

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051614.D
 Acq On : 31 Oct 2022 16:19
 Operator : JC/MD
 Sample : N5353-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWX9

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: VU051614.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	30	40	51	rBV	269227	497644	26.07%	5.151%
2	1.600	76	81	87	rBV2	131758	154341	8.08%	1.598%
3	1.909	172	177	195	rVB	84725	119517	6.26%	1.237%
4	2.565	370	381	394	rBV2	108045	177666	9.31%	1.839%
5	3.353	613	626	646	rBV	86159	171737	9.00%	1.778%
6	3.883	766	791	813	rVB	10487	49119	2.57%	0.508%
7	4.620	1007	1020	1023	rBV	207127	351368	18.40%	3.637%
8	4.665	1024	1034	1063	rVB	828518	1909168	100.00%	19.762%
9	5.060	1139	1157	1177	rBV	164276	362335	18.98%	3.751%
10	5.722	1343	1363	1396	rBV2	283861	791463	41.46%	8.193%
11	6.247	1513	1526	1546	rBV	226173	433238	22.69%	4.485%
12	6.542	1604	1618	1636	rBV2	121794	233279	12.22%	2.415%
13	6.690	1650	1664	1691	rBV	207126	409044	21.43%	4.234%
14	7.565	1924	1936	1951	rBV2	72671	129021	6.76%	1.336%
15	7.896	2026	2039	2056	rBV	261503	456310	23.90%	4.723%
16	8.179	2115	2127	2140	rBV2	45189	77395	4.05%	0.801%
17	8.552	2231	2243	2256	rBV	171429	288236	15.10%	2.984%
18	8.632	2256	2268	2307	rVV	597418	1103402	57.79%	11.422%
19	9.417	2499	2512	2537	rBV	345732	598852	31.37%	6.199%
20	10.754	2915	2928	2948	rBV	199303	318237	16.67%	3.294%
21	10.889	2959	2970	2982	rVB2	13235	21468	1.12%	0.222%
22	11.809	3243	3256	3279	rBV	286660	486551	25.48%	5.036%
23	12.060	3323	3334	3351	rBV3	26162	54875	2.87%	0.568%
24	12.192	3363	3375	3407	rVB	270860	466295	24.42%	4.827%

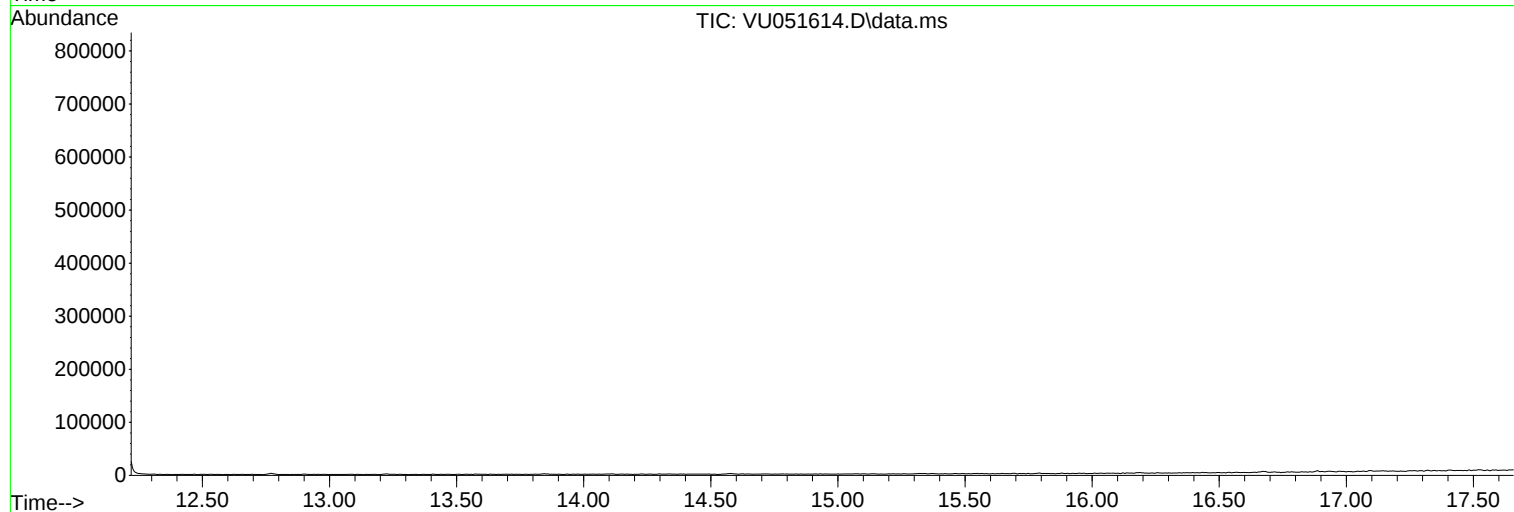
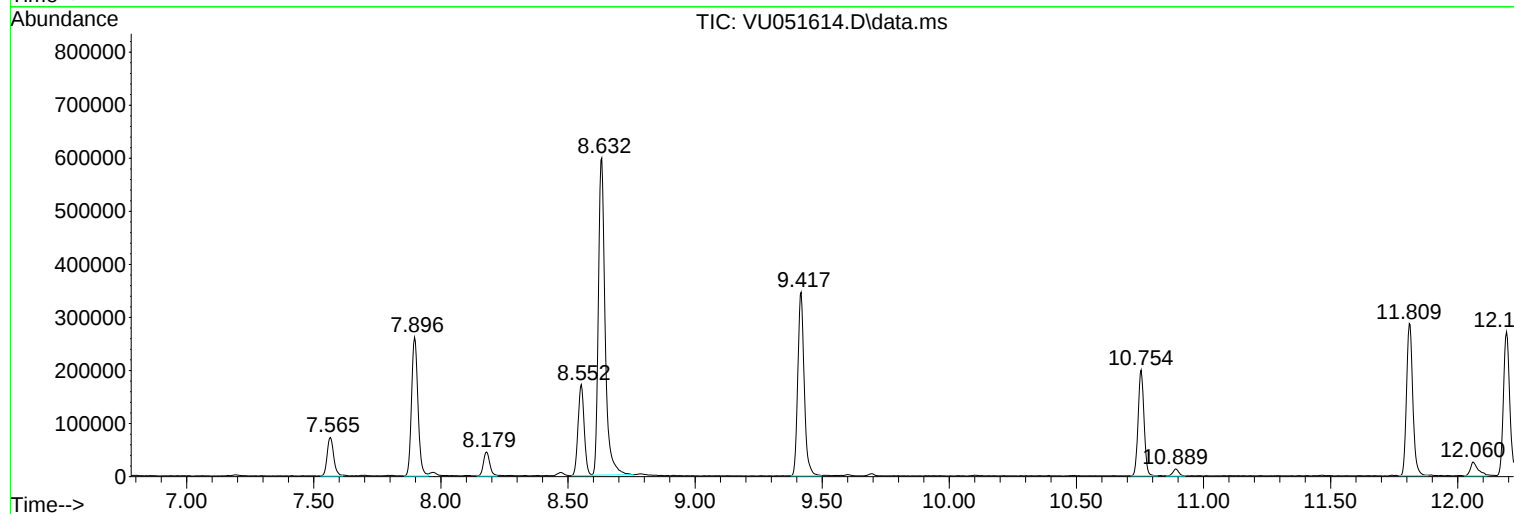
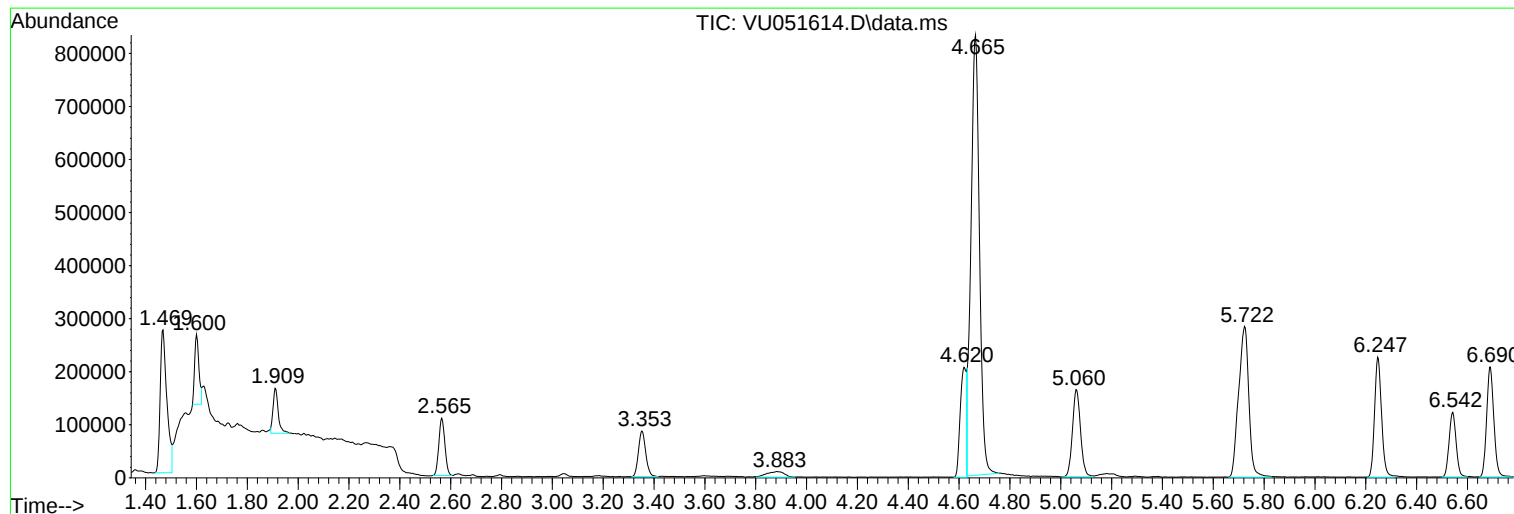
Sum of corrected areas: 9660561

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ALS Vial : 12 Sample Multiplier: 1

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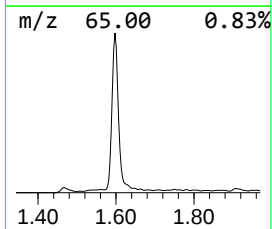
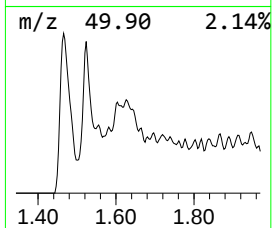
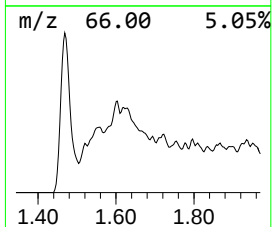
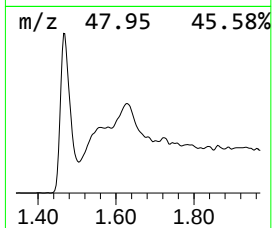
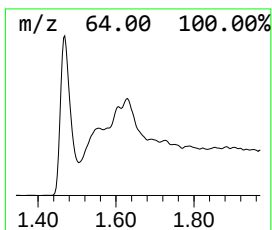
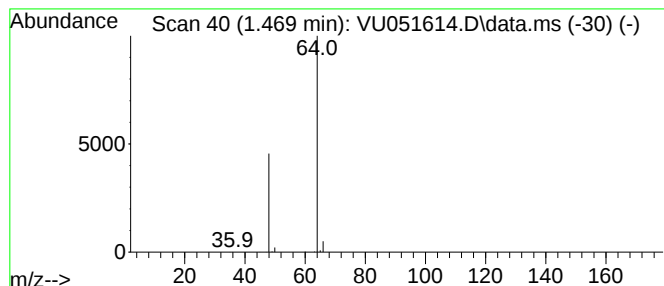
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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	5.74 ug/L	497644	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			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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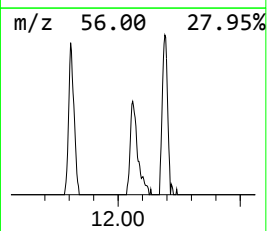
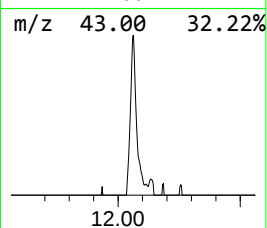
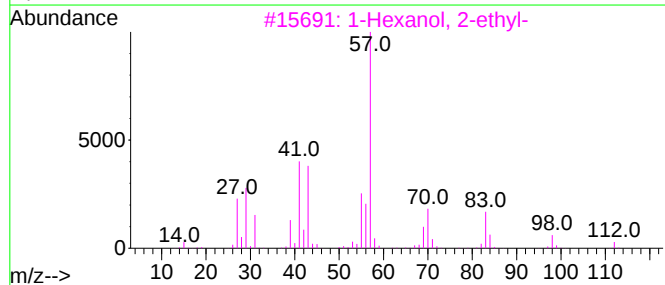
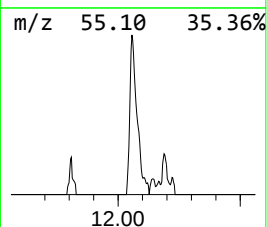
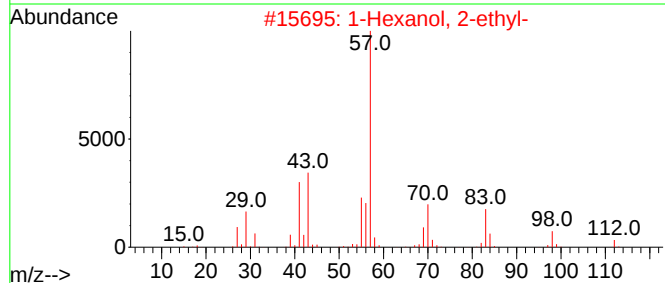
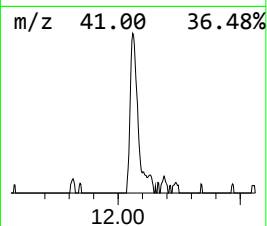
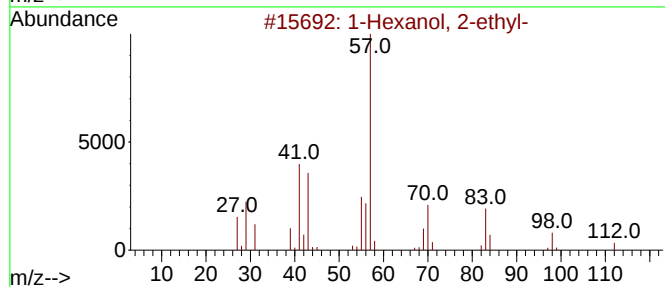
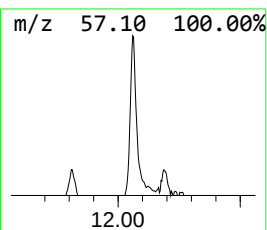
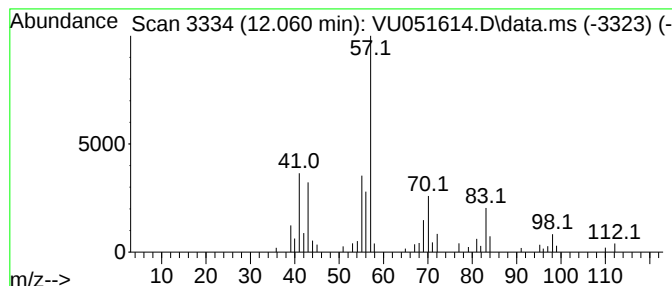
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	0.56 ug/L	54875	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	78
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	59
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	5.7	ug/L	497644	1	6.247	433238	5.0
1-Hexanol, 2-et...	12.060	0.6	ug/L	54875	3	11.812	486551	5.0