Supporting Information for

N-heterocyclic carbene-catalyzed sulfa-Michael addition of enals

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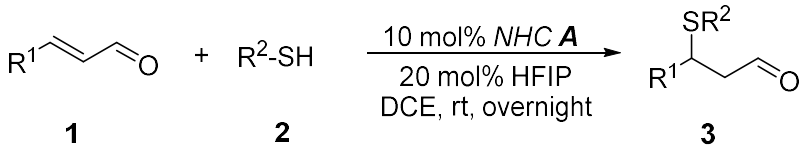
Contents

1. Experimental Section

All reactions were conducted under nitrogen atmosphere in oven-dried glassware with magnetic stirring bar. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) spectra were recorded using deuterated chloroform as solvent, with tetramethylsilane as an internal standard and reported in ppm (δ). Melting points was measured on a WRS-1B melting point apparatus and were uncorrected. High-resolution mass spectra (HRMS) were recorded on FTICRMS. Thiols, enals and other chemicals were obtained from Adamas-beta and used without purification. Anhydrous THF, MTBE and toluene were distilled from sodium and benzophenone. DMSO, DMF, CH_2Cl_2, $CHCl_3$ and CH_3CN were distilled from calcium hydride. 1, 2-dichloroethane was distilled from calcium chloride.

2. General procedure A: NHC-catalyzed sulfa-Michael addition of enals in 1, 2-dichloroethane

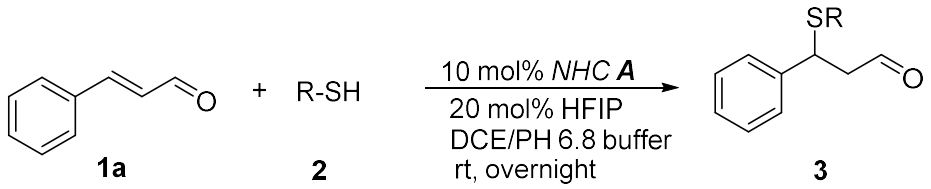


1 **2** **3**

IPr **A** (7.8 mg, 10 mol%) was dissolved in 2.0 mL dry 1,2-dichloroethane. Enal **1** (0.2 mmol), thiol **2** (0.6 mmol,) and 1,1,1,3,3,3-hexafluoro-2-propanol (6.7 mg, 20 mol%) were added subsequently via a syringe at ambient temperature. The reaction mixture was stirred overnight at the same temperature. Then, the mixture was diluted with Et_2O (5.0 mL×3) and concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel (PE) to give the desired product **3**.

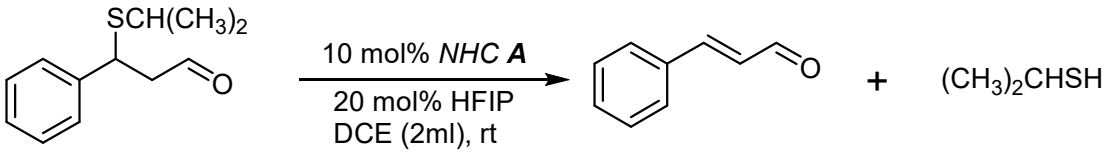
3. General procedure B: NHC-catalyzed sulfa-Michael addition of enals in DCM/

pH 6.8 phosphate aqueous mixture



IPr **A** (7.8 mg, 10 mol%) was dissolved in a mixture of 1.3 mL dry 1,2-dichloroethane and 1.0 ml pH 6.8 phosphate-based buffer solution. cinnamaldehyde **1a** (0.2 mmol), thiol **2** (0.6 mmol,) and HFIP (6.7 mg, 20 mol%) were added subsequently via a syringe at ambient temperature. The reaction mixture was stirred overnight at the same temperature. Then, the mixture was extracted with DCM (5.0 mL×3) and dried over anhydrous $MgSO_4$, then concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel (PE) to give the desired product **3**.

4. **Procedure for NHC-catalyzed reversible reaction of *sulfa*-Michael adduct**



To a solution of *NHC* **A** (7.8 mg, 10 mol%) in 2.0 mL 1,2-dichloroethane was added 1,1,1,3,3,3-hexafluoro-2-propanol (6.7mg, 20 mol%) and 3-(isopropylthio)-3-phenylpropanal (**3j**) (0.2 mmol). The reaction mixture was stirred at room temperature for 12 h, and then, the reaction mixture was filtered through a short silica pad and washed with EtOAc (15.0 mL) and concentrated in vacuum. The ratio of **3j** to cinnamaldehyde (2.4 : 1) was determined by ^{1}H NMR anaylsis of the crude reaction mixture. The crude product was further purified by flash column

chromatography on silica gel (PE) to give the product cinnamaldehyde in 29% yield.

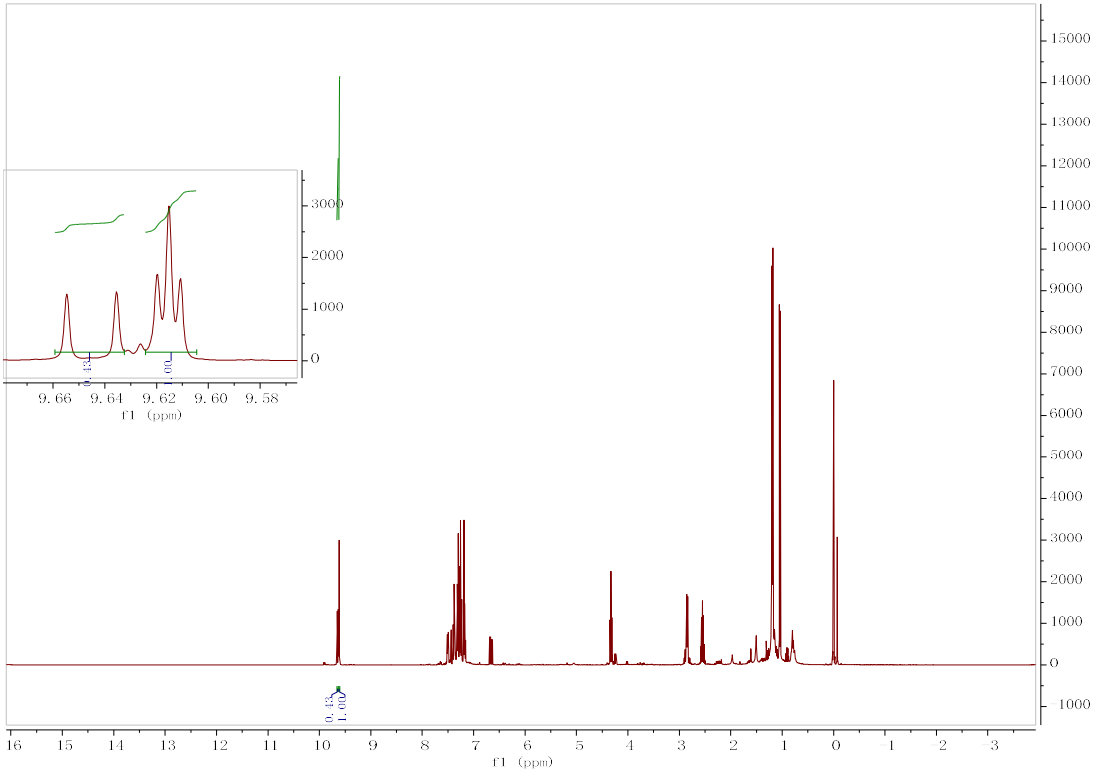
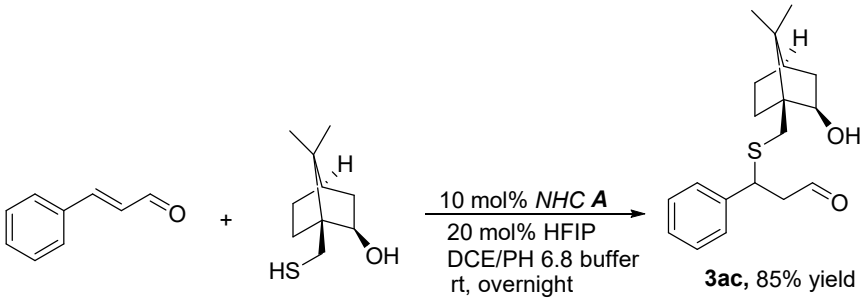


Fig.1 ^{1}H NMR ($CDCl_3$, 400 MHZ) of the crude reaction mixture of **3j**

5. 1 NHC-catalyzed Michael addition between mercaptoisoborneol and cinnamaldehyde

3ac was prepared according to **General Procedure B.**

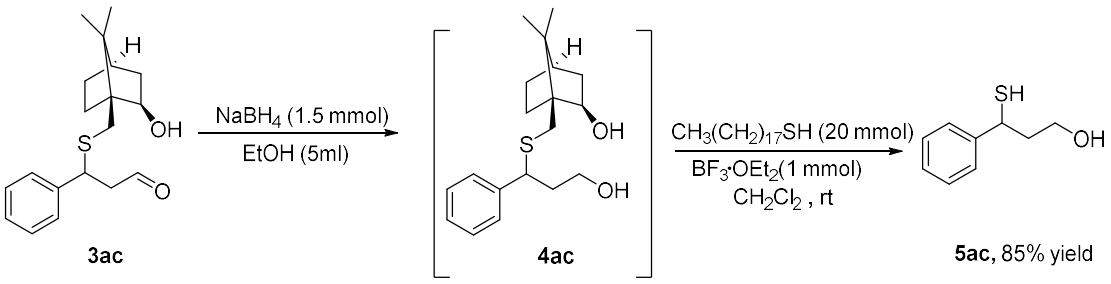


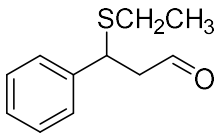
3ac, 85% yield

5. 2 Reduction and deprotection of compound 3ac

To a solution of **3ac** (1 mmol) in anhydrous EtOH (10.0 mL) was added $NaBH_4$ (1.5 mmol) at 0 ^{o}C, and after the addition of $NaBH_4$, the reaction mixture was stirred at room temperature for additional 2.0 hours. The reaction was quenched with water

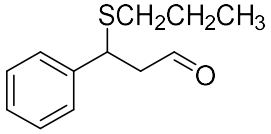
(30 ml) at 0 ^{o} and extracted with DCM (3×20 ml), the combined organic layer was washed with brine, and dried over magnesium sulfate, filtered, and concentrated in vacuum to give intermediate **4ac**, which was used directly in the next step. Intermediate **4ac** was dissolved in CH_2Cl_2 (12.0 mL), and then, $BF_3 \bullet OEt_2$ (1.0 mmol) was added at room temperature. The reaction mixture was stirred at room temperature until full consumption of **4ac** (about 3 hours). n-Octadecylmercaptan (20.0 mmol) was then added and the resultant mixture was stirred for 6 h at room temperature. The reaction mixture was poured into water, and extracted with ethyl acetate (3×30 mL). The combined organic layers were washed with brine, and dried over magnesium sulfate, filtered, and concentrated in vacuum. Purification of the residue by silica gel column chromatography (hexane/ethyl acetate = 10:1) gave the product **5ac**.





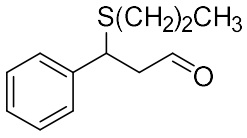
3-(Ethylthio)-3-phenylpropanal (3a) [1]

Pale yellow oil; 37.7 mg, 97% yield; $\mathbf{R}_f$ (PE/DCM = 2/1): 0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.8 Hz, 1H), 7.37 – 7.29 (m, 4H), 7.27 – 7.22 (m, 1H), 4.36 (t, *J* = 7.5 Hz, 1H), 2.95 (dt, *J* = 7.6, 1.9 Hz, 2H), 2.42–2.24 (m, 2H), 1.16 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.50, 141.33, 128.71, 127.64, 127.53, 49.76, 42.89, 25.19, 14.29.



3-Phenyl-3-(propylthio)propanal (3b)

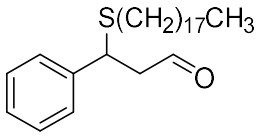
Colorless oil; 37.5 mg, 90% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.8 Hz, 1H), 7.38 – 7.30 (m, 4H), 7.27 – 7.22 (m, 1H), 4.32 (t, *J* = 7.5 Hz, 1H), 2.95 (ddd, *J* = 7.6, 1.8, 1.2 Hz, 2H), 2.43 – 2.21 (m, 2H), 1.57 – 1.43 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.55, 141.39, 128.70, 127.65, 127.52, 49.85, 43.16, 33.25, 22.46; FTIR (film) 3430, 3029, 2962, 2727, 1724, 1679, 1491, 1454, 1385, 1293, 1240, 1123, 1051, 751, 700 cm^{-1}; HRMS (ESI) *m/z* calcd for $C12H17OS^+$ $(M+H)^+$ 209.0995, found 209.0999.



3-(Butylthio)-3-phenylpropanal (3c) [2]

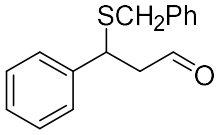
Colorless oil; 36.0 mg, 81% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (t, *J* = 1.8 Hz, 1H), 7.38 – 7.30 (m, 4H), 7.27 – 7.25 (m, 1H), 4.33 (t, *J* = 7.5 Hz, 1H), 2.95 (dt, *J* = 7.6, 1.7 Hz, 2H), 2.41 – 2.24 (m, 2H), 1.52 – 1.42 (m, 2H), 1.35 – 1.26 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.56,

141.36, 128.69, 127.65, 127.52, 49.83, 43.21, 31.17, 30.90, 21.93, 13.60.



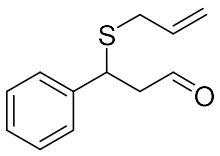
3-(Octadecylthio)-3-phenylpropanal (3d)

Colorless oil; 68.5 mg, 82%[b] yield; $\mathbf{R}_f$ (PE/DCM = 3/1): 0.21; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (t, *J* = 1.8 Hz, 1H), 7.37 – 7.26 (m, 4H), 7.26 – 7.22 (m, 1H), 4.32 (t, *J* = 7.5 Hz, 1H), 2.95 (dt, *J* = 7.6, 1.7 Hz, 2H), 2.44 – 2.19 (m, 2H), 1.53 – 1.41 (m, 2H), 1.24 (d, *J* = 9.2 Hz, 30H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.56, 141.38, 128.69, 127.65, 127.52, 49.83, 43.24, 31.94, 31.25, 29.71, 29.68, 29.65, 29.58, 29.46, 29.38, 29.14, 29.10, 28.82, 22.71, 14.14. FTIR (film) 3435, 3029, 2923, 2852, 1727, 1454, 1384, 1053, 911, 748, 698 cm^{-1}; HRMS (ESI) *m/z* calcd for $C27H47OS^+$ $(M+H)^+$ 419.3342, found 419.3347.



3-(Benzylthio)-3-phenylpropanal (3e) [3]

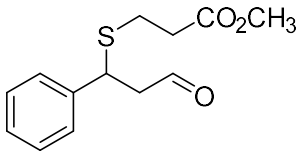
Pale yellow oil; 46.6 mg, 91% yield; $\mathbf{R}_f$ (PE/DCM = 1/1): 0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.58 (t, *J* = 1.9 Hz, 1H), 7.38 – 7.27 (m, 7H), 7.25 – 7.19 (m, 3H), 4.18 (t, *J* = 7.5 Hz, 1H), 3.59 – 3.42 (m, 2H), 2.89 (ddd, *J* = 7.6, 3.7, 1.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.39, 140.88, 128.94, 128.77, 128.52, 127.89, 127.67, 127.15, 49.58, 42.75, 35.57.



3-(Allylthio)-3-phenylpropanal (3f)

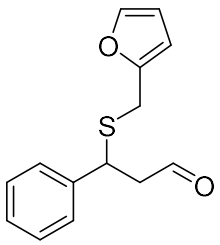
Pale yellow oil; 36.3 mg, 88% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.35; ^{1}H NMR (400

MHz, $CDCl_3$) δ 9.67 (t, *J* = 1.8 Hz, 1H), 7.38 – 7.30 (m, 4H), 7.28 – 7.24 (m, 1H), 5.81 – 5.70 (m, 1H), 5.13 – 5.01 (m, 2H), 4.31 (t, *J* = 7.5 Hz, 1H), 3.04 – 2.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.41, 141.02, 133.92, 128.74, 127.87, 127.61, 117.60, 49.68, 42.10, 34.13. FTIR (film) 3429, 3082, 3029, 2914, 2827, 2727, 1724, 1635, 1453, 1403, 1230, 991, 919, 751, 700 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{12}H_{15}OS^+$ $(M+H)^+$ 207.0838, found 207.0838.



Methyl 3-((3-oxo-1-phenylpropyl)thio)propanoate (3g)

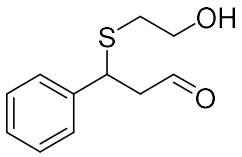
Colorless oil; 42.0 mg, 83% yield; $\mathbf{R}_f$ (PE/EtOAc = 5/1): 0.25; ^1H NMR (400 MHz, $CDCl_3$) δ 9.68 (t, *J* = 1.7 Hz, 1H), 7.39 – 7.30 (m, 4H), 7.30 – 7.26 (m, 1H), 4.38 (t, *J* = 7.4 Hz, 1H), 3.66 (s, 3H), 2.96 (dt, *J* = 7.5, 1.9 Hz, 2H), 2.60 (td, *J* = 7.1, 1.0 Hz, 2H), 2.50 – 2.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.12, 172.15, 140.89, 128.84, 127.77, 127.67, 51.81, 49.71, 43.35, 34.14, 26.14; FTIR (film) 3441, 2923, 1723, 1436, 1360, 1171, 1055, 751, 700 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{13}H_{16}O_3S^+$ $(M+H)^+$ 253.0893, found 253.0889.



3-((Furan-2-ylmethyl)thio)-3-phenylpropanal (3h)

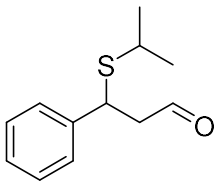
Colorless oil; 45.3 mg, 92% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.35; ^1H NMR (400 MHz, $CDCl_3$) δ 9.62 (t, *J* = 1.8 Hz, 1H), 7.39 – 7.31 (m, 5H), 7.31 – 7.26 (m, 1H), 6.30 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.11 (dd, *J* = 3.3, 0.8 Hz, 1H), 4.33 (t, *J* = 7.5 Hz, 1H), 3.63 – 3.40 (m, 2H), 3.03 – 2.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.21, 151.16, 142.21, 140.57, 128.78, 127.90, 127.74, 110.44, 107.73, 49.47, 42.88, 27.64; FTIR (film) 3463, 2728, 1723, 1638, 1502, 1384, 1150, 1010, 934, 740, 700 cm^{-1}; HRMS

(ESI) *m/z* calcd for C14H15O2S$^+$ (M+H)$^+$ 247.0787, found 247.0786.



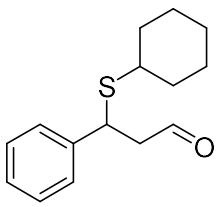
3-((2-Hydroxyethyl)thio)-3-phenylpropanal (3i)

Colorless oil; 36.8 mg, 87%[b] yield; $\mathbf{R}_f$ (PE/EtOAc = 1/1): 0.15; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (t, *J* = 1.5 Hz, 1H), 7.36 – 7.31 (m, 5H), 4.41 (t, *J* = 7.4 Hz, 1H), 3.74 – 3.55 (m, 3H), 2.99 (dt, *J* = 7.3, 1.5 Hz, 2H), 2.55 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.17, 141.13, 128.88, 127.80, 127.64, 60.64, 49.99, 42.71, 34.37. FTIR (film) 3428, 2919, 1721, 1453, 1384, 1057, 700 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{11}H_{14}O_2S^+$ (M+H)$^+$ 211.0787, found 211.0779.



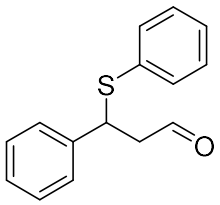
3-(Isopropylthio)-3-phenylpropanal (3j)

Colorless oil; 31.7 mg, 76%[b] yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (t, *J* = 1.8 Hz, 1H), 7.42 – 7.29 (m, 4H), 7.26 – 7.21 (m, 1H), 4.40 (t, *J* = 7.5 Hz, 1H), 2.92 (ddd, *J* = 7.5, 3.3, 1.8 Hz, 2H), 2.67 – 2.57 (m, 1H), 1.26 (d, *J* = 6.6 Hz, 3H), 1.11 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.56, 128.72, 127.60, 127.47, 50.19, 42.36, 34.55, 23.48, 22.90; FTIR (film) 3028, 2960, 2929, 2866, 2725, 2359, 1724, 1679, 1453, 1246, 1055, 752, 700 cm^{-1}; HRMS (ESI) *m/z* calcd for C12H17OS$^+$ (M+H)$^+$ 209.0995, found 209.0993.



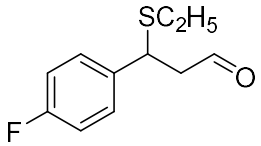
3-(Cyclohexylthio)-3-phenylpropanal (3k)

Pale yellow oil; 38.3 mg, 77%[b] yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.33; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (t, *J* = 1.8 Hz, 1H), 7.39 – 7.26 (m, 4H), 7.26 – 7.21 (m, 1H), 4.42 (t, *J* = 7.5 Hz, 1H), 2.92 (dt, *J* = 7.6, 2.0 Hz, 2H), 2.48 – 2.34 (m, 1H), 1.98 (d, *J* = 13.2 Hz, 1H), 1.77 – 1.57 (m, 3H), 1.40 – 1.11 (m, 5H), 0.94 – 0.80 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.70, 128.69, 127.55, 127.42, 50.27, 43.06, 41.81, 33.63, 33.14, 25.89, 25.75, 25.68. FTIR (film) 3436, 2929, 1724, 1637, 1449, 1384, 1073, 908, 734 cm^{-1}; HRMS (ESI) *m/z* calcd for $C15H21OS^+$ $(M+H)^+$ 249.1308, found 249.1307.



3-Phenyl-3-(phenylthio)propanal (3m)[4]

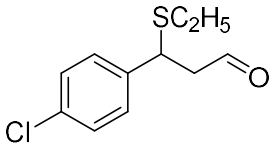
Pale yellow oil; 26.1 mg, 54%[b] yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.29; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.7 Hz, 1H), 7.53 – 7.16 (m, 10H), 4.69 (t, *J* = 7.5 Hz, 1H), 3.04 (ddd, *J* = 7.2, 3.5, 1.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.45, 140.44, 133.40, 129.06, 128.93, 128.63, 127.99, 127.67, 49.22, 47.26.



3-(Ethylthio)-3-(4-fluorophenyl)propanal (3n)

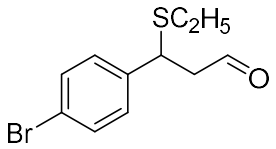
Colorless oil; 39.9 mg, 94% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.24; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.7 Hz, 1H), 7.37 – 7.30 (m, 2H), 7.06 – 6.98 (m, 2H), 4.36 (t, *J* = 7.4 Hz, 1H), 2.94 (dd, *J* = 7.5, 1.7 Hz, 2H), 2.38 –2.28 (m, 2H), 1.16 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 199.14, 161.95 (d, *J* = 246.4 Hz), 137.14 (d, *J* = 3.2 Hz), 129.22 (d, *J* = 8.0 Hz), 115.57 (d, *J* = 21.6 Hz), 49.97 (d, *J* = 0.7 Hz), 42.09, 25.20, 14.24; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.73; FTIR (film) 3430, 2969,

2928, 2828, 2730, 2360, 1725, 1683, 1601, 1509, 1224, 1159, 1124, 974, 841 cm^{-1}; HRMS (ESI) *m/z* calcd for $C11H14FOS^+$ $(M+H)^+$ 213.0744, found 213.0742.



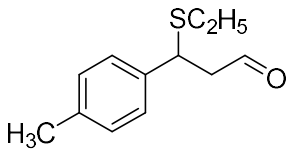
3-(4-Chlorophenyl)-3-(ethylthio)propanal (3o)

Yellow oil; 40.1 mg, 88% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.23; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.6 Hz, 1H), 7.30 (s, 4H), 4.34 (t, *J* = 7.4 Hz, 1H), 2.94 (dd, *J* = 7.4, 1.6 Hz, 2H), 2.38 –2.28 (m, 2H), 1.16 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.94, 139.99, 133.18, 129.02, 128.86, 49.79, 42.14, 25.23, 14.23. FTIR (film) 3431, 2968, 2926, 2851, 2728, 1724, 1682, 1490, 1409, 1265, 1091, 1013, 807 cm^{-1}; HRMS (ESI) *m/z* calcd for $C11H14ClOS^+$ $(M+H)^+$ 229.0448, found 229.0445.



3-(4-Bromophenyl)-3-(ethylthio)propanal (3p)[5]

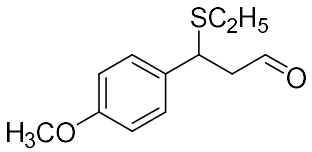
Yellow oil; 43.5 mg, 80% yield; $\mathbf{R}_f$ (PE/DCM = 1/1): 0.31; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (t, *J* = 1.6 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.29 – 7.24 (m, 2H), 4.35 (t, *J* = 7.4 Hz, 1H), 2.95 (dd, *J* = 7.4, 1.6 Hz, 2H), 2.40 – 2.30 (m, 2H), 1.18 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.91, 140.54, 131.82, 129.38, 121.25, 49.73, 42.19, 25.23, 14.23.



3-(Ethylthio)-3-(p-tolyl)propanal (3q)

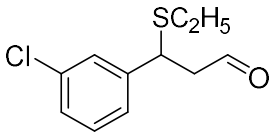
Pale yellow oil; 29.2 mg, 70% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.41; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.9 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 7.7 Hz,

2H), 4.33 (t, *J* = 7.5 Hz, 1H), 2.93 (dt, *J* = 7.5, 1.8 Hz, 2H), 2.39 – 2.30 (m, 5H), 1.16 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.70, 138.18, 137.24, 127.50, 49.81, 42.63, 25.15, 14.29; FTIR (film) 2966, 1686, 1629, 1488, 1073, 1010, 905, 868, 728, 649 cm^{-1}; HRMS (ESI) *m/z* calcd for C12H17OS$^+$ (M+H)$^+$ 209.0995, found 209.0997.



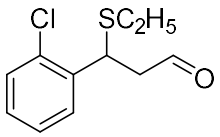
3-(Ethylthio)-3-(4-methoxyphenyl)propanal (3r)[6]

Yellow oil; 31.4 mg, 70% yield; $\mathbf{R}_f$ (PE/EtOAc = 5/1): 0.45; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (t, *J* = 1.8 Hz, 1H), 7.29 – 7.26 (m, 2H), 6.88 – 6.84 (m, 2H), 4.34 (t, *J* = 7.5 Hz, 1H), 3.80 (s, 3H), 2.92 (dt, *J* = 7.5, 1.8 Hz, 2H), 2.38 –2.28 (m, 2H), 1.16 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.72, 158.88, 128.70, 114.05, 55.28, 49.93, 42.31, 25.12, 14.30.



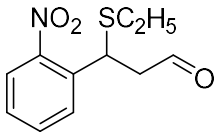
3-(3-Chlorophenyl)-3-(ethylthio)propanal (3s)

Yellow oil; 36.0 mg, 79% yield; $\mathbf{R}_f$ (PE/DCM = 2/1): 0.38; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (t, *J* = 1.5 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.26 – 7.21 (m, 3H), 4.33 (t, *J* = 7.4 Hz, 1H), 2.99 – 2.92 (m, 2H), 2.41 – 2.30 (m, 2H), 1.18 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.83, 143.65, 134.57, 129.94, 127.75, 125.94, 49.70, 42.35, 25.32, 14.22; FTIR (film) 3434, 2970, 2931, 1724, 1629, 1384, 1079, 786 cm^{-1}; HRMS (ESI) *m/z* calcd for C11H14ClOS$^+$(M+H)$^+$ 229.0448, found 229.0446.



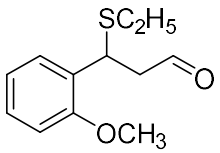
3-(2-Chlorophenyl)-3-(ethylthio)propanal (3t)

Yellow oil; 34.7 mg, 76% yield; $\mathbf{R}_f$ (PE/DCM = 2/1): 0.38; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.72 (t, *J* = 2.0 Hz, 1H), 7.58 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.36 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.29 (td, *J* = 7.6, 1.5 Hz, 1H), 7.19 (td, *J* = 7.6, 1.7 Hz, 1H), 4.97 (t, *J* = 7.5 Hz, 1H), 2.91 (dd, *J* = 7.5, 2.0 Hz, 2H), 2.51 – 2.35 (m, 2H), 1.20 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.15, 138.90, 133.32, 129.66, 129.00, 128.56, 127.49, 49.24, 39.02, 25.50, 14.48. FTIR (film) 3432, 2969, 2928, 1725, 1473, 1443, 1268, 1035, 753 cm^{-1}; HRMS (ESI) *m/z* calcd for $C11H14ClOS^+$ $(M+H)^+$ 229.0448, found 229.0449.



3-(Ethylthio)-3-(2-nitrophenyl)propanal (3u)

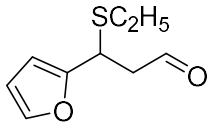
Yellow oil; 43.0 mg, 90% yield; $\mathbf{R}_f$ (PE/EtOAc = 5/1): 0.23; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.72 (dd, *J* = 2.1, 1.3 Hz, 1H), 7.84 (td, *J* = 8.0, 1.4 Hz, 2H), 7.67 – 7.61 (m, 1H), 7.42 (ddd, *J* = 8.1, 7.4, 1.4 Hz, 1H), 5.09 (t, *J* = 7.5 Hz, 1H), 3.08 – 2.92 (m, 2H), 2.54 – 2.36 (m, 2H), 1.18 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.33, 136.80, 133.21, 129.9, 128.19, 124.24, 50.10, 37.57, 25.95, 14.31. FTIR (film) 3436, 2967, 2927, 1723, 1686, 1526, 1350, 1119, 971, 785, 741 cm^{-1}; HRMS (ESI) *m/z* calcd for $C11H14NO3S^+$ $(M+H)^+$ 240.0689, found 240.0688.



3-(Ethylthio)-3-(2-methoxyphenyl)propanal (3v)

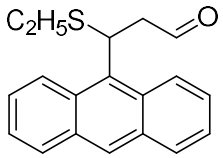
Yellow oil; 36.8 mg, 82% yield; $\mathbf{R}_f$ (PE/EtOAc = 5/1): 0.51; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (t, *J* = 2.2 Hz, 1H), 7.43 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.23 (ddd, *J* = 8.2, 7.4, 1.7 Hz, 1H), 6.96 (td, *J* = 7.5, 1.2 Hz, 1H), 6.88 (dd, *J* = 8.2, 1.1 Hz, 1H), 4.85 (t, *J* = 7.5 Hz, 1H), 3.85 (s, 3H), 2.90 (ddd, *J* = 7.4, 2.2, 0.7 Hz, 2H), 2.47 – 2.37 (m, 2H),

1.19 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.48, 156.63, 129.33, 128.42, 128.23, 120.95, 110.73, 55.51, 49.06, 36.26, 25.48, 14.45. FTIR (film) 3435, 2970, 2928, 1724, 1631, 1384, 1149, 1069, 1010, 925, 740 cm^{-1}; HRMS (ESI) *m/z* calcd for C12H17O2S$^+$ (M+H) $^+$ 225.0944, found 225.0943.



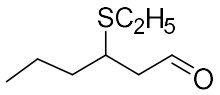
3-(Ethylthio)-3-(furan-2-yl)propanal (3w)

Pale yellow oil; 23.6 mg, 64% yield; $\mathbf{R}_f$ (PE/EtOAc = 5/1): 0.42; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (t, J = 1.7 Hz, 1H), 7.37 (dd, J = 1.9, 0.9 Hz, 1H), 6.31 (dd, J = 3.3, 1.8 Hz, 1H), 6.21 (d, J = 3.2 Hz, 1H), 4.44 (t, J = 7.3 Hz, 1H), 3.14 – 2.90 (m, 2H), 2.49 (qd, J = 7.4, 1.0 Hz, 2H), 1.20 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.11, 153.24, 142.25, 110.31, 107.06, 46.90, 35.74, 25.20, 14.37. FTIR (film) 3435, 2970, 2928, 1724, 1631, 1384, 1149, 1069, 1010, 925, 740 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_9H_{13}O_2S^+$ (M+H)$^+$ 185.0631, found 185.0631.



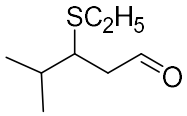
3-(anthracen-9-yl)-3-(ethylthio)propanal (3x)

Yellow oil; 23.6 mg, 78% yield; $\mathbf{R}_f$ (PE/DCM = 1/1): 0.53; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.74 (t, J = 1.2 Hz, 1H), 8.67 (d, J = 8.9 Hz, 1H), 8.51 – 8.36 (m, 2H), 8.05 – 7.96 (m, 2H), 7.59 – 7.51 (m, 2H), 7.50 – 7.43 (m, 2H), 6.11 (t, J = 6.6 Hz, 1H), 3.69 (ddd, J = 18.2, 7.1, 1.5 Hz, 1H), 3.47 (dd, J = 18.3, 6.1 Hz, 1H), 2.73 – 2.46 (m, 2H), 1.20 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.41, 133.32, 129.77, 129.53, 128.22, 126.70, 126.16, 125.54, 125.16, 124.97, 124.88, 123.05, 51.67, 35.56, 27.82, 14.79; FTIR (film) 3435, 3050, 2924, 2360, 1720, 1681, 1445, 888, 731 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{19}H_{18}OS^+$ (M+H)$^+$ 295.1151, found 295.1152.



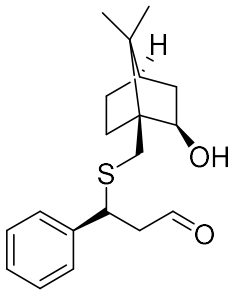
3-(Ethylthio)hexanal (3y)[7]

Colorless oil; 31.1 mg, 97% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.49; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.79 (t, *J* = 2.1 Hz, 1H), 3.18 – 3.10 (m, 1H), 2.68 – 2.63 (m, 2H), 2.56 (q, *J* = 7.4 Hz, 2H), 1.65 – 1.56 (m, 2H), 1.52 – 1.42 (m, 2H), 1.25 (t, *J* = 7.4 Hz, 3H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.15, 48.84, 39.04, 37.48, 24.48, 20.03, 14.74, 13.82.



3-(Ethylthio)-4-methylpentanal (3z)[5]

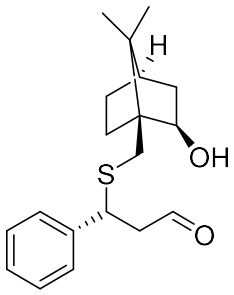
Colorless oil; 31.1 mg, 97% yield; $\mathbf{R}_f$ (PE/EtOAc = 10/1): 0.53; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.83 – 9.76 (m, 1H), 3.03 (ddd, *J* = 8.9, 5.3, 4.4 Hz, 1H), 2.69 – 2.54 (m, 4H), 1.98 – 1.90 (m, 1H), 1.25 (t, *J* = 7.4 Hz, 3H), 0.99 (dd, *J* = 11.9, 6.7 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.40, 46.40, 46.37, 32.37, 26.24, 19.34, 19.27, 14.85.



(R)-3-((((1S,2R,4R)-2-hydroxy-7,7-dimethylbicyclo[2.2.1]heptan-1-yl)methyl)thio)-3-phenylpropanal (*syn*-3ac)

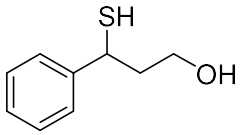
Colorless oil; 26.0 mg 31% yield. $\mathbf{R}_f$ (PE /EtOAc = 5/1): 0.35, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.71 (t, *J* = 1.8 Hz, 1H), 7.40 – 7.32 (m, 4H), 7.32 – 7.26 (m, 1H), 4.28 (t, *J* = 7.5 Hz, 1H), 3.75 (dd, *J* = 7.5, 3.7 Hz, 1H), 3.00 (dd, *J* = 7.5, 1.8 Hz, 2H), 2.54 – 2.44 (m, 2H), 1.75 – 1.59 (m, 6H), 1.51 – 1.44 (m, 1H), 1.18 – 1.11 (m, 1H), 1.05 – 0.98 (m, 1H), 0.89 (s, 3H), 0.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.30,

141.49, 128.95, 127.93, 127.46, 51.93, 49.65, 47.61, 44.98, 44.06, 38.95, 30.90, 30.21, 27.11, 20.59, 19.75. FTIR (film) 3435, 2931, 1723, 1453, 1388, 1265, 1072, 878, 739, 700 cm^{-1}; HRMS (ESI) m/z calcd for $C19H27O2S^+$ $(M+H)^+$ 319.1726, found 319.1722.



(R)-3-((((1S,2R,4R)-2-hydroxy-7,7-dimethylbicyclo[2.2.1]heptan-1-yl)methyl)thio)-3-phenylpropanal(*anti*-3ac)

Colorless oil; 34.3 mg 54% yield. $\mathbf{R}_f$ (PE /EtOAc = 5/1): 0.30, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.73 (t, *J* = 1.6 Hz, 1H), 7.37 – 7.33 (m, 4H), 7.30 – 7.26 (m, 1H), 4.34 (dd, *J* = 8.1, 6.8 Hz, 1H), 3.82 (dd, *J* = 8.0, 3.9 Hz, 1H), 3.08 – 2.95 (m, 2H), 2.69 (d, *J* = 11.0 Hz, 1H), 2.43 – 2.27 (m, 2H), 1.81 – 1.58 (m, 5H), 1.37 – 1.28 (m, 1H), 1.13 – 1.06 (m, 1H), 1.02 – 0.96 (m, 4H), 0.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.51, 141.42, 128.79, 127.63, 127.46, 51.90, 49.75, 47.62, 45.13, 44.51, 39.24, 30.93, 30.83, 27.06, 20.55, 19.89. FTIR (film) 3436, 2930, 1723, 1454, 1388, 1264, 1072, 879, 739, 700 cm^{-1}; HRMS (ESI) m/z calcd for $C19H27O2S^+$ $(M+H)^+$ 319.1726, found 319.1722.



3-Mercapto-3-phenylpropan-1-ol(5ac)

Colorless oil; 94% yield. R_f (Pet. ether /EtOAc = 3/1): 0.20,^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 4H), 7.27 – 7.22 (m, 1H), 4.21 (td, *J* = 7.6, 5.8 Hz, 1H), 3.80 – 3.61 (m, 2H), 2.28 – 2.08 (m, 2H), 1.96 (d, *J* = 5.9 Hz, 1H), 1.48 (d, *J* = 1.9 Hz, 1H).^{13}C NMR (100 MHz, CDCl3) δ 144.38, 128.77, 127.34, 126.87, 60.61, 42.04, 40.59.

Reference

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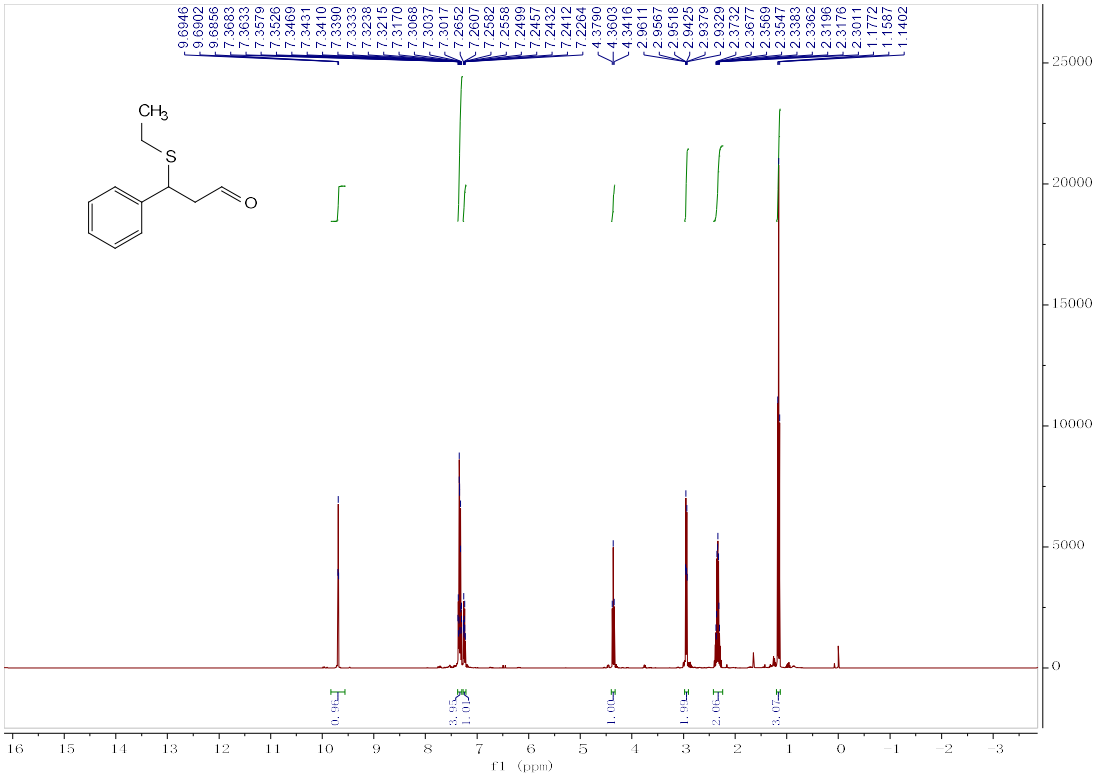
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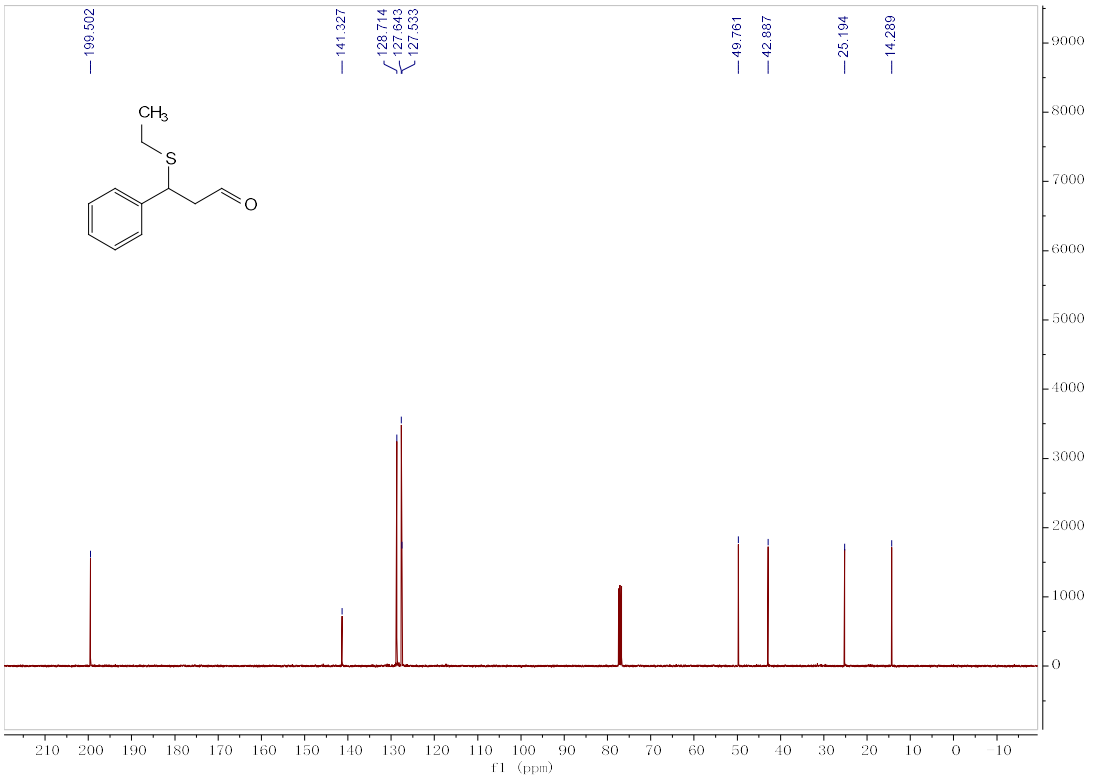
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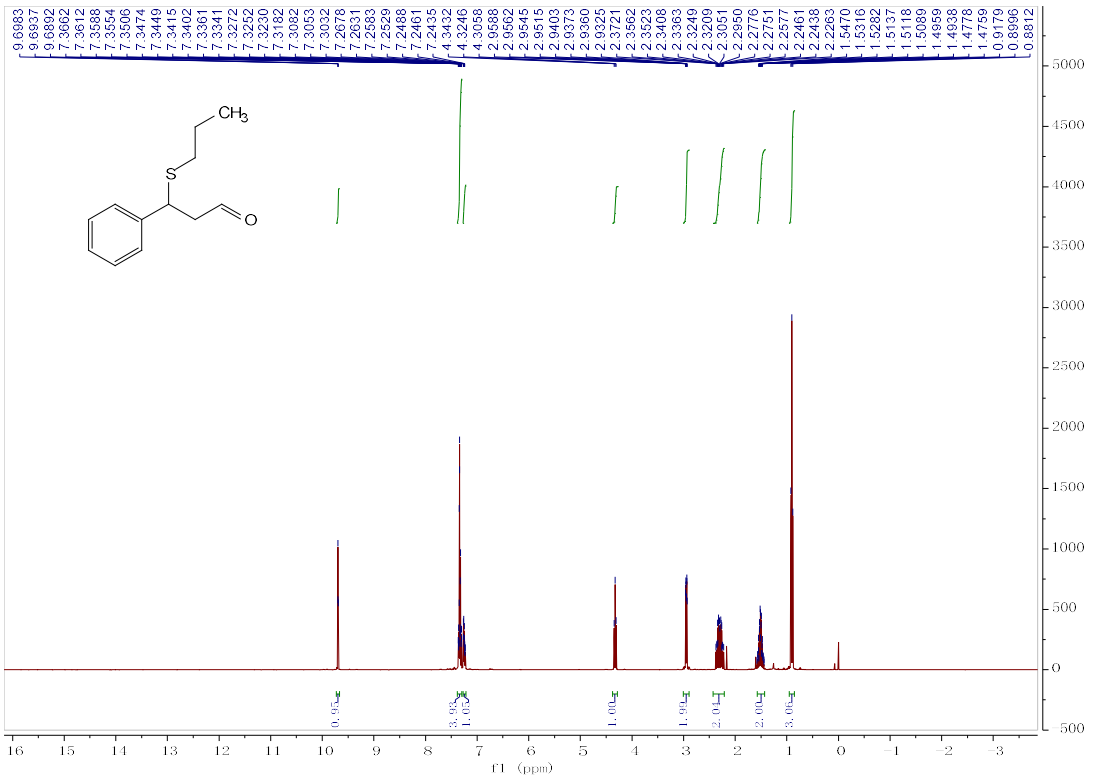
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7.2631
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2.2577
2.2461
2.2438
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1.5089
1.4959
1.4938
1.4778
1.4759
0.9179
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0.8812
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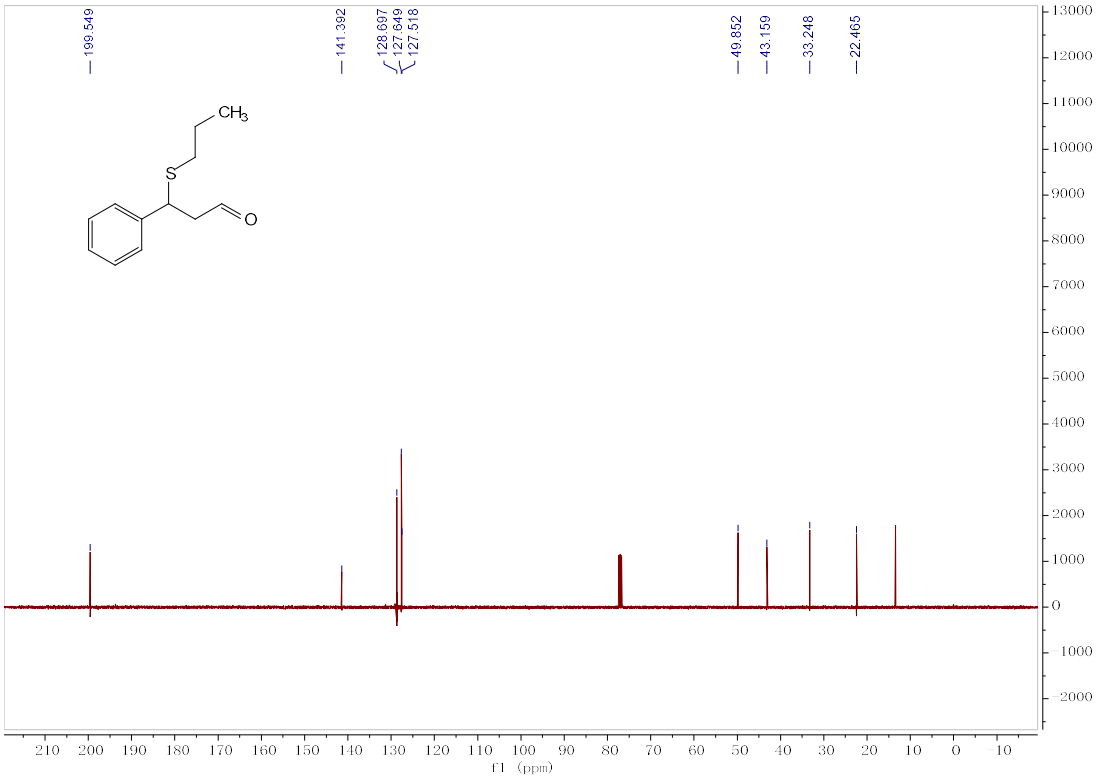
2.00
3.00
f1 (ppm)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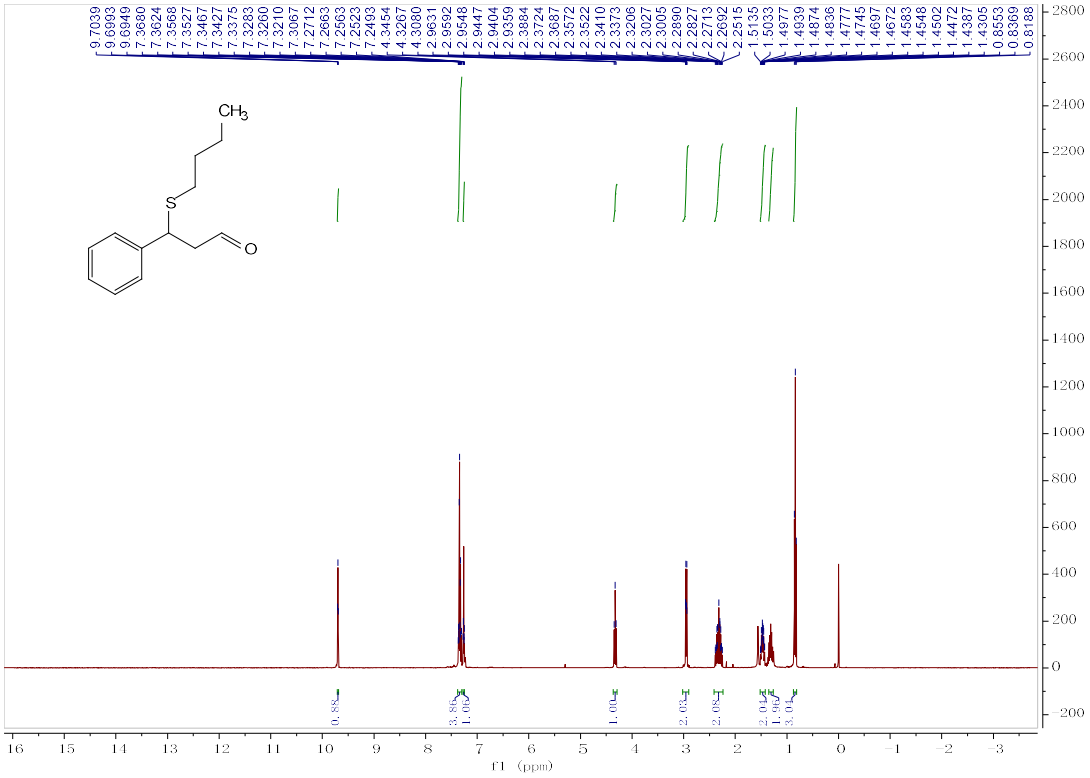
S
O
f1 (ppm)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7.3210
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7.2712
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7.2563
7.2523
7.2493
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4.3267
4.3080
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2.3687
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2.3522
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2.2827
2.2713
2.2692
2.2515
1.5135
1.5033
1.4977
1.4939
1.4874
1.4836
1.4777
1.4745
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1.4672
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1.4548
1.4502
1.4472
1.4387
1.4305
0.8553
0.8369
0.8188
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2.04
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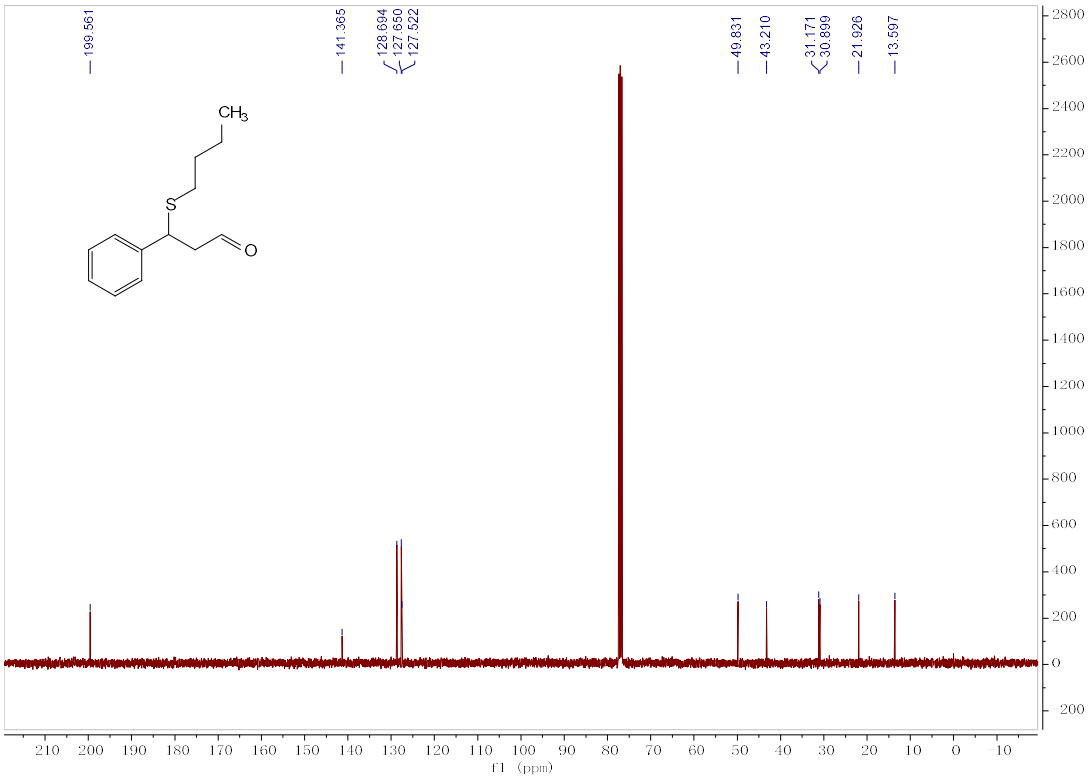
3.04
f1 (ppm)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31.171
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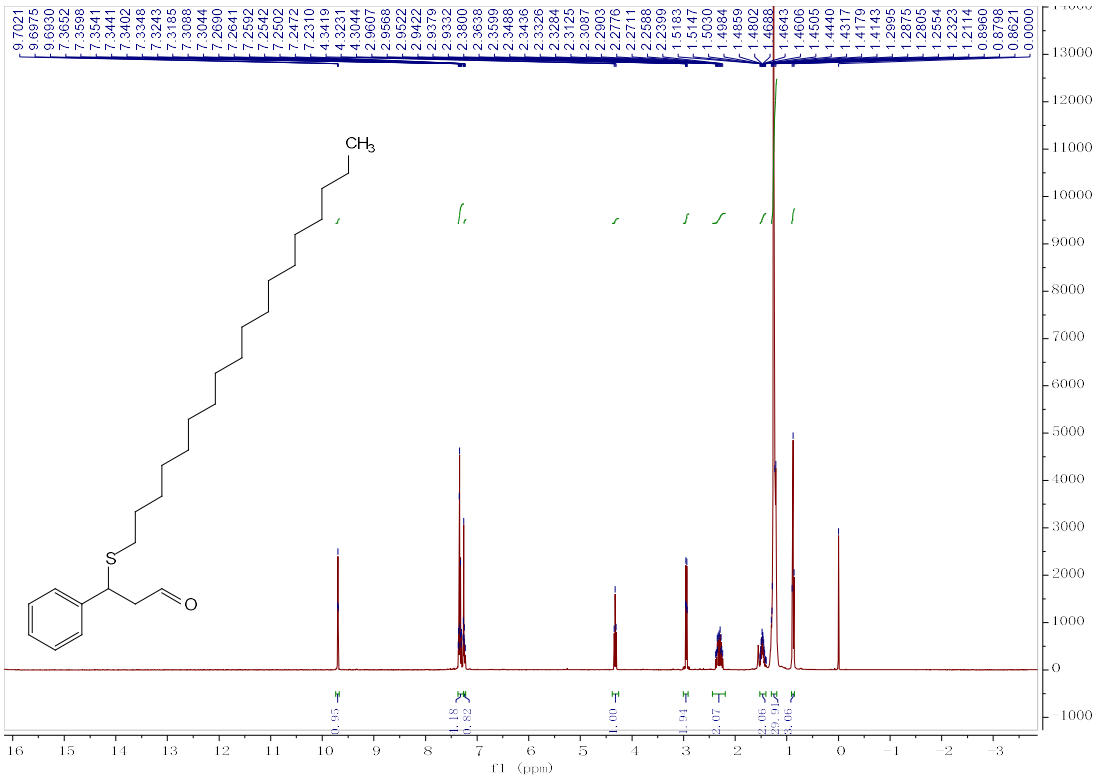
O
f1 (ppm)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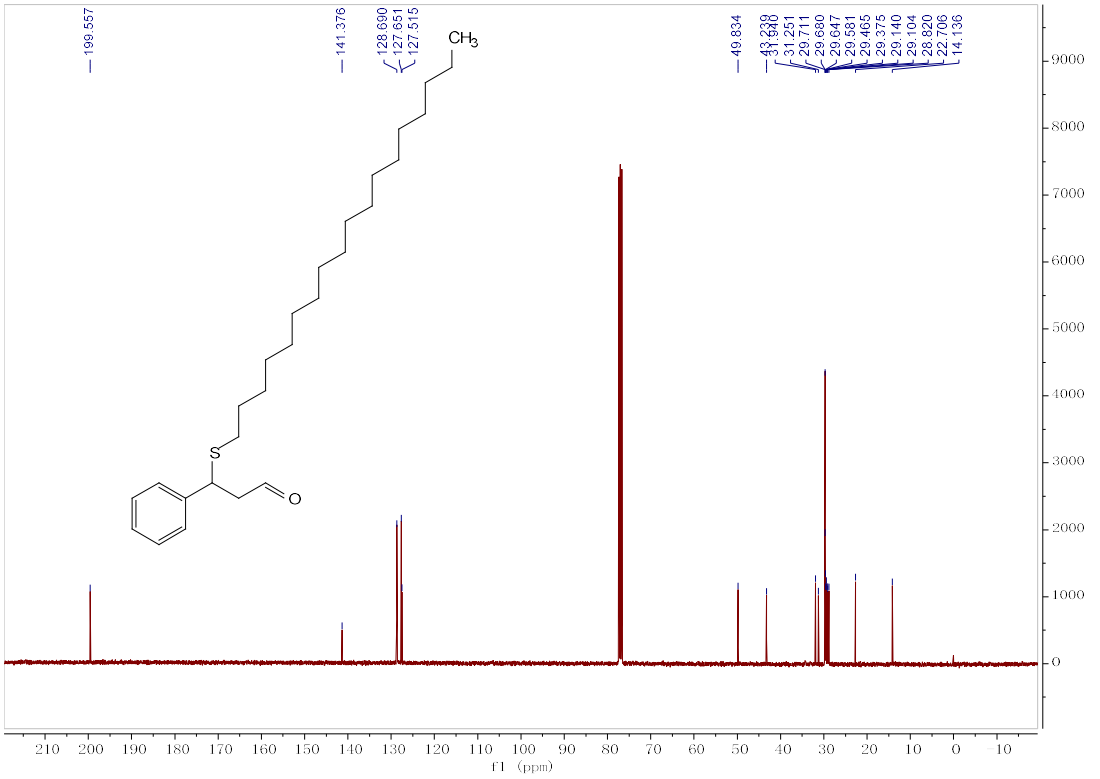
f1 (ppm)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29.680
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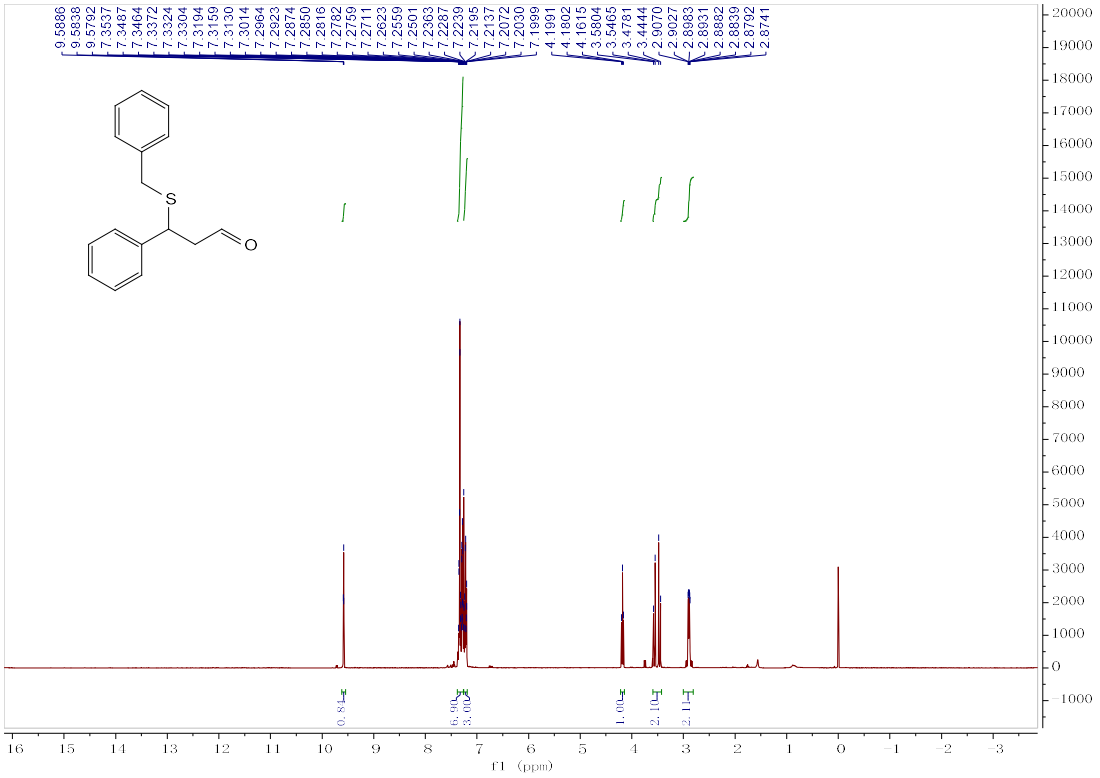
29.104
28.820
22.706
14.136
CH3
S
O
f1 (ppm)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7.3130
7.3014
7.2964
7.2923
7.2874
7.2850
7.2816
7.2782
7.2759
7.2711
7.2623
7.2559
7.2501
7.2363
7.2287
7.2239
7.2195
7.2137
7.2072
7.2030
7.1999
4.1991
4.1802
4.1615
3.5804
3.5465
3.4781
3.4444
2.9070
2.9027
2.8983
2.8931
2.8882
2.8839
2.8792
2.8741
S
O
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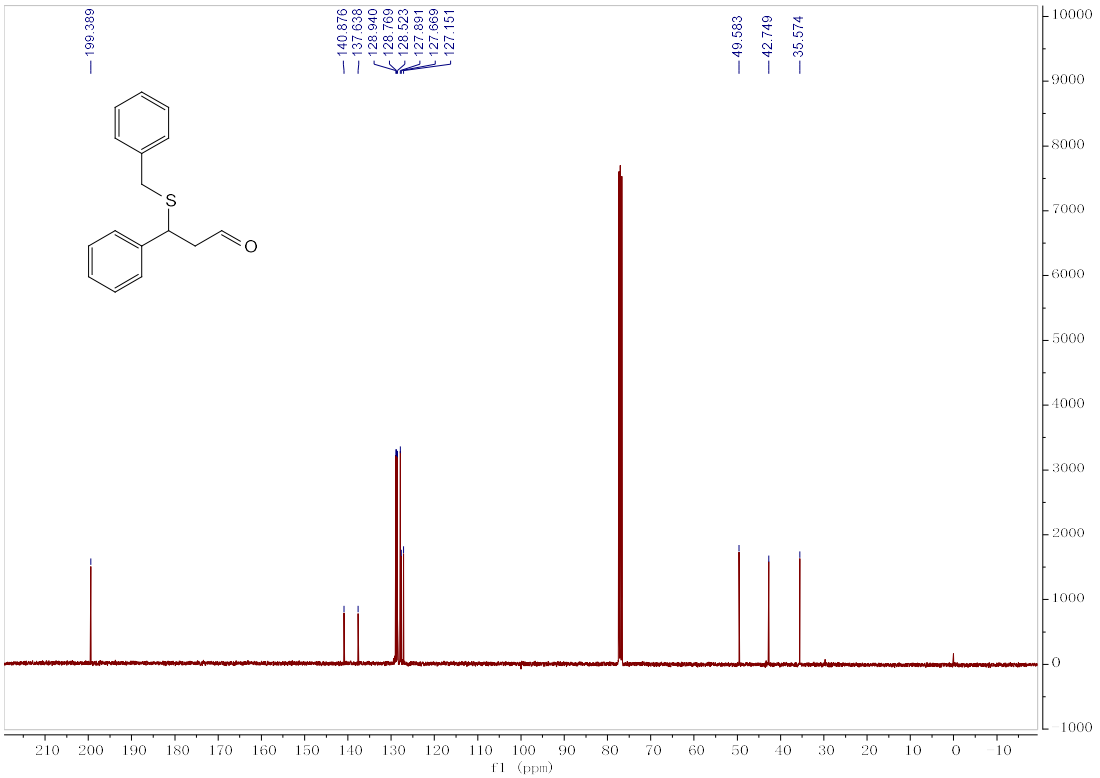
6.90
3.00
1.00
2.10
2.11
f1 (ppm)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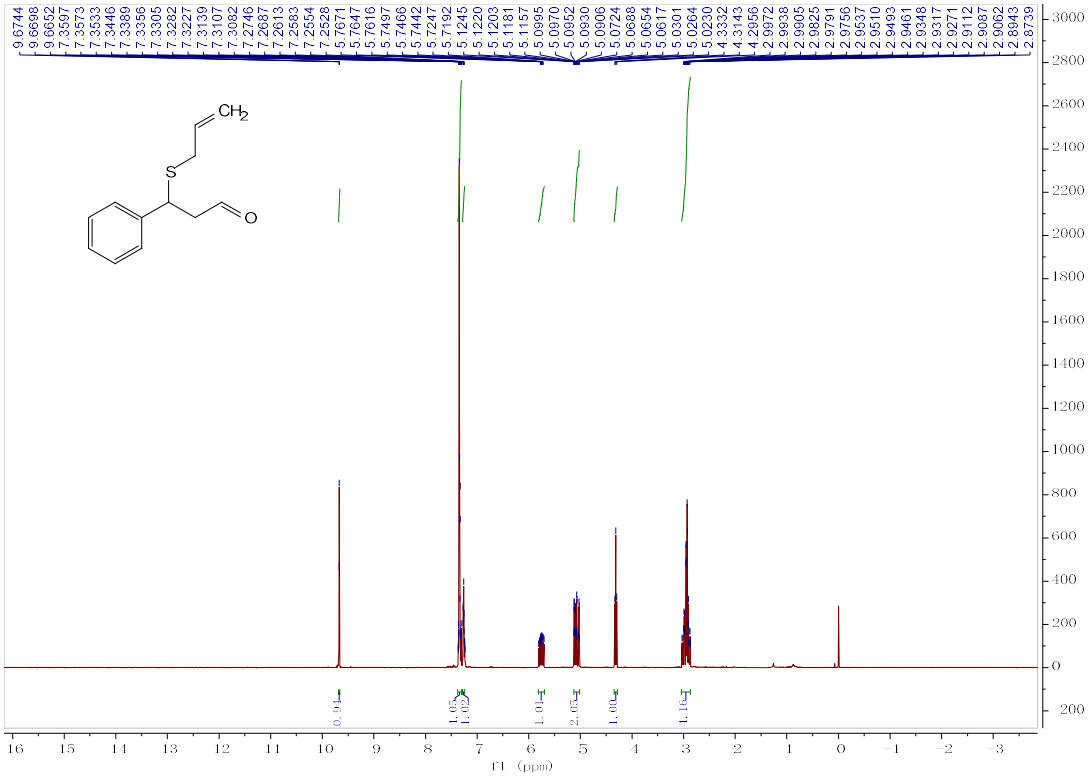
42.749
35.574
S
O
f1 (ppm)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7.3282
7.3227
7.3139
7.3107
7.3082
7.2746
7.2687
7.2613
7.2583
7.2554
7.2528
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5.7647
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5.7497
5.7466
5.7442
5.7247
5.7192
5.1245
5.1220
5.1203
5.1181
5.1157
5.0995
5.0970
5.0952
5.0930
5.0906
5.0724
5.0688
5.0654
5.0617
5.0301
5.0264
5.0230
4.3332
4.3143
4.2956
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2.9805
2.9625
2.9791
2.9756
2.9537
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2.9348
2.9317
2.9271
2.9112
2.9087
2.9062
2.8943
2.8739
CH2
S
O
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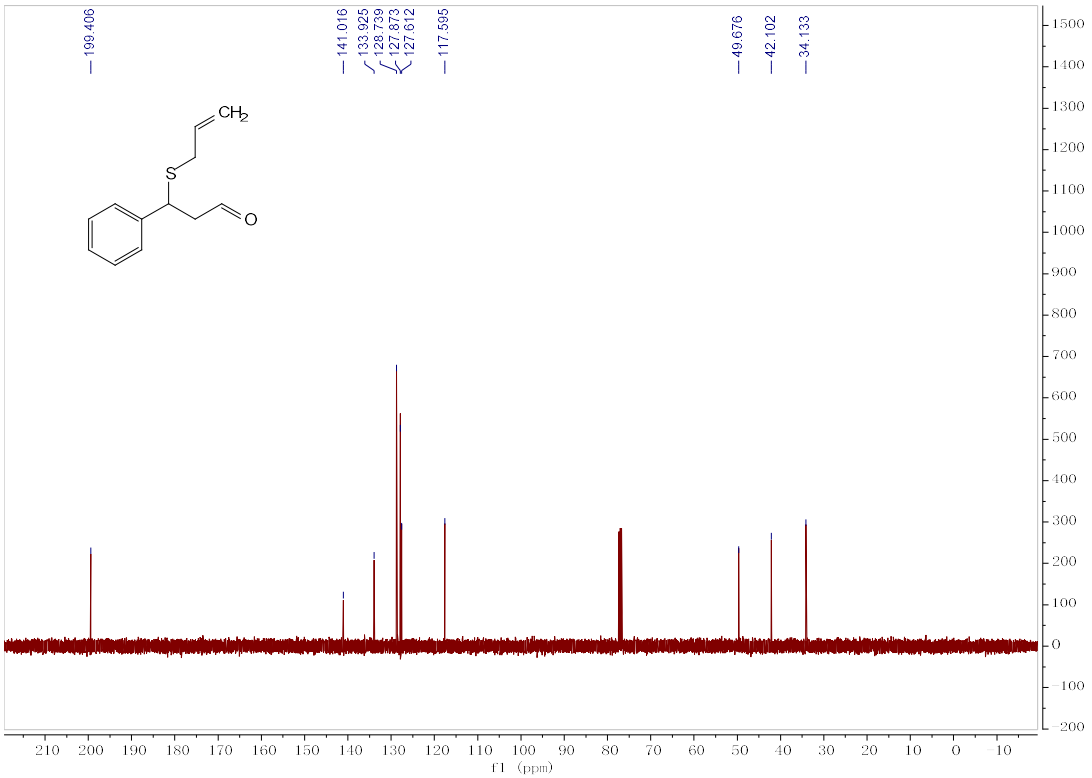
1.05
1.02
1.01
2.05
1.00
1.16
f1 (ppm)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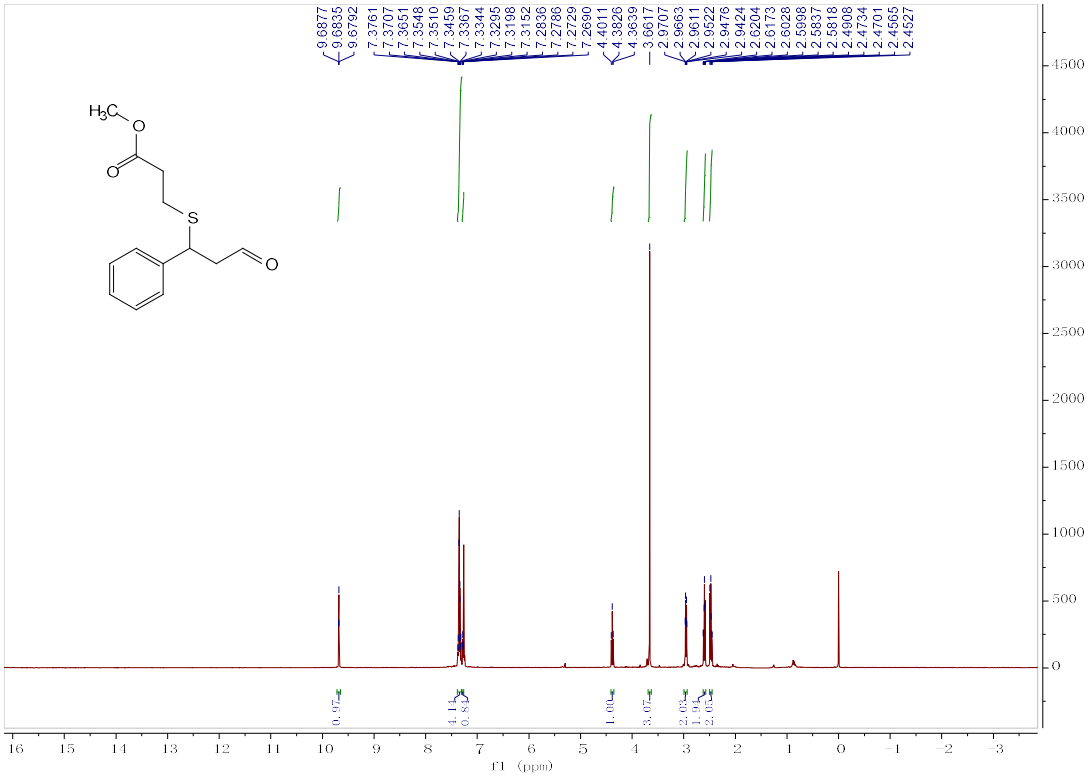
49.676
42.102
34.133
CH2
S
O
f1 (ppm)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7.3295
7.3198
7.3152
7.2836
7.2786
7.2729
7.2690
4.4011
4.3826
4.3639
3.6617
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2.9663
2.9611
2.9522
2.9476
2.9424
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2.6173
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2.5998
2.5837
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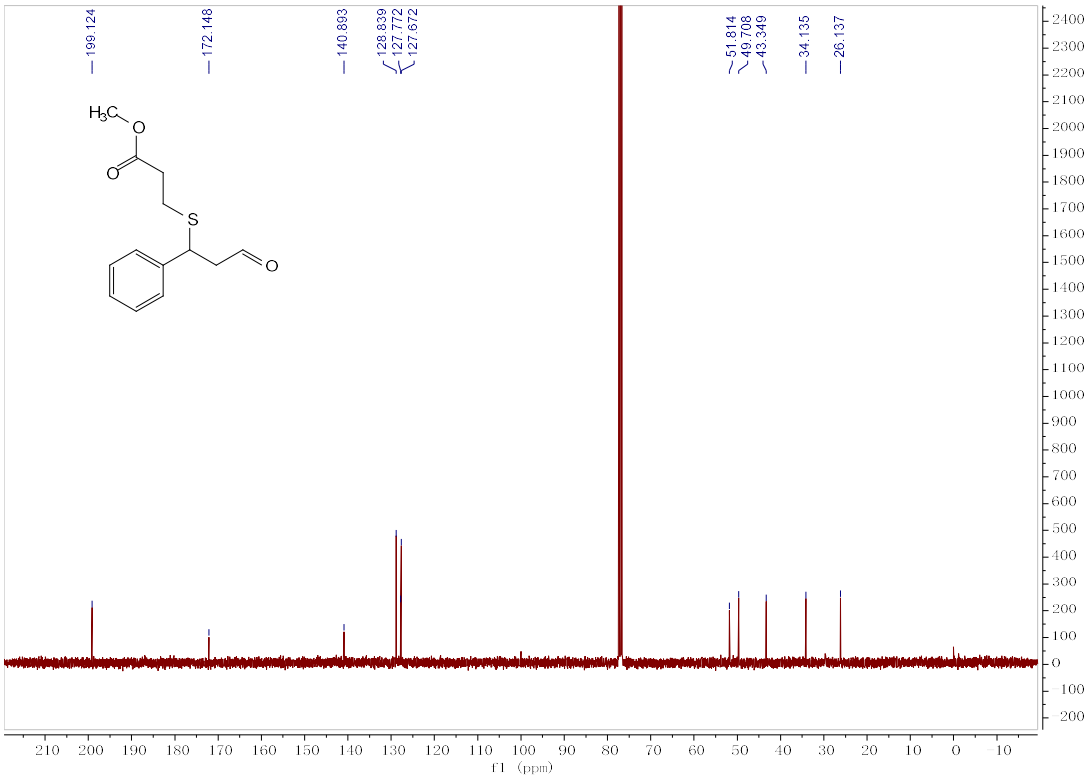
2.4701
2.4565
2.4527
H3C
O
O
S
O
f1 (ppm)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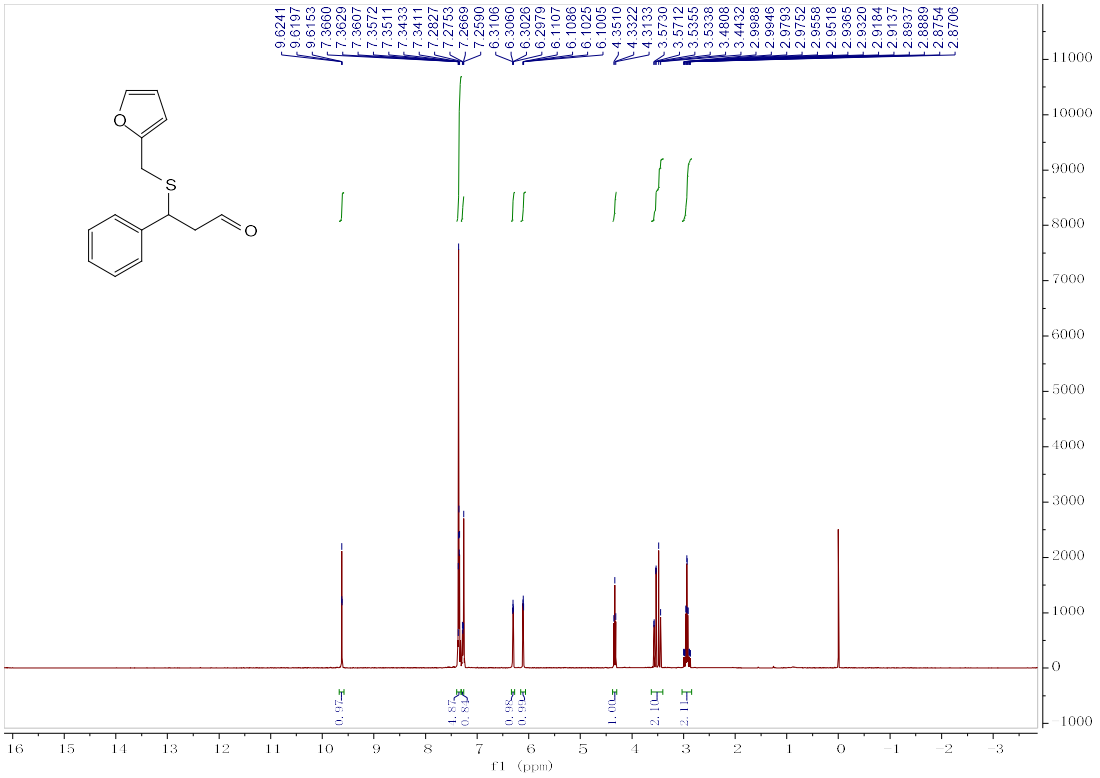
51.814
49.708
43.349
34.135
26.137
H3C
O
O
S
O
f1 (ppm)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7.3572
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7.3433
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7.2827
7.2753
7.2669
7.2590
6.3106
6.3060
6.3026
6.2979
6.1107
6.1086
6.1025
6.1005
4.3510
4.3322
4.3133
3.5730
3.5712
3.5355
3.5338
3.4808
3.4432
2.9688
2.9646
2.9793
2.9752
2.9558
2.9518
2.9365
2.9320
2.9184
2.9137
2.8937
2.8889
2.8754
2.8706
O
S
O
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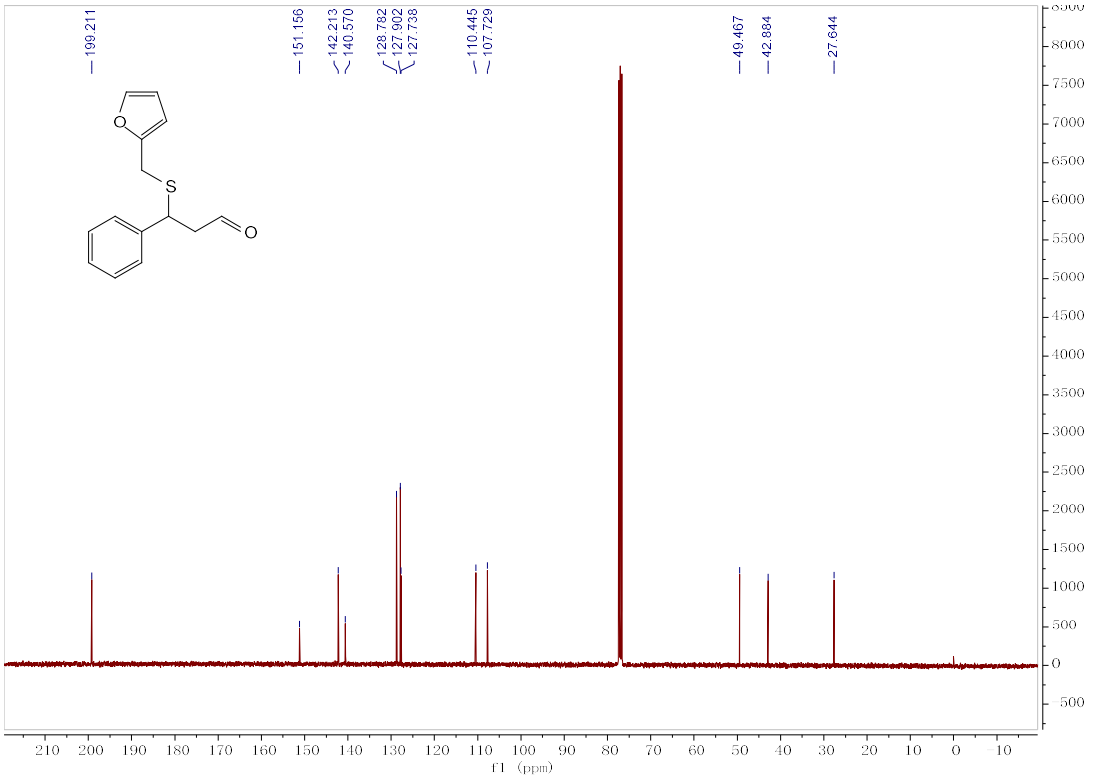
1.87
0.84
0.98
0.94
1.00
2.10
2.11
f1 (ppm)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142.213
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110.445
107.729
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42.884
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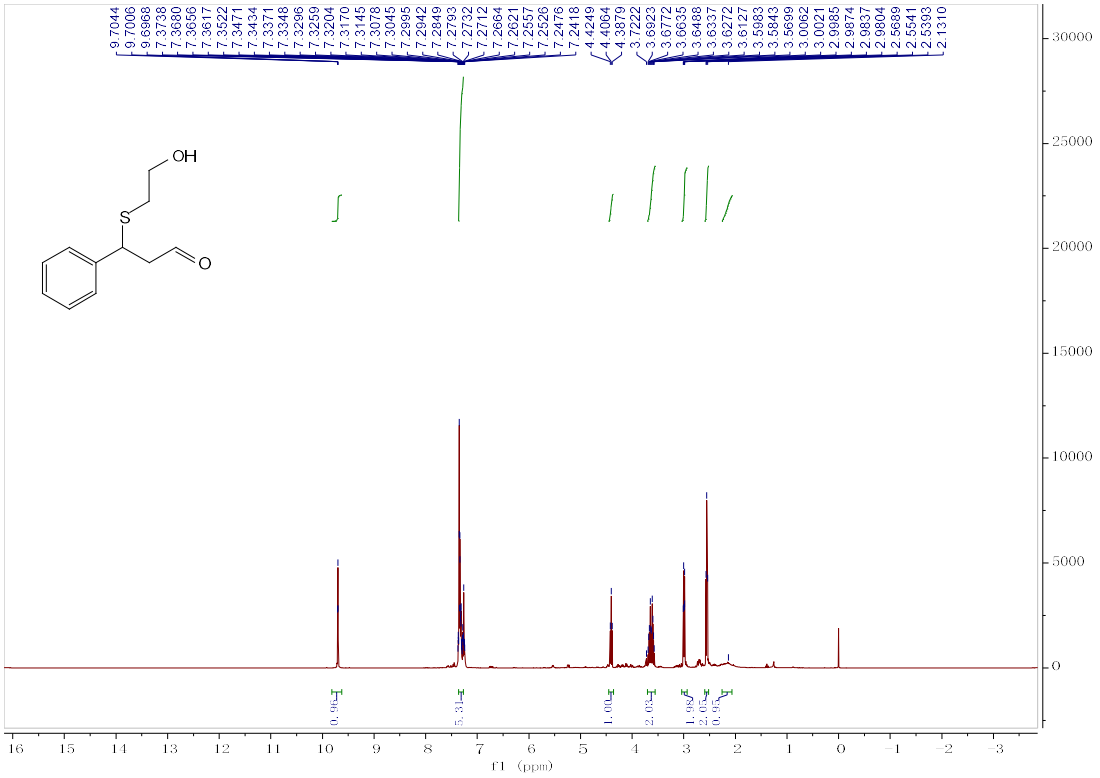
O
S
O
f1 (ppm)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7.2712
7.2664
7.2621
7.2557
7.2526
7.2476
7.2418
4.4249
4.4064
4.3879
3.7222
3.6923
3.6772
3.6635
3.6488
3.6337
3.6272
3.6127
3.5983
3.5843
3.5699
3.0062
3.0021
2.9985
2.9874
2.9837
2.9804
2.5689
2.5541
2.5393
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OH
S
O
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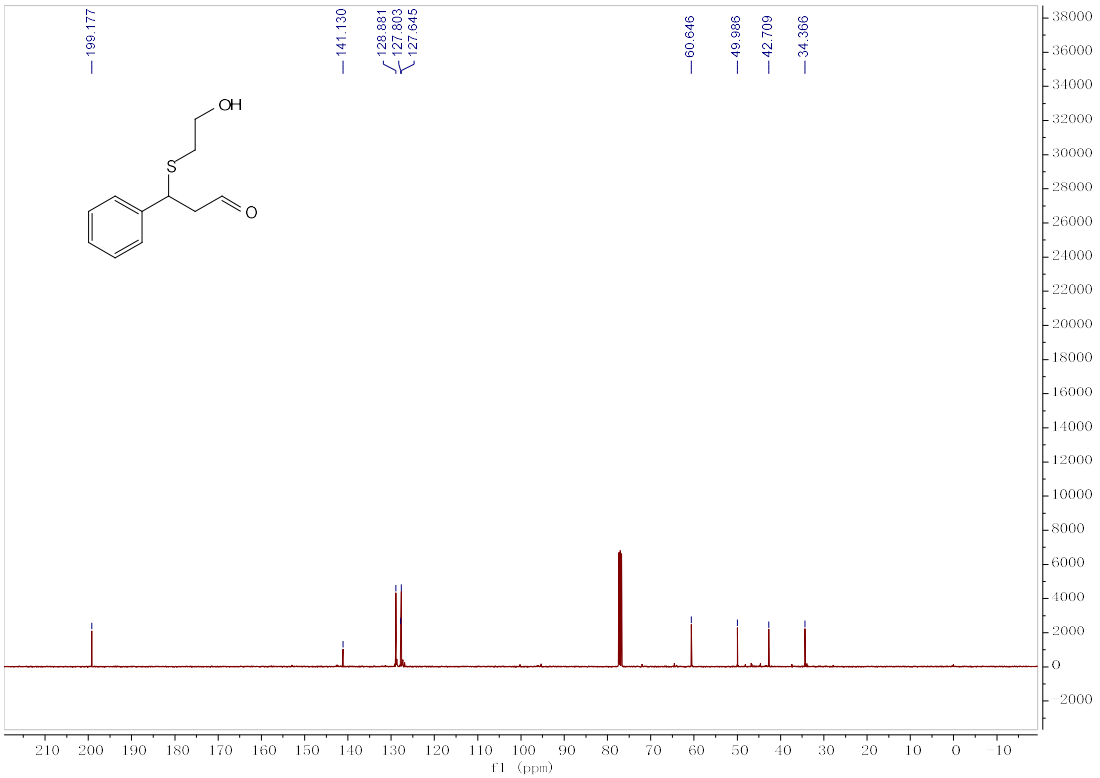
5.33
1.00
2.03
1.98
2.05
0.55
f1 (ppm)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42.709
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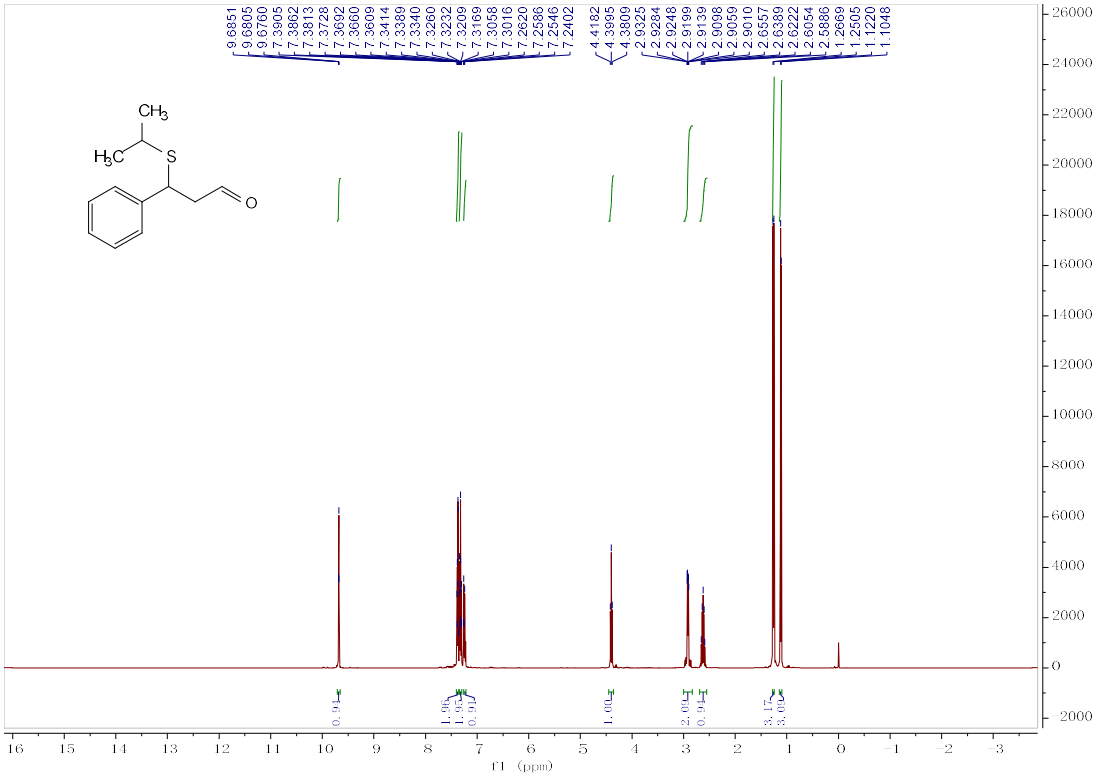
OH
S
O
f1 (ppm)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7.3813
7.3728
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7.3414
7.3389
7.3340
7.3260
7.3232
7.3209
7.3169
7.3058
7.3016
7.2620
7.2586
7.2546
7.2402
4.4182
4.3995
4.3809
2.9325
2.9284
2.9248
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2.9139
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2.9059
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2.6222
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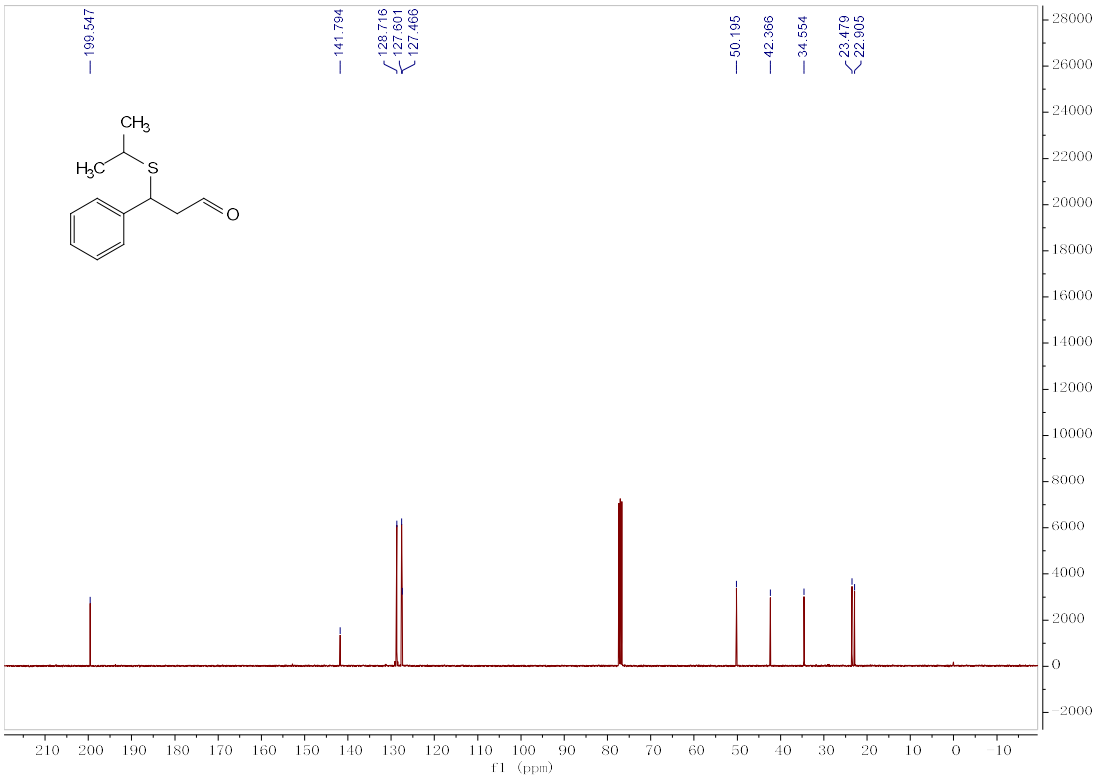
CH3
H3C
S
O
f1 (ppm)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23.479
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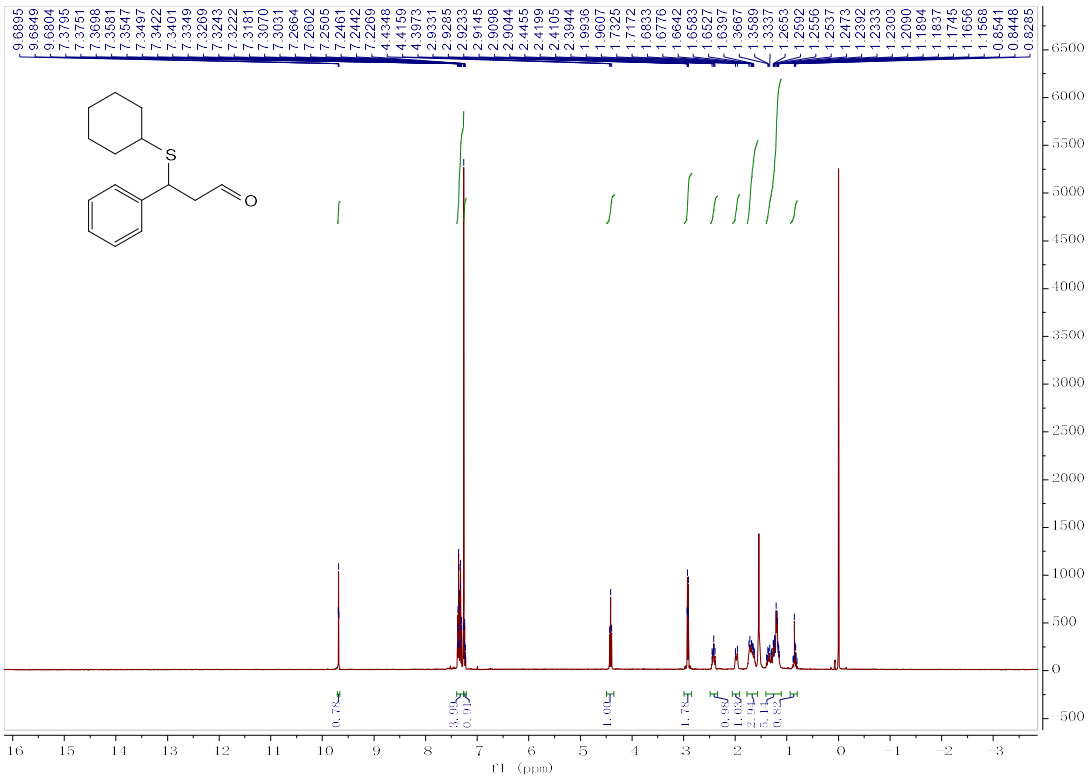
H3C
S
O
f1 (ppm)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7.3181
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7.3031
7.2664
7.2602
7.2505
7.2461
7.2442
7.2269
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4.4159
4.3973
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2.9285
2.9233
2.9145
2.9098
2.9044
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2.4199
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1.6642
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1.6397
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1.2653
1.2592
1.2556
1.2537
1.2473
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1.2090
1.1894
1.1837
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1.1568
0.8541
0.8448
0.8285
S
O
0.78
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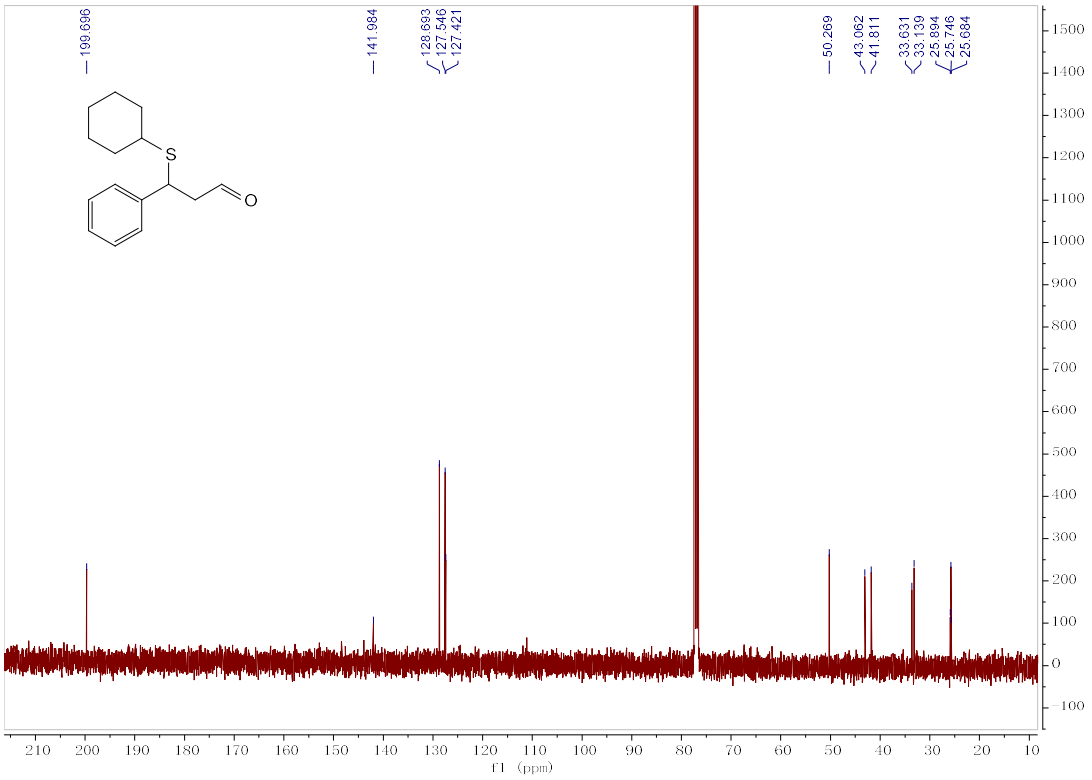
0.91
1.00
1.78
0.98
1.03
2.94
5.14
0.82
f1 (ppm)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43.062
41.811
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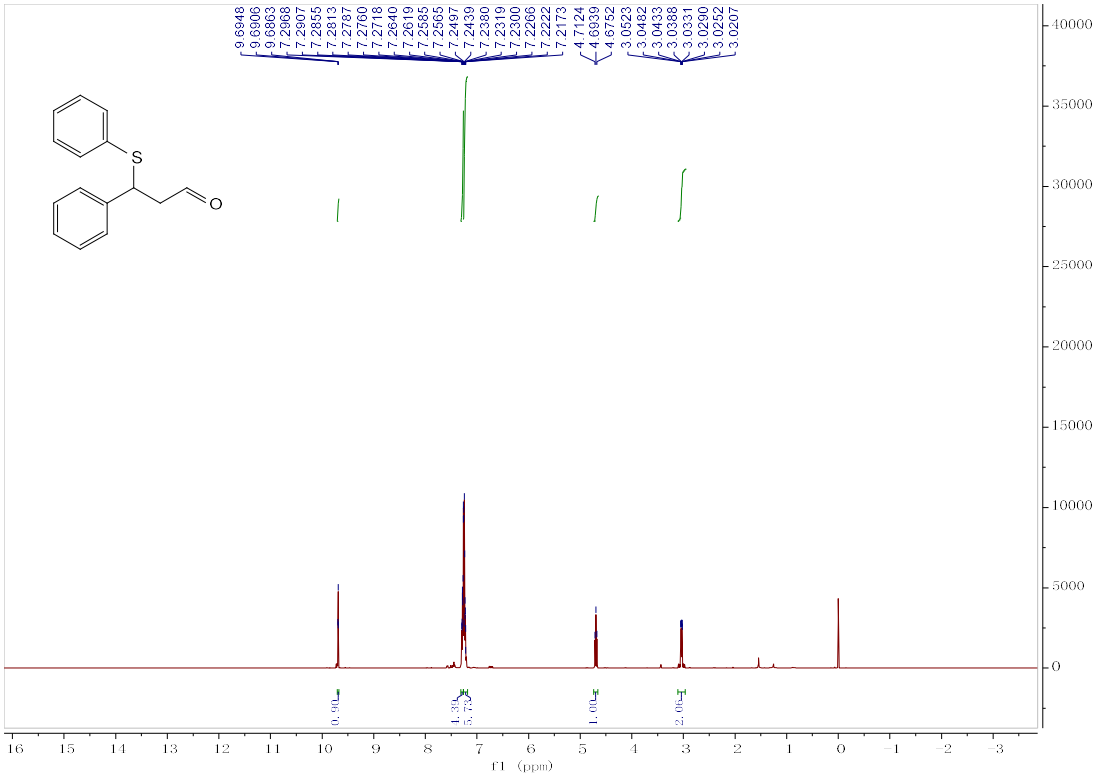
33.139
25.894
25.746
25.684
S
O
f1 (ppm)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7.2439
7.2380
7.2319
7.2300
7.2266
7.2222
7.2173
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4.6939
4.6752
3.0523
3.0482
3.0433
3.0388
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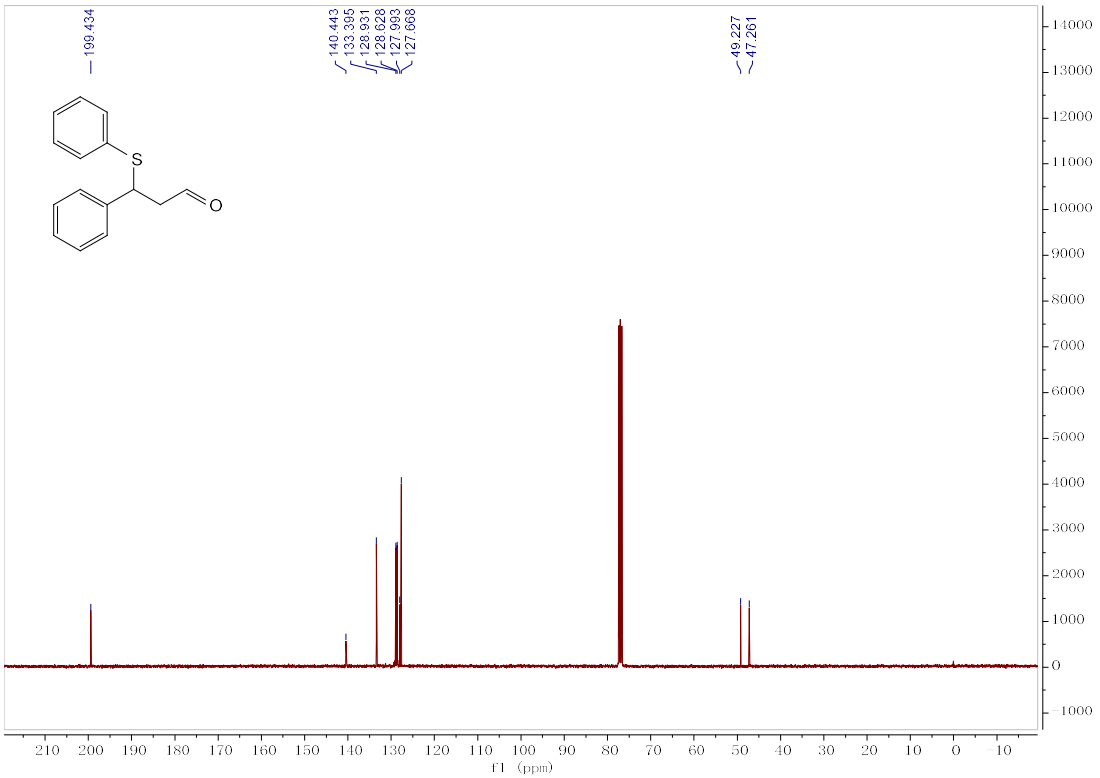
3.0252
3.0207
S
O
0.90
1.38
5.73
1.00
2.06
f1 (ppm)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127.993
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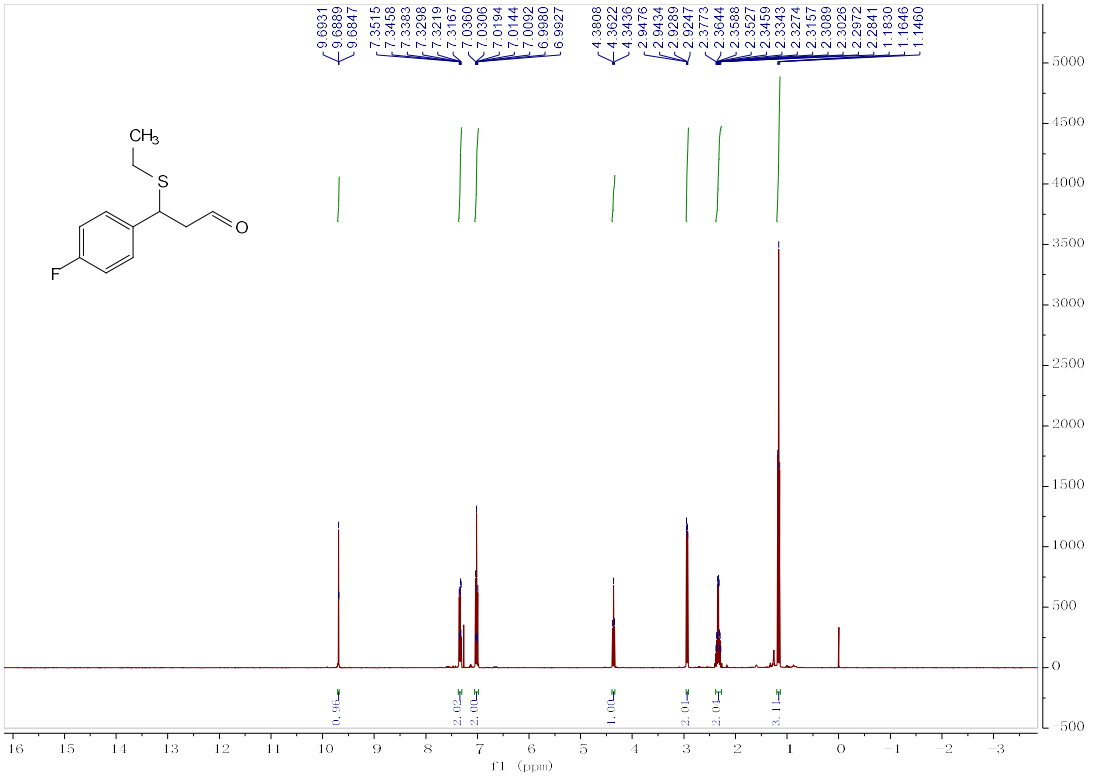
49.227
47.261
S
O
f1 (ppm)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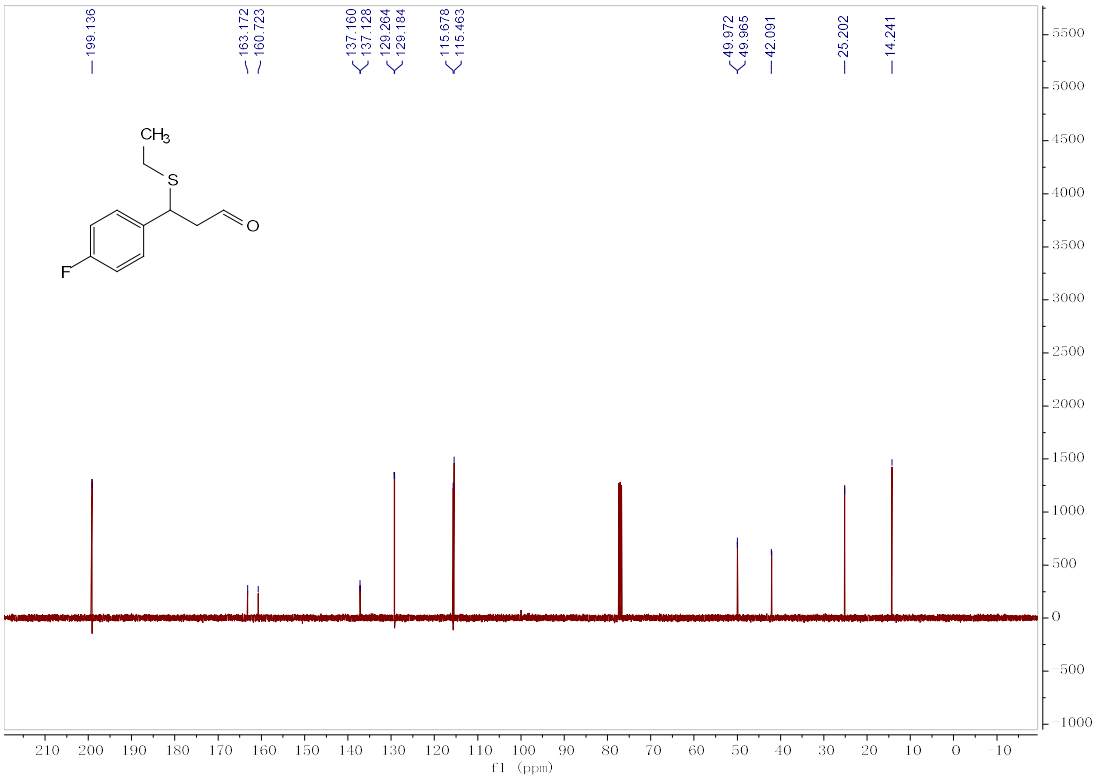
7.3458
7.3383
7.3298
7.3219
7.3167
7.0360
7.0306
7.0194
7.0144
7.0092
6.9880
6.9827
4.3808
4.3622
4.3436
2.9476
2.9434
2.9289
2.9247
2.3773
2.3644
2.3588
2.3527
2.3459
2.3343
2.3274
2.3157
2.3089
2.3026
2.2972
2.2841
1.1830
1.1646
1.1460
CH3
S
O
F
0.96
2.02
2.00
1.00
2.01
2.04
3.11
f1 (ppm)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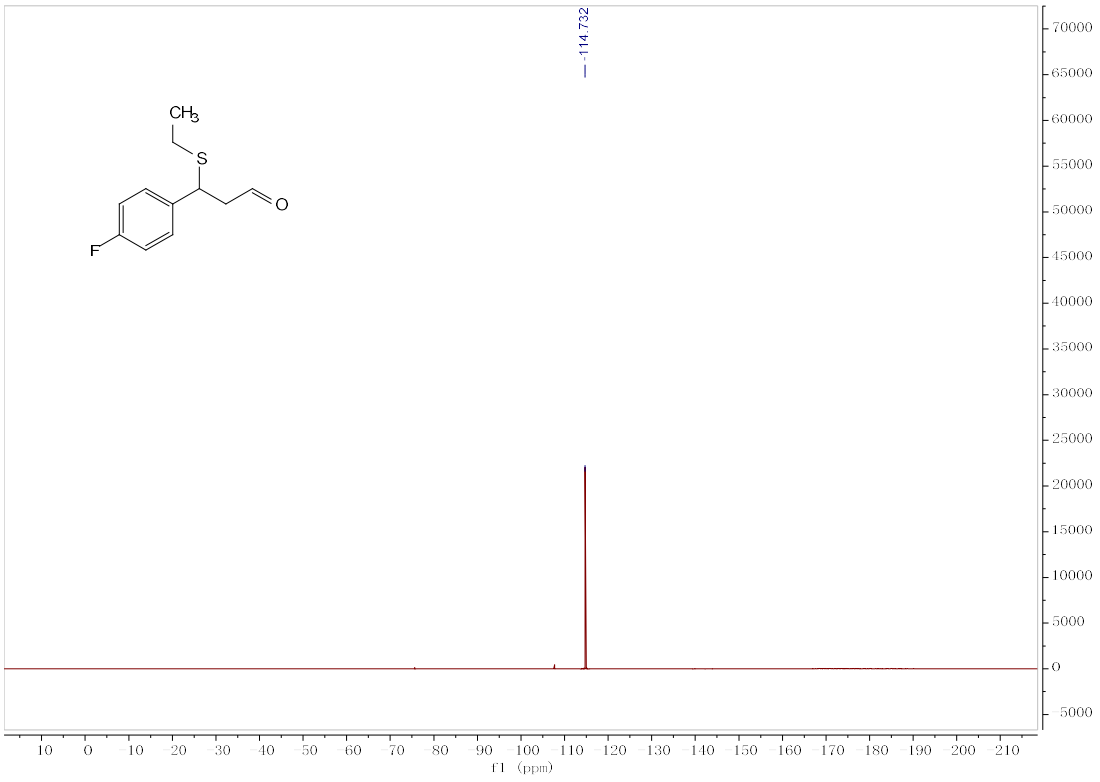
49.965
42.091
25.202
14.241
CH3
S
O
F
f1 (ppm)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S
O
F
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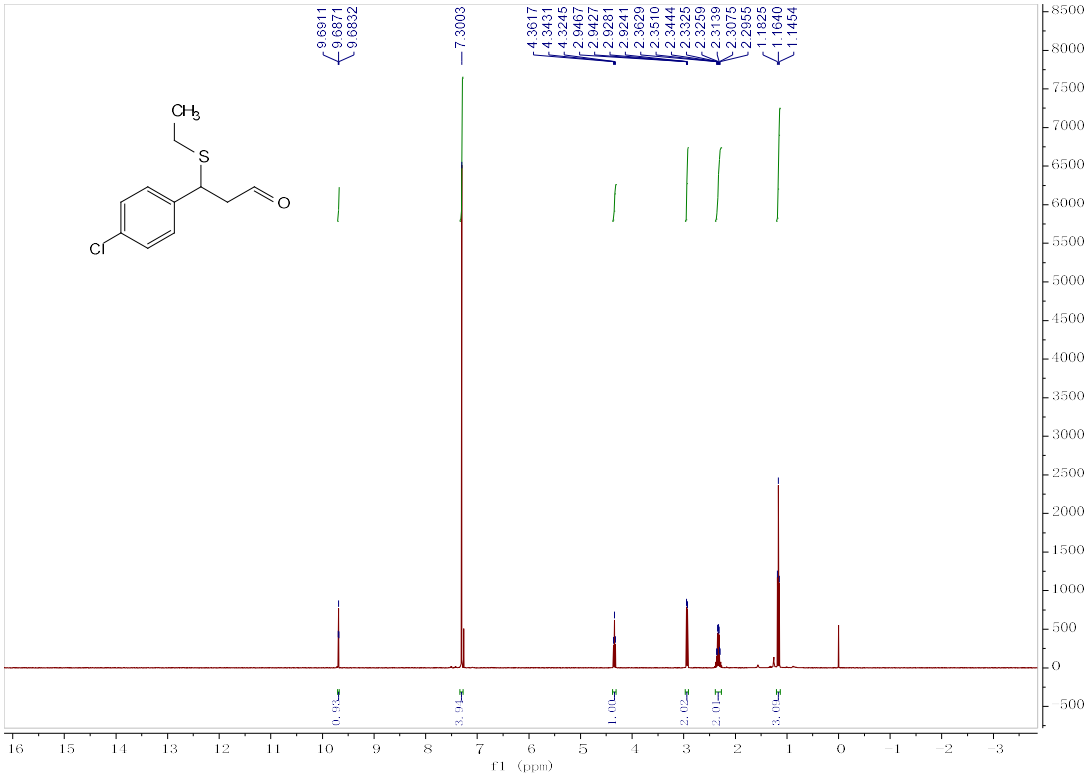
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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4.3431
4.3245
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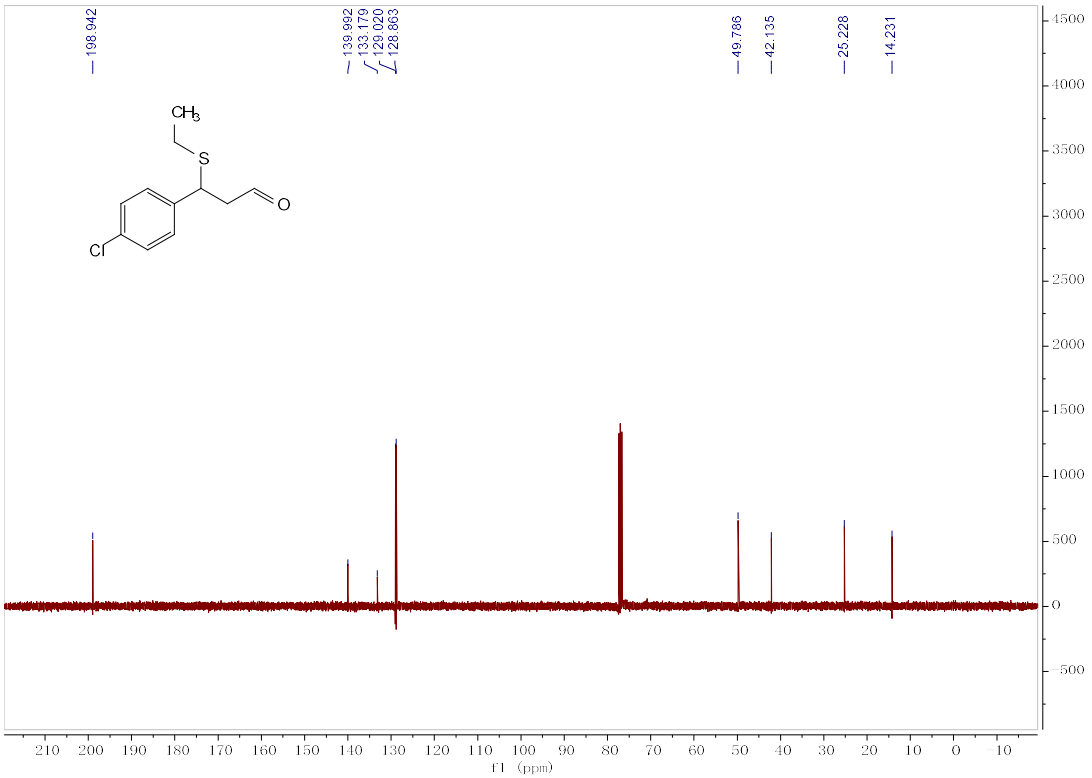
2.9427
2.9281
2.9241
2.3629
2.3510
2.3444
2.3325
2.3259
2.3139
2.3075
2.2955
1.1825
1.1640
1.1454
CH3
S
O
Cl
0.93
3.04
1.00
2.02
2.01
3.03
f1 (ppm)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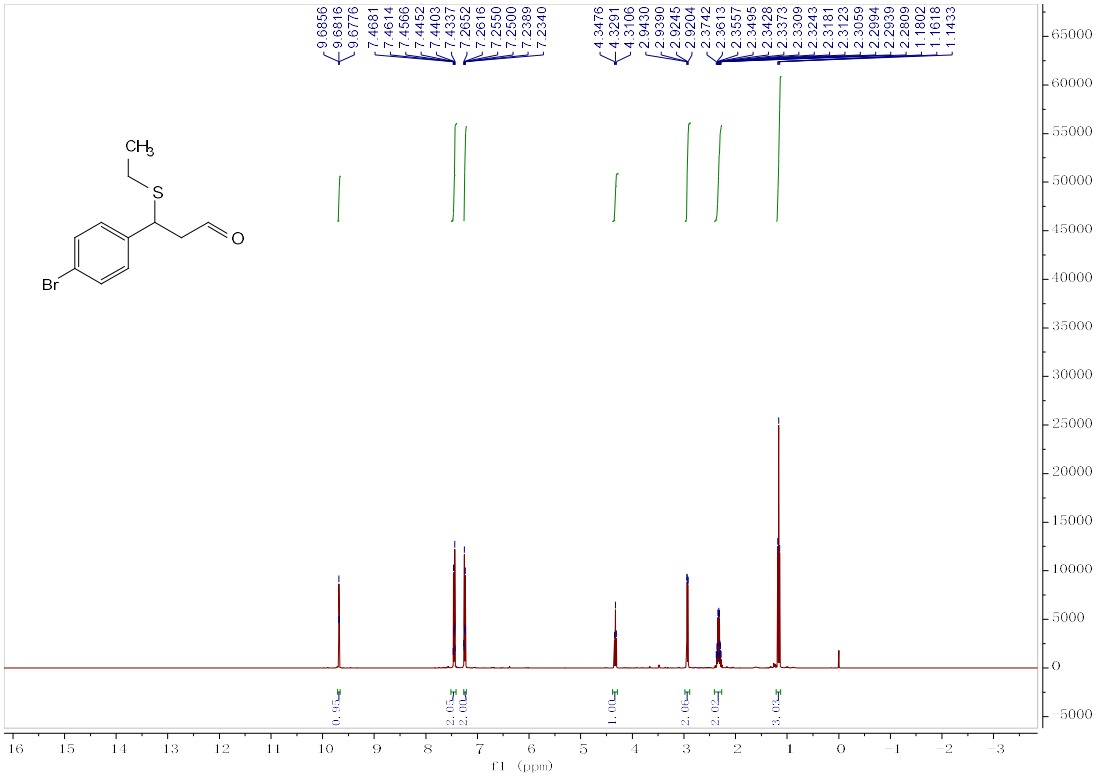
129.020
128.863
49.786
42.135
25.228
14.231
CH3
S
O
Cl
f1 (ppm)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9.6776
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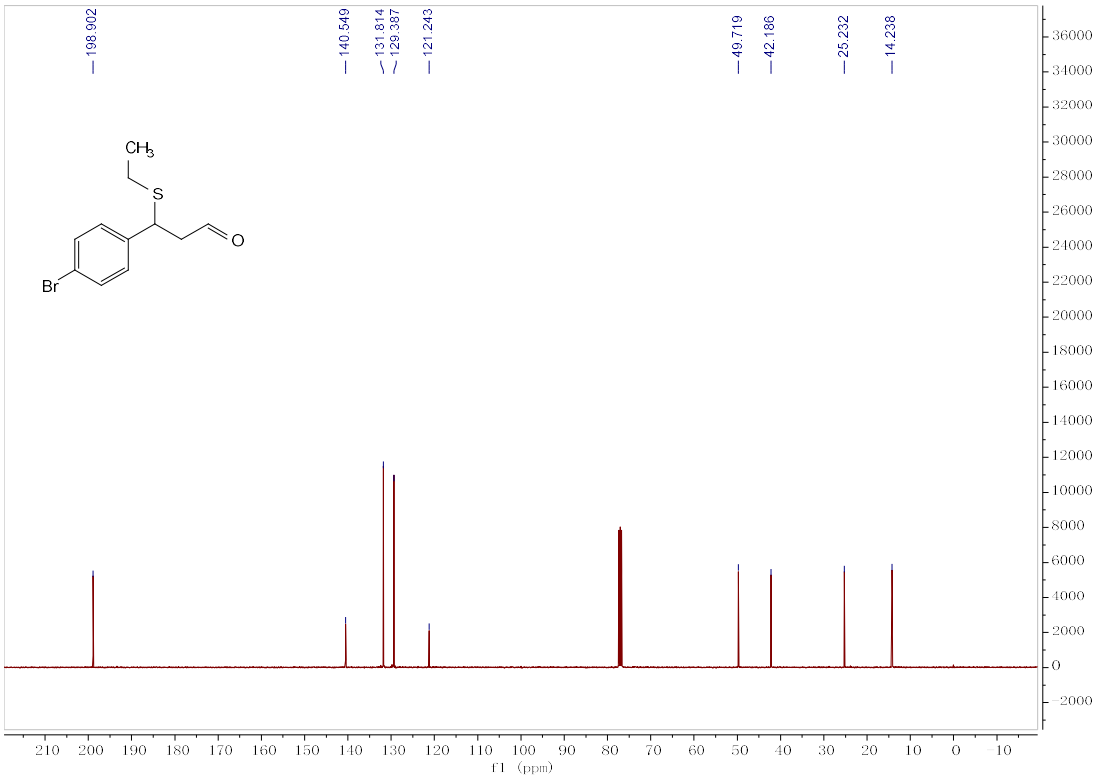
7.4614
7.4566
7.4452
7.4403
7.4337
7.2652
7.2616
7.2550
7.2500
7.2389
7.2340
4.3476
4.3291
4.3106
2.9430
2.9390
2.9245
2.9204
2.3742
2.3613
2.3557
2.3495
2.3428
2.3373
2.3309
2.3243
2.3181
2.3123
2.3059
2.2994
2.2939
2.2809
1.1802
1.1618
1.1433
CH3
S
O
Br
0.95
2.05
2.00
1.00
2.06
2.02
3.03
f1 (ppm)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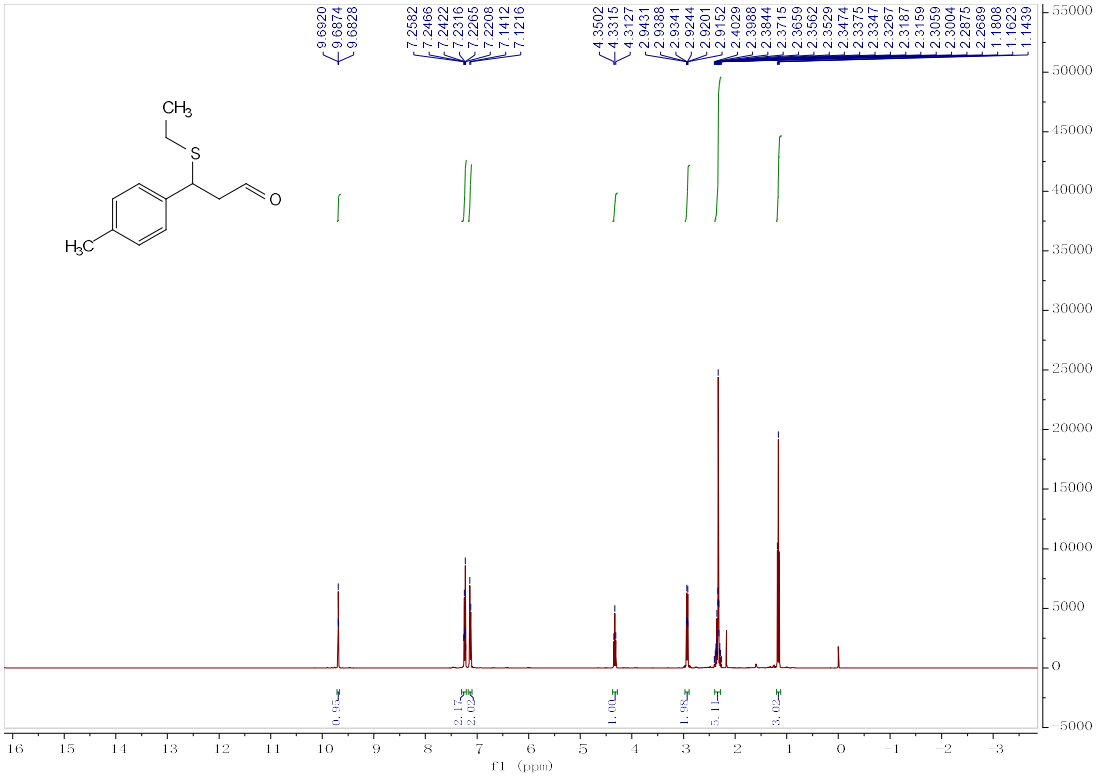
121.243
49.719
42.186
25.232
14.238
CH3
S
O
Br
f1 (ppm)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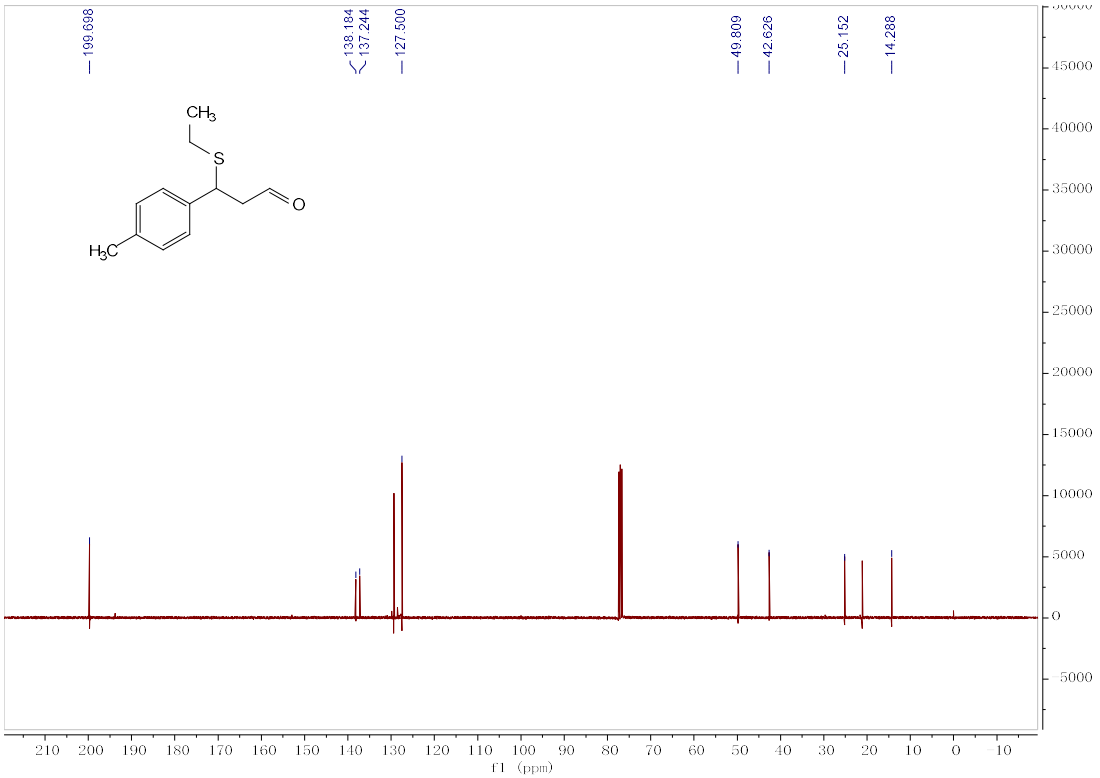
9.6874
9.6828
7.2582
7.2466
7.2422
7.2316
7.2265
7.2208
7.1412
7.1216
4.3502
4.3315
4.3127
2.9431
2.9388
2.9341
2.9244
2.9201
2.9152
2.4029
2.3988
2.3844
2.3715
2.3659
2.3562
2.3529
2.3474
2.3375
2.3347
2.3267
2.3187
2.3159
2.3059
2.3004
2.2875
2.2689
1.1808
1.1623
1.1439
CH3
S
O
H3C
0.95
2.17
2.02
1.00
1.98
5.11
3.02
f1 (ppm)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42.626
25.152
14.288
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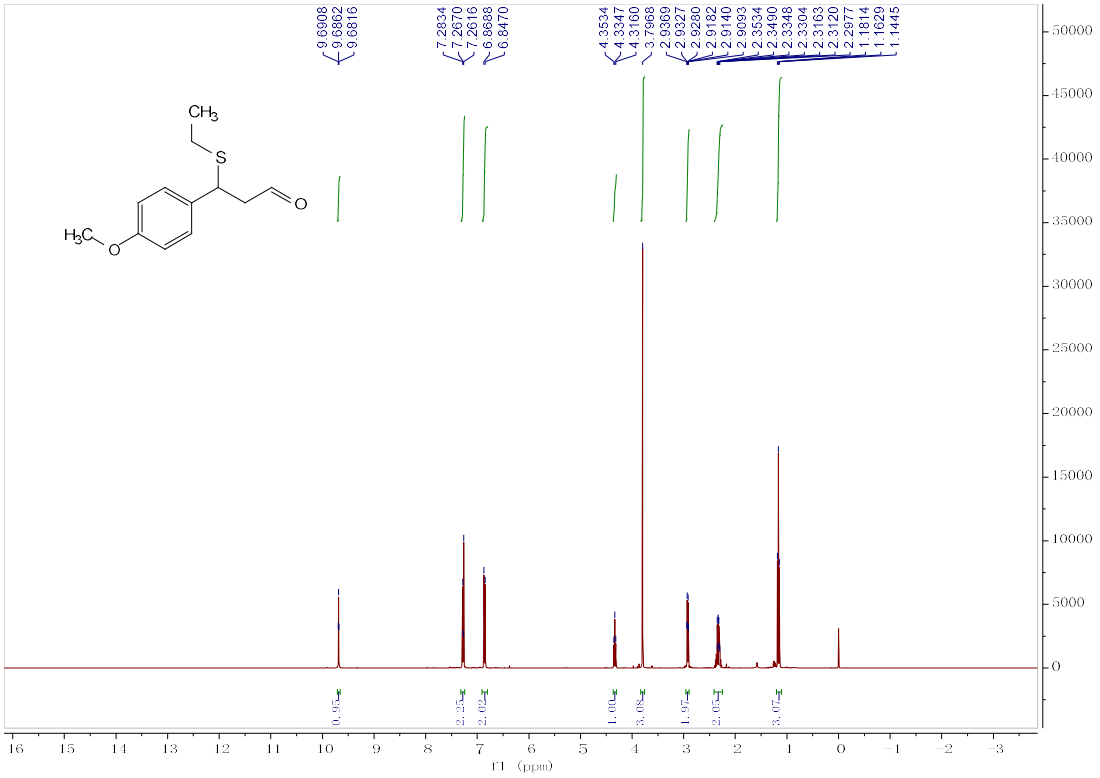
S
O
H3C
f1 (ppm)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7.2670
7.2616
6.8688
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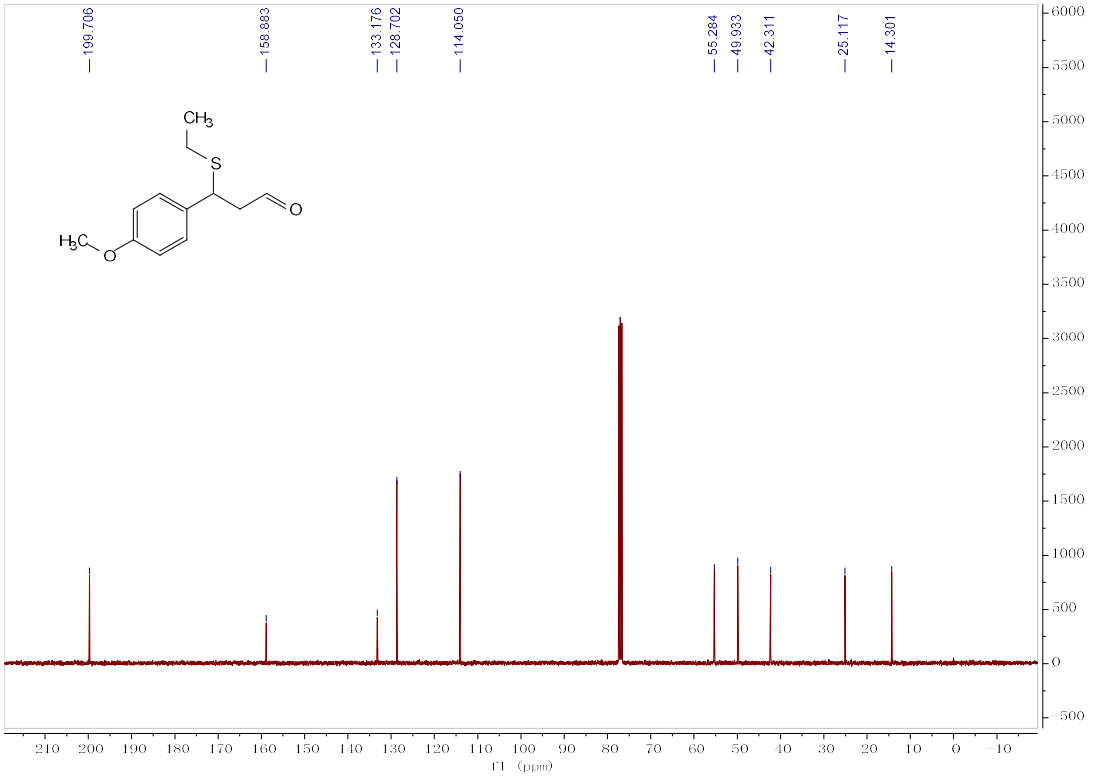
4.3534
4.3347
4.3160
3.7968
2.9369
2.9327
2.9280
2.9182
2.9140
2.9093
2.3534
2.3490
2.3348
2.3304
2.3163
2.3120
2.2977
1.1814
1.1629
1.1445
CH3
S
O
H3C
O
0.95
2.25
2.02
1.00
3.08
1.97
2.05
3.07
f1 (ppm)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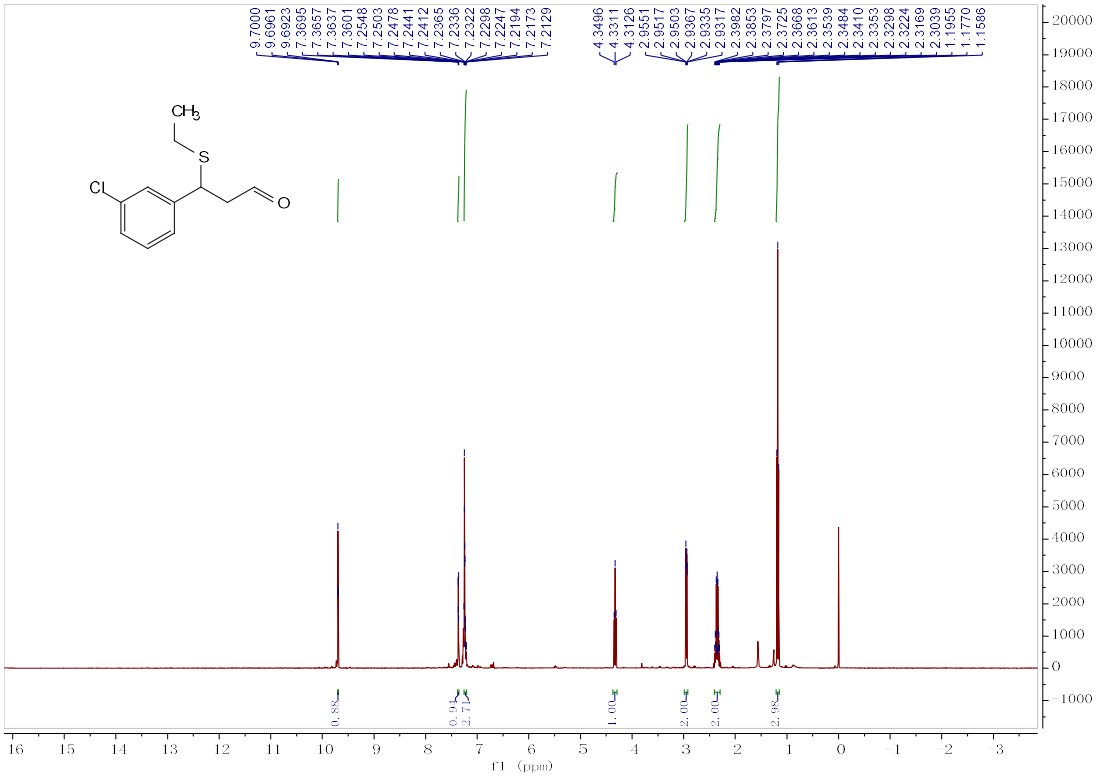
158.883
133.176
128.702
114.050
55.284
49.933
42.311
25.117
14.301
CH3
S
O
H3C
O
f1 (ppm)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9.6961
9.6923
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7.3657
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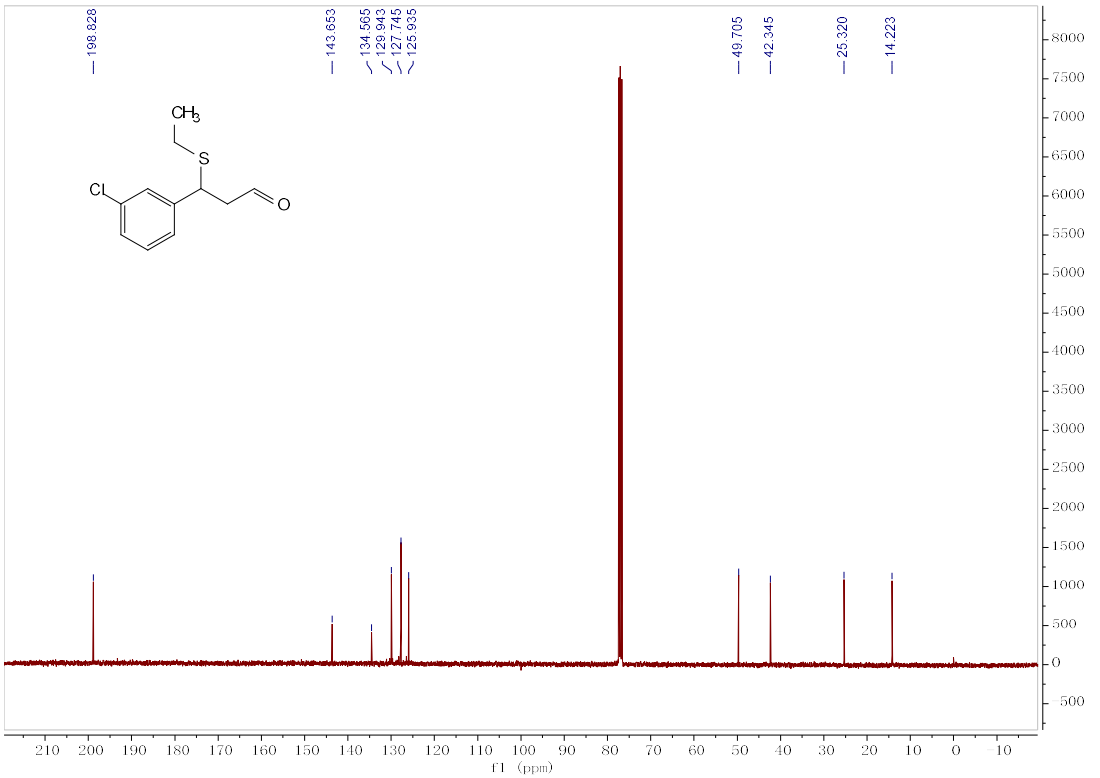
7.3601
7.2548
7.2503
7.2478
7.2441
7.2412
7.2365
7.2336
7.2322
7.2298
7.2247
7.2194
7.2173
7.2129
4.3496
4.3311
4.3126
2.9551
2.9517
2.9503
2.9367
2.9335
2.9317
2.3982
2.3853
2.3797
2.3725
2.3668
2.3613
2.3539
2.3484
2.3410
2.3353
2.3298
2.3224
2.3169
2.3039
1.1955
1.1770
1.1586
CH3
S
Cl
O
0.88
0.94
2.72
1.00
2.01
2.06
2.98
f1 (ppm)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129.943
127.745
125.935
49.705
42.345
25.320
14.223
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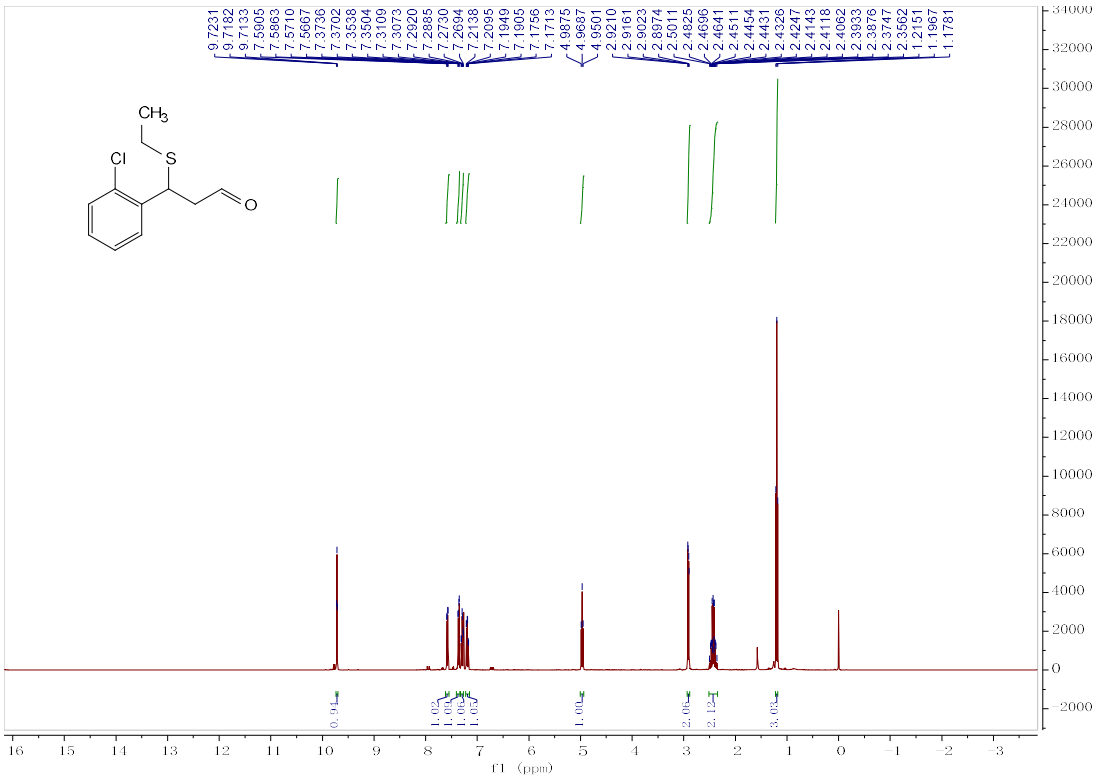
S
Cl
O
f1 (ppm)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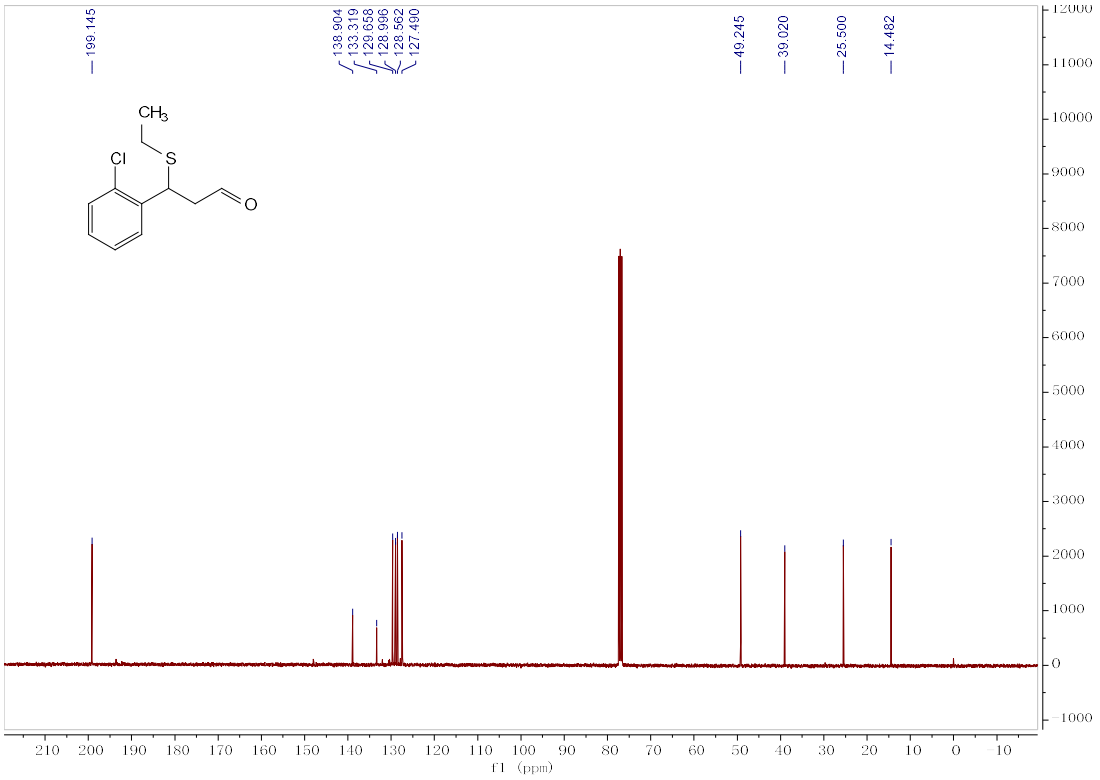
9.7182
9.7133
7.5905
7.5863
7.5710
7.5667
7.3736
7.3702
7.3538
7.3504
7.3109
7.3073
7.2920
7.2885
7.2730
7.2694
7.2138
7.2095
7.1949
7.1905
7.1756
7.1713
4.9875
4.9687
4.9501
2.9210
2.9161
2.9023
2.8974
2.5011
2.4825
2.4696
2.4641
2.4511
2.4454
2.4431
2.4326
2.4247
2.4143
2.4118
2.4062
2.3933
2.3876
2.3747
2.3562
1.2151
1.1967
1.1781
CH3
Cl
S
O
0.94
1.02
1.00
1.06
1.05
1.00
2.06
2.12
3.03
f1 (ppm)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133.319
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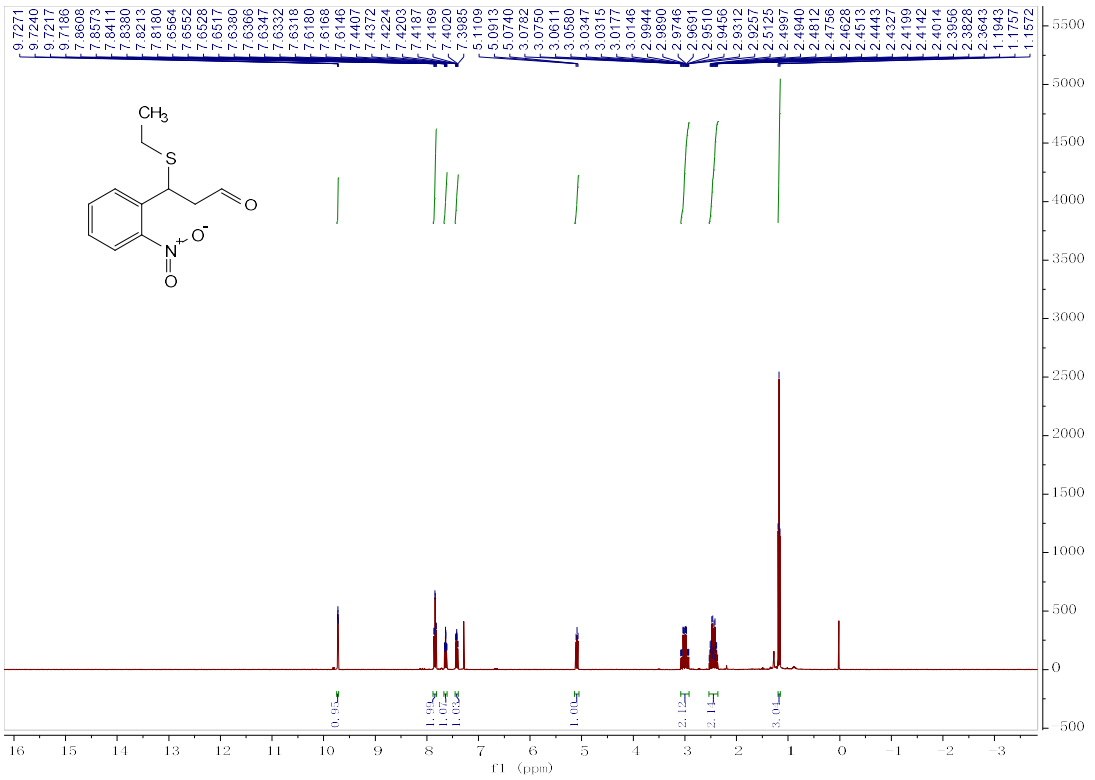
128.562
127.490
49.245
39.020
25.500
14.482
CH3
Cl
S
O
f1 (ppm)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9.7217
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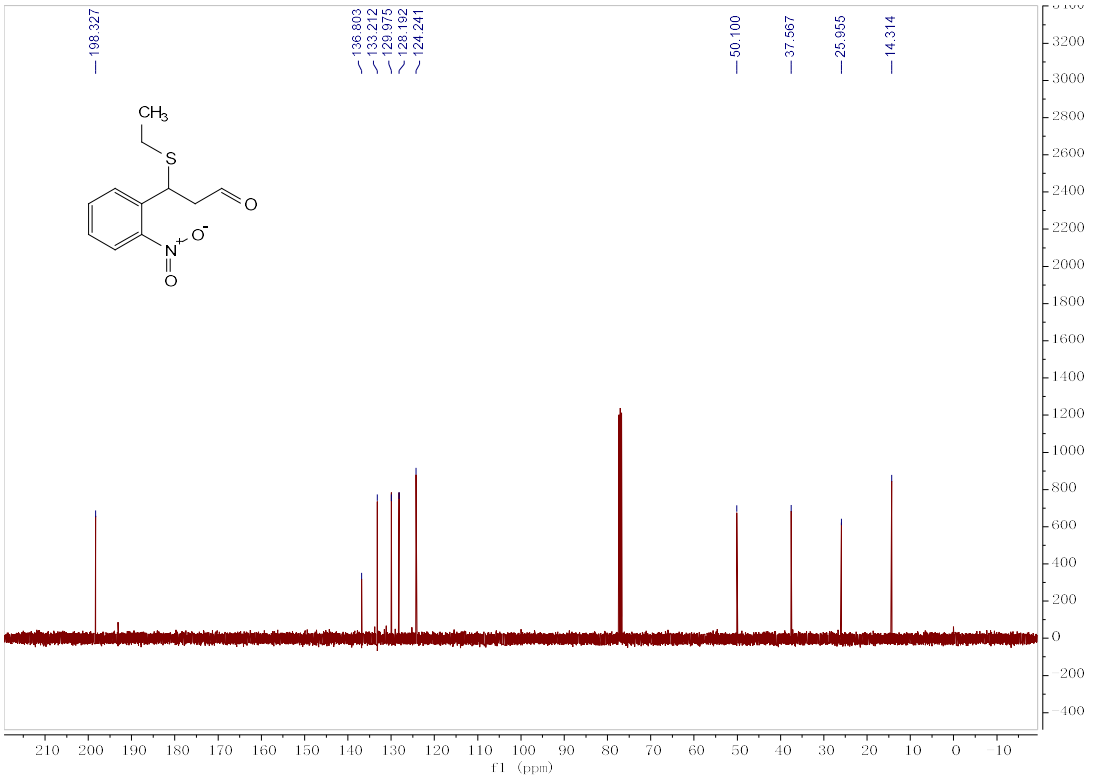
7.8608
7.8573
7.8411
7.8380
7.8213
7.8180
7.6564
7.6552
7.6528
7.6517
7.6380
7.6366
7.6347
7.6332
7.6318
7.6180
7.6168
7.6146
7.4407
7.4372
7.4224
7.4203
7.4187
7.4169
7.4020
7.3985
5.1109
5.0913
5.0740
3.0782
3.0750
3.0611
3.0580
3.0347
3.0315
3.0177
3.0146
2.9944
2.9900
2.9746
2.9691
2.9510
2.9456
2.9312
2.9257
2.5125
2.4997
2.4940
2.4912
2.4756
2.4628
2.4513
2.4443
2.4327
2.4199
2.4142
2.4014
2.3956
2.3828
2.3643
1.1943
1.1757
1.1572
CH3
S
O
N+
O-
O
0.95
1.94
1.07
1.03
1.00
2.12
2.14
3.04
f1 (ppm)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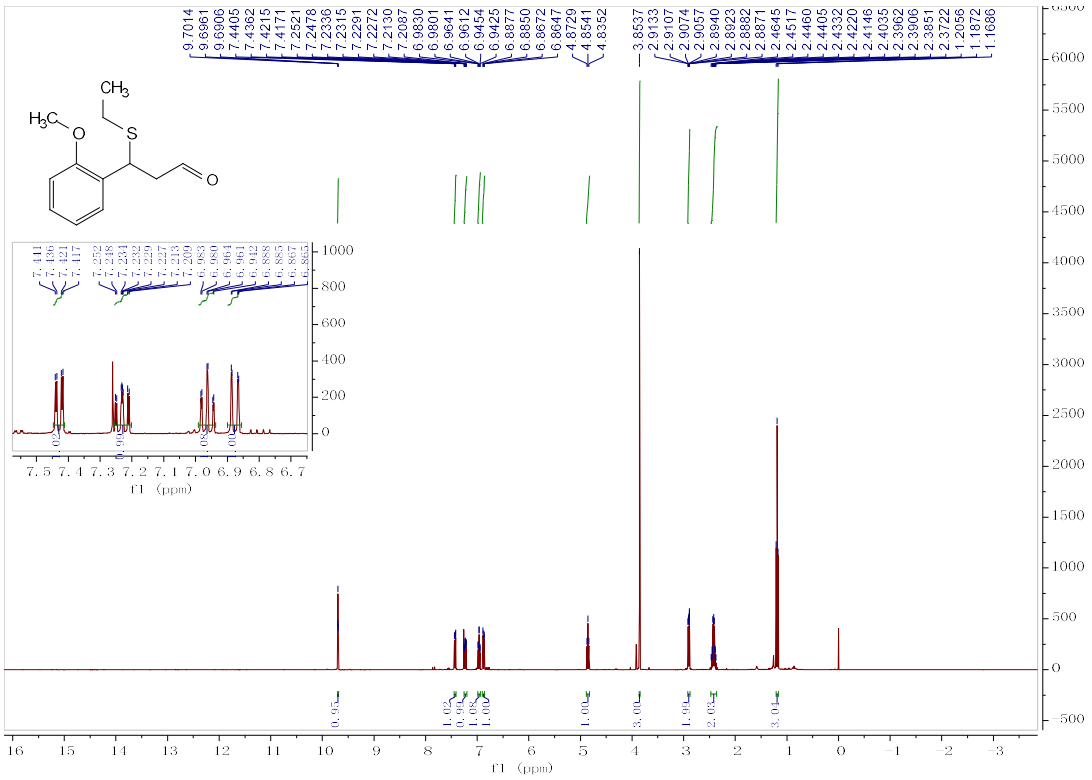
136.803
133.212
128.975
128.192
124.241
50.100
37.567
25.955
14.314
CH3
S
O
N+
O-
O
f1 (ppm)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9.6906
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7.4171
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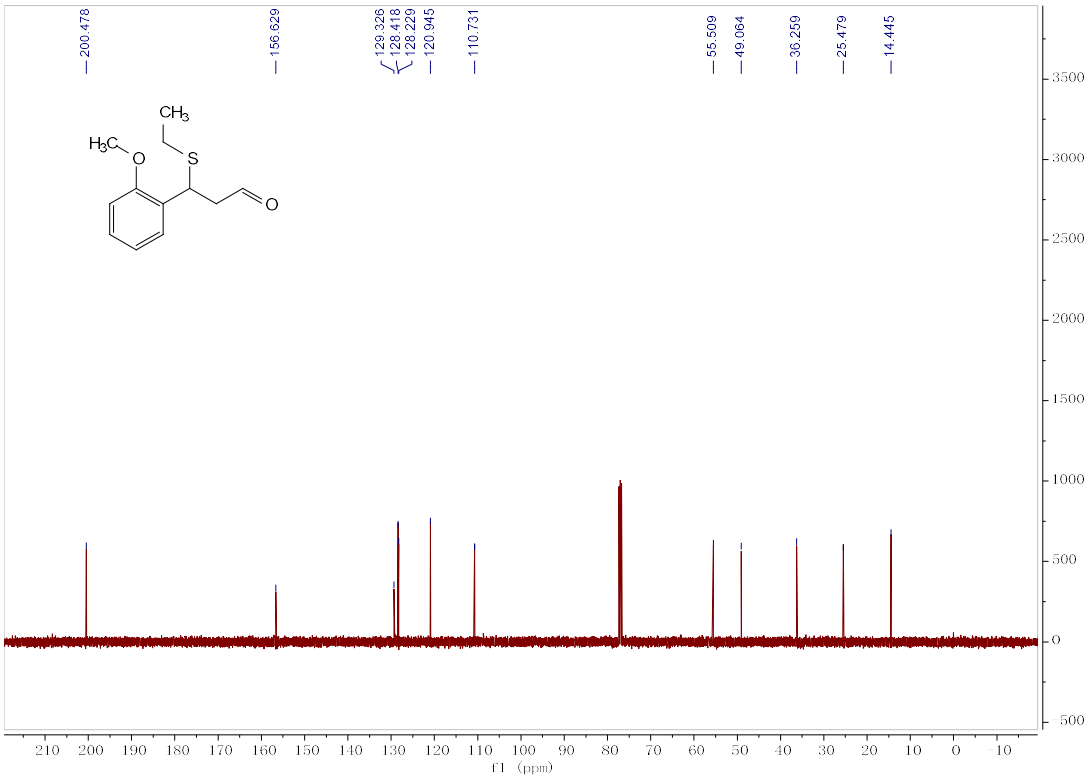
7.2478
7.2336
7.2315
7.2291
7.2272
7.2130
7.2087
6.9830
6.9801
6.9641
6.9612
6.9454
6.9425
6.8877
6.8850
6.8672
6.8647
4.8729
4.8541
4.8352
3.8537
2.9133
2.9107
2.9074
2.9057
2.8940
2.8923
2.8882
2.8871
2.4645
2.4517
2.4460
2.4405
2.4332
2.4220
2.4146
2.4035
2.3962
2.3906
2.3851
2.3722
2.2056
1.1872
1.1686
CH3
H3C
O
S
O
f1 (ppm)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128.418
128.229
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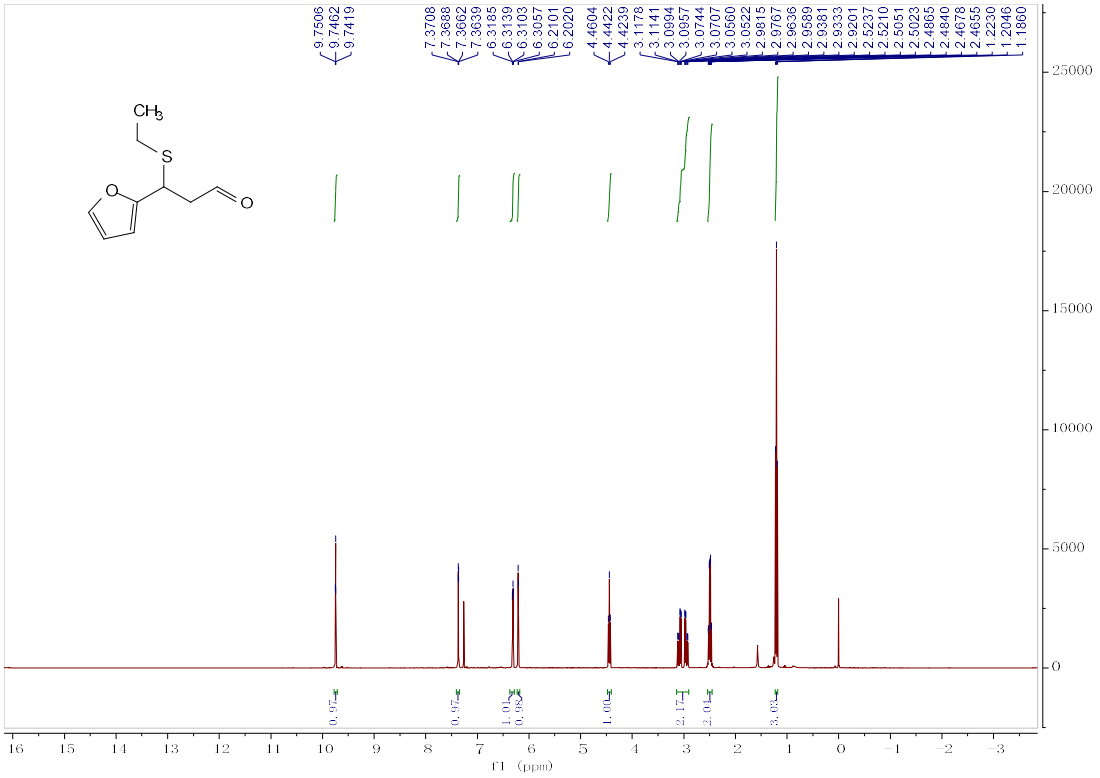
110.731
55.509
49.064
36.259
25.479
14.445
CH3
H3C
O
S
O
f1 (ppm)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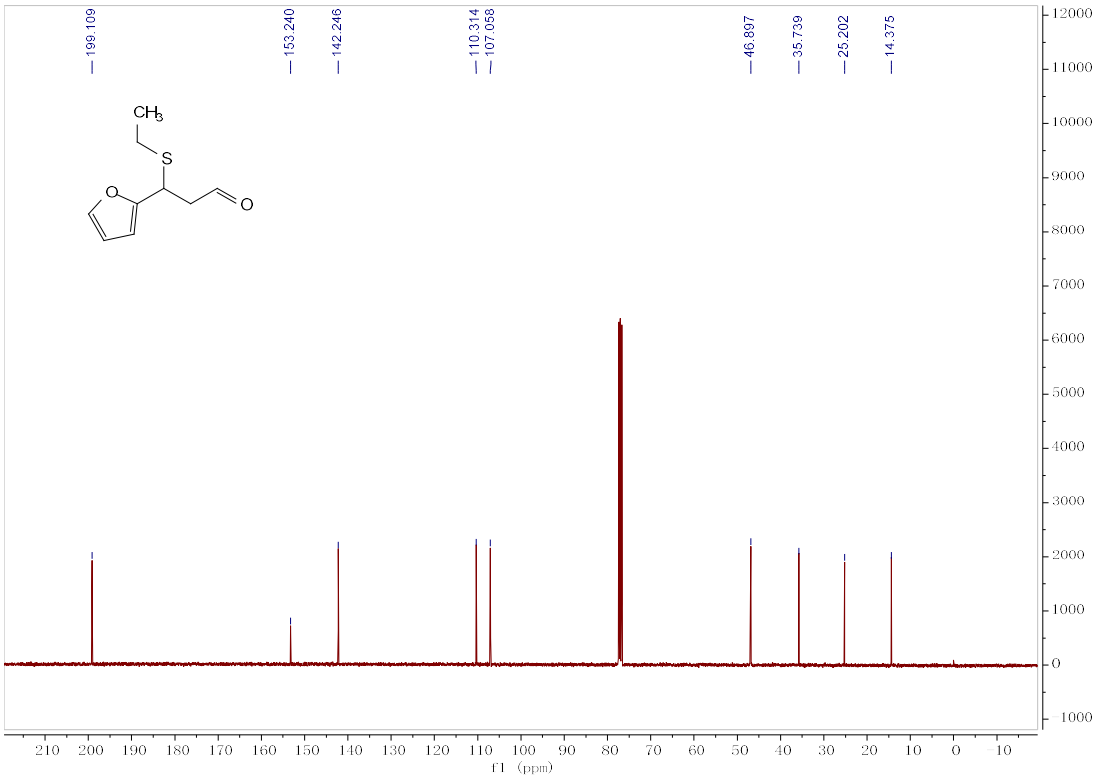
9.7419
7.3708
7.3688
7.3662
7.3639
6.3185
6.3139
6.3103
6.3057
6.2101
6.2020
4.4604
4.4422
4.4239
3.1178
3.1141
3.0894
3.0957
3.0744
3.0707
3.0560
3.0522
2.9815
2.9767
2.9636
2.9589
2.9381
2.9333
2.9201
2.5237
2.5210
2.5051
2.5023
2.4865
2.4840
2.4678
2.4655
1.2230
1.2046
1.1860
0.97
0.97
1.01
0.98
1.00
2.17
2.04
3.03
f1 (ppm)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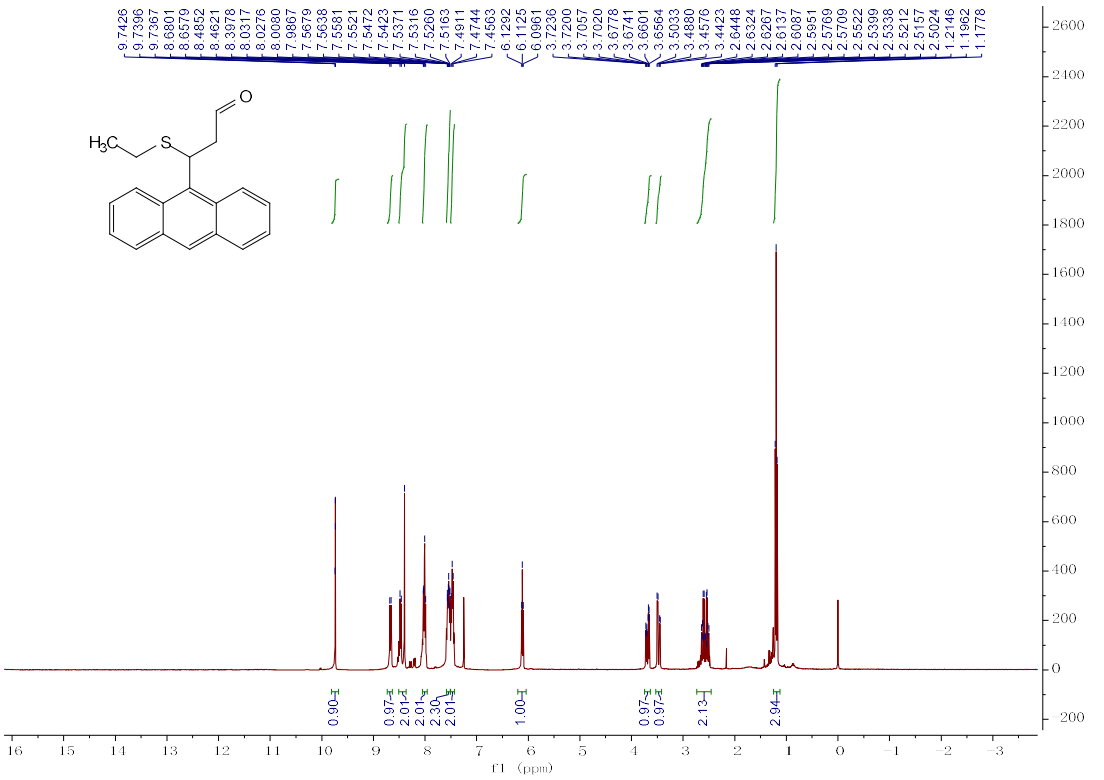
153.240
142.246
110.314
107.058
46.897
35.739
25.202
14.375
f1 (ppm)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9.7367
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8.6579
8.4652
8.4621
8.3978
8.0317
8.0276
8.0080
7.9867
7.5679
7.5638
7.5581
7.5521
7.5472
7.5423
7.5371
7.5316
7.5260
7.5163
7.4911
7.4744
7.4563
6.1292
6.1125
6.0961
3.7236
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3.7057
3.7020
3.6778
3.6741
3.6601
3.6564
3.5033
3.4880
3.4576
3.4423
2.6448
2.6324
2.6267
2.6137
2.6087
2.5951
2.5769
2.5709
2.5522
2.5399
2.5338
2.5212
2.5157
2.5024
1.2146
1.1962
1.1778
O
H3C
S
0.90
0.97
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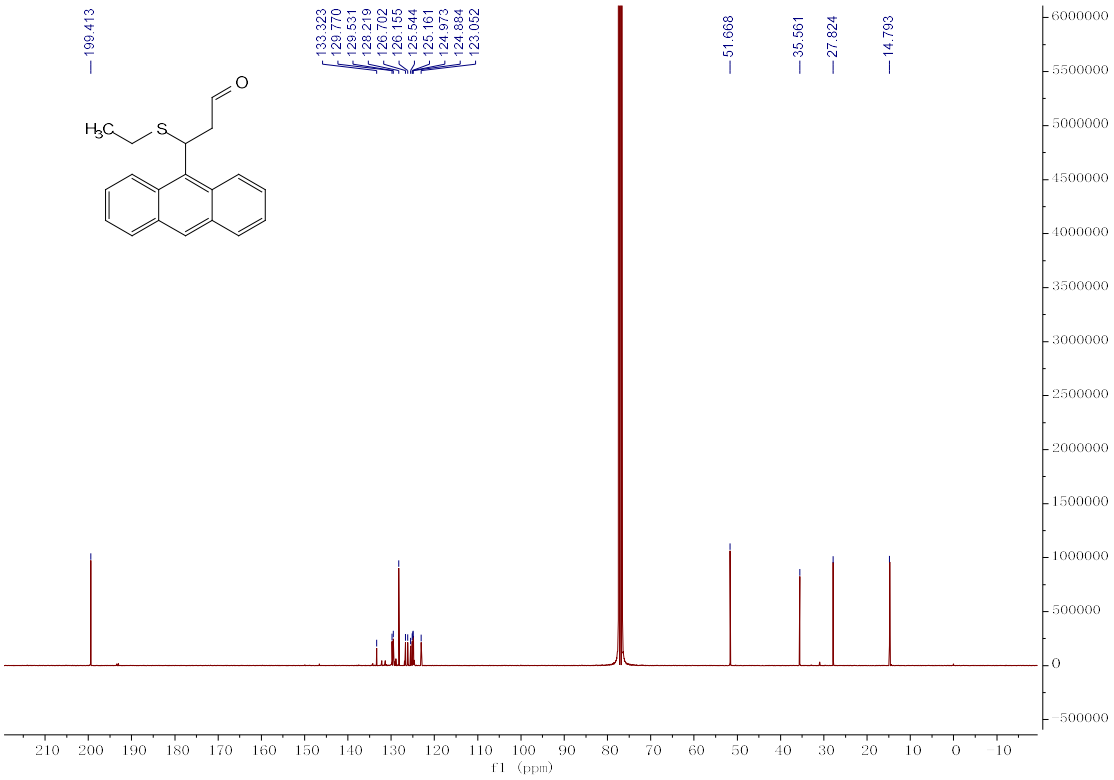
2.01
2.30
2.01
1.00
0.97
0.97
2.13
2.94
f1 (ppm)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126.155
125.544
125.161
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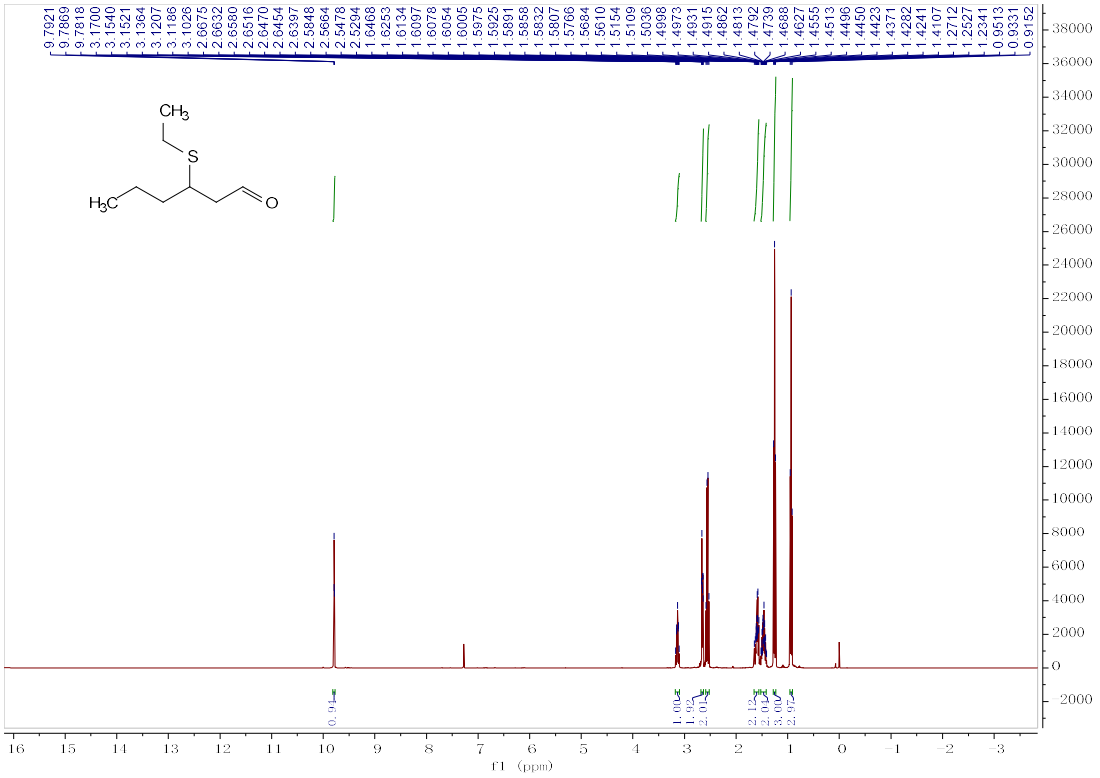
124.884
123.052
51.668
35.561
27.824
14.793
O
H3C
S
f1 (ppm)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9.7818
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3.1540
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3.1364
3.1207
3.1186
3.1026
2.6675
2.6632
2.6580
2.6516
2.6470
2.6454
2.6397
2.5848
2.5664
2.5478
2.5294
1.6468
1.6253
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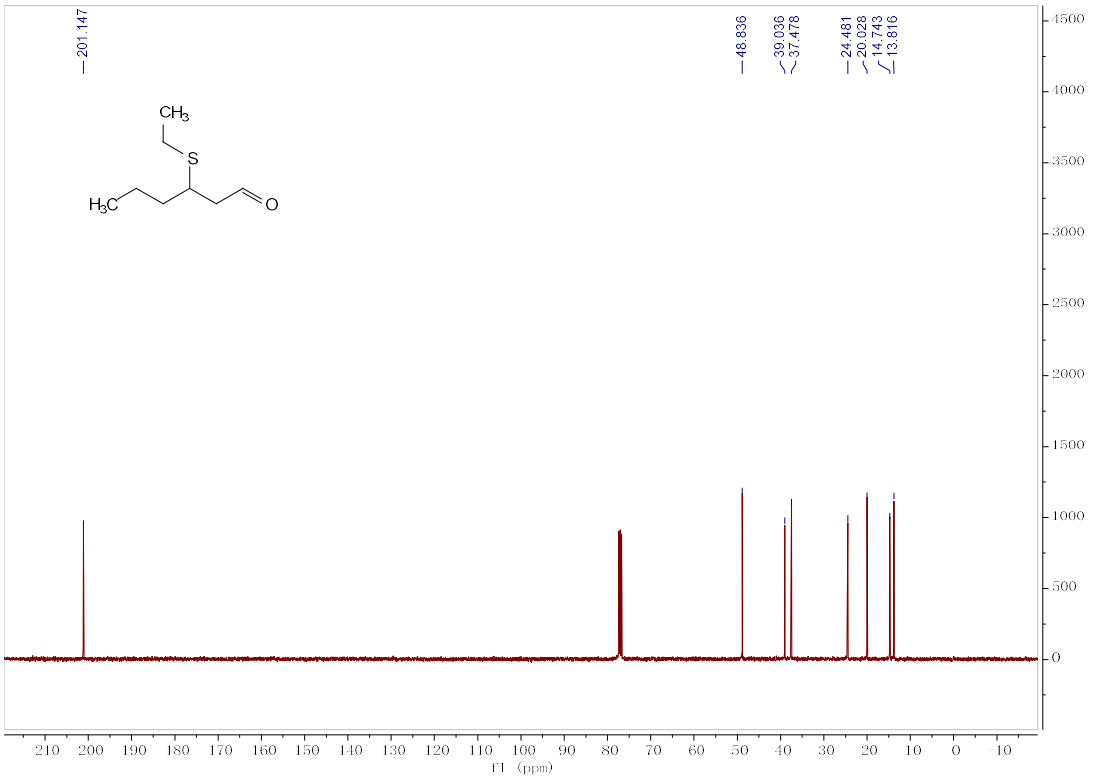
1.6097
1.6078
1.6054
1.6005
1.5975
1.5925
1.5891
1.5858
1.5832
1.5807
1.5766
1.5684
1.5610
1.5154
1.5109
1.5036
1.4998
1.4973
1.4931
1.4915
1.4862
1.4813
1.4792
1.4739
1.4688
1.4627
1.4555
1.4513
1.4496
1.4450
1.4423
1.4371
1.4282
1.4241
1.4107
1.2712
1.2527
1.2341
0.9513
0.9331
0.9152
CH3
S
H3C
O
0.94
1.00
1.92
2.01
2.12
2.04
3.00
2.97
f1 (ppm)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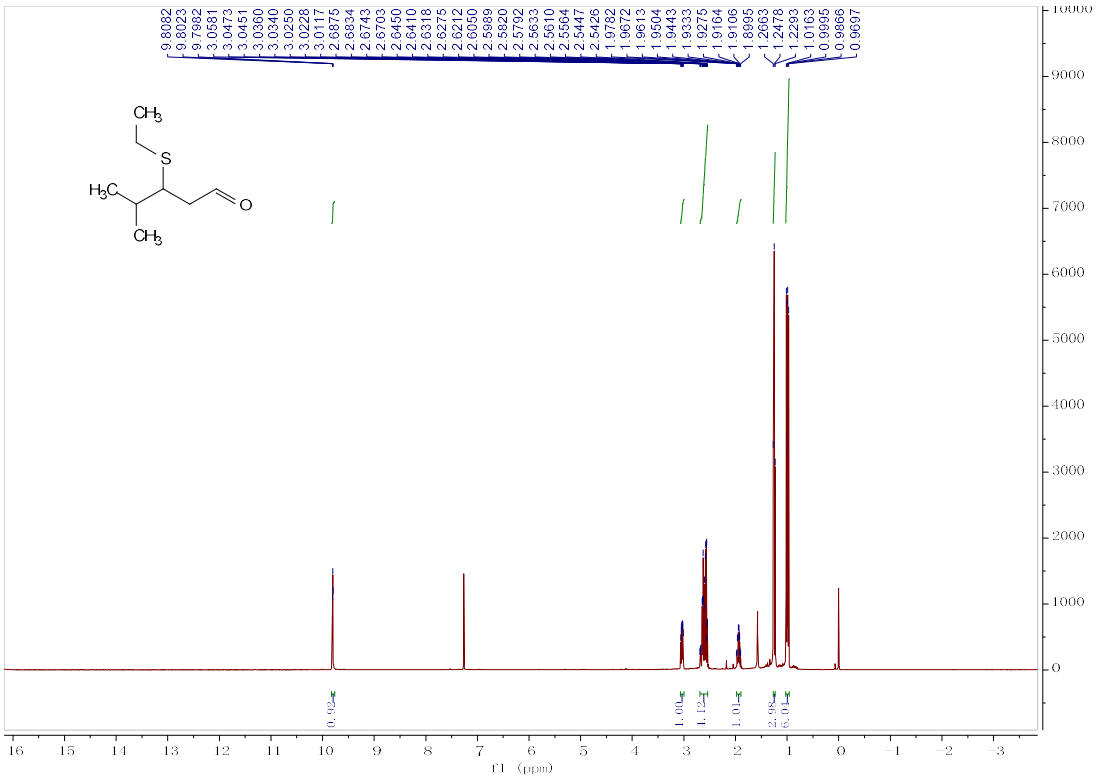
S
H3C
O
f1 (ppm)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9.8023
9.7982
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3.0473
3.0451
3.0360
3.0340
3.0250
3.0228
3.0117
2.6875
2.6834
2.6743
2.6703
2.6450
2.6410
2.6318
2.6275
2.6212
2.6050
2.5989
2.5820
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1.9672
1.9613
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1.9275
1.9164
1.9106
1.8995
1.2663
1.2478
1.2293
1.0163
0.9995
0.9866
0.9697
CH3
S
H3C
O
CH3
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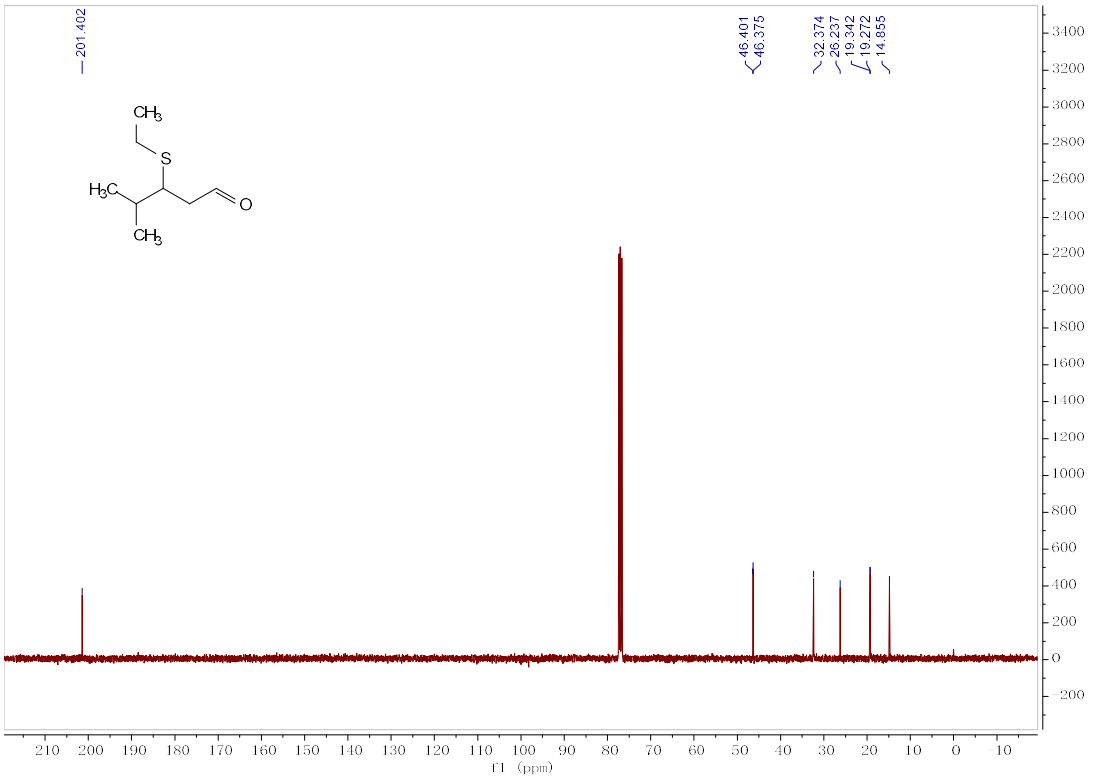
1.00
1.12
1.01
2.98
6.04
f1 (ppm)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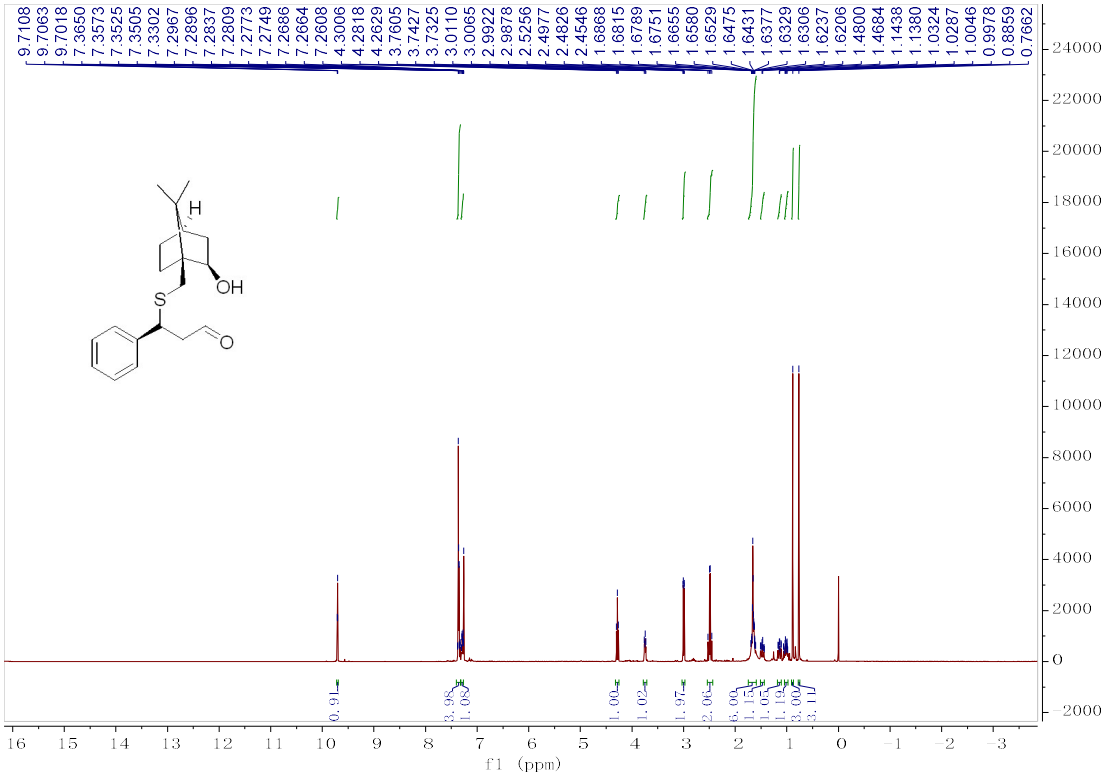
46.401
46.375
32.374
26.237
19.342
19.272
14.855
CH3
S
H3C
O
CH3
f1 (ppm)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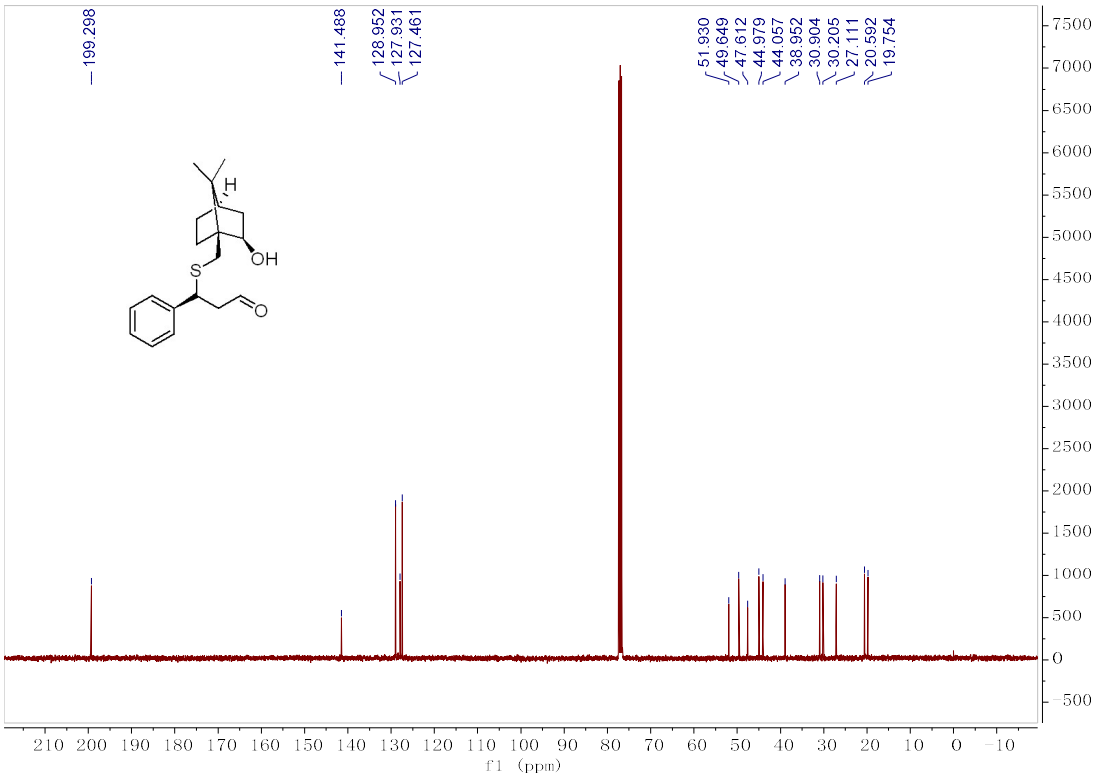
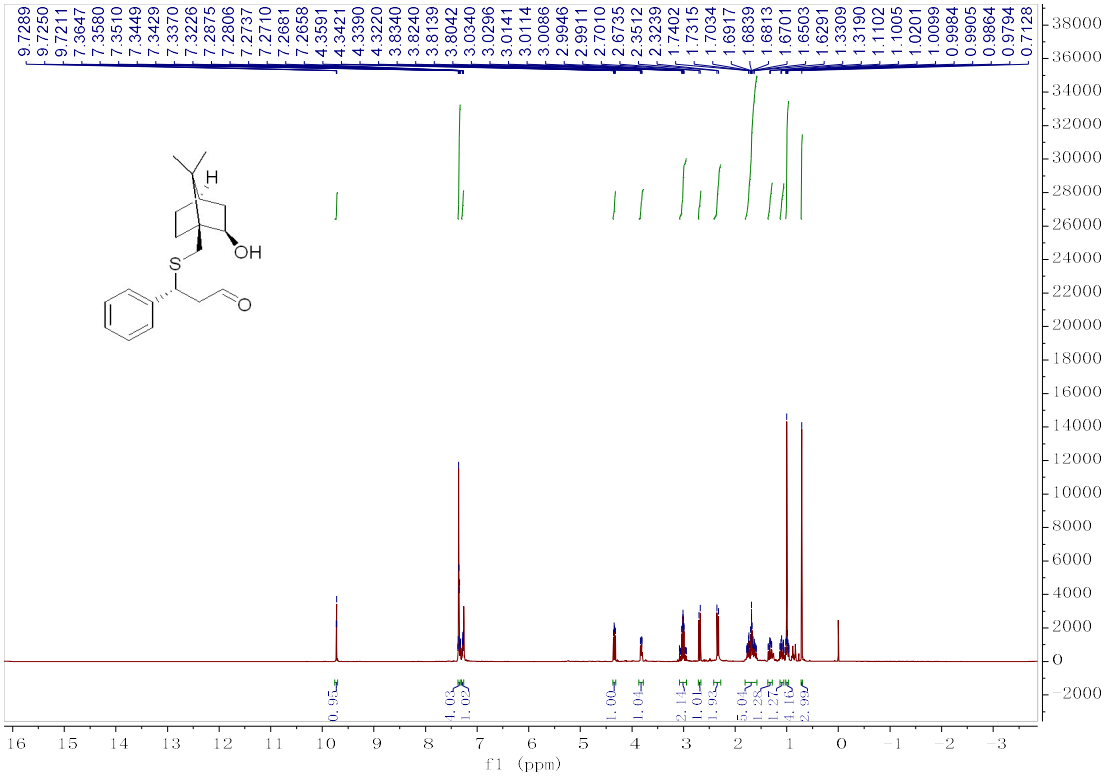
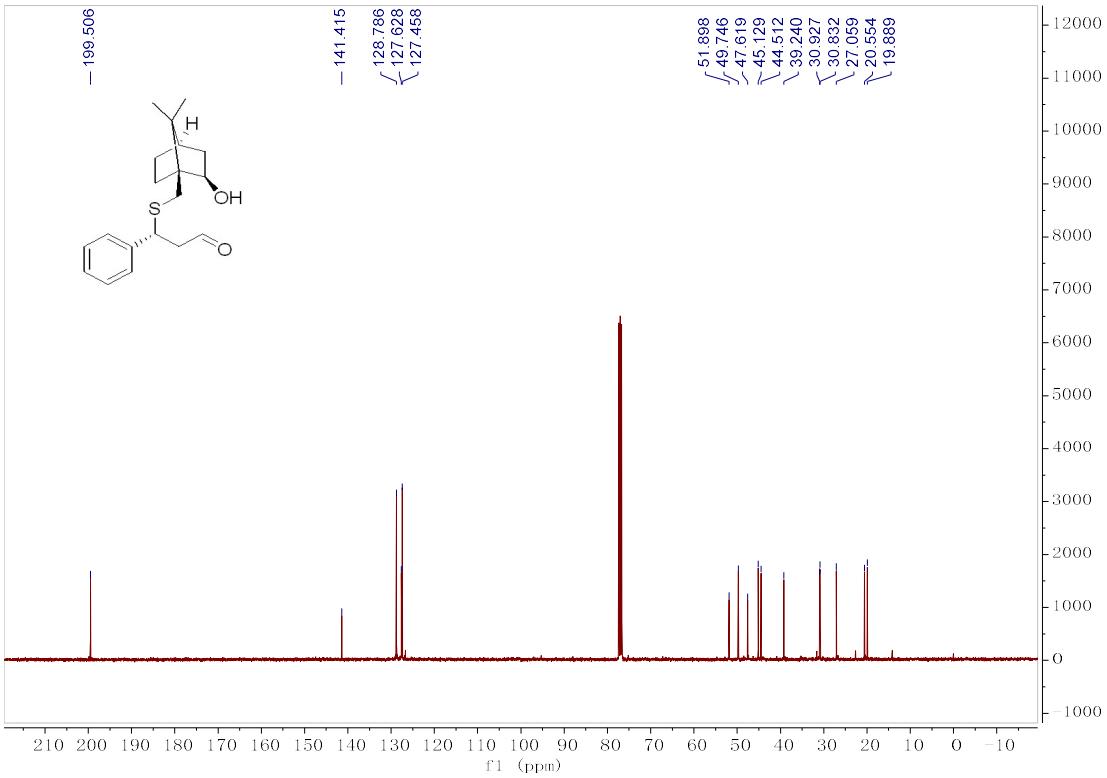
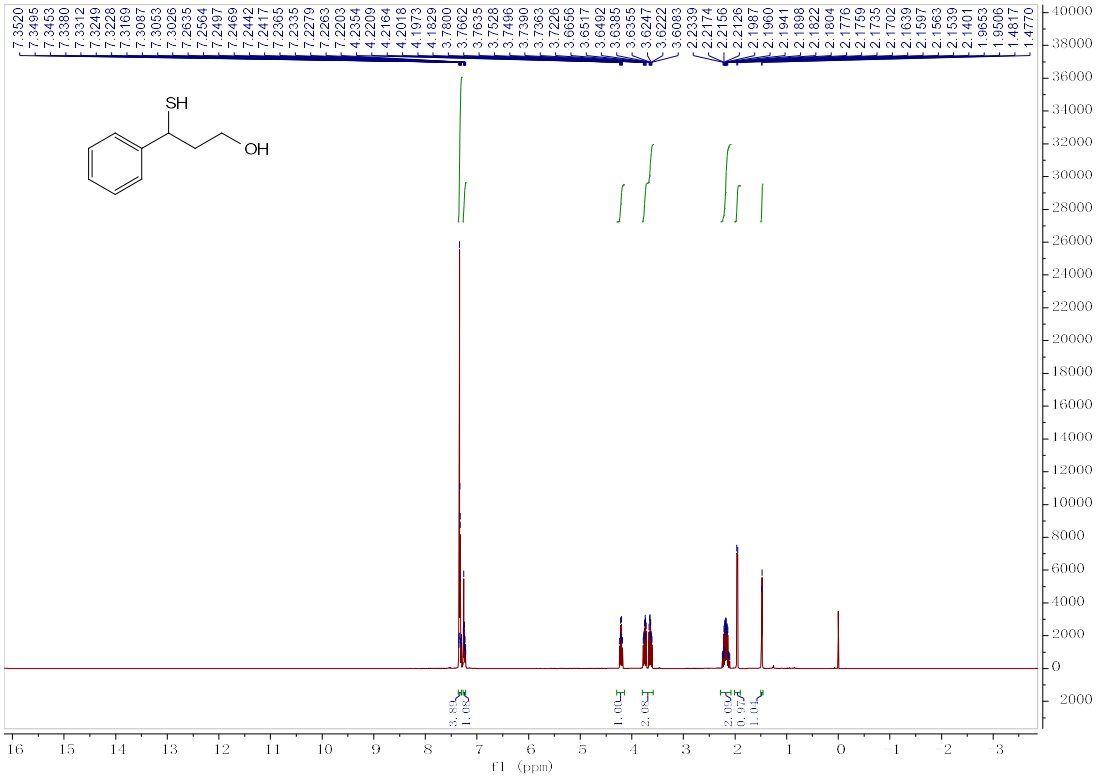
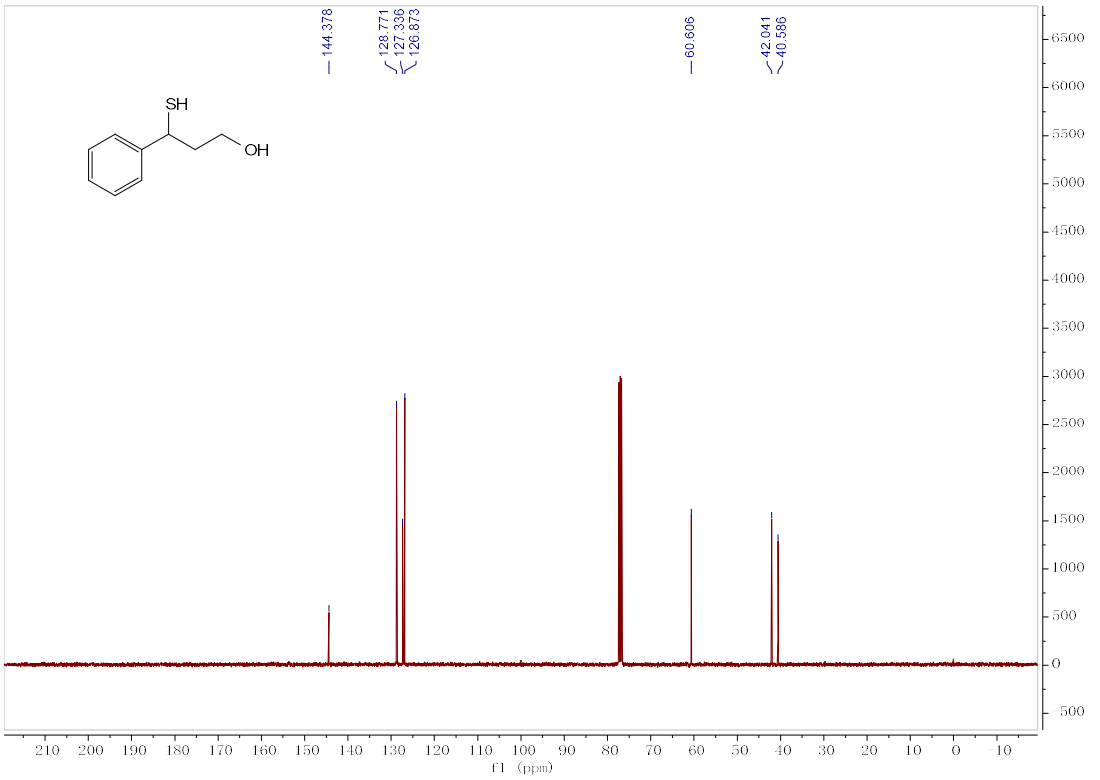
9.7063
9.7018
7.3650
7.3573
7.3525
7.3505
7.3302
7.2967
7.2896
7.2837
7.2809
7.2773
7.2749
7.2686
7.2664
7.2608
4.3006
4.2818
4.2629
3.7605
3.7427
3.7325
3.0110
3.0065
2.9922
2.9878
2.5256
2.4977
2.4826
2.4546
1.6868
1.6815
1.6789
1.6751
1.6655
1.6580
1.6529
1.6475
1.6431
1.6377
1.6329
1.6306
1.6237
1.6206
1.4800
1.4684
1.1438
1.1380
1.0324
1.0287
1.0046
0.9978
0.8859
0.7662
H
OH
S
O
0.91
3.98
1.02
1.00
1.02
1.97
2.06
6.00
1.13
1.05
1.19
3.00
3.11
f1 (ppm)


199.298
141.488
128.952
127.931
127.461
51.930
49.649
47.612
44.979
44.057
38.952
30.904
30.205
27.111
20.592
19.754
H
OH
S
O
f1 (ppm)


9.7289
9.7250
9.7211
7.3647
7.3580
7.3510
7.3449
7.3429
7.3370
7.3226
7.2875
7.2806
7.2737
7.2710
7.2681
7.2658
4.3591
4.3421
4.3390
4.3220
3.8340
3.8240
3.8139
3.8042
3.0340
3.0296
3.0141
3.0114
3.0086
2.9946
2.9911
2.7010
2.6735
2.3512
2.3239
1.7402
1.7315
1.7034
1.6917
1.6839
1.6813
1.6701
1.6503
1.6291
1.3309
1.3190
1.1102
1.1005
1.0201
1.0099
0.9984
0.9905
0.9864
0.9794
0.7128
H
OH
S
O
0.95
1.03
1.02
1.00
1.04
2.14
1.01
1.93
5.04
1.28
1.25
4.16
2.96
f1 (ppm)


199.506
141.415
128.786
127.628
127.458
51.898
49.746
47.619
45.129
44.512
39.240
30.927
30.832
27.059
20.554
19.889
H
OH
S
O
f1 (ppm)


SH
OH
f1 (ppm)


144.378
128.771
127.336
126.873
60.606
42.041
40.586
SH
OH
f1 (ppm)