

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045099.D
 Acq On : 04 Oct 2021 16:22
 Operator : SY/MD
 Sample : M3996-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A24

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: VU045099.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	37	44	65	rBV3	15660	39949	0.22%	0.143%
2	1.604	74	82	94	rBV	141271	167720	0.93%	0.600%
3	1.909	170	177	193	rVB	118532	162883	0.90%	0.583%
4	2.469	344	351	363	rVB2	3191	5075	0.03%	0.018%
5	2.572	369	383	404	rBV	231340	393167	2.18%	1.407%
6	2.797	445	453	457	rBV2	570	826	0.00%	0.003%
7	2.880	475	479	482	rBV	191	180	0.00%	0.001%
8	2.948	496	500	502	rBV2	331	273	0.00%	0.001%
9	3.019	517	522	527	rVV4	408	480	0.00%	0.002%
10	3.054	527	533	538	rVV4	643	716	0.00%	0.003%
11	3.089	541	544	546	rVB2	311	200	0.00%	0.001%
12	3.192	564	576	591	rVB2	4651	10588	0.06%	0.038%
13	3.369	621	631	644	rVB2	3616	8055	0.04%	0.029%
14	3.424	644	648	653	rVB2	215	169	0.00%	0.001%
15	3.456	653	658	662	rBV2	161	178	0.00%	0.001%
16	3.504	668	673	678	rBV2	226	282	0.00%	0.001%
17	3.533	678	682	686	rVB2	198	201	0.00%	0.001%
18	3.600	694	703	705	rBV	182	237	0.00%	0.001%
19	3.668	720	724	731	rBV2	199	272	0.00%	0.001%
20	3.896	792	795	798	rBV	225	178	0.00%	0.001%
21	4.057	842	845	850	rVB2	175	211	0.00%	0.001%
22	4.478	972	976	980	rBV2	233	240	0.00%	0.001%
23	4.533	987	993	994	rBV	262	218	0.00%	0.001%
24	4.543	994	996	1002	rVB3	516	486	0.00%	0.002%
25	4.629	1007	1023	1057	rBV	162160	407450	2.26%	1.458%
26	4.935	1115	1118	1123	rBV2	232	234	0.00%	0.001%
27	5.070	1143	1160	1183	rBV	220758	488411	2.71%	1.747%
28	5.221	1204	1207	1215	rVB3	491	531	0.00%	0.002%
29	5.301	1218	1232	1236	rBV4	666	1332	0.01%	0.005%
30	5.385	1255	1258	1262	rVV2	365	379	0.00%	0.001%
31	5.629	1331	1334	1340	rVB2	256	236	0.00%	0.001%
32	5.729	1340	1365	1394	rBV2	449743	1250925	6.93%	4.475%
33	6.047	1459	1464	1467	rVB	380	316	0.00%	0.001%
34	6.083	1472	1475	1480	rVB3	396	361	0.00%	0.001%
35	6.118	1480	1486	1488	rBV2	544	496	0.00%	0.002%
36	6.166	1497	1501	1504	rVB3	301	225	0.00%	0.001%

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

37	6.253	1512	1528	1548	rBV	362903	685436	3.80%	2.452%
38	6.433	1580	1584	1586	rBV3	324	243	0.00%	0.001%
39	6.546	1607	1619	1632	rVB5	28602	55171	0.31%	0.197%
40	6.697	1651	1666	1692	rBV	292101	572202	3.17%	2.047%
41	6.800	1696	1698	1700	rBV	552	312	0.00%	0.001%
42	6.980	1750	1754	1757	rVB2	237	233	0.00%	0.001%
43	7.015	1761	1765	1768	rBV	251	235	0.00%	0.001%
44	7.041	1768	1773	1774	rBV2	337	244	0.00%	0.001%
45	7.112	1790	1795	1799	rVB2	382	414	0.00%	0.001%
46	7.186	1809	1818	1829	rBV4	2449	4581	0.03%	0.016%
47	7.243	1834	1836	1840	rVB	257	174	0.00%	0.001%
48	7.279	1844	1847	1851	rBV	311	262	0.00%	0.001%
49	7.366	1870	1874	1877	rBV	178	174	0.00%	0.001%
50	7.452	1894	1901	1905	rBV2	250	385	0.00%	0.001%
51	7.504	1914	1917	1924	rBV2	213	270	0.00%	0.001%
52	7.568	1924	1937	1956	rBV	160216	281057	1.56%	1.006%
53	7.690	1968	1975	1986	rVB4	1785	3201	0.02%	0.011%
54	7.742	1989	1991	1996	rVB	303	233	0.00%	0.001%
55	7.806	2009	2011	2016	rVB2	280	229	0.00%	0.001%
56	7.903	2026	2041	2055	rBV	543765	918897	5.09%	3.288%
57	7.973	2055	2063	2080	rVB	22303	37563	0.21%	0.134%
58	8.182	2116	2128	2143	rBV	112152	186867	1.04%	0.669%
59	8.481	2212	2221	2229	rVB	789	1258	0.01%	0.005%
60	8.558	2229	2245	2260	rBV	10747005	18045538	100.00%	64.562%
61	8.636	2261	2269	2312	rVB	524209	990522	5.49%	3.544%
62	8.922	2356	2358	2360	rBV	273	168	0.00%	0.001%
63	9.066	2400	2403	2406	rBV2	270	238	0.00%	0.001%
64	9.285	2468	2471	2475	rVB2	313	262	0.00%	0.001%
65	9.420	2499	2513	2532	rBV	510896	834375	4.62%	2.985%
66	9.575	2553	2561	2574	rVB	6746	10168	0.06%	0.036%
67	9.700	2590	2600	2612	rVB	6718	10662	0.06%	0.038%
68	9.809	2631	2634	2640	rBV	207	239	0.00%	0.001%
69	9.896	2656	2661	2665	rBV	246	269	0.00%	0.001%
70	9.947	2674	2677	2681	rBV	258	250	0.00%	0.001%
71	10.102	2717	2725	2738	rBV2	3442	5449	0.03%	0.019%
72	10.298	2782	2786	2790	rBV2	191	205	0.00%	0.001%
73	10.484	2837	2844	2847	rBV3	370	387	0.00%	0.001%
74	10.677	2894	2904	2913	rBV7	1755	2892	0.02%	0.010%
75	10.761	2916	2930	2951	rVV	423744	682058	3.78%	2.440%
76	10.870	2960	2964	2967	rVV3	393	377	0.00%	0.001%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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 Title : VOC Analysis

77	10.902	2969	2974	2984	rVB3	784	1425	0.01%	0.005%
78	10.999	2999	3004	3010	rBV2	745	1052	0.01%	0.004%
79	11.092	3028	3033	3043	rVB4	550	852	0.00%	0.003%
80	11.205	3063	3068	3071	rBV2	222	233	0.00%	0.001%
81	11.295	3090	3096	3100	rBV3	605	677	0.00%	0.002%
82	11.375	3118	3121	3125	rBV2	211	211	0.00%	0.001%
83	11.472	3141	3151	3159	rVV3	4401	6615	0.04%	0.024%
84	11.700	3216	3222	3228	rBV3	908	1184	0.01%	0.004%
85	11.767	3240	3243	3245	rBV2	280	223	0.00%	0.001%
86	11.816	3245	3258	3278	rVV	510044	789355	4.37%	2.824%
87	11.973	3304	3307	3321	rVB3	1336	1646	0.01%	0.006%
88	12.060	3331	3334	3335	rBV	293	205	0.00%	0.001%
89	12.095	3340	3345	3352	rVV2	846	1096	0.01%	0.004%
90	12.195	3363	3376	3394	rBV	524986	845374	4.68%	3.025%
91	12.295	3405	3407	3416	rVB4	455	510	0.00%	0.002%
92	12.500	3468	3471	3473	rBV	242	190	0.00%	0.001%
93	12.983	3617	3621	3622	rBV2	266	191	0.00%	0.001%
94	13.455	3765	3768	3771	rBV2	325	204	0.00%	0.001%
95	13.719	3847	3850	3855	rBV2	226	243	0.00%	0.001%
96	14.092	3958	3966	3980	rVB2	7446	11551	0.06%	0.041%
97	14.742	4162	4168	4171	rBV3	452	582	0.00%	0.002%
98	15.108	4279	4282	4285	rBV2	328	228	0.00%	0.001%
99	15.230	4311	4320	4333	rBV2	3097	5307	0.03%	0.019%
100	15.417	4370	4378	4387	rBV4	2283	3987	0.02%	0.014%

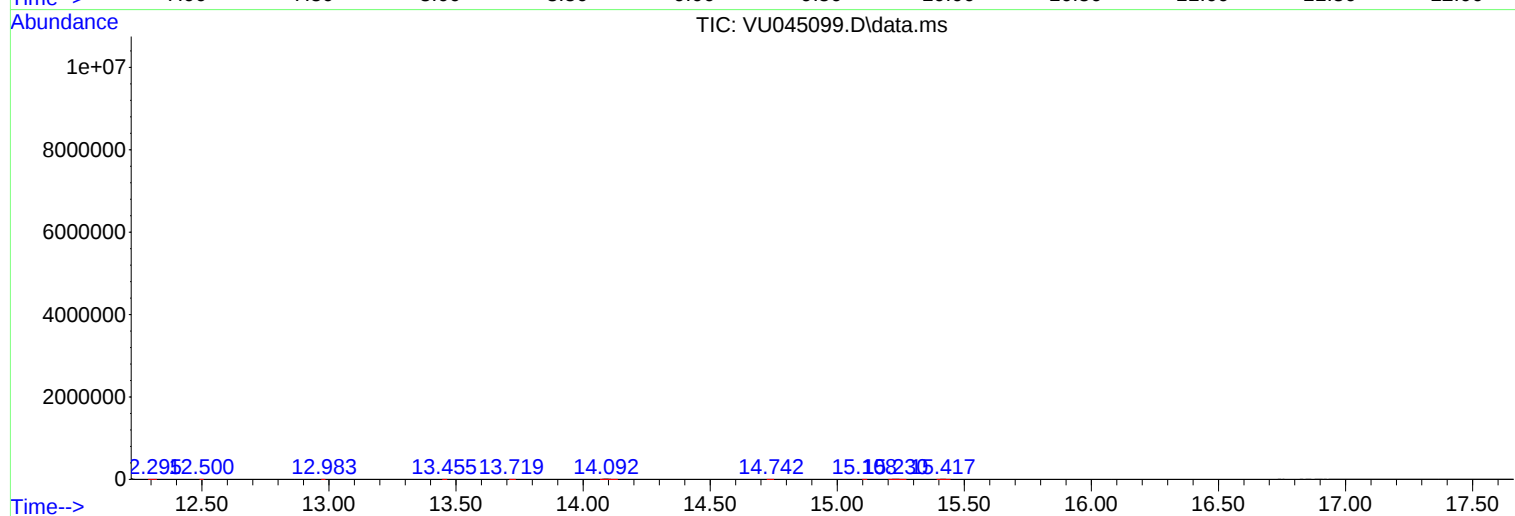
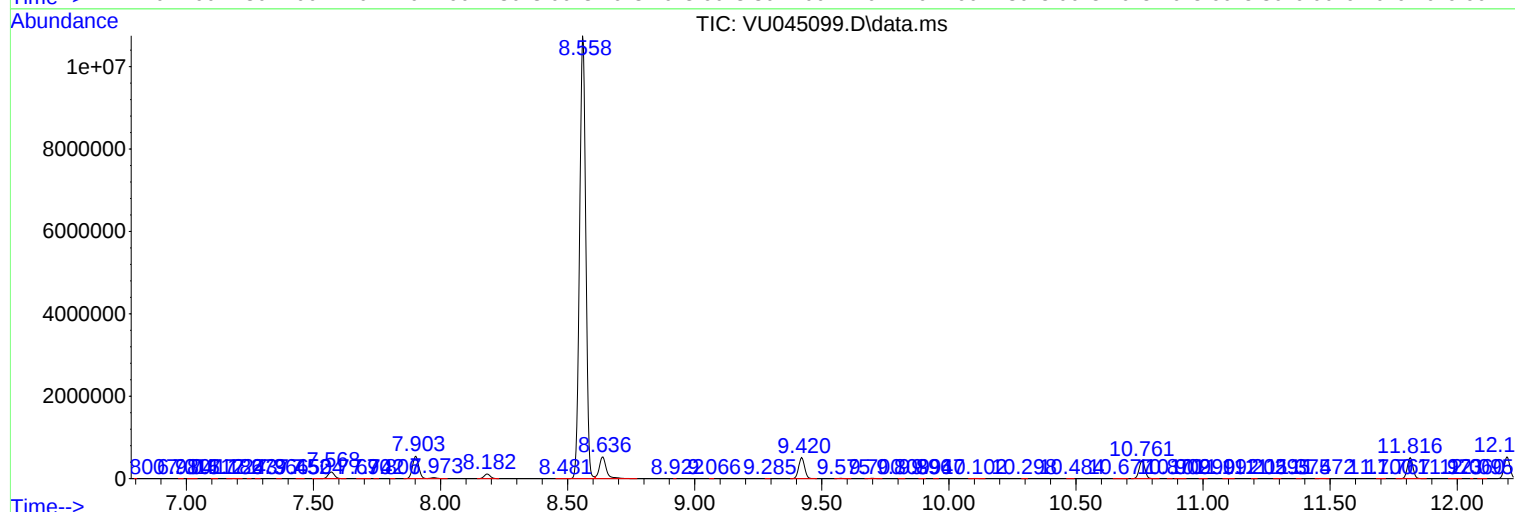
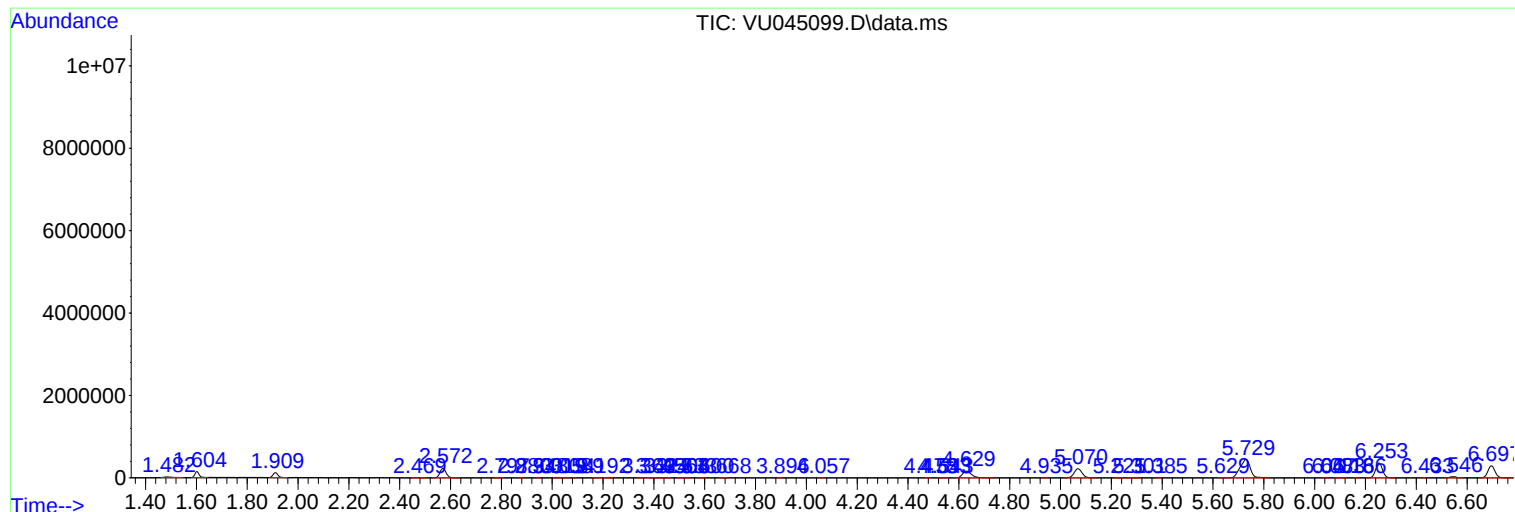
Sum of corrected areas: 27950521

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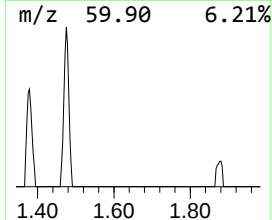
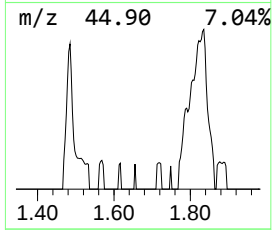
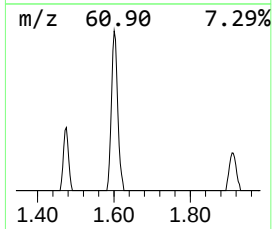
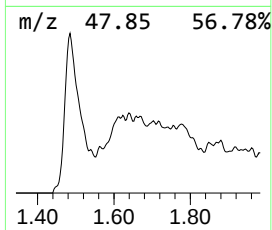
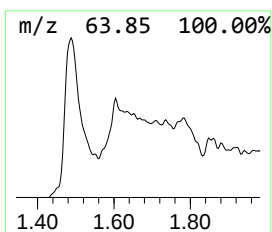
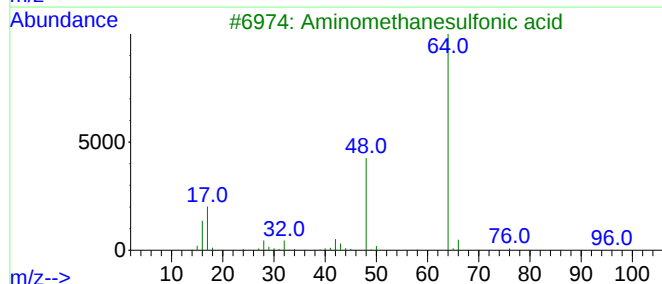
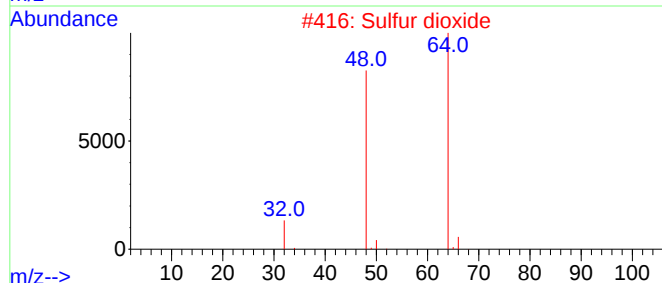
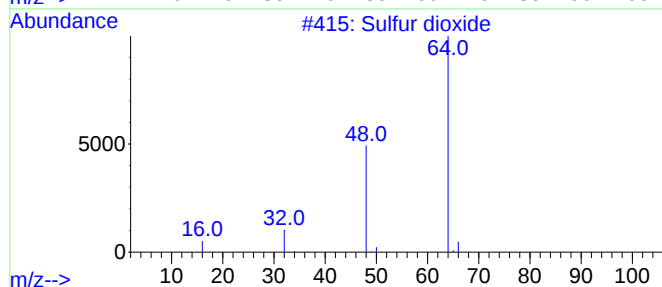
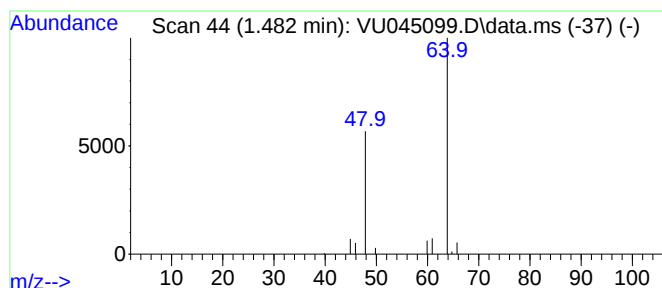
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.482	2.91 ug/L	39949	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.482	2.9	ug/L	39949	1	6.253	685436	50.0