

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011524\
 Data File : VU057535.D
 Acq On : 15 Jan 2024 17:25
 Operator : MD/SY
 Sample : P1062-20
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH273

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\SFAMUTR011124WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057535.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.371	21	25	32	rVB	27311	26260	2.44%	0.310%
2	1.451	42	50	63	rBV	82917	152611	14.20%	1.801%
3	1.589	86	93	112	rVB2	131489	168075	15.63%	1.983%
4	1.904	183	191	211	rVB2	112665	168248	15.65%	1.985%
5	2.117	249	257	258	rBV2	33969	39819	3.70%	0.470%
6	2.284	303	309	328	rVB2	34474	76848	7.15%	0.907%
7	2.567	383	397	414	rVB3	458493	838574	78.00%	9.894%
8	2.679	423	432	442	rBV3	13652	27302	2.54%	0.322%
9	2.779	455	463	476	rVB	27307	46041	4.28%	0.543%
10	2.994	521	530	533	rBV2	22593	34450	3.20%	0.406%
11	3.856	782	798	817	rBV	448285	1075042	100.00%	12.685%
12	4.660	1033	1048	1055	rBV4	25647	57038	5.31%	0.673%
13	4.731	1056	1070	1099	rVV2	50327	230638	21.45%	2.721%
14	5.055	1155	1171	1189	rBV	201082	441900	41.11%	5.214%
15	5.714	1357	1376	1417	rBV2	351375	989653	92.06%	11.677%
16	6.242	1518	1540	1565	rBV	186431	382520	35.58%	4.513%
17	6.534	1621	1631	1644	rBV2	24092	44080	4.10%	0.520%
18	6.685	1662	1678	1698	rBV	242896	481181	44.76%	5.678%
19	6.788	1698	1710	1721	rVB5	14594	30739	2.86%	0.363%
20	7.560	1938	1950	1965	rBV	81098	147131	13.69%	1.736%
21	7.891	2041	2053	2070	rBV	237955	464280	43.19%	5.478%
22	7.965	2072	2076	2088	rVB3	11074	17609	1.64%	0.208%
23	8.177	2131	2142	2161	rBV2	49813	90441	8.41%	1.067%
24	8.640	2273	2286	2332	rBV2	423046	991912	92.27%	11.704%
25	9.412	2514	2526	2548	rBV	241467	442684	41.18%	5.223%
26	10.750	2930	2942	2958	rBV	159632	263200	24.48%	3.106%
27	11.807	3257	3271	3292	rBV	186265	315808	29.38%	3.726%
28	12.065	3341	3351	3377	rBV3	14709	39150	3.64%	0.462%
29	12.187	3377	3389	3410	rVB	236900	391937	36.46%	4.625%

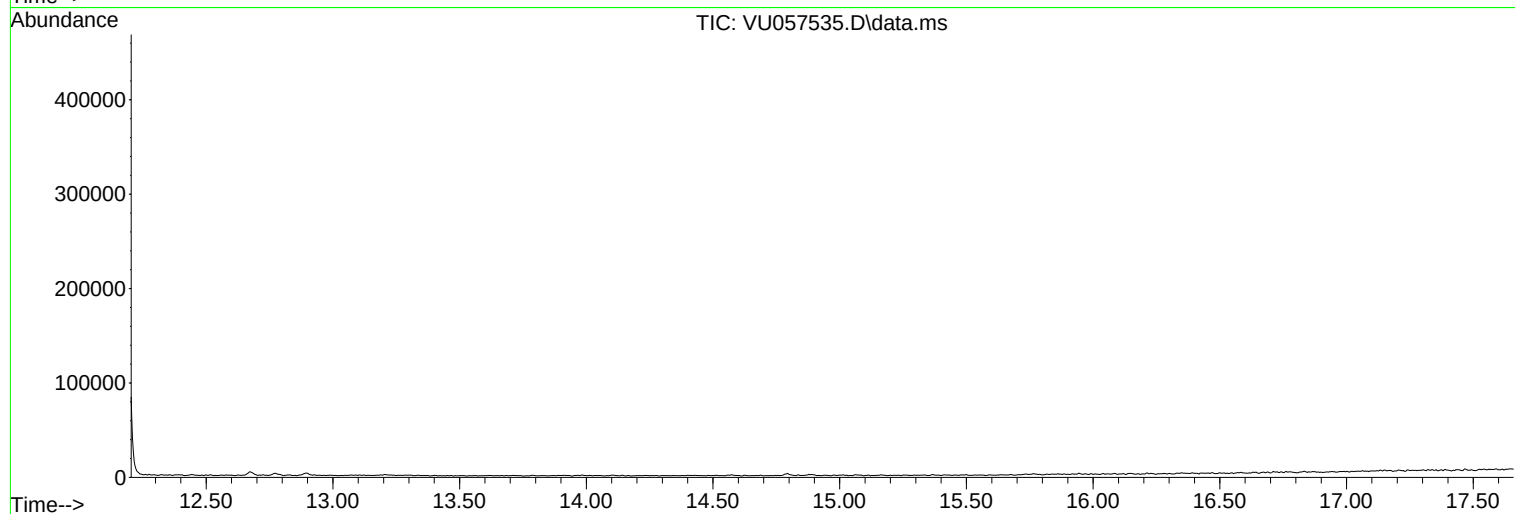
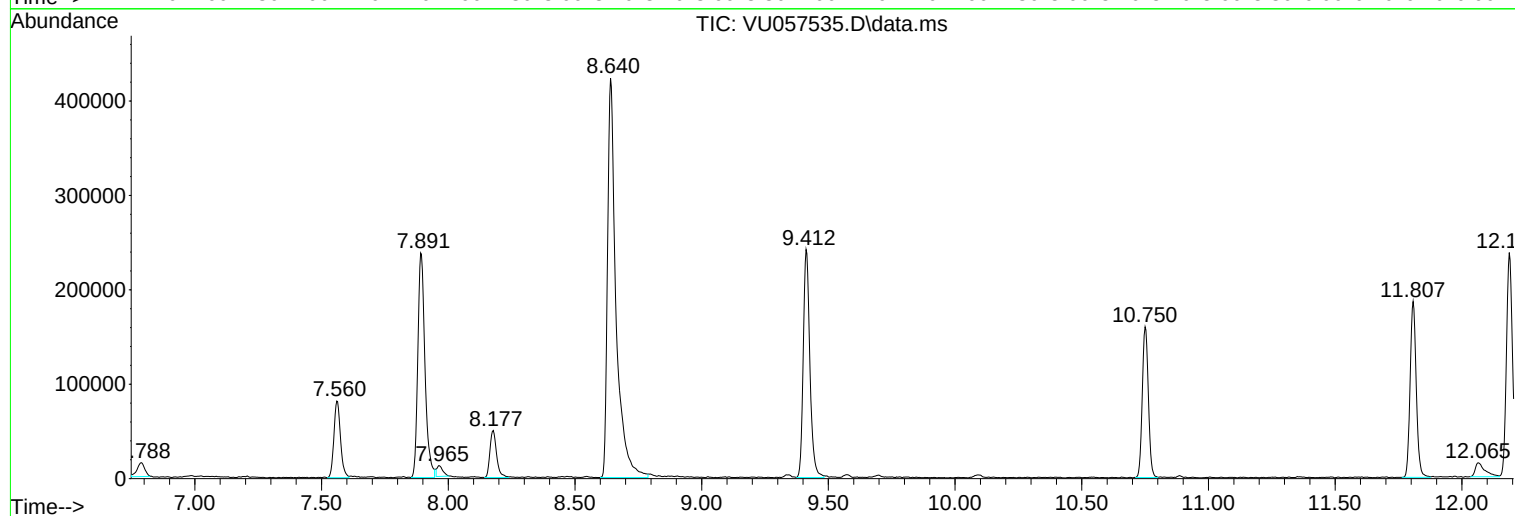
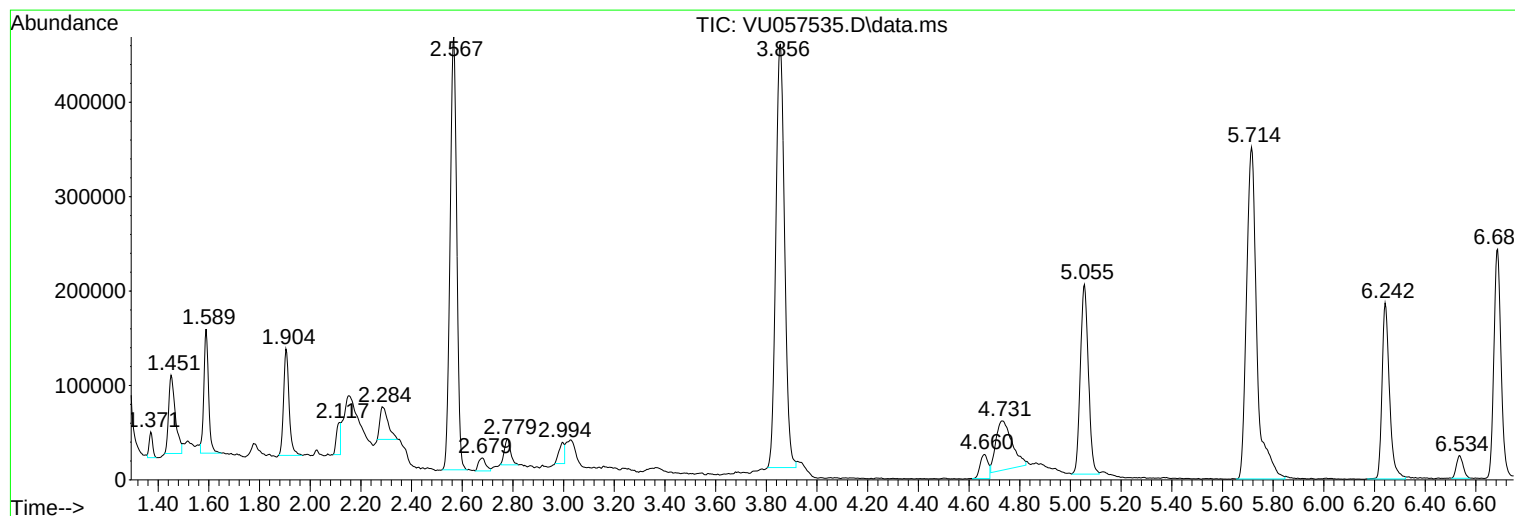
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011124WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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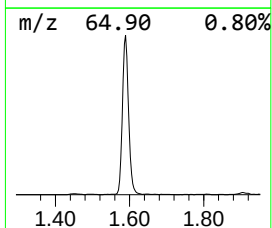
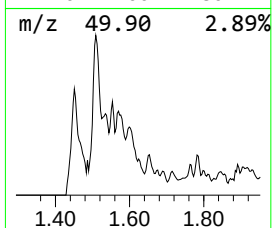
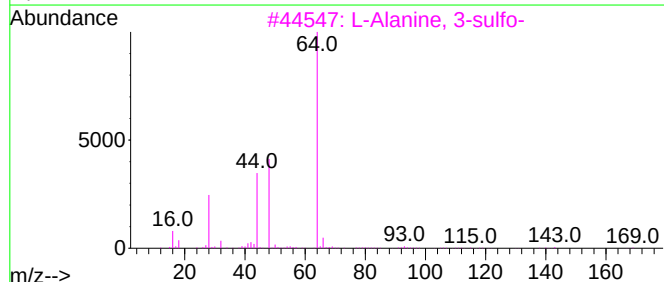
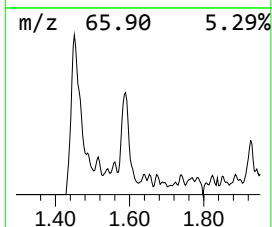
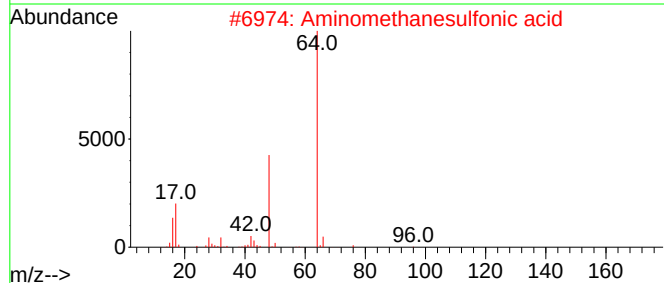
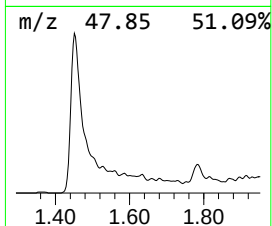
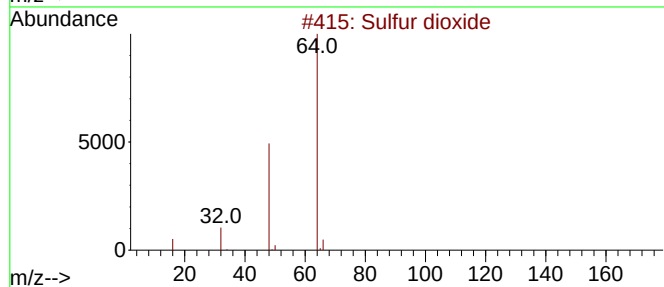
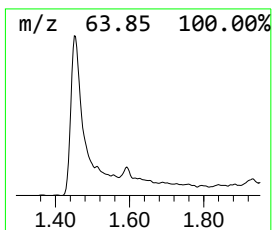
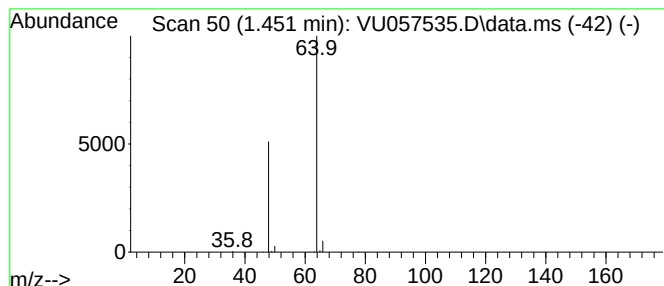
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.451	1.99 ug/L	152611	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			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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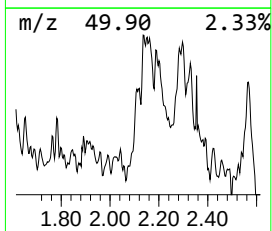
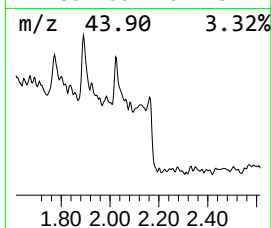
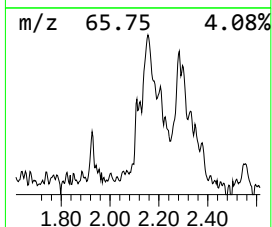
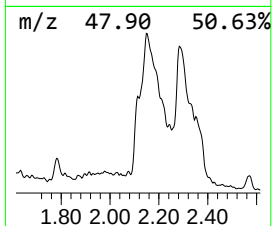
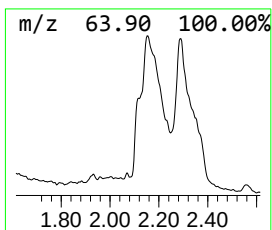
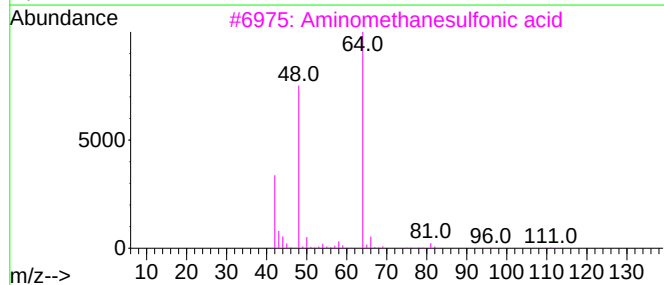
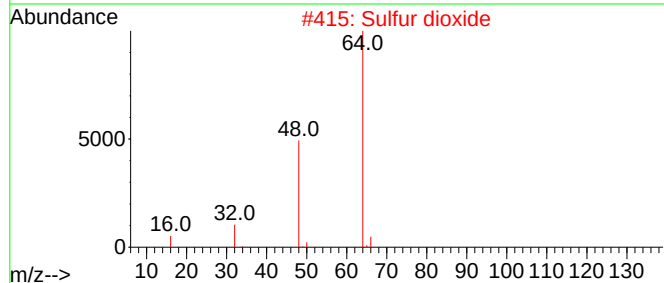
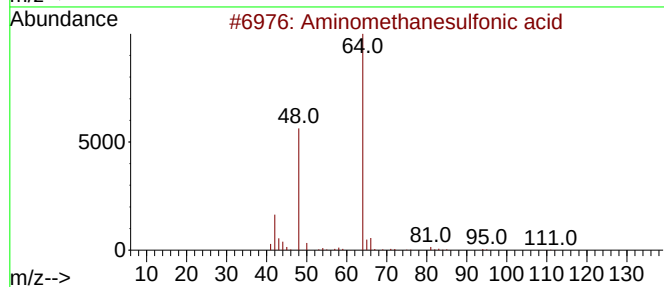
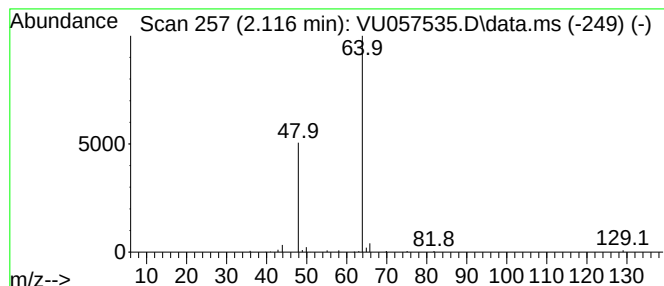
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011124WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	0.52 ug/L	39819	1,4-Difluorobenzene	6.242

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9



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ALS Vial : 21 Sample Multiplier: 1

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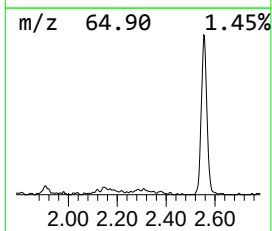
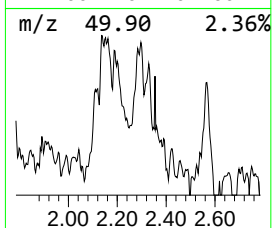
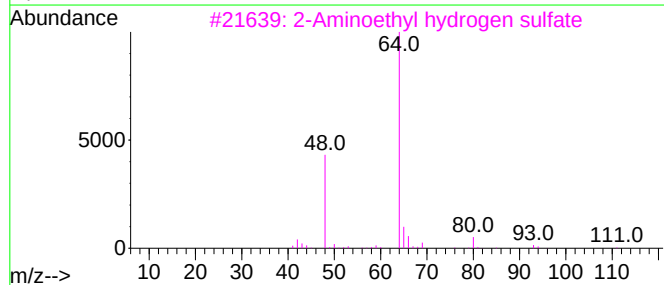
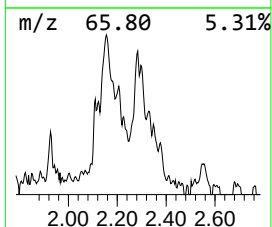
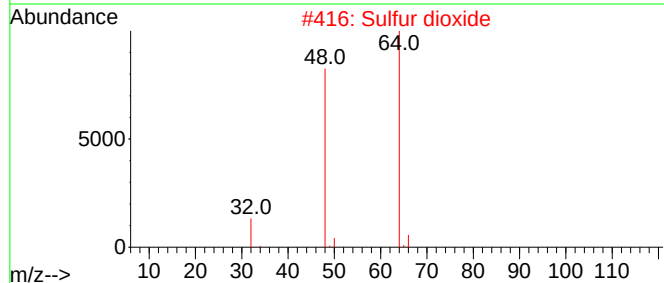
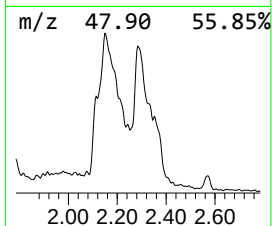
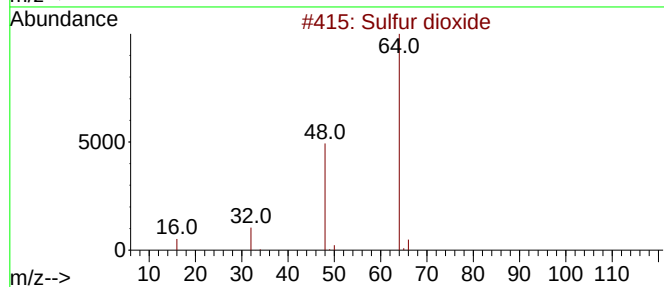
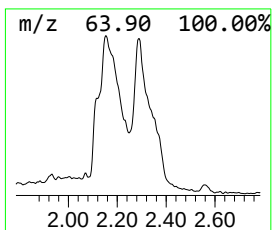
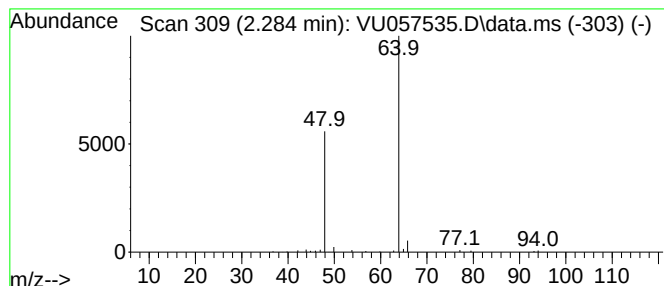
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011124WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2-Aminoethyl hydrogen sulfate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.284	1.00 ug/L	76848	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64



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ALS Vial : 21 Sample Multiplier: 1

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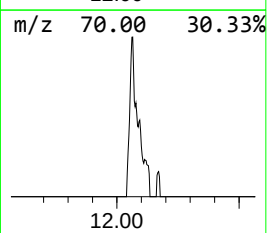
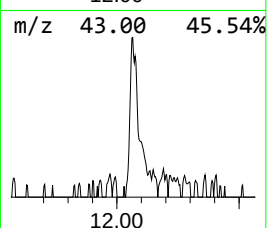
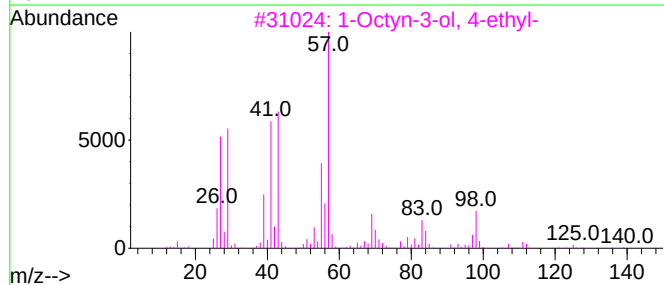
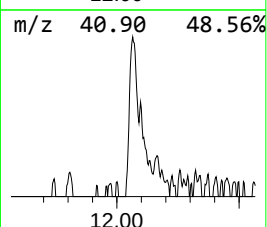
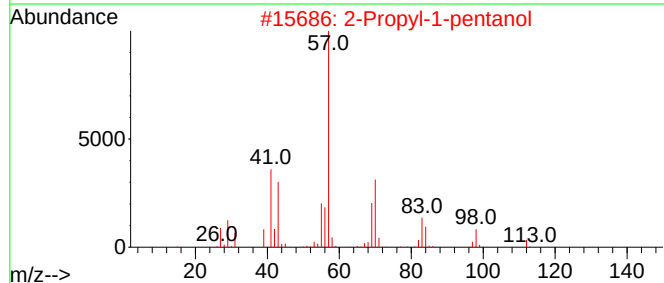
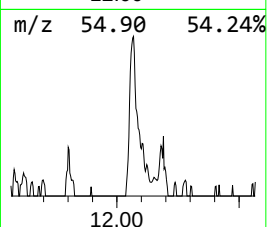
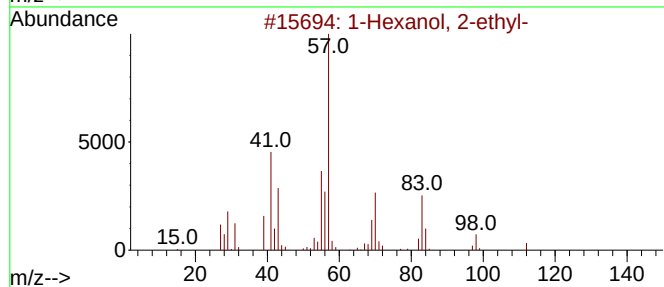
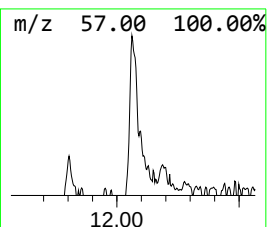
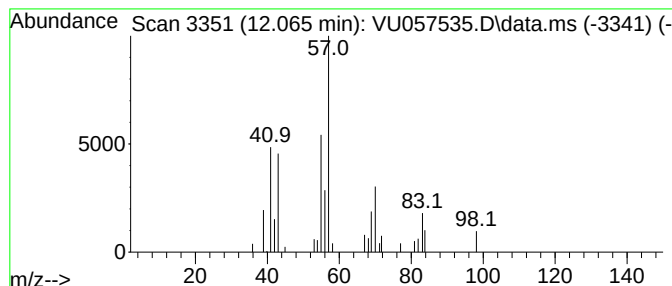
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.065	0.62 ug/L	39150	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3			1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	59
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.451	2.0	ug/L	152611	1	6.242	382520	5.0
Aminomethanesul...	2.116	0.5	ug/L	39819	1	6.242	382520	5.0
2-Aminoethyl hy...	2.284	1.0	ug/L	76848	1	6.242	382520	5.0
1-Hexanol, 2-et...	12.065	0.6	ug/L	39150	3	11.807	315808	5.0