

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012224\
 Data File : VV033798.D
 Acq On : 22 Jan 2024 13:25
 Operator : SY/MD
 Sample : P1190-15
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMT2

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: VV033798.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	53	rBV	147118	161529	0.20%	0.146%
2	1.285	63	76	91	rBV2	848803	1111075	1.37%	1.007%
3	1.532	147	153	169	rVB	101960	129050	0.16%	0.117%
4	2.063	309	318	341	rVB2	230279	375994	0.46%	0.341%
5	2.243	364	374	391	rBV	25787	42664	0.05%	0.039%
6	2.449	429	438	451	rBV	11568	18346	0.02%	0.017%
7	2.561	466	473	476	rBV4	674	927	0.00%	0.001%
8	2.693	503	514	547	rBV	609322	1071036	1.32%	0.970%
9	3.593	788	794	795	rBV3	658	615	0.00%	0.001%
10	3.815	837	863	928	rBV	31251500	81082028	100.00%	73.461%
11	4.249	986	998	1034	rVB2	123362	333636	0.41%	0.302%
12	4.773	1158	1161	1164	rBV3	266	213	0.00%	0.000%
13	4.799	1167	1169	1177	rVB3	510	464	0.00%	0.000%
14	4.957	1201	1218	1243	rBV2	292009	774783	0.96%	0.702%
15	5.182	1284	1288	1291	rBV4	322	290	0.00%	0.000%
16	5.256	1308	1311	1313	rBV2	276	233	0.00%	0.000%
17	5.349	1337	1340	1342	rBV3	319	211	0.00%	0.000%
18	5.532	1385	1397	1430	rBV	246801	510018	0.63%	0.462%
19	5.831	1467	1490	1525	rBV	3766108	7310625	9.02%	6.623%
20	5.989	1528	1539	1568	rVB	172967	367480	0.45%	0.333%
21	6.310	1637	1639	1642	rVB	493	267	0.00%	0.000%
22	6.822	1792	1798	1803	rVV2	159	233	0.00%	0.000%
23	6.912	1816	1826	1854	rBV	97466	182166	0.22%	0.165%
24	7.111	1885	1888	1893	rBV3	242	229	0.00%	0.000%
25	7.185	1909	1911	1916	rVB2	340	238	0.00%	0.000%
26	7.243	1917	1929	1970	rBV	369889	655421	0.81%	0.594%
27	7.551	2016	2025	2052	rBV	65149	117021	0.14%	0.106%
28	7.722	2074	2078	2084	rBV3	399	313	0.00%	0.000%
29	7.773	2084	2094	2112	rVB	32555	57107	0.07%	0.052%
30	7.905	2112	2135	2163	rBV	7959655	13076605	16.13%	11.847%
31	8.021	2164	2171	2206	rVB	181275	345036	0.43%	0.313%
32	8.281	2247	2252	2260	rVB6	1879	2586	0.00%	0.002%
33	8.358	2274	2276	2281	rVB4	338	219	0.00%	0.000%
34	8.445	2299	2303	2306	rVB3	378	314	0.00%	0.000%
35	8.529	2320	2329	2336	rVV3	865	1093	0.00%	0.001%
36	8.571	2341	2342	2349	rVB2	378	211	0.00%	0.000%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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

37	8.735	2384	2393	2398	rBV5	1007	1628	0.00%	0.001%
38	8.783	2398	2408	2443	rBV	384206	626203	0.77%	0.567%
39	9.047	2481	2490	2492	rBV4	1229	1470	0.00%	0.001%
40	9.162	2518	2526	2537	rVB3	3230	5692	0.01%	0.005%
41	9.252	2547	2554	2565	rVB3	1540	2032	0.00%	0.002%
42	9.387	2586	2596	2598	rBV4	1800	2346	0.00%	0.002%
43	9.403	2598	2601	2602	rBV2	1060	701	0.00%	0.001%
44	9.487	2621	2627	2640	rBV3	1830	2711	0.00%	0.002%
45	9.641	2659	2675	2687	rBV6	6471	12698	0.02%	0.012%
46	9.738	2696	2705	2713	rBV9	3430	6945	0.01%	0.006%
47	9.838	2733	2736	2737	rBV	405	231	0.00%	0.000%
48	9.863	2740	2744	2745	rBV3	1431	858	0.00%	0.001%
49	9.911	2756	2759	2766	rVB7	1590	1861	0.00%	0.002%
50	10.059	2797	2805	2813	rVV4	4626	7324	0.01%	0.007%
51	10.153	2820	2834	2865	rVB2	228835	502574	0.62%	0.455%
52	10.278	2870	2873	2874	rBV2	428	254	0.00%	0.000%
53	10.301	2874	2880	2885	rBV6	1995	3382	0.00%	0.003%
54	10.391	2899	2908	2927	rBV4	8212	18775	0.02%	0.017%
55	10.481	2930	2936	2948	rVB	5984	9091	0.01%	0.008%
56	10.670	2984	2995	3005	rVV7	5433	11605	0.01%	0.011%
57	10.731	3012	3014	3015	rBV	532	243	0.00%	0.000%
58	10.854	3033	3052	3067	rBV2	17054	32410	0.04%	0.029%
59	10.956	3073	3084	3093	rBV8	2645	4887	0.01%	0.004%
60	11.008	3094	3100	3101	rBV5	1428	1269	0.00%	0.001%
61	11.095	3120	3127	3130	rBV3	1094	1333	0.00%	0.001%
62	11.130	3133	3138	3144	rVV4	2466	3204	0.00%	0.003%
63	11.185	3144	3155	3175	rVV	428608	662560	0.82%	0.600%
64	11.275	3177	3183	3200	rVB2	11443	18742	0.02%	0.017%
65	11.397	3216	3221	3223	rBV3	923	794	0.00%	0.001%
66	11.484	3237	3248	3252	rBV6	2337	4263	0.01%	0.004%
67	11.561	3254	3272	3293	rVB	401949	649678	0.80%	0.589%
68	11.683	3305	3310	3312	rBV4	971	975	0.00%	0.001%
69	11.728	3322	3324	3326	rBV2	376	226	0.00%	0.000%
70	11.757	3327	3333	3344	rVB2	3687	5621	0.01%	0.005%
71	11.854	3355	3363	3364	rBV2	1819	1801	0.00%	0.002%
72	11.934	3384	3388	3389	rBV2	564	438	0.00%	0.000%
73	11.966	3390	3398	3412	rVB7	4540	11273	0.01%	0.010%
74	12.056	3418	3426	3429	rBV3	1762	1918	0.00%	0.002%
75	12.095	3431	3438	3440	rBV4	1844	2161	0.00%	0.002%
76	12.178	3455	3464	3466	rBV3	2539	3016	0.00%	0.003%

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ClientSampleId :
DCMT2

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	12.243	3476	3484	3485	rBV4	1358	1446	0.00%	0.001%
78	12.297	3497	3501	3502	rBV	803	543	0.00%	0.000%
79	12.355	3515	3519	3526	rVB3	1686	2046	0.00%	0.002%
80	12.407	3528	3535	3544	rVB6	2253	2813	0.00%	0.003%
81	12.493	3557	3562	3569	rBV5	957	1452	0.00%	0.001%
82	12.625	3598	3603	3613	rBV4	309	516	0.00%	0.000%
83	12.741	3634	3639	3644	rBV2	296	325	0.00%	0.000%
84	12.767	3644	3647	3650	rVV3	257	220	0.00%	0.000%
85	12.786	3650	3653	3655	rVV	373	231	0.00%	0.000%
86	12.818	3657	3663	3672	rVB4	2273	3373	0.00%	0.003%
87	12.882	3680	3683	3686	rBV3	398	276	0.00%	0.000%
88	12.940	3697	3701	3704	rBV2	278	223	0.00%	0.000%
89	12.985	3711	3715	3719	rBV2	412	361	0.00%	0.000%
90	13.037	3728	3731	3737	rVB3	529	344	0.00%	0.000%
91	13.159	3764	3769	3772	rBV2	239	240	0.00%	0.000%
92	13.452	3853	3860	3869	rVV5	1952	2708	0.00%	0.002%
93	13.979	4019	4024	4026	rBV2	477	420	0.00%	0.000%
94	14.133	4068	4072	4076	rBV	193	222	0.00%	0.000%
95	14.185	4085	4088	4092	rVB2	328	261	0.00%	0.000%
96	14.699	4246	4248	4250	rBV3	323	212	0.00%	0.000%
97	15.050	4355	4357	4361	rVB3	328	219	0.00%	0.000%
98	15.117	4375	4378	4381	rBV2	305	244	0.00%	0.000%
99	15.130	4381	4382	4389	rVB2	411	348	0.00%	0.000%
100	15.287	4428	4431	4432	rBV	354	241	0.00%	0.000%

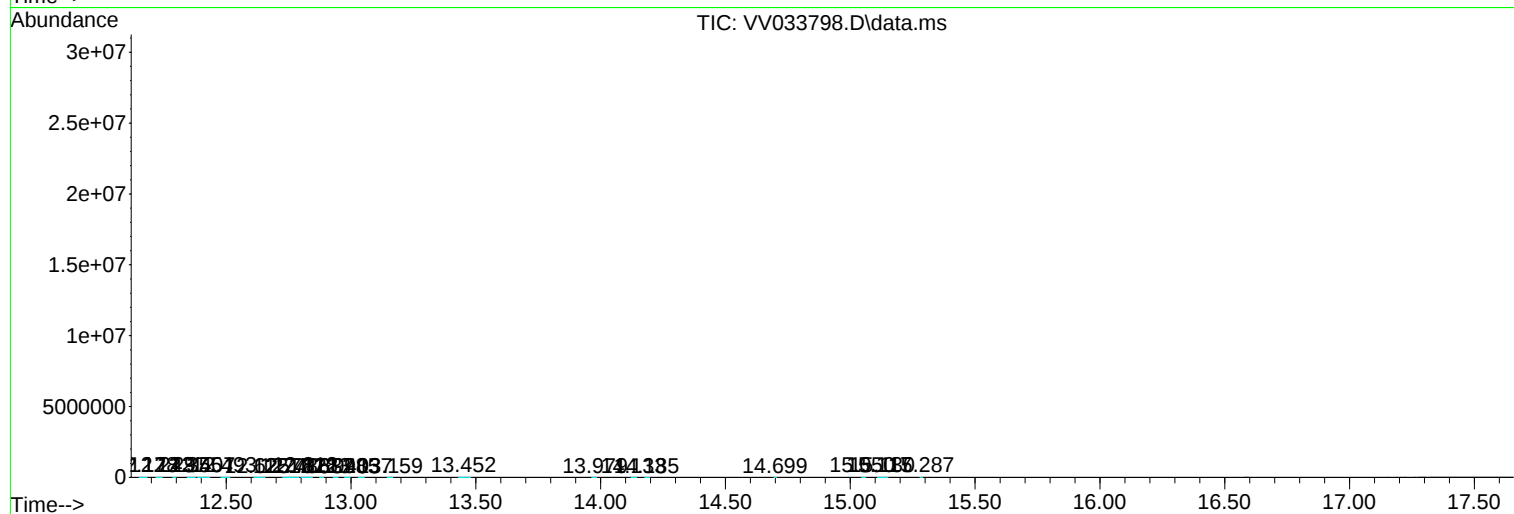
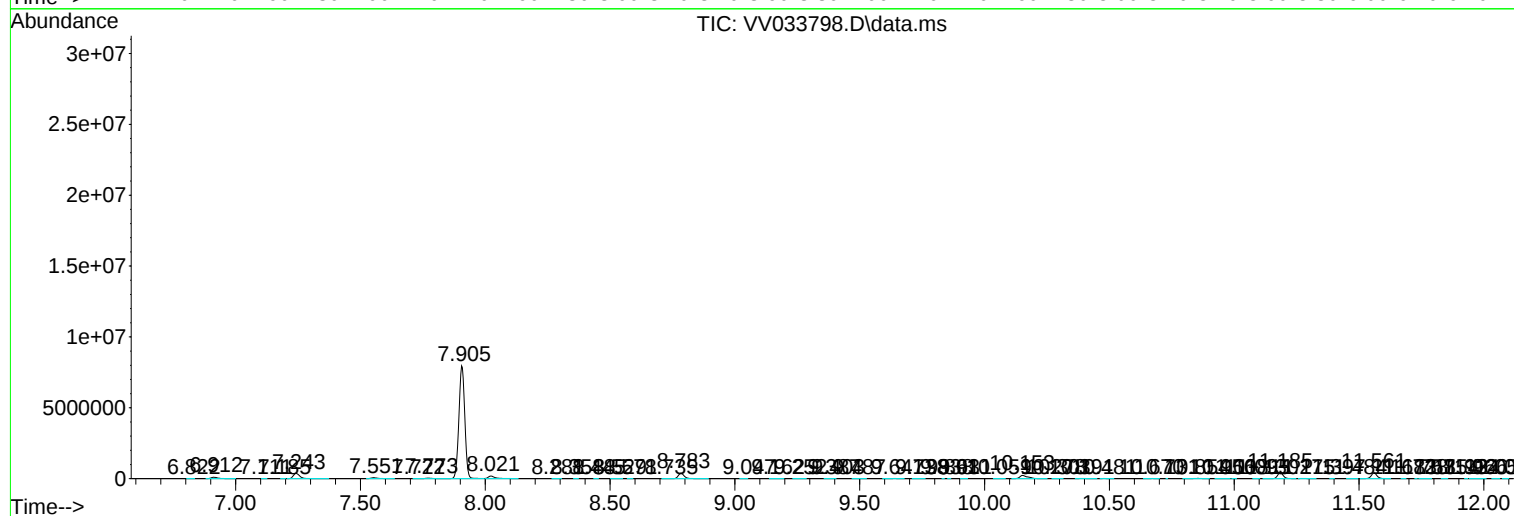
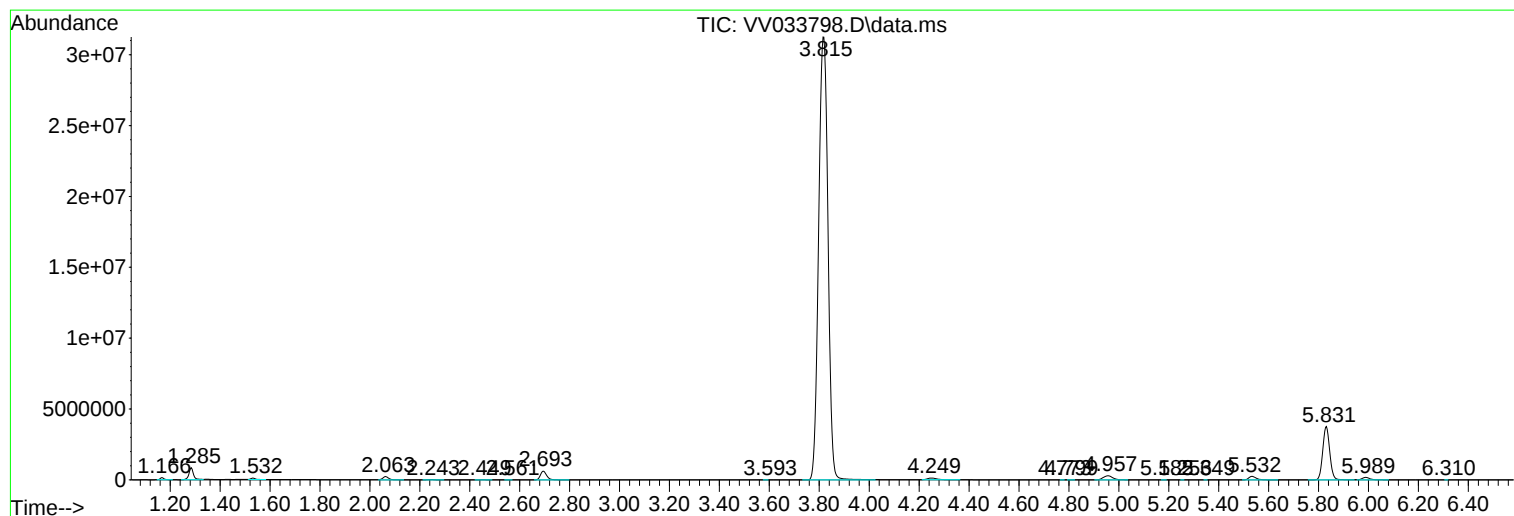
Sum of corrected areas: 110374753

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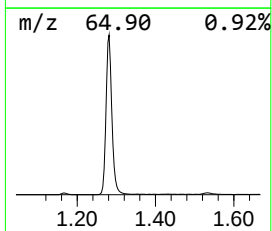
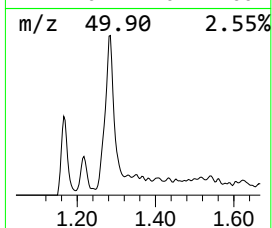
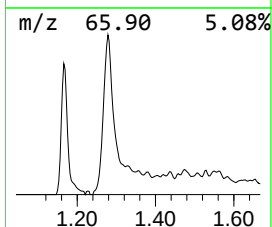
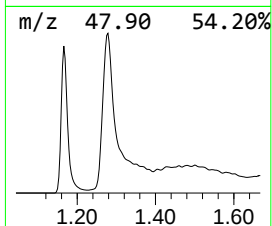
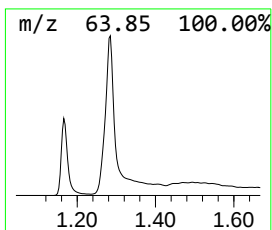
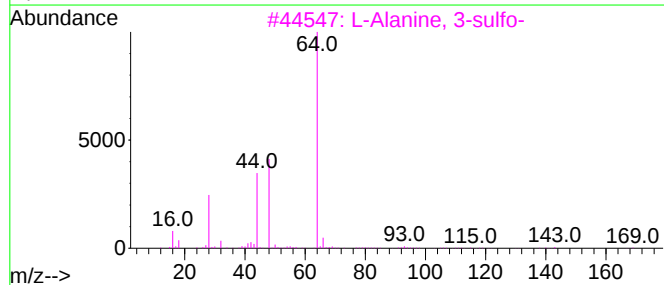
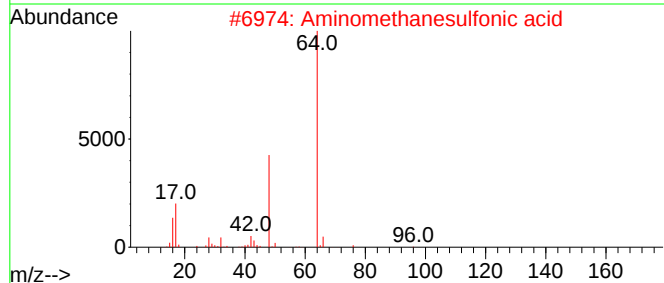
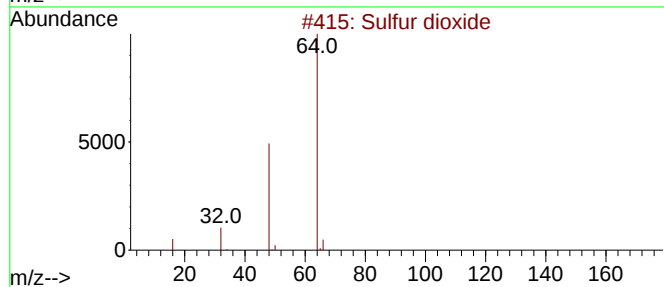
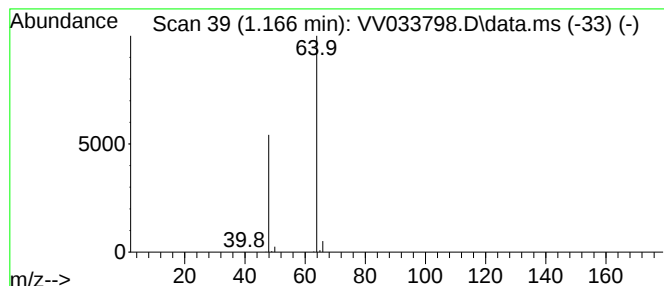
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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	15.84 ug/L	161529	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			Sulfur dioxide	64	O2S	007446-09-5	5



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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	15.8	ug/L	161529	1	5.535	510018	50.0