

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
Data File : VU060910.D
Acq On : 19 Sep 2024 19:56
Operator : MD/SY
Sample : P3987-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8Q1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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: VU060910.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	50	60	83	rBV	146865	513899	26.28%	8.376%
2	1.596	90	95	111	rVB3	89456	126850	6.49%	2.067%
3	1.911	187	193	206	rVB	48235	61609	3.15%	1.004%
4	2.563	378	396	411	rBV3	94444	170610	8.72%	2.781%
5	4.653	1024	1046	1073	rBV4	83509	291943	14.93%	4.758%
6	5.055	1154	1171	1190	rBV2	80182	178711	9.14%	2.913%
7	5.718	1356	1377	1406	rBV2	151851	403180	20.62%	6.571%
8	6.242	1527	1540	1562	rBV	143408	286821	14.67%	4.675%
9	6.534	1616	1631	1665	rBV	1029168	1955705	100.00%	31.875%
10	6.682	1665	1677	1697	rVB	96646	193880	9.91%	3.160%
11	7.560	1940	1950	1965	rBV	33072	60942	3.12%	0.993%
12	7.891	2041	2053	2070	rBV	172203	311049	15.90%	5.070%
13	8.177	2132	2142	2156	rBV4	20038	33786	1.73%	0.551%
14	8.627	2272	2282	2308	rBV	169723	349348	17.86%	5.694%
15	9.412	2512	2526	2553	rBV	216958	383390	19.60%	6.249%
16	10.750	2929	2942	2960	rVB	74809	123225	6.30%	2.008%
17	11.807	3259	3271	3292	rBV	184909	309916	15.85%	5.051%
18	12.055	3336	3348	3373	rBV	47920	100083	5.12%	1.631%
19	12.187	3377	3389	3406	rVB	170689	280508	14.34%	4.572%

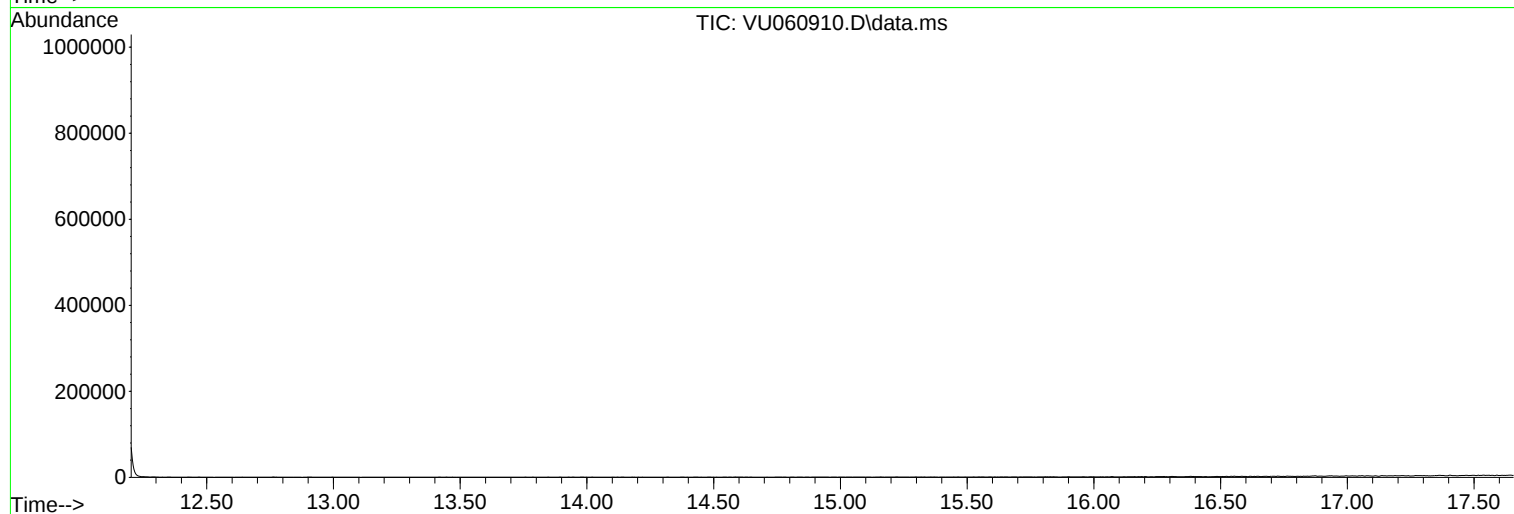
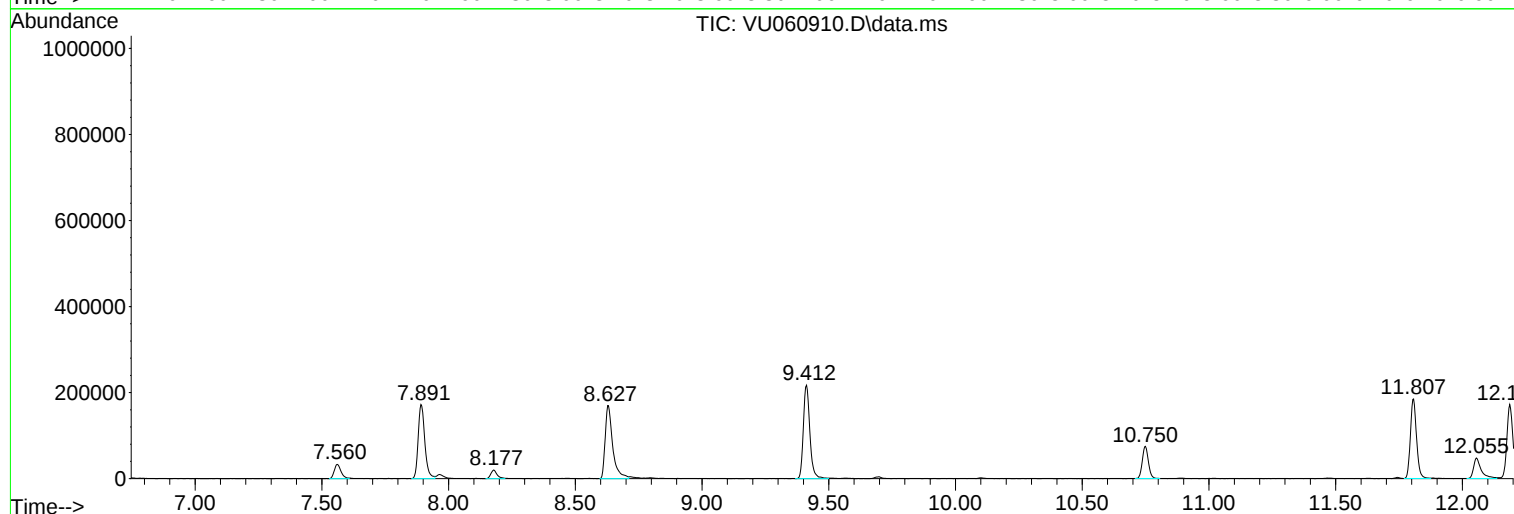
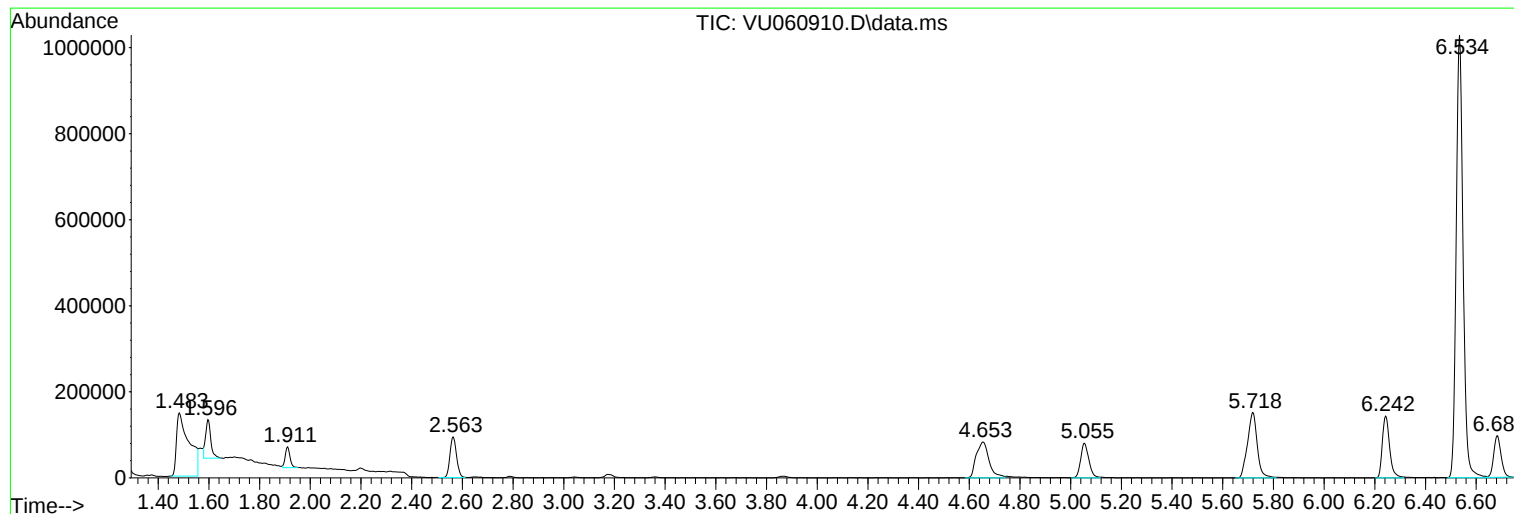
Sum of corrected areas: 6135455

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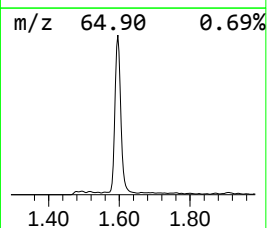
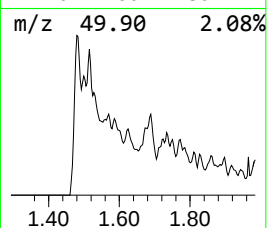
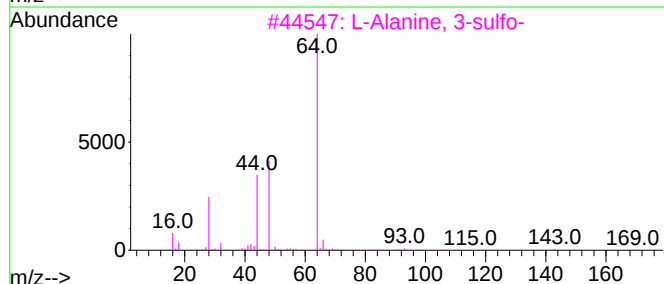
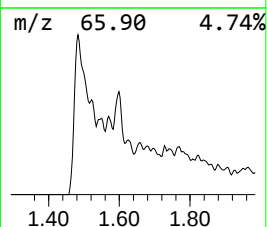
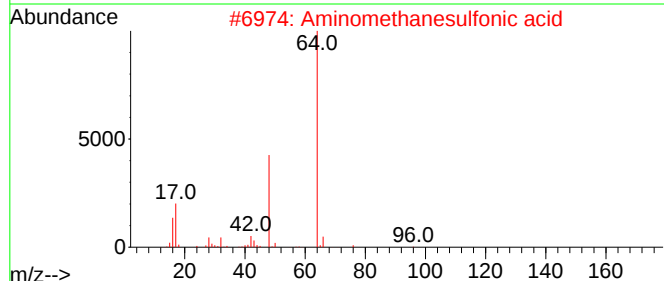
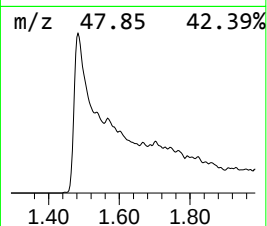
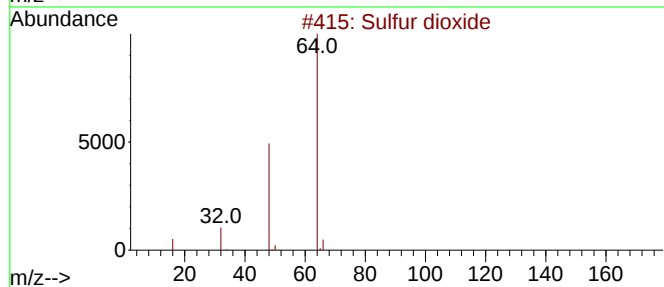
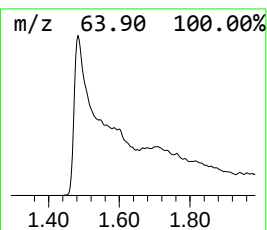
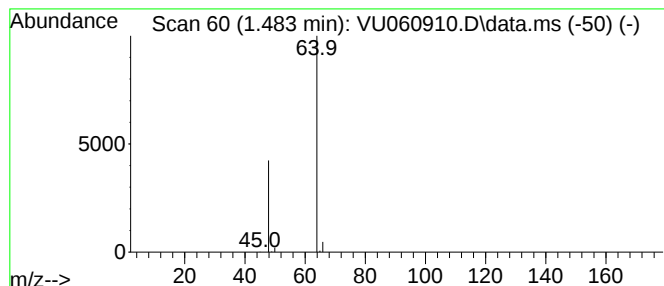
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.483	8.96 ug/L	513899	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			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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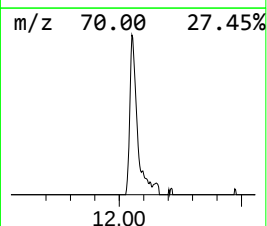
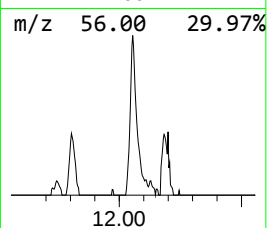
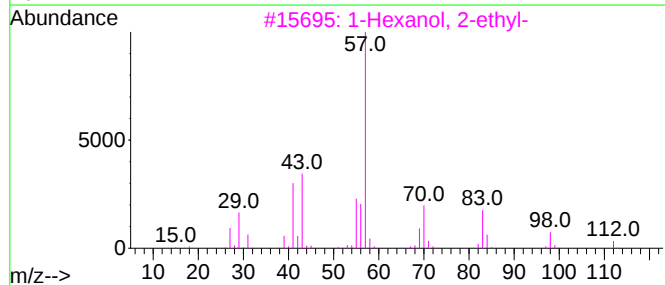
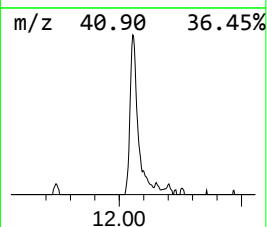
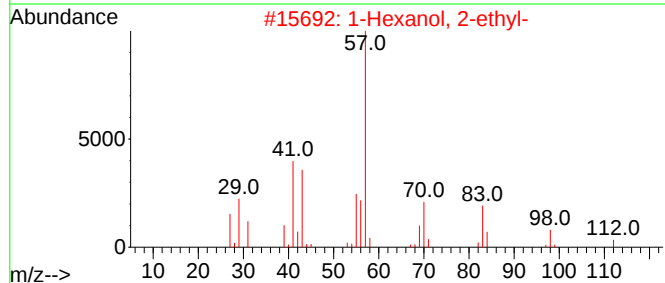
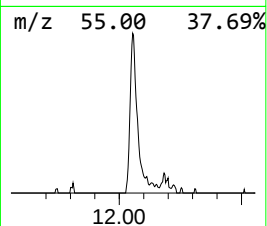
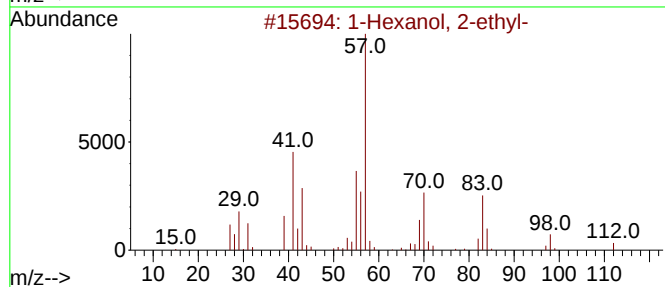
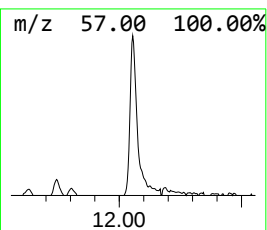
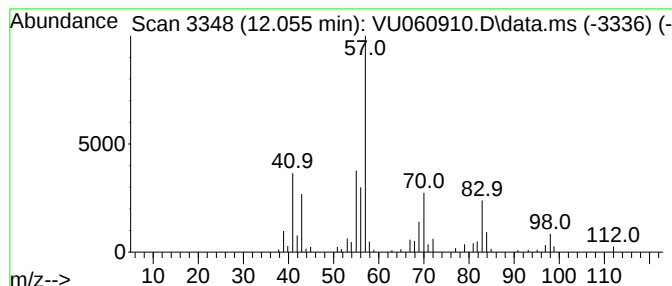
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.055	1.61 ug/L	100083	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	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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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	1.483	9.0	ug/L	513899	1	6.242	286821	5.0
1-Hexanol, 2-et...	12.055	1.6	ug/L	100083	3	11.807	309916	5.0