

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025379.D
 Acq On : 29 Nov 2021 18:55
 Operator : JC/MD
 Sample : M4837-09 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20929

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: VX025379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.056	152	159	178	rBV	528812	803467	68.79%	12.195%
2	2.532	227	237	245	rBV	31188	55373	4.74%	0.840%
3	3.867	443	456	474	rBV	446757	1167980	100.00%	17.728%
4	5.391	693	706	721	rBV2	70832	207246	17.74%	3.146%
5	5.556	721	733	749	rVV	122078	347241	29.73%	5.270%
6	5.964	789	800	818	rBV	74183	206128	17.65%	3.129%
7	6.763	921	931	945	rBV	190319	450421	38.56%	6.836%
8	7.208	996	1004	1022	rBV	214597	445141	38.11%	6.756%
9	8.653	1233	1241	1247	rBV	392687	616146	52.75%	9.352%
10	8.720	1247	1252	1258	rVB	151050	225326	19.29%	3.420%
11	9.232	1331	1336	1341	rBV	39908	62389	5.34%	0.947%
12	10.055	1465	1471	1484	rBV	408854	538550	46.11%	8.174%
13	10.195	1490	1494	1503	rVB	16696	21464	1.84%	0.326%
14	10.299	1503	1511	1518	rBV	63550	91913	7.87%	1.395%
15	10.579	1551	1557	1563	rBV	105365	146908	12.58%	2.230%
16	10.646	1563	1568	1579	rVB	36744	59755	5.12%	0.907%
17	11.085	1634	1640	1651	rVB	322418	419481	35.92%	6.367%
18	12.024	1789	1794	1803	rVB	424309	520312	44.55%	7.897%
19	12.219	1821	1826	1839	rBV	121394	162872	13.94%	2.472%
20	12.591	1877	1887	1896	rBV	23466	40387	3.46%	0.613%

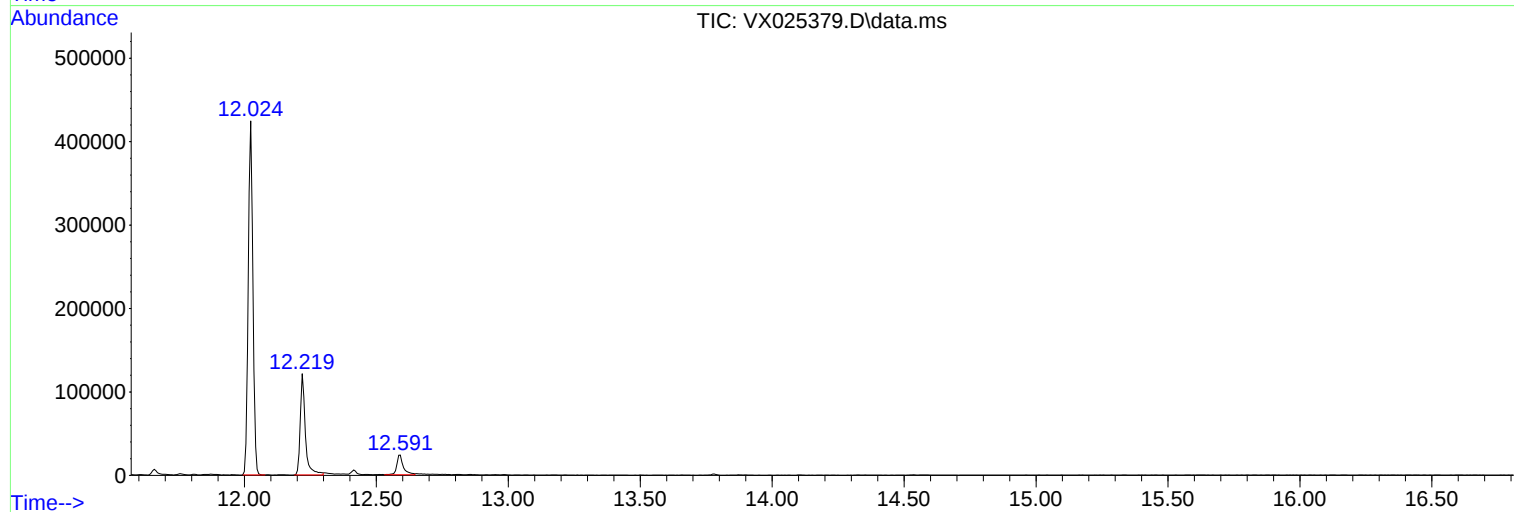
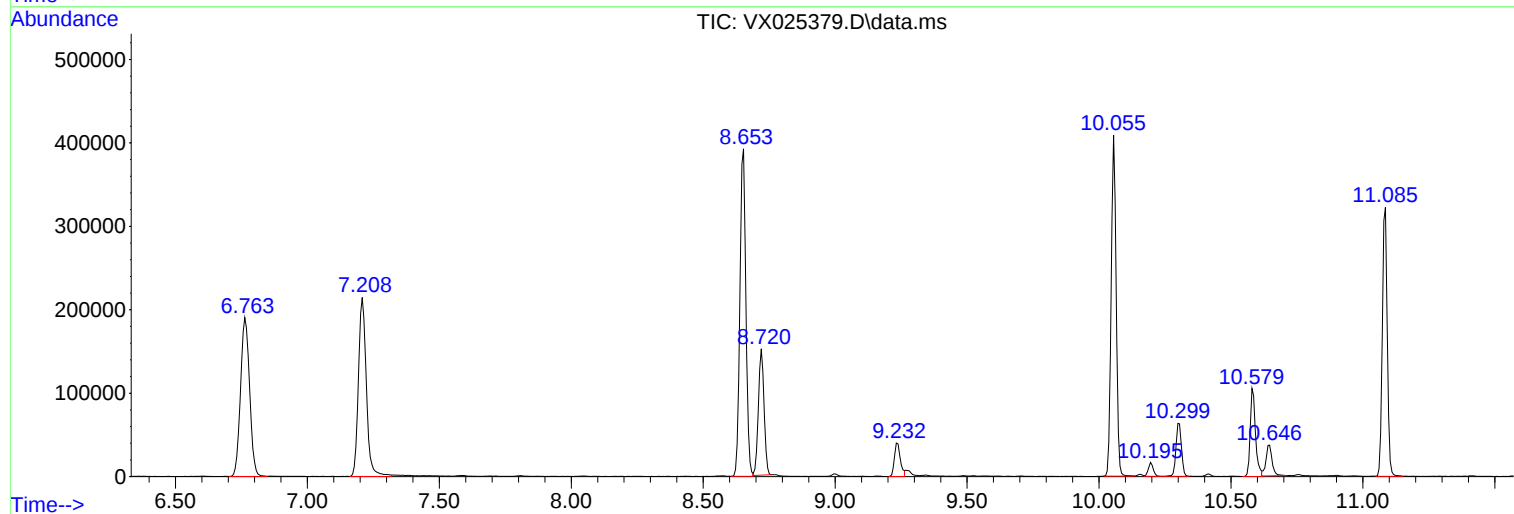
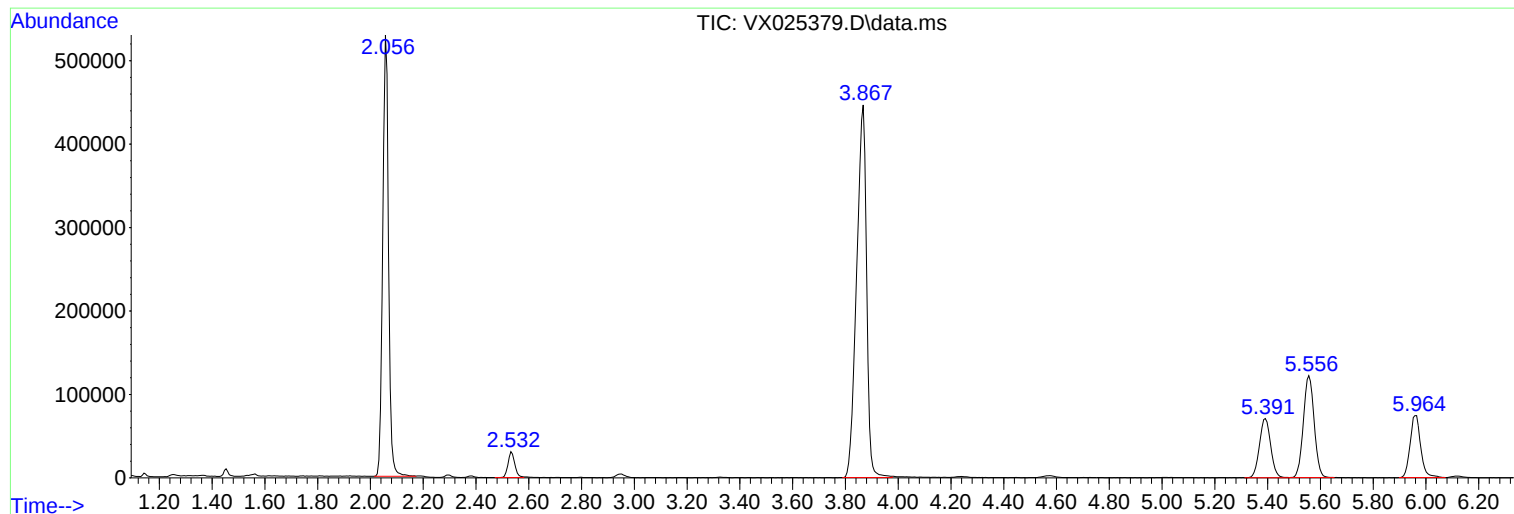
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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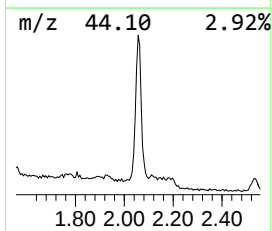
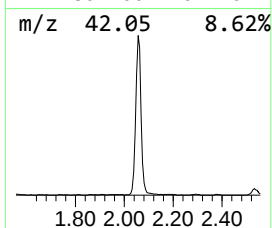
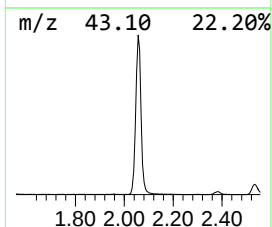
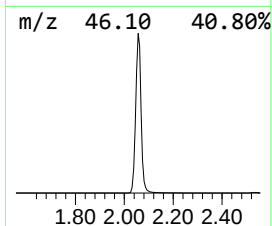
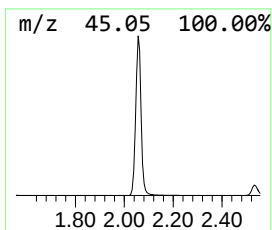
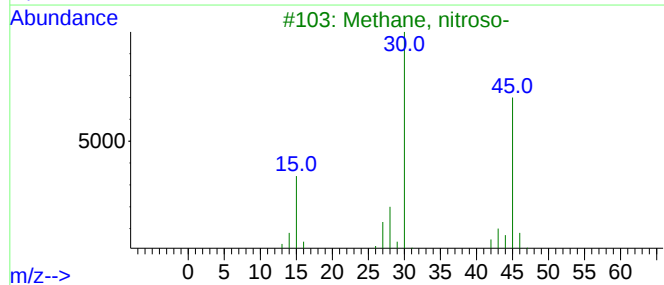
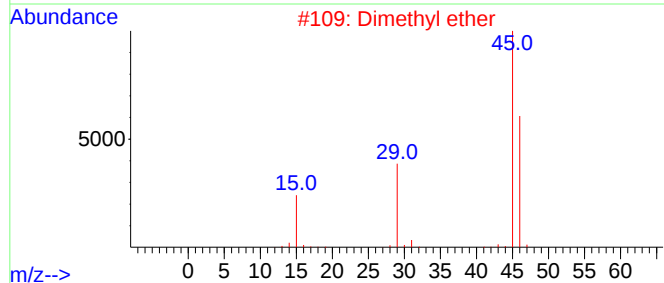
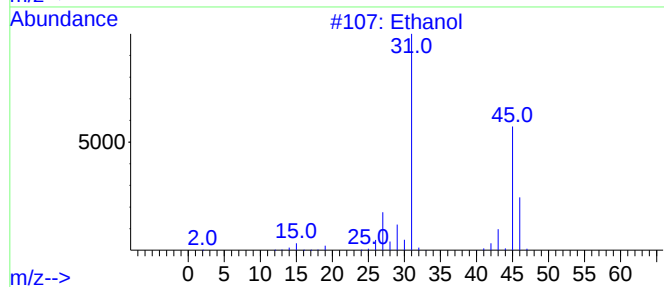
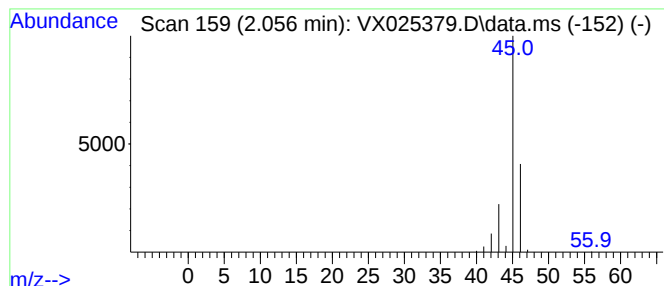
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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	115.69 ug/l	803467	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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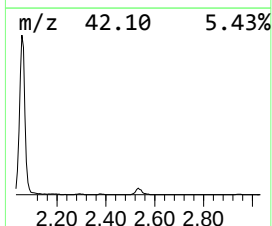
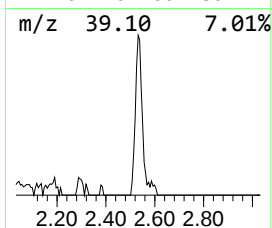
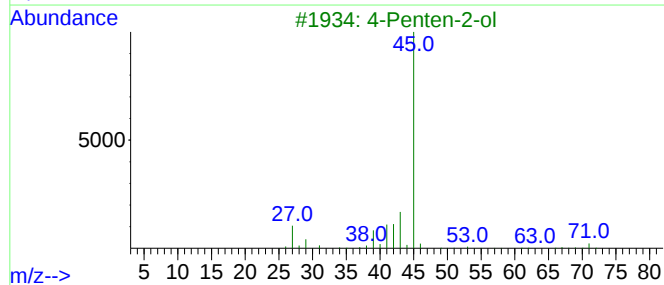
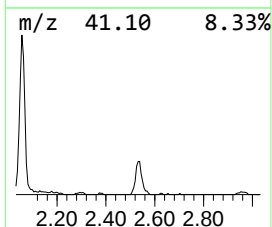
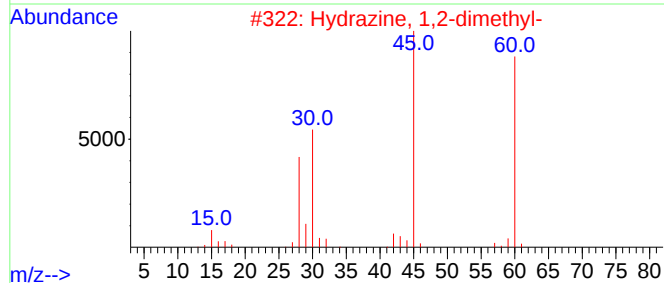
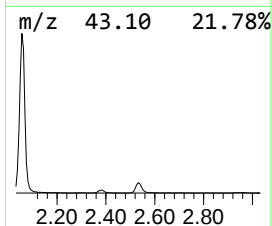
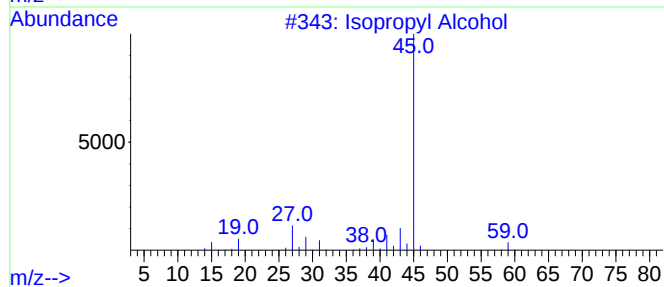
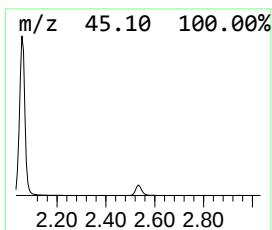
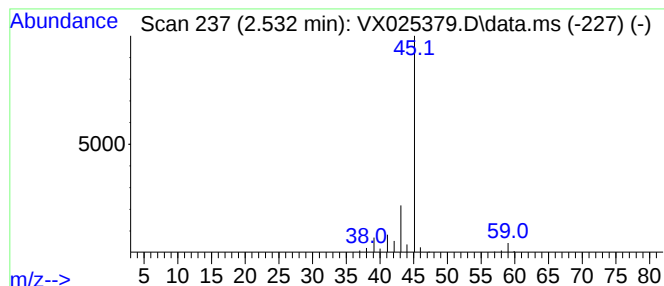
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	7.97 ug/l	55373	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			4-Penten-2-ol	86	C5H10O	000625-31-0	9
4			Ethylamine	45	C2H7N	000075-04-7	5
5			Formamide	45	CH3NO	000075-12-7	4



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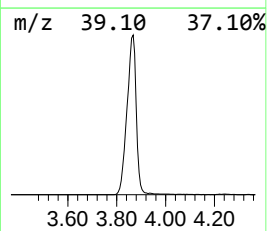
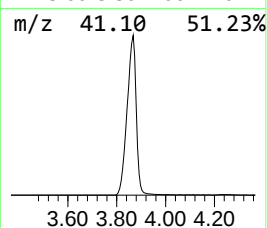
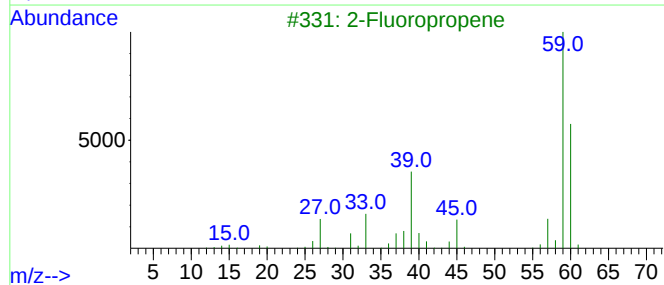
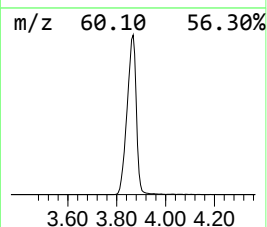
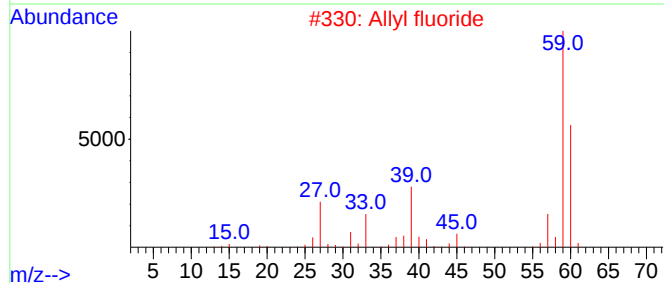
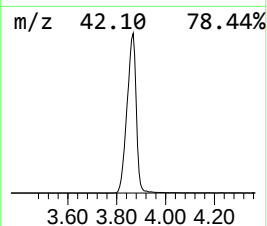
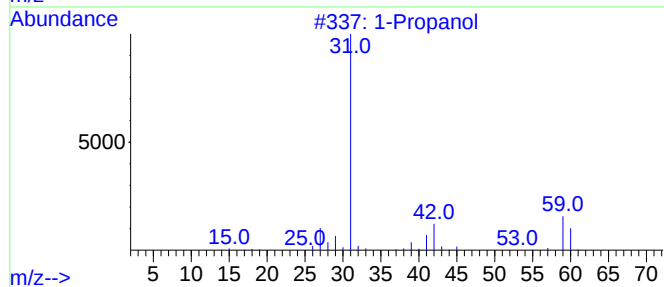
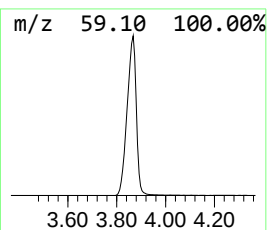
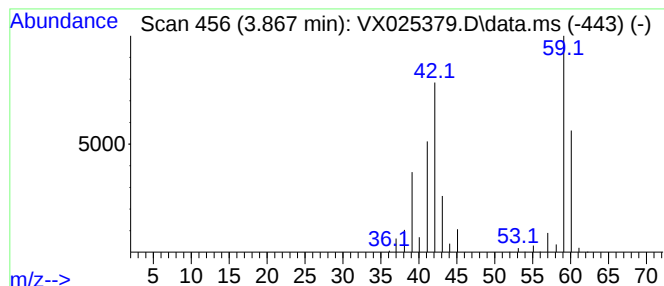
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.867	168.18 ug/l	1167980	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	47
3		2-Fluoropropene	60	C3H5F	001184-60-7	43
4		Cyclopropane	42	C3H6	000075-19-4	16
5		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9



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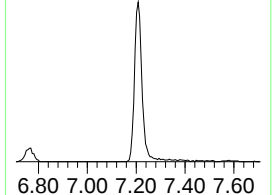
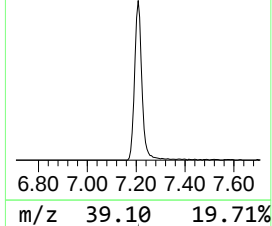
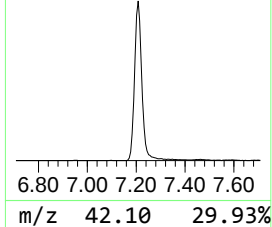
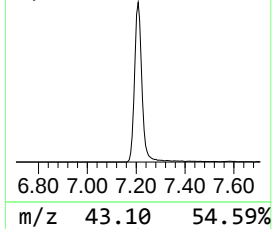
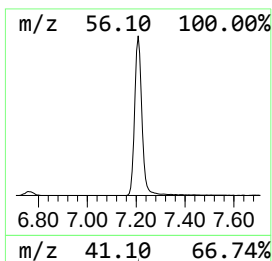
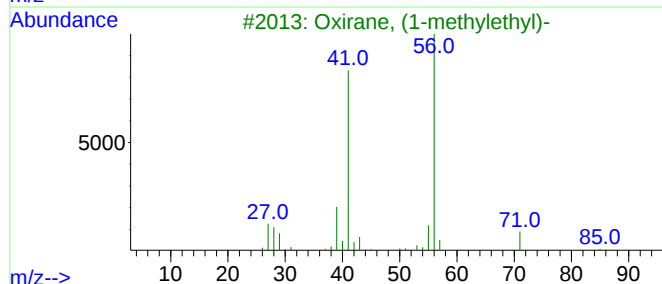
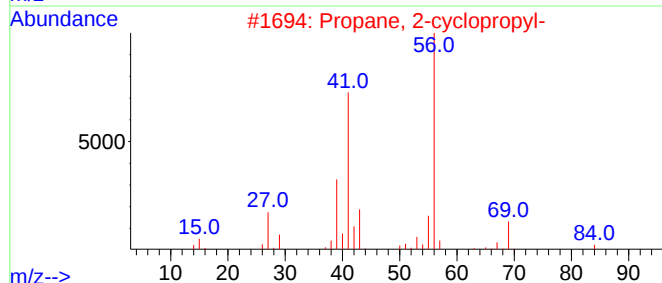
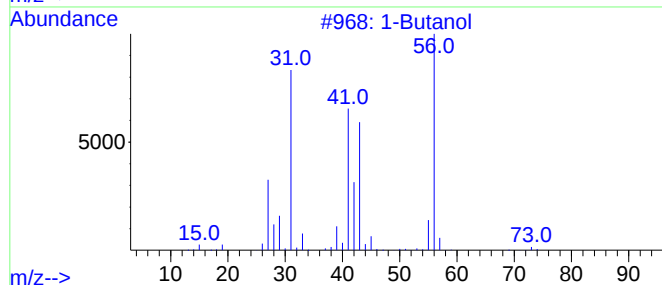
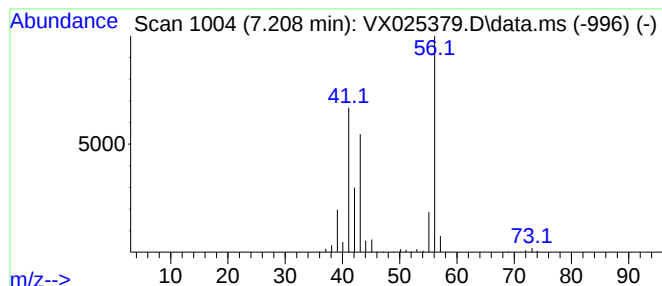
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Quant Title : SW846 8260

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

Peak Number 4 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	49.41 ug/l	445141	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	90
2	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	9
3	Oxirane, (1-methylethyl)-		86	C5H10O	001438-14-8	9
4	Butane, 1-chloro-		92	C4H9Cl	000109-69-3	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...		100	C6H12O	032347-12-9	9



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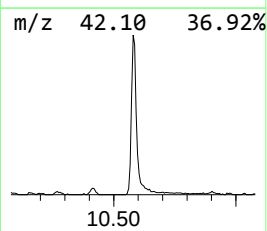
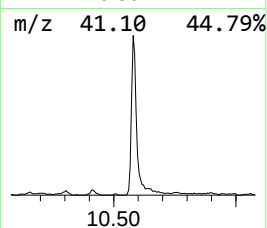
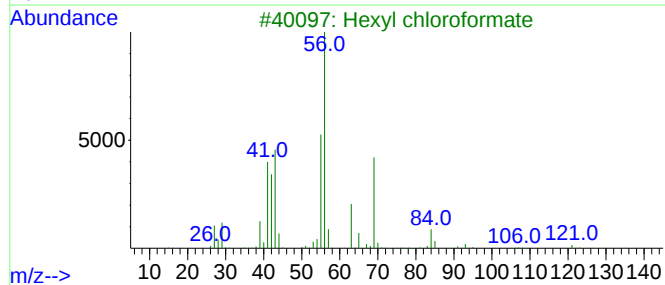
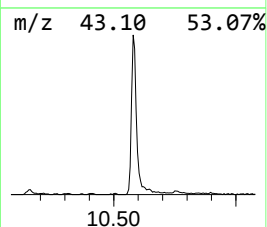
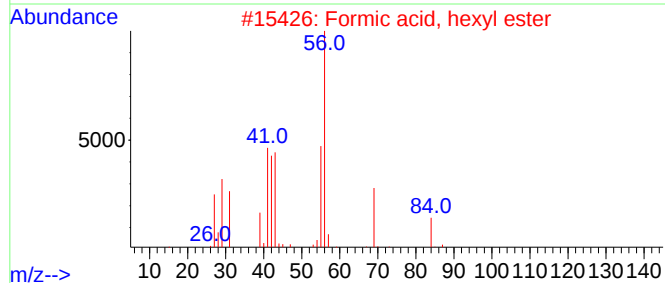
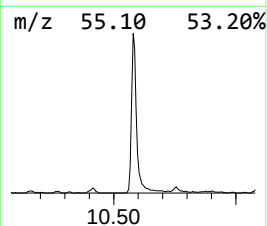
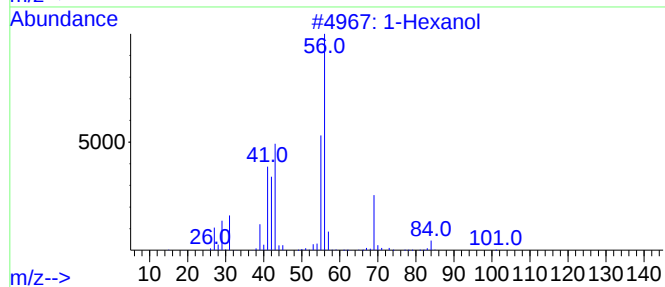
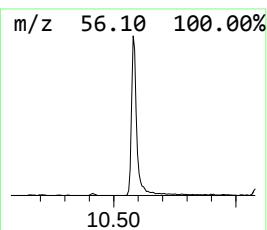
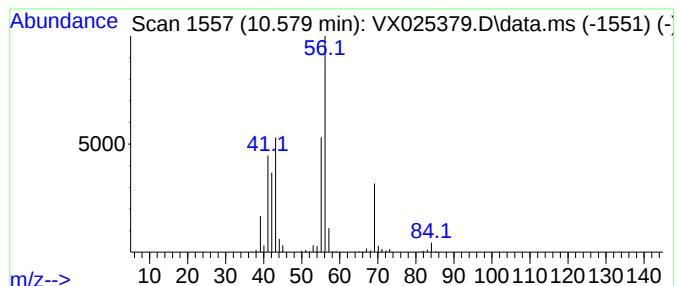
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	13.64 ug/l	146908	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	83
2			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	72
4			Cyclopropane, propyl-	84	C6H12	002415-72-7	72
5			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72



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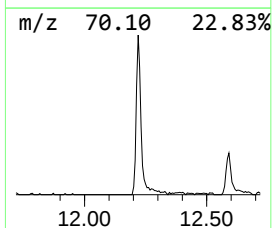
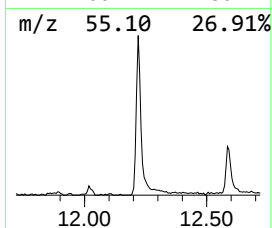
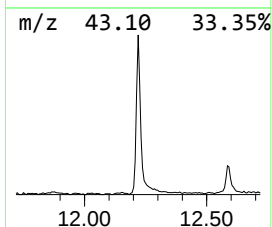
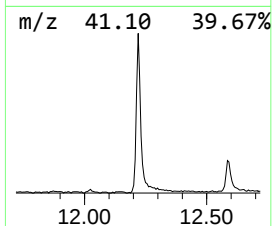
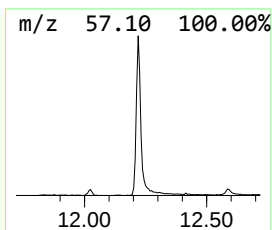
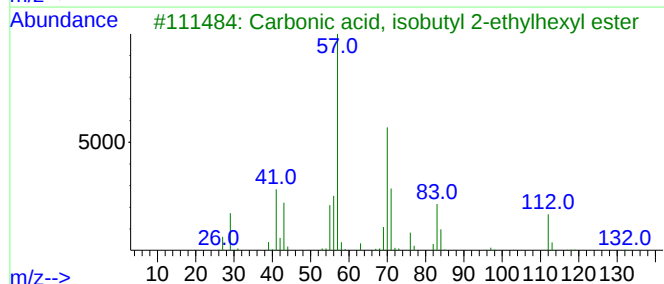
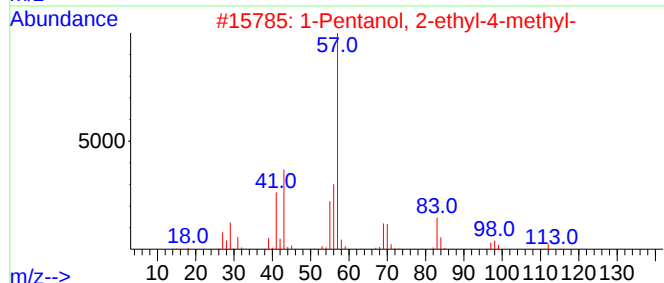
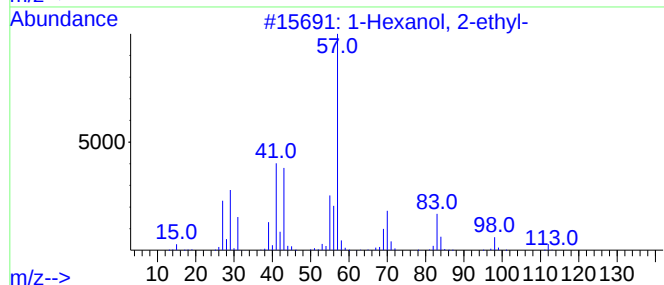
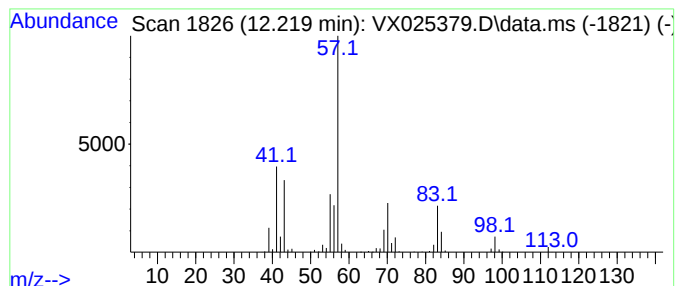
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	15.65 ug/l	162872	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-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025379.D
Acq On : 29 Nov 2021 18:55
Operator : JC/MD
Sample : M4837-09 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20929

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	2.056	115.7	ug/l	803467	1	5.556	347241	50.0
Isopropyl Alcohol	2.532	8.0	ug/l	55373	1	5.556	347241	50.0
1-Propanol	3.867	168.2	ug/l	1167980	1	5.556	347241	50.0
1-Butanol	7.208	49.4	ug/l	445141	2	6.763	450421	50.0
1-Hexanol	10.579	13.6	ug/l	146908	3	10.055	538550	50.0
1-Hexanol, 2-et...	12.219	15.7	ug/l	162872	4	12.024	520312	50.0