

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110422\
 Data File : VU051763.D
 Acq On : 04 Nov 2022 16:26
 Operator : JC/MD
 Sample : N5407-02DL 5X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4Y2DL

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: VU051763.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	12	rVB	43564	34433	4.59%	0.395%
2	1.494	38	48	49	rBV3	64096	77404	10.31%	0.888%
3	1.584	70	76	86	rBV2	113927	213049	28.38%	2.443%
4	1.909	173	177	196	rVB	73167	106937	14.25%	1.226%
5	2.562	369	380	395	rVB	123974	199649	26.60%	2.290%
6	2.681	395	417	439	rBV3	123302	356498	47.50%	4.089%
7	2.787	440	450	468	rVB	208524	357978	47.69%	4.106%
8	3.041	517	529	559	rVB	250581	491540	65.49%	5.637%
9	3.182	567	573	583	rVB2	14626	25746	3.43%	0.295%
10	3.867	769	786	802	rVV2	51307	128410	17.11%	1.473%
11	3.961	802	815	832	rVB5	12558	32559	4.34%	0.373%
12	4.652	1013	1030	1045	rBV2	83328	285702	38.06%	3.277%
13	5.060	1140	1157	1183	rBV2	142036	351359	46.81%	4.030%
14	5.723	1343	1363	1396	rBV3	244387	668627	89.08%	7.668%
15	6.169	1490	1502	1513	rBV	5225	12057	1.61%	0.138%
16	6.247	1513	1526	1547	rVV	195996	382195	50.92%	4.383%
17	6.690	1647	1664	1680	rBV	164759	321216	42.80%	3.684%
18	6.784	1681	1693	1713	rVB4	11850	33340	4.44%	0.382%
19	7.163	1793	1811	1813	rBV8	6174	12873	1.72%	0.148%
20	7.250	1830	1838	1850	rVB3	11688	19982	2.66%	0.229%
21	7.565	1923	1936	1951	rBV	66801	120501	16.05%	1.382%
22	7.800	1994	2009	2027	rBV3	78303	225800	30.08%	2.590%
23	7.896	2027	2039	2052	rVV	273675	493664	65.77%	5.662%
24	7.967	2052	2061	2076	rVV	124826	222579	29.65%	2.553%
25	8.034	2076	2082	2098	rVB6	6079	11964	1.59%	0.137%
26	8.179	2116	2127	2137	rBV2	42178	71999	9.59%	0.826%
27	8.237	2137	2145	2166	rVB3	18183	46238	6.16%	0.530%
28	8.468	2207	2217	2235	rVB2	16045	32320	4.31%	0.371%
29	8.636	2257	2269	2311	rBV	349946	750591	100.00%	8.608%
30	9.041	2385	2395	2409	rVB2	13332	21549	2.87%	0.247%
31	9.417	2499	2512	2531	rBV	311456	526526	70.15%	6.039%
32	9.571	2549	2560	2570	rBV	25980	42553	5.67%	0.488%
33	9.690	2584	2597	2613	rBV	72106	123980	16.52%	1.422%
34	10.099	2714	2724	2744	rBV5	26051	54458	7.26%	0.625%
35	10.240	2756	2768	2782	rBV2	8263	15026	2.00%	0.172%
36	10.369	2798	2808	2825	rBV7	7261	17460	2.33%	0.200%

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37	10.754	2916	2928	2947	rVB	143893	235019	31.31%	2.695%
38	10.890	2960	2970	2981	rVB	25283	41726	5.56%	0.479%
39	10.996	2997	3003	3014	rBV4	4524	7969	1.06%	0.091%
40	11.468	3140	3150	3158	rBV2	16237	25701	3.42%	0.295%
41	11.652	3199	3207	3216	rBV2	6254	12021	1.60%	0.138%
42	11.809	3244	3256	3274	rBV	331629	533441	71.07%	6.118%
43	11.893	3274	3282	3292	rVB3	9093	14606	1.95%	0.168%
44	12.060	3321	3334	3354	rBV	137094	293719	39.13%	3.369%
45	12.192	3363	3375	3396	rVB	316614	525352	69.99%	6.025%
46	12.542	3476	3484	3500	rBV9	11449	24786	3.30%	0.284%
47	12.770	3547	3555	3564	rBV2	8987	13325	1.78%	0.153%
48	12.947	3600	3610	3622	rBV4	10409	17314	2.31%	0.199%
49	13.288	3704	3716	3727	rBV9	7570	12953	1.73%	0.149%
50	13.449	3757	3766	3773	rBV4	6603	10389	1.38%	0.119%
51	13.516	3778	3787	3796	rBV6	8845	13513	1.80%	0.155%
52	13.735	3847	3855	3862	rBV9	6461	10397	1.39%	0.119%
53	14.037	3940	3949	3957	rVV9	5712	9470	1.26%	0.109%
54	16.513	4712	4719	4729	rBV5	6272	11350	1.51%	0.130%
55	16.764	4789	4797	4808	rBV6	10747	17523	2.33%	0.201%

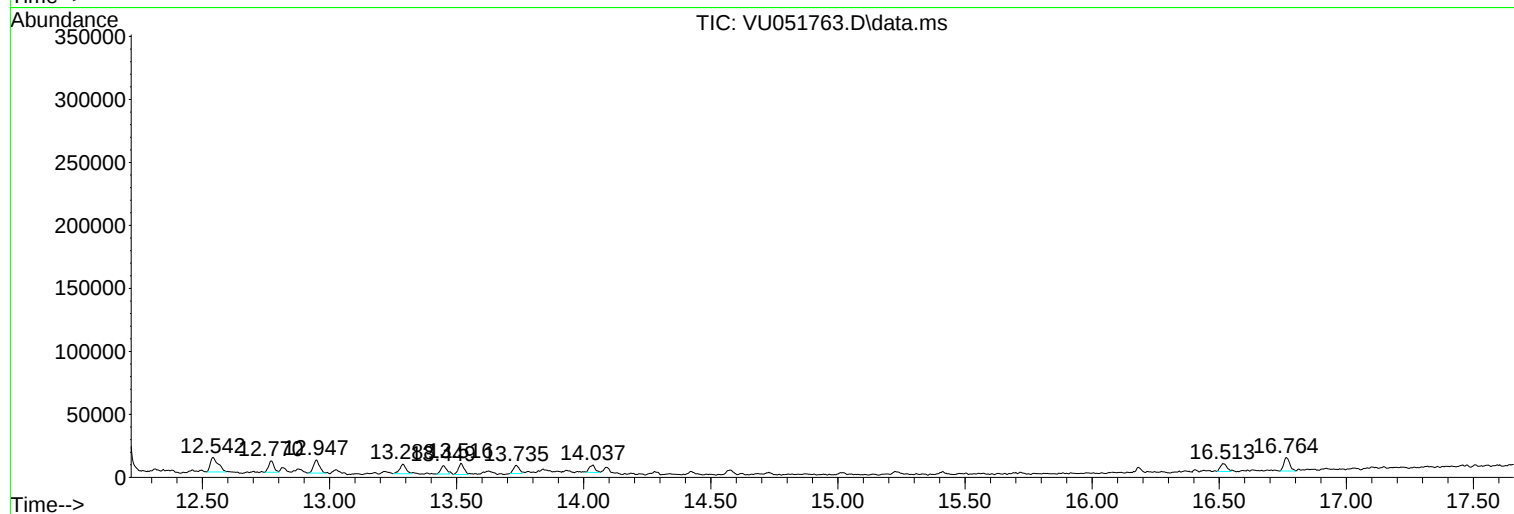
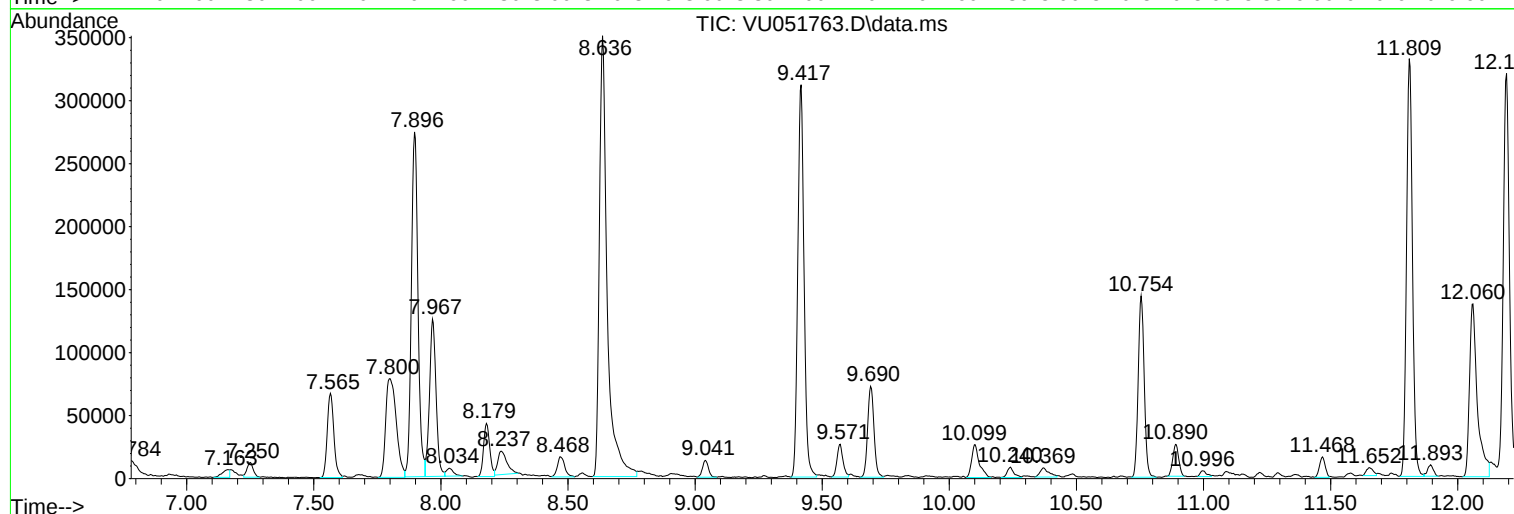
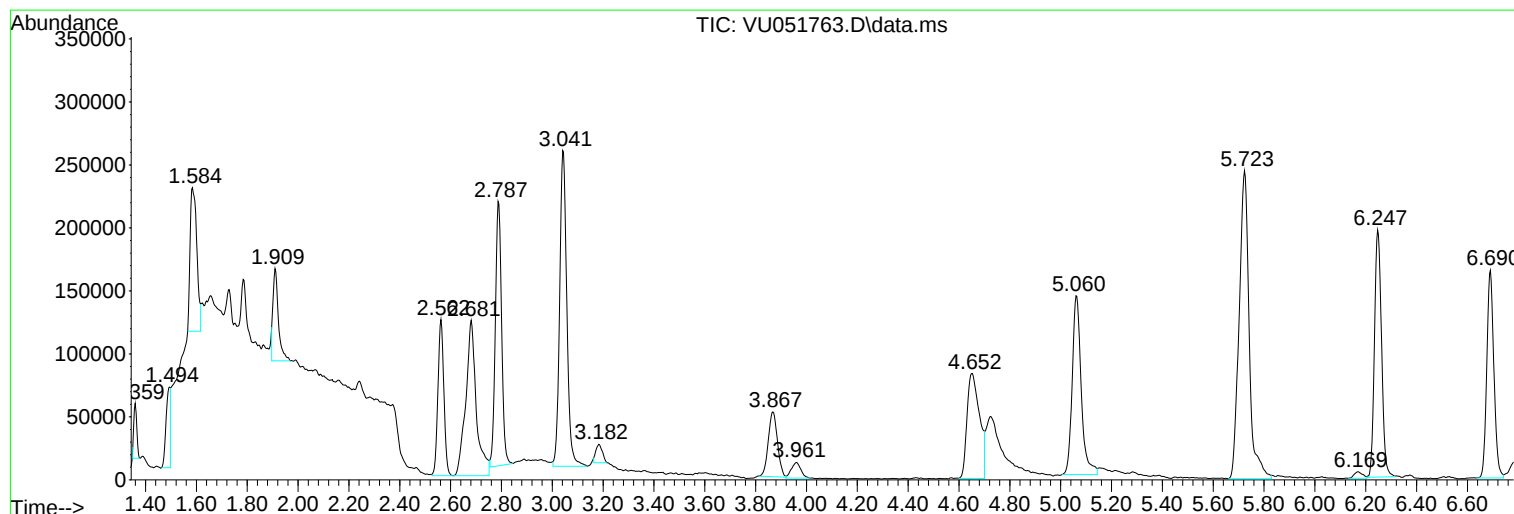
Sum of corrected areas: 8719336

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



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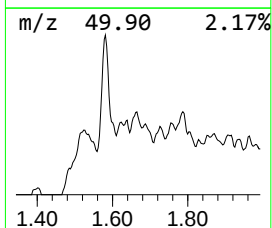
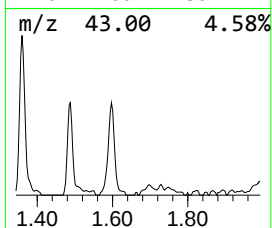
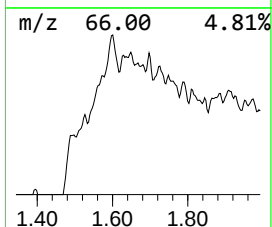
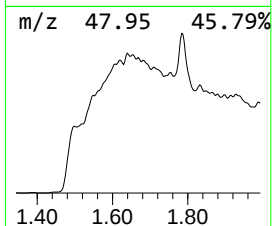
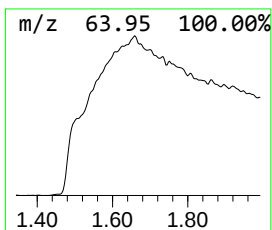
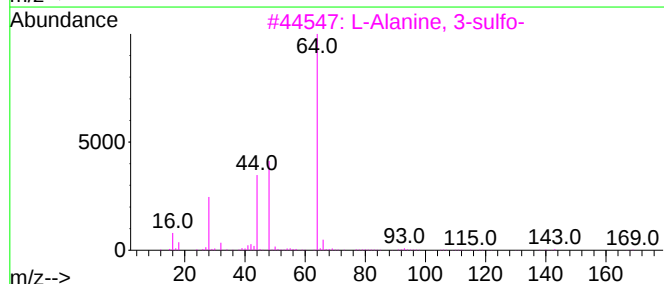
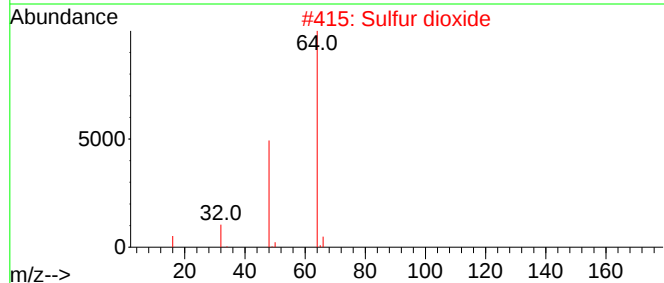
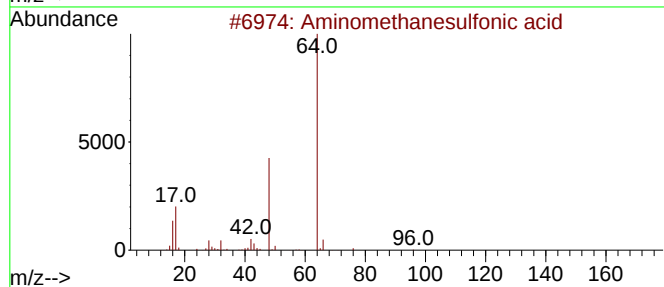
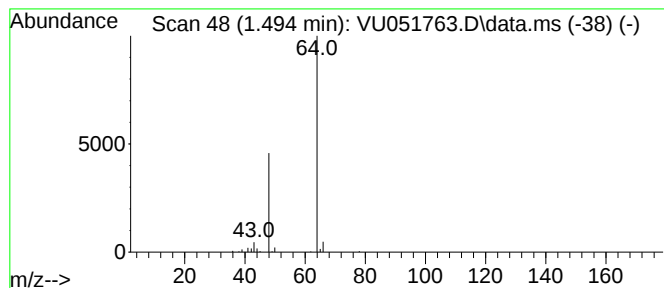
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.494	1.01 ug/L	77404	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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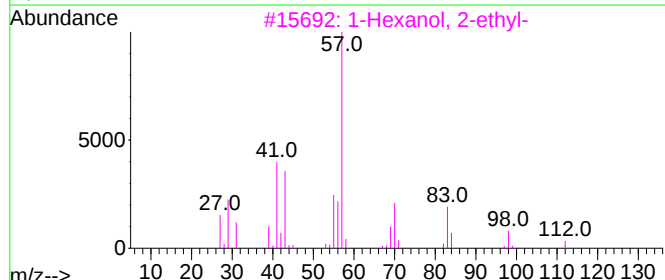
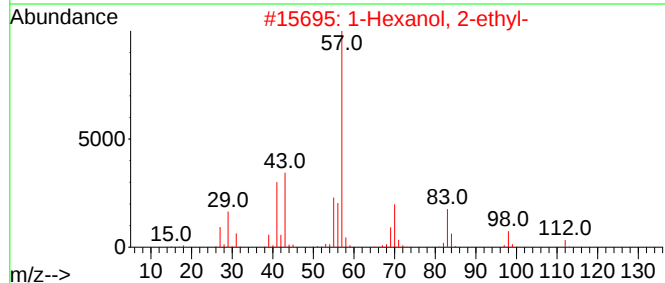
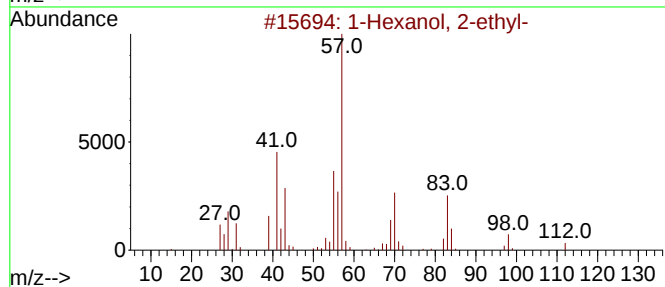
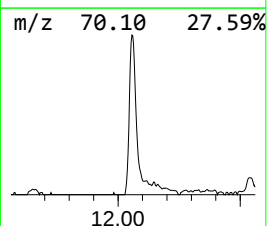
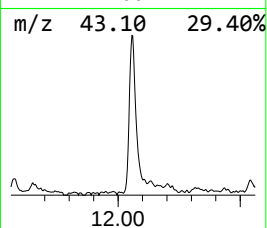
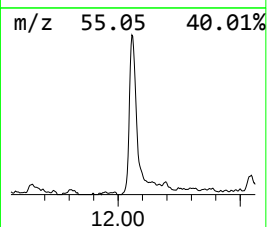
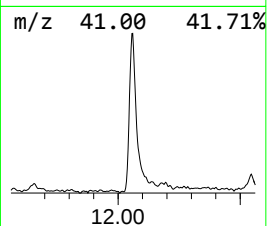
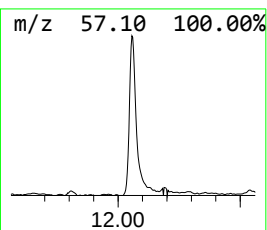
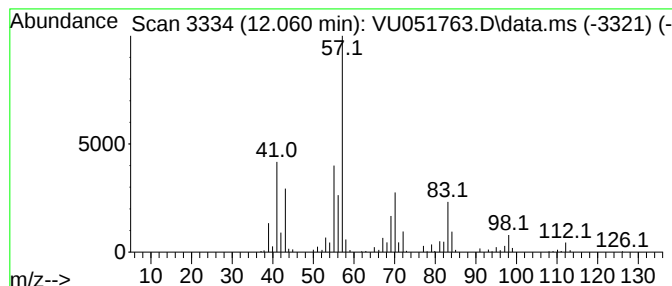
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	2.75 ug/L	293719	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	2-Ethyl-1-hexanol, trifluoroacetate			226	C10H17F3O2	053800-08-1	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.494	1.0	ug/L	77404	1	6.247	382195	5.0
1-Hexanol, 2-et...	12.060	2.8	ug/L	293719	3	11.809	533441	5.0