

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091422\
 Data File : VX031317.D
 Acq On : 14 Sep 2022 19:51
 Operator : JC/MD
 Sample : N4588-07 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AUD-1665

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\82X091422W.M
 Title : SW846 8260

Signal : TIC: VX031317.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.257	24	28	36	rBV	367892	339029	1.80%	0.858%
2	1.446	56	59	86	rBV	8703070	11011577	58.33%	27.853%
3	2.178	157	179	196	rBV	3407446	18877546	100.00%	47.750%
4	4.720	585	596	619	rVB	125667	373726	1.98%	0.945%
5	5.555	722	733	747	rVB	77189	216628	1.15%	0.548%
6	5.848	767	781	793	rBV	1929828	5323195	28.20%	13.465%
7	5.964	793	800	807	rVV	89249	231187	1.22%	0.585%
8	6.763	922	931	946	rVB	135872	321320	1.70%	0.813%
9	7.244	1001	1010	1026	rBV	119686	335822	1.78%	0.849%
10	8.652	1234	1241	1247	rBV	390367	604211	3.20%	1.528%
11	10.055	1460	1471	1484	rBV2	279753	419519	2.22%	1.061%
12	10.317	1508	1514	1527	rVB2	400123	570105	3.02%	1.442%
13	11.085	1634	1640	1645	rBV	299553	393577	2.08%	0.996%
14	12.024	1790	1794	1801	rVB	257103	312673	1.66%	0.791%
15	12.219	1818	1826	1836	rBV	116693	203904	1.08%	0.516%

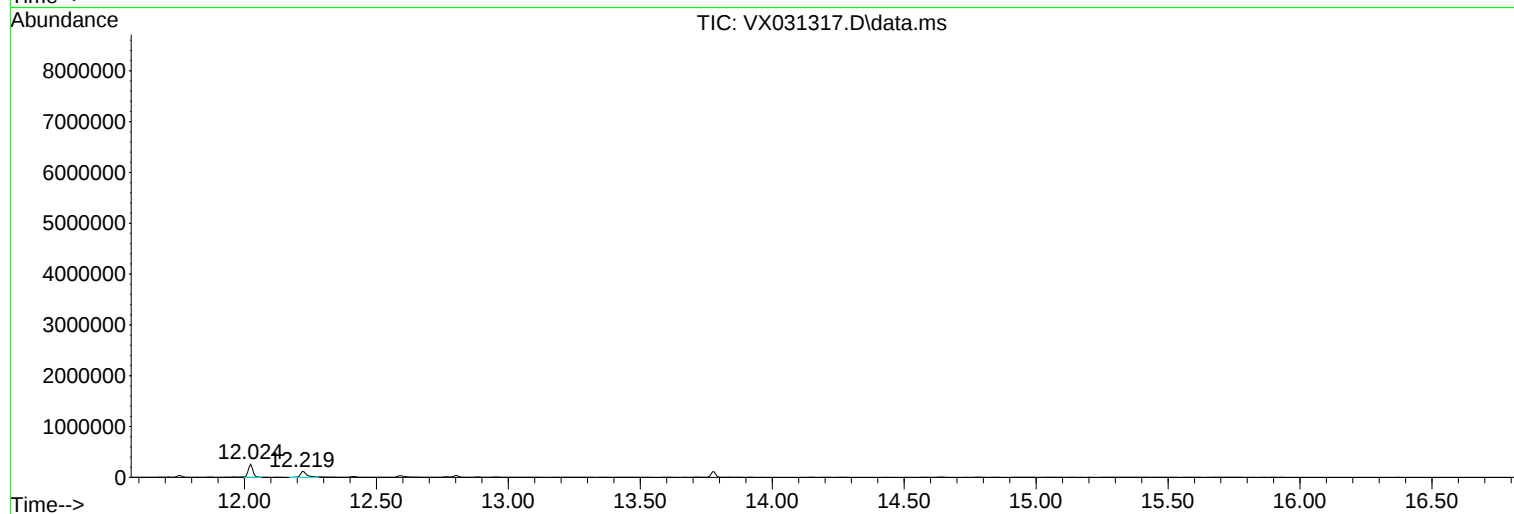
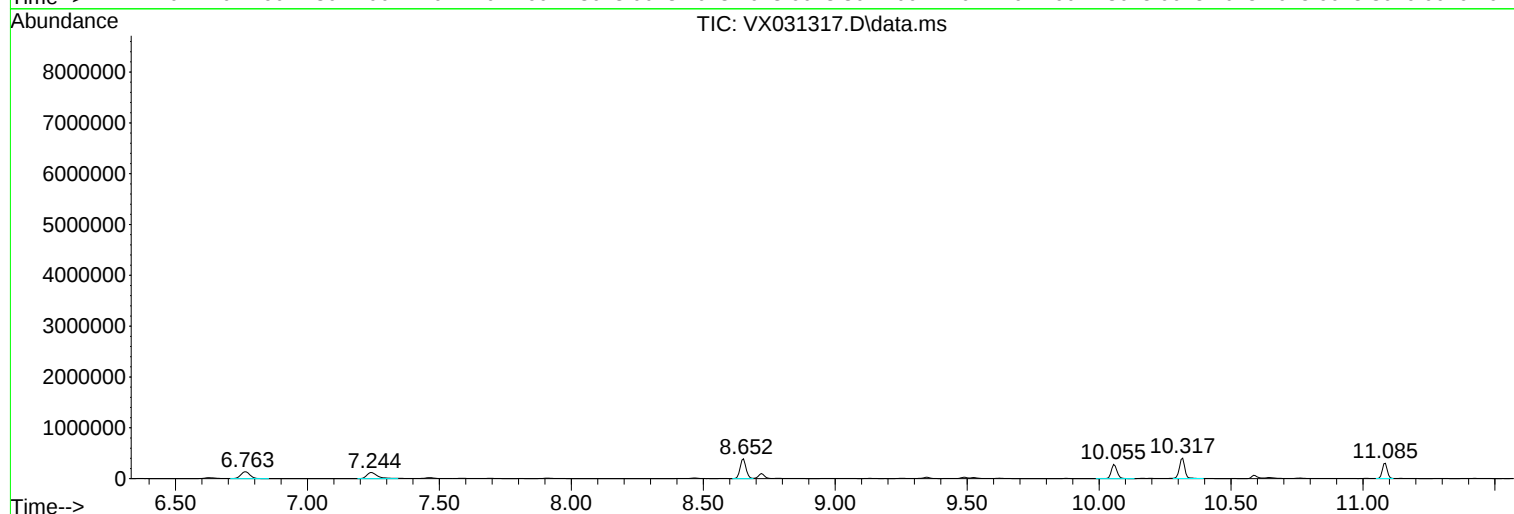
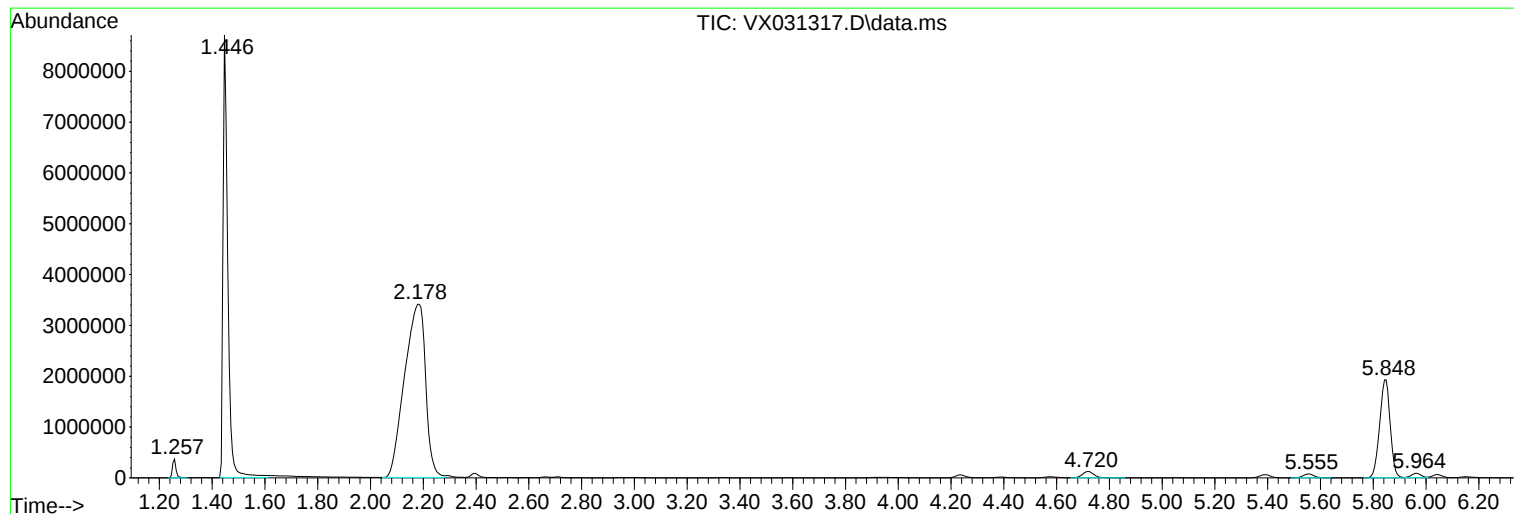
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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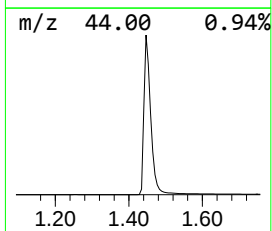
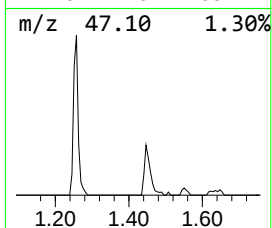
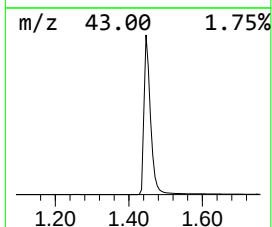
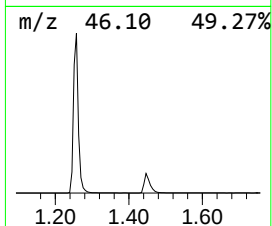
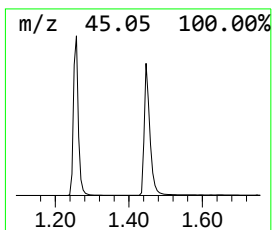
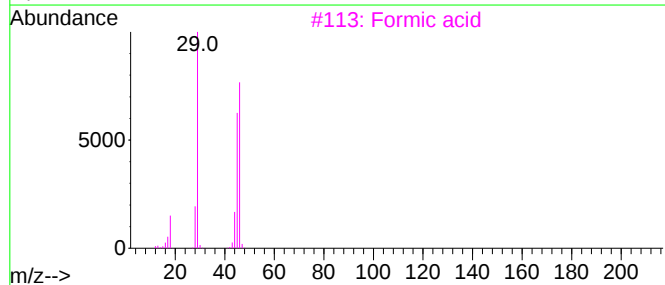
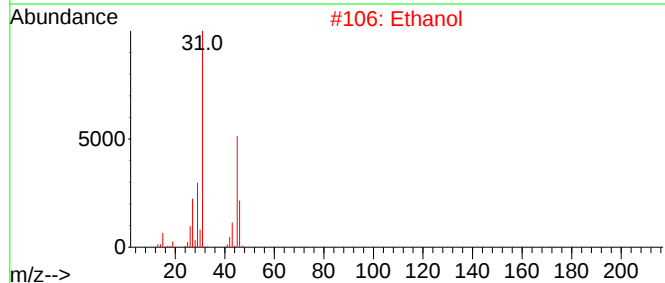
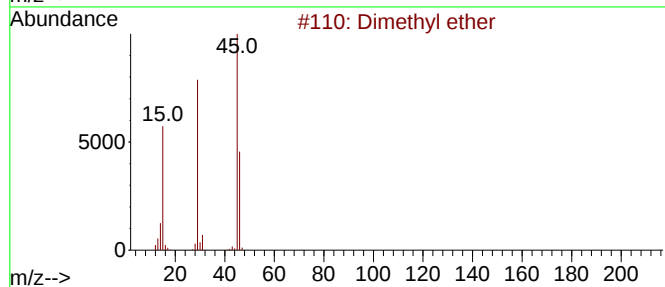
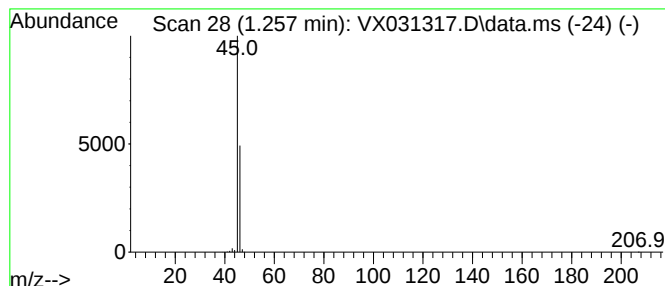
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.257	78.25 ug/l	339029	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	90
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	7
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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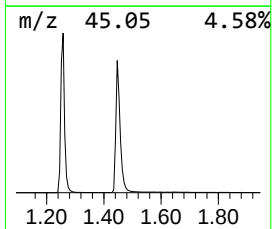
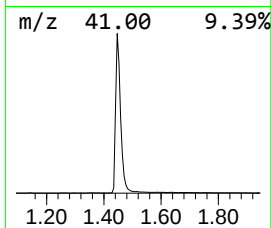
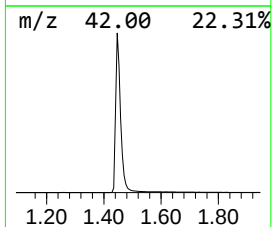
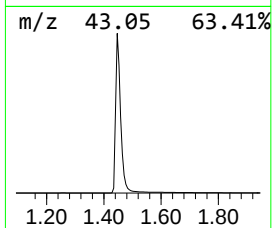
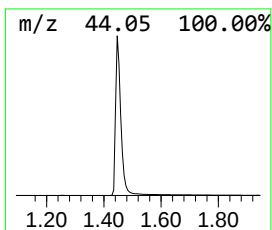
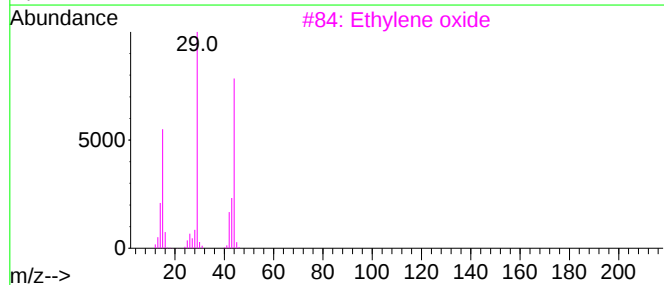
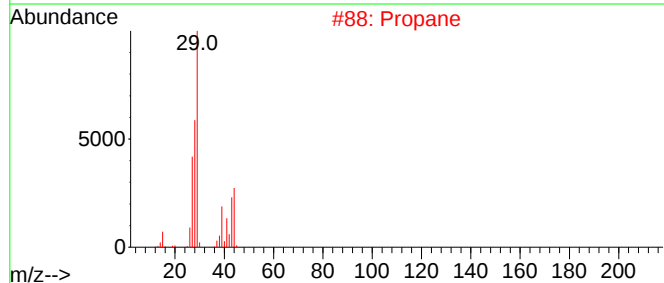
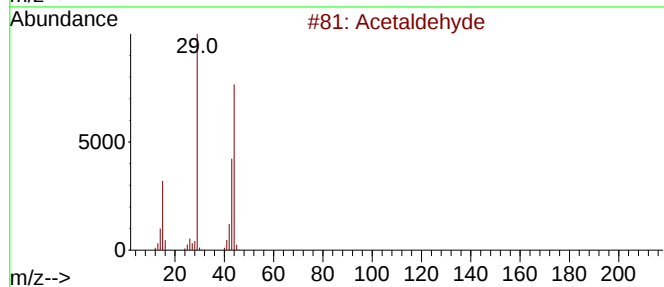
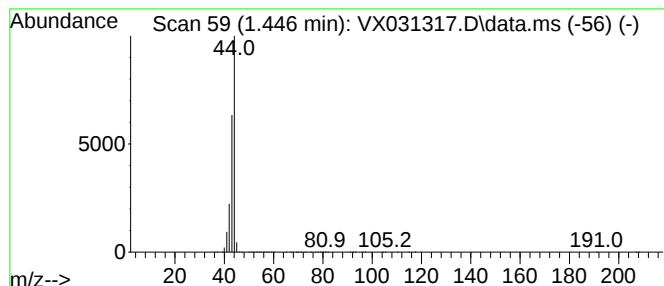
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.446	2541.59 ug/l	11011600	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	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			Carbon dioxide	44	CO2	000124-38-9	3



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Instrument :
MSVOA_X
ClientSampleId :
AUD-1665

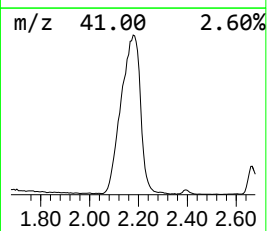
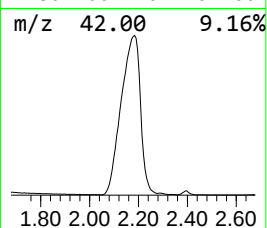
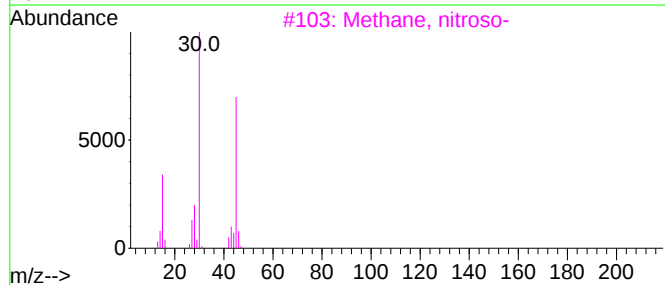
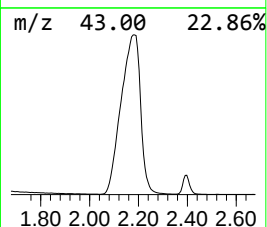
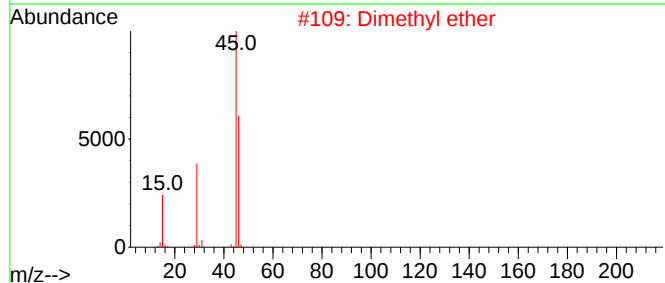
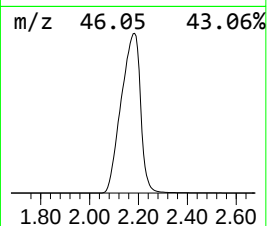
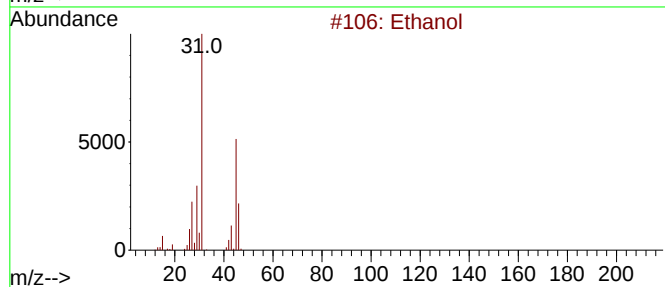
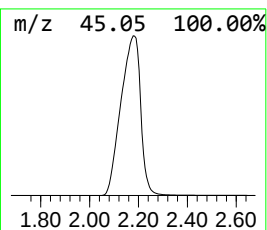
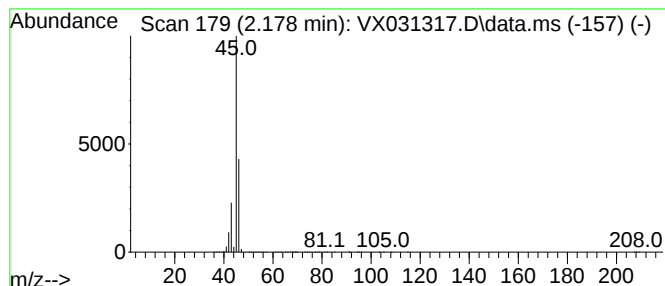
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Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.178	4357.13 ug/l	18877500	Pentafluorobenzene	5.555

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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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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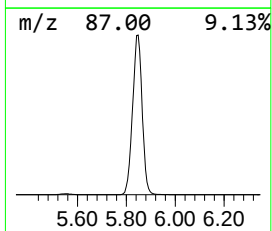
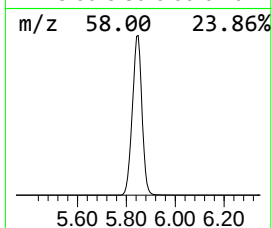
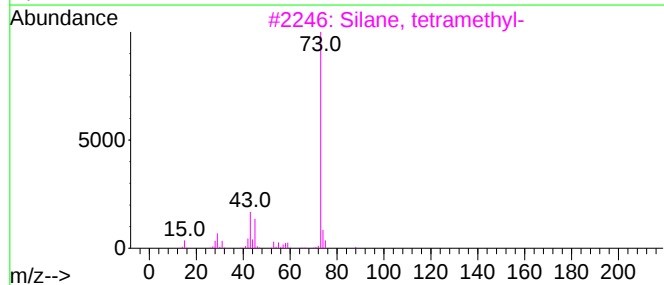
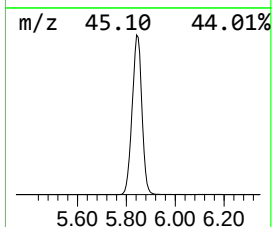
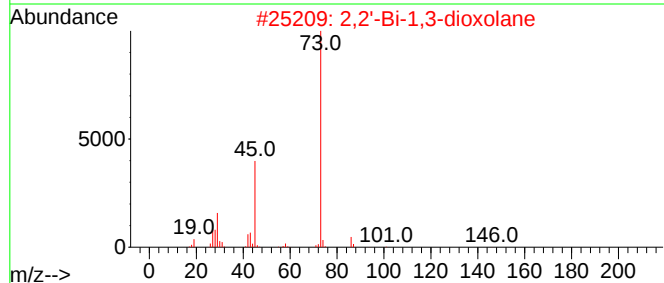
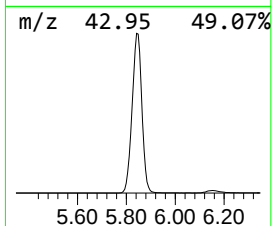
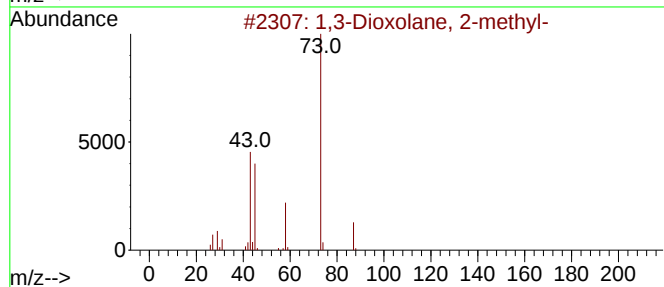
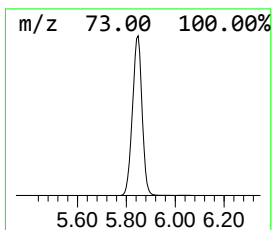
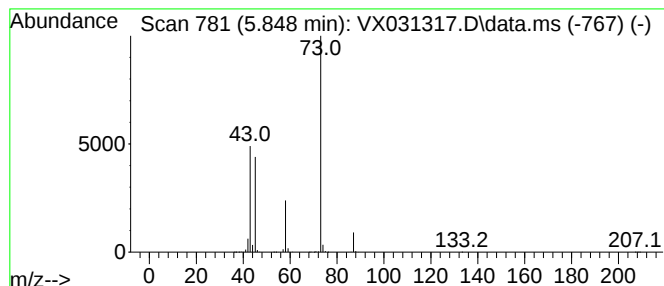
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.848	1228.65 ug/l	5323200	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	22
4			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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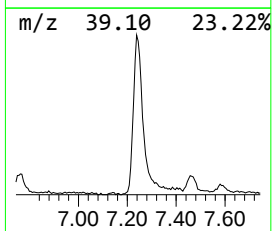
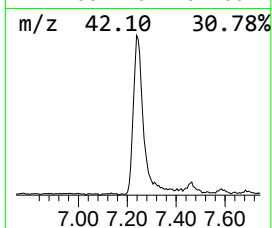
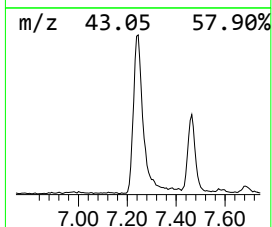
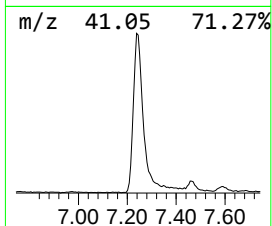
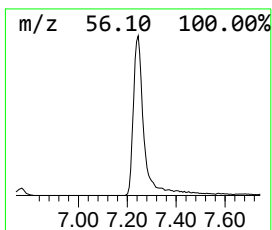
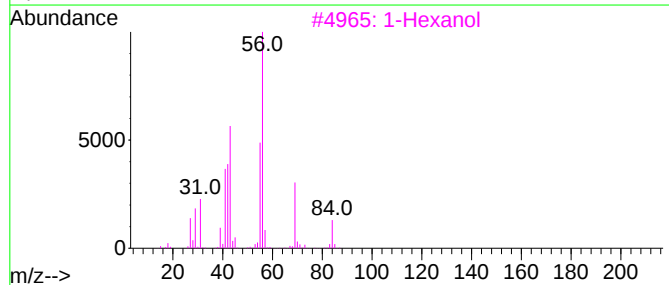
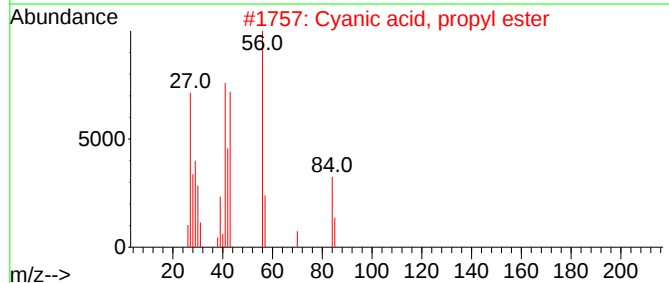
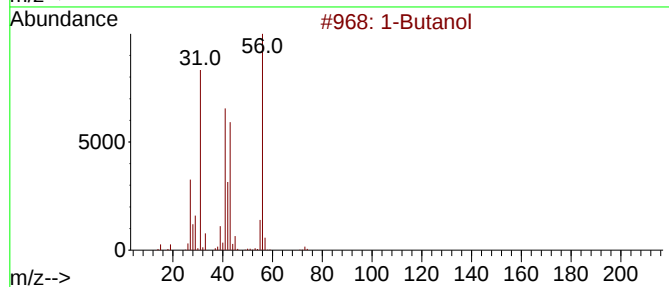
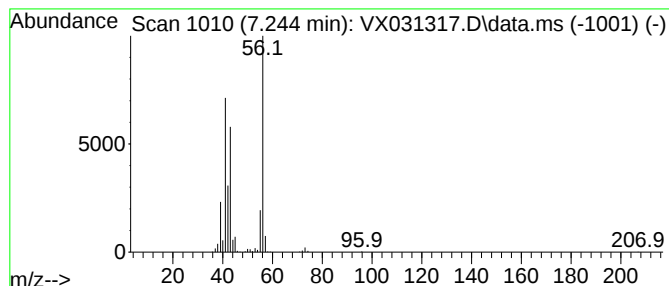
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.244	52.26 ug/l	335822	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	50
3			1-Hexanol	102	C6H14O	000111-27-3	43
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
5			2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	38



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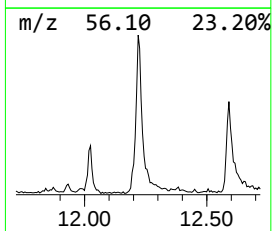
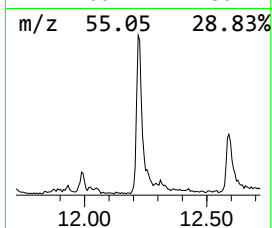
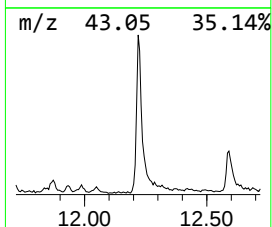
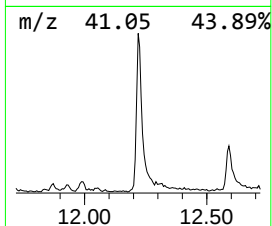
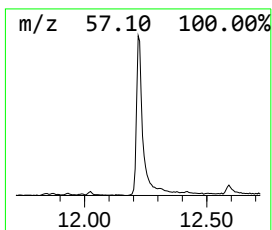
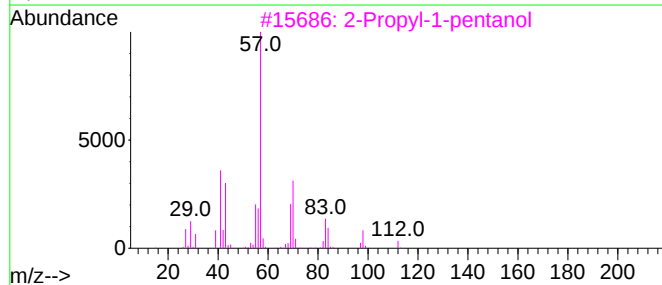
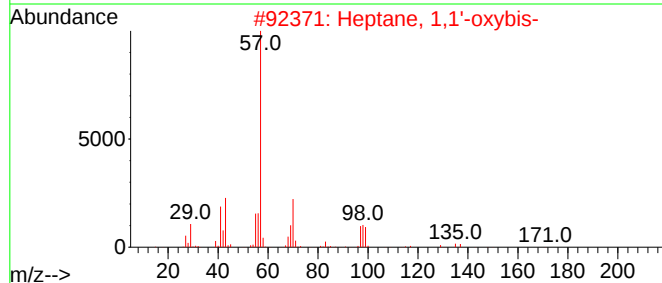
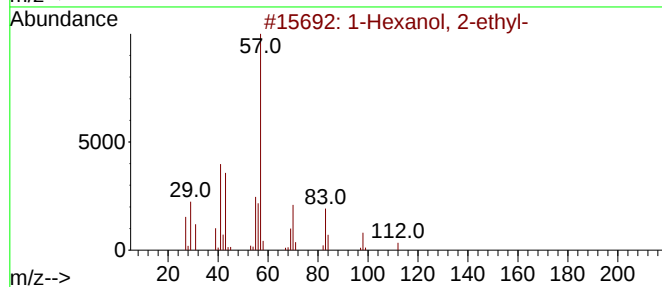
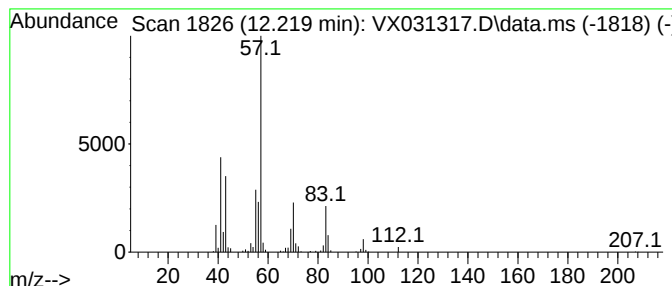
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	32.61 ug/l	203904	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50
5		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091422\
Data File : VX031317.D
Acq On : 14 Sep 2022 19:51
Operator : JC/MD
Sample : N4588-07 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1665

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.257	78.3	ug/l	339029	1	5.555	216628	50.0
Acetaldehyde	1.446	2541.6	ug/l	11011600	1	5.555	216628	50.0
Ethanol	2.178	4357.1	ug/l	18877500	1	5.555	216628	50.0
1,3-Dioxolane, ...	5.848	1228.7	ug/l	5323200	1	5.555	216628	50.0
1-Butanol	7.244	52.3	ug/l	335822	2	6.763	321320	50.0
1-Hexanol, 2-et...	12.219	32.6	ug/l	203904	4	12.024	312673	50.0