

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025375.D
 Acq On : 29 Nov 2021 17:21
 Operator : JC/MD
 Sample : M4837-12 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20932

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: VX025375.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	178	rBV	702042	1079847	81.03%	15.830%
2	2.532	229	237	244	rBV	15570	28816	2.16%	0.422%
3	3.867	442	456	470	rBV	496309	1332572	100.00%	19.535%
4	5.391	694	706	720	rBV	73394	211390	15.86%	3.099%
5	5.556	722	733	747	rBV	125387	350878	26.33%	5.144%
6	5.958	789	799	810	rBV	74782	204790	15.37%	3.002%
7	6.763	920	931	945	rBV	192433	455215	34.16%	6.673%
8	7.208	996	1004	1023	rBV	248092	511096	38.35%	7.493%
9	8.647	1234	1240	1248	rBV	384365	623949	46.82%	9.147%
10	9.232	1330	1336	1347	rBV	34210	56938	4.27%	0.835%
11	10.055	1465	1471	1484	rVB	408344	543477	40.78%	7.967%
12	10.579	1552	1557	1565	rBV	109253	147757	11.09%	2.166%
13	10.659	1565	1570	1580	rVB2	10599	19640	1.47%	0.288%
14	11.079	1634	1639	1650	rVB	324084	424863	31.88%	6.228%
15	12.024	1788	1794	1802	rVB	419844	527043	39.55%	7.726%
16	12.219	1821	1826	1838	rBV	151877	199710	14.99%	2.928%
17	12.414	1854	1858	1865	rVB	16092	20386	1.53%	0.299%
18	12.585	1880	1886	1898	rBV	33883	56244	4.22%	0.825%
19	13.731	2070	2074	2079	rBV	20827	26823	2.01%	0.393%

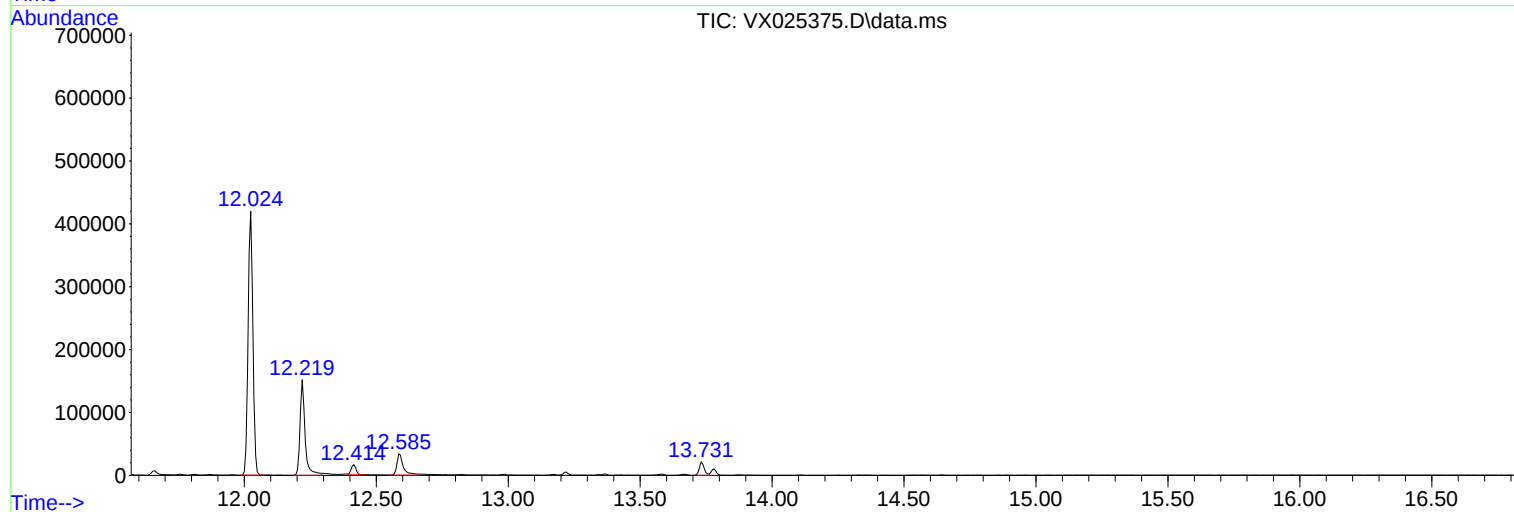
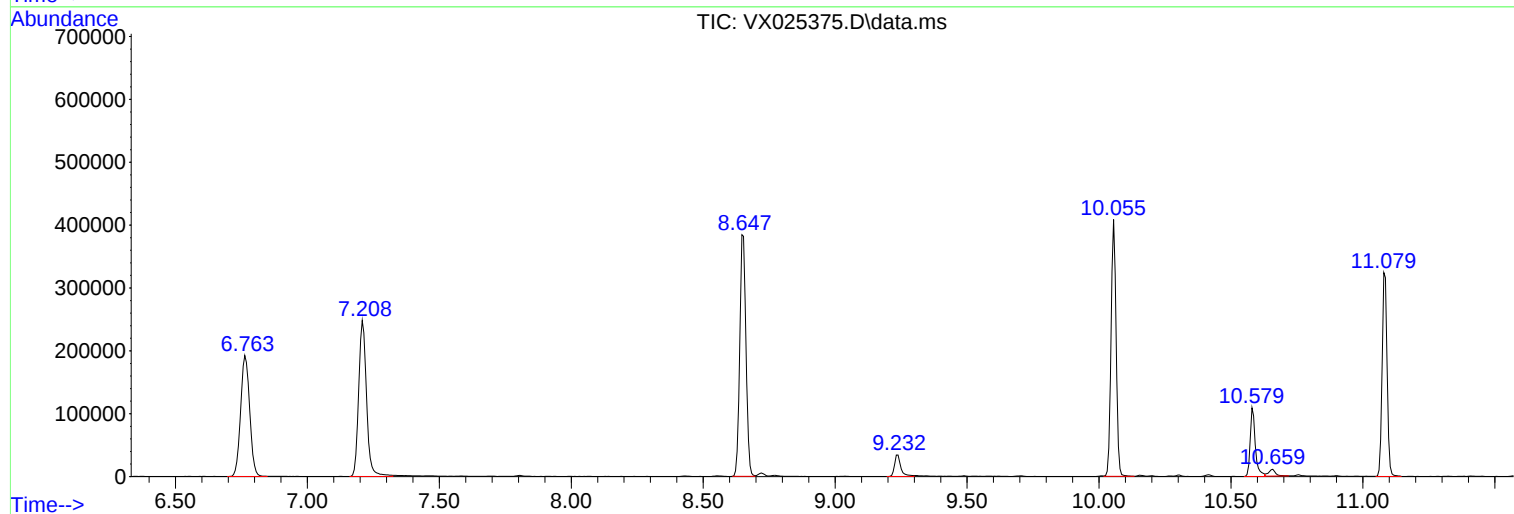
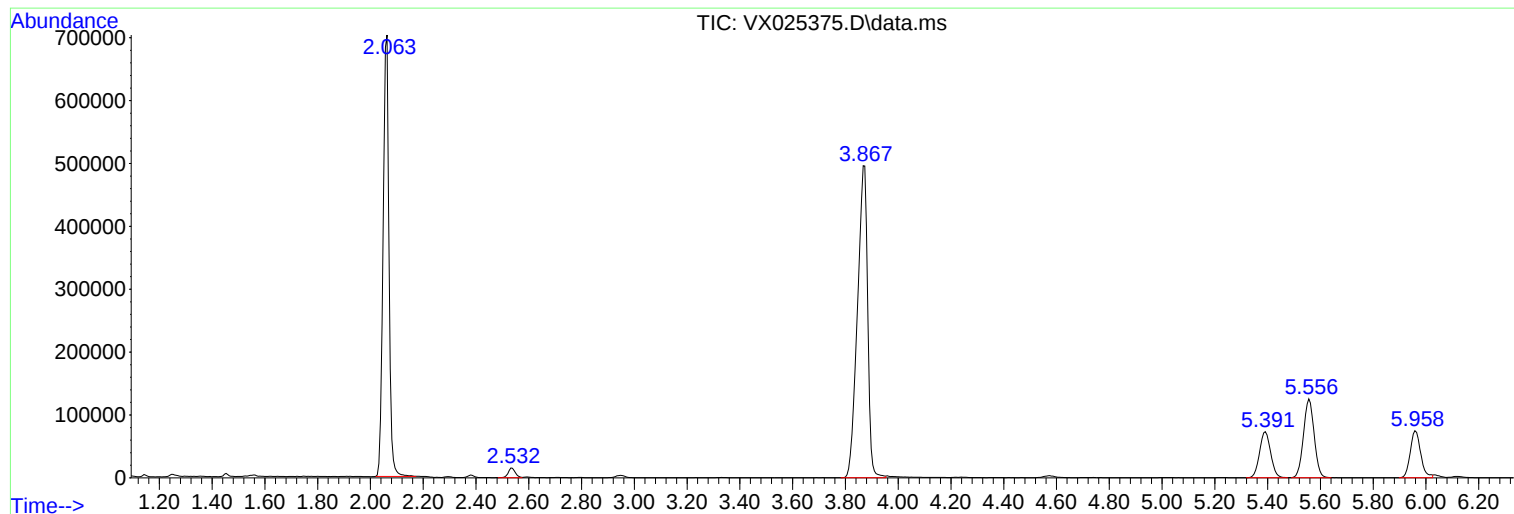
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Quant Title : SW846 8260

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



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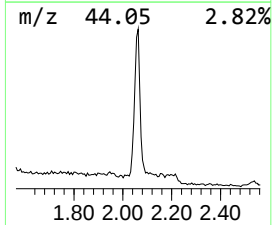
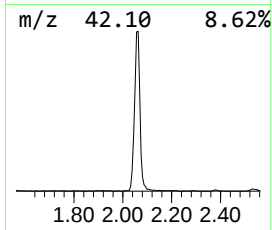
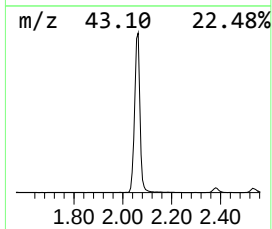
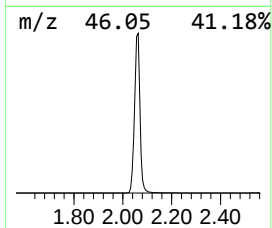
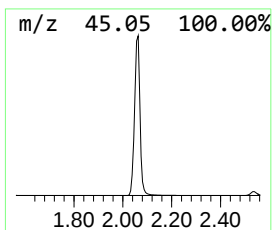
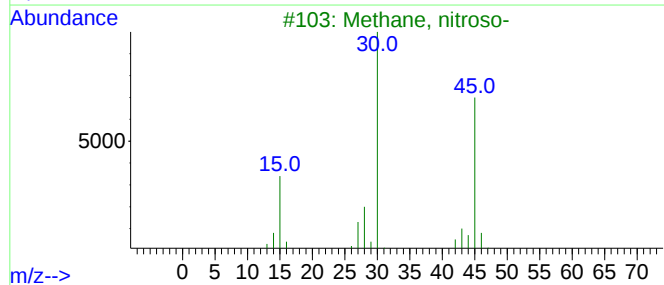
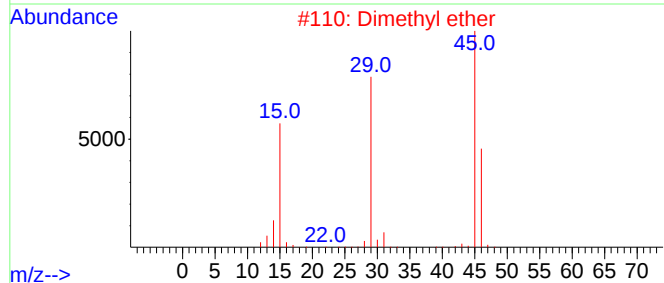
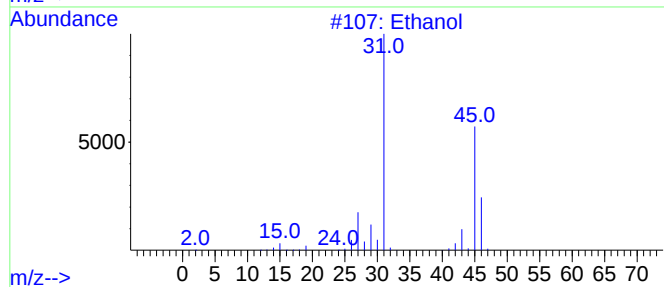
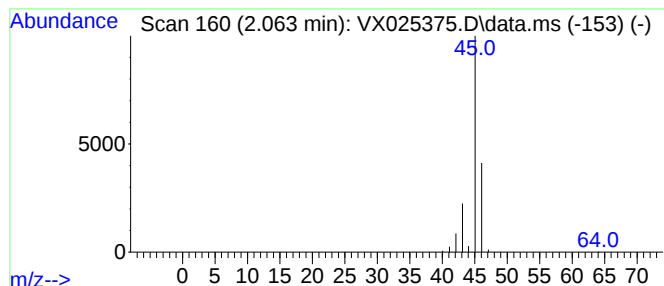
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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	153.88 ug/l	1079850	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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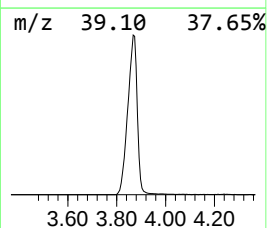
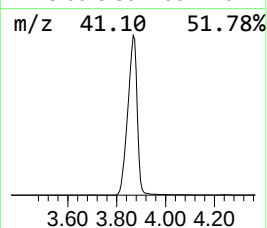
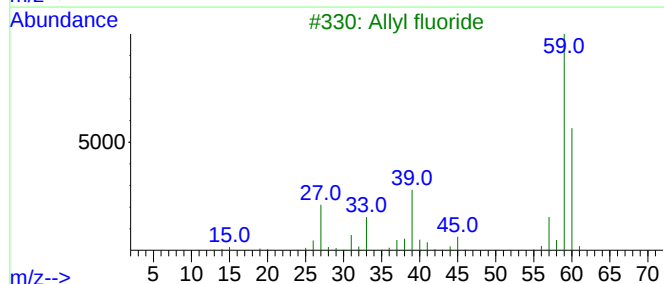
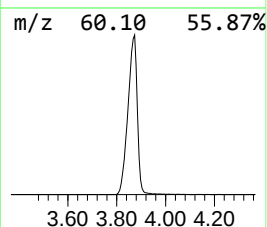
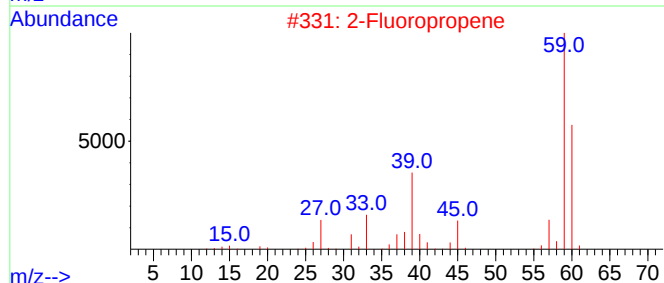
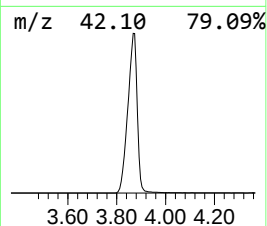
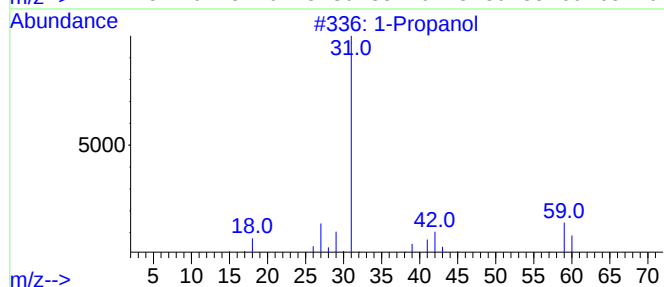
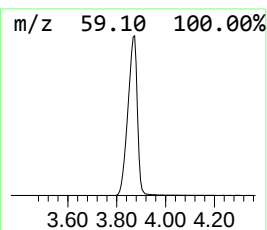
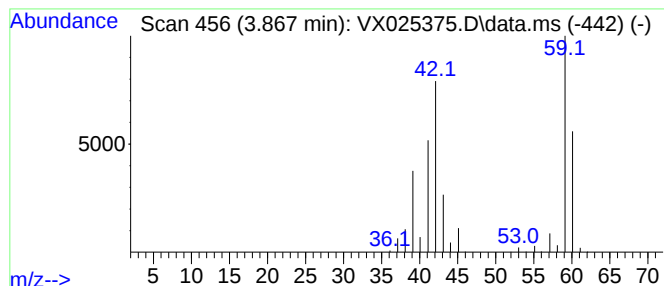
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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.
3.867	189.89 ug/l	1332570	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	43
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	16
5	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	9



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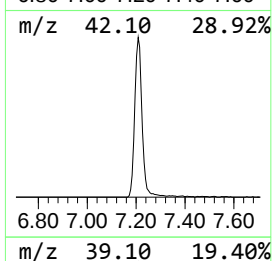
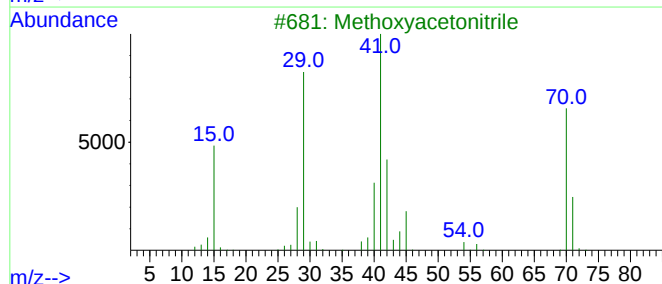
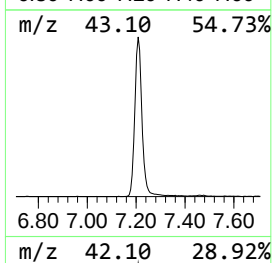
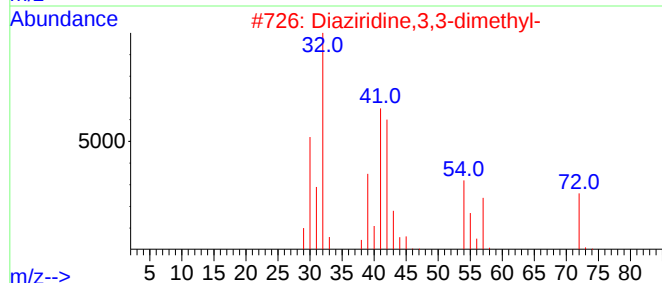
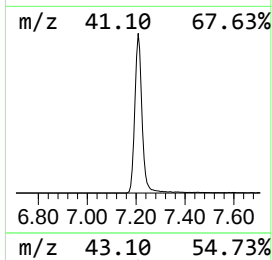
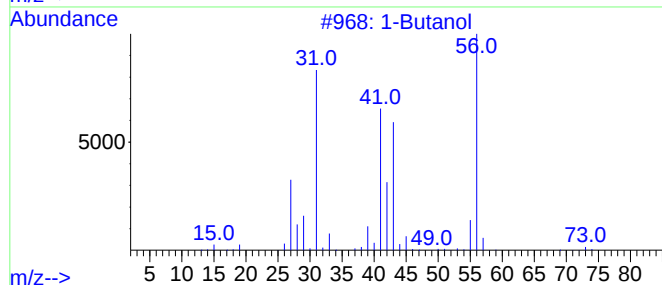
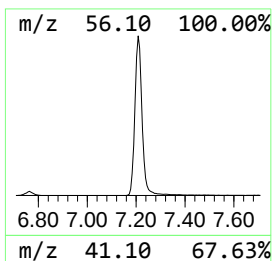
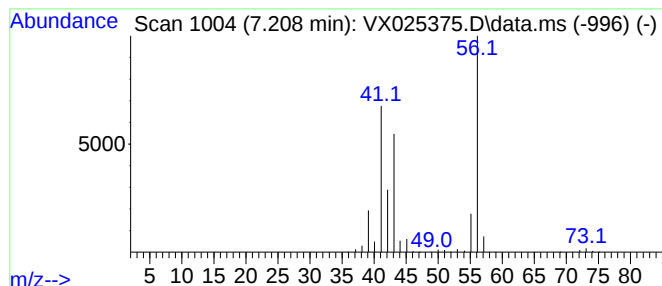
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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	56.14 ug/l	511096	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
3			Methoxyacetonitrile	71	C3H5NO	001738-36-9	9
4			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



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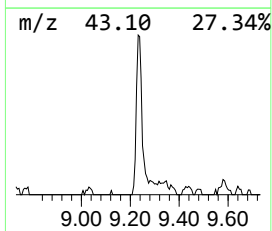
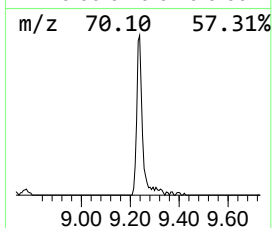
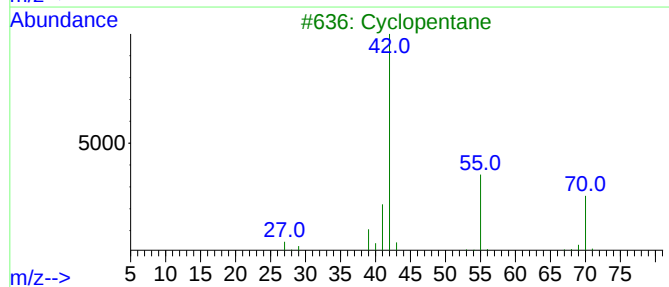
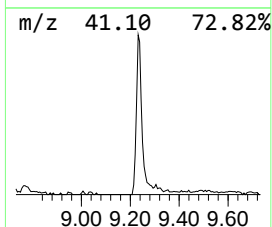
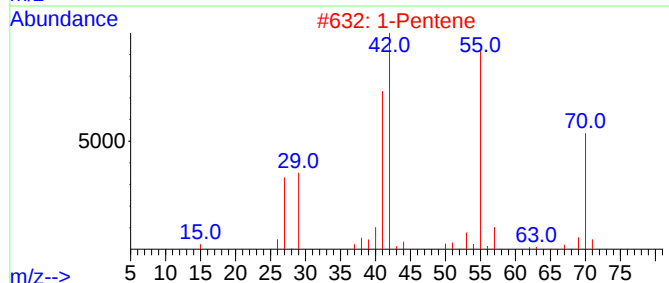
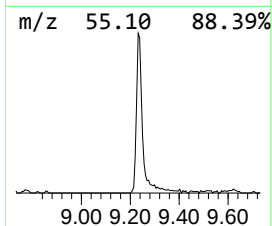
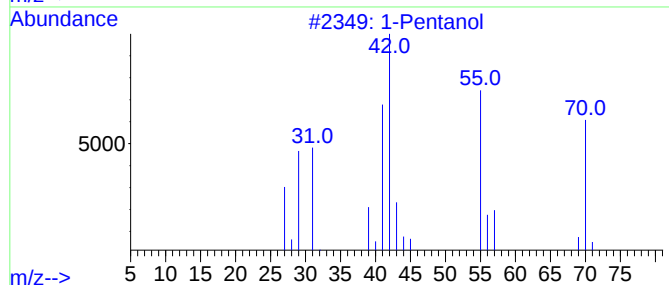
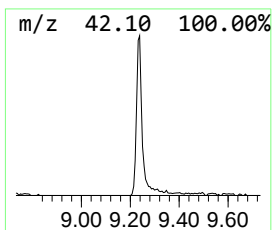
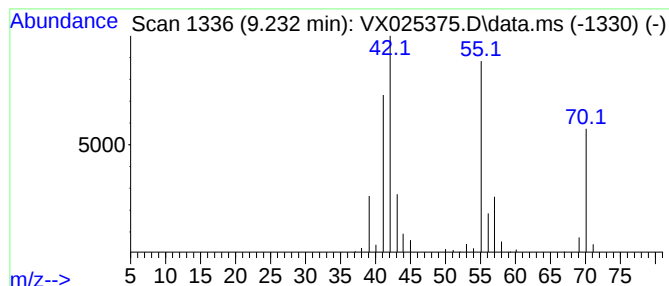
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Pentanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	5.24 ug/l	56938	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol	88	C5H12O	000071-41-0	90
2			1-Pentene	70	C5H10	000109-67-1	72
3			Cyclopentane	70	C5H10	000287-92-3	64
4			1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	64
5			Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	43



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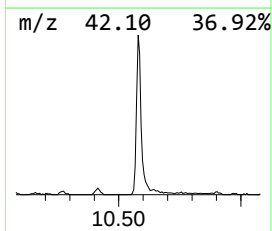
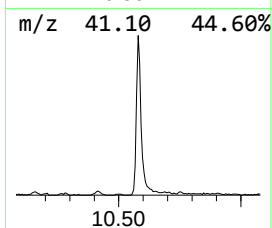
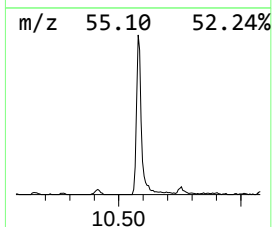
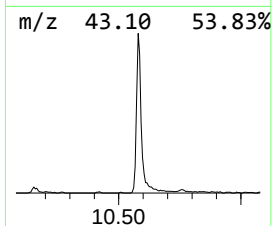
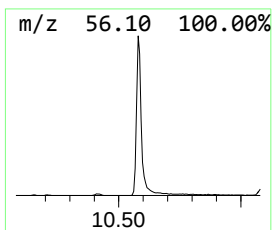
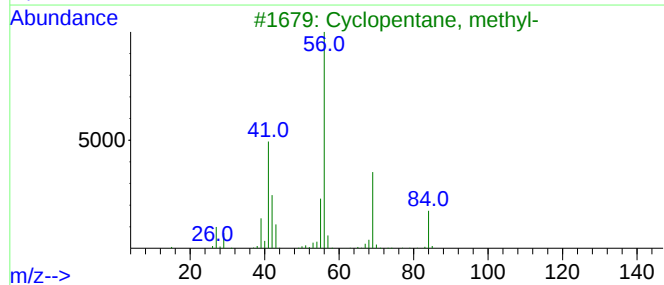
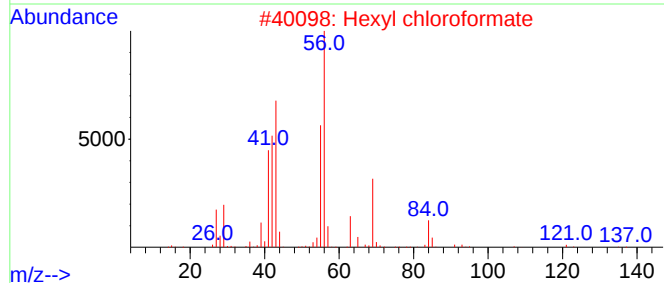
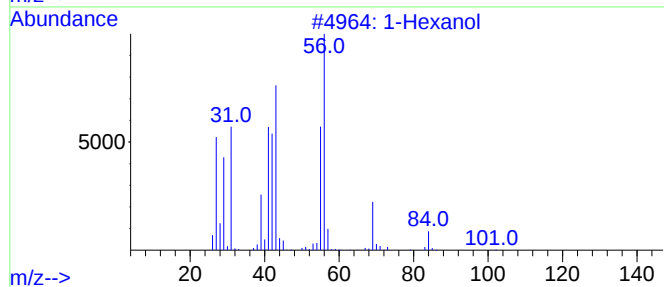
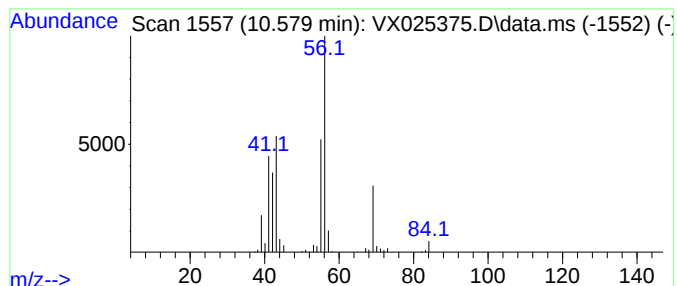
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.579	13.59 ug/l	147757	Chlorobenzene-d5	10.055	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
4	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	78



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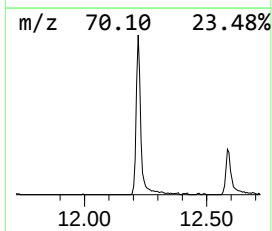
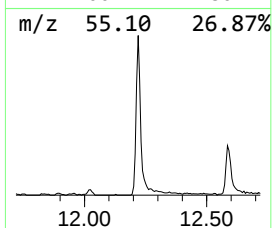
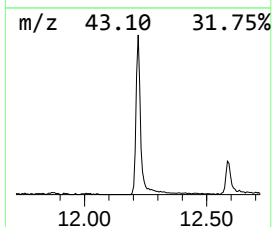
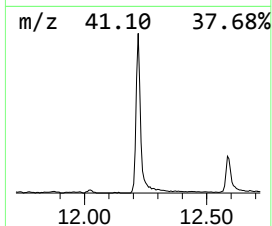
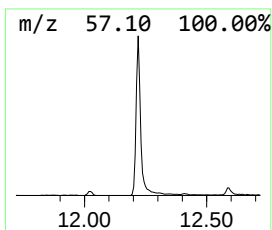
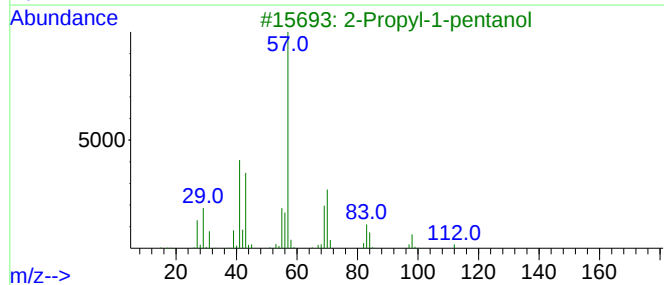
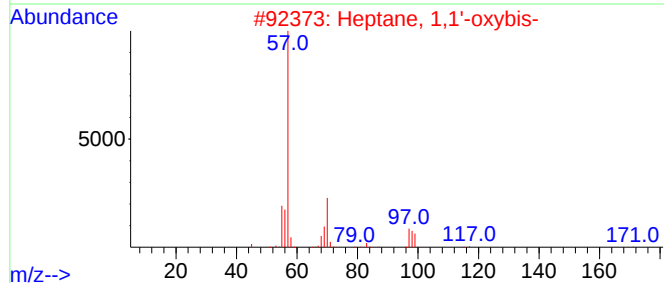
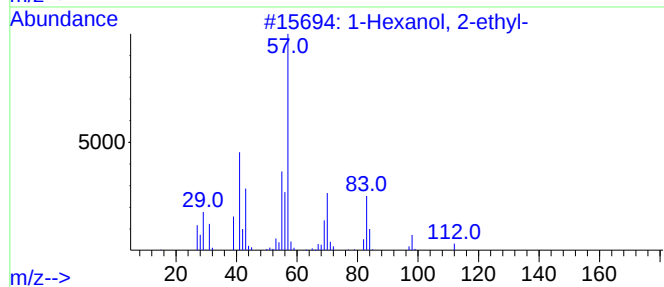
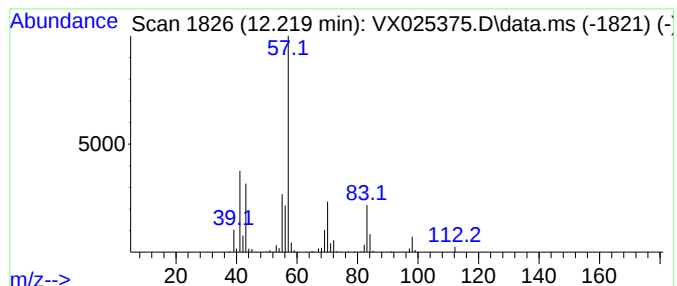
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	18.95 ug/l	199710	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			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025375.D
Acq On : 29 Nov 2021 17:21
Operator : JC/MD
Sample : M4837-12 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20932

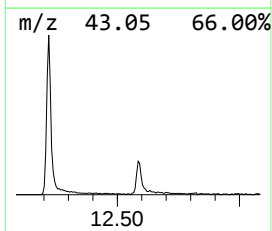
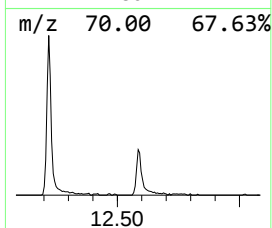
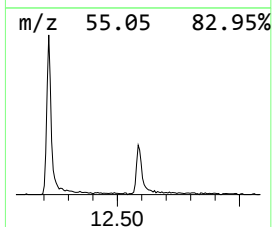
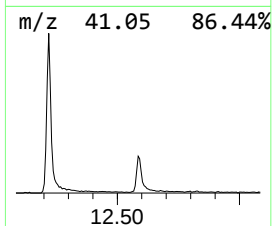
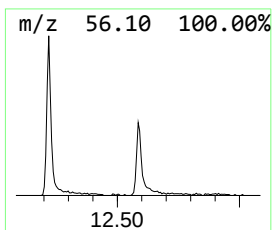
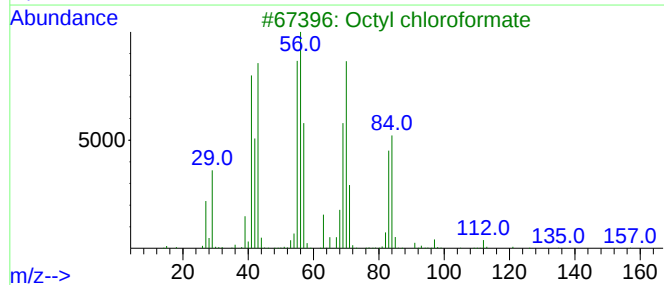
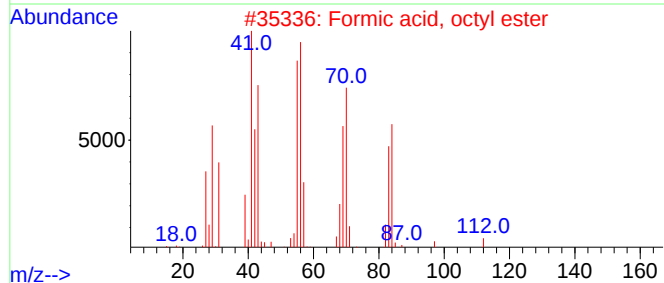
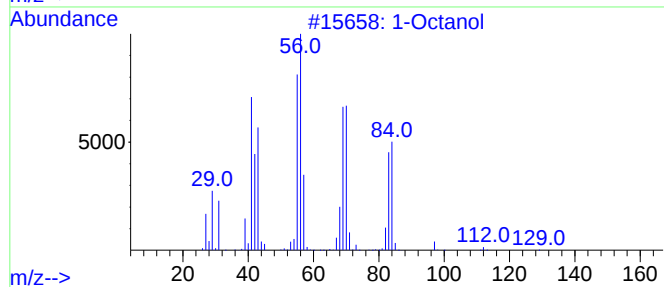
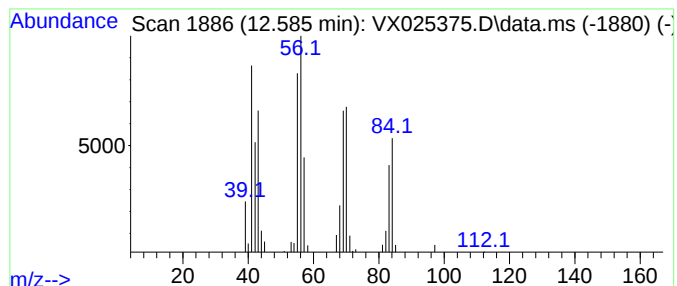
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Quant Title : SW846 8260

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

Peak Number 7 1-Octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	5.34 ug/l	56244	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	86
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 : VX025375.D
Acq On : 29 Nov 2021 17:21
Operator : JC/MD
Sample : M4837-12 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20932

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	153.9	ug/l	1079850	1	5.556	350878	50.0
1-Propanol	3.867	189.9	ug/l	1332570	1	5.556	350878	50.0
1-Butanol	7.208	56.1	ug/l	511096	2	6.763	455215	50.0
1-Pentanol	9.232	5.2	ug/l	56938	3	10.055	543477	50.0
1-Hexanol	10.579	13.6	ug/l	147757	3	10.055	543477	50.0
1-Hexanol, 2-et...	12.219	18.9	ug/l	199710	4	12.024	527043	50.0
1-Octanol	12.585	5.3	ug/l	56244	4	12.024	527043	50.0