

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
 Data File : VX008916.D
 Acq On : 13 Apr 2019 03:35
 Operator : JC/SP
 Sample : K2381-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 CL-COMP-3

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\82X040319W.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	1.453	47	49	111	rBV	29508846	87296231	100.00%	48.669%
2	2.202	151	172	175	rBV	9129678	35025139	40.12%	19.527%
3	2.355	191	197	206	rVB	713937	1234341	1.41%	0.688%
4	2.446	206	212	227	rVB	1235644	2162650	2.48%	1.206%
5	2.623	234	241	252	rVB	540634	947898	1.09%	0.528%
6	3.970	444	462	474	rBV	331811	947758	1.09%	0.528%
7	4.830	592	603	616	rBV	526792	1529426	1.75%	0.853%
8	5.933	774	784	796	rBV	336237	894987	1.03%	0.499%
9	7.299	1000	1008	1027	rVB	453384	931481	1.07%	0.519%
10	8.616	1217	1224	1234	rBV	844266	1438269	1.65%	0.802%
11	8.713	1234	1240	1247	rVB	685310	1070289	1.23%	0.597%
12	10.366	1497	1511	1516	rBV	1182690	1664514	1.91%	0.928%
13	11.134	1632	1637	1640	rBV	750702	1055203	1.21%	0.588%
14	11.530	1698	1702	1708	rVB	2365466	2709618	3.10%	1.511%
15	11.768	1737	1741	1744	rVV	769523	965133	1.11%	0.538%
16	11.804	1744	1747	1757	rVB	578253	1008555	1.16%	0.562%
17	12.060	1781	1789	1797	rVV	7348755	10376149	11.89%	5.785%
18	12.475	1846	1857	1861	rBV	3006458	3609388	4.13%	2.012%
19	12.633	1880	1883	1887	rVV	1989933	2496654	2.86%	1.392%
20	13.018	1942	1946	1953	rVB	741782	1101580	1.26%	0.614%
21	13.249	1972	1984	1990	rBV	5175699	11690157	13.39%	6.517%
22	13.322	1991	1996	1998	rVV	1112115	1588019	1.82%	0.885%
23	14.091	2118	2122	2126	rVB	1562434	1645376	1.88%	0.917%
24	14.810	2236	2240	2243	rBV	1070428	1146640	1.31%	0.639%
25	15.633	2369	2375	2381	rBV	3373446	4833436	5.54%	2.695%

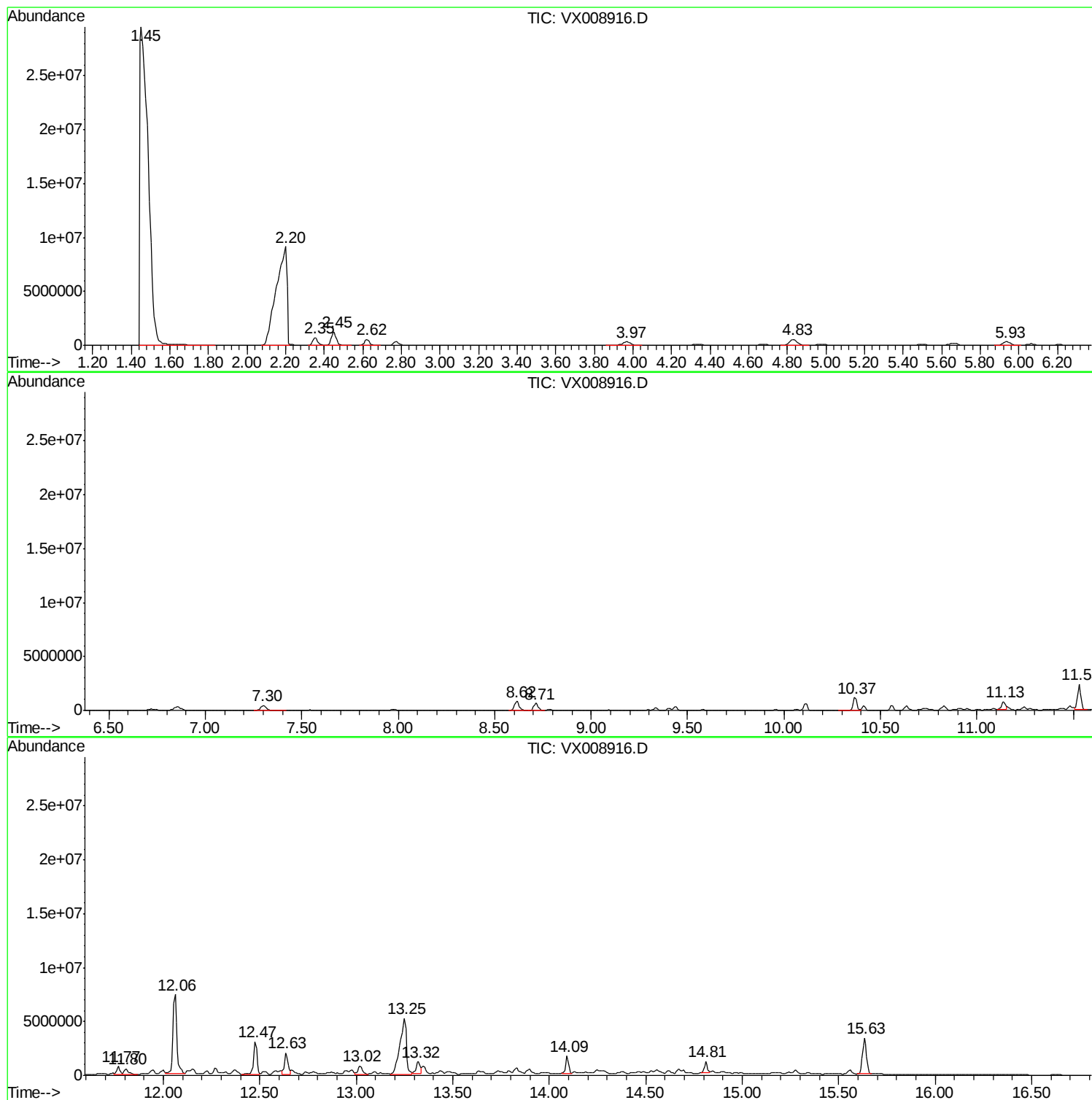
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampled :
CL-COMP-3

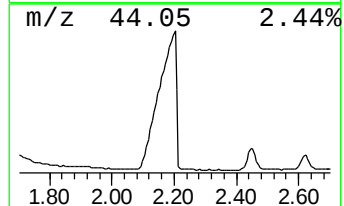
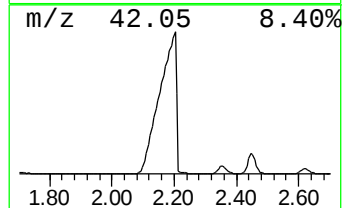
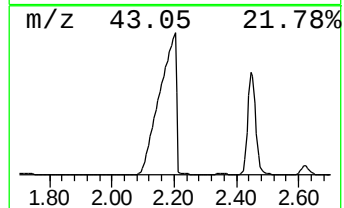
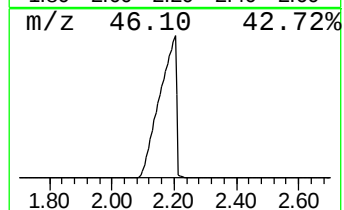
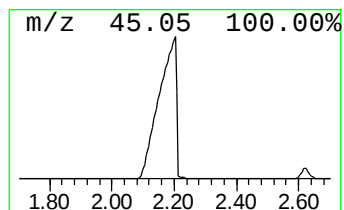
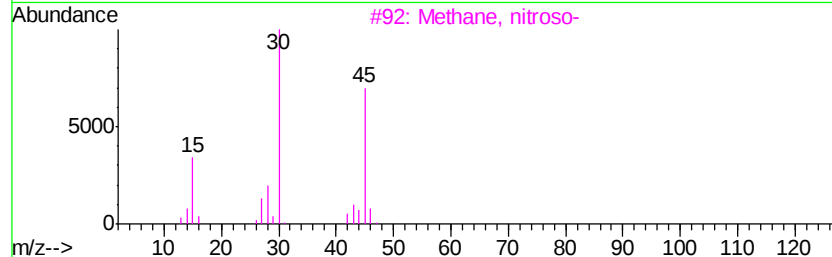
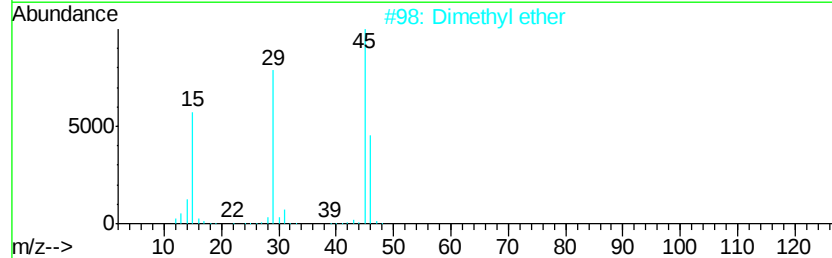
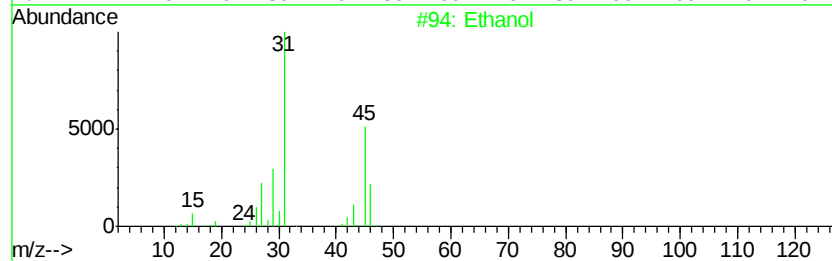
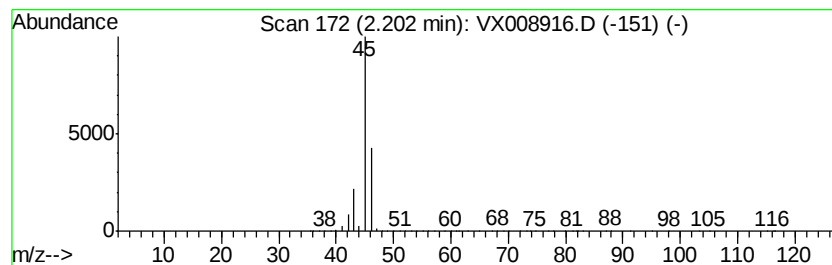
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	1956.74 ug/l	35025100	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	90
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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CL-COMP-3

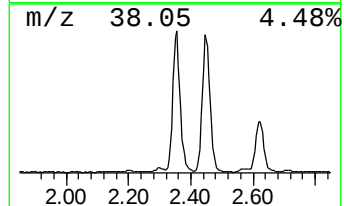
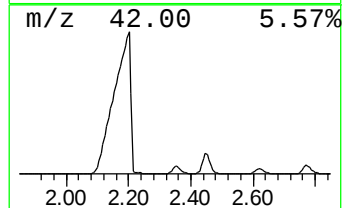
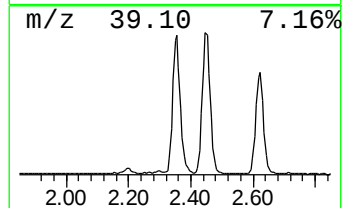
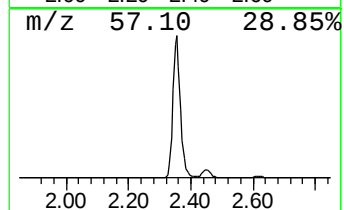
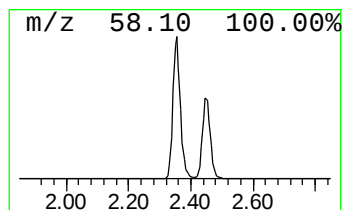
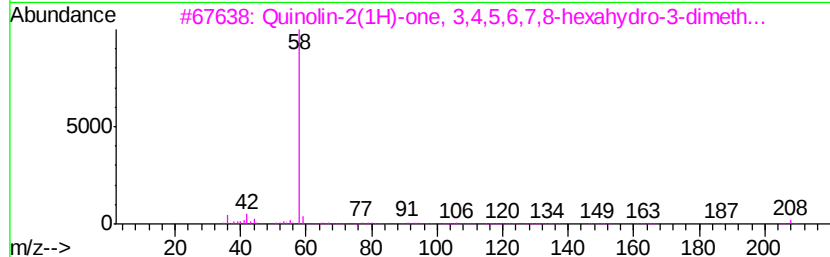
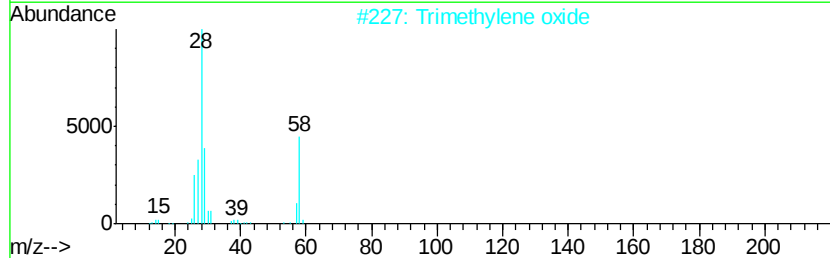
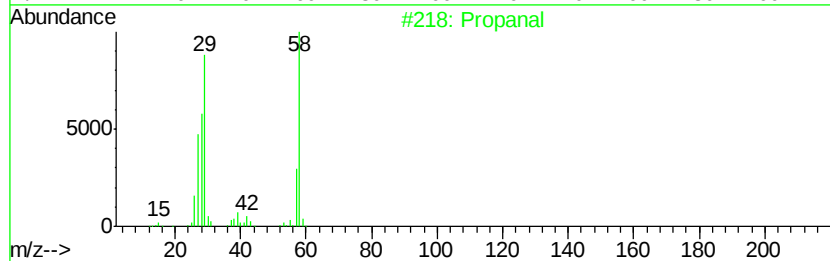
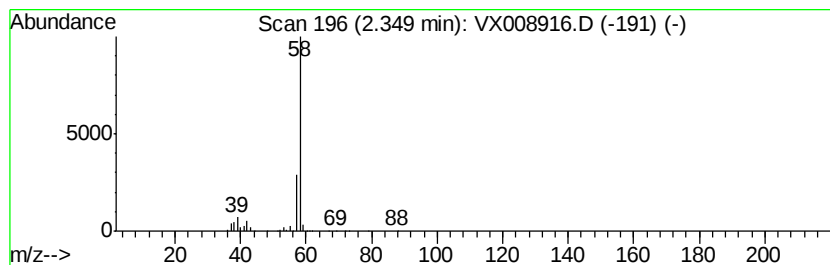
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Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	68.96 ug/l	1234340	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Propylene oxide	58	C3H6O	000075-56-9	7
5		Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	4



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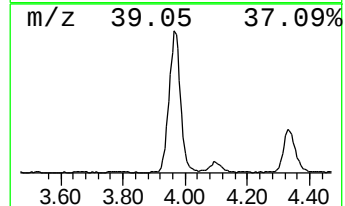
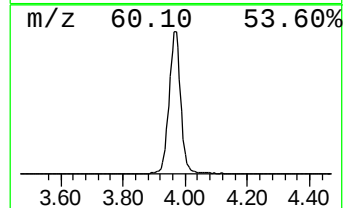
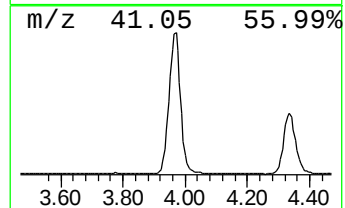
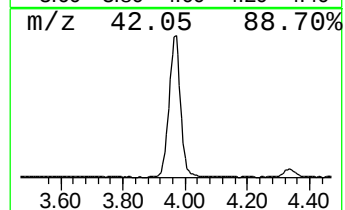
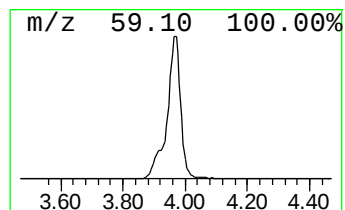
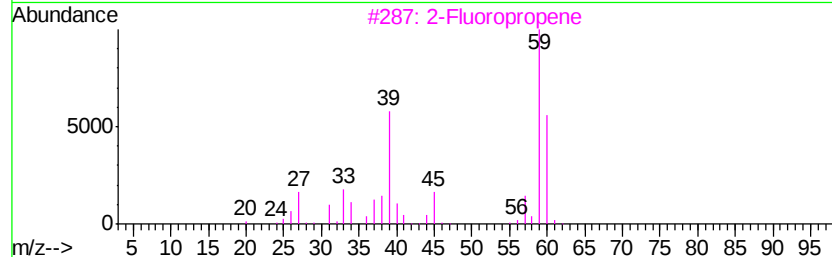
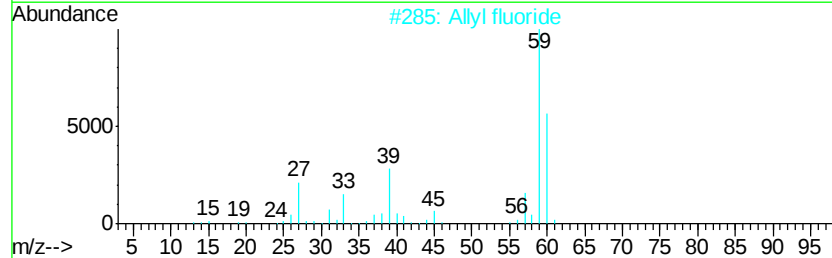
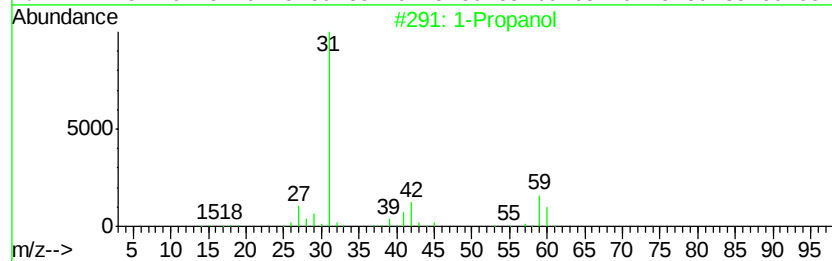
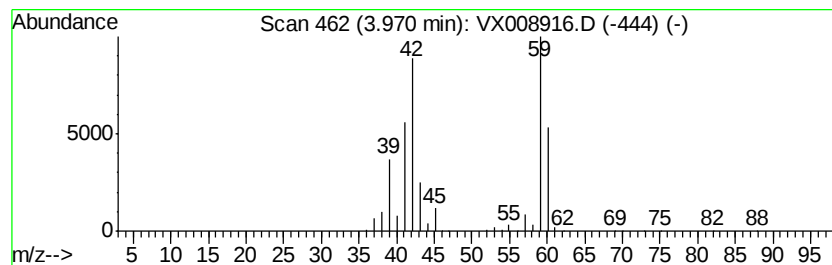
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Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.97	52.95 ug/l	947758	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	47
3		2-Fluoropropene	60	C3H5F	001184-60-7	37
4		Cyclopropane	42	C3H6	000075-19-4	16
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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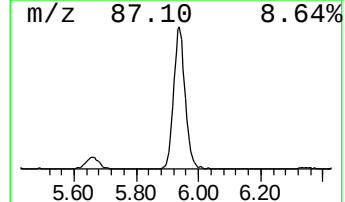
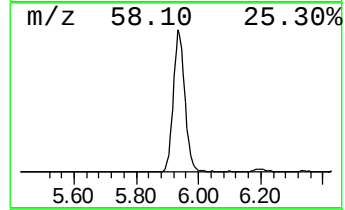
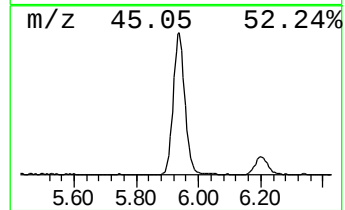
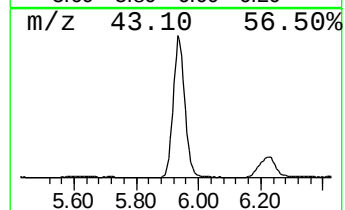
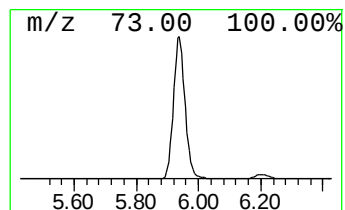
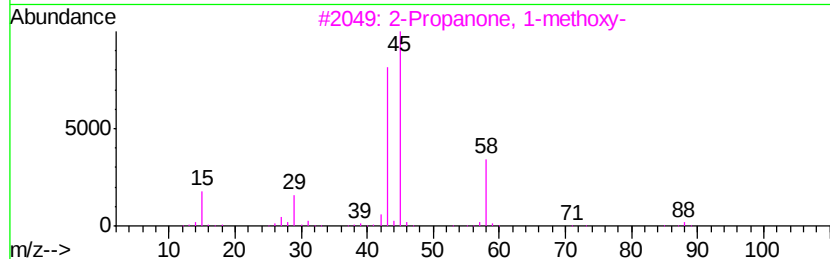
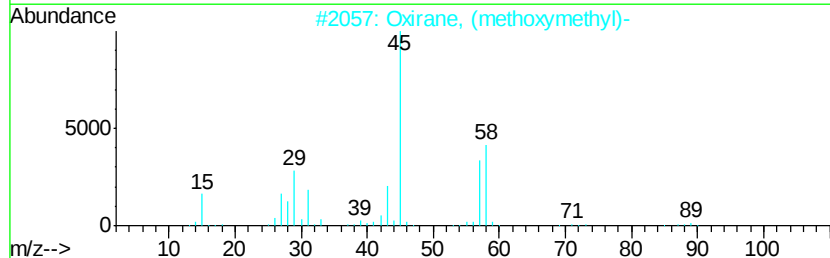
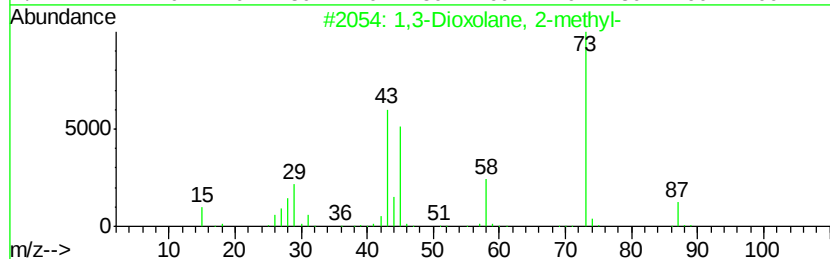
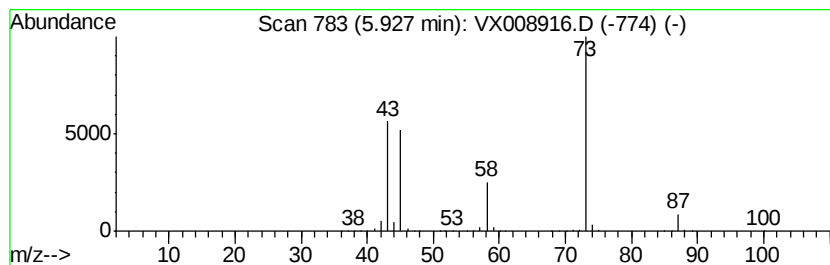
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	50.00 ug/l	894987	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2		Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	47
3		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	42
4		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	16



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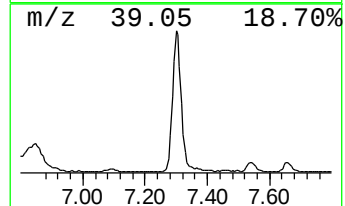
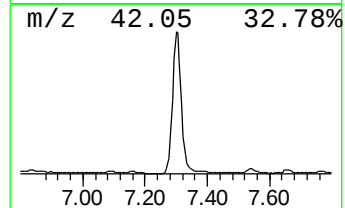
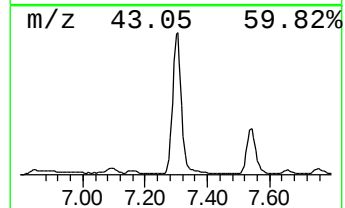
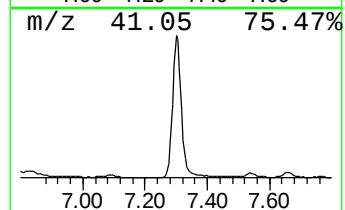
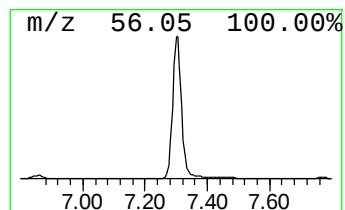
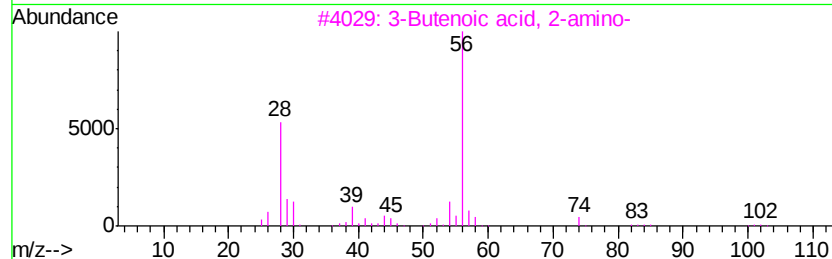
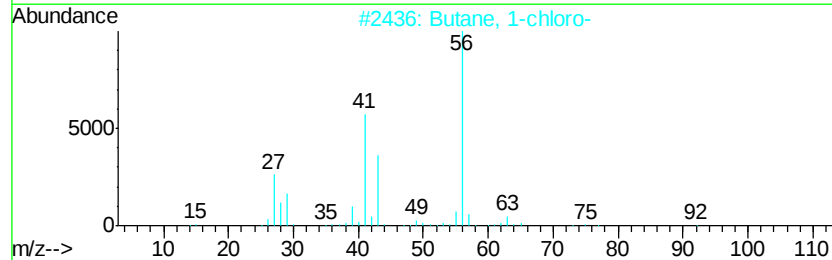
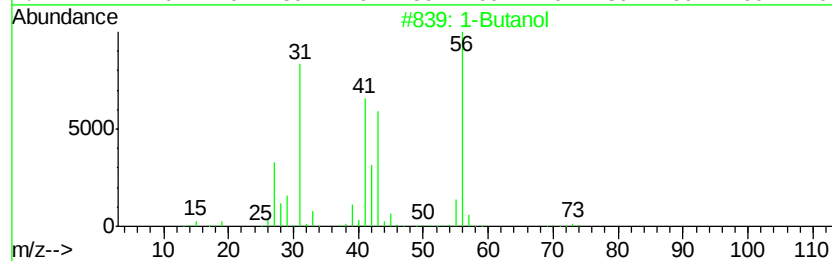
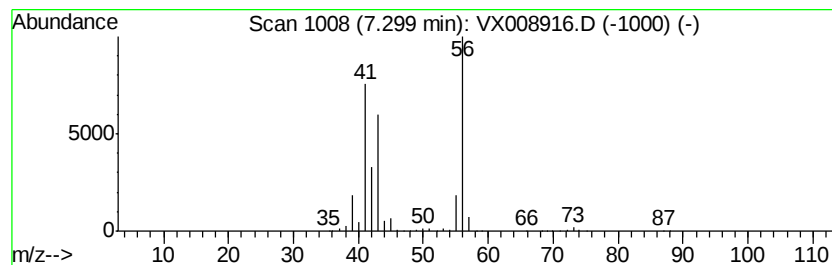
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	50.00 ug/l	931481	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	90
2		Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
3		3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
4		Methoxyacetoneitrile	71	C3H5NO	001738-36-9	9
5		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9



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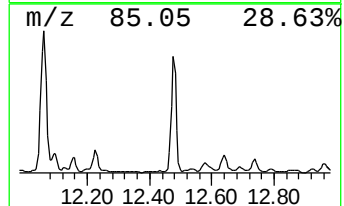
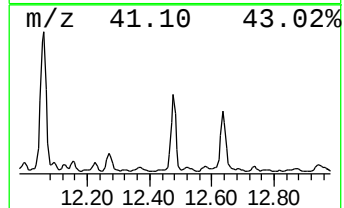
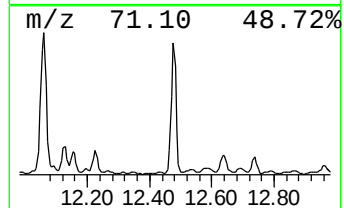
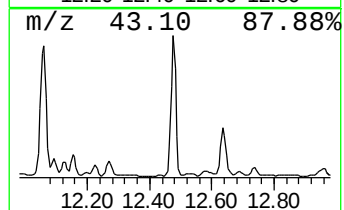
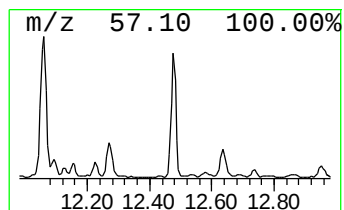
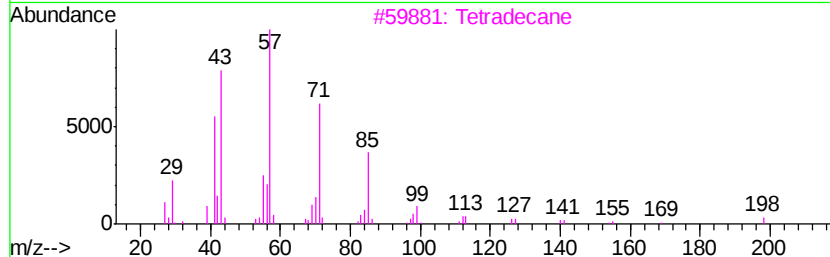
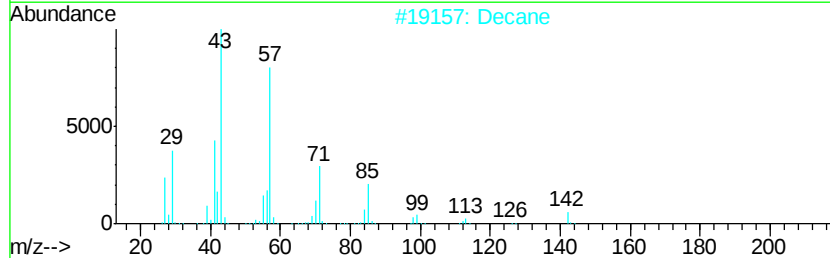
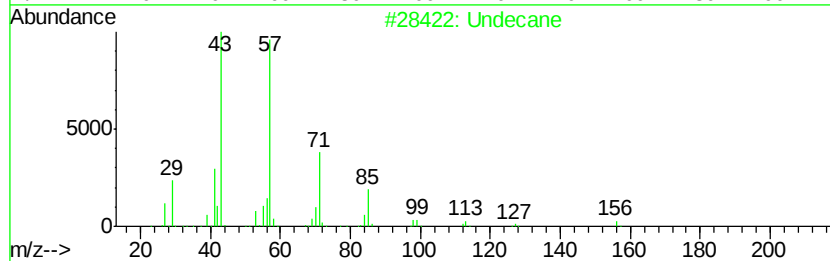
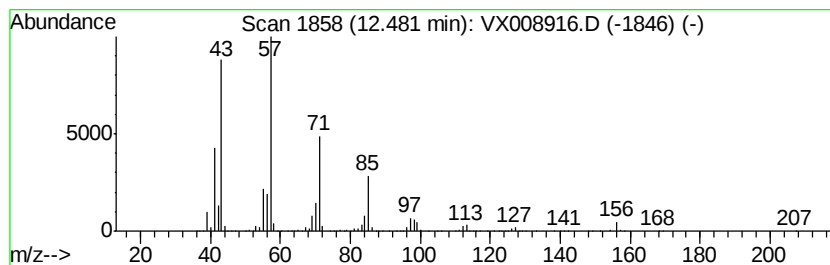
Instrument :
MSVOA_X
ClientSampled :
CL-COMP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

Peak Number 7 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	17.39 ug/l	3609390	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane	156 C11H24	001120-21-4	93
2	Decane	142 C10H22	000124-18-5	93
3	Tetradecane	198 C14H30	000629-59-4	86
4	Tridecane	184 C13H28	000629-50-5	80
5	Hexadecane	226 C16H34	000544-76-3	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008916.D
Acq On : 13 Apr 2019 03:35
Operator : JC/SP
Sample : K2381-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

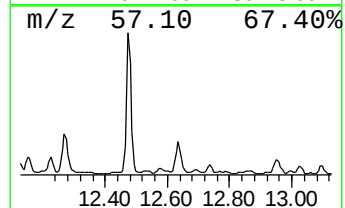
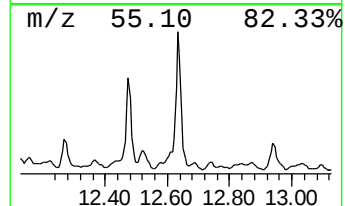
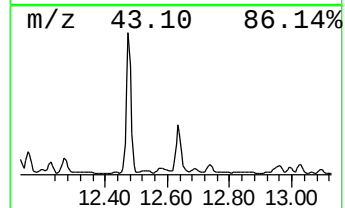
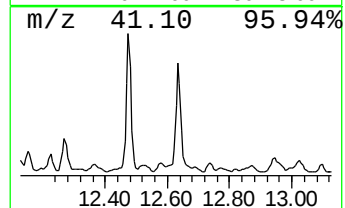
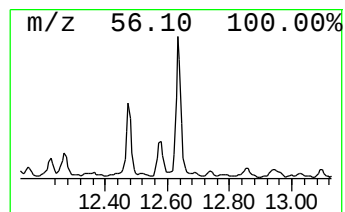
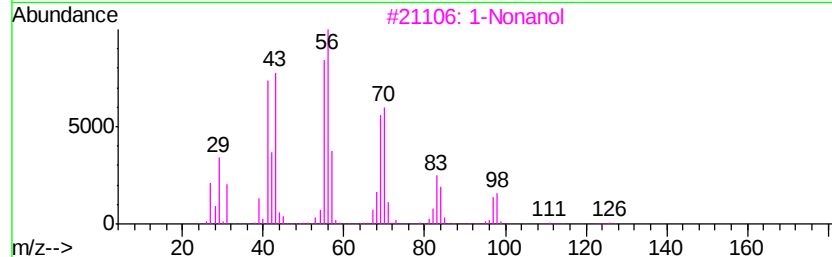
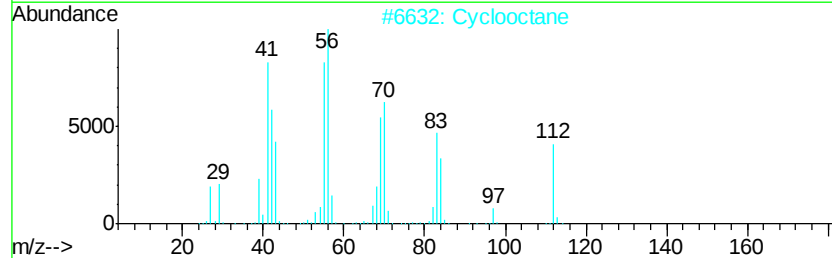
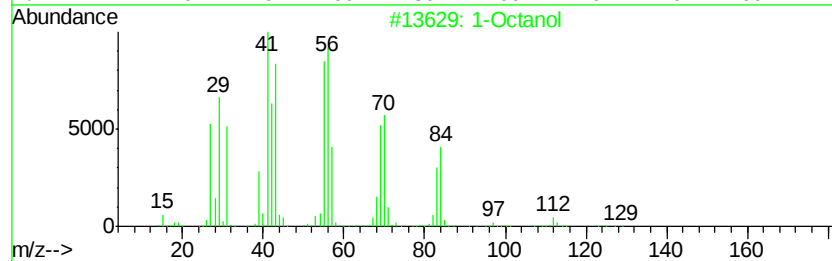
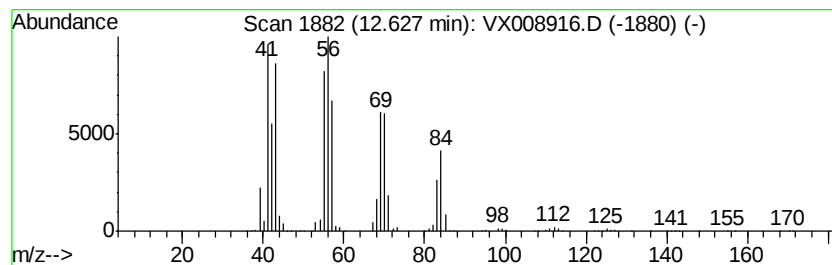
Instrument :
MSVOA_X
ClientSampled :
CL-COMP-3

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Octanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	12.03 ug/l	2496650	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octanol		130 C8H18O	000111-87-5 90
2	Cyclooctane		112 C8H16	000292-64-8 80
3	1-Nonanol		144 C9H20O	000143-08-8 80
4	Hexyl octyl ether		214 C14H30O	017071-54-4 64
5	1-Decene		140 C10H20	000872-05-9 59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008916.D
Acq On : 13 Apr 2019 03:35
Operator : JC/SP
Sample : K2381-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
CL-COMP-3

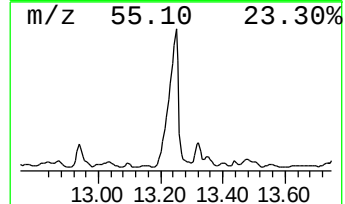
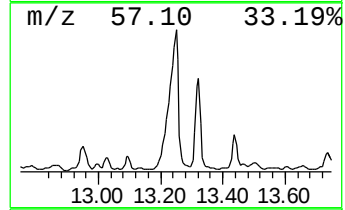
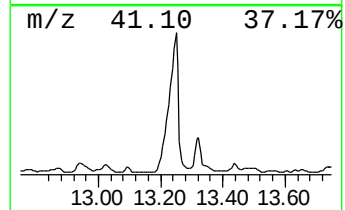
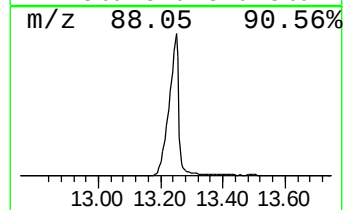
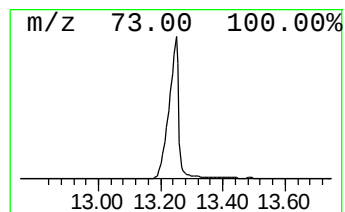
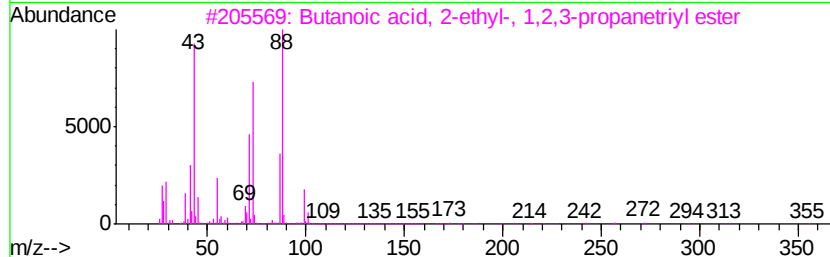
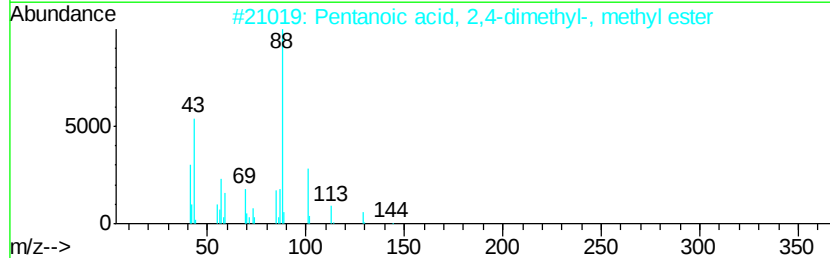
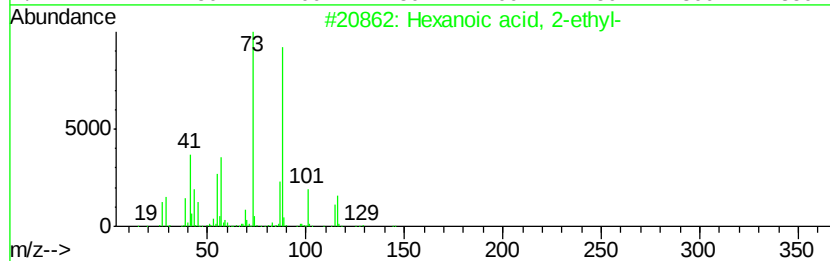
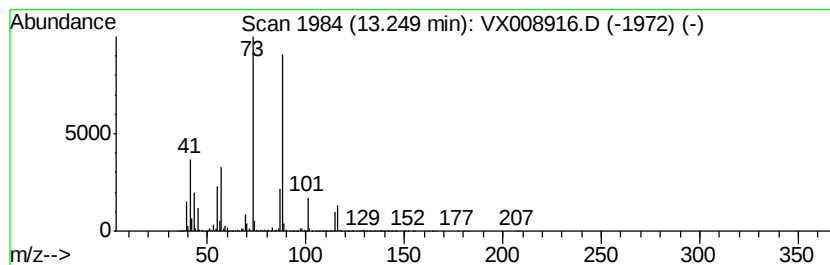
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	56.33 ug/l	11690200	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	50
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
4		L(-)-Fucose, tetramethyl ether	220	C10H20O5	1000332-75-0	42
5		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008916.D
Acq On : 13 Apr 2019 03:35
Operator : JC/SP
Sample : K2381-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-COMP-3

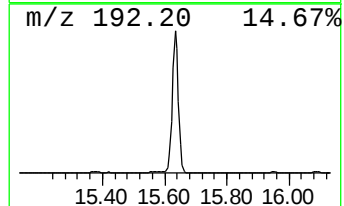
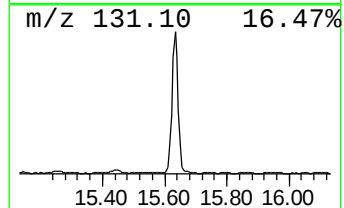
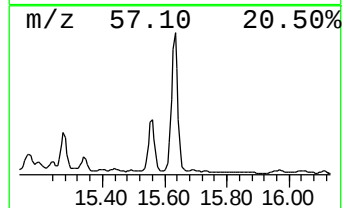
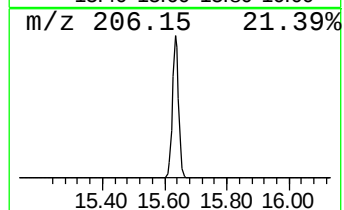
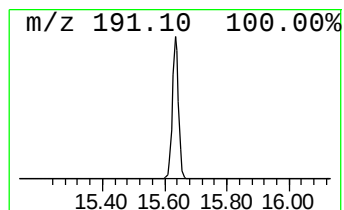
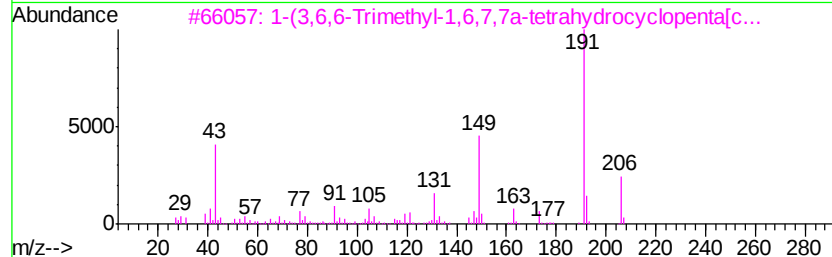
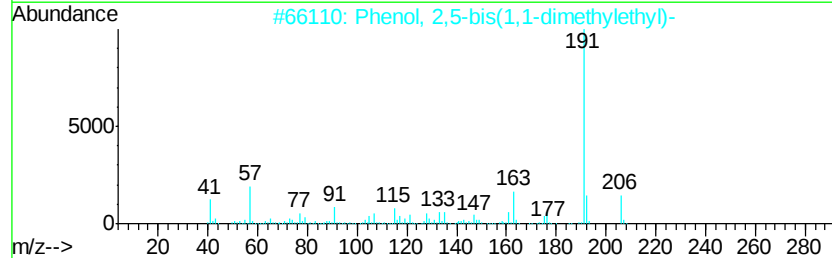
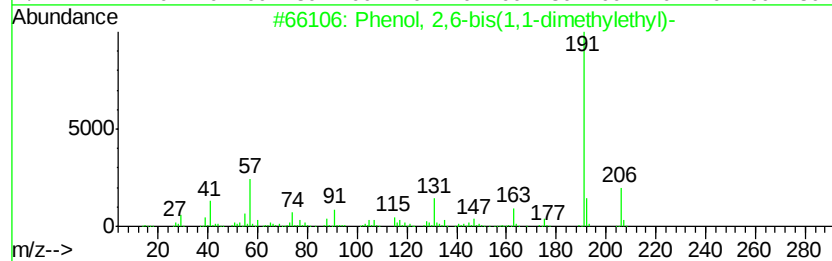
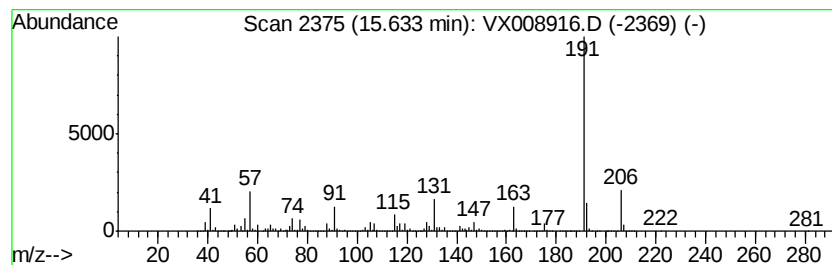
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	23.29 ug/l	4833440	1,4-Dichlorobenzene-d4	12.08

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, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	87
3		1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	83
4		Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	81
5		Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008916.D
Acq On : 13 Apr 2019 03:35
Operator : JC/SP
Sample : K2381-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
CL-COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.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
Ethanol	2.20	1956.7	ug/l	35025100	1	5.66	894987	50.0
Propanal	2.35	69.0	ug/l	1234340	1	5.66	894987	50.0
1-Propanol	3.97	53.0	ug/l	947758	1	5.66	894987	50.0
1,3-Dioxolane, 2-...	5.93	50.0	ug/l	894987	1	5.66	894987	50.0
1-Butanol	7.30	50.0	ug/l	931481	2	6.86	931481	50.0
Undecane	12.48	17.4	ug/l	3609390	4	12.08	10376100	50.0
1-Octanol	12.63	12.0	ug/l	2496650	4	12.08	10376100	50.0
Hexanoic acid, 2-...	13.25	56.3	ug/l	11690200	4	12.08	10376100	50.0
Phenol, 2,6-bis(1...	15.63	23.3	ug/l	4833440	4	12.08	10376100	50.0