

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061419\
 Data File : VX010310.D
 Acq On : 14 Jun 2019 18:59
 Operator : JC/SP
 Sample : K3387-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WASTE-TANK

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\82X060719W.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	1.276	16	20	23	rBV	122321	145171	9.83%	1.128%
2	1.312	23	26	37	rVV	84948	256641	17.38%	1.995%
3	1.404	38	41	46	rVB	67423	93240	6.31%	0.725%
4	1.489	51	55	68	rVB	188793	309917	20.98%	2.409%
5	2.251	176	180	189	rVB9	5476	15141	1.03%	0.118%
6	2.349	190	196	205	rVB	62501	103322	7.00%	0.803%
7	2.440	205	211	216	rBV	127014	214257	14.51%	1.665%
8	2.605	228	238	249	rBV	281701	537084	36.36%	4.175%
9	2.709	249	255	261	rVV	39516	93782	6.35%	0.729%
10	2.776	262	266	274	rVV	13192	34146	2.31%	0.265%
11	2.855	276	279	290	rVB5	7445	17962	1.22%	0.140%
12	3.416	363	371	379	rBV2	8589	20070	1.36%	0.156%
13	3.952	452	459	472	rBV2	13557	38332	2.60%	0.298%
14	4.464	537	543	554	rVB9	4834	15410	1.04%	0.120%
15	4.598	554	565	571	rBV2	17084	52465	3.55%	0.408%
16	4.678	571	578	589	rVB	54247	150791	10.21%	1.172%
17	5.129	640	652	668	rBV3	104003	333591	22.59%	2.593%
18	5.403	687	697	703	rBV2	9440	28475	1.93%	0.221%
19	5.501	703	713	727	rVV2	178580	515888	34.93%	4.010%
20	5.659	727	739	761	rVB	311151	888275	60.14%	6.905%
21	6.062	792	805	817	rBV	168169	446202	30.21%	3.468%
22	6.214	821	830	840	rVV2	33815	90434	6.12%	0.703%
23	6.458	863	870	880	rBV5	7327	18909	1.28%	0.147%
24	6.860	925	936	949	rBV	455100	1084025	73.40%	8.426%
25	7.720	1071	1077	1084	rVB	26097	46460	3.15%	0.361%
26	8.482	1193	1202	1212	rBV2	8724	20993	1.42%	0.163%
27	8.646	1219	1229	1234	rBV	61467	101037	6.84%	0.785%
28	8.714	1234	1240	1247	rBV	957742	1476929	100.00%	11.481%
29	8.787	1247	1252	1254	rBV	29456	48374	3.28%	0.376%
30	8.835	1254	1260	1263	rBV2	129240	295934	20.04%	2.300%
31	9.652	1388	1394	1411	rBV	98180	232932	15.77%	1.811%
32	10.043	1453	1458	1464	rBV	41358	104987	7.11%	0.816%
33	10.110	1464	1469	1479	rVV	958572	1315465	89.07%	10.225%
34	10.207	1480	1485	1499	rVB	432988	576431	39.03%	4.481%

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Integration Parameters: RTEINT.P

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35	10.677	1556	1562	1570	rBV	134045	220347	14.92%	1.713%
36	10.756	1570	1575	1592	rVV	203333	331405	22.44%	2.576%
37	10.908	1595	1600	1612	rVB5	10722	23453	1.59%	0.182%
38	11.134	1630	1637	1647	rBV	837153	1067636	72.29%	8.299%
39	11.646	1717	1721	1729	rBV	25721	35044	2.37%	0.272%
40	11.804	1743	1747	1755	rVB	37290	49937	3.38%	0.388%
41	12.079	1786	1792	1800	rVB	1003305	1291837	87.47%	10.042%
42	12.268	1818	1823	1831	rBV	69673	93646	6.34%	0.728%
43	13.213	1973	1978	1986	rBV	18098	28234	1.91%	0.219%

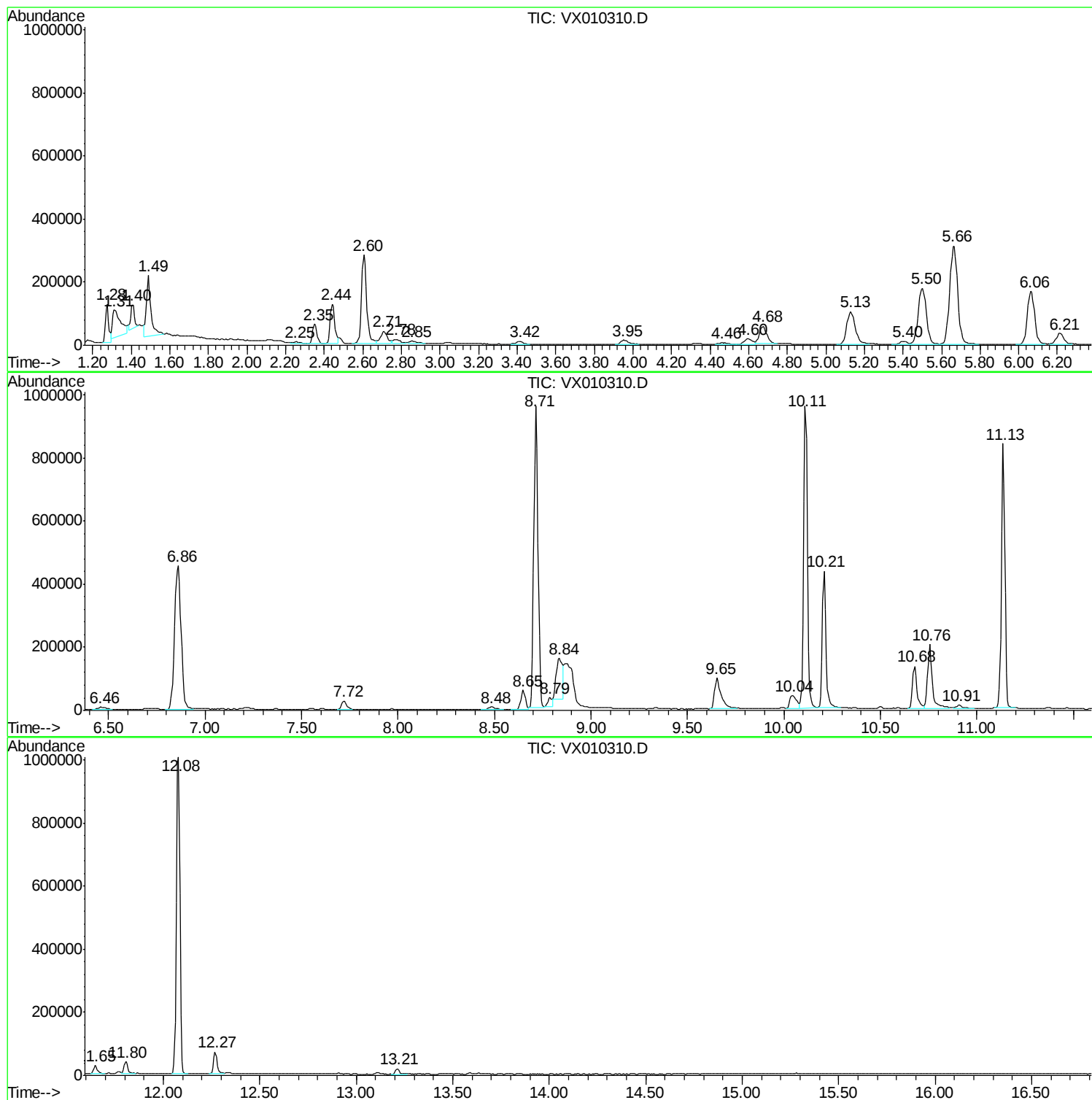
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Quant Title : SW846 8260

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



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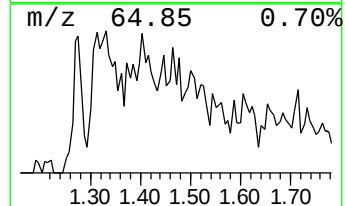
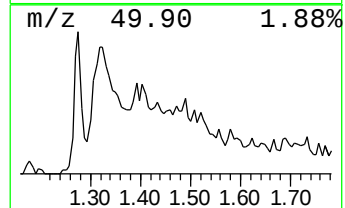
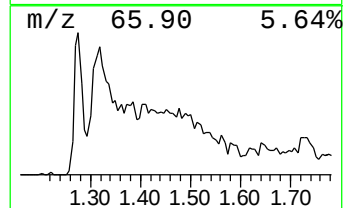
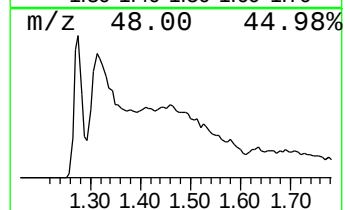
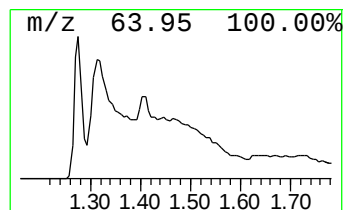
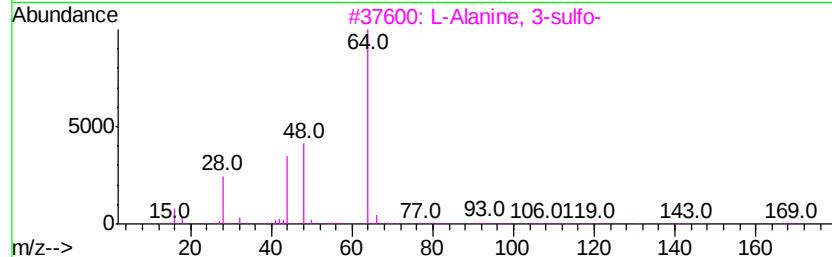
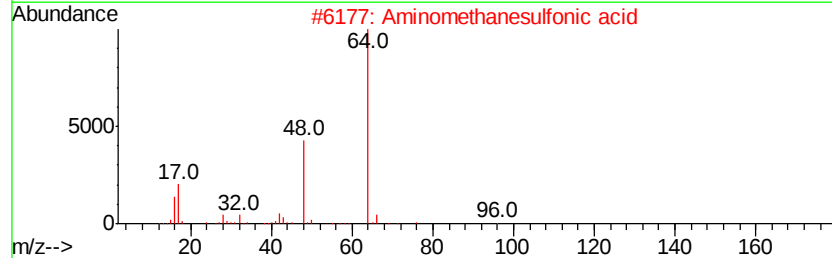
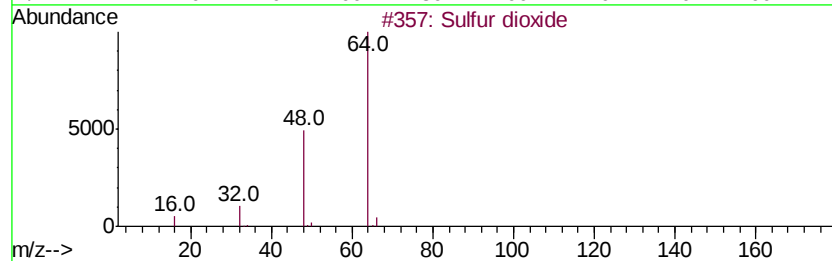
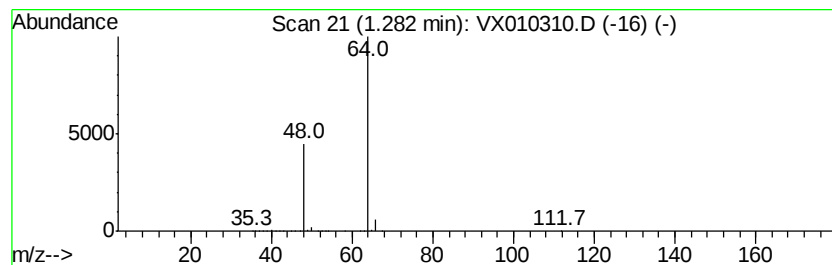
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	8.17 ug/l	145171	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide		64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-		64	C2H2F2	000075-38-7	4
5	Ethyl Chloride		64	C2H5Cl	000075-00-3	3



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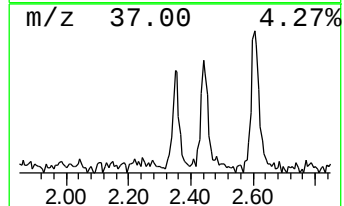
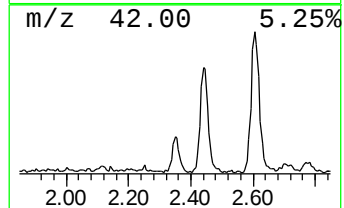
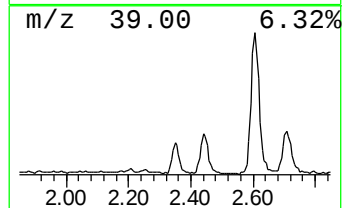
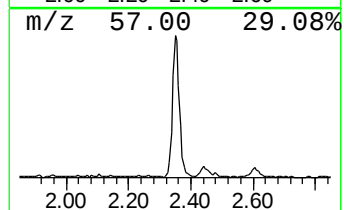
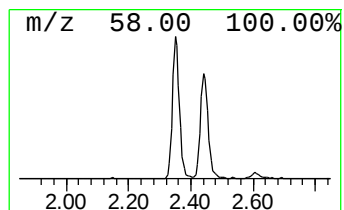
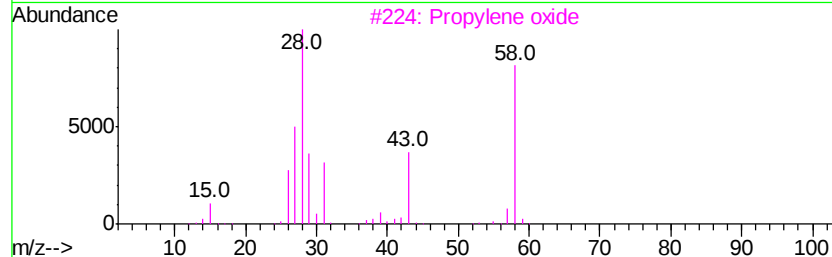
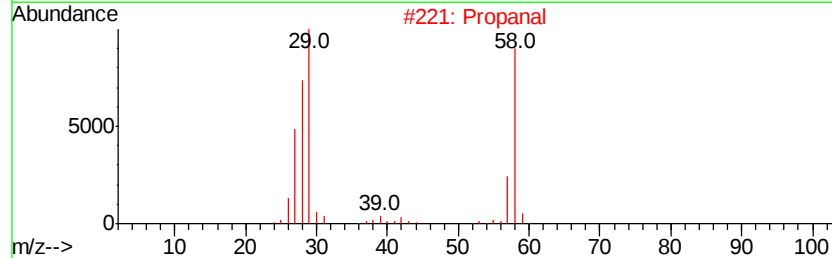
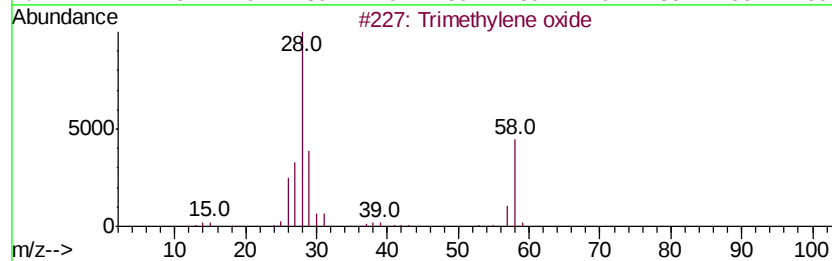
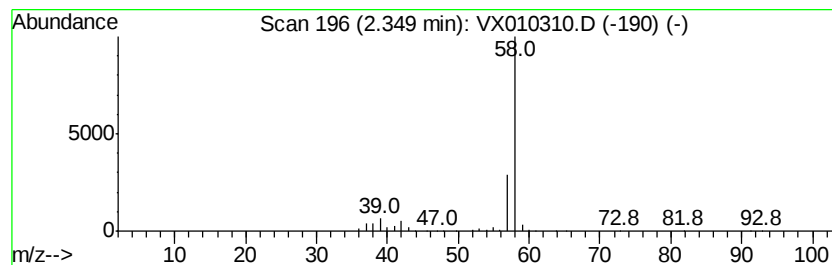
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Trimethylene oxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	5.82 ug/l	103322	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trimethylene oxide	58	C3H6O	000503-30-0	56
2			Propanal	58	C3H6O	000123-38-6	50
3			Propylene oxide	58	C3H6O	000075-56-9	9
4			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5			Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	5



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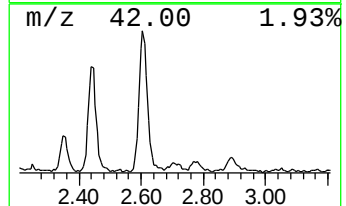
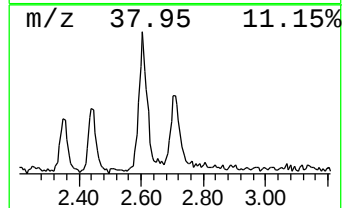
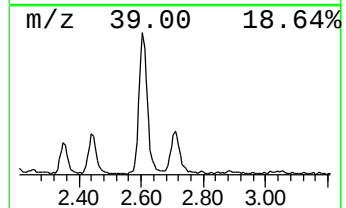
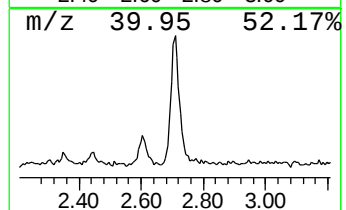
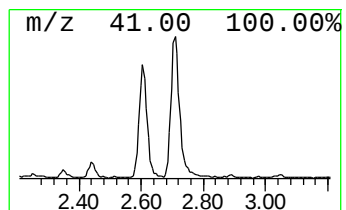
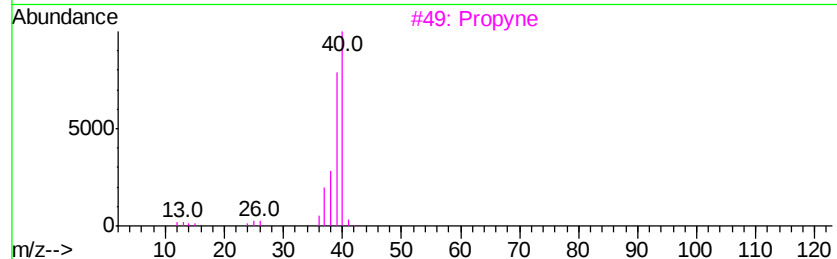
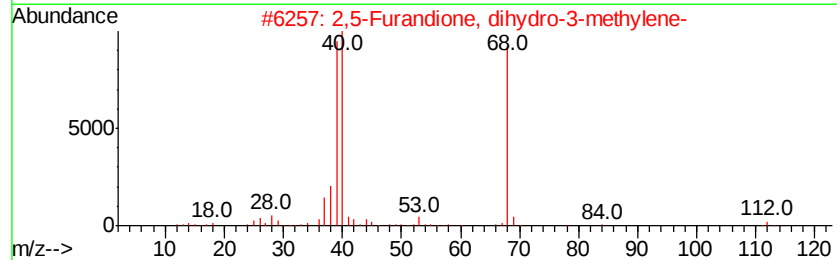
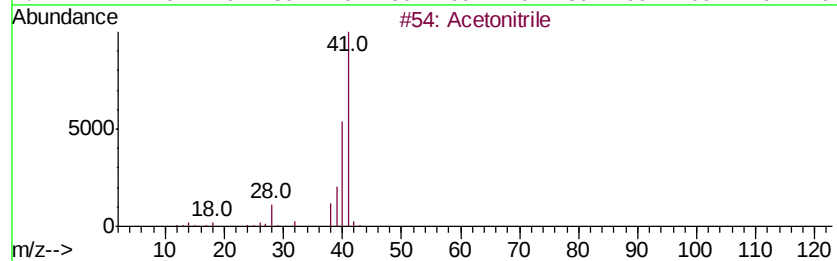
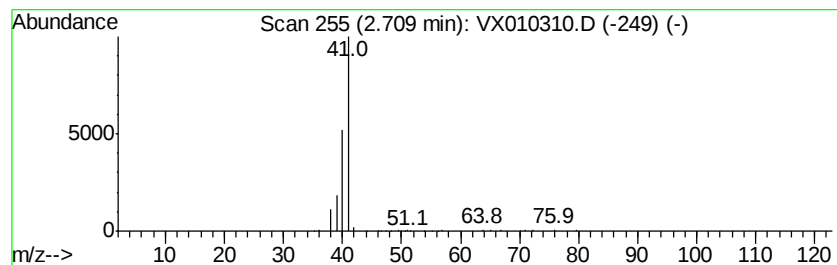
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown2.71 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.71	5.28 ug/l	93782	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetonitrile	41	C2H3N	000075-05-8	38
2		2,5-Furandione, dihydro-3-methyl...	112	C5H4O3	002170-03-8	9
3		Propyne	40	C3H4	000074-99-7	4
4		Methyl isocyanide	41	C2H3N	000593-75-9	4
5		Allyl chloride	76	C3H5Cl	000107-05-1	2



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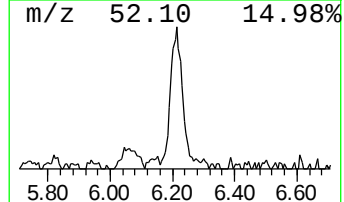
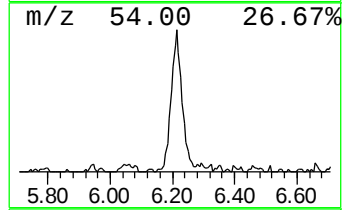
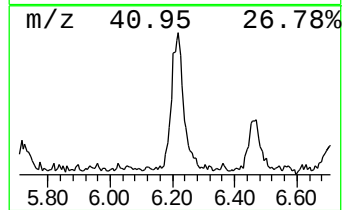
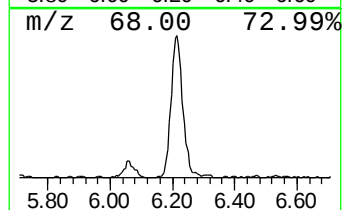
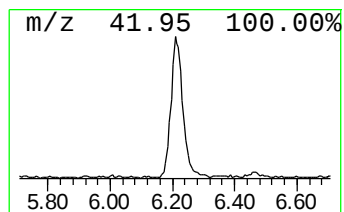
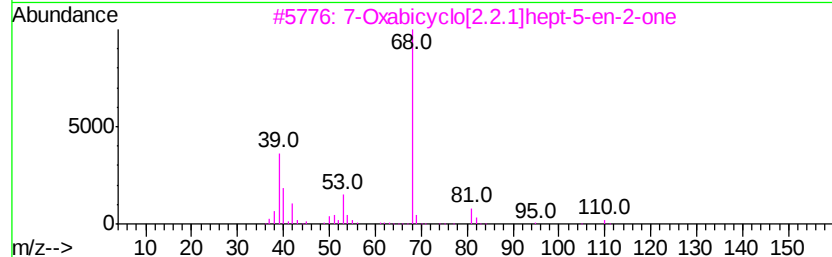
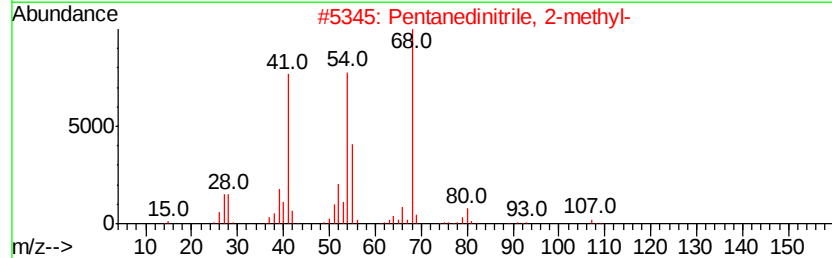
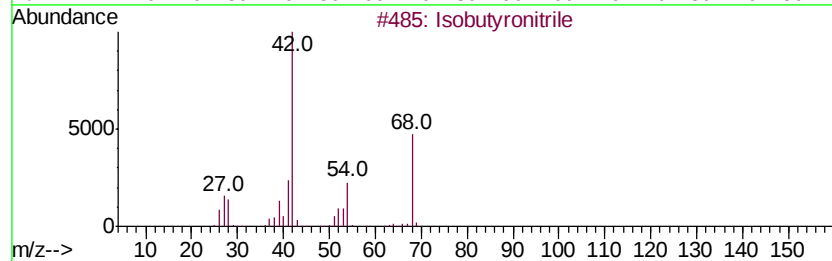
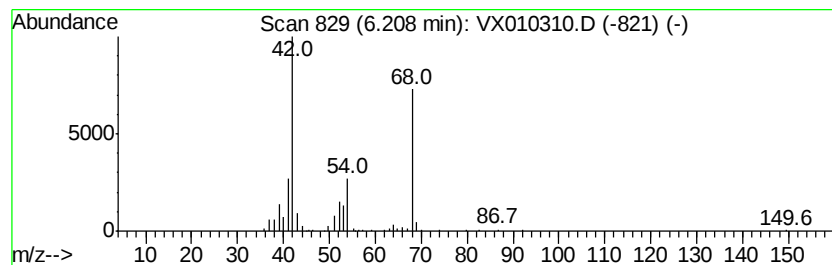
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Peak Number 6 Isobutyronitrile Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	5.09 ug/l	90434	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutyronitrile	69	C4H7N	000078-82-0	91
2		Pentanedinitrile, 2-methyl-	108	C6H8N2	004553-62-2	37
3		7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	32
4		Aziridine, 1-methyl-2-methylene-	69	C4H7N	025012-55-9	25
5		2-Pentyne	68	C5H8	000627-21-4	17



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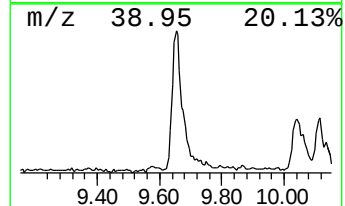
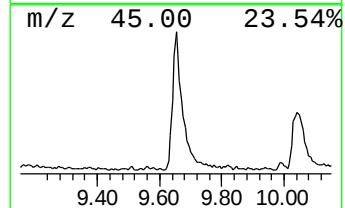
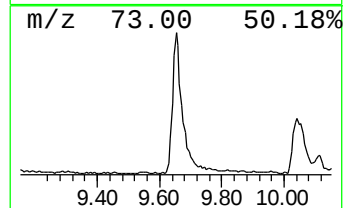
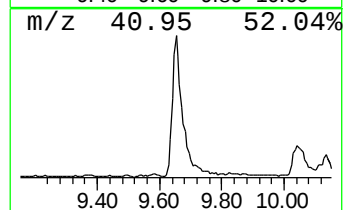
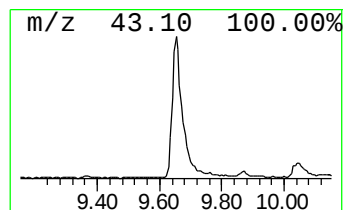
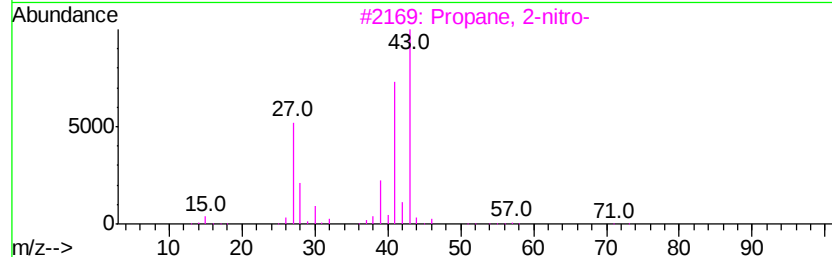
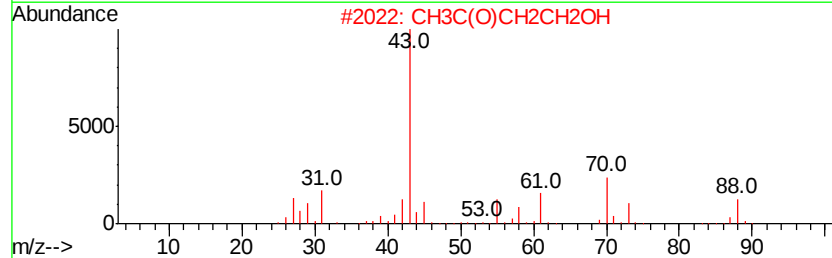
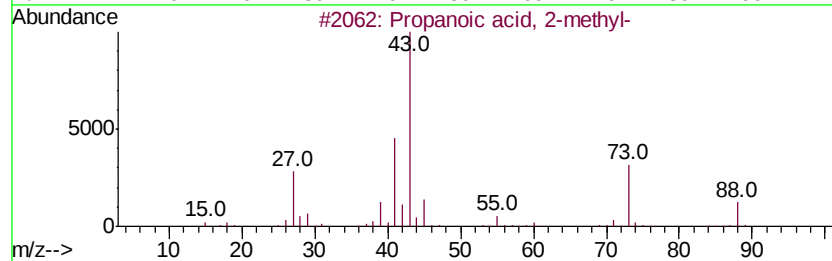
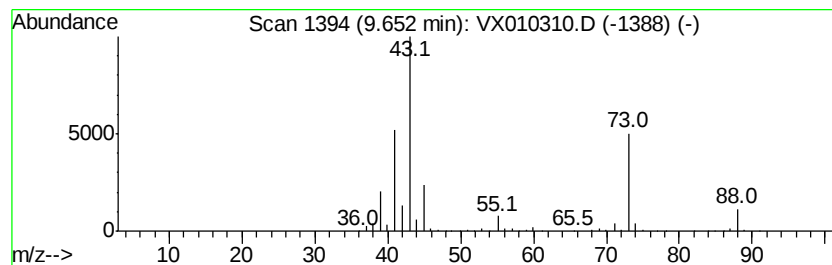
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Quant Title : SW846 8260

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

Peak Number 7 Propanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	8.85 ug/l	232932	Chlorobenzene-d5	10.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	86
2			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	64
3			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	10
4			Hydrazine, (1,1-dimethylethyl)-	88	C4H12N2	032064-67-8	9
5			Propane, 1-ethoxy-	88	C5H12O	000628-32-0	9



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061419\
Data File : VX010310.D
Acq On : 14 Jun 2019 18:59
Operator : JC/SP
Sample : K3387-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-TANK

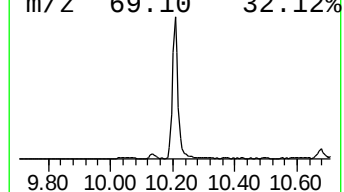
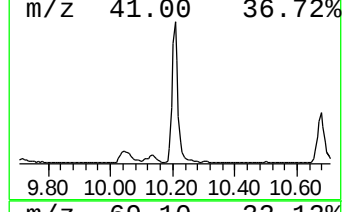
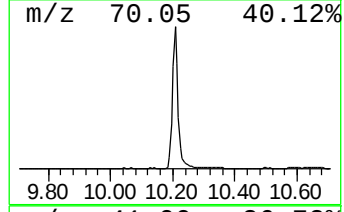
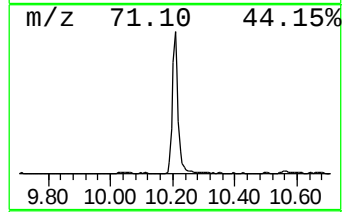
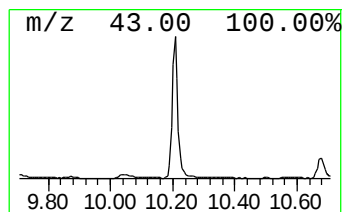
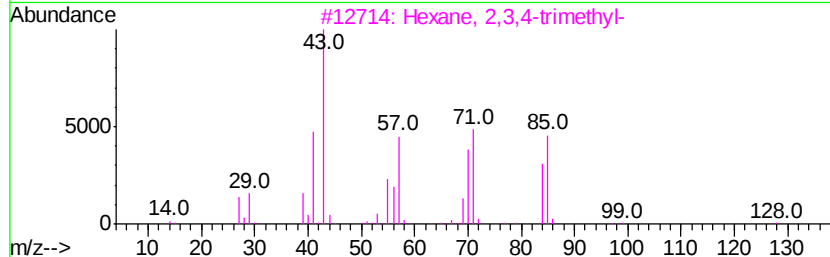
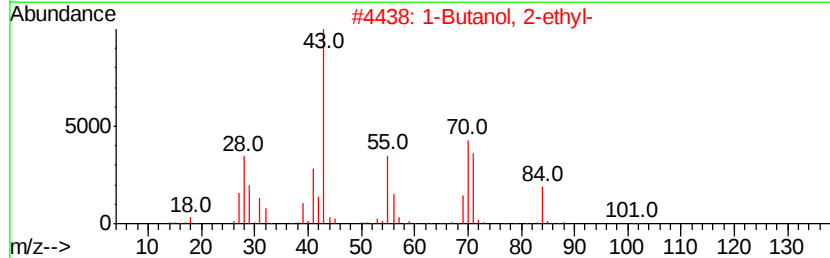
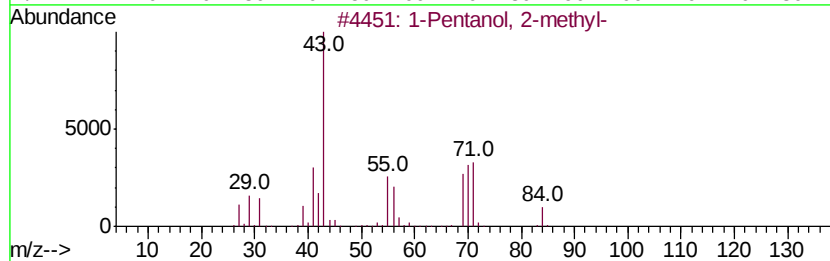
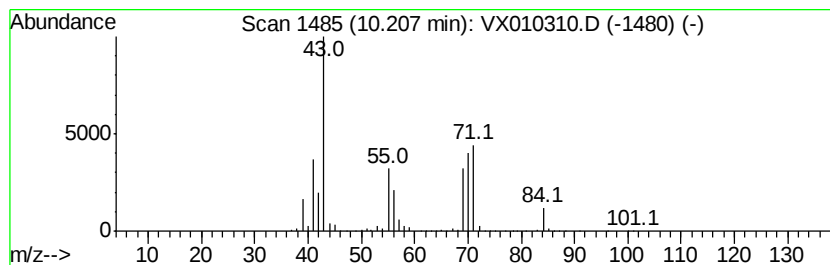
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Quant Title : SW846 8260

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

Peak Number 8 1-Pentanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.21	21.91 ug/l	576431	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	59
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	45
4		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	42
5		Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061419\
Data File : VX010310.D
Acq On : 14 Jun 2019 18:59
Operator : JC/SP
Sample : K3387-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

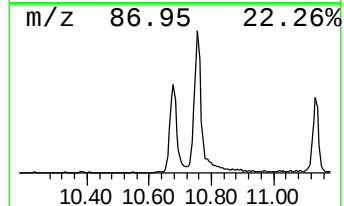
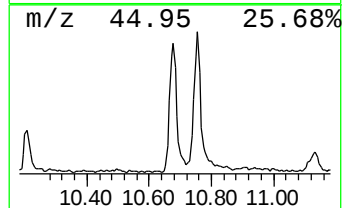
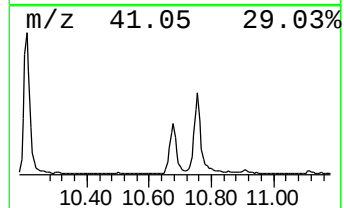
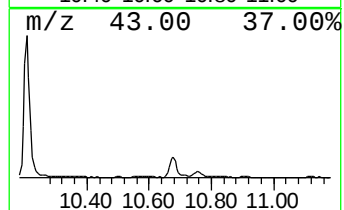
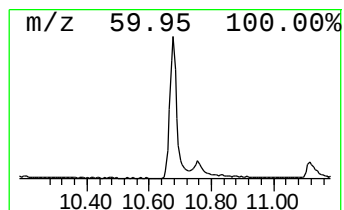
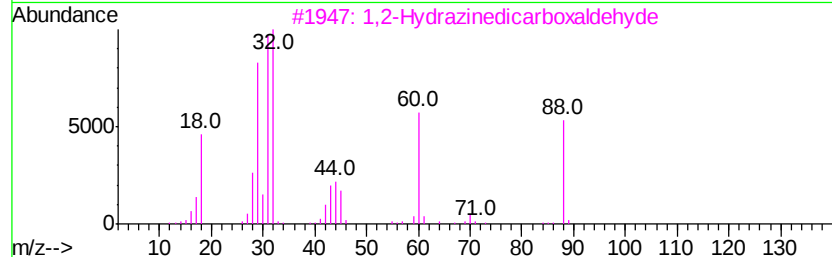
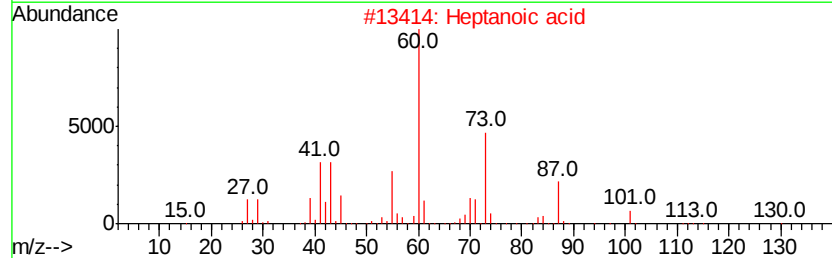
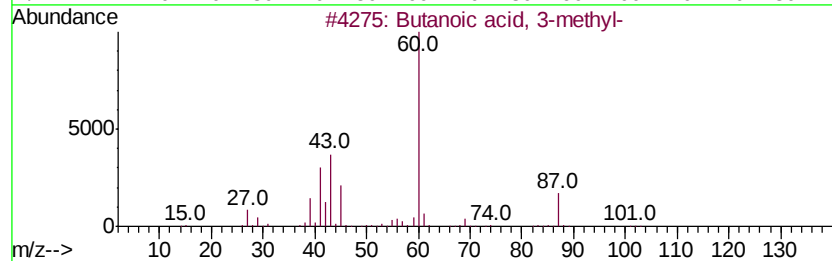
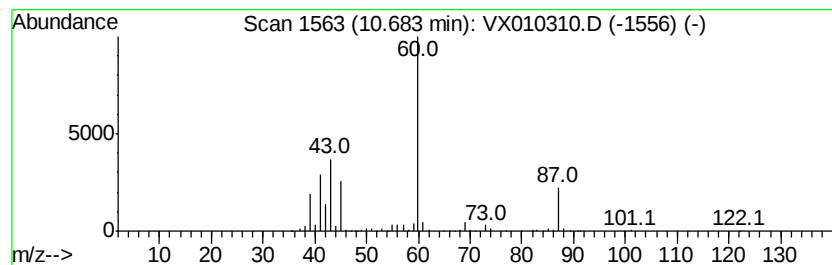
Instrument :
MSVOA_X
ClientSampleId :
WASTE-TANK

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 9 Butanoic acid, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.68	8.38 ug/l	220347	Chlorobenzene-d5	10.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2	Heptanoic acid	130	C7H14O2	000111-14-8	39
3	1,2-Hydrazinedicarboxaldehyd	88	C2H4N2O2	000628-36-4	38
4	Pentanoic acid	102	C5H10O2	000109-52-4	12
5	Morpholine	87	C4H9NO	000110-91-8	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061419\
Data File : VX010310.D
Acq On : 14 Jun 2019 18:59
Operator : JC/SP
Sample : K3387-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-TANK

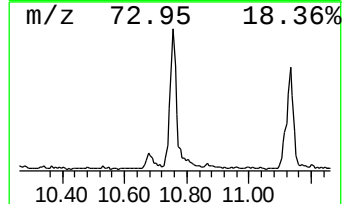
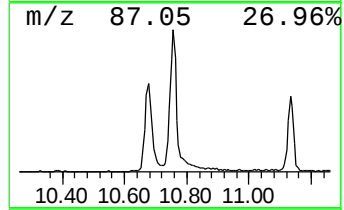
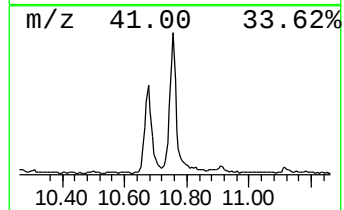
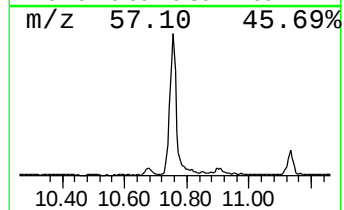
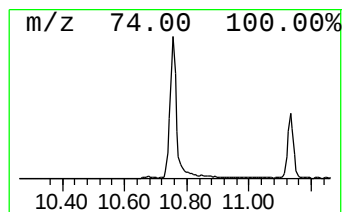
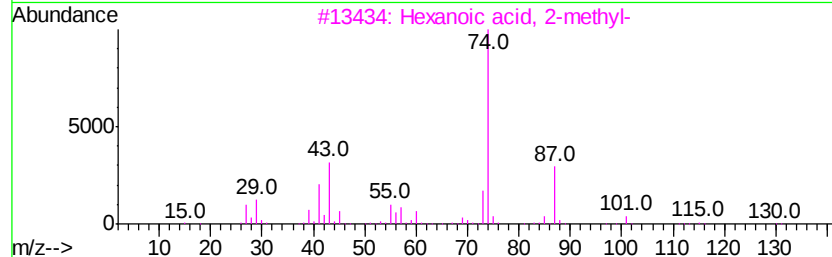
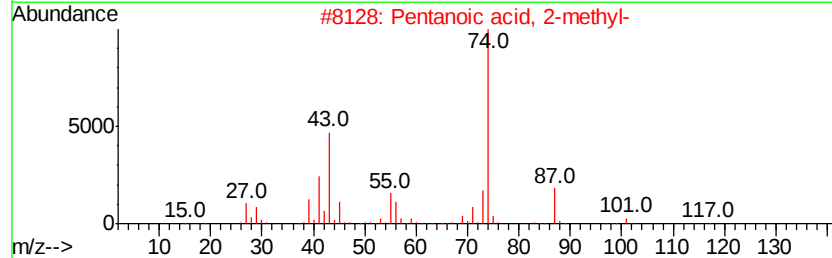
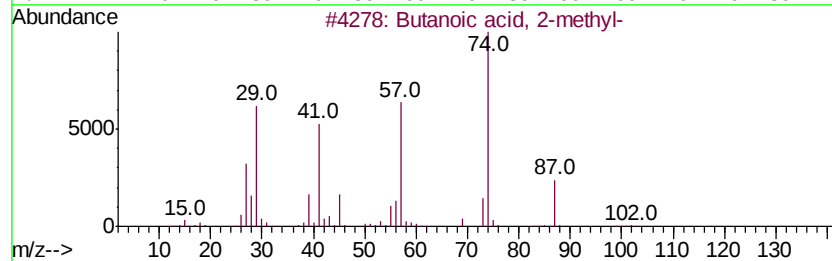
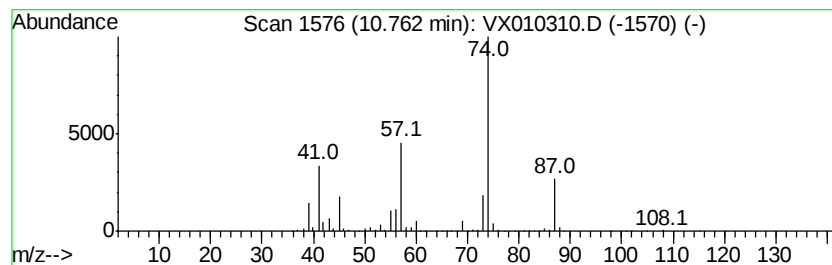
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 10 Butanoic acid, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	12.60 ug/l	331405	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	78
2		Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	59
3		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	50
4		Methyl valerate	116	C6H12O2	000624-24-8	38
5		Propanoic acid	74	C3H6O2	000079-09-4	28



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061419\
Data File : VX010310.D
Acq On : 14 Jun 2019 18:59
Operator : JC/SP
Sample : K3387-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.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
Sulfur dioxide	1.28	8.2	ug/l	145171	1	5.67	888275	50.0
Trimethylene oxide	2.35	5.8	ug/l	103322	1	5.67	888275	50.0
unknown2.71	2.71	5.3	ug/l	93782	1	5.67	888275	50.0
Isobutyronitrile	6.21	5.1	ug/l	90434	1	5.67	888275	50.0
Propanoic acid, 2...	9.65	8.8	ug/l	232932	3	10.11	1315470	50.0
1-Pentanol, 2-met...	10.21	21.9	ug/l	576431	3	10.11	1315470	50.0
Butanoic acid, 3-...	10.68	8.4	ug/l	220347	3	10.11	1315470	50.0
Butanoic acid, 2-...	10.76	12.6	ug/l	331405	3	10.11	1315470	50.0