

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
 Data File : VU057118.D
 Acq On : 21 Dec 2023 02:40
 Operator : MD/SY
 Sample : 05892-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B07

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\SFAMUTR121123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057118.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	9	20	33	rBV2	93637	166171	17.01%	2.559%
2	1.470	48	56	80	rBV	420384	976689	100.00%	15.042%
3	1.592	90	94	105	rVB	68234	75698	7.75%	1.166%
4	1.911	188	193	209	rVB	67619	101750	10.42%	1.567%
5	2.560	383	395	422	rVB	129675	217697	22.29%	3.353%
6	2.789	456	466	481	rBV	6378	12263	1.26%	0.189%
7	4.650	1032	1045	1074	rBV2	32245	121816	12.47%	1.876%
8	5.055	1156	1171	1195	rBV2	125401	278247	28.49%	4.285%
9	5.721	1353	1378	1400	rBV2	225364	592047	60.62%	9.118%
10	6.245	1524	1541	1564	rBV	215380	424741	43.49%	6.541%
11	6.685	1665	1678	1696	rBV	139525	280717	28.74%	4.323%
12	7.161	1813	1826	1849	rBV2	28141	58989	6.04%	0.908%
13	7.563	1939	1951	1970	rBV	66111	122639	12.56%	1.889%
14	7.894	2037	2054	2071	rBV	268796	479871	49.13%	7.390%
15	8.177	2132	2142	2156	rBV	37968	66037	6.76%	1.017%
16	8.634	2269	2284	2321	rBV	210261	486487	49.81%	7.492%
17	9.412	2514	2526	2550	rBV	311302	546549	55.96%	8.417%
18	10.081	2725	2734	2747	rBV2	17284	29691	3.04%	0.457%
19	10.341	2806	2815	2828	rBV7	12346	22010	2.25%	0.339%
20	10.750	2930	2942	2956	rBV2	97299	164772	16.87%	2.538%
21	11.737	3241	3249	3259	rVV4	23824	38119	3.90%	0.587%
22	11.807	3259	3271	3293	rVB	316989	507100	51.92%	7.810%
23	11.981	3315	3325	3338	rVB8	9273	19582	2.00%	0.302%
24	12.061	3338	3350	3359	rBV8	6512	15170	1.55%	0.234%
25	12.187	3373	3389	3413	rVB	274680	485212	49.68%	7.473%
26	12.888	3597	3607	3617	rBV8	9673	16740	1.71%	0.258%
27	12.971	3624	3633	3646	rVB7	18340	29749	3.05%	0.458%
28	15.685	4466	4477	4489	rBV6	23666	37145	3.80%	0.572%
29	16.762	4804	4812	4823	rBV8	11711	18026	1.85%	0.278%
30	16.878	4836	4848	4861	rBV2	64589	101369	10.38%	1.561%

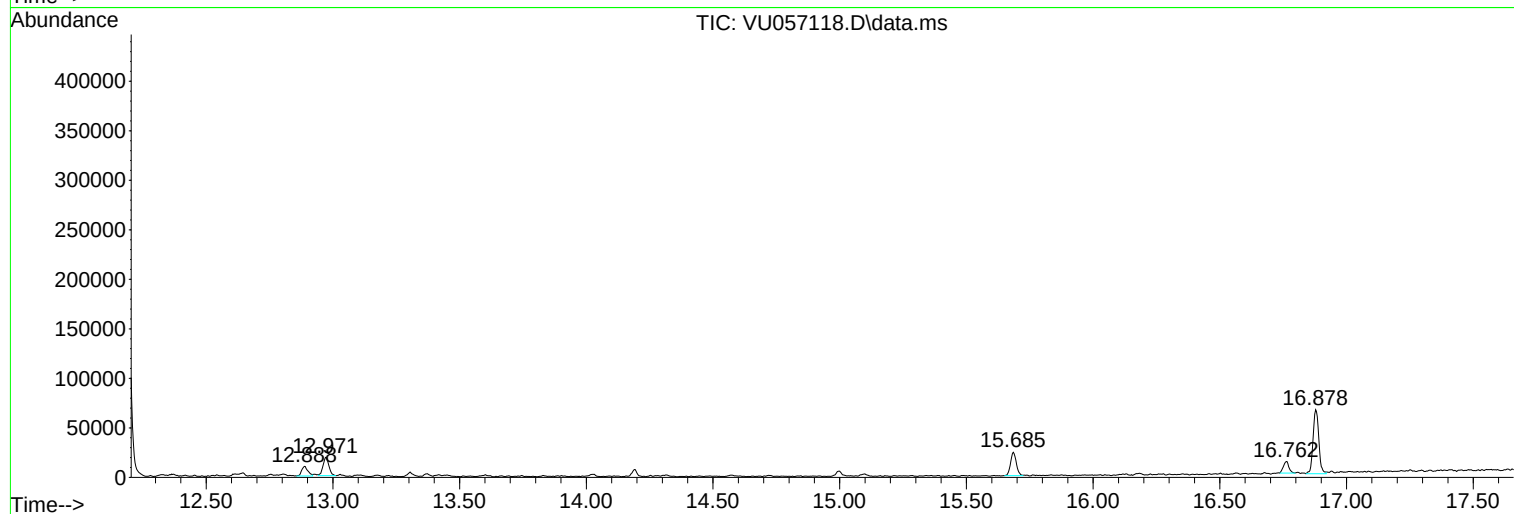
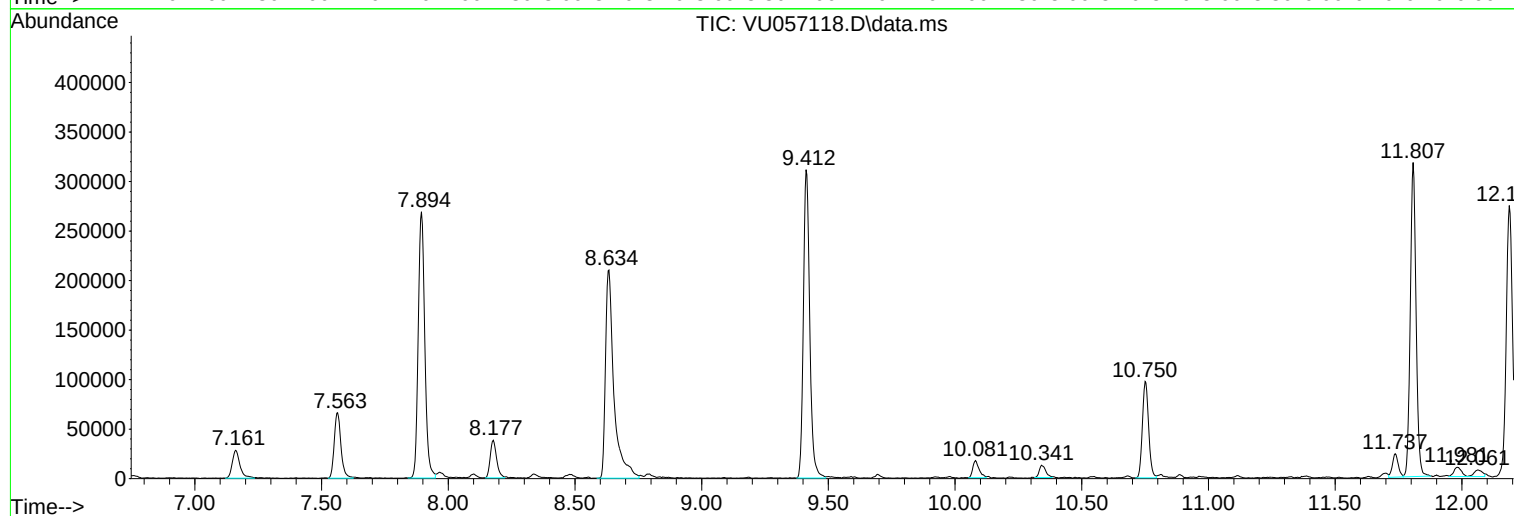
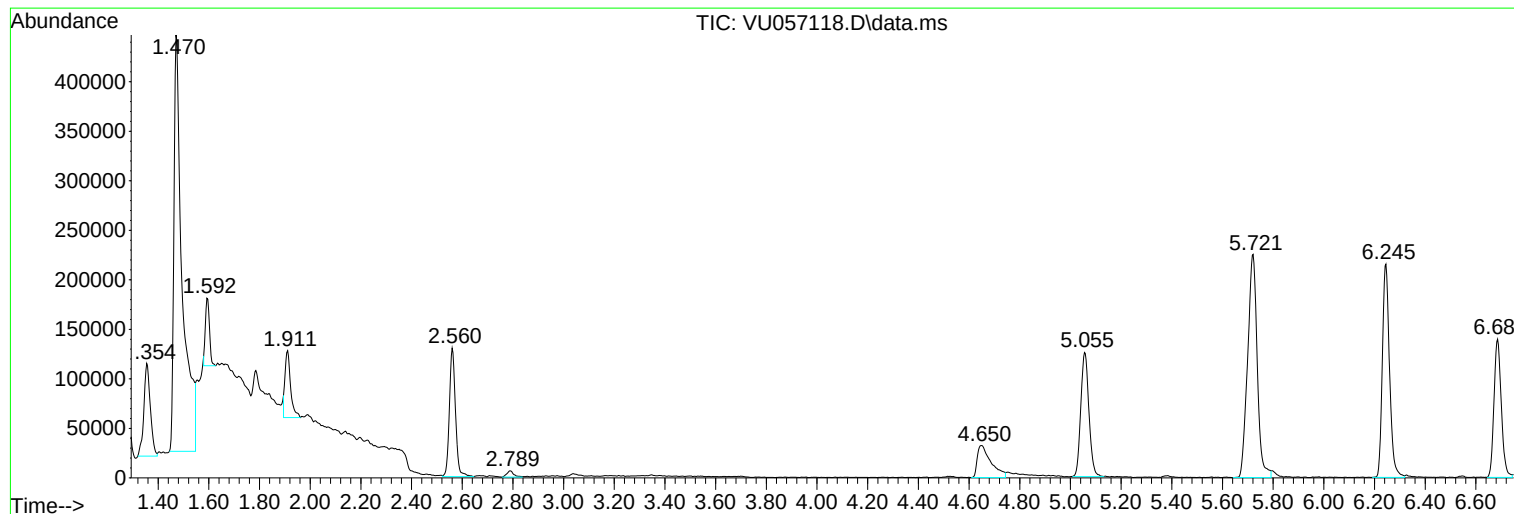
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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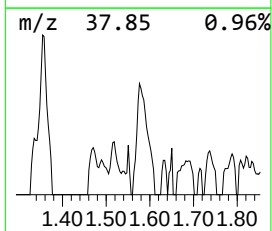
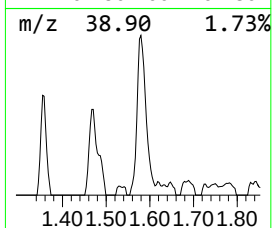
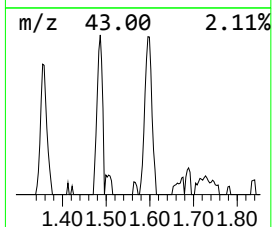
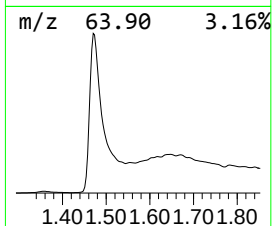
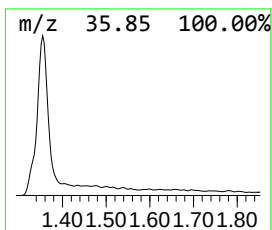
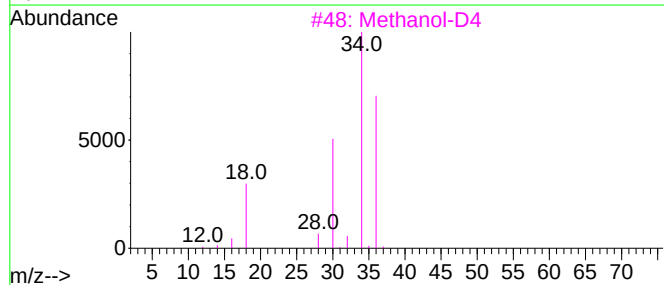
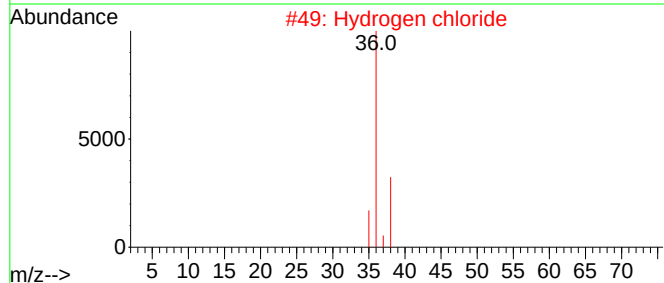
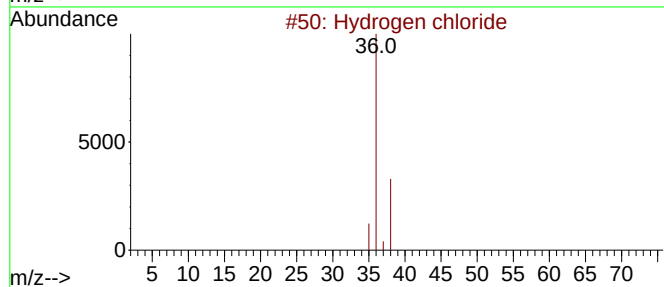
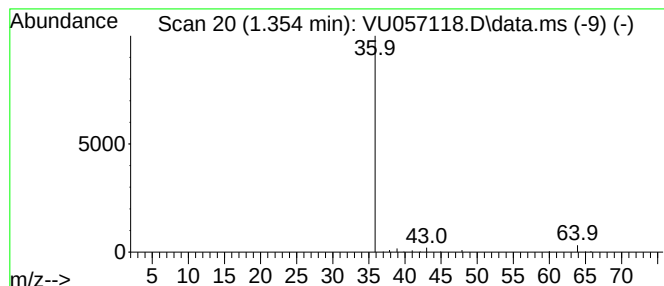
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.354	1.96 ug/L	166171	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hydrogen chloride	36	ClH	007647-01-0	2
2		Hydrogen chloride	36	ClH	007647-01-0	2
3		Methanol-D4	36	CD4O	000811-98-3	2
4		Ammonium Chloride	53	ClH4N	012125-02-9	1
5		2-Chloroethylamine	79	C2H6ClN	000689-98-5	1



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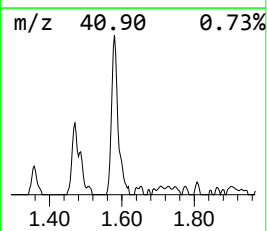
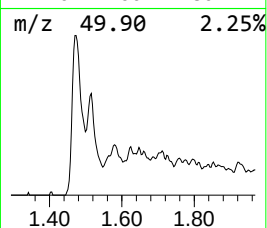
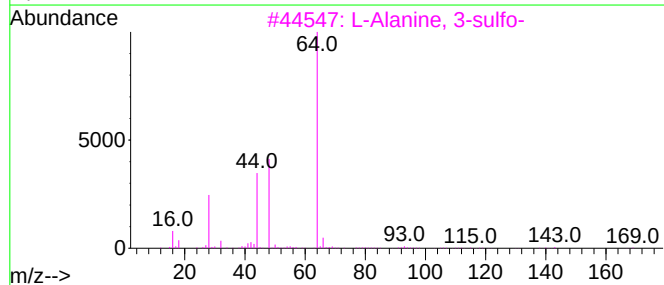
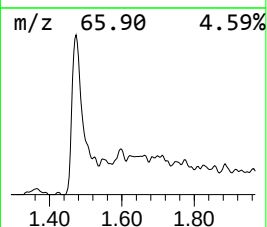
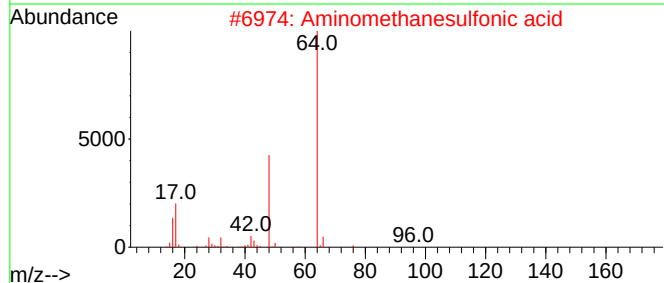
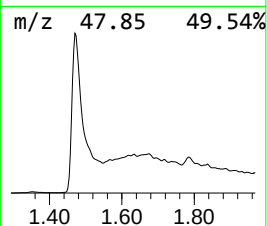
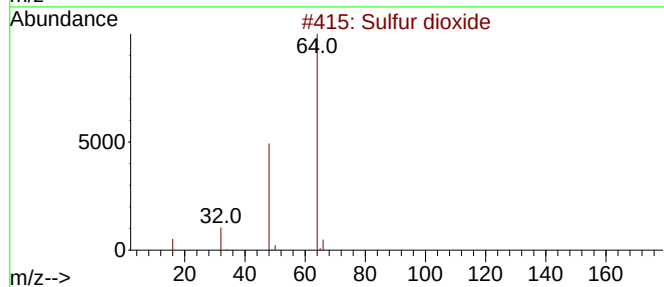
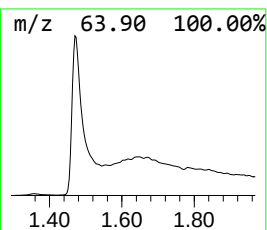
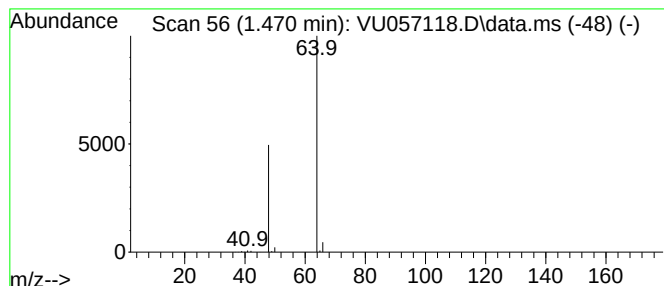
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.470	11.50 ug/L	976689	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	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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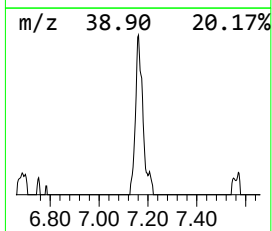
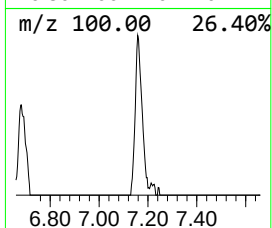
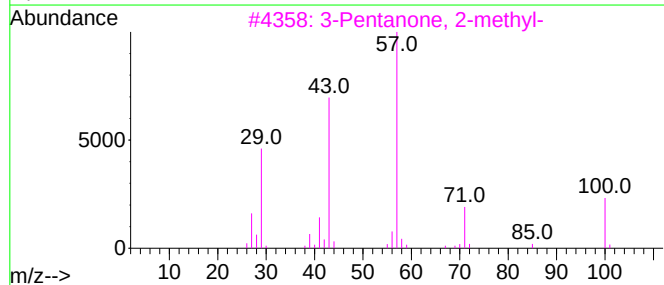
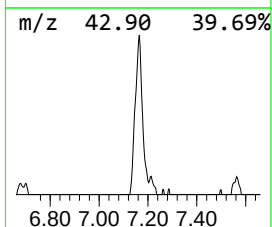
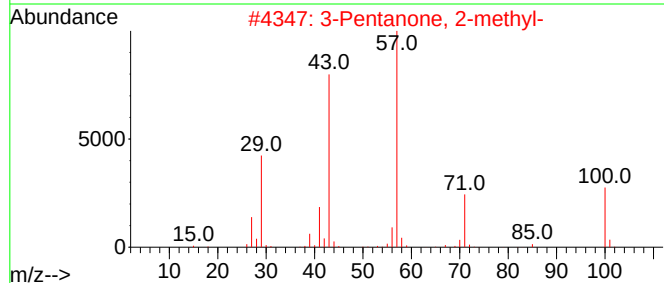
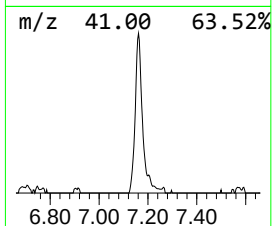
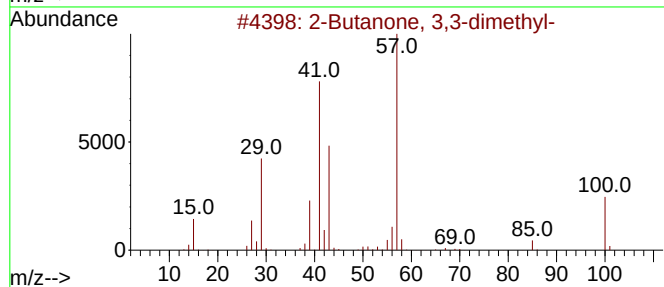
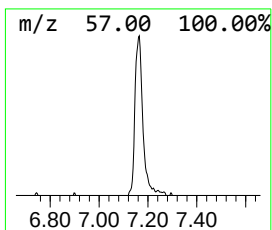
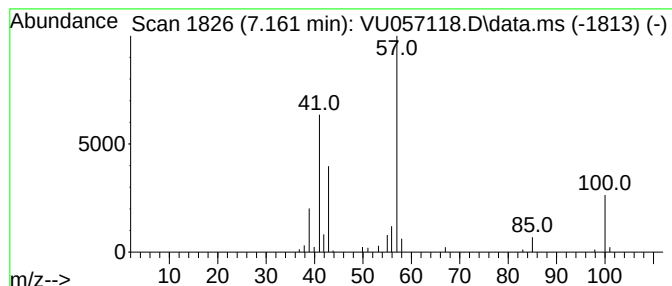
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	0.69 ug/L	58989	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	91	
2	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	80	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	80	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	80	
5	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	80	



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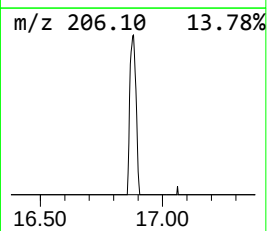
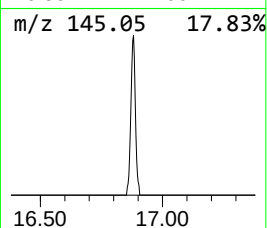
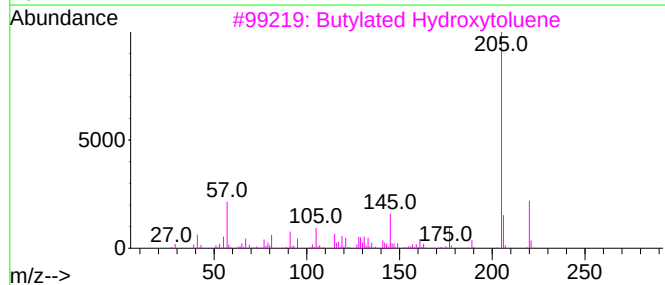
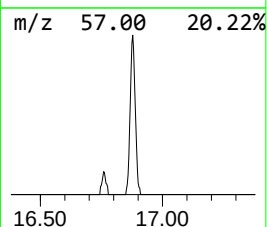
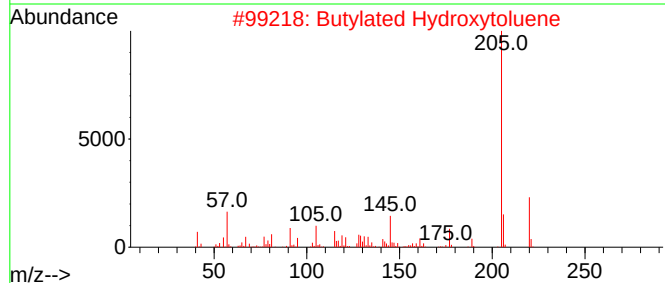
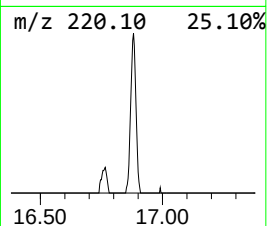
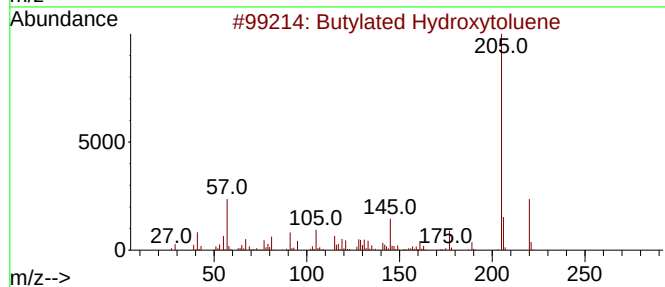
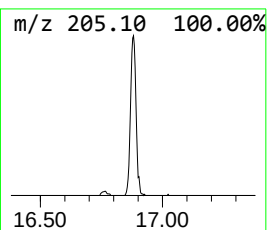
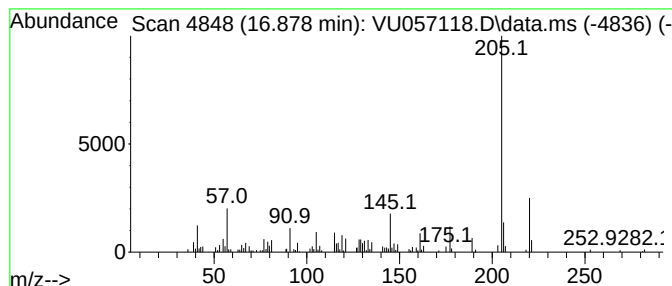
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butylated Hydroxytoluene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.878	1.00 ug/L	101369	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.354	2.0	ug/L	166171	1	6.245	424741	5.0
Sulfur dioxide	1.470	11.5	ug/L	976689	1	6.245	424741	5.0
2-Butanone, 3,3...	7.161	0.7	ug/L	58989	1	6.245	424741	5.0
Butylated Hydro...	16.878	1.0	ug/L	101369	3	11.807	507100	5.0