

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
 Data File : VX040053.D
 Acq On : 31 Jan 2024 17:23
 Operator : JC/MD
 Sample : P1282-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1242

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\82X013024W.M

Title : SW846 8260

Signal : TIC: VX040053.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	105	rBV	14586032	27720214	100.00%	64.218%
2	2.056	152	159	176	rBV	733931	1194402	4.31%	2.767%
3	2.288	191	197	207	rBV	1631152	2628657	9.48%	6.090%
4	4.227	504	515	538	rBV	696628	1824719	6.58%	4.227%
5	5.550	722	732	746	rBV	102945	286211	1.03%	0.663%
6	6.757	922	930	941	rBV	160863	378595	1.37%	0.877%
7	7.202	996	1003	1017	rBV2	157496	341592	1.23%	0.791%
8	8.647	1234	1240	1248	rBV	358171	548928	1.98%	1.272%
9	10.055	1464	1471	1482	rBV	362491	550101	1.98%	1.274%
10	10.750	1578	1585	1594	rBV	226061	310363	1.12%	0.719%
11	11.079	1634	1639	1644	rBV	322917	409472	1.48%	0.949%
12	11.683	1733	1738	1746	rVB	1863006	2074706	7.48%	4.806%
13	11.988	1783	1788	1791	rBV	1071359	1289032	4.65%	2.986%
14	12.018	1791	1793	1802	rVB	423062	539144	1.94%	1.249%
15	12.219	1819	1826	1836	rBV	2484151	3069962	11.07%	7.112%

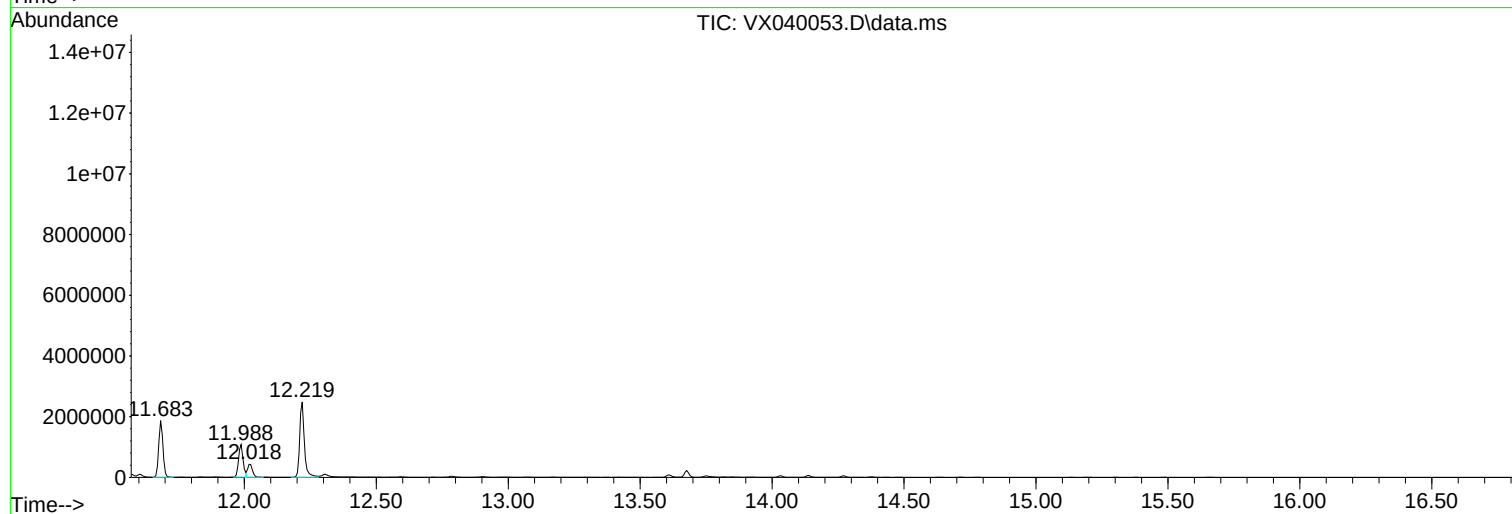
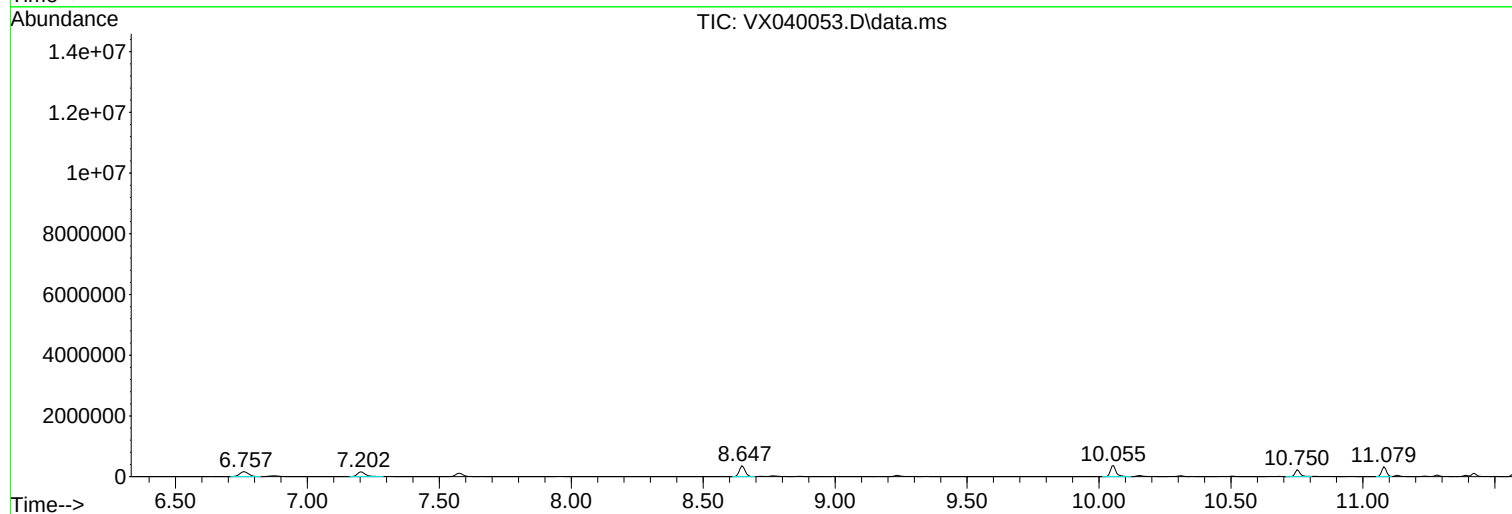
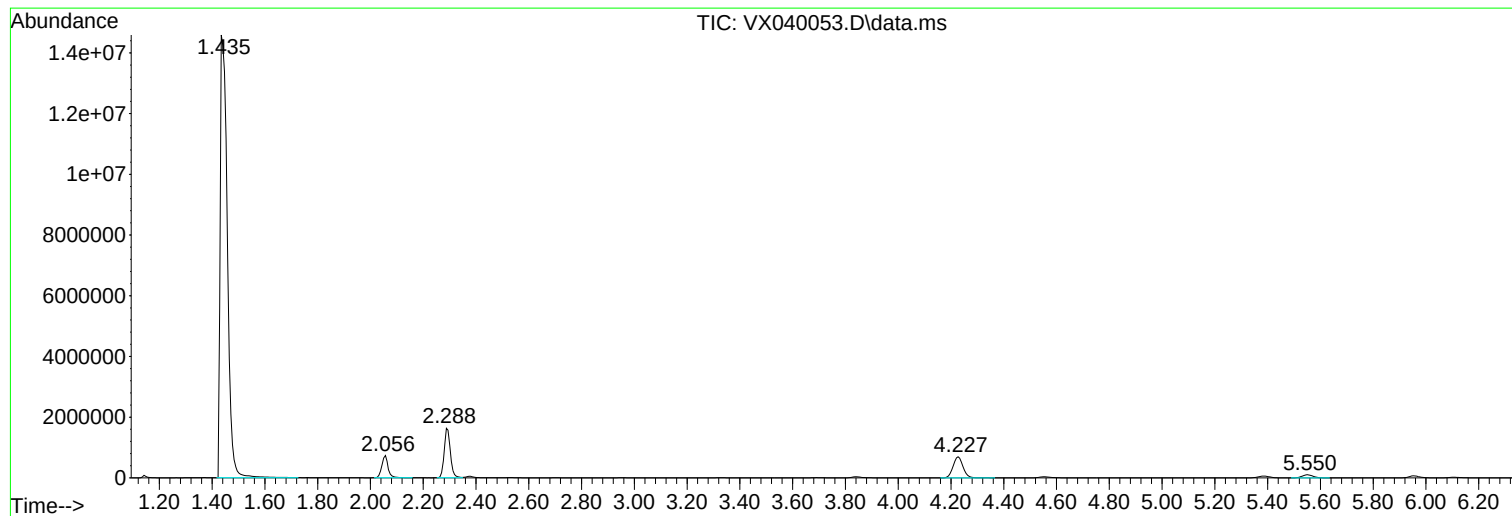
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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



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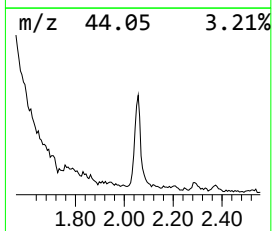
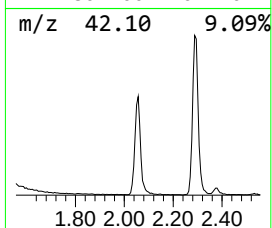
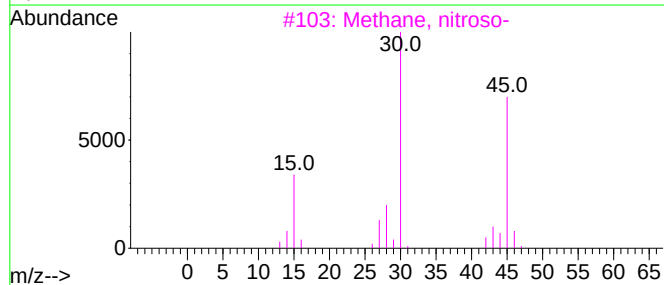
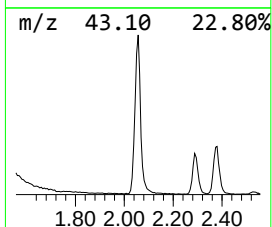
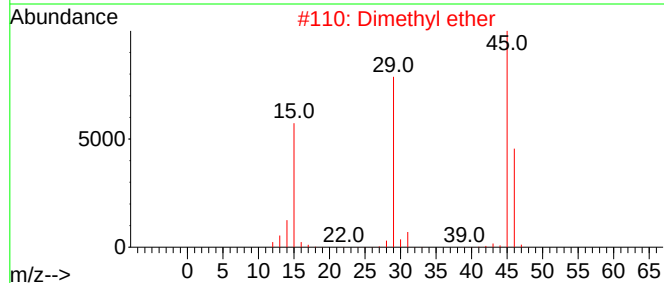
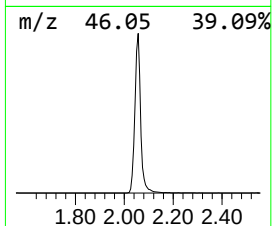
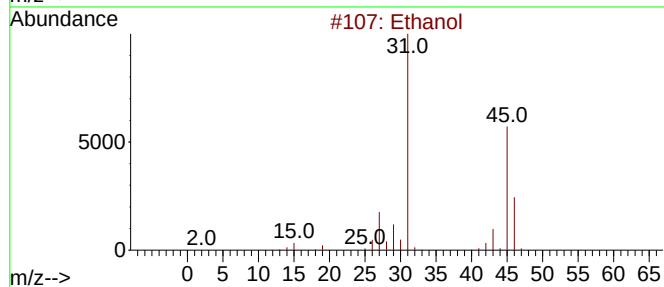
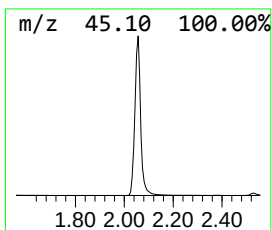
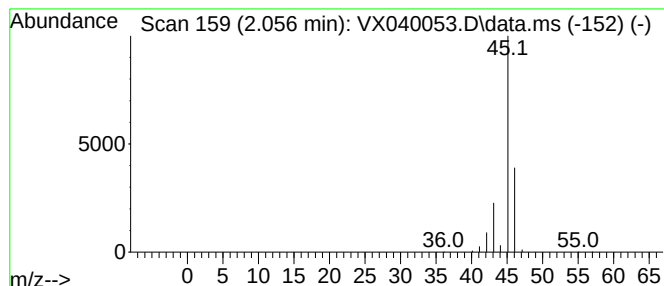
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	208.66 ug/l	1194400	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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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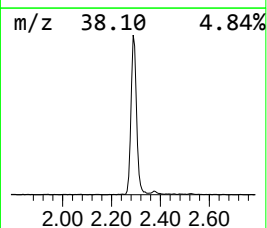
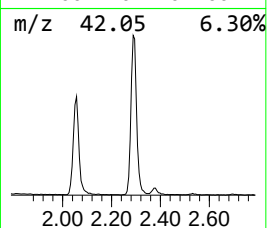
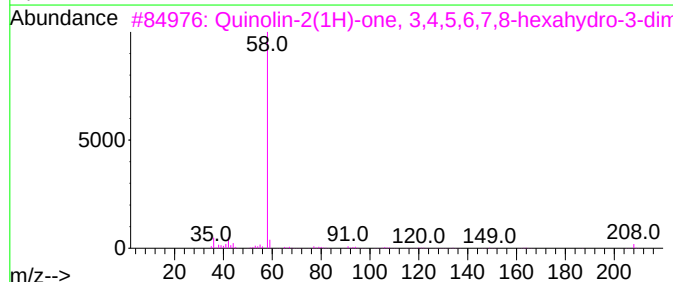
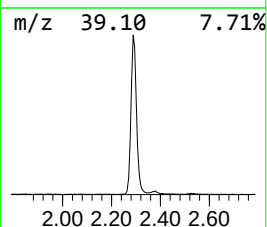
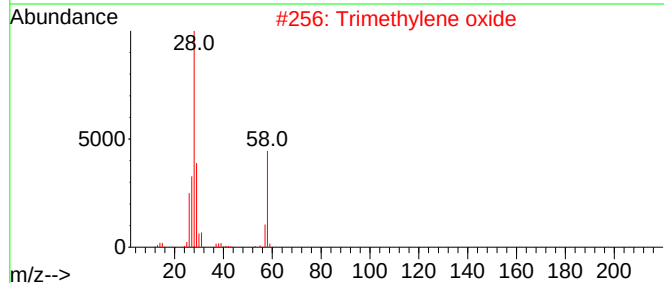
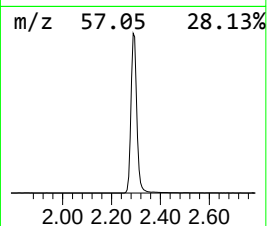
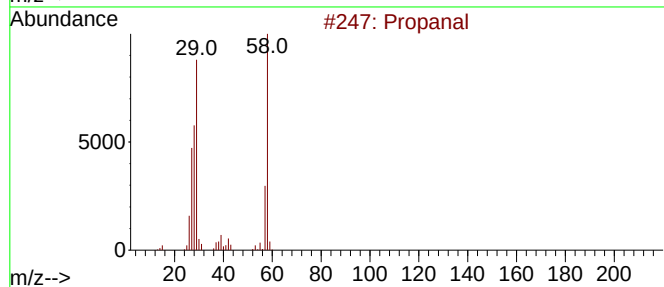
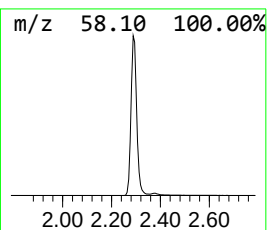
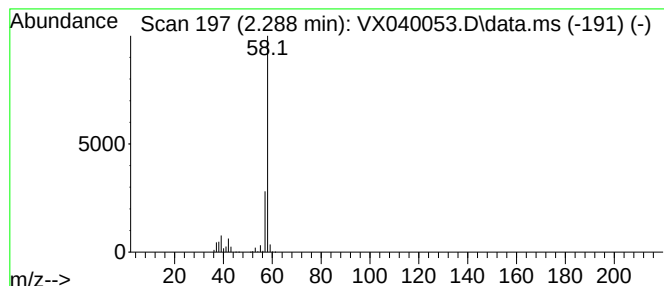
Instrument :
MSVOA_X
ClientSampleId :
1242

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.288	459.22 ug/l	2628660	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	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5	Propylene oxide	58	C3H6O	000075-56-9	7



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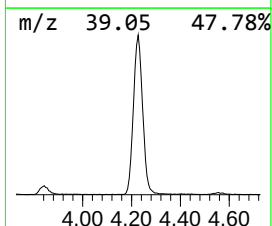
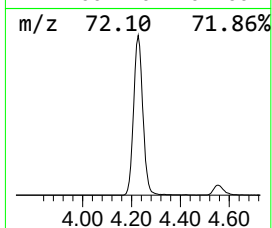
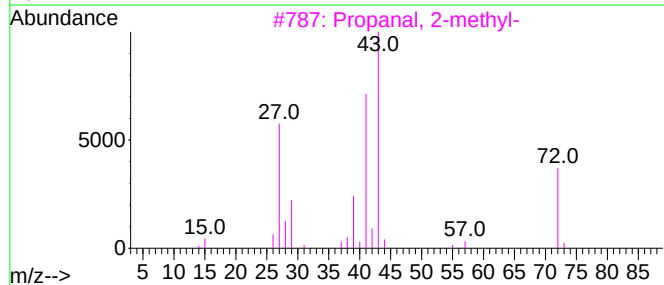
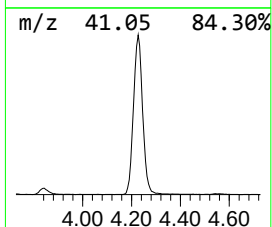
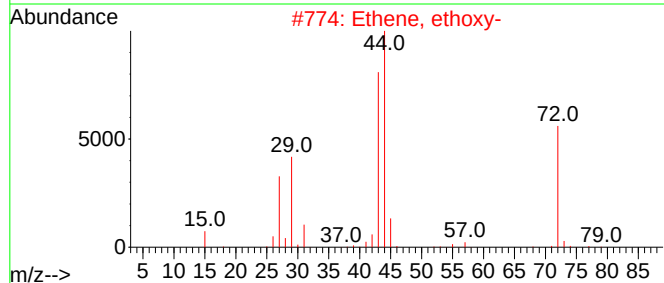
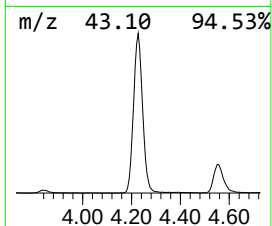
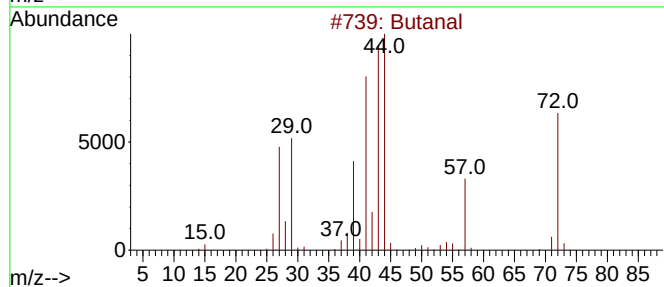
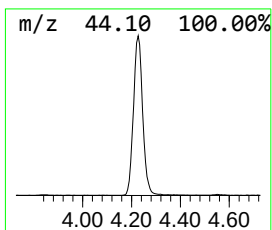
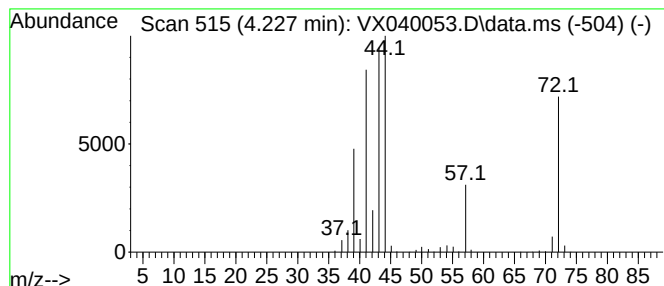
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Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	318.77 ug/l	1824720	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	32
4			Methacrolein	70	C4H6O	000078-85-3	27
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	27



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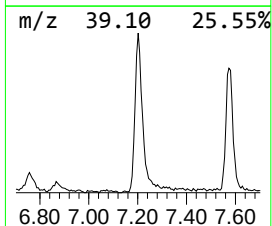
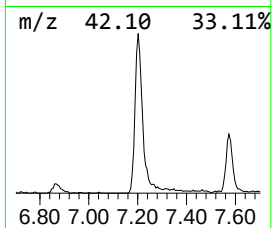
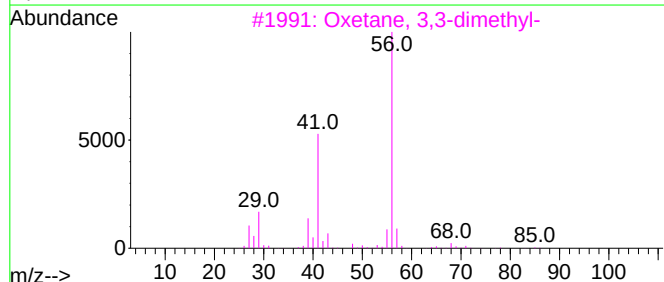
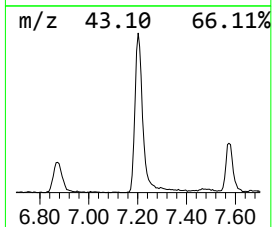
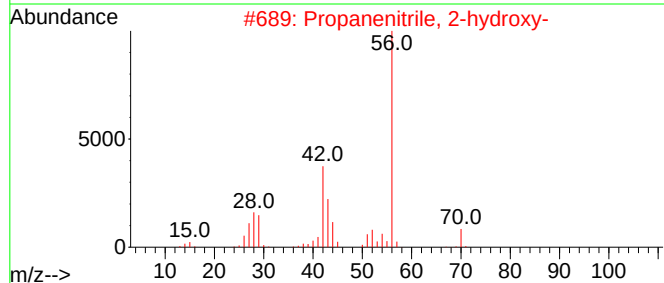
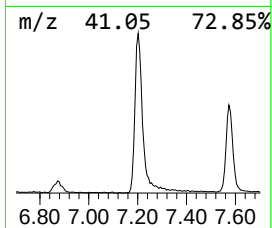
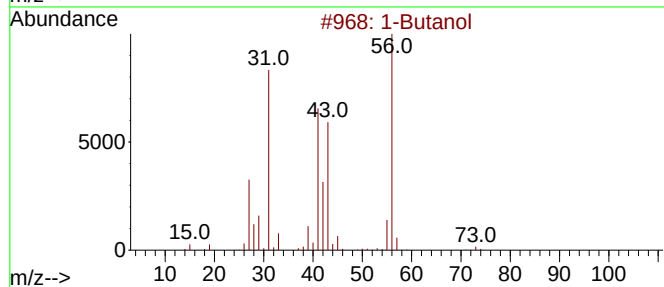
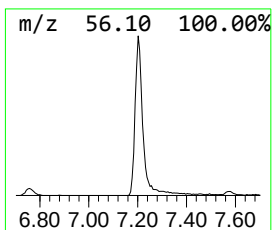
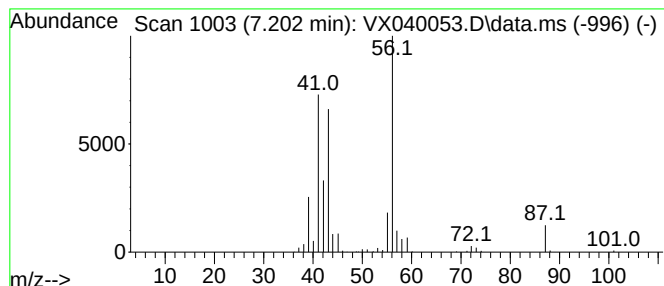
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Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	45.11 ug/l	341592	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	72
2			Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	42
3			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	42
4			3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	40
5			1-Hexanol	102	C6H14O	000111-27-3	39



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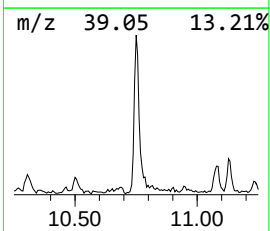
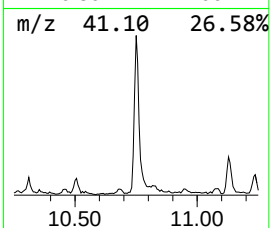
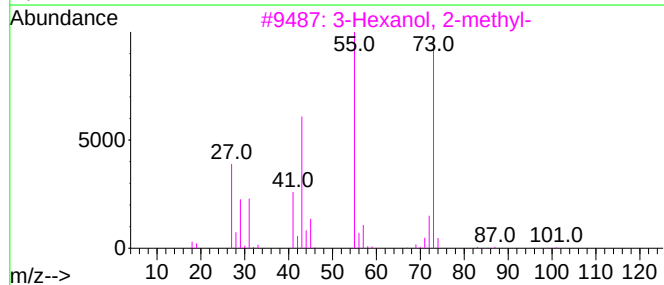
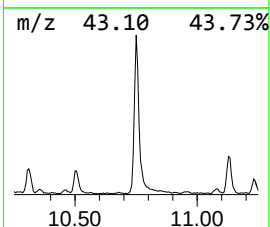
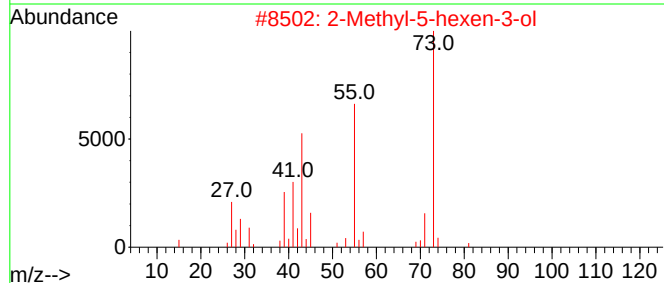
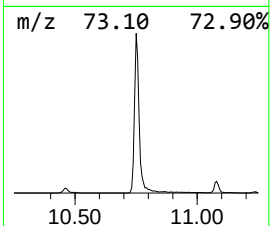
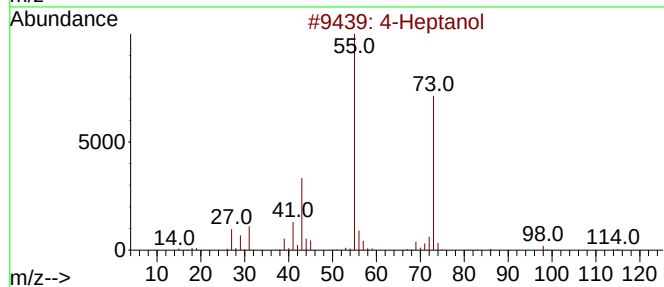
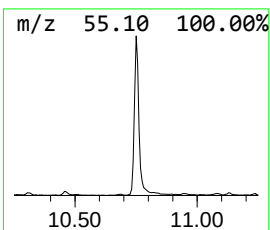
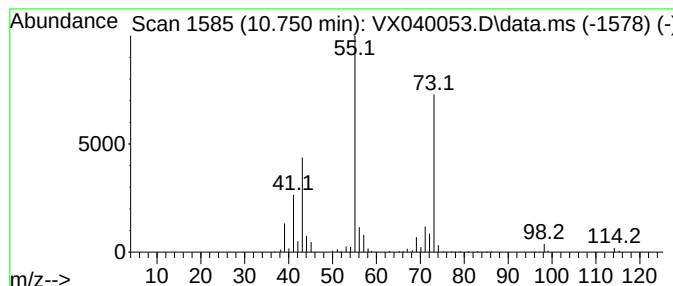
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Peak Number 6 4-Heptanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	28.21 ug/l	310363	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	72
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	47
4			Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	43
5			Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	43



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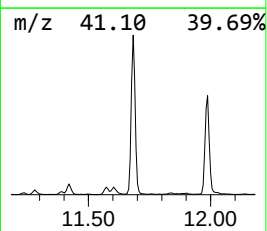
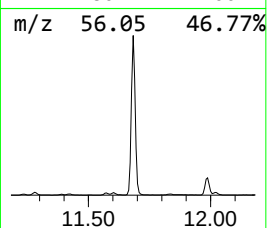
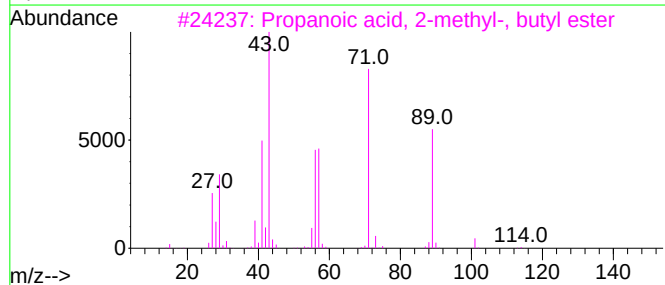
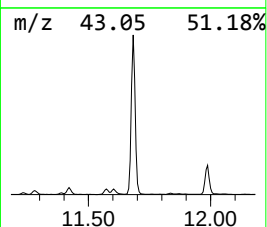
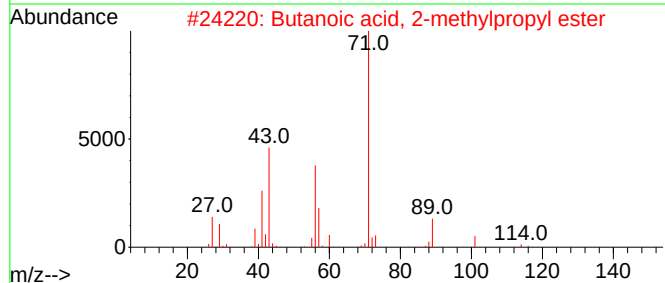
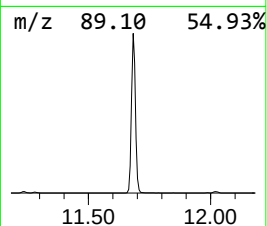
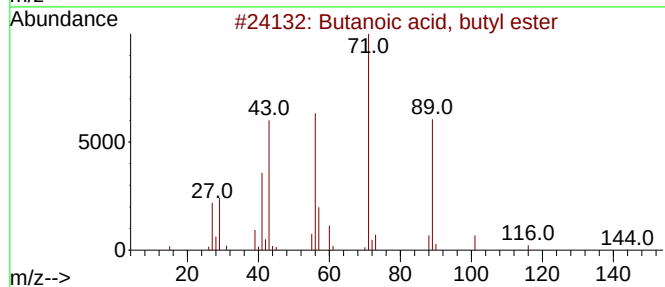
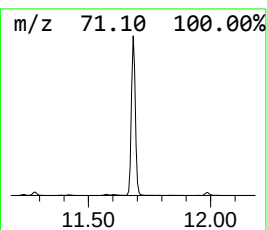
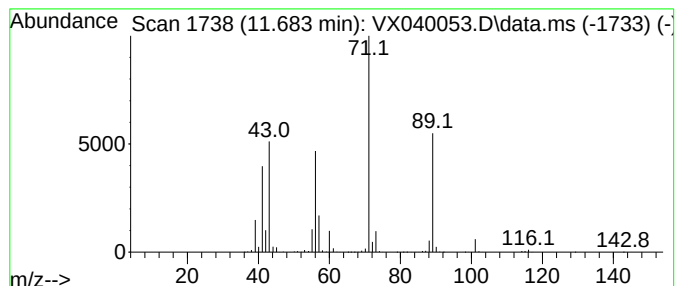
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Quant Title : SW846 8260

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

Peak Number 7 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	192.41 ug/l	2074710	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, octyl ester	200	C12H24O2	000110-39-4	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040053.D
Acq On : 31 Jan 2024 17:23
Operator : JC/MD
Sample : P1282-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1242

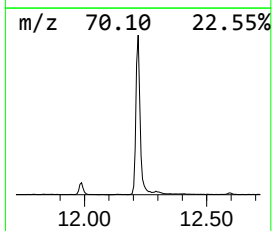
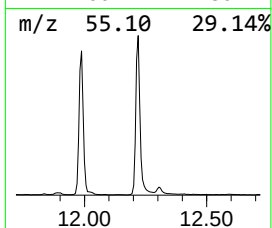
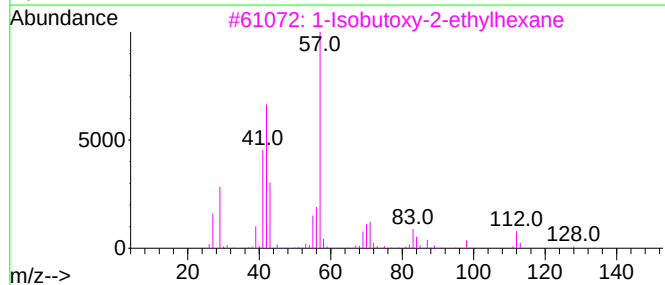
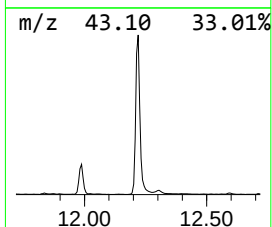
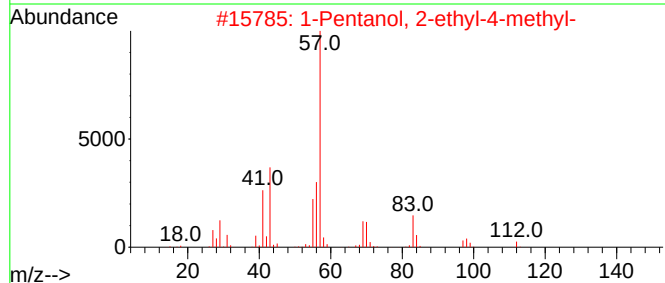
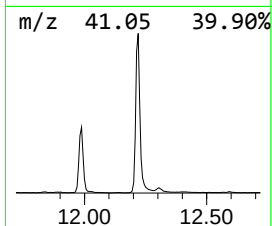
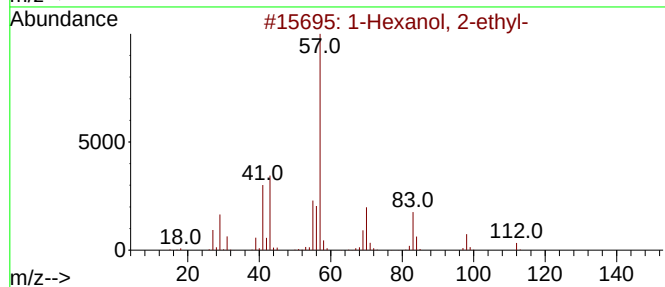
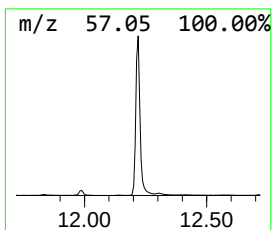
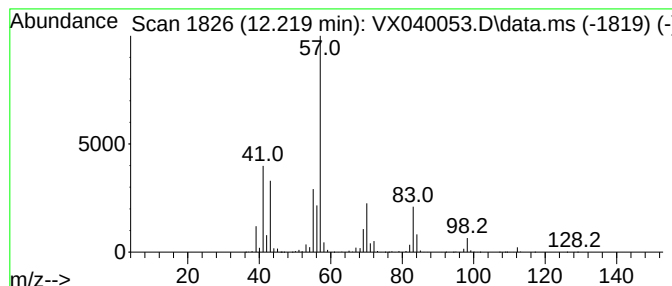
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	284.71 ug/l	3069960	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\VX013124\
Data File : VX040053.D
Acq On : 31 Jan 2024 17:23
Operator : JC/MD
Sample : P1282-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1242

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.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
Ethanol	2.056	208.7	ug/l	1194400	1	5.550	286211	50.0
Propanal	2.288	459.2	ug/l	2628660	1	5.550	286211	50.0
Butanal	4.227	318.8	ug/l	1824720	1	5.550	286211	50.0
1-Butanol	7.202	45.1	ug/l	341592	2	6.757	378595	50.0
4-Heptanol	10.750	28.2	ug/l	310363	3	10.055	550101	50.0
Butanoic acid, ...	11.683	192.4	ug/l	2074710	4	12.024	539144	50.0
1-Hexanol, 2-et...	12.219	284.7	ug/l	3069960	4	12.024	539144	50.0