

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052121\
 Data File : VX022119.D
 Acq On : 21 May 2021 16:39
 Operator : JC/MD
 Sample : M2481-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WASTE-WATER

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\82X051921W.M

Title : SW846 8260

Signal : TIC: VX022119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	24	27	33	rBV	25810	25321	1.31%	0.470%
2	1.374	43	47	56	rBV	25729	23718	1.23%	0.441%
3	1.453	56	60	75	rBV	1760554	1928169	100.00%	35.816%
4	2.069	154	161	170	rBV	42793	67176	3.48%	1.248%
5	4.251	508	519	530	rBV2	9823	27481	1.43%	0.510%
6	4.690	578	591	609	rBV	186466	538873	27.95%	10.010%
7	5.026	635	646	656	rBV2	24487	76749	3.98%	1.426%
8	5.397	696	707	721	rVB2	49605	140253	7.27%	2.605%
9	5.562	721	734	746	rBV2	75376	211013	10.94%	3.920%
10	5.842	768	780	792	rBV	131298	347802	18.04%	6.460%
11	5.964	792	800	812	rVB2	57940	150468	7.80%	2.795%
12	6.769	922	932	944	rBV	132047	314316	16.30%	5.838%
13	7.665	1072	1079	1089	rBV2	17896	37624	1.95%	0.699%
14	8.653	1234	1241	1250	rBV	281941	435592	22.59%	8.091%
15	10.061	1466	1472	1482	rVB	256488	354816	18.40%	6.591%
16	10.945	1612	1617	1628	rVB	130623	172228	8.93%	3.199%
17	11.085	1635	1640	1649	rVB	200378	249034	12.92%	4.626%
18	12.024	1789	1794	1805	rBV	234396	282919	14.67%	5.255%

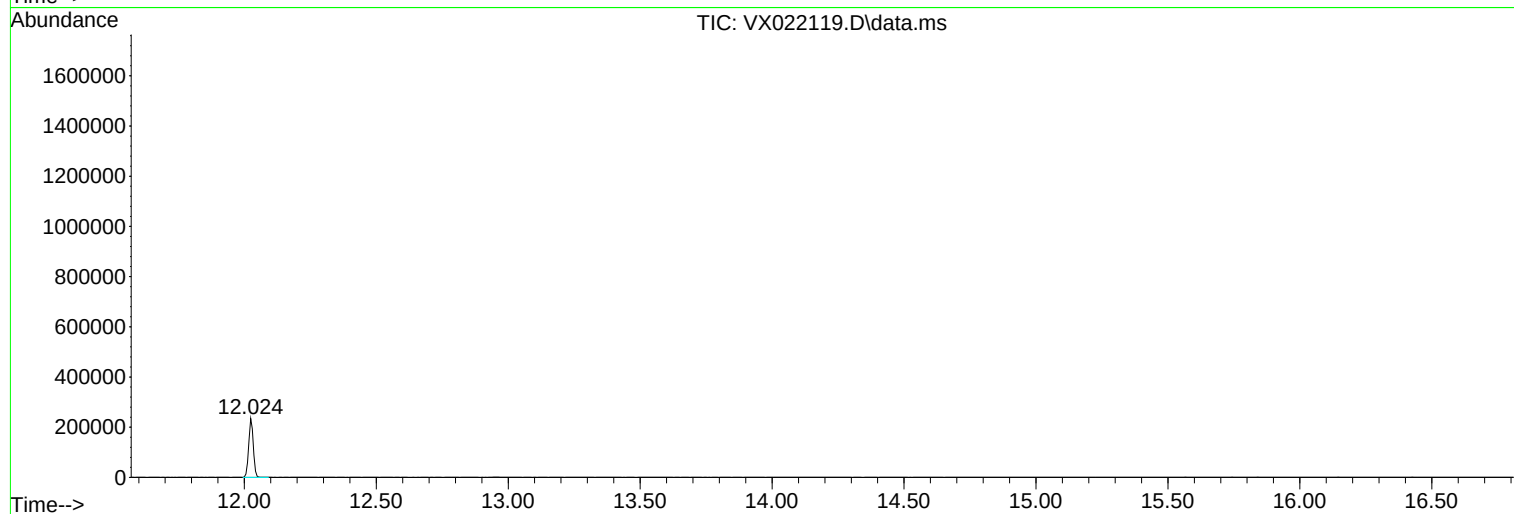
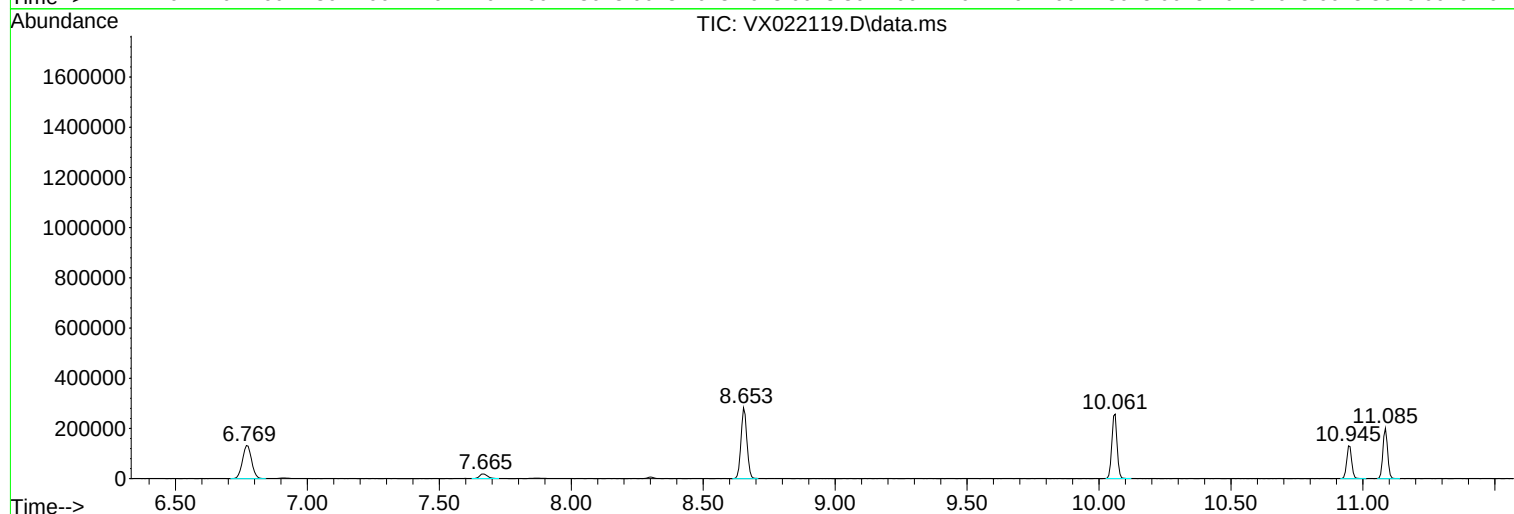
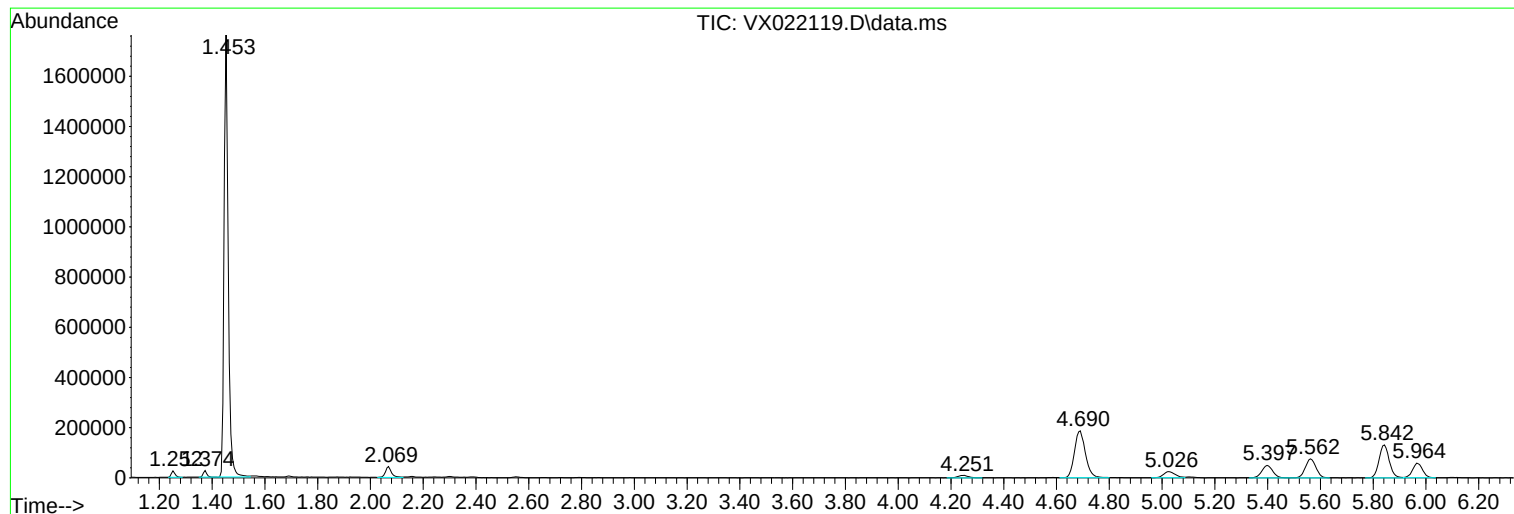
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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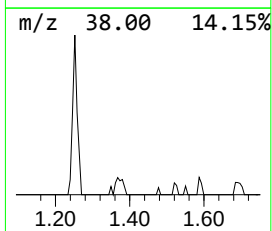
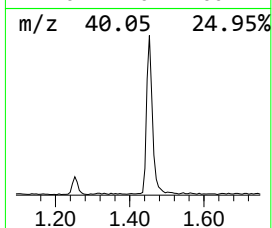
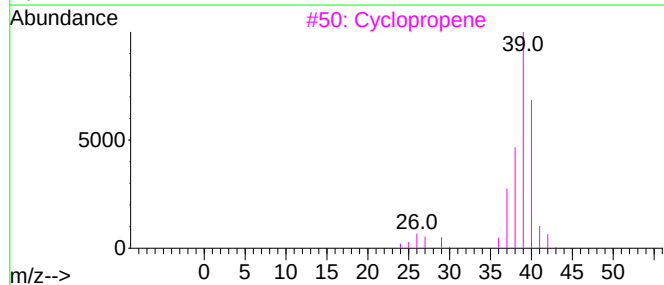
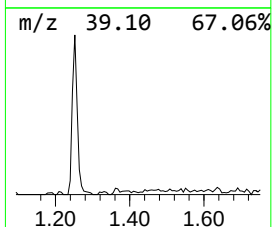
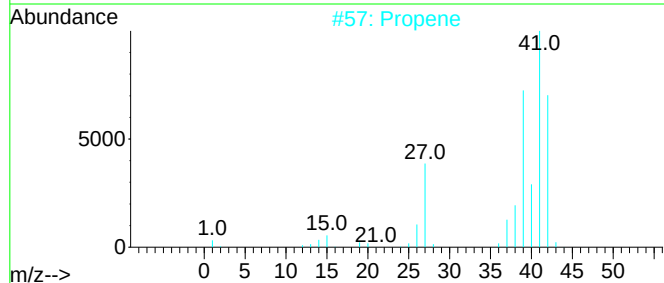
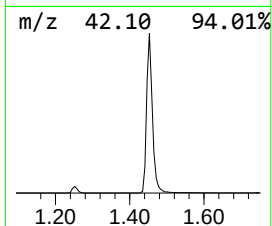
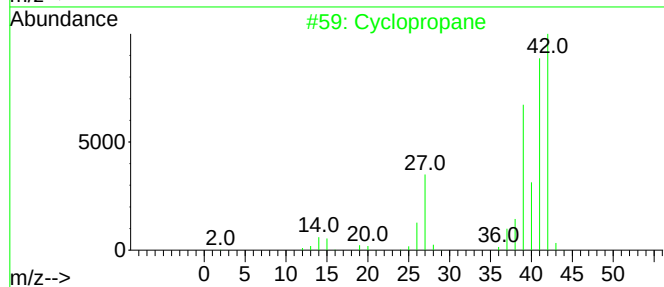
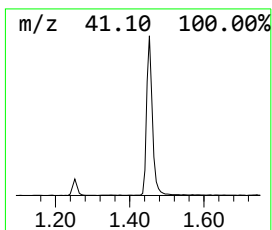
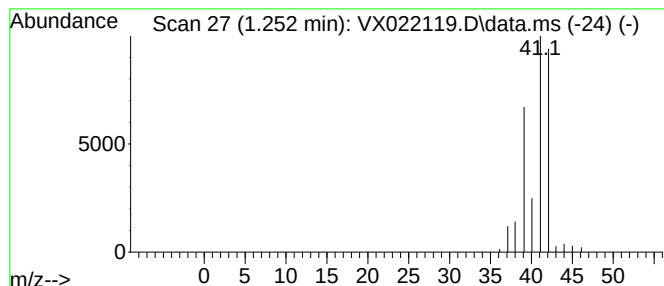
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclopropane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	6.00 ug/l	25321	Pentafluorobenzene	5.568

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane	42	C3H6	000075-19-4	90
2		Propene	42	C3H6	000115-07-1	83
3		Cyclopropene	40	C3H4	002781-85-3	10
4		2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
5		Cyanamide	42	CH2N2	000420-04-2	3



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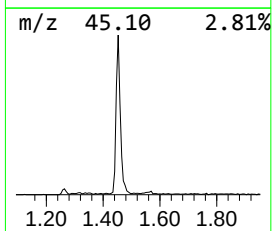
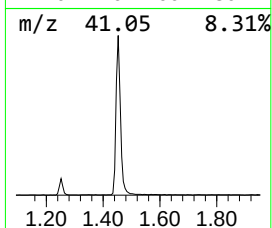
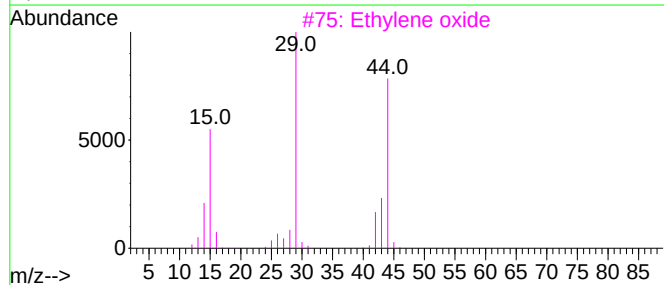
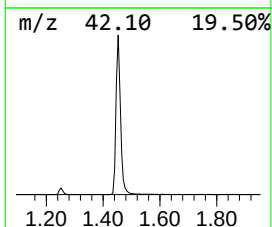
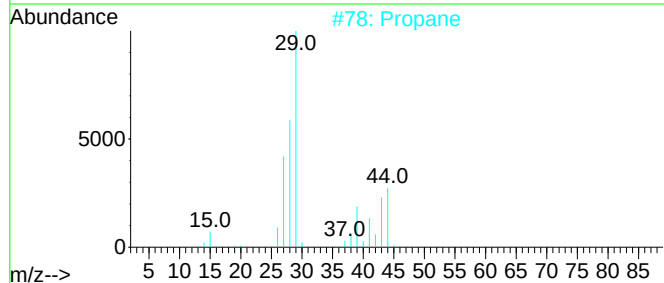
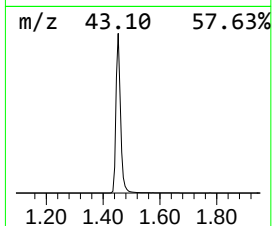
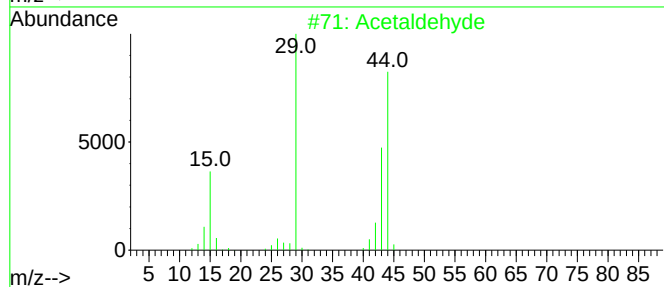
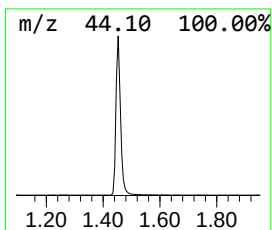
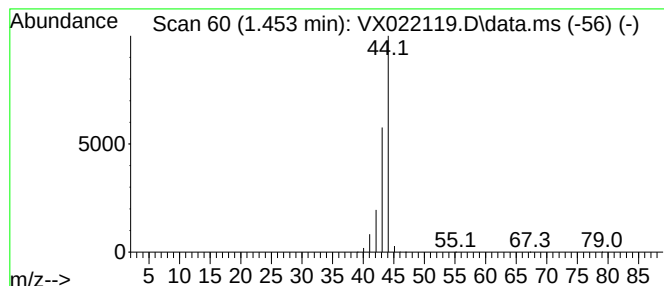
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	456.88 ug/l	1928170	Pentafluorobenzene	5.568

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			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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Instrument :
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WASTE-WATER

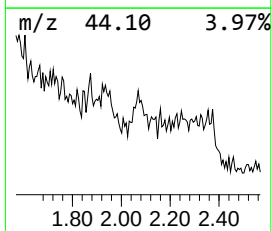
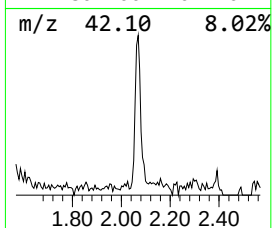
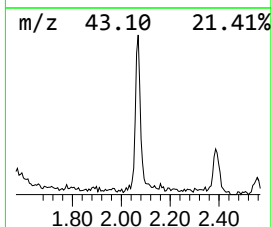
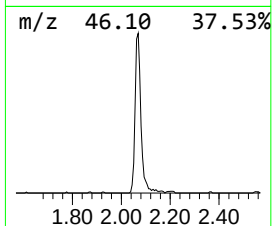
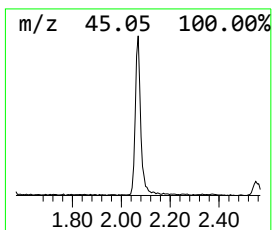
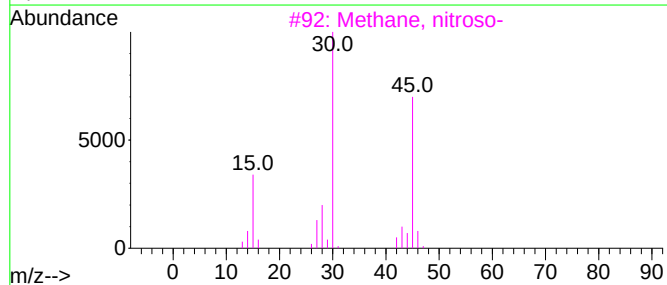
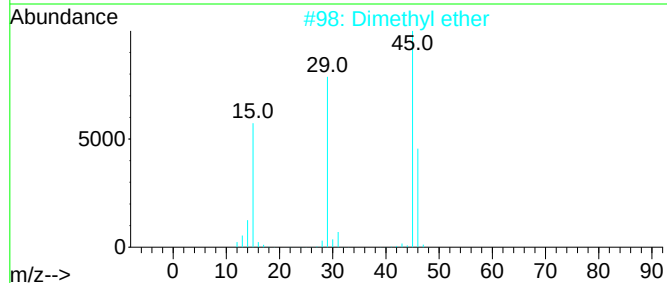
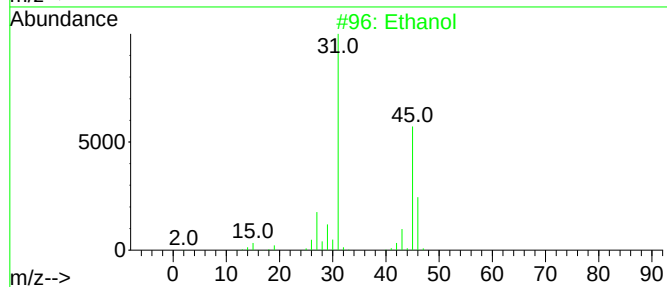
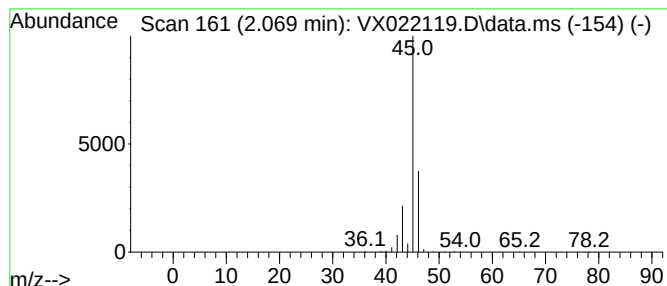
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	15.92 ug/l	67176	Pentafluorobenzene	5.568

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			Fluoroacetic acid	78	C2H3FO2	000144-49-0	2



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WASTE-WATER

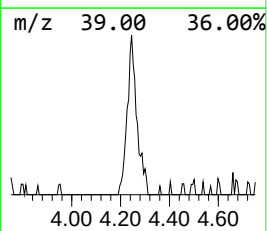
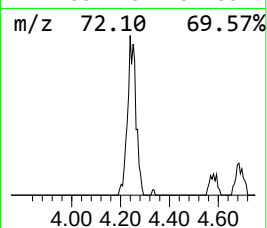
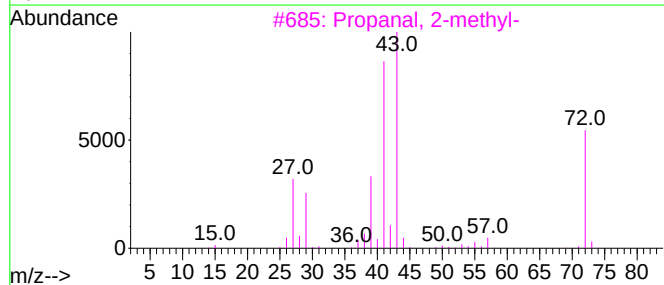
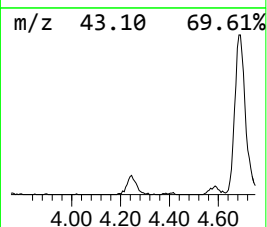
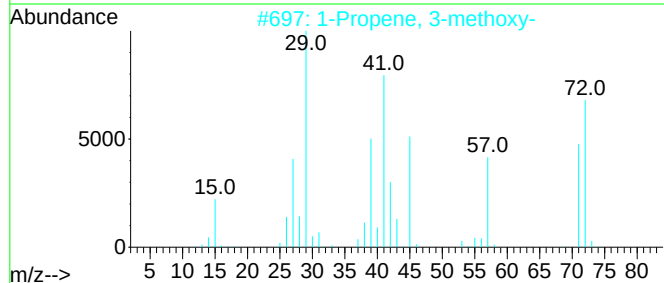
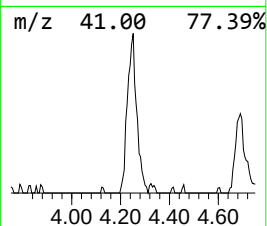
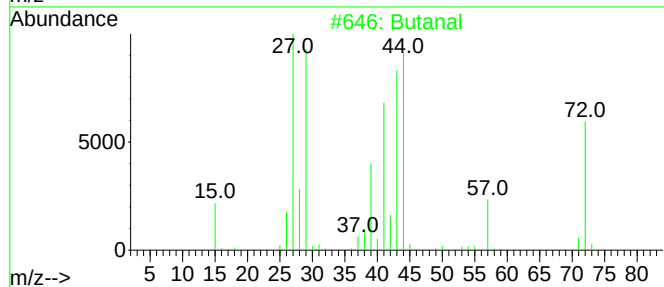
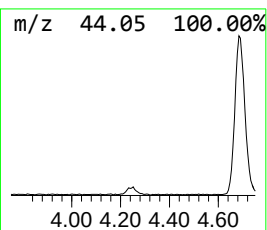
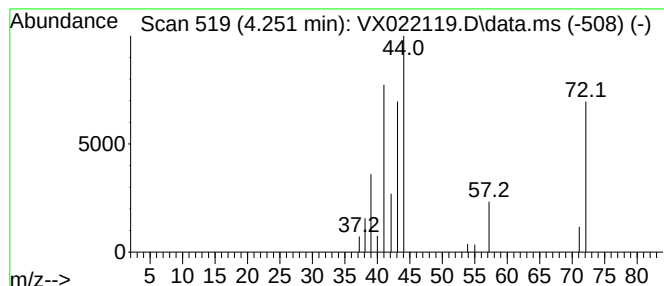
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.251	6.51 ug/l	27481	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	86
2			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	9
4			2,3-Epoxybutane	72	C4H8O	003266-23-7	9
5			Methoxyacetonitrile	71	C3H5NO	001738-36-9	9



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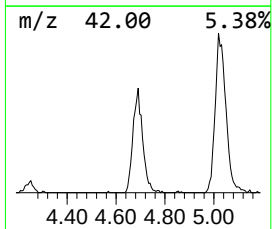
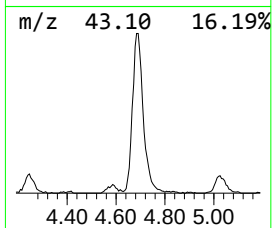
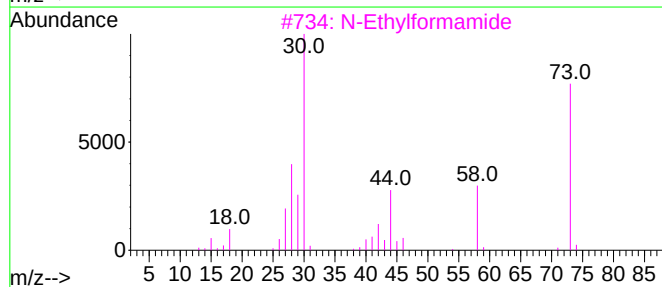
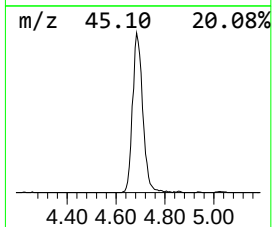
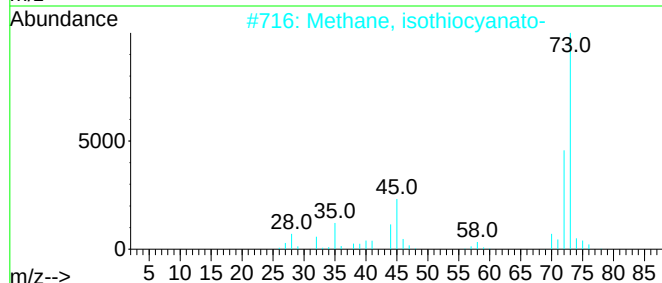
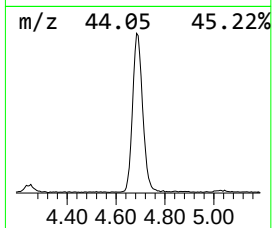
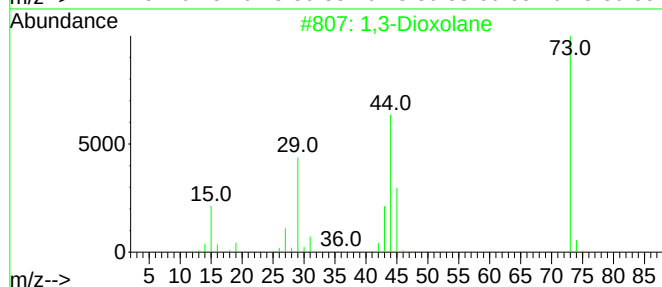
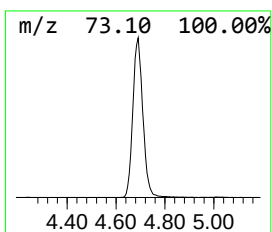
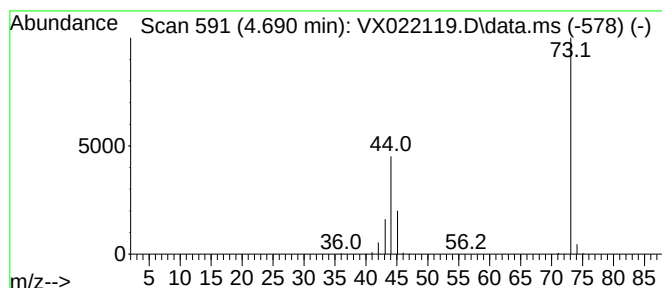
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3-Dioxolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.690	127.69 ug/l	538873	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane	74	C3H6O2	000646-06-0	86
2			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	5
3			N-Ethylformamide	73	C3H7NO	000627-45-2	5
4			Guanidine, methyl-	73	C2H7N3	000471-29-4	5
5			Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	4



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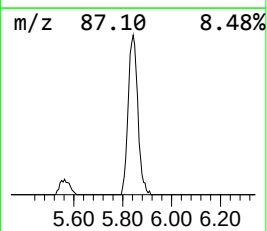
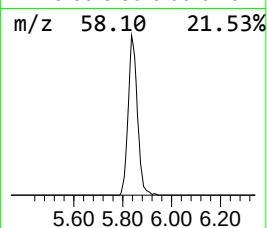
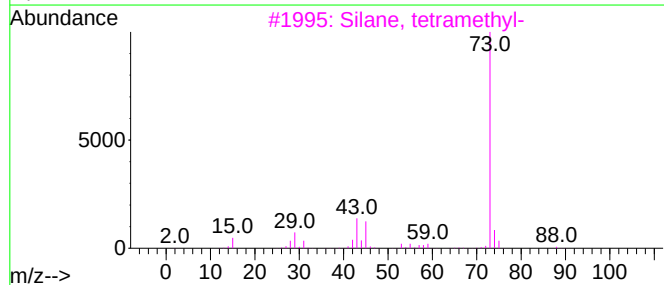
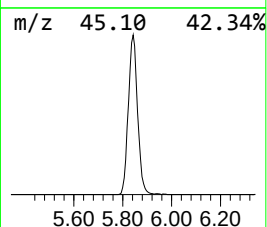
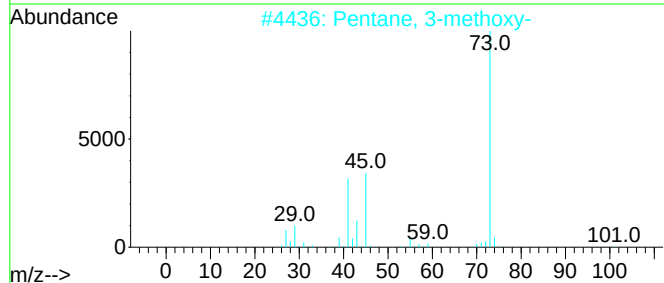
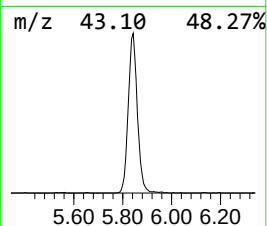
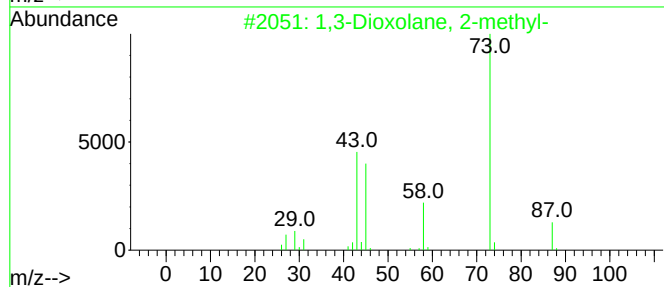
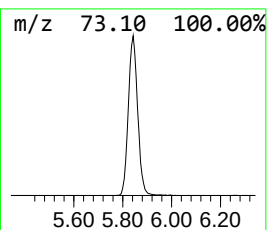
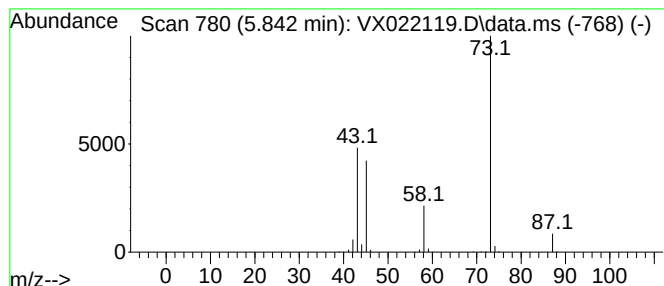
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.842	82.41 ug/l	347802	Pentafluorobenzene	5.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052121\
Data File : VX022119.D
Acq On : 21 May 2021 16:39
Operator : JC/MD
Sample : M2481-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-WATER

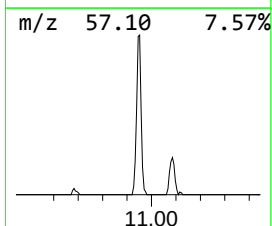
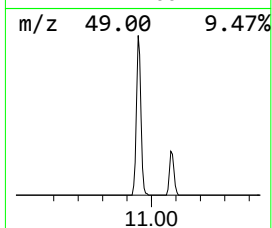
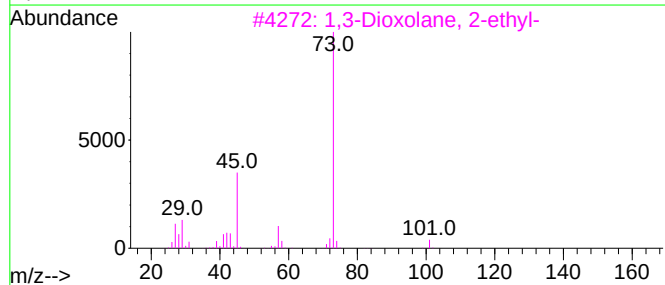
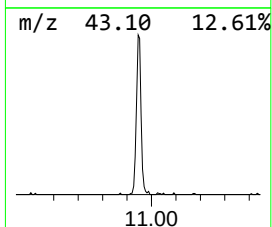
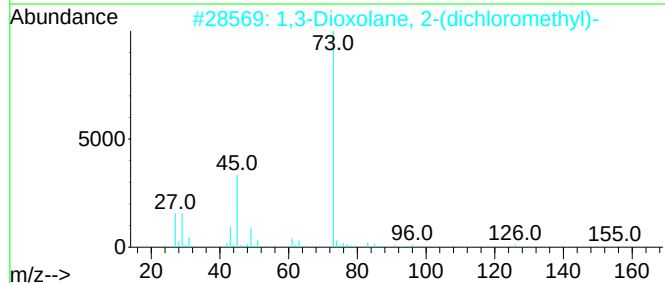
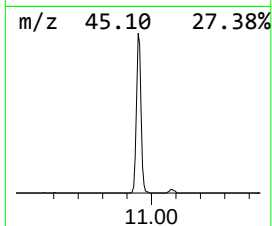
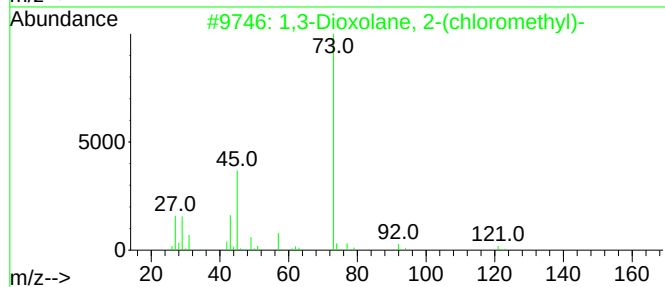
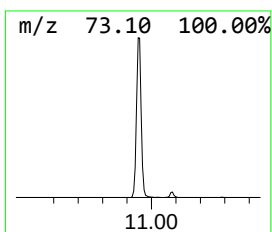
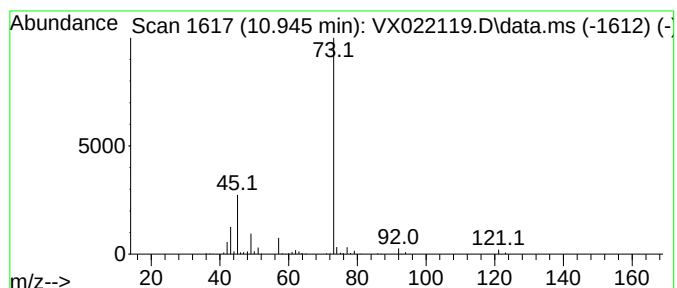
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,3-Dioxolane, 2-(chloromet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	24.27 ug/l	172228	Chlorobenzene-d5	10.061

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	72
2			1,3-Dioxolane, 2-(dichloromethyl)-	156	C4H6Cl2O2	002612-35-3	45
3			1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	33
4			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	33
5			1,3-Dioxolane, 2-(phenylmethyl)-	164	C10H12O2	000101-49-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052121\
Data File : VX022119.D
Acq On : 21 May 2021 16:39
Operator : JC/MD
Sample : M2481-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASTE-WATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopropane	1.252	6.0	ug/l	25321	1	5.568	211013	50.0
Acetaldehyde	1.453	456.9	ug/l	1928170	1	5.568	211013	50.0
Ethanol	2.069	15.9	ug/l	67176	1	5.568	211013	50.0
Butanal	4.251	6.5	ug/l	27481	1	5.568	211013	50.0
1,3-Dioxolane	4.690	127.7	ug/l	538873	1	5.568	211013	50.0
1,3-Dioxolane, ...	5.842	82.4	ug/l	347802	1	5.568	211013	50.0
1,3-Dioxolane, ...	10.945	24.3	ug/l	172228	3	10.061	354816	50.0