

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
 Data File : VU057119.D
 Acq On : 21 Dec 2023 03:20
 Operator : MD/SY
 Sample : 05892-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B08

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: VU057119.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	rVB2	44585	84596	5.14%	1.170%
2	1.473	48	57	87	rBV	459103	1647230	100.00%	22.789%
3	1.592	91	94	104	rVB	83598	121430	7.37%	1.680%
4	1.911	188	193	207	rVB	70909	97806	5.94%	1.353%
5	2.560	383	395	410	rVB	130363	216542	13.15%	2.996%
6	4.653	1034	1046	1079	rBV2	29171	133938	8.13%	1.853%
7	5.055	1156	1171	1194	rBV	127106	289581	17.58%	4.006%
8	5.721	1359	1378	1416	rVB2	230736	602380	36.57%	8.334%
9	6.245	1528	1541	1562	rBV	229311	447447	27.16%	6.190%
10	6.685	1665	1678	1697	rBV2	138993	279910	16.99%	3.872%
11	7.165	1814	1827	1844	rBV3	25126	55173	3.35%	0.763%
12	7.563	1940	1951	1969	rBV2	64516	120155	7.29%	1.662%
13	7.894	2042	2054	2072	rBV	271389	476322	28.92%	6.590%
14	8.177	2130	2142	2155	rBV3	38475	68293	4.15%	0.945%
15	8.634	2273	2284	2320	rBV	216981	485732	29.49%	6.720%
16	9.412	2515	2526	2550	rBV	315042	560581	34.03%	7.755%
17	10.078	2723	2733	2756	rVB2	20922	39353	2.39%	0.544%
18	10.344	2808	2816	2836	rVB8	9475	18428	1.12%	0.255%
19	10.753	2929	2943	2960	rBV	100870	170290	10.34%	2.356%
20	11.692	3226	3235	3241	rBV10	10110	16873	1.02%	0.233%
21	11.737	3241	3249	3258	rVV4	27490	45928	2.79%	0.635%
22	11.807	3259	3271	3295	rVB	328179	539508	32.75%	7.464%
23	12.190	3370	3390	3412	rVB	276201	485702	29.49%	6.719%
24	12.891	3598	3608	3619	rBV5	9246	17568	1.07%	0.243%
25	12.971	3623	3633	3643	rVB9	12189	18825	1.14%	0.260%
26	14.190	4003	4012	4021	rVB6	14211	21919	1.33%	0.303%
27	15.685	4467	4477	4487	rBV6	27323	43450	2.64%	0.601%
28	16.881	4839	4849	4861	rBV	83060	123348	7.49%	1.706%

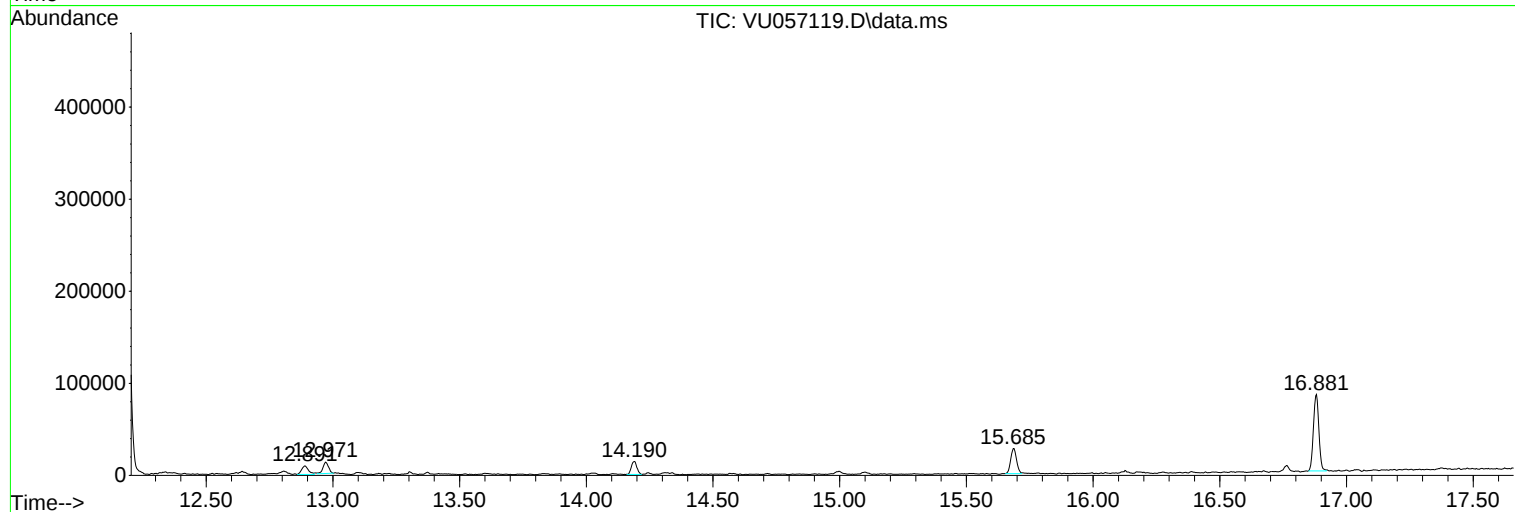
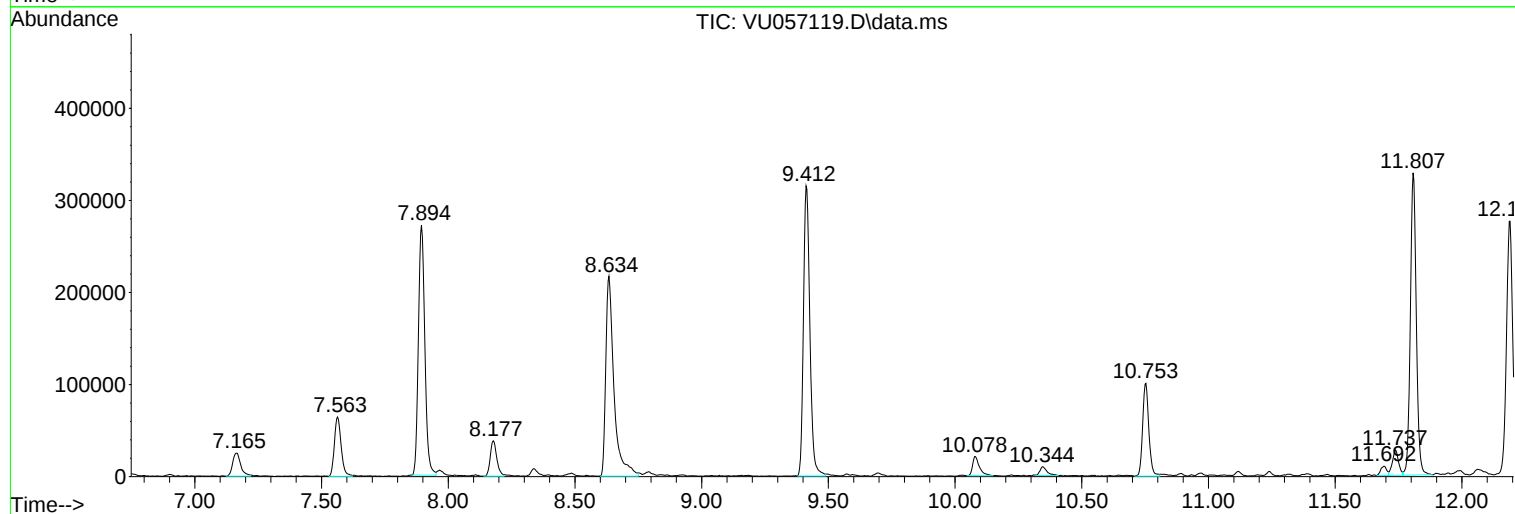
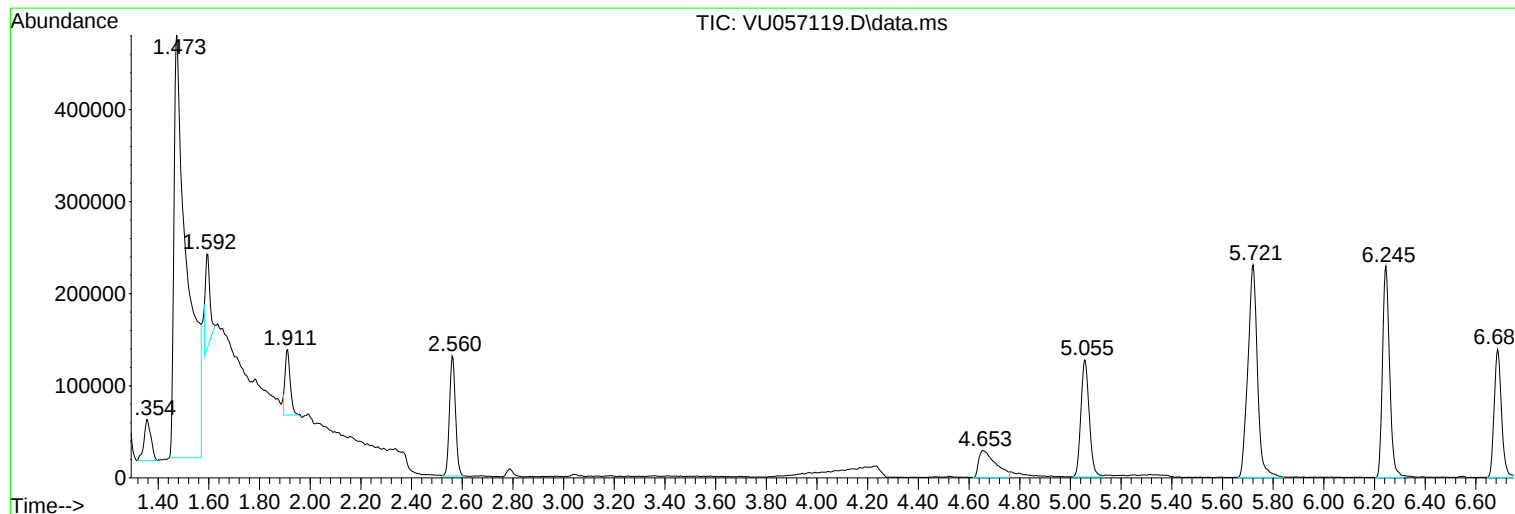
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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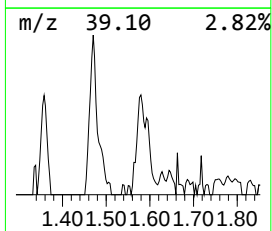
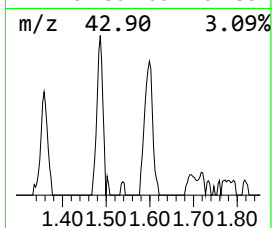
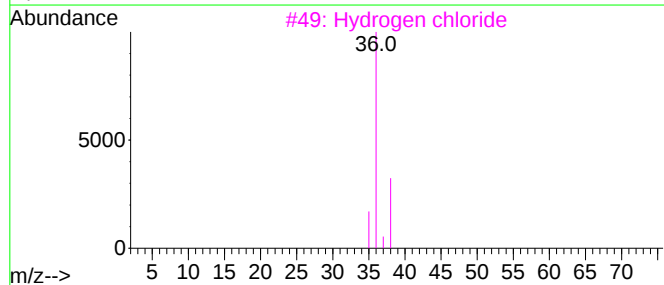
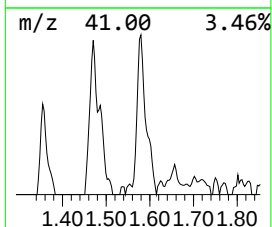
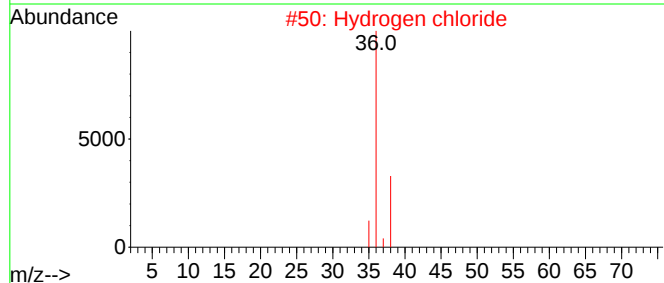
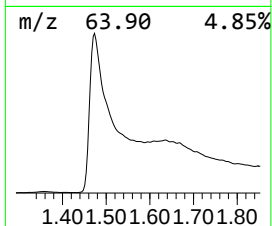
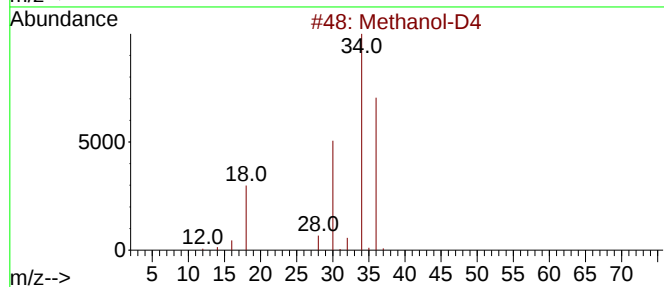
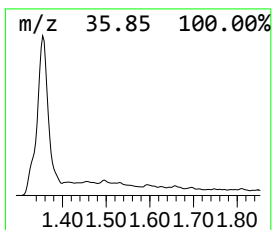
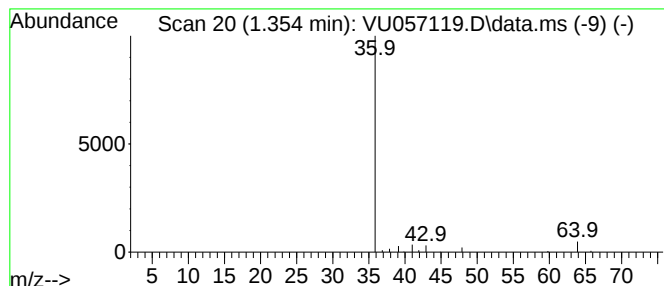
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.354	0.95 ug/L	84596	1,4-Difluorobenzene	6.245

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



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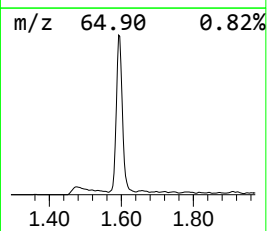
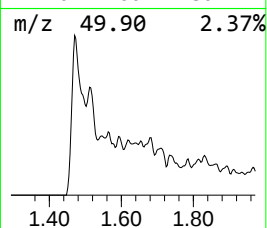
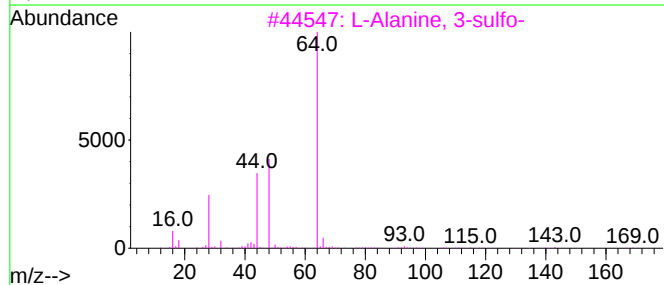
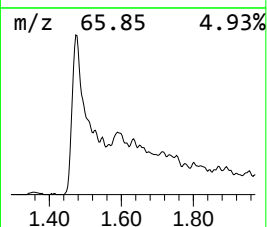
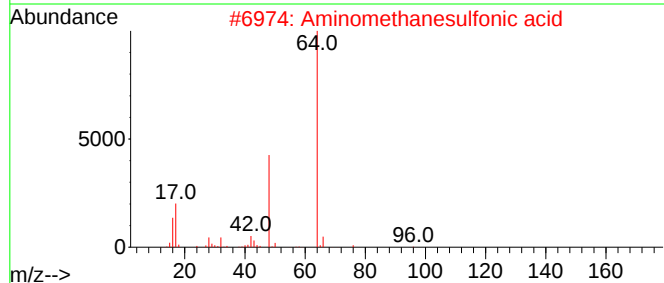
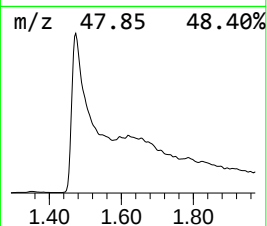
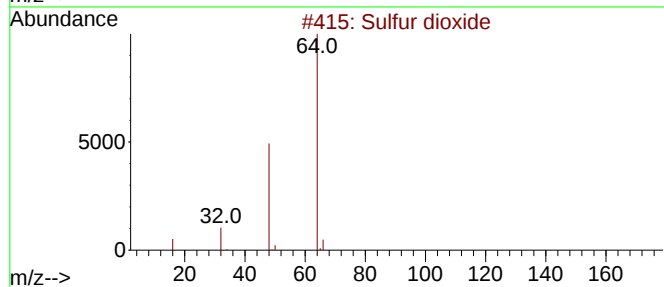
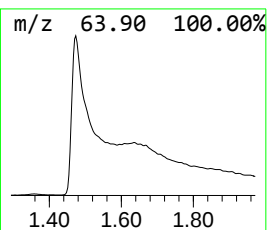
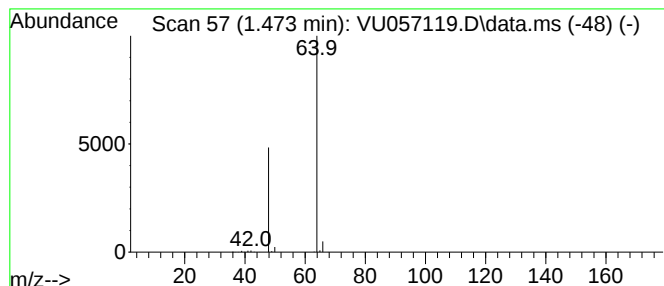
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.473	18.41 ug/L	1647230	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
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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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

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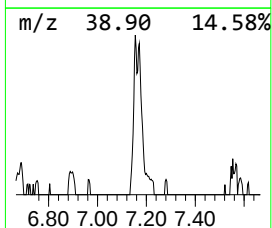
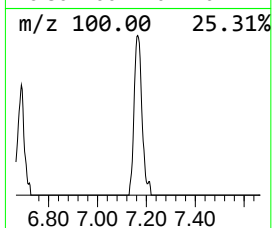
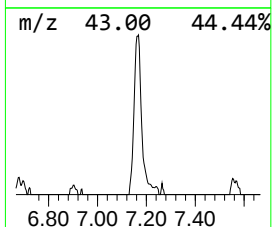
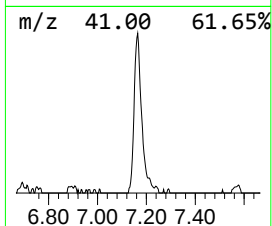
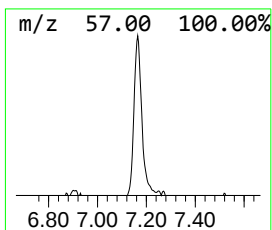
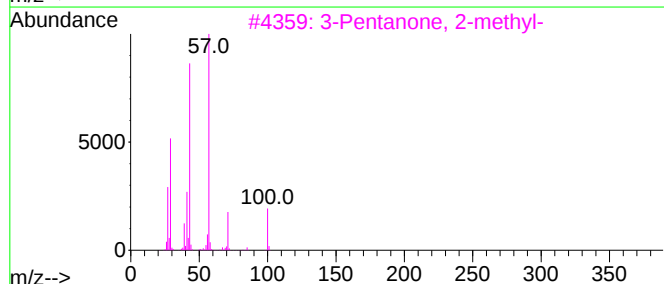
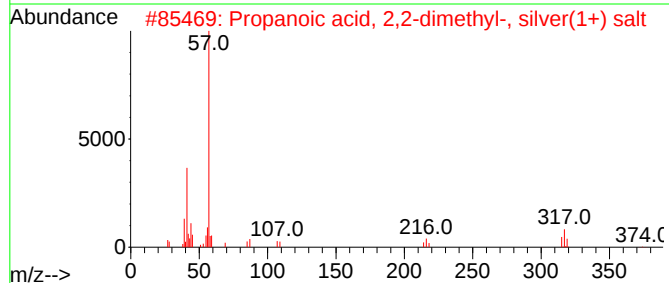
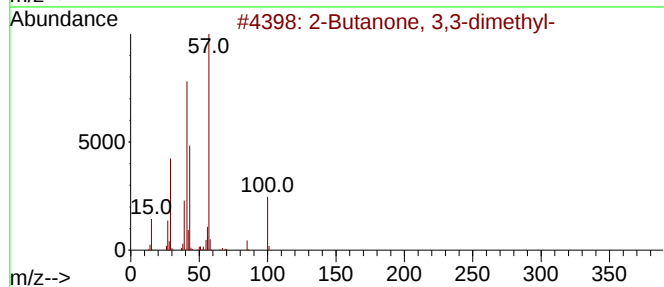
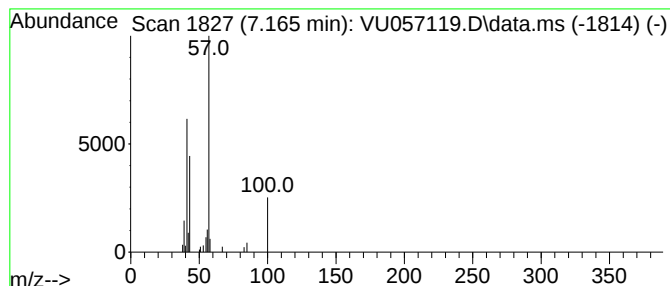
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.165	0.62 ug/L	55173	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	Propanoic acid, 2,2-dimethyl-, s...		208	C5H9AgO2		007324-58-5	50
3	3-Pentanone, 2-methyl-		100	C6H12O		000565-69-5	45
4	Propane, 2-methyl-2-nitro-		103	C4H9NO2		000594-70-7	43
5	2-Butanone, 3,3-dimethyl-		100	C6H12O		000075-97-8	42



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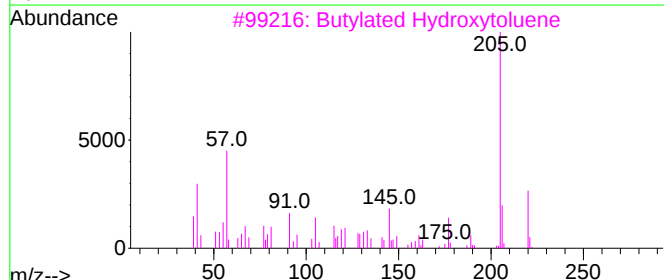
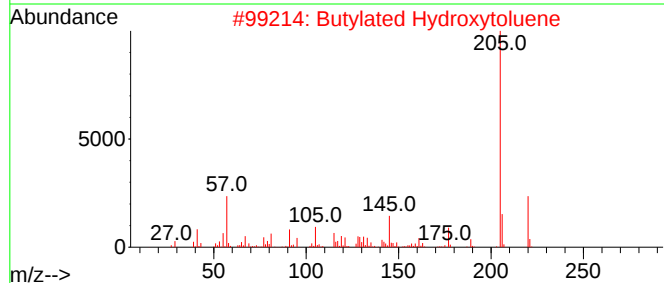
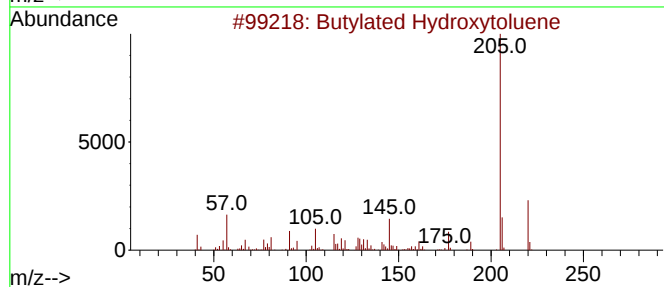
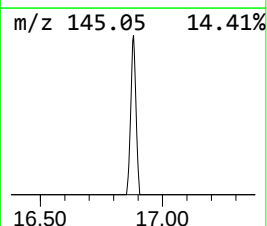
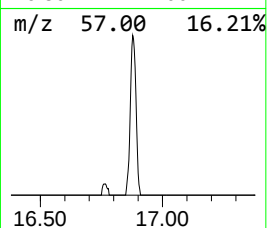
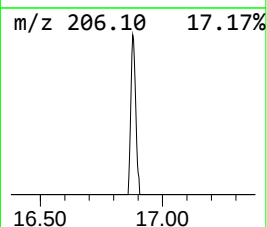
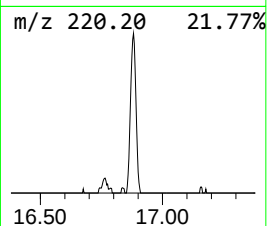
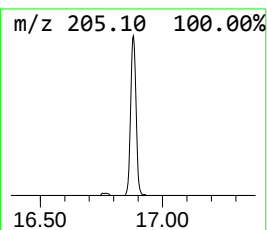
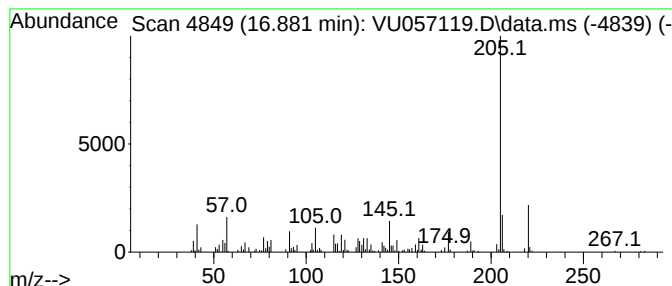
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.881	1.14 ug/L	123348	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	91
4			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	90
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.354	0.9	ug/L	84596	1	6.245	447447	5.0
Sulfur dioxide	1.473	18.4	ug/L	1647230	1	6.245	447447	5.0
2-Butanone, 3,3...	7.165	0.6	ug/L	55173	1	6.245	447447	5.0
Butylated Hydro...	16.881	1.1	ug/L	123348	3	11.807	539508	5.0