

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061719\
 Data File : VN056335.D
 Acq On : 17 Jun 2019 13:11
 Operator : JC/SP
 Sample : K3373-01 10X
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 13857-13964-13981

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.310	154	167	202	rBV	2401895	4109139	34.85%	12.498%
2	3.288	453	471	499	rBV	215859	608324	5.16%	1.850%
3	3.693	576	597	631	rBV	4515872	11789806	100.00%	35.858%
4	4.278	762	779	821	rVB3	51965	224089	1.90%	0.682%
5	6.059	1311	1333	1377	rBV2	211034	702601	5.96%	2.137%
6	7.590	1791	1809	1820	rBV	229113	567336	4.81%	1.726%
7	7.664	1820	1832	1864	rVB2	376538	917276	7.78%	2.790%
8	8.027	1925	1945	1975	rBV	239410	561658	4.76%	1.708%
9	8.587	2104	2119	2150	rVB	686418	1506815	12.78%	4.583%
10	8.844	2177	2199	2213	rBV3	73479	162577	1.38%	0.494%
11	9.876	2507	2520	2540	rBV	120532	225486	1.91%	0.686%
12	10.088	2569	2586	2619	rBV	967874	1857669	15.76%	5.650%
13	10.349	2649	2667	2692	rBV	479584	837630	7.10%	2.548%
14	10.493	2698	2712	2745	rVB	317824	558090	4.73%	1.697%
15	11.406	2979	2996	3024	rBV	908842	1660948	14.09%	5.052%
16	11.541	3025	3038	3070	rVB	704959	1196094	10.15%	3.638%
17	12.365	3276	3294	3302	rBV	2666063	4375358	37.11%	13.307%
18	13.342	3585	3598	3616	rVB	599540	1018371	8.64%	3.097%

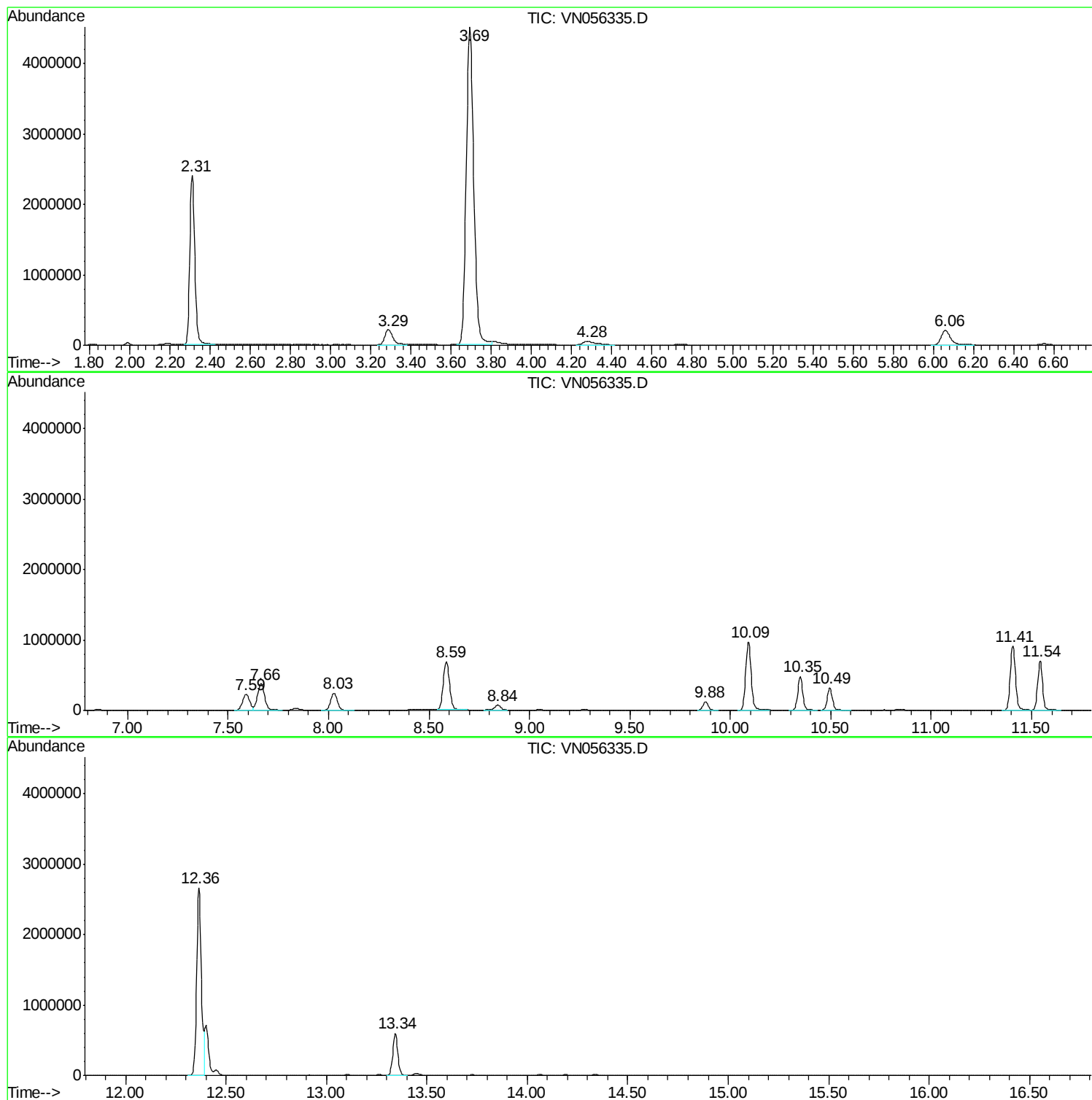
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Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M
Quant Title : SW846 8260

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



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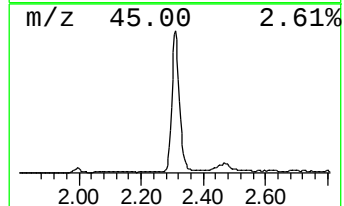
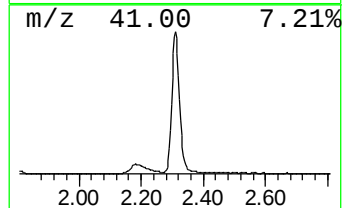
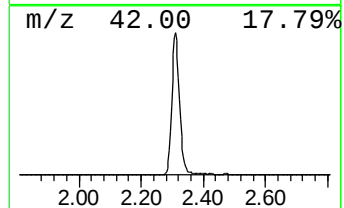
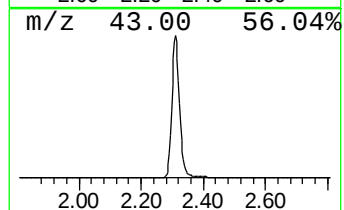
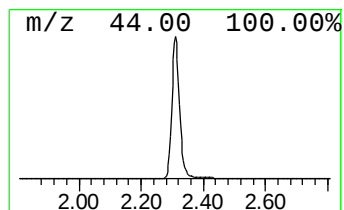
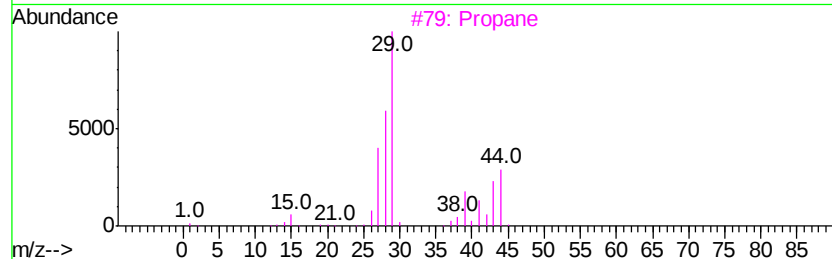
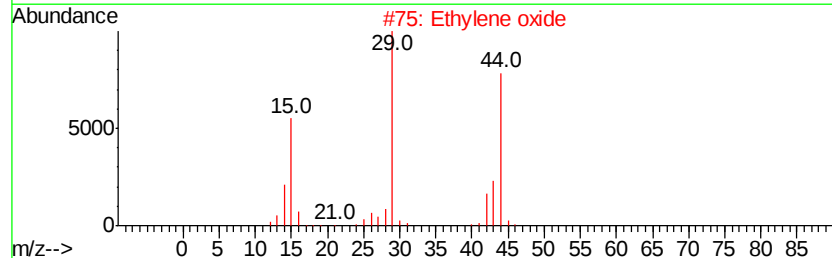
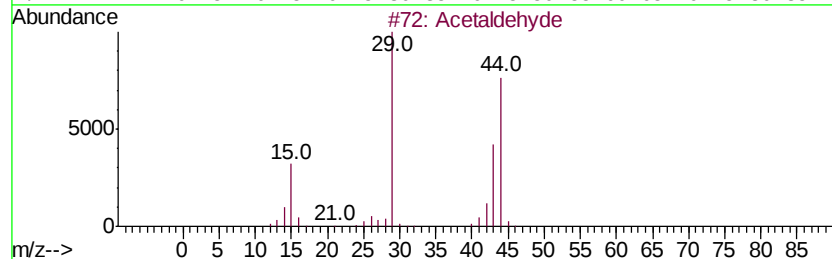
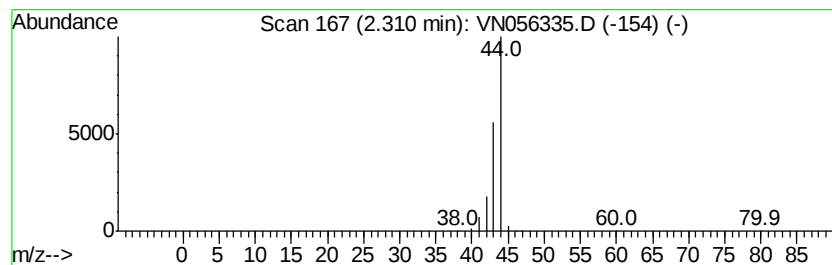
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	223.99 ug/l	4109140	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehydve	44	C2H4O	000075-07-0	64
2		Ethylene oxide	44	C2H4O	000075-21-8	5
3		Propane	44	C3H8	000074-98-6	4
4		1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5		Alanine	89	C3H7NO2	000056-41-7	4



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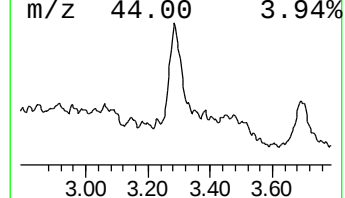
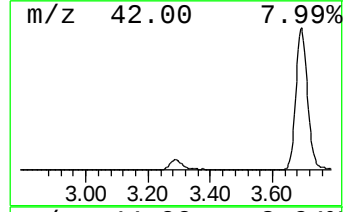
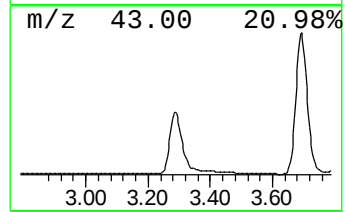
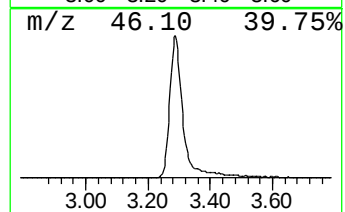
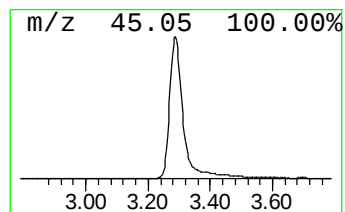
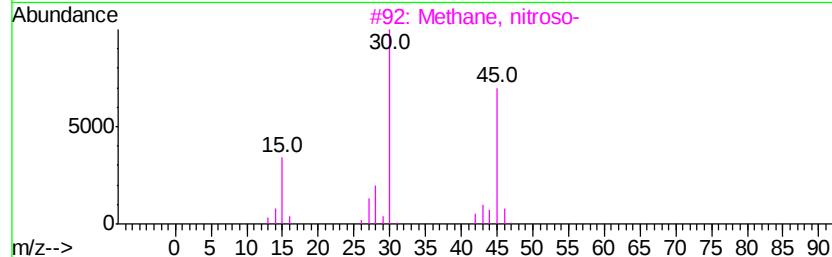
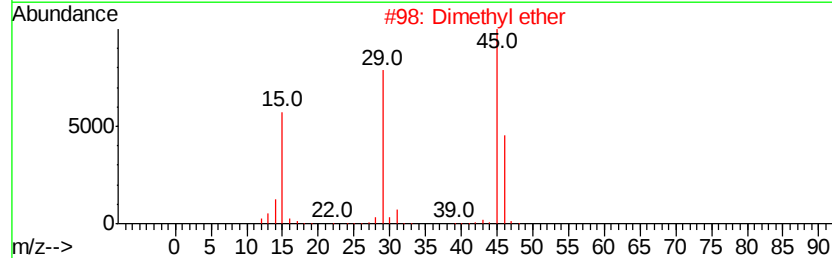
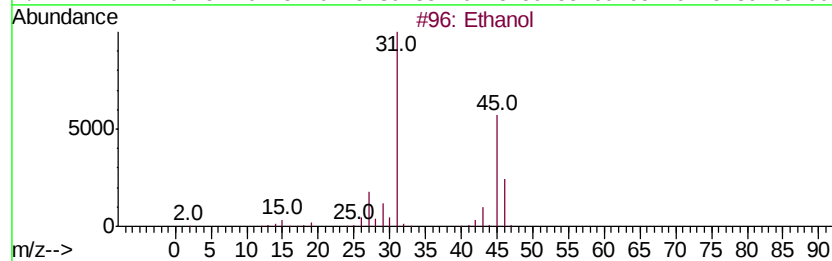
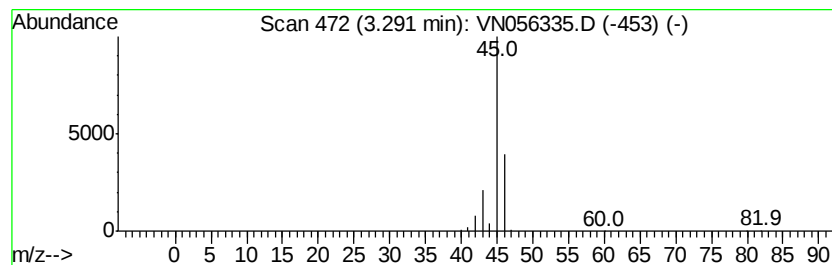
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	33.16 ug/l	608324	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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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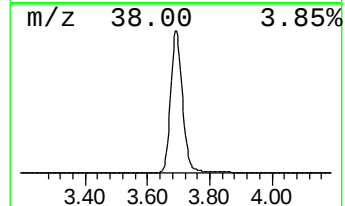
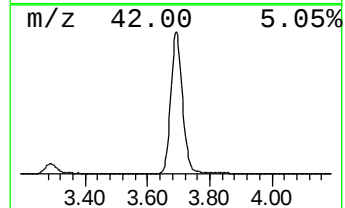
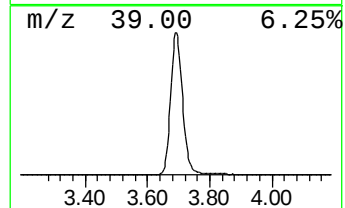
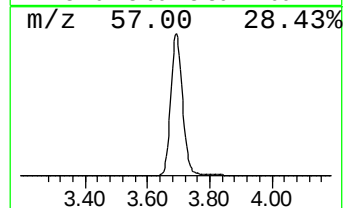
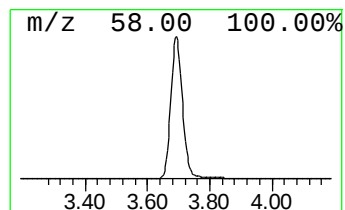
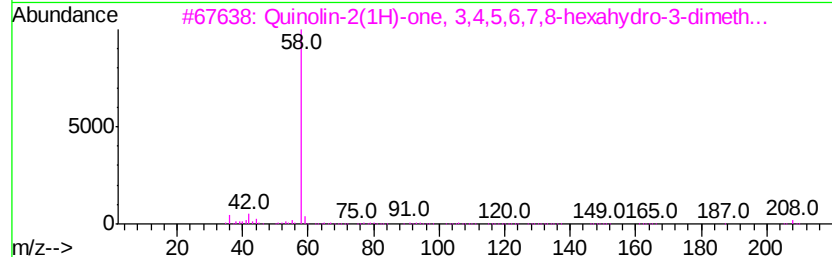
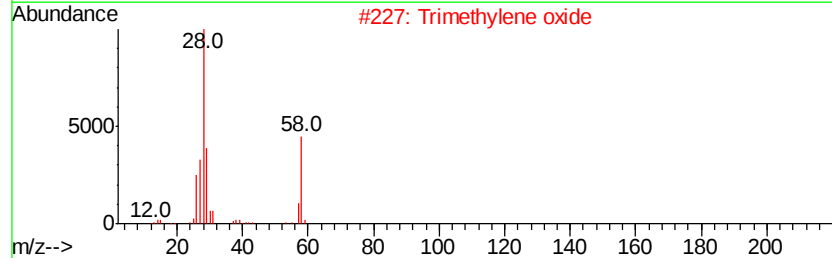
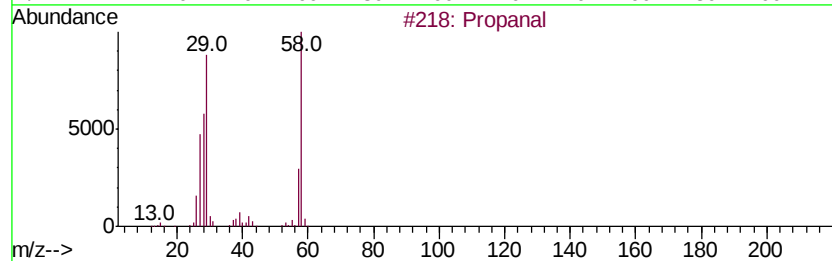
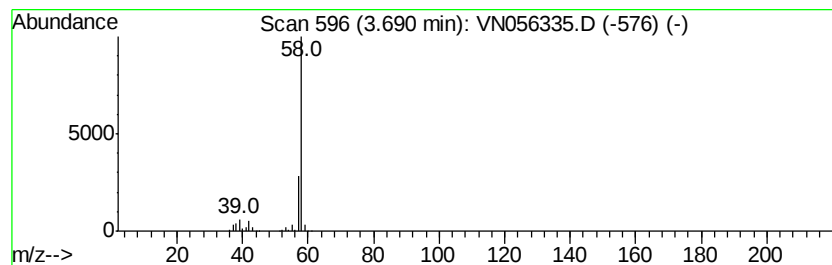
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Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
3.69	642.65 ug/l	11789800	Pentafluorobenzene	7.66		
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	Propylene oxide		58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-		58	C3H6O	016088-62-3	4



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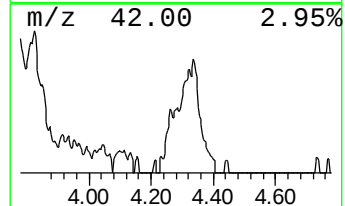
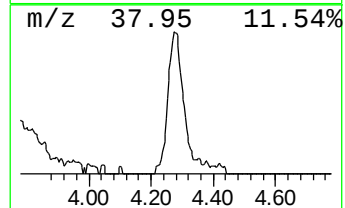
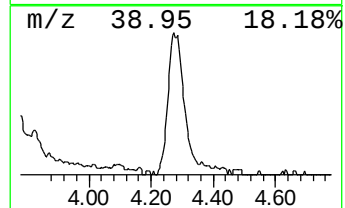
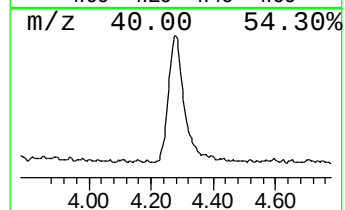
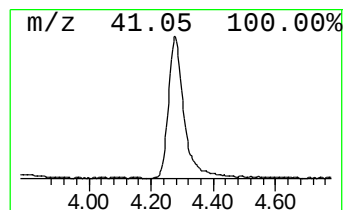
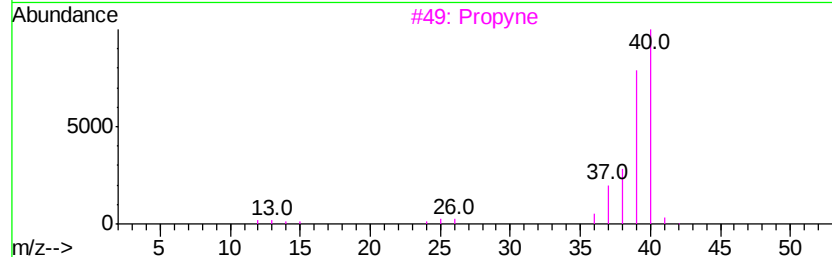
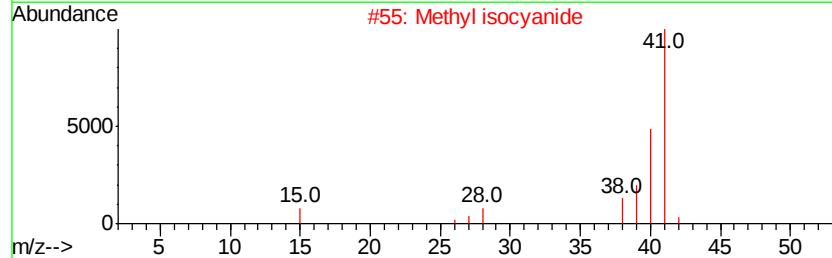
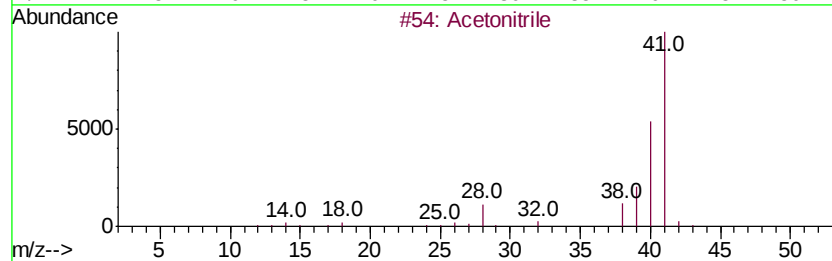
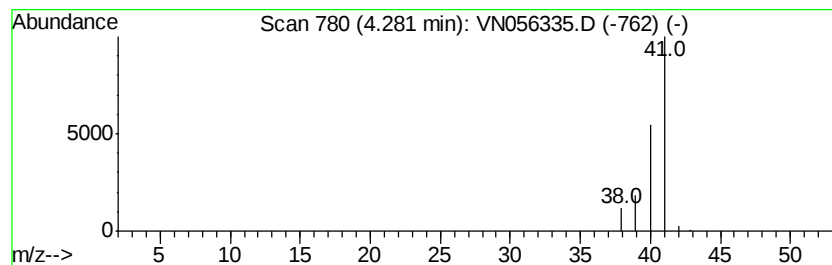
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Acetonitrile Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	12.21 ug/l	224089	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetonitrile	41	C2H3N	000075-05-8	74
2		Methyl isocyanide	41	C2H3N	000593-75-9	64
3		Propyne	40	C3H4	000074-99-7	4
4		Allene	40	C3H4	000463-49-0	1
5		Borane, trimethyl-	56	C3H9B	000593-90-8	1



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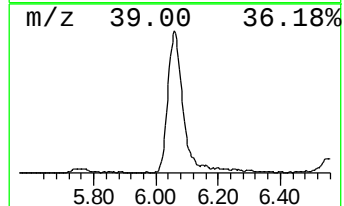
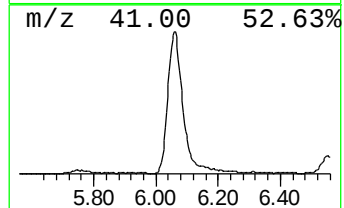
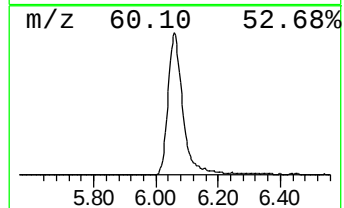
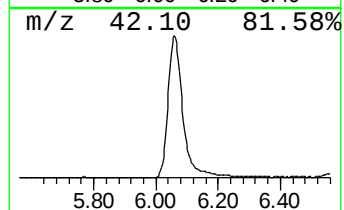
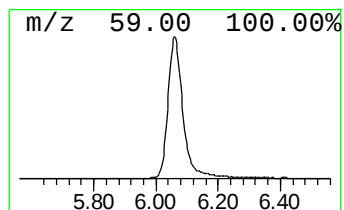
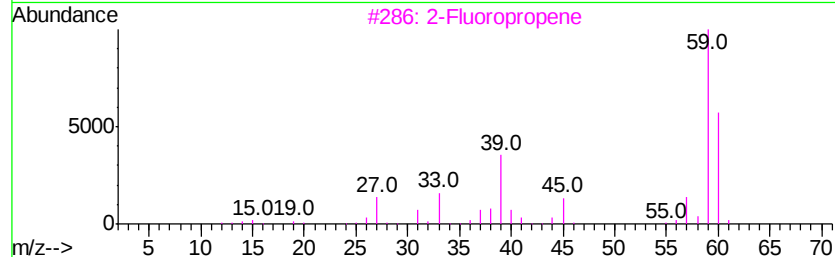
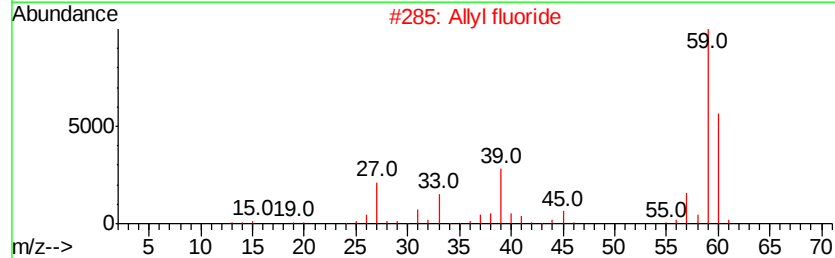
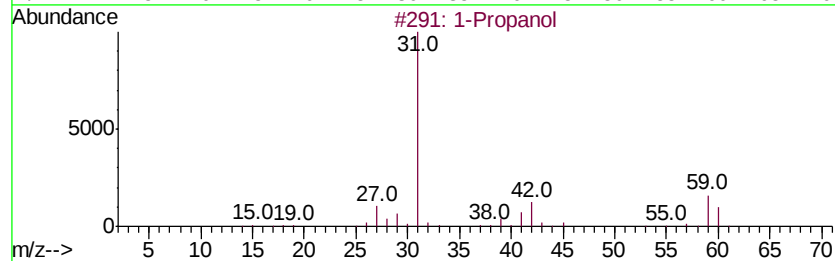
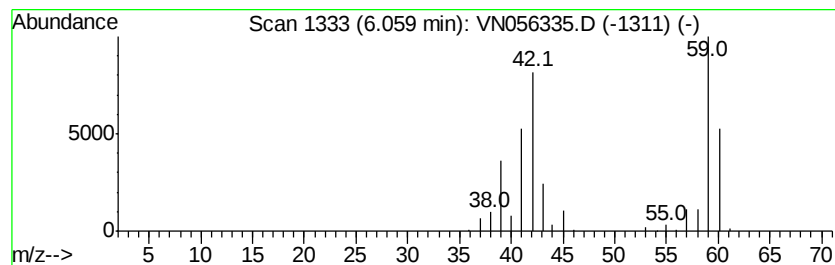
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Quant Title : SW846 8260

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

Peak Number 5 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	38.30 ug/l	702601	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	72
2		Allyl fluoride	60	C3H5F	000818-92-8	47
3		2-Fluoropropene	60	C3H5F	001184-60-7	43
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	23
5		Cyclopropane	42	C3H6	000075-19-4	12



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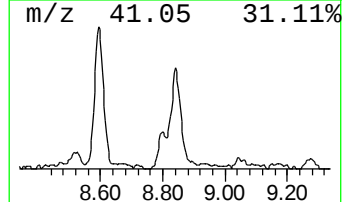
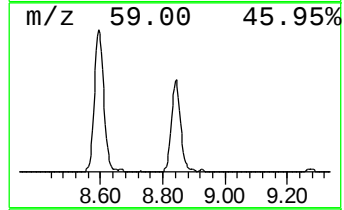
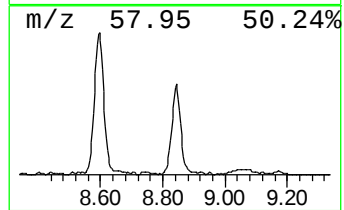
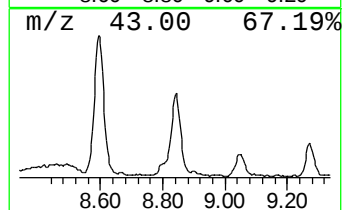
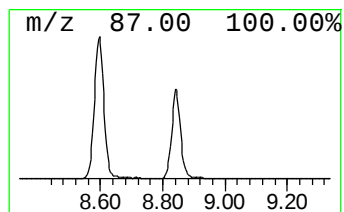
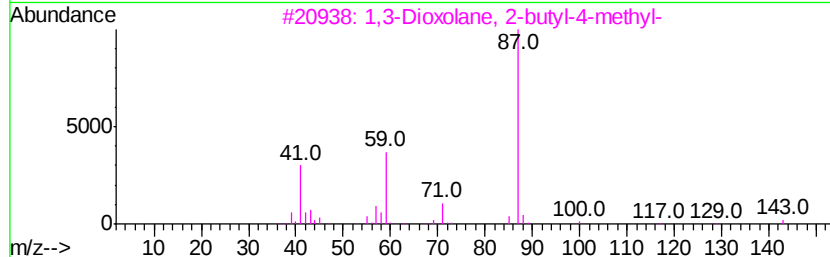
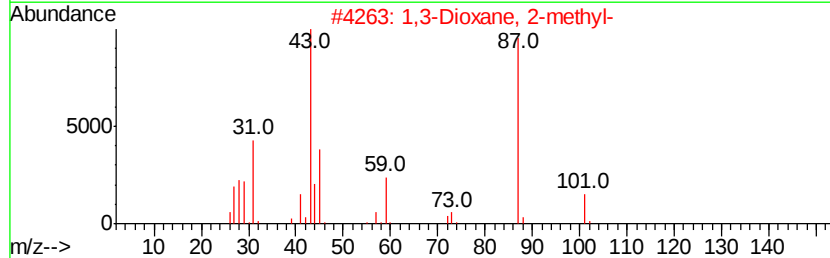
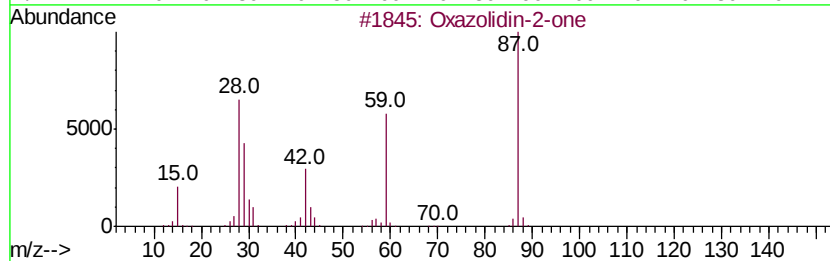
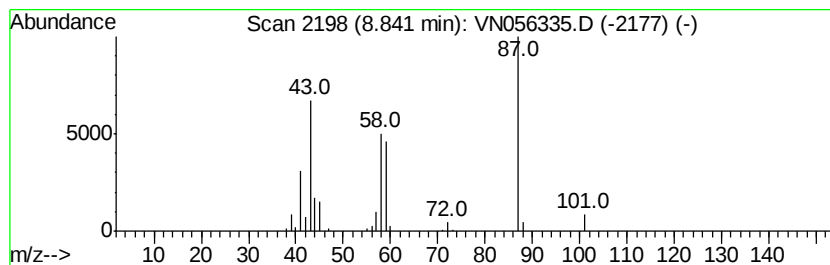
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ClientSampleId :
13857-13964-13981

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M
Quant Title : SW846 8260

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

Peak Number 6 Oxazolidin-2-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	5.39 ug/l	162577	1,4-Difluorobenzene	8.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxazolidin-2-one	87 C3H5NO2	000497-25-6 50
2		1,3-Dioxane, 2-methyl-	102 C5H10O2	000626-68-6 40
3		1,3-Dioxolane, 2-butyl-4-methyl-	144 C8H16O2	074094-60-3 36
4		N,N-Dimethylacetamide	87 C4H9NO	000127-19-5 35
5		Oxirane, (propoxymethyl)-	116 C6H12O2	003126-95-2 32



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN061719\
Data File : VN056335.D
Acq On : 17 Jun 2019 13:11
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 11 Sample Multiplier: 1

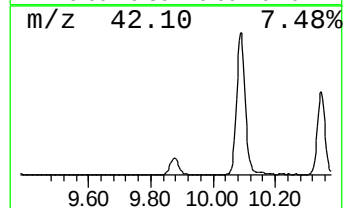
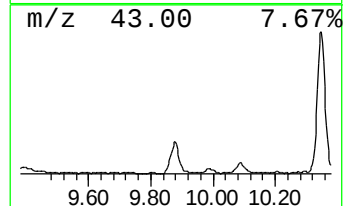
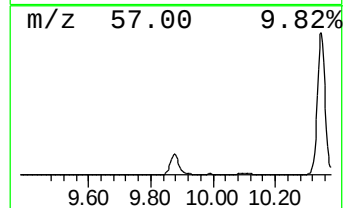
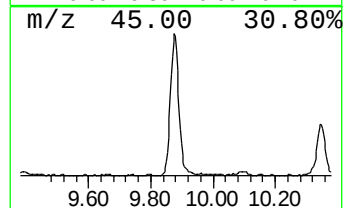
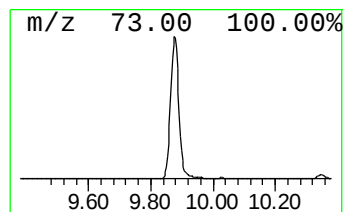
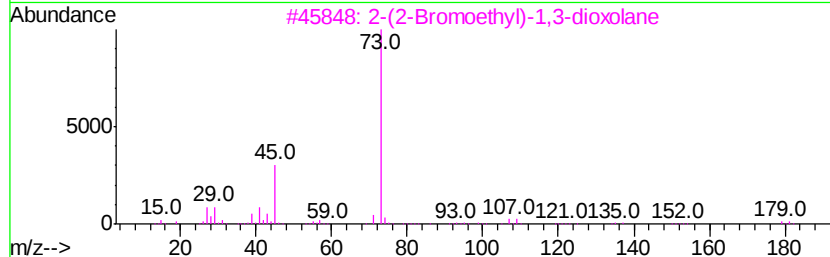
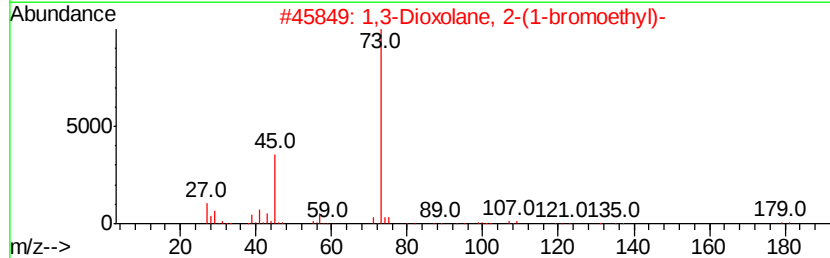
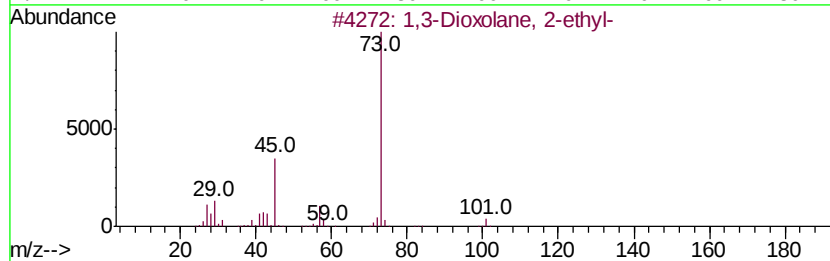
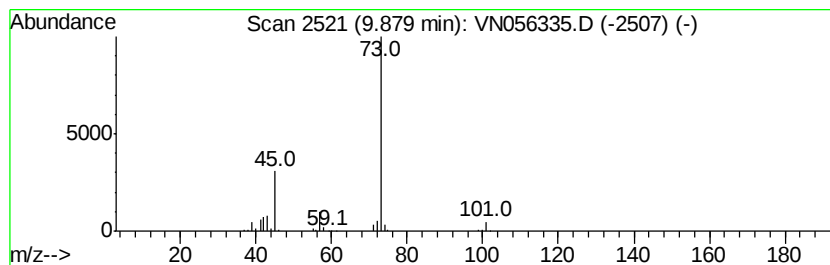
Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M
Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.88	7.48 ug/l	225486	1,4-Difluorobenzene	8.58	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	64
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	59
3	2-(2-Bromoethyl)-1,3-dioxolane	180	C5H9BrO2	018742-02-4	40
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	40
5	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061719\
Data File : VN056335.D
Acq On : 17 Jun 2019 13:11
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 11 Sample Multiplier: 1

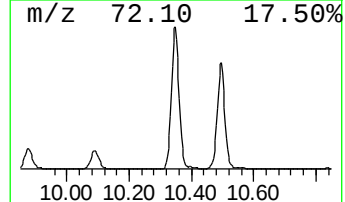
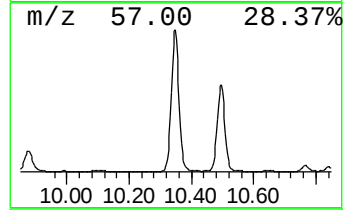
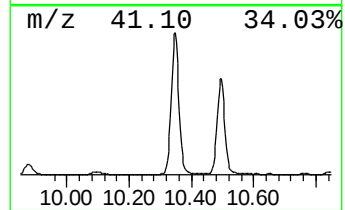
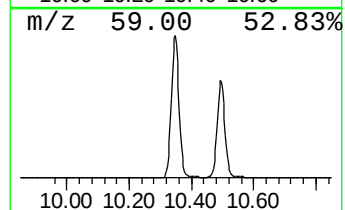
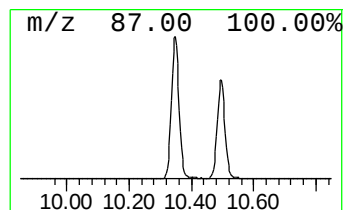
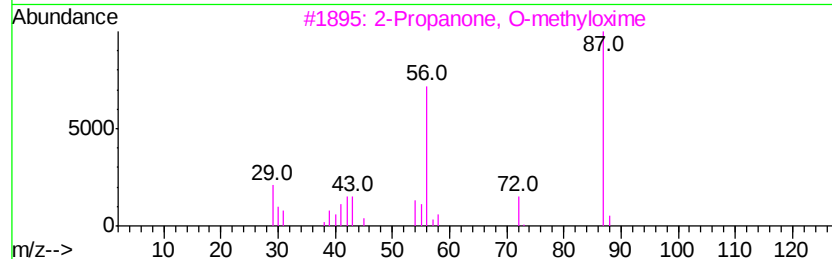
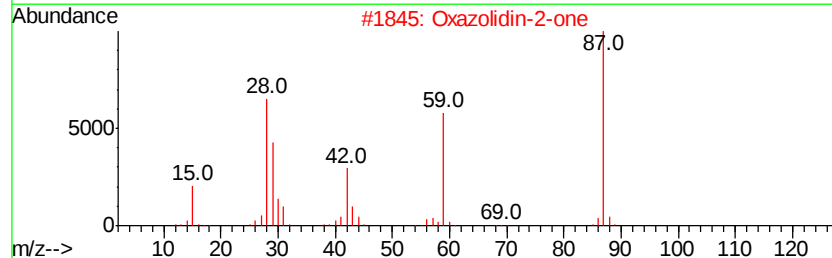
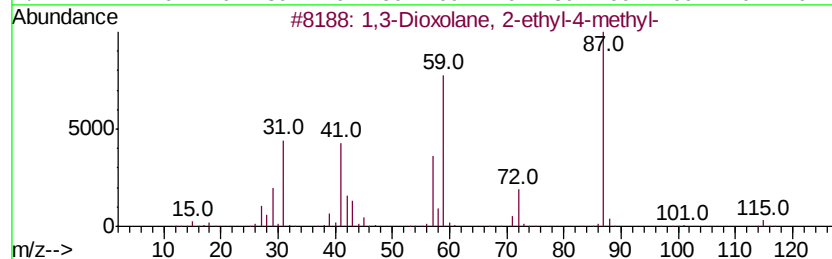
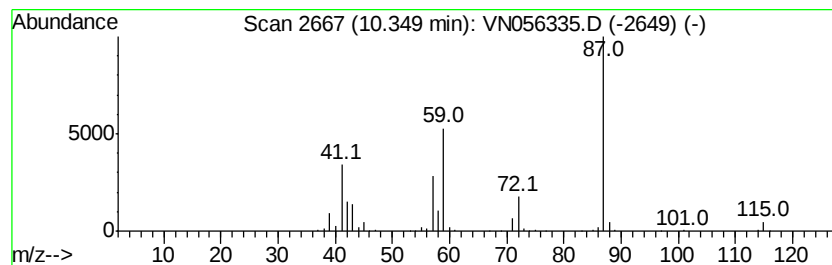
Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M
Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	25.22 ug/l	837630	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116 C6H12O2	004359-46-0	90
2	Oxazolidin-2-one	87 C3H5NO2	000497-25-6	64
3	2-Propanone, O-methylloxime	87 C4H9NO	003376-35-0	52
4	Thiocyanic acid, ethyl ester	87 C3H5NS	000542-90-5	50
5	Acetamide, N-ethyl-	87 C4H9NO	000625-50-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN061719\
Data File : VN056335.D
Acq On : 17 Jun 2019 13:11
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

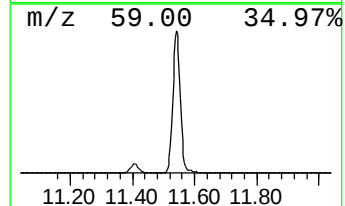
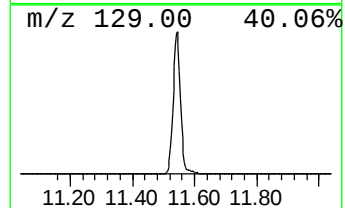
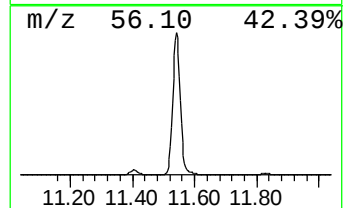
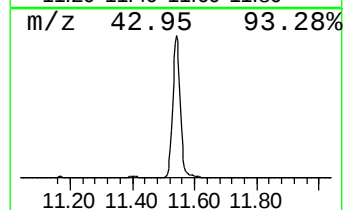
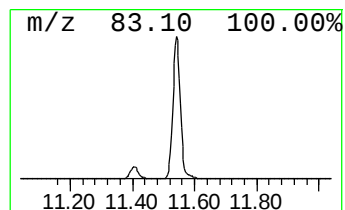
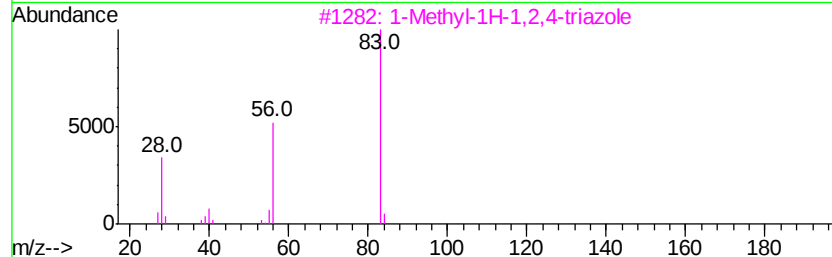
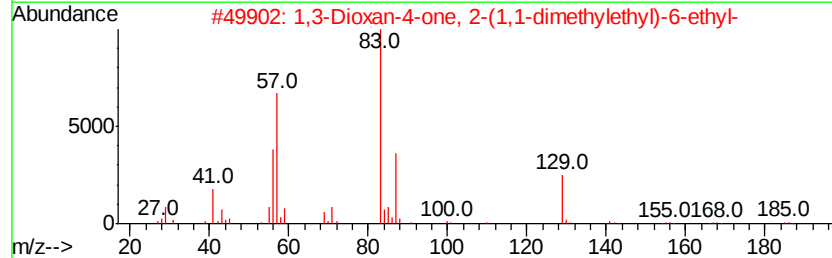
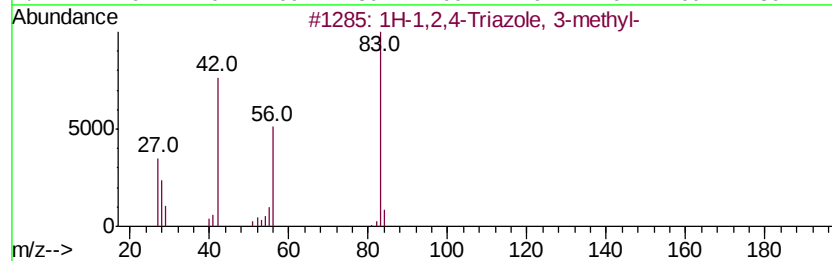
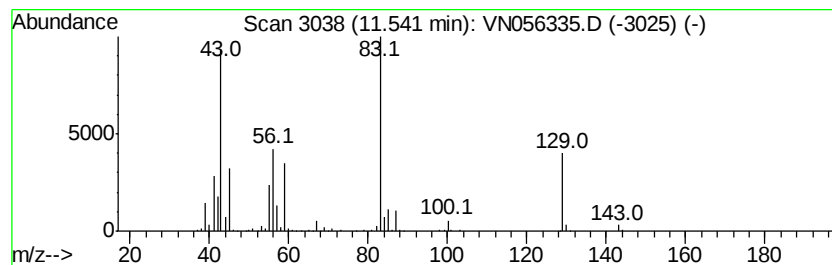
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown11.54 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	36.01 ug/l	1196090	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	38
2		1,3-Dioxan-4-one, 2-(1,1-dimethyl-...)	186	C10H18O3	113505-80-9	33
3		1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	32
4		Cyclohexanecarboxylic acid, 2-me...	184	C11H20O2	037139-85-8	23
5		1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	17



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN061719\
Data File : VN056335.D
Acq On : 17 Jun 2019 13:11
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061719W.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
Acetaldehyde	2.31	224.0	ug/l	4109140	1	7.66	917276	50.0
Ethanol	3.29	33.2	ug/l	608324	1	7.66	917276	50.0
Propanal	3.69	642.6	ug/l	11789800	1	7.66	917276	50.0
Acetonitrile	4.28	12.2	ug/l	224089	1	7.66	917276	50.0
1-Propanol	6.06	38.3	ug/l	702601	1	7.66	917276	50.0
Oxazolidin-2-one	8.84	5.4	ug/l	162577	2	8.58	1506820	50.0
1,3-Dioxolane, 2-...	9.88	7.5	ug/l	225486	2	8.58	1506820	50.0
1,3-Dioxolane, 2-...	10.35	25.2	ug/l	837630	3	11.41	1660950	50.0
unknown11.54	11.54	36.0	ug/l	1196090	3	11.41	1660950	50.0