

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045261.D
 Acq On : 08 Oct 2021 19:02
 Operator : SY/MD
 Sample : M4026-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AP6

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: VU045261.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	53	rBV	25825	47312	3.43%	0.469%
2	1.600	74	81	96	rVB	213672	232379	16.87%	2.303%
3	1.896	165	173	191	rVB	150182	205184	14.89%	2.033%
4	2.565	367	381	397	rBV	281670	477376	34.65%	4.730%
5	2.790	438	451	465	rVB2	4760	9848	0.71%	0.098%
6	3.047	526	531	538	rVB3	685	997	0.07%	0.010%
7	3.115	549	552	556	rBV2	177	152	0.01%	0.002%
8	3.192	562	576	589	rBV4	5432	12155	0.88%	0.120%
9	3.452	654	657	663	rBV2	233	316	0.02%	0.003%
10	3.652	714	719	722	rBV2	176	209	0.02%	0.002%
11	3.861	781	784	786	rBV2	170	144	0.01%	0.001%
12	4.044	839	841	844	rBV2	158	128	0.01%	0.001%
13	4.140	863	871	874	rBV2	188	195	0.01%	0.002%
14	4.182	881	884	888	rVB2	187	136	0.01%	0.001%
15	4.211	888	893	895	rBV2	129	130	0.01%	0.001%
16	4.317	923	926	929	rVV	186	147	0.01%	0.001%
17	4.427	956	960	962	rBV2	212	179	0.01%	0.002%
18	4.491	976	980	987	rBV2	169	254	0.02%	0.003%
19	4.523	988	990	993	rVB2	235	129	0.01%	0.001%
20	4.552	993	999	1001	rBV2	216	254	0.02%	0.003%
21	4.629	1007	1023	1058	rBV	151922	356291	25.86%	3.531%
22	4.803	1075	1077	1081	rVB	309	138	0.01%	0.001%
23	5.066	1138	1159	1186	rBV	241413	529195	38.41%	5.244%
24	5.295	1219	1230	1237	rBV3	619	1267	0.09%	0.013%
25	5.382	1255	1257	1259	rVB	257	138	0.01%	0.001%
26	5.401	1259	1263	1268	rBV2	221	290	0.02%	0.003%
27	5.536	1298	1305	1307	rBV2	246	322	0.02%	0.003%
28	5.600	1323	1325	1329	rVB2	249	185	0.01%	0.002%
29	5.645	1336	1339	1342	rVB	262	188	0.01%	0.002%
30	5.729	1342	1365	1383	rBV2	517499	1377646	100.00%	13.651%
31	6.070	1468	1471	1478	rBV3	174	218	0.02%	0.002%
32	6.115	1482	1485	1491	rVB4	337	295	0.02%	0.003%
33	6.153	1491	1497	1503	rVB3	255	336	0.02%	0.003%
34	6.185	1503	1507	1511	rBV2	291	273	0.02%	0.003%
35	6.253	1514	1528	1545	rBV	354419	665627	48.32%	6.596%
36	6.491	1599	1602	1605	rBV3	189	186	0.01%	0.002%

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

37	6.536	1606	1616	1625	rVB6	4147	7825	0.57%	0.078%
38	6.574	1625	1628	1630	rBV2	240	144	0.01%	0.001%
39	6.603	1634	1637	1640	rBV2	175	158	0.01%	0.002%
40	6.697	1651	1666	1686	rBV	324601	627383	45.54%	6.217%
41	6.935	1736	1740	1743	rBV	172	176	0.01%	0.002%
42	7.012	1762	1764	1768	rVB2	156	133	0.01%	0.001%
43	7.050	1769	1776	1786	rBV2	631	1085	0.08%	0.011%
44	7.102	1789	1792	1794	rBV	164	135	0.01%	0.001%
45	7.179	1807	1816	1827	rBV4	1261	2104	0.15%	0.021%
46	7.426	1890	1893	1900	rVB2	242	302	0.02%	0.003%
47	7.465	1900	1905	1909	rBV2	169	224	0.02%	0.002%
48	7.500	1909	1916	1922	rVB2	221	344	0.02%	0.003%
49	7.568	1922	1937	1954	rBV	175687	304756	22.12%	3.020%
50	7.668	1964	1968	1970	rBV3	230	172	0.01%	0.002%
51	7.687	1970	1974	1981	rVB4	1047	1281	0.09%	0.013%
52	7.726	1981	1986	1993	rBV2	150	225	0.02%	0.002%
53	7.902	2026	2041	2056	rBV	628213	1063540	77.20%	10.539%
54	7.973	2056	2063	2075	rVB	9757	16083	1.17%	0.159%
55	8.182	2115	2128	2146	rBV	122593	203030	14.74%	2.012%
56	8.353	2176	2181	2190	rBV	554	850	0.06%	0.008%
57	8.475	2212	2219	2228	rBV2	877	1191	0.09%	0.012%
58	8.635	2256	2269	2322	rBV	444097	777214	56.42%	7.702%
59	9.192	2439	2442	2451	rBV2	114	139	0.01%	0.001%
60	9.420	2500	2513	2529	rBV	514763	829845	60.24%	8.223%
61	9.700	2591	2600	2607	rBV4	1850	2846	0.21%	0.028%
62	9.796	2627	2630	2632	rBV2	180	151	0.01%	0.001%
63	10.047	2706	2708	2717	rBV2	190	304	0.02%	0.003%
64	10.098	2721	2724	2727	rBV	380	297	0.02%	0.003%
65	10.307	2785	2789	2792	rVB2	160	159	0.01%	0.002%
66	10.375	2807	2810	2812	rBV	207	163	0.01%	0.002%
67	10.632	2887	2890	2894	rBV	187	156	0.01%	0.002%
68	10.674	2894	2903	2912	rVV	3595	4901	0.36%	0.049%
69	10.761	2916	2930	2950	rVV	448346	707898	51.38%	7.015%
70	10.870	2959	2964	2967	rBV2	675	589	0.04%	0.006%
71	10.889	2968	2970	2972	rBV2	501	228	0.02%	0.002%
72	10.925	2979	2981	2983	rBV	257	141	0.01%	0.001%
73	10.960	2990	2992	2995	rBV	151	130	0.01%	0.001%
74	11.012	3005	3008	3011	rVB3	261	162	0.01%	0.002%
75	11.111	3036	3039	3041	rBV	346	245	0.02%	0.002%
76	11.320	3098	3104	3107	rBV2	249	295	0.02%	0.003%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.359	3113	3116	3120	rBV2	186	144	0.01%	0.001%
78	11.458	3140	3147	3159	rVB3	2259	4008	0.29%	0.040%
79	11.577	3179	3184	3186	rBV2	553	414	0.03%	0.004%
80	11.632	3198	3201	3205	rBV	163	158	0.01%	0.002%
81	11.696	3214	3221	3230	rBV4	1522	2257	0.16%	0.022%
82	11.815	3245	3258	3280	rBV	462566	719952	52.26%	7.134%
83	11.918	3287	3290	3292	rBV	267	197	0.01%	0.002%
84	11.950	3292	3300	3302	rVV4	1111	1557	0.11%	0.015%
85	11.973	3303	3307	3317	rVB3	2110	3020	0.22%	0.030%
86	12.092	3342	3344	3347	rVB3	247	140	0.01%	0.001%
87	12.111	3347	3350	3352	rBV2	253	164	0.01%	0.002%
88	12.195	3360	3376	3397	rBV	541856	878020	63.73%	8.701%
89	12.269	3397	3399	3408	rVB4	766	906	0.07%	0.009%
90	12.330	3413	3418	3424	rBV2	749	889	0.06%	0.009%
91	12.401	3438	3440	3446	rVB3	295	229	0.02%	0.002%
92	12.455	3454	3457	3459	rBV2	178	159	0.01%	0.002%
93	12.642	3512	3515	3524	rVB4	627	683	0.05%	0.007%
94	12.725	3537	3541	3543	rBV	281	248	0.02%	0.002%
95	12.770	3552	3555	3558	rBV2	347	320	0.02%	0.003%
96	12.822	3567	3571	3572	rBV	196	176	0.01%	0.002%
97	12.867	3582	3585	3587	rBV	213	159	0.01%	0.002%
98	13.082	3649	3652	3656	rBV2	198	183	0.01%	0.002%
99	13.327	3723	3728	3731	rBV	218	192	0.01%	0.002%
100	13.587	3806	3809	3811	rBV	191	142	0.01%	0.001%

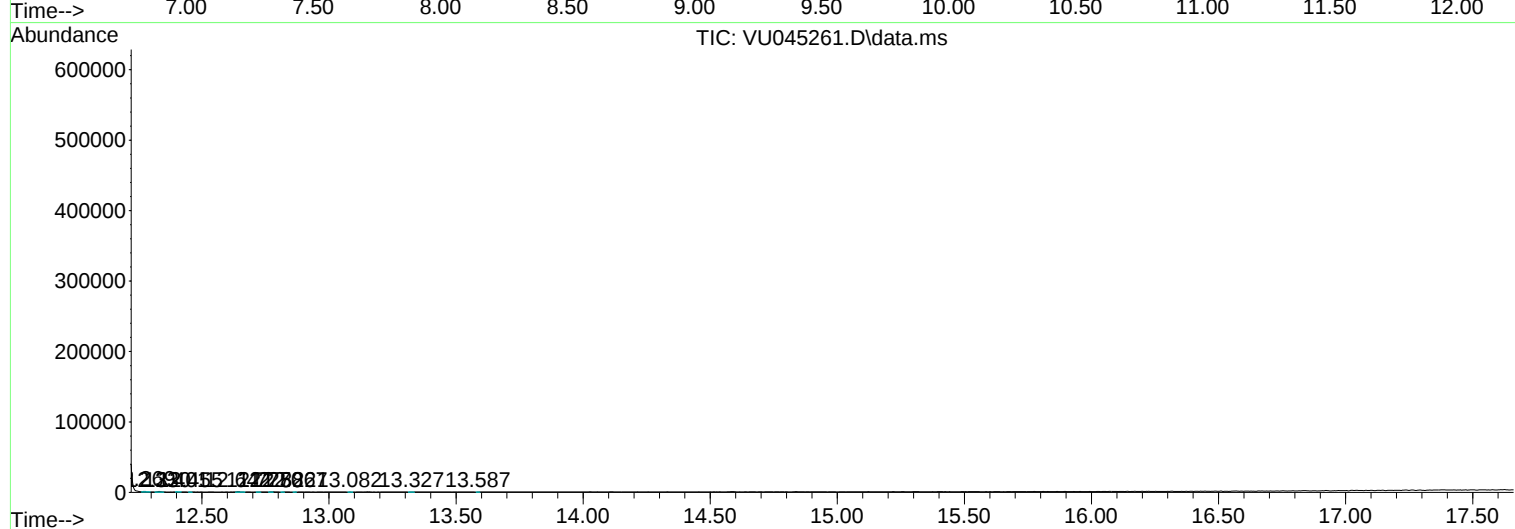
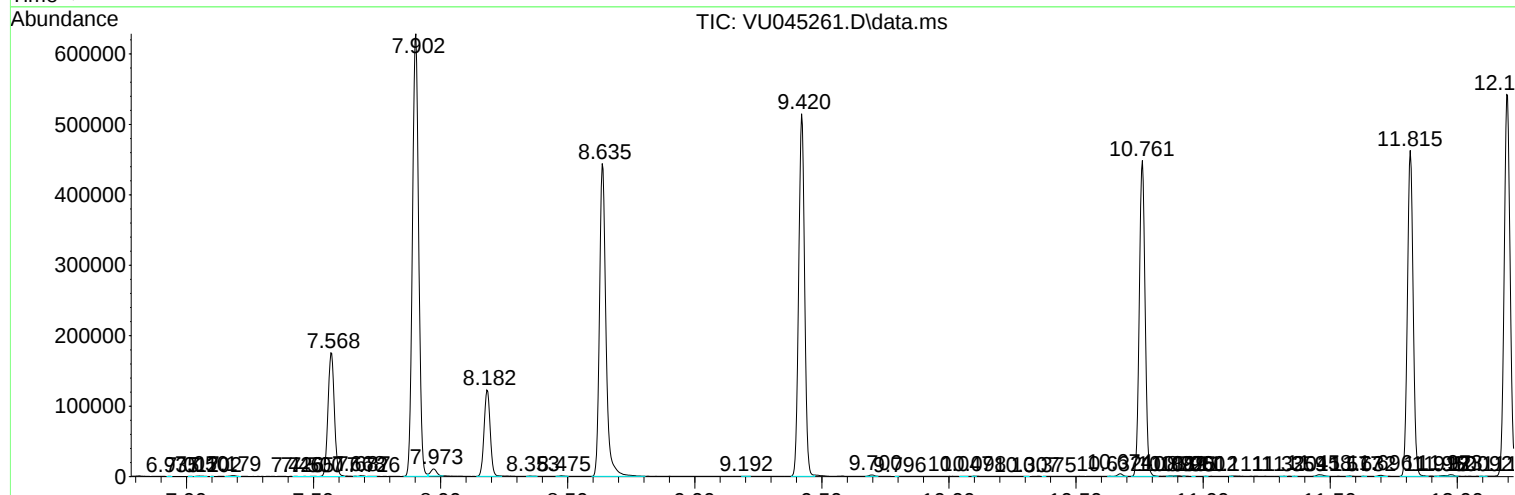
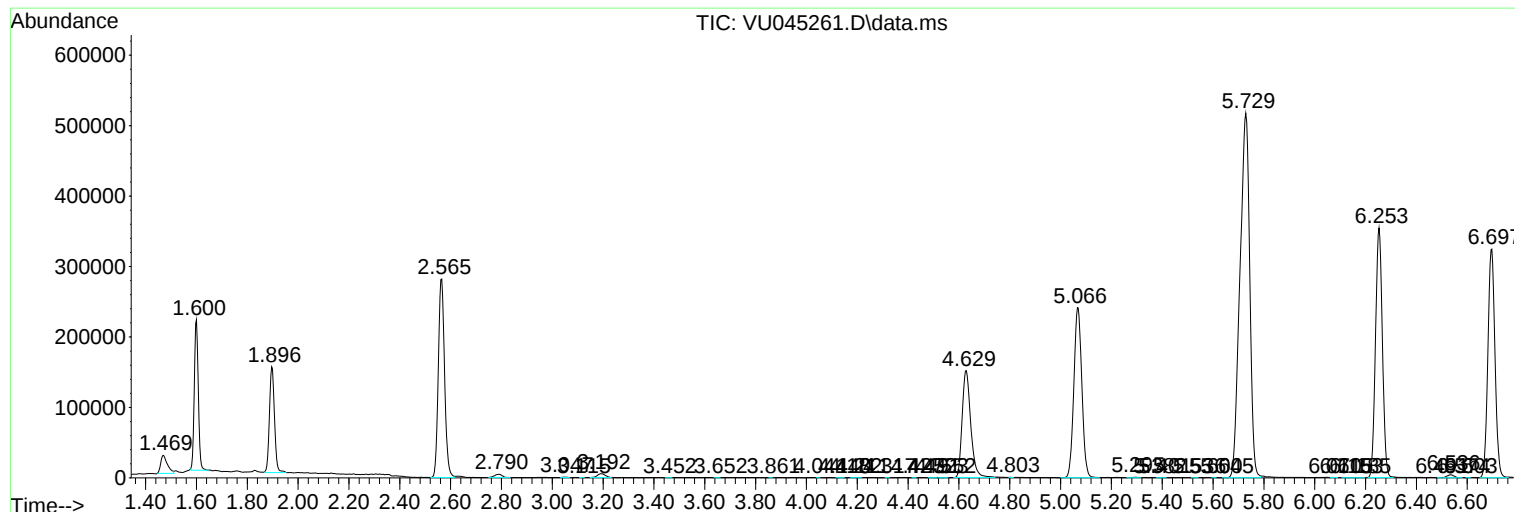
Sum of corrected areas: 10091540

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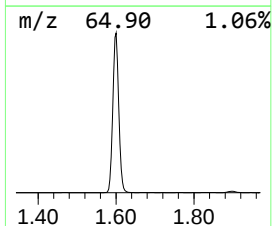
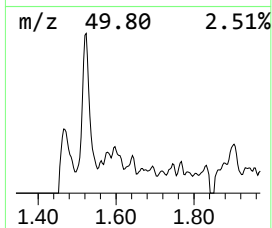
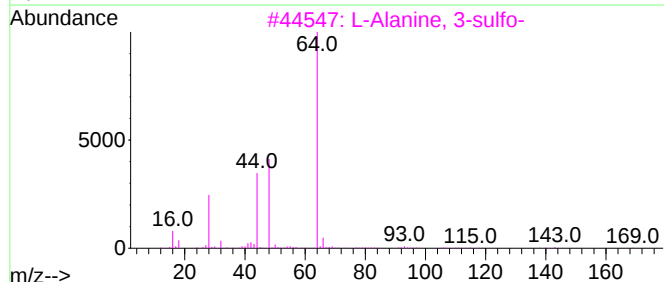
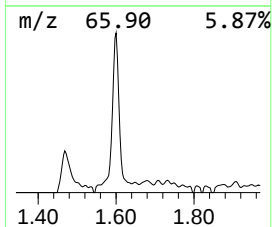
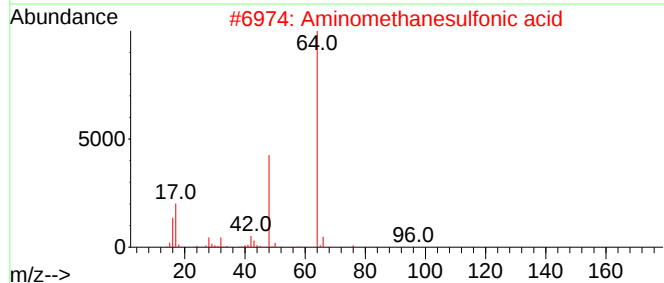
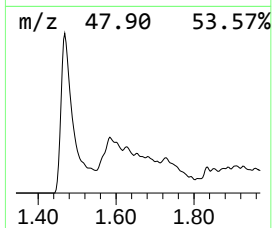
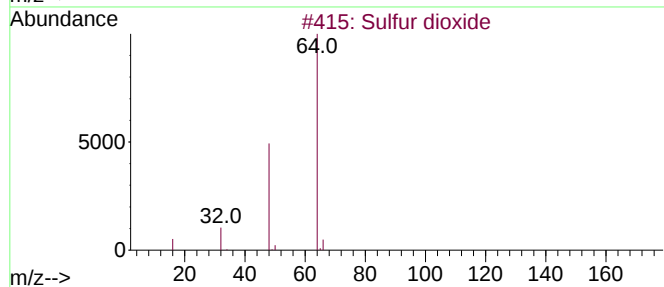
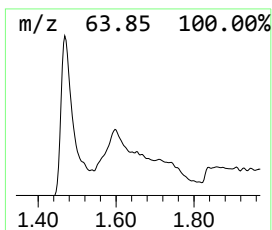
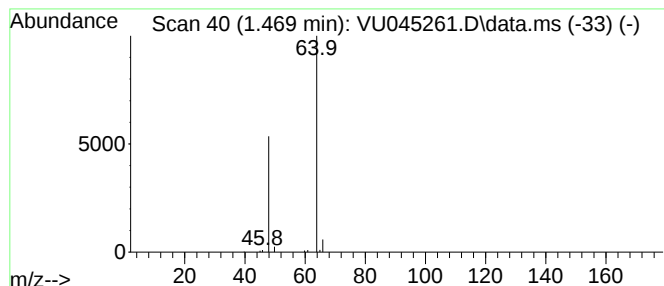
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	3.55 ug/L	47312	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			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.5	ug/L	47312	1	6.253	665627	50.0