

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039598.D
 Acq On : 03 Jan 2024 13:43
 Operator : JC/MD
 Sample : P1002-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1210

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: VX039598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.422	53	55	67	rBV2	13352943	36056661	100.00%	62.553%
2	1.526	67	72	93	rVV2	1691063	7988819	22.16%	13.860%
3	1.666	93	95	132	rVB	196810	709088	1.97%	1.230%
4	2.099	156	166	191	rVB	740825	1887207	5.23%	3.274%
5	4.227	503	515	524	rBV	882967	2428195	6.73%	4.213%
6	4.318	526	530	560	rVV2	85526	372126	1.03%	0.646%
7	6.757	921	930	947	rVB	215008	521254	1.45%	0.904%
8	7.226	999	1007	1025	rBV	254620	581838	1.61%	1.009%
9	8.647	1233	1240	1249	rBV	457543	706155	1.96%	1.225%
10	10.055	1465	1471	1483	rBV	462266	686565	1.90%	1.191%
11	11.079	1634	1639	1645	rBV	432529	546458	1.52%	0.948%
12	11.683	1733	1738	1746	rVB	594141	675236	1.87%	1.171%
13	11.988	1779	1788	1791	rBV2	1054022	1431032	3.97%	2.483%
14	12.018	1791	1793	1802	rVB	472884	599361	1.66%	1.040%
15	12.219	1818	1826	1837	rBV	1832950	2451356	6.80%	4.253%

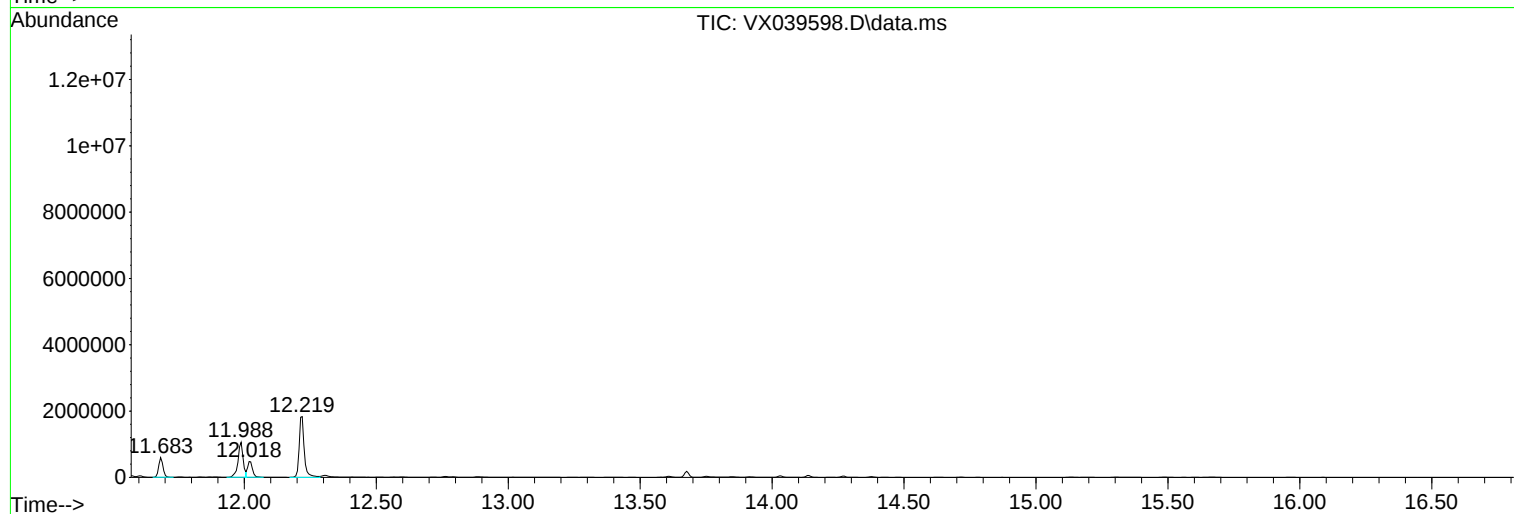
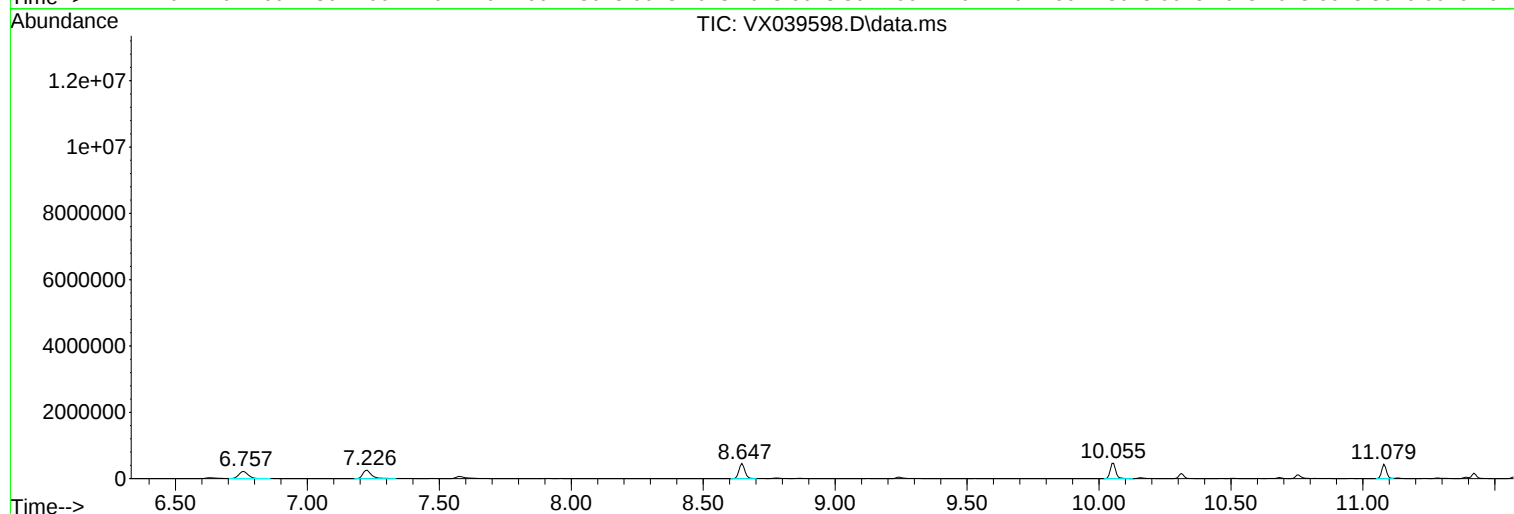
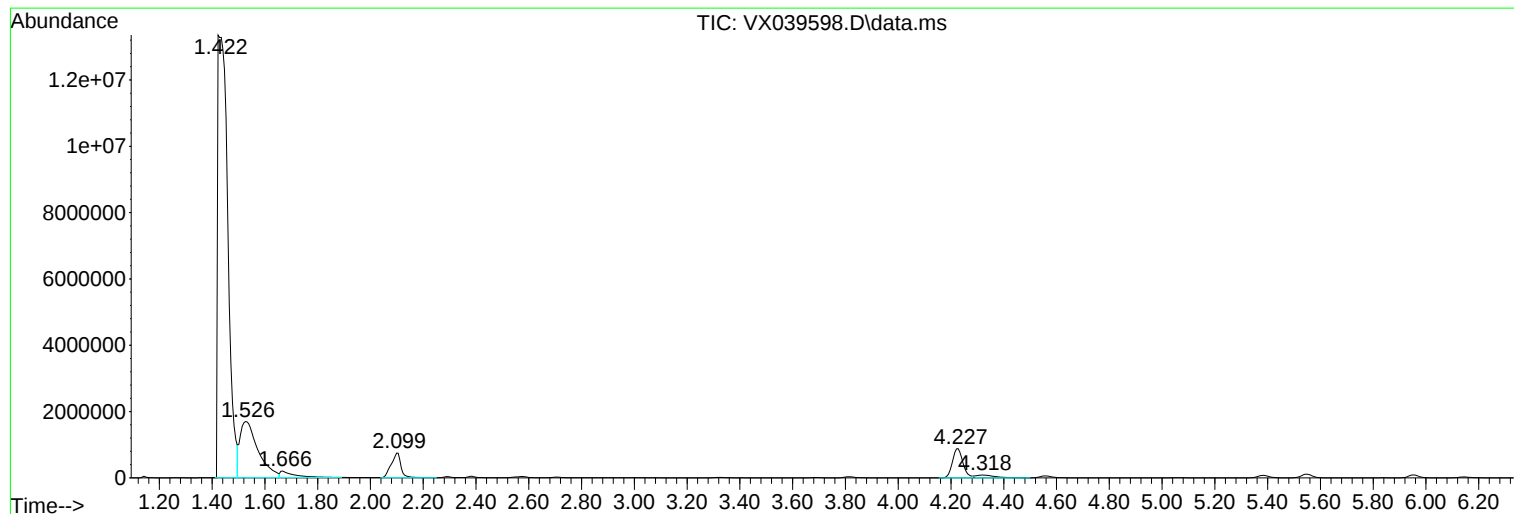
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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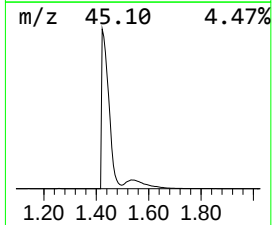
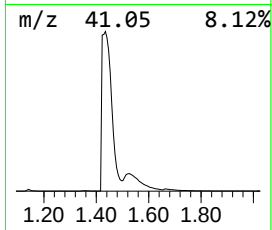
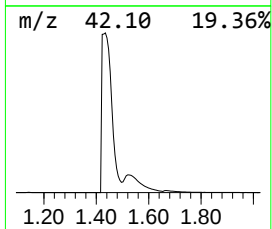
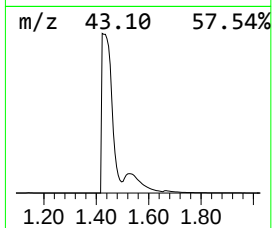
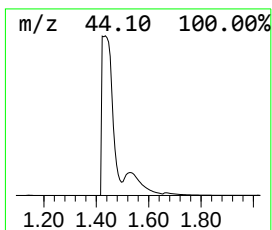
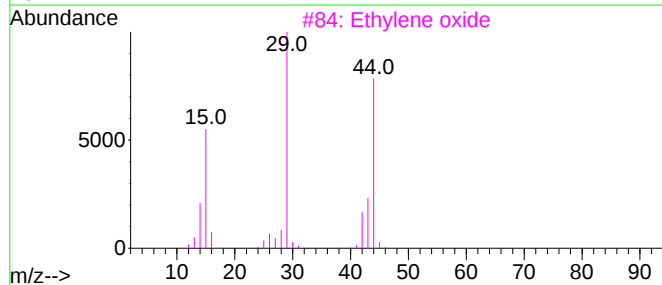
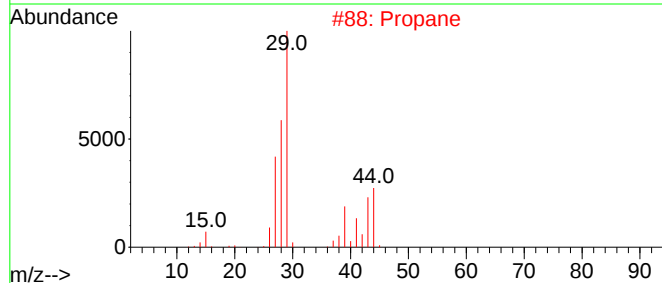
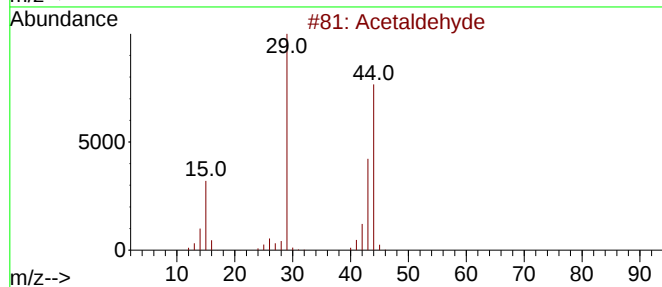
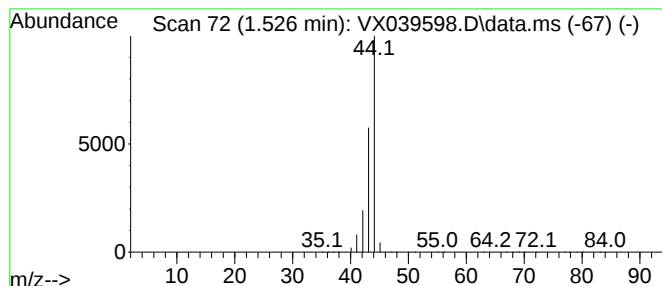
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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.
1.526	766.31 ug/l	7988820	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			Alanine	89	C3H7NO2	000056-41-7	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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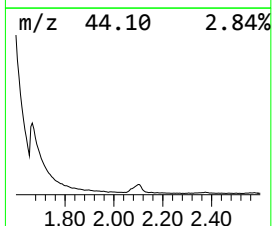
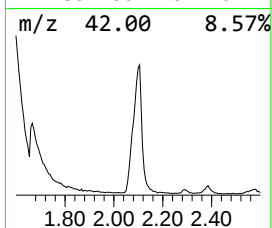
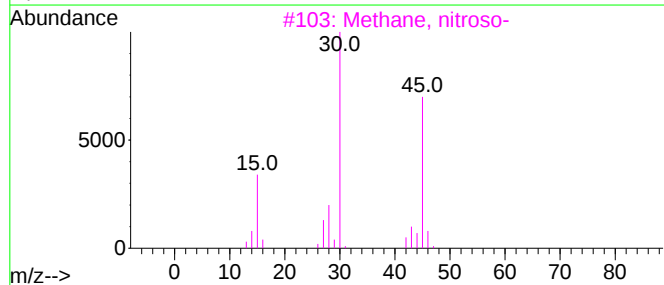
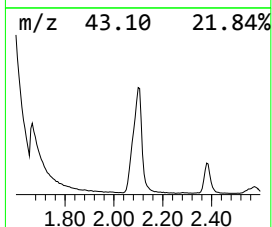
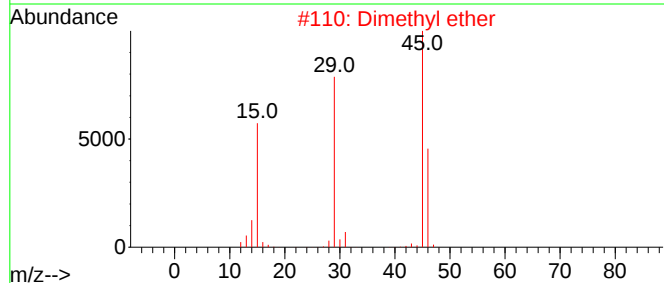
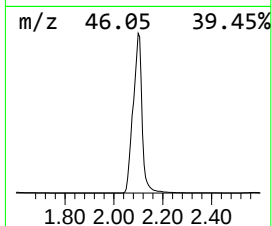
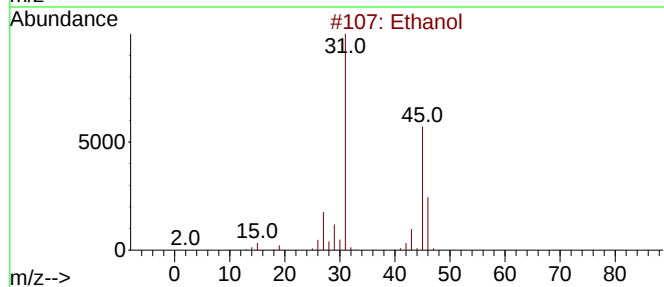
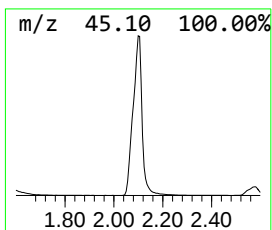
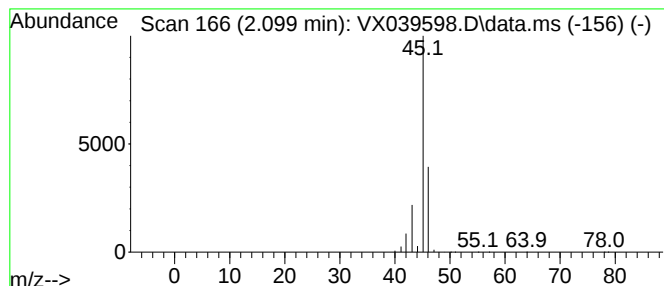
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 4 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	181.03 ug/l	1887210	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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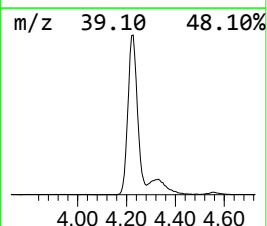
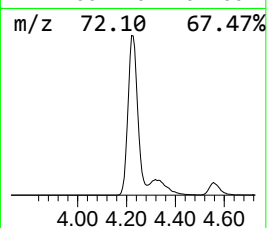
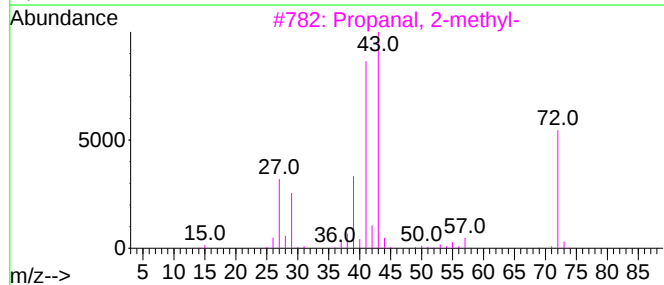
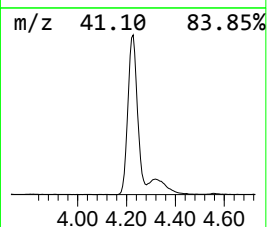
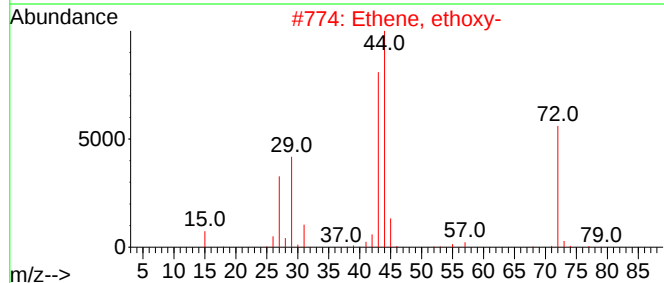
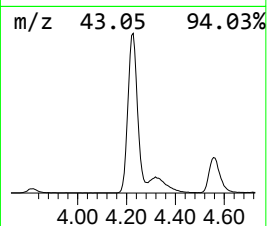
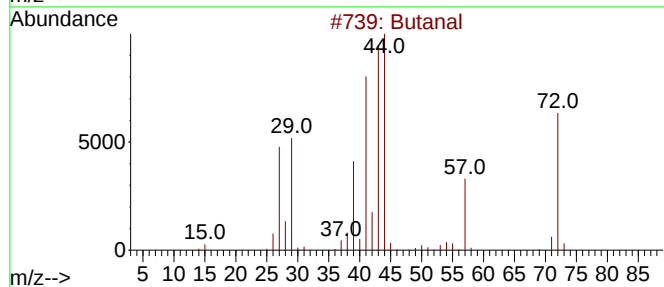
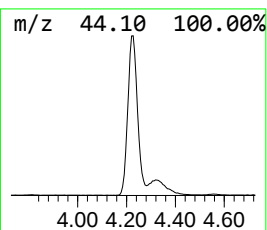
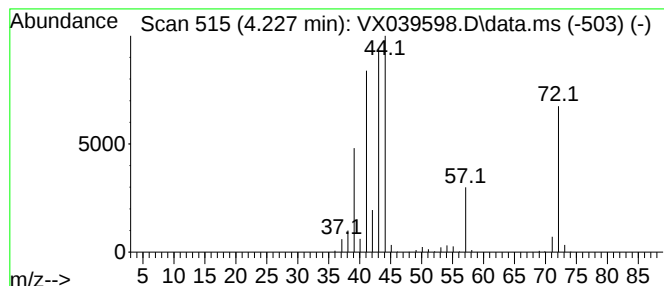
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	232.92 ug/l	2428200	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			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	32
5			Dimethylketene	70	C4H6O	000598-26-5	27



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Instrument :
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ClientSampleId :
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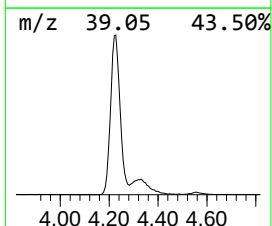
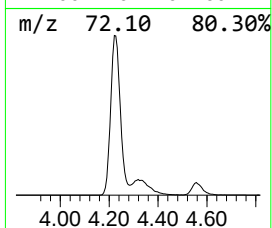
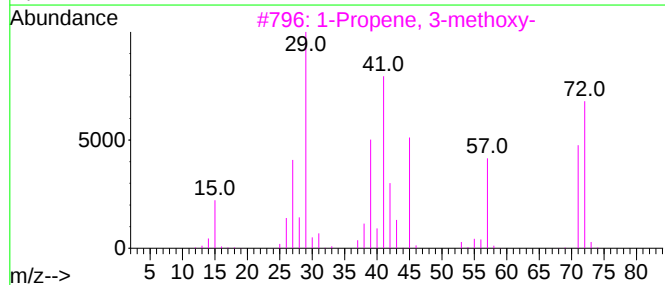
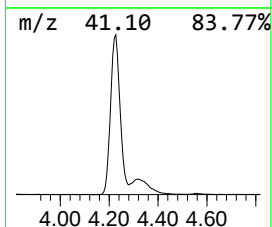
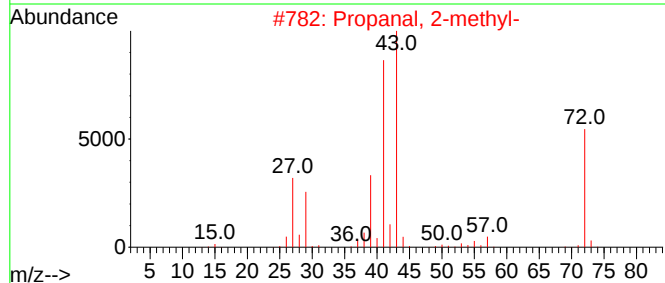
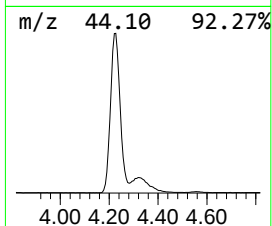
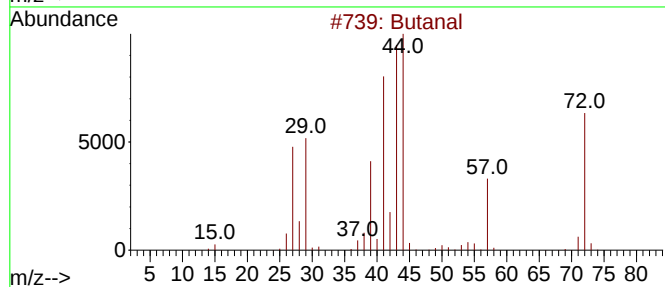
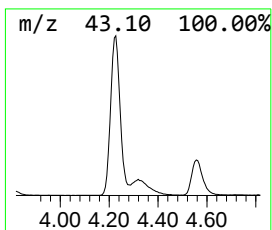
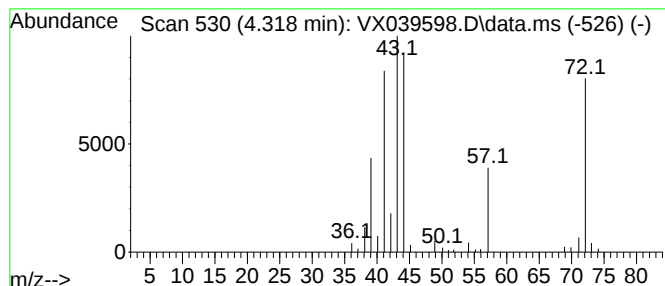
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown4.318 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.318	35.70 ug/l	372126	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	37
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	23
5			Acetaldehyde, methylhydrazone	72	C3H8N2	017167-73-6	9



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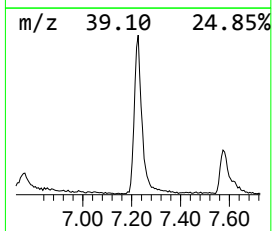
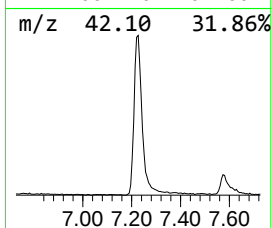
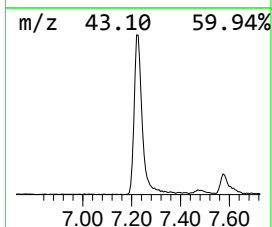
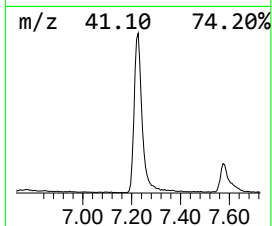
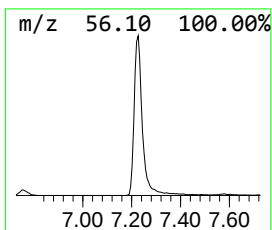
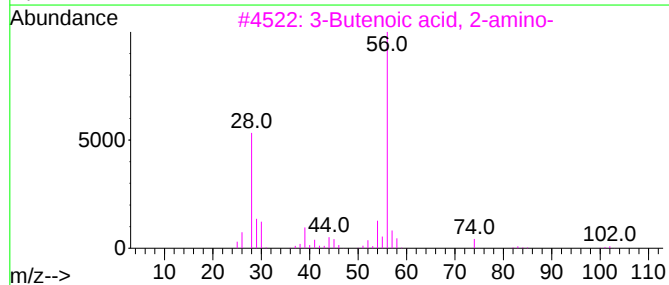
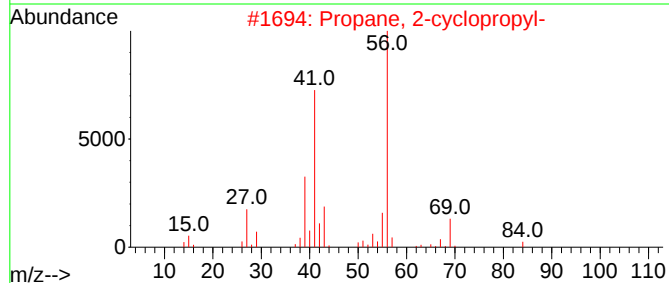
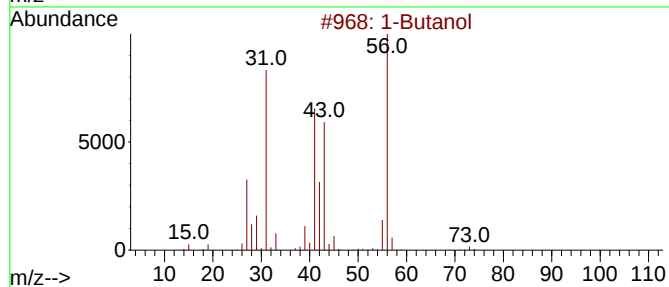
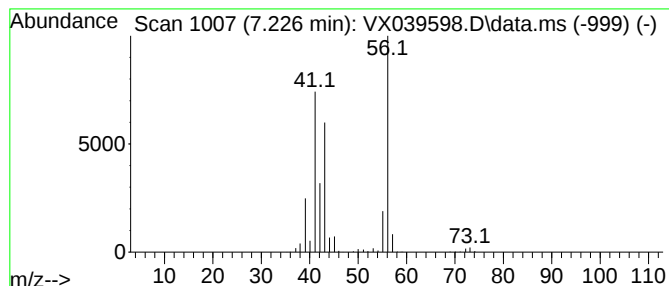
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	55.81 ug/l	581838	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3			3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
4			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	9



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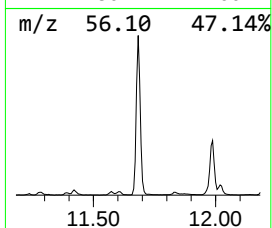
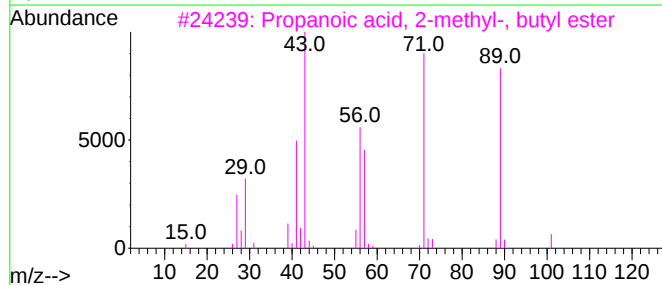
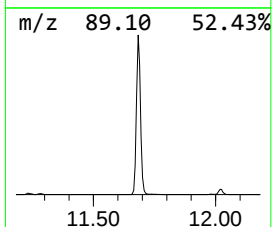
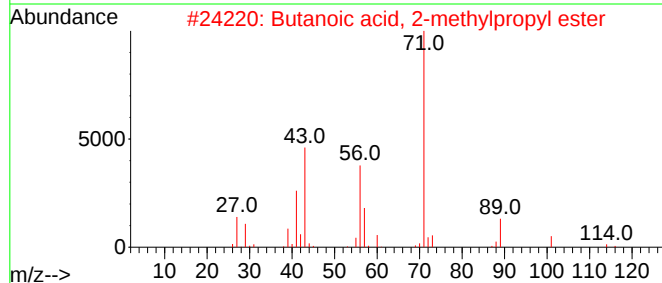
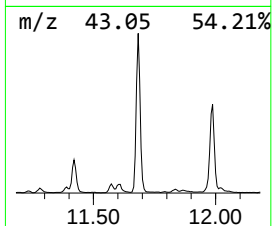
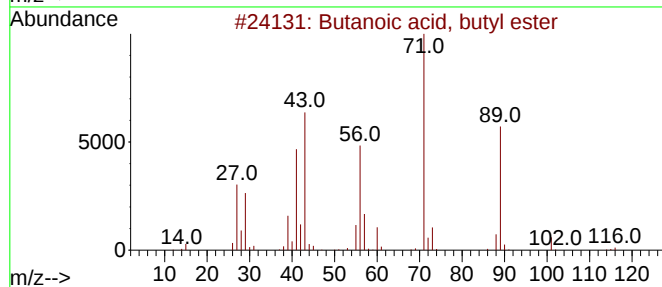
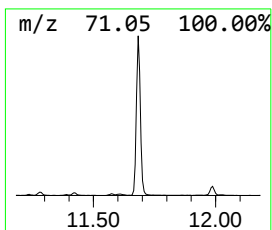
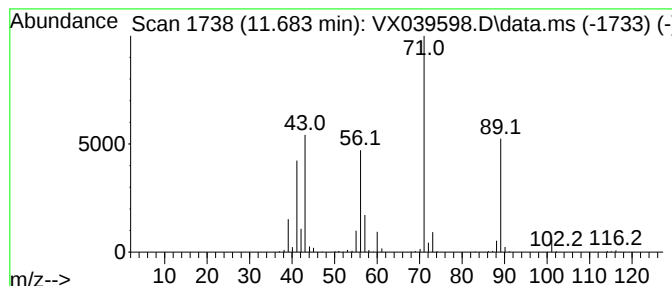
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	56.33 ug/l	675236	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	59
5			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039598.D
Acq On : 03 Jan 2024 13:43
Operator : JC/MD
Sample : P1002-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1210

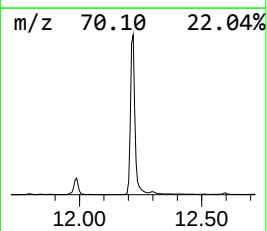
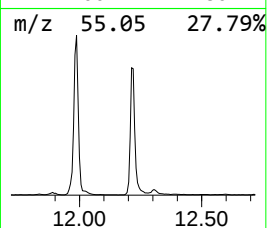
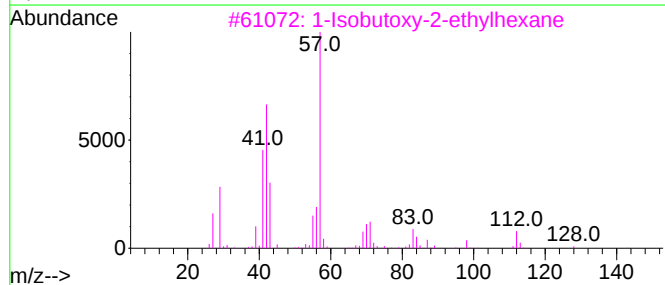
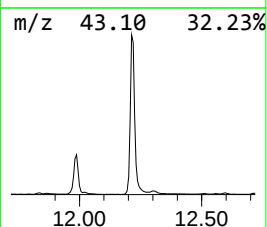
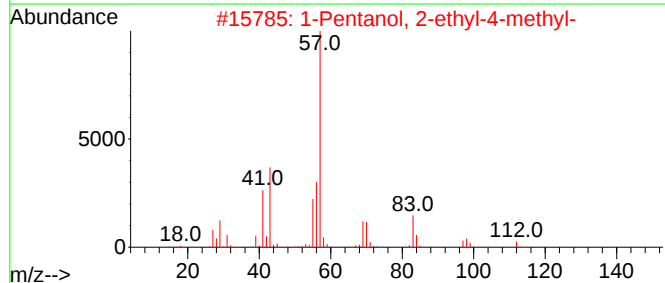
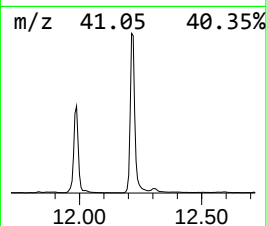
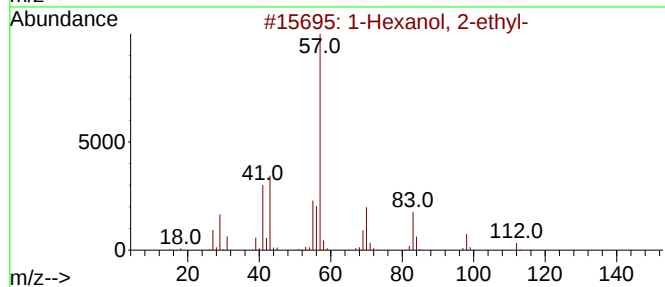
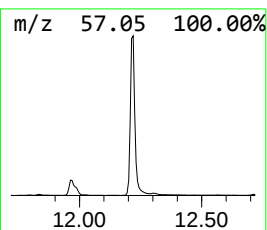
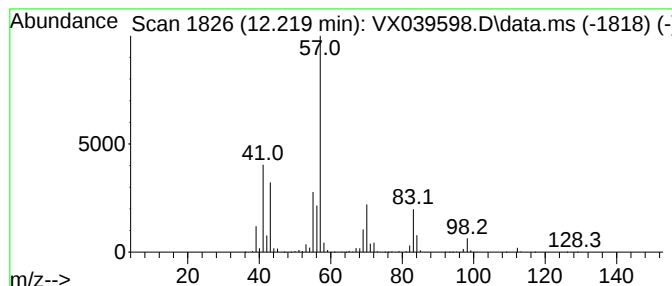
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	204.50 ug/l	2451360	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		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039598.D
Acq On : 03 Jan 2024 13:43
Operator : JC/MD
Sample : P1002-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1210

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	1.526	766.3	ug/l	7988820	1	5.550	521254	50.0
Ethanol	2.099	181.0	ug/l	1887210	1	5.550	521254	50.0
Butanal	4.227	232.9	ug/l	2428200	1	5.550	521254	50.0
unknown4.318	4.318	35.7	ug/l	372126	1	5.550	521254	50.0
1-Butanol	7.226	55.8	ug/l	581838	2	6.757	521254	50.0
Butanoic acid, ...	11.683	56.3	ug/l	675236	4	12.024	599361	50.0
1-Hexanol, 2-et...	12.219	204.5	ug/l	2451360	4	12.024	599361	50.0