

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051621.D
 Acq On : 31 Oct 2022 19:15
 Operator : JC/MD
 Sample : N5353-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWU7

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: VU051621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	35	45	56	rBV	113659	251950	2.97%	1.275%
2	1.601	73	81	122	rBV	6752198	8486644	100.00%	42.960%
3	1.913	172	178	191	rVB	87846	120808	1.42%	0.612%
4	2.565	369	381	393	rVB	102838	163588	1.93%	0.828%
5	3.350	609	625	646	rBV	1214386	2392713	28.19%	12.112%
6	4.665	1009	1034	1077	rBV2	995614	2646472	31.18%	13.397%
7	5.060	1141	1157	1182	rBV	163305	370550	4.37%	1.876%
8	5.723	1341	1363	1382	rBV2	280611	771829	9.09%	3.907%
9	6.247	1512	1526	1550	rBV	242227	462338	5.45%	2.340%
10	6.690	1650	1664	1679	rBV	199979	403252	4.75%	2.041%
11	7.379	1865	1878	1901	rBV3	42848	89693	1.06%	0.454%
12	7.565	1922	1936	1949	rBV	73207	135279	1.59%	0.685%
13	7.896	2028	2039	2056	rVB	263523	449527	5.30%	2.276%
14	8.633	2255	2268	2298	rBV	602245	1127737	13.29%	5.709%
15	9.417	2499	2512	2534	rBV	356493	608474	7.17%	3.080%
16	10.755	2915	2928	2942	rBV	191517	308218	3.63%	1.560%
17	11.809	3243	3256	3275	rBV	311003	505340	5.95%	2.558%
18	12.192	3362	3375	3394	rBV	274060	460121	5.42%	2.329%

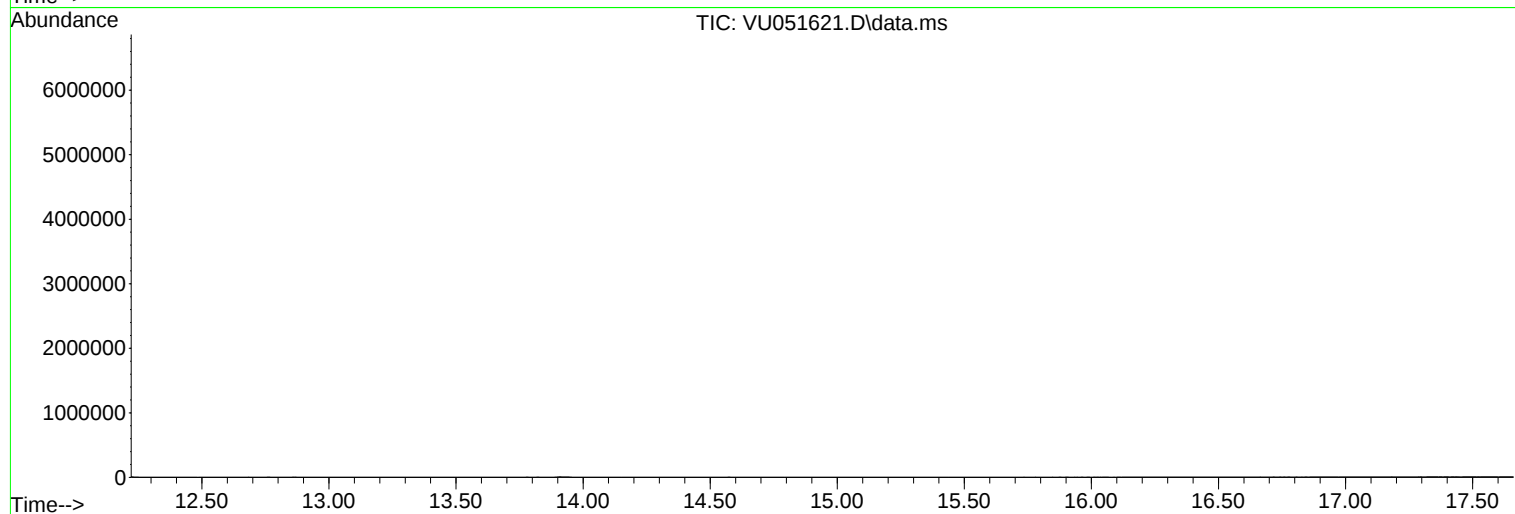
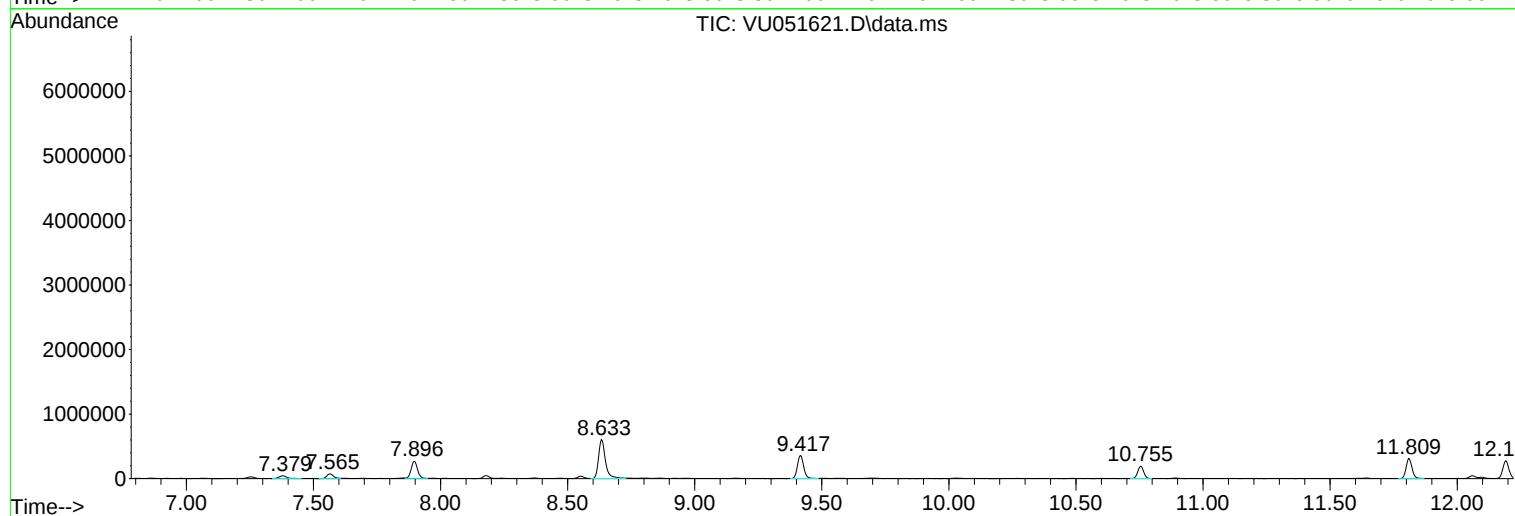
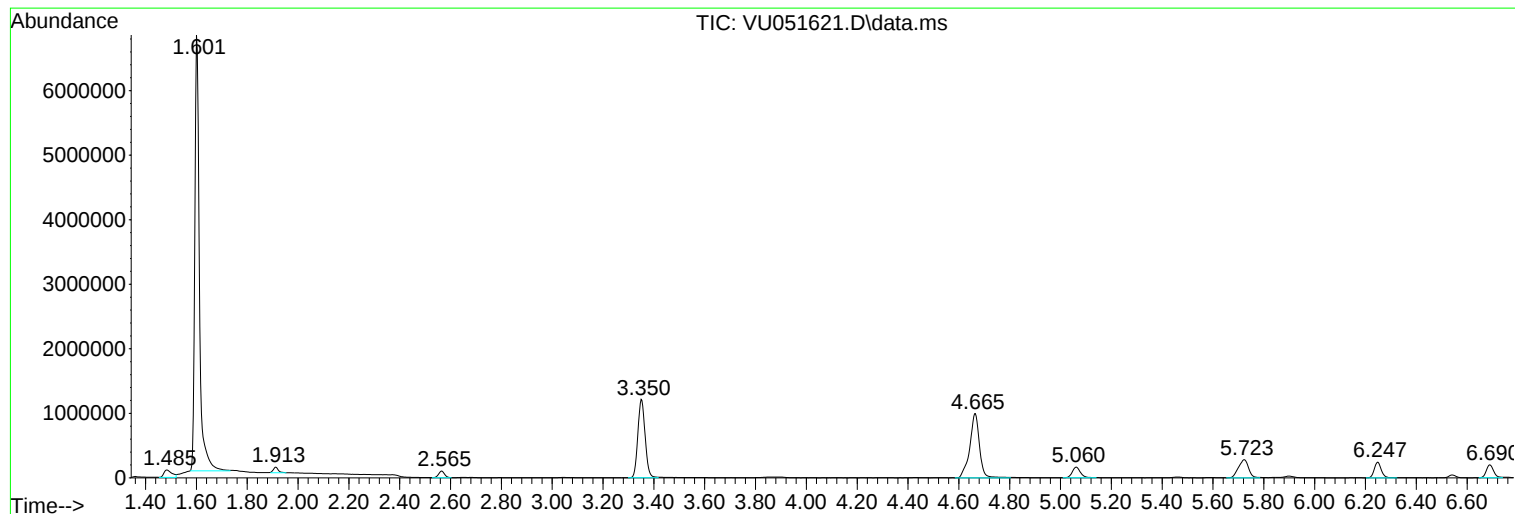
Sum of corrected areas: 19754533

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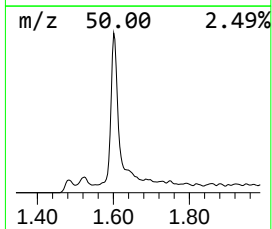
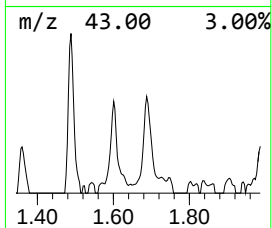
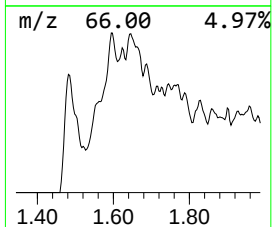
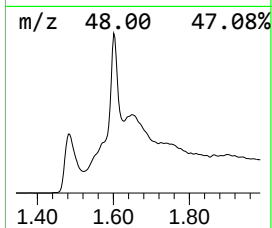
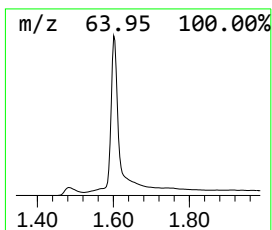
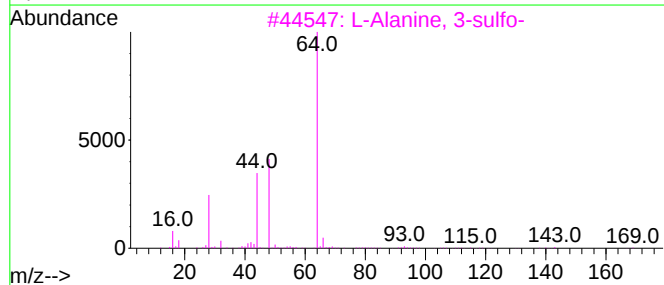
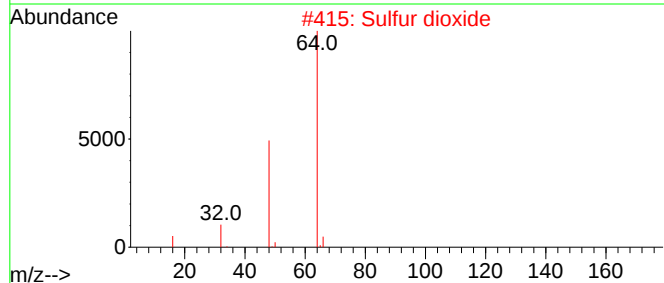
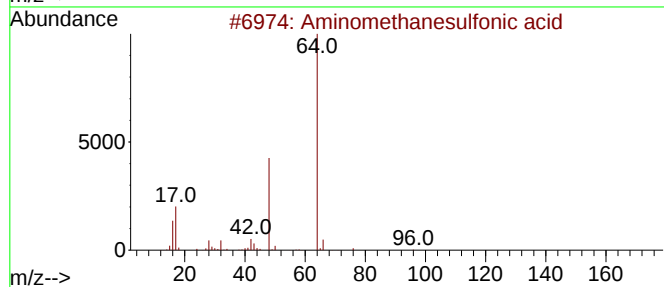
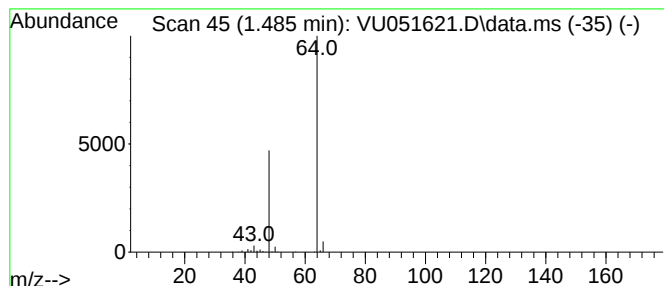
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.485	2.72 ug/L	251950	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
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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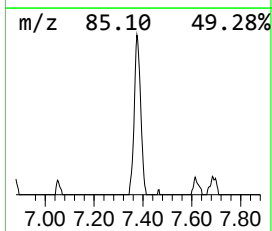
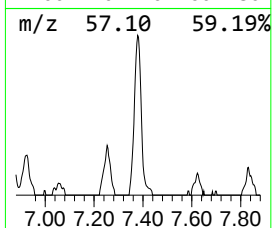
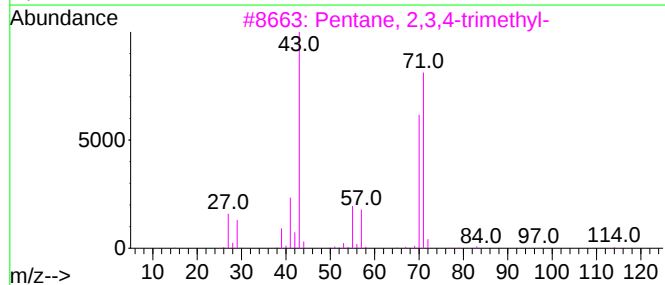
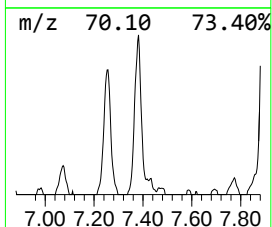
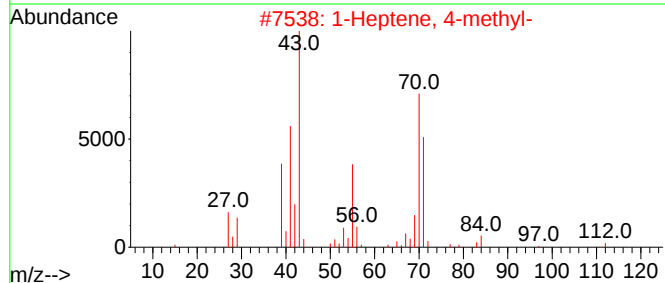
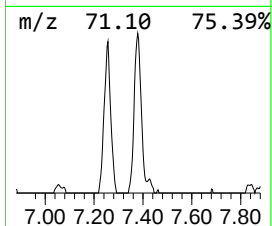
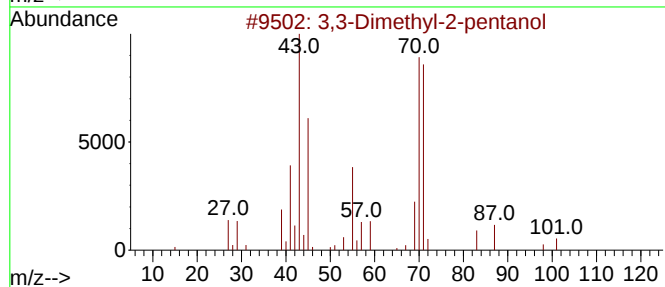
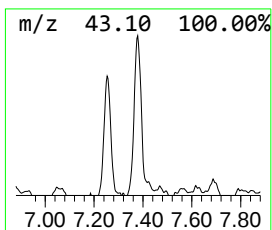
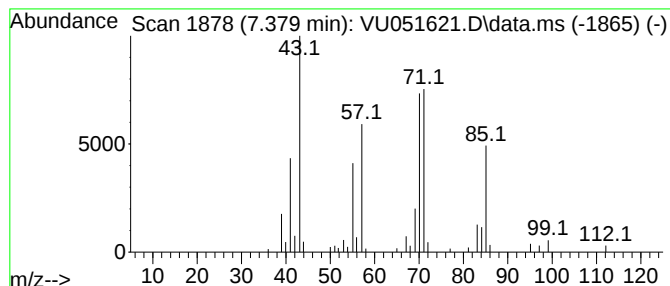
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Quant Title : TRACE VOA SFAM1.0

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Peak Number 2 3,3-Dimethyl-2-pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.379	0.97 ug/L	89693	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	59
2		1-Heptene, 4-methyl-	112	C8H16	013151-05-8	58
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	50



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.485	2.7	ug/L	251950	1	6.247	462338	5.0
3,3-Dimethyl-2-...	7.379	1.0	ug/L	89693	1	6.247	462338	5.0