-1.51263000	-1.21234700
C	3.72084800	2.22077700	-0.55340700
H	4.77717000	2.50304300	-0.62488900
H	3.22862000	2.42095900	-1.51036300
H	3.23804900	2.82381900	0.22191700

TS-S3

C	-3.95371900	-0.45008400	-0.43382100
O	-5.08935000	-1.00694400	-0.08855800
C	-5.17198400	-2.45947300	-0.12346100
H	-6.18841300	-2.68602600	0.19431800
H	-4.99443900	-2.81591200	-1.13973900
H	-4.44323700	-2.89074500	0.56572700
O	-3.00089700	-1.14421200	-0.84876300
C	-3.92809400	1.03422800	-0.32999900
C	-3.11478500	1.85992400	-1.28324700
H	-2.22836600	2.27480400	-0.78952700
H	-2.79546600	1.27463400	-2.14712700
H	-3.71987200	2.70349500	-1.63126300
N	-4.65420900	1.49450600	0.63091700
O	-4.58180200	2.86502000	0.71503700
H	-5.16708200	3.07730500	1.46747300
C	-1.21141400	-0.66412200	-0.75157000
H	-1.05201300	-0.61943500	-1.81216000
C	-0.67965300	-0.62826100	0.41553900
C	-1.19654700	-0.80379500	1.80916900
H	-1.04036800	0.11279900	2.38906500
H	-2.26308000	-1.05214700	1.83153100
H	-0.64426500	-1.60066000	2.31891400
Au	1.38190300	-0.19644000	0.09228300
P	3.66858100	0.24727700	-0.12238600
C	4.45964800	-0.63602400	-1.52370500
H	5.52827500	-0.39869700	-1.57082400
H	4.33499700	-1.71582900	-1.39504500
H	3.98207000	-0.33962600	-2.46299700
C	4.06849100	2.01824500	-0.39047900
H	3.69656100	2.61042700	0.45166000
H	5.15171600	2.15688300	-0.47893500
H	3.58302000	2.37102700	-1.30605400
C	4.64479900	-0.23857900	1.35375200
H	4.51677100	-1.30883000	1.54436500
H	5.70768200	-0.02463200	1.19569400
H	4.29184500	0.31596300	2.22913400

TS-S4

C	-4.09239100	-0.53979300	-0.15671400
O	-5.22814400	-1.19506200	-0.17681600
C	-5.18447300	-2.64052400	-0.01572500
H	-6.22849200	-2.94980800	-0.01376200
H	-4.64807200	-3.08970400	-0.85380100

H	-4.70002600	-2.89640500	0.92865600
O	-3.00668700	-1.15326900	-0.08527500
C	-4.23057900	0.93946300	-0.25529700
C	-3.19019700	1.77066200	-0.94738700
H	-2.54623100	2.28345400	-0.22272500
H	-2.56354100	1.16187600	-1.59993900
H	-3.68856200	2.54137100	-1.54312300
N	-5.30195600	1.38858400	0.30477200
O	-5.38554200	2.75844300	0.23006000
H	-6.22720600	2.95771900	0.68350700
C	-0.47117400	-0.67793200	-0.51465400
H	-0.75324000	-1.04576400	-1.49662500
C	-1.31876900	-0.52079800	0.44253400
C	-1.58652400	-0.17439400	1.84499100
H	-1.98747300	-1.02955100	2.39917600
H	-0.63246500	0.11573800	2.29871700
H	-2.28138700	0.66620400	1.94054400
Au	1.54421300	-0.21368900	-0.18374100
P	3.81377300	0.27912300	0.11615800
C	4.94229900	-0.74412300	-0.90783000
H	5.98679400	-0.48371000	-0.70325700
H	4.78402100	-1.80348200	-0.68204800
H	4.72973500	-0.57787200	-1.96870700
C	4.25414700	2.01539700	-0.28727000
H	3.66912400	2.69722800	0.33821400
H	5.32141800	2.19172000	-0.11283600
H	4.02112500	2.21918200	-1.33725400
C	4.39455900	0.03576300	1.84096700
H	4.23843300	-1.00619200	2.13804500
H	5.45952000	0.27889300	1.92564900
H	3.82237700	0.68038500	2.51594300

INT-S1

C	-0.72466800	0.37517200	0.00218800
O	-1.38317700	-0.79195000	0.00208700
C	-2.82130700	-0.69492500	-0.00276900
H	-3.17995800	-1.72462900	-0.00127900
H	-3.17443200	-0.16768500	0.88760900
H	-3.16848700	-0.17239400	-0.89828200
O	-1.27172300	1.46389000	-0.00039300
C	0.76814600	0.22416200	0.00375900
C	1.61316100	1.46281000	-0.00004500
H	2.21014600	1.51477500	-0.91873100
H	0.98667600	2.35260300	0.06845700
H	2.31858400	1.44655400	0.83845400
N	1.22093500	-0.98052900	0.00278000
O	2.60929000	-1.00121100	-0.00386700
H	2.81381500	-1.95466000	0.00289900

INT-S2

C	2.49960500	-1.08809600	-0.00341800
H	2.52230500	-2.16241900	-0.00678400
C	2.81884000	0.10014700	-0.00039500
C	3.32417100	1.46978300	0.00057100
H	2.99572700	2.01117200	0.89350100
H	4.42068100	1.43915700	-0.00201000
H	2.99161400	2.01361200	-0.88936300
Au	0.42537100	-0.22189200	0.00175200
P	-1.86033700	0.18418600	0.00142500
C	-2.76179500	-0.85570200	-1.20710200
H	-3.83347800	-0.63071900	-1.17126500
H	-2.38429700	-0.65914800	-2.21522000
H	-2.60626900	-1.91332100	-0.97268200
C	-2.65465300	-0.13243600	1.62133300
H	-2.20473600	0.51050100	2.38409500
H	-3.72886700	0.07472400	1.56035000
H	-2.50312100	-1.17758100	1.90843300
C	-2.27569400	1.91611700	-0.42805400
H	-1.88719900	2.15129200	-1.42362100
H	-3.36274500	2.05321100	-0.42110300
H	-1.82172300	2.59728000	0.29827300

For L=PPh$_3$

TS1 (1h)

C	-5.19873900	0.07461800	0.32851500
O	-4.43543500	-1.00067700	0.43405200
C	-3.10430600	-0.87776700	1.00812500
C	-2.32434000	0.29438200	0.47877400
C	-2.81281600	1.44182800	0.21031600
O	-4.80968300	1.22332000	0.58835200
C	-6.58709600	-0.17381500	-0.14384600
N	-6.91283600	-1.41814200	-0.23874100
O	-8.20973500	-1.57102100	-0.66653700
C	-7.48859000	0.98616200	-0.43870600
Au	-0.23238200	0.17366300	0.20388800
H	-3.21565500	-0.78870200	2.09458500
H	-2.63412400	-1.82972900	0.77290900
H	-8.32704800	-2.54028300	-0.69162600
H	-8.35949900	0.96695700	0.22685900
H	-6.96344000	1.93271600	-0.30886600
H	-7.86558900	0.91895700	-1.46539500
P	2.08219000	-0.08364600	-0.05281600
C	-2.86636900	2.83031300	-0.22395700
H	-3.47436300	2.94613600	-1.12706100
H	-3.26091200	3.47829700	0.56534400
H	-1.84165900	3.14704700	-0.45376400
C	2.92047900	-0.45703700	1.53410000
C	2.23709900	-1.22471200	2.49210800
C	4.22448700	-0.01445900	1.80551000
C	2.85418300	-1.55231200	3.69985200
H	1.22304600	-1.56284000	2.29360800
C	4.83534700	-0.34137400	3.01832100
H	4.76336700	0.58448000	1.07798600
C	4.15318200	-1.10971200	3.96465300
H	2.31810900	-2.14555800	4.43533400
H	5.84428800	0.00638200	3.22165300
H	4.63045000	-1.35968700	4.90811000
C	2.48790700	-1.45434500	-1.20188800
C	3.57994900	-2.30880100	-0.98738500
C	1.67481400	-1.64060500	-2.33325300
C	3.85407000	-3.33376400	-1.89629800
H	4.21477700	-2.18047300	-0.11625700
C	1.95806500	-2.66112000	-3.24109800
H	0.82072300	-0.98887300	-2.50126400
C	3.04654300	-3.51057100	-3.02190800
H	4.69882000	-3.99404800	-1.72099200
H	1.32454400	-2.79793900	-4.11306100
H	3.26164400	-4.31061600	-3.72488500
C	2.87863000	1.42608100	-0.72508900
C	3.91983600	1.36340600	-1.66322100
C	2.43054600	2.67877500	-0.27143600
C	4.50697600	2.53973100	-2.13623800
H	4.27431900	0.40404600	-2.02681000
C	3.02451600	3.84947200	-0.74307900
H	1.61868100	2.73806900	0.44946300
C	4.06217100	3.78143100	-1.67753900
H	5.31203400	2.48270400	-2.86353000
H	2.67241900	4.81332900	-0.38614500
H	4.51982100	4.69416100	-2.04886900

TS5 (1h)

C	5.29506500	1.52101300	-0.25174200
C	5.92325900	0.17827400	0.01646400
N	5.12294400	-0.77135000	0.34776200
C	3.02440700	-0.40113200	0.39502200
C	3.29331700	0.89650600	1.02463500
O	4.02942000	1.78042700	0.14514800
O	5.90619100	2.37521900	-0.85429700
C	2.33588500	-1.31245800	-0.15913600
Au	0.32590800	-0.56349600	-0.03566100
P	-1.92076400	0.08712800	-0.00427500
O	5.71525300	-2.00090400	0.48682800
C	7.39525700	0.01122600	-0.18734700
H	2.35244800	1.41483800	1.21794800
H	3.83244500	0.78182400	1.96903500

H	5.01472200	-2.56567700	0.87066800
H	7.82481100	-0.57320200	0.63212400
H	7.58367300	-0.53778300	-1.11878600
H	7.88252800	0.98401900	-0.25161200
C	2.56804200	-2.63825400	-0.80868900
H	3.63385900	-2.81464800	-0.98773800
H	2.17287500	-3.44141600	-0.17646800
H	2.04116900	-2.69244000	-1.76579300
C	-2.22604200	1.58862500	-1.00977400
C	-3.42920100	1.77934900	-1.70715500
C	-1.22911700	2.57713900	-1.06507100
C	-3.63053600	2.94800600	-2.44507300
H	-4.20596800	1.02145000	-1.67967000
C	-1.43807100	3.74445800	-1.80002100
H	-0.29027500	2.43123900	-0.53641100
C	-2.63832300	3.93018900	-2.49172900
H	-4.56310800	3.08762600	-2.98465500
H	-0.66120300	4.50291100	-1.83925000
H	-2.79778500	4.83625400	-3.06967600
C	-2.49791400	0.45511900	1.69655900
C	-3.37178200	1.51756500	1.97181800
C	-2.04939700	-0.36356800	2.74752800
C	-3.79354100	1.75326100	3.28278000
H	-3.72208100	2.16180200	1.17153200
C	-2.47970000	-0.12737900	4.05316700
H	-1.36535600	-1.18376600	2.54277400
C	-3.35070900	0.93269500	4.32233100
H	-4.46822300	2.57963000	3.48848700
H	-2.12981800	-0.76556700	4.85982100
H	-3.67951600	1.12056000	5.34070500
C	-3.01758500	-1.22324500	-0.66787000
C	-4.27588600	-1.49291100	-0.10902900
C	-2.58061200	-1.96303600	-1.78021800
C	-5.08619400	-2.48868500	-0.66031800
H	-4.62588300	-0.93275000	0.75236700
C	-3.39678200	-2.95182100	-2.32965000
H	-1.60440900	-1.76481600	-2.21601700
C	-4.64971900	-3.21700400	-1.76902100
H	-6.05844300	-2.69305700	-0.22063000
H	-3.05192900	-3.51813700	-3.19028600
H	-5.28208600	-3.99173000	-2.19365800

TS5 (1v)

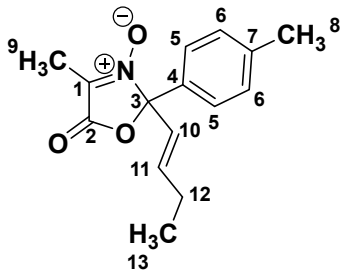
C	5.28996300	0.29970800	-0.32081900
O	4.60127500	-0.82658900	-0.50786300
C	3.27147800	-0.79156400	-1.07647100
C	2.41141700	0.27534500	-0.46652900
C	2.73803800	1.43301100	-0.09719700
O	4.84293700	1.43204100	-0.52285400
C	6.67809400	0.09413100	0.18114600
N	7.08047800	-1.13062500	0.19925400
O	8.37124000	-1.23229800	0.66587500
C	7.49171400	1.28282800	0.59596200
Au	0.30656500	0.19748800	-0.15879500
H	3.35528600	-0.60824100	-2.15324600
H	2.88062700	-1.79299100	-0.90967500
H	8.55401300	-2.19034200	0.61988700
H	8.41150500	1.34019100	0.00265900
H	6.92599200	2.20588000	0.46752700
H	7.79097900	1.18664200	1.64610300
P	-2.01476500	-0.03526000	0.06228900
C	-2.64642100	0.70126600	1.61649700
C	-2.04104600	1.87295800	2.10189500
C	-3.72051700	0.13437900	2.31965600
C	-2.51286100	2.47379200	3.26929100
H	-1.20215100	2.31280900	1.56767300
C	-4.18473600	0.73798000	3.49052500
H	-4.19427500	-0.77388300	1.96062200
C	-3.58395000	1.90608000	3.96541700
H	-2.03997200	3.37939200	3.63886700
H	-5.01531700	0.29184900	4.03024000
H	-3.94671800	2.37078600	4.87802900
C	-2.90347700	0.77070000	-1.32260600
C	-4.13454800	1.41880300	-1.14068000
C	-2.32850300	0.72192600	-2.60410800
C	-4.78112900	2.00699400	-2.23045300
H	-4.58945600	1.46963700	-0.15647600
C	-2.98211800	1.30568500	-3.68931300
H	-1.36984400	0.23006800	-2.75041300
C	-4.20822400	1.95076400	-3.50296300
H	-5.73226900	2.51042600	-2.08151200
H	-2.53062000	1.26395000	-4.67655900
H	-4.71292200	2.41244900	-4.34705200
C	-2.51675700	-1.79831200	0.06715300
C	-3.66451600	-2.24485000	-0.60466600
C	-1.72855300	-2.71836600	0.77994400
C	-4.01812500	-3.59589400	-0.56085000
H	-4.28170500	-1.54632100	-1.16077800
C	-2.09034800	-4.06468600	0.82465800
H	-0.83483400	-2.38260500	1.30047300
C	-3.23427800	-4.50525900	0.15228600
H	-4.90687200	-3.93459900	-1.08586800
H	-1.47601200	-4.76942600	1.37806600
H	-3.51106000	-5.55544000	0.18208600
H	2.73791800	2.43175800	0.29710100

TS5 (1v)

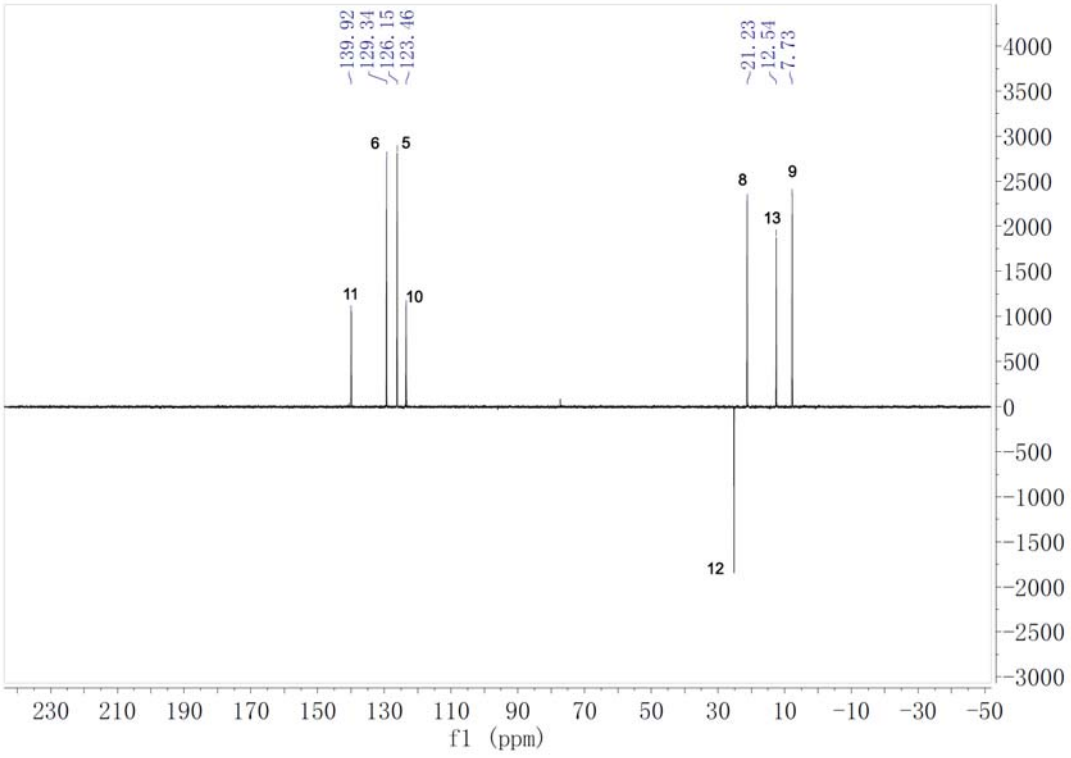
C	5.59024100	1.32822500	-0.10264000
C	6.14769800	-0.06737300	-0.08788000
N	5.29720200	-1.01308800	0.09669300
C	3.10993000	-0.50416400	0.41391100
C	3.59206200	0.65639300	1.16291100
O	4.33392700	1.58109800	0.34514400
O	6.23039700	2.24483000	-0.56644300
C	2.34100000	-1.33793800	-0.12929400
Au	0.35411300	-0.57157100	-0.00228800
P	-1.89610500	0.06309900	-0.01923000
O	5.81371900	-2.27561100	-0.02627100
C	7.60031100	-0.27066800	-0.38328800
H	2.72965900	1.22340200	1.52469200
H	4.18571900	0.34378800	2.02681900
H	5.06546700	-2.86373500	0.20129400
H	8.01570400	-1.03549300	0.27990200
H	7.72968900	-0.62157000	-1.41501700
H	8.14775500	0.66469400	-0.26459100
C	-2.16571000	1.67588000	-0.84577700
C	-3.31987600	1.93630700	-1.60109600
C	-1.19267100	2.67873000	-0.69909100
C	-3.49678700	3.18746400	-2.19626800
H	-4.07787000	1.16987400	-1.72922700
C	-1.37718100	3.92762100	-1.29274500
H	-0.29040200	2.48020000	-0.12607600
C	-2.52907600	4.18294500	-2.04210700
H	-4.39152700	3.38168300	-2.78106200
H	-0.61862200	4.69667600	-1.17669600
H	-2.66842400	5.15336800	-2.51036600
C	-2.59218500	0.19861000	1.67074200
C	-3.57847400	1.14349500	1.99378800
C	-2.13079200	-0.68665000	2.65984700
C	-4.09857600	1.19463600	3.28914000
H	-3.94076900	1.83906300	1.24337000
C	-2.65804400	-0.63390400	3.95035300
H	-1.36008400	-1.41507700	2.41967600
C	-3.64143600	0.30772400	4.26658400
H	-4.86059600	1.92978700	3.53220200
H	-2.29583700	-1.32238600	4.70867000
H	-4.04691800	0.35266800	5.27351800
C	-2.90716500	-1.17203800	-0.92102900
C	-4.18313800	-1.55451500	-0.48126300
C	-2.37919400	-1.73942300	-2.09385500
C	-4.92075400	-2.49158300	-1.20947600
H	-4.60290500	-1.12842600	0.42443300
C	-3.12313800	-2.66946700	-2.81956900
H	-1.38775500	-1.45438900	-2.43742100
C	-4.39393000	-3.04839800	-2.37671700
H	-5.90698100	-2.78562200	-0.86133700

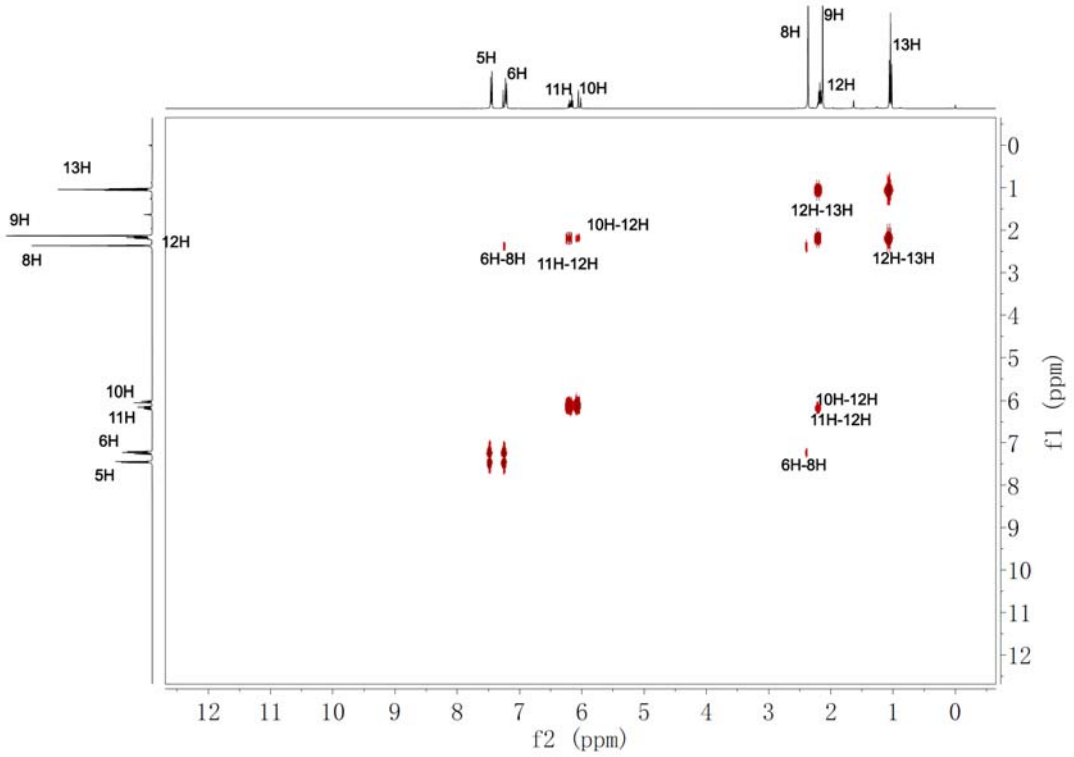
H	-2.70731700	-3.10295700	-3.72484900
H	-4.96919600	-3.77932700	-2.93816900
H	2.45444300	-2.28101000	-0.64789800

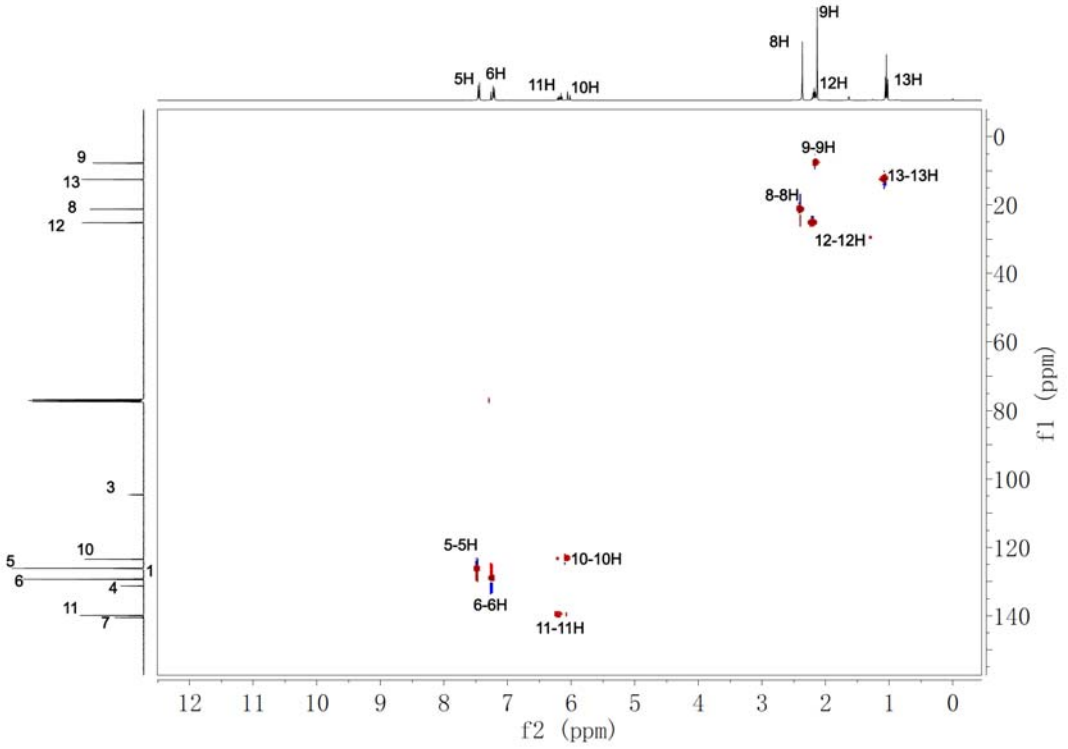
5. ^{1}H NMR and ^{13}C NMR Spectra

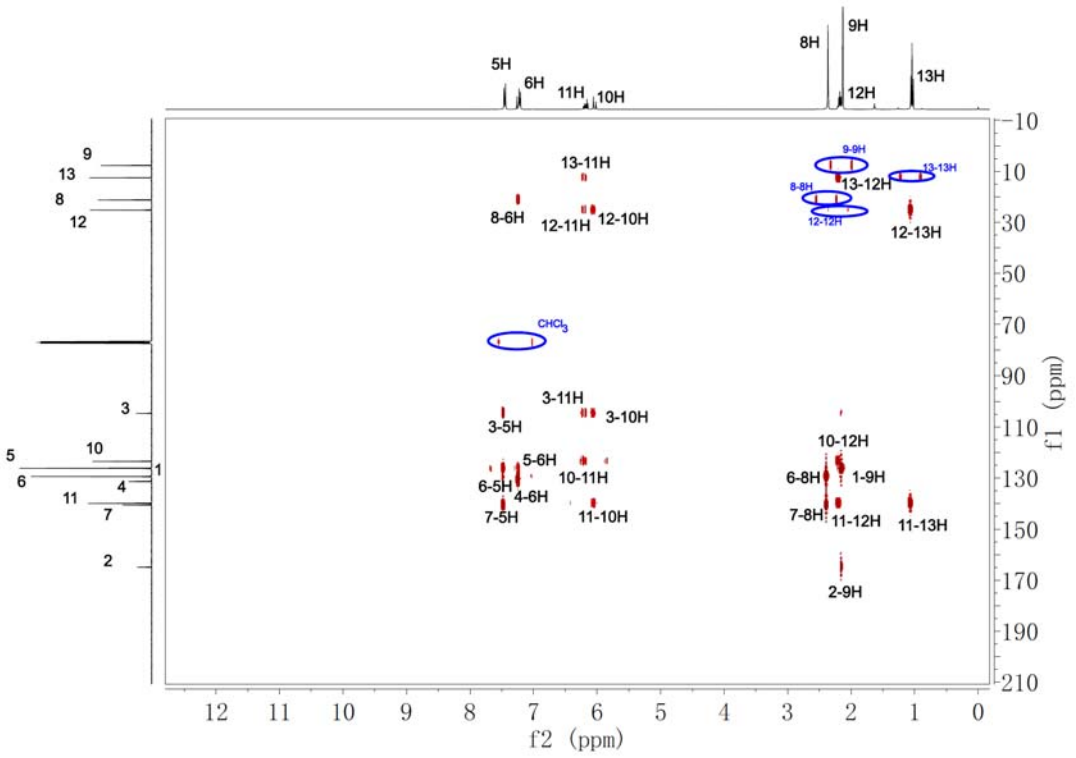


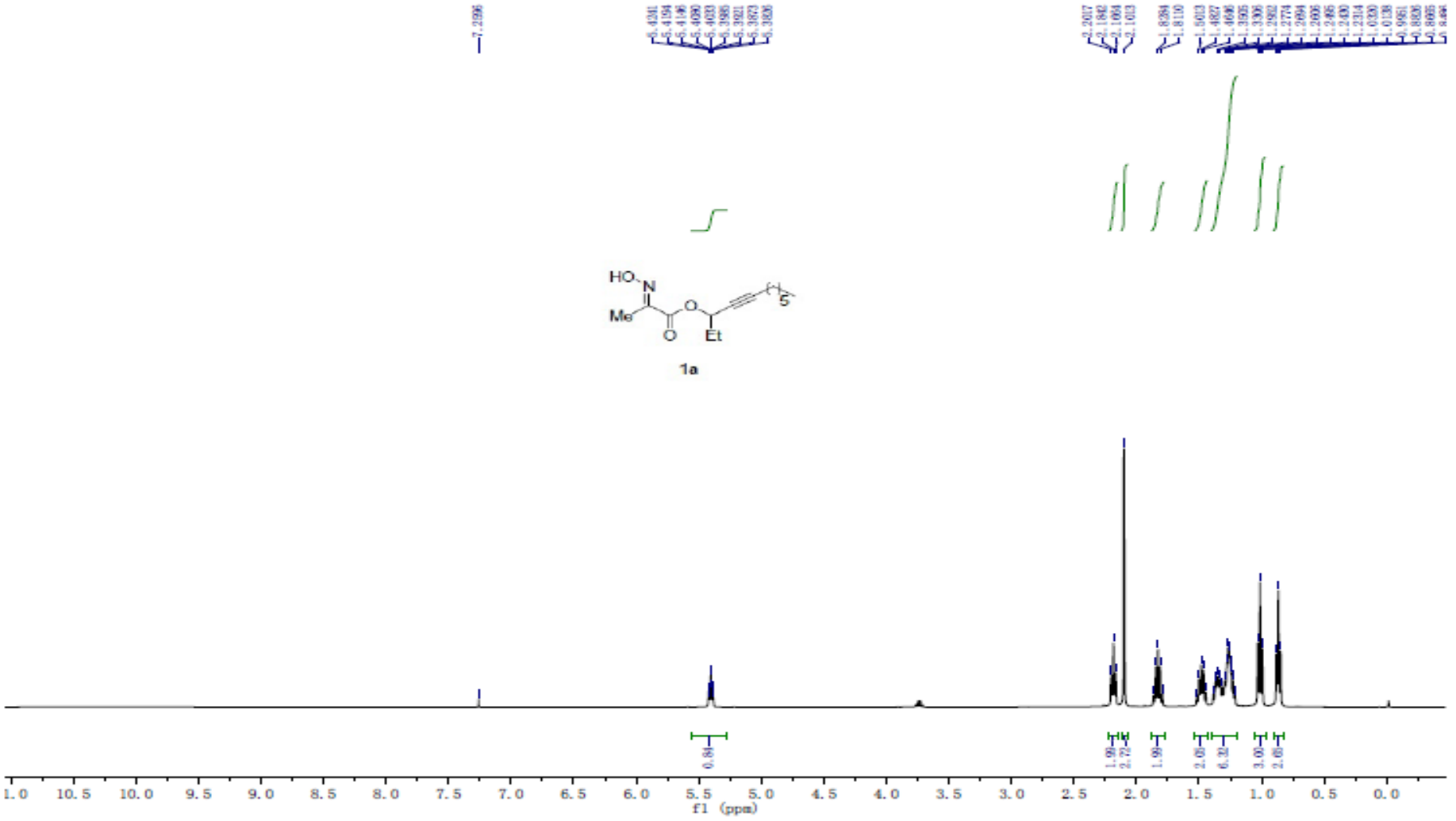
2k

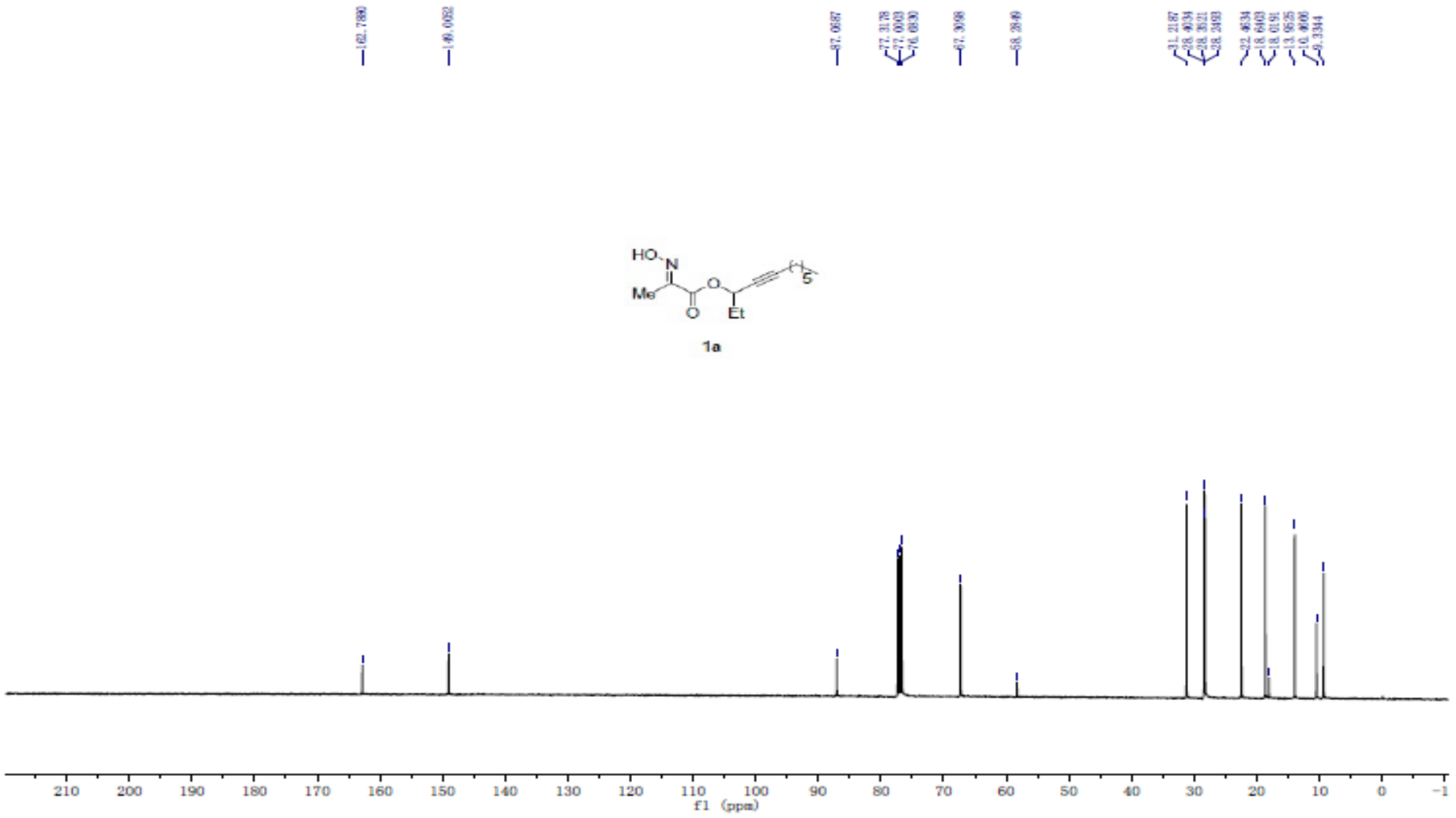



8H
9H
13H
5H
6H
11H
10H
12H
13H
9H
8H
12H
10H
11H
6H
5H
10H-12H
6H-8H
11H-12H
12H-13H
12H-13H
10H-12H
11H-12H
6H-8H
f2 (ppm)
f1 (ppm)


9H
8H
5H
6H
11H
10H
12H
13H
9
13
8
12
3
10
5
1
6
4
11
7
9-9H
13-13H
8-8H
12-12H
5-5H
10-10H
6-6H
11-11H
0
20
40
60
80
100
120
140
f1 (ppm)
12
11
10
9
8
7
6
5
4
3
2
1
0
f2 (ppm)


5H
6H
11H
10H
8H
9H
12H
13H
13-11H
8-6H
12-11H
12-10H
9-9H
13-13H
13-12H
8-8H
12-12H
12-13H
CHCl3
3-11H
3-5H
3-10H
10-12H
5-6H
10-11H
6-8H
1-9H
6-5H
4-6H
7-8H
11-12H
11-13H
7-5H
11-10H
2-9H
9
13
8
12
3
10
5
1
6
4
11
7
2
f1 (ppm)
f2 (ppm)


HO
N
Me
O
O
Et
5
1a
f1 (ppm)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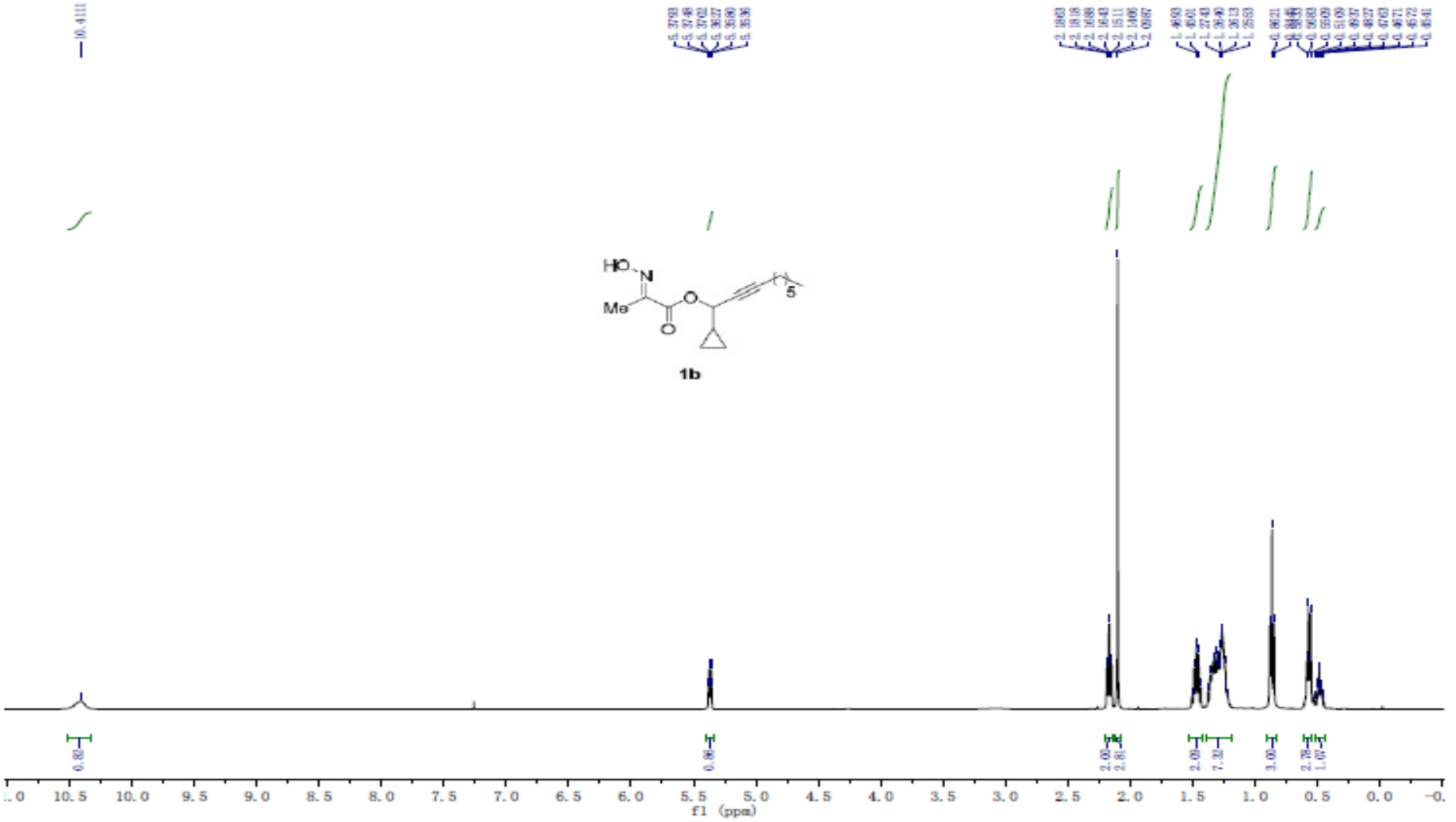
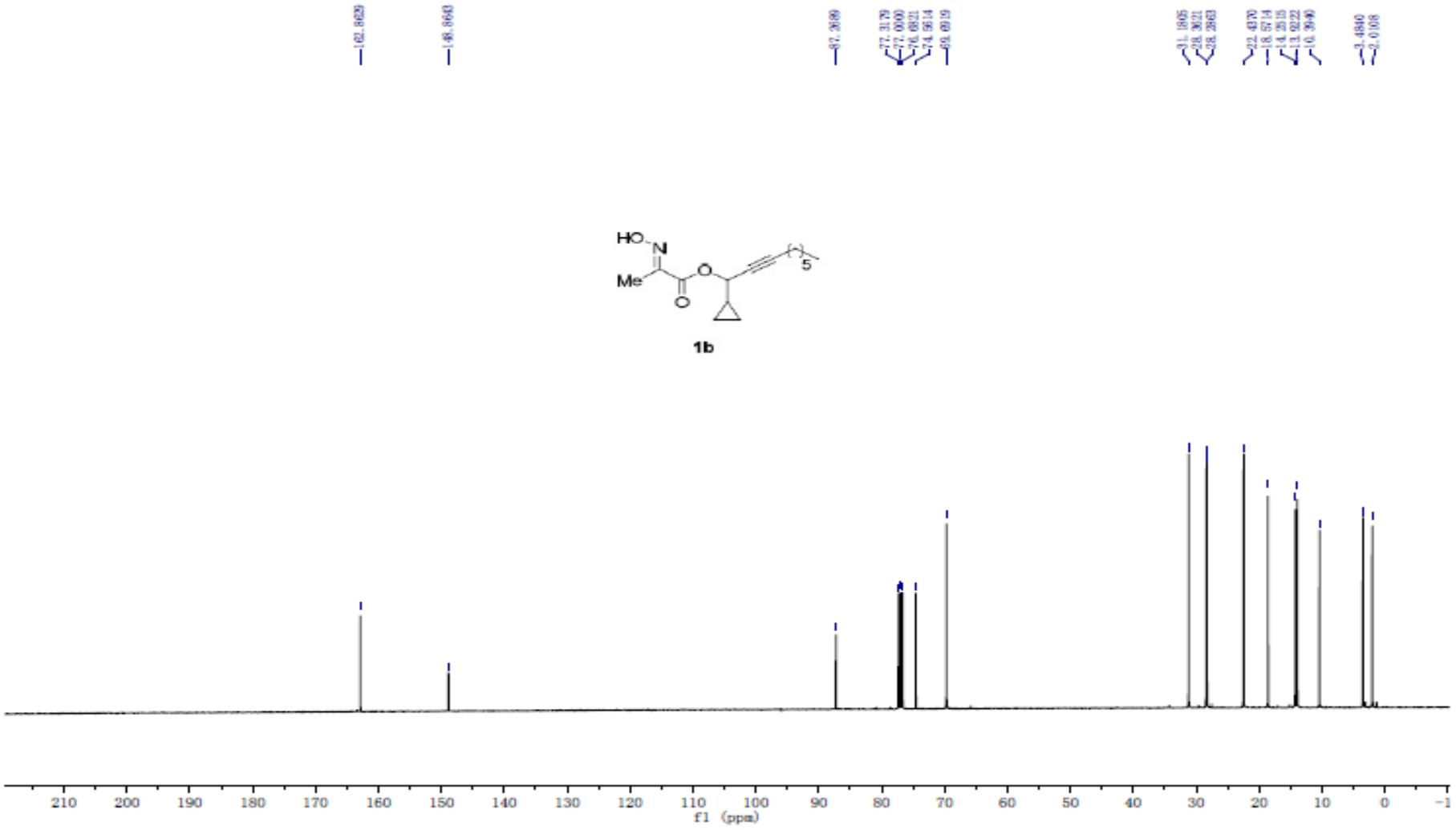
87.0687
77.3178
77.0063
76.6830
67.3098
58.3849
31.2187
28.4034
28.3521
28.3493
22.4634
18.6403
18.0191
13.9535
10.4806
9.3344
HO
N
Me
O
O
Et
5
1a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)


HO
N
Me
O
O
5
1b
f1 (ppm)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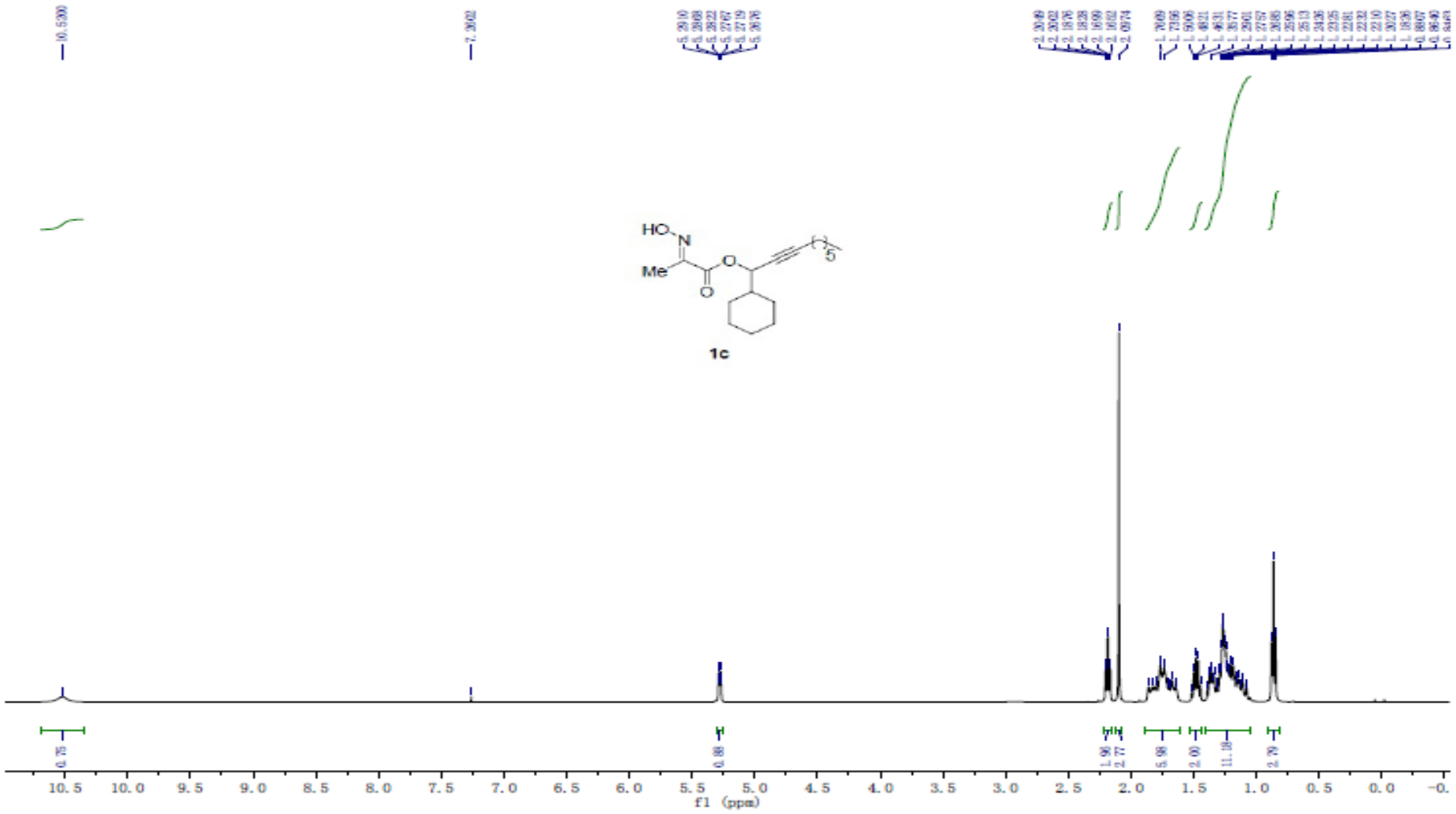
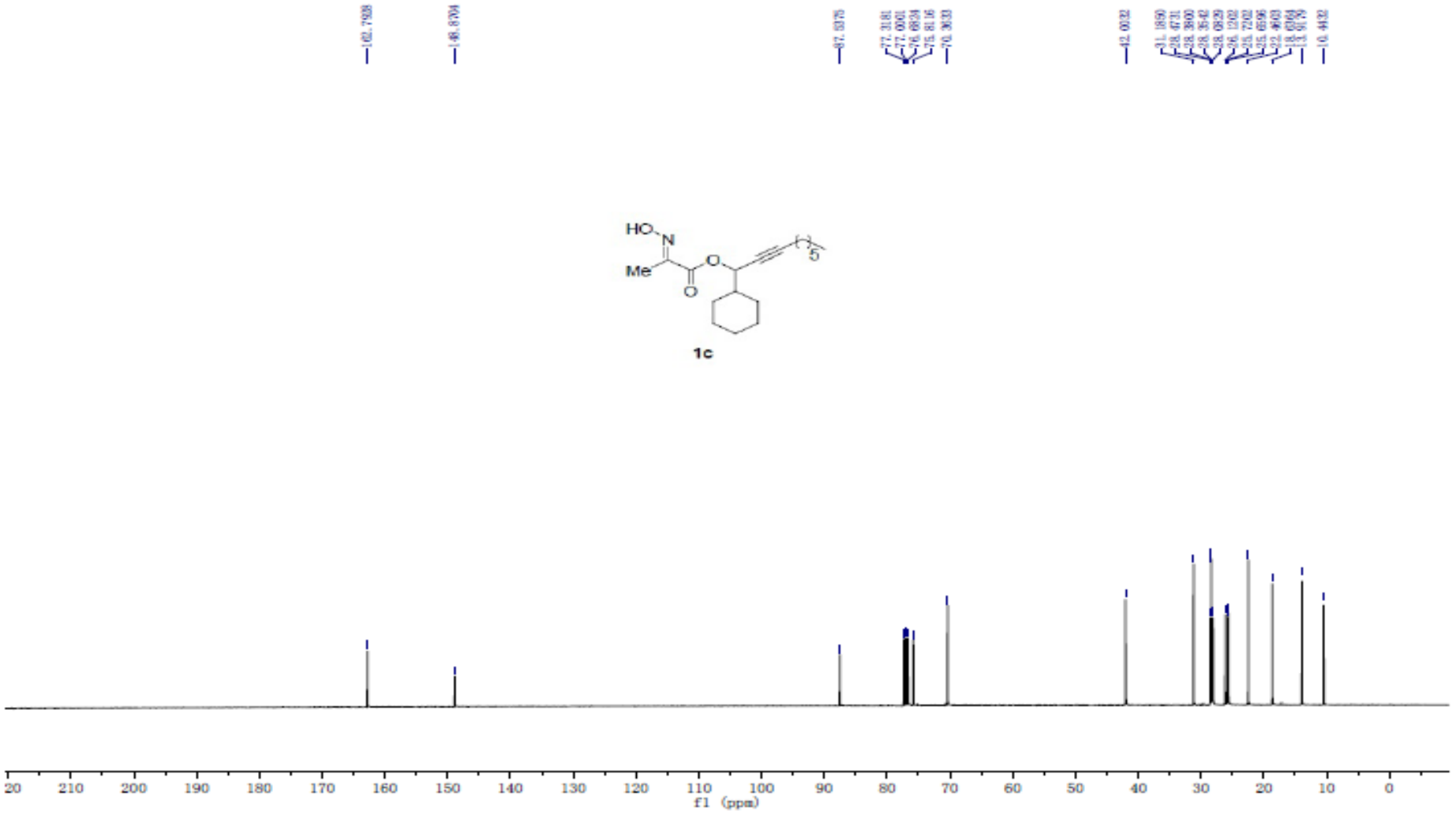
97.3689
77.3179
77.0000
76.6821
74.9614
69.6919
31.1805
28.3021
28.2863
22.4370
18.5714
14.2515
13.9222
10.3949
3.4840
2.0108
HO
N
Me
O
O
5
1b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


HO
N
Me
O
O
5
1c
f1 (ppm)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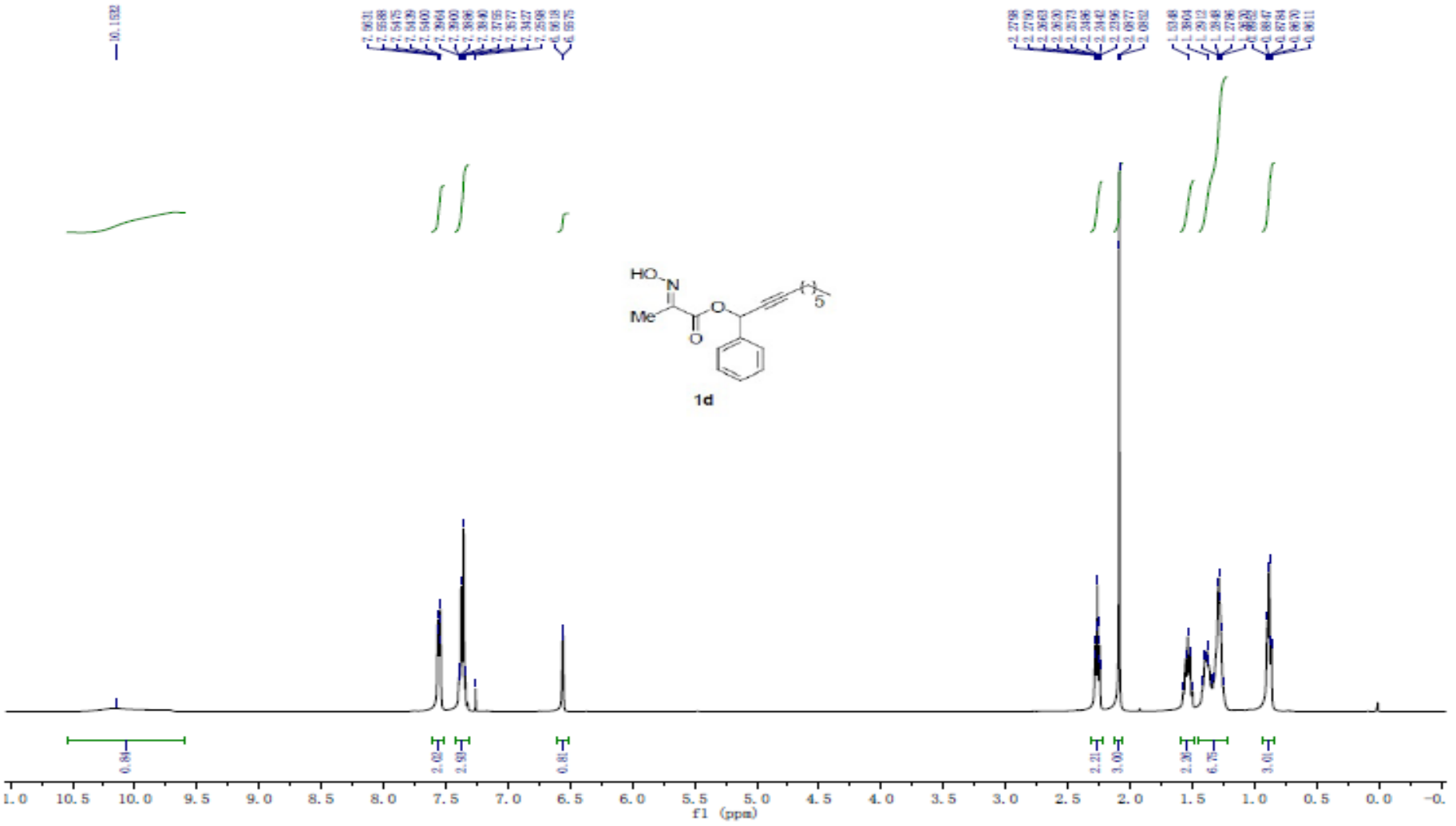
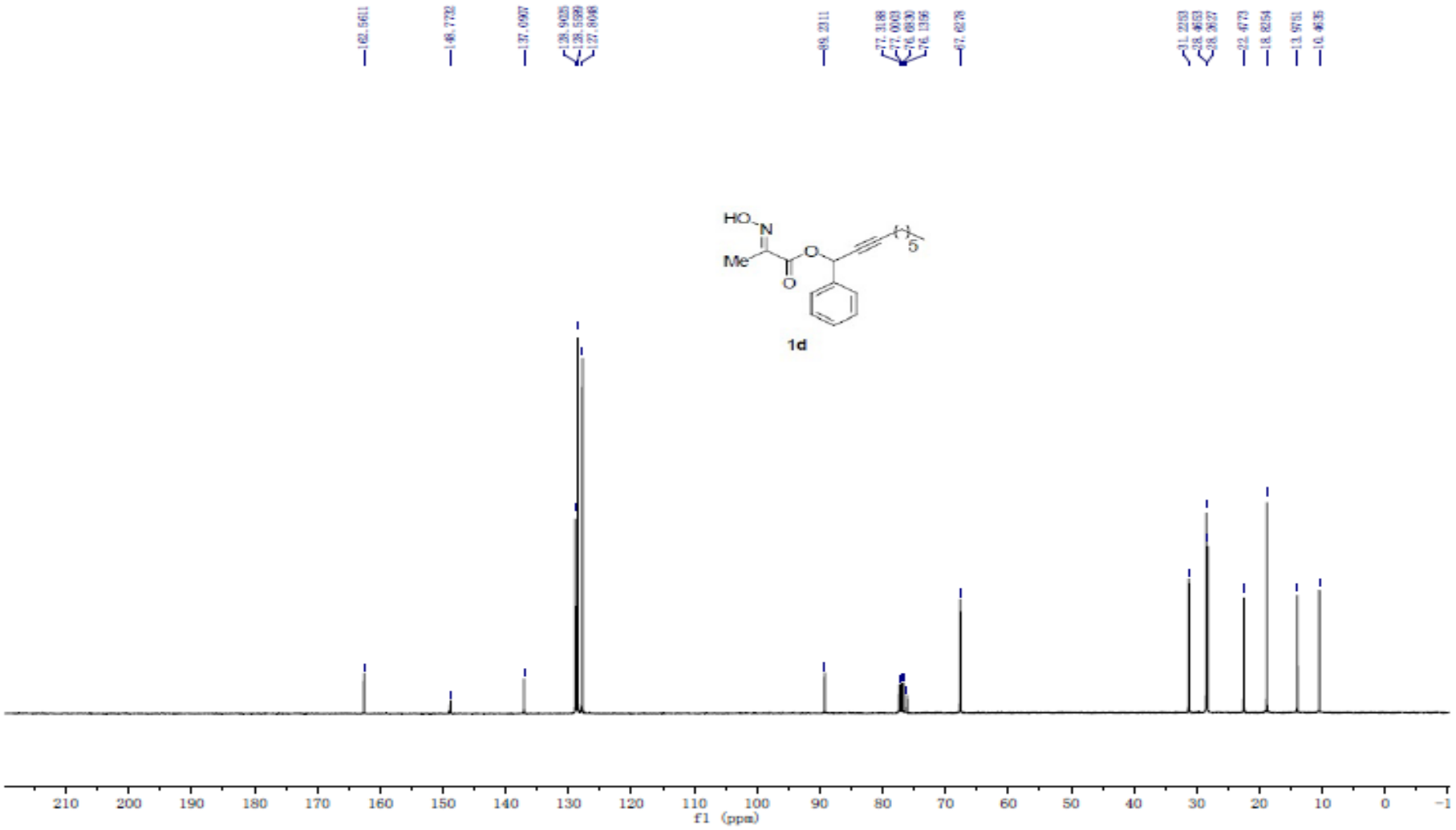
87.5375
77.3181
77.0001
76.6824
75.8116
70.3633
42.0032
31.1899
28.4731
28.3900
28.3542
28.0829
26.1202
25.7202
25.6596
22.9403
18.6264
13.9179
10.4432
HO
N
Me
O
O
5
1c
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


HO
N
Me
O
O
5
1d
f1 (ppm)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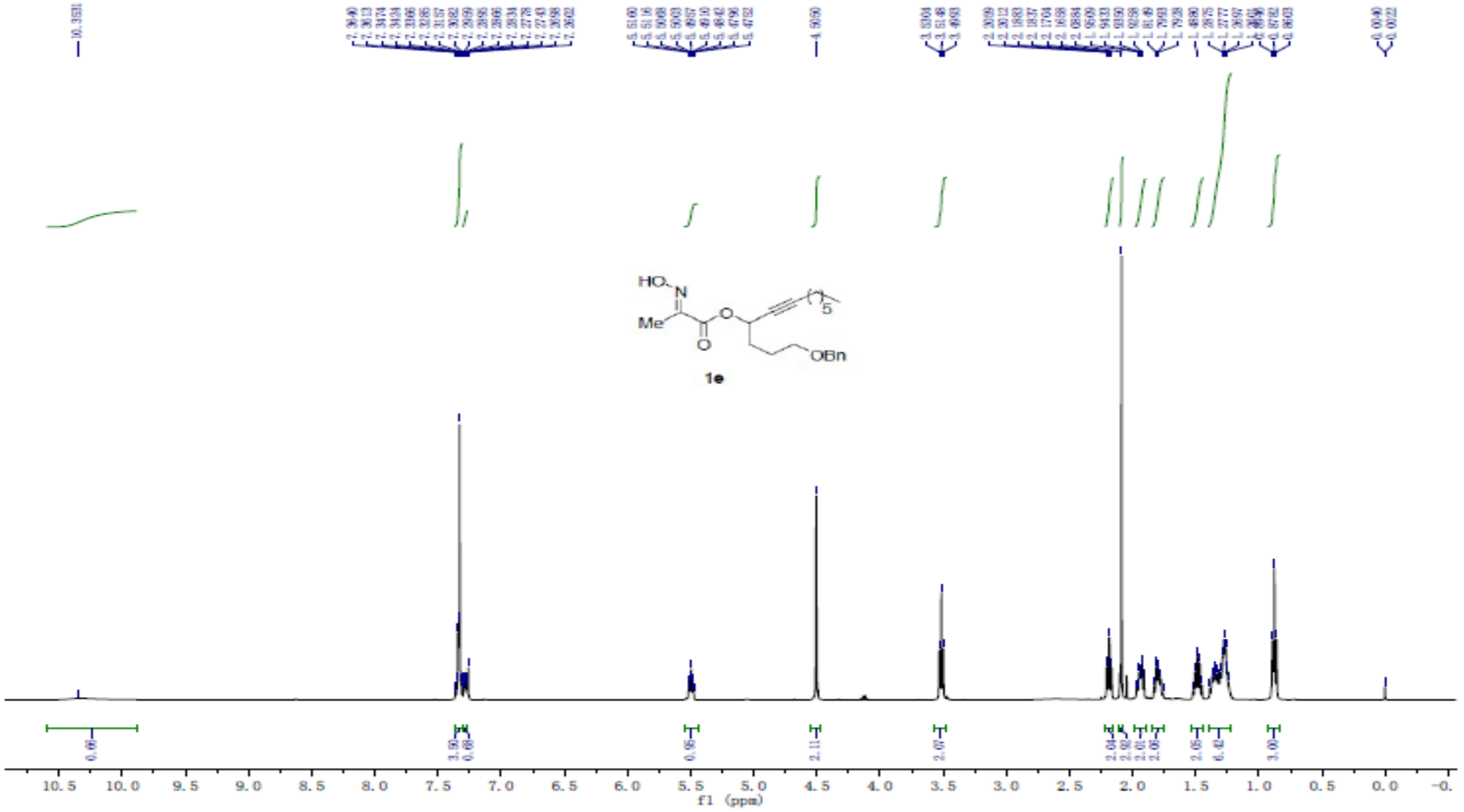
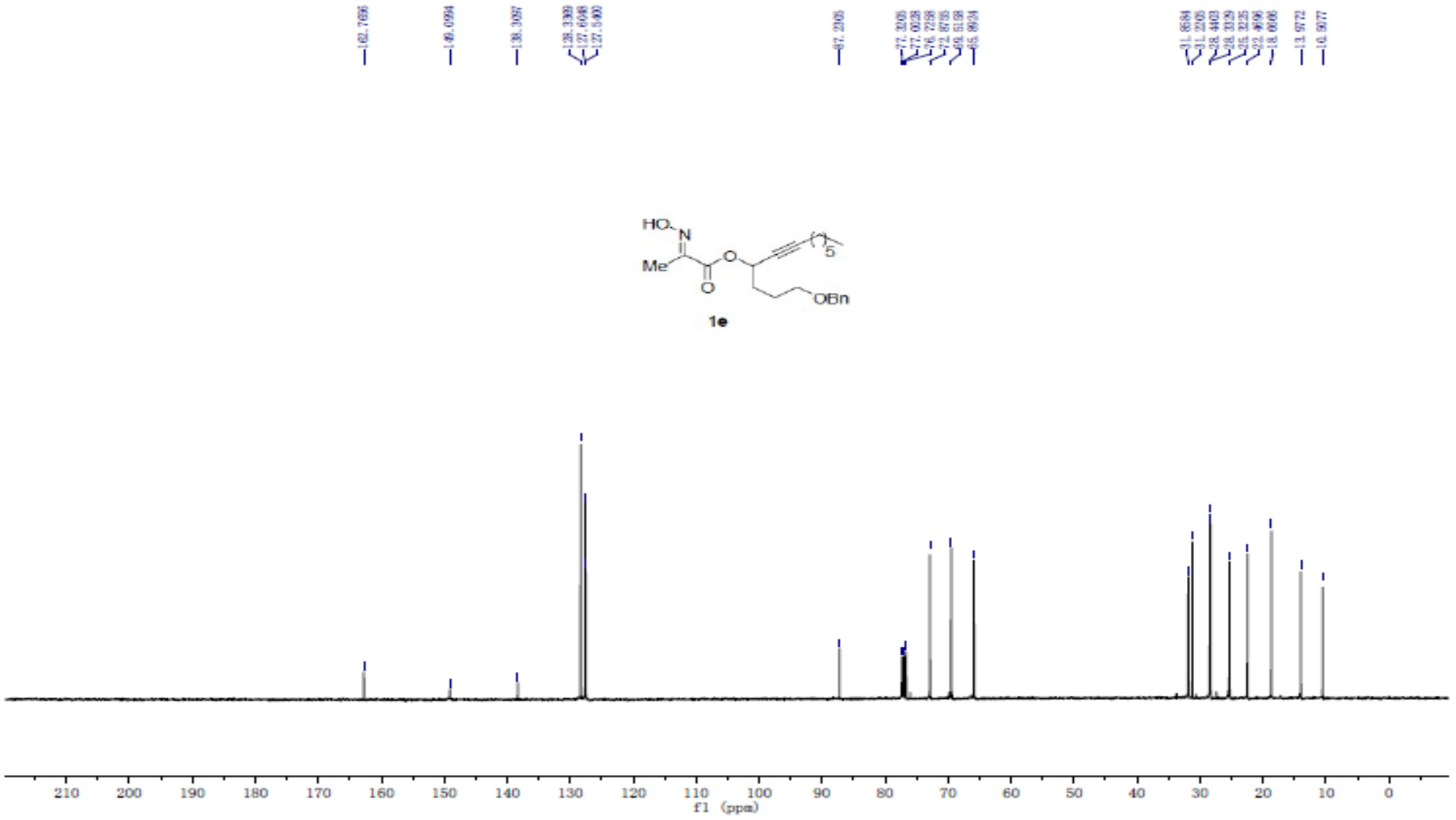
137.0907
128.9035
128.5599
127.8048
89.2311
77.3188
77.0003
76.6830
76.1356
67.6278
31.2253
28.4653
28.3622
22.4773
18.8254
13.9751
10.4635
HO
N
Me
O
O
5
1d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)


HO
N
Me
O
O
5
OBn
1e
f1 (ppm)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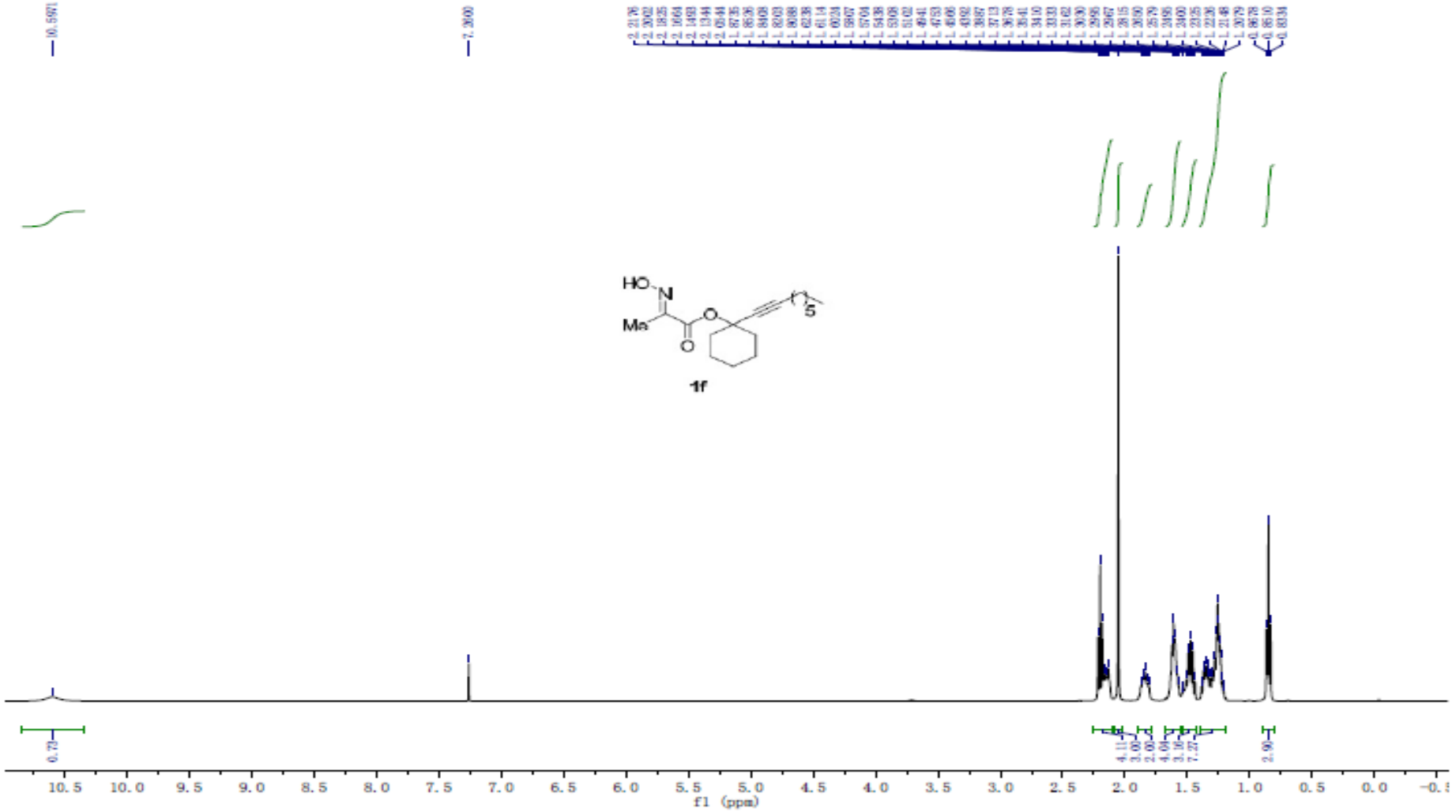
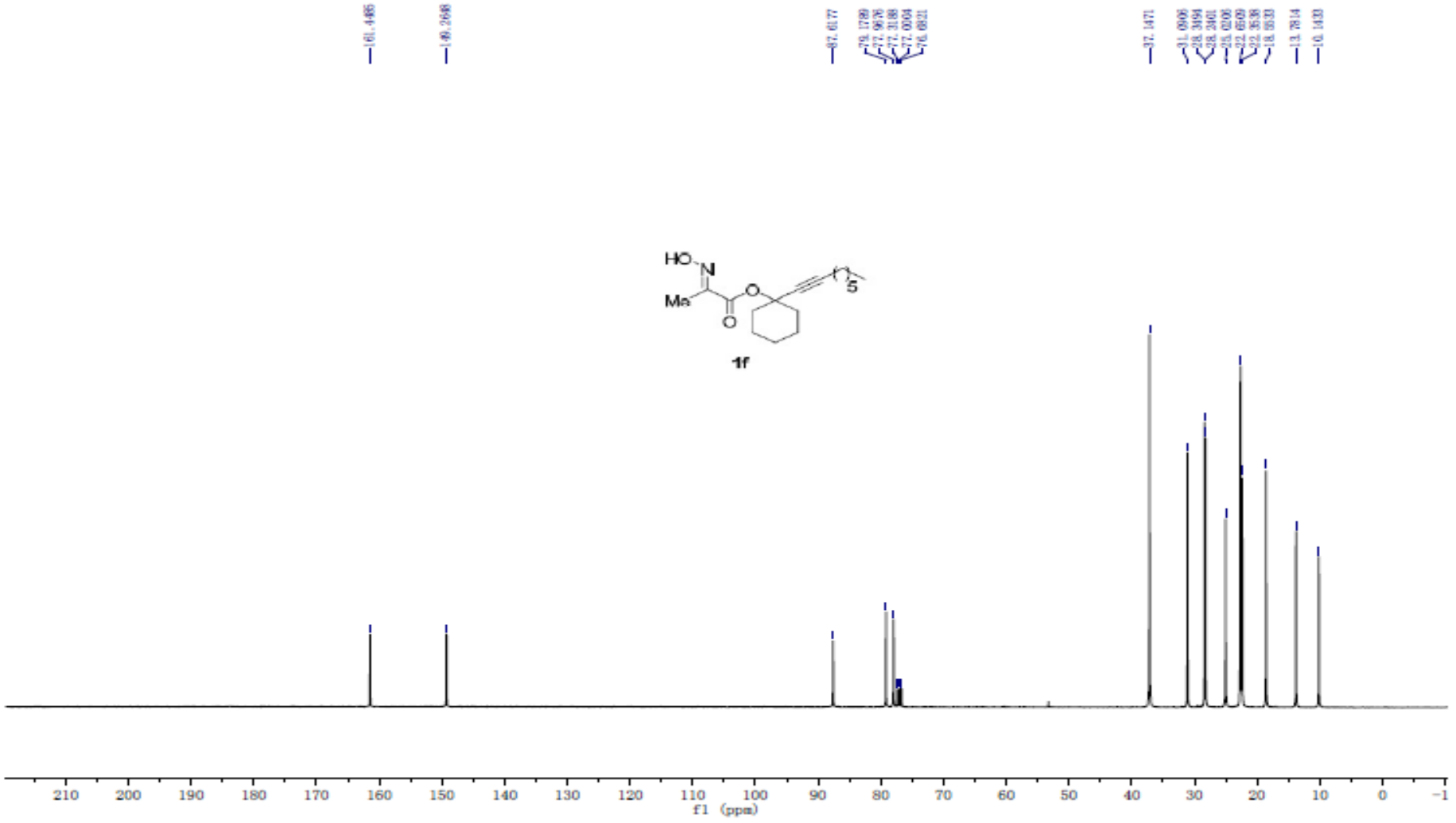
128.3393
127.6048
127.5900
97.2305
77.3205
77.0028
76.7238
72.8735
69.5138
65.8924
31.6584
31.2205
28.4483
28.3329
25.3225
22.4990
18.6666
13.9772
10.9077
HO
N
Me
O
O
5
OBn
1e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.5971
7.3000
HO
N
Me
O
O
5
1f
0.73
4.11
3.03
2.00
4.05
3.16
7.27
2.90
10.5
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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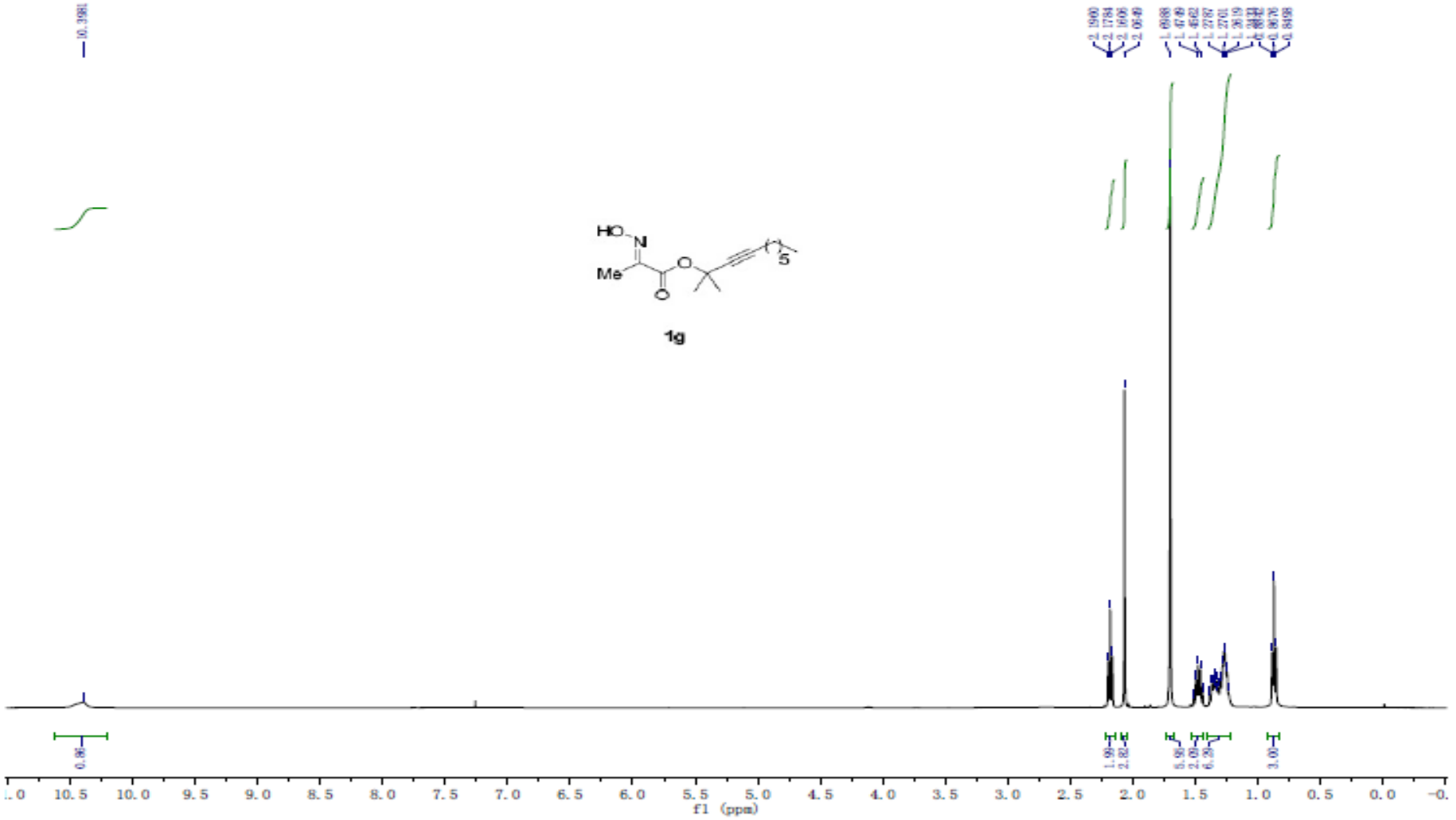
97.6177
79.1799
77.9978
77.3188
77.0004
76.6821
37.1471
31.0906
28.3994
28.2901
25.6206
22.8569
22.3538
18.5533
13.7814
10.1433
HO
N
Me
O
O
5
1f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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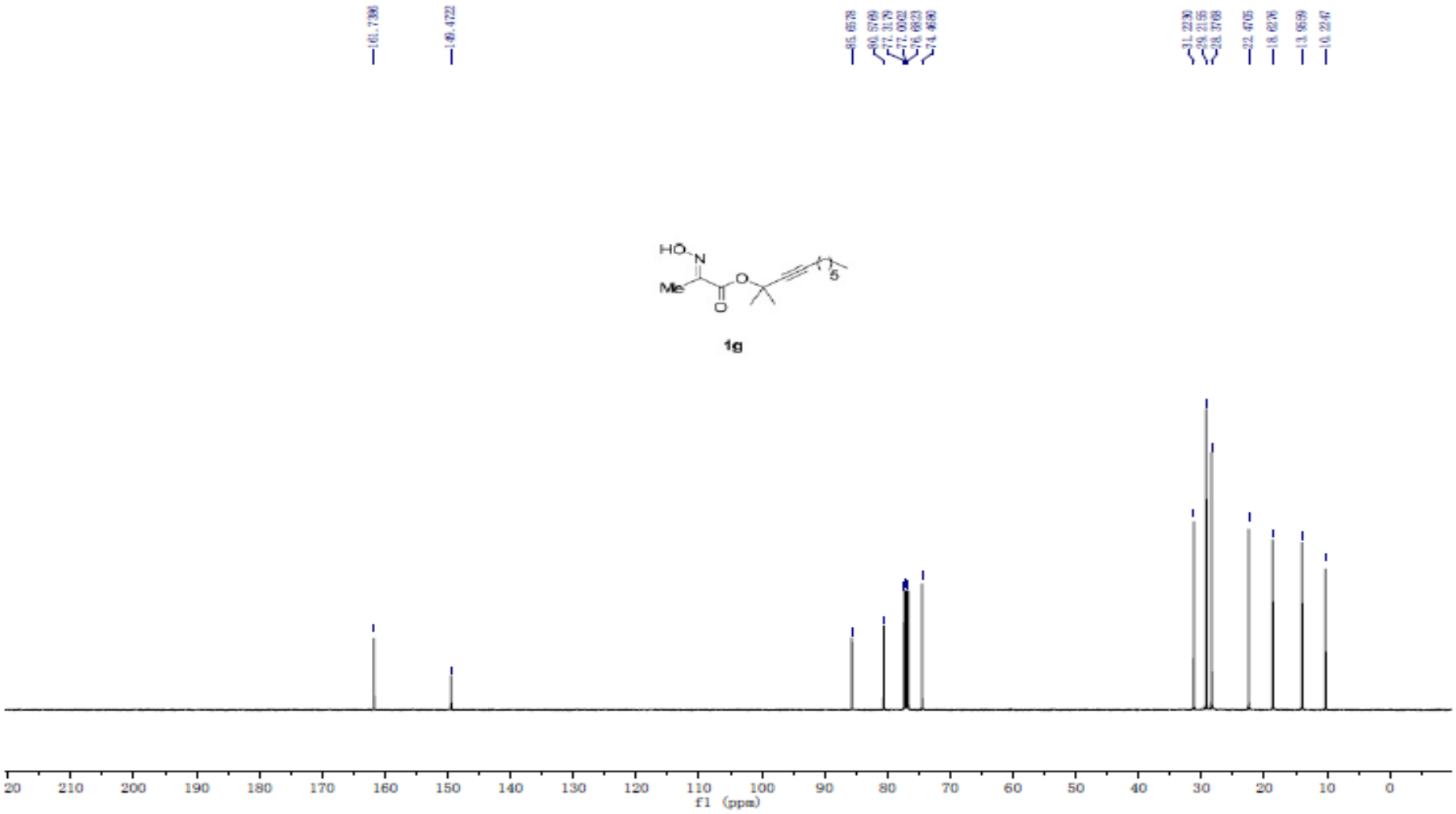
2.1900
2.1784
2.1609
2.0549
1.6988
1.4749
1.4562
1.2787
1.2701
1.2619
HO
N
Me
O
O
S
1g
0.86
1.90
2.82
5.90
2.08
6.20
3.00
f1 (ppm)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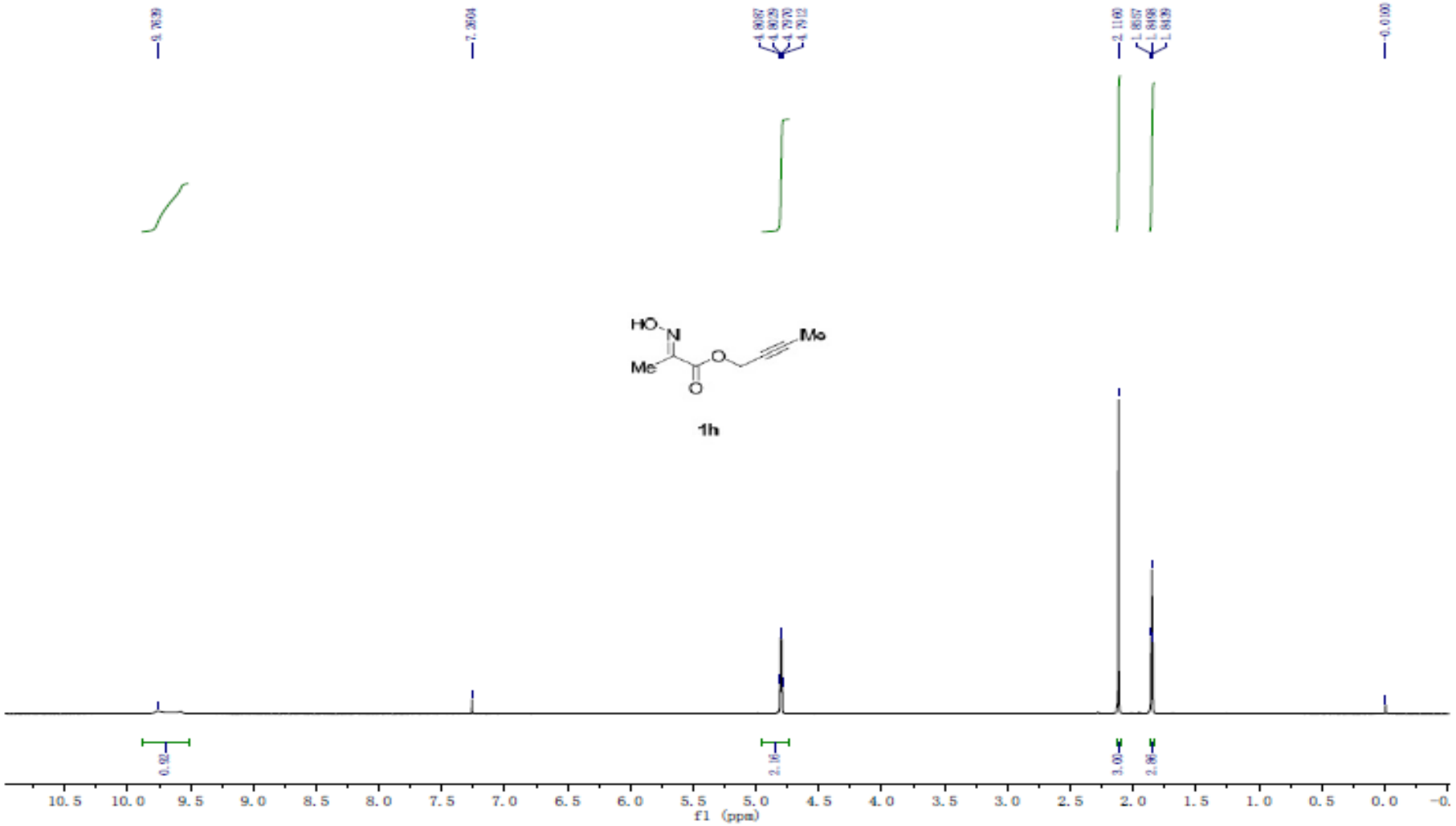
80.5749
77.3179
77.0002
76.6823
74.4680
31.2230
29.2155
28.3768
22.4705
18.6276
13.9659
10.2247
HO
N
Me
O
O
5
1g
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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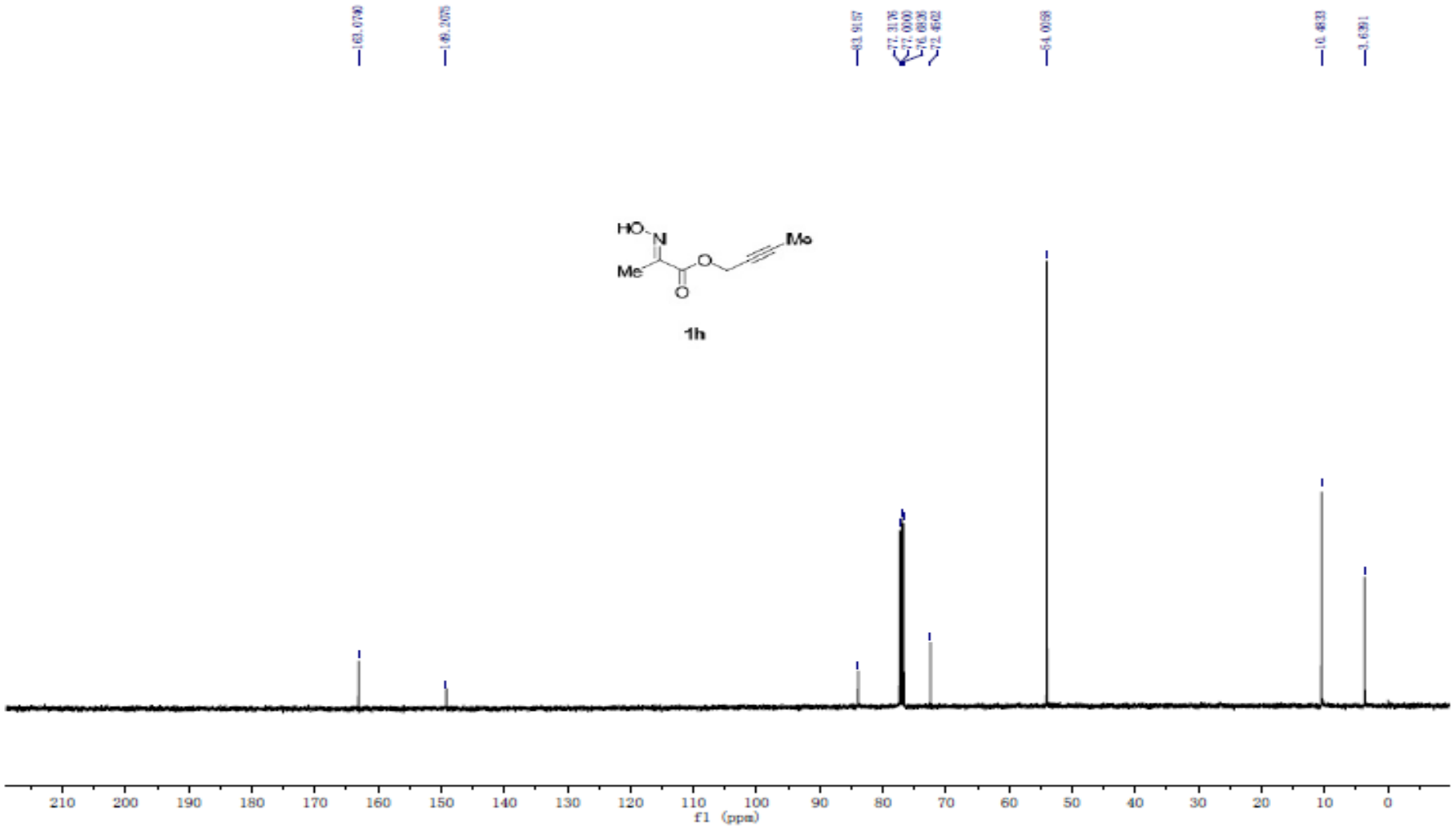
4.8029
4.7970
4.7912
2.1160
1.8557
1.8498
1.8439
0.0000
HO
N
Me
O
O
Me
1h
0.92
2.16
3.00
2.86
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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83.9157
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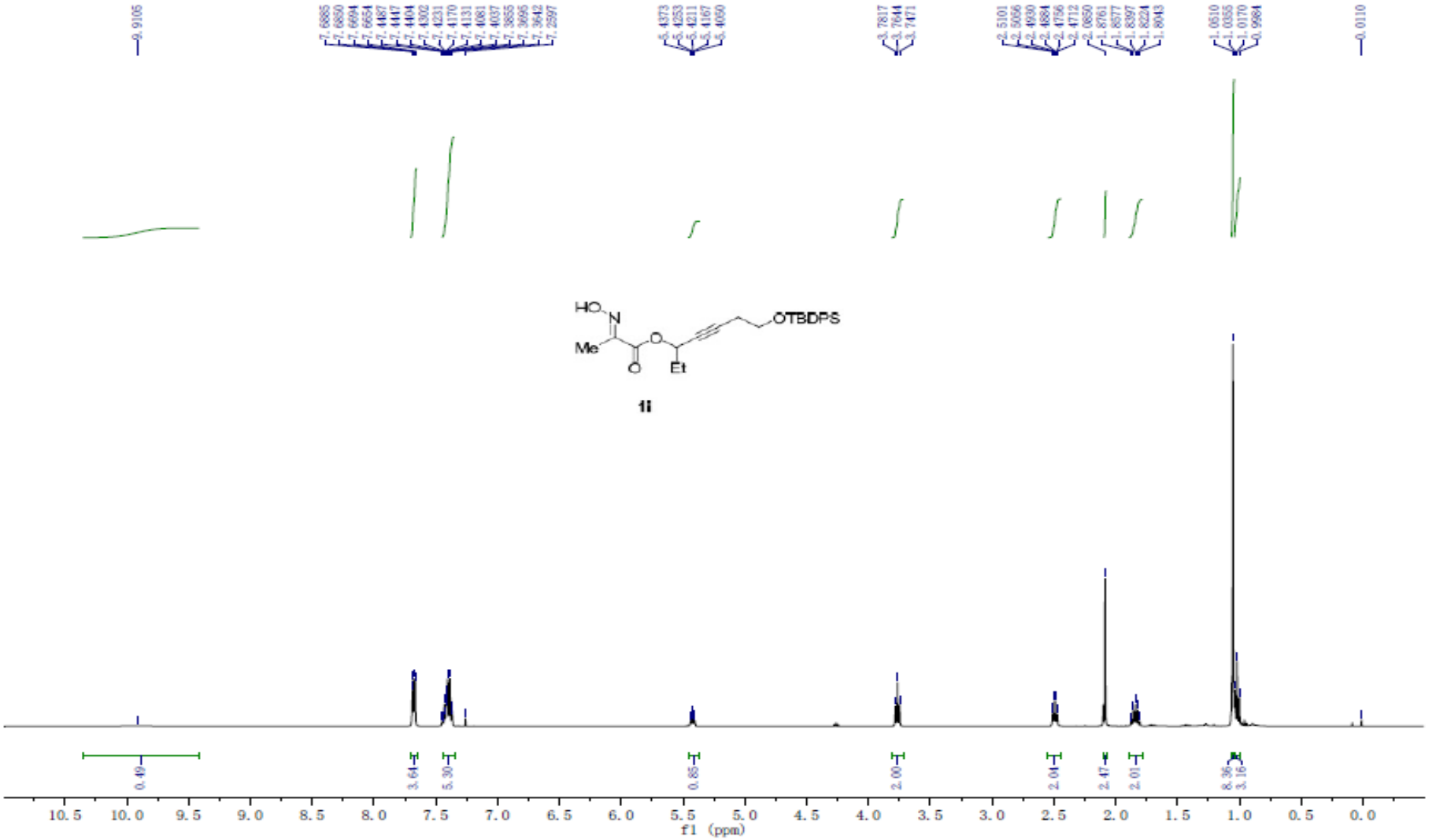
54.0058
10.4633
3.6391
HO
N
Me
O
O
Me
1h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6850
7.6694
7.6654
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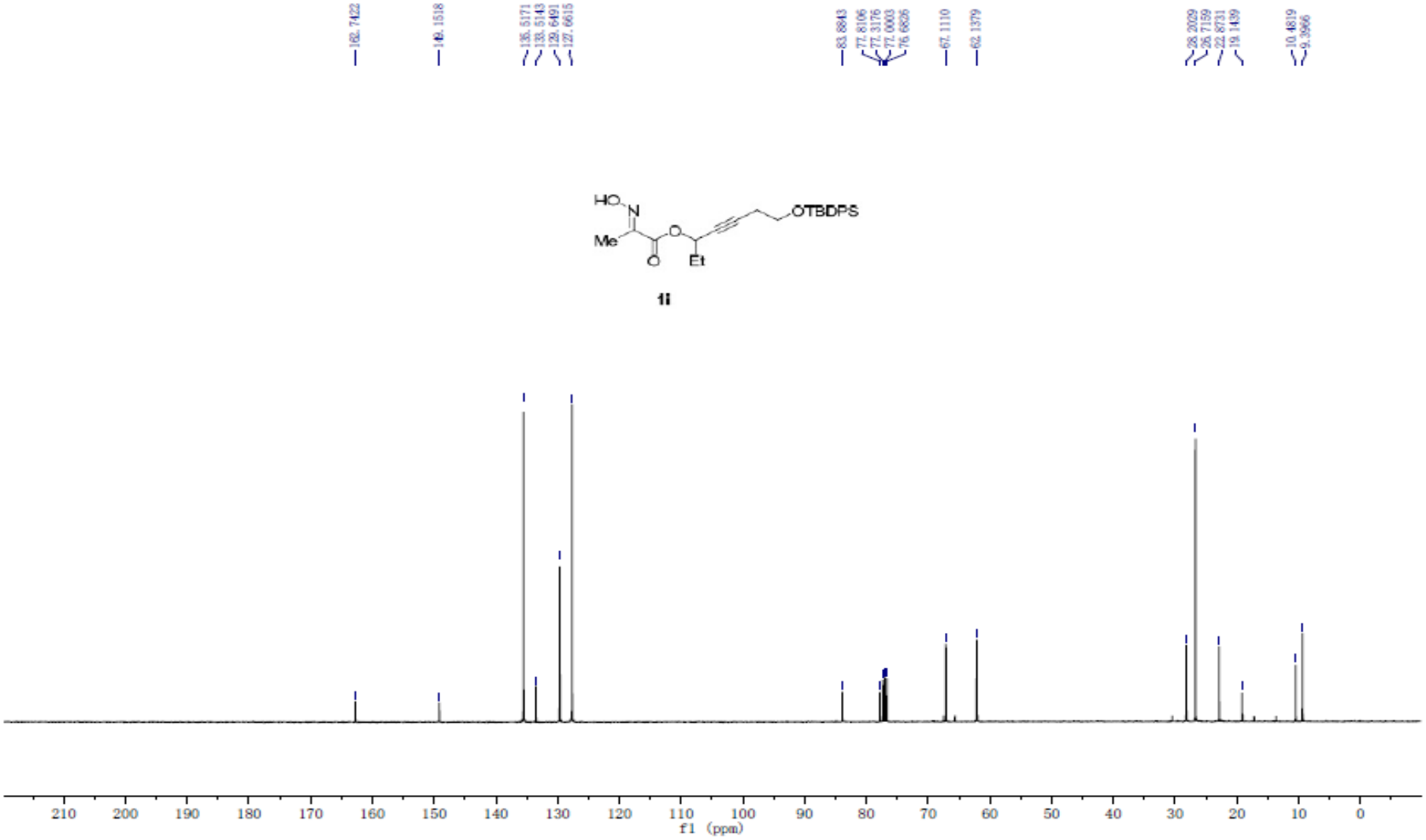
7.4447
7.4404
7.4302
7.4231
7.4170
7.4131
7.4081
7.4037
7.3655
7.3595
7.3642
7.2597
5.4373
5.4253
5.4211
5.4167
5.4050
3.7817
3.7644
3.7471
2.5101
2.5056
2.4930
2.4884
2.4756
2.4712
2.0650
1.8761
1.8577
1.8397
1.8224
1.6943
1.0510
1.0355
1.0170
0.9984
0.0110
HO
N
Me
O
O
Et
OTBDPS
1i
0.49
3.64
5.30
0.85
2.00
2.04
2.47
2.01
8.36
3.16
10.5
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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133.5143
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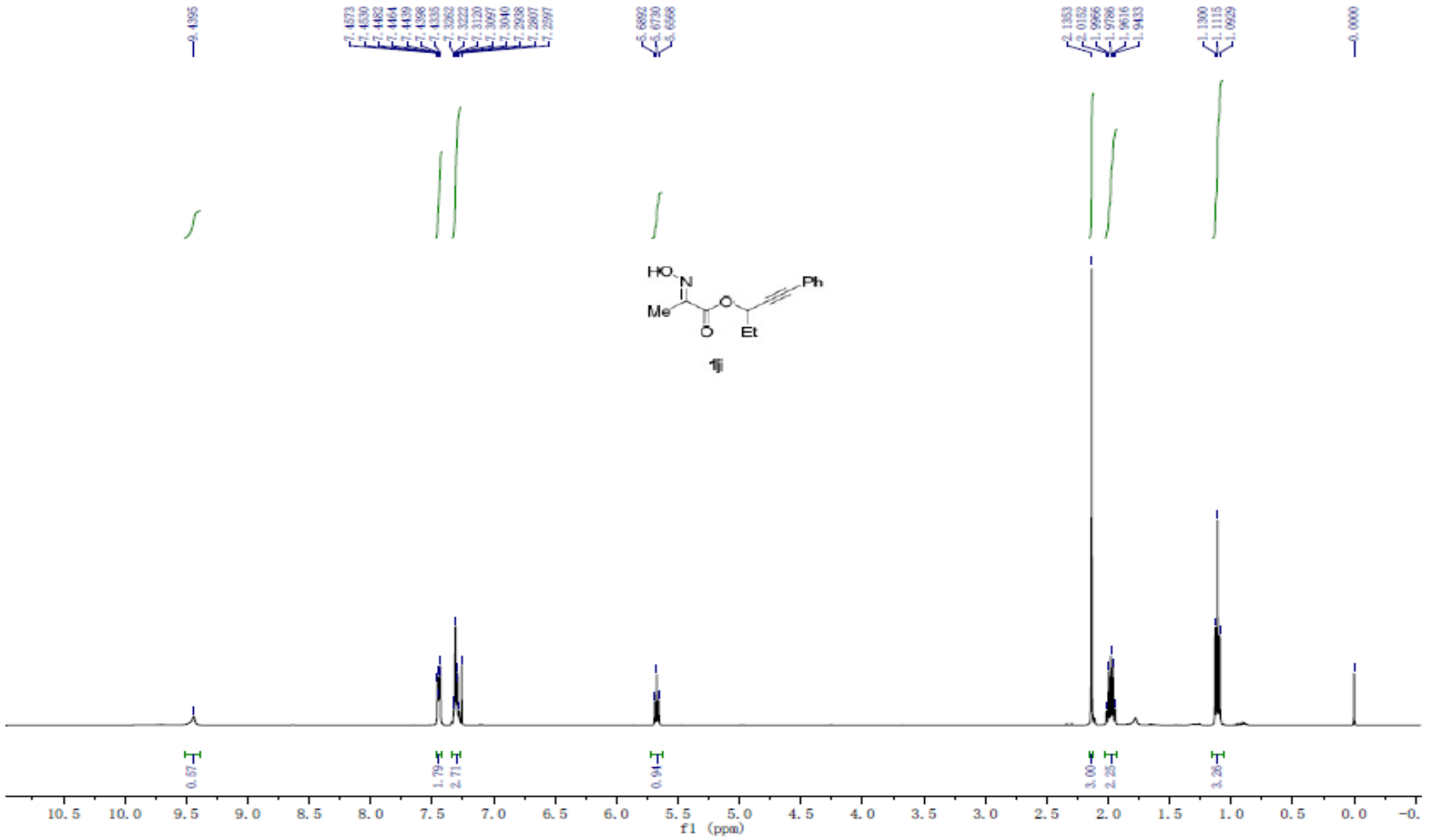
83.8843
77.8106
77.3176
77.0003
76.6826
67.1110
62.1379
28.2029
26.7159
22.8731
19.1439
10.4819
9.3966
HO
N
Me
O
O
Et
OTBDPS
1i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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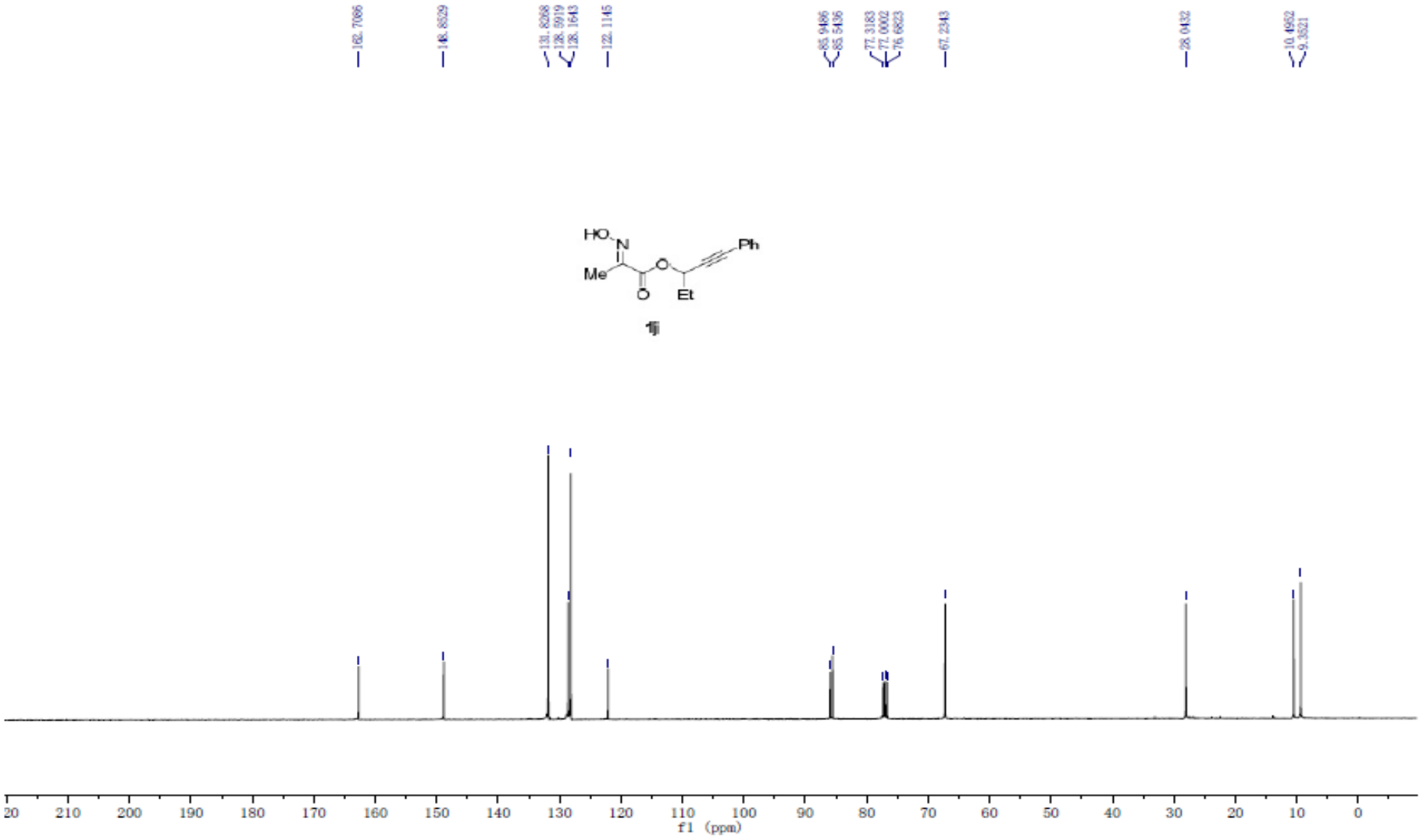
7.4530
7.4482
7.4464
7.4439
7.4398
7.4335
7.3262
7.3222
7.3120
7.3097
7.3040
7.2938
7.2807
7.2597
5.6892
5.6730
5.6568
2.1353
2.0152
1.9966
1.9786
1.9616
1.9433
1.1300
1.1115
1.0929
0.0000
HO
N
Me
O
O
Et
Ph
1j
0.57
1.79
2.71
0.94
3.00
2.25
3.26
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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131.8268
128.5919
128.1643
122.1145
85.9486
85.5436
77.3183
77.0002
76.6823
67.2343
26.0432
10.4952
9.3521
HO
N
Me
O
O
Et
Ph
1fj
20
210
200
190
180
170
160
150
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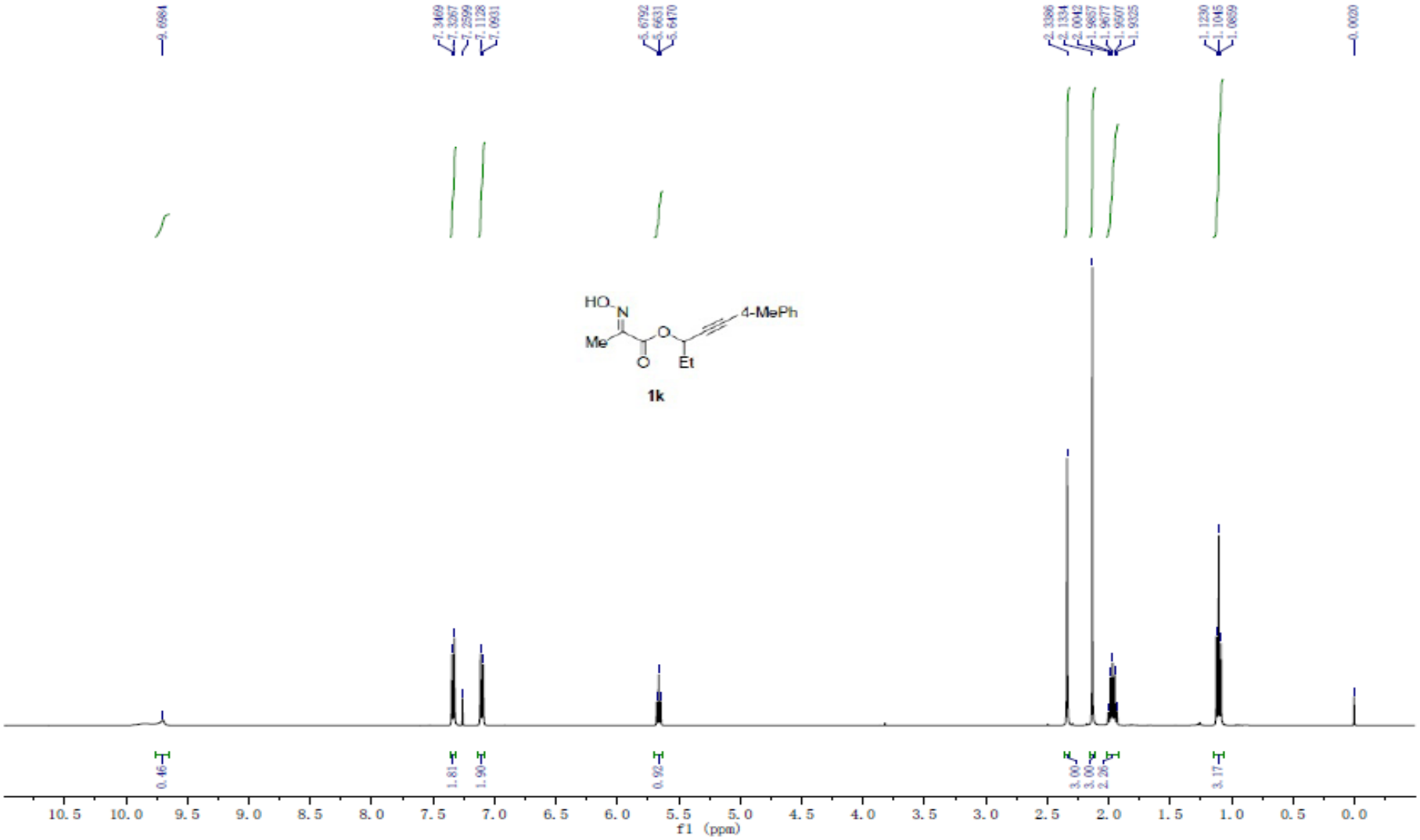
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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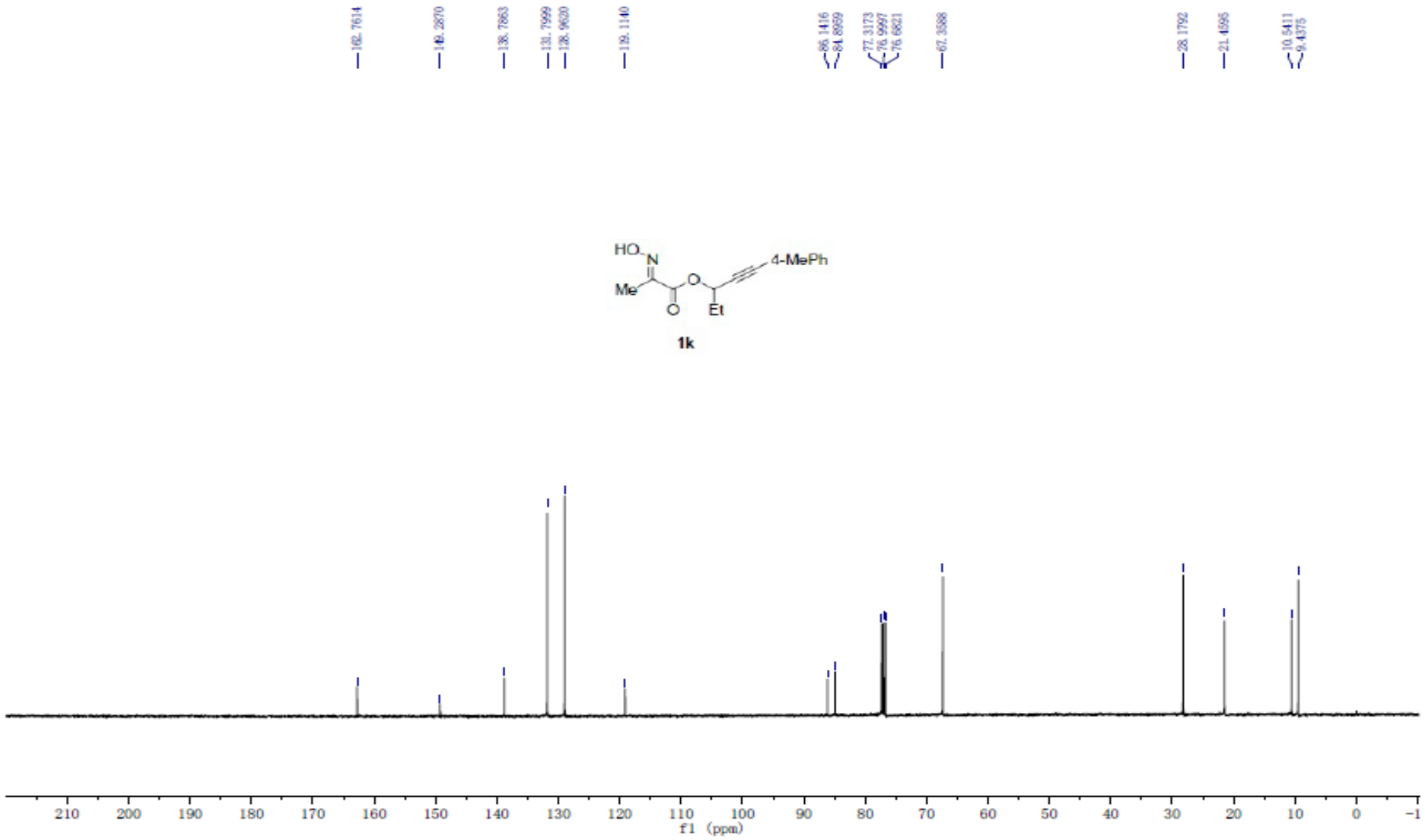
7.3267
7.2599
7.1128
7.0931
5.6792
5.6631
5.6470
2.3386
2.1334
2.0042
1.9857
1.9677
1.9507
1.9325
1.1230
1.1045
1.0859
0.0020
HO
N
Me
O
O
Et
4-MePh
1k
0.46
1.81
1.90
0.92
3.00
3.00
2.28
3.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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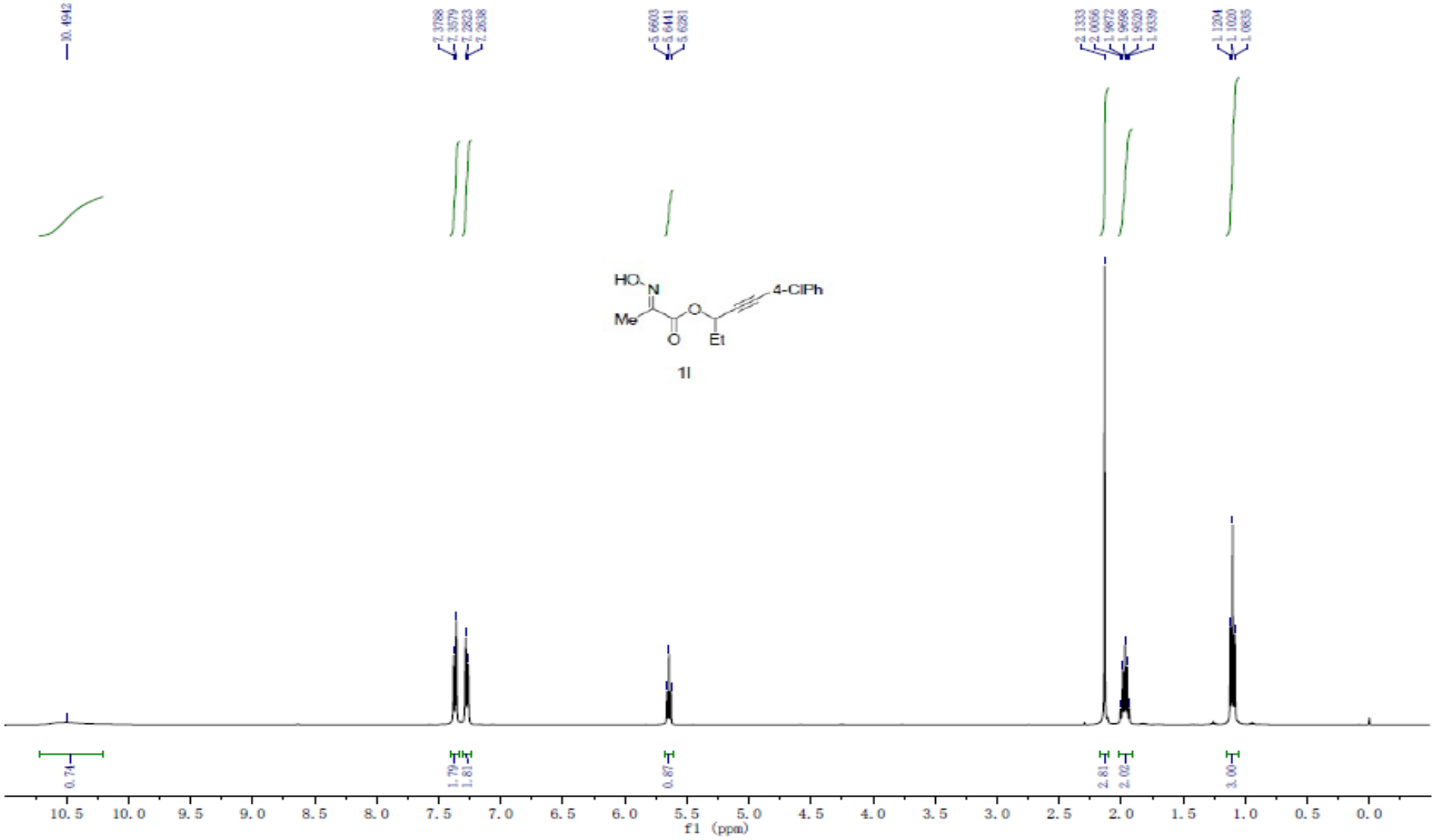
138.7863
131.7999
128.9620
119.1140
86.1416
84.8959
77.3173
76.9997
76.6821
67.3588
28.1792
21.4595
10.5411
9.4375
HO
N
Me
O
O
Et
4-MePh
1k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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7.3579
7.2823
7.2638
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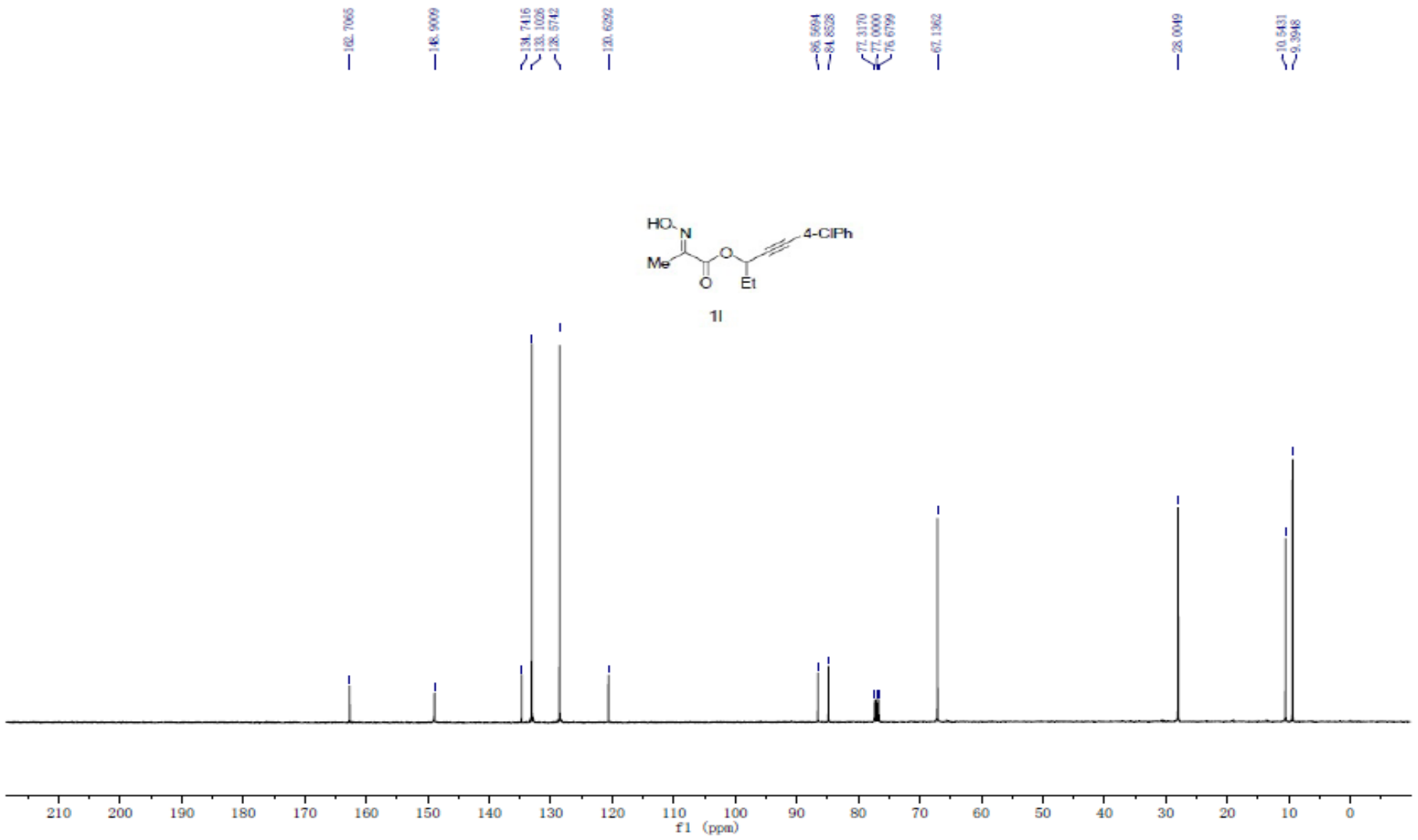
5.6441
5.6281
2.1333
2.0056
1.9872
1.9698
1.9520
1.9339
1.1204
1.1020
1.0835
HO
N
Me
O
O
Et
4-ClPh
1l
0.74
1.79
1.81
0.87
2.81
2.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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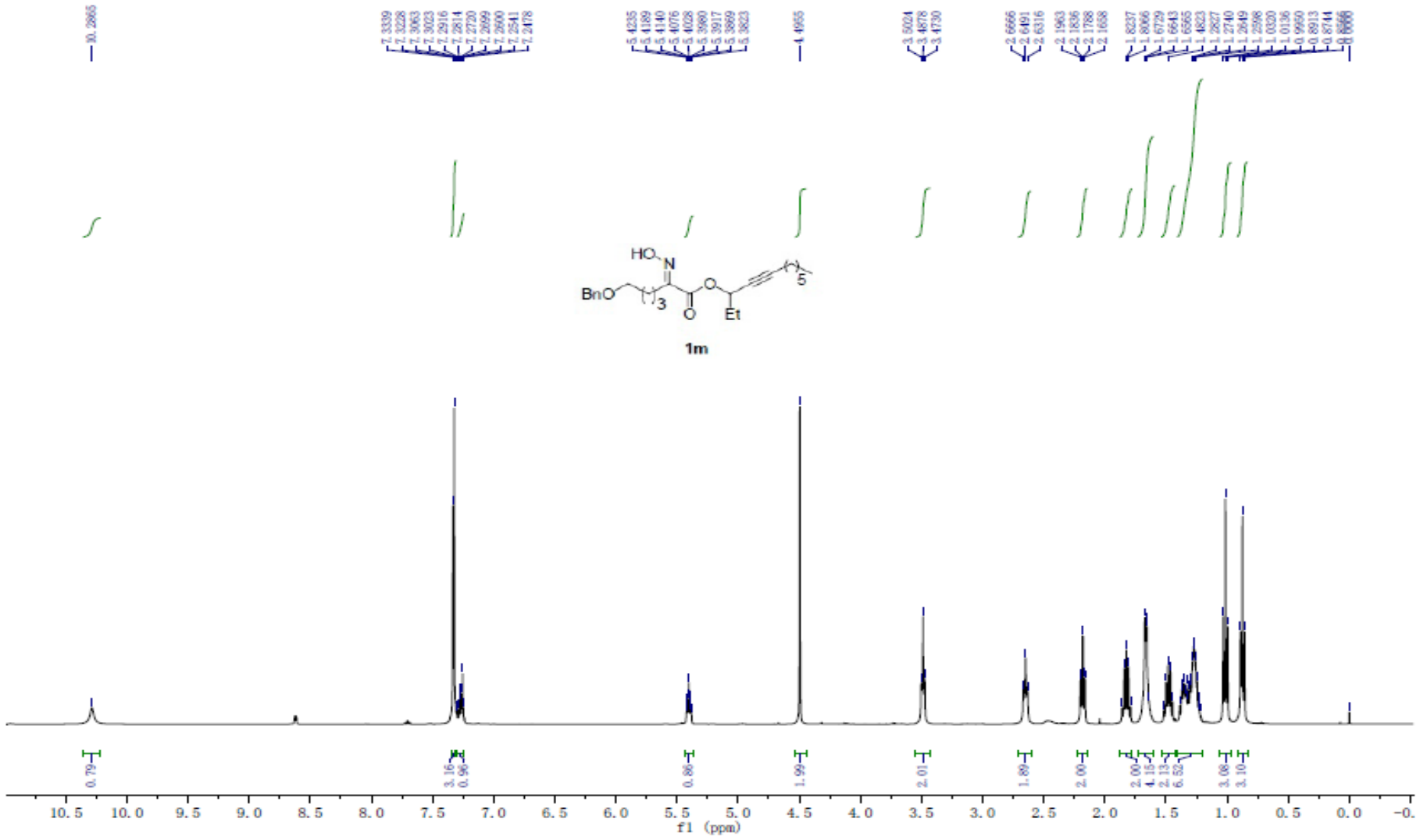
133.1026
128.5742
120.6292
86.5694
84.8528
77.3170
77.0000
76.6799
67.1362
28.0049
10.5431
9.3948
HO
N
Me
O
O
Et
4-ClPh
1l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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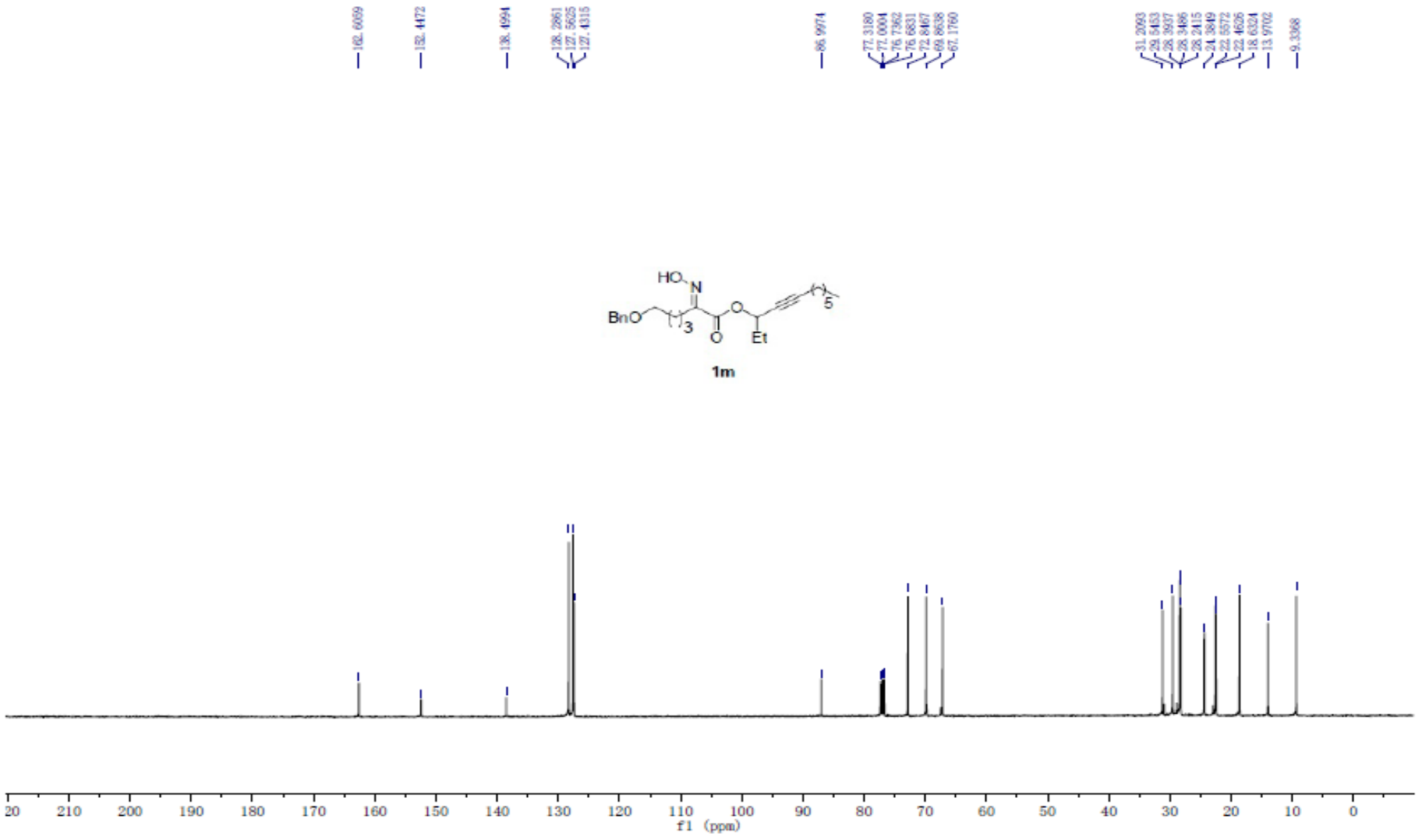
BnO
3
O
O
Et
5
1m
f1 (ppm)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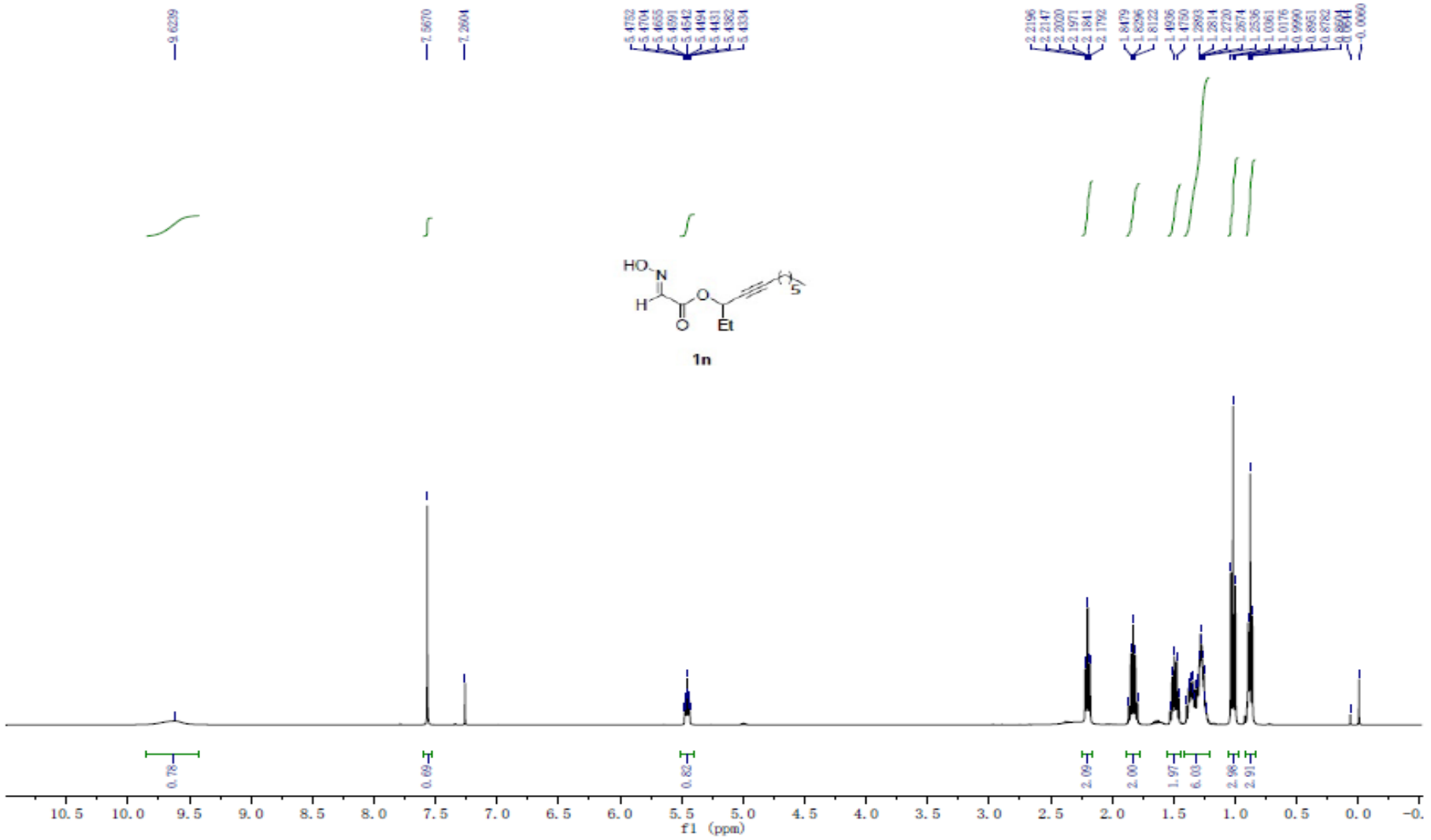
76.6831
72.8467
69.8638
67.1760
31.2093
29.5453
26.3937
26.3486
26.2415
24.3849
22.5572
22.4626
18.6324
13.9702
9.3368
HO
N
BnO
3
O
O
Et
5
1m
f1 (ppm)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5.4542
5.4494
5.4431
5.4382
5.4334
2.2196
2.2147
2.2020
2.1971
2.1841
2.1792
1.8479
1.8296
1.8122
1.4936
1.4750
1.2893
1.2814
1.2720
1.2674
1.2536
1.0061
1.0176
0.9990
0.8951
0.8782
0.8661
0.8611
-0.0060
HO
N
H
O
O
Et
S
1n
0.78
0.69
0.82
2.09
2.00
1.97
6.03
2.98
2.91
10.5
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
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2.0
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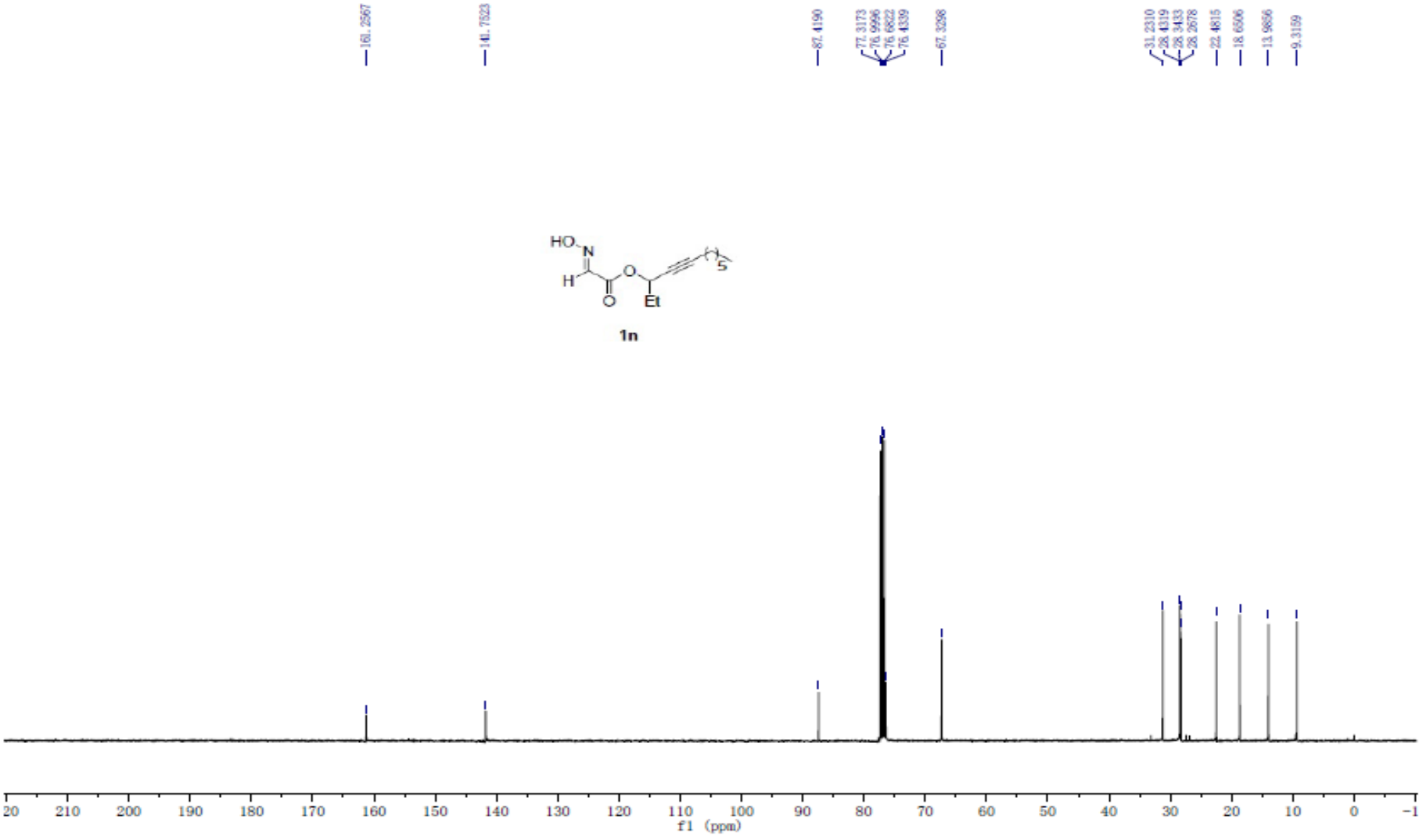
0.5
0.0
-0.
f1 (ppm)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67.3298
31.2310
28.4319
28.3433
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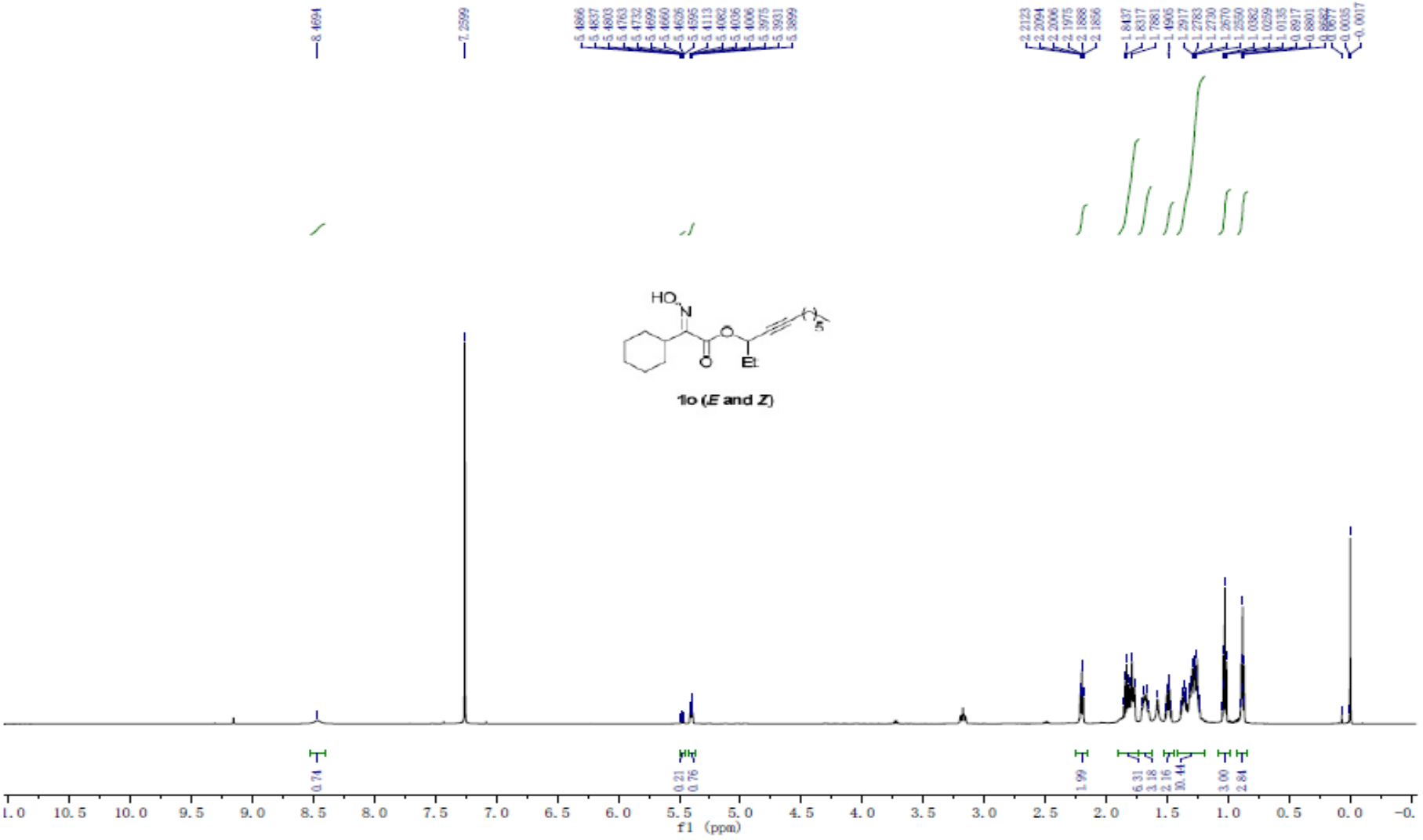
18.6506
13.9656
9.3159
HO
N
H
O
O
Et
1n
f1 (ppm)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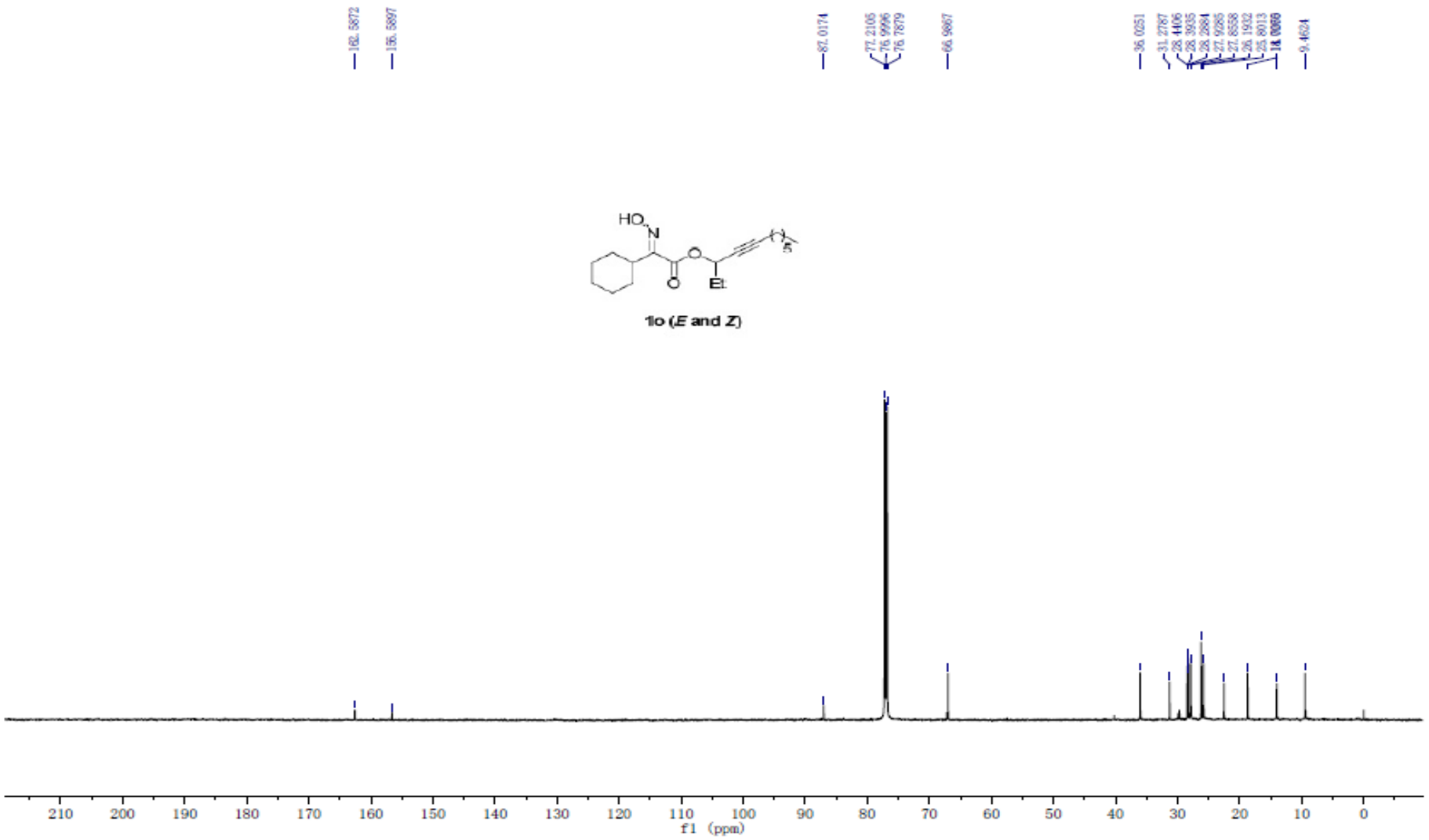
5.4603
5.4763
5.4732
5.4699
5.4660
5.4626
5.4595
5.4113
5.4082
5.4036
5.4006
5.3975
5.3931
5.3899
2.2123
2.2094
2.2006
2.1975
2.1888
2.1856
1.8437
1.8317
1.7881
1.4905
1.2917
1.2783
1.2730
1.2570
1.2550
1.0382
1.0259
1.0135
0.8917
0.8801
0.0035
-0.0017
HO
N
O
O
Et
5
1lo (E and Z)
0.74
0.21
0.76
1.99
6.31
3.18
2.16
20.44
3.00
2.84
f1 (ppm)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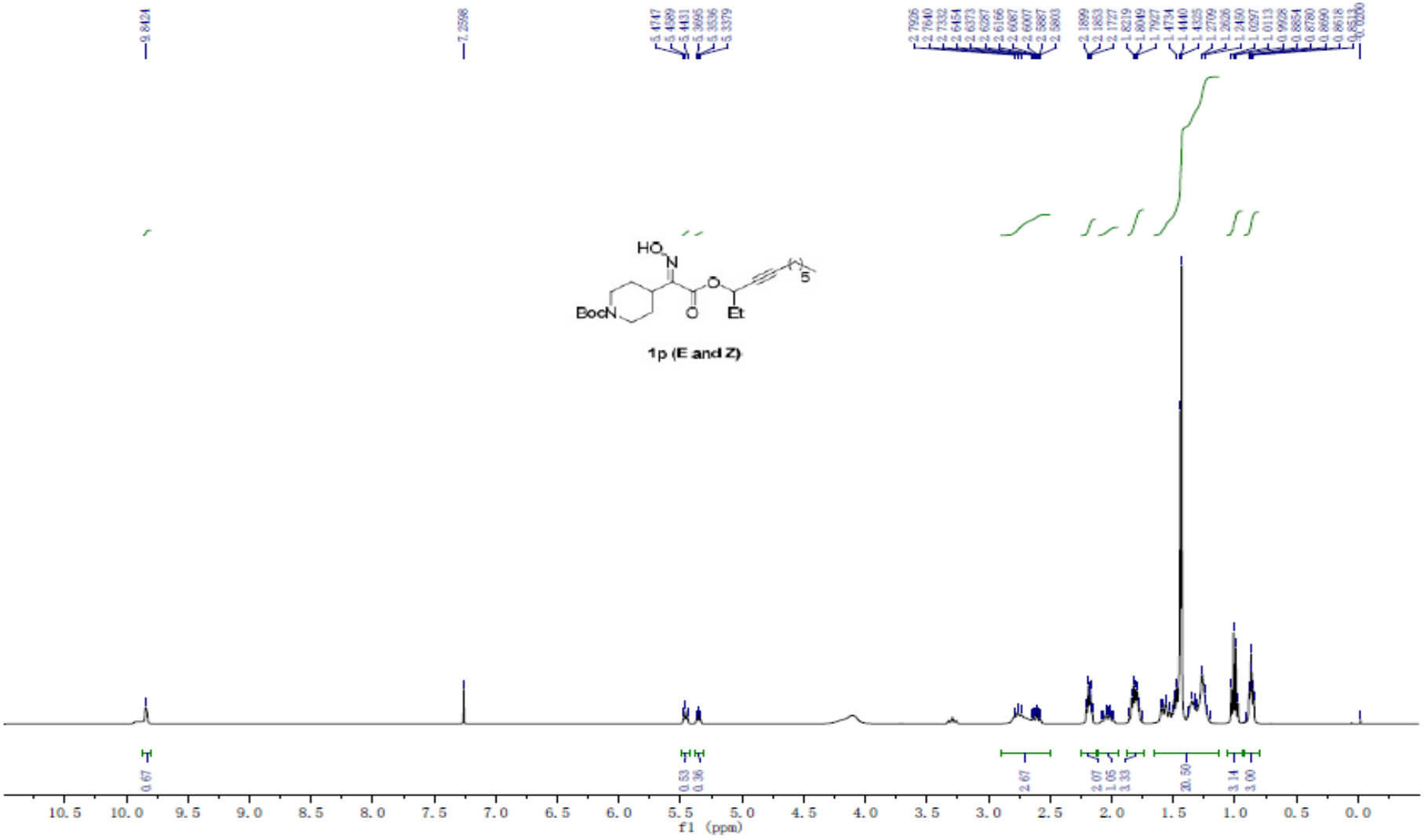
155.5897
87.0174
77.2105
76.9996
76.7879
66.9867
36.0251
31.2787
28.4406
28.3935
28.2884
27.9285
27.8558
26.1932
25.8013
14.0060
9.4624
HO
N
O
O
Et
1o (E and Z)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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5.4431
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5.3536
5.3379
2.7926
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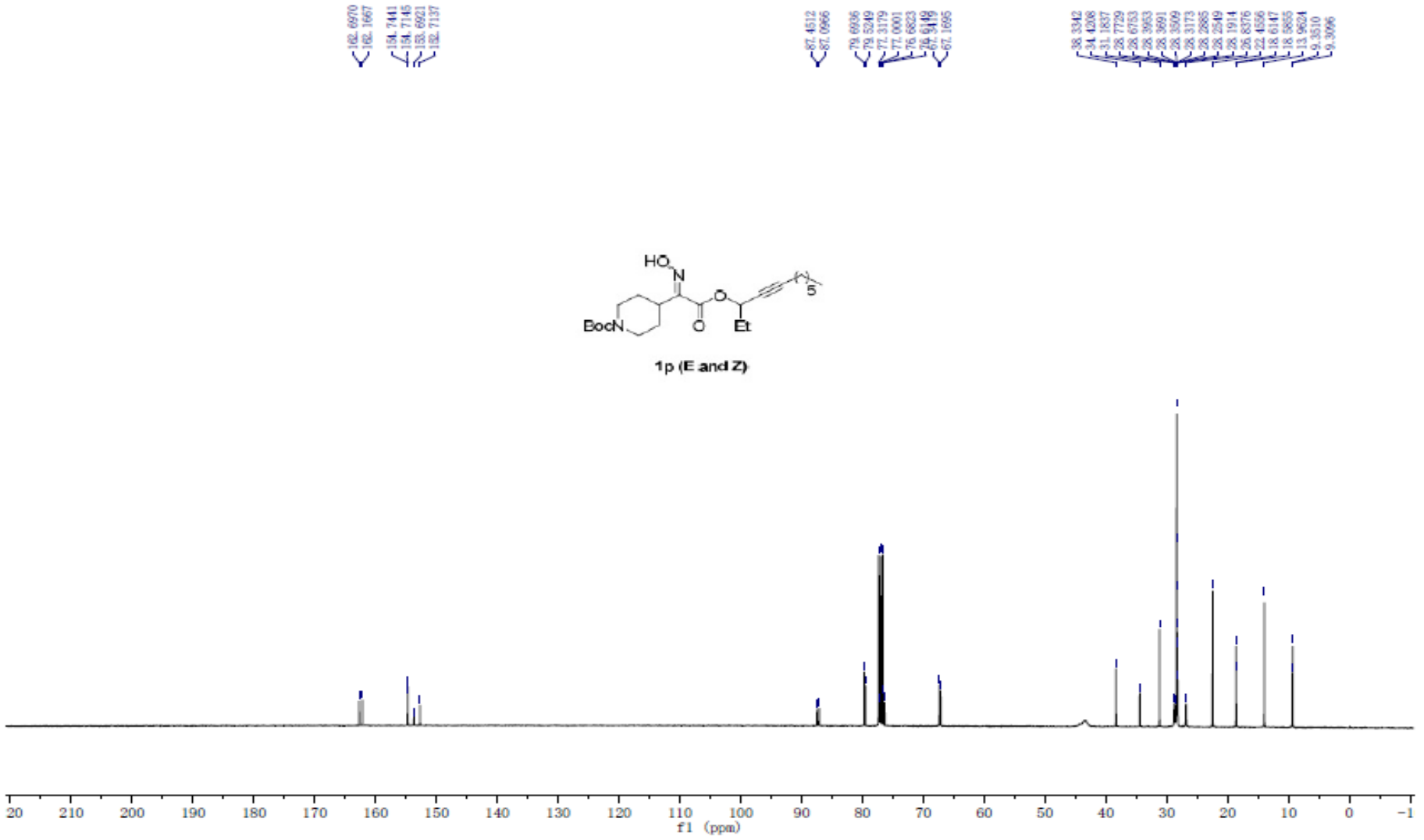
2.7332
2.6454
2.6373
2.6267
2.6166
2.6067
2.6007
2.5887
2.5803
2.1899
2.1853
2.1727
2.1219
2.1049
1.7927
1.4734
1.4440
1.4325
1.2709
1.2626
1.2490
1.0297
1.0113
0.9928
0.8854
0.8780
0.8690
0.8618
0.8513
0.0260
HO
N
O
O
5
BocN
Et
1p (E and Z)
0.67
0.53
0.36
2.67
2.07
1.05
3.33
20.50
3.14
3.00
10.5
10.0
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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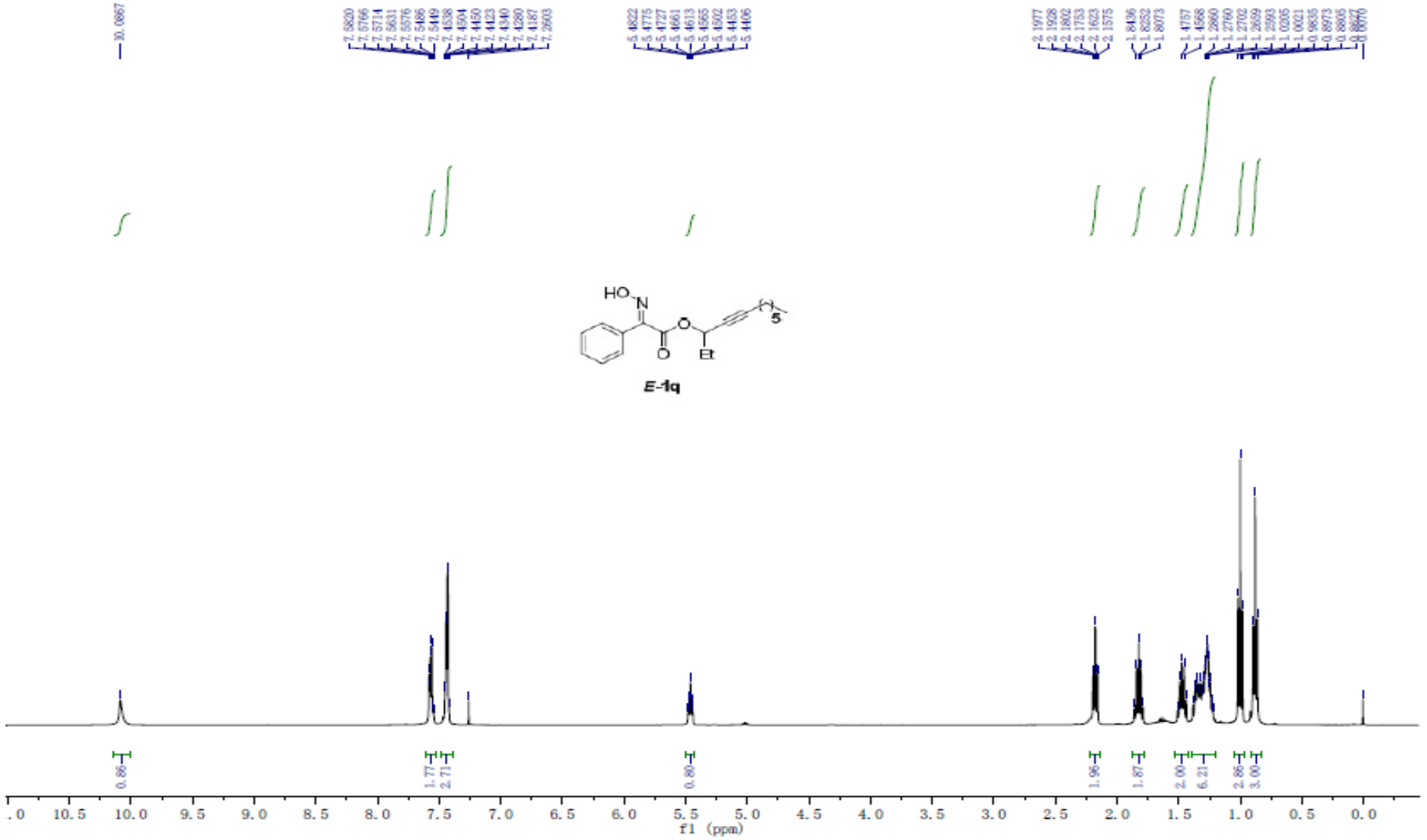
153.6921
152.7137
87.4512
87.0996
79.6936
79.5249
77.3179
77.0001
76.6823
67.9419
67.1695
38.3342
34.4206
31.1837
28.7729
28.6753
28.3963
28.3691
28.3509
28.3173
28.2885
28.2549
28.1914
26.8376
22.4556
18.6147
18.5855
13.9624
9.3510
9.3066
HO
N
O
O
BocN
Et
5
1p (E and Z)
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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7.5419
7.4538
7.4504
7.4450
7.4423
7.4340
7.4290
7.4187
7.2603
5.4822
5.4775
5.4727
5.4661
5.4613
5.4565
5.4502
5.4453
5.4406
2.1977
2.1928
2.1802
2.1753
2.1623
2.1575
1.8436
1.8252
1.8073
1.4757
1.4568
1.2860
1.2760
1.2702
1.2659
1.2593
1.0035
1.0021
0.9635
0.8973
0.8805
0.8647
0.8570
HO
N
O
O
Et
5
E-1q
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1.77
2.71
0.80
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6.21
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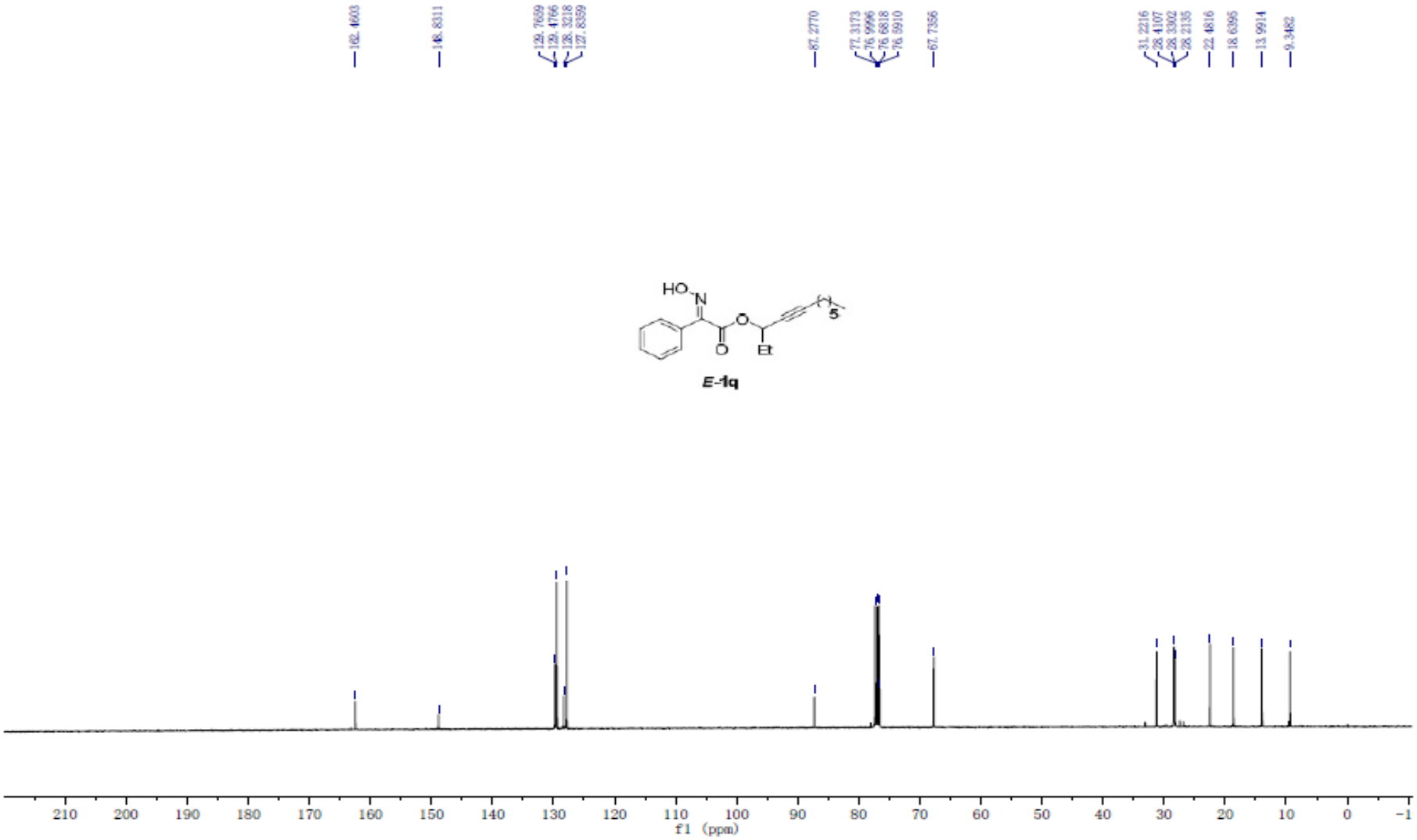
3.00
f1 (ppm)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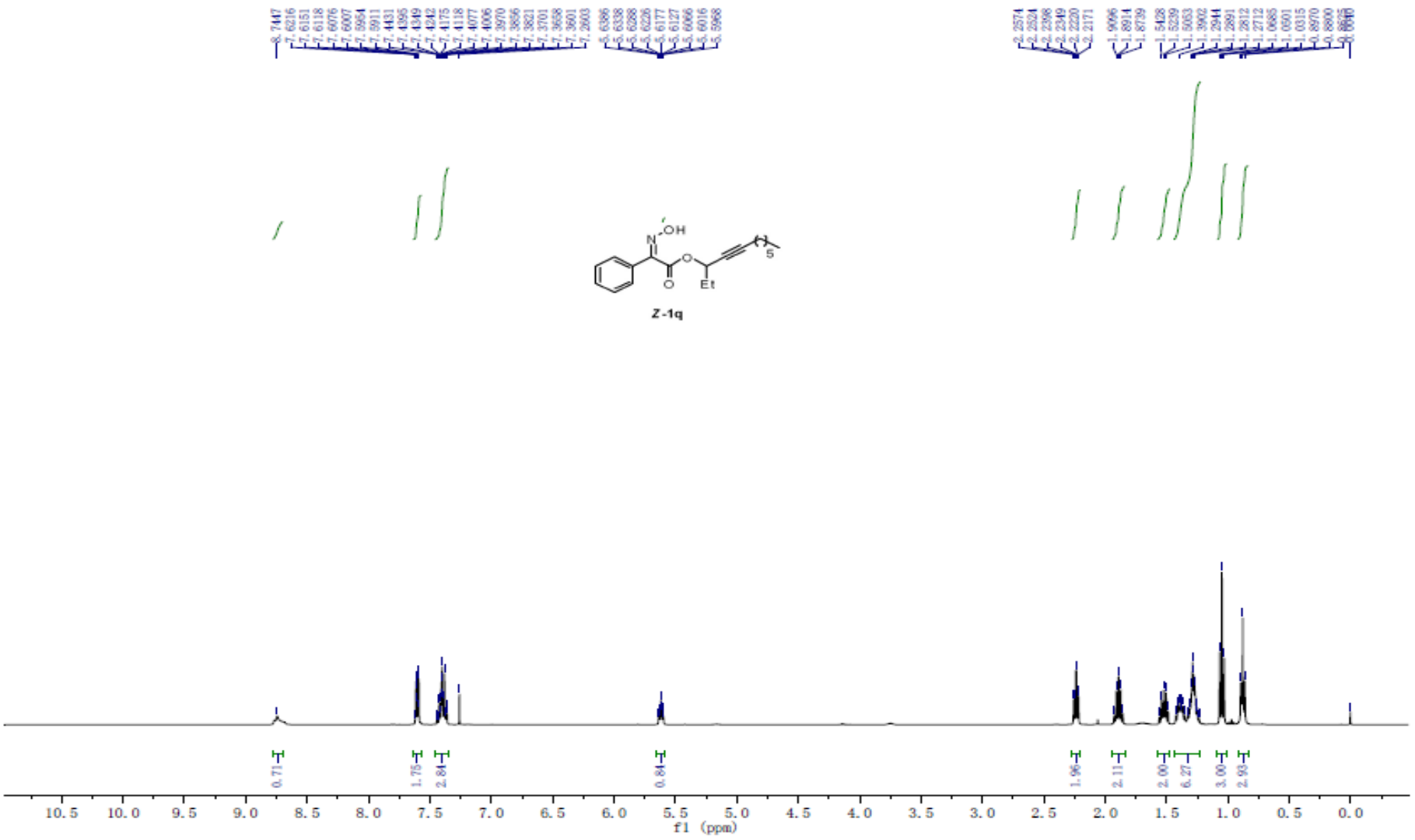
76.6818
76.6910
67.7356
31.2216
28.4107
28.3302
28.2135
22.4816
18.6395
13.9914
9.3482
HO
N
O
O
Et
5
E-1q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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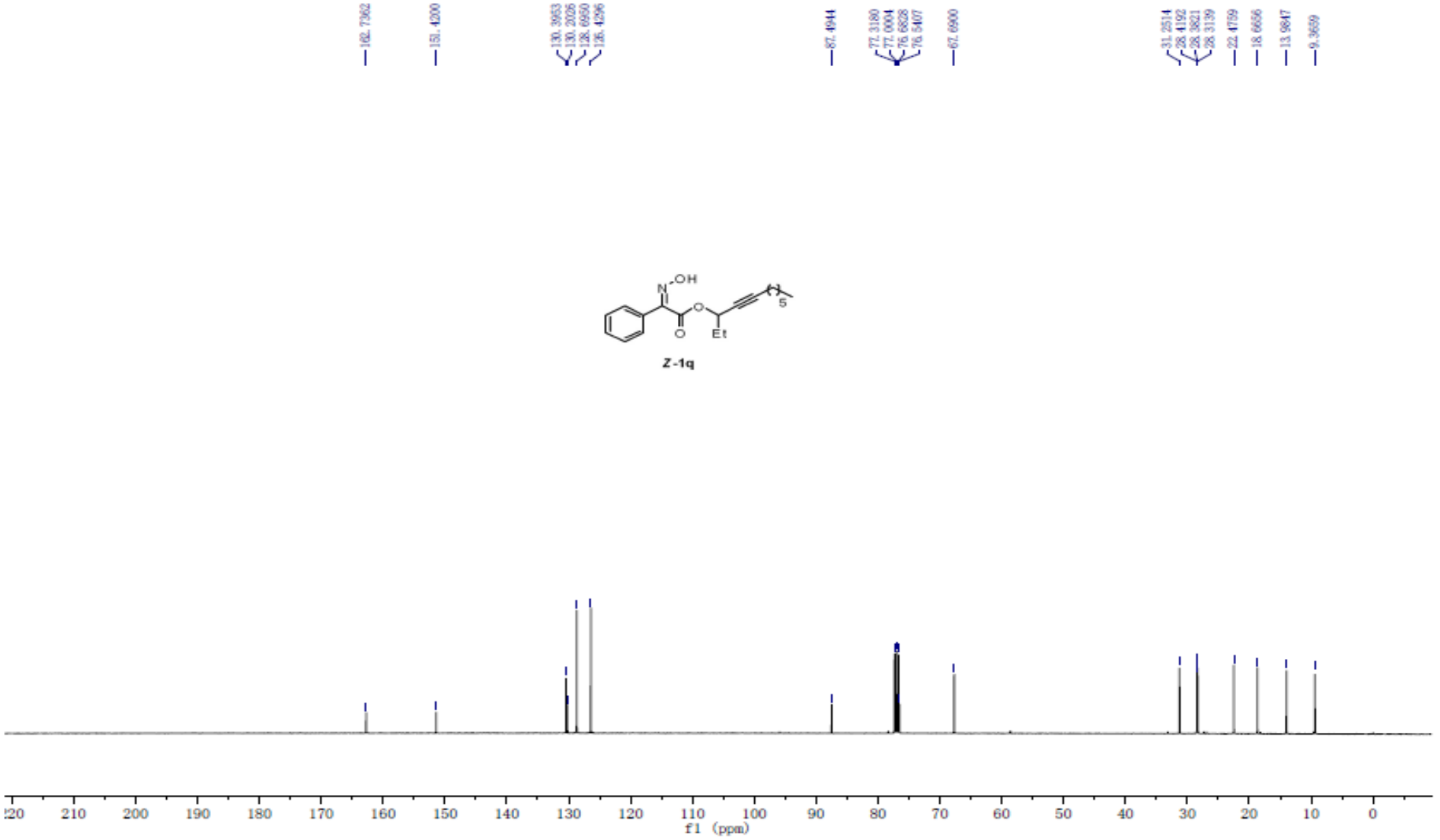
7.4242
7.4175
7.4118
7.4077
7.4006
7.3970
7.3856
7.3821
7.3701
7.3658
7.3601
7.2603
5.6386
5.6338
5.6288
5.6226
5.6177
5.6127
5.6066
5.6016
5.5968
2.2574
2.2524
2.2396
2.2349
2.2220
2.2171
1.9096
1.8914
1.8739
1.5428
1.5239
1.5053
1.3902
1.2944
1.2891
1.2812
1.2712
1.0685
1.0501
1.0315
0.8970
0.8800
0.8615
OH
N
O
O
Et
5
Z-1q
0.71
1.75
2.84
0.84
1.96
2.11
2.00
6.27
3.00
2.93
10.5
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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67.6900
31.2514
28.4192
28.3821
28.3139
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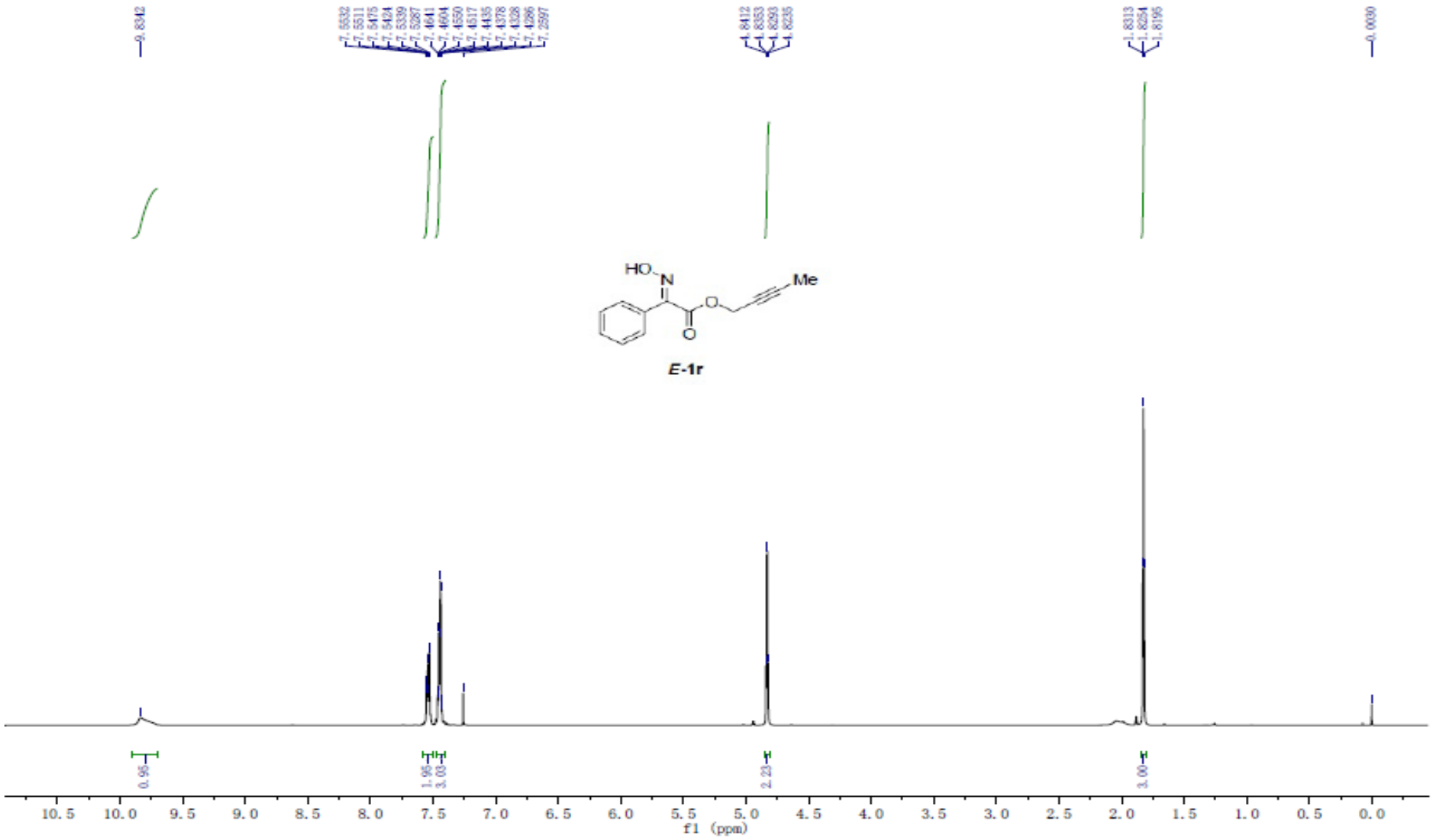
13.9847
9.3659
N
OH
O
O
Et
5
Z-1q
f1 (ppm)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7.4604
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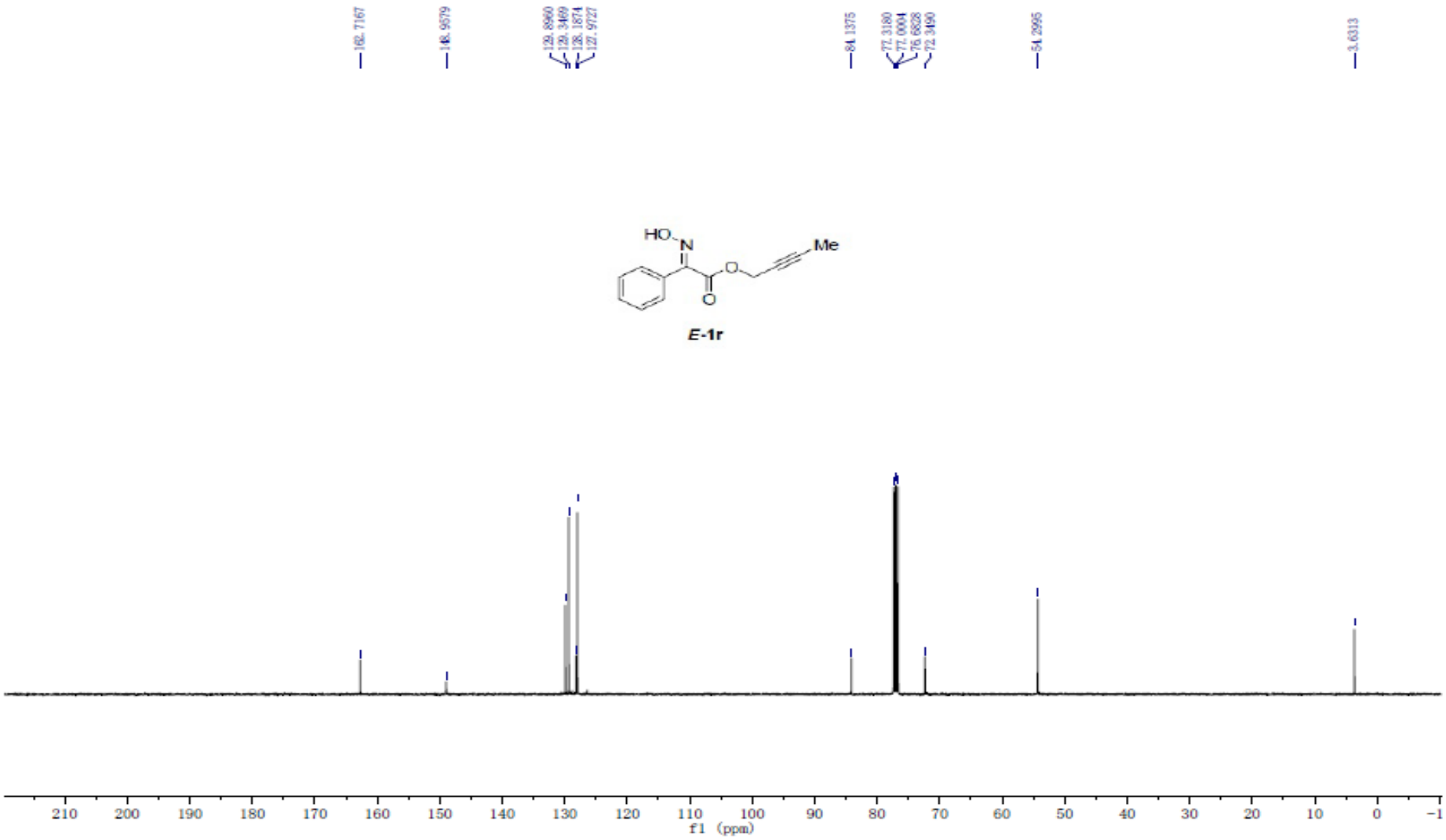
7.4517
7.4435
7.4378
7.4328
7.4286
7.2597
4.8412
4.8353
4.8293
4.8235
1.8313
1.8254
1.8196
0.0039
HO
N
O
O
Me
E-1r
0.95
1.96
3.03
2.23
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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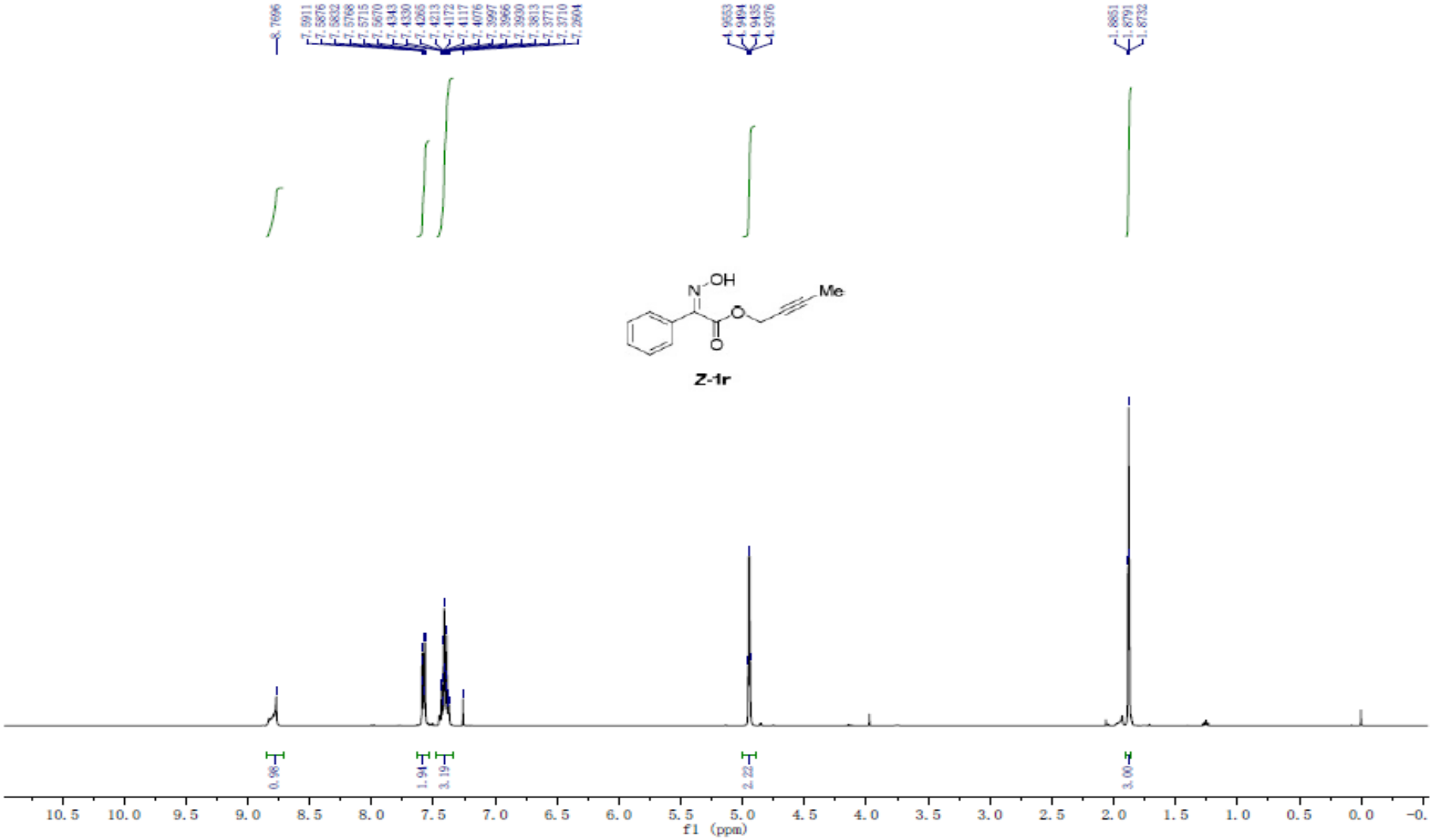
76.6828
72.3490
54.2995
3.6313
HO
N
O
O
Me
E-1r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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7.4213
7.4172
7.4117
7.4076
7.3997
7.3966
7.3930
7.3813
7.3771
7.3710
7.2604
4.9553
4.9494
4.9435
4.9376
1.8851
1.8791
1.8732
OH
N
O
O
Me
Z-1r
0.98
1.94
3.19
2.22
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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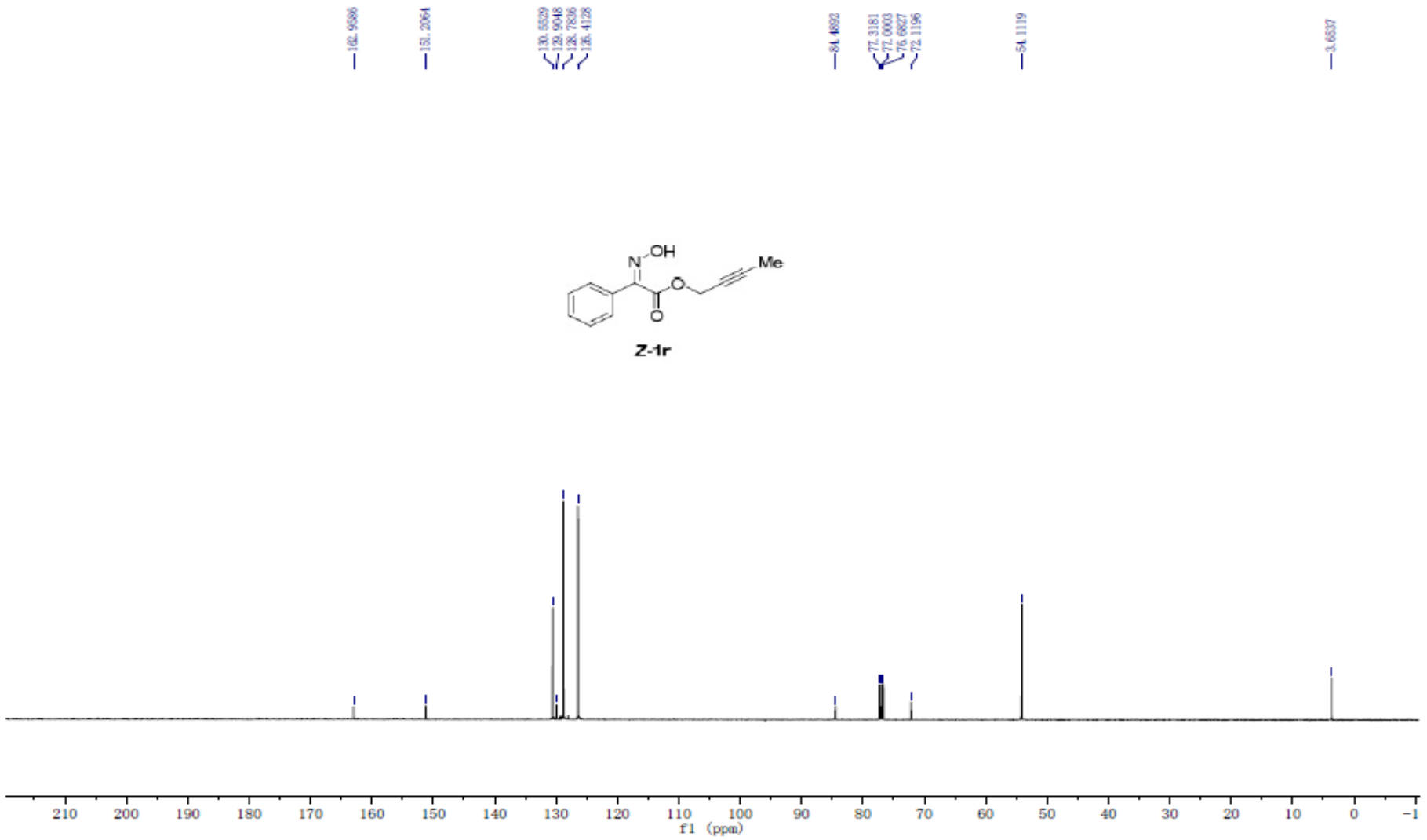
1.0
0.5
0.0
f1 (ppm)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77.0003
76.6827
72.1196
54.1119
3.6537
N
OH
O
O
Me
Z-1r
210
200
190
180
170
160
150
140
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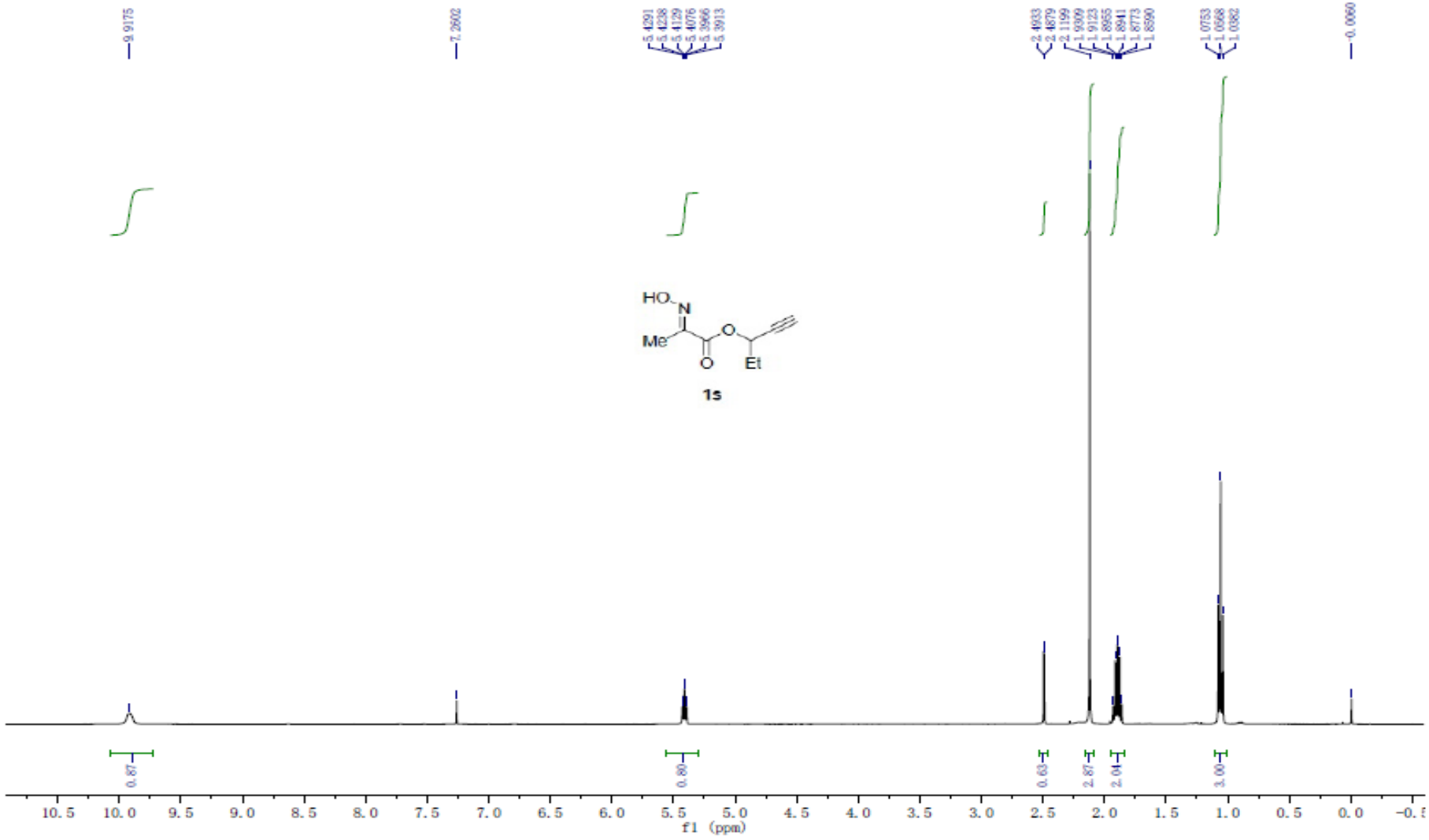
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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5.3966
5.3913
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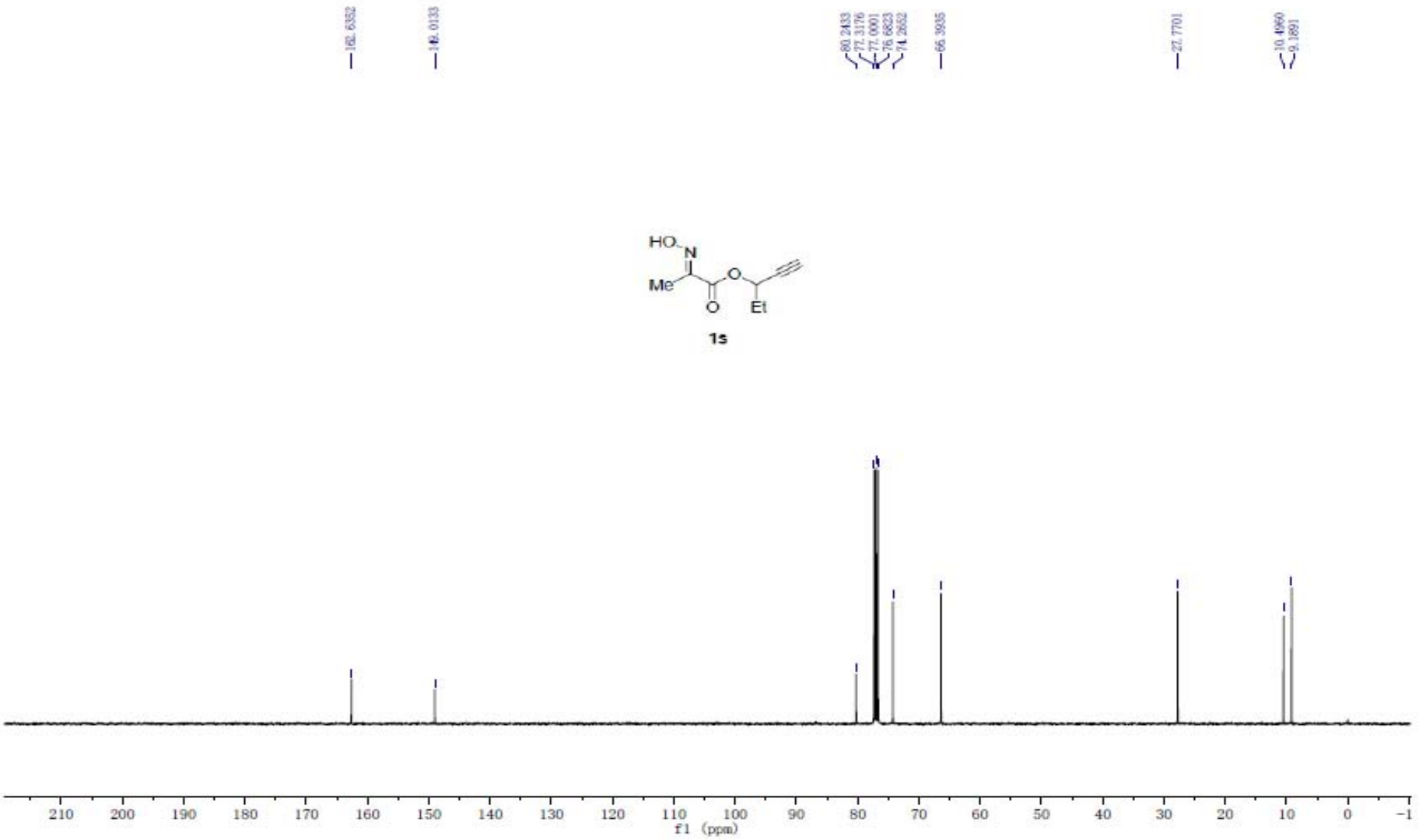
2.1199
1.9309
1.9123
1.8955
1.8941
1.8773
1.8590
1.0753
1.0568
1.0382
0.0060
HO
N
Me
O
O
Et
1s
0.87
0.80
0.63
2.87
2.04
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.0001
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74.2652
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27.7701
10.4960
9.1891
HO
N
Me
O
O
Et
1s
210
200
190
180
170
160
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140
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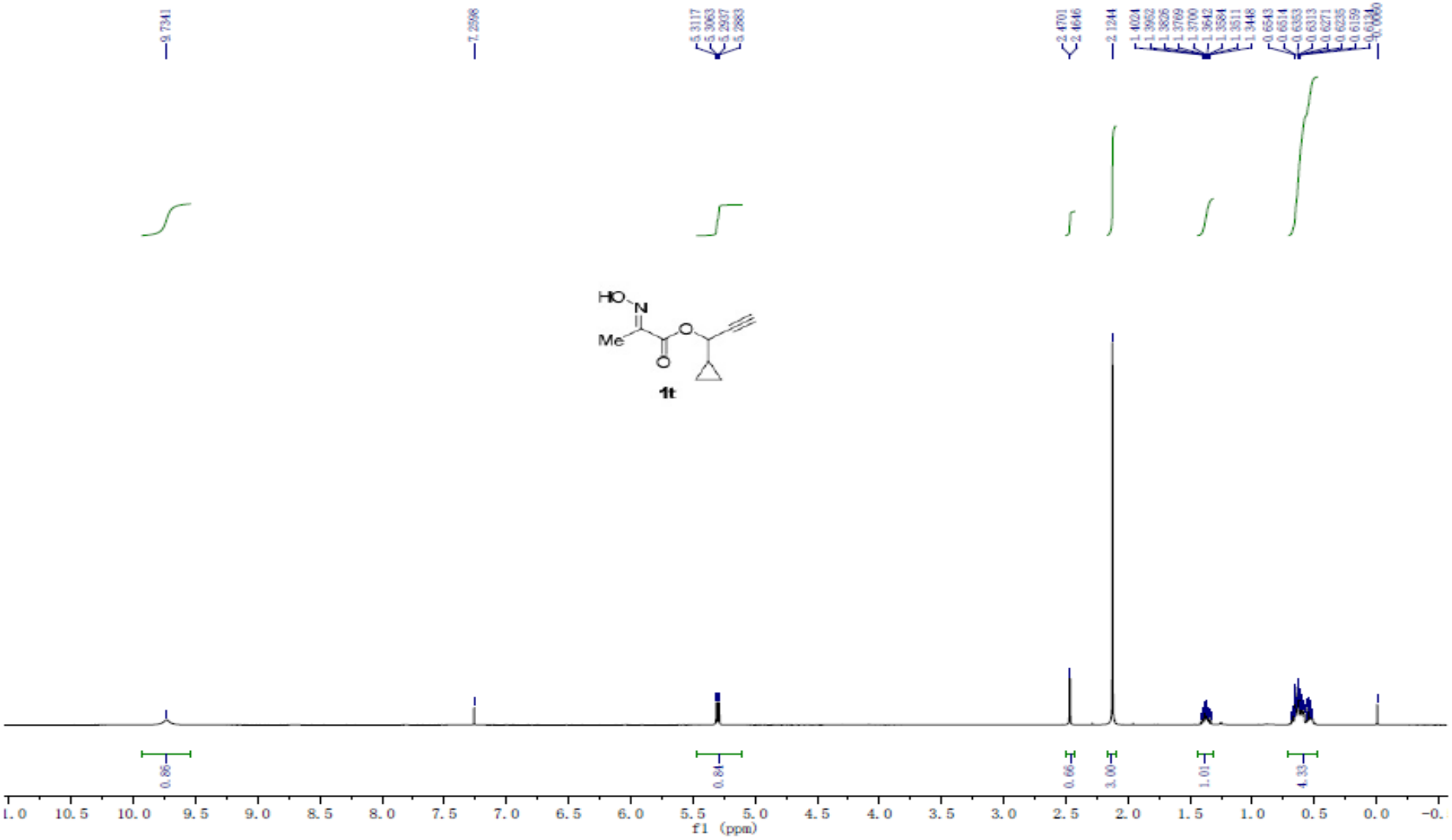
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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1.3826
1.3769
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1.3642
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1.3511
1.3446
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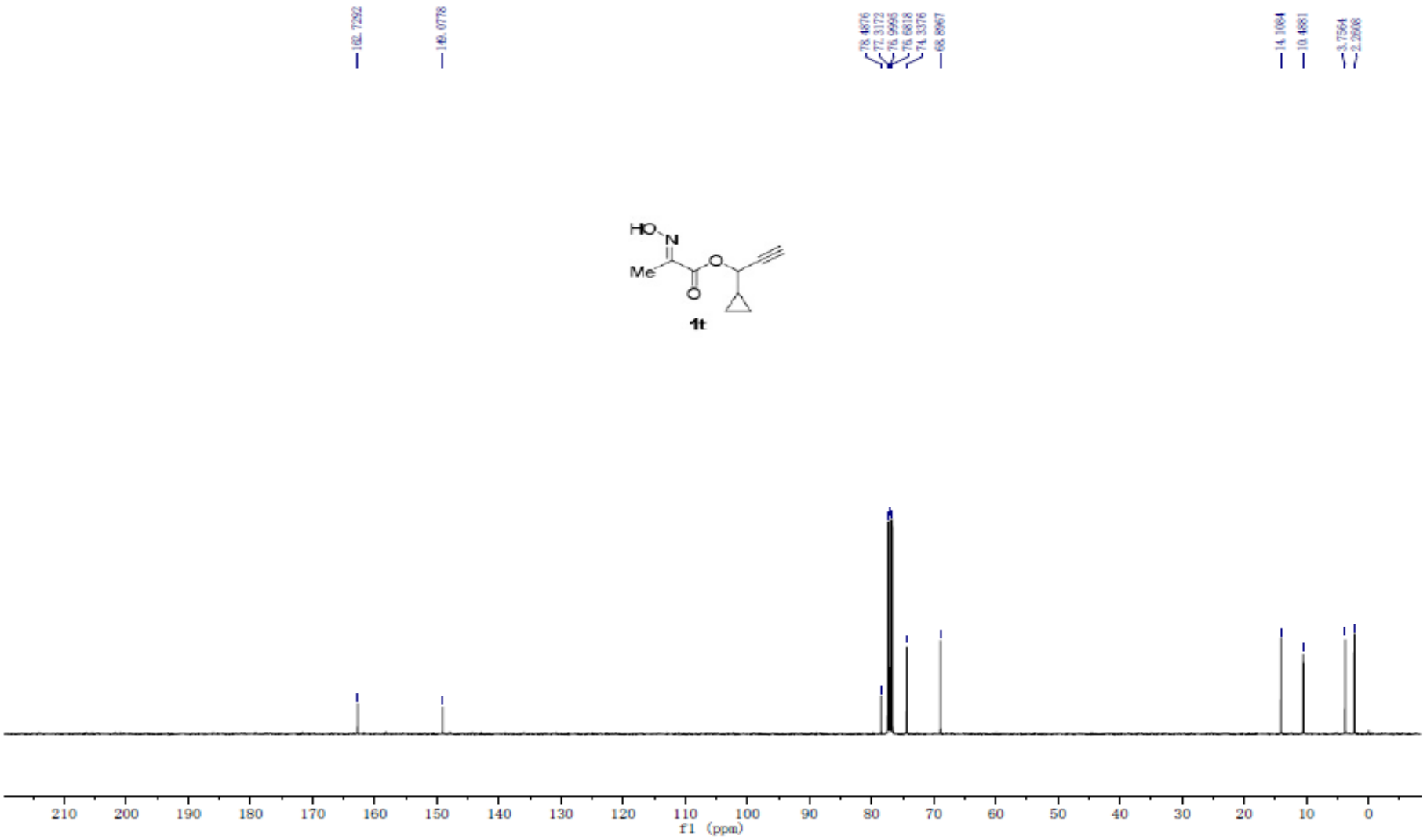
0.6514
0.6353
0.6313
0.6271
0.6235
0.6159
0.6124
0.0000
HO
N
Me
O
O
1t
0.86
0.84
0.66
3.00
1.01
4.33
f1 (ppm)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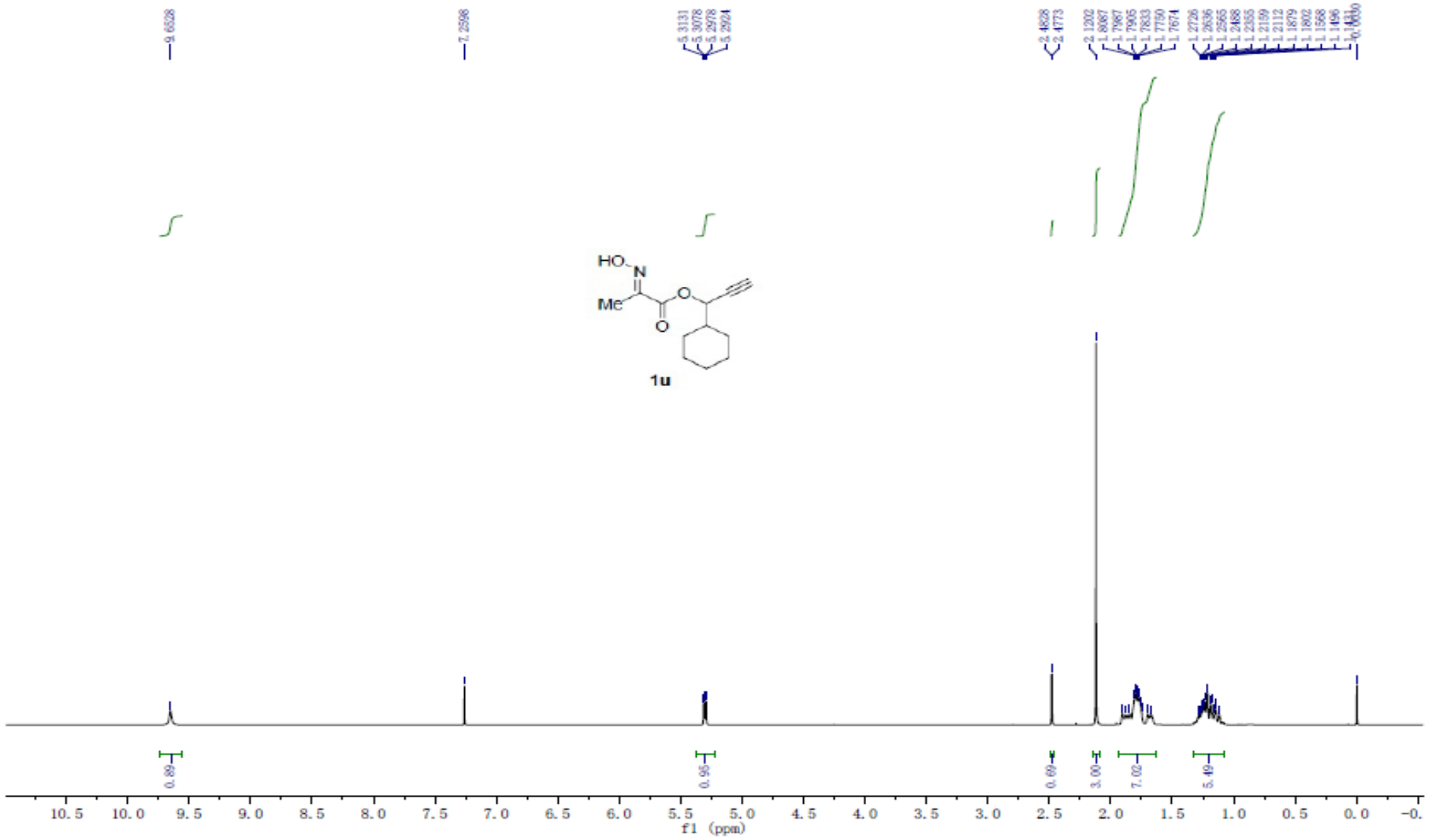
149.0778
78.4876
77.3172
76.9995
76.6818
74.3376
68.8967
14.1064
10.4881
3.7564
2.2906
HO
N
Me
O
O
1t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2598
5.3131
5.3078
5.2978
5.2924
2.4828
2.4773
2.1202
1.8067
1.7967
1.7905
1.7833
1.7750
1.7674
1.2726
1.2636
1.2565
1.2488
1.2353
1.2159
1.2112
1.1879
1.1802
1.1568
1.1496
1.1431
0.0000
HO
N
Me
O
O
1u
0.89
0.95
0.69
3.00
7.02
5.49
10.5
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
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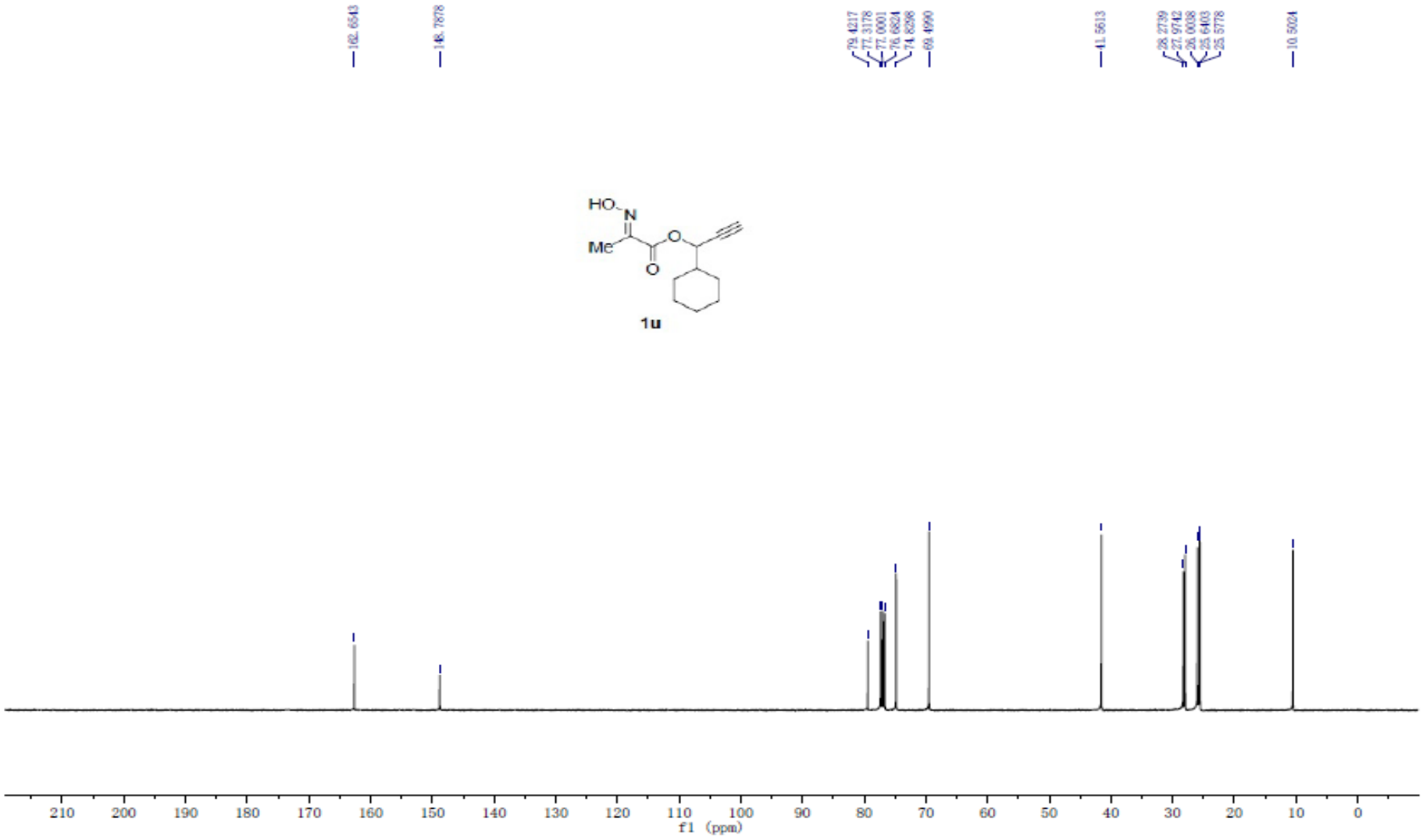
0.0
f1 (ppm)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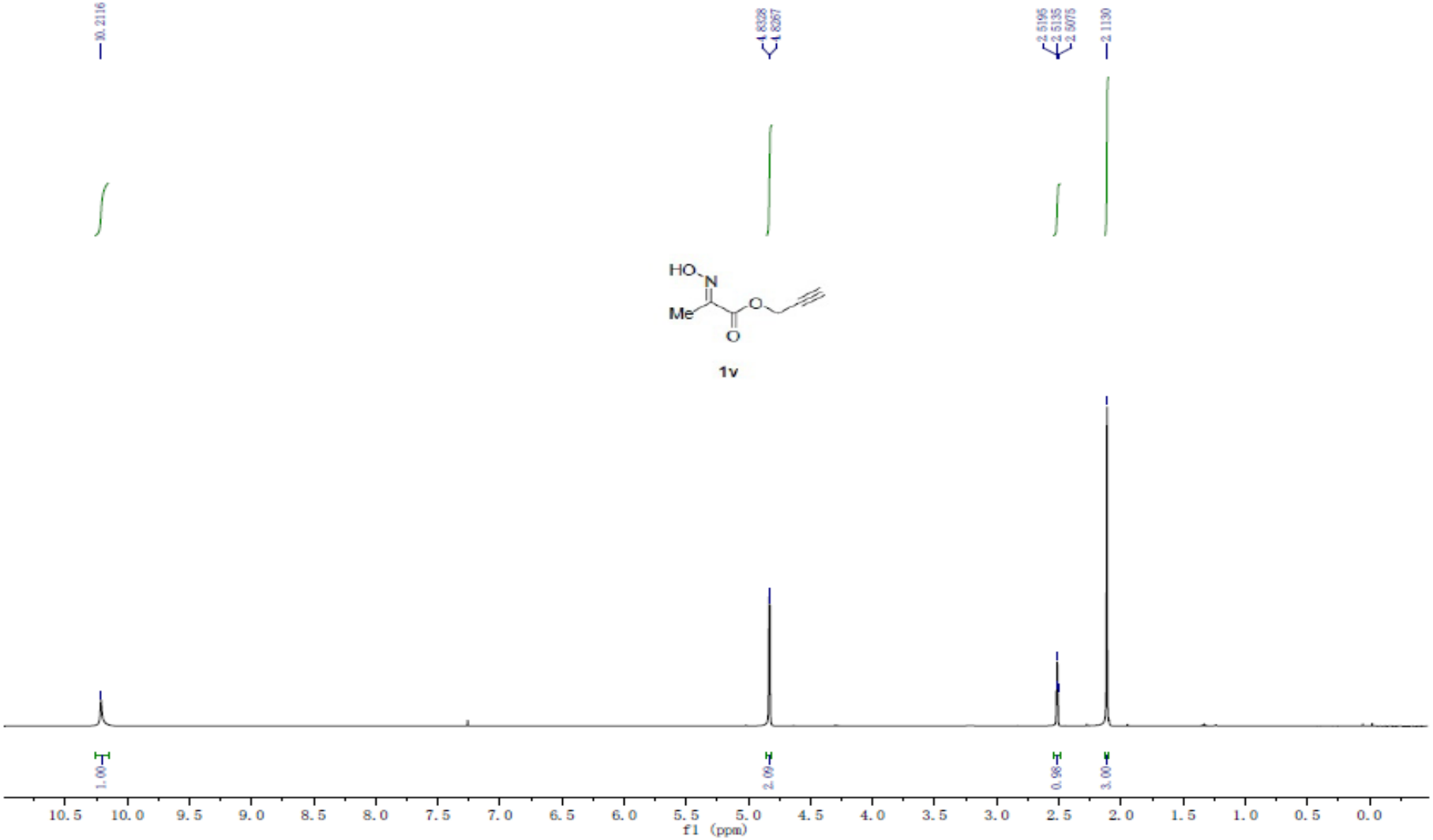
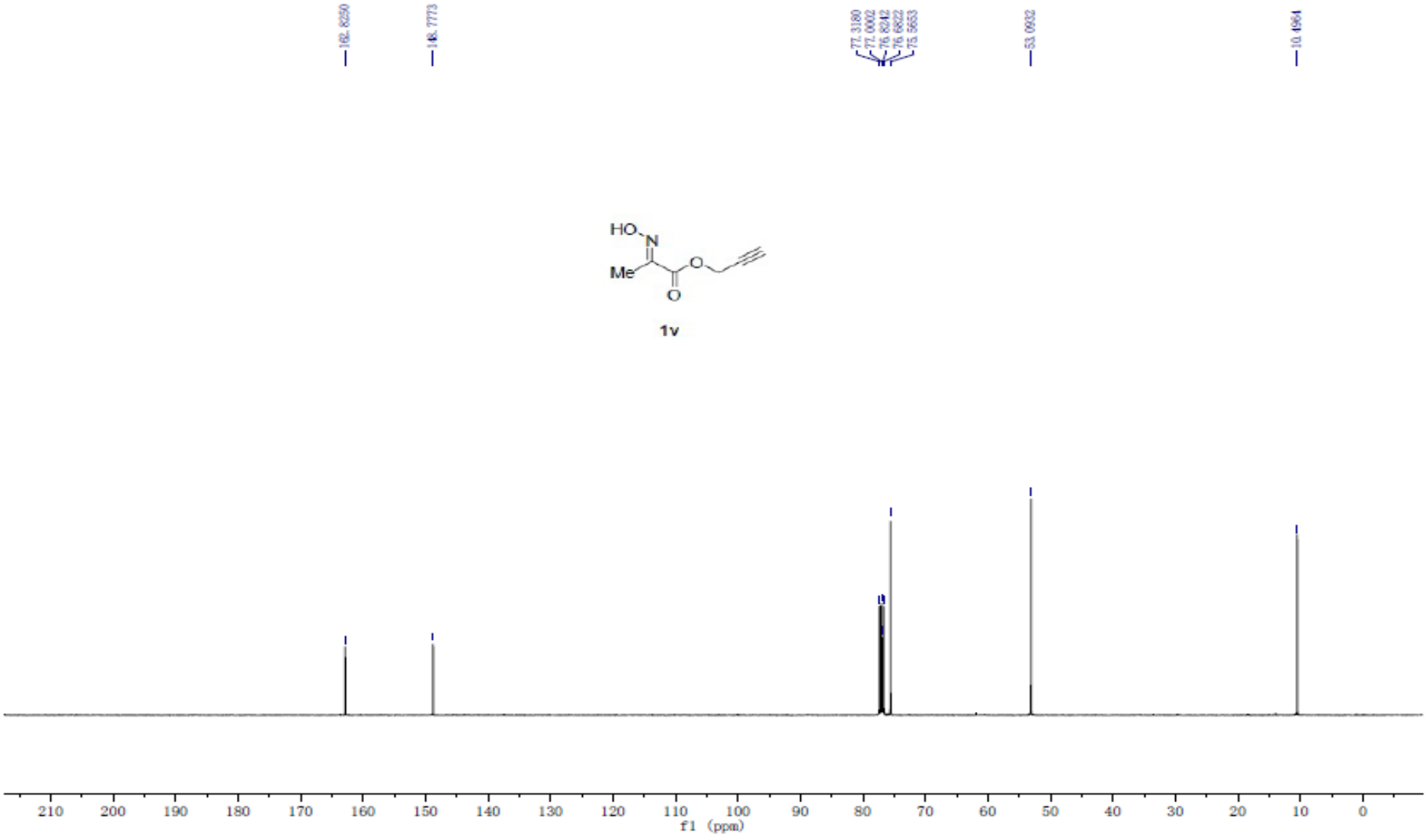
77.0001
76.6824
74.8286
69.4990
41.5613
28.2739
27.9742
26.0038
25.6403
25.5778
10.5024
HO
N
Me
O
O
1u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.2116
4.8328
4.8267
2.5195
2.5135
2.5075
2.1130
HO
N
Me
O
O
1v
1.00
2.09
0.98
3.00
10.5
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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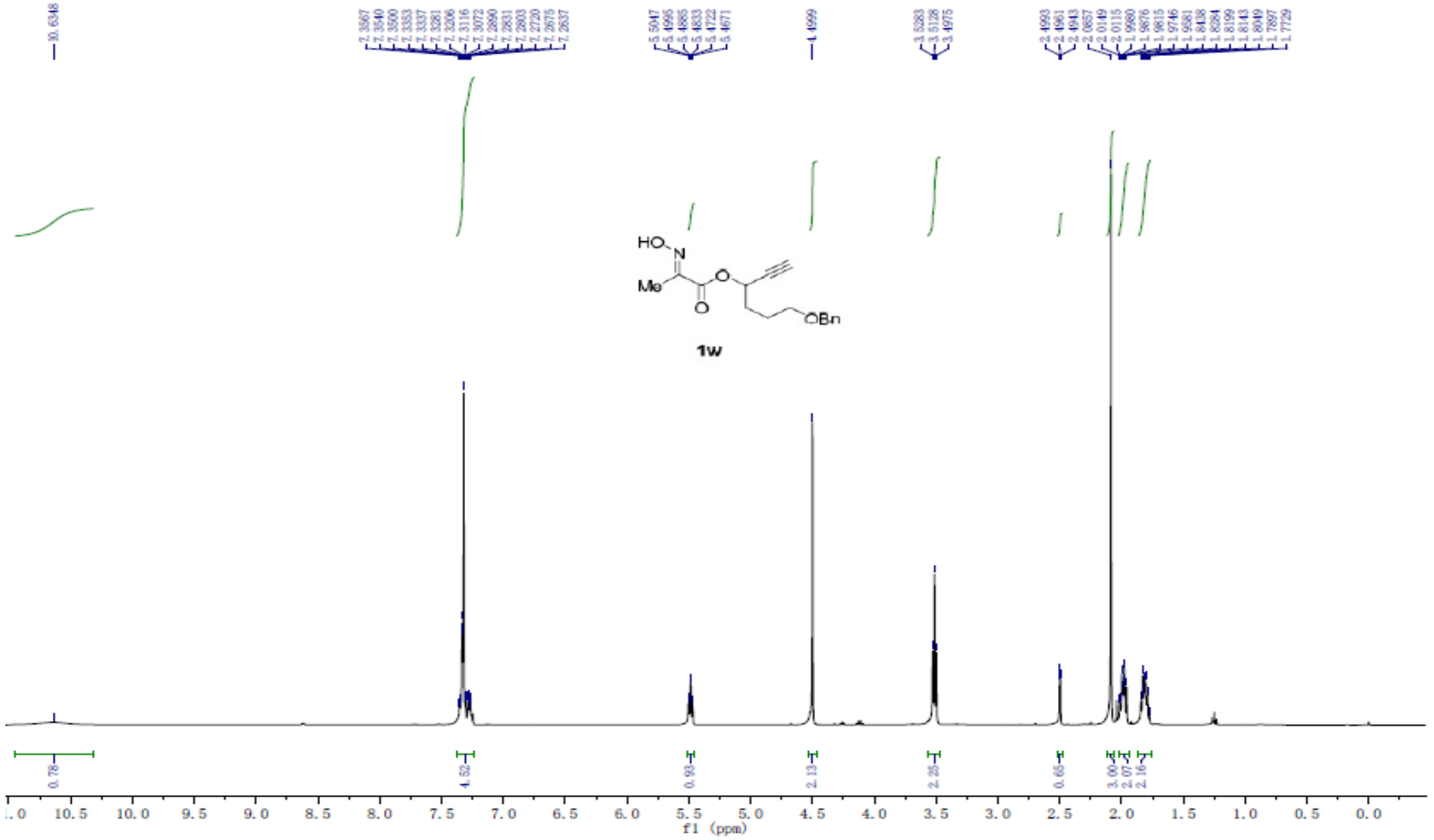
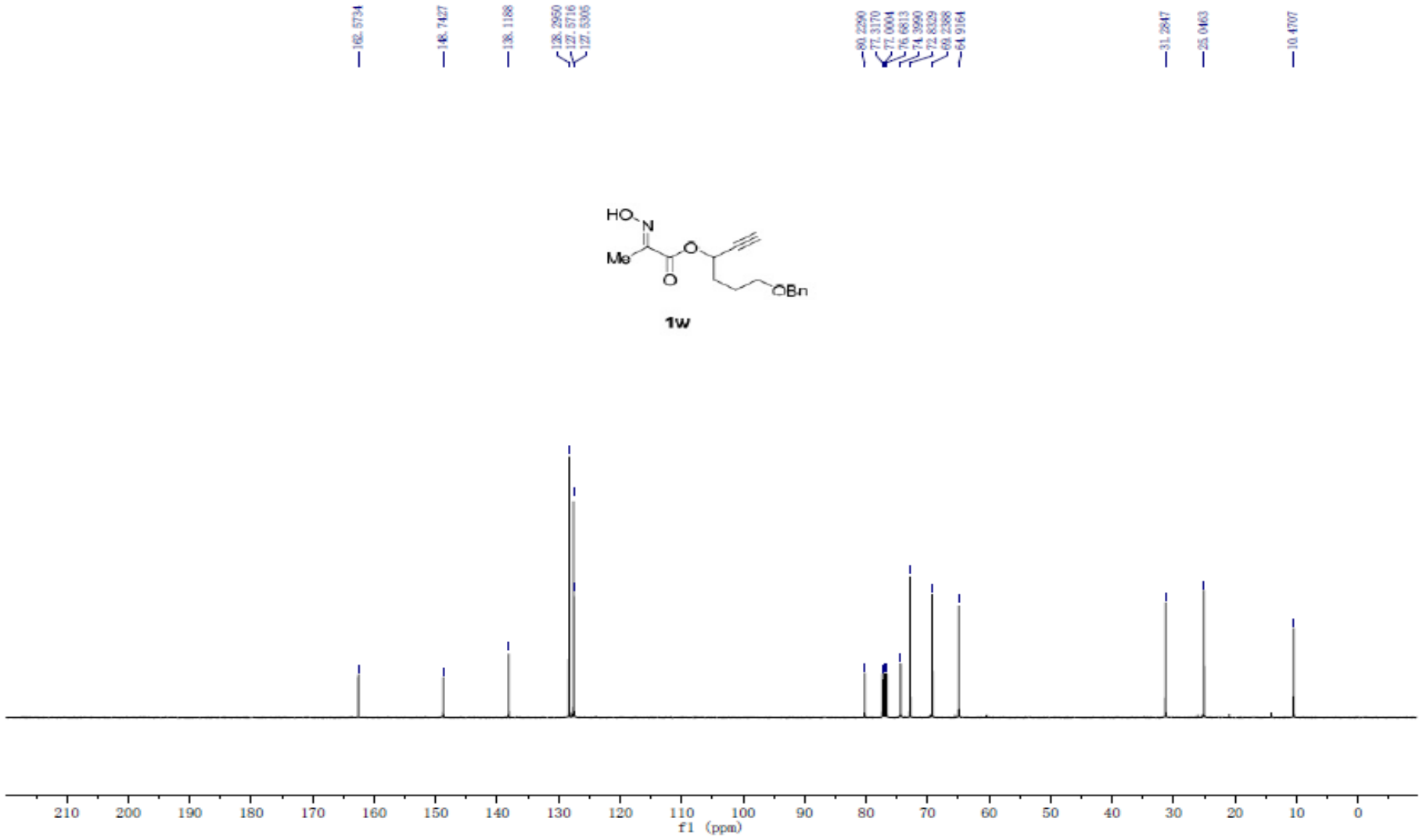
77.3180
77.0002
76.6842
76.6822
75.5653
53.0932
10.4964
HO
N
Me
O
O
1v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


HO
N
Me
O
O
OBn
1w
f1 (ppm)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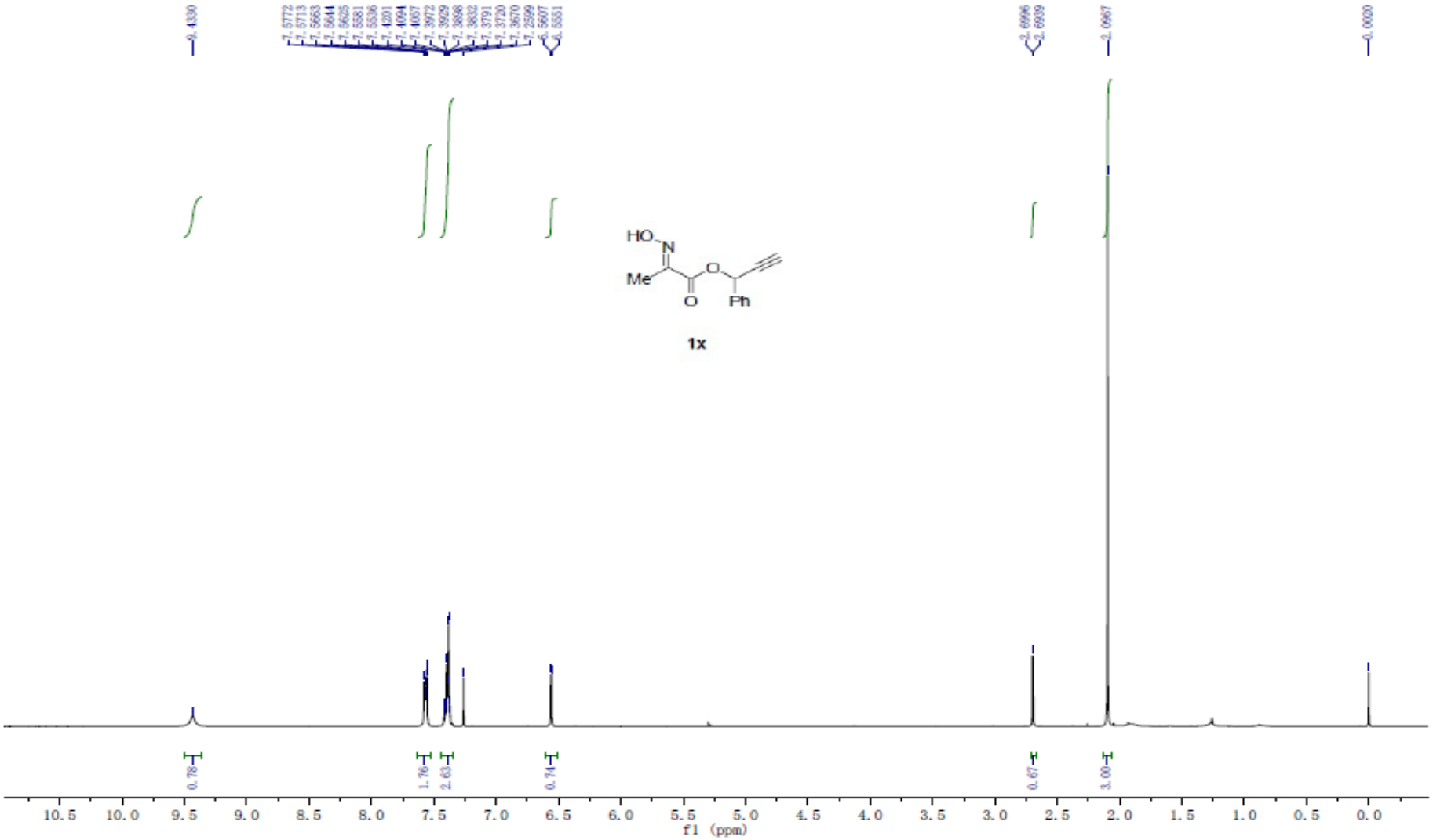
138.1188
128.2950
127.5716
127.5305
80.2290
77.3170
77.0004
76.6813
74.3990
72.8329
69.2388
64.9164
31.2847
25.0463
10.4707
HO
N
Me
O
O
OBn
1w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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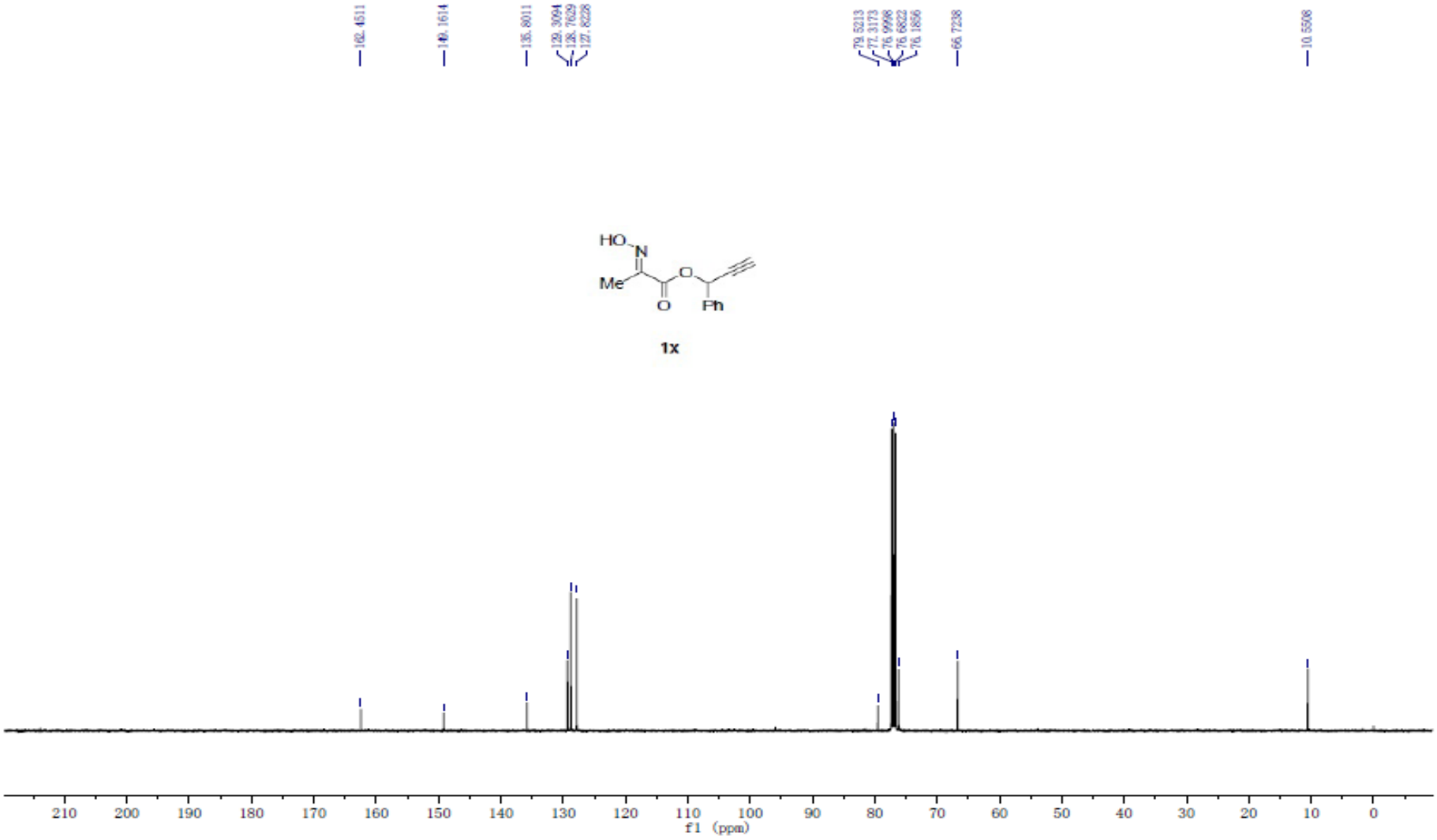
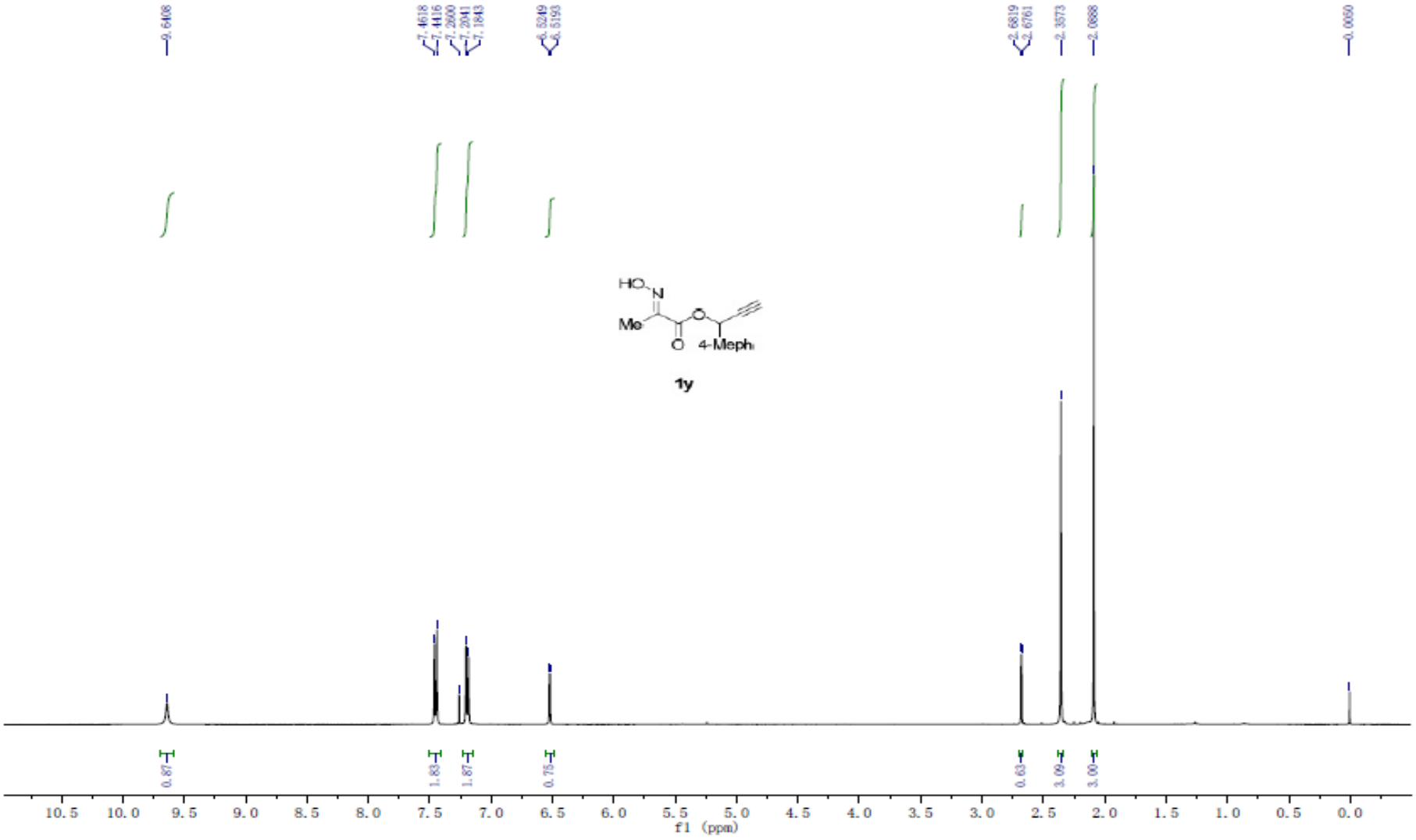
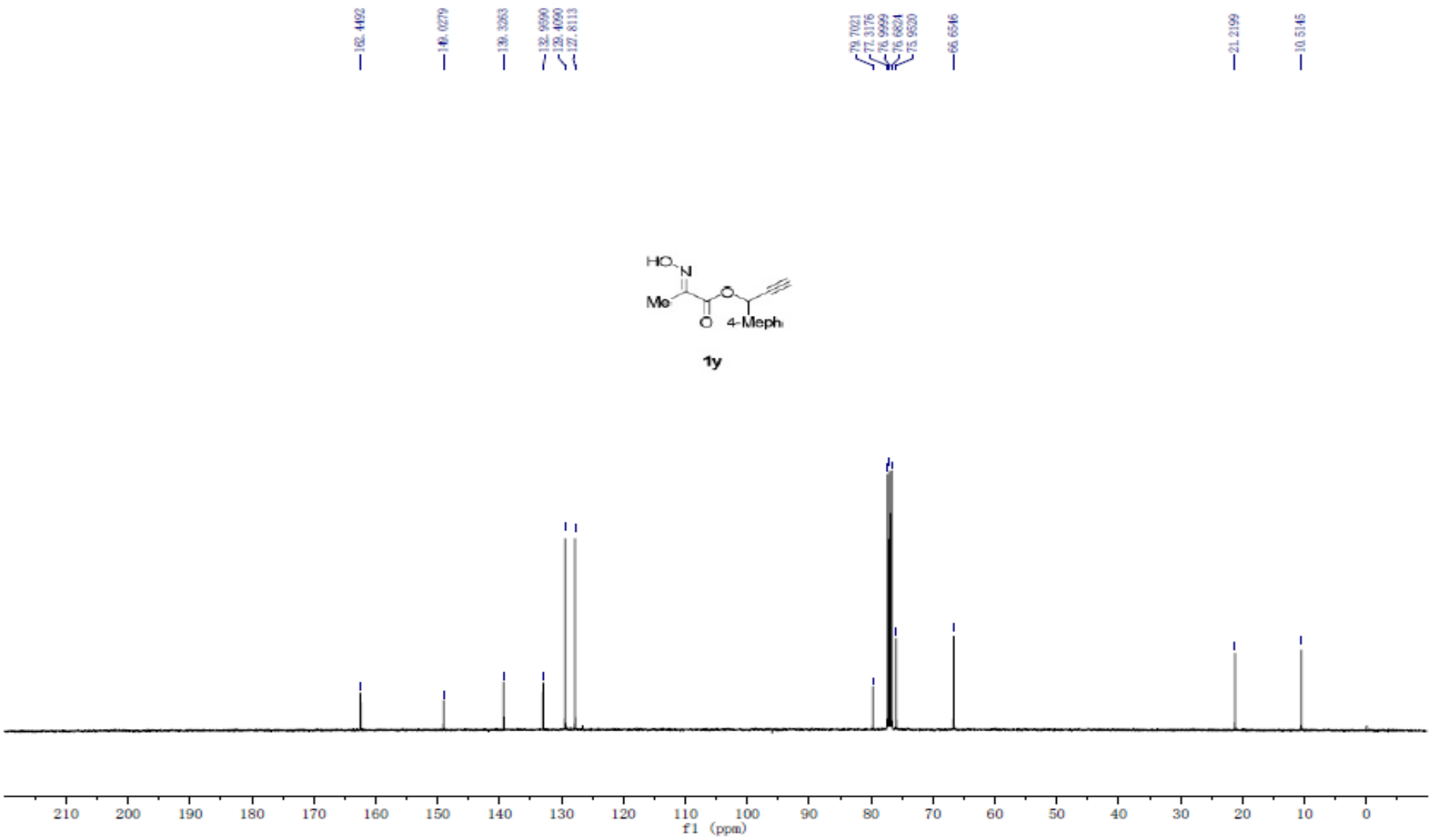
7.5772
7.5713
7.5663
7.5644
7.5625
7.5381
7.5336
7.4301
7.4094
7.4057
7.3972
7.3929
7.3898
7.3832
7.3791
7.3720
7.3670
7.2599
6.5607
6.5551
2.6966
2.6939
2.0967
0.0020
HO
N
Me
O
O
Ph
1x
0.78
1.76
2.63
0.74
0.67
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


162.4511
149.1614
135.8011
129.3094
128.7629
127.8226
79.5213
77.3173
76.9998
76.6822
76.1856
66.7238
10.5508
HO
N
Me
O
O
Ph
1x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.6408
7.4618
7.4416
7.2600
7.2041
7.1843
6.5249
6.5193
2.6819
2.6761
2.3573
2.0888
0.0050
HO
N
Me
O
O
4-Meph
1y
0.87
1.83
1.87
0.75
0.63
3.09
3.00
10.5 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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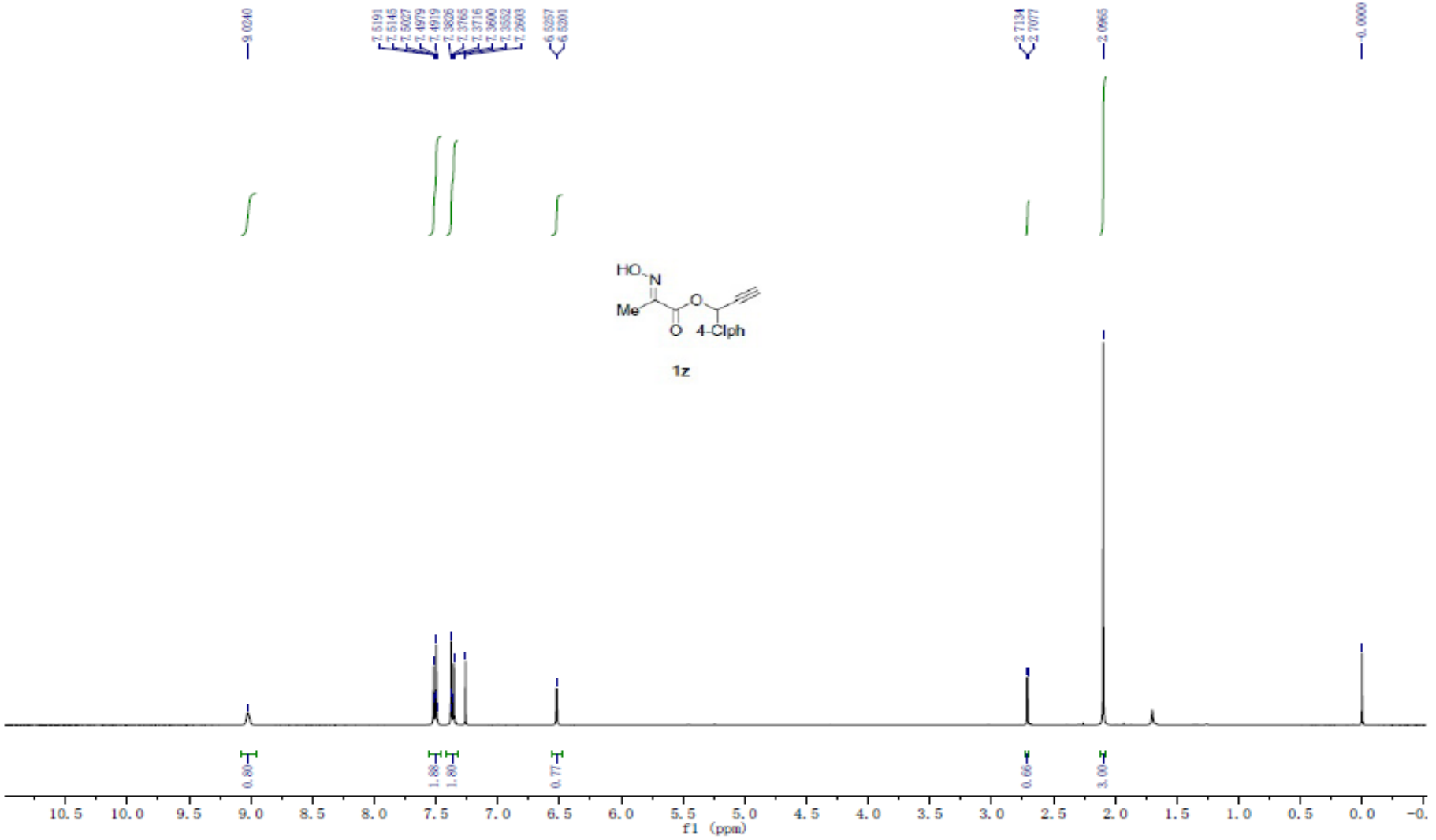
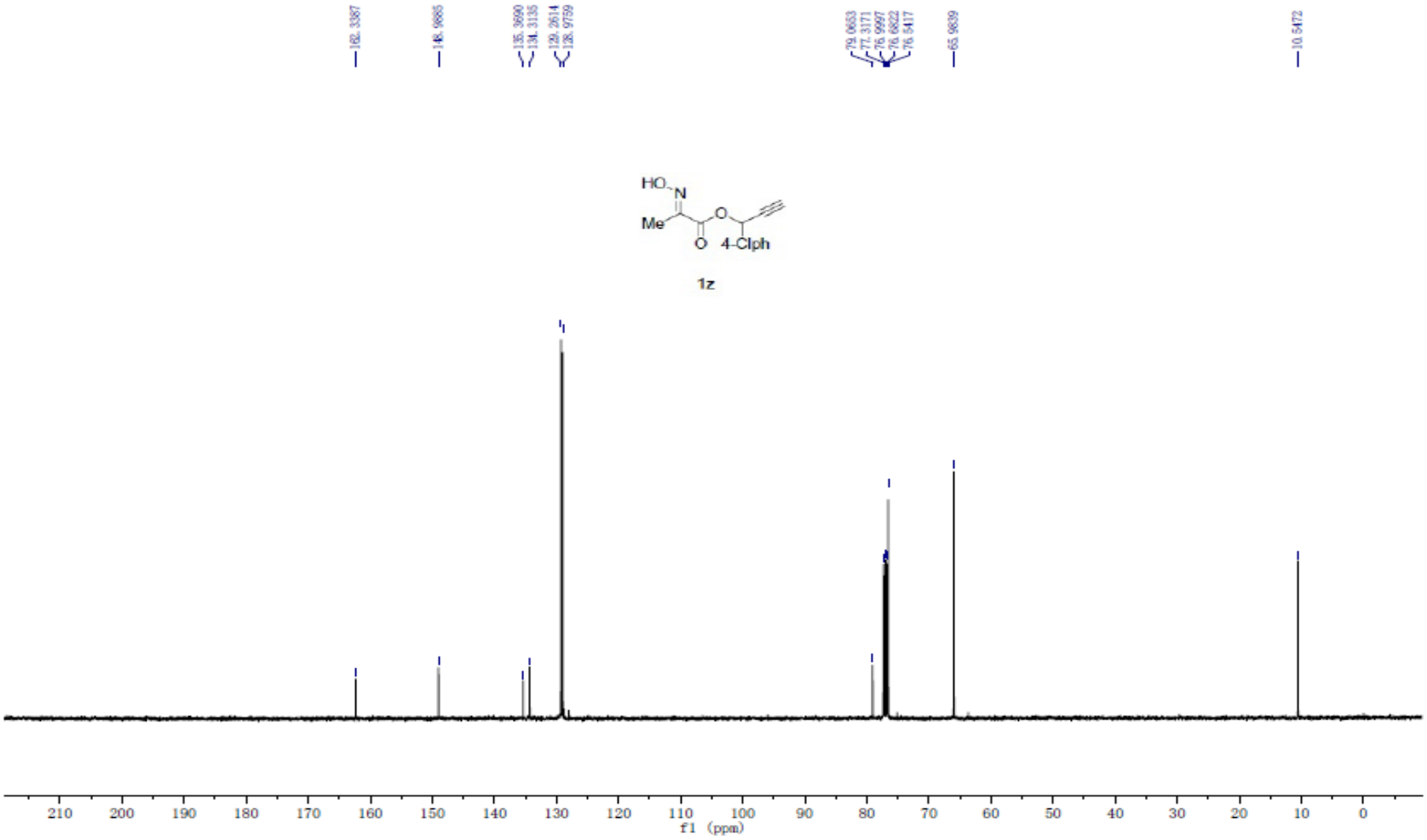
139.3263
132.9990
129.4090
127.8113
79.7021
77.3176
76.9999
76.6824
75.9520
66.6546
21.2199
10.5145
HO
N
Me
O
O
4-Meph
1y
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.0240
7.5191
7.5145
7.5027
7.4979
7.4919
7.3826
7.3765
7.3716
7.3600
7.3552
7.2603
6.5257
6.5201
2.7134
2.7077
2.0965
0.0000
HO
N
Me
O
O
4-ClPh
1z
0.80
1.88
1.80
0.77
0.66
3.00
10.5
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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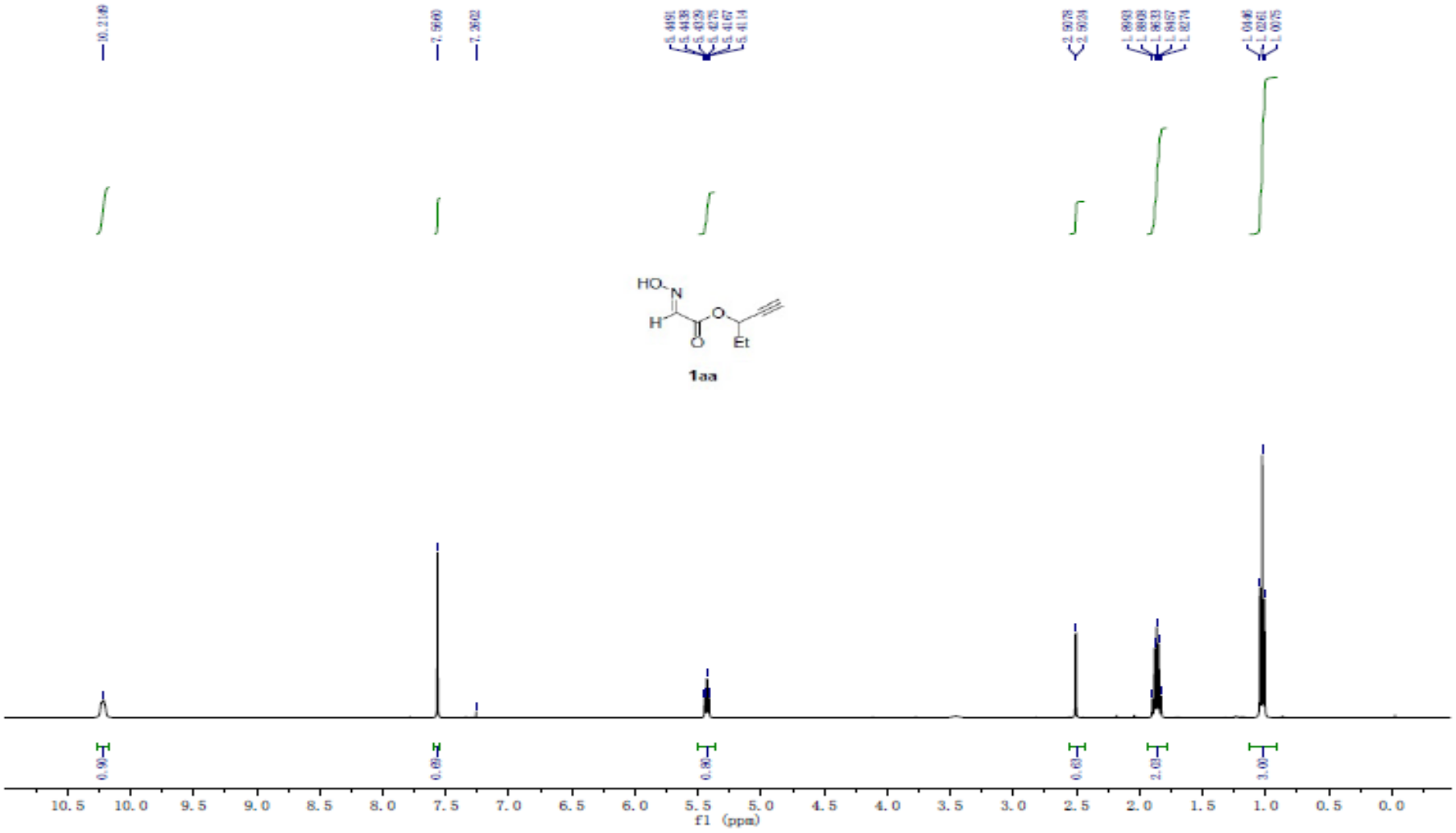
148.9685
135.9690
134.3135
129.2614
128.9759
79.0653
77.3171
76.9997
76.6822
76.5417
65.9839
10.5472
HO
N
Me
O
O
4-Clph
1z
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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5.4451
5.4438
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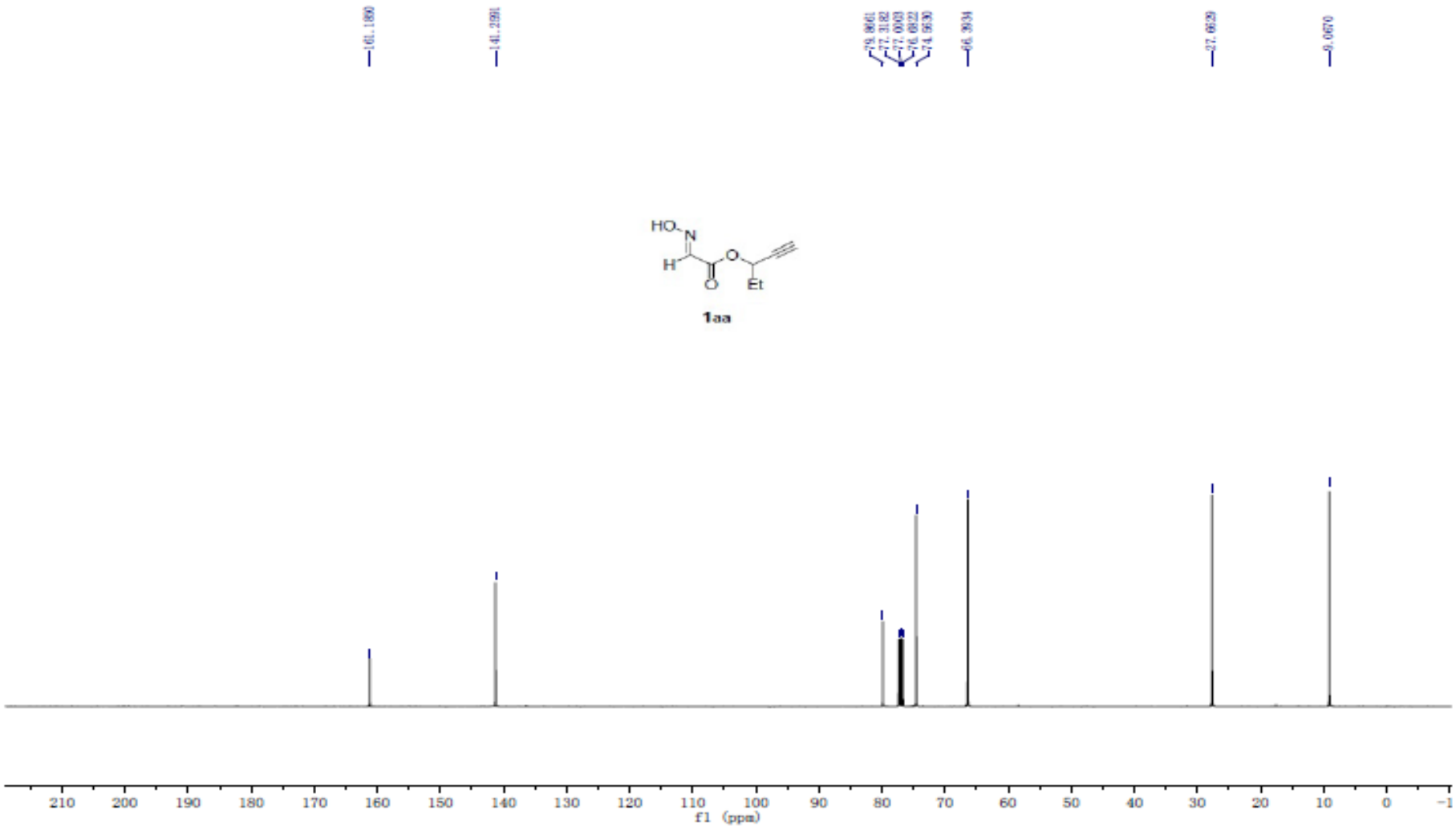
5.4275
5.4167
5.4114
2.5078
2.5034
1.8993
1.8808
1.8633
1.8457
1.8274
1.0486
1.0361
1.0075
HO
N
H
O
O
Et
1aa
0.90
0.89
0.86
0.68
2.03
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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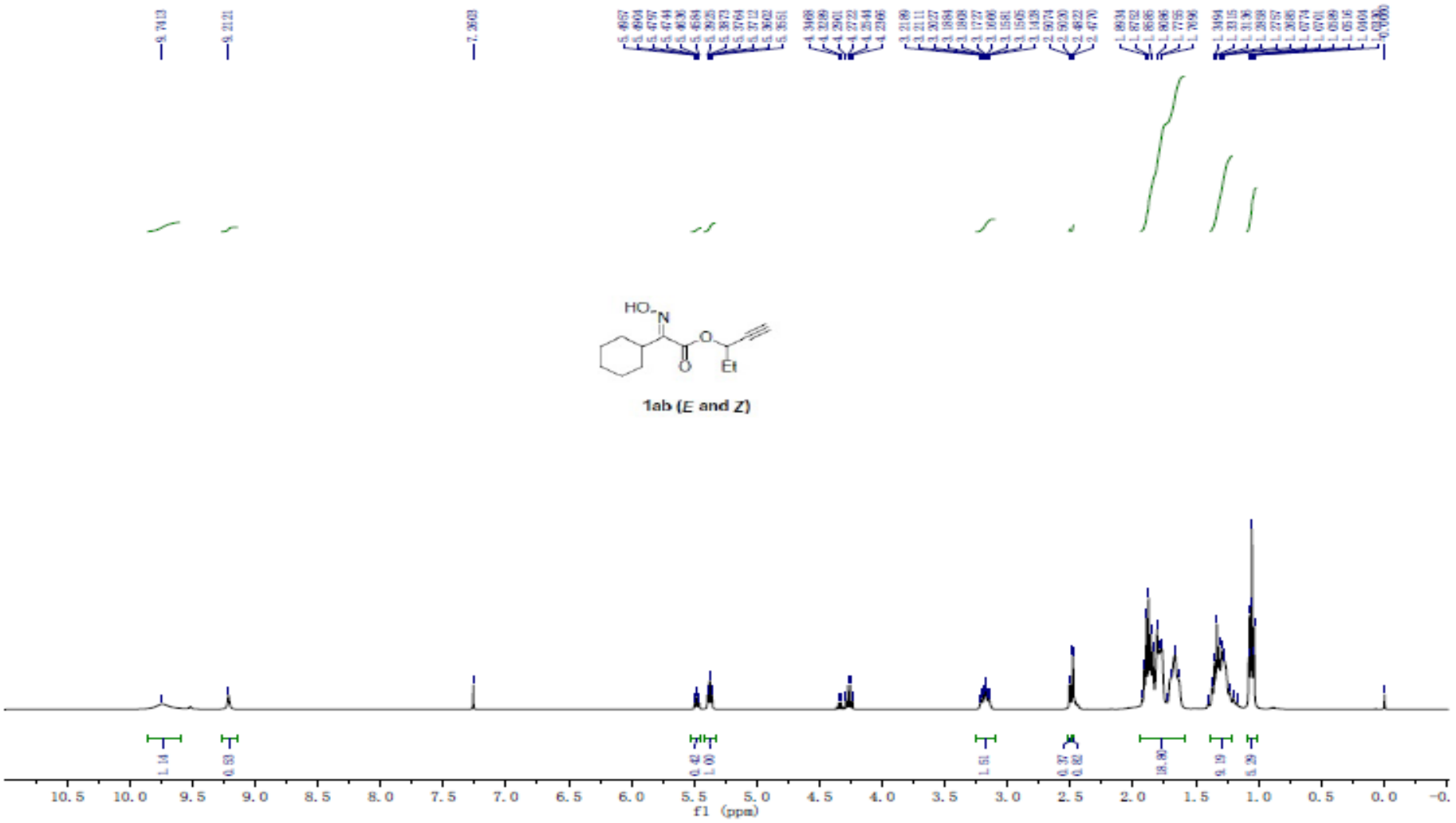
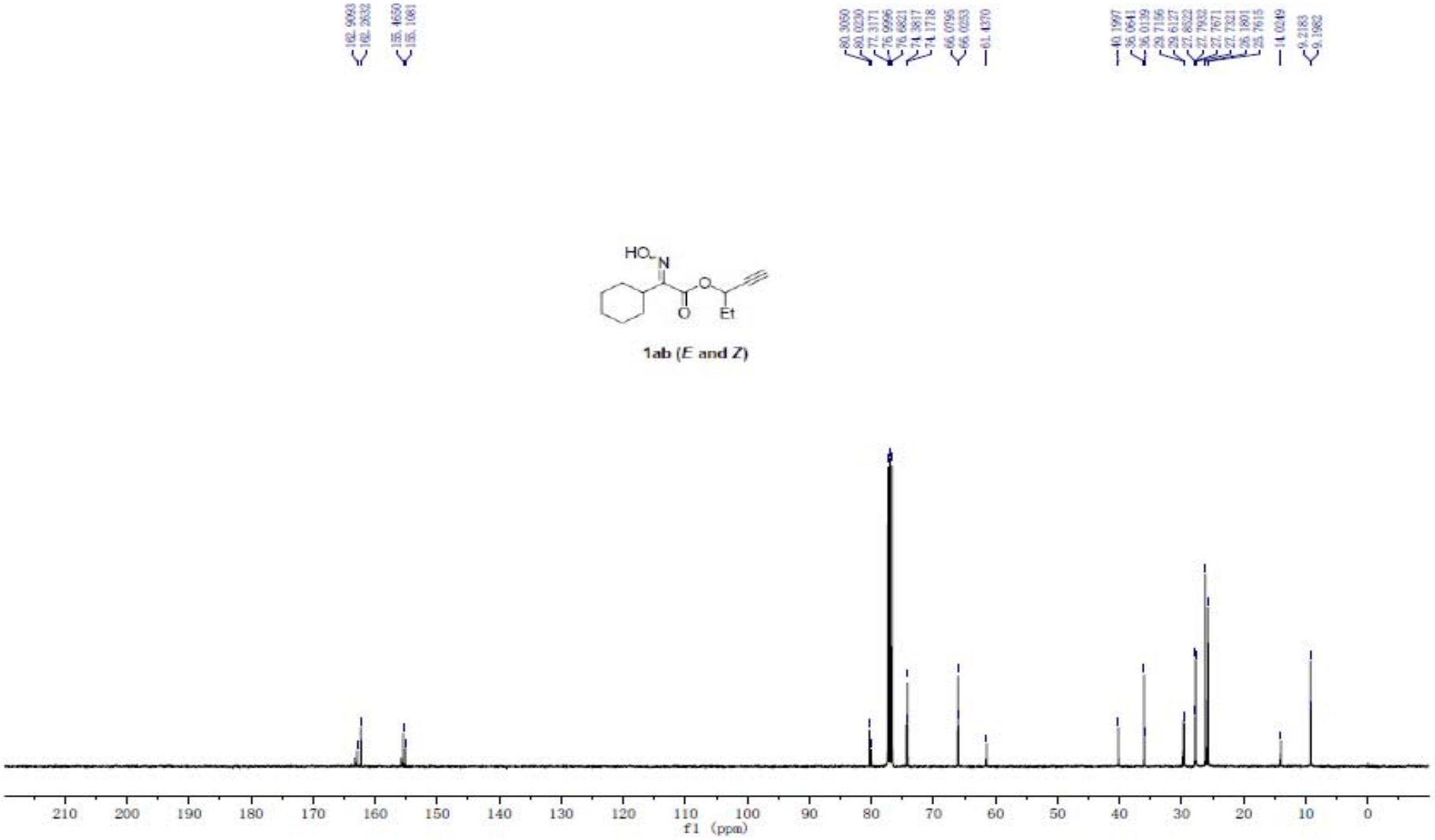
141.2991
79.8661
77.3182
77.0003
76.6822
74.9630
66.3934
27.6629
9.0670
HO
N
H
O
O
Et
1aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


HO
N
O
O
Et
1ab (E and Z)
f1 (ppm)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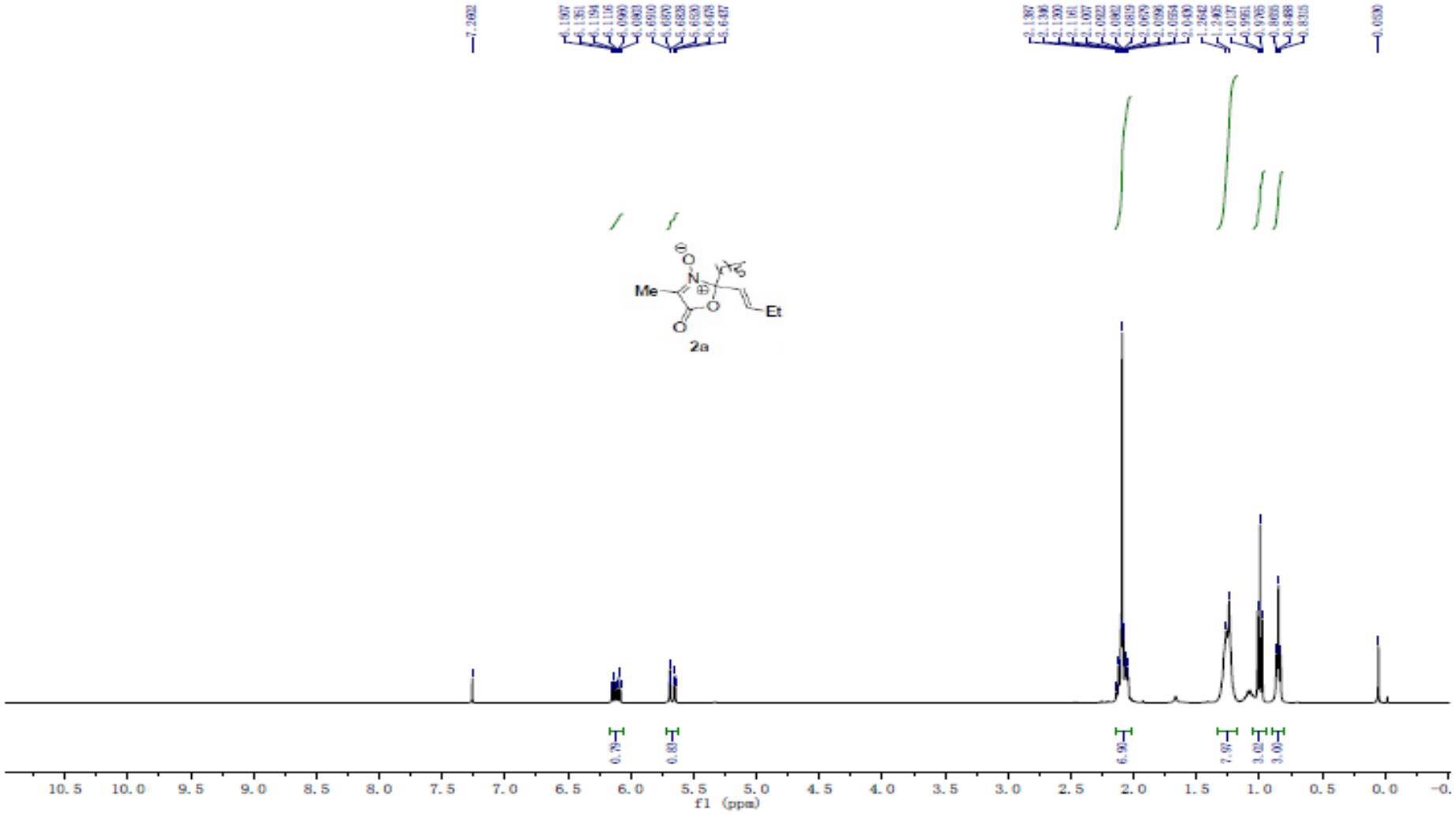
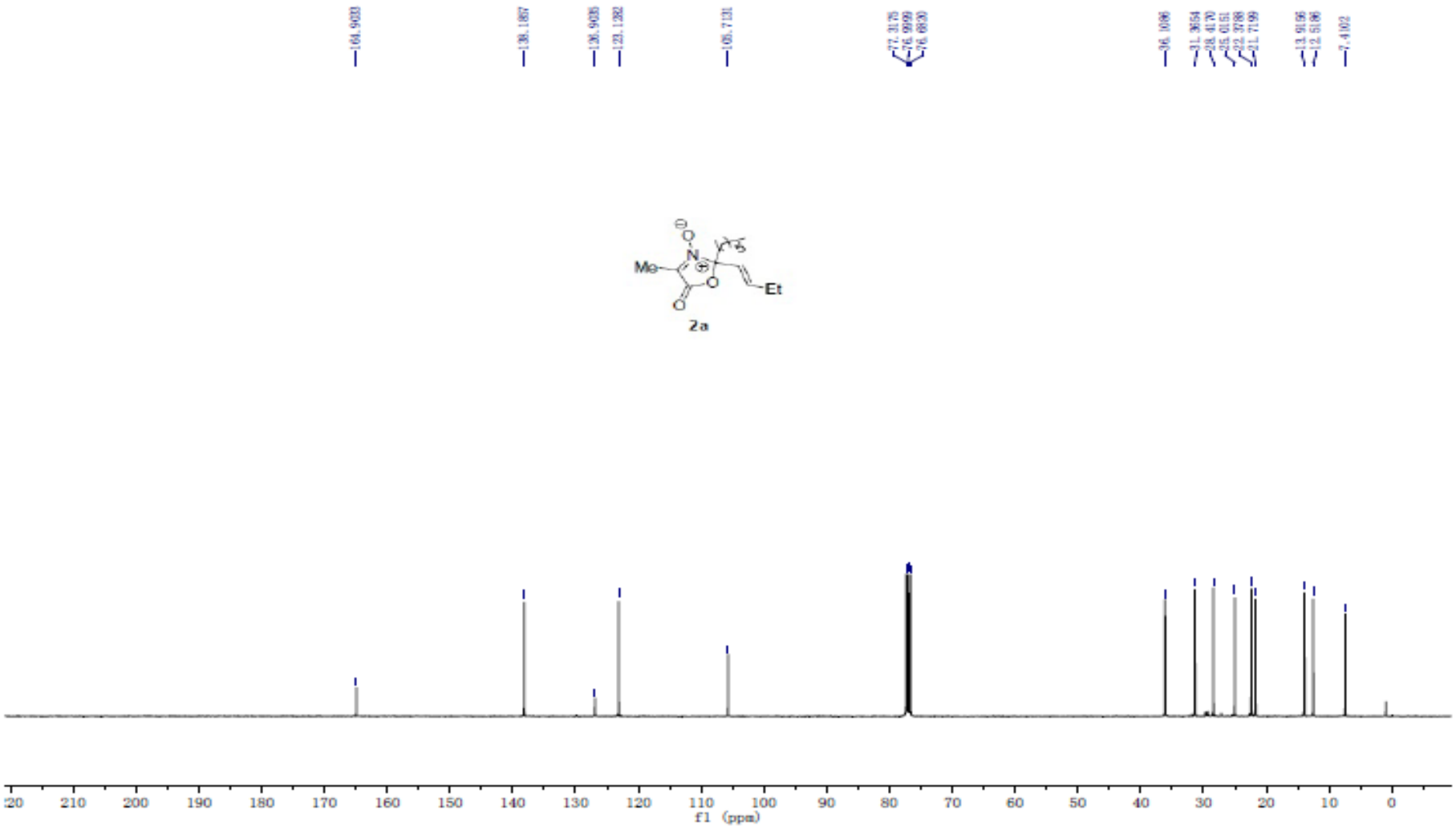
76.9996
76.6821
74.3817
74.1718
66.0795
66.0253
61.4370
40.1997
36.0641
36.0139
29.7196
29.6127
27.8522
27.7932
27.7671
27.7321
26.1801
25.7615
14.0249
9.2183
9.1962
HO
N
O
O
Et
1ab (E and Z)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
Et
2a
f1 (ppm)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76.9999
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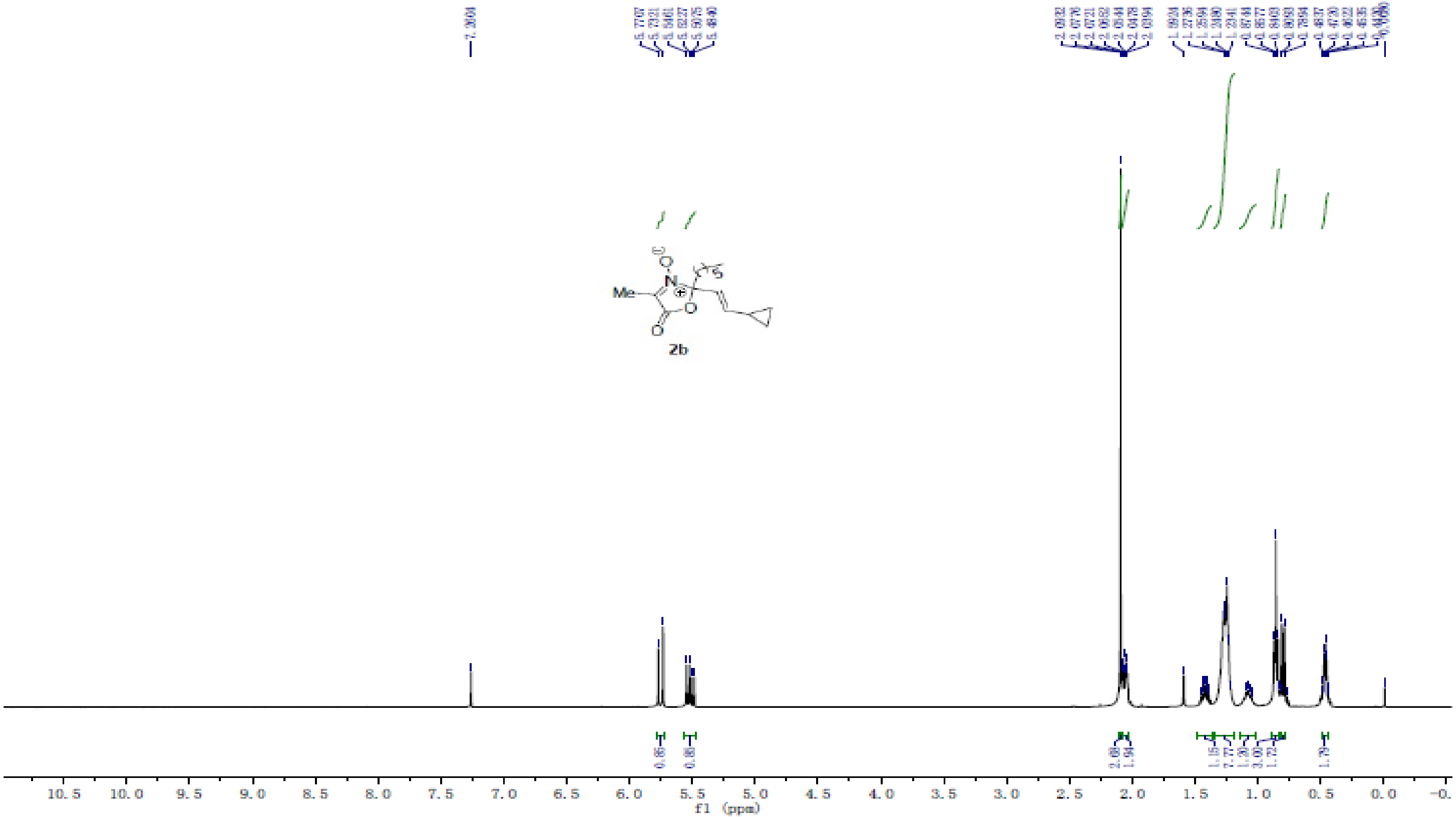
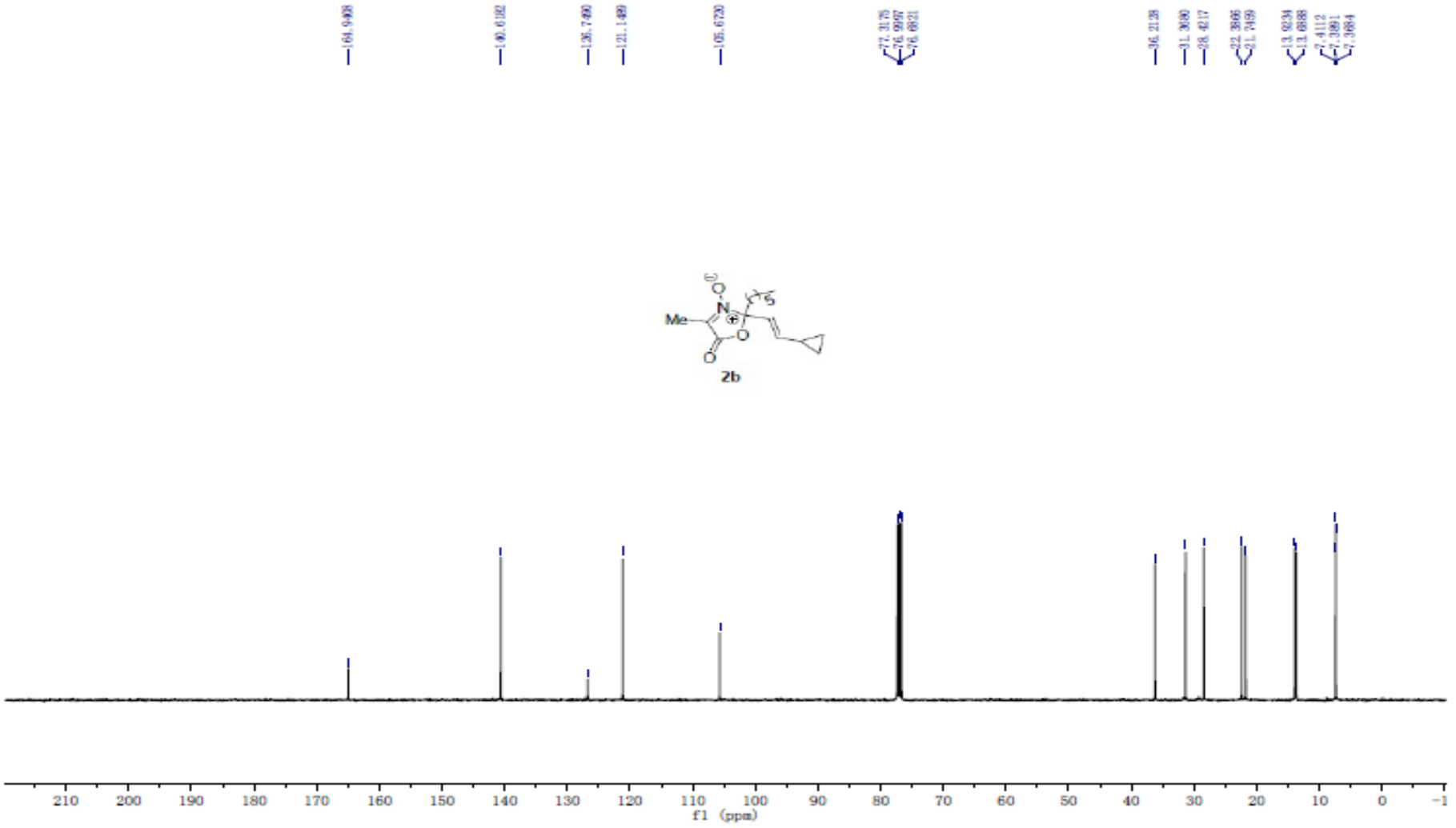
12.5106
7.4102
Me
Et
2a
f1 (ppm)


Me
2b
10.5 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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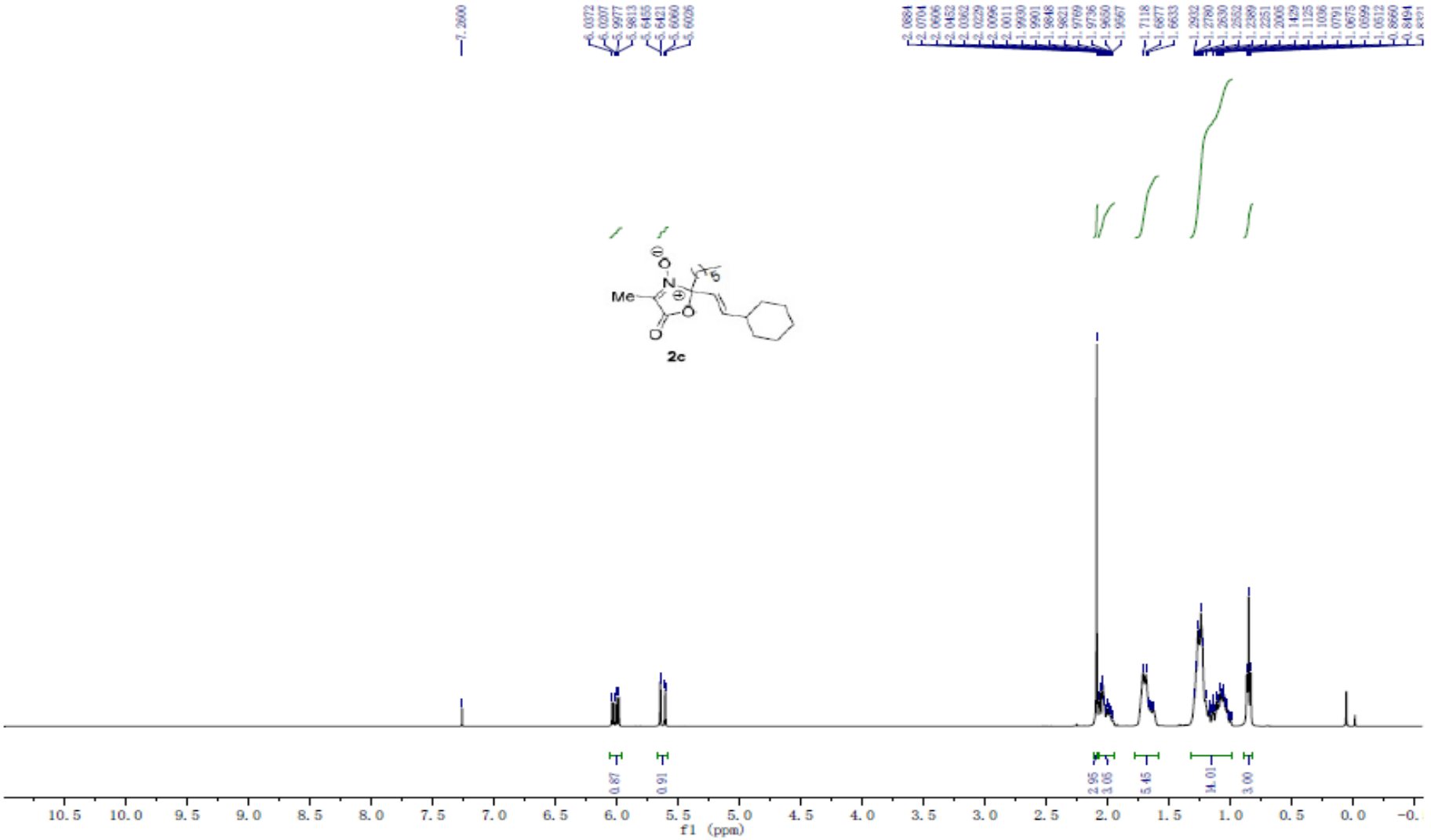
28.4217
22.3866
21.7459
13.9234
13.6888
7.4112
7.3891
7.3684
Me
O
N
O
O
2b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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6.0307
5.9977
5.9813
5.6455
5.6421
5.6060
5.6026
2.0884
2.0704
2.0606
2.0452
2.0362
2.0229
2.0096
2.0011
1.9930
1.9901
1.9848
1.9821
1.9769
1.9736
1.9650
1.9567
1.7118
1.6877
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1.2932
1.2780
1.2630
1.2532
1.2389
1.2251
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1.1429
1.1125
1.1036
1.0791
1.0675
1.0599
1.0512
0.8860
0.8494
Me
2c
0.87
0.91
2.95
3.05
5.45
14.01
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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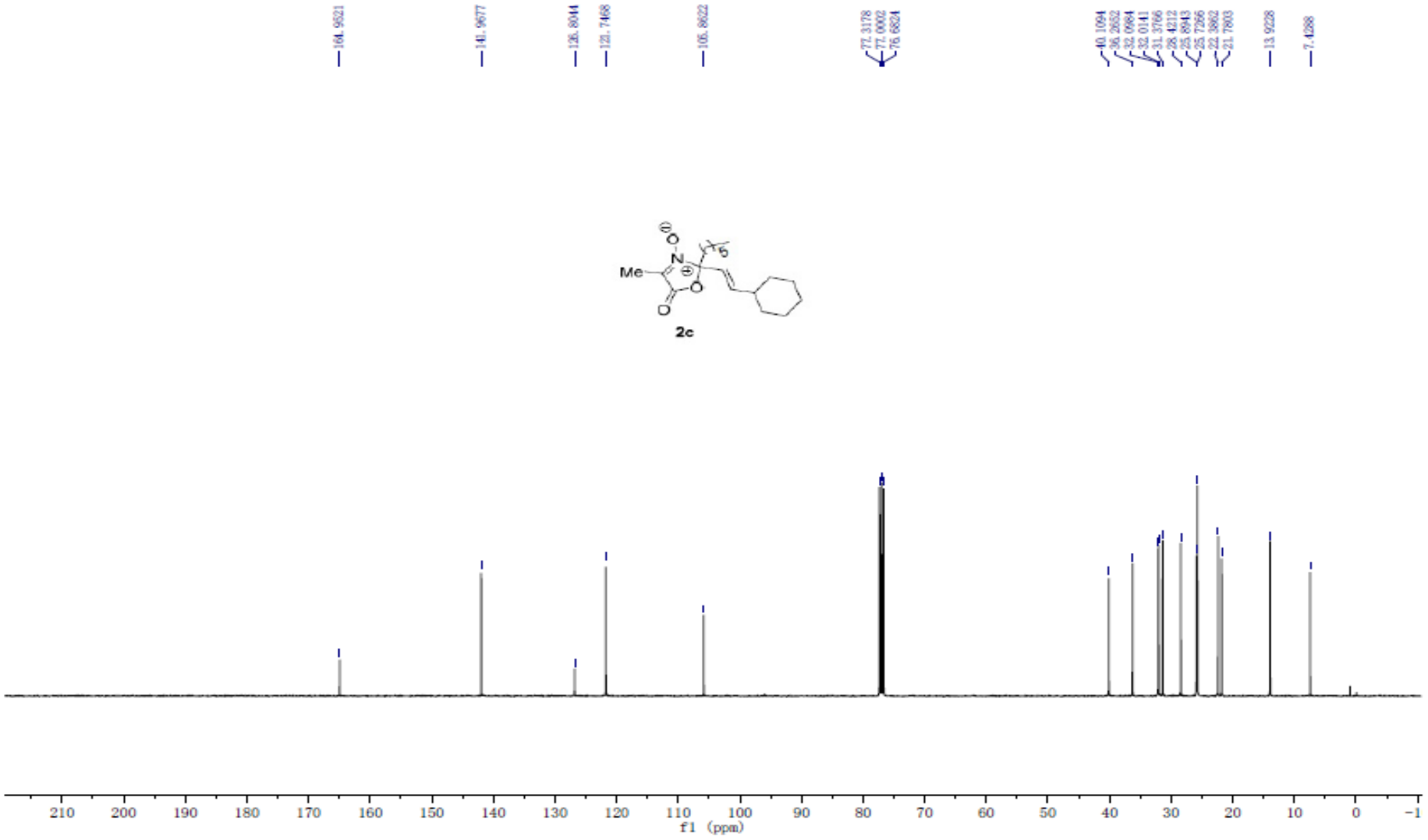
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.0002
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32.0984
32.0141
31.3766
28.4212
25.8943
25.7296
22.3862
21.7803
13.9228
7.4288
Me
2c
210
200
190
180
170
160
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120
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100
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80
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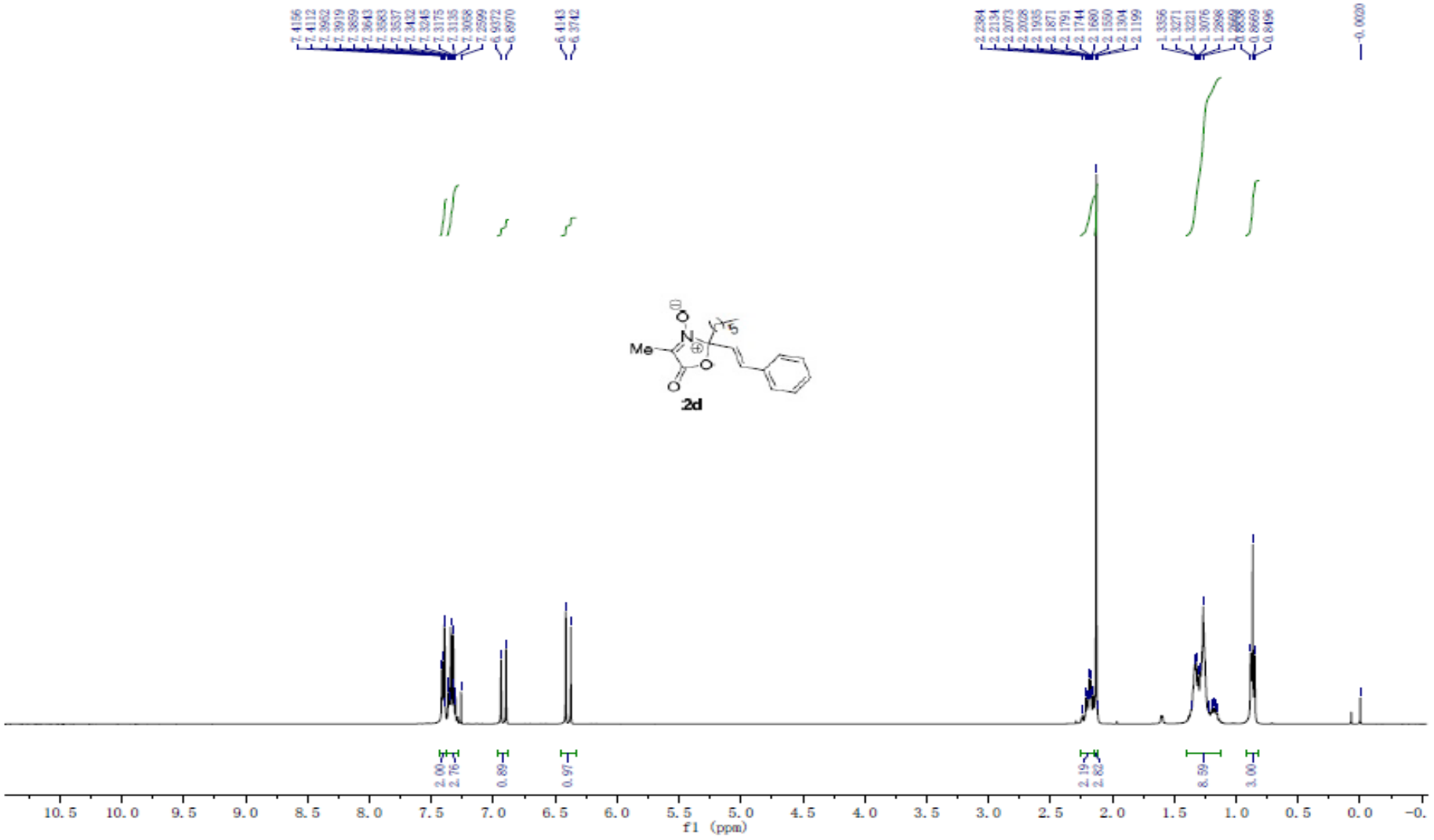
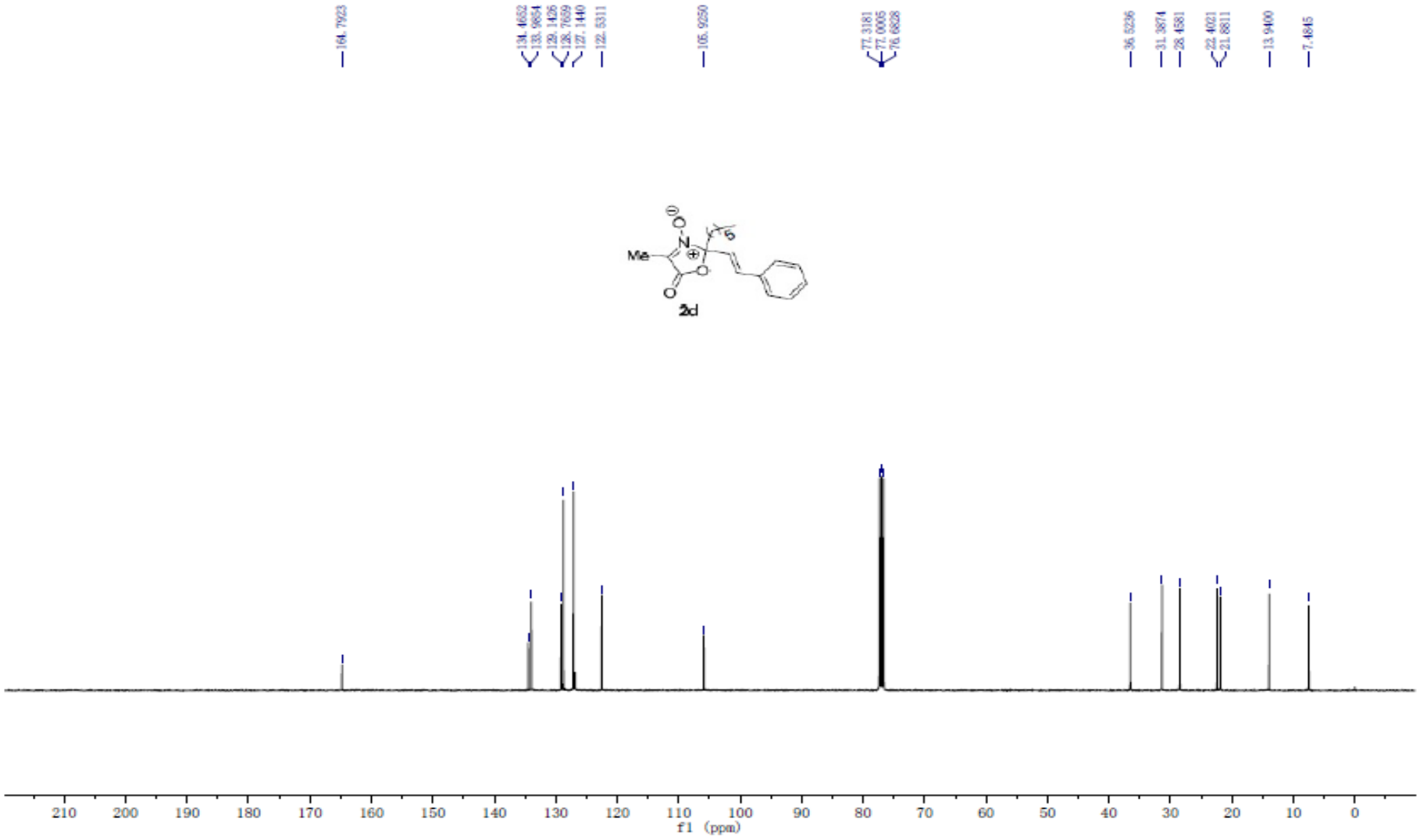
60
50
40
30
20
10
0
−1
f1 (ppm)


Me
2d
f1 (ppm)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128.7659
127.1440
122.5311
105.9250
77.3181
77.0005
76.6828
36.5236
31.3874
28.4581
22.4021
21.8811
13.9400
7.4845
Me
2cl
210
200
190
180
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100
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70
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50
40
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10
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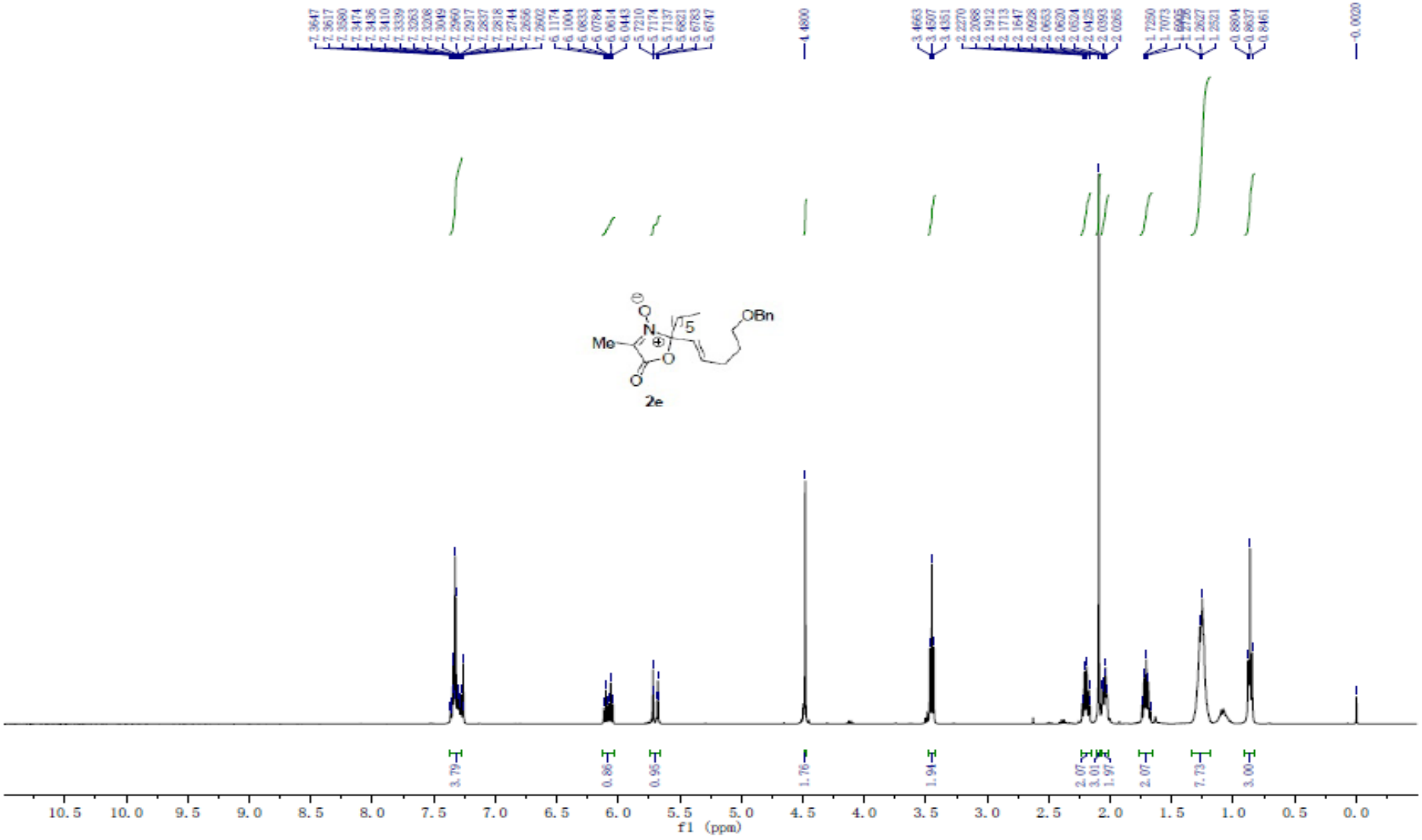
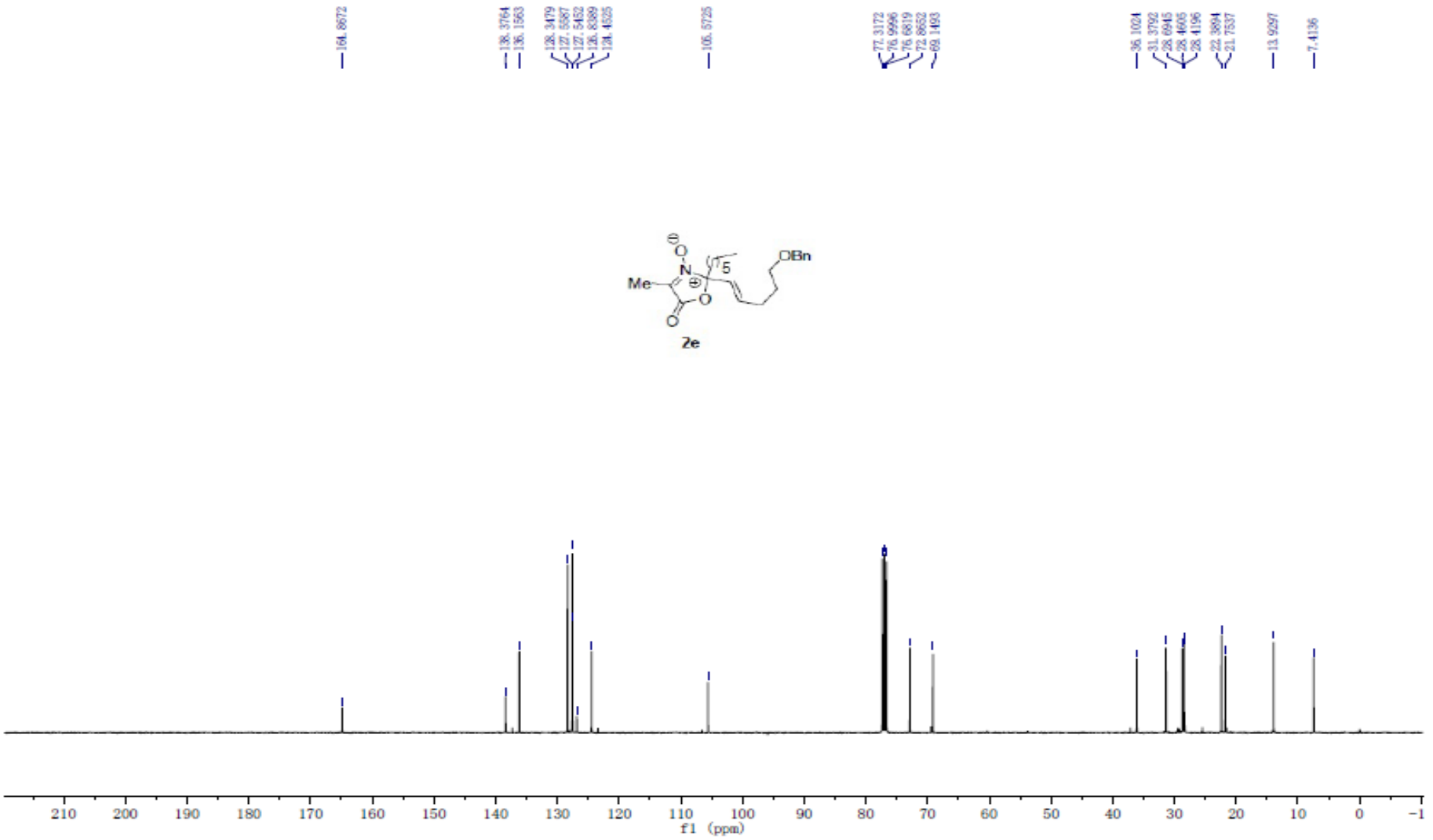
f1 (ppm)


OBn
Me
2e
f1 (ppm)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136.1563
128.3479
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124.4025
105.5725
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76.9996
76.6819
72.8652
69.1493
36.1024
31.3792
28.6945
26.4605
26.4196
22.3894
21.7537
13.9297
7.4136
Me
OBn
5
Ze
210
200
190
180
170
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100
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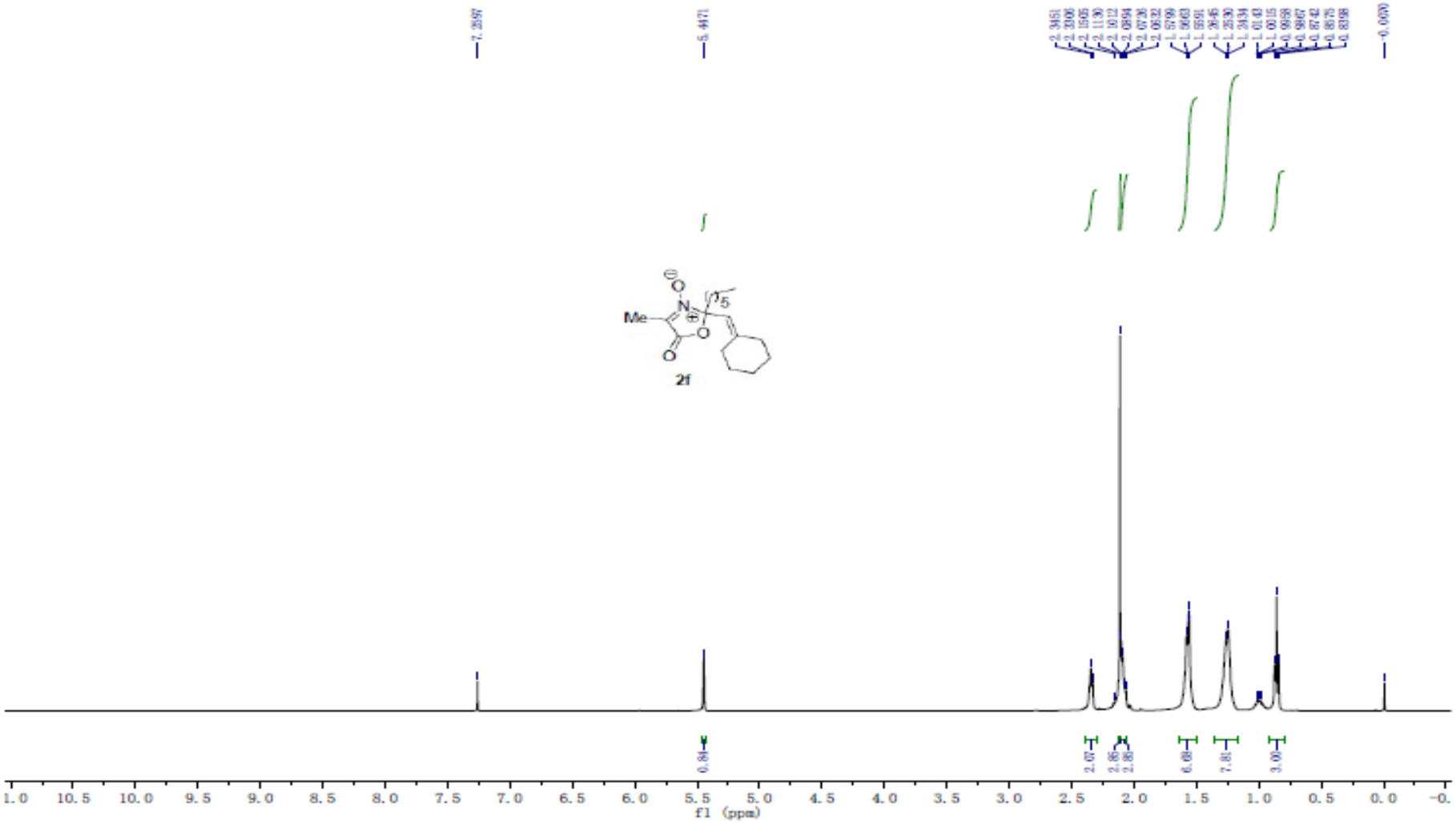
f1 (ppm)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2.1130
2.1012
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2.0720
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1.5799
1.5663
1.5591
1.3645
1.3530
1.3434
1.0143
1.0015
0.9958
0.9867
0.8742
0.8675
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2.85
2.88
6.08
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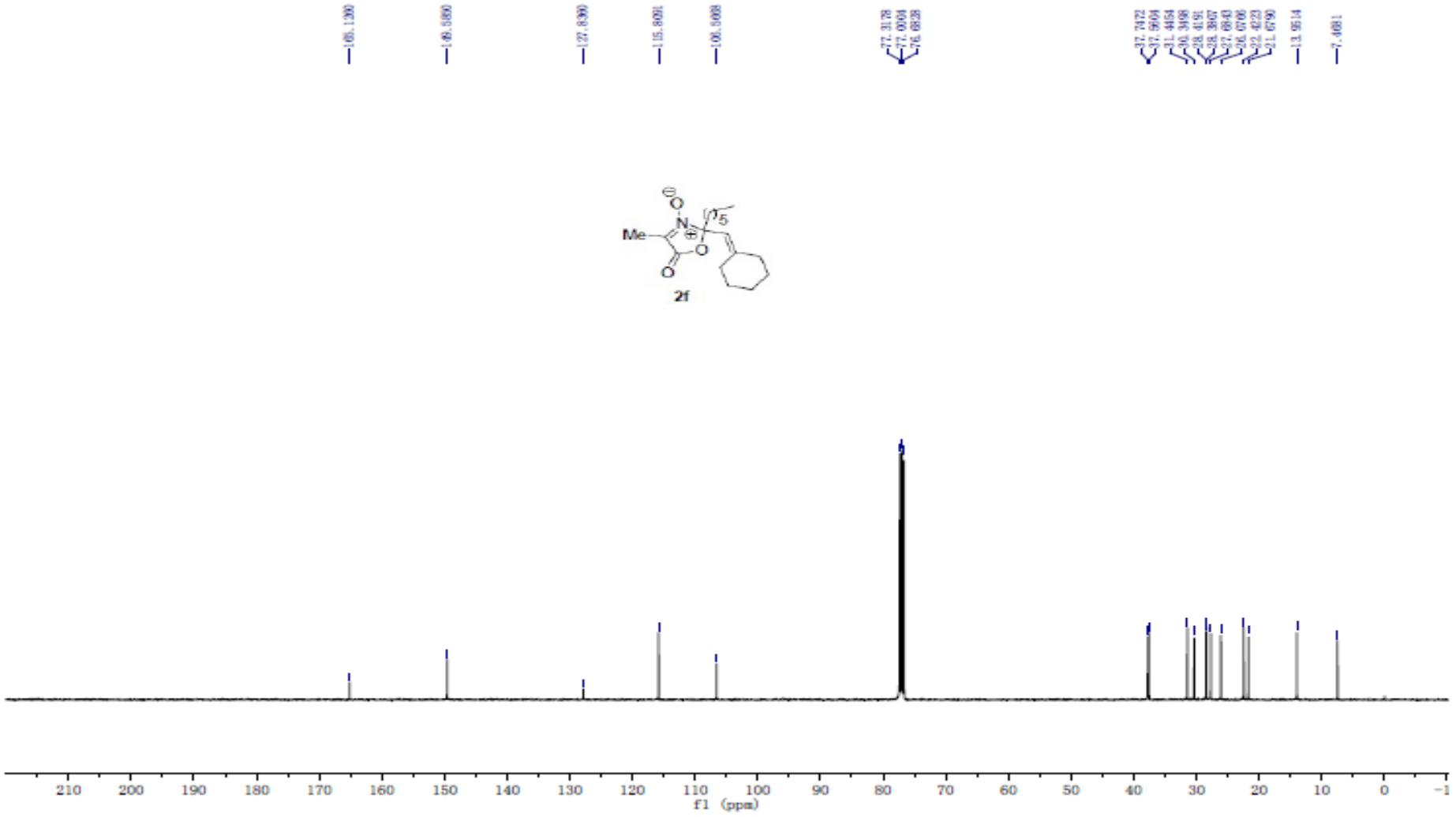
3.00
f1 (ppm)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30.3498
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27.6843
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13.9514
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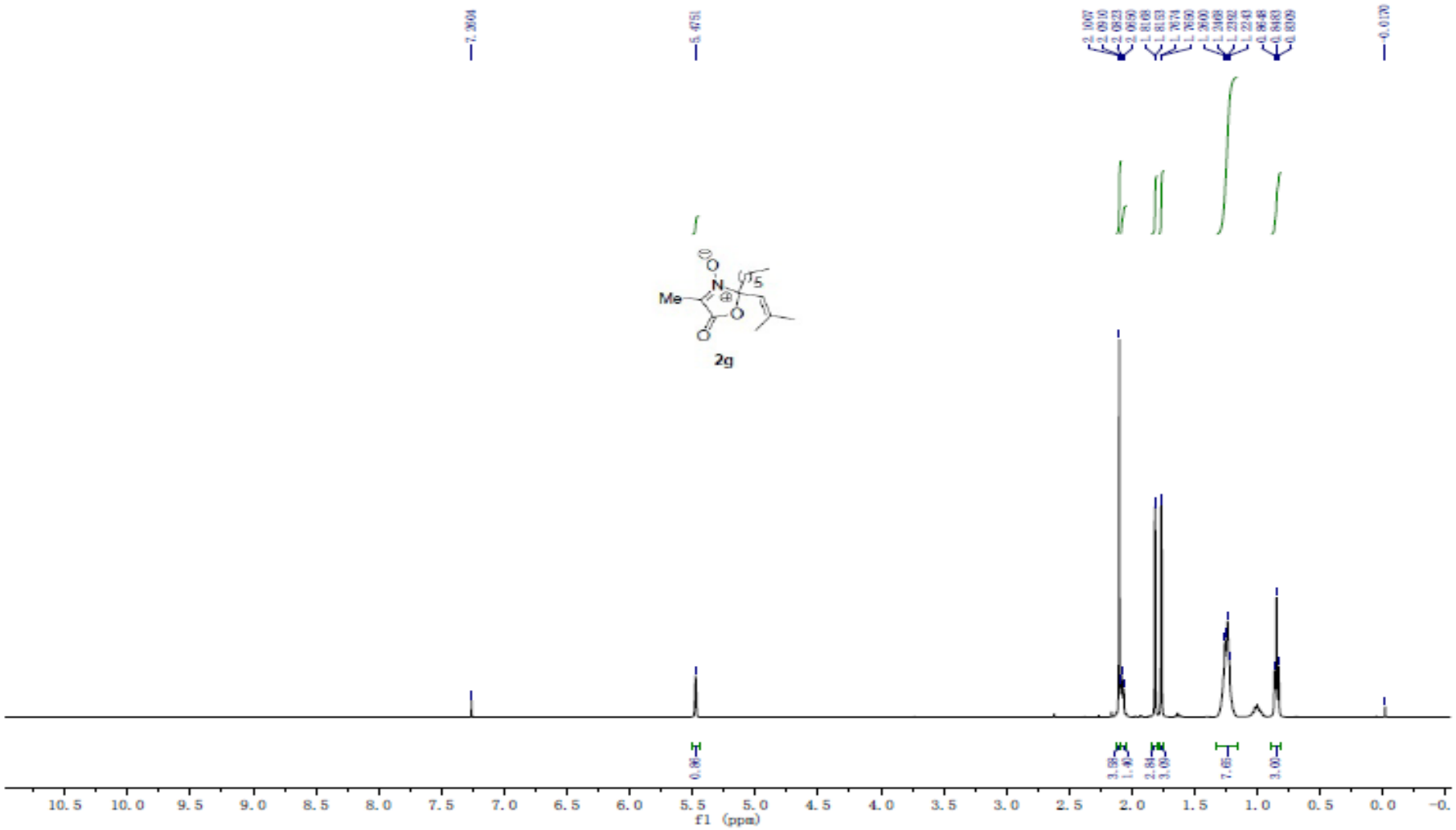
Me
2f
f1 (ppm)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1.3468
1.2392
1.2243
0.8648
0.8483
0.8309
-0.0170
Me
2g
0.98
3.58
1.49
2.84
3.00
7.65
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
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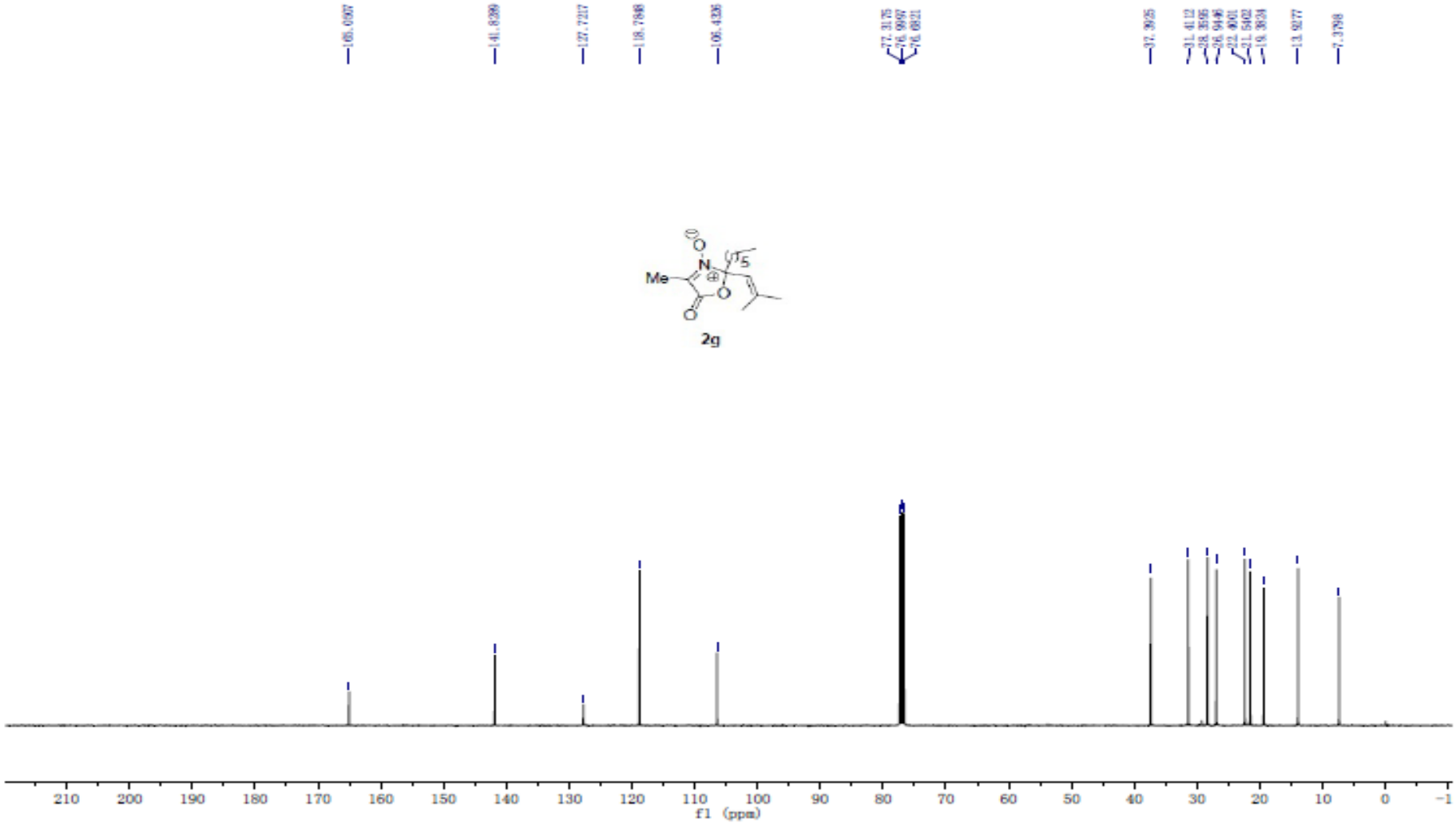
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26.9496
22.8061
21.5492
19.3834
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7.3798
Me
2g
210
200
190
180
170
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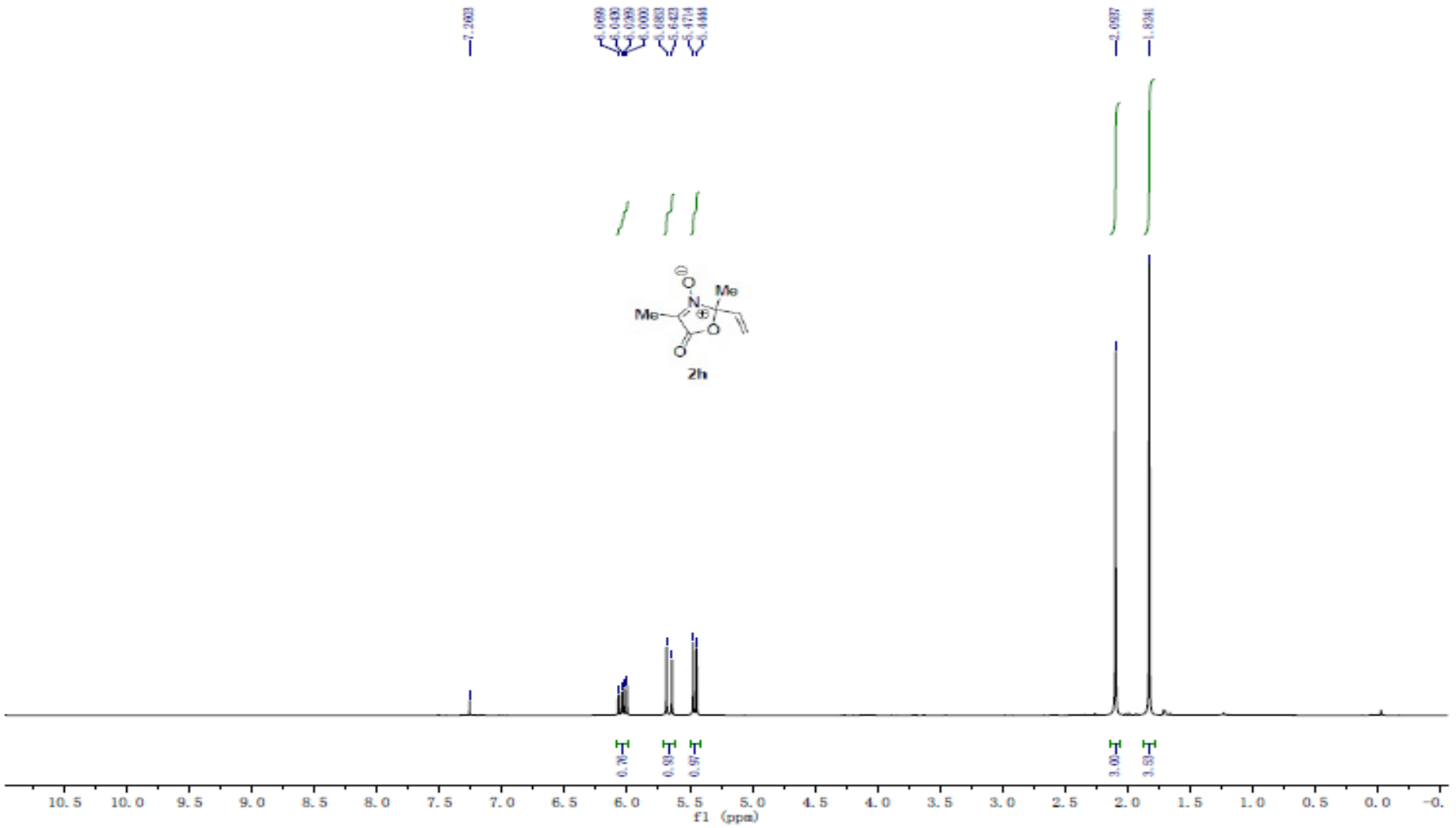
−1
f1 (ppm)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2.0337
1.8341
Me
Me
2h
0.70
0.98
0.97
3.00
3.83
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
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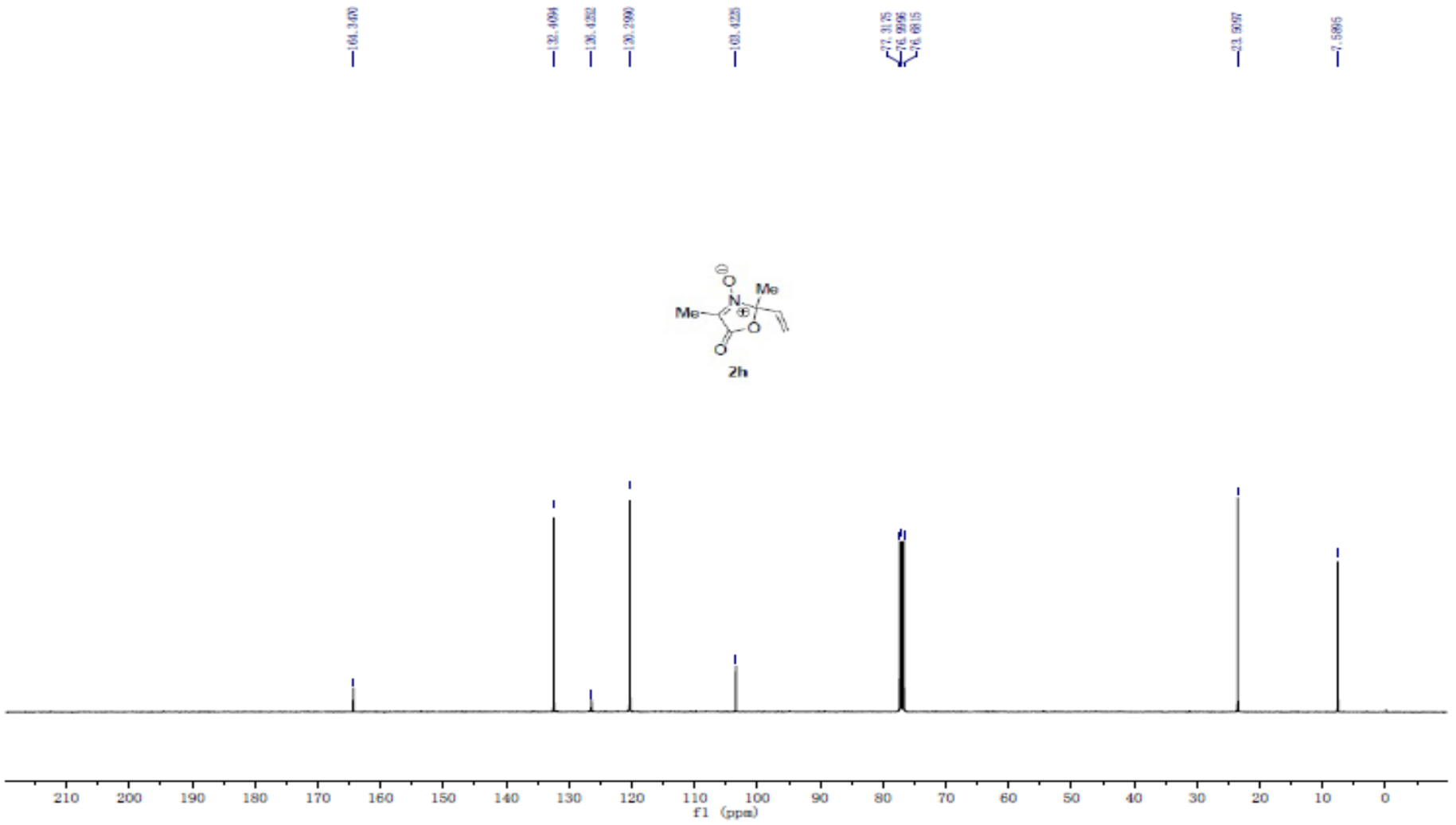
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Me
Me
2h
210
200
190
180
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150
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130
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90
80
70
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50
40
30
20
10
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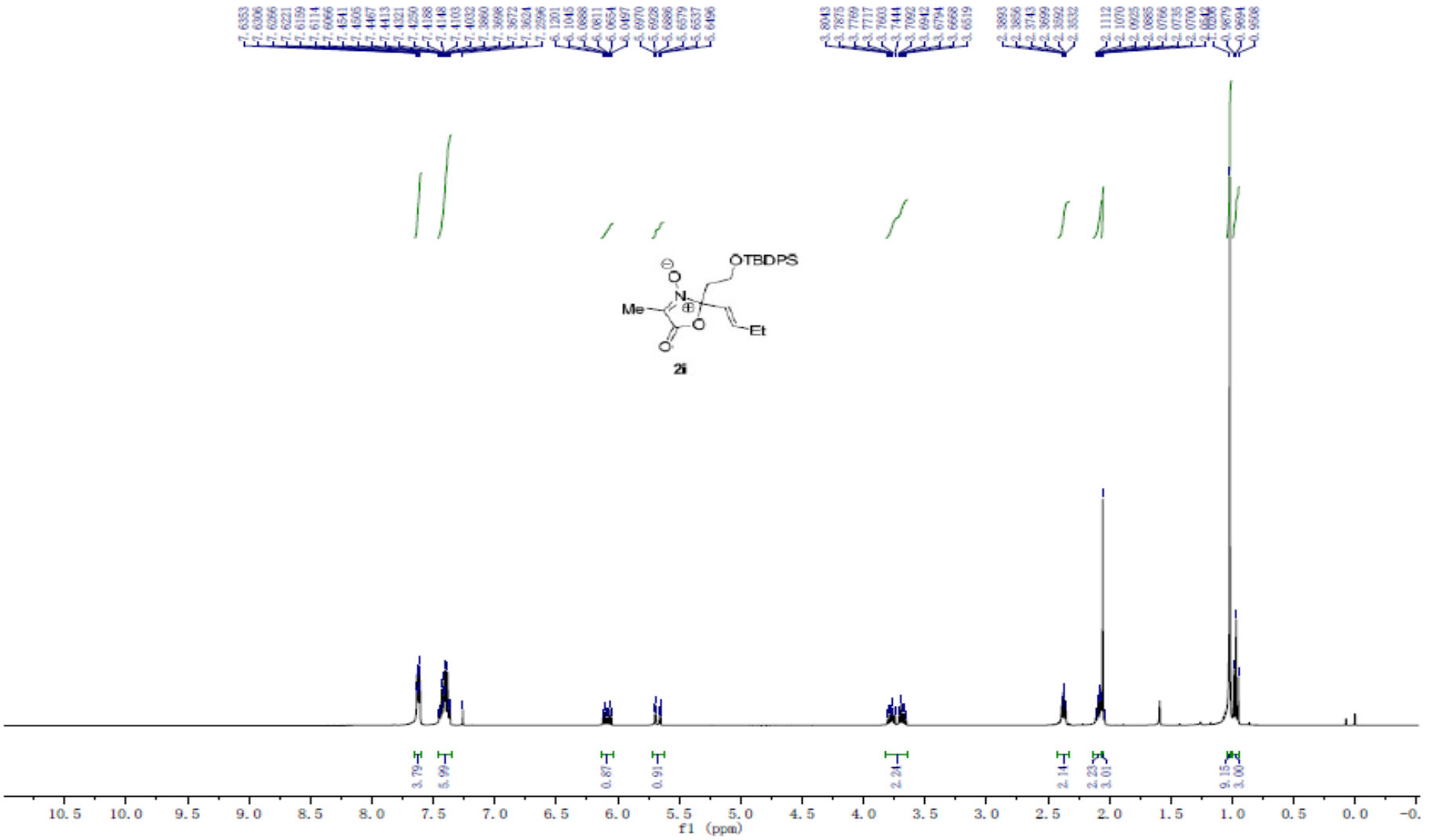
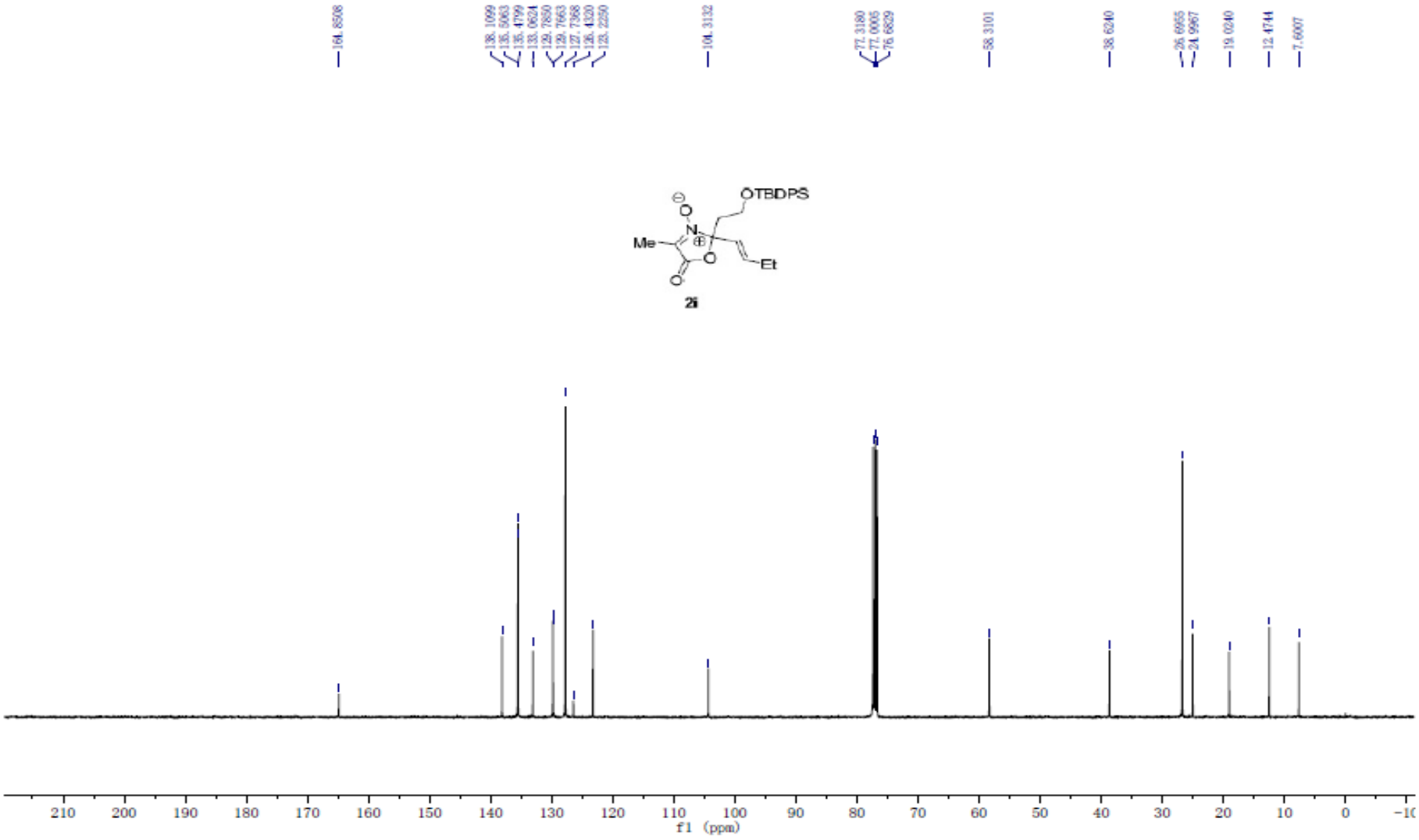
f1 (ppm)


OTBDPS
Me
Et
2i
f1 (ppm)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77.3180
77.0005
76.6829
58.3101
38.6240
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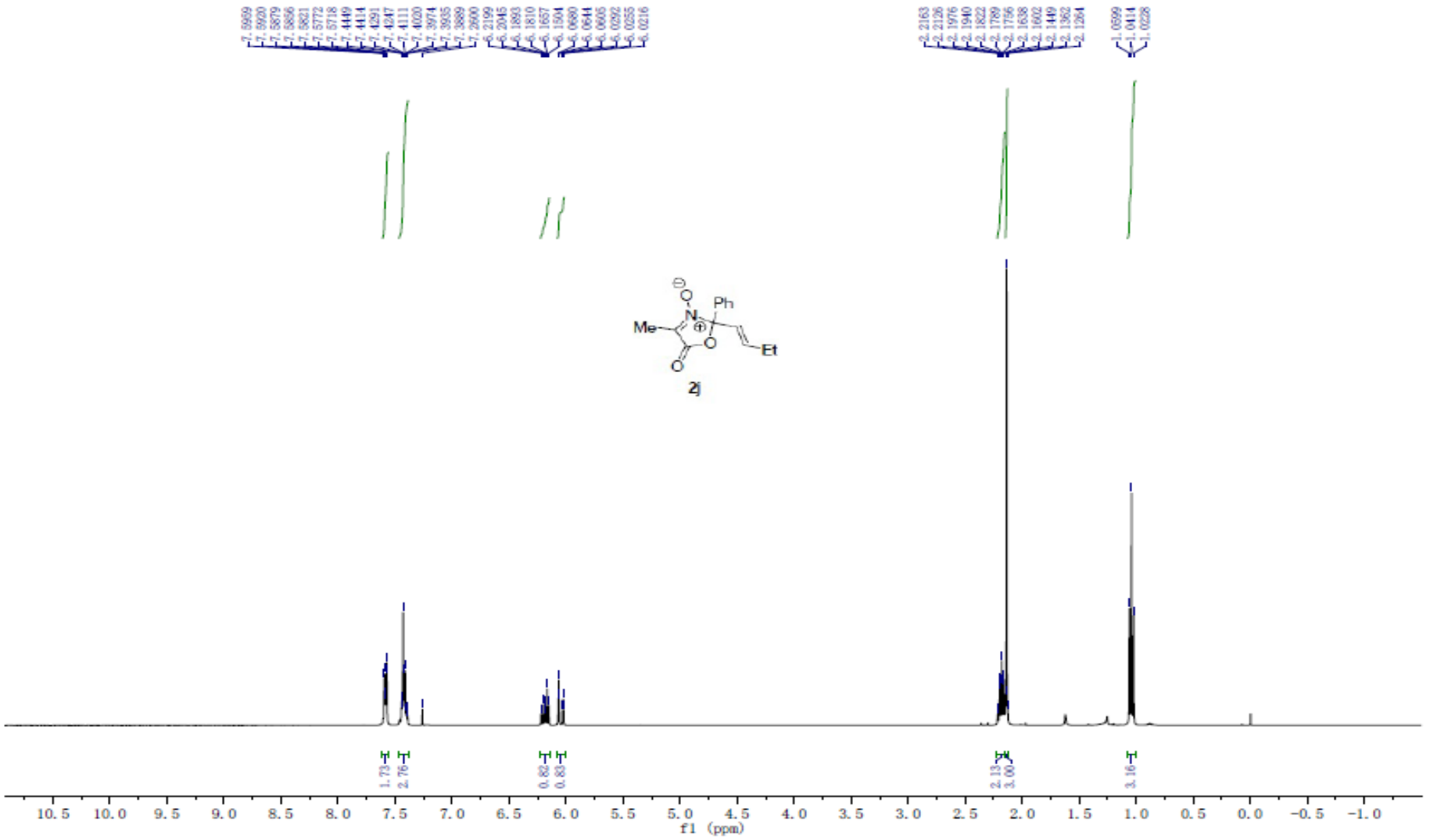
7.6007
OTBDPS
Me
Et
O
N
2i
f1 (ppm)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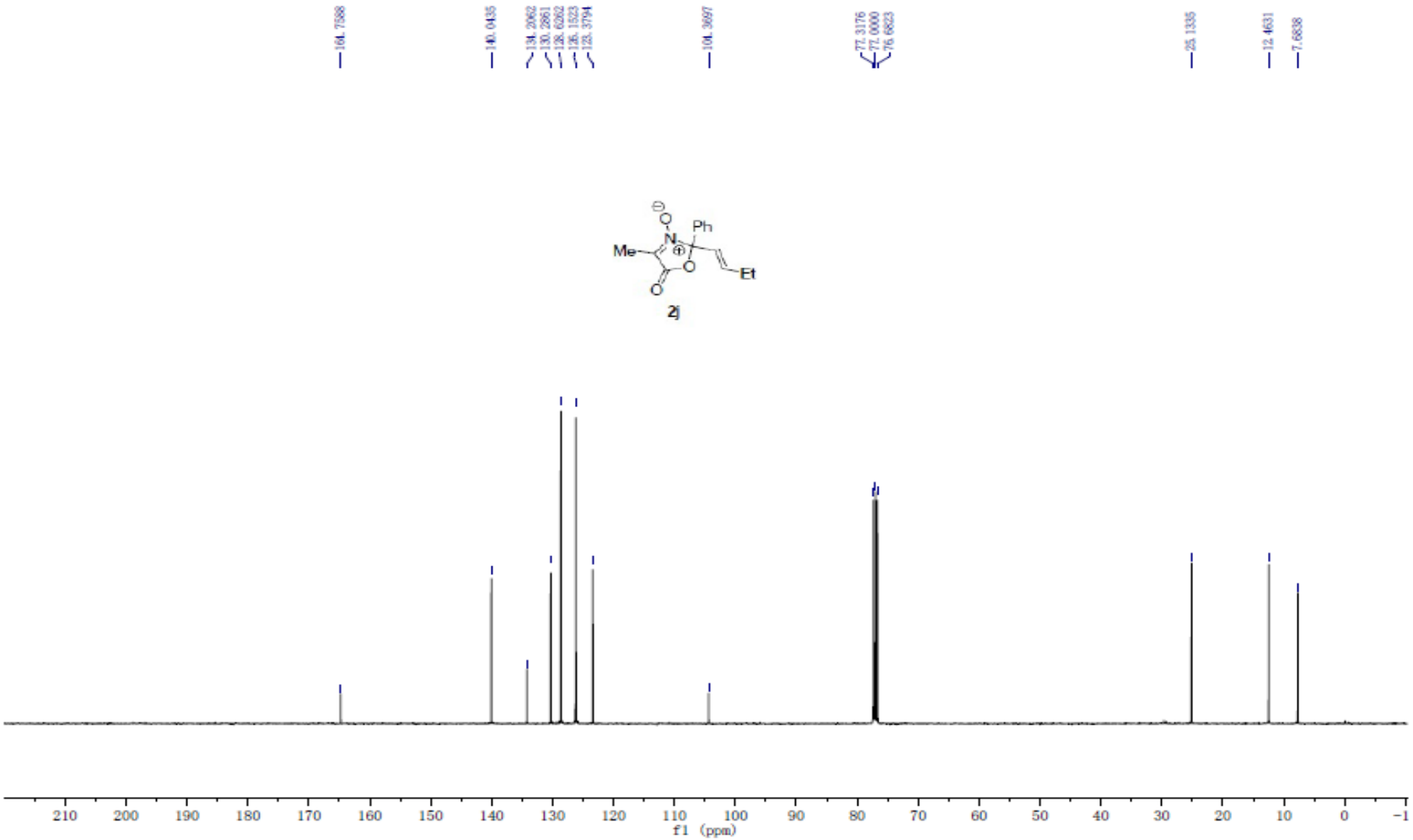
7.4247
7.4111
7.4020
7.3974
7.3935
7.3889
7.2900
6.2199
6.2045
6.1893
6.1810
6.1657
6.1504
6.0680
6.0644
6.0605
6.0292
6.0255
6.0216
2.2163
2.2126
2.1976
2.1940
2.1822
2.1789
2.1756
2.1638
2.1602
2.1449
2.1362
2.1264
1.0599
1.0414
1.0228
Ph
Me
Et
2j
1.73
2.76
0.62
0.83
2.13
3.00
3.16
10.5 10.0 9.5 9.0 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 -1.0
f1 (ppm)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25.1335
12.4631
7.6838
Ph
Me
Et
2j
210
200
190
180
170
160
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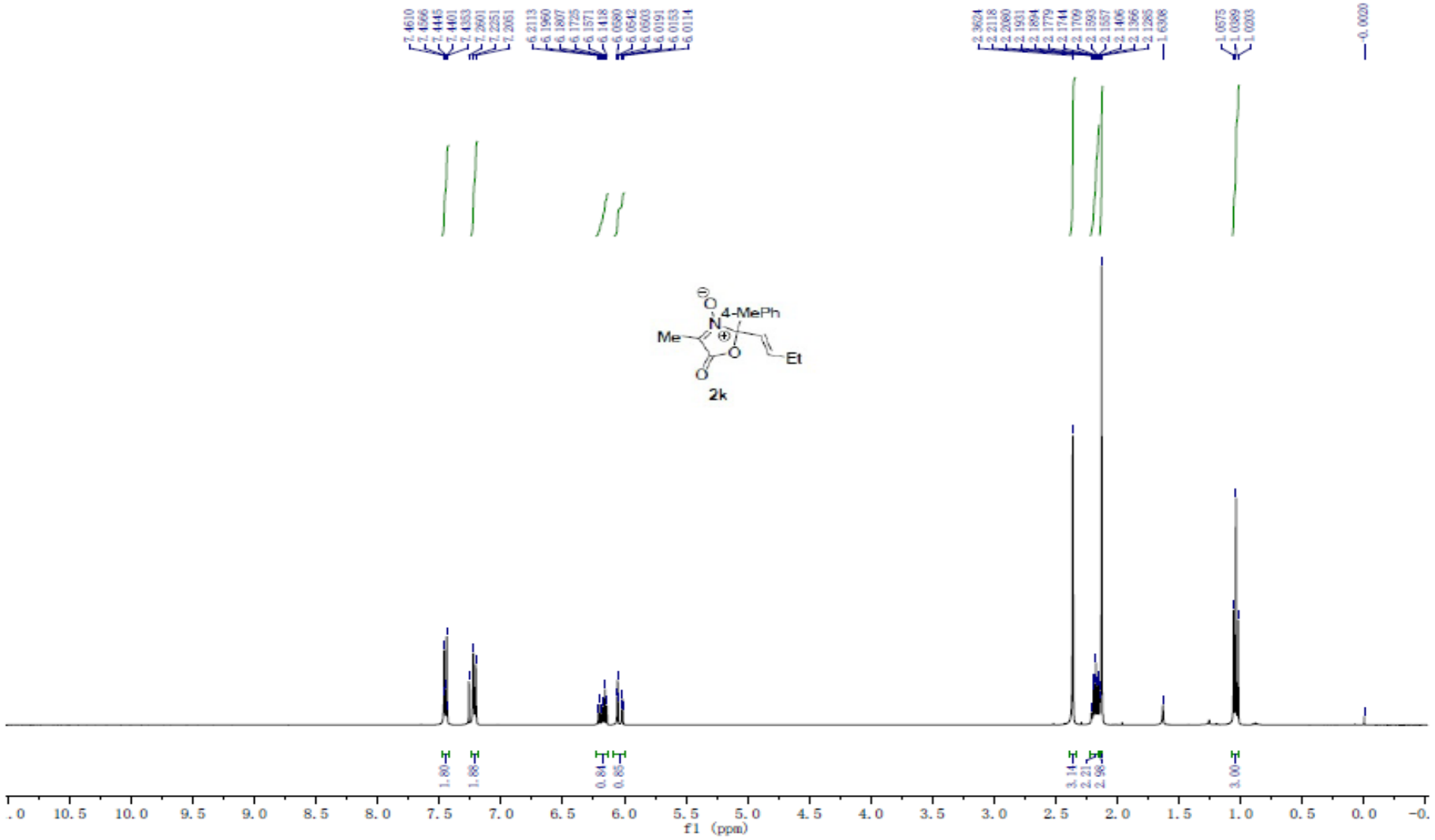
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)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6.2113
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6.1571
6.1418
6.0590
6.0542
6.0503
6.0191
6.0153
6.0114
2.3624
2.2118
2.2060
2.1931
2.1894
2.1779
2.1744
2.1709
2.1593
2.1557
2.1405
2.1366
2.1265
1.6308
1.0575
1.0389
1.0203
0.0020
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Me
Et
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0.84
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2.21
2.98
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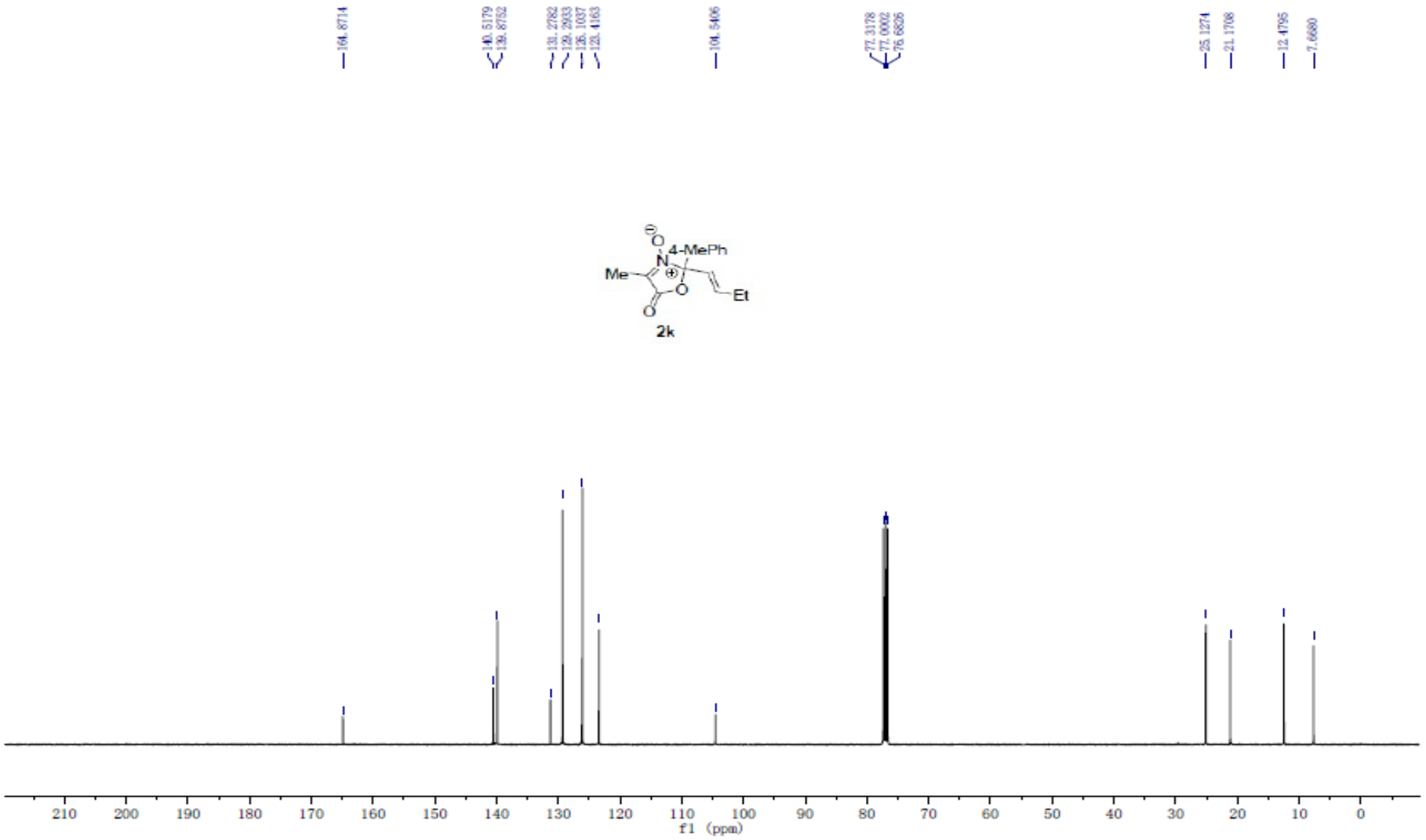
f1 (ppm)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25.1274
21.1708
12.4795
7.6680
4-MePh
Me
Et
2k
210
200
190
180
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130
120
110
100
90
80
70
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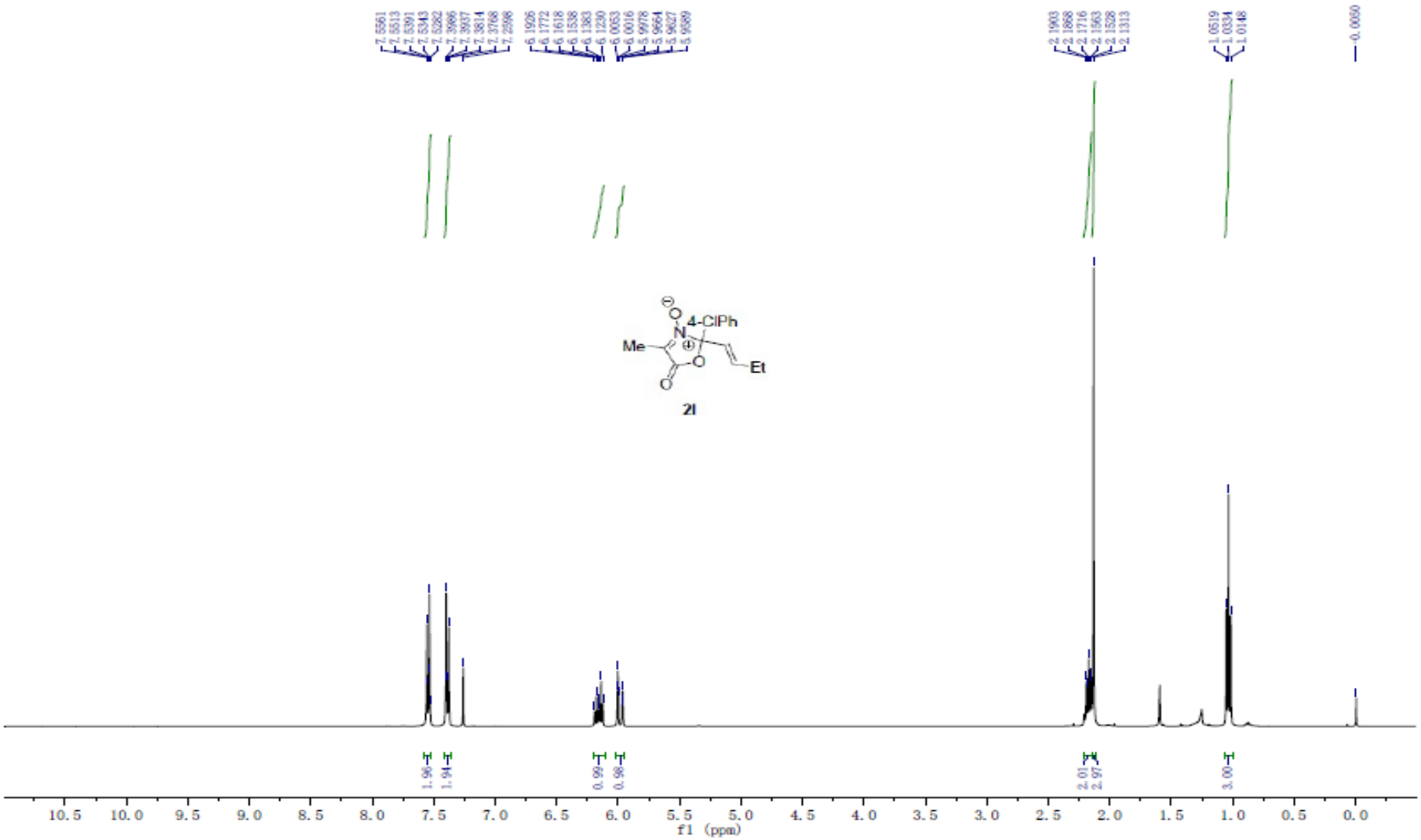
50
40
30
20
10
0
f1 (ppm)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6.1618
6.1538
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6.1230
6.0053
6.0016
5.9978
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5.9627
5.9589
2.1903
2.1868
2.1716
2.1563
2.1528
2.1313
1.0519
1.0334
1.0148
0.0050
4-ClPh
Me
Et
2l
1.96
1.94
0.99
0.98
2.01
2.97
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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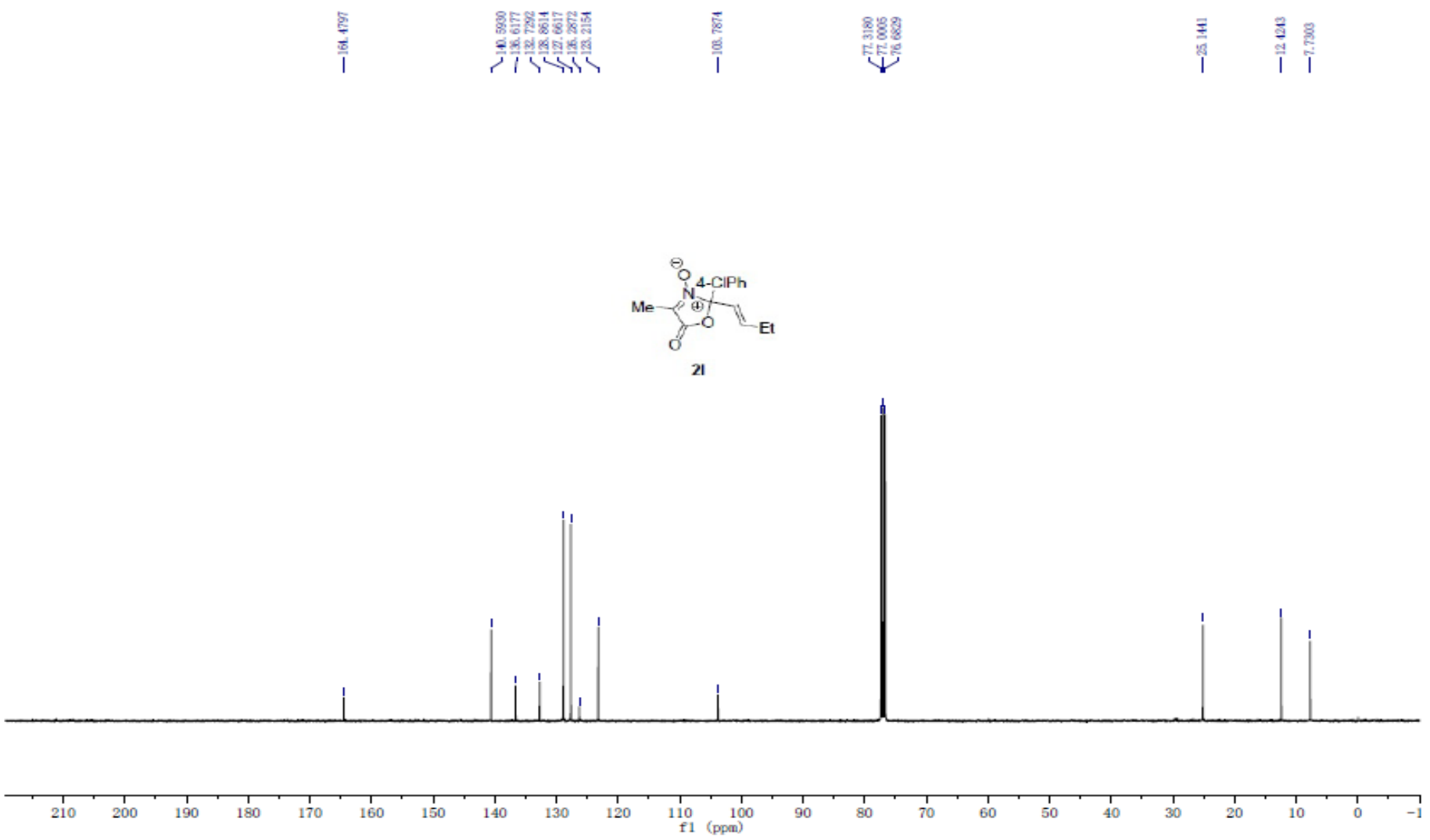
f1 (ppm)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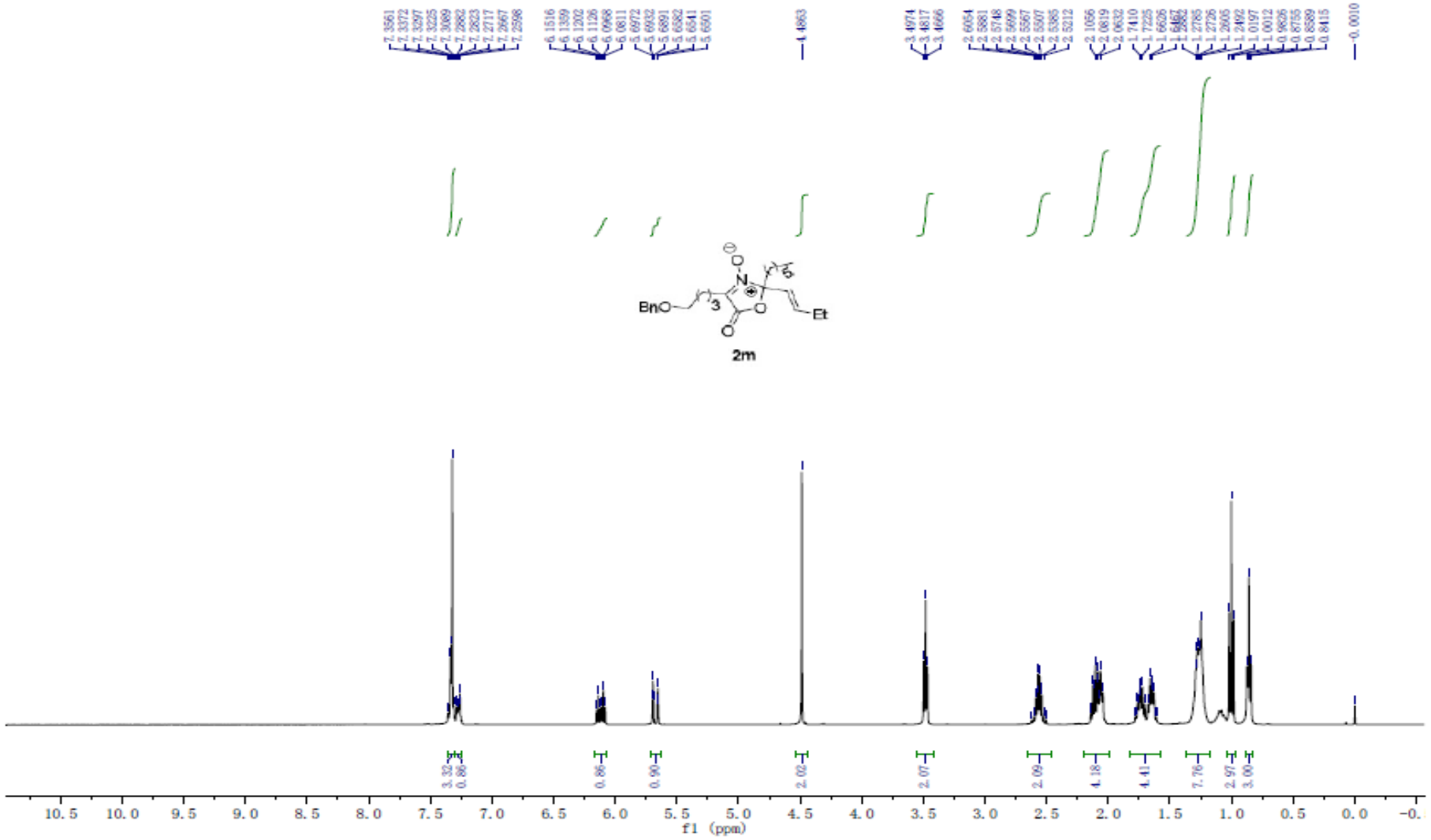
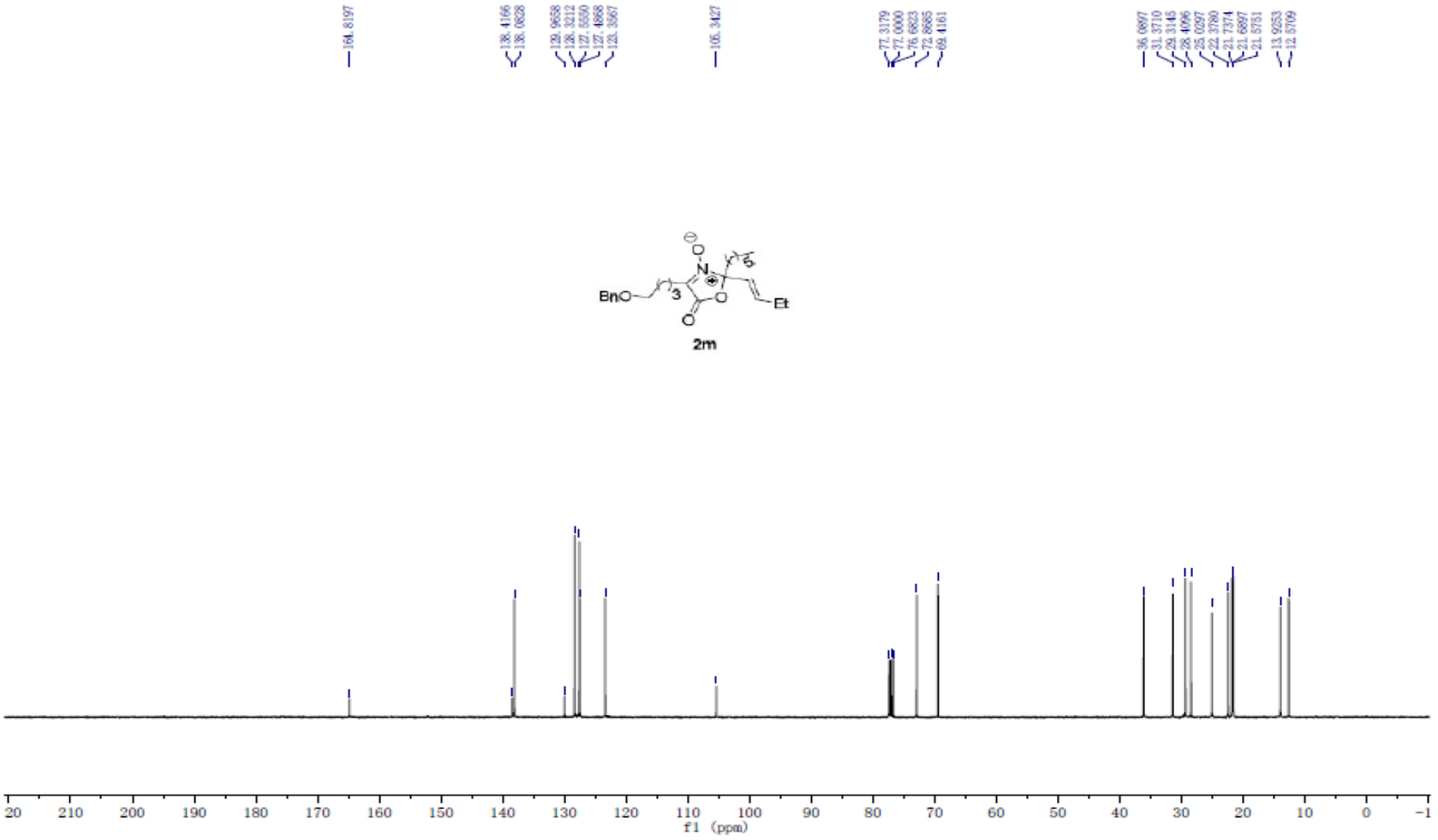
4-ClPh
Me
Et
2l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


BnO
Et
2m
f1 (ppm)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26.4096
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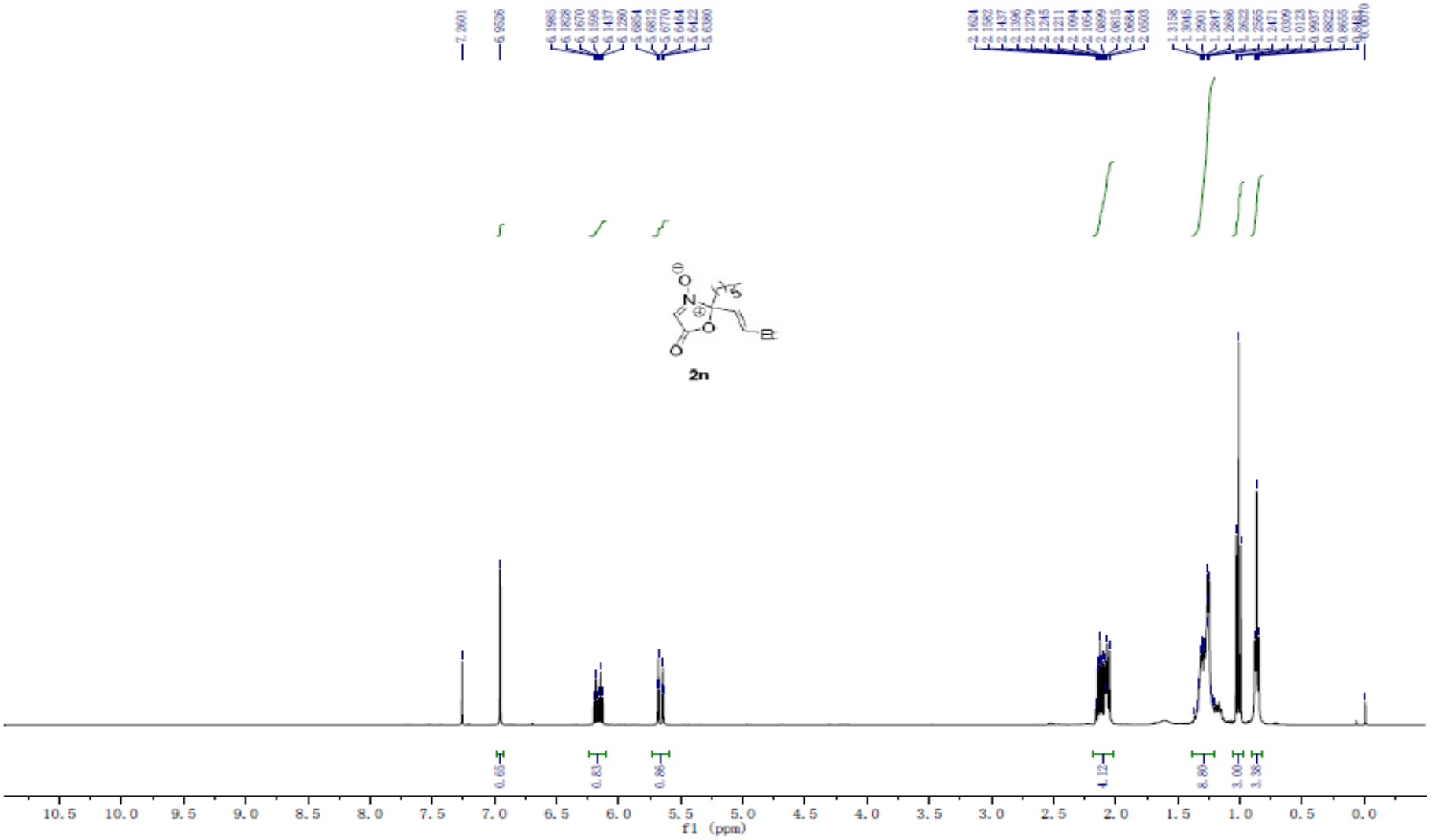
BnO
3
5
Et
2m
f1 (ppm)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2.1582
2.1437
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2.1279
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1.2847
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0.0010
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0.83
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
1.5
1.0
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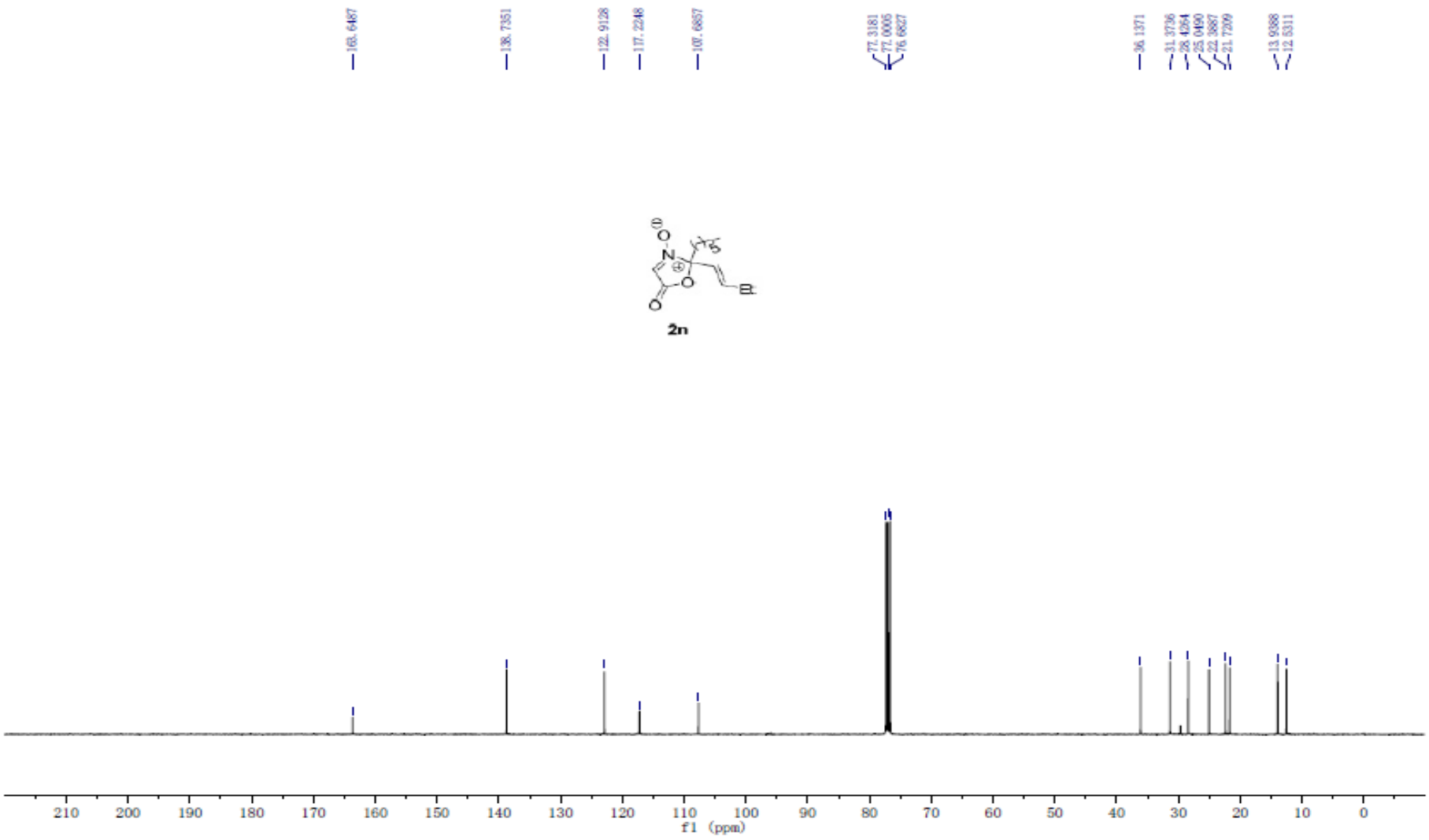
f1 (ppm)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28.4264
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22.3867
21.7209
13.9388
12.5311
2n
210
200
190
180
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120
110
100
90
80
70
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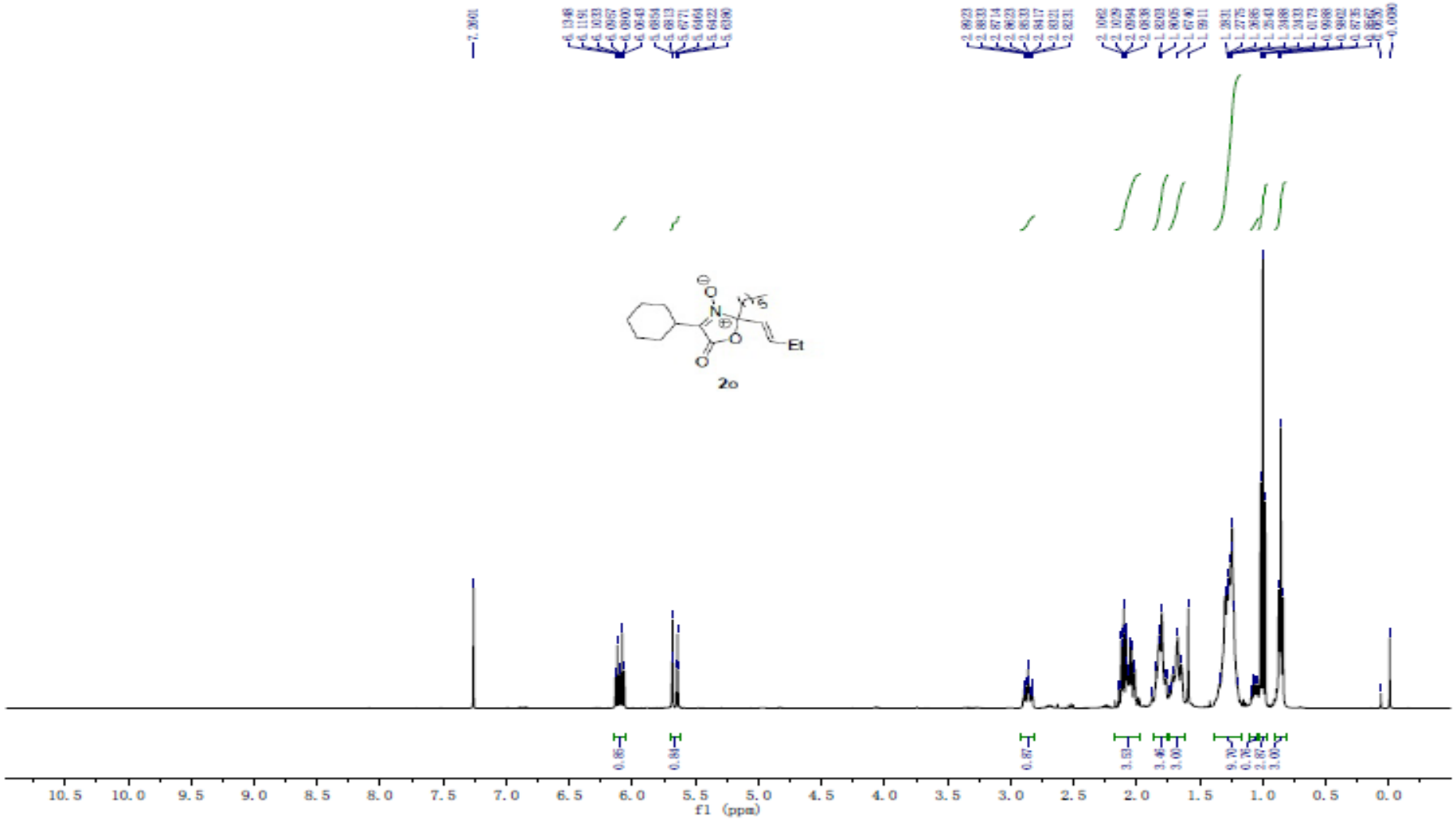
50
40
30
20
10
0
f1 (ppm)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-0.0000
O
N
O
O
Et
2o
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0.84
0.87
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9.5
9.0
8.5
8.0
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6.5
6.0
5.5
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1.0
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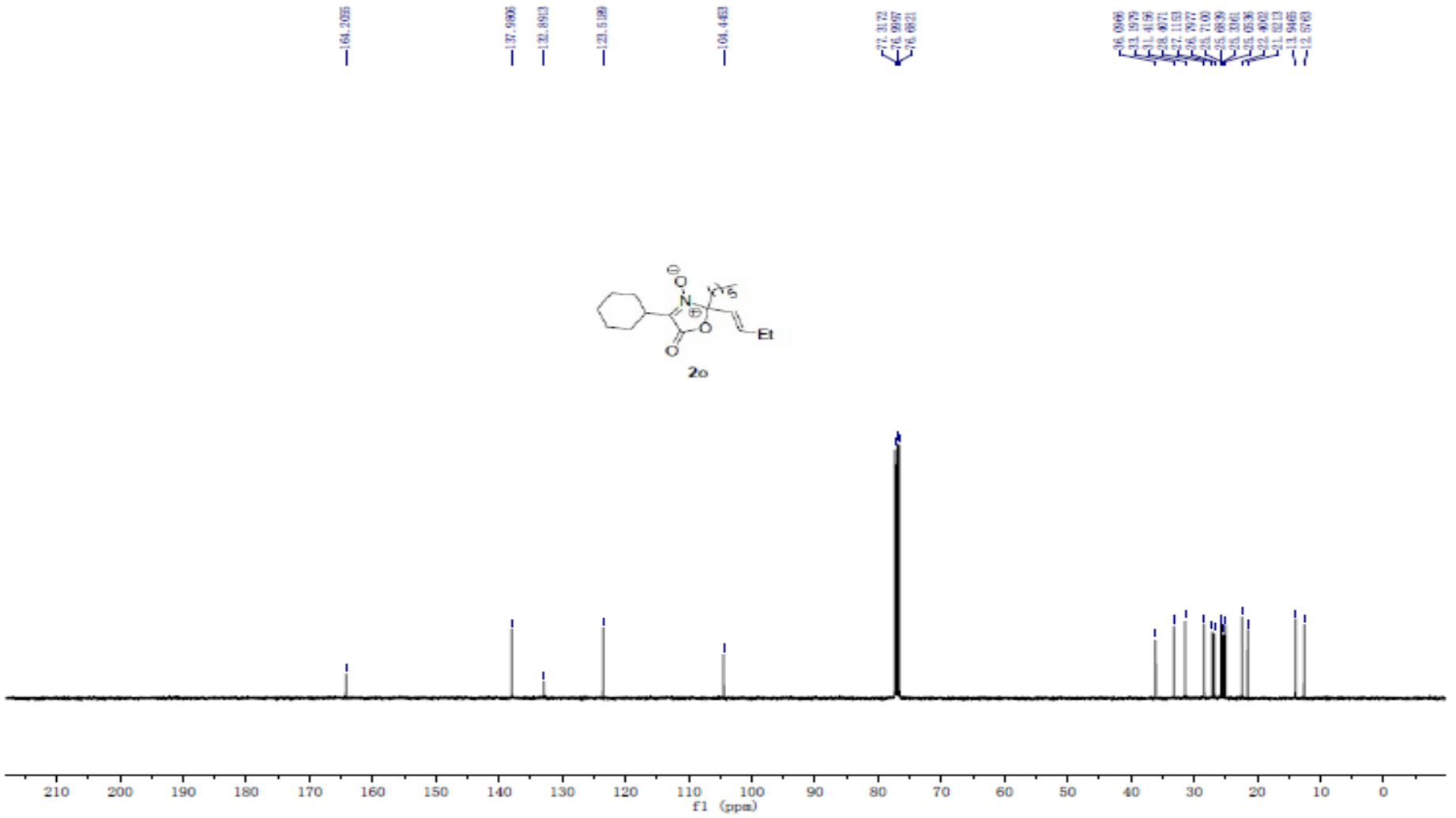
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21.9213
13.9465
12.5763
Et
2o
210
200
190
180
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50
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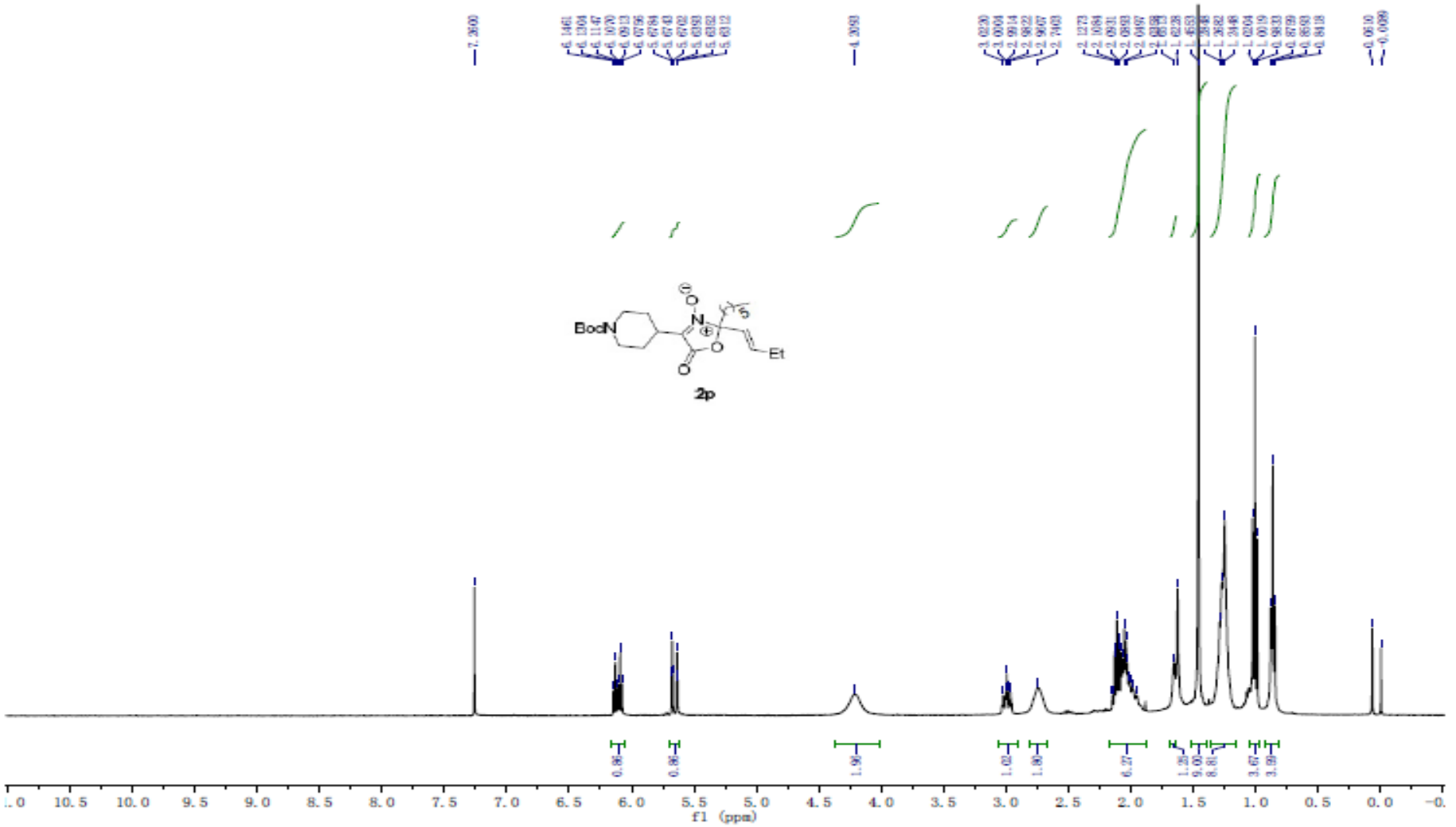
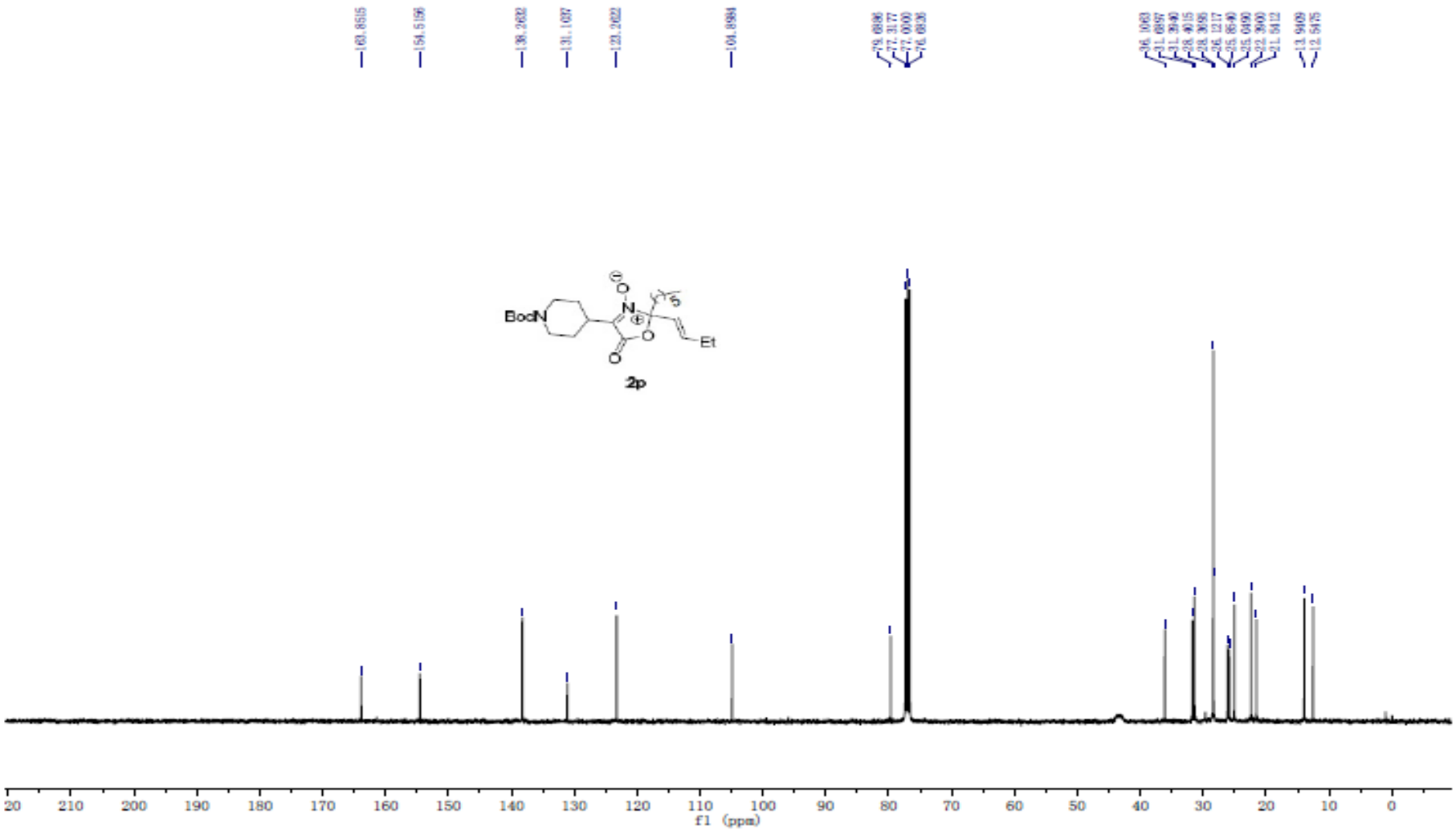
f1 (ppm)


BocN
Et
2p
f1 (ppm)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31.3940
28.4015
28.3056
26.1217
25.8540
25.6490
22.3900
21.5412
13.9409
12.5475
BocN
O
N
O
O
O
5
Et
2p
20
210
200
190
180
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50
40
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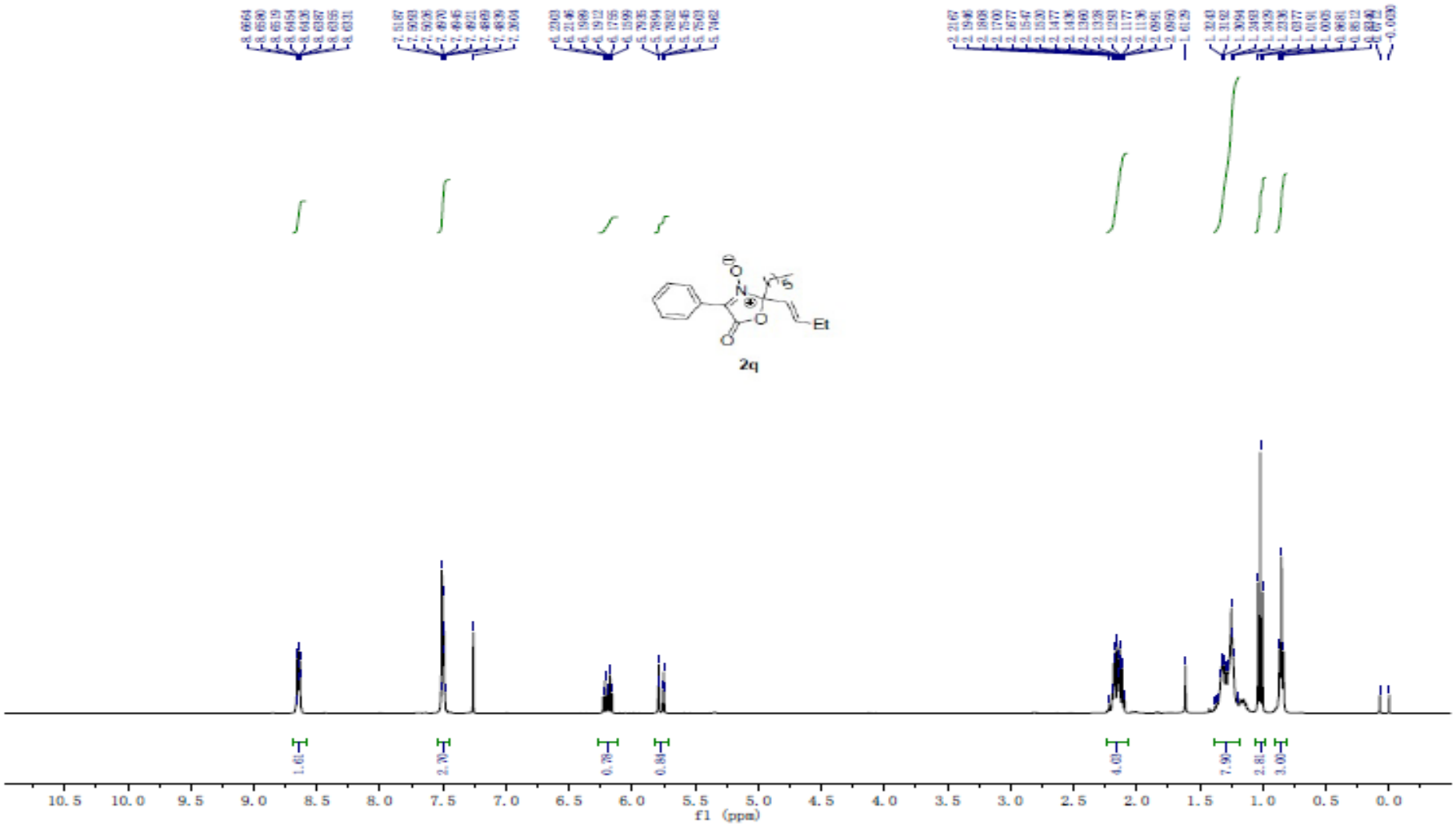
10
0
f1 (ppm)


Et
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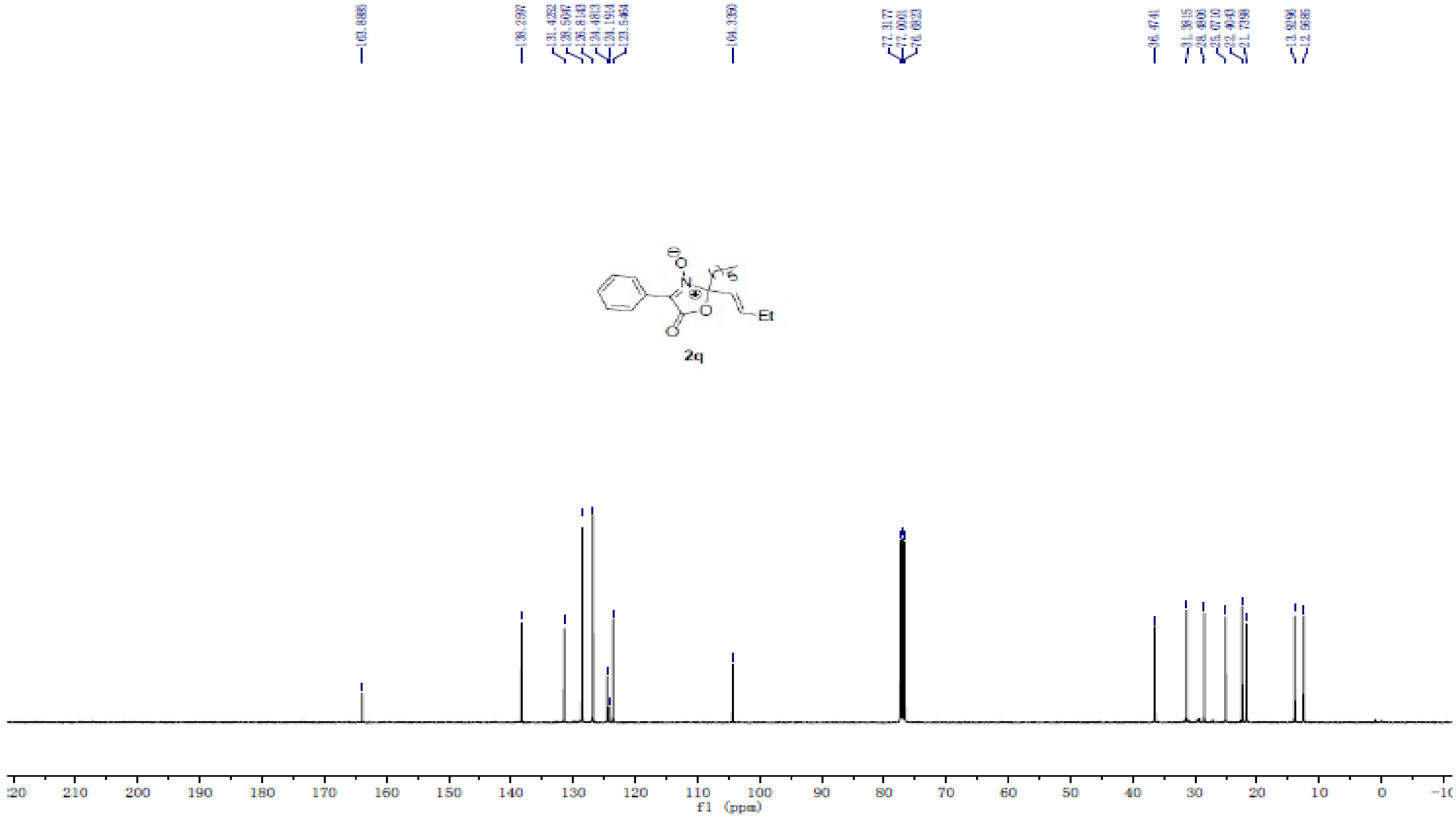
2.70
0.78
0.84
4.03
7.90
2.81
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Et
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180
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160
150
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120
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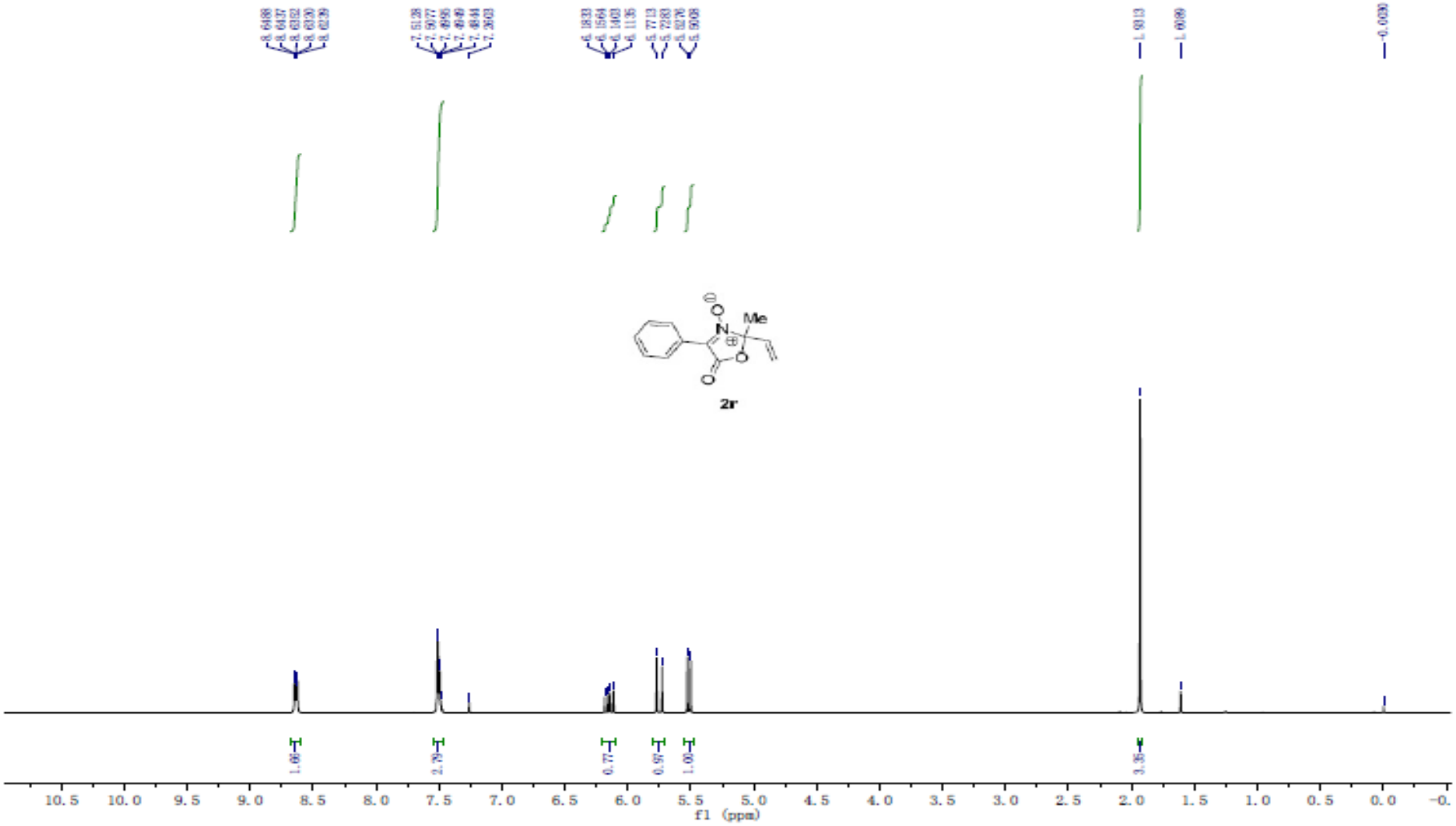
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

2q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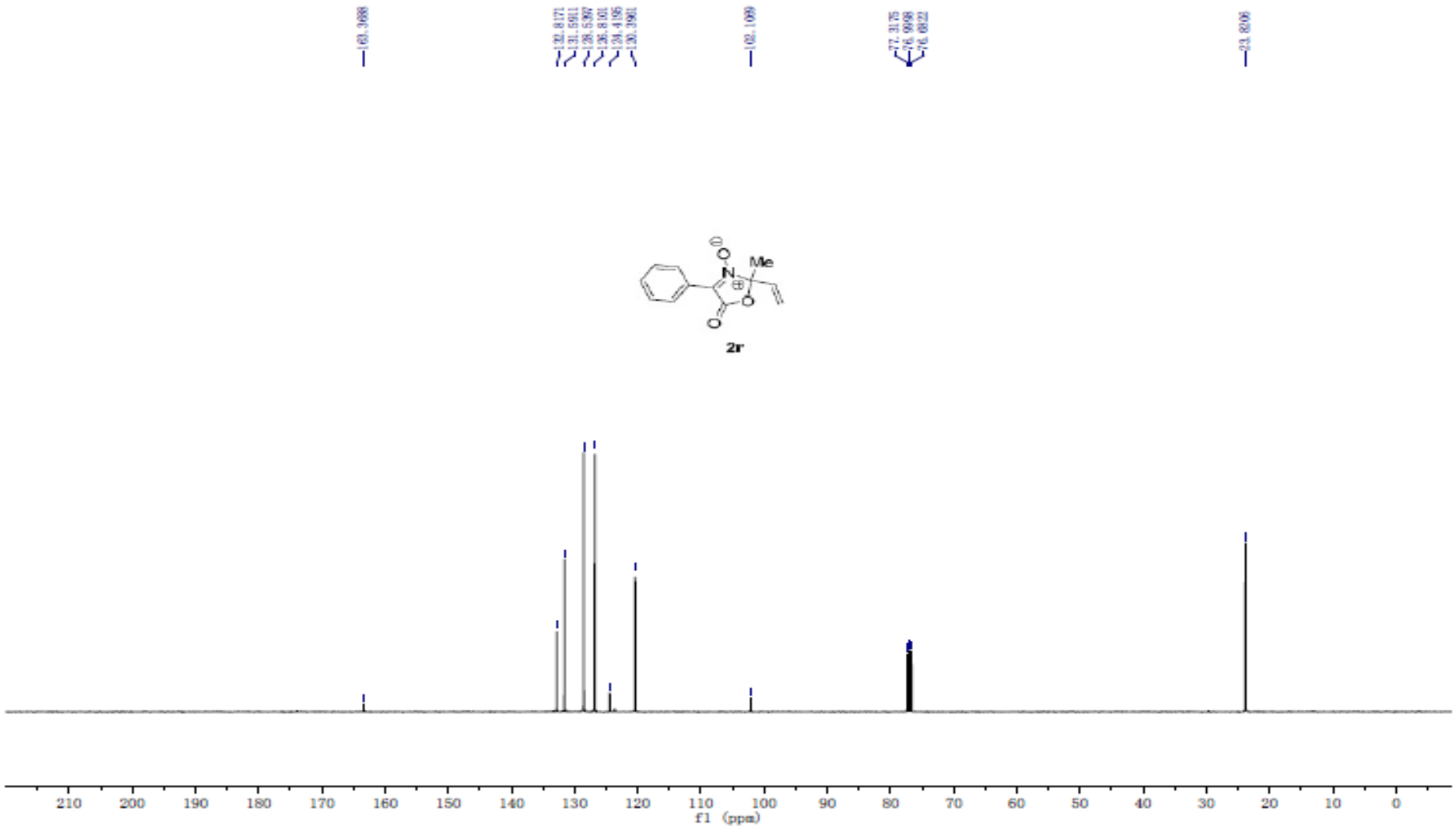
8.6352
8.6330
8.6239
7.5138
7.5077
7.4896
7.4849
7.4844
7.3903
6.1833
6.1564
6.1403
6.1135
5.7713
5.7283
5.5276
5.5008
1.9813
1.9089
-0.0030
Me
N
O
O
O
2r
1.05
2.70
0.77
0.97
1.00
3.35
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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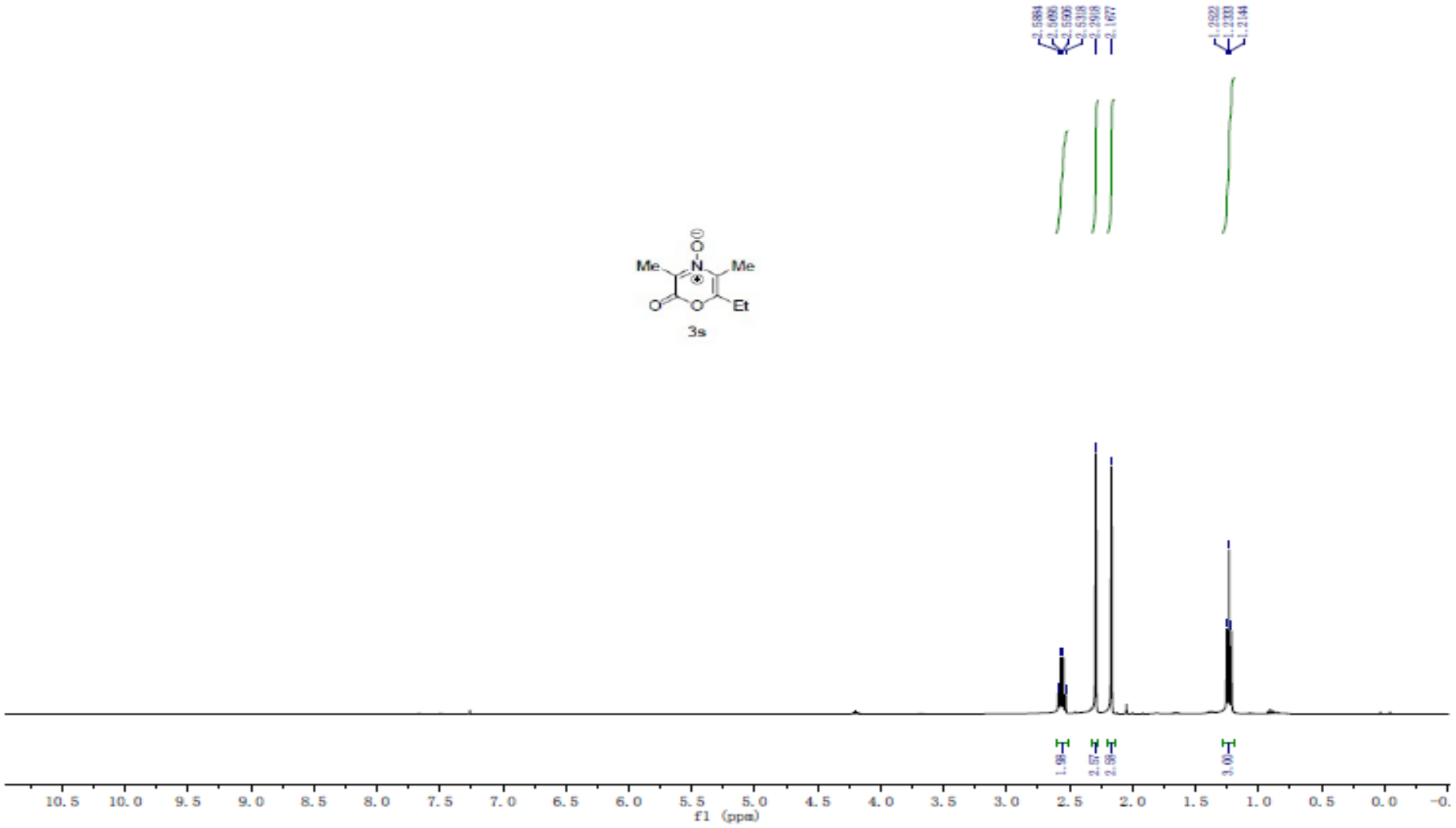
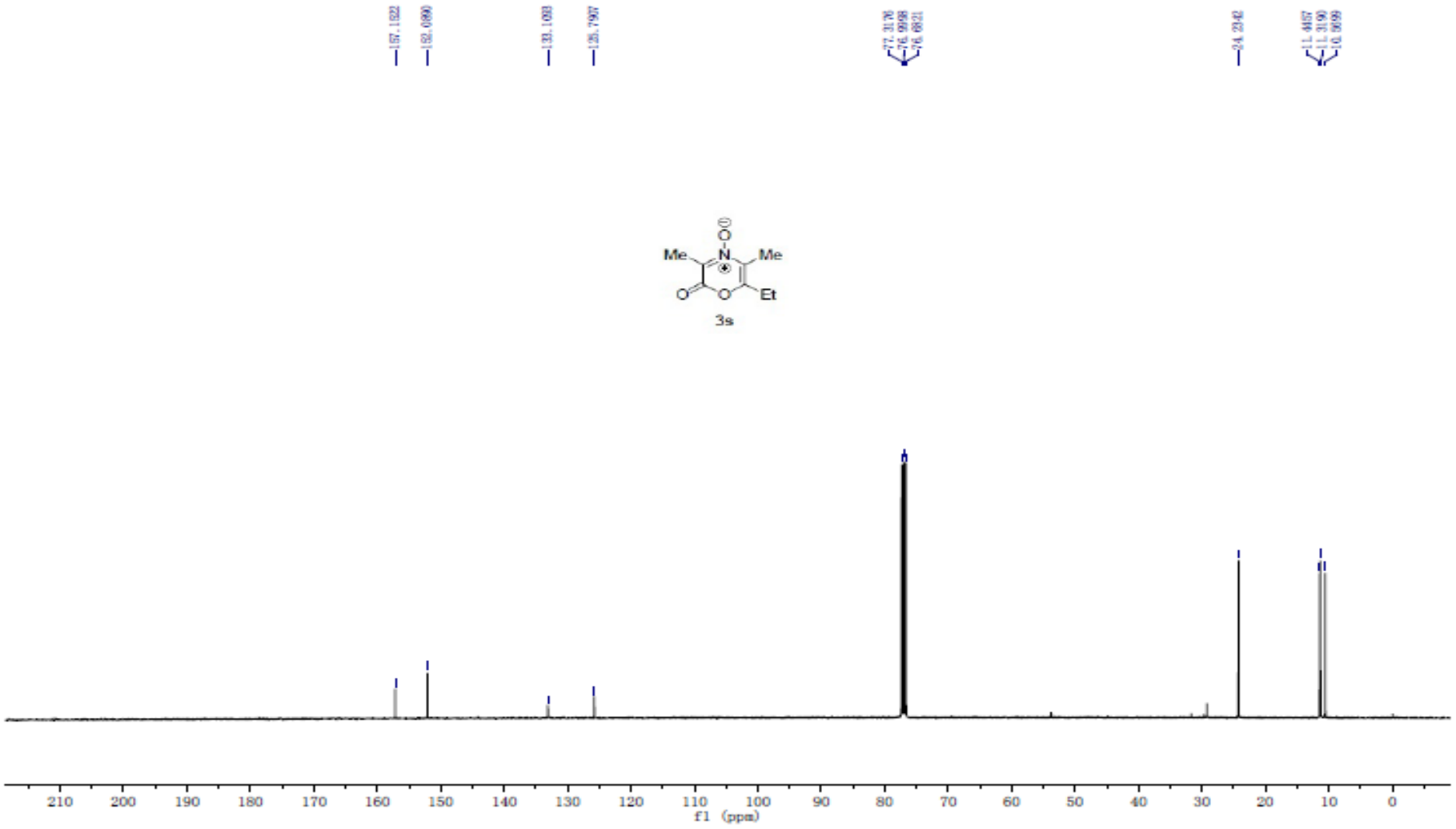
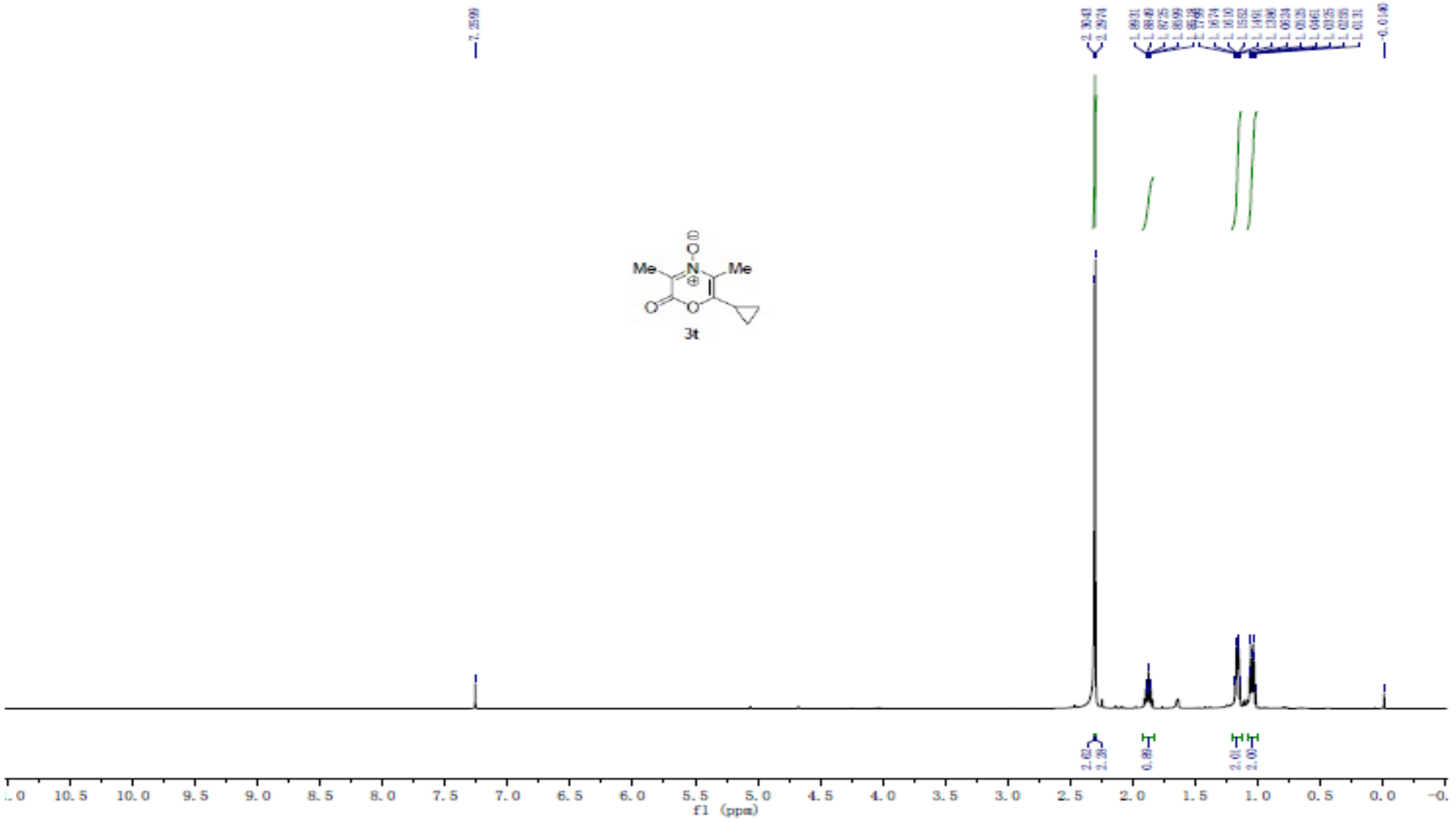
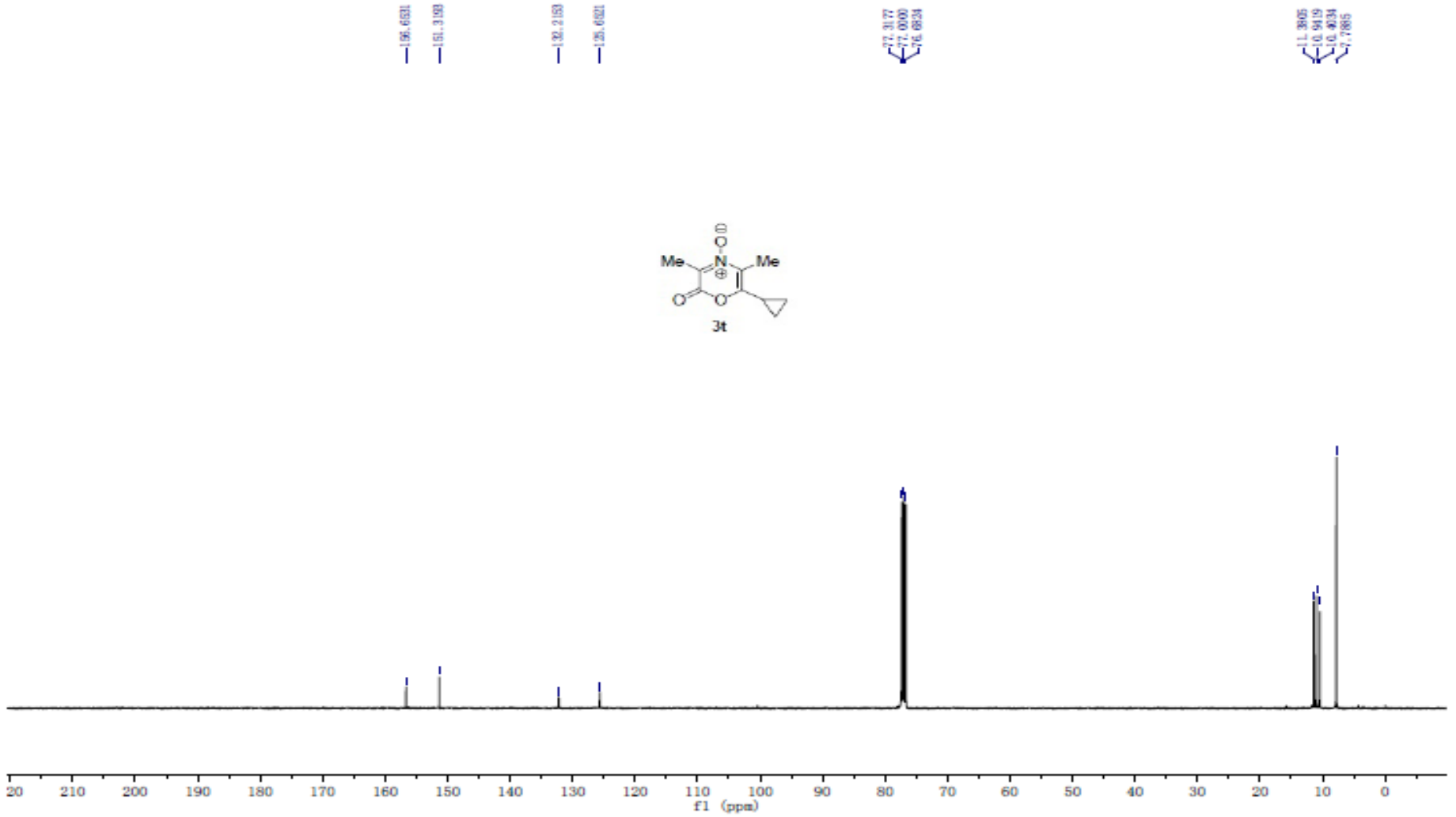
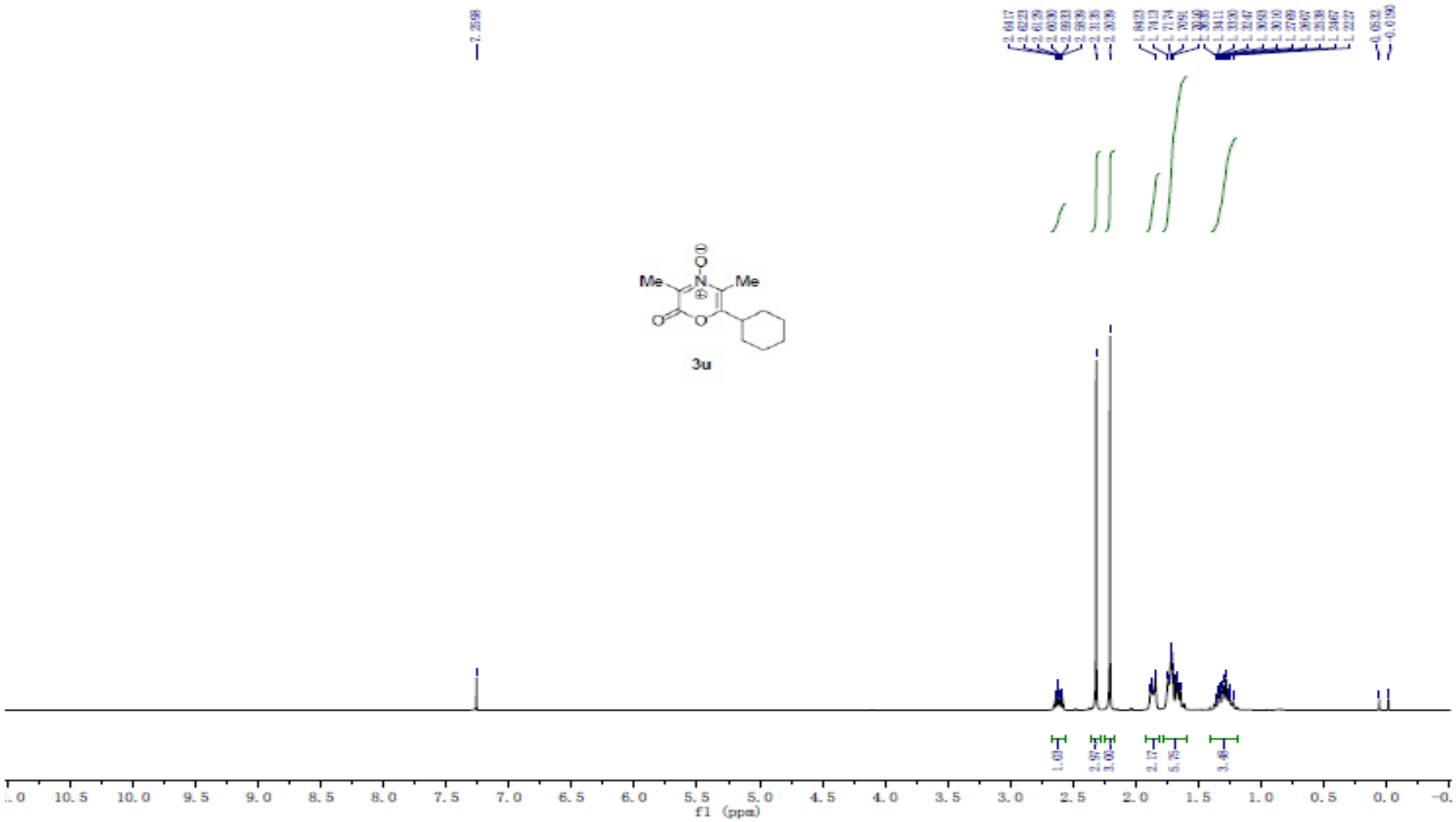
132.8171
131.5911
128.5367
126.8101
124.4195
120.3961
102.1099
77.3175
76.9998
76.6822
23.8206
Me
O
N
O
O
2r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

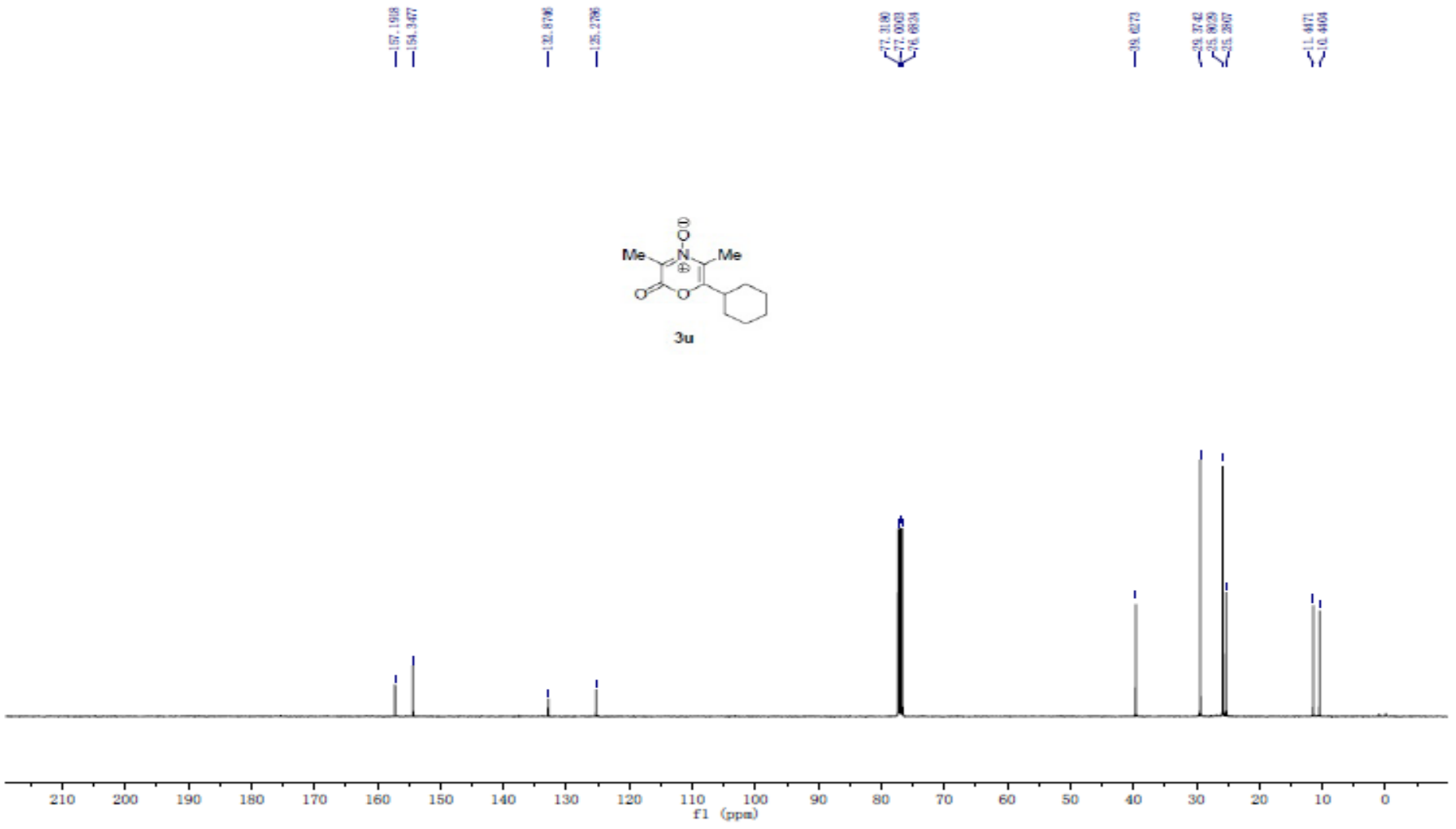

2.5884
2.5696
2.5506
2.5318
2.2918
2.1677
1.2922
1.2733
1.2544
Me
Me
Et
3s
1.98
2.57
2.58
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.
f1 (ppm)

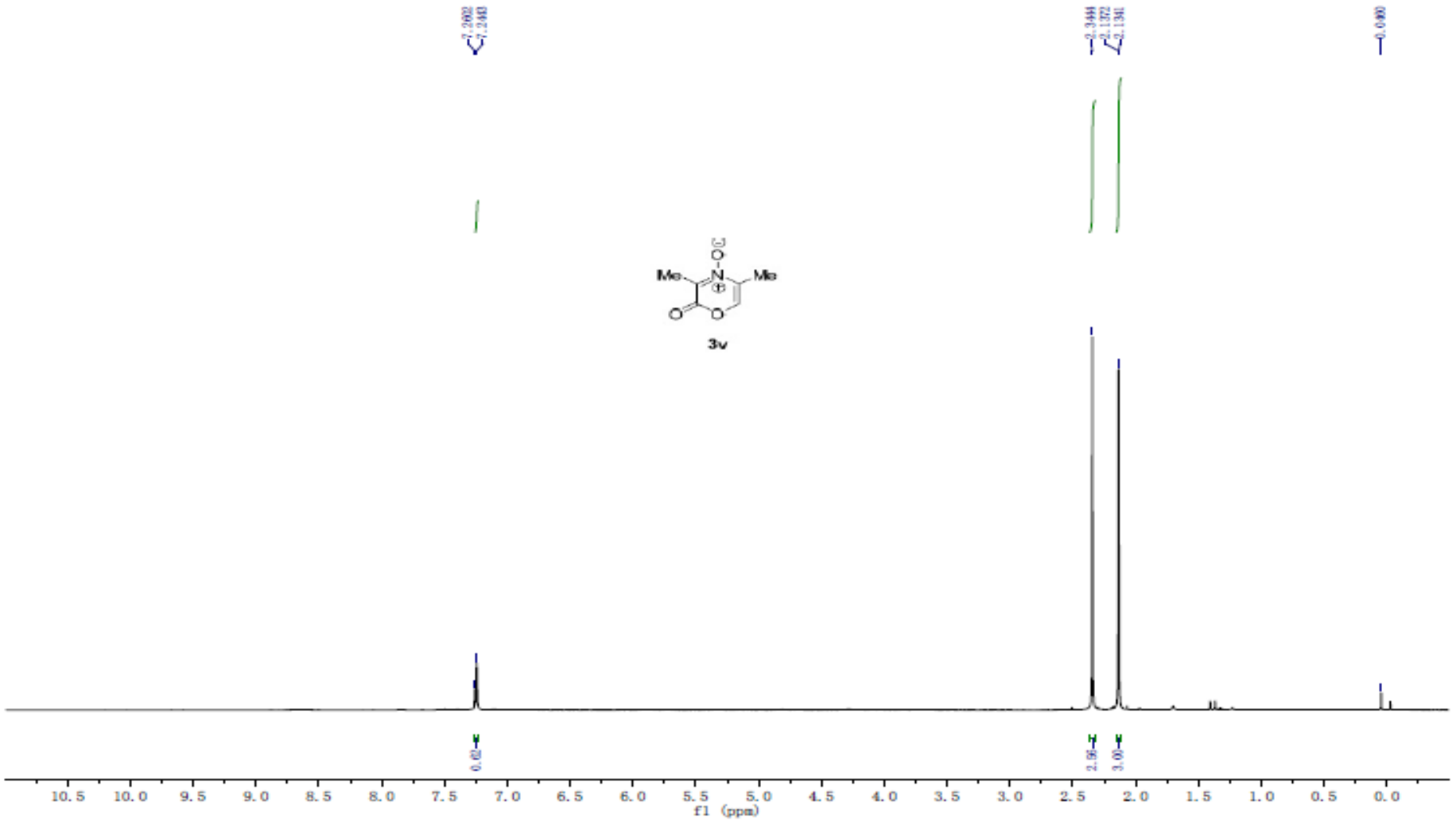

157.1522
152.0899
133.1083
125.7907
77.3176
76.9998
76.6821
24.2342
11.4457
11.3190
10.9699
Me
Me
Et
3s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

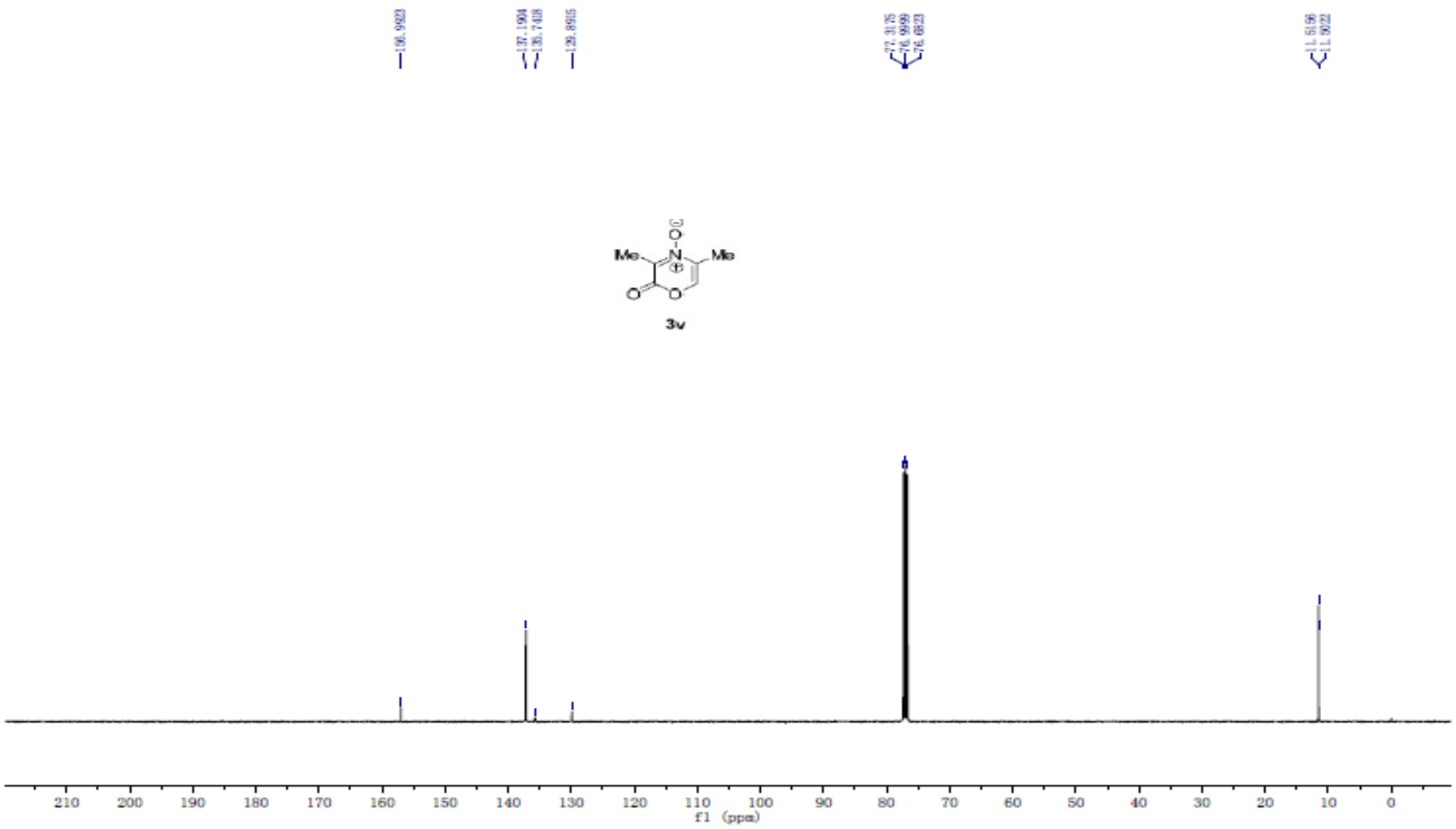

7.2599
2.3043
2.2974
-0.0140
Me
Me
3t
2.62
2.39
0.89
2.01
2.00
f1 (ppm)

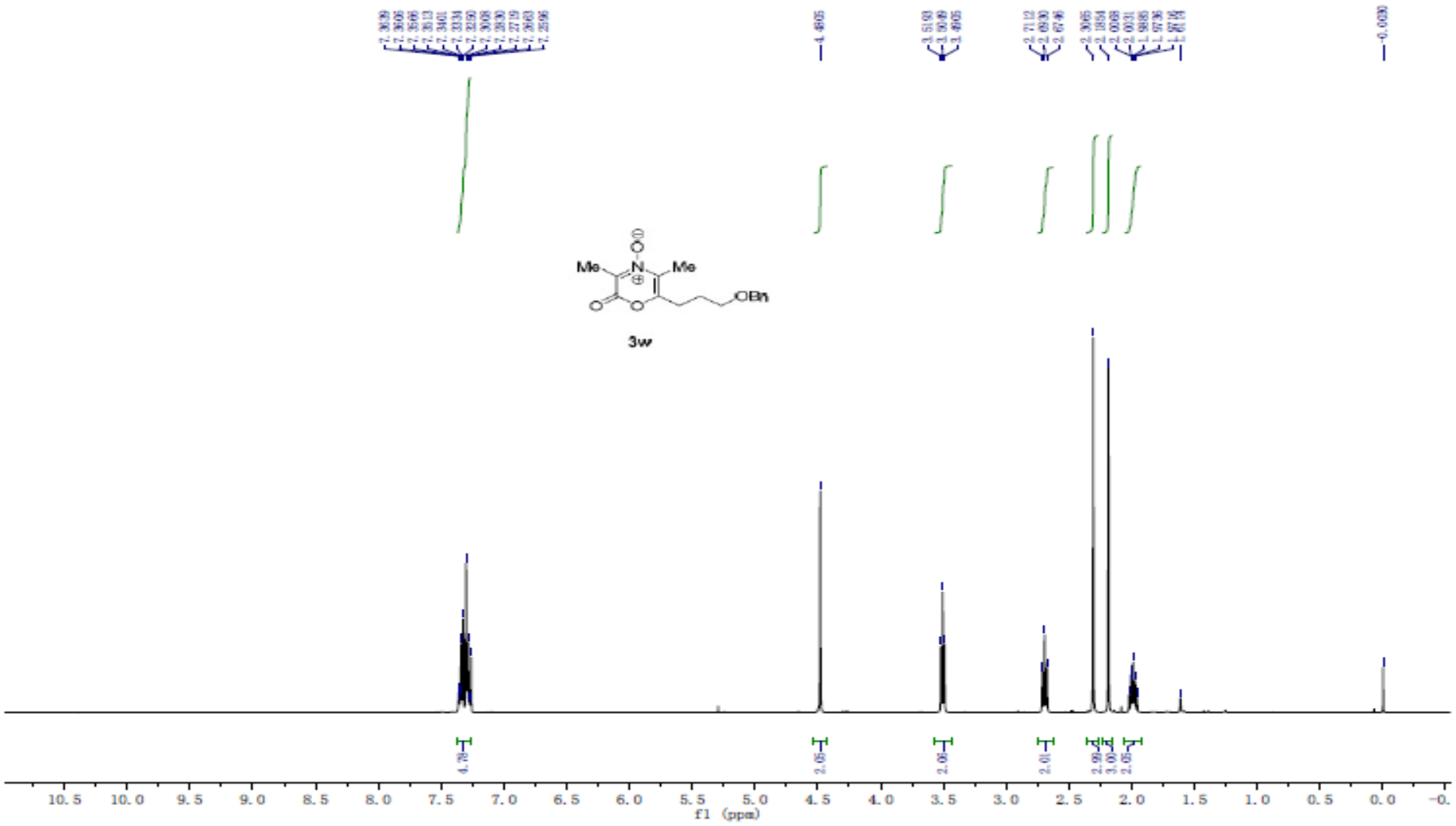

156.6531
151.3193
132.2153
125.6021
77.3177
77.0000
76.6834
11.3805
10.9419
10.4034
7.7865
Me
N
Me
O
O
3t
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.2598
2.6417
2.6223
2.6129
2.6030
2.5933
2.5839
2.3135
2.3039
1.8423
1.7413
1.7174
1.7091
1.3411
1.3300
1.3247
1.3063
1.3010
1.2769
1.2607
1.2538
1.2467
1.2227
0.0532
-0.0190
Me
Me
O
O
O
3u
1.03
2.97
3.03
2.17
5.75
3.48
f1 (ppm)

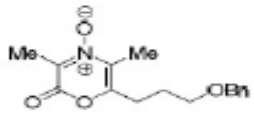

157.1918
154.3477
132.8798
125.2765
77.3180
77.0003
76.6834
39.6273
29.3742
25.8029
25.2807
11.4471
10.4404
Me
Me
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.2602
7.2483
2.3444
2.1372
2.1341
0.0000
Me
Me
3v
0.82
2.56
3.00
10.5 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)

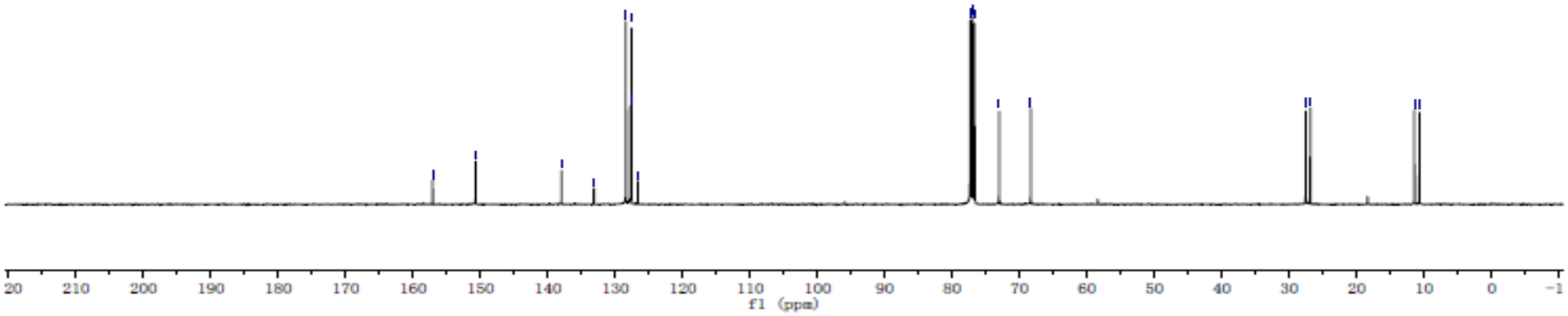

156.9923
137.1904
135.7418
129.8915
77.3175
76.9999
76.6823
11.5196
11.3022
Me
Me
3v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

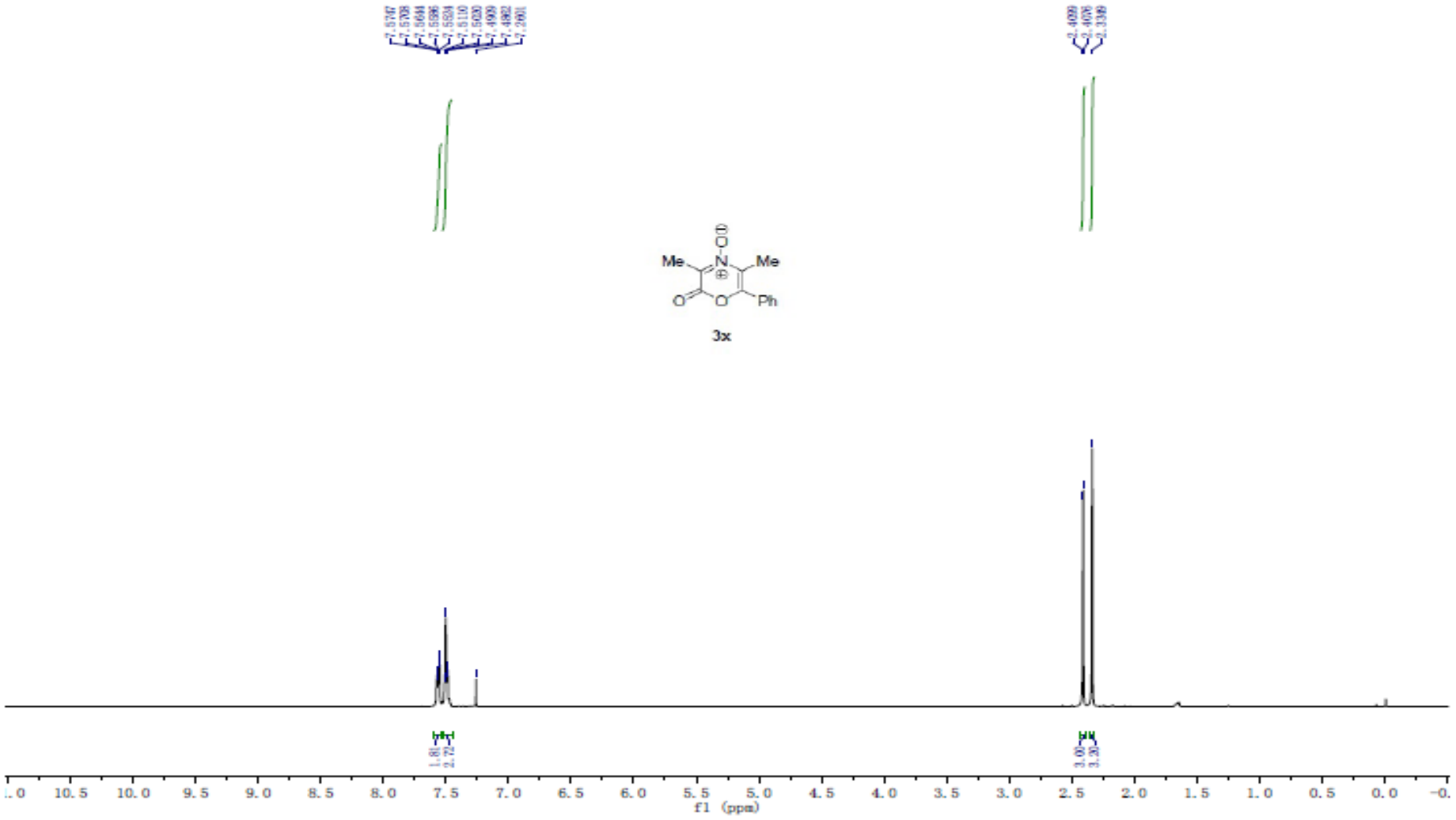

Me
Me
OBn
3w
f1 (ppm)

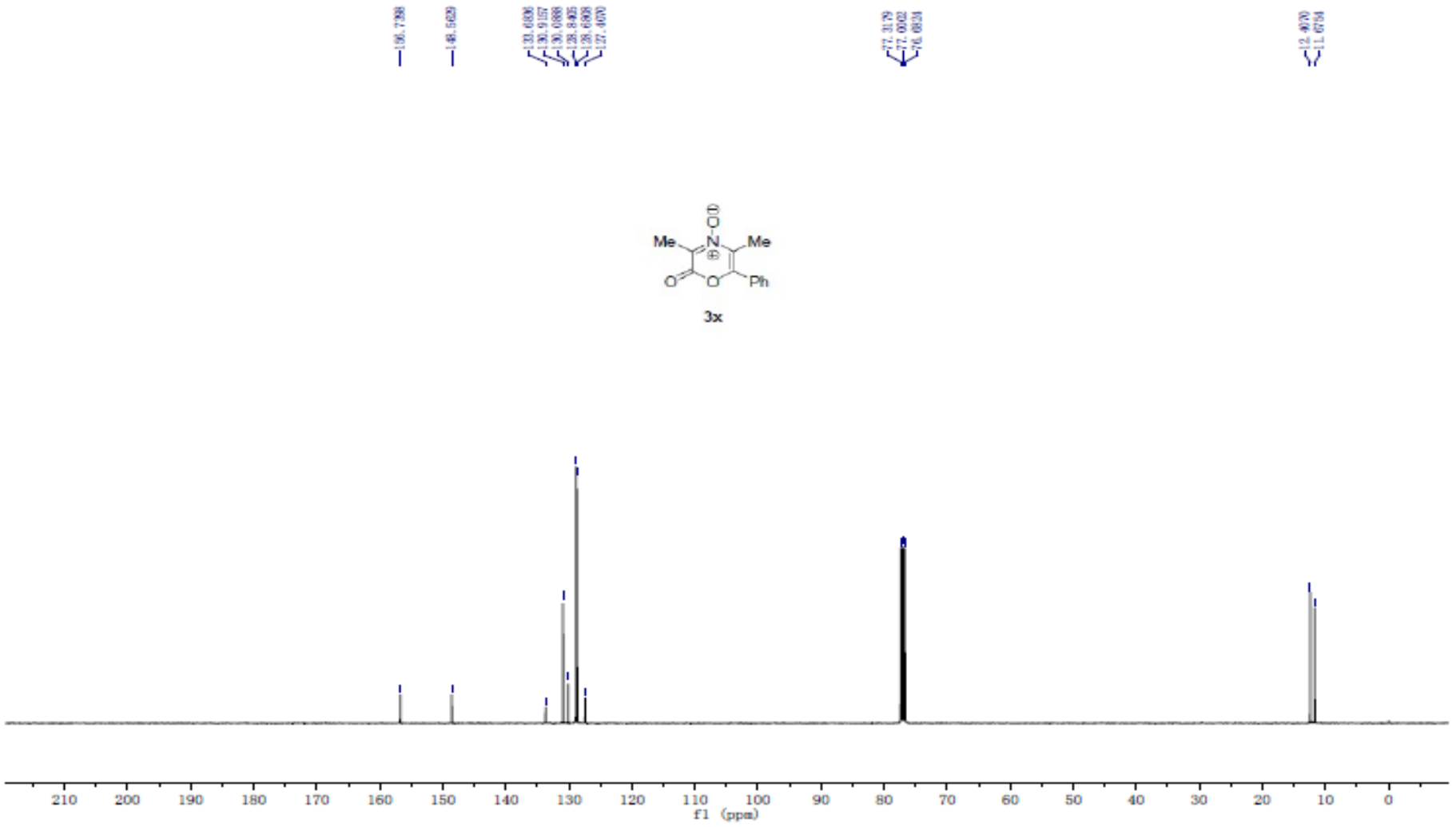

157.0394
150.6969
137.9651
133.1464
128.3992
127.6999
127.5792
126.6193
77.3180
77.0004
76.6827
73.0361
68.3475
27.9657
26.8910
11.4395
10.7146


Me
N
Me
OBn
O
O

3w


20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)


Me
Me
Ph
3x
f1 (ppm)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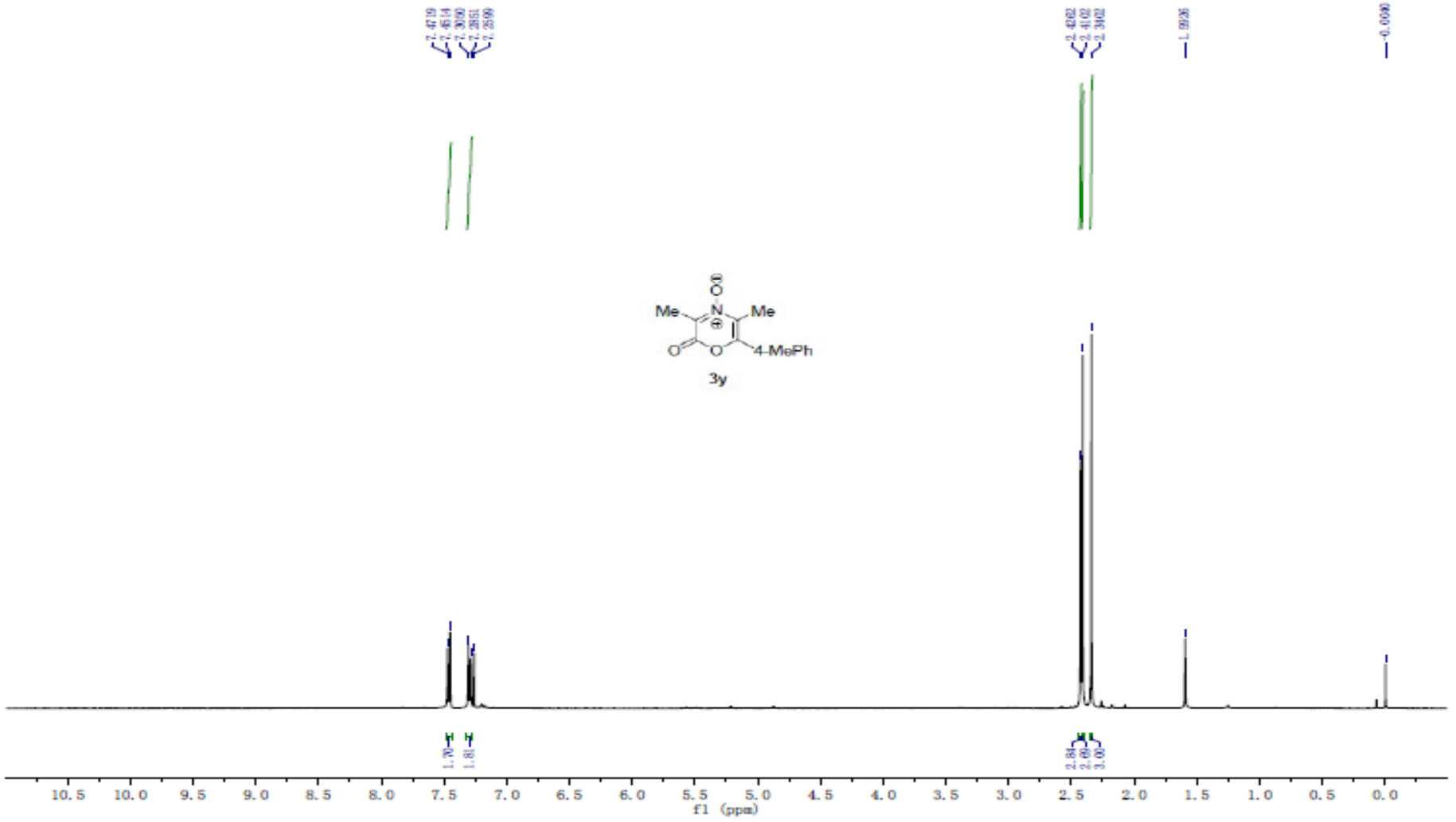
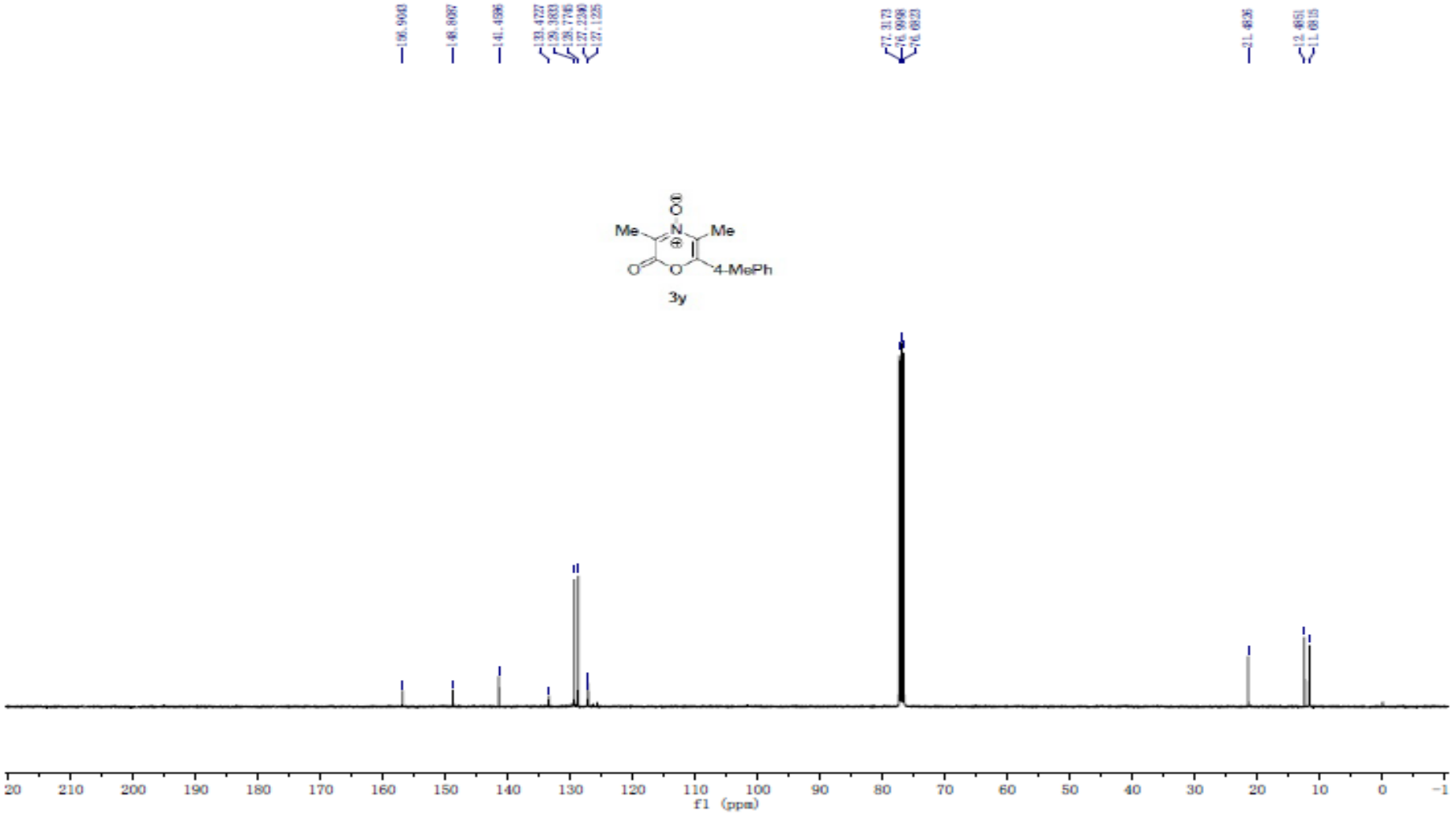
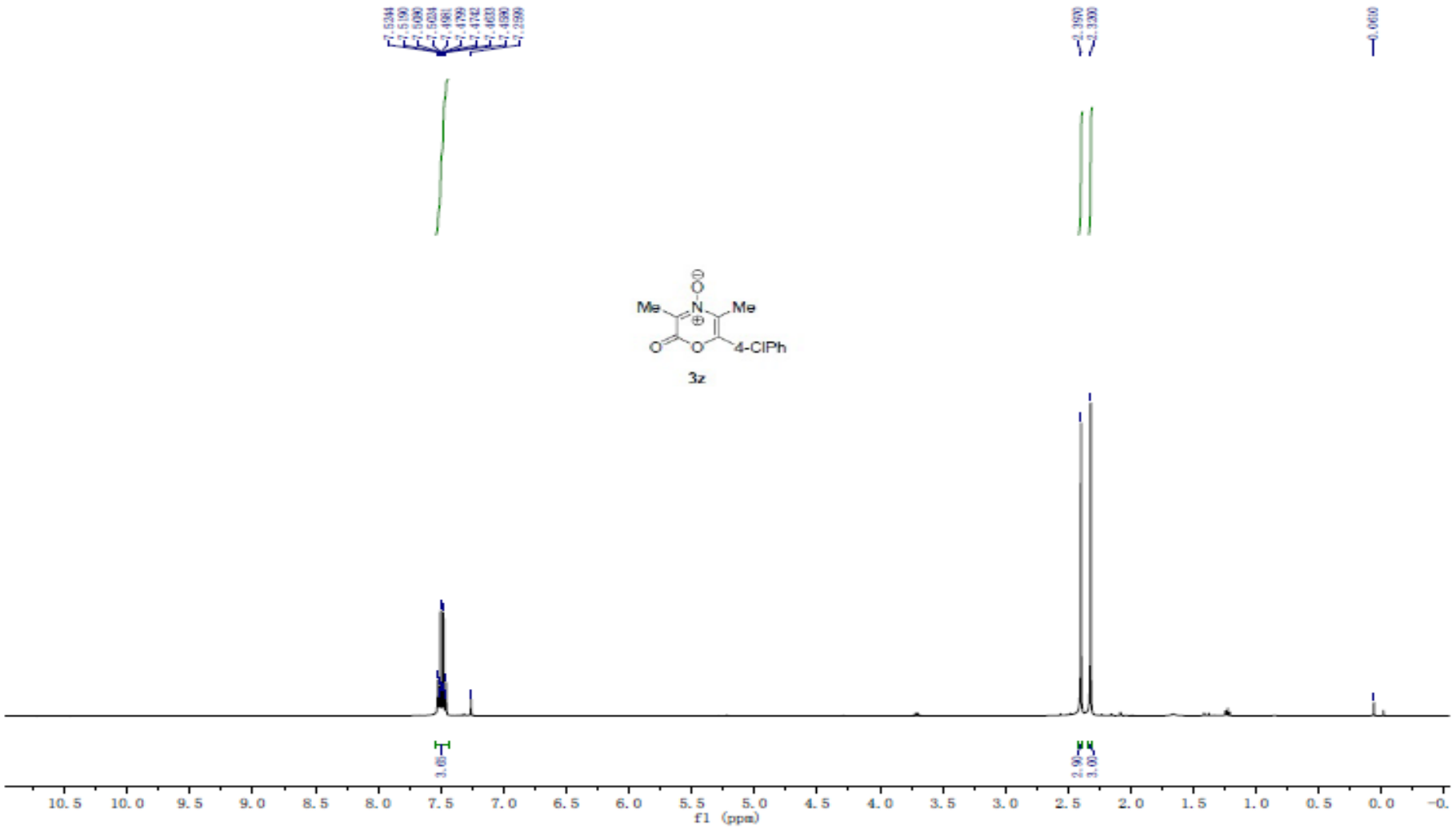
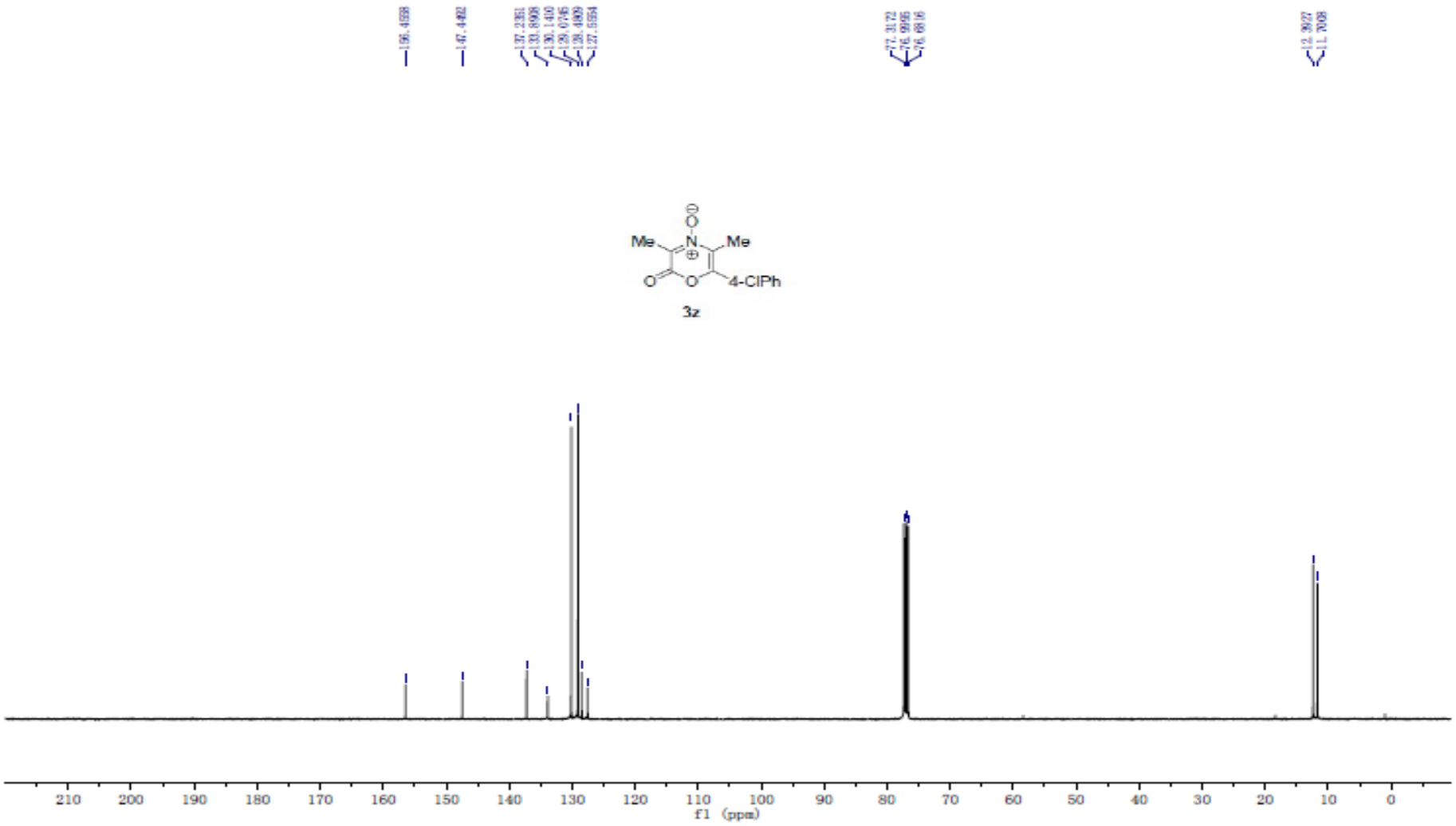
148.5629
133.6836
130.9157
130.0886
128.8405
128.6905
127.4670
77.3179
77.0002
76.6824
12.4670
11.6754
Me
Me
Ph
3x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.4719
7.4614
7.3090
7.2851
7.2599
2.4262
2.4102
2.3942
1.9936
-0.0000
Me
Me
4-MePh
3y
1.70
1.81
2.88
2.68
3.00
10.5 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)


156.9043
146.8067
141.4396
133.4727
129.3833
128.7745
127.2230
127.1225
77.3173
76.9998
76.6823
21.4635
12.4651
11.6915
Me
Me
4-MePh
3y
f1 (ppm)


7.5344
7.5190
7.5090
7.5024
7.4981
7.4799
7.4742
7.4633
7.4590
7.2599
2.3570
2.3300
0.0010
Me
Me
4-ClPh
3z
3.68
2.90
3.00
10.5 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.
f1 (ppm)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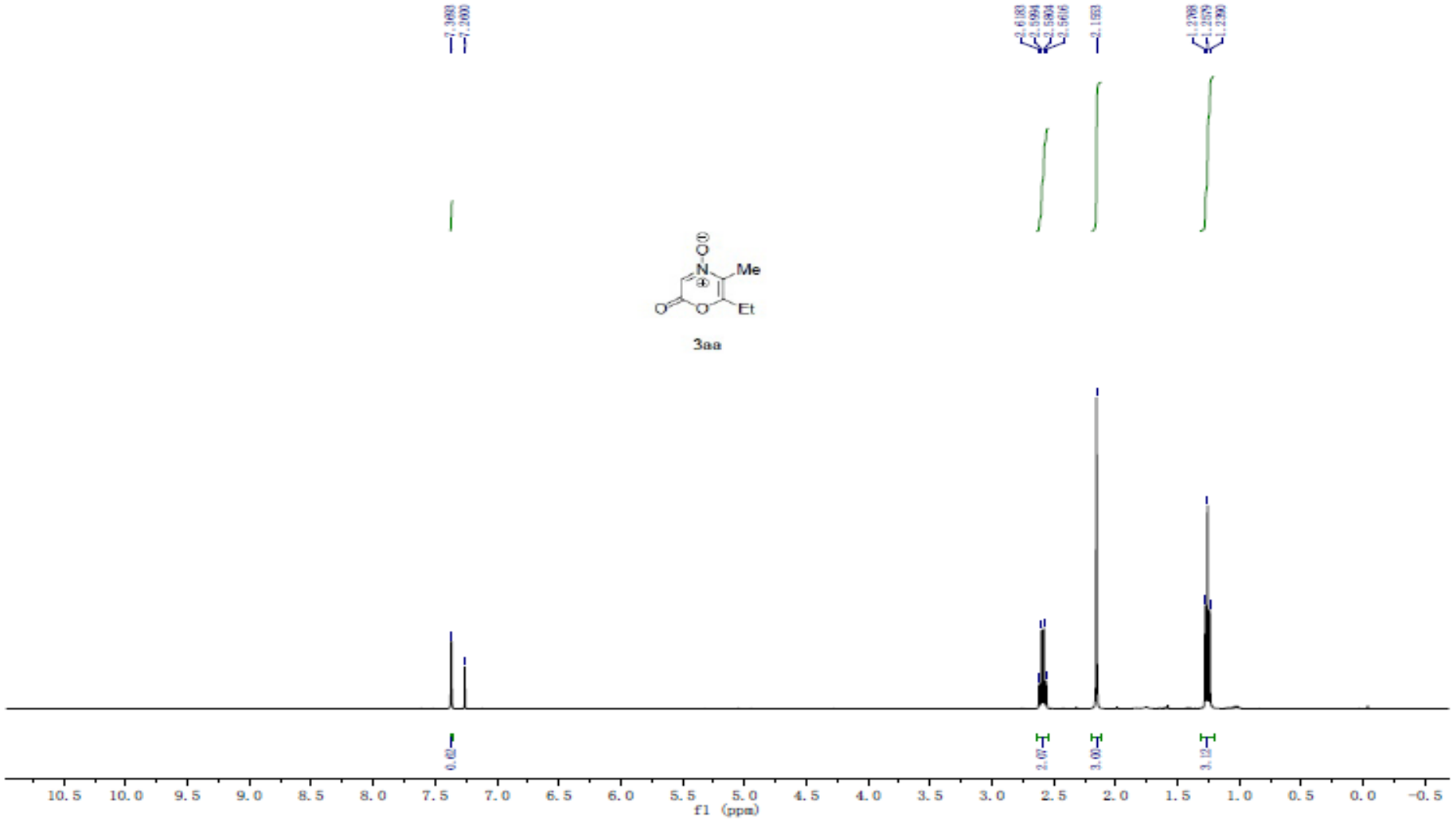
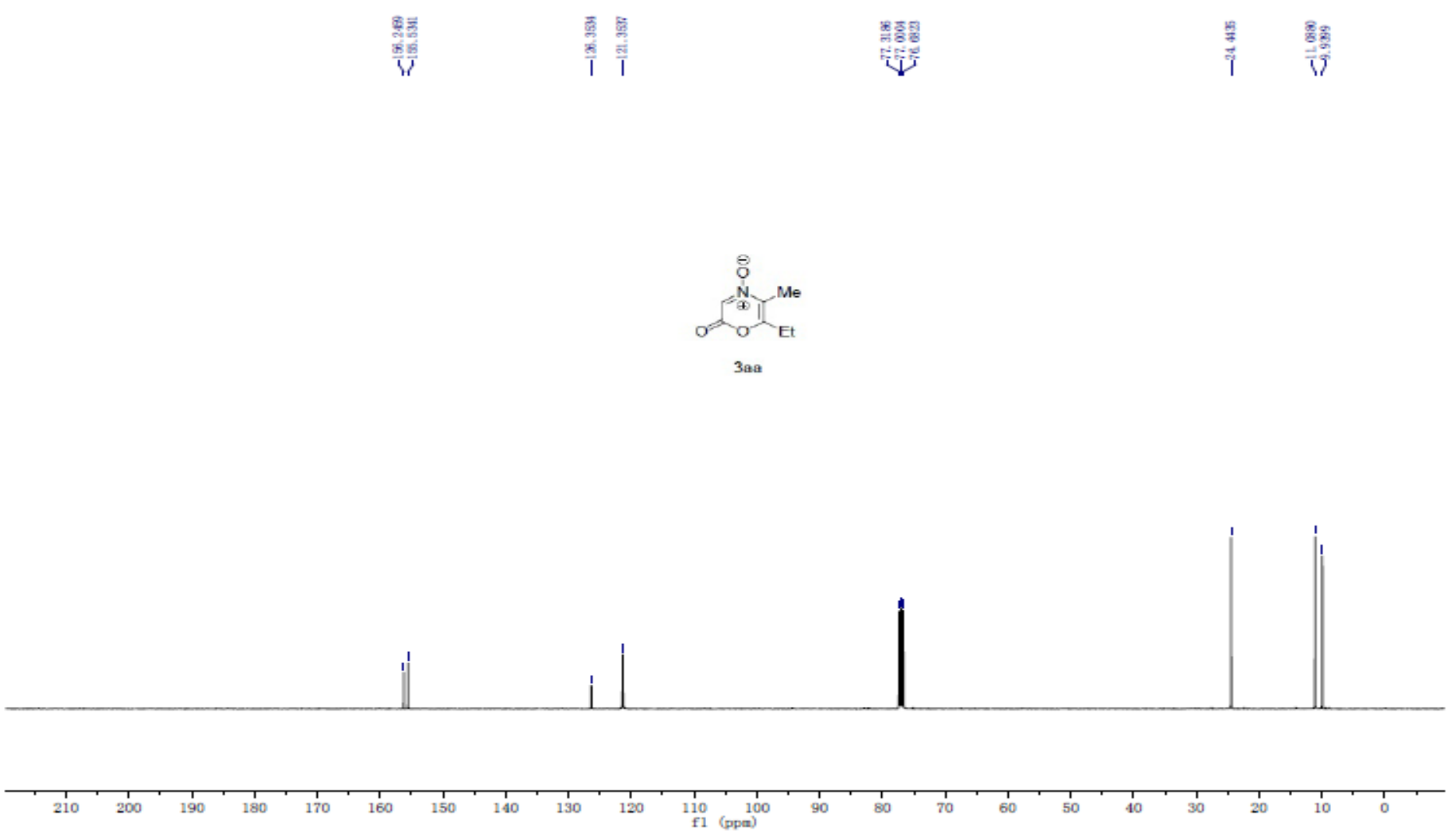
147.4482
137.2351
133.8908
130.1410
129.6746
128.4809
127.5554
77.3172
76.9995
76.6816
12.3627
11.7008
Me
Me
4-ClPh
3z
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.3683
7.2000
2.6183
2.5994
2.5804
2.5616
2.1553
1.2288
1.2079
1.1890
Me
Et
3aa
0.62
2.07
3.00
3.19
10.5 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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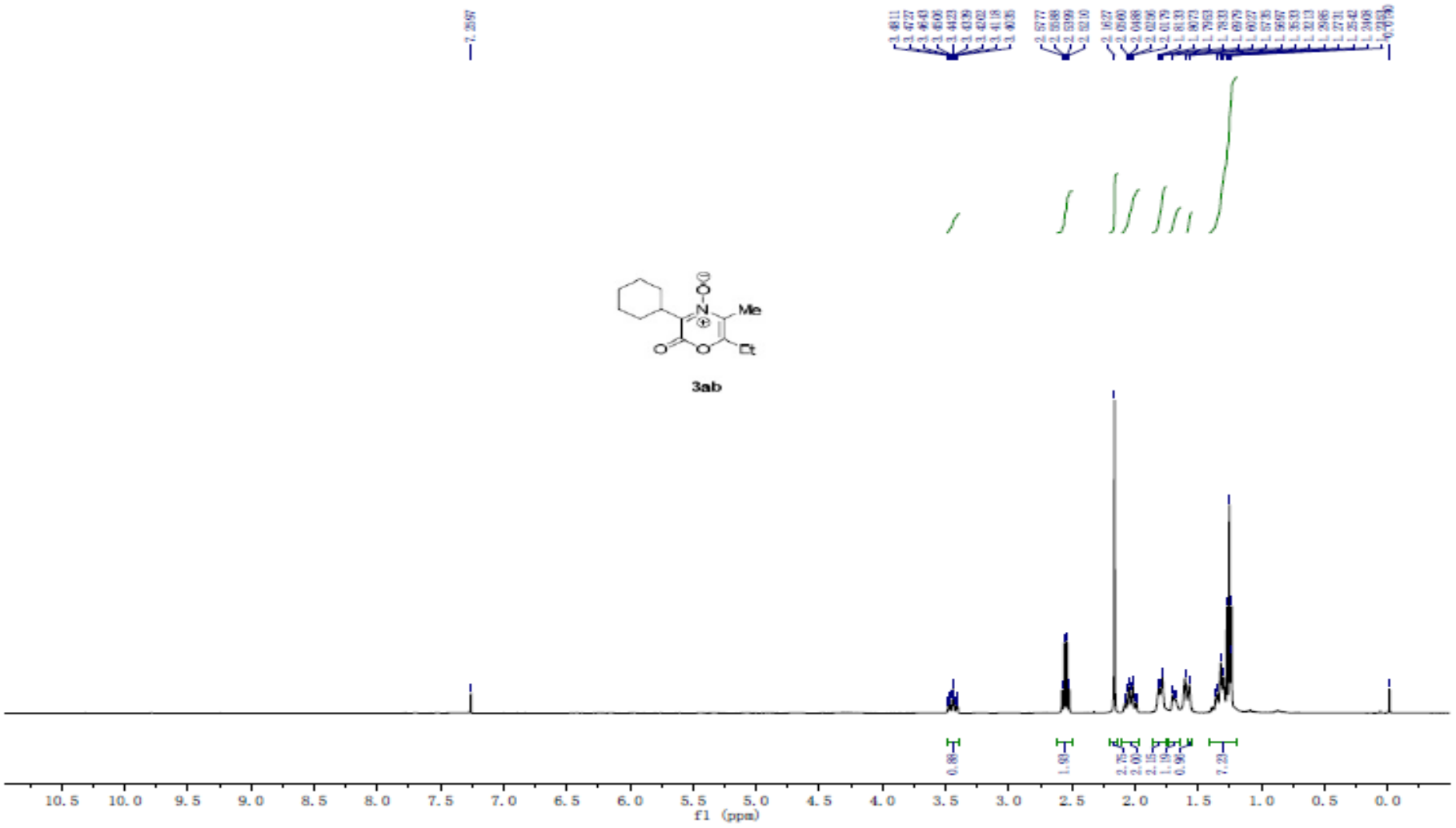
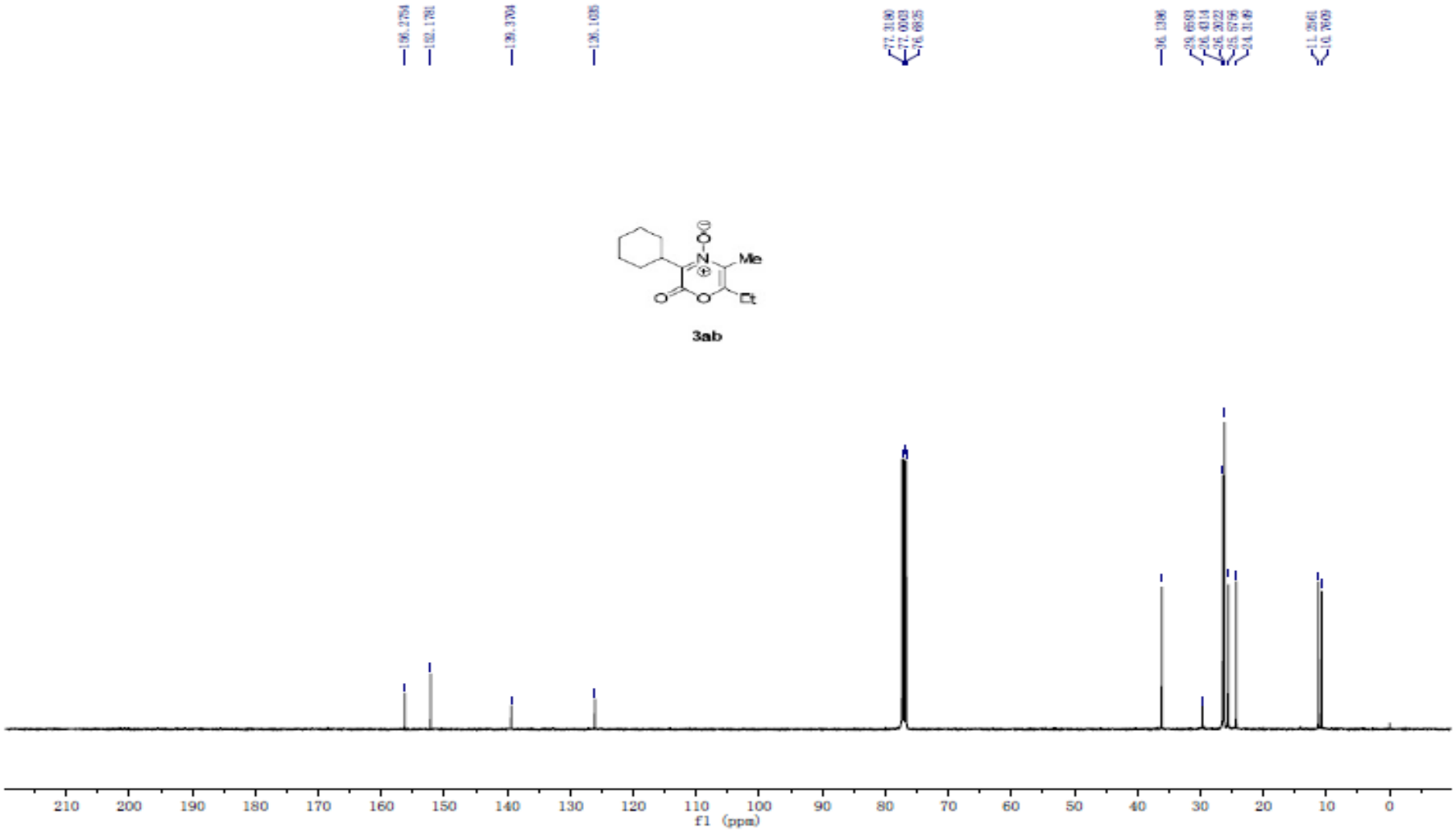
155.5341
136.3534
121.3537
77.3186
77.0004
76.6823
24.4435
11.0680
9.9399
Me
Et
3aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
Et
3ab
f1 (ppm)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152.1781
139.3704
136.1035
77.3180
77.0003
76.6825
36.1388
29.6593
26.4314
26.2022
25.5795
24.3149
11.2561
10.7609
Me
Et
3ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)