

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081222\
 Data File : VV027356.D
 Acq On : 13 Aug 2022 03:28
 Operator : SY/MD
 Sample : N4115-17
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F5D84

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_V\Method\SFAMVTR081122WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV027356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	16	20	37	rVB3	27528	47377	8.88%	0.791%
2	1.291	71	78	86	rBV2	241679	320144	59.99%	5.344%
3	1.339	86	93	120	rVB	185827	411627	77.13%	6.871%
4	1.561	157	162	173	rVB	67766	83901	15.72%	1.400%
5	2.028	301	307	316	rVB2	25176	33822	6.34%	0.565%
6	2.105	322	331	342	rVB	126175	192358	36.05%	3.211%
7	2.163	344	349	356	rVB	7347	9173	1.72%	0.153%
8	2.291	381	389	399	rVB3	5311	7915	1.48%	0.132%
9	2.761	527	535	546	rVB8	3994	7567	1.42%	0.126%
10	3.876	872	882	911	rBV2	74881	259815	48.69%	4.337%
11	4.343	1012	1027	1048	rBV	105393	265766	49.80%	4.436%
12	5.043	1227	1245	1264	rBV2	200631	520929	97.62%	8.695%
13	5.613	1410	1422	1438	rBV2	176817	366270	68.63%	6.114%
14	5.918	1507	1517	1520	rBV8	4421	6246	1.17%	0.104%
15	6.066	1550	1563	1595	rBV	127626	281428	52.74%	4.698%
16	6.989	1836	1850	1865	rBV2	40755	82768	15.51%	1.382%
17	7.313	1940	1951	1964	rBV	205932	379953	71.20%	6.342%
18	7.384	1964	1973	1998	rVB	238320	445979	83.57%	7.444%
19	7.625	2039	2048	2063	rBV3	23174	42726	8.01%	0.713%
20	8.088	2182	2192	2221	rBV	267849	533651	100.00%	8.908%
21	8.252	2234	2243	2262	rVB6	14282	32910	6.17%	0.549%
22	8.850	2418	2429	2453	rBV	290698	504318	94.50%	8.418%
23	9.018	2472	2481	2488	rBV3	6504	11138	2.09%	0.186%
24	9.108	2501	2509	2515	rBV2	11339	18777	3.52%	0.313%
25	10.214	2843	2853	2869	rBV	97409	159382	29.87%	2.660%
26	10.416	2906	2916	2927	rBV	27702	47086	8.82%	0.786%
27	10.526	2941	2950	2952	rBV5	4075	5831	1.09%	0.097%
28	10.719	3002	3010	3025	rVB	21576	34626	6.49%	0.578%
29	10.918	3065	3072	3080	rBV5	4582	7099	1.33%	0.118%
30	11.249	3163	3175	3195	rBV	281182	445487	83.48%	7.436%
31	11.410	3215	3225	3229	rBV8	5676	8101	1.52%	0.135%
32	11.622	3280	3291	3314	rBV	223236	362104	67.85%	6.044%
33	12.879	3671	3682	3691	rBV5	9343	16757	3.14%	0.280%
34	14.085	4047	4057	4070	rVB5	5944	11679	2.19%	0.195%
35	16.307	4734	4748	4759	rBV5	15893	26244	4.92%	0.438%

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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_V\Method\SFAMVTR081122WMA.M
Title : TRACE VOA SFAM1.0

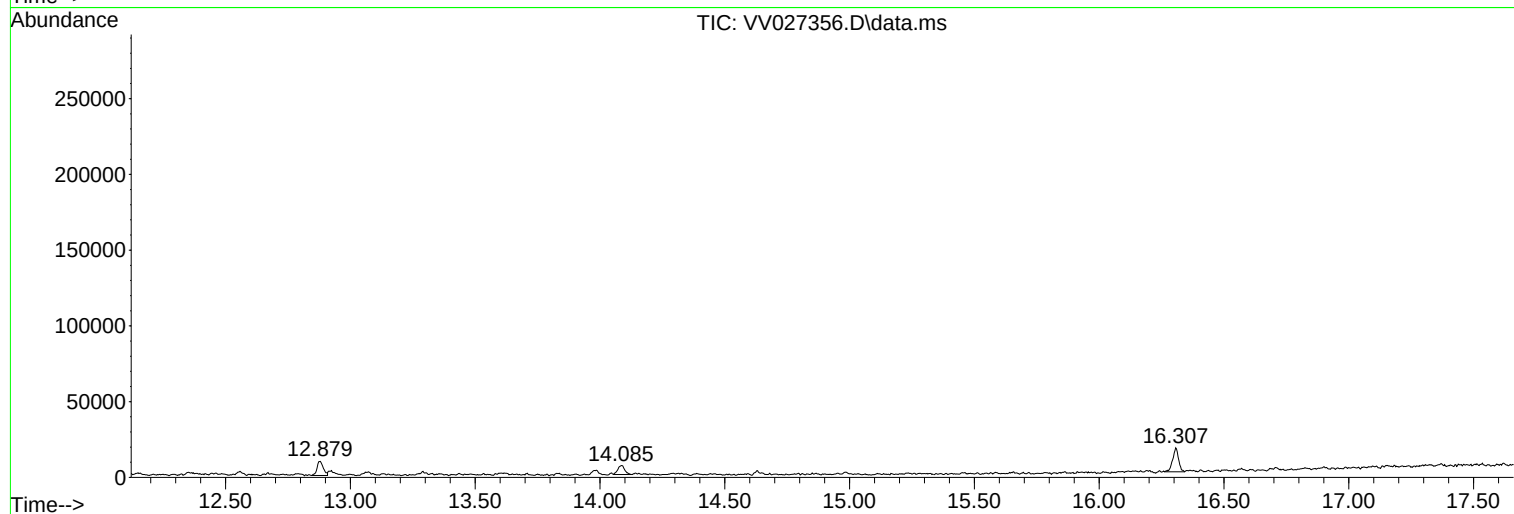
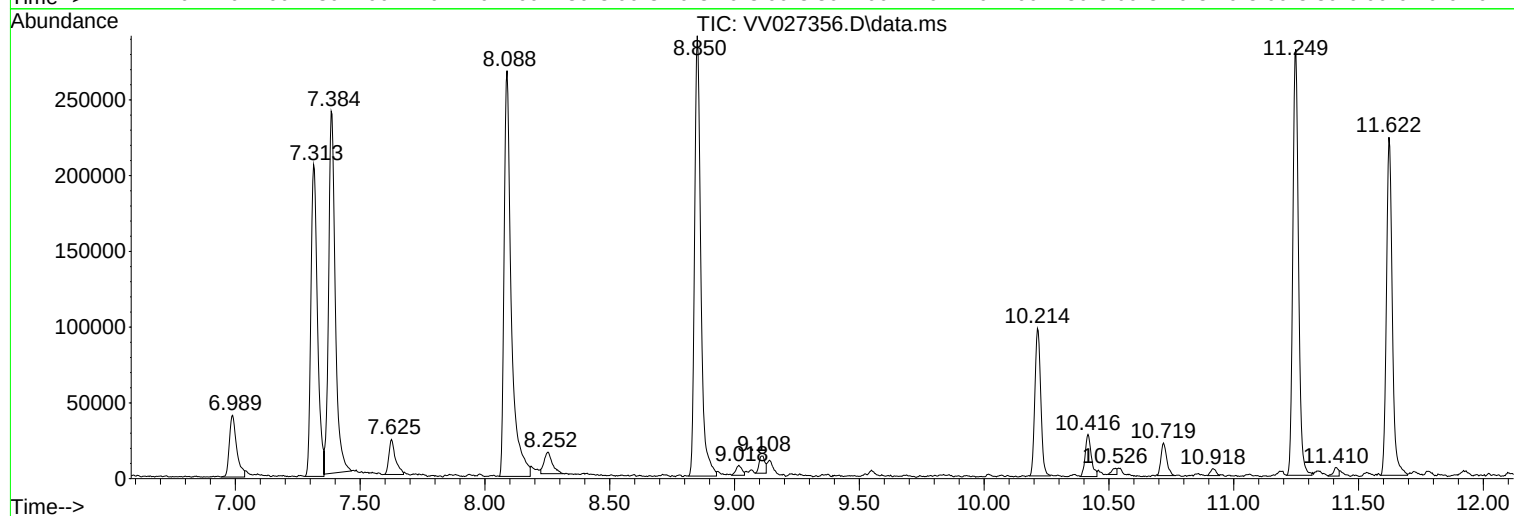
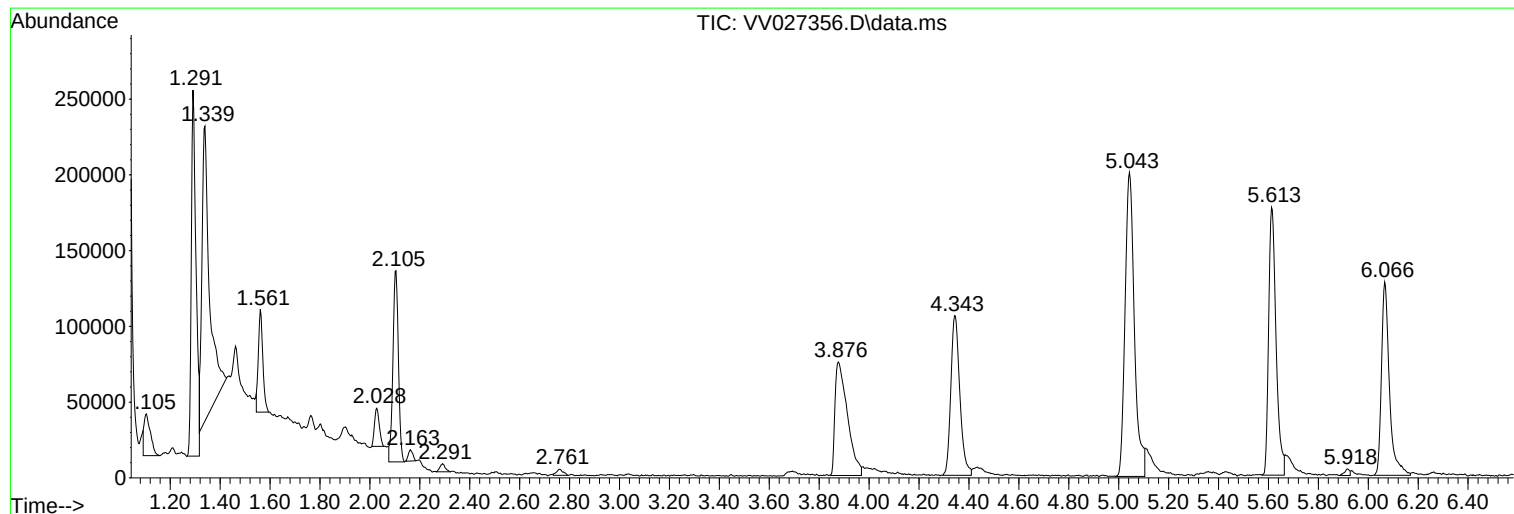
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081122WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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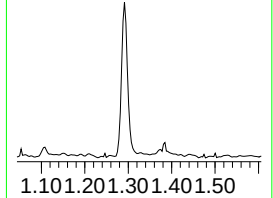
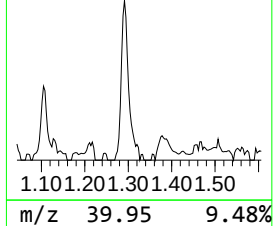
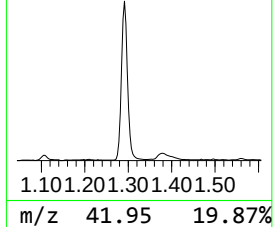
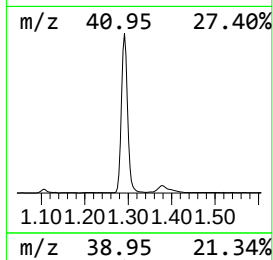
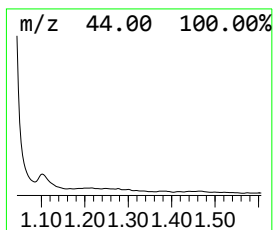
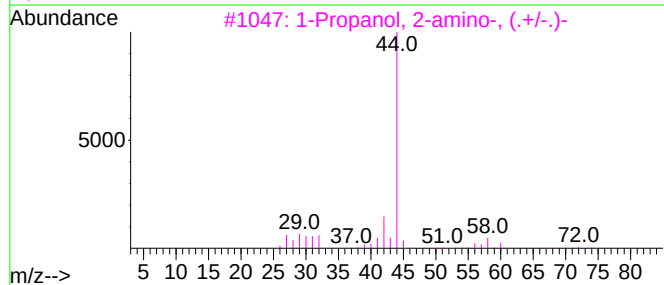
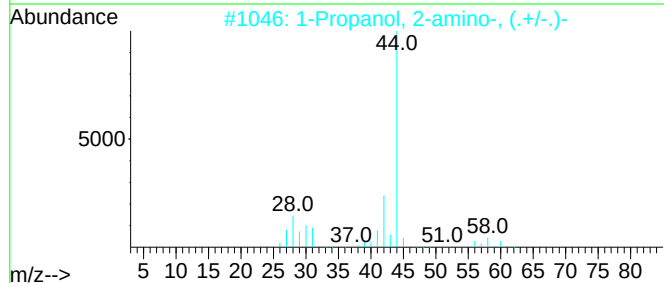
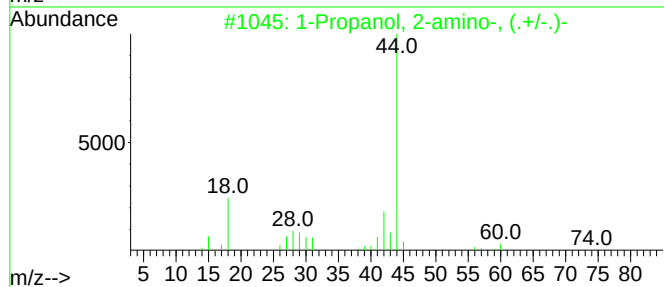
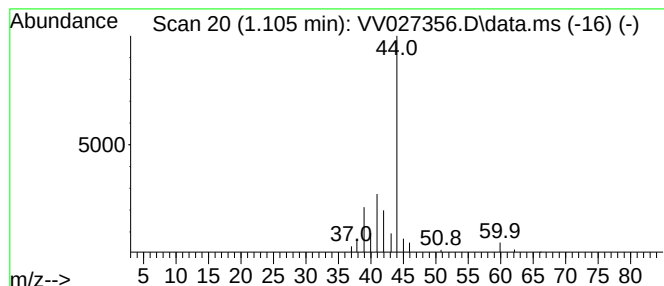
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.105	0.65 ug/L	47377	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-amino-, (+/-)-			75	C3H9NO	006168-72-5	9
2	1-Propanol, 2-amino-, (+/-)-			75	C3H9NO	006168-72-5	9
3	1-Propanol, 2-amino-, (+/-)-			75	C3H9NO	006168-72-5	9
4	D-Alanine			89	C3H7NO2	000338-69-2	9
5	Acetaldehyde			44	C2H4O	000075-07-0	5



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Instrument :
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ClientSampleId :
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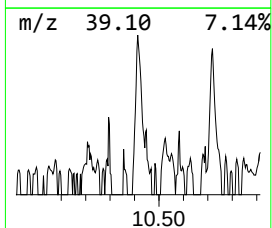
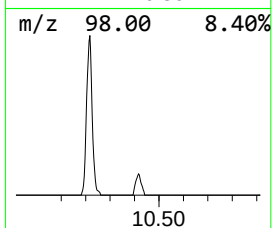
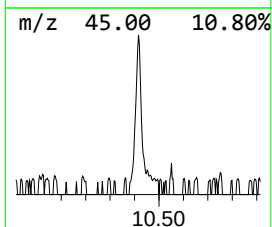
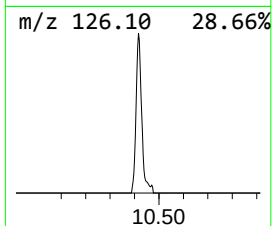
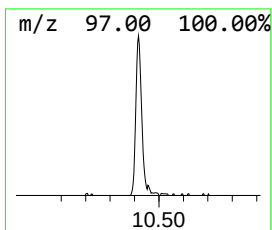
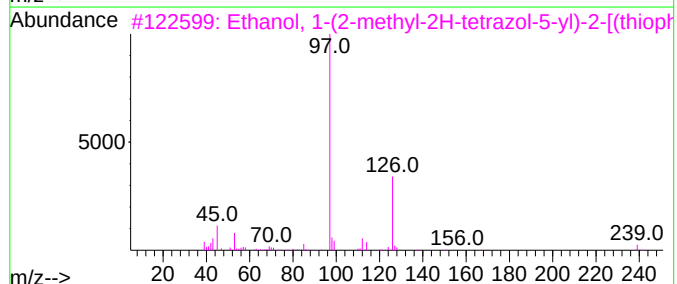
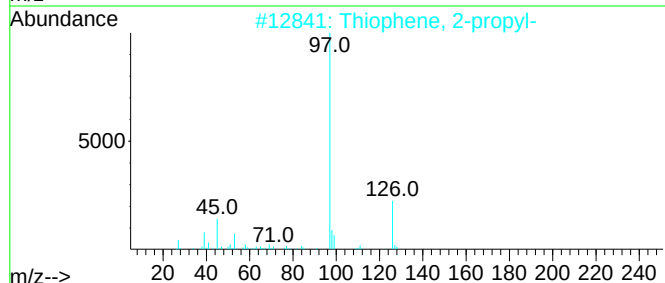
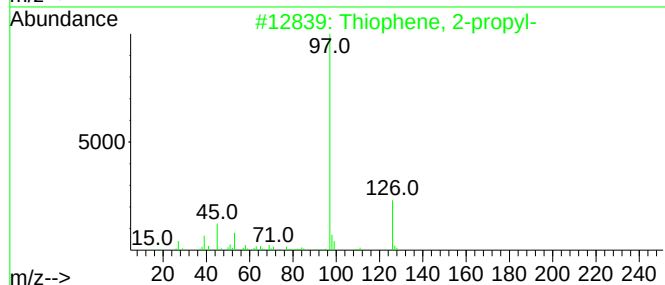
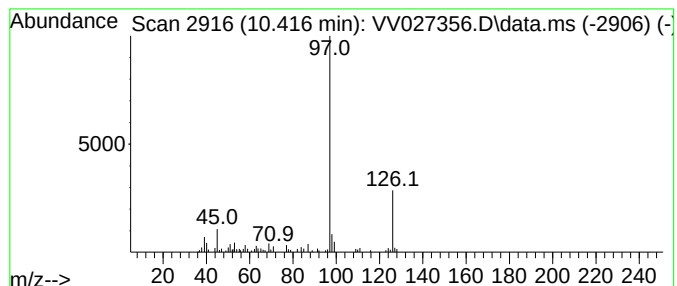
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Thiophene, 2-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.416	0.53 ug/L	47086	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-propyl-	126	C7H10S	001551-27-5	90
2			Thiophene, 2-propyl-	126	C7H10S	001551-27-5	80
3			Ethanol, 1-(2-methyl-2H-tetrazol...	239	C9H13N5OS	1000316-81-4	64
4			1H-Pyrazole, 4,5-dihydro-3-methy...	126	C7H14N2	026964-49-8	64
5			1H-Pyrazole, 4,5-dihydro-3-methy...	126	C7H14N2	026964-49-8	64



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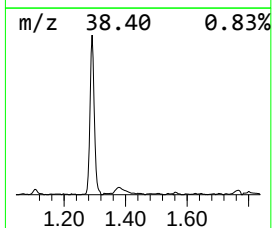
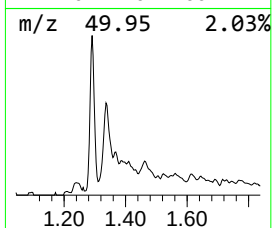
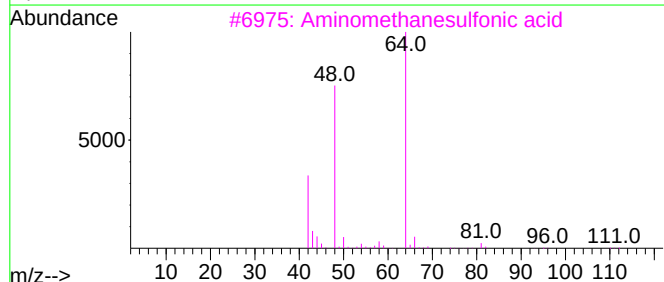
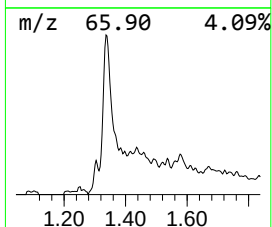
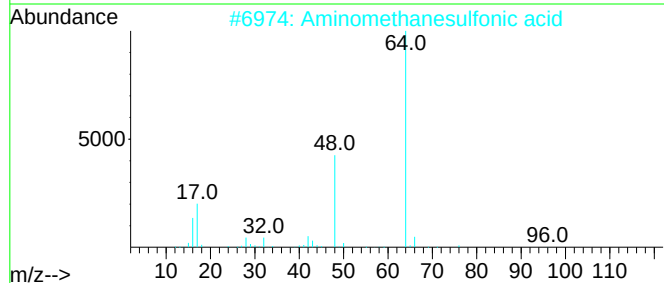
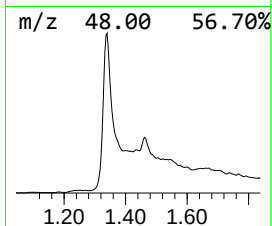
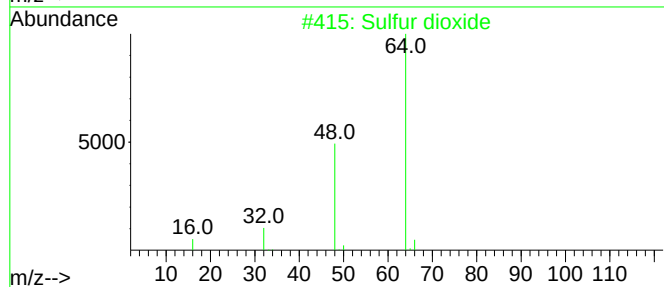
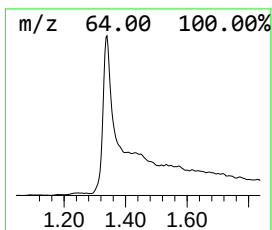
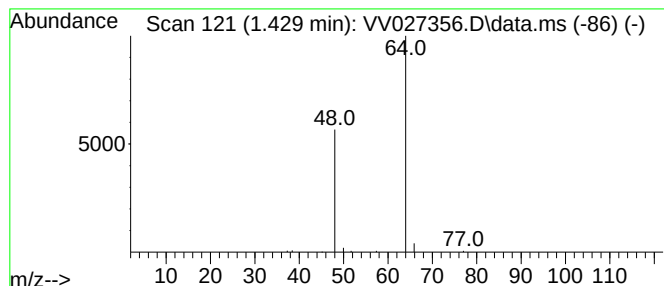
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.339	5.62 ug/L	411627	1,4-Difluorobenzene	5.613

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	25
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	1.105	0.7	ug/L	47377	1	5.613	366270	5.0
Thiophene, 2-pr...	10.416	0.5	ug/L	47086	3	11.249	445487	5.0
Sulfur dioxide	1.339	5.6	ug/L	411627	1	5.613	366270	5.0