

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025376.D
 Acq On : 29 Nov 2021 17:45
 Operator : JC/MD
 Sample : M4837-13 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20933

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\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.063	152	160	172	rBV	775796	1157334	68.83%	15.650%
2	2.538	230	238	244	rBV	24155	44945	2.67%	0.608%
3	3.879	443	458	489	rBV	604436	1681522	100.00%	22.739%
4	5.391	693	706	721	rBV	71458	207358	12.33%	2.804%
5	5.556	721	733	751	rVB2	124391	350924	20.87%	4.745%
6	5.958	787	799	808	rBV	76574	201284	11.97%	2.722%
7	6.031	808	811	820	rVB4	7851	19429	1.16%	0.263%
8	6.763	921	931	945	rBV	190344	449131	26.71%	6.074%
9	7.208	995	1004	1021	rBV	292544	615460	36.60%	8.323%
10	8.653	1234	1241	1248	rBV	383159	606744	36.08%	8.205%
11	9.232	1331	1336	1351	rBV	60420	95084	5.65%	1.286%
12	10.055	1465	1471	1484	rVB	387429	520247	30.94%	7.035%
13	10.579	1552	1557	1565	rBV	174572	224045	13.32%	3.030%
14	10.659	1565	1570	1578	rVB2	14305	26930	1.60%	0.364%
15	11.085	1634	1640	1651	rVB	301602	397763	23.65%	5.379%
16	12.024	1789	1794	1801	rVB	396129	481974	28.66%	6.518%
17	12.219	1821	1826	1839	rBV	158765	211995	12.61%	2.867%
18	12.414	1854	1858	1863	rVB	22448	28193	1.68%	0.381%
19	12.585	1881	1886	1907	rBV	43512	74547	4.43%	1.008%

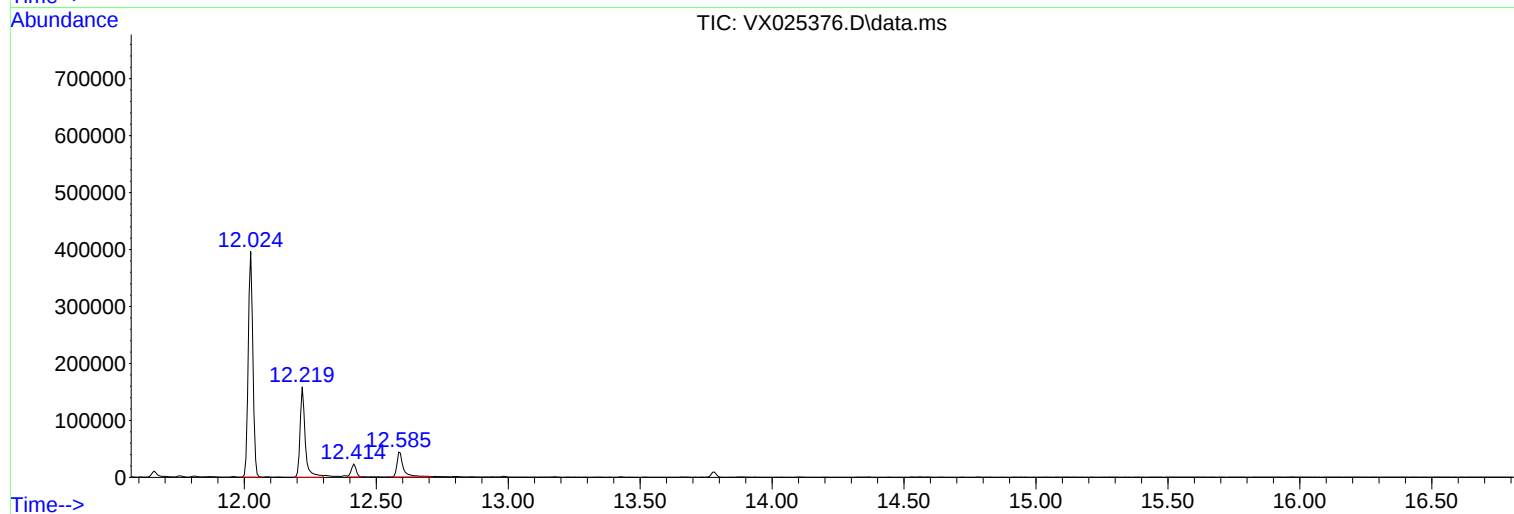
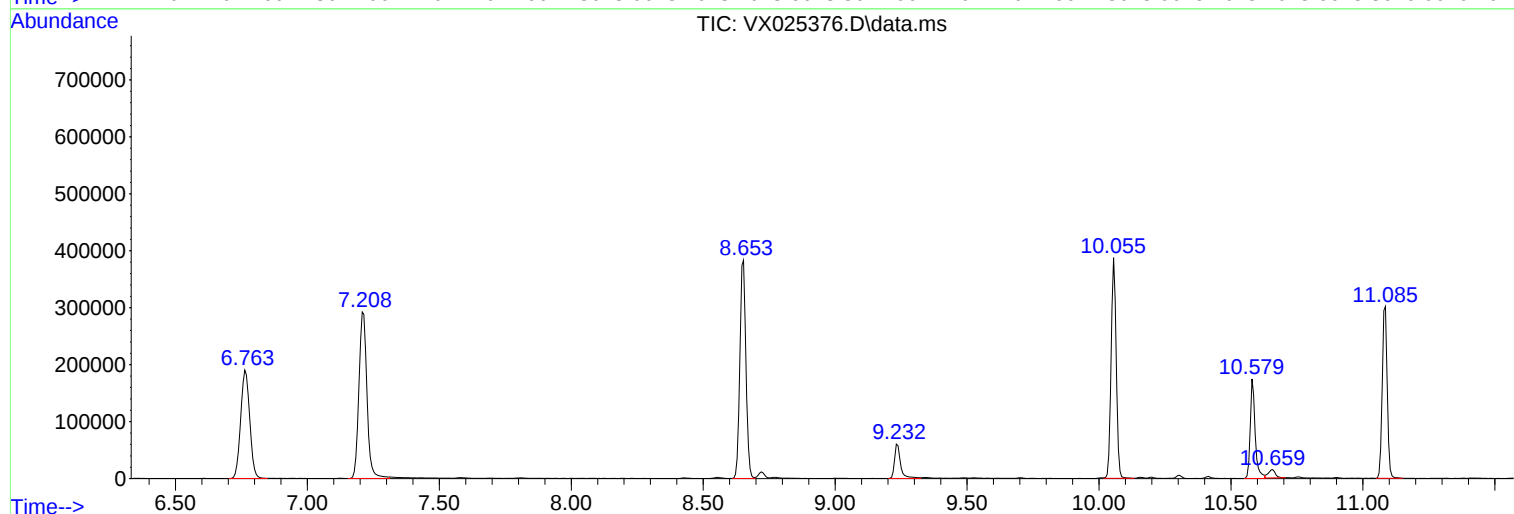
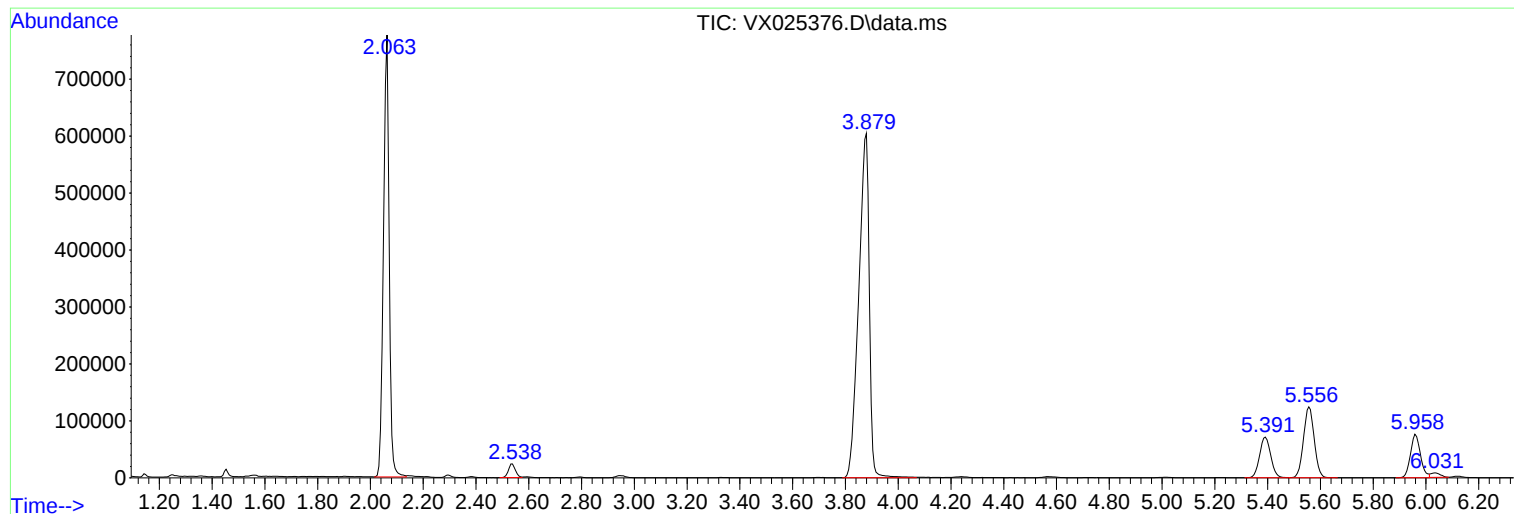
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Quant Title : SW846 8260

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



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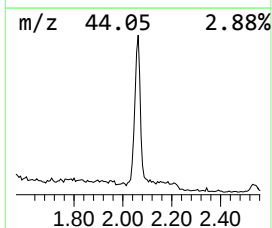
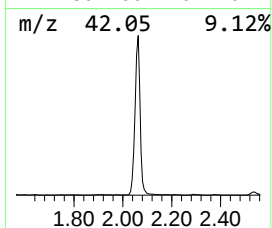
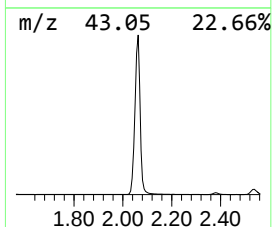
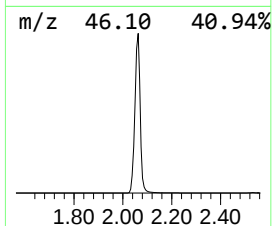
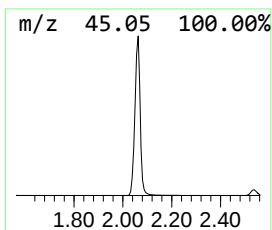
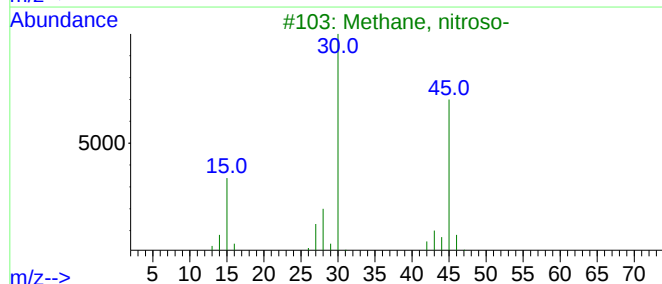
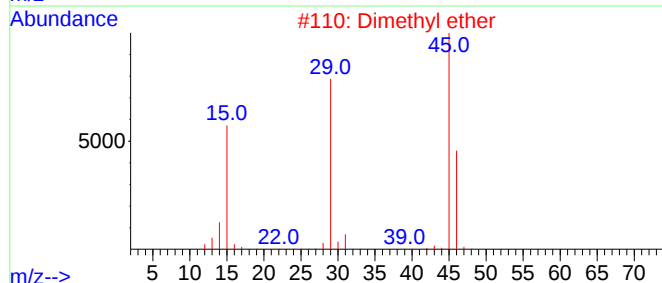
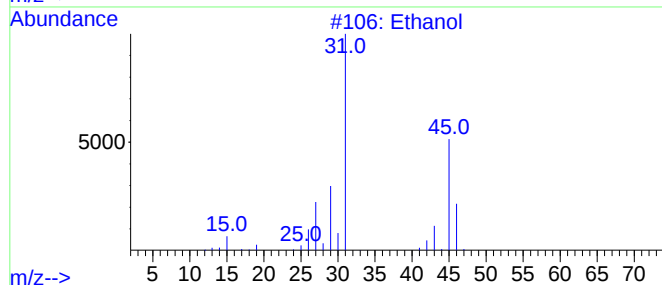
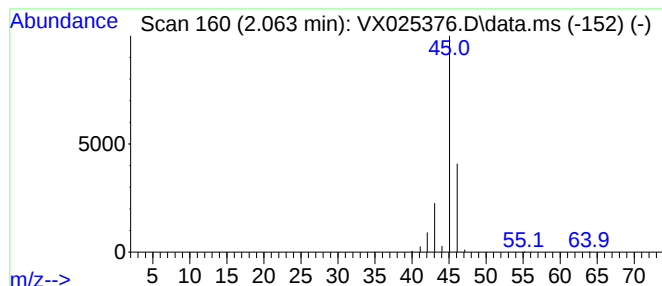
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Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	164.90 ug/l	1157330	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
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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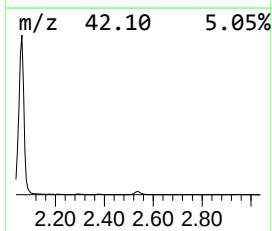
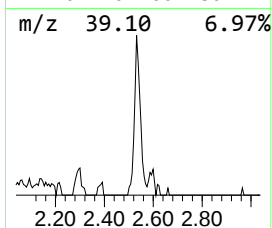
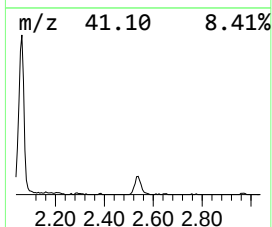
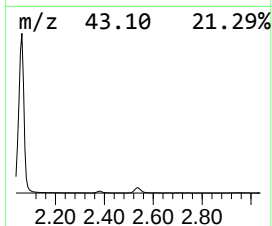
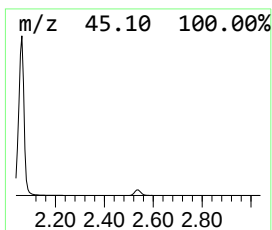
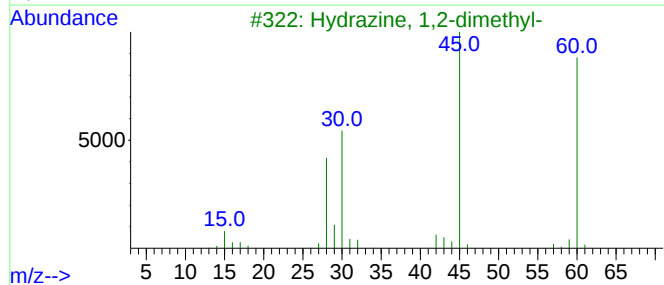
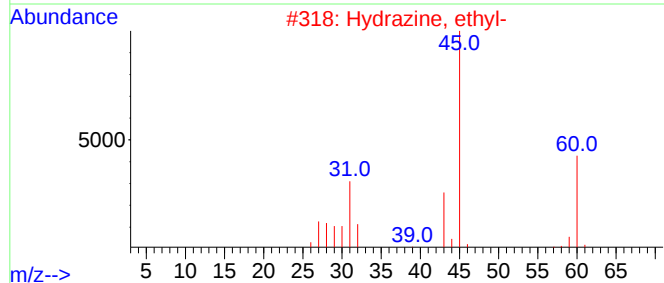
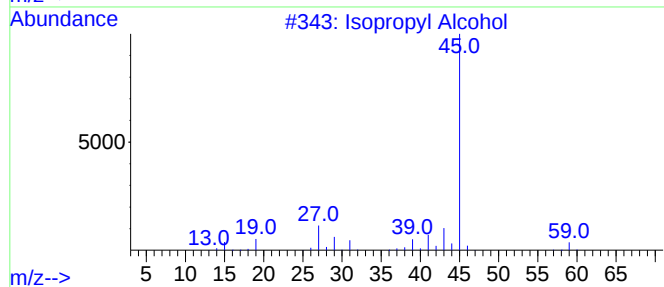
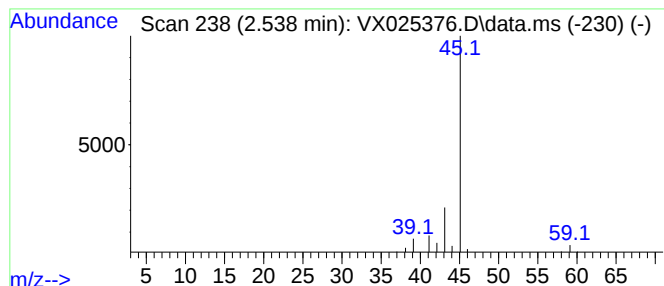
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.538	6.40 ug/l	44945	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	43
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			2-Butanol	74	C4H10O	000078-92-2	4
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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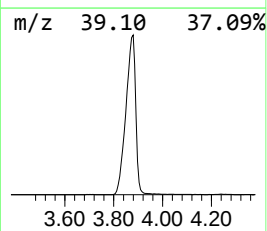
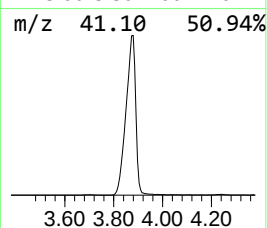
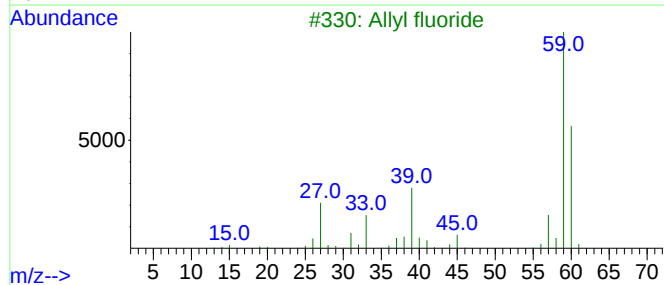
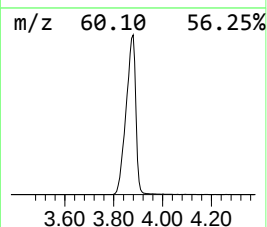
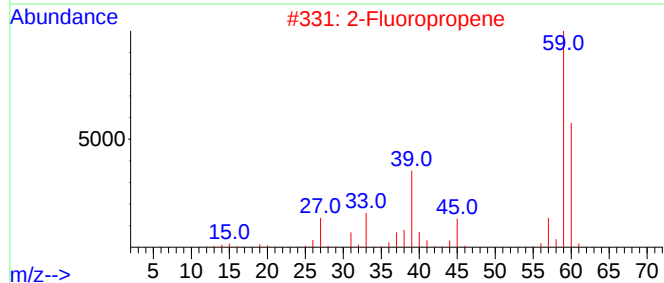
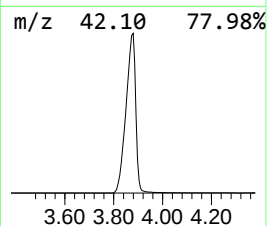
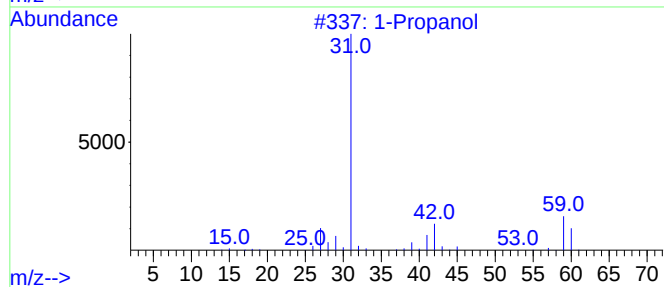
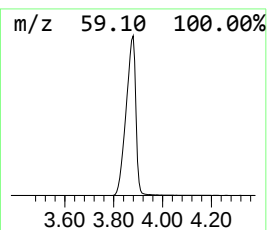
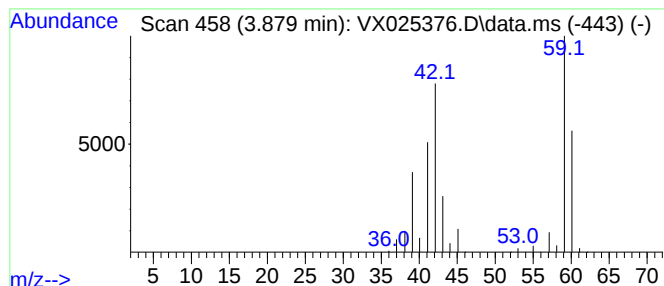
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.879	239.59 ug/l	1681520	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	78
2			2-Fluoropropene	60	C3H5F	001184-60-7	49
3			Allyl fluoride	60	C3H5F	000818-92-8	47
4			Cyclopropane	42	C3H6	000075-19-4	16
5			Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9



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Instrument :
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ClientSampleId :
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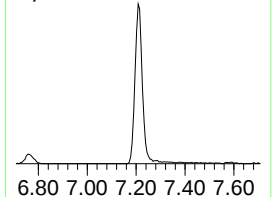
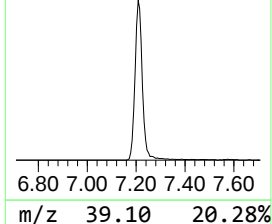
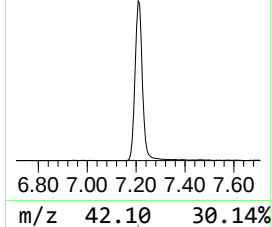
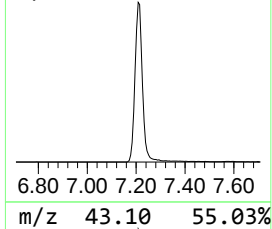
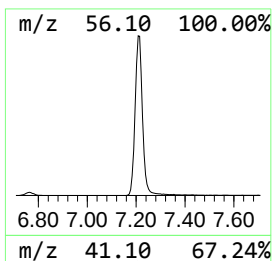
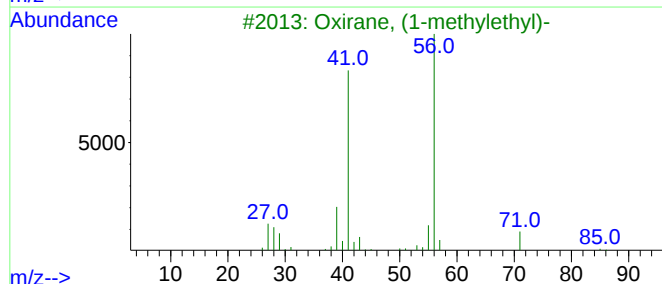
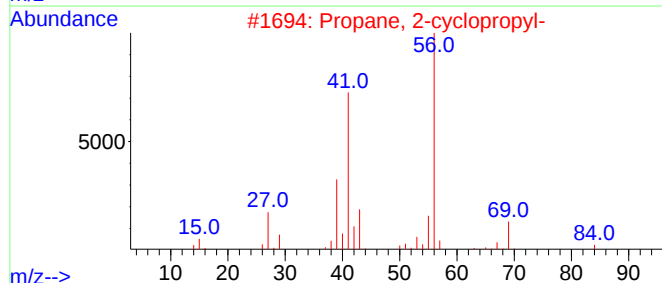
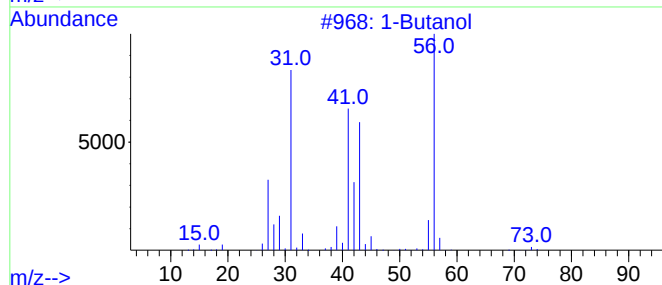
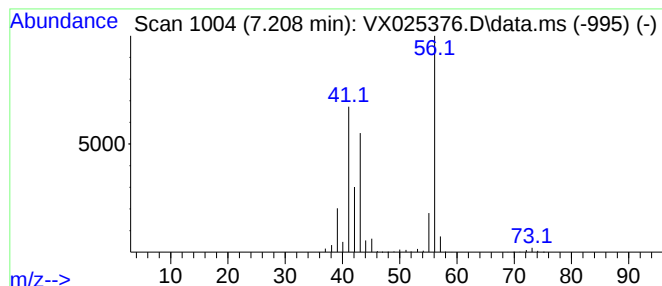
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	68.52 ug/l	615460	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	33
3			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
4			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9



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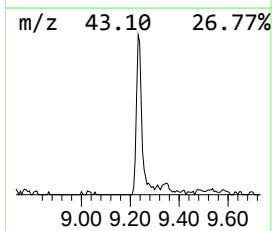
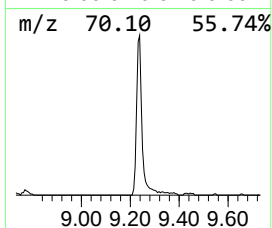
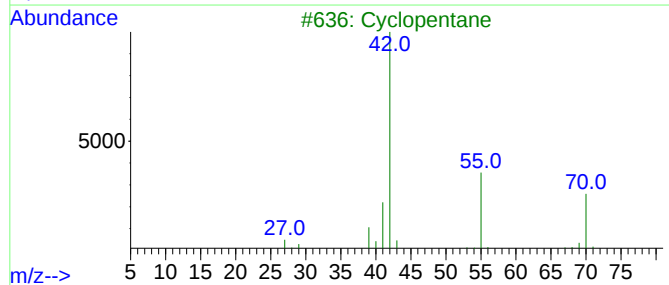
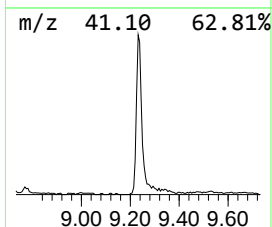
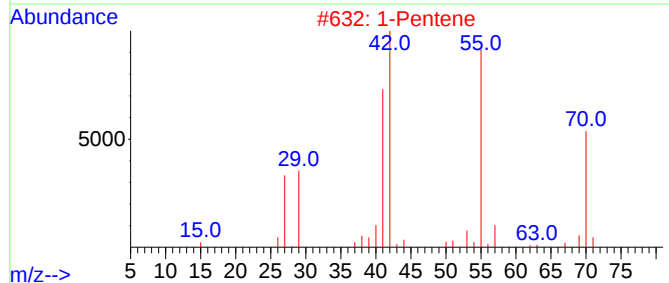
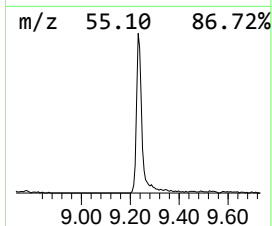
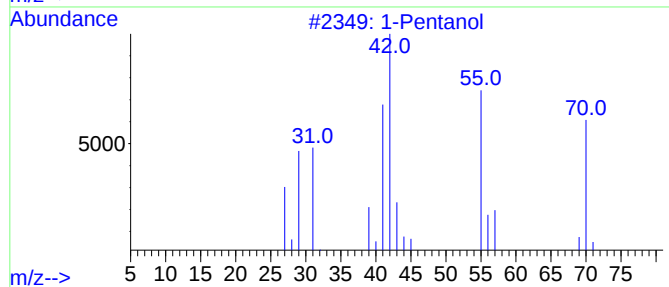
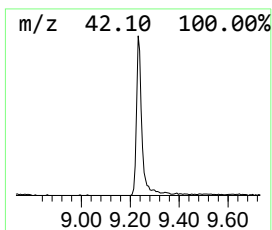
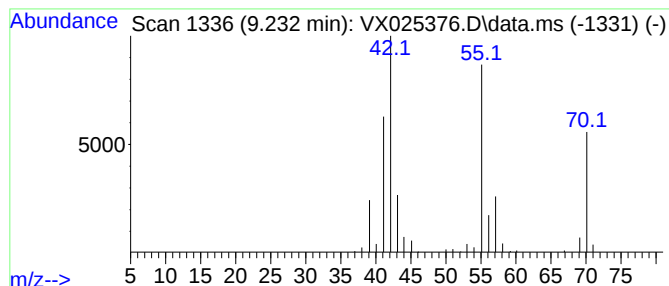
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Quant Title : SW846 8260

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

Peak Number 5 1-Pentanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	9.14 ug/l	95084	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol	88	C5H12O	000071-41-0	86
2			1-Pentene	70	C5H10	000109-67-1	72
3			Cyclopentane	70	C5H10	000287-92-3	72
4			1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	50
5			Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	40



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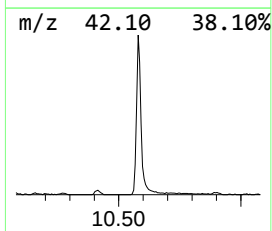
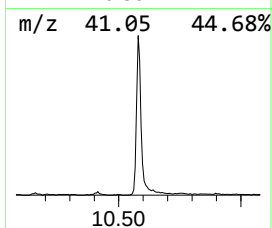
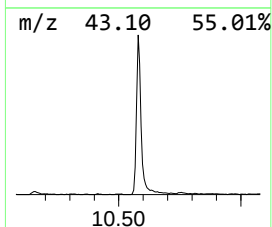
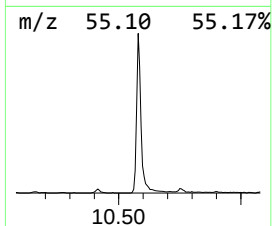
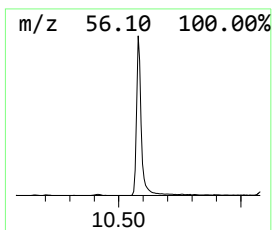
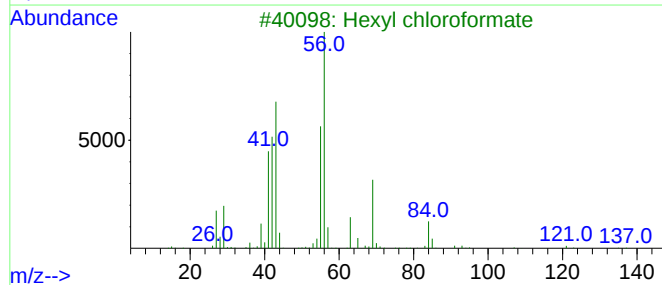
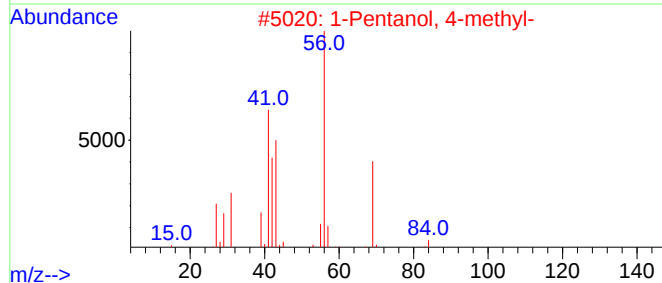
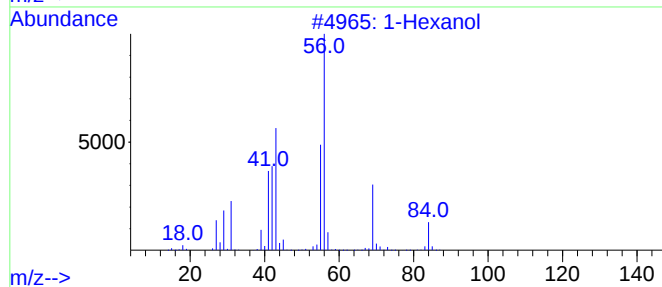
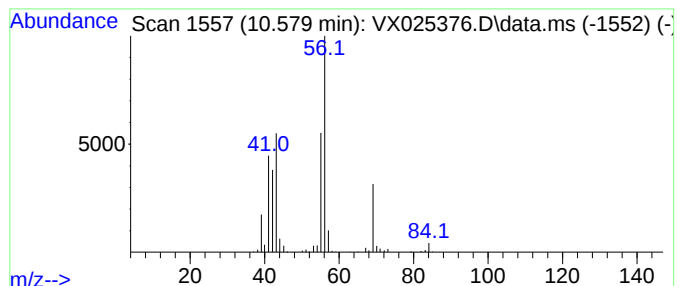
Instrument :
MSVOA_X
ClientSampleId :
20933

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.579	21.53 ug/l	224045	Chlorobenzene-d5	10.055	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	86
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	59
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025376.D
Acq On : 29 Nov 2021 17:45
Operator : JC/MD
Sample : M4837-13 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20933

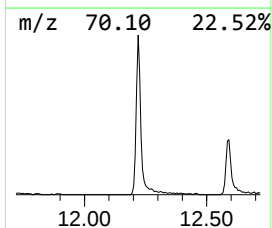
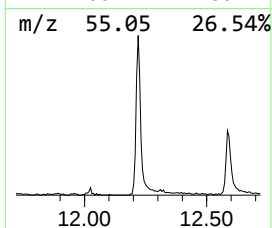
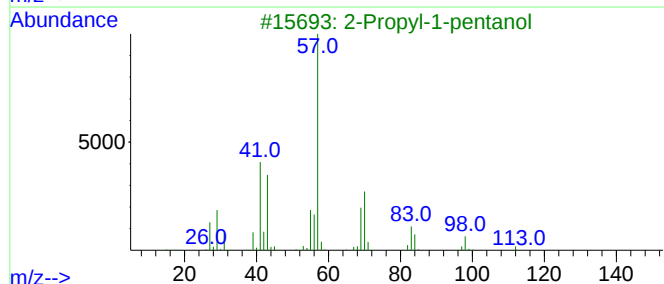
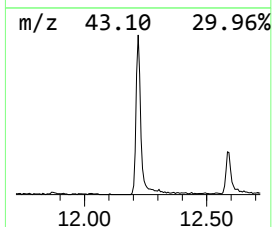
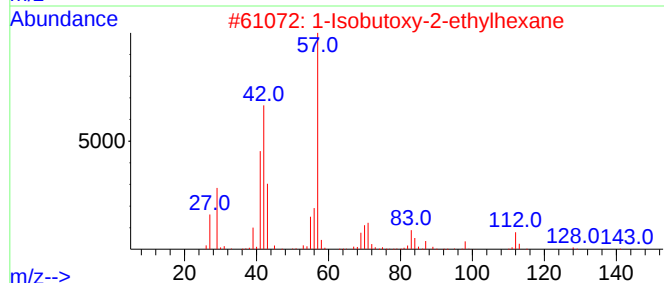
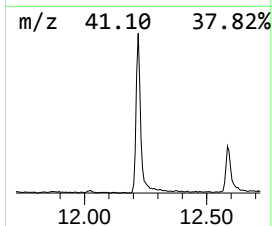
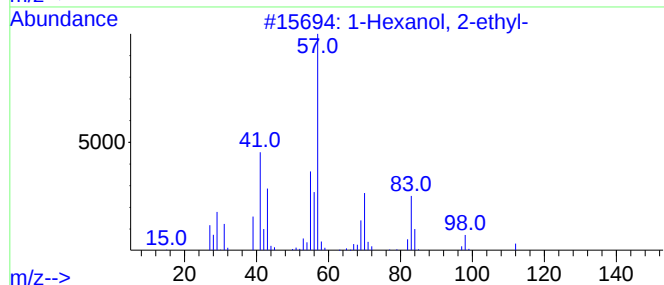
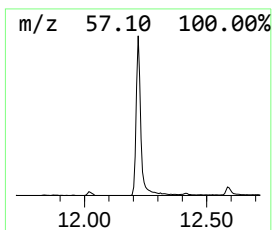
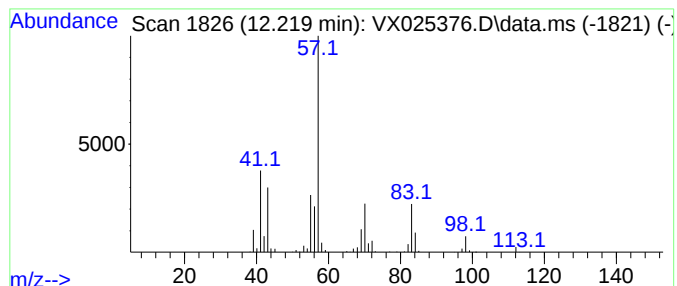
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	21.99 ug/l	211995	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	90
2		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025376.D
Acq On : 29 Nov 2021 17:45
Operator : JC/MD
Sample : M4837-13 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

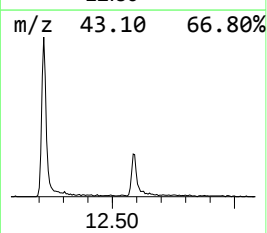
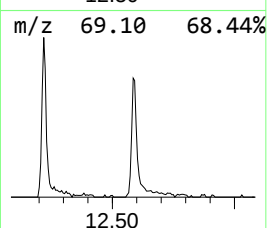
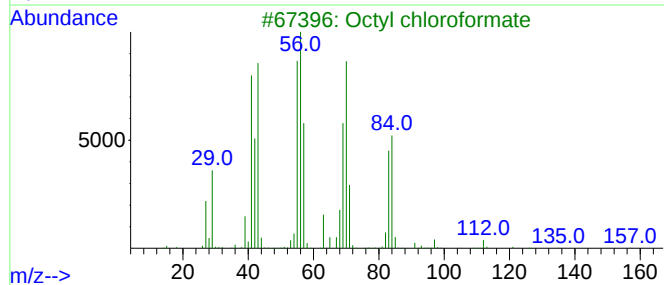
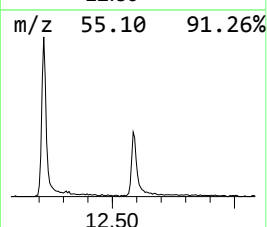
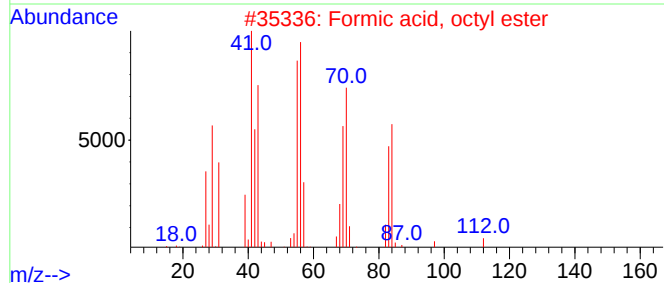
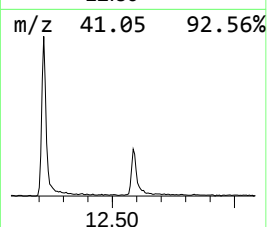
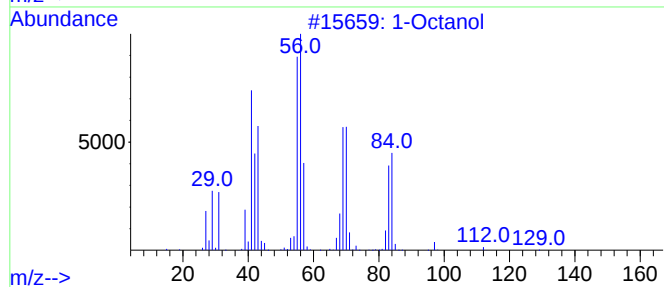
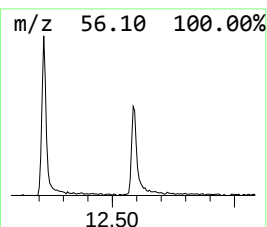
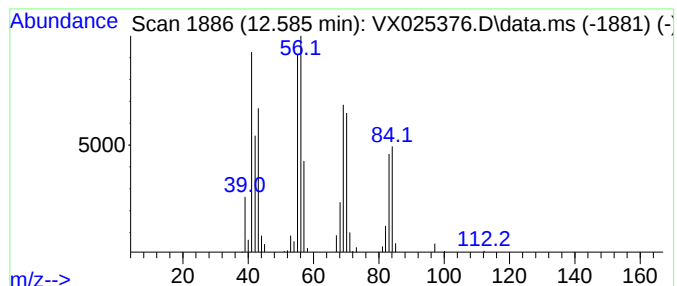
Instrument :
MSVOA_X
ClientSampleId :
20933

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Octanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.585	7.73 ug/l	74547	1,4-Dichlorobenzene-d4		12.024	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Octanol		130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester		158	C9H18O2	000112-32-3	90
3	Octyl chloroformate		192	C9H17ClO2	007452-59-7	78
4	1-Nonanol		144	C9H20O	000143-08-8	72
5	Formic acid, heptyl ester		144	C8H16O2	000112-23-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025376.D
Acq On : 29 Nov 2021 17:45
Operator : JC/MD
Sample : M4837-13 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20933

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.063	164.9	ug/l	1157330	1	5.562	350924	50.0
Isopropyl Alcohol	2.538	6.4	ug/l	44945	1	5.562	350924	50.0
1-Propanol	3.879	239.6	ug/l	1681520	1	5.562	350924	50.0
1-Butanol	7.208	68.5	ug/l	615460	2	6.763	449131	50.0
1-Pentanol	9.232	9.1	ug/l	95084	3	10.055	520247	50.0
1-Hexanol	10.579	21.5	ug/l	224045	3	10.055	520247	50.0
1-Hexanol, 2-et...	12.219	22.0	ug/l	211995	4	12.024	481974	50.0
1-Octanol	12.585	7.7	ug/l	74547	4	12.024	481974	50.0