

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
 Data File : VU060923.D
 Acq On : 20 Sep 2024 03:50
 Operator : MD/SY
 Sample : P3987-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH8P4

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: VU060923.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.608	91	99	112	rVB	47606	57415	1.14%	0.432%
2	1.882	171	184	193	rBV2	23611	73130	1.45%	0.550%
3	2.084	240	247	265	rBV	27920	58805	1.16%	0.442%
4	2.586	388	403	420	rBV	864807	1421941	28.17%	10.697%
5	3.055	534	549	562	rBV3	26874	54567	1.08%	0.411%
6	3.875	786	804	830	rBV	772134	1804687	35.75%	13.577%
7	4.679	1036	1054	1071	rBV2	603753	1394441	27.62%	10.491%
8	5.081	1164	1179	1194	rBV2	69582	160152	3.17%	1.205%
9	5.753	1370	1388	1400	rBV2	145067	352585	6.98%	2.653%
10	6.271	1537	1549	1565	rBV	137022	261055	5.17%	1.964%
11	6.557	1623	1638	1674	rBV	2692064	5048013	100.00%	37.977%
12	6.708	1674	1685	1701	rVB	86184	172711	3.42%	1.299%
13	7.576	1945	1955	1974	rBV2	36197	64641	1.28%	0.486%
14	7.904	2044	2057	2069	rBV	142326	257397	5.10%	1.936%
15	7.975	2070	2079	2104	rVB	137786	264209	5.23%	1.988%
16	8.647	2272	2288	2330	rBV	194529	411610	8.15%	3.097%
17	9.418	2515	2528	2546	rBV	199333	353028	6.99%	2.656%
18	9.692	2597	2613	2631	rBV2	87449	158225	3.13%	1.190%
19	10.097	2729	2739	2754	rBV	34173	58548	1.16%	0.440%
20	10.753	2928	2943	2961	rVB	80588	132097	2.62%	0.994%
21	11.807	3259	3271	3288	rBV	195282	321516	6.37%	2.419%
22	12.058	3338	3349	3378	rBV4	43818	127317	2.52%	0.958%
23	12.187	3378	3389	3404	rVB	173973	284239	5.63%	2.138%

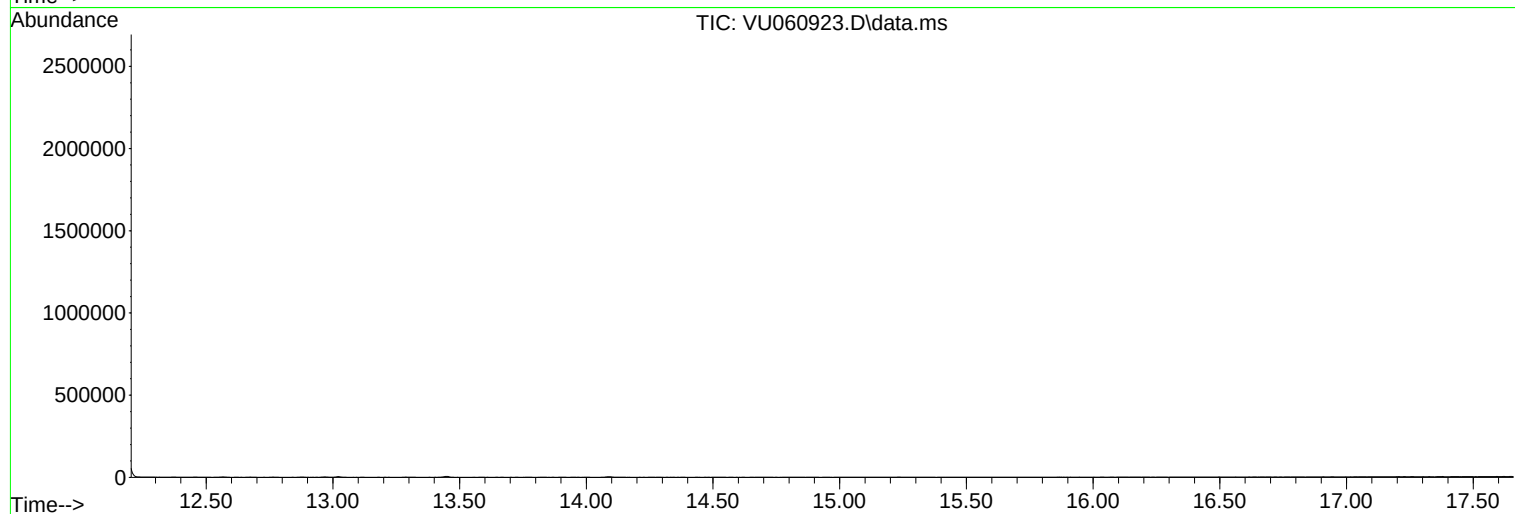
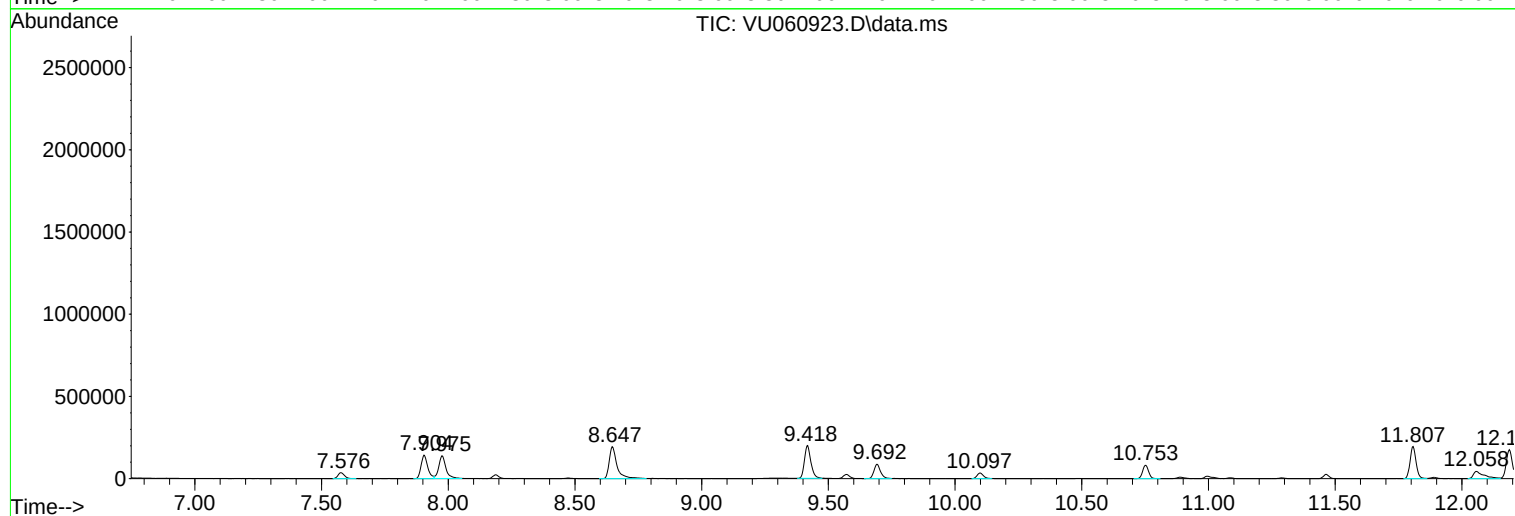
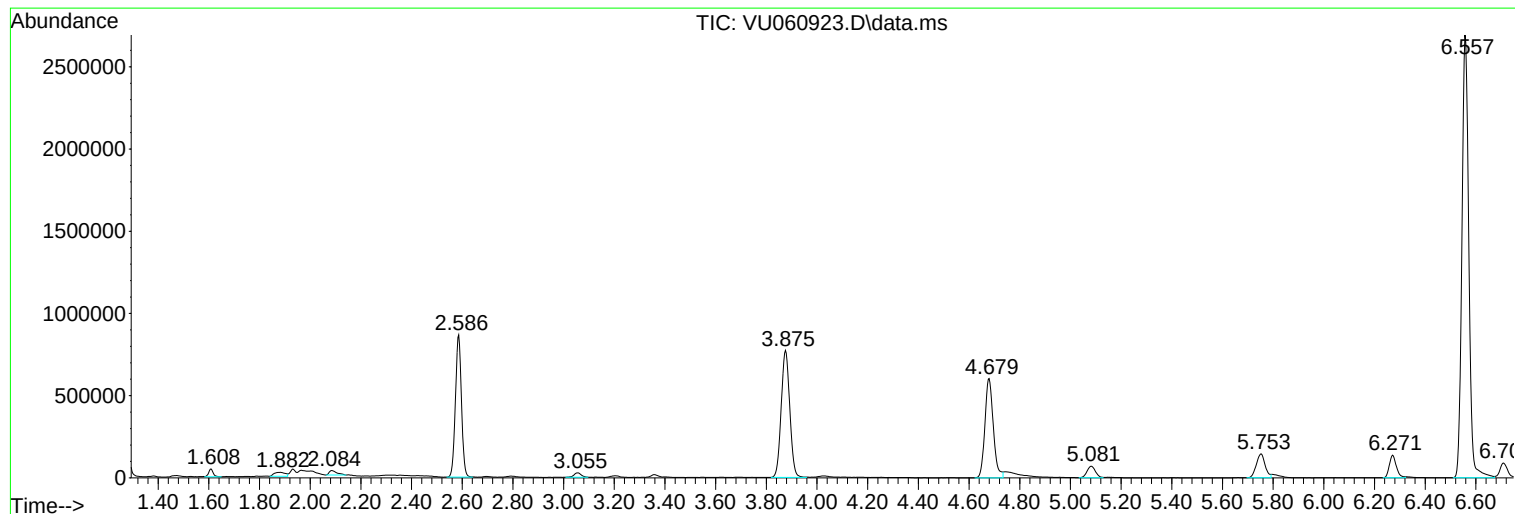
Sum of corrected areas: 13292329

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ClientSampleId :
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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



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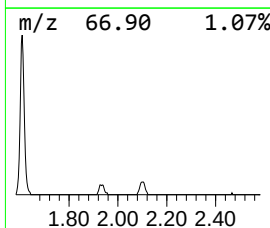
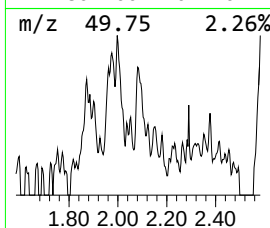
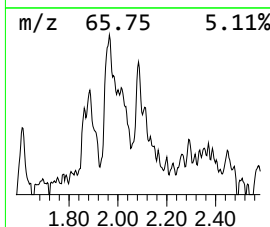
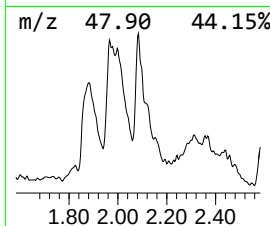
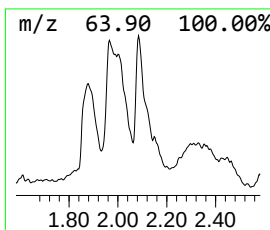
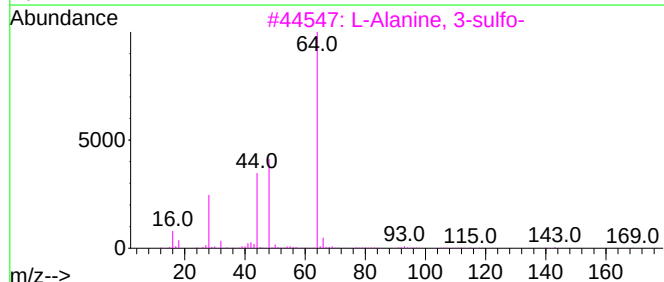
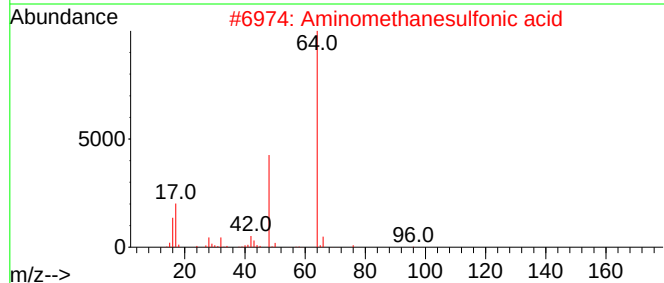
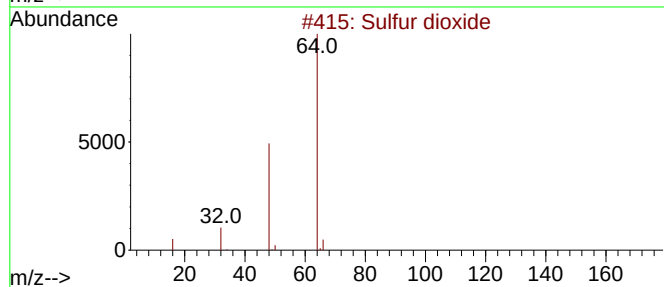
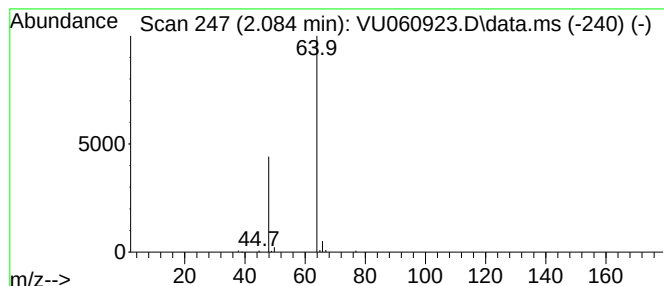
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.084	1.13 ug/L	58805	1,4-Difluorobenzene	6.271

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			Sulfur dioxide	64	O2S	007446-09-5	5



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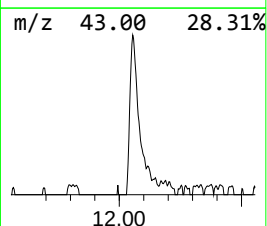
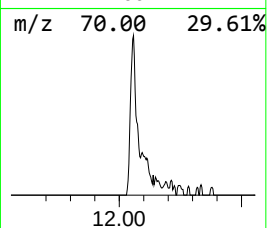
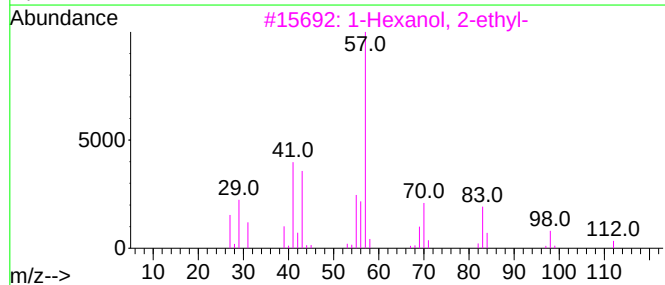
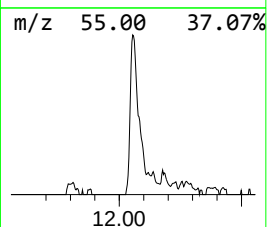
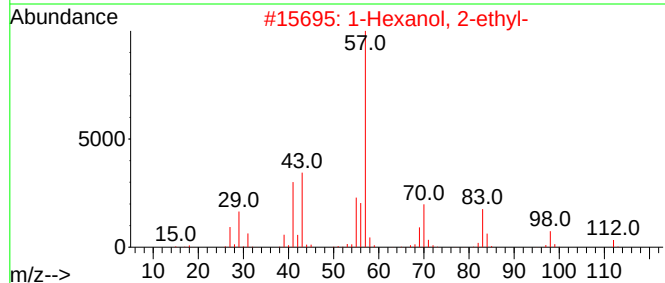
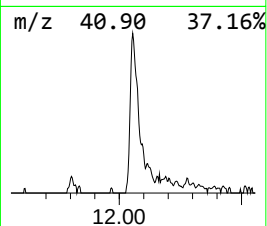
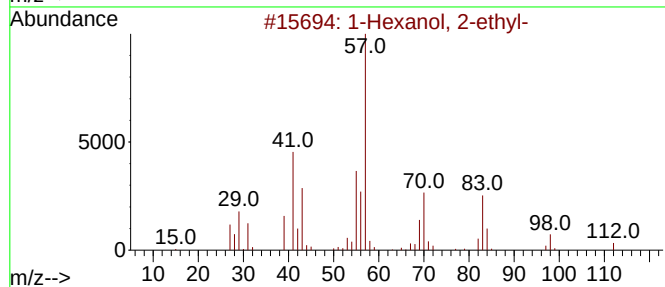
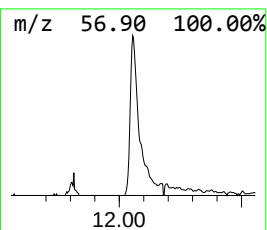
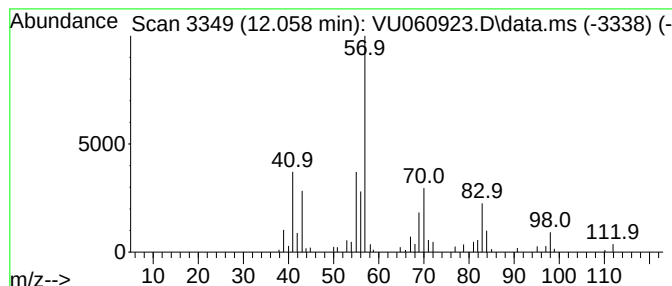
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Quant Title : TRACE VOA SFAM1.0

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.058	1.98 ug/L	127317	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	90
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59



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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
Sulfur dioxide	2.084	1.1	ug/L	58805	1	6.271	261055	5.0
1-Hexanol, 2-et...	12.058	2.0	ug/L	127317	3	11.807	321516	5.0