

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX053119\
 Data File : VX009978.D
 Acq On : 31 May 2019 12:01
 Operator : JC/SP
 Sample : K2964-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-1

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\82X052819W.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	1.318	19	27	44	rBV2	124665	633328	1.80%	0.562%
2	1.489	51	55	67	rVB	384681	467558	1.33%	0.415%
3	2.184	151	169	172	rBV	7562353	23179565	65.91%	20.584%
4	2.452	205	213	229	rBV	8586865	14522954	41.30%	12.896%
5	2.629	233	242	260	rVV	3824613	6869293	19.53%	6.100%
6	2.775	260	266	275	rVB	305533	540917	1.54%	0.480%
7	3.995	449	466	479	rBV	1293949	3914131	11.13%	3.476%
8	4.836	593	604	620	rVB	376683	1073616	3.05%	0.953%
9	5.665	725	740	753	rBV	169825	483746	1.38%	0.430%
10	6.226	823	832	844	rBV	142345	372126	1.06%	0.330%
11	6.860	926	936	952	rBV	273503	662937	1.89%	0.589%
12	7.305	1001	1009	1027	rVB	1106806	2245270	6.38%	1.994%
13	8.713	1234	1240	1246	rBV	570285	887128	2.52%	0.788%
14	9.293	1330	1335	1340	rBV	373524	531420	1.51%	0.472%
15	9.439	1354	1359	1364	rVB	365853	522696	1.49%	0.464%
16	10.110	1464	1469	1481	rVB	556553	766022	2.18%	0.680%
17	10.634	1550	1555	1560	rBV	791911	984220	2.80%	0.874%
18	11.134	1632	1637	1647	rBV	493566	695597	1.98%	0.618%
19	11.530	1691	1702	1705	rBV2	215035	356641	1.01%	0.317%
20	11.804	1743	1747	1757	rVB3	262068	423752	1.20%	0.376%
21	12.073	1786	1791	1797	rVB2	578428	908178	2.58%	0.806%
22	12.152	1797	1804	1810	rBV4	234323	543840	1.55%	0.483%
23	12.268	1819	1823	1830	rBV	1298324	1626676	4.63%	1.444%
24	12.475	1853	1857	1861	rVB	479937	511428	1.45%	0.454%
25	12.652	1879	1886	1897	rBV	25882717	35166426	100.00%	31.228%
26	13.018	1941	1946	1953	rVB3	234567	441212	1.25%	0.392%
27	13.200	1972	1976	1984	rVB2	393362	583346	1.66%	0.518%
28	13.316	1990	1995	1998	rBV	316509	428893	1.22%	0.381%
29	13.475	2017	2021	2031	rBV	2220549	2573409	7.32%	2.285%
30	13.639	2043	2048	2057	rVB2	347076	551304	1.57%	0.490%
31	14.091	2118	2122	2126	rVB	348699	362992	1.03%	0.322%
32	14.249	2143	2148	2165	rBV	5361563	6712046	19.09%	5.960%
33	15.188	2297	2302	2308	rBV	564183	843710	2.40%	0.749%
34	15.279	2313	2317	2324	rVB	534511	828976	2.36%	0.736%

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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 >
Peak separation: 5

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35	16.176	2458	2464	2471	rBV	217873	396710	1.13%	0.352%
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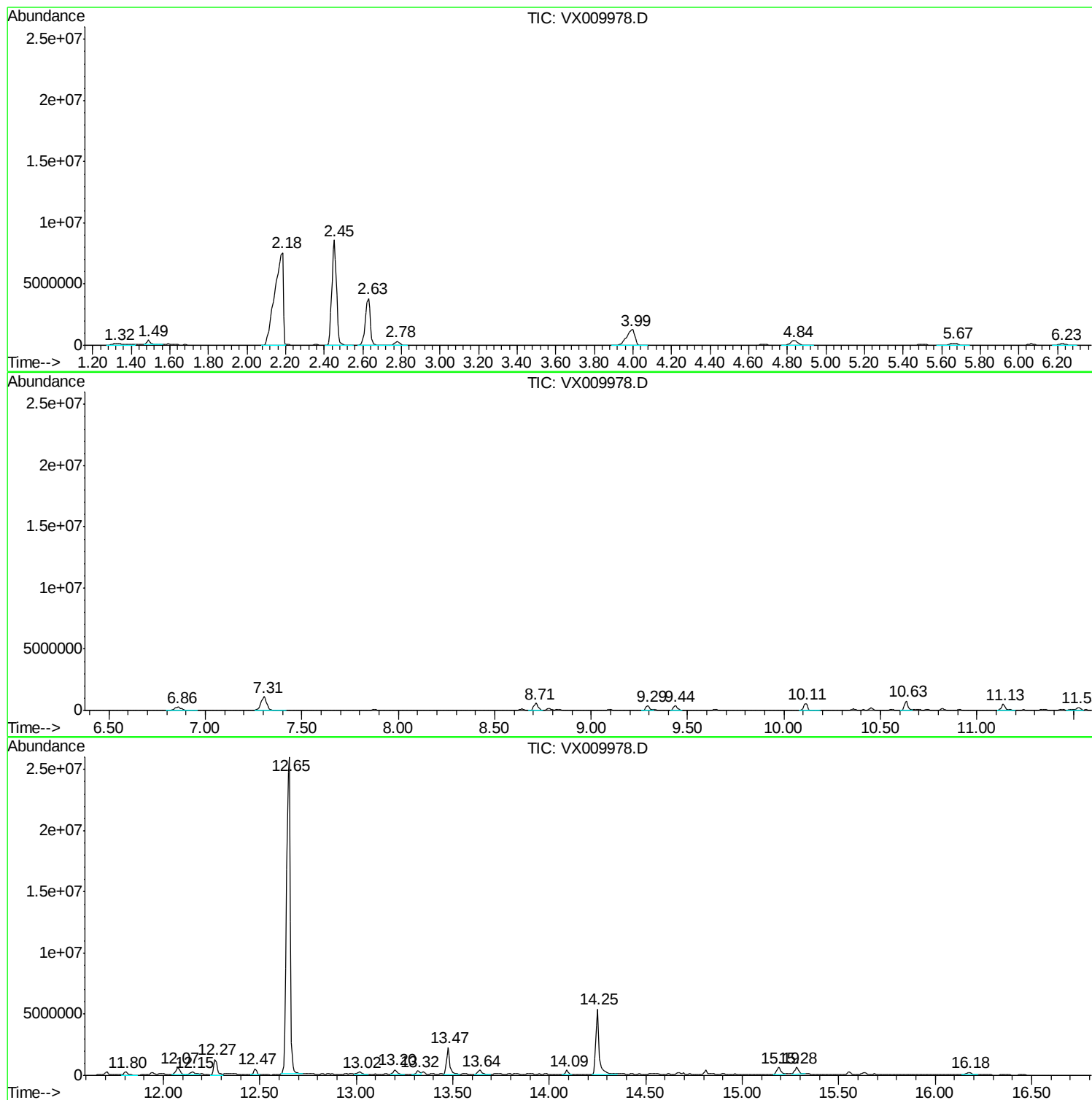
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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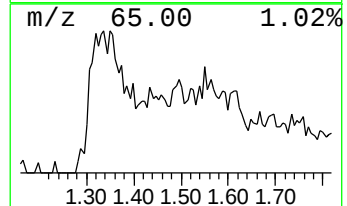
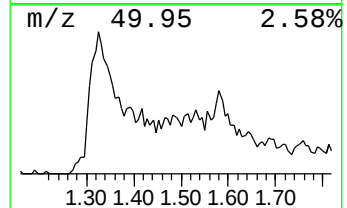
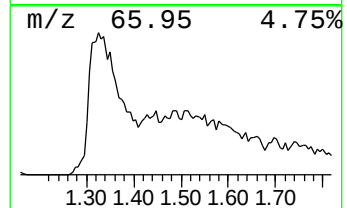
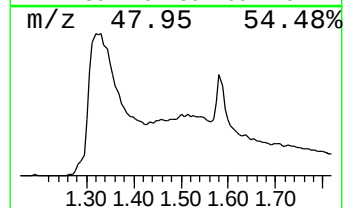
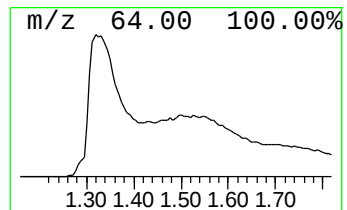
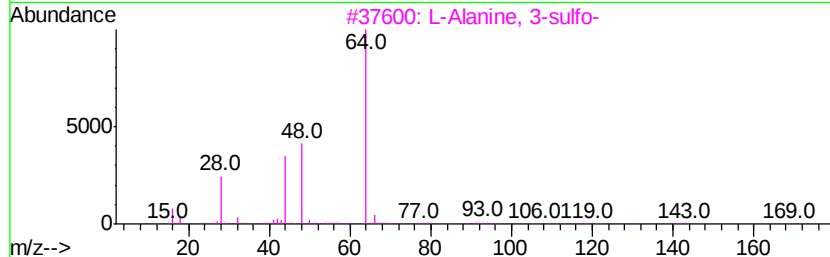
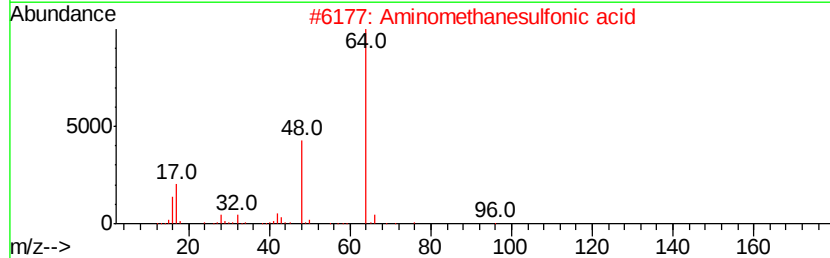
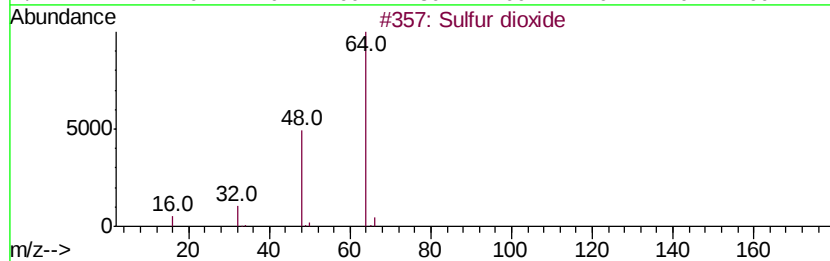
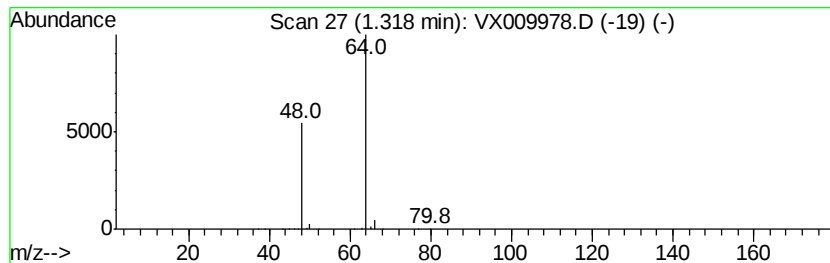
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	65.46 ug/l	633328	Pentafluorobenzene	5.67
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	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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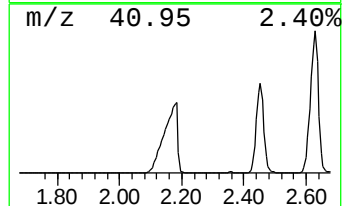
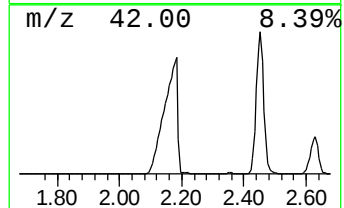
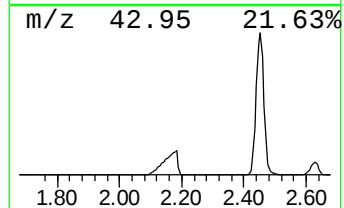
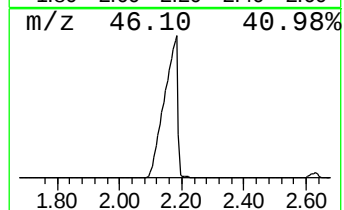
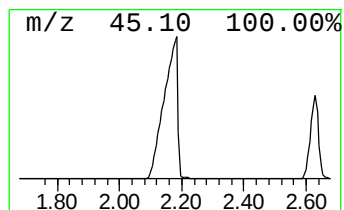
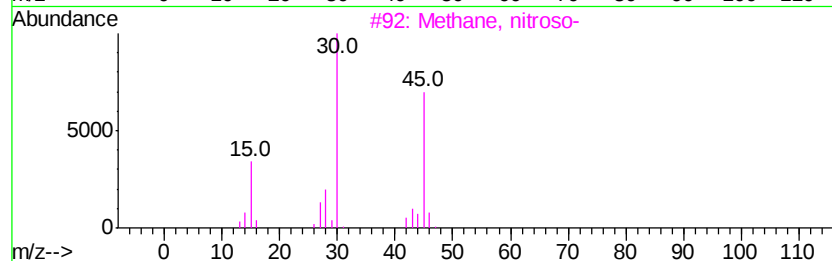
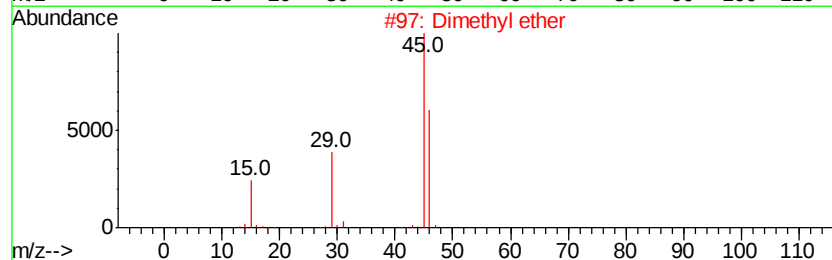
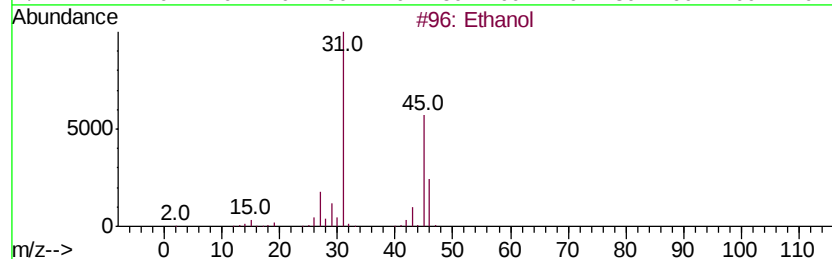
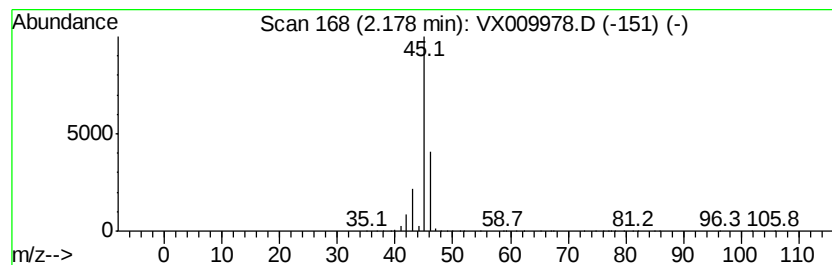
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	2395.84 ug/l	23179600	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	83
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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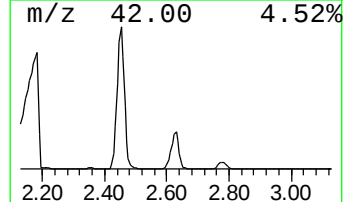
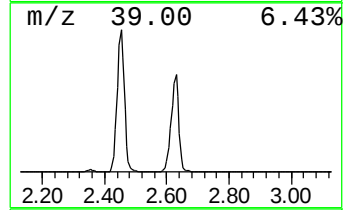
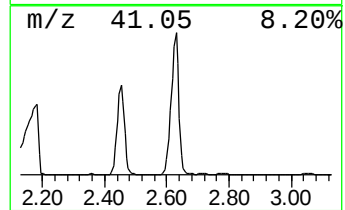
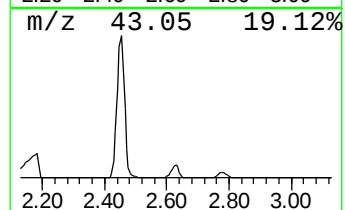
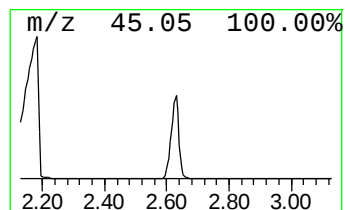
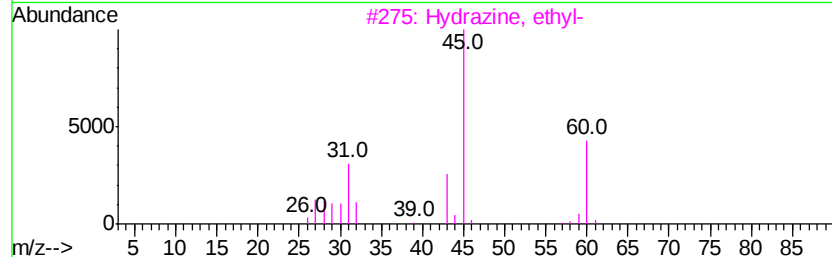
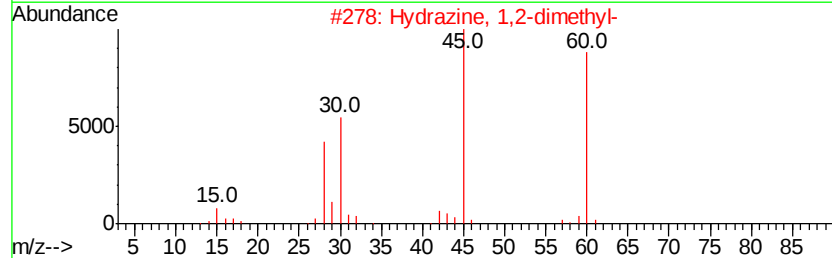
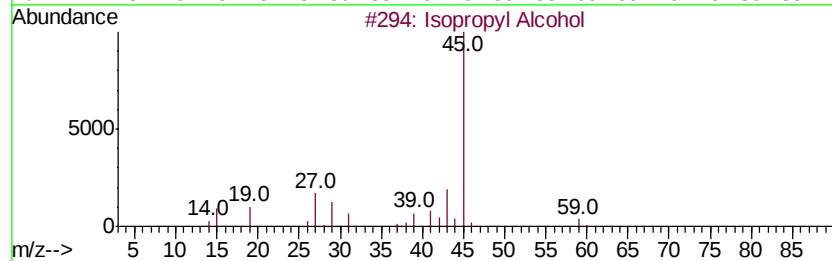
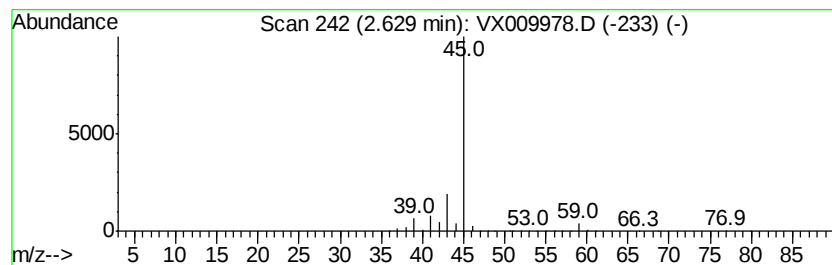
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.63	710.01 ug/l	6869290	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4		Formamide	45	CH3NO	000075-12-7	5
5		4-Penten-2-ol	86	C5H10O	000625-31-0	4



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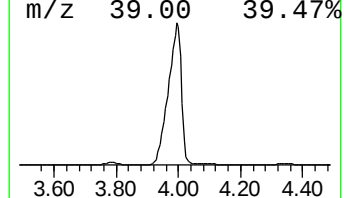
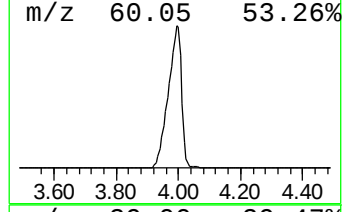
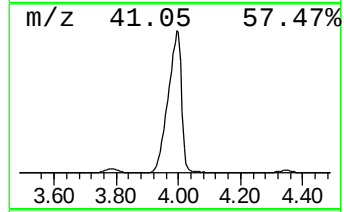
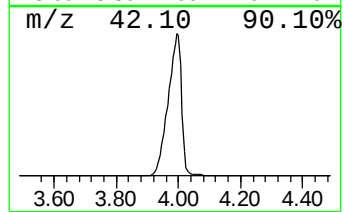
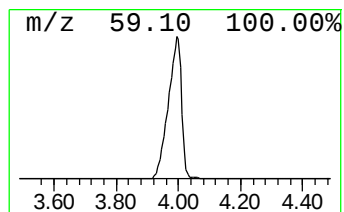
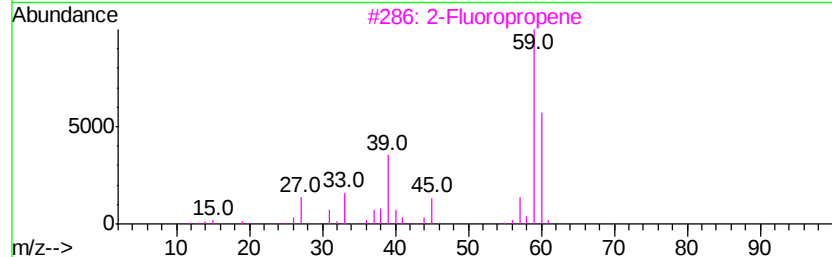
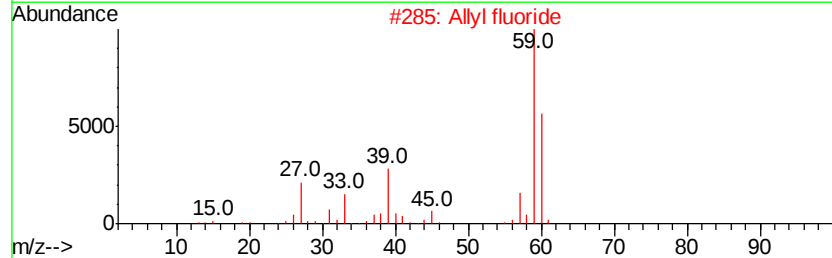
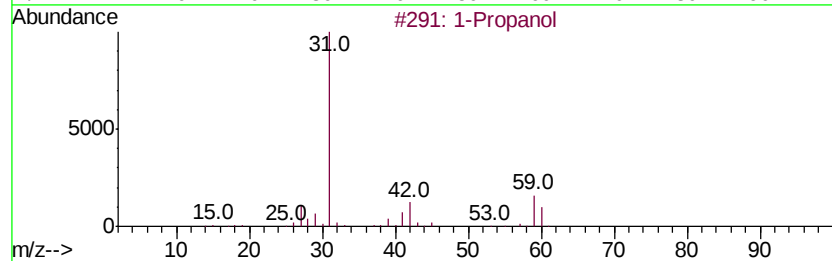
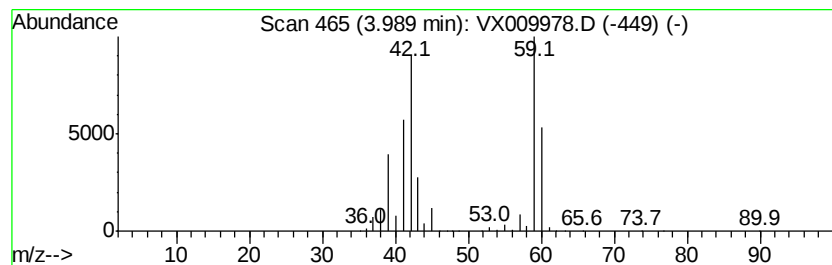
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Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	404.57 ug/l	3914130	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	64
2		Allyl fluoride	60	C3H5F	000818-92-8	32
3		2-Fluoropropene	60	C3H5F	001184-60-7	27
4		Cyclopropane	42	C3H6	000075-19-4	9
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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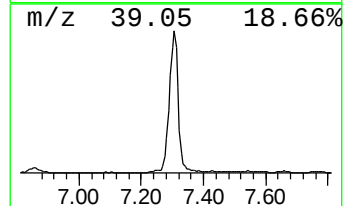
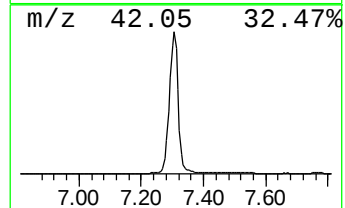
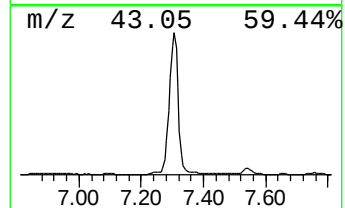
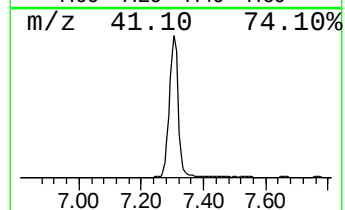
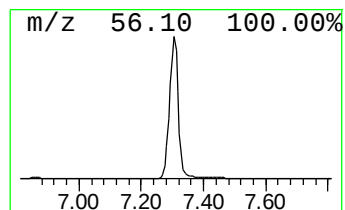
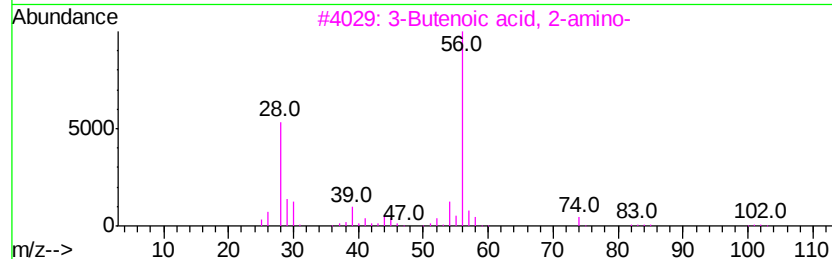
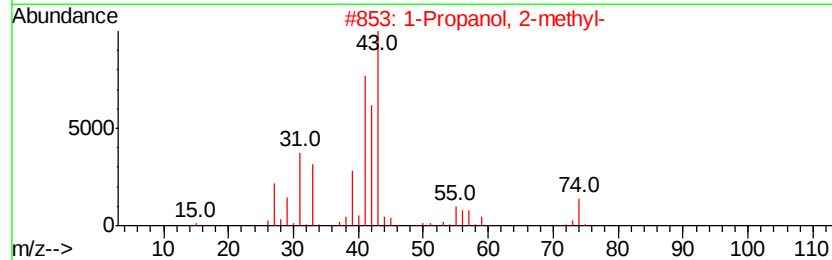
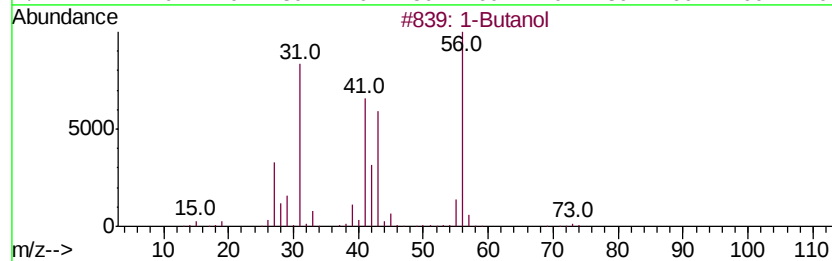
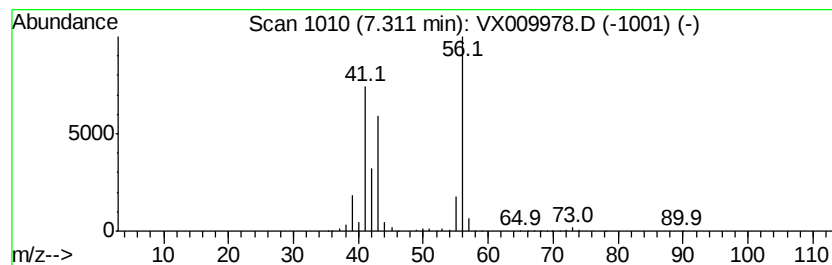
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	169.34 ug/l	2245270	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	90
2		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12
3		3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
4		Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5		Isobutylene epoxide	72	C4H8O	000558-30-5	9



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ClientSampleId :
COMP-1

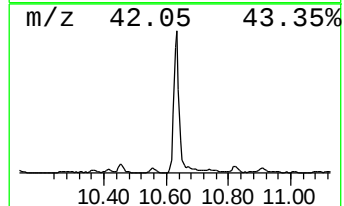
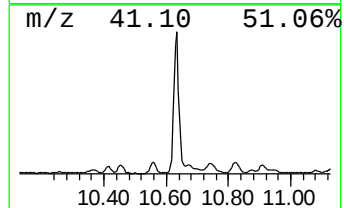
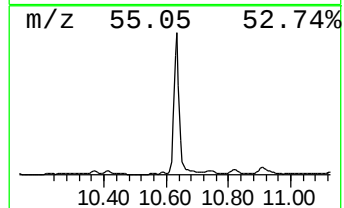
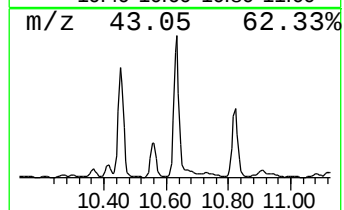
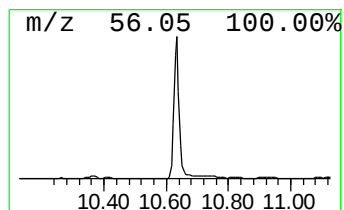
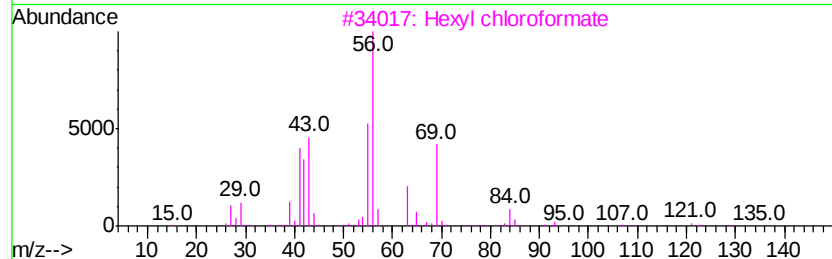
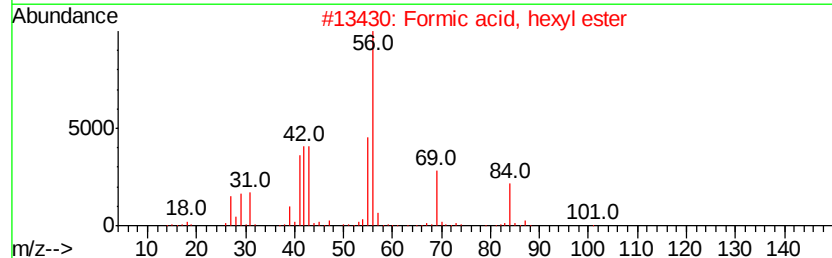
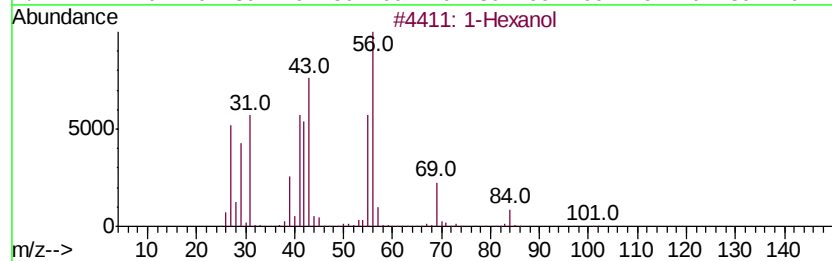
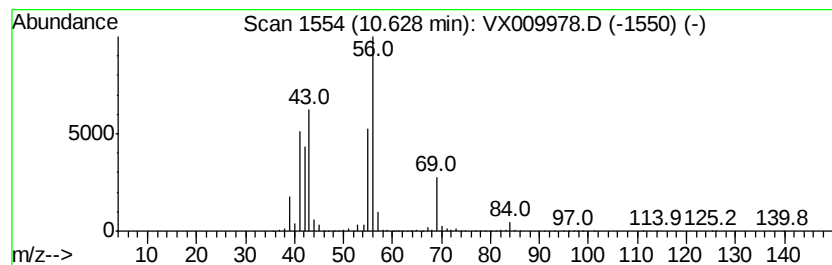
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	64.24 ug/l	984220	Chlorobenzene-d5	10.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol		102	C6H14O	000111-27-3	90
2	Formic acid, hexyl ester		130	C7H14O2	000629-33-4	78
3	Hexyl chloroformate		164	C7H13ClO2	006092-54-2	64
4	Cyclopropane, propyl-		84	C6H12	002415-72-7	59
5	1-Pentanol, 4-methyl-		102	C6H14O	000626-89-1	56



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009978.D
Acq On : 31 May 2019 12:01
Operator : JC/SP
Sample : K2964-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

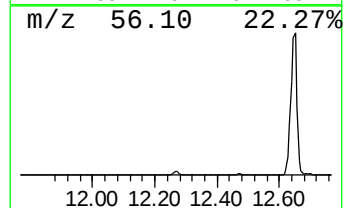
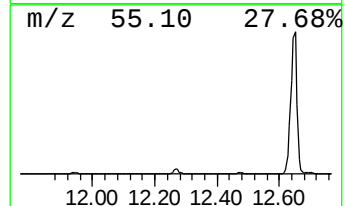
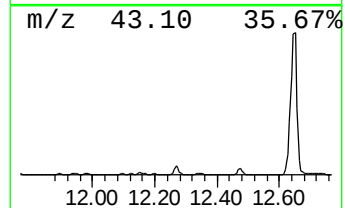
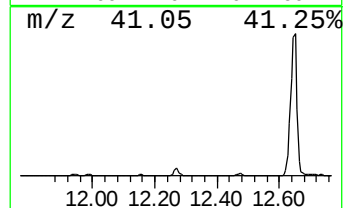
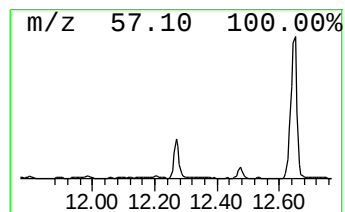
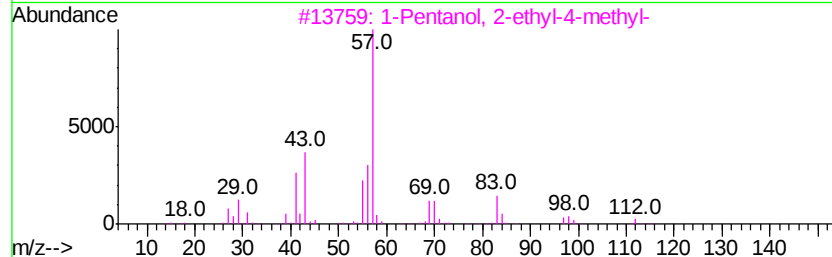
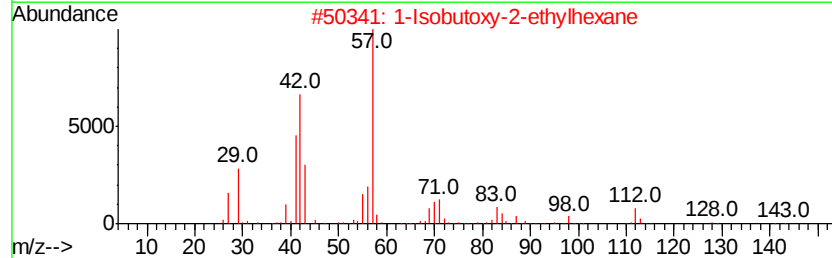
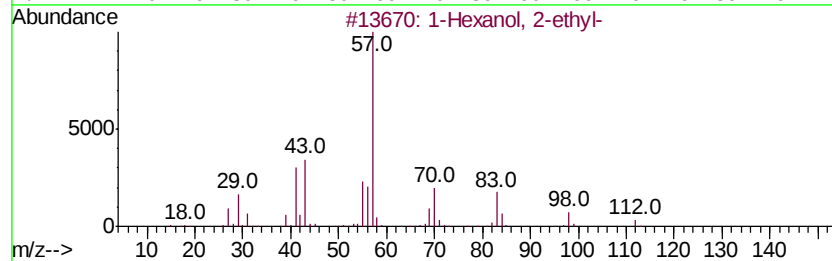
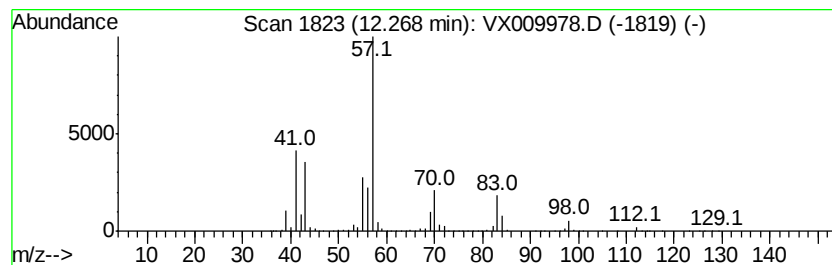
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	89.56 ug/l	1626680	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	78
2	1-Isobutoxy-2-ethylhexane	186 C12H26O	1000139-90-3	56
3	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	53
5	Heptane, 1,1'-oxybis-	214 C14H30O	000629-64-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009978.D
Acq On : 31 May 2019 12:01
Operator : JC/SP
Sample : K2964-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

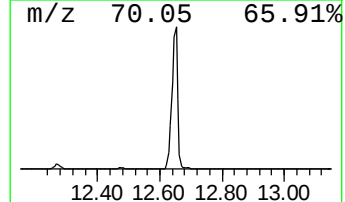
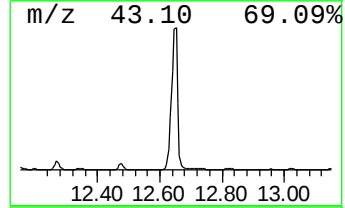
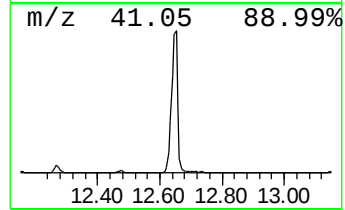
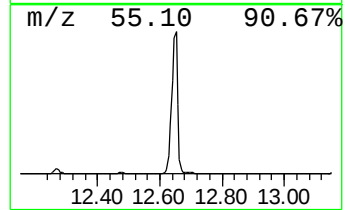
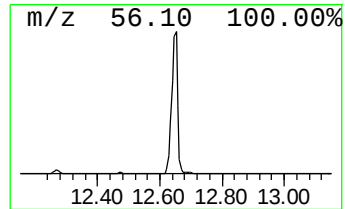
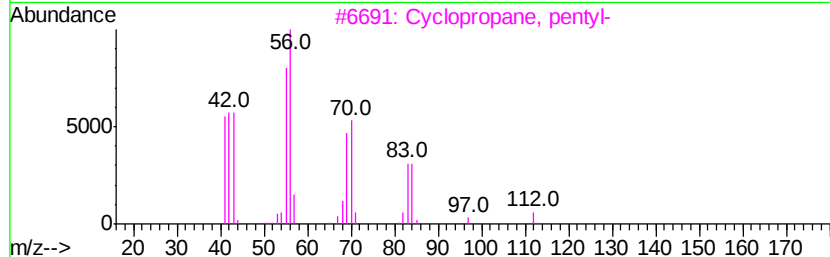
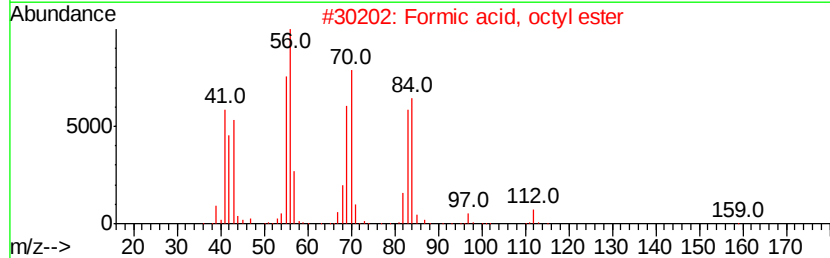
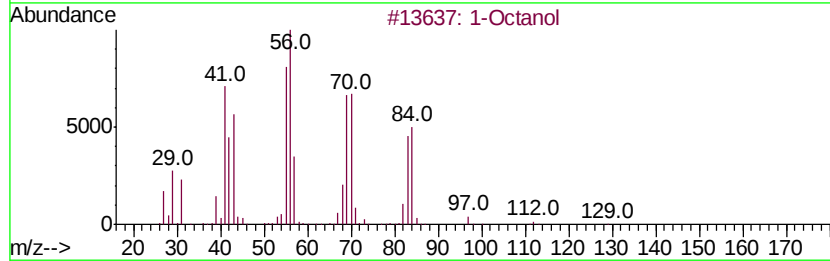
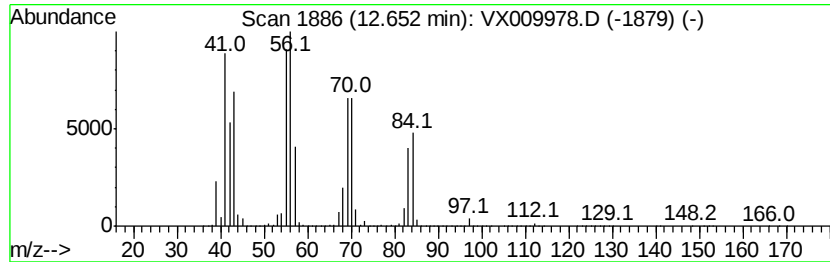
Instrument :
MSVOA_X
ClientSampleId :
COMP-1

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.65	1936.10 ug/l	35166400	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3	Cyclopropane, pentyl-	112	C8H16	002511-91-3	78
4	Cyclooctane	112	C8H16	000292-64-8	78
5	1-Nonanol	144	C9H20O	000143-08-8	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
 Data File : VX009978.D
 Acq On : 31 May 2019 12:01
 Operator : JC/SP
 Sample : K2964-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-1

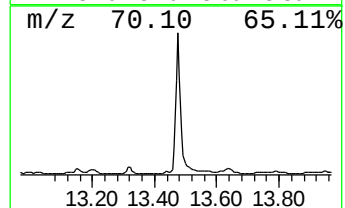
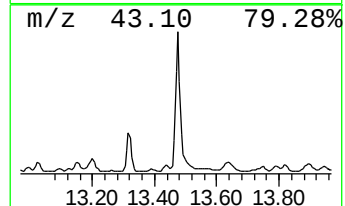
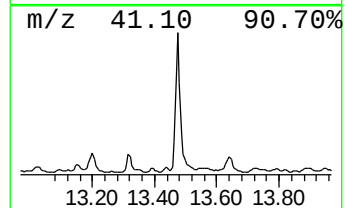
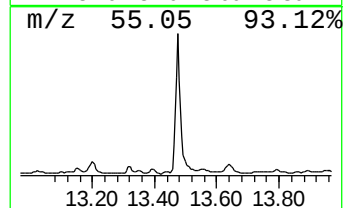
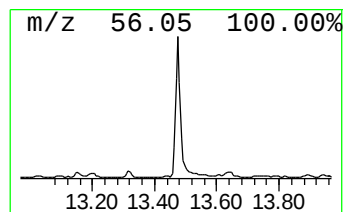
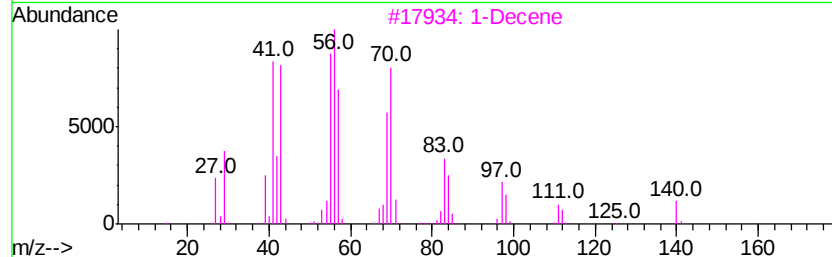
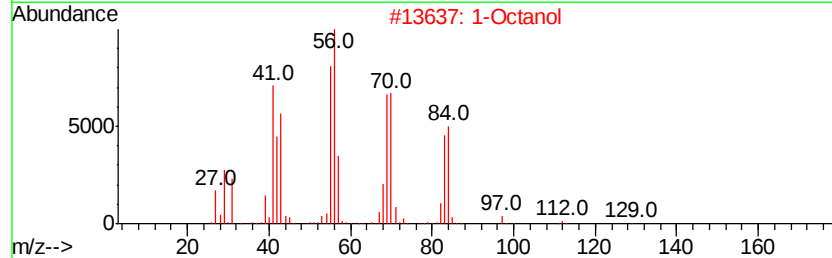
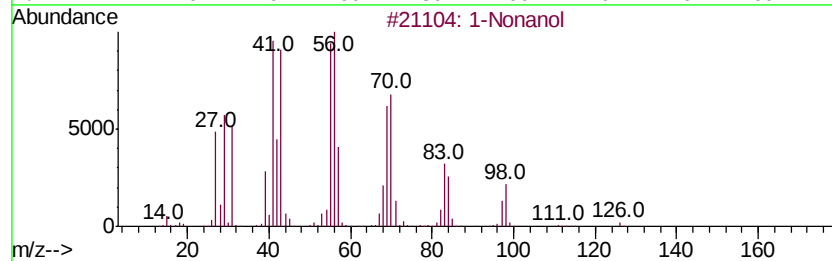
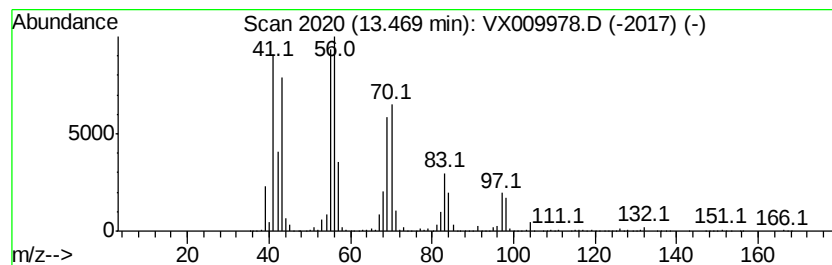
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 Quant Title : SW846 8260

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

 Peak Number 9 1-Nonanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	141.68 ug/l	2573410	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonanol	144	C9H20O	000143-08-8	91
2		1-Octanol	130	C8H18O	000111-87-5	80
3		1-Decene	140	C10H20	000872-05-9	72
4		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	68
5		Isopropylcyclobutane	98	C7H14	000872-56-0	68



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009978.D
Acq On : 31 May 2019 12:01
Operator : JC/SP
Sample : K2964-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

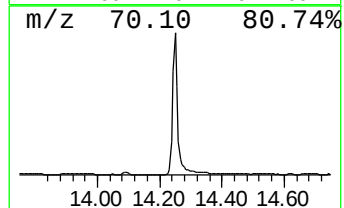
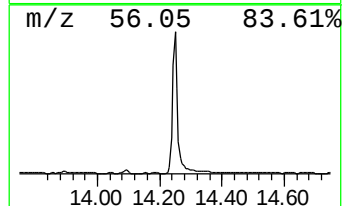
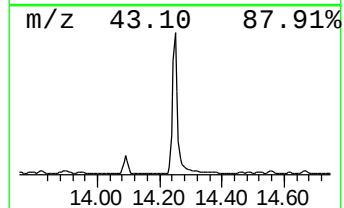
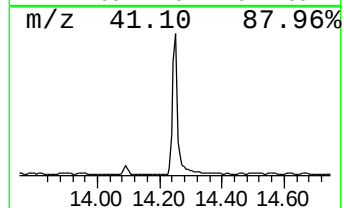
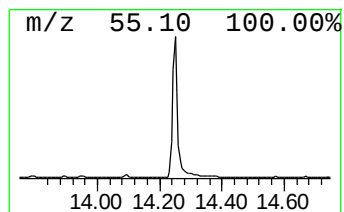
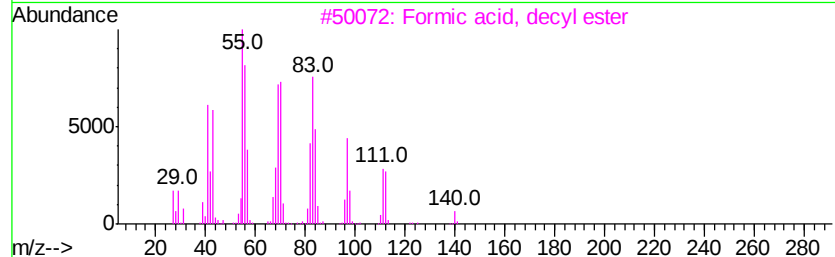
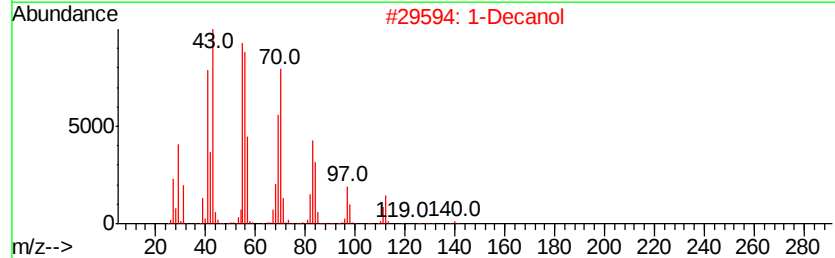
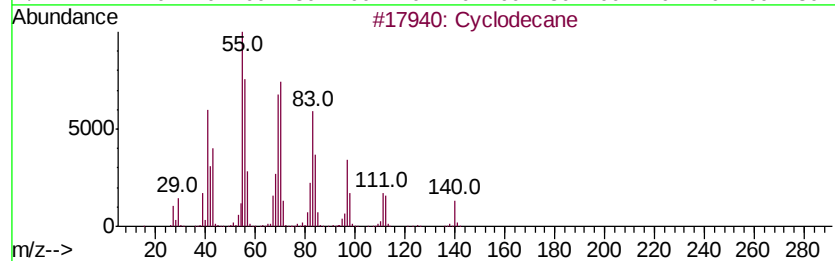
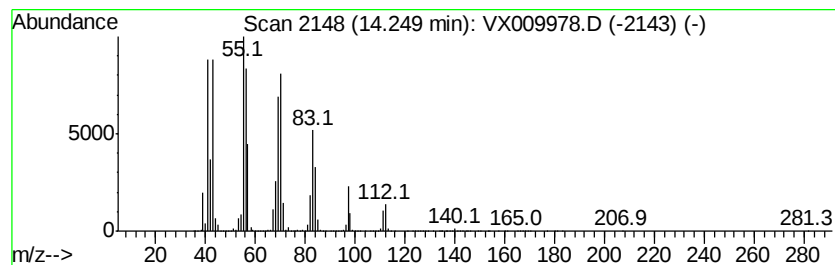
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 10 Cyclodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	369.53 ug/l	6712050	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclodecane	140	C10H20	000293-96-9	91
2		1-Decanol	158	C10H22O	000112-30-1	91
3		Formic acid, decyl ester	186	C11H22O2	005451-52-5	90
4		Cyclopropane, octyl-	154	C11H22	001472-09-9	87
5		Cyclodecane, methyl-	154	C11H22	013151-43-4	87



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX053119\
 Data File : VX009978.D
 Acq On : 31 May 2019 12:01
 Operator : JC/SP
 Sample : K2964-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.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	1.32	65.5	ug/l	633328	1	5.67	483746	50.0
Ethanol	2.18	2395.8	ug/l	23179600	1	5.67	483746	50.0
Isopropyl Alcohol	2.63	710.0	ug/l	6869290	1	5.67	483746	50.0
1-Propanol	3.99	404.6	ug/l	3914130	1	5.67	483746	50.0
1-Butanol	7.31	169.3	ug/l	2245270	2	6.86	662937	50.0
1-Hexanol	10.63	64.2	ug/l	984220	3	10.11	766022	50.0
1-Hexanol, 2-ethyl-	12.27	89.6	ug/l	1626680	4	12.08	908178	50.0
1-Octanol	12.65	1936.1	ug/l	35166400	4	12.08	908178	50.0
1-Nonanol	13.47	141.7	ug/l	2573410	4	12.08	908178	50.0
Cyclodecane	14.25	369.5	ug/l	6712050	4	12.08	908178	50.0