

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122418\
Data File : VX006805.D
Acq On : 24 Dec 2018 19:44
Operator : JC/MD
Sample : J6533-19
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

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\82X121818W.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	1.489	51	55	68	rBV	12031944	14907151	100.00%	30.588%
2	2.129	152	160	181	rBV	4116195	6709390	45.01%	13.767%
3	2.446	207	212	225	rVB	220258	375437	2.52%	0.770%
4	2.782	258	267	275	rBV	90377	174322	1.17%	0.358%
5	3.068	300	314	322	rBV	167960	425689	2.86%	0.873%
6	4.348	511	524	538	rBV	273533	805229	5.40%	1.652%
7	4.696	568	581	599	rBV	1522589	4269697	28.64%	8.761%
8	5.184	648	661	674	rBV2	161137	508965	3.41%	1.044%
9	5.501	699	713	725	rBV	360304	1034334	6.94%	2.122%
10	5.665	727	740	755	rVV	669617	1892317	12.69%	3.883%
11	6.068	796	806	814	rBV	384567	981805	6.59%	2.015%
12	6.860	925	936	948	rBV	974137	2264186	15.19%	4.646%
13	7.323	1004	1012	1025	rBV	202888	445003	2.99%	0.913%
14	8.713	1233	1240	1247	rBV	2045445	3129067	20.99%	6.421%
15	8.787	1247	1252	1258	rVB	113403	180362	1.21%	0.370%
16	10.110	1461	1469	1481	rBV	2008689	2745345	18.42%	5.633%
17	10.366	1501	1511	1517	rBV2	317103	517133	3.47%	1.061%
18	10.707	1561	1567	1580	rVB3	132836	245956	1.65%	0.505%
19	11.134	1632	1637	1643	rBV	1727350	2212446	14.84%	4.540%
20	11.920	1759	1766	1775	rVB	94222	162216	1.09%	0.333%
21	12.079	1787	1792	1799	rVB	2230152	2711245	18.19%	5.563%
22	12.274	1818	1824	1835	rBV	1306319	1856204	12.45%	3.809%
23	12.469	1851	1856	1862	rVB	146156	181776	1.22%	0.373%

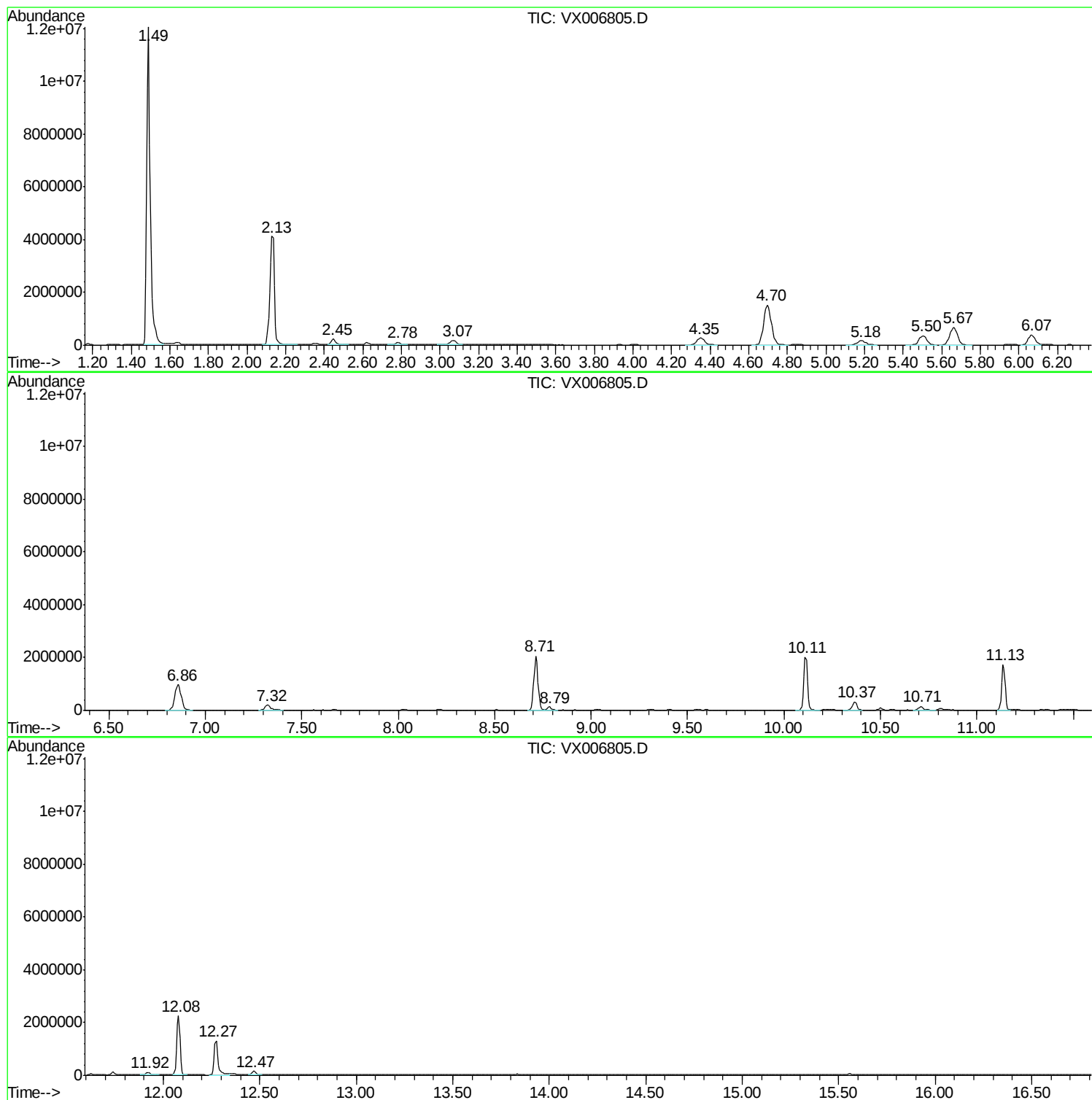
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Quant Title : SW846 8260

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



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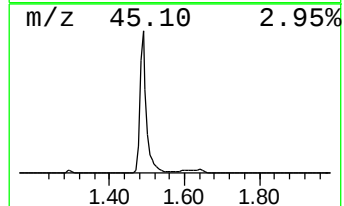
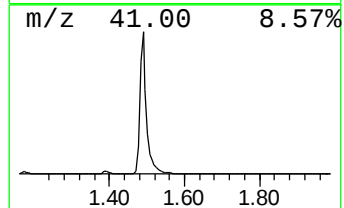
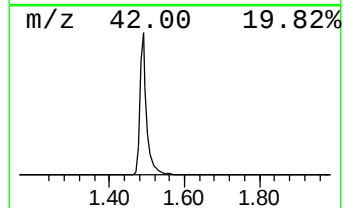
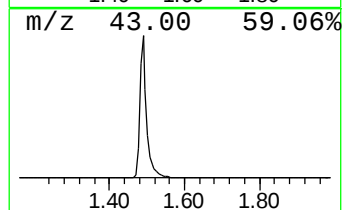
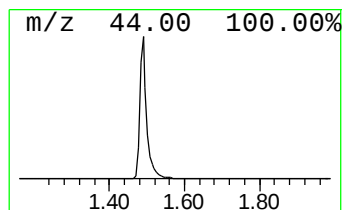
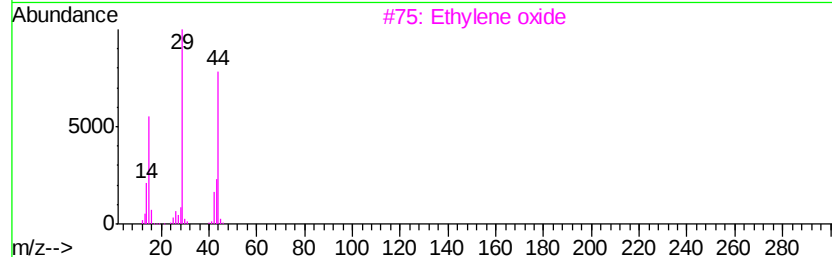
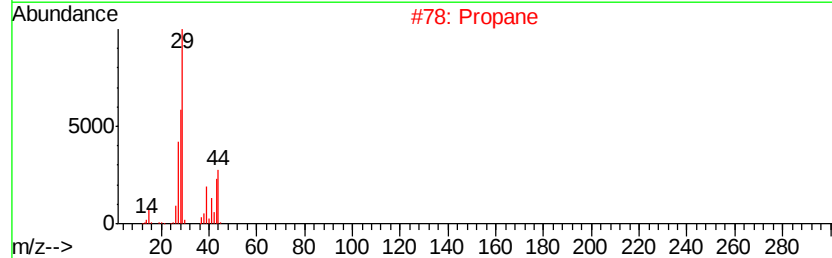
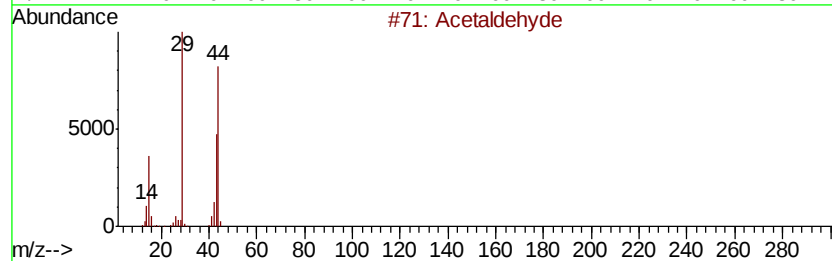
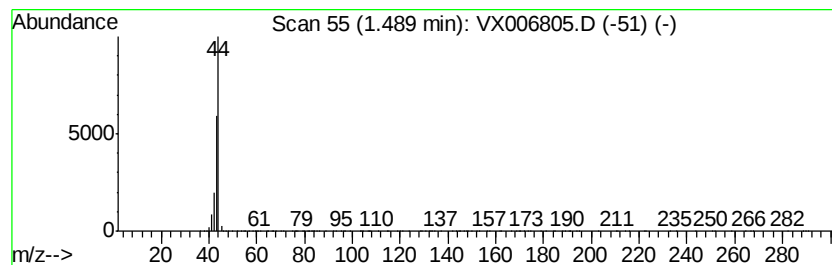
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	393.89 ug/l	14907200	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehydve	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		Ethyne, fluoro-	44	C2HF	002713-09-9	3



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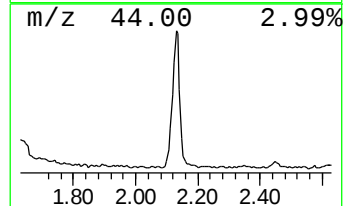
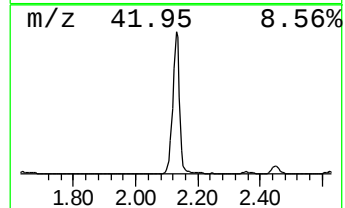
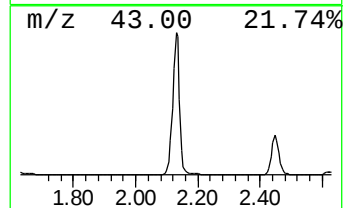
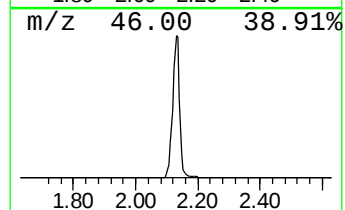
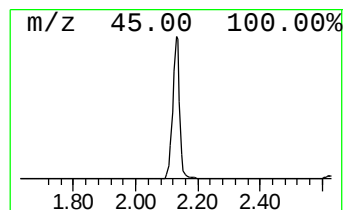
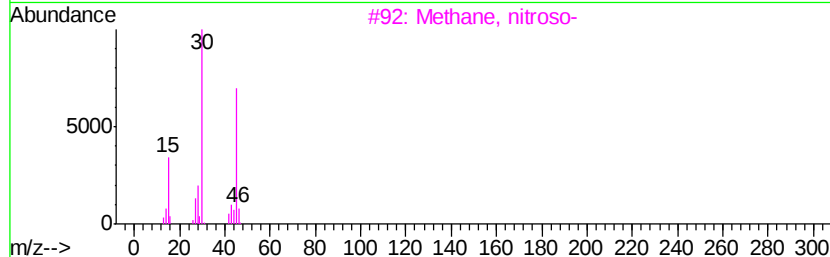
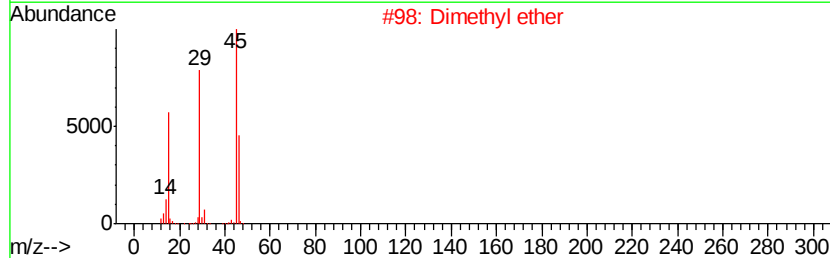
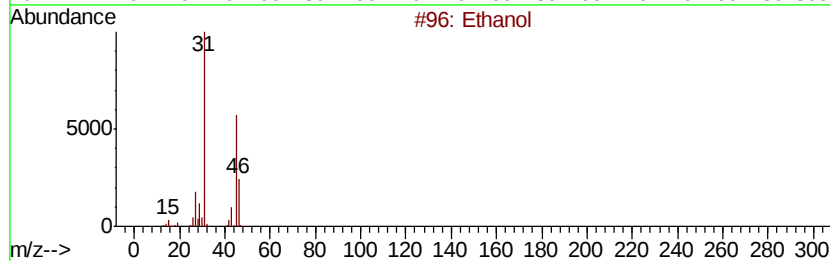
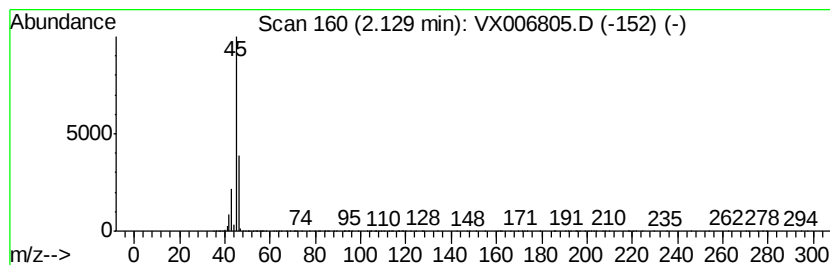
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	177.28 ug/l	6709390	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	64
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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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
COMP-5

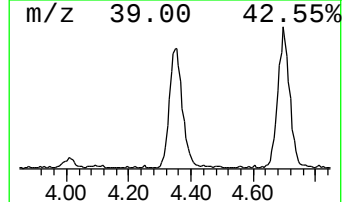
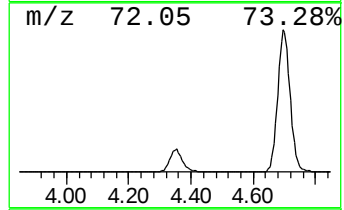
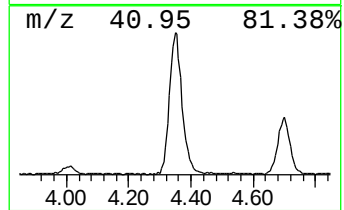
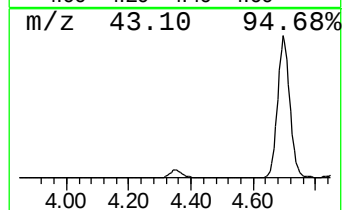
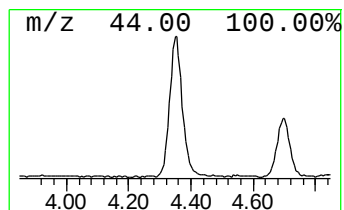
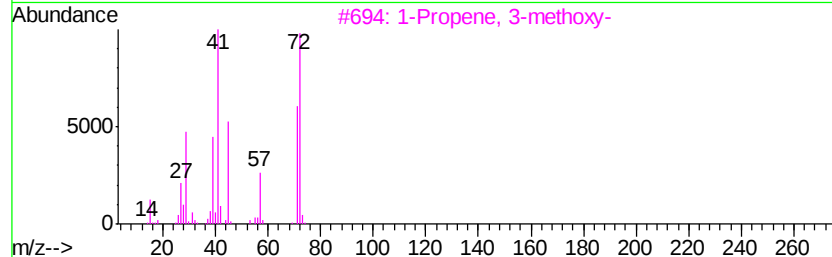
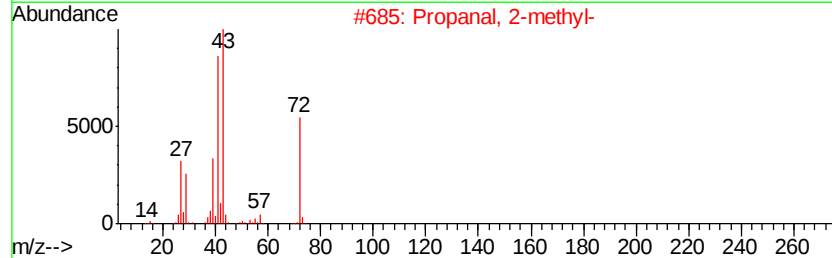
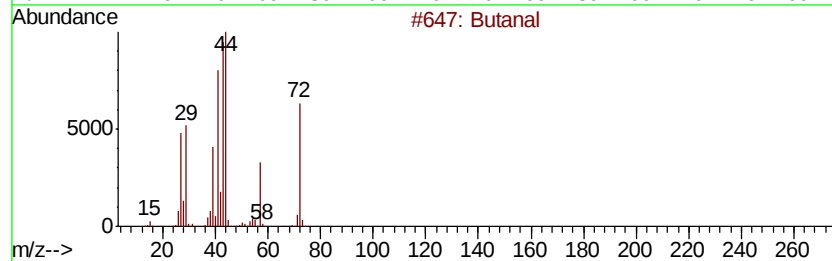
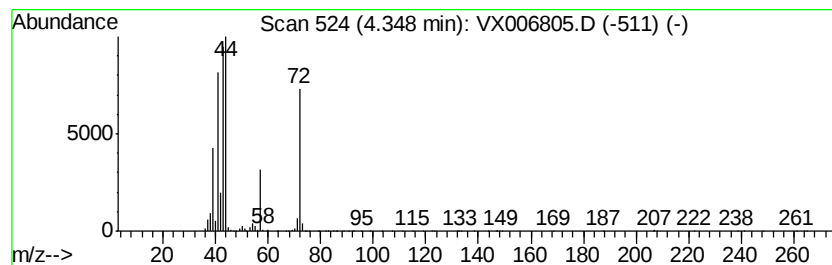
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Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	21.28 ug/l	805229	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4		Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5		O-Methylisourea	74	C2H6N2O	002440-60-0	25



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Instrument :
MSVOA_X
ClientSampleId :
COMP-5

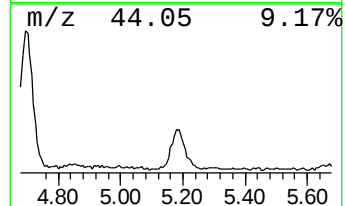
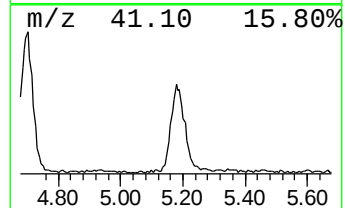
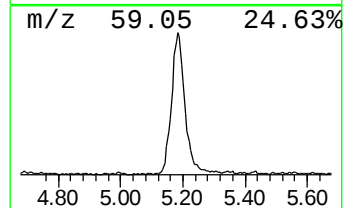
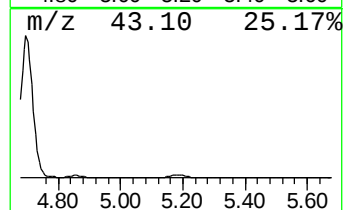
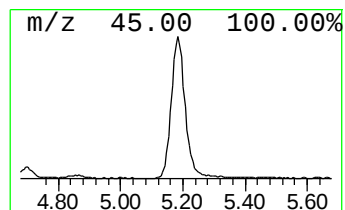
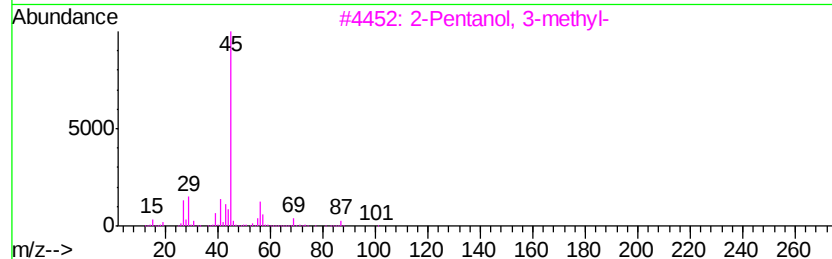
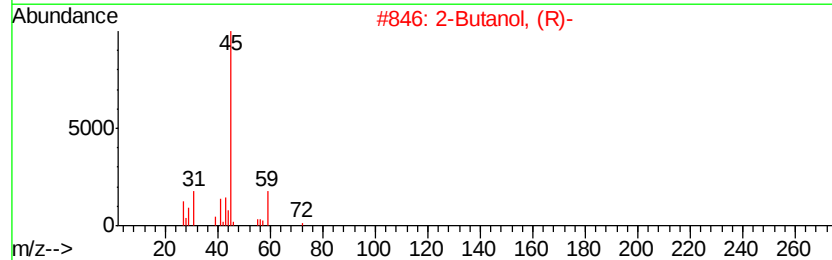
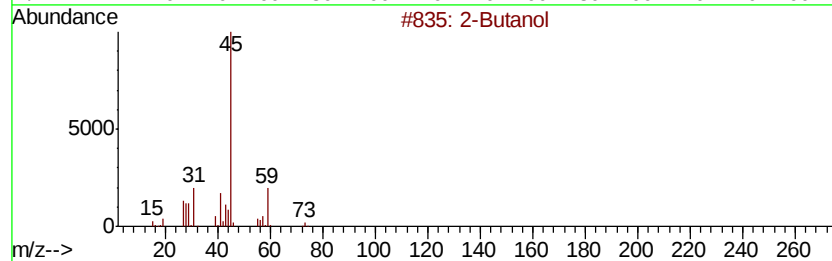
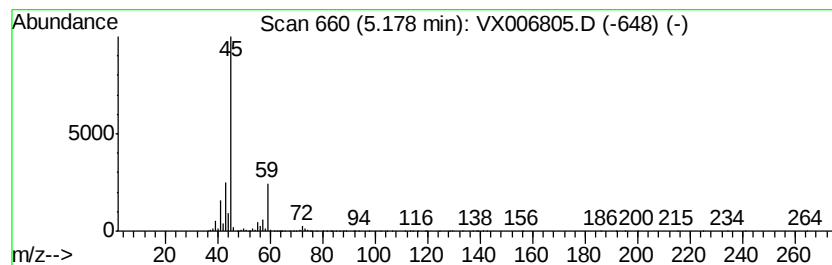
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Quant Title : SW846 8260

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

Peak Number 4 2-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	13.45 ug/l	508965	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanol	74	C4H10O	000078-92-2	83
2		2-Butanol, (R)-	74	C4H10O	014898-79-4	83
3		2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	42
5		Butane, 2-ethoxy-	102	C6H14O	002679-87-0	40



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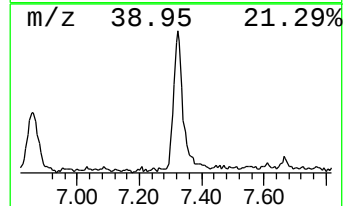
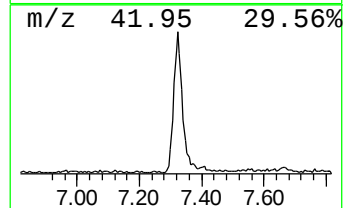
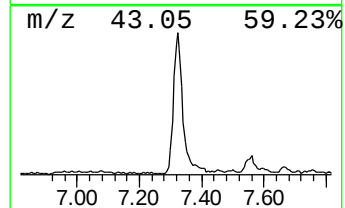
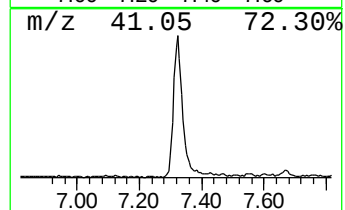
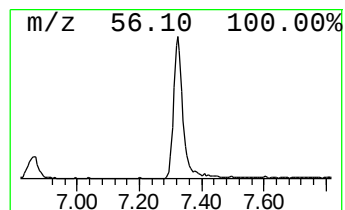
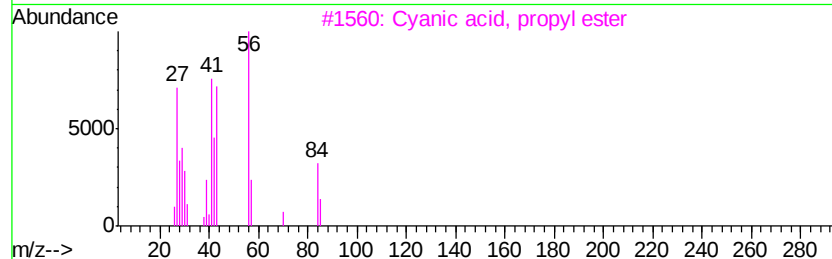
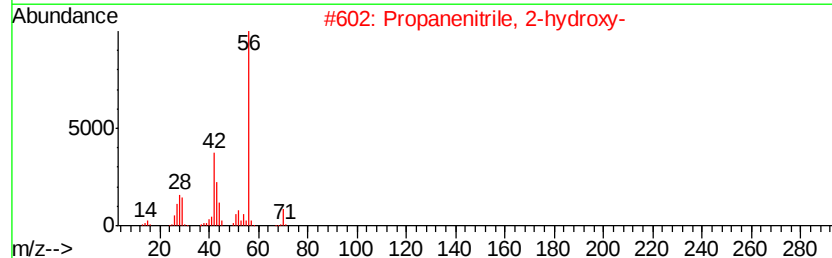
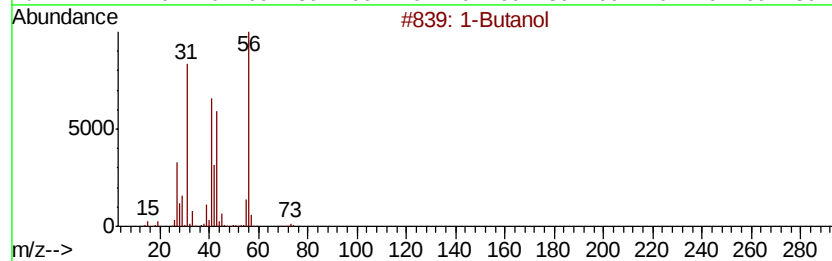
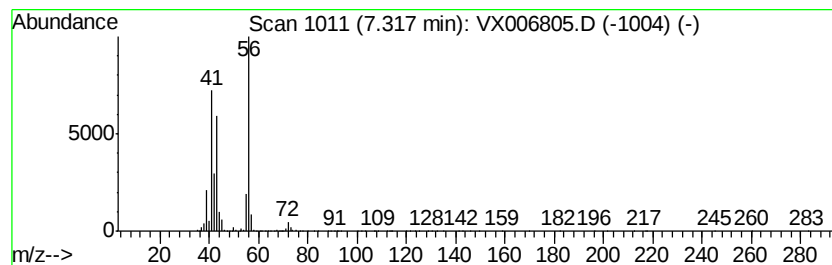
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	9.83 ug/l	445003	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	87
2		Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	50
3		Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	45
4		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
5		Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	39



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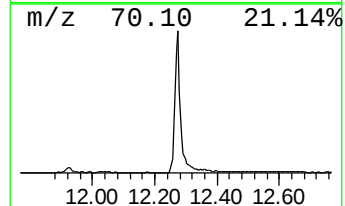
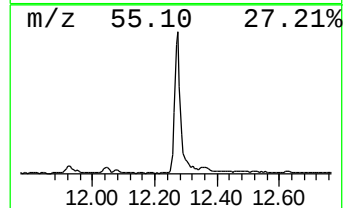
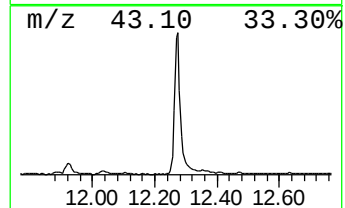
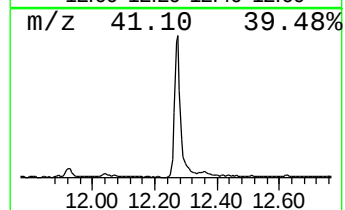
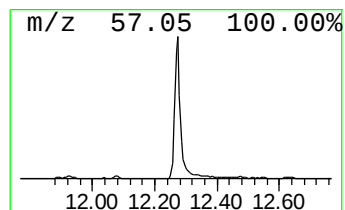
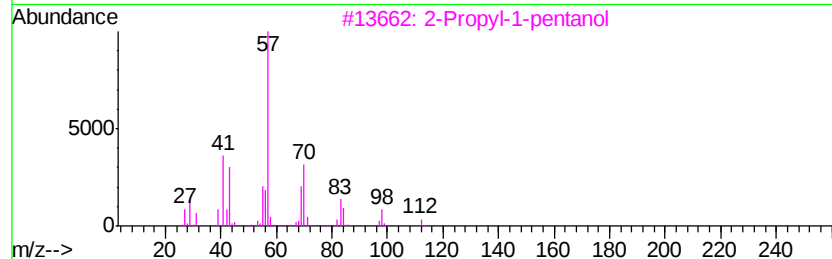
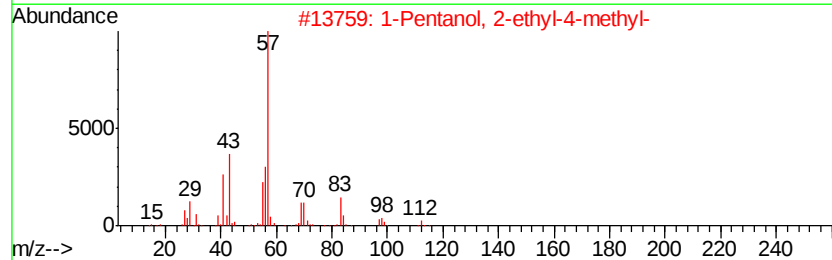
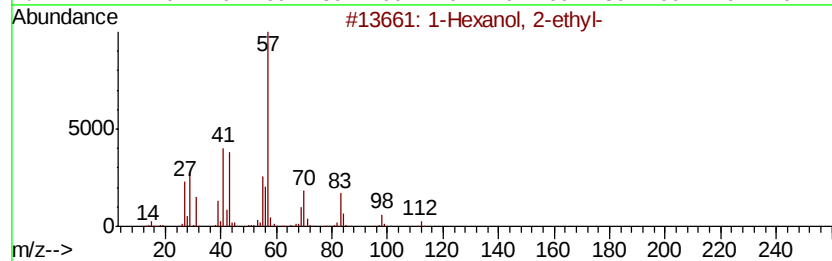
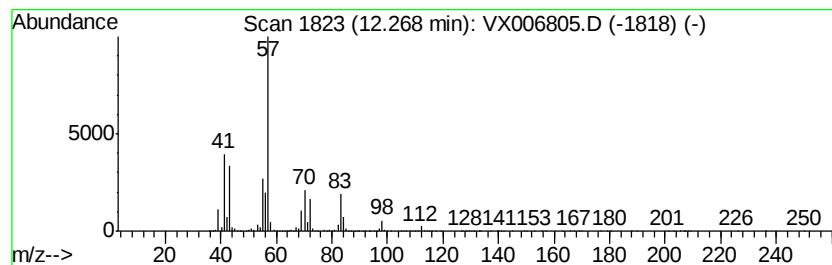
Instrument :
MSVOA_X
ClientSampleId :
COMP-5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	34.23 ug/l	1856200	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	86
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	50
3	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	47
4	1-Decene, 2,4-dimethyl-	168 C12H24	055170-80-4	43
5	2-Ethyl-1-hexanol, methyl ether	144 C9H20O	1000365-10-2	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX122418\
Data File : VX006805.D
Acq On : 24 Dec 2018 19:44
Operator : JC/MD
Sample : J6533-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-5

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.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	1.49	393.9	ug/l	14907200	1	5.67	1892320	50.0
Ethanol	2.13	177.3	ug/l	6709390	1	5.67	1892320	50.0
Butanal	4.35	21.3	ug/l	805229	1	5.67	1892320	50.0
2-Butanol	5.18	13.4	ug/l	508965	1	5.67	1892320	50.0
1-Butanol	7.32	9.8	ug/l	445003	2	6.86	2264190	50.0
1-Hexanol, 2-ethyl-	12.27	34.2	ug/l	1856200	4	12.08	2711250	50.0