

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050824\
 Data File : VX041418.D
 Acq On : 08 May 2024 14:06
 Operator : JC/MD
 Sample : P2389-02 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1401

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\82X043024W.M
 Title : SW846 8260

Signal : TIC: VX041418.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	56	59	64	rBV	1807206	2159609	100.00%	26.169%
2	1.490	64	66	88	rVB	279890	561368	25.99%	6.802%
3	2.087	158	164	177	rBV	118346	183224	8.48%	2.220%
4	4.239	507	517	539	rBV	14545	53481	2.48%	0.648%
5	5.385	693	705	720	rBV2	93942	277805	12.86%	3.366%
6	5.550	720	732	748	rVV	167174	479595	22.21%	5.811%
7	5.952	788	798	821	rBV	100009	273858	12.68%	3.318%
8	6.757	921	930	942	rBV	282061	684133	31.68%	8.290%
9	6.879	942	950	962	rVB	48342	120325	5.57%	1.458%
10	7.208	998	1004	1019	rBV3	29889	82203	3.81%	0.996%
11	8.647	1233	1240	1249	rBV	570316	893438	41.37%	10.826%
12	10.055	1465	1471	1486	rBV	530961	746918	34.59%	9.051%
13	10.311	1504	1513	1524	rBV2	49951	72695	3.37%	0.881%
14	11.079	1634	1639	1655	rBV	538278	699126	32.37%	8.472%
15	12.024	1781	1794	1802	rBV	675808	872334	40.39%	10.570%
16	12.213	1818	1825	1835	rBV3	23307	49055	2.27%	0.594%
17	12.415	1854	1858	1866	rBV	33787	43505	2.01%	0.527%

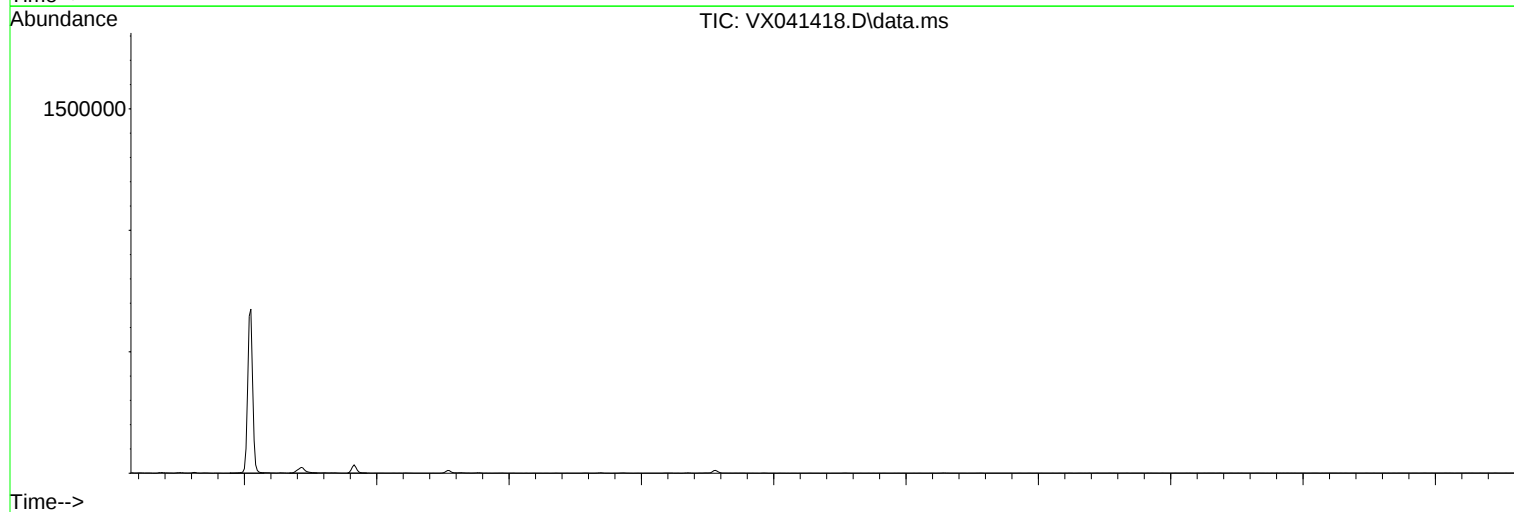
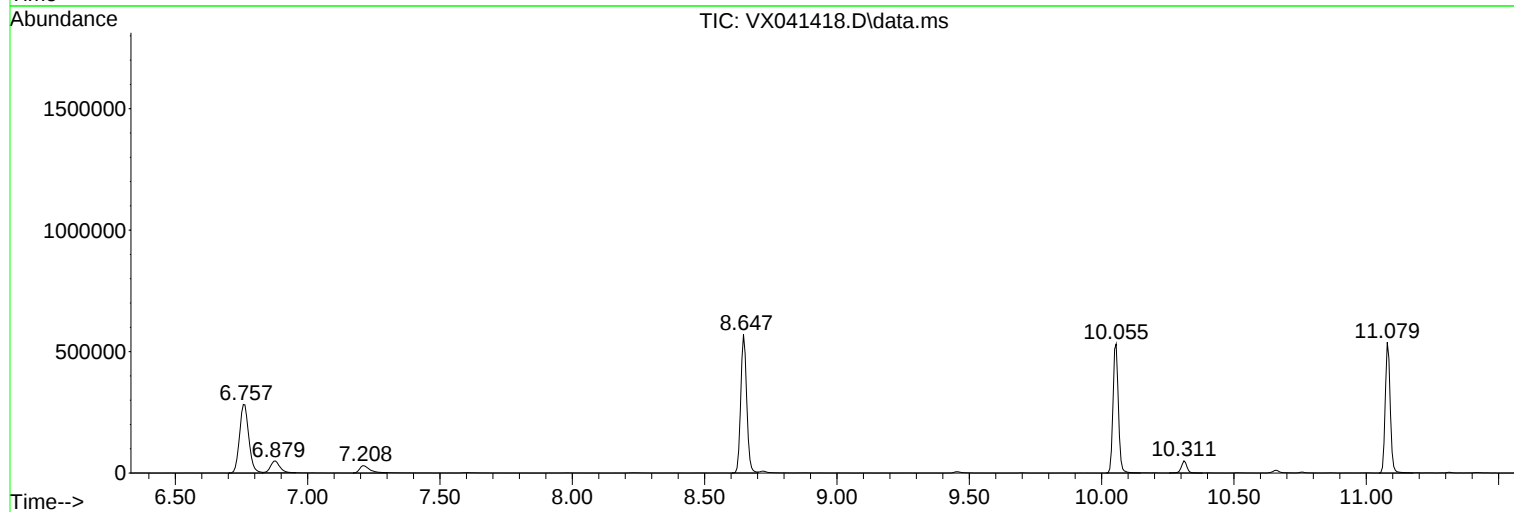
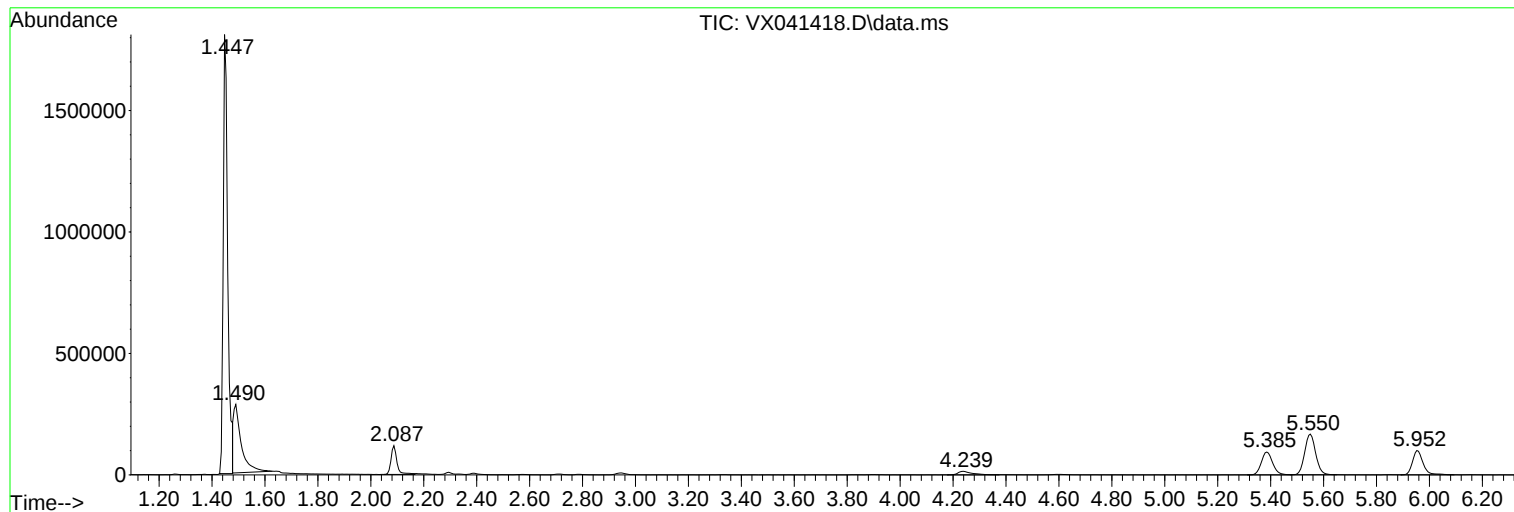
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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



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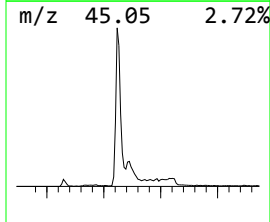
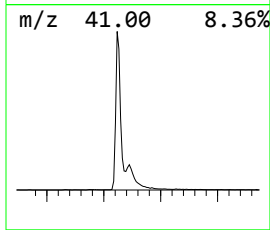
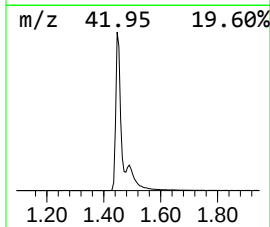
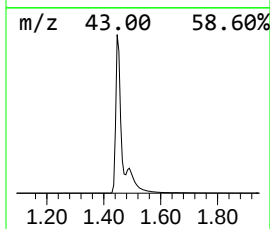
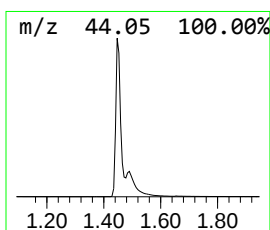
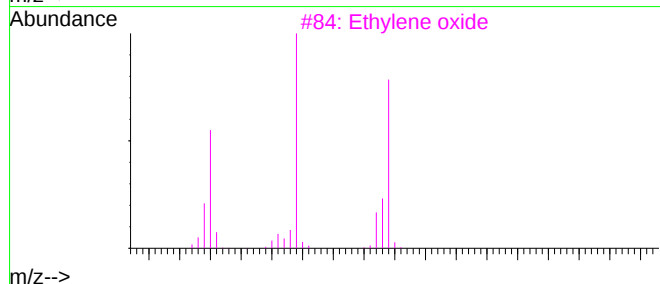
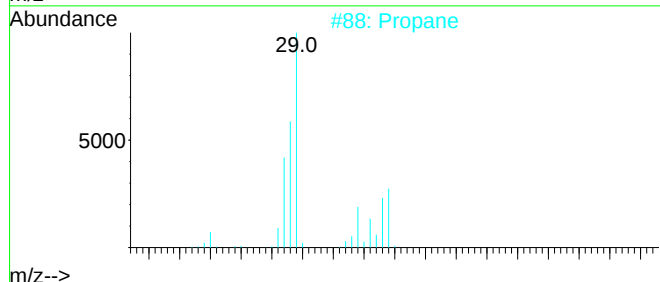
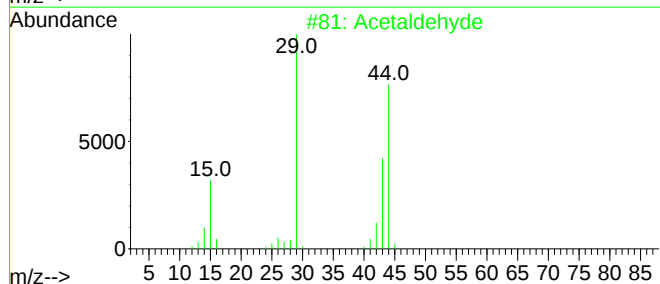
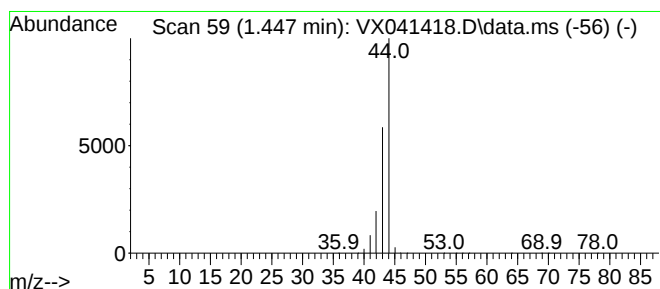
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	225.15 ug/l	2159610	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Acetonitrile-d3	44	C2D3N	002206-26-0	3



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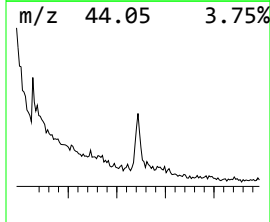
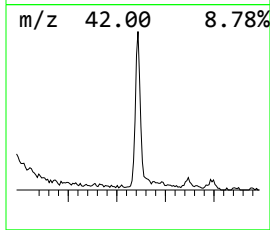
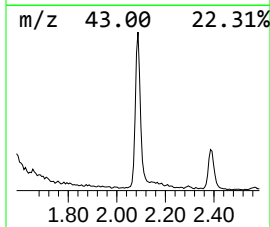
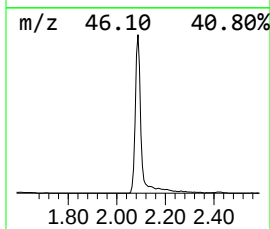
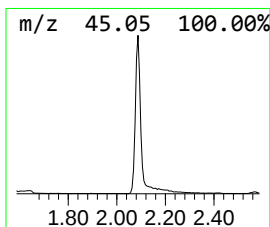
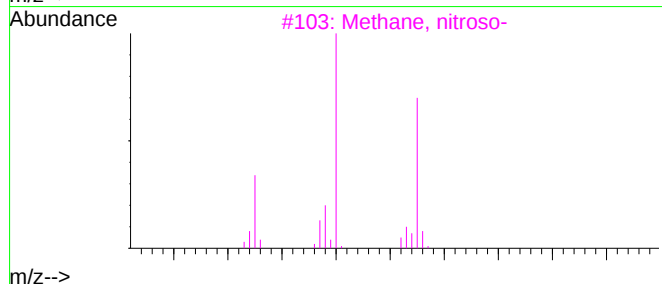
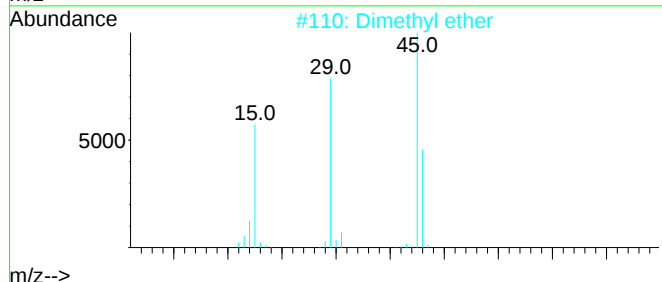
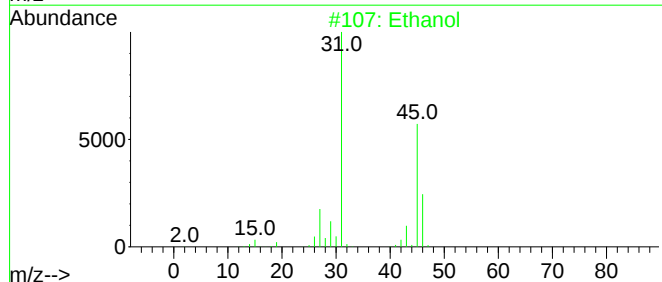
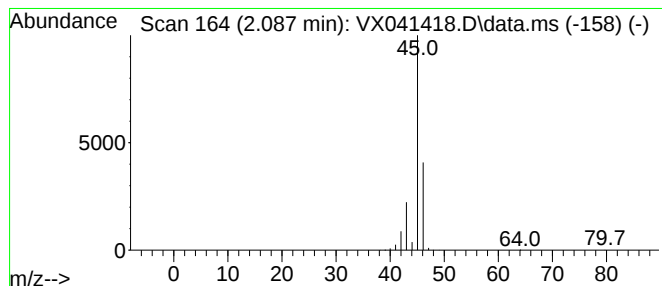
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.087	19.10 ug/l	183224	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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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

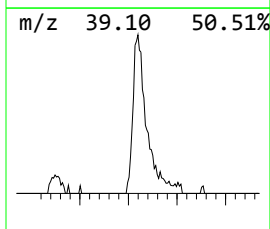
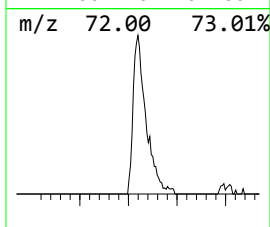
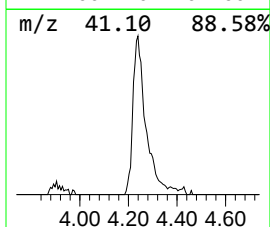
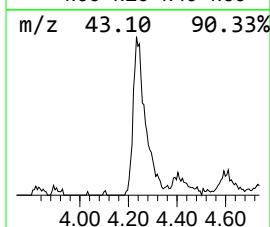
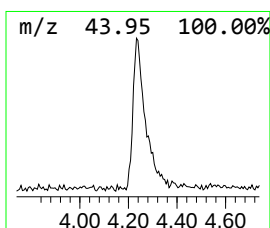
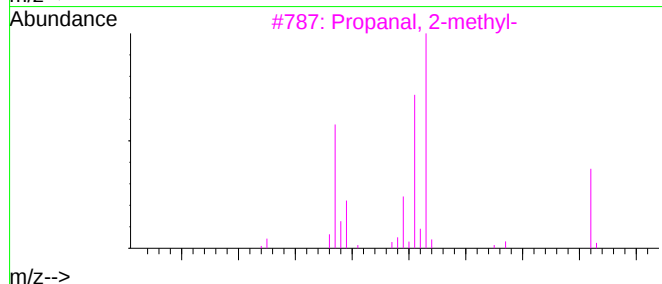
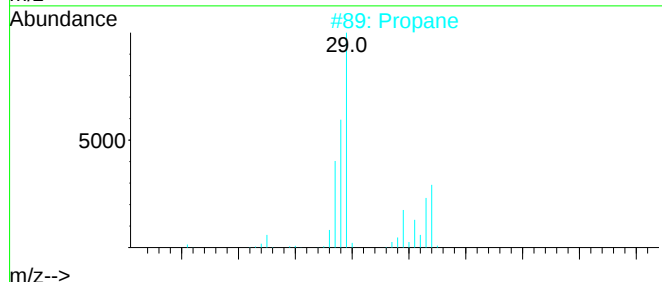
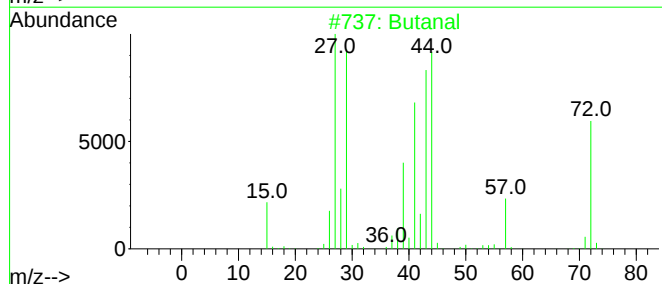
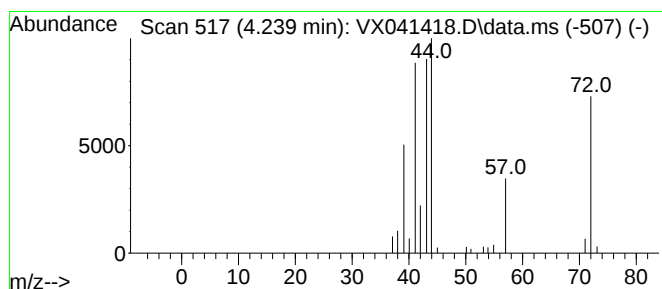
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.239	5.58 ug/l	53481	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	59
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	Ethene, ethoxy-	72	C4H8O	000109-92-2	38



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Instrument :
MSVOA_X
ClientSampleId :
1401

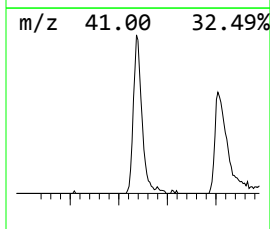
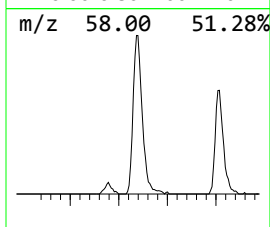
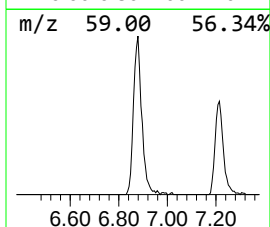
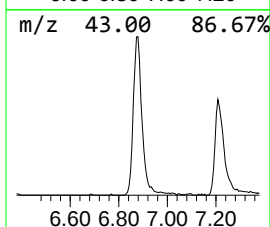
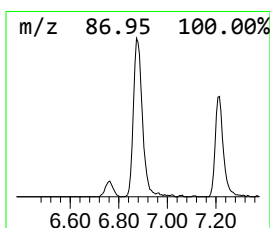
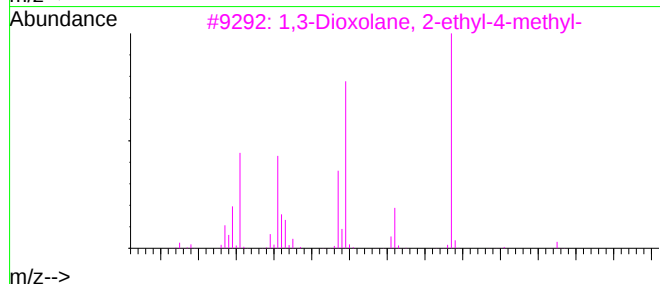
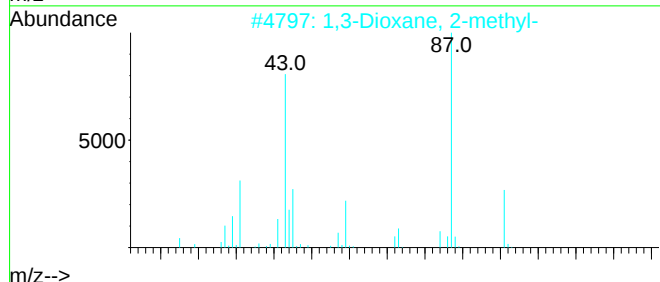
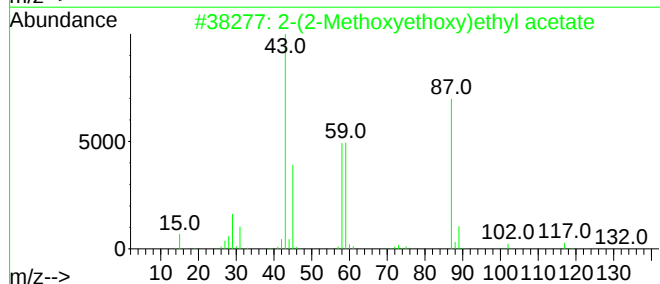
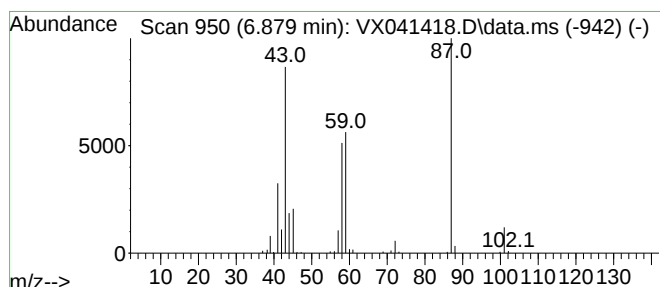
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown6.879 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	8.79 ug/l	120325	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	38
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	38
3	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	37
4	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	23
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	23



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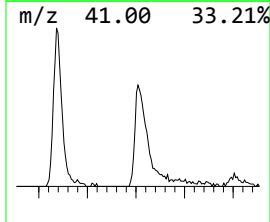
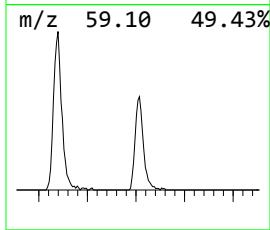
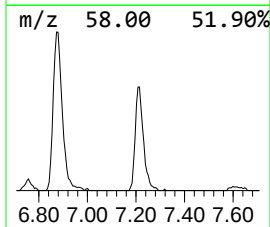
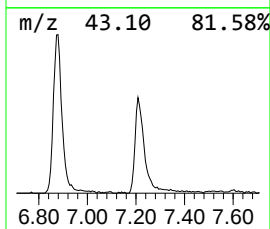
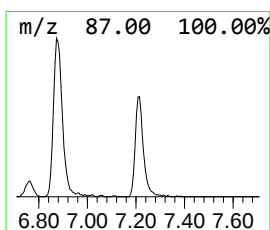
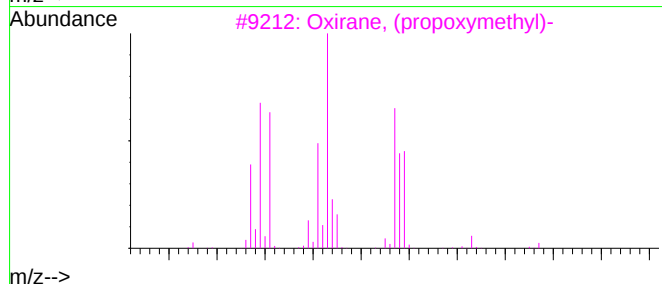
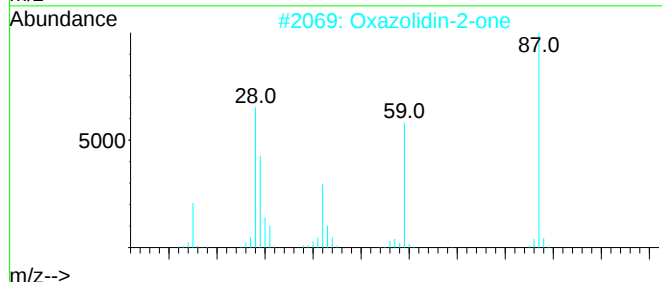
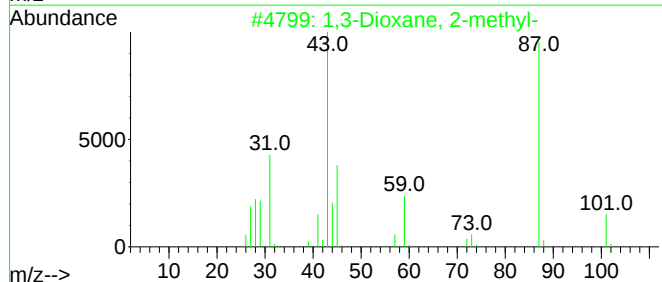
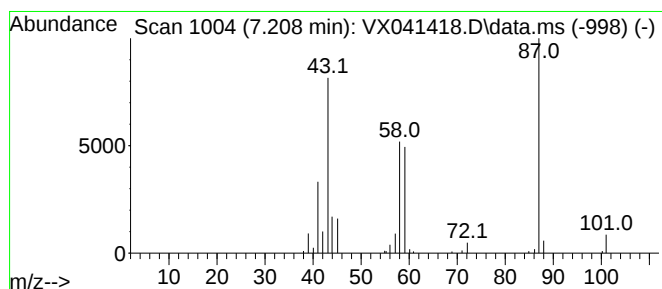
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3-Dioxane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	6.01 ug/l	82203	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	43
3	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	43
4	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	38



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.447	225.2	ug/l	2159610	1	5.550	479595	50.0
Ethanol	2.087	19.1	ug/l	183224	1	5.550	479595	50.0
Butanal	4.239	5.6	ug/l	53481	1	5.550	479595	50.0
unknown6.879	6.879	8.8	ug/l	120325	2	6.763	684133	50.0
1,3-Dioxane, 2-...	7.208	6.0	ug/l	82203	2	6.763	684133	50.0