

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
 Data File : VU055882.D
 Acq On : 25 Oct 2023 16:21
 Operator : MD/SY
 Sample : 04952-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOAR3

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: VU055882.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.467	47	55	59	rBV	112214	164762	6.37%	0.791%
2	1.599	89	96	110	rVB2	430237	516538	19.98%	2.481%
3	1.882	177	184	202	rVB	213023	333659	12.91%	1.602%
4	2.454	359	362	379	rVB	10222	14956	0.58%	0.072%
5	2.557	379	394	411	rBV	551425	907595	35.11%	4.359%
6	2.682	426	433	446	rVB	2778	5817	0.23%	0.028%
7	2.750	450	454	456	rVB4	907	651	0.03%	0.003%
8	2.782	456	464	466	rBV2	4205	4906	0.19%	0.024%
9	2.949	512	516	518	rBV4	909	609	0.02%	0.003%
10	3.013	525	536	539	rBV5	4476	7766	0.30%	0.037%
11	3.129	560	572	582	rBV2	28149	57918	2.24%	0.278%
12	3.357	628	643	657	rBV3	15575	36738	1.42%	0.176%
13	3.454	668	673	677	rBV4	782	679	0.03%	0.003%
14	3.586	705	714	718	rBV4	634	836	0.03%	0.004%
15	3.685	741	745	746	rBV2	744	567	0.02%	0.003%
16	3.917	813	817	820	rBV3	707	478	0.02%	0.002%
17	3.949	824	827	831	rVV3	620	609	0.02%	0.003%
18	4.148	882	889	894	rBV2	639	771	0.03%	0.004%
19	4.335	940	947	949	rBV	891	1026	0.04%	0.005%
20	4.367	954	957	960	rVB	791	503	0.02%	0.002%
21	4.518	995	1004	1007	rBV5	4549	6609	0.26%	0.032%
22	4.615	1022	1034	1067	rBV	212841	556759	21.54%	2.674%
23	5.055	1154	1171	1195	rVV	460204	1035170	40.05%	4.971%
24	5.325	1243	1255	1264	rBV2	6848	16100	0.62%	0.077%
25	5.717	1356	1377	1402	rBV2	955069	2584705	100.00%	12.413%
26	5.955	1449	1451	1453	rBV2	902	557	0.02%	0.003%
27	6.023	1469	1472	1477	rBV5	991	891	0.03%	0.004%
28	6.245	1526	1541	1571	rBV	686338	1349327	52.20%	6.480%
29	6.589	1642	1648	1652	rBV5	2024	2627	0.10%	0.013%
30	6.685	1663	1678	1698	rBV	573750	1140377	44.12%	5.477%
31	6.975	1763	1768	1770	rBV4	922	760	0.03%	0.004%
32	7.094	1800	1805	1807	rBV3	551	467	0.02%	0.002%
33	7.184	1822	1833	1834	rBV6	6738	8517	0.33%	0.041%
34	7.560	1938	1950	1969	rBV	321460	570255	22.06%	2.739%
35	7.711	1985	1997	2006	rBV	4617	11023	0.43%	0.053%
36	7.791	2019	2022	2024	rBV3	857	570	0.02%	0.003%

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

37	7.894	2035	2054	2088	rBV	1205990	2092029	80.94%	10.047%
38	8.052	2100	2103	2104	rBV2	800	464	0.02%	0.002%
39	8.110	2119	2121	2127	rVB2	820	662	0.03%	0.003%
40	8.174	2130	2141	2169	rBV	219009	388955	15.05%	1.868%
41	8.296	2175	2179	2181	rBV4	1076	575	0.02%	0.003%
42	8.344	2190	2194	2198	rVB2	905	852	0.03%	0.004%
43	8.383	2204	2206	2211	rBV2	466	487	0.02%	0.002%
44	8.489	2223	2239	2248	rBV5	7622	19882	0.77%	0.095%
45	8.550	2249	2258	2271	rVB2	31028	56006	2.17%	0.269%
46	8.634	2272	2284	2317	rBV	840457	1616831	62.55%	7.765%
47	8.894	2361	2365	2369	rVB5	1092	958	0.04%	0.005%
48	8.959	2383	2385	2388	rVB3	793	491	0.02%	0.002%
49	9.004	2395	2399	2401	rVB4	921	668	0.03%	0.003%
50	9.029	2401	2407	2411	rBV5	1087	1500	0.06%	0.007%
51	9.274	2475	2483	2494	rVB5	3254	5139	0.20%	0.025%
52	9.338	2497	2503	2505	rBV4	2086	2117	0.08%	0.010%
53	9.412	2514	2526	2551	rBV	1030850	1761302	68.14%	8.458%
54	9.598	2581	2584	2590	rVB7	2103	1919	0.07%	0.009%
55	9.682	2607	2610	2612	rBV4	828	593	0.02%	0.003%
56	9.746	2627	2630	2631	rBV2	1084	644	0.02%	0.003%
57	9.762	2633	2635	2637	rBV3	1294	757	0.03%	0.004%
58	9.830	2647	2656	2664	rBV9	4377	7665	0.30%	0.037%
59	9.936	2686	2689	2692	rVV3	665	530	0.02%	0.003%
60	10.007	2708	2711	2715	rBV5	1230	955	0.04%	0.005%
61	10.026	2715	2717	2720	rBV3	764	484	0.02%	0.002%
62	10.100	2734	2740	2745	rBV5	1561	2320	0.09%	0.011%
63	10.190	2763	2768	2769	rBV	887	715	0.03%	0.003%
64	10.261	2786	2790	2792	rBV2	976	651	0.03%	0.003%
65	10.274	2792	2794	2796	rVV	1098	570	0.02%	0.003%
66	10.299	2800	2802	2805	rVV2	920	490	0.02%	0.002%
67	10.364	2816	2822	2826	rBV6	1440	1637	0.06%	0.008%
68	10.383	2826	2828	2831	rVV3	1003	609	0.02%	0.003%
69	10.402	2831	2834	2837	rVV2	779	524	0.02%	0.003%
70	10.524	2868	2872	2873	rBV2	741	482	0.02%	0.002%
71	10.547	2873	2879	2884	rVB6	2606	3529	0.14%	0.017%
72	10.582	2884	2890	2891	rBV3	1066	684	0.03%	0.003%
73	10.640	2900	2908	2917	rBV7	2491	3862	0.15%	0.019%
74	10.695	2919	2925	2930	rBV6	953	1121	0.04%	0.005%
75	10.753	2930	2943	2970	rBV	937640	1515791	58.64%	7.279%
76	10.884	2980	2984	2988	rBV6	2376	2642	0.10%	0.013%

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 Title : VOC Analysis

77	10.946	3000	3003	3005	rBV3	763	455	0.02%	0.002%
78	10.975	3009	3012	3016	rVB3	1179	639	0.02%	0.003%
79	11.386	3133	3140	3142	rBV4	674	704	0.03%	0.003%
80	11.405	3142	3146	3148	rBV3	1269	932	0.04%	0.004%
81	11.692	3233	3235	3241	rVB4	922	846	0.03%	0.004%
82	11.733	3241	3248	3251	rBV5	1346	1499	0.06%	0.007%
83	11.807	3259	3271	3296	rBV	1143595	1873440	72.48%	8.997%
84	12.090	3348	3359	3371	rBV	5613	11302	0.44%	0.054%
85	12.190	3376	3390	3419	rVV	1268234	2081921	80.55%	9.998%
86	12.402	3454	3456	3460	rVB3	1755	1007	0.04%	0.005%
87	12.515	3488	3491	3497	rVB5	985	923	0.04%	0.004%
88	12.560	3503	3505	3509	rVB4	1377	913	0.04%	0.004%
89	12.843	3591	3593	3599	rBV3	596	531	0.02%	0.003%
90	12.900	3609	3611	3614	rBV2	789	466	0.02%	0.002%
91	12.994	3638	3640	3644	rVB3	962	495	0.02%	0.002%
92	13.232	3711	3714	3720	rVB4	1506	1252	0.05%	0.006%
93	13.415	3768	3771	3777	rVB4	594	552	0.02%	0.003%
94	13.457	3780	3784	3788	rVV3	1058	977	0.04%	0.005%
95	13.614	3831	3833	3838	rVB2	777	522	0.02%	0.003%
96	13.871	3911	3913	3918	rBV3	1133	907	0.04%	0.004%
97	14.068	3970	3974	3980	rVV4	770	718	0.03%	0.003%
98	14.450	4090	4093	4097	rBV3	837	704	0.03%	0.003%
99	14.781	4194	4196	4198	rBV2	841	465	0.02%	0.002%
100	14.907	4233	4235	4238	rBV2	934	592	0.02%	0.003%

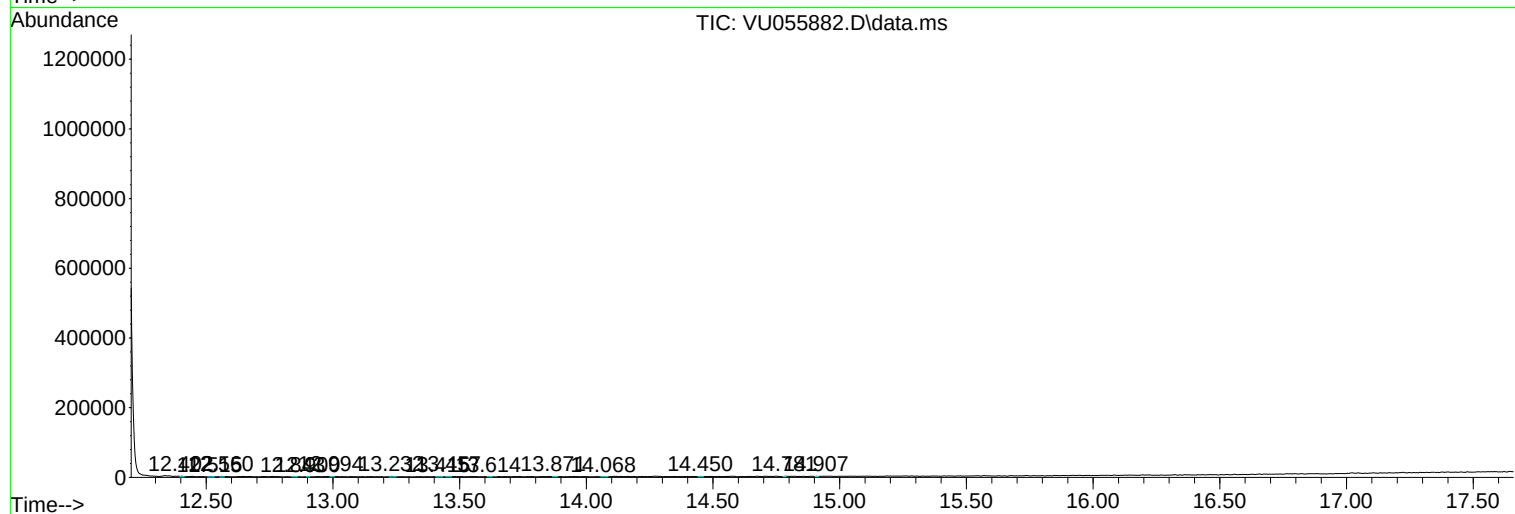
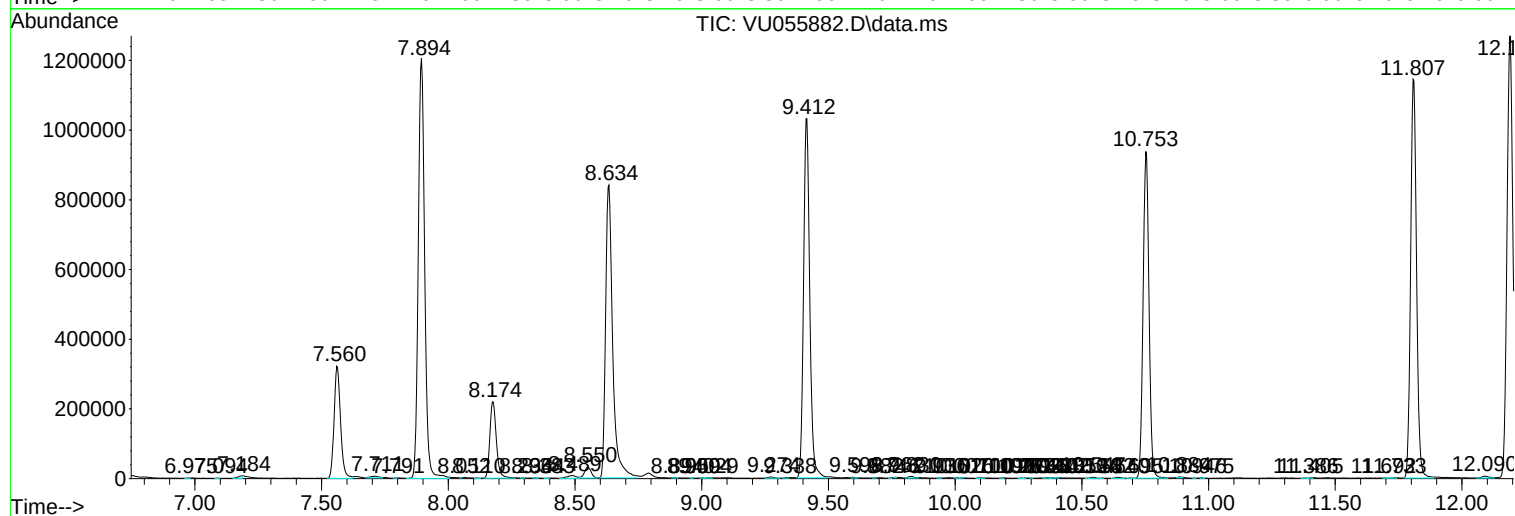
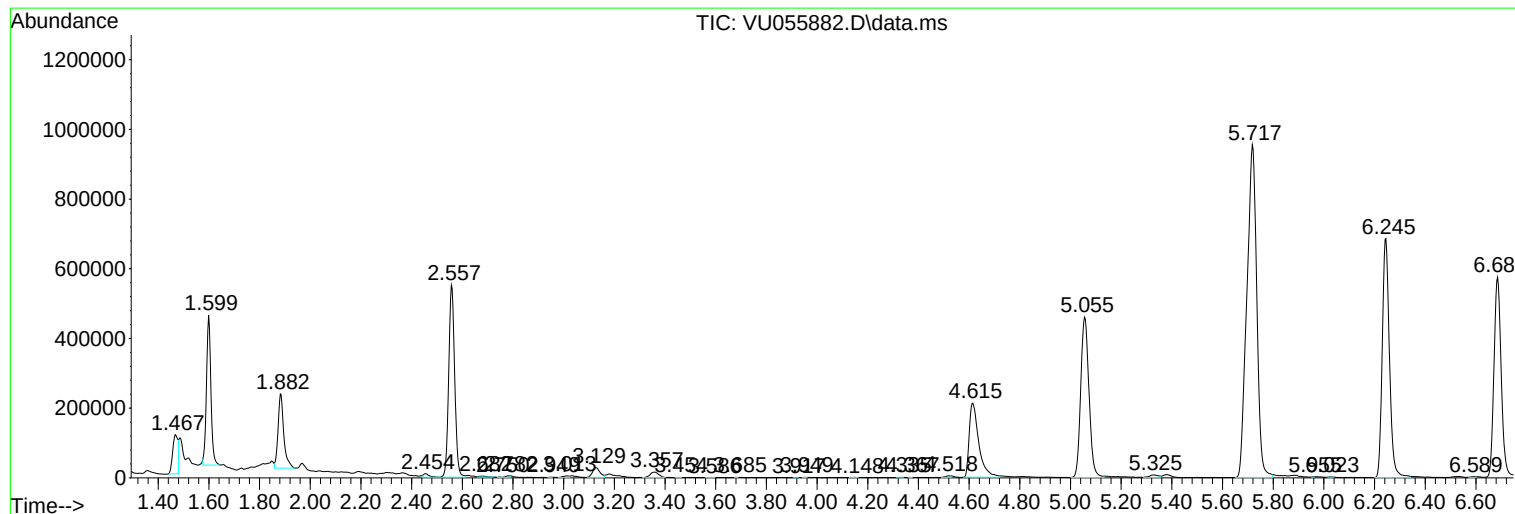
Sum of corrected areas: 20822952

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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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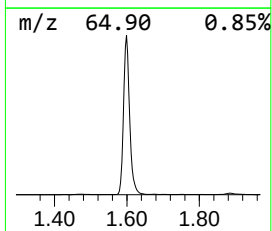
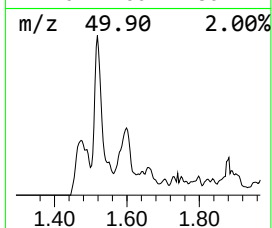
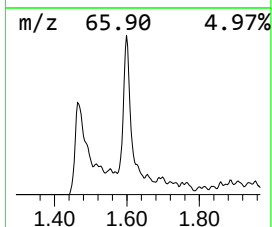
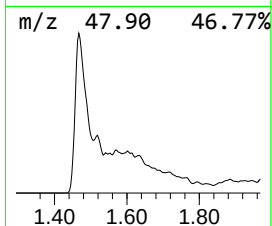
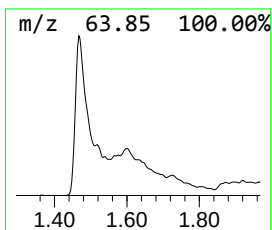
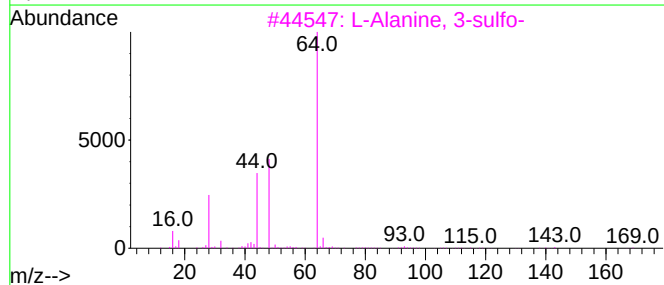
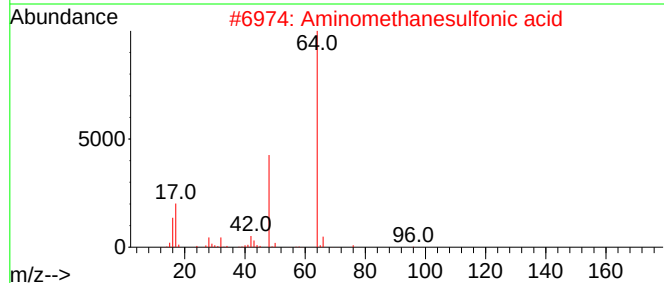
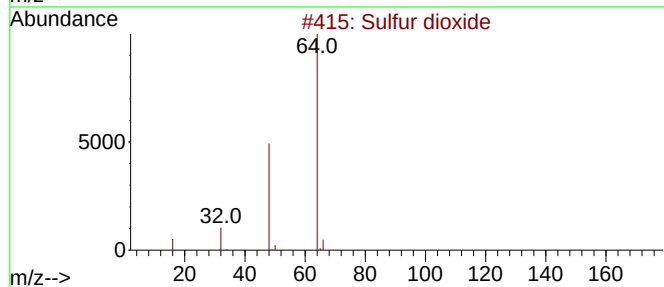
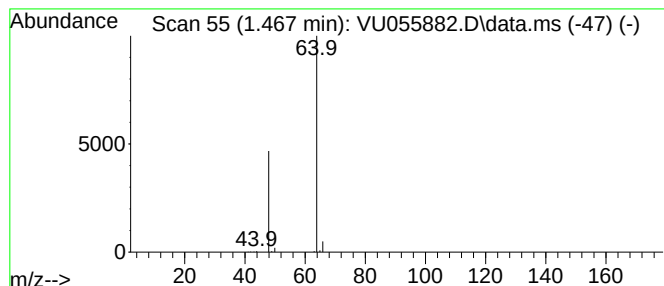
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.467	6.11 ug/L	164762	1,4-Difluorobenzene	6.245

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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.467	6.1	ug/L	164762	1	6.245	1349330	50.0