

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030621\
 Data File : VX021018.D
 Acq On : 04 Mar 2021 16:45
 Operator : JC/MD
 Sample : M1507-08 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 41116

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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M

Title : SW846 8260

Signal : TIC: VX021018.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	62	66	89	rBV	3559042	4388838	100.00%	30.103%
2	2.105	164	173	204	rVB	916691	1866026	42.52%	12.799%
3	4.299	537	546	561	rBV2	39722	114398	2.61%	0.785%
4	4.635	593	603	616	rBV2	18852	56003	1.28%	0.384%
5	5.464	730	744	758	rBV2	147797	429281	9.78%	2.944%
6	5.629	760	772	788	rBV2	241756	664749	15.15%	4.559%
7	6.029	828	840	850	rBV	165660	435386	9.92%	2.986%
8	6.829	965	976	997	rBV	415218	980664	22.34%	6.726%
9	7.270	1043	1051	1060	rBV2	18982	46321	1.06%	0.318%
10	8.694	1285	1293	1301	rBV	888172	1382903	31.51%	9.485%
11	9.529	1429	1435	1445	rVB	40511	62936	1.43%	0.432%
12	10.094	1525	1531	1544	rBV	906086	1235636	28.15%	8.475%
13	10.347	1569	1574	1585	rVB	334485	458531	10.45%	3.145%
14	11.118	1700	1705	1711	rBV	729544	946389	21.56%	6.491%
15	12.059	1860	1865	1873	rVB	904775	1146959	26.13%	7.867%
16	12.253	1892	1898	1909	rBV2	62438	125727	2.86%	0.862%
17	12.453	1928	1932	1937	rVB	71385	83492	1.90%	0.573%
18	13.818	2159	2164	2170	rVB	124194	155329	3.54%	1.065%

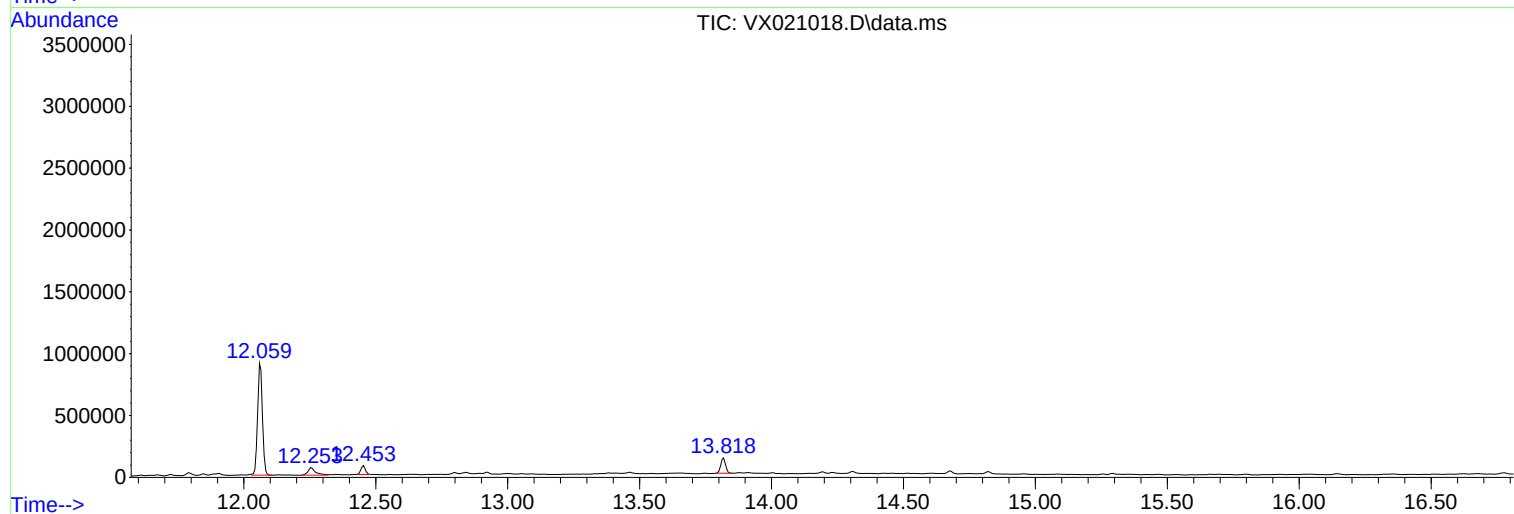
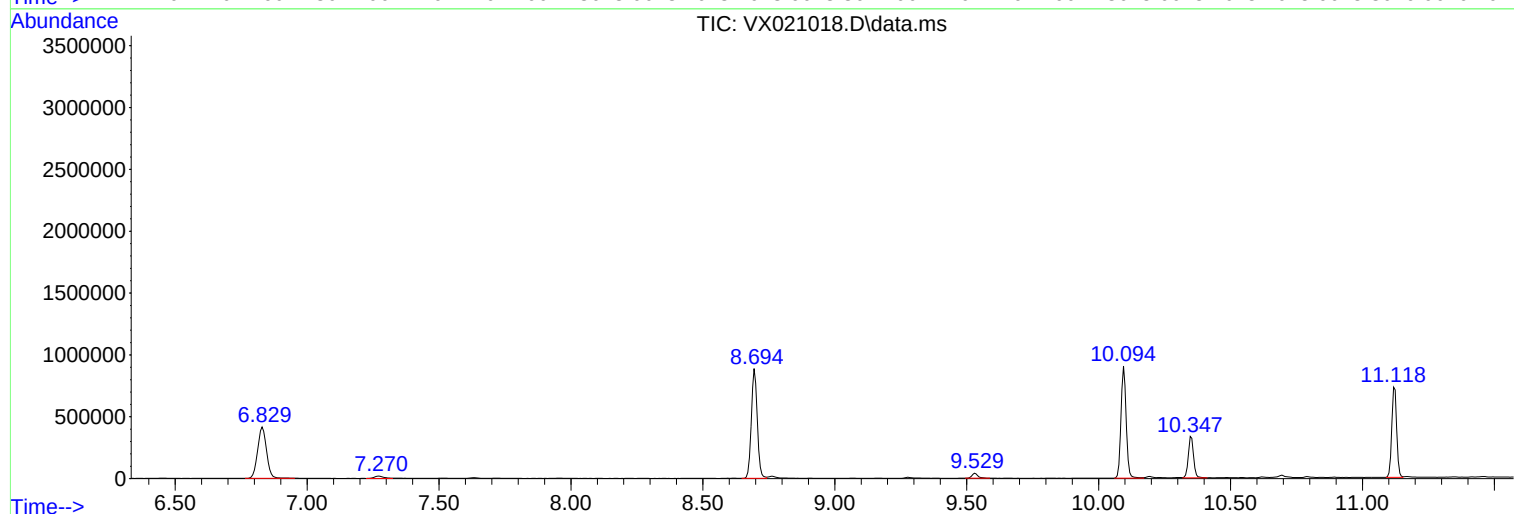
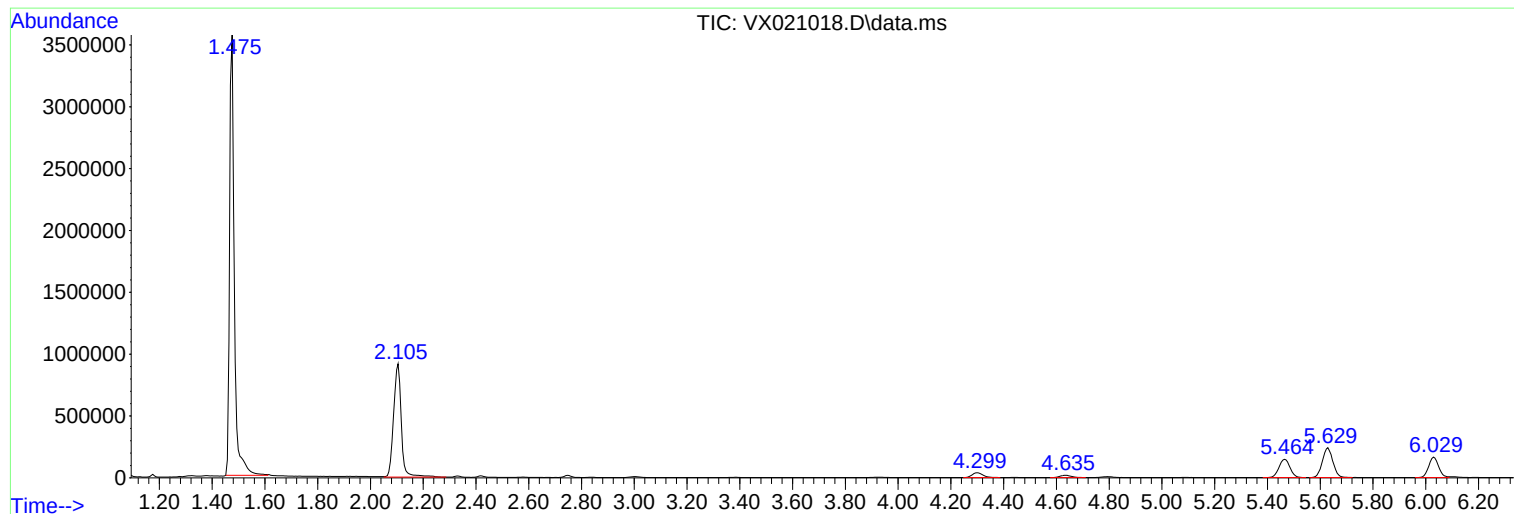
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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



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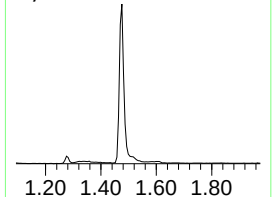
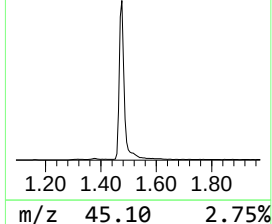
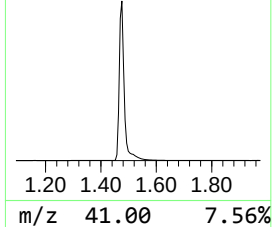
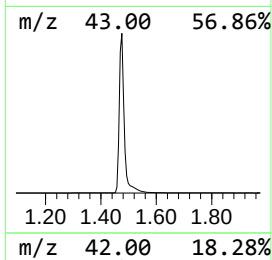
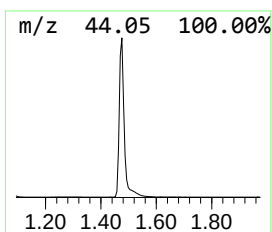
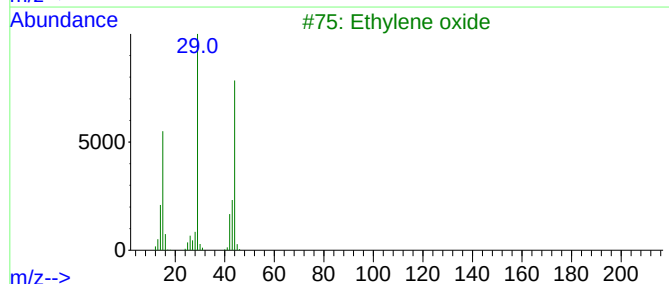
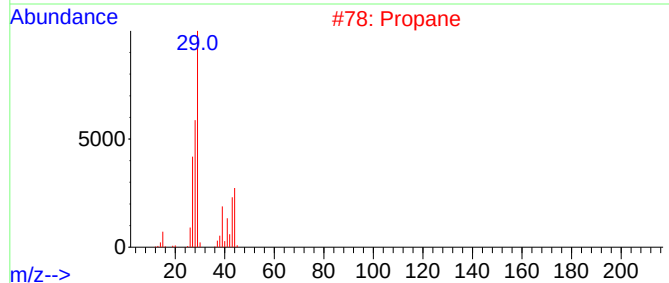
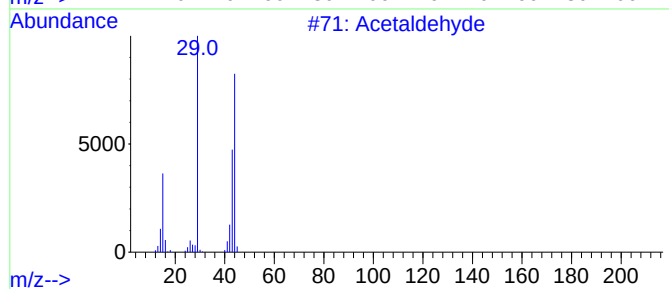
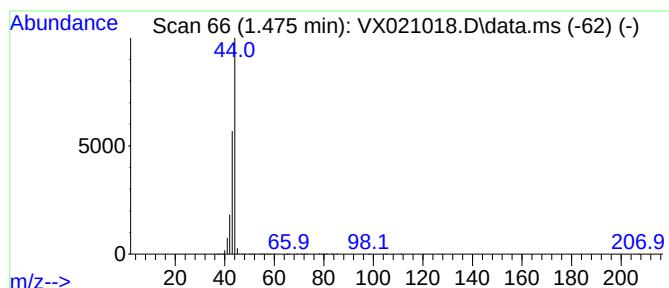
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	330.11 ug/l	4388840	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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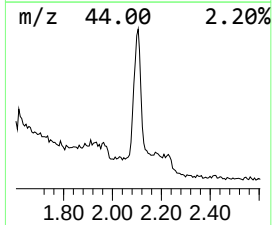
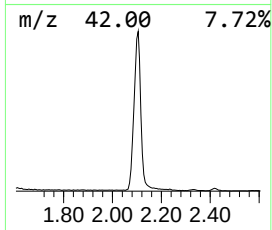
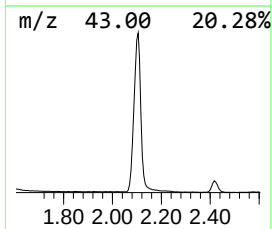
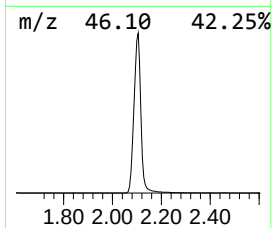
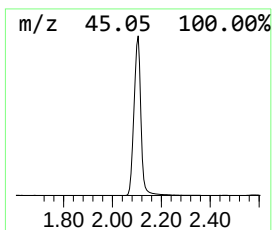
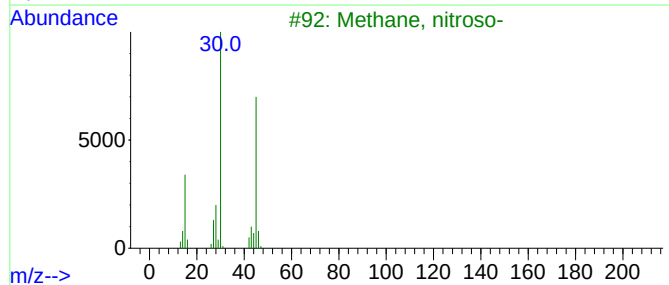
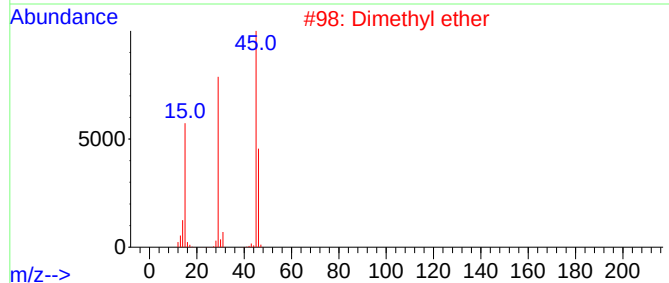
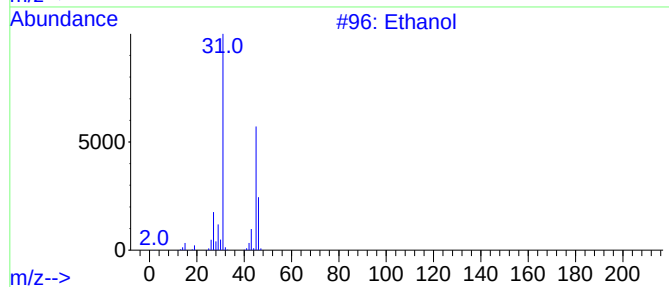
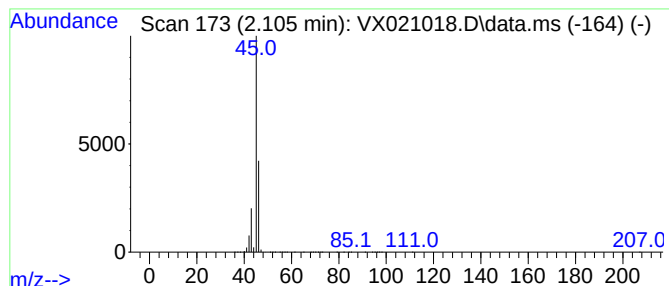
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	140.36 ug/l	1866030	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	78
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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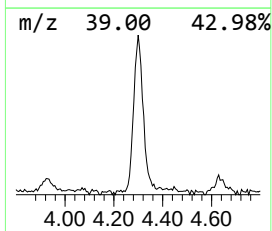
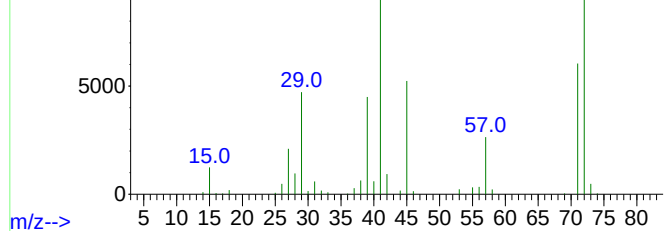
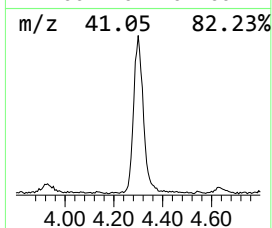
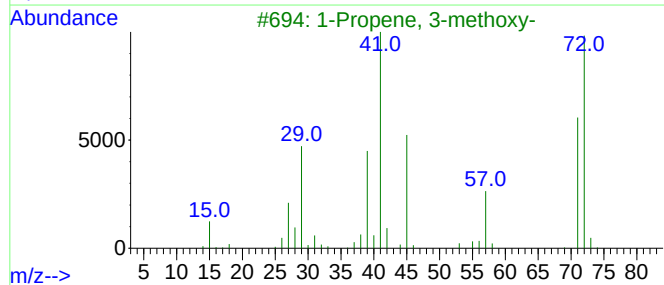
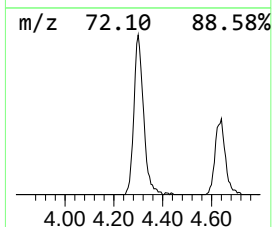
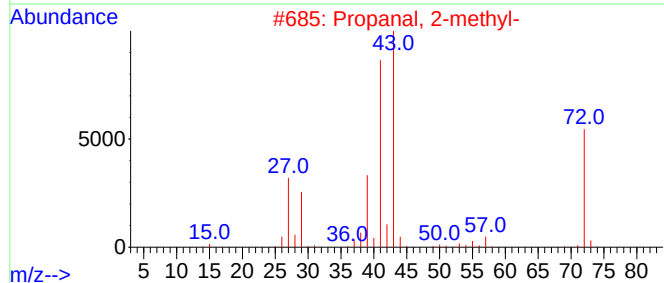
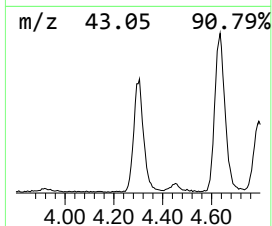
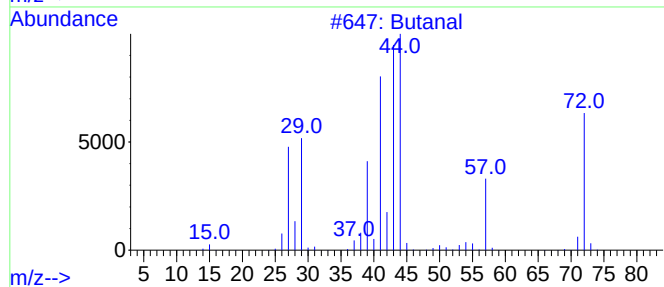
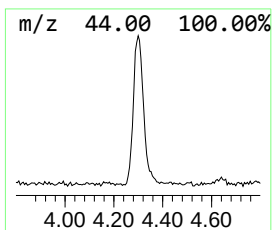
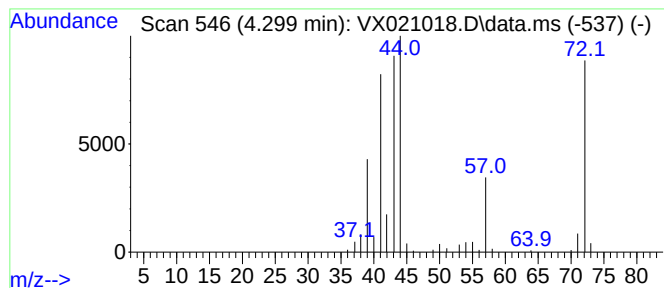
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	8.60 ug/l	114398	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4			1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	27
5			Isobutylene epoxide	72	C4H8O	000558-30-5	27



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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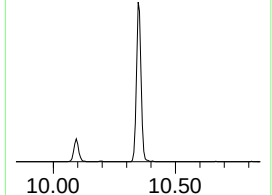
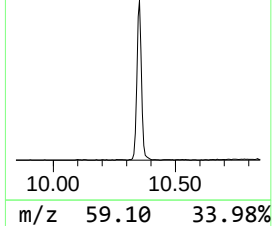
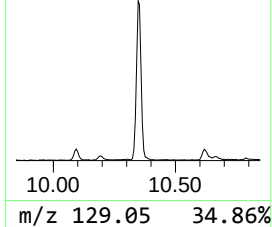
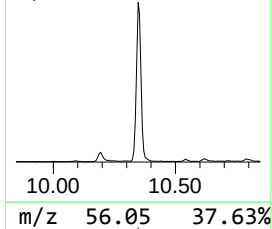
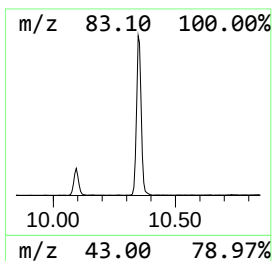
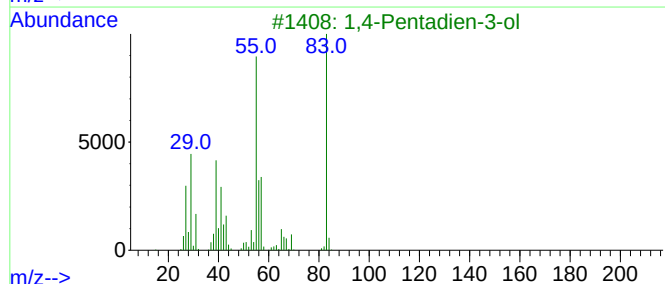
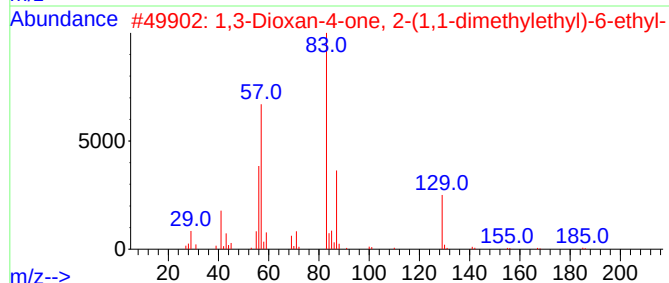
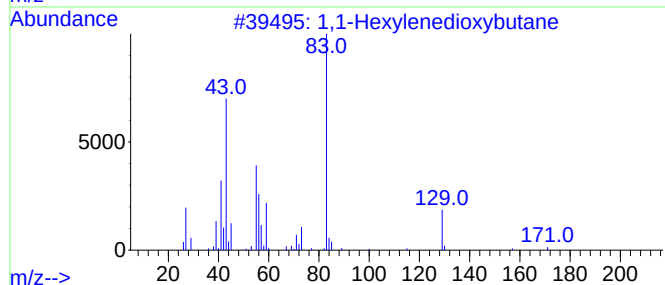
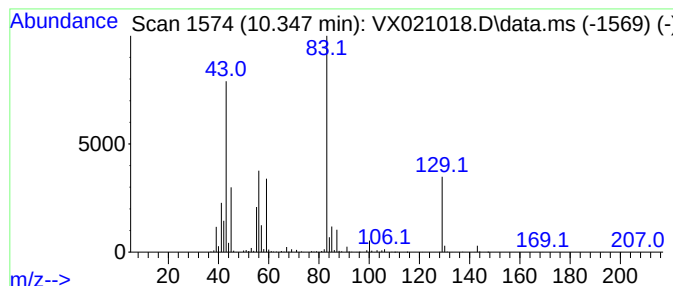
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown10.347 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.347	18.55 ug/l	458531	Chlorobenzene-d5	10.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	39
2			1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	36
3			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	32
4			Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	25
5			1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	23



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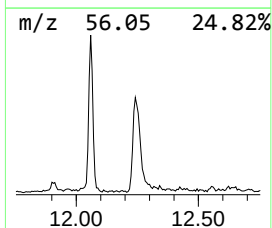
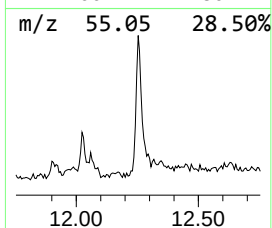
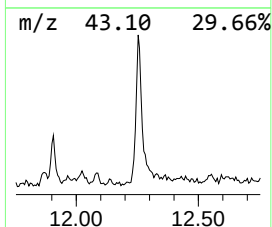
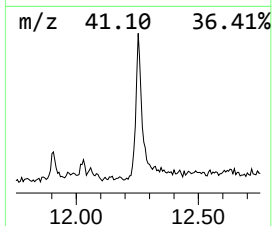
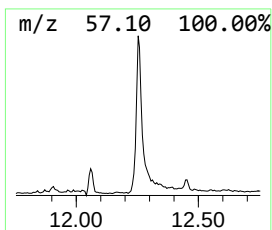
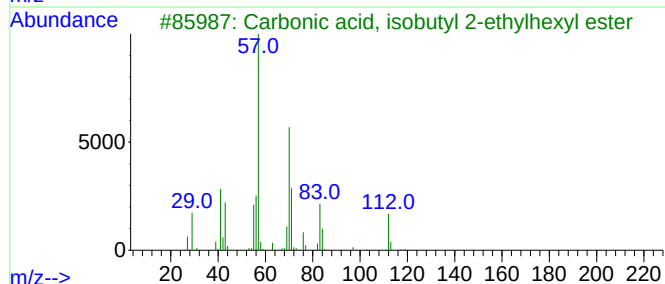
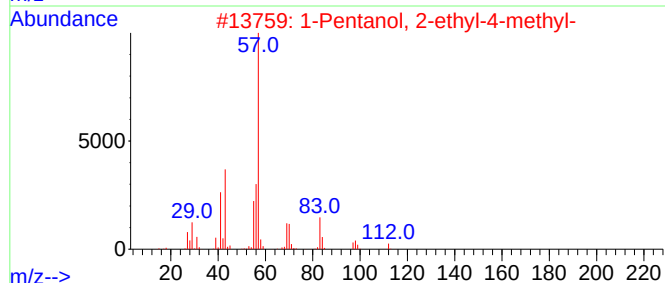
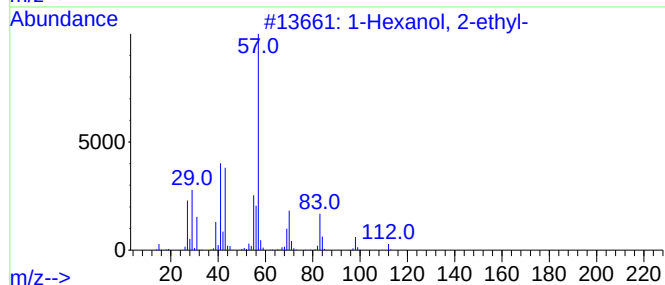
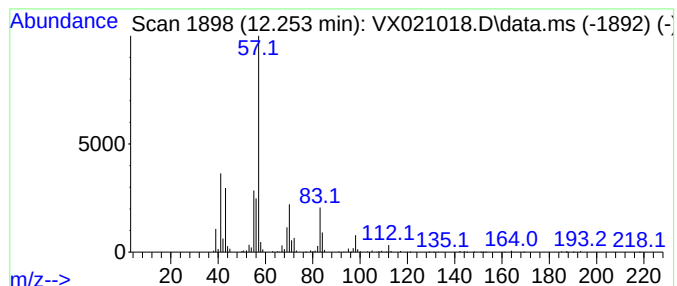
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	5.48 ug/l	125727	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	53
4			1-Decene, 3,4-dimethyl-	168	C12H24	050871-03-9	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



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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	1.475	330.1	ug/l	4388840	1	5.629	664749	50.0
Ethanol	2.105	140.4	ug/l	1866030	1	5.629	664749	50.0
Butanal	4.299	8.6	ug/l	114398	1	5.629	664749	50.0
unknown10.347	10.347	18.6	ug/l	458531	3	10.094	1235640	50.0
1-Hexanol, 2-et...	12.253	5.5	ug/l	125727	4	12.065	1146960	50.0