

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033780.D
 Acq On : 20 Jan 2024 02:22
 Operator : SY/MD
 Sample : P1189-21
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMR8

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: VV033780.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	121190	139043	18.59%	2.202%
2	1.281	66	75	105	rBV	166305	290017	38.77%	4.593%
3	1.532	146	153	166	rVB	86056	102984	13.77%	1.631%
4	2.060	308	317	345	rVB	172812	270944	36.22%	4.291%
5	2.214	363	365	366	rBV2	480	245	0.03%	0.004%
6	2.397	418	422	423	rBV	340	227	0.03%	0.004%
7	2.452	434	439	443	rVB4	671	531	0.07%	0.008%
8	2.516	455	459	461	rBV	181	149	0.02%	0.002%
9	2.529	461	463	467	rVB2	311	161	0.02%	0.003%
10	2.561	467	473	476	rBV3	670	941	0.13%	0.015%
11	2.789	541	544	548	rVB2	189	139	0.02%	0.002%
12	2.870	567	569	575	rVB2	152	129	0.02%	0.002%
13	3.095	632	639	641	rBV	146	134	0.02%	0.002%
14	3.699	821	827	831	rBV2	96	130	0.02%	0.002%
15	3.741	832	840	844	rBV2	151	189	0.03%	0.003%
16	3.786	845	854	888	rBV	47882	130598	17.46%	2.068%
17	4.059	936	939	942	rBV	273	206	0.03%	0.003%
18	4.249	982	998	1022	rBV	116974	297923	39.82%	4.718%
19	4.577	1097	1100	1101	rBV2	300	157	0.02%	0.002%
20	4.587	1101	1103	1106	rVB2	298	145	0.02%	0.002%
21	4.625	1110	1115	1118	rBV2	195	183	0.02%	0.003%
22	4.641	1118	1120	1124	rVB	183	151	0.02%	0.002%
23	4.802	1164	1170	1174	rBV	149	136	0.02%	0.002%
24	4.957	1202	1218	1253	rBV2	279441	748121	100.00%	11.847%
25	5.230	1301	1303	1306	rBV	206	123	0.02%	0.002%
26	5.378	1346	1349	1352	rBV2	256	207	0.03%	0.003%
27	5.410	1354	1359	1364	rVV2	252	211	0.03%	0.003%
28	5.490	1381	1384	1385	rBV	196	130	0.02%	0.002%
29	5.532	1386	1397	1426	rBV	264856	542173	72.47%	8.586%
30	5.834	1485	1491	1492	rBV2	803	694	0.09%	0.011%
31	5.892	1506	1509	1512	rBV	144	123	0.02%	0.002%
32	5.921	1515	1518	1522	rVB	257	204	0.03%	0.003%
33	5.944	1522	1525	1527	rBV2	203	157	0.02%	0.002%
34	5.989	1527	1539	1566	rBV	165142	339397	45.37%	5.375%
35	6.191	1597	1602	1604	rVB3	369	341	0.05%	0.005%
36	6.252	1617	1621	1623	rBV2	227	142	0.02%	0.002%

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

37	6.346	1645	1650	1654	rBV2	147	159	0.02%	0.003%
38	6.477	1684	1691	1694	rVB2	162	195	0.03%	0.003%
39	6.497	1694	1697	1701	rBV	285	240	0.03%	0.004%
40	6.542	1706	1711	1716	rVB2	222	212	0.03%	0.003%
41	6.606	1725	1731	1736	rBV3	306	450	0.06%	0.007%
42	6.657	1744	1747	1752	rVB3	321	262	0.04%	0.004%
43	6.812	1791	1795	1800	rBV2	165	168	0.02%	0.003%
44	6.915	1816	1827	1858	rBV	86189	165332	22.10%	2.618%
45	7.146	1890	1899	1900	rBV2	535	626	0.08%	0.010%
46	7.243	1918	1929	1964	rBV	337396	601036	80.34%	9.518%
47	7.554	2016	2026	2053	rBV	58278	105625	14.12%	1.673%
48	7.731	2078	2081	2084	rVV2	240	167	0.02%	0.003%
49	7.876	2118	2126	2132	rBV2	1063	1581	0.21%	0.025%
50	7.911	2133	2137	2144	rVB5	1131	1387	0.19%	0.022%
51	8.024	2162	2172	2212	rBV	174451	337120	45.06%	5.339%
52	8.304	2256	2259	2261	rBV2	262	188	0.03%	0.003%
53	8.336	2267	2269	2274	rVB3	293	166	0.02%	0.003%
54	8.365	2275	2278	2282	rVB	190	175	0.02%	0.003%
55	8.390	2282	2286	2287	rBV	218	134	0.02%	0.002%
56	8.516	2322	2325	2328	rVV	276	213	0.03%	0.003%
57	8.706	2381	2384	2388	rVB2	173	137	0.02%	0.002%
58	8.744	2388	2396	2398	rBV2	139	188	0.03%	0.003%
59	8.783	2398	2408	2454	rBV	399984	663299	88.66%	10.504%
60	9.207	2537	2540	2547	rVB	137	152	0.02%	0.002%
61	9.323	2571	2576	2581	rVB2	132	152	0.02%	0.002%
62	9.580	2653	2656	2662	rVB2	171	185	0.02%	0.003%
63	9.837	2732	2736	2739	rBV	202	165	0.02%	0.003%
64	9.979	2776	2780	2785	rBV2	147	185	0.02%	0.003%
65	10.101	2812	2818	2823	rBV2	139	158	0.02%	0.003%
66	10.152	2823	2834	2862	rBV	217678	338166	45.20%	5.355%
67	10.297	2873	2879	2880	rVV	197	182	0.02%	0.003%
68	10.326	2880	2888	2896	rVB3	2089	3082	0.41%	0.049%
69	10.432	2914	2921	2923	rBV2	132	161	0.02%	0.003%
70	10.529	2943	2951	2955	rBV2	134	191	0.03%	0.003%
71	10.580	2963	2967	2974	rBV2	159	220	0.03%	0.003%
72	10.812	3035	3039	3044	rBV2	184	178	0.02%	0.003%
73	10.837	3044	3047	3052	rVV2	187	156	0.02%	0.002%
74	11.185	3144	3155	3182	rBV	412871	646922	86.47%	10.245%
75	11.410	3222	3225	3228	rVB2	293	127	0.02%	0.002%
76	11.519	3256	3259	3260	rBV2	214	128	0.02%	0.002%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.561	3260	3272	3295	rVV	344484	559948	74.85%	8.867%
78	11.850	3357	3362	3366	rBV2	150	151	0.02%	0.002%
79	12.127	3445	3448	3451	rVB2	187	126	0.02%	0.002%
80	12.194	3463	3469	3479	rVB3	537	799	0.11%	0.013%
81	12.541	3574	3577	3581	rBV2	166	127	0.02%	0.002%
82	12.892	3682	3686	3693	rBV2	172	235	0.03%	0.004%
83	13.455	3860	3861	3866	rVV	225	146	0.02%	0.002%
84	13.985	4021	4026	4029	rBV2	367	364	0.05%	0.006%
85	14.085	4050	4057	4062	rBV6	1944	3422	0.46%	0.054%
86	14.220	4094	4099	4102	rBV3	393	455	0.06%	0.007%
87	14.236	4102	4104	4108	rVB	535	286	0.04%	0.005%
88	14.268	4111	4114	4116	rBV	178	138	0.02%	0.002%
89	14.316	4125	4129	4132	rBV3	353	323	0.04%	0.005%
90	14.361	4141	4143	4146	rVB2	213	143	0.02%	0.002%
91	14.487	4179	4182	4184	rVV2	227	130	0.02%	0.002%
92	14.554	4200	4203	4206	rVB	319	228	0.03%	0.004%
93	14.754	4263	4265	4273	rVB2	318	250	0.03%	0.004%
94	14.808	4279	4282	4287	rVB	427	298	0.04%	0.005%
95	15.037	4351	4353	4358	rBV2	289	227	0.03%	0.004%
96	15.059	4358	4360	4361	rBV	364	148	0.02%	0.002%
97	15.127	4379	4381	4386	rVB2	412	296	0.04%	0.005%
98	15.194	4400	4402	4406	rBV4	440	267	0.04%	0.004%
99	15.294	4431	4433	4436	rBV3	308	201	0.03%	0.003%
100	16.252	4724	4731	4738	rVB5	6350	9005	1.20%	0.143%

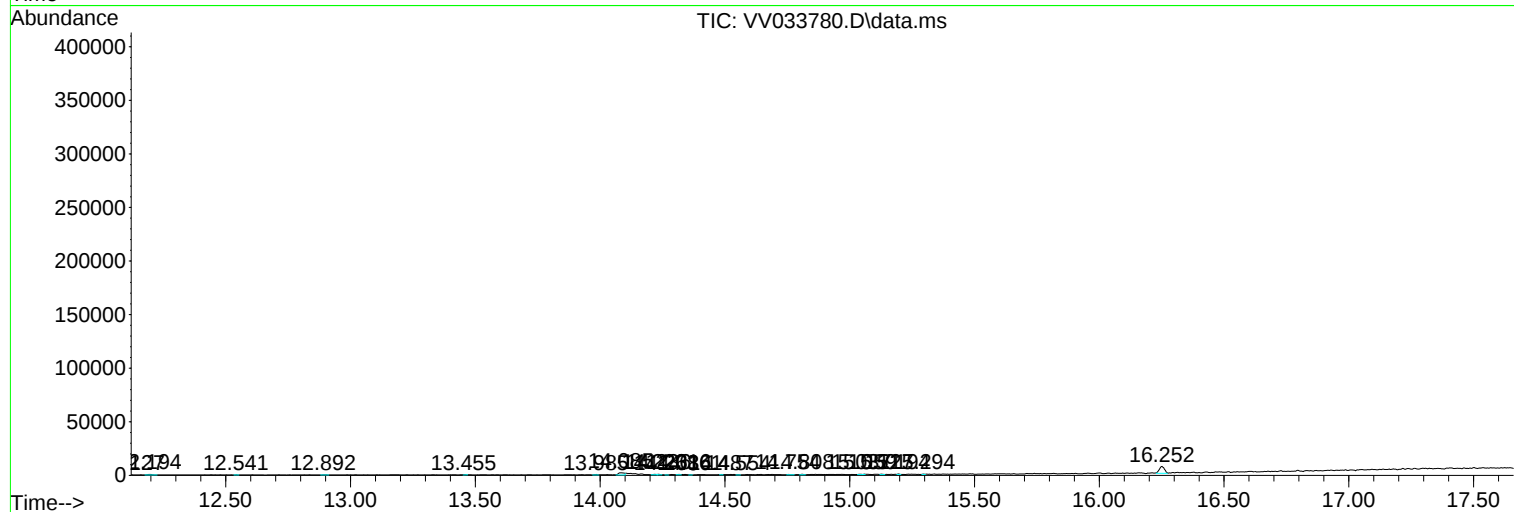
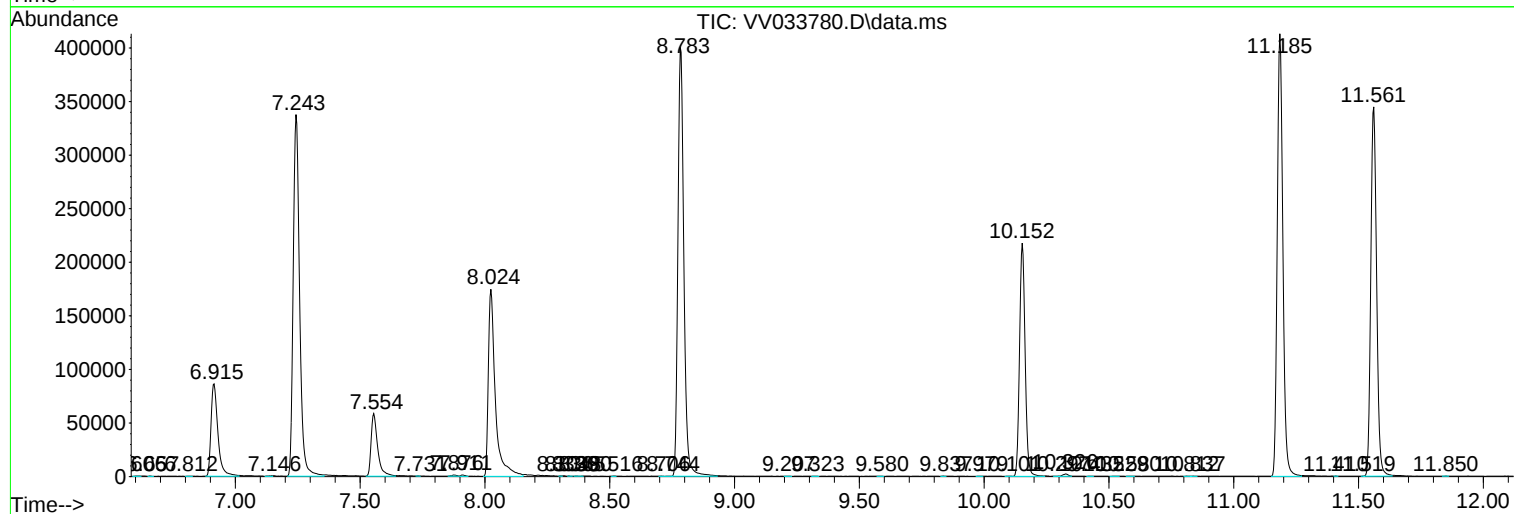
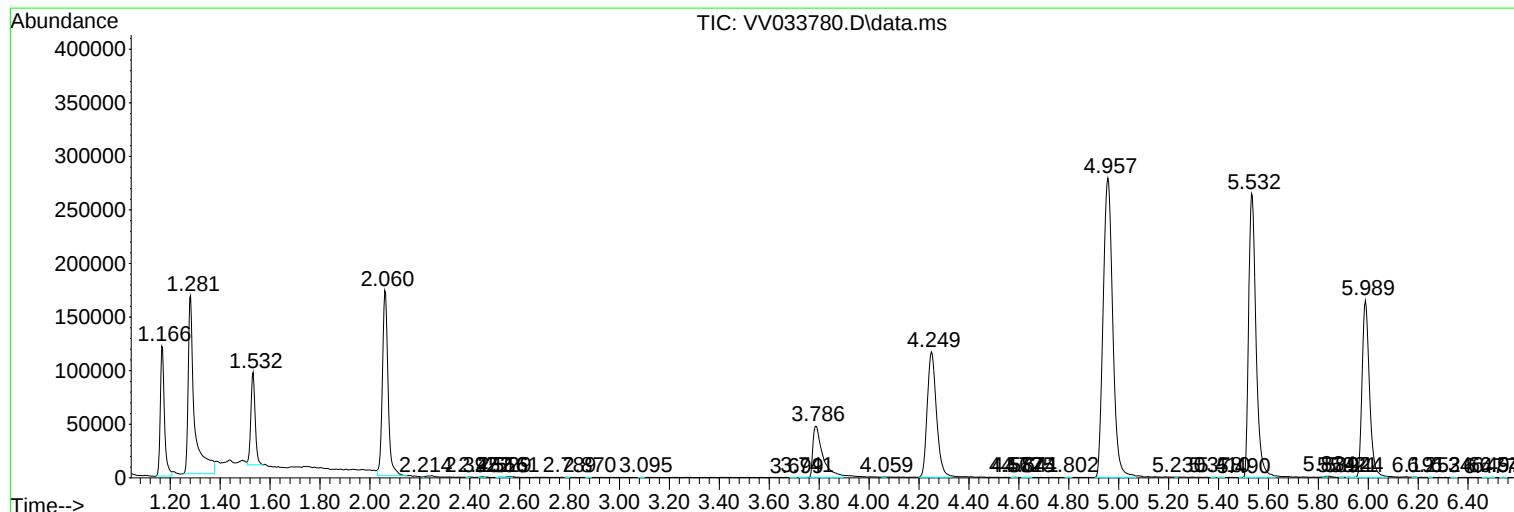
Sum of corrected areas: 6314768

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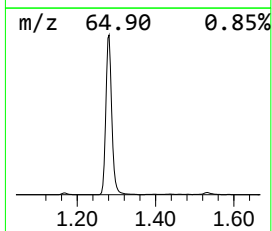
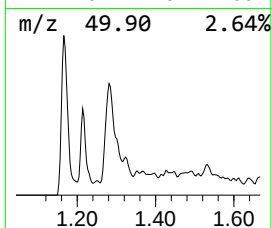
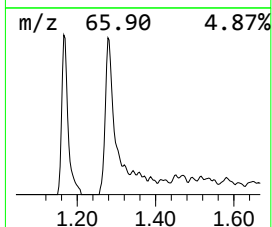
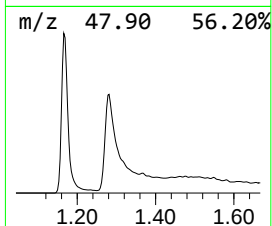
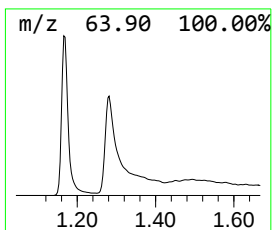
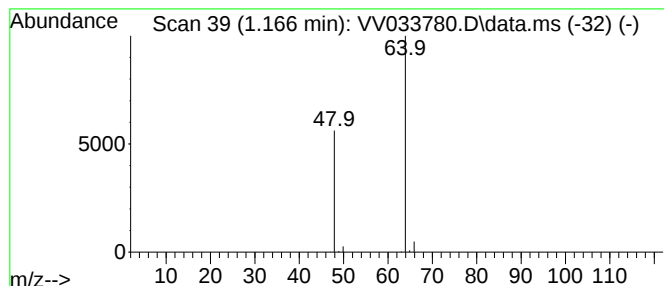
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	12.82 ug/L	139043	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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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	12.8	ug/L	139043	1	5.532	542173	50.0