

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
 Data File : VU055903.D
 Acq On : 26 Oct 2023 13:55
 Operator : MD/SY
 Sample : 04961-12ME
 Misc : 5.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0LJ6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055903.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.477	49	58	67	rBV3	31979	76658	4.34%	0.512%
2	1.599	89	96	134	rVB2	251501	402703	22.81%	2.687%
3	2.544	378	390	410	rBV	190086	329791	18.68%	2.201%
4	2.759	451	457	458	rBV3	1990	1601	0.09%	0.011%
5	2.856	485	487	493	rVB4	721	578	0.03%	0.004%
6	2.891	493	498	499	rBV2	722	565	0.03%	0.004%
7	3.036	530	543	558	rBV8	8532	26741	1.51%	0.178%
8	3.113	558	567	575	rVV3	11184	21099	1.20%	0.141%
9	3.177	576	587	605	rVB2	18896	48187	2.73%	0.322%
10	3.338	626	637	652	rVV6	4267	10173	0.58%	0.068%
11	3.673	732	741	743	rBV4	2002	2053	0.12%	0.014%
12	3.962	825	831	834	rBV	525	485	0.03%	0.003%
13	3.988	836	839	845	rVV2	596	449	0.03%	0.003%
14	4.046	852	857	860	rVV2	406	381	0.02%	0.003%
15	4.184	895	900	904	rBV	436	407	0.02%	0.003%
16	4.393	958	965	967	rBV4	531	552	0.03%	0.004%
17	4.406	967	969	972	rBV3	757	511	0.03%	0.003%
18	4.422	972	974	978	rVB3	967	658	0.04%	0.004%
19	4.509	989	1001	1002	rBV3	2316	2955	0.17%	0.020%
20	4.628	1026	1038	1077	rBV	139570	465760	26.39%	3.108%
21	4.930	1128	1132	1136	rBV3	651	483	0.03%	0.003%
22	5.055	1155	1171	1198	rBV	282045	672425	38.09%	4.487%
23	5.206	1216	1218	1223	rVB4	792	544	0.03%	0.004%
24	5.335	1239	1258	1267	rBV4	7184	19302	1.09%	0.129%
25	5.447	1285	1293	1306	rVB8	3075	7093	0.40%	0.047%
26	5.557	1323	1327	1329	rBV3	689	547	0.03%	0.004%
27	5.579	1330	1334	1340	rVV5	1325	1765	0.10%	0.012%
28	5.624	1344	1348	1351	rBV2	725	585	0.03%	0.004%
29	5.714	1356	1376	1409	rBV2	553334	1499206	84.93%	10.004%
30	5.878	1425	1427	1429	rBV2	632	408	0.02%	0.003%
31	5.981	1448	1459	1464	rBV6	4956	9005	0.51%	0.060%
32	6.058	1481	1483	1486	rVB2	761	457	0.03%	0.003%
33	6.126	1502	1504	1508	rVB3	715	528	0.03%	0.004%
34	6.242	1524	1540	1578	rBV	651977	1331454	75.43%	8.885%
35	6.525	1619	1628	1642	rVV	6000	13825	0.78%	0.092%
36	6.598	1642	1651	1662	rVV4	6279	14000	0.79%	0.093%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	6.685	1665	1678	1706	rVB	364710	744504	42.18%	4.968%
38	7.193	1827	1836	1859	rBV10	6816	22836	1.29%	0.152%
39	7.380	1890	1894	1897	rVV4	1007	940	0.05%	0.006%
40	7.396	1897	1899	1905	rVB4	802	709	0.04%	0.005%
41	7.563	1939	1951	1978	rBV	176985	359248	20.35%	2.397%
42	7.705	1989	1995	1997	rBV5	1835	2330	0.13%	0.016%
43	7.791	2013	2022	2029	rBV8	5902	10494	0.59%	0.070%
44	7.894	2041	2054	2074	rBV	542796	1006647	57.03%	6.717%
45	8.078	2108	2111	2117	rVB3	1003	840	0.05%	0.006%
46	8.123	2122	2125	2126	rBV3	688	388	0.02%	0.003%
47	8.180	2131	2143	2164	rBV	118069	253073	14.34%	1.689%
48	8.351	2192	2196	2197	rBV3	1182	741	0.04%	0.005%
49	8.460	2227	2230	2231	rBV2	1169	536	0.03%	0.004%
50	8.550	2245	2258	2269	rBV8	13374	26431	1.50%	0.176%
51	8.650	2275	2289	2315	rBV	576224	1206877	68.37%	8.053%
52	8.920	2369	2373	2374	rBV4	1426	1087	0.06%	0.007%
53	9.042	2409	2411	2415	rVB3	801	413	0.02%	0.003%
54	9.209	2454	2463	2471	rVB6	2561	3732	0.21%	0.025%
55	9.283	2483	2486	2488	rVB2	818	435	0.02%	0.003%
56	9.338	2496	2503	2510	rVB5	1702	2654	0.15%	0.018%
57	9.418	2510	2528	2554	rBV	921104	1721261	97.51%	11.486%
58	9.579	2571	2578	2583	rBV8	2028	2479	0.14%	0.017%
59	9.692	2608	2613	2614	rBV4	2676	2182	0.12%	0.015%
60	9.801	2641	2647	2650	rVB2	439	492	0.03%	0.003%
61	9.817	2650	2652	2655	rBV	607	403	0.02%	0.003%
62	9.984	2701	2704	2708	rVV4	416	393	0.02%	0.003%
63	10.007	2708	2711	2714	rVB3	793	459	0.03%	0.003%
64	10.029	2714	2718	2721	rBV2	589	402	0.02%	0.003%
65	10.119	2743	2746	2749	rBV4	1115	851	0.05%	0.006%
66	10.180	2763	2765	2769	rBV2	530	450	0.03%	0.003%
67	10.241	2778	2784	2785	rBV2	1648	1332	0.08%	0.009%
68	10.341	2811	2815	2819	rBV3	1160	931	0.05%	0.006%
69	10.360	2819	2821	2824	rVV2	632	393	0.02%	0.003%
70	10.393	2824	2831	2837	rVB6	2022	2743	0.16%	0.018%
71	10.540	2875	2877	2879	rBV2	708	416	0.02%	0.003%
72	10.621	2896	2902	2907	rBV8	2512	3084	0.17%	0.021%
73	10.643	2907	2909	2925	rVB5	2194	3454	0.20%	0.023%
74	10.714	2925	2931	2932	rBV2	564	505	0.03%	0.003%
75	10.759	2932	2945	2965	rBV	739419	1210132	68.56%	8.075%
76	10.984	3012	3015	3018	rBV2	952	617	0.03%	0.004%

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 ClientSampleId :
 E0LJ6ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Start Thrs: 0.2

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

77	11.010	3018	3023	3027	rBV5	583	663	0.04%	0.004%
78	11.116	3048	3056	3066	rVB6	9131	14778	0.84%	0.099%
79	11.177	3071	3075	3078	rVB4	772	681	0.04%	0.005%
80	11.200	3078	3082	3084	rBV3	1282	951	0.05%	0.006%
81	11.251	3093	3098	3099	rBV4	834	587	0.03%	0.004%
82	11.306	3106	3115	3122	rBV7	2794	4731	0.27%	0.032%
83	11.373	3132	3136	3141	rBV4	1678	2082	0.12%	0.014%
84	11.412	3142	3148	3157	rVB5	8489	11443	0.65%	0.076%
85	11.553	3188	3192	3193	rBV2	601	416	0.02%	0.003%
86	11.618	3206	3212	3213	rBV5	1599	1477	0.08%	0.010%
87	11.711	3232	3241	3244	rBV3	1485	2149	0.12%	0.014%
88	11.814	3260	3273	3300	rBV	1066026	1765186	100.00%	11.779%
89	11.981	3321	3325	3327	rBV4	2073	1702	0.10%	0.011%
90	12.097	3350	3361	3372	rBV9	4262	8067	0.46%	0.054%
91	12.193	3375	3391	3414	rBV	840750	1398560	79.23%	9.332%
92	12.328	3424	3433	3442	rBV3	21082	32908	1.86%	0.220%
93	12.524	3489	3494	3497	rBV5	3329	3289	0.19%	0.022%
94	12.659	3529	3536	3543	rBV7	4489	8298	0.47%	0.055%
95	12.926	3610	3619	3621	rBV9	5217	8197	0.46%	0.055%
96	13.132	3675	3683	3688	rBV10	4130	5487	0.31%	0.037%
97	13.177	3694	3697	3699	rBV4	1696	1216	0.07%	0.008%
98	13.428	3766	3775	3783	rBV	42807	64641	3.66%	0.431%
99	13.585	3816	3824	3833	rBV3	21036	33674	1.91%	0.225%
100	14.447	4085	4092	4100	rBV	40763	52950	3.00%	0.353%

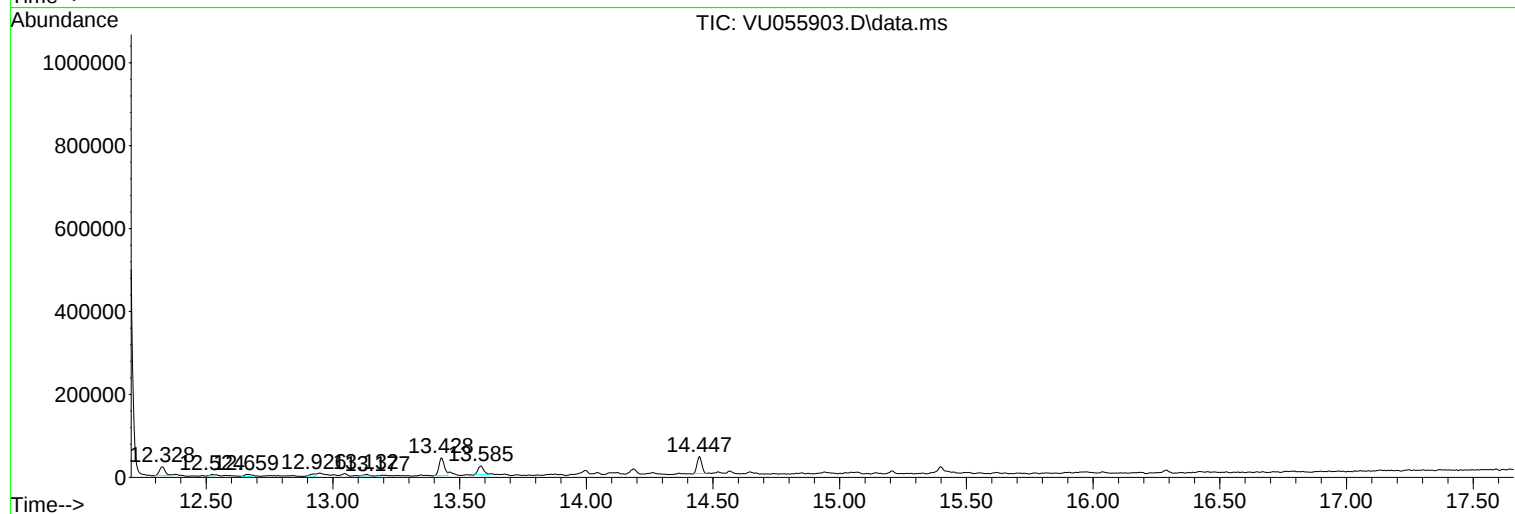
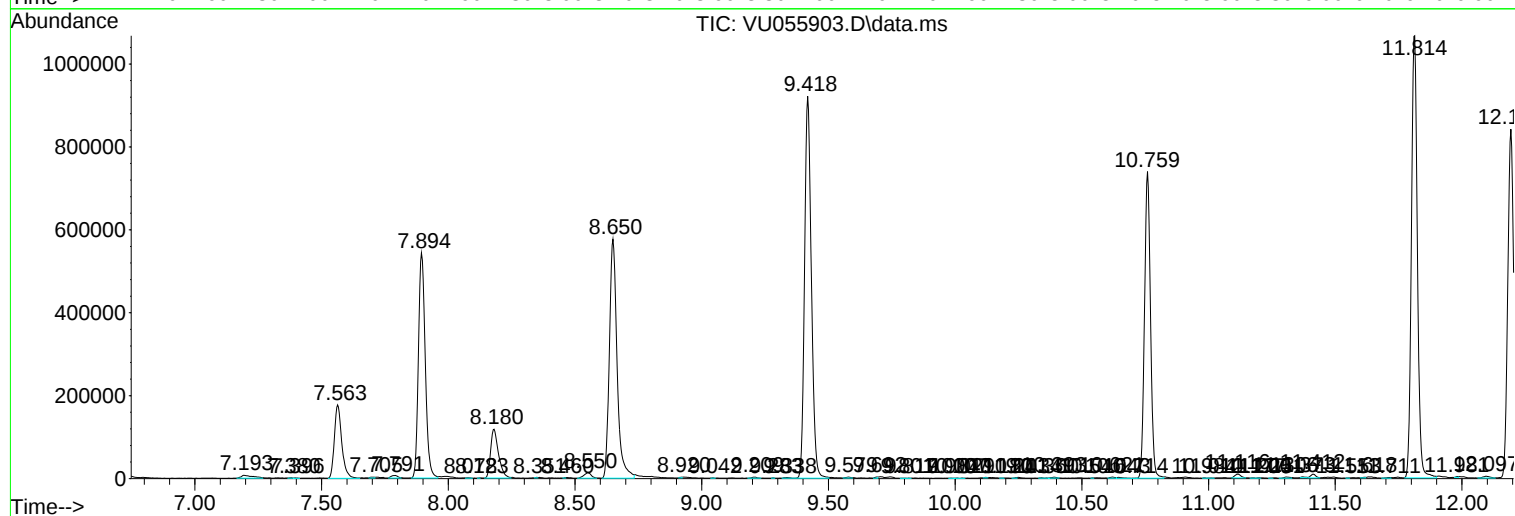
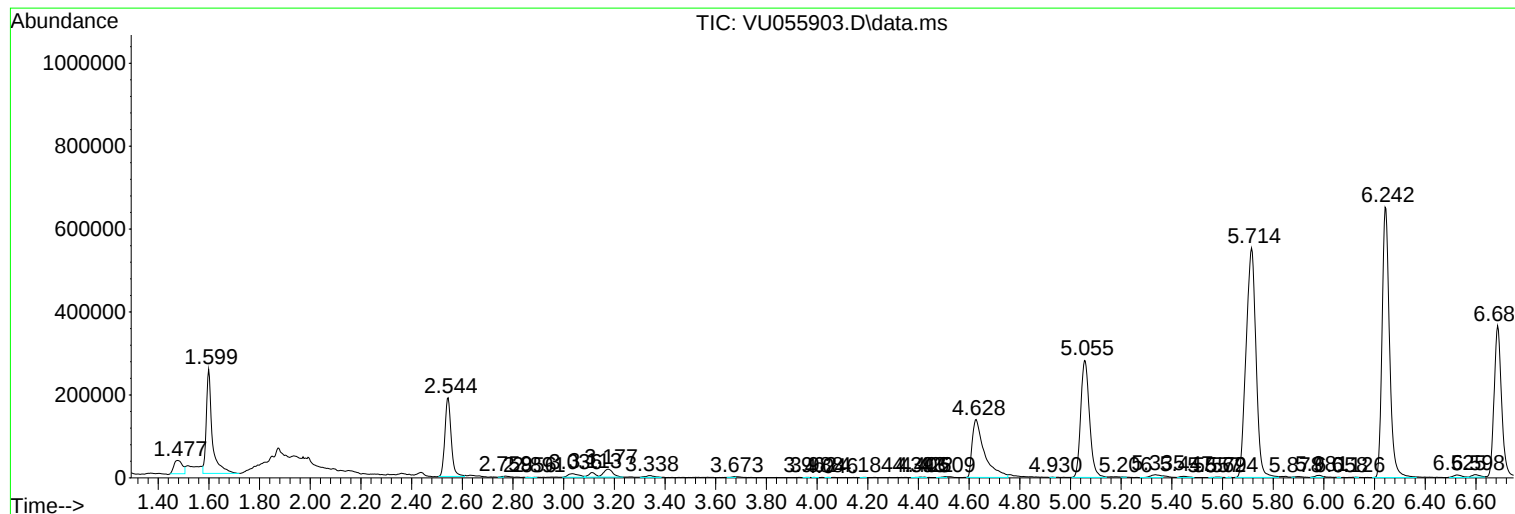
Sum of corrected areas: 14985961

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Instrument :
MSVOA_U
ClientSampleId :
EOLJ6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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E0LJ6ME

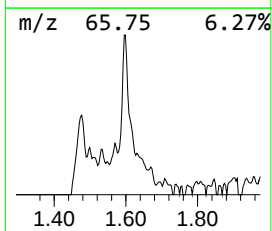
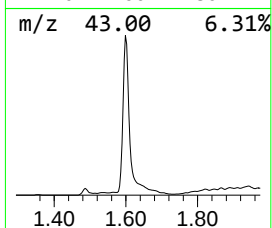
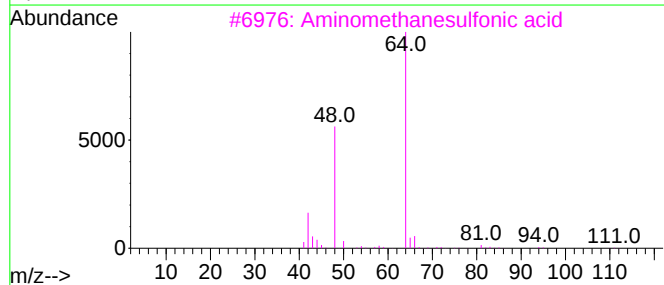
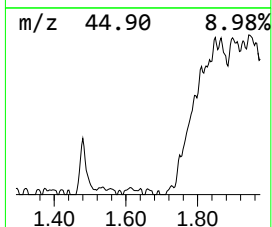
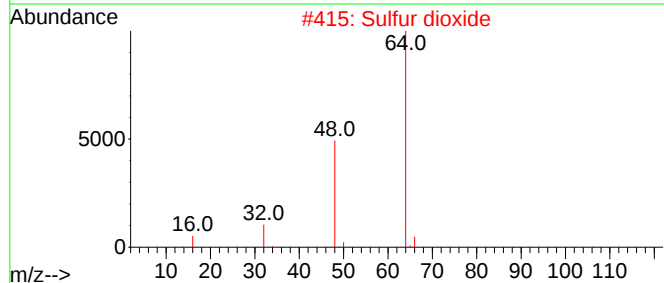
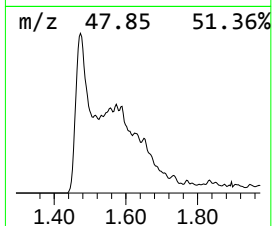
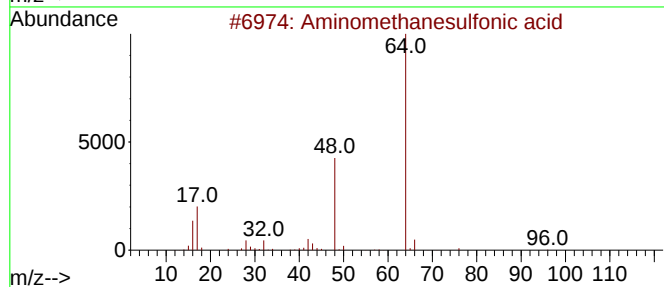
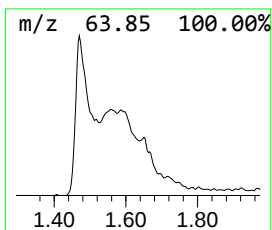
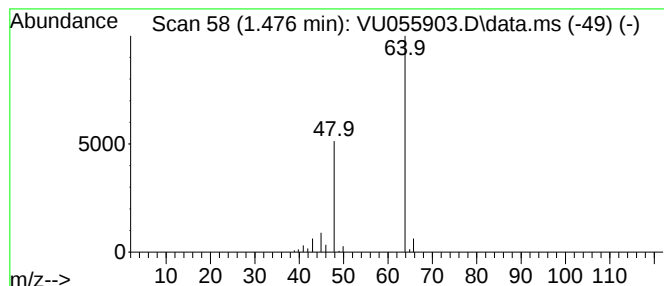
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.476	2.88 ug/L	76658	1,4-Difluorobenzene	6.242

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.476	2.9	ug/L	76658	1	6.242	1331450	50.0