

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011924\
 Data File : VV033762.D
 Acq On : 19 Jan 2024 18:24
 Operator : SY/MD
 Sample : P1190-13
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMS4

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: VV033762.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	53	rBV	98345	114742	0.11%	0.074%
2	1.285	67	76	103	rBV2	730187	863802	0.83%	0.561%
3	1.532	146	153	170	rVB	92977	117105	0.11%	0.076%
4	2.063	308	318	343	rVB2	203895	331399	0.32%	0.215%
5	2.249	371	376	386	rVB2	1431	1936	0.00%	0.001%
6	2.696	503	515	541	rBV	225638	402928	0.39%	0.262%
7	2.892	572	576	581	rBV2	274	224	0.00%	0.000%
8	2.982	601	604	609	rVV2	244	184	0.00%	0.000%
9	3.124	641	648	655	rBV3	447	611	0.00%	0.000%
10	3.349	713	718	723	rBV2	276	400	0.00%	0.000%
11	3.391	728	731	734	rBV	169	160	0.00%	0.000%
12	3.812	844	862	907	rBV	5534941	13237723	12.68%	8.591%
13	4.249	985	998	1027	rVB	121055	305913	0.29%	0.199%
14	4.777	1159	1162	1165	rVB2	257	190	0.00%	0.000%
15	4.957	1201	1218	1262	rBV2	297238	790679	0.76%	0.513%
16	5.211	1294	1297	1305	rBV3	476	485	0.00%	0.000%
17	5.416	1358	1361	1366	rVB2	361	253	0.00%	0.000%
18	5.532	1386	1397	1425	rBV	274545	558882	0.54%	0.363%
19	5.751	1462	1465	1466	rBV	371	213	0.00%	0.000%
20	5.834	1473	1491	1527	rBV	14962172	28682076	27.48%	18.615%
21	5.989	1530	1539	1586	rVB	182190	435671	0.42%	0.283%
22	6.397	1663	1666	1671	rVB4	483	284	0.00%	0.000%
23	6.420	1671	1673	1680	rVB3	286	202	0.00%	0.000%
24	6.449	1680	1682	1686	rVB	378	171	0.00%	0.000%
25	6.535	1707	1709	1713	rBV2	303	203	0.00%	0.000%
26	6.584	1720	1724	1725	rBV2	336	212	0.00%	0.000%
27	6.725	1762	1768	1771	rBV2	126	157	0.00%	0.000%
28	6.802	1785	1792	1795	rBV2	218	304	0.00%	0.000%
29	6.915	1816	1827	1854	rBV	96740	180452	0.17%	0.117%
30	7.143	1893	1898	1901	rBV3	341	341	0.00%	0.000%
31	7.243	1917	1929	1952	rBV	360186	629085	0.60%	0.408%
32	7.551	2012	2025	2049	rBV2	71882	133362	0.13%	0.087%
33	7.841	2110	2115	2120	rBV	222	275	0.00%	0.000%
34	7.931	2120	2143	2165	rBV	44368624	104359256	100.00%	67.731%
35	8.024	2166	2172	2211	rVB	250758	574614	0.55%	0.373%
36	8.336	2266	2269	2277	rVB6	1186	1337	0.00%	0.001%

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 Title : VOC Analysis

37	8.397	2286	2288	2291	rVB2	326	152	0.00%	0.000%
38	8.442	2296	2302	2305	rBV2	1175	1440	0.00%	0.001%
39	8.522	2324	2327	2328	rBV4	736	386	0.00%	0.000%
40	8.584	2340	2346	2348	rBV4	575	403	0.00%	0.000%
41	8.728	2385	2391	2398	rBV5	1282	2146	0.00%	0.001%
42	8.783	2398	2408	2433	rBV	395035	641681	0.61%	0.416%
43	8.960	2458	2463	2469	rVB6	1164	1385	0.00%	0.001%
44	9.082	2495	2501	2503	rBV5	1786	1796	0.00%	0.001%
45	9.127	2513	2515	2517	rVB	397	164	0.00%	0.000%
46	9.149	2517	2522	2524	rVB4	556	449	0.00%	0.000%
47	9.182	2529	2532	2533	rBV2	300	205	0.00%	0.000%
48	9.194	2533	2536	2542	rVB3	613	480	0.00%	0.000%
49	9.246	2550	2552	2558	rVB4	435	407	0.00%	0.000%
50	9.384	2590	2595	2596	rBV2	700	460	0.00%	0.000%
51	9.490	2621	2628	2635	rBV4	1945	2619	0.00%	0.002%
52	9.519	2635	2637	2643	rVB2	555	428	0.00%	0.000%
53	9.641	2661	2675	2682	rBV6	2023	3789	0.00%	0.002%
54	9.686	2686	2689	2692	rBV2	254	159	0.00%	0.000%
55	9.735	2697	2704	2712	rBV3	1987	2923	0.00%	0.002%
56	9.789	2712	2721	2723	rVV4	860	1181	0.00%	0.001%
57	9.850	2737	2740	2743	rBV	555	392	0.00%	0.000%
58	9.873	2743	2747	2753	rVB3	572	690	0.00%	0.000%
59	9.911	2756	2759	2763	rVV2	400	216	0.00%	0.000%
60	9.956	2769	2773	2776	rVB2	332	303	0.00%	0.000%
61	9.992	2776	2784	2787	rBV2	333	369	0.00%	0.000%
62	10.008	2787	2789	2792	rBV	271	168	0.00%	0.000%
63	10.059	2798	2805	2816	rVB4	1667	2159	0.00%	0.001%
64	10.153	2823	2834	2851	rBV	215290	347606	0.33%	0.226%
65	10.294	2872	2878	2879	rBV2	1042	737	0.00%	0.000%
66	10.391	2901	2908	2914	rBV7	3829	5574	0.01%	0.004%
67	10.439	2921	2923	2924	rBV	387	150	0.00%	0.000%
68	10.484	2931	2937	2949	rVB6	2120	3820	0.00%	0.002%
69	10.551	2952	2958	2965	rVB5	1190	1603	0.00%	0.001%
70	10.673	2985	2996	3006	rBV8	2633	5079	0.00%	0.003%
71	10.757	3020	3022	3024	rBV2	433	240	0.00%	0.000%
72	10.825	3040	3043	3044	rBV	508	242	0.00%	0.000%
73	10.857	3045	3053	3069	rVB	5713	9953	0.01%	0.006%
74	10.953	3080	3083	3084	rBV	384	247	0.00%	0.000%
75	10.998	3094	3097	3101	rBV2	547	478	0.00%	0.000%
76	11.088	3122	3125	3133	rVB4	652	699	0.00%	0.000%

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 Title : VOC Analysis

77	11.133	3137	3139	3142	rBV2	299	149	0.00%	0.000%
78	11.185	3144	3155	3177	rBV	454961	695997	0.67%	0.452%
79	11.352	3204	3207	3208	rBV2	313	219	0.00%	0.000%
80	11.464	3238	3242	3244	rBV3	457	442	0.00%	0.000%
81	11.480	3244	3247	3256	rVB4	880	1105	0.00%	0.001%
82	11.561	3260	3272	3296	rBV	388039	607396	0.58%	0.394%
83	11.734	3322	3326	3328	rBV2	170	152	0.00%	0.000%
84	11.853	3360	3363	3368	rBV	225	213	0.00%	0.000%
85	11.963	3389	3397	3400	rBV3	444	541	0.00%	0.000%
86	11.998	3407	3408	3414	rVB	352	186	0.00%	0.000%
87	12.027	3414	3417	3420	rBV	213	163	0.00%	0.000%
88	12.046	3420	3423	3426	rBV2	403	361	0.00%	0.000%
89	12.101	3437	3440	3442	rBV2	232	169	0.00%	0.000%
90	12.243	3476	3484	3488	rBV2	384	494	0.00%	0.000%
91	12.352	3515	3518	3521	rBV2	181	162	0.00%	0.000%
92	12.824	3660	3665	3672	rVB2	348	520	0.00%	0.000%
93	13.448	3855	3859	3861	rBV3	395	302	0.00%	0.000%
94	13.702	3935	3938	3941	rVB2	278	175	0.00%	0.000%
95	13.728	3942	3946	3949	rBV2	166	151	0.00%	0.000%
96	14.078	4051	4055	4057	rBV	256	196	0.00%	0.000%
97	14.387	4146	4151	4154	rBV3	211	249	0.00%	0.000%
98	14.426	4160	4163	4166	rBV	219	162	0.00%	0.000%
99	14.988	4336	4338	4342	rVB2	282	176	0.00%	0.000%
100	15.467	4482	4487	4489	rBV4	455	484	0.00%	0.000%

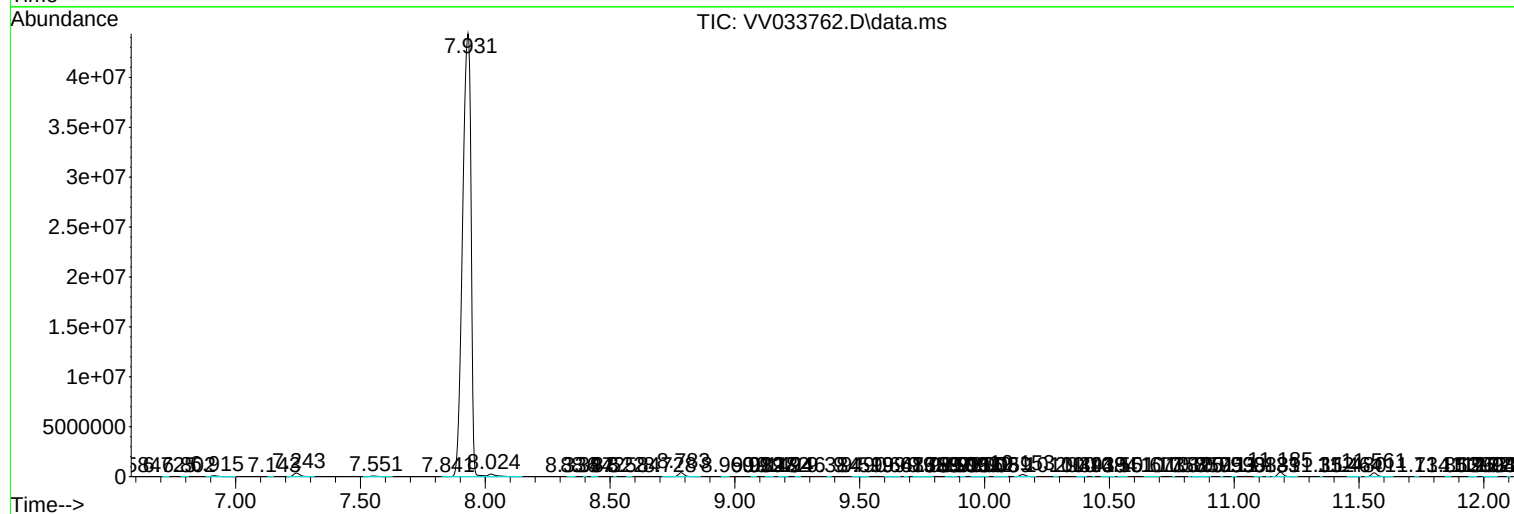
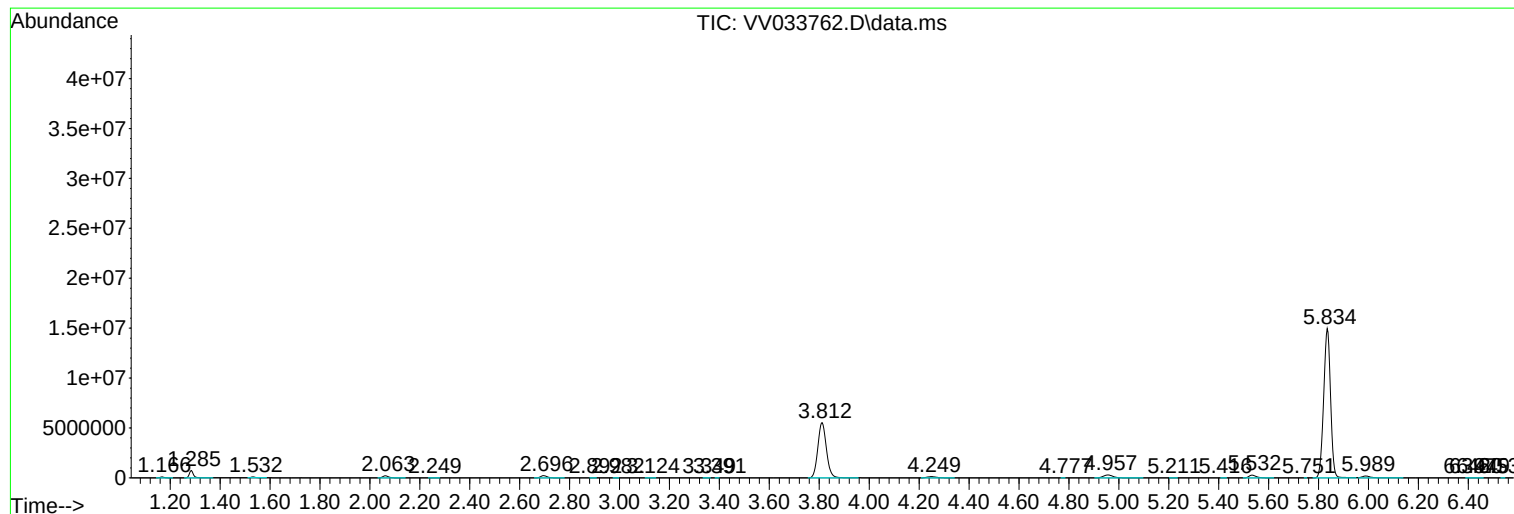
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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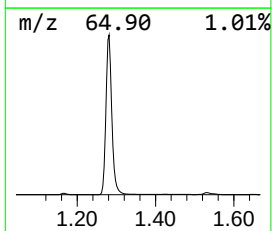
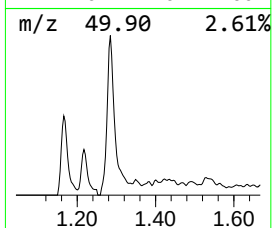
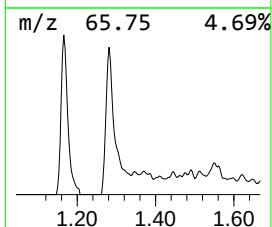
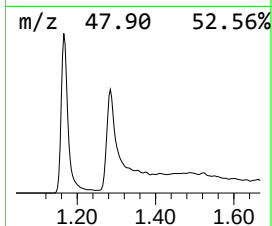
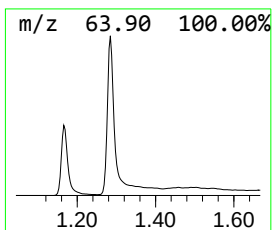
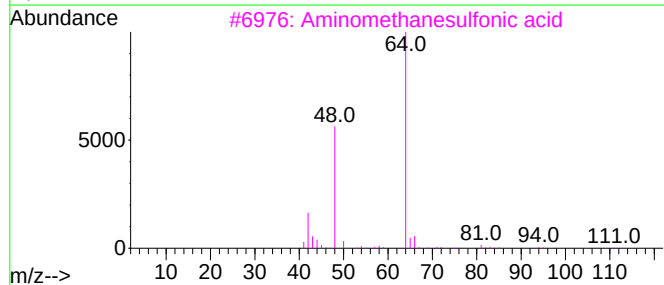
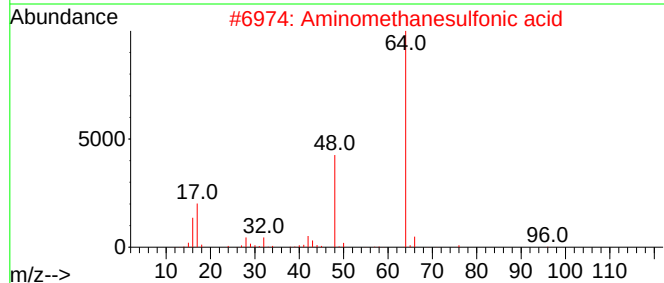
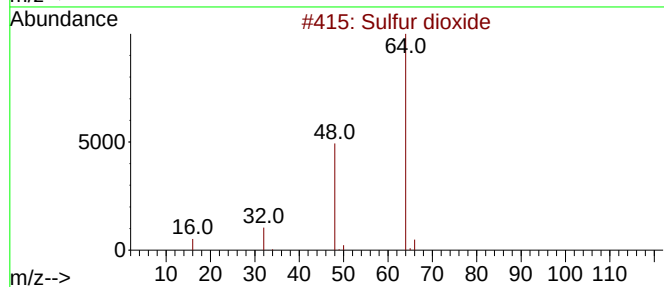
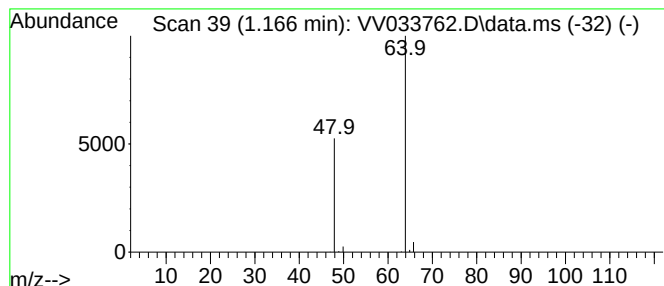
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	10.27 ug/L	114742	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			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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	10.3	ug/L	114742	1	5.535	558882	50.0