

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122618\
 Data File : VX006823.D
 Acq On : 26 Dec 2018 17:23
 Operator : JC/MD
 Sample : J6533-16
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-4

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	1.483	51	54	70	rBV	41454662	61851588	100.00%	51.647%
2	2.148	151	163	167	rBV	15232461	31557424	51.02%	26.351%
3	4.348	513	524	540	rBV	950862	2615844	4.23%	2.184%
4	4.696	571	581	597	rVB	773194	2152281	3.48%	1.797%
5	5.501	700	713	726	rBV	381067	1086235	1.76%	0.907%
6	5.659	728	739	758	rVB	690332	1946140	3.15%	1.625%
7	5.952	778	787	797	rBV	295342	771471	1.25%	0.644%
8	6.068	797	806	814	rBV	383911	960160	1.55%	0.802%
9	6.860	926	936	949	rBV	989837	2314556	3.74%	1.933%
10	7.317	1004	1011	1027	rBV	381014	785648	1.27%	0.656%
11	8.713	1233	1240	1247	rBV	2081695	3200706	5.17%	2.673%
12	10.110	1462	1469	1481	rVB	2057877	2808887	4.54%	2.345%
13	10.366	1504	1511	1520	rBV2	878434	1243645	2.01%	1.038%
14	11.134	1632	1637	1643	rBV	1876853	2338751	3.78%	1.953%
15	12.079	1787	1792	1799	rVB	2272965	2854012	4.61%	2.383%
16	12.268	1817	1823	1834	rBV	822231	1270968	2.05%	1.061%

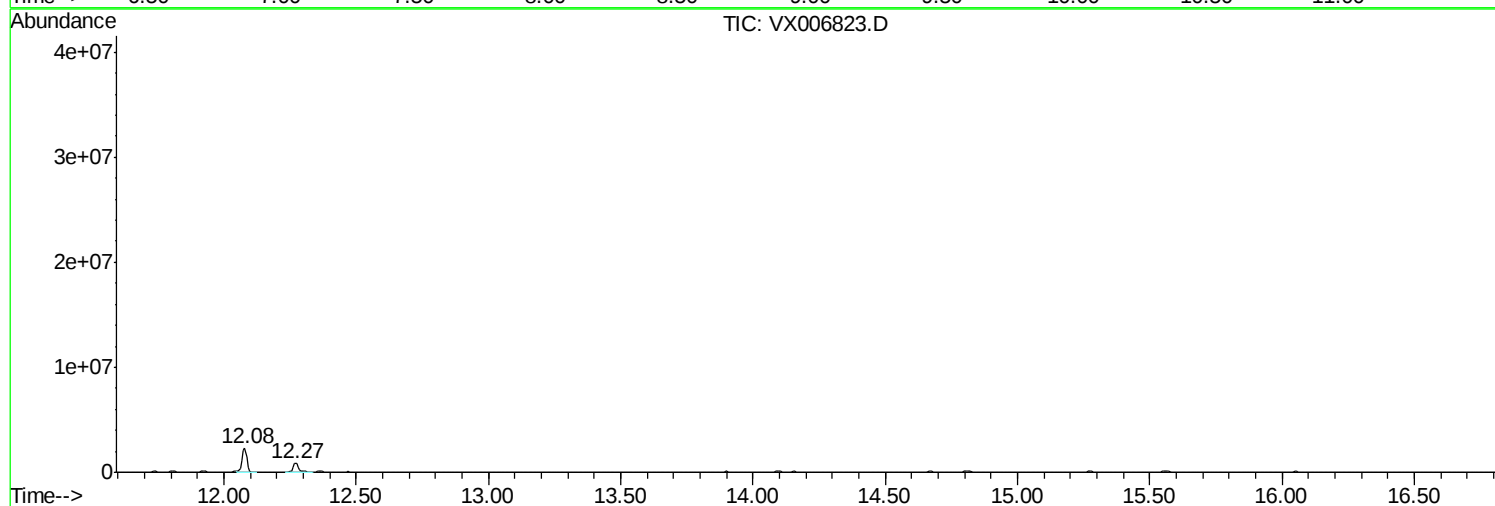
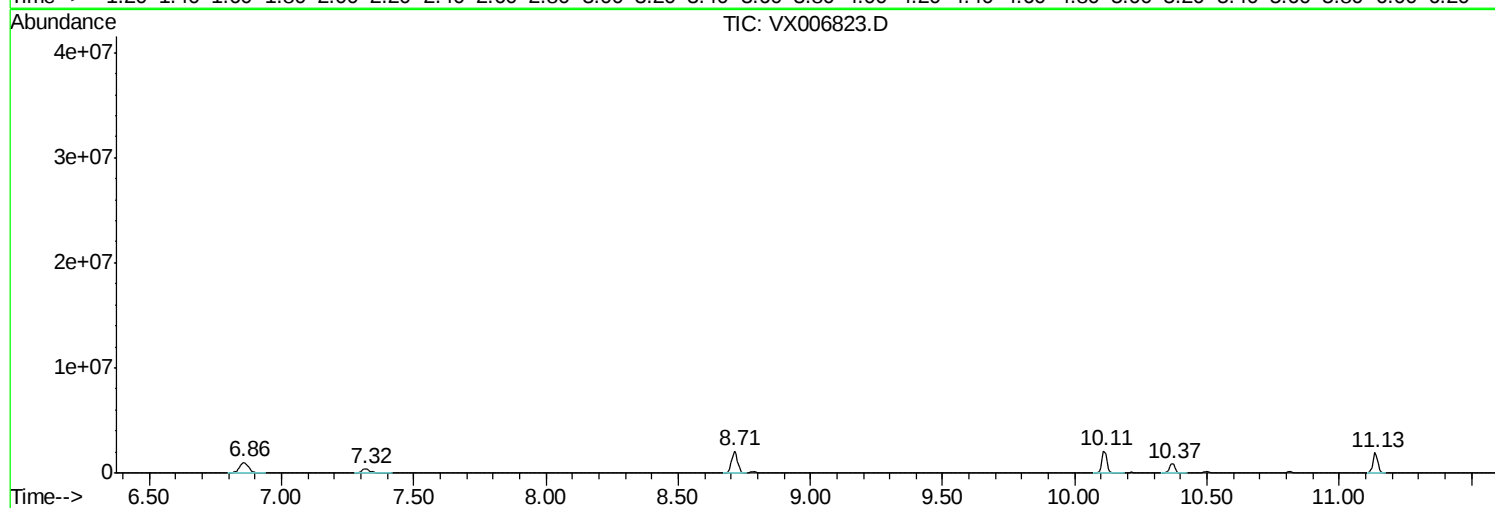
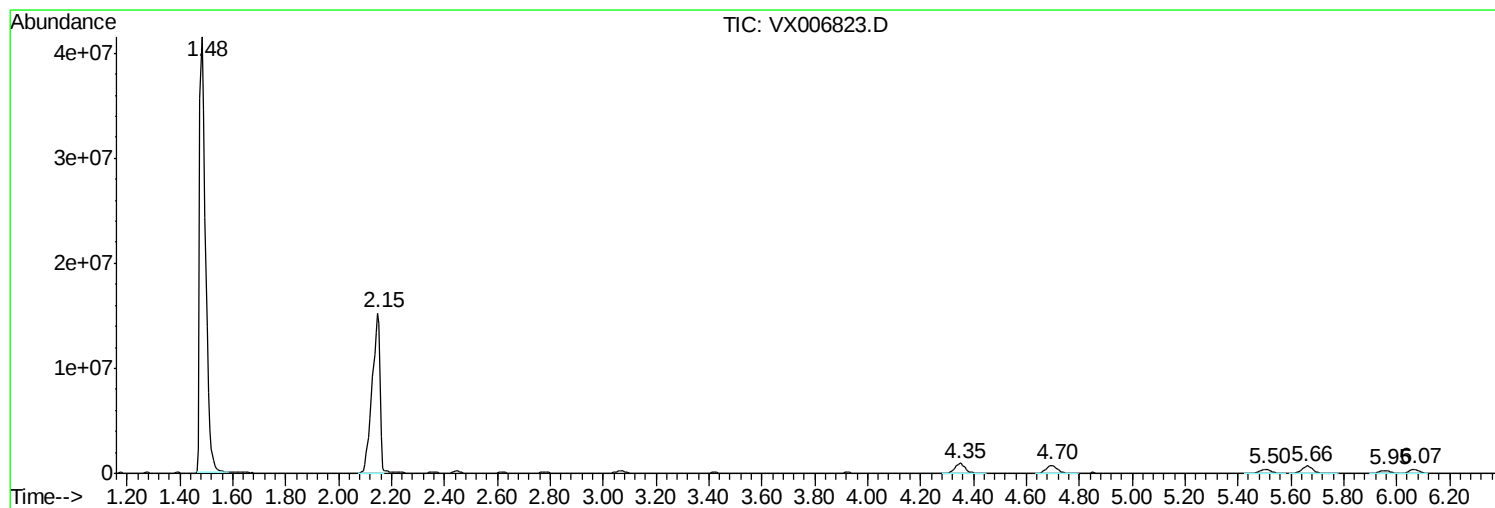
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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



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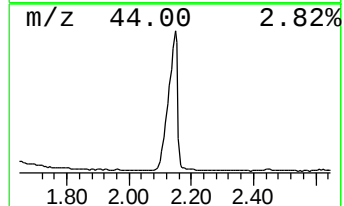
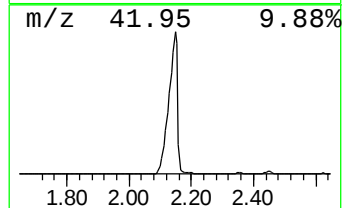
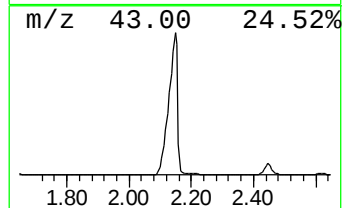
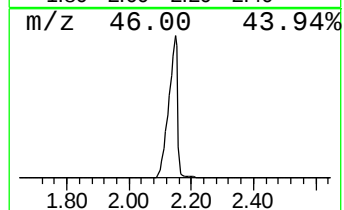
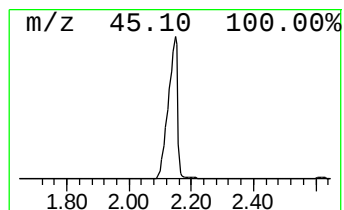
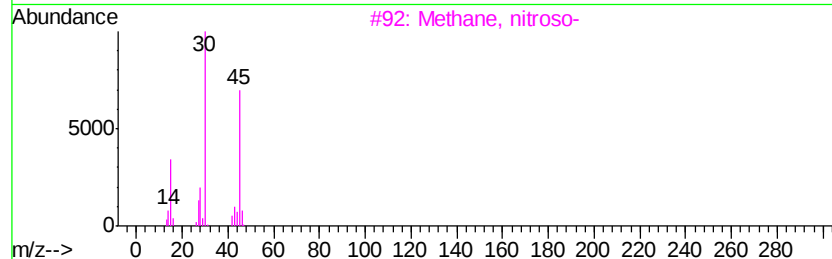
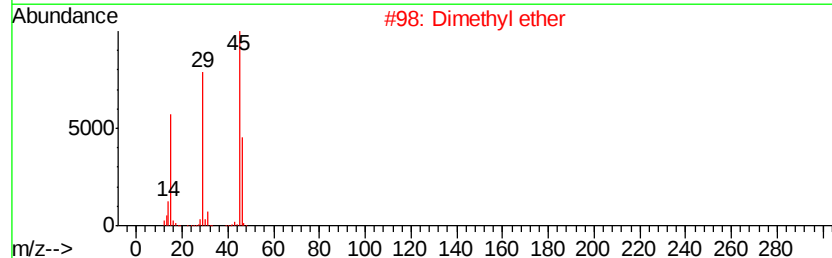
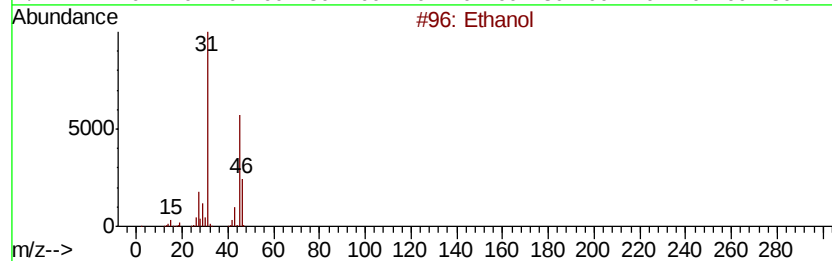
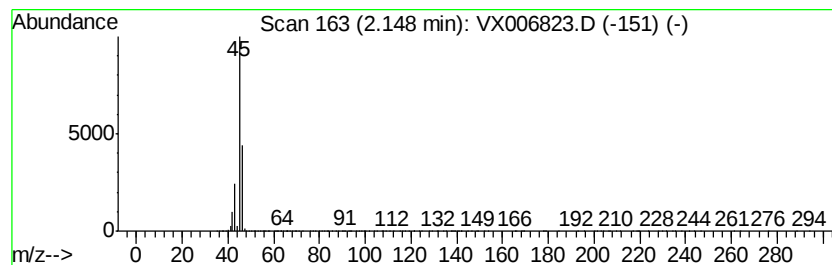
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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.
2.15	810.77 ug/l	31557400	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	83
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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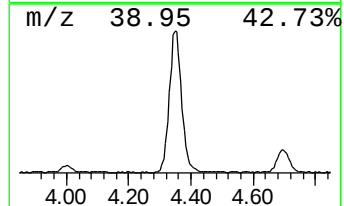
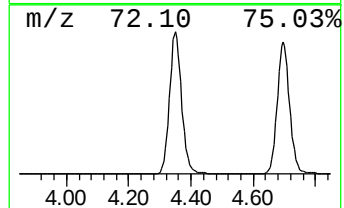
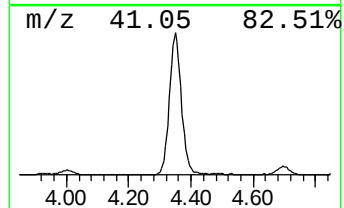
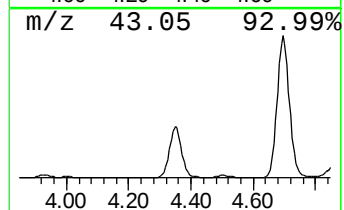
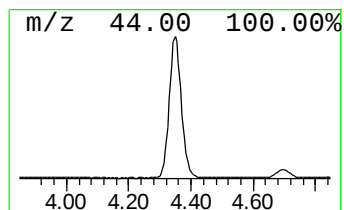
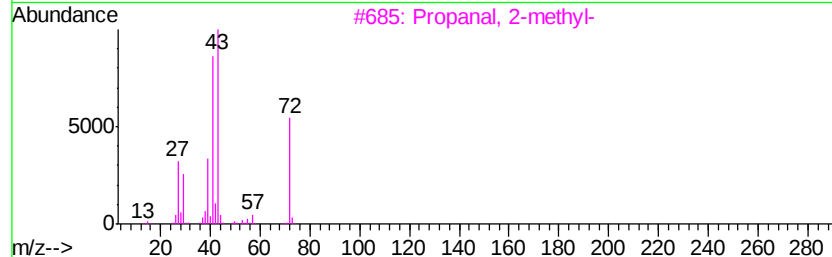
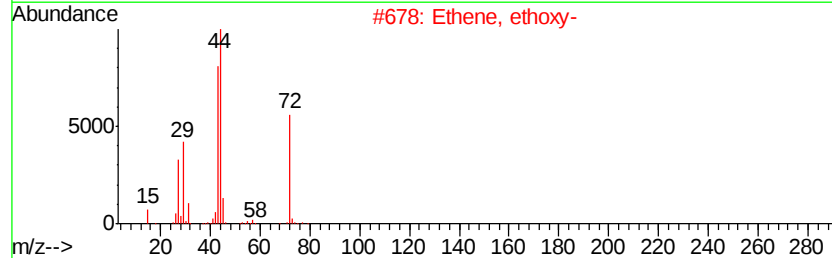
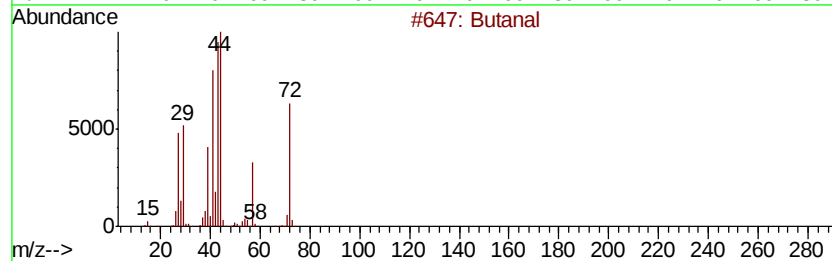
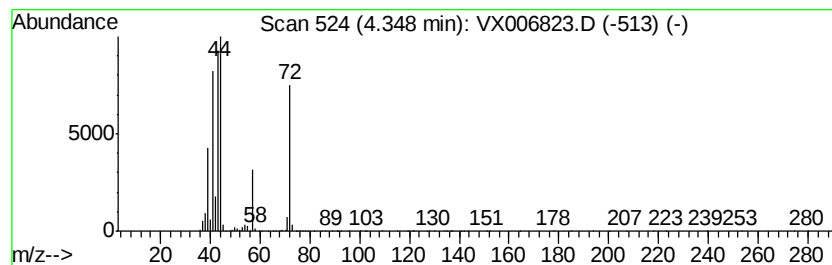
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	67.21 ug/l	2615840	Pentafluorobenzene	5.66

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	58
3		Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
5		Isobutylene epoxide	72	C4H8O	000558-30-5	35



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Instrument :
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ClientSampleId :
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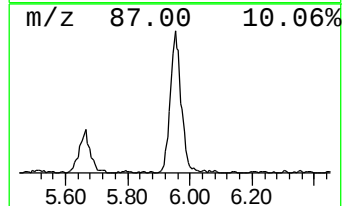
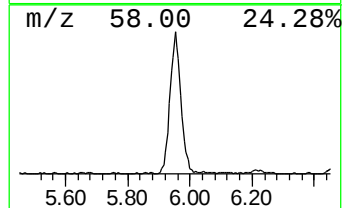
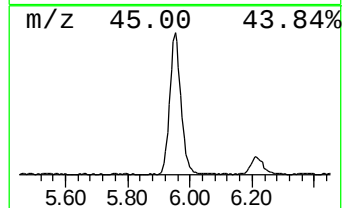
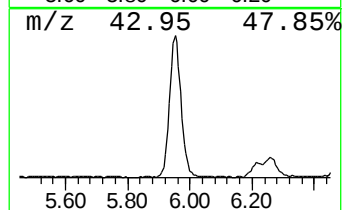
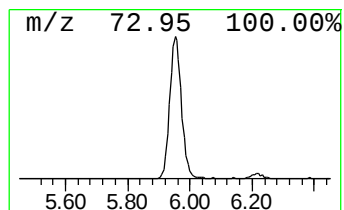
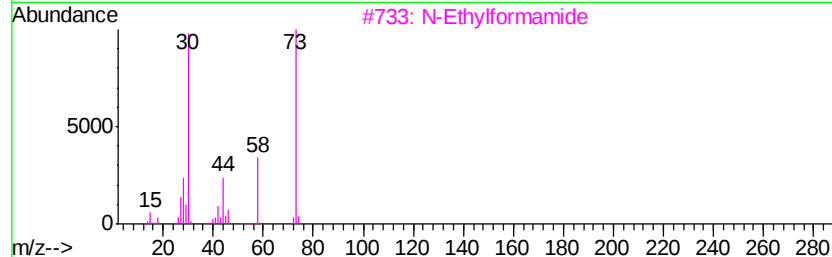
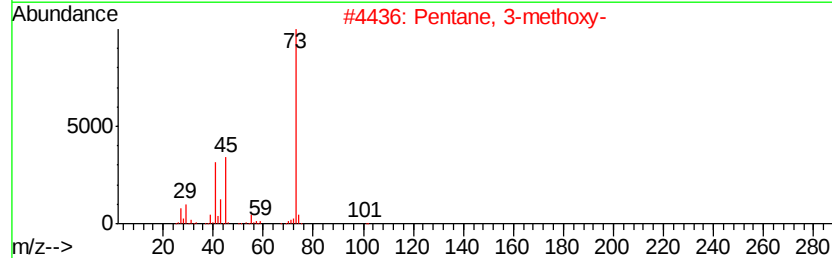
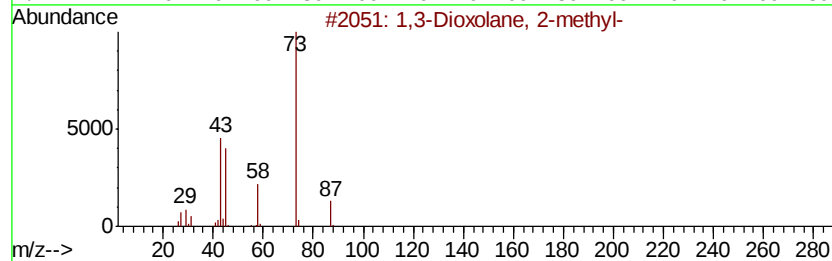
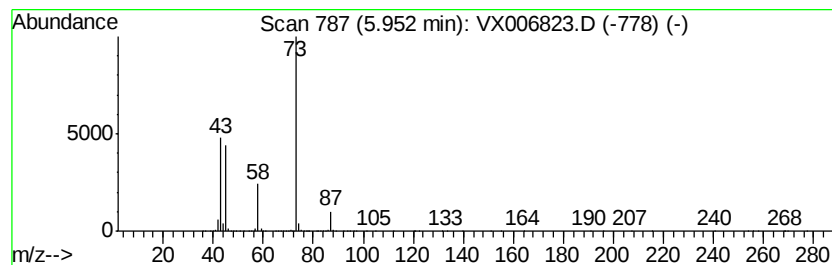
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Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	19.82 ug/l	771471	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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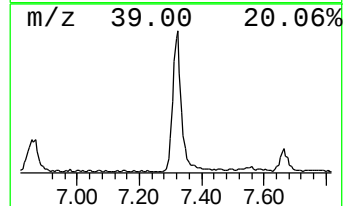
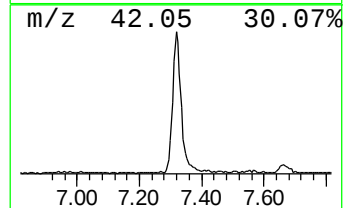
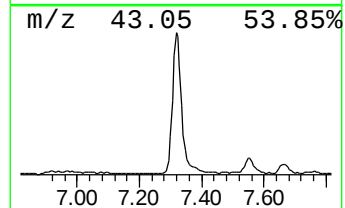
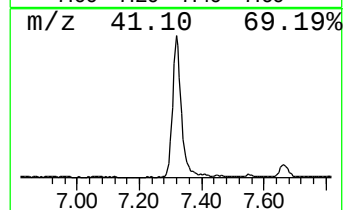
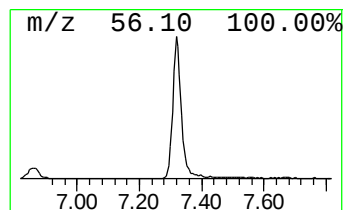
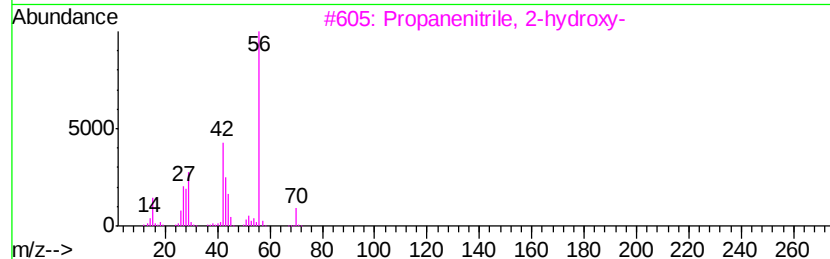
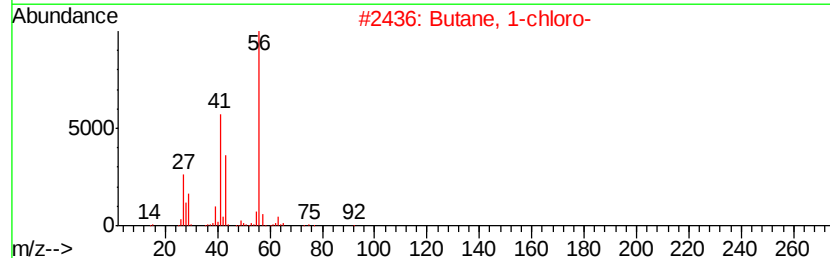
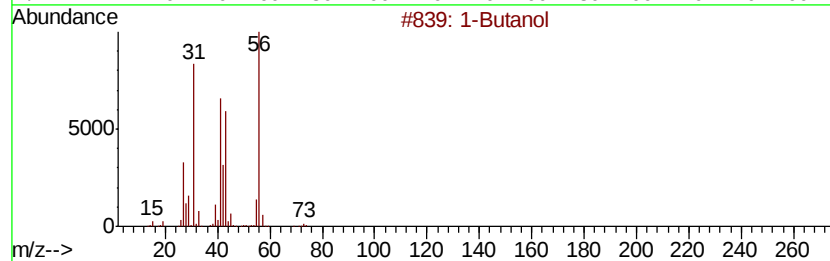
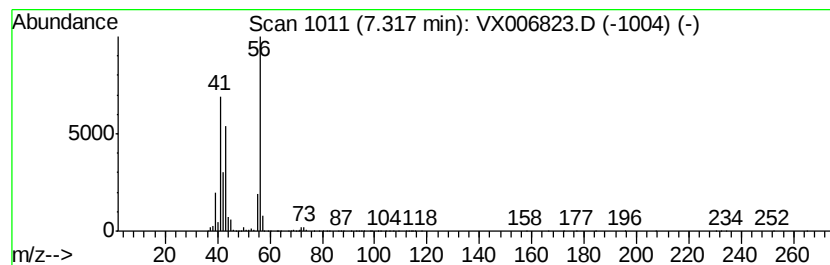
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	16.97 ug/l	785648	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	90
2		Butane, 1-chloro-	92	C4H9Cl	000109-69-3	38
3		Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	9
4		Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
5		Methoxyacetoneitrile	71	C3H5NO	001738-36-9	9



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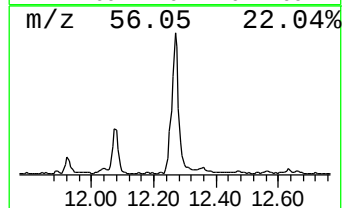
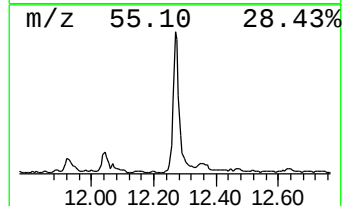
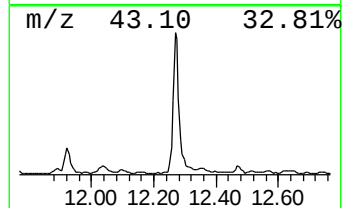
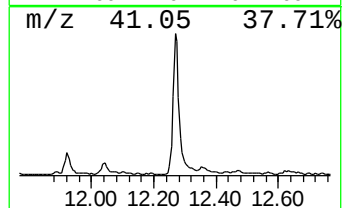
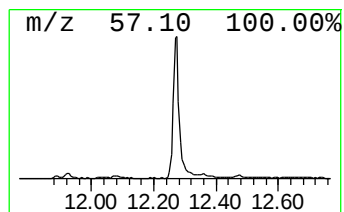
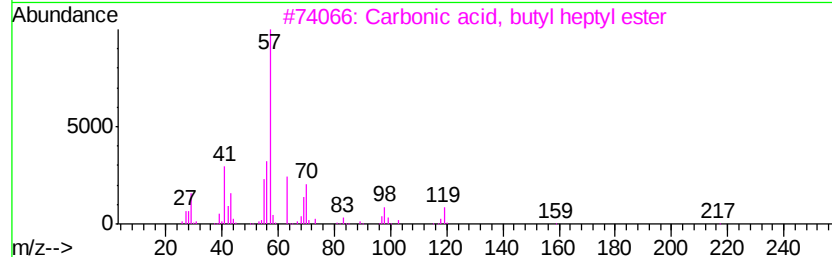
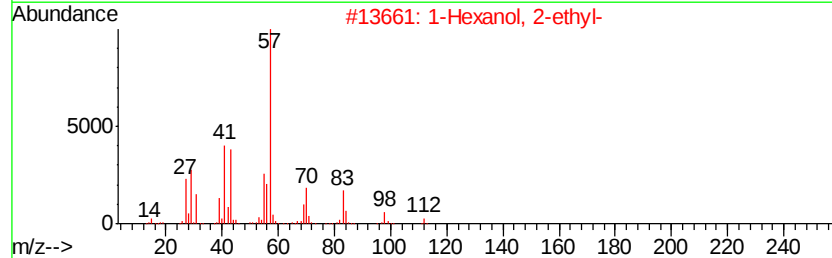
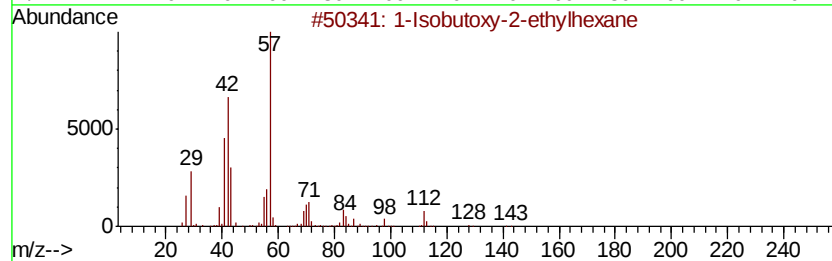
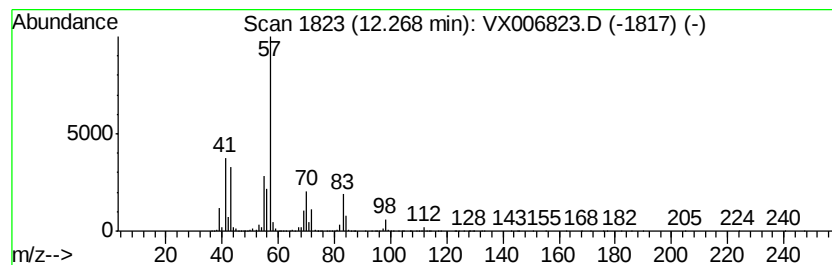
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Isobutoxy-2-ethylhexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	22.27 ug/l	1270970	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3		Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	53
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50



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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	2.15	810.8	ug/l	31557400	1	5.66	1946140	50.0
Butanal	4.35	67.2	ug/l	2615840	1	5.66	1946140	50.0
1,3-Dioxolane, 2-...	5.95	19.8	ug/l	771471	1	5.66	1946140	50.0
1-Butanol	7.32	17.0	ug/l	785648	2	6.86	2314560	50.0
1-Isobutoxy-2-eth...	12.27	22.3	ug/l	1270970	4	12.08	2854010	50.0