

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039596.D
 Acq On : 03 Jan 2024 12:57
 Operator : JC/MD
 Sample : P1001-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-1208

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.435	54	57	67	rBV	13256970	22927789	100.00%	59.864%
2	1.532	67	73	94	rVV	1305769	5650926	24.65%	14.754%
3	1.666	94	95	127	rVB	106929	353292	1.54%	0.922%
4	2.105	156	167	188	rVB	537859	1308117	5.71%	3.415%
5	2.288	191	197	205	rBV	228313	381121	1.66%	0.995%
6	4.227	501	515	524	rBV	395258	1081605	4.72%	2.824%
7	5.544	722	731	745	rBV	104317	299440	1.31%	0.782%
8	6.757	922	930	943	rVB	199728	478234	2.09%	1.249%
9	7.226	996	1007	1027	rBV	166158	378868	1.65%	0.989%
10	8.647	1233	1240	1249	rBV	423532	662034	2.89%	1.729%
11	10.055	1465	1471	1484	rBV	460171	649582	2.83%	1.696%
12	11.079	1634	1639	1645	rBV	389381	490810	2.14%	1.281%
13	11.683	1733	1738	1746	rVB	598701	682597	2.98%	1.782%
14	11.988	1779	1788	1791	rBV	665744	848735	3.70%	2.216%
15	12.018	1791	1793	1802	rVB	457750	564674	2.46%	1.474%
16	12.219	1819	1826	1836	rBV	1118373	1542102	6.73%	4.026%

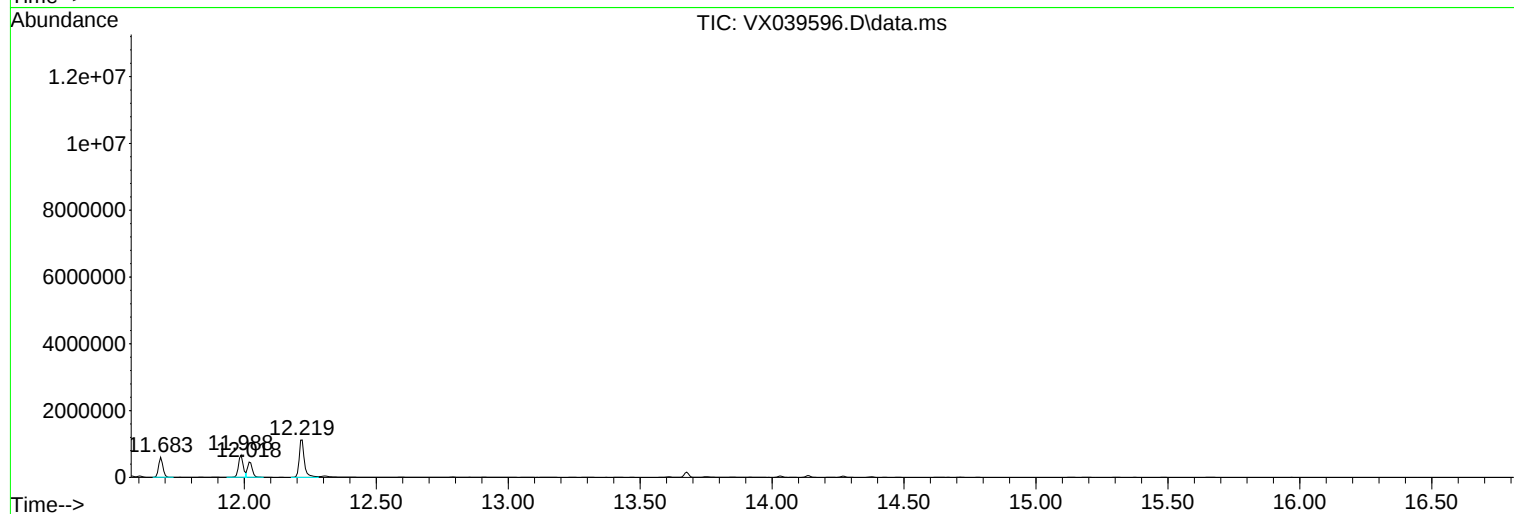
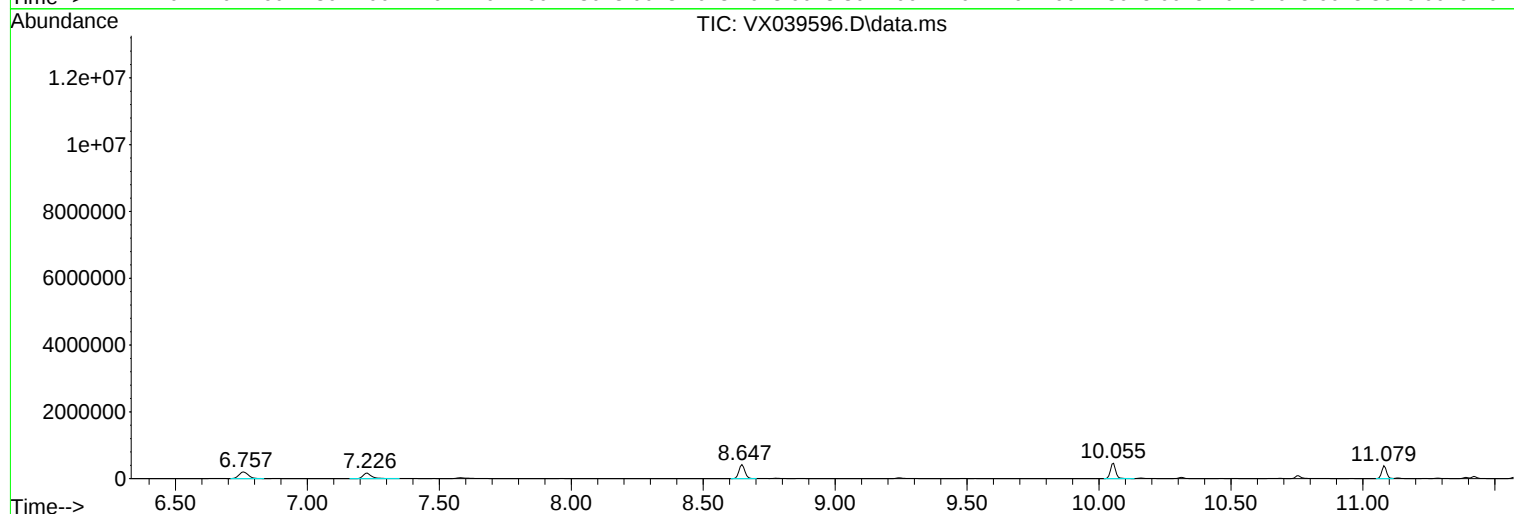
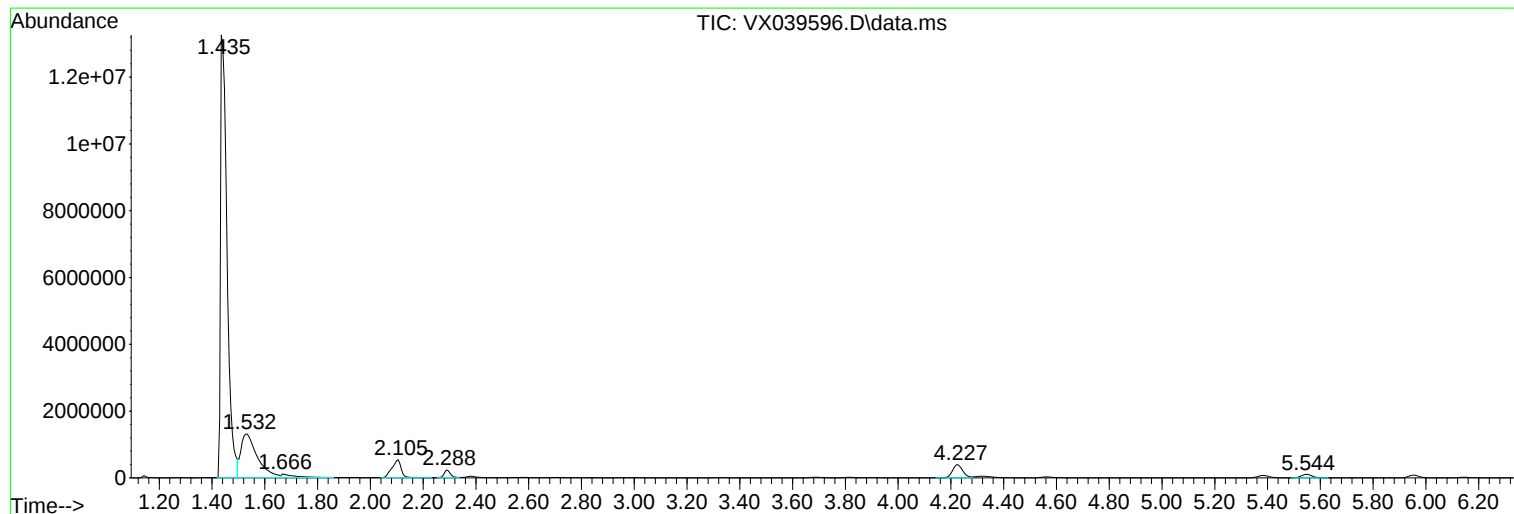
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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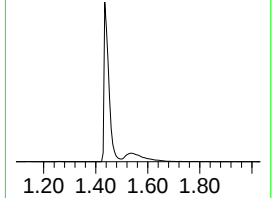
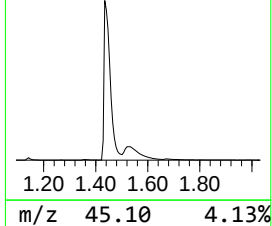
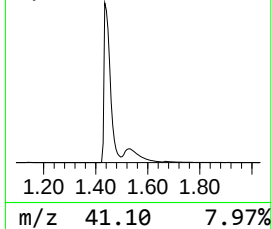
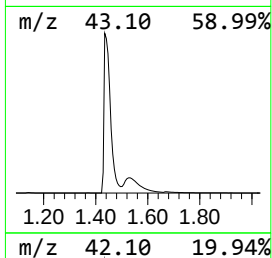
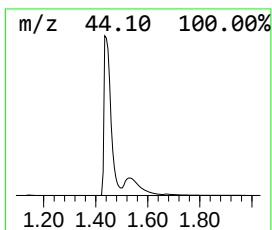
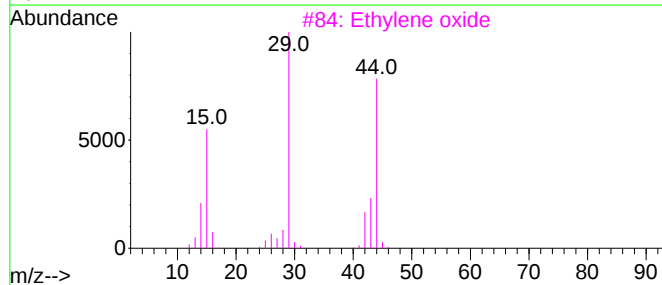
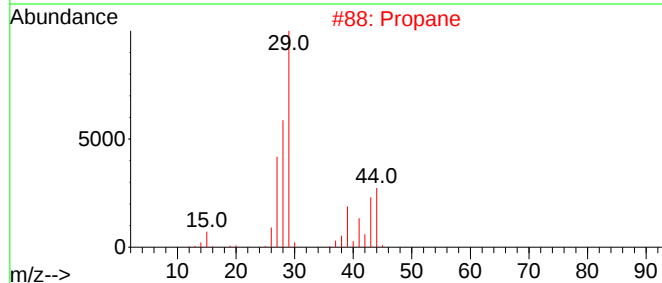
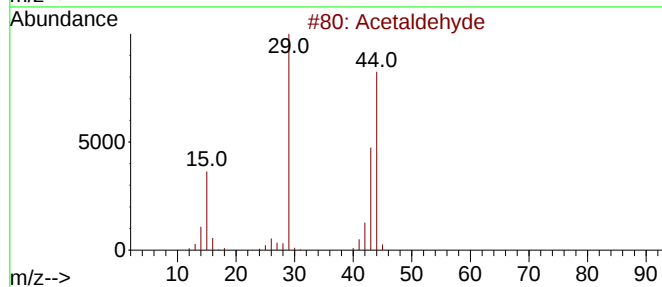
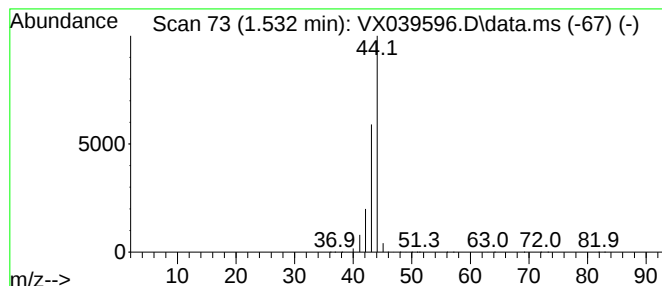
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.532	943.58 ug/l	5650930	Pentafluorobenzene	5.550

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-(Methylamino)propan-2-ol	89	C4H11NO	1000486-79-1	4
5			Alanine	89	C3H7NO2	000056-41-7	4



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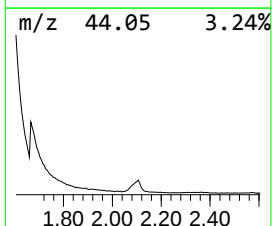
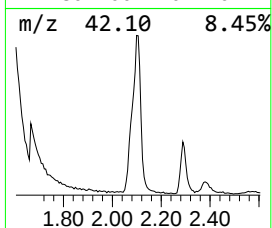
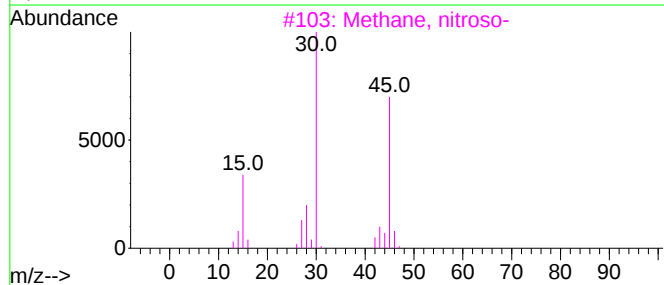
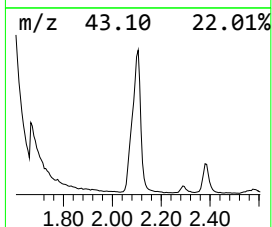
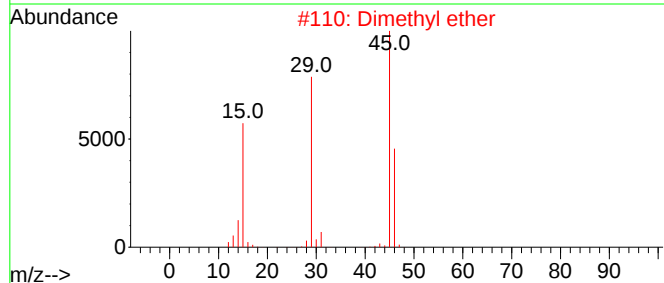
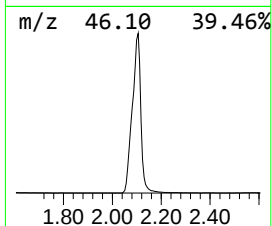
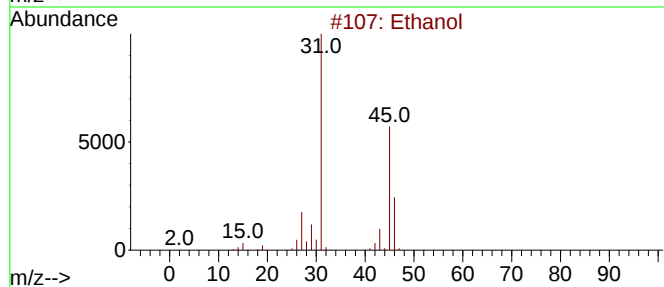
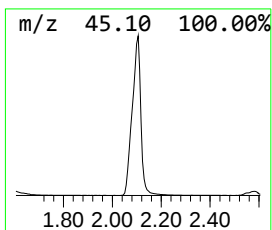
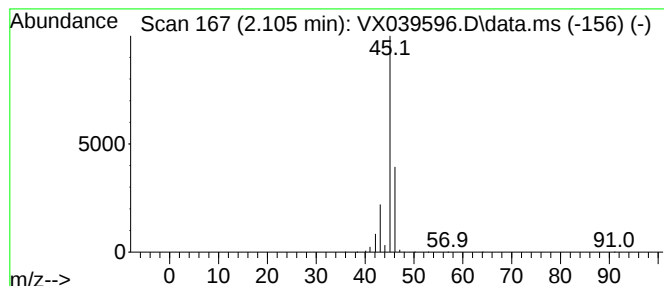
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.105	218.43 ug/l	1308120	Pentafluorobenzene	5.550

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			Oxalic acid	90	C2H2O4	000144-62-7	4



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ORA-1208

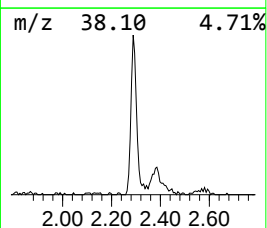
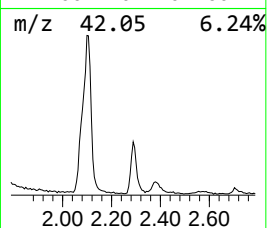
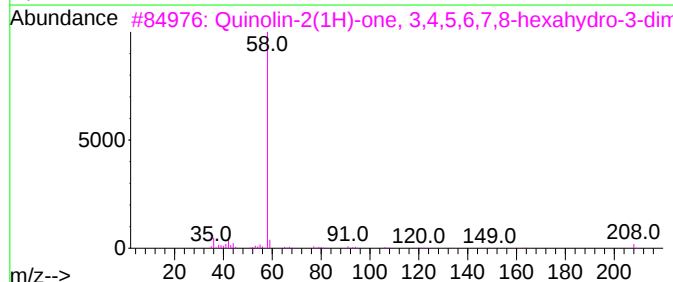
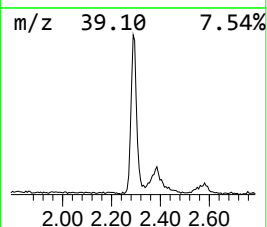
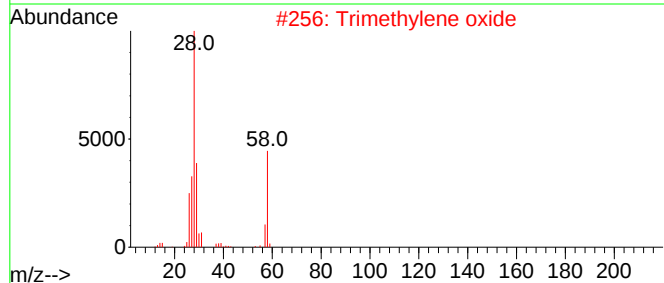
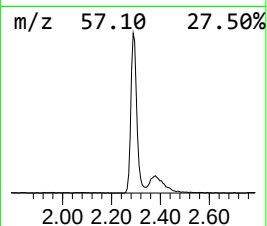
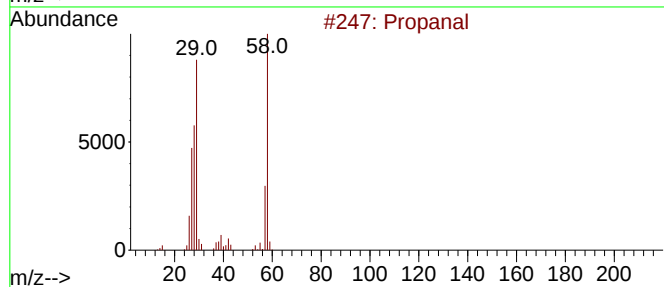
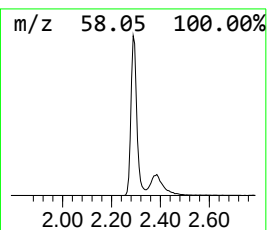
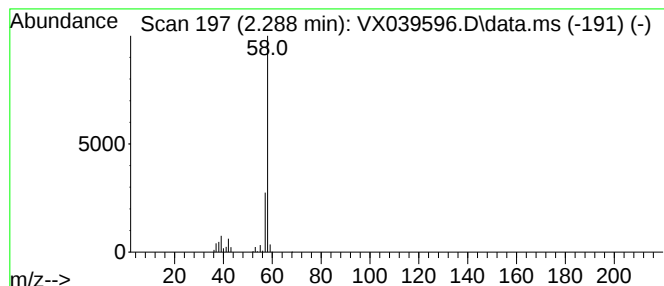
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Propanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.288	63.64 ug/l	381121	Pentafluorobenzene	5.550

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	9
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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Instrument :
MSVOA_X
ClientSampleId :
ORA-1208

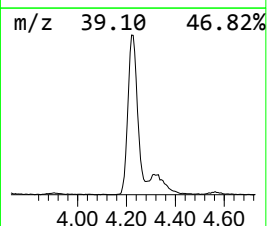
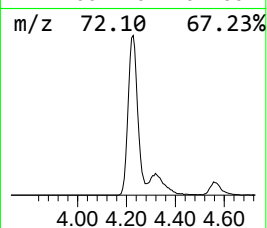
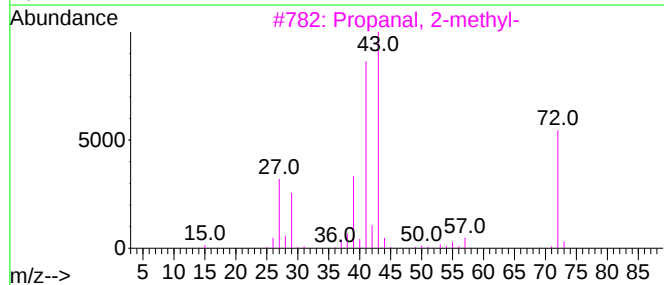
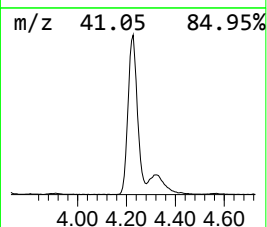
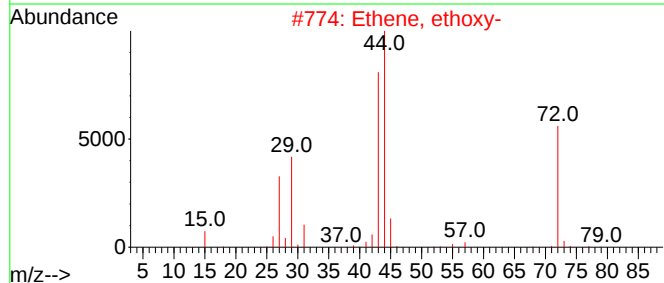
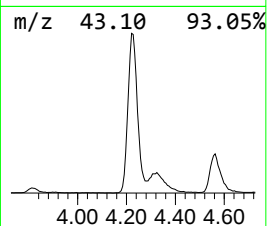
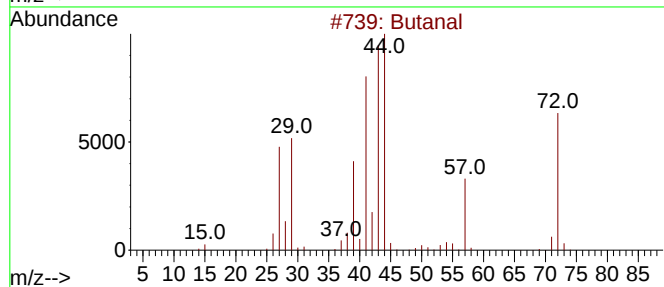
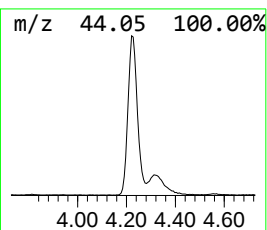
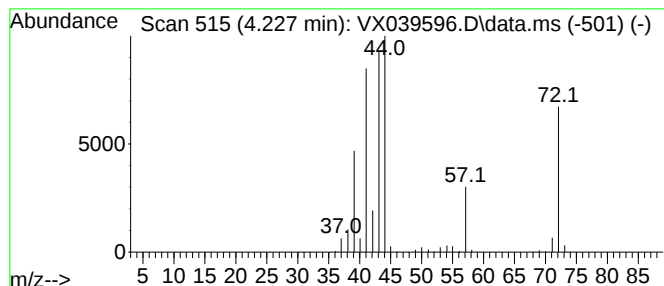
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	180.60 ug/l	1081610	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	49
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4			Methacrolein	70	C4H6O	000078-85-3	27
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	17



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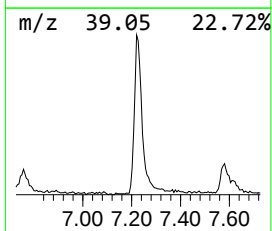
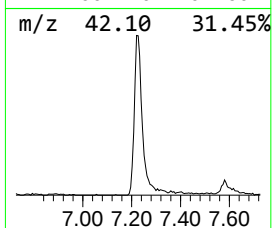
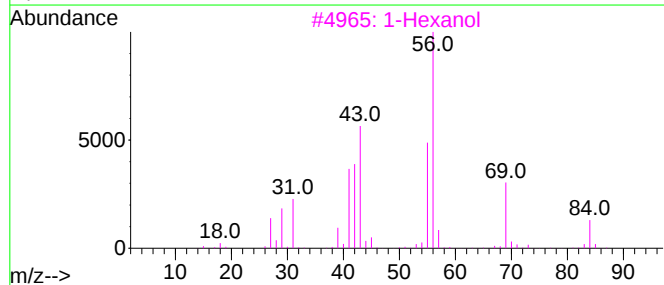
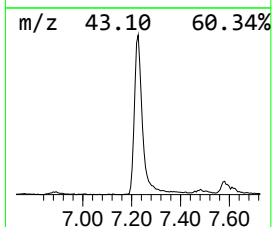
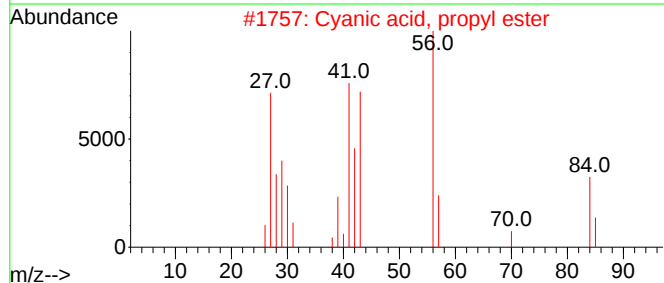
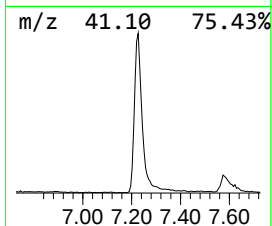
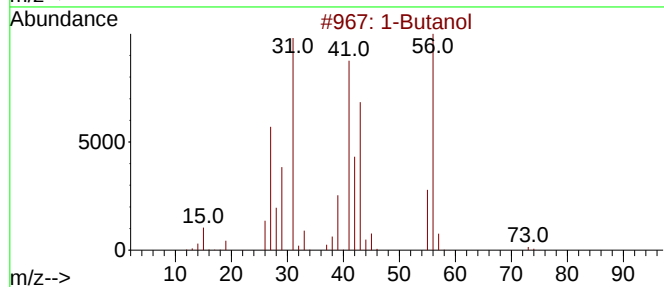
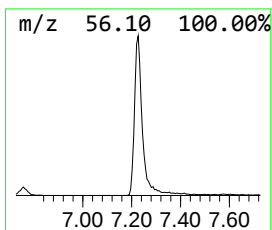
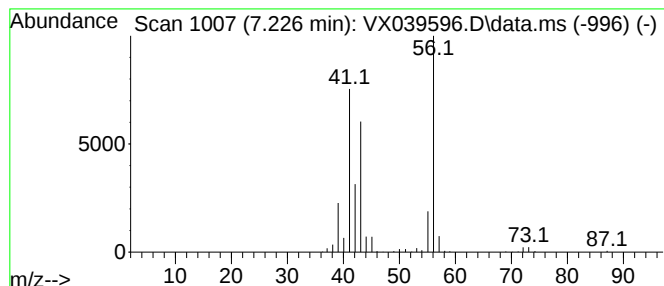
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Butanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	39.61 ug/l	378868	1,4-Difluorobenzene	6.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	90
2	Cyanic acid, propyl ester		85	C4H7NO	001768-36-1	50
3	1-Hexanol		102	C6H14O	000111-27-3	38
4	1-Pentene, 4-methyl-		84	C6H12	000691-37-2	28
5	5-Methyloxazolidine		87	C4H9NO	058328-22-6	9



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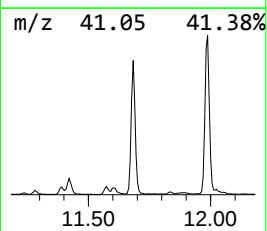
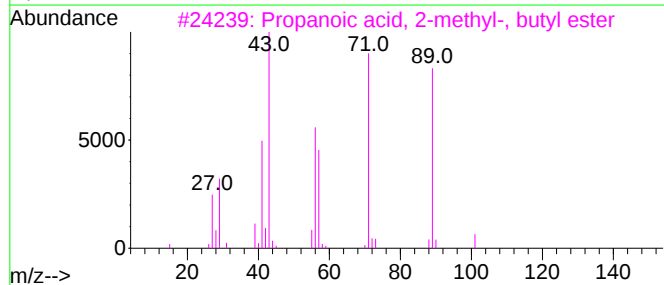
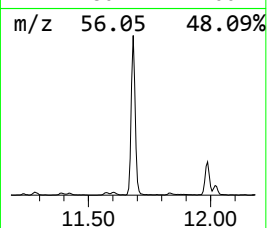
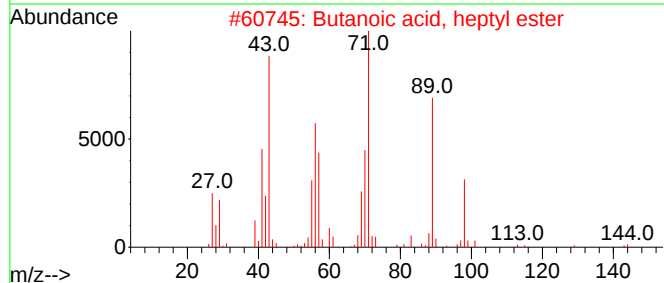
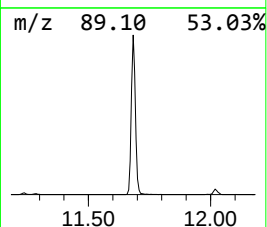
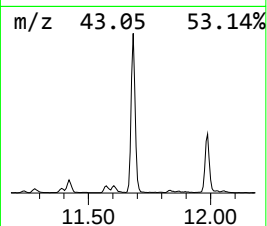
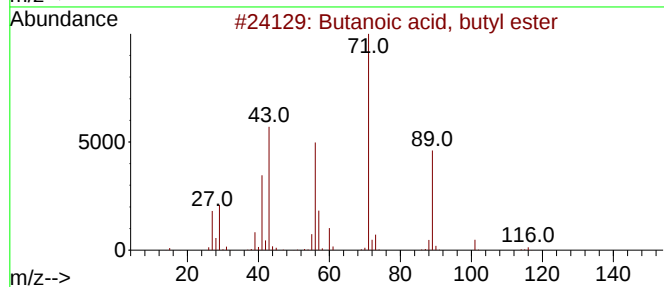
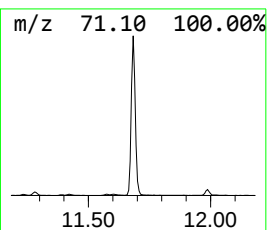
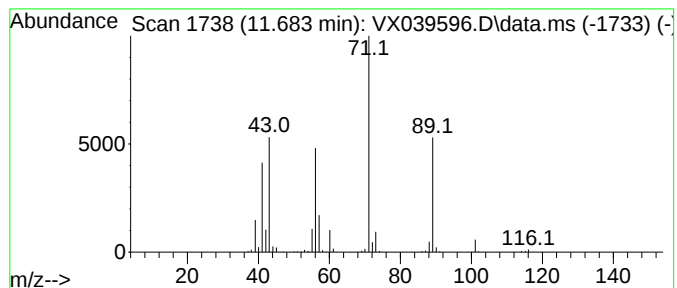
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	60.44 ug/l	682597	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039596.D
Acq On : 03 Jan 2024 12:57
Operator : JC/MD
Sample : P1001-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1208

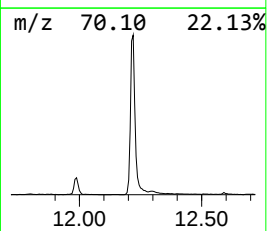
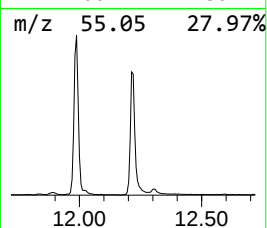
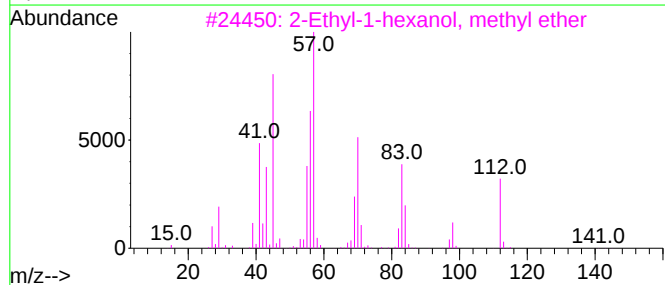
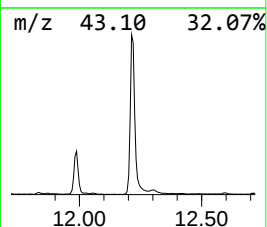
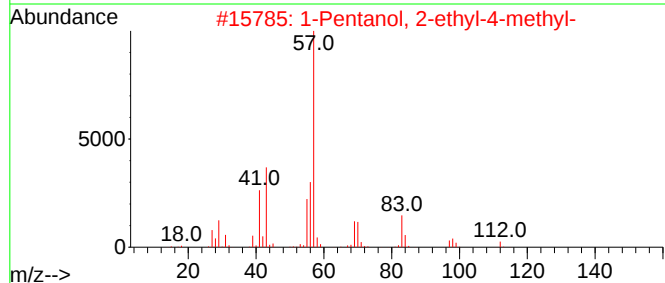
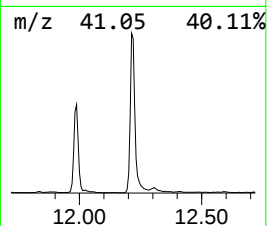
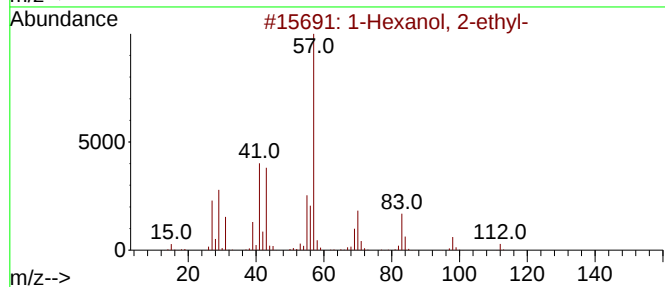
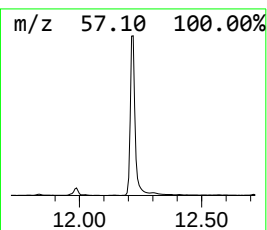
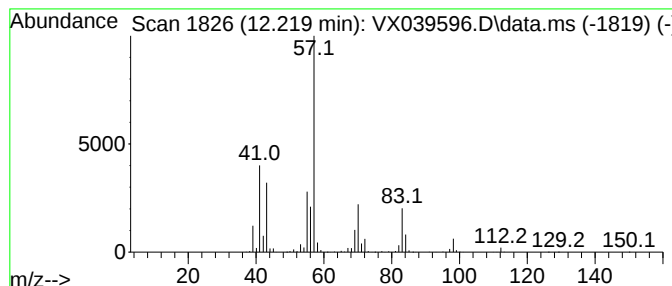
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	136.55 ug/l	1542100	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039596.D
Acq On : 03 Jan 2024 12:57
Operator : JC/MD
Sample : P1001-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1208

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.532	943.6	ug/l	5650930	1	5.550	299440	50.0
Ethanol	2.105	218.4	ug/l	1308120	1	5.550	299440	50.0
Propanal	2.288	63.6	ug/l	381121	1	5.550	299440	50.0
Butanal	4.227	180.6	ug/l	1081610	1	5.550	299440	50.0
1-Butanol	7.226	39.6	ug/l	378868	2	6.757	478234	50.0
Butanoic acid, ...	11.683	60.4	ug/l	682597	4	12.024	564674	50.0
1-Hexanol, 2-et...	12.219	136.6	ug/l	1542100	4	12.024	564674	50.0