

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045209.D
 Acq On : 07 Oct 2021 14:06
 Operator : SY/MD
 Sample : M4025-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN3

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045209.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	32	39	54	rBV	63826	111971	8.91%	1.171%
2	1.601	74	81	102	rVB	178733	209740	16.70%	2.193%
3	1.893	164	172	186	rVB	130083	175687	13.99%	1.837%
4	2.562	367	380	398	rBV	256058	427760	34.05%	4.472%
5	2.691	417	420	424	rBV2	265	187	0.01%	0.002%
6	2.784	437	449	459	rBV4	1752	3696	0.29%	0.039%
7	2.961	498	504	515	rVB3	469	939	0.07%	0.010%
8	3.006	515	518	521	rBV	232	178	0.01%	0.002%
9	3.047	525	531	537	rBV3	809	1186	0.09%	0.012%
10	3.189	563	575	587	rBV	2885	6250	0.50%	0.065%
11	3.369	626	631	635	rBV3	285	274	0.02%	0.003%
12	3.459	652	659	663	rBV2	227	349	0.03%	0.004%
13	3.523	675	679	683	rVB2	235	243	0.02%	0.003%
14	3.555	686	689	694	rBV	172	157	0.01%	0.002%
15	3.665	720	723	725	rBV	184	153	0.01%	0.002%
16	3.819	768	771	775	rBV2	283	278	0.02%	0.003%
17	3.871	784	787	791	rBV	193	165	0.01%	0.002%
18	3.893	791	794	798	rVB	222	177	0.01%	0.002%
19	3.932	803	806	810	rBV2	157	176	0.01%	0.002%
20	4.096	854	857	861	rVV	194	192	0.02%	0.002%
21	4.266	907	910	914	rVB	224	178	0.01%	0.002%
22	4.629	1008	1023	1052	rBV	136338	319731	25.45%	3.343%
23	4.809	1076	1079	1083	rVB2	291	252	0.02%	0.003%
24	4.867	1094	1097	1100	rBV2	234	181	0.01%	0.002%
25	4.909	1107	1110	1114	rBV3	313	296	0.02%	0.003%
26	5.067	1142	1159	1187	rVV	222108	482909	38.44%	5.049%
27	5.282	1223	1226	1227	rBV	512	304	0.02%	0.003%
28	5.372	1250	1254	1260	rVB2	238	269	0.02%	0.003%
29	5.501	1290	1294	1298	rBV2	175	201	0.02%	0.002%
30	5.565	1310	1314	1319	rBB	141	179	0.01%	0.002%
31	5.729	1342	1365	1389	rBV2	468220	1256180	100.00%	13.133%
32	5.996	1443	1448	1451	rBV3	209	253	0.02%	0.003%
33	6.047	1460	1464	1469	rVB3	186	231	0.02%	0.002%
34	6.079	1469	1474	1479	rVB3	277	312	0.02%	0.003%
35	6.112	1479	1484	1485	rBV	307	203	0.02%	0.002%
36	6.253	1513	1528	1551	rBV	368267	688104	54.78%	7.194%

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 Title : VOC Analysis

37	6.430	1578	1583	1588	rBV	283	360	0.03%	0.004%
38	6.497	1600	1604	1606	rBV2	304	211	0.02%	0.002%
39	6.533	1607	1615	1626	rVV7	2263	3906	0.31%	0.041%
40	6.694	1651	1665	1683	rBV	295895	572950	45.61%	5.990%
41	6.800	1695	1698	1699	rBV	319	175	0.01%	0.002%
42	7.015	1760	1765	1768	rBV	146	151	0.01%	0.002%
43	7.034	1768	1771	1773	rBV	225	177	0.01%	0.002%
44	7.086	1784	1787	1793	rBV2	196	219	0.02%	0.002%
45	7.176	1808	1815	1816	rBV2	816	779	0.06%	0.008%
46	7.301	1852	1854	1860	rVV2	227	220	0.02%	0.002%
47	7.340	1860	1866	1869	rVB2	226	248	0.02%	0.003%
48	7.404	1881	1886	1888	rBV	251	239	0.02%	0.002%
49	7.488	1907	1912	1915	rBV2	196	215	0.02%	0.002%
50	7.568	1924	1937	1958	rVV	150560	260139	20.71%	2.720%
51	7.687	1970	1974	1982	rVB3	663	889	0.07%	0.009%
52	7.899	2026	2040	2055	rBV	580067	980956	78.09%	10.255%
53	7.973	2057	2063	2076	rVB	8208	12962	1.03%	0.136%
54	8.182	2115	2128	2146	rVV	105132	173804	13.84%	1.817%
55	8.340	2175	2177	2184	rVB3	363	369	0.03%	0.004%
56	8.636	2257	2269	2304	rBV	409964	720395	57.35%	7.531%
57	9.086	2406	2409	2412	rBV	157	153	0.01%	0.002%
58	9.166	2427	2434	2436	rBV	202	270	0.02%	0.003%
59	9.240	2454	2457	2460	rBV2	225	218	0.02%	0.002%
60	9.420	2500	2513	2538	rBV	534324	861918	68.61%	9.011%
61	9.568	2554	2559	2561	rBV2	410	362	0.03%	0.004%
62	9.700	2592	2600	2607	rVB3	1222	1868	0.15%	0.020%
63	9.735	2607	2611	2615	rBV2	206	238	0.02%	0.002%
64	9.761	2616	2619	2623	rVV	224	174	0.01%	0.002%
65	9.787	2623	2627	2633	rVV2	171	181	0.01%	0.002%
66	10.102	2722	2725	2730	rVB2	239	246	0.02%	0.003%
67	10.337	2793	2798	2806	rVB2	322	458	0.04%	0.005%
68	10.378	2806	2811	2814	rBV2	207	192	0.02%	0.002%
69	10.423	2823	2825	2830	rVB2	199	174	0.01%	0.002%
70	10.462	2833	2837	2840	rBV	241	226	0.02%	0.002%
71	10.533	2856	2859	2862	rVB	278	156	0.01%	0.002%
72	10.674	2896	2903	2911	rVB2	1539	1876	0.15%	0.020%
73	10.761	2917	2930	2950	rBV	419394	670483	53.37%	7.010%
74	10.899	2970	2973	2976	rBV2	361	244	0.02%	0.003%
75	11.099	3028	3035	3038	rBV2	391	487	0.04%	0.005%
76	11.295	3094	3096	3104	rVB	282	224	0.02%	0.002%

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Smoothing : OFF

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Min Area: 0 % of largest Peak

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

77	11.372	3116	3120	3122	rBV2	212	203	0.02%	0.002%
78	11.462	3140	3148	3149	rBV3	779	727	0.06%	0.008%
79	11.697	3218	3221	3229	rVB5	599	660	0.05%	0.007%
80	11.754	3235	3239	3242	rBV2	179	158	0.01%	0.002%
81	11.816	3245	3258	3274	rBV	488067	762524	60.70%	7.972%
82	11.941	3293	3297	3299	rBV2	365	274	0.02%	0.003%
83	11.973	3304	3307	3313	rVB2	670	713	0.06%	0.007%
84	12.115	3345	3351	3355	rBV2	312	406	0.03%	0.004%
85	12.195	3363	3376	3397	rVV	519286	836427	66.58%	8.744%
86	12.330	3414	3418	3422	rBV3	244	214	0.02%	0.002%
87	12.507	3469	3473	3480	rVB2	272	336	0.03%	0.004%
88	12.536	3480	3482	3486	rBV2	213	176	0.01%	0.002%
89	12.581	3486	3496	3499	rBV2	185	338	0.03%	0.004%
90	12.960	3610	3614	3620	rVB2	272	389	0.03%	0.004%
91	13.031	3631	3636	3639	rBV	213	235	0.02%	0.002%
92	13.147	3668	3672	3676	rBV2	294	343	0.03%	0.004%
93	13.378	3739	3744	3747	rBV2	317	268	0.02%	0.003%
94	13.417	3753	3756	3763	rVB2	191	210	0.02%	0.002%
95	13.610	3811	3816	3819	rBV2	202	264	0.02%	0.003%
96	13.896	3901	3905	3906	rBV	233	172	0.01%	0.002%
97	14.089	3962	3965	3968	rBV2	545	474	0.04%	0.005%
98	14.356	4045	4048	4053	rBV2	339	290	0.02%	0.003%
99	14.725	4160	4163	4164	rBV	352	233	0.02%	0.002%
100	14.957	4232	4235	4237	rBV3	253	168	0.01%	0.002%

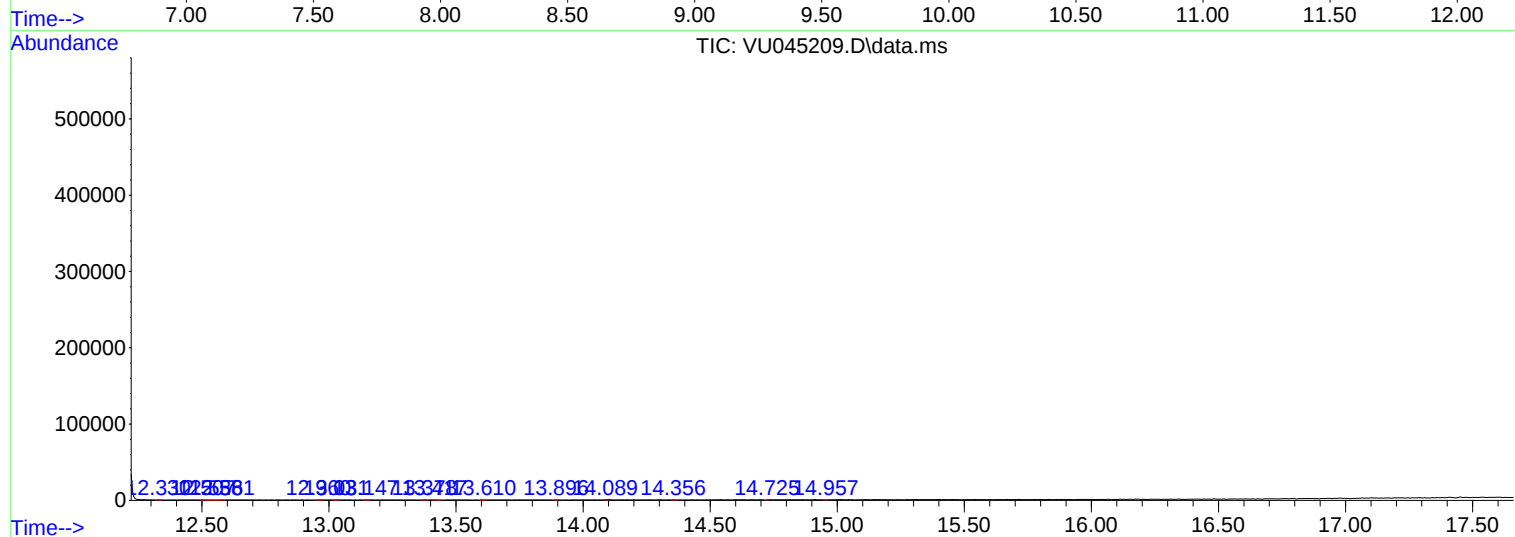
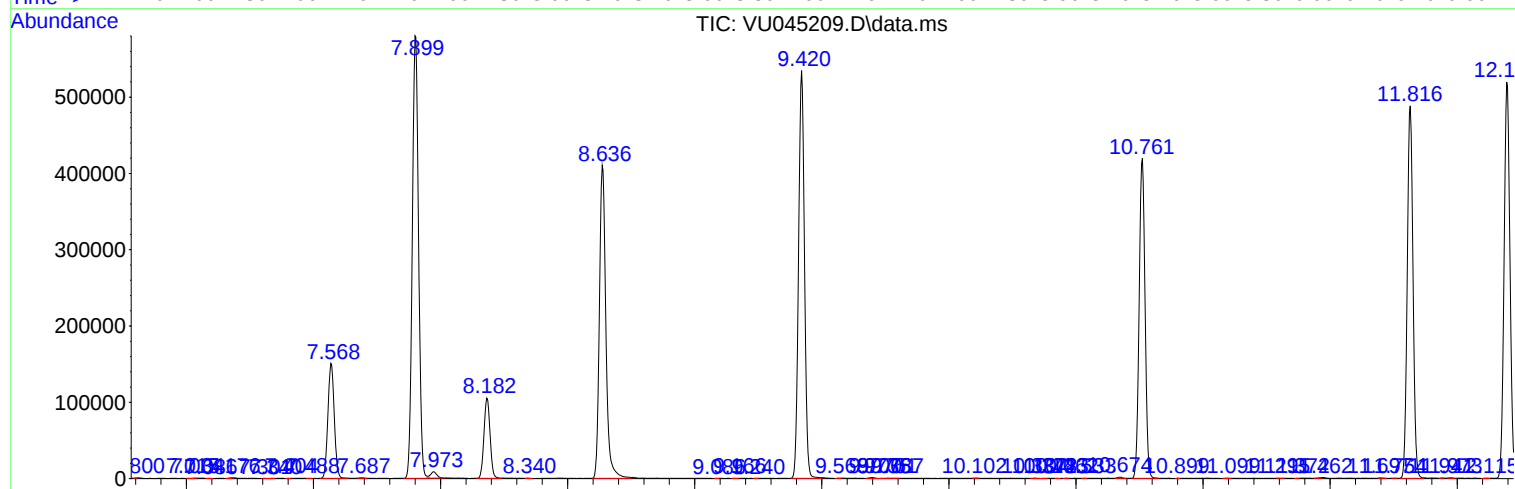
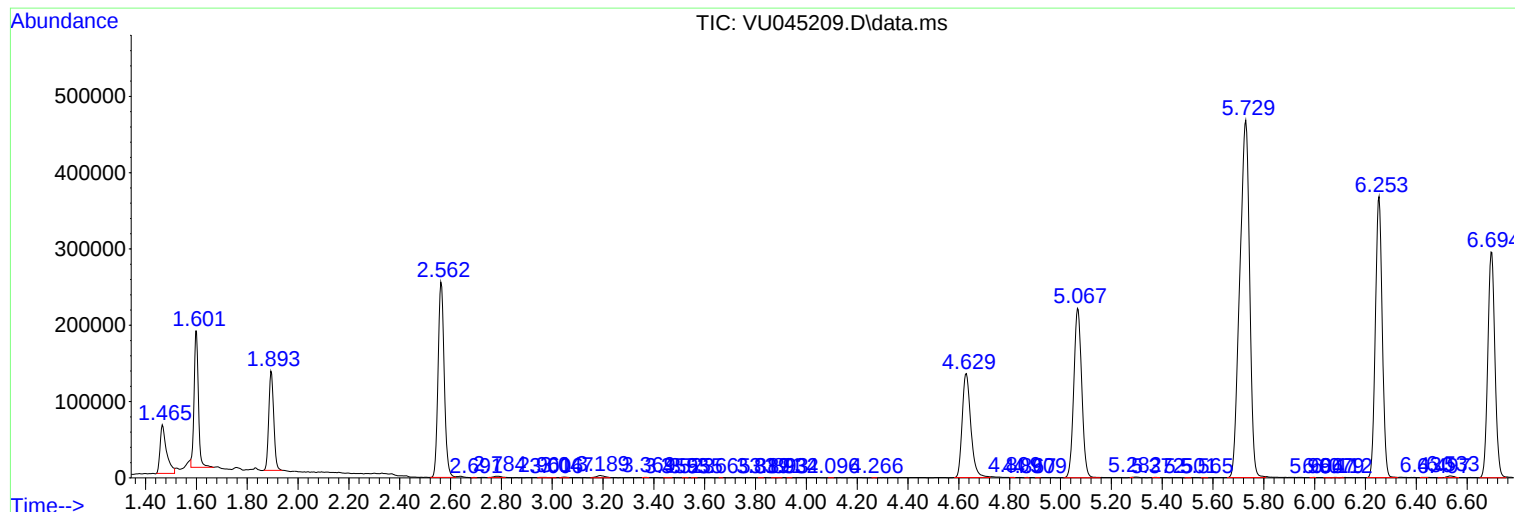
Sum of corrected areas: 9565255

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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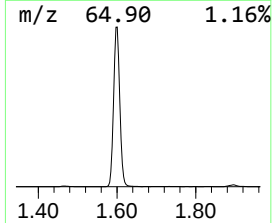
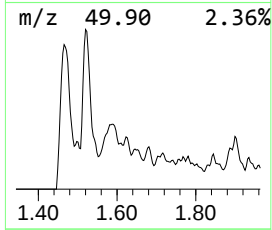
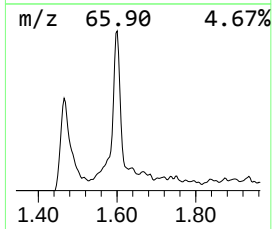
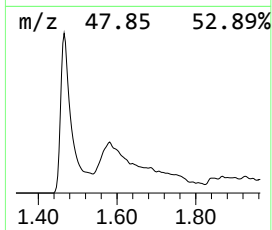
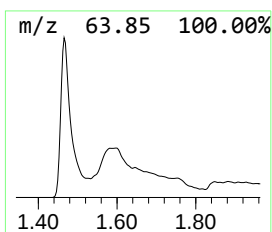
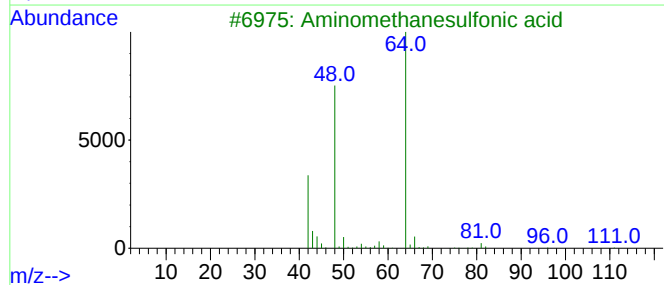
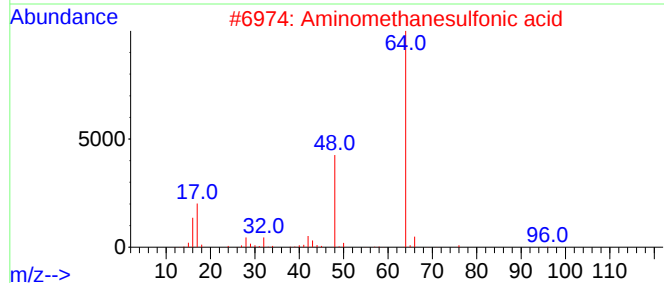
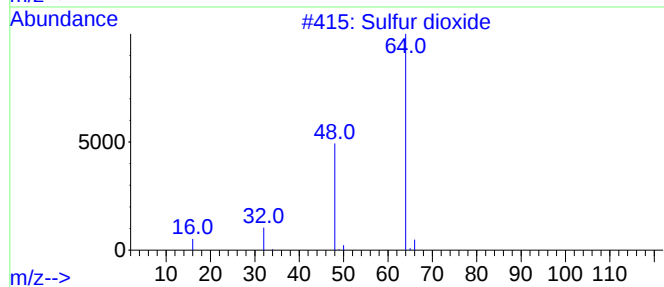
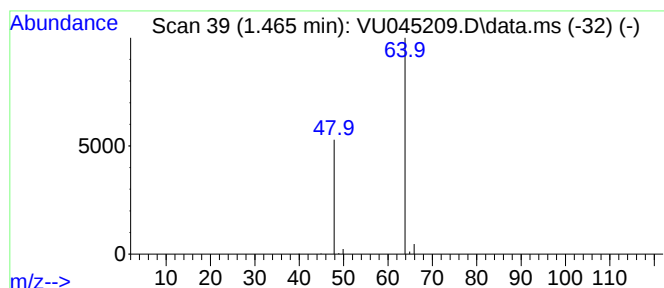
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.465	8.14 ug/L	111971	1,4-Difluorobenzene	6.253

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



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.465	8.1	ug/L	111971	1	6.253	688104	50.0