

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012324\
 Data File : VV033825.D
 Acq On : 23 Jan 2024 13:12
 Operator : SY/MD
 Sample : P1190-18
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VHBLK001

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: VV033825.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	32	39	52	rBV	44584	52344	6.81%	0.859%
2	1.281	68	75	89	rBV	97997	109003	14.18%	1.790%
3	1.529	145	152	169	rVB	89273	107150	13.94%	1.759%
4	2.060	307	317	340	rVB	181222	272290	35.43%	4.471%
5	2.156	346	347	351	rVB2	412	262	0.03%	0.004%
6	2.240	367	373	378	rBV3	528	832	0.11%	0.014%
7	2.445	434	437	438	rBV3	330	214	0.03%	0.004%
8	2.551	463	470	471	rBV2	926	830	0.11%	0.014%
9	2.635	492	496	499	rBV2	269	208	0.03%	0.003%
10	2.815	547	552	553	rBV	154	122	0.02%	0.002%
11	3.330	706	712	715	rBV	214	153	0.02%	0.003%
12	3.477	755	758	761	rVB2	190	120	0.02%	0.002%
13	3.516	765	770	772	rBV2	313	239	0.03%	0.004%
14	3.648	805	811	816	rBV	164	163	0.02%	0.003%
15	3.783	845	853	891	rBV	50113	139002	18.09%	2.282%
16	4.249	982	998	1027	rBV	118327	302592	39.37%	4.968%
17	4.484	1066	1071	1072	rBV2	400	276	0.04%	0.005%
18	4.519	1080	1082	1087	rVB2	303	253	0.03%	0.004%
19	4.555	1089	1093	1094	rBV2	291	178	0.02%	0.003%
20	4.564	1094	1096	1100	rVB	212	119	0.02%	0.002%
21	4.696	1134	1137	1140	rBV2	213	158	0.02%	0.003%
22	4.754	1152	1155	1161	rVB2	131	121	0.02%	0.002%
23	4.867	1187	1190	1192	rBV	176	141	0.02%	0.002%
24	4.957	1201	1218	1249	rBV2	289455	768492	100.00%	12.618%
25	5.133	1271	1273	1279	rVB3	402	215	0.03%	0.004%
26	5.201	1291	1294	1301	rVB2	254	214	0.03%	0.004%
27	5.281	1316	1319	1325	rVB2	307	263	0.03%	0.004%
28	5.342	1335	1338	1340	rBV	324	213	0.03%	0.003%
29	5.391	1350	1353	1354	rBV2	178	118	0.02%	0.002%
30	5.487	1381	1383	1386	rBV	185	168	0.02%	0.003%
31	5.532	1386	1397	1423	rBV	260569	530140	68.98%	8.704%
32	5.828	1483	1489	1490	rBV2	1411	1299	0.17%	0.021%
33	5.989	1526	1539	1571	rBV	169706	348242	45.31%	5.718%
34	6.137	1582	1585	1587	rBV3	364	235	0.03%	0.004%
35	6.220	1608	1611	1617	rBV3	281	189	0.02%	0.003%
36	6.571	1715	1720	1724	rBV	170	153	0.02%	0.003%

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

37	6.596	1724	1728	1729	rBV2	162	140	0.02%	0.002%
38	6.683	1753	1755	1759	rBV2	220	135	0.02%	0.002%
39	6.706	1759	1762	1767	rVV2	128	134	0.02%	0.002%
40	6.911	1815	1826	1849	rBV	96068	180542	23.49%	2.964%
41	7.175	1905	1908	1912	rVB2	277	136	0.02%	0.002%
42	7.243	1918	1929	1965	rBV	350826	626541	81.53%	10.287%
43	7.554	2014	2026	2052	rBV	65264	117654	15.31%	1.932%
44	7.905	2131	2135	2141	rVB2	124	154	0.02%	0.003%
45	7.982	2153	2159	2162	rBV2	232	271	0.04%	0.004%
46	8.024	2162	2172	2211	rBV	176357	339079	44.12%	5.567%
47	8.268	2245	2248	2254	rVB5	399	373	0.05%	0.006%
48	8.403	2285	2290	2294	rBV	255	287	0.04%	0.005%
49	8.471	2308	2311	2314	rBV	223	133	0.02%	0.002%
50	8.522	2324	2327	2331	rBV2	125	116	0.02%	0.002%
51	8.641	2360	2364	2368	rBV	191	168	0.02%	0.003%
52	8.718	2385	2388	2391	rBV	186	138	0.02%	0.002%
53	8.783	2397	2408	2429	rBV	393193	642332	83.58%	10.547%
54	9.001	2472	2476	2478	rBV2	198	203	0.03%	0.003%
55	9.120	2510	2513	2516	rBV	154	121	0.02%	0.002%
56	9.149	2519	2522	2529	rVV2	147	129	0.02%	0.002%
57	9.461	2615	2619	2622	rBV	148	132	0.02%	0.002%
58	10.107	2817	2820	2823	rBV	148	124	0.02%	0.002%
59	10.152	2823	2834	2857	rVV	214563	337748	43.95%	5.546%
60	10.323	2883	2887	2892	rVB2	259	300	0.04%	0.005%
61	10.349	2892	2895	2899	rVB2	162	116	0.02%	0.002%
62	10.368	2899	2901	2905	rVB	213	131	0.02%	0.002%
63	10.686	2997	3000	3003	rBV2	145	118	0.02%	0.002%
64	10.866	3053	3056	3061	rBV2	130	136	0.02%	0.002%
65	10.947	3078	3081	3084	rVB	202	132	0.02%	0.002%
66	11.185	3144	3155	3178	rBV	413922	632388	82.29%	10.383%
67	11.352	3204	3207	3210	rBV3	239	133	0.02%	0.002%
68	11.390	3215	3219	3223	rBV2	224	154	0.02%	0.003%
69	11.561	3260	3272	3301	rBV	357222	567051	73.79%	9.311%
70	11.728	3321	3324	3325	rBV	197	118	0.02%	0.002%
71	11.818	3347	3352	3355	rBV2	131	156	0.02%	0.003%
72	12.339	3510	3514	3516	rBV2	169	127	0.02%	0.002%
73	12.721	3629	3633	3636	rBV	166	134	0.02%	0.002%
74	12.828	3662	3666	3668	rBV2	190	131	0.02%	0.002%
75	12.966	3704	3709	3712	rBV	225	191	0.02%	0.003%
76	13.133	3758	3761	3764	rBV2	180	135	0.02%	0.002%

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 Title : VOC Analysis

77	13.255	3797	3799	3803	rVB2	225	120	0.02%	0.002%
78	13.461	3857	3863	3868	rBV2	252	299	0.04%	0.005%
79	13.705	3934	3939	3942	rBV2	126	145	0.02%	0.002%
80	13.815	3968	3973	3974	rBV	238	190	0.02%	0.003%
81	13.908	3999	4002	4004	rBV	245	139	0.02%	0.002%
82	13.934	4007	4010	4012	rBV	171	117	0.02%	0.002%
83	13.982	4018	4025	4031	rBV4	456	807	0.11%	0.013%
84	14.075	4051	4054	4056	rBV2	264	168	0.02%	0.003%
85	14.130	4068	4071	4077	rBV2	268	219	0.03%	0.004%
86	14.162	4077	4081	4084	rBV3	208	205	0.03%	0.003%
87	14.201	4090	4093	4096	rBV2	181	123	0.02%	0.002%
88	14.217	4096	4098	4102	rBV2	173	156	0.02%	0.003%
89	14.239	4102	4105	4109	rBV2	247	204	0.03%	0.003%
90	14.326	4128	4132	4136	rBV2	294	302	0.04%	0.005%
91	14.422	4159	4162	4163	rBV	200	138	0.02%	0.002%
92	14.512	4183	4190	4191	rBV	268	307	0.04%	0.005%
93	14.599	4214	4217	4219	rBV	231	134	0.02%	0.002%
94	14.808	4279	4282	4283	rBV2	403	195	0.03%	0.003%
95	14.863	4298	4299	4304	rBV2	266	141	0.02%	0.002%
96	15.053	4355	4358	4363	rVB3	385	251	0.03%	0.004%
97	15.078	4363	4366	4369	rBV3	353	298	0.04%	0.005%
98	15.123	4378	4380	4385	rBV3	314	234	0.03%	0.004%
99	15.168	4392	4394	4397	rBV	384	192	0.02%	0.003%
100	15.345	4448	4449	4452	rBV	363	197	0.03%	0.003%

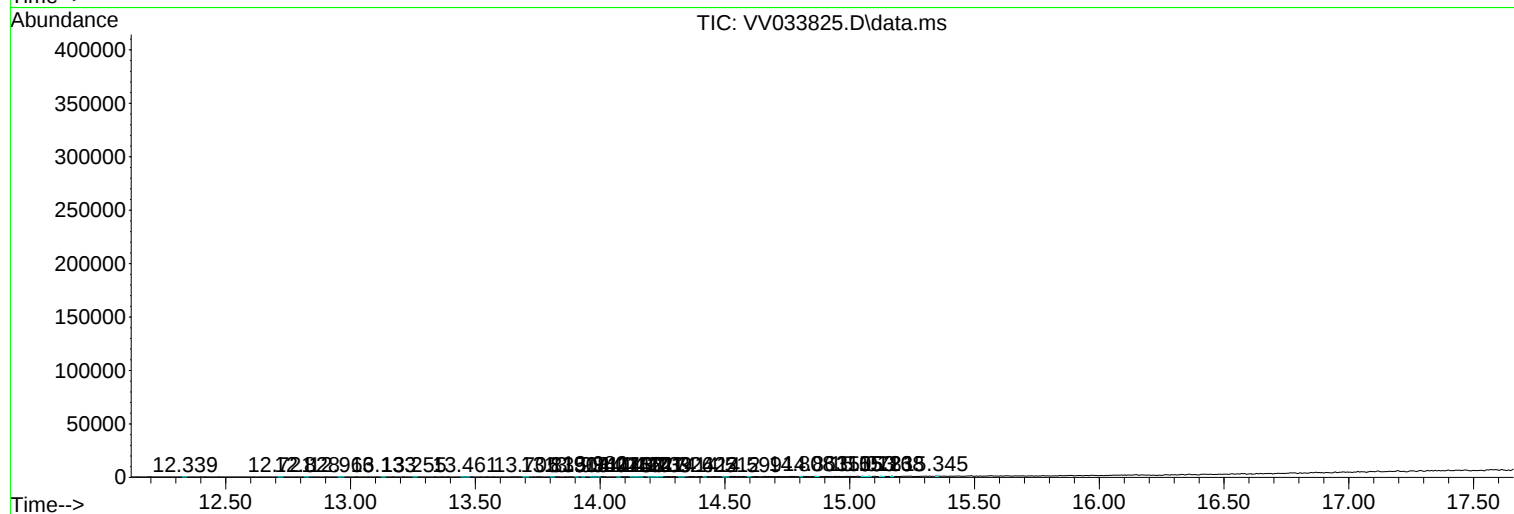
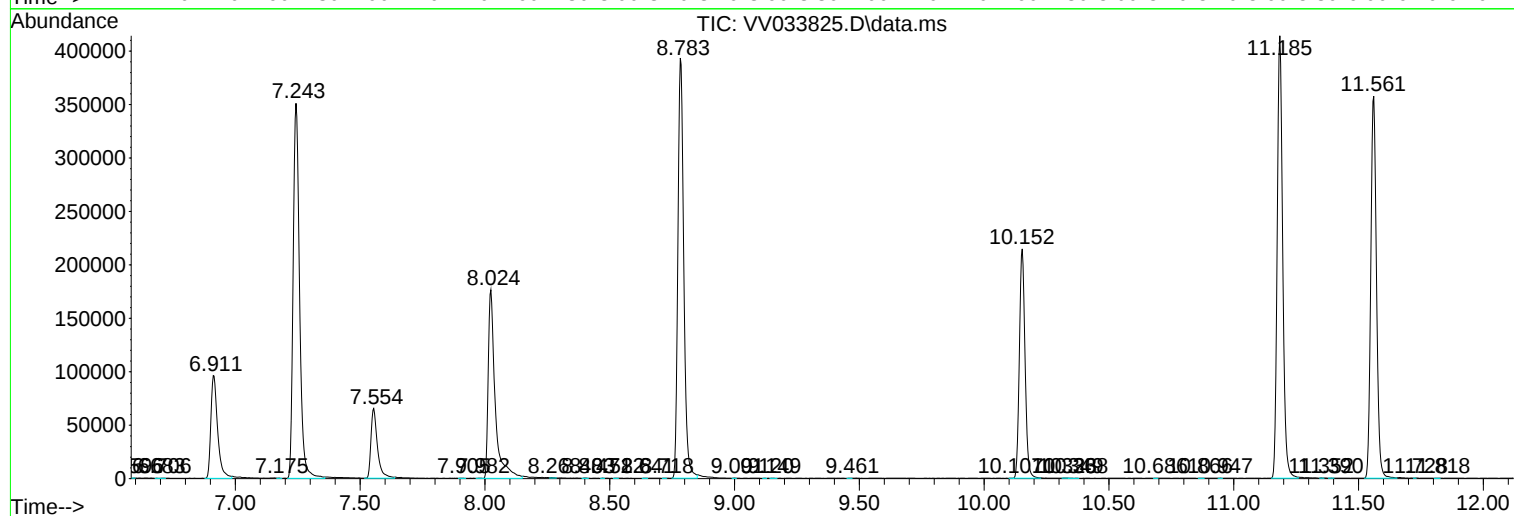
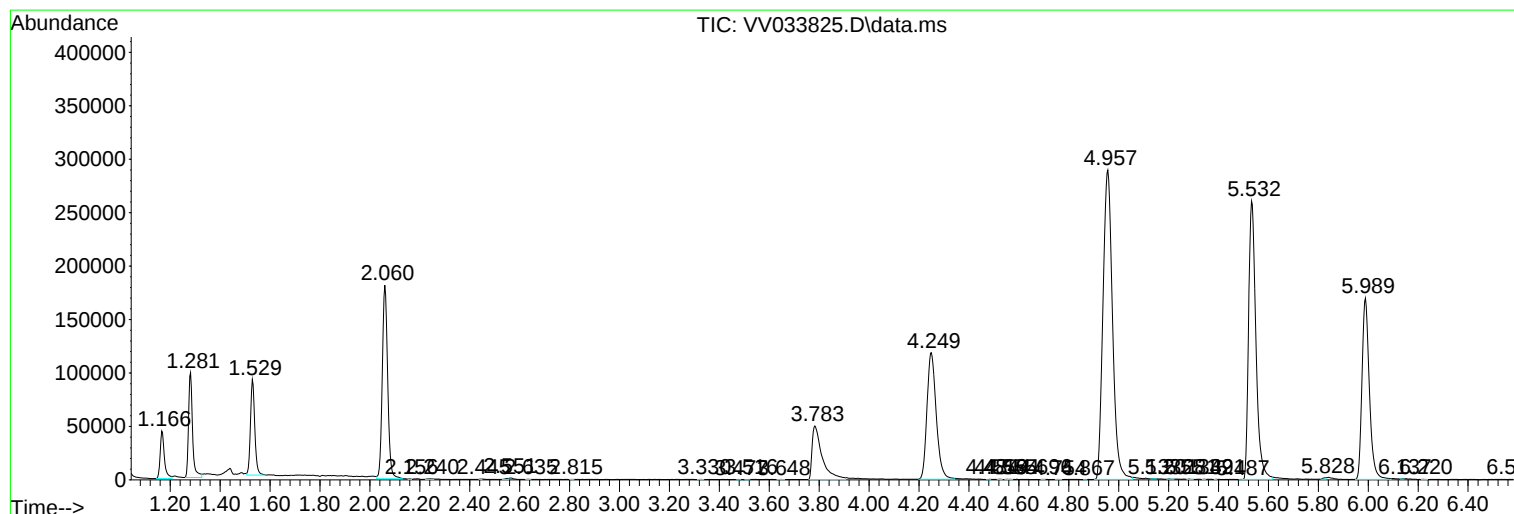
Sum of corrected areas: 6090433

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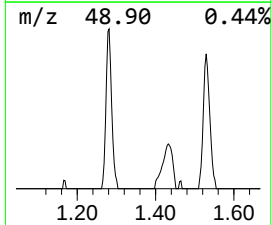
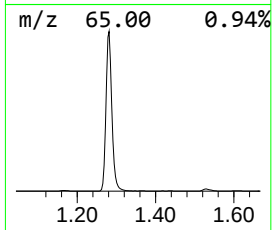
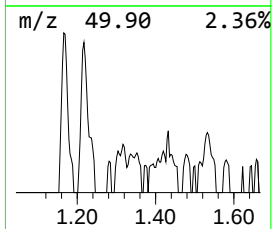
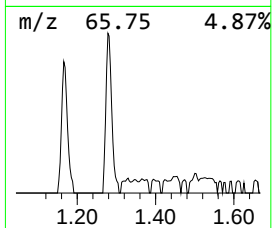
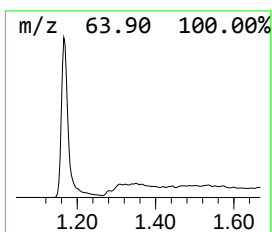
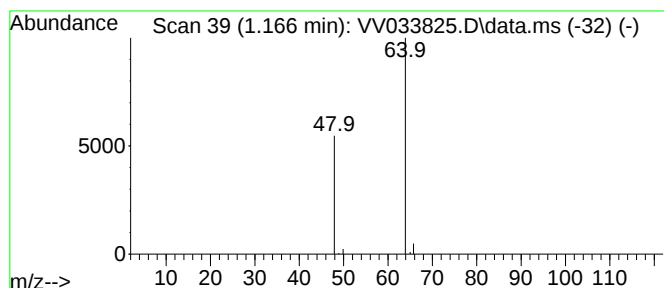
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	4.94 ug/L	52344	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 Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	4.9	ug/L	52344	1	5.532	530140	50.0