

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
 Data File : VX039605.D
 Acq On : 03 Jan 2024 16:21
 Operator : JC/MD
 Sample : P1002-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1217

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.441	55	58	98	rBV	12723661	18992348	100.00%	70.986%
2	2.050	151	158	170	rBV	595046	981877	5.17%	3.670%
3	4.221	502	514	532	rBV	351959	939782	4.95%	3.513%
4	5.385	692	705	716	rBV2	73019	215182	1.13%	0.804%
5	5.550	722	732	748	rVB	102058	296707	1.56%	1.109%
6	5.952	788	798	807	rBV	82848	224284	1.18%	0.838%
7	6.757	921	930	944	rVB	197936	480158	2.53%	1.795%
8	7.196	995	1002	1019	rBV	93429	214962	1.13%	0.803%
9	8.647	1234	1240	1248	rBV	441419	683291	3.60%	2.554%
10	10.049	1465	1470	1483	rBV	498925	702233	3.70%	2.625%
11	11.079	1634	1639	1645	rBV	451757	567452	2.99%	2.121%
12	11.683	1733	1738	1746	rBV	364886	416563	2.19%	1.557%
13	11.987	1779	1788	1790	rBV2	195356	284599	1.50%	1.064%
14	12.018	1790	1793	1801	rVB	579847	735513	3.87%	2.749%
15	12.213	1819	1825	1836	rBV	776894	1020110	5.37%	3.813%

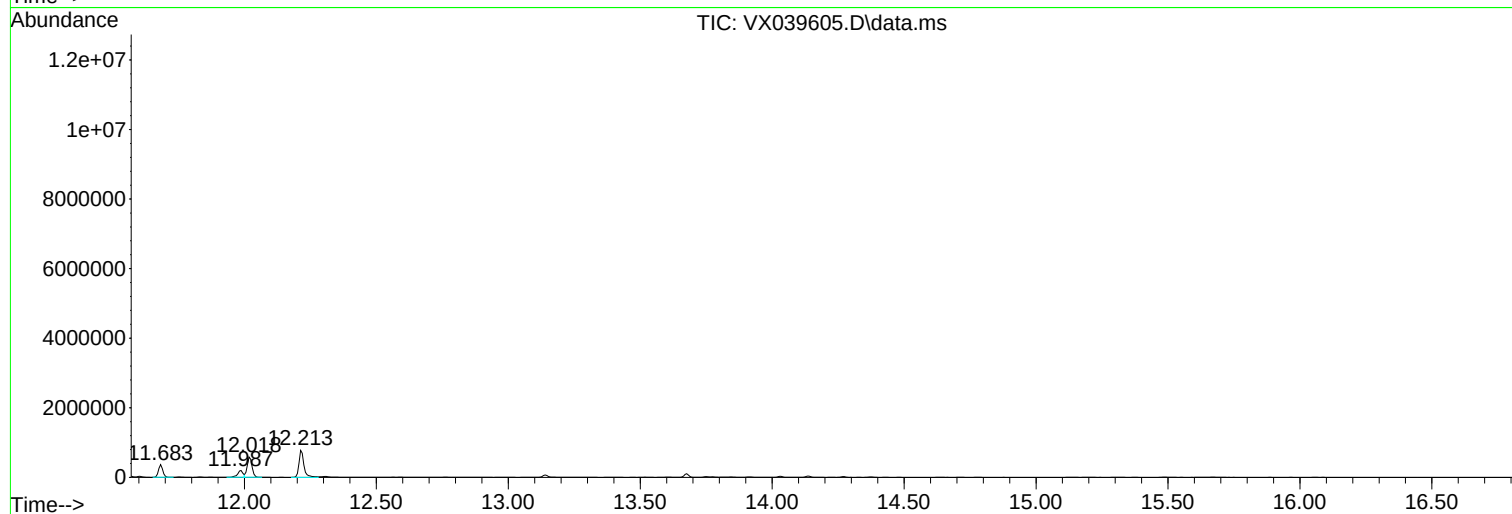
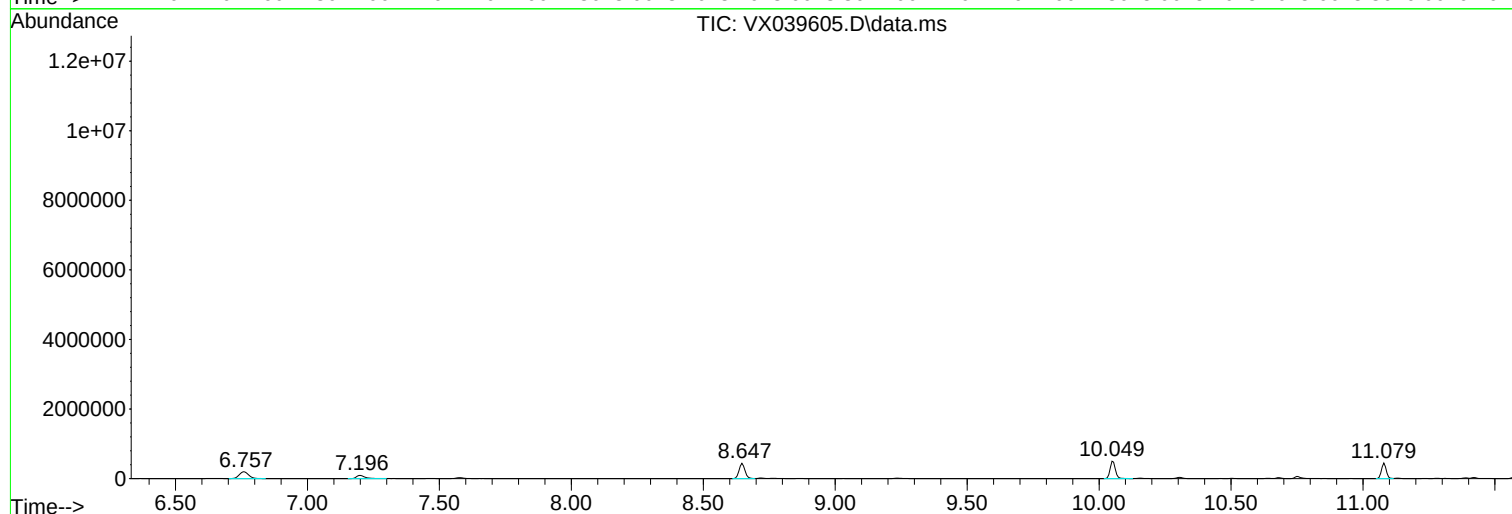
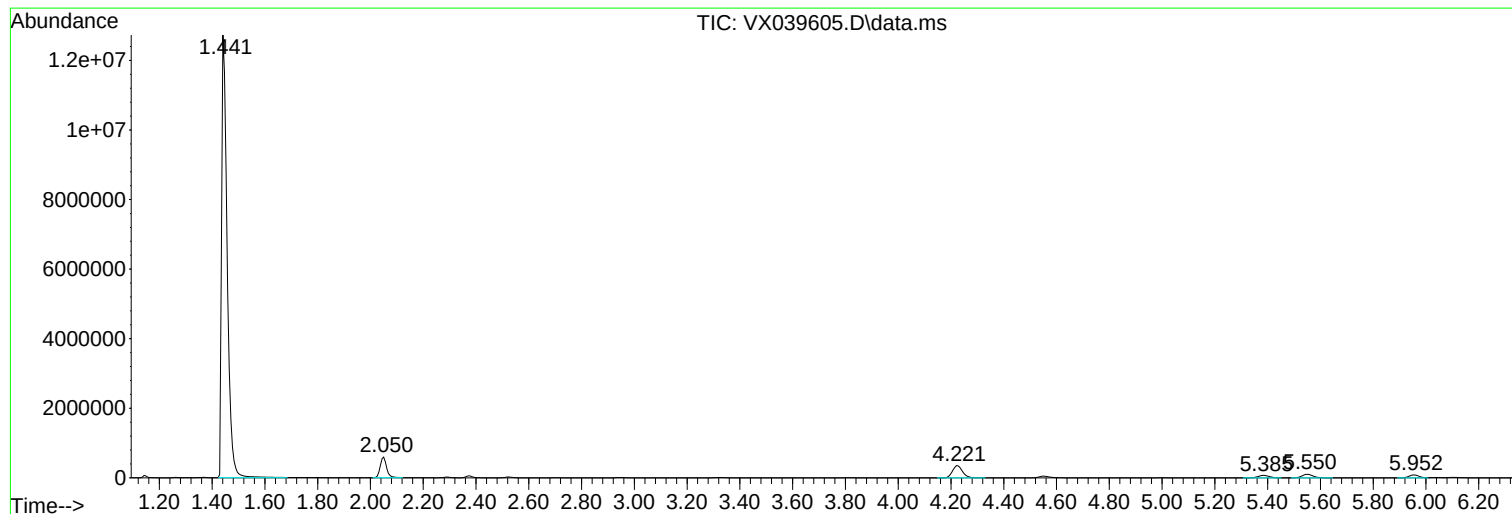
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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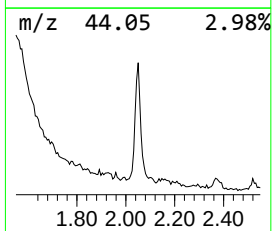
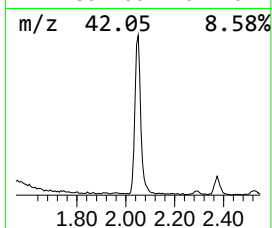
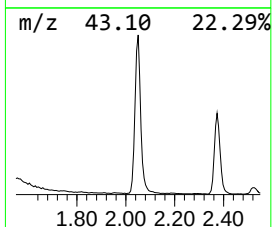
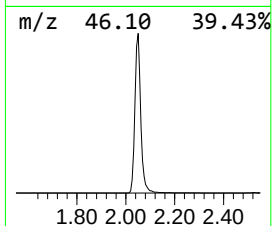
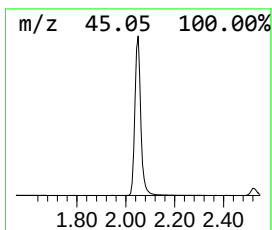
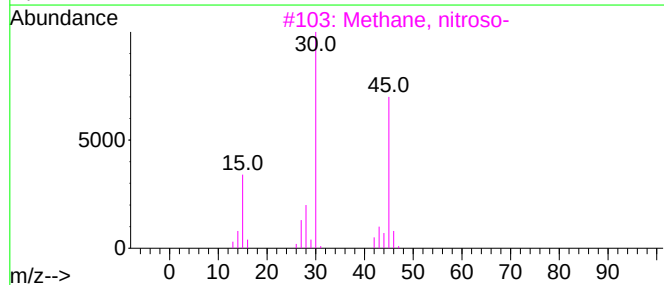
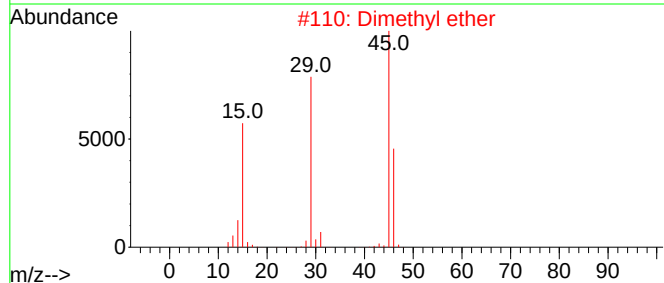
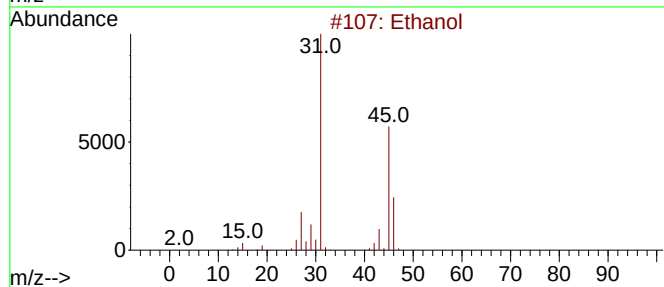
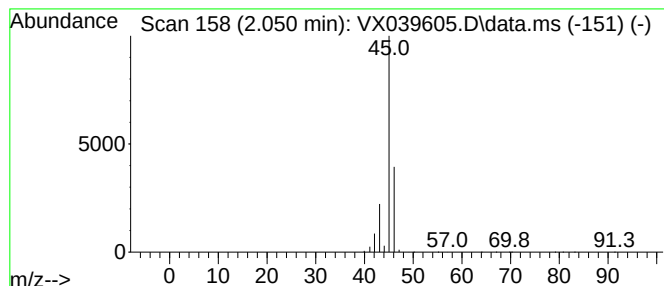
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	165.46 ug/l	981877	Pentafluorobenzene	5.550

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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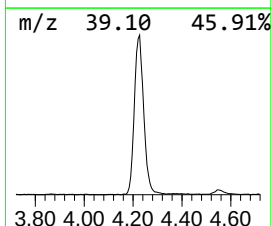
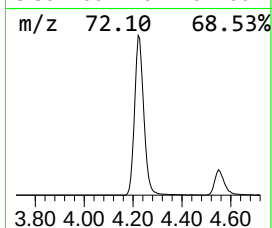
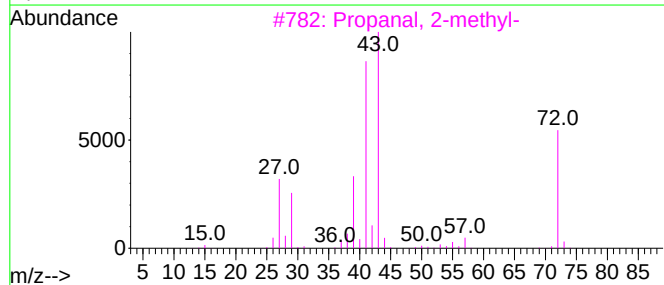
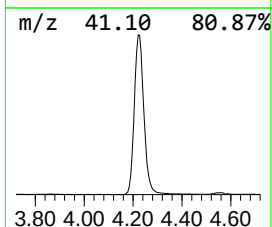
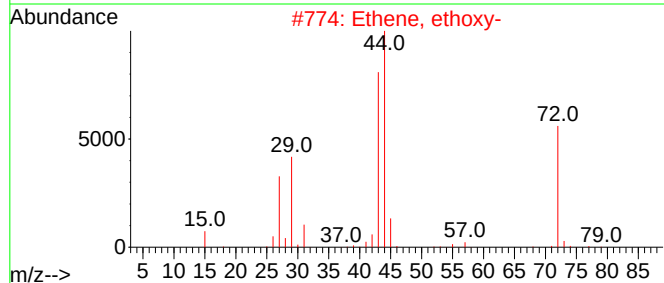
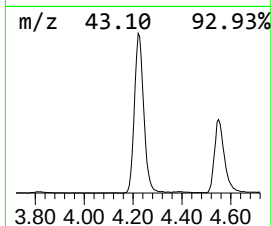
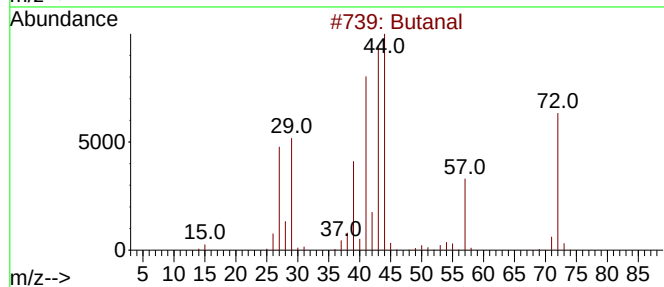
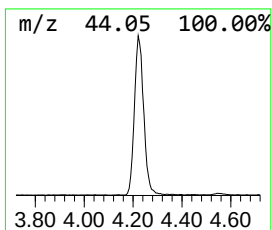
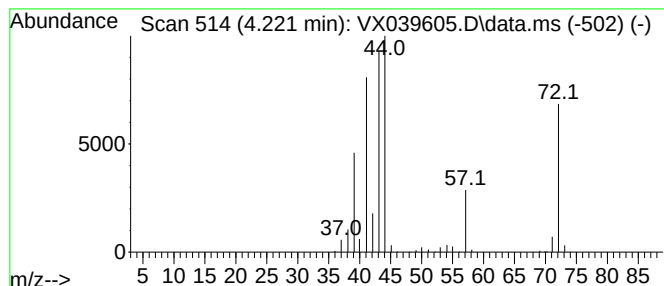
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.221	158.37 ug/l	939782	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	49
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23



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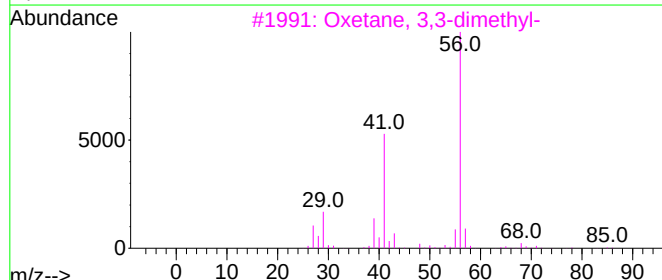
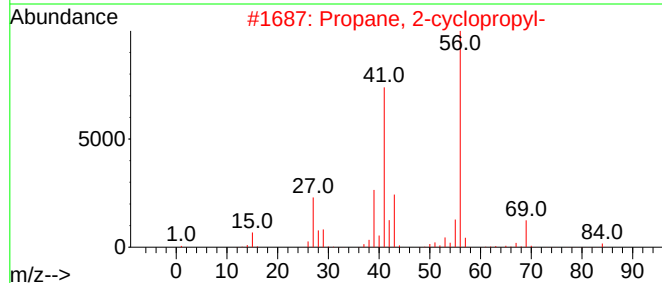
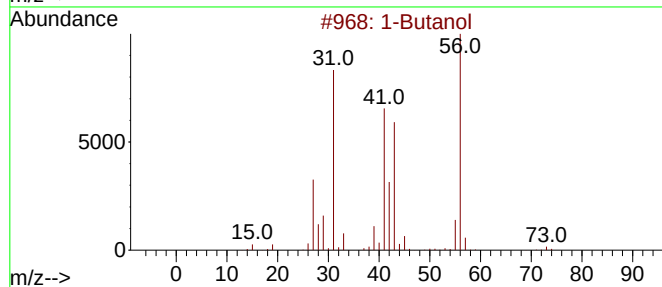
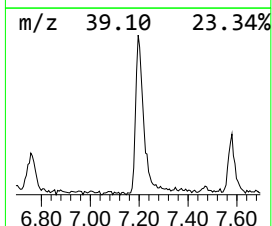
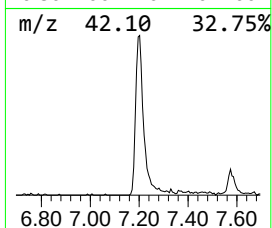
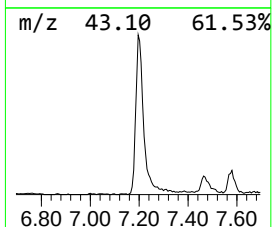
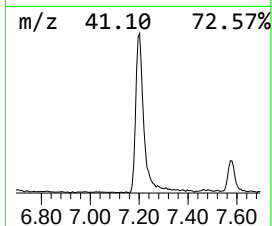
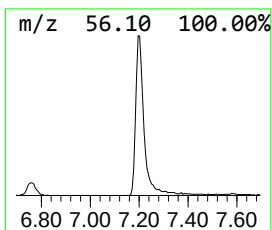
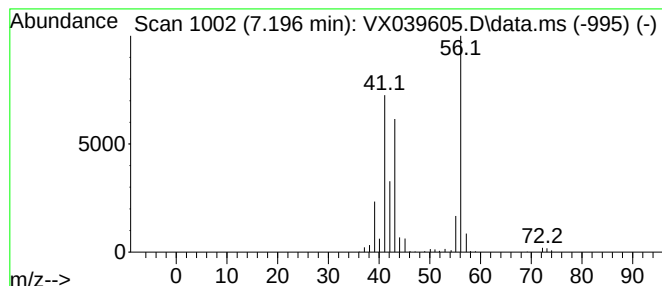
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Peak Number 4 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.196	22.38 ug/l	214962	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	86
2	Propane, 2-cyclopropyl-			84	C6H12	003638-35-5	38
3	Oxetane, 3,3-dimethyl-			86	C5H10O	006921-35-3	36
4	Propane, 1-chloro-2-methyl-			92	C4H9Cl	000513-36-0	9
5	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	9



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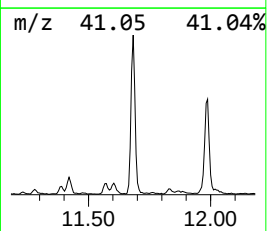
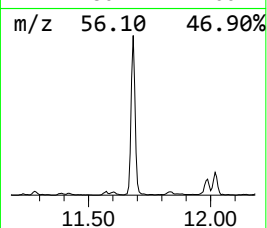
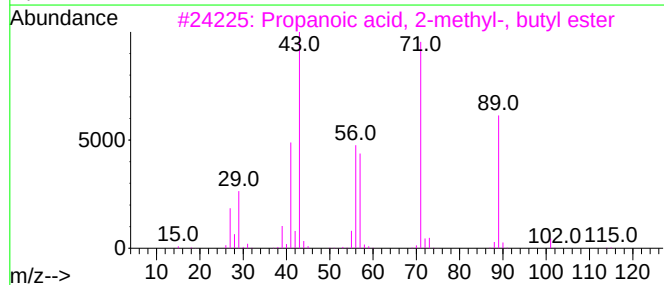
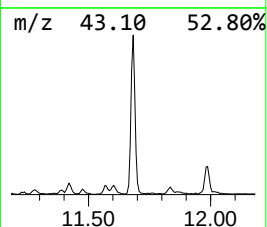
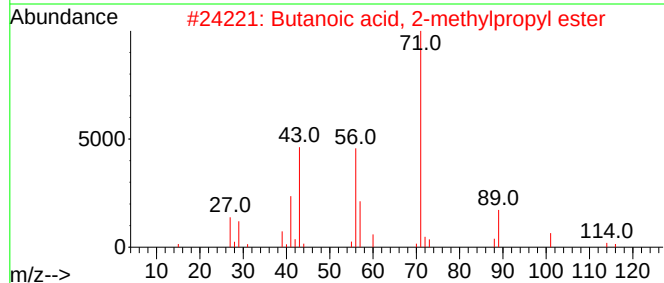
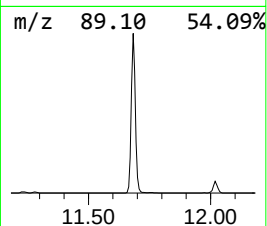
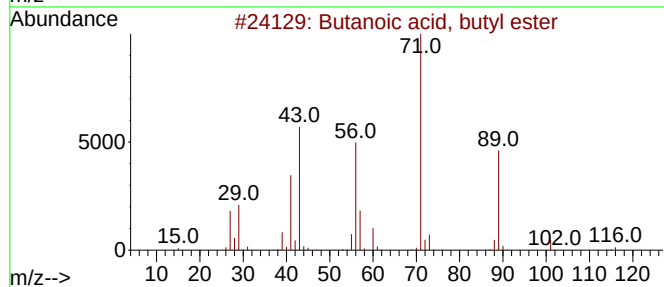
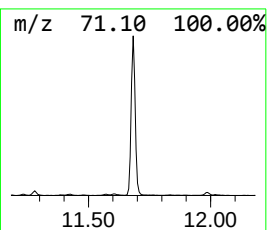
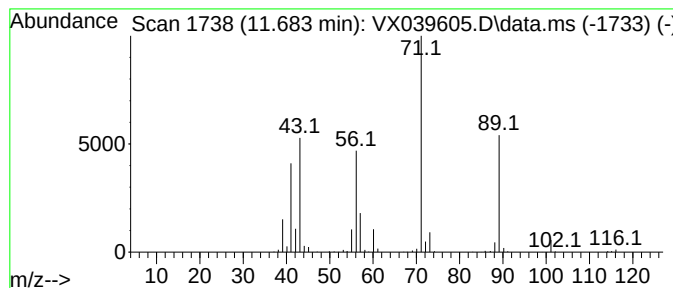
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	28.32 ug/l	416563	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
5			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56



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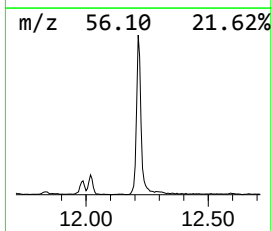
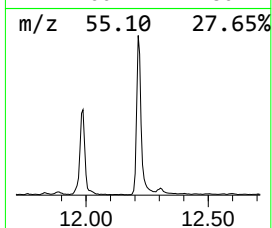
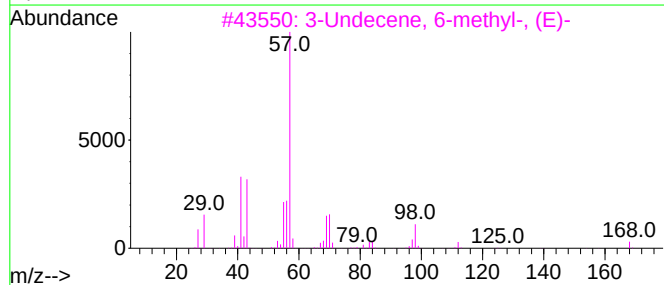
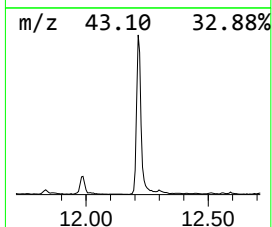
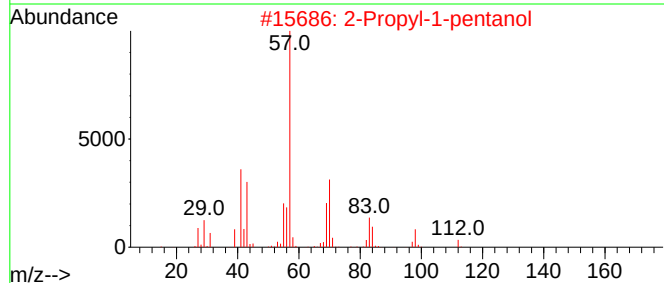
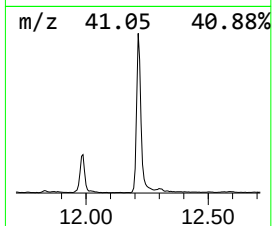
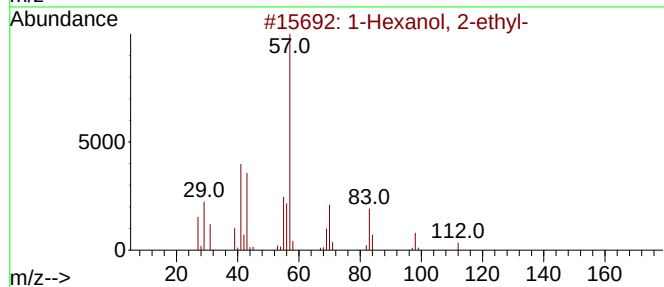
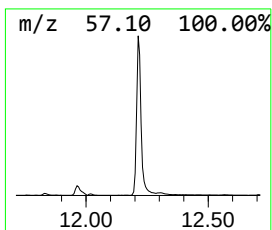
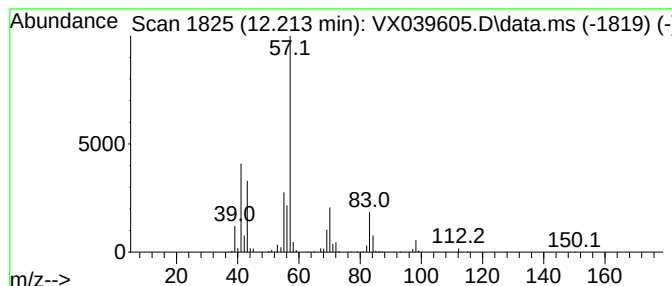
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	69.35 ug/l	1020110	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50



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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	2.050	165.5	ug/l	981877	1	5.550	296707	50.0
Butanal	4.221	158.4	ug/l	939782	1	5.550	296707	50.0
1-Butanol	7.196	22.4	ug/l	214962	2	6.757	480158	50.0
Butanoic acid, ...	11.683	28.3	ug/l	416563	4	12.018	735513	50.0
1-Hexanol, 2-et...	12.213	69.3	ug/l	1020110	4	12.018	735513	50.0