Supporting Information

A General Platinum-catalyzed Alkoxycarbonylation of Olefins

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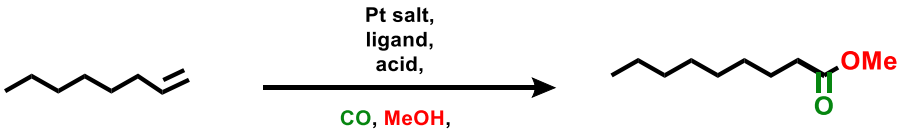
Contents

S1. General information: Materials and methods

All commercial reagents were ordered from Alfa Aesar, Aldrich, TCI or Strem. Unless otherwise stated, commercial reagents were used without purification. Air- and moisture-sensitive syntheses were performed under argon atmosphere in heating gun vacuum dried glassware. Analytical data of literature known compounds were in agree with reported data. NMR spectra were recorded on Bruker Avance 300 (300 MHz) or 400 (400 MHz) NMR spectrometers. Chemical shifts δ (ppm) are given relative to solvent: references for $CDCl_3$ were 7.26 ppm (^{1}H NMR) and 77.16 ppm (^{13}C NMR), for CD_2Cl_2 were 5.32 ppm (^{1}H NMR) and 53.84 ppm (^{13}C NMR), for d_6-benzene were 7.16 ppm (^{1}H NMR) and 128.26 ppm (^{13}C NMR), and for d_8-toluene were 2.08 ppm (^{1}H NMR) and 20.43 ppm (^{13}C NMR). Signals were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210 Time-of-Flight LC/MS (Agilent) with electrospray ionization (ESI). The data are given as mass units per charge (m/z) and intensities of signals are given in brackets. For GC analyses, HP 6890 chromatograph with a 29 m HP5 column was used.

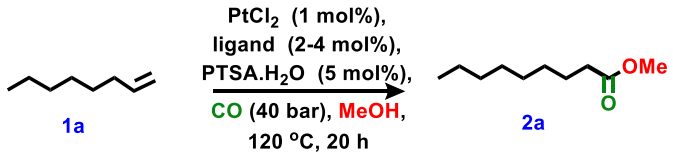
S2. General procedure of platinum catalysed alkoxycarbonylation of alkenes



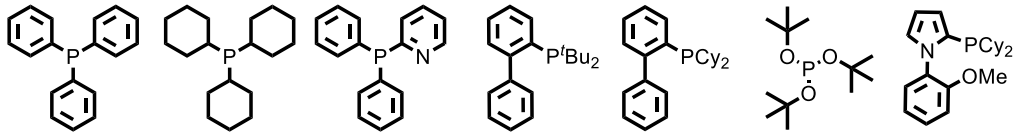
A 4 mL screw-cap vial was charged with platinum salt, ligand, acid, and an oven-dried stirring bar. The vial was closed by PTFE/white rubber septum (Wheaton 13 mm Septa) and phenolic cap and connected with atmosphere with a needle. Then, the vial was evacuated under vacuum and recharged with argon for three times. After MeOH and **1** were injected by syringe; the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave was flushed with carbon monoxide for three times and carbon monoxide was charged. The reaction was heated at the specified temperature. Afterwards, the autoclave was cooled to room temperature and the pressure was carefully released. Mesitylene was added into the reaction as internal standard. A sample of the mixture was analysed by gas chromatography. Pure products were obtained by column chromatography on silica gel.

S3. Optimisation of reaction conditions

Table S3.1. The effect of ligand [a]

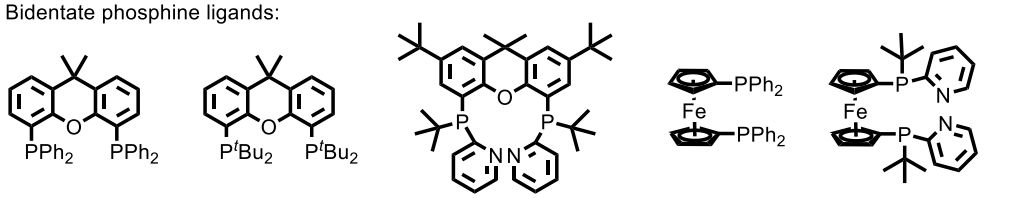


Monodentate phosphine ligands:

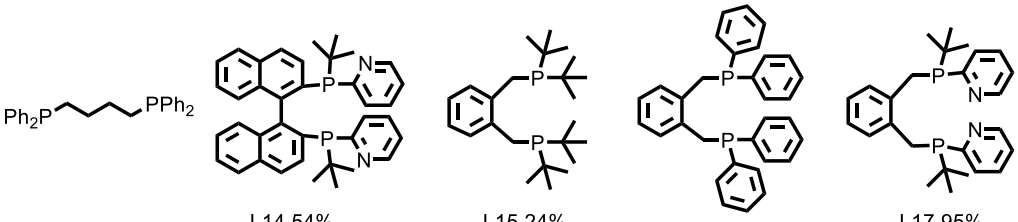


L1 0% L2 0% L3 0% L4 0% L5 0% L6 0% L7 0%

Bidentate phosphine ligands:



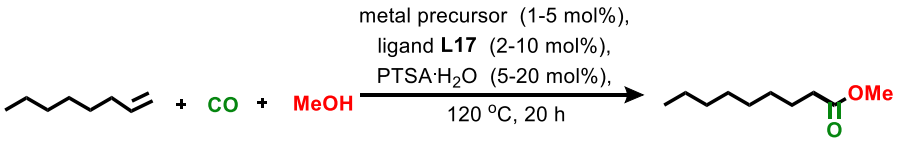
L8 38%, (*n/iso*=78/22) L9 17%, (*n/iso*=78/22) L10 0% L11 0% L12 78%, (*n/iso*=64/36)



L13 0% L14 54%, (*n/iso*=73/27) L15 24%, (*n/iso*=77/23) L16 0% L17 95%, (*n/iso*=73/27)

[a]. Standard reaction conditions: 1-Octene (1.0 mmol), $PtCl_2$ (0.01 mmol, 1.0 mol%), ligands (for monodentate phosphine ligand: 0.04 mmol, 4.0 mol%; for bidentate phosphine ligand: 0.02 mmol, 2.0 mol%), PTSA·H_2O (5.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 20 h; The selectivity and yield were determined by GC analysis with mesitylene as the internal standard.

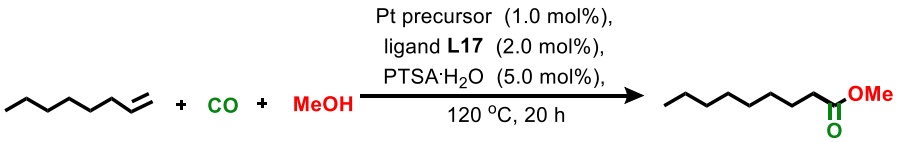
Table S3.2. The effect of different metal catalyst precursors



Entry	Metal precursor	Yield (%)	Selectivity (n/iso)
1.	$Fe_3(CO)_{12}$ [a]	0	
2.	$Cu(CH_3CN)_4PF_6$ [a]	0	
3.	$[Ru(p\text{-}cym)Cl_2]_2$ [b]	0	
4.	Rh(cod)(acac) [b]	0	
5.	$PdCl_2$ [b]	96	72/28
6.	$PtCl_2$ [b]	95	73/27

[a]. Reaction conditions: 1-Octene (1.0 mmol), metal precursor (refer to Fe or Cu, 0.05 mmol, 5.0 mol%), ligand (0.1 mmol, 10.0 mol%), PTSA·H_2O (20.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 20 h; the selectivity and yield were determined by GC analysis with mesitylene as the internal standard. [b]. reaction conditions: 1-Octene (1.0 mmol), metal precursor (refer to Ru, Rh, Pd or Pt, 0.01 mmol, 1.0 mol%), ligand (0.02 mmol, 2.0 mol%), PTSA·H_2O (5.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 20 h; the selectivity and yield were determined by GC analysis with mesitylene as the internal standard.

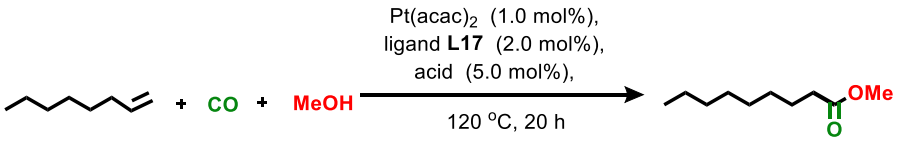
Table S3.3. The effect of Pt precursors



Entry	Pt precursor	Yield	Selectivity (n/iso)
1.	$PtCl_2$	95	73/27
2.	$PtBr_2$	58	68/32
3.	$Pt(acac)_2$	98	79/21
4.	$Pt(cod)Cl_2$	63	68/32

[a]. reaction conditions: 1-octene (1.0 mmol), Pt precursor (0.01 mmol, 1.0 mol%), ligand (0.02 mmol, 2.0 mol%), PTSA·H_2O (5.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 20 h; the selectivity and yield were determined by GC analysis with mesitylene as the internal standard.

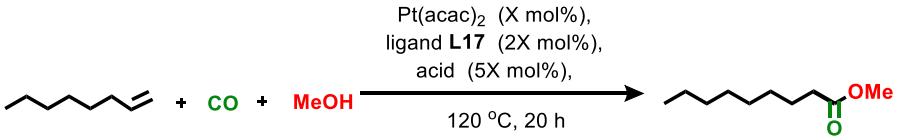
Table S3.4. The effect of acid [a]



Entry	Acid	Yield	Selectivity (n/iso)
1.	HCl, aqueous solution	65	70/30
2.	CF_3COOH	72	69/31
3.	MSA	93	77/23
4.	CSA	90	68/32
5.	PTSA	98	79/21
6.	H_2SO_4	67	71/29

[a]. reaction conditions: 1-octene (1.0 mmol), $Pt(acac)_2$ (0.01 mmol, 1.0 mol%), ligand (0.02 mmol, 2.0 mol%), acid (5.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 20 h; the selectivity and yield were determined by GC analysis with mesitylene as the internal standard.

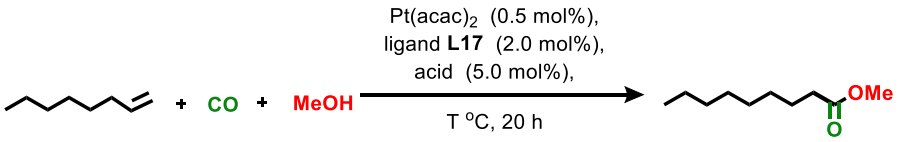
Table S3.5. The effect of catalyst loading [a]



Entry	Catalyst loading (Pt)	Yield	Selectivity (n/iso)
1.	0.1 mmol%	54	79/21
2.	0.2 mmol%	57	79/21
3.	0.5 mmol%	95	74/26
4.	1.0 mmol%	98	79/21

[a]. reaction conditions: 1-octene (1.0 mmol), $Pt(acac)_2$ (0.001-0.01 mmol, 0.1-1.0 mol%), ligand (0.02 mmol, 2.0 mol%), PTSA· H_2O (5.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 20 h; the selectivity and yield were determined by GC analysis with mesitylene as the internal standard.

Table S3.6. The effect of tempature [a]



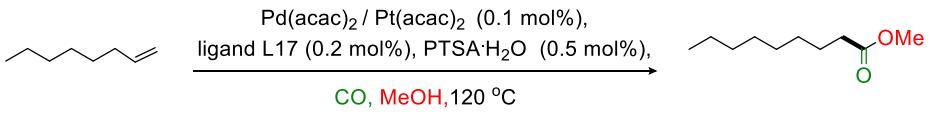
Entry	Temperature (°C)	Yield	Selectivity (*n/iso*)
1	120 °C	95	74/26
2	60 °C	trace	

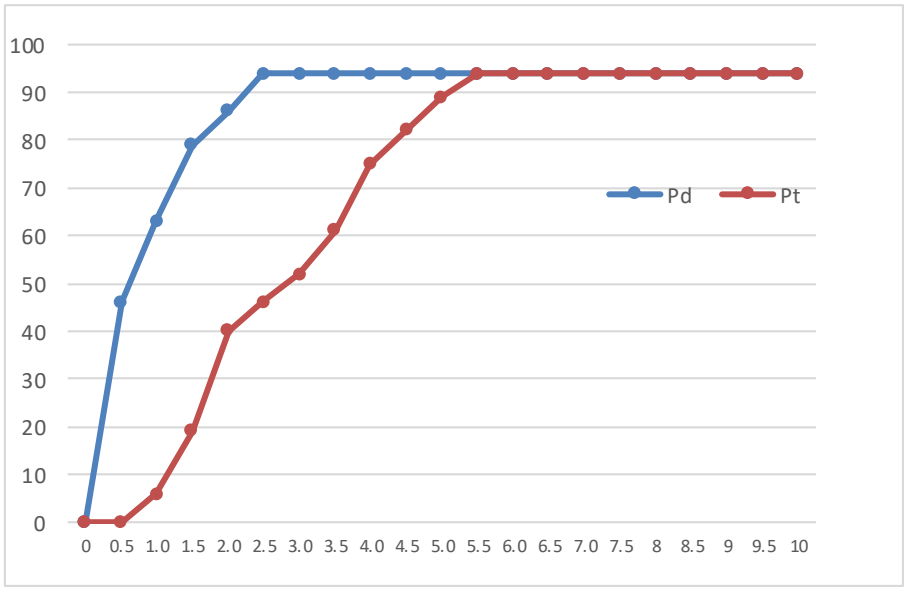
[a]. reaction conditions: 1-octene (1.0 mmol), $Pt(acac)_2$ (0.005 mmol, 0.5 mol%), ligand (0.02 mmol, 2.0 mol%), PTSA· H_2O (5.0 mol%), MeOH (2.0 mL), CO (40 atm), 20 h; the selectivity and yield were determined by GC analysis with mesitylene as the internal standard.

S4. Kinetic monitoring experiment

In order to understand the process in more detail, kinetic monitoring experiments were conducted. In general, all catalytic experiments an excess of ligand was used to ensure stability of the active complex at low metal concentration. By comparison, we observe that the Pd catalysed reaction is basically completed in about 2.5 hours; the rate of Pt-catalysed reaction is slower. It takes about 5.5 hours to complete the reaction. However, for 1-octene, the final yield of the product is the same for both catalysts.

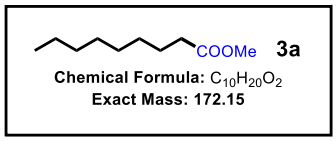
Figure S4. Kinetic monitoring experiment.





The ***X***-axis represents the reaction time and the ***Y***-axis represents the reaction yield. Reaction conditions: 1-octene (20 mmol), $Pd(acac)_2$ or $Pt(acac)_2$ (0.02 mmol, 0.1 mol%), ligand (0.04 mmol, 0.2 mol%), $PTSA{\cdot}H_2O$ (0.5 mol%), MeOH (30 mL), CO (40 atm), 120 °C; the GC yield were determined by GC analysis with mesitylene as the internal standard.

S5. Characterization of the products

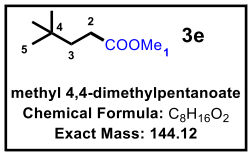


Colorless oil, 95% yield, *n*/*iso* = 74/26.

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.66 (s, 3H), 2.34-2.24 (m, 2H), 1.67-1.54 (m, 2H), 1.34-1.19 (m, 10H), 0.92-0.79 (m, 3H) ppm;

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.5, 51.6, 34.2, 32.0, 29.4, 29.3, 29.3, 25.1, 22.8, 14.2.

DEPT135-^{13}C NMR (75 MHz, $CDCl_3$) δ 51.6 (-), 34.3, 31.9, 29.4, 29.3, 29.3, 25.1, 22.8, 14.2 (-).

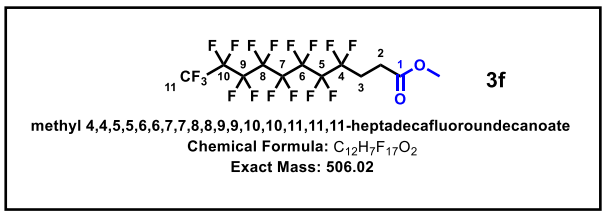


Colorless oil, 93% yield, *n*/*iso* > 99/1.

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.65 (s, 3H), 2.31-2.21 (m, 2H), 1.58-1.48 (m, 2H), 0.88 (s, 9H) ppm;

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.0, 51.6, 38.7, 30.2, 30.0, 29.1.

DEPT135-^{13}C NMR (75 MHz, $CDCl_3$) δ 51.6, 38.7 (-), 30.0 (-), 29.1.

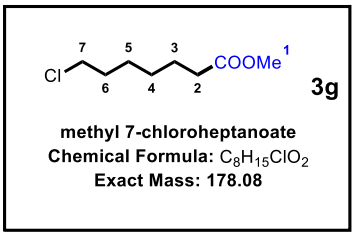


Colorless oil, 87% yield, *n*/*iso* > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.67 (s, 3H), 2.62-2.52 (m, 2H), 2.51-2.32 (m, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 120.7, 118.8, 118.1, 116.0, 113.8, 111.4, 111.1, 108.9, 108.5, 106.2, 52.0, 26.7, 25.3.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 52.0, 26.7 (-), 25.3 (-).

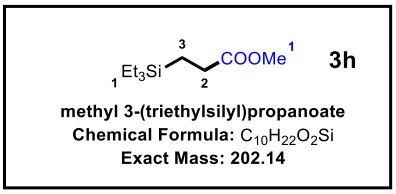


Colorless oil, 87% yield, *n*/*iso* = 66/34.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.59 (s, 3H), 3.49-3.39 (t, *J* = 6.7 Hz, 2H), 2.30-2.19 (m, 2H), 1.76-1.25 (m, 8H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 51.4, 44.9, 33.9, 32.4, 28.4, 26.5, 24.7.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.4, 44.9 (-), 33.9 (-), 32.4 (-), 28.4 (-), 26.5 (-), 24.7 (-).

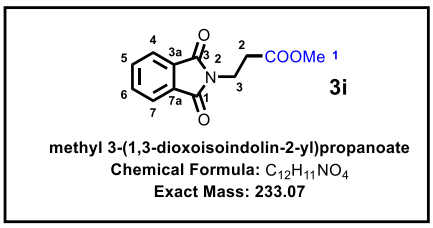


Colorless oil, 82% yield, *n*/*iso* = 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (s, 3H), 2.32-2.18 (m, 2H), 1.02-0.77 (m, 11H), 0.58-0.44 (q, *J* = 7.9 Hz, 6H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 51.6, 28.6, 7.3, 6.6, 3.1.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.6, 28.6 (-), 7.3, 6.6 (-), 3.1 (-).

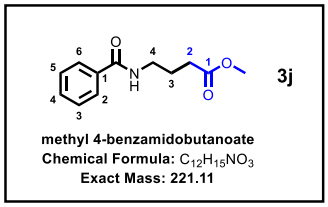


White solid, 77% yield, n/iso > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.70 (m, 2H), 7.70-7.58 (m, 2H), 3.96-3.84 (t, *J* = 7.2 Hz, 2H), 3.60 (s, 3H), 2.73-2.60 (t, *J* = 7.2 Hz, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 167.9, 134.0, 132.0, 123.3, 51.9, 33.8, 32.8.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 134.0, 123.3, 51.9, 33.8 (-), 32.8 (-).

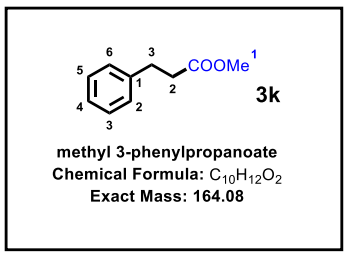


Colorless oil, 66% yield, *n*/*iso* = 68/32.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79-7.70 (m, 2H), 7.43-7.24 (m, 4H), 3.56 (s, 3H), 3.45-3.32 (m, 2H), 2.38-2.27 (t, *J* = 7.2 Hz, 2H), 1.93-1.78 (m, 2H) ppm;

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.9, 167.7, 134.4, 131.1, 128.2, 126.9, 51.5, 39.4, 31.5, 24.4.

DEPT135-^{13}C NMR (75 MHz, $CDCl_3$) δ 131.1, 128.2, 126.9, 51.5, 39.4 (-), 31.5 (-), 24.4 (-).

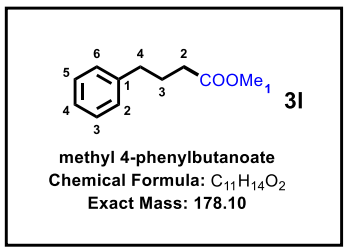


Colorless oil, 95% yield, *n*/*iso* = 71/29.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.24 (m, 5H), 3.71 (s, 3H), 3.07-2.95 (t, *J* = 7.8 Hz, 2H), 2.73-2.64 (m, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.1, 140.5, 128.4, 128.2, 126.2, 51.4, 35.6, 30.9.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 128.4, 128.2, 126.2, 51.4, 35.6 (-), 30.9 (-).

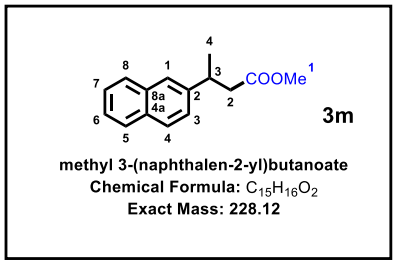


Colorless oil, 94% yield, *n*/*iso* = 65/35.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.22 (m, 5H), 3.70 (s, 3H), 2.75-2.62 (m, 2H), 2.45-2.33 (t, *J* = 7.5 Hz, 2H), 2.08-1.96 (m, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 141.3, 128.4, 128.3, 125.9, 51.3, 35.1, 33.3, 26.4.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 128.5, 128.4, 126.0, 51.5, 35.2 (-), 33.4 (-), 26.6 (-).

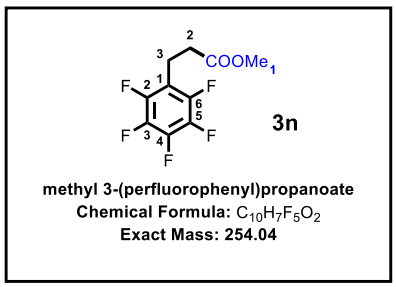


Light yellow solid, 97% yield, *n*/*iso* > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.82 (m, 3H), 7.78-7.72 (m, 1H), 7.57-7.40 (m, 3H), 3.68 (s, 3H), 3.64-3.48 (m, 1H), 2.89-2.67 (m, 2H), 1.52-1.44 (d, *J* = 7.0 Hz, 3H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.7, 143.1, 133.6, 132.3, 128.2, 127.6, 127.6, 125.9, 125.4, 125.4, 124.9, 51.4, 42.6, 36.5, 21.8.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 128.2, 127.6, 127.6, 125.9, 125.4, 125.4, 124.9, 51.4, 42.6 (-), 36.5, 21.8.

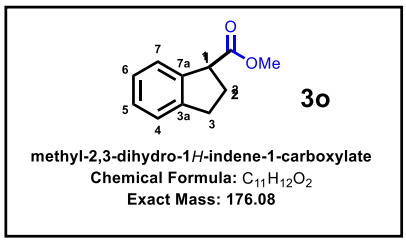


Colorless oil, 87% yield, *n*/*iso* > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.65 (s, 3H), 3.03-2.95 (t, *J* = 7.7 Hz, 2H), 2.63-2.54 (t, *J* = 7.7 Hz, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 146.5, 144.0, 141.3, 138.8, 136.3, 113.5, 51.8, 32.9, 18.0.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.8, 32.9 (-), 18.0 (-).

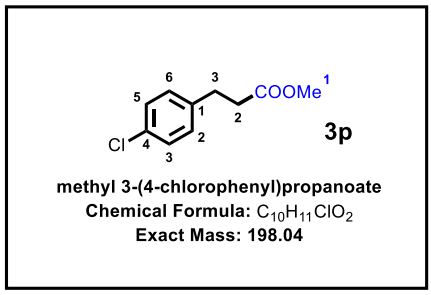


Colorless oil, 87% yield, *1:2* = 88:12.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.46 (m, 1H), 7.39-7.22 (m, 3H), 4.20-4.10 (m, 1H), 3.82 (s, 3H), 3.24-2.95 (m, 2H), 2.60-2.37 (m, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 144.0, 140.6, 127.5, 126.4, 124.7, 124.6, 51.9, 50.0, 31.7, 28.7.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 127.5 (-), 126.4 (-), 124.7 (-), 124.6 (-), 51.9 (-), 50.0 (-), 31.7, 28.7.

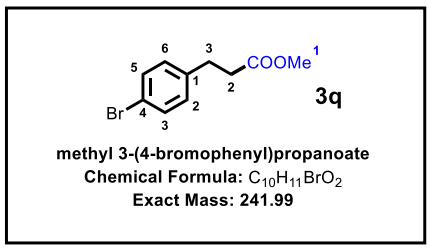


Colorless oil, 89% yield, *n*/*iso* = 71/29.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.21 (m, 2H), 7.15-7.09 (m, 2H), 3.65 (s, 3H), 2.91 (t, *J* = 7.7 Hz, 2H), 2.60 (t, *J* = 7.7 Hz, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 138.9, 132.0, 129.6, 128.5, 51.5, 35.4, 30.2.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 129.6, 128.5, 51.5, 35.4 (-), 30.2 (-).

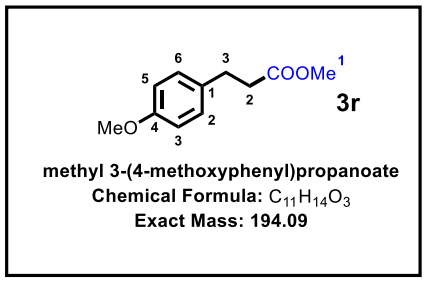


Colorless oil, 86% yield, *n*/*iso* = 72/28.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 2H), 7.09-7.03 (m, 2H), 3.65 (s, 3H), 2.89 (t, *J* = 7.7 Hz, 2H), 2.60 (t, *J* = 7.7 Hz, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 139.4, 131.4, 130.0, 120.0, 51.5, 35.3, 30.2.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 131.4, 130.0, 51.5, 35.3 (-), 30.2 (-).

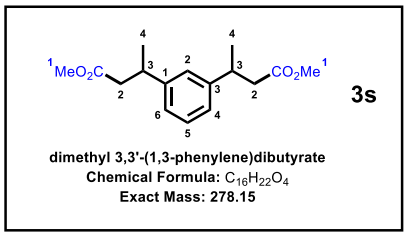


Colorless oil, 85% yield, *n*/*iso* = 52/48.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17-7.09 (m, 2H), 6.91-6.86 (m, 2H), 3.78 (s, 3H), 3.68 (s, 3H), 2.92 (t, *J* = 7.8 Hz, 2H), 2.62 (t, *J* = 7.8 Hz, 2H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.3, 158.0, 132.5, 129.2, 113.8, 55.1, 51.4, 35.9, 30.0.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 129.2, 113.8, 55.1, 51.4, 35.9 (-), 30.0 (-).

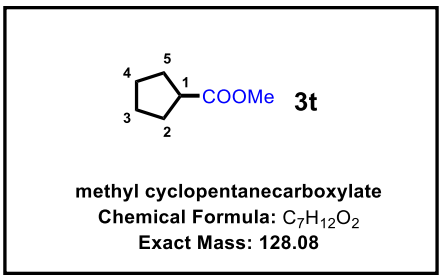


Colorless oil, 86% yield, *n*/*iso* > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.19 (m, 1H), 7.12-7.01 (m, 3H), 3.63 (s, 6H), 3.36-3.19 (m, 2H), 2.70-2.46 (m, 4H), 1.30 (d, *J* = 7.0 Hz, 6H) ppm;

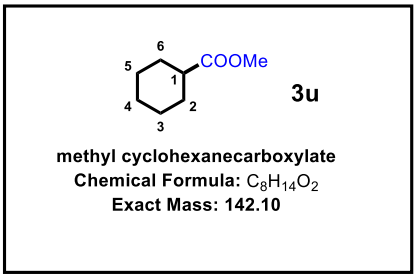
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 145.9, 128.7, 125.4, 124.7, 51.5, 42.8, 36.5, 21.7.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 128.7 (-), 125.4 (-), 124.7 (-), 51.5 (-), 42.8, 36.5(-), 21.7 (-).



Colorless oil, 97% yield.

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.65 (s, 3H), 2.79-2.63 (m, 1H), 1.93-1.48 (m, 8H) ppm;
^{13}C NMR (75 MHz, $CDCl_3$) δ 177.4, 51.7, 43.8, 30.1, 25.9.
DEPT135-^{13}C NMR (75 MHz, $CDCl_3$) δ 51.7 (-), 43.8 (-), 30.1, 25.9.

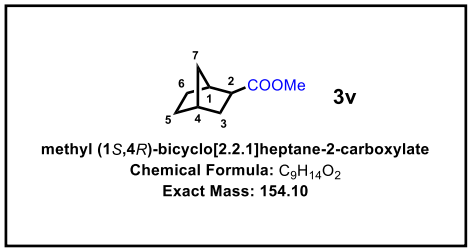


Colorless oil, 96% yield.

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.60 (s, 3H), 2.32-2.17 (m, 1H), 1.92-1.76 (m, 2H), 1.74-1.13 (m, 8H) ppm;

^{13}C NMR (75 MHz, $CDCl_3$) δ 176.5, 51.4, 43.1, 29.1, 25.8, 25.5.

DEPT135-^{13}C NMR (75 MHz, $CDCl_3$) δ 51.4 (-), 43.1 (-), 29.1, 25.8, 25.5.

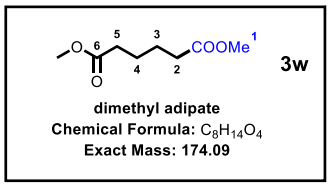


Colorless oil, 88% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.61 (s, 3H), 2.48-2.39 (m, 1H), 2.32-2.19 (m, 2H), 1.85-1.72 (m, 1H), 1.54-1.36 (m, 4H), 1.22-1.06 (m, 3H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.5, 51.6, 46.4, 41.0, 36.5, 36.1, 34.2, 29.5, 28.7.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.6 (-), 46.4 (-), 40.9 (-), 36.5, 36.1 (-), 34.2, 29.5, 28.7.

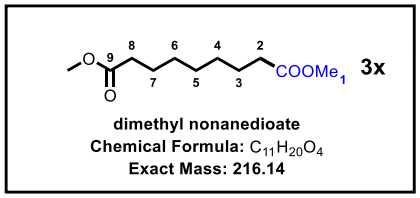


Colorless oil, 98% yield, *n*/*iso* = 69/31.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.65 (s, 6H), 2.36-2.27 (m, 4H), 1.68-1.60 (m, 4H), ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 77.5, 77.2, 76.8, 51.7, 33.8, 24.5.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.7 (-), 33.8, 24.5.

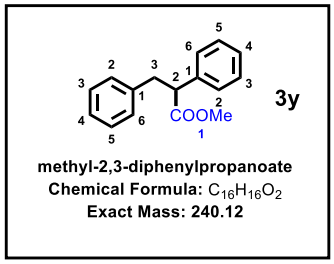


Colorless oil, 88% yield, *n*/*iso* = 42/58.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56 (s, 6H), 2.20 (t, *J* = 7.5 Hz, 4H), 1.52 (m, 4H), 1.28-1.17 (m, 6H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 51.3, 33.9, 28.9, 28.8, 24.8.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.3, 33.9 (-), 28.8 (-), 24.8 (-).

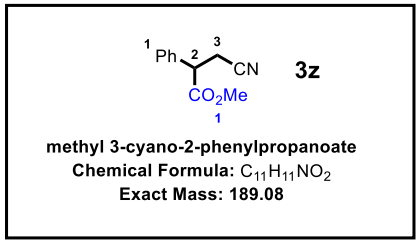


Light yellow solid, 89% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-6.95 (m, 10H), 3.78 (dd, *J* = 8.8, 6.7 Hz, 1H), 3.52 (s, 3H), 3.40-3.27 (m, 1H), 2.95 (dd, J = 13.7, 6.7 Hz, 1H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 139.2, 138.8, 129.0, 128.8, 128.5, 128.1, 127.5, 126.5, 53.7, 52.1, 40.0.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 129.0, 128.8, 128.5, 128.1, 127.5, 126.5, 53.7, 52.1, 39.9 (-).

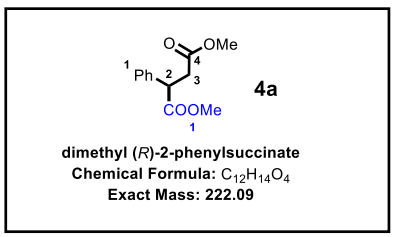


Colorless oil, 84% yield, *n*/*iso* = 78/22.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.21 (m, 5H), 3.97 (t, *J* = 7.6 Hz, 1H), 3.74 (s, 3H), 3.05 (dd, *J* = 16.8, 7.5 Hz, 1H), 2.82 (dd, *J* = 16.8, 7.6 Hz, 1H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 135.8, 129.3, 128.6, 127.6, 117.6, 52.8, 47.6, 21.7.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 129.3, 128.6, 127.6, 52.8, 47.6, 21.7 (-).

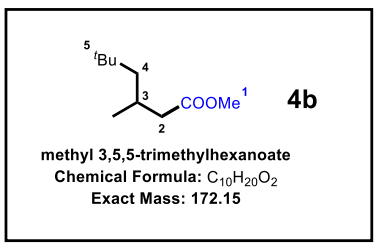


Colorless oil, 86% yield, 2:3 = 95:5.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.20 (m, 5H), 4.15-4.05 (m, 1H), 3.66 (s, 6H), 3.27-3.14 (m, 1H), 2.67 (dd, *J* = 17.0, 5.2 Hz, 1H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.4, 171.9, 144.1, 128.9, 127.7, 127.6, 52.3, 51.8, 47.1, 37.6.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 128.9, 127.7, 127.6, 52.3, 51.5, 46.3, 37.6 (-).

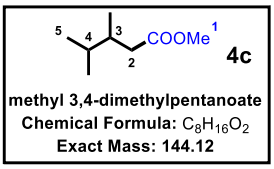


Colorless oil, 94% yield, *n*/*iso* > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 3H), 2.33-2.23 (m, 1H), 2.15-2.06 (m, 1H), 2.06-1.93 (m, 1H), 1.21 (dd, *J* = 14.0, 4.0 Hz, 1H), 1.09 (dd, *J* = 14.1, 6.3 Hz, 1H), 0.97-0.92 (d, 3H), 0.88 (s, 9H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7, 51.4, 50.6, 43.9, 31.2, 30.0, 27.1, 22.8.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.4, 50.6 (-), 43.9 (-), 30.0, 27.1, 22.8.

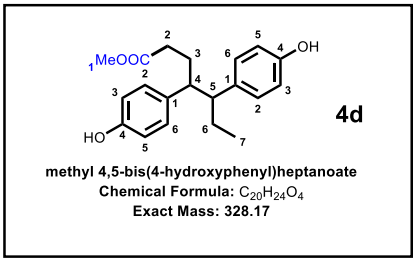


Colorless oil, 70% yield, *n*/*iso* > 99/1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 3H), 2.32 (dd, *J* = 14.6, 5.2 Hz, 1H), 2.05 (dd, *J* = 14.6, 9.1 Hz, 1H), 1.92-1.75 (m, 1H), 1.62- 1.45 (m, 1H), 0.89- 0.77 (m, 9H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3, 51.5, 39.1, 36.0, 32.2, 19.9, 18.4, 15.9.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 51.5, 39.1 (-), 36.0, 32.2, 19.9, 18.3, 15.9.



White solid, 32% yield, *n/iso* = 90/10.

For this product, linear and branched products were not easily separated by column chromatography and we obtained a mixture of products. The ratio of linear and branched products is determined by GC. Corresponding low-resolution mass spectra, ^{13}C characteristic peaks were compared to the known spectra. For the ^{1}H spectrum, here we list the spectrum of the mixture products.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98-6.82 (m, 6H), 6.76-6.52 (m, 8H), 4.12-3.99 (m, 1H), 3.58-3.47 (s, 1.45 H), 3.47-3.35 (s, 2.94H), 2.70-2.31 (m, 3.04H), 2.15-1.78 (m, 5.62H), 1.24-1.11 (m, 3.38H), 0.67-0.59 (t, *J* = 7.2 Hz, 1H), 0.51-0.40 (t, *J* = 7.3 Hz, 3H) ppm;

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 175.6, 154.4, 154.2, 154.1, 153.8, 135.6, 135.0, 134.1, 133.3, 130.1, 130.0, 129.3, 115.5, 115.3, 114.8, 114.6, 77.5, 77.2, 76.8, 61.0, 53.6, 52.7, 51.9, 51.8, 51.0, 50.0, 32.6, 32.1, 29.7, 28.2, 27.4, 26.0, 21.1, 14.1, 12.4, 12.2.

DEPT135-^{13}C NMR (101 MHz, $CDCl_3$) δ 130.1, 130.0, 129.3, 115.5, 115.3, 114.8, 114.6, 61.0, 53.6, 52.7, 51.9, 51.8, 51.0, 50.0, 32.6, 32.6, 29.7, 28.6, 27.4, 26.0, 21.1, 14.1, 12.4, 12.2.

References

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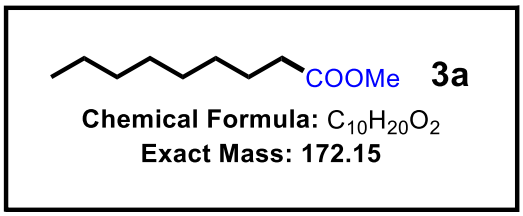
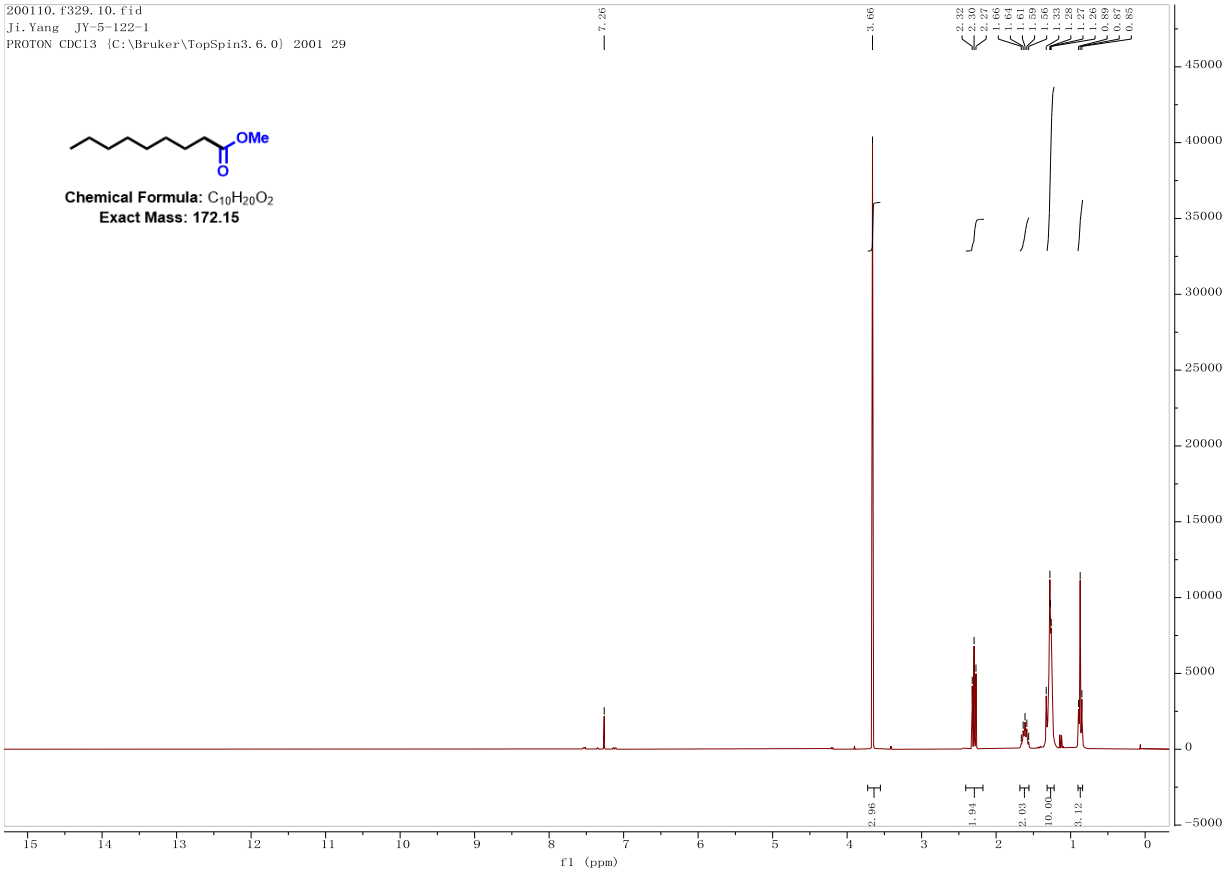
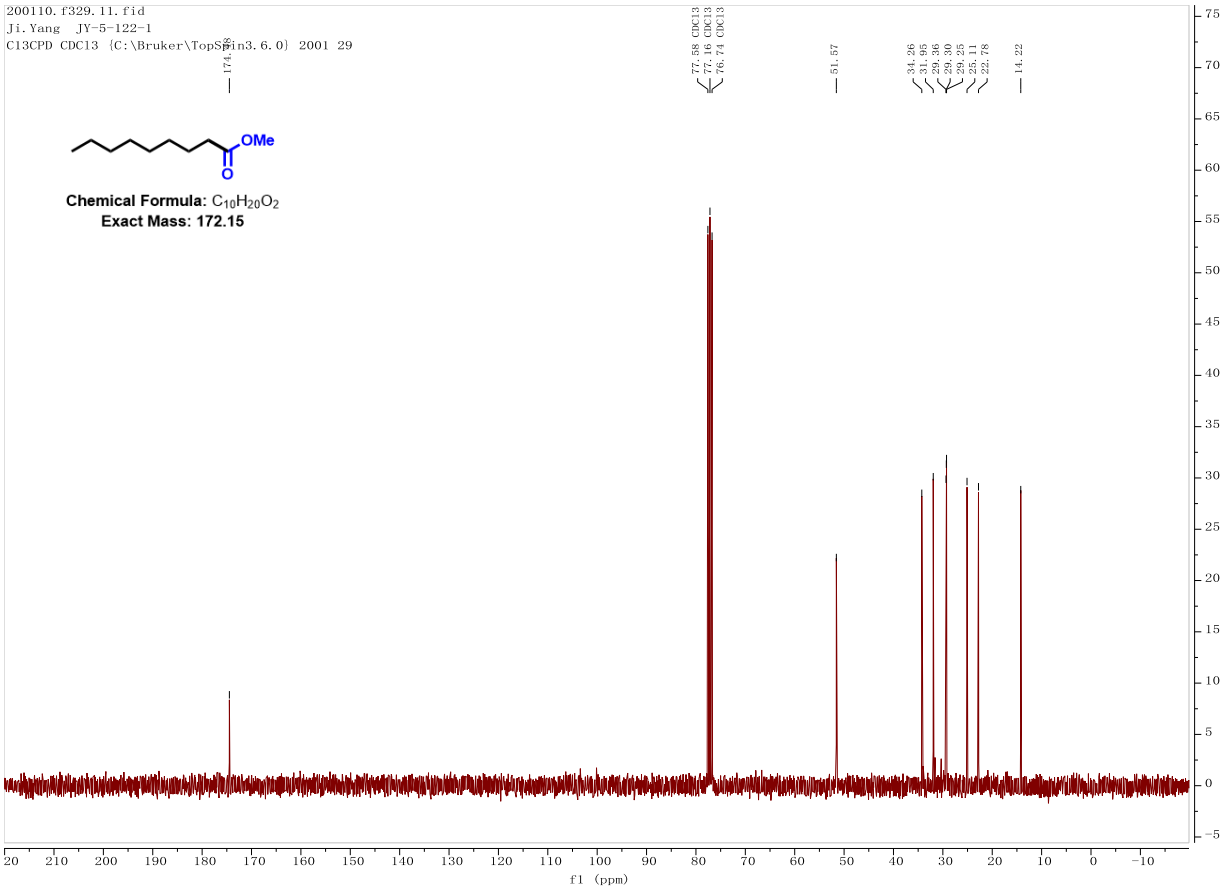
S6. NMR, GC and GC-MS spectra:



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76.74 CDCl3
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OMe
O
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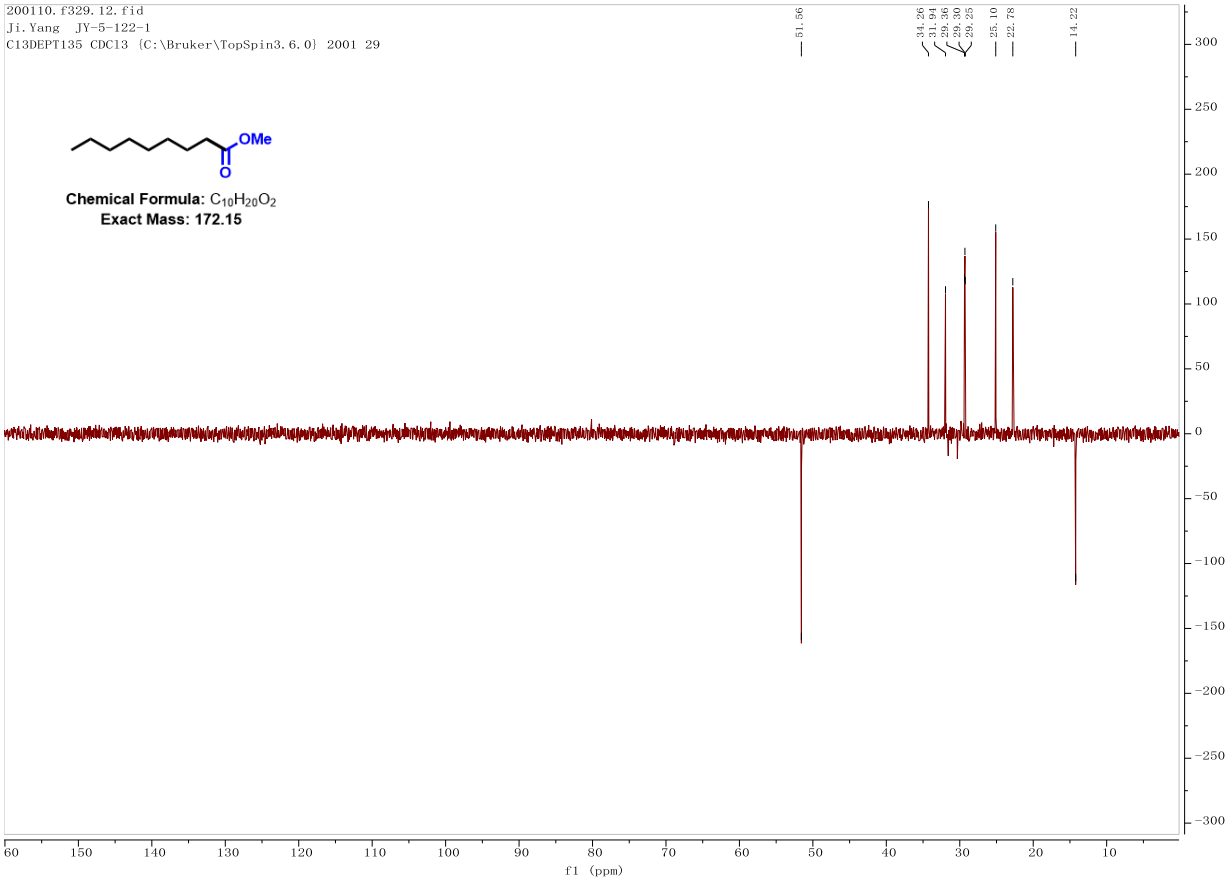
Exact Mass: 172.15
f1 (ppm)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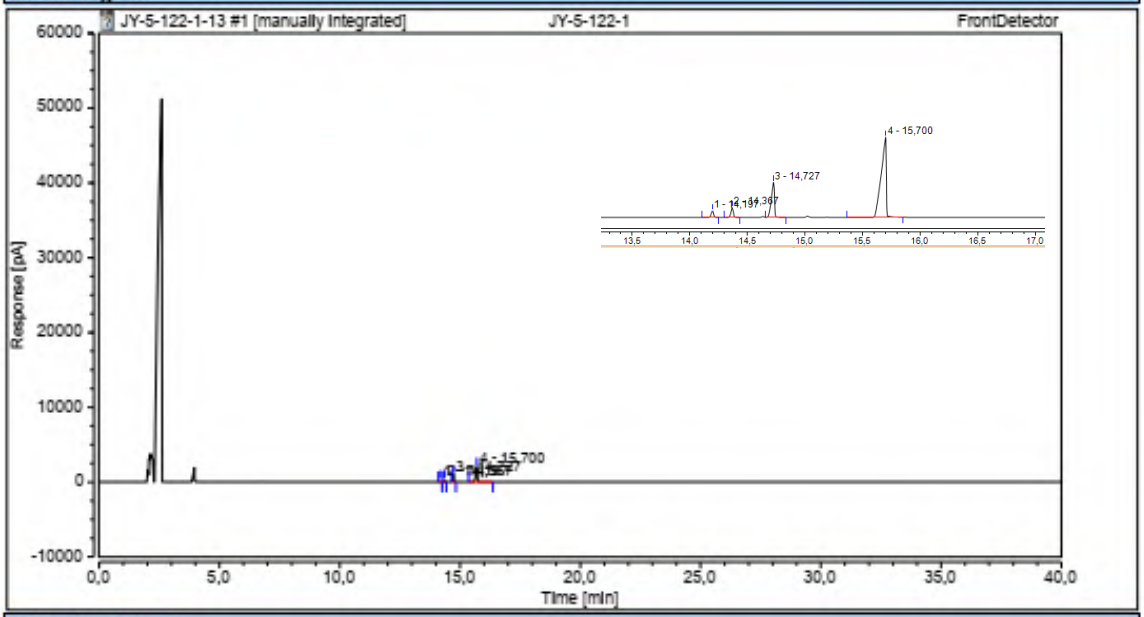
29.30
29.25
25.10
22.78
14.22
OMe
O
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-1**	*Run Time (min):*	**40,00**
Vial Number:	**61**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 15:22**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,197	3,643	155,521	2,77	5,08	n.a.
2		14,367	5,439	232,981	4,13	7,61	n.a.
3		14,727	25,100	809,661	19,07	26,46	n.a.
4		15,700	97,436	1861,618	74,03	60,84	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**131,618**	**3059,782**	**100,00**	**100,00**	

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Instrument : GC-MSD
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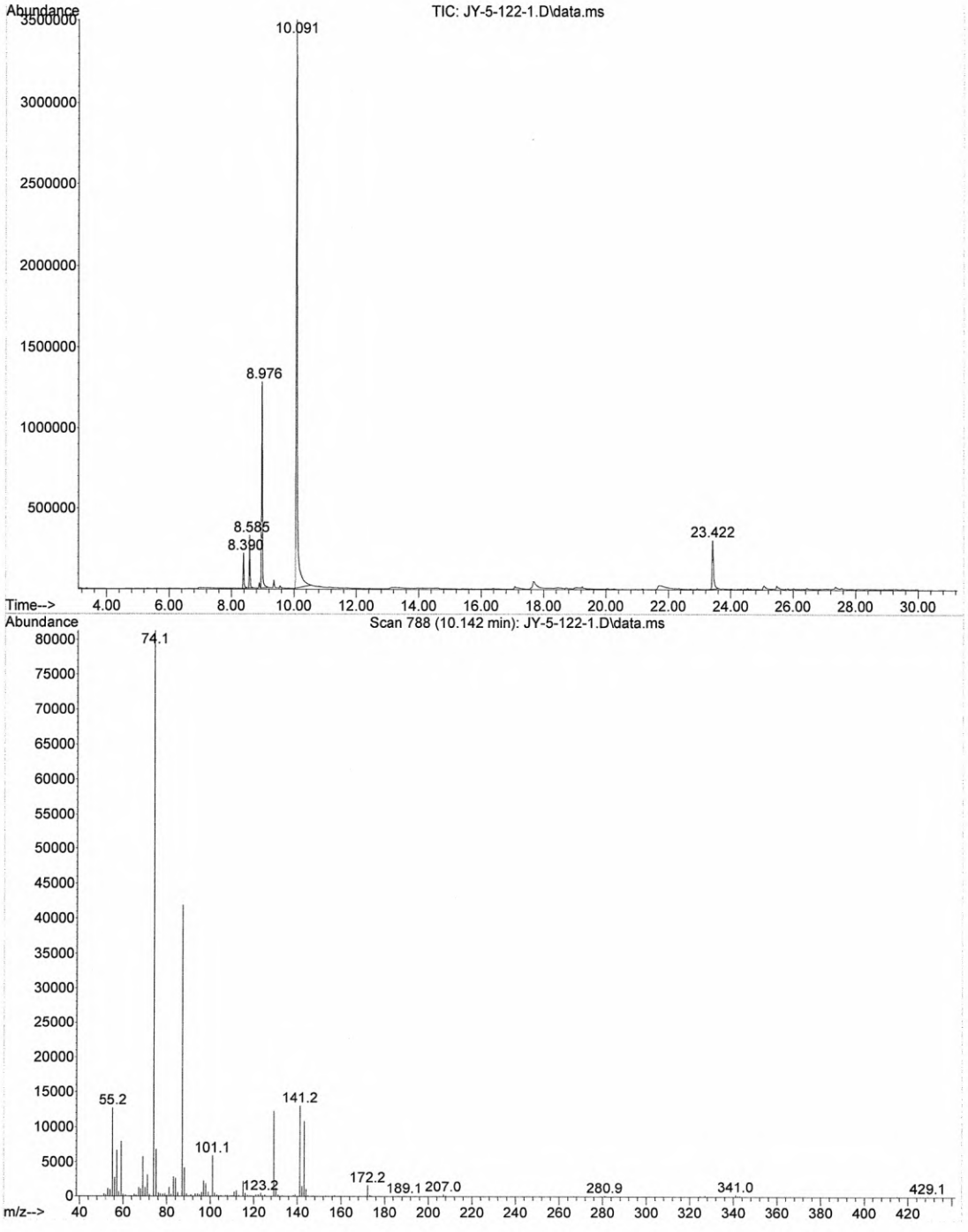

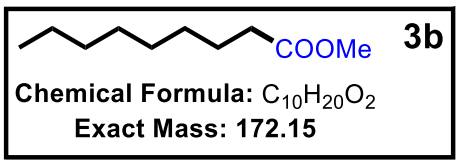
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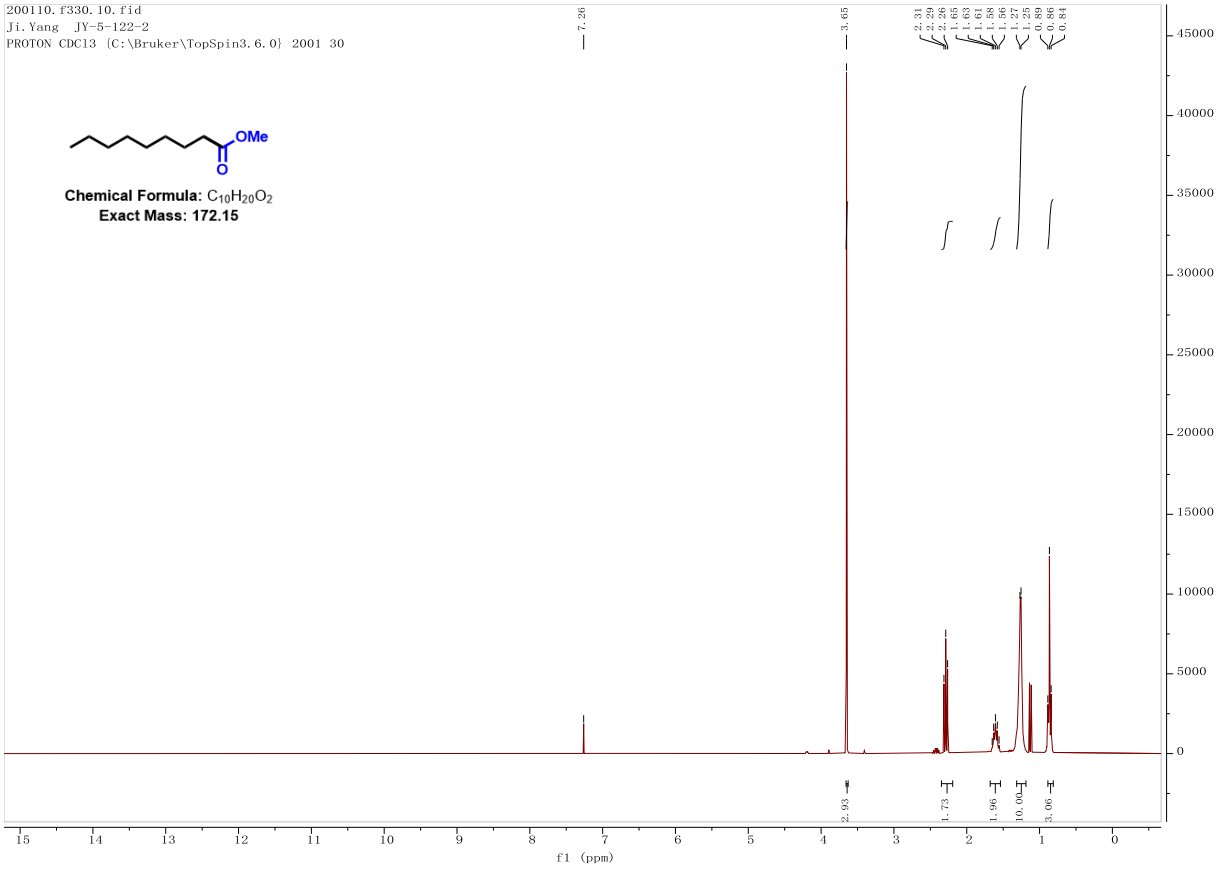
Exact Mass: 172.15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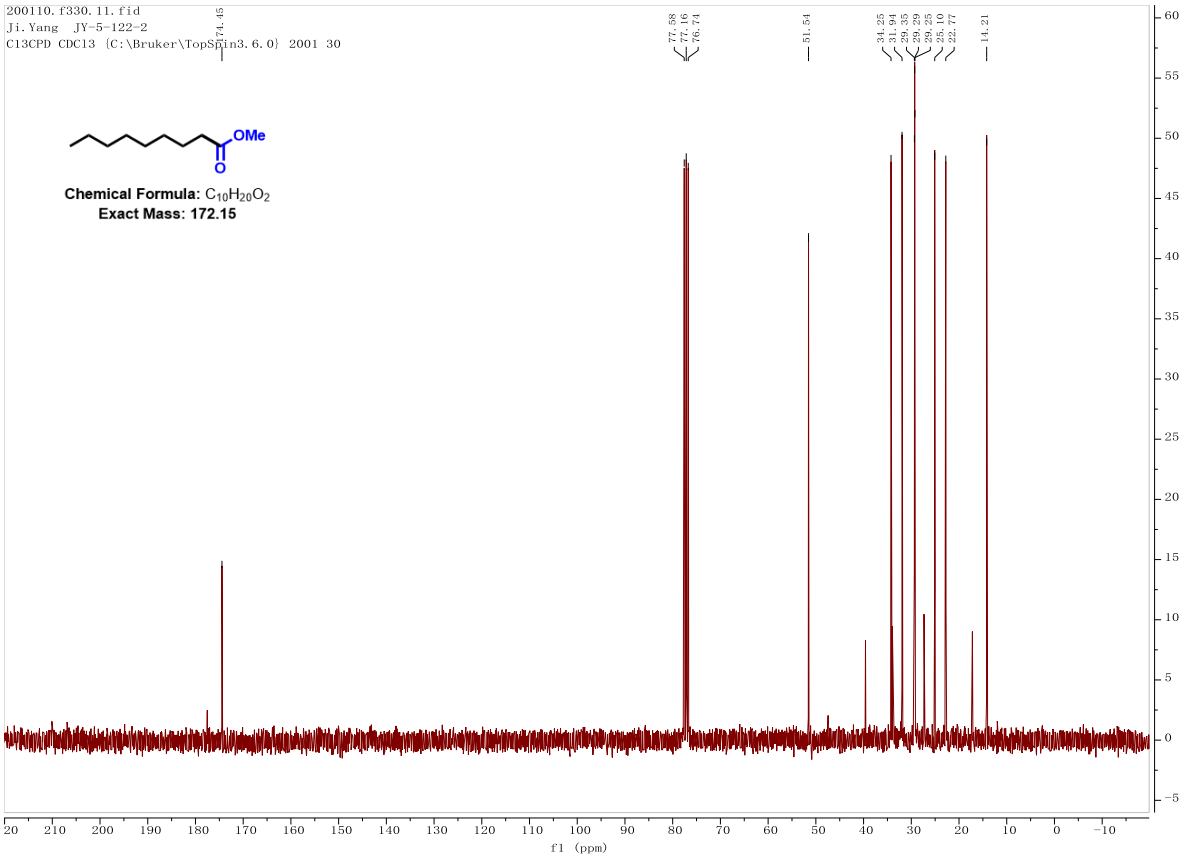
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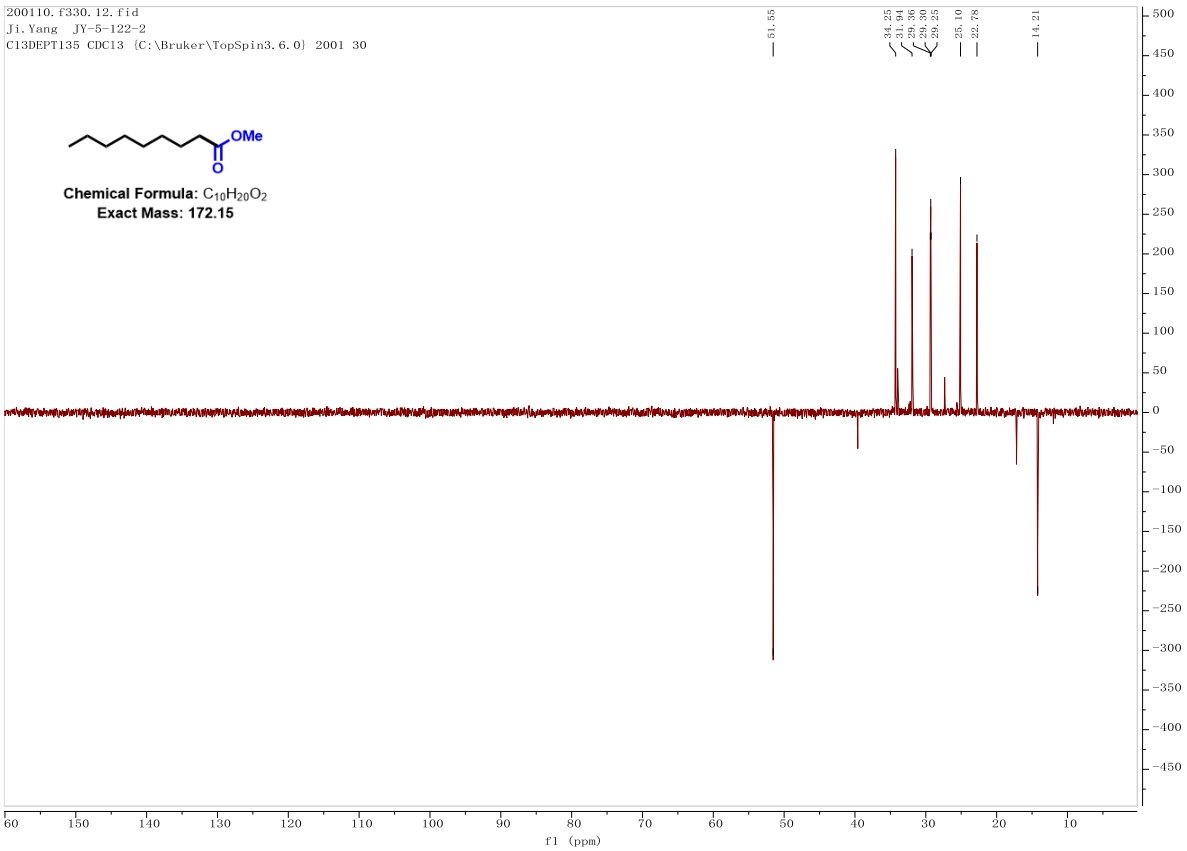
29.25
25.10
22.77
14.21
OMe
O
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)

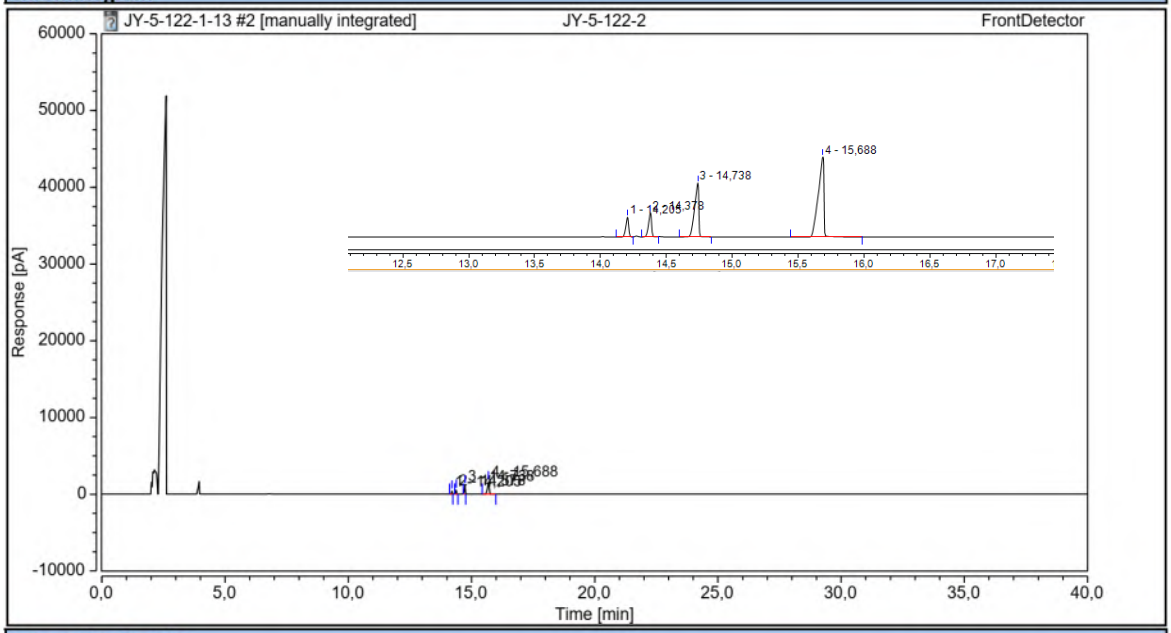

200110.f330.12.fid
Ji.Yang JY-5-122-2
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 30
51.55
34.25
31.94
29.36
29.30
29.25
25.10
22.78
14.21
OMe
O
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-2**	*Run Time (min):*	**40,00**
Vial Number:	**62**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 16:24**	*Sample Weight:*	**1,0000**

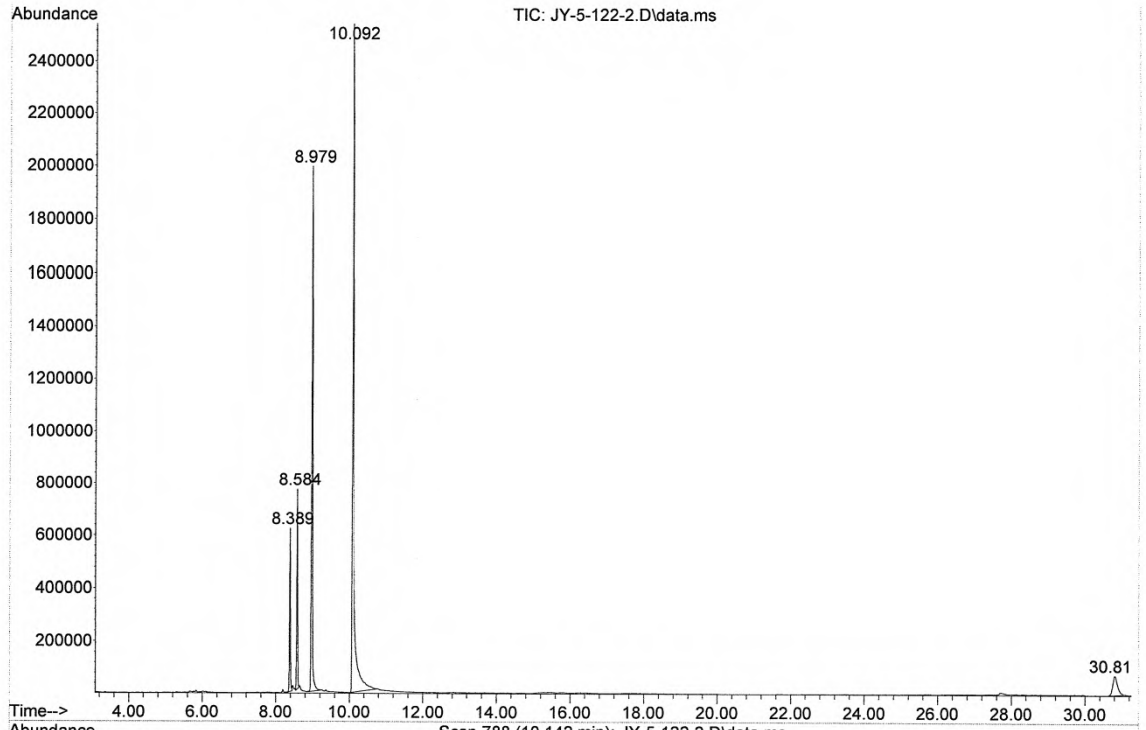
Chromatogram

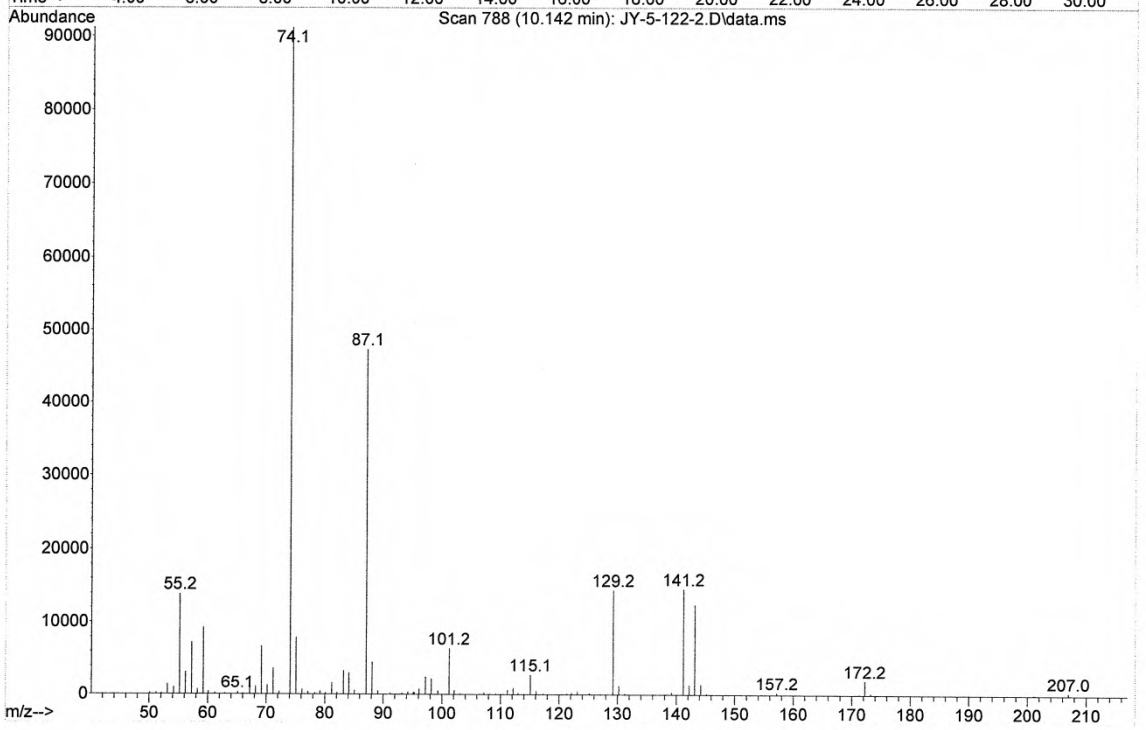


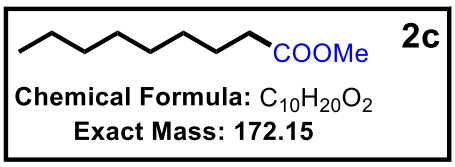
Integration Results

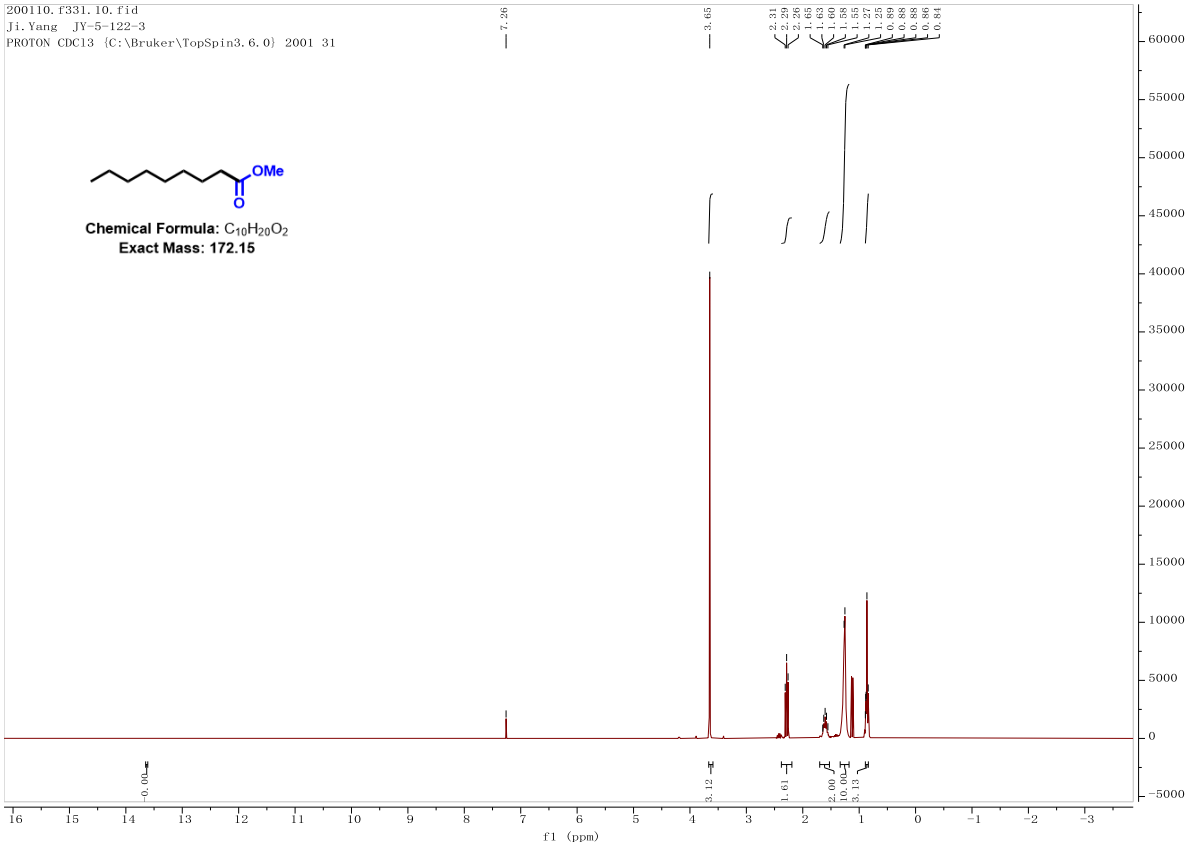
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,205	9,933	402,636	6,97	11,19	n.a.
2		14,378	12,442	486,257	8,73	13,51	n.a.
3		14,738	39,244	1087,904	27,54	30,22	n.a.
4		15,688	80,895	1622,894	56,76	45,08	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**142,514**	**3599,691**	**100,00**	**100,00**	

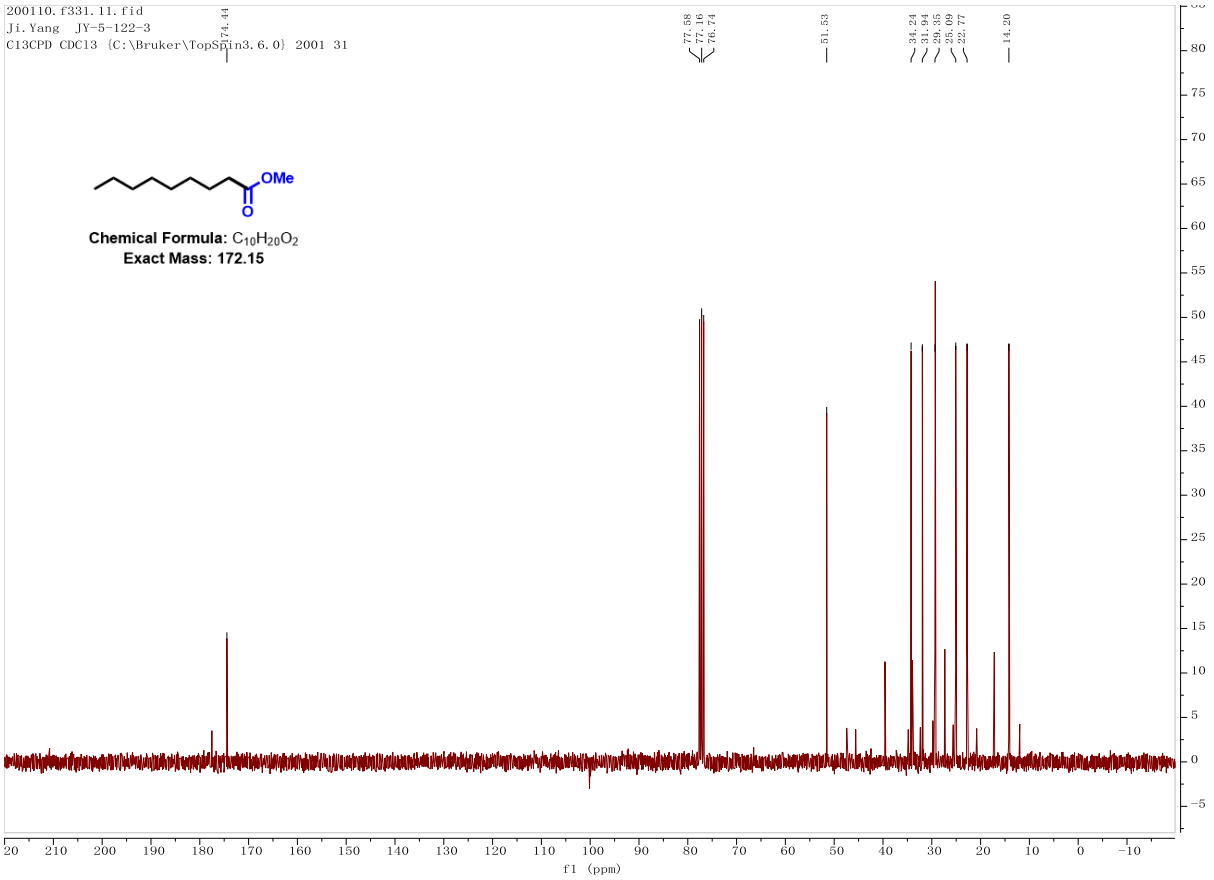
File :D:\MSDChem\1\DATA\2001\JY-5-122-2.D
Operator :
Acquired : 9 Jan 2020 15:47 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-2
Misc Info :
Vial Number: 37

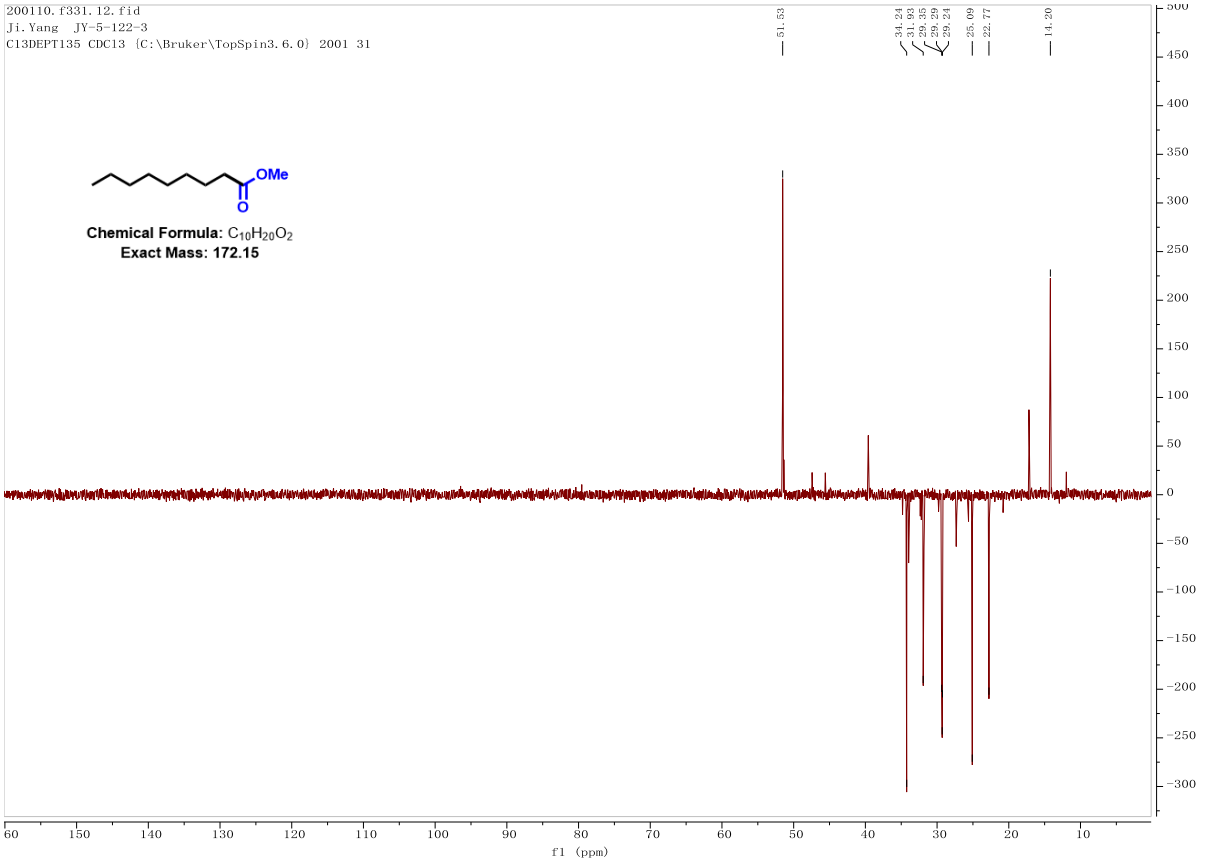





COOMe
2c
Chemical Formula: C10H20O2
Exact Mass: 172.15


200110.f331.10.fid
Ji.Yang JY-5-122-3
PROTON CDC13 {C:\Bruker\TopSpin3.6.0} 2001 31
OMe
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)


200110.f331.11.fid
Ji.Yang JY-5-122-3
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 31
174.44
77.58
77.16
76.74
51.53
34.24
31.94
29.35
25.09
22.77
14.20
OMe
O
Chemical Formula: $C_{10}H_{20}O_2$
Exact Mass: 172.15
f1 (ppm)

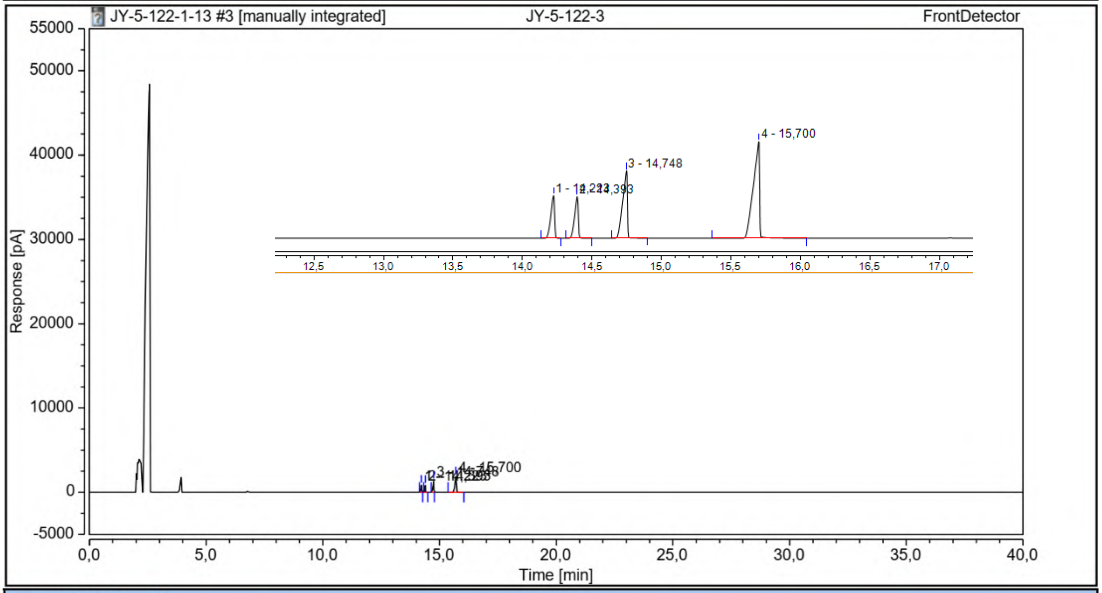

200110.f331.12.fid
Ji.Yang JY-5-122-3
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 31
51.53
34.24
31.93
29.35
29.29
29.24
25.09
22.77
14.20
OMe
O
Chemical Formula: $C_{10}H_{20}O_2$
Exact Mass: 172.15
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-3**	*Run Time (min):*	**40,00**
Vial Number:	**63**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 17:25**	*Sample Weight:*	**1,0000**

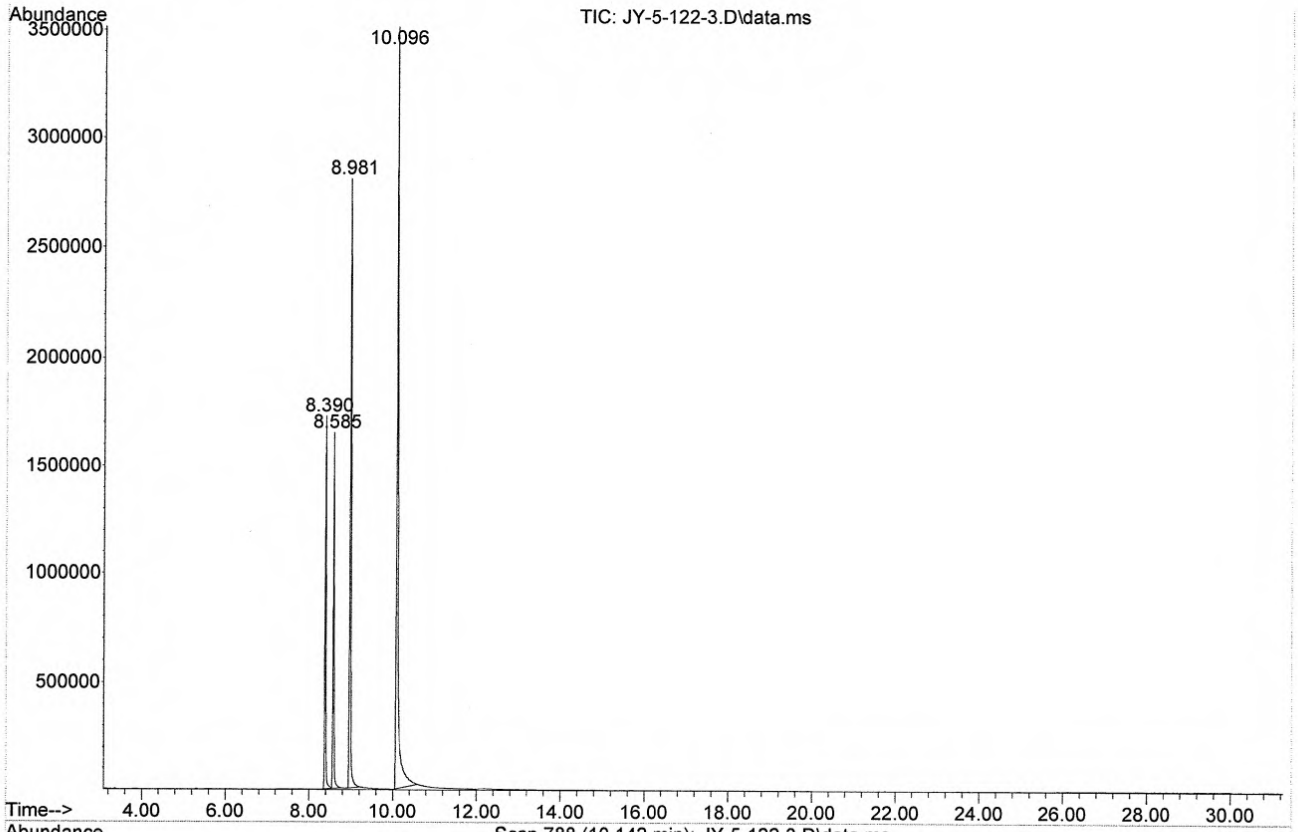
Chromatogram

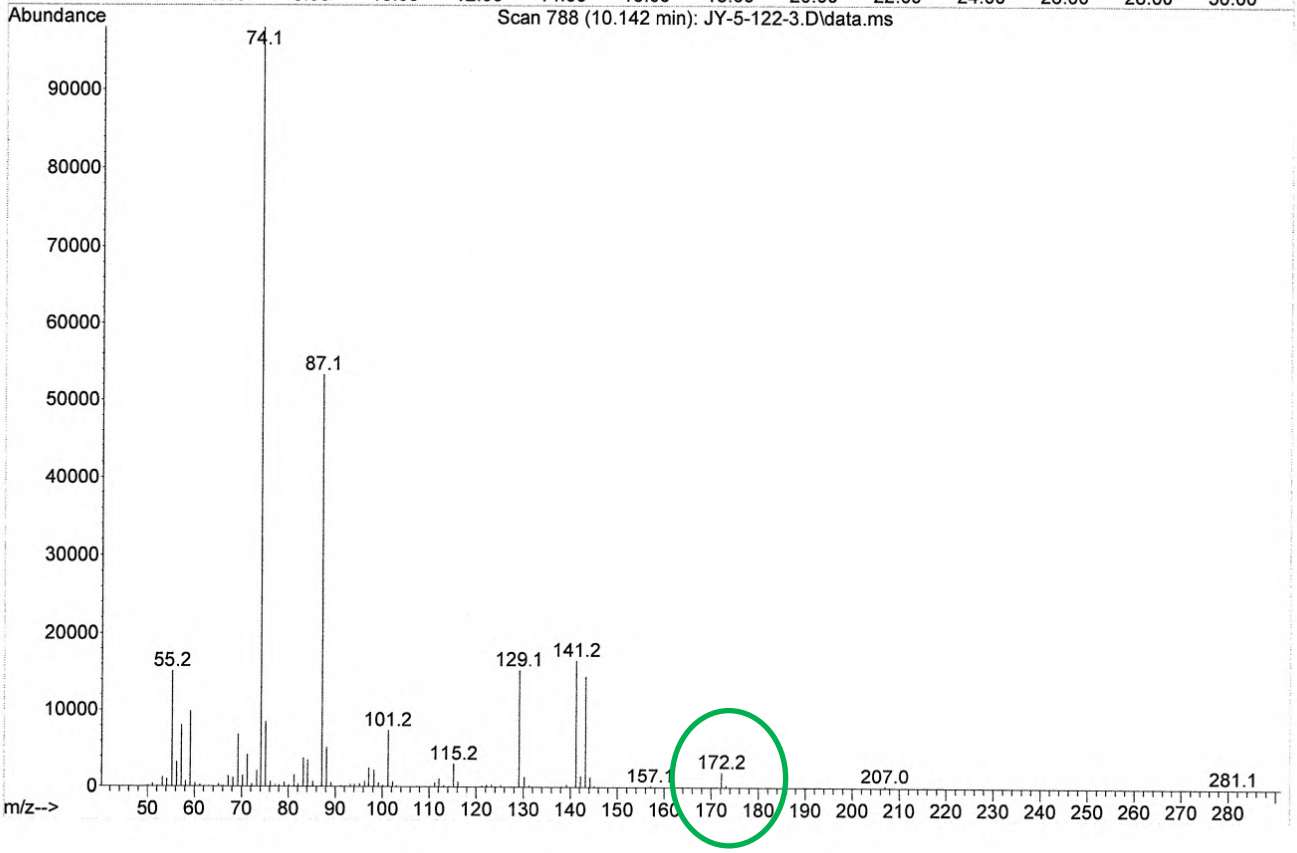


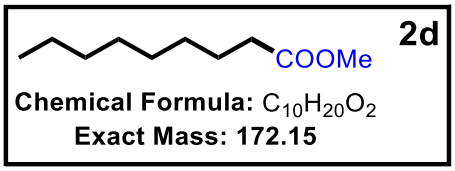
Integration Results

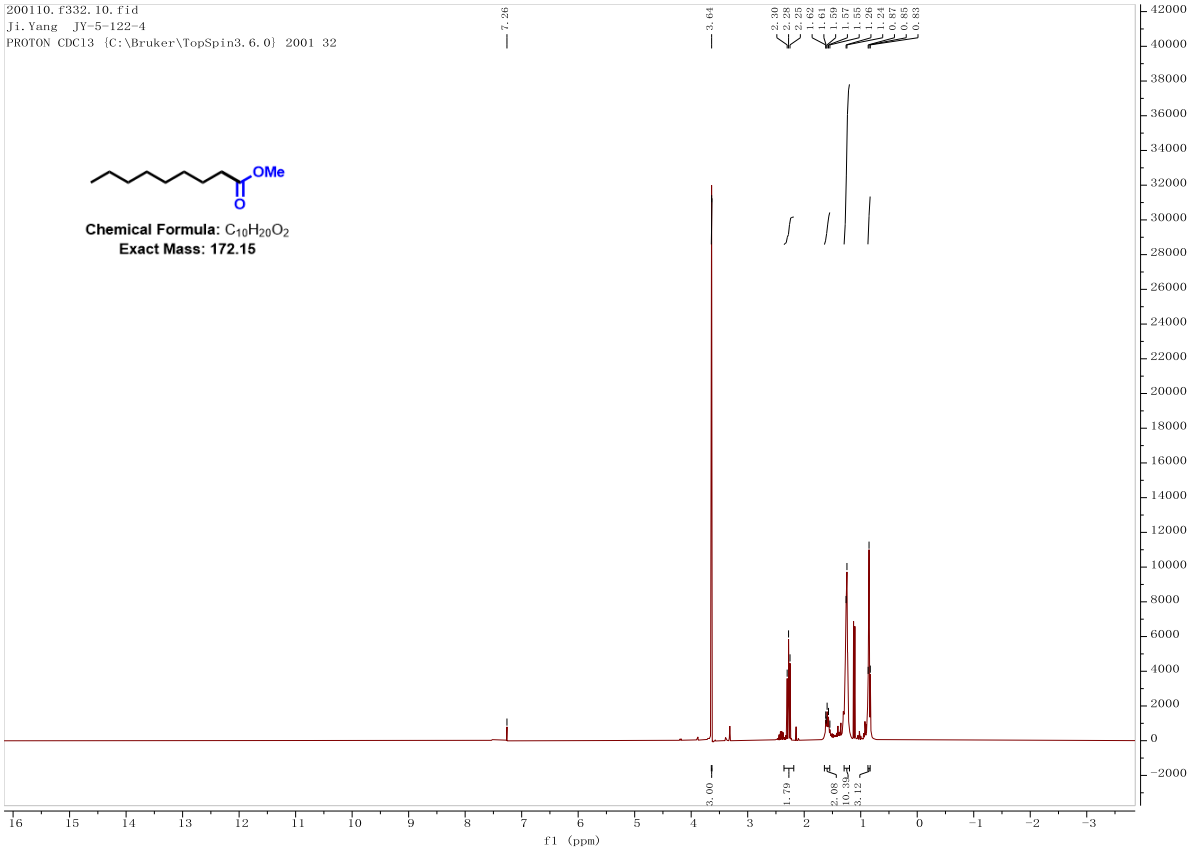
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,223	25,427	819,360	12,95	17,19	n.a.
2		14,393	24,045	797,381	12,25	16,73	n.a.
3		14,748	49,991	1293,989	25,47	27,15	n.a.
4		15,700	96,828	1856,073	49,33	38,94	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**196,291**	**4766,803**	**100,00**	**100,00**	

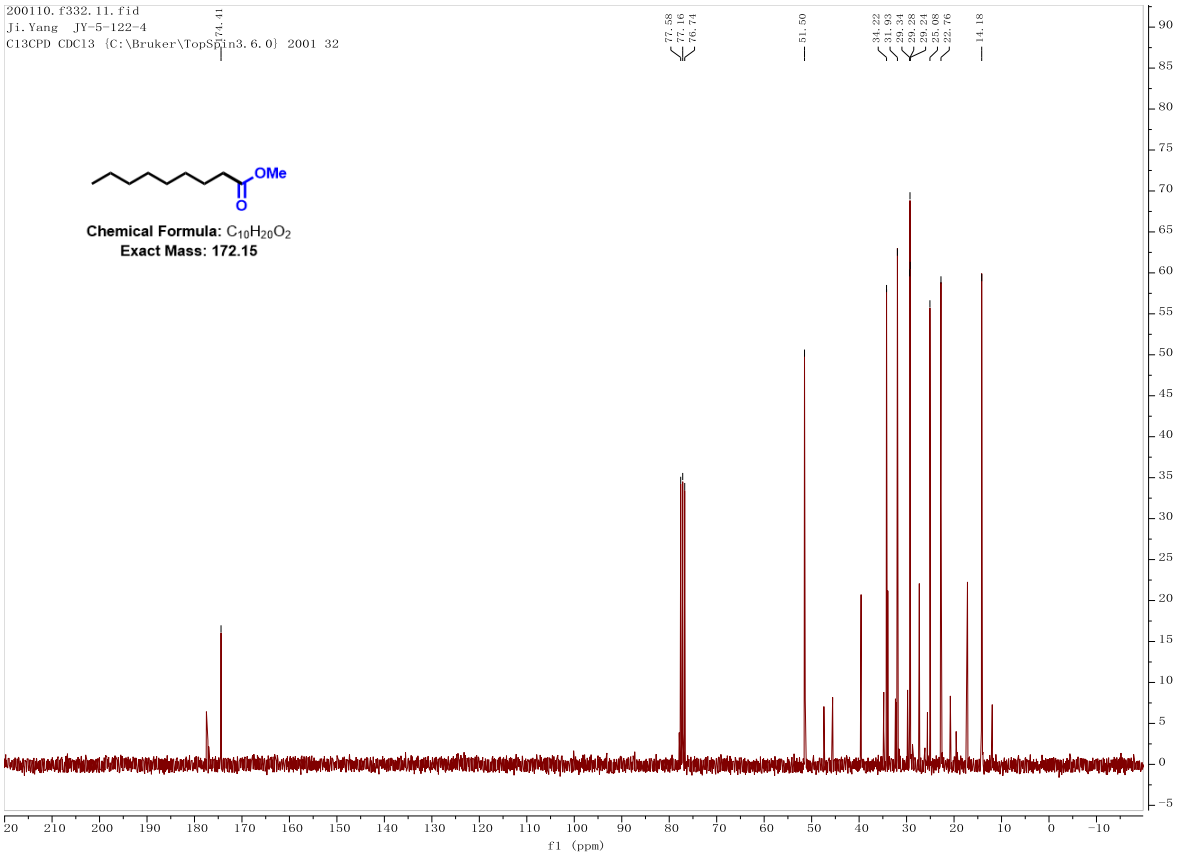
File :D:\MSDChem\1\DATA\2001\JY-5-122-3.D
Operator :
Acquired : 9 Jan 2020 16:26 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-3
Misc Info :
Vial Number: 38

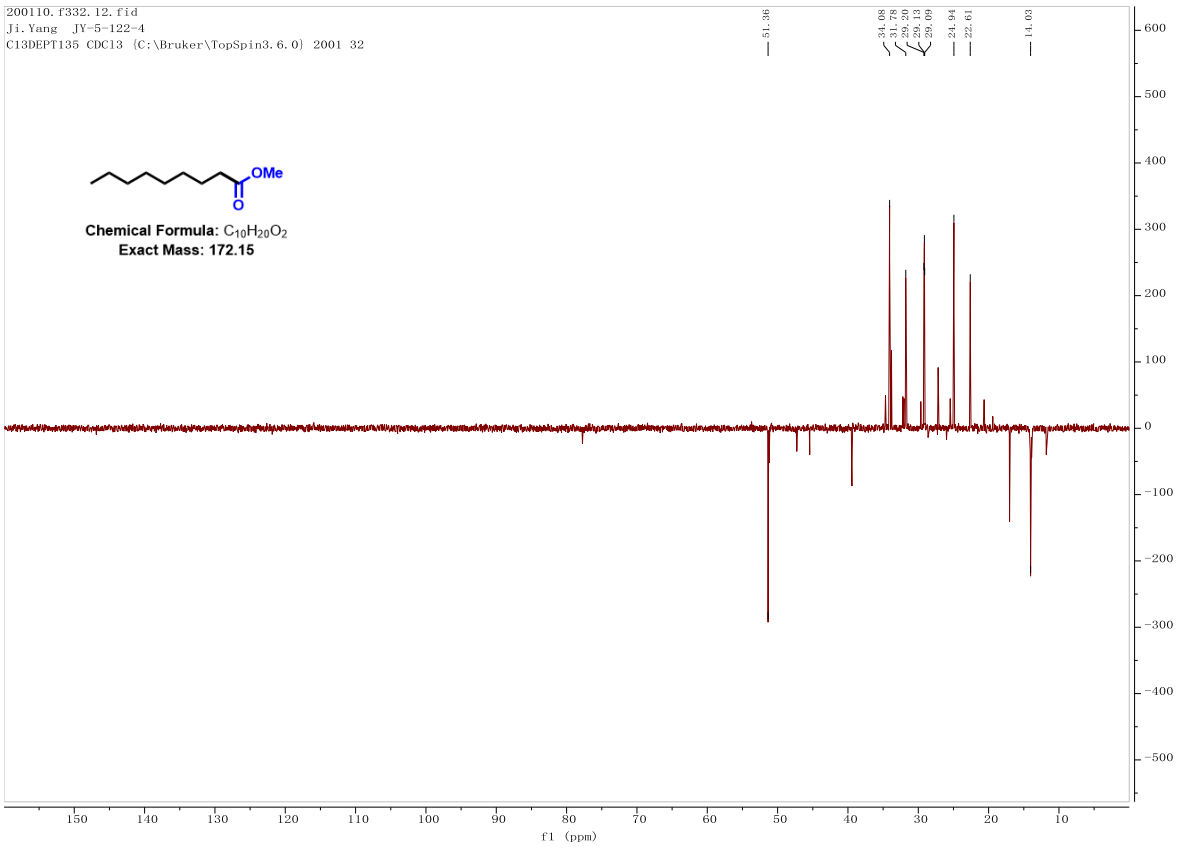





COOMe
2d
Chemical Formula: C10H20O2
Exact Mass: 172.15


200110.f332.10.fid
Ji.Yang JY-5-122-4
PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 32
OMe
O
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)


200110.f332.11.fid
Ji.Yang JY-5-122-4
C13CPD CDC13 {C:\Bruker\TopSpin3.6.0} 2001 32
174.41
77.58
77.16
76.74
51.50
34.22
31.93
29.34
29.28
29.24
25.08
22.76
14.18
OMe
O
Chemical Formula: $C_{10}H_{20}O_2$
Exact Mass: 172.15
f1 (ppm)

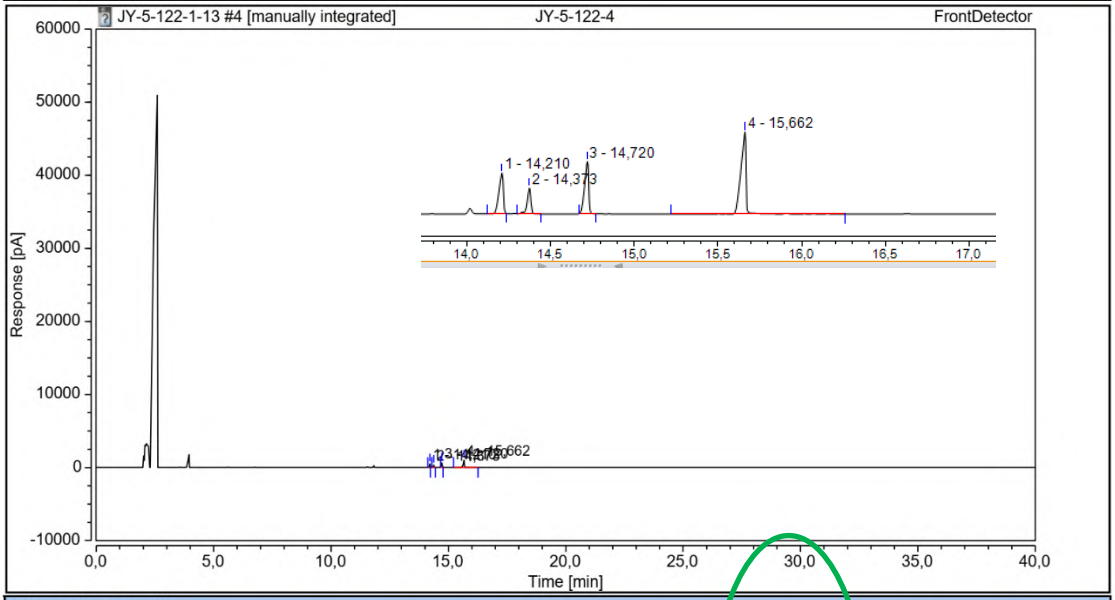

200110.f332.12.fid
Ji.Yang JY-5-122-4
C13DEPT135 CDC13 {C:\Bruker\TopSpin3.6.0} 2001 32
51.36
34.08
31.78
29.30
29.13
29.09
24.94
22.61
14.03
OMe
O
Chemical Formula: $C_{10}H_{20}O_2$
Exact Mass: 172.15
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-4**	*Run Time (min):*	**40,00**
Vial Number:	**64**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 18:27**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,210	14,769	488,239	19,40	20,26	n.a.
2		14,373	7,810	309,592	10,26	12,85	n.a.
3		14,720	17,556	627,524	23,06	26,04	n.a.
4		15,662	35,984	984,437	47,27	40,85	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**76,119**	**2409,792**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-4.D
Operator   :
Acquired   :  9 Jan 2020  17:05     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-4
Misc Info  :
Vial Number: 39
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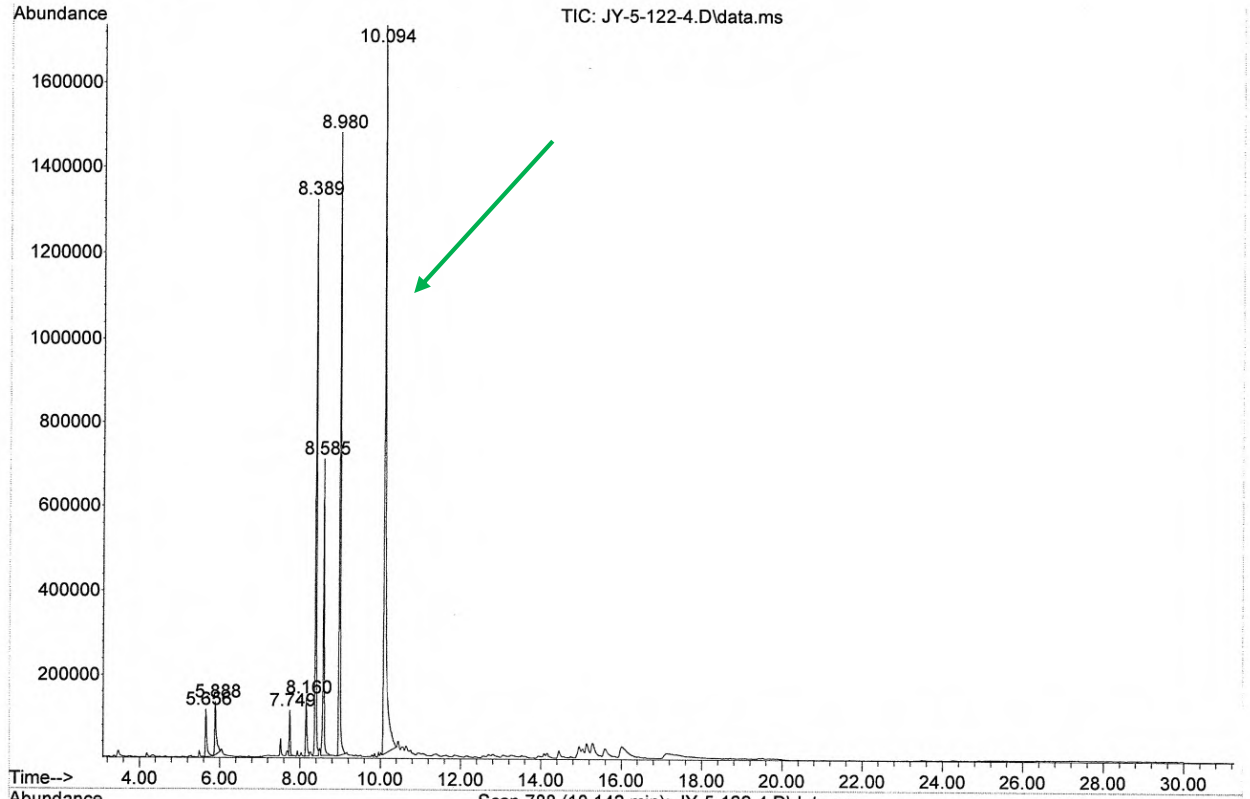
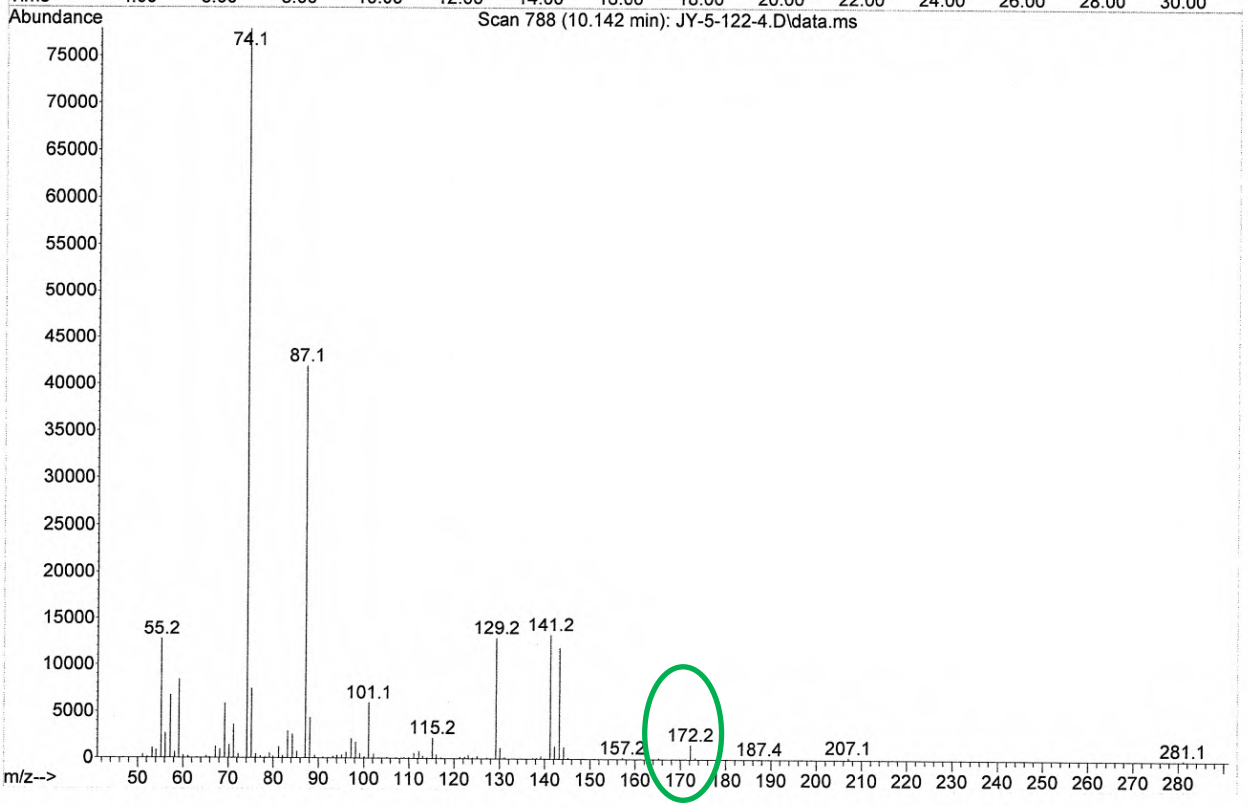
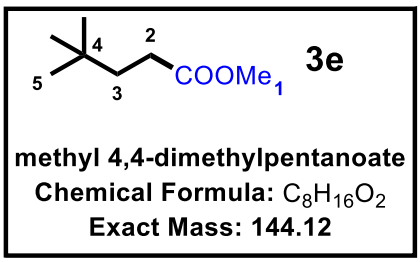
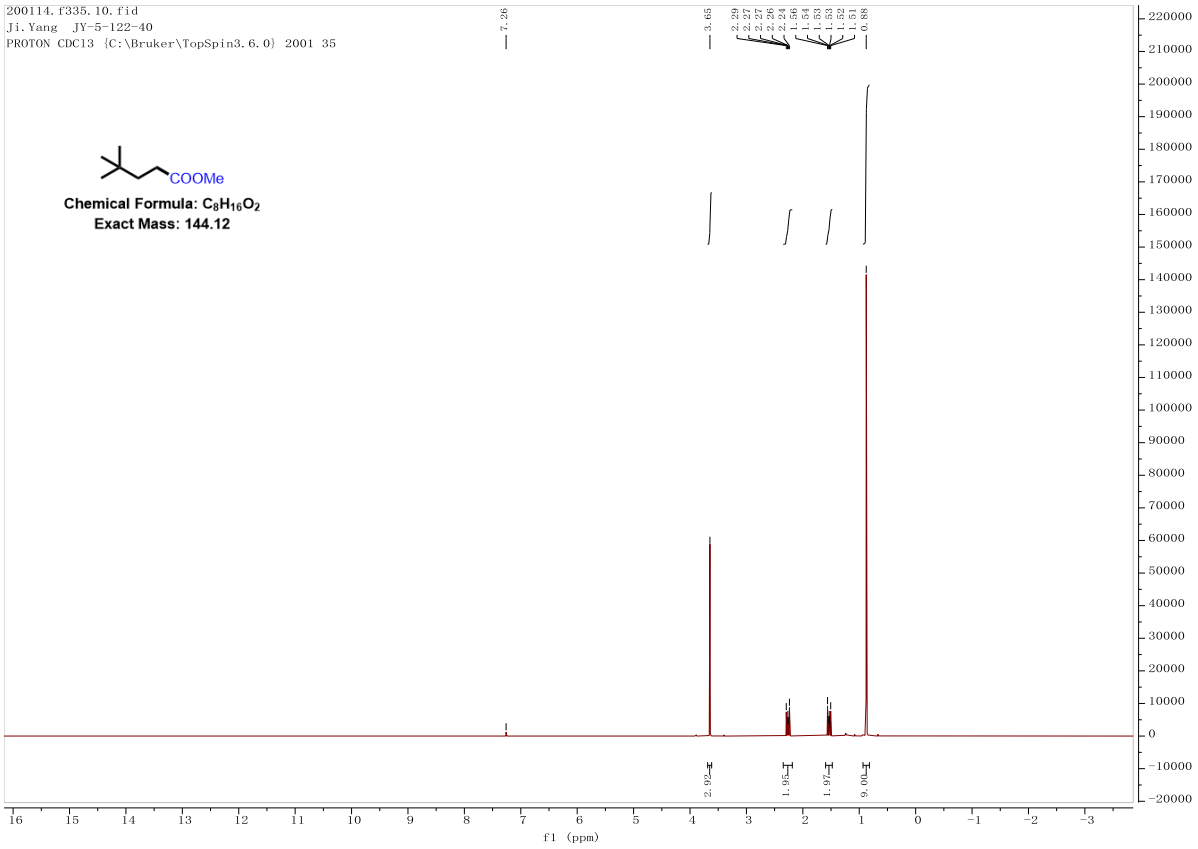


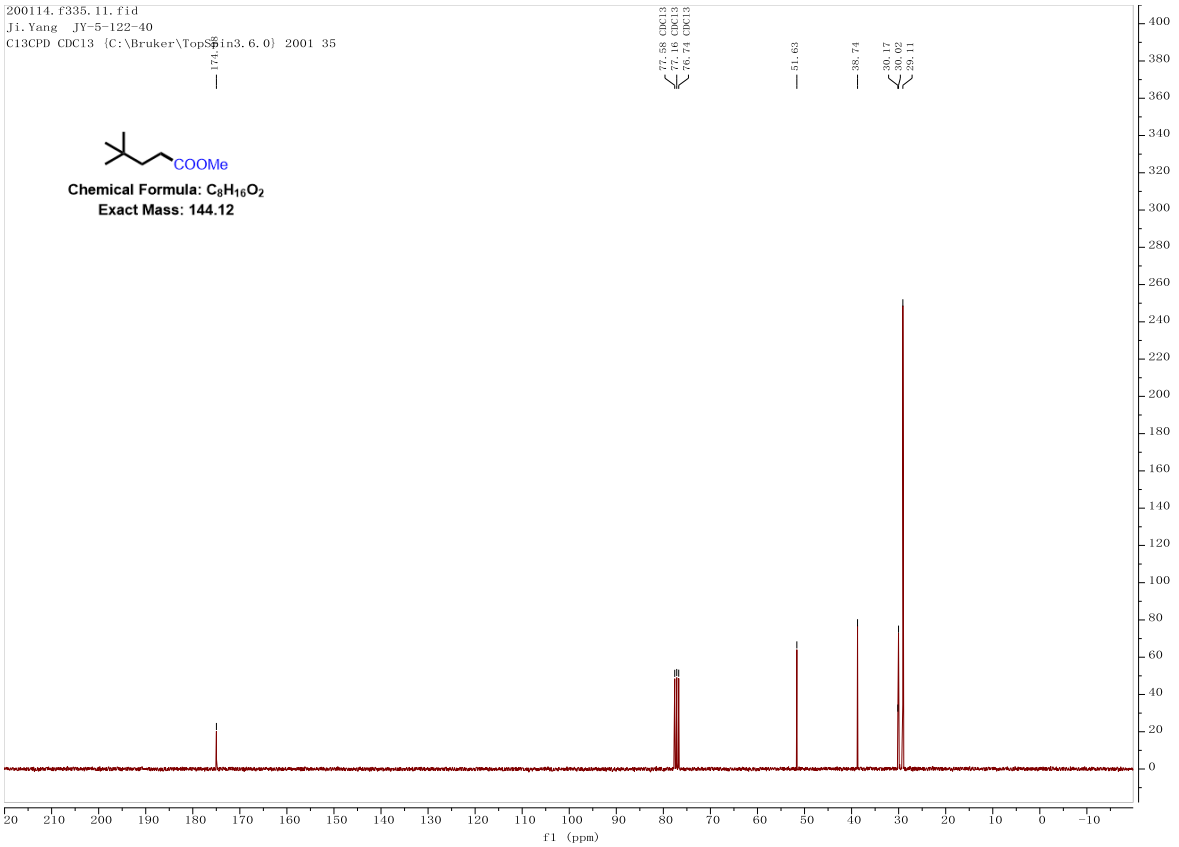




3e

methyl 4,4-dimethylpentanoate
Chemical Formula: $C_8H_{16}O_2$
Exact Mass: 144.12

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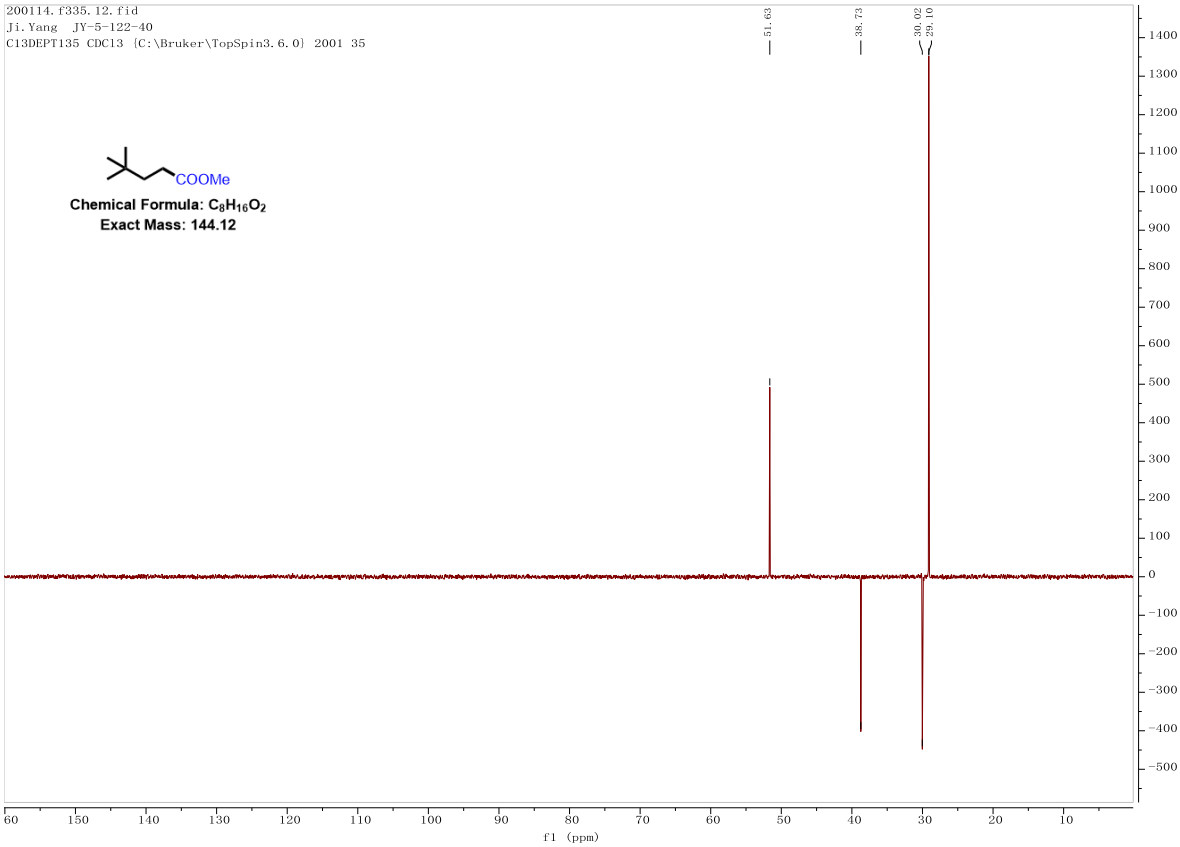
Ji.Yang JY-5-122-40
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 35
174.56
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
51.63
38.74
30.17
30.02
29.11
COOMe
Chemical Formula: C8H16O2
Exact Mass: 144.12
f1 (ppm)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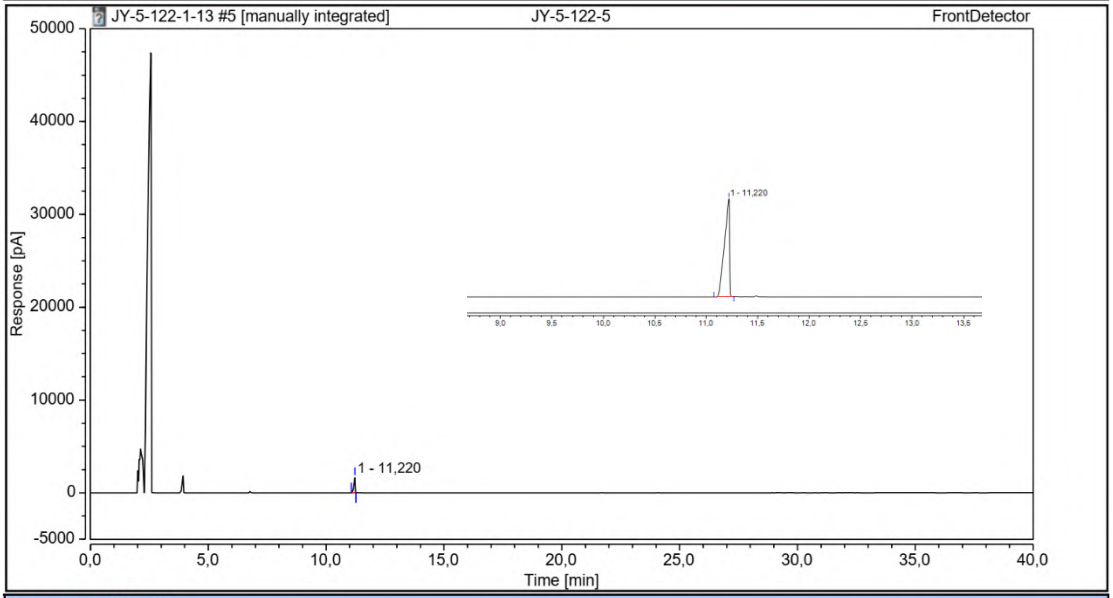
Ji.Yang JY-5-122-40
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 35
51.63
38.73
30.02
29.10
COOMe
Chemical Formula: C8H16O2
Exact Mass: 144.12
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-5**	*Run Time (min):*	**40,00**
Vial Number:	**65**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 19:29**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		11,220	92,026	1617,879	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**92,026**	**1617,879**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-5.D
Operator   :
Acquired   :  9 Jan 2020  17:44     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-5
Misc Info  :
Vial Number: 40
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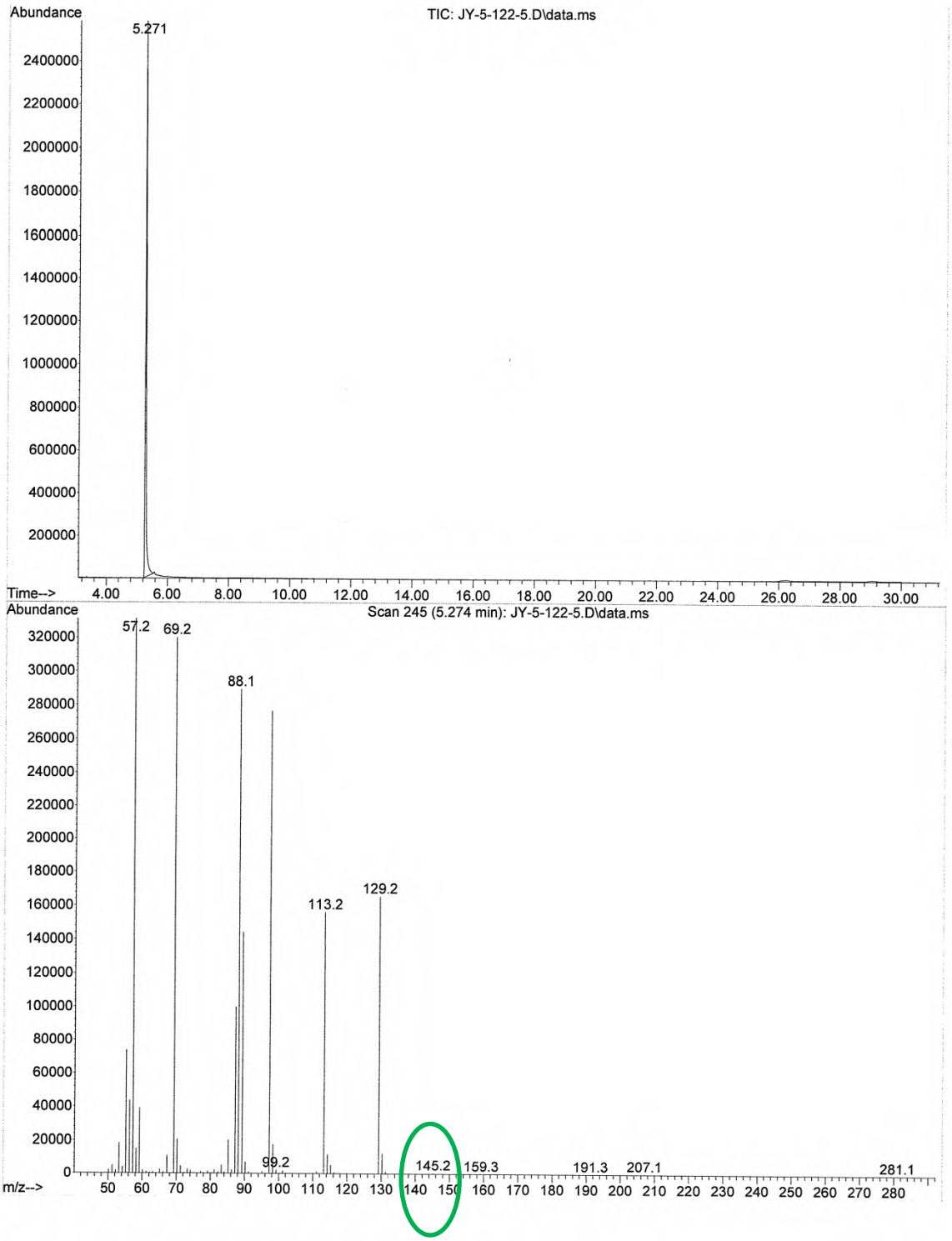
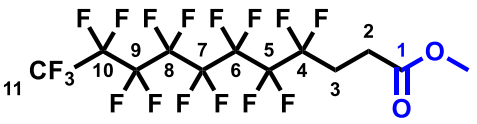


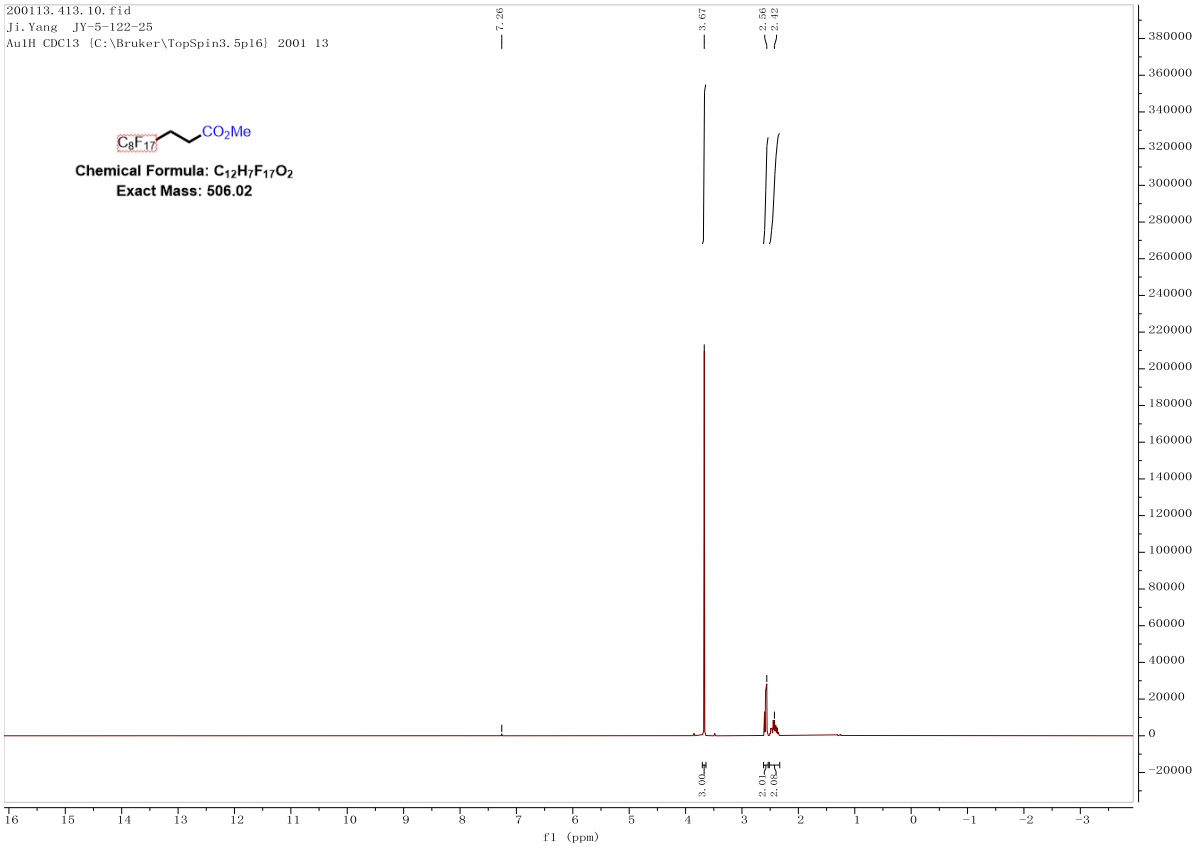


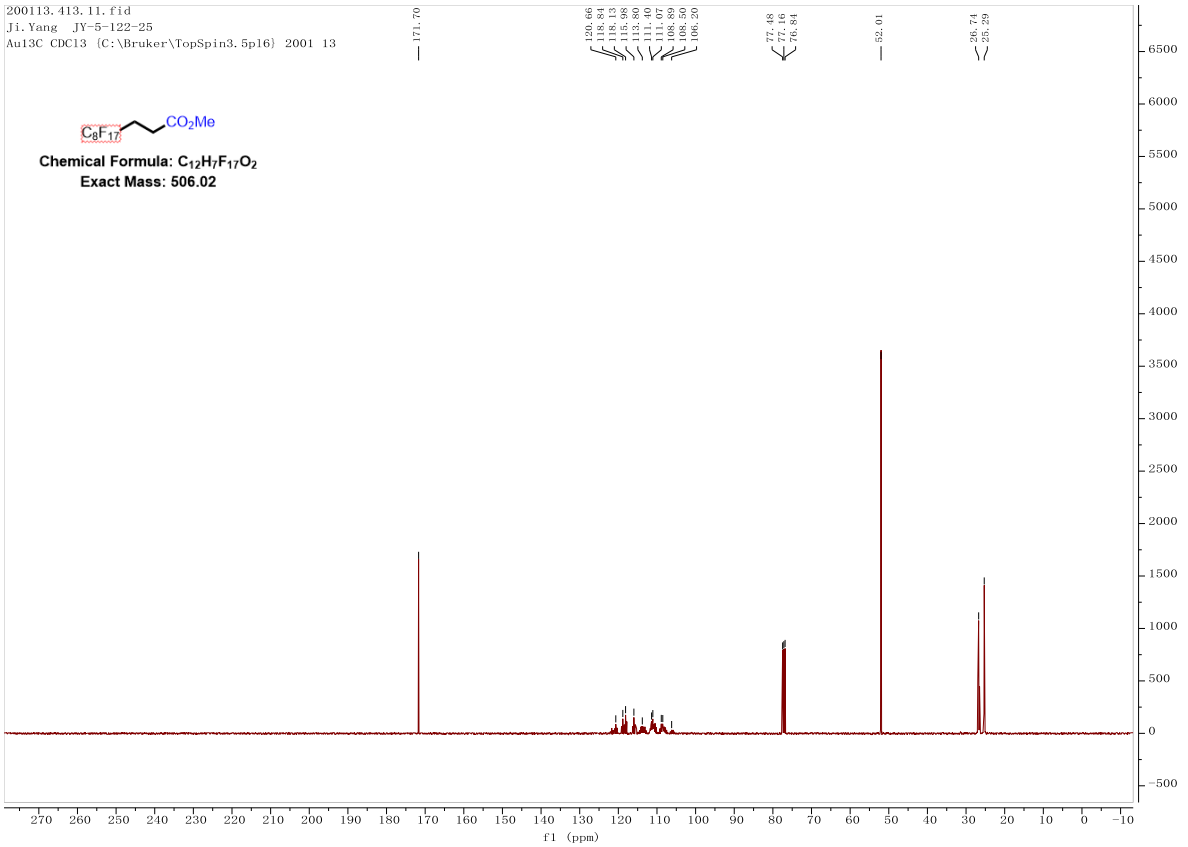
3f

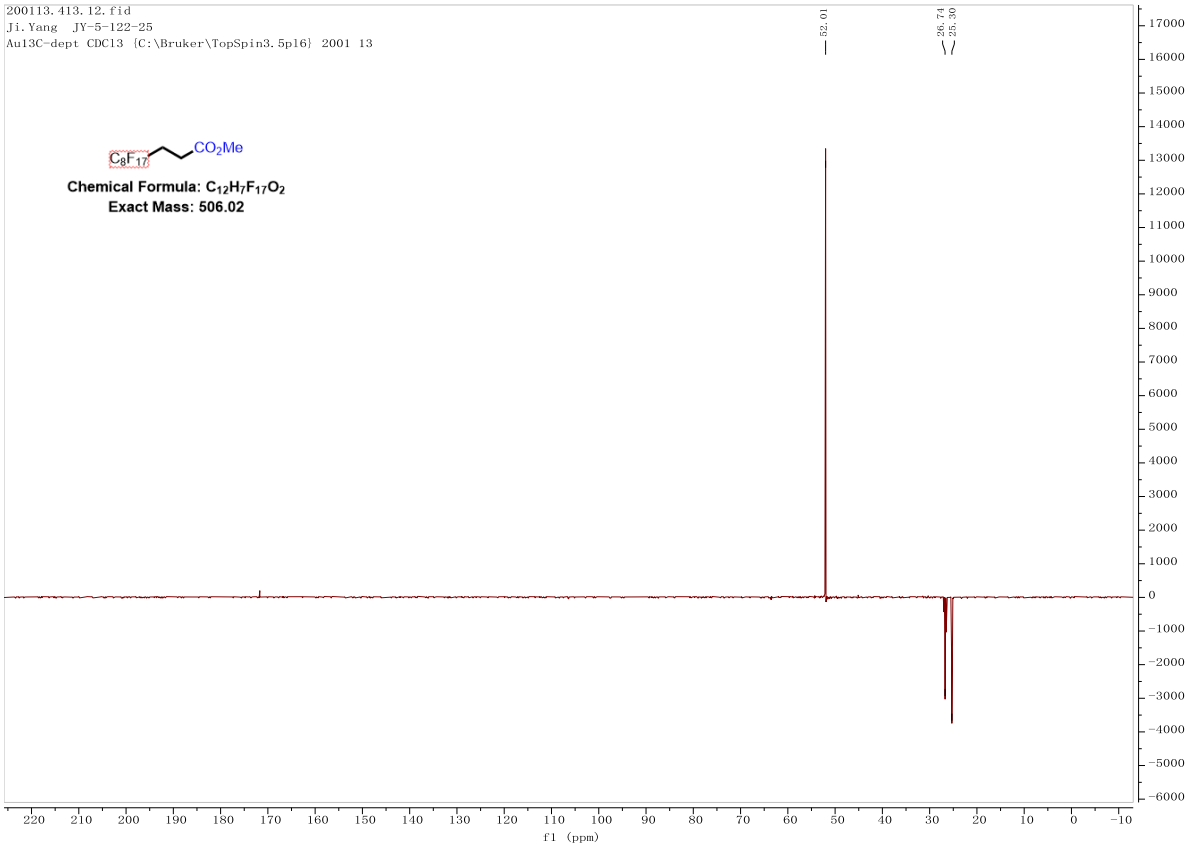
methyl 4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecanoate

Chemical Formula: $C_{12}H_7F_{17}O_2$

Exact Mass: 506.02




200113.413.11.fid
Ji.Yang JY-5-122-25
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 13
171.70
120.66
118.84
118.13
115.98
113.80
111.40
111.07
108.89
108.50
106.20
77.48
77.16
76.84
52.01
26.74
25.29
C8F17
CO2Me
Chemical Formula: C12H7F17O2
Exact Mass: 506.02
f1 (ppm)

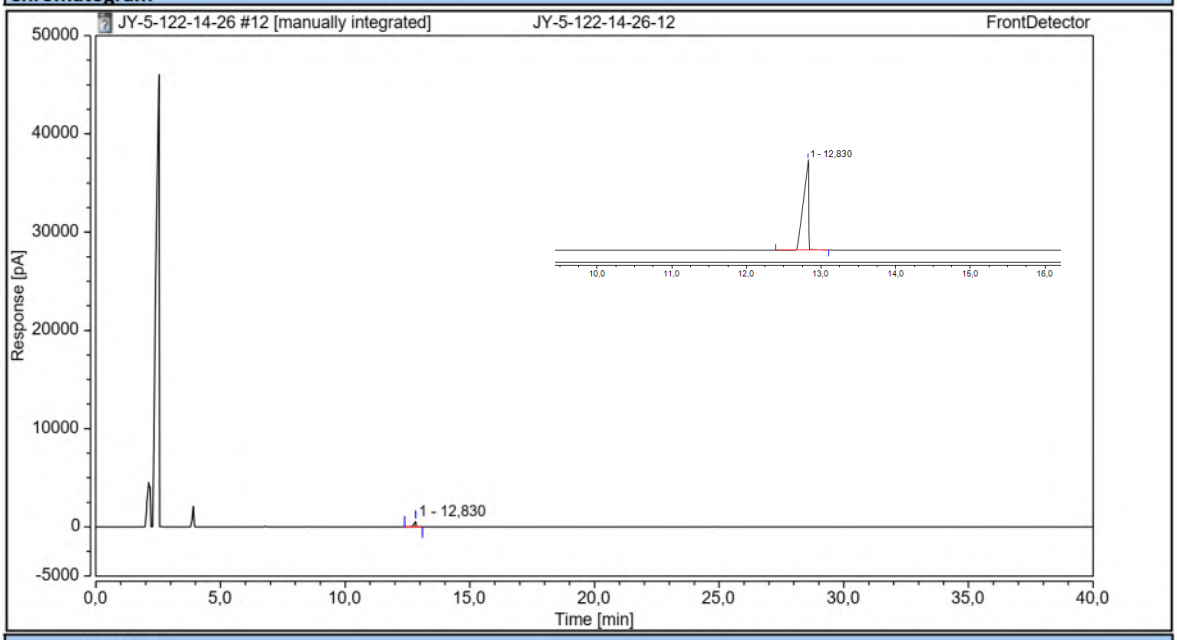

200113.413.12.fid
Ji.Yang JY-5-122-25
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 13
52.01
26.74
25.30
C8F17
CO2Me
Chemical Formula: C12H7F17O2
Exact Mass: 506.02
f1 (ppm)

Chromatogram and Results

Injection Details

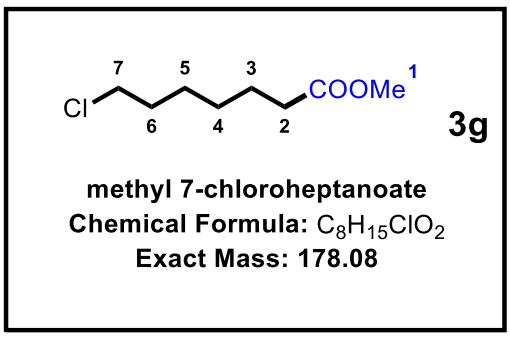
Injection Name:	**JY-5-122-14-26-12**	*Run Time (min):*	**40,00**
Vial Number:	**122**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 18:06**	*Sample Weight:*	**1,0000**

Chromatogram

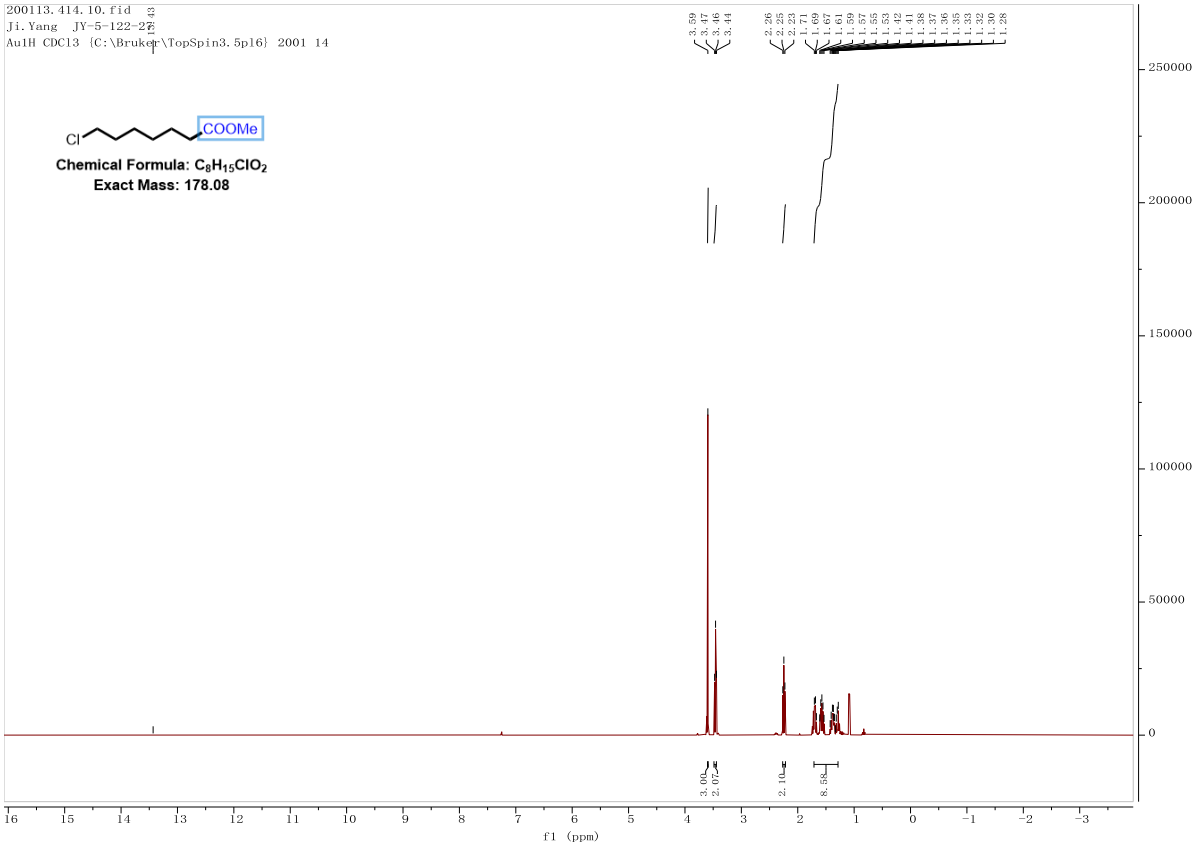


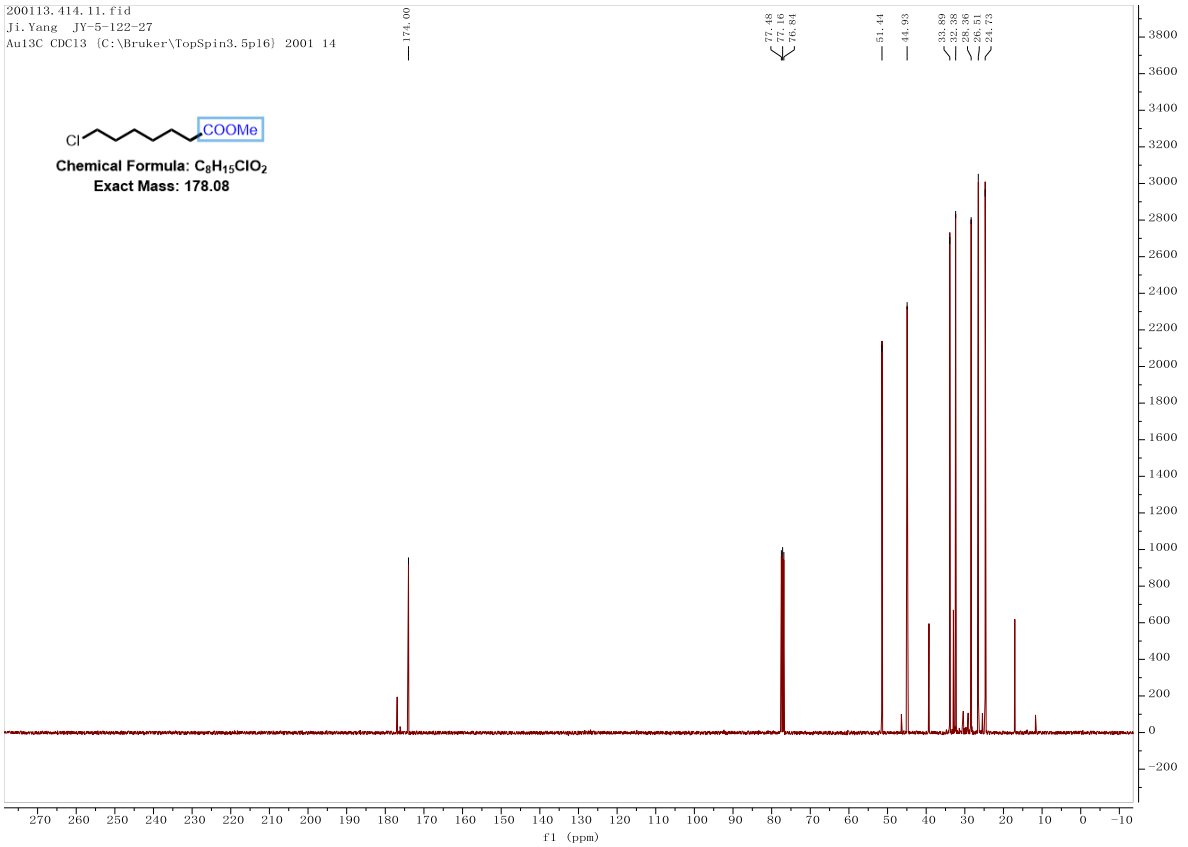
Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		12,830	45,757	565,361	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**45,757**	**565,361**	**100,00**	**100,00**	



methyl 7-chloroheptanoate
Chemical Formula: $C_8H_{15}ClO_2$
Exact Mass: 178.08

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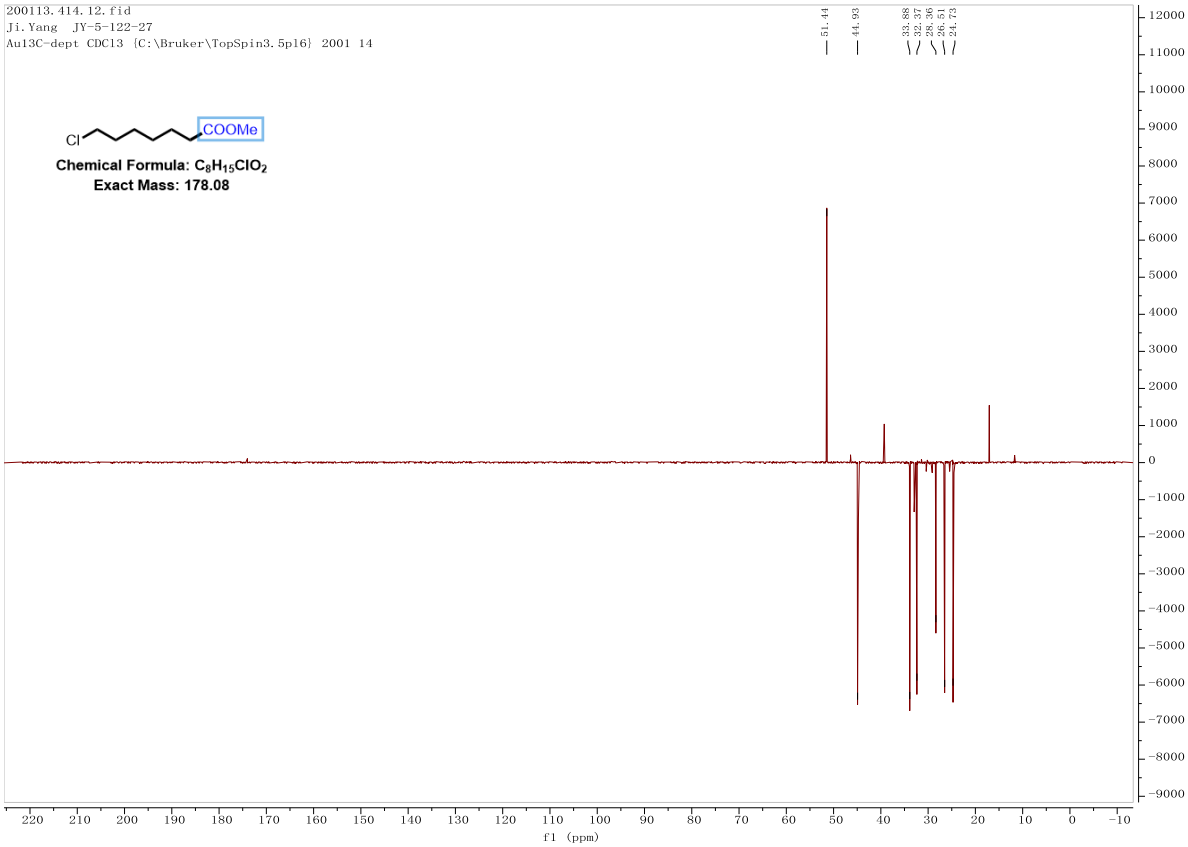
Ji.Yang JY-5-122-27
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 14
174.00
77.48
77.16
76.84
51.44
44.93
33.89
32.38
28.36
26.51
24.73
Cl
COOMe
Chemical Formula: C8H15ClO2
Exact Mass: 178.08
f1 (ppm)

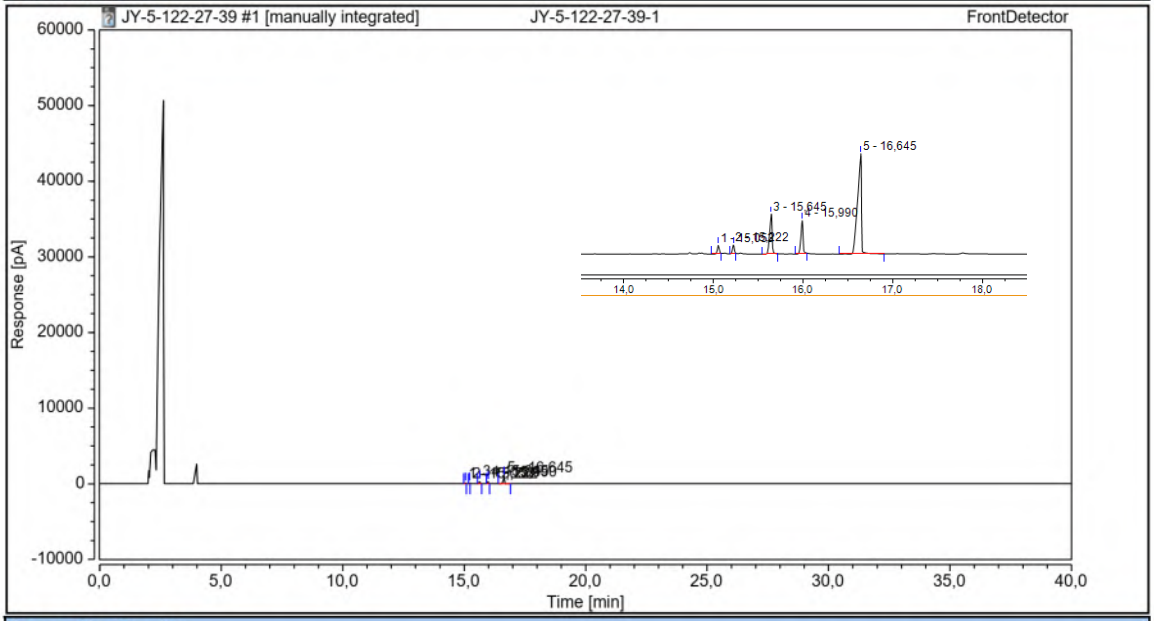

200113.414.12.fid
Ji.Yang JY-5-122-27
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 14
51.44
44.93
33.89
32.37
28.36
26.51
24.73
Cl
COOMe
Chemical Formula: C8H15ClO2
Exact Mass: 178.08
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-1**	*Run Time (min):*	**40,00**
Vial Number:	**25**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 21:31**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		15,053	1,641	74,872	2,46	4,44	n.a.
2		15,222	1,668	75,188	2,50	4,45	n.a.
3		15,645	11,316	354,707	16,99	21,02	n.a.
4		15,990	7,802	291,892	11,72	17,29	n.a.
5		16,645	44,172	891,211	66,33	52,80	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**66,600**	**1687,870**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-27.D
Operator   :
Acquired   : 11 Jan 2020  14:32     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-27
Misc Info  :
Vial Number: 31
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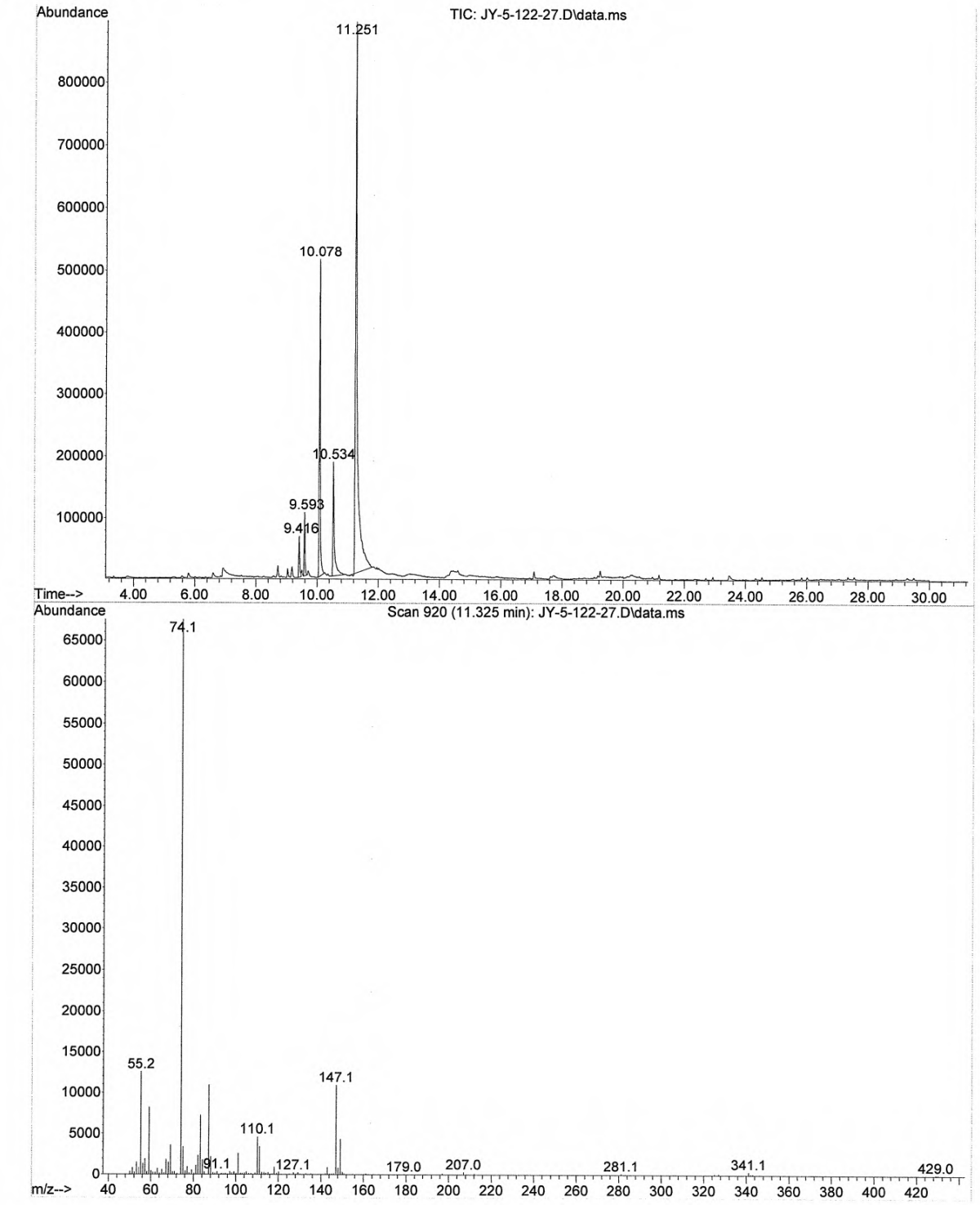
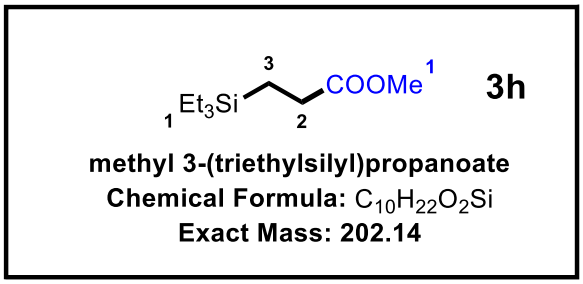
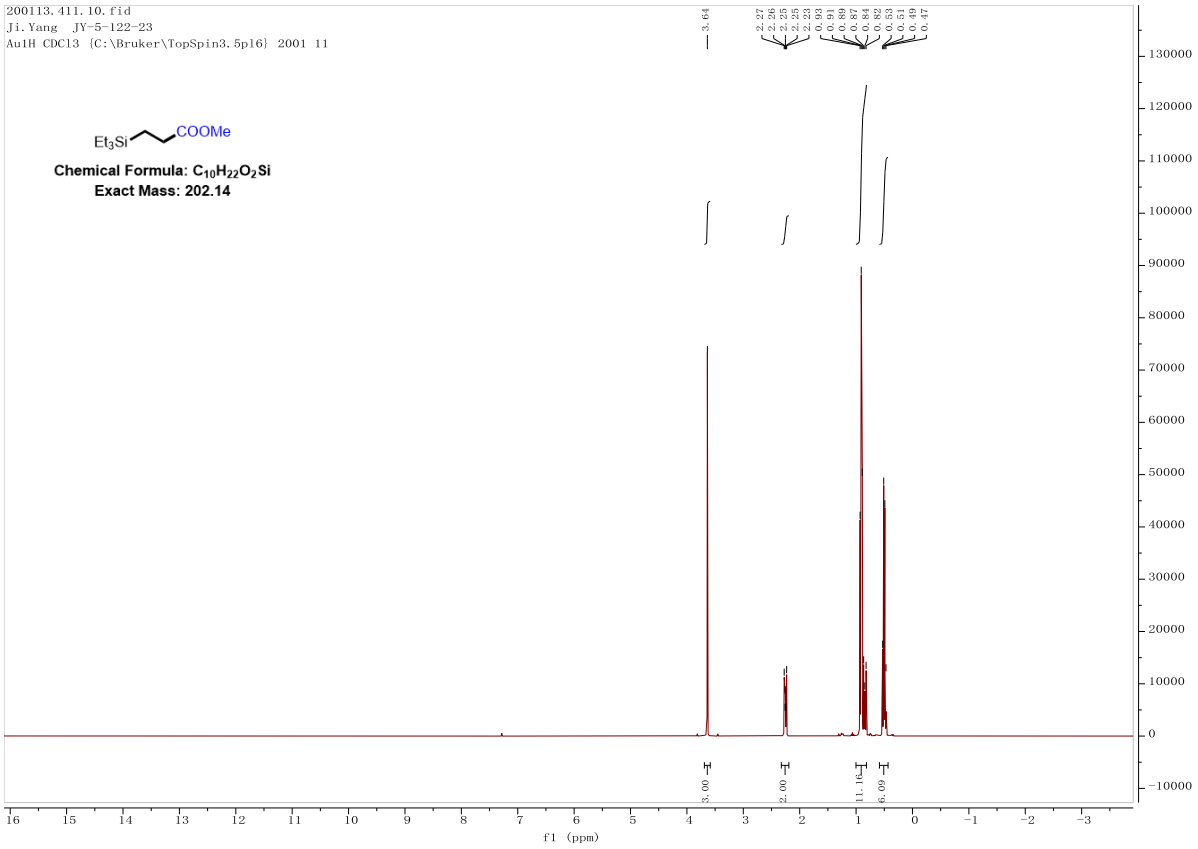
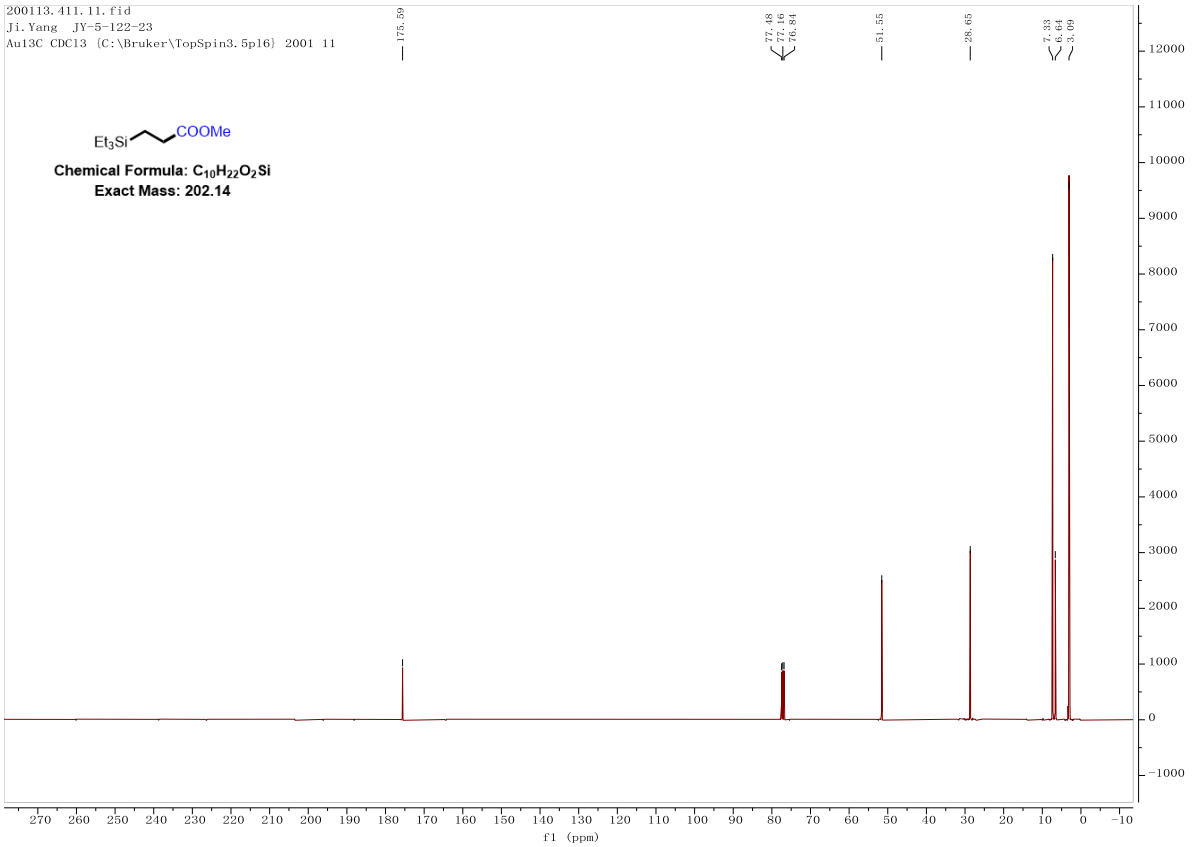




methyl 3-(triethylsilyl)propanoate
Chemical Formula: $C_{10}H_{22}O_2Si$
Exact Mass: 202.14

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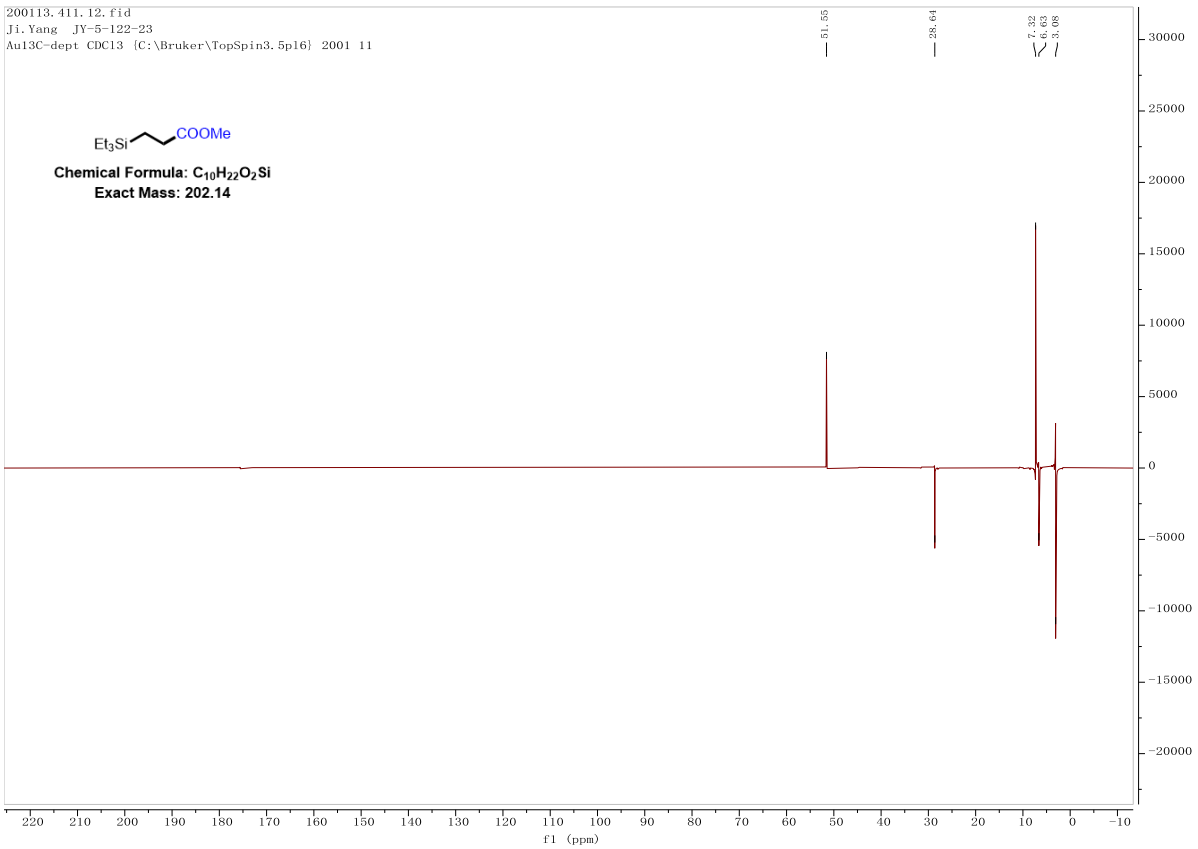
Ji.Yang JY-5-122-23
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 11
175.59
77.48
77.16
76.84
51.55
28.65
7.33
6.64
3.09
Et3Si
COOMe
Chemical Formula: C10H22O2Si
Exact Mass: 202.14
f1 (ppm)

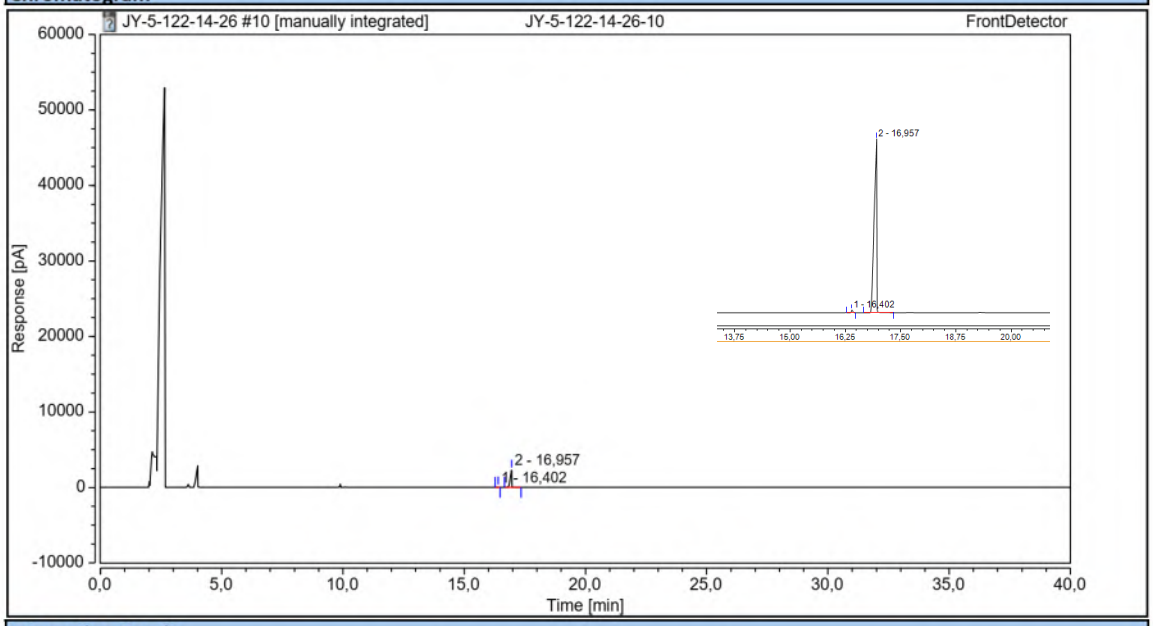

200113.411.12.fid
Ji.Yang JY-5-122-23
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 11
51.55
28.64
7.32
6.63
3.08
Et3Si
COOMe
Chemical Formula: C10H22O2Si
Exact Mass: 202.14
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-14-26-10**	*Run Time (min):*	**40,00**
Vial Number:	**120**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 16:02**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		16,402	1,006	36,134	0,64	1,56	n.a.
2		16,957	155,836	2276,370	99,36	98,44	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**156,842**	**2312,504**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-23.D
Operator   :
Acquired   : 10 Jan 2020  16:58     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-23
Misc Info  :
Vial Number: 45
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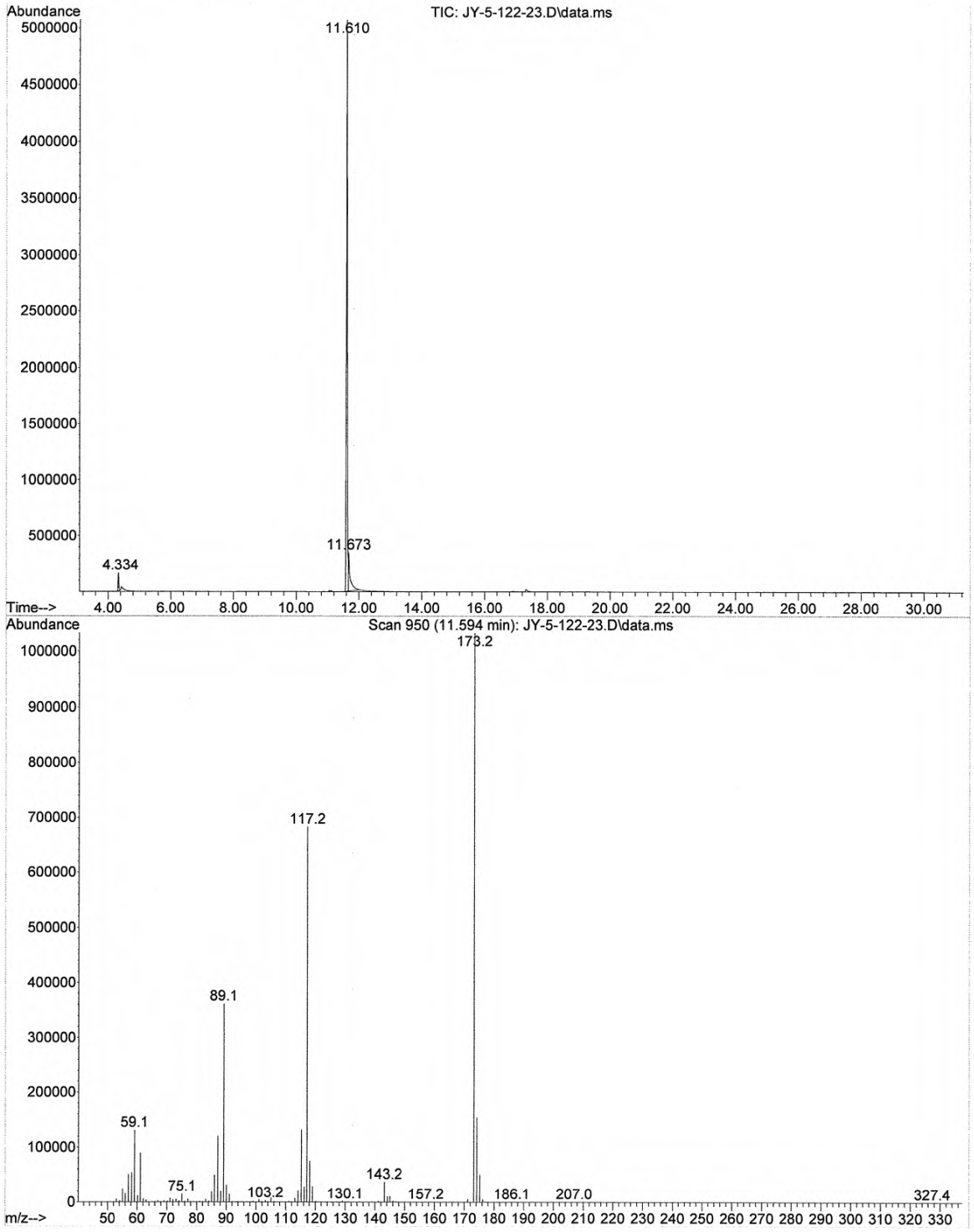
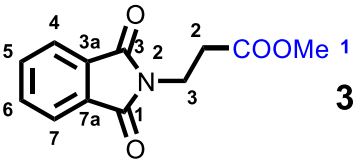


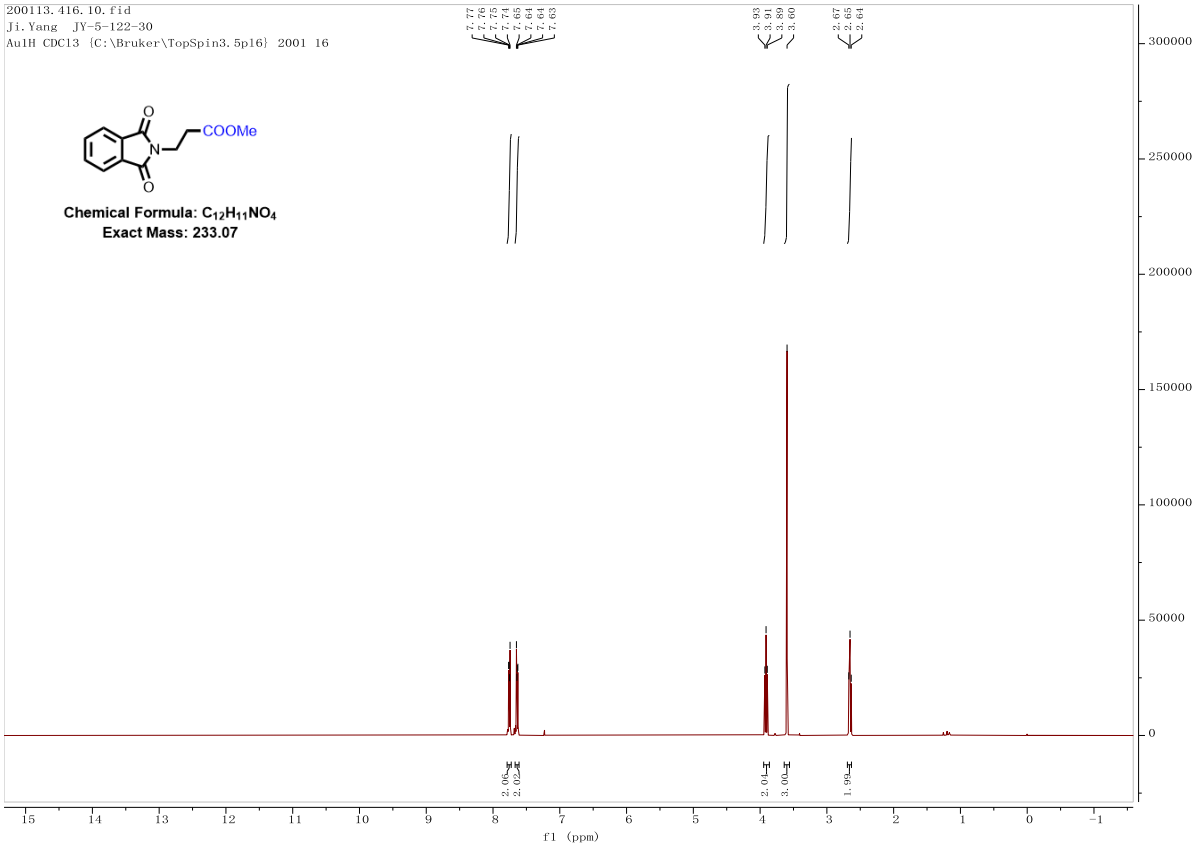


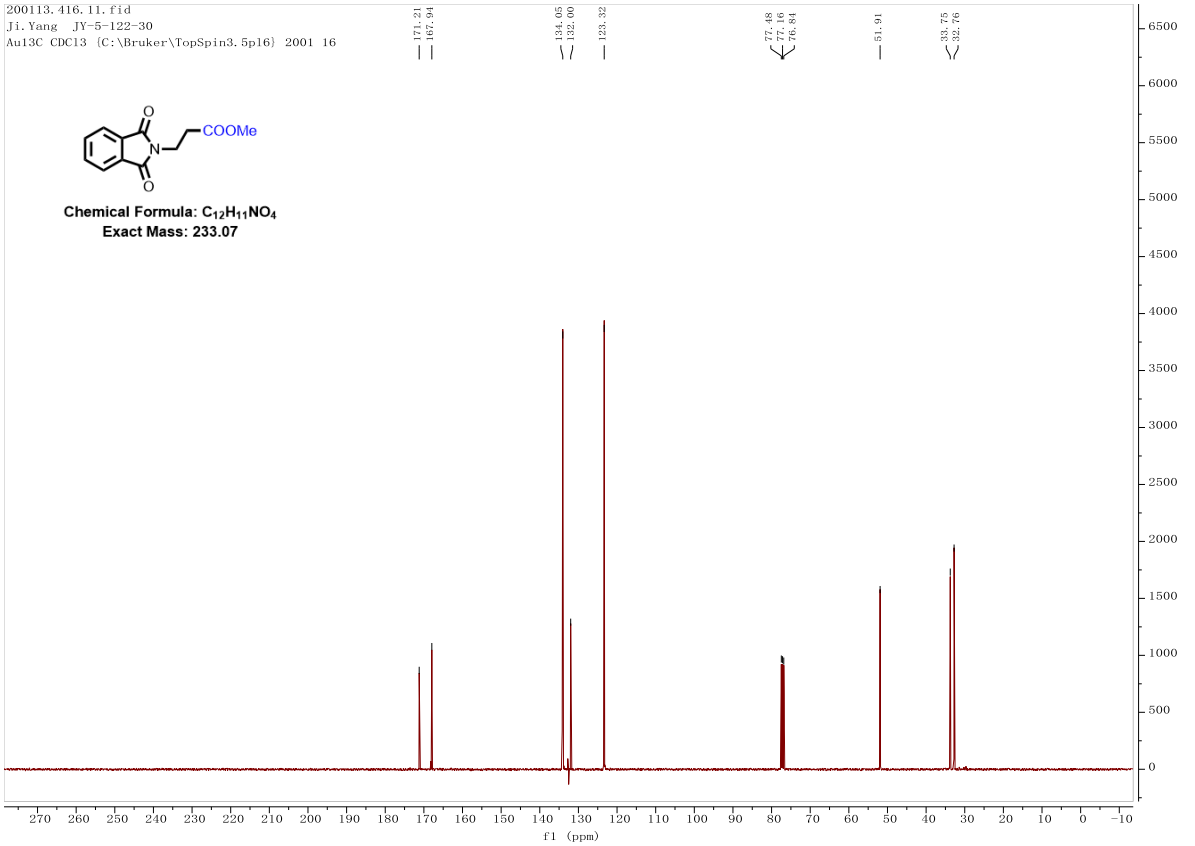
3i

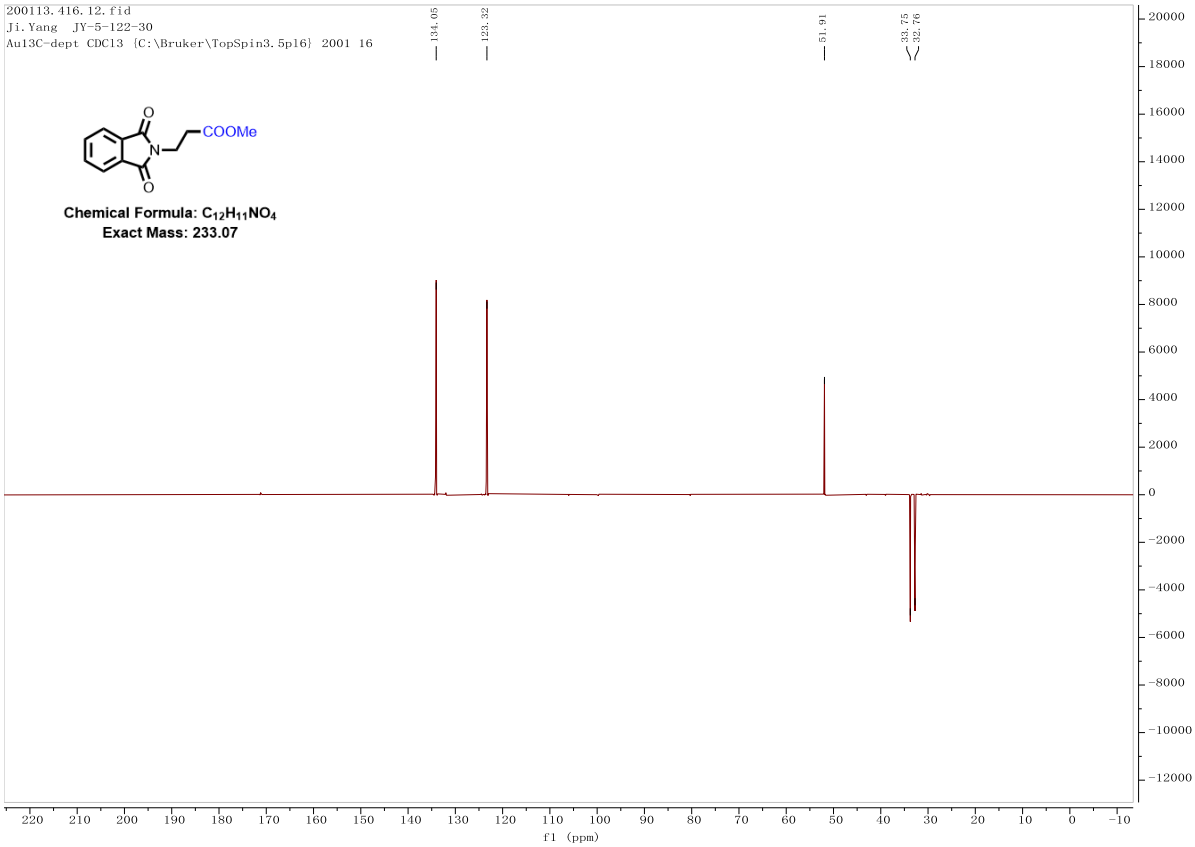
methyl 3-(1,3-dioxoisoindolin-2-yl)propanoate

Chemical Formula: $C_{12}H_{11}NO_4$

Exact Mass: 233.07




200113.416.11.fid
Ji.Yang JY-5-122-30
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 16
171.21
167.94
134.05
132.00
123.32
77.48
77.16
76.84
51.91
33.75
32.76
COOMe
Chemical Formula: C12H11NO4
Exact Mass: 233.07
f1 (ppm)

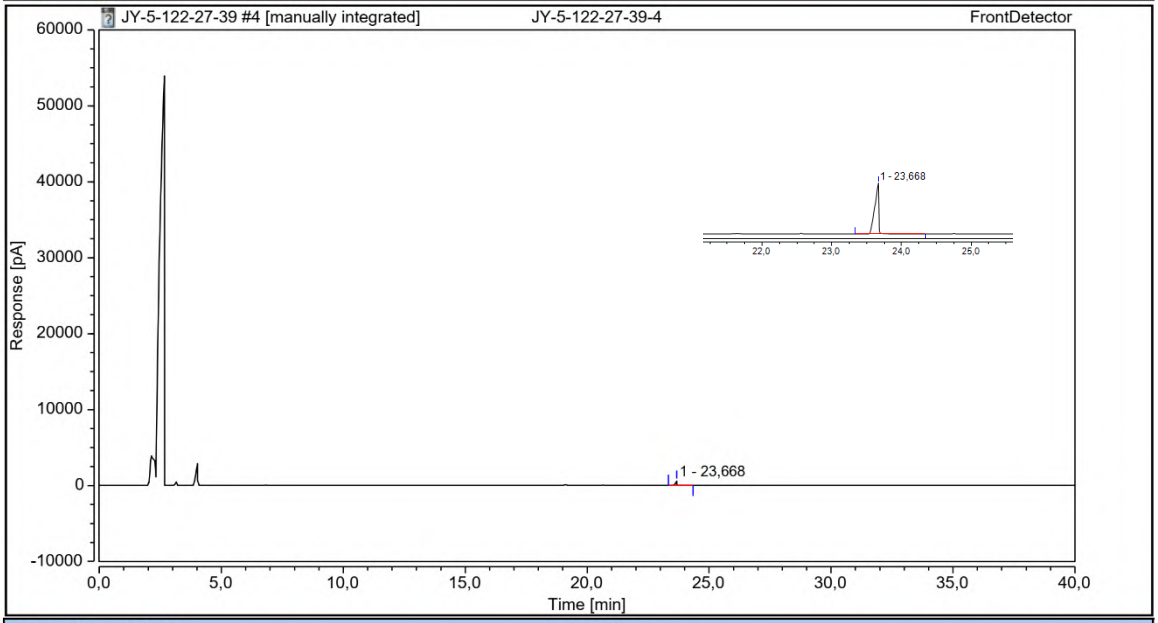

200113.416.12.fid
Ji.Yang JY-5-122-30
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 16
134.05
123.32
51.91
33.75
32.76
COOMe
Chemical Formula: C12H11NO4
Exact Mass: 233.07
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-4**	*Run Time (min):*	**40,00**
Vial Number:	**28**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Jan.20 16:26**	*Sample Weight:*	**1,0000**

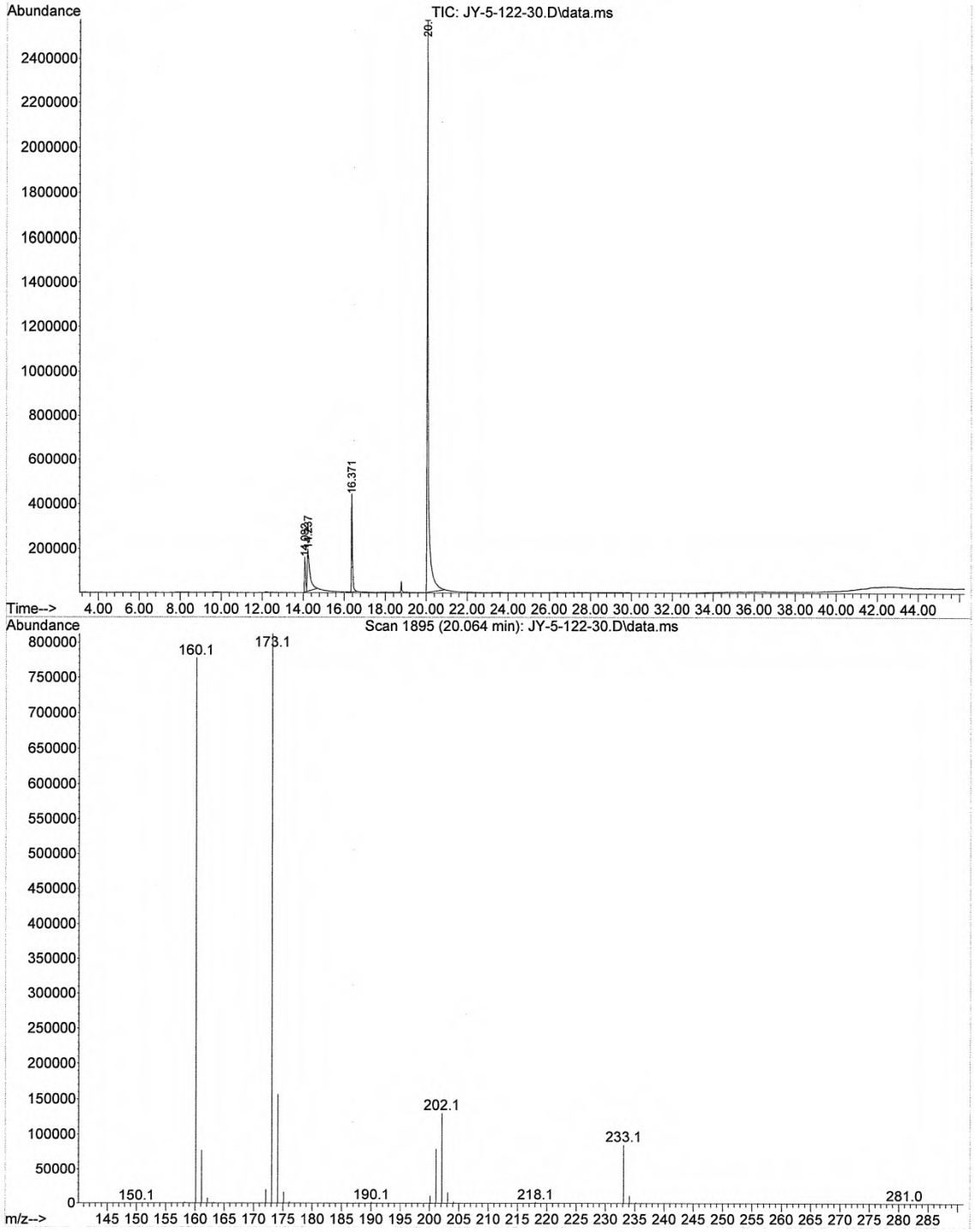
Chromatogram

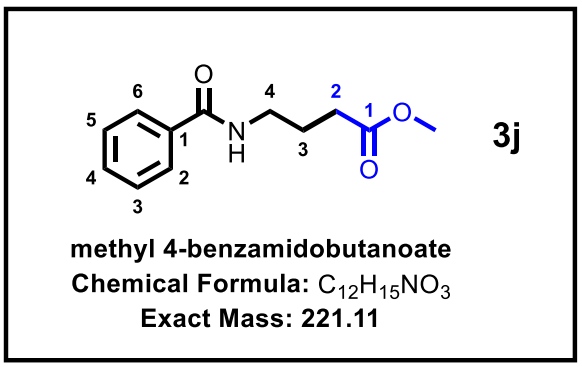


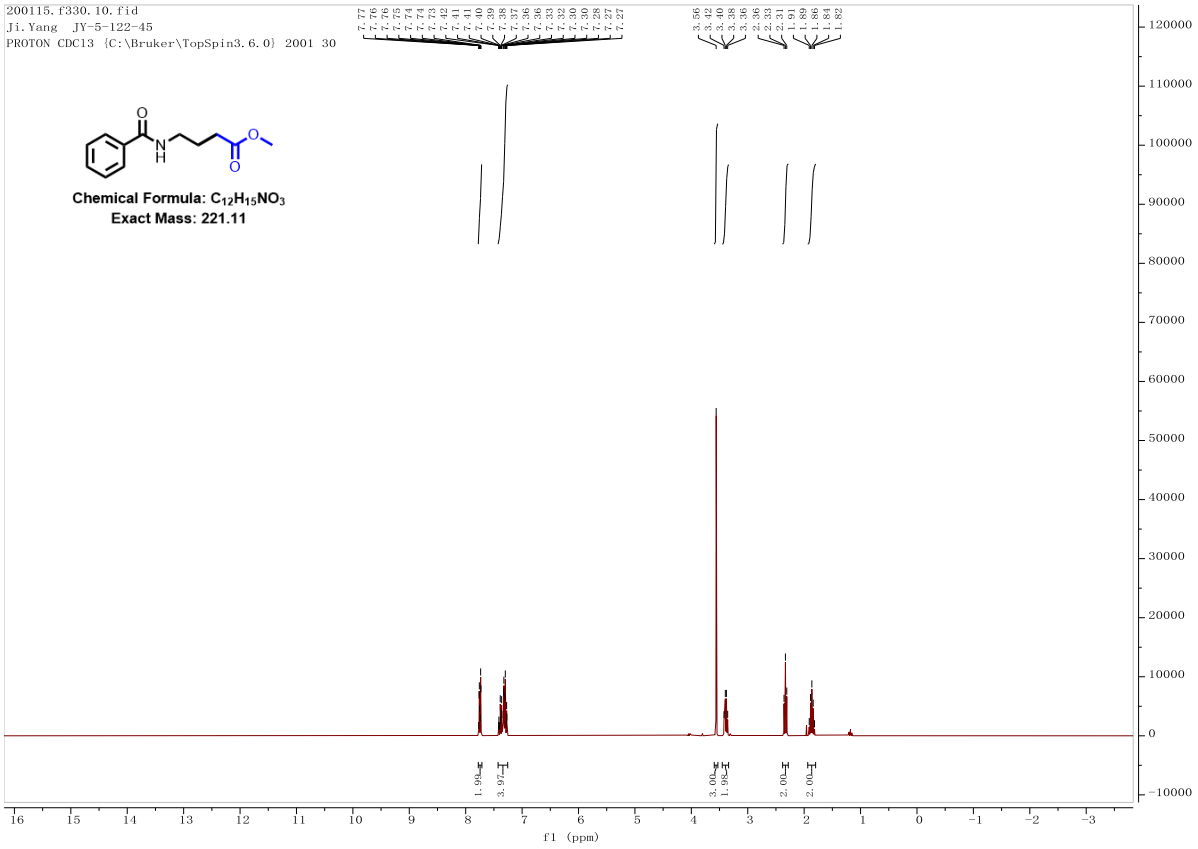
Integration Results

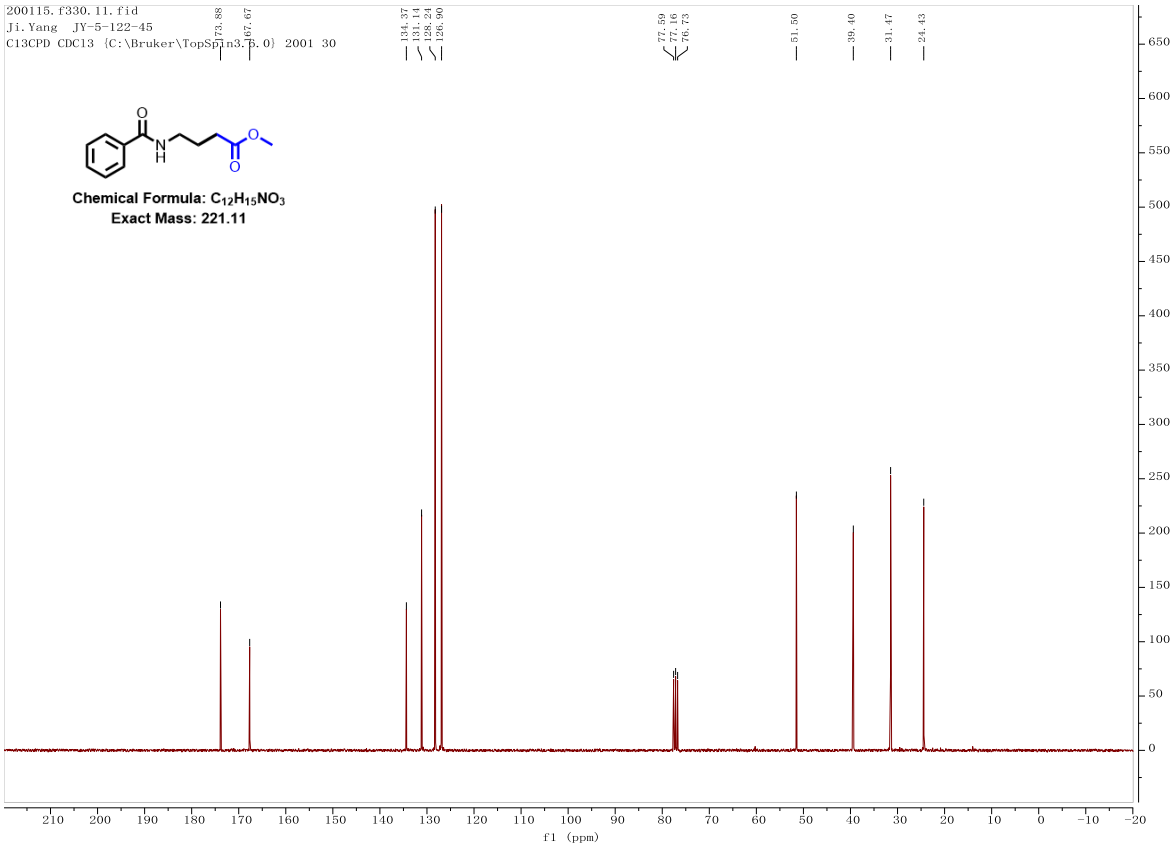
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		23,668	37,672	555,035	100,00	100,00	n.a.
Total:			**37,672**	**555,035**	**100,00**	**100,00**	

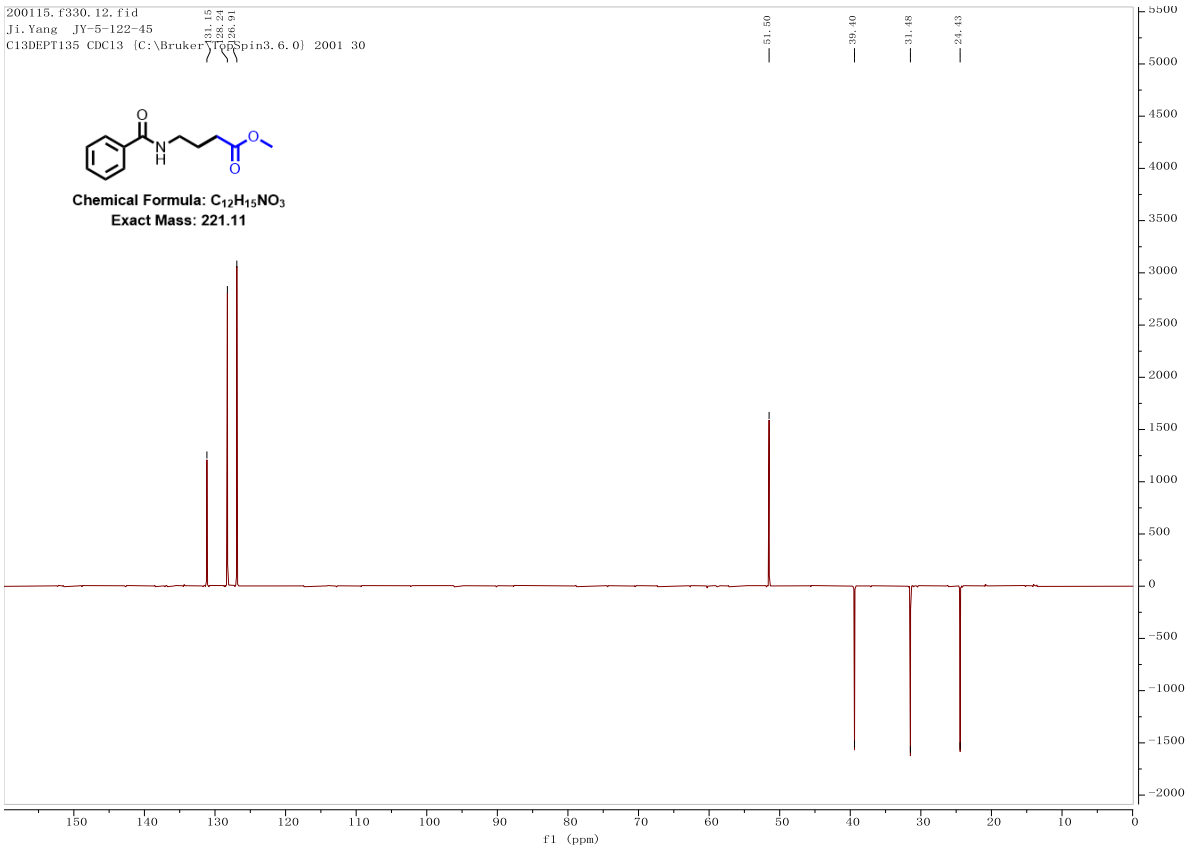
File :D:\MSDChem\1\DATA\2001\JY-5-122-30.D
Operator :
Acquired : 11 Jan 2020 17:06 using AcqMethod SK3-45X.M
Instrument : GC-MSD
Sample Name: JY-5-122-30
Misc Info :
Vial Number: 34




3j
methyl 4-benzamidobutanoate
Chemical Formula: C12H15NO3
Exact Mass: 221.11


200115.f330.10.fid
Ji.Yang JY-5-122-45
PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 30
Chemical Formula: C12H15NO3
Exact Mass: 221.11
f1 (ppm)


200115.f330.11.fid
Ji.Yang JY-5-122-45
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 30
173.88
167.67
134.37
131.14
128.53
126.90
77.59
77.16
76.73
51.50
39.40
31.47
24.43
Chemical Formula: C12H15NO3
Exact Mass: 221.11
f1 (ppm)

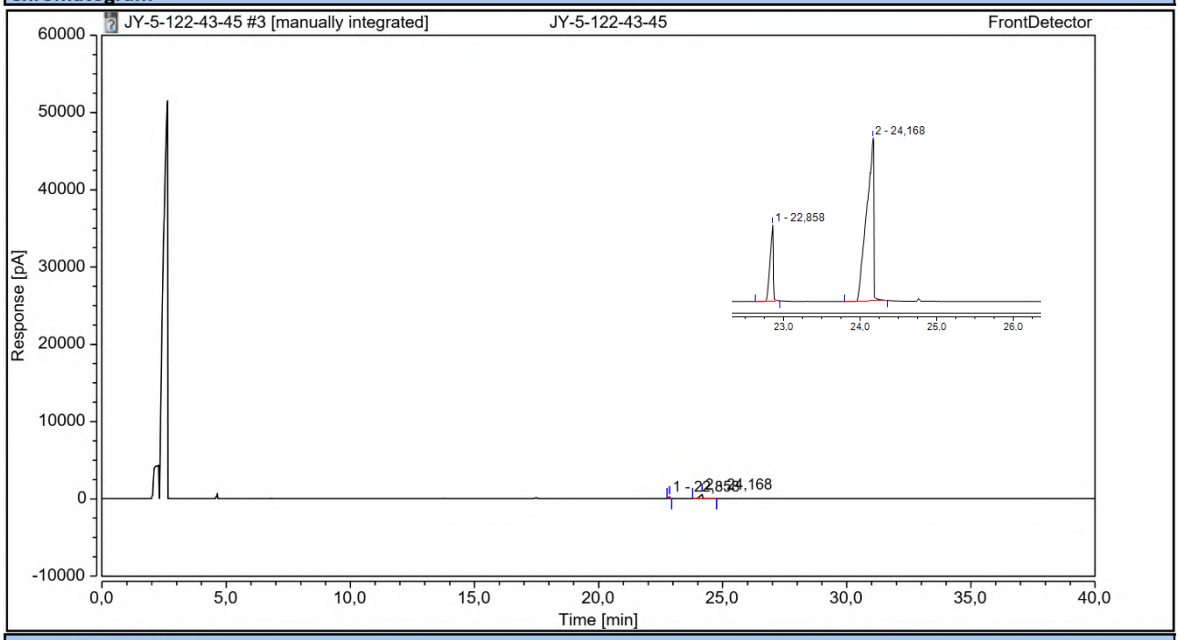

200115.f330.12.fid
Ji.Yang JY-5-122-45
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 30
131.15
128.54
126.91
51.50
39.40
31.48
24.43
Chemical Formula: C12H15NO3
Exact Mass: 221.11
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-43-45**	*Run Time (min):*	**40,00**
Vial Number:	**75**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**13.Jan.20 16:34**	*Sample Weight:*	**1,0000**

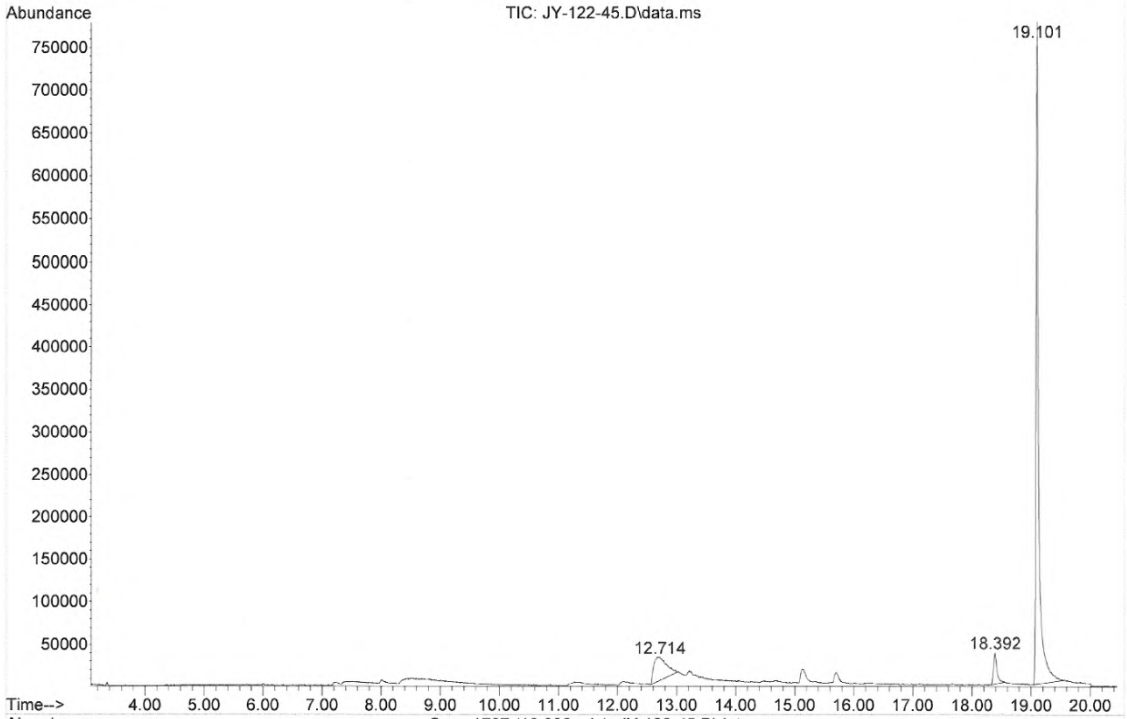
Chromatogram

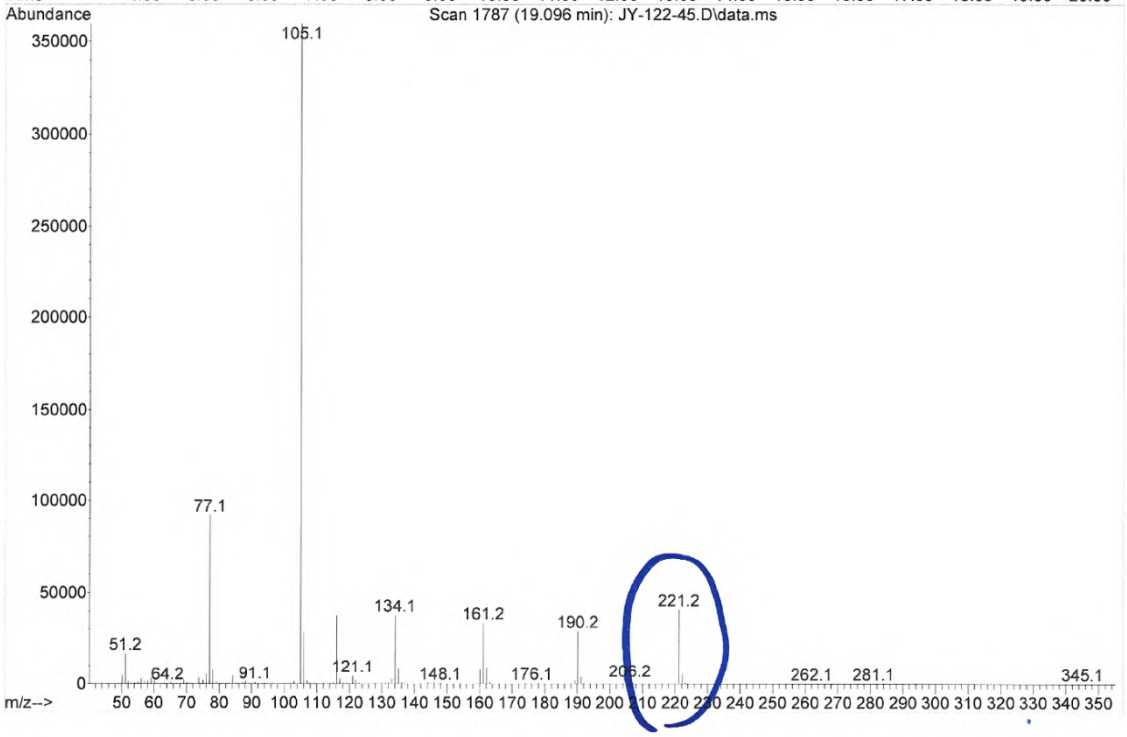


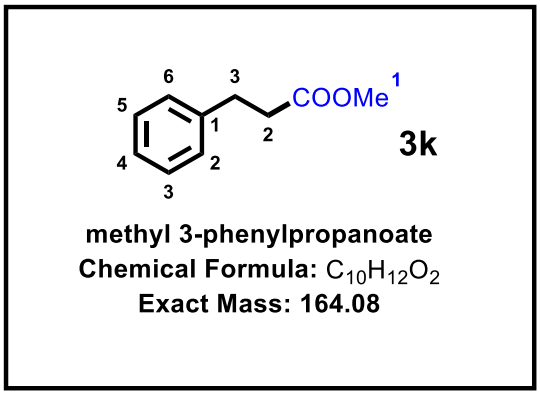
Integration Results

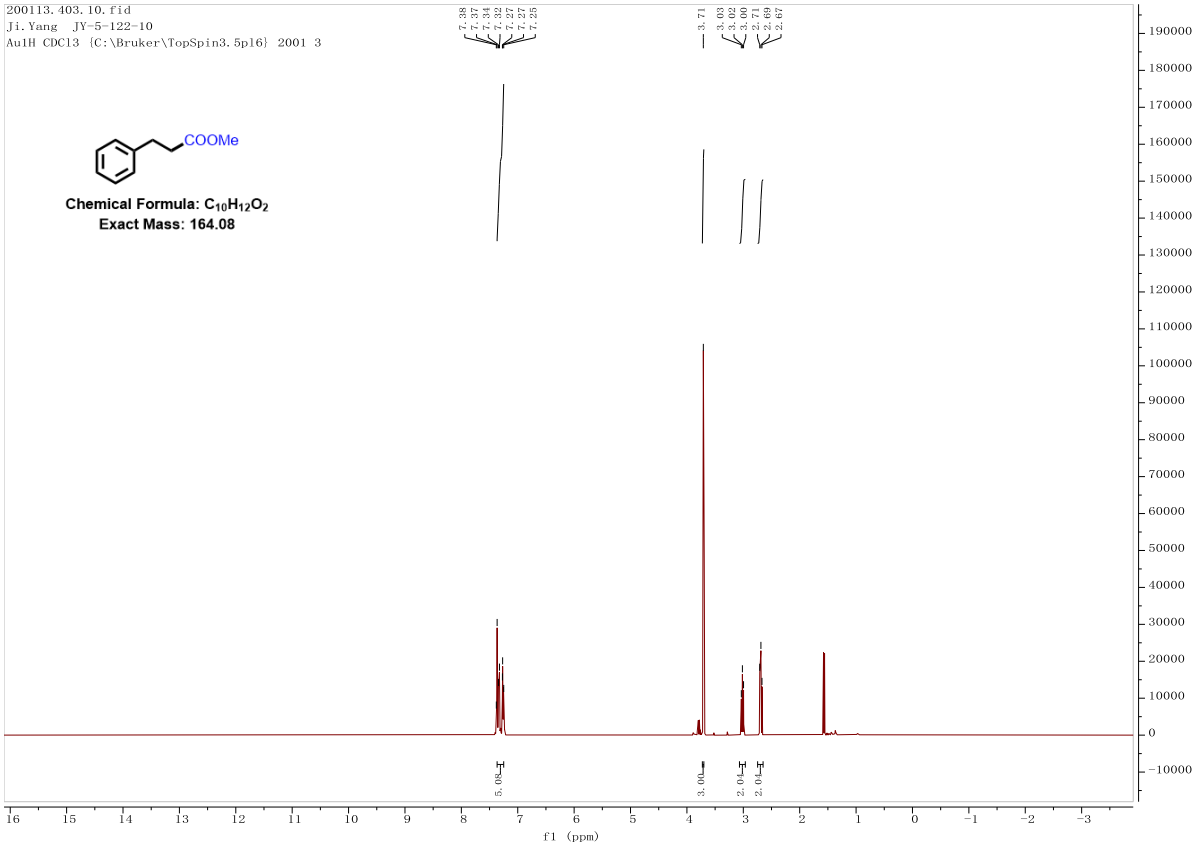
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		22,858	12,569	264,111	17,91	31,93	n.a.
2		24,168	57,625	562,972	82,09	68,07	n.a.
Total:			**70,193**	**827,083**	**100,00**	**100,00**	

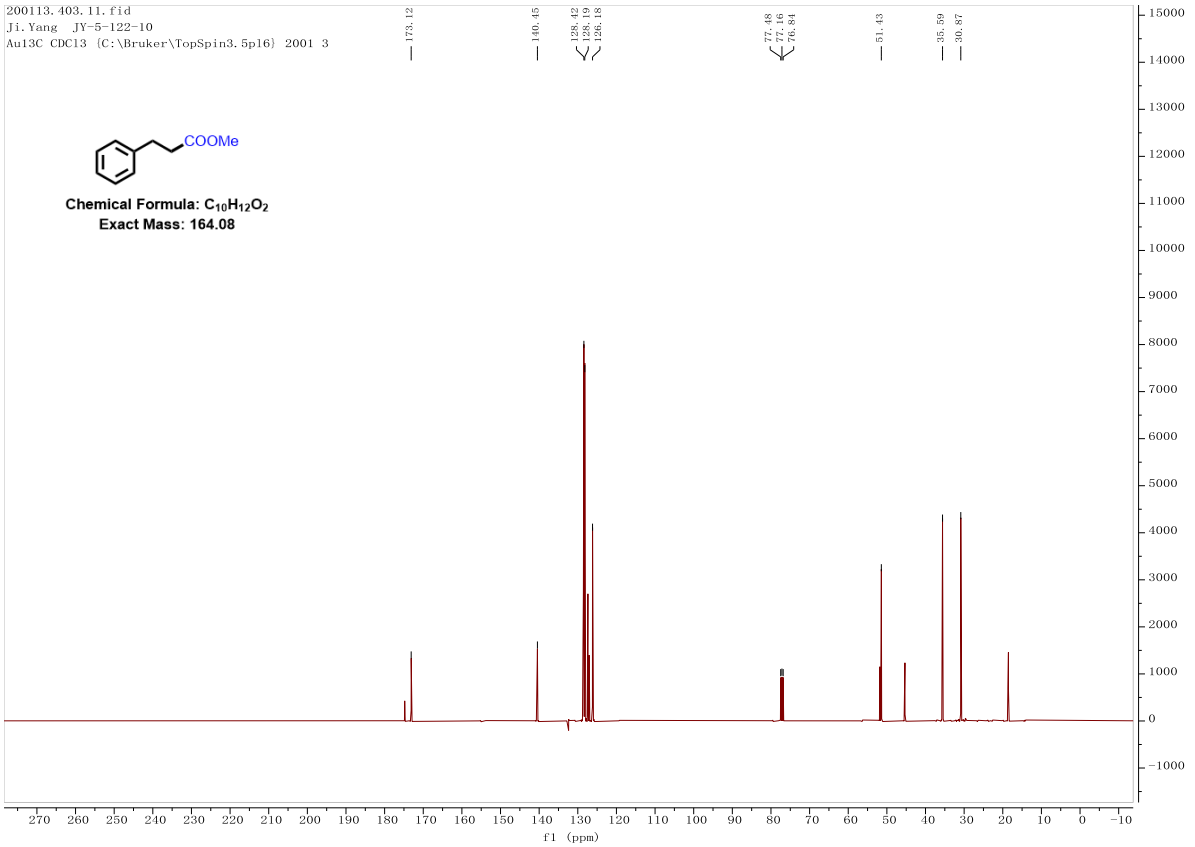
File :D:\MSDChem\1\DATA\2001\JY-122-45.D
Operator :
Acquired : 13 Jan 2020 16:33 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-122-45
Misc Info :
Vial Number: 48

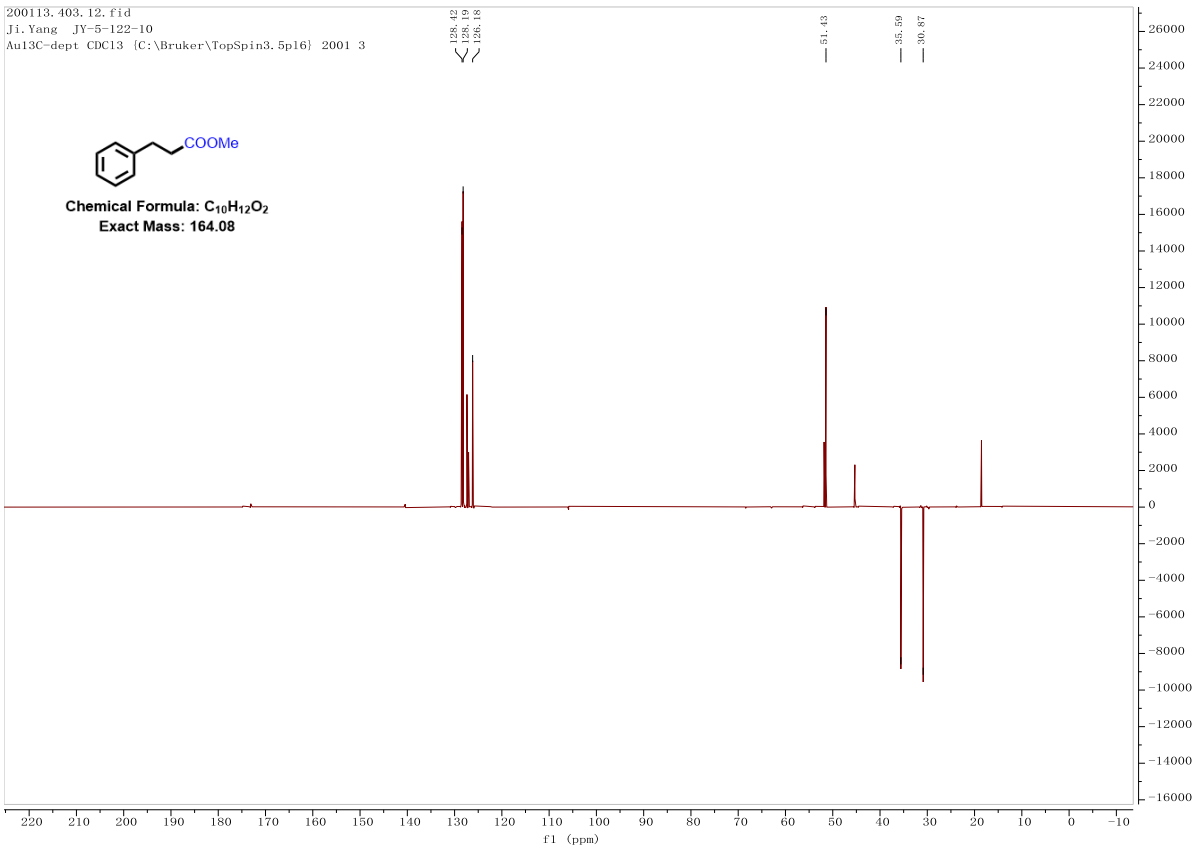





6
3
5
1
COOMe
1
2
4
2
3
3k
methyl 3-phenylpropanoate
Chemical Formula: C10H12O2
Exact Mass: 164.08


200113.403.10.fid
Ji.Yang JY-5-122-10
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 3
COOMe
Chemical Formula: C10H12O2
Exact Mass: 164.08
f1 (ppm)


200113.403.11.fid
Ji.Yang JY-5-122-10
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 3
173.12
140.45
128.42
128.19
126.18
77.48
77.16
76.84
51.43
35.59
30.87
COOMe
Chemical Formula: C10H12O2
Exact Mass: 164.08
f1 (ppm)

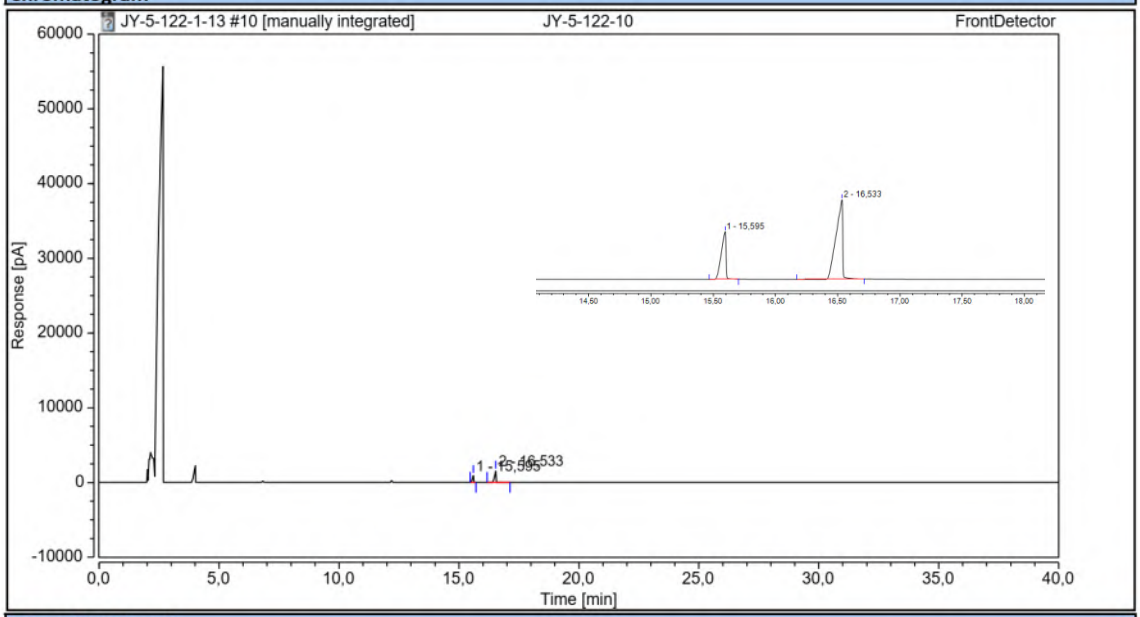

200113.403.12.fid
Ji.Yang JY-5-122-10
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 3
128.42
128.19
126.18
51.43
35.59
30.87
COOMe
Chemical Formula: C10H12O2
Exact Mass: 164.08
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-10**	*Run Time (min):*	**40,00**
Vial Number:	**70**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 00:37**	*Sample Weight:*	**1,0000**

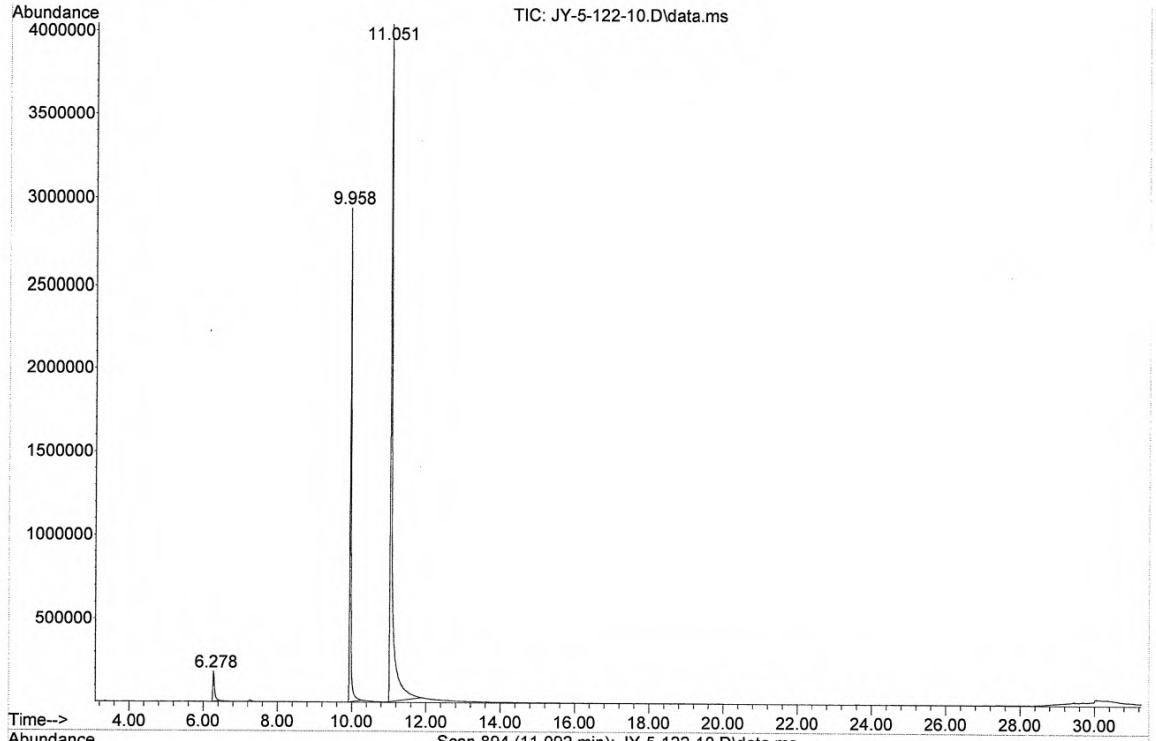
Chromatogram

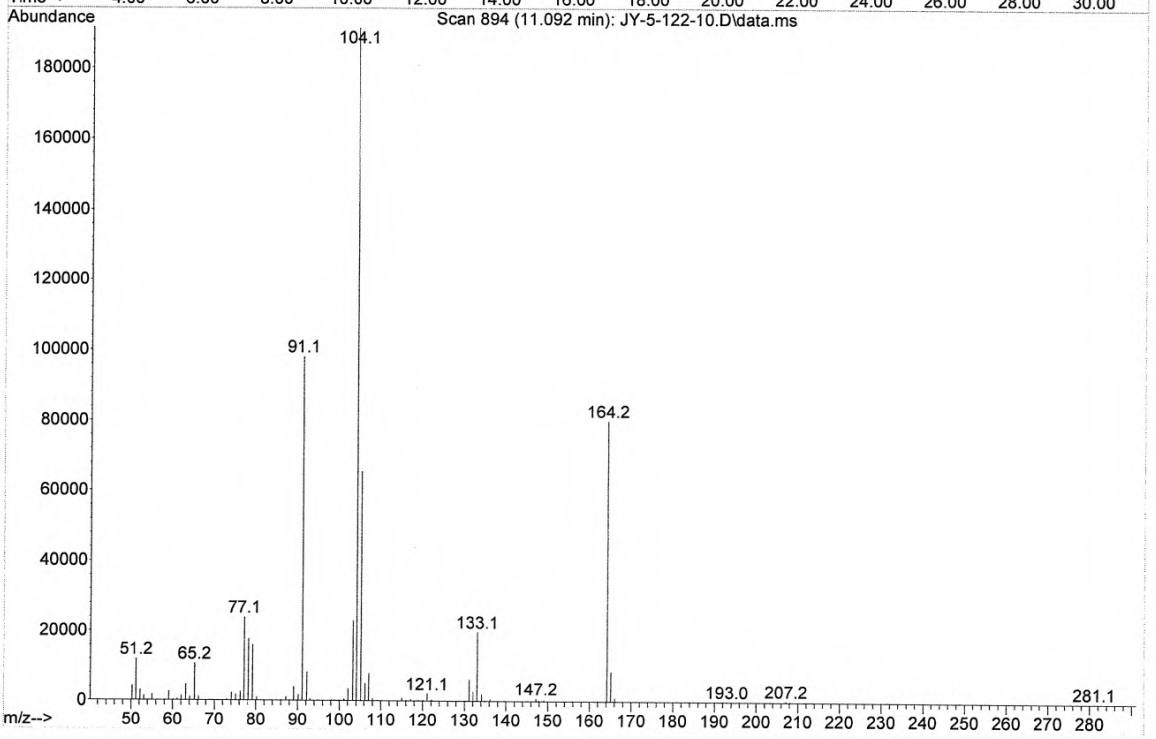


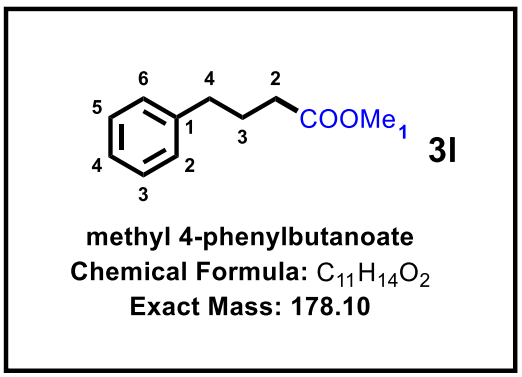
Integration Results

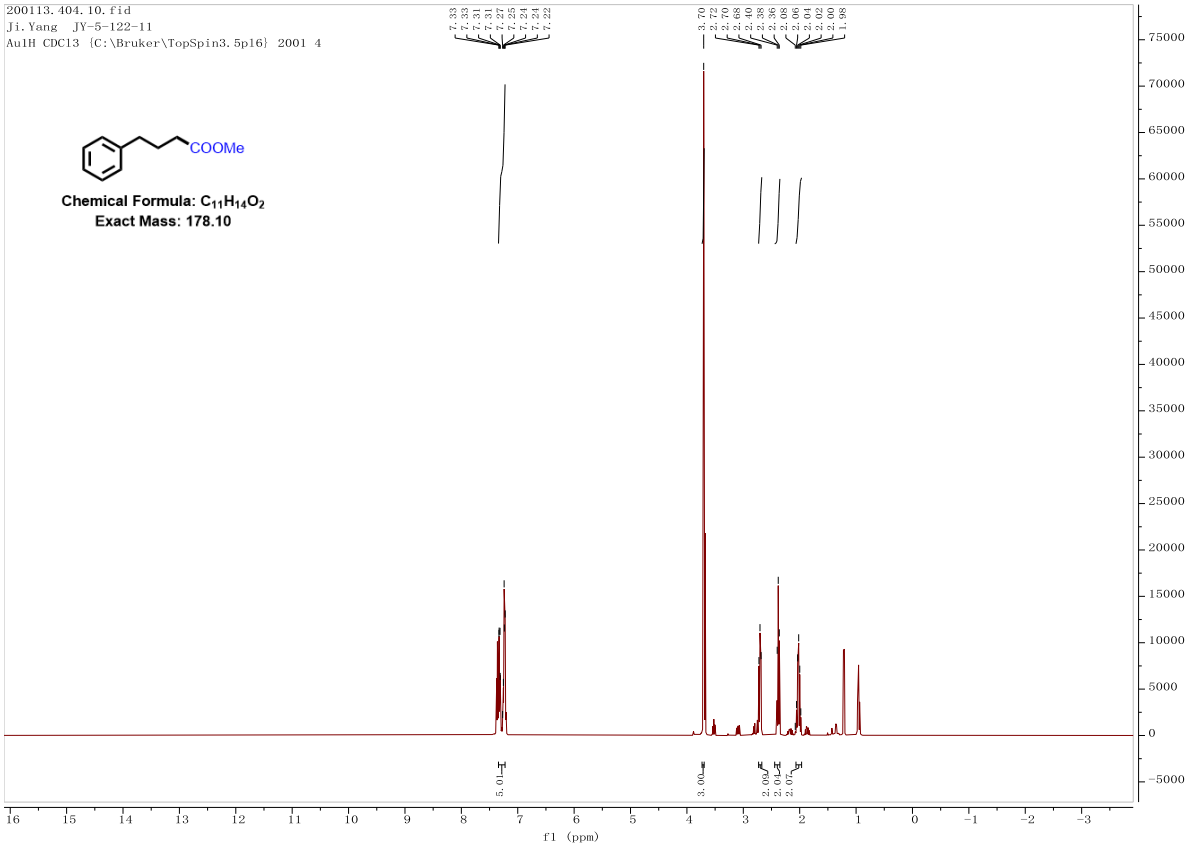
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		15,595	39,382	905,350	28,99	37,44	n.a.
2		16,533	96,450	1512,600	71,01	62,56	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**135,831**	**2417,950**	**100,00**	**100,00**	

File :D:\MSDChem\1\DATA\2001\JY-5-122-10.D
Operator :
Acquired : 9 Jan 2020 20:57 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-10
Misc Info :
Vial Number: 45

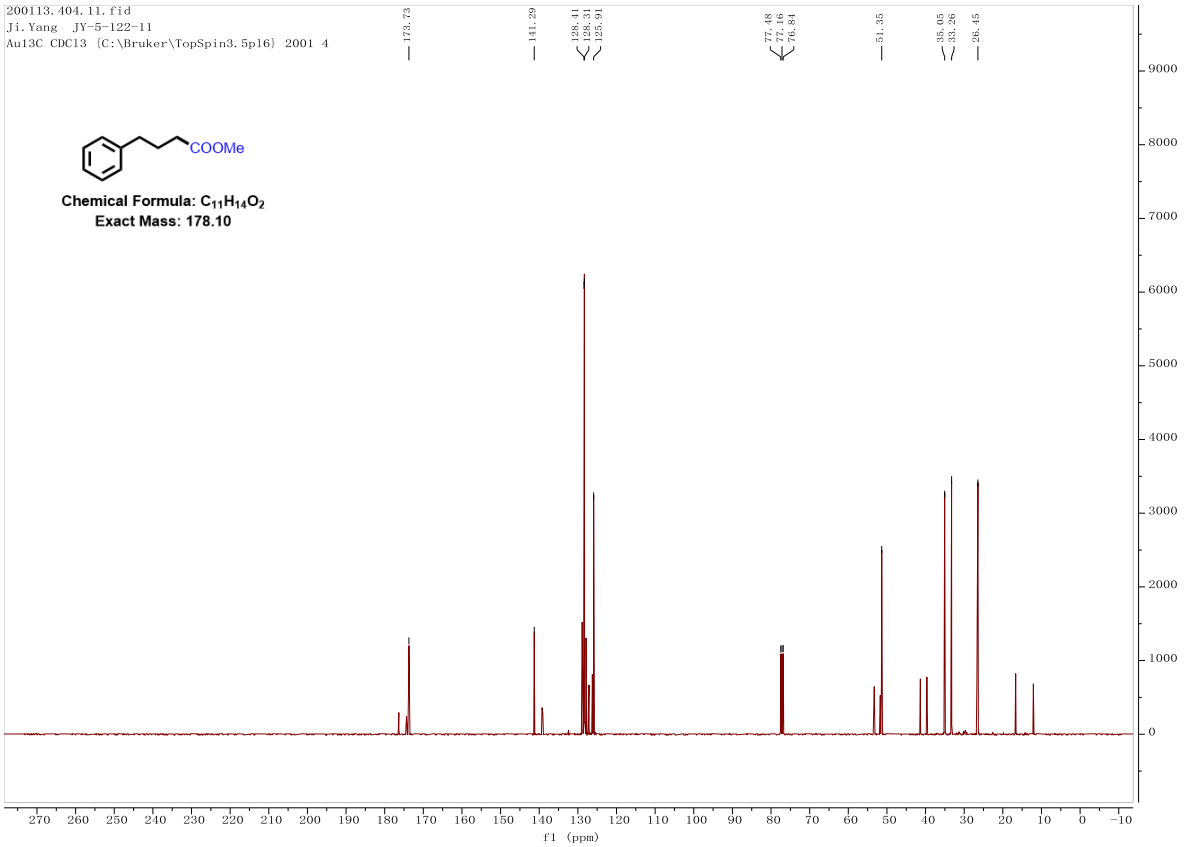


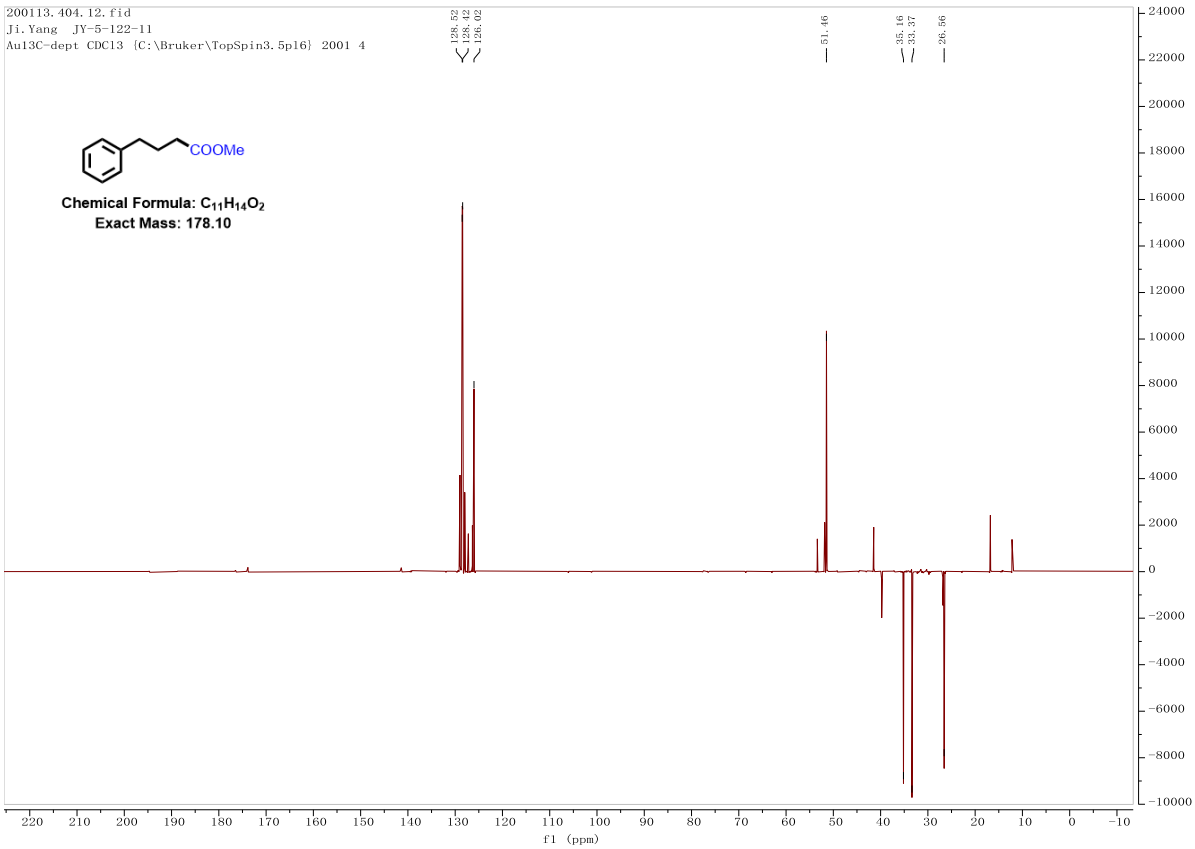



6
4
2
5
1
3
COOMe
1
4
2
3
3l
methyl 4-phenylbutanoate
Chemical Formula: C11H14O2
Exact Mass: 178.10


200113.404.10.fid
Ji.Yang JY-5-122-11
AulH CDC13 {C:\Bruker\TopSpin3.5p16} 2001 4
COOMe
Chemical Formula: C11H14O2
Exact Mass: 178.10
f1 (ppm)

.


200113.404.11.fid
Ji.Yang JY-5-122-11
Au13C CDCl3 {C:\Bruker\TopSpin3.5p16} 2001 4
173.73
141.29
128.41
128.31
125.91
77.48
77.16
76.84
51.35
35.05
33.26
26.45
COOMe
Chemical Formula: C11H14O2
Exact Mass: 178.10
f1 (ppm)

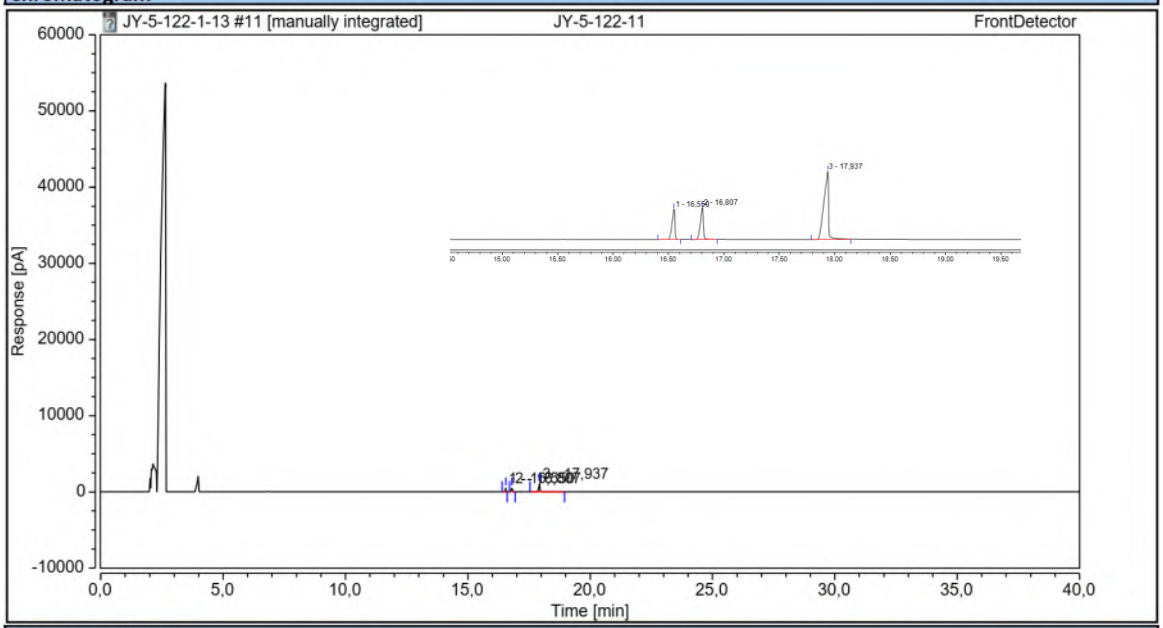

200113.404.12.fid
Ji.Yang JY-5-122-11
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5p16} 2001 4
128.52
128.42
126.02
51.46
35.16
33.37
26.56
COOMe
Chemical Formula: C11H14O2
Exact Mass: 178.10
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-11**	*Run Time (min):*	**40,00**
Vial Number:	**71**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 01:38**	*Sample Weight:*	**1,0000**

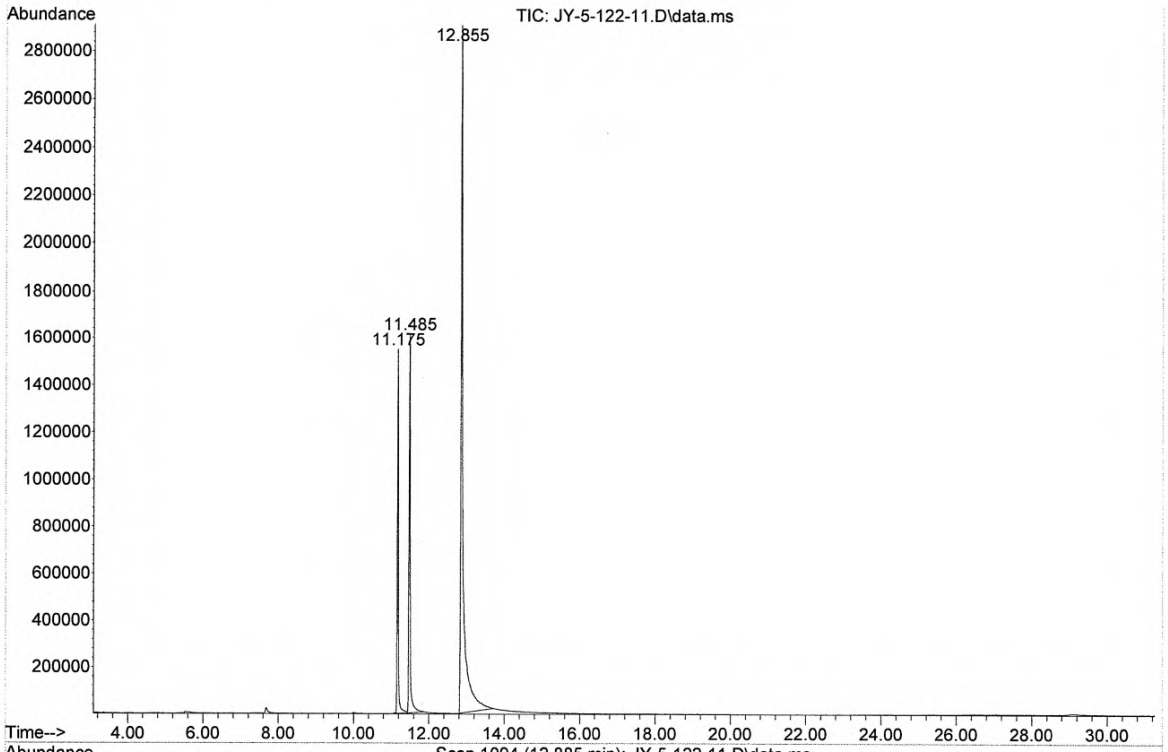
Chromatogram

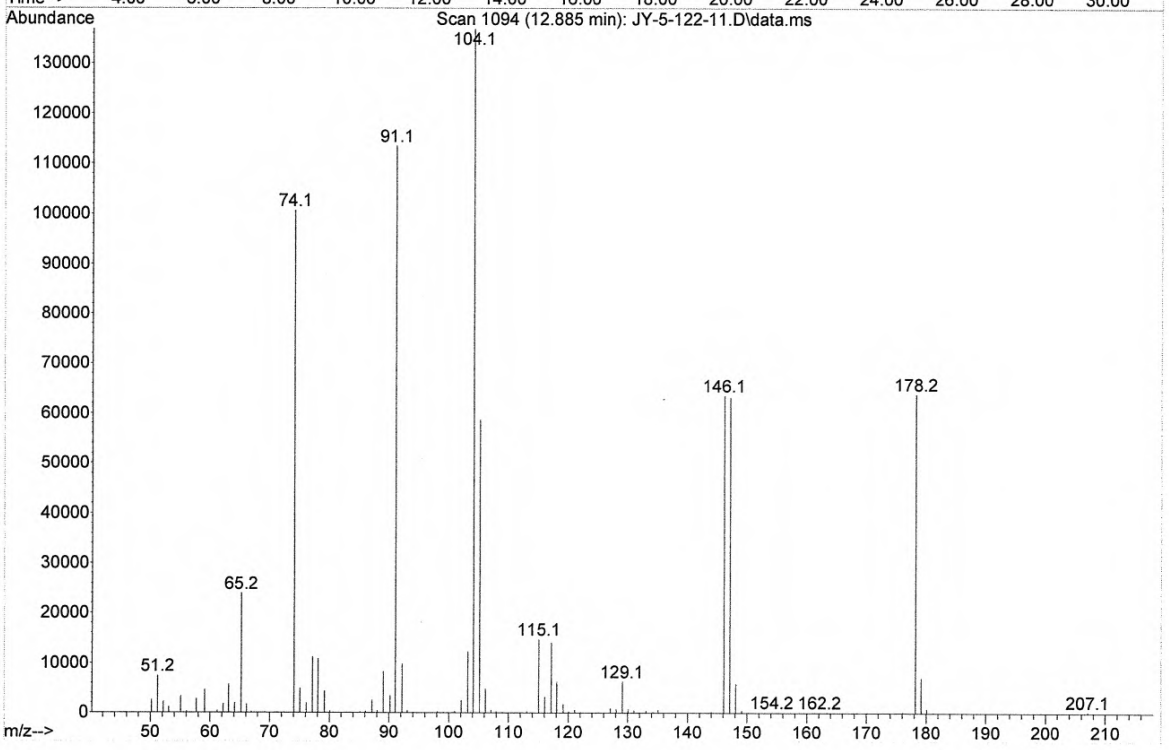


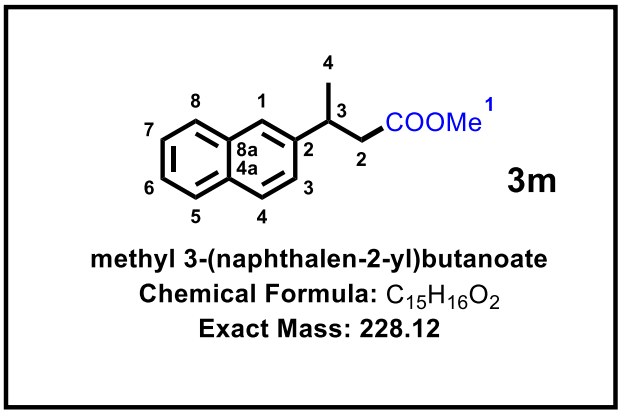
Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		16,550	14,635	489,660	16,92	23,31	n.a.
2		16,807	16,094	513,243	18,61	24,43	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
3		17,937	55,742	1097,985	64,46	52,26	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**86,472**	**2100,888**	**100,00**	**100,00**	

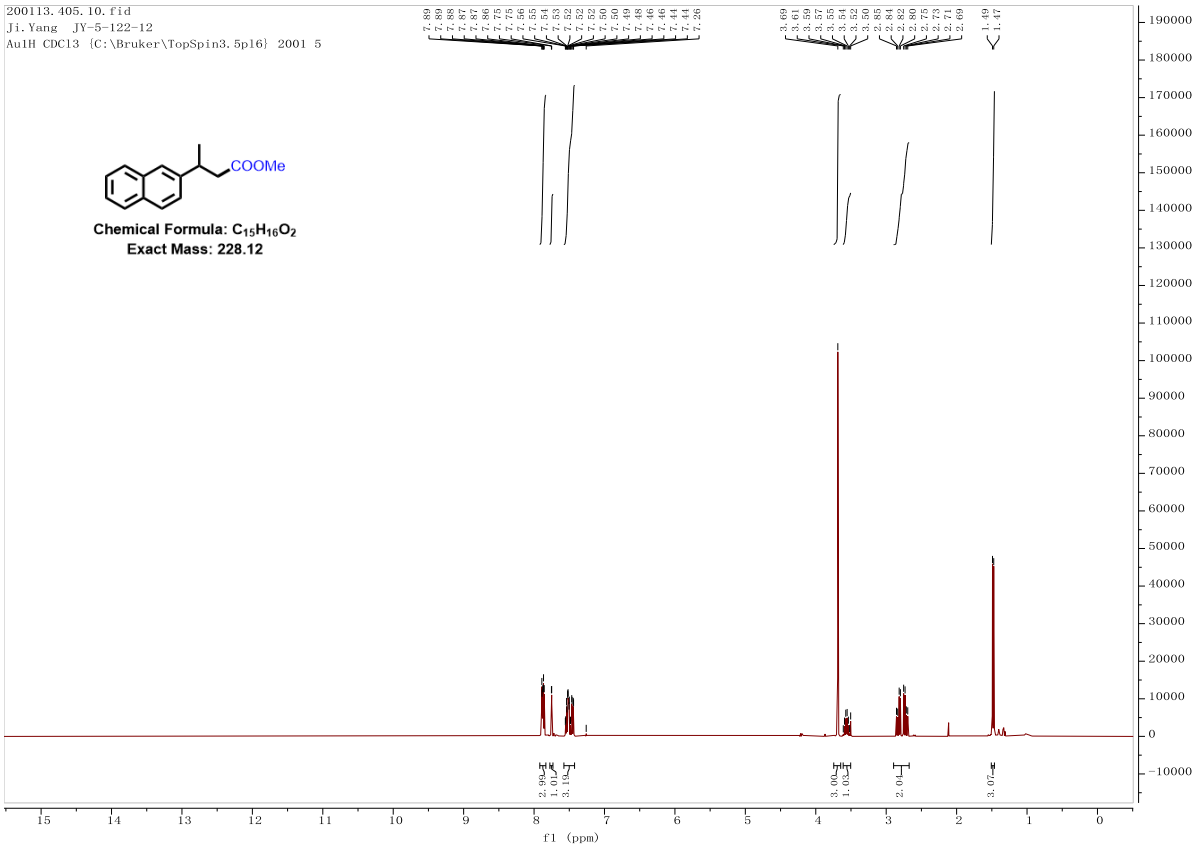
```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-11.D
Operator   :
Acquired   :  9 Jan 2020  21:36     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-11
Misc Info  :
Vial Number: 46
```

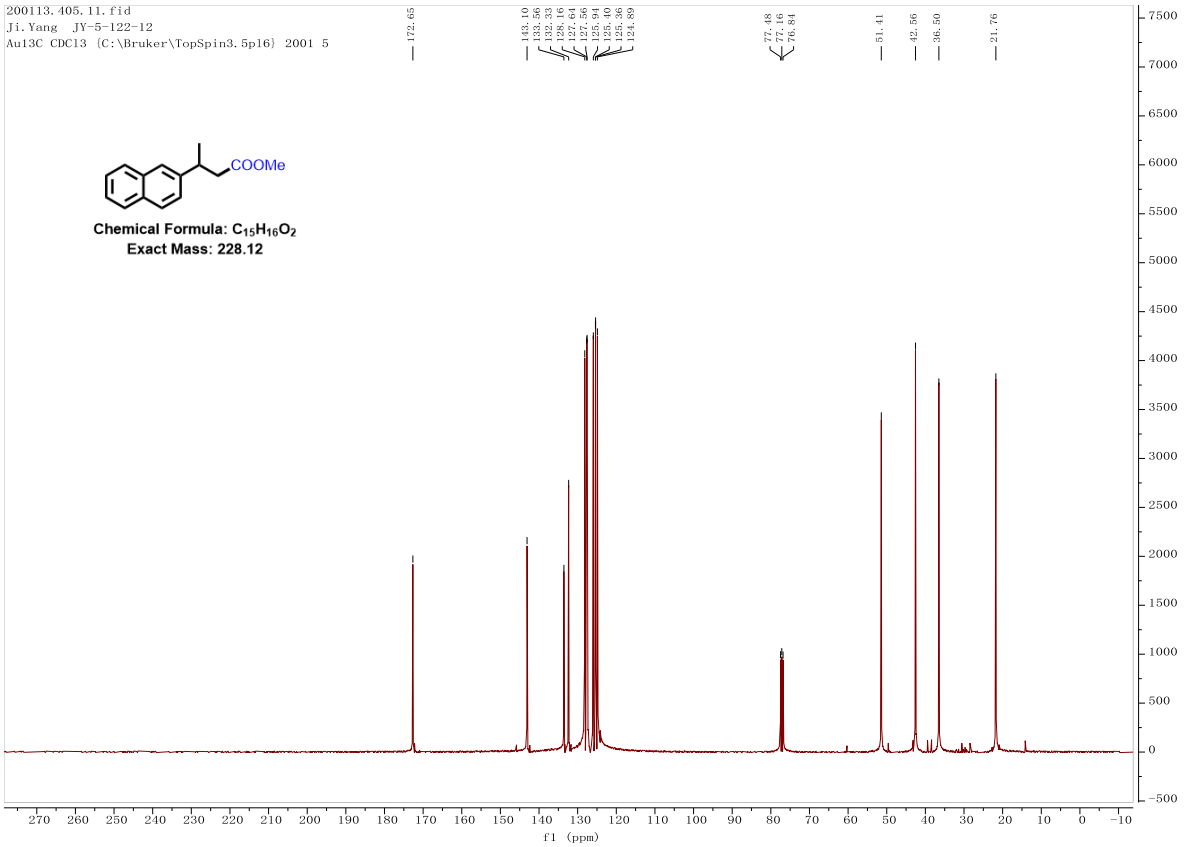


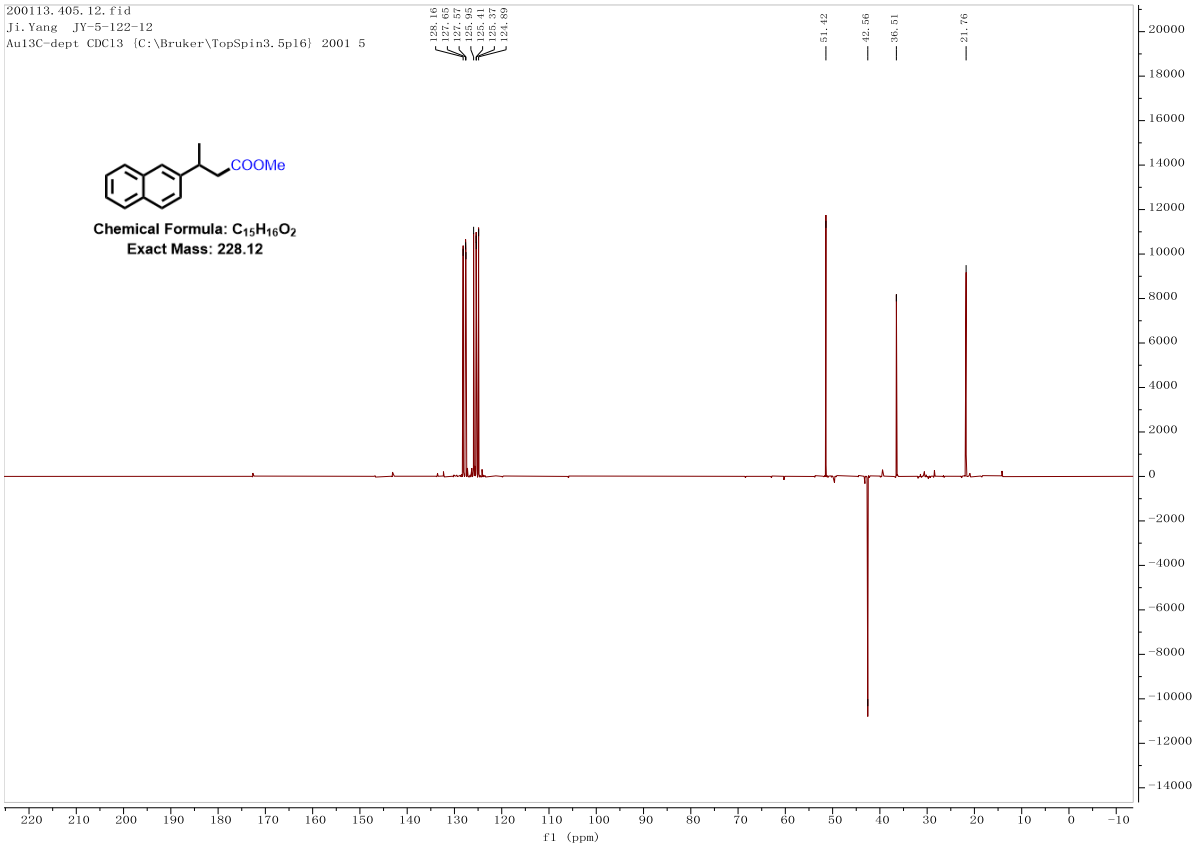




methyl 3-(naphthalen-2-yl)butanoate
Chemical Formula: $C_{15}H_{16}O_2$
Exact Mass: 228.12




200113.405.11.fid
Ji.Yang JY-5-122-12
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 5
172.65
143.10
133.56
132.33
128.16
127.64
127.56
125.94
125.40
125.36
124.89
77.48
77.16
76.84
51.41
42.56
36.50
21.76
COOMe
Chemical Formula: C15H16O2
Exact Mass: 228.12
f1 (ppm)

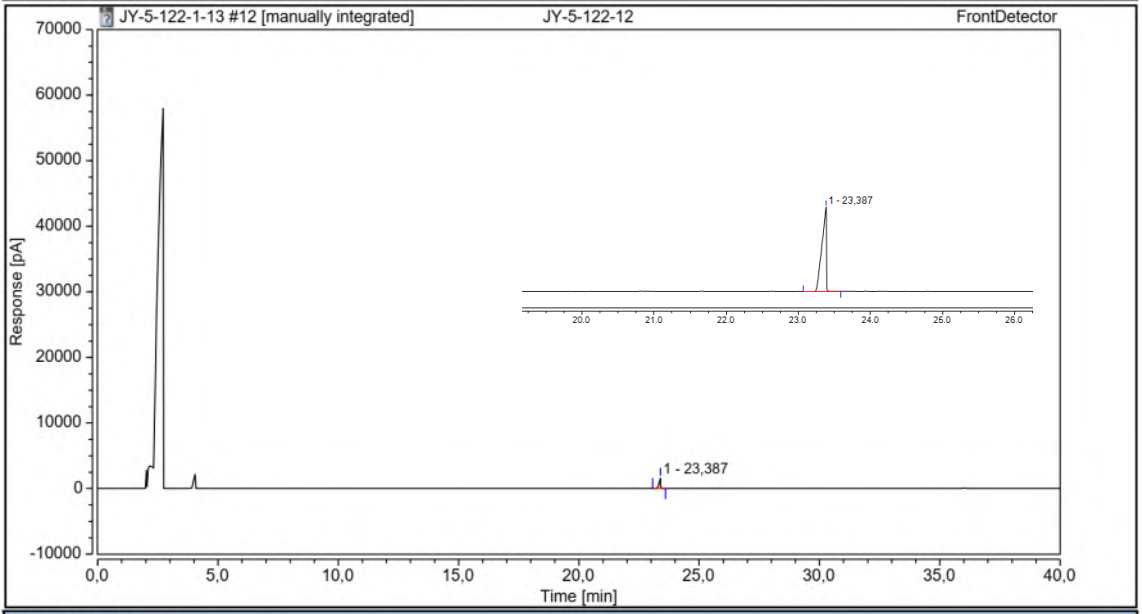

200113.405.12.fid
Ji.Yang JY-5-122-12
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 5
128.16
127.65
127.57
125.95
125.41
125.37
124.89
51.42
42.56
36.51
21.76
COOMe
Chemical Formula: C15H16O2
Exact Mass: 228.12
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-12**	*Run Time (min):*	**40,00**
Vial Number:	**72**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 02:40**	*Sample Weight:*	**1,0000**

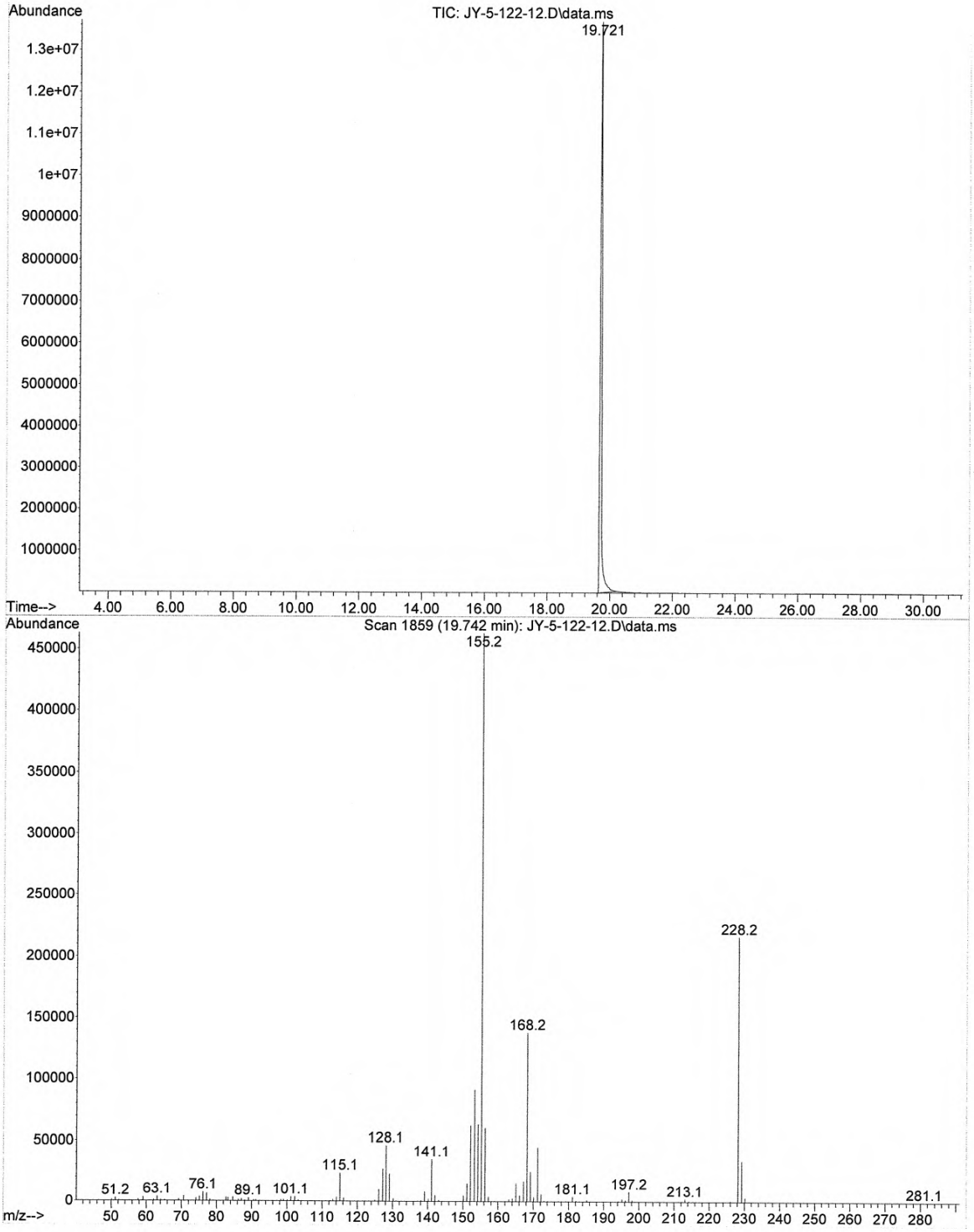
Chromatogram

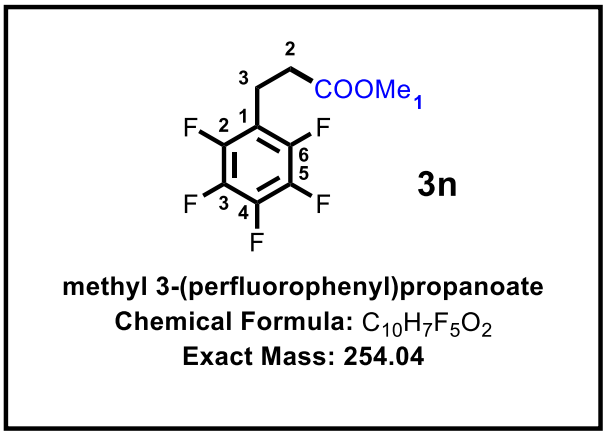


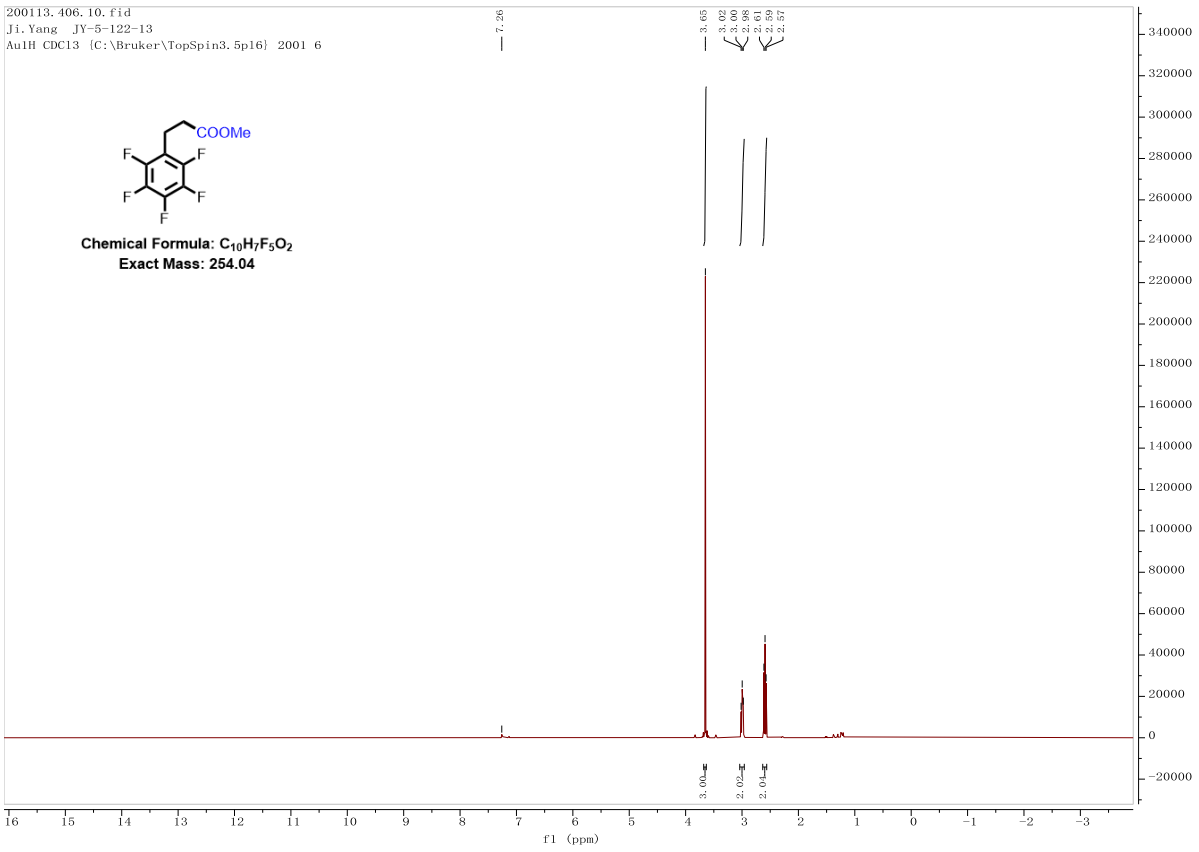
Integration Results

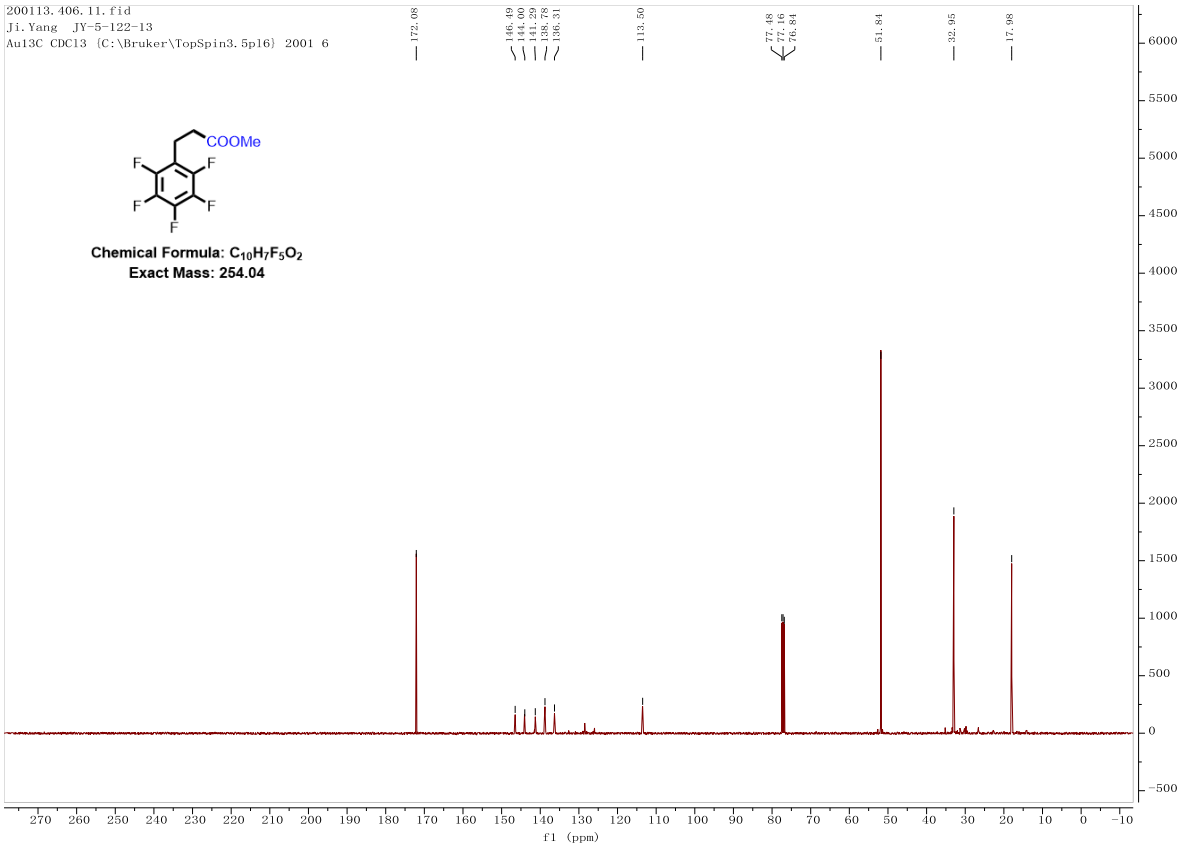
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		23,387	112,198	1546,722	100,00	100,00	n.a.
Total:			**112,198**	**1546,722**	**100,00**	**100,00**	

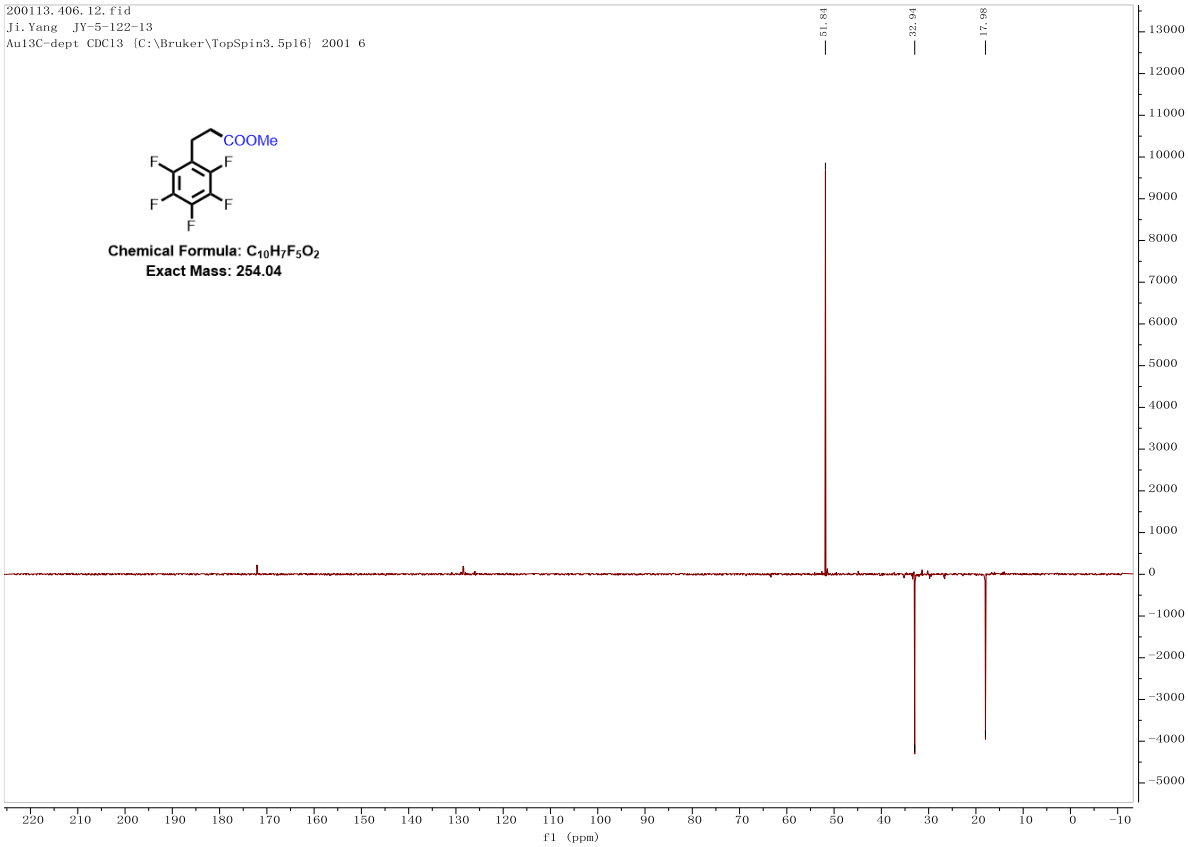
```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-12.D
Operator   :
Acquired   :  9 Jan 2020  22:15     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-12
Misc Info  :
Vial Number: 47
```




COOMe
F
F
F
F
F
3n
methyl 3-(perfluorophenyl)propanoate
Chemical Formula: C10H7F5O2
Exact Mass: 254.04


200113.406.10.fid
Ji.Yang JY-5-122-13
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 6
7.26
3.65
3.02
3.00
2.98
2.61
2.59
2.57
COOMe
F
F
F
F
F
Chemical Formula: C10H7F5O2
Exact Mass: 254.04
3.04
2.02
2.04
f1 (ppm)


200113.406.11.fid
Ji.Yang JY-5-122-13
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 6
172.08
146.49
144.00
141.29
138.78
136.31
113.50
77.48
77.16
76.84
51.84
32.95
17.98
COOMe
F
F
F
F
F
Chemical Formula: C10H7F5O2
Exact Mass: 254.04
f1 (ppm)

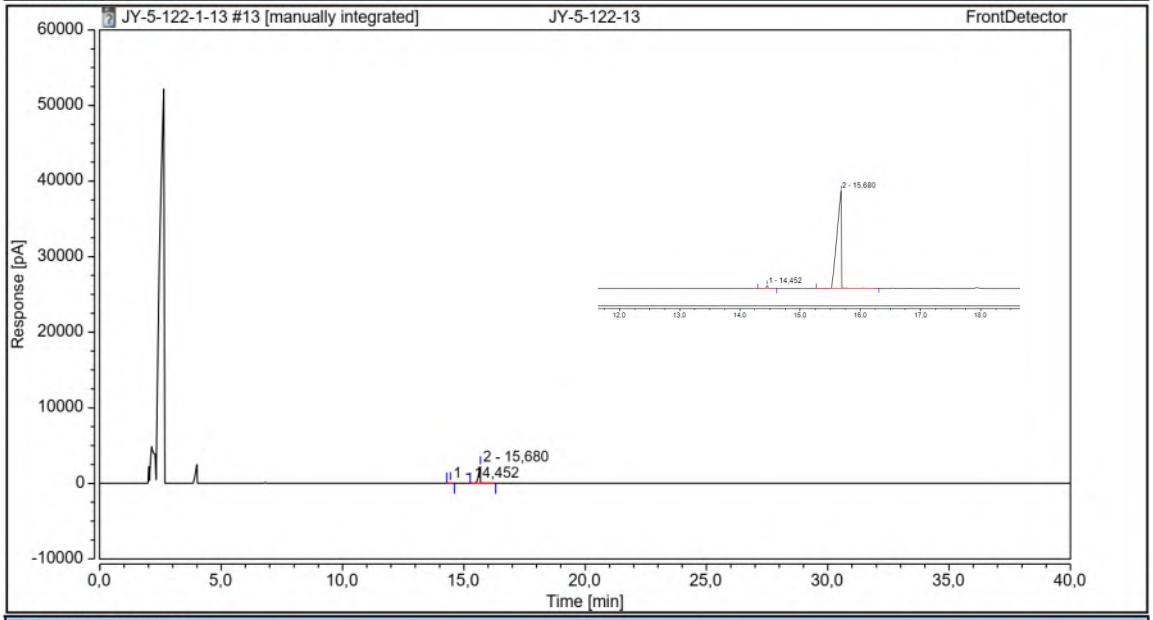

200113.406.12.fid
Ji.Yang JY-5-122-13
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 6
51.84
32.94
17.98
COOMe
F
F
F
F
F
Chemical Formula: C10H7F5O2
Exact Mass: 254.04
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-13**	*Run Time (min):*	**40,00**
Vial Number:	**73**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 03:41**	*Sample Weight:*	**1,0000**

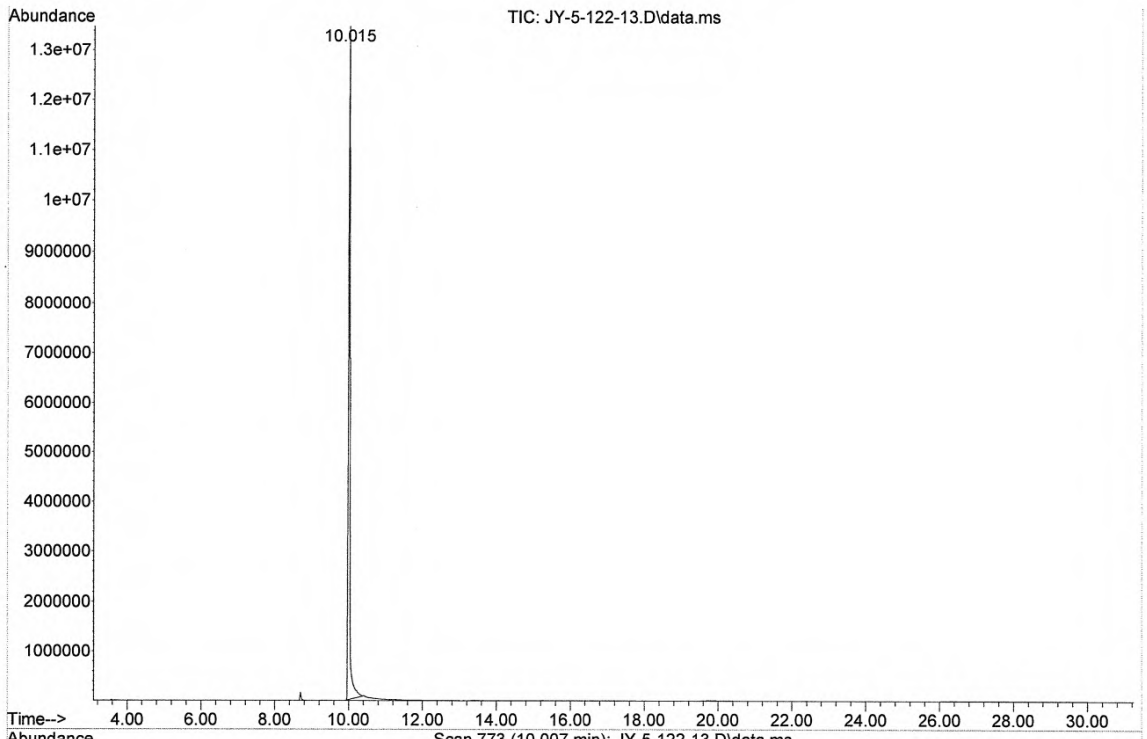
Chromatogram

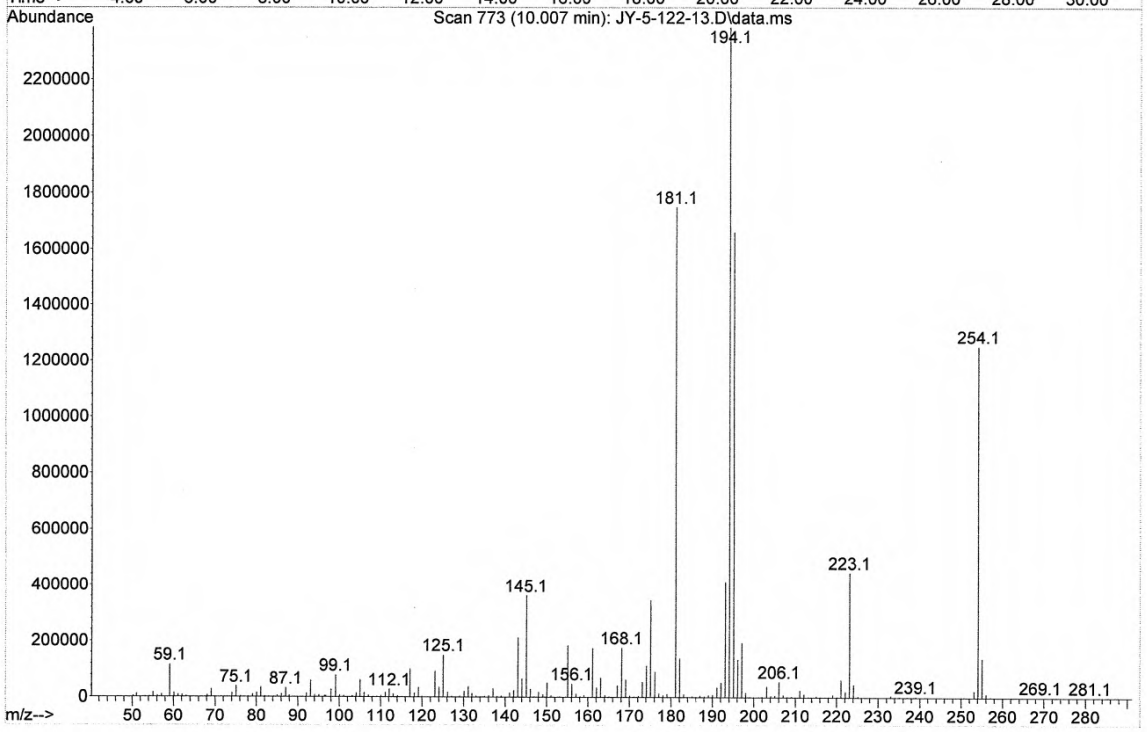


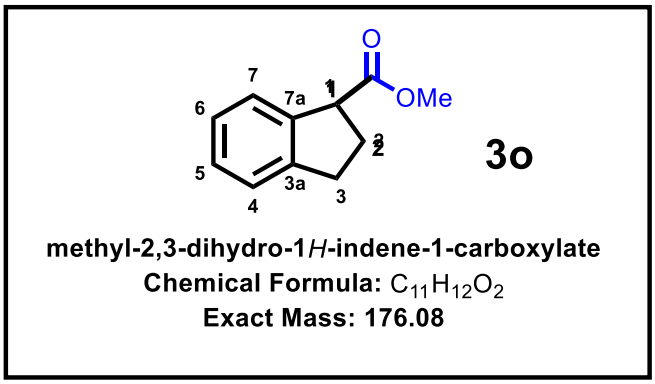
Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,452	1,676	66,785	0,91	2,98	n.a.
2		15,680	181,537	2172,601	99,09	97,02	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**183,214**	**2239,387**	**100,00**	**100,00**	

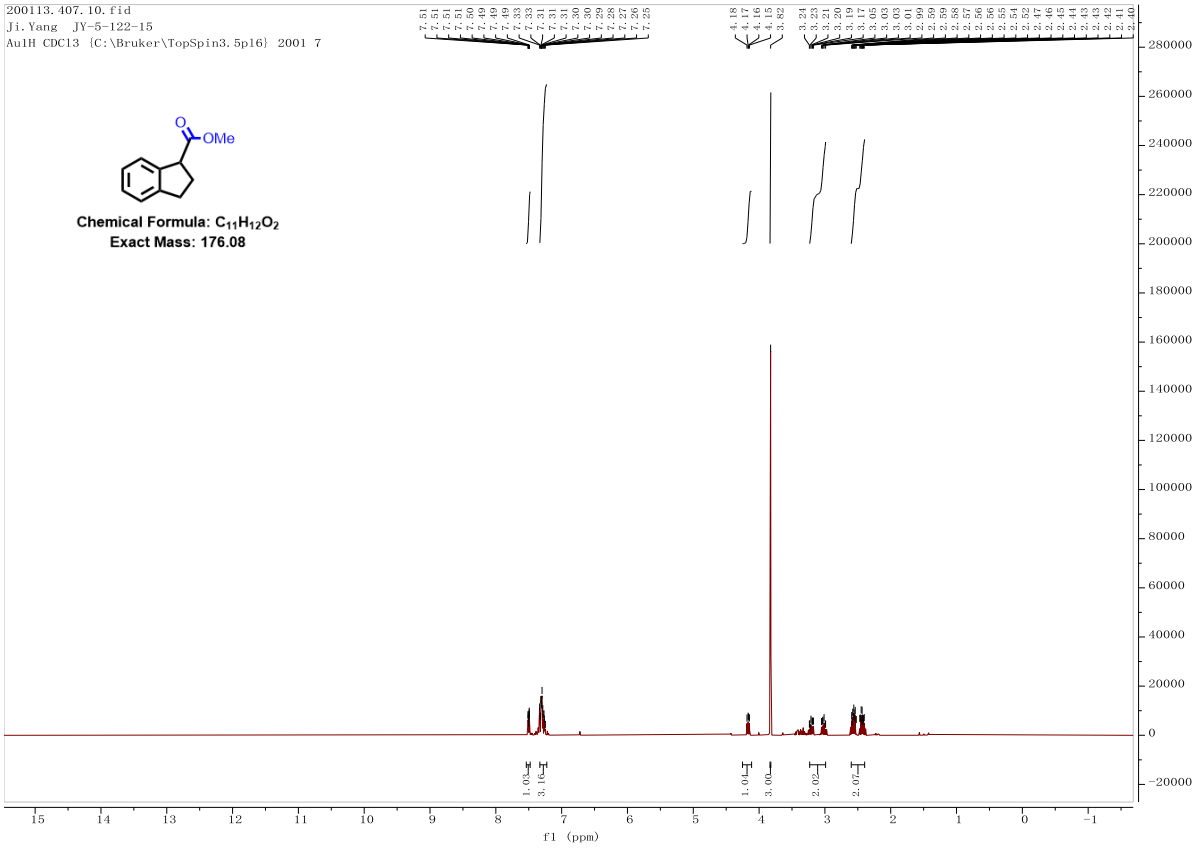
File :D:\MSDChem\1\DATA\2001\JY-5-122-13.D
Operator :
Acquired : 9 Jan 2020 22:54 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-13
Misc Info :
Vial Number: 48

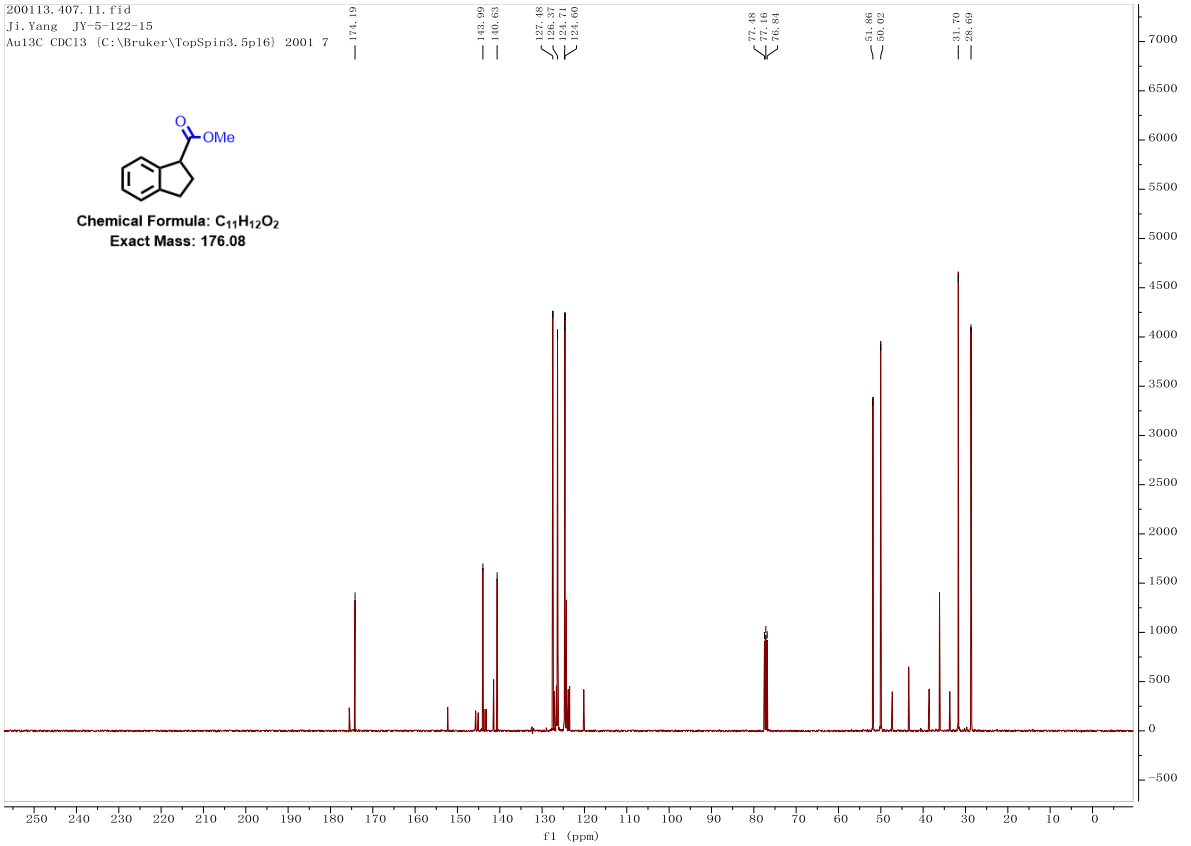


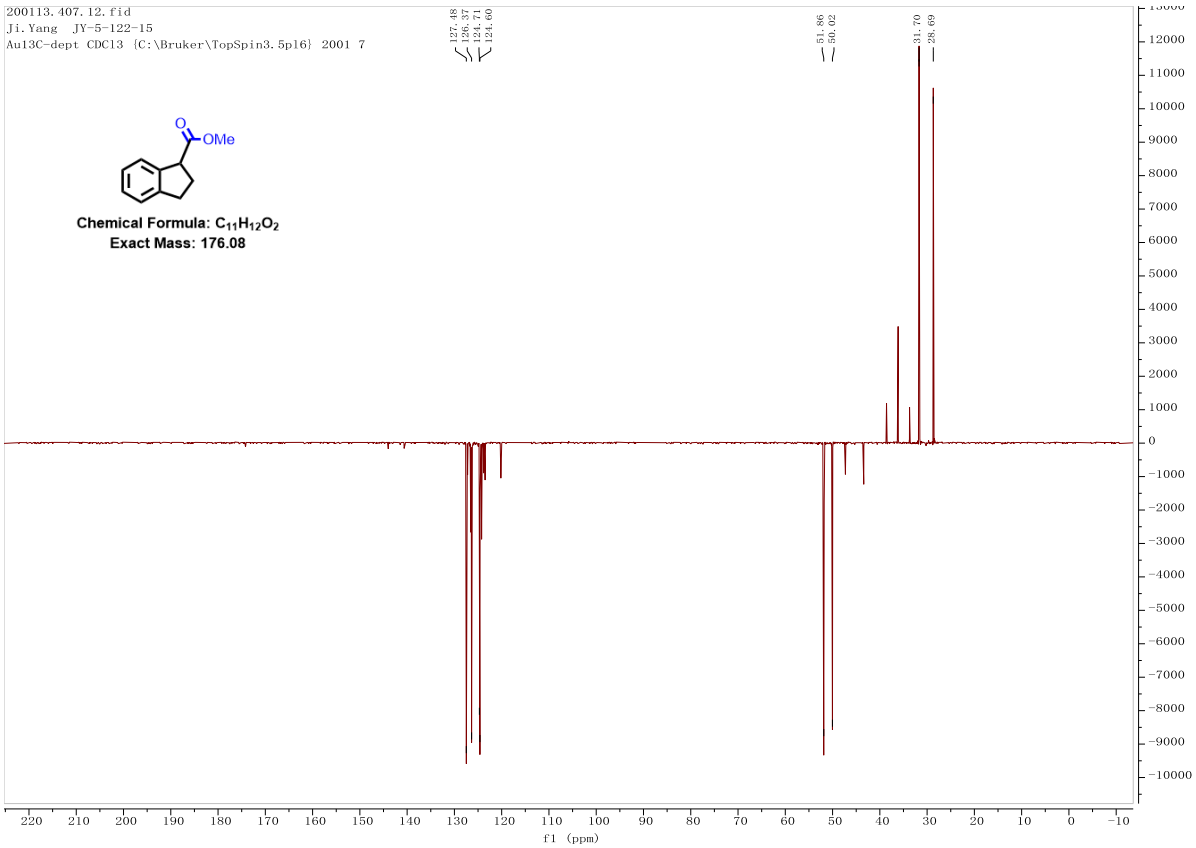




methyl-2,3-dihydro-1*H*-indene-1-carboxylate
Chemical Formula: $C_{11}H_{12}O_2$
Exact Mass: 176.08




200113.407.11.fid
Ji.Yang JY-5-122-15
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 7
174.19
143.99
140.63
127.48
126.37
124.71
124.60
77.48
77.16
76.84
51.86
50.02
31.70
28.69
OMe
Chemical Formula: C11H12O2
Exact Mass: 176.08
f1 (ppm)

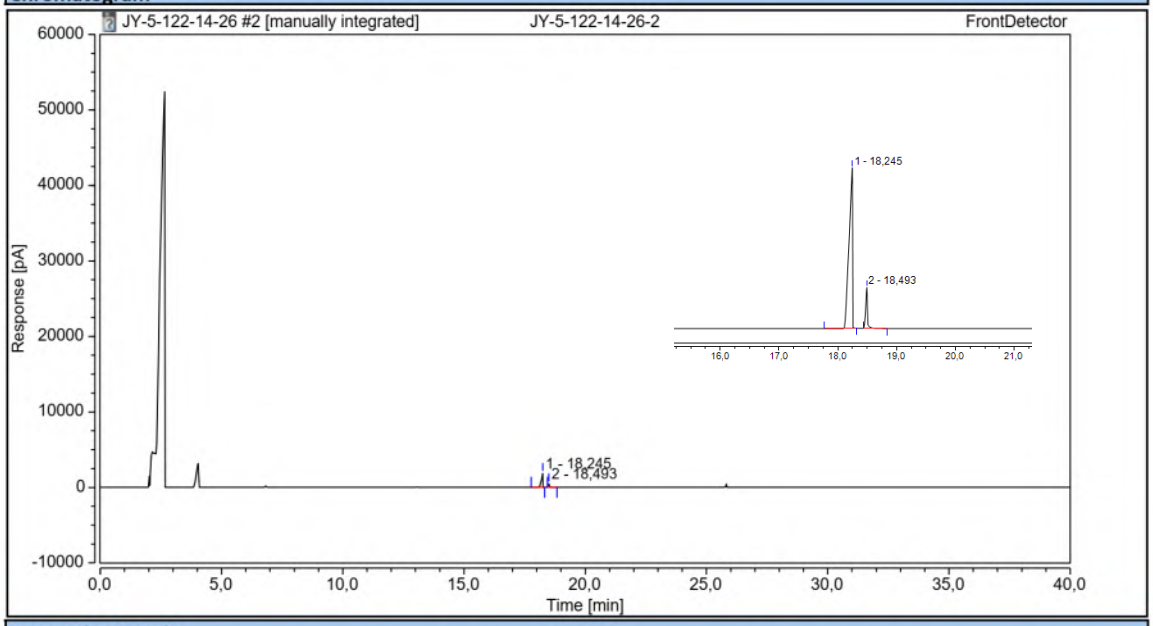

200113.407.12.fid
Ji.Yang JY-5-122-15
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 7
127.48
126.37
124.71
124.60
51.86
50.02
31.70
28.69
OMe
Chemical Formula: C11H12O2
Exact Mass: 176.08
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-14-26-2**	*Run Time (min):*	**40,00**
Vial Number:	**112**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 07:47**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		18,245	121,600	1824,910	88,49	79,75	n.a.
2		18,493	15,824	463,334	11,51	20,25	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**137,424**	**2288,244**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-15.D
Operator   :
Acquired   : 10 Jan 2020  10:38     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-15
Misc Info  :
Vial Number: 37
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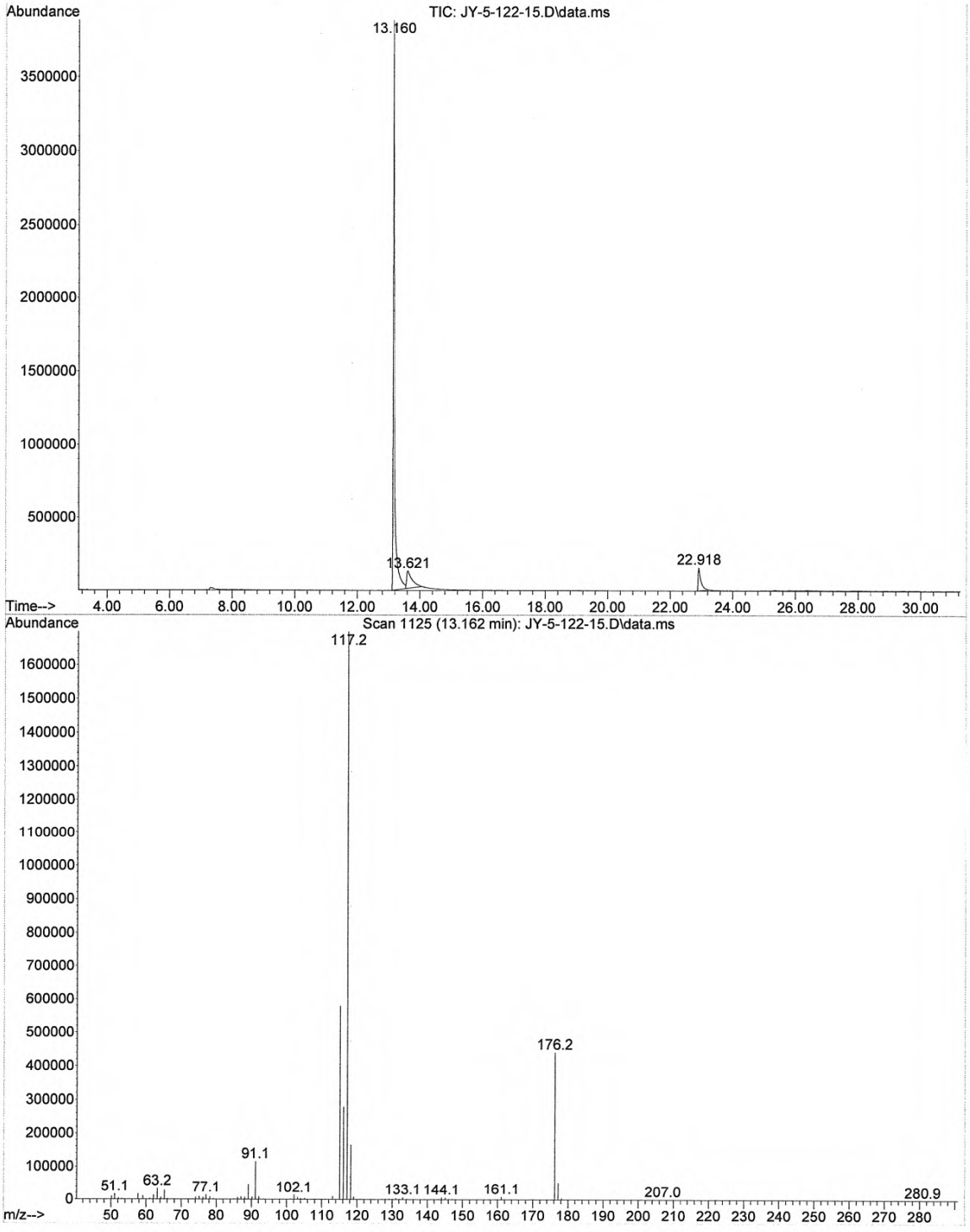
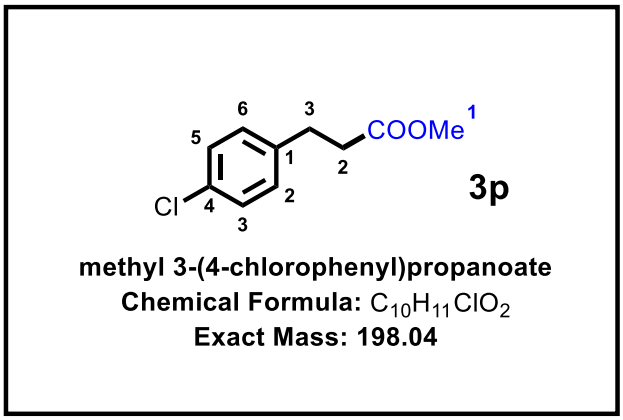
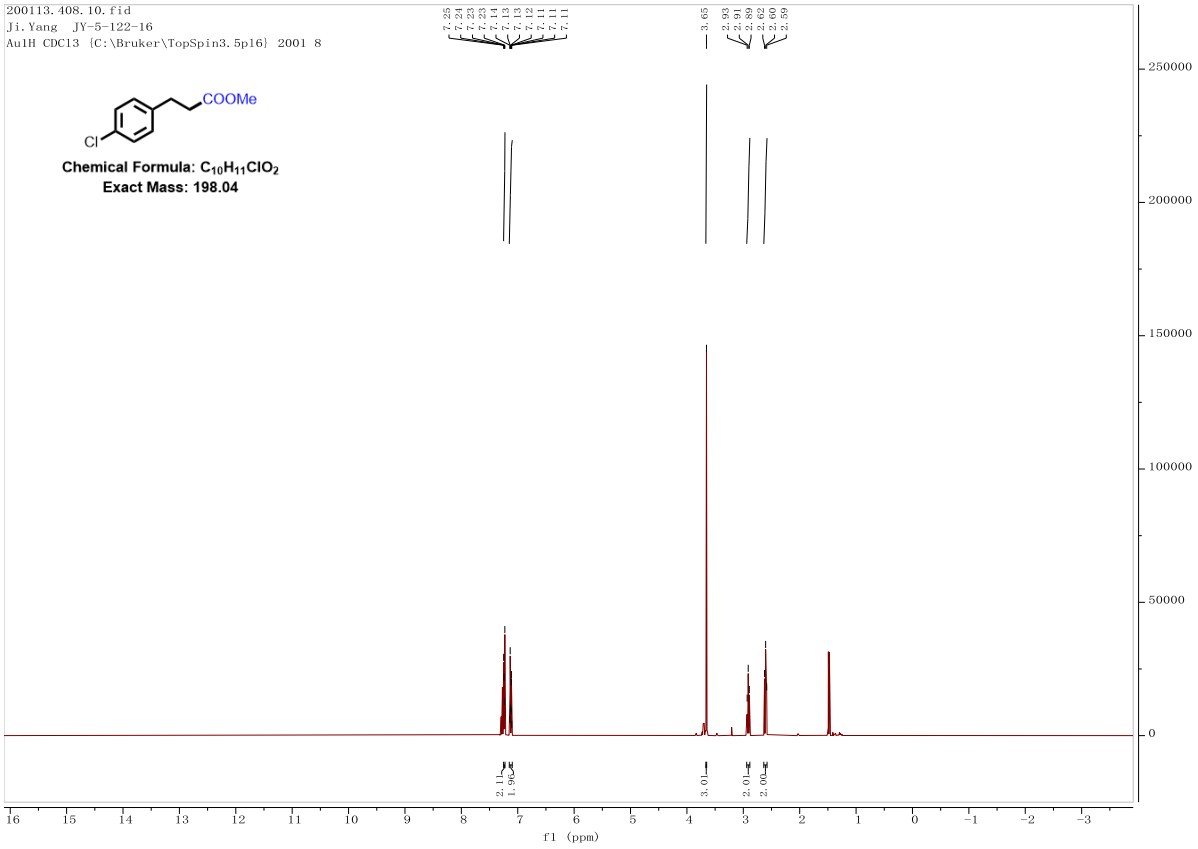
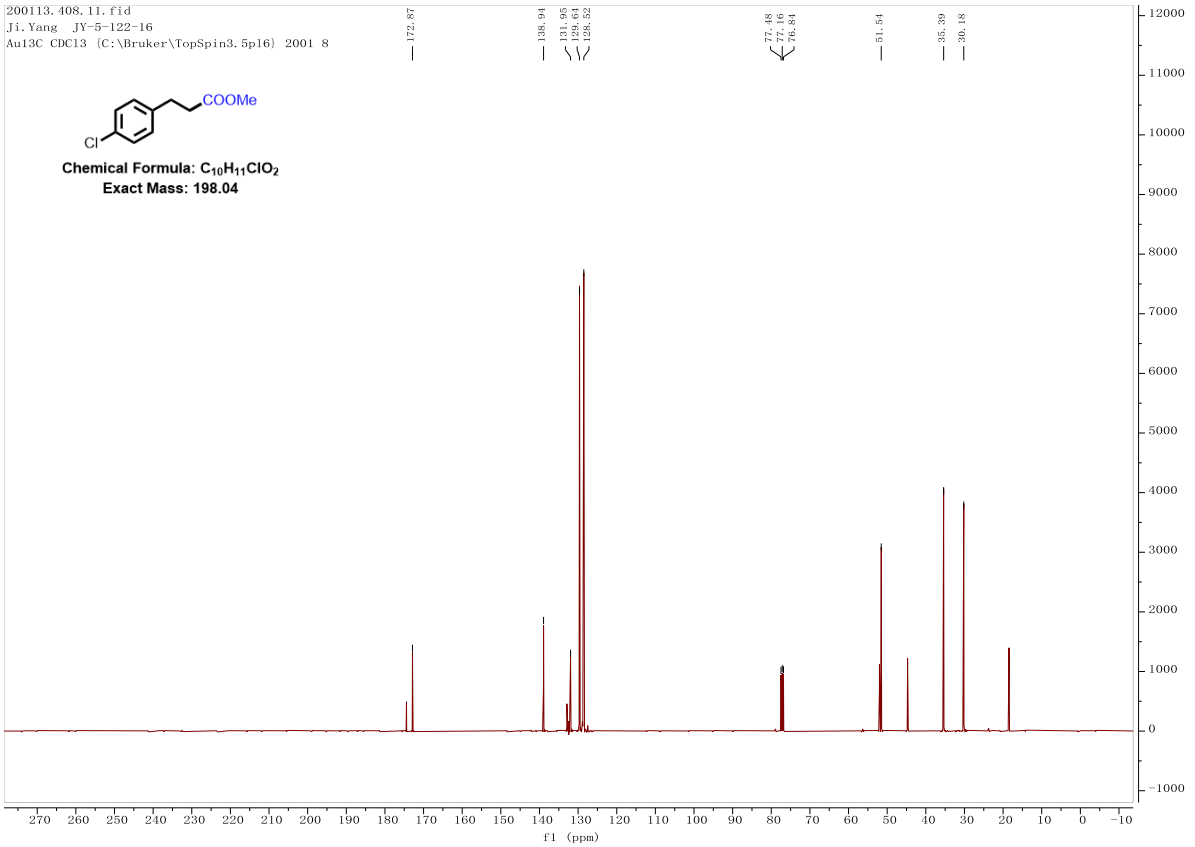
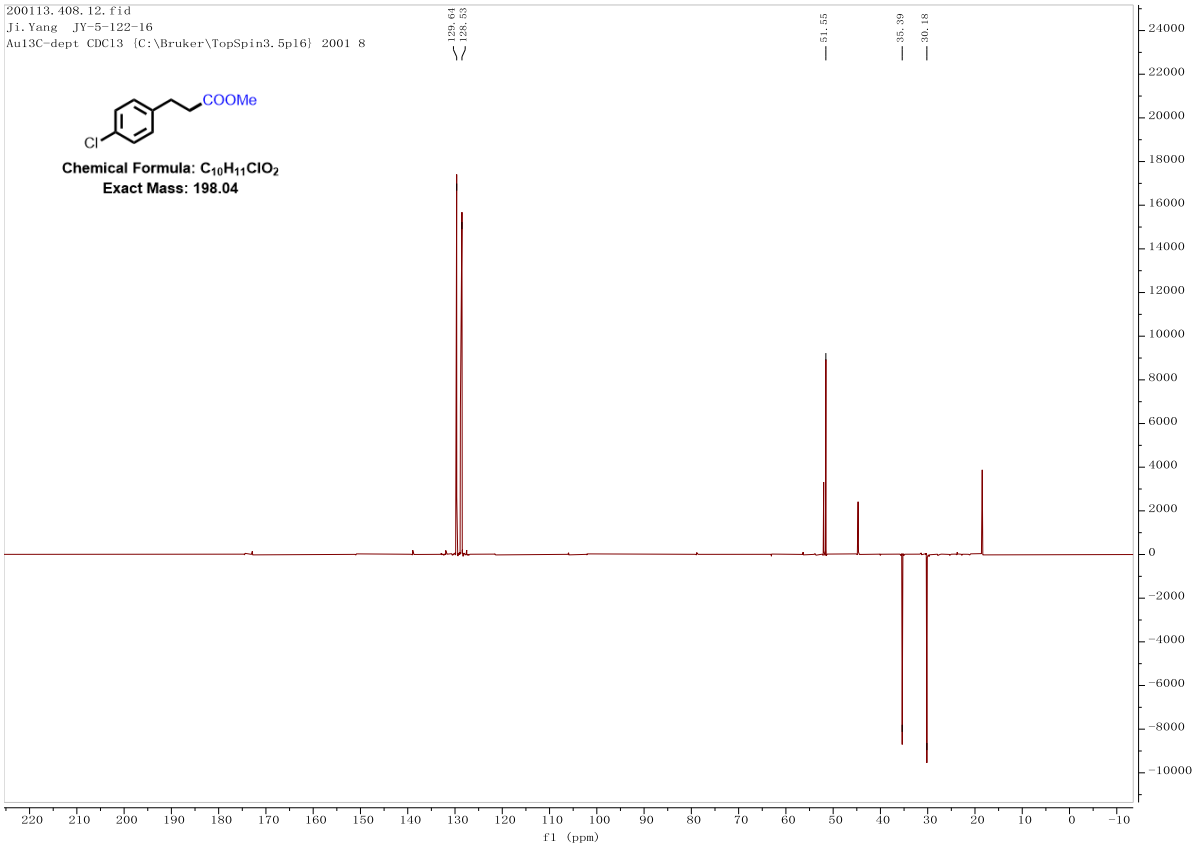




methyl 3-(4-chlorophenyl)propanoate
Chemical Formula: $C_{10}H_{11}ClO_2$
Exact Mass: 198.04




200113.408.11.fid
Ji.Yang JY-5-122-16
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 8
172.87
138.94
131.95
129.64
128.52
77.48
77.16
76.84
51.64
35.39
30.18
COOMe
Cl
Chemical Formula: C10H11ClO2
Exact Mass: 198.04
f1 (ppm)

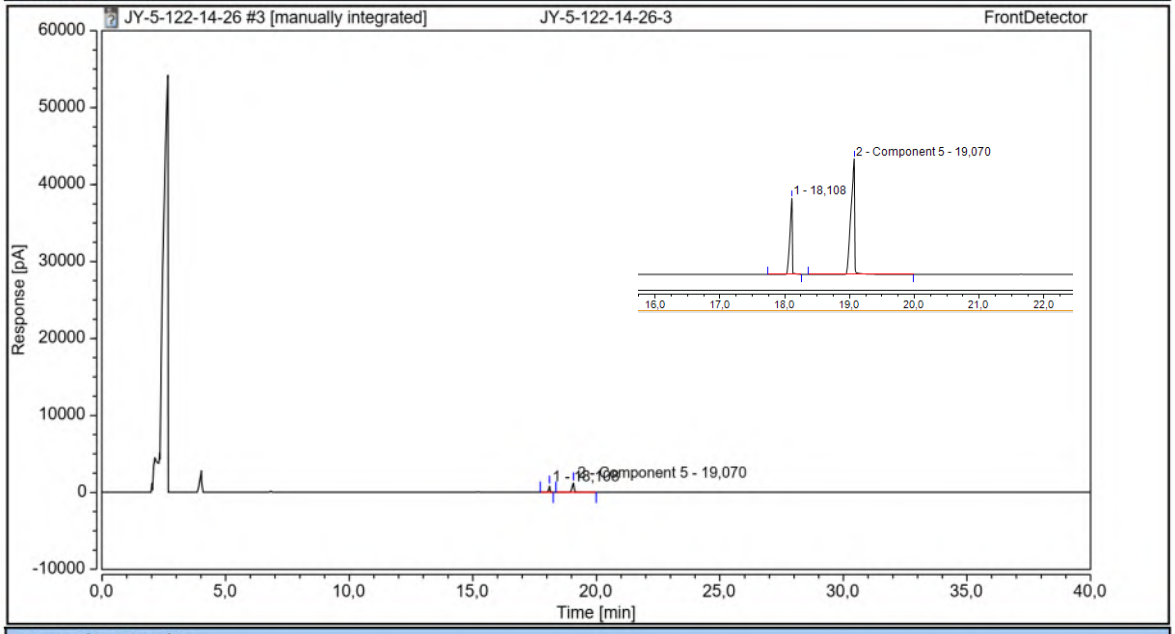

200113.408.12.fid
Ji.Yang JY-5-122-16
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 8
129.64
128.53
51.55
35.39
30.18
COOMe
Cl
Chemical Formula: C10H11ClO2
Exact Mass: 198.04
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-14-26-3**	*Run Time (min):*	**40,00**
Vial Number:	**113**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 08:48**	*Sample Weight:*	**1,0000**

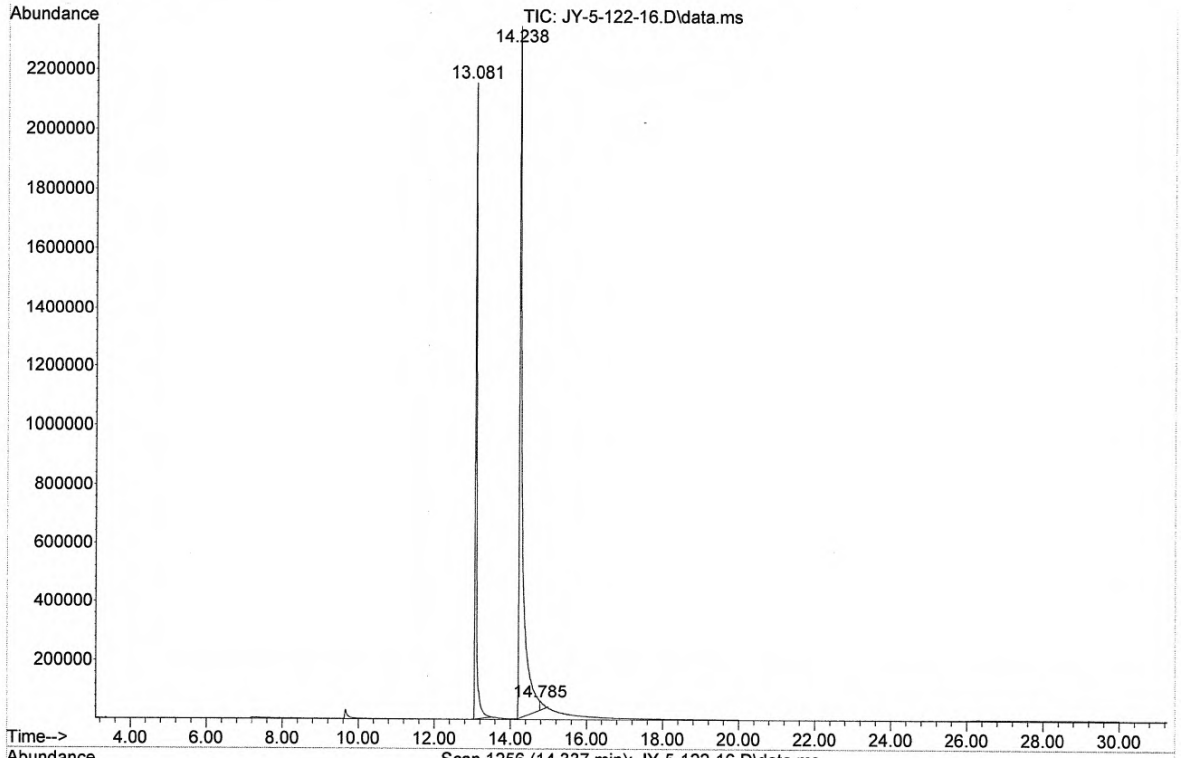
Chromatogram

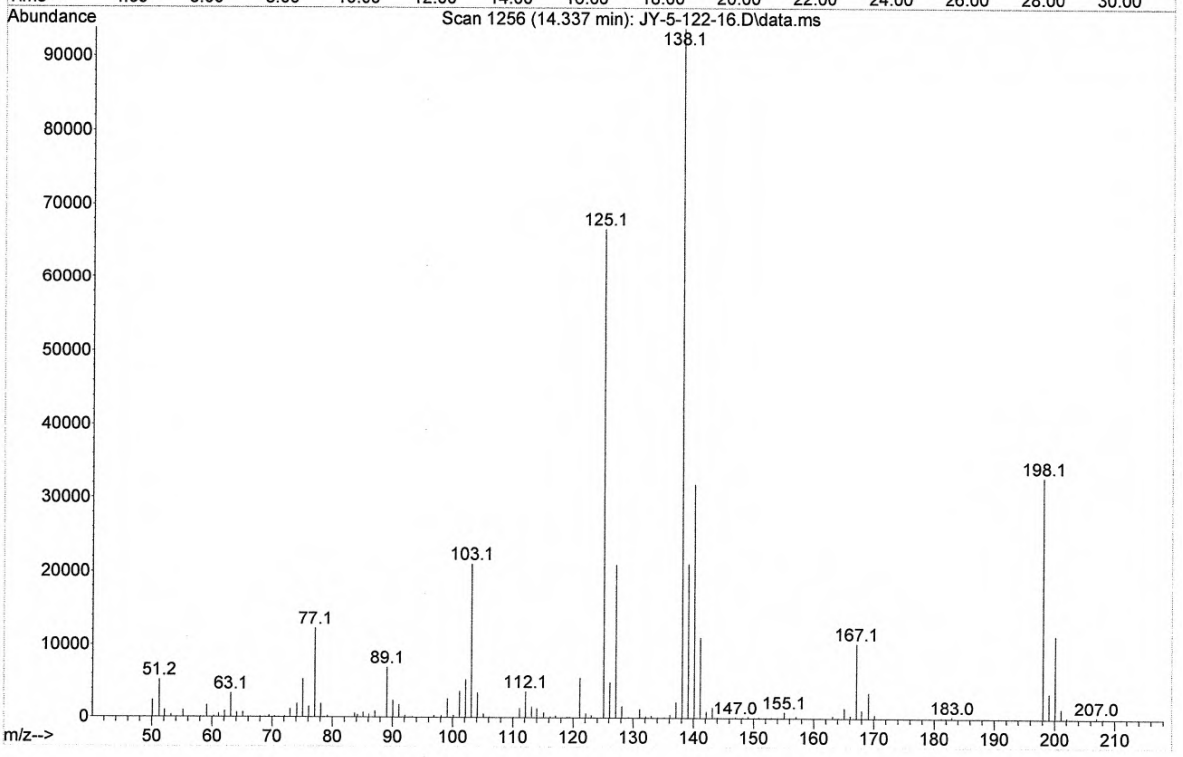


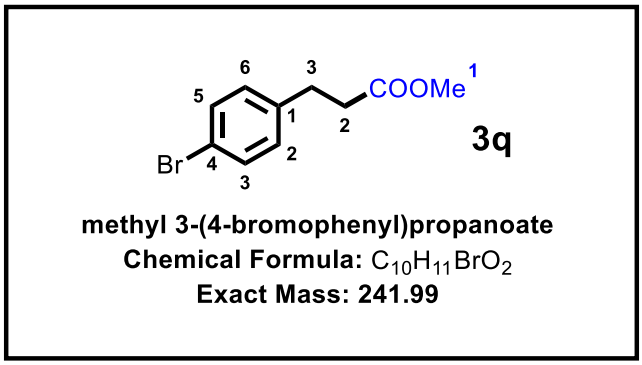
Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		18,108	32,949	786,789	28,98	39,72	n.a.
2	Component 5	19,070	80,751	1193,904	71,02	60,28	n.a.
Total:			**113,699**	**1980,692**	**100,00**	**100,00**	

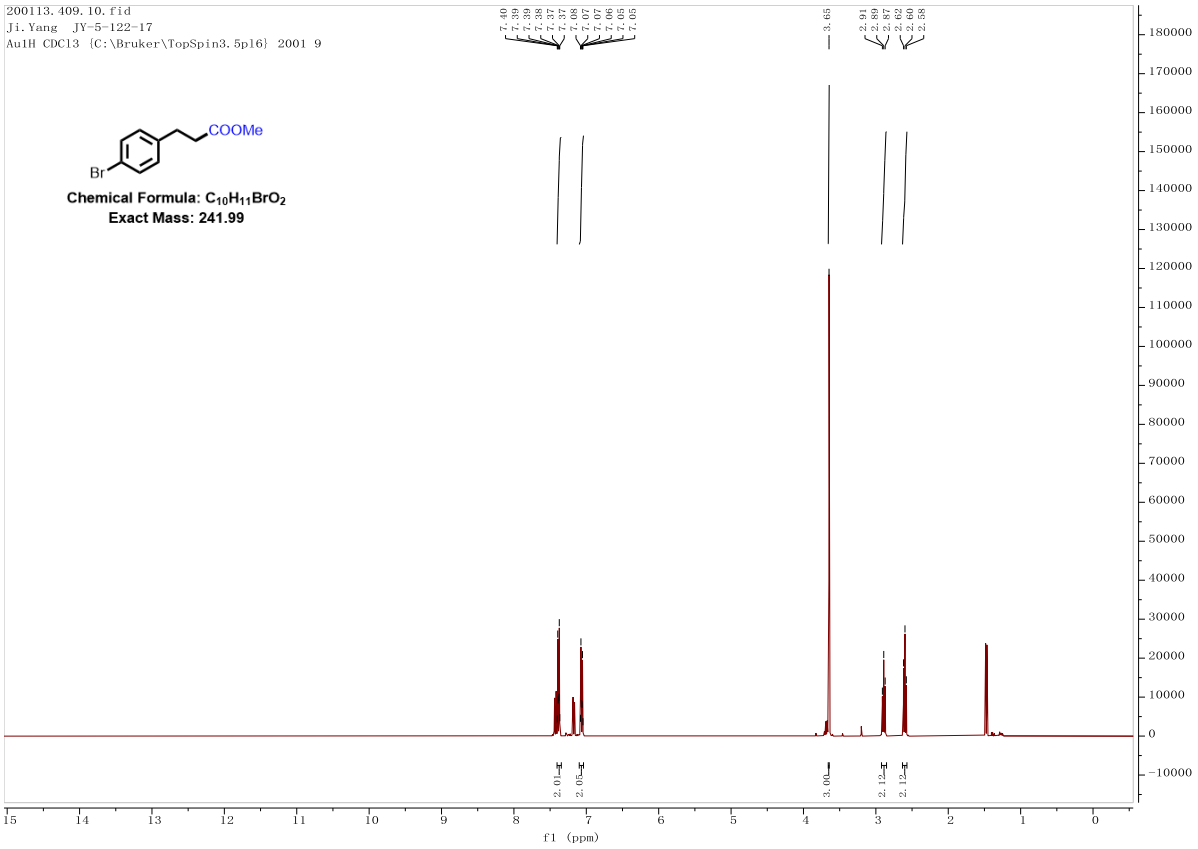
File :D:\MSDChem\1\DATA\2001\JY-5-122-16.D
Operator :
Acquired : 10 Jan 2020 11:55 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-16
Misc Info :
Vial Number: 38

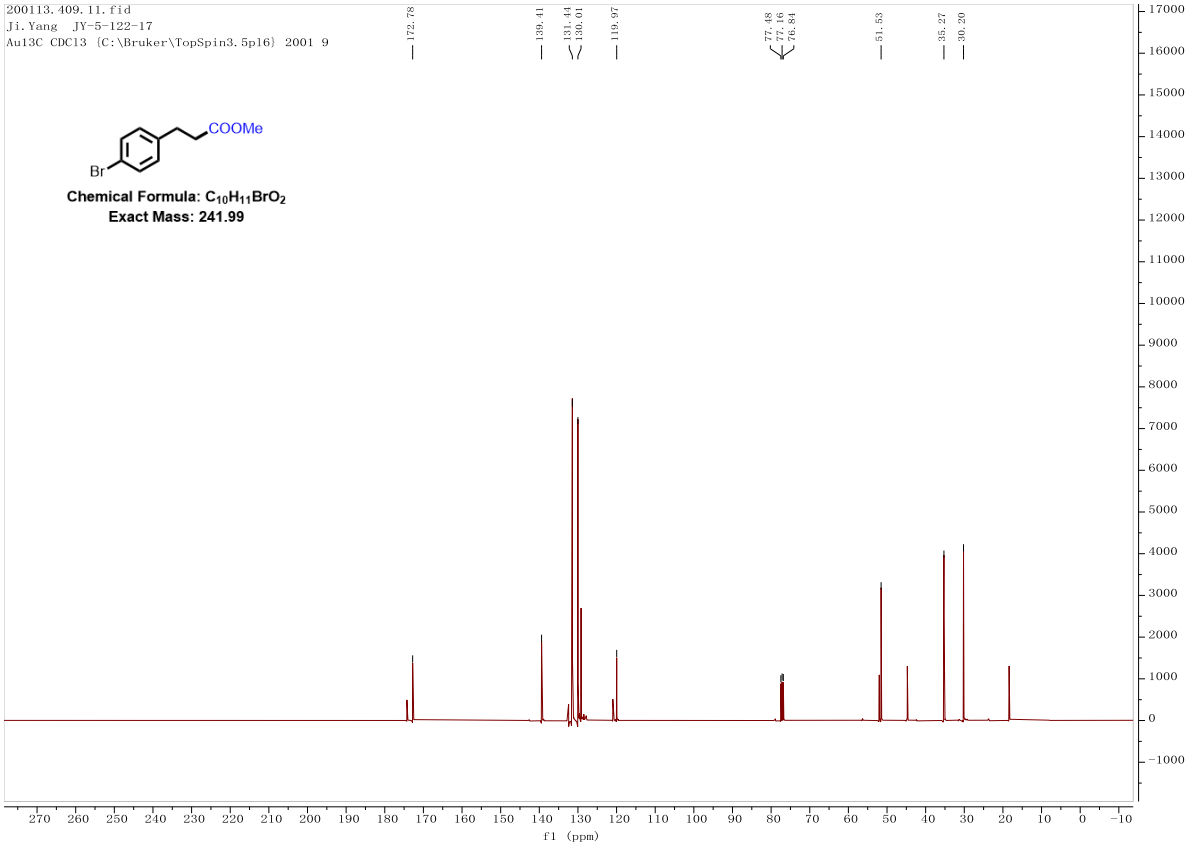


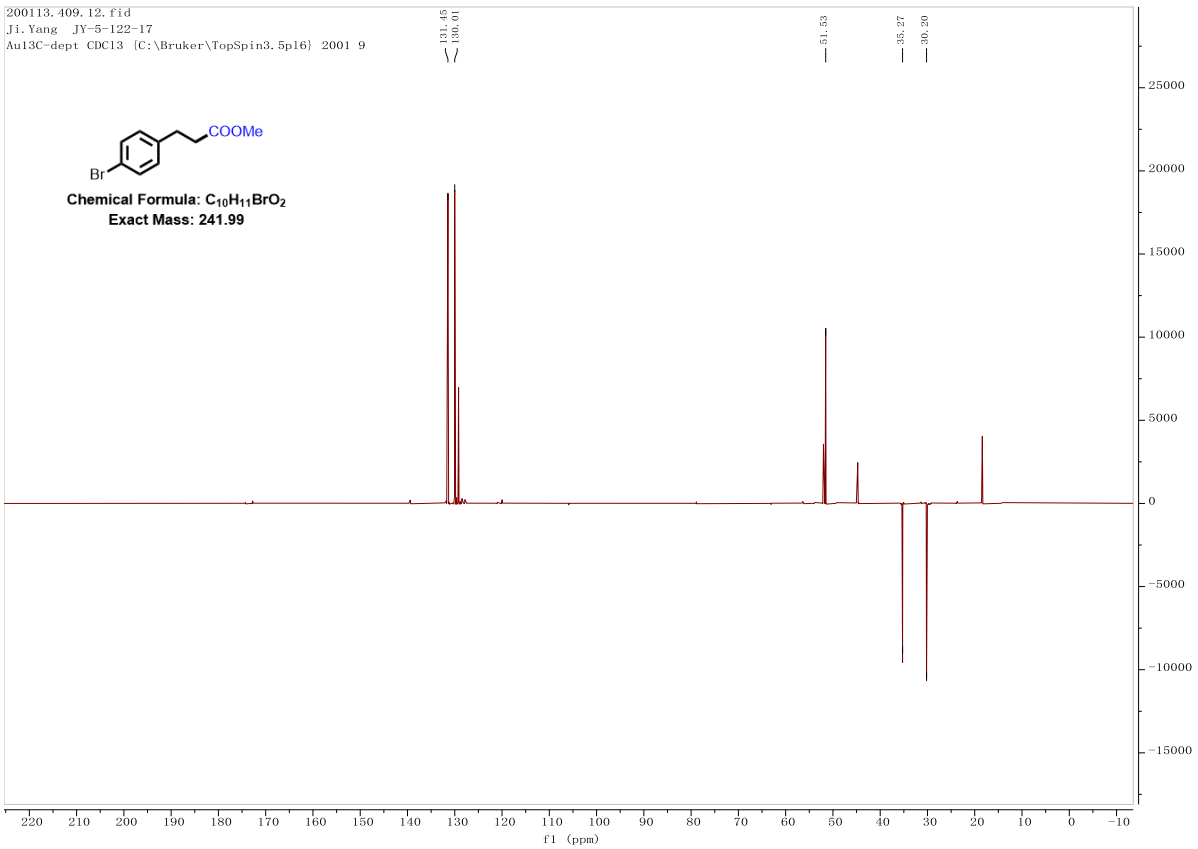




methyl 3-(4-bromophenyl)propanoate
Chemical Formula: $C_{10}H_{11}BrO_2$
Exact Mass: 241.99




200113.409.11.fid
Ji.Yang JY-5-122-17
Au13C CDCl3 {C:\Bruker\TopSpin3.5p16} 2001 9
172.78
139.41
131.44
130.01
119.97
77.48
77.16
76.84
51.53
35.27
30.20
COOMe
Br
Chemical Formula: C10H11BrO2
Exact Mass: 241.99
f1 (ppm)

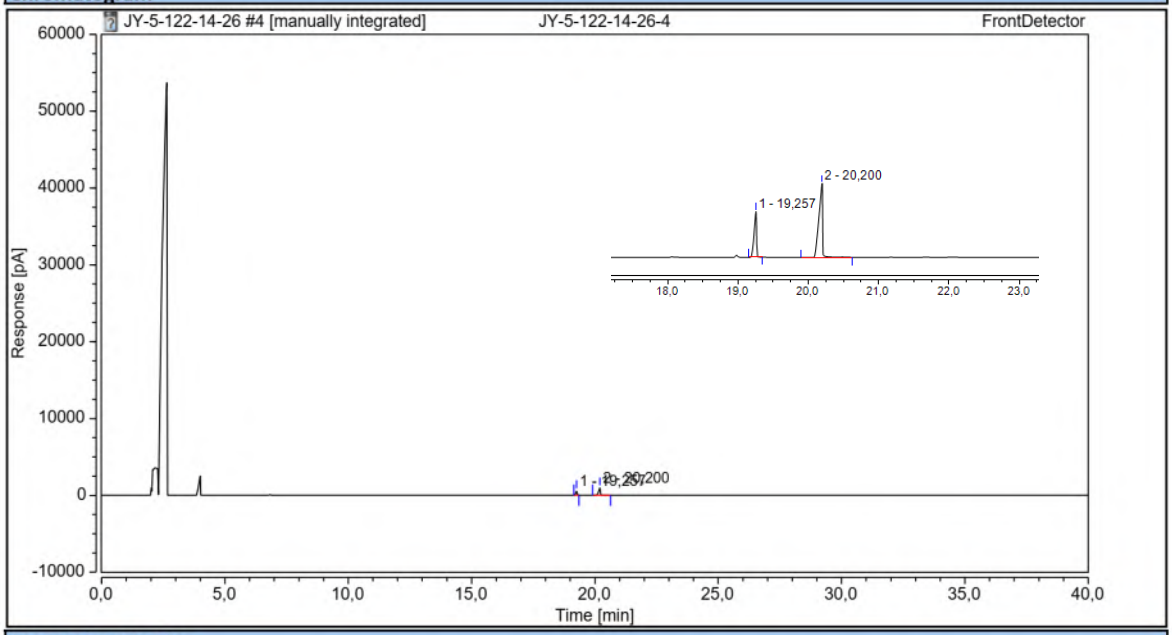

200113.409.12.fid
Ji.Yang JY-5-122-17
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5p16} 2001 9
131.45
130.01
51.53
35.27
30.20
COOMe
Br
Chemical Formula: C10H11BrO2
Exact Mass: 241.99
f1 (ppm)

Chromatogram and Results

Injection Details

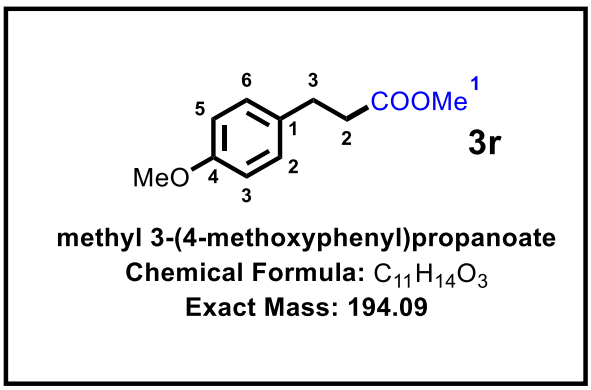
Injection Name:	**JY-5-122-14-26-4**	*Run Time (min):*	**40,00**
Vial Number:	**114**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 09:49**	*Sample Weight:*	**1,0000**

Chromatogram

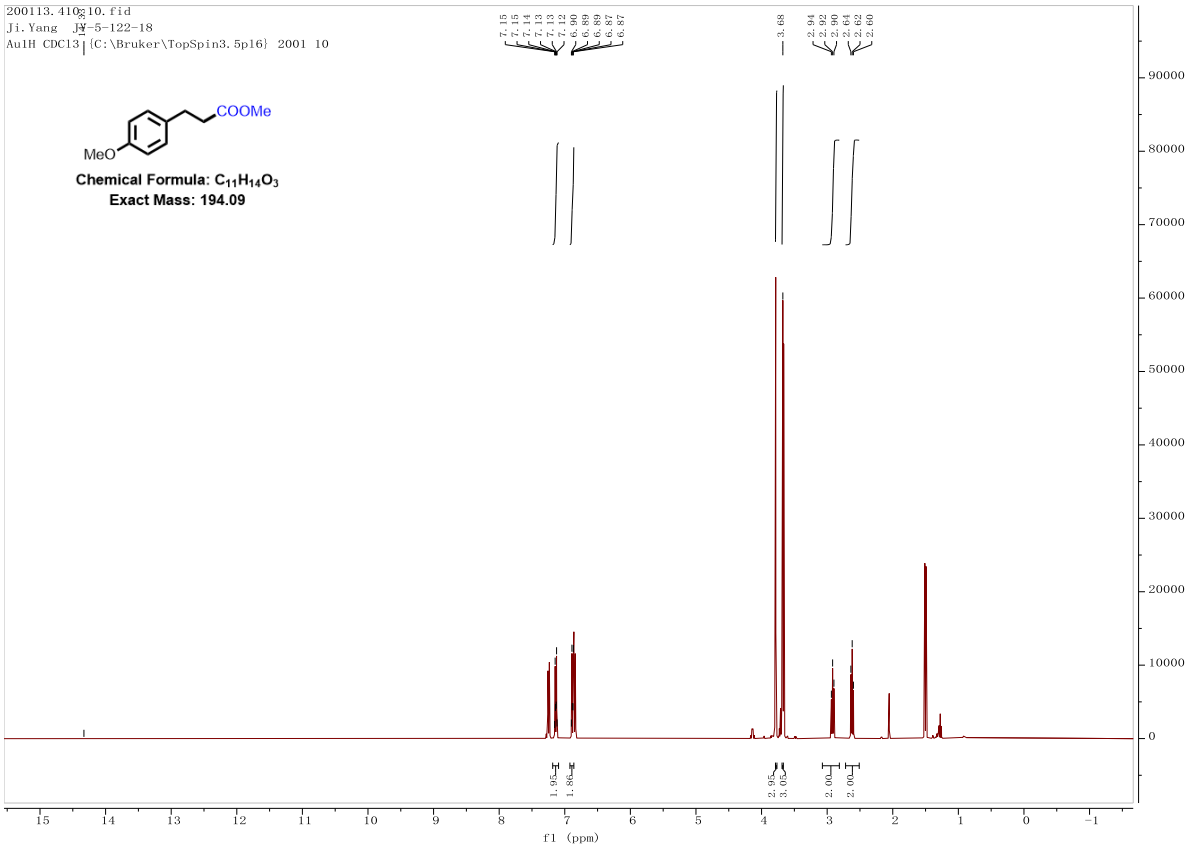


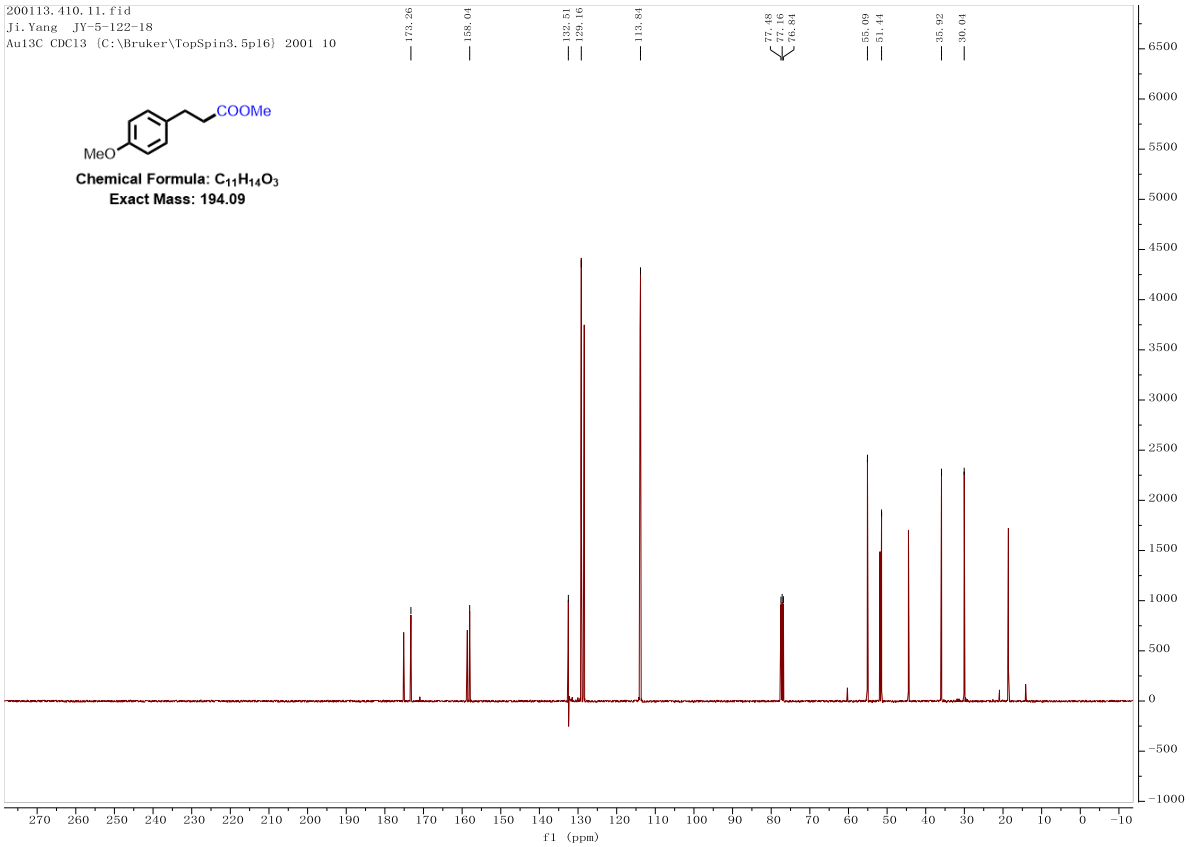
Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		19,257	22,686	579,135	28,26	38,22	n.a.
2		20,200	57,588	936,177	71,74	61,78	n.a.
Total:			**80,273**	**1515,312**	**100,00**	**100,00**	



methyl 3-(4-methoxyphenyl)propanoate
Chemical Formula: $C_{11}H_{14}O_3$
Exact Mass: 194.09

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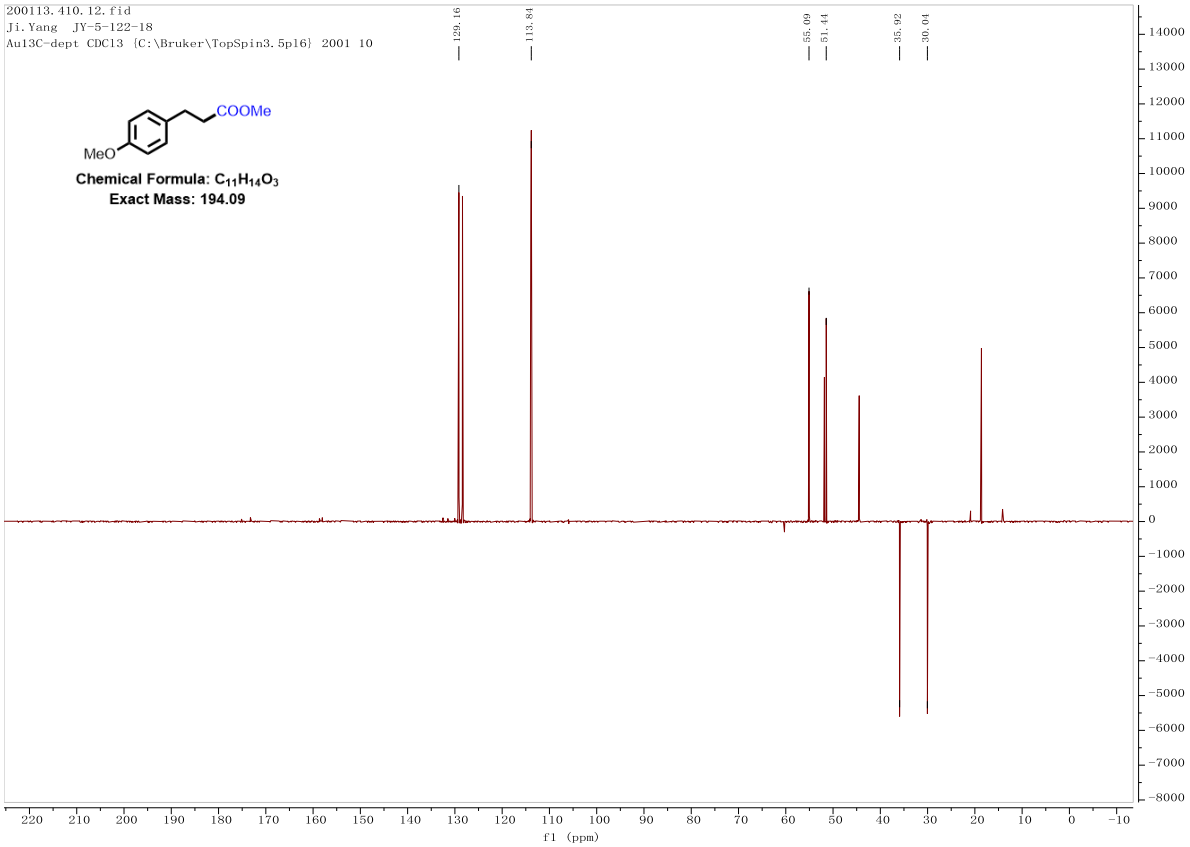
Ji.Yang JY-5-122-18
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 10
173.26
158.04
132.51
129.16
113.84
77.48
77.16
76.84
55.09
51.44
35.92
30.04
COOMe
MeO
Chemical Formula: C11H14O3
Exact Mass: 194.09
f1 (ppm)

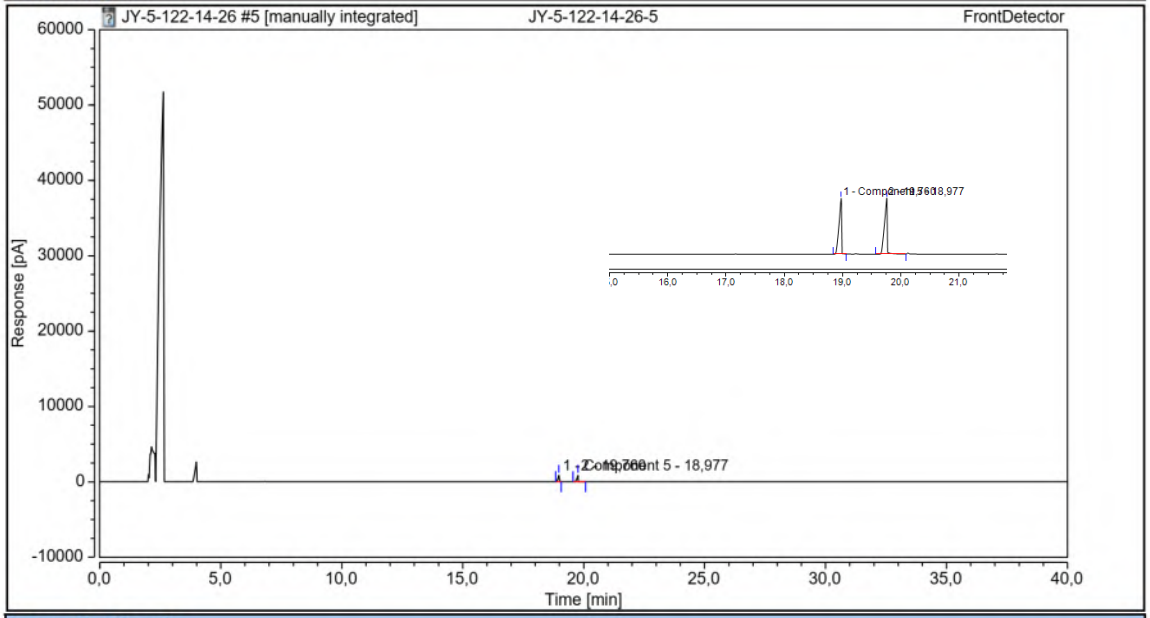

200113.410.12.fid
Ji.Yang JY-5-122-18
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 10
129.16
113.84
55.09
51.44
35.92
30.04
COOMe
MeO
Chemical Formula: C11H14O3
Exact Mass: 194.09
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-14-26-5**	*Run Time (min):*	**40,00**
Vial Number:	**115**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**10.Jan.20 10:51**	*Sample Weight:*	**1,0000**

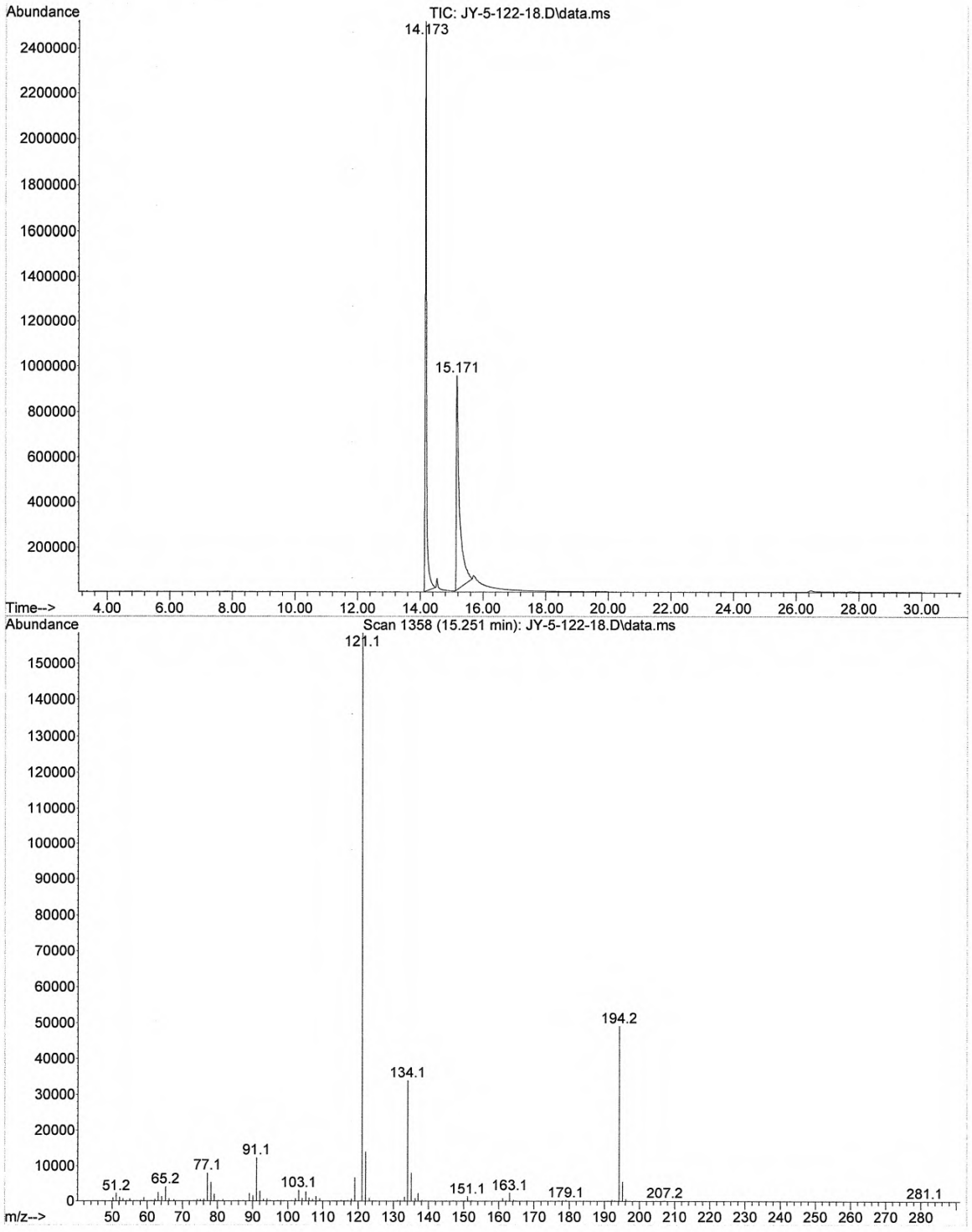
Chromatogram

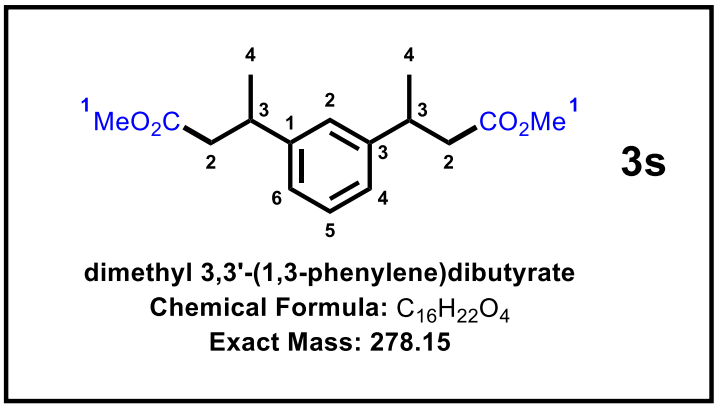


Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1	Component 5	18,977	43,034	853,471	47,63	49,84	n.a.
2		19,760	47,318	858,890	52,37	50,16	n.a.
Total:			**90,352**	**1712,361**	**100,00**	**100,00**	

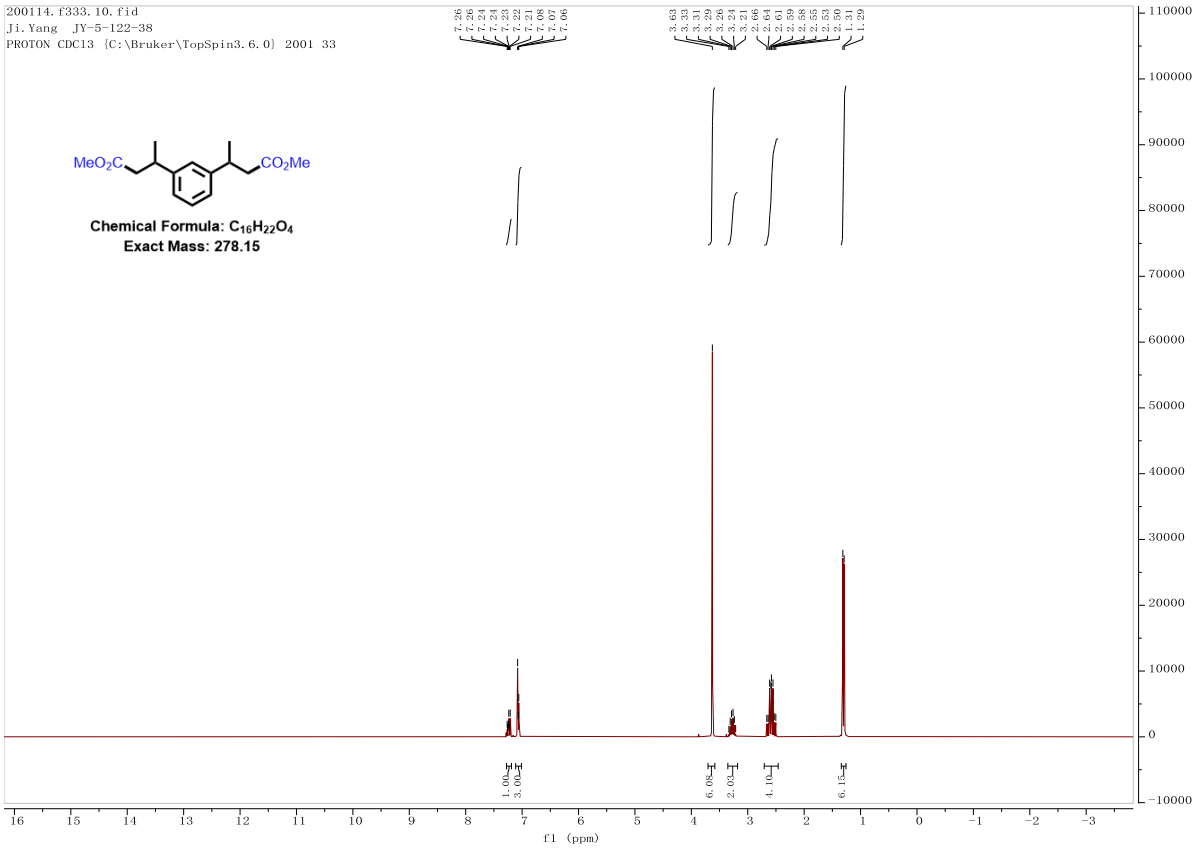
File :D:\MSDChem\1\DATA\2001\JY-5-122-18.D
Operator :
Acquired : 10 Jan 2020 13:13 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-18
Misc Info :
Vial Number: 40

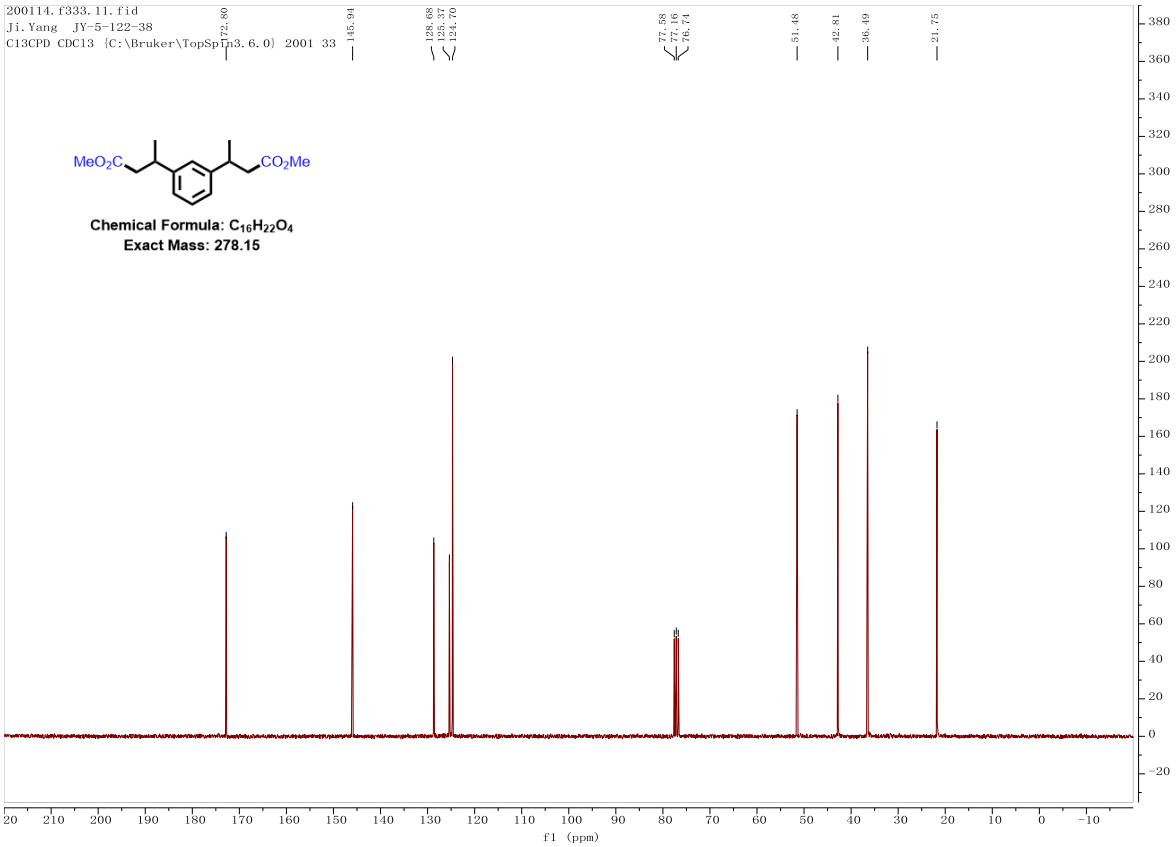


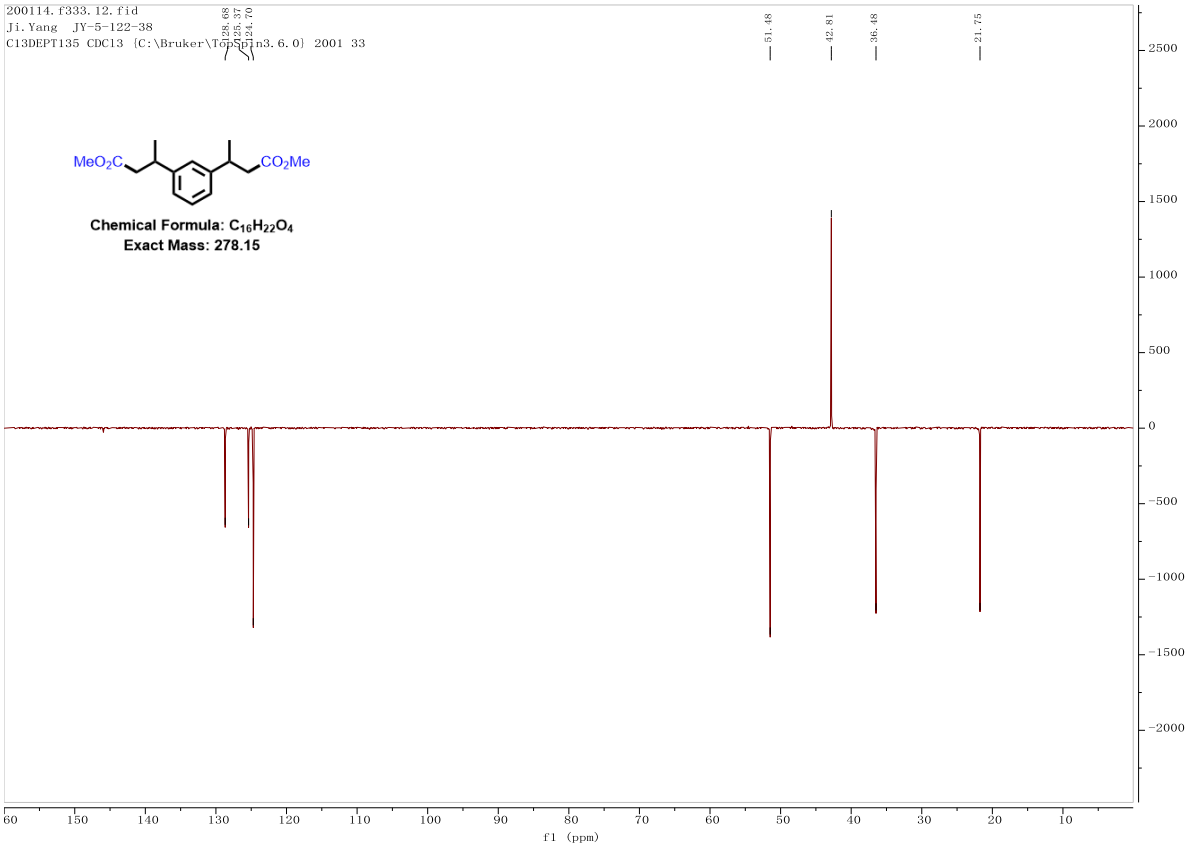


3s

dimethyl 3,3'-(1,3-phenylene)dibutyrate
Chemical Formula: $C_{16}H_{22}O_4$
Exact Mass: 278.15




200114.f333.11.fid
Ji.Yang JY-5-122-38
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 33
172.80
145.94
138.68
125.37
124.70
77.58
77.16
76.74
51.48
42.81
36.49
21.75
MeO2C
CO2Me
Chemical Formula: C16H22O4
Exact Mass: 278.15
f1 (ppm)

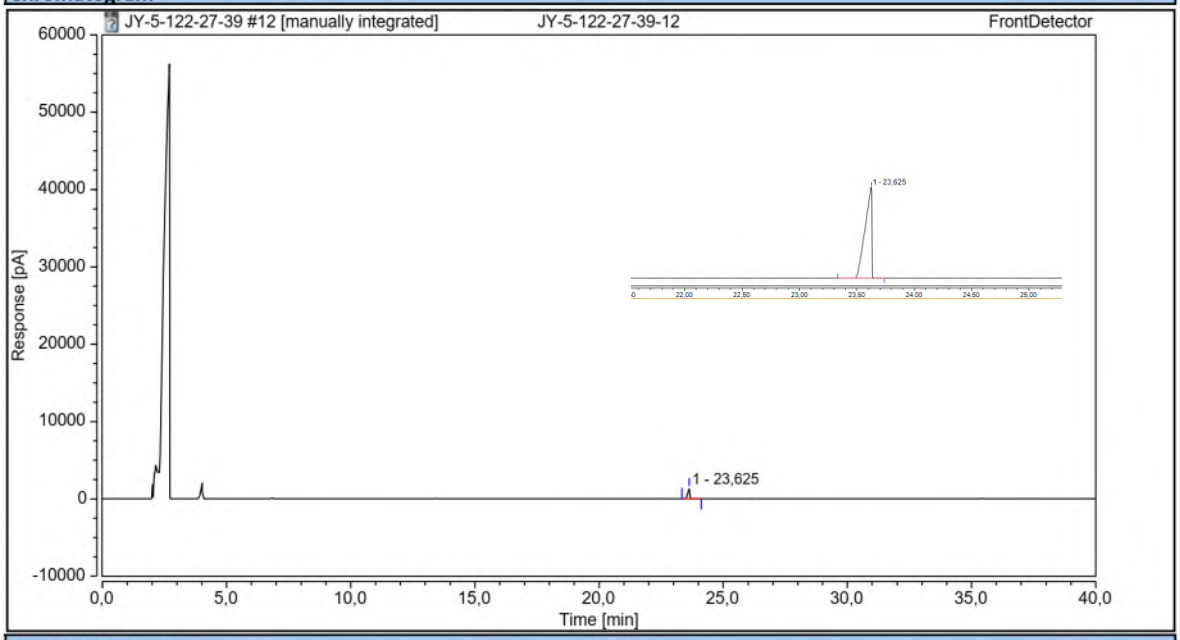

200114.f333.12.fid
Ji.Yang JY-5-122-38
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 33
128.68
125.37
124.70
51.48
42.81
36.48
21.75
MeO2C
CO2Me
Chemical Formula: C16H22O4
Exact Mass: 278.15
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-12**	*Run Time (min):*	**40,00**
Vial Number:	**36**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**12.Jan.20 00:32**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		23,625	88,066	1289,907	100,00	100,00	n.a.
Total:			**88,066**	**1289,907**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-38.D
Operator   :
Acquired   : 11 Jan 2020  23:03     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-38
Misc Info  :
Vial Number: 42
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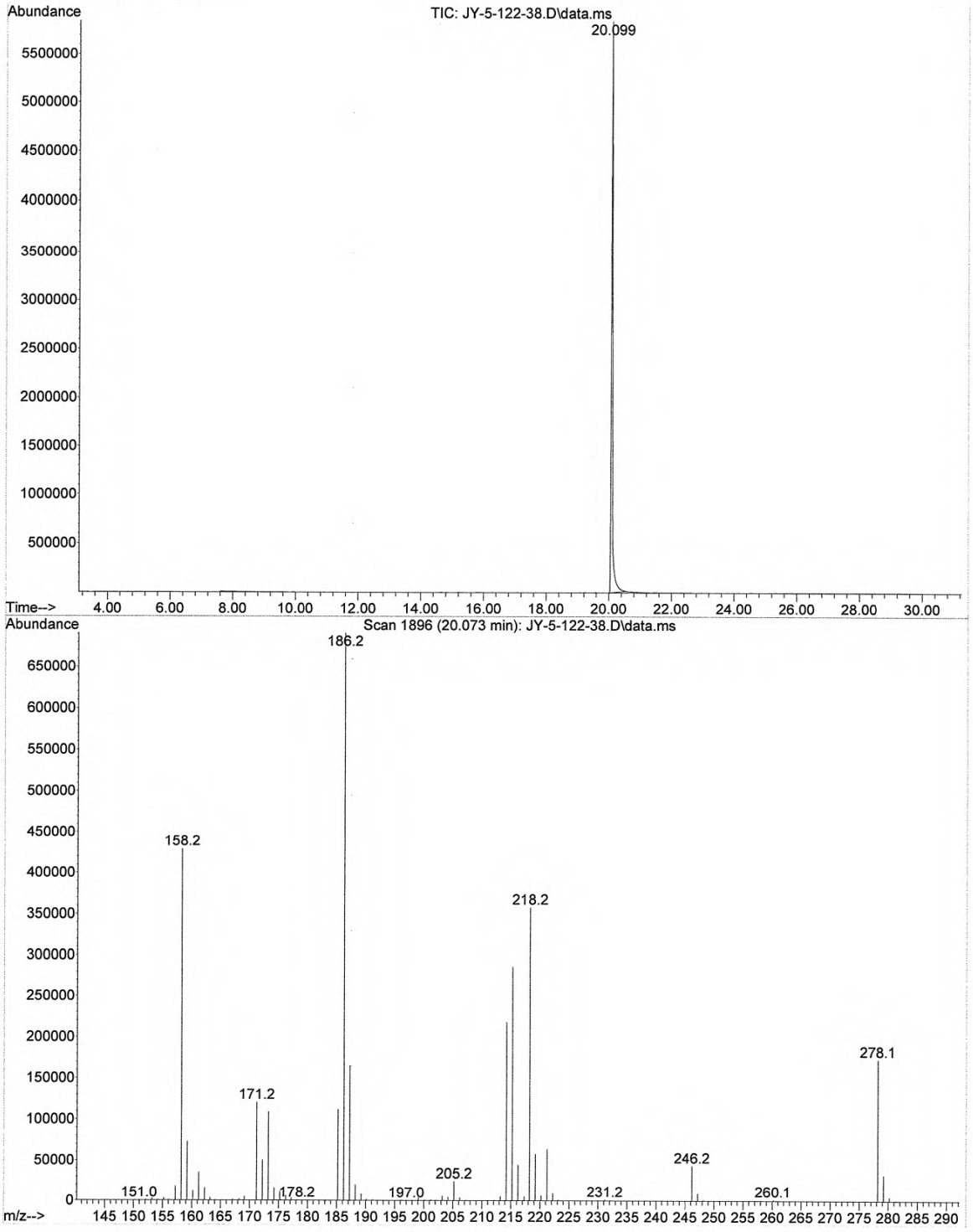
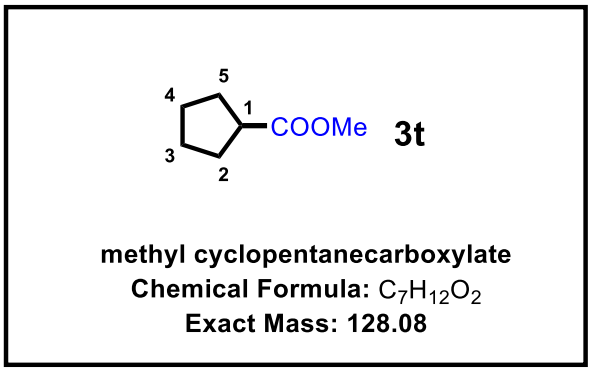
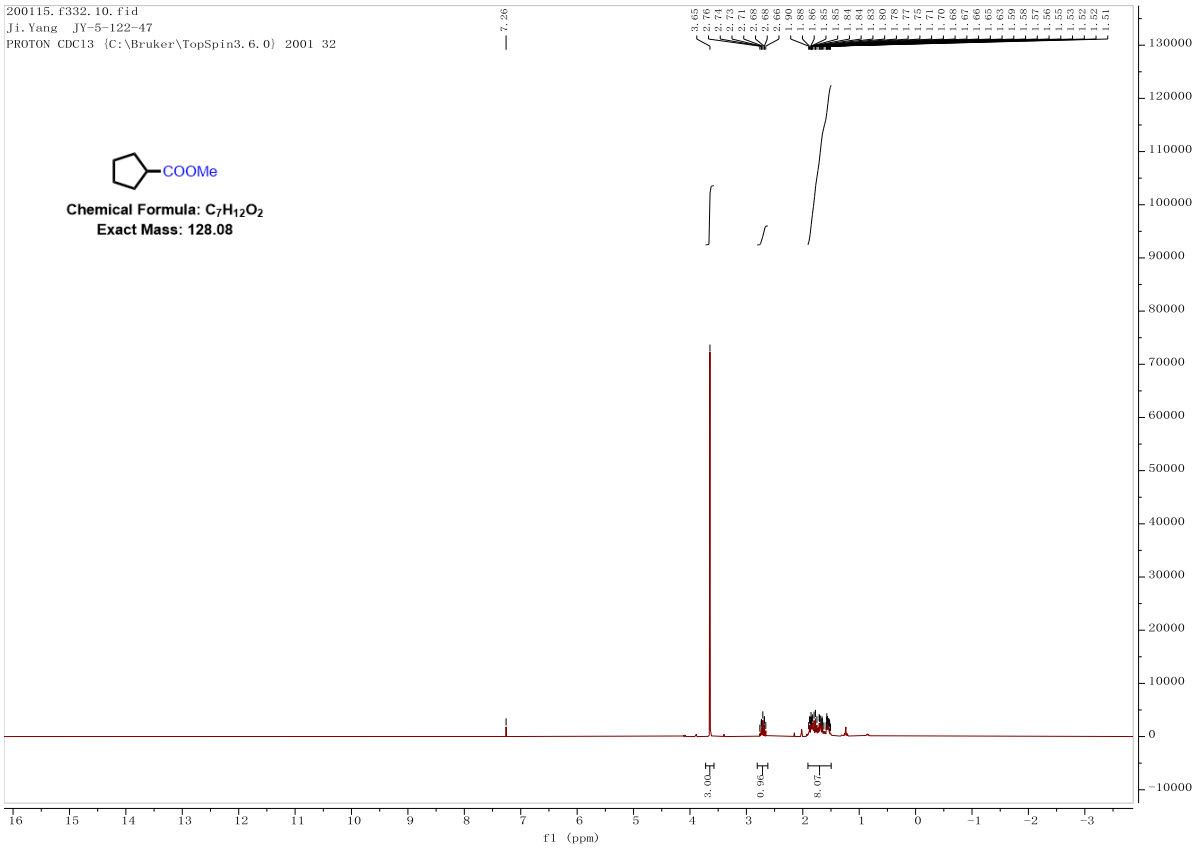
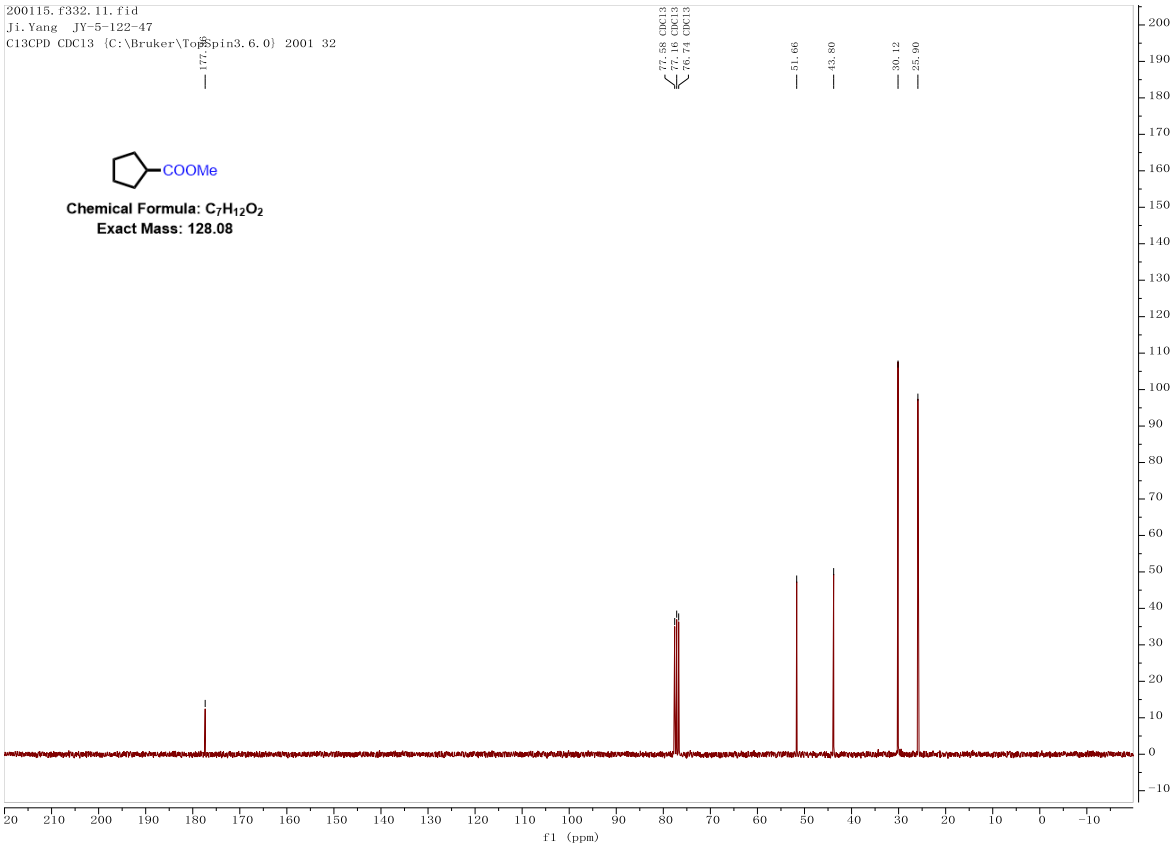
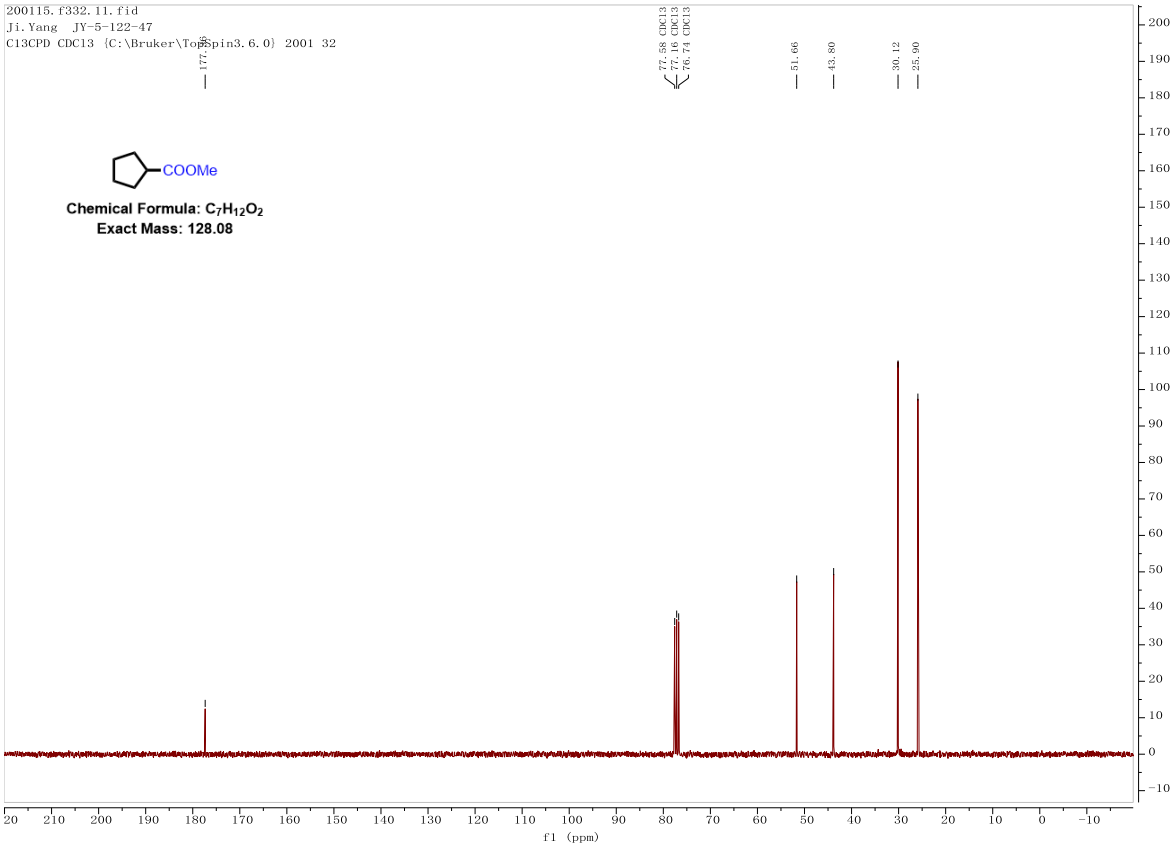



5
4
1
COOMe
3t
3
2
methyl cyclopentanecarboxylate
Chemical Formula: C7H12O2
Exact Mass: 128.08


200115.f332.10.fid
Ji.Yang JY-5-122-47
PROTON CDC13 {C:\Bruker\TopSpin3.6.0} 2001 32
COOMe
Chemical Formula: C7H12O2
Exact Mass: 128.08
f1 (ppm)


200115.f332.11.fid
Ji.Yang JY-5-122-47
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 32
177.26
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
51.66
43.80
30.12
25.90
COOMe
Chemical Formula: C7H12O2
Exact Mass: 128.08
f1 (ppm)

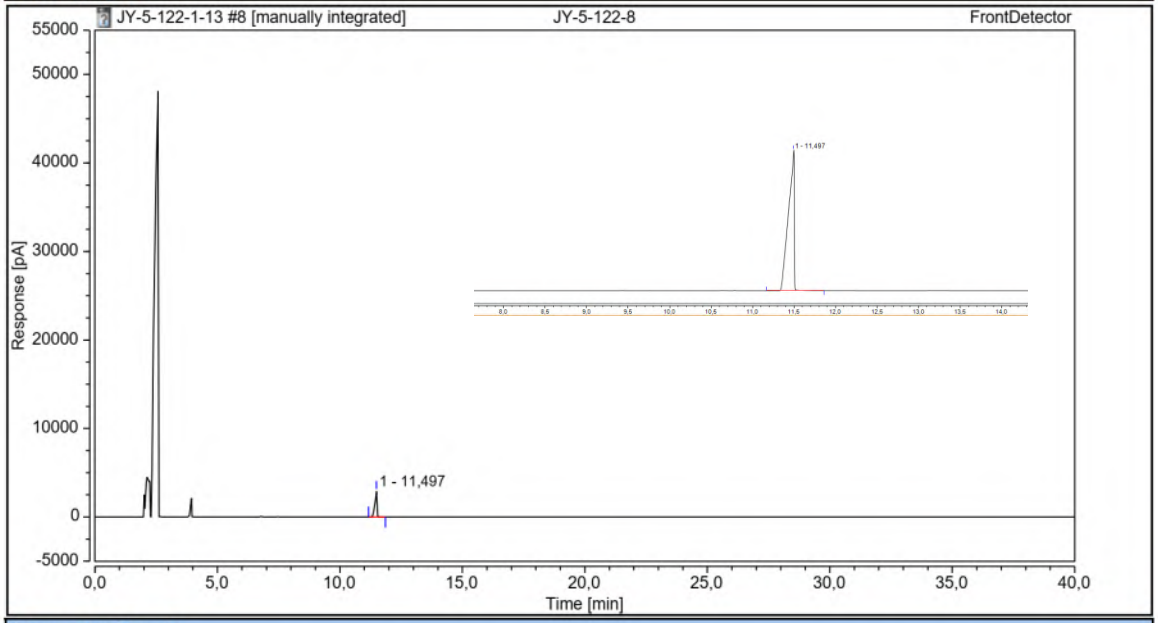

200115.f332.11.fid
Ji.Yang JY-5-122-47
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 32
177.26
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
51.66
43.80
30.12
25.90
COOMe
Chemical Formula: C7H12O2
Exact Mass: 128.08
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-8**	*Run Time (min):*	**40,00**
Vial Number:	**68**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 22:34**	*Sample Weight:*	**1,0000**

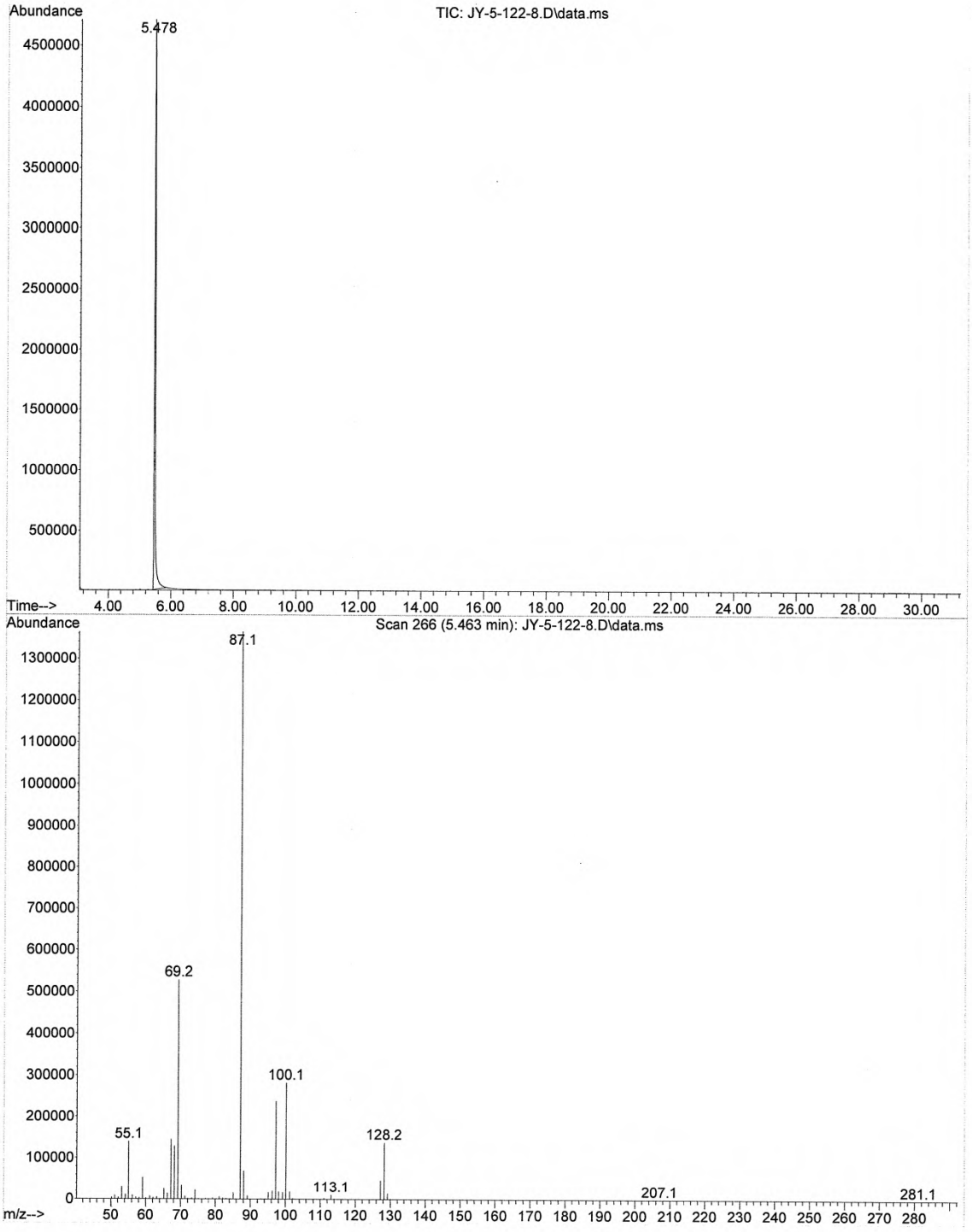
Chromatogram

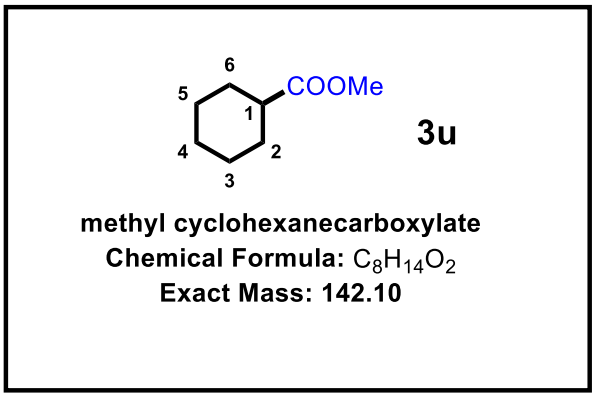


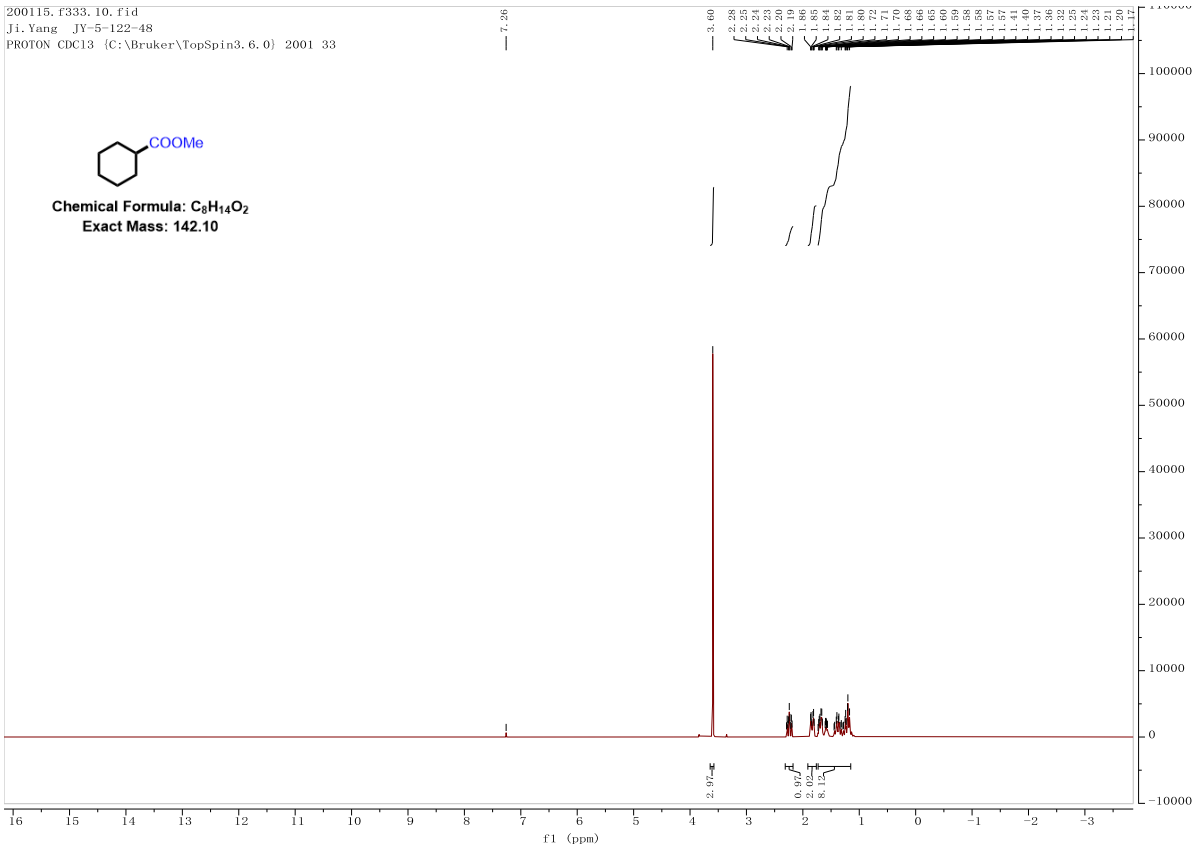
Integration Results

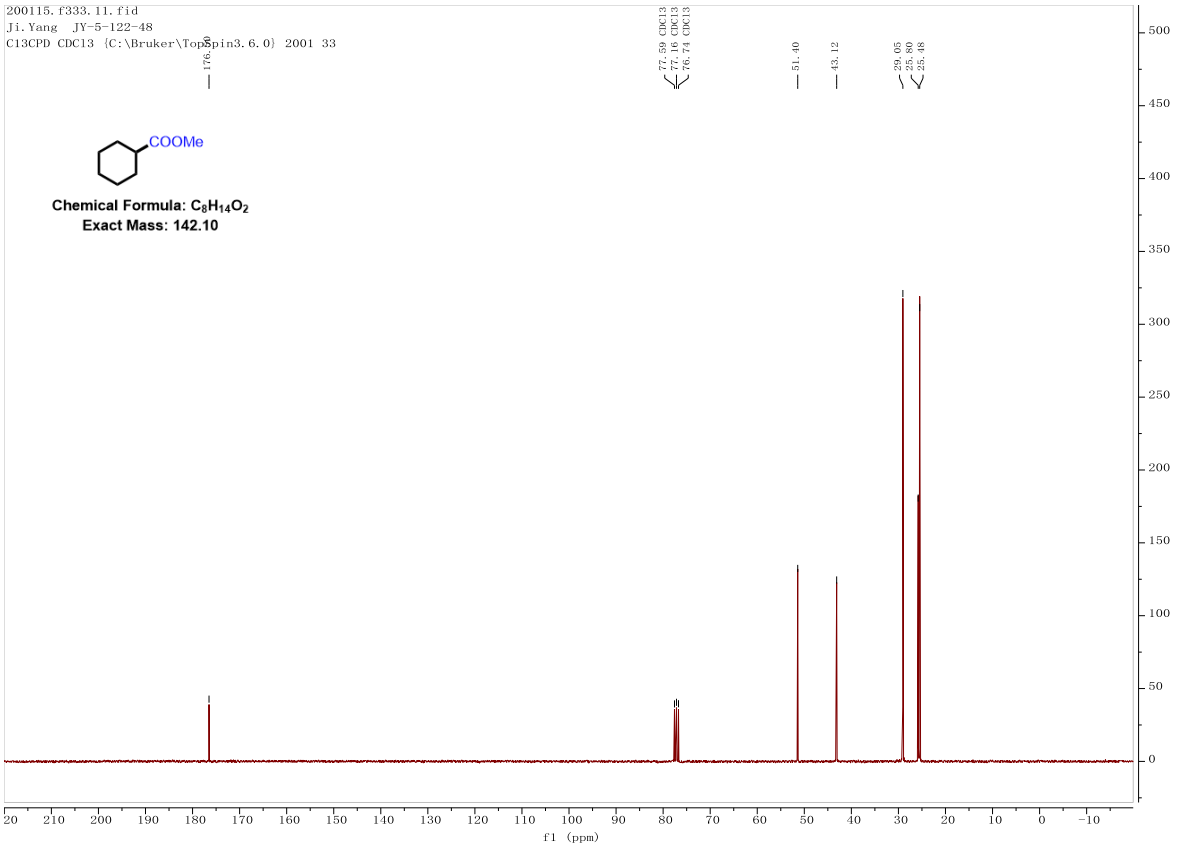
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		11,497	233,454	2874,648	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**233,454**	**2874,648**	**100,00**	**100,00**	

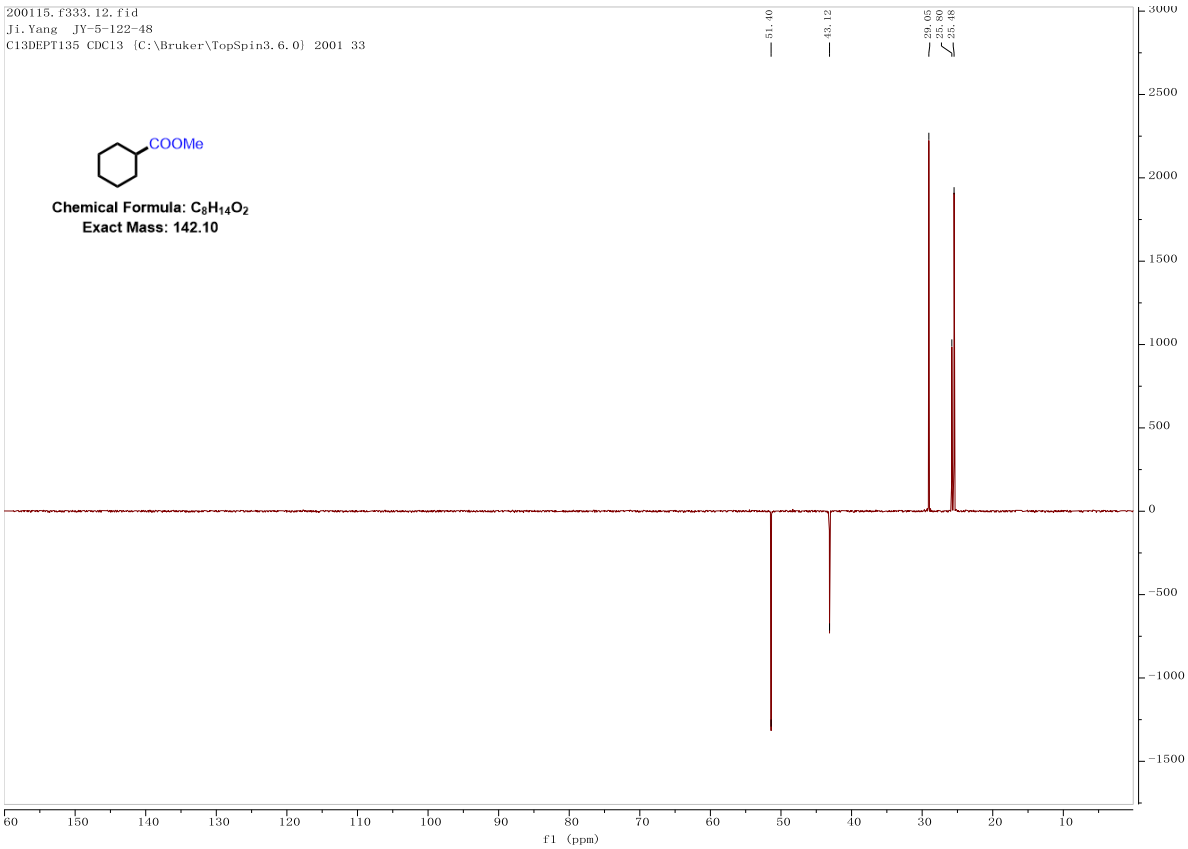
File :D:\MSDChem\1\DATA\2001\JY-5-122-8.D
Operator :
Acquired : 9 Jan 2020 19:40 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-8
Misc Info :
Vial Number: 43




6
5
1
COOMe
4
2
3
3u
methyl cyclohexanecarboxylate
Chemical Formula: C8H14O2
Exact Mass: 142.10


200115.f333.10.fid
Ji.Yang JY-5-122-48
PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 33
COOMe
Chemical Formula: C8H14O2
Exact Mass: 142.10
f1 (ppm)


200115.f333.11.fid
Ji.Yang JY-5-122-48
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 33
176.90
77.59 CDCl3
77.16 CDCl3
76.74 CDCl3
51.40
43.12
29.05
25.80
25.48
COOMe
Chemical Formula: C8H14O2
Exact Mass: 142.10
f1 (ppm)

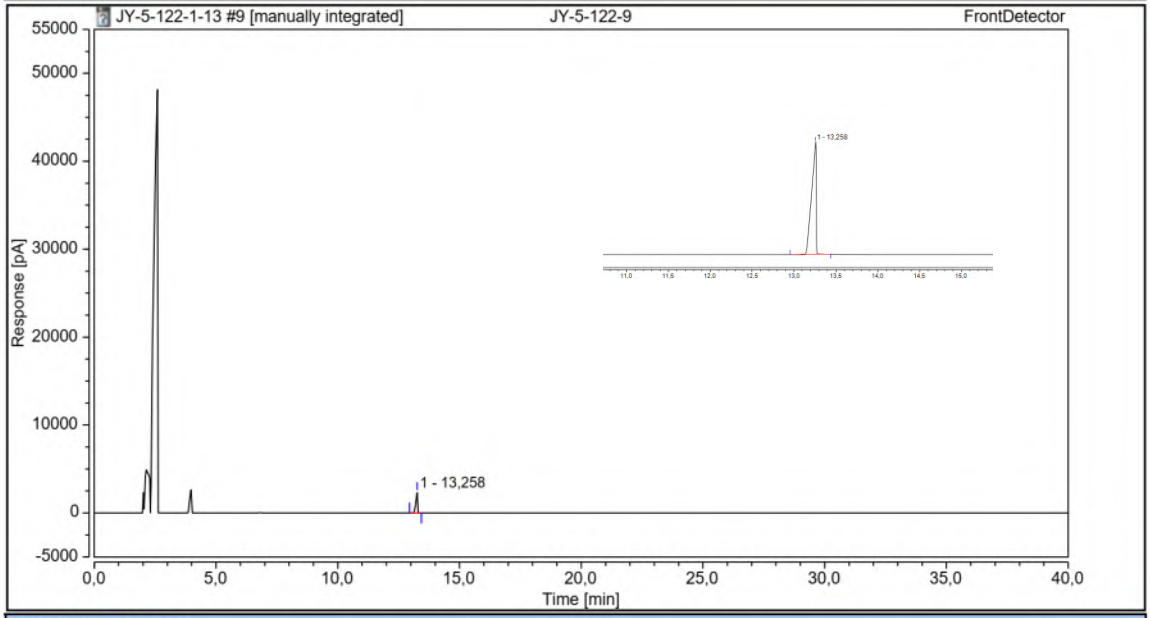

200115.f333.12.fid
Ji.Yang JY-5-122-48
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 33
51.40
43.12
29.05
25.80
25.48
COOMe
Chemical Formula: C8H14O2
Exact Mass: 142.10
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-9**	*Run Time (min):*	**40,00**
Vial Number:	**69**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 23:36**	*Sample Weight:*	**1,0000**

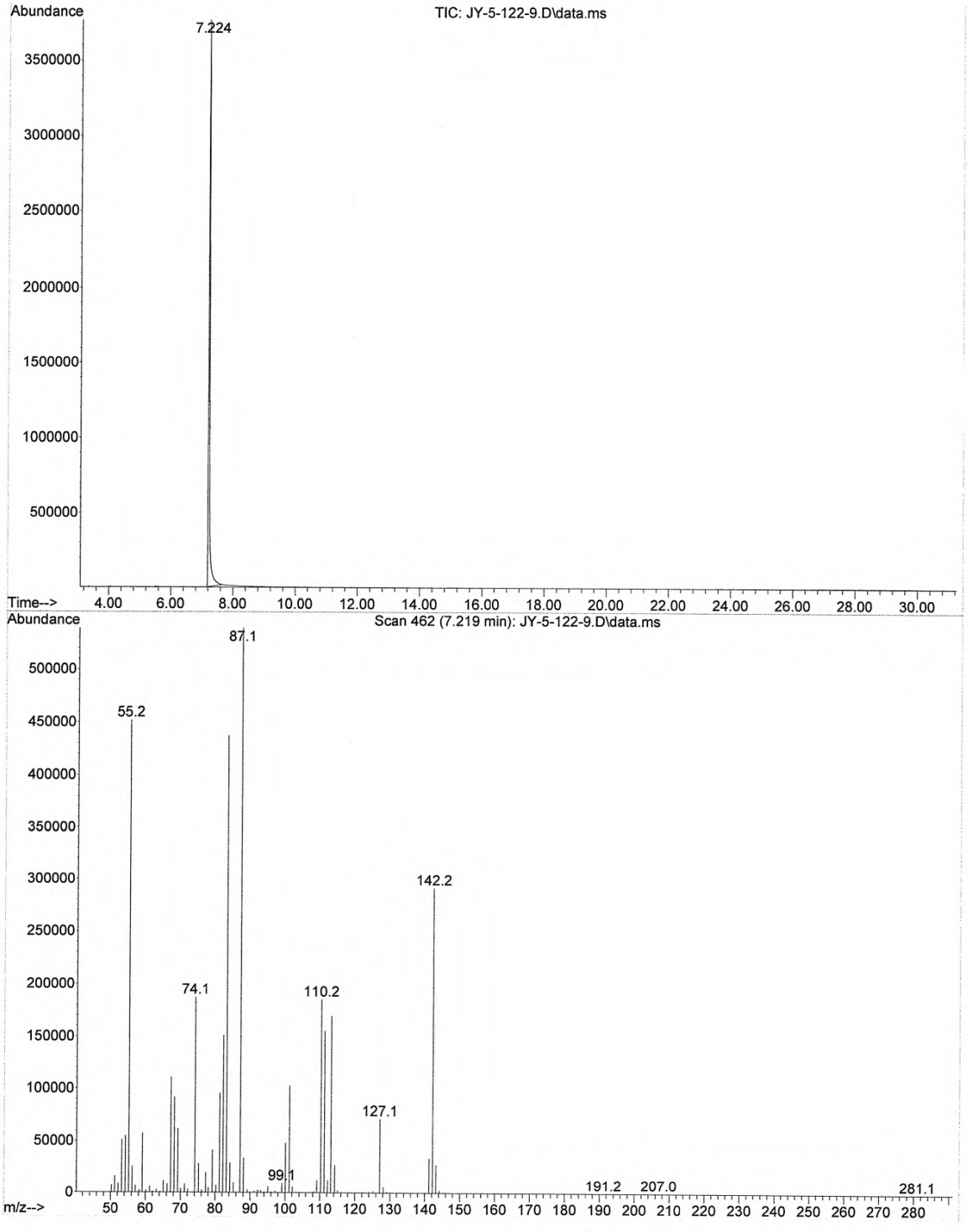
Chromatogram

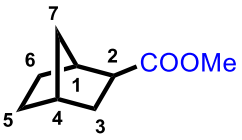


Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		13,258	141,526	2288,091	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**141,526**	**2288,091**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-9.D
Operator   :
Acquired   :  9 Jan 2020  20:19     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-9
Misc Info  :
Vial Number: 44
```



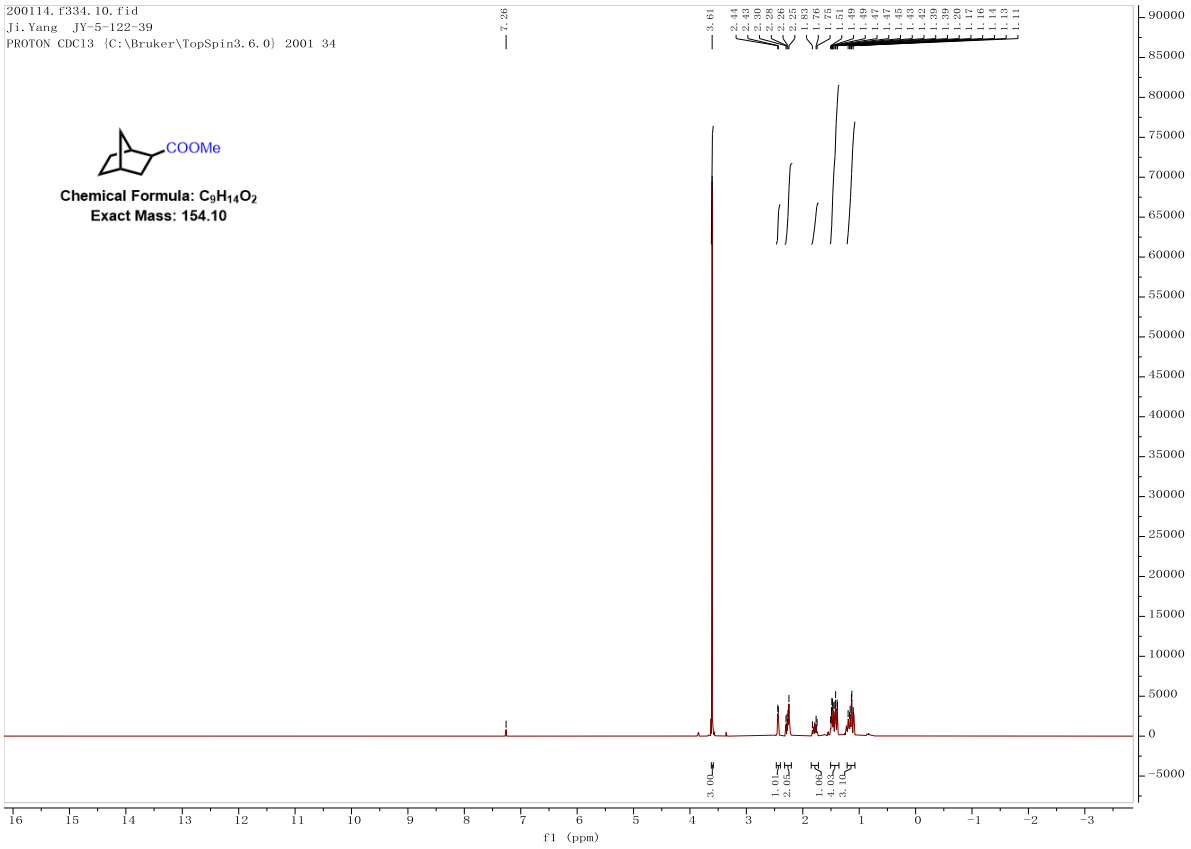


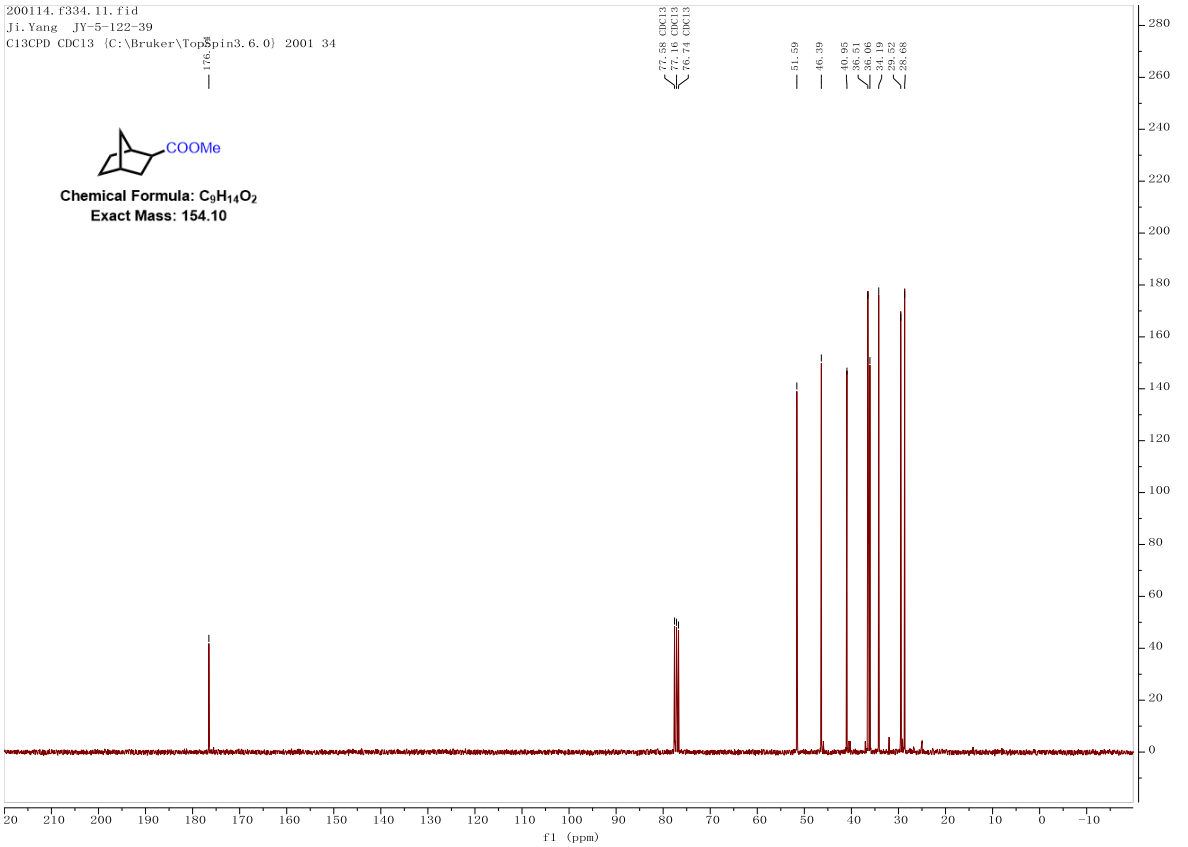
3v

methyl (1*S*,4*R*)-bicyclo[2.2.1]heptane-2-carboxylate

Chemical Formula: $C_9H_{14}O_2$

Exact Mass: 154.10

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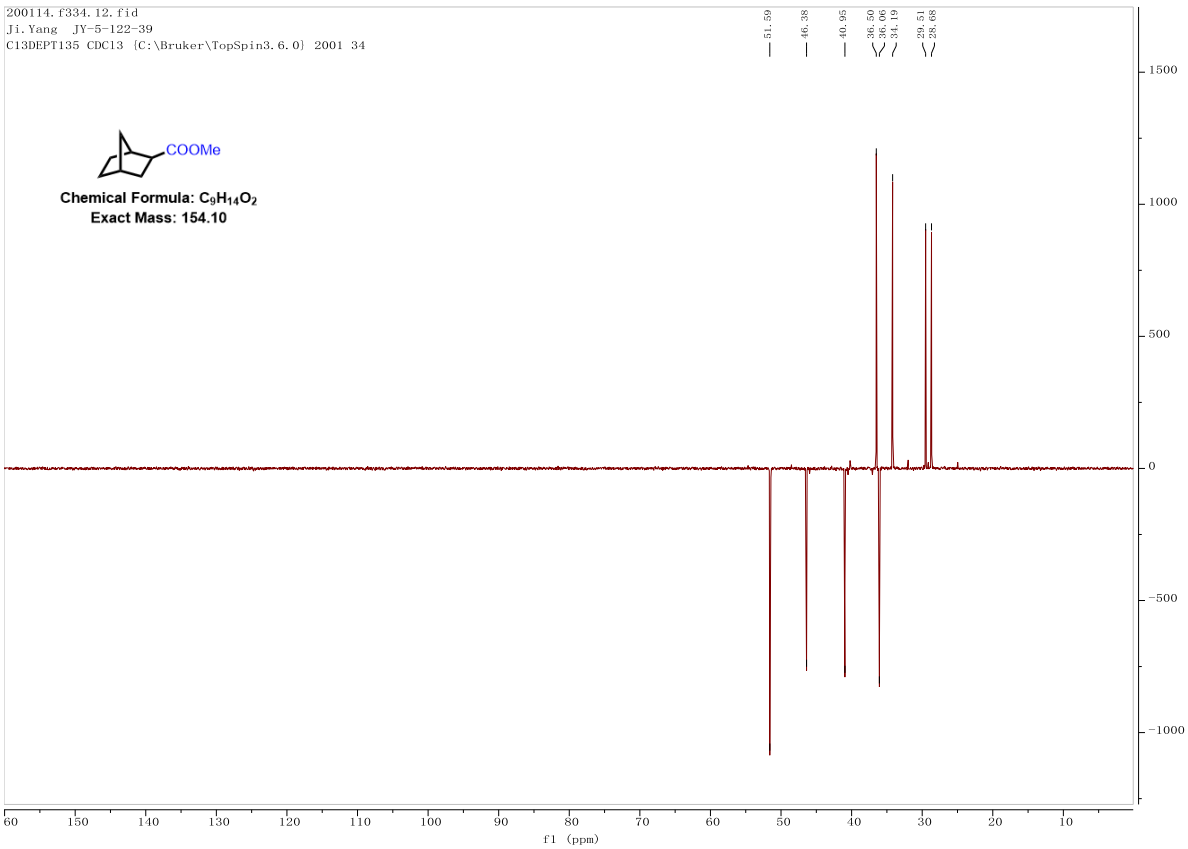
Ji.Yang JY-5-122-39
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 34
176.35
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
51.59
46.39
40.95
36.51
36.06
34.19
29.32
28.68
COOMe
Chemical Formula: C9H14O2
Exact Mass: 154.10
f1 (ppm)

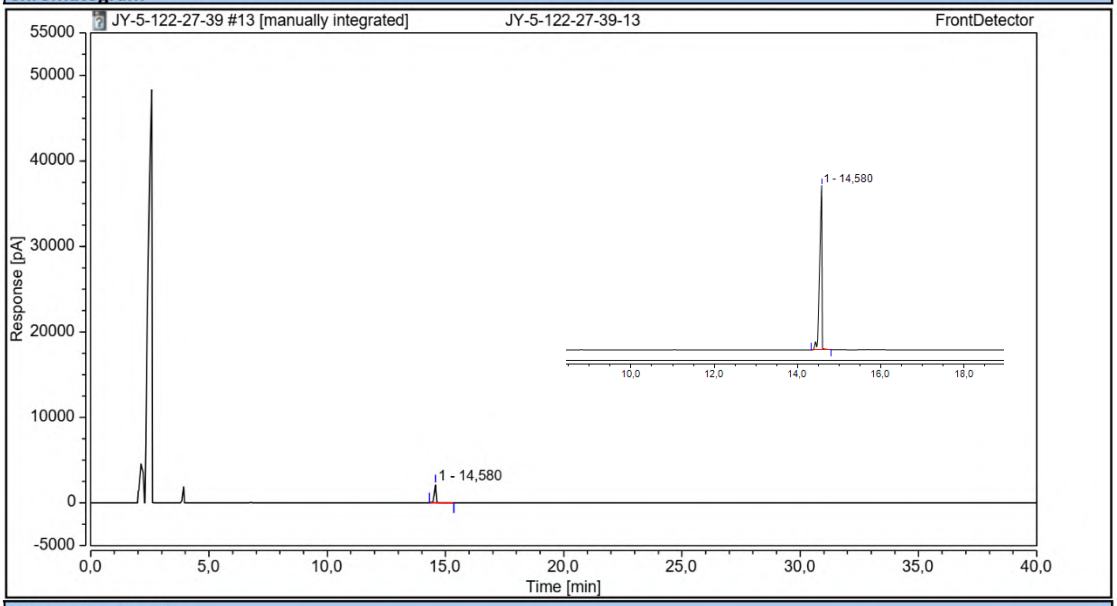

200114.f334.12.fid
Ji.Yang JY-5-122-39
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 34
51.59
46.38
40.95
36.50
36.06
34.19
29.51
28.68
COOMe
Chemical Formula: C9H14O2
Exact Mass: 154.10
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-13**	*Run Time (min):*	**40,00**
Vial Number:	**37**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**12.Jan.20 01:33**	*Sample Weight:*	**1,0000**

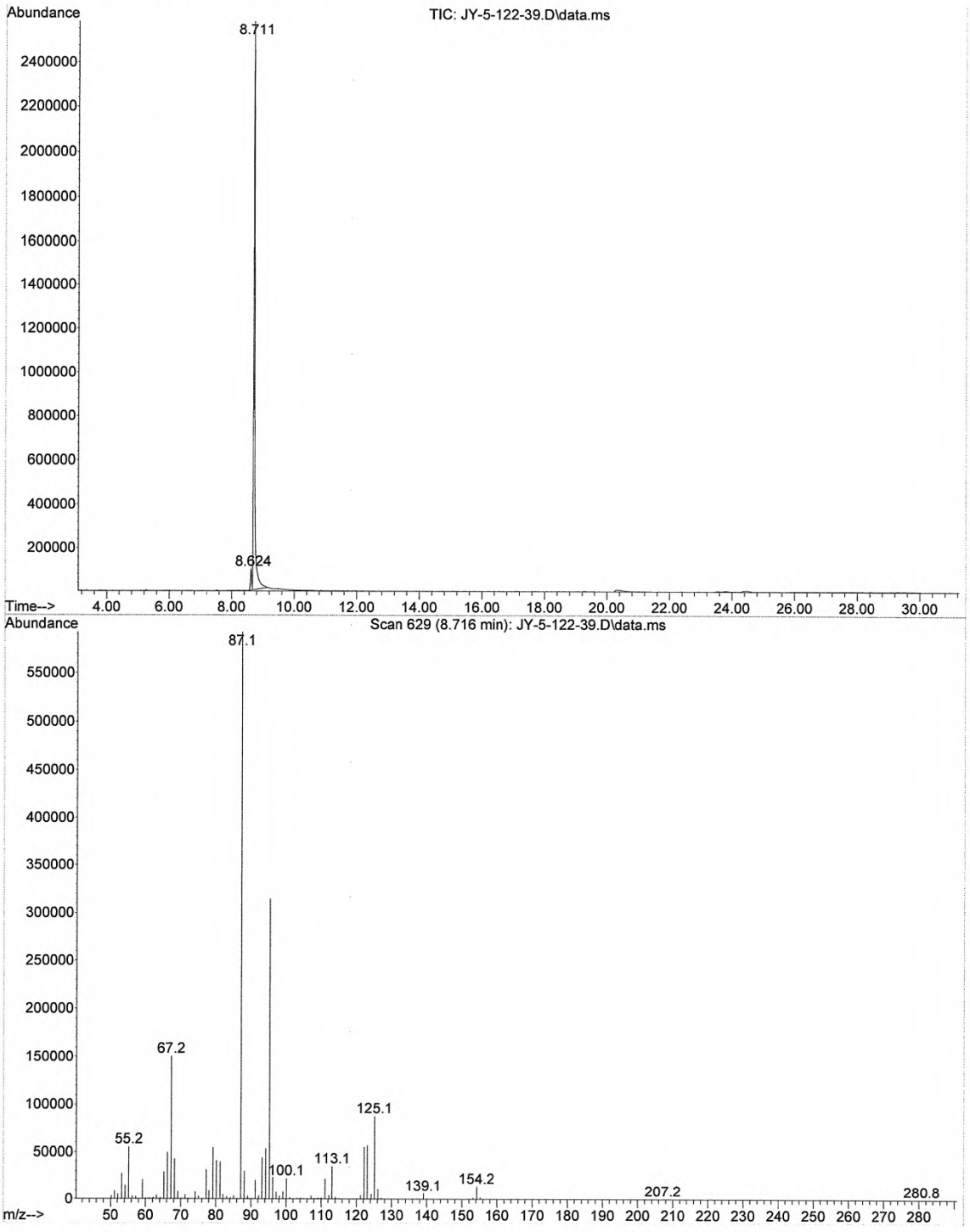
Chromatogram

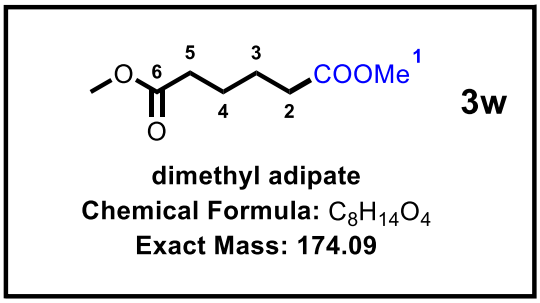


Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,580	129,613	2094,455	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**129,613**	**2094,455**	**100,00**	**100,00**	

File :D:\MSDChem\1\DATA\2001\JY-5-122-39.D
Operator :
Acquired : 11 Jan 2020 23:42 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-39
Misc Info :
Vial Number: 43



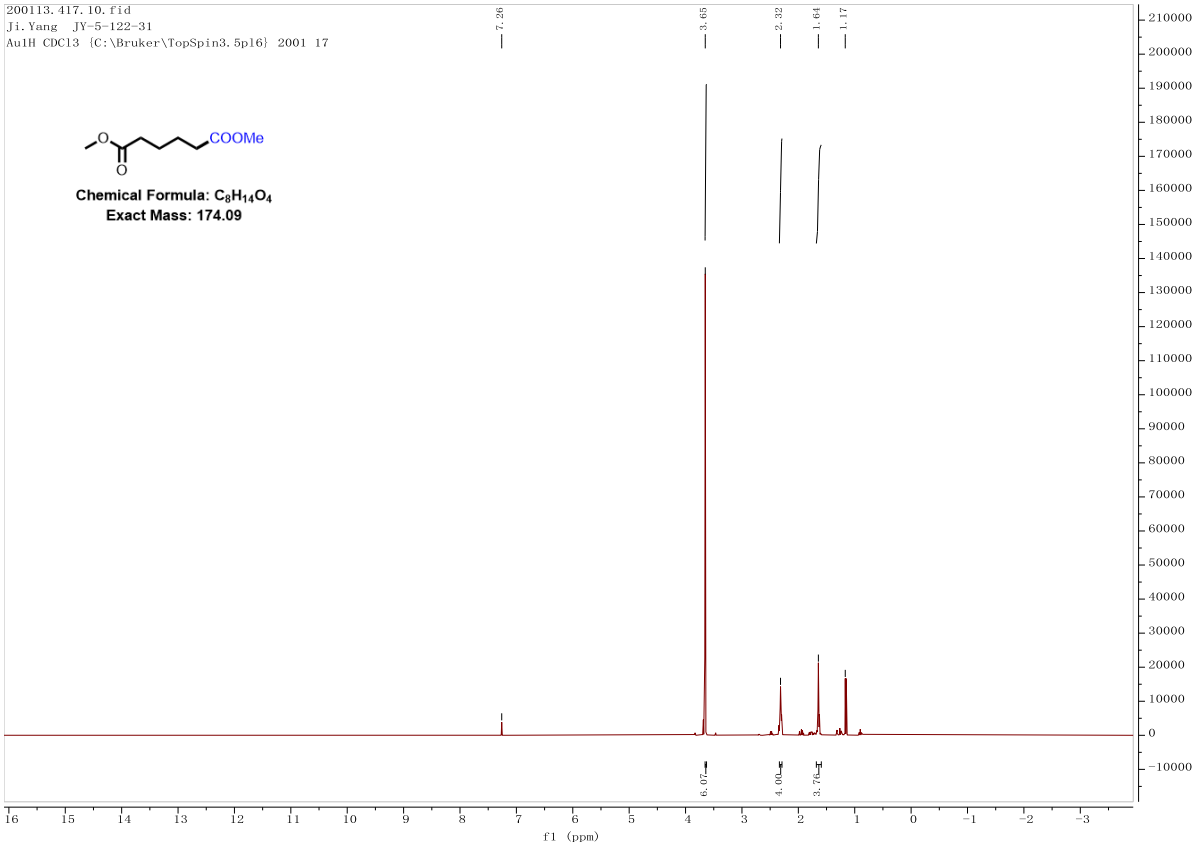


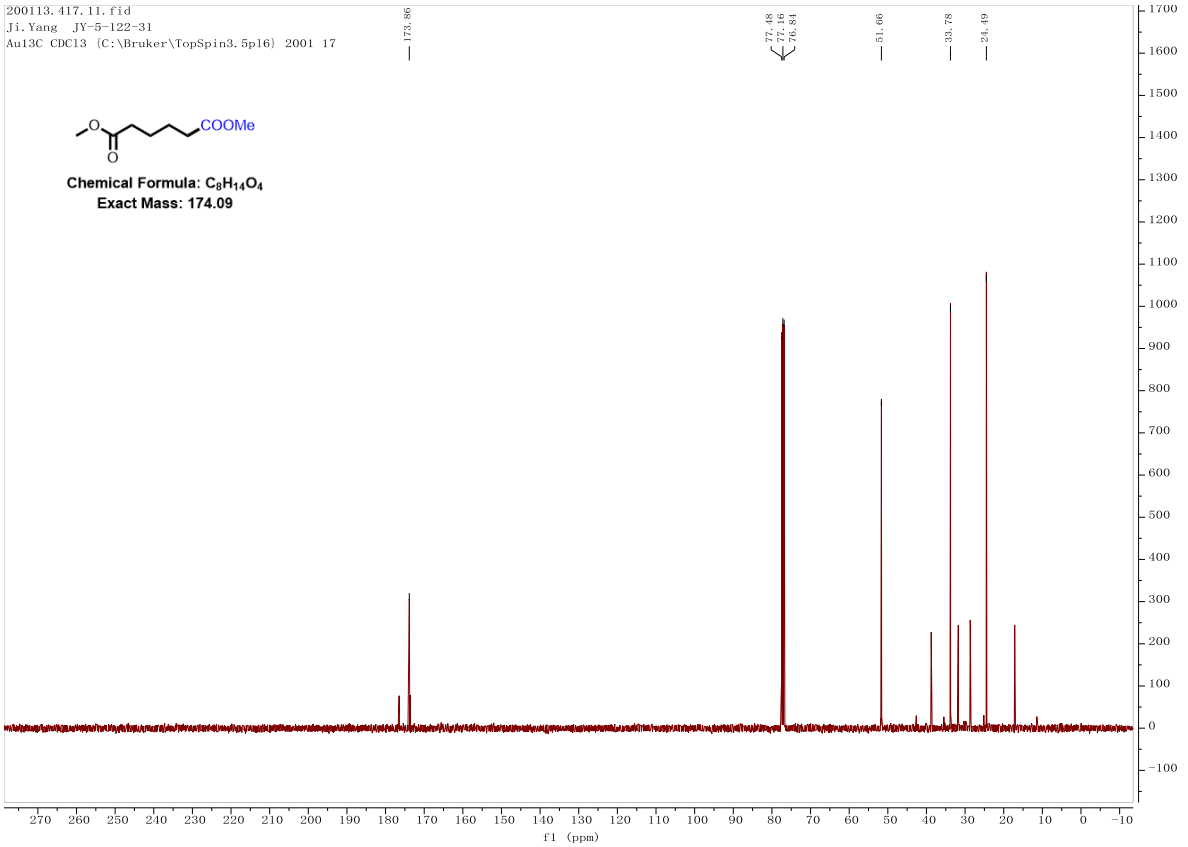
3w

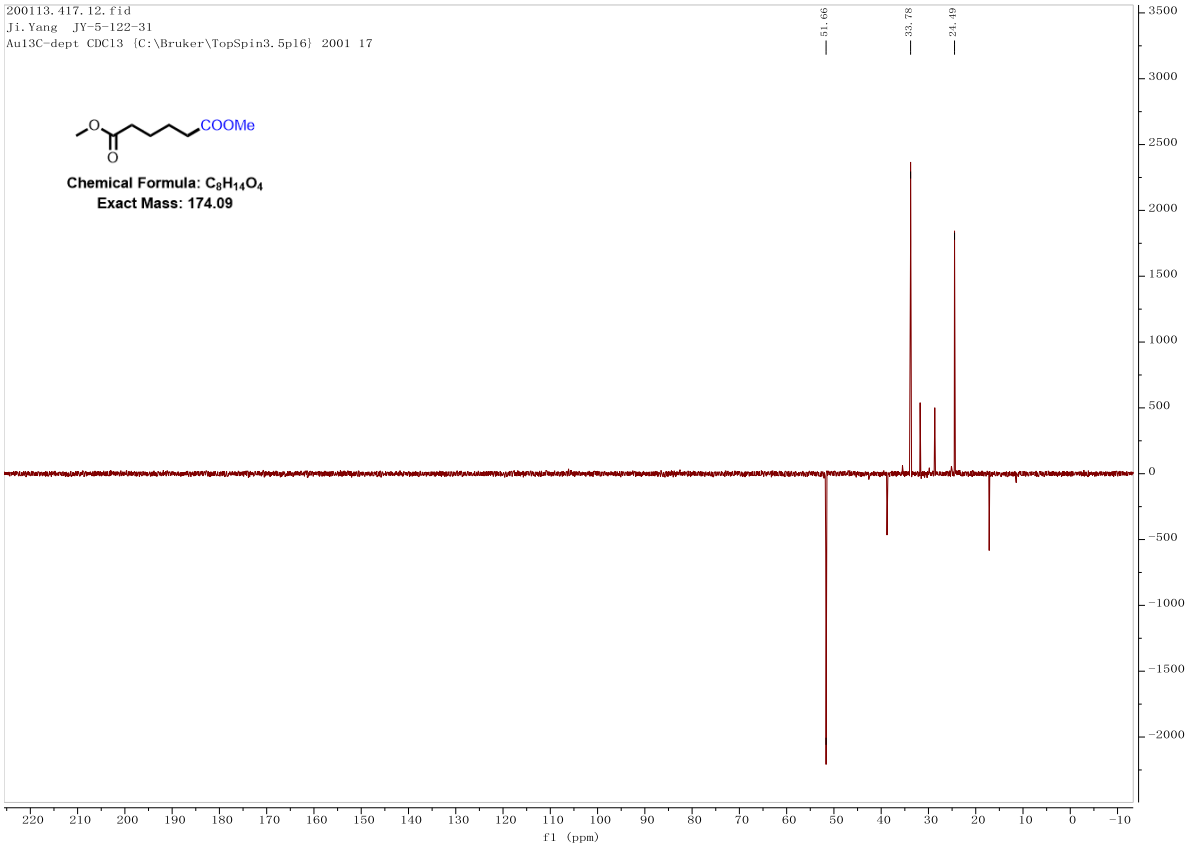
dimethyl adipate

Chemical Formula: $C_8H_{14}O_4$

Exact Mass: 174.09




200113.417.11.fid
Ji.Yang JY-5-122-31
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 17
173.86
77.48
77.16
76.84
51.66
33.78
24.49
COOMe
Chemical Formula: C8H14O4
Exact Mass: 174.09
f1 (ppm)

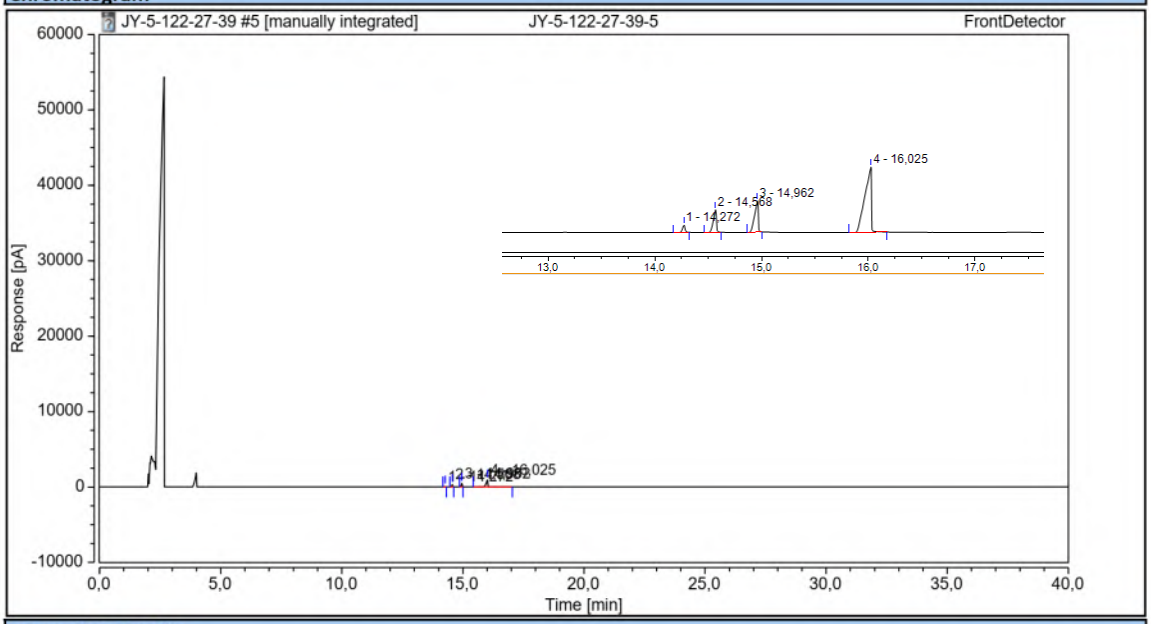

200113.417.12.fid
Ji.Yang JY-5-122-31
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 17
51.66
33.78
24.49
COOMe
Chemical Formula: C8H14O4
Exact Mass: 174.09
f1 (ppm)

Chromatogram and Results

Injection Details

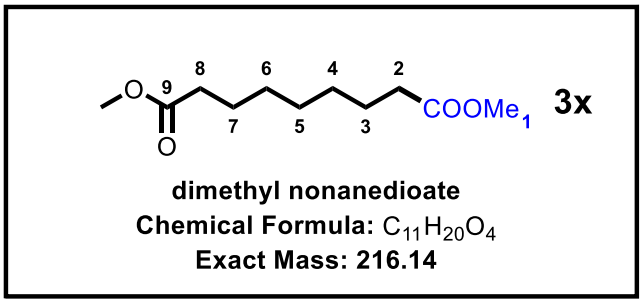
Injection Name:	**JY-5-122-27-39-5**	*Run Time (min):*	**40,00**
Vial Number:	**29**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Jan.20 17:26**	*Sample Weight:*	**1,0000**

Chromatogram

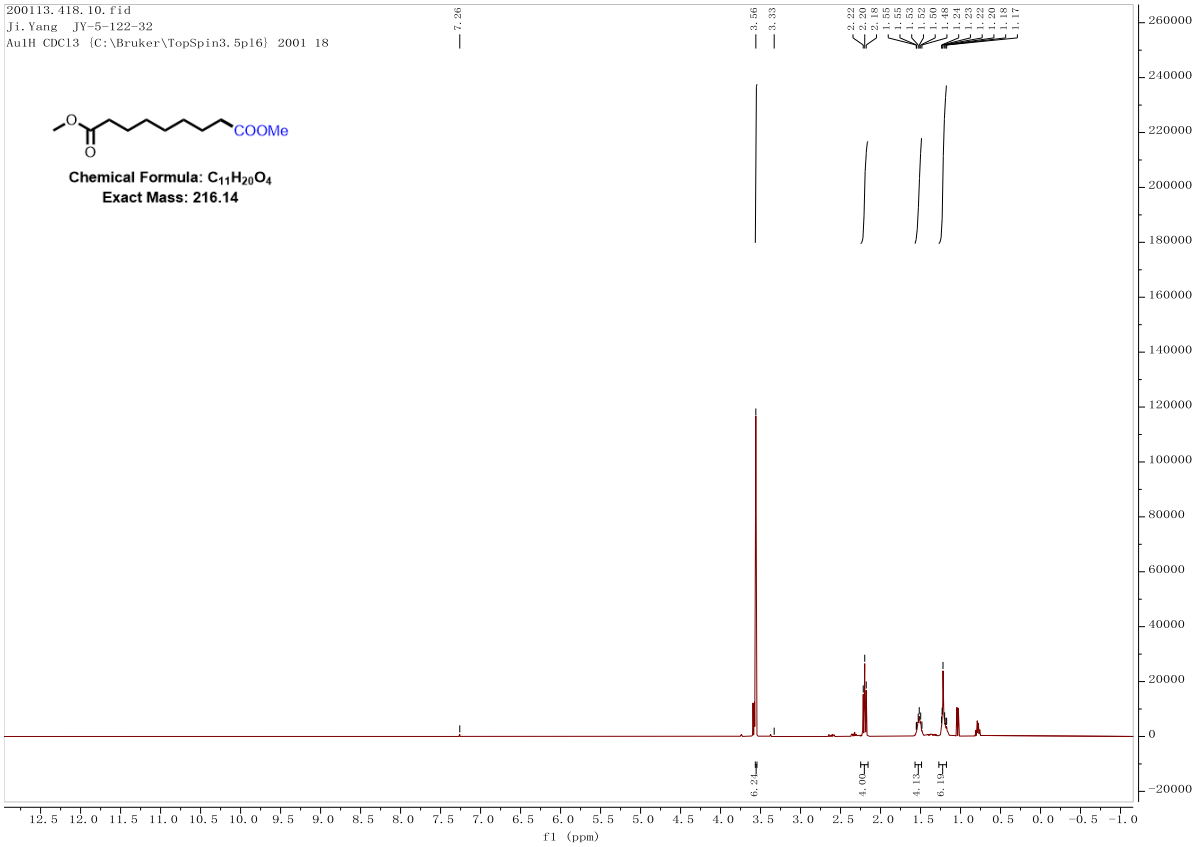


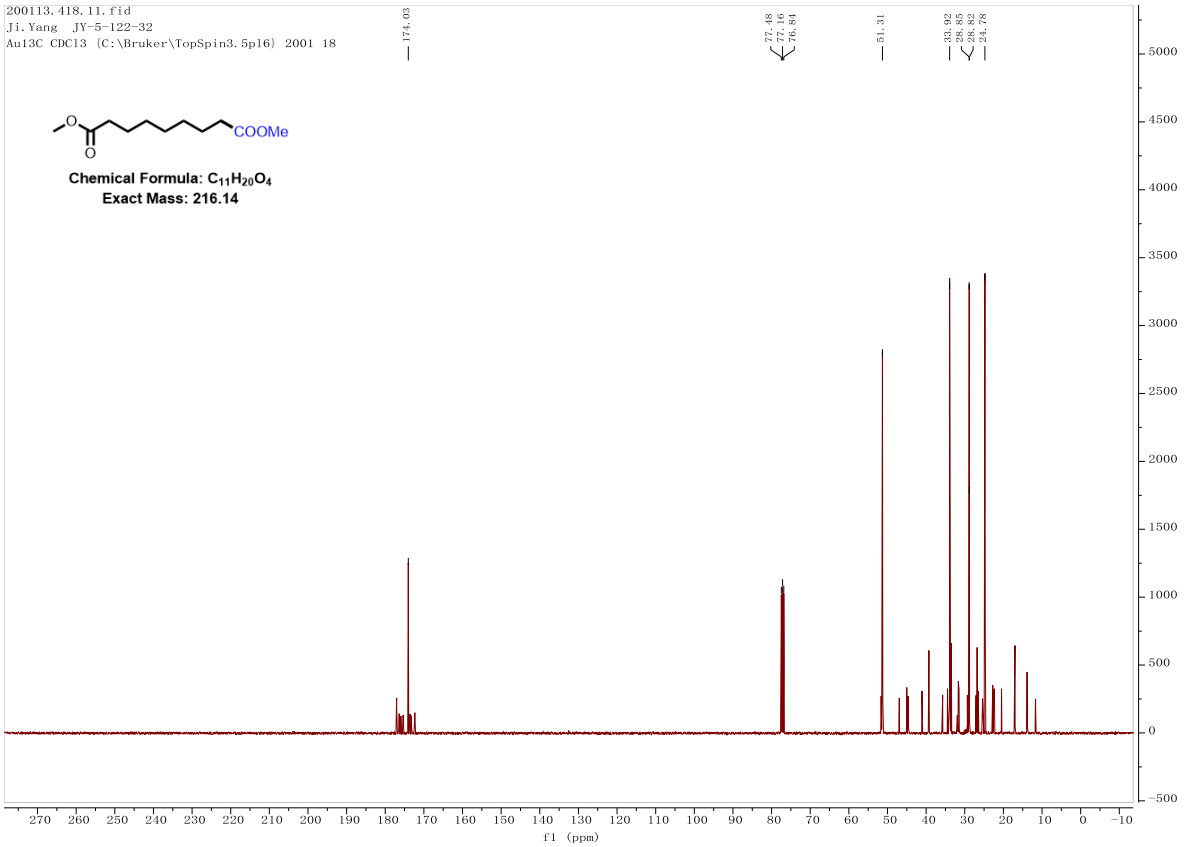
Integration Results

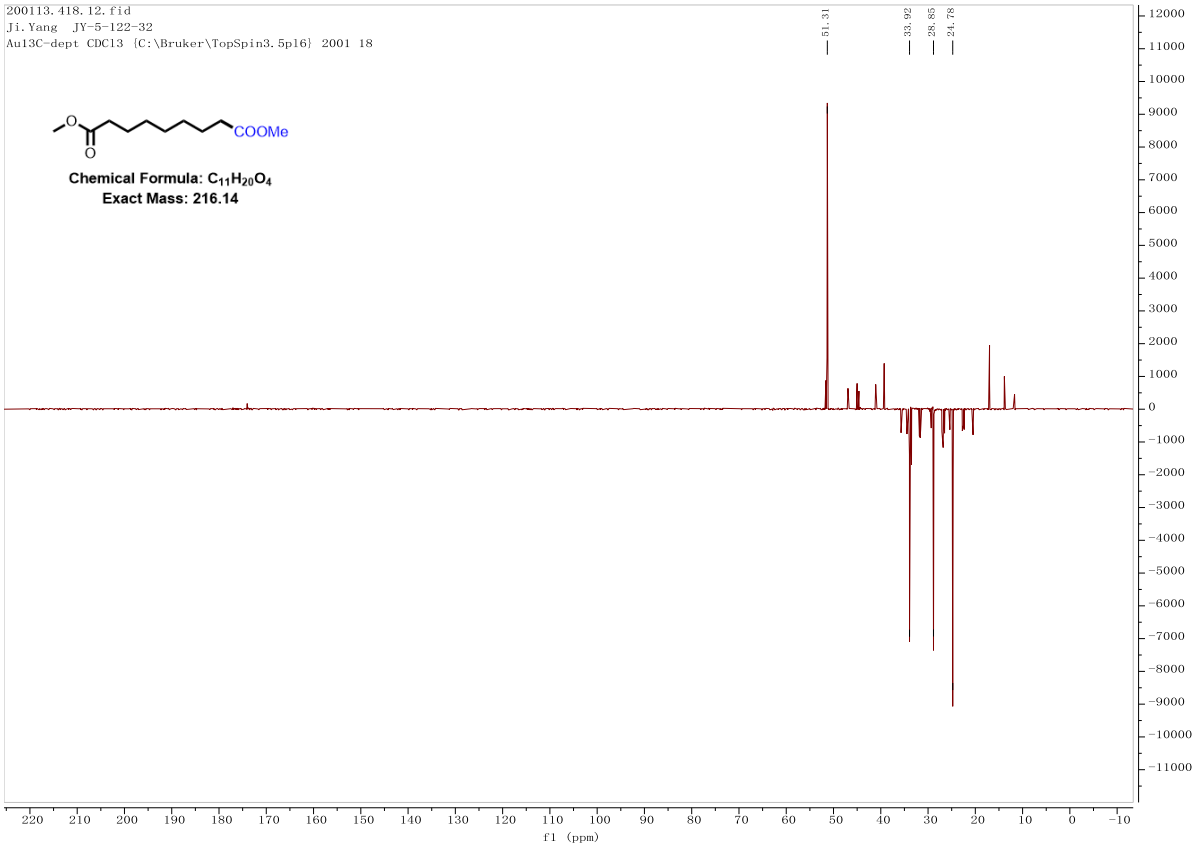
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		14,272	2,794	109,620	2,82	6,05	n.a.
2		14,568	10,701	322,992	10,81	17,83	n.a.
3		14,962	17,399	445,334	17,57	24,59	n.a.
4		16,025	68,141	933,392	68,81	51,53	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**99,035**	**1811,338**	**100,00**	**100,00**	



dimethyl nonanedioate
Chemical Formula: $C_{11}H_{20}O_4$
Exact Mass: 216.14




200113.418.11.fid
Ji.Yang JY-5-122-32
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 18
174.03
77.48
77.16
76.84
51.31
33.92
28.85
28.82
24.78
COOMe
Chemical Formula: C11H20O4
Exact Mass: 216.14
f1 (ppm)

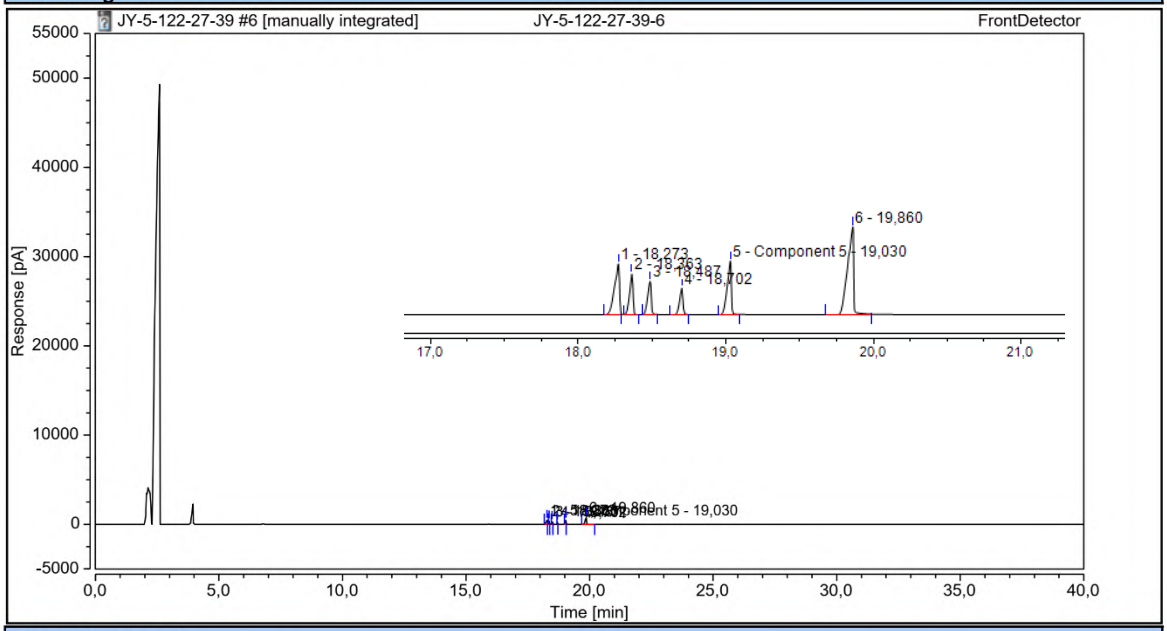

200113.418.12.fid
Ji.Yang JY-5-122-32
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 18
51.31
33.92
28.85
24.78
COOMe
Chemical Formula: C11H20O4
Exact Mass: 216.14
f1 (ppm)

Chromatogram and Results

Injection Details

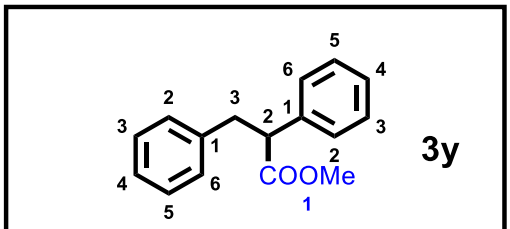
Injection Name:	**JY-5-122-27-39-6**	*Run Time (min):*	**40,00**
Vial Number:	**30**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Jan.20 18:27**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		18,273	16,605	426,289	19,31	17,59	n.a.
2		18,363	7,982	329,251	9,28	13,58	n.a.
3		18,487	7,502	277,608	8,73	11,45	n.a.
4		18,702	4,700	205,873	5,47	8,49	n.a.
5	Component 5	19,030	13,365	444,069	15,55	18,32	n.a.
6		19,860	35,817	740,961	41,66	30,57	n.a.
Total:			**85,970**	**2424,051**	**100,00**	**100,00**	

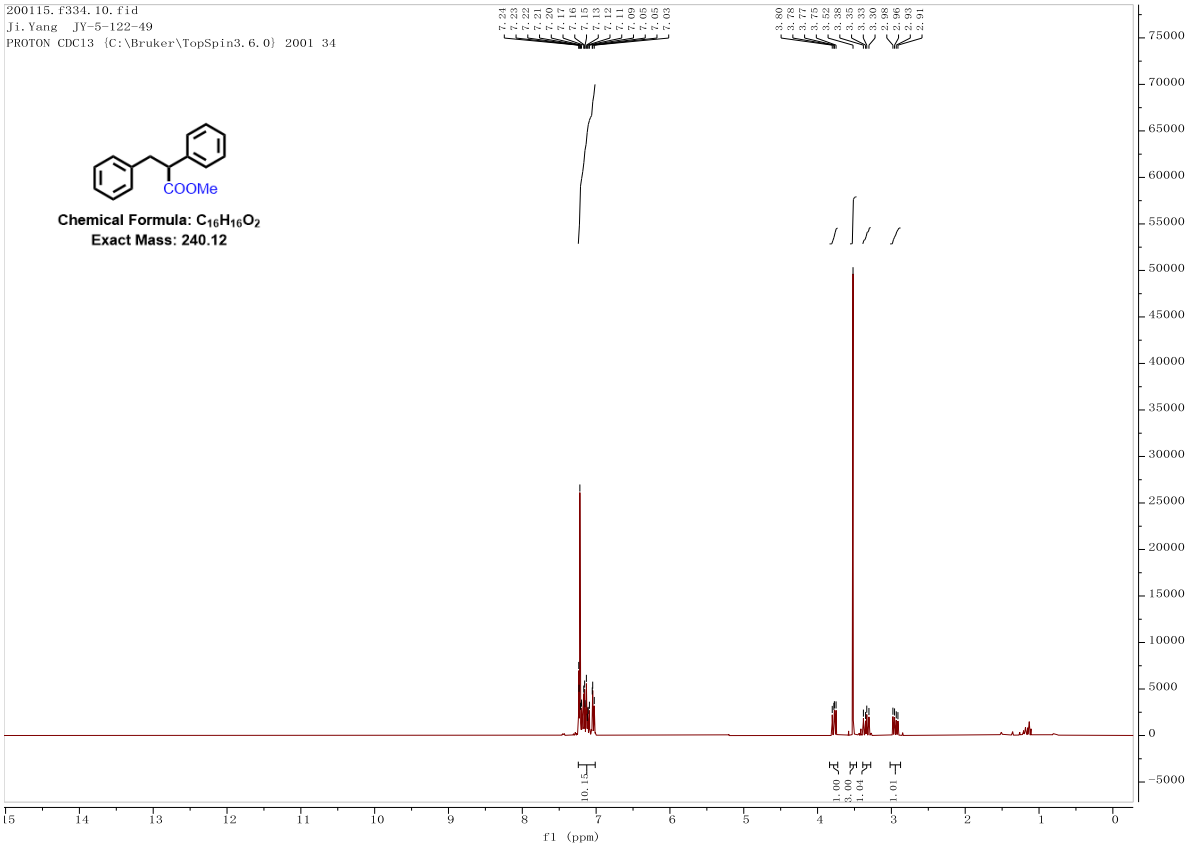


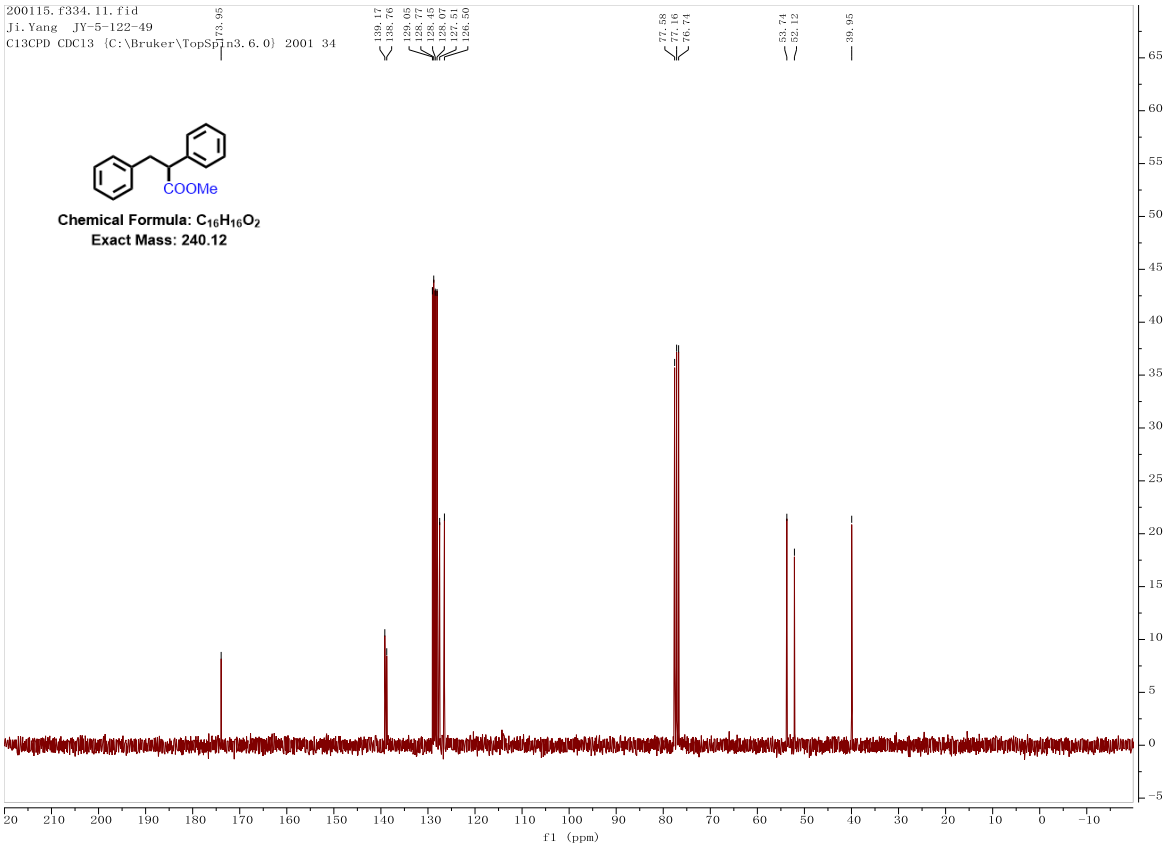
3y

methyl-2,3-diphenylpropanoate

Chemical Formula: $C_{16}H_{16}O_2$

Exact Mass: 240.12

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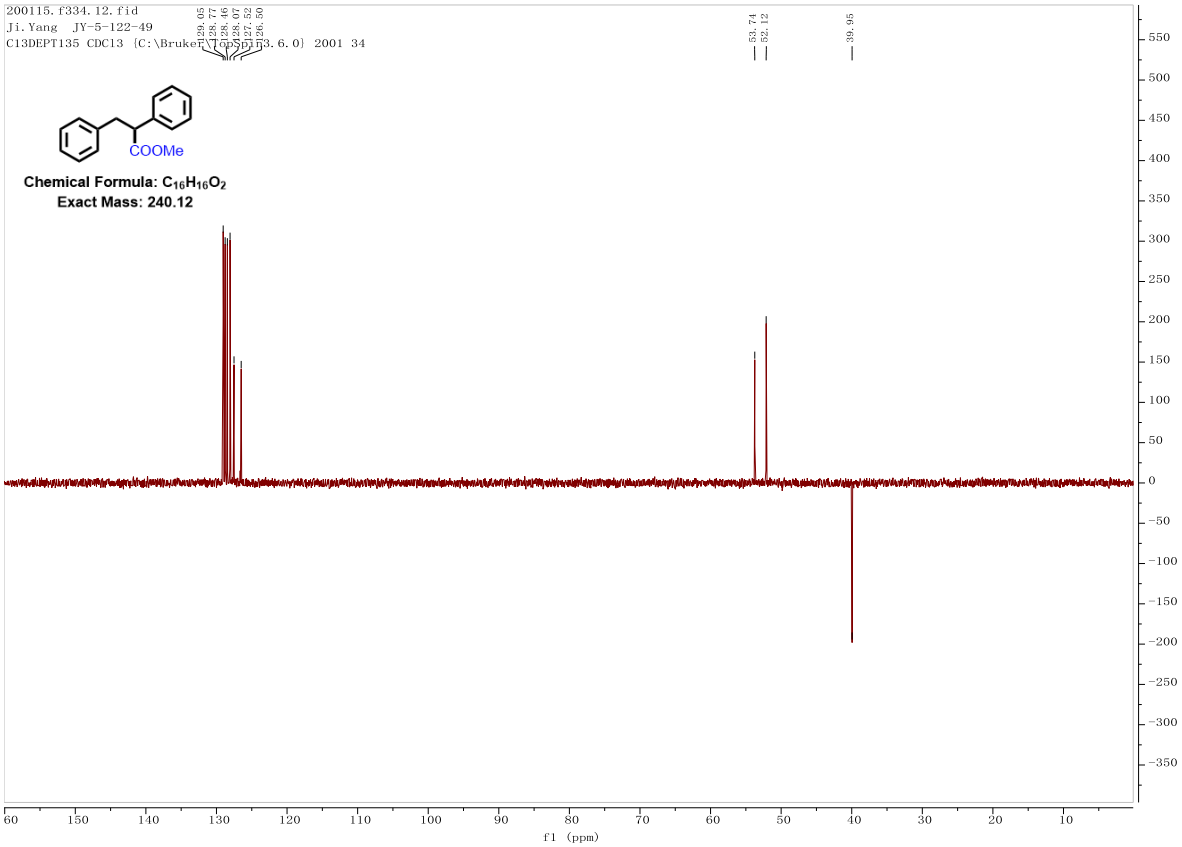
Ji.Yang JY-5-122-49
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 34
173.95
139.17
138.76
129.05
128.77
128.45
128.07
127.51
126.50
77.58
77.16
76.74
53.74
52.12
39.95
COOMe
Chemical Formula: C16H16O2
Exact Mass: 240.12
f1 (ppm)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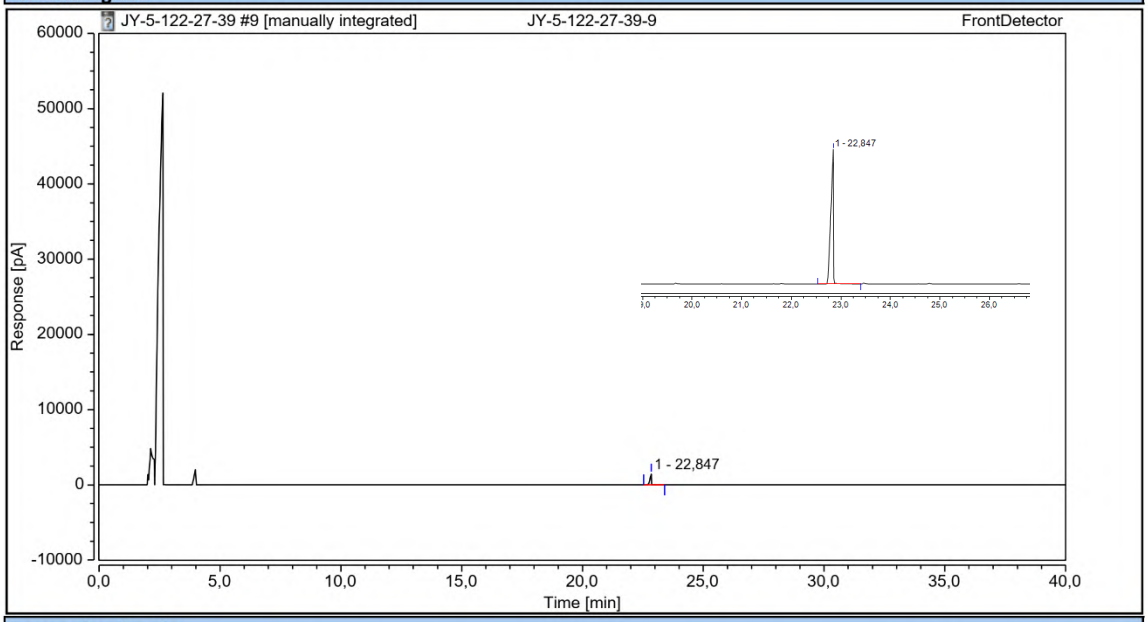
Ji.Yang JY-5-122-49
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 34
129.05
128.77
128.46
128.07
127.52
126.50
53.74
52.12
39.95
COOMe
Chemical Formula: C16H16O2
Exact Mass: 240.12
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-9**	*Run Time (min):*	**40,00**
Vial Number:	**33**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Jan.20 21:30**	*Sample Weight:*	**1,0000**

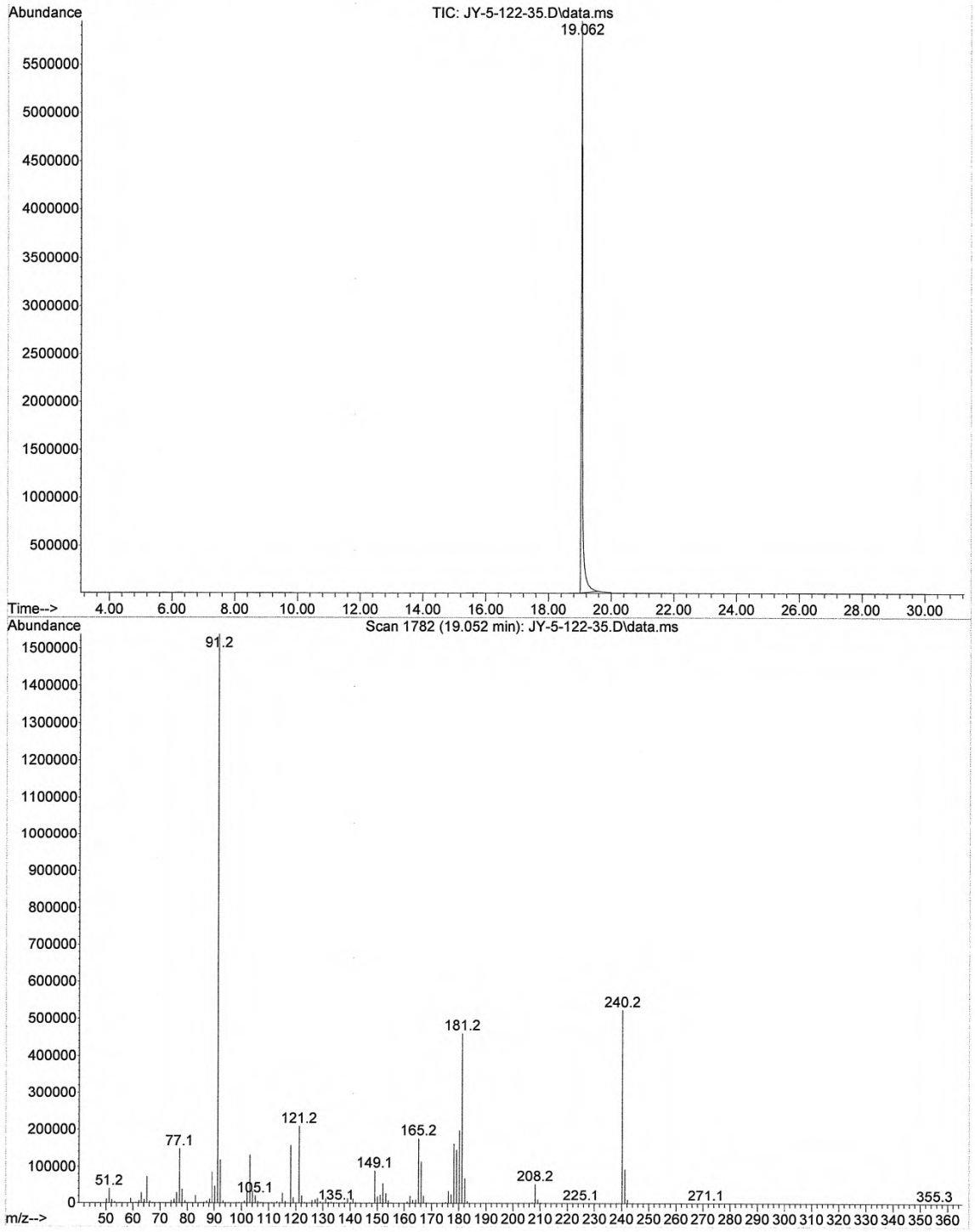
Chromatogram

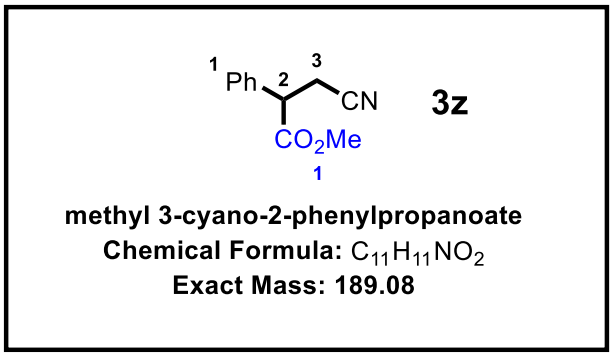


Integration Results

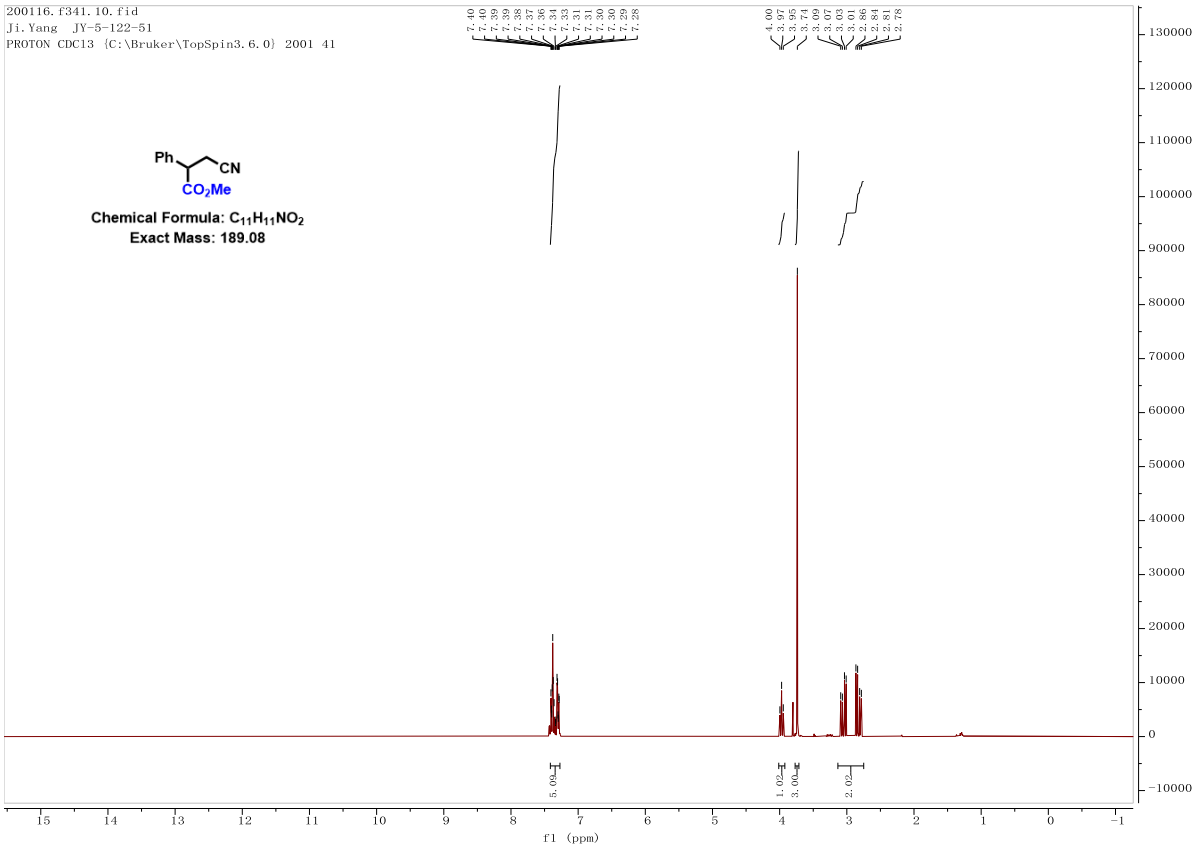
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		22,847	87,088	1411,970	100,00	100,00	n.a.
Total:			**87,088**	**1411,970**	**100,00**	**100,00**	

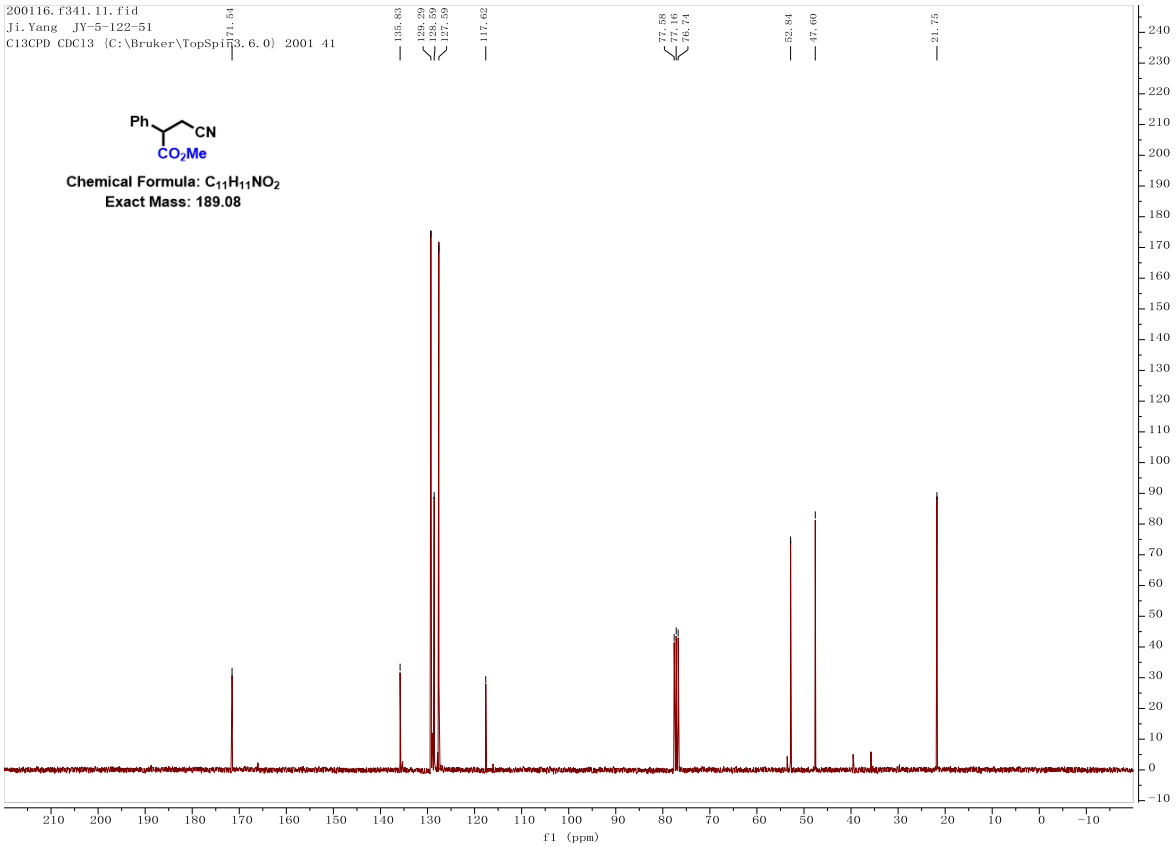
File :D:\MSDChem\1\DATA\2001\JY-5-122-35.D
Operator :
Acquired : 11 Jan 2020 21:07 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-35
Misc Info :
Vial Number: 39





methyl 3-cyano-2-phenylpropanoate
Chemical Formula: $C_{11}H_{11}NO_2$
Exact Mass: 189.08

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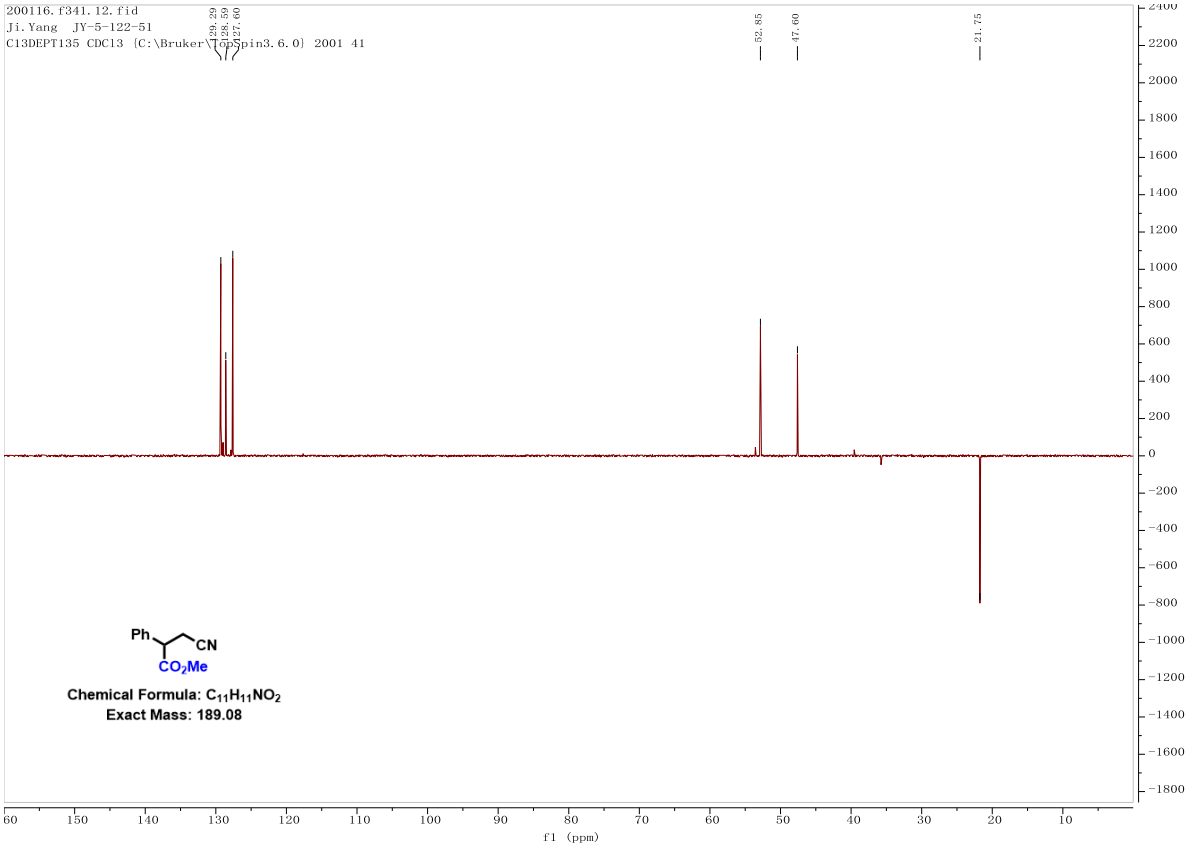
Ji.Yang JY-5-122-51
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 41
171.54
135.83
129.29
128.59
127.59
117.62
77.58
77.16
76.74
52.84
47.60
21.75
Ph
CN
CO2Me
Chemical Formula: C11H11NO2
Exact Mass: 189.08
f1 (ppm)

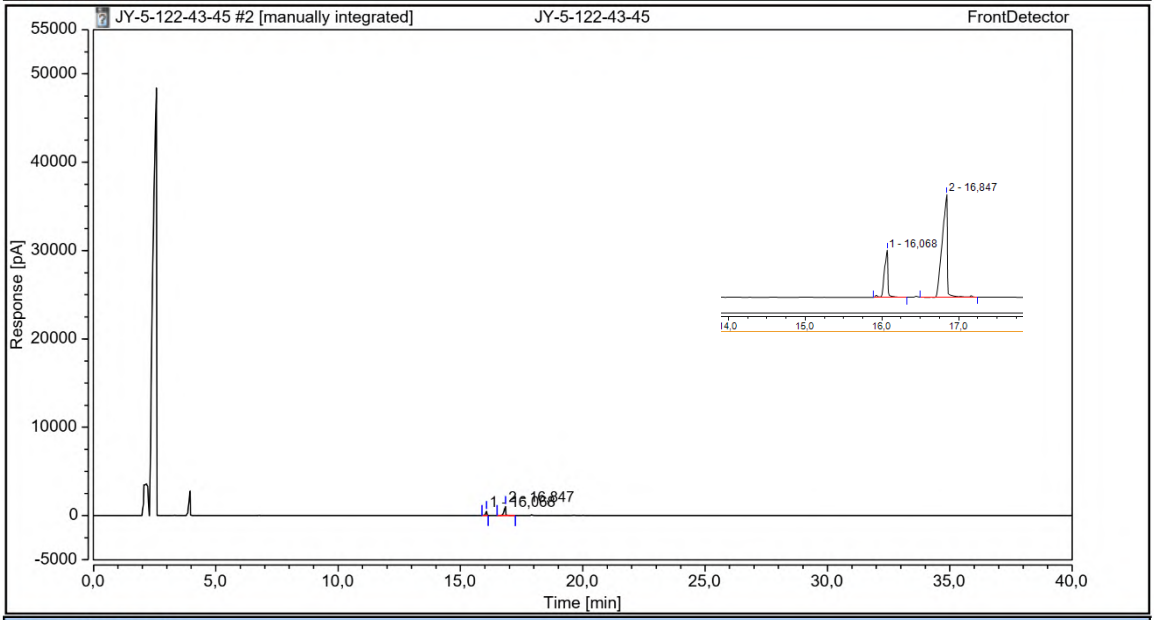

200116.f341.12.fid
Ji.Yang JY-5-122-51
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 41
129.29
128.59
127.60
52.85
47.60
21.75
Ph
CN
CO2Me
Chemical Formula: C11H11NO2
Exact Mass: 189.08
f1 (ppm)

Chromatogram and Results

Injection Details

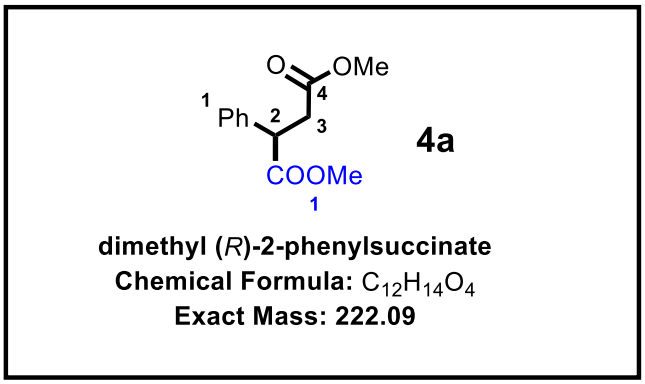
Injection Name:	**JY-5-122-43-45**	*Run Time (min):*	**40,00**
Vial Number:	**74**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**13.Jan.20 15:32**	*Sample Weight:*	**1,0000**

Chromatogram

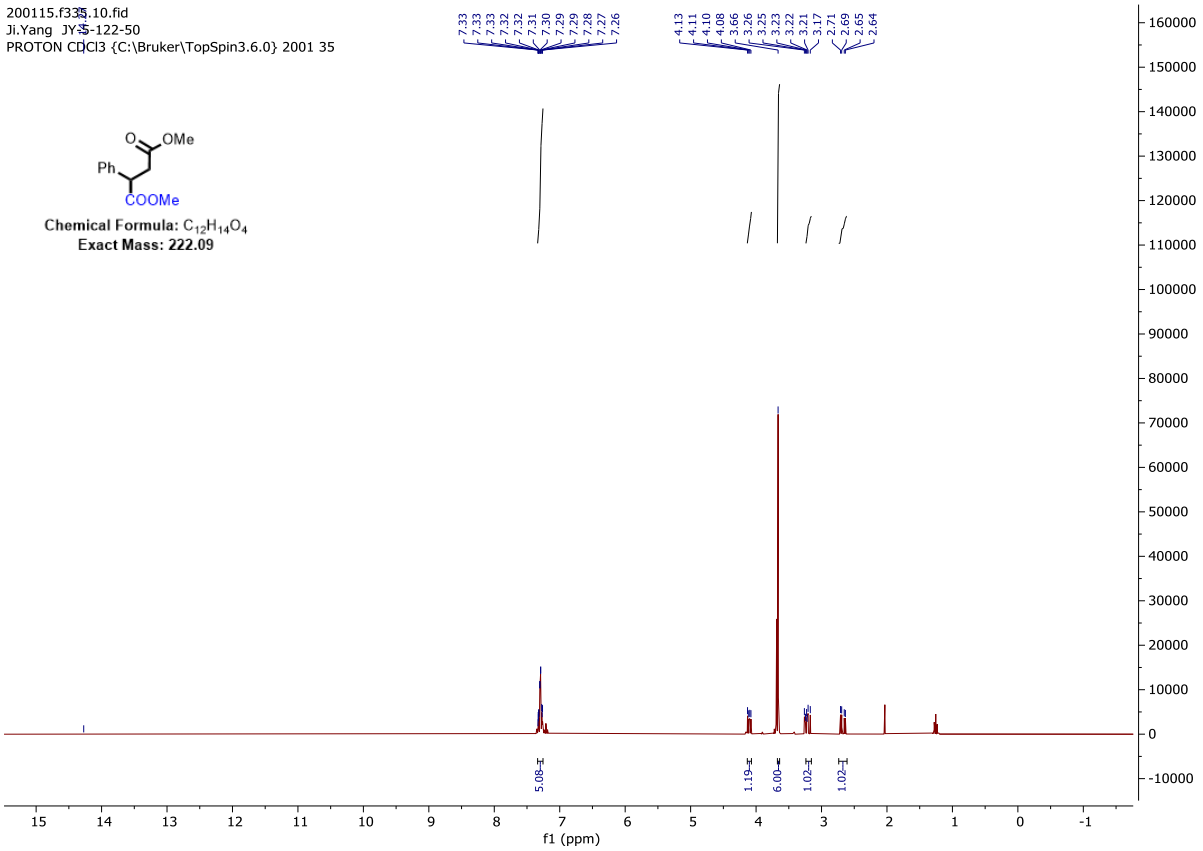


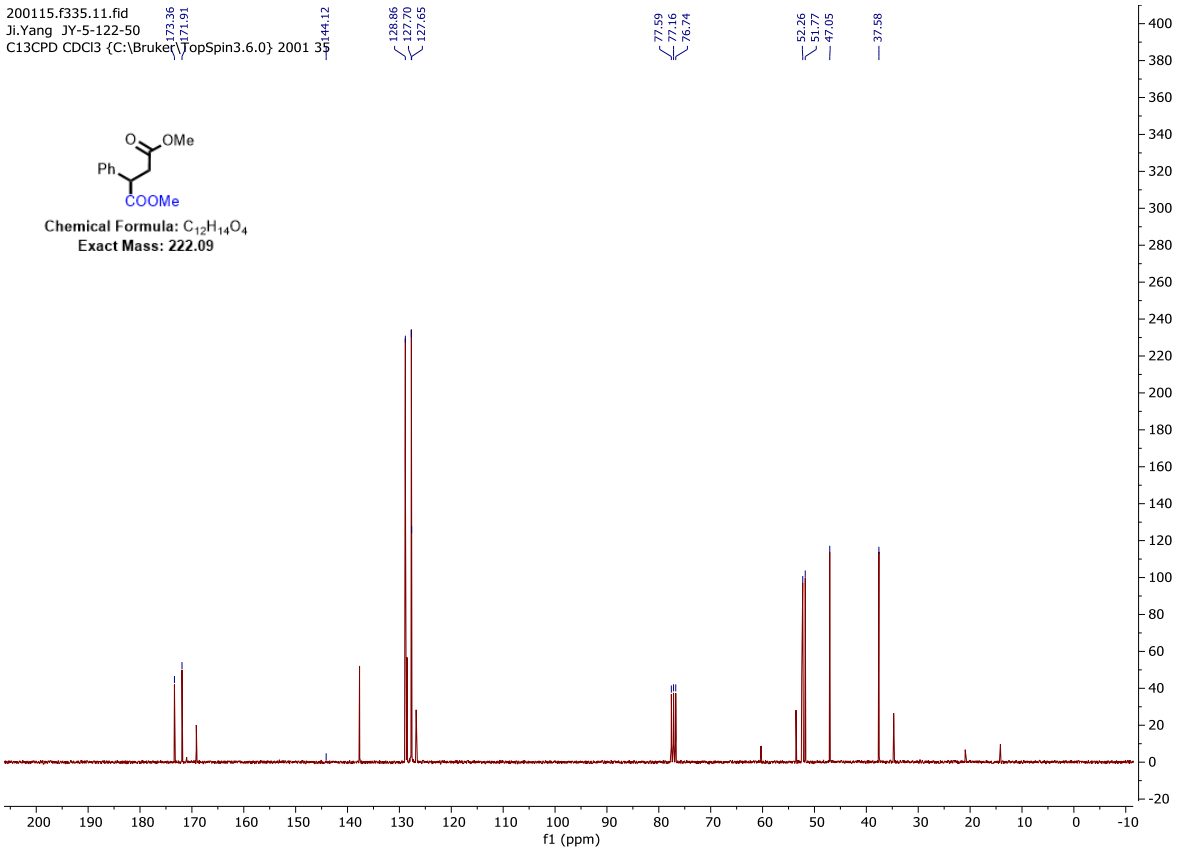
Integration Results

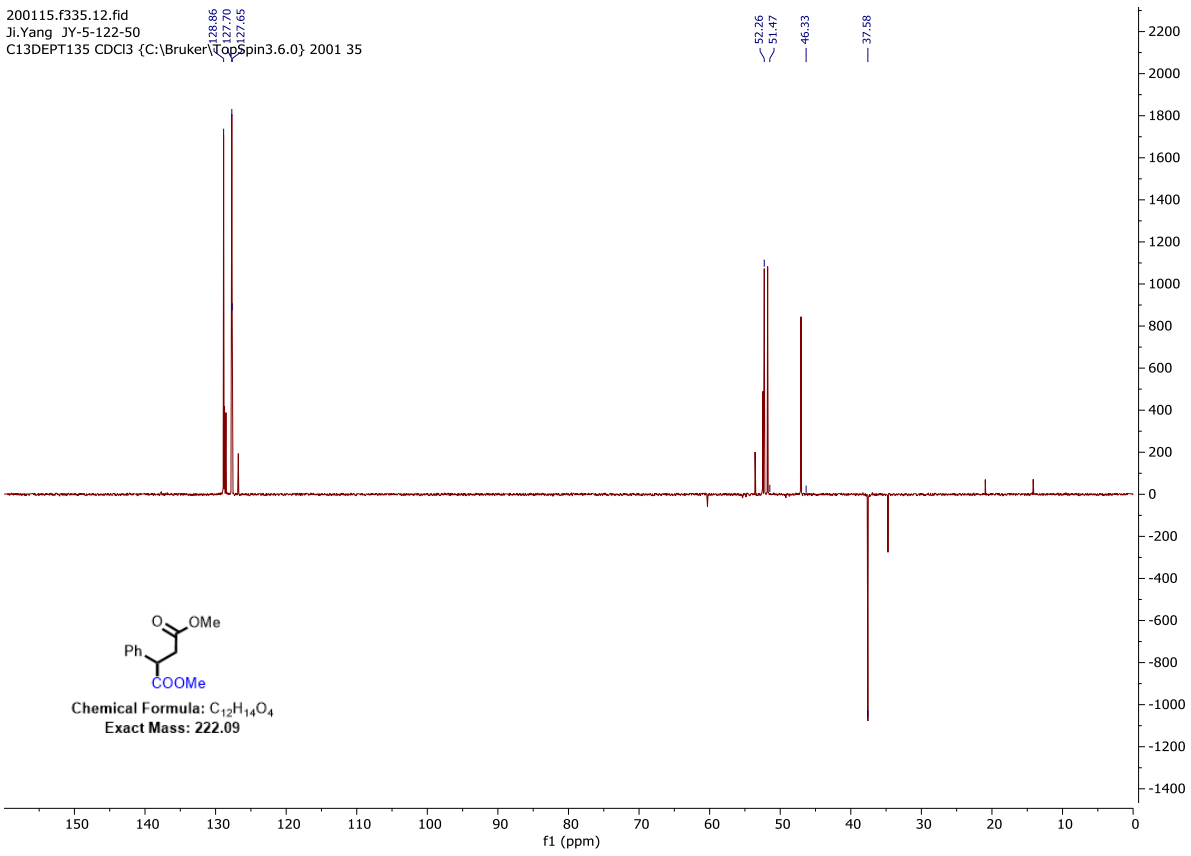
No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		16,068	22,163	451,922	22,29	31,14	n.a.
2		16,847	77,249	999,182	77,71	68,86	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**99,412**	**1451,105**	**100,00**	**100,00**	



dimethyl (*R*)-2-phenylsuccinate
Chemical Formula: $C_{12}H_{14}O_4$
Exact Mass: 222.09




200115.f335.11.fid
Ji.Yang JY-5-122-50
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 35
173.36
171.91
144.12
128.86
127.70
127.65
77.59
77.16
76.74
52.26
51.77
47.05
37.58
OMe
Ph
COOMe
Chemical Formula: C12H14O4
Exact Mass: 222.09
f1 (ppm)

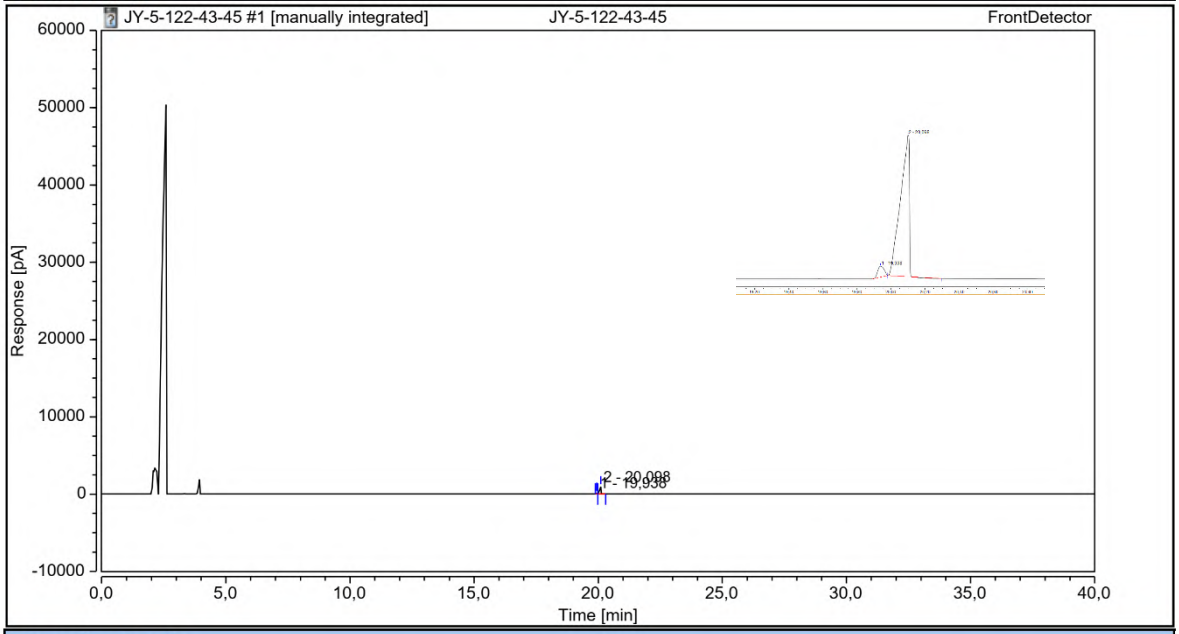

200115.f335.12.fid
Ji.Yang JY-5-122-50
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 35
128.86
127.70
127.65
52.26
51.47
46.33
37.58
OMe
Ph
COOMe
Chemical Formula: C12H14O4
Exact Mass: 222.09
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-43-45**	*Run Time (min):*	**40,00**
Vial Number:	**73**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**13.Jan.20 14:30**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		19,938	3,040	70,365	5,31	7,24	n.a.
2		20,098	54,255	901,678	94,69	92,76	n.a.
Total:			**57,295**	**972,043**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-122-43.D
Operator   :
Acquired   : 13 Jan 2020  15:16     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-122-43
Misc Info  :
Vial Number: 46
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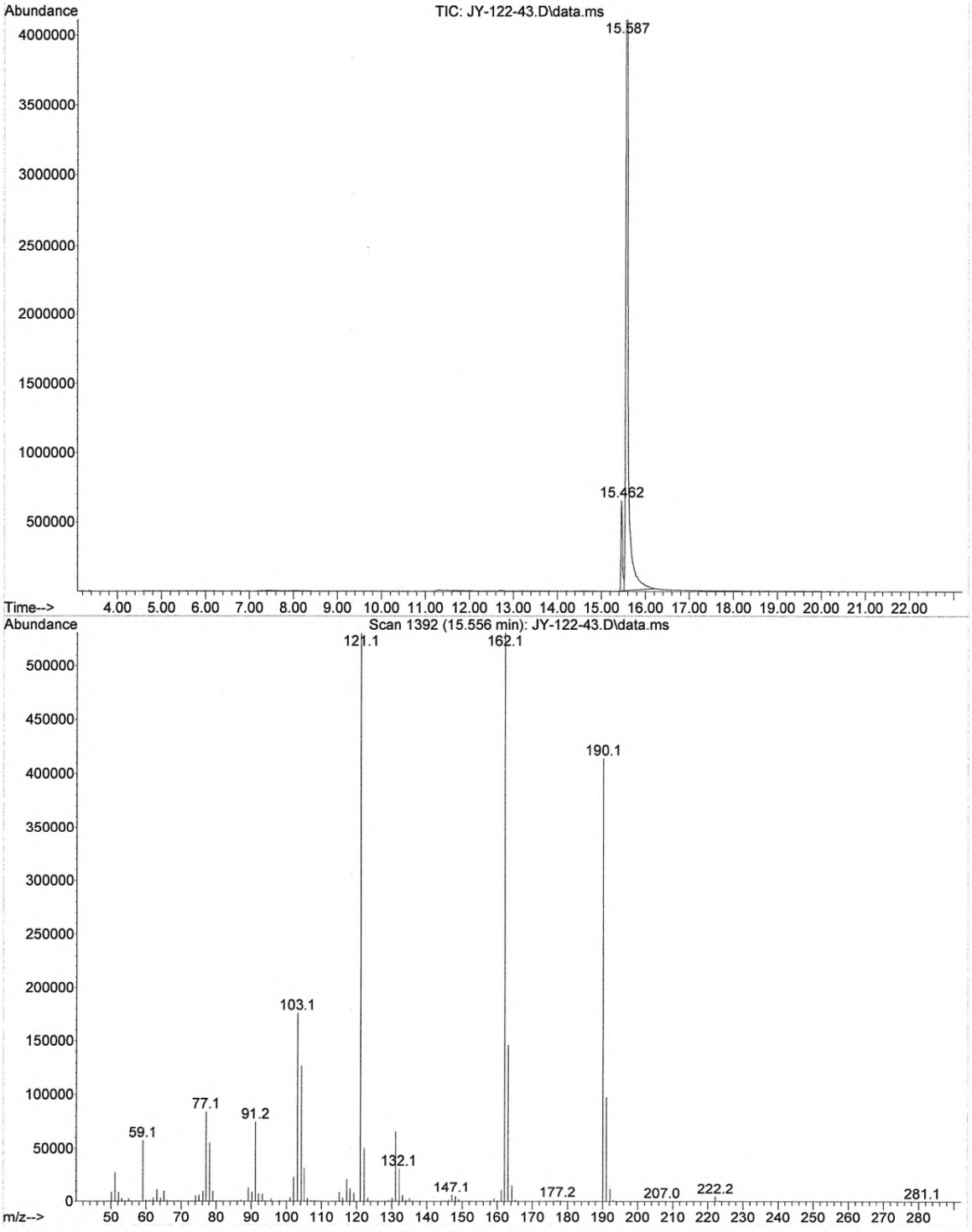
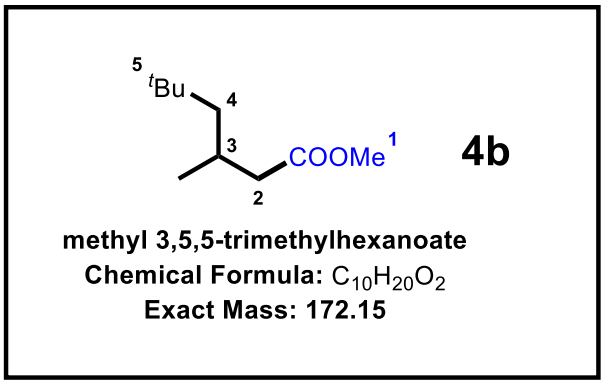
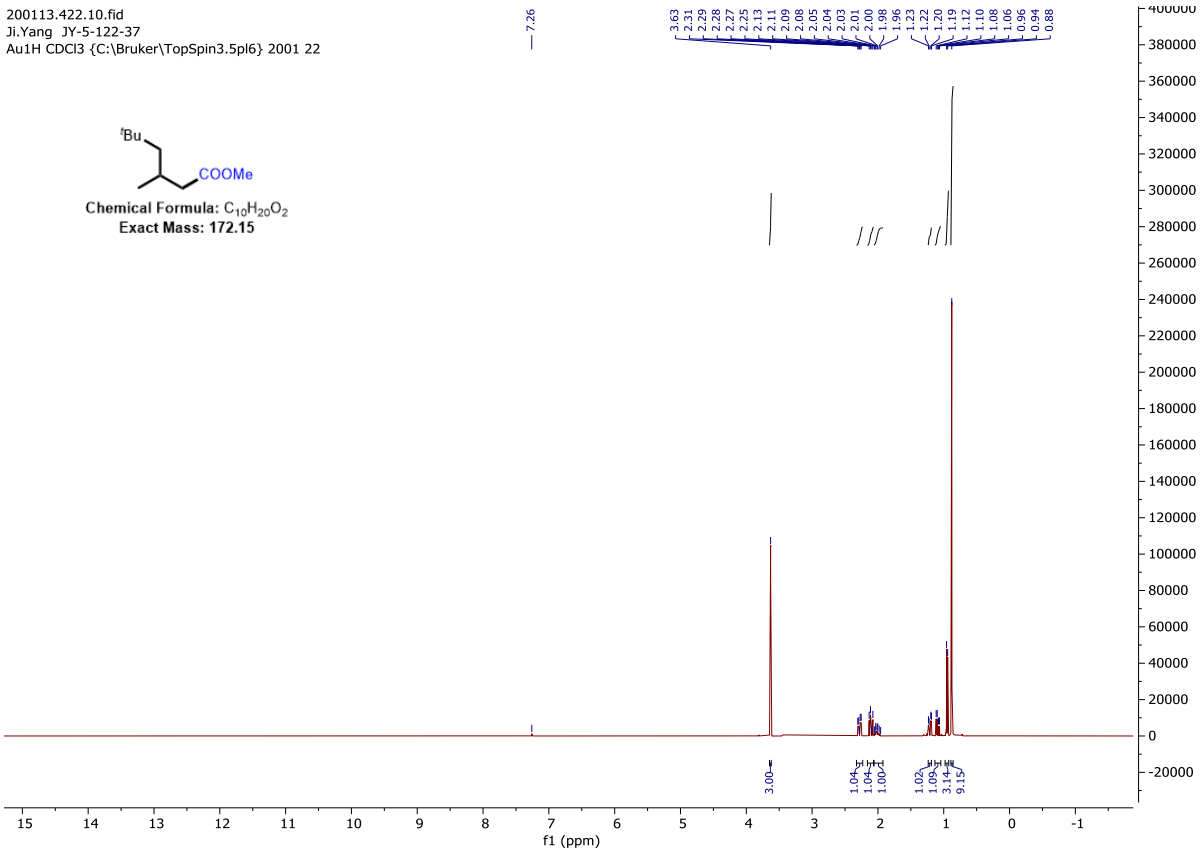
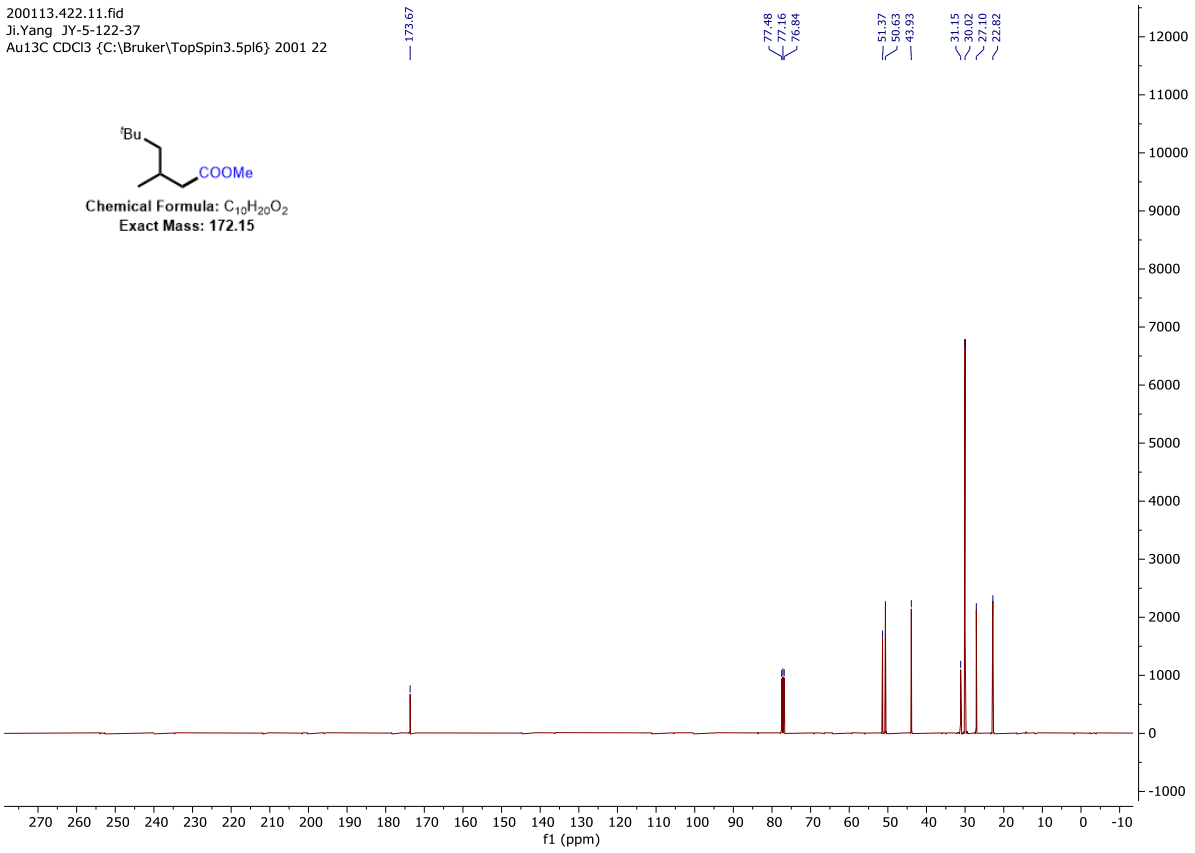


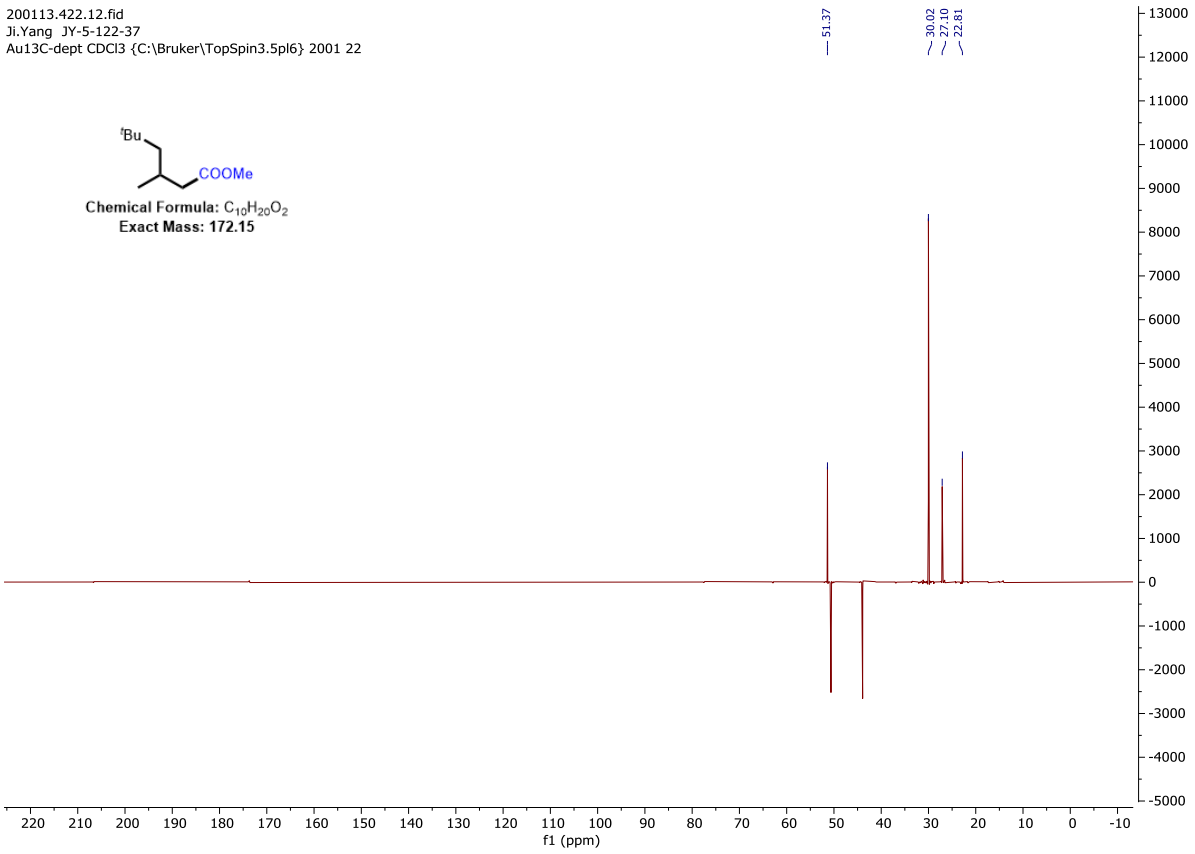


4b

methyl 3,5,5-trimethylhexanoate
Chemical Formula: $C_{10}H_{20}O_2$
Exact Mass: 172.15




200113.422.11.fid
Ji.Yang JY-5-122-37
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 22
173.67
77.48
77.16
76.84
51.37
50.63
43.93
31.15
30.02
27.10
22.82
tBu
COOMe
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)

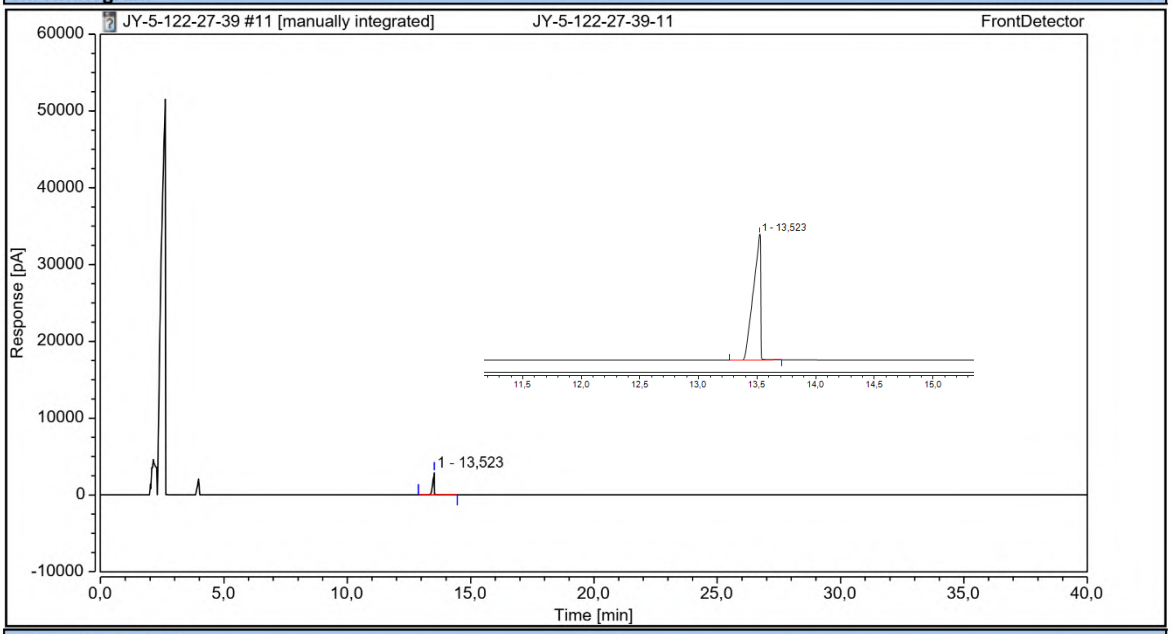

200113.422.12.fid
Ji.Yang JY-5-122-37
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5pl6} 2001 22
51.37
30.02
27.10
22.81
tBu
COOMe
Chemical Formula: C10H20O2
Exact Mass: 172.15
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-11**	*Run Time (min):*	**40,00**
Vial Number:	**35**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Jan.20 23:31**	*Sample Weight:*	**1,0000**

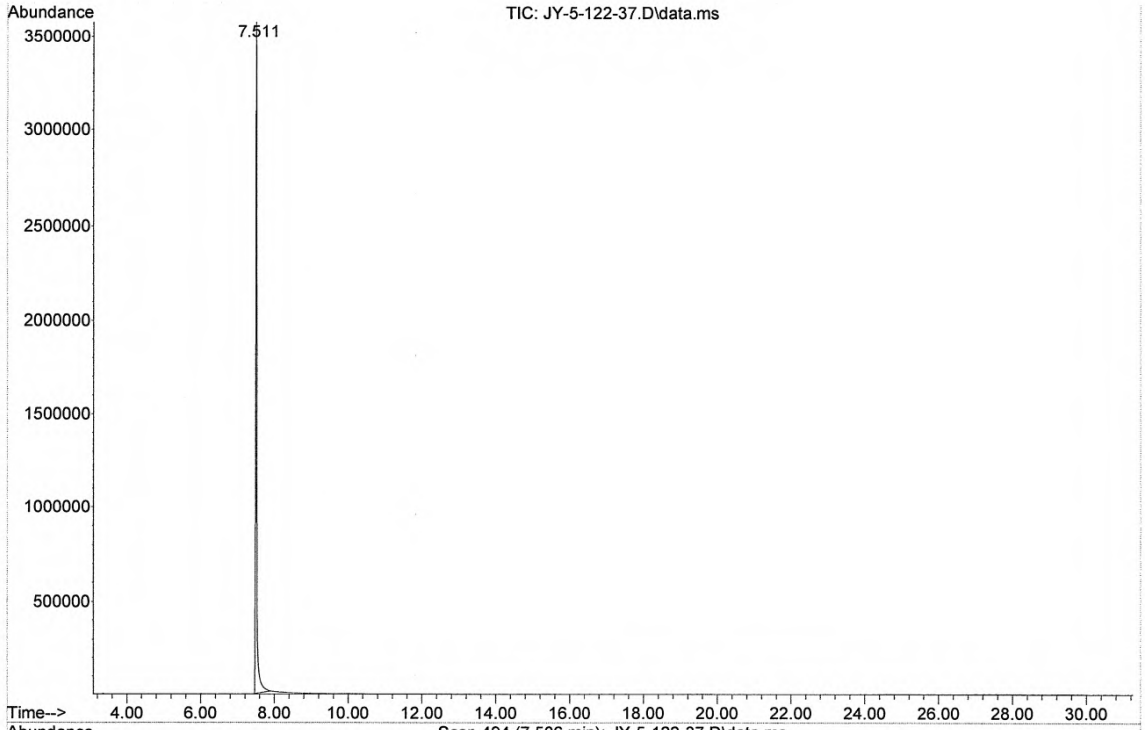
Chromatogram

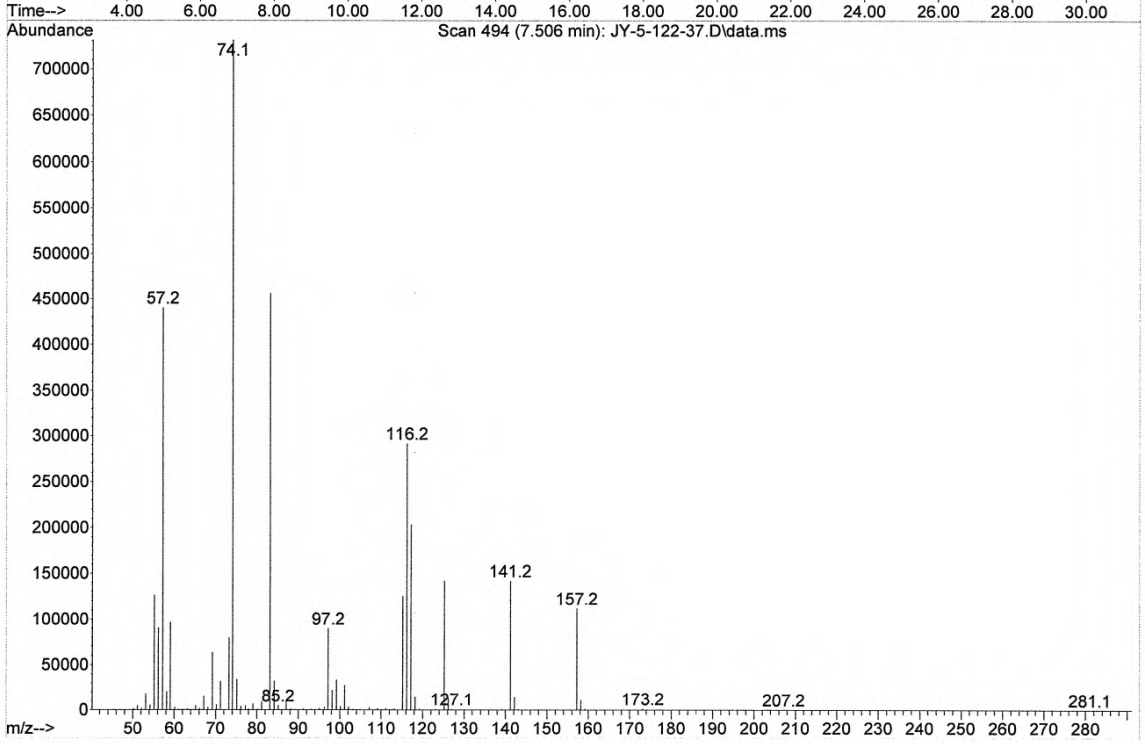


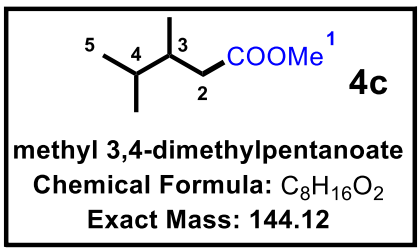
Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		13,523	208,485	2869,076	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**208,485**	**2869,076**	**100,00**	**100,00**	

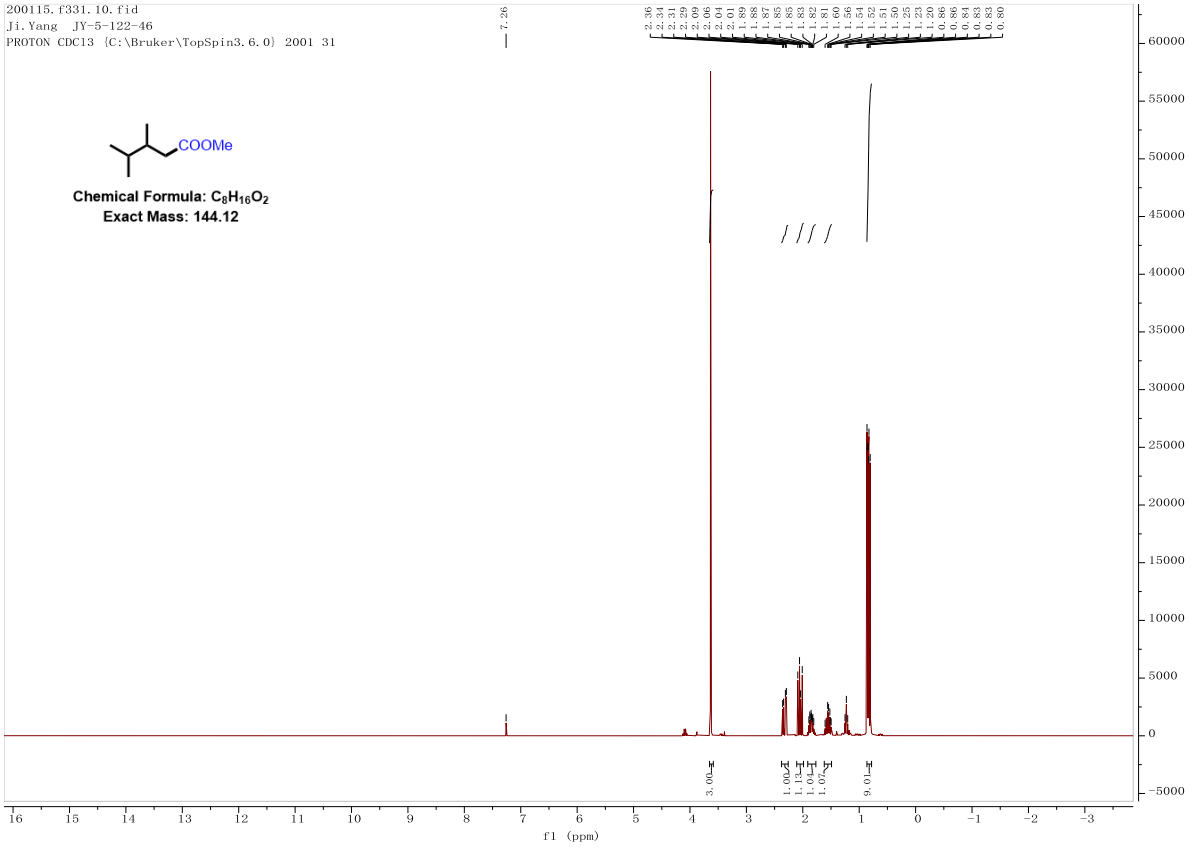
File :D:\MSDChem\1\DATA\2001\JY-5-122-37.D
Operator :
Acquired : 11 Jan 2020 22:25 using AcqMethod SK3-30X.M
Instrument : GC-MSD
Sample Name: JY-5-122-37
Misc Info :
Vial Number: 41

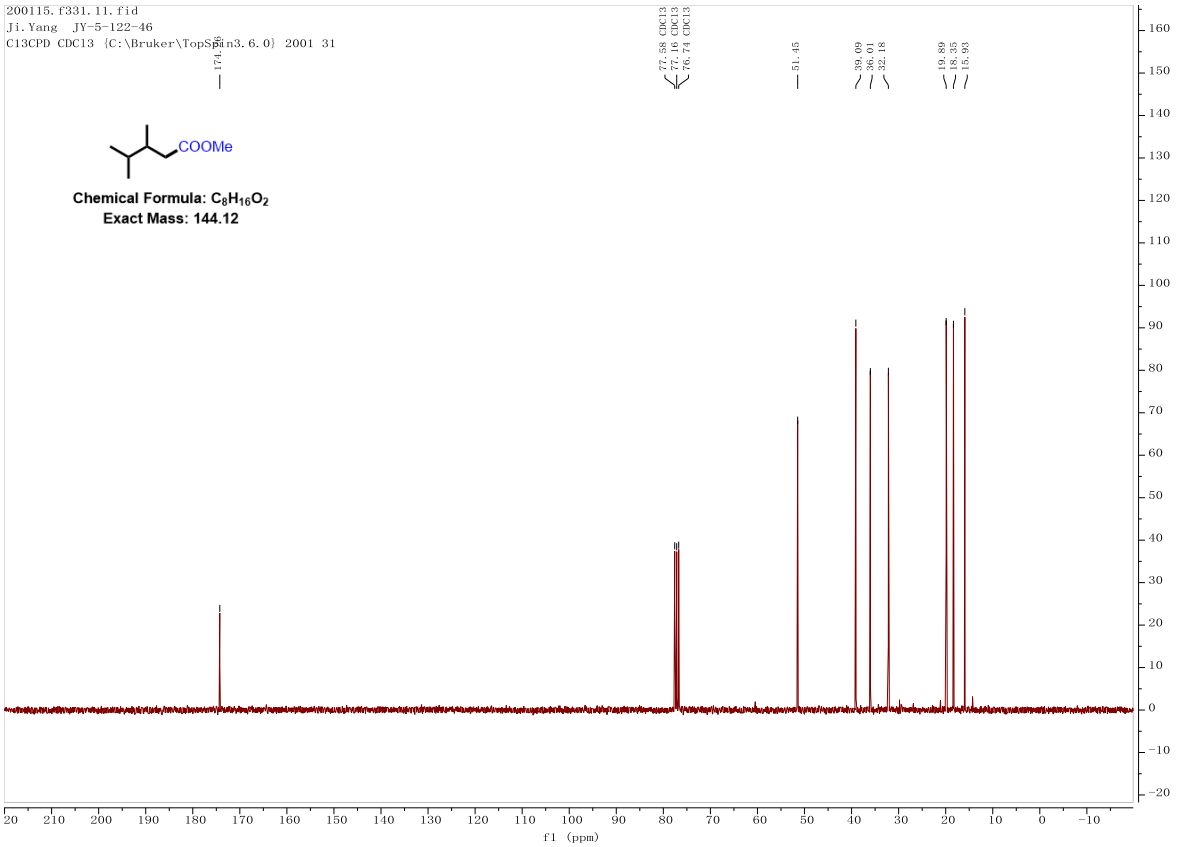


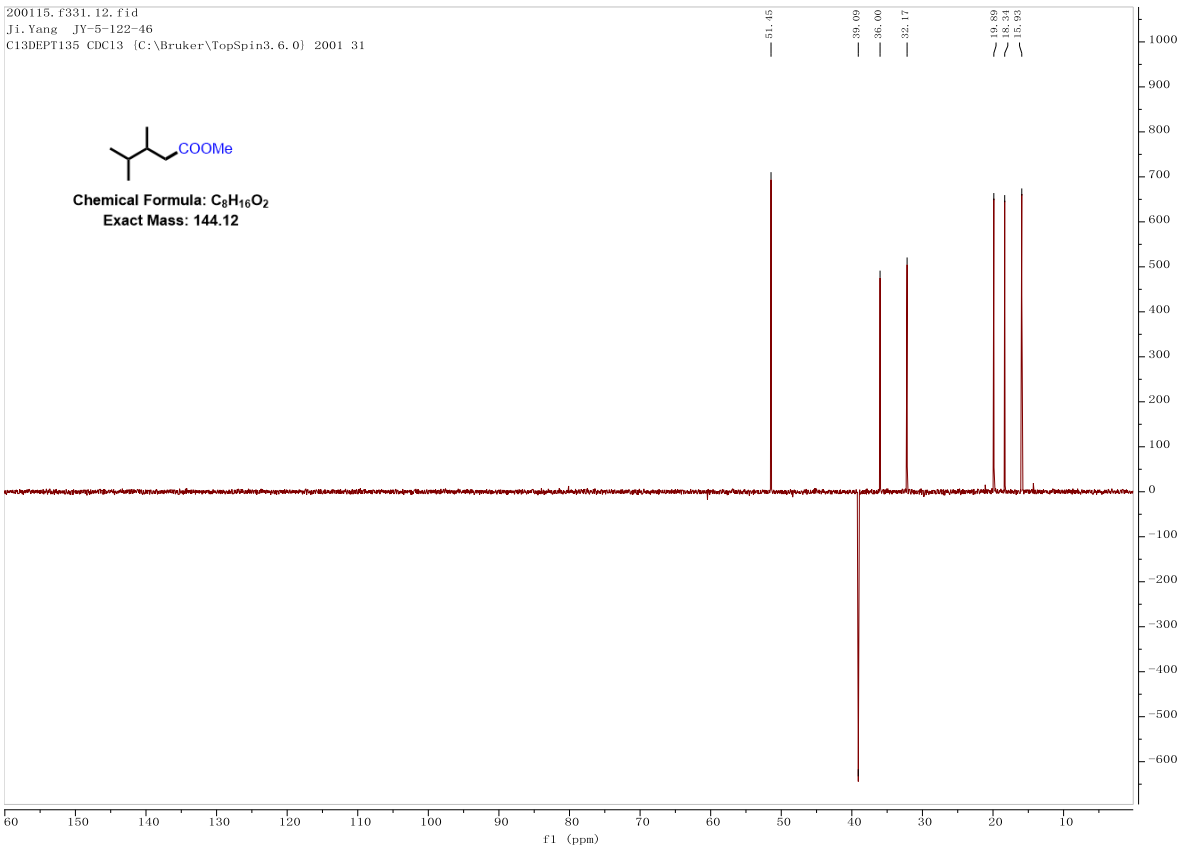




methyl 3,4-dimethylpentanoate
Chemical Formula: $C_8H_{16}O_2$
Exact Mass: 144.12




200115.f331.11.fid
Ji.Yang JY-5-122-46
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 31
174.89
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
51.45
39.09
36.01
32.18
19.89
18.35
15.93
COOMe
Chemical Formula: C8H16O2
Exact Mass: 144.12
f1 (ppm)

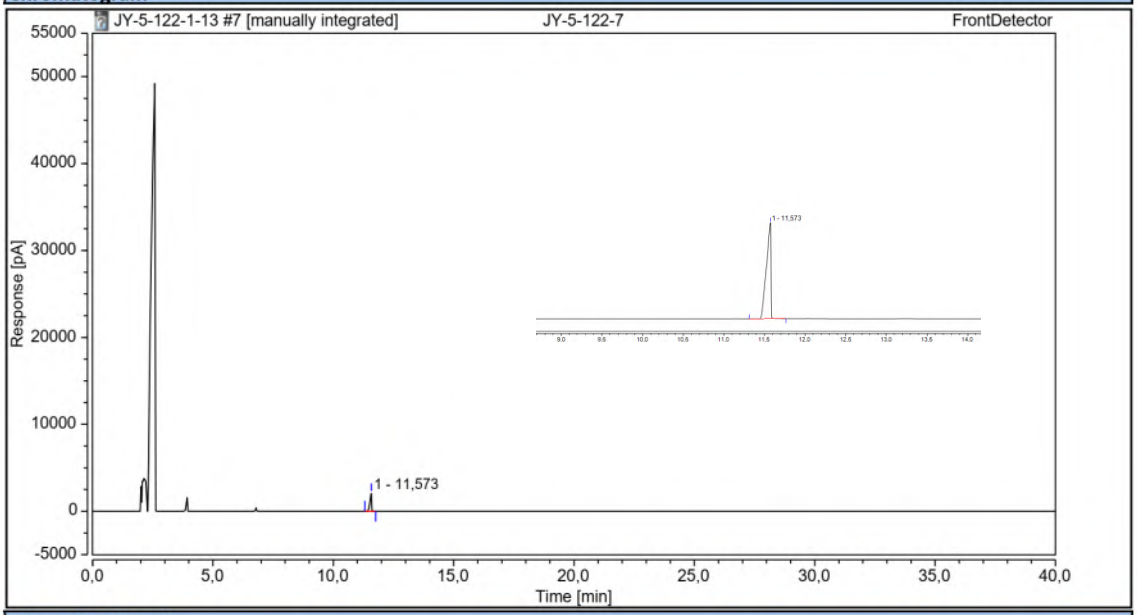

200115.f331.12.fid
Ji.Yang JY-5-122-46
C13DEPT135 CDCl3 {C:\Bruker\TopSpin3.6.0} 2001 31
51.45
39.09
36.00
32.17
19.89
18.34
15.93
COOMe
Chemical Formula: C8H16O2
Exact Mass: 144.12
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-7**	*Run Time (min):*	**40,00**
Vial Number:	**67**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**09.Jan.20 21:33**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		11,573	127,703	2011,701	100,00	100,00	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Total:			**127,703**	**2011,701**	**100,00**	**100,00**	

```
File       :D:\MSDChem\1\DATA\2001\JY-5-122-7.D
Operator   :
Acquired   :  9 Jan 2020  19:01     using AcqMethod SK3-30X.M
Instrument :    GC-MSD
Sample Name: JY-5-122-7
Misc Info  :
Vial Number: 42
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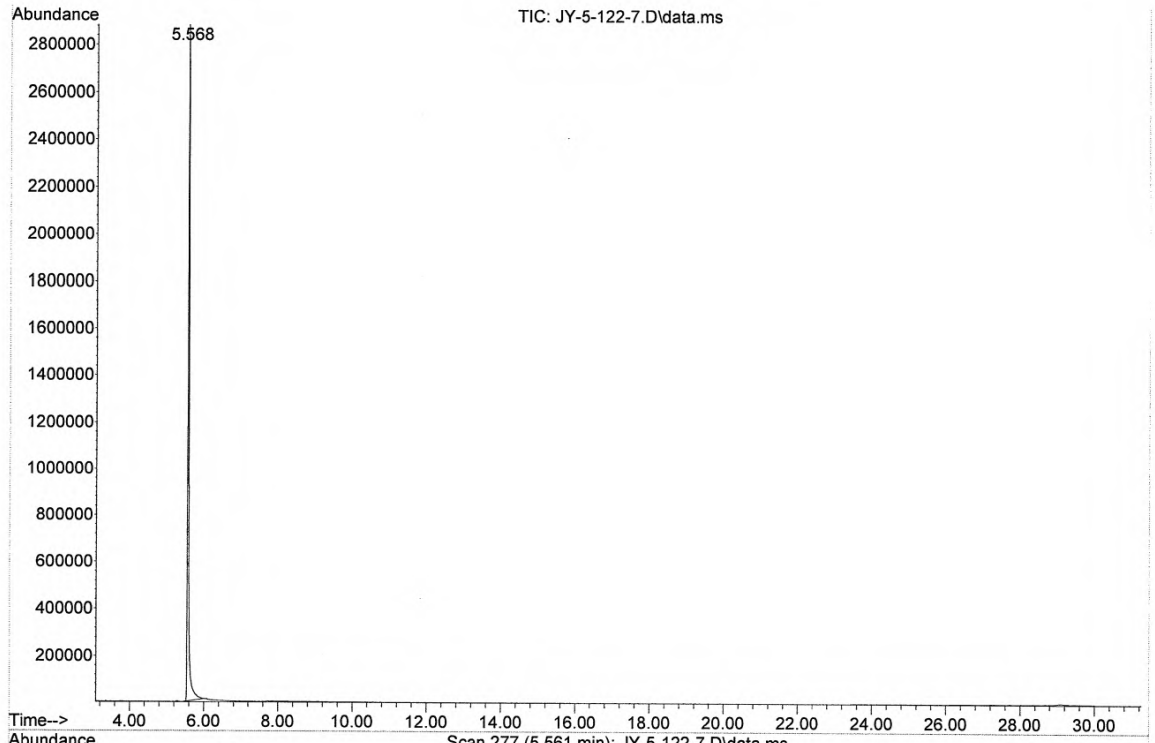
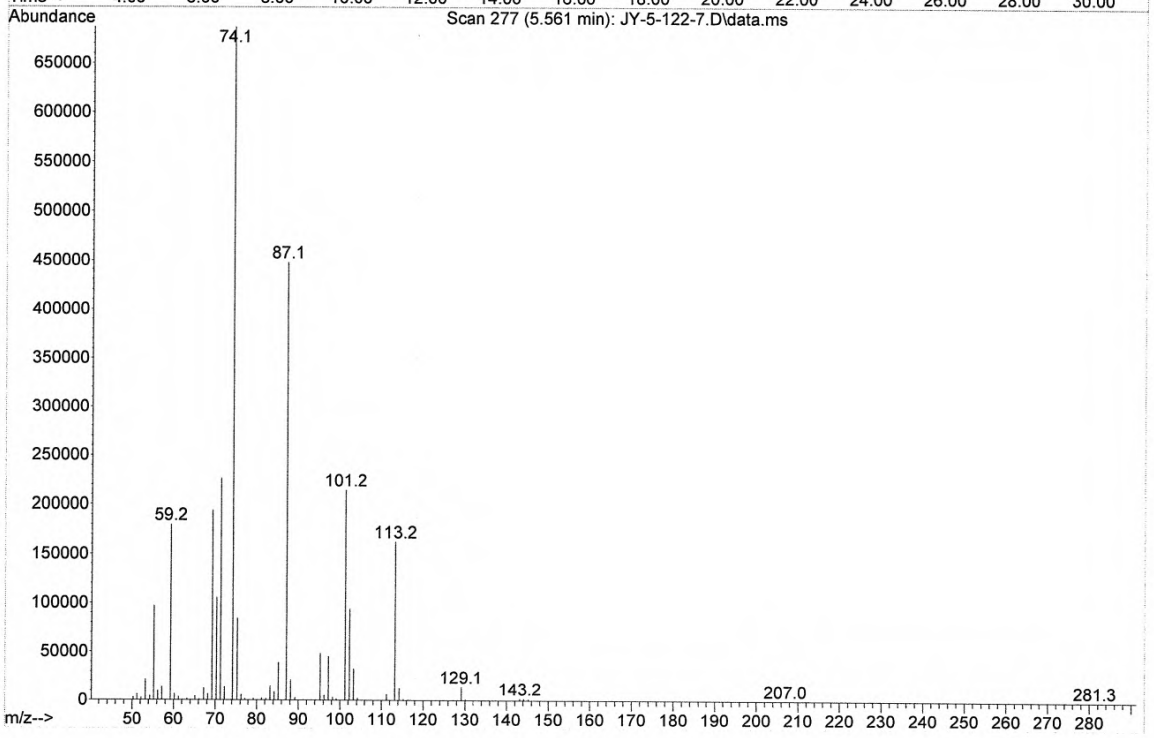
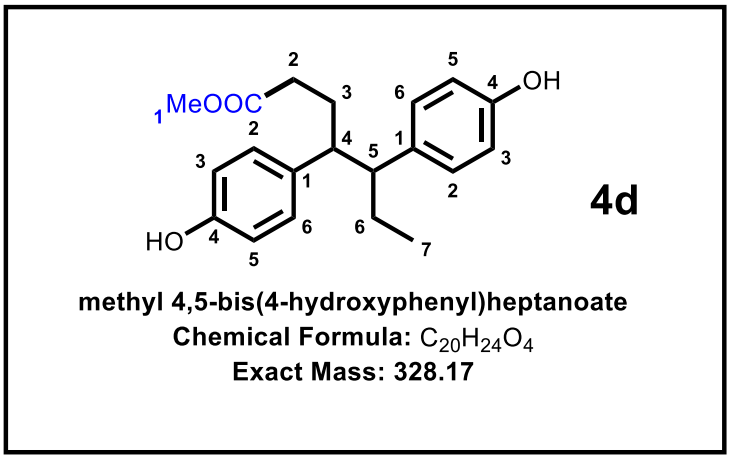
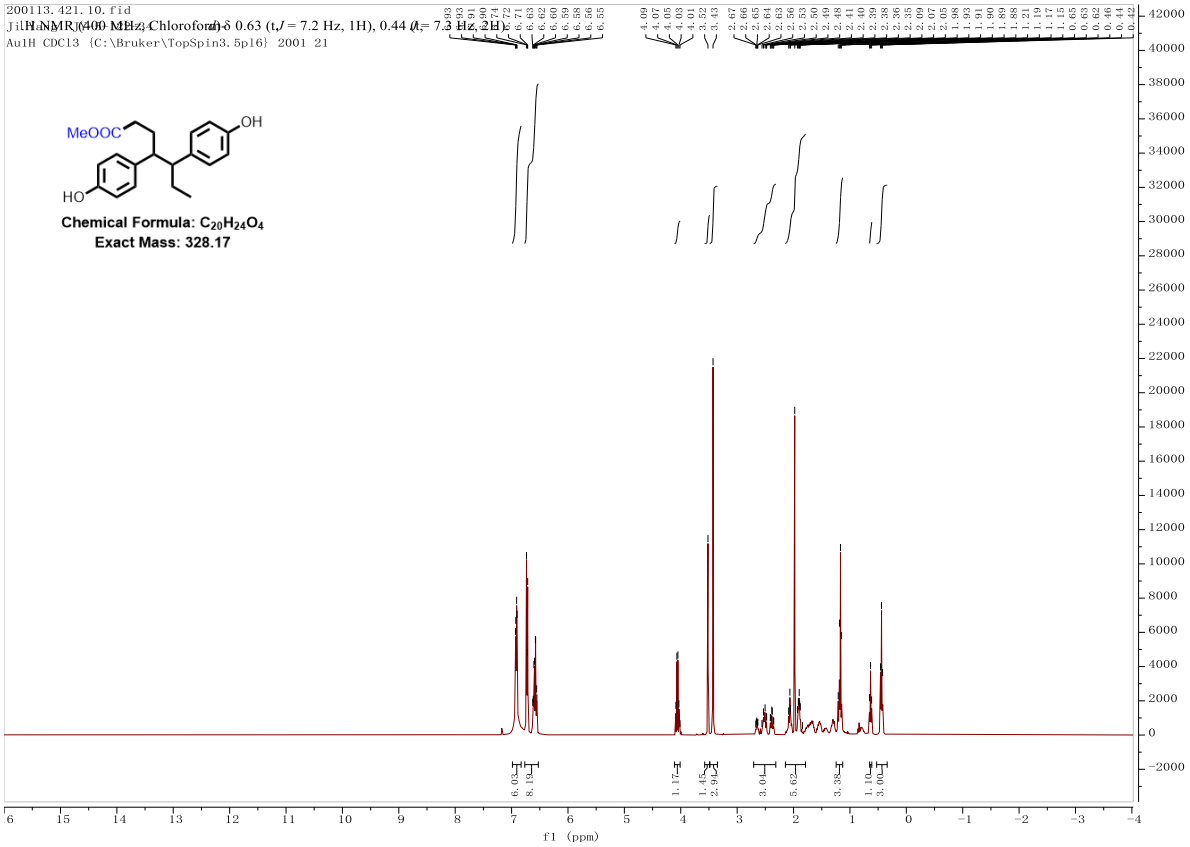
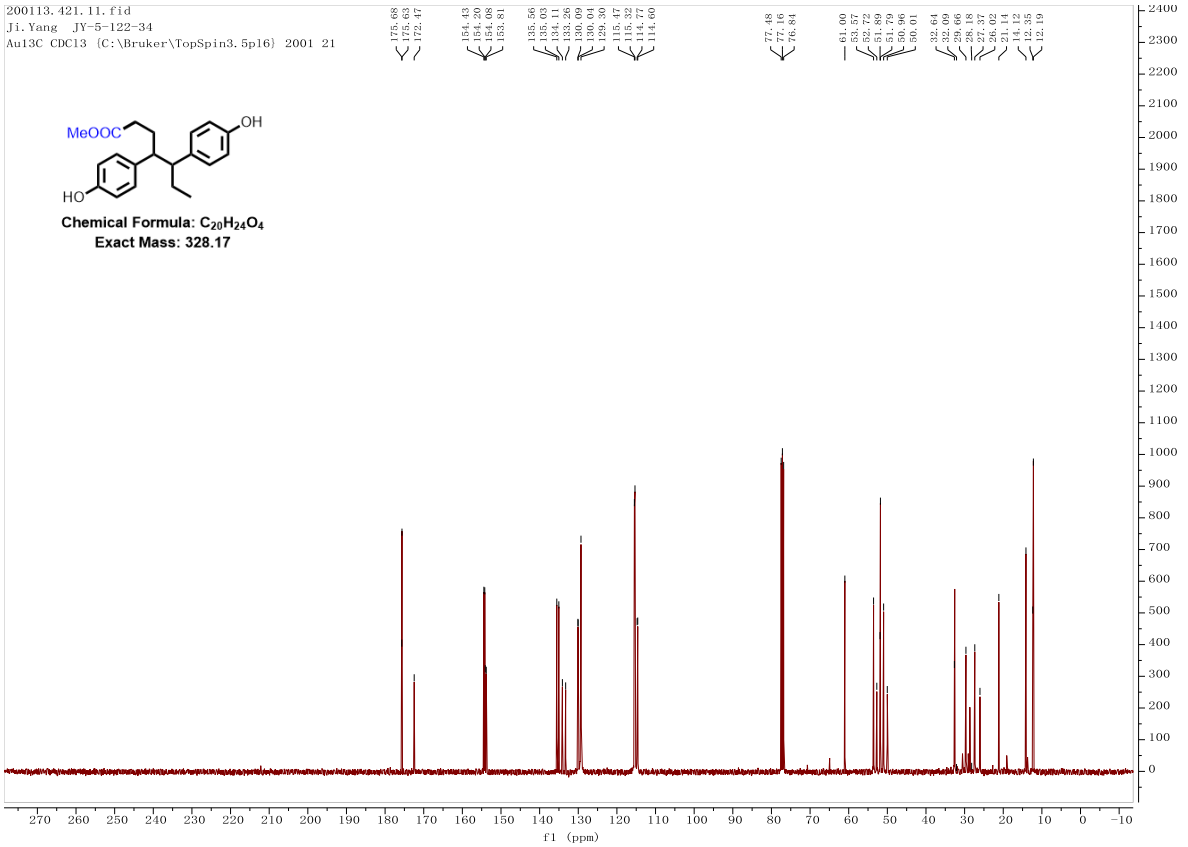
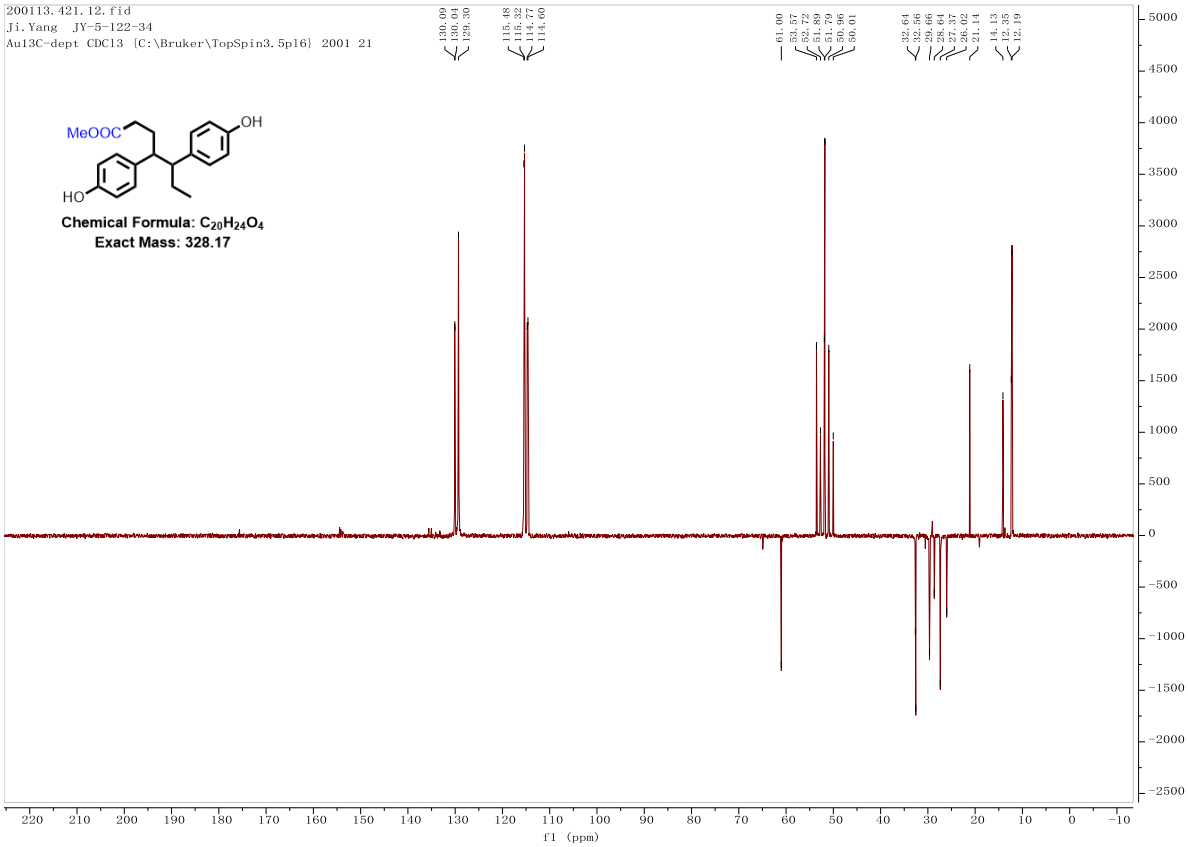





MeOOC
OH
HO
4d
methyl 4,5-bis(4-hydroxyphenyl)heptanoate
Chemical Formula: $C_{20}H_{24}O_4$
Exact Mass: 328.17


200113. 421. 10. fid
AulH CDC13 {C:\Bruker\TopSpin3. 5p16} 2001 21
MeOOC
OH
HO
Chemical Formula: $C_{20}H_{24}O_4$
Exact Mass: 328.17
f1 (ppm)


200113.421.11.fid
Ji.Yang JY-5-122-34
Au13C CDCl3 {C:\Bruker\TopSpin3.5p16} 2001 21
MeOOC
OH
HO
Chemical Formula: C20H24O4
Exact Mass: 328.17
f1 (ppm)

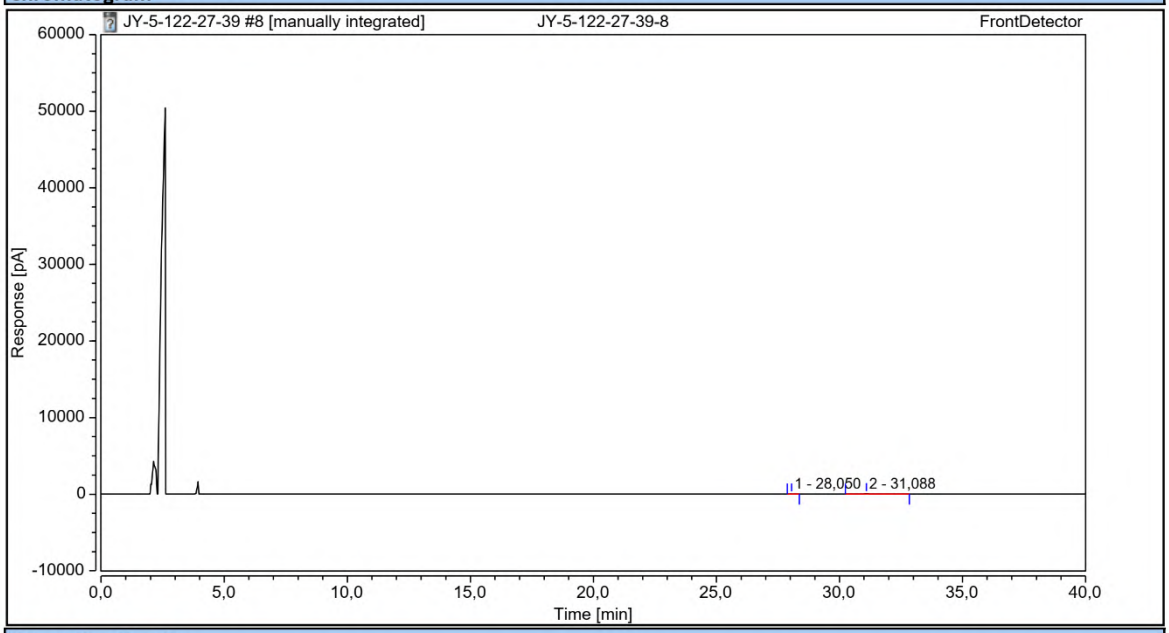

200113.421.12.fid
Ji.Yang JY-5-122-34
Au13C-dept CDCl3 {C:\Bruker\TopSpin3.5p16} 2001 21
MeOOC
OH
HO
Chemical Formula: C20H24O4
Exact Mass: 328.17
f1 (ppm)

Chromatogram and Results

Injection Details

Injection Name:	**JY-5-122-27-39-8**	*Run Time (min):*	**40,00**
Vial Number:	**32**	*Injection Volume:*	**2,00**
Injection Type:	**Unknown**	*Channel:*	**FrontDetector**
Calibration Level:		*Wavelength:*	**n.a.**
Instrument Method:	**dong-40min**	*Bandwidth:*	**n.a.**
Processing Method:	**dong**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Jan.20 20:29**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area pA*min	Height pA	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	Component 5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1		28,050	1,870	11,640	10,30	22,28	n.a.
2		31,088	16,286	40,616	89,70	77,72	n.a.
Total:			**18,156**	**52,256**	**100,00**	**100,00**	

File :D:\MSDChem\1\DATA\2001\JY-5-122-34.D
Operator :
Acquired : 11 Jan 2020 20:13 using AcqMethod SK3-45X.M
Instrument : GC-MSD
Sample Name: JY-5-122-34
Misc Info :
Vial Number: 38