

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033761.D
 Acq On : 19 Jan 2024 18:00
 Operator : SY/MD
 Sample : P1190-12
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMS3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	31	39	65	rBV	112032	136960	17.16%	1.966%
2	1.281	68	75	92	rBV2	148666	196037	24.57%	2.815%
3	1.532	146	153	163	rVB	90408	106517	13.35%	1.529%
4	2.060	308	317	331	rVB	184148	265214	33.24%	3.808%
5	2.233	369	371	372	rBV	361	149	0.02%	0.002%
6	2.568	468	475	484	rVB4	519	558	0.07%	0.008%
7	2.699	506	516	532	rBV	16230	28937	3.63%	0.415%
8	2.789	538	544	553	rVB2	151	273	0.03%	0.004%
9	3.288	696	699	706	rVB2	144	155	0.02%	0.002%
10	3.494	759	763	768	rVB	164	173	0.02%	0.002%
11	3.693	822	825	830	rVB2	223	210	0.03%	0.003%
12	3.812	845	862	899	rBV2	80453	298923	37.46%	4.292%
13	4.249	982	998	1024	rBV	121693	314479	39.41%	4.515%
14	4.796	1164	1168	1169	rBV2	218	180	0.02%	0.003%
15	4.957	1201	1218	1256	rBV2	298724	797949	100.00%	11.457%
16	5.330	1332	1334	1337	rBV	380	298	0.04%	0.004%
17	5.423	1361	1363	1366	rVB2	277	174	0.02%	0.002%
18	5.442	1366	1369	1372	rBV	183	164	0.02%	0.002%
19	5.532	1386	1397	1425	rBV	282006	580407	72.74%	8.333%
20	5.838	1482	1492	1523	rVB5	29331	63406	7.95%	0.910%
21	5.989	1526	1539	1578	rBV	173104	359636	45.07%	5.164%
22	6.146	1586	1588	1593	rVB4	401	226	0.03%	0.003%
23	6.201	1603	1605	1609	rBV	335	238	0.03%	0.003%
24	6.516	1699	1703	1710	rBV2	197	293	0.04%	0.004%
25	6.915	1815	1827	1847	rBV	97092	182109	22.82%	2.615%
26	7.178	1906	1909	1911	rBV3	555	345	0.04%	0.005%
27	7.243	1918	1929	1956	rBV	364258	633900	79.44%	9.102%
28	7.555	2015	2026	2063	rBV	65359	122288	15.33%	1.756%
29	7.731	2079	2081	2084	rVB2	276	143	0.02%	0.002%
30	7.799	2096	2102	2108	rBV2	127	182	0.02%	0.003%
31	7.828	2108	2111	2117	rBV2	146	176	0.02%	0.003%
32	7.908	2117	2136	2153	rBV2	67535	116777	14.63%	1.677%
33	8.024	2163	2172	2211	rBV	179539	347883	43.60%	4.995%
34	8.278	2248	2251	2257	rVB5	847	848	0.11%	0.012%
35	8.426	2295	2297	2302	rVB	212	149	0.02%	0.002%
36	8.522	2325	2327	2330	rVB	412	234	0.03%	0.003%

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 Title : VOC Analysis

37	8.609	2349	2354	2355	rBV	181	141	0.02%	0.002%
38	8.783	2398	2408	2438	rBV	435276	707319	88.64%	10.156%
39	8.992	2469	2473	2476	rVB	293	190	0.02%	0.003%
40	9.034	2482	2486	2490	rVB3	284	223	0.03%	0.003%
41	9.056	2490	2493	2494	rBV	256	141	0.02%	0.002%
42	9.088	2500	2503	2513	rVB2	1018	1082	0.14%	0.016%
43	9.255	2550	2555	2558	rVB	267	277	0.03%	0.004%
44	9.410	2593	2603	2604	rBV4	1072	1508	0.19%	0.022%
45	9.445	2610	2614	2617	rBV3	212	168	0.02%	0.002%
46	9.490	2625	2628	2636	rVB2	277	226	0.03%	0.003%
47	9.609	2661	2665	2666	rBV	710	479	0.06%	0.007%
48	9.641	2667	2675	2682	rVB4	2526	4025	0.50%	0.058%
49	9.735	2696	2704	2712	rBV4	2282	3936	0.49%	0.057%
50	9.792	2719	2722	2728	rVB3	843	644	0.08%	0.009%
51	9.870	2738	2746	2747	rBV	286	263	0.03%	0.004%
52	9.960	2772	2774	2777	rVB	371	226	0.03%	0.003%
53	10.062	2799	2806	2814	rVB5	1202	1597	0.20%	0.023%
54	10.153	2823	2834	2854	rBV	227139	361160	45.26%	5.186%
55	10.294	2875	2878	2879	rBV	355	219	0.03%	0.003%
56	10.313	2880	2884	2885	rBV	950	559	0.07%	0.008%
57	10.387	2901	2907	2908	rBV3	830	767	0.10%	0.011%
58	10.445	2916	2925	2934	rVB5	1372	2181	0.27%	0.031%
59	10.497	2938	2941	2942	rBV	359	206	0.03%	0.003%
60	10.551	2953	2958	2966	rVB4	964	1188	0.15%	0.017%
61	10.667	2986	2994	3002	rBV5	1818	2973	0.37%	0.043%
62	10.702	3003	3005	3010	rVB4	577	339	0.04%	0.005%
63	10.828	3038	3044	3047	rVV6	1119	1112	0.14%	0.016%
64	10.857	3051	3053	3058	rBV3	401	305	0.04%	0.004%
65	10.995	3091	3096	3098	rBV3	462	412	0.05%	0.006%
66	11.014	3098	3102	3103	rVV2	346	239	0.03%	0.003%
67	11.027	3103	3106	3113	rVB4	913	855	0.11%	0.012%
68	11.091	3120	3126	3137	rVB4	1113	1439	0.18%	0.021%
69	11.185	3144	3155	3185	rBV	451550	699728	87.69%	10.047%
70	11.394	3218	3220	3227	rVB3	328	255	0.03%	0.004%
71	11.461	3234	3241	3245	rBV2	237	389	0.05%	0.006%
72	11.484	3245	3248	3250	rBV2	317	267	0.03%	0.004%
73	11.561	3257	3272	3296	rBV	375742	597179	74.84%	8.574%
74	11.693	3311	3313	3319	rVB2	720	409	0.05%	0.006%
75	11.725	3321	3323	3327	rVB2	359	222	0.03%	0.003%
76	11.760	3327	3334	3346	rBV4	1175	1621	0.20%	0.023%

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 Title : VOC Analysis

77	11.863	3361	3366	3369	rBV2	225	245	0.03%	0.004%
78	11.956	3389	3395	3403	rBV4	1020	1405	0.18%	0.020%
79	12.053	3420	3425	3430	rBV3	558	550	0.07%	0.008%
80	12.406	3531	3535	3538	rBV3	230	228	0.03%	0.003%
81	12.786	3650	3653	3658	rVB3	224	171	0.02%	0.002%
82	12.824	3658	3665	3670	rBV4	529	727	0.09%	0.010%
83	12.943	3700	3702	3707	rBV3	203	165	0.02%	0.002%
84	13.107	3749	3753	3755	rBV2	165	143	0.02%	0.002%
85	13.136	3759	3762	3766	rVB	188	148	0.02%	0.002%
86	13.168	3767	3772	3773	rBV	170	149	0.02%	0.002%
87	13.246	3792	3796	3799	rBV	216	227	0.03%	0.003%
88	13.410	3843	3847	3850	rBV2	194	181	0.02%	0.003%
89	13.445	3855	3858	3859	rBV2	297	168	0.02%	0.002%
90	13.947	4011	4014	4017	rVB2	279	176	0.02%	0.003%
91	14.062	4047	4050	4053	rBV	204	173	0.02%	0.002%
92	14.162	4077	4081	4085	rBV	301	293	0.04%	0.004%
93	14.657	4230	4235	4238	rBV2	431	481	0.06%	0.007%
94	14.834	4286	4290	4298	rBV2	359	512	0.06%	0.007%
95	14.992	4337	4339	4341	rBV	358	216	0.03%	0.003%
96	15.291	4426	4432	4437	rBV4	576	820	0.10%	0.012%
97	15.406	4465	4468	4469	rBV	368	189	0.02%	0.003%
98	15.609	4529	4531	4534	rVB4	462	239	0.03%	0.003%
99	15.680	4551	4553	4558	rBV4	421	284	0.04%	0.004%
100	16.252	4725	4731	4736	rVB5	3449	3819	0.48%	0.055%

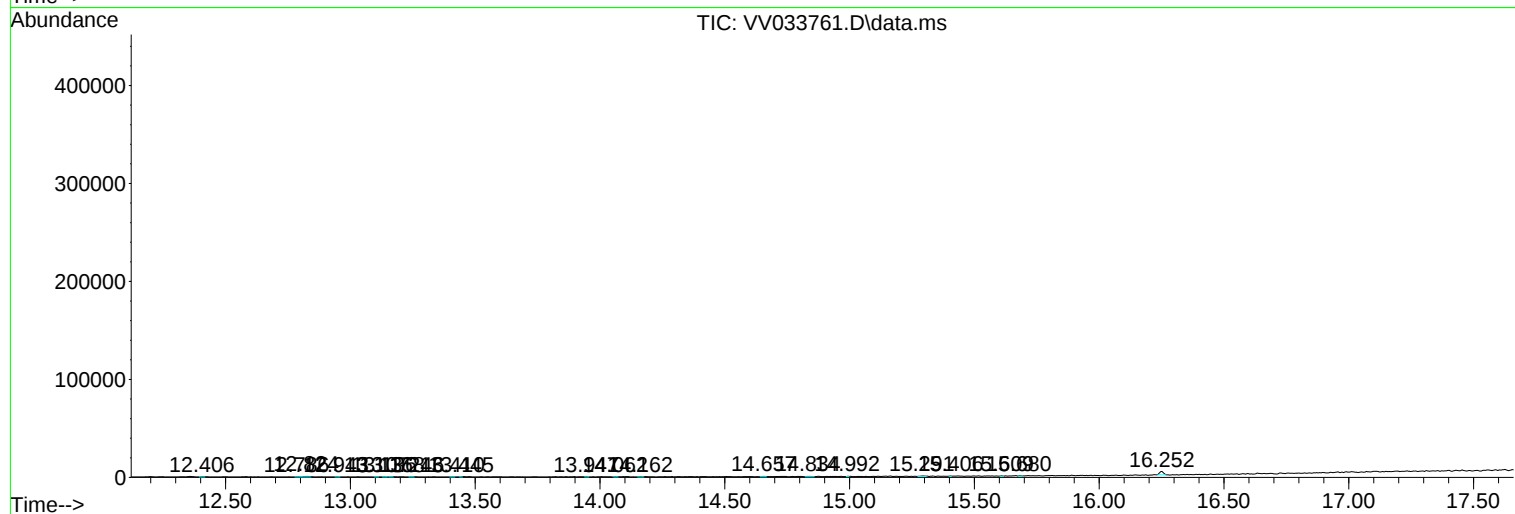
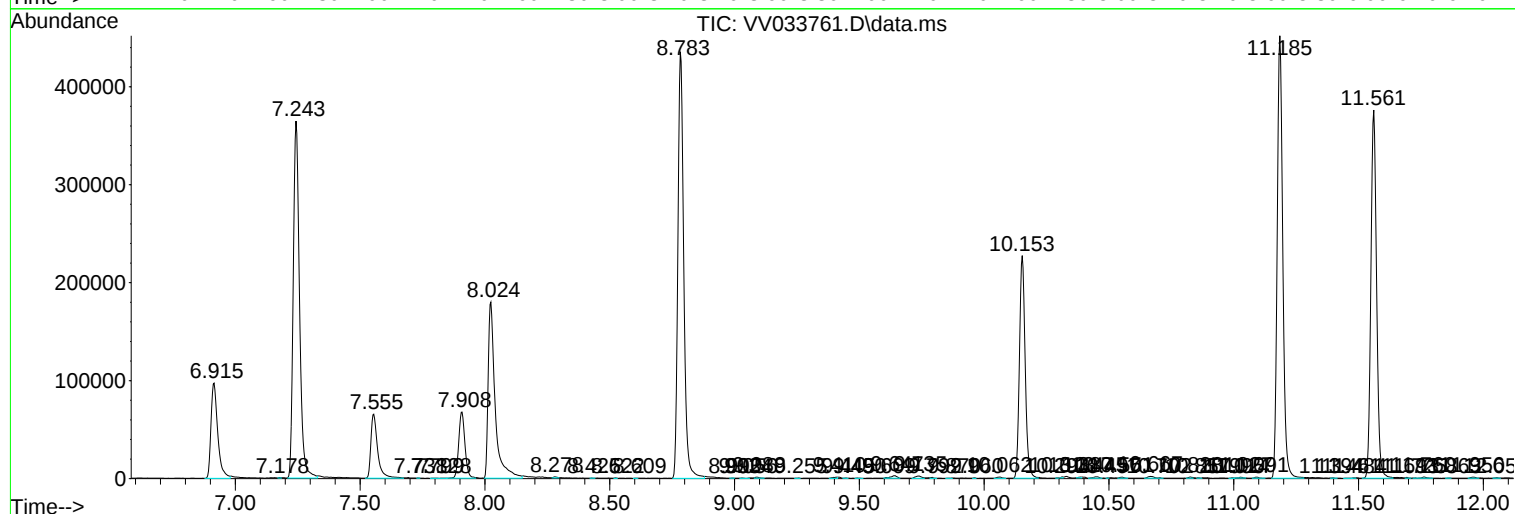
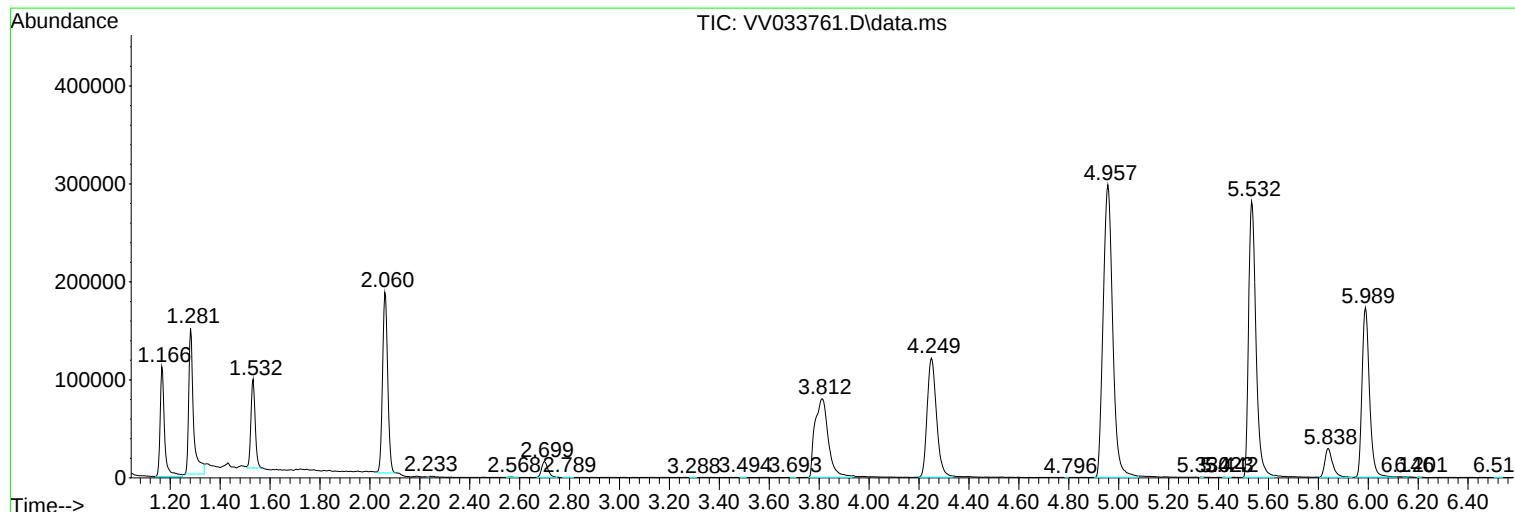
Sum of corrected areas: 6964768

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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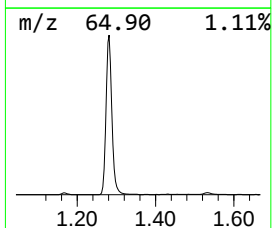
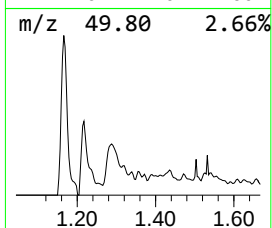
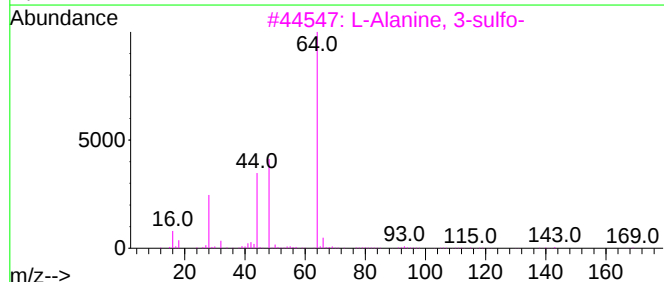
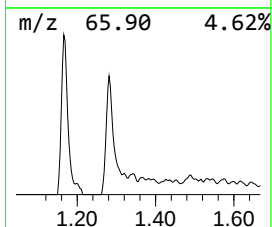
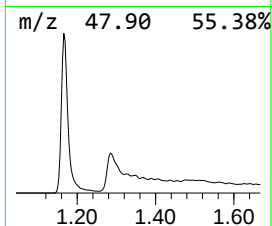
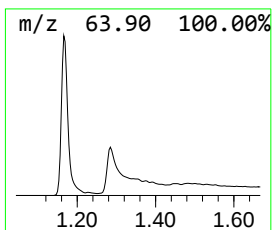
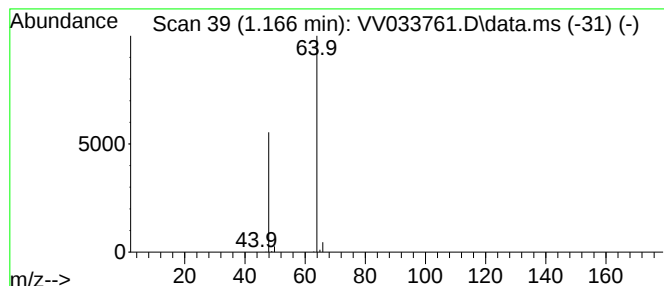
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	11.80 ug/L	136960	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	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	1.166	11.8	ug/L	136960	1	5.532	580407	50.0