

Supplementary Information

Controllable transformation of biomass-derived diols over ammonia-modified H-Beta zeolite

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Fig. S1 GC-MS data of the volatile reaction products.



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Data File:	12	Original Data Path:	E:\GCMS Data\ChemLab
Current Data Path:	E:\GCMS Data\ChemLab	Sample Type:	Unknown
Sample ID:	4	Sample Name:	
Operator:	W. T	Acquisition Date:	08/14/19 11:25:14 AM
Run Time(min):	16.58	Comments:	
Vial:	1	Injection Volume(μl):	10.00
Scans:	4877	Low Mass(m/z):	50
High Mass(m/z):	400	Sample Volume(μl):	0.00
Sample Weight:	0.00	ISTD Amount:	0.000
Calibration Level:		Dilution Factor:	1.00
Instrument Method:	E:\GCMS Methods\ChemLab\CLT.meth	Original Processing Method:	
Current Processing Method:	N/A	Calibration File:	N/A

Method type:	Acquisition - General
MS transfer line temperature:	270 °C
Ion source temperature:	260 °C
Use acquisition threshold:	No
Ionization mode:	EI
Run completion:	GC run time
Segment #1:	
Start time:	0.5 min
Filament/multiplier/dynode on:	Yes
Chromatography filter on:	Yes
Chrom. filter peak width time:	1 sec
Use tune file emission current:	Yes
Use last tuned detector gain:	Yes
Use tune file electron energy:	Yes
Calibration gas:	Off
Scan #1	
Tune file:	(Last Saved)
Ion polarity:	Positive
Data type:	Centroid
Start mass:	50 amu
End mass:	400 amu
Scan time:	0.2 sec

NOTICE: If this method uses a linked external file in timed mode or is used for an AutoSIM acquisition run, please see the scan header report in the raw file for scan event source information.

Acquisition Time	
Use oven run time:	Yes
Oven Method	
Maximum temperature:	280.0 °C
Prep-run timeout:	10.00 min
Equilibration time:	0.50 min
Ready delay:	0.00 min
Oven on/off:	On
Cryogenics enable:	Off
Cryogenics threshold:	50.0 °C
Cryogenics timeout:	60.00 min
Initial temperature:	60.0 °C
Initial hold time:	5.00 min
Number of ramps:	1
Ramp 01 rate:	30.0 °C/min
Ramp 01 final temperature:	270.0 °C
Ramp 01 hold time:	5.00 min

S/SL - Front Method	
S/SL mode:	Split
Temperature enable:	On
Temperature:	250 °C
Split flow enable:	On
Split flow:	20.0 mL/min
Purge flow:	5.0 mL/min
Constant septum purge:	On
Carrier mode:	Constant Pressure



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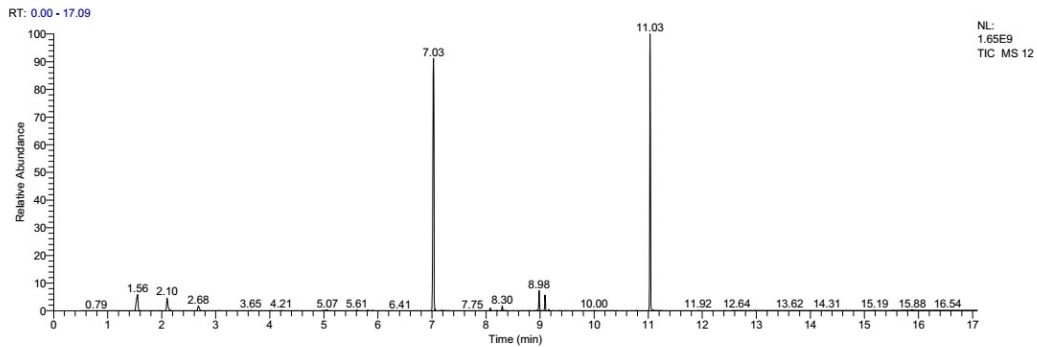
Carrier pressure enable: On
Carrier pressure: 80.00 kPa
Vacuum compensation: On
Carrier gas saver enable: On
Carrier gas saver flow: 25.0 mL/min
Carrier gas saver time: 2.00 min
Backflush enable: On
Backflush start time: 1.50 min
Backflush duration: GC Run Time

Run Table Method
Ext. event #1 prep-run value: Off
Ext. event #2 prep-run value: Off
Ext. event #3 prep-run value: Off
Ext. event #4 prep-run value: Off
Ext. event #5 prep-run value: Off
Ext. event #6 prep-run value: Off
Ext. event #7 prep-run value: Off
Ext. event #8 prep-run value: Off
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Aux. oven event #5 prep-run value: Off
Aux. oven event #6 prep-run value: Off
Aux. oven event #7 prep-run value: Off
Aux. oven event #8 prep-run value: Off

Sampling
Sample volume (µl): 0.10
Plunger strokes: 3
Viscous sample: Yes
Sampling depth in vial: Center

Injection
Injection depth: Standard
Pre-Inj dwell time (s): 0.0
Post-Inj dwell time (s): 0.0

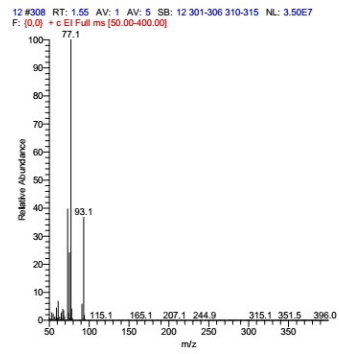
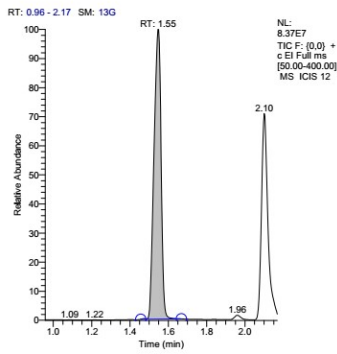
Washes
Pre-Inj solvent: C
Pre-Inj solvent cycles: 3
Sample rinses: 3
Post-Inj solvent: D
Post-Inj solvent cycles: 3





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RT	Peak Height	Peak Width	Peak Area	Area %	S/N	BL	Saturated
1.55	83355384.23	0.21	214237490.37	4.61	35175.59	BB	No
1.96	1162446.26	0.06	2308725.54	0.05	490.55	BB	No
2.10	59292739.24	0.14	139854125.69	3.01	25021.27	BB	No
2.40	592622.78	0.05	1090843.76	0.02	250.08	BB	No
2.68	23804719.33	0.15	61232793.58	1.32	10045.48	BB	No
3.07	1573377.80	0.09	3842102.85	0.08	663.96	BB	No
3.64	1987226.79	0.07	4705592.22	0.10	838.60	BB	No
4.02	1799746.81	0.09	4810867.06	0.10	759.48	BB	No
4.21	2081716.91	0.09	5766889.26	0.12	878.48	BB	No
4.40	808900.75	0.07	2189193.07	0.05	341.35	BB	No
5.06	3619155.64	0.18	19215111.95	0.41	1527.27	BB	No
5.20	411748.74	0.05	799819.64	0.02	173.76	BB	No
5.61	3579719.03	0.07	7418134.08	0.16	1510.63	BB	No
5.81	3244262.83	0.07	6435784.87	0.14	1369.06	BB	No
5.90	2837849.73	0.06	5385612.05	0.12	1197.56	BB	No
6.41	443263.06	0.04	658277.36	0.01	187.06	BB	No
7.02	1202812221.19	0.17	2188553364.20	47.11	507581.30	BB	No
7.17	2469016.97	0.09	5747448.72	0.12	1041.91	BB	No
7.23	1936245.91	0.06	3827874.04	0.08	817.09	BB	No
7.30	1104699.42	0.05	1776275.22	0.04	466.18	BB	No
7.75	454428.62	0.06	1153748.21	0.02	191.77	BB	No
8.08	10731010.88	0.09	19465126.14	0.42	4528.44	BB	No
8.20	2122314.62	0.09	5722391.30	0.12	895.61	BB	No
8.30	18178673.74	0.09	32486440.09	0.70	7671.32	BB	No
8.38	1160399.44	0.10	3074077.43	0.07	489.68	BB	No
8.50	539599.23	0.06	1321522.39	0.03	227.71	BB	No
8.67	700598.03	0.06	1315253.52	0.03	295.65	BB	No
8.79	731578.08	0.08	2166702.17	0.05	308.72	BB	No
8.90	597080.63	0.03	809051.49	0.02	251.97	BB	No
8.98	74220834.19	0.14	121774724.57	2.62	31320.86	BB	No
9.09	57691954.07	0.07	91078670.14	1.96	24345.74	BB	No
9.16	3945115.92	0.06	6390612.50	0.14	1664.82	BB	No
9.24	451897.10	0.03	616832.01	0.01	190.70	BB	No
9.36	1210044.08	0.05	1831396.39	0.04	510.63	BB	No
9.47	541146.60	0.05	877537.05	0.02	228.36	BB	No
9.65	417906.27	0.05	873024.60	0.02	176.35	BB	No
10.00	1171646.82	0.12	2573186.81	0.06	494.43	BB	No
10.24	463599.80	0.05	754200.90	0.02	195.64	BB	No
10.29	538086.34	0.05	858265.49	0.02	227.07	BB	No
10.35	691780.49	0.04	1025556.68	0.02	291.93	BB	No
10.79	911812.35	0.10	2312454.98	0.05	384.78	BB	No
11.03	1054498022.70	0.30	1653093272.69	35.58	444993.38	BB	No
11.92	720292.42	0.05	1199282.76	0.03	303.96	BB	No
15.19	507814.10	0.08	1349664.03	0.03	214.30	BB	No
15.88	3339590.51	0.14	9914307.00	0.21	1409.29	BB	No
16.40	504976.66	0.17	1699663.53	0.04	213.10	BB	No





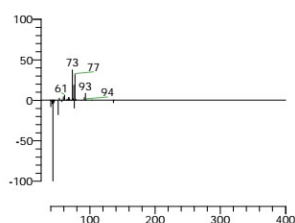
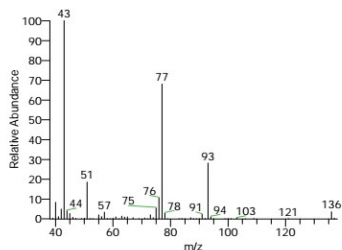
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RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
1.55	610	615	46.35	mainlib	C5H6F2O2	136
1.55	587	675	16.92	mainlib	C8H12	108
1.55	521	550	2.67	mainlib	C6H9NSi	123
1.55	520	620	2.56	nist_msms	C7H8O2	124
1.55	519	529	2.46	mainlib	C7H9Br	172

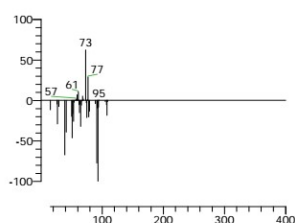
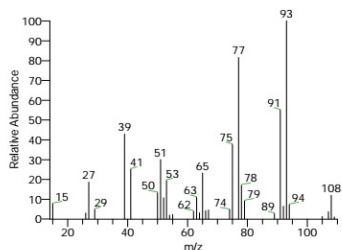
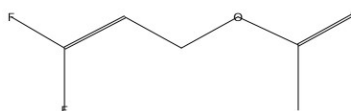
Hit Spectrum

Delta

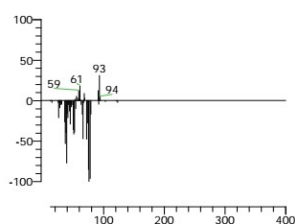
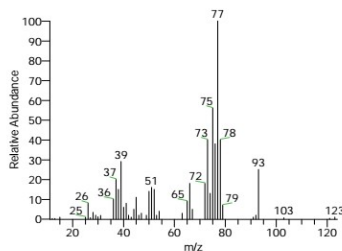
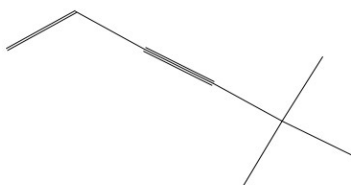
Compound Structure



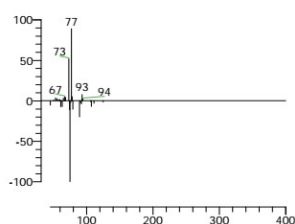
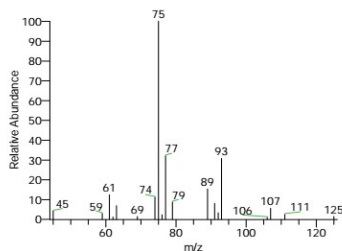
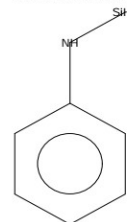
2-Propen-1-ol, 3,3-difluoro-, acetate
Formula C5H6F2O2, MW 136, CAS# 159740-6, Entry# 8836
3,3-Difluoro-2-propenyl acetate #



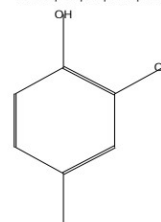
1-Hexen-3-yne, 5,5-dimethyl-
Formula C8H12, MW 108, CAS# 4911-58-4, Entry# 60086
5,5-Dimethyl-1-hexen-3-yne #



Silanamine, N-phenyl-
Formula C6H9NSi, MW 123, CAS# 5578-85-8, Entry# 42604
Silylamine, N-phenyl-



4-Methylcatechol
Formula C7H8O2, MW 124, CAS# 452-86-8, Entry# 6249
\$.06QqQ/triple quadrupole



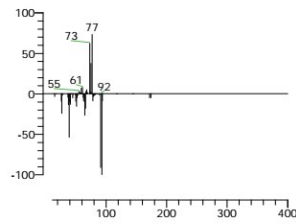
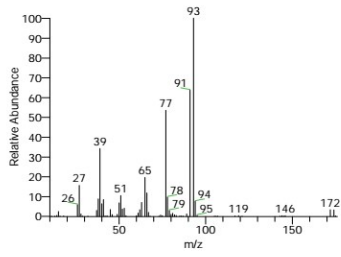


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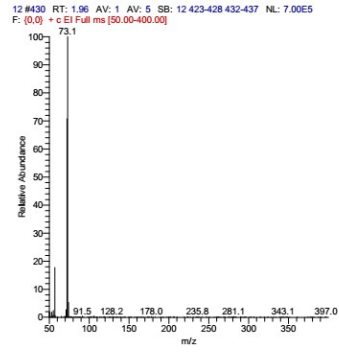
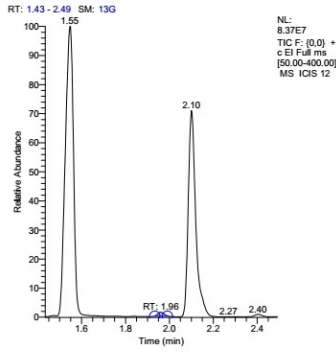
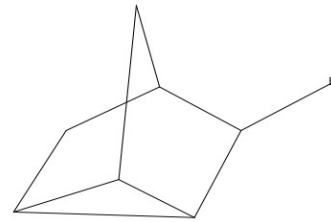
Hit Spectrum

Delta

Compound Structure



Nortriclyl bromide
Formula C₇H₉Br, MW 172, CAS# NA, Entry# 60212

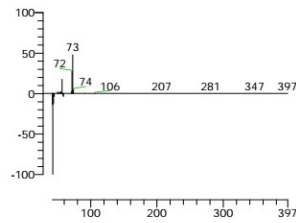
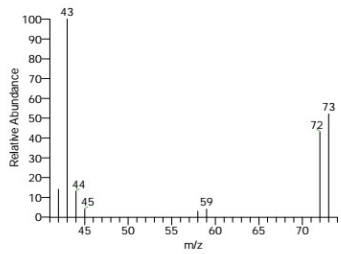


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
<u>1.96</u>	836	945	41.93	mainlib	C ₄ H ₇ NO ₂	101
1.96	809	879	35.42	replib	C ₃ H ₇ NO	73
1.96	832	935	35.42	replib	C ₃ H ₇ NO	73
1.96	750	754	3.61	replib	C ₄ H ₁₁ BO ₂	102
1.96	739	773	2.47	nist_msms	C ₄ H ₈ N ₂ O ₃	132

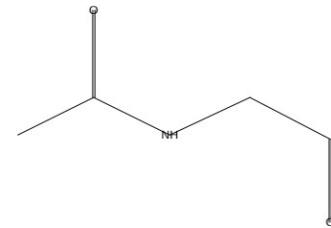
Hit Spectrum

Delta

Compound Structure



Acetamidoacetaldehyde
Formula C₄H₇NO₂, MW 101, CAS# 64790-08-5, Entry# 8695
N-(2-Oxoethyl)acetamide #



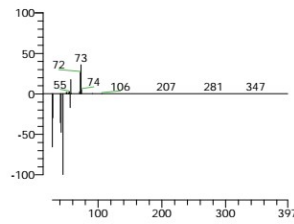
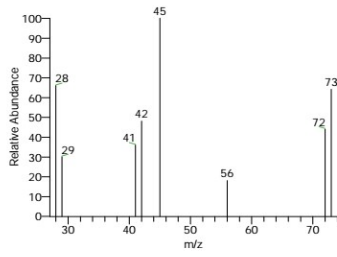


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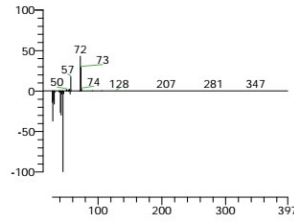
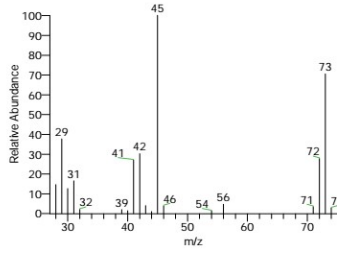
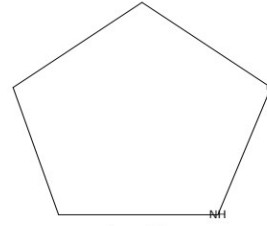
Hit Spectrum

Delta

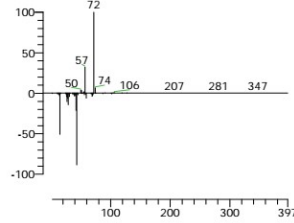
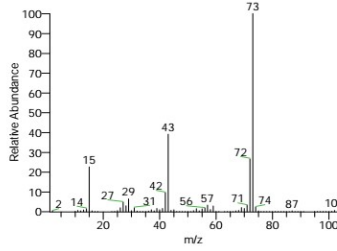
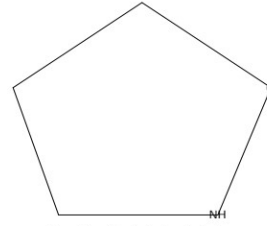
Compound Structure



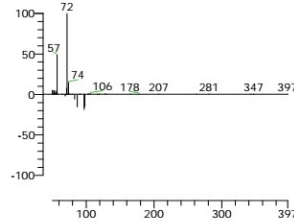
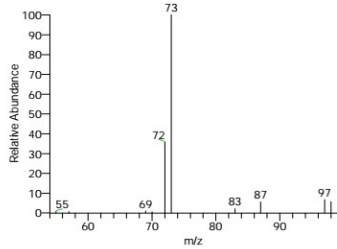
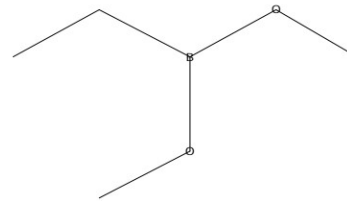
Isoxazolidine
Formula C3H7NO, MW 73, CAS# 504-72-3, Entry# 3700
Isoxazole, tetrahydro-



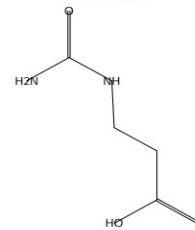
Isoxazolidine
Formula C3H7NO, MW 73, CAS# 504-72-3, Entry# 3928
Isoxazole, tetrahydro-



Boronic acid, ethyl-, dimethyl ester
Formula C4H11BO2, MW 102, CAS# 7318-82-3, Entry# 8944
Ethaneboronic acid, dimethyl ester

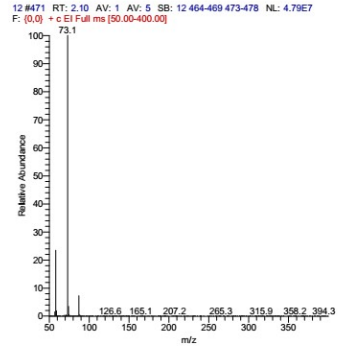
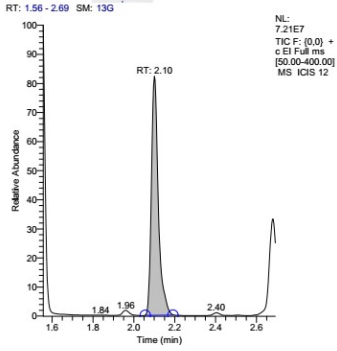


3-Ureidopropionic acid
Formula C4H8N2O3, MW 132, CAS# 462-88-4, Entry# 12279
\$.061/ton trap



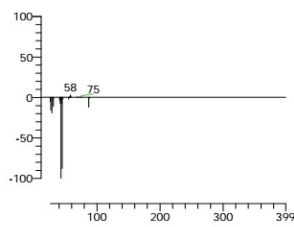
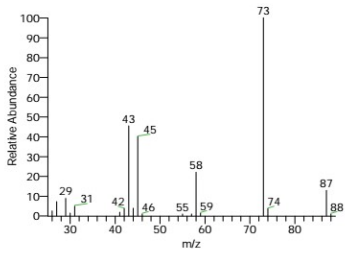


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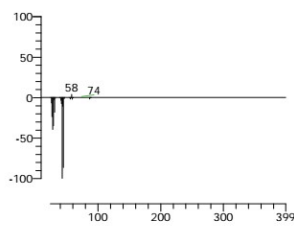
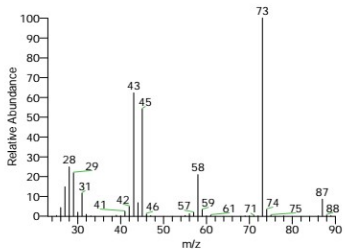
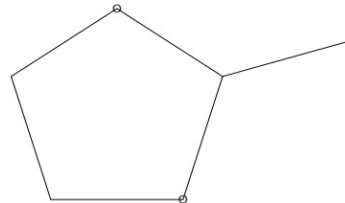


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
2.10	937	937	70.40	replib	C4H8O2	88
2.10	938	942	70.40	mainlib	C4H8O2	88
2.10	884	927	13.79	mainlib	C3H7NO	73
2.10	871	987	8.90	nist_msms	C4H9NO2	103
2.10	841	953	2.47	nist_msms	C2H5NO3	91

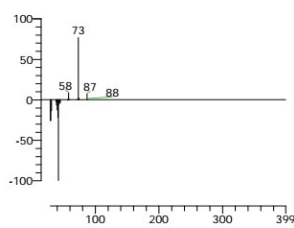
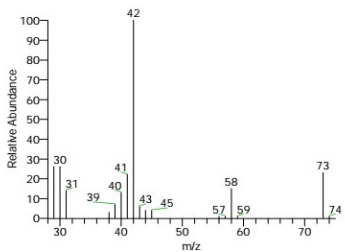
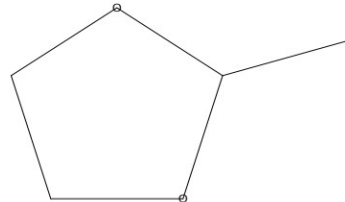
Hit Spectrum Delta Compound Structure



1,3-Dioxolane, 2-methyl-
Formula C4H8O2, MW 88, CAS# 497-26-7, Entry# 36954
2-Methyl-1,3-dioxolane



1,3-Dioxolane, 2-methyl-
Formula C4H8O2, MW 88, CAS# 497-26-7, Entry# 8927
2-Methyl-1,3-dioxolane



Acetaldehyde, O-methylxime
Formula C3H7NO, MW 73, CAS# 33581-43-0, Entry# 4172
(1E)-Ethanal o-methylxime #



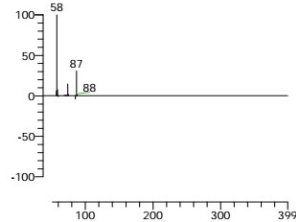
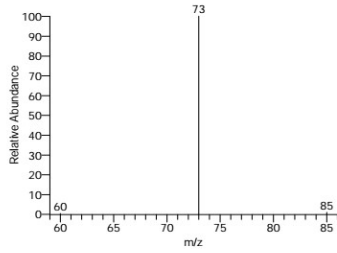


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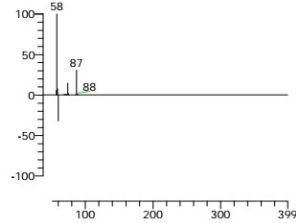
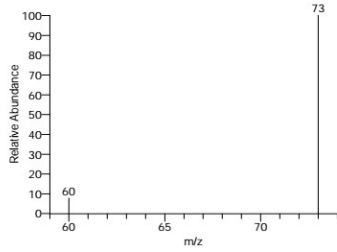
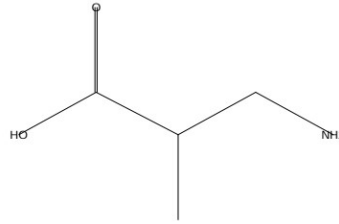
Hit Spectrum

Delta

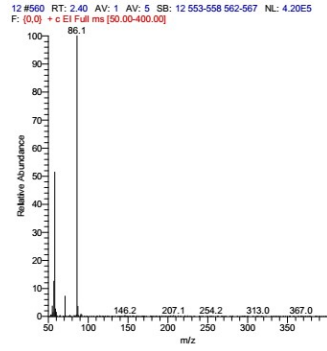
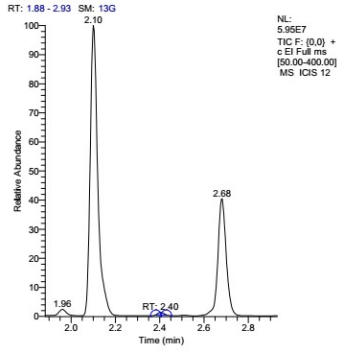
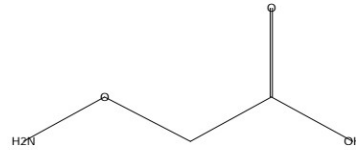
Compound Structure



DL-3-Aminoisobutyric acid
 Formula C₄H₉NO₂, MW 103, CAS# 144-90-1, Entry# 12270
 \$.0617/ion trap



O-(Carboxymethyl)hydroxylamine
 Formula C₂H₅NO₃, MW 91, CAS# 645-88-5, Entry# 12333
 \$.0617/ion trap



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
2.40	894	910	65.11	replib	C ₄ H ₆ O ₂	86
2.40	898	913	65.11	mainlib	C ₄ H ₆ O ₂	86
2.40	840	953	11.98	nist_msms	C ₁₉ H ₂₃ N ₃ O	309
2.40	825	932	7.26	nist_msms	C ₁₄ H ₂₂ N ₂ O	234
2.40	815	835	5.12	replib	C ₅ H ₁₀ O	86

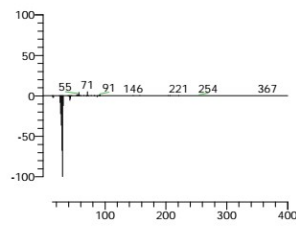
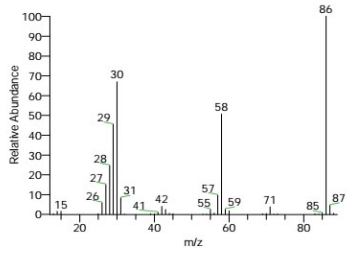


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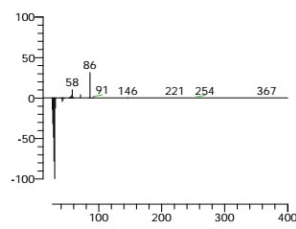
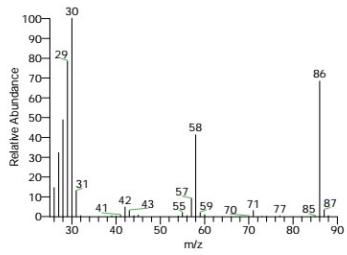
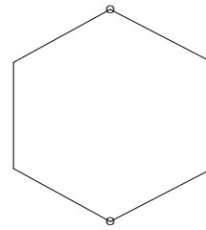
Hit Spectrum

Delta

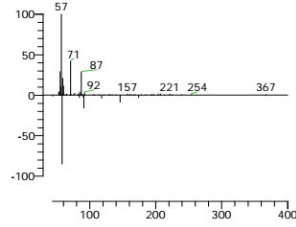
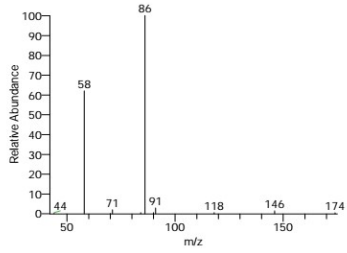
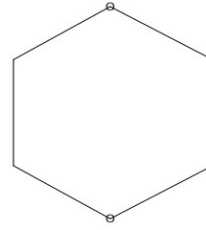
Compound Structure



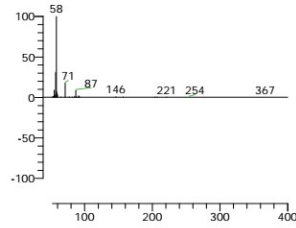
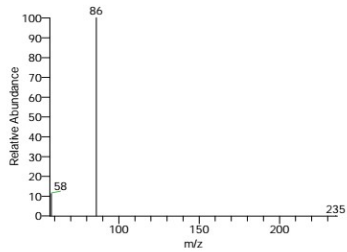
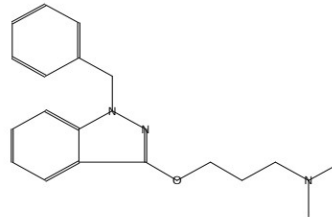
1,4-Dioxin, 2,3-dihydro-
Formula C4H6O2, MW 86, CAS# 543-75-9, Entry# 50594
p-Dioxin, 2,3-dihydro-



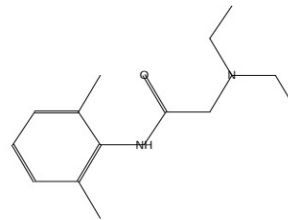
1,4-Dioxin, 2,3-dihydro-
Formula C4H6O2, MW 86, CAS# 543-75-9, Entry# 331
p-Dioxin, 2,3-dihydro-



Formula C19H23N3O, MW 309, CAS# 642-72-8, Entry# 4967
\$.06QqQ/triple quadrupole



Lidocaine
Formula C14H22N2O, MW 234, CAS# 137-58-6, Entry# 793
\$.06QqQ/triple quadrupole



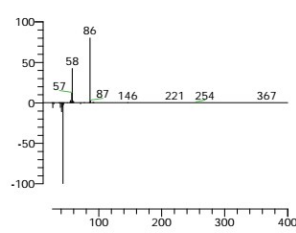
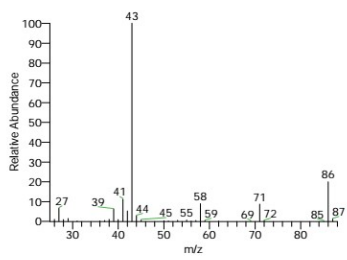


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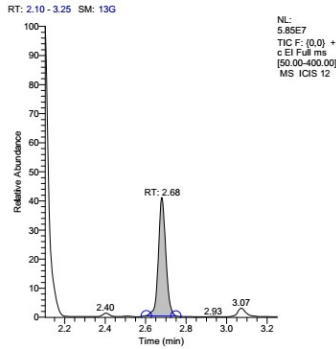
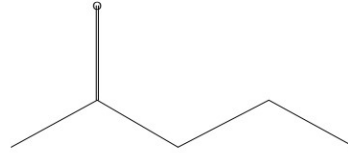
Hit Spectrum

Delta

Compound Structure

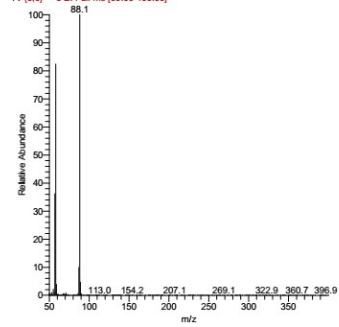


2-Pentanone
Formula C₅H₁₀O, MW 86, CAS# 107-87-9, Entry# 2807
Ethyl acetone



NL: 5.85E7
TIC F: (0.0) +
c EI Full.ms
[50.00-400.00]
MS ICIS 12

12 #642 RT: 2.68 AV: 1 AV: 5 SB: 12 635-640 644-649 NL: 1.06E7
F: (0.0) + c EI Full.ms [50.00-400.00]



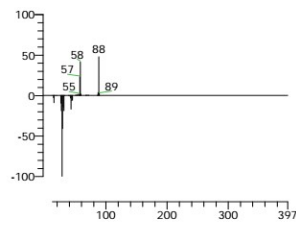
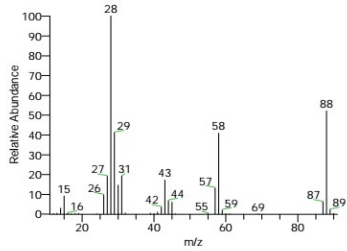
RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
2.68	917	923	78.93	replib	C ₄ H ₈ O ₂	88
2.68	907	913	78.93	replib	C ₄ H ₈ O ₂	88
2.68	914	922	78.93	replib	C ₄ H ₈ O ₂	88
2.68	951	961	78.93	mainlib	C ₄ H ₈ O ₂	88
2.68	916	934	19.81	replib	C ₅ H ₁₀ O ₃	118

Hit Spectrum

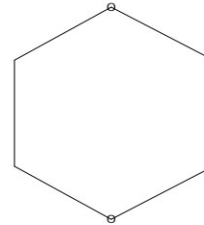
Delta

Compound Structure

SI 951, RSI 961, mainlib, Entry# 236, CAS# 123-91-1, 1,4-Dioxane



1,4-Dioxane
Formula C₄H₈O₂, MW 88, CAS# 123-91-1, Entry# 236
p-Dioxane



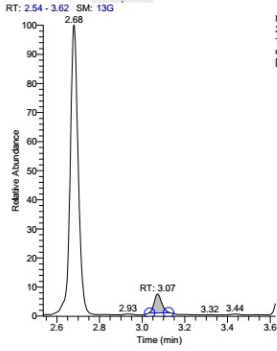


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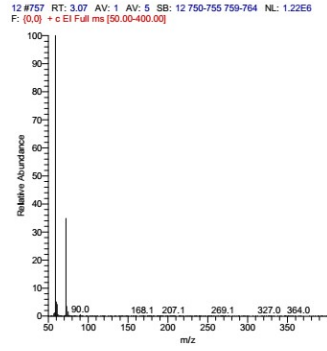
Hit Spectrum	Delta	Compound Structure
<p>SI 917, RSI 923, replib, Entry# 98, CAS# 123-91-1, 1,4-Dioxane</p> <p>Mass spectrum showing relative abundance versus m/z. The base peak is at m/z 28. Other significant peaks are labeled at m/z 15, 19, 27, 29, 31, 43, 45, 57, 59, 69, 87, and 89.</p>	<p>Delta spectrum showing relative abundance versus m/z. The base peak is at m/z 58. Other significant peaks are labeled at m/z 55, 57, and 89.</p>	<p>1,4-Dioxane Formula C₄H₈O₂, MW 88, CAS# 123-91-1, Entry# 98 p-Dioxane</p>
<p>Mass spectrum showing relative abundance versus m/z. The base peak is at m/z 28. Other significant peaks are labeled at m/z 26, 27, 31, 42, 43, 44, 45, 59, 73, 87, 89, and 118.</p>	<p>Delta spectrum showing relative abundance versus m/z. The base peak is at m/z 58. Other significant peaks are labeled at m/z 55, 57, and 89.</p>	<p>1,3,6-Trioxocane Formula C₅H₁₀O₃, MW 118, CAS# 1779-19-7, Entry# 94 Diethylene glycol formal</p>
<p>SI 914, RSI 922, replib, Entry# 100, CAS# 123-91-1, 1,4-Dioxane</p> <p>Mass spectrum showing relative abundance versus m/z. The base peak is at m/z 28. Other significant peaks are labeled at m/z 15, 26, 27, 29, 31, 43, 45, 56, 57, 59, 61, 77, 87, and 89.</p>	<p>Delta spectrum showing relative abundance versus m/z. The base peak is at m/z 58. Other significant peaks are labeled at m/z 55, 57, and 89.</p>	<p>1,4-Dioxane Formula C₄H₈O₂, MW 88, CAS# 123-91-1, Entry# 100 p-Dioxane</p>
<p>SI 907, RSI 913, replib, Entry# 99, CAS# 123-91-1, 1,4-Dioxane</p> <p>Mass spectrum showing relative abundance versus m/z. The base peak is at m/z 28. Other significant peaks are labeled at m/z 29, 31, 32, 42, 43, 44, 56, 57, 59, 67, 71, 85, 87, and 89.</p>	<p>Delta spectrum showing relative abundance versus m/z. The base peak is at m/z 58. Other significant peaks are labeled at m/z 55, 57, and 89.</p>	<p>1,4-Dioxane Formula C₄H₈O₂, MW 88, CAS# 123-91-1, Entry# 99 p-Dioxane</p>



ChemLab Technologies - GC/MS Report



NL: 2.41E7
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICS 12

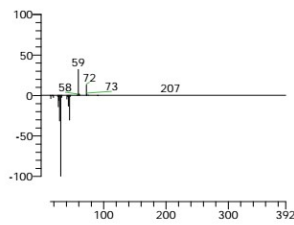
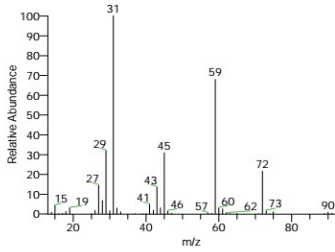


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
3.07	923	923	95.07	NISTDEMO	C4H10O2	90
3.07	923	923	95.07	mainlib	C4H10O2	90
3.07	914	926	95.07	replib	C4H10O2	90
3.07	929	929	95.07	replib	C4H10O2	90
3.07	744	775	1.52	replib	C4H9NO	87

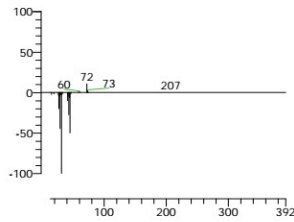
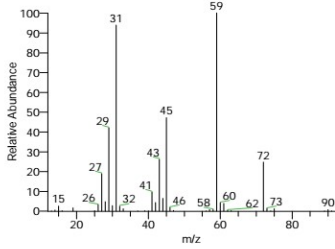
Hit Spectrum

Delta

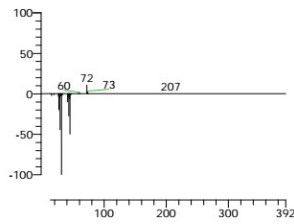
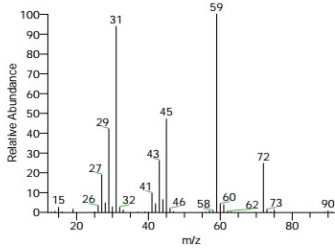
Compound Structure



Ethanol, 2-ethoxy-
Formula C4H10O2, MW 90, CAS# 110-80-5, Entry# 614
 α -Ethoxyethanol



Ethanol, 2-ethoxy-
Formula C4H10O2, MW 90, CAS# 110-80-5, Entry# 1992
 α -Ethoxyethanol



Ethanol, 2-ethoxy-
Formula C4H10O2, MW 90, CAS# 110-80-5, Entry# 27147
 α -Ethoxyethanol



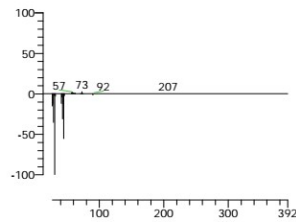
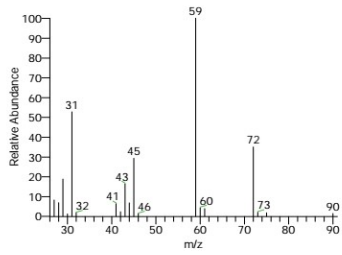


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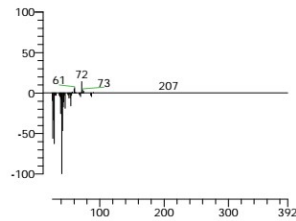
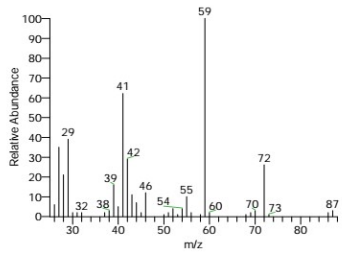
Hit Spectrum

Delta

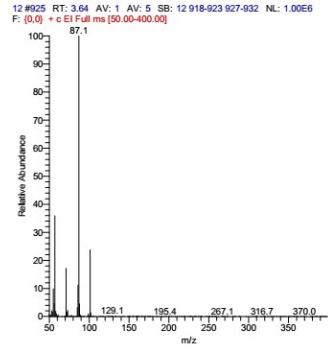
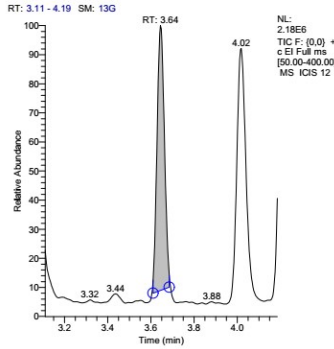
Compound Structure



Ethanol, 2-ethoxy-
Formula C₄H₁₀O₂, MW 90, CAS# 110-80-5, Entry# 6834
 α -Ethoxyethanol



Butanal, oxime
Formula C₄H₉NO, MW 87, CAS# 110-69-0, Entry# 6841
Butyraldehyde, oxime



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
3.64	888	892	95.06	mainlib	C ₆ H ₁₂ O ₂	116
3.64	697	795	2.85	replib	C ₅ H ₁₀ O ₂	102
3.64	683	716	2.85	replib	C ₅ H ₁₀ O ₂	102
3.64	743	809	2.85	mainlib	C ₅ H ₁₀ O ₂	102
3.64	685	693	0.52	mainlib	C ₈ H ₁₈ O	130

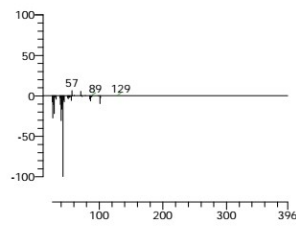
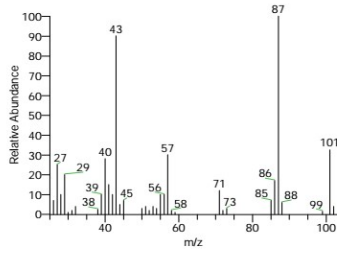


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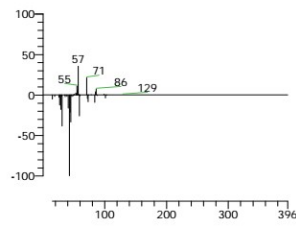
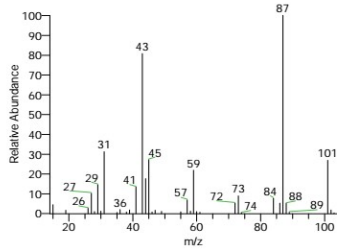
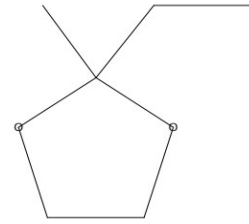
Hit Spectrum

Delta

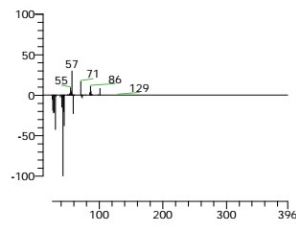
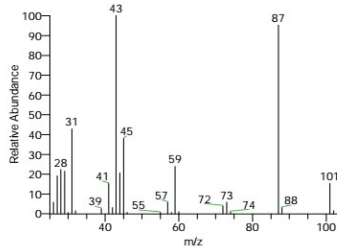
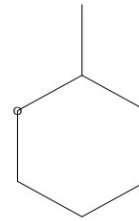
Compound Structure



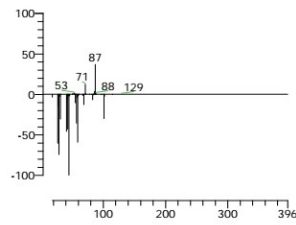
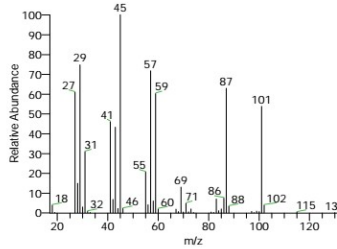
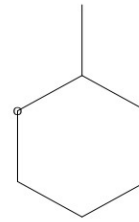
1,3-Dioxolane, 2-ethyl-2-methyl-
Formula C₆H₁₂O₂, MW 116, CAS# 126-39-6, Entry# 51953
2-Butanone, cyclic ethylene acetal



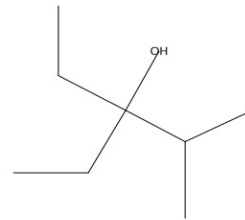
1,3-Dioxane, 2-methyl-
Formula C₅H₁₀O₂, MW 102, CAS# 626-68-6, Entry# 51873
m-Dioxane, 2-methyl-



1,3-Dioxane, 2-methyl-
Formula C₅H₁₀O₂, MW 102, CAS# 626-68-6, Entry# 2821
m-Dioxane, 2-methyl-



3-Pentanol, 3-ethyl-2-methyl-
Formula C₈H₁₈O, MW 130, CAS# 597-05-7, Entry# 15658
2-Methyl-3-ethyl-3-pentanol



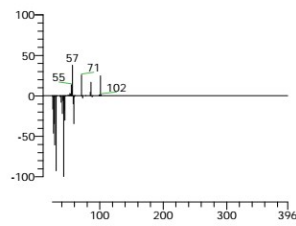
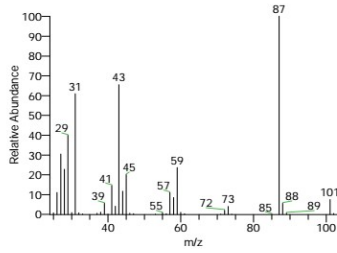


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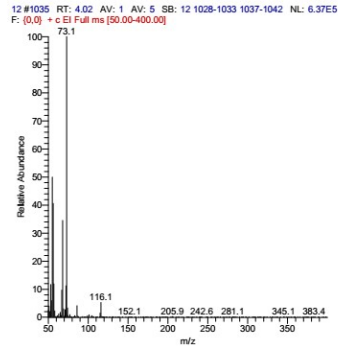
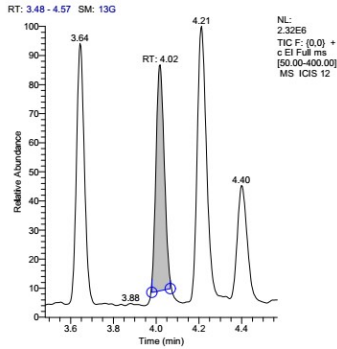
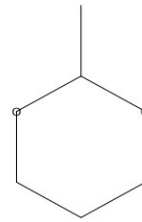
Hit Spectrum

Delta

Compound Structure



1,3-Dioxane, 2-methyl-
Formula C5H10O2, MW 102, CAS# 626-68-6, Entry# 11810
m-Dioxane, 2-methyl-



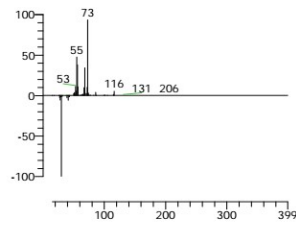
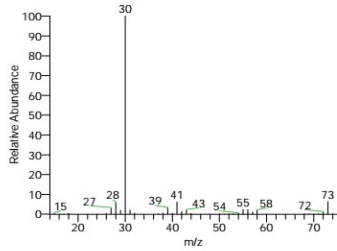
RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
4.02	708	762	16.99	replib	C4H11N	73
4.02	688	779	7.74	replib	C7H16O	116
4.02	688	825	7.74	mainlib	C8H16O	128
4.02	682	708	6.08	replib	C7H14O	114
4.02	680	748	5.61	replib	C5H12O2	104

Hit Spectrum

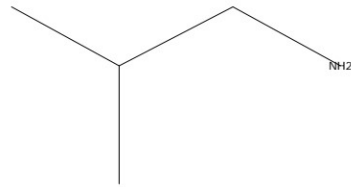
Delta

Compound Structure

SI 708, RSI 762, replib, Entry# 468, CAS# 78-81-9, Isobutylamine



Isobutylamine
Formula C4H11N, MW 73, CAS# 78-81-9, Entry# 468
1-Propanamine, 2-methyl-



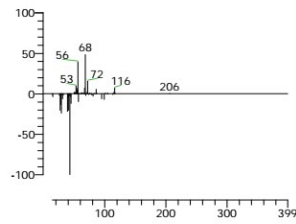
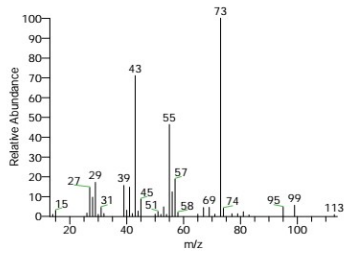


ChemLab Technologies - GC/MS Report

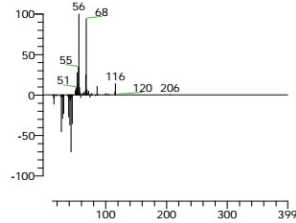
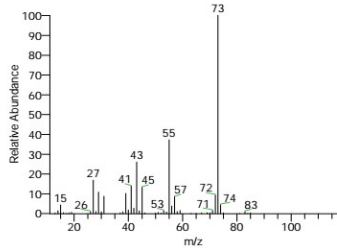
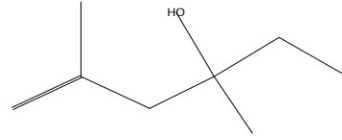
Hit Spectrum

Delta

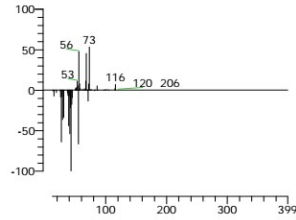
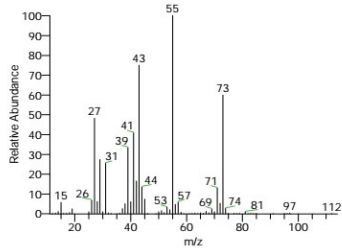
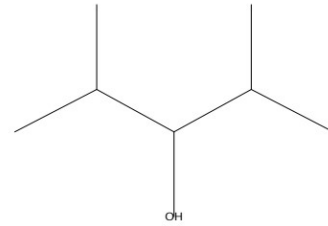
Compound Structure



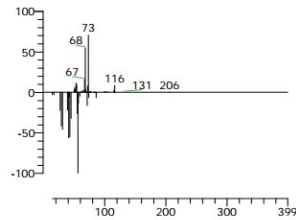
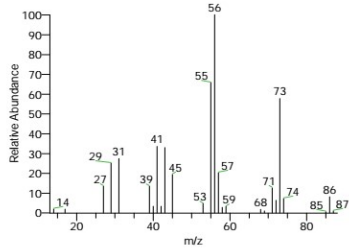
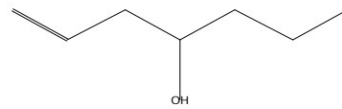
3,5-Dimethyl-5-hexen-3-ol
Formula C₈H₁₆O, MW 128, CAS# 1569-46-6, Entry# 36970



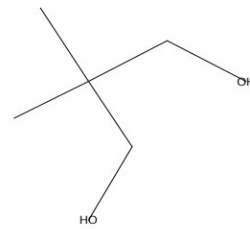
3-Pentanol, 2,4-dimethyl-
Disopropylcarbinol
Formula C₇H₁₆O, MW 116, CAS# 600-36-2, Entry# 9003



1-Hepten-4-ol
Formula C₇H₁₄O, MW 114, CAS# 3521-91-3, Entry# 4621

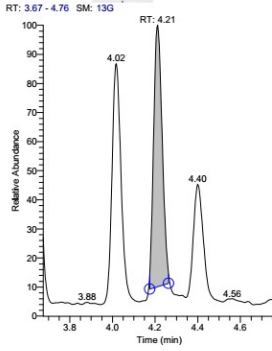


Neopentyl glycol
Formula C₅H₁₂O₂, MW 104, CAS# 126-30-7, Entry# 5227
1,3-Propanediol, 2,2-dimethyl-



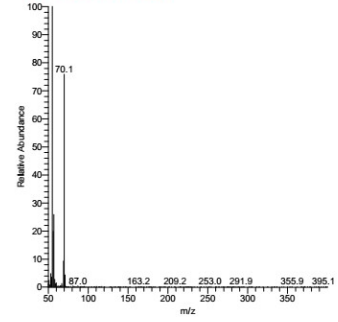


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NL: 2.32E6
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICS 12

12 #1092 RT: 4.21 AV: 1 AV: 5 SB: 12 1085-1090 1094-1099 NL: 8.89E5
F: (0.0) + c EI Full ms (50.00-400.00)

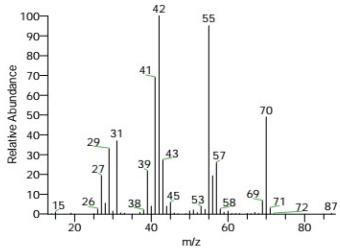


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
4.21	948	952	71.77	mainlib	C5H12O	88
4.21	942	949	71.77	replib	C5H12O	88
4.21	913	961	71.77	replib	C5H12O	88
4.21	890	908	71.77	replib	C5H12O	88
4.21	948	952	71.77	NISTDEMO	C5H12O	88

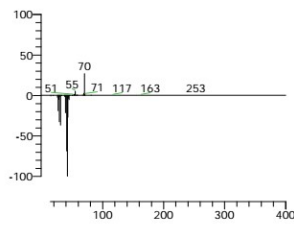
Hit Spectrum

Delta

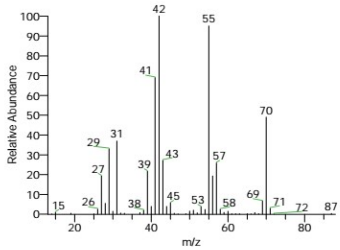
Compound Structure



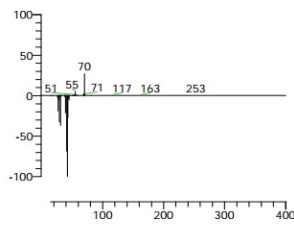
SI 948, RSI 952, mainlib, Entry# 4447, CAS# 71-41-0, 1-Pentanol



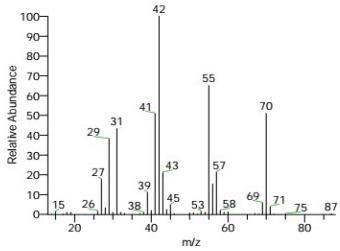
1-Pentanol
Formula C5H12O, MW 88, CAS# 71-41-0, Entry# 2234
Pentyl alcohol



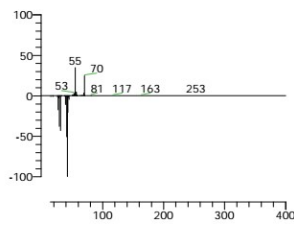
SI 942, RSI 949, replib, Entry# 1443, CAS# 71-41-0, 1-Pentanol



1-Pentanol
Formula C5H12O, MW 88, CAS# 71-41-0, Entry# 4447
Pentyl alcohol



SI 942, RSI 949, replib, Entry# 1443, CAS# 71-41-0, 1-Pentanol



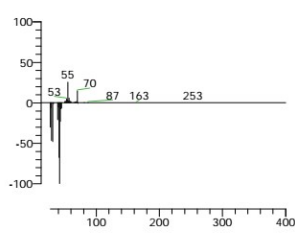
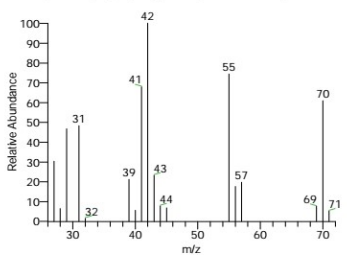
1-Pentanol
Formula C5H12O, MW 88, CAS# 71-41-0, Entry# 1443
Pentyl alcohol



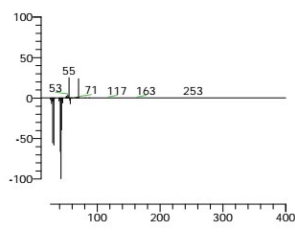
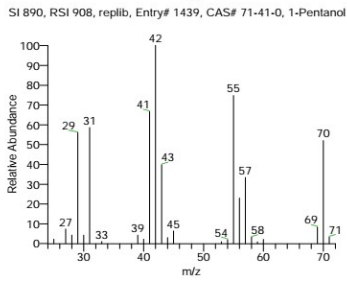


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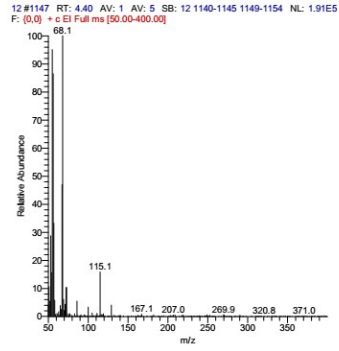
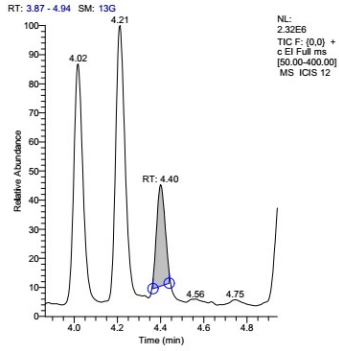
SI 913, RSI 961, replib, Entry# 1438, CAS# 71-41-0, 1-Pentanol Delta Compound Structure



1-Pentanol
Formula C5H12O, MW 88, CAS# 71-41-0, Entry# 1438
Pentyl alcohol



1-Pentanol
Formula C5H12O, MW 88, CAS# 71-41-0, Entry# 1439
Pentyl alcohol



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
4.40	780	878	32.95	mainlib	C5H10O	86
4.40	779	878	31.67	mainlib	C5H10O	86
4.40	770	866	22.99	mainlib	C5H10O	86
4.40	728	808	6.89	replib	C5H10O	86
4.40	744	848	6.89	replib	C5H10O	86

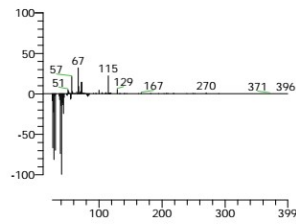
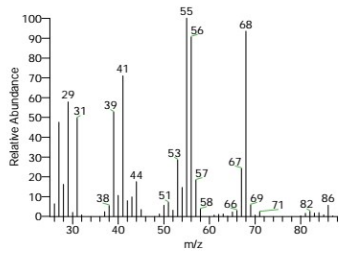


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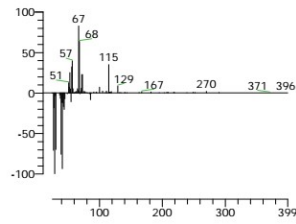
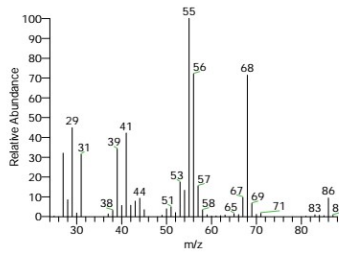
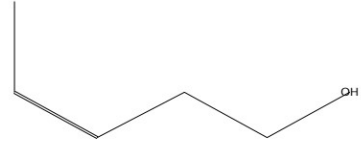
Hit Spectrum

Delta

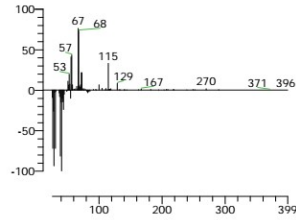
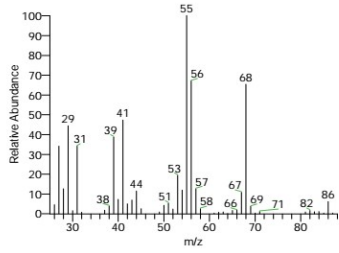
Compound Structure



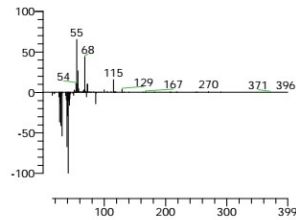
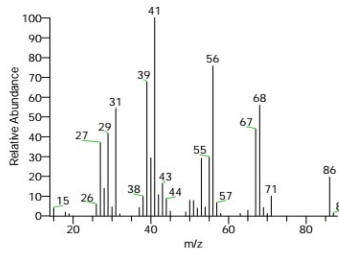
3-Penten-1-ol, (Z)-
Formula C₅H₁₀O, MW 86, CAS# 764-38-5, Entry# 18745
(3Z)-3-Penten-1-ol #



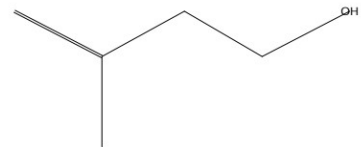
3-Penten-1-ol
Formula C₅H₁₀O, MW 86, CAS# 39161-19-8, Entry# 18574
3-Pentenol



3-Penten-1-ol, (E)-
Formula C₅H₁₀O, MW 86, CAS# 374-37-4, Entry# 18575
trans-3-Pentenol-1



3-Buten-1-ol, 3-methyl-
Formula C₅H₁₀O, MW 86, CAS# 763-32-6, Entry# 1009
Isobutenylcarbinol



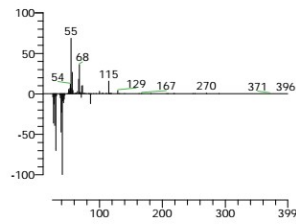
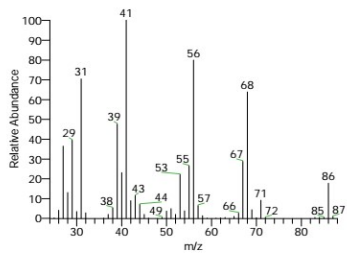


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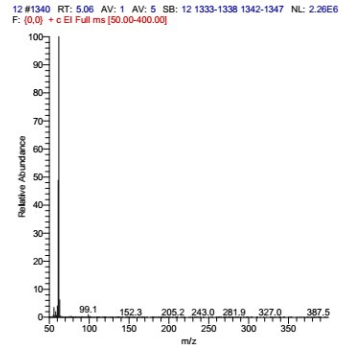
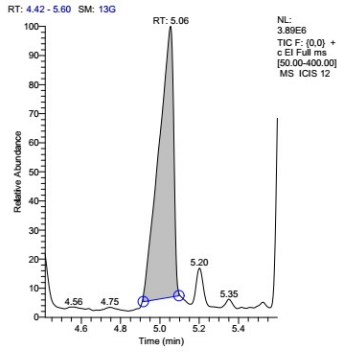
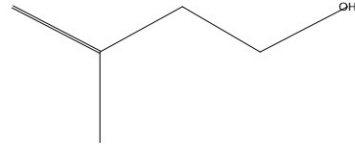
Hit Spectrum

Delta

Compound Structure



3-Buten-1-ol, 3-methyl-
Formula C5H10O, MW 86, CAS# 763-32-6, Entry# 1001
Isobutenylcarbinol

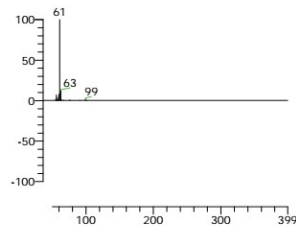
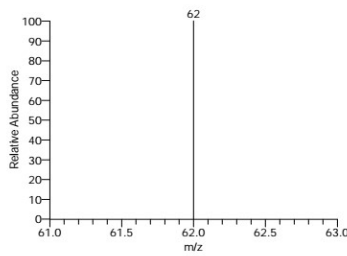


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
5.06	914	999	47.86	nist_msms	KNO3	101
5.06	914	999	47.86	nist_msms	NNaO3	85
5.06	797	831	2.72	replib	C2H6S	62
5.06	763	805	0.99	replib	C2H6O2	62
5.06	774	800	0.99	replib	C2H6O2	62

Hit Spectrum

Delta

Compound Structure



Sodium nitrate
Formula NNaO3, MW 85, CAS# 7631-99-4, Entry# 2074
\$.0617 Ion trap



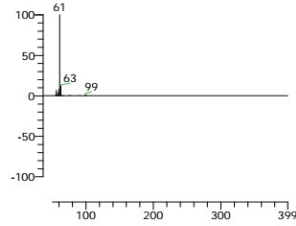
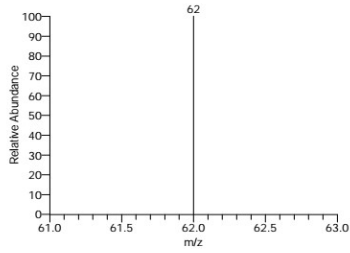


ChemLab Technologies - GC/MS Report

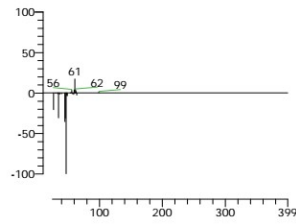
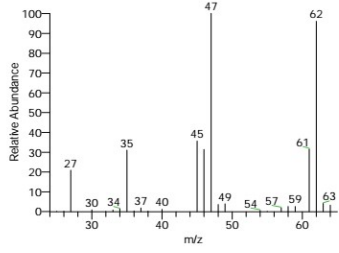
Hit Spectrum

Delta

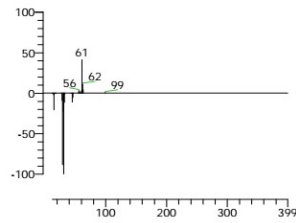
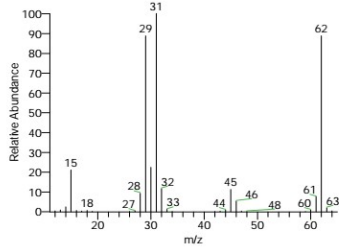
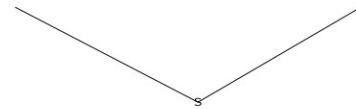
Compound Structure



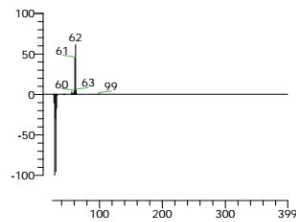
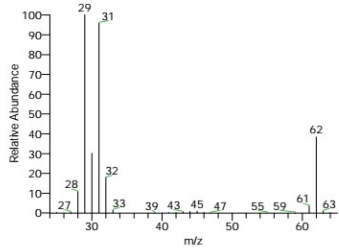
Potassium nitrate
Formula KNO_3 , MW 101, CAS# 7757-79-1, Entry# 2079
\$.0617/ion trap



Dimethyl sulfide
Formula $\text{C}_2\text{H}_6\text{S}$, MW 62, CAS# 75-18-3, Entry# 4066
Methane, thiois-



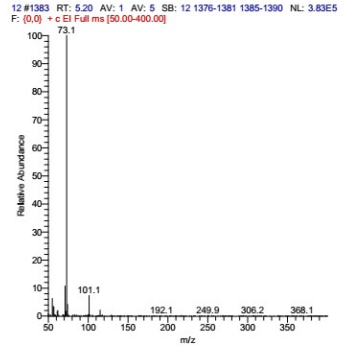
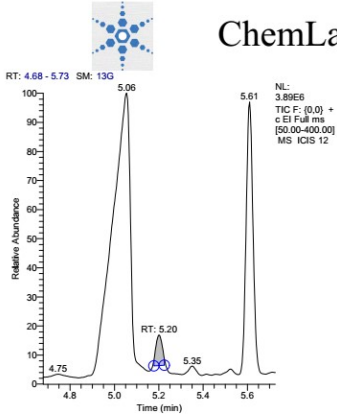
Peroxide, dimethyl
Formula $\text{C}_2\text{H}_6\text{O}_2$, MW 62, CAS# 690-02-8, Entry# 578
Methyl peroxide



Peroxide, dimethyl
Formula $\text{C}_2\text{H}_6\text{O}_2$, MW 62, CAS# 690-02-8, Entry# 159
Methyl peroxide



ChemLab Technologies - GC/MS Report



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
5.20	811	860	55.23	mainlib	C6H12O2	116
5.20	843	893	55.23	replib	C6H12O2	116
5.20	799	889	11.97	mainlib	C6H12O2	116
5.20	792	945	9.17	replib	C3H6O2	74
5.20	776	859	5.28	mainlib	C5H8O3	116

Hit Spectrum	Delta	Compound Structure
		<p>1,3-Dioxolane, 2-(1-methylethyl)- Formula C6H12O2, MW 116, CAS# 822-83-3, Entry# 8924 1,3-Dioxolane, 2-isopropyl-</p>
		<p>1,3-Dioxolane, 2-(1-methylethyl)- Formula C6H12O2, MW 116, CAS# 822-83-3, Entry# 37058 1,3-Dioxolane, 2-isopropyl-</p>
		<p>1,3-Dioxolane, 2-propyl- Formula C6H12O2, MW 116, CAS# 3390-13-4, Entry# 37065 Butanal, cyclic 1,2-ethanediyyl acetal</p>

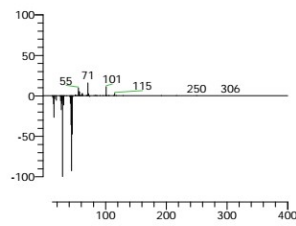
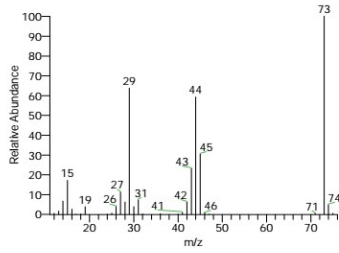


ChemLab Technologies - GC/MS Report

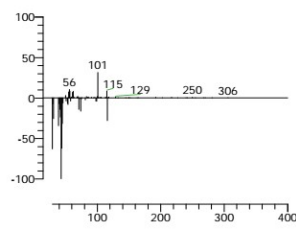
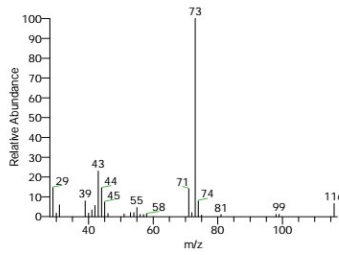
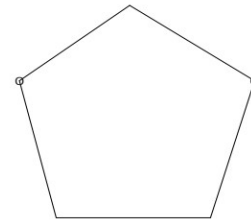
Hit Spectrum

Delta

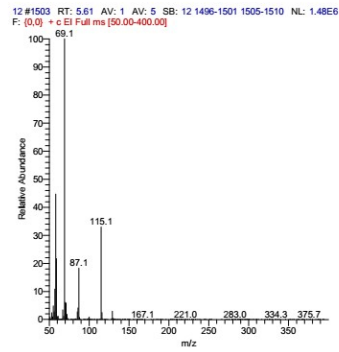
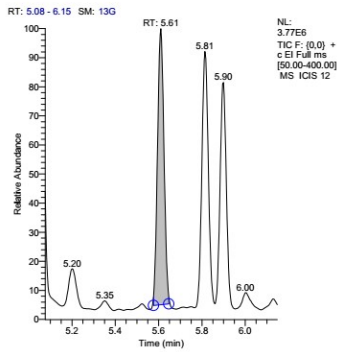
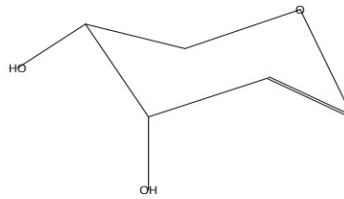
Compound Structure



1,3-Dioxolane
Formula C3H6O2, MW 74, CAS# 646-06-0, Entry# 8899
Ethylene glycol formal



d-Arabinol
Formula C5H8O3, MW 116, CAS# 496-61-7, Entry# 36940



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
5.61	702	716	24.84	mainlib	C9H16O3	172
5.61	674	678	17.54	replib	C8H16O3	160
5.61	692	711	17.54	replib	C8H16O3	160
5.61	688	700	14.82	mainlib	C9H16O3	172
5.61	682	684	11.64	mainlib	C12H22O3	214

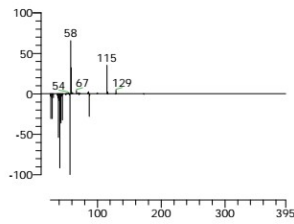
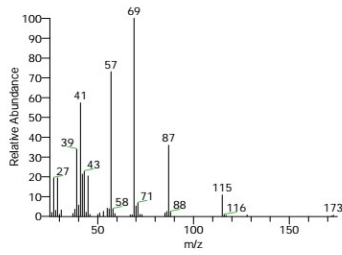


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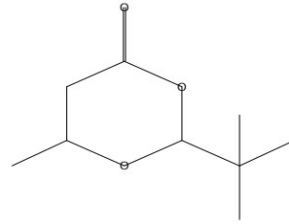
Hit Spectrum

Delta

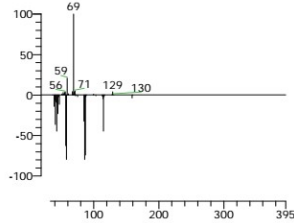
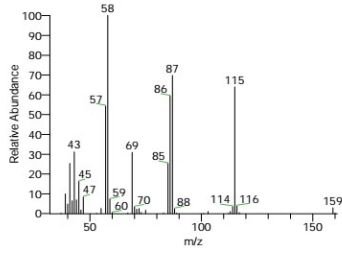
Compound Structure



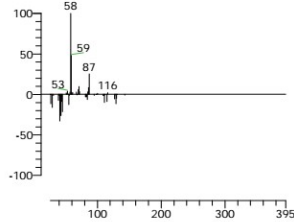
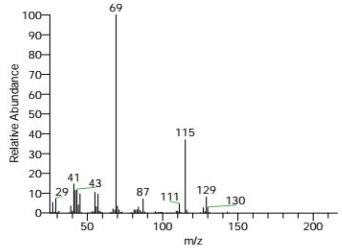
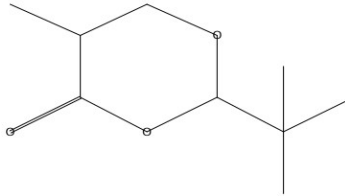
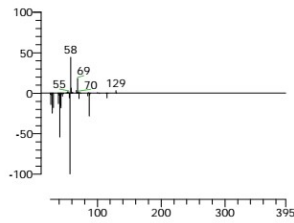
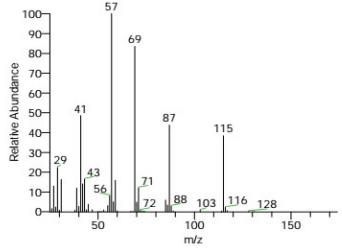
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-6-methyl-
Formula C₉H₁₆O₃, MW 172, CAS# 113505-75-2, Entry# 32217
2-tert-Butyl-6-methyl-1,3-dioxan-4-one #



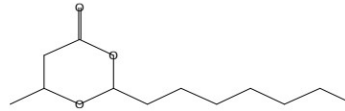
Furan, 2,5-diethoxytetrahydro-
Formula C₈H₁₆O₃, MW 160, CAS# 3320-90-9, Entry# 6616
2,5-Diethoxytetrahydrofuran



1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5-methyl-, (2s-cis)-
Formula C₉H₁₆O₃, MW 172, CAS# 107289-32-7, Entry# 23371
2-tert-Butyl-5-methyl-1,3-dioxan-4-one #



1,3-Dioxan-4-one, 2-heptyl-6-methyl
Formula C₁₂H₂₂O₃, MW 214, CAS# 95902-24-6, Entry# 33005
2-Heptyl-6-methyl-1,3-dioxan-4-one #



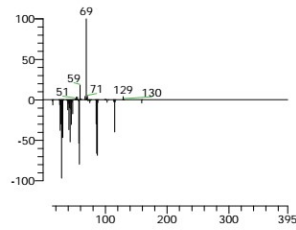
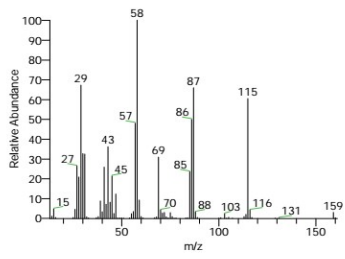


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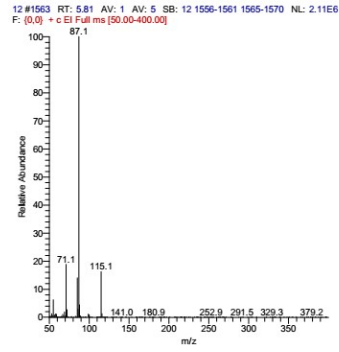
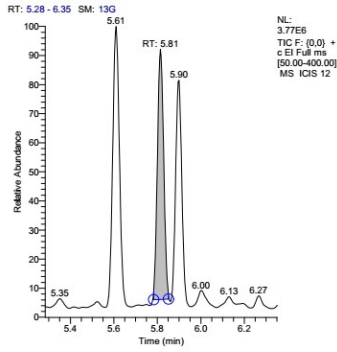
Hit Spectrum

Delta

Compound Structure



Furan, 2,5-diethoxytetrahydro-
Formula C₈H₁₆O₃, MW 160, CAS# 3320-90-9, Entry# 6327
2,5-Diethoxytetrahydrofuran

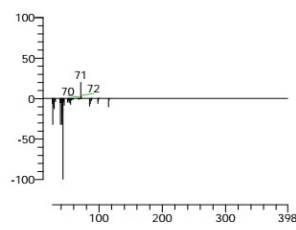
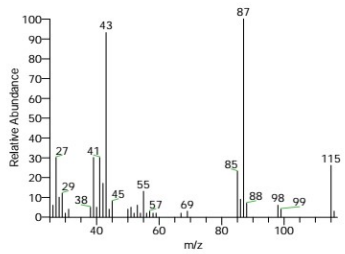


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
5.81	787	849	32.44	mainlib	C ₇ H ₁₄ O ₂	130
5.81	766	789	13.80	mainlib	C ₇ H ₁₄ O ₂	130
5.81	763	769	12.19	replib	C ₈ H ₁₈ O	130
5.81	753	960	8.61	nist_msms	C ₄ H ₄ O ₅	132
5.81	743	745	6.07	mainlib	C ₈ H ₁₈ O	130

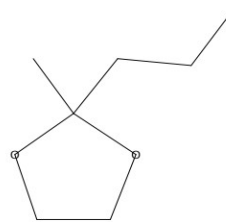
Hit Spectrum

Delta

Compound Structure



1,3-Dioxolane, 2-methyl-2-propyl-
Formula C₇H₁₄O₂, MW 130, CAS# 4352-98-1, Entry# 51871
2-Pentanone, cyclic 1,2-ethanediyf acetal



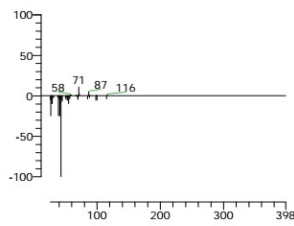
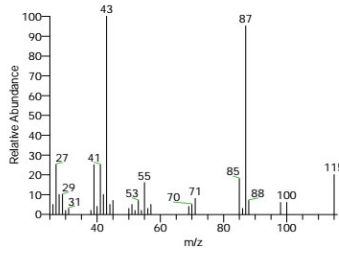


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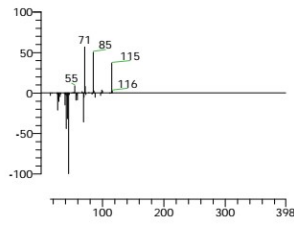
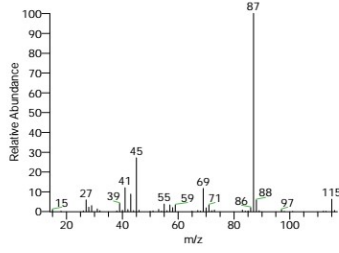
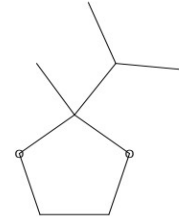
Hit Spectrum

Delta

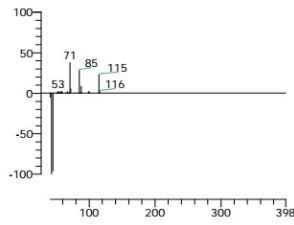
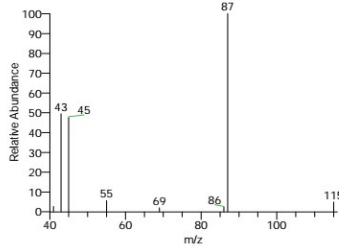
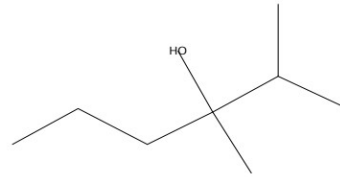
Compound Structure



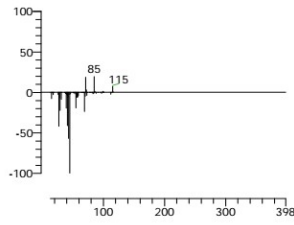
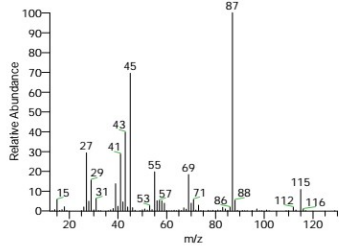
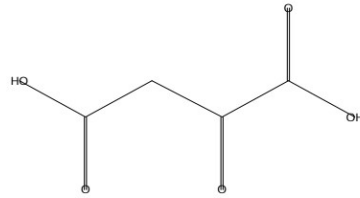
1,3-Dioxolane, 2-methyl-2-(1-methylethyl)-
Formula C7H14O2, MW 130, CAS# 4405-16-7, Entry# 9468
1,3-Dioxolane, 2-isopropyl-2-methyl-



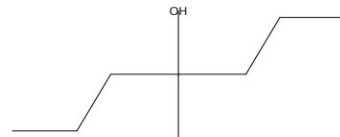
3-Hexanol, 2,3-dimethyl-
Formula C8H18O, MW 130, CAS# 4166-46-5, Entry# 11828
2,3-Dimethyl-3-hexanol



Oxalacetic acid
Formula C4H4O5, MW 132, CAS# 328-42-7, Entry# 14374
\$:06Q-TOF

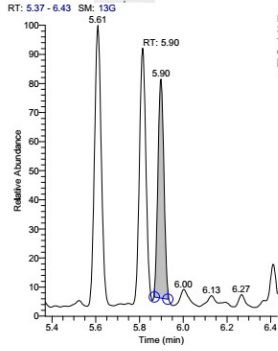


4-Heptanol, 4-methyl-
Formula C8H18O, MW 130, CAS# 598-01-6, Entry# 52013
4-Hydroxy-4-methylheptane



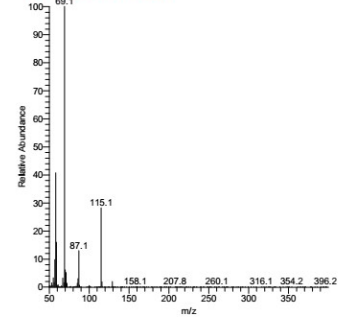


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NL:
3.77E6
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICIS 12

12 #1588 RT: 5.90 AV: 1 AV: 5 SB: 12 1581-1586 1590-1595 NL: 1.38E6
F: (0.0) + c EI Full ms (50.00-400.00)

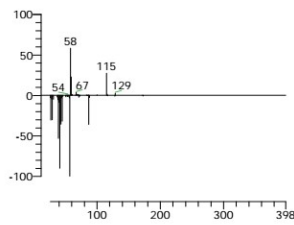
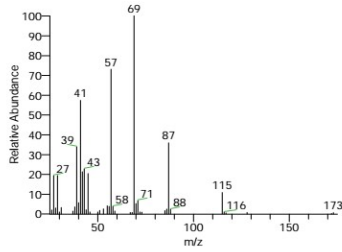


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
5.90	715	726	27.08	mainlib	C9H16O3	172
5.90	704	713	18.58	mainlib	C9H16O3	172
5.90	686	700	9.58	replib	C8H16O3	160
5.90	676	677	6.76	mainlib	C12H22O3	214
5.90	675	685	6.50	replib	C7H16O	116

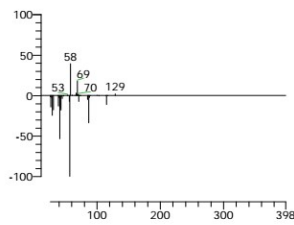
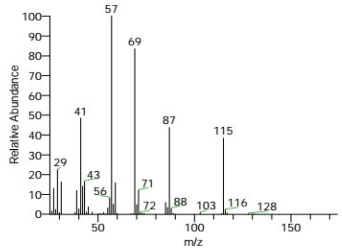
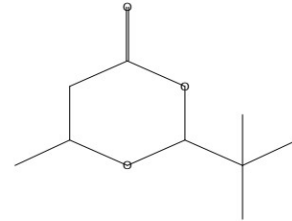
Hit Spectrum

Delta

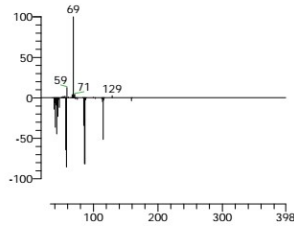
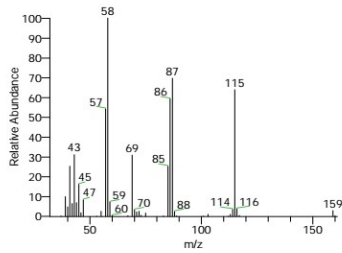
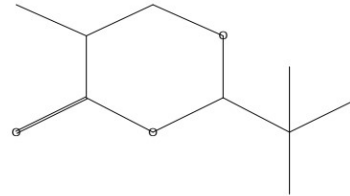
Compound Structure



1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-6-methyl-
Formula C9H16O3, MW 172, CAS# 113505-75-2, Entry# 32217
2-tert-Butyl-6-methyl-1,3-dioxan-4-one #



1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5-methyl-, (2s-cis)-
Formula C9H16O3, MW 172, CAS# 107289-32-7, Entry# 23371
2-tert-Butyl-5-methyl-1,3-dioxan-4-one #



Furan, 2,5-diethoxytetrahydro-
Formula C8H16O3, MW 160, CAS# 3320-90-9, Entry# 6616
2,5-Diethoxytetrahydrofuran



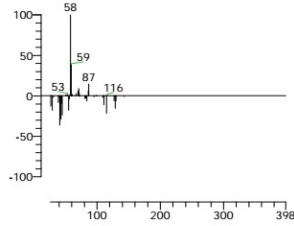
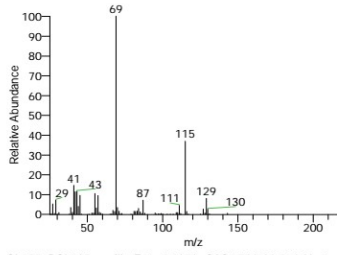


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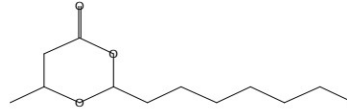
Hit Spectrum

Delta

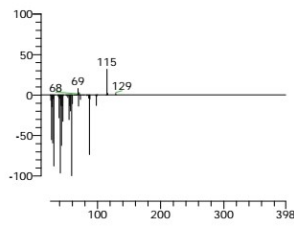
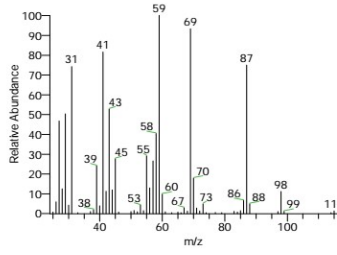
Compound Structure



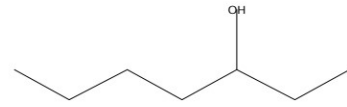
1,3-Dioxan-4-one, 2-heptyl-6-methyl
 Formula C₁₂H₂₂O₃, MW 214, CAS# 99902-24-6, Entry# 33005
 2-Heptyl-6-methyl-1,3-dioxan-4-one #



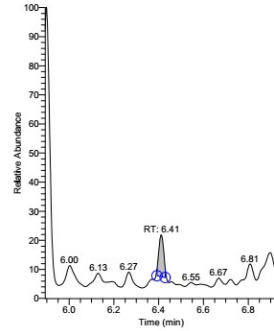
SI 675, RSI 685, replib, Entry# 6979, CAS# 589-82-2, 3-Heptanol



3-Heptanol
 Formula C₇H₁₆O, MW 116, CAS# 589-82-2, Entry# 6979
 3-Hydroxyheptane

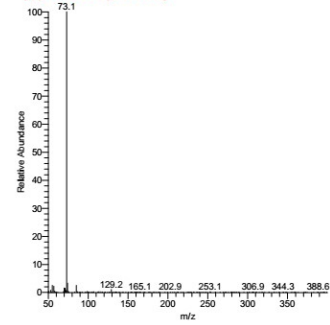


RT: 5.89 - 6.93 SM: 13G



NL:
 3.07E6
 TIC F: (0.0) +
 c EI Full ms
 [50.00-400.00]
 MS ICIS 12

12 #1739 RT: 6.41 AV: 1 AV: 5 SB: 12 1732-1737 1741-1746 NL: 5.39E5
 F: (0.0) + c EI Full ms [50.00-400.00]



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
6.41	903	995	51.00	nist_msms	C ₄ H ₉ NO ₂	103
6.41	876	949	15.00	replib	C ₃ H ₆ O ₂	74
6.41	846	999	4.17	nist_msms	C ₄ H ₁₀ O ₂	90
6.41	846	999	4.17	nist_msms	C ₄ H ₁₁ NO	89
6.41	844	898	3.84	mainlib	C ₄ H ₈ O ₃	104

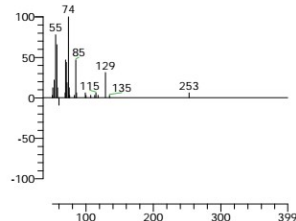
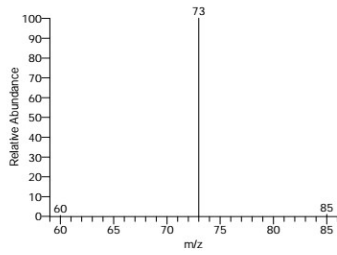


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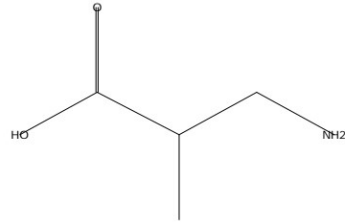
Hit Spectrum

Delta

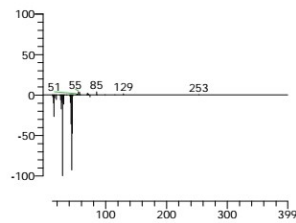
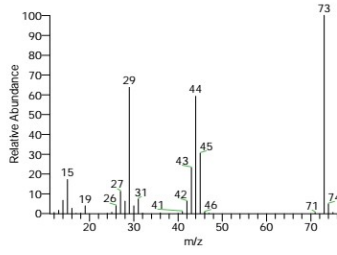
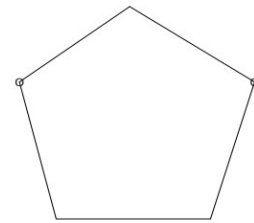
Compound Structure



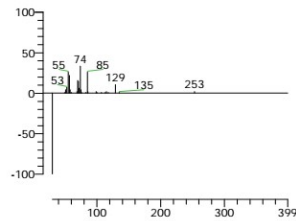
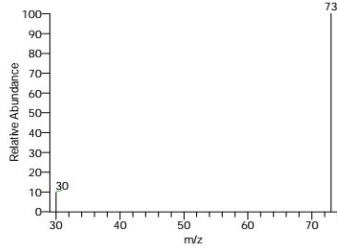
DL-3-Aminoisobutyric acid
Formula C₄H₉NO₂, MW 103, CAS# 144-90-1, Entry# 12270
\$.0617/ion trap



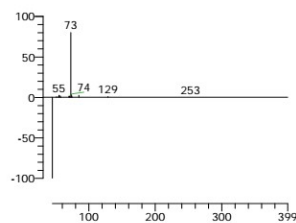
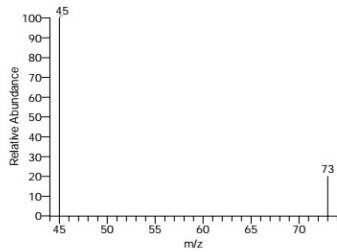
1,3-Dioxolane
Formula C₃H₆O₂, MW 74, CAS# 646-06-0, Entry# 8899
Ethylene glycol formal



4-Amino-1-butanol
Formula C₄H₁₁NO, MW 89, CAS# 13325-10-5, Entry# 11062
\$.0617/ion trap

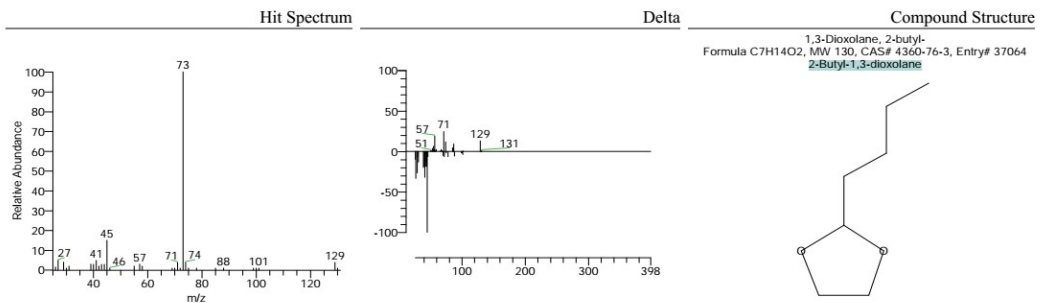
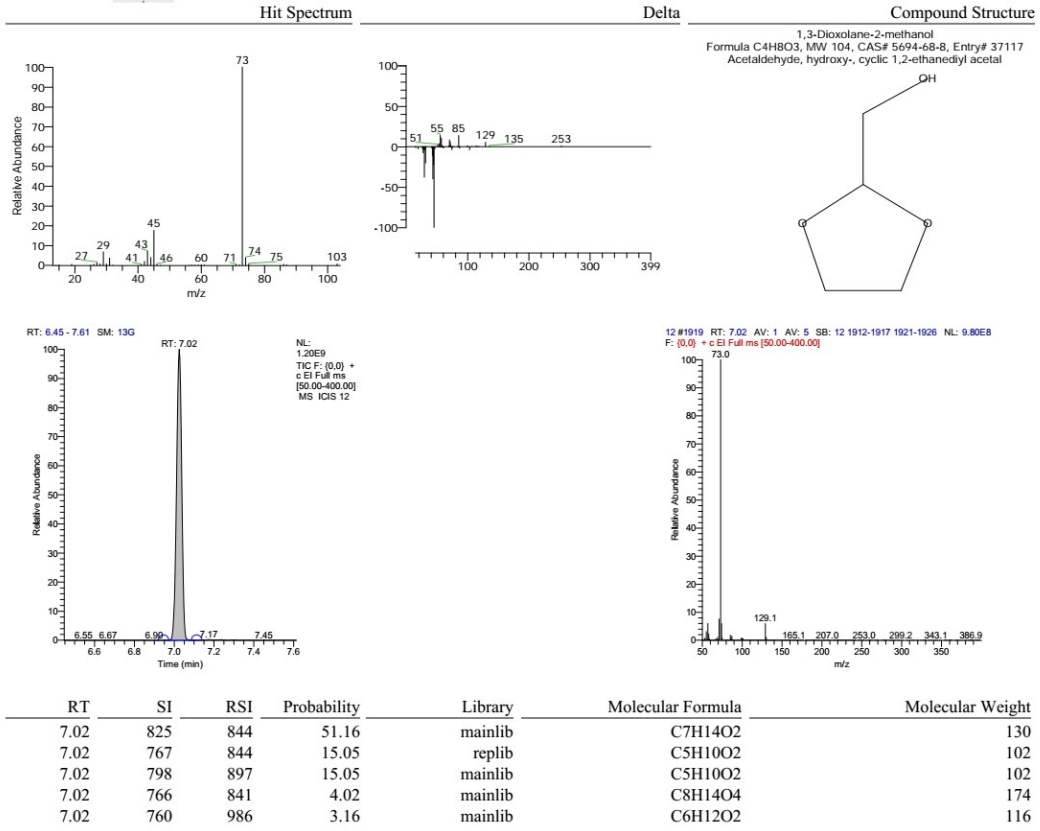


2-Ethoxyethanol
Formula C₄H₁₀O₂, MW 90, CAS# 110-80-5, Entry# 25170
\$.06Q-TOF





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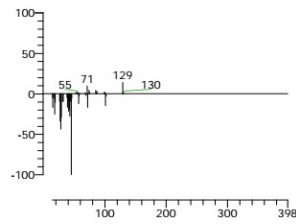
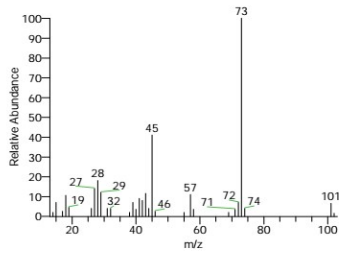


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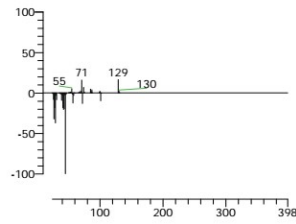
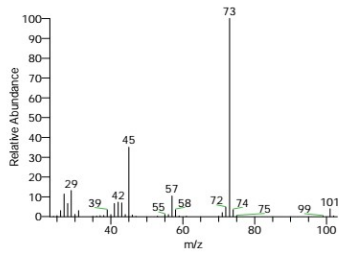
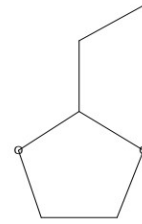
Hit Spectrum

Delta

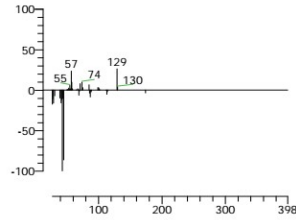
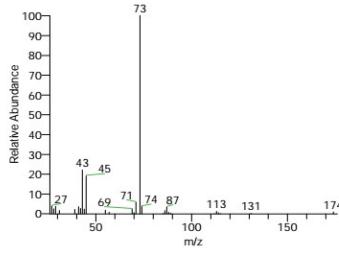
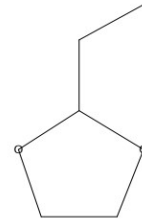
Compound Structure



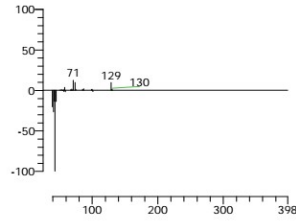
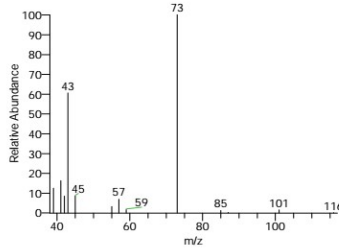
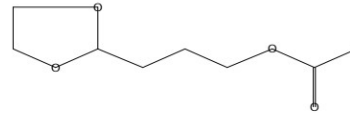
1,3-Dioxolane, 2-ethyl-
Formula C5H10O2, MW 102, CAS# 2568-96-9, Entry# 37066
Propanal, cyclic 1,2-ethanediyil acetal



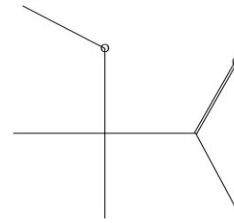
1,3-Dioxolane, 2-ethyl-
Formula C5H10O2, MW 102, CAS# 2568-96-9, Entry# 8959
Propanal, cyclic 1,2-ethanediyil acetal



Acetic acid, 3-[1,3]dioxolan-2-ylpropyl ester
Formula C8H14O4, MW 174, CAS# NA, Entry# 36951
3-(1,3-Dioxolan-2-yl)propyl acetate #

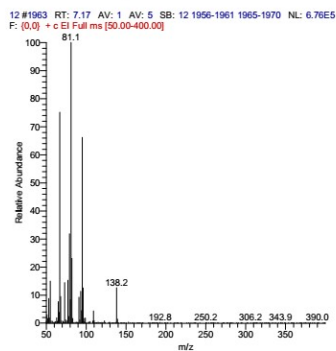
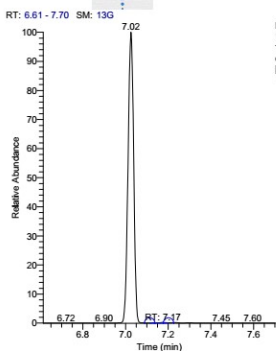


2-Butanone, 3-methoxy-3-methyl-
Formula C6H12O2, MW 116, CAS# 36687-98-6, Entry# 36944
3-Methoxy-3-methyl-2-butanone #





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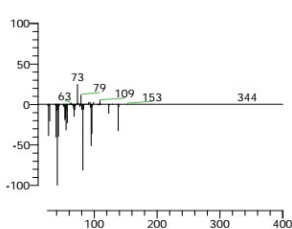
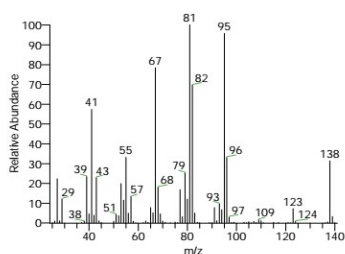


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
7.17	822	825	15.04	mainlib	C10H18	138
7.17	804	821	7.75	mainlib	C10H18	138
7.17	798	817	6.09	mainlib	C10H18	138
7.17	797	819	5.86	replib	C10H18	138
7.17	788	812	4.25	mainlib	C10H18	138

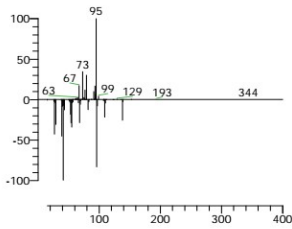
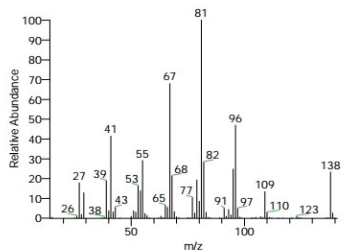
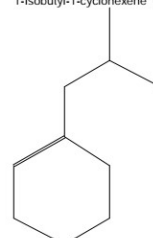
Hit Spectrum

Delta

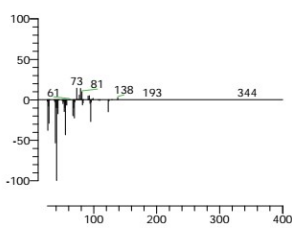
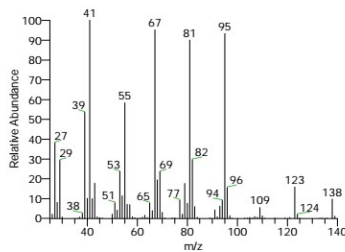
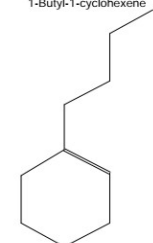
Compound Structure



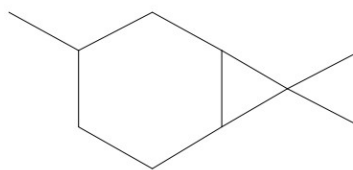
Cyclohexene, 1-(2-methylpropyl)-
Formula C10H18, MW 138, CAS# 3983-03-7, Entry# 45931
1-Isobutyl-1-cyclohexene #



Cyclohexene, 1-butyl-
Formula C10H18, MW 138, CAS# 3282-53-9, Entry# 45677
1-Butyl-1-cyclohexene



Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1a,3a,6a)]-
Formula C10H18, MW 138, CAS# 6069-97-2, Entry# 3035
3,7,7-Trimethylbicyclo[4.1.0]heptane #



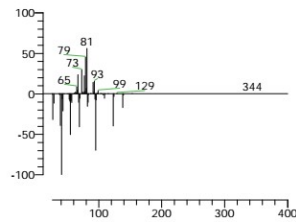
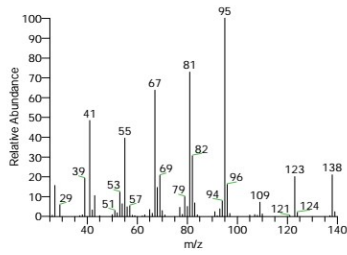


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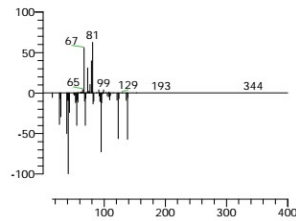
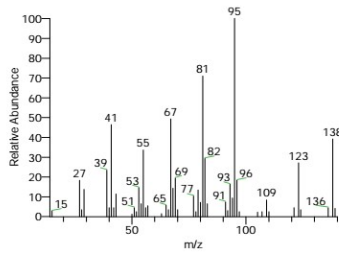
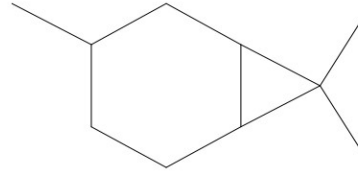
Hit Spectrum

Delta

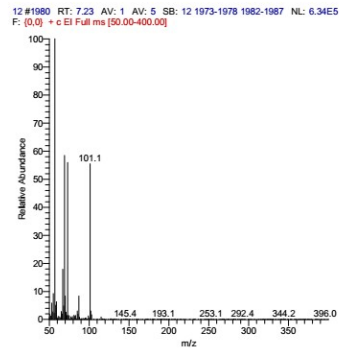
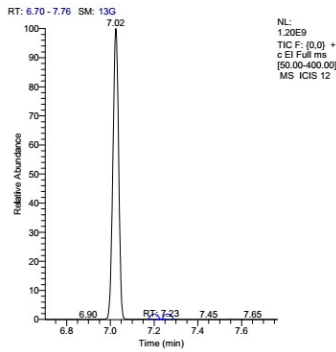
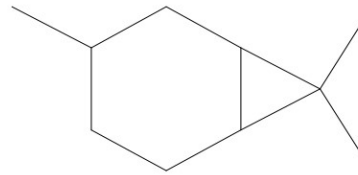
Compound Structure



Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-
Formula C10H18, MW 138, CAS# 554-59-6, Entry# 13537
Carane



Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1a,3a,6a)]-
Formula C10H18, MW 138, CAS# 2778-68-9, Entry# 61997
Carane, (1S,3S,6R)-(-)-



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
7.23	694	696	19.21	mainlib	C9H14O5	202
7.23	692	709	17.72	mainlib	C10H22O	158
7.23	661	688	10.20	replib	C8H18O	130
7.23	676	676	10.20	replib	C8H18O	130
7.23	665	683	7.00	mainlib	C10H22O4S	238

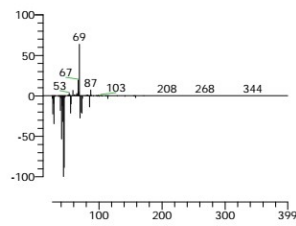
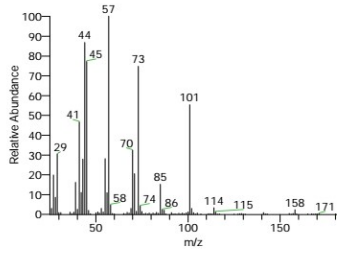


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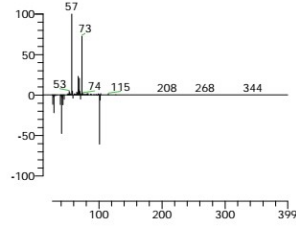
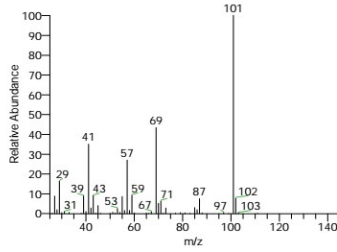
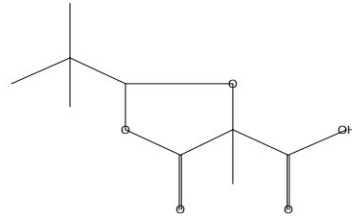
Hit Spectrum

Delta

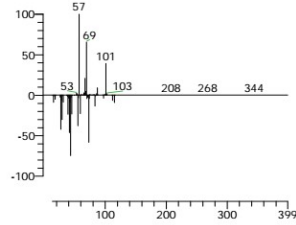
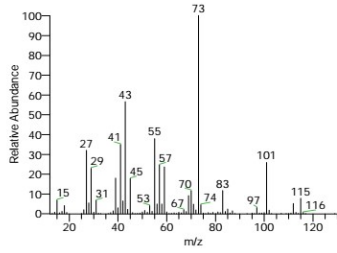
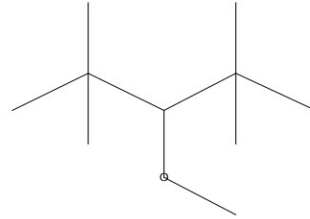
Compound Structure



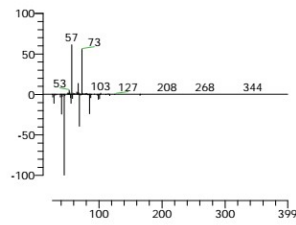
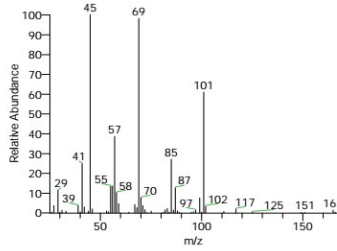
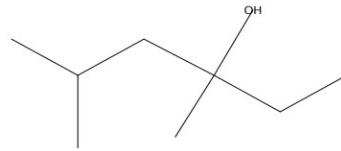
2-tert-Butyl-4-methyl-5-oxo-1,3-dioxolane-4-carboxylic acid
Formula C₉H₁₄O₅, MW 202, CAS# NA, Entry# 22882
2-tert-Butyl-4-methyl-5-oxo-1,3-dioxolane-4-carboxylic acid #



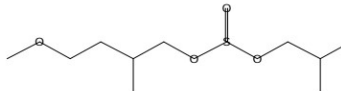
Pentane, 2,2,4,4-tetramethyl-3-methoxy-
Formula C₁₀H₂₂O, MW 158, CAS# NA, Entry# 67348
3-Methoxy-2,2,4,4-tetramethylpentane #



3-Hexanol, 3,5-dimethyl-
Formula C₈H₁₈O, MW 130, CAS# 4209-91-0, Entry# 8934
3,5-Dimethyl-3-hexanol



Sulfurous acid, isobutyl 2-methyl-4-methoxybutyl ester
Formula C₁₀H₂₂O₄S, MW 238, CAS# NA, Entry# 16114



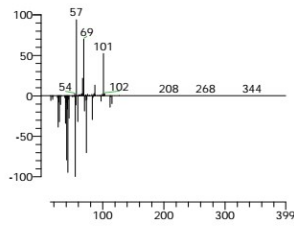
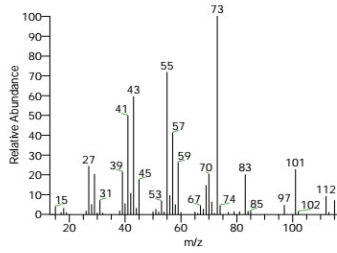


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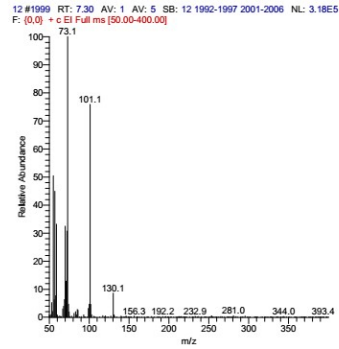
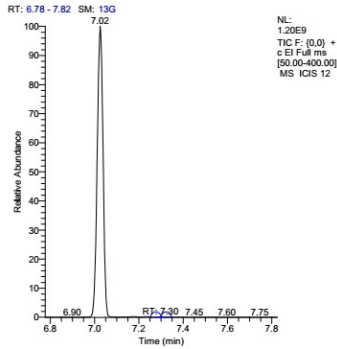
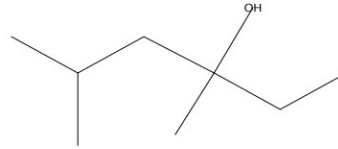
Hit Spectrum

Delta

Compound Structure



3-Hexanol, 3,5-dimethyl-
Formula C₈H₁₈O, MW 130, CAS# 4209-91-0, Entry# 9008
3,5-Dimethyl-3-hexanol

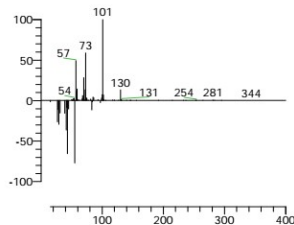
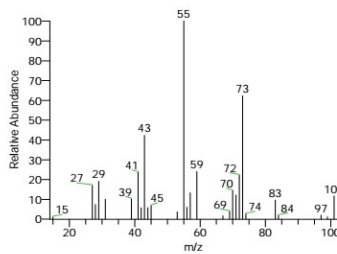


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
7.30	744	825	38.96	mainlib	C ₉ H ₂₀ O	144
7.30	717	746	11.46	replib	C ₈ H ₁₈ O	130
7.30	708	765	8.55	replib	C ₉ H ₂₀ O	144
7.30	709	723	8.55	mainlib	C ₉ H ₂₀ O	144
7.30	695	707	5.35	mainlib	C ₉ H ₁₄ O ₅	202

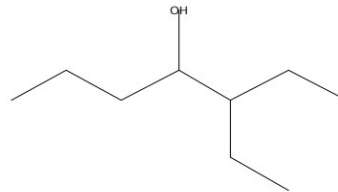
Hit Spectrum

Delta

Compound Structure



4-Heptanol, 3-ethyl-
Formula C₉H₂₀O, MW 144, CAS# 19780-42-8, Entry# 19080
3-Ethyl-4-heptanol



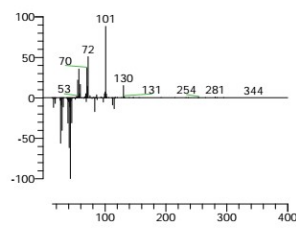
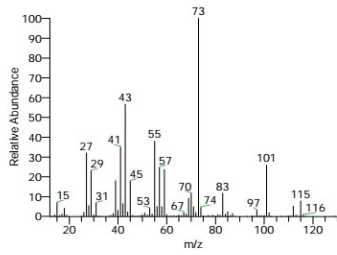


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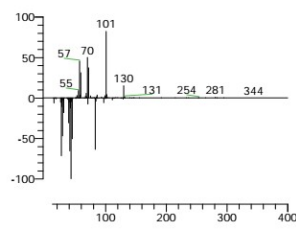
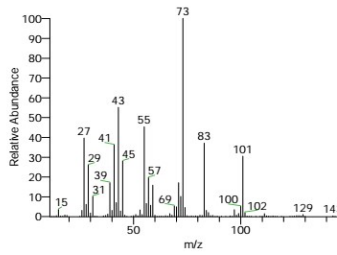
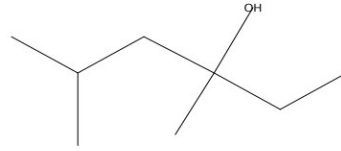
Hit Spectrum

Delta

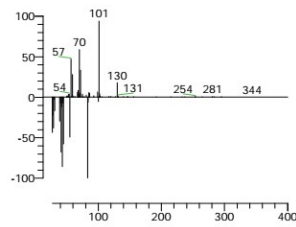
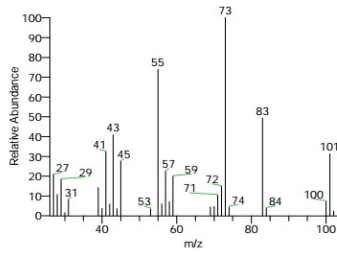
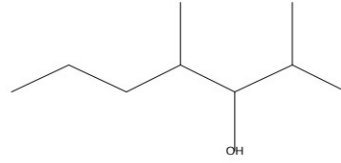
Compound Structure



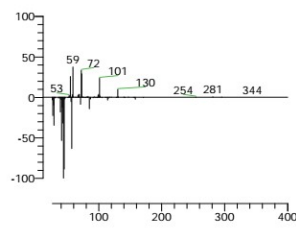
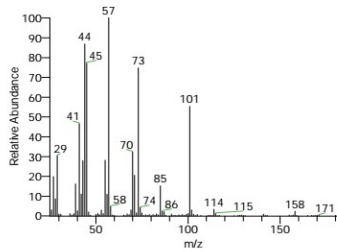
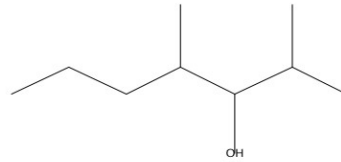
3-Hexanol, 3,5-dimethyl-
Formula C₈H₁₈O, MW 130, CAS# 4209-91-0, Entry# 8934
3,5-Dimethyl-3-hexanol



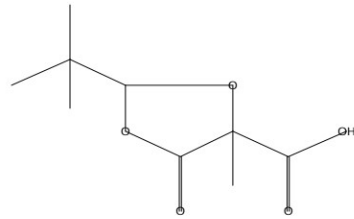
3-Heptanol, 2,4-dimethyl-
Formula C₉H₂₀O, MW 144, CAS# 19549-72-5, Entry# 36963
2,4-Dimethyl-3-heptanol



3-Heptanol, 2,4-dimethyl-
Formula C₉H₂₀O, MW 144, CAS# 19549-72-5, Entry# 9012
2,4-Dimethyl-3-heptanol

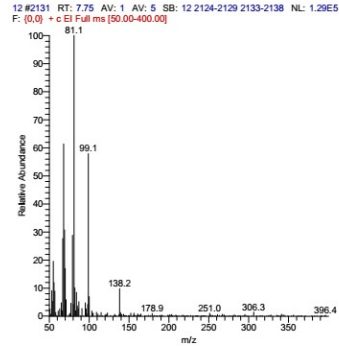
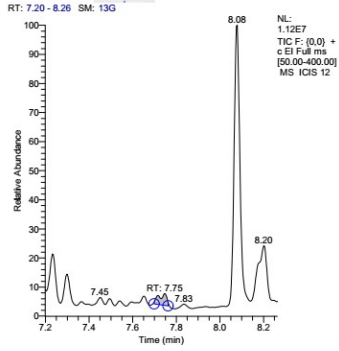


2-tert-Butyl-4-methyl-5-oxo-1,3-dioxolane-4-carboxylic acid #
Formula C₉H₁₄O₅, MW 202, CAS# NA, Entry# 22882
2-tert-Butyl-4-methyl-5-oxo-1,3-dioxolane-4-carboxylic acid #





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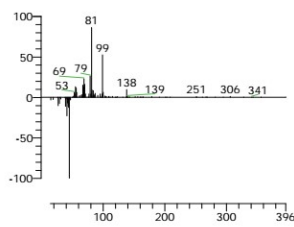
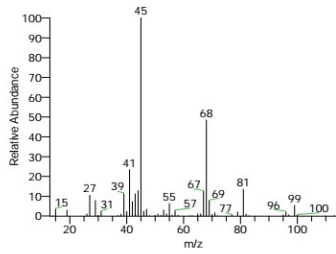


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
7.75	637	703	10.45	replib	C7H14O	114
7.75	652	752	10.45	mainlib	C7H14O	114
7.75	633	679	5.39	mainlib	C10H20O	156
7.75	634	688	5.39	replib	C10H20O	156
7.75	630	683	4.55	mainlib	C10H20O	156

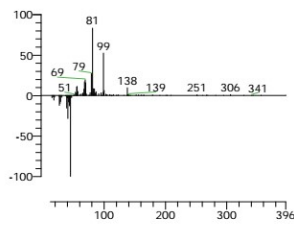
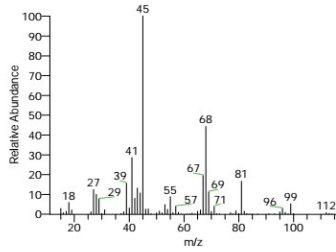
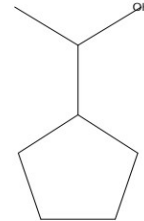
Hit Spectrum

Delta

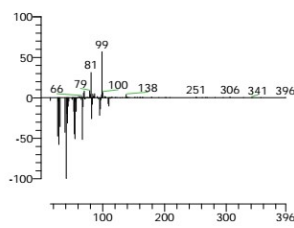
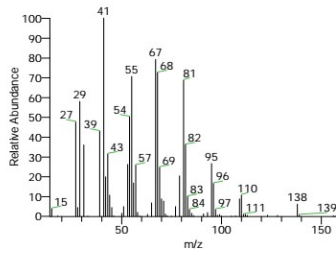
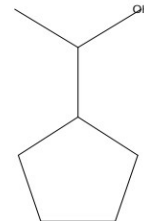
Compound Structure



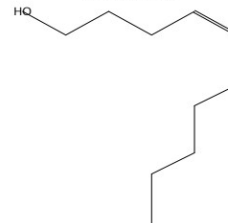
Cyclopentanemethanol, 3-methyl-
Formula C7H14O, MW 114, CAS# 52829-98-8, Entry# 16093
1-Cyclopentylethanol



Cyclopentanemethanol, 3-methyl-
Formula C7H14O, MW 114, CAS# 52829-98-8, Entry# 3910
1-Cyclopentylethanol



(Z)-4-Decen-1-ol
Formula C10H20O, MW 156, CAS# 57074-37-0, Entry# 1090
cis-4-Decen-1-ol



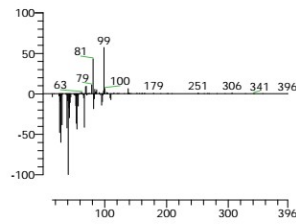
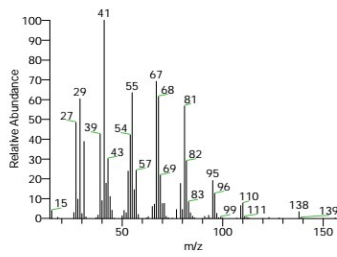


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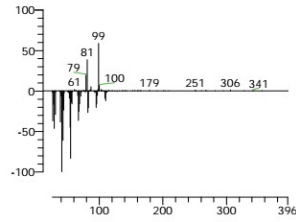
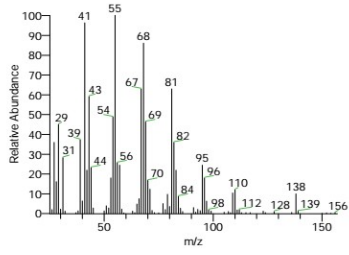
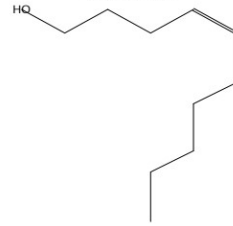
Hit Spectrum

Delta

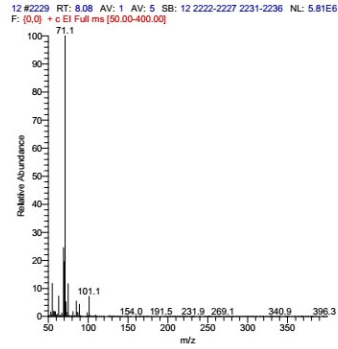
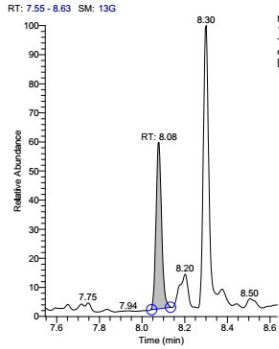
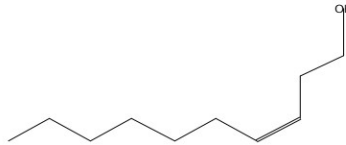
Compound Structure



(Z)-4-Decen-1-ol
Formula C10H20O, MW 156, CAS# 57074-37-0, Entry# 3002
cis-4-Decen-1-ol



3-Decen-1-ol, (Z)-
Formula C10H20O, MW 156, CAS# 10340-22-4, Entry# 17967
cis-3-Decen-1-ol



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.08	734	797	29.84	replib	C10H22O	158
8.08	720	775	29.84	mainlib	C10H22O	158
8.08	747	800	29.84	replib	C10H22O	158
8.08	717	796	8.29	replib	C10H22O	158
8.08	711	780	6.52	mainlib	C9H18O	142



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Hit Spectrum	Delta	Compound Structure	
SI 747, RSI 800, replib, Entry# 8599, CAS# 693-65-2, n-Amyl ether			n-Amyl ether Formula C ₁₀ H ₂₂ O, MW 158, CAS# 693-65-2, Entry# 8599 Pentane, 1,1'-oxybis- <chem>CCCCCOCCCC</chem>
SI 734, RSI 797, replib, Entry# 2568, CAS# 693-65-2, n-Amyl ether			n-Amyl ether Formula C ₁₀ H ₂₂ O, MW 158, CAS# 693-65-2, Entry# 2568 Pentane, 1,1'-oxybis- <chem>CCCCCOCCCC</chem>
			n-Amyl ether Formula C ₁₀ H ₂₂ O, MW 158, CAS# 693-65-2, Entry# 35145 Pentane, 1,1'-oxybis- <chem>CCCCCOCCCC</chem>
			Butane, 1,1'-oxybis[3-methyl-] Formula C ₁₀ H ₂₂ O, MW 158, CAS# 544-01-4, Entry# 8594 Isopentyl ether <chem>CC(C)CCOC(C)C</chem>

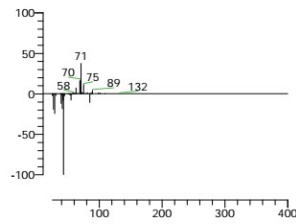
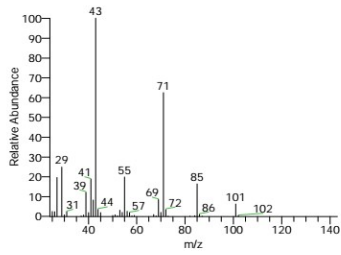


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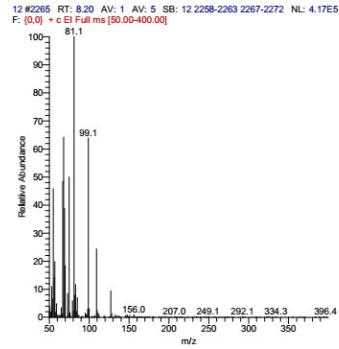
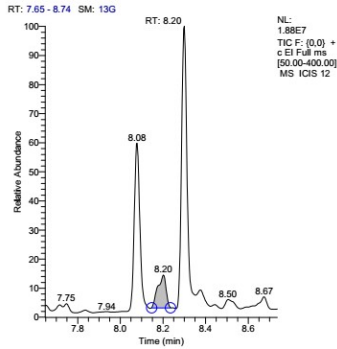
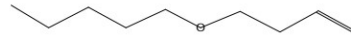
Hit Spectrum

Delta

Compound Structure



Ether, 3-butenyl pentyl
Formula C₉H₁₈O, MW 142, CAS# 34061-78-4, Entry# 8274
3-Butenyl pentyl ether #

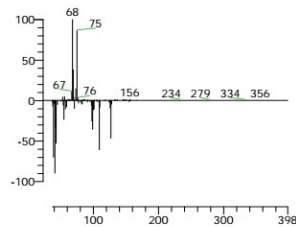
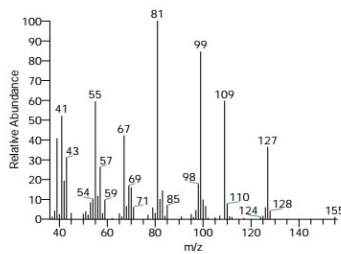


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.20	741	800	44.61	mainlib	C ₁₀ H ₂₀ O	156
8.20	646	655	3.61	mainlib	C ₉ H ₁₄ O ₂	154
8.20	635	682	2.47	mainlib	C ₉ H ₁₈ O	142
8.20	635	693	2.47	mainlib	C ₈ H ₁₅ NO ₃	173
8.20	631	687	2.09	mainlib	C ₁₀ H ₁₈ O ₂	170

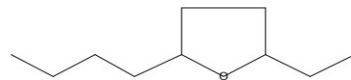
Hit Spectrum

Delta

Compound Structure



Tetrahydrofuran, 2-ethyl-5-butyl-
Formula C₁₀H₂₀O, MW 156, CAS# 164584-36-5, Entry# 46058
2-Butyl-5-ethyltetrahydrofuran #



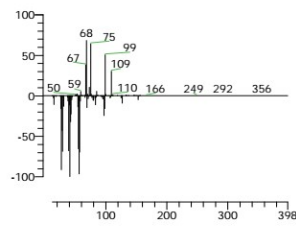
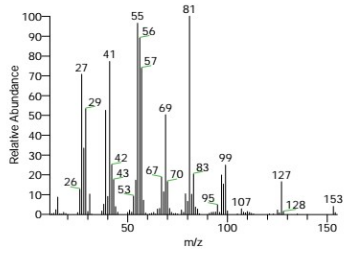


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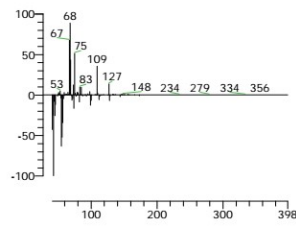
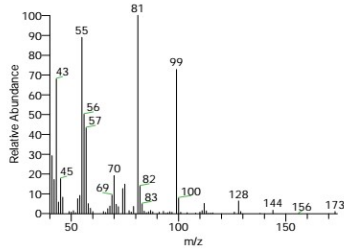
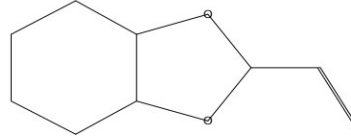
Hit Spectrum

Delta

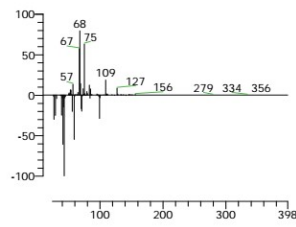
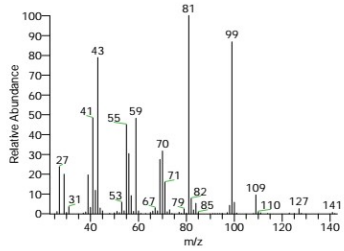
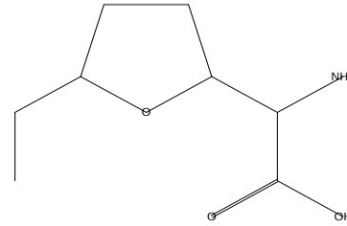
Compound Structure



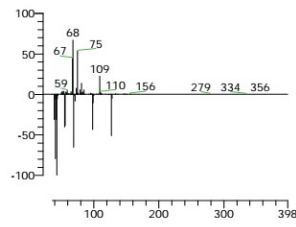
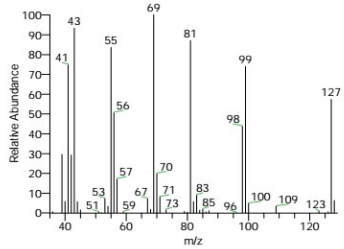
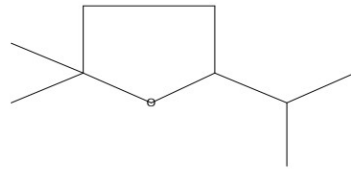
1,3-Benzodioxole, 2-ethenylhexahydro-
Formula C₉H₁₄O₂, MW 154, CAS# 55702-63-1, Entry# 45543
2-Vinylhexahydro-1,3-benzodioxole #



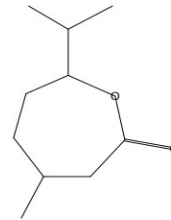
Δ-[5-Ethyl-2,3,4,5-tetrahydro-2-furyl]glycine
Formula C₈H₁₅NO₃, MW 173, CAS# NA, Entry# 45571
2-Amino-3,6-anhydro-2,4,5-trideoxy-6-ethylhexonic acid #



Furan, tetrahydro-2,2-dimethyl-5-(1-methylethyl)-
Formula C₉H₁₈O, MW 142, CAS# 97265-00-4, Entry# 46050
5-Isopropyl-2,2-dimethyltetrahydrofuran #

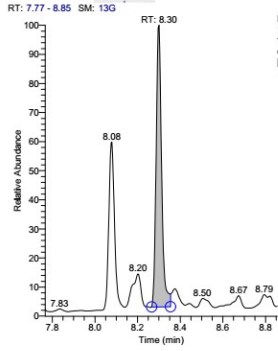


2-Oxepanone, 4-methyl-7-(1-methylethyl)-
Formula C₁₀H₁₈O₂, MW 170, CAS# 499-54-7, Entry# 31881
3-Methyl-6-isopropyl-6-hexanolide



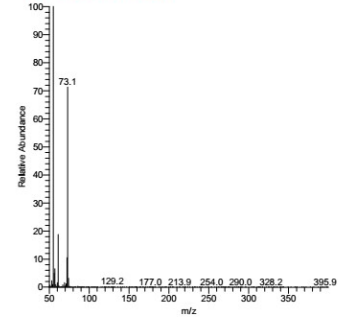


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NL: 1.88E7
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICS 12

12 #2294 RT: 8.30 AV: 1 AV: 5 SB: 12 2287-2292 2296-2301 NL: 9.75E6
F: (0.0) + c EI Full ms (50.00-400.00)

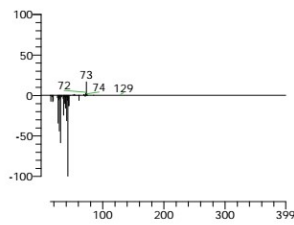
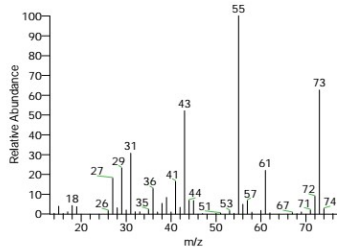


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.30	884	884	75.21	mainlib	C5H12O2	104
8.30	931	933	75.21	replib	C5H12O2	104
8.30	853	901	11.87	mainlib	C7H16O	116
8.30	865	917	11.87	replib	C7H16O	116
8.30	847	901	6.12	replib	C7H16O	116

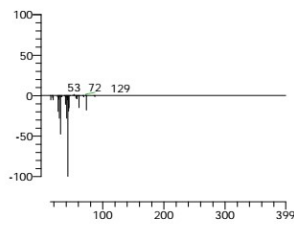
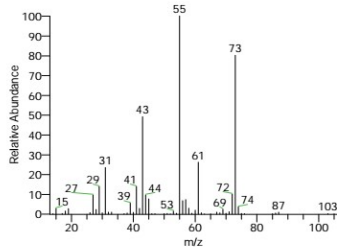
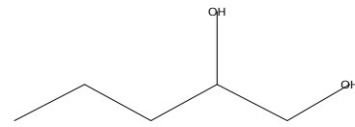
Hit Spectrum

Delta

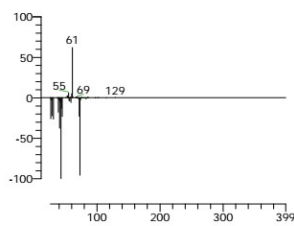
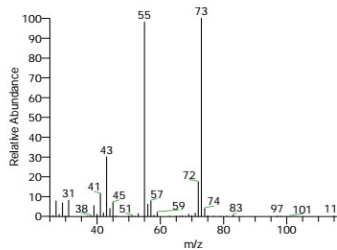
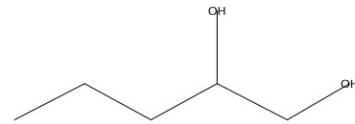
Compound Structure



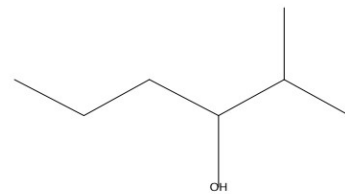
1,2-Pentanediol
Formula C5H12O2, MW 104, CAS# 5343-92-0, Entry# 4801



1,2-Pentanediol
Formula C5H12O2, MW 104, CAS# 5343-92-0, Entry# 19085



3-Hexanol, 2-methyl-
1-isopropyl-1-butanol
Formula C7H16O, MW 116, CAS# 617-29-8, Entry# 9005



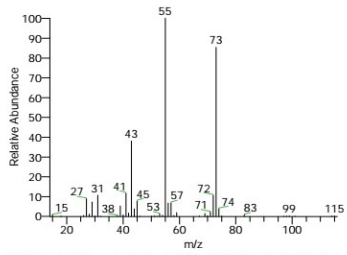


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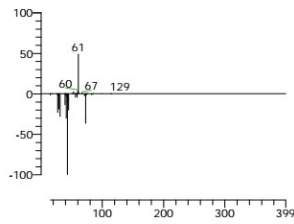
Hit Spectrum

Delta

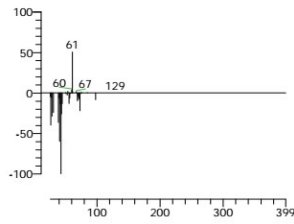
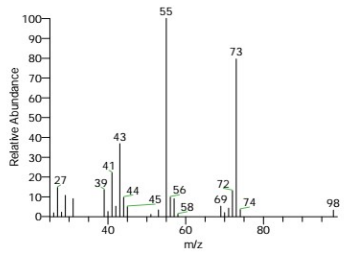
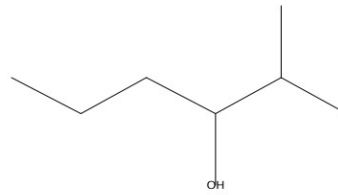
Compound Structure



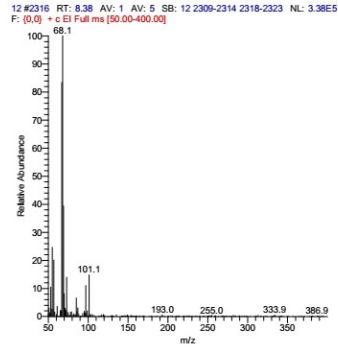
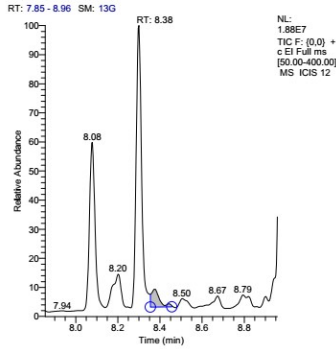
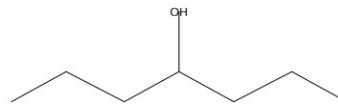
SI 847, RSI 901, replib, Entry# 4803, CAS# 589-55-9, 4-Heptanol



3-Hexanol, 2-methyl-1-isopropyl-1-butanol
Formula C7H16O, MW 116, CAS# 617-29-8, Entry# 19081



4-Heptanol
Formula C7H16O, MW 116, CAS# 589-55-9, Entry# 4803
Dipropylcarbinol



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.38	708	792	29.11	mainlib	C10H18O	154
8.38	703	795	23.46	mainlib	C10H18O3	186
8.38	679	803	7.86	replib	C10H18O	154
8.38	677	752	7.25	mainlib	C7H9F3O2	182
8.38	664	742	4.68	mainlib	C10H18O3	186

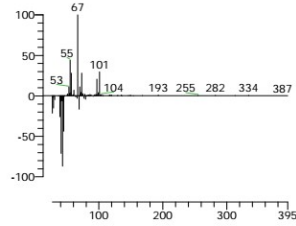
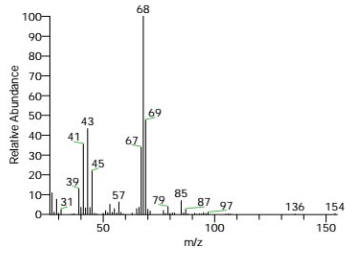


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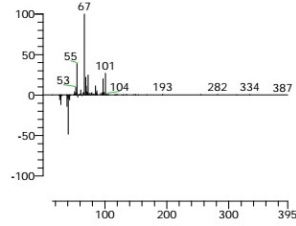
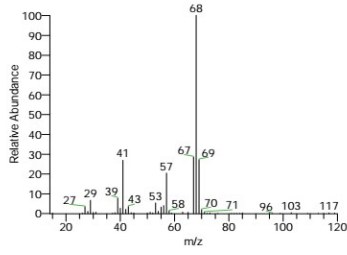
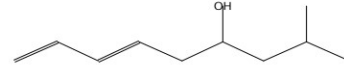
Hit Spectrum

Delta

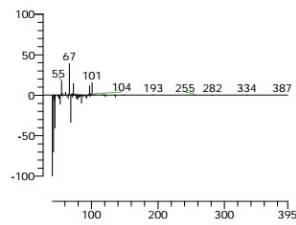
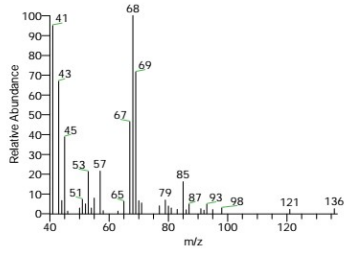
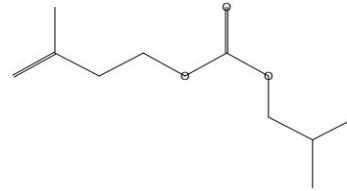
Compound Structure



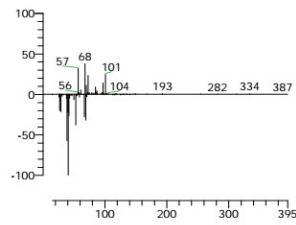
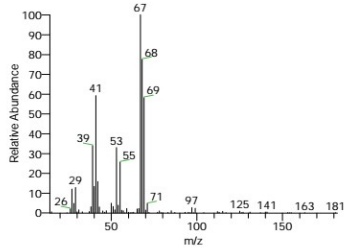
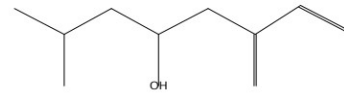
1,3-Nonadien-6-ol, 8-methyl-
Formula C₁₀H₁₈O, MW 154, CAS# NA, Entry# 30766
(6E)-2-Methyl-6,8-nonadien-4-ol #



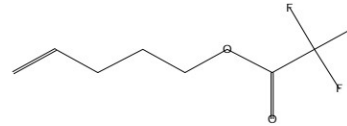
Isobutyl 3-methylbut-3-enyl carbonate
Formula C₁₀H₁₈O₃, MW 186, CAS# NA, Entry# 30712



7-Octen-4-ol, 2-methyl-6-methylene-, (S)-
Formula C₁₀H₁₈O, MW 154, CAS# 35628-05-8, Entry# 7820
7-Octen-4-ol, 2-methyl-6-methylene-, (-)-



4-Penten-1-ol, trifluoroacetate
Formula C₇H₉F₃O₂, MW 182, CAS# NA, Entry# 29969



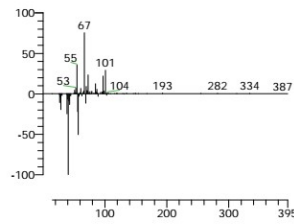
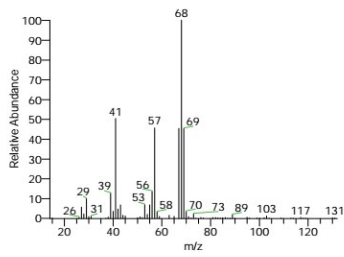


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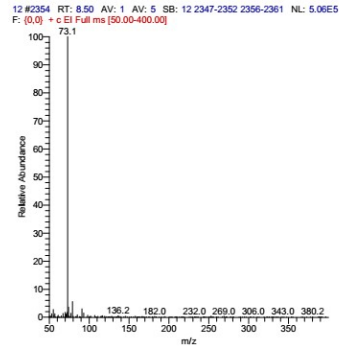
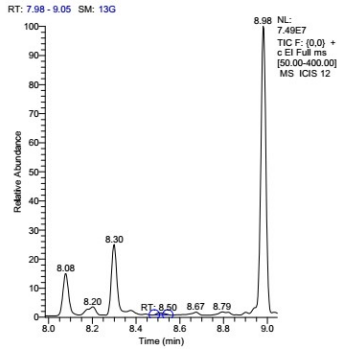
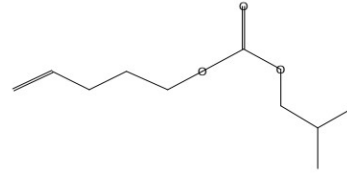
Hit Spectrum

Delta

Compound Structure



Isobutyl pent-4-enyl carbonate
Formula C10H18O3, MW 186, CAS# NA, Entry# 30568

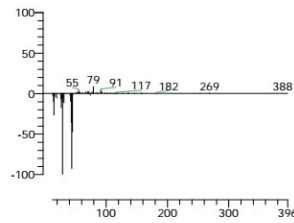
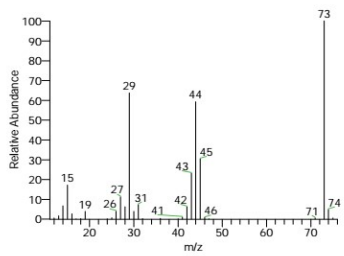


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.50	798	963	30.33	replib	C3H6O2	74
8.50	769	877	8.59	mainlib	C6H14O	102
8.50	762	818	6.58	mainlib	C10H16O2	168
8.50	758	932	5.56	nist_msms	C4H10O2	90
8.50	755	879	4.91	mainlib	C10H16BrCl3O2	352

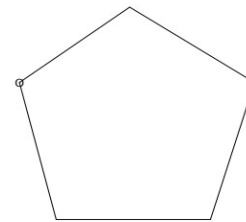
Hit Spectrum

Delta

Compound Structure



1,3-Dioxolane
Formula C3H6O2, MW 74, CAS# 646-06-0, Entry# 8899
Ethylene glycol formal



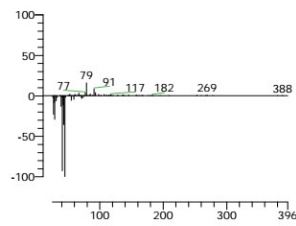
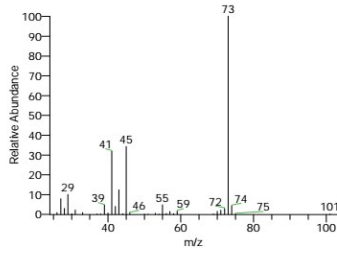


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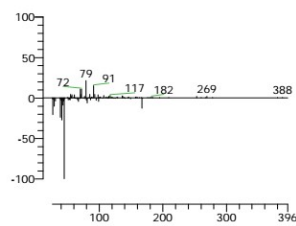
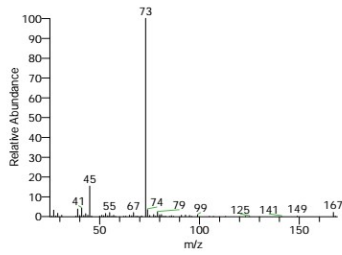
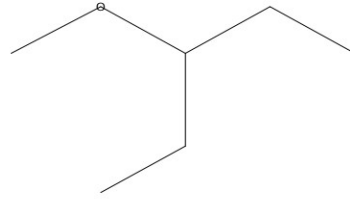
Hit Spectrum

Delta

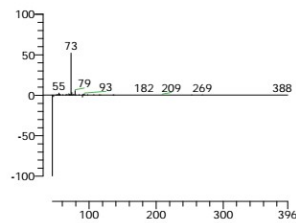
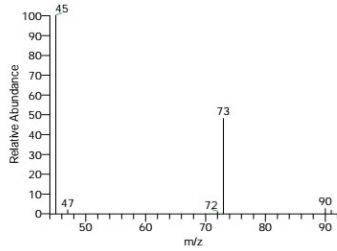
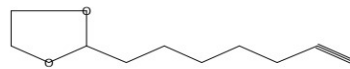
Compound Structure



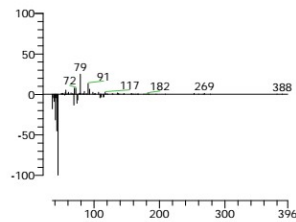
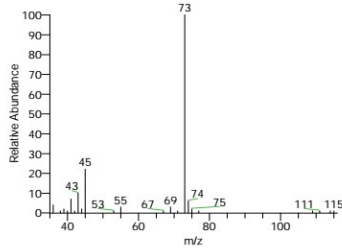
Pentane, 3-methoxy-
Formula C₆H₁₄O, MW 102, CAS# 36839-67-5, Entry# 37087
1-Ethylpropyl methyl ether



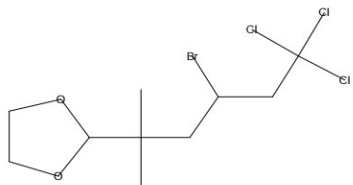
1,3-Dioxolane, 2-(6-heptynyl)-
Formula C₁₀H₁₆O₂, MW 168, CAS# 25595-82-8, Entry# 37084
2-(6-Heptynyl)-1,3-dioxolane #



2-Ethoxyethanol
Formula C₄H₁₀O₂, MW 90, CAS# 110-80-5, Entry# 25158
\$.06Q-TOF

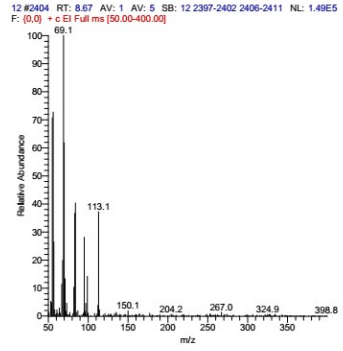
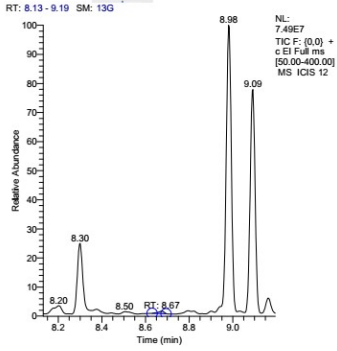


1,3-Dioxolane, 2-(3-bromo-5,5,5-trichloro-2,2-dimethylpentyl)-
Formula C₁₀H₁₆BrCl₃O₂, MW 352, CAS# NA, Entry# 37089
2-(3-Bromo-5,5,5-trichloro-1,1-dimethylpentyl)-1,3-dioxolane #





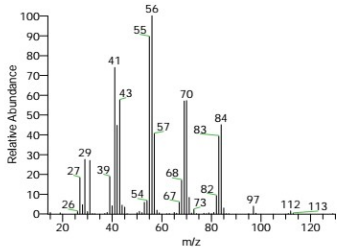
ChemLab Technologies - GC/MS Report



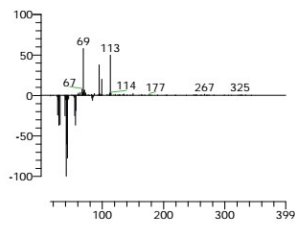
RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.67	686	801	8.78	replib	C8H18O	130
8.67	696	758	8.78	replib	C8H18O	130
8.67	700	784	8.78	replib	C8H18O	130
8.67	698	759	8.09	mainlib	C10H17F3O2	226
8.67	691	818	6.20	mainlib	C8H16	112

Hit Spectrum

SI 700, RSI 784, replib, Entry# 5209, CAS# 111-87-5, 1-Octanol

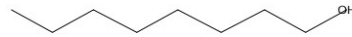


Delta

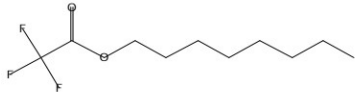


Compound Structure

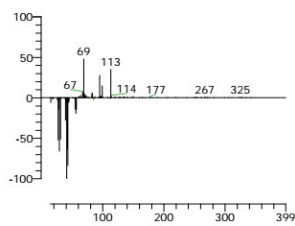
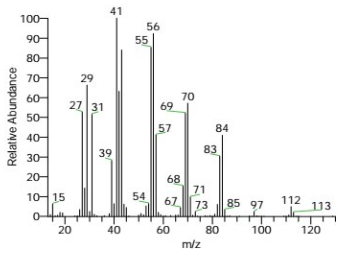
1-Octanol
Formula C8H18O, MW 130, CAS# 111-87-5, Entry# 5209
Octyl alcohol



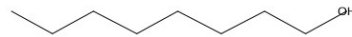
1-Octyl trifluoroacetate
Formula C10H17F3O2, MW 226, CAS# 2561-21-9, Entry# 32070
Octyl trifluoroacetate



SI 696, RSI 758, replib, Entry# 1017, CAS# 111-87-5, 1-Octanol



1-Octanol
Formula C8H18O, MW 130, CAS# 111-87-5, Entry# 1017
Octyl alcohol



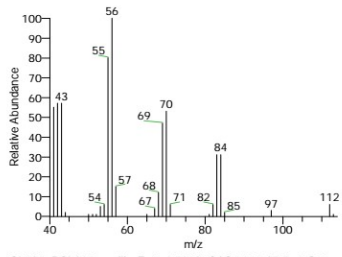


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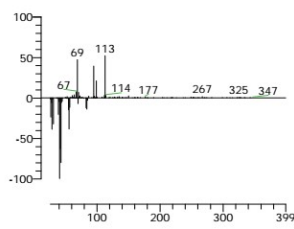
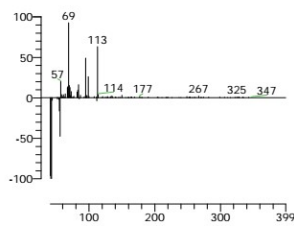
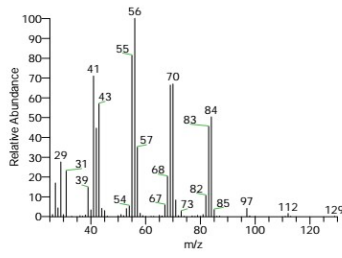
Hit Spectrum

Delta

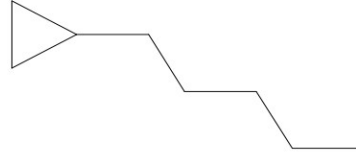
Compound Structure



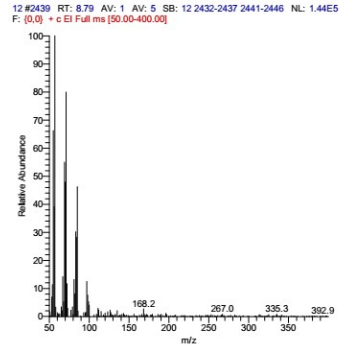
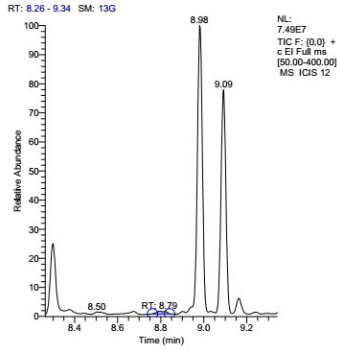
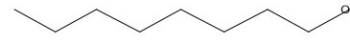
SI 686, RSI 801, replib, Entry# 5208, CAS# 111-87-5, 1-Octanol



Cyclopropane, pentyl-
Formula C8H16, MW 112, CAS# 2511-91-3, Entry# 20792
Pentane, 1-cyclopropyl-



1-Octanol
Formula C8H18O, MW 130, CAS# 111-87-5, Entry# 5208
Octyl alcohol



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.79	774	825	7.25	mainlib	C22H45Cl3Si	442
8.79	770	839	6.40	mainlib	C12H26O	186
8.79	771	820	6.40	replib	C12H26O	186
8.79	762	822	4.65	mainlib	C10H22O	158
8.79	761	781	4.47	replib	C20H40O	296

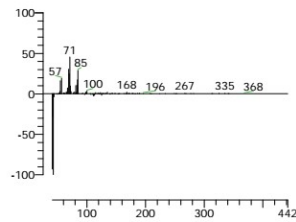
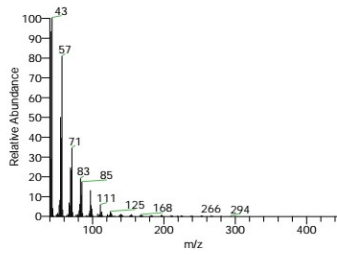


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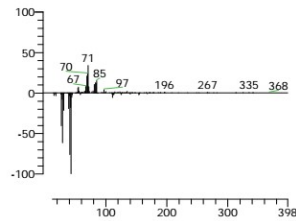
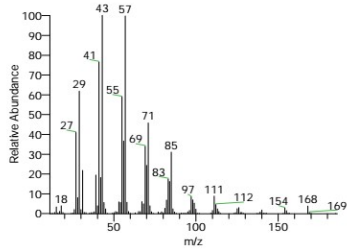
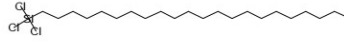
Hit Spectrum

Delta

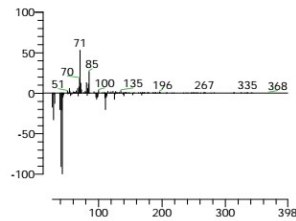
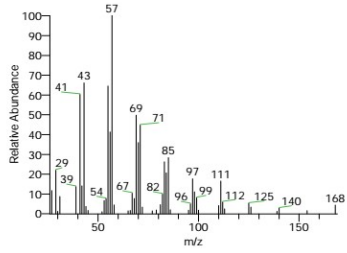
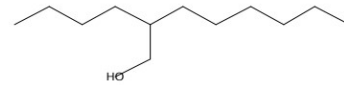
Compound Structure



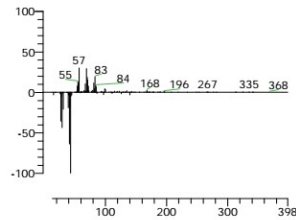
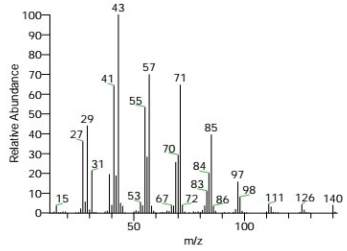
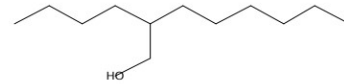
Silane, trichlorodocosyl-
Formula C₂₂H₄₅Cl₃Si, MW 442, CAS# 7325-84-0, Entry# 5777
Docosyltrichlorosilane



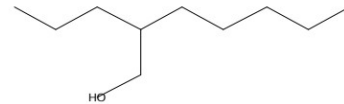
1-Octanol, 2-butyl-
Formula C₁₂H₂₆O, MW 186, CAS# 3913-02-8, Entry# 2140
2-Butyl-1-octanol



1-Octanol, 2-butyl-
Formula C₁₂H₂₆O, MW 186, CAS# 3913-02-8, Entry# 22453
2-Butyl-1-octanol



1-Heptanol, 2-propyl-
Formula C₁₀H₂₂O, MW 158, CAS# 10042-59-8, Entry# 7476
2-Propylheptanol



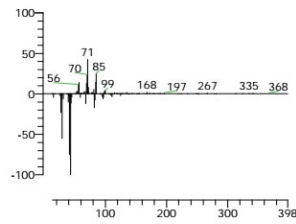
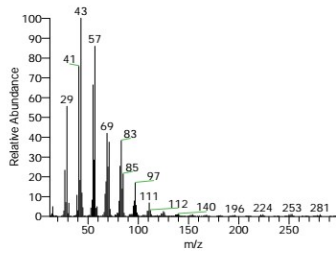


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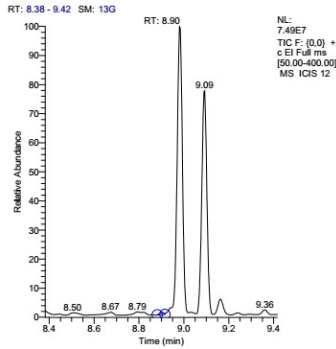
Hit Spectrum

Delta

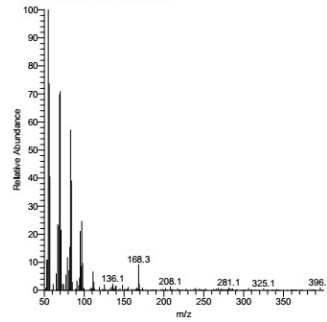
Compound Structure



Octadecane, 1-(ethenoxy)-
Formula C₂₀H₄₀O, MW 296, CAS# 930-02-9, Entry# 2167
Ether, octadecyl vinyl



12 #2471 RT: 8.90 AV: 1 AV: 5 SB: 12 2464-2469 2473-2478 NL: 1.29E5
F: [0.0] + c EI Full ms [50.00-400.00]

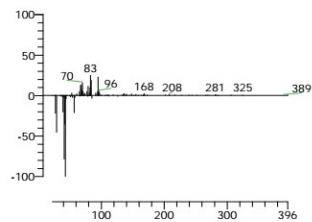
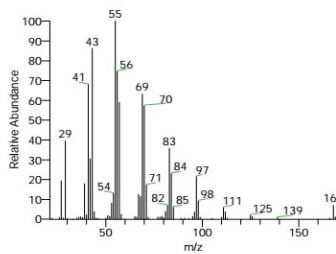


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.90	791	839	7.86	replib	C ₁₂ H ₂₄	168
8.90	805	861	7.86	mainlib	C ₁₂ H ₂₄	168
8.90	794	848	5.39	mainlib	C ₁₂ H ₂₄	168
8.90	792	842	4.97	replib	C ₁₂ H ₂₄	168
8.90	792	845	4.97	replib	C ₁₂ H ₂₄	168

Hit Spectrum

Delta

Compound Structure



2-Dodecene, (E)-
Formula C₁₂H₂₄, MW 168, CAS# 7206-13-5, Entry# 18390
(2E)-2-Dodecene



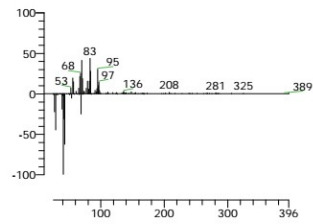
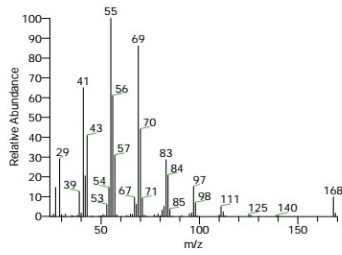


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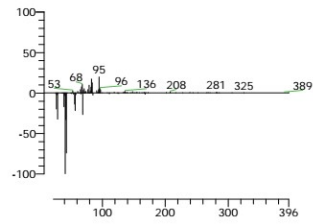
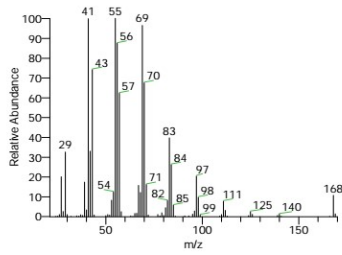
Hit Spectrum

Delta

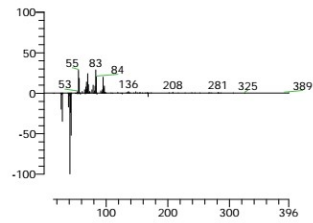
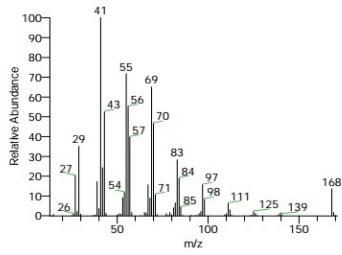
Compound Structure



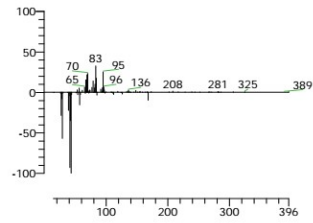
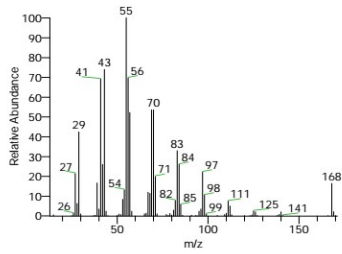
6-Dodecene, (E)-
Formula C₁₂H₂₄, MW 168, CAS# 7206-17-9, Entry# 18775
(6E)-6-Dodecene



3-Dodecene, (E)-
Formula C₁₂H₂₄, MW 168, CAS# 7206-14-6, Entry# 4455
trans-3-Dodecene



3-Dodecene, (E)-
Formula C₁₂H₂₄, MW 168, CAS# 7206-14-6, Entry# 953
trans-3-Dodecene

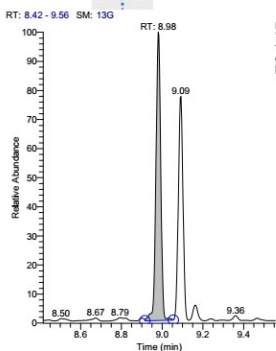


2-Dodecene, (E)-
Formula C₁₂H₂₄, MW 168, CAS# 7206-13-5, Entry# 4598
(2E)-2-Dodecene

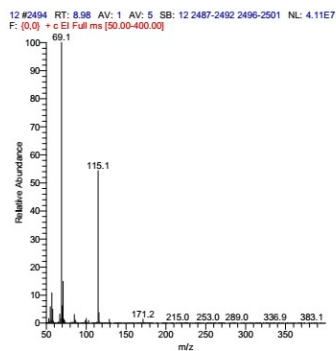




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NL:
7.49E7
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICS 12

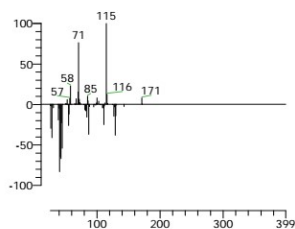
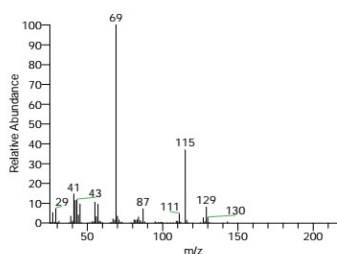


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
8.98	709	716	40.37	mainlib	C12H22O3	214
8.98	681	691	11.65	mainlib	C21H42O2	326
8.98	674	676	8.93	mainlib	C10H20O2	172
8.98	667	684	6.84	mainlib	C9H16O3	172
8.98	658	664	4.96	mainlib	C21H42O2	326

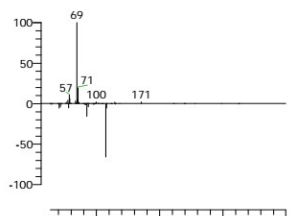
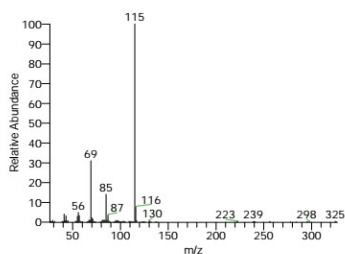
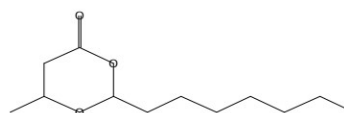
Hit Spectrum

Delta

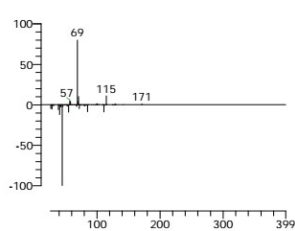
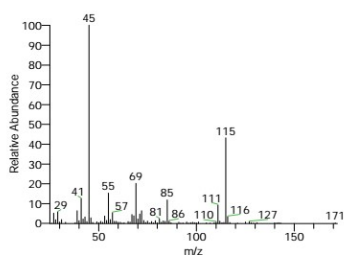
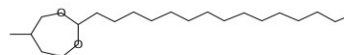
Compound Structure



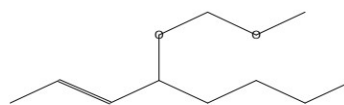
1,3-Dioxan-4-one, 2-heptyl-6-methyl
Formula C12H22O3, MW 214, CAS# 95902-24-6, Entry# 33005
2-Heptyl-6-methyl-1,3-dioxan-4-one #



1,3-Dioxepane, 5-methyl-2-pentadecyl-
Formula C21H42O2, MW 326, CAS# 56599-34-9, Entry# 83314
5-Methyl-2-pentadecyl-1,3-dioxepane #



4-Methoxymethoxy-oct-2-ene
Formula C10H20O2, MW 172, CAS# NA, Entry# 16453
(2E)-4-(Methoxymethoxy)-2-octene #



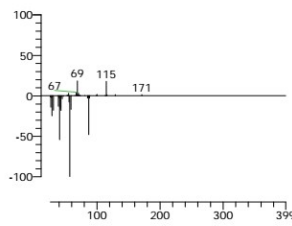
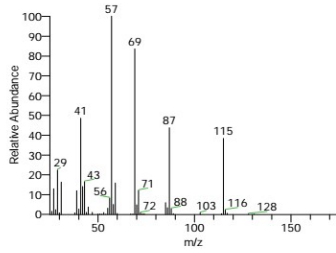


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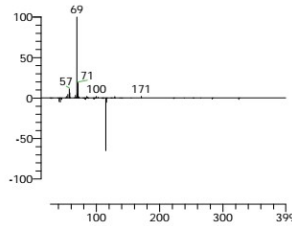
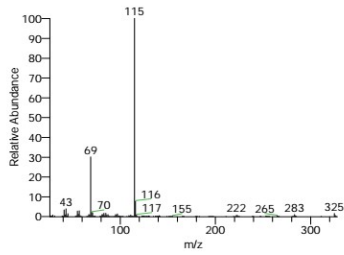
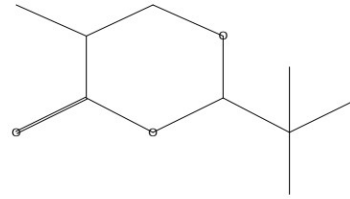
Hit Spectrum

Delta

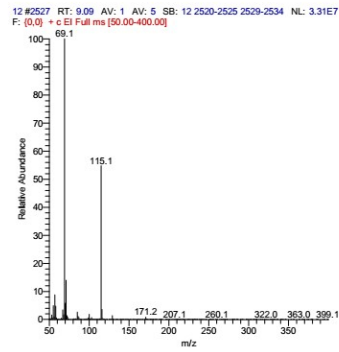
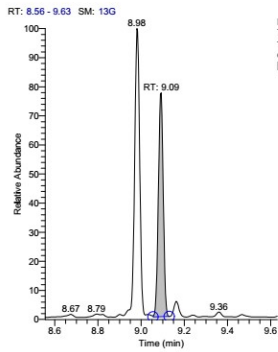
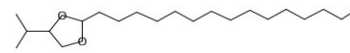
Compound Structure



1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5-methyl-, (2s-cis)-
 Formula C₉H₁₆O₃, MW 172, CAS# 107289-32-7, Entry# 23371
 2-tert-Butyl-5-methyl-1,3-dioxan-4-one #



1,3-Dioxolane, 4-(1-methylethyl)-2-pentadecyl-
 Formula C₂₁H₄₂O₂, MW 326, CAS# 56599-35-0, Entry# 83333
 4-Isopropyl-2-pentadecyl-1,3-dioxolane #



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
9.09	725	729	36.14	mainlib	C ₁₂ H ₂₂ O ₃	214
9.09	711	809	22.62	mainlib	C ₇ H ₁₄ O ₂	130
9.09	700	707	15.52	mainlib	C ₂₁ H ₄₂ O ₂	326
9.09	686	689	9.71	mainlib	C ₂₁ H ₄₂ O ₂	326
9.09	662	675	3.25	mainlib	C ₉ H ₁₆ O ₃	172

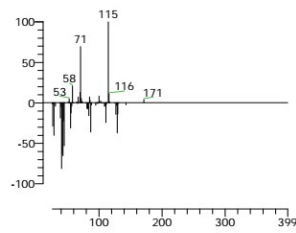
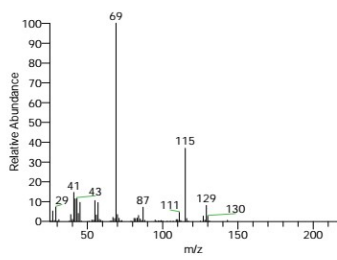


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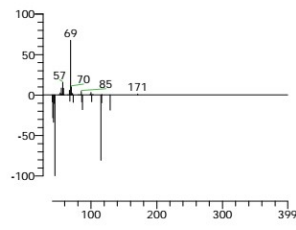
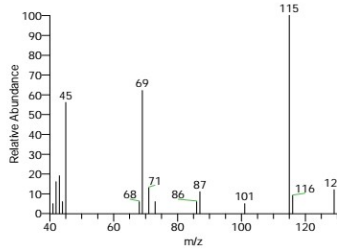
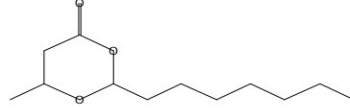
Hit Spectrum

Delta

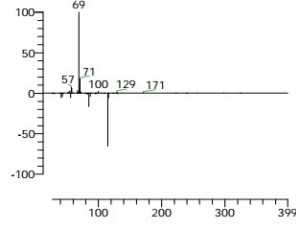
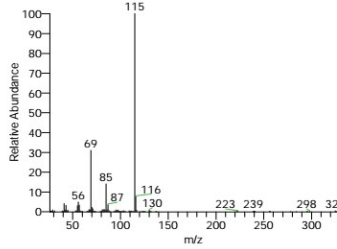
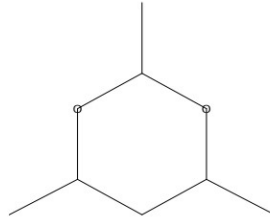
Compound Structure



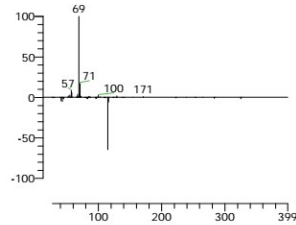
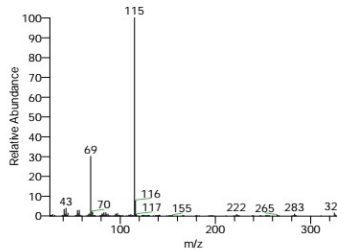
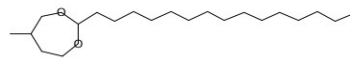
1,3-Dioxan-4-one, 2-heptyl-6-methyl
Formula C12H22O3, MW 214, CAS# 99902-24-6, Entry# 33005
2-Heptyl-6-methyl-1,3-dioxan-4-one #



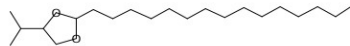
1,3-Dioxane, 2,4,6-trimethyl-, (2a,4a,6a)-
Formula C7H14O2, MW 130, CAS# 19145-91-6, Entry# 83285
m-Dioxane, 2,4,6-trimethyl-, cis-2,4,cis-2,6-



1,3-Dioxepane, 5-methyl-2-pentadecyl-
Formula C21H42O2, MW 326, CAS# 56599-34-9, Entry# 83314
5-Methyl-2-pentadecyl-1,3-dioxepane #



1,3-Dioxolane, 4-(1-methylethyl)-2-pentadecyl-
Formula C21H42O2, MW 326, CAS# 56599-35-0, Entry# 83333
4-Isopropyl-2-pentadecyl-1,3-dioxolane #



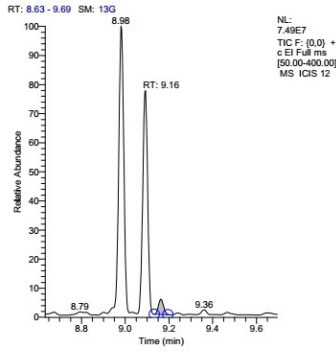
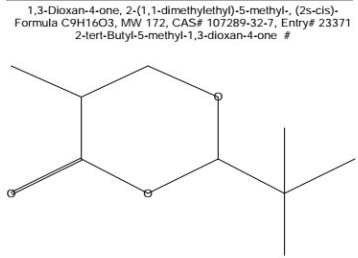
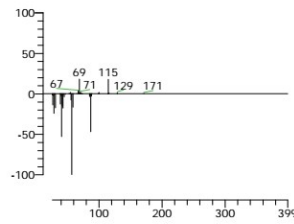
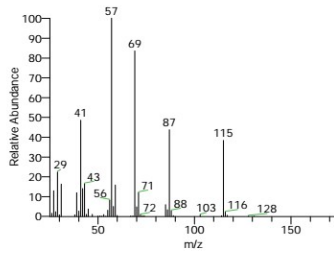


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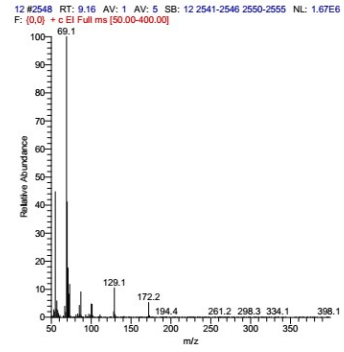
Hit Spectrum

Delta

Compound Structure



NL: 7.49E7
TIC F: (0.0) +
c EI Full ms
[50.00-400.00]
MS ICIS 12

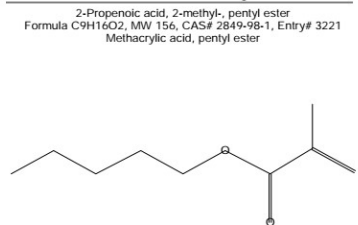
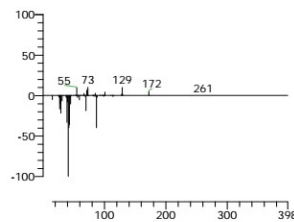
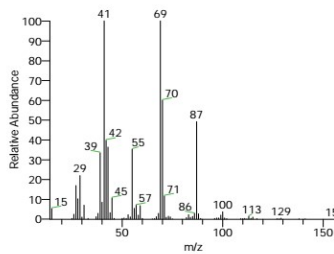


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
9.16	691	711	16.72	mainlib	C ₉ H ₂₀ O ₂	160
9.16	678	697	16.72	replib	C ₉ H ₂₀ O ₂	160
9.16	691	717	16.72	mainlib	C ₉ H ₁₆ O ₂	156
9.16	673	911	8.62	mainlib	C ₉ H ₁₆ O ₂	156
9.16	659	717	5.40	replib	C ₆ H ₁₄ O ₂	118

Hit Spectrum

Delta

Compound Structure



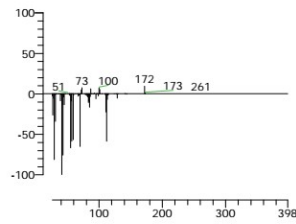
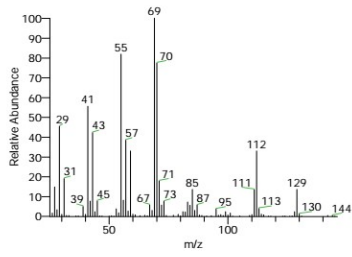


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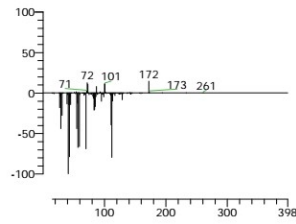
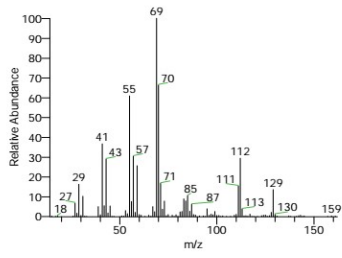
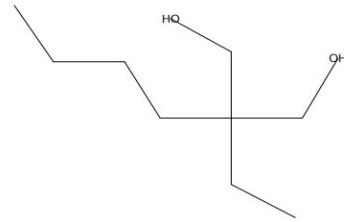
Hit Spectrum

Delta

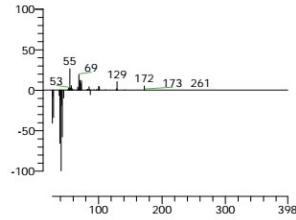
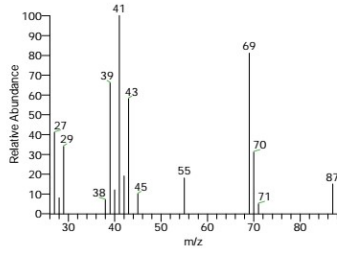
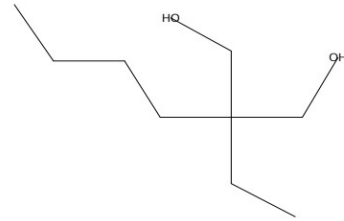
Compound Structure



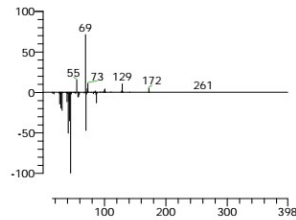
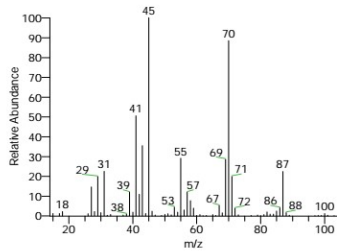
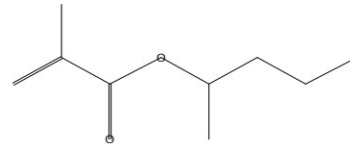
1,3-Propanediol, 2-butyl-2-ethyl-
Formula C₉H₂₀O₂, MW 160, CAS# 115-84-4, Entry# 32085
BEP



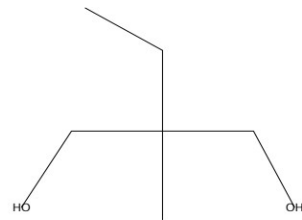
1,3-Propanediol, 2-butyl-2-ethyl-
Formula C₉H₂₀O₂, MW 160, CAS# 115-84-4, Entry# 8189
BEP



2-Propenoic acid, 2-methyl-, 1-methylbutyl ester
Formula C₉H₁₆O₂, MW 156, CAS# 94159-12-3, Entry# 3100
1-Methylbutyl methacrylate

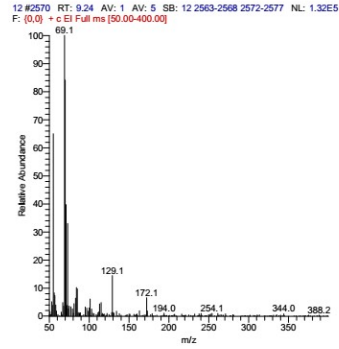
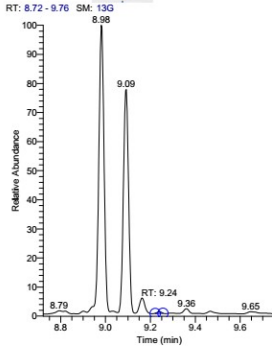


2-Ethyl-2-methyl-1,3-propanediol
Formula C₆H₁₄O₂, MW 118, CAS# 77-84-9, Entry# 3918
2-Methyl-2-ethyl-1,3-propanediol





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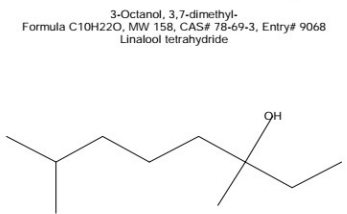
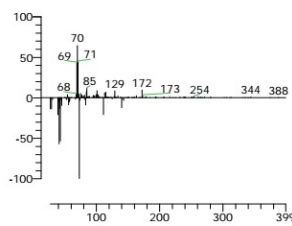
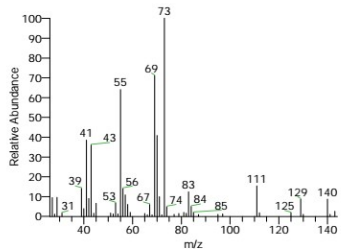
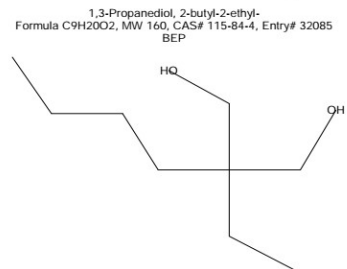
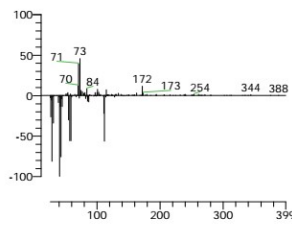
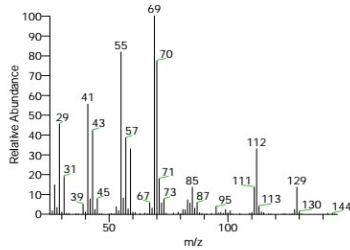
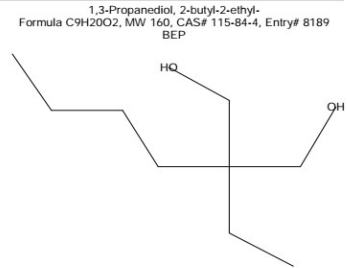
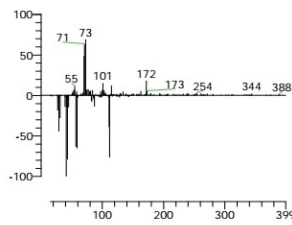
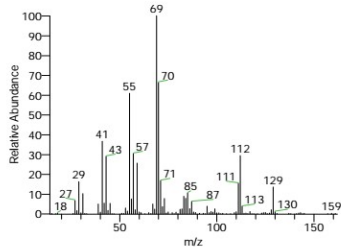


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
9.24	642	725	21.60	mainlib	C9H20O2	160
9.24	656	727	21.60	replib	C9H20O2	160
9.24	628	751	6.23	replib	C10H22O	158
9.24	622	770	4.90	mainlib	C7H16O	116
9.24	621	749	4.71	mainlib	C7H16O	116

Hit Spectrum

Delta

Compound Structure



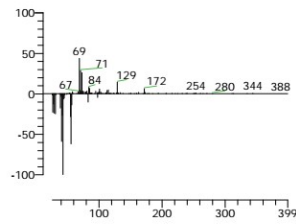
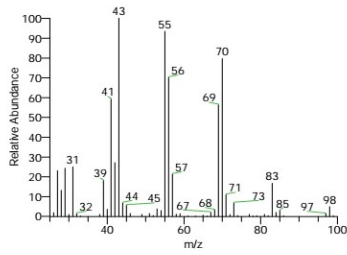


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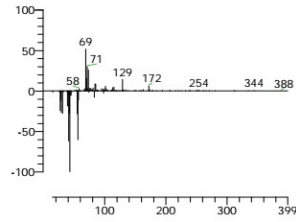
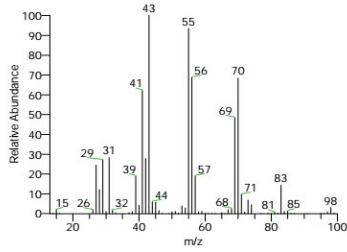
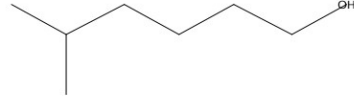
Hit Spectrum

Delta

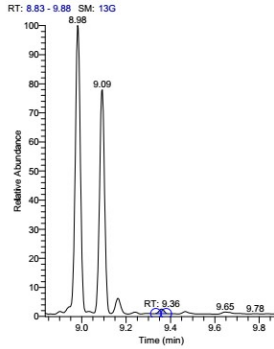
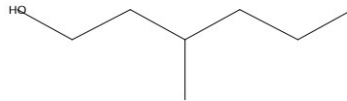
Compound Structure



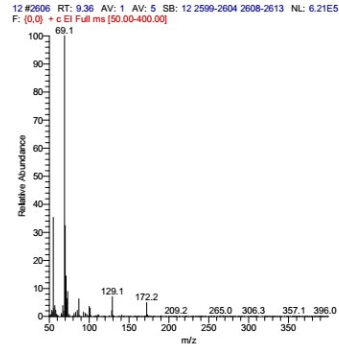
1-Hexanol, 5-methyl-5-Methyl-1-hexanol
Formula C7H16O, MW 116, CAS# 627-98-5, Entry# 6922



1-Hexanol, 3-methyl-3-Methyl-1-hexanol
Formula C7H16O, MW 116, CAS# 13231-81-7, Entry# 6824



NL: 7.49E7
TIC F: (0,0) +
c EI Full ms
[50.00-400.00]
MS ICIS 12



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
9.36	685	716	13.92	mainlib	C9H16O2	156
9.36	684	791	13.38	mainlib	C9H16O2	156
9.36	679	903	10.78	mainlib	C9H16O2	156
9.36	664	816	6.53	mainlib	C5H10O2S	134
9.36	660	684	5.52	mainlib	C9H20O2	160

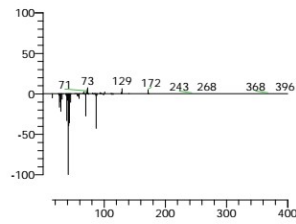
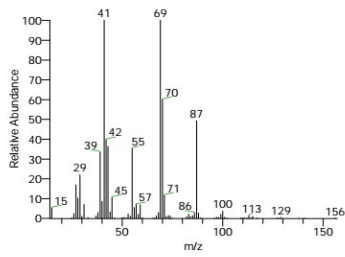


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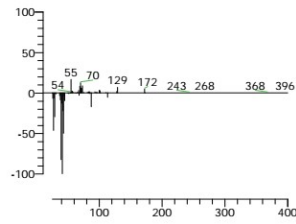
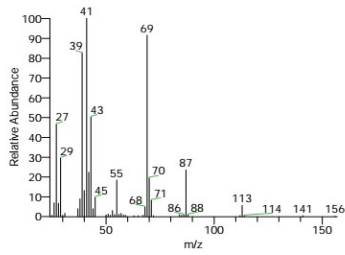
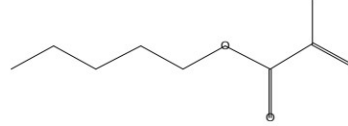
Hit Spectrum

Delta

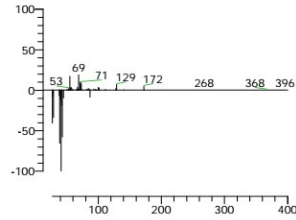
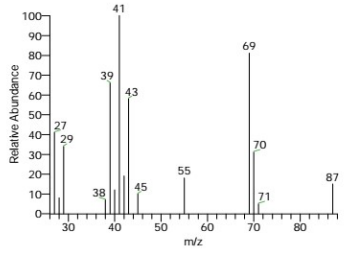
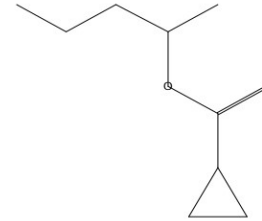
Compound Structure



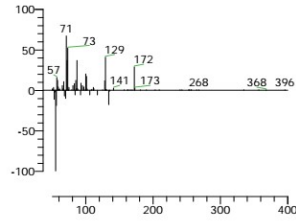
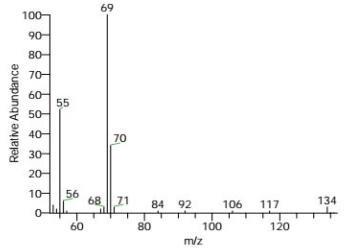
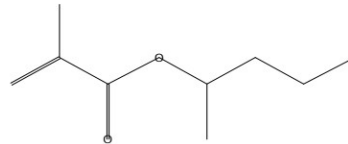
2-Propenoic acid, 2-methyl-, pentyl ester
Formula C9H16O2, MW 156, CAS# 2849-98-1, Entry# 3221
Methacrylic acid, pentyl ester



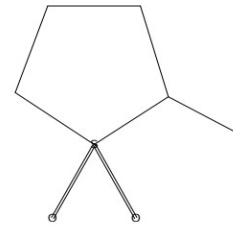
Cyclopropanecarboxylic acid, 2-pentyl ester
Formula C9H16O2, MW 156, CAS# NA, Entry# 3093
1-Methylbutyl cyclopropanecarboxylate #



2-Propenoic acid, 2-methyl-, 1-methylbutyl ester
Formula C9H16O2, MW 156, CAS# 94159-12-3, Entry# 3100
1-Methylbutyl methacrylate



2-Methylthiolane, S,S-dioxide
Formula C5H10O2S, MW 134, CAS# 1003-46-9, Entry# 32086
2-Methyltetrahydrothiophene 1,1-dioxide #



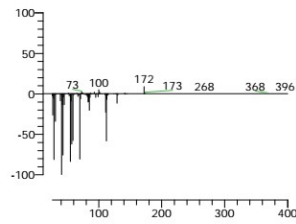
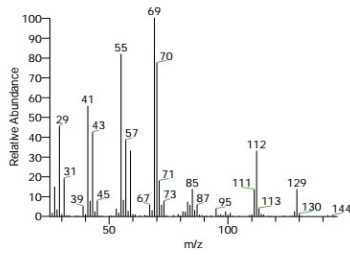


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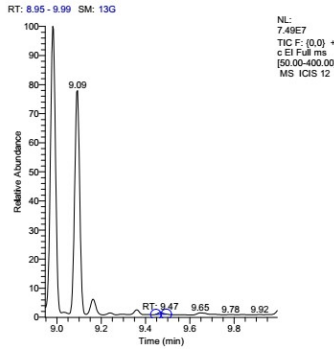
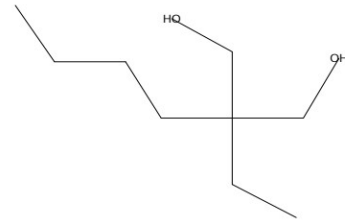
Hit Spectrum

Delta

Compound Structure

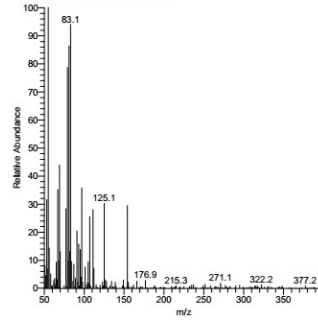


1,3-Propanediol, 2-butyl-2-ethyl-
Formula C₉H₂₀O₂, MW 160, CAS# 115-84-4, Entry# 32085
BEP



NL: 7.49E7
TIC F: (0.0) +
c EI Full ms
[50.00-400.00]
MS ICIS 12

12 #2637 RT: 9.47 AV: 1 AV: 5 SB: 12 2630-2636 2639-2644 NL: 7.87E4
F: (0.0) + c EI Full ms [50.00-400.00]

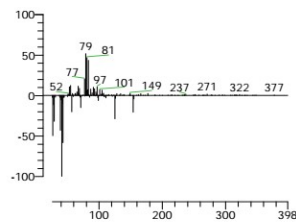
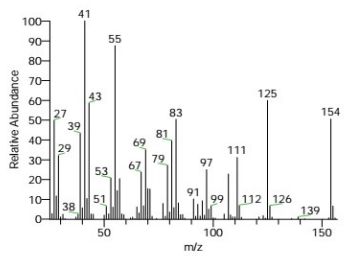


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
9.47	707	788	66.41	replib	C ₁₀ H ₁₈ O	154
9.47	745	814	66.41	mainlib	C ₁₀ H ₁₈ O	154
9.47	679	752	10.48	mainlib	C ₁₀ H ₁₈ O	154
9.47	628	778	2.11	mainlib	C ₇ H ₁₂ O	112
9.47	621	697	1.61	mainlib	C ₁₀ H ₁₈ O	154

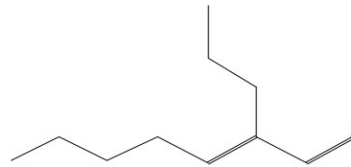
Hit Spectrum

Delta

Compound Structure



2-Heptenal, 2-propyl-
Formula C₁₀H₁₈O, MW 154, CAS# 34880-43-8, Entry# 2744
2-Propyl-2-heptenal



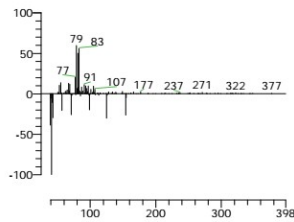
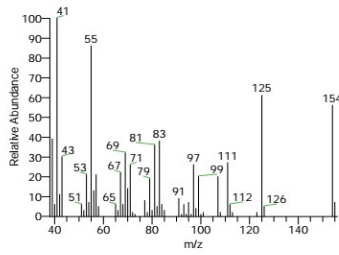


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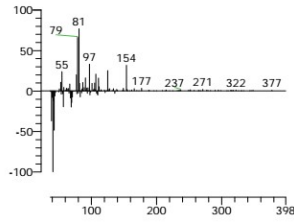
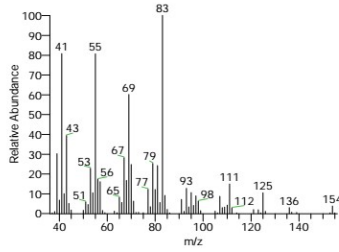
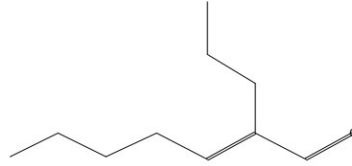
Hit Spectrum

Delta

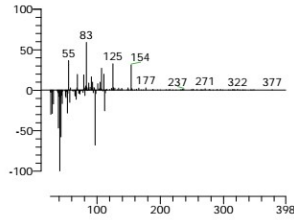
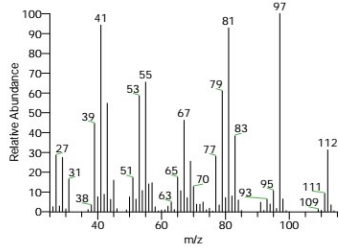
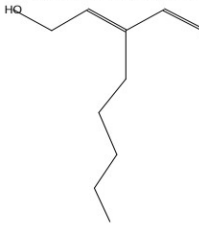
Compound Structure



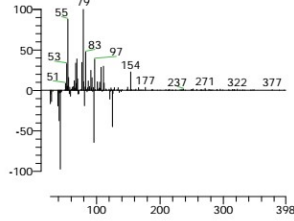
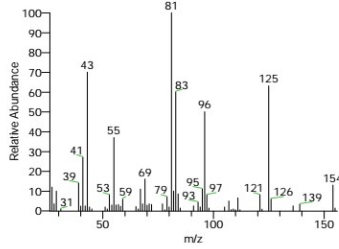
2-Heptenal, 2-propyl-
Formula C₁₀H₁₈O, MW 154, CAS# 34880-43-8, Entry# 992
2-Propyl-2-heptenal



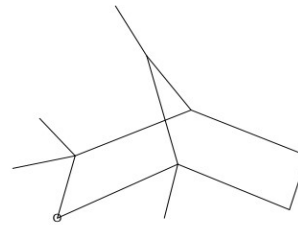
2,4-Pentadien-1-ol, 3-pentyl-, (2Z)-
Formula C₁₀H₁₈O, MW 154, CAS# NA, Entry# 47252
(2E)-3-Pentyl-2,4-pentadien-1-ol #



4-Methyl-2,3-hexadien-1-ol
Formula C₇H₁₂O, MW 112, CAS# NA, Entry# 63336

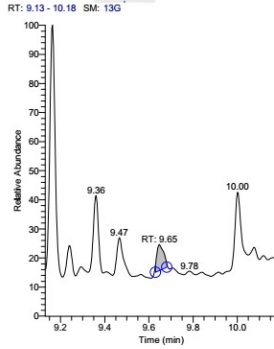


2-Oxabicyclo[2.2.1]heptane, 1,3,3,7-tetramethyl-, (1R,4S,7S)-(+)-
Formula C₁₀H₁₈O, MW 154, CAS# 15404-57-6, Entry# 45421
1,3,3,7-Tetramethyl-2-oxabicyclo[2.2.1]heptane #

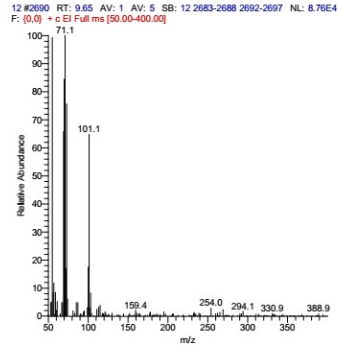




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NL:
4.66E6
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICIS 12

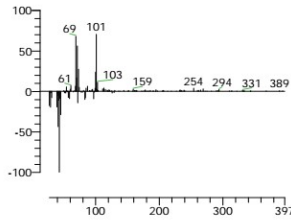
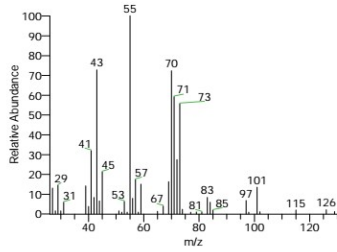


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
9.65	638	781	26.01	mainlib	C9H20O	144
9.65	616	749	10.28	mainlib	C6H12O2	116
9.65	597	695	4.99	mainlib	C10H22O	158
9.65	596	658	4.79	replib	C9H18O2	158
9.65	594	717	4.42	replib	C6H14O	102

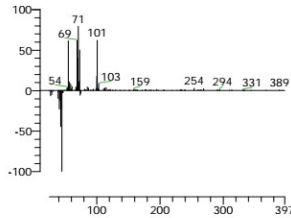
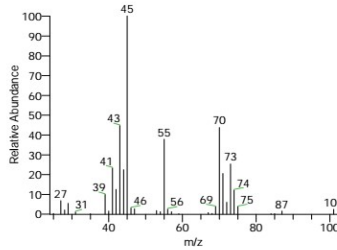
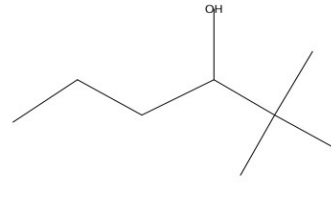
Hit Spectrum

Delta

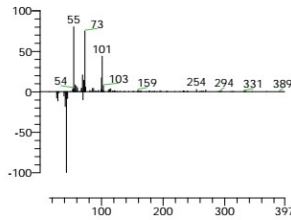
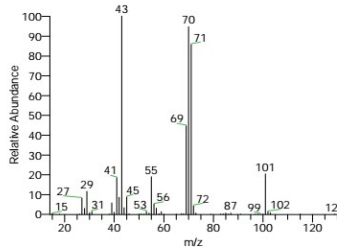
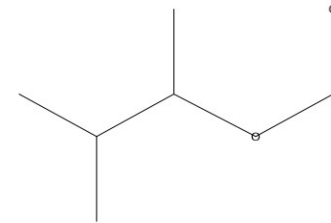
Compound Structure



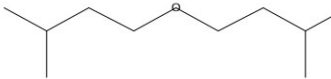
3,3-Dimethyl-4-heptanol
Formula C9H20O, MW 144, CAS# 19549-78-1, Entry# 18430



Formic acid, 3-methylbut-2-yl ester
Formula C6H12O2, MW 116, CAS# NA, Entry# 15819



Butane, 1,1'-oxybis[3-methyl-Isopentyl ether]
Formula C10H22O, MW 158, CAS# 544-01-4, Entry# 8222



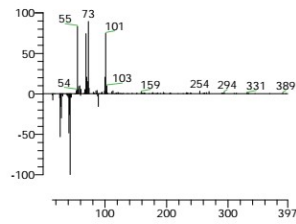
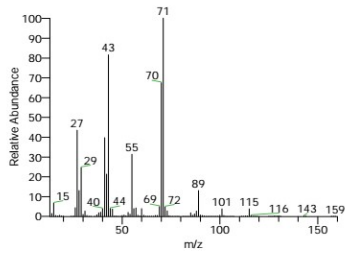


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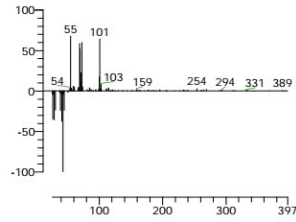
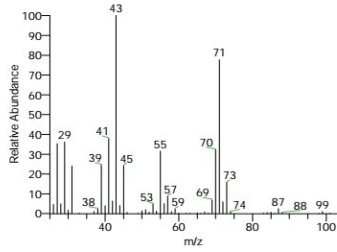
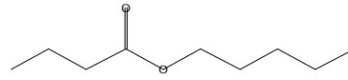
Hit Spectrum

Delta

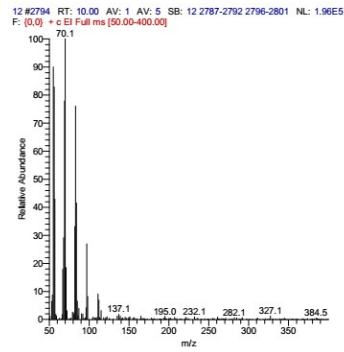
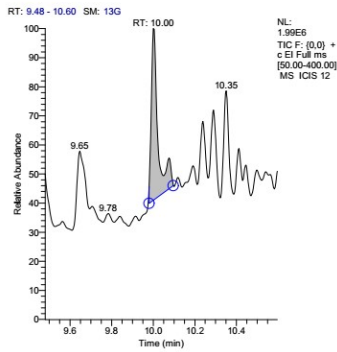
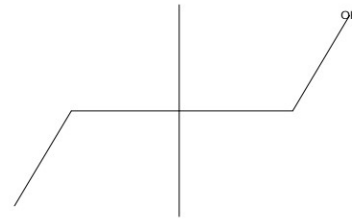
Compound Structure



Butanoic acid, pentyl ester
 Formula C₉H₁₈O₂, MW 158, CAS# 540-18-1, Entry# 8595
 Butyric acid, pentyl ester



1-Butanol, 2,2-dimethyl-
 Formula C₆H₁₄O, MW 102, CAS# 1185-33-7, Entry# 2502
 2,2-Dimethyl-1-butanol



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
10.00	820	890	9.20	mainlib	C ₁₁ H ₂₄ O	172
10.00	820	890	9.20	NISTDEMO	C ₁₁ H ₂₄ O	172
10.00	802	859	7.05	replib	C ₁₀ H ₂₂ O	158
10.00	813	877	7.05	replib	C ₁₀ H ₂₂ O	158
10.00	802	865	4.83	mainlib	C ₁₁ H ₂₂	154

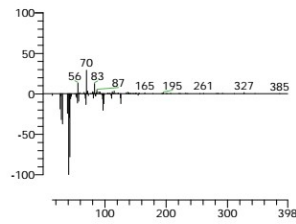
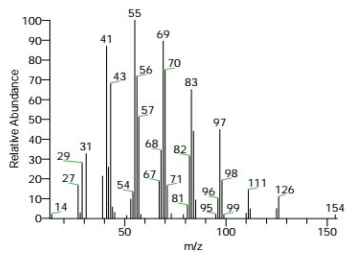


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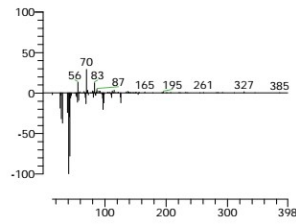
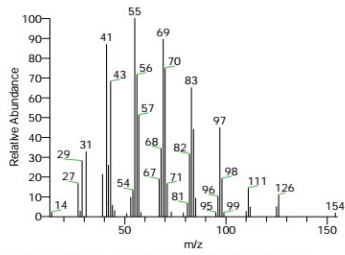
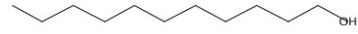
Hit Spectrum

Delta

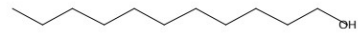
Compound Structure



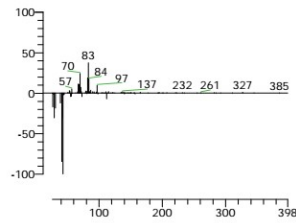
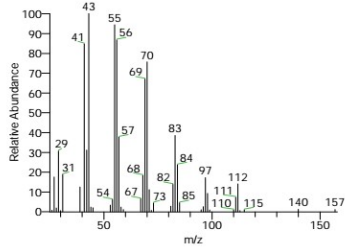
1-Undecanol
Formula C₁₁H₂₄O, MW 172, CAS# 112-42-5, Entry# 409
Undecyl alcohol



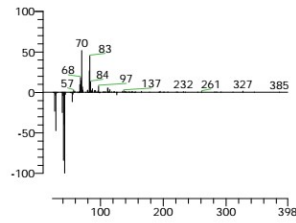
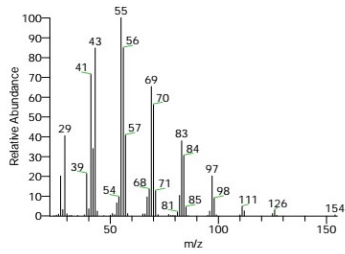
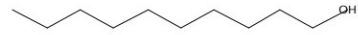
1-Undecanol
Formula C₁₁H₂₄O, MW 172, CAS# 112-42-5, Entry# 18777
Undecyl alcohol



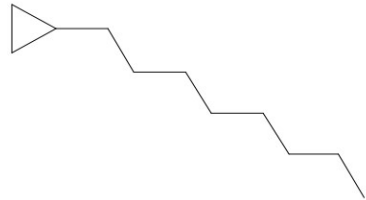
SI 813, RSI 877, replib, Entry# 2011, CAS# 112-30-1, 1-Decanol



1-Decanol
Formula C₁₀H₂₂O, MW 158, CAS# 112-30-1, Entry# 2011
Decyl alcohol



Cyclopropane, octyl-
Formula C₁₁H₂₂, MW 154, CAS# 1472-09-9, Entry# 18565
Octane, 1-cyclopropyl-



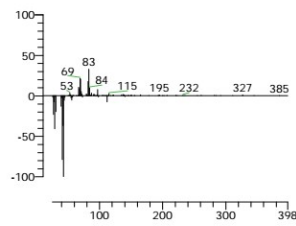
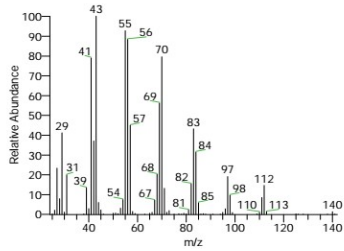


ChemLab Technologies - GC/MS Report

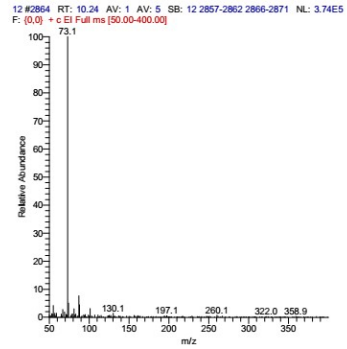
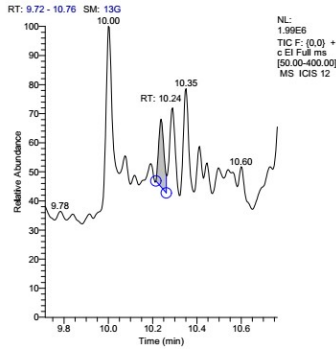
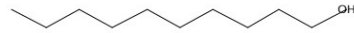
SI 802, RSI 859, replib, Entry# 2010, CAS# 112-30-1, 1-Decanol

Delta

Compound Structure



1-Decanol
Formula C₁₀H₂₂O, MW 158, CAS# 112-30-1, Entry# 2010
Decyl alcohol

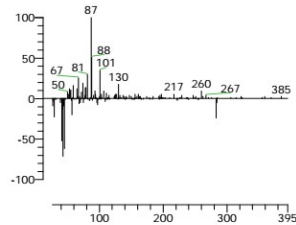
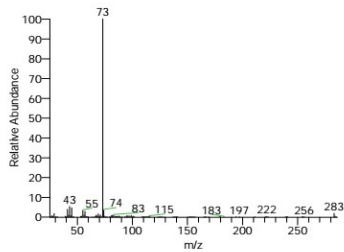


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
10.24	701	761	20.81	mainlib	C ₁₈ H ₃₆ O ₂	284
10.24	680	995	8.85	replib	C ₃ H ₆ O ₂	74
10.24	667	874	5.72	mainlib	C ₆ H ₁₂ O ₂	116
10.24	664	861	5.05	mainlib	C ₆ H ₁₂ O ₂	116
10.24	659	816	4.07	NISTDEMO	C ₅ H ₁₂ O	88

Hit Spectrum

Delta

Compound Structure



1,3-Dioxolane, 2-pentadecyl-
Formula C₁₈H₃₆O₂, MW 284, CAS# 4360-57-0, Entry# 36955
Hexadecanal cyclic ethylene acetal



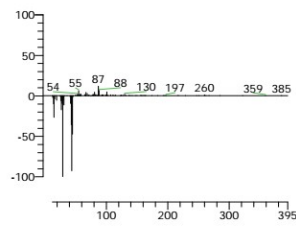
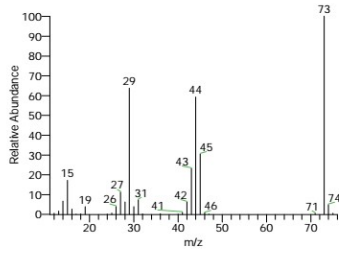


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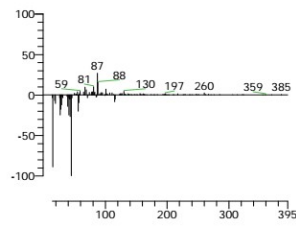
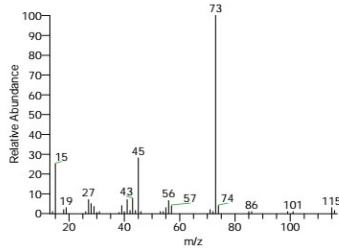
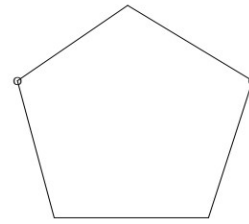
Hit Spectrum

Delta

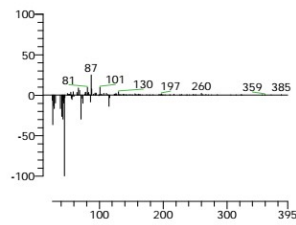
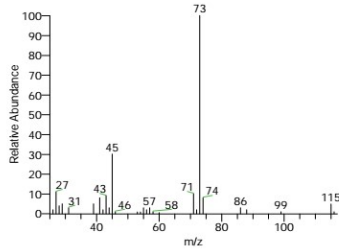
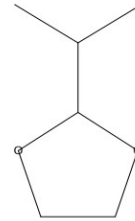
Compound Structure



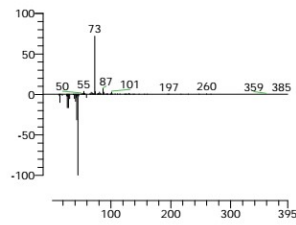
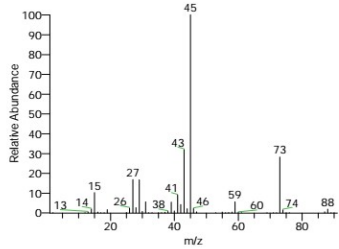
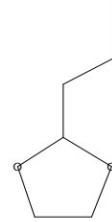
1,3-Dioxolane
Formula C3H6O2, MW 74, CAS# 646-06-0, Entry# 8899
Ethylene glycol formal



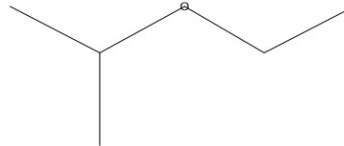
1,3-Dioxolane, 2-(1-methylethyl)-
Formula C6H12O2, MW 116, CAS# 822-83-3, Entry# 37058
1,3-Dioxolane, 2-isopropyl-



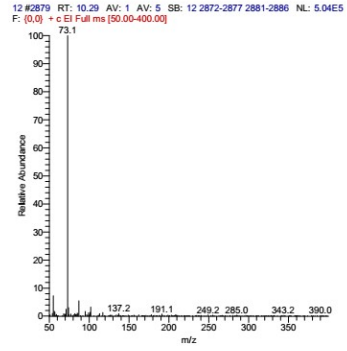
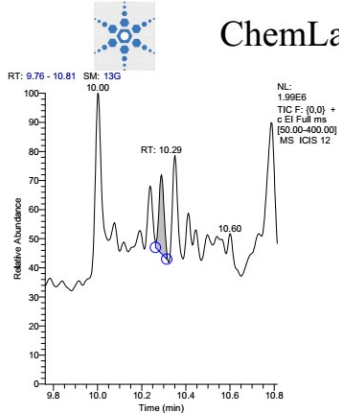
1,3-Dioxolane, 2-propyl-
Formula C6H12O2, MW 116, CAS# 3390-13-4, Entry# 37065
Butanal, cyclic 1,2-ethanediy acetal



Propane, 2-ethoxy-
Formula C5H12O, MW 88, CAS# 625-54-7, Entry# 1293
Ether, ethyl isopropyl



ChemLab Technologies - GC/MS Report



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
10.29	727	814	12.79	mainlib	C10H20O2	172
10.29	727	814	12.79	NISTDEMO	C10H20O2	172
10.29	713	751	8.01	mainlib	C18H36O2	284
10.29	710	804	7.07	mainlib	C6H10O2	114
10.29	710	921	7.07	mainlib	C6H12O2	116

Hit Spectrum	Delta	Compound Structure
		<p>1,3-Dioxolane, 2-heptyl- Formula C10H20O2, MW 172, CAS# 4359-57-3, Entry# 1394 2-Heptyl-1,3-dioxolane #</p>
		<p>1,3-Dioxolane, 2-heptyl- Formula C10H20O2, MW 172, CAS# 4359-57-3, Entry# 37083 2-Heptyl-1,3-dioxolane #</p>
		<p>1,3-Dioxolane, 2-pentadecyl- Formula C18H36O2, MW 284, CAS# 4360-57-0, Entry# 36955 Hexadecanal cyclic ethylene acetal</p>

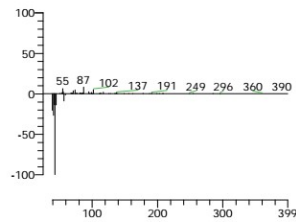
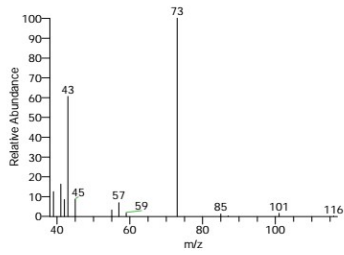


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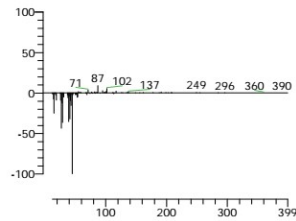
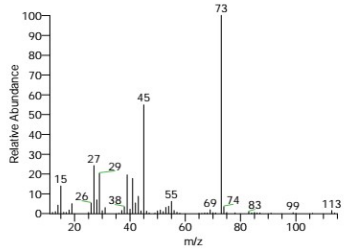
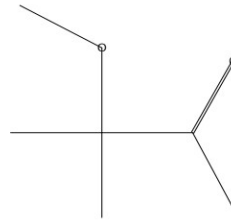
Hit Spectrum

Delta

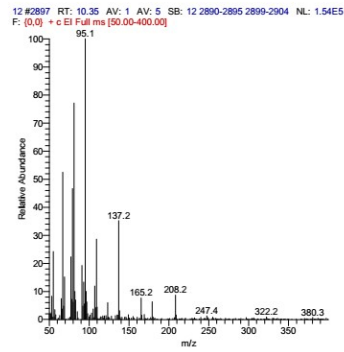
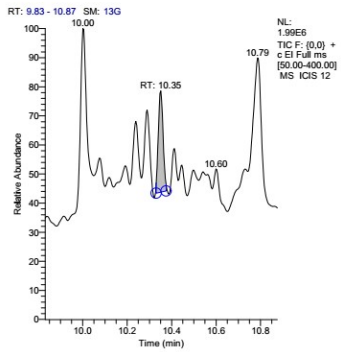
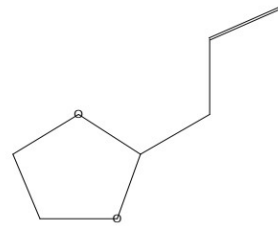
Compound Structure



2-Butanone, 3-methoxy-3-methyl-
 Formula C₆H₁₂O₂, MW 116, CAS# 36687-98-6, Entry# 36944
 3-Methoxy-3-methyl-2-butanone #



1,3-Dioxolane, 2-(2-propenyl)-
 Formula C₆H₁₀O₂, MW 114, CAS# 38653-49-5, Entry# 37063
 2-Allyl-1,3-dioxolane #



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
10.35	717	822	11.11	replib	C ₁₀ H ₁₆ O	152
10.35	702	774	6.73	mainlib	C ₁₂ H ₂₂	166
10.35	701	795	6.47	mainlib	C ₁₀ H ₁₆ O	152
10.35	696	774	5.21	mainlib	C ₁₀ H ₁₇ Br	216
10.35	693	756	4.60	mainlib	C ₁₂ H ₂₂	166

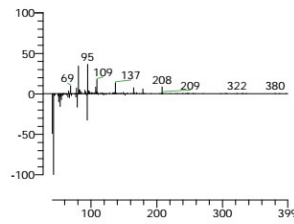
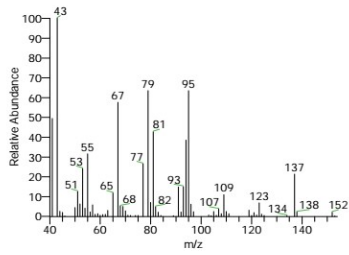


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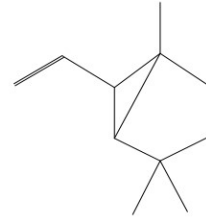
Hit Spectrum

Delta

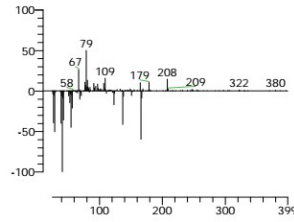
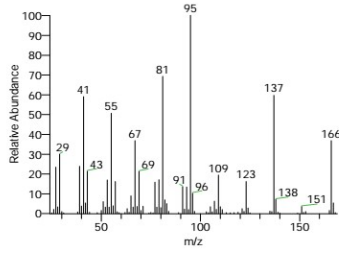
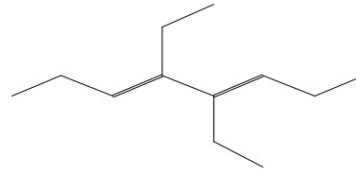
Compound Structure



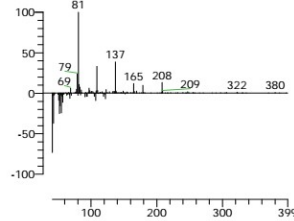
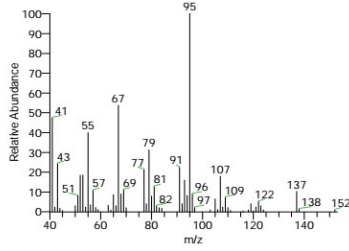
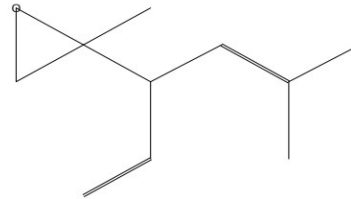
Artemiseole
Formula C₁₀H₁₆O, MW 152, CAS# 60485-46-3, Entry# 2699
1,6,6-Trimethyl-4-ethenyl-exo-2-oxabicyclo[3.1.0] hexane



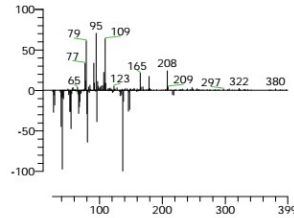
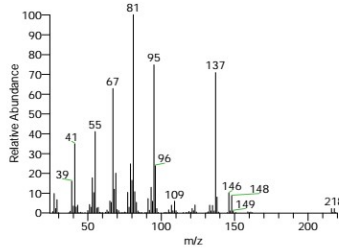
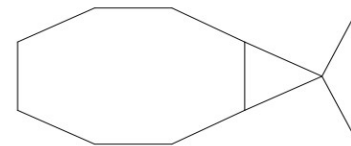
3,5-Octadiene, 4,5-diethyl-
Formula C₁₂H₂₂, MW 166, CAS# 67652-84-0, Entry# 62027
4,5-Diethyl-3,5-octadiene



Santolina epoxide
Formula C₁₀H₁₆O, MW 152, CAS# 60485-45-2, Entry# 61795
2-Methyl-2-(3-methyl-1-vinyl-2-butenyl)oxirane #



Bicyclo[6.1.0]nonane, 9-bromo-9-methyl-, (1a,8a,9a)-
Formula C₁₀H₁₇Br, MW 216, CAS# 59474-03-2, Entry# 45957
9-Bromo-9-methylbicyclo[6.1.0]nonane #



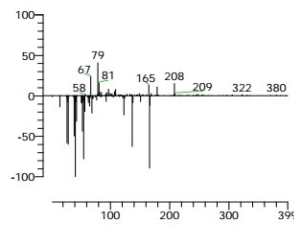
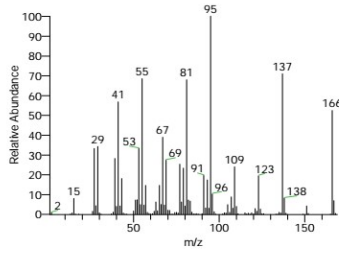


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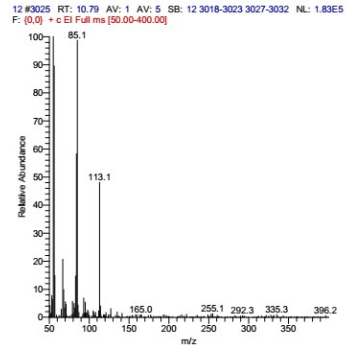
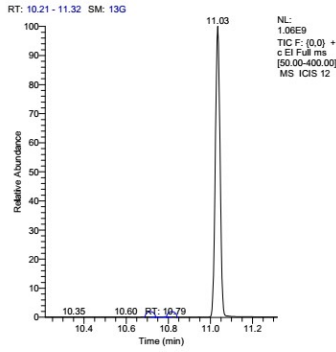
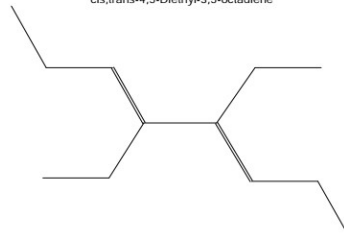
Hit Spectrum

Delta

Compound Structure



3,5-Octadiene, 4,5-diethyl-, (E,Z)-
Formula C₁₂H₂₂, MW 166, CAS# 21293-02-7, Entry# 62407
cis,trans-4,5-Diethyl-3,5-octadiene



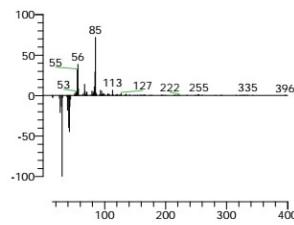
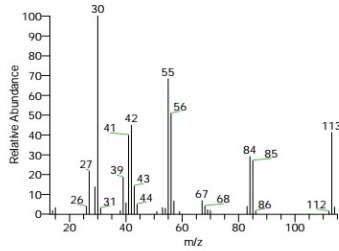
RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
10.79	693	797	65.18	replib	C ₆ H ₁₁ NO	113
10.79	725	868	65.18	replib	C ₆ H ₁₁ NO	113
10.79	756	899	65.18	replib	C ₆ H ₁₁ NO	113
10.79	730	819	19.53	mainlib	C ₁₀ H ₁₈ O ₂	170
10.79	701	773	5.53	mainlib	C ₁₂ H ₂₂ O ₂	198

Hit Spectrum

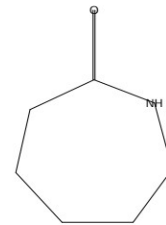
Delta

Compound Structure

SI 756, RSI 899, replib, Entry# 424, CAS# 105-60-2, Caprolactam



Caprolactam
Formula C₆H₁₁NO, MW 113, CAS# 105-60-2, Entry# 424
2H-Azepin-2-one, hexahydro-



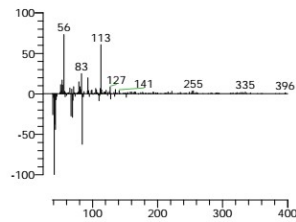
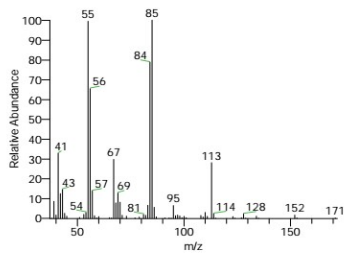


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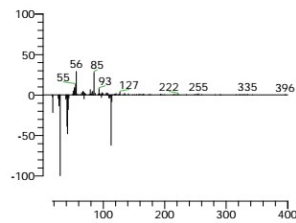
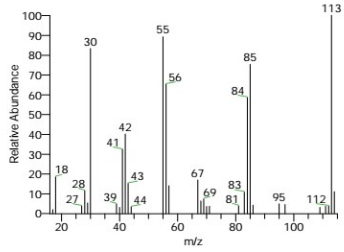
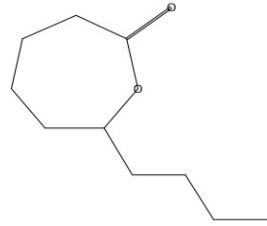
Hit Spectrum

Delta

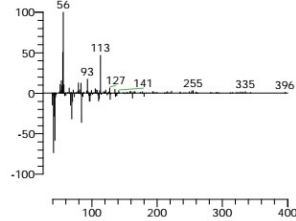
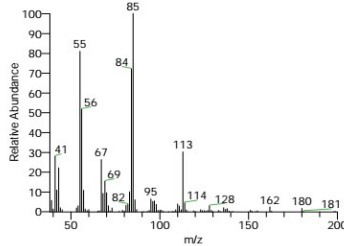
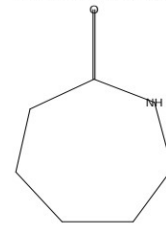
Compound Structure



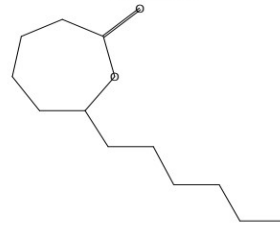
2-Oxepanone, 7-butyl-7-butyl-2-oxepanone
Formula C₁₀H₁₈O₂, MW 170, CAS# 5579-78-2, Entry# 49926



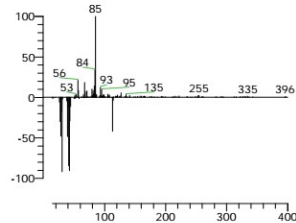
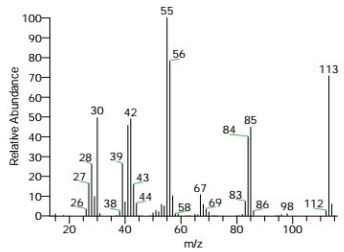
Caprolactam
Formula C₆H₁₁NO, MW 113, CAS# 105-60-2, Entry# 16493



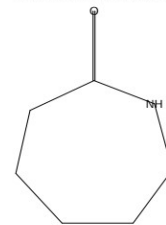
2-Oxepanone, 7-hexyl-7-hexyl-2-oxepanone
Formula C₁₂H₂₂O₂, MW 198, CAS# 16429-21-3, Entry# 49927



SI 693, RSI 797, replib, Entry# 4669, CAS# 105-60-2, Caprolactam

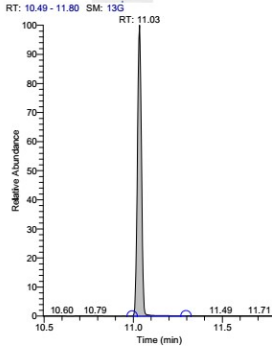


Caprolactam
Formula C₆H₁₁NO, MW 113, CAS# 105-60-2, Entry# 4669



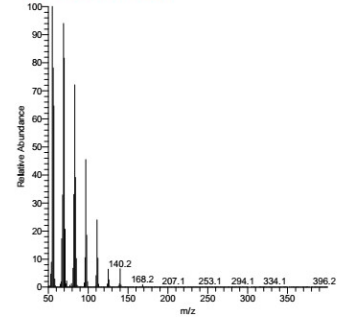


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NL: 1.06E9
TIC F: (0.0) +
c EI Full ms
(50.00-400.00)
MS ICS 12

12 #3098 RT: 11.03 AV: 1 AV: 5 SB: 12 3091-3096 3100-3105 NL: 1.66E8
F: (0.0) + c EI Full ms (50.00-400.00)

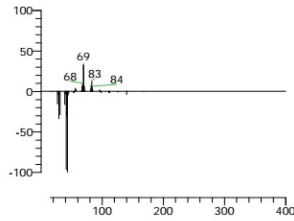
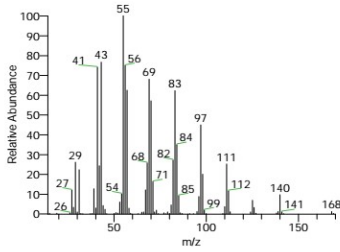


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
11.03	926	926	27.74	replib	C12H26O	186
11.03	928	929	27.74	replib	C12H26O	186
11.03	926	927	27.74	replib	C12H26O	186
11.03	964	964	27.74	replib	C12H26O	186
11.03	931	933	7.26	replib	C12H24	168

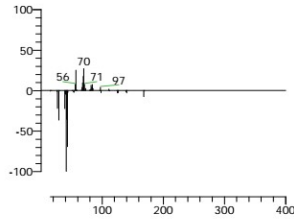
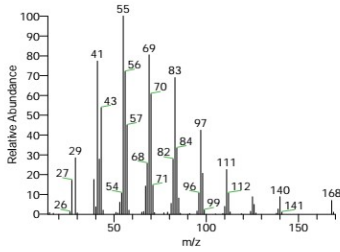
Hit Spectrum

Delta

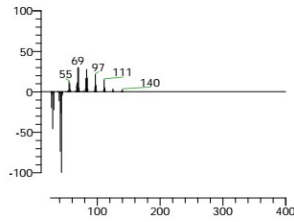
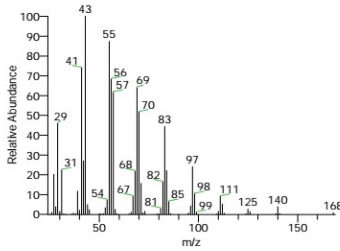
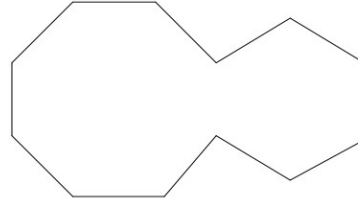
Compound Structure



1-Dodecanol
Formula C12H26O, MW 186, CAS# 112-53-8, Entry# 4595
Dodecyl alcohol



Cyclododecane
Formula C12H24, MW 168, CAS# 294-62-2, Entry# 4733



1-Dodecanol
Formula C12H26O, MW 186, CAS# 112-53-8, Entry# 2001
Dodecyl alcohol



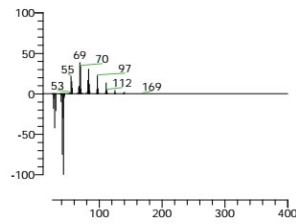
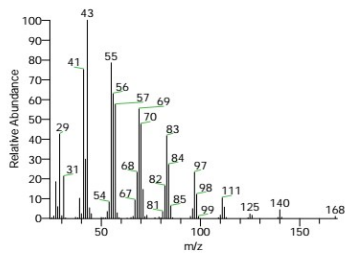


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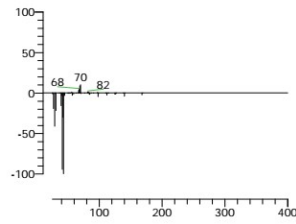
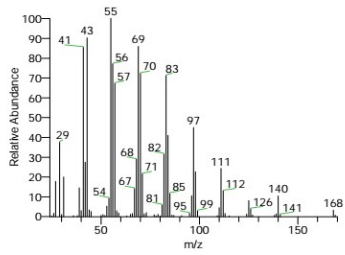
Hit Spectrum

Delta

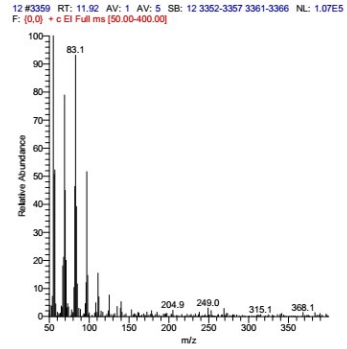
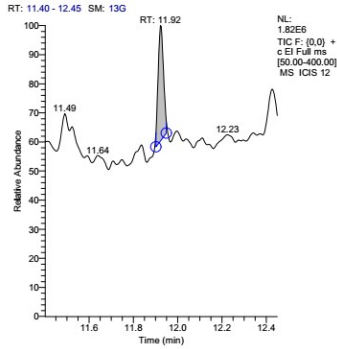
Compound Structure



1-Dodecanol
Formula C₁₂H₂₆O, MW 186, CAS# 112-53-8, Entry# 2000
Dodecyl alcohol



1-Dodecanol
Formula C₁₂H₂₆O, MW 186, CAS# 112-53-8, Entry# 4614
Dodecyl alcohol



RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
11.92	766	904	7.73	replib	C ₁₄ H ₂₈	196
11.92	760	893	6.08	NISTDEMO	C ₁₃ H ₂₈ O	200
11.92	753	876	4.78	replib	C ₁₆ H ₃₄ O	242
11.92	754	880	4.78	mainlib	C ₁₆ H ₃₄ O	242
11.92	753	886	4.59	replib	C ₁₄ H ₂₈	196

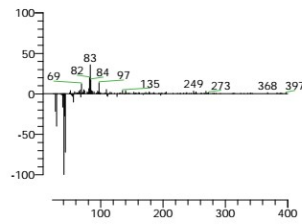
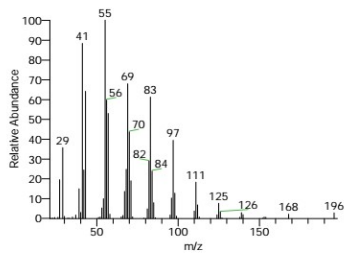


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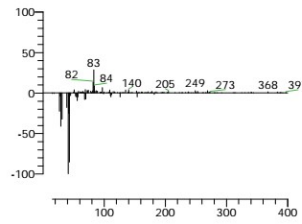
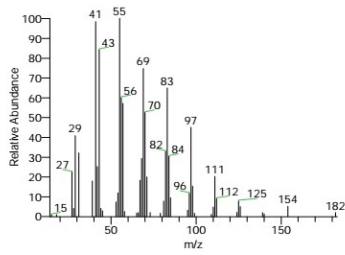
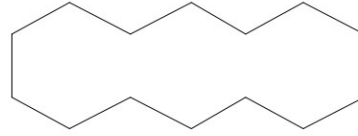
Hit Spectrum

Delta

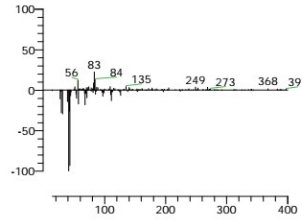
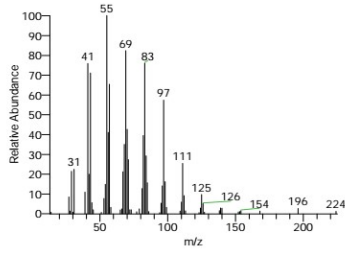
Compound Structure



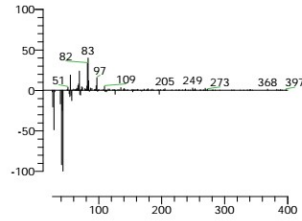
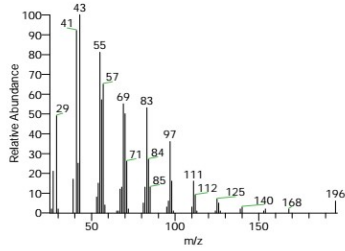
Cyclohexadecane
Formula C₁₄H₂₈, MW 196, CAS# 295-17-0, Entry# 4454



n-Tridecan-1-ol
Formula C₁₃H₂₈O, MW 200, CAS# 112-70-9, Entry# 646



1-Hexadecanol
Formula C₁₆H₃₄O, MW 242, CAS# 36653-82-4, Entry# 18939



1-Tetradecene
Formula C₁₄H₂₈, MW 196, CAS# 1120-36-1, Entry# 1735



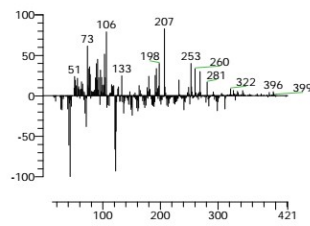
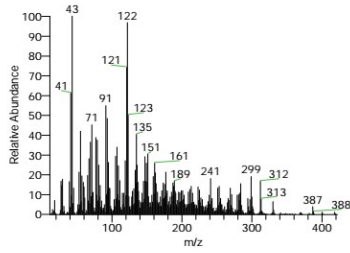


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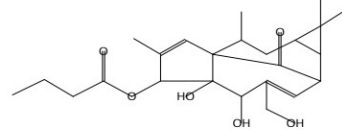
Hit Spectrum

Delta

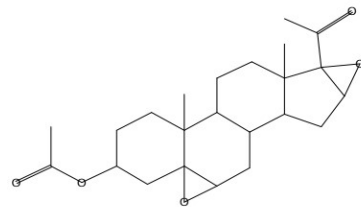
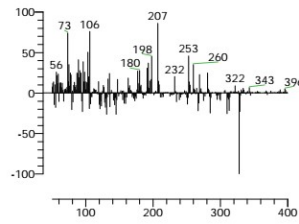
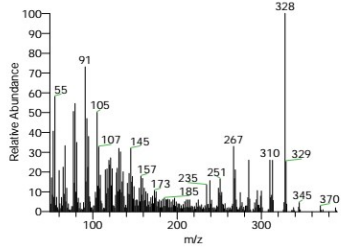
Compound Structure



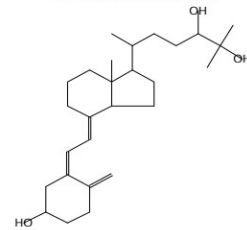
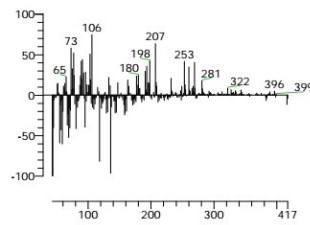
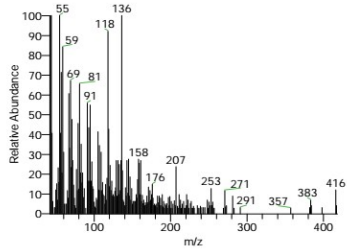
Formula C₂₄H₃₄O₆, MW 418, CAS# 77508-67-9, Entry# 10997



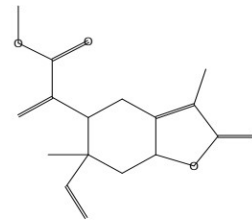
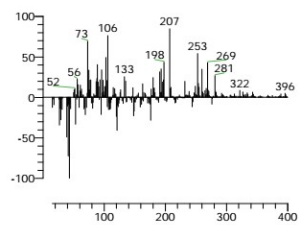
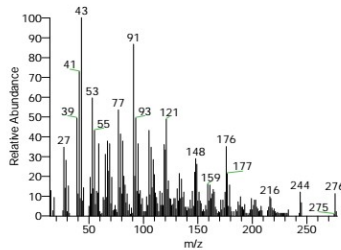
Pregnan-20-one, 3-(acetyloxy)-5,6,16,17-diepoxy-, (3a,5a,6a,16a)-
Formula C₂₃H₃₂O₅, MW 388, CAS# 14231-06-2, Entry# 202587
5a-Pregnan-20-one, 5,6a,16a,17-diepoxy-3a-hydroxy-, acetate



9,10-Secocholesta-5,7,10(19)-triene-3,24,25-triol, (3a,5Z,7E)-
Formula C₂₇H₄₄O₃, MW 416, CAS# 40013-87-4, Entry# 6382
24,25-Dihydroxycholecalciferol

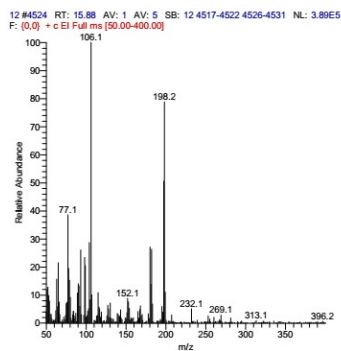
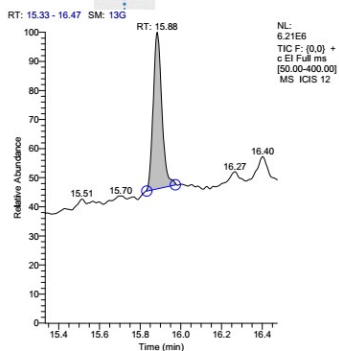


Formula C₁₆H₂₀O₄, MW 276, CAS# 19892-19-4, Entry# 9616





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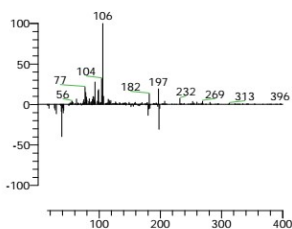
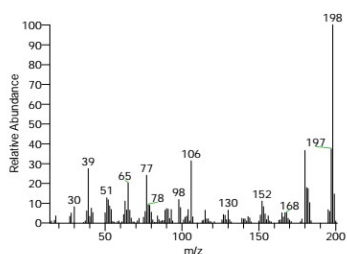


RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
15.88	813	876	52.53	mainlib	C13H14N2	198
15.88	813	876	52.53	NISTDEMO	C13H14N2	198
15.88	796	856	34.98	replib	C13H14N2	198
15.88	774	825	34.98	NISTDEMO	C13H14N2	198
15.88	801	858	34.98	replib	C13H14N2	198

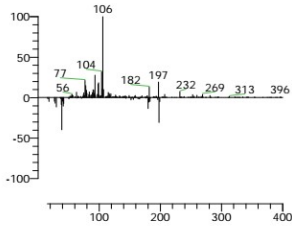
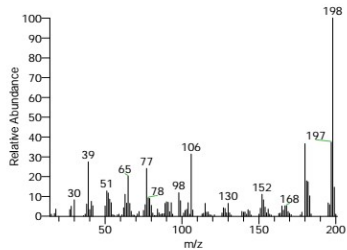
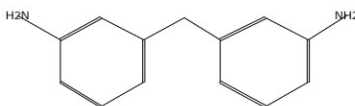
Hit Spectrum

Delta

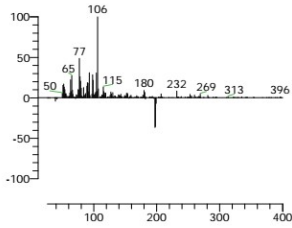
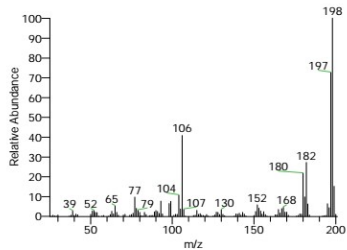
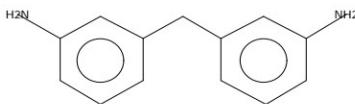
Compound Structure



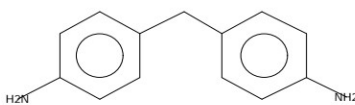
3,3'-Diaminodiphenylmethane
Formula C13H14N2, MW 198, CAS# 19471-12-6, Entry# 215
3-(3-Aminobenzyl)phenylamine #



3,3'-Diaminodiphenylmethane
Formula C13H14N2, MW 198, CAS# 19471-12-6, Entry# 161610
3-(3-Aminobenzyl)phenylamine #

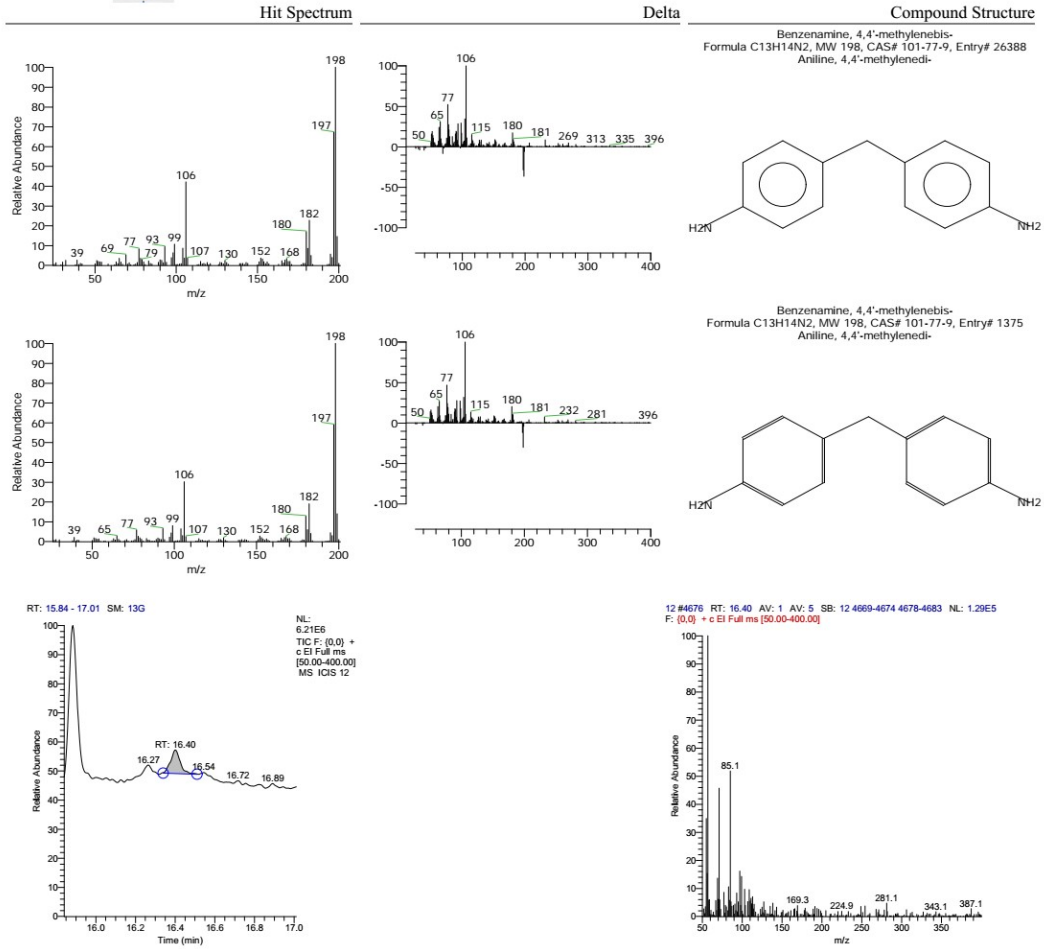


Benzenamine, 4,4'-methylenebis-
Formula C13H14N2, MW 198, CAS# 101-77-9, Entry# 26389
Aniline, 4,4'-methylene-





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RT	SI	RSI	Probability	Library	Molecular Formula	Molecular Weight
16.40	580	642	18.21	replib	C ₂₆ H ₅₄	366
16.40	618	647	18.21	mainlib	C ₂₆ H ₅₄	366
16.40	587	681	4.96	mainlib	C ₂₆ H ₅₄	366
16.40	584	665	4.38	replib	C ₄₄ H ₉₀	618
16.40	583	682	4.21	mainlib	C ₂₆ H ₅₄	366

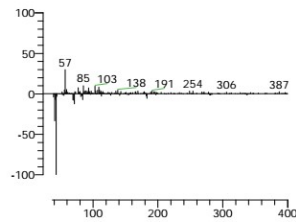
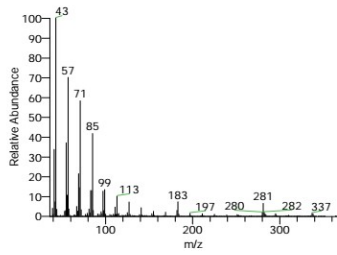


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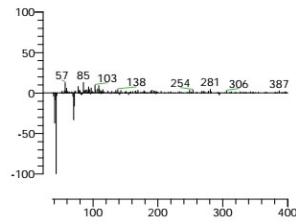
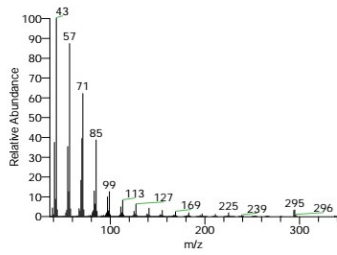
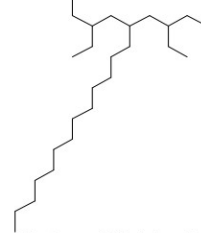
Hit Spectrum

Delta

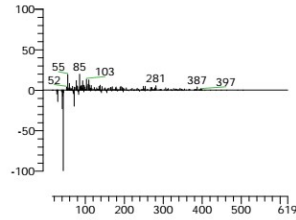
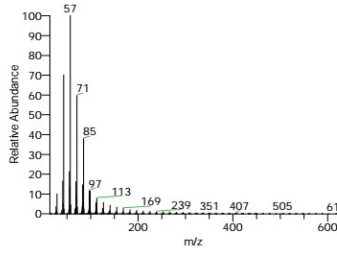
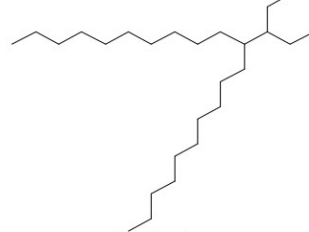
Compound Structure



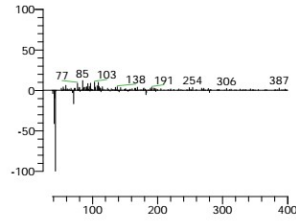
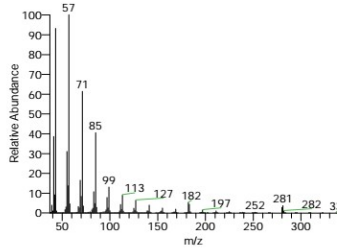
Octadecane, 3-ethyl-5-(2-ethylbutyl)-
Formula C₂₆H₅₄, MW 366, CAS# 55282-12-7, Entry# 7471
3-Ethyl-5-(2-ethylbutyl)octadecane



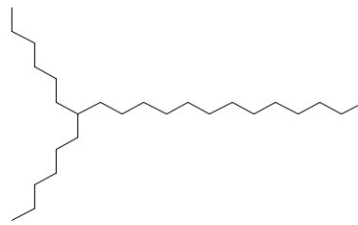
Heneicosane, 11-(1-ethylpropyl)-
Formula C₂₆H₅₄, MW 366, CAS# 55282-11-6, Entry# 7468
11-(1-Ethylpropyl)heneicosane



Tetratetracontane
Formula C₄₄H₉₀, MW 618, CAS# 7098-22-8, Entry# 5823
n-Tetratetracontane



Eicosane, 7-hexyl-
Formula C₂₆H₅₄, MW 366, CAS# 55333-99-8, Entry# 22628
7-n-Hexyleicosane





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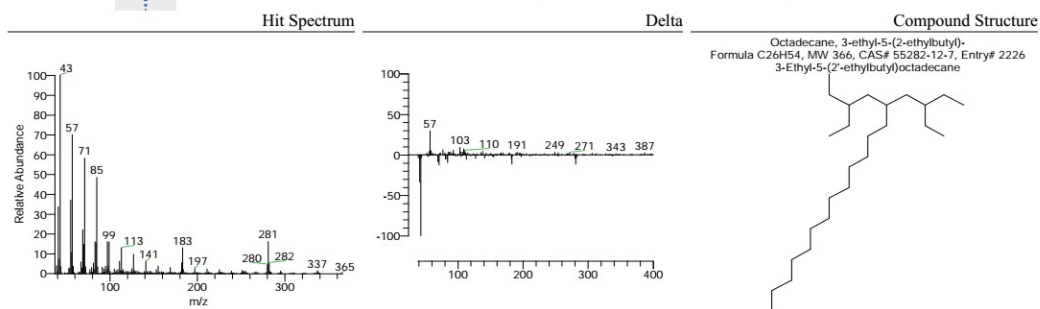


Fig. S1 GC-MS data of the volatile reaction products.