

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025374.D
 Acq On : 29 Nov 2021 16:58
 Operator : JC/MD
 Sample : M4837-11 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20931

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: VX025374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	33	rBV	4384	8438	1.12%	0.157%
2	2.056	150	159	181	rBV	426028	633229	83.73%	11.762%
3	2.538	230	238	245	rBV	8432	16244	2.15%	0.302%
4	2.946	297	305	314	rBV	4205	9729	1.29%	0.181%
5	3.861	444	455	477	rBV	297038	756279	100.00%	14.048%
6	4.574	562	572	584	rVB2	2733	8686	1.15%	0.161%
7	5.391	693	706	719	rBV	73858	211717	27.99%	3.933%
8	5.556	722	733	750	rVB	126005	357034	47.21%	6.632%
9	5.958	788	799	818	rBV	77134	208021	27.51%	3.864%
10	6.763	922	931	947	rBV	194169	460131	60.84%	8.547%
11	7.208	996	1004	1023	rBV	138200	293729	38.84%	5.456%
12	8.653	1234	1241	1249	rBV	394617	629048	83.18%	11.685%
13	9.238	1332	1337	1351	rBV	18052	33556	4.44%	0.623%
14	10.055	1465	1471	1485	rVB	410851	546896	72.31%	10.159%
15	10.585	1552	1558	1566	rBV	55709	85261	11.27%	1.584%
16	10.658	1566	1570	1580	rVB3	6025	10675	1.41%	0.198%
17	11.085	1634	1640	1651	rBV	327392	423007	55.93%	7.857%
18	12.024	1788	1794	1803	rBV	428389	525849	69.53%	9.768%
19	12.219	1820	1826	1839	rBV	90957	126813	16.77%	2.356%
20	12.414	1854	1858	1863	rVB	11059	14154	1.87%	0.263%
21	12.591	1881	1887	1899	rBV	14094	24990	3.30%	0.464%

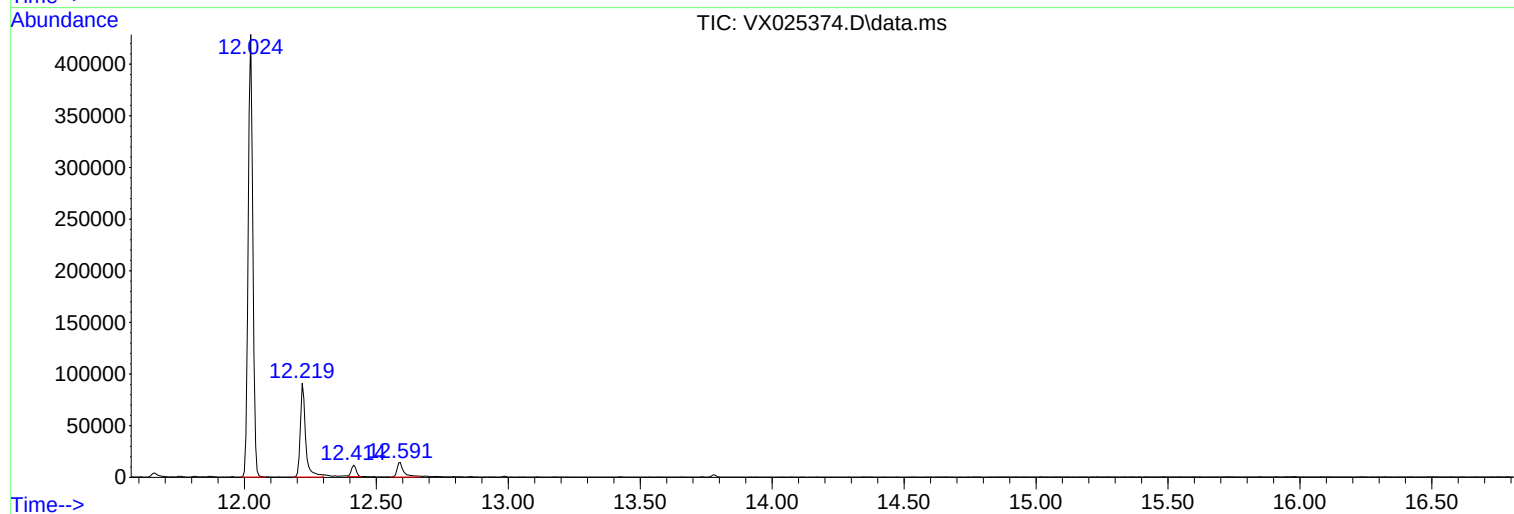
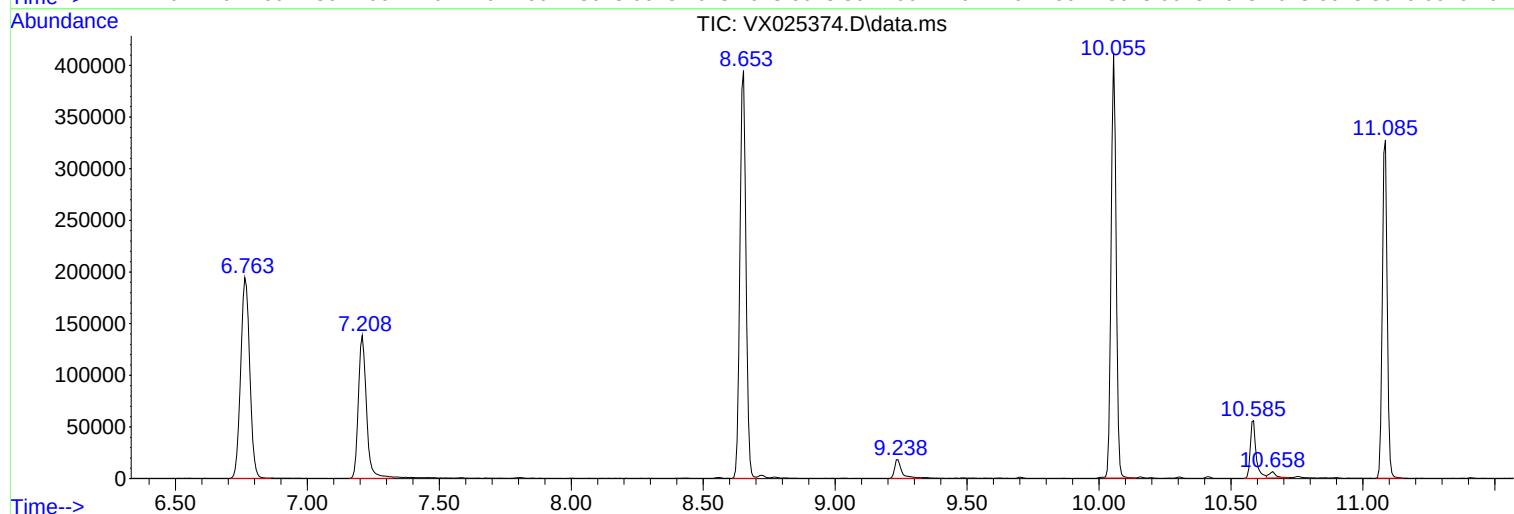
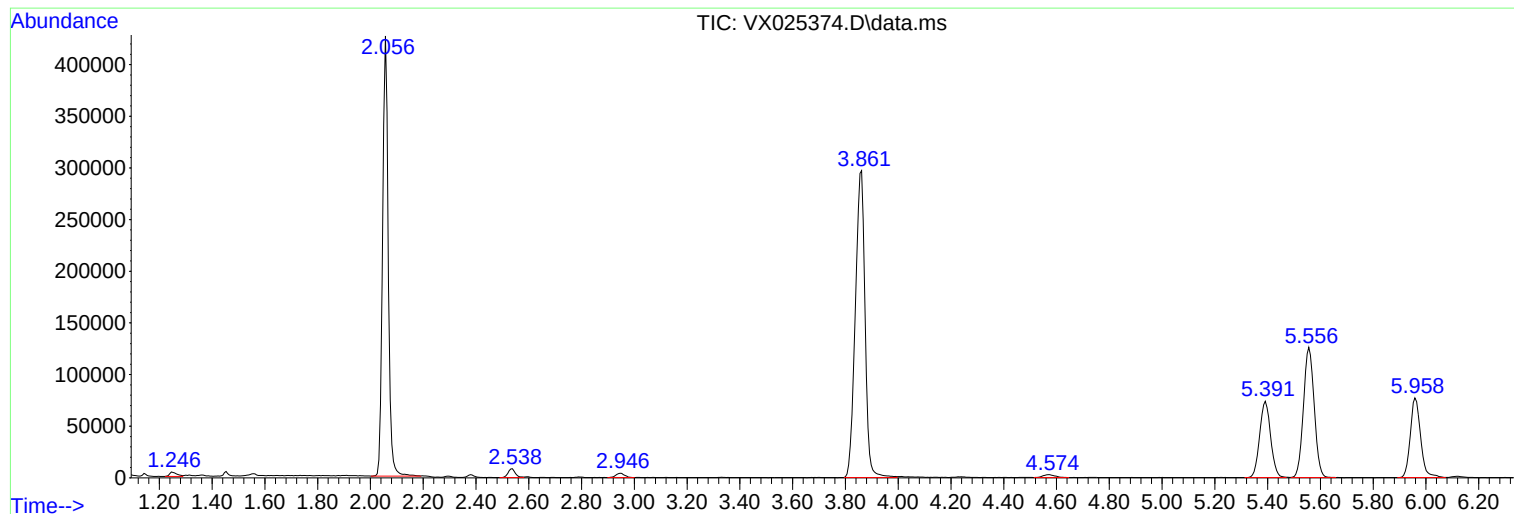
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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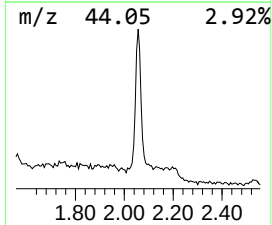
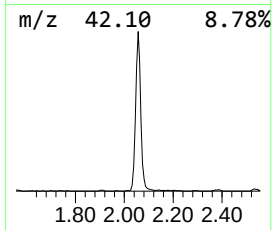
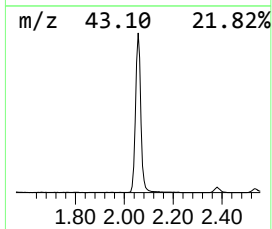
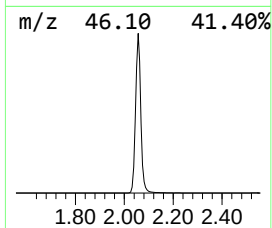
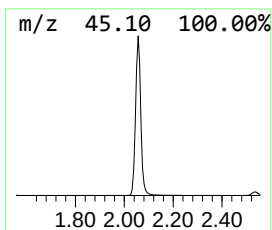
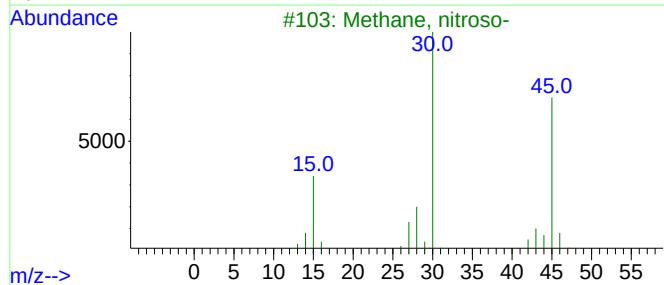
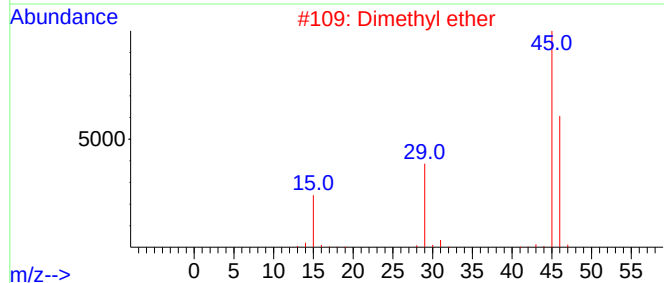
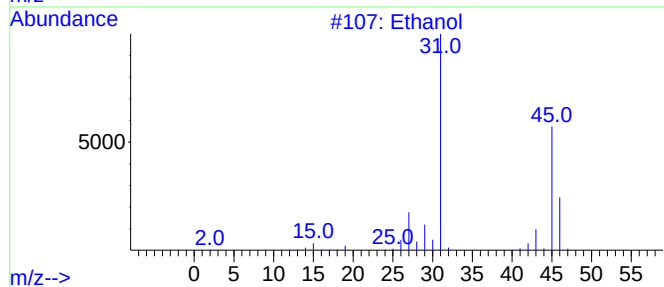
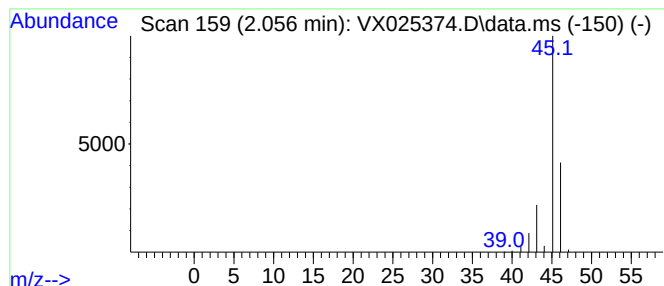
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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.
2.056	88.68 ug/l	633229	Pentafluorobenzene	5.556

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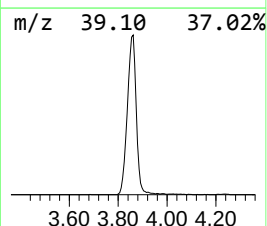
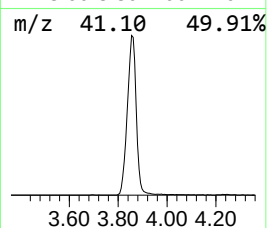
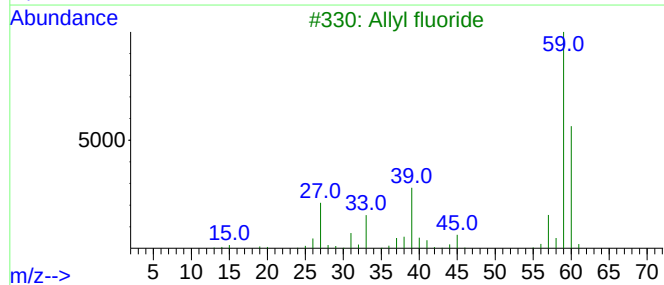
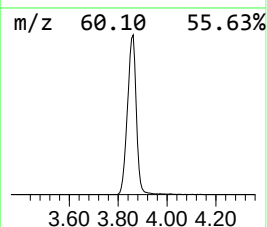
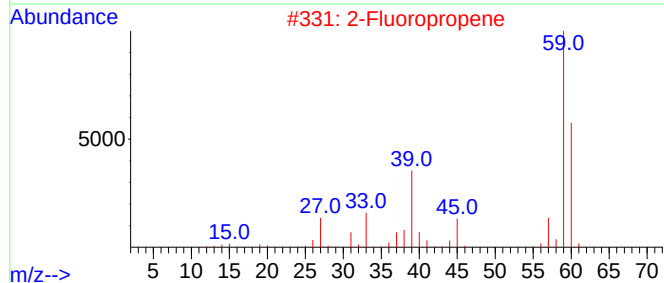
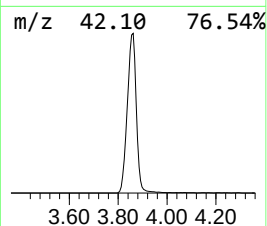
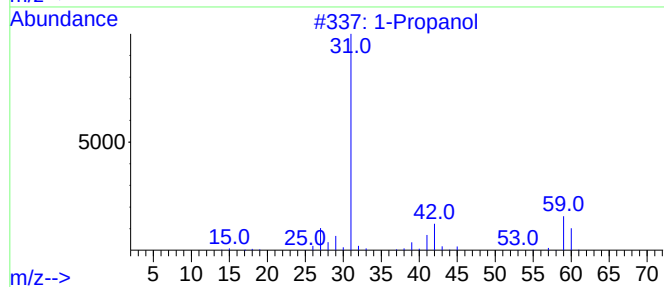
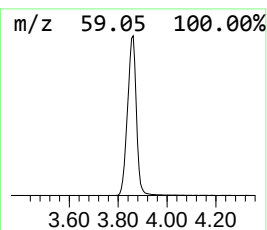
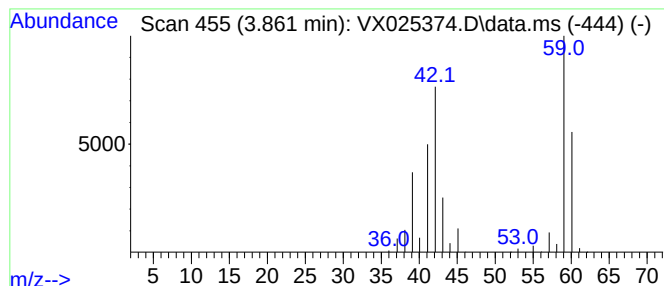
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.861	105.91 ug/l	756279	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	37
4		2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	17
5		Cyclopropane	42	C3H6	000075-19-4	12



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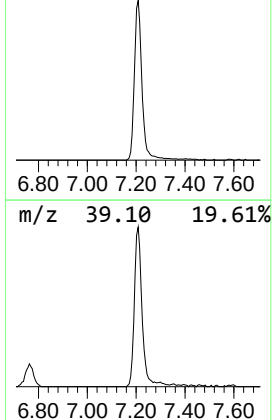
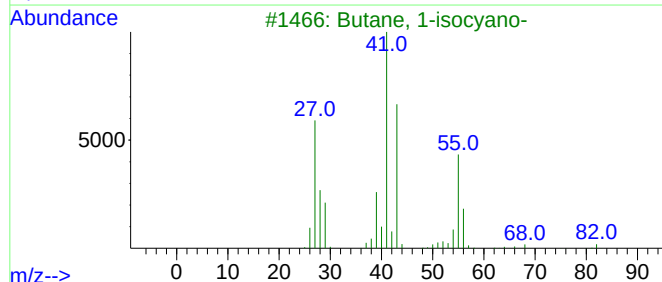
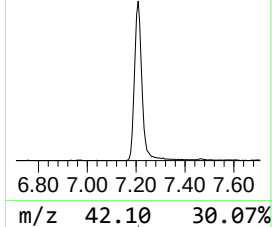
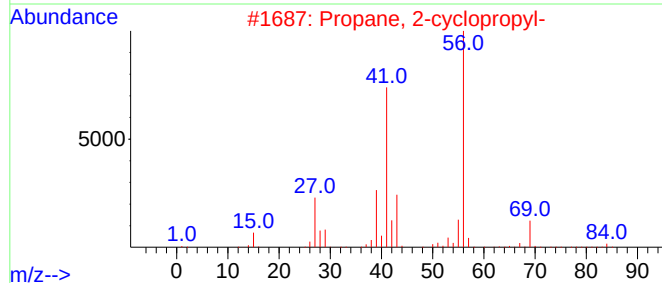
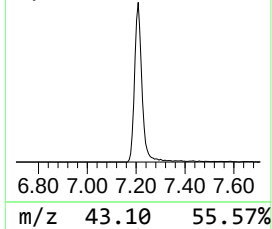
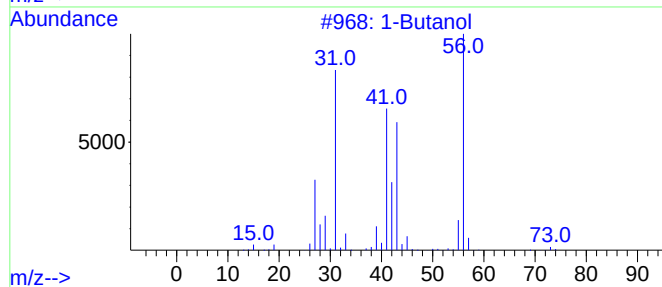
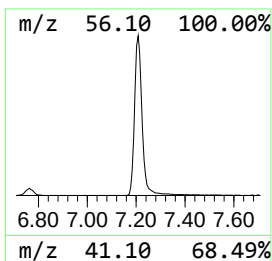
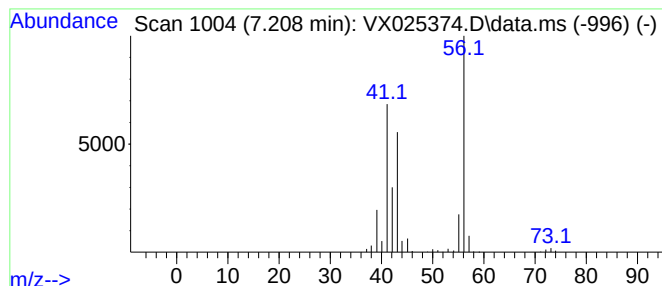
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Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	31.92 ug/l	293729	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	36
3			Butane, 1-isocyano-	83	C5H9N	002769-64-4	9
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5			.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	9



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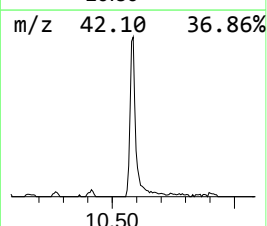
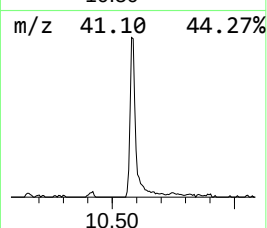
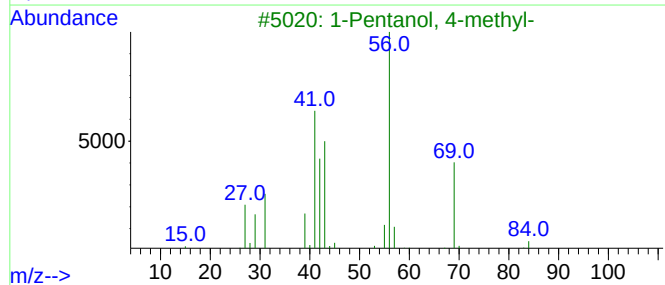
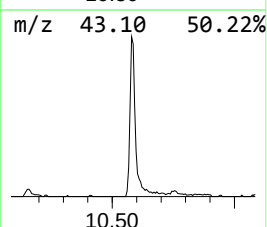
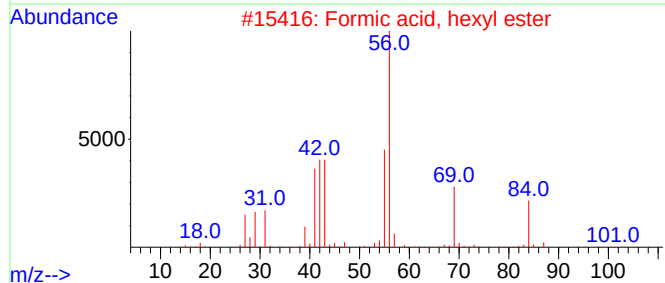
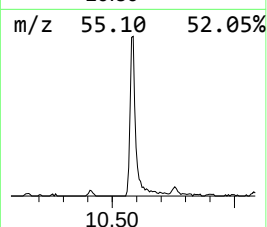
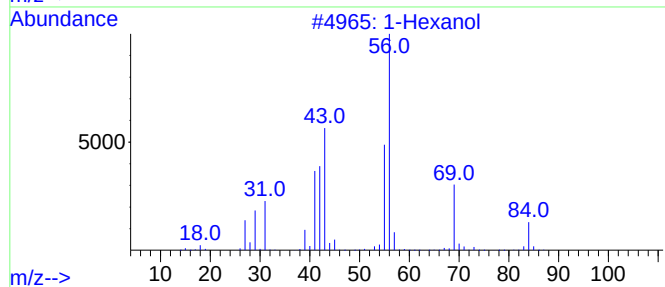
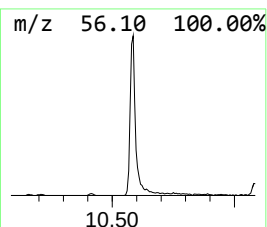
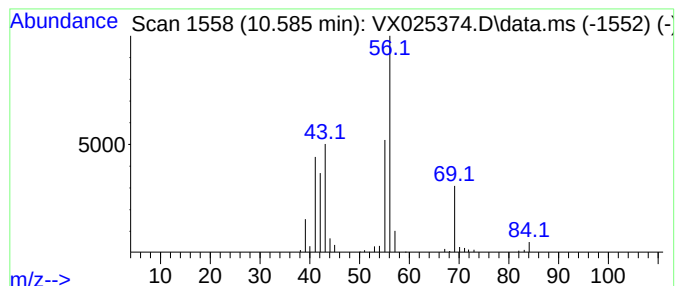
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.585	7.79 ug/l	85261	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	90
2			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	72



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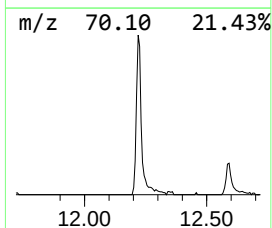
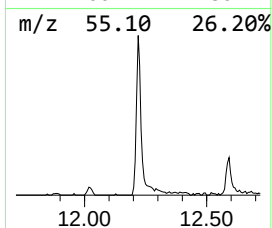
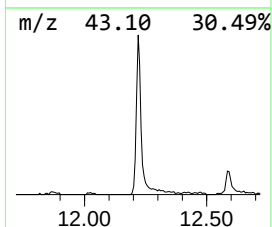
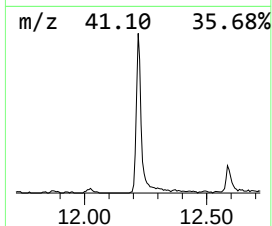
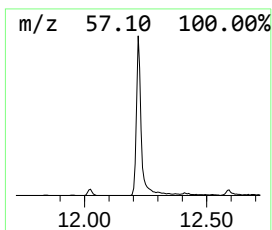
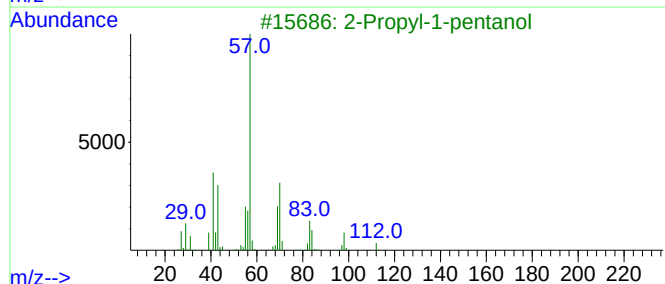
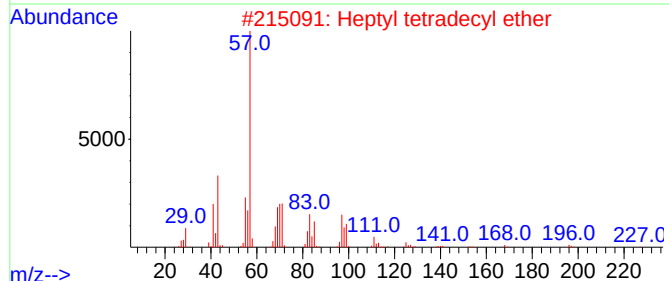
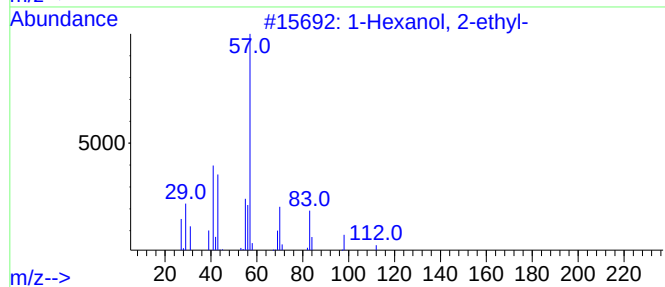
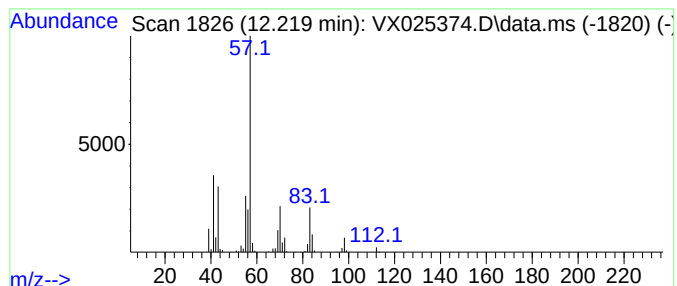
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Quant Title : SW846 8260

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	12.06 ug/l	126813	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			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.056	88.7	ug/l	633229	1	5.556	357034	50.0
1-Propanol	3.861	105.9	ug/l	756279	1	5.556	357034	50.0
1-Butanol	7.208	31.9	ug/l	293729	2	6.763	460131	50.0
1-Hexanol	10.585	7.8	ug/l	85261	3	10.055	546896	50.0
1-Hexanol, 2-et...	12.219	12.1	ug/l	126813	4	12.024	525849	50.0