

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011623\
 Data File : VU052702.D
 Acq On : 16 Jan 2023 14:40
 Operator : JC/MD
 Sample : 01139-04DL 20X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH1Y7DL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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_U\Method\SFAMUTR011023WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052702.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	70	80	92	rBV	50599	62251	7.04%	0.881%
2	1.732	114	122	130	rVB2	12207	15255	1.73%	0.216%
3	1.912	169	178	196	rBV	45862	65559	7.41%	0.928%
4	2.565	369	381	394	rBV	105557	184035	20.81%	2.604%
5	2.678	404	416	418	rBV3	17065	33110	3.74%	0.469%
6	3.044	523	530	549	rVB2	23880	51072	5.78%	0.723%
7	4.655	1012	1031	1041	rBV4	76342	248645	28.12%	3.518%
8	4.726	1046	1053	1104	rVB	110137	488159	55.20%	6.907%
9	5.060	1141	1157	1176	rBV	112863	275244	31.12%	3.895%
10	5.722	1341	1363	1385	rBV3	216377	564853	63.87%	7.993%
11	6.243	1509	1525	1547	rBV	174496	335323	37.92%	4.745%
12	6.629	1602	1645	1647	rBV2	242221	884337	100.00%	12.513%
13	7.562	1923	1935	1952	rBV2	70184	124035	14.03%	1.755%
14	7.893	2025	2038	2056	rBV	260319	447564	50.61%	6.333%
15	8.156	2107	2120	2140	rBV2	101276	237220	26.82%	3.357%
16	8.571	2236	2249	2258	rBV	81451	132474	14.98%	1.875%
17	8.632	2258	2268	2302	rVB2	342902	694477	78.53%	9.827%
18	8.832	2320	2330	2348	rVB2	40249	67335	7.61%	0.953%
19	9.414	2493	2511	2530	rBV	252183	415943	47.03%	5.886%
20	10.025	2689	2701	2708	rBV5	4525	9382	1.06%	0.133%
21	10.070	2708	2715	2729	rVB3	6058	10062	1.14%	0.142%
22	10.565	2861	2869	2879	rBV2	14346	21257	2.40%	0.301%
23	10.751	2916	2927	2937	rBV	108271	171520	19.40%	2.427%
24	10.960	2982	2992	3007	rBV2	29537	45490	5.14%	0.644%
25	11.153	3042	3052	3065	rBV	19844	31345	3.54%	0.444%
26	11.369	3107	3119	3146	rBV	373161	564789	63.87%	7.992%
27	11.806	3243	3255	3274	rBV	279558	438253	49.56%	6.201%
28	12.188	3361	3374	3389	rBV	252407	402421	45.51%	5.694%
29	13.298	3708	3719	3733	rBV	31025	45726	5.17%	0.647%

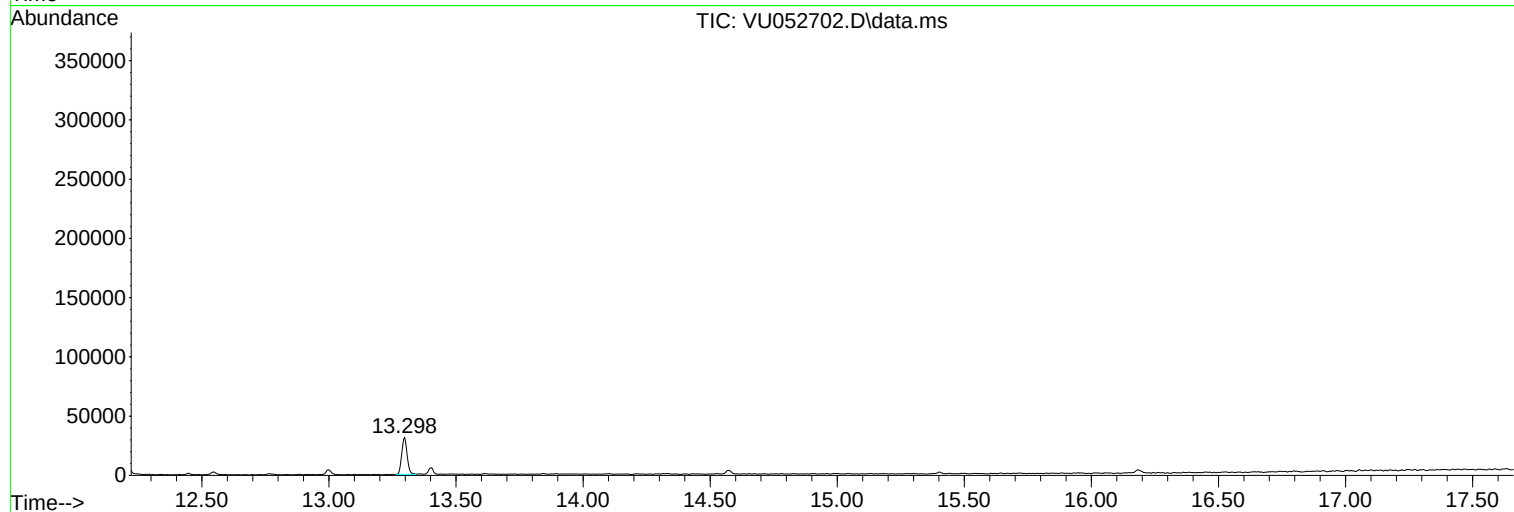
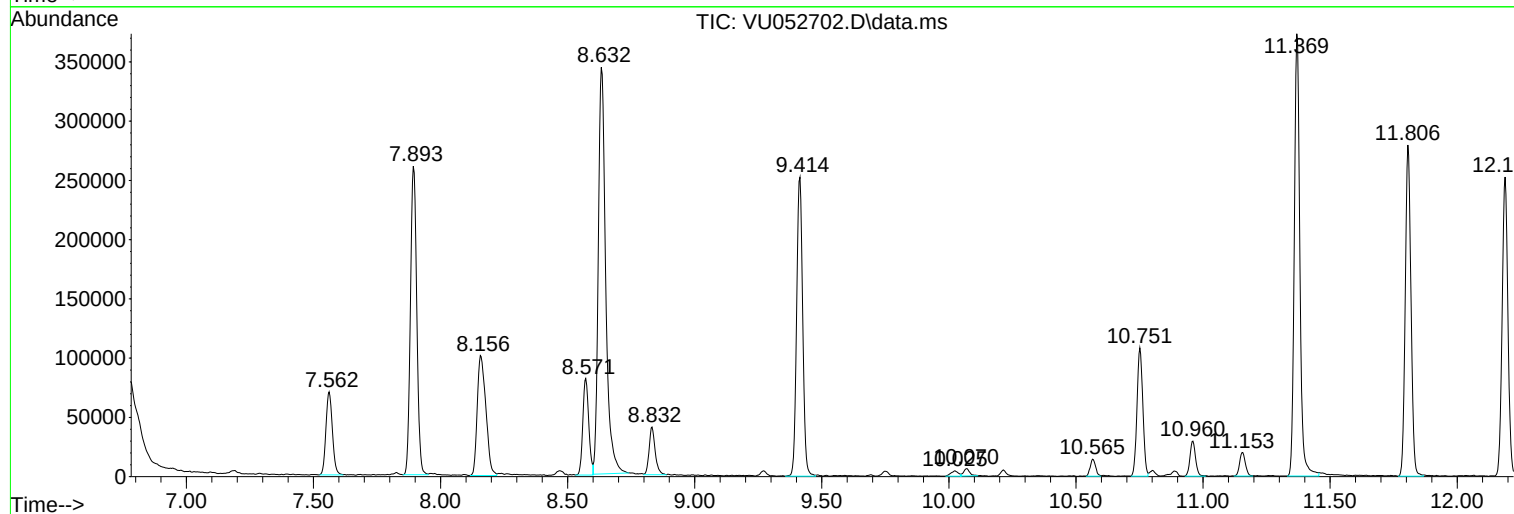
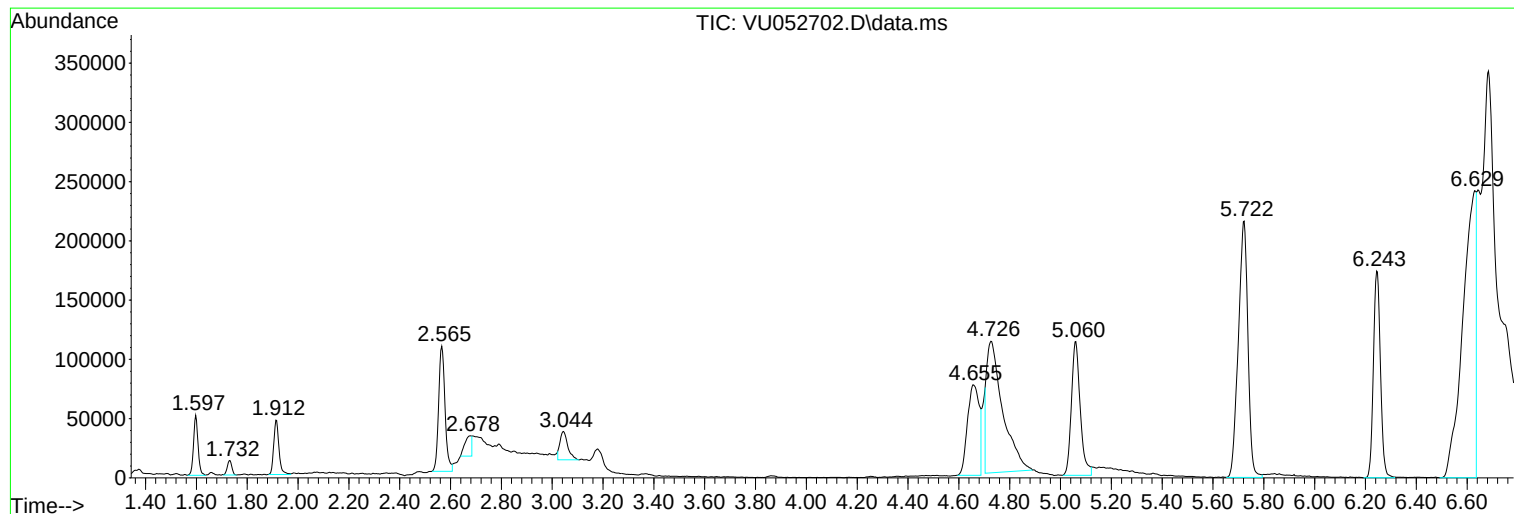
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Instrument :
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ClientSampleId :
BH1Y7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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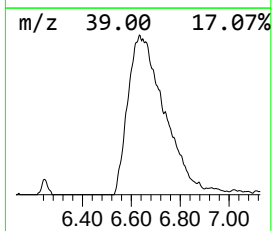
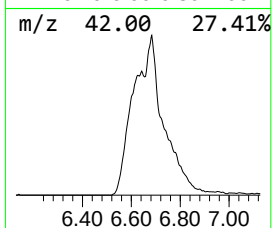
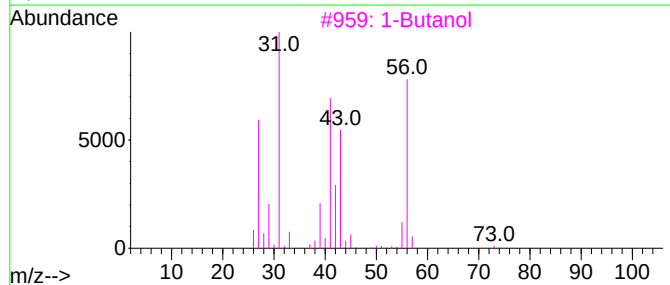
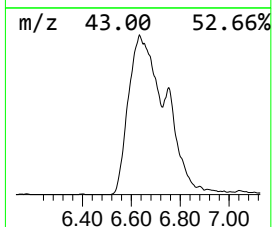
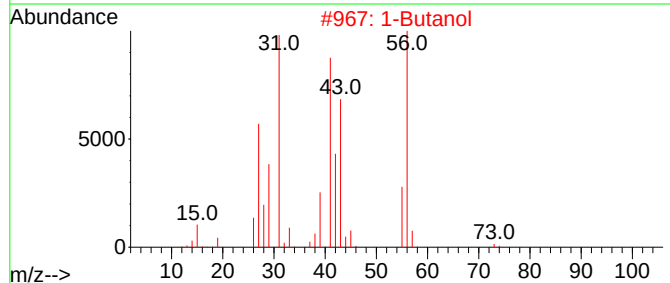
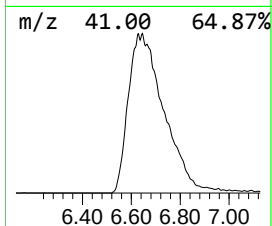
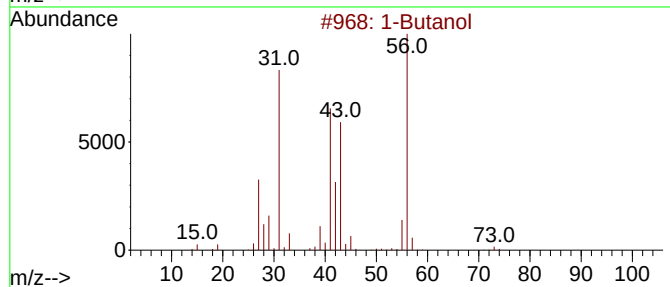
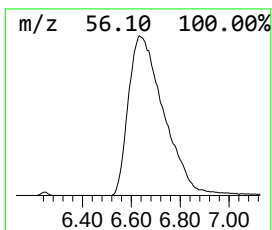
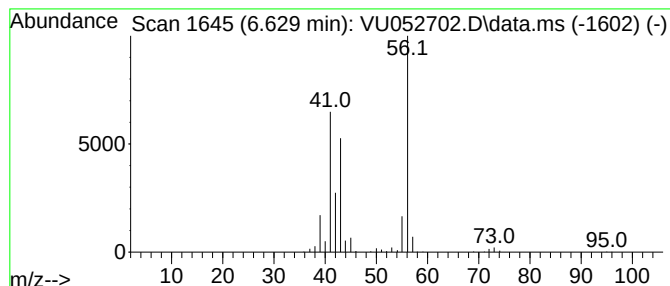
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.629	13.19 ug/L	884337	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	91
2	1-Butanol			74	C4H10O	000071-36-3	90
3	1-Butanol			74	C4H10O	000071-36-3	86
4	1-Butanol			74	C4H10O	000071-36-3	83
5	1-Butanol			74	C4H10O	000071-36-3	50



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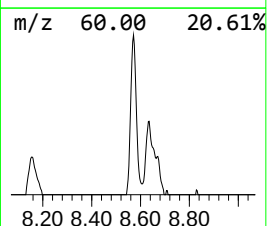
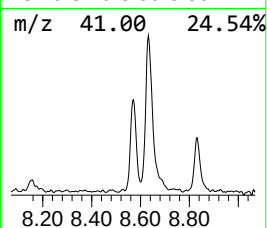
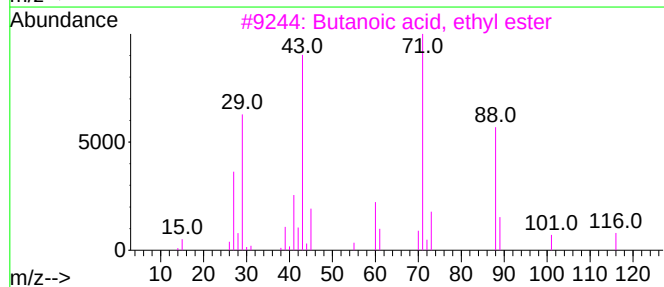
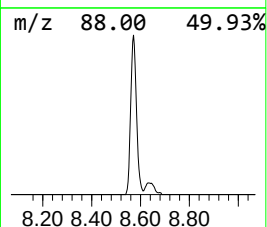
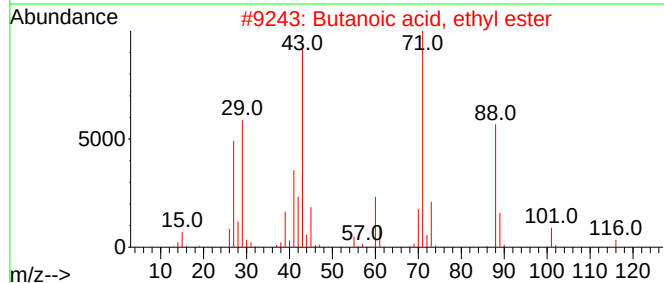
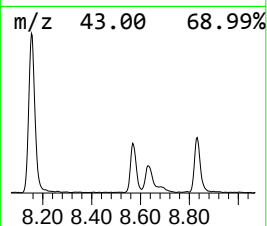
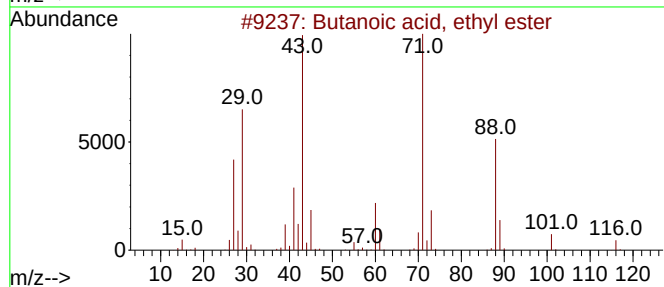
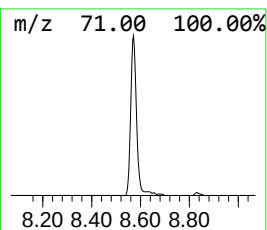
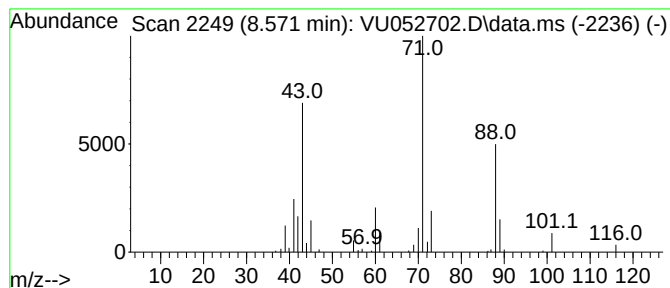
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.571	1.59 ug/L	132474	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
4			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	83
5			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	49



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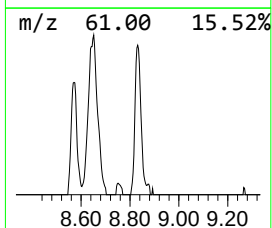
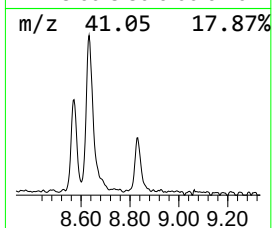
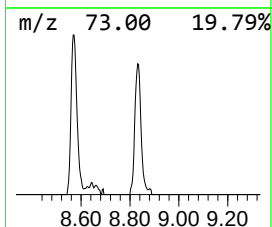
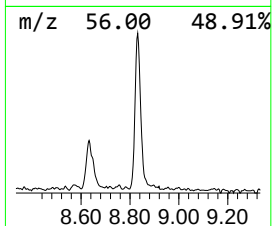
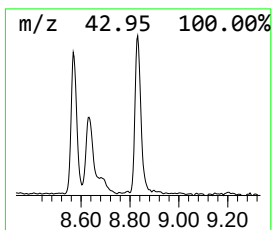
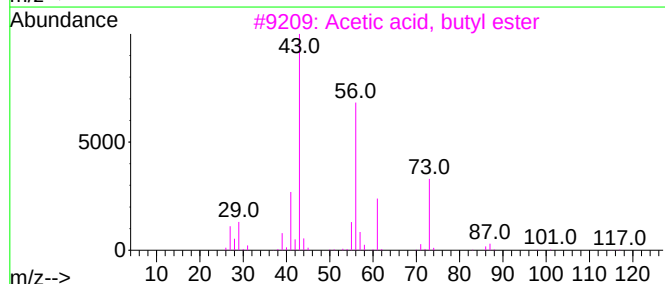
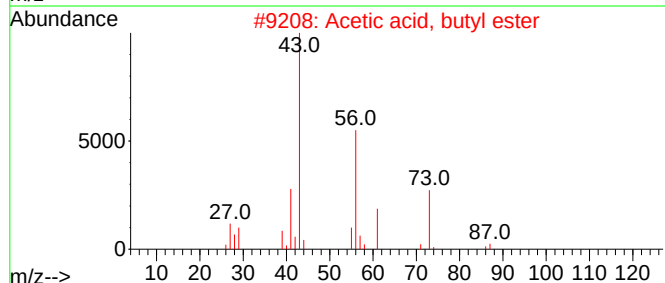
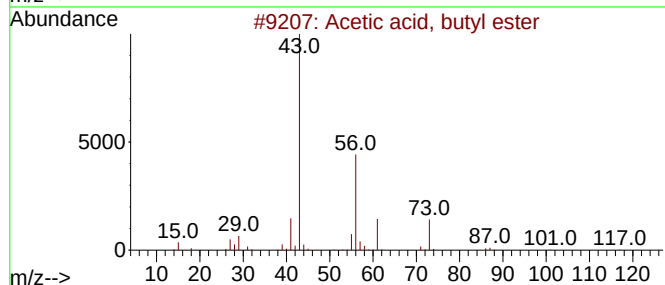
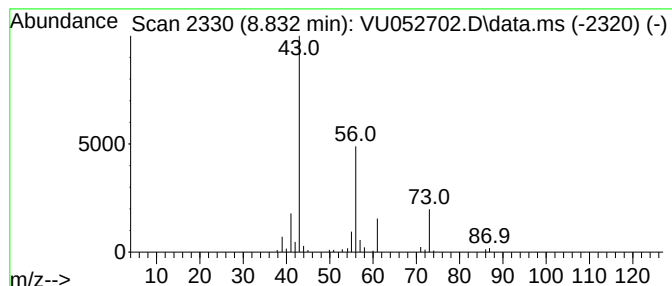
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.832	0.81 ug/L	67335	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



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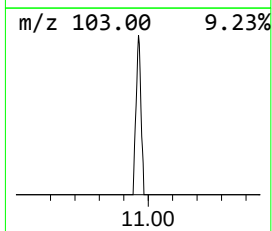
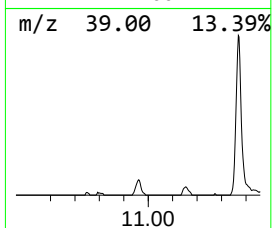
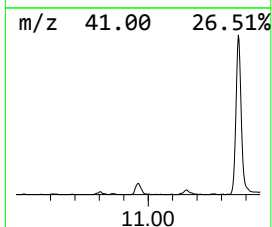
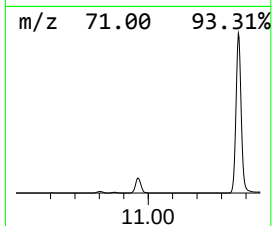
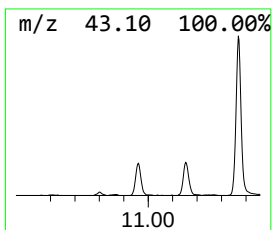
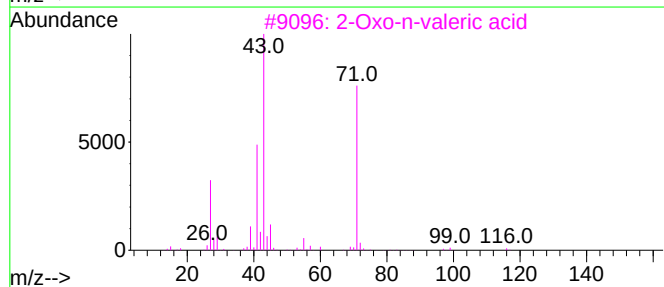
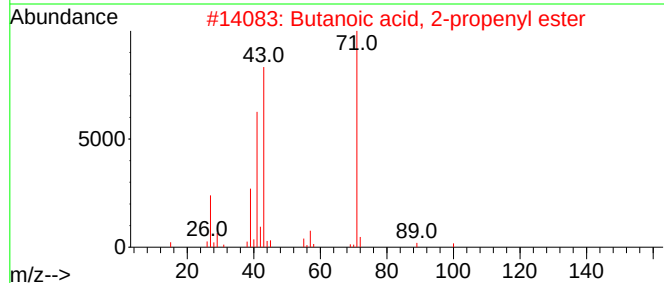
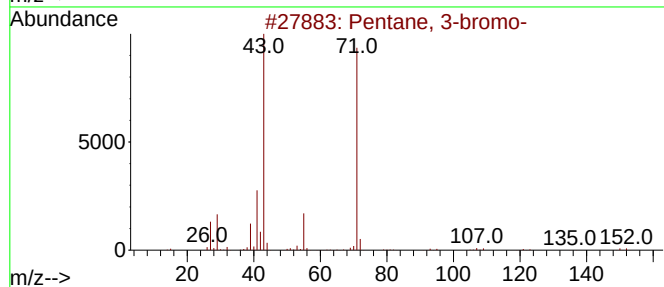
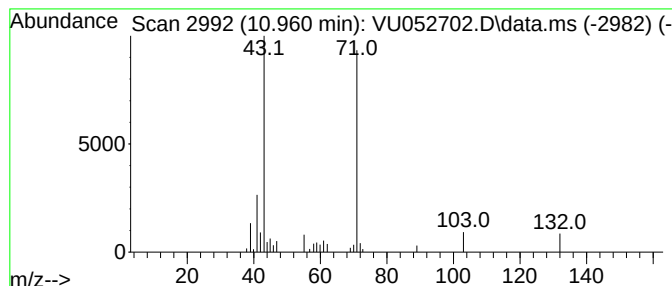
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Pentane, 3-bromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.960	0.52 ug/L	45490	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-bromo-	150	C5H11Br	001809-10-5	50
2			Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	50
3			2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	42
4			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	40
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	40



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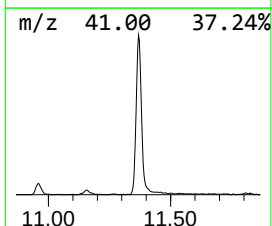
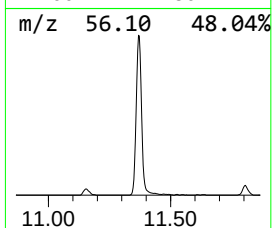
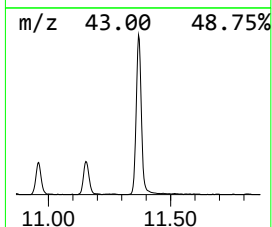
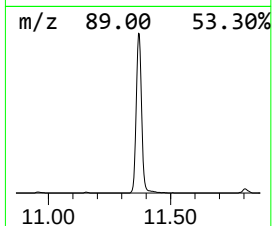
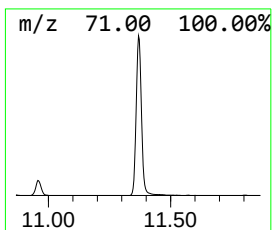
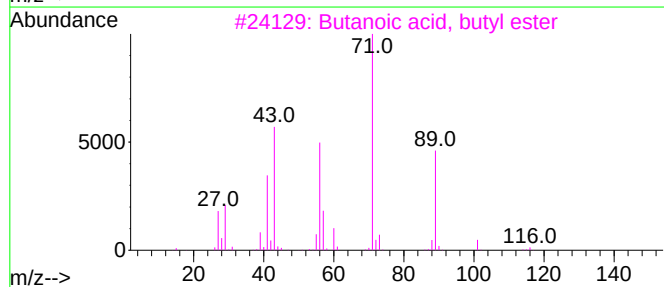
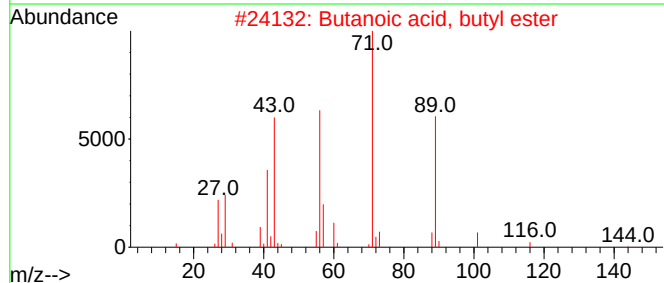
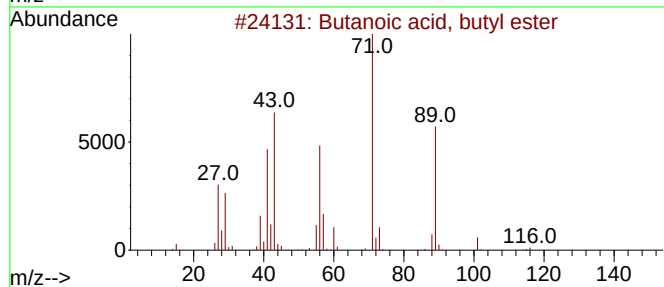
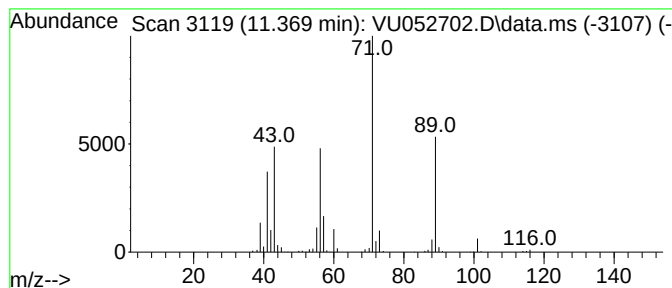
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.368	6.44 ug/L	564789	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
3			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
5			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72



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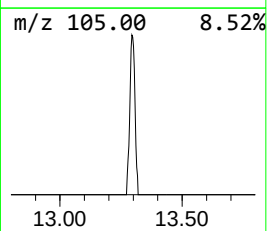
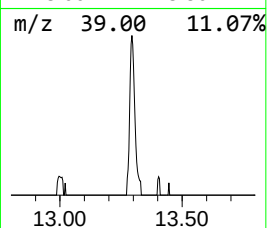
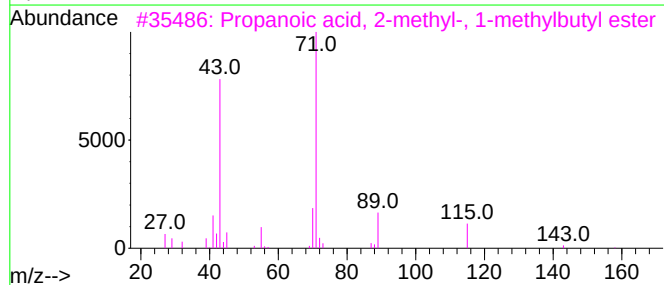
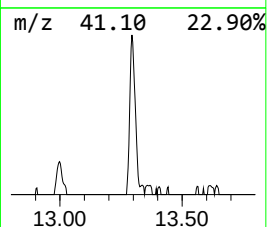
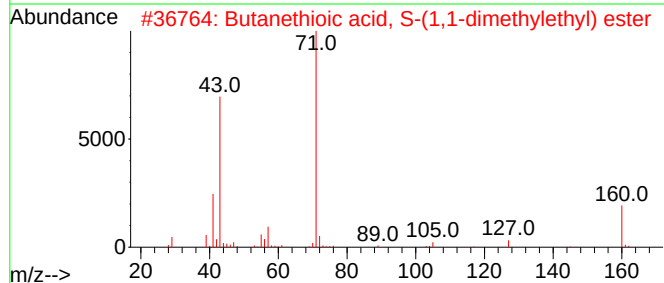
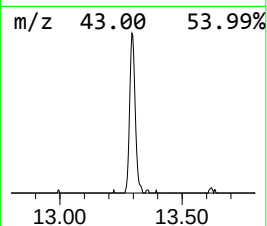
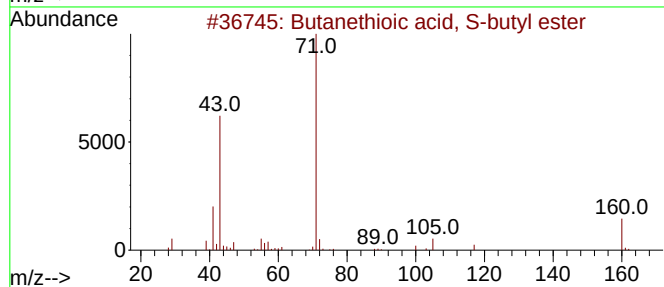
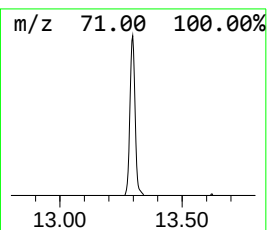
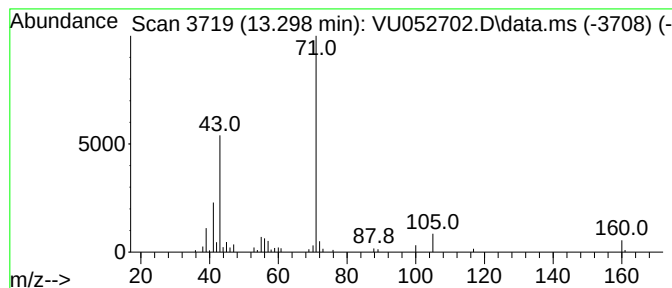
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Butanethioic acid, S-butyl ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.298	0.52 ug/L	45726	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanethioic acid, S-butyl ester	160	C8H16OS	002432-52-2	78
2			Butanethioic acid, S-(1,1-dimeth...	160	C8H16OS	006330-43-4	72
3			Propanoic acid, 2-methyl-, 1-met...	158	C9H18O2	054340-93-1	59
4			Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	59
5			2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011623\
Data File : VU052702.D
Acq On : 16 Jan 2023 14:40
Operator : JC/MD
Sample : 01139-04DL 20X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH1Y7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Butanol	6.629	13.2	ug/L	884337	1	6.243	335323	5.0
Butanoic acid, ...	8.571	1.6	ug/L	132474	2	9.414	415943	5.0
Acetic acid, bu...	8.832	0.8	ug/L	67335	2	9.414	415943	5.0
Pentane, 3-bromo-	10.960	0.5	ug/L	45490	3	11.806	438253	5.0
Butanoic acid, ...	11.368	6.4	ug/L	564789	3	11.806	438253	5.0
Butanethioic ac...	13.298	0.5	ug/L	45726	3	11.806	438253	5.0