

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX060319\
Data File : VX010048.D
Acq On : 03 Jun 2019 19:55
Operator : JC/SP
Sample : K3165-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
13911

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\82X052819W.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	1.483	50	54	85	rBV	14196191	20157130	12.44%	4.332%
2	2.367	183	199	209	rBV2	21592207	48222524	29.75%	10.363%
3	2.446	209	212	234	rVB	1180805	2253783	1.39%	0.484%
4	4.147	439	491	495	rBV	4768549	36518125	22.53%	7.848%
5	7.013	945	961	986	rVB	19795383	55399857	34.18%	11.906%
6	7.324	998	1012	1018	rBV	14555957	32708639	20.18%	7.029%
7	9.110	1290	1305	1310	rBV2	56091433	162069298	100.00%	34.829%
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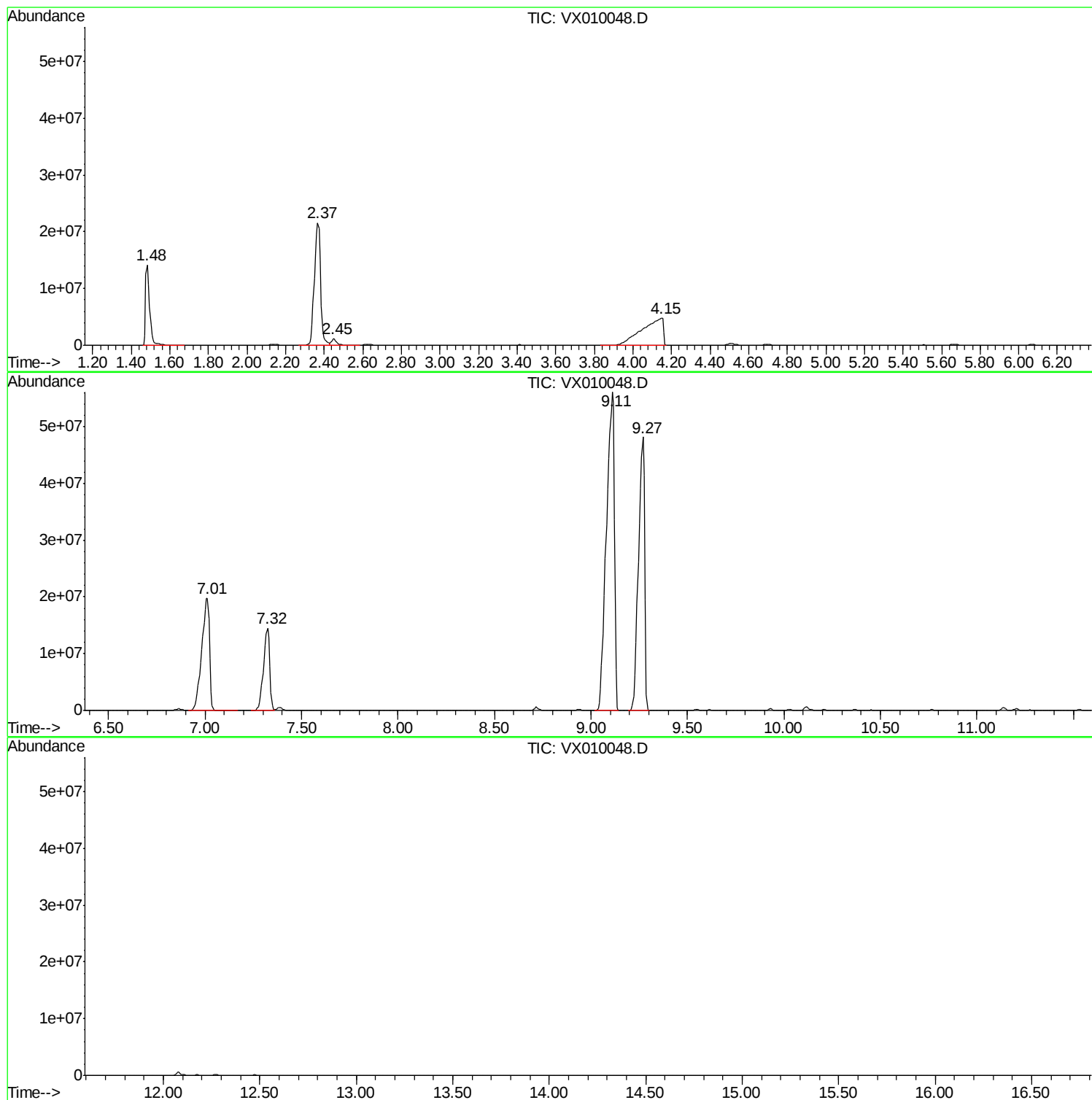
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Quant Title : SW846 8260

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



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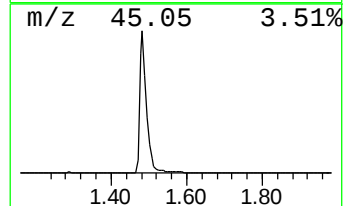
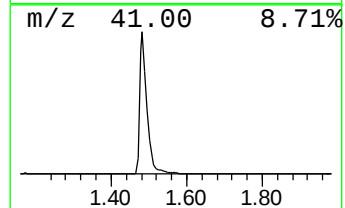
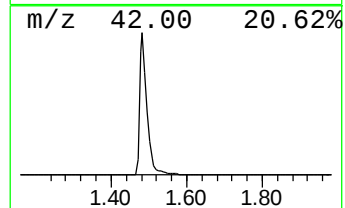
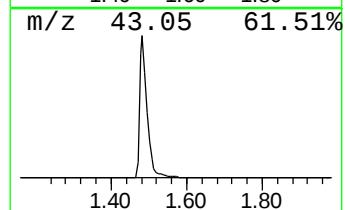
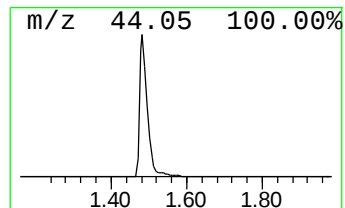
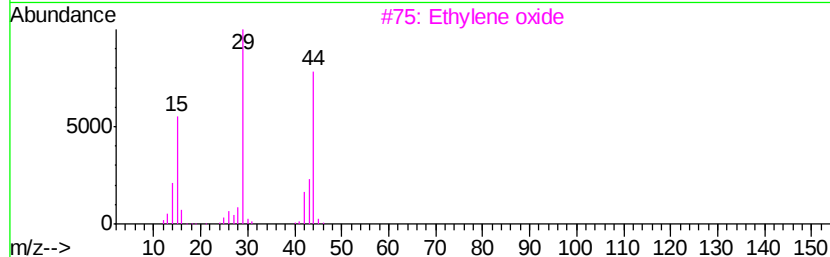
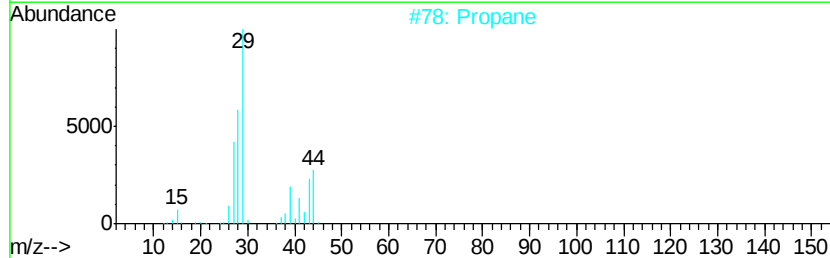
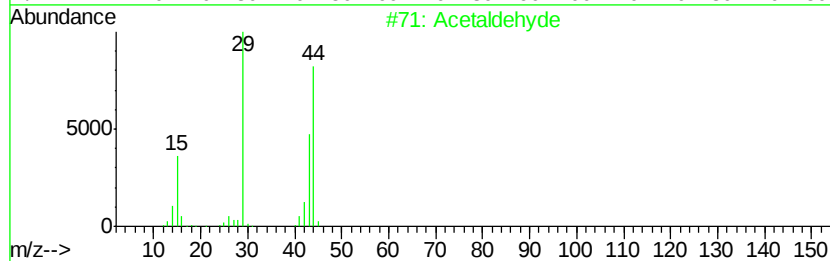
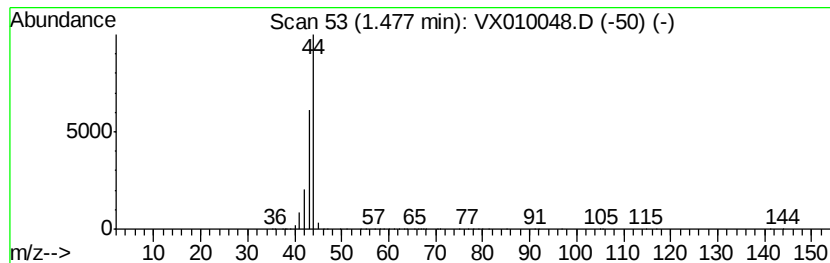
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	18.19 ug/l	20157100	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyd		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	Carbon dioxide		44	CO2	000124-38-9	3



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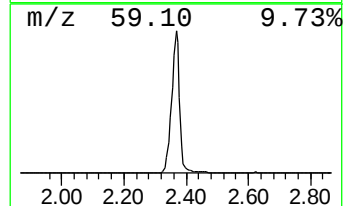
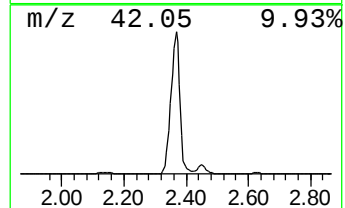
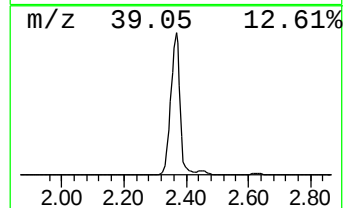
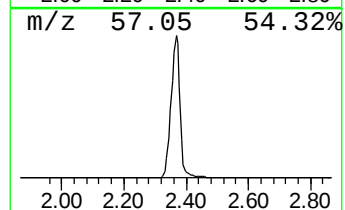
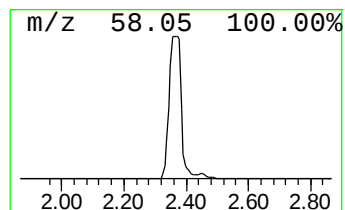
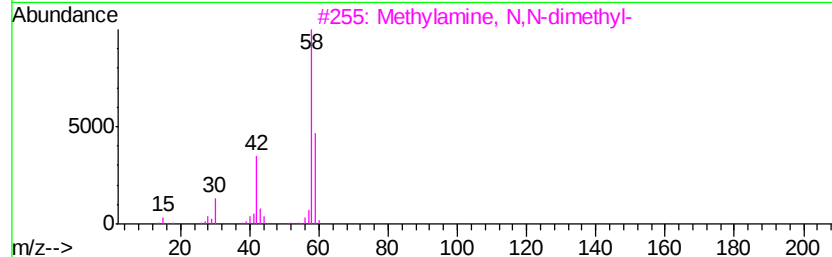
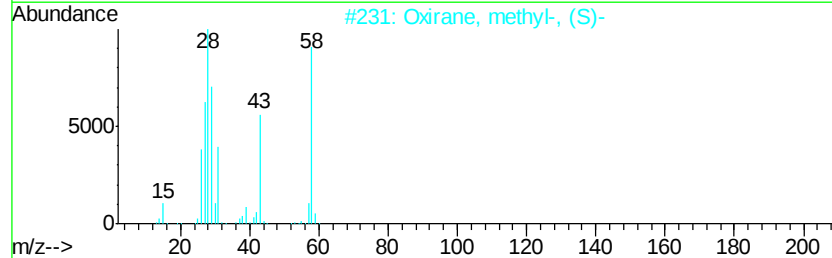
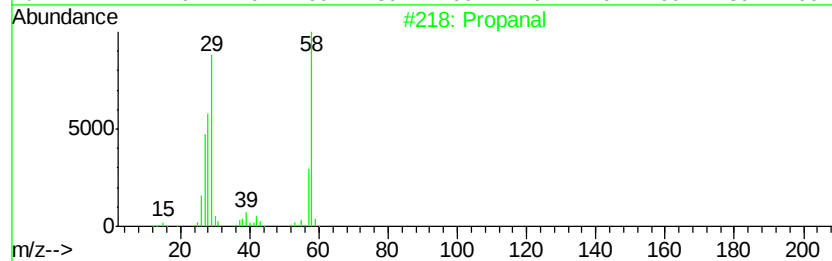
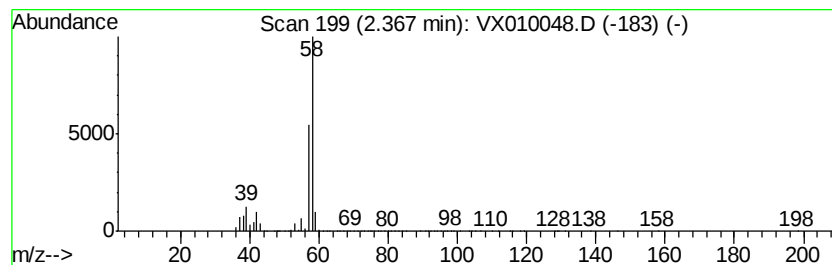
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Peak Number 2 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.37	43.52 ug/l	48222500	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal	58	C3H6O	000123-38-6	50
2		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
3		Methvlamine, N,N-dimethyl-	59	C3H9N	000075-50-3	4
4		2-Propen-1-amine	57	C3H7N	000107-11-9	4
5		2-Propyn-1-ol, propionate	112	C6H8O2	001932-92-9	4



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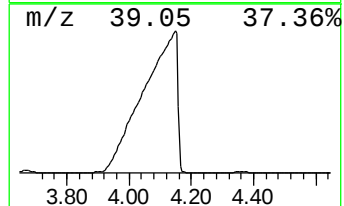
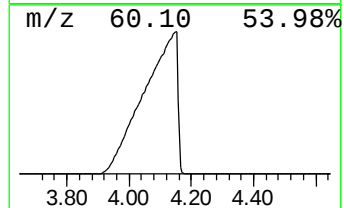
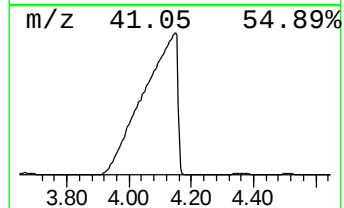
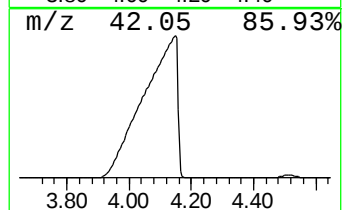
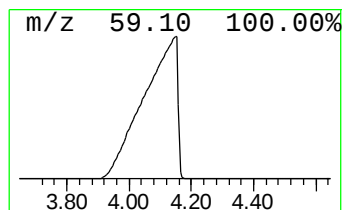
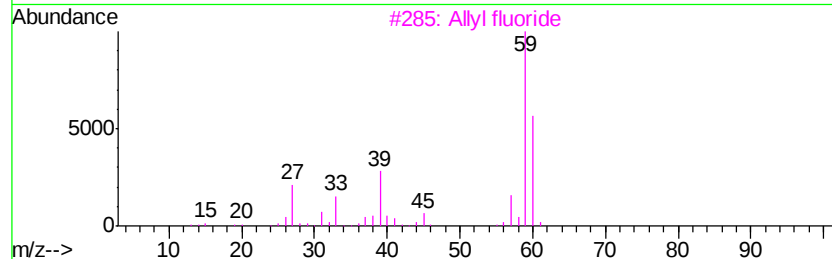
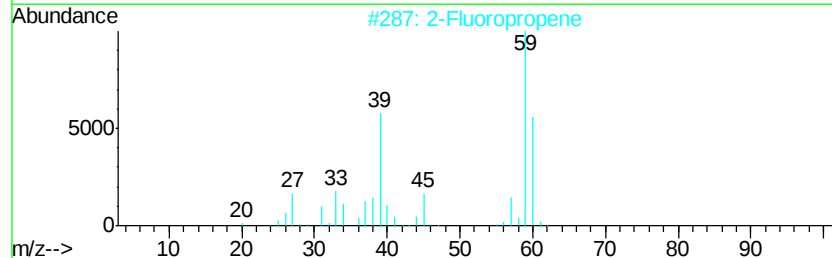
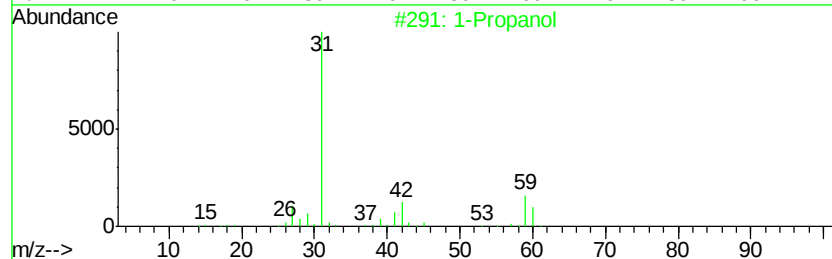
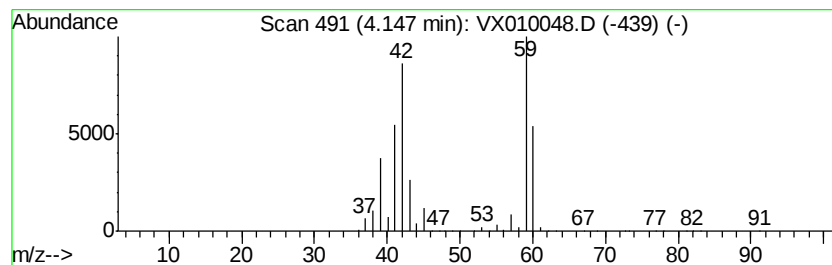
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	32.96 ug/l	36518100	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	47
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Cyclopropane	42	C3H6	000075-19-4	9
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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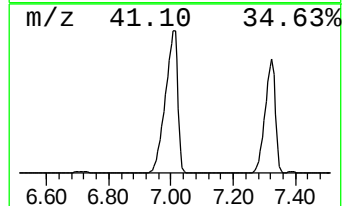
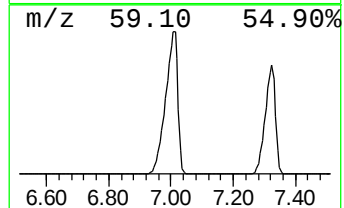
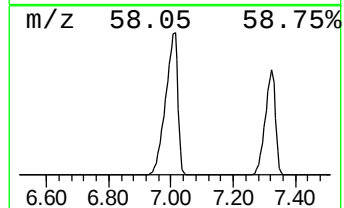
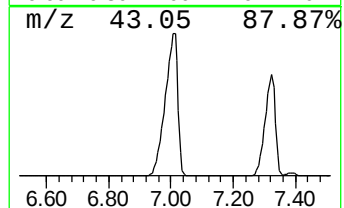
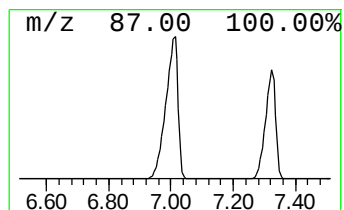
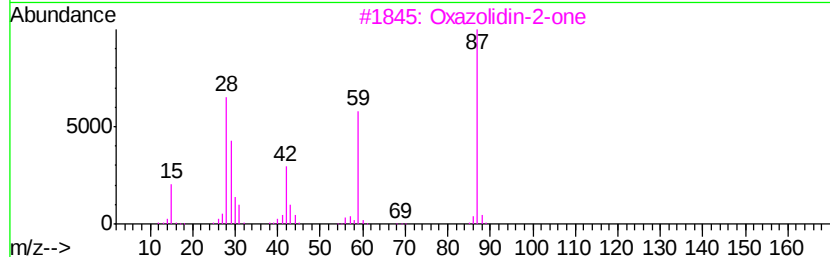
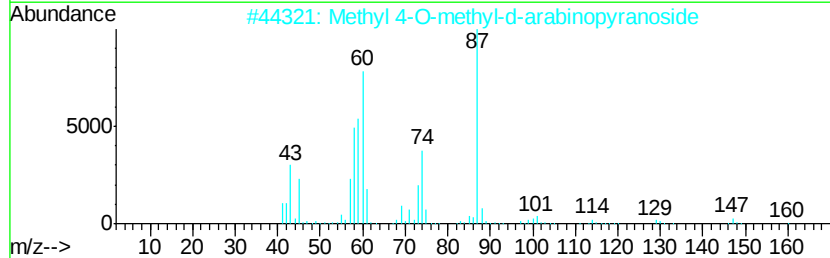
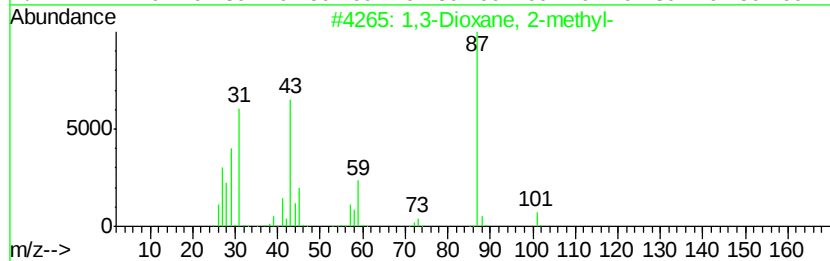
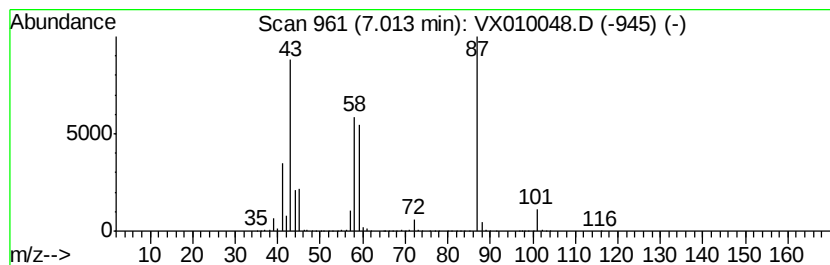
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.01	50.00 ug/l	55399900	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	40
2		Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	36
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	32
4		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	28
5		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	28



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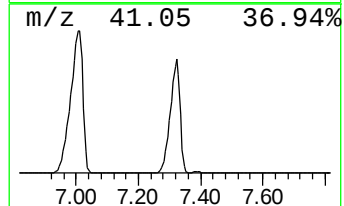
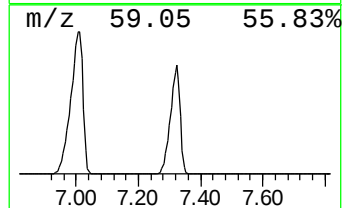
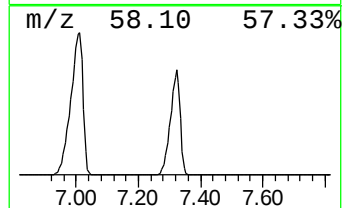
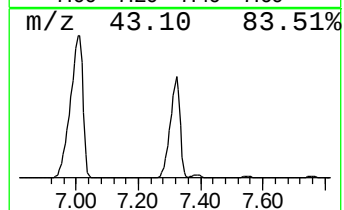
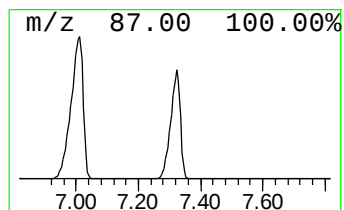
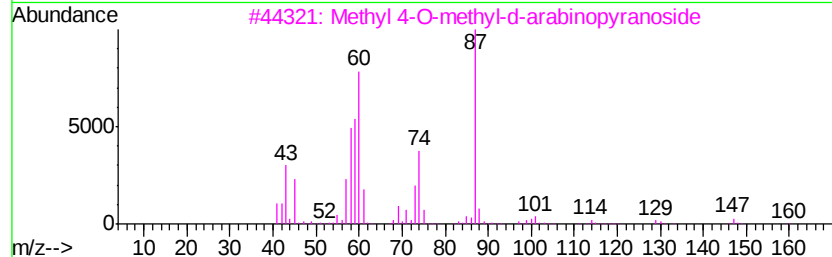
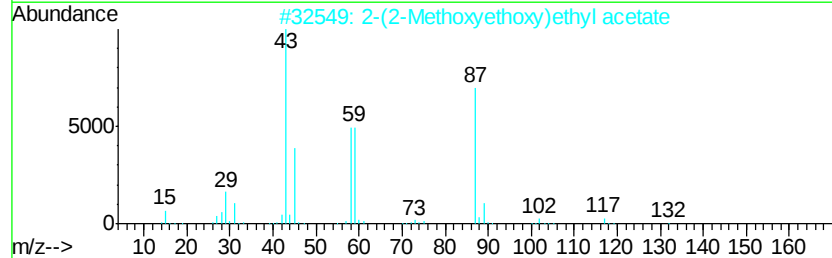
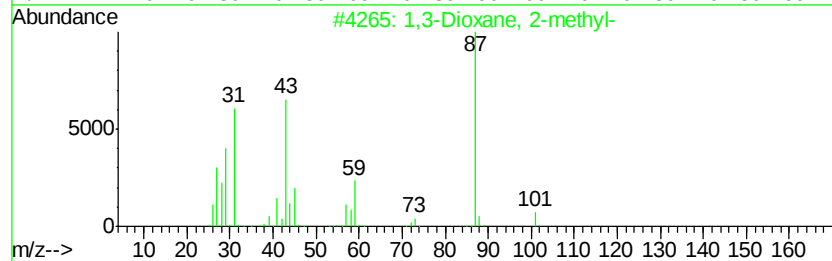
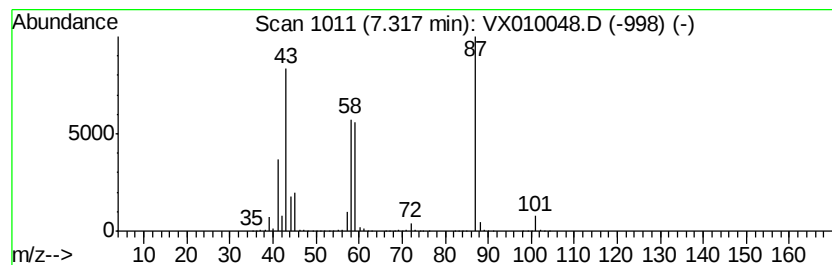
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	29.52 ug/l	32708600	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
3		Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
5		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33



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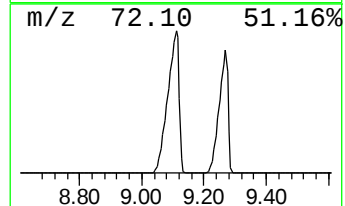
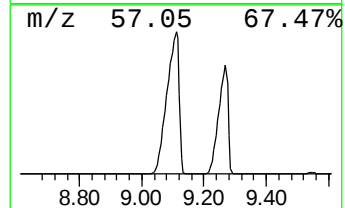
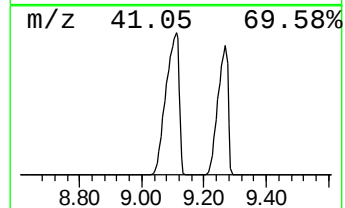
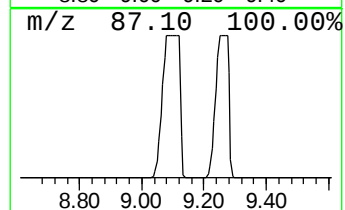
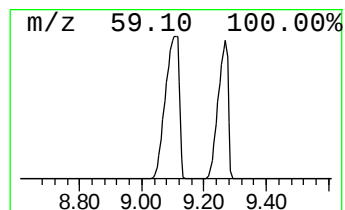
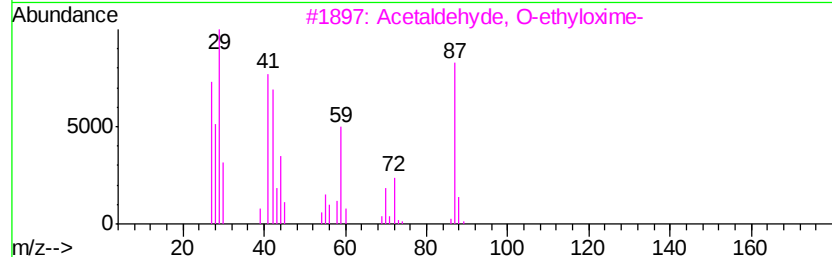
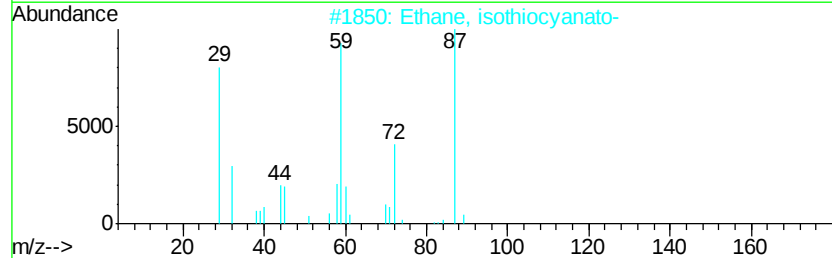
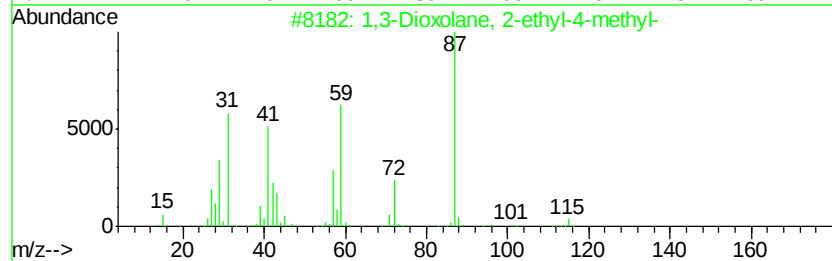
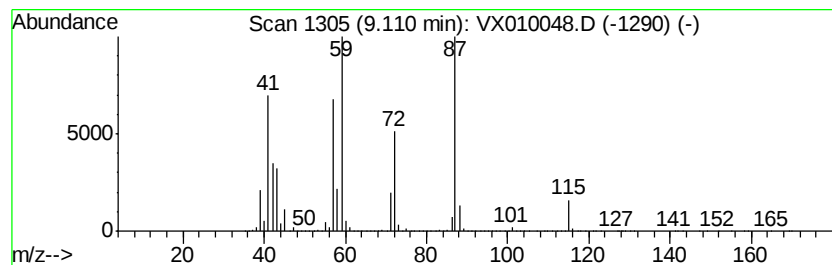
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Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.11	75.04 ug/l	162069000	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	72
2		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	59
3		Acetaldehyde, O-ethylxime-	87	C4H9NO	1000288-34-6	59
4		Urea, (2-hydroxyethyl)-	104	C3H8N2O2	002078-71-9	50
5		(Methylthio)-acetonitrile	87	C3H5NS	035120-10-6	32



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Operator : JC/SP
Sample : K3165-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
13911

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.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	1.48	18.2	ug/l	20157100	1	5.67	55399900	50.0
Propanal	2.37	43.5	ug/l	48222500	1	5.67	55399900	50.0
1-Propanol	4.15	33.0	ug/l	36518100	1	5.67	55399900	50.0
unknown7.01	7.01	50.0	ug/l	55399900	2	6.87	55399900	50.0
1,3-Dioxane, 2-me...	7.32	29.5	ug/l	32708600	2	6.87	55399900	50.0
1,3-Dioxolane, 2-...	9.11	75.0	ug/l	162069000	3	10.12	107994000	50.0