

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041723\
 Data File : VX035107.D
 Acq On : 17 Apr 2023 14:29
 Operator : JC/MD
 Sample : 02353-03 200X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BUR-1261

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\82X032923W.M

Title : SW846 8260

Signal : TIC: VX035107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	77	rBV	430790	544803	33.40%	5.652%
2	4.385	532	541	560	rBV2	42636	148466	9.10%	1.540%
3	5.385	694	705	719	rBV2	178772	522525	32.04%	5.421%
4	5.550	721	732	751	rVB	317155	915523	56.13%	9.499%
5	5.952	787	798	820	rBV	199239	546392	33.50%	5.669%
6	6.757	920	930	941	rBV	493044	1195572	73.30%	12.404%
7	6.873	942	949	967	rVB	85872	217849	13.36%	2.260%
8	7.214	996	1005	1015	rBV2	14180	34205	2.10%	0.355%
9	8.647	1233	1240	1249	rBV	1040039	1630956	100.00%	16.921%
10	10.055	1465	1471	1486	rBV	1027525	1417317	86.90%	14.705%
11	11.079	1634	1639	1654	rBV	858203	1097569	67.30%	11.387%
12	12.024	1788	1794	1802	rVB	1030969	1332068	81.67%	13.820%
13	12.219	1821	1826	1831	rBV	22935	35349	2.17%	0.367%

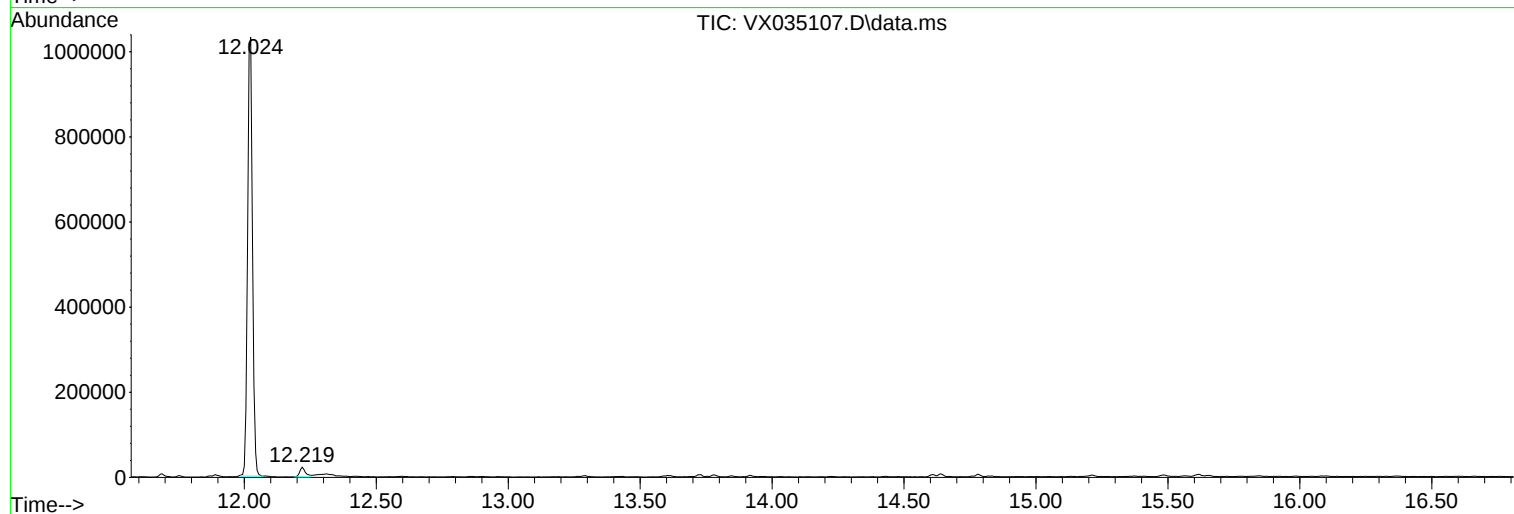
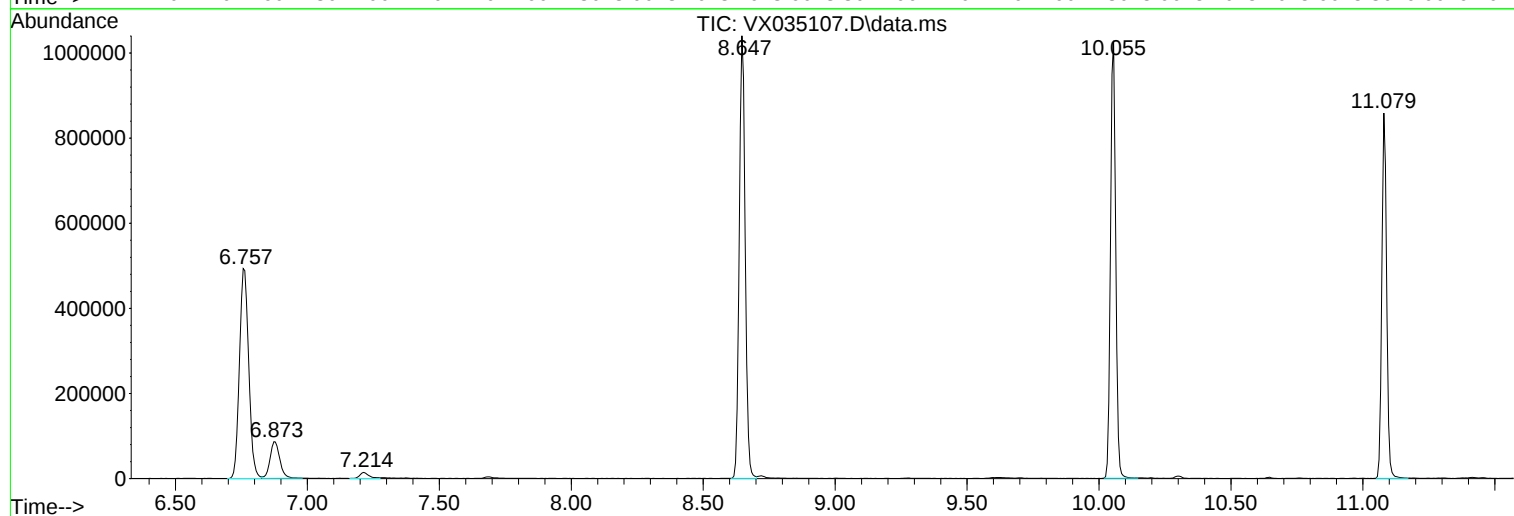
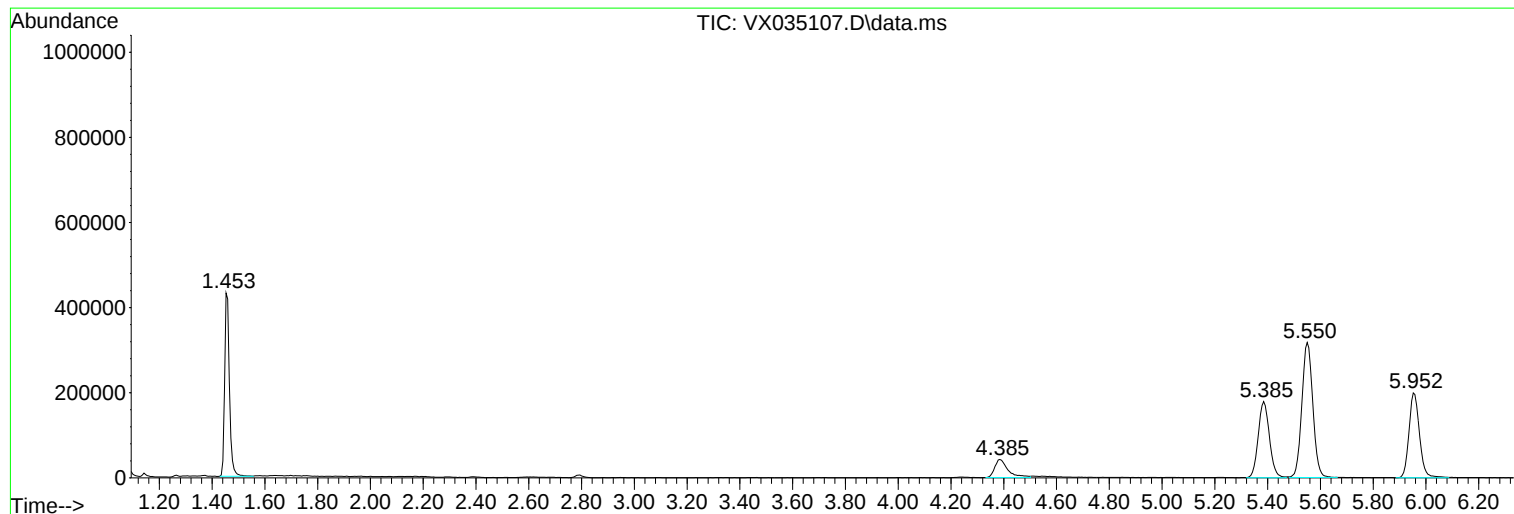
Sum of corrected areas: 9638594

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



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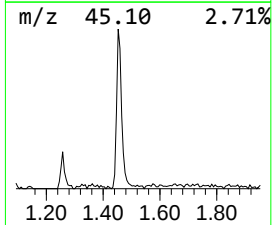
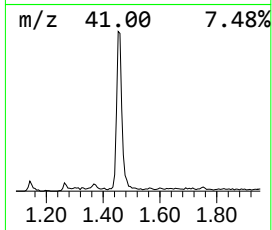
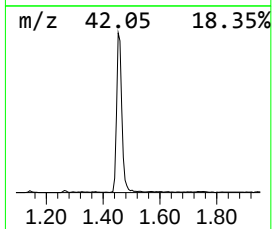
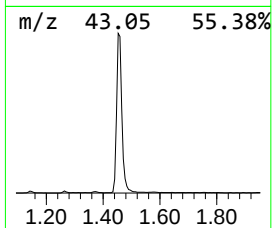
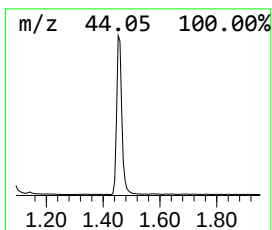
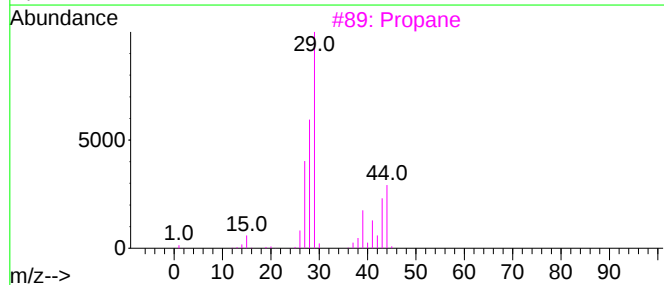
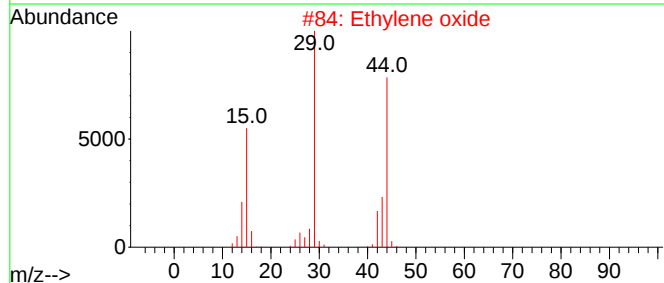
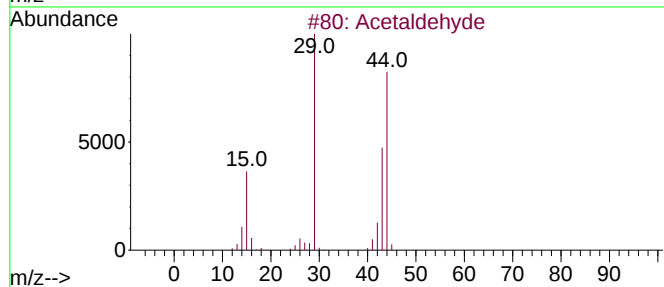
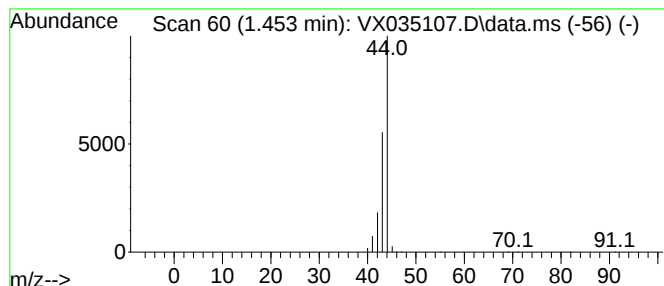
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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.
1.453	29.75 ug/l	544803	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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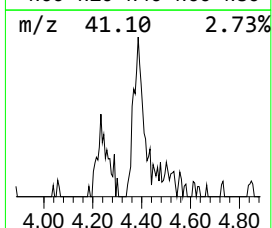
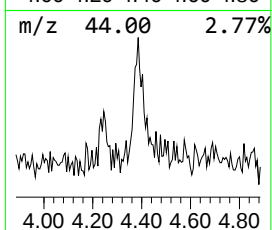
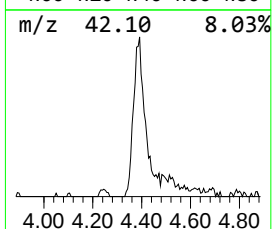
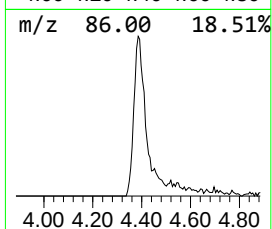
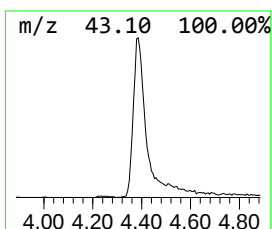
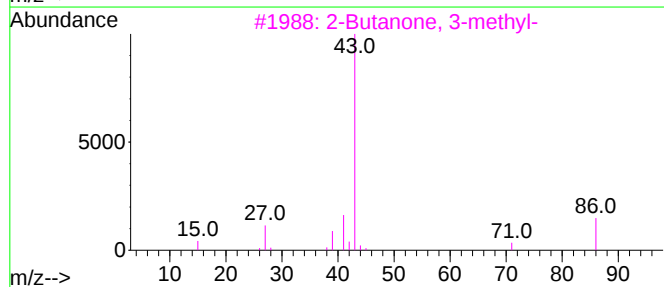
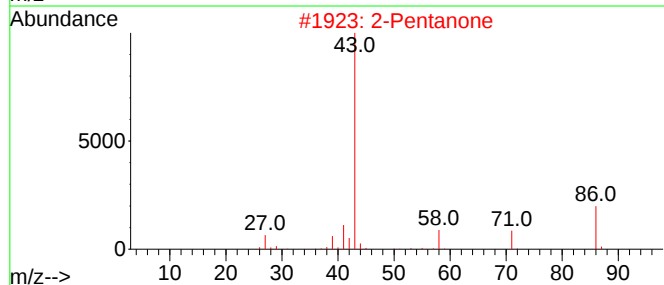
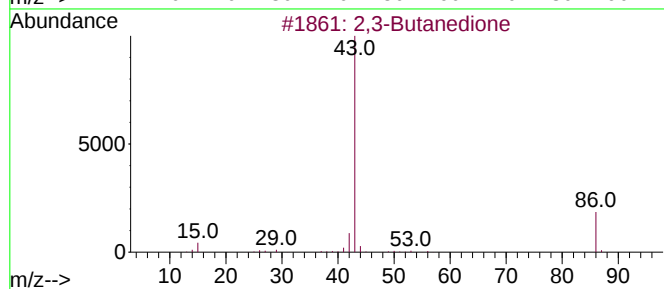
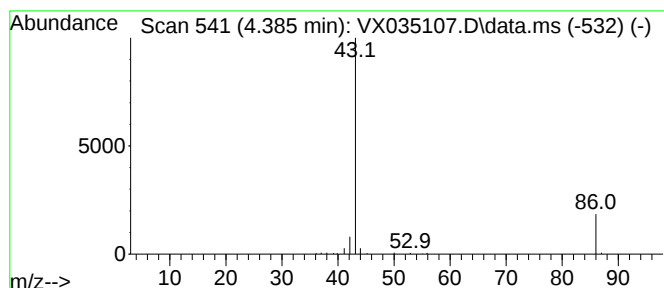
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Peak Number 2 2,3-Butanedione Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.385	8.11 ug/l	148466	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Butanedione	86	C4H6O2	000431-03-8	90
2			2-Pentanone	86	C5H10O	000107-87-9	50
3			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
4			Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	5
5			Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	4



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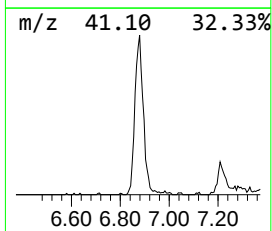
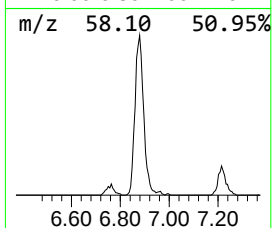
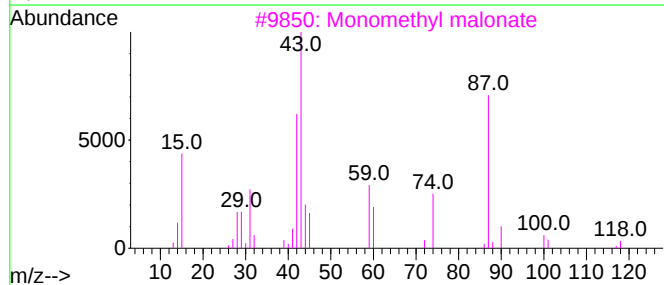
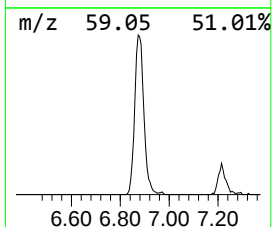
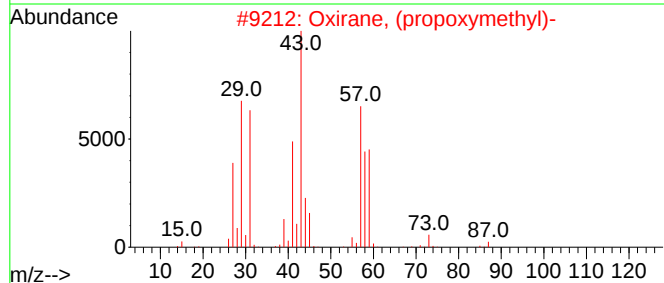
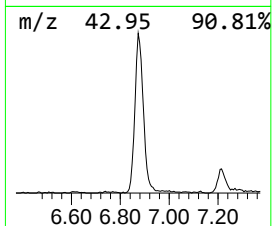
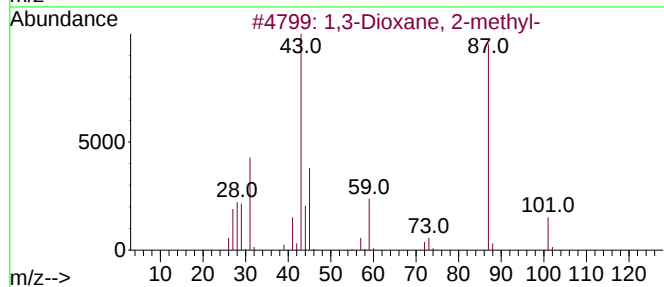
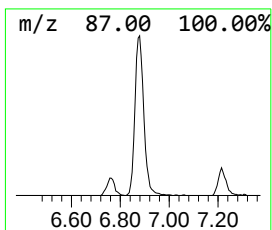
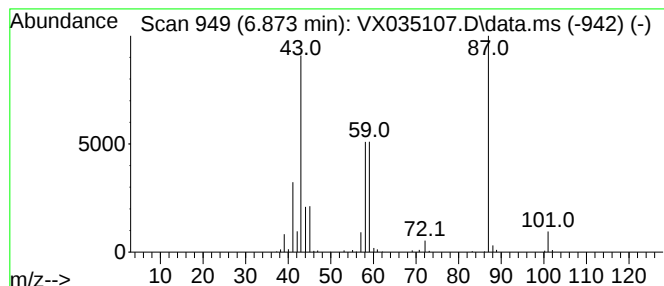
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Peak Number 3 unknown6.873 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	9.11 ug/l	217849	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	47
2		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	43
3		Monomethyl malonate	118	C4H6O4	016695-14-0	33
4		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	25
5		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	23



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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	29.8	ug/l	544803	1	5.550	915523	50.0
2,3-Butanedione	4.385	8.1	ug/l	148466	1	5.550	915523	50.0
unknown6.873	6.873	9.1	ug/l	217849	2	6.763	1195570	50.0