

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
 Data File : VV033884.D
 Acq On : 26 Jan 2024 13:57
 Operator : SY/MD
 Sample : P1252-07
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMT8

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: VV033884.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	52	rBV	100267	112142	14.89%	1.817%
2	1.278	67	74	111	rBV2	115875	222857	29.60%	3.611%
3	1.529	145	152	171	rVB	93033	116364	15.45%	1.885%
4	2.059	307	317	331	rVB	192317	281127	37.33%	4.555%
5	2.182	351	355	362	rVB2	777	1064	0.14%	0.017%
6	2.230	367	370	372	rBV3	526	415	0.06%	0.007%
7	2.445	435	437	440	rBV3	322	245	0.03%	0.004%
8	2.519	456	460	465	rBV2	149	161	0.02%	0.003%
9	2.571	473	476	480	rBV4	397	357	0.05%	0.006%
10	2.783	537	542	549	rBV2	256	357	0.05%	0.006%
11	2.838	554	559	566	rBV2	151	243	0.03%	0.004%
12	2.931	585	588	591	rVB2	211	140	0.02%	0.002%
13	3.143	652	654	663	rVB2	155	186	0.02%	0.003%
14	3.217	675	677	682	rVB	268	198	0.03%	0.003%
15	3.368	720	724	732	rVB2	157	189	0.03%	0.003%
16	3.670	813	818	823	rVB2	222	233	0.03%	0.004%
17	3.706	823	829	831	rBV2	272	226	0.03%	0.004%
18	3.783	845	853	891	rBV	57249	149472	19.85%	2.422%
19	4.075	942	944	950	rVB2	307	194	0.03%	0.003%
20	4.249	982	998	1034	rBV	117110	303744	40.34%	4.921%
21	4.400	1043	1045	1050	rVB2	546	373	0.05%	0.006%
22	4.468	1065	1066	1071	rVB	292	153	0.02%	0.002%
23	4.506	1075	1078	1082	rVV2	220	189	0.03%	0.003%
24	4.529	1082	1085	1089	rVB3	229	181	0.02%	0.003%
25	4.603	1104	1108	1112	rBV	278	179	0.02%	0.003%
26	4.725	1143	1146	1151	rVB2	165	150	0.02%	0.002%
27	4.956	1202	1218	1253	rBV2	284740	752993	100.00%	12.200%
28	5.326	1330	1333	1336	rBV	292	267	0.04%	0.004%
29	5.474	1371	1379	1383	rBV	186	258	0.03%	0.004%
30	5.535	1386	1398	1421	rBV	249506	507185	67.36%	8.218%
31	5.841	1486	1493	1500	rVB5	1065	1698	0.23%	0.028%
32	5.886	1500	1507	1510	rBV3	253	324	0.04%	0.005%
33	5.905	1510	1513	1516	rBV2	238	191	0.03%	0.003%
34	5.989	1527	1539	1568	rBV	164209	335698	44.58%	5.439%
35	6.149	1586	1589	1592	rVB2	604	409	0.05%	0.007%
36	6.169	1592	1595	1596	rVV3	251	185	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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

37	6.191	1600	1602	1606	rVB2	298	143	0.02%	0.002%
38	6.413	1665	1671	1678	rBV2	242	334	0.04%	0.005%
39	6.445	1678	1681	1686	rVV2	217	234	0.03%	0.004%
40	6.474	1686	1690	1697	rVV2	189	262	0.03%	0.004%
41	6.587	1720	1725	1727	rBV2	236	164	0.02%	0.003%
42	6.915	1815	1827	1854	rBV	94153	175552	23.31%	2.844%
43	7.243	1915	1929	1963	rBV	341906	607029	80.62%	9.835%
44	7.554	2016	2026	2054	rBV	62869	115255	15.31%	1.867%
45	7.763	2088	2091	2097	rVB3	256	225	0.03%	0.004%
46	7.866	2119	2123	2126	rBV2	217	213	0.03%	0.003%
47	8.024	2163	2172	2212	rBV	209408	377152	50.09%	6.111%
48	8.468	2307	2310	2314	rBV2	239	137	0.02%	0.002%
49	8.493	2314	2318	2321	rBV	272	185	0.02%	0.003%
50	8.542	2328	2333	2337	rBV	268	197	0.03%	0.003%
51	8.667	2367	2372	2374	rBV	272	157	0.02%	0.003%
52	8.728	2385	2391	2397	rBV2	197	258	0.03%	0.004%
53	8.786	2397	2409	2430	rBV	374270	608964	80.87%	9.867%
54	9.008	2475	2478	2480	rBV2	289	150	0.02%	0.002%
55	9.104	2504	2508	2512	rBV2	193	182	0.02%	0.003%
56	9.217	2540	2543	2546	rVB2	226	139	0.02%	0.002%
57	9.342	2579	2582	2588	rVB2	191	152	0.02%	0.002%
58	9.374	2588	2592	2594	rBV	190	142	0.02%	0.002%
59	9.850	2735	2740	2742	rBV	133	141	0.02%	0.002%
60	9.940	2761	2768	2772	rBV2	174	256	0.03%	0.004%
61	10.056	2801	2804	2809	rVB2	240	181	0.02%	0.003%
62	10.152	2822	2834	2858	rBV	222669	350454	46.54%	5.678%
63	10.316	2883	2885	2888	rBV	188	157	0.02%	0.003%
64	10.596	2966	2972	2974	rBV	197	194	0.03%	0.003%
65	10.847	3047	3050	3058	rVB2	126	140	0.02%	0.002%
66	10.882	3058	3061	3068	rBV	277	300	0.04%	0.005%
67	10.940	3073	3079	3082	rBV2	178	196	0.03%	0.003%
68	11.140	3137	3141	3144	rBV2	226	163	0.02%	0.003%
69	11.185	3145	3155	3179	rBV	382855	593635	78.84%	9.618%
70	11.320	3195	3197	3205	rVB2	346	225	0.03%	0.004%
71	11.512	3248	3257	3261	rBV6	1765	2898	0.38%	0.047%
72	11.561	3261	3272	3295	rVB	341649	538774	71.55%	8.729%
73	11.676	3306	3308	3310	rBV2	278	154	0.02%	0.002%
74	11.837	3356	3358	3363	rBV	191	143	0.02%	0.002%
75	11.966	3395	3398	3402	rVB	256	158	0.02%	0.003%
76	11.998	3402	3408	3411	rBV2	176	224	0.03%	0.004%

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 ClientSampleId :
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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

77	12.049	3421	3424	3428	rBV2	160	142	0.02%	0.002%
78	12.123	3442	3447	3452	rBV2	152	201	0.03%	0.003%
79	12.197	3466	3470	3475	rBV3	259	244	0.03%	0.004%
80	12.268	3488	3492	3495	rBV2	200	188	0.02%	0.003%
81	12.316	3505	3507	3513	rVB2	182	162	0.02%	0.003%
82	12.352	3516	3518	3526	rVV2	158	173	0.02%	0.003%
83	12.390	3527	3530	3534	rVB2	213	166	0.02%	0.003%
84	12.541	3574	3577	3581	rBV2	167	144	0.02%	0.002%
85	12.850	3670	3673	3676	rBV2	238	197	0.03%	0.003%
86	13.043	3730	3733	3735	rBV	214	140	0.02%	0.002%
87	13.461	3860	3863	3868	rVB3	285	314	0.04%	0.005%
88	13.644	3917	3920	3925	rBV2	275	191	0.03%	0.003%
89	13.741	3948	3950	3954	rVB	317	196	0.03%	0.003%
90	13.834	3975	3979	3982	rBV2	240	185	0.02%	0.003%
91	13.885	3993	3995	3999	rVB	280	160	0.02%	0.003%
92	13.950	4012	4015	4017	rBV2	304	241	0.03%	0.004%
93	13.988	4021	4027	4032	rVB2	590	819	0.11%	0.013%
94	14.078	4051	4055	4059	rVB3	213	198	0.03%	0.003%
95	14.467	4171	4176	4180	rBV2	392	503	0.07%	0.008%
96	14.564	4203	4206	4210	rBV2	264	202	0.03%	0.003%
97	14.760	4264	4267	4269	rBV	347	210	0.03%	0.003%
98	14.950	4323	4326	4328	rBV2	413	216	0.03%	0.003%
99	14.988	4332	4338	4341	rBV3	392	458	0.06%	0.007%
100	16.400	4775	4777	4780	rVB3	691	296	0.04%	0.005%

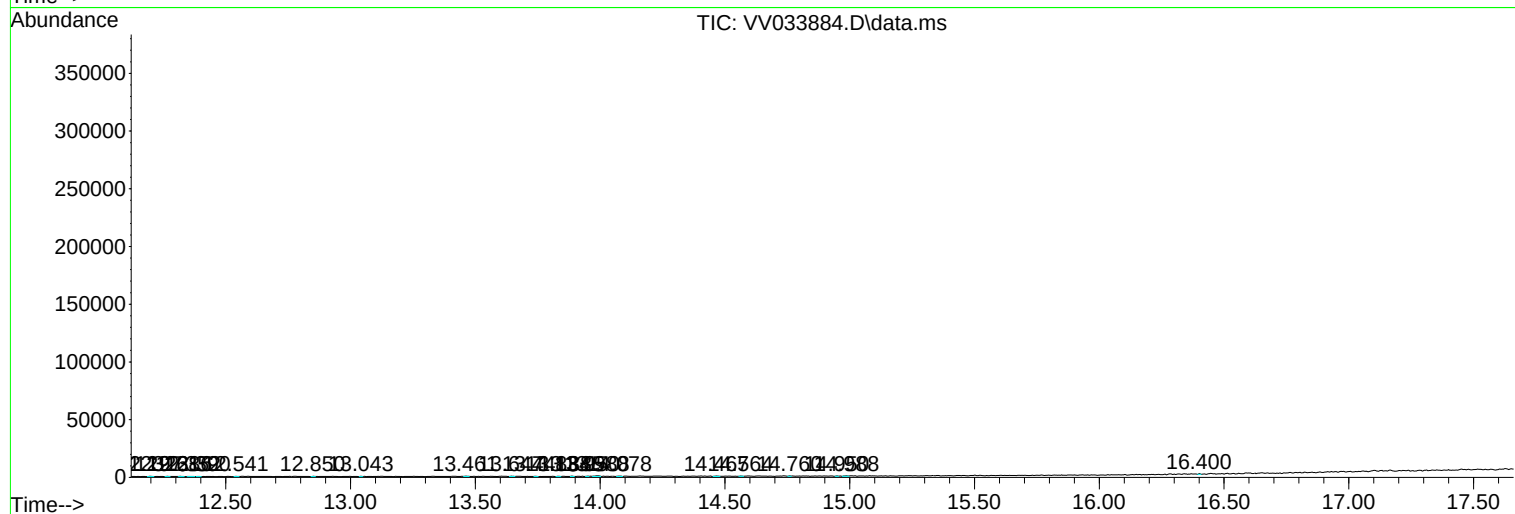
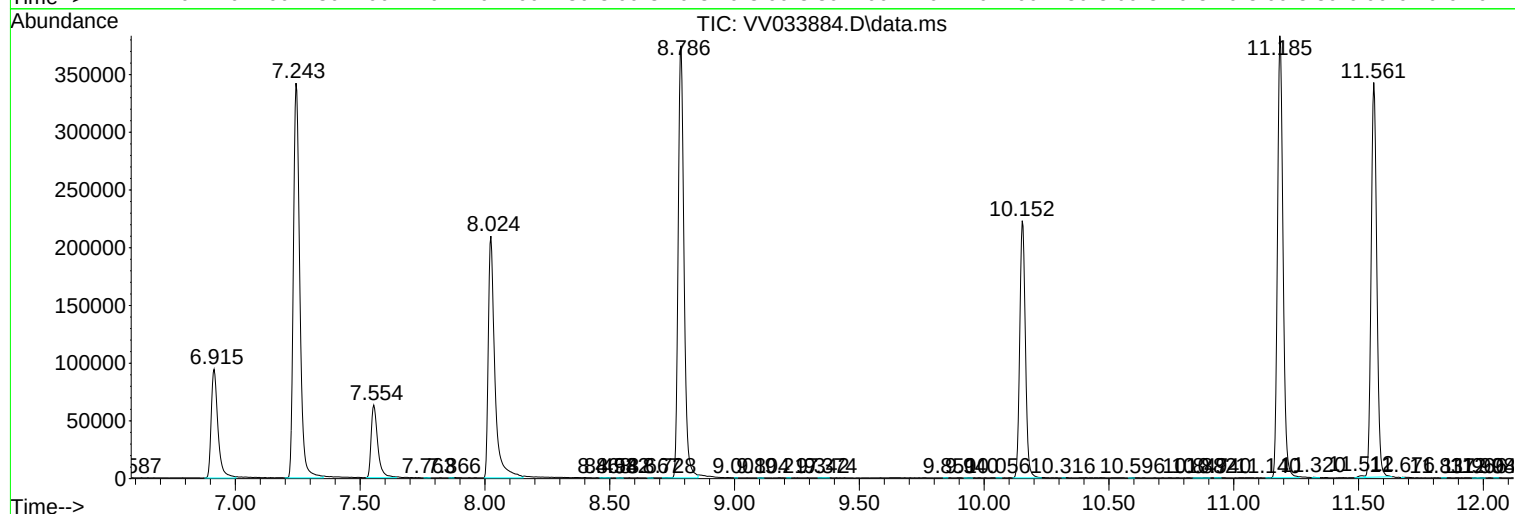
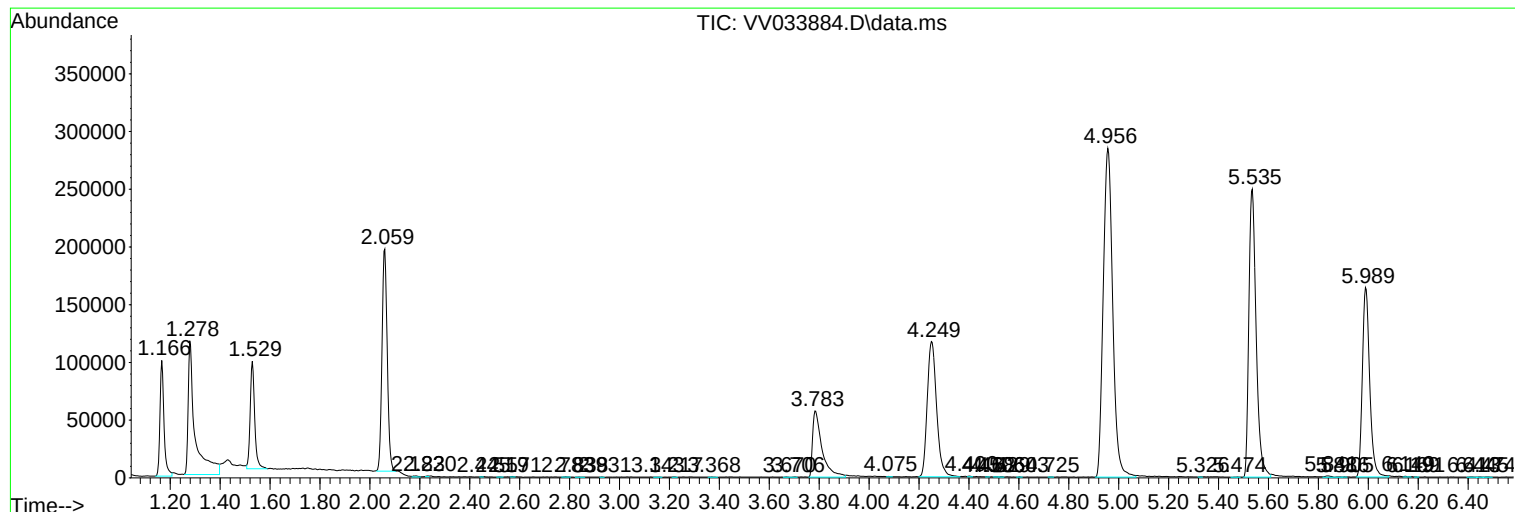
Sum of corrected areas: 6171912

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMT8

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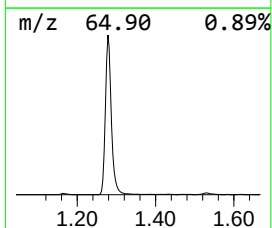
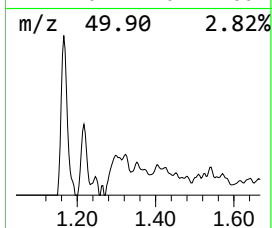
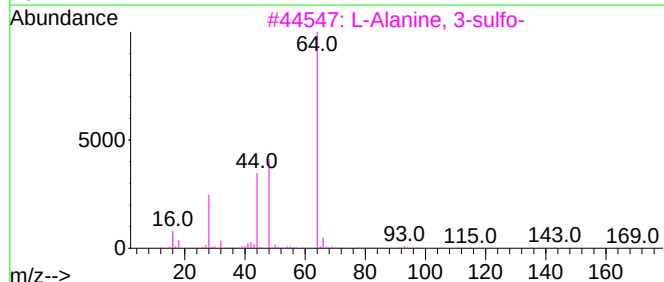
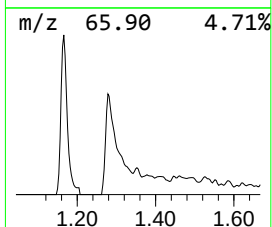
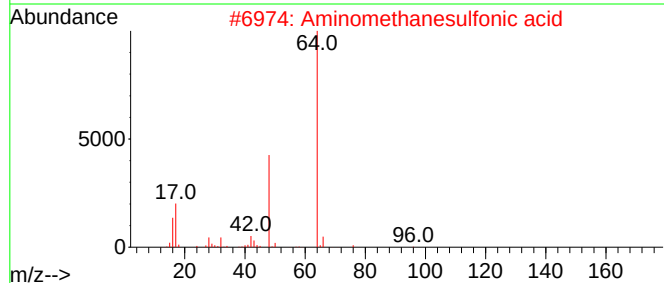
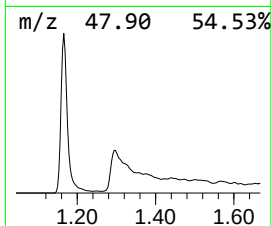
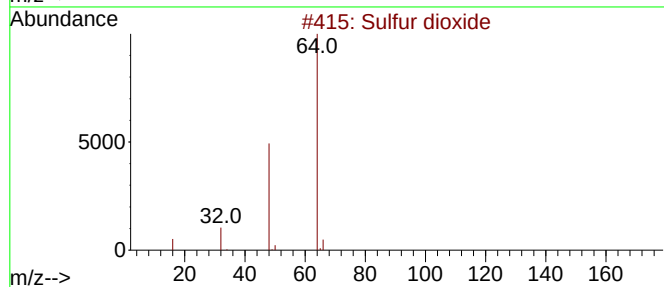
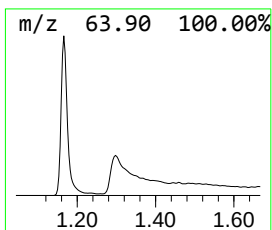
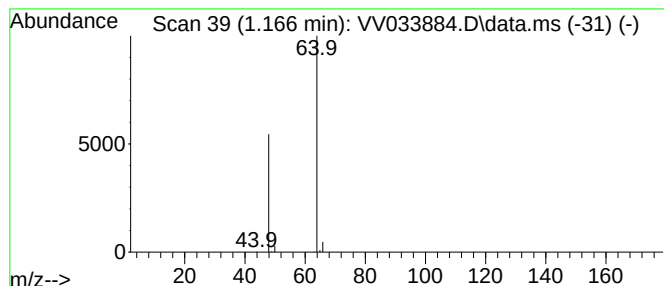
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	11.06 ug/L	112142	1,4-Difluorobenzene	5.535

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			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	11.1	ug/L	112142	1	5.535	507185	50.0