

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033756.D
 Acq On : 19 Jan 2024 16:01
 Operator : SY/MD
 Sample : P1190-07
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ4

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: VV033756.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	33	39	52	rVB	63295	73142	9.09%	1.095%
2	1.282	67	75	94	rBV	188032	308441	38.34%	4.617%
3	1.532	147	153	168	rVB	93198	118968	14.79%	1.781%
4	2.060	309	317	341	rVB	186535	298229	37.07%	4.464%
5	2.224	361	368	385	rVB3	4174	10390	1.29%	0.156%
6	2.384	415	418	421	rVB2	298	218	0.03%	0.003%
7	2.449	433	438	443	rVV3	699	599	0.07%	0.009%
8	2.497	449	453	457	rBV2	288	257	0.03%	0.004%
9	2.561	462	473	485	rVV2	2600	5250	0.65%	0.079%
10	2.700	509	516	528	rVB3	2554	4500	0.56%	0.067%
11	2.761	532	535	538	rBV	160	122	0.02%	0.002%
12	2.921	583	585	588	rBV2	220	147	0.02%	0.002%
13	3.220	674	678	684	rVB2	212	241	0.03%	0.004%
14	3.413	733	738	745	rVB2	143	179	0.02%	0.003%
15	3.535	771	776	782	rBV2	112	156	0.02%	0.002%
16	3.783	842	853	892	rBV	53222	153282	19.05%	2.295%
17	4.034	928	931	935	rVB	265	176	0.02%	0.003%
18	4.249	981	998	1028	rBV	125719	317171	39.43%	4.748%
19	4.568	1090	1097	1101	rBV3	342	414	0.05%	0.006%
20	4.590	1101	1104	1107	rVV2	354	222	0.03%	0.003%
21	4.896	1190	1199	1201	rBV2	146	175	0.02%	0.003%
22	4.957	1201	1218	1252	rBV2	300310	804447	100.00%	12.042%
23	5.150	1276	1278	1287	rVB	396	300	0.04%	0.004%
24	5.352	1337	1341	1343	rBV2	235	164	0.02%	0.002%
25	5.413	1355	1360	1363	rBV2	232	243	0.03%	0.004%
26	5.532	1386	1397	1433	rBV	270809	561124	69.75%	8.400%
27	5.722	1453	1456	1461	rVB3	409	330	0.04%	0.005%
28	5.831	1485	1490	1493	rBV6	894	900	0.11%	0.013%
29	5.921	1515	1518	1523	rVV	170	161	0.02%	0.002%
30	5.989	1526	1539	1568	rBV	175279	366761	45.59%	5.490%
31	6.230	1610	1614	1616	rVV2	192	163	0.02%	0.002%
32	6.256	1619	1622	1628	rVB2	219	216	0.03%	0.003%
33	6.317	1638	1641	1645	rVB2	166	120	0.01%	0.002%
34	6.587	1718	1725	1728	rBV2	249	309	0.04%	0.005%
35	6.825	1792	1799	1804	rBV	207	253	0.03%	0.004%
36	6.915	1815	1827	1851	rBV	96812	182587	22.70%	2.733%

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

37	7.127	1891	1893	1895	rBV	256	142	0.02%	0.002%
38	7.149	1895	1900	1903	rBV3	430	454	0.06%	0.007%
39	7.243	1918	1929	1965	rBV	363075	643791	80.03%	9.637%
40	7.555	2015	2026	2051	rBV	63478	115933	14.41%	1.736%
41	7.741	2082	2084	2090	rVB3	308	216	0.03%	0.003%
42	7.879	2116	2127	2139	rVB4	1805	3122	0.39%	0.047%
43	7.937	2139	2145	2149	rVB2	140	136	0.02%	0.002%
44	8.024	2162	2172	2219	rBV	182405	362593	45.07%	5.428%
45	8.387	2282	2285	2288	rVB4	283	194	0.02%	0.003%
46	8.452	2300	2305	2309	rBV2	224	302	0.04%	0.005%
47	8.474	2310	2312	2320	rVB2	190	223	0.03%	0.003%
48	8.516	2320	2325	2328	rBV3	193	192	0.02%	0.003%
49	8.690	2374	2379	2385	rVV2	256	189	0.02%	0.003%
50	8.783	2397	2408	2443	rBV	413320	687122	85.42%	10.286%
51	8.985	2467	2471	2473	rBV3	204	185	0.02%	0.003%
52	9.153	2517	2523	2527	rVV2	115	139	0.02%	0.002%
53	9.188	2531	2534	2540	rVB2	157	163	0.02%	0.002%
54	9.490	2626	2628	2633	rVB2	221	197	0.02%	0.003%
55	9.712	2694	2697	2700	rBV	169	132	0.02%	0.002%
56	9.828	2731	2733	2738	rVB2	207	148	0.02%	0.002%
57	9.866	2738	2745	2748	rBV2	221	235	0.03%	0.004%
58	10.027	2791	2795	2798	rBV2	153	148	0.02%	0.002%
59	10.153	2822	2834	2861	rBV	231952	364053	45.26%	5.450%
60	10.326	2877	2888	2900	rVB3	2280	3558	0.44%	0.053%
61	10.432	2918	2921	2925	rVB	164	123	0.02%	0.002%
62	10.461	2925	2930	2932	rBV2	120	123	0.02%	0.002%
63	10.612	2975	2977	2980	rBV2	178	121	0.02%	0.002%
64	10.706	3003	3006	3009	rBV2	154	124	0.02%	0.002%
65	10.857	3049	3053	3056	rBV2	145	132	0.02%	0.002%
66	10.953	3079	3083	3087	rBV2	133	145	0.02%	0.002%
67	11.133	3136	3139	3144	rBV3	335	284	0.04%	0.004%
68	11.185	3144	3155	3184	rBV	430472	675178	83.93%	10.107%
69	11.423	3227	3229	3237	rVB2	226	124	0.02%	0.002%
70	11.471	3237	3244	3248	rBV	133	165	0.02%	0.002%
71	11.561	3259	3272	3295	rBV	373322	596883	74.20%	8.935%
72	11.718	3319	3321	3324	rBV	246	151	0.02%	0.002%
73	11.776	3335	3339	3344	rBV	190	199	0.02%	0.003%
74	12.091	3432	3437	3443	rBV	211	204	0.03%	0.003%
75	12.185	3463	3466	3469	rBV3	266	186	0.02%	0.003%
76	12.571	3583	3586	3592	rBV2	172	151	0.02%	0.002%

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 Title : VOC Analysis

77	12.641	3605	3608	3615	rBV	192	199	0.02%	0.003%
78	13.220	3785	3788	3794	rBV4	324	254	0.03%	0.004%
79	13.265	3799	3802	3807	rBV	158	156	0.02%	0.002%
80	13.455	3853	3861	3862	rBV2	461	505	0.06%	0.008%
81	13.545	3884	3889	3891	rBV2	143	129	0.02%	0.002%
82	13.651	3919	3922	3928	rVV2	154	122	0.02%	0.002%
83	13.712	3937	3941	3947	rBV2	198	234	0.03%	0.004%
84	13.773	3953	3960	3965	rBV2	208	262	0.03%	0.004%
85	13.802	3966	3969	3972	rBV	198	145	0.02%	0.002%
86	13.818	3972	3974	3978	rVB	242	135	0.02%	0.002%
87	13.976	4019	4023	4025	rBV2	512	420	0.05%	0.006%
88	14.075	4051	4054	4057	rVB	189	132	0.02%	0.002%
89	14.098	4057	4061	4066	rBV2	351	352	0.04%	0.005%
90	14.181	4085	4087	4091	rVB	238	185	0.02%	0.003%
91	14.297	4120	4123	4129	rBV4	322	341	0.04%	0.005%
92	14.323	4129	4131	4135	rVB	242	172	0.02%	0.003%
93	14.821	4284	4286	4289	rBV2	297	131	0.02%	0.002%
94	15.004	4341	4343	4346	rVB2	283	141	0.02%	0.002%
95	15.278	4426	4428	4431	rBV2	415	314	0.04%	0.005%
96	15.365	4453	4455	4460	rBV4	297	322	0.04%	0.005%
97	15.477	4488	4490	4493	rBV3	461	311	0.04%	0.005%
98	15.702	4557	4560	4563	rBV3	606	391	0.05%	0.006%
99	15.976	4644	4645	4646	rBV3	510	168	0.02%	0.003%
100	16.252	4726	4731	4742	rVB4	4723	6335	0.79%	0.095%

Sum of corrected areas: 6680073

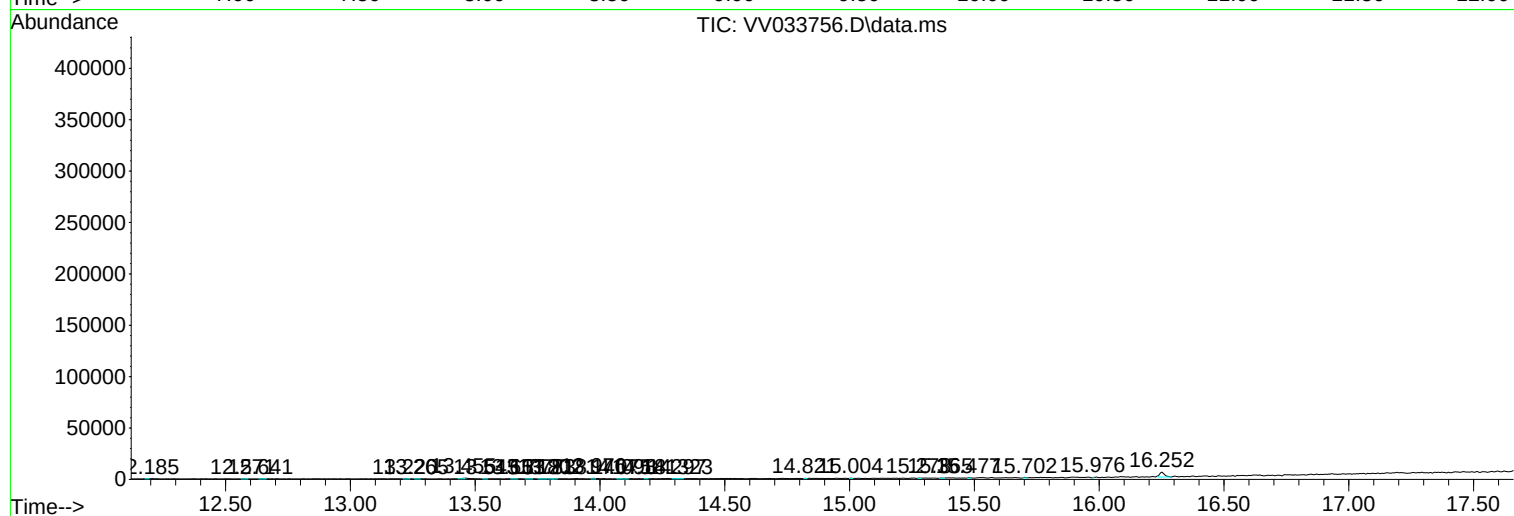
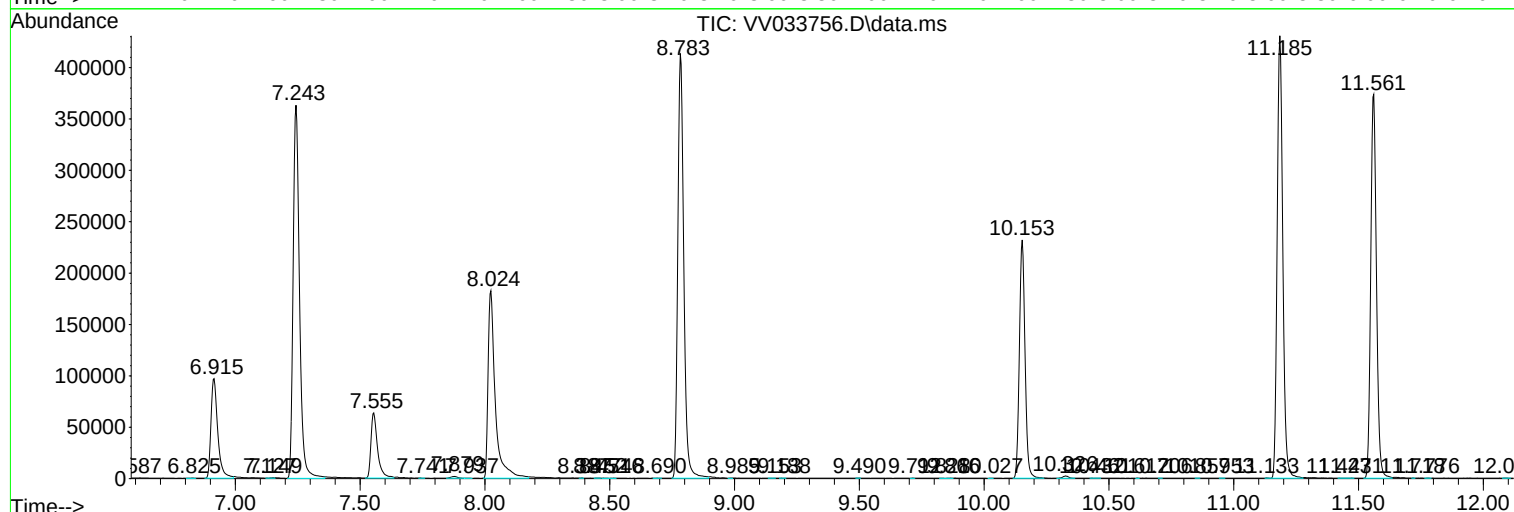
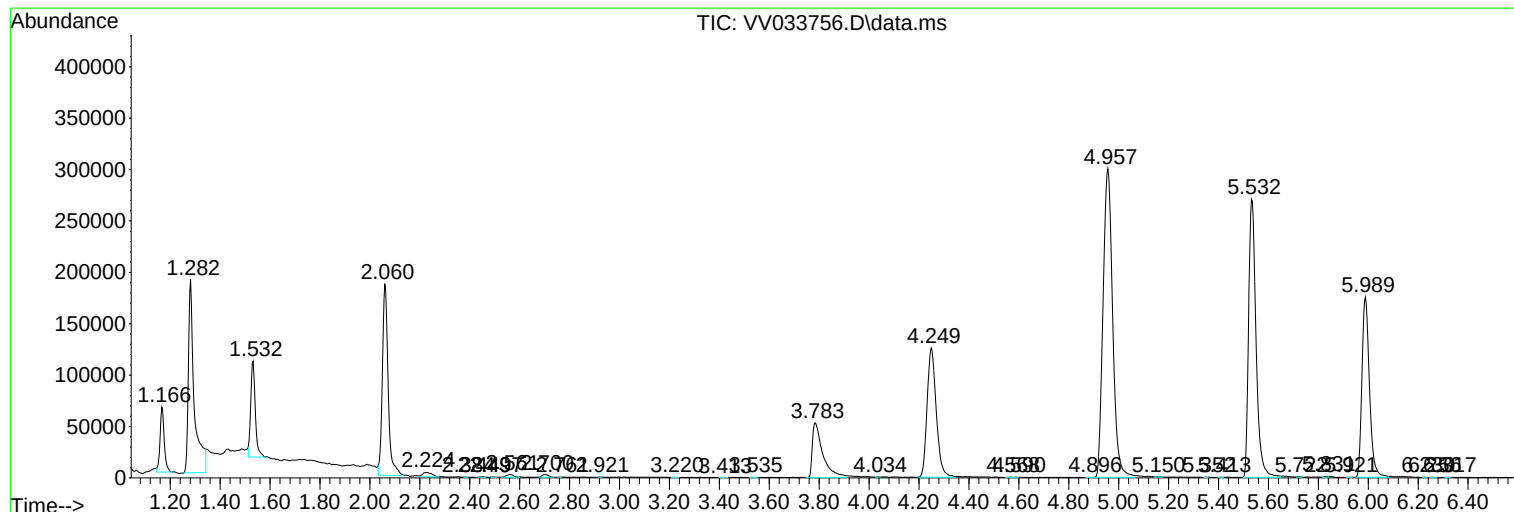
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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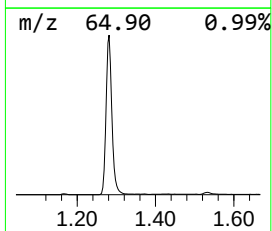
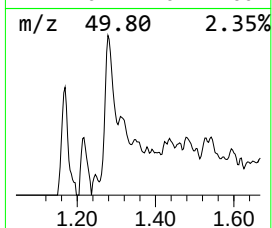
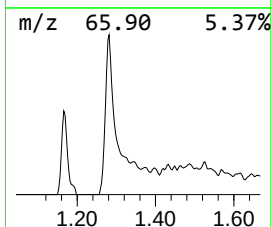
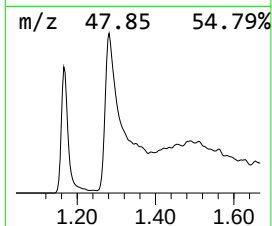
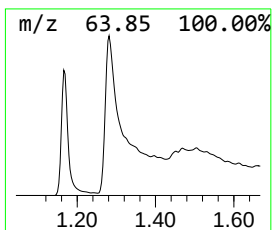
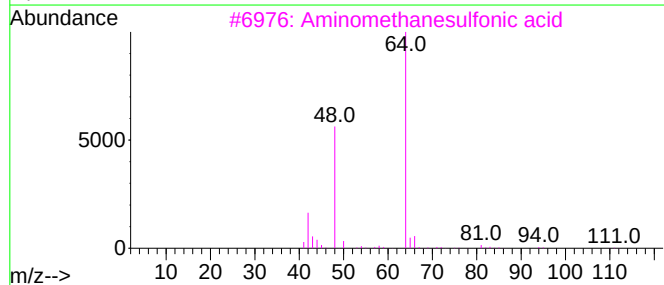
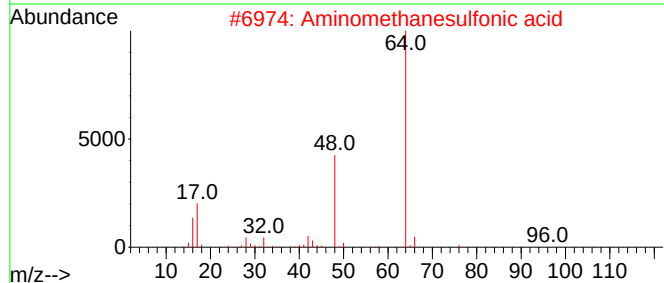
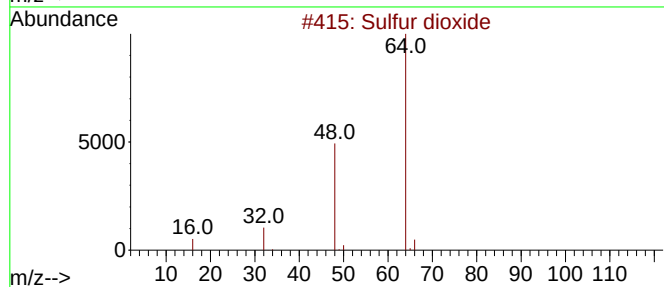
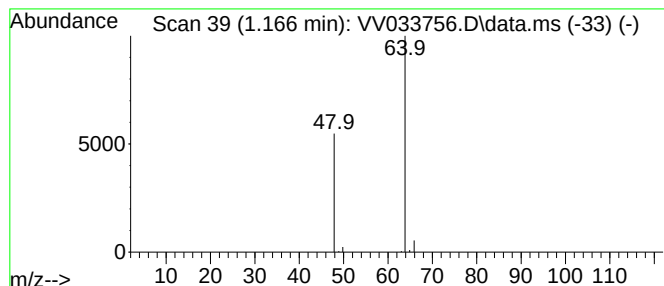
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
1.166	6.52 ug/L	73142	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	6.5	ug/L	73142	1	5.532	561124	50.0