

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
 Data File : VV037353.D
 Acq On : 18 Sep 2024 23:54
 Operator : SY/MD
 Sample : P3988-14 50X
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH8S3

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_V\Method\SFAMVTR091024WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV037353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.217	43	55	66	rBV3	16797	50716	3.53%	0.394%
2	1.278	67	74	83	rBV2	188616	198084	13.78%	1.541%
3	1.333	83	91	94	rBV	129901	179762	12.51%	1.398%
4	1.532	146	153	164	rVB	136784	162908	11.33%	1.267%
5	2.056	308	316	331	rVB	297594	478005	33.25%	3.718%
6	2.134	332	340	366	rVB	77625	215688	15.00%	1.678%
7	3.111	634	644	660	rBV3	6138	14535	1.01%	0.113%
8	3.429	728	743	747	rBV8	16158	40583	2.82%	0.316%
9	3.809	845	861	877	rBV2	176291	564615	39.28%	4.391%
10	4.243	982	996	1046	rBV2	180705	597316	41.55%	4.646%
11	4.953	1201	1217	1244	rBV2	423149	1106507	76.97%	8.606%
12	5.532	1386	1397	1426	rBV	324666	711824	49.52%	5.536%
13	5.850	1481	1496	1505	rBV6	13670	31510	2.19%	0.245%
14	5.912	1505	1515	1530	rBV	452491	1437489	100.00%	11.180%
15	5.982	1532	1537	1576	rVB	366995	837201	58.24%	6.512%
16	6.307	1630	1638	1648	rBV2	17321	32360	2.25%	0.252%
17	6.915	1817	1827	1844	rBV2	85678	175315	12.20%	1.364%
18	7.239	1917	1928	1956	rBV	498297	934220	64.99%	7.266%
19	7.558	2019	2027	2042	rBV2	44800	90574	6.30%	0.704%
20	7.969	2146	2155	2164	rBV	162378	249093	17.33%	1.937%
21	8.024	2164	2172	2216	rVB	541454	1206394	83.92%	9.383%
22	8.255	2235	2244	2261	rBV3	21591	46512	3.24%	0.362%
23	8.365	2271	2278	2294	rVB6	9756	18428	1.28%	0.143%
24	8.780	2396	2407	2435	rBV	533079	930256	64.71%	7.235%
25	9.493	2620	2629	2649	rBV3	33998	74743	5.20%	0.581%
26	9.641	2667	2675	2696	rBV2	15412	36890	2.57%	0.287%
27	10.149	2820	2833	2851	rBV	200168	337998	23.51%	2.629%
28	10.786	3021	3031	3057	rBV	190432	346094	24.08%	2.692%
29	11.181	3143	3154	3180	rBV	563386	914420	63.61%	7.112%
30	11.554	3256	3270	3294	rBV	492933	837182	58.24%	6.511%

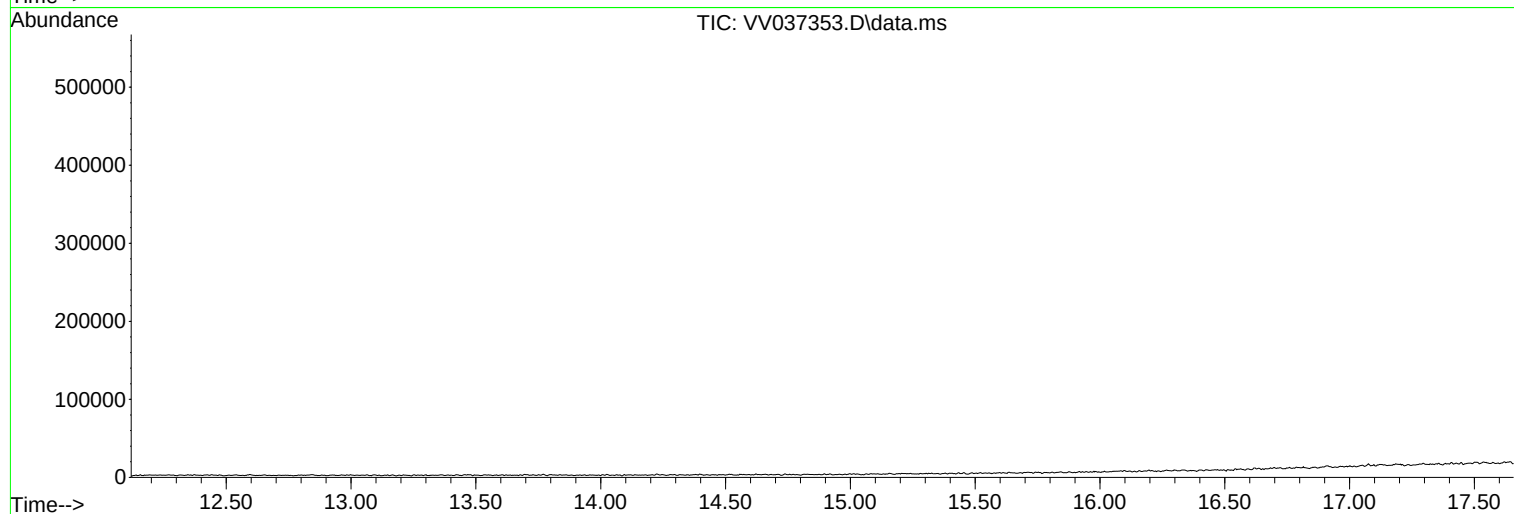
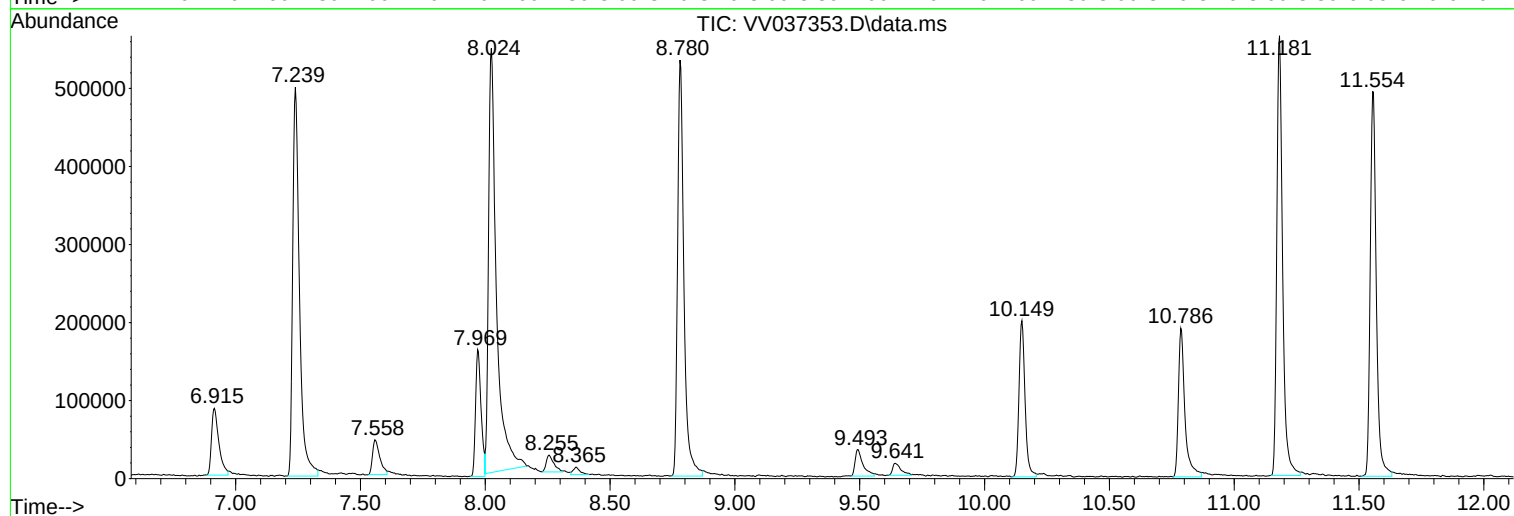
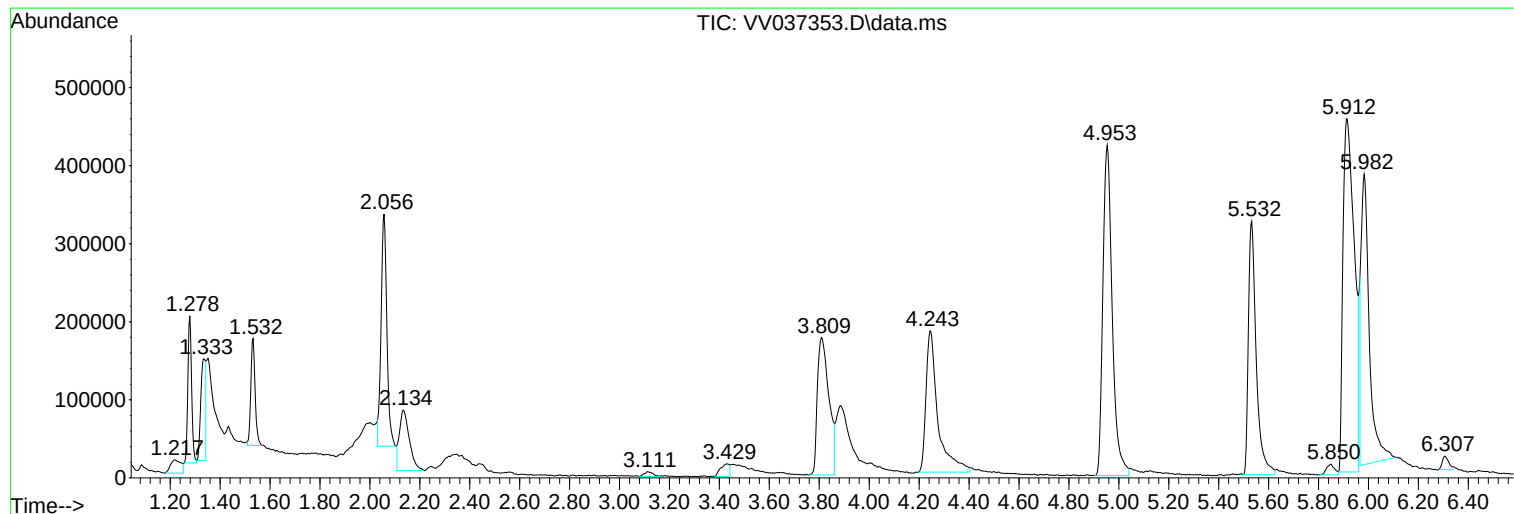
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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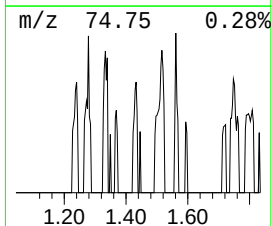
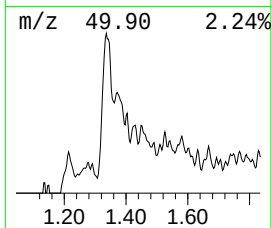
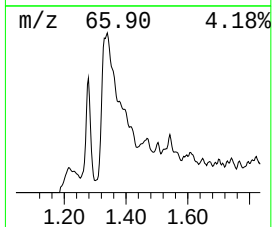
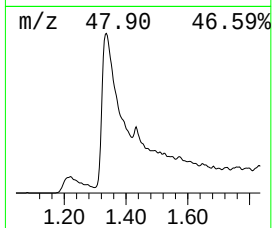
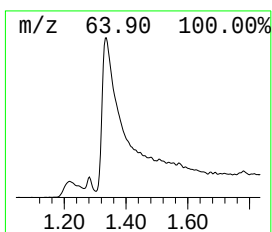
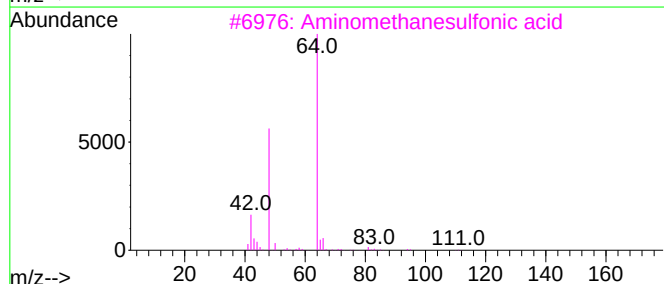
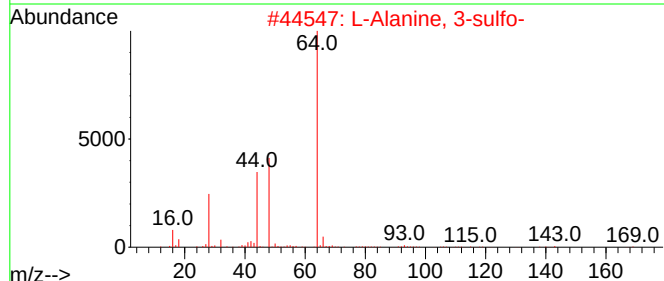
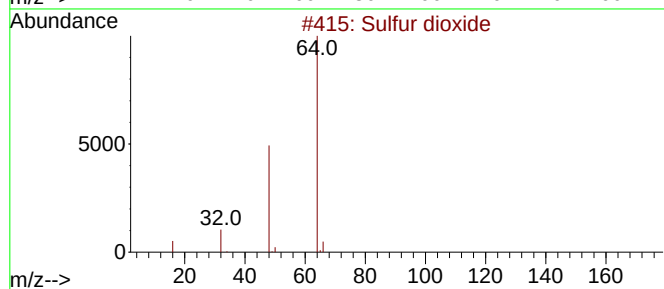
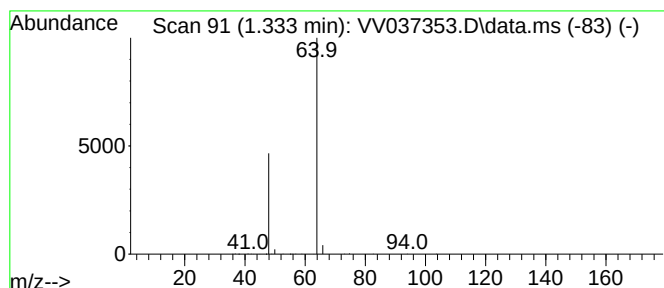
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.333	1.26 ug/L	179762	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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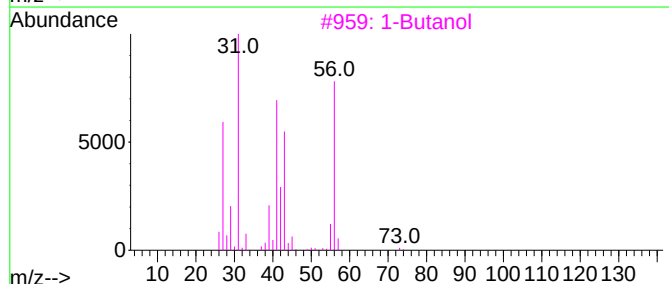
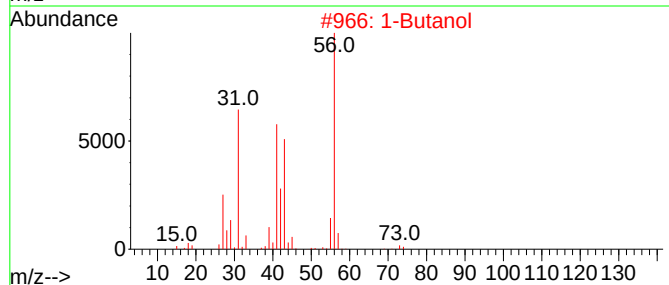
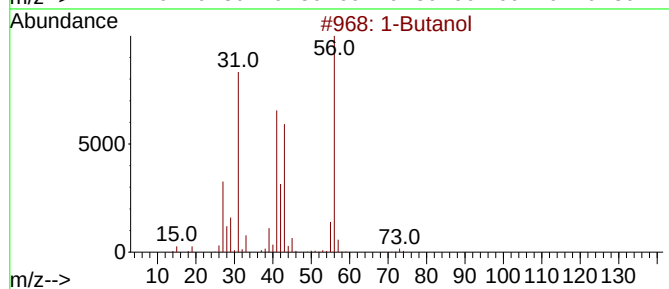
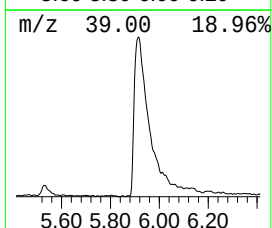
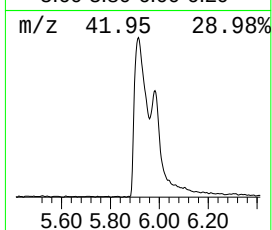
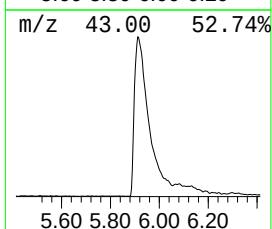
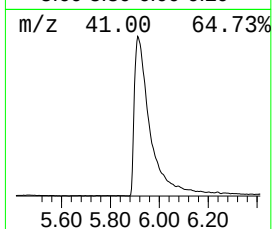
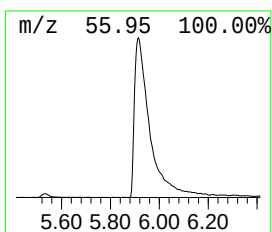
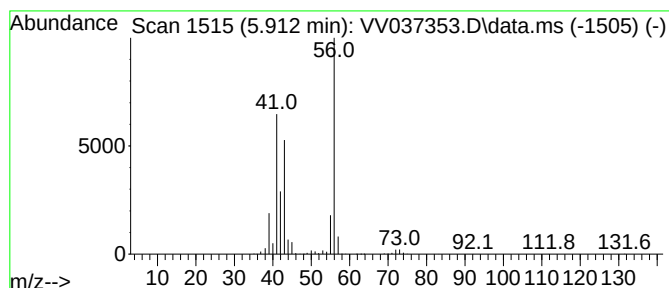
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.912	10.10 ug/L	1437490	1,4-Difluorobenzene	5.532

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	90
2	1-Butanol		74	C4H10O	000071-36-3	83
3	1-Butanol		74	C4H10O	000071-36-3	72
4	1-Butanol		74	C4H10O	000071-36-3	50
5	1-Butanol		74	C4H10O	000071-36-3	49



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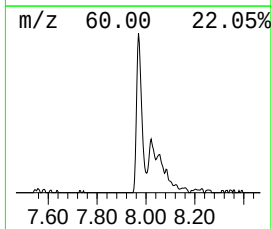
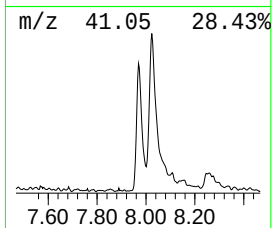
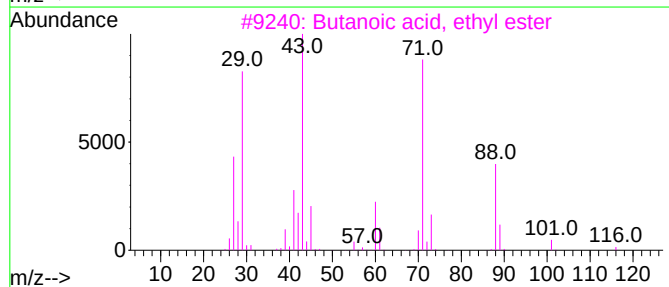
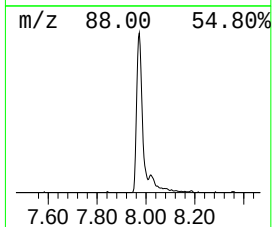
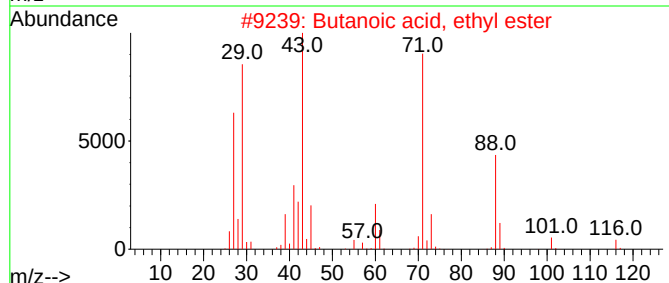
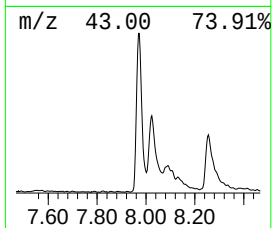
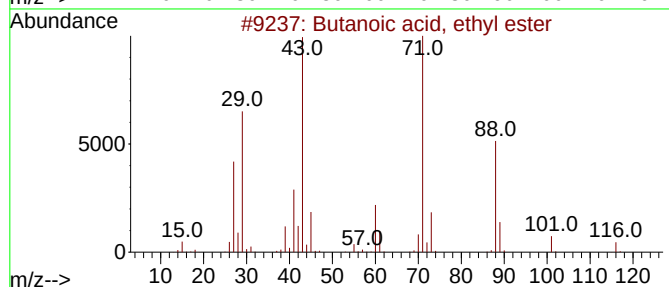
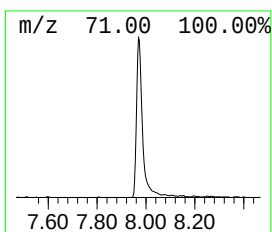
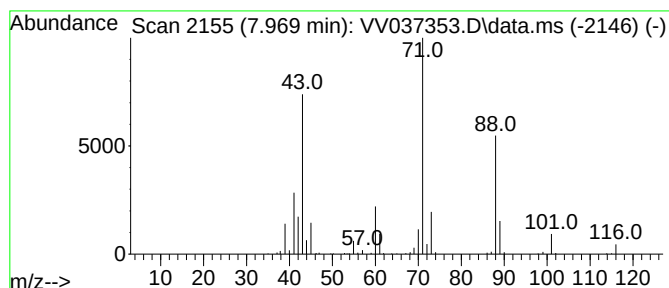
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
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Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	1.34 ug/L	249093	Chlorobenzene-d5	8.780

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	91
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	83
4			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	83
5			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

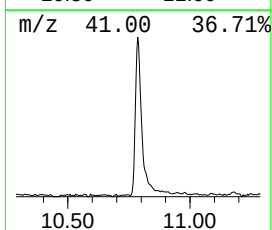
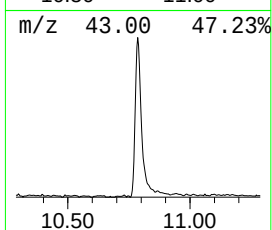
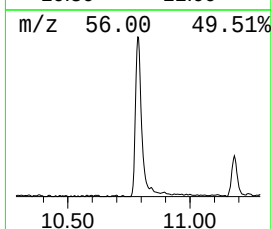
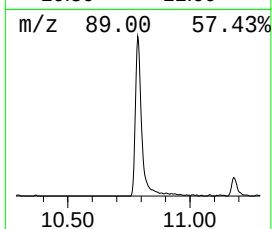
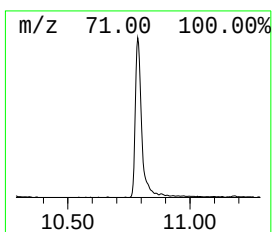
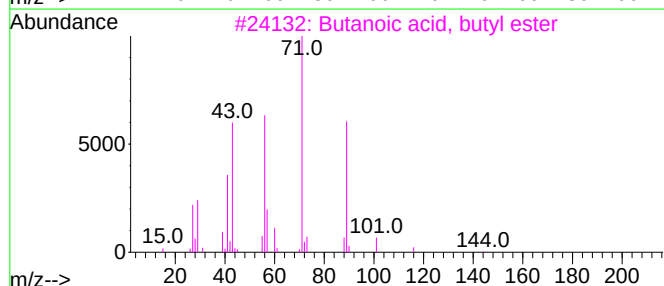
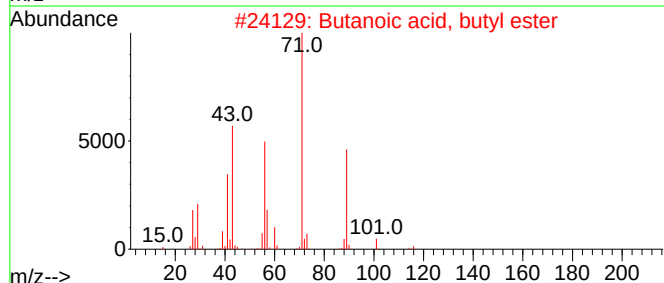
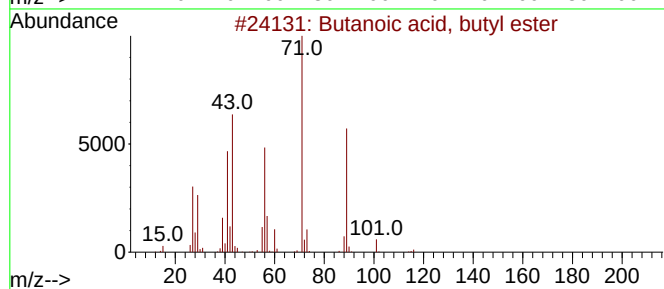
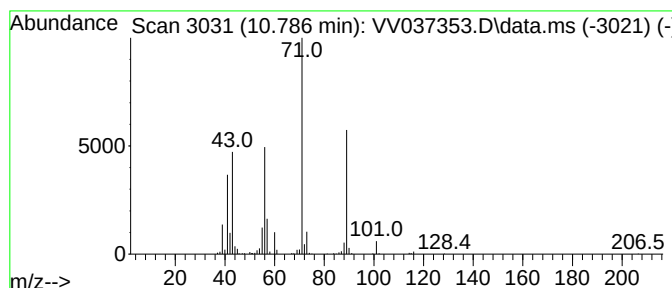
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.786	1.89 ug/L	346094	1,4-Dichlorobenzene-d4	11.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
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	64
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.333	1.3	ug/L	179762	1	5.532	711824	5.0
1-Butanol	5.912	10.1	ug/L	1437490	1	5.532	711824	5.0
Butanoic acid, ...	7.969	1.3	ug/L	249093	2	8.780	930256	5.0
Butanoic acid, ...	10.786	1.9	ug/L	346094	3	11.181	914420	5.0