

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025363.D
 Acq On : 29 Nov 2021 12:41
 Operator : JC/MD
 Sample : M4837-06 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20926

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: VX025363.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	153	160	176	rBV	512134	772176	85.28%	12.996%
2	2.538	230	238	246	rBV	11046	21547	2.38%	0.363%
3	2.947	296	305	315	rVB	4580	10647	1.18%	0.179%
4	3.867	444	456	475	rBV	345938	905420	100.00%	15.238%
5	5.391	692	706	722	rBV	75222	218665	24.15%	3.680%
6	5.556	722	733	751	rVB	130420	368312	40.68%	6.199%
7	5.958	789	799	819	rBV	81946	216509	23.91%	3.644%
8	6.763	920	931	949	rBV	200674	474061	52.36%	7.978%
9	7.208	996	1004	1024	rBV	173864	373524	41.25%	6.286%
10	8.647	1233	1240	1249	rBV	403041	649634	71.75%	10.933%
11	9.238	1329	1337	1341	rBV	29329	44176	4.88%	0.743%
12	10.055	1465	1471	1480	rBV	433848	564941	62.40%	9.508%
13	10.579	1552	1557	1566	rBV	80756	118951	13.14%	2.002%
14	10.659	1566	1570	1581	rVB2	5426	10488	1.16%	0.177%
15	11.085	1634	1640	1654	rVB	335981	438564	48.44%	7.381%
16	11.659	1729	1734	1741	rBV2	5973	9669	1.07%	0.163%
17	12.024	1788	1794	1804	rBV	446439	543604	60.04%	9.149%
18	12.219	1821	1826	1839	rBV	120913	163163	18.02%	2.746%
19	12.415	1854	1858	1863	rVB	7367	9543	1.05%	0.161%
20	12.591	1882	1887	1898	rBV	16324	28258	3.12%	0.476%

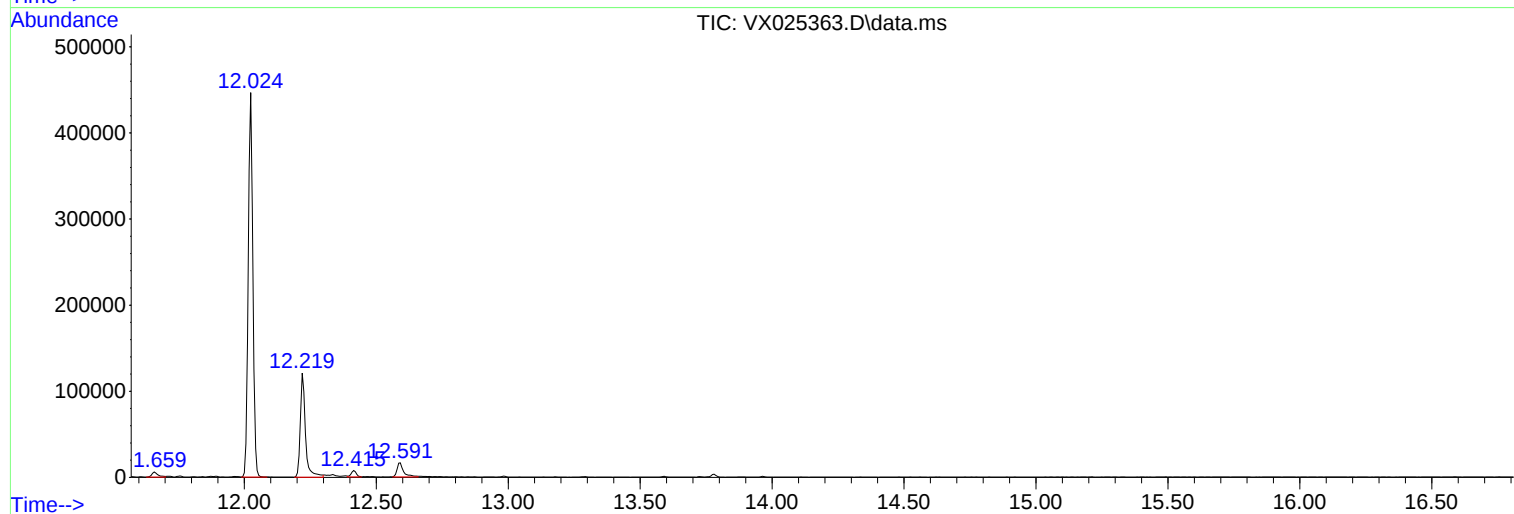
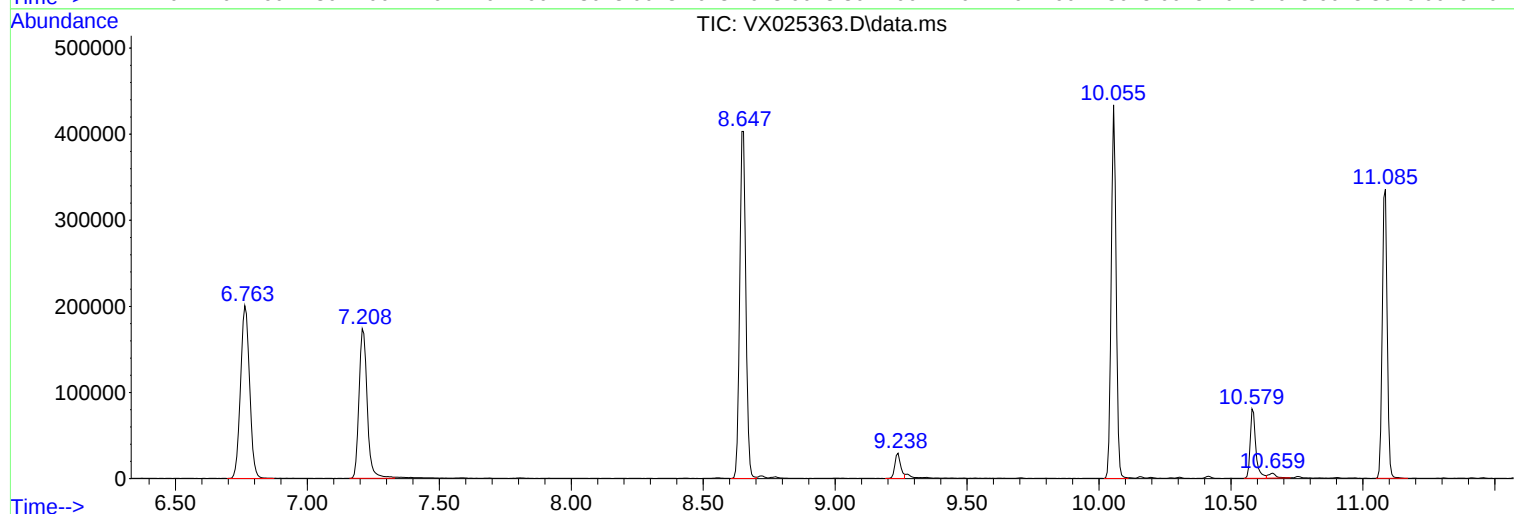
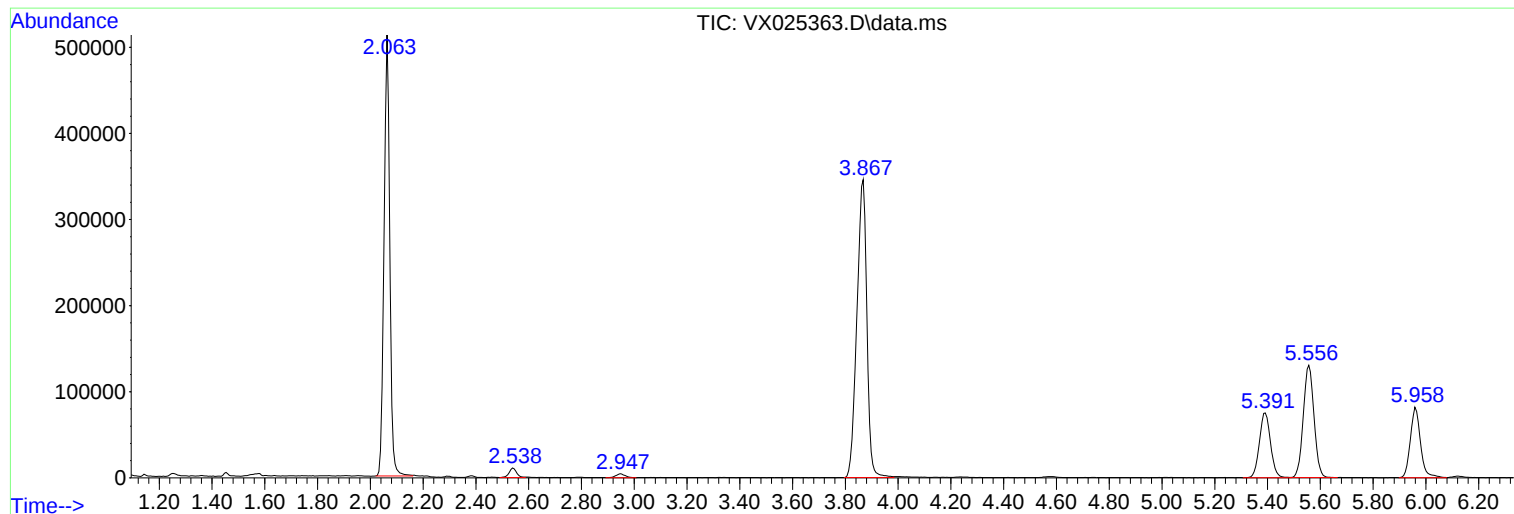
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Quant Title : SW846 8260

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



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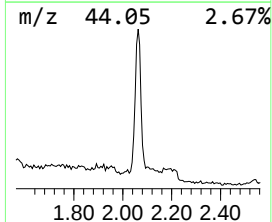
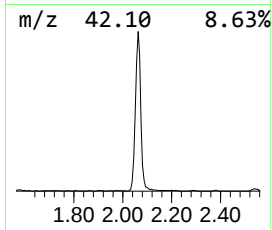
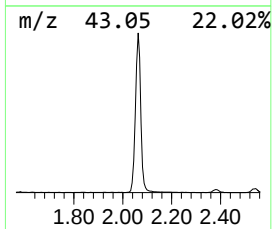
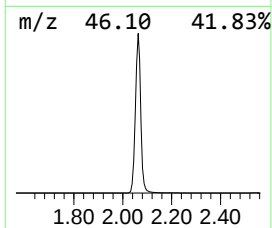
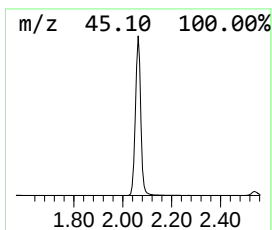
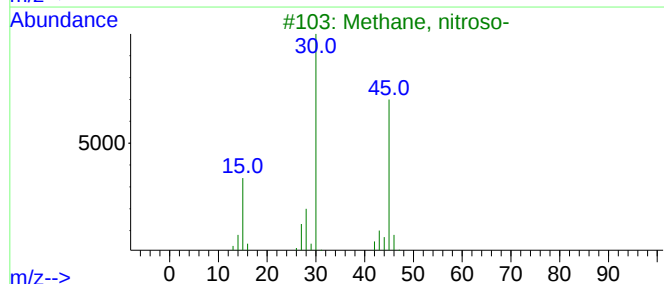
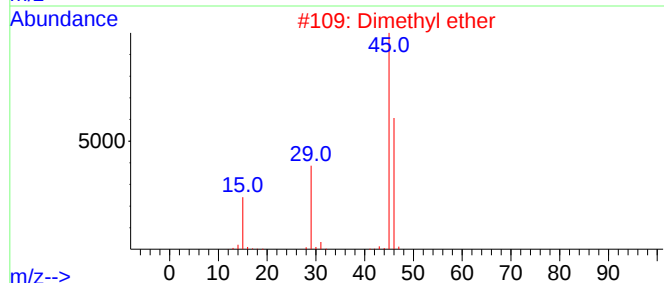
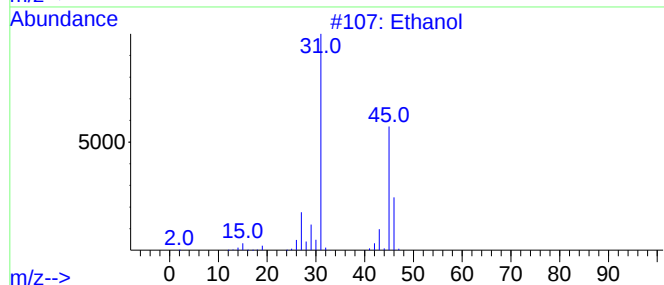
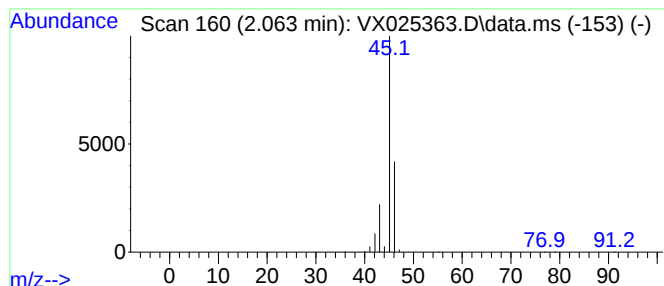
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	104.83 ug/l	772176	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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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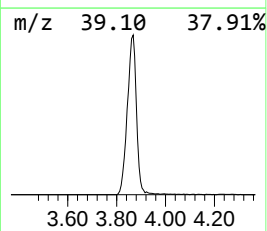
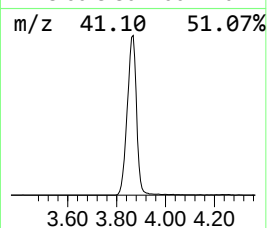
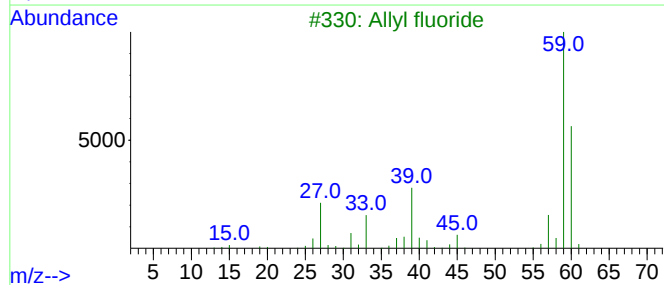
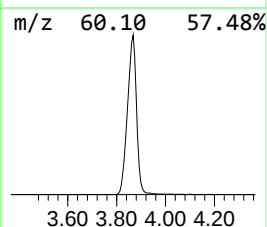
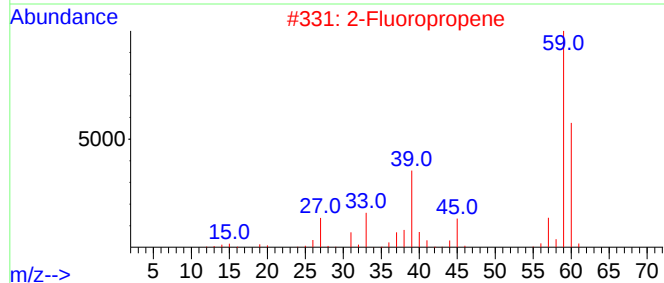
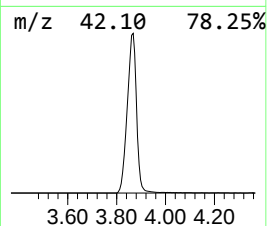
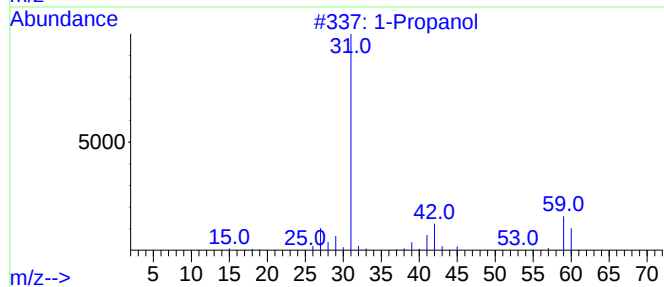
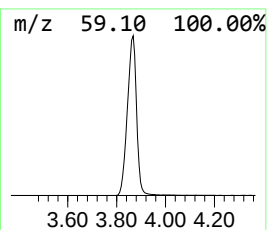
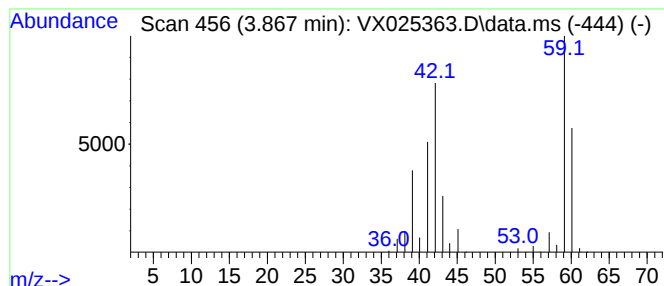
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.867	122.92 ug/l	905420	Pentafluorobenzene	5.556

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	52
3	Allyl fluoride			60	C3H5F	000818-92-8	47
4	Cyclopropane			42	C3H6	000075-19-4	12
5	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	9



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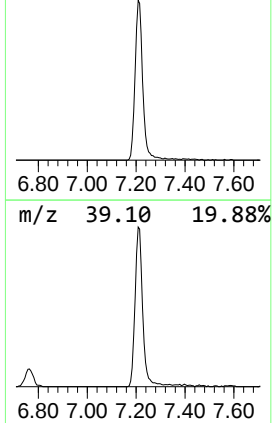
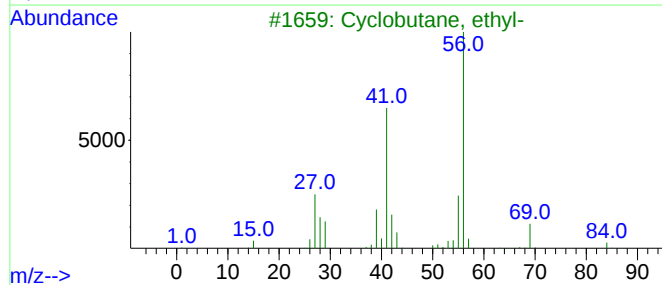
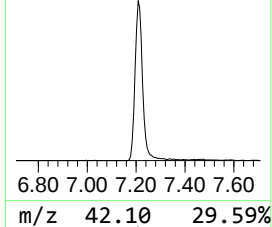
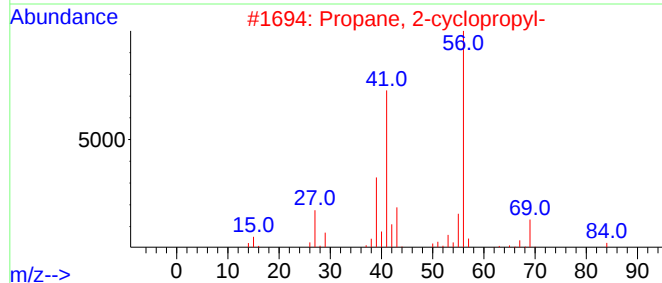
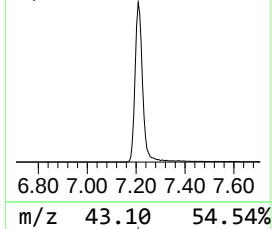
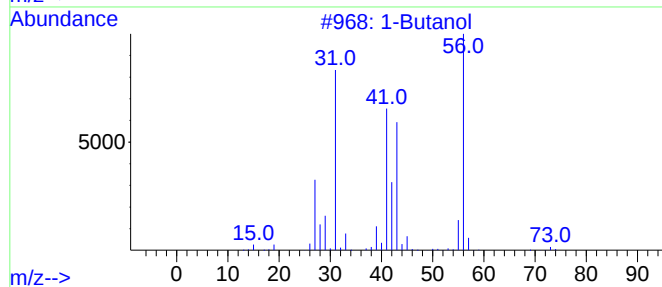
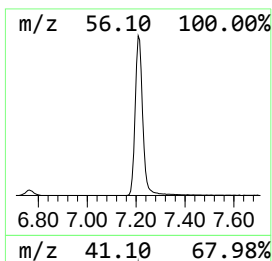
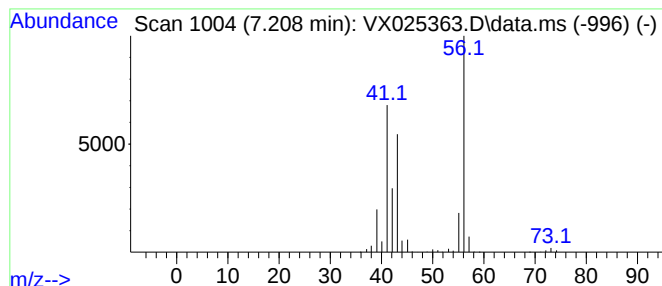
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	39.40 ug/l	373524	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	9
3	Cyclobutane, ethyl-		84	C6H12	004806-61-5	9
4	Oxirane, (1-methylethyl)-		86	C5H10O	001438-14-8	9
5	Methoxyacetonitrile		71	C3H5NO	001738-36-9	9



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Sample : M4837-06 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

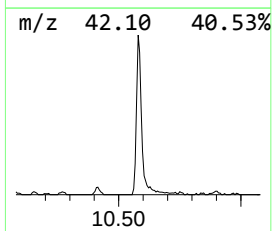
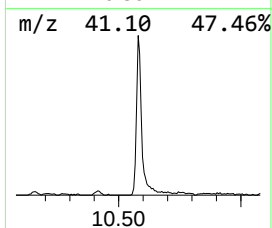
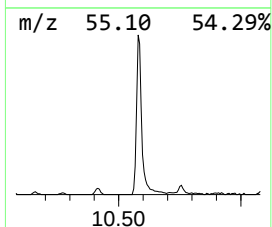
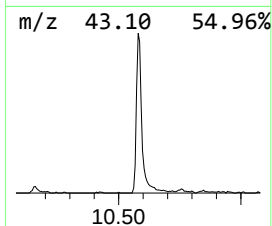
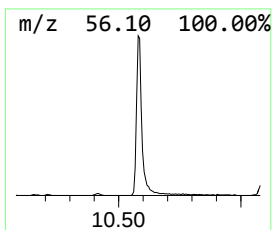
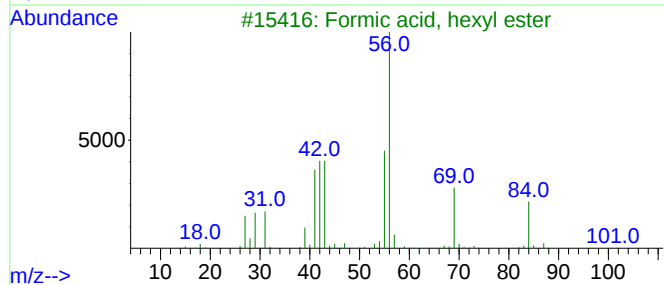
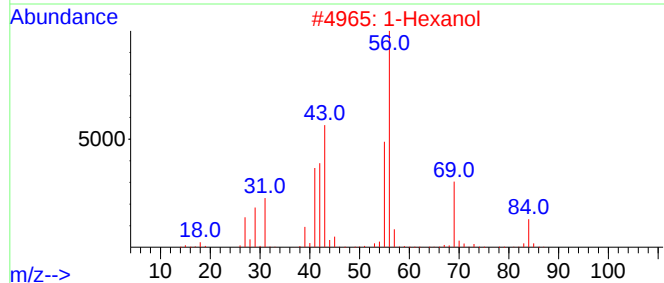
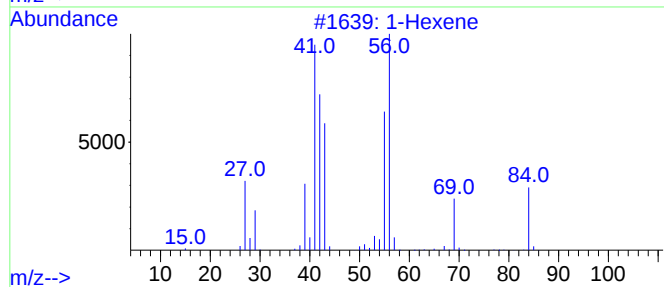
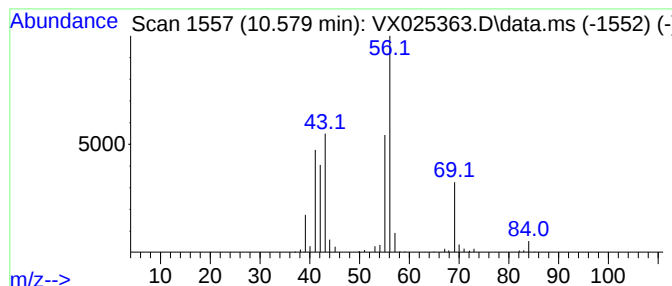
Instrument :
MSVOA_X
ClientSampleId :
20926

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-Hexene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.579	10.53 ug/l	118951	Chlorobenzene-d5	10.055	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene	84	C6H12	000592-41-6	90
2	1-Hexanol	102	C6H14O	000111-27-3	90
3	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
4	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	64



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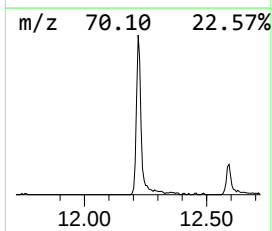
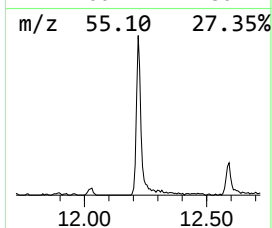
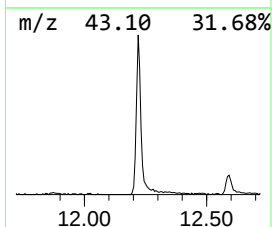
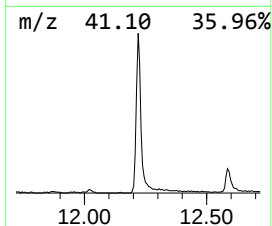
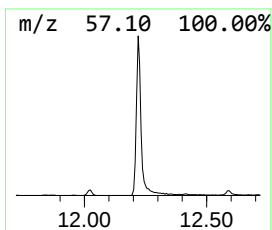
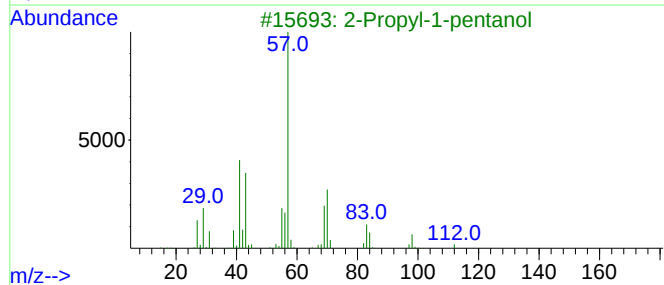
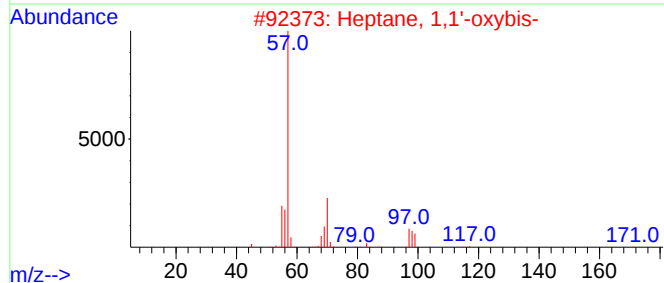
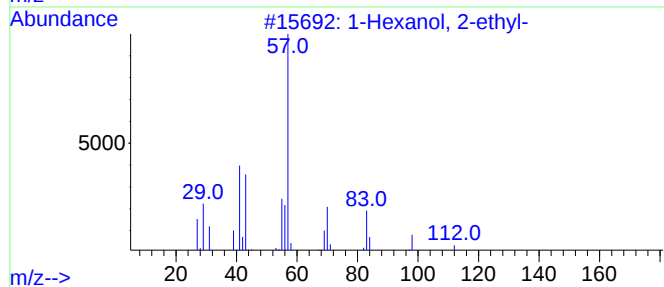
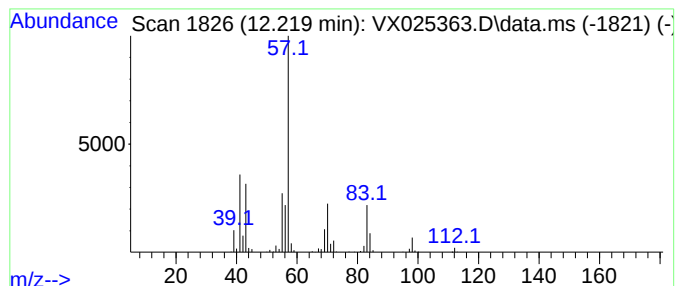
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	15.01 ug/l	163163	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	83
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47



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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	104.8	ug/l	772176	1	5.556	368312	50.0
1-Propanol	3.867	122.9	ug/l	905420	1	5.556	368312	50.0
1-Butanol	7.208	39.4	ug/l	373524	2	6.763	474061	50.0
1-Hexene	10.579	10.5	ug/l	118951	3	10.055	564941	50.0
1-Hexanol, 2-et...	12.219	15.0	ug/l	163163	4	12.024	543604	50.0