

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051619.D
 Acq On : 31 Oct 2022 18:25
 Operator : JC/MD
 Sample : N5353-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWR2

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\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	23	rVB3	12211	15356	1.46%	0.221%
2	1.466	30	39	52	rBV	215279	380105	36.03%	5.458%
3	1.597	75	80	115	rVB3	111939	295439	28.01%	4.242%
4	1.909	170	177	191	rVB	77356	105842	10.03%	1.520%
5	2.565	368	381	393	rBV	99401	161201	15.28%	2.315%
6	3.044	519	530	544	rVB3	7946	15782	1.50%	0.227%
7	3.861	759	784	789	rBV6	10633	33775	3.20%	0.485%
8	4.617	1008	1019	1063	rBV	185830	487275	46.19%	6.997%
9	5.060	1139	1157	1188	rBV2	153796	363550	34.46%	5.221%
10	5.723	1340	1363	1393	rBV2	261721	721672	68.41%	10.363%
11	6.247	1512	1526	1544	rBV2	214096	413135	39.16%	5.933%
12	6.543	1605	1618	1632	rBV3	39241	75043	7.11%	1.078%
13	6.690	1650	1664	1683	rBV	193338	381060	36.12%	5.472%
14	7.565	1924	1936	1955	rBV2	70500	125925	11.94%	1.808%
15	7.896	2026	2039	2056	rBV	233896	410192	38.88%	5.890%
16	8.179	2116	2127	2144	rBV	45082	77706	7.37%	1.116%
17	8.552	2234	2243	2256	rBV2	20054	33264	3.15%	0.478%
18	8.632	2256	2268	2305	rBV	563188	1054926	100.00%	15.149%
19	9.417	2497	2512	2535	rBV	333766	562529	53.32%	8.078%
20	10.755	2913	2928	2941	rBV	192077	304797	28.89%	4.377%
21	10.893	2959	2971	2981	rVB2	10679	17007	1.61%	0.244%
22	11.809	3244	3256	3281	rBV	265083	439503	41.66%	6.311%
23	12.060	3323	3334	3349	rBV2	45143	85582	8.11%	1.229%
24	12.192	3363	3375	3391	rBV	243062	403145	38.22%	5.789%

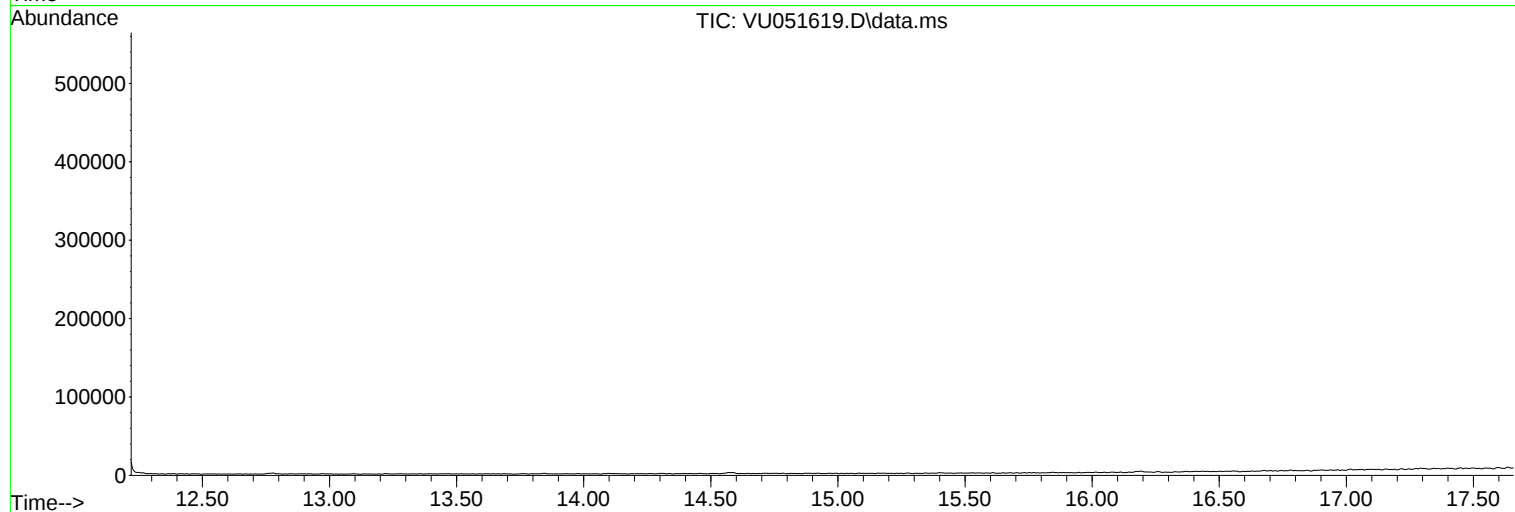
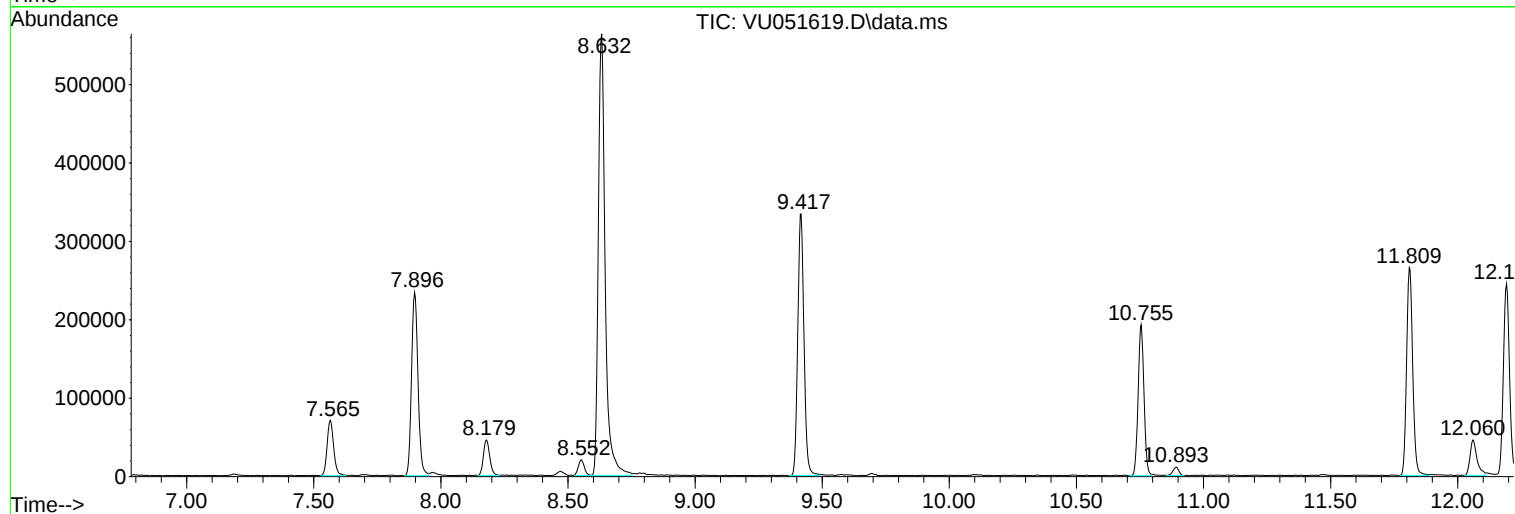
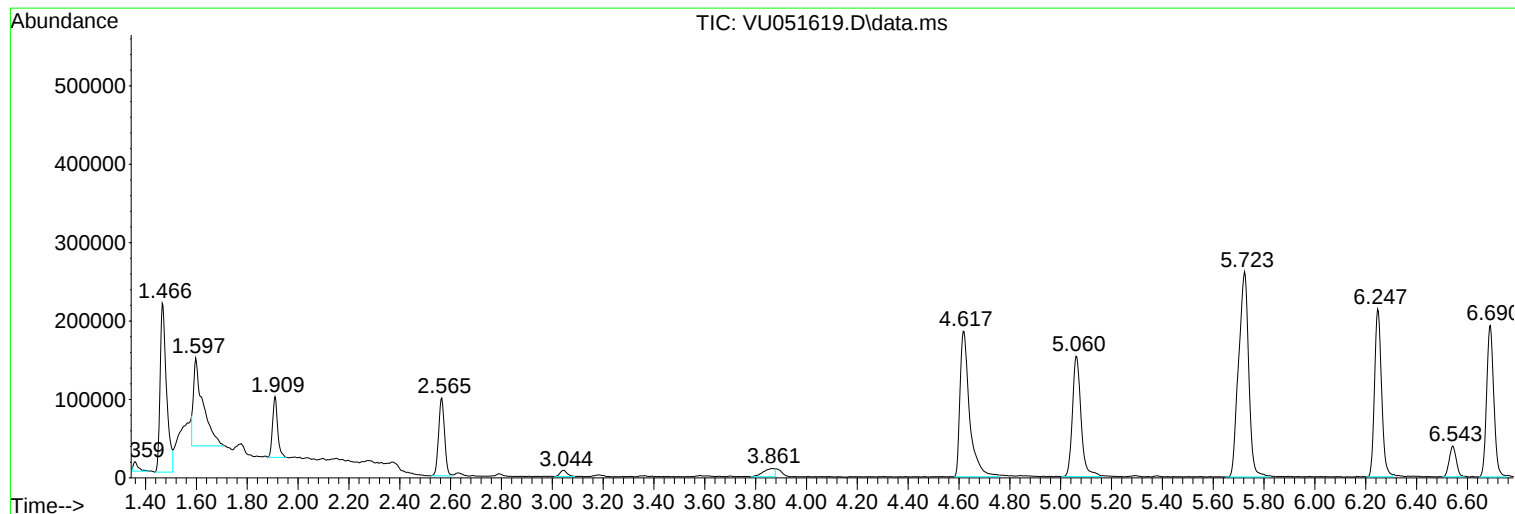
Sum of corrected areas: 6963811

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ALS Vial : 17 Sample Multiplier: 1

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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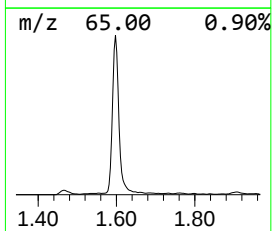
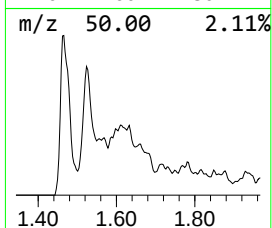
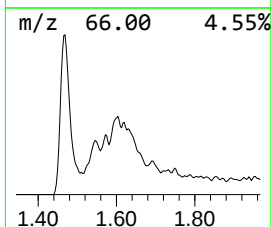
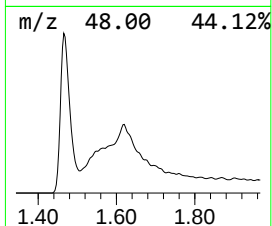
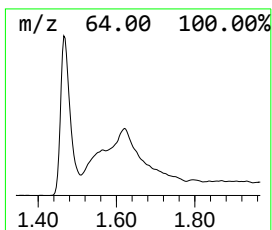
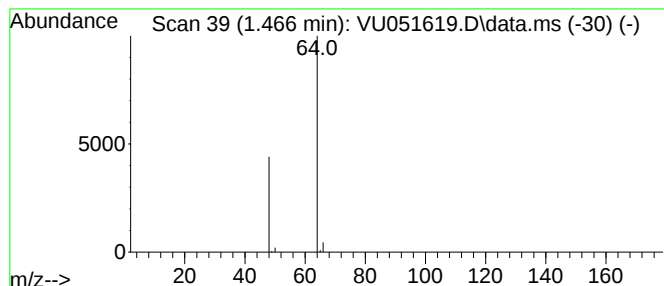
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.466	4.60 ug/L	380105	1,4-Difluorobenzene	6.250

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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4



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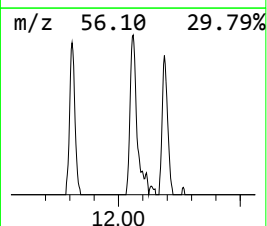
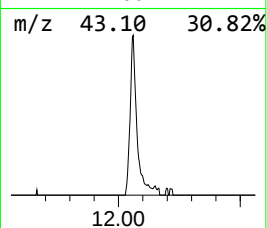
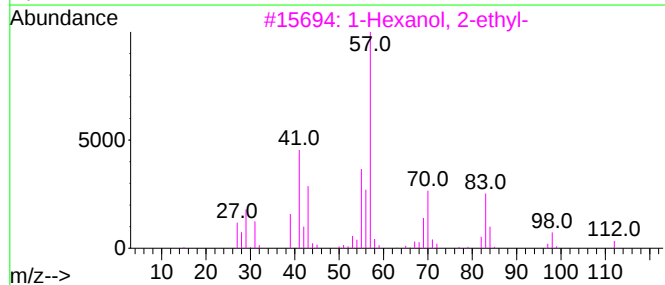
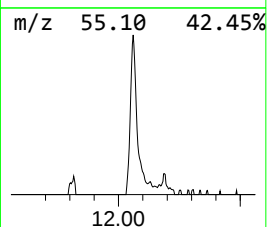
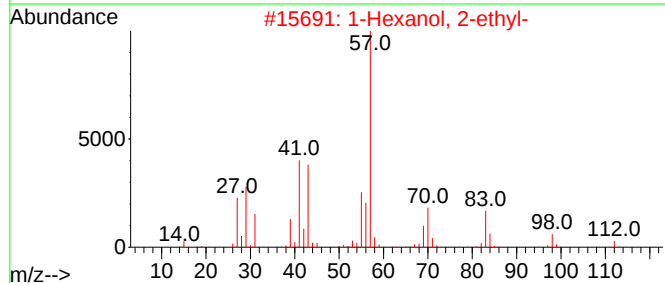
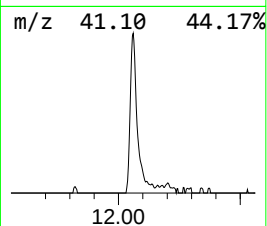
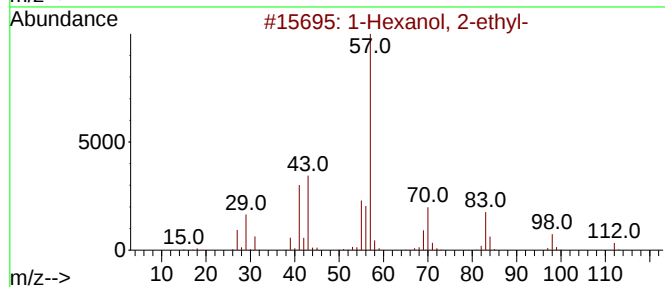
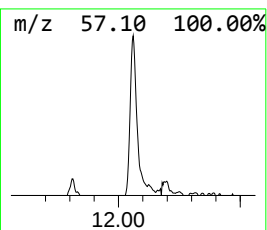
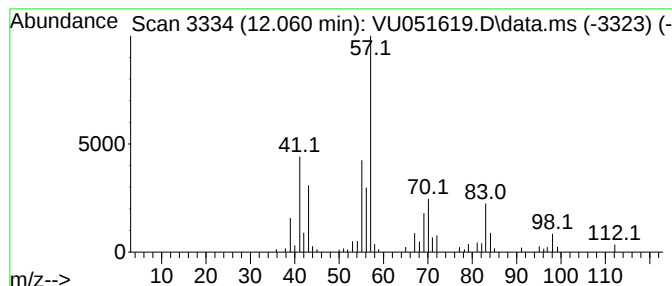
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	0.97 ug/L	85582	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



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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	1.466	4.6	ug/L	380105	1	6.250	413135	5.0
1-Hexanol, 2-et...	12.060	1.0	ug/L	85582	3	11.809	439503	5.0