

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX040620\
 Data File : VX015510.D
 Acq On : 06 Apr 2020 14:18
 Operator : JC/SP
 Sample : L2097-14
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40789

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\82X032720W.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	1.064	25	29	42	rBV	4933349	5646762	25.13%	5.886%
2	1.472	92	96	109	rBV	13882413	15048200	66.96%	15.686%
3	2.088	192	197	206	rBV	386048	559420	2.49%	0.583%
4	2.332	231	237	246	rBV	2419432	3769933	16.77%	3.930%
5	2.417	246	251	261	rVB	568410	934169	4.16%	0.974%
6	3.832	474	483	488	rBV	92985	246177	1.10%	0.257%
7	3.947	488	502	523	rVB	7817706	22474666	100.00%	23.427%
8	4.453	576	585	601	rVB	896703	2464858	10.97%	2.569%
9	5.472	740	752	763	rBV	659306	1879946	8.36%	1.960%
10	5.636	768	779	795	rVB	1162194	3263865	14.52%	3.402%
11	6.039	835	845	863	rBV	727738	1903424	8.47%	1.984%
12	6.837	965	976	988	rBV	1808686	4322271	19.23%	4.505%
13	7.276	1041	1048	1061	rBV	119387	305829	1.36%	0.319%
14	8.697	1275	1281	1288	rBV	3802421	5935203	26.41%	6.187%
15	10.099	1505	1511	1521	rBV	3928555	5290706	23.54%	5.515%
16	10.343	1546	1551	1558	rVB	251225	366949	1.63%	0.383%
17	11.123	1674	1679	1685	rBV	3295216	4139265	18.42%	4.315%
18	11.422	1723	1728	1736	rBV	242361	485768	2.16%	0.506%
19	11.495	1736	1740	1747	rVB2	246774	421566	1.88%	0.439%
20	11.720	1773	1777	1781	rVV	242267	293290	1.30%	0.306%
21	11.794	1784	1789	1795	rVB	611398	757196	3.37%	0.789%
22	11.909	1802	1808	1816	rVB	318286	472010	2.10%	0.492%
23	12.013	1821	1825	1829	rVV2	436325	845758	3.76%	0.882%
24	12.062	1829	1833	1840	rVV	4122239	5192781	23.11%	5.413%
25	12.129	1840	1844	1849	rVB	218032	272840	1.21%	0.284%
26	12.257	1862	1865	1868	rBV	638751	763323	3.40%	0.796%
27	12.361	1877	1882	1888	rVB4	217806	364696	1.62%	0.380%
28	12.836	1956	1960	1966	rBV5	125329	236320	1.05%	0.246%
29	13.001	1984	1987	1995	rBV	179715	250943	1.12%	0.262%
30	13.330	2038	2041	2046	rVB2	275866	433809	1.93%	0.452%
31	13.464	2061	2063	2073	rVB6	211110	336559	1.50%	0.351%
32	13.793	2113	2117	2120	rBV	275333	362937	1.61%	0.378%
33	13.885	2128	2132	2139	rVB2	526271	770190	3.43%	0.803%
34	13.958	2139	2144	2151	rBV3	467664	776022	3.45%	0.809%

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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

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35	14.269	2190	2195	2202	rVB5	282585	475173	2.11%	0.495%
36	14.525	2233	2237	2244	rBV4	188526	320530	1.43%	0.334%
37	14.659	2255	2259	2265	rBV3	422624	783861	3.49%	0.817%
38	14.714	2265	2268	2272	rVB	277142	325949	1.45%	0.340%
39	14.891	2294	2297	2301	rVB4	217768	268941	1.20%	0.280%
40	15.226	2348	2352	2355	rBV3	178963	287633	1.28%	0.300%
41	15.299	2360	2364	2371	rVB5	175886	390287	1.74%	0.407%
42	15.531	2398	2402	2406	rBV3	201448	290485	1.29%	0.303%
43	15.665	2420	2424	2428	rBV2	207481	286234	1.27%	0.298%
44	15.708	2428	2431	2439	rVB5	153541	277585	1.24%	0.289%
45	16.147	2499	2503	2514	rVB7	130784	281050	1.25%	0.293%
46	16.360	2530	2538	2545	rBV3	128380	358440	1.59%	0.374%

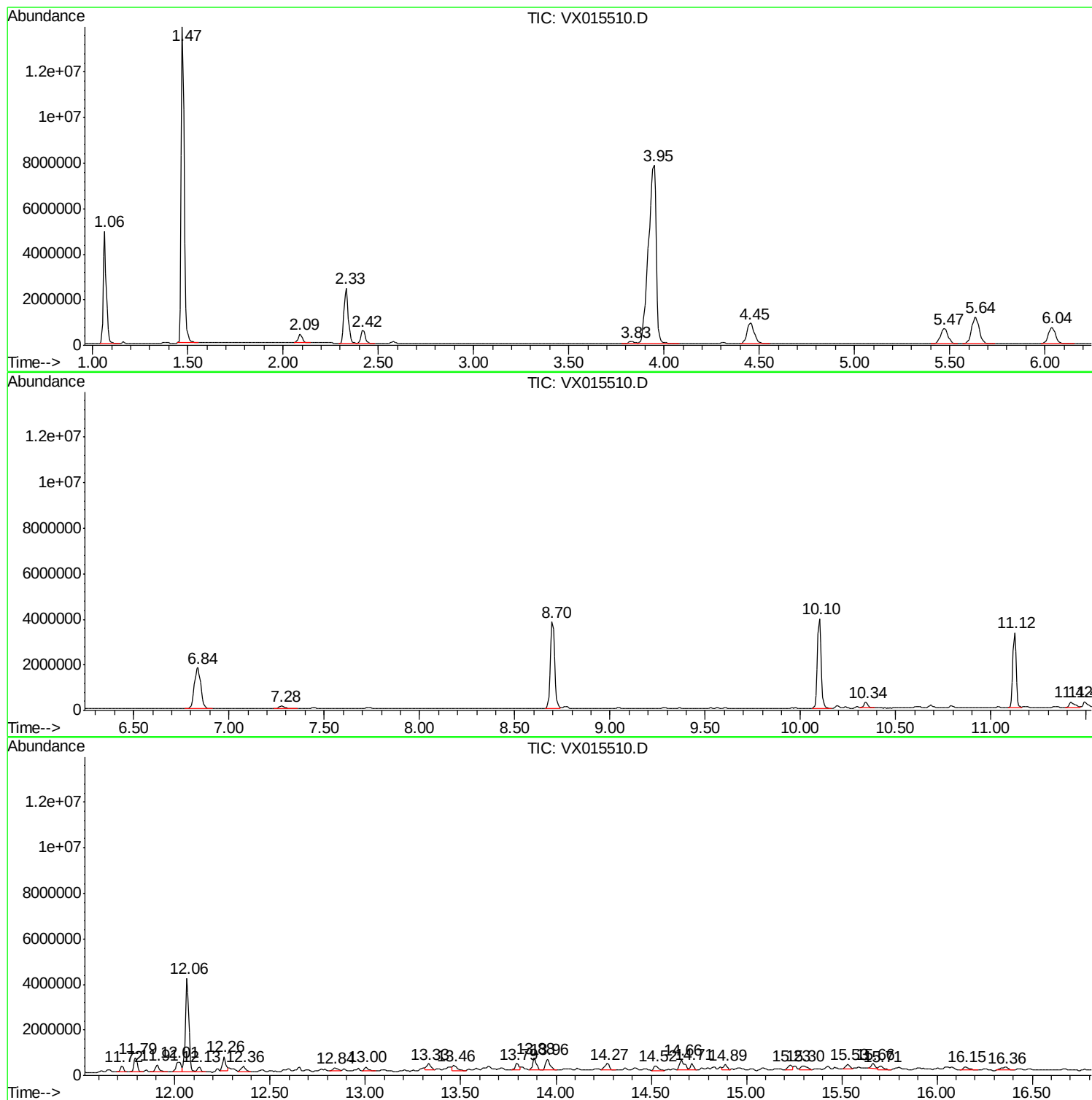
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



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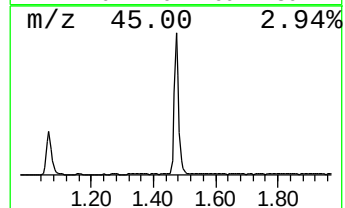
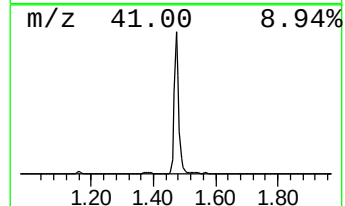
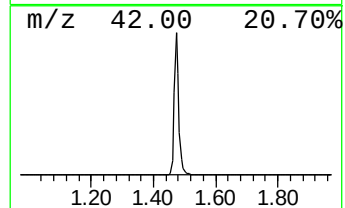
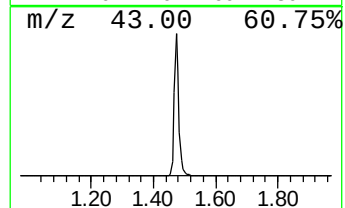
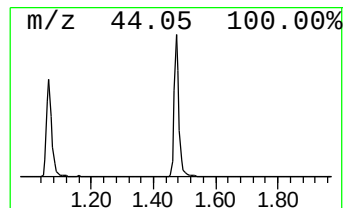
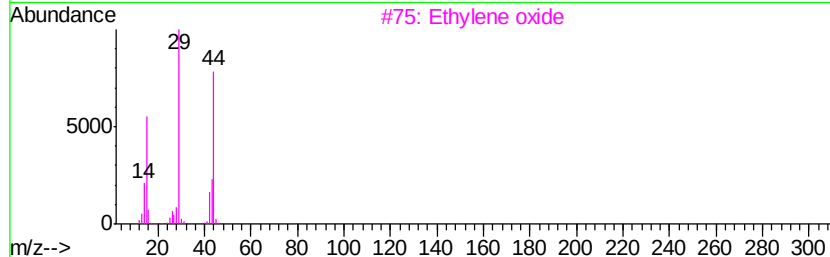
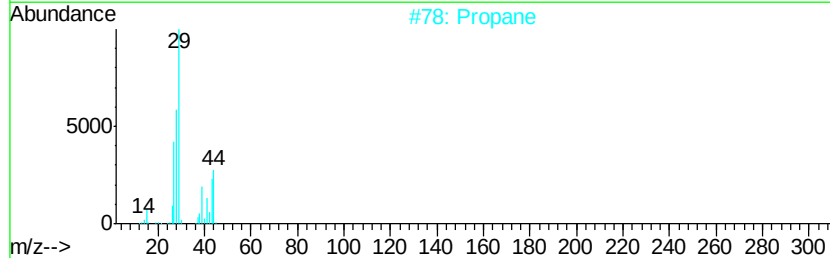
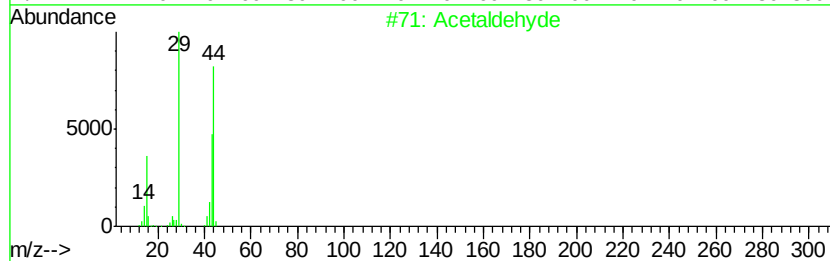
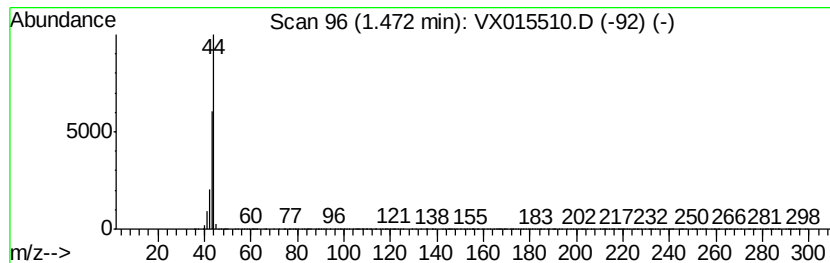
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	230.53 ug/l	15048200	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehyd	44	C2H4O	000075-07-0	74
2		Propane	44	C3H8	000074-98-6	5
3		Ethylene oxide	44	C2H4O	000075-21-8	5
4		Alanine	89	C3H7NO2	000056-41-7	4
5		Ethyne, fluoro-	44	C2HF	002713-09-9	3



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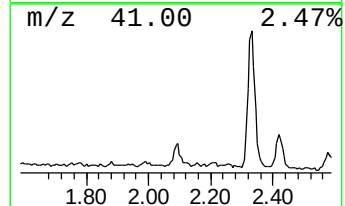
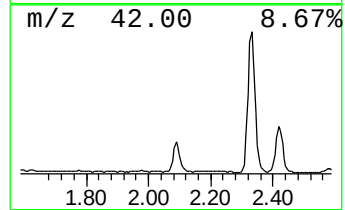
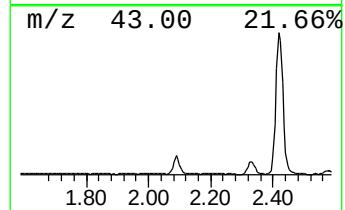
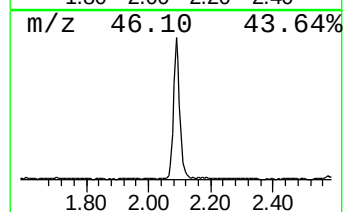
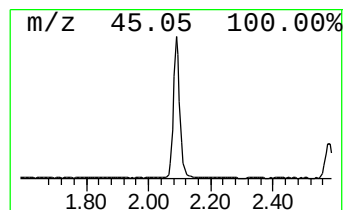
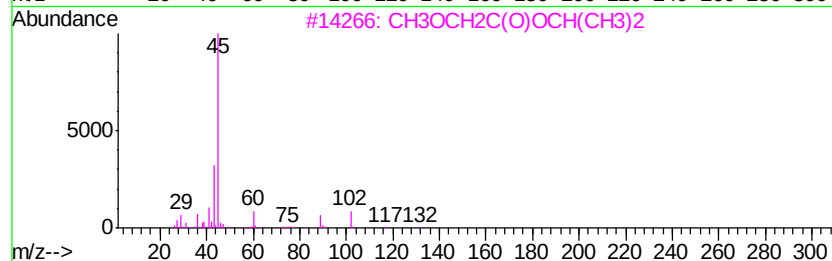
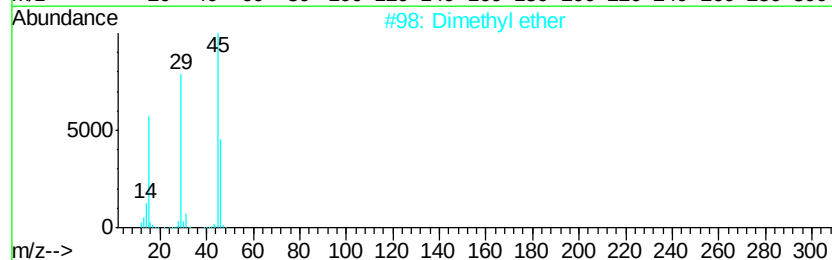
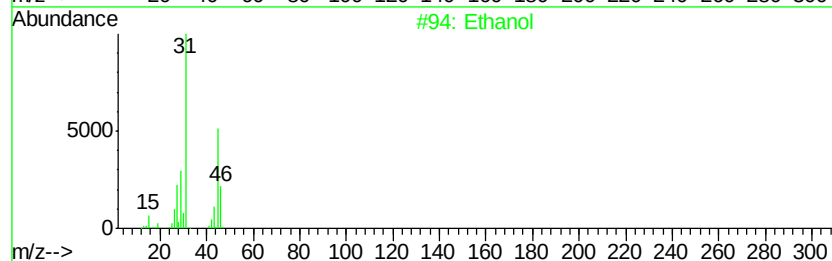
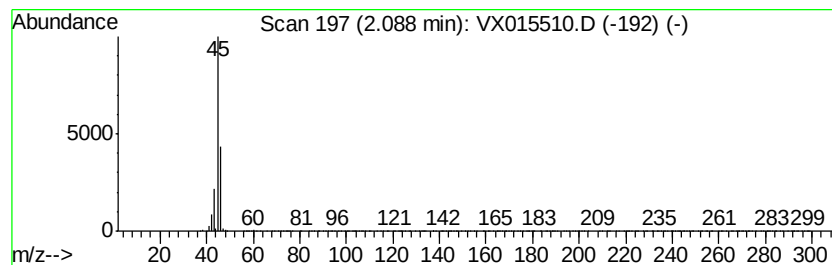
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	8.57 ug/l	559420	Pentafluorobenzene	5.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ethanol	46 C2H6O	000064-17-5	86
2	Dimethyl ether	46 C2H6O	000115-10-6	9
3	CH3OCH2C(O)OCH(CH3)2	132 C6H12O3	017640-21-0	7
4	Isopropyl Alcohol	60 C3H8O	000067-63-0	4
5	Methane, nitroso-	45 CH3NO	000865-40-7	4



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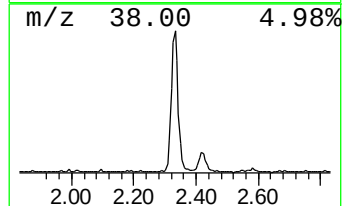
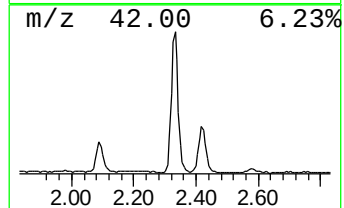
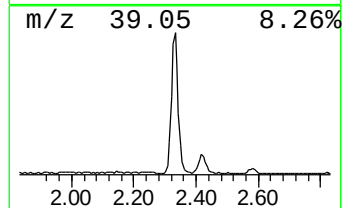
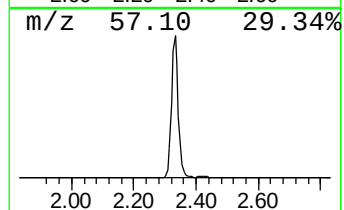
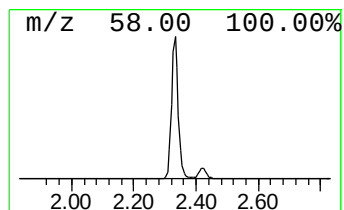
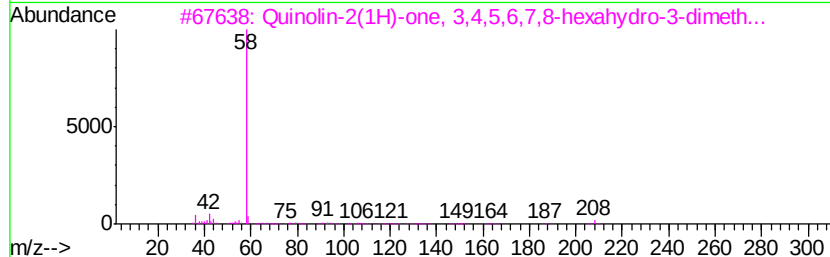
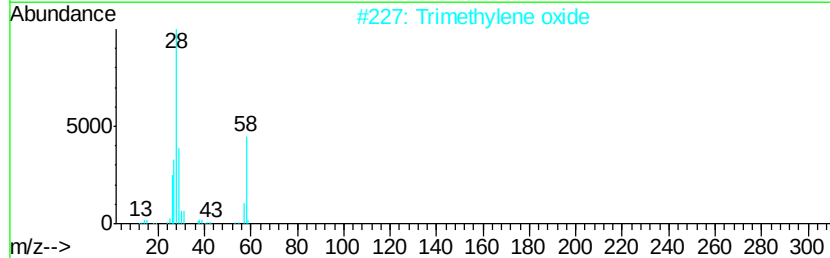
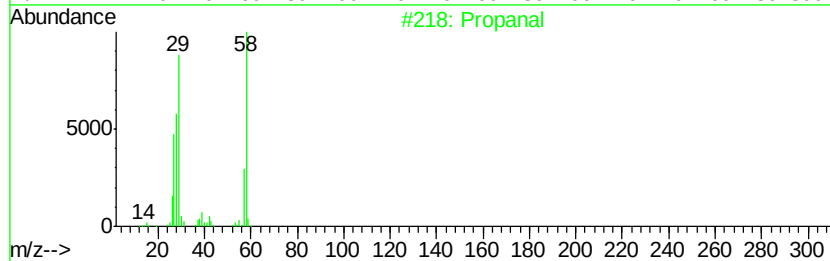
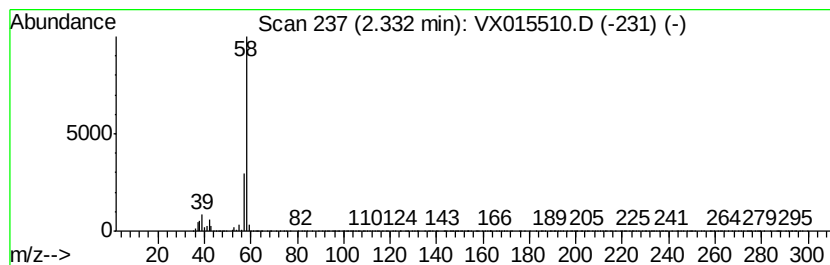
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 4 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	57.75 ug/l	3769930	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal		58	C3H6O	000123-38-6	78
2	Trimethylene oxide		58	C3H6O	000503-30-0	9
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...		208	C12H20N2O	1000259-95-6	9
4	Oxirane, methyl-, (S)-		58	C3H6O	016088-62-3	7
5	Propylene oxide		58	C3H6O	000075-56-9	7



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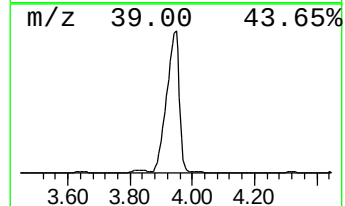
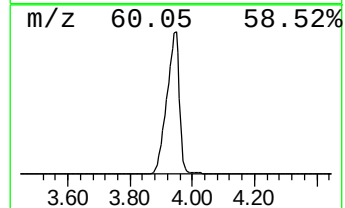
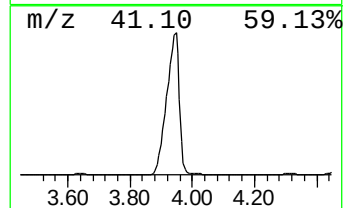
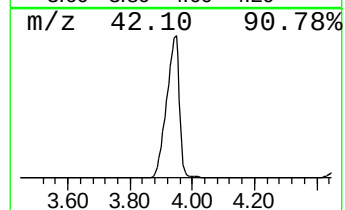
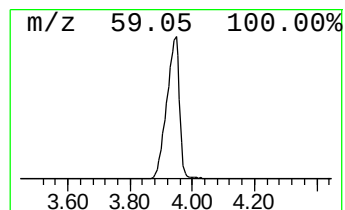
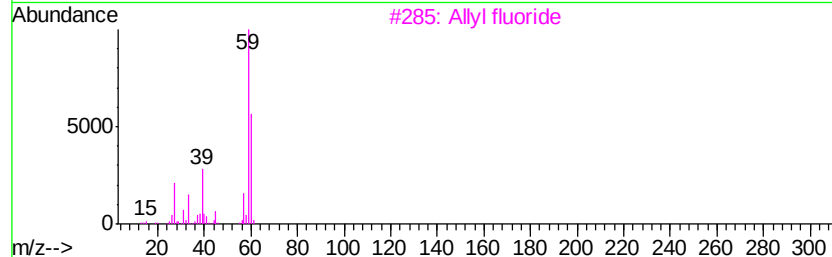
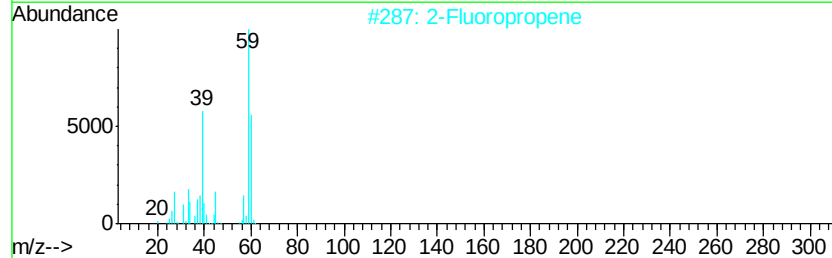
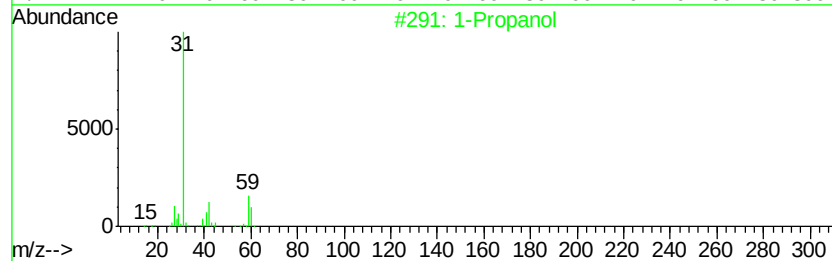
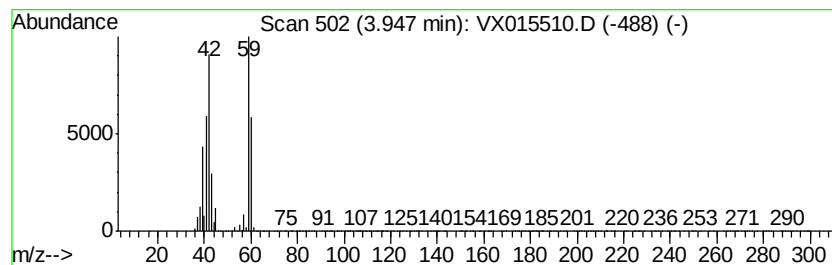
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.95	344.30 ug/l	22474700	Pentafluorobenzene	5.64

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	38
3	Allyl fluoride	60	C3H5F	000818-92-8	32
4	Cyclopropane	42	C3H6	000075-19-4	32
5	Propene	42	C3H6	000115-07-1	23



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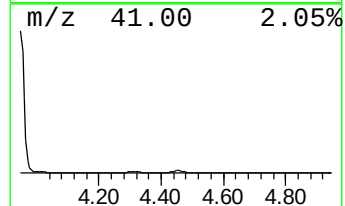
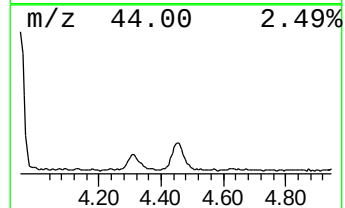
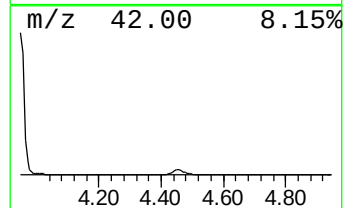
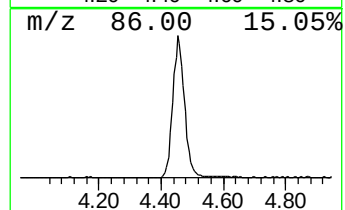
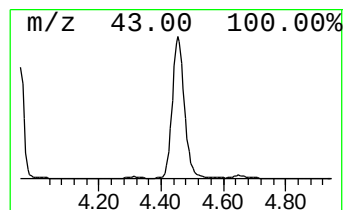
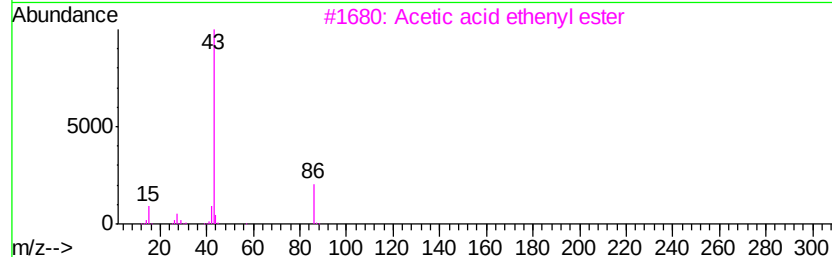
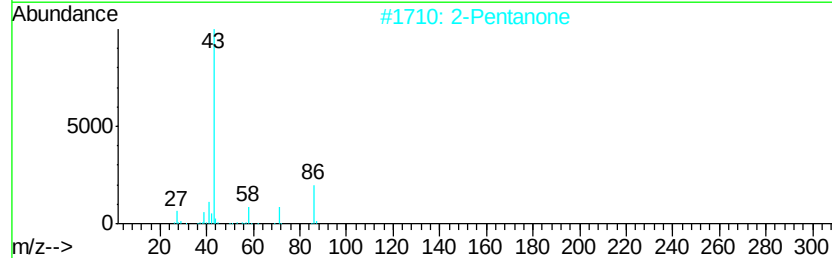
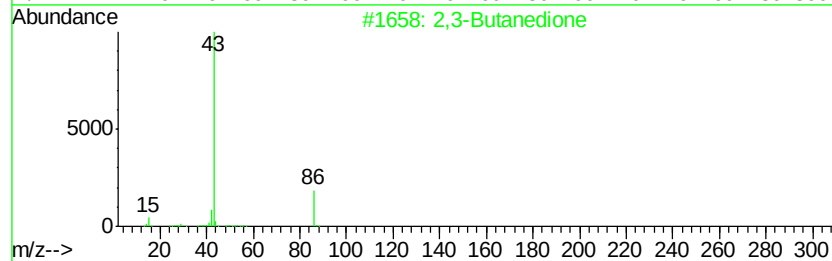
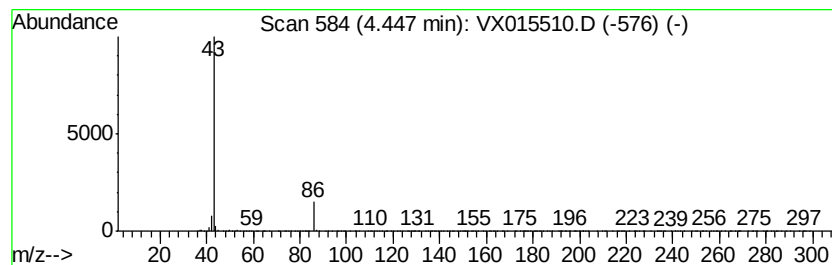
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Quant Title : SW846 8260

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

Peak Number 6 2,3-Butanedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	37.76 ug/l	2464860	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Butanedione	86	C4H6O2	000431-03-8	80
2		2-Pentanone	86	C5H10O	000107-87-9	50
3		Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
4		Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5		Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	5



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX040620\
Data File : VX015510.D
Acq On : 06 Apr 2020 14:18
Operator : JC/SP
Sample : L2097-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

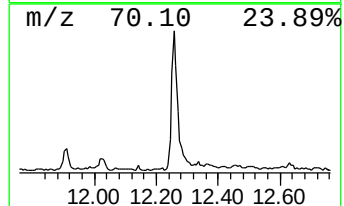
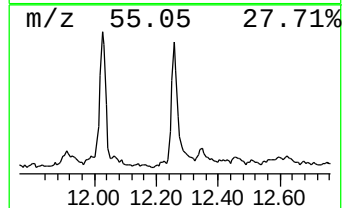
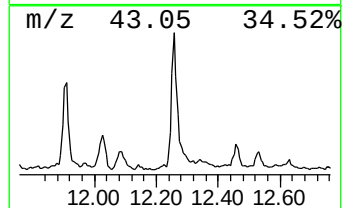
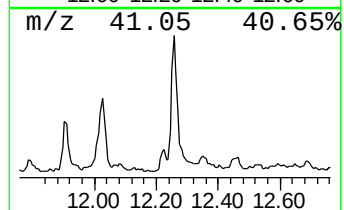
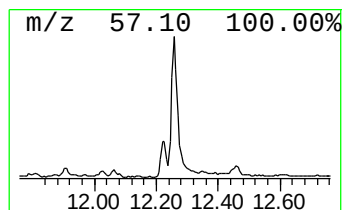
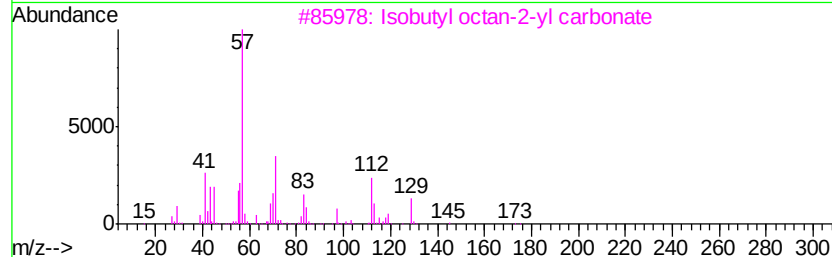
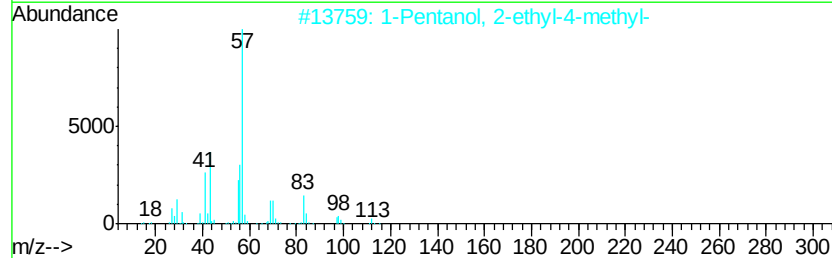
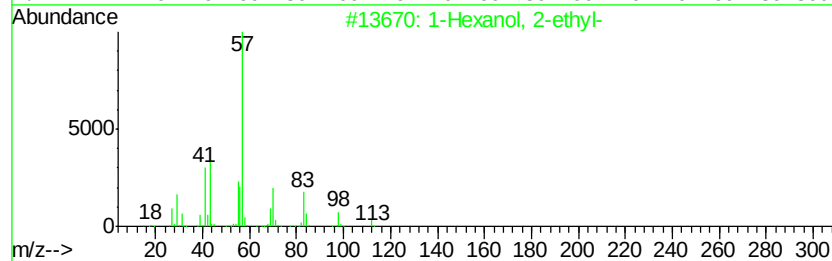
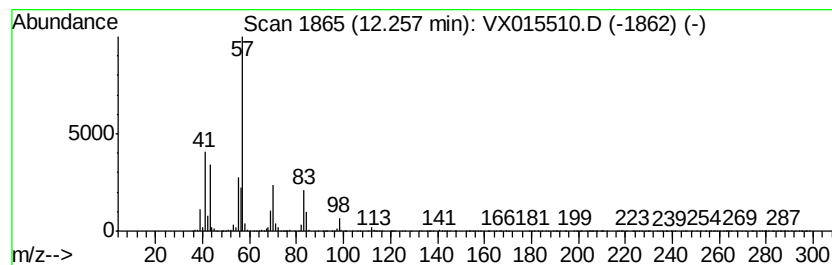
Instrument :
MSVOA_X
ClientSampleId :
40789

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	7.35 ug/l	763323	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	83
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	59
3	Isobutyl octan-2-yl carbonate	230 C13H26O3	1000372-74-7	56
4	Carbonic acid, isobutyl 2-ethylh...	230 C13H26O3	1000357-82-9	53
5	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX040620\
Data File : VX015510.D
Acq On : 06 Apr 2020 14:18
Operator : JC/SP
Sample : L2097-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40789

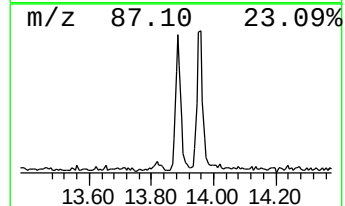
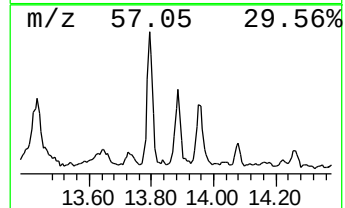
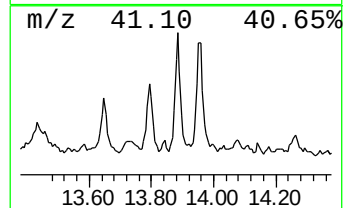
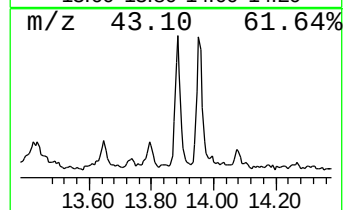
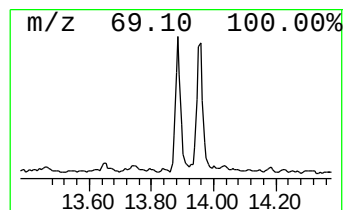
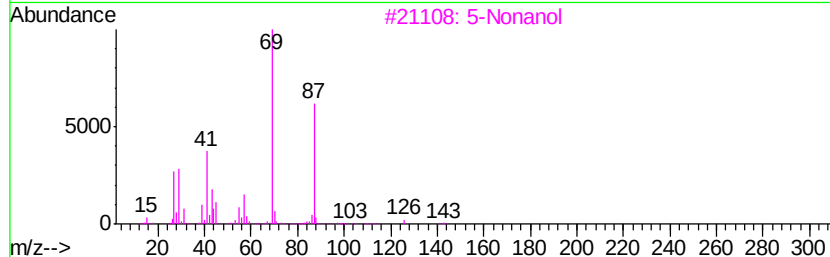
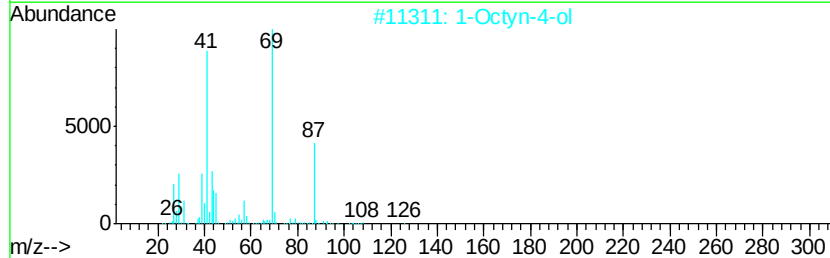
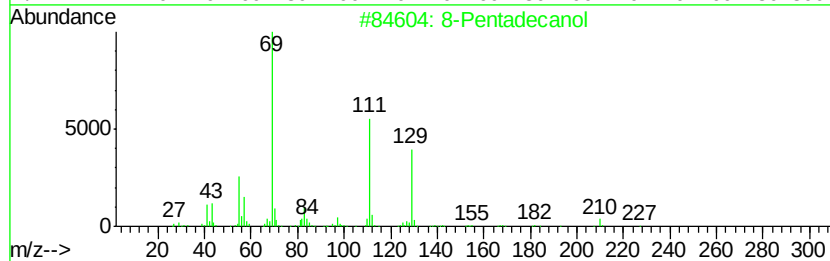
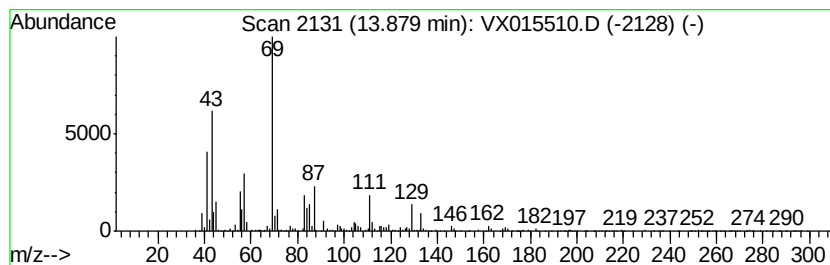
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown13.88 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.42 ug/l	770190	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	8-Pentadecanol	228	C15H32O	001653-35-6	47
2		1-Octyn-4-ol	126	C8H14O	052517-92-7	43
3		5-Nonanol	144	C9H20O	000623-93-8	43
4		2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	43
5		2-Propenoic acid, 2-methyl-, 1-m...	128	C7H12O2	004655-34-9	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX040620\
Data File : VX015510.D
Acq On : 06 Apr 2020 14:18
Operator : JC/SP
Sample : L2097-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40789

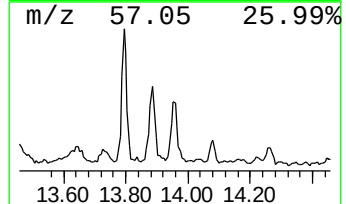
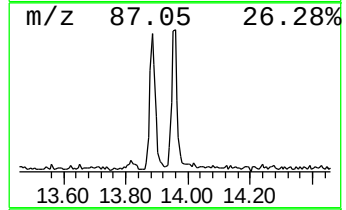
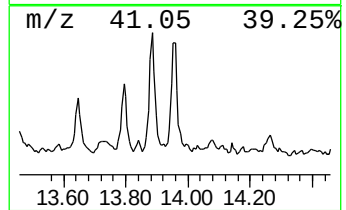
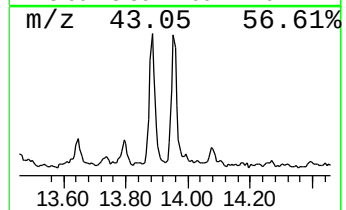
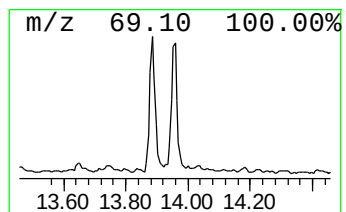
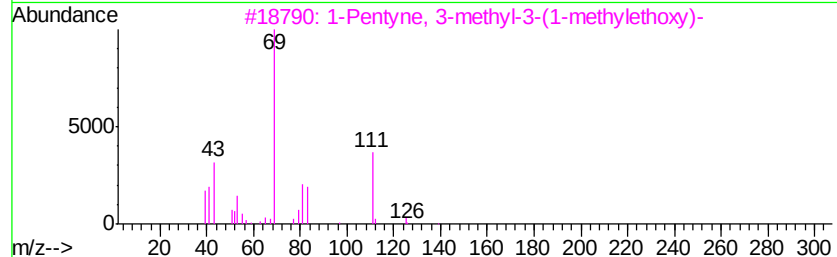
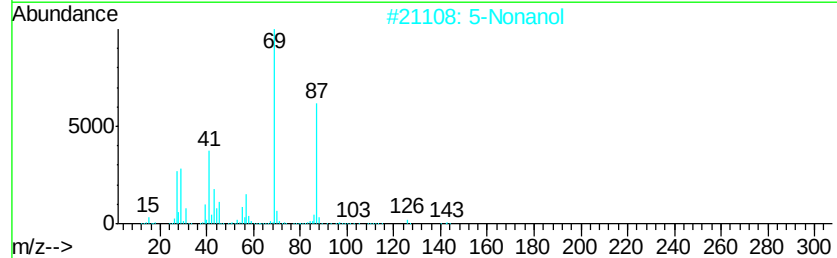
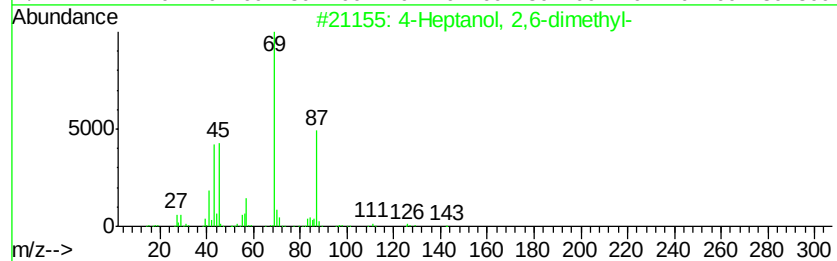
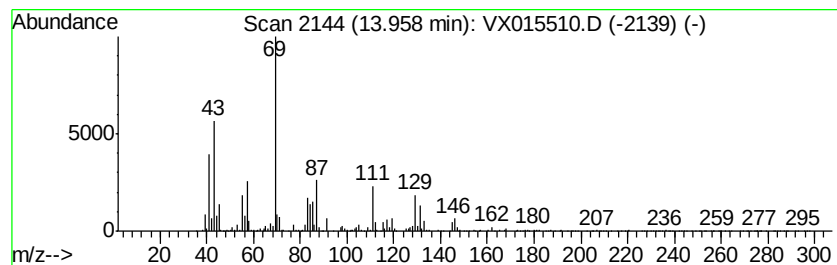
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown13.96 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	7.47 ug/l	776022	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	47
2		5-Nonanol	144	C9H20O	000623-93-8	43
3		1-Pentyne, 3-methyl-3-(1-methyle...	140	C9H16O	053966-55-5	43
4		2-Cyclopropylcarbonyloxododecane	254	C16H30O2	1000245-58-0	42
5		5-Dodecanol	186	C12H26O	010203-33-5	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX040620\
Data File : VX015510.D
Acq On : 06 Apr 2020 14:18
Operator : JC/SP
Sample : L2097-14
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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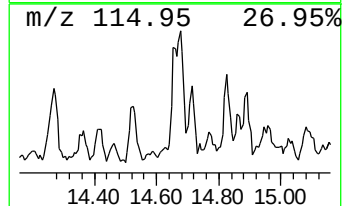
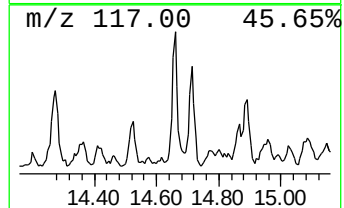
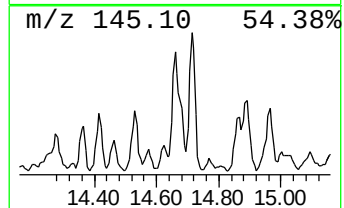
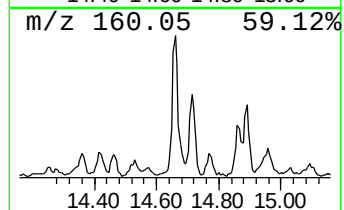
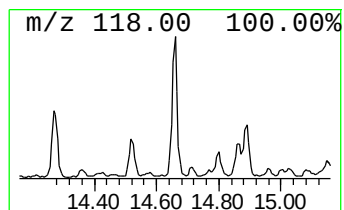
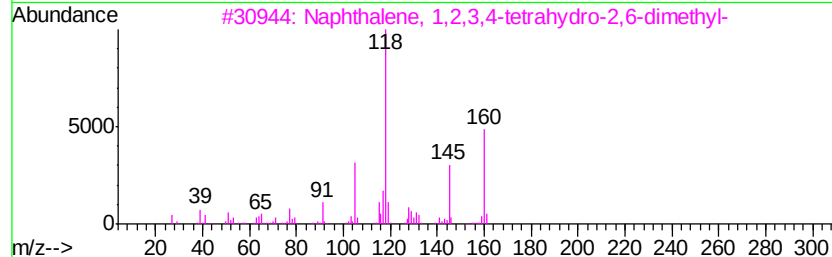
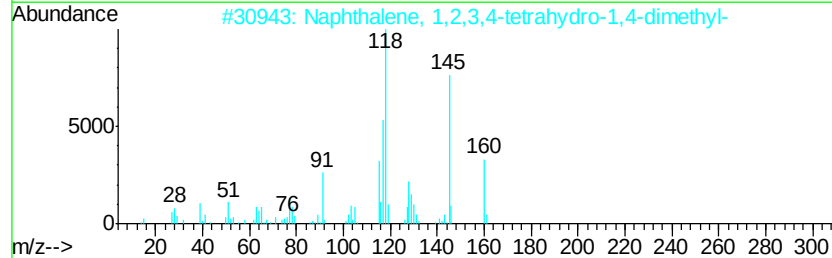
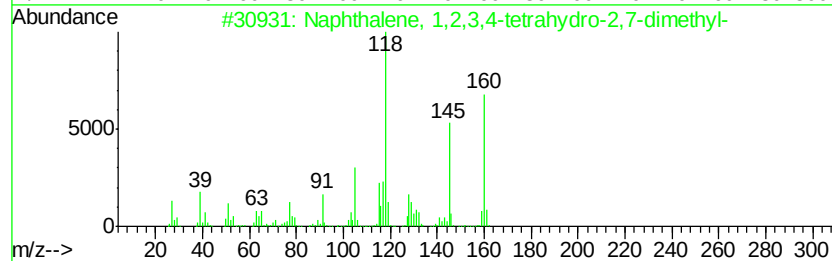
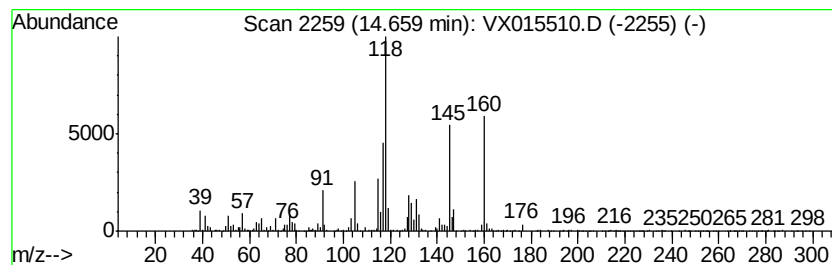
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	7.55 ug/l	783861	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	91
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	90
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	72
4		1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	64
5		Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	46



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX040620\
Data File : VX015510.D
Acq On : 06 Apr 2020 14:18
Operator : JC/SP
Sample : L2097-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40789

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.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	230.5	ug/l	15048200	1	5.64	3263870	50.0
Ethanol	2.09	8.6	ug/l	559420	1	5.64	3263870	50.0
Propanal	2.33	57.8	ug/l	3769930	1	5.64	3263870	50.0
1-Propanol	3.95	344.3	ug/l	22474700	1	5.64	3263870	50.0
2,3-Butanedione	4.45	37.8	ug/l	2464860	1	5.64	3263870	50.0
1-Hexanol, 2-ethyl-	12.26	7.3	ug/l	763323	4	12.06	5192780	50.0
unknown13.88	13.88	7.4	ug/l	770190	4	12.06	5192780	50.0
unknown13.96	13.96	7.5	ug/l	776022	4	12.06	5192780	50.0
Naphthalene, 1,2,...	14.66	7.5	ug/l	783861	4	12.06	5192780	50.0