

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
 Data File : VU057116.D
 Acq On : 21 Dec 2023 01:20
 Operator : MD/SY
 Sample : 05892-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B00

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: VU057116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	17	26	32	rBV	33826	50838	8.15%	0.816%
2	1.486	58	61	63	rBV	10248	7665	1.23%	0.123%
3	1.554	63	82	87	rBV2	116609	367303	58.86%	5.893%
4	1.596	91	95	106	rVB	102586	150328	24.09%	2.412%
5	1.911	188	193	202	rVB	66950	87487	14.02%	1.404%
6	2.563	384	396	410	rVB	136565	229662	36.81%	3.685%
7	2.792	452	467	479	rBV	12396	22259	3.57%	0.357%
8	3.354	635	642	656	rVB8	3825	8341	1.34%	0.134%
9	4.650	1032	1045	1063	rBV2	35454	125374	20.09%	2.012%
10	5.055	1155	1171	1194	rBV	129954	291498	46.72%	4.677%
11	5.718	1358	1377	1412	rBV2	236645	623980	100.00%	10.012%
12	6.242	1528	1540	1567	rBV	216829	429739	68.87%	6.895%
13	6.541	1620	1633	1647	rBV4	4817	9240	1.48%	0.148%
14	6.685	1663	1678	1694	rBV	146179	289991	46.47%	4.653%
15	7.161	1810	1826	1842	rBV3	51507	110423	17.70%	1.772%
16	7.563	1937	1951	1972	rBV	68310	125828	20.17%	2.019%
17	7.891	2041	2053	2070	rBV	274634	491388	78.75%	7.884%
18	7.965	2071	2076	2090	rVB3	9893	17790	2.85%	0.285%
19	8.177	2131	2142	2156	rBV3	39831	71309	11.43%	1.144%
20	8.335	2182	2191	2204	rBV3	10005	18210	2.92%	0.292%
21	8.480	2222	2236	2247	rBV9	8267	20523	3.29%	0.329%
22	8.634	2269	2284	2304	rBV2	229509	487536	78.13%	7.822%
23	9.412	2514	2526	2552	rBV	310441	547457	87.74%	8.784%
24	9.570	2566	2575	2585	rBV2	6960	12263	1.97%	0.197%
25	9.692	2603	2613	2625	rVB4	4647	8093	1.30%	0.130%
26	10.078	2722	2733	2756	rVB	25514	48512	7.77%	0.778%
27	10.344	2805	2816	2828	rBV8	9930	17123	2.74%	0.275%
28	10.750	2931	2942	2956	rBV	102218	174116	27.90%	2.794%
29	10.888	2975	2985	2997	rVB4	10545	16767	2.69%	0.269%
30	11.692	3223	3235	3240	rBV10	5612	10158	1.63%	0.163%
31	11.737	3240	3249	3259	rVV4	27916	47789	7.66%	0.767%
32	11.807	3259	3271	3294	rVB	320364	525978	84.29%	8.439%
33	11.981	3315	3325	3338	rVB8	7764	15851	2.54%	0.254%
34	12.061	3338	3350	3367	rVV9	11121	30287	4.85%	0.486%
35	12.187	3368	3389	3411	rVB	284011	498406	79.88%	7.997%
36	12.891	3600	3608	3618	rBV9	7272	13272	2.13%	0.213%

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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

37	12.971	3624	3633	3646	rVB5	20818	33296	5.34%	0.534%
38	13.303	3728	3736	3743	rBV7	5382	6927	1.11%	0.111%
39	14.190	4004	4012	4020	rBV6	10800	14510	2.33%	0.233%
40	14.994	4254	4262	4270	rBV8	5526	8789	1.41%	0.141%
41	15.685	4466	4477	4488	rBV7	19392	31608	5.07%	0.507%
42	16.762	4803	4812	4821	rBV7	8806	12814	2.05%	0.206%
43	16.878	4838	4848	4861	rBV2	78943	121758	19.51%	1.954%

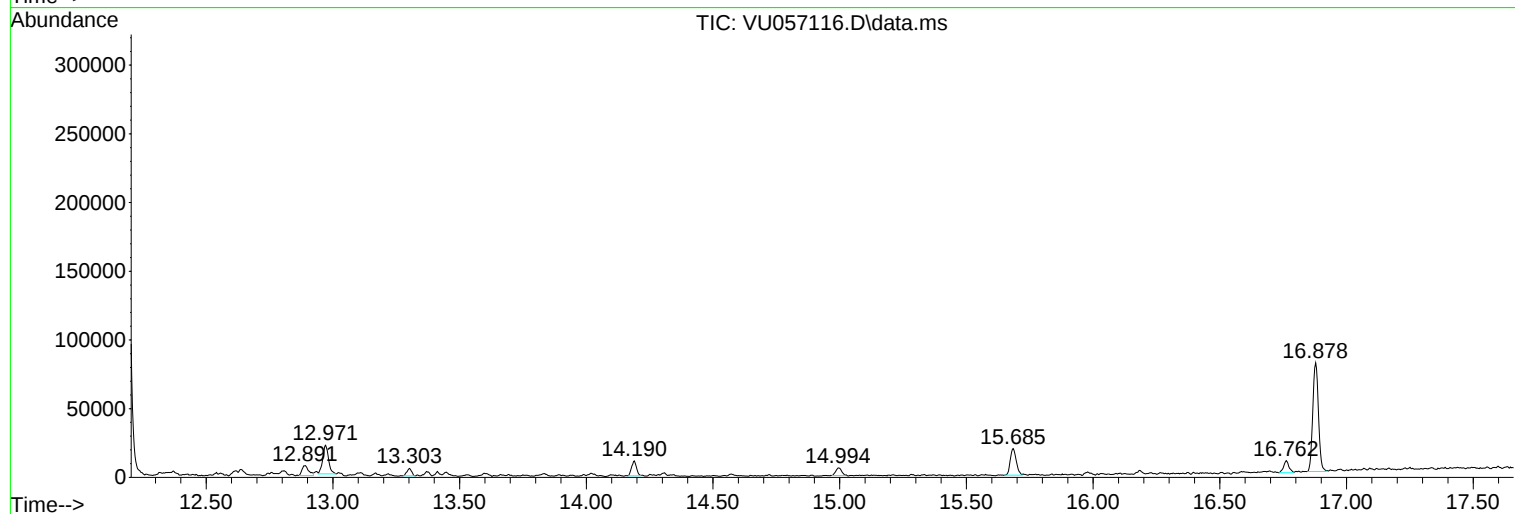
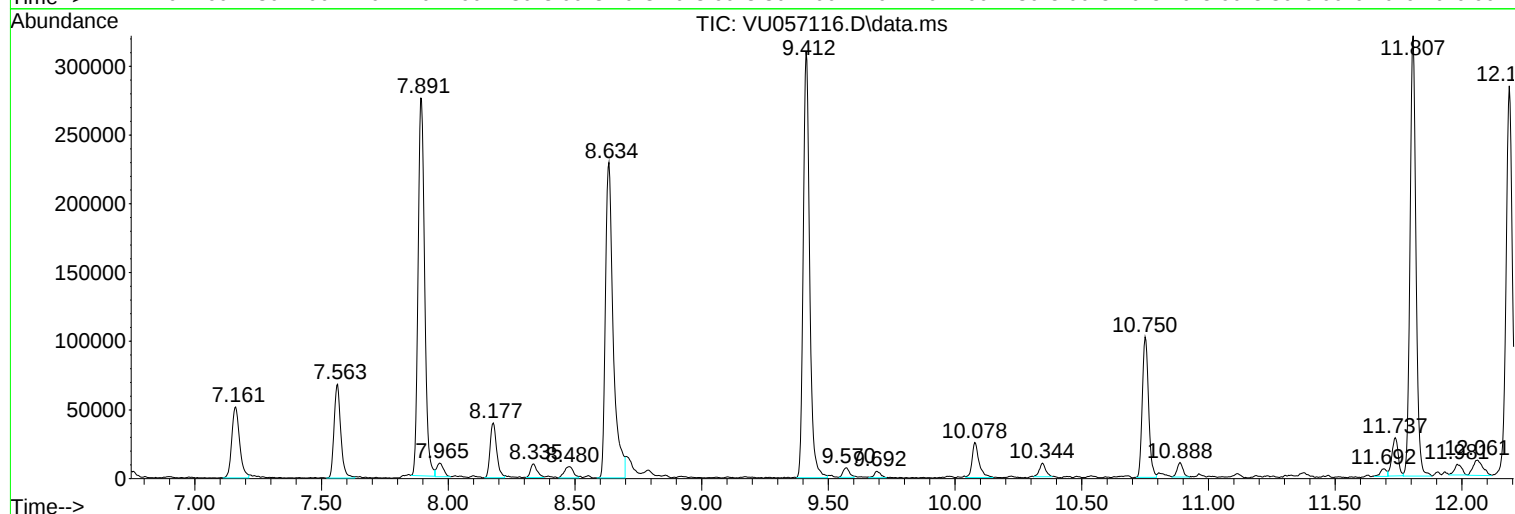
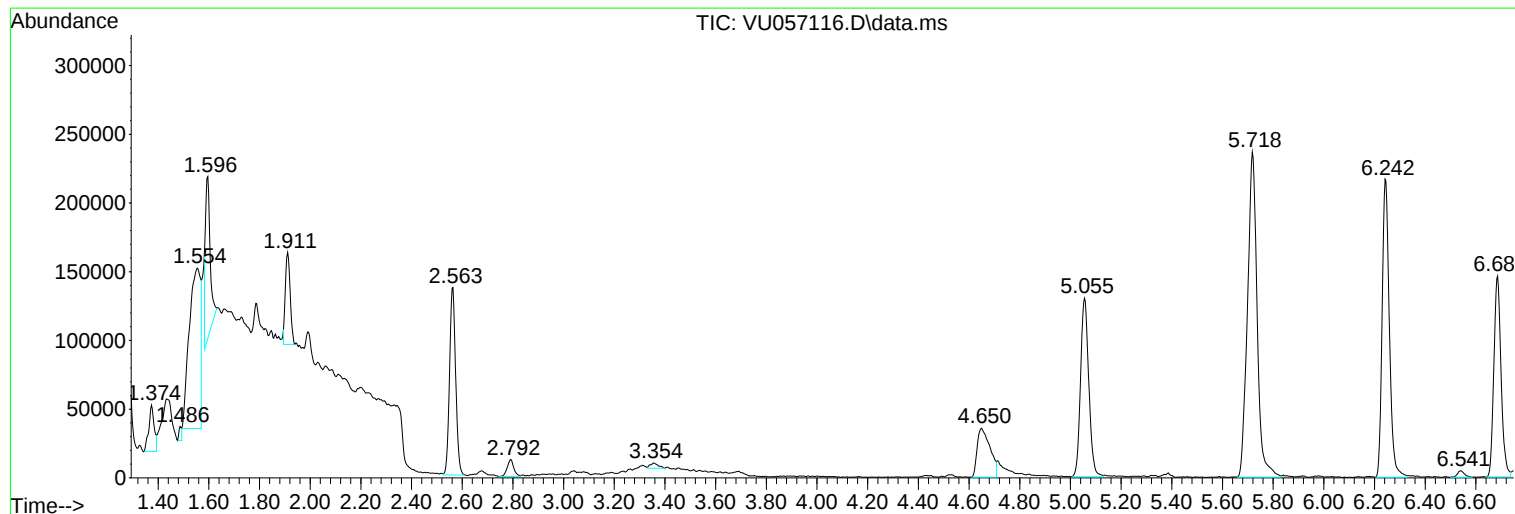
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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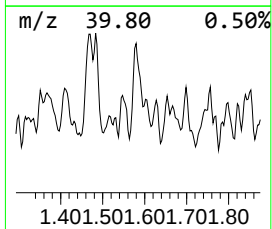
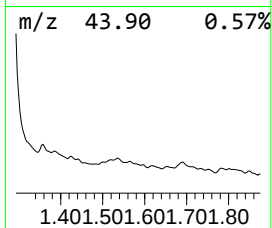
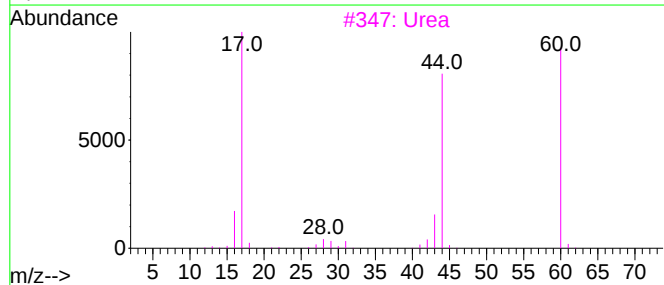
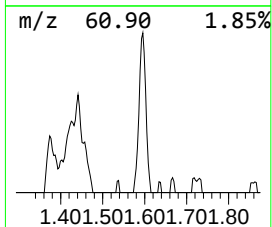
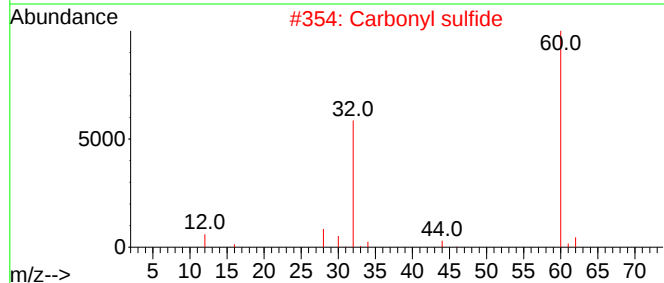
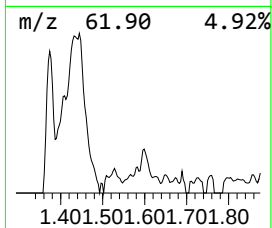
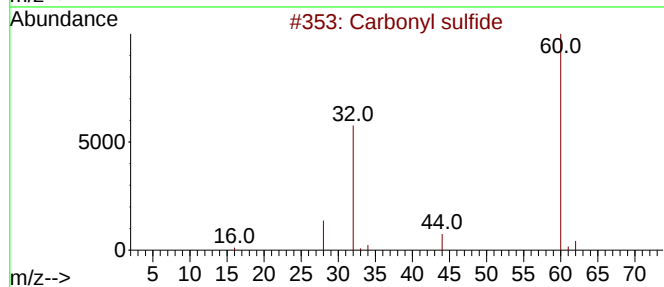
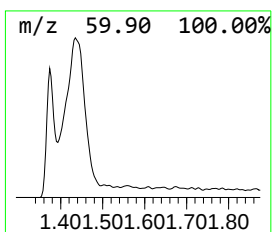
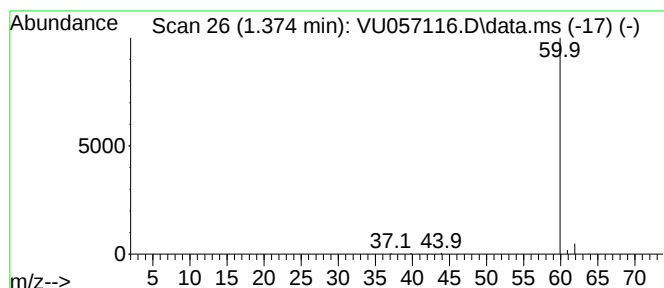
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	0.59 ug/L	50838	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonyl sulfide	60	COS	000463-58-1	5
2			Carbonyl sulfide	60	COS	000463-58-1	5
3			Urea	60	CH4N2O	000057-13-6	4
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	4
5			Formamidoxime	60	CH4N2O	000624-82-8	4



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
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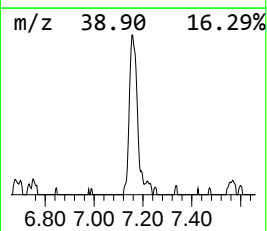
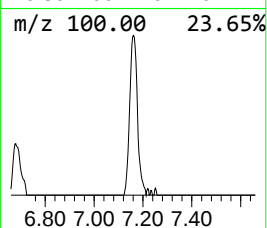
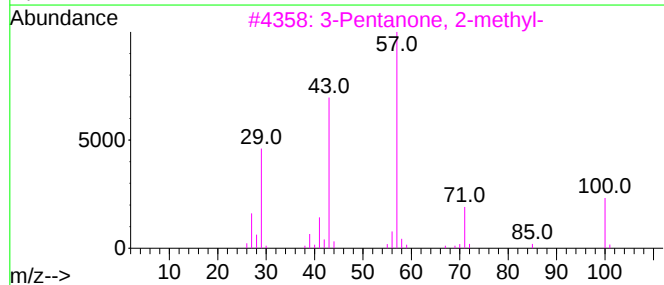
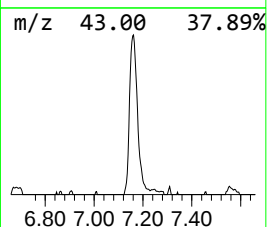
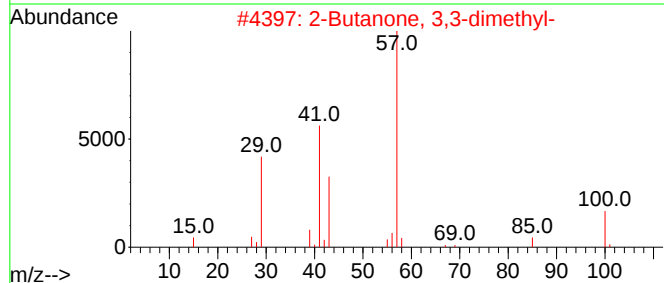
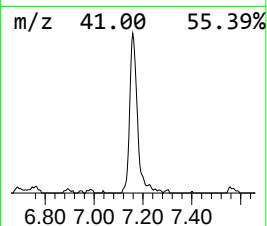
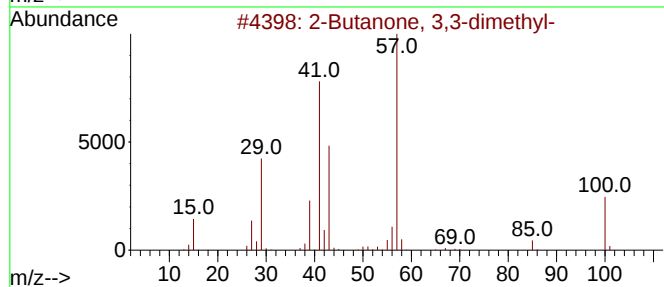
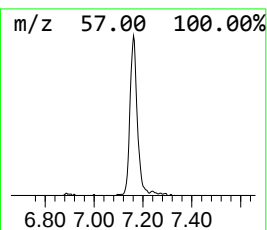
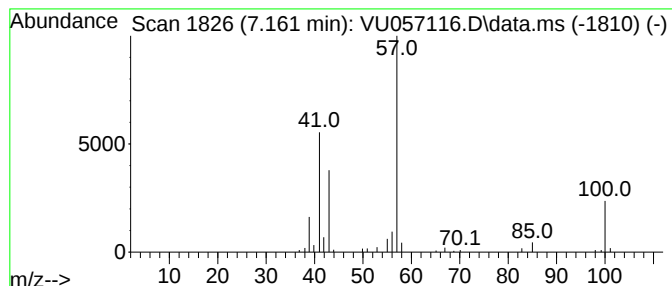
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.161	1.28 ug/L	110423	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	91
2	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	91
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	59
4	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	58
5	3-Hexanone			100	C6H12O	000589-38-8	50



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F7B00

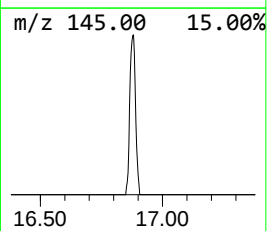
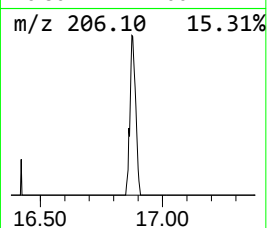
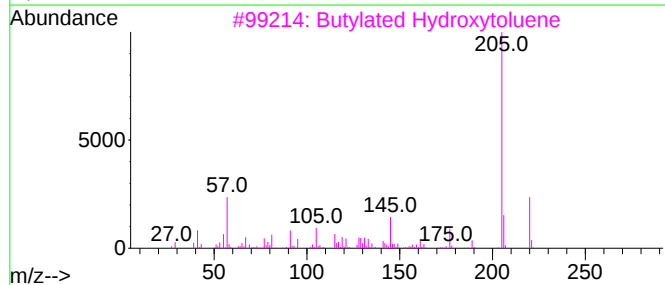
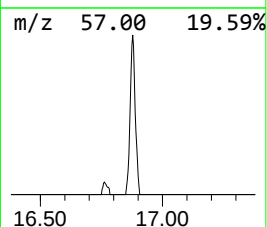
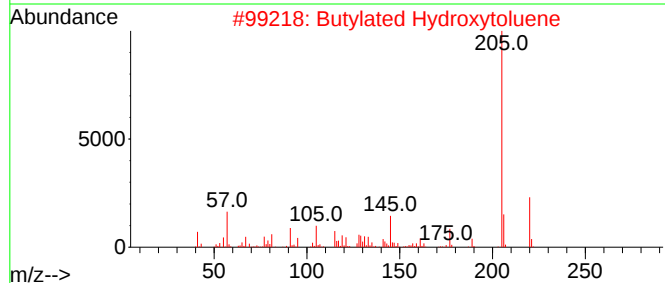
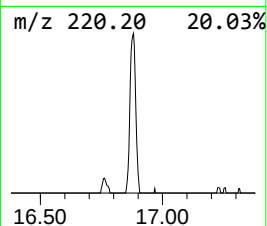
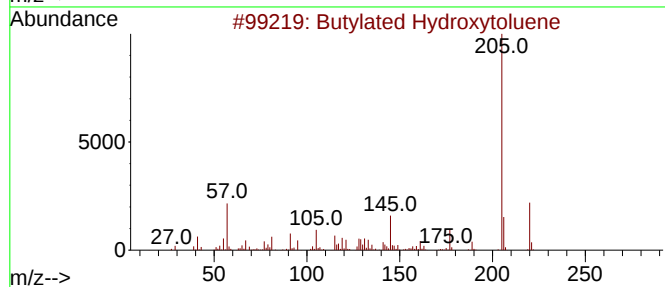
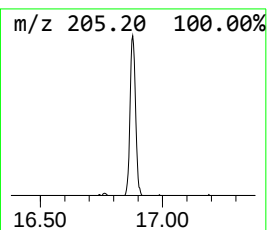
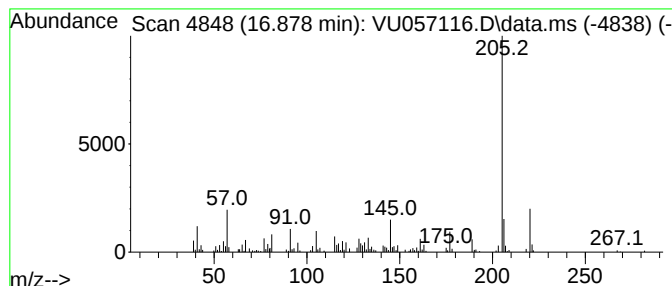
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.878	1.16 ug/L	121758	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96



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ALS Vial : 41 Sample Multiplier: 1

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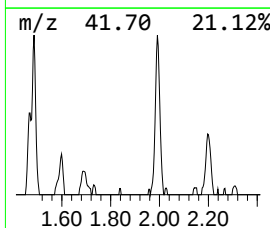
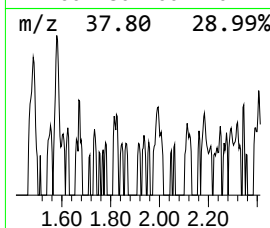
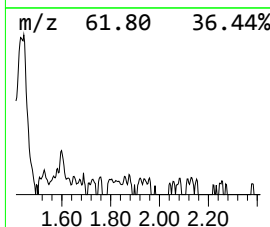
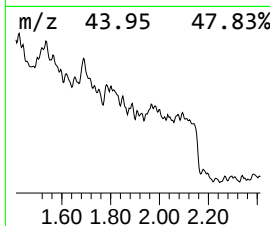
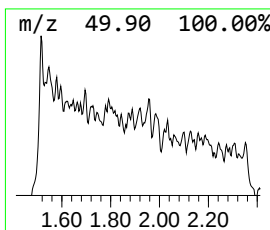
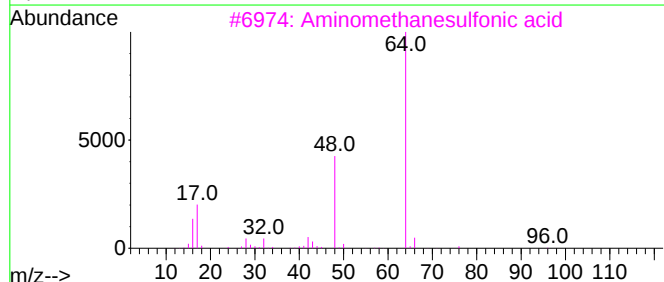
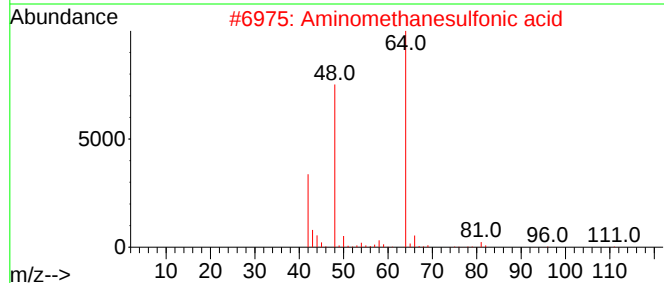
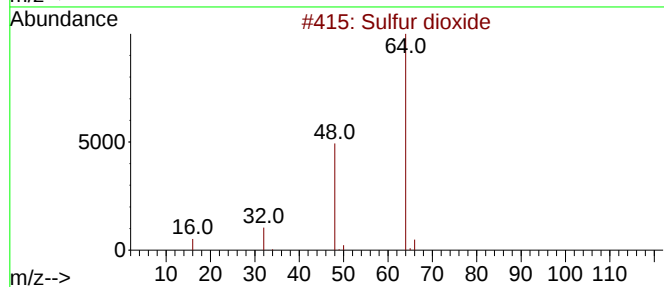
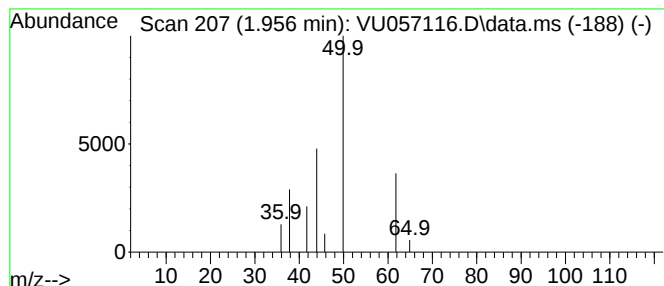
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.911	1.02 ug/L	87487	1,4-Difluorobenzene	6.242

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.374	0.6	ug/L	50838	1	6.242	429739	5.0
2-Butanone, 3,3...	7.161	1.3	ug/L	110423	1	6.242	429739	5.0
Butylated Hydro...	16.878	1.2	ug/L	121758	3	11.807	525978	5.0
Sulfur dioxide	1.911	1.0	ug/L	87487	1	6.242	429739	5.0