

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061523\
 Data File : VU054544.D
 Acq On : 15 Jun 2023 23:31
 Operator : MD/SY
 Sample : 03253-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXYY8

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\SFAMUTR060723WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.518	55	71	82	rBV2	33408	117094	12.40%	1.449%
2	1.599	89	96	110	rVB	79137	93877	9.94%	1.162%
3	1.914	186	194	206	rVB	99555	130610	13.83%	1.616%
4	2.566	384	397	409	rBV	146644	237779	25.18%	2.943%
5	2.647	412	422	441	rVV2	14827	38983	4.13%	0.482%
6	2.795	458	468	478	rBV	16772	29055	3.08%	0.360%
7	3.049	536	547	558	rVB4	5231	10111	1.07%	0.125%
8	4.631	1021	1039	1063	rBV	131565	394005	41.72%	4.876%
9	5.058	1157	1172	1196	rVB	180271	406304	43.02%	5.029%
10	5.721	1357	1378	1413	rBV2	343568	909425	96.30%	11.256%
11	6.245	1527	1541	1565	rBV	319493	626005	66.29%	7.748%
12	6.685	1664	1678	1698	rBV	225478	454966	48.18%	5.631%
13	7.563	1939	1951	1966	rBV	86953	158347	16.77%	1.960%
14	7.894	2041	2054	2069	rBV	386246	686617	72.71%	8.498%
15	7.968	2071	2077	2095	rVB2	18359	35373	3.75%	0.438%
16	8.177	2132	2142	2162	rBV	51960	95916	10.16%	1.187%
17	8.470	2224	2233	2243	rVB2	11185	17863	1.89%	0.221%
18	8.631	2270	2283	2315	rBV	469957	944365	100.00%	11.688%
19	8.788	2323	2332	2341	rBV3	16516	27782	2.94%	0.344%
20	9.412	2511	2526	2548	rBV	443153	758507	80.32%	9.388%
21	9.692	2603	2613	2626	rBV4	8514	14902	1.58%	0.184%
22	10.100	2729	2740	2748	rBV4	6315	10885	1.15%	0.135%
23	10.753	2930	2943	2966	rVB2	165486	278770	29.52%	3.450%
24	10.888	2976	2985	2998	rBV2	23457	37934	4.02%	0.469%
25	11.688	3224	3234	3245	rBV4	7759	14273	1.51%	0.177%
26	11.807	3258	3271	3293	rBV	458795	744438	78.83%	9.214%
27	12.061	3338	3350	3367	rBV2	43999	103847	11.00%	1.285%
28	12.187	3378	3389	3405	rBV	382447	632059	66.93%	7.823%
29	12.884	3597	3606	3618	rBV3	38158	59600	6.31%	0.738%
30	14.093	3965	3982	3992	rBV3	3988	10111	1.07%	0.125%

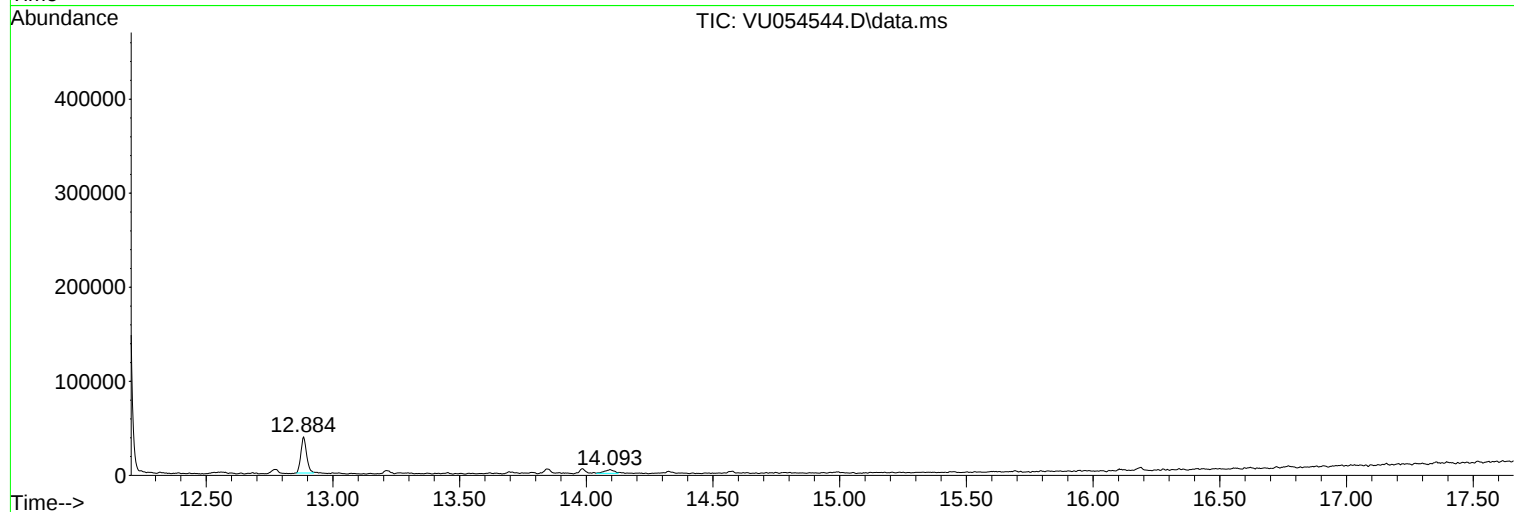
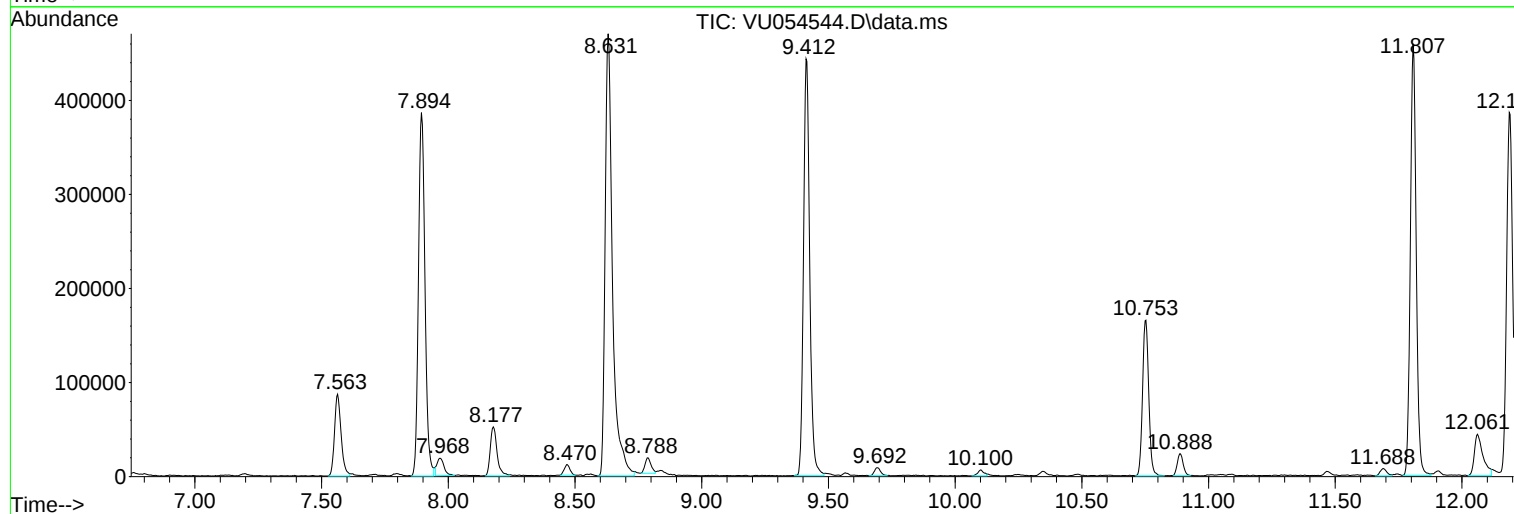
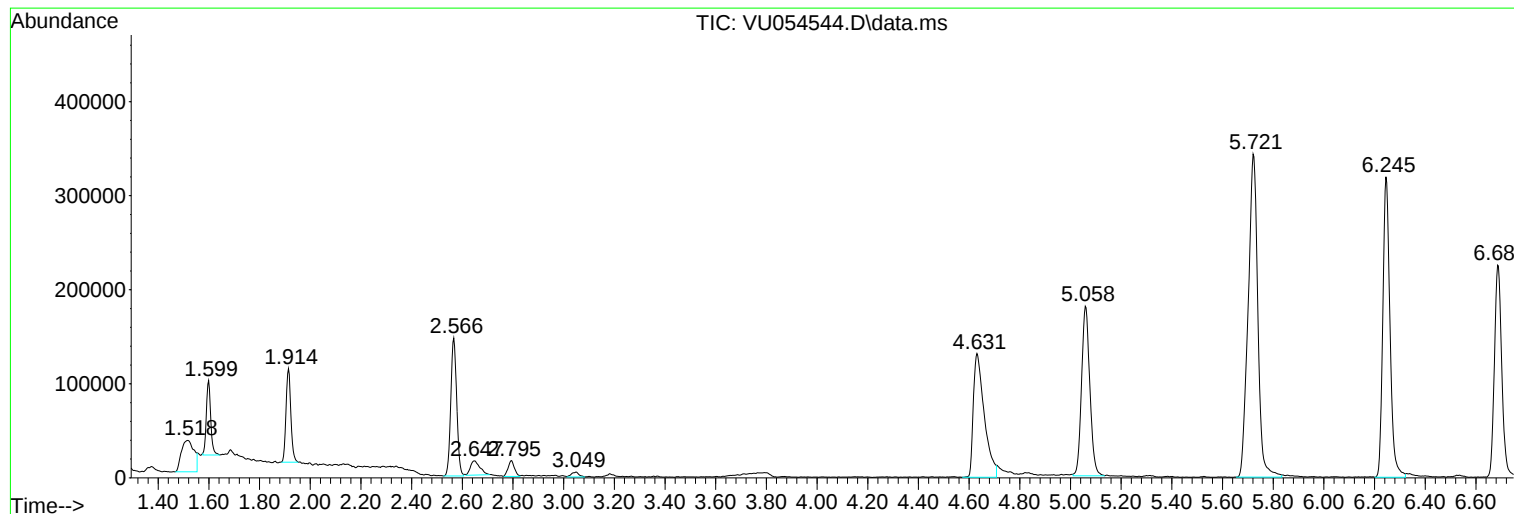
Sum of corrected areas: 8079803

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ClientSampleId :
EXYY8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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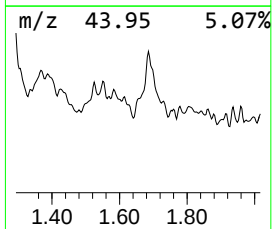
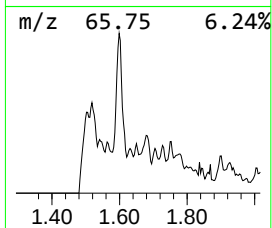
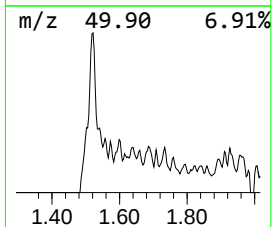
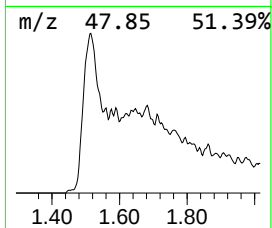
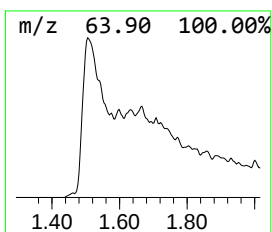
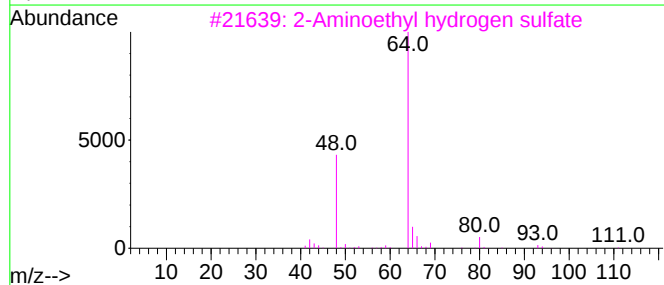
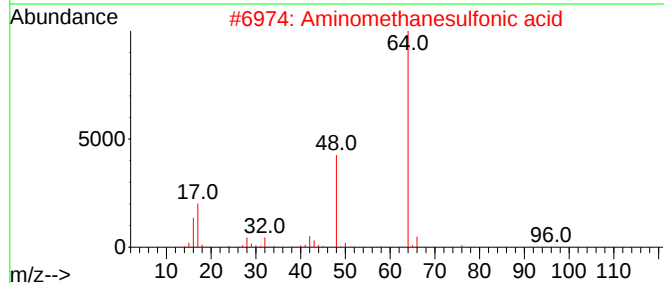
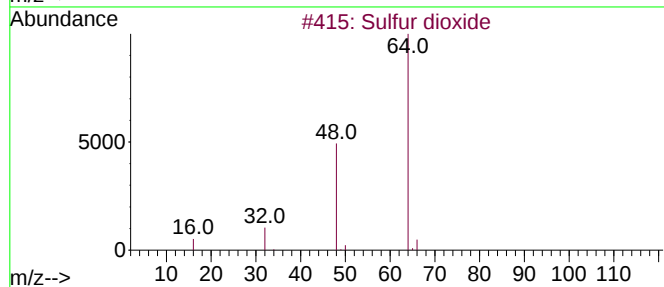
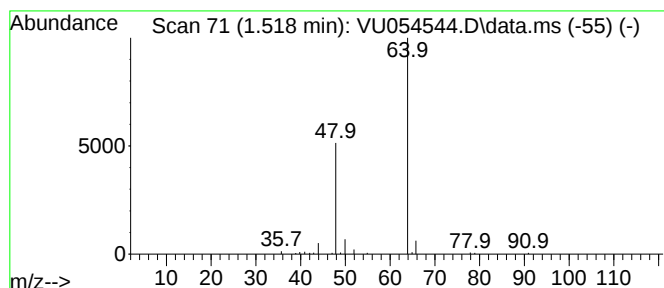
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.518	0.94 ug/L	117094	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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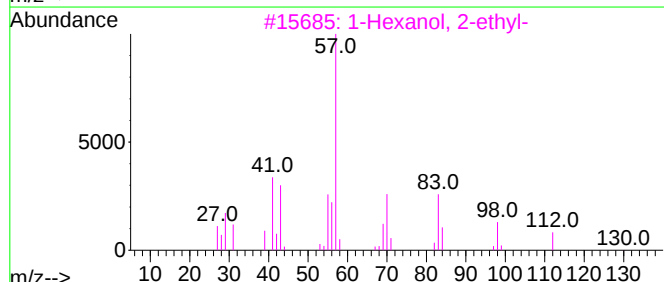
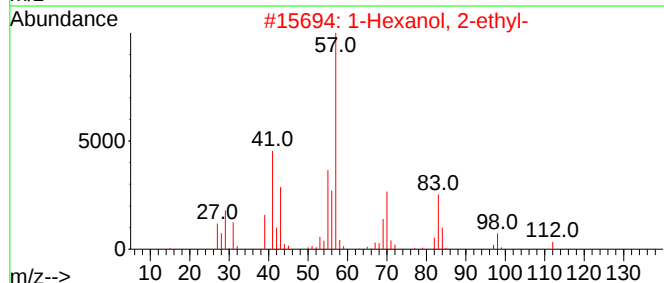
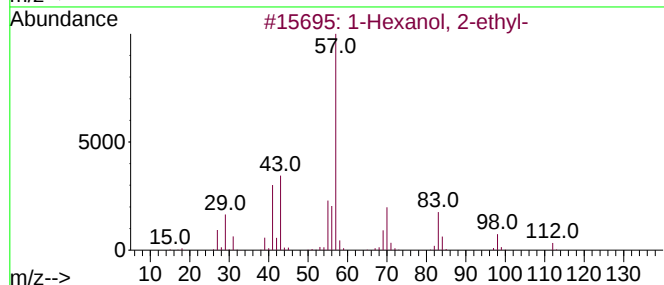
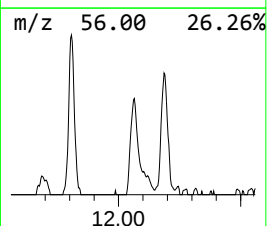
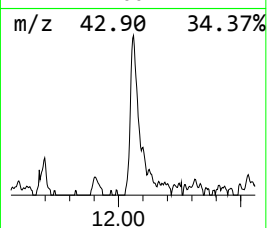
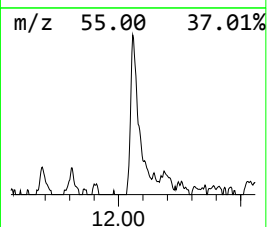
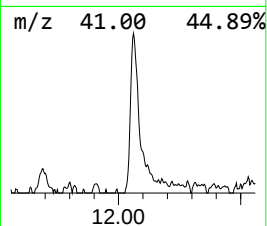
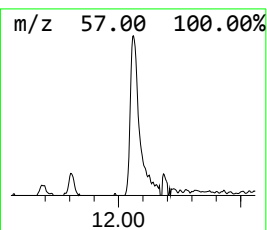
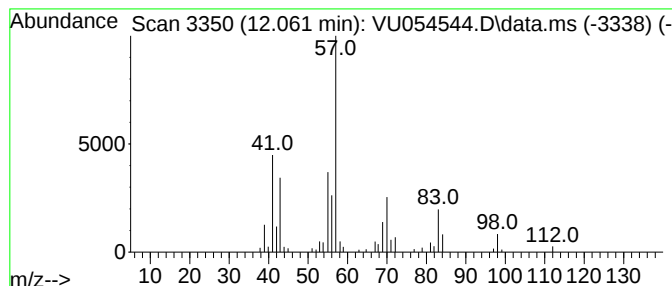
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Quant Title : TRACE VOA SFAM1.0

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.
12.061	0.70 ug/L	103847	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	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.518	0.9	ug/L	117094	1	6.245	626005	5.0
1-Hexanol, 2-et...	12.061	0.7	ug/L	103847	3	11.807	744438	5.0