

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051613.D
 Acq On : 31 Oct 2022 15:54
 Operator : JC/MD
 Sample : N5353-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWX5

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: VU051613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	31	39	50	rBV	256833	459381	42.91%	6.390%
2	1.597	75	80	102	rVB2	148627	282601	26.40%	3.931%
3	1.909	172	177	202	rVB	84975	136150	12.72%	1.894%
4	2.565	369	381	393	rBV	103949	168399	15.73%	2.342%
5	3.874	759	788	789	rBV	11513	34727	3.24%	0.483%
6	4.617	1006	1019	1051	rBV	192465	475881	44.45%	6.620%
7	5.060	1141	1157	1175	rBV	153181	346084	32.33%	4.814%
8	5.723	1343	1363	1395	rBV2	262842	731119	68.29%	10.170%
9	6.247	1510	1526	1554	rBV	218069	418973	39.14%	5.828%
10	6.539	1605	1617	1636	rBV3	39975	83720	7.82%	1.165%
11	6.687	1650	1663	1683	rBV	191433	376550	35.17%	5.238%
12	7.565	1924	1936	1951	rBV	70193	125539	11.73%	1.746%
13	7.896	2025	2039	2059	rBV	242192	428712	40.05%	5.964%
14	8.179	2113	2127	2145	rBV2	47527	79929	7.47%	1.112%
15	8.552	2232	2243	2256	rBV2	62321	106079	9.91%	1.476%
16	8.629	2256	2267	2310	rVV	575801	1070572	100.00%	14.892%
17	9.414	2499	2511	2536	rBV	319635	554886	51.83%	7.719%
18	10.755	2915	2928	2948	rBV	190939	304567	28.45%	4.237%
19	10.893	2960	2971	2981	rBV2	9063	15473	1.45%	0.215%
20	11.809	3245	3256	3278	rBV	272146	455525	42.55%	6.336%
21	12.060	3323	3334	3355	rBV2	42290	87404	8.16%	1.216%
22	12.192	3363	3375	3393	rVB	252126	424754	39.68%	5.908%
23	16.886	4827	4835	4844	rBV3	15227	21882	2.04%	0.304%

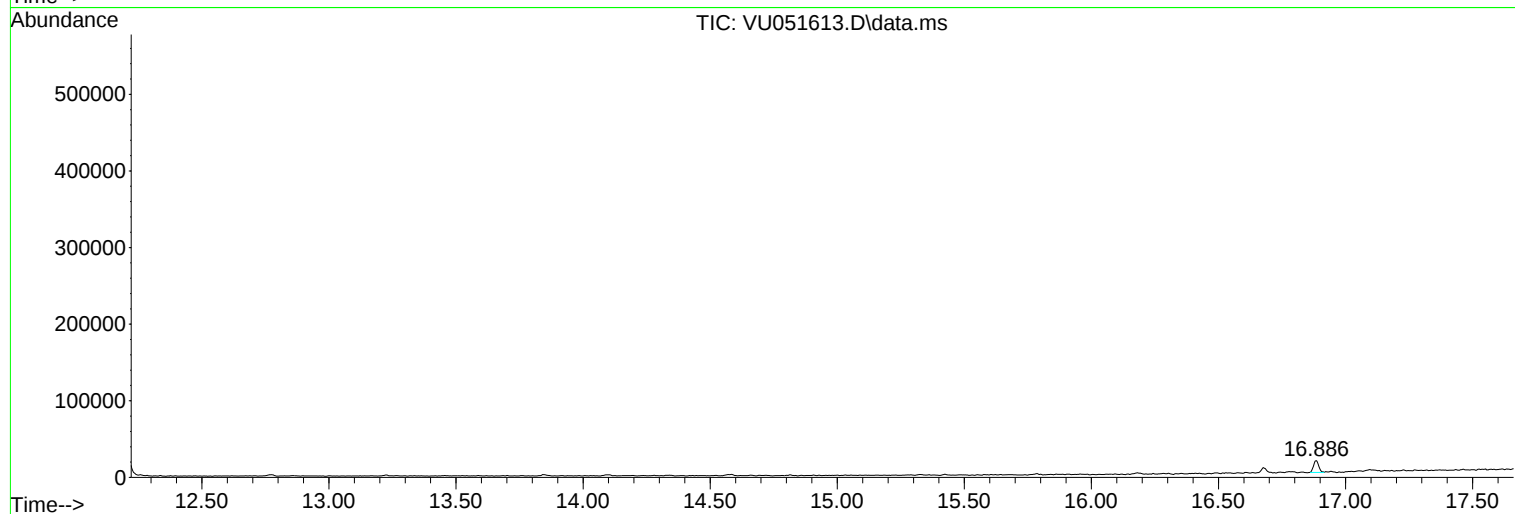
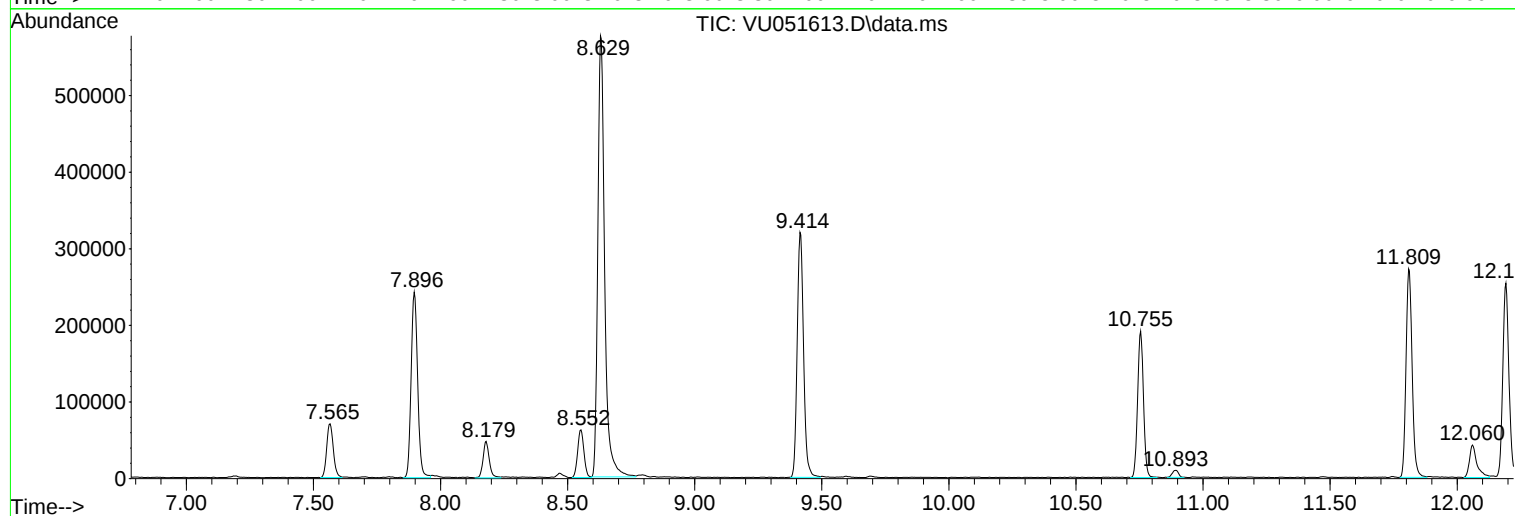
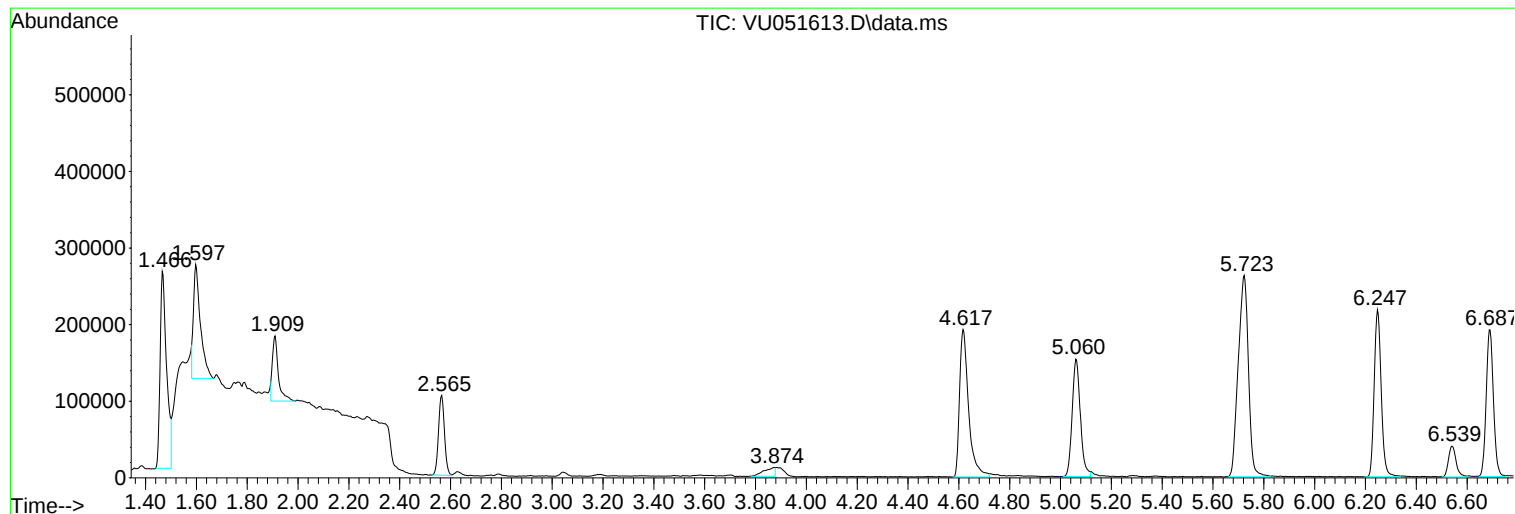
Sum of corrected areas: 7188907

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ClientSampleId :
DBWX5

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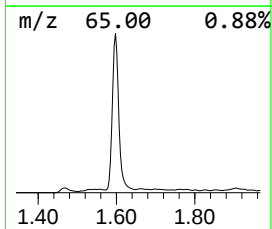
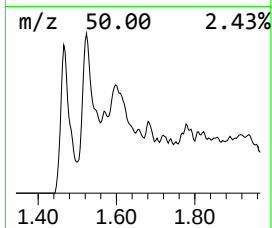
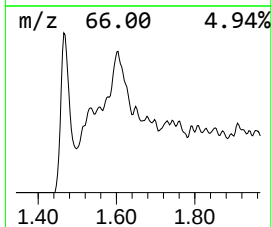
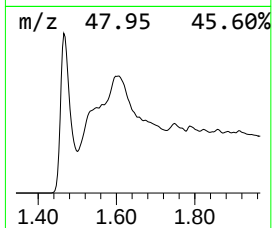
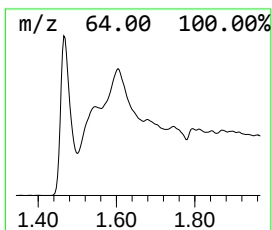
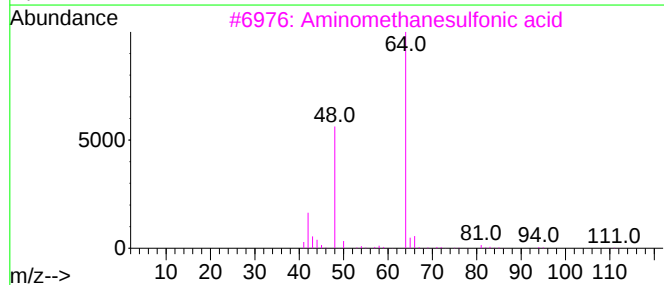
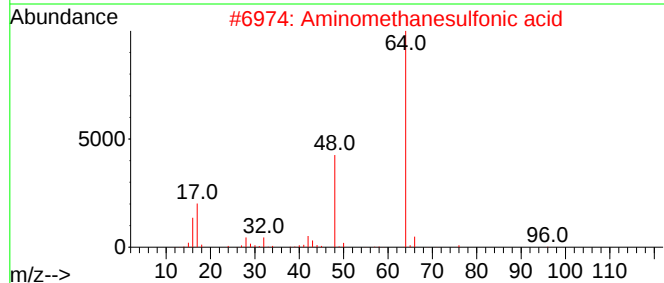
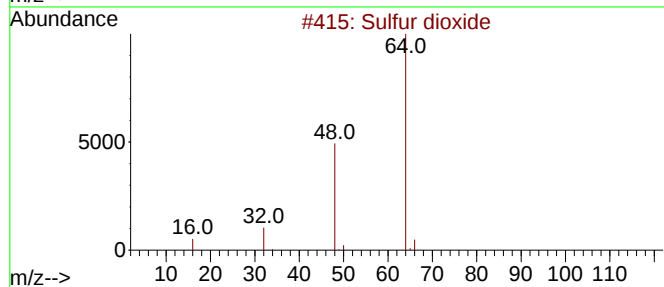
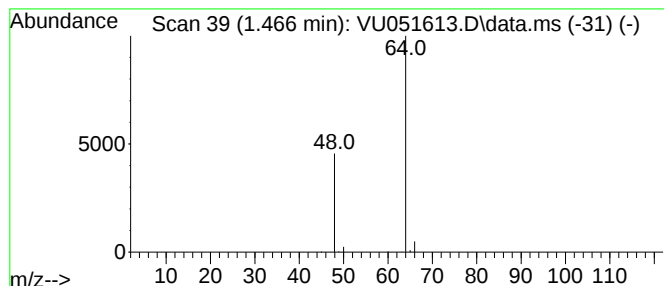
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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	5.48 ug/L	459381	1,4-Difluorobenzene	6.247

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	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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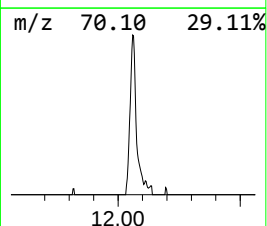
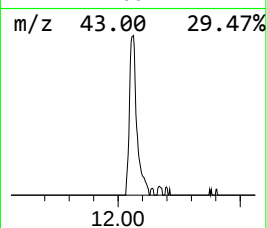
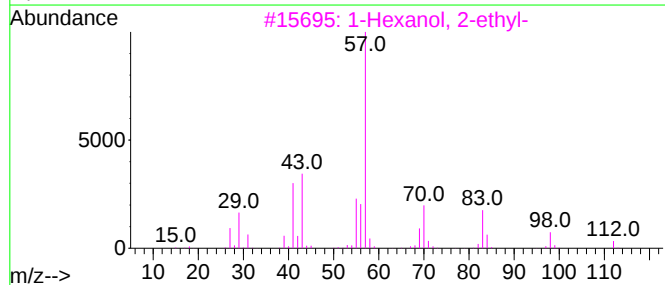
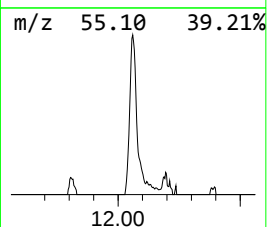
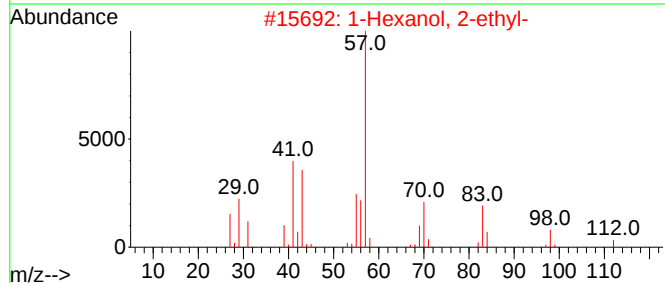
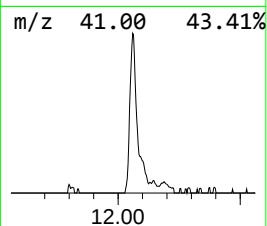
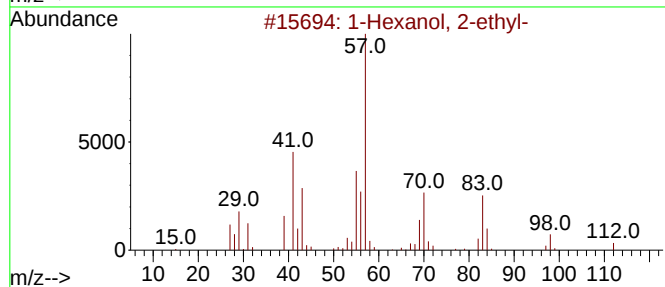
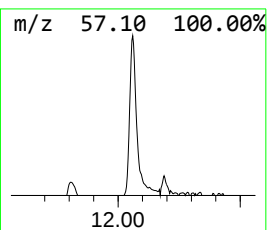
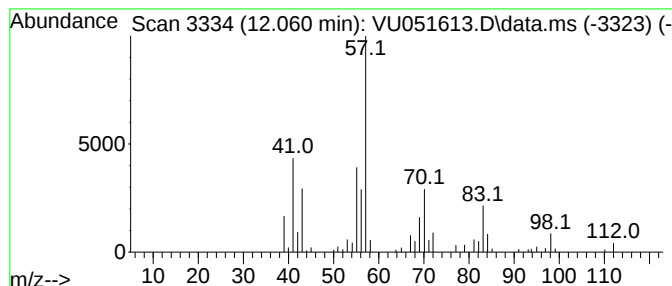
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	0.96 ug/L	87404	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	80
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	58
5			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.466	5.5	ug/L	459381	1	6.247	418973	5.0
1-Hexanol, 2-et...	12.060	1.0	ug/L	87404	3	11.809	455525	5.0