

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045250.D
 Acq On : 08 Oct 2021 14:42
 Operator : SY/MD
 Sample : M4024-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AN1

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: VU045250.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	29583	52844	4.04%	0.544%
2	1.600	74	81	102	rVB	156547	171507	13.10%	1.767%
3	1.900	166	174	191	rVB	125632	170158	13.00%	1.753%
4	2.565	368	381	400	rBV	234265	393425	30.06%	4.053%
5	2.684	415	418	424	rVB2	299	209	0.02%	0.002%
6	2.713	424	427	431	rBV	179	153	0.01%	0.002%
7	2.780	438	448	453	rBV5	1127	1942	0.15%	0.020%
8	2.951	496	501	503	rBV2	263	241	0.02%	0.002%
9	3.044	524	530	540	rVB4	836	1280	0.10%	0.013%
10	3.192	565	576	586	rBV3	1841	3907	0.30%	0.040%
11	3.375	628	633	636	rVB3	236	224	0.02%	0.002%
12	3.417	642	646	649	rVB	173	164	0.01%	0.002%
13	3.452	649	657	659	rBV2	199	248	0.02%	0.003%
14	3.517	673	677	679	rVV	147	142	0.01%	0.001%
15	3.784	756	760	763	rBV2	168	148	0.01%	0.002%
16	3.864	781	785	786	rBV2	179	142	0.01%	0.001%
17	3.948	808	811	814	rBV	235	202	0.02%	0.002%
18	4.015	825	832	835	rVB2	183	185	0.01%	0.002%
19	4.044	835	841	844	rBV	186	235	0.02%	0.002%
20	4.105	856	860	867	rVB2	233	280	0.02%	0.003%
21	4.292	915	918	920	rBV2	217	176	0.01%	0.002%
22	4.366	938	941	944	rBV	212	172	0.01%	0.002%
23	4.440	959	964	970	rVB2	182	204	0.02%	0.002%
24	4.629	1008	1023	1058	rBV	149417	353179	26.98%	3.638%
25	4.957	1122	1125	1128	rVB	216	152	0.01%	0.002%
26	5.002	1133	1139	1142	rBV	336	372	0.03%	0.004%
27	5.070	1142	1160	1180	rBV	230041	504348	38.53%	5.196%
28	5.298	1223	1231	1241	rBV3	810	1682	0.13%	0.017%
29	5.372	1251	1254	1257	rBV	358	304	0.02%	0.003%
30	5.729	1343	1365	1385	rBV2	487162	1308939	100.00%	13.484%
31	6.044	1458	1463	1464	rBV3	339	314	0.02%	0.003%
32	6.157	1495	1498	1500	rBV	247	180	0.01%	0.002%
33	6.253	1513	1528	1546	rBV	368800	684578	52.30%	7.052%
34	6.542	1606	1618	1630	rVB7	6050	12028	0.92%	0.124%
35	6.697	1650	1666	1691	rBV	316923	606845	46.36%	6.252%
36	6.957	1745	1747	1753	rVV	188	157	0.01%	0.002%

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 Title : VOC Analysis

37	7.025	1765	1768	1770	rBV2	238	185	0.01%	0.002%
38	7.054	1770	1777	1784	rVB2	519	735	0.06%	0.008%
39	7.185	1809	1818	1830	rBV3	2836	4756	0.36%	0.049%
40	7.436	1892	1896	1899	rBV2	166	183	0.01%	0.002%
41	7.568	1925	1937	1956	rBV	164692	287927	22.00%	2.966%
42	7.687	1967	1974	1988	rVB3	2214	3393	0.26%	0.035%
43	7.902	2026	2041	2056	rBV	585677	999009	76.32%	10.292%
44	7.973	2056	2063	2075	rVB2	8366	13581	1.04%	0.140%
45	8.182	2116	2128	2144	rBV	117947	193695	14.80%	1.995%
46	8.292	2159	2162	2169	rVB3	322	310	0.02%	0.003%
47	8.423	2200	2203	2212	rVB2	233	405	0.03%	0.004%
48	8.481	2216	2221	2225	rVB2	267	357	0.03%	0.004%
49	8.636	2255	2269	2298	rBV	423454	751578	57.42%	7.743%
50	8.899	2349	2351	2356	rVB2	285	222	0.02%	0.002%
51	8.938	2359	2363	2365	rBV2	238	232	0.02%	0.002%
52	9.041	2390	2395	2396	rBV2	175	170	0.01%	0.002%
53	9.201	2442	2445	2447	rBV	226	180	0.01%	0.002%
54	9.327	2481	2484	2488	rVB2	270	186	0.01%	0.002%
55	9.349	2488	2491	2498	rVB2	250	296	0.02%	0.003%
56	9.420	2498	2513	2546	rBV	532095	858028	65.55%	8.839%
57	9.571	2556	2560	2561	rBV	354	279	0.02%	0.003%
58	9.697	2589	2599	2607	rBV3	1773	2906	0.22%	0.030%
59	9.947	2672	2677	2680	rBV2	199	241	0.02%	0.002%
60	10.108	2721	2727	2733	rBV3	545	742	0.06%	0.008%
61	10.189	2748	2752	2756	rBV2	223	269	0.02%	0.003%
62	10.674	2894	2903	2910	rVB3	2211	3188	0.24%	0.033%
63	10.761	2917	2930	2952	rVB	437754	705609	53.91%	7.269%
64	10.864	2957	2962	2963	rBV2	274	186	0.01%	0.002%
65	10.928	2979	2982	2988	rVB3	436	396	0.03%	0.004%
66	10.970	2988	2995	2998	rBV2	214	302	0.02%	0.003%
67	11.008	3004	3007	3013	rVB	250	185	0.01%	0.002%
68	11.073	3023	3027	3032	rBV2	214	194	0.01%	0.002%
69	11.124	3038	3043	3048	rVB4	268	310	0.02%	0.003%
70	11.150	3049	3051	3054	rVB2	383	239	0.02%	0.002%
71	11.169	3054	3057	3060	rBV	250	222	0.02%	0.002%
72	11.211	3068	3070	3073	rVB2	322	156	0.01%	0.002%
73	11.426	3135	3137	3140	rVB	204	144	0.01%	0.001%
74	11.462	3140	3148	3160	rBV4	1560	2943	0.22%	0.030%
75	11.574	3180	3183	3185	rBV	289	216	0.02%	0.002%
76	11.697	3217	3221	3227	rVB3	871	1098	0.08%	0.011%

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Min Area: 0 % of largest Peak

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Peak Location: TOP

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

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

77	11.729	3227	3231	3237	rBV	252	342	0.03%	0.004%
78	11.816	3246	3258	3274	rBV	471029	736605	56.27%	7.588%
79	11.912	3286	3288	3291	rVB2	342	197	0.02%	0.002%
80	11.947	3291	3299	3302	rBV4	1142	1639	0.13%	0.017%
81	11.976	3303	3308	3315	rVB3	1603	2231	0.17%	0.023%
82	12.076	3335	3339	3345	rBV2	198	258	0.02%	0.003%
83	12.137	3355	3358	3361	rBV2	231	180	0.01%	0.002%
84	12.195	3361	3376	3393	rBV	528835	854447	65.28%	8.802%
85	12.333	3415	3419	3421	rBV3	385	259	0.02%	0.003%
86	12.626	3505	3510	3511	rBV	250	193	0.01%	0.002%
87	12.639	3512	3514	3519	rVB2	296	309	0.02%	0.003%
88	12.754	3546	3550	3559	rVV2	298	449	0.03%	0.005%
89	12.912	3596	3599	3602	rBV	226	204	0.02%	0.002%
90	13.153	3672	3674	3678	rVB2	309	202	0.02%	0.002%
91	13.185	3678	3684	3688	rBV2	295	432	0.03%	0.004%
92	13.262	3704	3708	3711	rBV2	160	157	0.01%	0.002%
93	13.356	3729	3737	3740	rBV2	262	340	0.03%	0.004%
94	13.857	3889	3893	3895	rBV2	259	206	0.02%	0.002%
95	13.899	3901	3906	3909	rBV2	197	270	0.02%	0.003%
96	14.102	3962	3969	3974	rBV2	429	611	0.05%	0.006%
97	14.542	4103	4106	4110	rBV2	234	227	0.02%	0.002%
98	14.799	4183	4186	4191	rVB2	348	335	0.03%	0.003%
99	14.831	4193	4196	4198	rBV	297	207	0.02%	0.002%
100	14.909	4218	4220	4226	rBV2	268	271	0.02%	0.003%

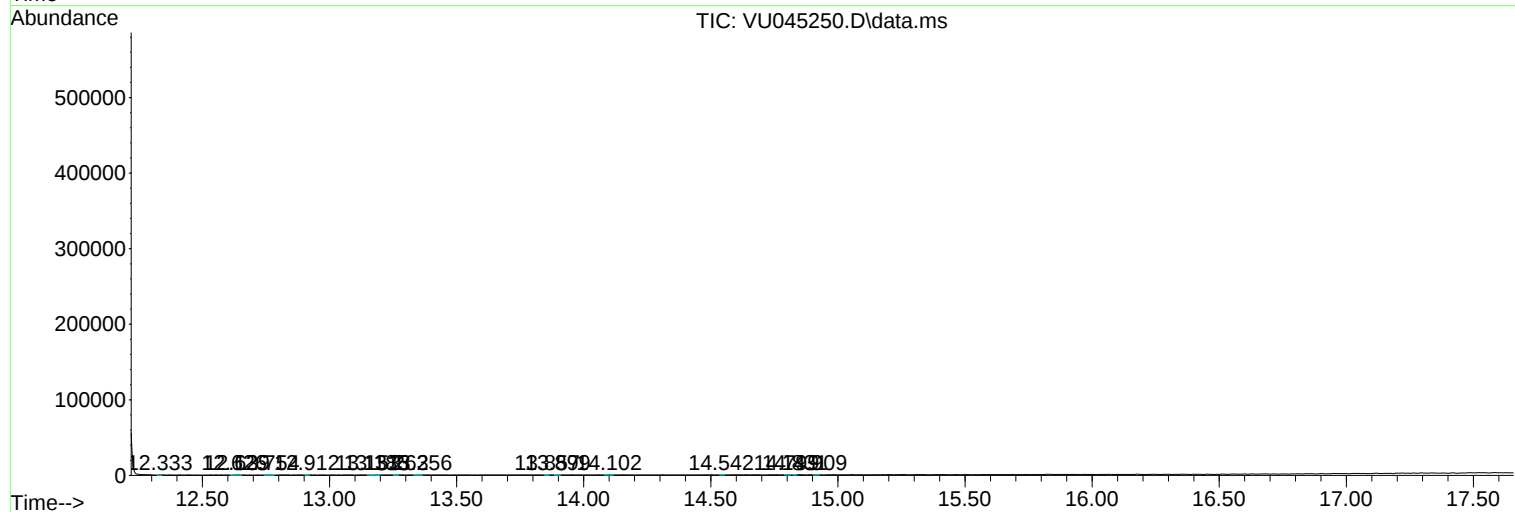
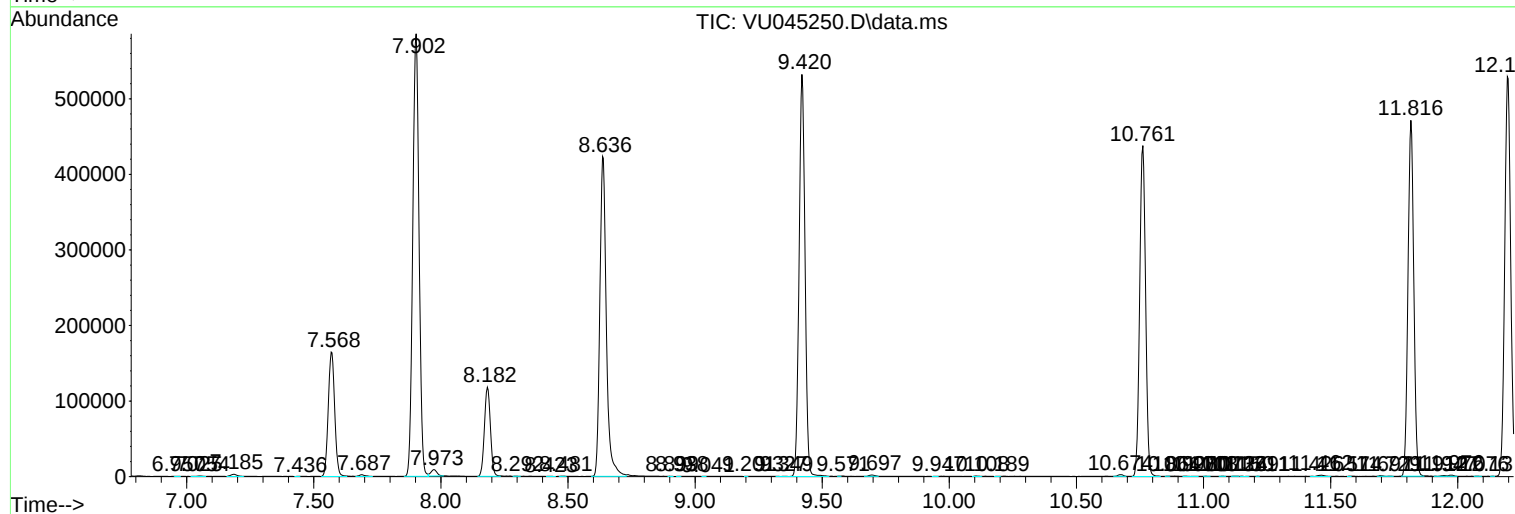
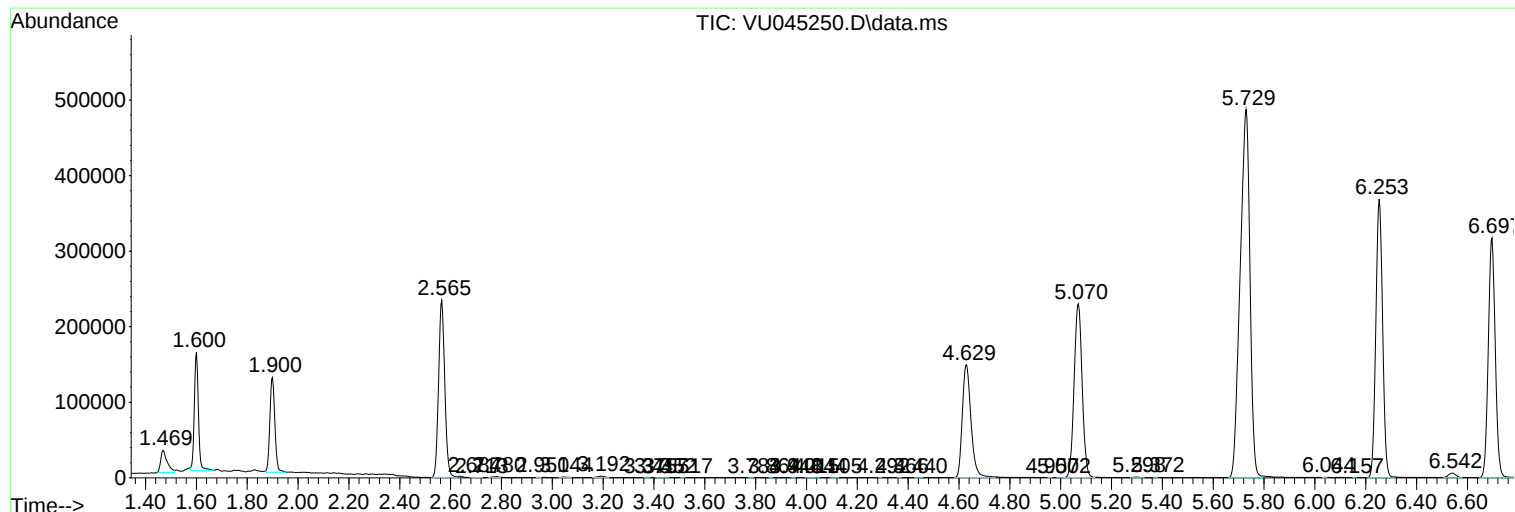
Sum of corrected areas: 9707090

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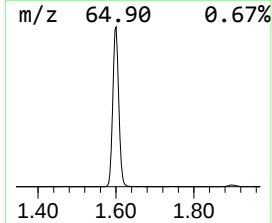
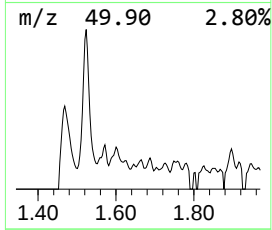
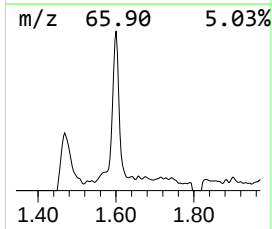
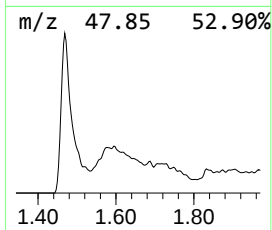
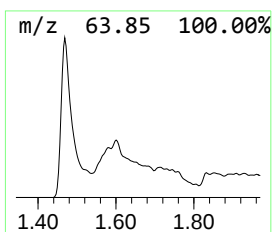
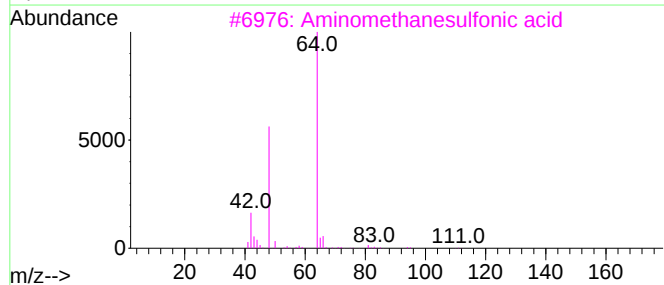
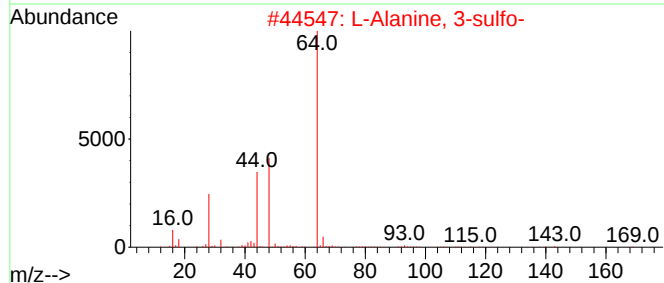
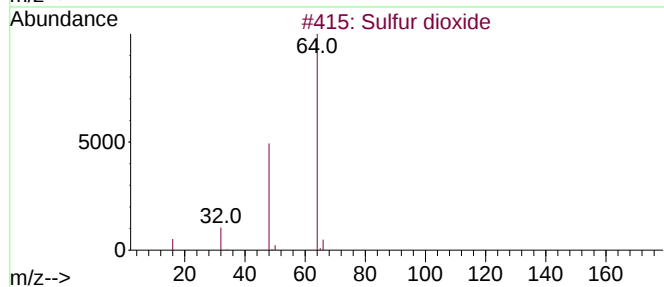
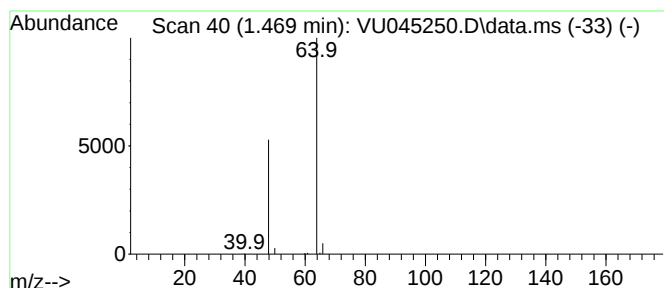
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.86 ug/L	52844	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.469	3.9	ug/L	52844	1	6.253	684578	50.0