

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051635.D
 Acq On : 01 Nov 2022 01:34
 Operator : JC/MD
 Sample : N5321-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWS3

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: VU051635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	31	40	53	rBV	121915	223763	21.34%	3.379%
2	1.597	74	80	86	rBV	65524	73973	7.06%	1.117%
3	1.909	169	177	188	rBV	77336	103324	9.85%	1.560%
4	2.565	369	381	394	rBV	97465	156055	14.88%	2.356%
5	3.041	521	529	542	rVB2	6221	10890	1.04%	0.164%
6	3.854	756	782	783	rBV2	9001	22502	2.15%	0.340%
7	4.616	1008	1019	1053	rBV	189006	491385	46.87%	7.420%
8	5.060	1139	1157	1191	rBV	166930	399583	38.11%	6.034%
9	5.722	1342	1363	1392	rBV2	271750	751108	71.64%	11.342%
10	6.247	1513	1526	1554	rBV	230324	447515	42.68%	6.757%
11	6.539	1606	1617	1635	rVB9	9790	20005	1.91%	0.302%
12	6.690	1649	1664	1684	rBV	201826	394986	37.67%	5.964%
13	7.565	1923	1936	1957	rBV2	69096	124390	11.86%	1.878%
14	7.896	2022	2039	2058	rBV	244150	424371	40.48%	6.408%
15	8.179	2116	2127	2150	rBV	43889	76602	7.31%	1.157%
16	8.632	2255	2268	2300	rBV	552825	1048454	100.00%	15.832%
17	9.417	2498	2512	2538	rBV	355090	602822	57.50%	9.103%
18	10.754	2912	2928	2947	rBV	188643	306966	29.28%	4.635%
19	10.889	2960	2970	2985	rVB3	8045	13817	1.32%	0.209%
20	11.812	3244	3257	3279	rBV	283394	465432	44.39%	7.028%
21	12.060	3324	3334	3348	rBV3	26659	53127	5.07%	0.802%
22	12.192	3361	3375	3398	rBV	248247	411505	39.25%	6.214%

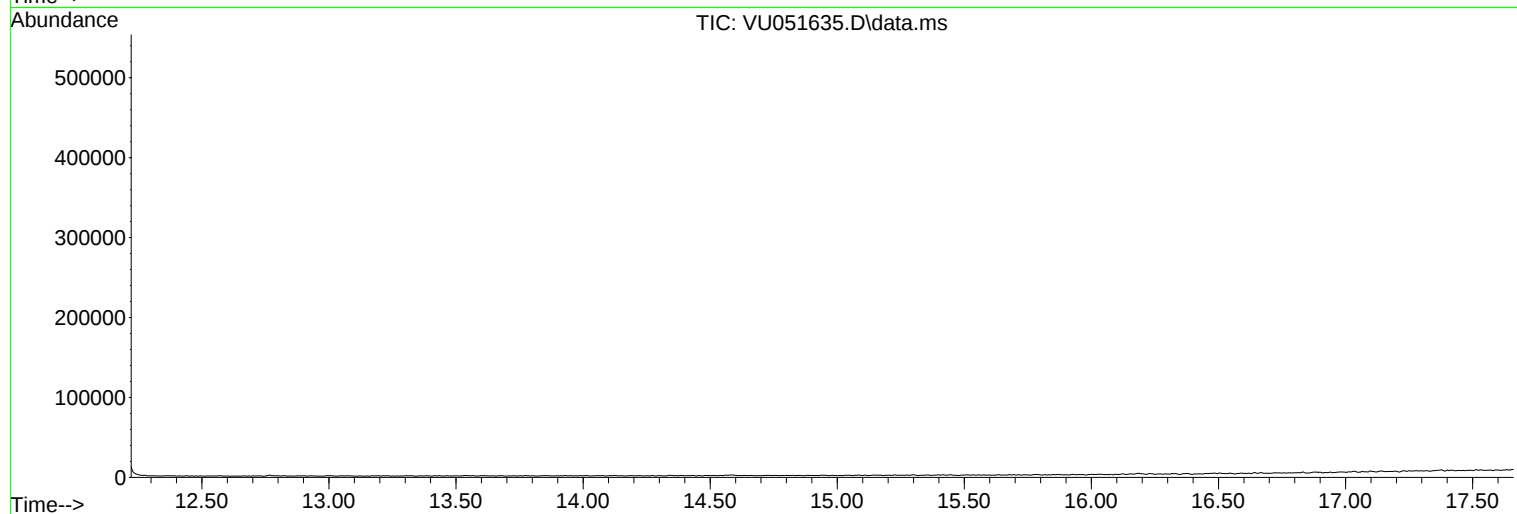
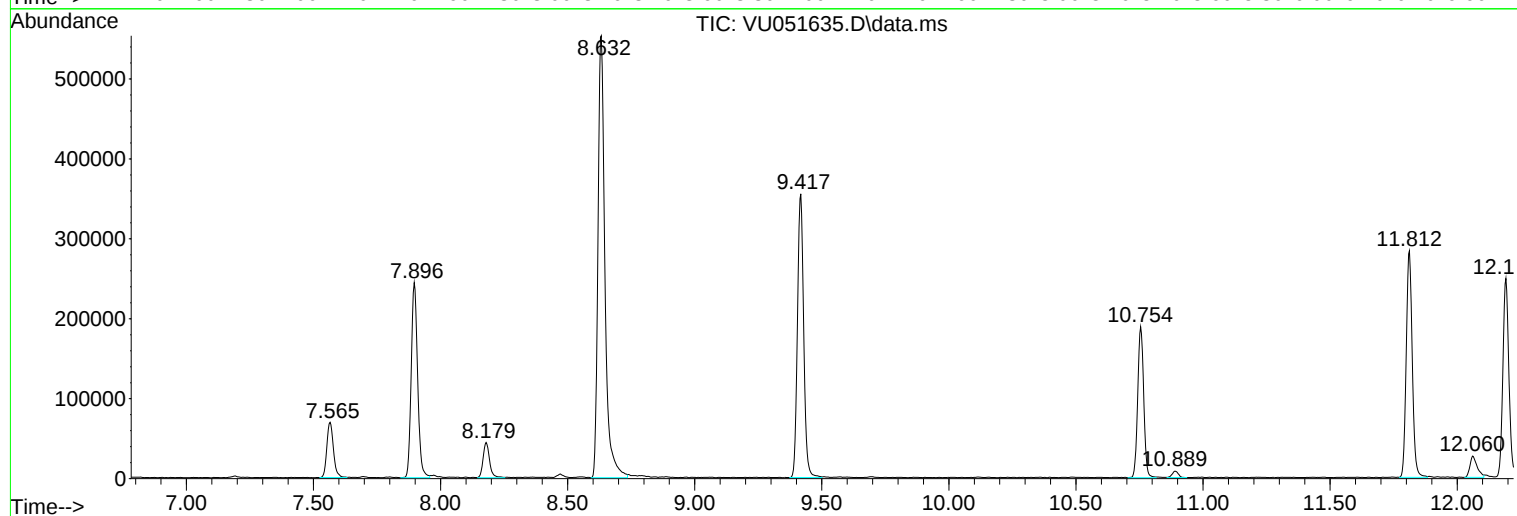
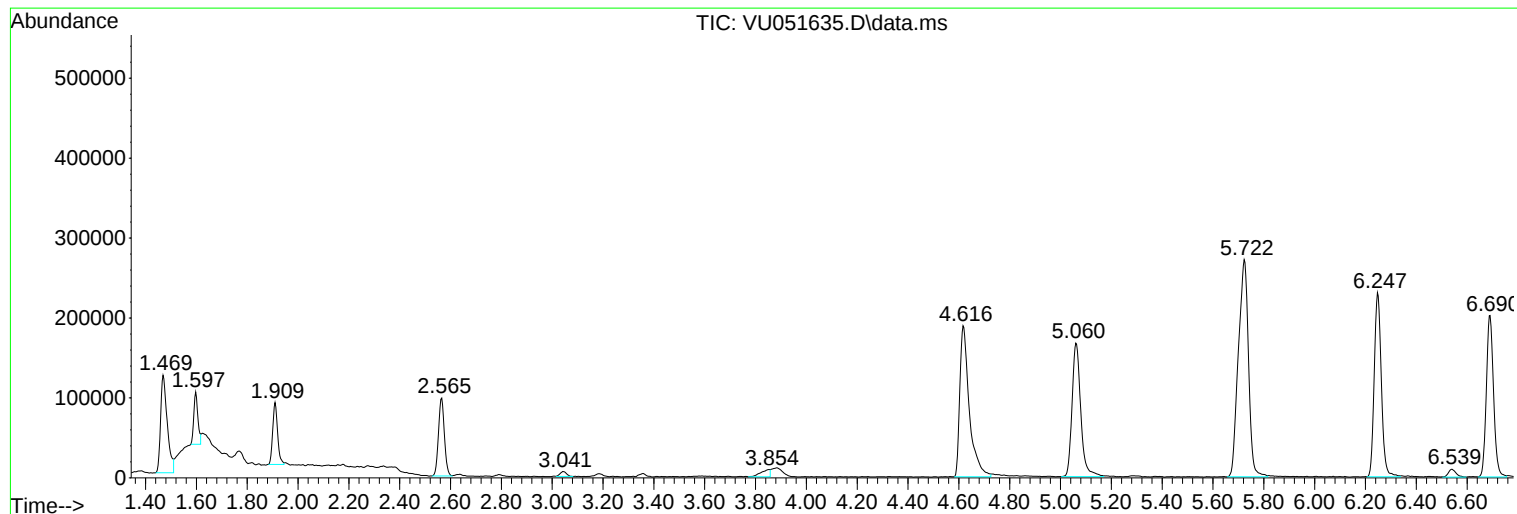
Sum of corrected areas: 6622575

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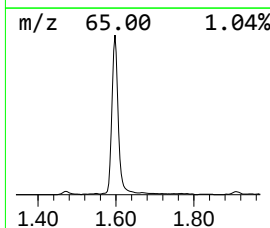
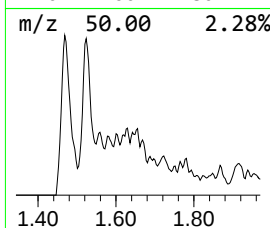
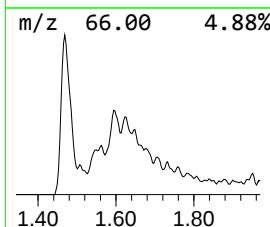
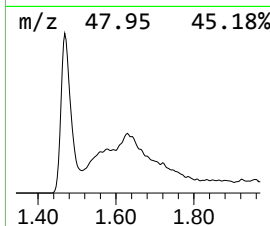
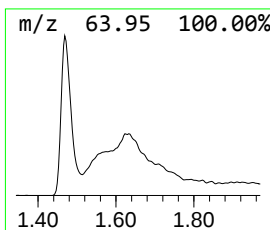
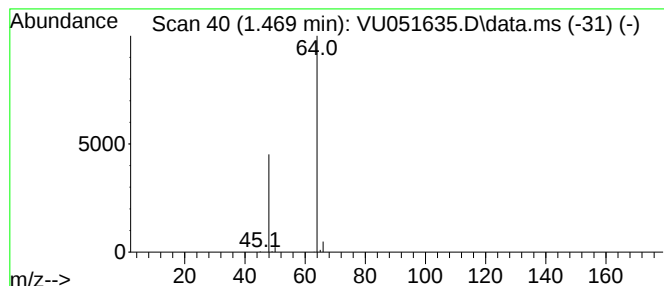
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.469	2.50 ug/L	223763	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			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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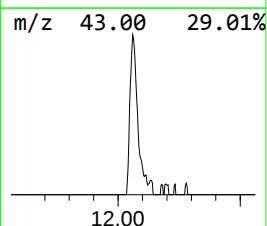
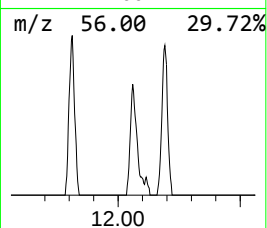
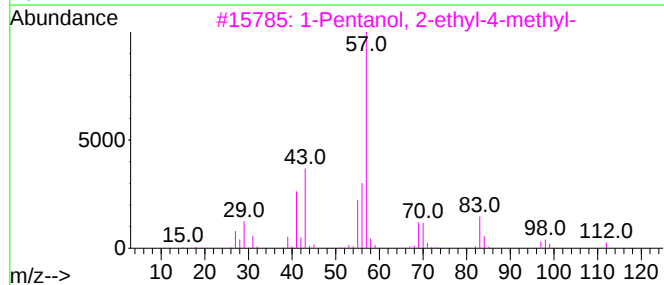
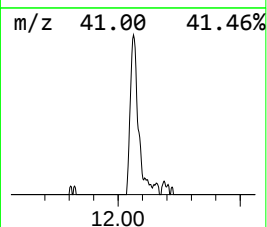
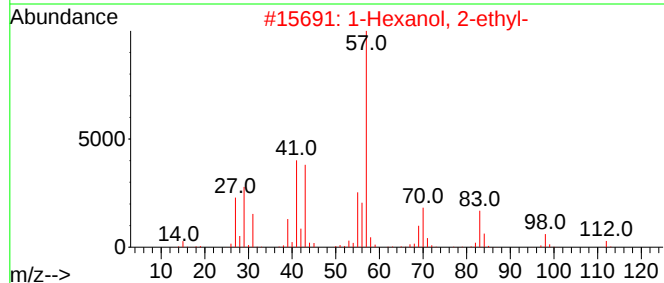
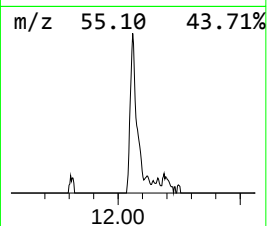
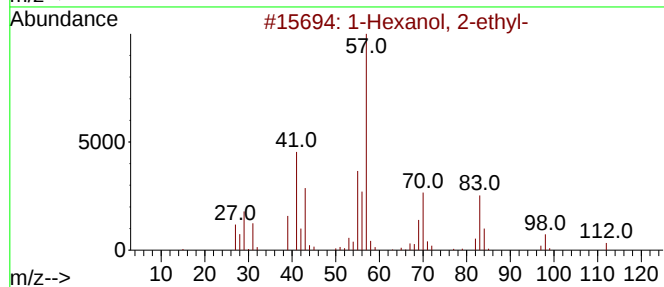
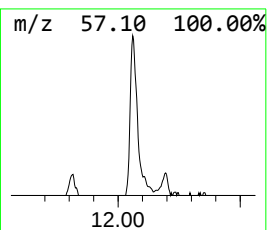
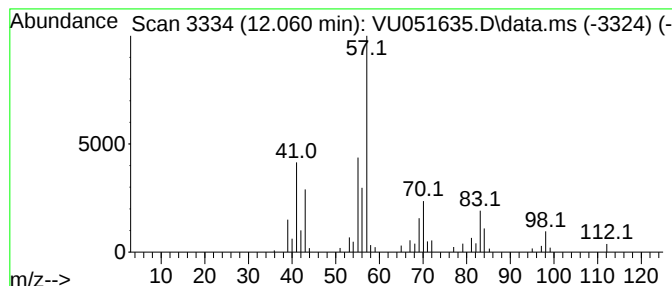
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Quant Title : TRACE VOA SFAM1.0

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	0.57 ug/L	53127	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	2.5	ug/L	223763	1	6.247	447515	5.0
1-Hexanol, 2-et...	12.060	0.6	ug/L	53127	3	11.812	465432	5.0