

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
 Data File : VX016338.D
 Acq On : 19 May 2020 16:36
 Operator : JC/SP
 Sample : L2673-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 102

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_X\METHOD\82X050420W.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	1.471	59	63	83	rVB	6400738	8088006	8.26%	1.988%
2	2.380	191	212	218	rBV2	21975266	92329745	94.34%	22.700%
3	4.093	450	493	497	rBV	5540497	39512745	40.37%	9.714%
4	6.946	952	961	972	rVV	1538883	3504863	3.58%	0.862%
5	7.275	1006	1015	1022	rBV	986442	2100399	2.15%	0.516%
6	8.696	1241	1248	1252	rBV	816349	1463243	1.50%	0.360%
7	8.915	1277	1284	1298	rVB	4653570	7511736	7.68%	1.847%
8	9.074	1298	1310	1315	rBV2	38752596	97871248	100.00%	24.062%
9	9.232	1326	1336	1341	rBV	34184813	69957096	71.48%	17.199%
10	10.140	1472	1485	1490	rBV	33723110	63330478	64.71%	15.570%
11	10.195	1490	1494	1504	rVB	2650597	3379692	3.45%	0.831%
12	10.756	1578	1586	1598	rVB3	703252	1412580	1.44%	0.347%
13	11.122	1640	1646	1652	rBV	823004	1073984	1.10%	0.264%
14	11.701	1730	1741	1747	rBV	5746507	9075336	9.27%	2.231%
15	11.994	1781	1789	1796	rBV	2263858	2776473	2.84%	0.683%
16	12.061	1796	1800	1803	rBV	919888	1307144	1.34%	0.321%
17	12.256	1827	1832	1838	rBV	1663443	2045591	2.09%	0.503%

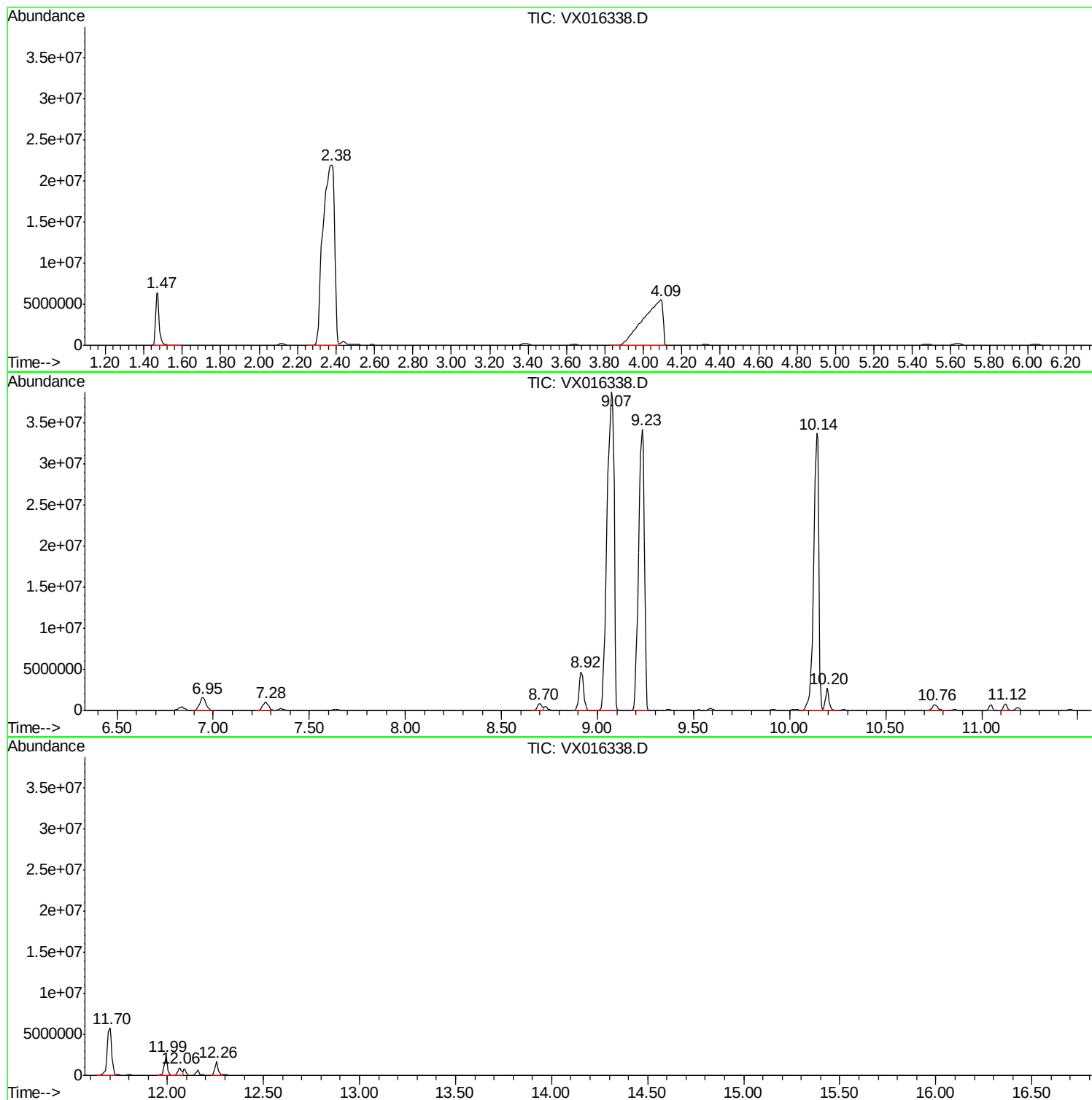
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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



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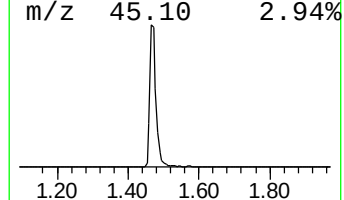
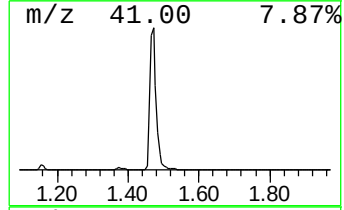
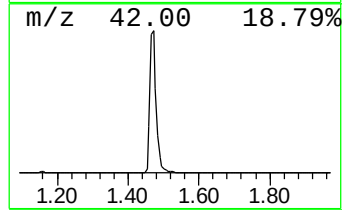
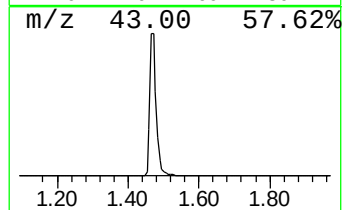
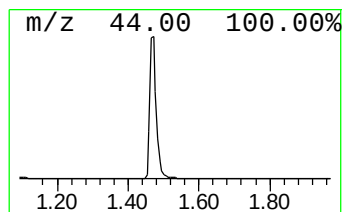
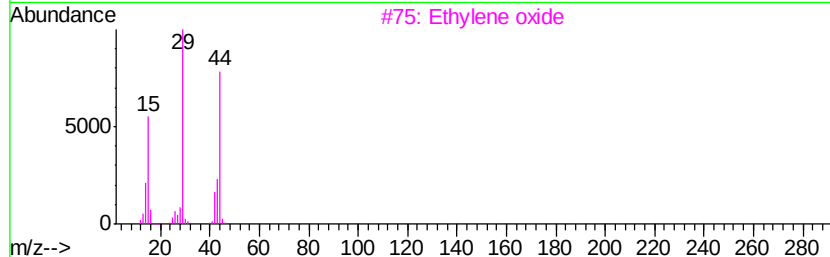
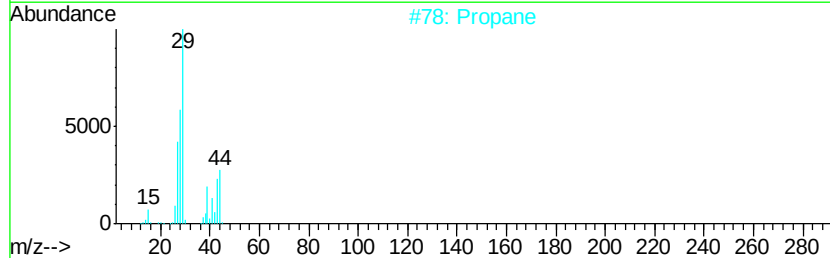
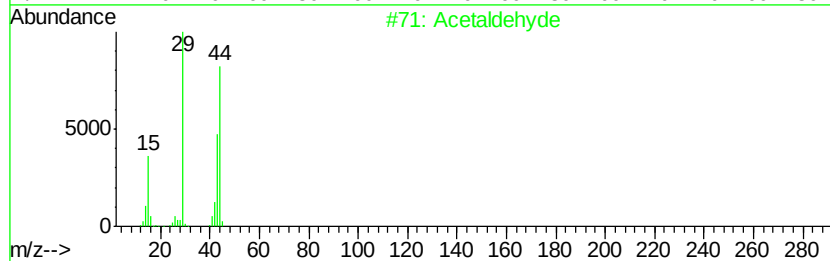
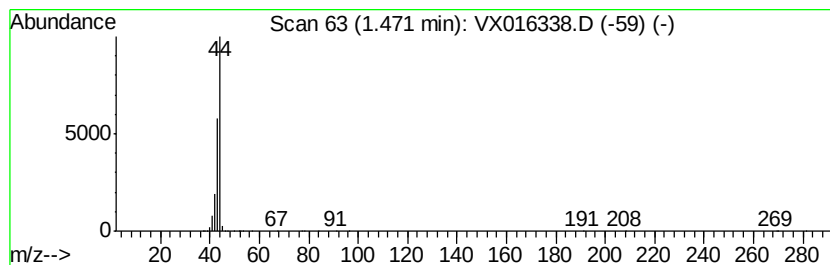
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	115.38 ug/l	8088010	Pentafluorobenzene	5.64

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	1,2-Propanediamine		74	C3H10N2	000078-90-0	4
5	Alanine		89	C3H7NO2	000056-41-7	4



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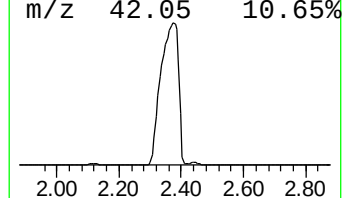
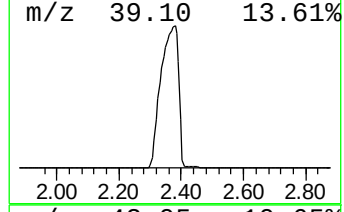
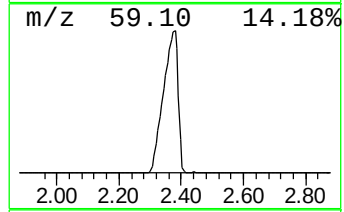
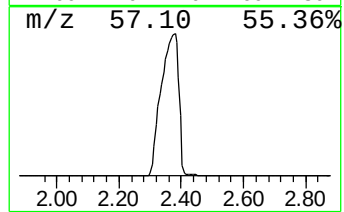
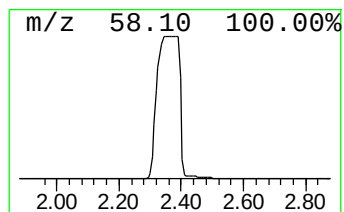
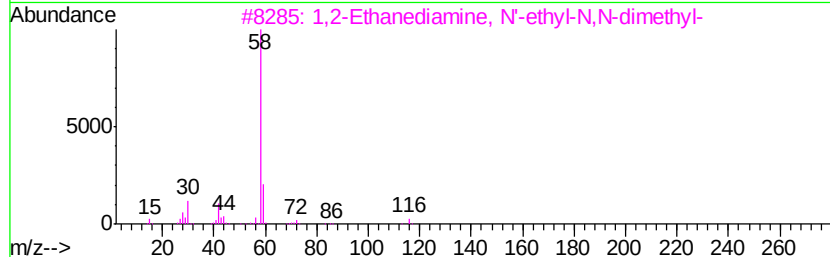
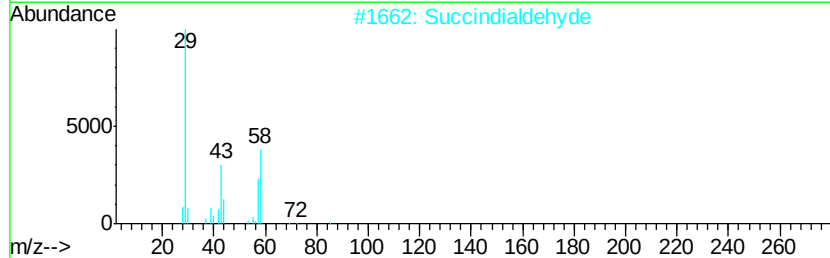
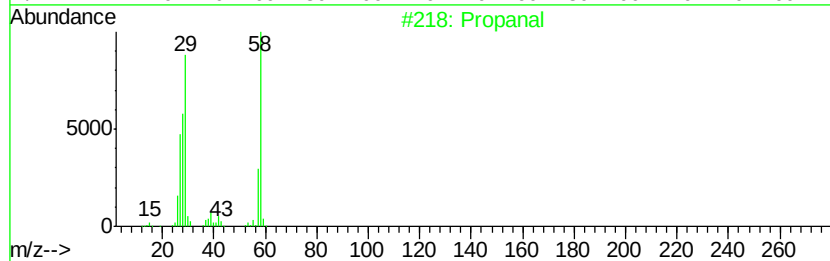
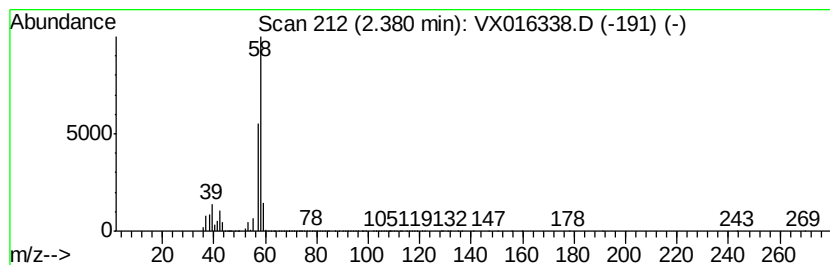
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	1317.17 ug/l	92329700	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal		58	C3H6O	000123-38-6	50
2	Succindialdehyde		86	C4H6O2	000638-37-9	9
3	1,2-Ethanediamine, N'-ethyl-N,N-...		116	C6H16N2	000123-83-1	9
4	Methylamine, N,N-dimethyl-		59	C3H9N	000075-50-3	7
5	Oxirane, methyl-, (S)-		58	C3H6O	016088-62-3	4



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Instrument :
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ClientSampleId :
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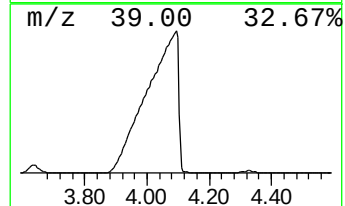
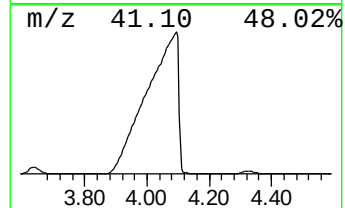
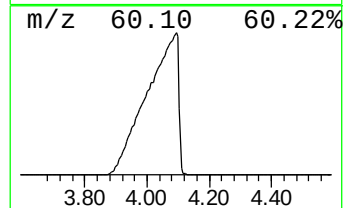
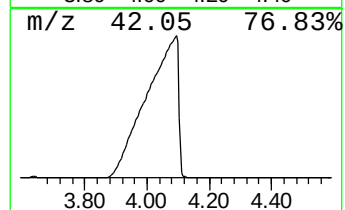
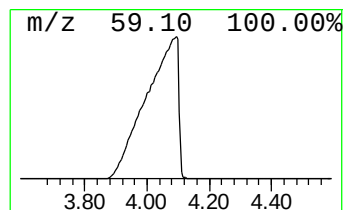
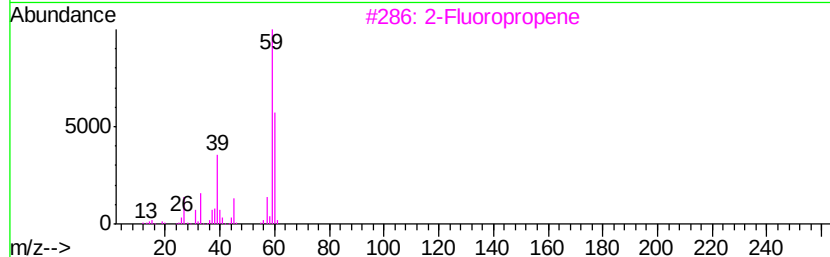
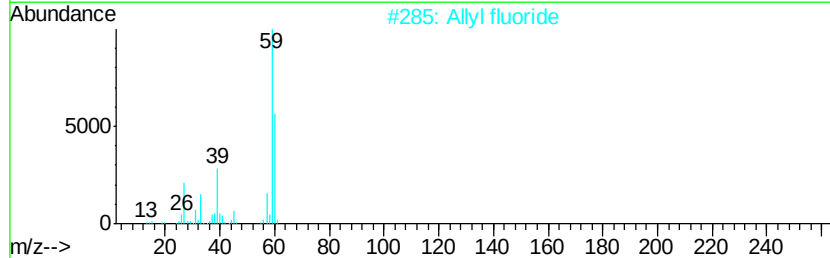
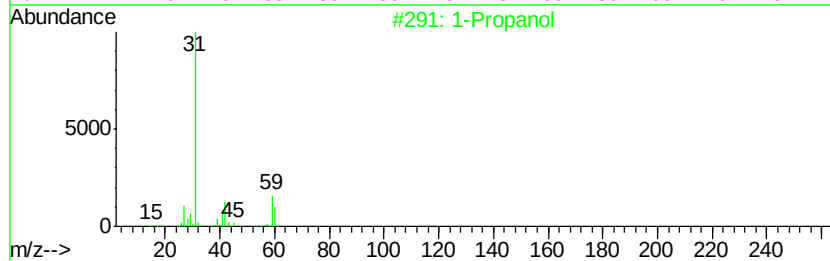
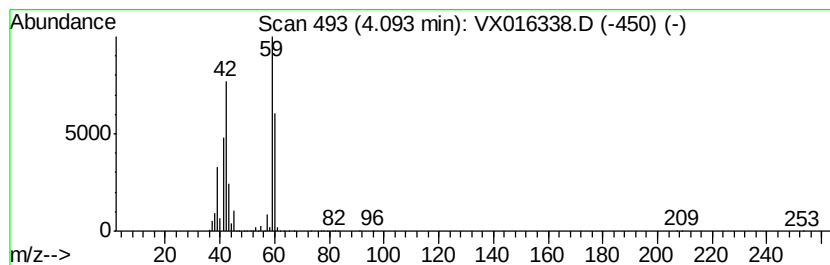
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Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	563.69 ug/l	39512700	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	47
3		2-Fluoropropene	60	C3H5F	001184-60-7	47
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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ALS Vial : 18 Sample Multiplier: 1

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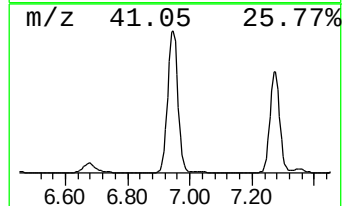
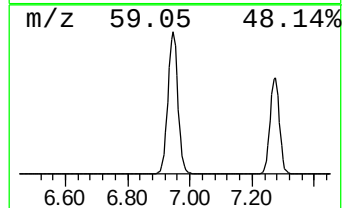
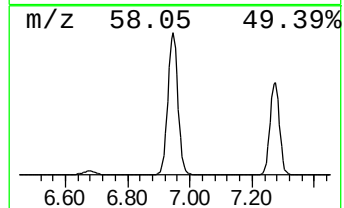
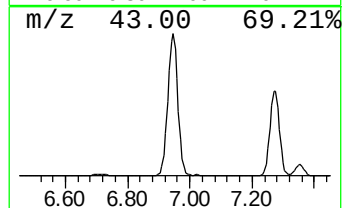
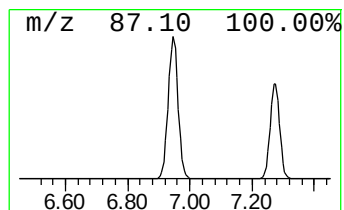
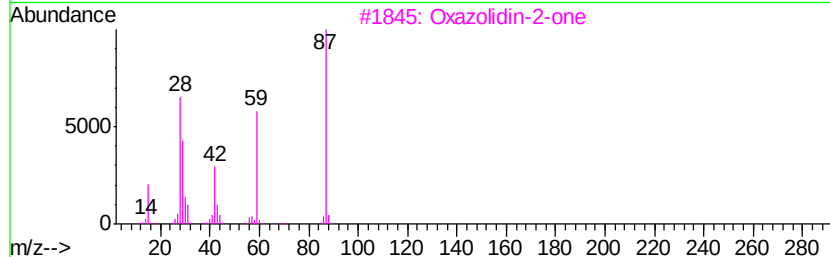
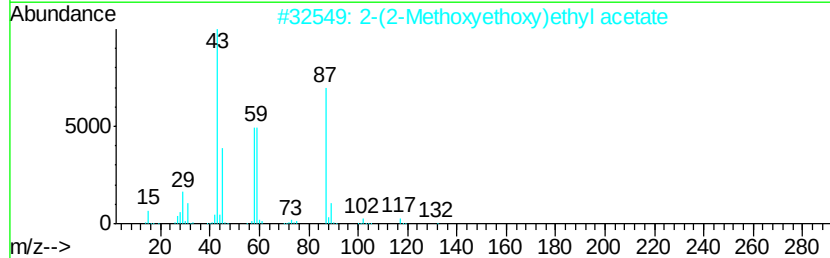
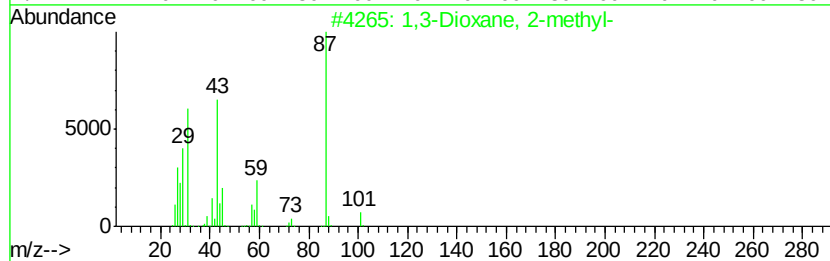
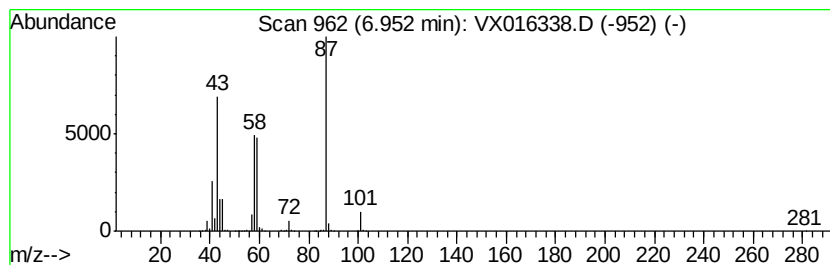
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,3-Dioxane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	50.00 ug/l	3504860	1,4-Difluorobenzene	6.84

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	50
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
4		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
5		Diethylsilane	88	C4H12Si	000542-91-6	17



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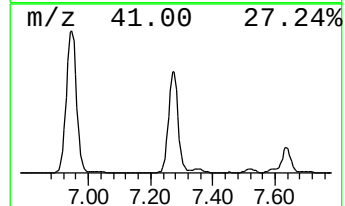
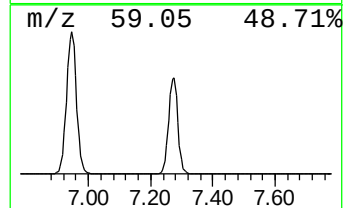
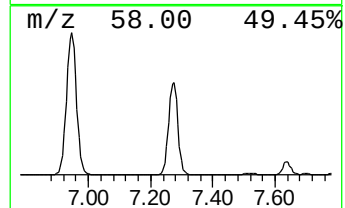
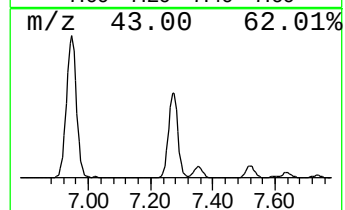
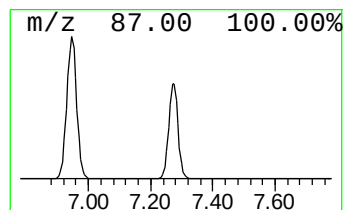
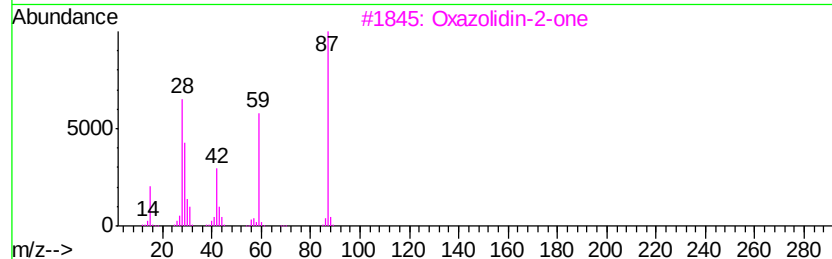
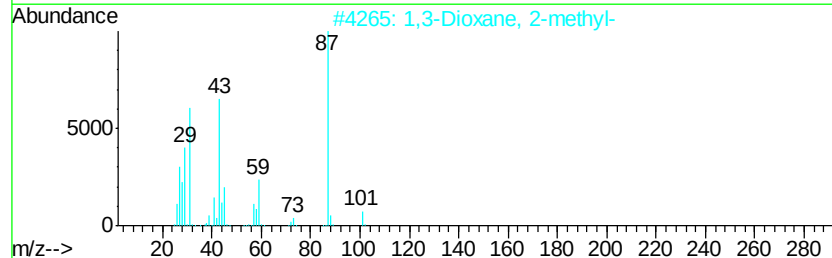
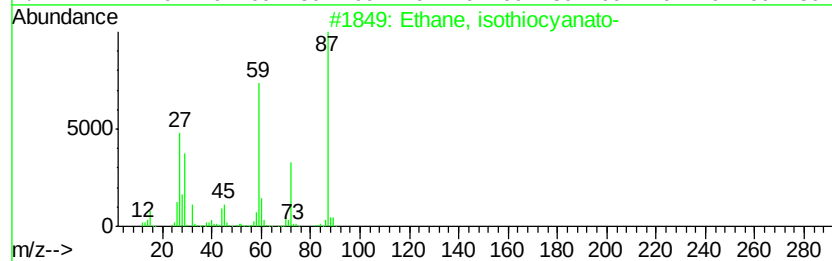
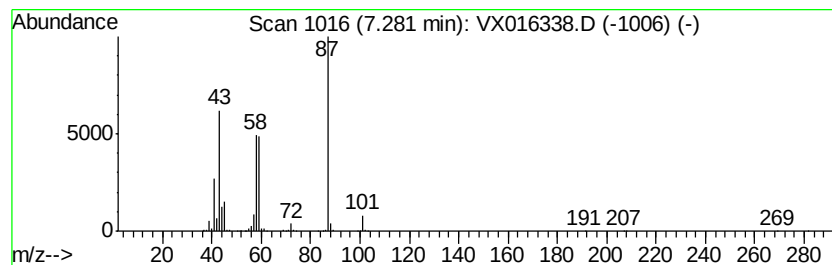
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Peak Number 5 Ethane, isothiocyanato- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	29.96 ug/l	2100400	1,4-Difluorobenzene	6.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethane, isothiocyano-	87	C3H5NS	000542-85-8	53
2		1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	49
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
4		Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	39
5		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36



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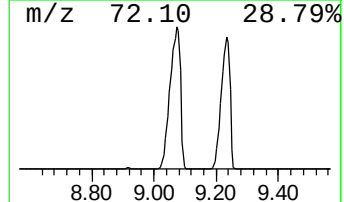
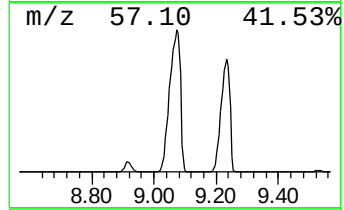
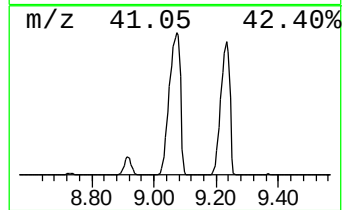
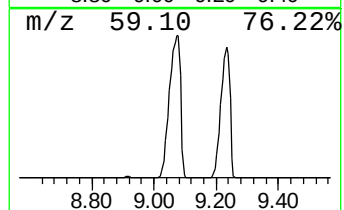
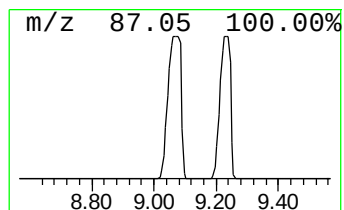
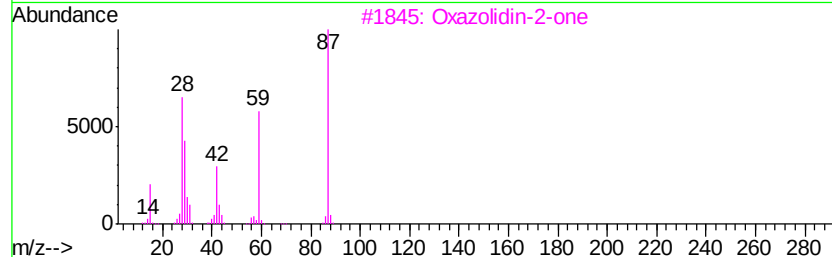
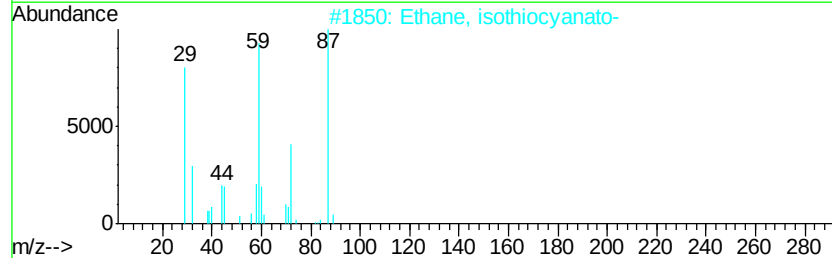
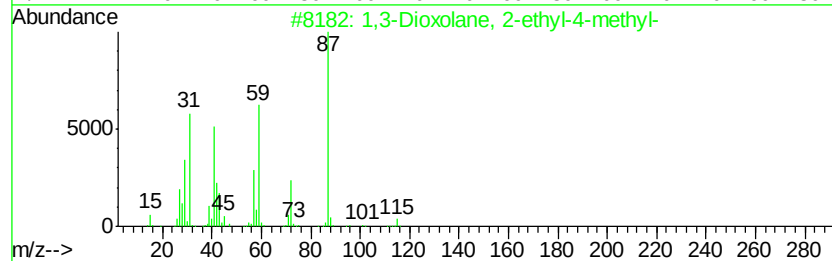
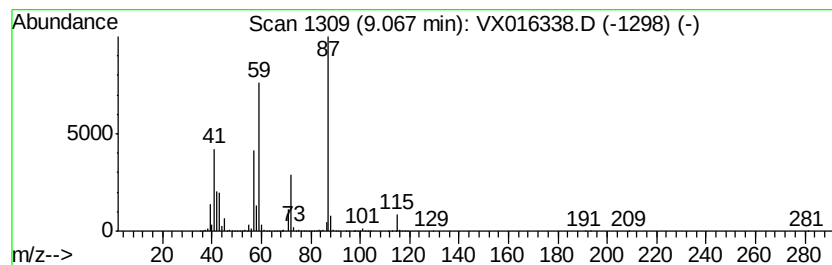
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	77.27 ug/l	97871200	Chlorobenzene-d5	10.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	83
2		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	64
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	53
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	43
5		2-[2-[2-(2-Methoxyethoxy)etho...	294	C13H26O7	1000351-91-3	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016338.D
Acq On : 19 May 2020 16:36
Operator : JC/SP
Sample : L2673-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
102

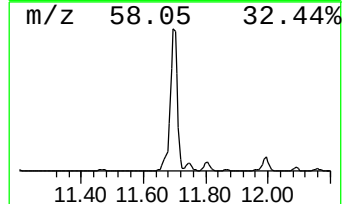
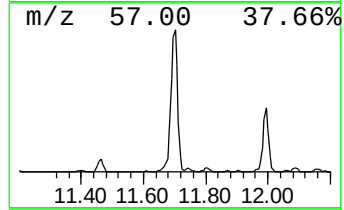
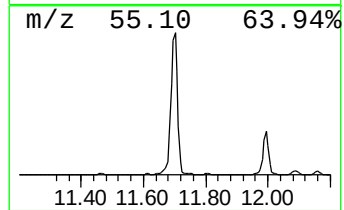
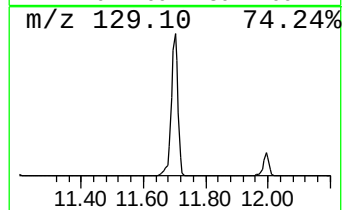
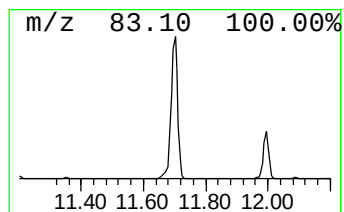
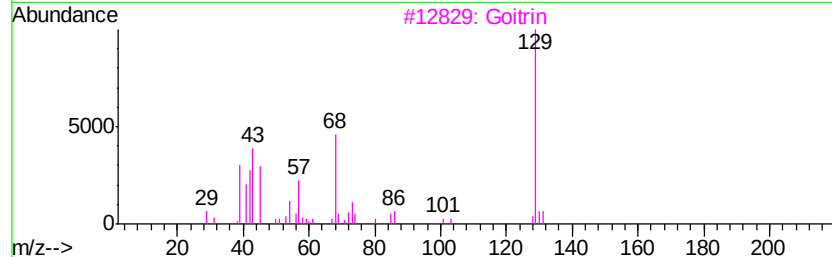
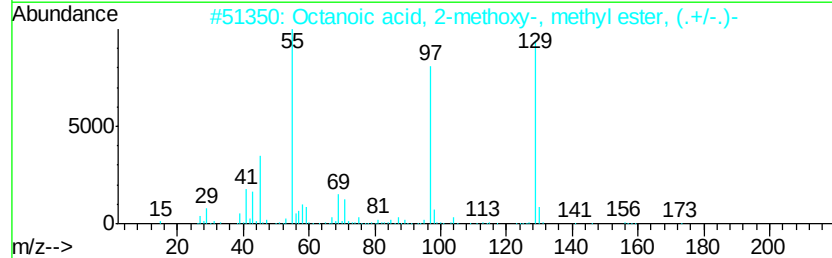
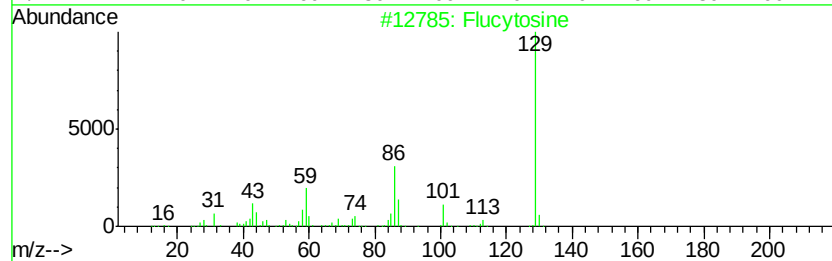
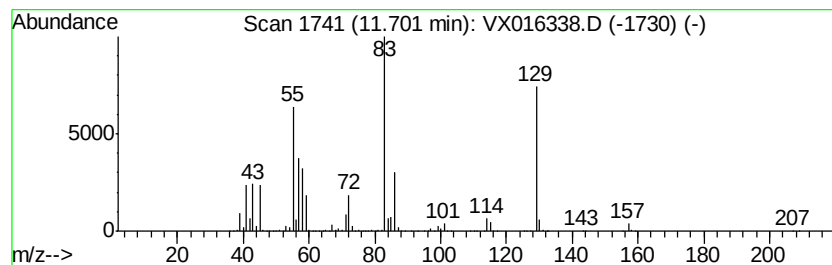
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown11.70 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	347.14 ug/l	9075340	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Flucytosine	129	C4H4FN3O	002022-85-7	35
2		Octanoic acid, 2-methoxy-, methy...	188	C10H20O3	1000332-74-2	35
3		Goitrin	129	C5H7NOS	000500-12-9	25
4		2,5,8,11-Tetraoxatridecan-13-yl ...	292	C14H28O6	1000366-96-8	25
5		2-(2-(2-Methoxyethoxy)ethoxy)eth...	248	C12H24O5	1000367-01-3	23



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016338.D
Acq On : 19 May 2020 16:36
Operator : JC/SP
Sample : L2673-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
102

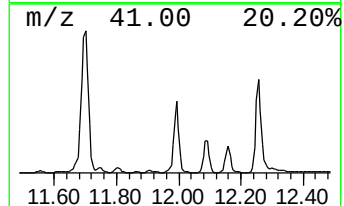
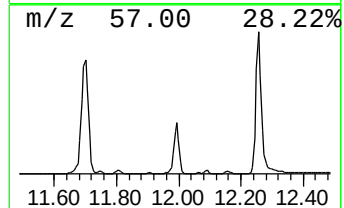
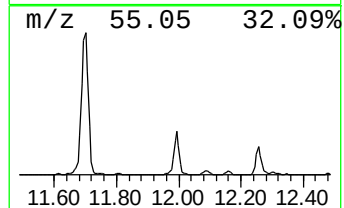
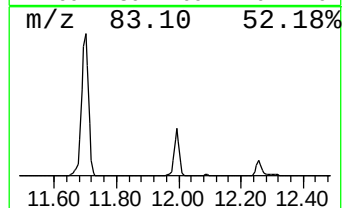
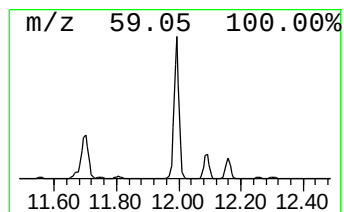
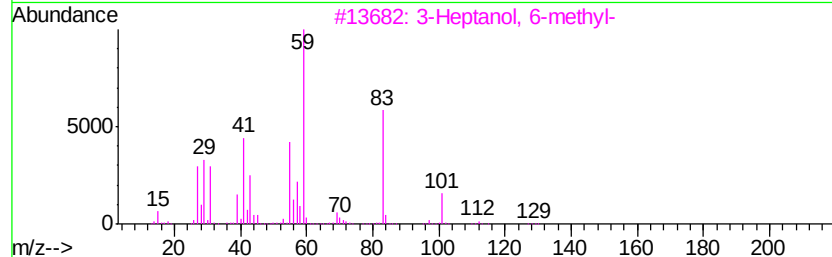
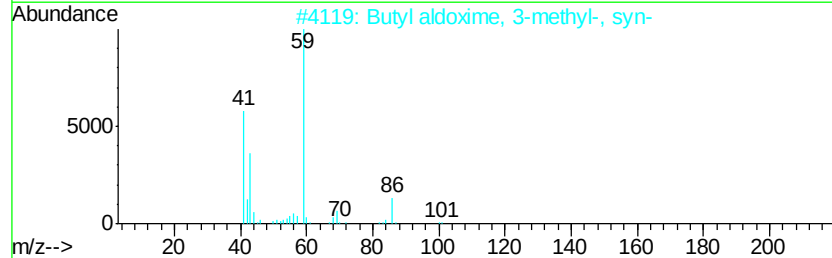
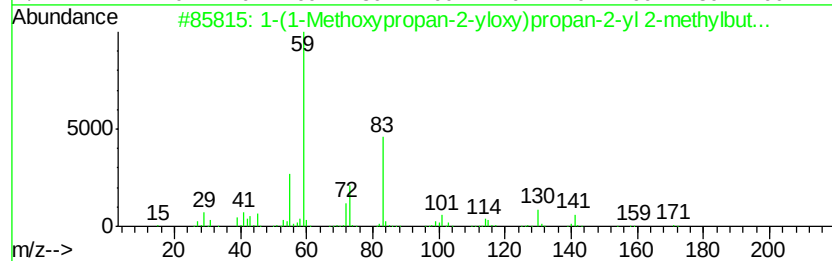
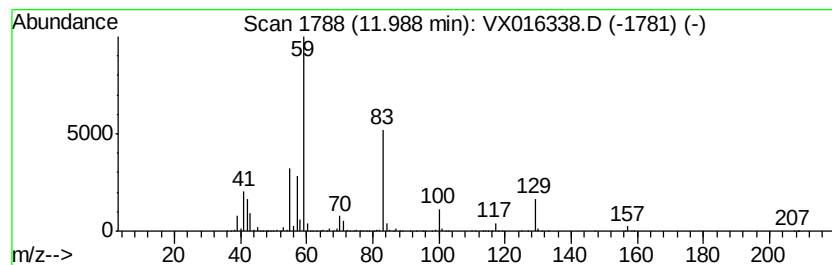
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown11.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	106.20 ug/l	2776470	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(1-Methoxypropan-2-yloxy)propan...	230	C12H22O4	1000367-11-3	45
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	37
3		3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	36
4		Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	33
5		Undecanol-3	172	C11H24O	006929-08-4	28



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016338.D
Acq On : 19 May 2020 16:36
Operator : JC/SP
Sample : L2673-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

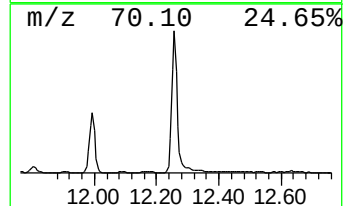
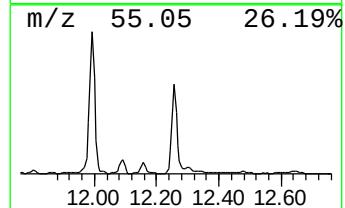
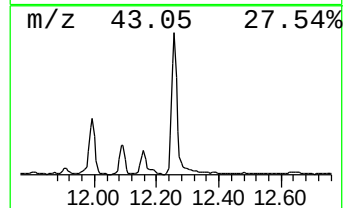
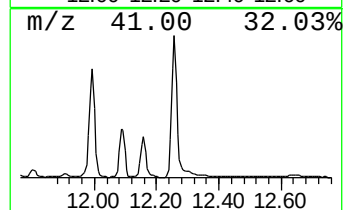
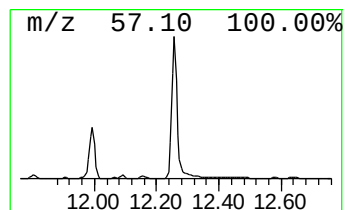
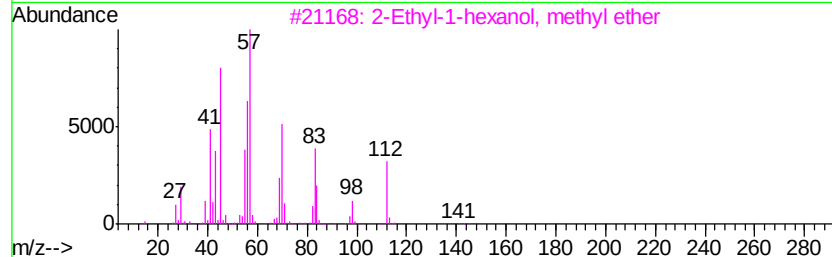
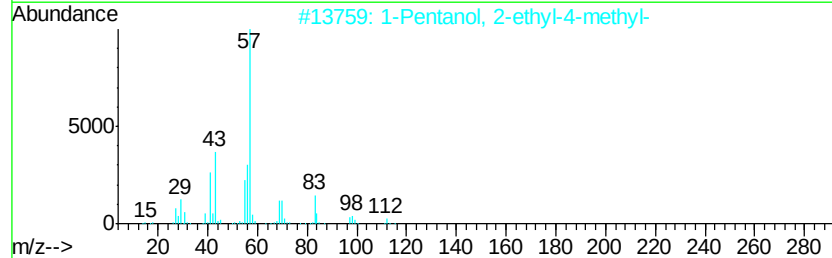
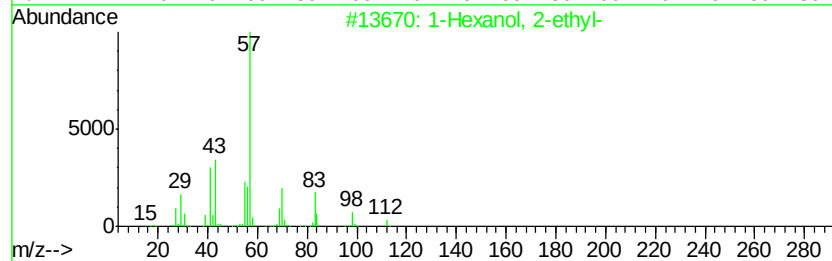
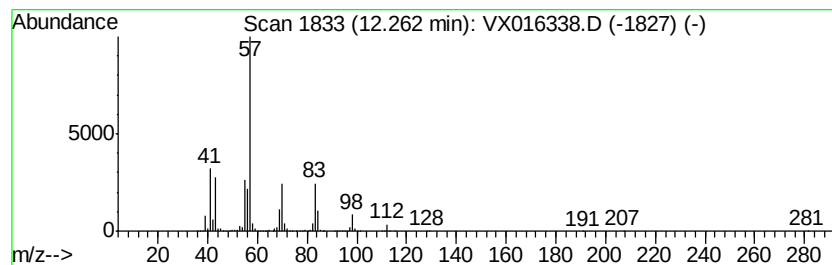
Instrument :
MSVOA_X
ClientSampled :
102

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	78.25 ug/l	2045590	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	56
3	2-Ethyl-1-hexanol, methyl ether	144 C9H20O	1000365-10-2	50
4	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50
5	Heptane, 1,1'-oxybis-	214 C14H30O	000629-64-1	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016338.D
Acq On : 19 May 2020 16:36
Operator : JC/SP
Sample : L2673-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
102

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.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	1.47	115.4	ug/l	8088010	1	5.64	3504860	50.0
Propanal	2.38	1317.2	ug/l	92329700	1	5.64	3504860	50.0
1-Propanol	4.09	563.7	ug/l	39512700	1	5.64	3504860	50.0
1,3-Dioxane, 2-me...	6.95	50.0	ug/l	3504860	2	6.84	3504860	50.0
Ethane, isothiocy...	7.28	30.0	ug/l	2100400	2	6.84	3504860	50.0
1,3-Dioxolane, 2-...	9.07	77.3	ug/l	97871200	3	10.10	63330500	50.0
unknown11.70	11.70	347.1	ug/l	9075340	4	12.06	1307140	50.0
unknown11.99	11.99	106.2	ug/l	2776470	4	12.06	1307140	50.0
1-Hexanol, 2-ethyl-	12.26	78.3	ug/l	2045590	4	12.06	1307140	50.0