

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112520\
 Data File : VX019659.D
 Acq On : 25 Nov 2020 16:18
 Operator : JC/MD
 Sample : L4841-02 5X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 16855

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\82X112120W.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	68	rBV	632560	735734	6.67%	2.218%
2	1.514	68	70	91	rVB	75268	148789	1.35%	0.449%
3	2.124	162	170	190	rBV	1842666	2861914	25.96%	8.630%
4	2.331	198	204	209	rBV	234260	385051	3.49%	1.161%
5	2.422	214	219	236	rVB	453013	779318	7.07%	2.350%
6	2.605	242	249	261	rBV	147022	294779	2.67%	0.889%
7	3.995	447	477	518	rBV	2947299	11025545	100.00%	33.246%
8	5.464	707	718	734	rBV	169621	483902	4.39%	1.459%
9	5.623	734	744	765	rVB	313471	884464	8.02%	2.667%
10	6.031	799	811	819	rBV	195213	513283	4.66%	1.548%
11	6.830	930	942	953	rBV	481815	1145771	10.39%	3.455%
12	6.940	953	960	970	rVB	140375	321655	2.92%	0.970%
13	8.696	1240	1248	1254	rBV	1004751	1548645	14.05%	4.670%
14	8.763	1254	1259	1265	rVV	247190	388597	3.52%	1.172%
15	9.043	1297	1305	1318	rBV	359247	551974	5.01%	1.664%
16	9.598	1392	1396	1405	rVV	185368	319351	2.90%	0.963%
17	10.098	1471	1478	1489	rBV	939137	1330794	12.07%	4.013%
18	10.342	1507	1518	1524	rBV	212411	299017	2.71%	0.902%
19	10.683	1569	1574	1585	rVB	115802	162407	1.47%	0.490%
20	11.122	1640	1646	1654	rBV	793214	999015	9.06%	3.012%
21	11.421	1689	1695	1702	rBV	150660	273576	2.48%	0.825%
22	11.488	1702	1706	1714	rVB	118005	151920	1.38%	0.458%
23	11.652	1728	1733	1742	rBV	90519	114861	1.04%	0.346%
24	11.793	1751	1756	1761	rBV	459324	556797	5.05%	1.679%
25	12.061	1795	1800	1806	rVB	1060472	1268588	11.51%	3.825%
26	12.128	1806	1811	1815	rBV	169378	204912	1.86%	0.618%
27	12.256	1827	1832	1834	rBV	131868	170773	1.55%	0.515%
28	12.280	1834	1836	1839	rVV	117098	175133	1.59%	0.528%
29	12.305	1839	1840	1844	rVV	103165	112928	1.02%	0.341%
30	12.353	1844	1848	1858	rVV3	173849	288034	2.61%	0.869%
31	12.573	1879	1884	1885	rBV	95546	119625	1.08%	0.361%
32	12.591	1885	1887	1891	rVV	103085	123610	1.12%	0.373%
33	12.652	1891	1897	1900	rVV	176313	220604	2.00%	0.665%
34	12.738	1907	1911	1923	rBV3	85601	160509	1.46%	0.484%

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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	12.957	1940	1947	1951	rVV	144882	190941	1.73%	0.576%
36	13.000	1951	1954	1960	rVB	239104	290058	2.63%	0.875%
37	13.207	1980	1988	1992	rBV2	161096	225375	2.04%	0.680%
38	13.329	2004	2008	2014	rVB2	355783	471810	4.28%	1.423%
39	13.463	2025	2030	2038	rVB	134822	179855	1.63%	0.542%
40	13.585	2046	2050	2052	rVV	85566	114515	1.04%	0.345%
41	13.622	2052	2056	2062	rVV4	108094	220436	2.00%	0.665%
42	13.701	2066	2069	2075	rVB2	102335	162872	1.48%	0.491%
43	13.817	2081	2088	2095	rBV	506875	648681	5.88%	1.956%
44	13.963	2106	2112	2117	rBV4	84509	132491	1.20%	0.400%
45	14.115	2132	2137	2144	rBV	107838	134956	1.22%	0.407%
46	14.268	2155	2162	2170	rBV3	147336	291834	2.65%	0.880%
47	14.518	2198	2203	2209	rBV2	87591	122533	1.11%	0.369%
48	14.676	2219	2229	2233	rBV	425854	589267	5.34%	1.777%
49	14.823	2248	2253	2257	rBV	199217	266438	2.42%	0.803%

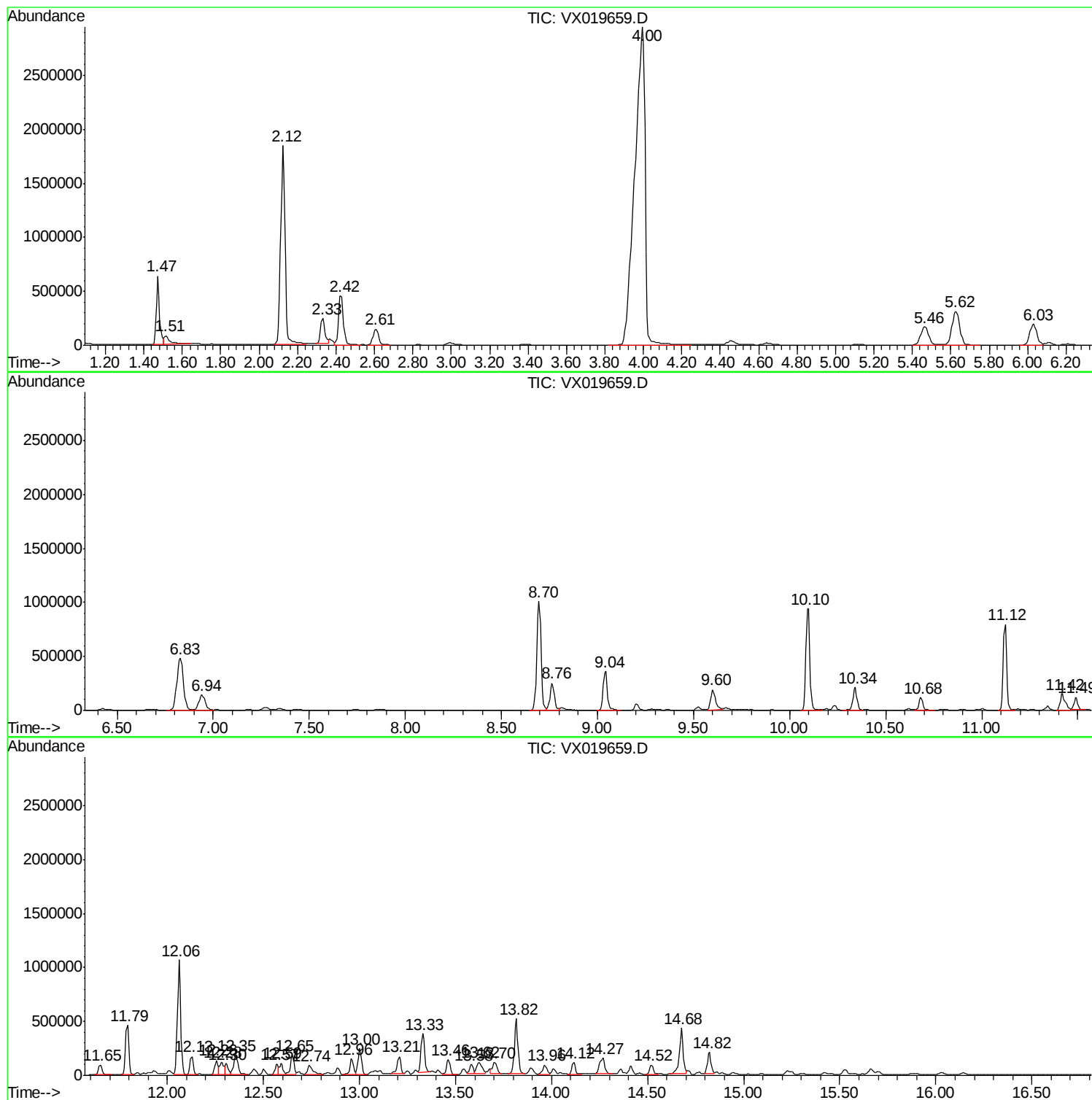
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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



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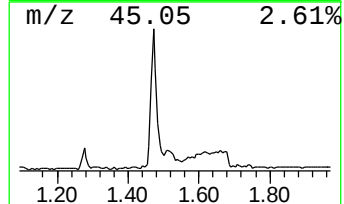
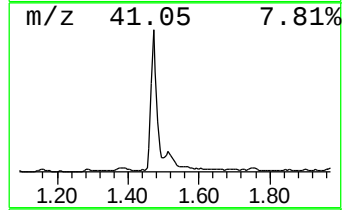
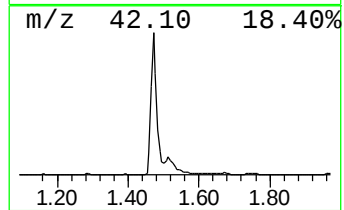
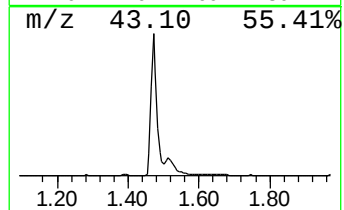
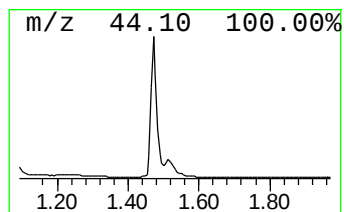
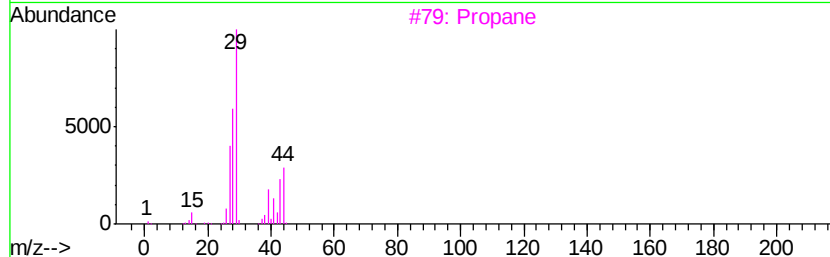
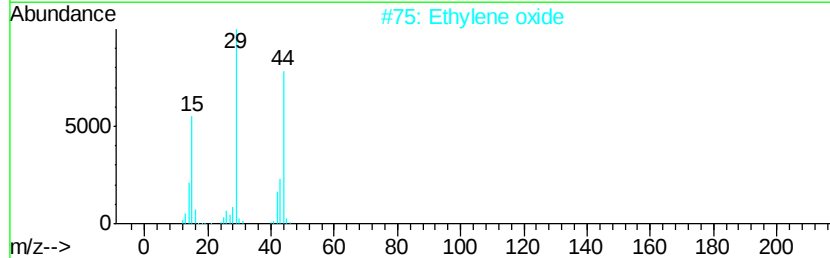
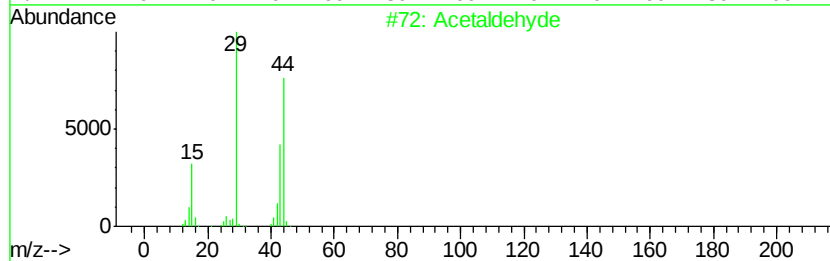
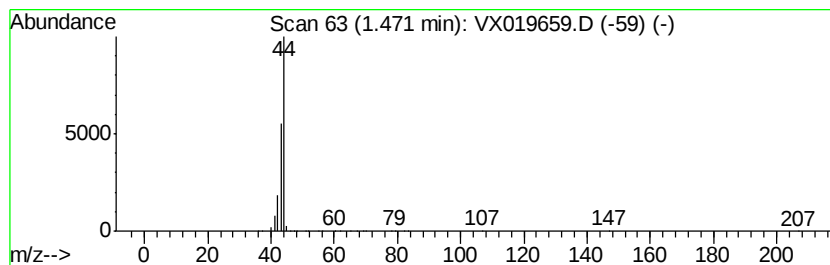
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	41.59 ug/l	735734	Pentafluorobenzene	5.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyd		44	C2H4O	000075-07-0	56
2	Ethylene oxide		44	C2H4O	000075-21-8	5
3	Propane		44	C3H8	000074-98-6	4
4	Alanine		89	C3H7NO2	000056-41-7	4
5	Carbon dioxide		44	CO2	000124-38-9	3



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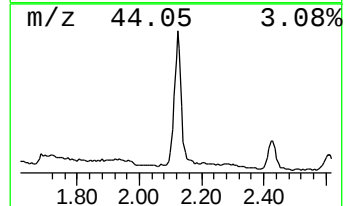
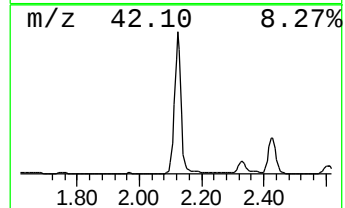
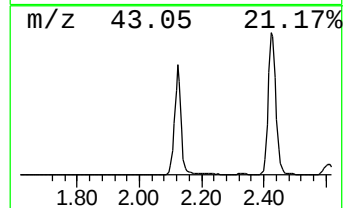
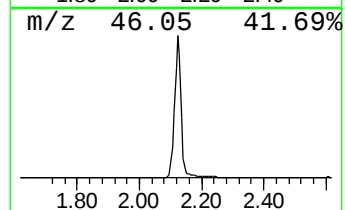
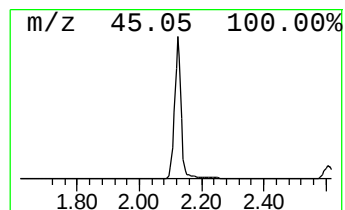
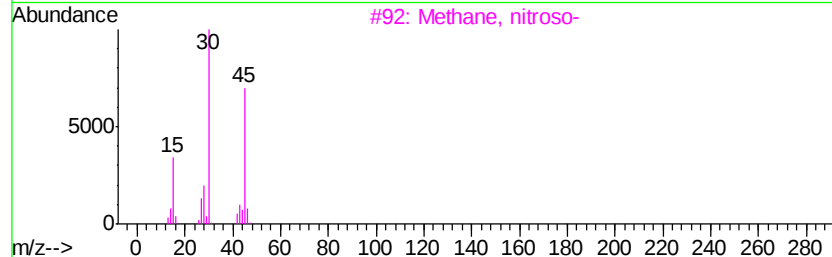
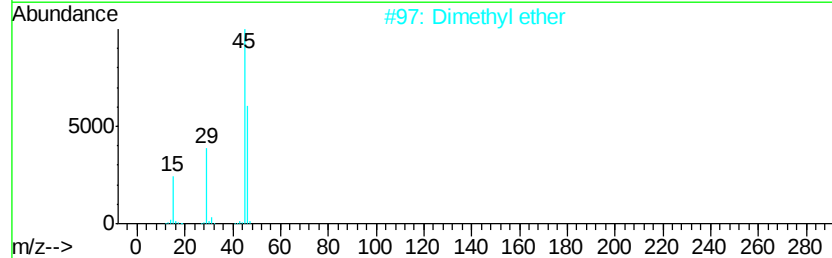
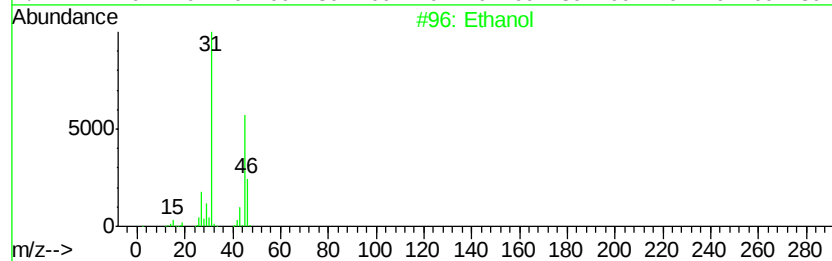
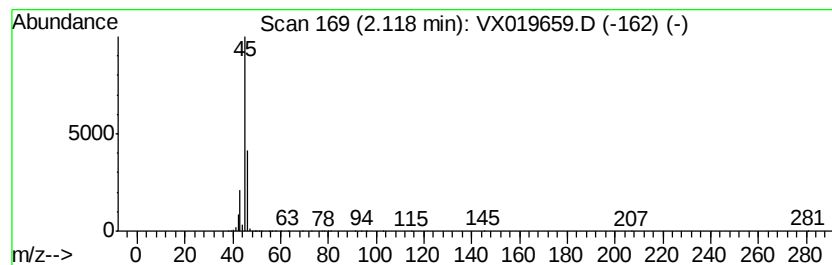
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Quant Title : SW846 8260

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.
2.12	161.79 ug/l	2861910	Pentafluorobenzene	5.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	74
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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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

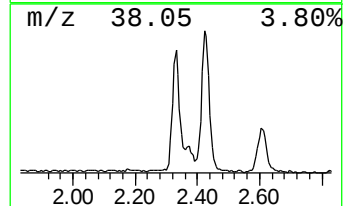
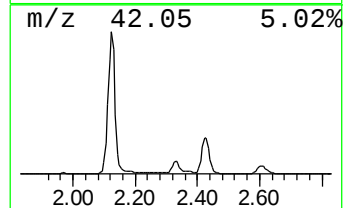
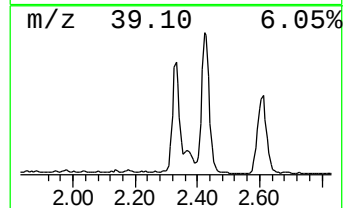
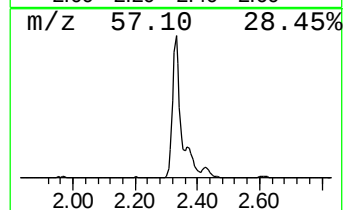
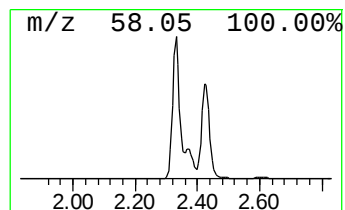
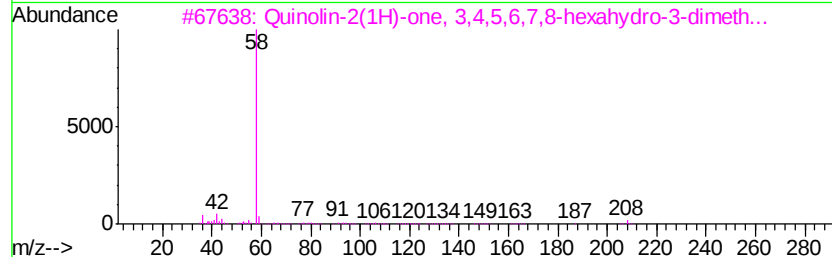
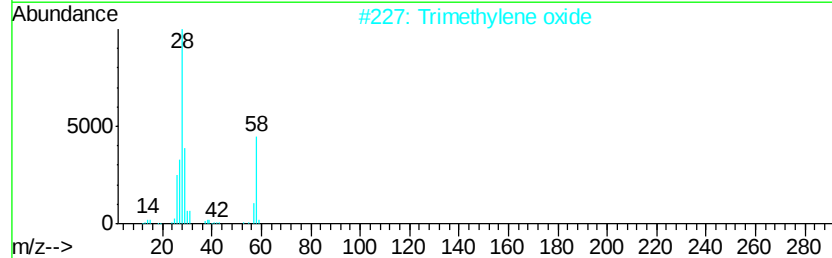
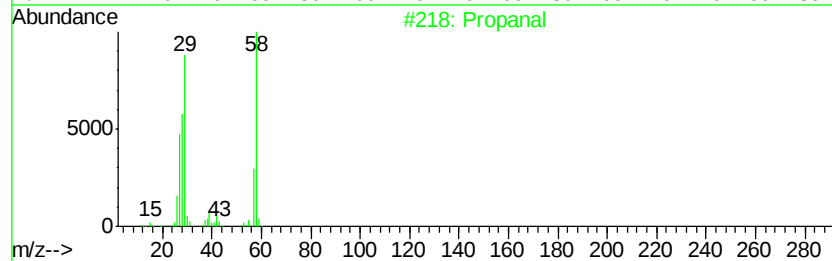
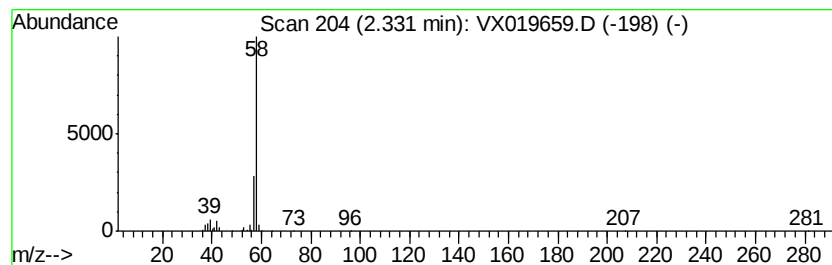
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	21.77 ug/l	385051	Pentafluorobenzene	5.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Propanal		58 C3H6O	000123-38-6 78
2	Trimethylene oxide		58 C3H6O	000503-30-0 56
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	Oxirane, methyl-, (S)-		58 C3H6O	016088-62-3 4



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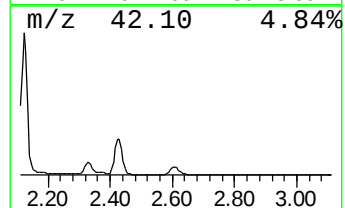
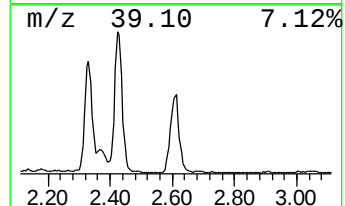
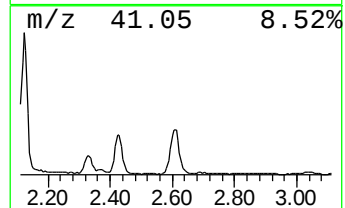
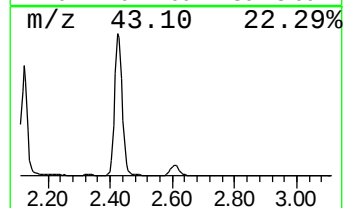
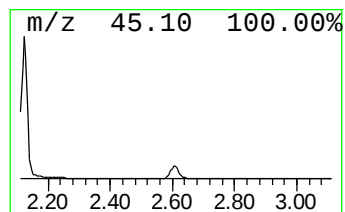
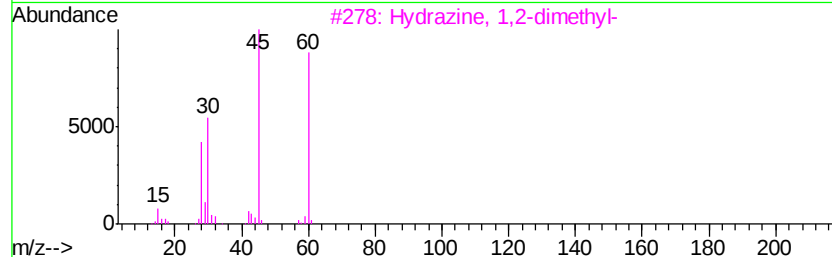
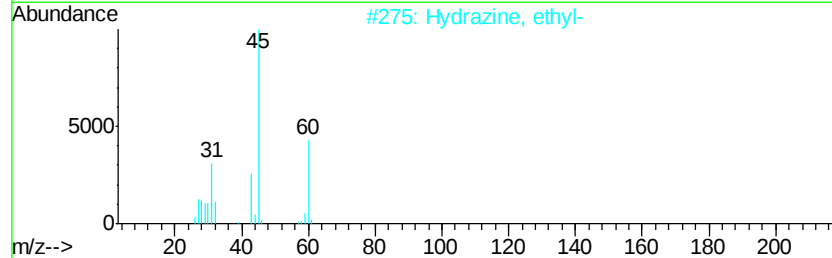
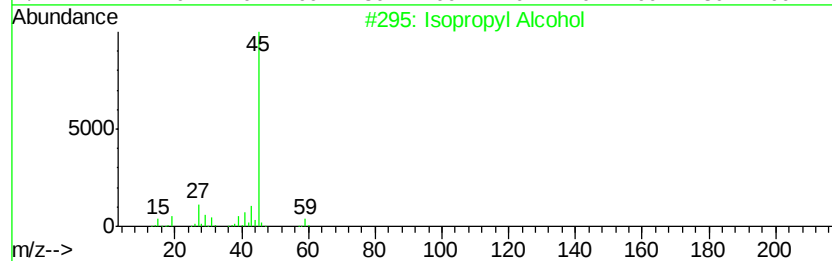
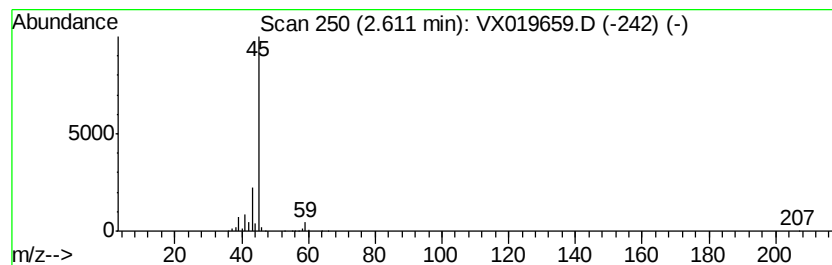
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.61	16.66 ug/l	294779	Pentafluorobenzene	5.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4		Formamide	45	CH3NO	000075-12-7	5
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	2



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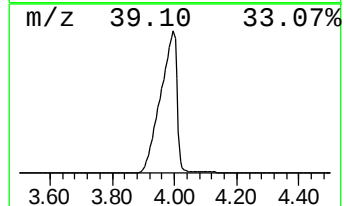
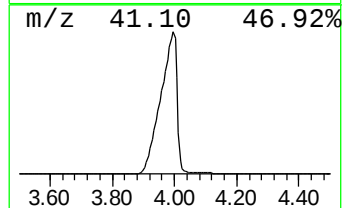
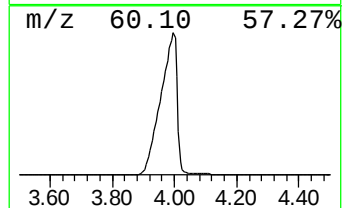
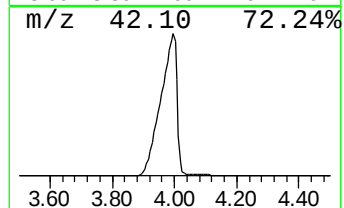
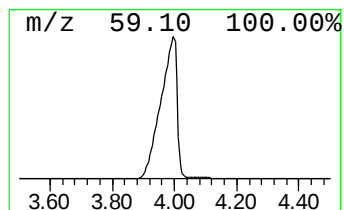
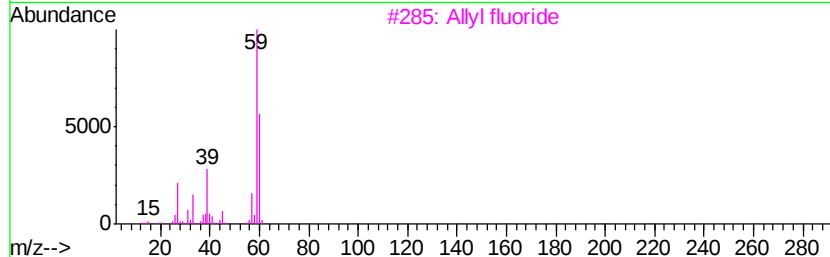
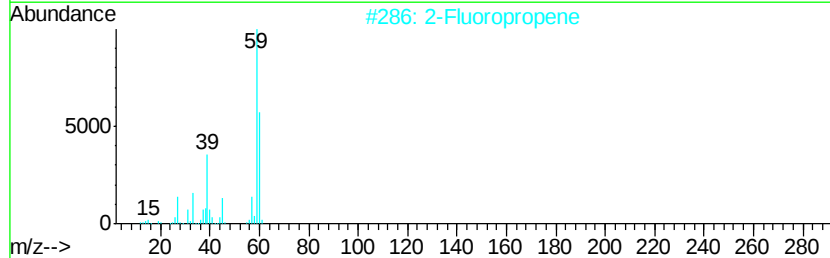
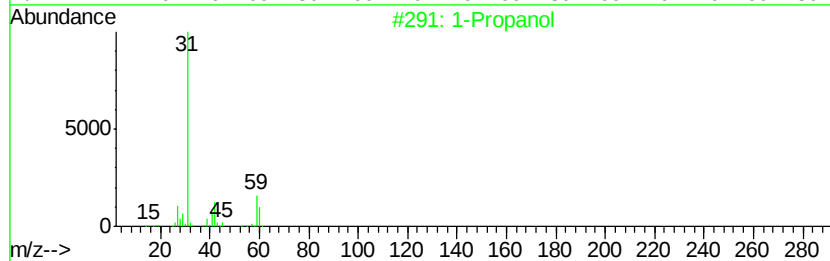
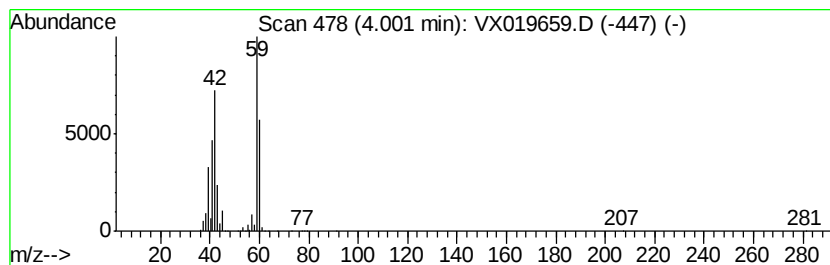
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Quant Title : SW846 8260

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

Peak Number 5 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	623.29 ug/l	11025500	Pentafluorobenzene	5.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol		60	C3H8O	000071-23-8	78
2	2-Fluoropropene		60	C3H5F	001184-60-7	49
3	Allyl fluoride		60	C3H5F	000818-92-8	47
4	Cyclopropane		42	C3H6	000075-19-4	27
5	Methanamine, N-hydroxy-N-methyl-		61	C2H7NO	005725-96-2	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019659.D
Acq On : 25 Nov 2020 16:18
Operator : JC/MD
Sample : L4841-02 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleID :
16855

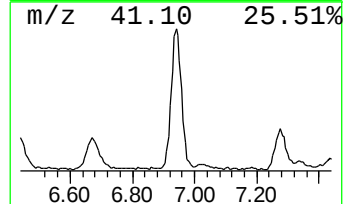
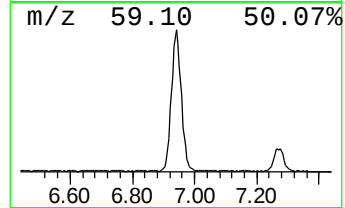
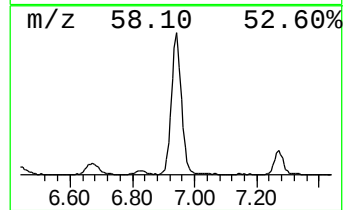
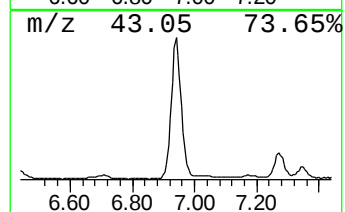
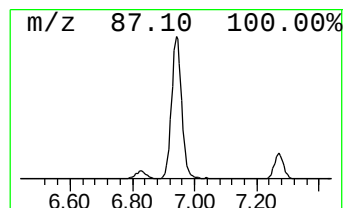
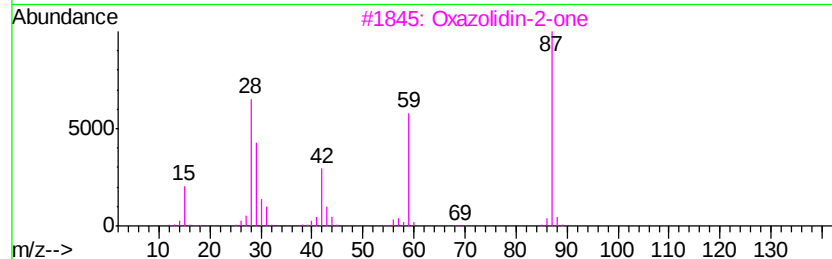
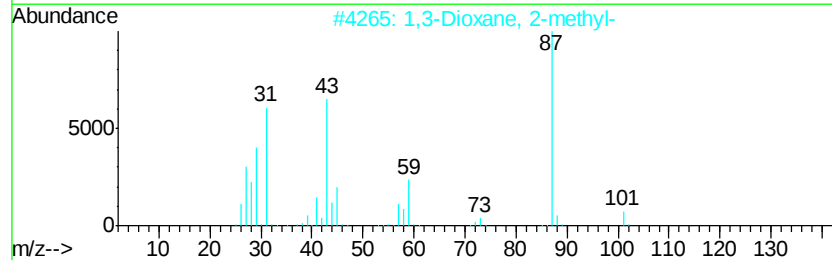
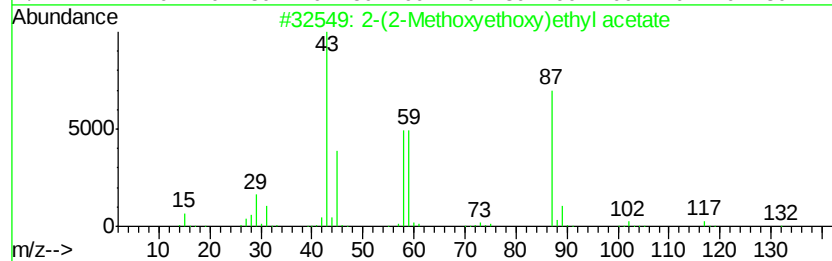
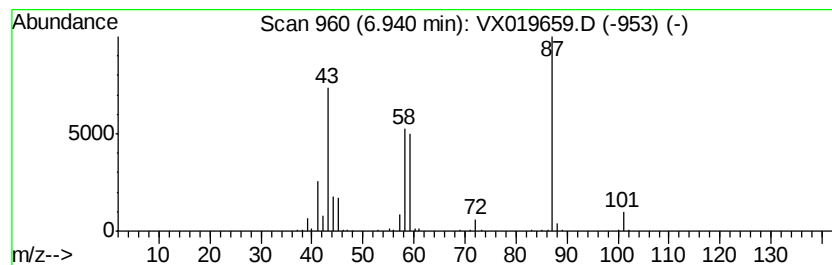
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Quant Title : SW846 8260

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

Peak Number 6 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	14.04 ug/l	321655	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	56
2		1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
4		3-Ethoxycarbonyl-5-hydroxytetrahydro-2H-pyran-2-one	188	C8H12O5	1000222-74-7	17
5		Diethylsilane	88	C4H12Si	000542-91-6	16



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019659.D
Acq On : 25 Nov 2020 16:18
Operator : JC/MD
Sample : L4841-02 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16855

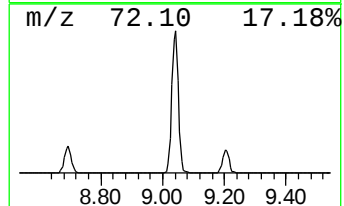
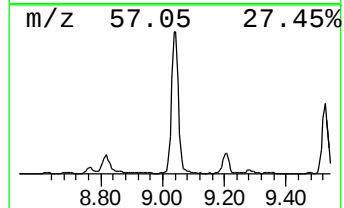
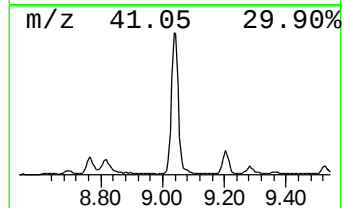
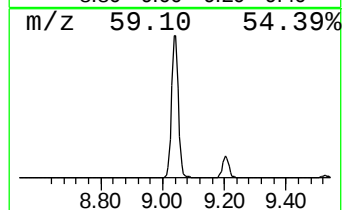
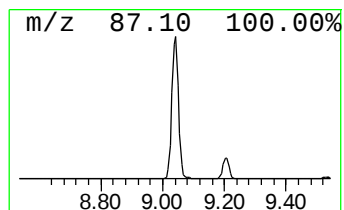
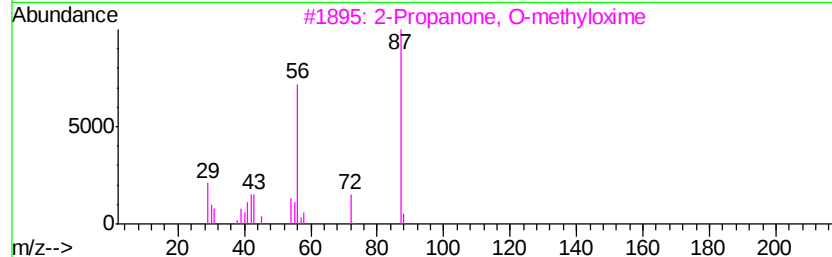
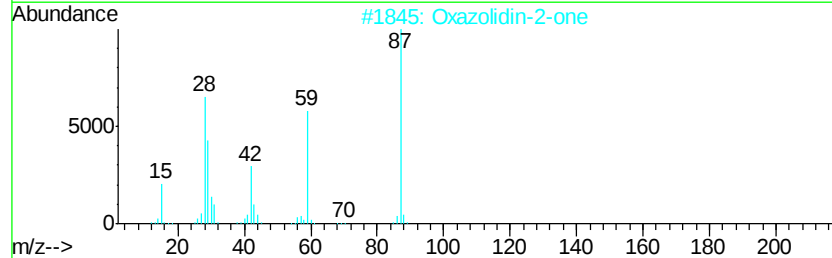
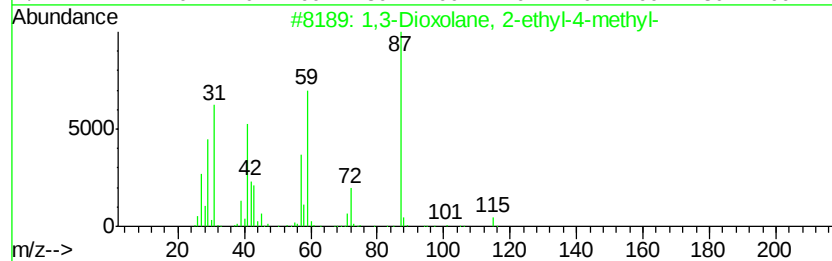
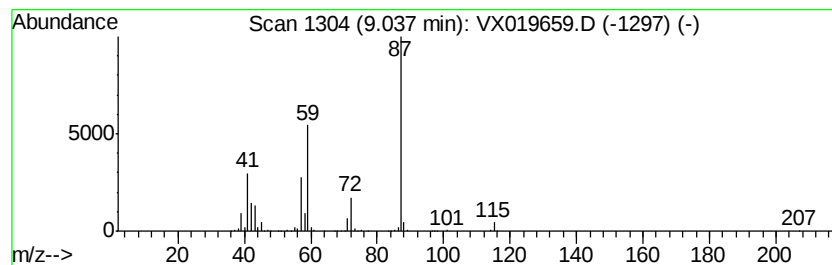
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Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	20.74 ug/l	551974	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	91
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3		2-Propanone, O-methylloxime	87	C4H9NO	003376-35-0	52
4		Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019659.D
Acq On : 25 Nov 2020 16:18
Operator : JC/MD
Sample : L4841-02 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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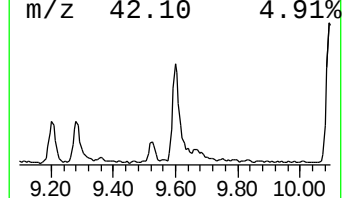
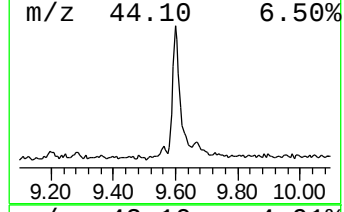
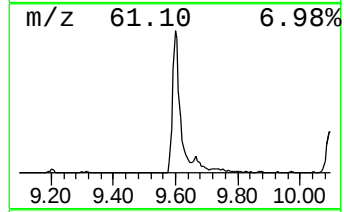
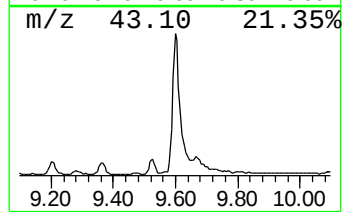
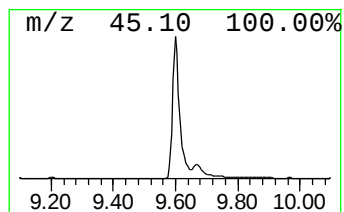
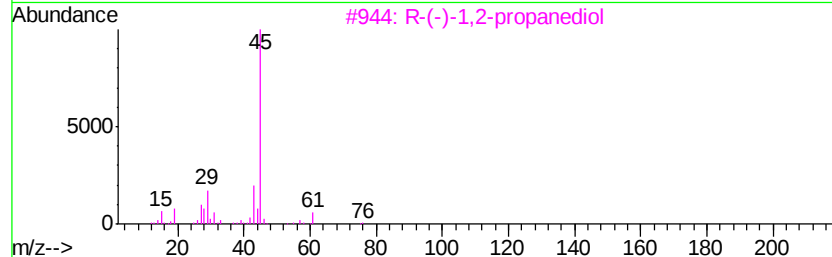
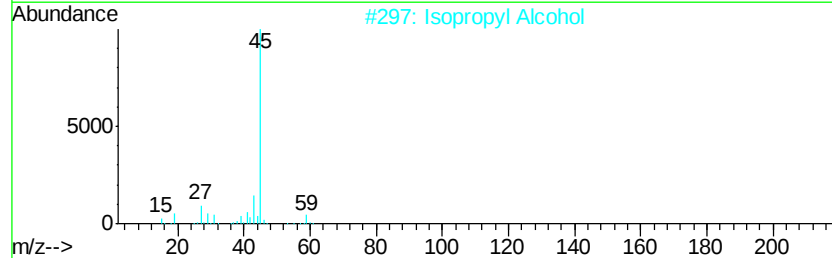
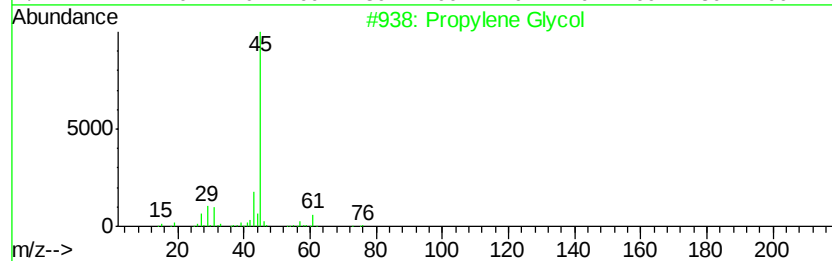
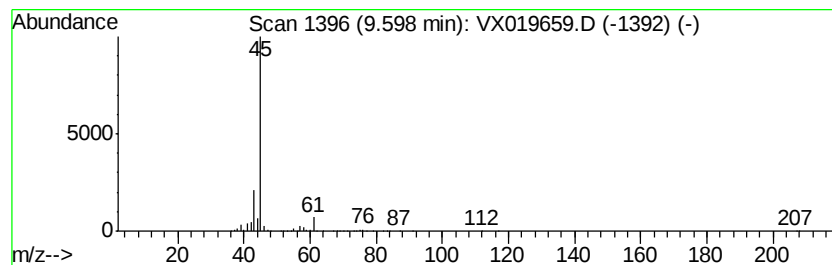
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

Peak Number 8 Propylene Glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	12.00 ug/l	319351	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	90
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	80
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
4		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019659.D
Acq On : 25 Nov 2020 16:18
Operator : JC/MD
Sample : L4841-02 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16855

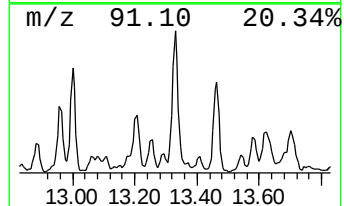
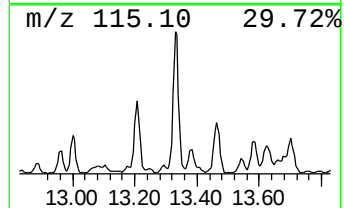
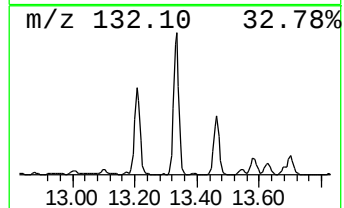
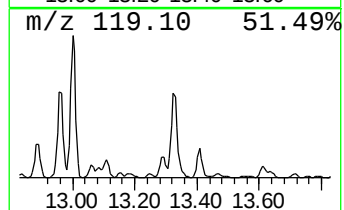
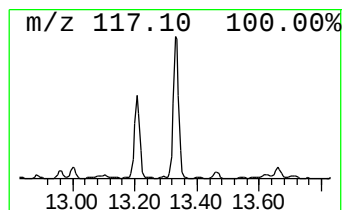
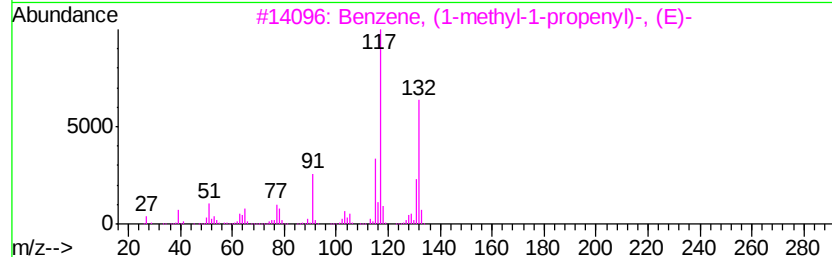
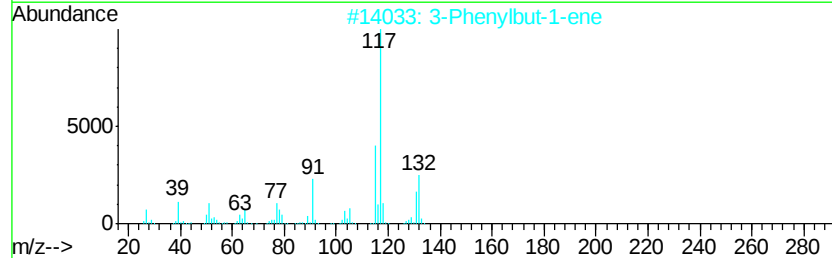
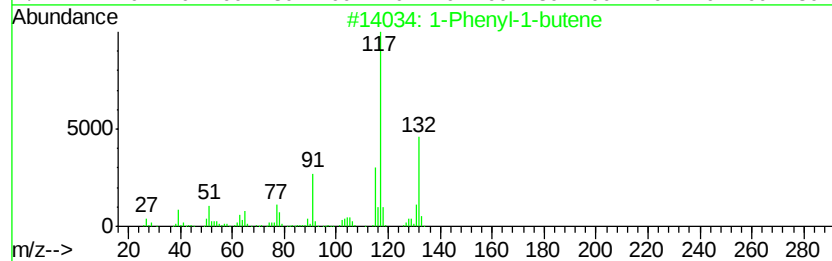
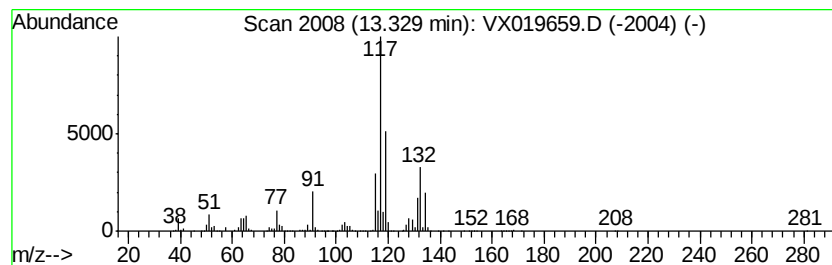
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Quant Title : SW846 8260

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

Peak Number 9 1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	18.60 ug/l	471810	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenyl-1-butene	132	C10H12	000824-90-8	86
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
4		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	64
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019659.D
Acq On : 25 Nov 2020 16:18
Operator : JC/MD
Sample : L4841-02 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16855

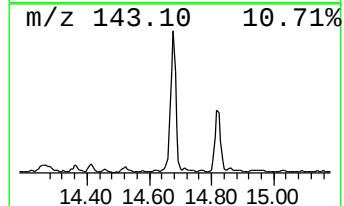
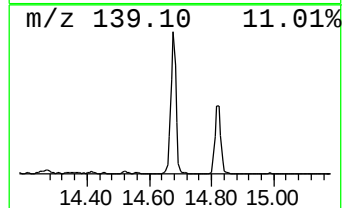
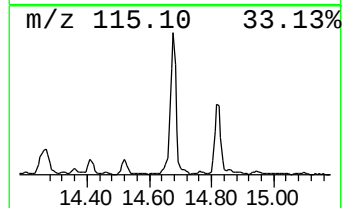
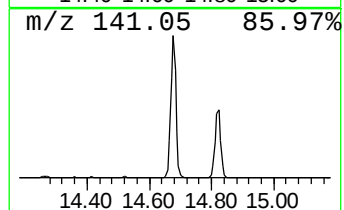
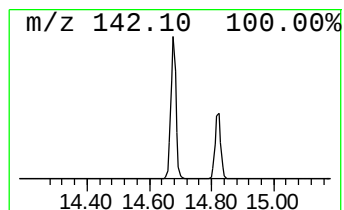
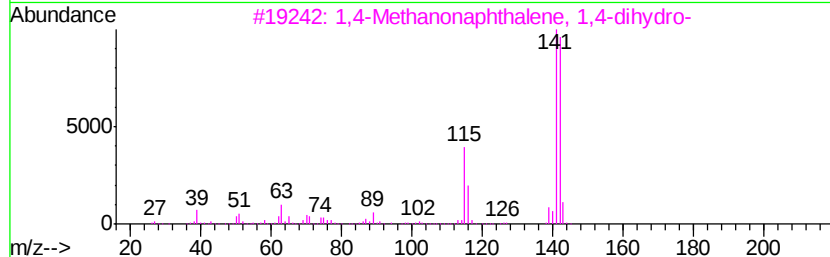
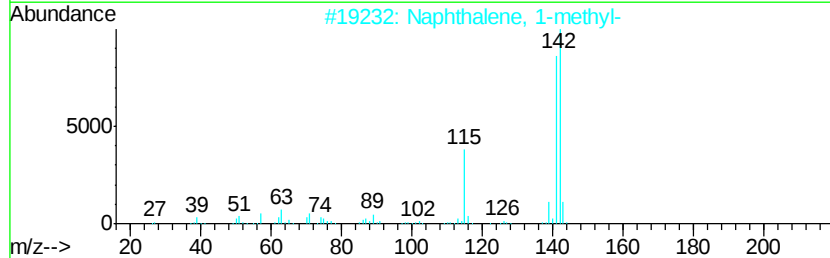
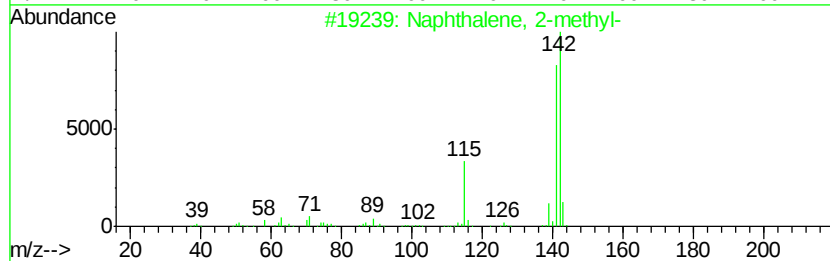
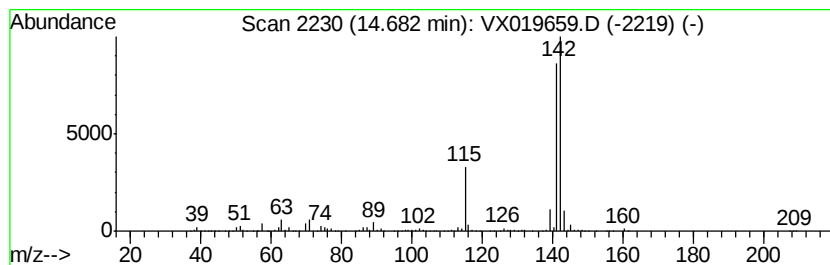
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	23.23 ug/l	589267	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019659.D
Acq On : 25 Nov 2020 16:18
Operator : JC/MD
Sample : L4841-02 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
16855

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.47	41.6	ug/l	735734	1	5.62	884464	50.0
Ethanol	2.12	161.8	ug/l	2861910	1	5.62	884464	50.0
Propanal	2.33	21.8	ug/l	385051	1	5.62	884464	50.0
Isopropyl Alcohol	2.61	16.7	ug/l	294779	1	5.62	884464	50.0
1-Propanol	4.00	623.3	ug/l	11025500	1	5.62	884464	50.0
2-(2-Methoxyethox...	6.94	14.0	ug/l	321655	2	6.83	1145770	50.0
1,3-Dioxolane, 2-...	9.04	20.7	ug/l	551974	3	10.10	1330790	50.0
Propylene Glycol	9.60	12.0	ug/l	319351	3	10.10	1330790	50.0
1-Phenyl-1-butene	13.33	18.6	ug/l	471810	4	12.06	1268590	50.0
Naphthalene, 2-me...	14.68	23.2	ug/l	589267	4	12.06	1268590	50.0