

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX110720\
 Data File : VX019346.D
 Acq On : 06 Nov 2020 16:51
 Operator : JC/MD
 Sample : L4636-09
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DRUM-COMP-1-AU

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102720W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	59	63	89	rBV	1993055	2285323	78.70%	11.276%
2	2.093	158	165	178	rBV	338217	587886	20.24%	2.901%
3	2.331	198	204	211	rVB	29123	46943	1.62%	0.232%
4	2.416	211	218	231	rBV	194321	323132	11.13%	1.594%
5	2.575	236	244	259	rBV	267525	505231	17.40%	2.493%
6	3.910	455	463	480	rBV2	28314	83159	2.86%	0.410%
7	4.300	514	527	539	rBV4	16508	56091	1.93%	0.277%
8	4.641	573	583	597	rBV3	33226	108050	3.72%	0.533%
9	5.465	706	718	733	rBV	188510	540331	18.61%	2.666%
10	5.629	733	745	763	rVB	318379	892862	30.75%	4.405%
11	6.031	799	811	822	rBV	215263	560376	19.30%	2.765%
12	6.830	931	942	959	rBV	508776	1202783	41.42%	5.934%
13	7.269	1007	1014	1024	rBV2	23687	56166	1.93%	0.277%
14	8.622	1227	1236	1241	rBV	39158	63614	2.19%	0.314%
15	8.696	1241	1248	1255	rVV	1072267	1652827	56.92%	8.155%
16	8.763	1255	1259	1265	rVB2	22143	38805	1.34%	0.191%
17	9.074	1302	1310	1321	rBV	30287	52741	1.82%	0.260%
18	10.098	1471	1478	1490	rBV	1074790	1474190	50.77%	7.274%
19	10.543	1544	1551	1560	rBV	29158	40505	1.39%	0.200%
20	10.720	1577	1580	1588	rVB	25483	32097	1.11%	0.158%
21	10.805	1588	1594	1599	rBV	27525	36832	1.27%	0.182%
22	10.878	1599	1606	1620	rVB	73939	115342	3.97%	0.569%
23	11.018	1624	1629	1635	rBV	46137	60049	2.07%	0.296%
24	11.122	1641	1646	1655	rVB	923949	1164882	40.11%	5.747%
25	12.061	1795	1800	1808	rVV	1286247	1554169	53.52%	7.668%
26	12.140	1808	1813	1819	rVB	85088	112757	3.88%	0.556%
27	12.256	1827	1832	1850	rBV	2330495	2903923	100.00%	14.328%
28	12.500	1867	1872	1885	rBV	81318	142332	4.90%	0.702%
29	12.616	1886	1891	1907	rVB	2245618	2566875	88.39%	12.665%
30	12.860	1925	1931	1934	rBV	102243	132721	4.57%	0.655%
31	13.006	1951	1955	1968	rBV	34233	59941	2.06%	0.296%
32	13.109	1968	1972	1974	rVV	32764	46310	1.59%	0.228%
33	13.140	1974	1977	1999	rVB	62167	126486	4.36%	0.624%
34	13.463	2025	2030	2034	rBV	35505	58689	2.02%	0.290%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : SW846 8260

35	13.548	2040	2044	2052	rVB	80024	114027	3.93%	0.563%
36	13.750	2072	2077	2078	rBV	24599	33380	1.15%	0.165%
37	13.786	2078	2083	2096	rVB3	92205	199283	6.86%	0.983%
38	13.926	2104	2106	2119	rVB5	19054	37938	1.31%	0.187%
39	14.445	2187	2191	2195	rBV	27893	31744	1.09%	0.157%
40	15.609	2376	2382	2389	rBV	110169	166910	5.75%	0.824%

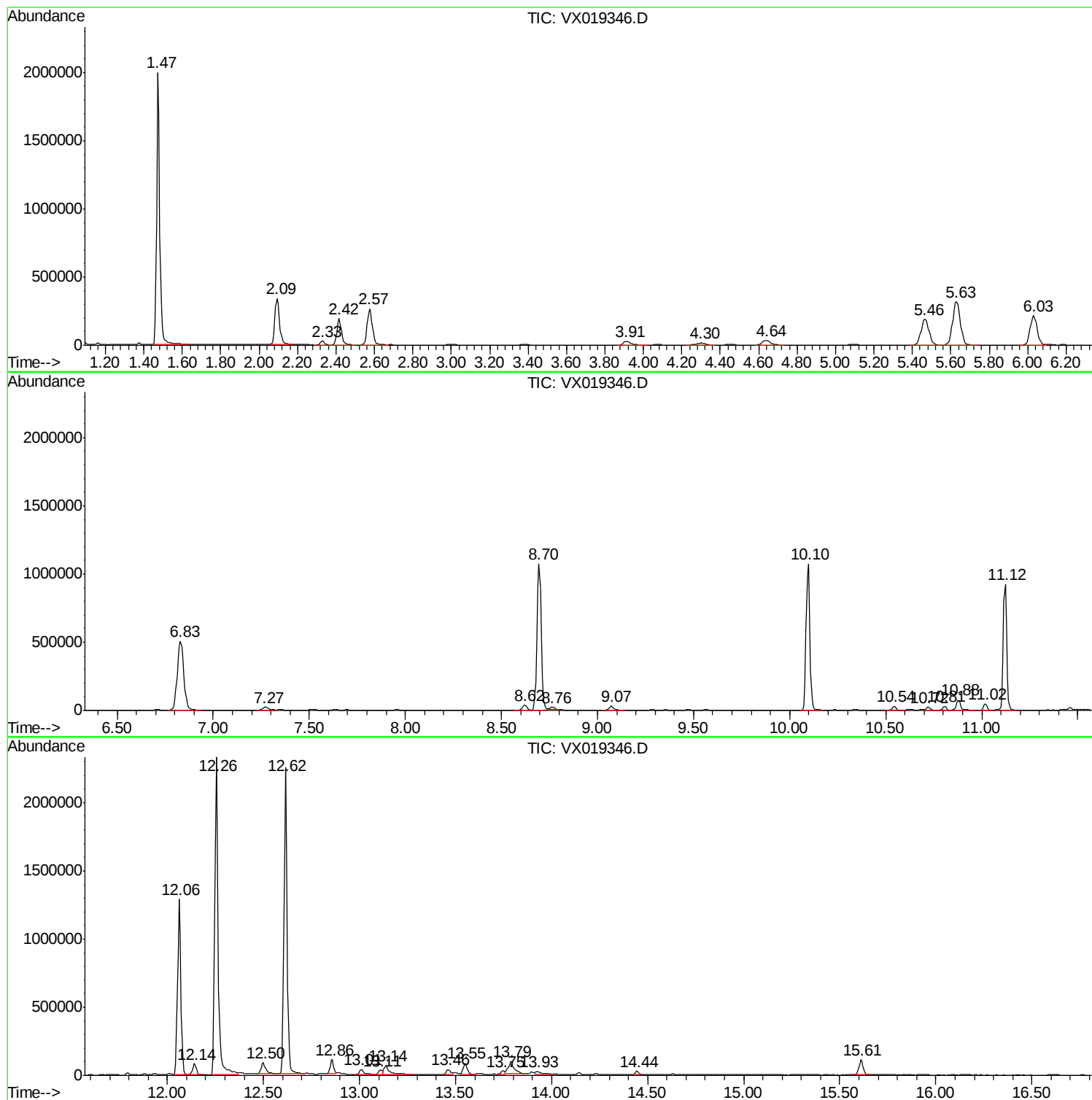
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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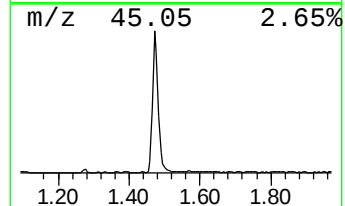
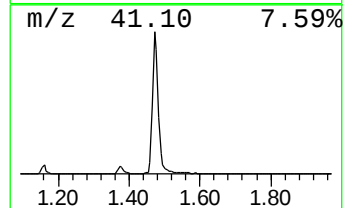
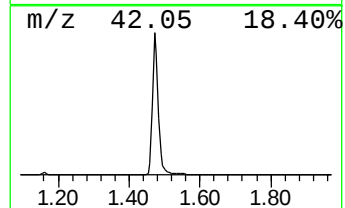
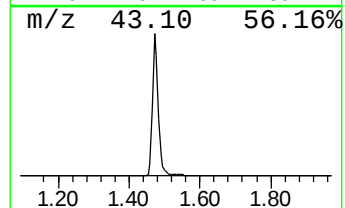
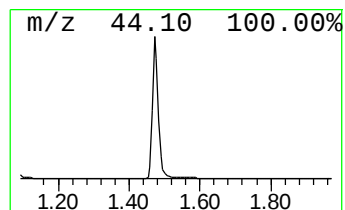
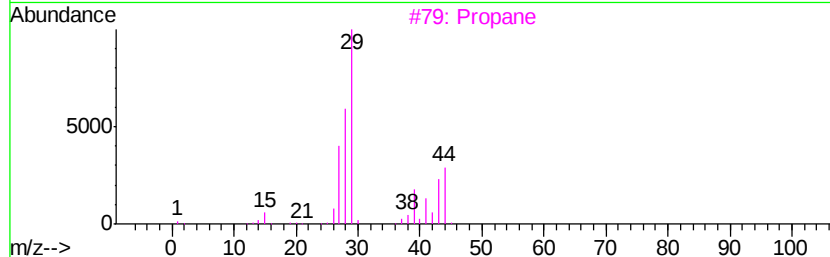
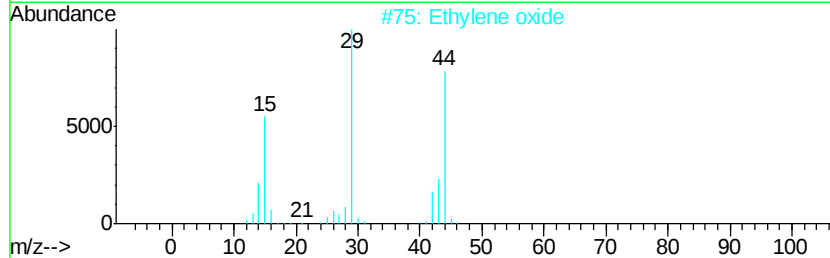
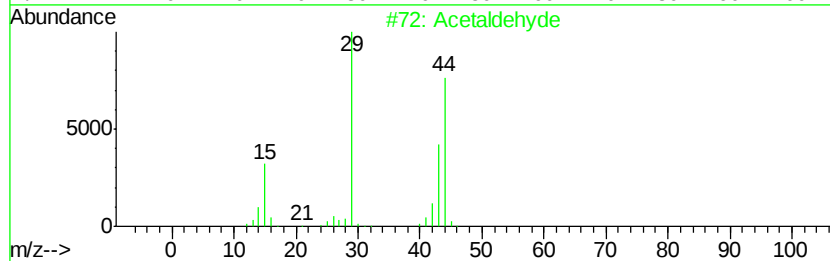
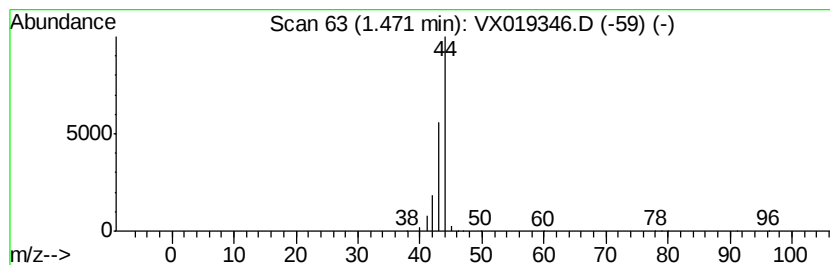
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	127.98 ug/l	2285320	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehydve	44	C2H4O	000075-07-0	64
2		Ethylene oxide	44	C2H4O	000075-21-8	5
3		Propane	44	C3H8	000074-98-6	4
4		Alanine	89	C3H7NO2	000056-41-7	4
5		Ethyne, fluoro-	44	C2HF	002713-09-9	3



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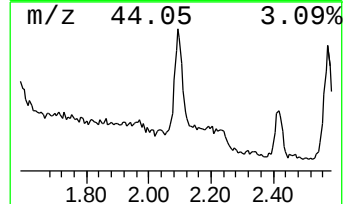
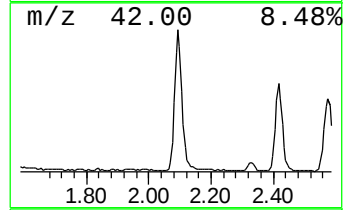
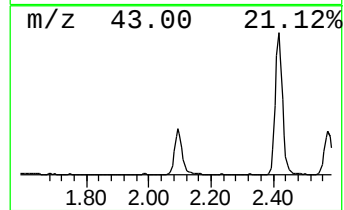
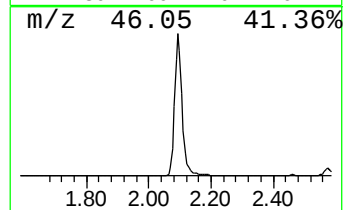
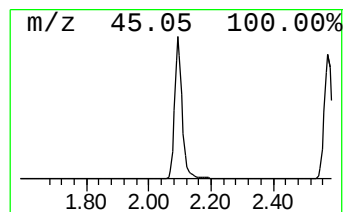
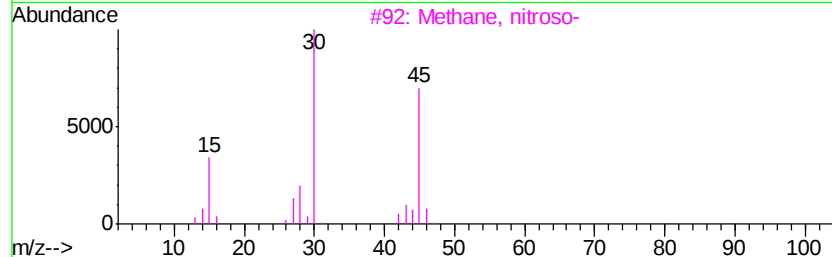
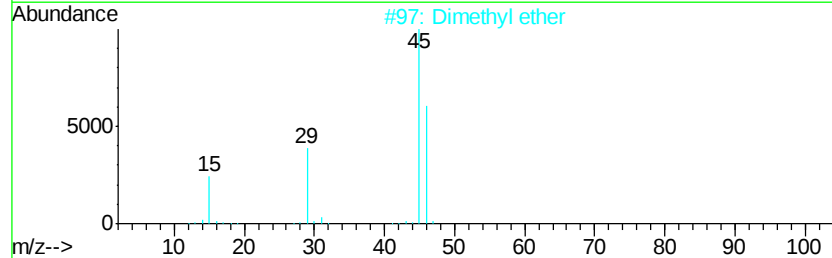
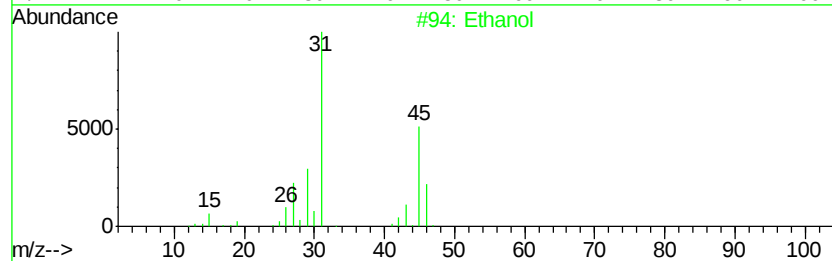
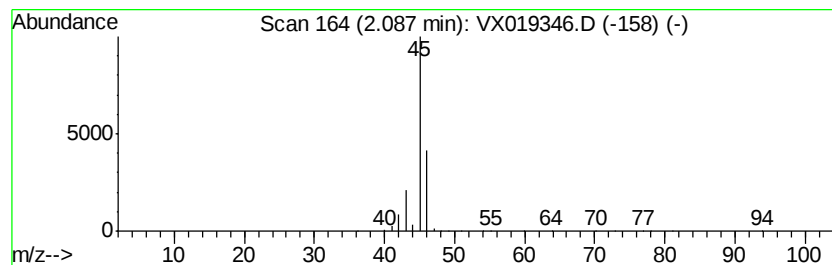
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	32.92 ug/l	587886	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	64
2		Dimethyl ether	46	C2H6O	000115-10-6	9
3		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Formic acid	46	CH2O2	000064-18-6	4
5		Oxalic acid	90	C2H2O4	000144-62-7	4



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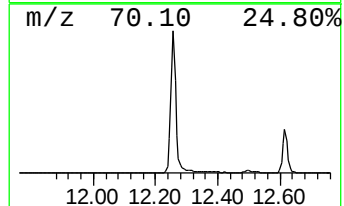
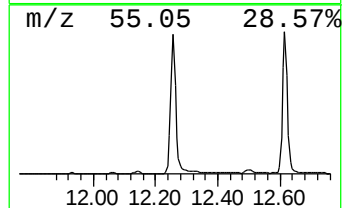
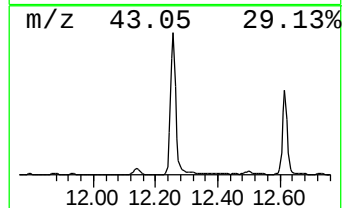
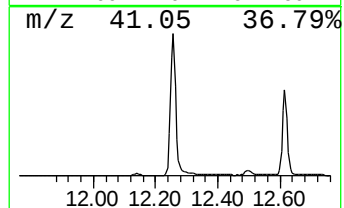
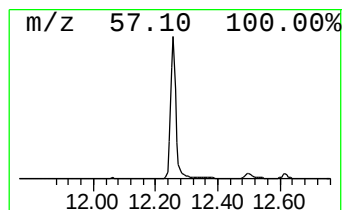
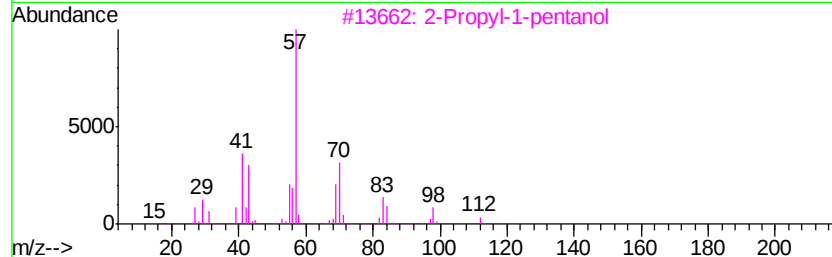
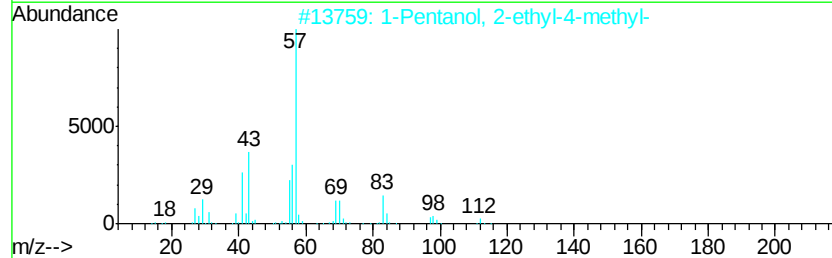
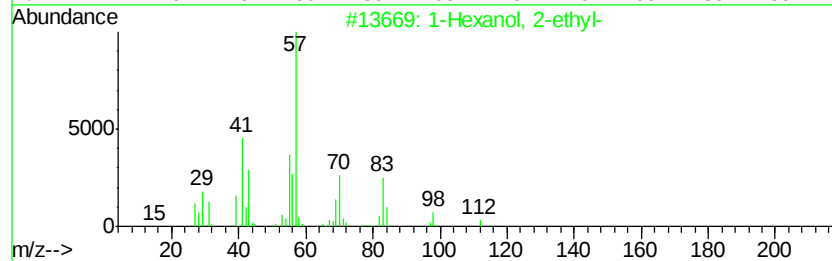
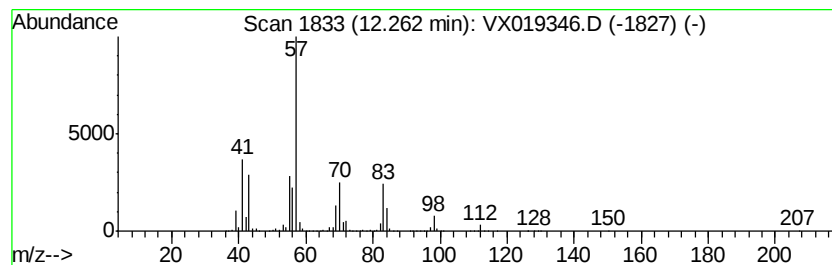
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	93.42 ug/l	2903920	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	90
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50
4	Heptyl isobutyl carbonate	216 C12H24O3	959068-08-7	47
5	2-Ethyl-1-hexanol, methyl ether	144 C9H20O	1000365-10-2	47



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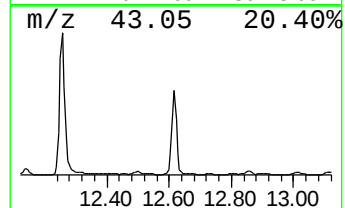
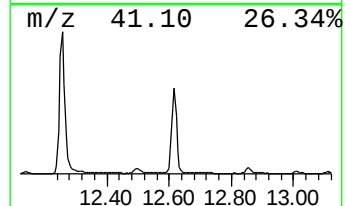
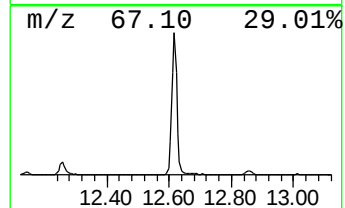
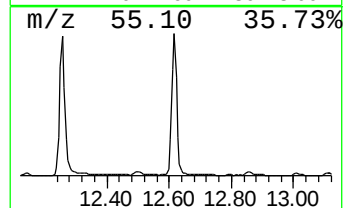
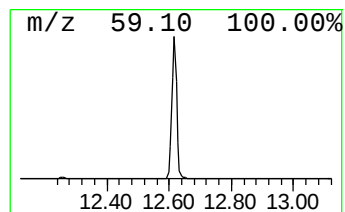
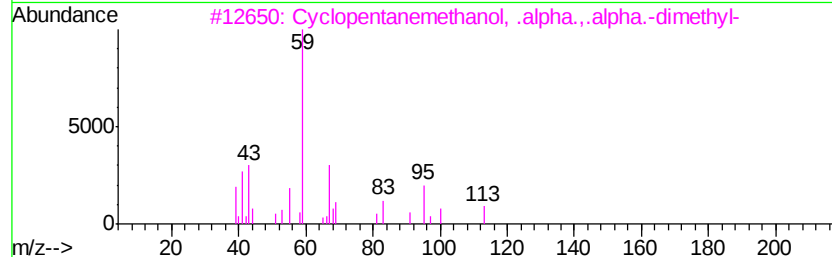
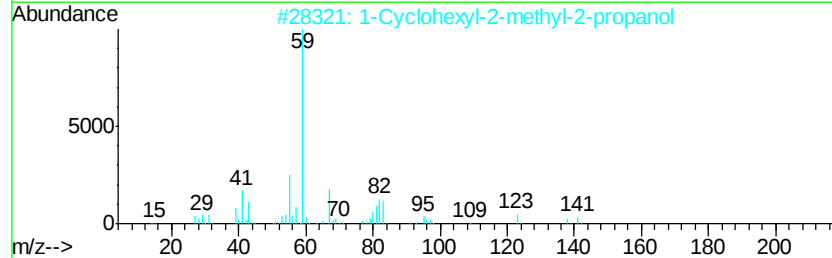
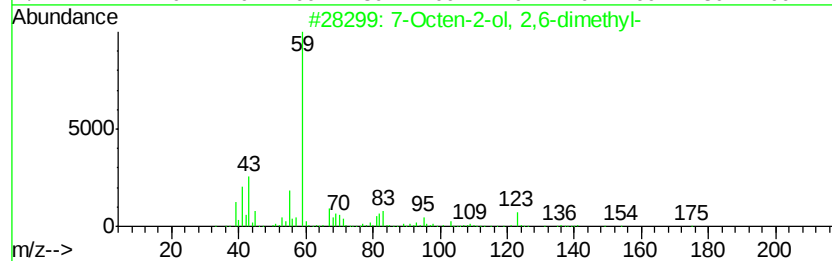
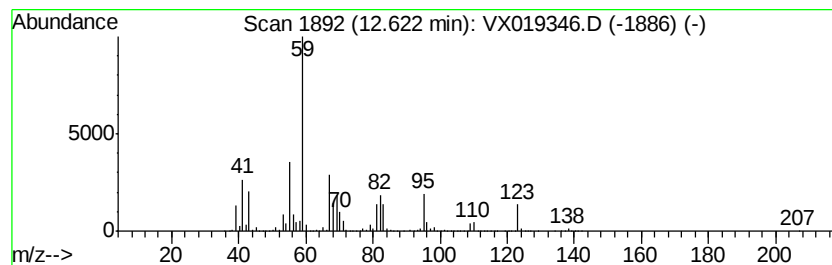
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	82.58 ug/l	2566880	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	72
2		1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	72
3		Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	59
4		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	50
5		1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	50



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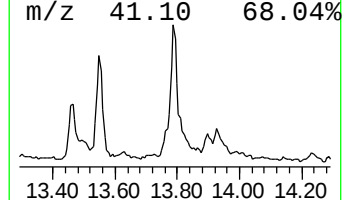
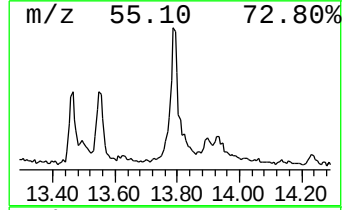
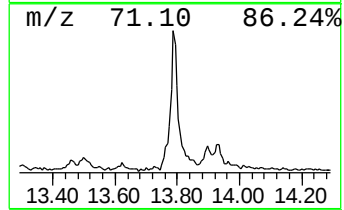
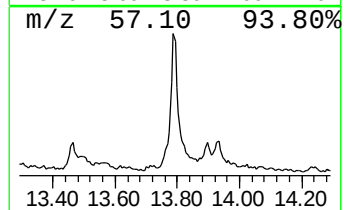
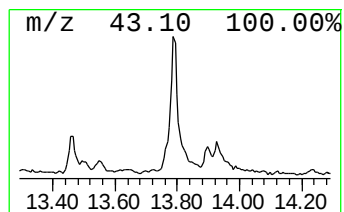
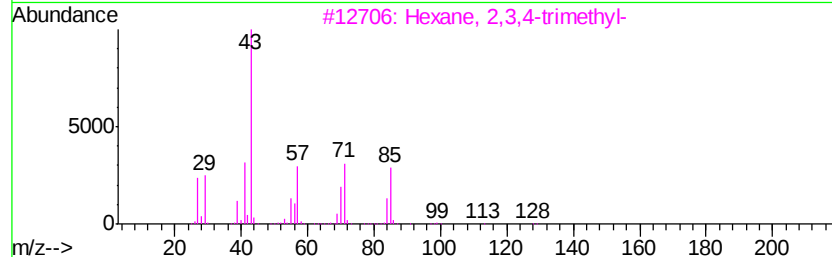
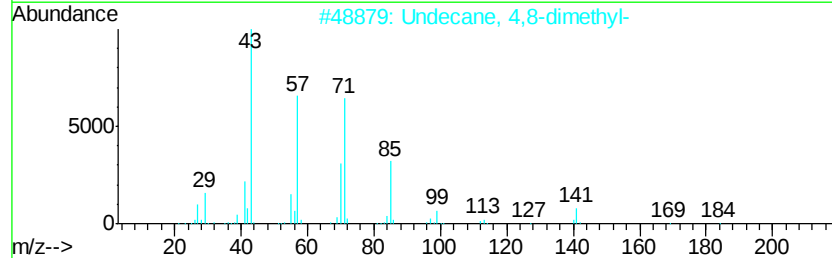
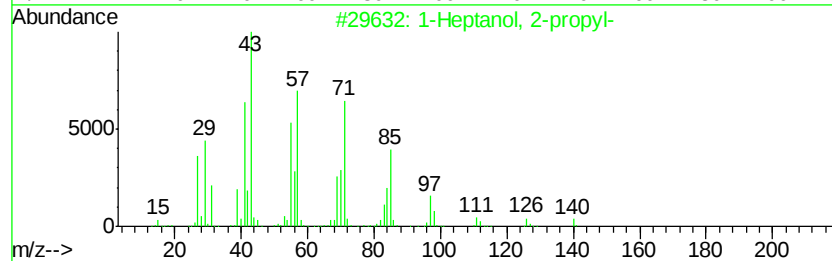
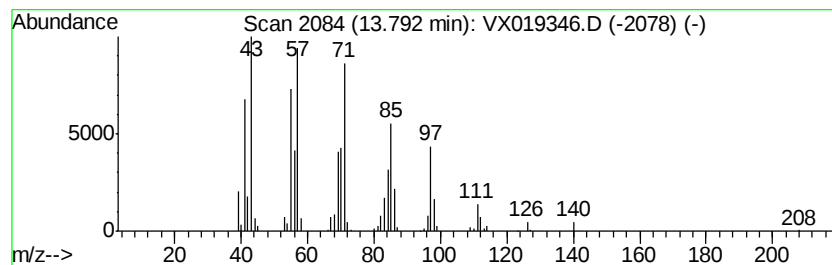
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heptanol, 2-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	6.41 ug/l	199283	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	64
2		Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	50
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	47
4		1-Octadecene	252	C18H36	000112-88-9	43
5		Octane, 4-methyl-	128	C9H20	002216-34-4	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX110720\
Data File : VX019346.D
Acq On : 06 Nov 2020 16:51
Operator : JC/MD
Sample : L4636-09
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DRUM-COMP-1-AU

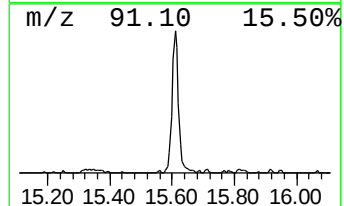
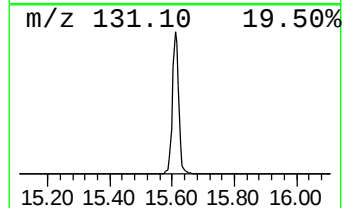
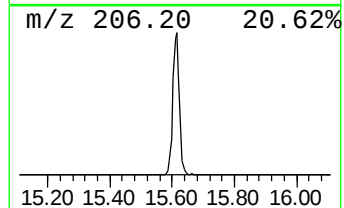
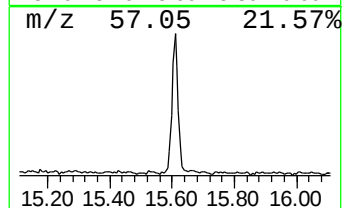
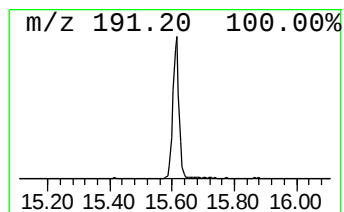
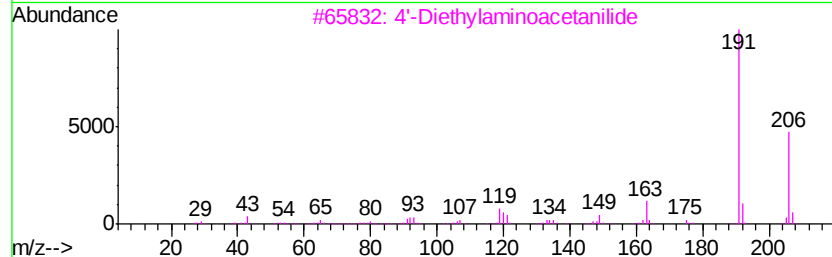
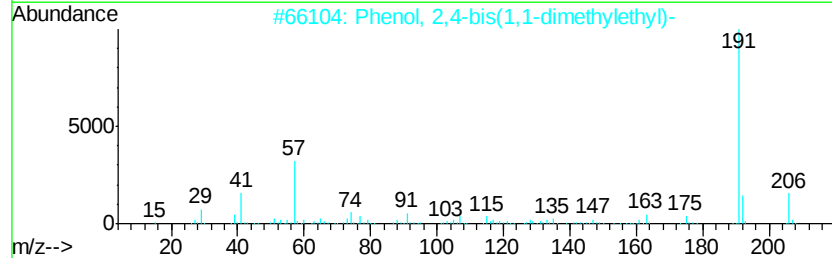
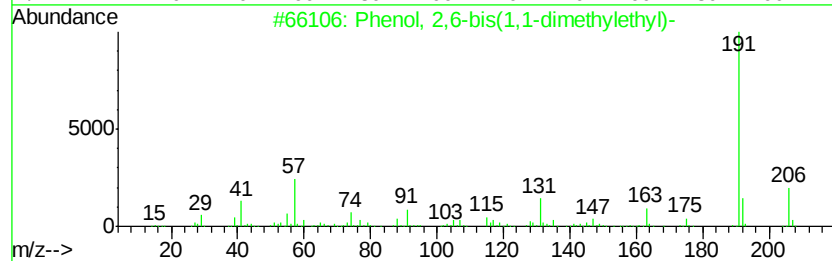
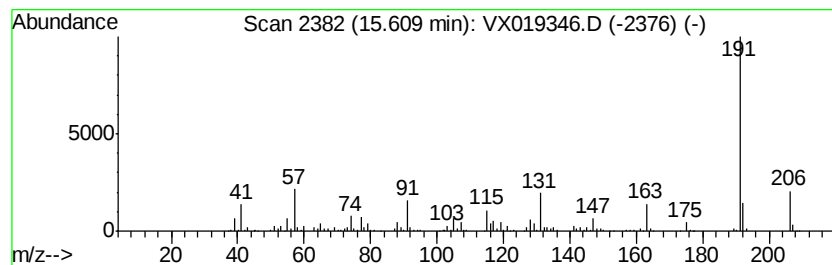
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	5.37 ug/l	166910	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
2		Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	83
3		4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	72
4		Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
5		Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	68



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX110720\
Data File : VX019346.D
Acq On : 06 Nov 2020 16:51
Operator : JC/MD
Sample : L4636-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DRUM-COMP-1-AU

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X102720W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.47	128.0	ug/l	2285320	1	5.63	892862	50.0
Ethanol	2.09	32.9	ug/l	587886	1	5.63	892862	50.0
1-Hexanol, 2-ethyl-	12.26	93.4	ug/l	2903920	4	12.06	1554170	50.0
7-Octen-2-ol, 2,6...	12.62	82.6	ug/l	2566880	4	12.06	1554170	50.0
1-Heptanol, 2-pro...	13.79	6.4	ug/l	199283	4	12.06	1554170	50.0
Phenol, 2,6-bis(1...	15.61	5.4	ug/l	166910	4	12.06	1554170	50.0