

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061419\
 Data File : VN056311.D
 Acq On : 14 Jun 2019 14:52
 Operator : JC/SP
 Sample : K3373-01 10X
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 13 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\82N060419W.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	2386364	4054544	35.16%	13.649%
2	3.288	451	471	506	rBV	209091	590721	5.12%	1.989%
3	3.693	577	597	630	rBV	4438455	11532356	100.00%	38.823%
4	4.275	759	778	820	rBV3	65651	249837	2.17%	0.841%
5	6.059	1311	1333	1371	rBV2	196841	659771	5.72%	2.221%
6	7.590	1788	1809	1820	rBV	220963	550047	4.77%	1.852%
7	7.664	1820	1832	1861	rVB	358746	865138	7.50%	2.912%
8	8.027	1925	1945	1971	rBV	231291	533432	4.63%	1.796%
9	8.587	2104	2119	2157	rVB	646835	1411057	12.24%	4.750%
10	8.844	2175	2199	2215	rBV3	54815	133877	1.16%	0.451%
11	9.876	2507	2520	2539	rBV	108989	199211	1.73%	0.671%
12	10.091	2572	2587	2623	rBV	906035	1731564	15.01%	5.829%
13	10.349	2650	2667	2694	rBV	401380	704258	6.11%	2.371%
14	10.496	2700	2713	2738	rVB	261034	453162	3.93%	1.526%
15	11.406	2977	2996	3026	rBV	859694	1536266	13.32%	5.172%
16	11.541	3026	3038	3060	rVV	287278	476155	4.13%	1.603%
17	12.365	3281	3294	3301	rBV	1358127	2236660	19.39%	7.529%
18	12.400	3301	3305	3317	rVB	607743	893379	7.75%	3.007%
19	13.342	3585	3598	3614	rBV	528019	893859	7.75%	3.009%

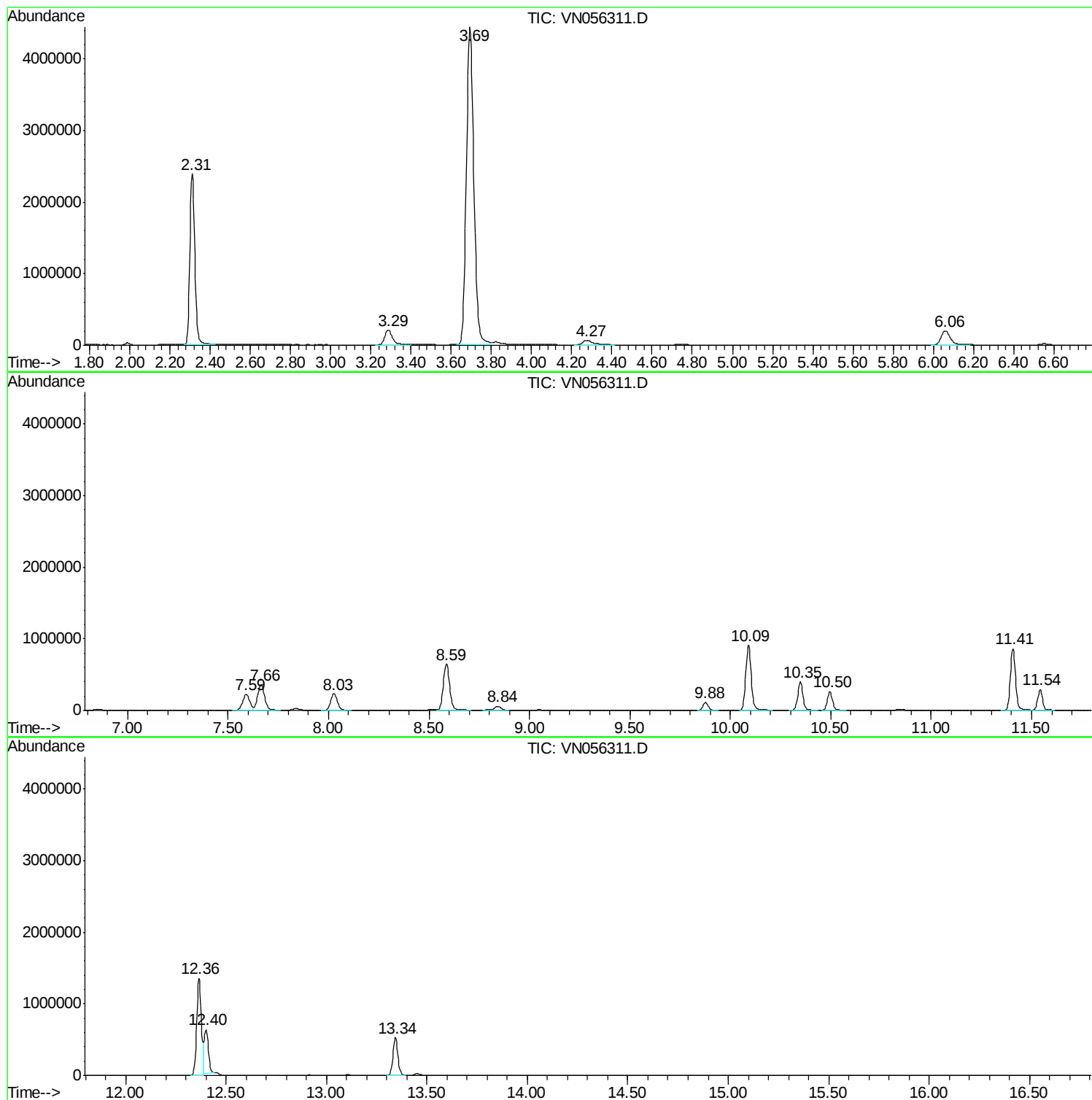
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N060419W.M
Quant Title : SW846 8260

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



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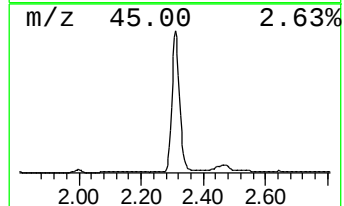
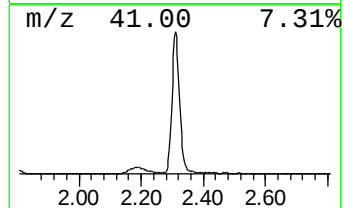
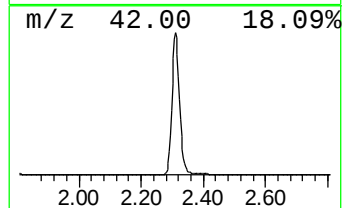
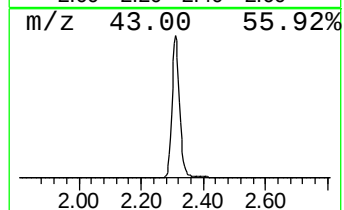
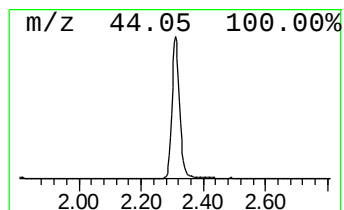
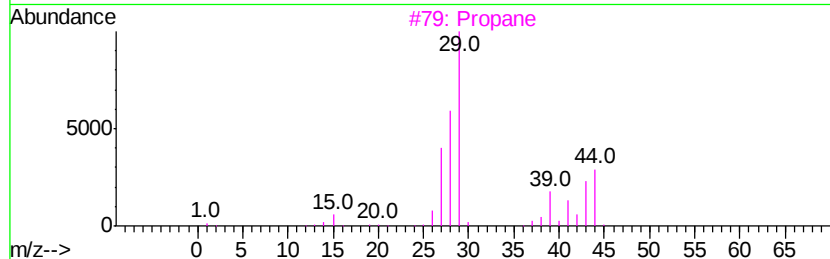
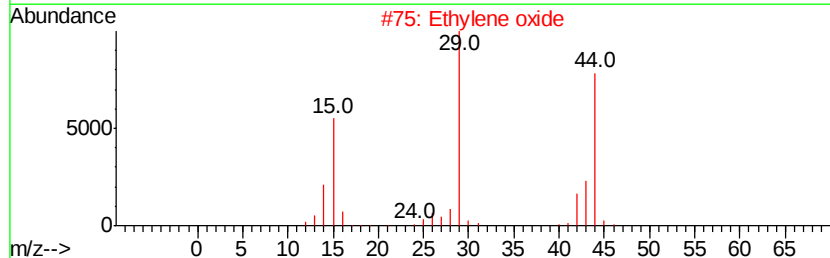
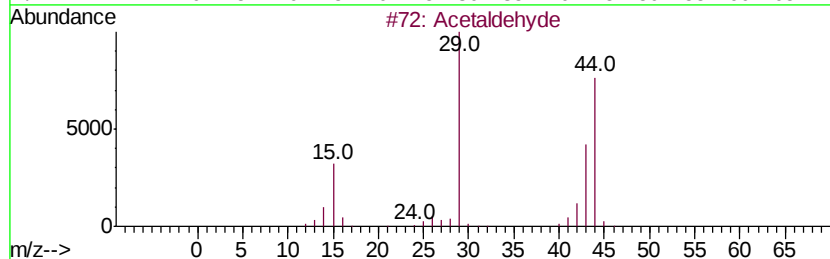
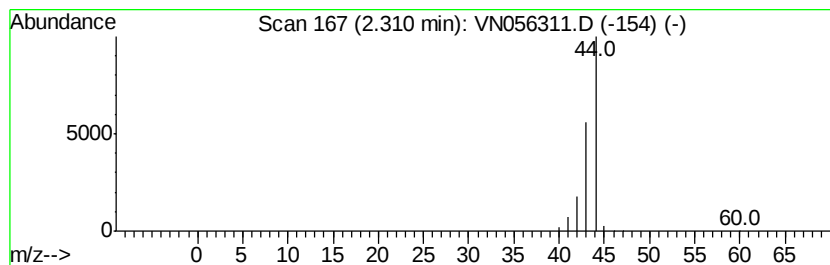
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N060419W.M
Quant Title : SW846 8260

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	234.33 ug/l	4054540	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehydve	44	C2H4O	000075-07-0	74
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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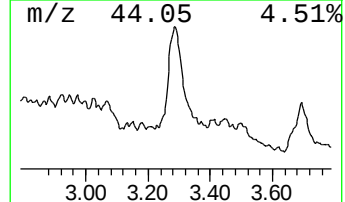
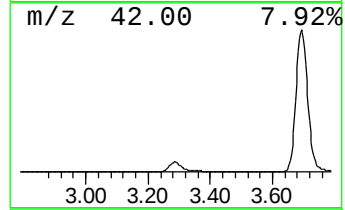
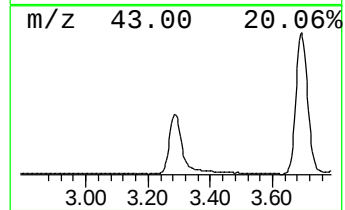
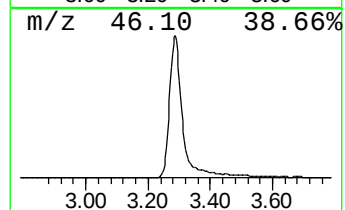
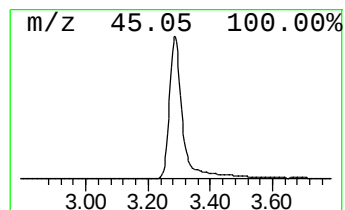
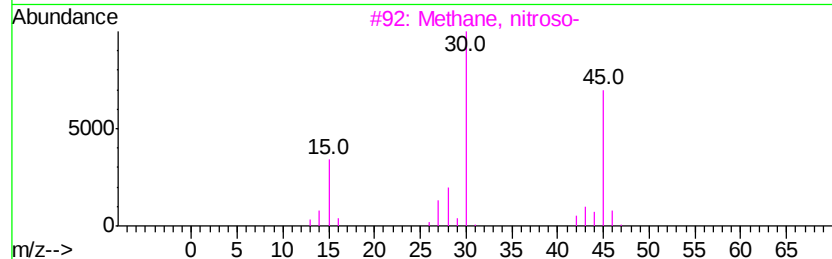
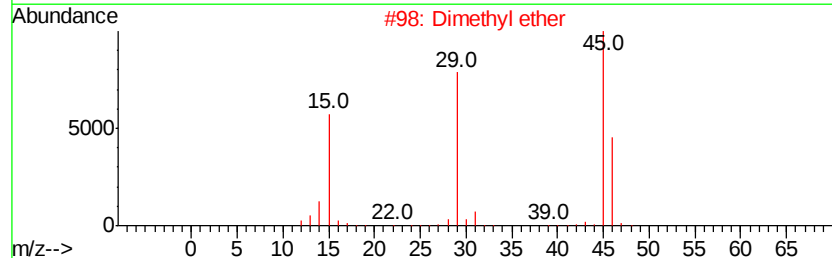
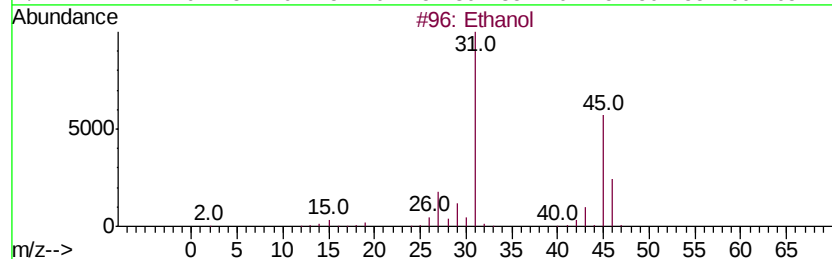
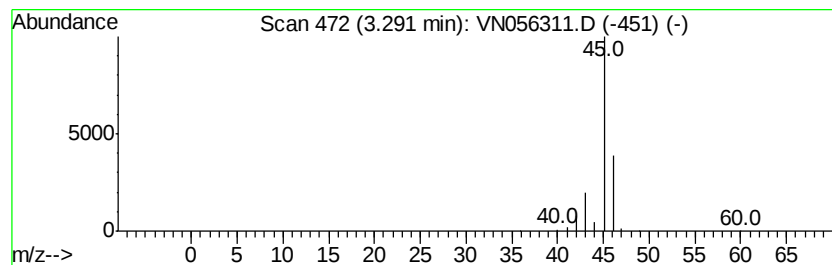
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	34.14 ug/l	590721	Pentafluorobenzene	7.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Formamide		45	CH3NO	000075-12-7	3



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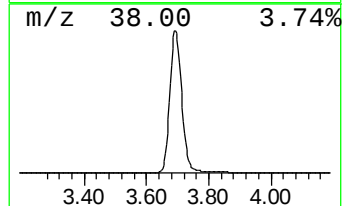
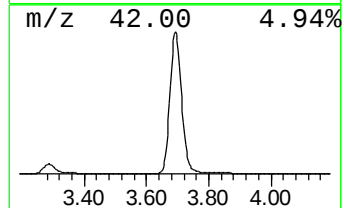
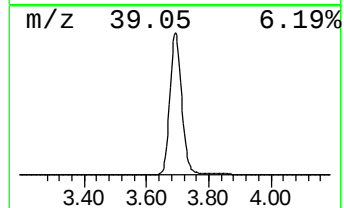
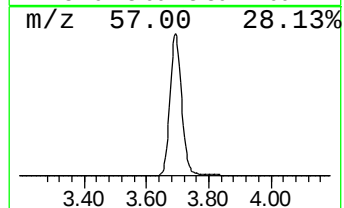
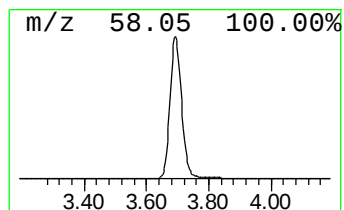
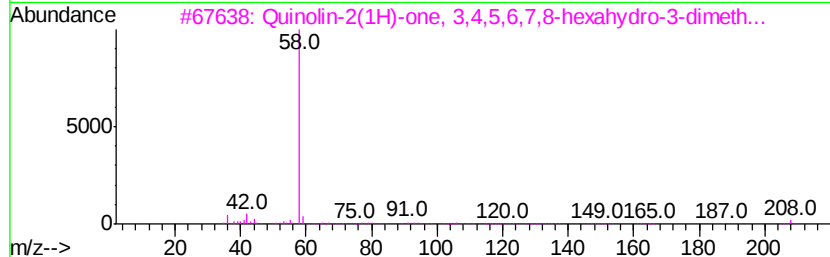
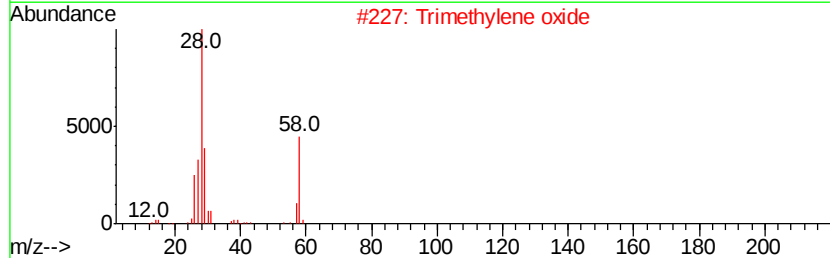
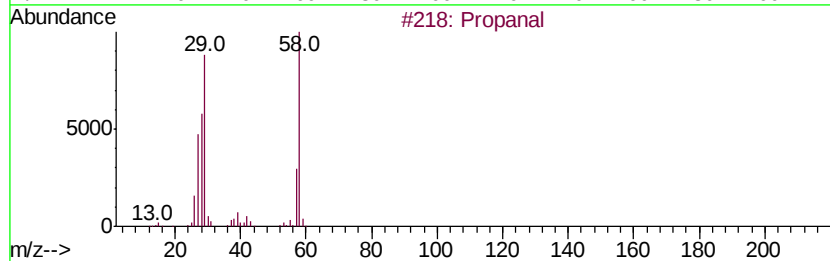
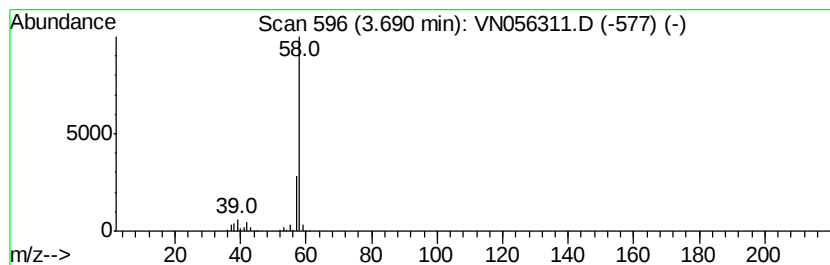
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Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
3.69	666.50 ug/l	11532400	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	64
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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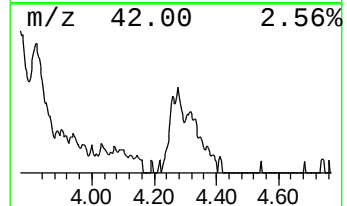
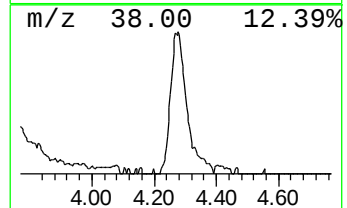
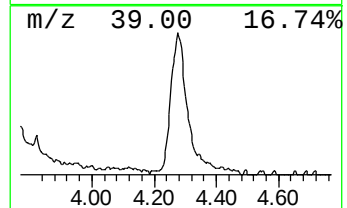
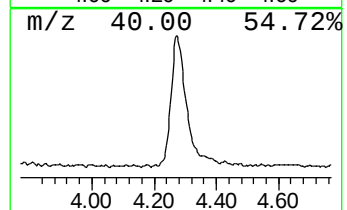
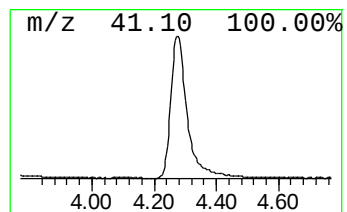
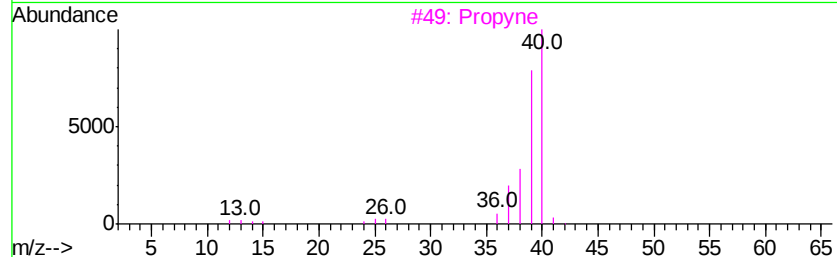
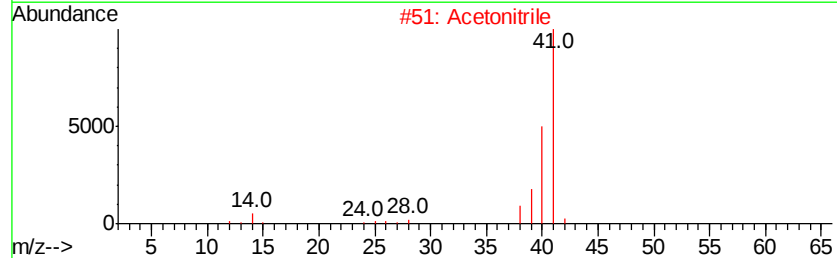
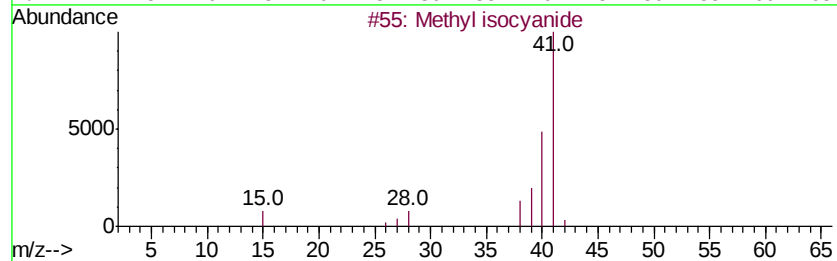
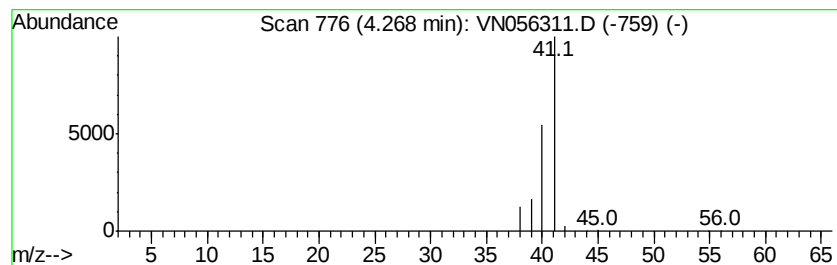
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Peak Number 4 Methyl isocyanide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	14.44 ug/l	249837	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl isocyanide	41	C2H3N	000593-75-9	50
2		Acetonitrile	41	C2H3N	000075-05-8	50
3		Propyne	40	C3H4	000074-99-7	4
4		Allene	40	C3H4	000463-49-0	1
5		Oxalic acid, diallyl ester	170	C8H10O4	1000309-22-9	1



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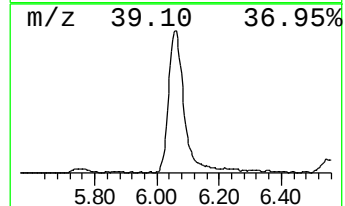
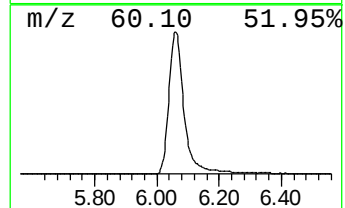
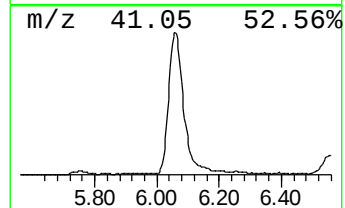
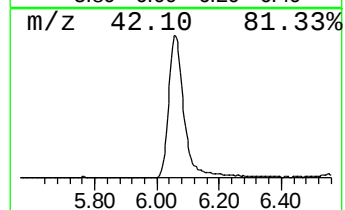
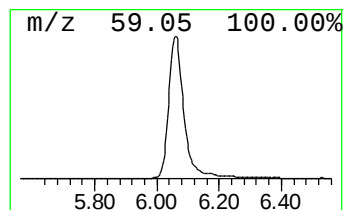
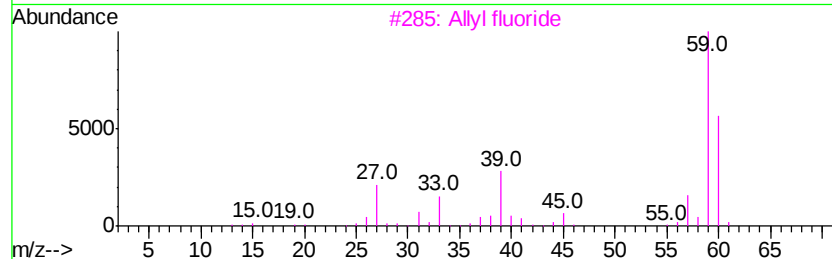
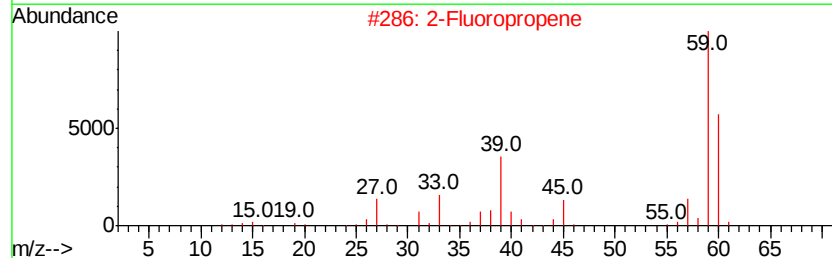
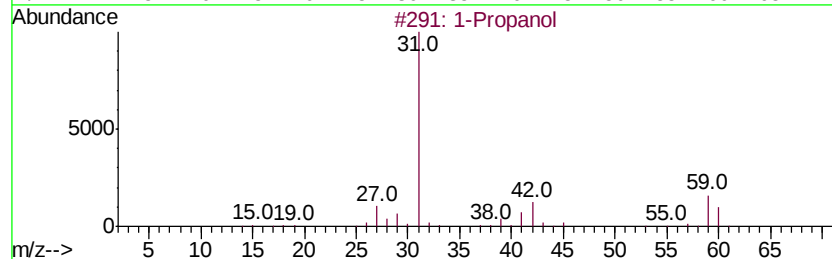
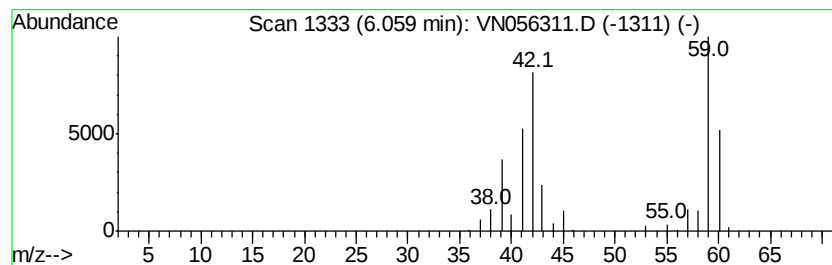
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Quant Title : SW846 8260

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	38.13 ug/l	659771	Pentafluorobenzene	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	72
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	43
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	17
5		Cyclopropane	42	C3H6	000075-19-4	9



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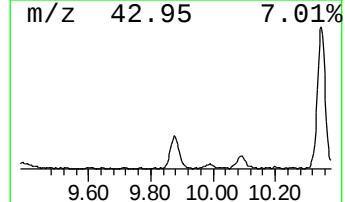
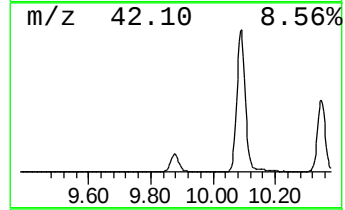
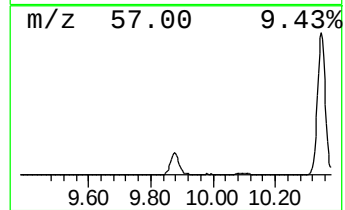
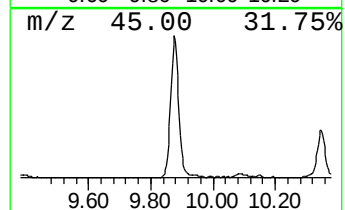
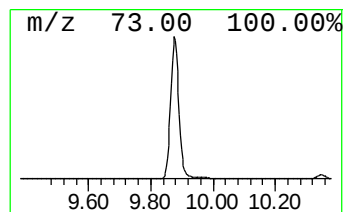
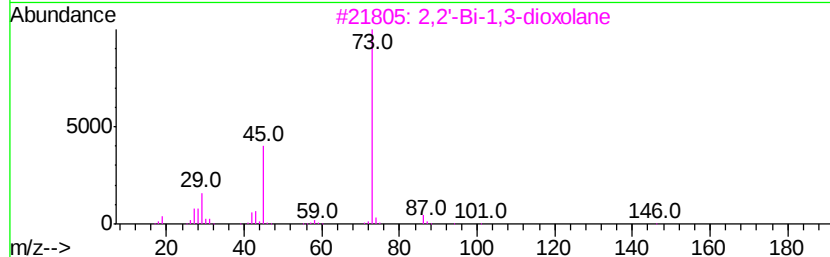
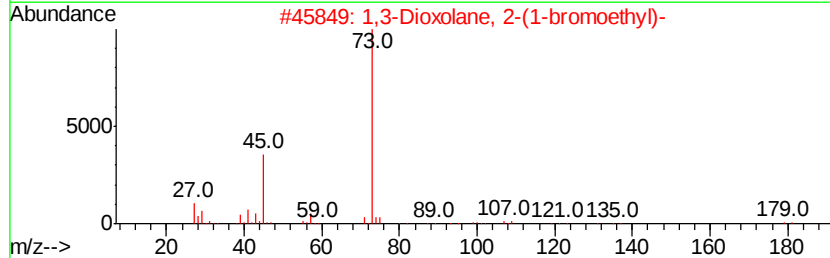
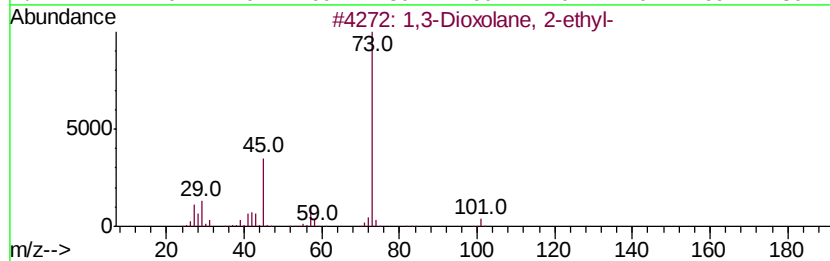
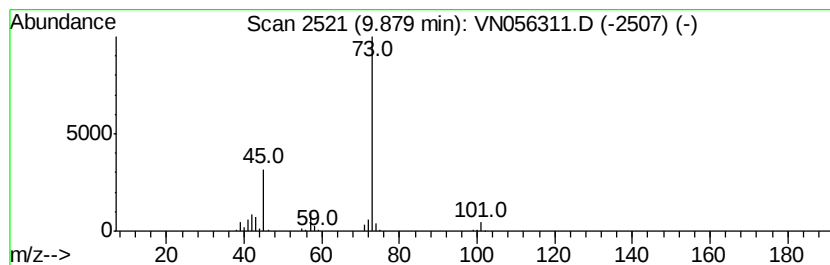
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Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxolane, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	7.06 ug/l	199211	1,4-Difluorobenzene	8.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	78
2			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	59
3			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	53
4			2-(2-Bromoethyl)-1,3-dioxolane	180	C5H9BrO2	018742-02-4	40
5			2,2'-Trimethylenebis-1,3-dioxolane	188	C9H16O4	006543-04-0	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN061419\
Data File : VN056311.D
Acq On : 14 Jun 2019 14:52
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

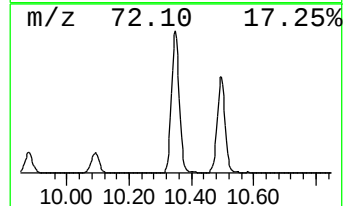
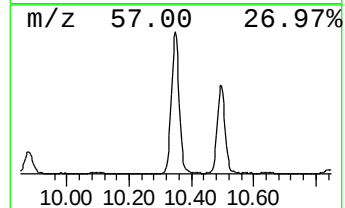
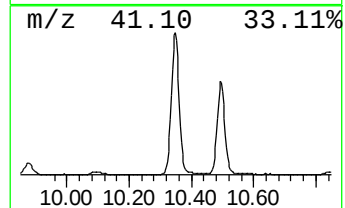
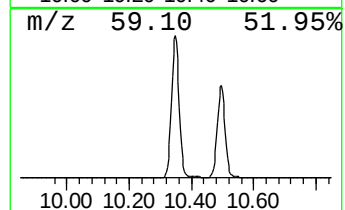
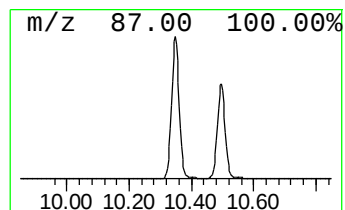
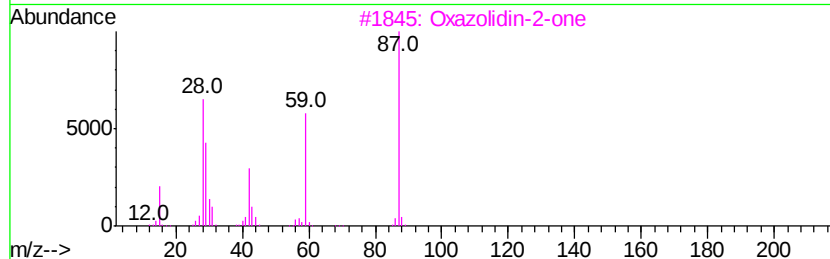
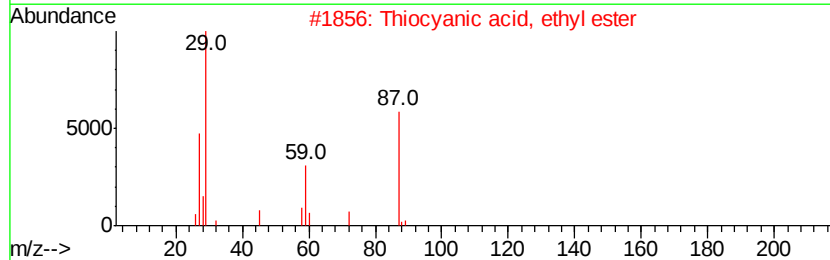
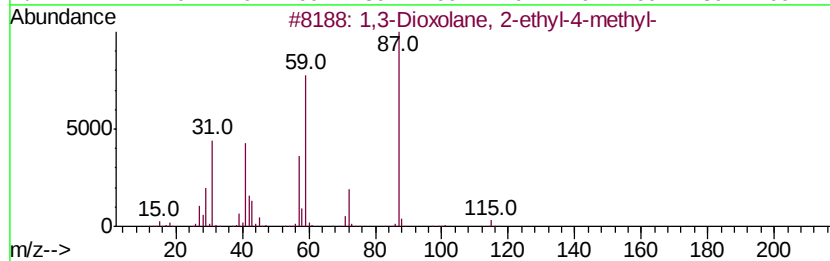
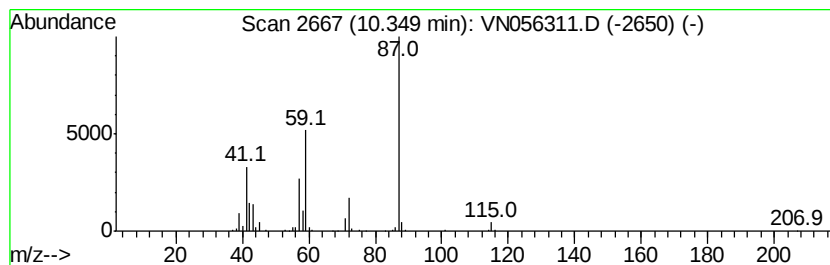
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Quant Title : SW846 8260

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

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	22.92 ug/l	704258	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	Thiocyanic acid, ethyl ester	87	C3H5NS		000542-90-5	72
3	Oxazolidin-2-one	87	C3H5NO2		000497-25-6	64
4	2-Propanone, O-methyloxime	87	C4H9NO		003376-35-0	52
5	Acetamide, N-ethyl-	87	C4H9NO		000625-50-3	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061419\
Data File : VN056311.D
Acq On : 14 Jun 2019 14:52
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

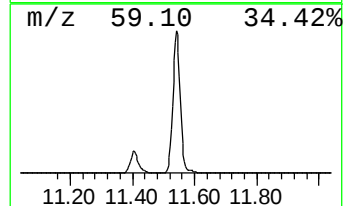
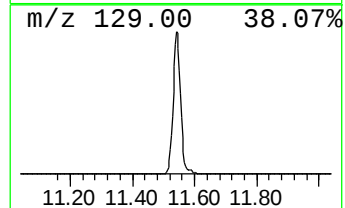
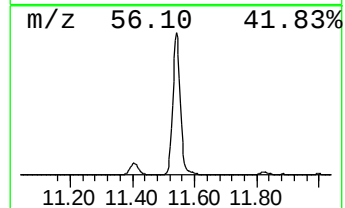
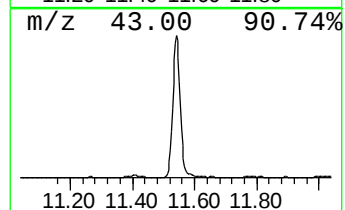
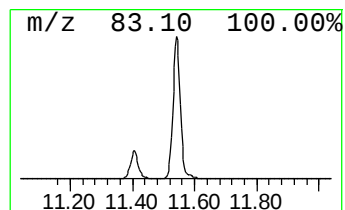
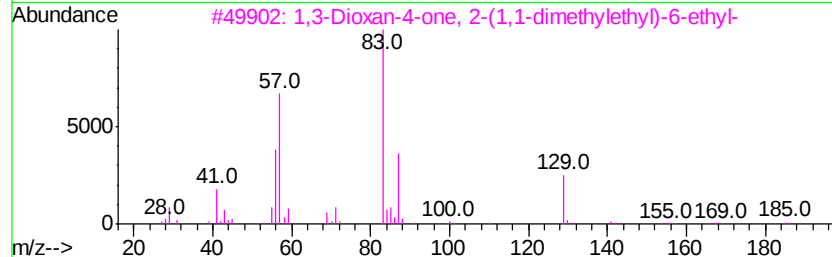
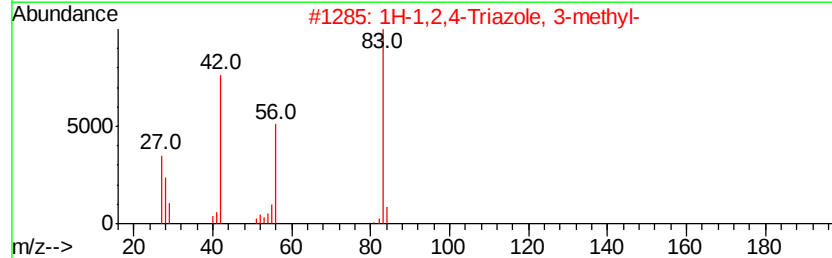
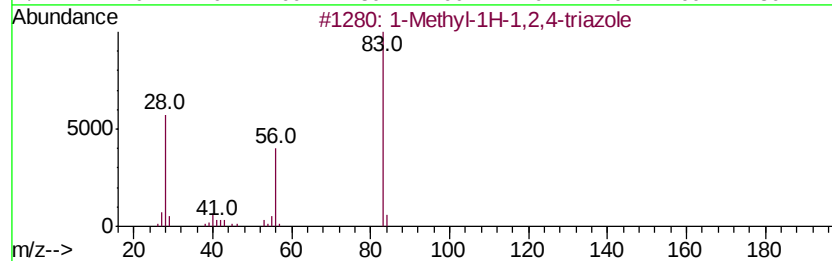
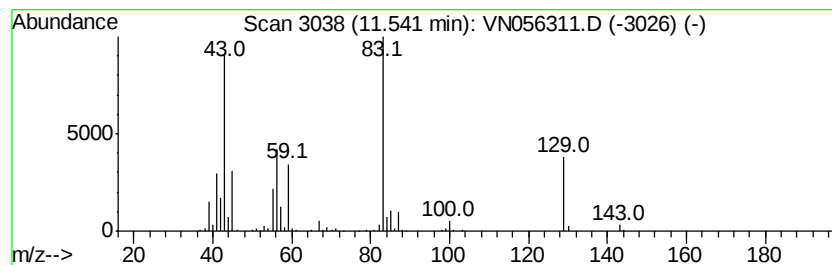
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N060419W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown11.54 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	15.50 ug/l	476155	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	43
2		1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	38
3		1,3-Dioxan-4-one, 2-(1,1-dimethv...	186	C10H18O3	113505-80-9	33
4		1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	32
5		Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	17



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN061419\
Data File : VN056311.D
Acq On : 14 Jun 2019 14:52
Operator : JC/SP
Sample : K3373-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
13857-13964-13981

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N060419W.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	234.3	ug/l	4054540	1	7.66	865138	50.0
Ethanol	3.29	34.1	ug/l	590721	1	7.66	865138	50.0
Propanal	3.69	666.5	ug/l	11532400	1	7.66	865138	50.0
Methyl isocyanide	4.27	14.4	ug/l	249837	1	7.66	865138	50.0
1-Propanol	6.06	38.1	ug/l	659771	1	7.66	865138	50.0
1,3-Dioxolane, 2-...	9.88	7.1	ug/l	199211	2	8.59	1411060	50.0
1,3-Dioxolane, 2-...	10.35	22.9	ug/l	704258	3	11.41	1536270	50.0
unknown11.54	11.54	15.5	ug/l	476155	3	11.41	1536270	50.0