

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122418\  
 Data File : VX006803.D  
 Acq On : 24 Dec 2018 18:51  
 Operator : JC/MD  
 Sample : J6533-13  
 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampled :  
 COMP-3

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\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	69	rBV	22190277	28372033	100.00%	50.062%
2	2.123	152	159	175	rBV	1356839	2185862	7.70%	3.857%
3	2.355	192	197	205	rVV	186208	301339	1.06%	0.532%
4	2.446	206	212	224	rVB	508537	842318	2.97%	1.486%
5	3.068	303	314	329	rBV	2621057	5907340	20.82%	10.423%
6	4.354	511	525	540	rBV2	107937	318277	1.12%	0.562%
7	4.696	572	581	592	rBV2	134980	374341	1.32%	0.661%
8	5.500	700	713	725	rBV	363045	1039149	3.66%	1.834%
9	5.659	727	739	755	rVV	680461	1901307	6.70%	3.355%
10	6.067	794	806	815	rBV	388568	1012327	3.57%	1.786%
11	6.860	925	936	950	rBV	976898	2274078	8.02%	4.013%
12	8.713	1233	1240	1247	rBV	2076176	3159053	11.13%	5.574%
13	10.109	1463	1469	1482	rBV	2054935	2758232	9.72%	4.867%
14	10.365	1504	1511	1521	rVB2	225405	348646	1.23%	0.615%
15	11.134	1632	1637	1643	rBV	1785271	2262748	7.98%	3.993%
16	12.079	1786	1792	1799	rVB	2254826	2813207	9.92%	4.964%
17	12.274	1818	1824	1836	rBV	268515	464457	1.64%	0.820%
18	16.175	2453	2464	2471	rBV	189037	338836	1.19%	0.598%

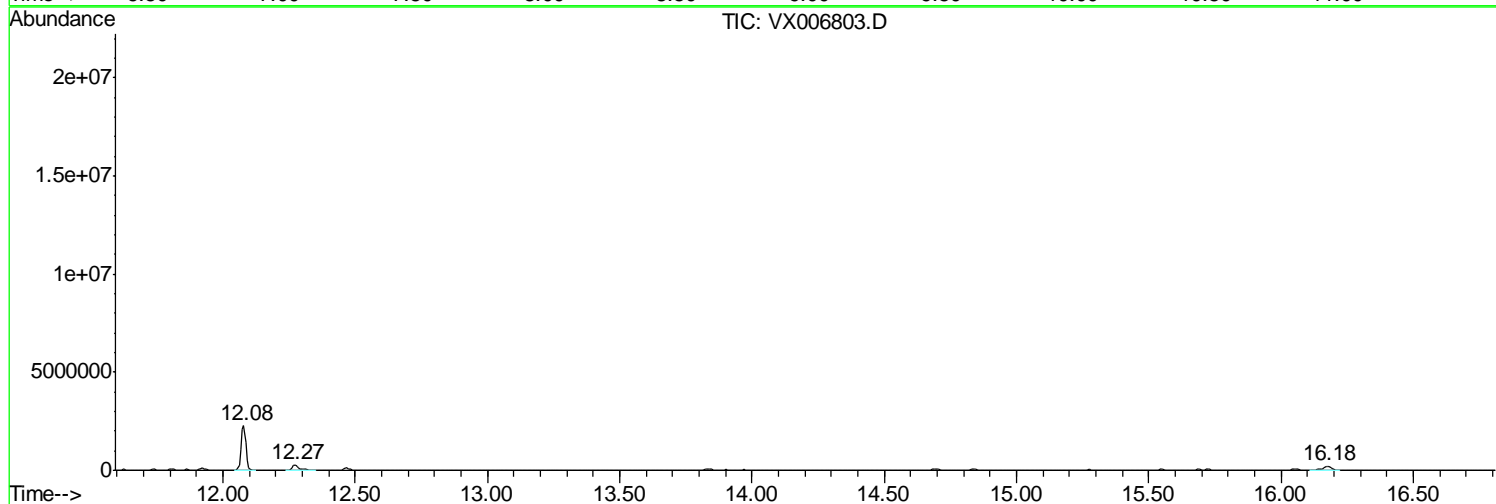
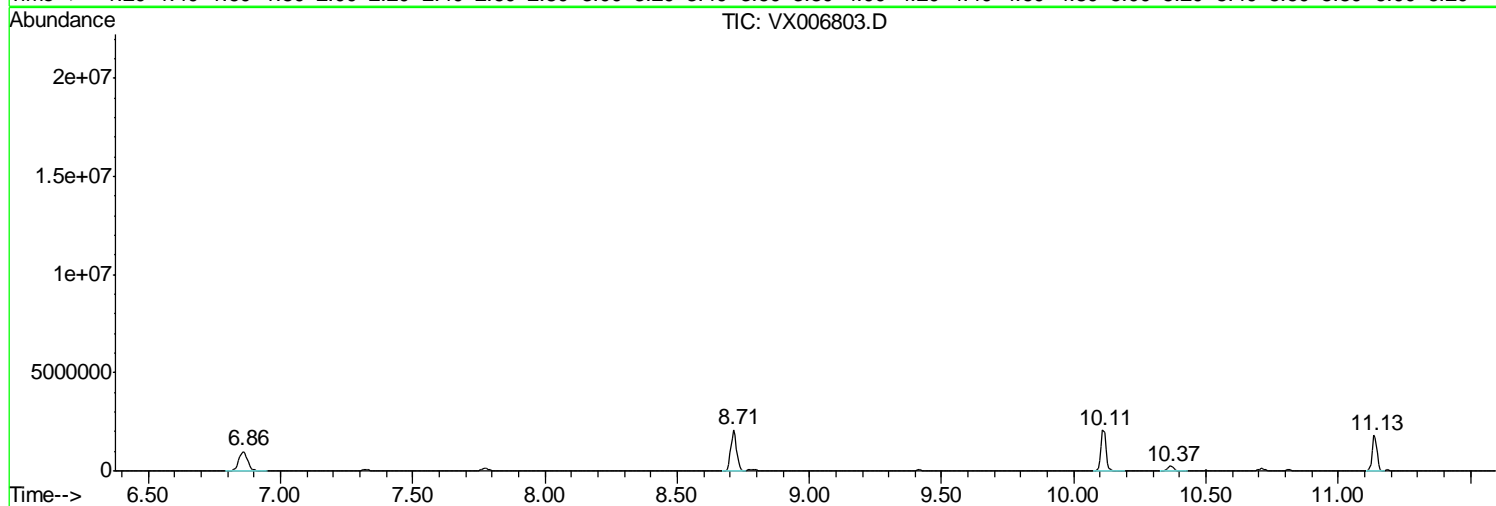
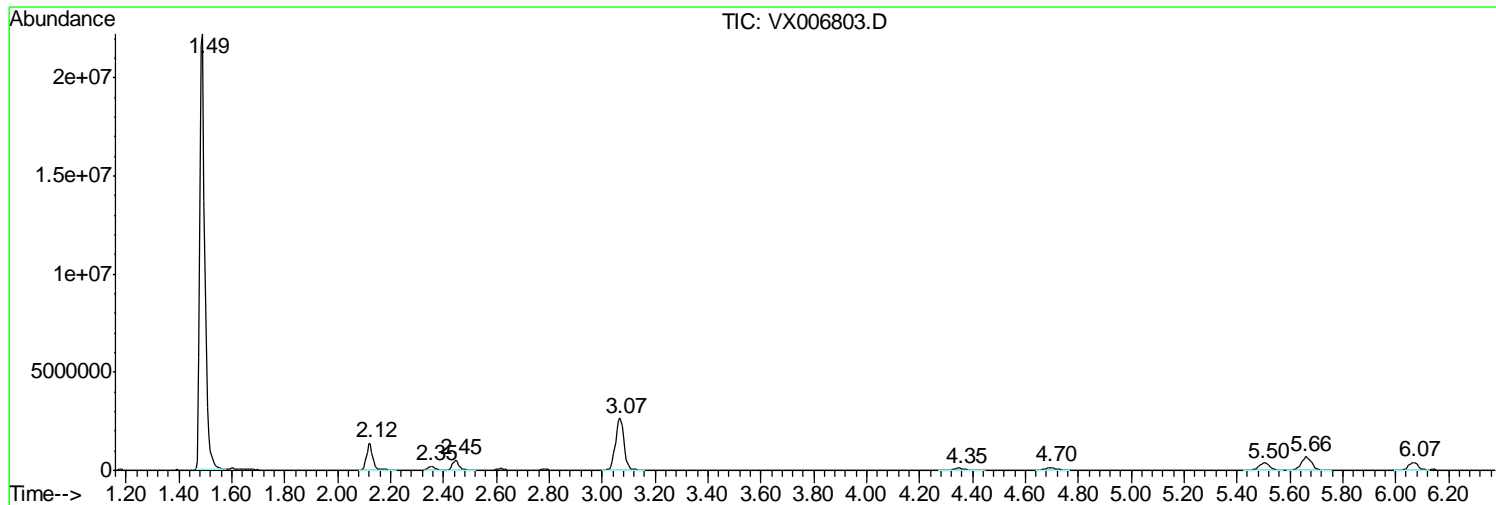
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121818W.M  
Quant Title : SW846 8260

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



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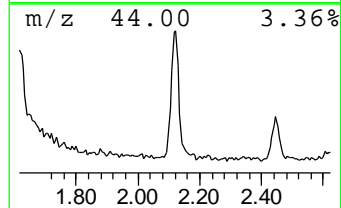
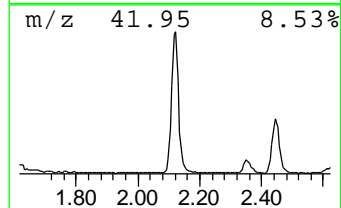
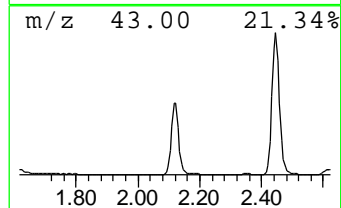
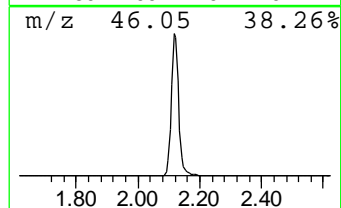
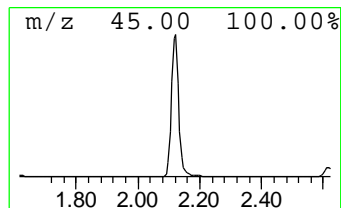
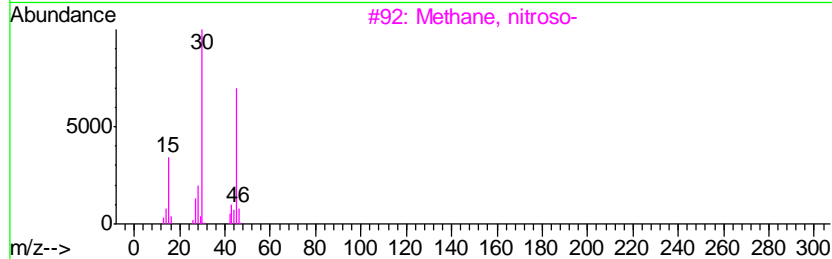
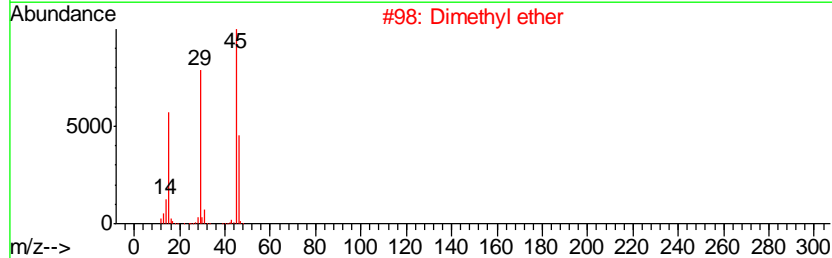
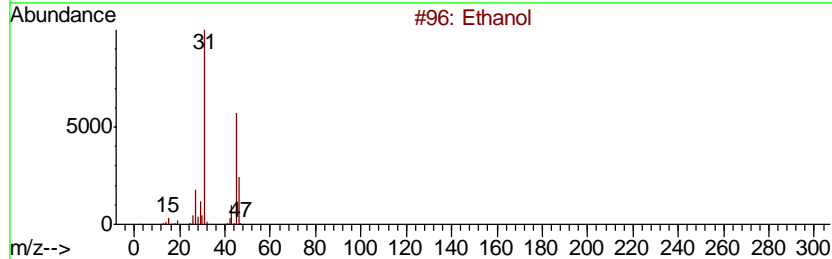
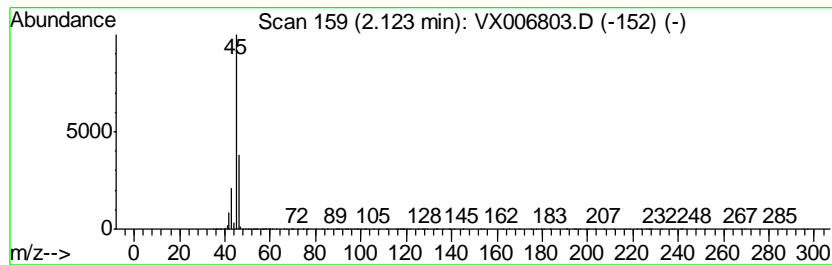
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121818W.M  
 Quant Title : SW846 8260

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

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 Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	57.48 ug/l	2185860	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		L-Lactic acid	90	C3H6O3	000079-33-4	2



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 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 COMP-3

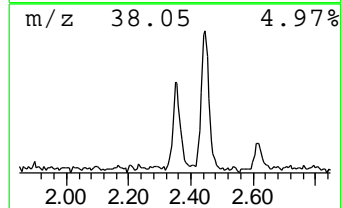
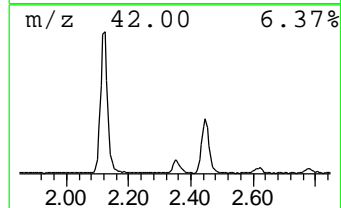
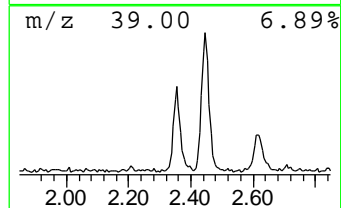
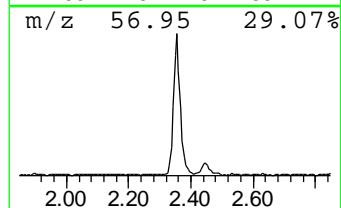
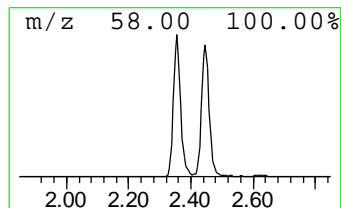
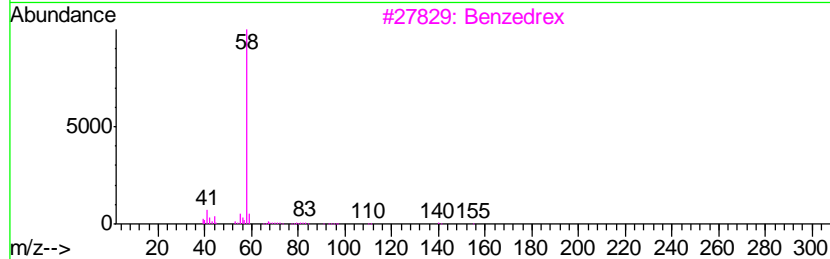
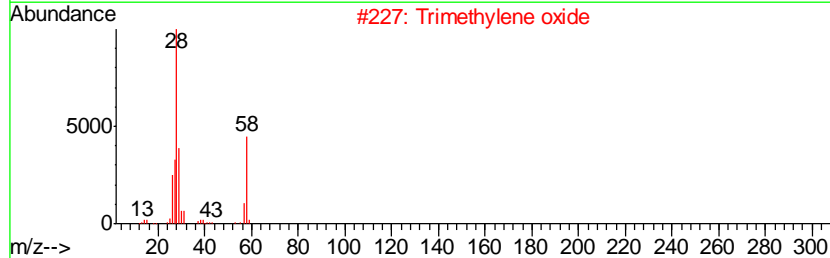
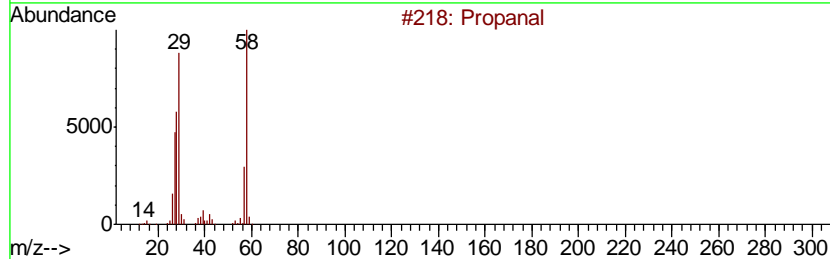
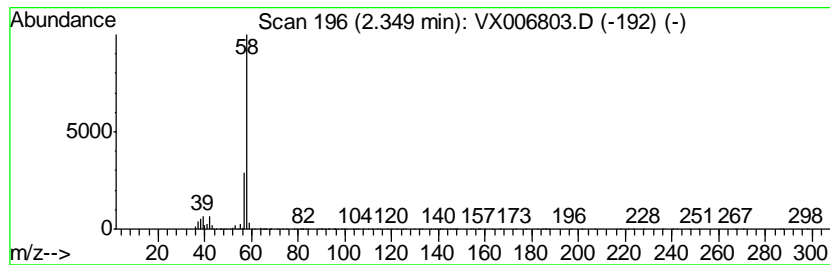
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121818W.M  
 Quant Title : SW846 8260

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

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 Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	7.92 ug/l	301339	Pentafluorobenzene	5.67

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		Benzedrex	155	C10H21N	000101-40-6	9
4		Propylene oxide	58	C3H6O	000075-56-9	7
5		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampled :  
 COMP-3

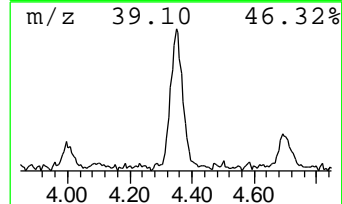
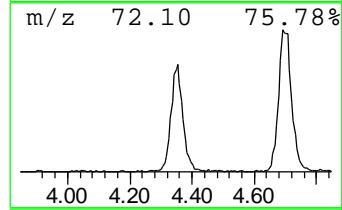
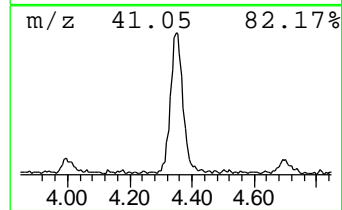
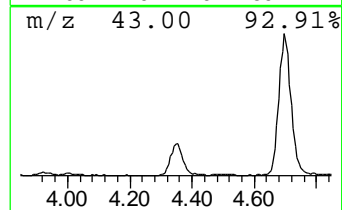
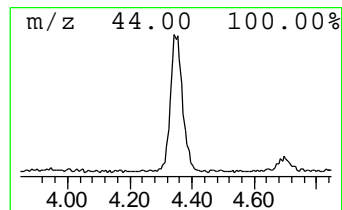
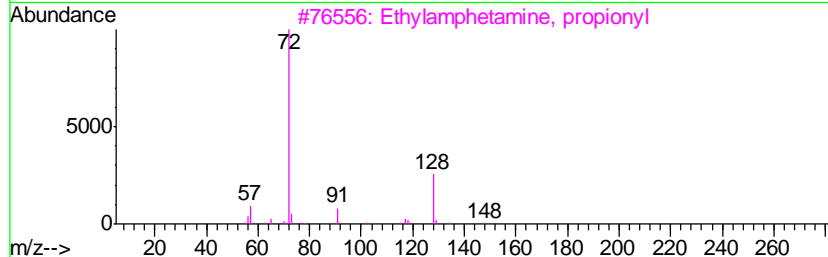
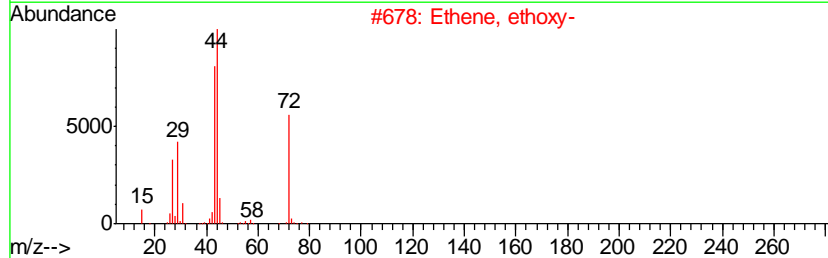
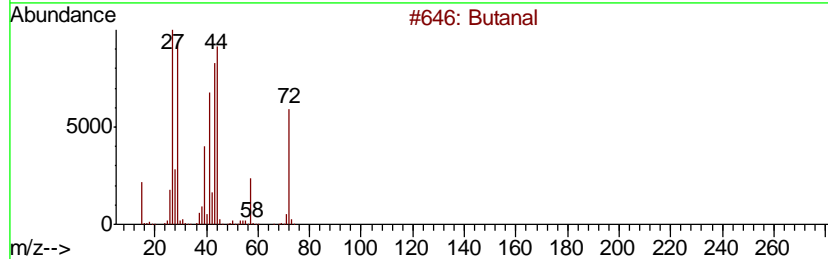
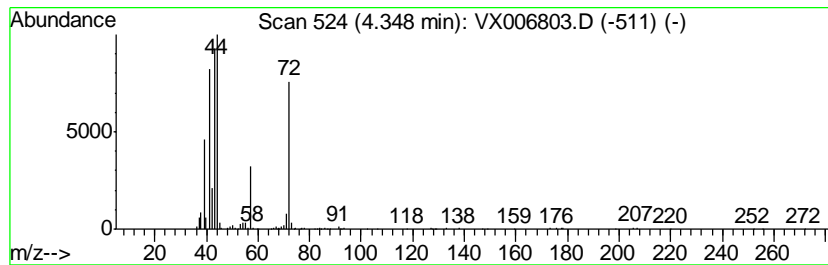
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121818W.M  
 Quant Title : SW846 8260

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

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 Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	8.37 ug/l	318277	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	91
2		Ethene, ethoxy-	72	C4H8O	000109-92-2	59
3		Ethylamphetamine, propionyl	219	C14H21NO	1000123-80-9	43
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38



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 Sample : J6533-13  
 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampled :  
 COMP-3

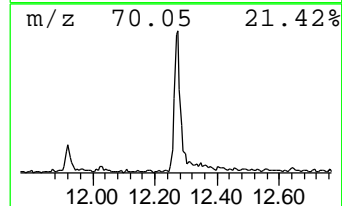
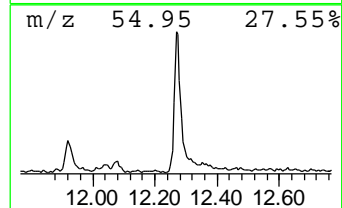
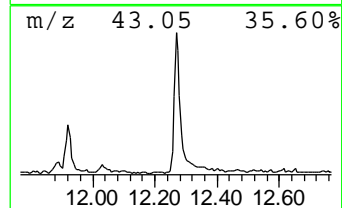
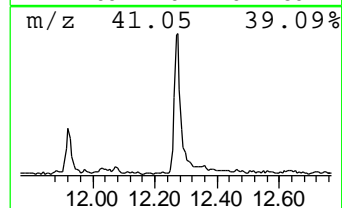
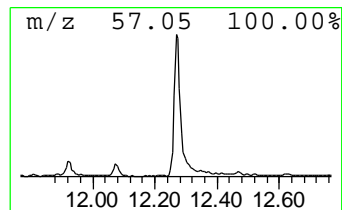
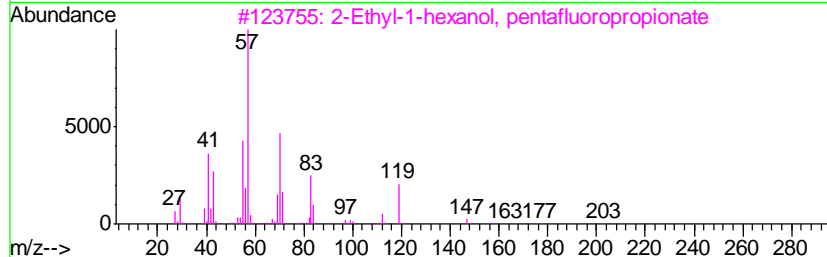
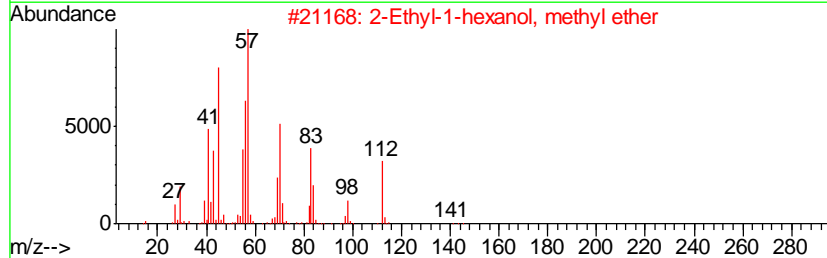
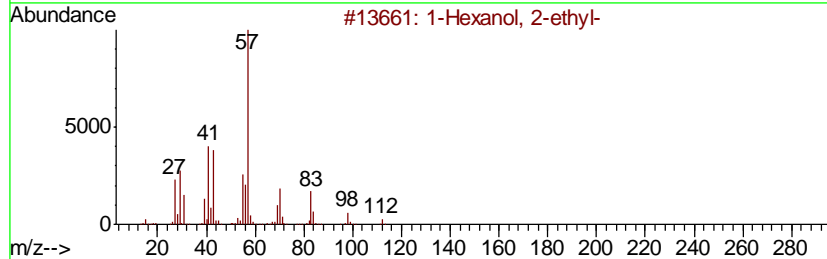
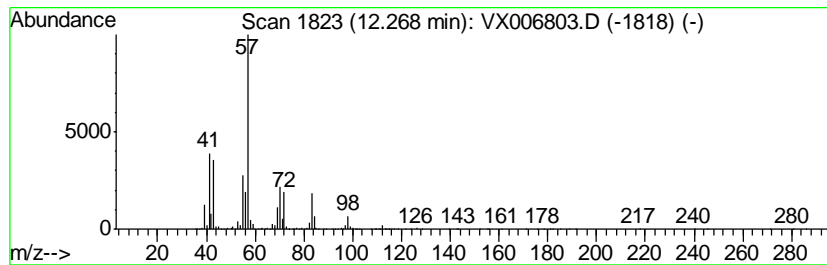
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_X\METHOD\82X121818W.M  
 Quant Title : SW846 8260

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

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 Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	8.25 ug/l	464457	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
3		2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	43
4		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	38
5		2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	38



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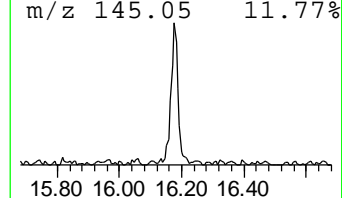
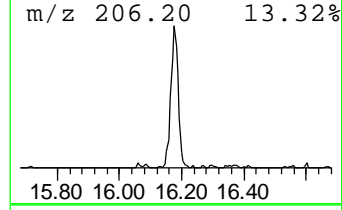
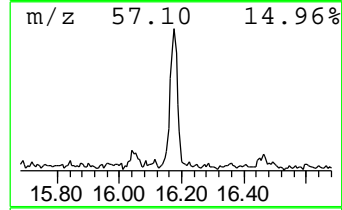
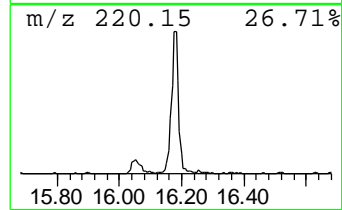
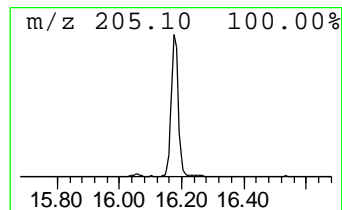
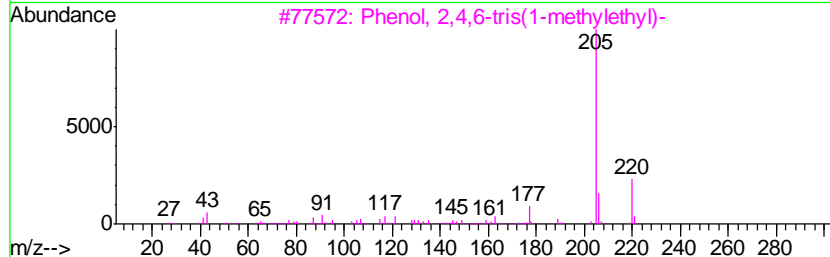
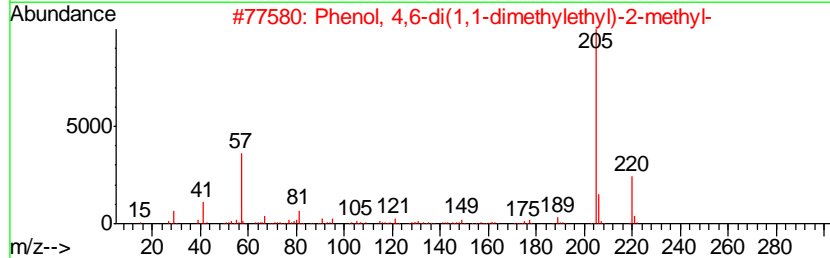
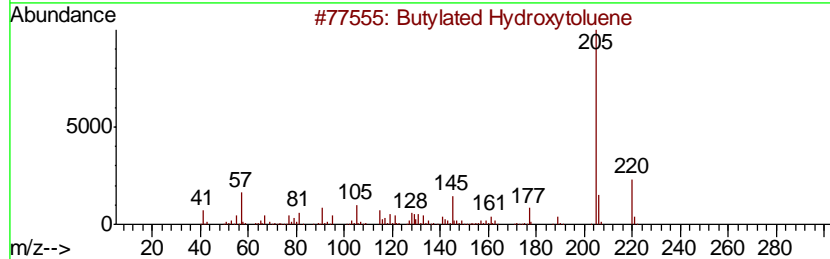
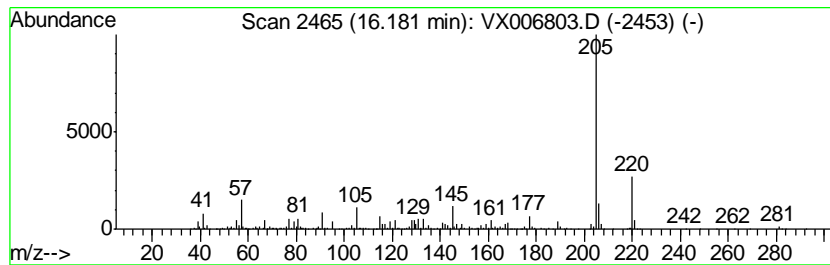
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 Butylated Hydroxytoluene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	6.02 ug/l	338836	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2		Phenol, 4,6-di(1,1-dimethylethyl)...	220	C15H24O	000616-55-7	90
3		Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87
4		2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	72
5		4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	72



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Instrument :  
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.12	57.5	ug/l	2185860	1	5.67	1901310	50.0
Propanal	2.35	7.9	ug/l	301339	1	5.67	1901310	50.0
Butanal	4.35	8.4	ug/l	318277	1	5.67	1901310	50.0
1-Hexanol, 2-ethyl-	12.27	8.3	ug/l	464457	4	12.08	2813210	50.0
Butylated Hydroxy...	16.18	6.0	ug/l	338836	4	12.08	2813210	50.0