

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091020\
 Data File : VX018346.D
 Acq On : 10 Sep 2020 17:57
 Operator : JC/SP
 Sample : L3952-05 10X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 16744

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\82X082120W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	59	63	74	rBV	1434556	1741431	24.26%	4.401%
2	2.093	158	165	178	rBV	2434450	3845394	53.57%	9.717%
3	2.416	213	218	230	rBV	567580	933201	13.00%	2.358%
4	2.580	237	245	254	rVB	90147	167778	2.34%	0.424%
5	3.916	456	464	477	rVB3	48274	125451	1.75%	0.317%
6	4.452	540	552	563	rVB	110612	309667	4.31%	0.783%
7	4.641	574	583	593	rBV2	56455	164609	2.29%	0.416%
8	5.464	708	718	732	rBV2	282878	835440	11.64%	2.111%
9	5.629	732	745	760	rVB	506321	1420155	19.78%	3.589%
10	6.031	800	811	823	rBV	323485	844885	11.77%	2.135%
11	6.830	931	942	951	rBV	728014	1743227	24.28%	4.405%
12	6.939	951	960	980	rVB	3146509	7178696	100.00%	18.140%
13	7.269	1004	1014	1022	rBV	1868929	3800914	52.95%	9.605%
14	7.348	1022	1027	1035	rVB	86699	183164	2.55%	0.463%
15	8.695	1241	1248	1256	rBV	1506715	2353918	32.79%	5.948%
16	9.043	1299	1305	1316	rVB	186387	290943	4.05%	0.735%
17	9.201	1323	1331	1338	rVB	118253	169893	2.37%	0.429%
18	9.604	1386	1397	1405	rBV	962180	1785214	24.87%	4.511%
19	10.097	1472	1478	1488	rVB	1587331	2164279	30.15%	5.469%
20	10.353	1513	1520	1530	rBV	2676451	3596442	50.10%	9.088%
21	11.122	1640	1646	1653	rBV	1479108	1771412	24.68%	4.476%
22	11.189	1653	1657	1663	rVB	99068	128262	1.79%	0.324%
23	12.012	1787	1792	1795	rBV2	59822	72371	1.01%	0.183%
24	12.060	1795	1800	1807	rVV	1825961	2257399	31.45%	5.704%
25	13.816	2079	2088	2094	rBV	118799	178161	2.48%	0.450%
26	14.267	2157	2162	2170	rVB5	46755	82060	1.14%	0.207%
27	14.523	2199	2204	2209	rBV7	38459	87573	1.22%	0.221%
28	14.658	2222	2226	2227	rBV2	83151	101236	1.41%	0.256%
29	14.676	2227	2229	2232	rVV	113851	135646	1.89%	0.343%
30	14.822	2250	2253	2257	rVV2	87961	107223	1.49%	0.271%
31	15.231	2315	2320	2321	rBV4	47216	71813	1.00%	0.181%
32	15.255	2321	2324	2327	rVB3	116334	147009	2.05%	0.371%
33	15.468	2355	2359	2363	rVB3	77444	110941	1.55%	0.280%
34	15.529	2364	2369	2377	rBV2	118355	220990	3.08%	0.558%

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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	15.663	2387	2391	2394	rBV2	93471	121759	1.70%	0.308%
36	15.798	2408	2413	2417	rVB4	89203	150478	2.10%	0.380%
37	16.145	2465	2470	2476	rBV2	86645	174005	2.42%	0.440%

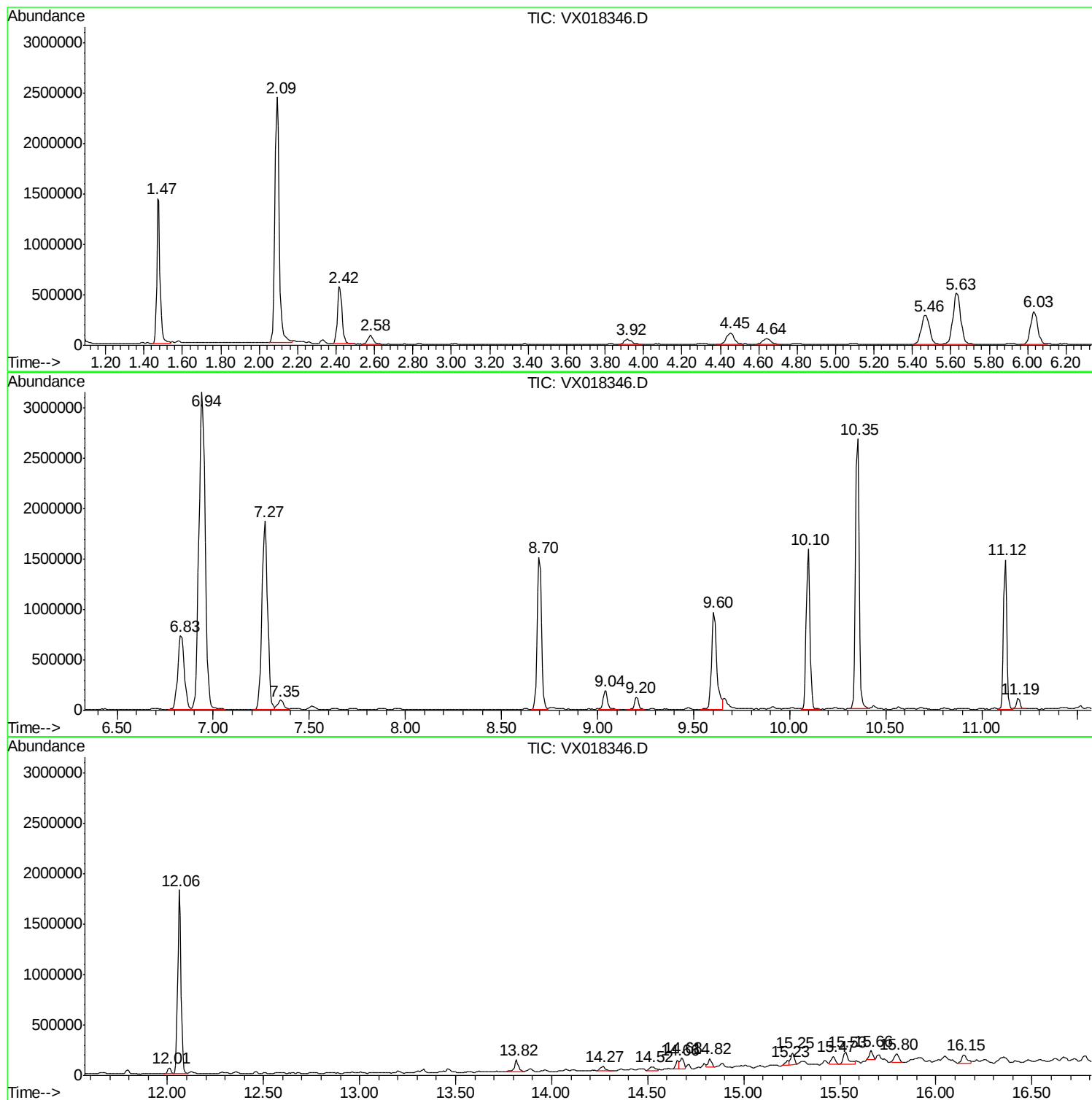
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Quant Title : SW846 8260

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



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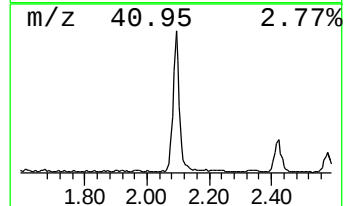
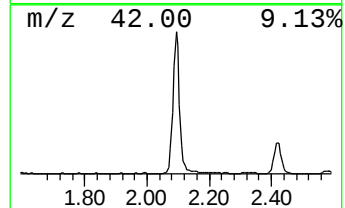
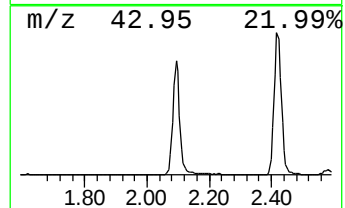
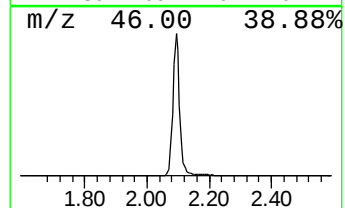
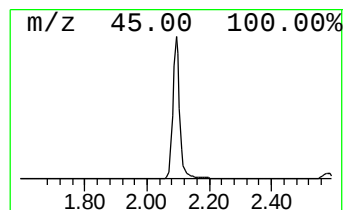
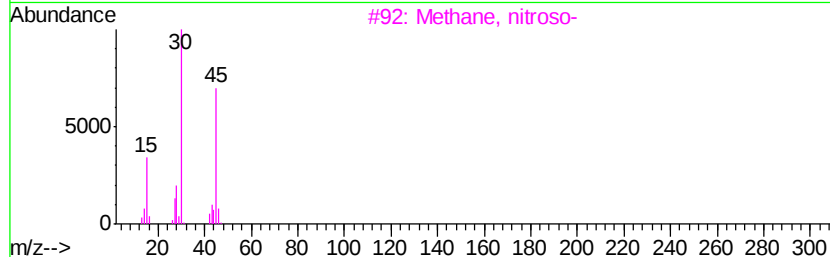
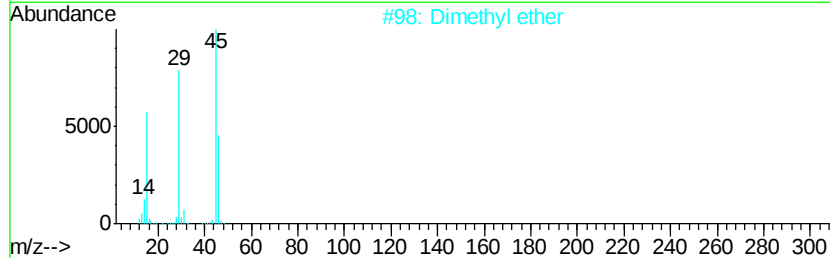
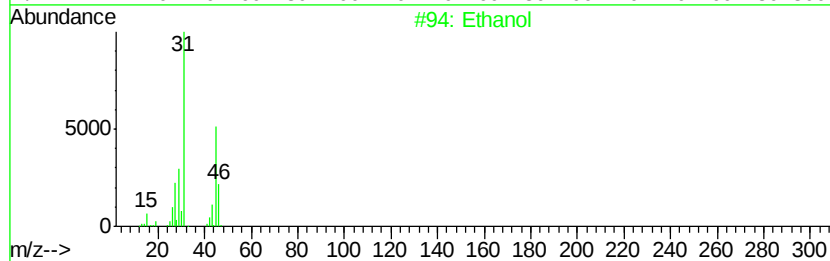
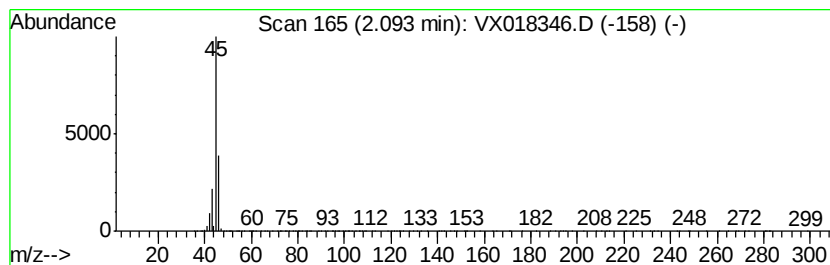
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	135.39 ug/l	3845390	Pentafluorobenzene	5.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	64
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	L-Lactic acid		90	C3H6O3	000079-33-4	2



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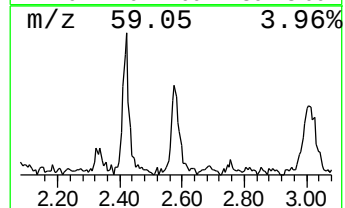
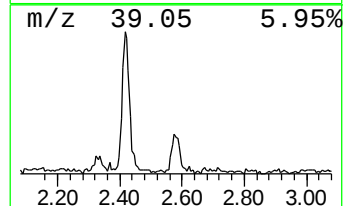
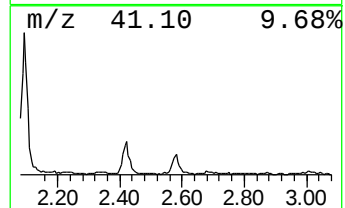
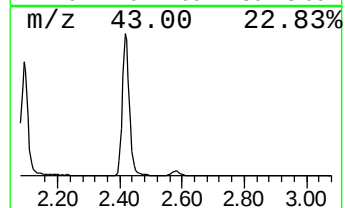
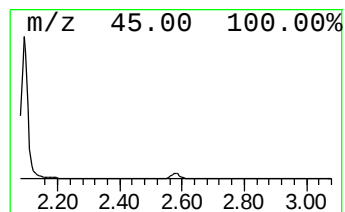
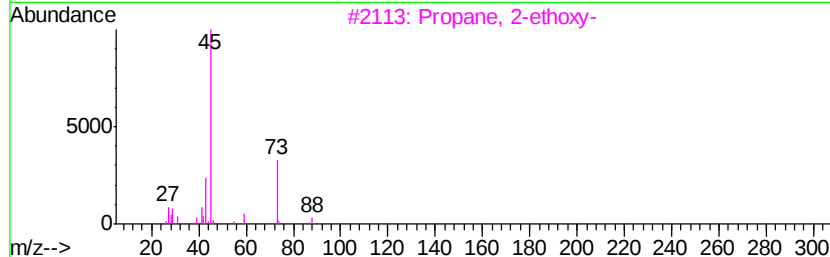
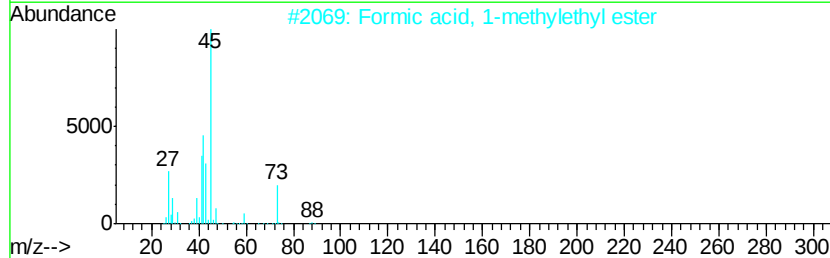
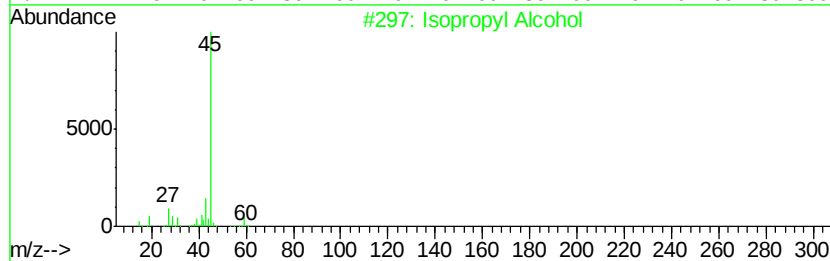
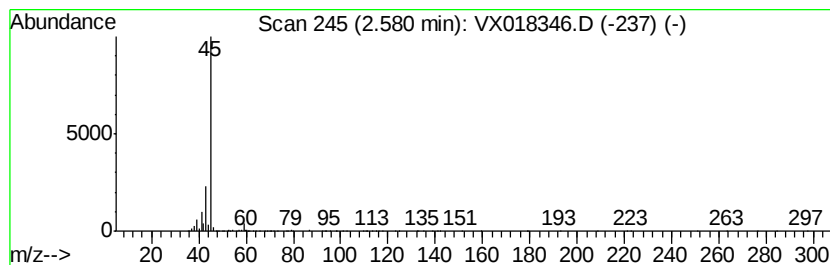
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.58	5.91 ug/l	167778	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2		Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
3		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
4		2-Pentanol	88	C5H12O	006032-29-7	9
5		Paraldehyde	132	C6H12O3	000123-63-7	9



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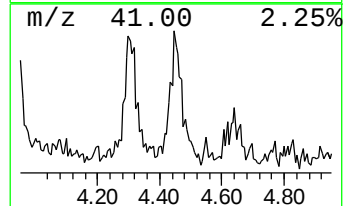
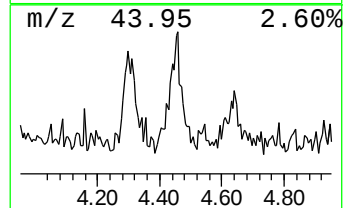
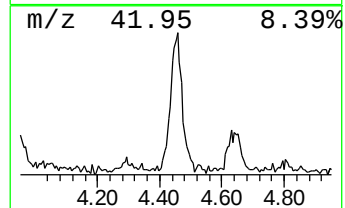
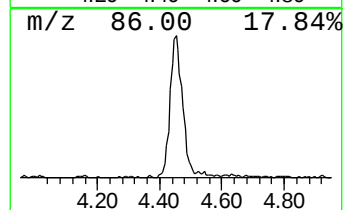
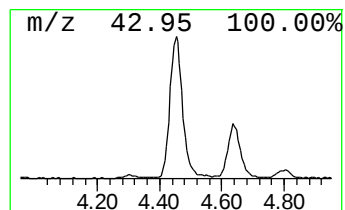
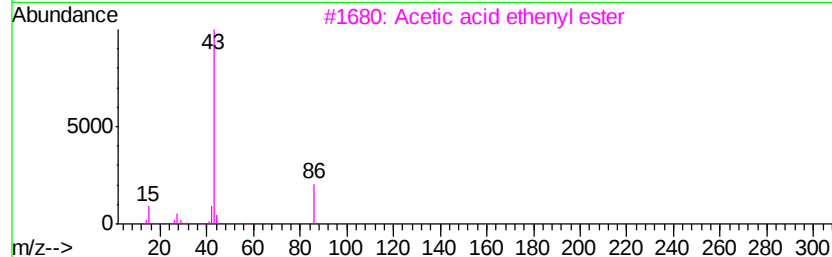
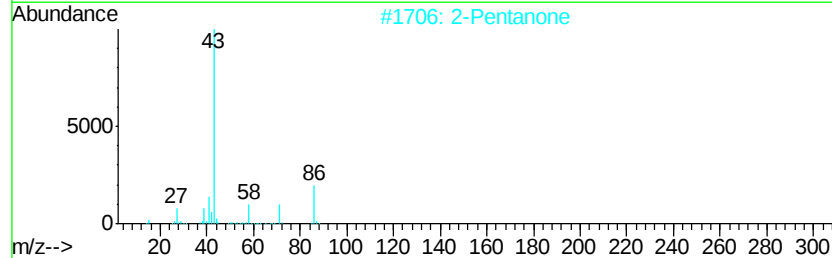
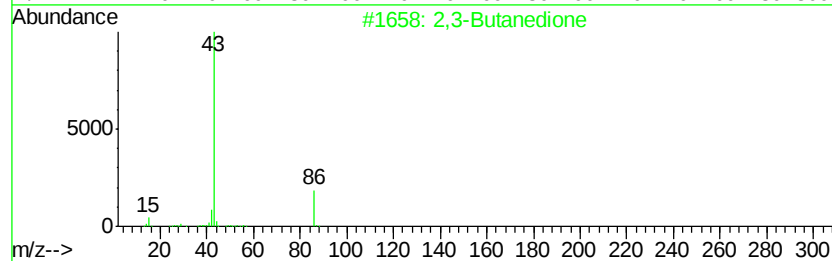
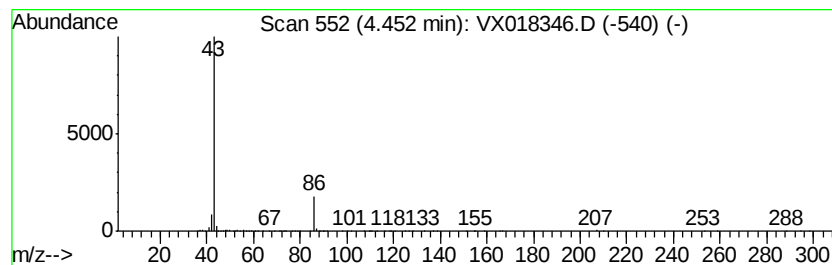
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,3-Butanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	10.90 ug/l	309667	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Butanedione	86	C4H6O2	000431-03-8	72
2		2-Pentanone	86	C5H10O	000107-87-9	72
3		Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
4		Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7



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ALS Vial : 14 Sample Multiplier: 1

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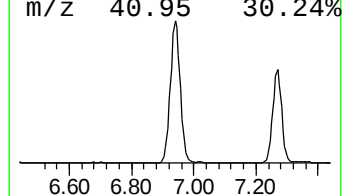
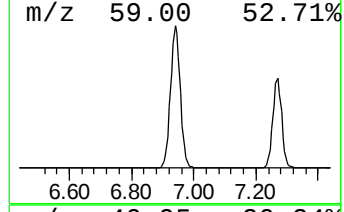
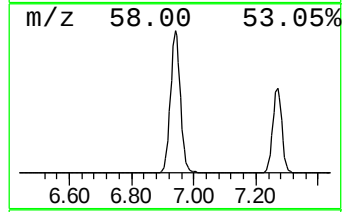
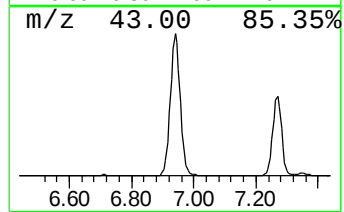
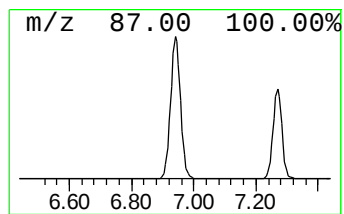
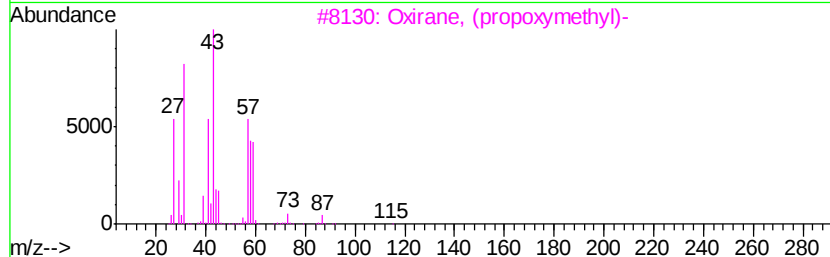
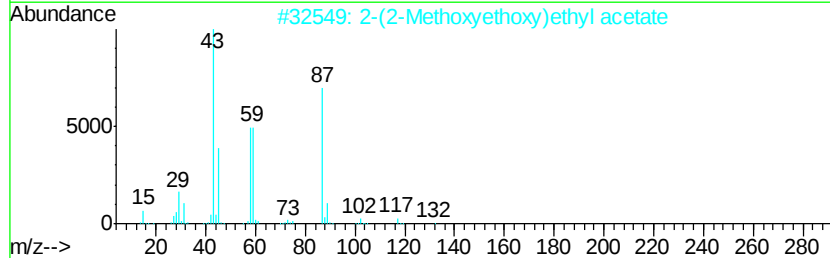
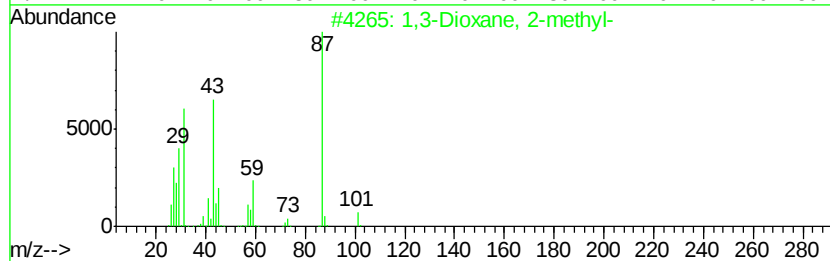
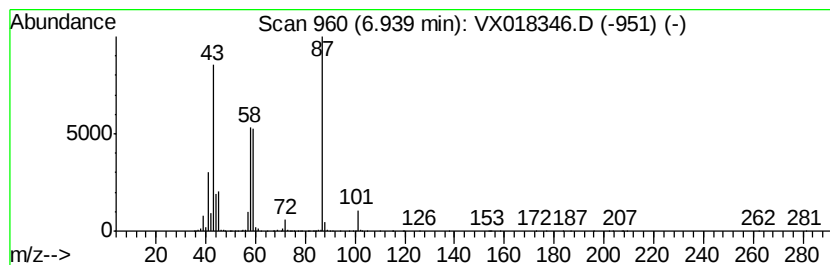
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.94 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	205.90 ug/l	7178700	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	40
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	38
3		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
4		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	32
5		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	28



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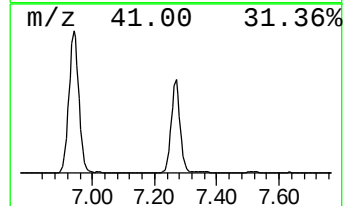
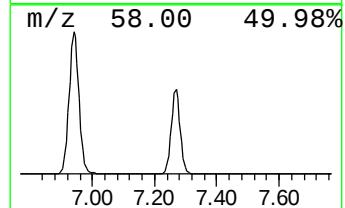
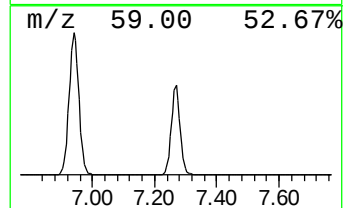
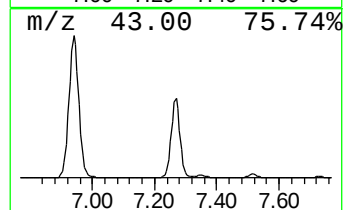
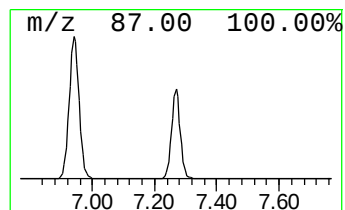
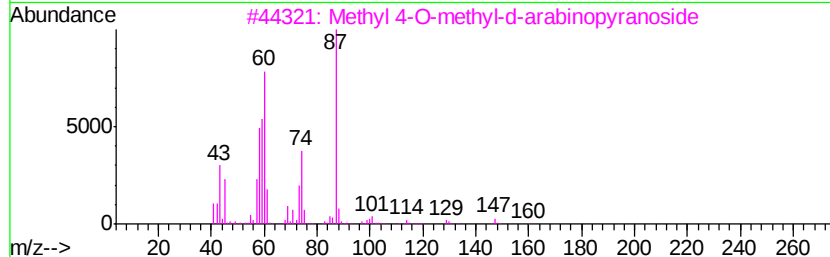
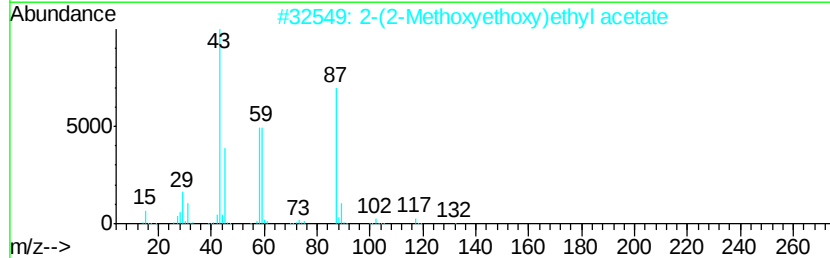
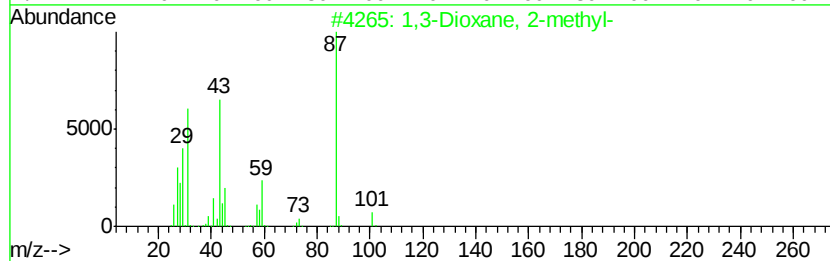
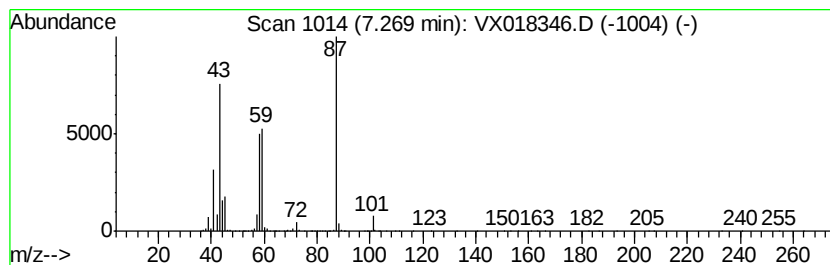
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Peak Number 6 unknown7.27 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	109.02 ug/l	3800910	1,4-Difluorobenzene	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	47
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	39
4			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	38
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091020\
Data File : VX018346.D
Acq On : 10 Sep 2020 17:57
Operator : JC/SP
Sample : L3952-05 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16744

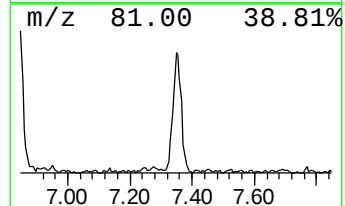
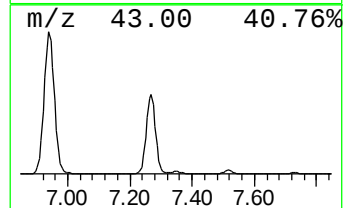
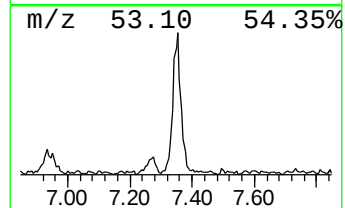
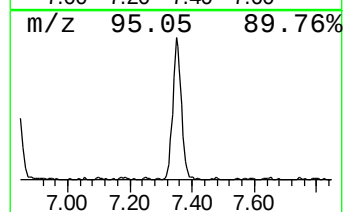
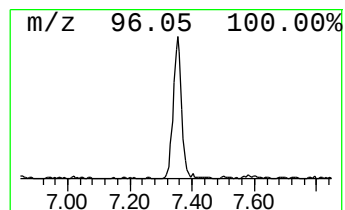
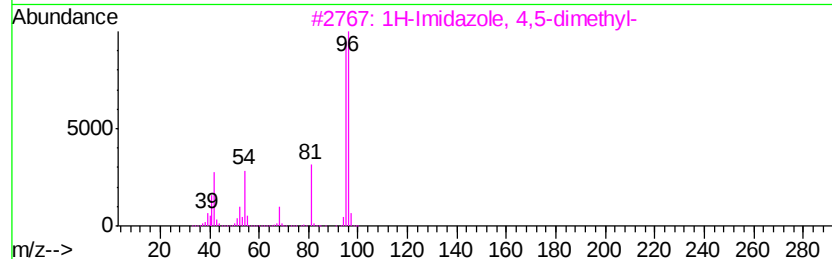
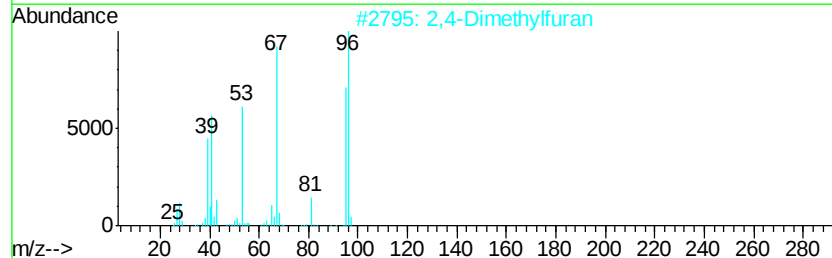
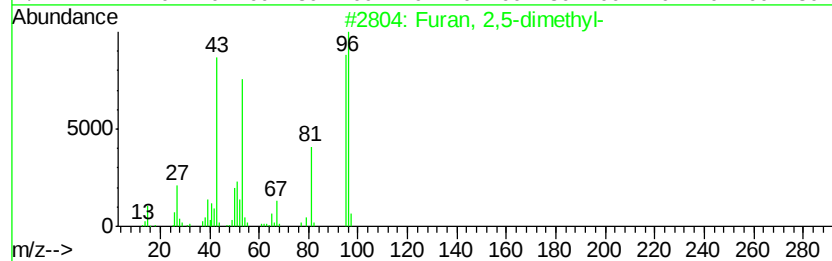
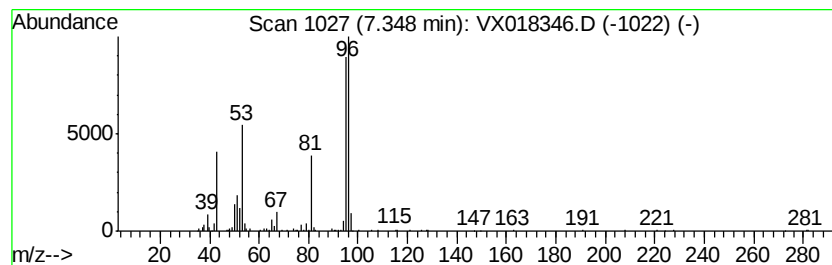
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 7 Furan, 2,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	5.25 ug/l	183164	1,4-Difluorobenzene	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	91
2			2,4-Dimethylfuran	96	C6H8O	003710-43-8	78
3			1H-Imidazole, 4,5-dimethyl-	96	C5H8N2	002302-39-8	46
4			1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	000694-48-4	43
5			Furfural	96	C5H4O2	000098-01-1	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091020\
Data File : VX018346.D
Acq On : 10 Sep 2020 17:57
Operator : JC/SP
Sample : L3952-05 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16744

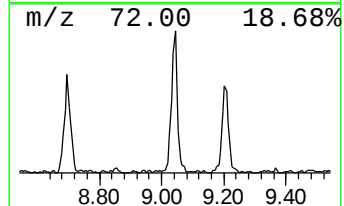
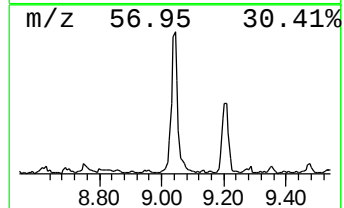
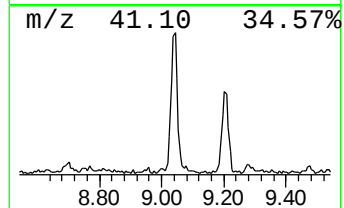
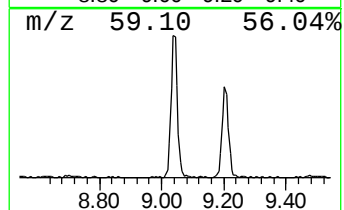
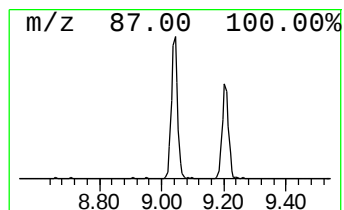
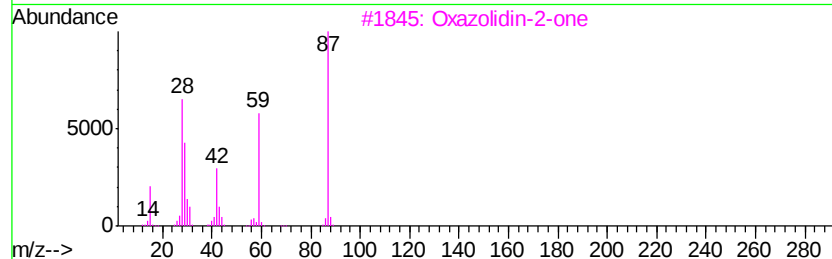
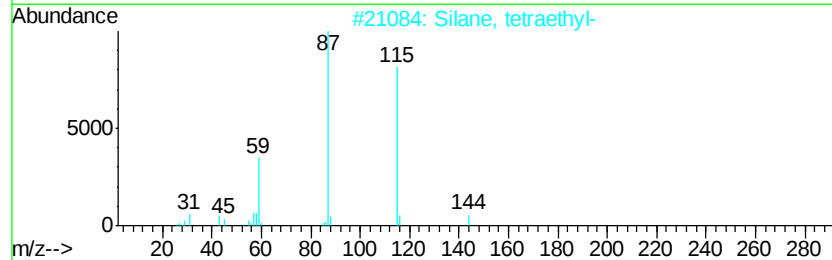
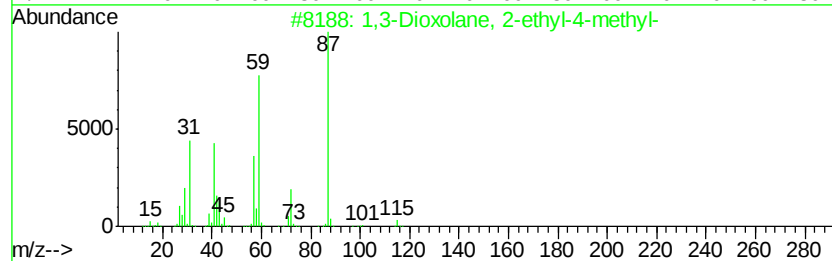
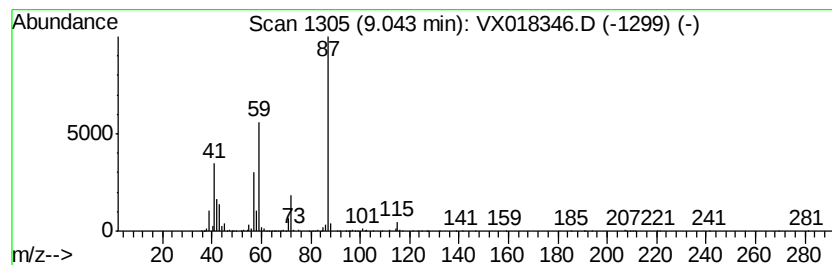
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	6.72 ug/l	290943	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	78
2		Silane, tetraethyl-	144	C8H20Si	000631-36-7	64
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
4		2-[2-[2-[2-[2-[2-[2-[2-[2-...	602	C27H54O14	1000351-89-6	64
5		2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091020\
Data File : VX018346.D
Acq On : 10 Sep 2020 17:57
Operator : JC/SP
Sample : L3952-05 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16744

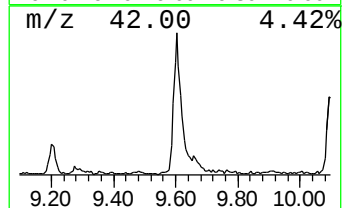
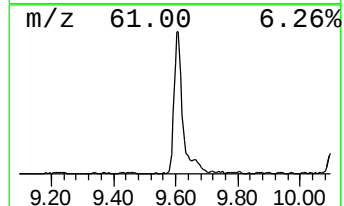
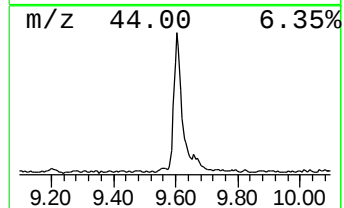
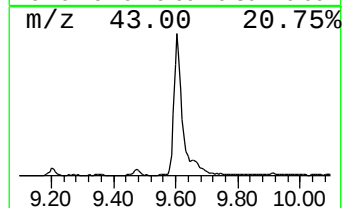
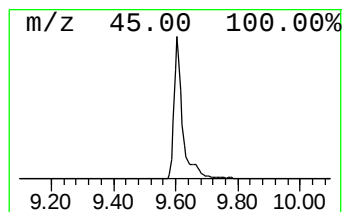
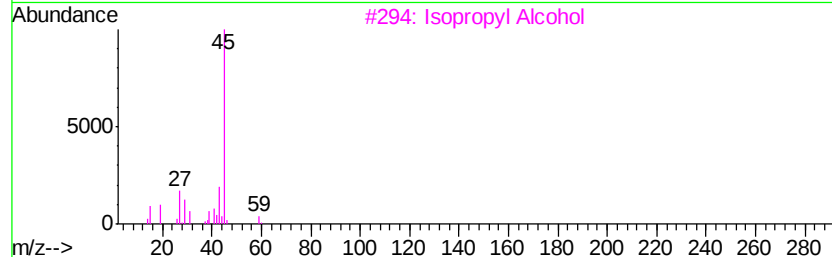
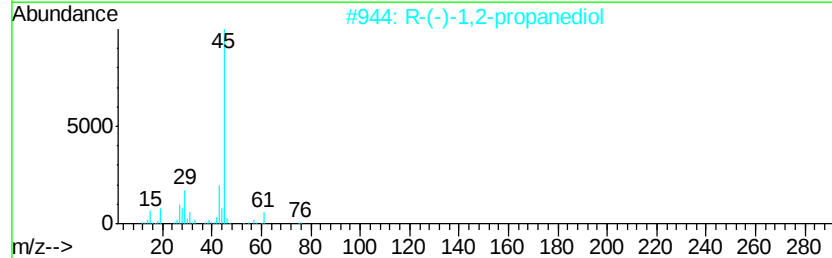
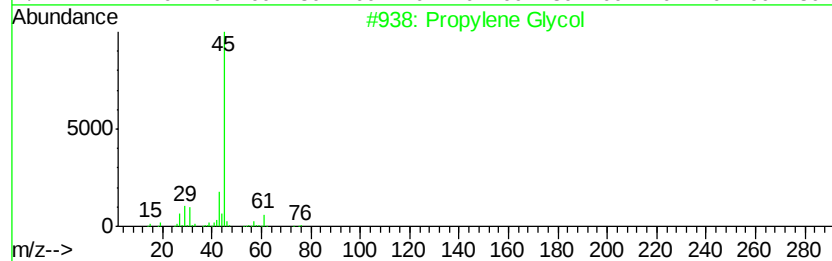
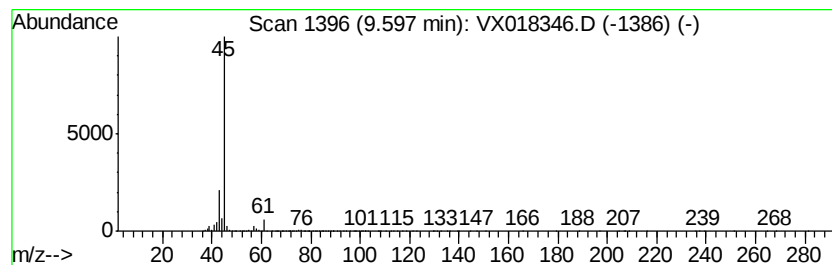
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 9 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	41.24 ug/l	1785210	Chlorobenzene-d5	10.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propylene Glycol	76	C3H8O2	000057-55-6	90
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5		2-Heptanol	116	C7H16O	000543-49-7	9



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091020\
Data File : VX018346.D
Acq On : 10 Sep 2020 17:57
Operator : JC/SP
Sample : L3952-05 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16744

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.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	2.09	135.4	ug/l	3845390	1	5.63	1420160	50.0
Isopropyl Alcohol	2.58	5.9	ug/l	167778	1	5.63	1420160	50.0
2,3-Butanedione	4.45	10.9	ug/l	309667	1	5.63	1420160	50.0
unknown6.94	6.94	205.9	ug/l	7178700	2	6.83	1743230	50.0
unknown7.27	7.27	109.0	ug/l	3800910	2	6.83	1743230	50.0
Furan, 2,5-dimethyl-	7.35	5.3	ug/l	183164	2	6.83	1743230	50.0
1,3-Dioxolane, 2-...	9.04	6.7	ug/l	290943	3	10.10	2164280	50.0
Propylene Glycol	9.60	41.2	ug/l	1785210	3	10.10	2164280	50.0