

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025368.D
 Acq On : 29 Nov 2021 14:37
 Operator : JC/MD
 Sample : M4837-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30850

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: VX025368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.081	152	163	182	rBV	1874970	3888344	20.08%	12.412%
2	2.380	206	212	228	rVB	522760	856635	4.42%	2.734%
3	2.544	228	239	257	rBV	494761	1086286	5.61%	3.467%
4	4.013	443	480	484	rBV	3036163	19363434	100.00%	61.809%
5	5.391	696	706	718	rVB	71917	205799	1.06%	0.657%
6	5.556	722	733	748	rVB	125989	354684	1.83%	1.132%
7	5.964	789	800	811	rBV	77062	202662	1.05%	0.647%
8	6.763	919	931	946	rBV	192765	462779	2.39%	1.477%
9	7.214	997	1005	1014	rBV	131803	274666	1.42%	0.877%
10	8.653	1234	1241	1247	rBV	397735	623915	3.22%	1.992%
11	9.238	1331	1337	1351	rBV	544836	783301	4.05%	2.500%
12	9.482	1372	1377	1392	rVB	162278	213824	1.10%	0.683%
13	10.055	1466	1471	1479	rVB	411739	551729	2.85%	1.761%
14	11.079	1632	1639	1646	rBV2	343508	486000	2.51%	1.551%
15	12.024	1789	1794	1801	rVB	446644	546942	2.82%	1.746%
16	12.219	1821	1826	1834	rBV	1212465	1426980	7.37%	4.555%

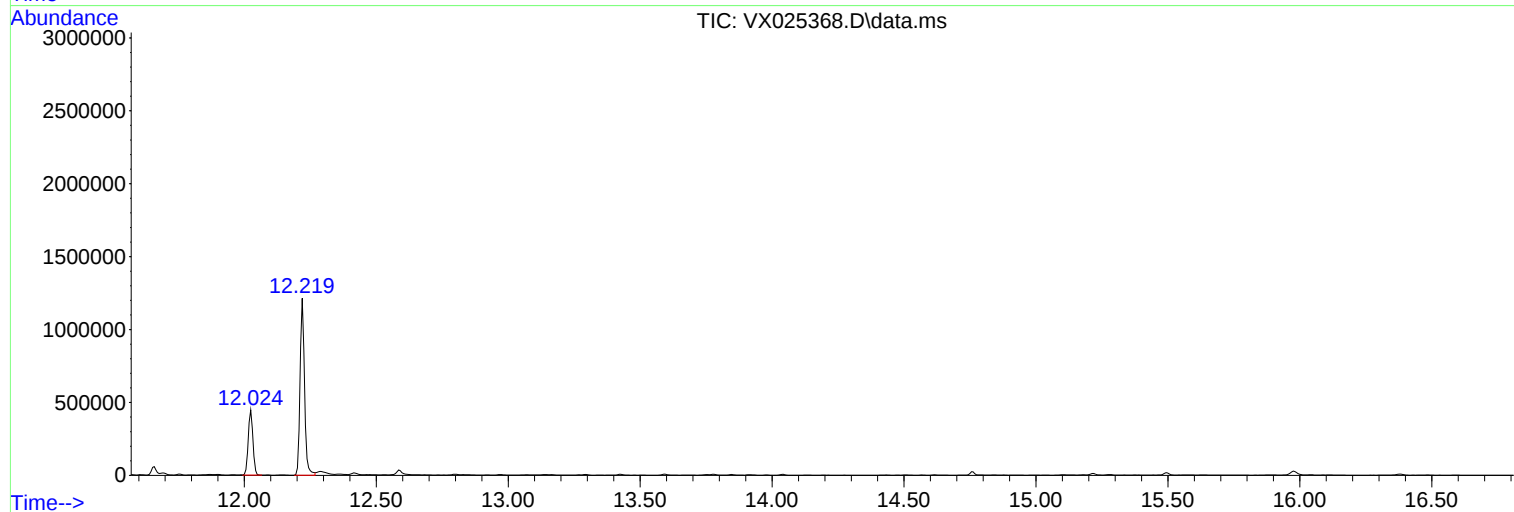
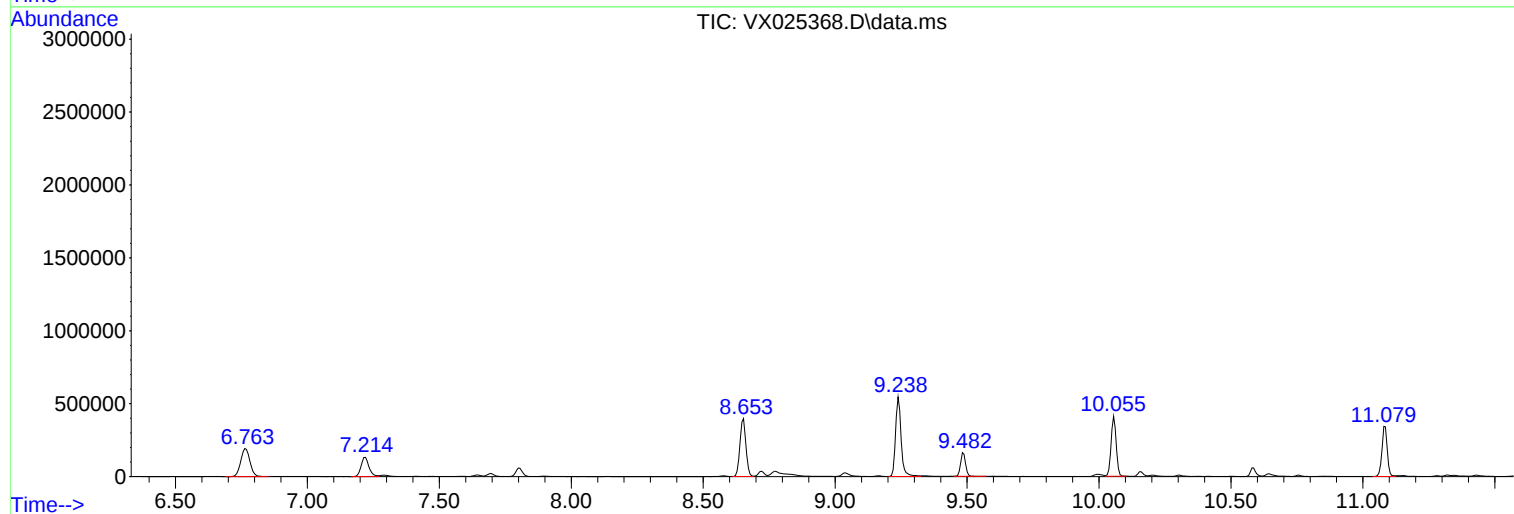
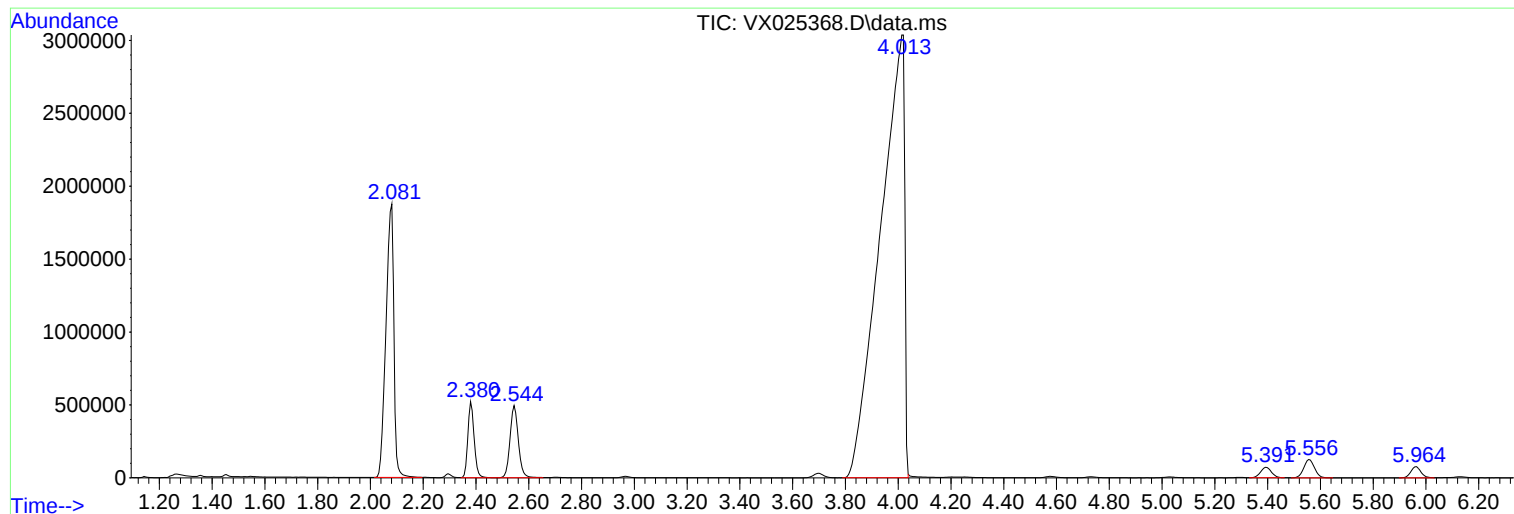
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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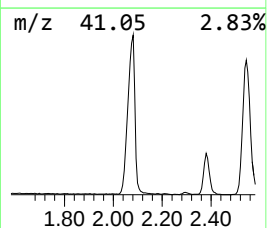
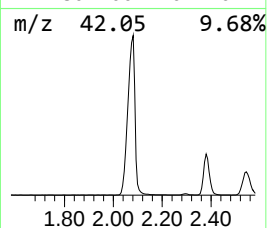
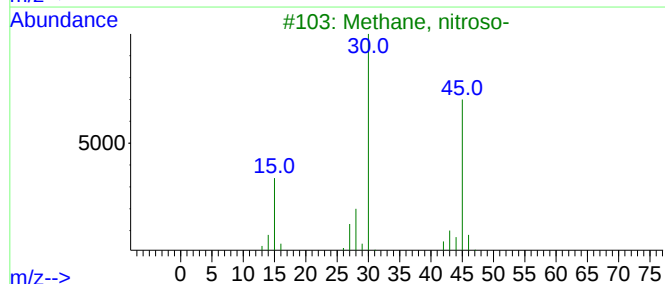
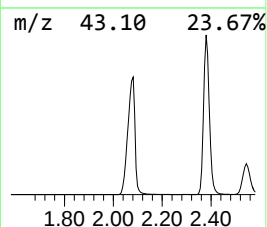
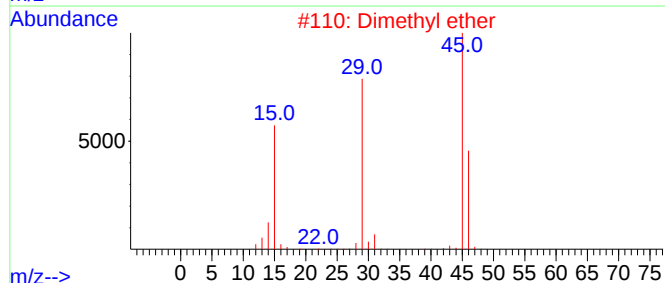
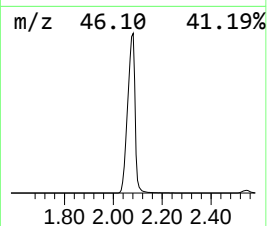
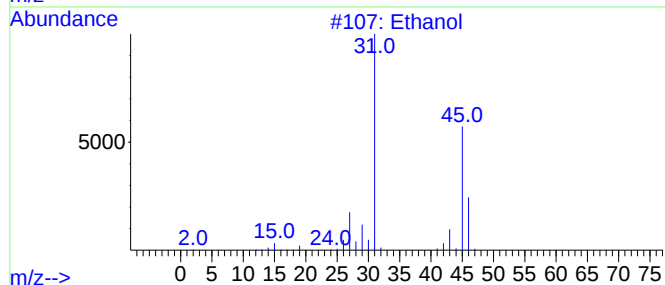
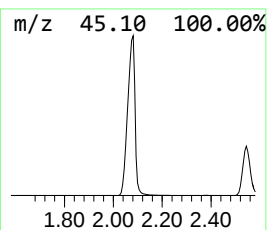
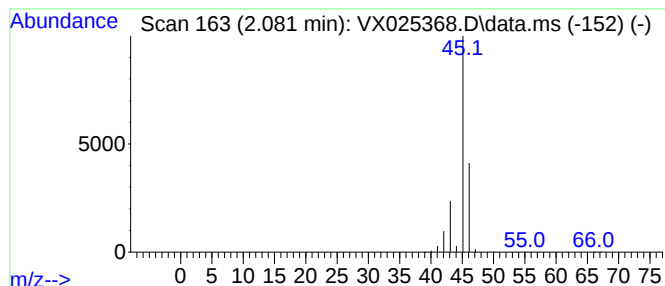
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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.
2.081	548.14 ug/l	3888340	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
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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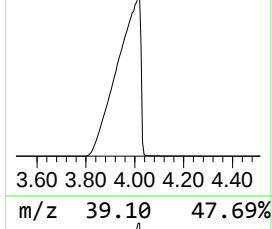
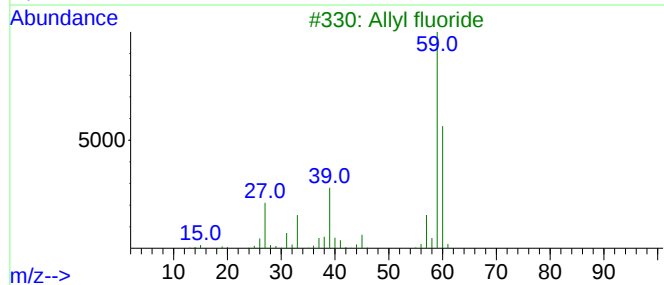
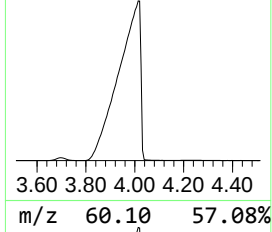
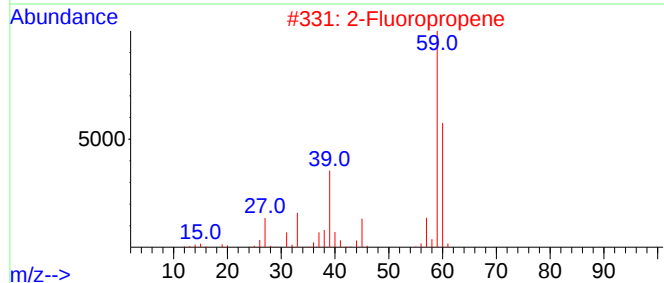
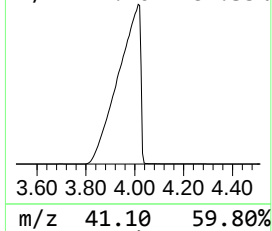
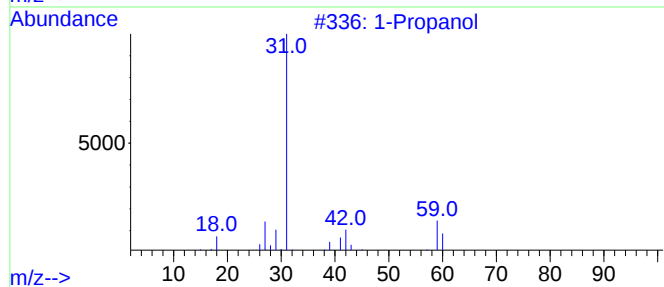
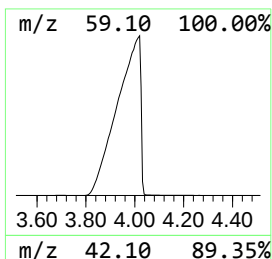
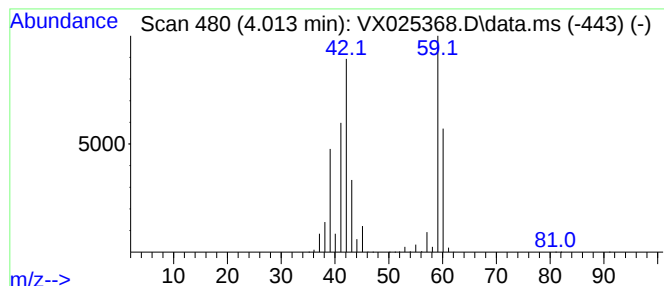
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.013	2729.67 ug/l	19363400	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	59
2		2-Fluoropropene	60	C3H5F	001184-60-7	38
3		Allyl fluoride	60	C3H5F	000818-92-8	32
4		Cyclopropane	42	C3H6	000075-19-4	25
5		Propene	42	C3H6	000115-07-1	25



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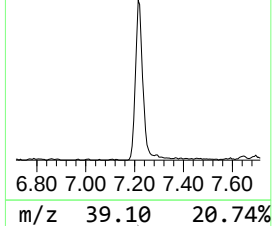
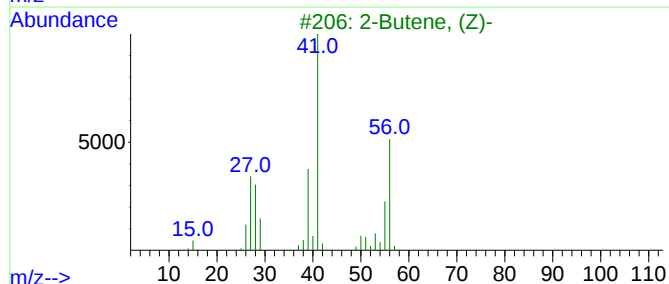
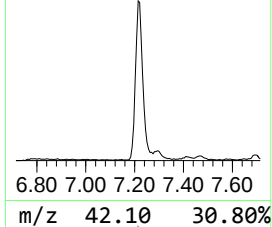
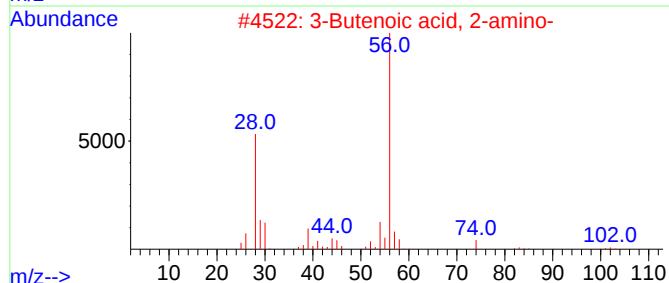
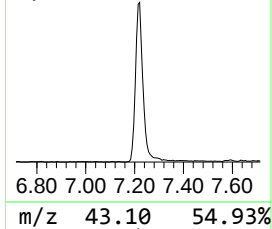
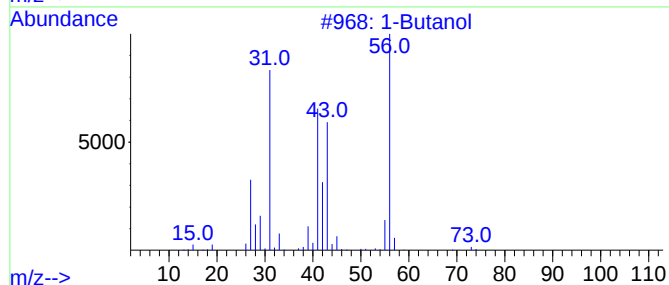
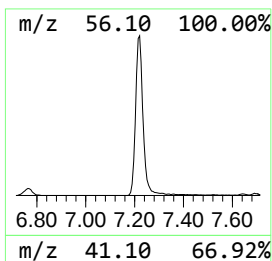
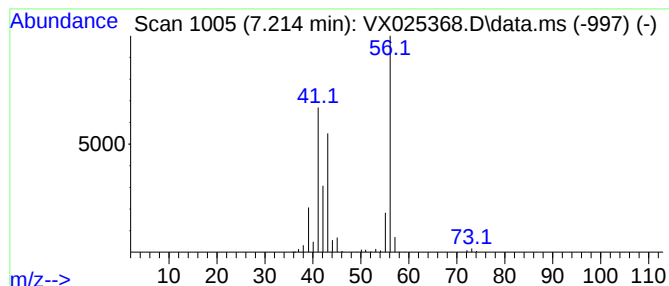
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Peak Number 3 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.214	29.68 ug/l	274666	1,4-Difluorobenzene	6.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
3	2-Butene, (Z)-	56	C4H8	000590-18-1	9
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9



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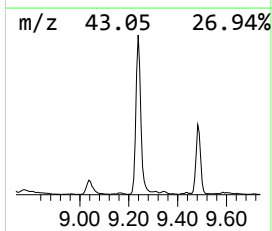
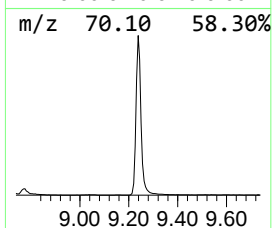
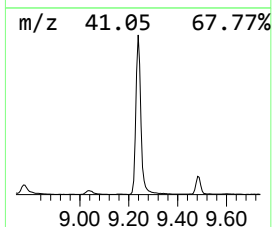
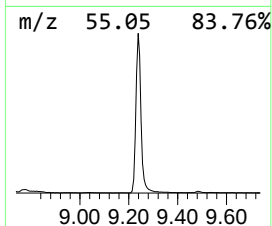
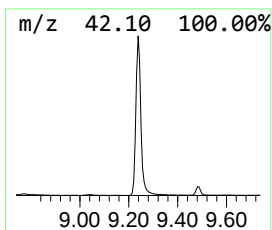
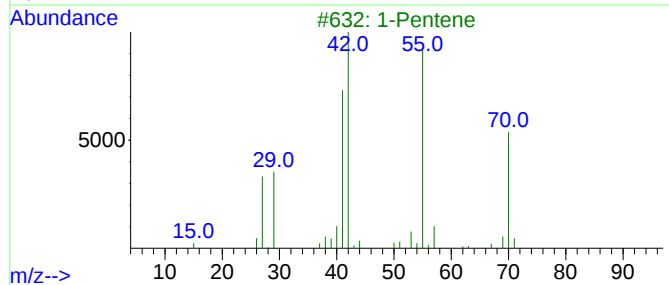
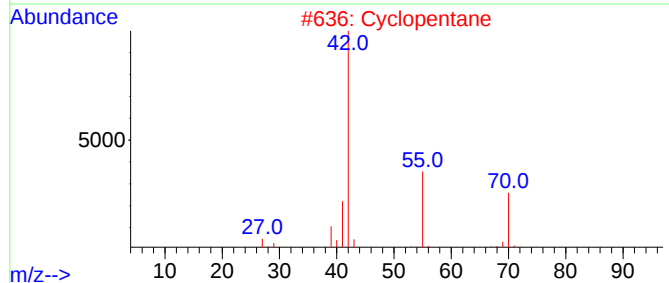
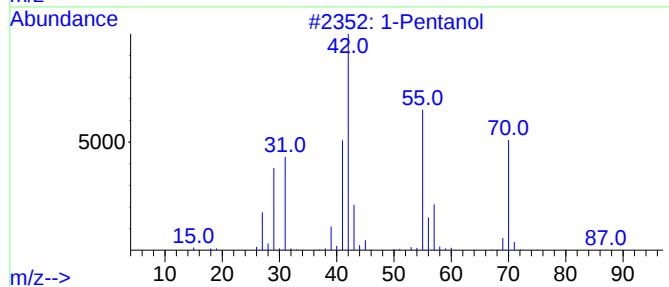
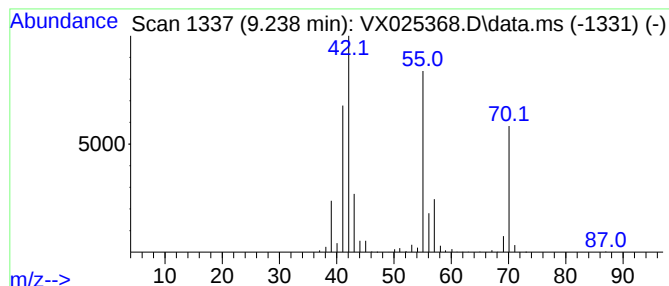
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Peak Number 4 1-Pentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.238	70.99 ug/l	783301	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol	88	C5H12O	000071-41-0	90
2			Cyclopentane	70	C5H10	000287-92-3	72
3			1-Pentene	70	C5H10	000109-67-1	72
4			Formic acid, pentyl ester	116	C6H12O2	000638-49-3	64
5			1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	42



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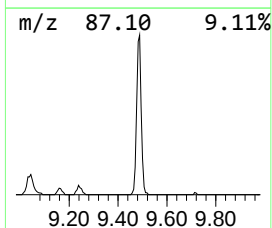
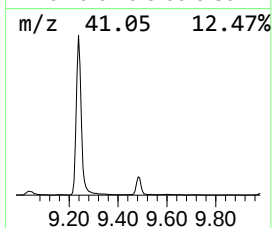
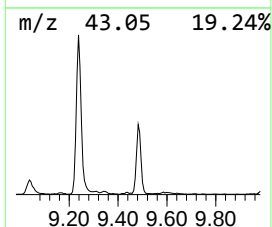
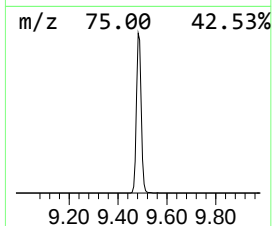
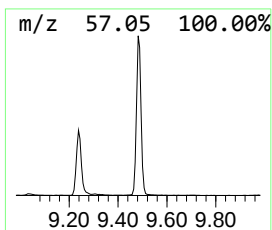
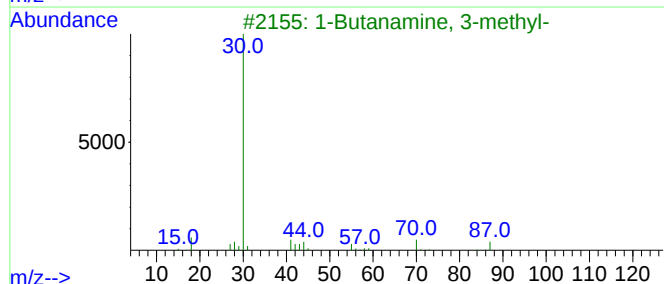
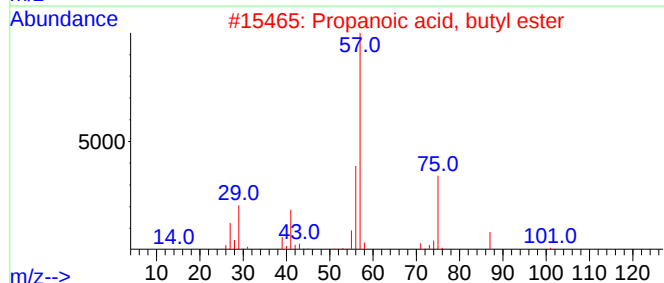
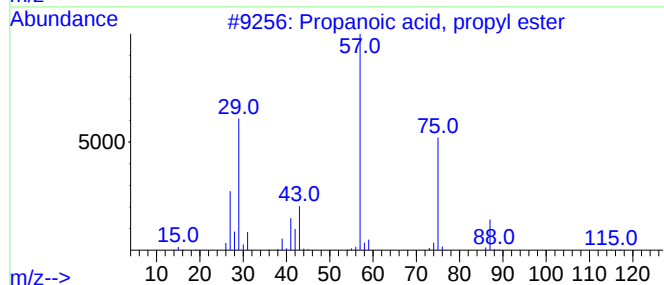
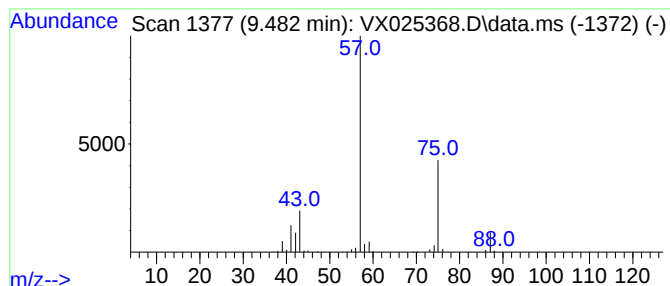
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	19.38 ug/l	213824	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4			1-Pentanamine	87	C5H13N	000110-58-7	9
5			Isobutyl ether	130	C8H18O	000628-55-7	9



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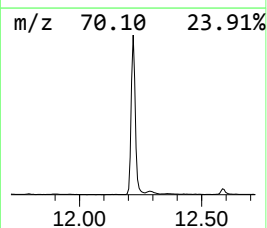
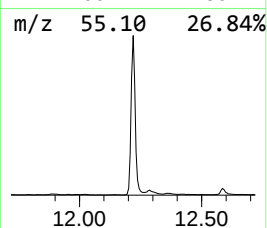
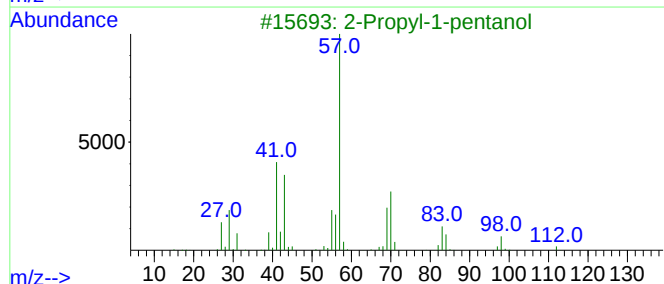
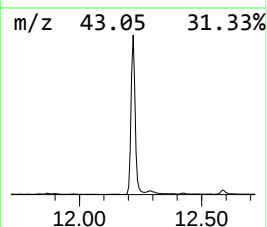
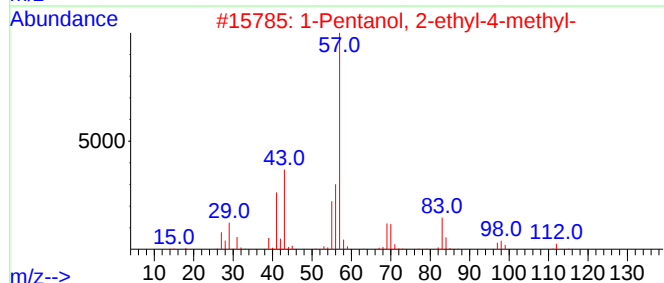
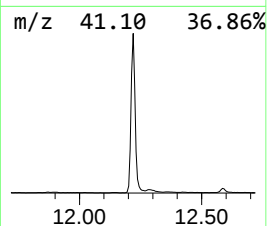
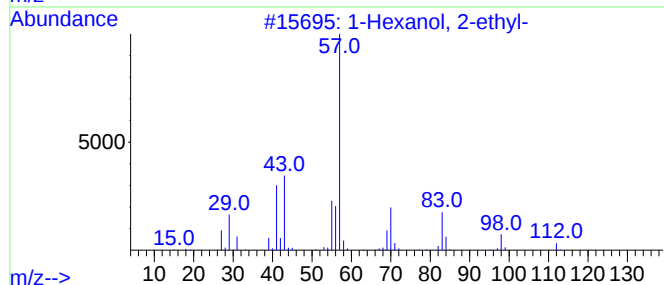
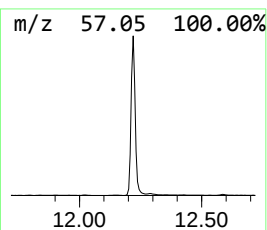
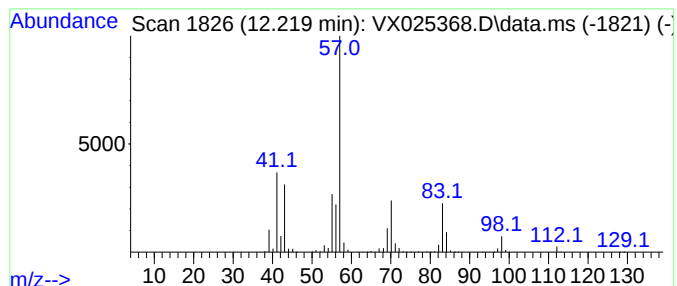
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	130.45 ug/l	1426980	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			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025368.D
Acq On : 29 Nov 2021 14:37
Operator : JC/MD
Sample : M4837-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30850

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	2.081	548.1	ug/l	3888340	1	5.556	354684	50.0
1-Propanol	4.013	2729.7	ug/l	19363400	1	5.556	354684	50.0
1-Butanol	7.214	29.7	ug/l	274666	2	6.763	462779	50.0
1-Pentanol	9.238	71.0	ug/l	783301	3	10.055	551729	50.0
Propanoic acid,...	9.482	19.4	ug/l	213824	3	10.055	551729	50.0
1-Hexanol, 2-et...	12.219	130.4	ug/l	1426980	4	12.024	546942	50.0