

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062121\
 Data File : VN067414.D
 Acq On : 21 Jun 2021 14:12
 Operator : JC/MD
 Sample : M2782-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WASTE-WATER-SAMPLE

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_N\methods\82N061421W.M

Title : SW846 8260

Signal : TIC: VN067414.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.220	74	86	109	rBV2	70966	121044	3.60%	0.629%
2	2.587	208	223	251	rBV	1867145	3360292	100.00%	17.450%
3	2.834	303	315	331	rVB	50866	106066	3.16%	0.551%
4	3.692	616	635	654	rBV2	47433	127013	3.78%	0.660%
5	7.402	1994	2018	2061	rBV	858488	2342945	69.72%	12.167%
6	7.694	2109	2127	2151	rBV2	120238	309513	9.21%	1.607%
7	8.024	2227	2250	2261	rBV	274664	649802	19.34%	3.374%
8	8.088	2262	2274	2299	rVB2	475801	1094548	32.57%	5.684%
9	8.257	2320	2337	2365	rBV	329339	757958	22.56%	3.936%
10	8.440	2387	2405	2433	rBV	353103	797609	23.74%	4.142%
11	8.971	2584	2603	2634	rBV	767971	1612713	47.99%	8.375%
12	9.574	2806	2828	2851	rBV2	78634	169159	5.03%	0.878%
13	10.443	3131	3152	3184	rBV	1187822	2291739	68.20%	11.901%
14	10.596	3188	3209	3221	rVV3	52253	156853	4.67%	0.815%
15	10.663	3222	3234	3258	rVB	175421	340646	10.14%	1.769%
16	11.749	3619	3639	3676	rBV	1081648	1995924	59.40%	10.365%
17	12.736	3990	4007	4029	rBV	805751	1440889	42.88%	7.482%
18	13.677	4340	4358	4379	rBV	932308	1582328	47.09%	8.217%

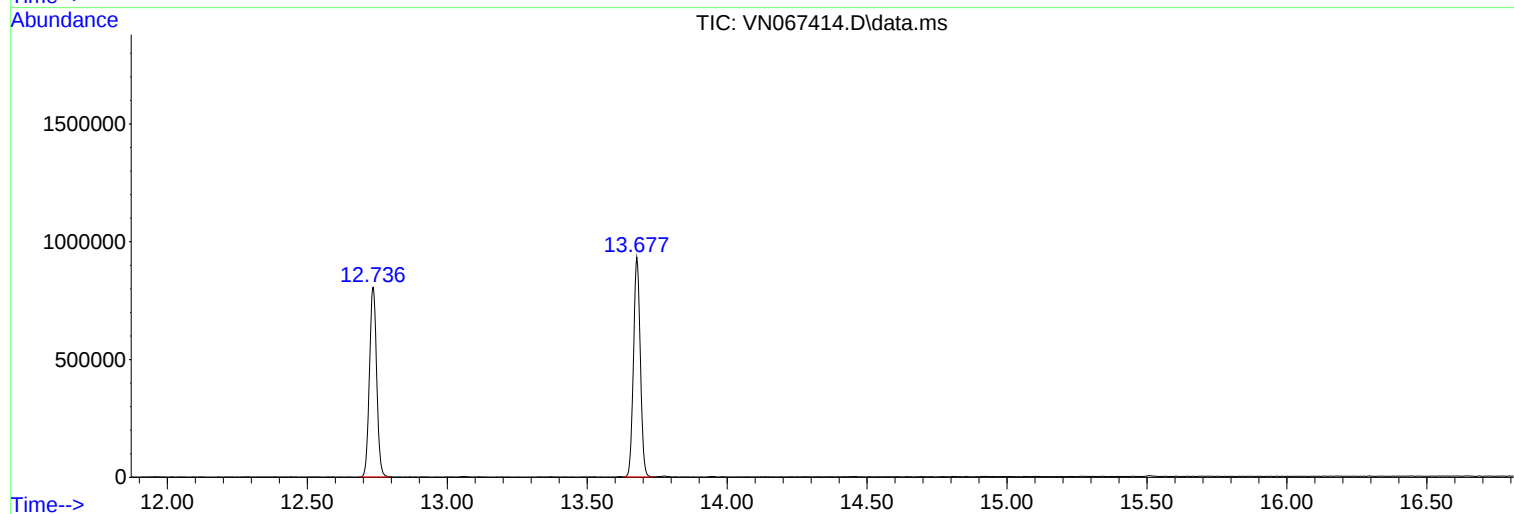
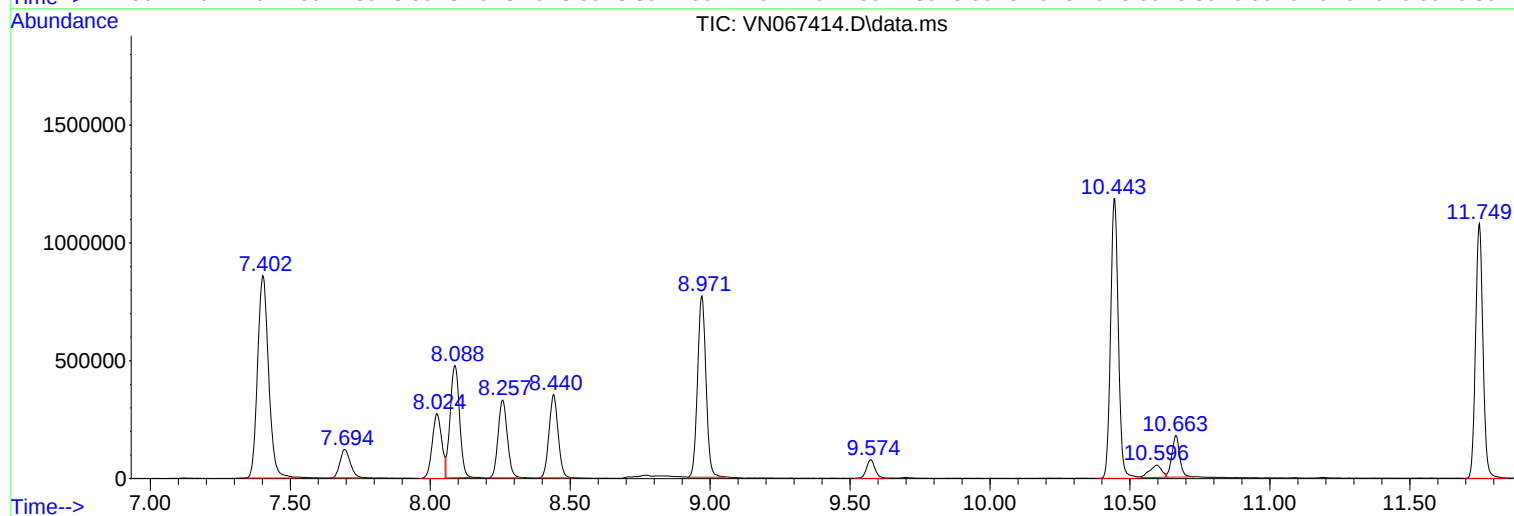
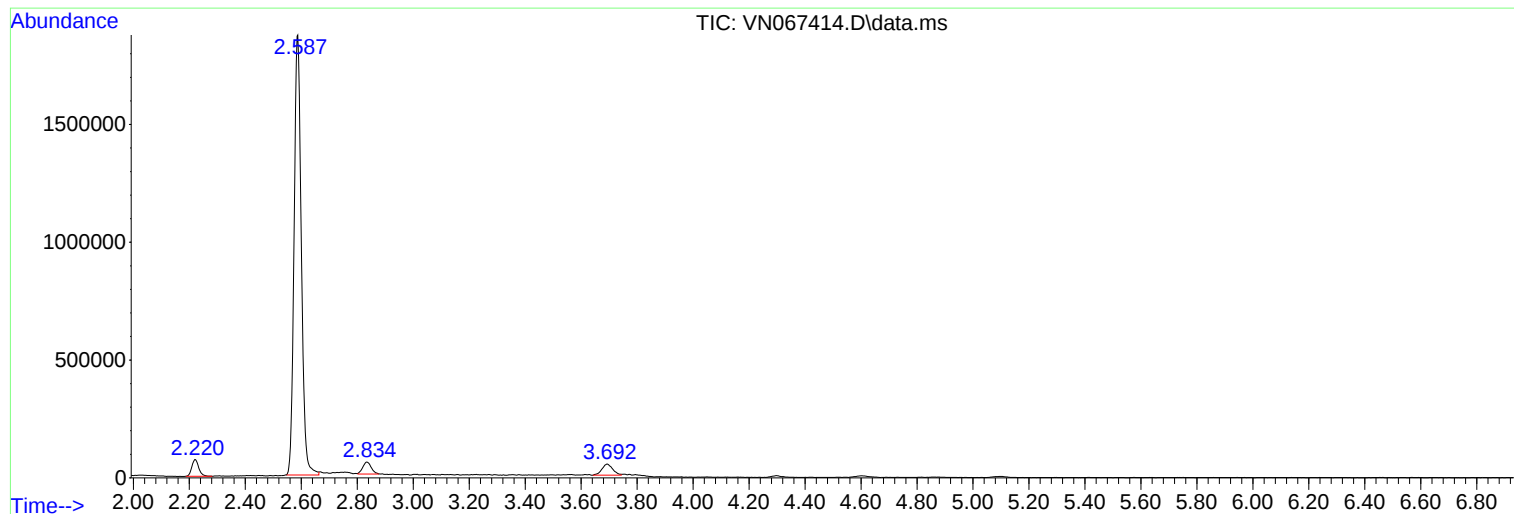
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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



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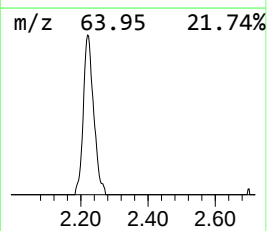
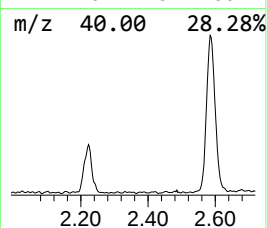
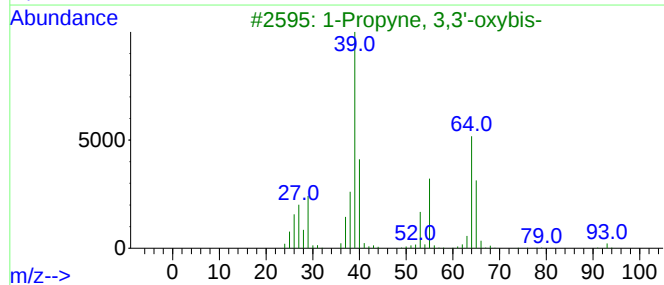
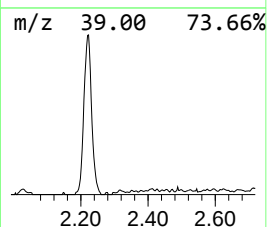
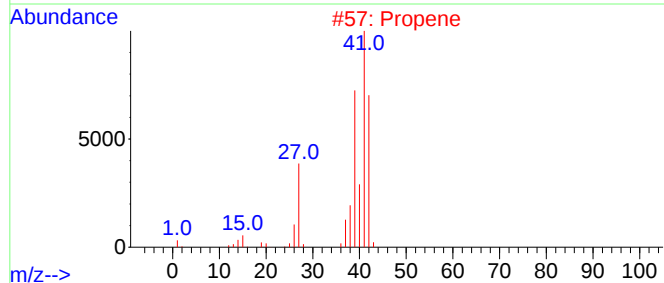
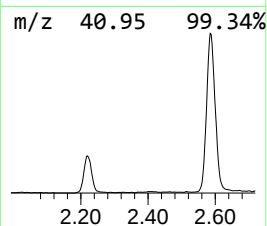
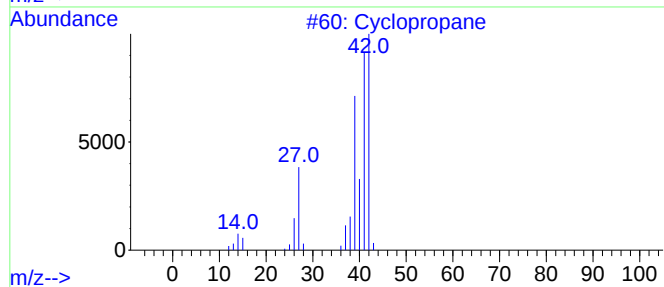
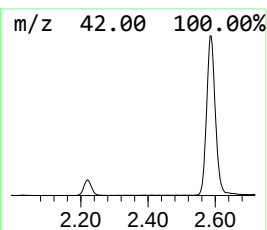
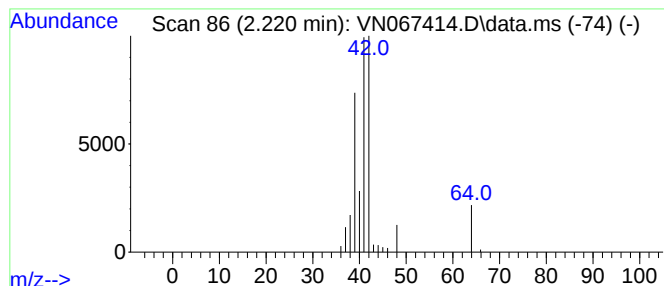
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopropane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.220	5.53 ug/l	121044	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane	42	C3H6	000075-19-4	86
2			Propene	42	C3H6	000115-07-1	78
3			1-Propyne, 3,3'-oxybis-	94	C6H6O	006921-27-3	38
4			Methylenecyclopropane	54	C4H6	006142-73-0	9
5			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	2



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WASTE-WATER-SAMPLE

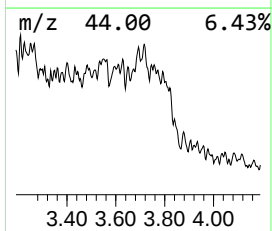
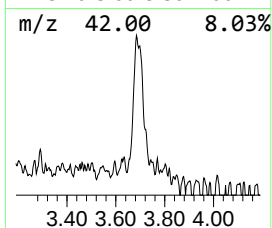
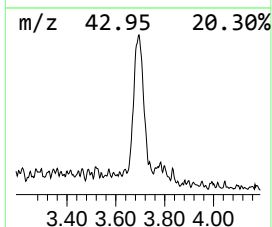
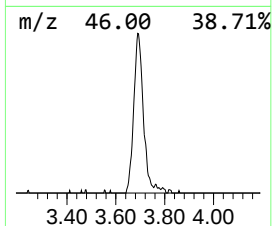
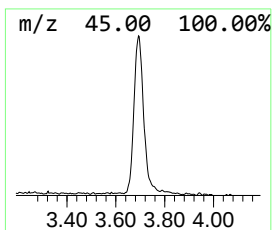
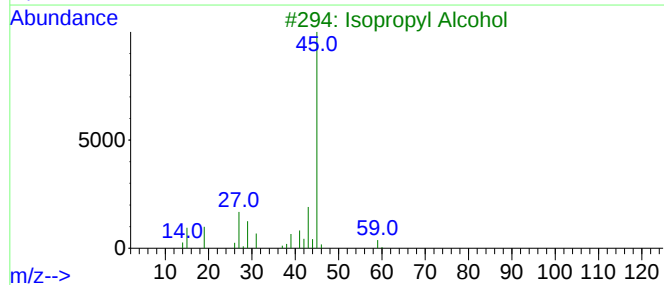
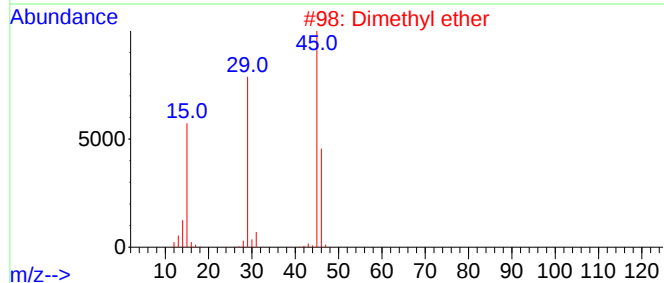
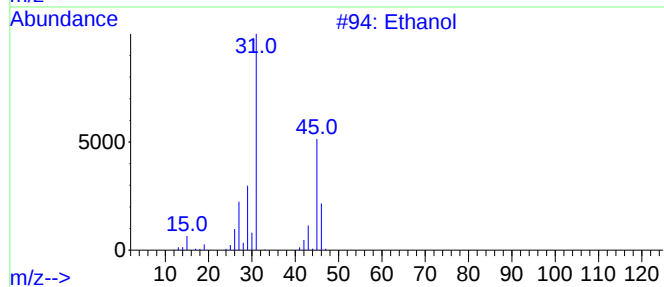
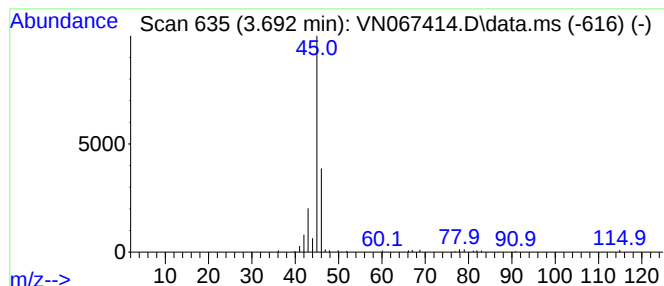
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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.
3.692	5.80 ug/l	127013	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	80
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Formic acid	46	CH2O2	000064-18-6	5
5			Methane, nitroso-	45	CH3NO	000865-40-7	4



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Instrument :
MSVOA_N
ClientSampleId :
WASTE-WATER-SAMPLE

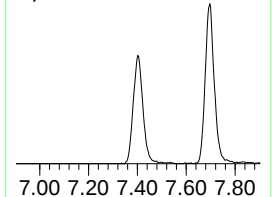
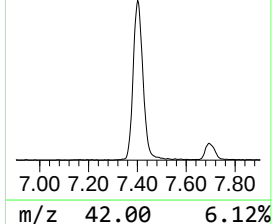
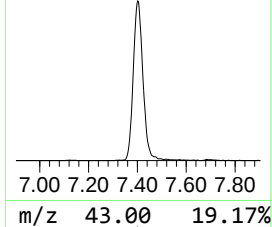
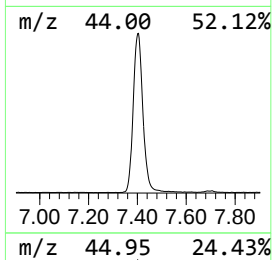
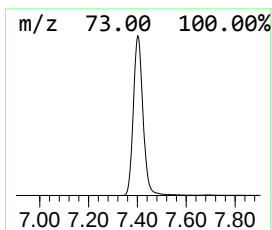
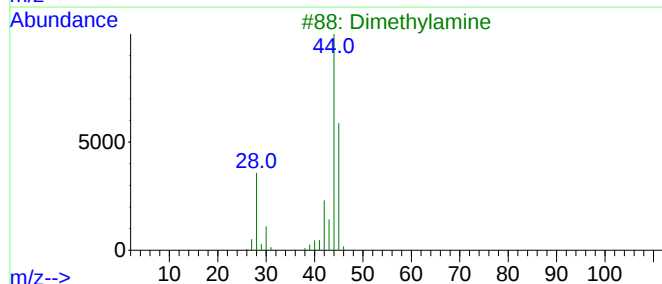
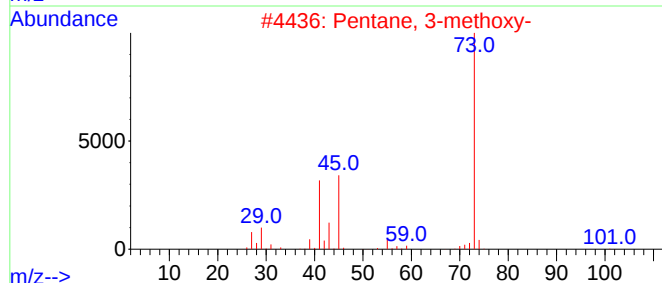
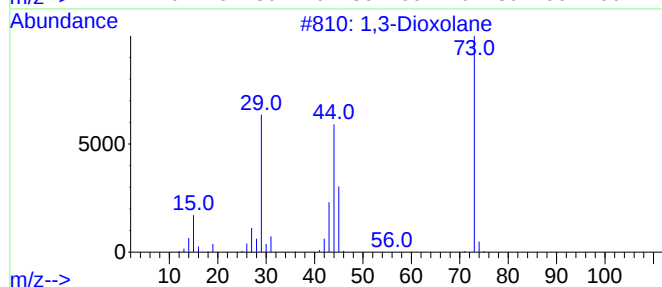
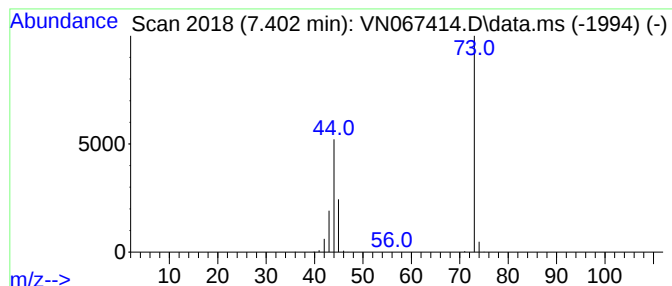
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Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.402	107.03 ug/l	2342950	Pentafluorobenzene	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane	74	C3H6O2	000646-06-0	90
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3		Dimethylamine	45	C2H7N	000124-40-3	5
4		1,2-Ethanediamine, N-methyl-	74	C3H10N2	000109-81-9	5
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WASTE-WATER-SAMPLE

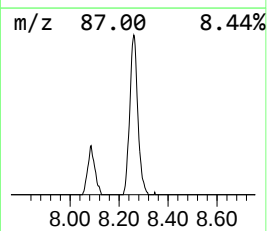
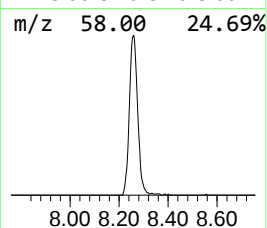
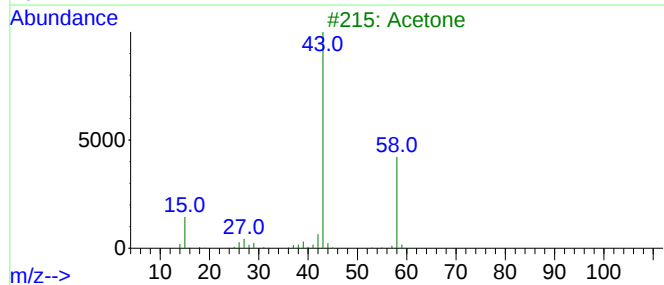
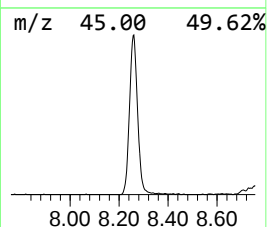
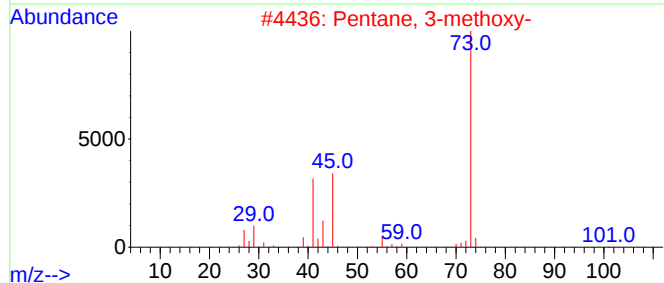
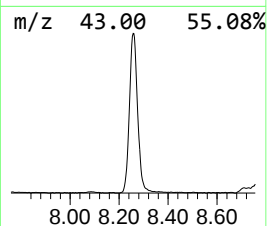
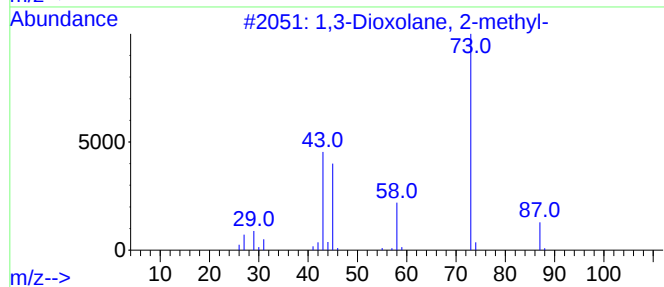
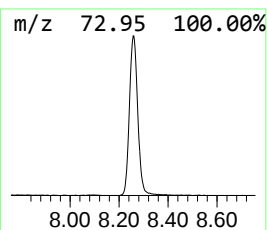
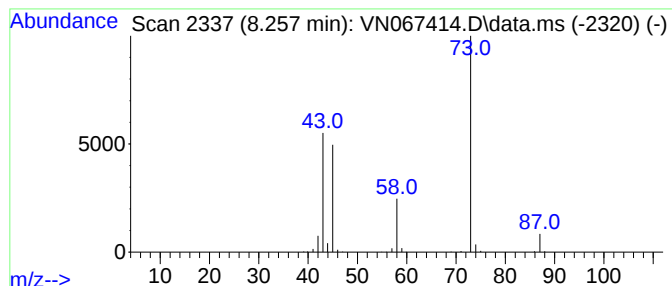
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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

Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.257	34.62 ug/l	757958	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	90
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
3			Acetone	58	C3H6O	000067-64-1	9
4			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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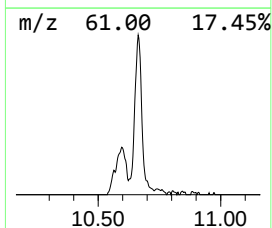
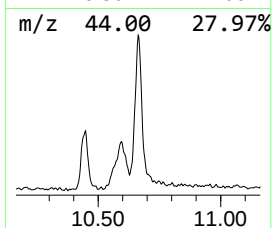
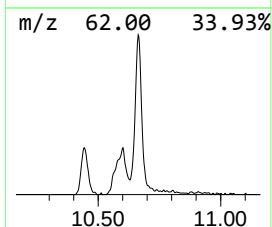
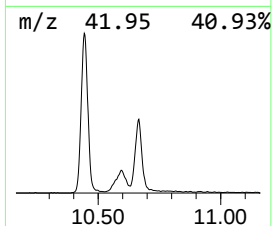
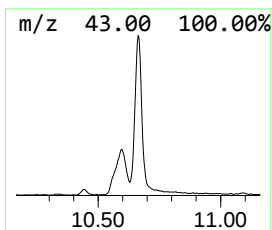
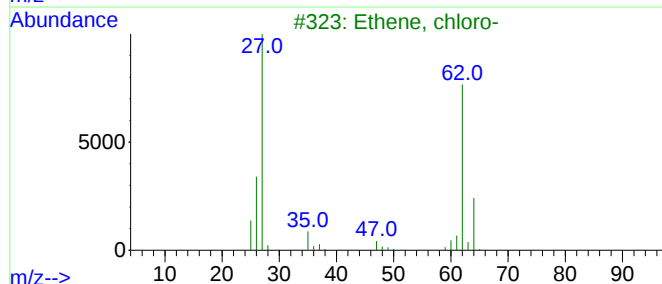
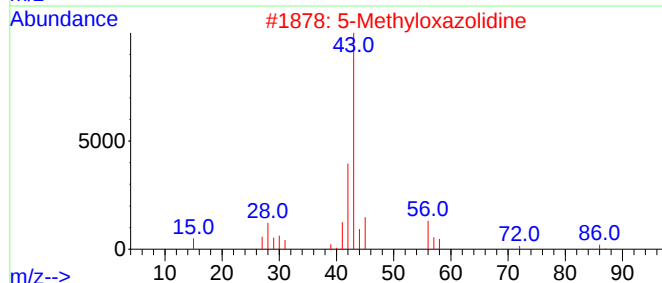
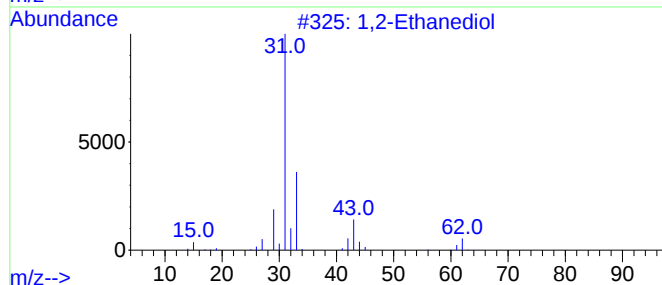
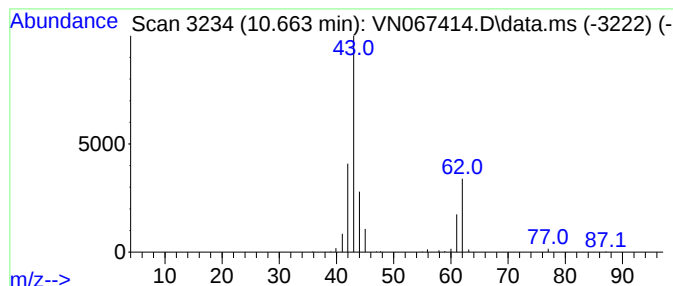
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Quant Title : SW846 8260

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

Peak Number 6 unknown10.663 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.663	8.53 ug/l	340646	Chlorobenzene-d5	11.749

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Ethanediol	62	C2H6O2	000107-21-1	42
2			5-Methyloxazolidine	87	C4H9NO	058328-22-6	9
3			Ethene, chloro-	62	C2H3Cl	000075-01-4	7
4			Ethanethiol	62	C2H6S	000075-08-1	5
5			Acetic acid, anhydride with form...	88	C3H4O3	002258-42-6	4



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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	2.220	5.5	ug/l	121044	1	8.088	1094550	50.0
Ethanol	3.692	5.8	ug/l	127013	1	8.088	1094550	50.0
1,3-Dioxolane	7.402	107.0	ug/l	2342950	1	8.088	1094550	50.0
1,3-Dioxolane, ...	8.257	34.6	ug/l	757958	1	8.088	1094550	50.0
unknown10.663	10.663	8.5	ug/l	340646	3	11.749	1995920	50.0