

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033757.D
 Acq On : 19 Jan 2024 16:25
 Operator : SY/MD
 Sample : P1190-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ6

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: VV033757.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	64	rBV	112725	136376	16.88%	2.026%
2	1.281	67	75	93	rBV2	163304	238452	29.52%	3.542%
3	1.532	146	153	169	rVB	92785	117598	14.56%	1.747%
4	2.059	308	317	350	rVB	191679	306191	37.90%	4.548%
5	2.185	351	356	360	rBV2	669	747	0.09%	0.011%
6	2.339	402	404	408	rBV2	182	125	0.02%	0.002%
7	2.445	433	437	438	rBV	448	237	0.03%	0.004%
8	2.551	466	470	471	rBV2	515	367	0.05%	0.005%
9	2.658	499	503	507	rBV	226	143	0.02%	0.002%
10	2.699	507	516	526	rBV2	3641	6673	0.83%	0.099%
11	2.773	536	539	546	rVB2	222	198	0.02%	0.003%
12	2.821	546	554	557	rBV2	272	278	0.03%	0.004%
13	2.924	582	586	591	rVB2	151	143	0.02%	0.002%
14	3.066	627	630	636	rVB2	183	181	0.02%	0.003%
15	3.140	652	653	663	rVB2	191	143	0.02%	0.002%
16	3.786	845	854	891	rBV3	54138	199947	24.75%	2.970%
17	4.030	928	930	936	rVB	317	237	0.03%	0.004%
18	4.079	942	945	948	rBV	241	150	0.02%	0.002%
19	4.182	974	977	980	rVB2	322	188	0.02%	0.003%
20	4.249	981	998	1028	rBV	123592	318011	39.36%	4.723%
21	4.423	1049	1052	1055	rBV3	250	214	0.03%	0.003%
22	4.474	1067	1068	1075	rVB3	476	445	0.06%	0.007%
23	4.538	1085	1088	1091	rBV3	173	122	0.02%	0.002%
24	4.600	1105	1107	1112	rVB3	251	182	0.02%	0.003%
25	4.628	1112	1116	1118	rBV3	183	142	0.02%	0.002%
26	4.767	1157	1159	1164	rVV2	163	136	0.02%	0.002%
27	4.956	1202	1218	1251	rBV2	302961	807861	100.00%	11.999%
28	5.252	1308	1310	1315	rVB2	278	206	0.03%	0.003%
29	5.288	1319	1321	1324	rVV2	237	124	0.02%	0.002%
30	5.320	1328	1331	1336	rVB2	372	217	0.03%	0.003%
31	5.416	1358	1361	1364	rBV	225	206	0.03%	0.003%
32	5.448	1368	1371	1375	rVB3	230	173	0.02%	0.003%
33	5.474	1375	1379	1383	rBV3	169	187	0.02%	0.003%
34	5.532	1386	1397	1433	rBV	274337	561850	69.55%	8.345%
35	5.841	1485	1493	1501	rVB6	795	1481	0.18%	0.022%
36	5.989	1524	1539	1569	rBV	176586	367794	45.53%	5.463%

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 Title : VOC Analysis

37	6.210	1607	1608	1612	rVB	328	139	0.02%	0.002%
38	6.272	1624	1627	1633	rBV	258	172	0.02%	0.003%
39	6.352	1649	1652	1656	rVB	242	163	0.02%	0.002%
40	6.378	1656	1660	1662	rVB2	183	153	0.02%	0.002%
41	6.400	1662	1667	1669	rBV2	224	238	0.03%	0.004%
42	6.606	1728	1731	1735	rVV	230	181	0.02%	0.003%
43	6.751	1774	1776	1781	rVB2	147	117	0.01%	0.002%
44	6.780	1781	1785	1792	rVB2	151	179	0.02%	0.003%
45	6.812	1792	1795	1800	rBV2	122	119	0.01%	0.002%
46	6.857	1804	1809	1812	rBV2	138	152	0.02%	0.002%
47	6.911	1815	1826	1857	rBV	97424	186881	23.13%	2.776%
48	7.091	1878	1882	1887	rVB3	302	305	0.04%	0.005%
49	7.194	1912	1914	1917	rBV	157	126	0.02%	0.002%
50	7.243	1918	1929	1952	rBV	372424	648005	80.21%	9.625%
51	7.419	1982	1984	1986	rBV	275	124	0.02%	0.002%
52	7.554	2016	2026	2057	rBV	65269	121742	15.07%	1.808%
53	7.776	2092	2095	2098	rBV3	198	124	0.02%	0.002%
54	7.873	2118	2125	2136	rVV2	1134	1812	0.22%	0.027%
55	8.024	2162	2172	2211	rBV	186064	358100	44.33%	5.319%
56	8.371	2277	2280	2283	rBV2	213	213	0.03%	0.003%
57	8.435	2298	2300	2303	rVB2	292	121	0.01%	0.002%
58	8.464	2306	2309	2313	rVV	155	149	0.02%	0.002%
59	8.493	2315	2318	2323	rVB2	237	230	0.03%	0.003%
60	8.525	2323	2328	2333	rBV2	256	286	0.04%	0.004%
61	8.686	2374	2378	2381	rBV3	299	244	0.03%	0.004%
62	8.783	2397	2408	2445	rBV	411367	689938	85.40%	10.247%
63	9.213	2539	2542	2546	rBV2	149	139	0.02%	0.002%
64	9.474	2619	2623	2627	rVB2	204	162	0.02%	0.002%
65	9.513	2627	2635	2636	rBV	151	142	0.02%	0.002%
66	9.722	2697	2700	2707	rBV2	133	157	0.02%	0.002%
67	9.844	2735	2738	2743	rBV2	131	142	0.02%	0.002%
68	10.078	2801	2811	2814	rBV2	207	290	0.04%	0.004%
69	10.152	2823	2834	2859	rBV	228578	362525	44.87%	5.384%
70	10.323	2877	2887	2899	rBV2	1421	2161	0.27%	0.032%
71	10.416	2913	2916	2922	rBV2	146	142	0.02%	0.002%
72	10.603	2971	2974	2980	rBV2	157	156	0.02%	0.002%
73	10.831	3039	3045	3047	rBV	108	121	0.01%	0.002%
74	11.184	3144	3155	3179	rBV	437561	676008	83.68%	10.040%
75	11.561	3256	3272	3294	rBV	374286	602157	74.54%	8.944%
76	11.747	3327	3330	3333	rBV2	203	121	0.01%	0.002%

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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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

77	12.040	3418	3421	3423	rBV	195	121	0.01%	0.002%
78	12.249	3479	3486	3488	rBV	164	161	0.02%	0.002%
79	12.274	3489	3494	3497	rBV2	201	216	0.03%	0.003%
80	12.358	3516	3520	3522	rBV	164	125	0.02%	0.002%
81	12.583	3587	3590	3593	rVV	172	116	0.01%	0.002%
82	13.117	3753	3756	3760	rBV2	183	120	0.01%	0.002%
83	13.454	3855	3861	3864	rBV2	726	725	0.09%	0.011%
84	13.500	3872	3875	3878	rBV2	258	203	0.03%	0.003%
85	13.702	3935	3938	3943	rVB2	233	176	0.02%	0.003%
86	13.744	3949	3951	3954	rVB	247	117	0.01%	0.002%
87	13.982	4020	4025	4028	rBV3	313	300	0.04%	0.004%
88	14.020	4034	4037	4039	rBV	184	127	0.02%	0.002%
89	14.049	4042	4046	4048	rBV2	198	190	0.02%	0.003%
90	14.091	4053	4059	4060	rBV2	344	253	0.03%	0.004%
91	14.329	4122	4133	4134	rBV3	288	491	0.06%	0.007%
92	14.371	4144	4146	4149	rBV3	269	143	0.02%	0.002%
93	14.403	4153	4156	4157	rBV	221	120	0.01%	0.002%
94	14.554	4201	4203	4205	rBV2	246	167	0.02%	0.002%
95	14.590	4211	4214	4219	rBV3	427	436	0.05%	0.006%
96	14.737	4257	4260	4262	rBV	249	211	0.03%	0.003%
97	15.216	4407	4409	4412	rVB2	443	233	0.03%	0.003%
98	15.252	4415	4420	4421	rBV2	415	318	0.04%	0.005%
99	15.406	4466	4468	4471	rBV2	327	218	0.03%	0.003%
100	16.252	4725	4731	4740	rVB5	3886	5368	0.66%	0.080%

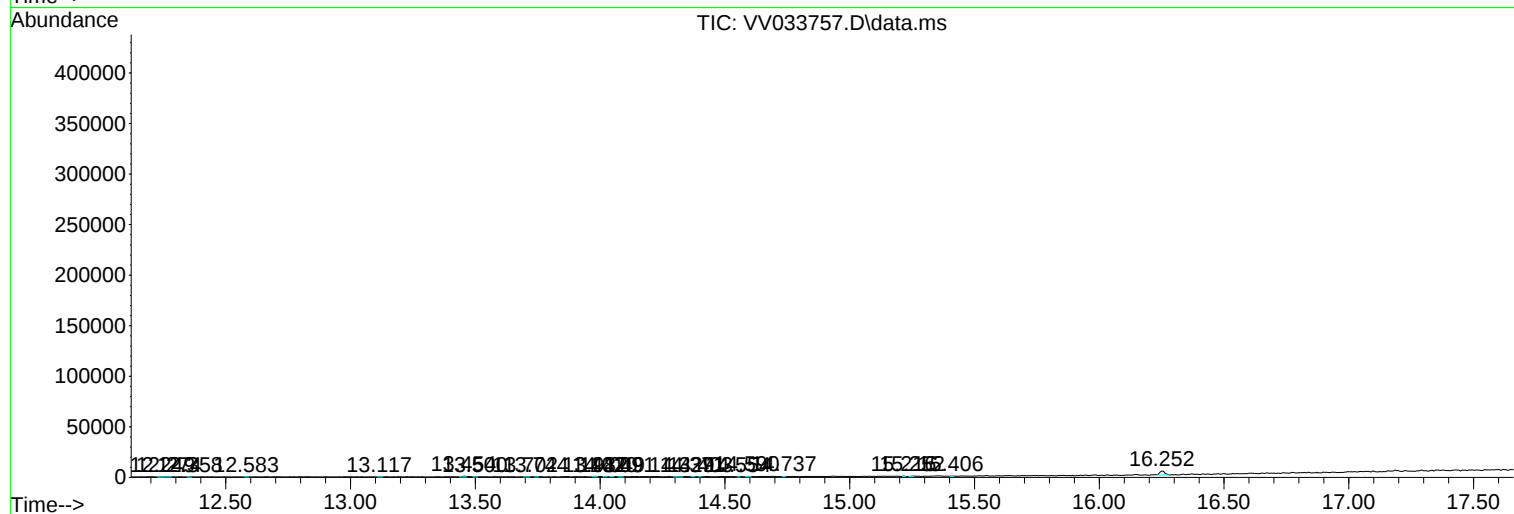
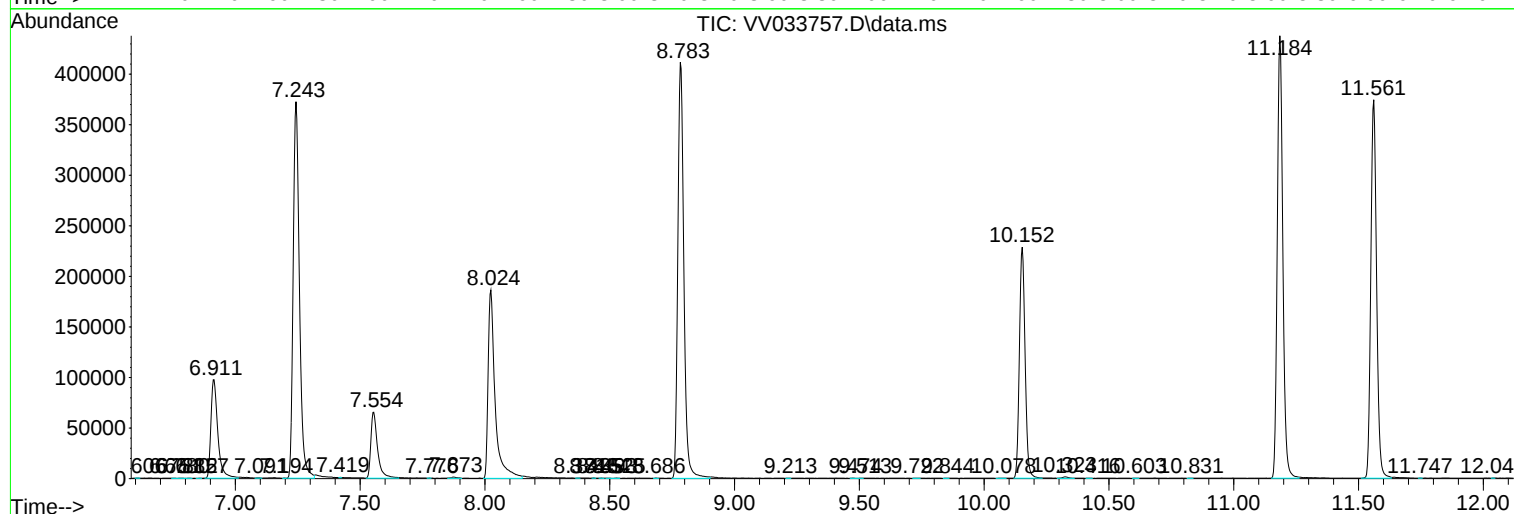
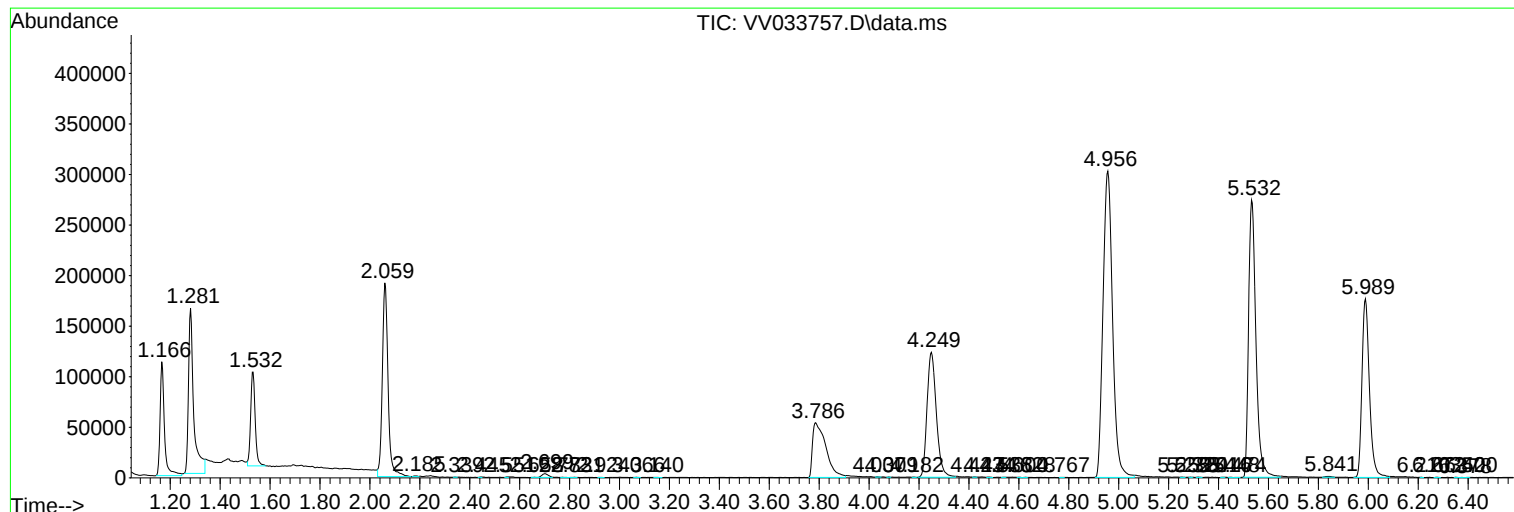
Sum of corrected areas: 6732816

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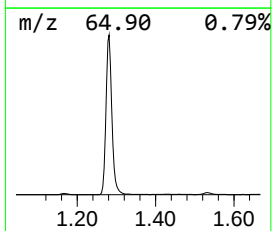
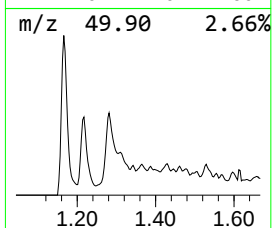
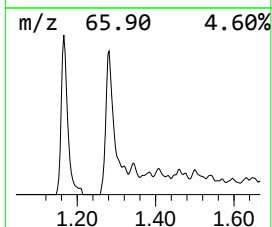
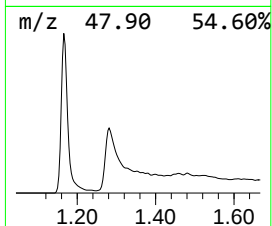
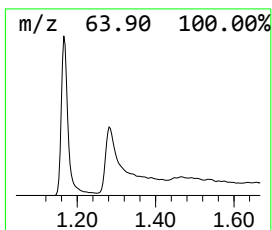
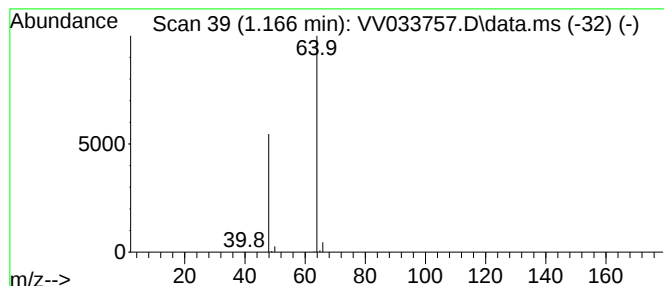
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	12.14 ug/L	136376	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 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	12.1	ug/L	136376	1	5.532	561850	50.0