

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020620\
 Data File : VX014859.D
 Acq On : 06 Feb 2020 19:40
 Operator : JC/SP
 Sample : L1419-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-1

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	1245872	1531603	3.81%	1.776%
2	1.472	93	96	128	rBV	28145380	40184801	100.00%	46.603%
3	2.119	193	202	228	rVB	8529437	14908780	37.10%	17.290%
4	2.344	233	239	247	rVV	300350	491669	1.22%	0.570%
5	2.430	247	253	270	rVB	536409	887775	2.21%	1.030%
6	4.326	553	564	585	rBV	2628140	7164835	17.83%	8.309%
7	5.490	745	755	766	rBV2	253257	714408	1.78%	0.829%
8	5.655	770	782	795	rVB	451270	1272450	3.17%	1.476%
9	6.051	839	847	857	rBV	285037	715361	1.78%	0.830%
10	6.850	967	978	990	rVB	691590	1642782	4.09%	1.905%
11	7.289	1041	1050	1068	rBV	2418375	4959374	12.34%	5.752%
12	8.709	1277	1283	1289	rBV	1502482	2286200	5.69%	2.651%
13	8.776	1289	1294	1300	rVB	816857	1247197	3.10%	1.446%
14	10.105	1502	1512	1523	rBV	1470295	2034339	5.06%	2.359%
15	10.361	1547	1554	1560	rBV2	630369	856230	2.13%	0.993%
16	11.129	1675	1680	1686	rBV	1229193	1614762	4.02%	1.873%
17	12.074	1830	1835	1842	rVB	1647289	2016113	5.02%	2.338%
18	12.263	1862	1866	1878	rBV	594420	853401	2.12%	0.990%
19	15.683	2421	2427	2430	rBV	268956	437145	1.09%	0.507%
20	16.744	2596	2601	2608	rVB2	222537	408151	1.02%	0.473%

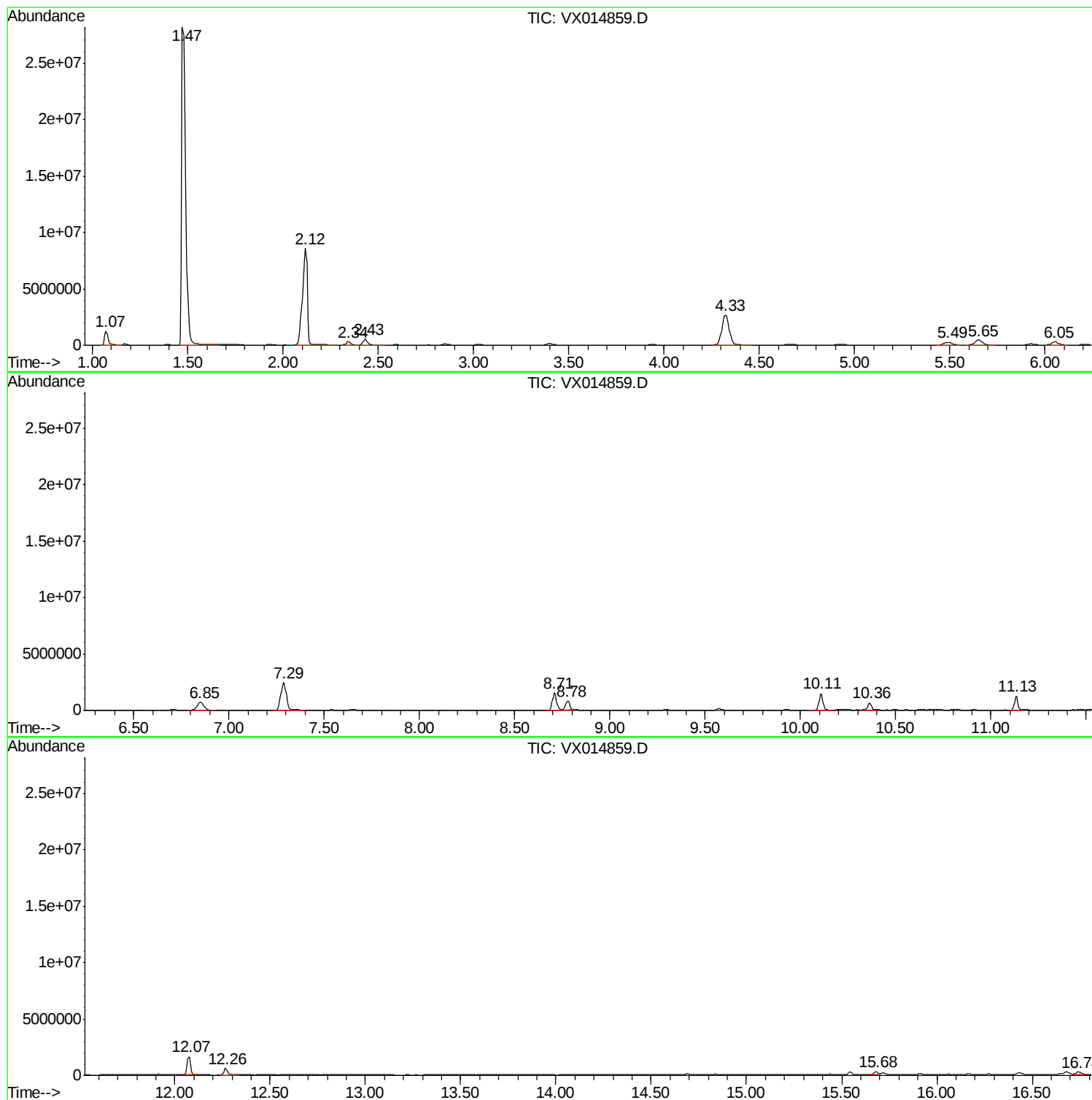
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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



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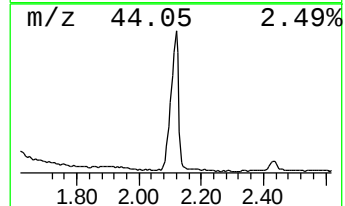
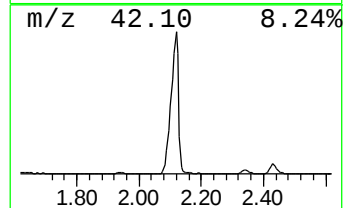
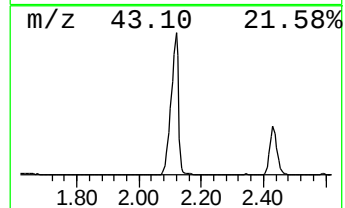
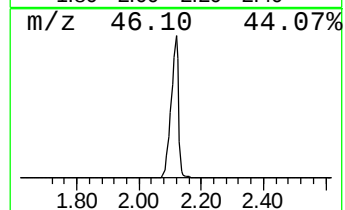
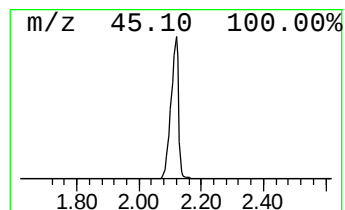
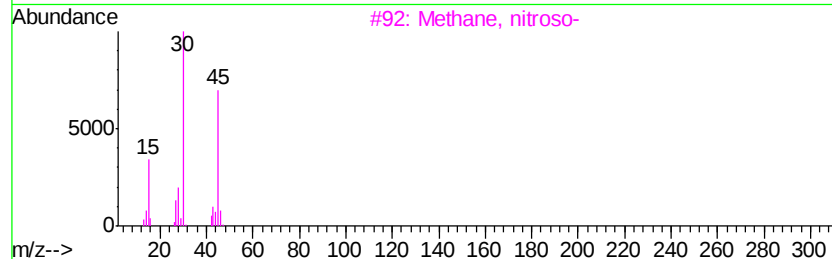
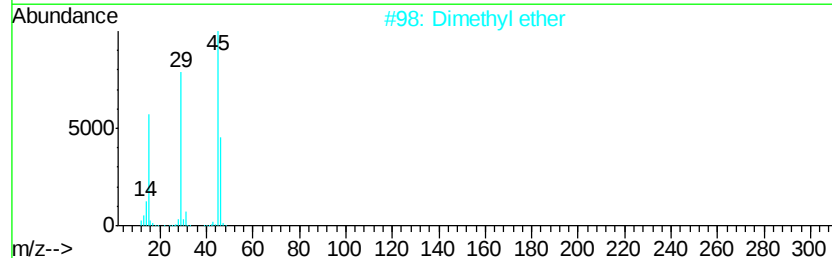
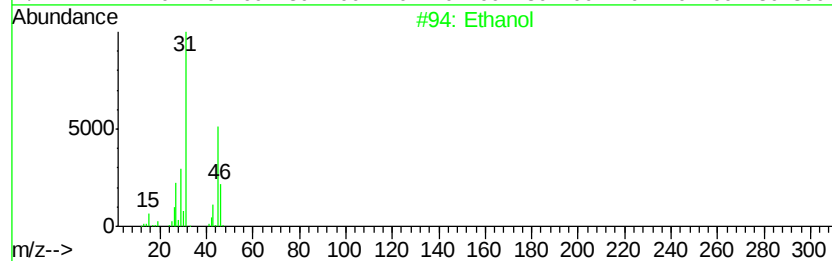
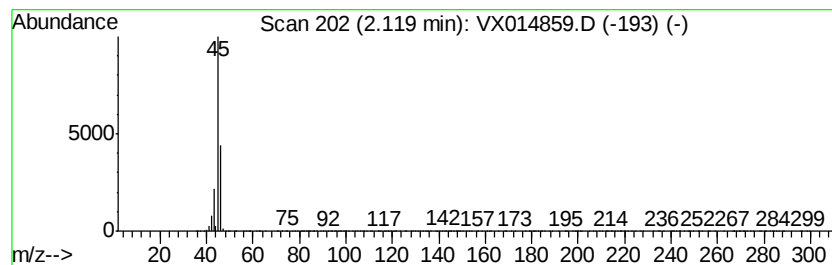
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	585.83 ug/l	14908800	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	86
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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Instrument :
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ClientSampleId :
COMP-1

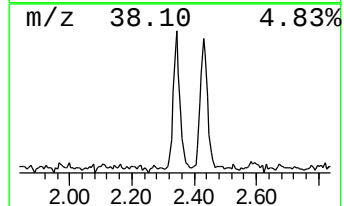
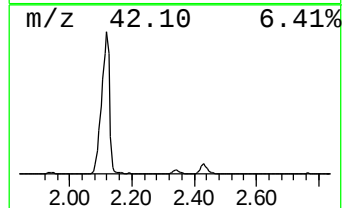
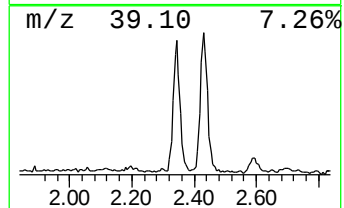
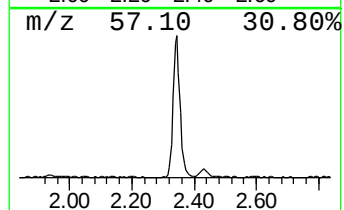
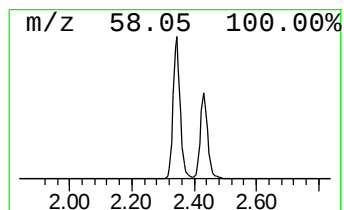
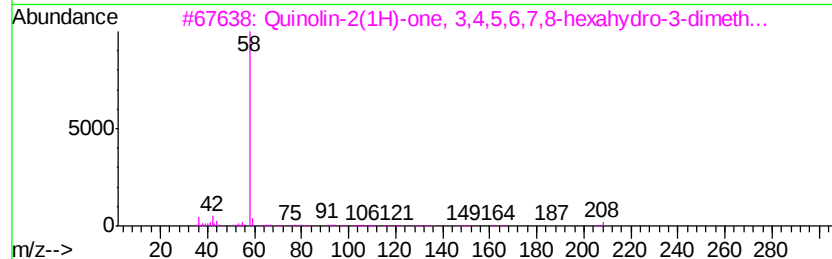
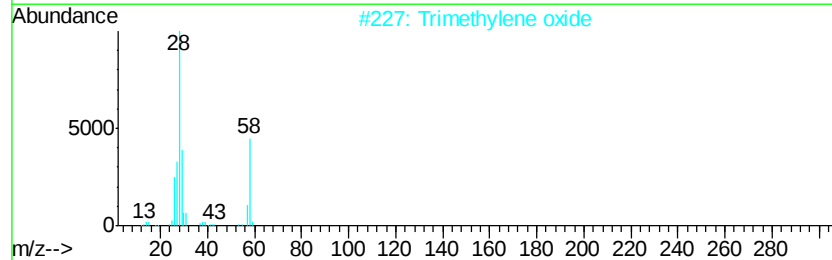
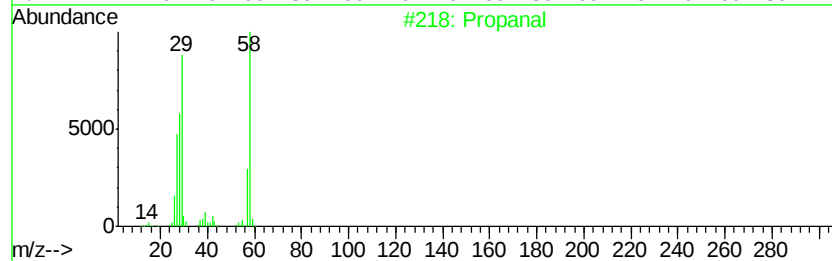
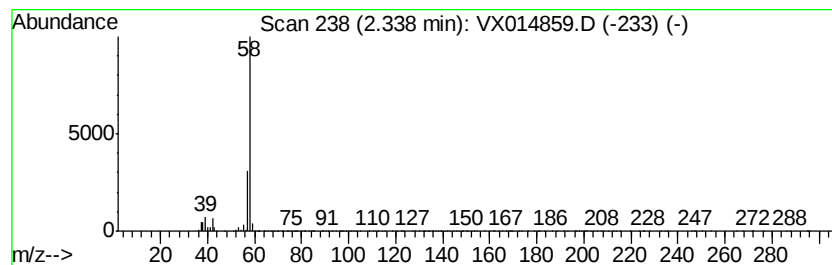
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 4 Propanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	19.32 ug/l	491669	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	9
5		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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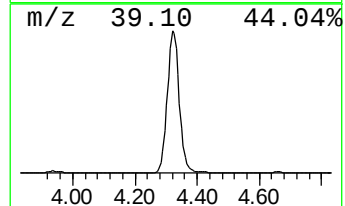
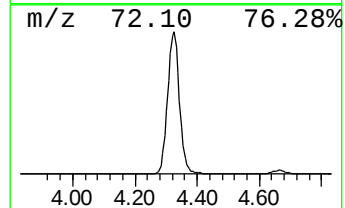
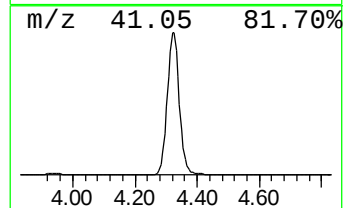
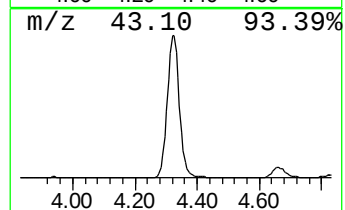
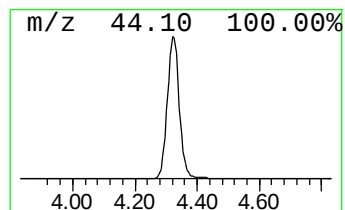
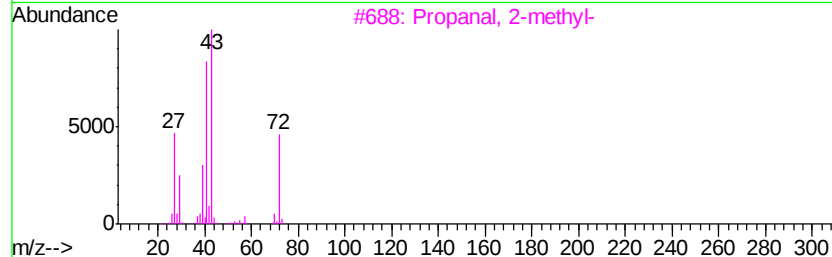
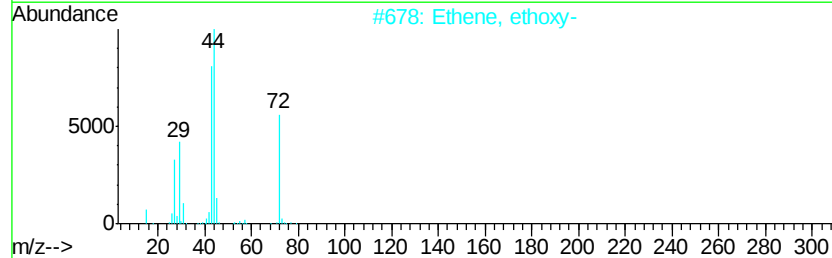
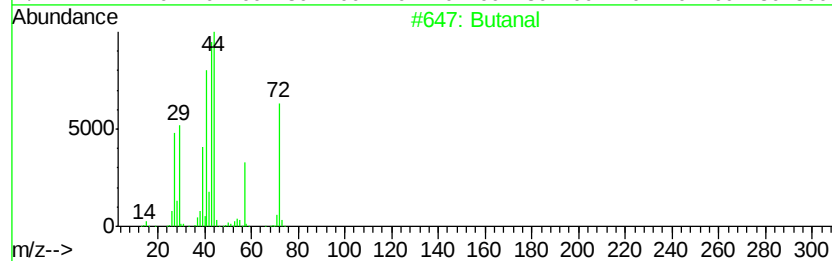
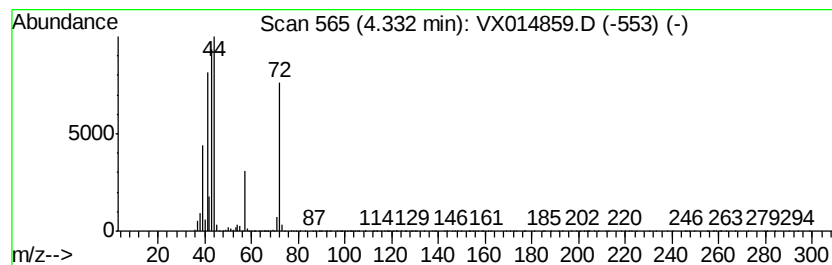
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	281.54 ug/l	7164840	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	94
2		Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5		Isobutylene epoxide	72	C4H8O	000558-30-5	35



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Misc : 5.0mL/MSVOA X/WATER
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Instrument :
MSVOA_X
ClientSampleId :
COMP-1

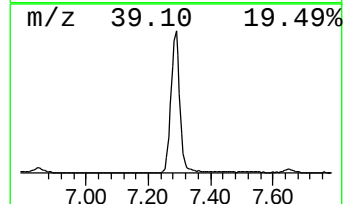
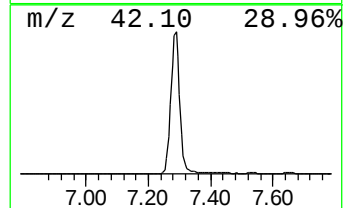
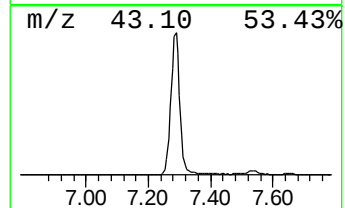
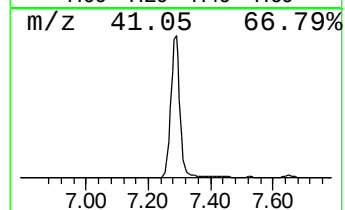
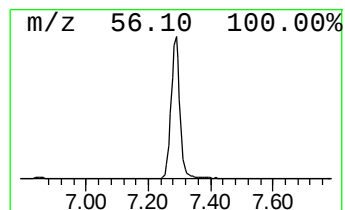
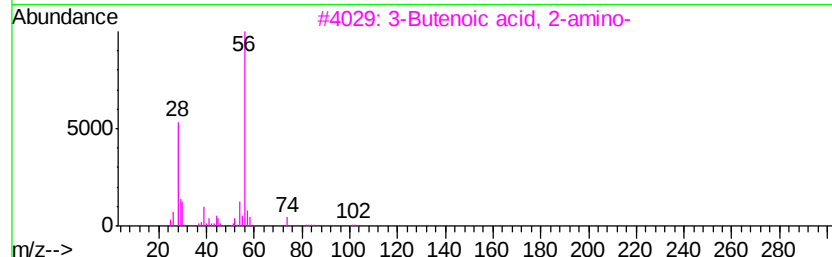
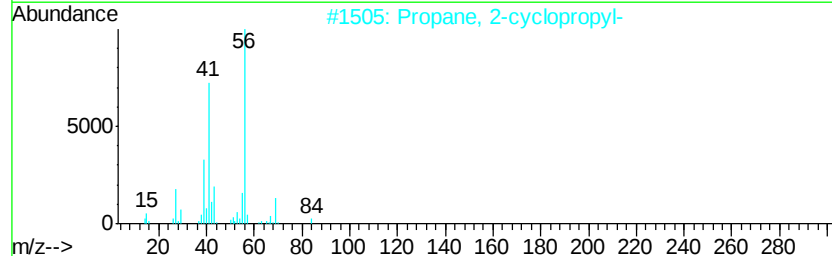
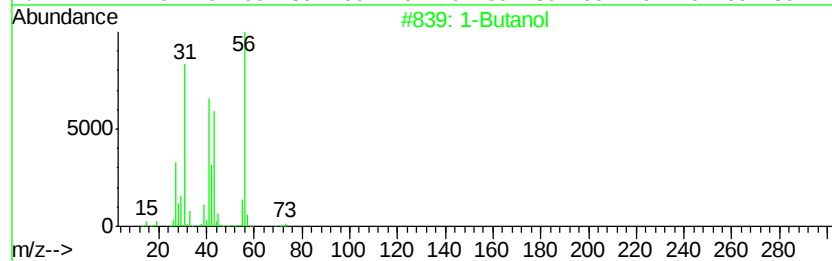
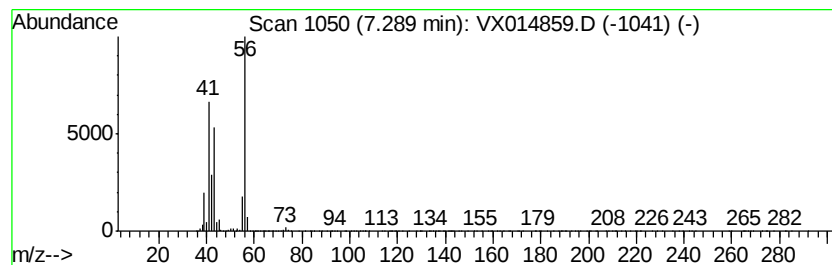
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	150.94 ug/l	4959370	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	90
2		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
3		3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
4		Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	9



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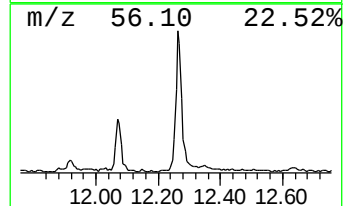
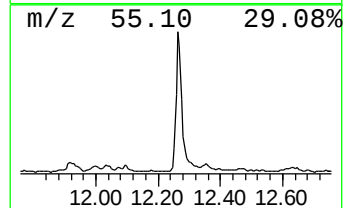
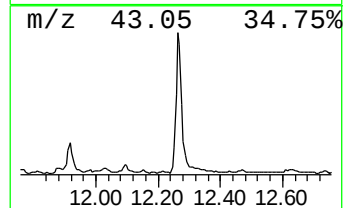
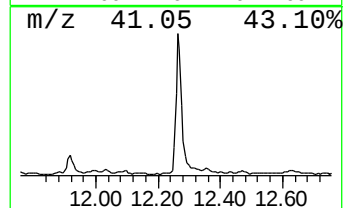
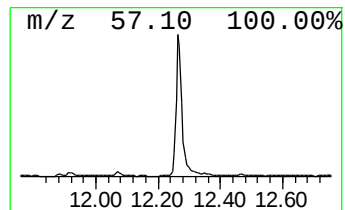
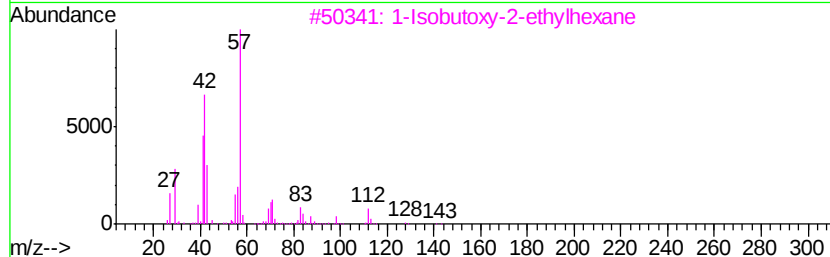
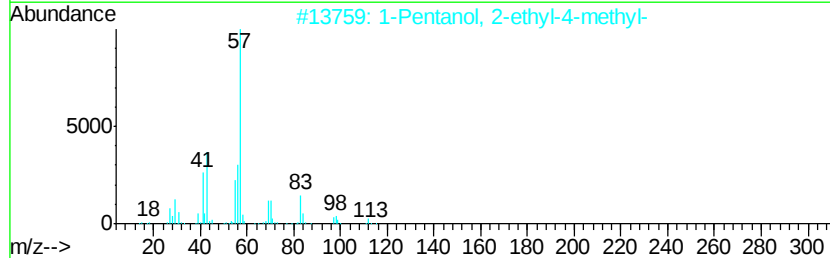
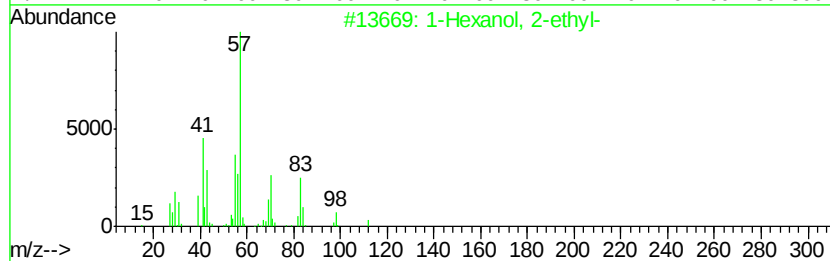
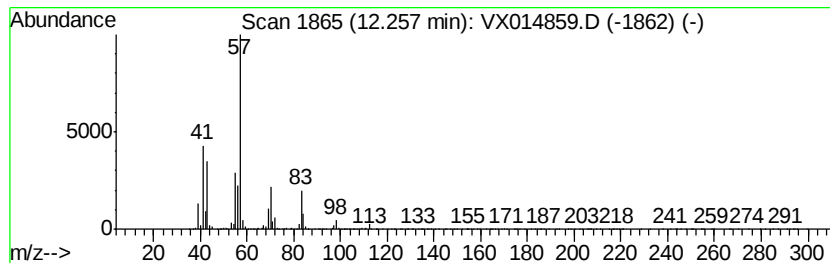
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	21.16 ug/l	853401	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	78
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4		Isobutyl octan-2-yl carbonate	230	C13H26O3	1000372-74-7	56
5		Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	50



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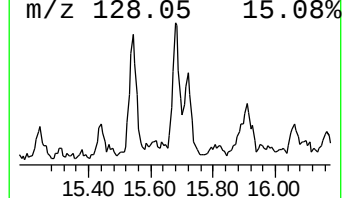
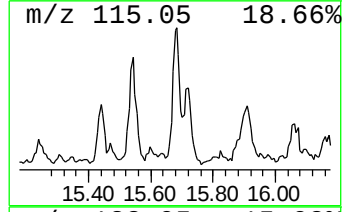
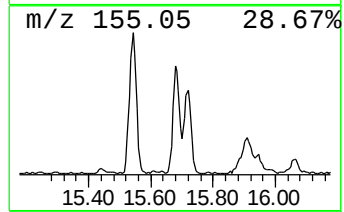
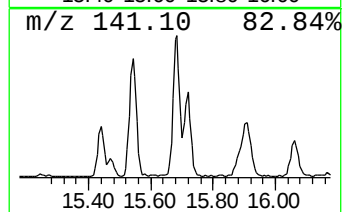
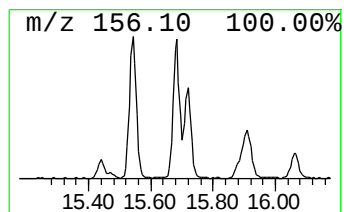
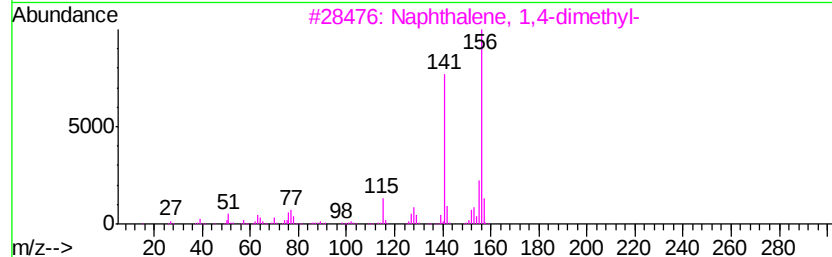
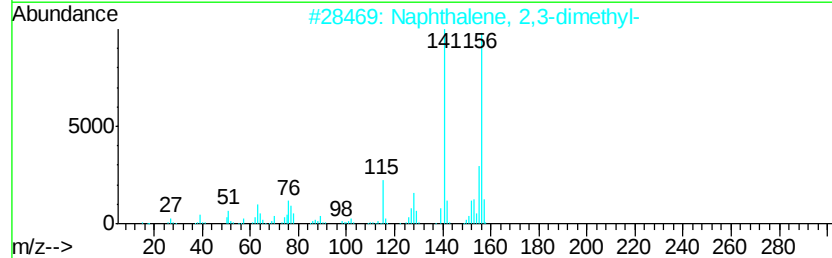
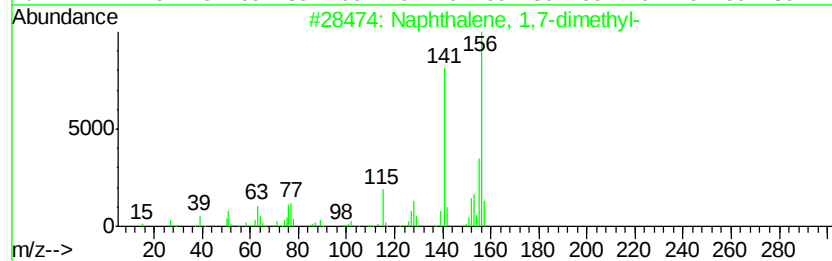
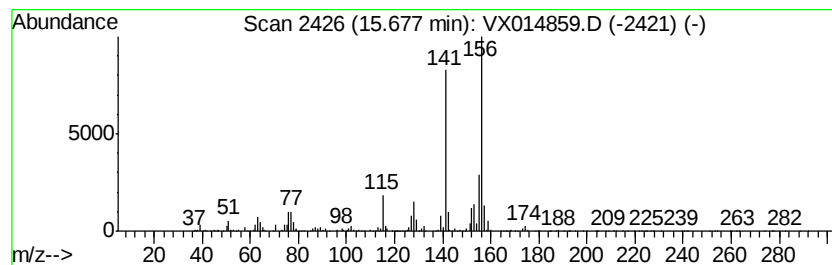
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,7-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	10.84 ug/l	437145	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
2		Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
3		Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4		Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5		Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX020620\
Data File : VX014859.D
Acq On : 06 Feb 2020 19:40
Operator : JC/SP
Sample : L1419-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

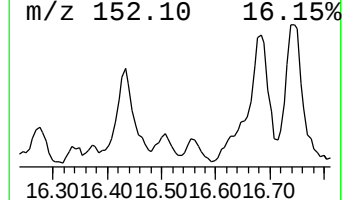
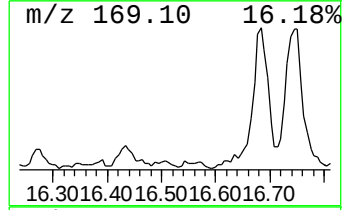
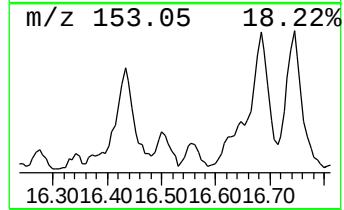
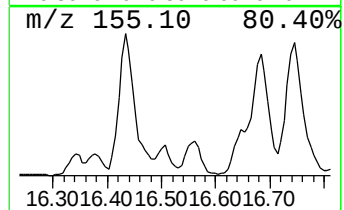
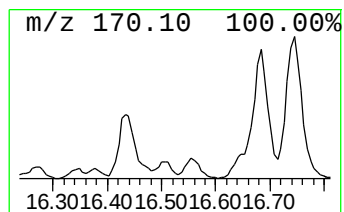
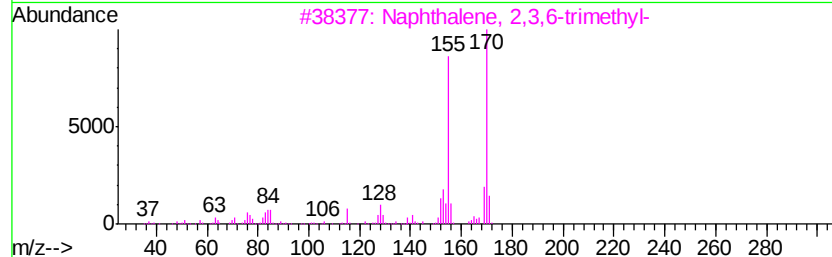
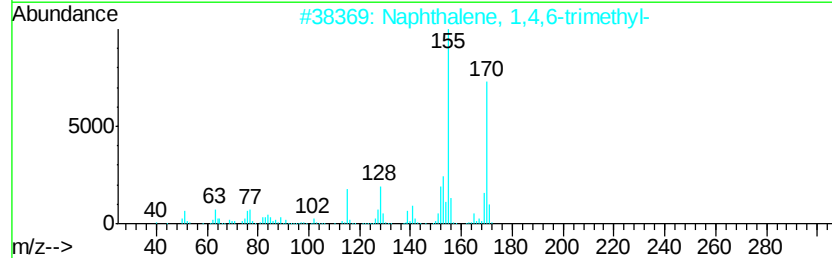
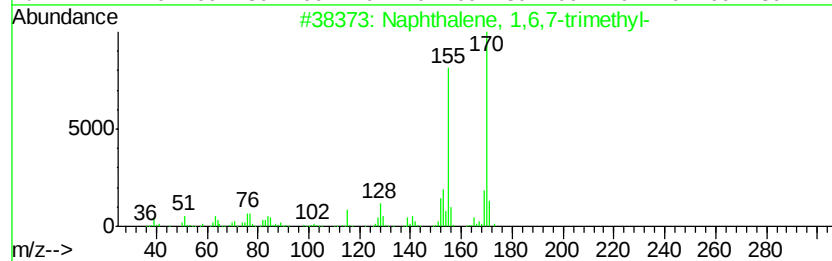
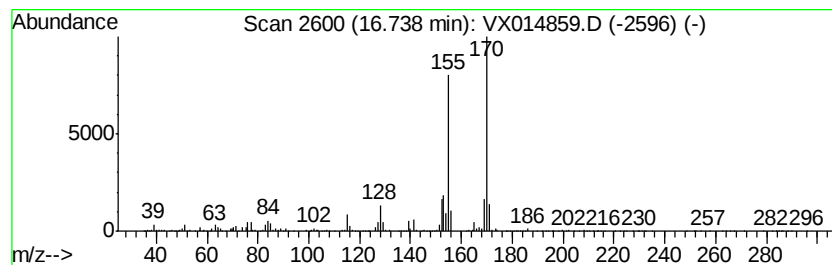
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,6,7-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	10.12 ug/l	408151	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	98
2		Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	97
3		Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	95
4		4,6,8-Trimethylazulene	170	C13H14	000941-81-1	94
5		Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX020620\
Data File : VX014859.D
Acq On : 06 Feb 2020 19:40
Operator : JC/SP
Sample : L1419-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

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
Ethanol	2.12	585.8	ug/l	14908800	1	5.65	1272450	50.0
Propanal	2.34	19.3	ug/l	491669	1	5.65	1272450	50.0
Butanal	4.33	281.5	ug/l	7164840	1	5.65	1272450	50.0
1-Butanol	7.29	150.9	ug/l	4959370	2	6.85	1642780	50.0
1-Hexanol, 2-ethyl-	12.26	21.2	ug/l	853401	4	12.07	2016110	50.0
Naphthalene, 1,7-...	15.68	10.8	ug/l	437145	4	12.07	2016110	50.0
Naphthalene, 1,6,...	16.74	10.1	ug/l	408151	4	12.07	2016110	50.0