

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX012720\
 Data File : VX014722.D
 Acq On : 27 Jan 2020 13:34
 Operator : JC/SP
 Sample : L1266-01 5X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40652

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\82X012220W.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	1.070	26	30	43	rBV	678613	852349	1.76%	0.793%
2	1.484	94	98	108	rBV	1051353	1202018	2.48%	1.118%
3	2.350	232	240	249	rBV2	26645107	48529124	100.00%	45.155%
4	2.435	249	254	274	rVB	2113293	3521400	7.26%	3.277%
5	3.966	489	505	524	rBV	3217359	9372858	19.31%	8.721%
6	5.490	744	755	769	rBV	257982	735390	1.52%	0.684%
7	5.654	771	782	796	rVB	452855	1257436	2.59%	1.170%
8	6.057	838	848	859	rBV	294376	764404	1.58%	0.711%
9	6.849	969	978	989	rBV	717720	1665007	3.43%	1.549%
10	8.709	1277	1283	1290	rBV	1492979	2410667	4.97%	2.243%
11	8.776	1290	1294	1300	rVB	348549	539608	1.11%	0.502%
12	8.922	1312	1318	1326	rBV	987897	1442664	2.97%	1.342%
13	9.056	1333	1340	1354	rVB	11075966	15549834	32.04%	14.469%
14	9.215	1360	1366	1375	rBV	6975900	9601509	19.79%	8.934%
15	10.111	1506	1513	1514	rBV	1580807	2165643	4.46%	2.015%
16	10.129	1514	1516	1523	rVV	2325600	2660220	5.48%	2.475%
17	10.202	1523	1528	1540	rVB	733290	982513	2.02%	0.914%
18	11.135	1675	1681	1687	rBV	1200808	1560701	3.22%	1.452%
19	12.074	1830	1835	1844	rVB	1570923	1965769	4.05%	1.829%
20	12.263	1862	1866	1877	rBV	495350	693392	1.43%	0.645%

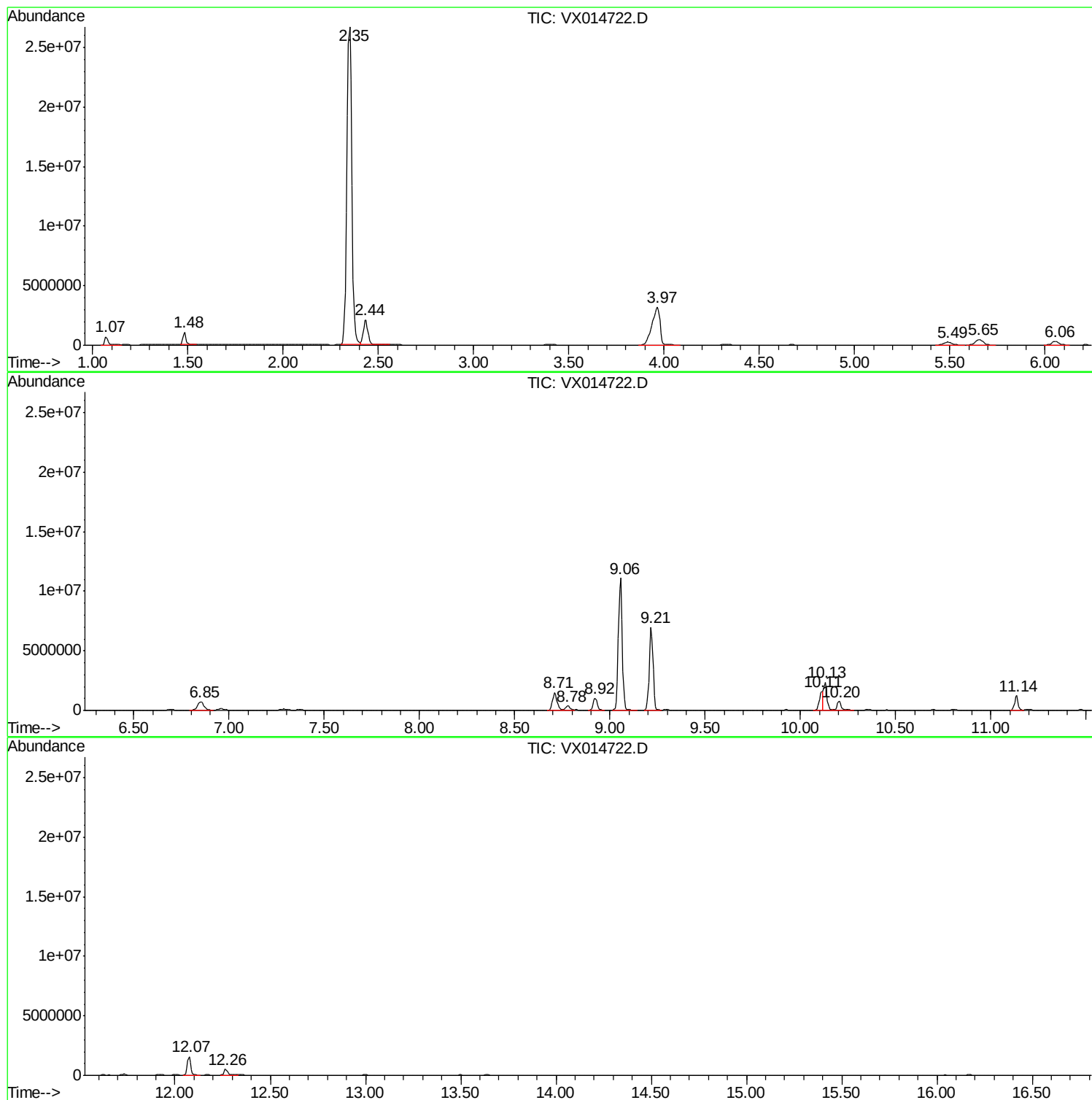
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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



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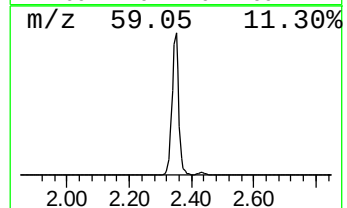
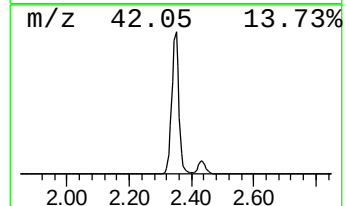
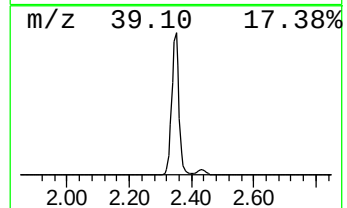
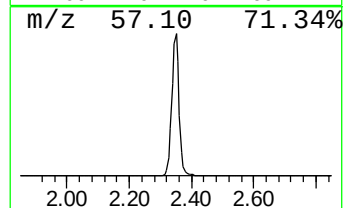
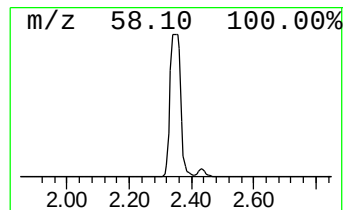
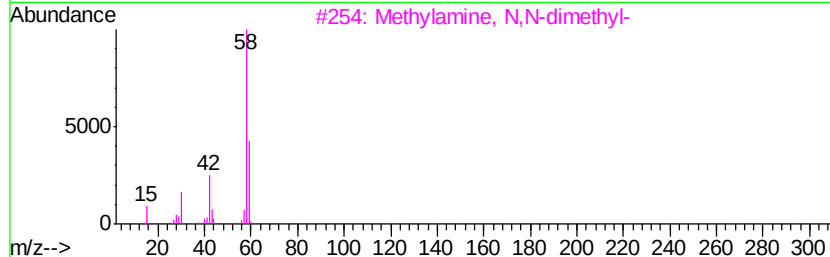
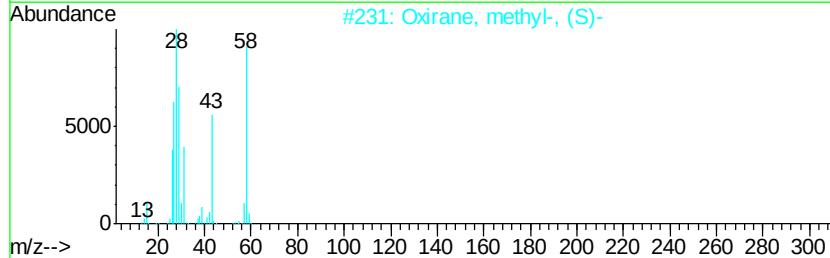
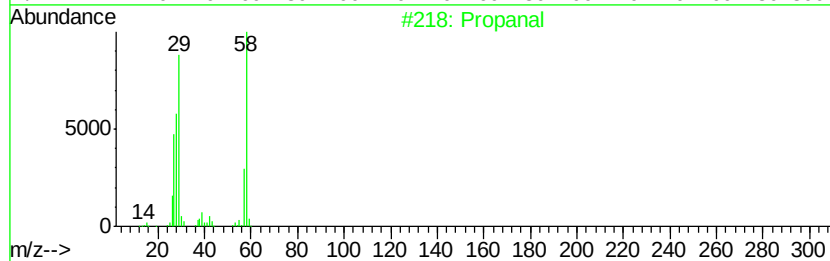
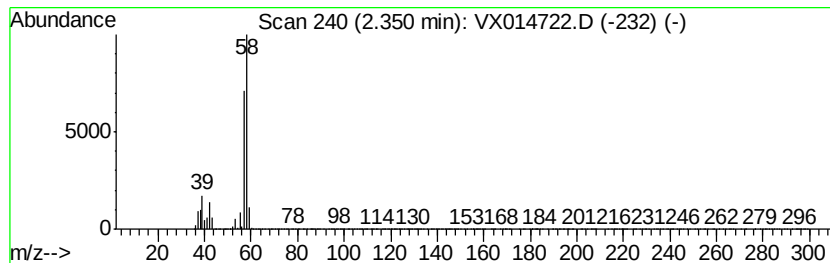
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown2.35 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	1929.69 ug/l	48529100	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal	58	C3H6O	000123-38-6	28
2		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
3		Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	5
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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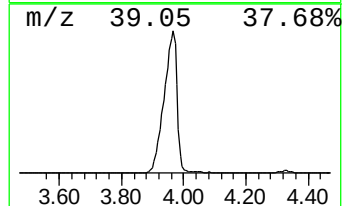
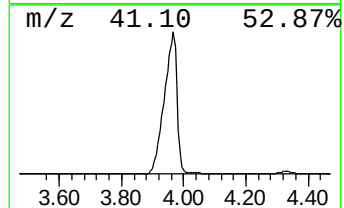
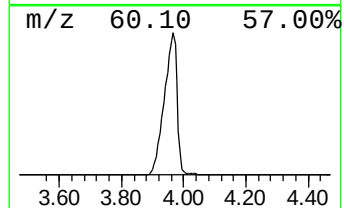
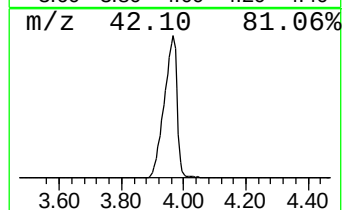
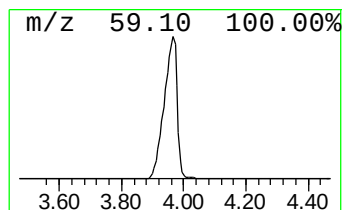
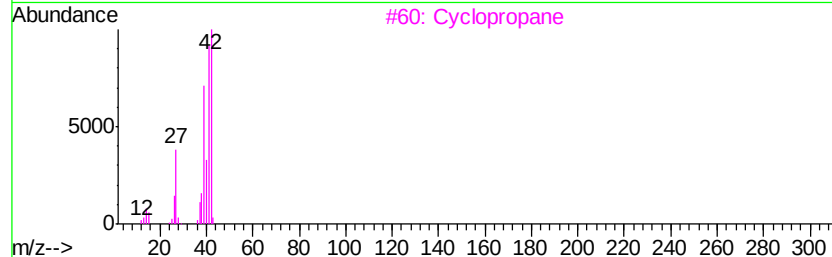
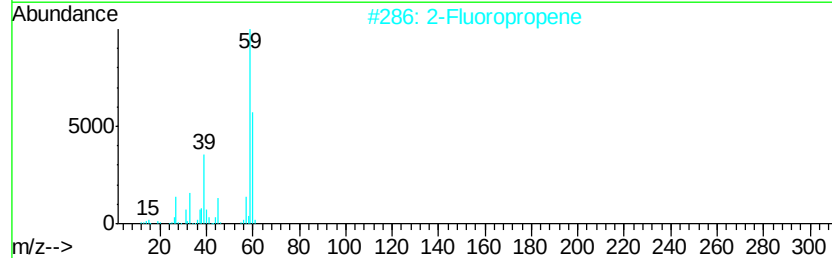
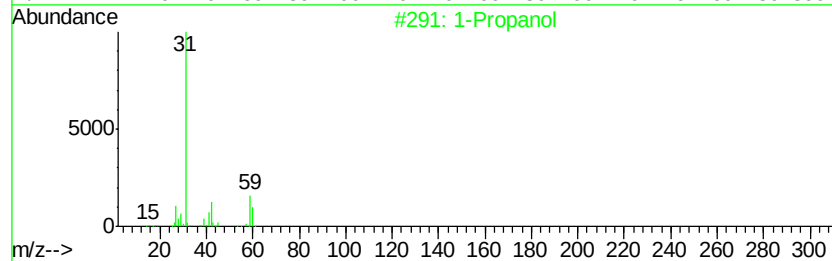
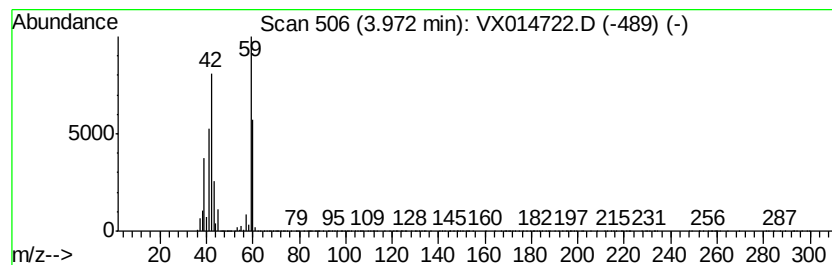
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.97	372.70 ug/l	9372860	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	64
2		2-Fluoropropene	60	C3H5F	001184-60-7	52
3		Cyclopropane	42	C3H6	000075-19-4	32
4		Allyl fluoride	60	C3H5F	000818-92-8	32
5		Propene	42	C3H6	000115-07-1	9



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Instrument :
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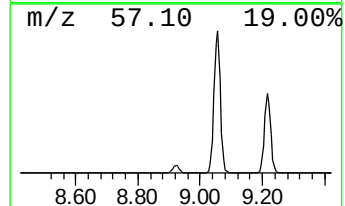
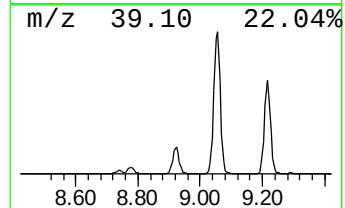
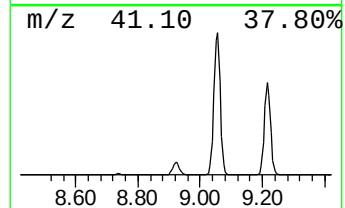
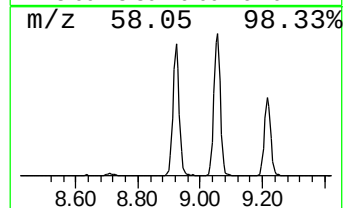
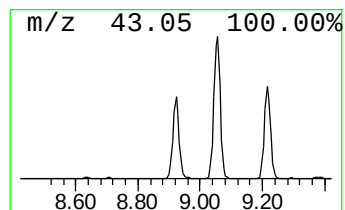
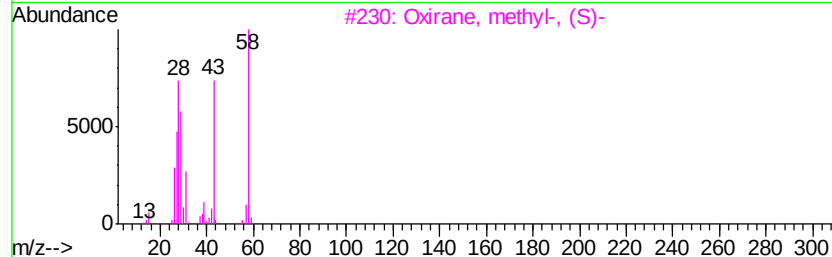
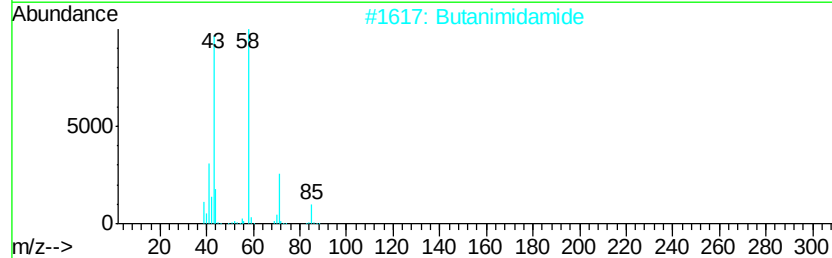
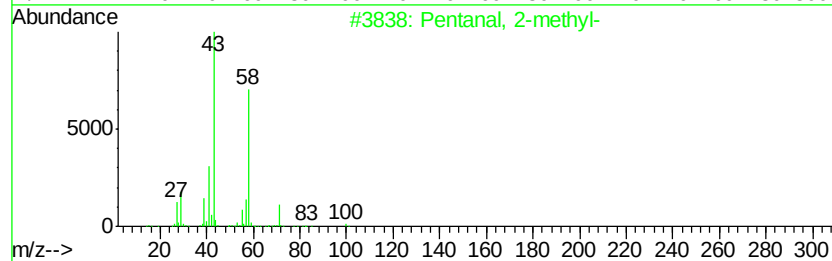
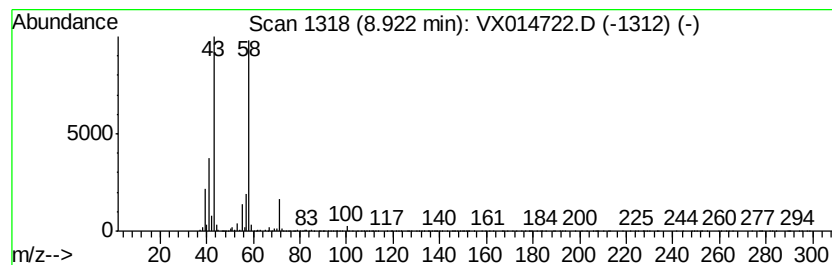
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Quant Title : SW846 8260

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

Peak Number 5 Pentanal, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.92	33.31 ug/l	1442660	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	91
2		Butanimidamide	86	C4H10N2	000107-90-4	64
3		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	64
4		Propanenitrile, 3-(dimethylamino)-	98	C5H10N2	001738-25-6	53
5		2-Propenoic acid, 2-(dimethylami...	143	C7H13NO2	002439-35-2	42



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Instrument :
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ClientSampleId :
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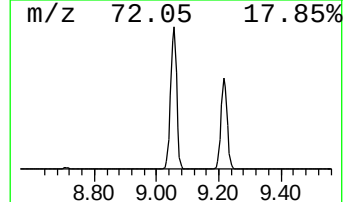
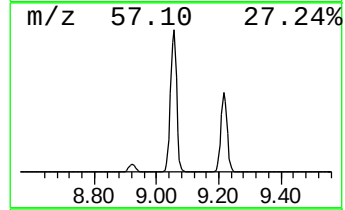
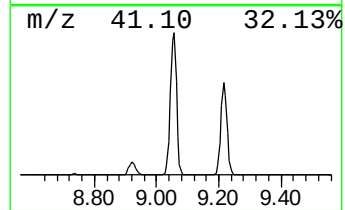
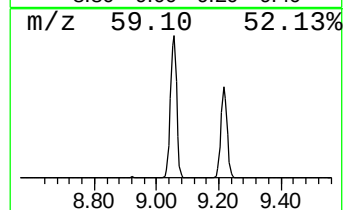
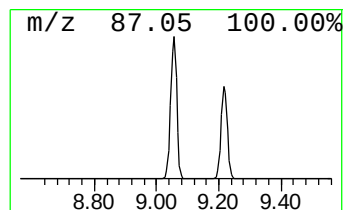
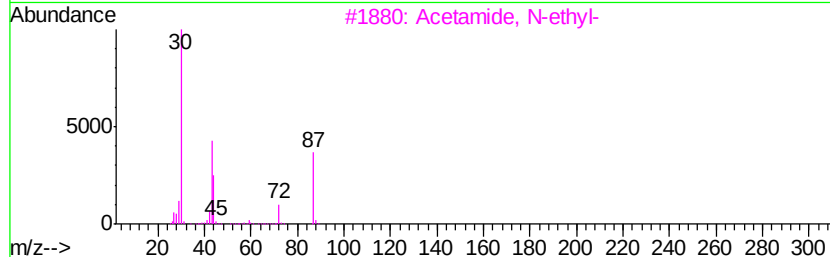
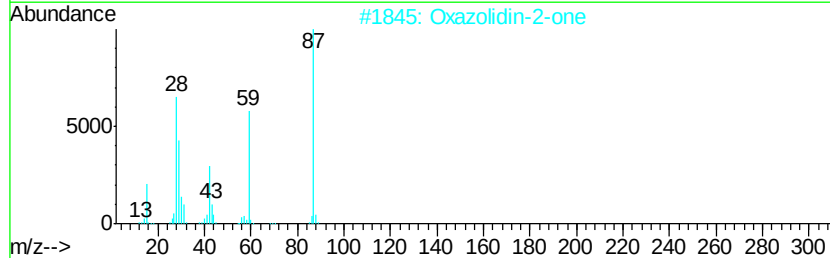
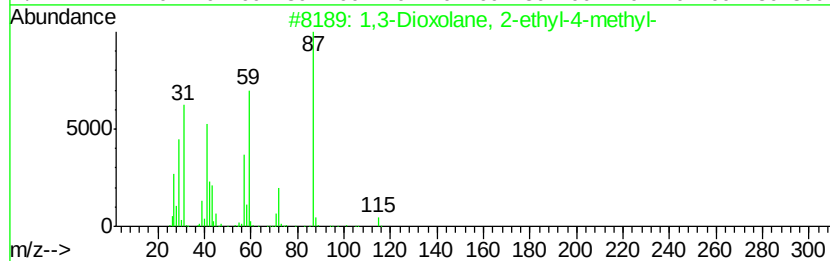
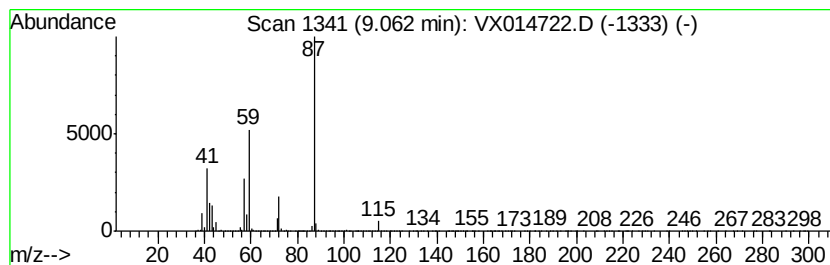
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	359.01 ug/l	15549800	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
4		2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	45



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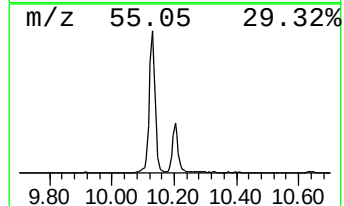
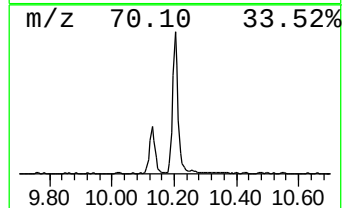
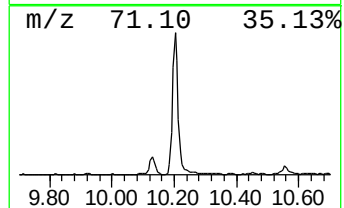
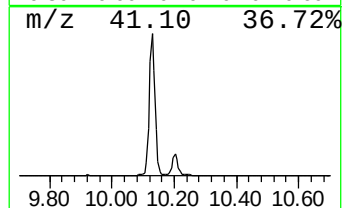
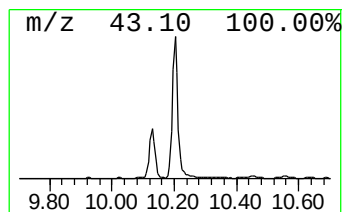
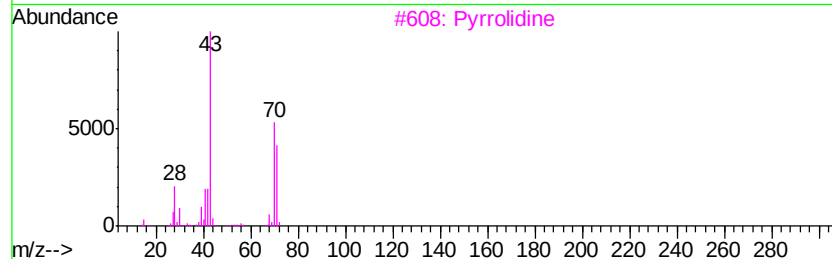
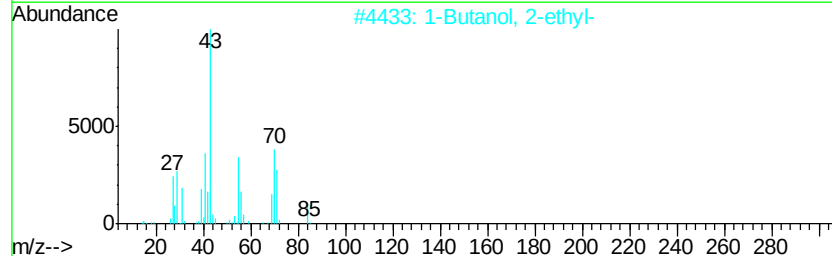
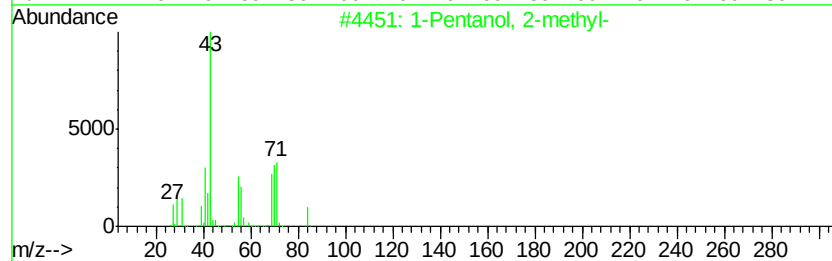
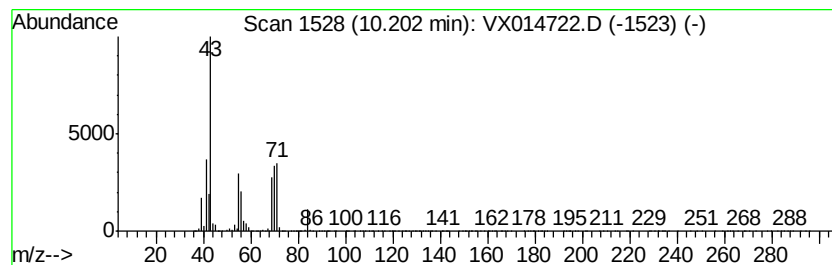
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Pentanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.20	22.68 ug/l	982513	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
3		Pyrrolidine	71	C4H9N	000123-75-1	50
4		2,4,6-Trimethyl-1-nonene	168	C12H24	055771-40-9	50
5		Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	50



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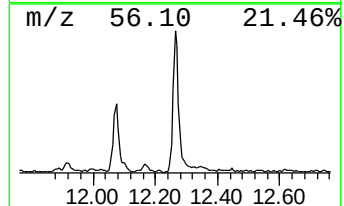
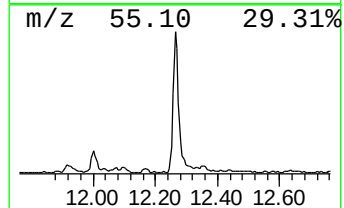
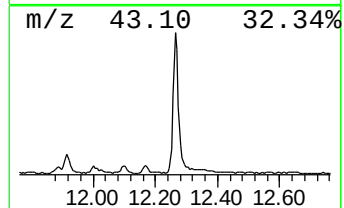
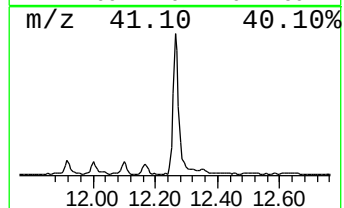
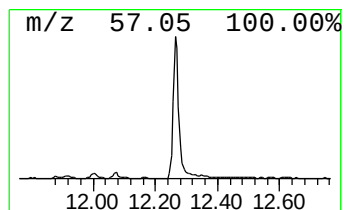
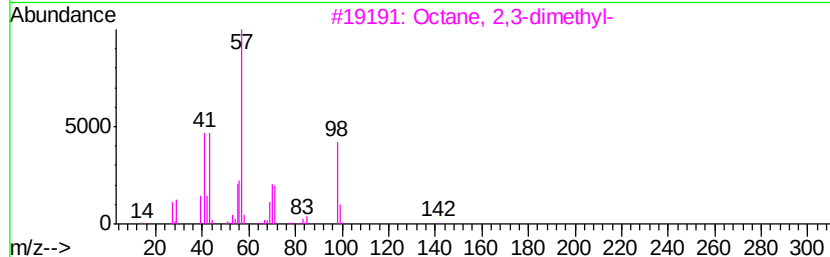
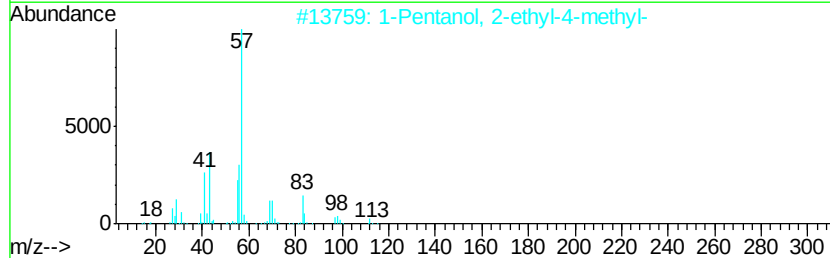
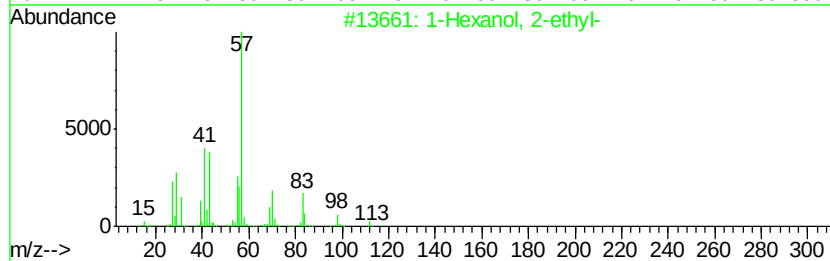
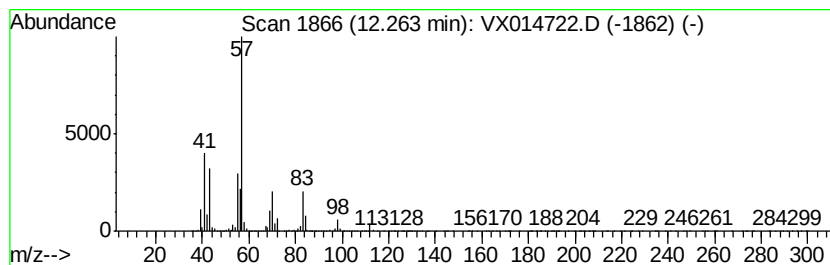
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
 Quant Title : SW846 8260

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

 Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	17.64 ug/l	693392	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
3		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
4		3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47
5		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX012720\
Data File : VX014722.D
Acq On : 27 Jan 2020 13:34
Operator : JC/SP
Sample : L1266-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40652

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.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
unknown2.35	2.35	1929.7	ug/l	48529100	1	5.65	1257440	50.0
1-Propanol	3.97	372.7	ug/l	9372860	1	5.65	1257440	50.0
Pentanal, 2-methyl-	8.92	33.3	ug/l	1442660	3	10.11	2165640	50.0
1,3-Dioxolane, 2-...	9.06	359.0	ug/l	15549800	3	10.11	2165640	50.0
1-Pentanol, 2-met...	10.20	22.7	ug/l	982513	3	10.11	2165640	50.0
1-Hexanol, 2-ethyl-	12.26	17.6	ug/l	693392	4	12.07	1965770	50.0