

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045211.D
 Acq On : 07 Oct 2021 14:54
 Operator : SY/MD
 Sample : M4025-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN5

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: VU045211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	54	rBV	32674	58488	4.60%	0.604%
2	1.601	74	81	98	rVB	185997	200375	15.76%	2.070%
3	1.900	165	174	195	rVB	132627	184368	14.50%	1.904%
4	2.565	367	381	398	rBV	260149	439085	34.53%	4.536%
5	2.774	435	446	459	rVB2	2045	4254	0.33%	0.044%
6	3.002	512	517	518	rBV	224	179	0.01%	0.002%
7	3.047	525	531	537	rVB4	763	977	0.08%	0.010%
8	3.086	537	543	544	rBV2	188	180	0.01%	0.002%
9	3.192	564	576	589	rBV	3132	6735	0.53%	0.070%
10	3.301	605	610	612	rBV	215	203	0.02%	0.002%
11	3.472	658	663	665	rBV2	143	181	0.01%	0.002%
12	3.629	708	712	716	rVB2	234	260	0.02%	0.003%
13	3.652	716	719	722	rBV	249	212	0.02%	0.002%
14	3.797	761	764	770	rBV	152	156	0.01%	0.002%
15	3.835	773	776	780	rVB2	258	232	0.02%	0.002%
16	3.861	780	784	789	rBV	222	270	0.02%	0.003%
17	3.916	794	801	804	rBV2	185	237	0.02%	0.002%
18	3.993	822	825	830	rVB2	189	160	0.01%	0.002%
19	4.160	872	877	880	rBV2	166	155	0.01%	0.002%
20	4.189	882	886	889	rBV2	164	166	0.01%	0.002%
21	4.330	926	930	932	rBV	240	215	0.02%	0.002%
22	4.465	970	972	977	rVB2	216	175	0.01%	0.002%
23	4.494	977	981	986	rBV2	184	278	0.02%	0.003%
24	4.629	1003	1023	1046	rBV	139802	328751	25.85%	3.396%
25	4.954	1122	1124	1130	rVB2	264	238	0.02%	0.002%
26	5.002	1137	1139	1143	rBV2	172	169	0.01%	0.002%
27	5.067	1143	1159	1179	rBV	224930	488507	38.42%	5.046%
28	5.170	1189	1191	1195	rVB	246	186	0.01%	0.002%
29	5.292	1221	1229	1240	rVB3	591	1205	0.09%	0.012%
30	5.372	1251	1254	1255	rBV	348	173	0.01%	0.002%
31	5.549	1303	1309	1313	rVB2	256	289	0.02%	0.003%
32	5.729	1341	1365	1391	rBV2	479419	1271600	100.00%	13.135%
33	6.118	1482	1486	1491	rVB3	475	480	0.04%	0.005%
34	6.163	1497	1500	1506	rBV4	209	263	0.02%	0.003%
35	6.253	1512	1528	1549	rBV	383019	710946	55.91%	7.344%
36	6.353	1557	1559	1565	rVB3	261	172	0.01%	0.002%

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 Title : VOC Analysis

37	6.401	1571	1574	1579	rBV2	185	169	0.01%	0.002%
38	6.536	1607	1616	1630	rBV7	3791	7803	0.61%	0.081%
39	6.633	1642	1646	1650	rBV2	192	209	0.02%	0.002%
40	6.694	1650	1665	1683	rBV	301998	578675	45.51%	5.977%
41	6.813	1696	1702	1706	rVB4	550	570	0.04%	0.006%
42	6.989	1755	1757	1761	rBV2	203	177	0.01%	0.002%
43	7.012	1761	1764	1767	rVV	161	157	0.01%	0.002%
44	7.054	1774	1777	1780	rVB2	371	296	0.02%	0.003%
45	7.134	1799	1802	1807	rBV2	245	254	0.02%	0.003%
46	7.179	1808	1816	1821	rBV4	944	1271	0.10%	0.013%
47	7.391	1877	1882	1886	rBV2	217	286	0.02%	0.003%
48	7.417	1887	1890	1894	rVB	223	157	0.01%	0.002%
49	7.568	1925	1937	1956	rBV	149854	261480	20.56%	2.701%
50	7.655	1961	1964	1965	rBV	316	184	0.01%	0.002%
51	7.774	1997	2001	2004	rBV	162	169	0.01%	0.002%
52	7.903	2026	2041	2056	rBV	590603	999945	78.64%	10.329%
53	7.973	2056	2063	2074	rVB2	8295	13803	1.09%	0.143%
54	8.182	2116	2128	2146	rBV	106685	175295	13.79%	1.811%
55	8.285	2155	2160	2163	rBV4	347	336	0.03%	0.003%
56	8.398	2190	2195	2198	rBV2	187	170	0.01%	0.002%
57	8.478	2208	2220	2225	rBV2	746	1258	0.10%	0.013%
58	8.636	2255	2269	2305	rBV	415919	725475	57.05%	7.494%
59	8.864	2333	2340	2341	rBV2	272	240	0.02%	0.002%
60	8.989	2376	2379	2383	rVB	221	173	0.01%	0.002%
61	9.041	2390	2395	2397	rBV	225	175	0.01%	0.002%
62	9.144	2423	2427	2430	rBV	200	197	0.02%	0.002%
63	9.253	2455	2461	2468	rVB2	205	332	0.03%	0.003%
64	9.292	2468	2473	2476	rBV2	267	300	0.02%	0.003%
65	9.420	2500	2513	2546	rVV	544061	888479	69.87%	9.178%
66	9.568	2555	2559	2560	rBV	363	257	0.02%	0.003%
67	9.693	2592	2598	2599	rBV2	843	714	0.06%	0.007%
68	9.732	2605	2610	2612	rBV2	169	167	0.01%	0.002%
69	9.851	2644	2647	2652	rVB2	262	233	0.02%	0.002%
70	9.912	2660	2666	2668	rBV2	259	256	0.02%	0.003%
71	10.099	2720	2724	2726	rBV2	224	205	0.02%	0.002%
72	10.295	2781	2785	2787	rBV2	198	195	0.02%	0.002%
73	10.433	2825	2828	2832	rVB2	184	158	0.01%	0.002%
74	10.674	2896	2903	2912	rVB4	1452	2056	0.16%	0.021%
75	10.761	2916	2930	2949	rVB	418814	671117	52.78%	6.932%
76	10.899	2971	2973	2979	rVB3	383	370	0.03%	0.004%

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Integrator: RTE

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Peak Location: TOP

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

77	10.989	2997	3001	3003	rBV2	264	206	0.02%	0.002%
78	11.092	3030	3033	3037	rBV2	247	209	0.02%	0.002%
79	11.214	3069	3071	3076	rVB2	231	184	0.01%	0.002%
80	11.288	3089	3094	3096	rBV2	259	204	0.02%	0.002%
81	11.356	3111	3115	3119	rVB2	241	253	0.02%	0.003%
82	11.404	3125	3130	3133	rBV2	264	243	0.02%	0.003%
83	11.468	3141	3150	3159	rVB4	1006	1851	0.15%	0.019%
84	11.513	3159	3164	3168	rBV2	259	310	0.02%	0.003%
85	11.578	3178	3184	3186	rBV2	234	257	0.02%	0.003%
86	11.632	3198	3201	3208	rVB	787	955	0.08%	0.010%
87	11.693	3217	3220	3228	rVB3	591	719	0.06%	0.007%
88	11.816	3245	3258	3281	rBV	502310	790712	62.18%	8.168%
89	12.195	3363	3376	3397	rBV	527274	846864	66.60%	8.748%
90	12.359	3421	3427	3431	rBV2	282	376	0.03%	0.004%
91	12.510	3471	3474	3479	rBB2	257	254	0.02%	0.003%
92	12.542	3479	3484	3488	rBV	227	213	0.02%	0.002%
93	12.565	3488	3491	3495	rBV2	203	205	0.02%	0.002%
94	12.632	3508	3512	3516	rBV2	193	240	0.02%	0.002%
95	12.787	3554	3560	3563	rBV3	475	608	0.05%	0.006%
96	13.250	3701	3704	3711	rBV2	220	258	0.02%	0.003%
97	13.369	3738	3741	3744	rBV2	203	199	0.02%	0.002%
98	14.478	4083	4086	4089	rBV	297	210	0.02%	0.002%
99	14.561	4110	4112	4115	rBV2	315	237	0.02%	0.002%
100	16.327	4654	4661	4664	rBV3	654	923	0.07%	0.010%

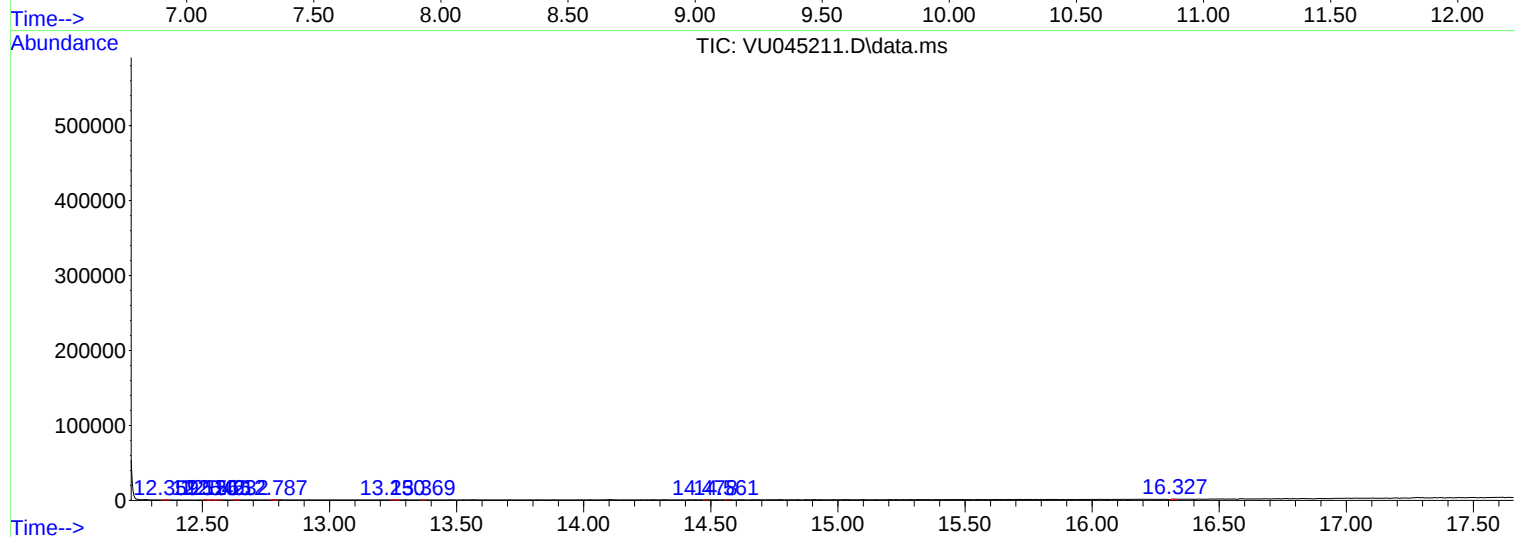
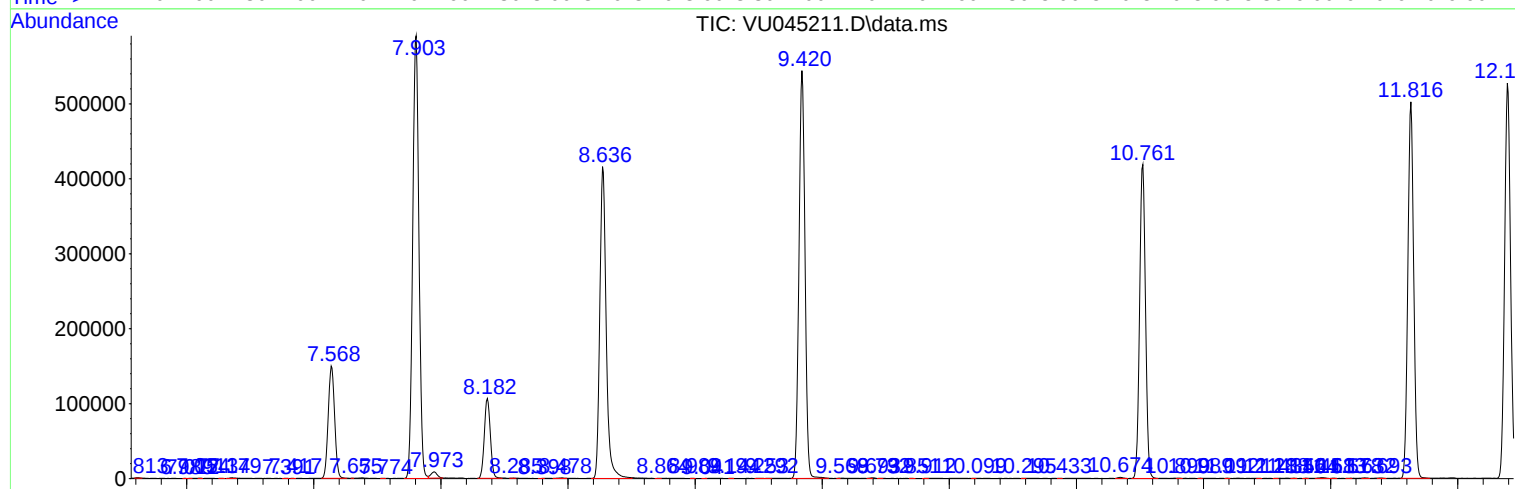
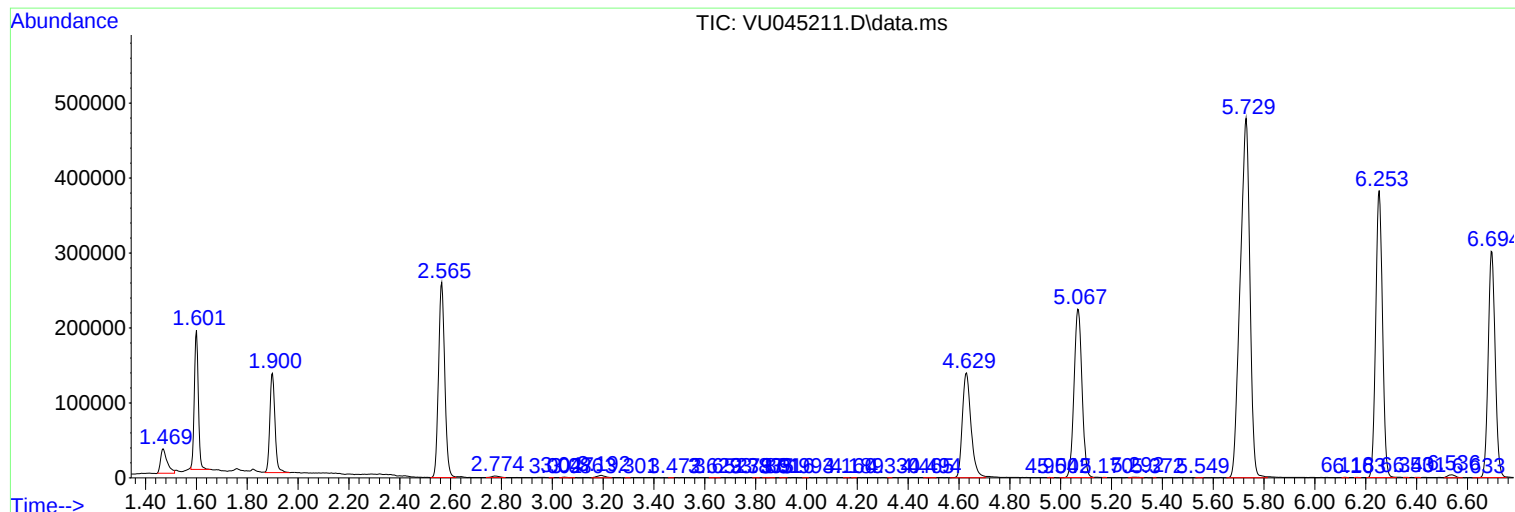
Sum of corrected areas: 9680973

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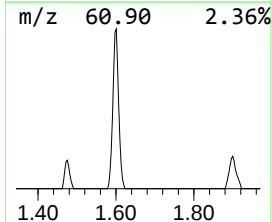
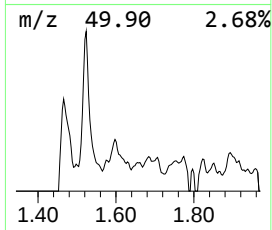
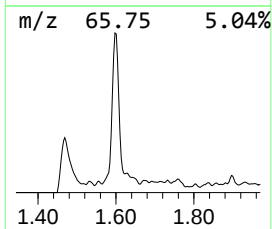
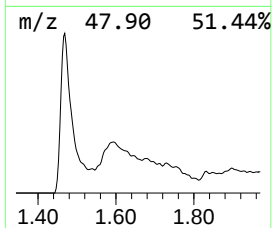
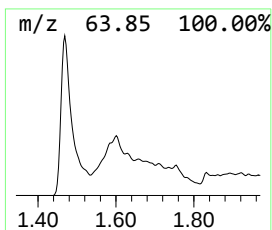
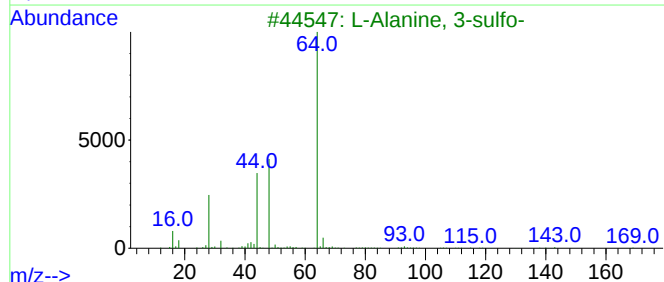
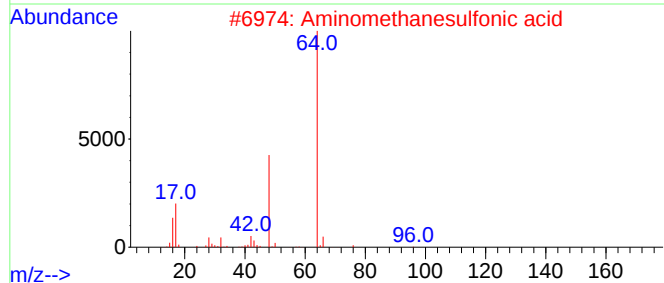
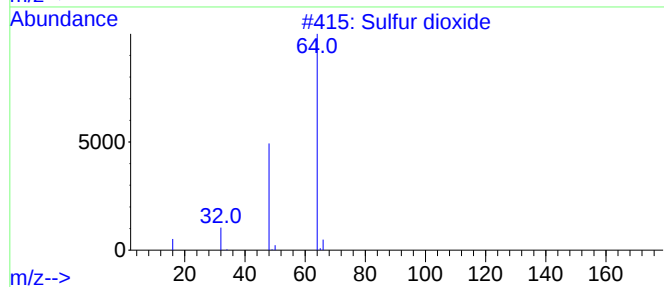
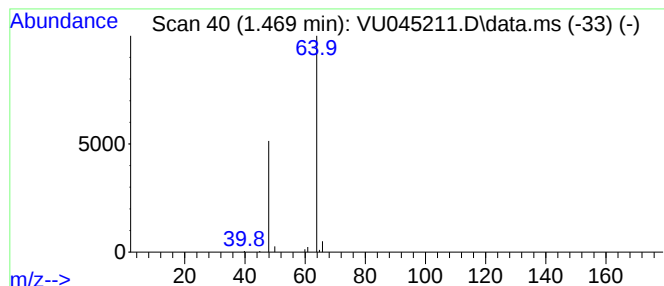
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.469	4.11 ug/L	58488	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	4.1	ug/L	58488	1	6.253	710946	50.0