Electronic Supplementary Information For:

Oxidation of olefins using molecular oxygen catalyzed by part-per-million level of recyclable copper catalyst under mild conditions

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1. Experimental methods

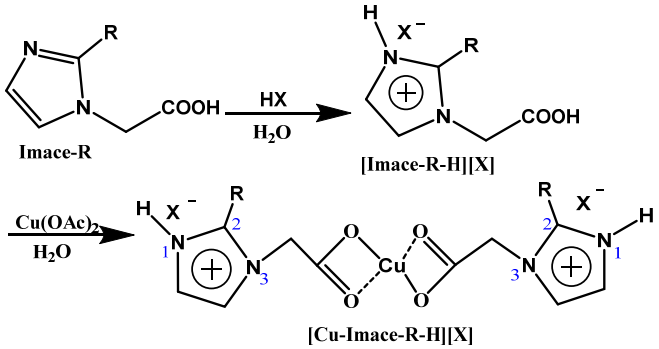
1.1 Materials and characterization methods

All solvents and chemicals were analytically pure agents purchased from commercial sources and were used without further purification unless otherwise indicated. The quantitative analysis of reactants and products was performed on a Shimadzu GC2014 gas chromatograph equipped with a WondaCAP-5 capillary column (5% Diphenyl 95% Dimethylpolysiloxane 30m×0.32mm×0.25μm) with a flame-ionization detector. A Shimadzu GCMS-QP2010 was used to identify substrates and their oxidation products resulting from catalysis. ^{1}H NMR and ^{13}C NMR spectra of ligands were recorded on a Bruker 400 MHz spectrometer. Ultraviolet-visible spectrum of different catalysts were recorded using a Shimadzu UV-3600 spectrophotometer (acetic acid as solvent). ESI Mass spectra of different catalysts were recorded using a Shimadzu LCMS-8030 ESI Mass Spectrometer.

1.2 General procedure for the synthesis of copper catalysts with an imidazole salt tag [Cu-Imace-R-H] [X] (X^-=F^-, Cl^-, Br^-, I^-, $CF_3CO_2^-$, HSO_4^-, NO_3^-, PF_6^-, or BF_4^-; R=H or CH_3)

The catalysts were synthesized according our previous procedures (ref. 49). In a typical experiment, 12.6 g (0.01 mol) 1-imidazoleacetic acid (Imace-H) was reacted with 11.0 g (0.11 mol) hydrochloric acid (36%) in 60 ml water at 50 °C for 3 h. The reaction mixture was evaporated under reduced pressure at 80 °C, and a white powder was obtained. Water was used to recrystallize the powder, and pure [Imace-H-H][Cl] was obtained. Subsequently, 14.6 g (0.090 mol) [Imace-H-H][Cl] was reacted with 8.9 g (0.045 mol) $Cu(OAc)_2$•H_2O in 100 ml water at 100 °C. The generated acetic acid was removed using water vapor. New amount of water (50 ml) was continuously added into the reaction system until the reaction was completed. The reaction mixture was then evaporated under reduced pressure at 80 °C, and a light-green

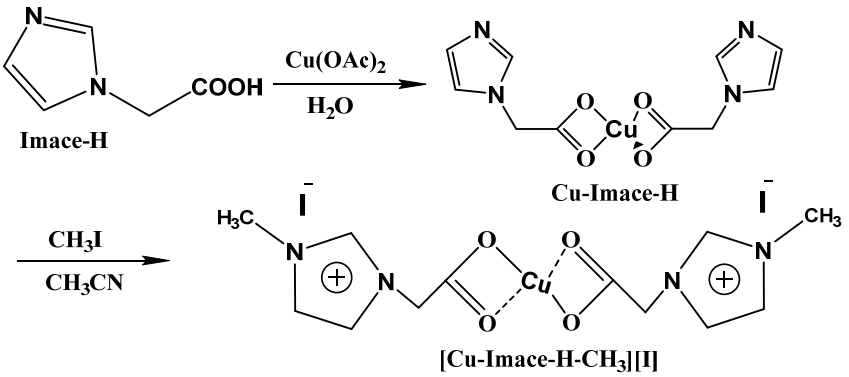
powder was obtained. Water was used to recrystallize the powder to obtain pure [Cu-Imace-H-H][Cl] (yield: 88.4%).



Scheme S1 Generation method for preparing [Cu-Imace-R-H][X] (X^-=F^-, Cl^-, Br^-, I^-, $CF_3CO_2^-$, HSO_4^-, NO_3^-, PF_6^-, or BF_4^-; R=H or CH_3)

1.3 Procedure for the synthesis of [Cu-Imace-H-CH_3][I]

2.52g (0.02 mol) 1-imidazoleacetic acid (Imace-H) was reacted with 2.0 g (0.01 mol) $Cu(OAc)_2$•H_2O in 30 ml water at 100 °C. The generated acetic acid was removed using water vapor. New water was continuously added into the reaction system until the reaction was completed. The reaction mixture was then evaporated until the mixture left about 15mL under reduced pressure at 80 °C. The suspended mixture was cooled to room temperature. After filtration, the precipitate was washed repeatedly with water, and dried under vacuum at 60 °C. The pure Cu-Imace-H was obtained. Subsequently, 1.57g (0.005 mol) Cu-Imace-H was reacted with 1.7g (0.012 mol) CH_3I in 20 ml acetonitrile at 30 °C. The suspended mixture was stirred continuously for 24 h, then the reaction mixture was evaporated under reduced pressure at 50 °C, and a blue powder was obtained. Water was used to recrystallize the powder, and pure [Cu-Imace-H-CH_3][I] was obtained. (Yield: 83.6%).



Scheme S2 Method for preparing [Cu-Imace-H-CH_3][I]

1.4 General procedure for cyclohexene epoxidation

The epoxidation reactions were carried out in tailored tubes equipped with a condensing unit (-30℃ ethanol as a cooling medium for the condensing to prevent the volatilization of solvent). Typically, 50 mL acetonitrile, 0.2 mol substrate, 0.2mol isobutylaldehyde and 0.08%mol (relative to the molar equivalent of substrate) catalysts were mixed with stirring at 60 °C. Then, molecular oxygen (>99.0%) was bubbled through the solution and the reaction times were given in the tables or figures of the manuscript. o-dichlorobenzene was used as an internal standard for the determination of yield and selectivity. The filtered liquid samples were analyzed by GC and GC-MS.

1.5 General procedure for catalyst recycling

The epoxidation reactions were carried out in tailored tubes equipped with a condensing unit (-30℃ ethanol as a cooling medium for the condensing to prevent the volatilization of solvent). 50 mL acetonitrile, 0.2 mol substrate, 0.2mol isobutylaldehyde and 0.08%mol (relative to the molar equivalent of substrate) catalysts were mixed with stirring at 60 °C. Then, molecular oxygen (>99.0%) was bubbled through the solution. The catalyst can be performed by simple filtration after the completion of the reactions, the recycled catalyst was washed by

diethyl ether, then dried at 60 °C overnight. The reactions were performed under the same conditions using the recovered catalyst.

2. The influence of BHT for the oxidation

Procedure for cyclohexene epoxidation in the presence of BHT (3,5-di-tert-butyl-p-hydroxytoluene): The epoxidation reactions were carried out in tailored tubes equipped with a condensing unit (-30℃ ethanol as a cooling medium for the condensing to prevent the volatilization of solvent). 50 mL acetonitrile, 0.2 mol substrate, 0.2mol isobutylaldehyde and 0.08%mol (relative to the molar equivalent of substrate) catalysts were mixed with stirring at 60 °C. Then, molecular oxygen (>99.0%) was bubbled through the solution. After 2 hours, 0.1g BHT was added into the catalytic system.

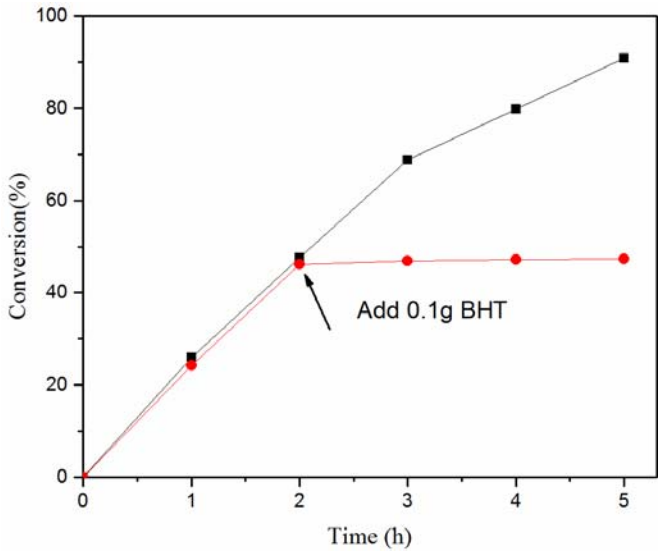


Fig. S1. The influence of BHT for the oxidation. Black line: normal reaction. Red line, 0.1g BHT was added after 2 hours.

3. The results of different reaction conditions

3.1 Reaction temperature

3.1 Solvent

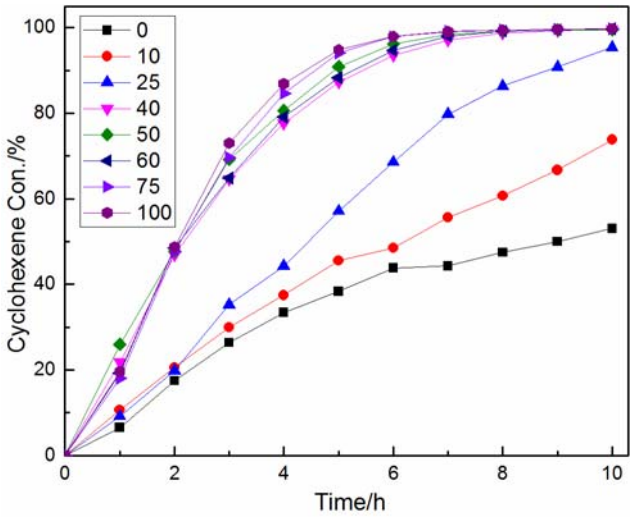


Fig. S2 Profile of the conversion rates of cyclohexene oxide for different amount of solvent (cyclohexene (0.2mol), solvent (CH_3CN, mL),isobutyraldehyde (0.2mol), the catalyst-to-substrate molar ratio is 800ppm, 60 ℃, O_2 bubbling (1atm).Products formed in the epoxidation reactions with olefins were identified by GC and GC-MS.)

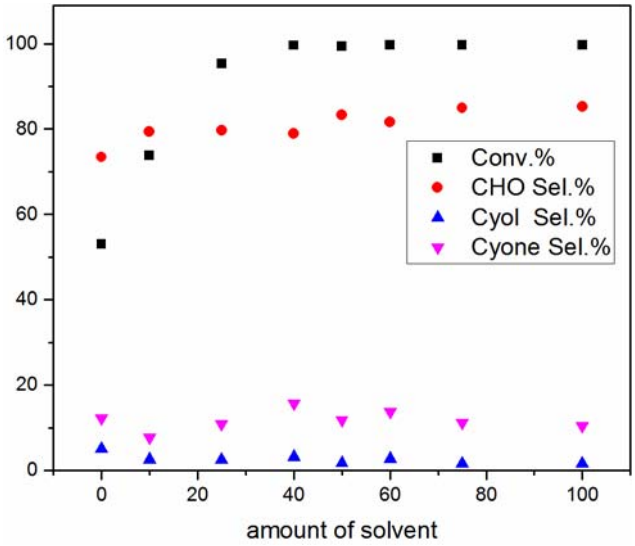


Fig. S3 The performance of loading different amount of solvent in the cyclohexene (cyclohexene (0.2mol), solvent (CH_3CN, mL),isobutyraldehyde (0.2mol), the catalyst-to-substrate molar ratio is 800ppm, 60 ℃, O_2 bubbling (1atm), 10h.Products formed in the epoxidation reactions with olefins were identified by GC and GC-MS.)

3.2 The molar ratio of isobutyraldehyde-to- cyclohexene

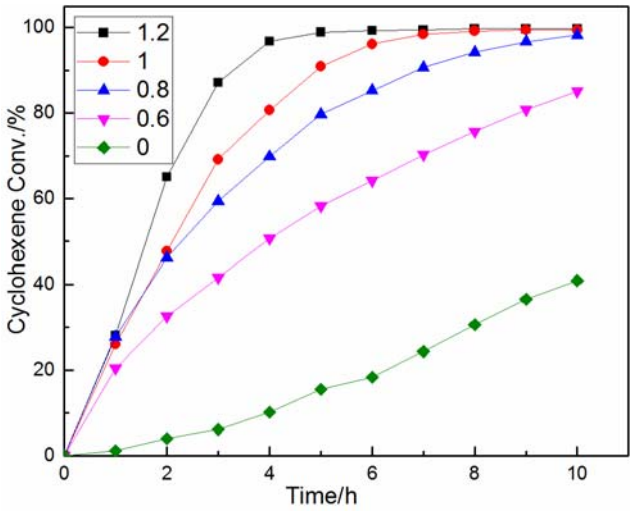


Fig. S4 Profile of the conversion rates of cyclohexene oxide for different molar ratios of isobutyraldehyde-to- cyclohexene (cyclohexene (0.2mol), solvent (CH_3CN, 50mL), the molar ratio of isobutyraldehyde-to- cyclohexene is 0, 0.6, 0.8, 1, 1.2., the catalyst-to-substrate molar ratio is 800ppm, 60 ℃, O_2 bubbling (1atm).Products formed in the epoxidation reactions with olefins were identified by GC and GC-MS.)

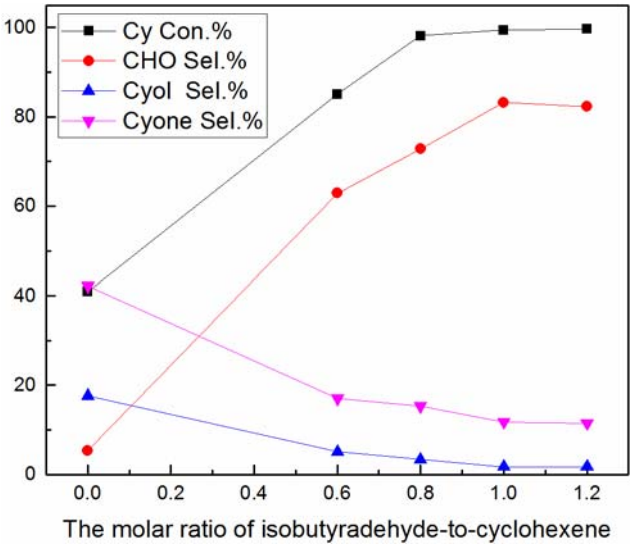


Fig. S5 The performance of different molar ratios of isobutyraldehyde-to- cyclohexene (cyclohexene (0.2mol), solvent (CH_3CN, 50mL), the molar ratio of isobutyraldehyde-to-cyclohexene is 0, 0.6, 0.8, 1, 1.2., the catalyst-to-substrate molar ratio is 800ppm, 60 ℃, O_2 bubbling (1atm),10h.Products formed in the epoxidation reactions with olefins were identified by GC and GC-MS.)

4 The characterization results of the catalysts

[Imace-H-H][F]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.76 (2H, s, CH_2), 7.32 (H, m, N-CH), 8.58 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 51.34 (-CH_2-), 119.23 (N-CH), 122.87 (N-CH), 135.38 (N-CH-N), 172.01 (-COOH). [Cu-Imace-H-H][F]: UV-vis (Acetic acid) λ_{max} (nm) 247.38. Elemental analysis: $C_{10}H_{12}F_2N_4O_4Cu{\cdot}0.5H_2O$, Calc. C 33.11, H 3.61, N 15.44; Found C 32.85, H 3.21, N 15.12. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][Cl]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.99 (2H, s, CH_2), 7.31 (H, s, N-CH), 8.63 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 49.66 (-CH_2-), 119.43 (N-CH), 122.97 (N-CH), 135.81 (N-CH-N), 169.77(-COOH). [Cu-Imace-H-H][Cl]: UV-vis (Acetic acid) λ_{max} (nm) 249.13. Elemental analysis: $C_{10}H_{12}Cl_2N_4O_4Cu$, Calc. C 31.06, H 3.13, N 14.49; Found C 30.04, H 2.90, N 15.07. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][Br]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.99 (2H, s, CH_2), 7.32 (H, d, N-CH), 8.64 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 49.85 (-CH_2-), 119.47 (N-CH), 123.04 (N-CH), 135.84 (N-CH-N), 169.63(-COOH). [Cu-Imace-H-H][Br]: UV-vis (Acetic acid) λ_{max} (nm) 249.48. Elemental analysis: $C_{10}H_{12}Br_2N_4O_4Cu$, Calc. C 25.26, H 2.54, N 11.78; Found C 26.20, H 2.45, N 12.32. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][I]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.92 (2H, s, CH_2), 7.39 (H, s, N-CH), 8.67 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 50.79 (-CH_2-), 119.39 (N-CH), 123.01 (N-CH), 135.64 (N-CH-N), 171.11(-COOH). [Cu-Imace-H-H][I]: UV-vis (Acetic acid) λ_{max} (nm) 248.77. Elemental analysis: $C_{10}H_{12}I_2N_4O_4Cu$, Calc. C 21.09, H 2.12, N 9.84; Found C 21.31, H 2.41, N 10.05. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][NO_3]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.98 (2H, s, CH_2), 7.32 (H, d, N-CH), 8.62 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 49.57 (-CH_2-), 119.42 (N-CH), 122.94 (N-CH), 135.88 (N-CH-N), 169.83(-COOH). [Cu-Imace-H-H][NO_3]: UV-vis (Acetic acid) λ_{max} (nm) 250.34. Elemental analysis: $C_{10}H_{12}N_6O_{10}Cu$, Calc. C 27.31, H 2.75, N 19.11; Found C 27.99, H 3.02, N 19.30. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][HSO_4]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.86 (2H, s, CH_2), 7.24 (H, s, N-CH), 8.53 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 49.80 (-CH_2-), 119.40 (N-CH), 122.85 (N-CH), 135.77 (N-CH-N), 170.09(-COOH). [Cu-Imace-H-H][HSO_4]: UV-vis (Acetic acid) λ_{max} (nm) 250.88. Elemental analysis: $C_{10}H_{14}S_2N_4O_{12}Cu$, Calc. C 23.56, H 2.77, N 10.99;

Found C 23.47, H 2.83, N 11.33. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][CF_3COO]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.92 (2H, s, CH_2), 7.28 (H, d, N-CH), 8.58 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 49.61 (-CH_2-), 119.39 (N-CH), 122.90 (N-CH), 135.72 (N-CH-N), 169.82(-COOH). [Cu-Imace-H-H][CF_3COO]: UV-vis (Acetic acid) λ_{max} (nm) 247.01. Elemental analysis: $C_{14}H_{12}F_6N_4O_8Cu$, Calc. C 31.04, H 2.23, N 10.34; Found C 32.07, H 2.43, N 10.04. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][BF_4]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 4.92 (2H, s, CH_2), 7.38 (H, s, N-CH), 8.65 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 50.85 (-CH_2-), 119.37 (N-CH), 122.96 (N-CH), 135.64 (N-CH-N), 170.89(-COOH). [Cu-Imace-H-H][BF_4]: UV-vis (Acetic acid) λ_{max} (nm) 246.48. Elemental analysis: $C_{10}H_{12}B_2F_8N_4O_4Cu$, Calc. C 24.54, H 2.47, N 11.45; Found C 23.81, H 2.56, N 12.03. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

[Imace-H-H][PF_6]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 5.02 (2H, s, CH_2), 7.39 (H, dt, N-CH), 8.68 (H, t, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 49.83 (-CH_2-), 119.47 (N-CH), 122.97 (N-CH), 135.89 (N-CH-N), 170.27(-COOH). [Cu-Imace-H-H][PF_6]: UV-vis (Acetic acid) λ_{max} (nm) 247.18. Elemental analysis: $C_{10}H_{12}Cl_2N_4O_4Cu$, Calc. C 24.54, H 2.47, N 11.45; Found C 25.08, H 2.66, N 11.62. MS (ESI) m/z=157 ([Cu-Imace-H-H]$^{2+}$).

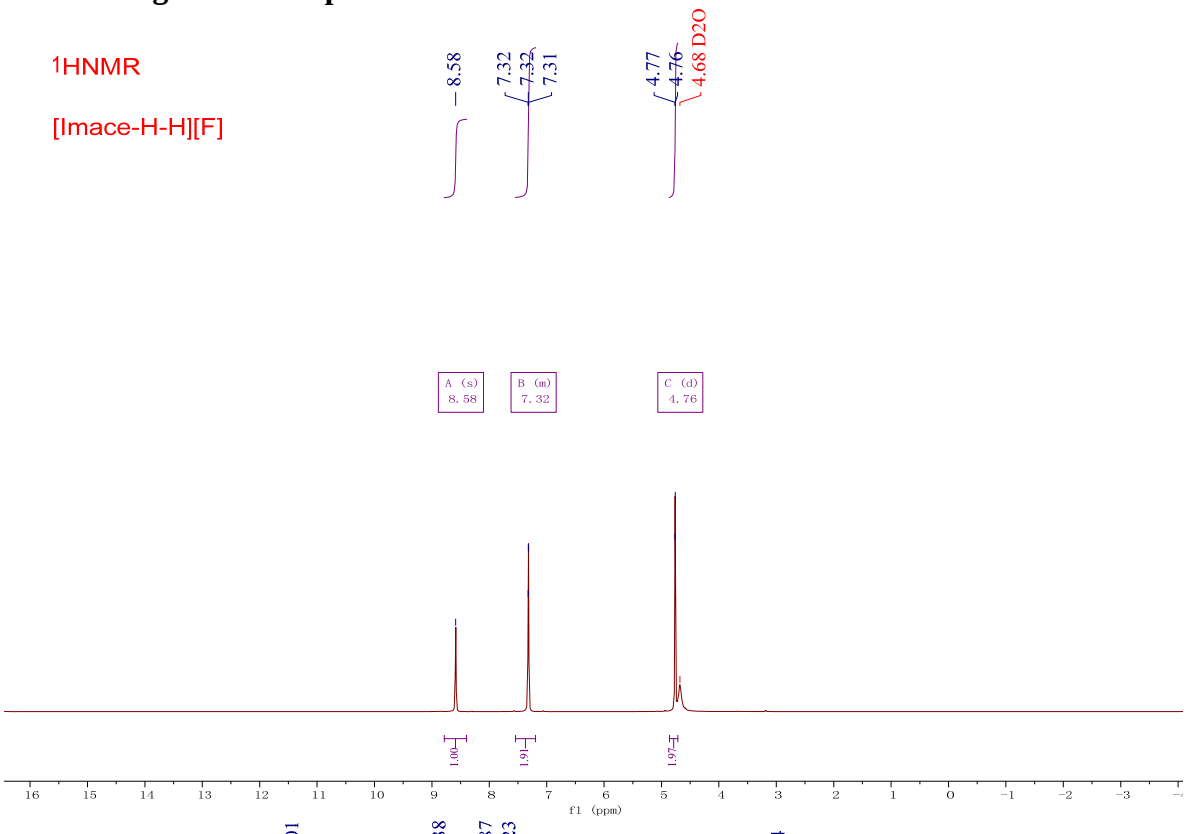
[Imace-CH_3-H][Cl]: ^{1}H-NMR (400MHz, D_2O) δ (ppm) 2.46 (H, s, -CH_3), 5.01 (2H, s, CH_2), 7.36 (H, s, N-CH). ^{13}C-NMR (100MHz, D_2O) δ (ppm) 9.13 (-CH_3), 49.14 (-CH_2-), 122.36 (N-CH), 122.37 (N-CH), 146.86 (N-CH-N), 169.41 (-COOH). [Cu-Imace-CH_3-H][Cl]: UV-vis (Acetic acid) λ_{max} (nm) 251.78. Elemental analysis: $C_{12}H_{16}Cl_2N_4O_4Cu$: Calc. C 34.75, H 3.89, N 13.51; Found C 35.01, H 3.30, N 14.04. MS (ESI) m/z=171 ([Cu-Imace-CH_3-H]$^{2+}$).

[Cu-Imace-H-CH_3][I]: UV-vis (Acetic acid) λ_{max} (nm) 248.80. Elemental analysis: $C_{12}H_{16}I_2N_4O_4Cu$, Calc. C 24.12, H 2.70, N 9.37; Found C 25.16, H 3.09, N 10.32. MS (ESI) m/z=171 ([Cu-Imace-H-CH_3]$^{2+}$).

5 The original NMR spectrum

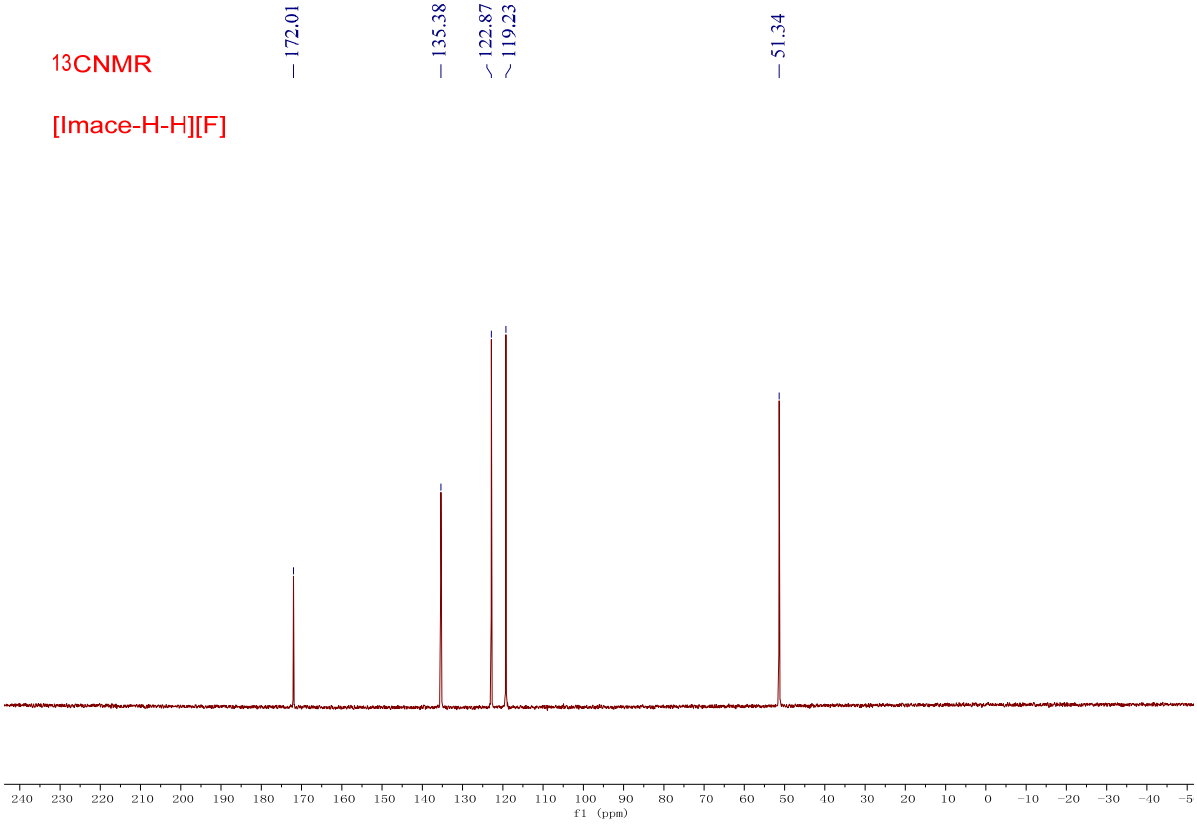
^{1}HNMR

[Imace-H-H][F]



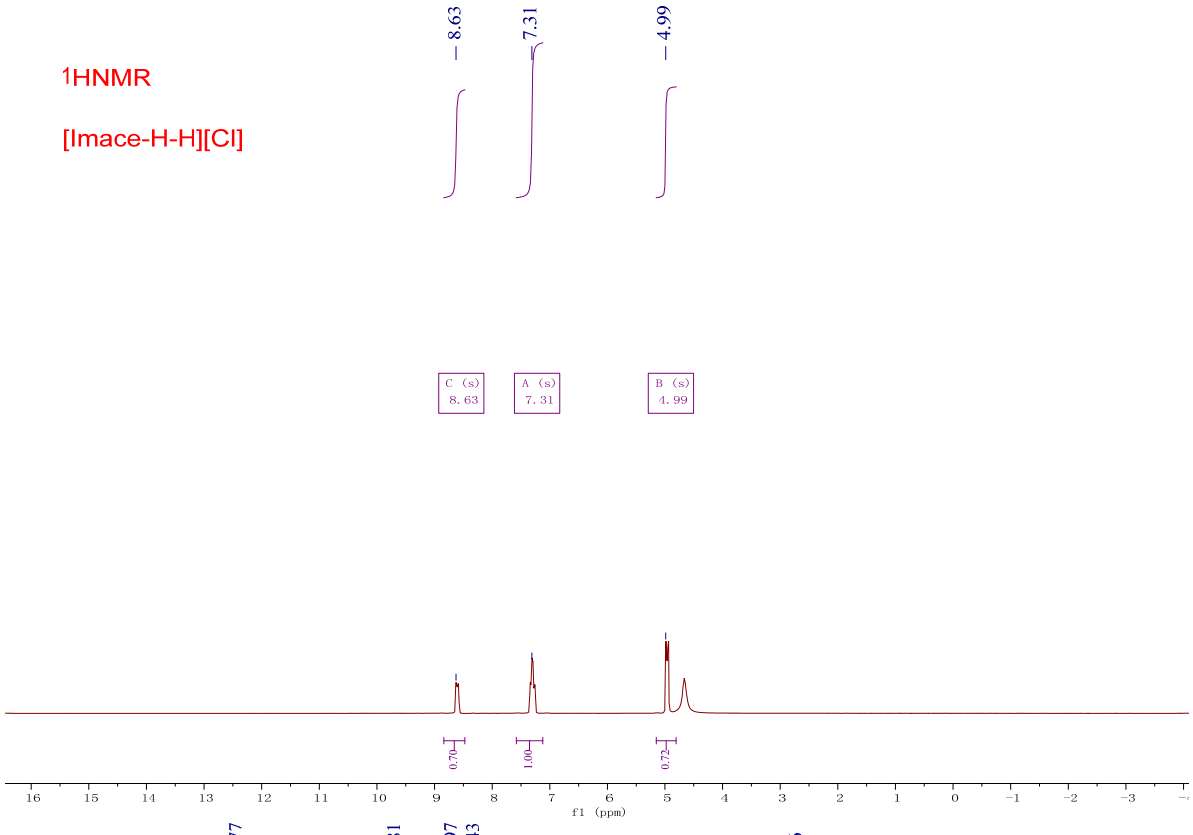
^{13}CNMR

[Imace-H-H][F]



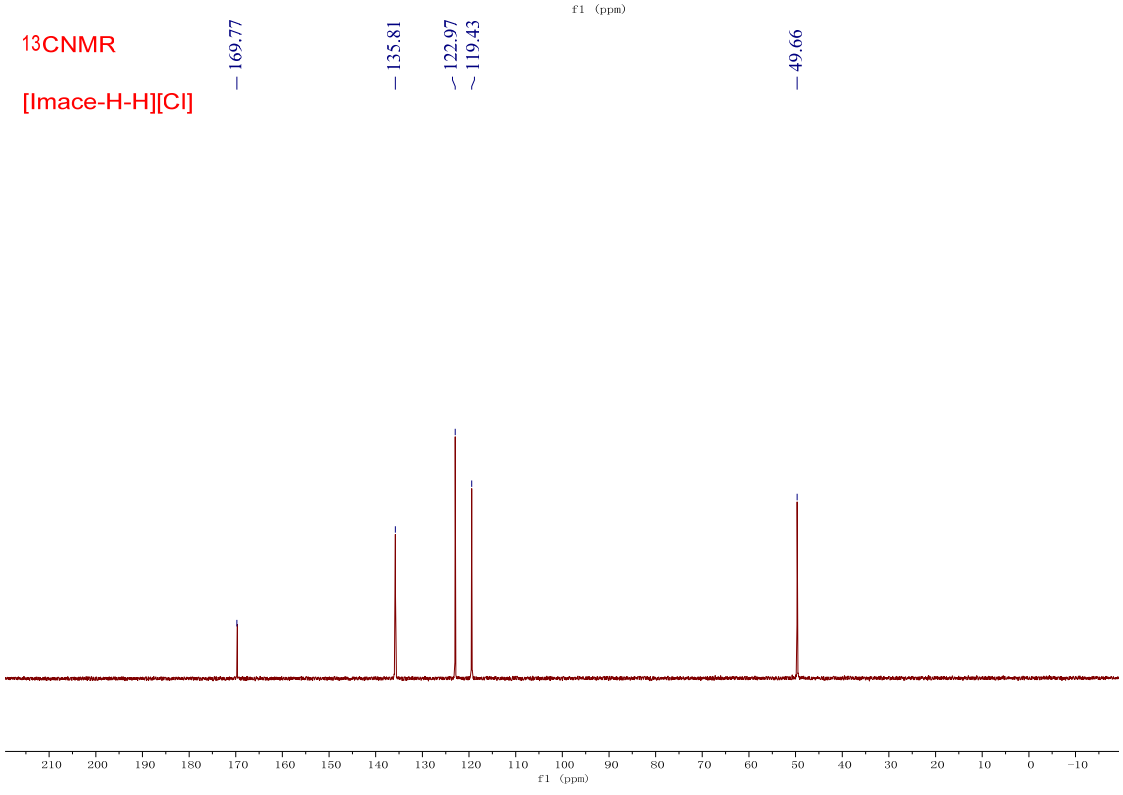
1HNMR

[Imace-H-H][Cl]



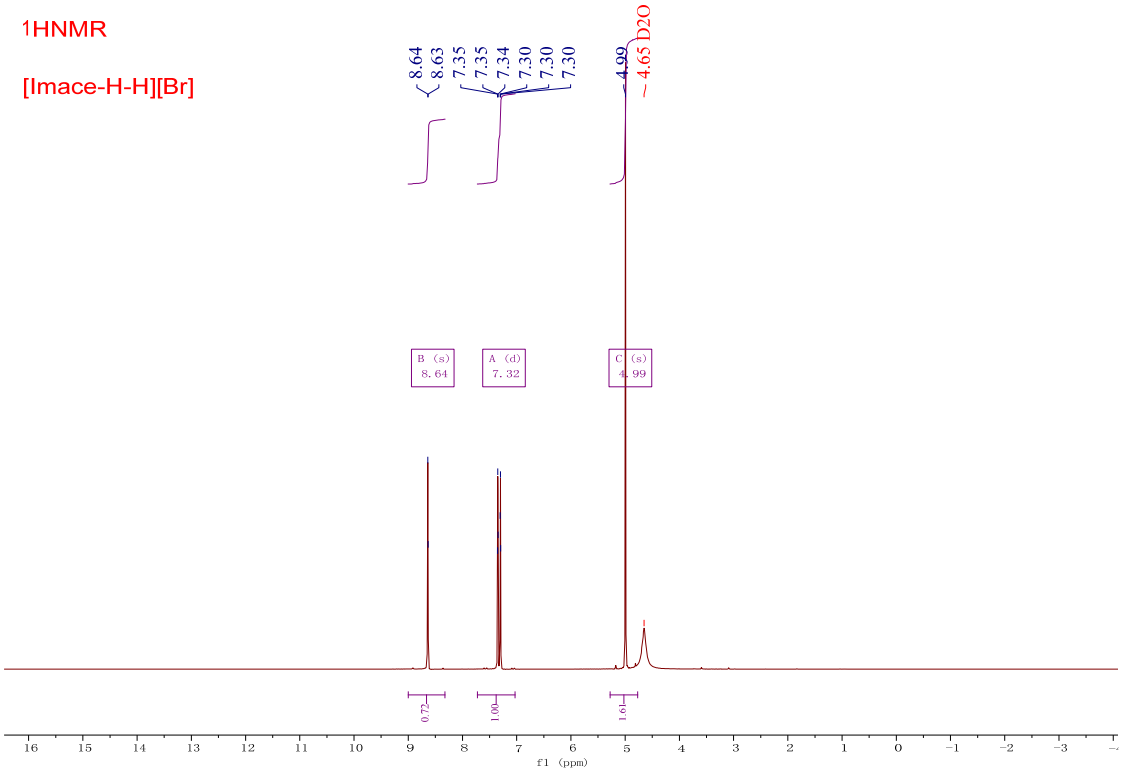
13CNMR

[Imace-H-H][Cl]



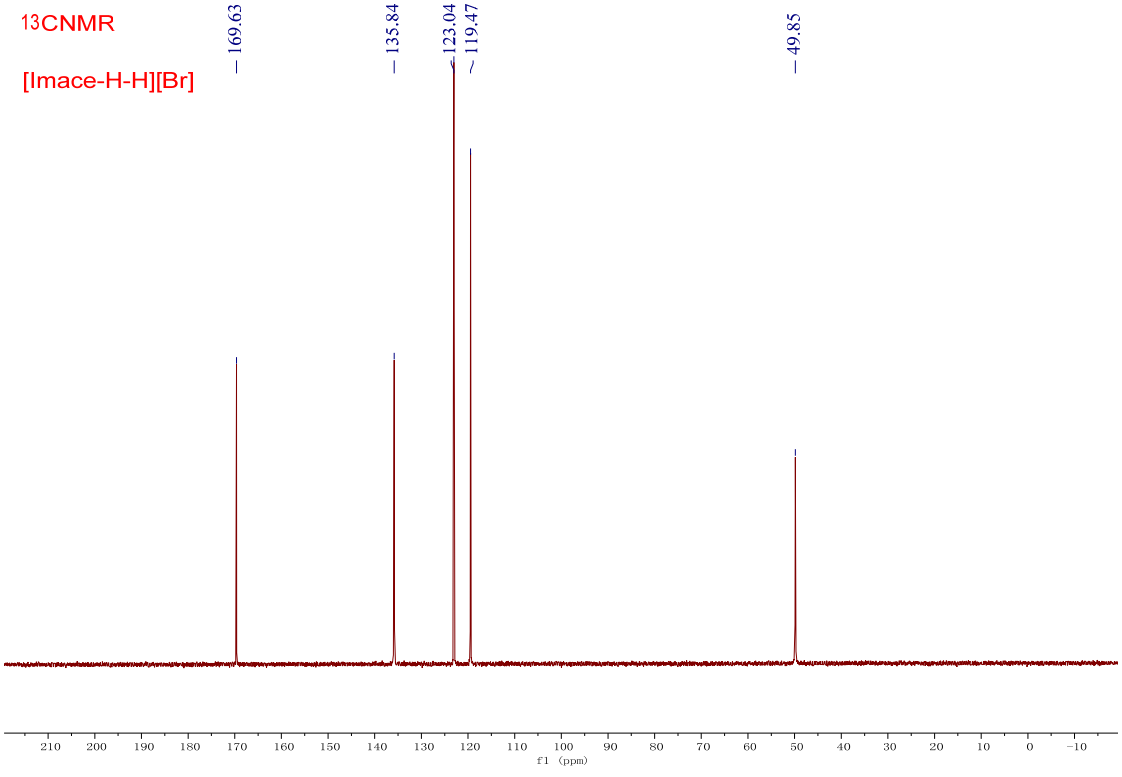
1HNMR

[Imace-H-H][Br]



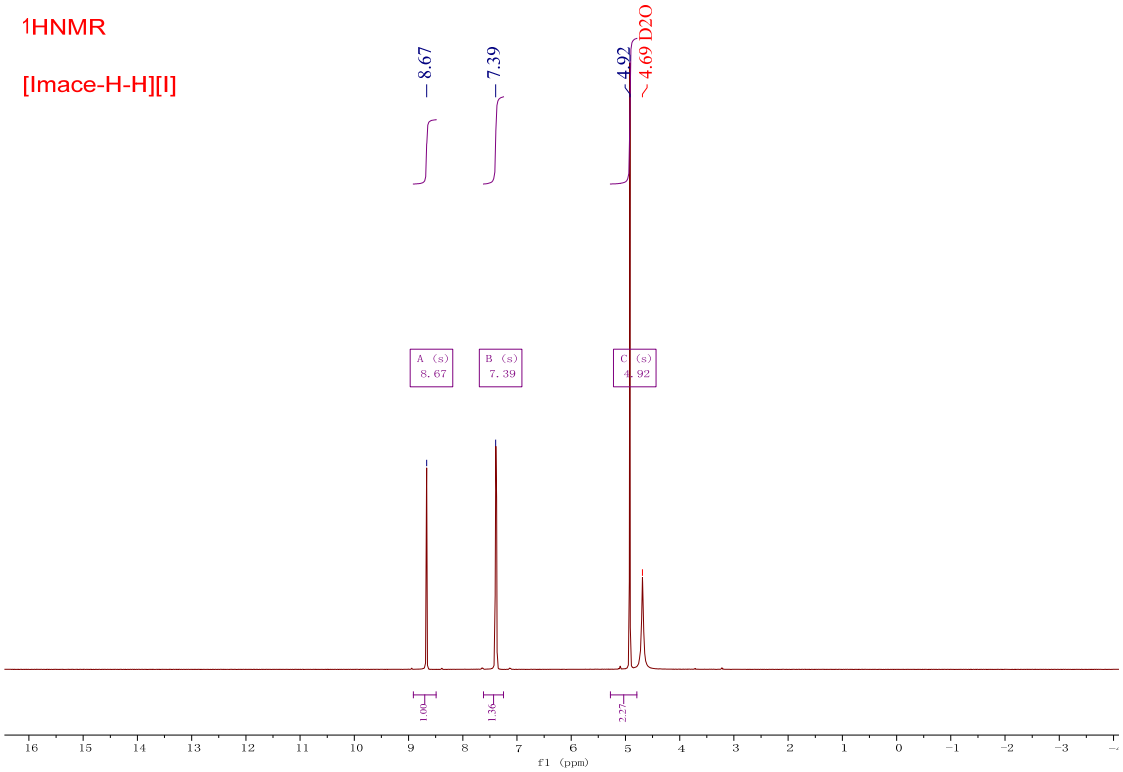
13CNMR

[Imace-H-H][Br]



1HNMR

[Imace-H-H][I]



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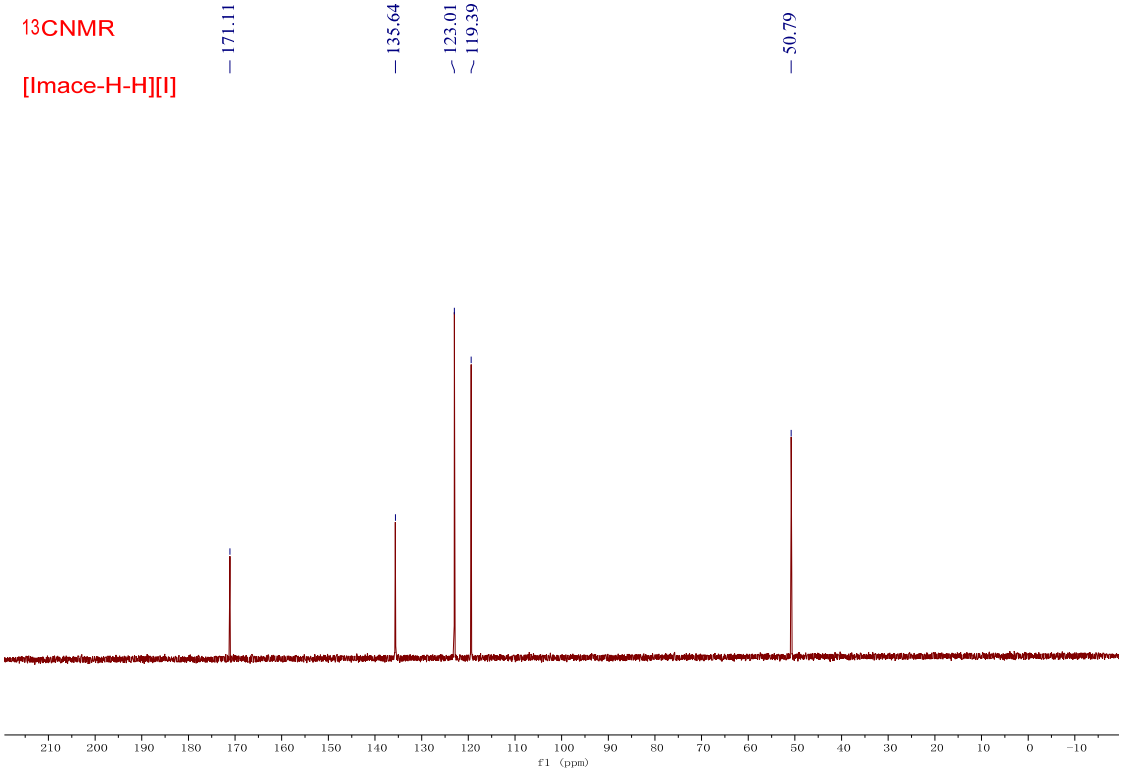
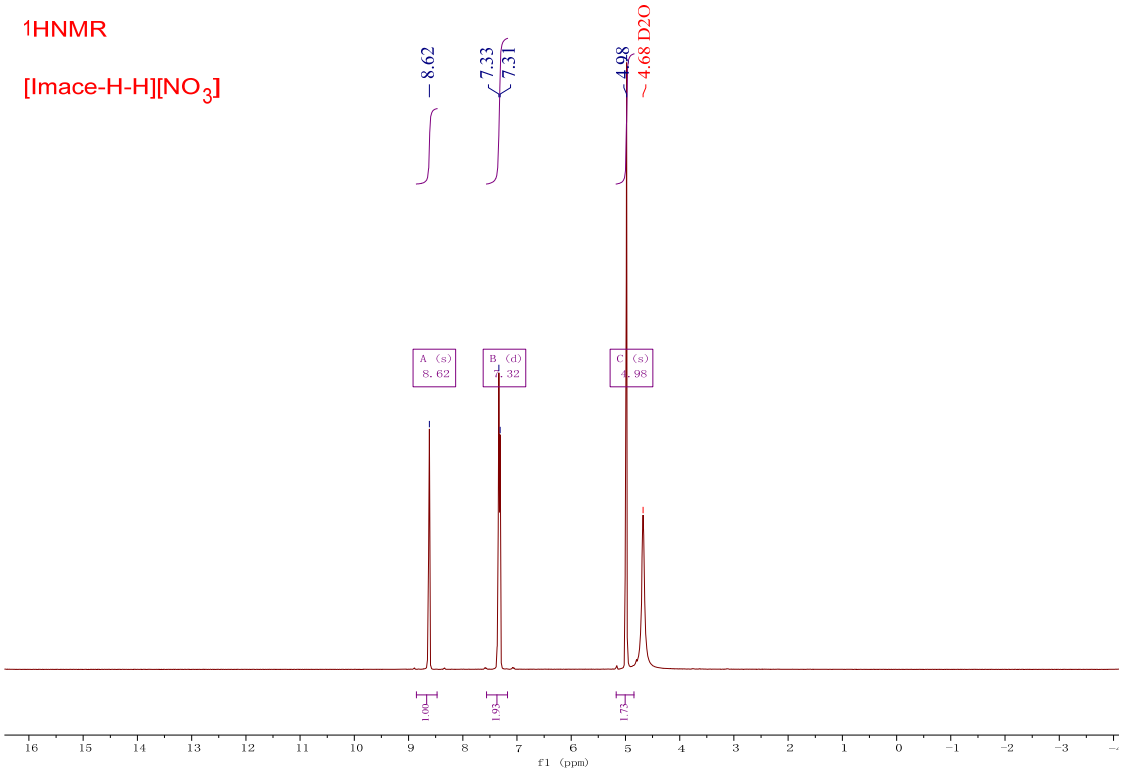
[Imace-H-H][I]



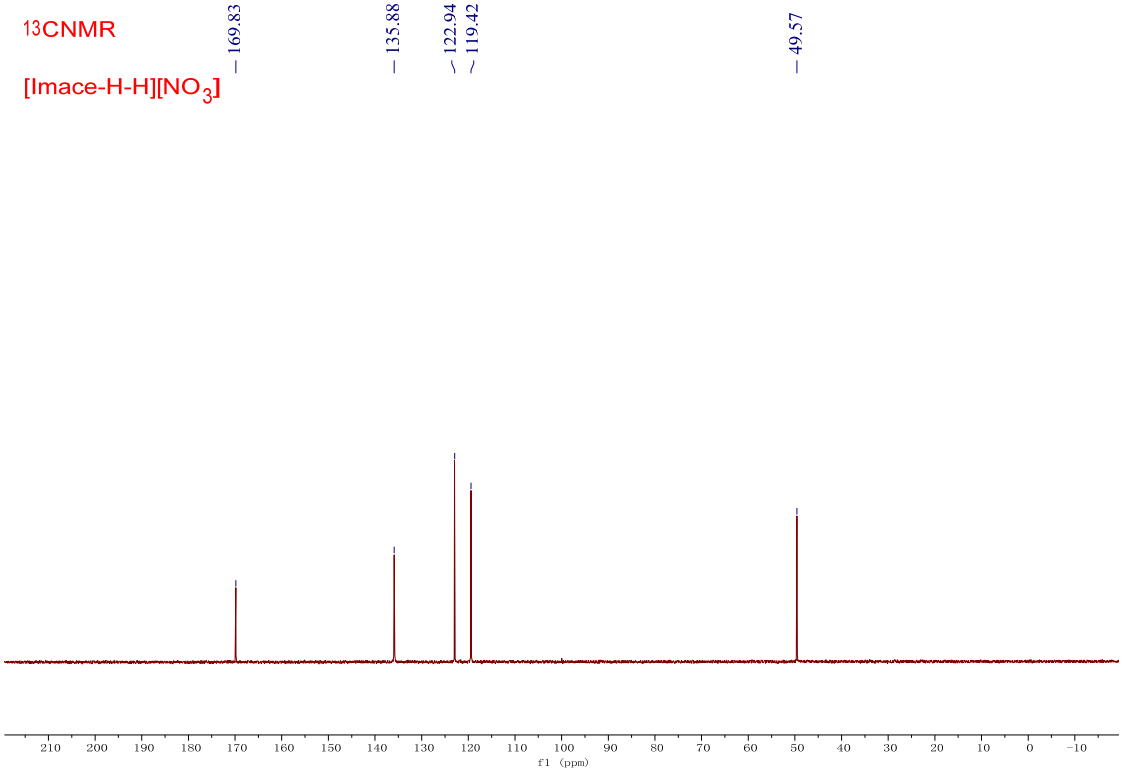
1HNMR

[Imace-H-H][NO_3]



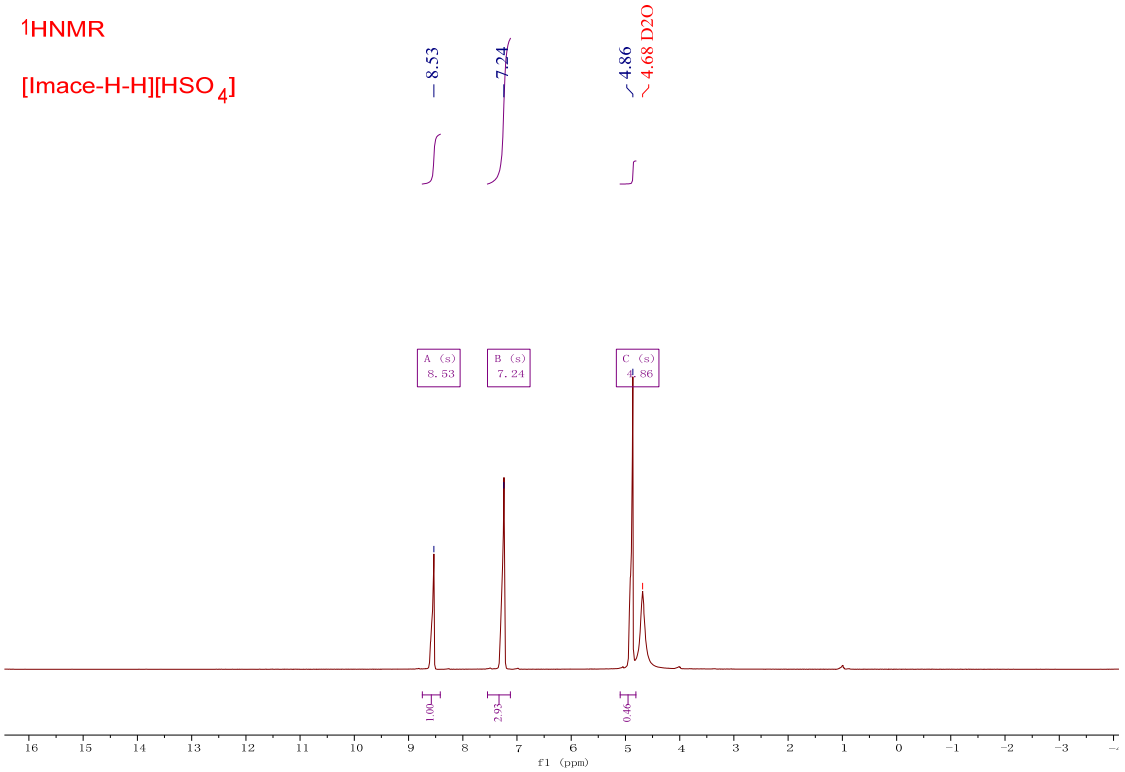
13CNMR

[Imace-H-H][NO_3]



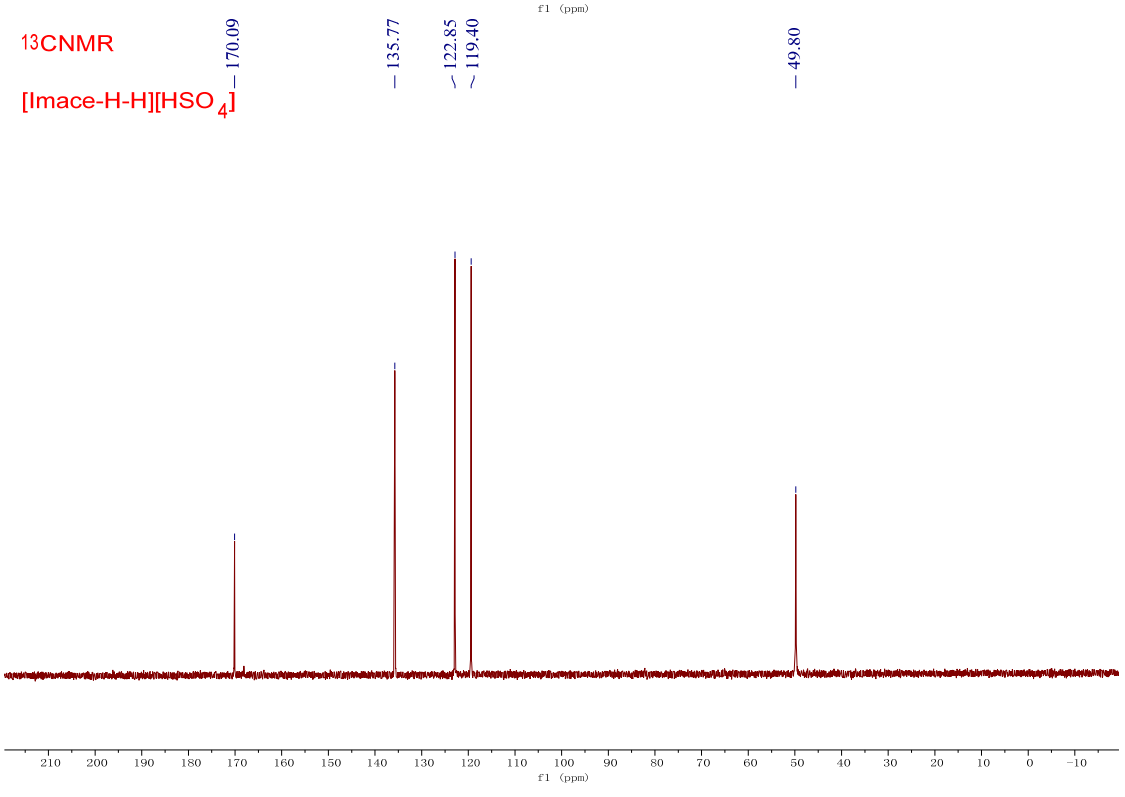
^{1}HNMR

[Imace-H-H][HSO_4]



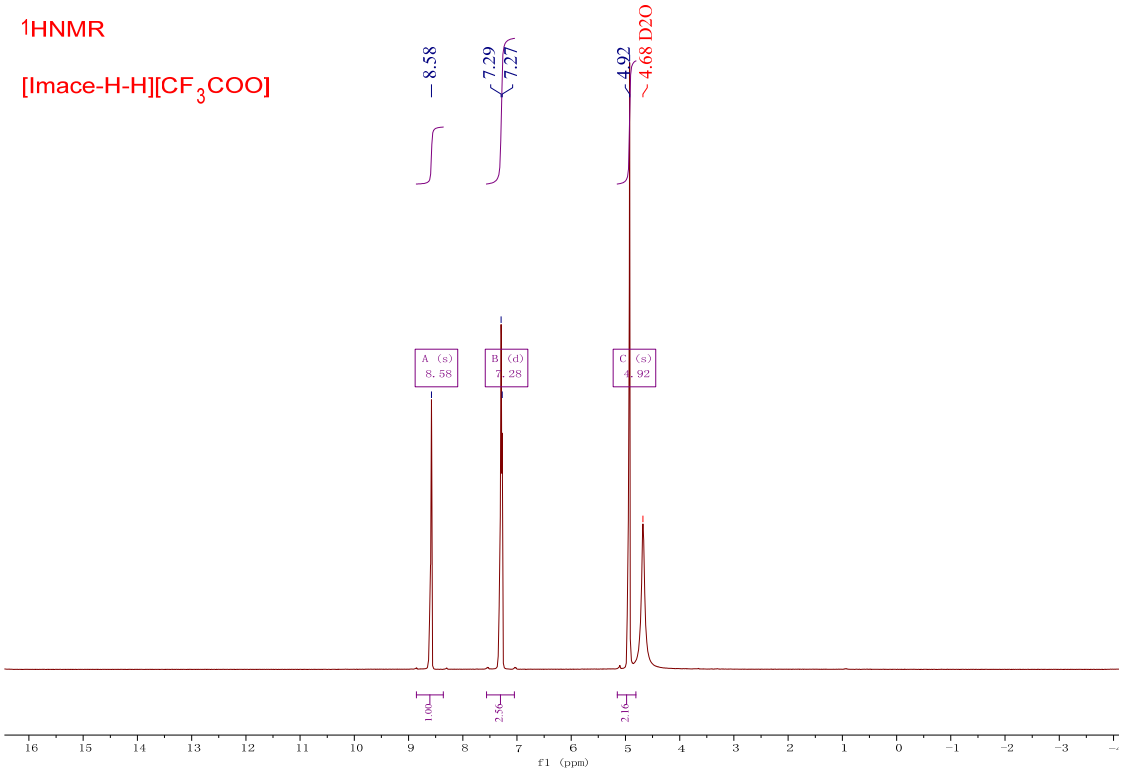
^{13}CNMR

[Imace-H-H][HSO_4]



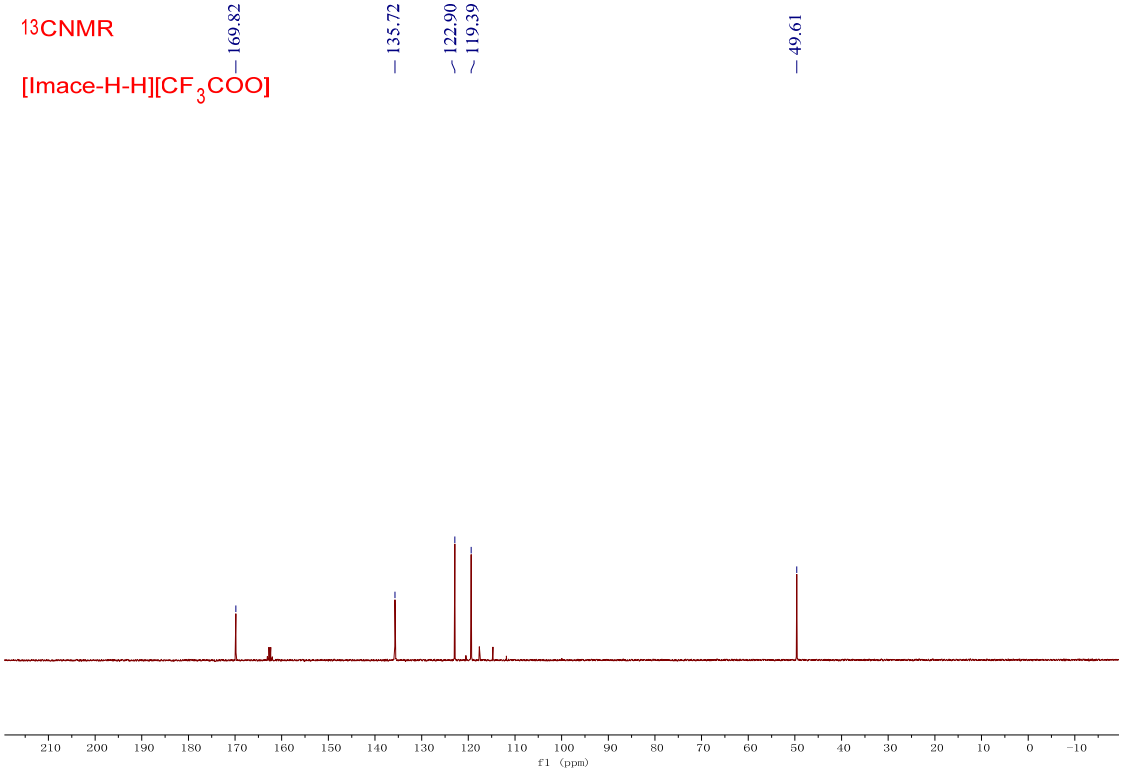
^{1}HNMR

[Imace-H-H][CF_3COO]



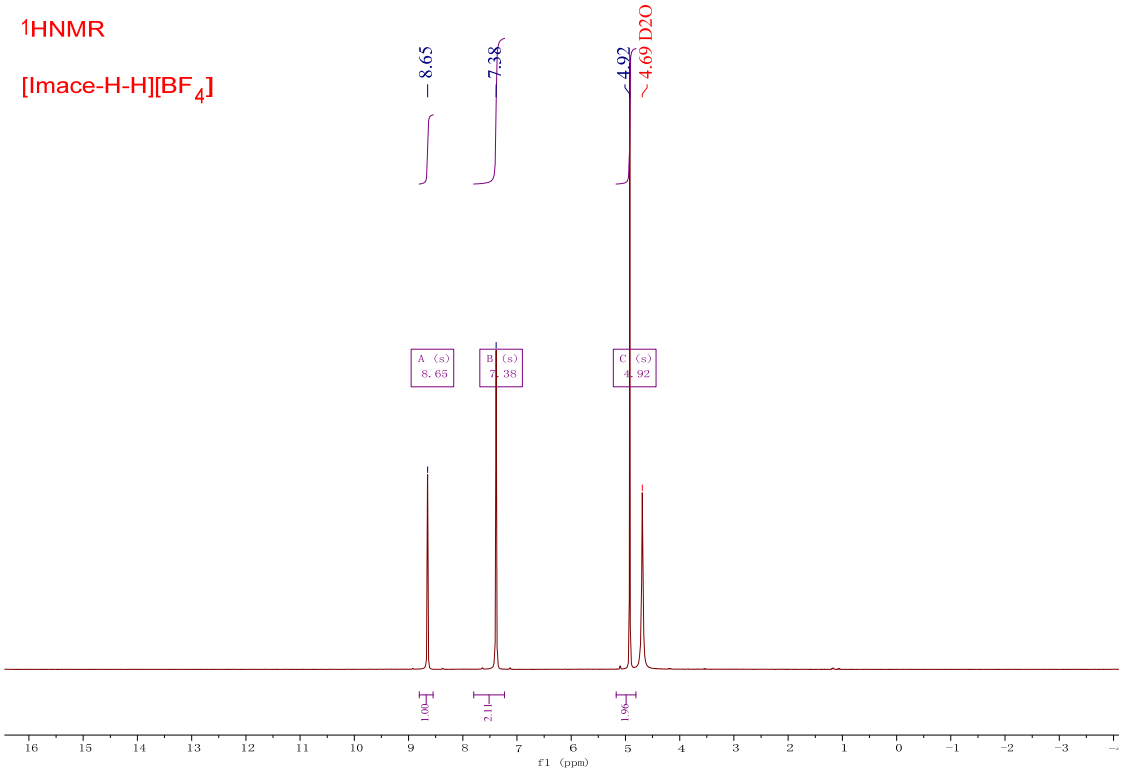
^{13}CNMR

[Imace-H-H][CF_3COO]



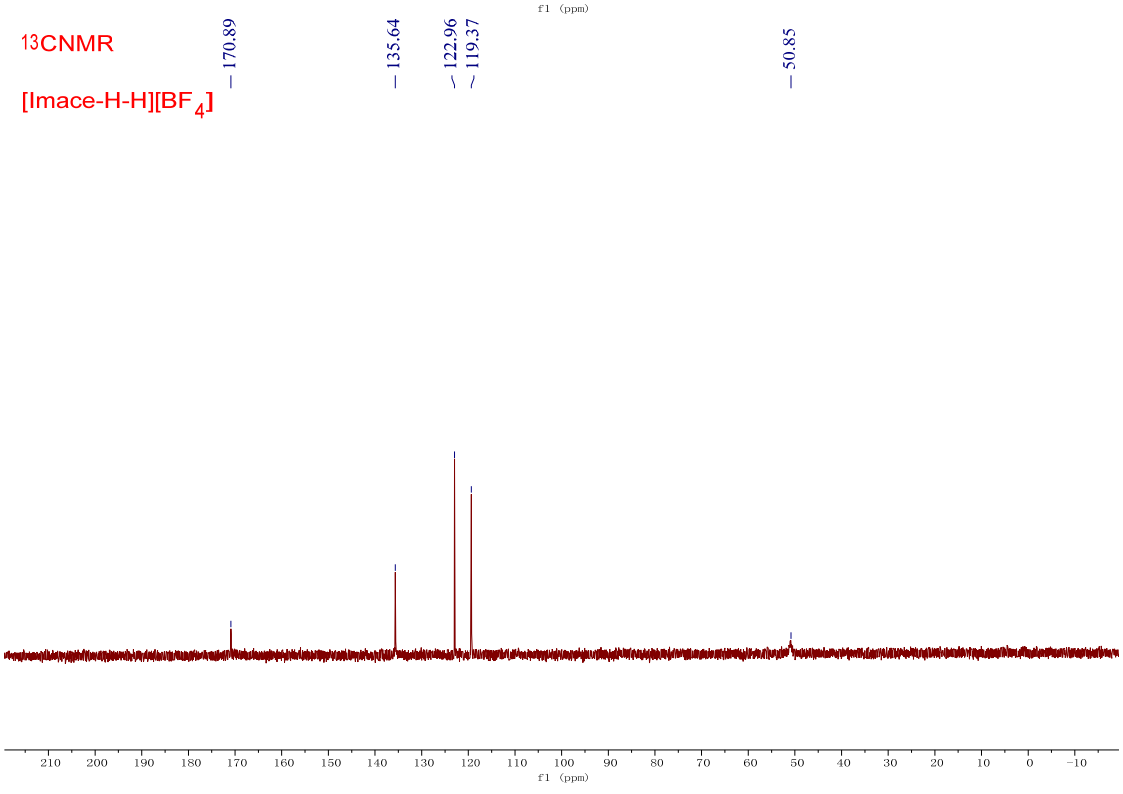
^{1}HNMR

[Imace-H-H][BF_4]



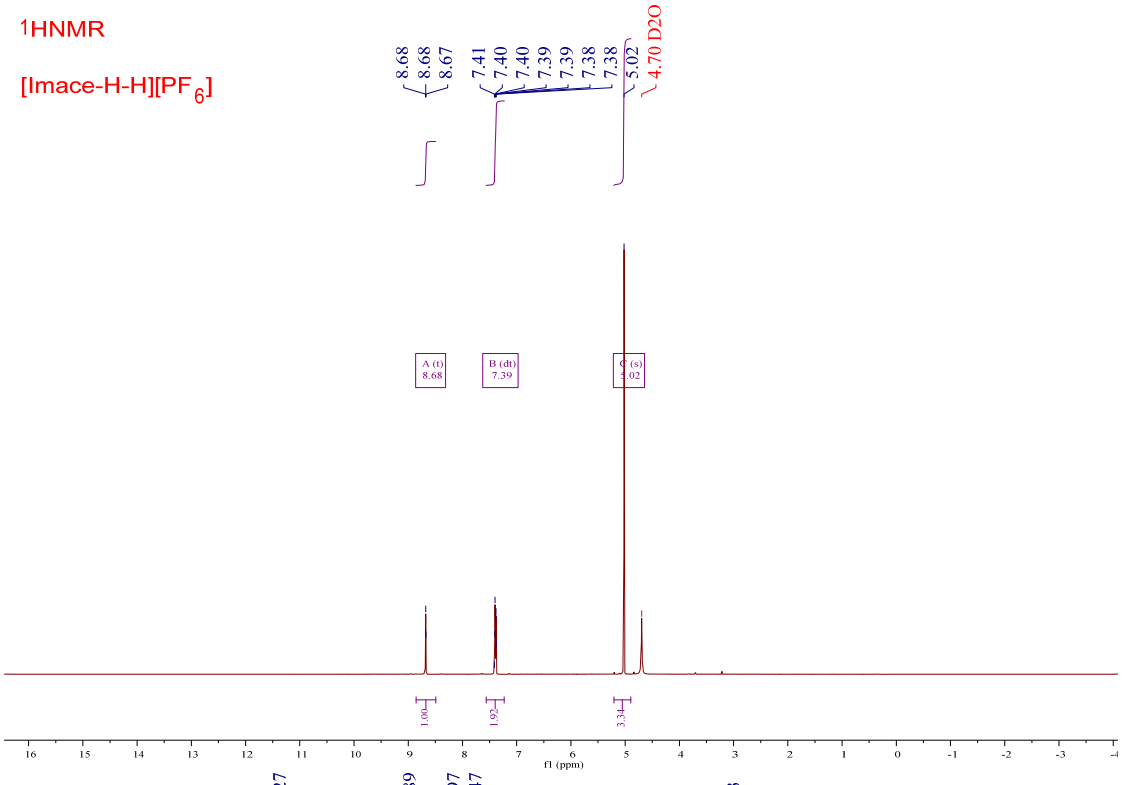
^{13}CNMR

[Imace-H-H][BF_4]



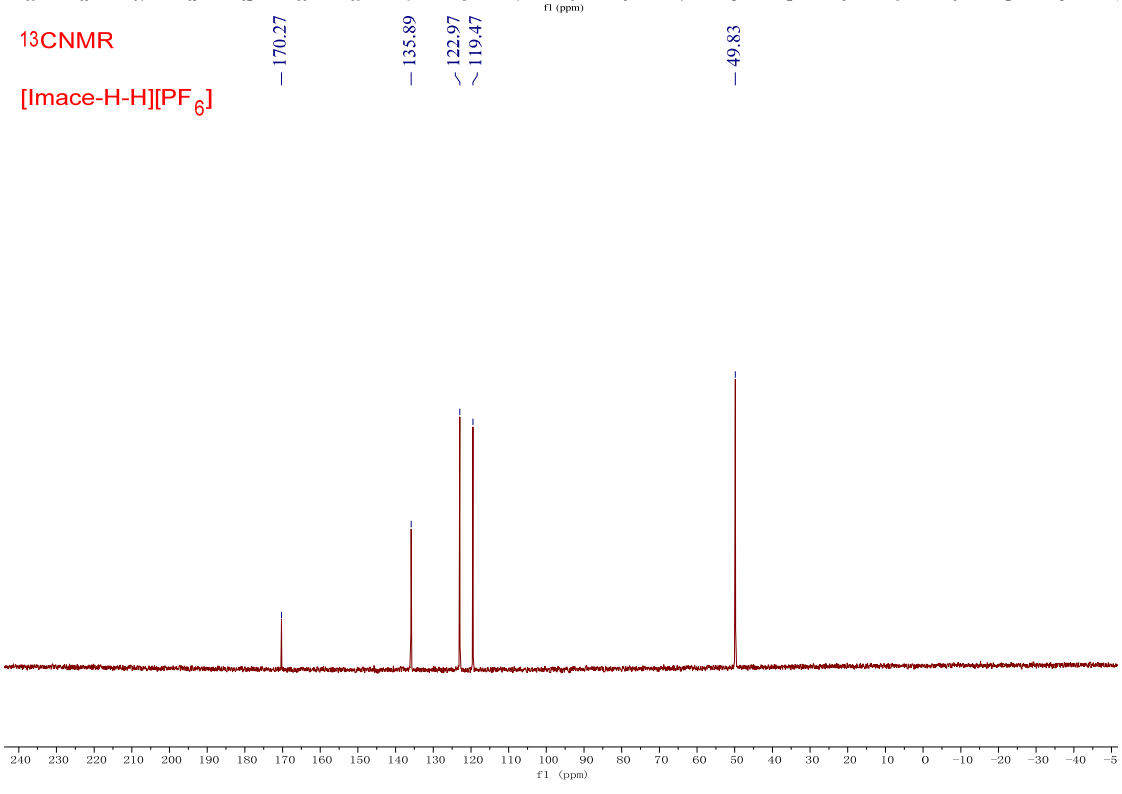
^{1}HNMR

[Imace-H-H][PF_6]



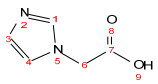
^{13}CNMR

[Imace-H-H][PF_6]



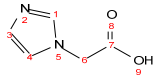
^{1}HNMR

[Imace-H-H]



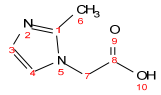
^{13}CNMR

[Imace-H-H]



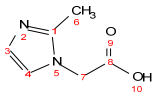
^{1}HNMR

[Imace-CH_3-H]



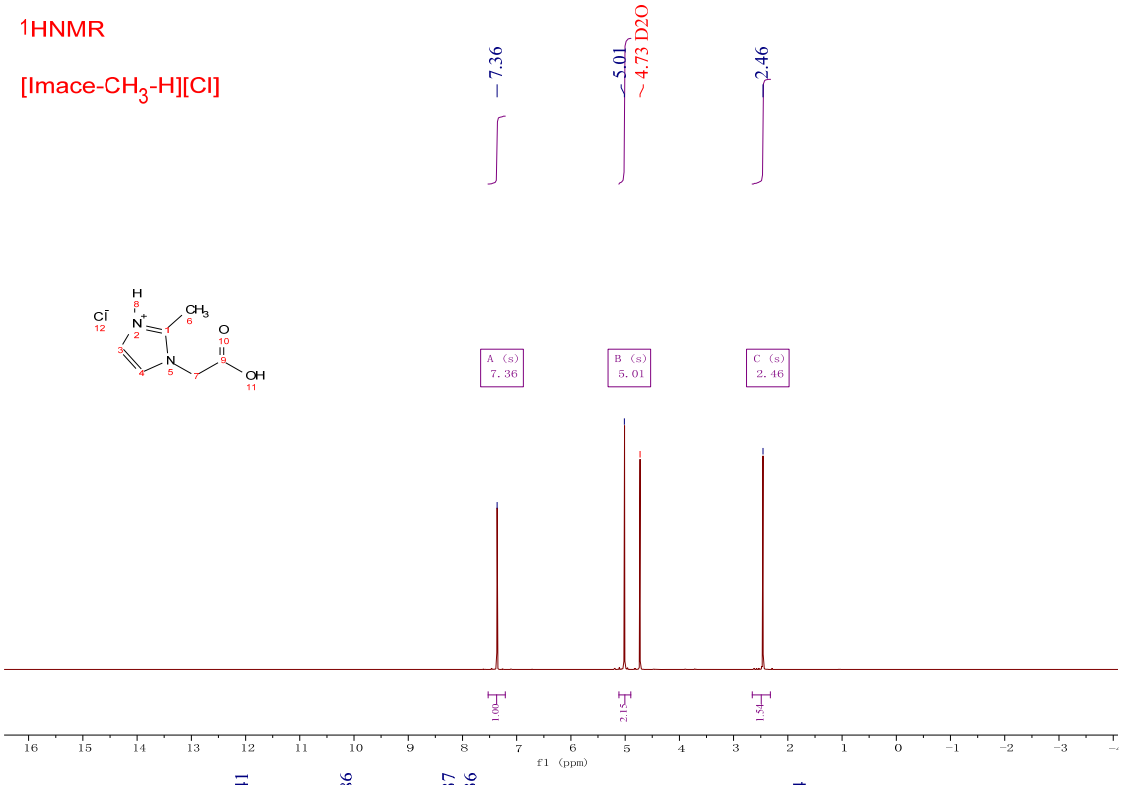
^{13}CNMR

[Imace-CH_3-H]



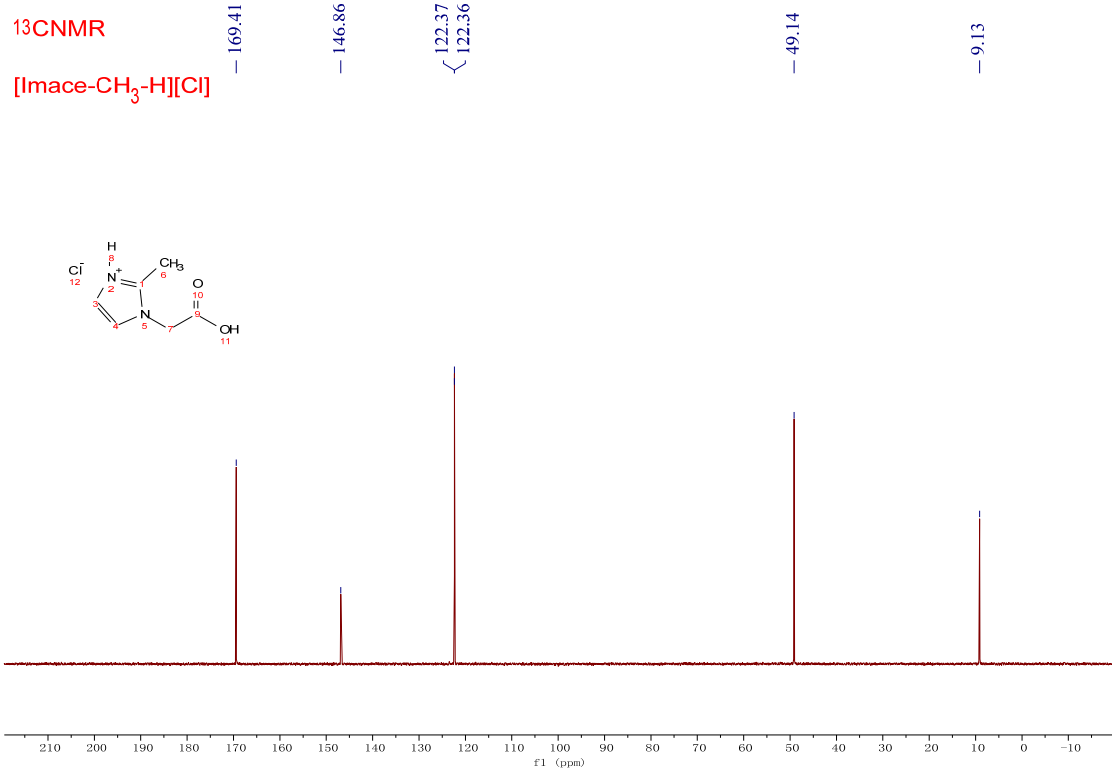
^{1}HNMR

[Imace-CH_3-H][Cl]



^{13}CNMR

[Imace-CH_3-H][Cl]



6 The GC conditions for each of the substrates tested

The quantitative analysis of reactants and products was performed on a Shimadzu GC2014 gas chromatograph equipped with a WondaCAP-5 capillary column (5% Diphenyl 95% Dimethylpolysiloxane 30m×0.32mm×0.25μm) with a flame-ionization detector. A Shimadzu GCMS-QP2010 was used to identify substrates and their oxidation products resulting from catalysis.

GC Condition:
Injection Port SPL1
Injection Mode: Split
Carrier Gas: N2
Flow Control: Pressure
Pressure: 45.8 KPa
Total Flow: 37.7 mL/min
Column Flow: 1.33 mL/min
Purge Flow: 3.0 mL/min
Splitter Ratio: 25

GC methods:

Method 1
Injection Port temperature: 280 ℃
FID Detector Temperature: 290 ℃
[Column Oven]
Initial Temperature: 50 ℃
Equilibration Time: 2.0 min
=Column Oven Temperature Program=
Total Program Time: 10.67min

	Rate(℃/min)	Temperature(℃)	Hold Time(min)
0	-	50.0	1.00
1	15.0	180.0	1.00

Method 2
Injection Port temperature: 280 ℃
FID Detector Temperature: 290 ℃
[Column Oven]
Initial Temperature: 50 ℃
Equilibration Time: 2.0 min
=Column Oven Temperature Program=
Total Program Time: 15.67 min

	Rate(℃/min)	Temperature(℃)	Hold Time(min)
0	-	50.0	1.00
1	15.0	180.0	1.00
2	20.0	240.0	2

Method 3
Injection Port temperature: 280 ℃
FID Detector Temperature: 290 ℃
[Column Oven]
Initial Temperature: 40 ℃
Equilibration Time: 2.0 min
=Column Oven Temperature Program=
Total Program Time: 11.0 min

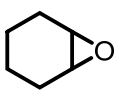
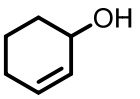
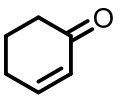
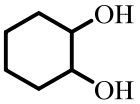
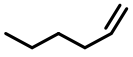
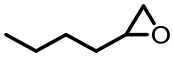
	Rate(℃/min)	Temperature(℃)	Hold Time(min)
0	-	40.0	3.00
1	20.0	180.0	1.00

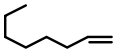
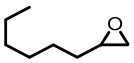
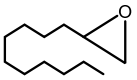
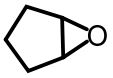
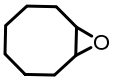
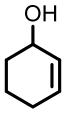
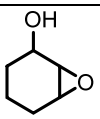
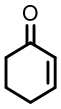
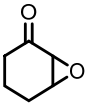
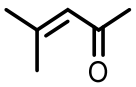
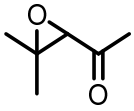
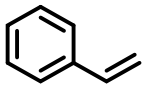
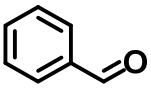
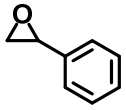
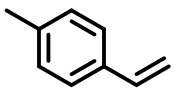
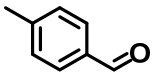
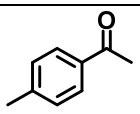
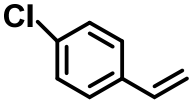
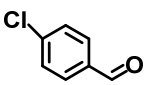
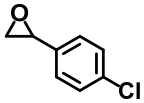
Method 4
Injection Port temperature: 290 ℃
FID Detector Temperature: 300 ℃
[Column Oven]
Initial Temperature: 120 ℃
Equilibration Time: 2.0 min
=Column Oven Temperature Program=
Total Program Time: 15.17 min

	Rate(℃/min)	Temperature(℃)	Hold Time(min)
0	-	120.0	1.00
1	15.0	220.0	1.00
2	20.0	250.0	5.00

Method 5
Injection Port temperature: 290 ℃
FID Detector Temperature: 300 ℃
[Column Oven]
Initial Temperature: 70 ℃
Equilibration Time: 2.0 min
=Column Oven Temperature Program=
Total Program Time: 13.00 min

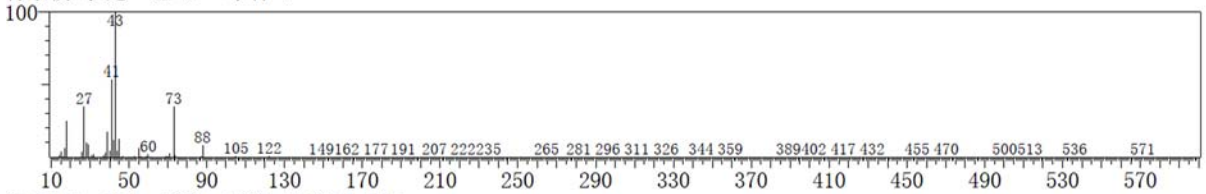
	Rate(℃/min)	Temperature(℃)	Hold Time(min)
0	-	70.0	1.00
1	20.0	250.0	3.00

substrate	GC Method	Substrate Ret. Time(min)	Products & Ret. Time (min)			
	Method 1	3.426	 5.196	 5.550	 6.128	 7.829
	Method 1	3.165	 5.942			

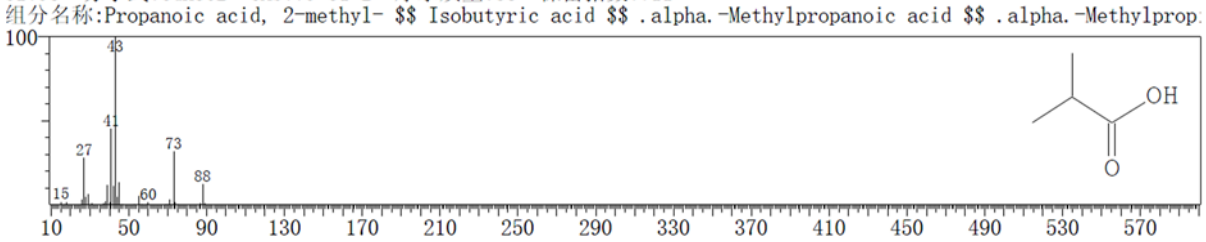
	Method 2	7.224	 10.632	
	Method 2	9.215	 11.741	
	Method 3	3.113	 4.937	
	Method 2	5.767	 6.008	
	Method 1	4.080	 5.165	
	Method 5	4.021	 5.214	
	Method 5	4.660	 5.504	
	Method 2	3.779	 7.371	
	Method 1	3.077	 3.444	
	Method 2	3.985	 5.137	
	Method 4	4.309	 4.731	 6.609
	Method 4	3.910	 4.420	 4.860
	Method 4	4.374	 4.731	 5.735

7 The original GC-MS of products

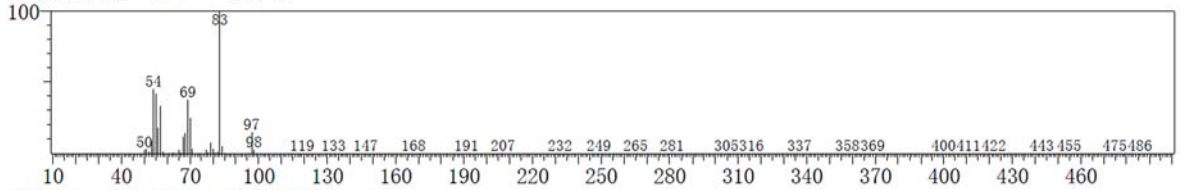
行号#:3　保留时间:2.055(扫描数#:212)　质量峰:391
原始模式:单个 2.055(212)　基峰:43.05(2903257)
背景模式:无　组 1 - 事件 1



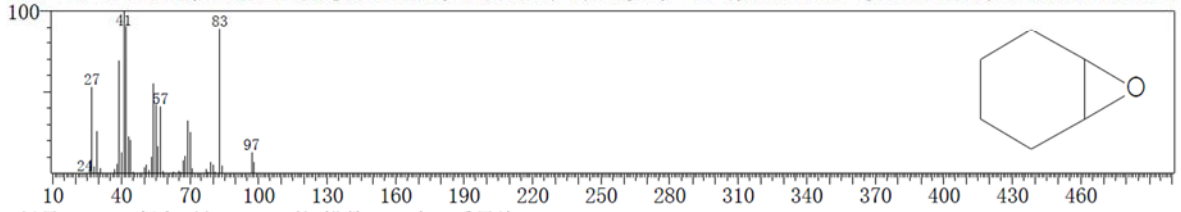
命中#:1　输入:1029　谱库:NIST14s.lib
SI:93　分子式:C4H8O2　CAS:79-31-2　摩尔质量:88　保留指数:711
组分名称:Propanoic acid, 2-methyl- $$ Isobutyric acid $$ .alpha.-Methylpropanoic acid $$ .alpha.-Methylprop



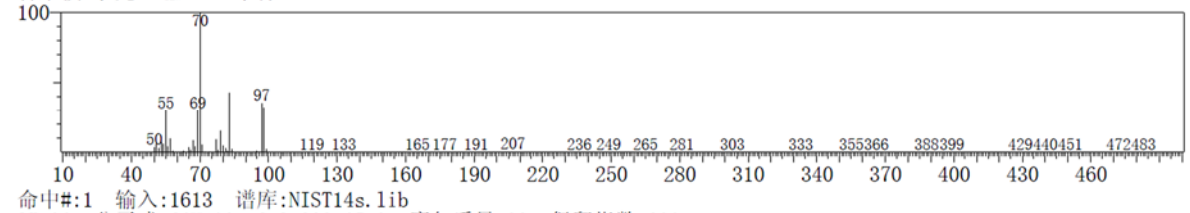
行号#:8　保留时间:3.510(扫描数#:603)　质量峰:300
原始模式:单个 3.510(603)　基峰:83.00(3254030)
背景模式:无　组 1 - 事件 1



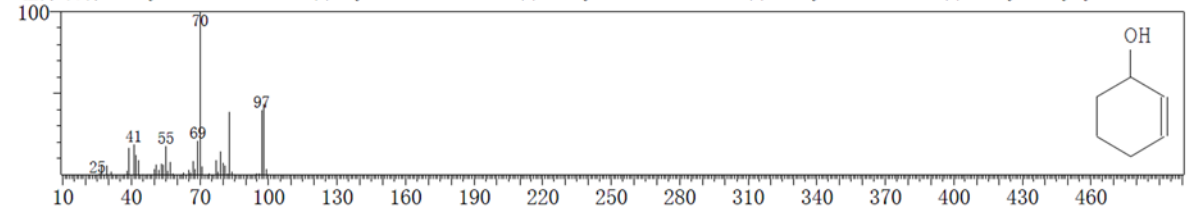
命中#:1　输入:1558　谱库:NIST14s.lib
SI:96　分子式:C6H10O　CAS:286-20-4　摩尔质量:98　保留指数:731
组分名称:7-Oxabicyclo[4.1.0]heptane $$ Cyclohexane, 1,2-epoxy- $$ Cyclohexene epoxide $$ Cyclohexene oxide



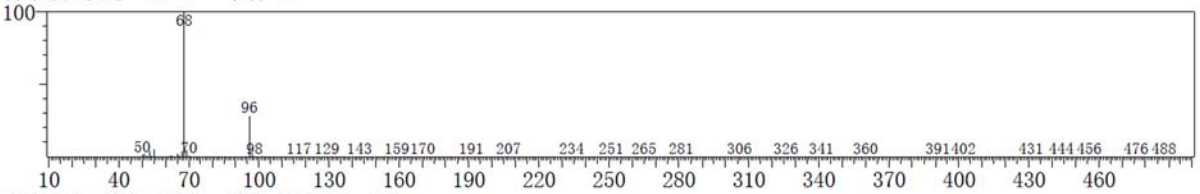
行号#:11　保留时间:3.805(扫描数#:662)　质量峰:308
原始模式:单个 3.805(662)　基峰:70.00(8212481)
背景模式:无　组 1 - 事件 1



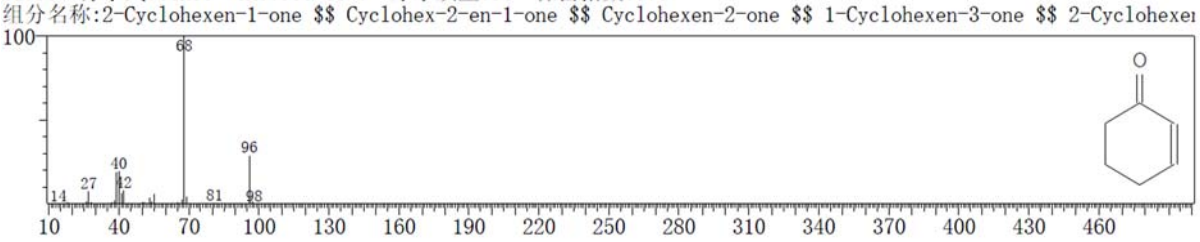
命中#:1　输入:1613　谱库:NIST14s.lib
SI:96　分子式:C6H10O　CAS:822-67-3　摩尔质量:98　保留指数:890
组分名称:2-Cyclohexen-1-ol $$ Cyclohexen-3-ol $$ 1-Cyclohexen-3-ol $$ 2-Cyclohexenol $$ 3-Hydroxycyclohexen



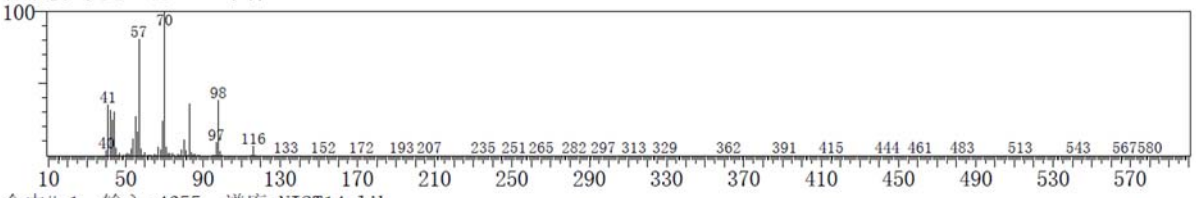
行号#:8　保留时间:4.360(扫描数#:773)　质量峰:314
原始模式:单个 4.360(773)　基峰:68.00(3558417)
背景模式:无　组 1 - 事件 1



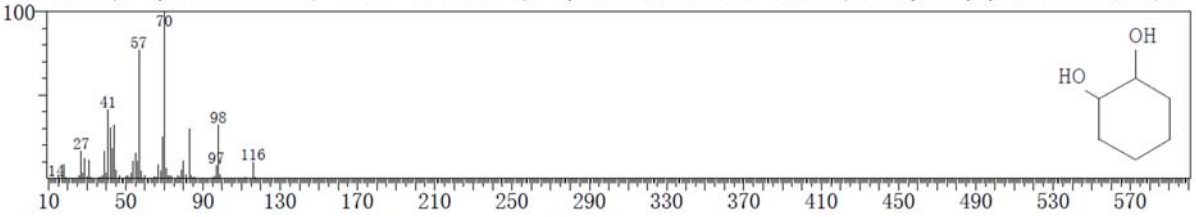
命中#:1　输入:1427　谱库:NIST14s.lib
SI:98　分子式:C6H8O　CAS:930-68-7　摩尔质量:96　保留指数:873
组分名称:2-Cyclohexen-1-one $$ Cyclohex-2-en-1-one $$ Cyclohexen-2-one $$ 1-Cyclohexen-3-one $$ 2-Cyclohexer



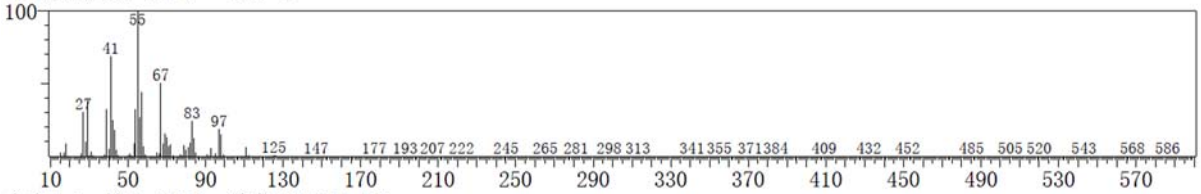
原始模式:单个 8.450(1291)　基峰:70.05(6278360)
背景模式:无　组 1 - 事件 1



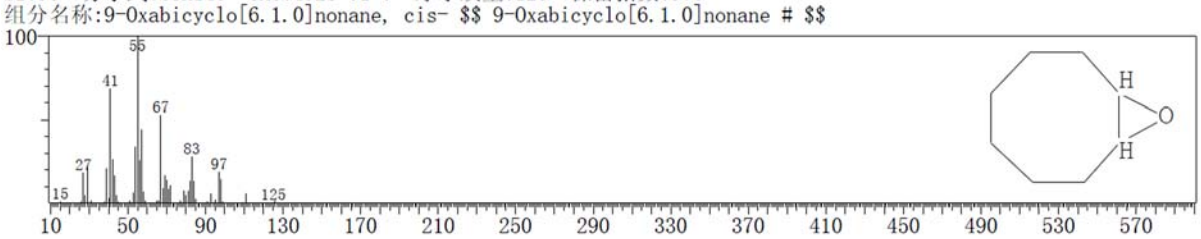
命中#:1　输入:4655　谱库:NIST14.lib
SI:97　分子式:C6H12O2　CAS:1460-57-7　摩尔质量:116　保留指数:1096
组分名称:1,2-Cyclohexanediol, trans- $$ trans-1,2-Cyclohexanediol $$ trans-1,2-Dihydroxycyclohexane $$ 1,2-



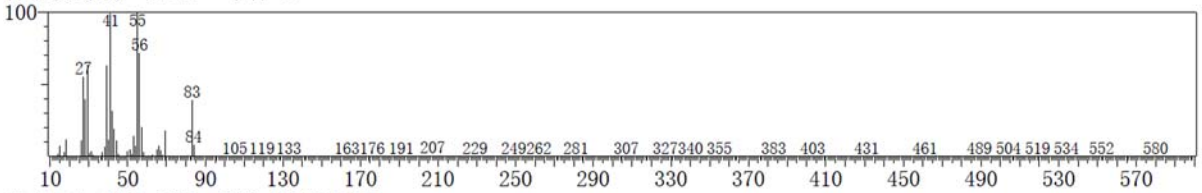
行号#:13　保留时间:4.750(扫描数#:751)　质量峰:397
原始模式:单个 4.750(751)　基峰:55.05(5724454)
背景模式:无　组 1 - 事件 1



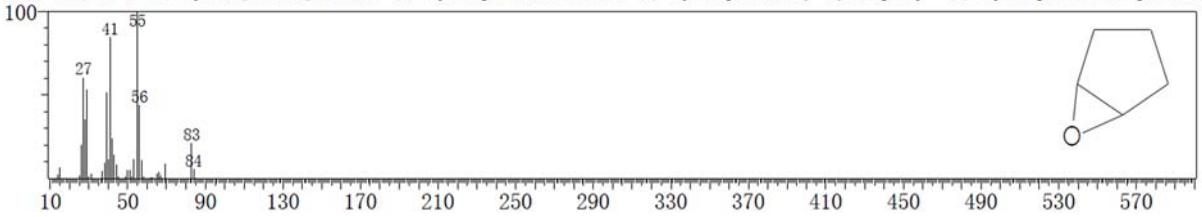
命中#:1　输入:6652　谱库:NIST14.lib
SI:96　分子式:C8H14O　CAS:4925-71-7　摩尔质量:126　保留指数:970
组分名称:9-Oxabicyclo[6.1.0]nonane, cis- $$ 9-Oxabicyclo[6.1.0]nonane # $$



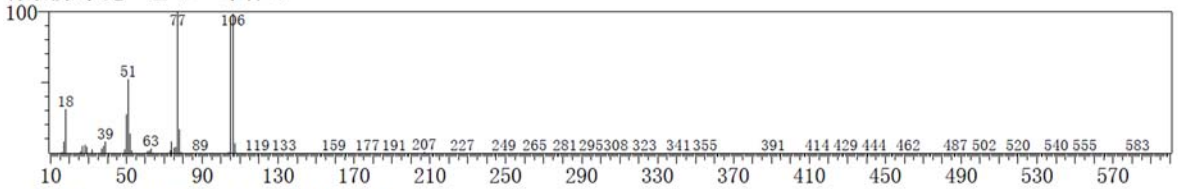
行号#:4　保留时间:2.680(扫描数#:437)　质量峰:393
原始模式:单个 2.680(437)　基峰:55.05(8405105)
背景模式:无　组 1 - 事件 1



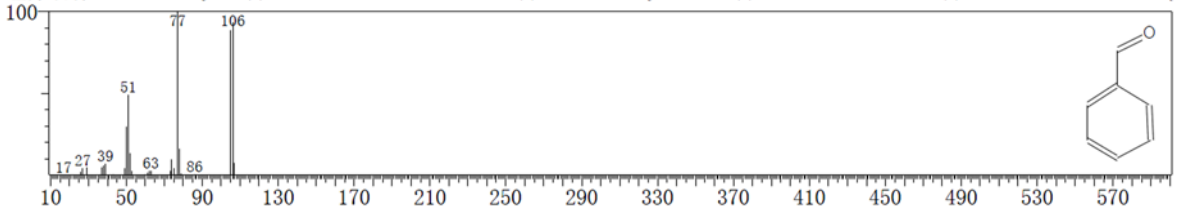
命中#:1　输入:695　谱库:NIST14.lib
SI:93　分子式:C5H8O　CAS:285-67-6　摩尔质量:84　保留指数:611
组分名称:6-Oxabicyclo[3.1.0]hexane $$ Cyclopentane oxide $$ Cyclopentane, 1,2-epoxy- $$ Cyclopentene epoxid



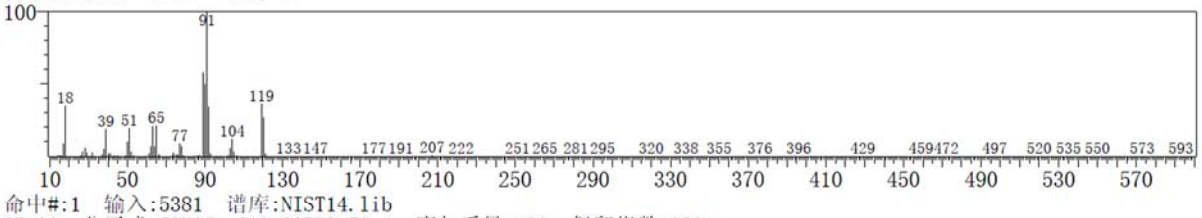
行号#:3　保留时间:2.850(扫描数#:371)　质量峰:376
原始模式:单个 2.850(371)　基峰:77.05(2290663)
背景模式:无　组 1 - 事件 1



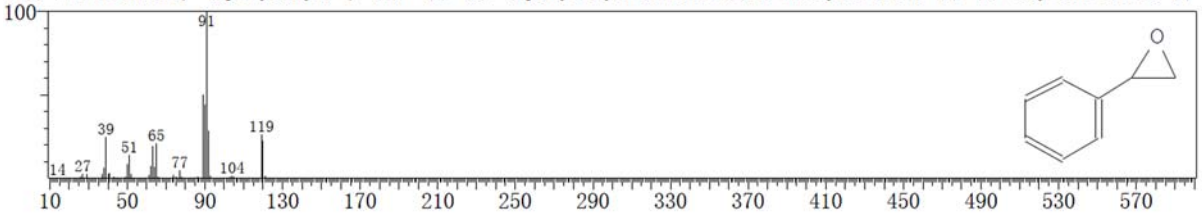
命中#:1　输入:2701　谱库:NIST14.lib
SI:95　分子式:C7H6O　CAS:100-52-7　摩尔质量:106　保留指数:982
组分名称:Benzaldehyde $$ Artificial Almond Oil $$ Benzaldehyde FFC $$ Benzenecarbonal $$ Benzenecarboxaldeh



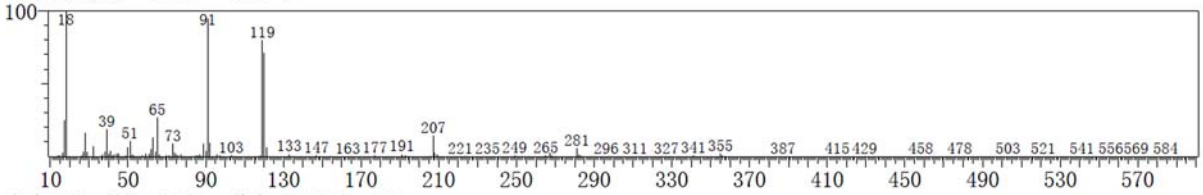
行号#:5　保留时间:3.550(扫描数#:511)　质量峰:357
原始模式:单个 3.550(511)　基峰:91.05(1992884)
背景模式:无　组 1 - 事件 1



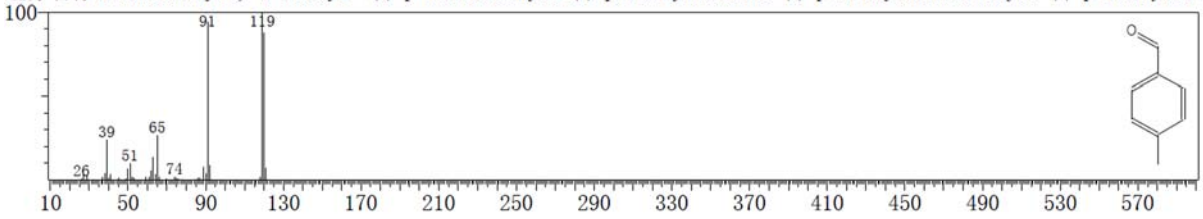
命中#:1　输入:5381　谱库:NIST14.lib
SI:90　分子式:C8H8O　CAS:20780-53-4　摩尔质量:120　保留指数:983
组分名称:Benzene, (epoxyethyl)-, (R)- $$ (R)-(Epoxyethyl)benzene $$ R-Phenyloxirane $$ (R)-Styrene oxide $$



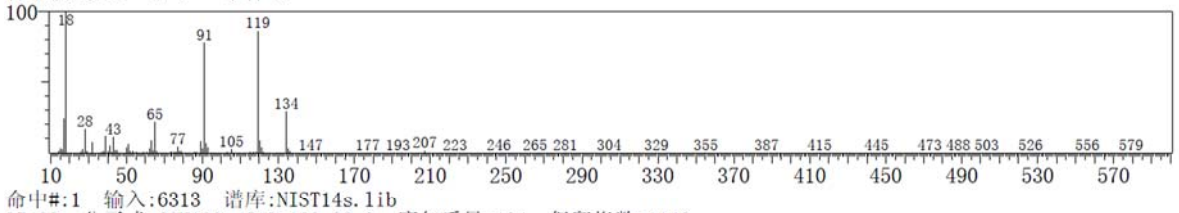
行号#:1　保留时间:3.710(扫描数#:543)　质量峰:423
原始模式:单个 3.710(543)　基峰:18.05(637160)
背景模式:无　组 1 - 事件 1



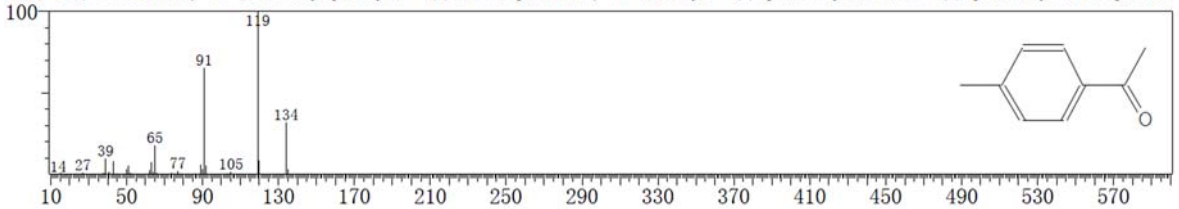
命中#:3　输入:4181　谱库:NIST14s.lib
SI:78　分子式:C8H8O　CAS:104-87-0　摩尔质量:120　保留指数:1095
组分名称:Benzaldehyde, 4-methyl- $$ p-Tolualdehyde $$ p-Formyltoluene $$ p-Methylbenzaldehyde $$ p-Toluylal



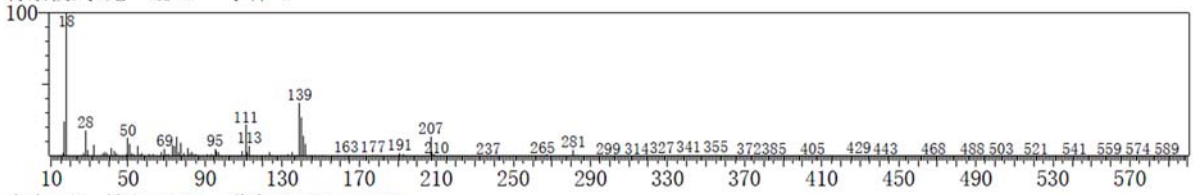
行号#:11　保留时间:5.440(扫描数#:889)　质量峰:400
原始模式:单个 5.440(889)　基峰:18.10(531943)
背景模式:无　组 1 - 事件 1



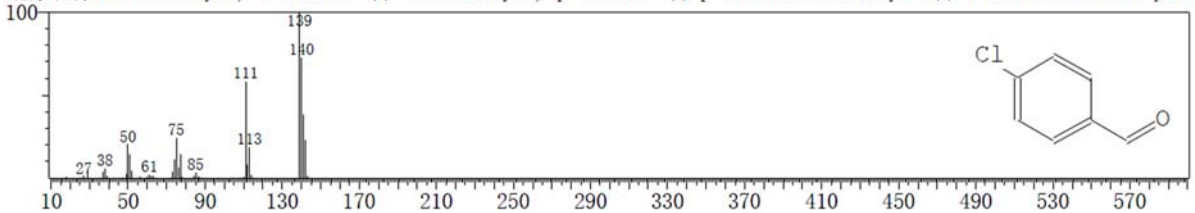
命中#:1　输入:6313　谱库:NIST14s.lib
SI:83　分子式:C9H10O　CAS:122-00-9　摩尔质量:134　保留指数:1142
组分名称:Ethanone, 1-(4-methylphenyl)- $$ Acetophenone, 4'-methyl- $$ p-Acetyltoluene $$ p-Methylacetophenor



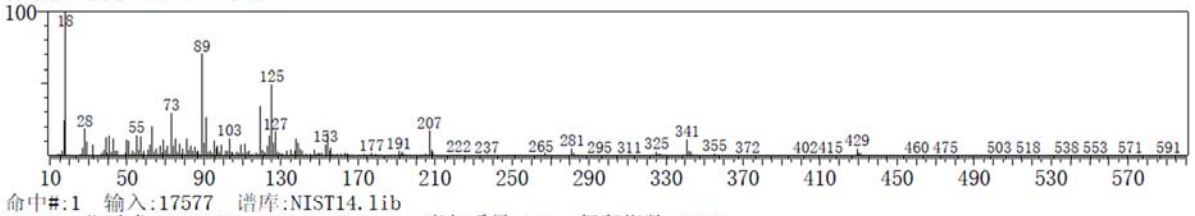
行号#:1　保留时间:4.085(扫描数#:618)　质量峰:434
原始模式:单个 4.085(618)　基峰:18.05(604536)
背景模式:无　组 1 - 事件 1



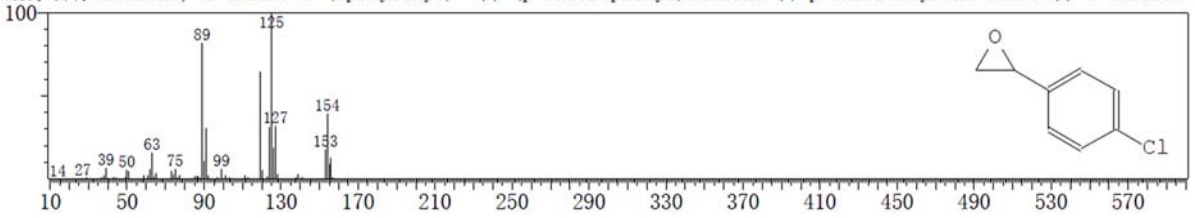
命中#:3　输入:7385　谱库:NIST14s.lib
SI:64　分子式:C7H5ClO　CAS:104-88-1　摩尔质量:140　保留指数:1162
组分名称:Benzaldehyde, 4-chloro- $$ Benzaldehyde, p-chloro- $$ p-Chlorobenzaldehyde $$ 4-Chlorobenzaldehyde



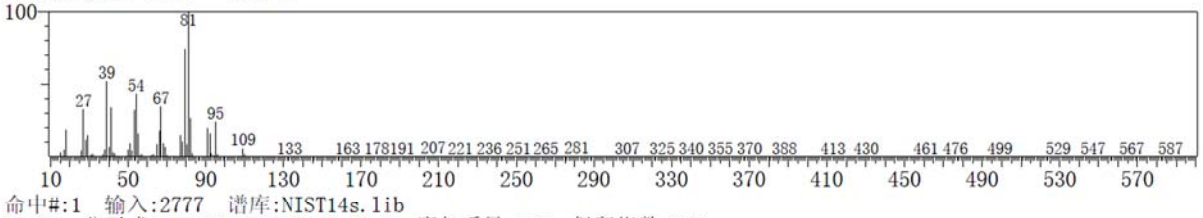
行号#:3　保留时间:5.040(扫描数#:809)　质量峰:439
原始模式:单个 5.040(809)　基峰:18.05(560039)
背景模式:无　组 1 - 事件 1



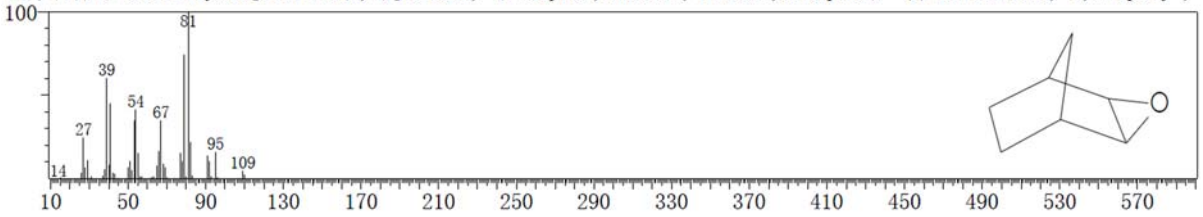
命中#:1　输入:17577　谱库:NIST14.lib
SI:63　分子式:C8H7ClO　CAS:2788-86-5　摩尔质量:154　保留指数:1163
组分名称:Benzene, 1-chloro-4-(epoxyethyl)- $$ (p-Chlorophenyl)oxirane $$ p-Chlorostyrene oxide $$ 4-Chloros



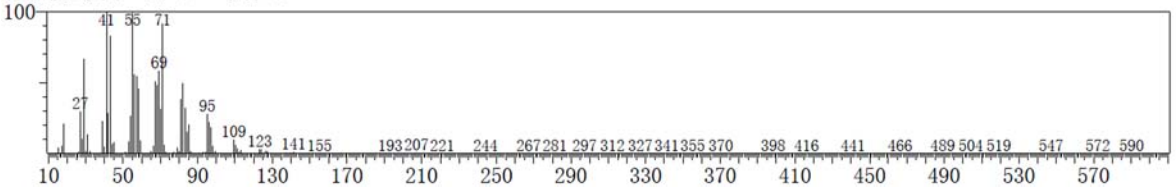
行号#:5　保留时间:2.765(扫描数#:354)　质量峰:388
原始模式:单个 2.765(354)　基峰:81.05(3698665)
背景模式:无　组 1 - 事件 1



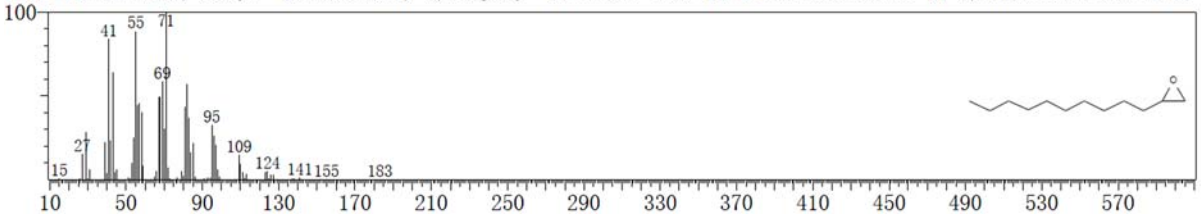
命中#:1　输入:2777　谱库:NIST14s.lib
SI:95　分子式:C7H10O　CAS:3146-39-2　摩尔质量:110　保留指数:630
组分名称:3-Oxatricyclo[3.2.1.0(2,4)]octane, (1.alpha.,2.beta.,4.beta.,5.alpha.)- $$ Norbornane, 2,3-epoxy-,



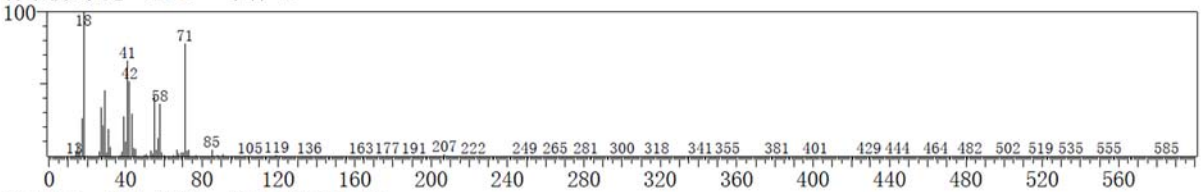
行号#:5　保留时间:6.220(扫描数#:1045)　质量峰:412
原始模式:单个 6.220(1045)　基峰:41.05(3200828)
背景模式:无　组 1 - 事件 1



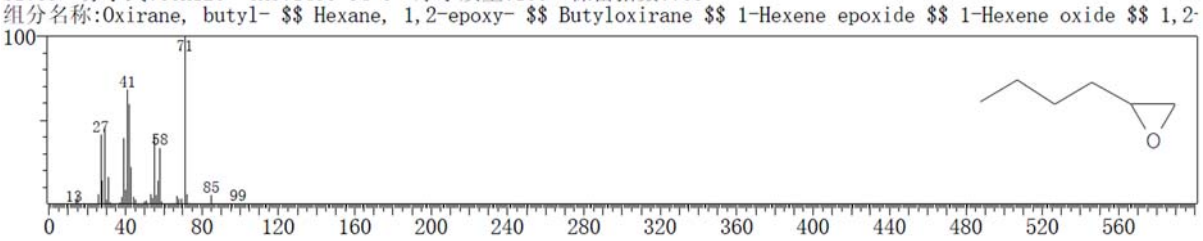
命中#:2　输入:36010　谱库:NIST14.lib
SI:94　分子式:C12H24O　CAS:2855-19-8　摩尔质量:184　保留指数:1304
组分名称:Oxirane, decyl- $$ Dodecane, 1,2-epoxy- $$ Nedox 1200 $$ 1-Dodecene oxide $$ 1,2-Dodecane oxide $$

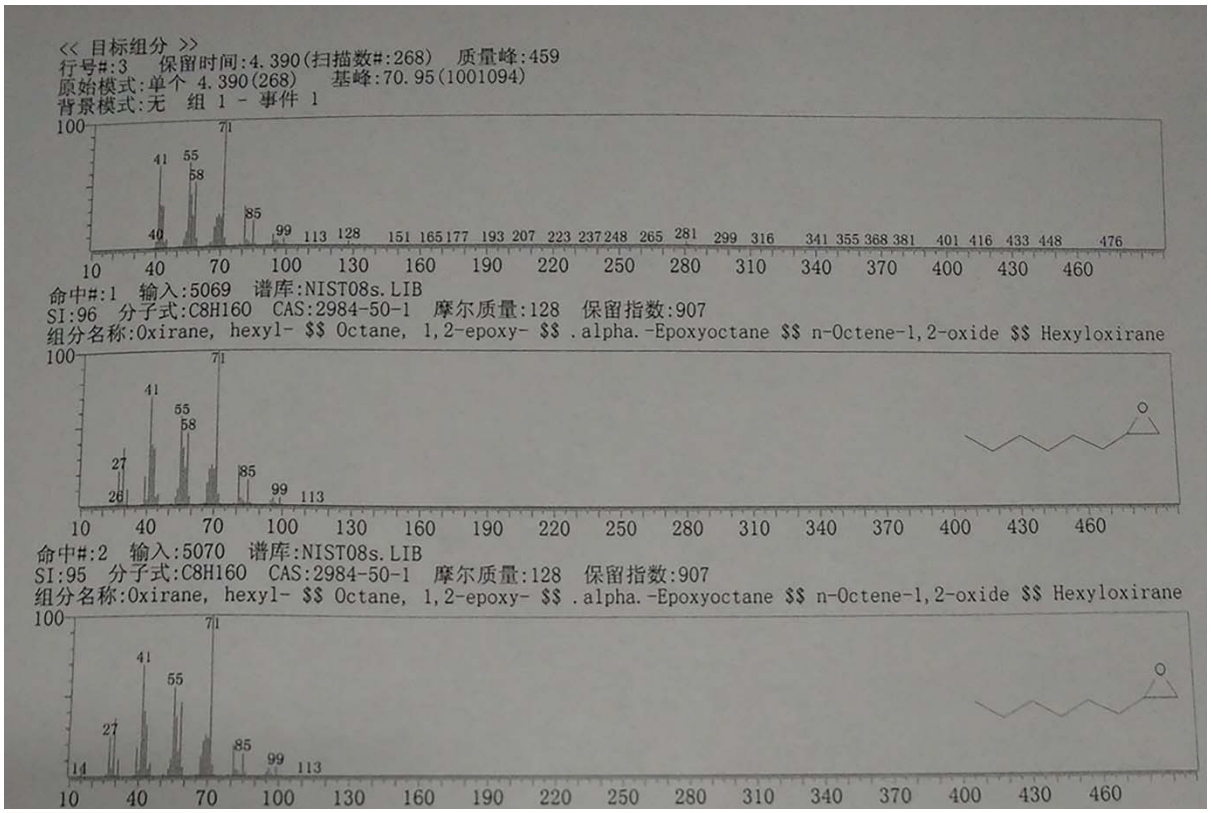


行号#:4　保留时间:2.040(扫描数#:209)　质量峰:381
原始模式:单个 2.040(209)　基峰:18.10(1013583)
背景模式:无　组 1 - 事件 1

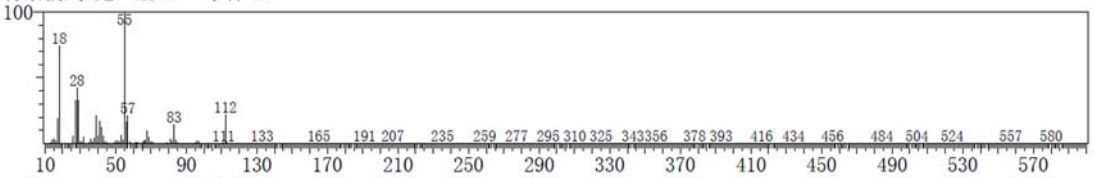


命中#:1　输入:2092　谱库:NIST14.lib
SI:89　分子式:C6H12O　CAS:1436-34-6　摩尔质量:100　保留指数:708
组分名称:Oxirane, butyl- $$ Hexane, 1,2-epoxy- $$ Butyloxirane $$ 1-Hexene epoxide $$ 1-Hexene oxide $$ 1,2-

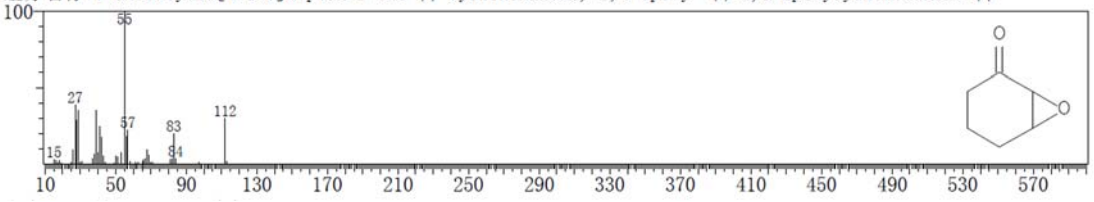




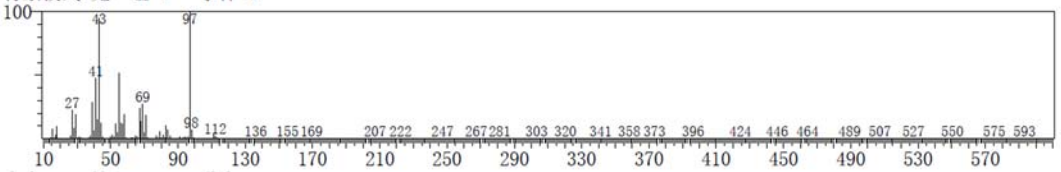
<< 目标组分 >>
行号#:6　保留时间:5.735(扫描数#:748)　质量峰:429
原始模式:单个 5.735(748)　基峰:55.00(851582)
背景模式:无　组 1 - 事件 1



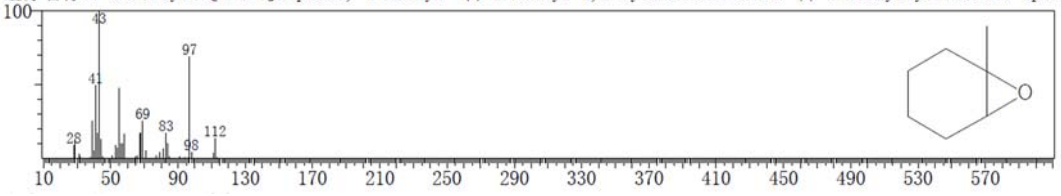
命中#:1　输入:3492　谱库:NIST14.lib
SI:89　分子式:C6H8O2　CAS:6705-49-3　摩尔质量:112　保留指数:902
组分名称:7-Oxabicyclo[4.1.0]heptan-2-one $$ Cyclohexanone, 2,3-epoxy- $$ 2,3-Epoxycyclohexanone $$



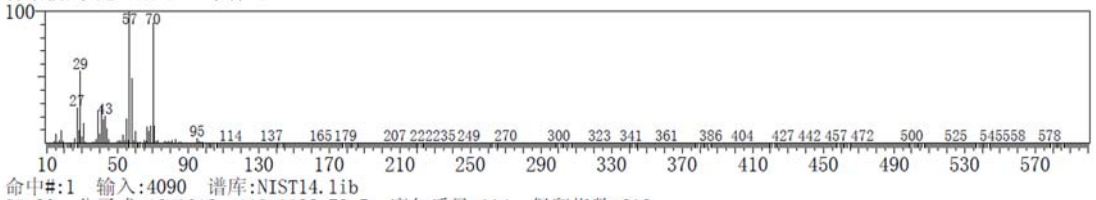
<< 目标组分 >>
行号#:2　保留时间:4.105(扫描数#:322)　质量峰:432
原始模式:单个 4.105(322)　基峰:97.05(7758143)
背景模式:无　组 1 - 事件 1



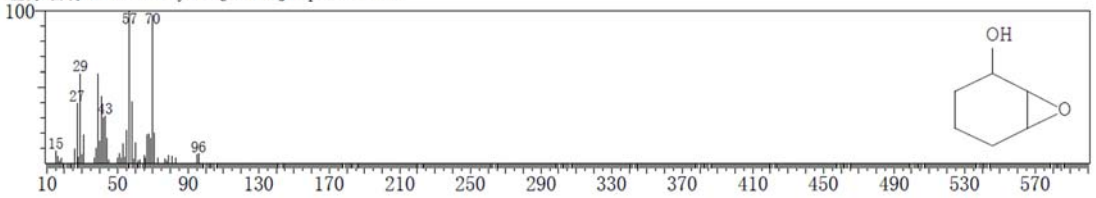
命中#:1　输入:3616　谱库:NIST14.lib
SI:90　分子式:C7H12O　CAS:1713-33-3　摩尔质量:112　保留指数:804
组分名称:7-Oxabicyclo[4.1.0]heptane, 1-methyl- $$ 1-Methyl-1,2-cyclohexene oxide $$ 1-Methylcyclohexene epo:



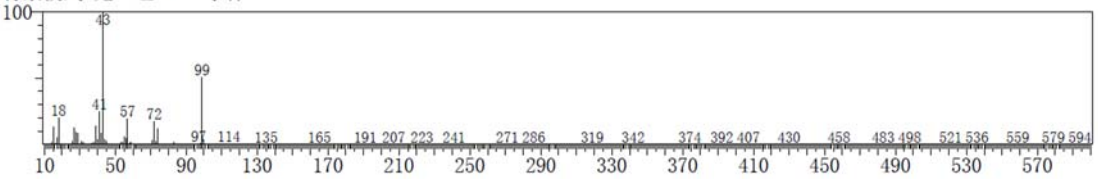
<< 目标组分 >>
行号#:7　保留时间:5.765(扫描数#:754)　质量峰:438
原始模式:单个 5.765(754)　基峰:57.00(6969066)
背景模式:无　组 1 - 事件 1



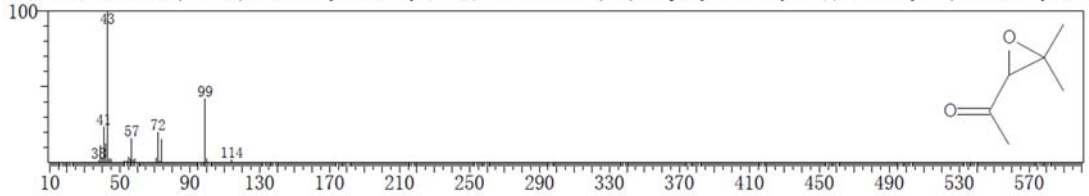
命中#:1　输入:4090　谱库:NIST14.lib
SI:90　分子式:C6H10O2　CAS:1192-78-5　摩尔质量:114　保留指数:919
组分名称:7-Oxabicyclo[4.1.0]heptan-2-ol



<< 目标组分 >>
行号#:1　保留时间:3.575(扫描数#:216)　质量峰:427
原始模式:单个 3.575(216)　基峰:43.00(4556396)
背景模式:无　组 1 - 事件 1

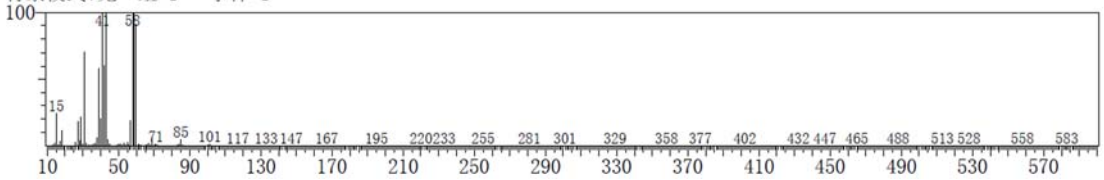


SI:84　分子式:C6H10O2　CAS:4478-63-1　摩尔质量:114　保留指数:780
组分名称:Ethanone, 1-(3,3-dimethyloxiranyl)- $$ 2-Pentanone, 3,4-epoxy-4-methyl- $$ 3-Acetyl-2,2-dimethylox



谱库

<< 目标组分 >>
行号#:1　保留时间:2.165(扫描数#:34)　质量峰:406
原始模式:单个 2.165(34)　基峰:57.95(8411490)
背景模式:无　组 1 - 事件 1



SI:83　分子式:C6H12O　CAS:5076-20-0　摩尔质量:100　保留指数:618
组分名称:Oxirane, tetramethyl- $$ Tetramethylethylene oxide $$ Butane, 2,3-epoxy-2,3-dimethyl- $$ Tetrameth