

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045249.D
 Acq On : 08 Oct 2021 14:18
 Operator : SY/MD
 Sample : M4023-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AJ3

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: VU045249.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	32	41	56	rBV2	39786	72076	5.30%	0.712%
2	1.601	74	81	99	rVB	156821	176990	13.02%	1.750%
3	1.890	163	171	186	rVB	131054	176972	13.02%	1.749%
4	2.562	368	380	400	rBV	244012	411454	30.27%	4.067%
5	2.790	445	451	457	rVB4	726	1046	0.08%	0.010%
6	2.951	498	501	504	rBV3	380	387	0.03%	0.004%
7	3.089	540	544	547	rBV2	313	307	0.02%	0.003%
8	3.160	561	566	567	rBV	164	135	0.01%	0.001%
9	3.186	567	574	577	rBV2	1144	1461	0.11%	0.014%
10	3.343	618	623	624	rBV	167	176	0.01%	0.002%
11	3.372	630	632	638	rVB2	307	252	0.02%	0.002%
12	3.700	730	734	737	rBV2	274	289	0.02%	0.003%
13	3.755	745	751	754	rBV2	252	304	0.02%	0.003%
14	3.797	761	764	767	rBV2	220	154	0.01%	0.002%
15	3.816	767	770	777	rBV	225	267	0.02%	0.003%
16	4.018	828	833	835	rBV	148	172	0.01%	0.002%
17	4.128	863	867	869	rBV2	224	180	0.01%	0.002%
18	4.205	886	891	894	rBV	179	215	0.02%	0.002%
19	4.224	895	897	901	rVB	335	246	0.02%	0.002%
20	4.256	901	907	912	rBV2	282	377	0.03%	0.004%
21	4.430	956	961	965	rBV2	122	133	0.01%	0.001%
22	4.510	981	986	989	rBV2	165	156	0.01%	0.002%
23	4.629	1008	1023	1054	rBV	160366	381008	28.03%	3.766%
24	4.919	1111	1113	1119	rVB2	236	171	0.01%	0.002%
25	5.067	1142	1159	1189	rVV	241638	535356	39.39%	5.292%
26	5.218	1205	1206	1209	rBV	239	140	0.01%	0.001%
27	5.295	1223	1230	1236	rBV2	627	1086	0.08%	0.011%
28	5.404	1260	1264	1267	rBV2	147	136	0.01%	0.001%
29	5.488	1285	1290	1295	rBV2	200	245	0.02%	0.002%
30	5.510	1295	1297	1302	rVB2	168	136	0.01%	0.001%
31	5.559	1309	1312	1321	rVV2	105	138	0.01%	0.001%
32	5.729	1342	1365	1388	rBV2	504234	1359159	100.00%	13.435%
33	6.073	1469	1472	1475	rBV2	223	147	0.01%	0.001%
34	6.089	1475	1477	1481	rVB2	176	152	0.01%	0.002%
35	6.112	1481	1484	1486	rBV3	230	169	0.01%	0.002%
36	6.253	1512	1528	1550	rBV	360226	674704	49.64%	6.669%

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 Title : VOC Analysis

37	6.481	1595	1599	1602	rVB3	213	163	0.01%	0.002%
38	6.542	1606	1618	1631	rVB7	10115	19656	1.45%	0.194%
39	6.694	1650	1665	1686	rBV	329578	635103	46.73%	6.278%
40	6.816	1694	1703	1710	rVB5	864	1362	0.10%	0.013%
41	7.051	1771	1776	1783	rVB3	388	474	0.03%	0.005%
42	7.182	1807	1817	1831	rVB4	3183	5615	0.41%	0.056%
43	7.237	1831	1834	1837	rBV	165	154	0.01%	0.002%
44	7.443	1892	1898	1901	rBV	154	181	0.01%	0.002%
45	7.514	1913	1920	1924	rBV2	124	156	0.01%	0.002%
46	7.568	1924	1937	1953	rBV	174194	301226	22.16%	2.978%
47	7.690	1966	1975	1983	rVB3	1963	3198	0.24%	0.032%
48	7.735	1987	1989	1992	rVV	200	133	0.01%	0.001%
49	7.825	2014	2017	2023	rBV	152	168	0.01%	0.002%
50	7.903	2027	2041	2055	rBV	615130	1040512	76.56%	10.285%
51	7.973	2057	2063	2075	rVB	8587	14294	1.05%	0.141%
52	8.182	2116	2128	2145	rBV	123934	203498	14.97%	2.012%
53	8.398	2190	2195	2199	rBV	182	208	0.02%	0.002%
54	8.472	2210	2218	2222	rBV3	751	958	0.07%	0.009%
55	8.526	2231	2235	2238	rBV2	271	250	0.02%	0.002%
56	8.546	2238	2241	2244	rBV	155	148	0.01%	0.001%
57	8.636	2257	2269	2297	rBV	459983	809545	59.56%	8.002%
58	8.864	2337	2340	2342	rBV	275	200	0.01%	0.002%
59	8.906	2350	2353	2358	rVB2	260	167	0.01%	0.002%
60	9.038	2389	2394	2397	rBV	203	233	0.02%	0.002%
61	9.292	2468	2473	2477	rBV	181	212	0.02%	0.002%
62	9.317	2477	2481	2484	rBV2	178	156	0.01%	0.002%
63	9.420	2500	2513	2534	rBV	519493	845345	62.20%	8.356%
64	9.565	2554	2558	2559	rBV2	261	165	0.01%	0.002%
65	9.578	2559	2562	2567	rVB2	460	413	0.03%	0.004%
66	9.693	2589	2598	2606	rBV3	1902	2879	0.21%	0.028%
67	9.729	2606	2609	2614	rBV	224	156	0.01%	0.002%
68	10.070	2711	2715	2720	rBV	147	166	0.01%	0.002%
69	10.105	2720	2726	2731	rVB4	535	570	0.04%	0.006%
70	10.147	2734	2739	2745	rBV	222	247	0.02%	0.002%
71	10.423	2821	2825	2830	rBV2	200	194	0.01%	0.002%
72	10.468	2836	2839	2841	rBV	246	192	0.01%	0.002%
73	10.555	2862	2866	2868	rBV2	217	190	0.01%	0.002%
74	10.674	2895	2903	2914	rVB3	2379	3643	0.27%	0.036%
75	10.761	2914	2930	2949	rBV	477959	762868	56.13%	7.541%
76	10.976	2993	2997	3001	rBV2	186	174	0.01%	0.002%

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 Title : VOC Analysis

77	10.999	3001	3004	3007	rVB2	266	186	0.01%	0.002%
78	11.079	3026	3029	3032	rBV	151	153	0.01%	0.002%
79	11.234	3073	3077	3080	rBV2	214	197	0.01%	0.002%
80	11.433	3134	3139	3140	rBV	178	147	0.01%	0.001%
81	11.459	3140	3147	3162	rVV5	1560	2804	0.21%	0.028%
82	11.584	3181	3186	3190	rBV2	231	252	0.02%	0.002%
83	11.632	3196	3201	3209	rVB2	655	868	0.06%	0.009%
84	11.697	3215	3221	3227	rBV3	1030	1239	0.09%	0.012%
85	11.816	3246	3258	3277	rBV	480064	742849	54.66%	7.343%
86	11.947	3290	3299	3302	rBV4	909	1294	0.10%	0.013%
87	11.976	3303	3308	3316	rVB3	1712	2333	0.17%	0.023%
88	12.195	3362	3376	3395	rBV	560459	909198	66.89%	8.987%
89	12.291	3402	3406	3407	rBV	223	154	0.01%	0.002%
90	12.407	3439	3442	3445	rVB2	332	173	0.01%	0.002%
91	12.629	3505	3511	3512	rBV2	294	266	0.02%	0.003%
92	12.774	3551	3556	3561	rBV2	270	329	0.02%	0.003%
93	13.153	3671	3674	3681	rBV2	315	381	0.03%	0.004%
94	13.725	3849	3852	3854	rBV	196	170	0.01%	0.002%
95	14.057	3951	3955	3959	rBV	228	207	0.02%	0.002%
96	14.282	4023	4025	4027	rBV	238	136	0.01%	0.001%
97	14.423	4066	4069	4074	rVB	326	284	0.02%	0.003%
98	14.523	4093	4100	4106	rBV3	318	463	0.03%	0.005%
99	14.918	4220	4223	4230	rBV	302	250	0.02%	0.002%
100	14.999	4245	4248	4252	rBV3	449	343	0.03%	0.003%

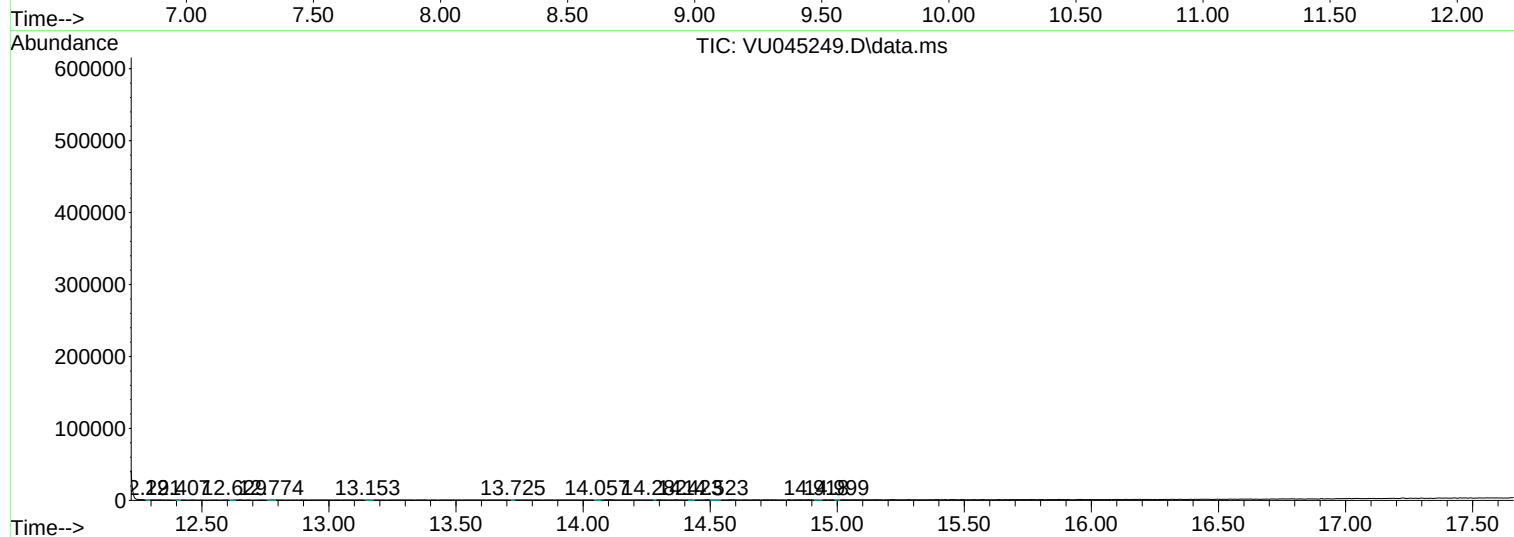
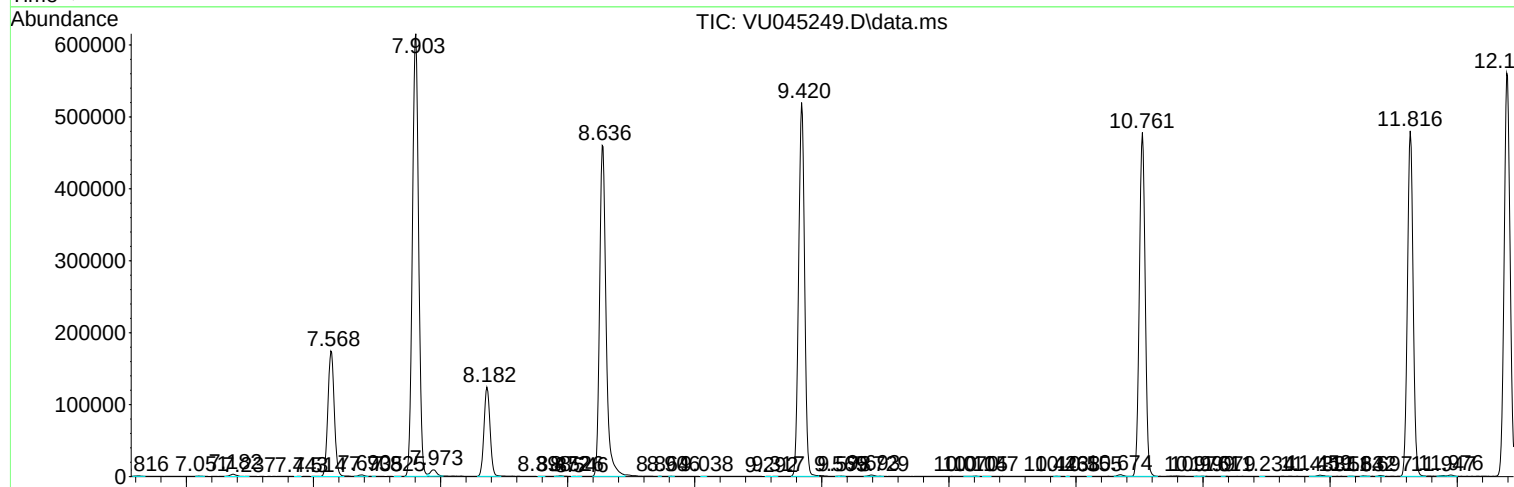
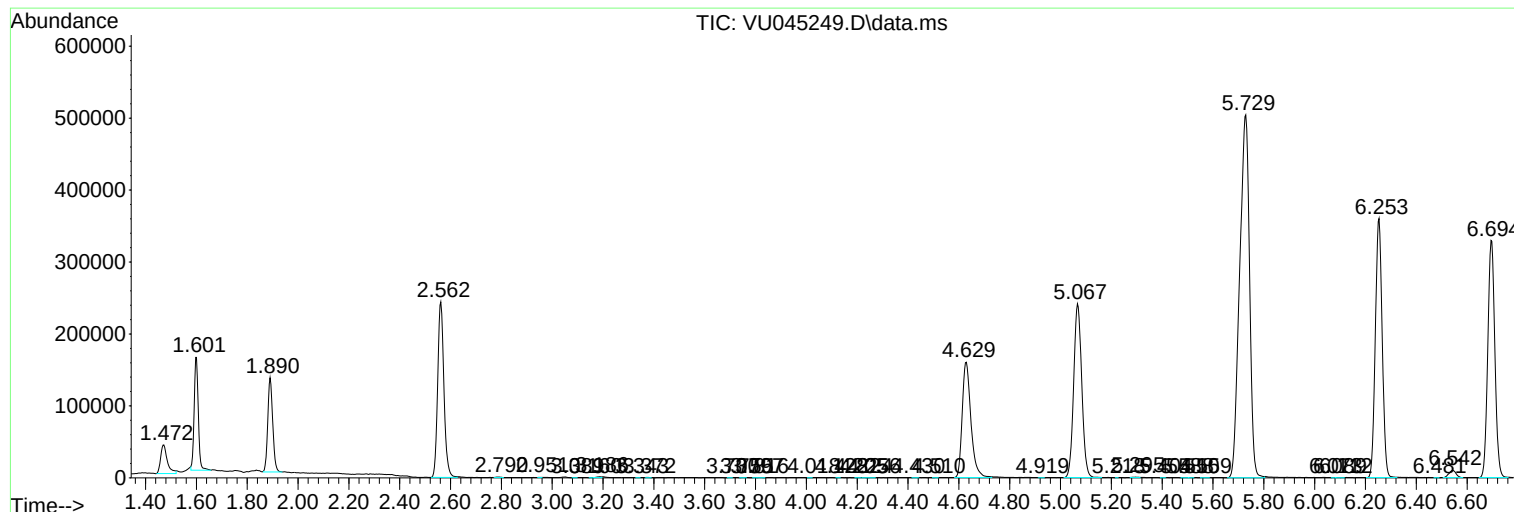
Sum of corrected areas: 10116344

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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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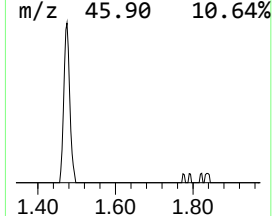
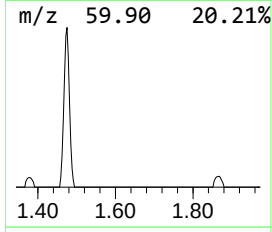
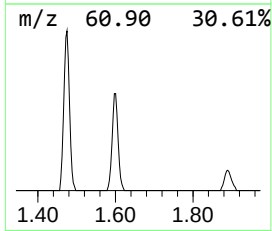
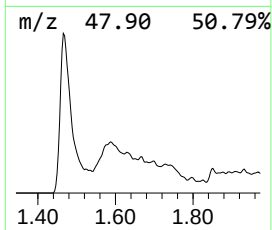
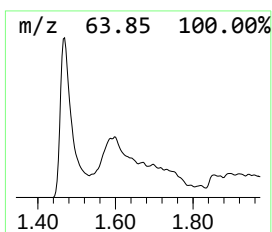
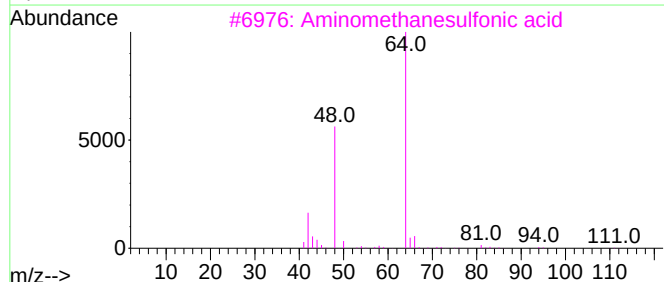
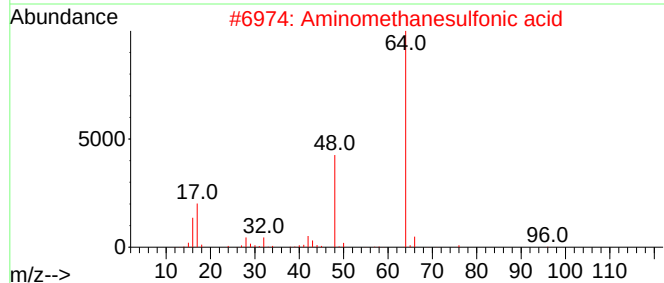
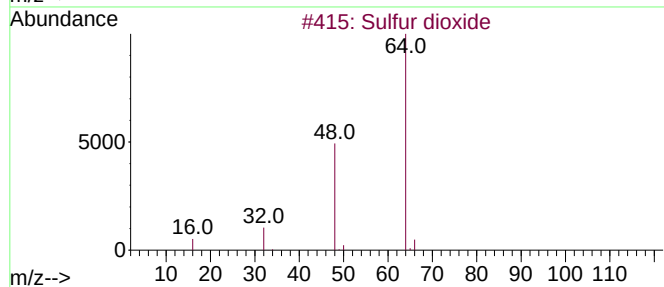
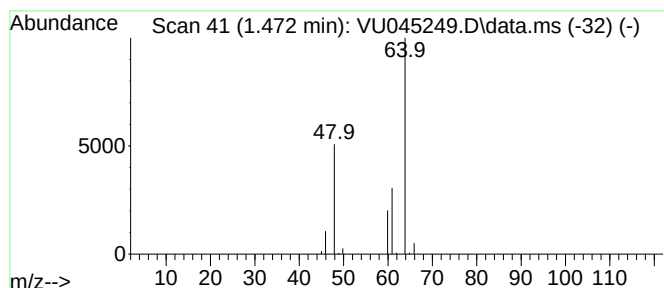
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.472	5.34 ug/L	72076	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	80
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	56
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	40
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	40
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.472	5.3	ug/L	72076	1	6.253	674704	50.0