

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
 Data File : VU060921.D
 Acq On : 20 Sep 2024 03:01
 Operator : MD/SY
 Sample : P3987-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH8Q0

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\SFAMUTR091624WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU060921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	52	59	72	rBV3	10052	21269	1.31%	0.301%
2	1.641	98	109	125	rBV2	149039	204837	12.60%	2.896%
3	1.856	169	176	180	rBV	23777	29604	1.82%	0.419%
4	1.892	181	187	201	rBV	18235	51408	3.16%	0.727%
5	1.962	202	209	213	rBV	40045	57833	3.56%	0.818%
6	2.036	226	232	246	rVB	45838	88478	5.44%	1.251%
7	2.107	247	254	269	rVB	55145	106402	6.55%	1.504%
8	2.188	275	279	294	rVB	25886	49152	3.02%	0.695%
9	2.551	383	392	405	rVB	29835	48389	2.98%	0.684%
10	2.660	411	426	443	rBV3	412032	770188	47.39%	10.889%
11	2.773	452	461	474	rBV2	19294	34945	2.15%	0.494%
12	3.448	659	671	695	rVB2	67851	142217	8.75%	2.011%
13	3.969	818	833	855	rBV	65143	155305	9.56%	2.196%
14	4.740	1056	1073	1090	rBV	725951	1625179	100.00%	22.977%
15	5.133	1182	1195	1211	rVB2	96366	208599	12.84%	2.949%
16	5.824	1391	1410	1422	rBV4	129156	348377	21.44%	4.925%
17	5.875	1422	1426	1447	rVB2	34427	54729	3.37%	0.774%
18	6.342	1557	1571	1587	rBV	146269	279719	17.21%	3.955%
19	6.621	1645	1658	1674	rBV	320532	588949	36.24%	8.327%
20	6.769	1694	1704	1721	rVB2	89923	177343	10.91%	2.507%
21	6.866	1726	1734	1748	rVB9	7865	16683	1.03%	0.236%
22	7.615	1955	1967	1984	rBV2	38157	67949	4.18%	0.961%
23	7.940	2055	2068	2081	rBV	140688	248169	15.27%	3.509%
24	8.010	2082	2090	2107	rVB3	19657	40057	2.46%	0.566%
25	8.216	2141	2154	2169	rBV2	22976	40536	2.49%	0.573%
26	8.666	2280	2294	2321	rBV	190953	396523	24.40%	5.606%
27	9.435	2522	2533	2562	rVB	217393	409198	25.18%	5.785%
28	10.756	2932	2944	2962	rVB	78393	129697	7.98%	1.834%
29	11.759	3243	3256	3262	rBV7	17054	36578	2.25%	0.517%
30	11.811	3262	3272	3293	rVB	206133	367993	22.64%	5.203%
31	12.190	3377	3390	3407	rBV	165790	276824	17.03%	3.914%

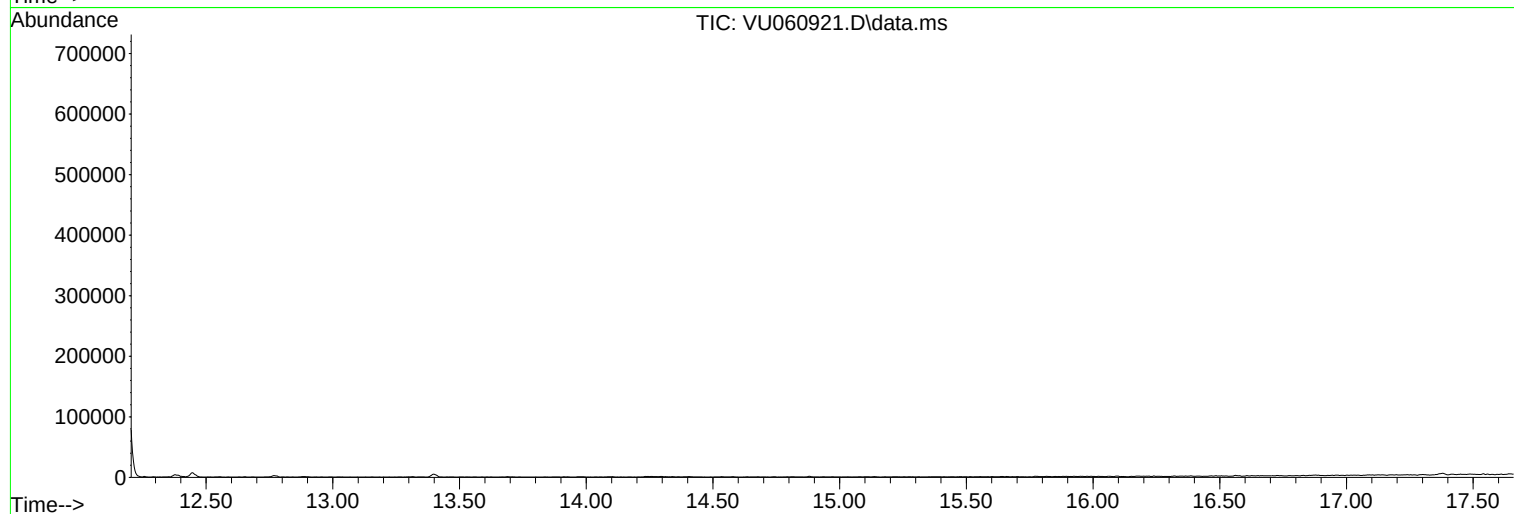
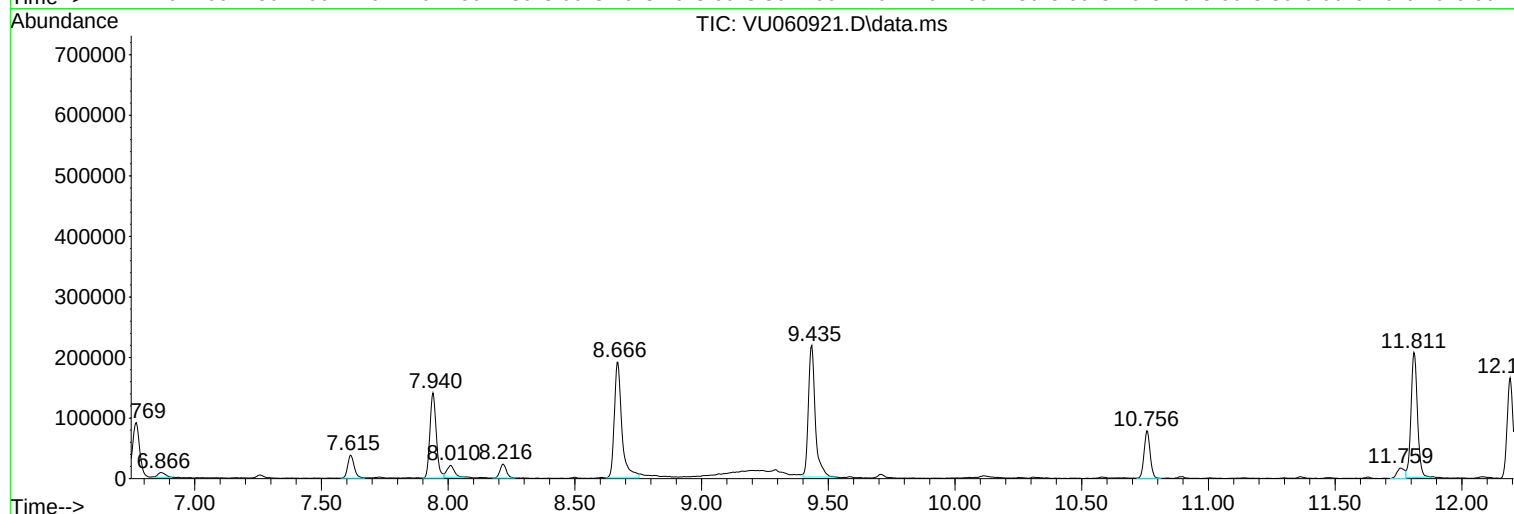
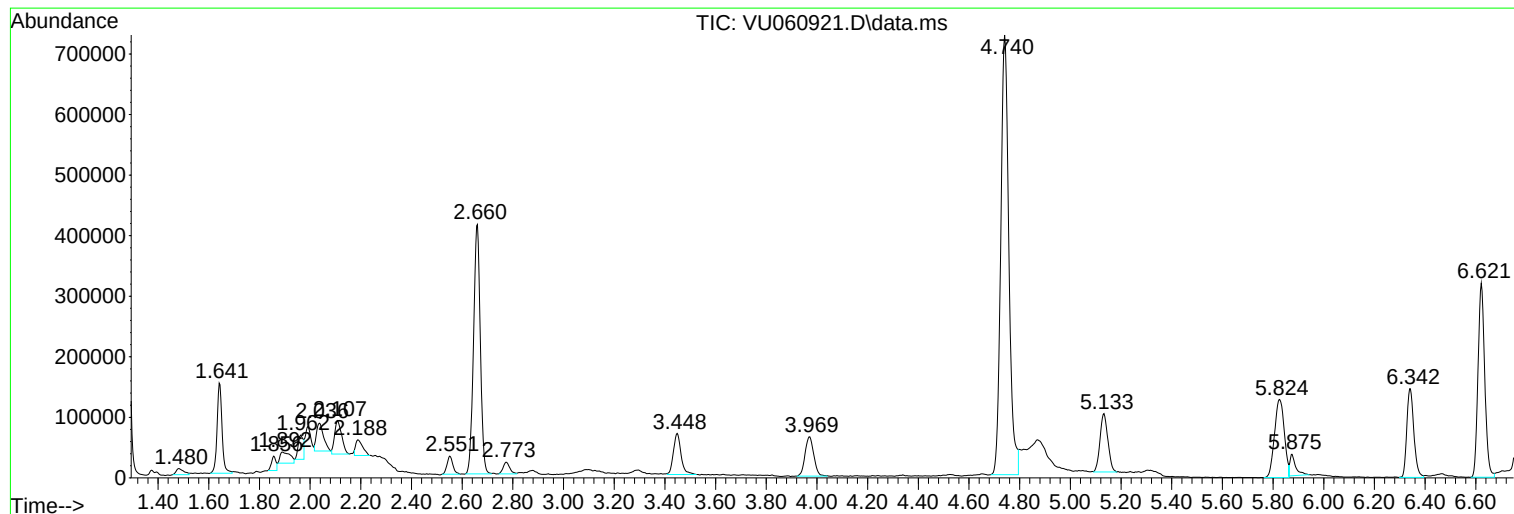
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Instrument :
MSVOA_U
ClientSampleId :
BH8Q0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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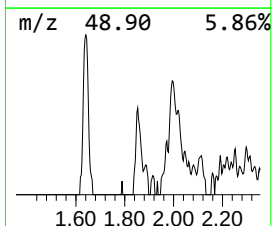
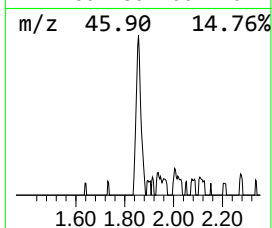
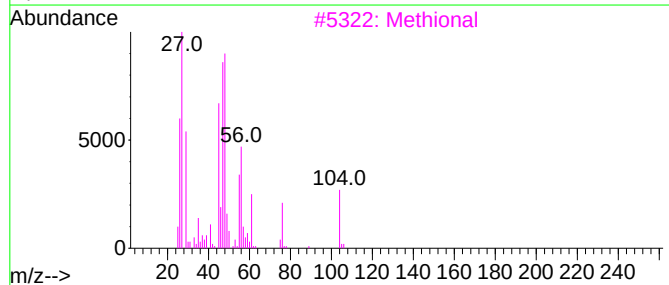
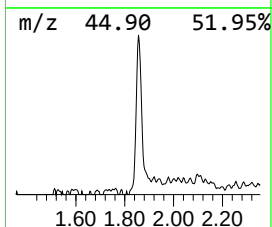
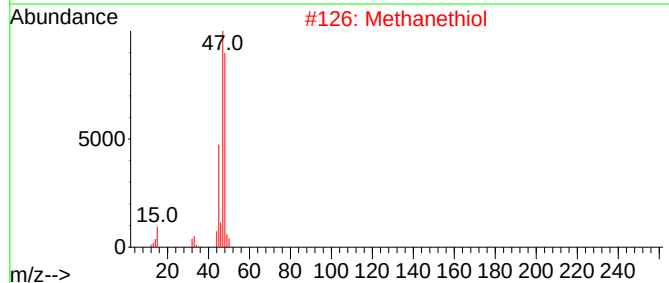
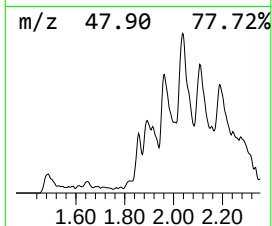
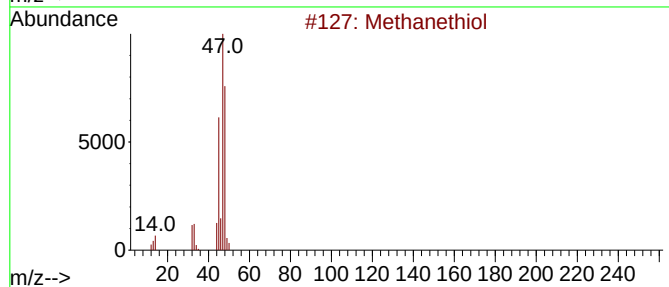
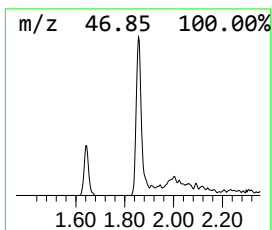
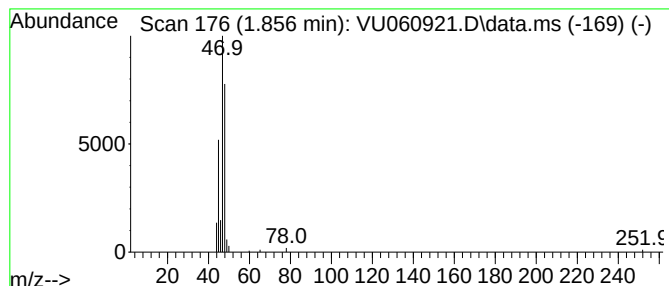
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Methanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.856	0.53 ug/L	29604	1,4-Difluorobenzene	6.342

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
2			Methanethiol	48	CH4S	000074-93-1	90
3			Methional	104	C4H8OS	003268-49-3	64
4			3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	28
5			Trisulfide, methyl 2-propenyl	152	C4H8S3	034135-85-8	9



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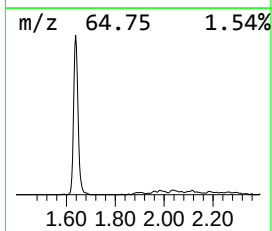
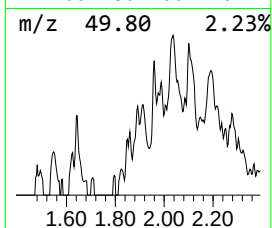
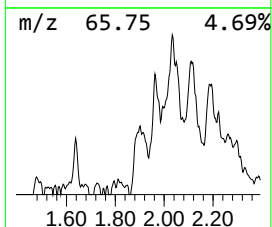
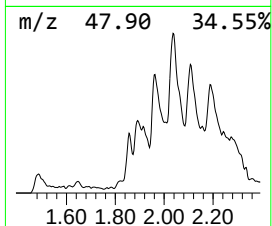
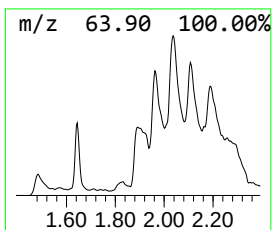
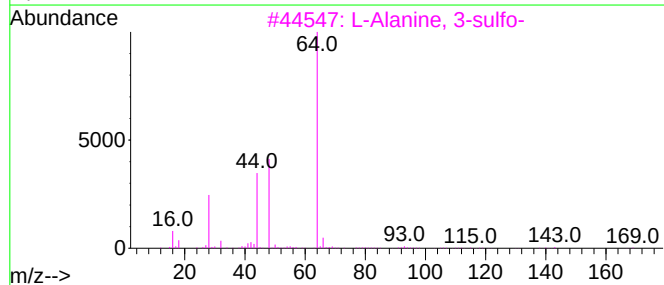
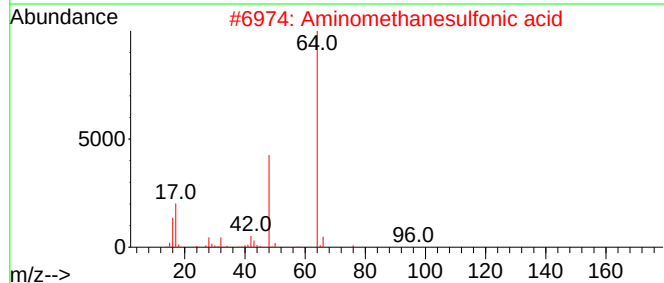
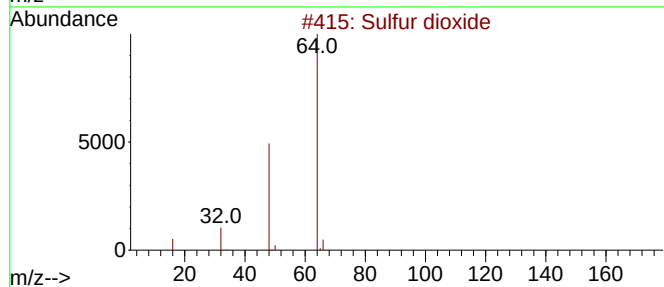
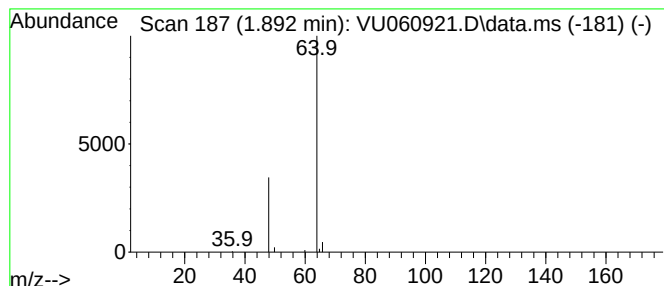
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.892	0.92 ug/L	51408	1,4-Difluorobenzene	6.342

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	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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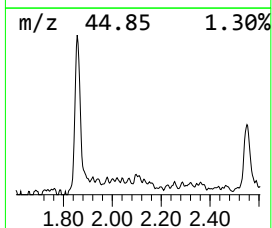
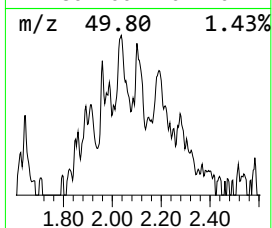
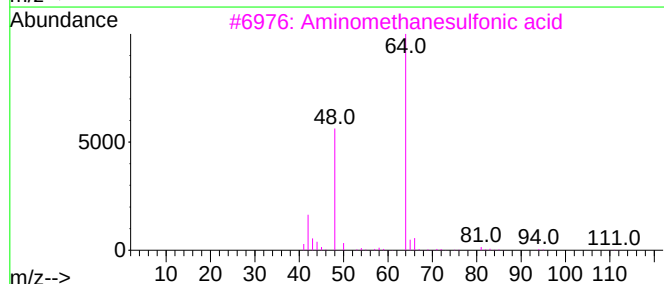
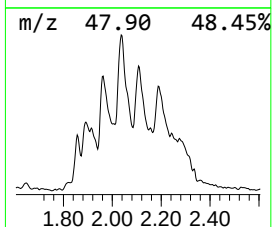
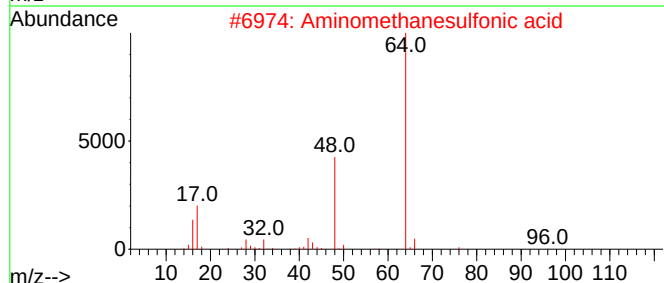
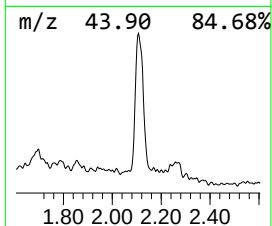
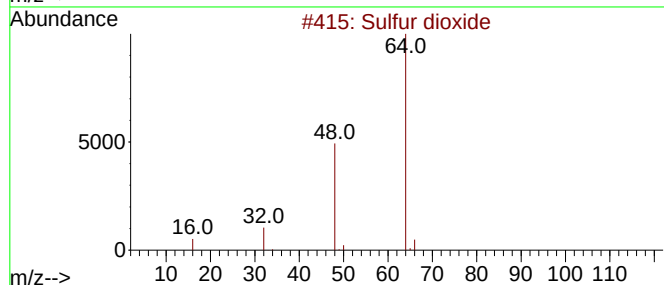
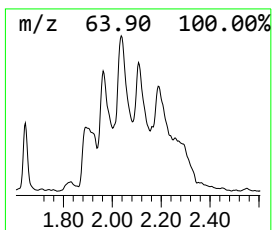
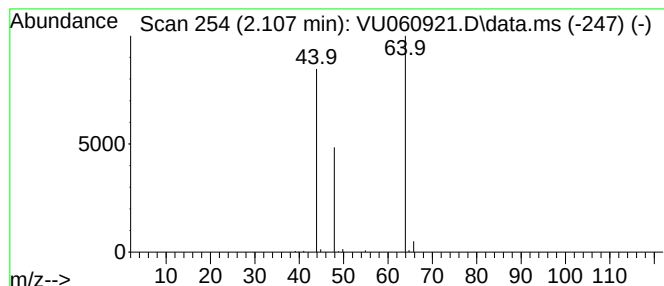
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.107	1.90 ug/L	106402	1,4-Difluorobenzene	6.342

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	50
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	39
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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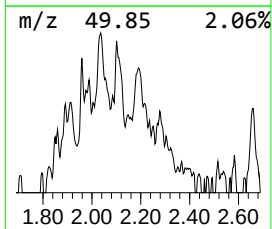
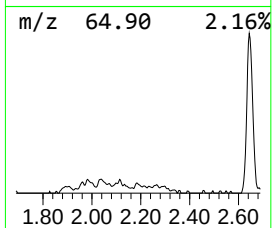
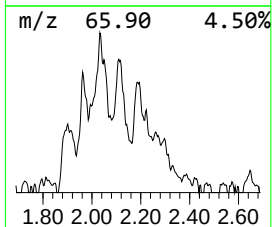
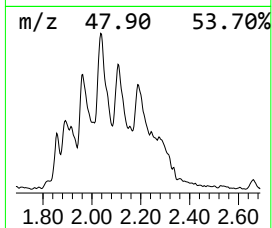
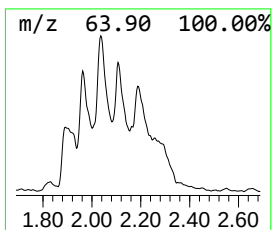
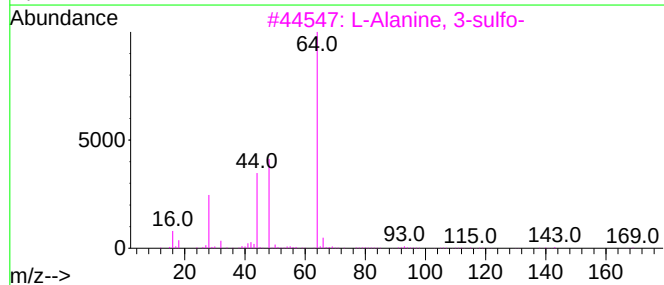
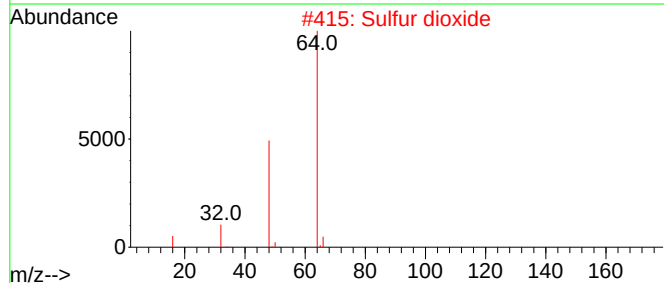
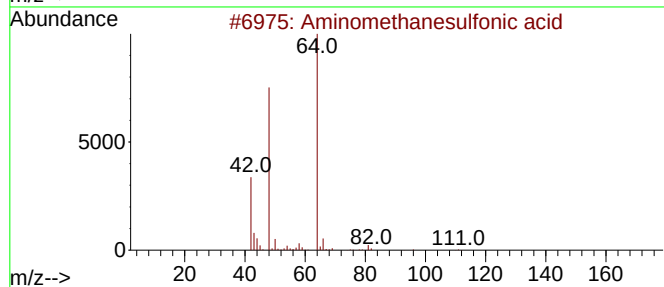
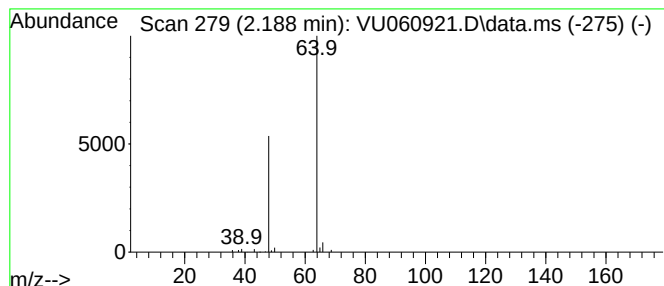
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Aminomethanesulfonic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.188	0.88 ug/L	49152	1,4-Difluorobenzene	6.342

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



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ALS Vial : 38 Sample Multiplier: 1

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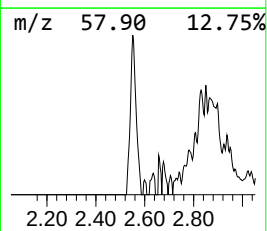
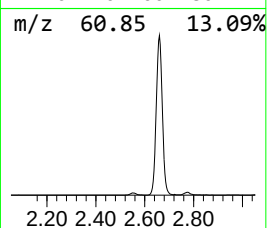
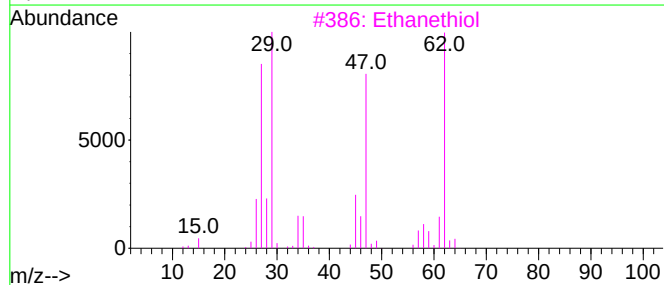
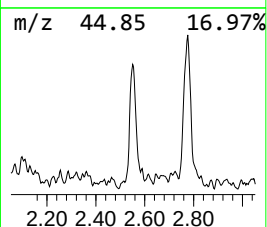
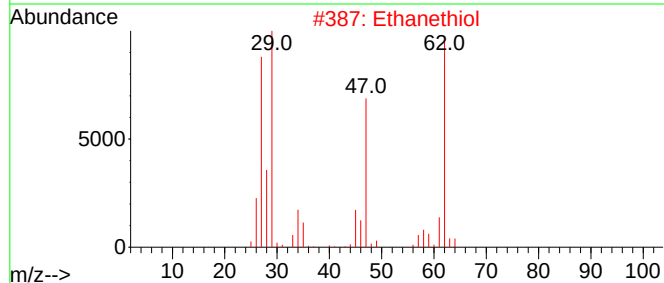
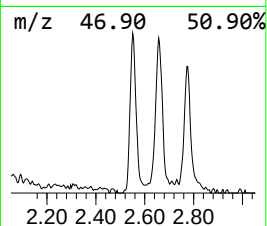
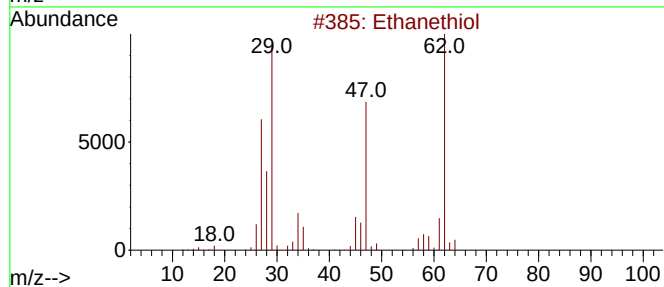
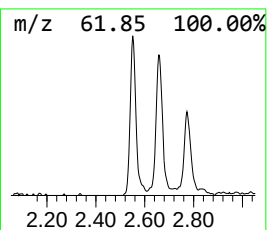
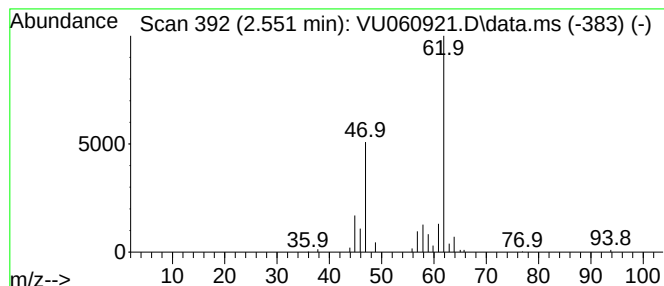
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Ethanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.551	0.86 ug/L	48389	1,4-Difluorobenzene	6.342

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanethiol	62	C2H6S	000075-08-1	91
2			Ethanethiol	62	C2H6S	000075-08-1	91
3			Ethanethiol	62	C2H6S	000075-08-1	83
4			Ethanethiol	62	C2H6S	000075-08-1	83
5			Peroxide, dimethyl	62	C2H6O2	000690-02-8	64



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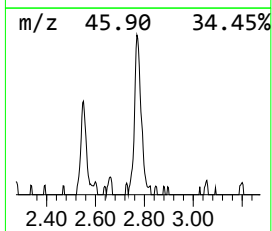
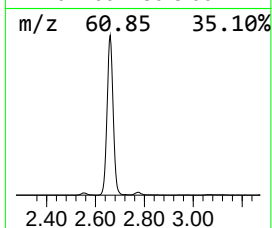
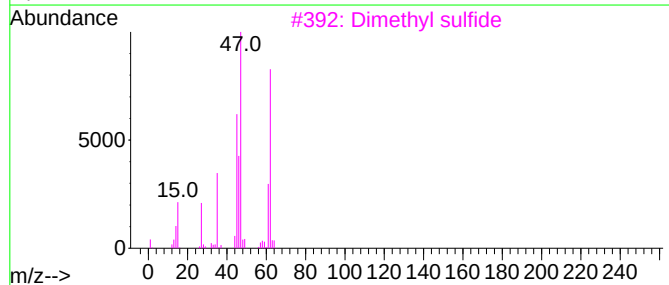
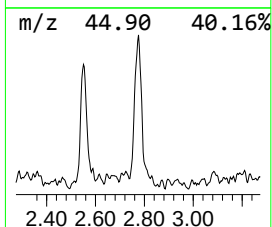
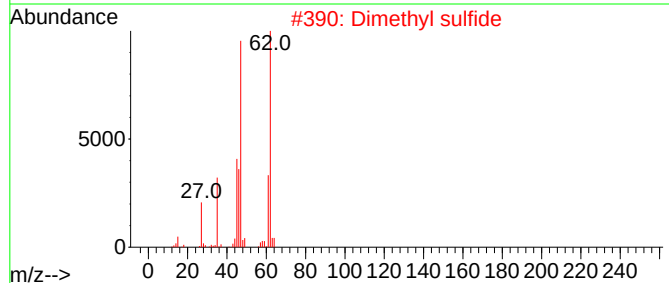
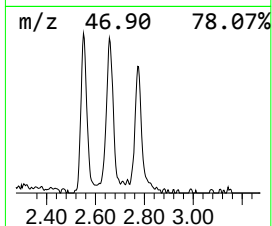
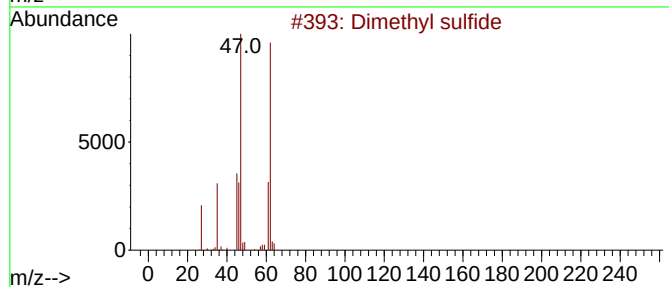
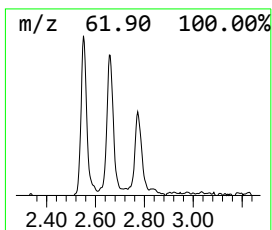
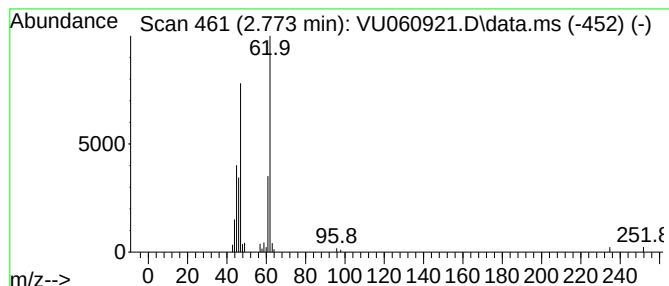
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Dimethyl sulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.773	0.62 ug/L	34945	1,4-Difluorobenzene	6.342

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	91
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	90
5			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
Data File : VU060921.D
Acq On : 20 Sep 2024 03:01
Operator : MD/SY
Sample : P3987-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8Q0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.856	0.5	ug/L	29604	1	6.342	279719	5.0
Sulfur dioxide	1.892	0.9	ug/L	51408	1	6.342	279719	5.0
unknown-01	2.107	1.9	ug/L	106402	1	6.342	279719	5.0
Aminomethanesul...	2.188	0.9	ug/L	49152	1	6.342	279719	5.0
Ethanethiol	2.551	0.9	ug/L	48389	1	6.342	279719	5.0
Dimethyl sulfide	2.773	0.6	ug/L	34945	1	6.342	279719	5.0