

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
 Data File : VU052360.D
 Acq On : 12 Dec 2022 18:08
 Operator : JC/MD
 Sample : N5961-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5N34

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\SFAMUTR111822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052360.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.379	6	12	21	rBV	38091	48720	4.06%	0.501%
2	1.600	43	81	92	rBV2	244730	1059682	88.21%	10.905%
3	1.916	174	179	200	rVB	116041	167434	13.94%	1.723%
4	2.568	370	382	398	rVB	194812	317571	26.43%	3.268%
5	2.687	403	419	426	rBV7	8661	21312	1.77%	0.219%
6	2.793	444	452	465	rVB	14408	24788	2.06%	0.255%
7	4.649	1012	1029	1082	rBV2	99499	480193	39.97%	4.941%
8	5.060	1141	1157	1180	rBV	174877	386969	32.21%	3.982%
9	5.723	1342	1363	1378	rBV2	352245	927321	77.19%	9.543%
10	5.793	1379	1385	1402	rVB2	31819	64645	5.38%	0.665%
11	6.247	1512	1526	1550	rBV	280738	542500	45.16%	5.583%
12	6.687	1640	1663	1680	rBV	222784	446600	37.18%	4.596%
13	7.166	1789	1812	1830	rBV2	22242	54078	4.50%	0.556%
14	7.565	1921	1936	1955	rBV2	93165	167736	13.96%	1.726%
15	7.896	2024	2039	2053	rBV	397007	694116	57.78%	7.143%
16	7.967	2054	2061	2076	rVB	25888	46842	3.90%	0.482%
17	8.176	2114	2126	2139	rBV	60213	102747	8.55%	1.057%
18	8.488	2212	2223	2232	rBV3	7412	14152	1.18%	0.146%
19	8.636	2255	2269	2306	rBV	571435	1201338	100.00%	12.362%
20	8.787	2308	2316	2328	rVB5	12240	22987	1.91%	0.237%
21	9.414	2499	2511	2538	rBV	423296	710454	59.14%	7.311%
22	9.976	2676	2686	2704	rBV2	14972	28345	2.36%	0.292%
23	10.539	2850	2861	2874	rBV4	11197	19058	1.59%	0.196%
24	10.681	2896	2905	2913	rBV2	10610	17007	1.42%	0.175%
25	10.754	2913	2928	2944	rVB	204952	343821	28.62%	3.538%
26	11.684	3207	3217	3227	rBV7	14051	21739	1.81%	0.224%
27	11.809	3243	3256	3282	rBV	392475	644491	53.65%	6.632%
28	12.002	3302	3316	3324	rVB3	11680	19749	1.64%	0.203%
29	12.057	3324	3333	3345	rBV2	31020	56532	4.71%	0.582%
30	12.188	3361	3374	3392	rBV	414312	676928	56.35%	6.966%
31	12.883	3580	3590	3600	rBV4	19556	30589	2.55%	0.315%
32	15.687	4453	4462	4479	rVB5	27959	47465	3.95%	0.488%
33	16.767	4787	4798	4815	rBV2	129097	223976	18.64%	2.305%
34	16.883	4825	4834	4844	rBV	57781	85910	7.15%	0.884%

Sum of corrected areas: 9717795

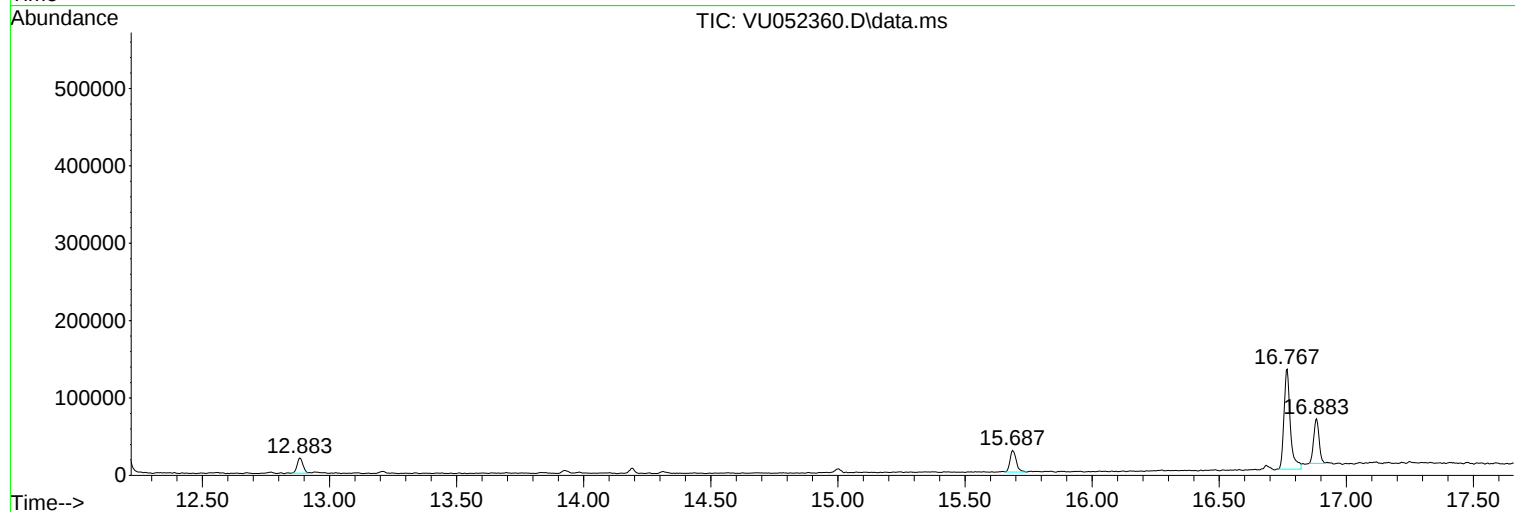
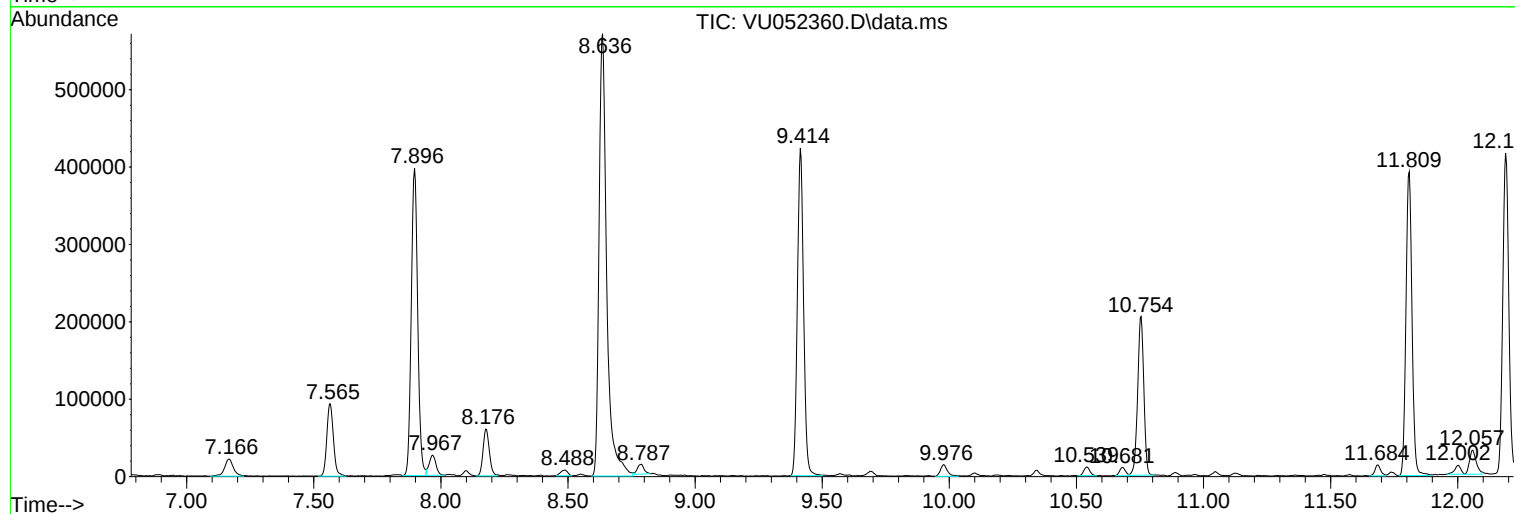
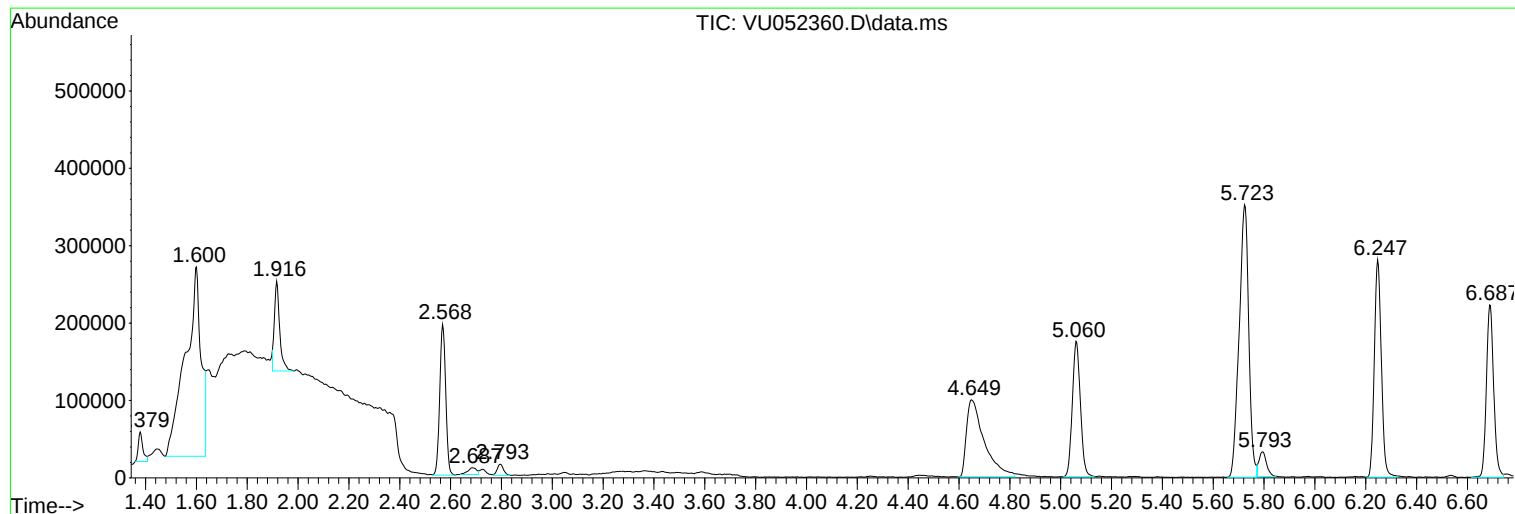
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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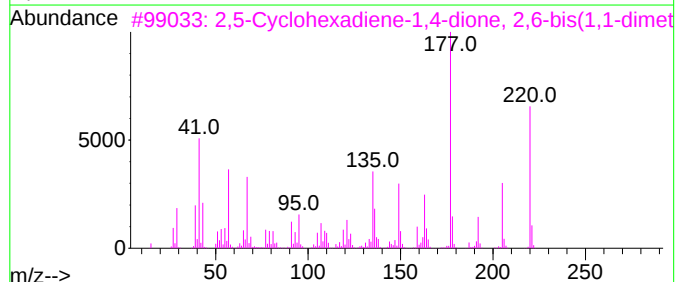
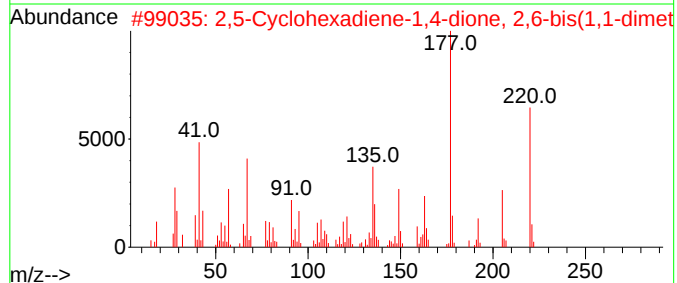
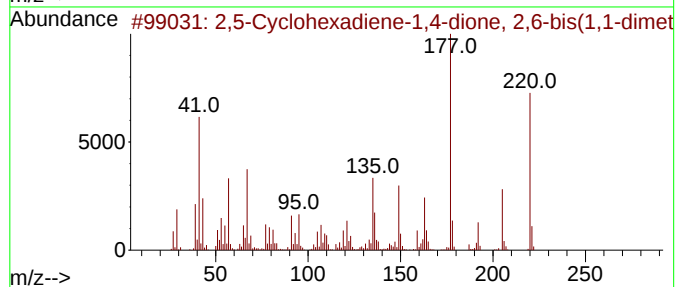
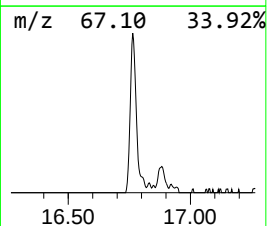
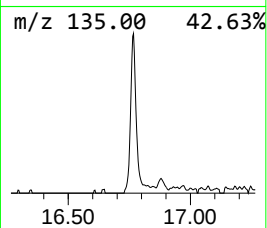
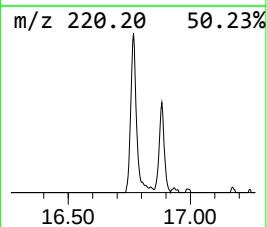
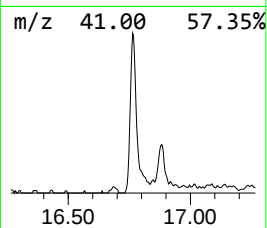
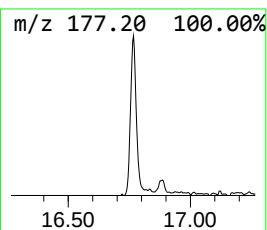
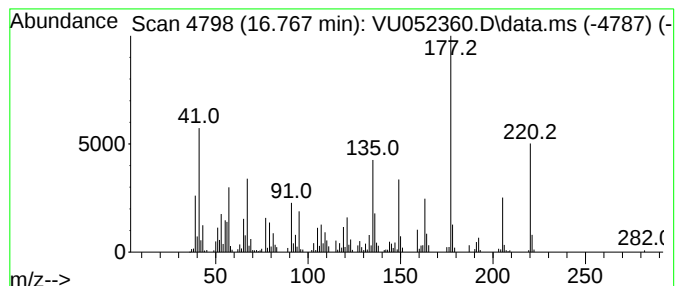
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.767	1.74 ug/L	223976	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	83		



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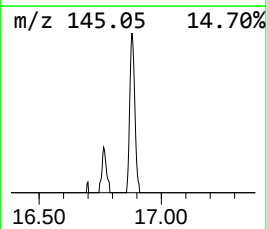
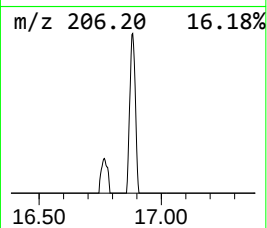
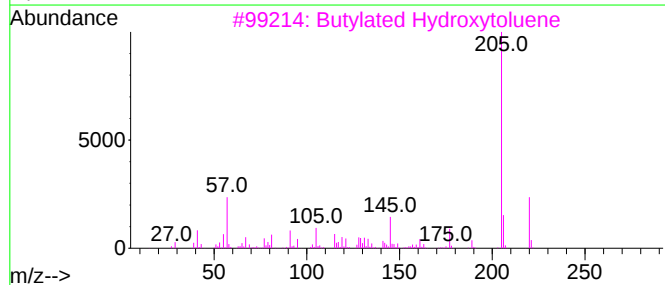
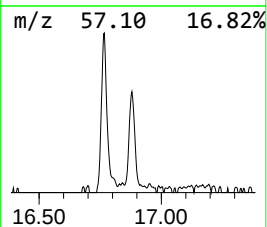
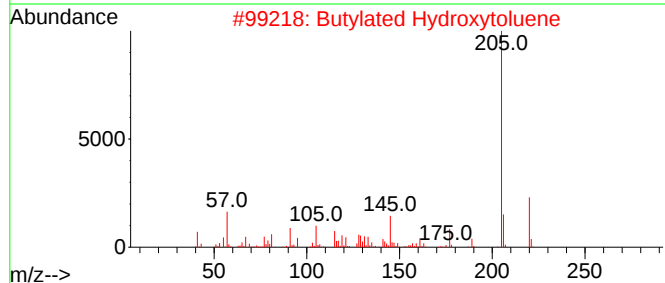
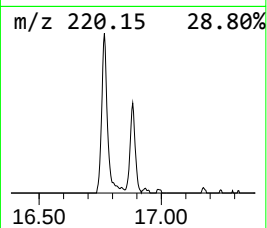
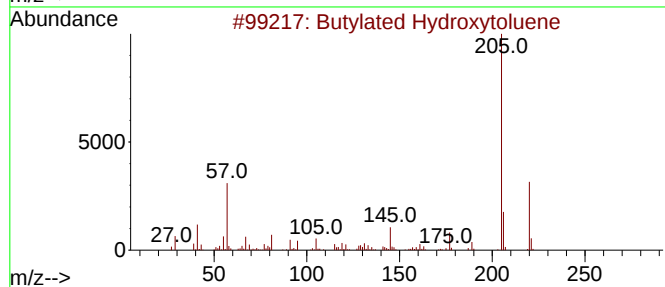
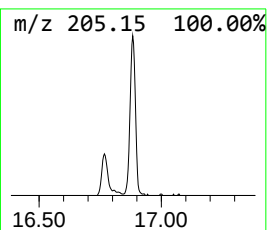
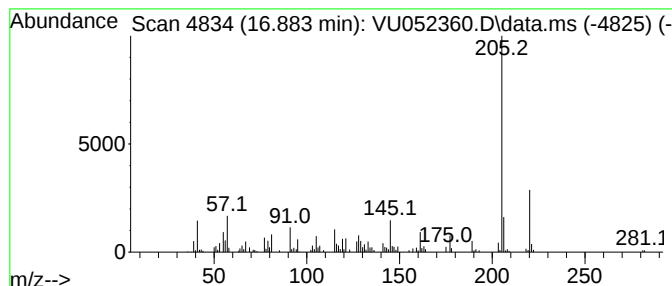
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	0.67 ug/L	85910	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
4			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	91
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	91



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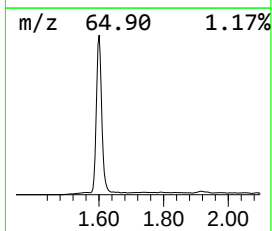
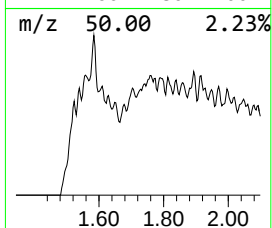
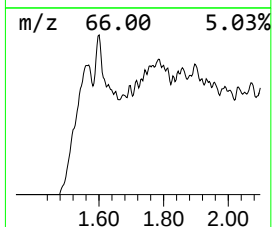
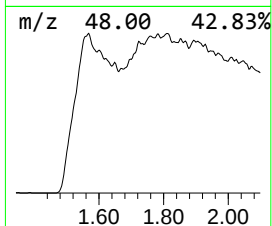
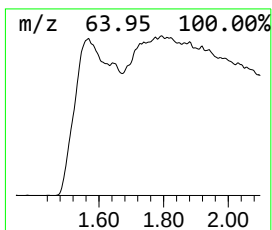
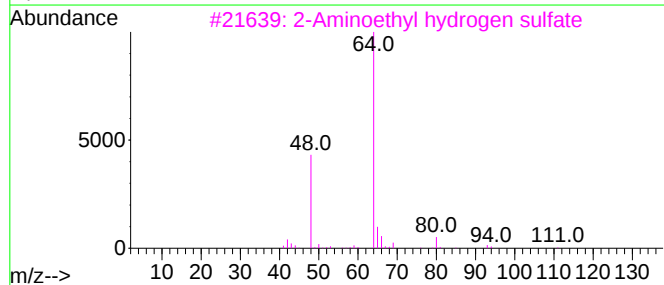
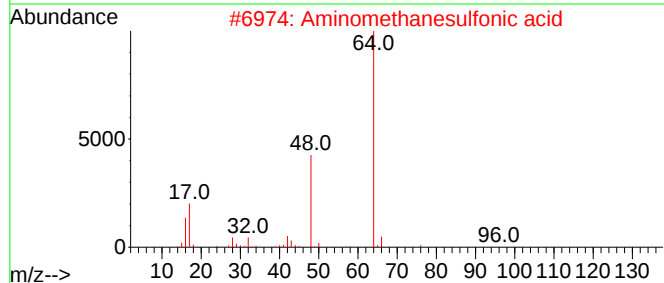
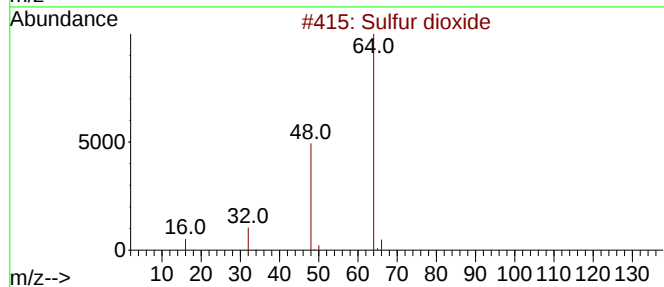
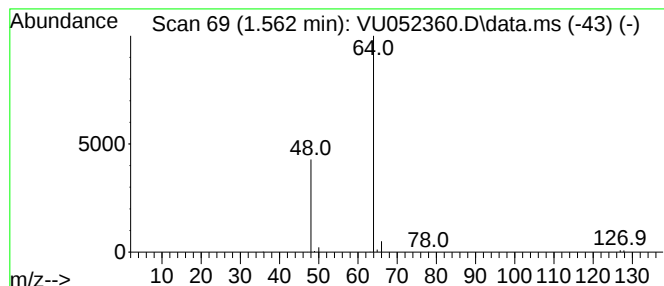
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.600	9.77 ug/L	1059680	1,4-Difluorobenzene	6.247

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			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	64
4			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
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
2,5-Cyclohexadi...	16.767	1.7	ug/L	223976	3	11.809	644491	5.0
Butylated Hydro...	16.883	0.7	ug/L	85910	3	11.809	644491	5.0
Sulfur dioxide	1.600	9.8	ug/L	1059680	1	6.247	542500	5.0