

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082624\
 Data File : VV037059.D
 Acq On : 27 Aug 2024 03:35
 Operator : SY/MD
 Sample : P3691-14
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K59

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\SFAMVLM082624WMA.M
 Title : VOC Analysis

Signal : TIC: VV037059.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.175	35	42	46	rBV	95981	134155	5.70%	0.783%
2	1.278	68	74	91	rVB2	338208	384836	16.34%	2.245%
3	1.532	146	153	171	rVB	258632	321279	13.64%	1.874%
4	2.056	307	316	329	rBV	524734	753494	32.00%	4.395%
5	3.471	751	756	758	rBV6	879	773	0.03%	0.005%
6	3.519	766	771	773	rBV5	1535	1141	0.05%	0.007%
7	3.561	781	784	787	rVB4	1571	1040	0.04%	0.006%
8	3.802	847	859	897	rBV2	191910	582432	24.73%	3.397%
9	4.243	978	996	1031	rBV	377715	947104	40.22%	5.524%
10	4.442	1055	1058	1063	rVB6	1740	1094	0.05%	0.006%
11	4.474	1063	1068	1072	rBV8	1594	1570	0.07%	0.009%
12	4.497	1072	1075	1078	rBV4	1085	911	0.04%	0.005%
13	4.558	1090	1094	1096	rBV5	1014	693	0.03%	0.004%
14	4.841	1178	1182	1184	rBV3	814	682	0.03%	0.004%
15	4.867	1187	1190	1193	rVB4	1460	901	0.04%	0.005%
16	4.886	1193	1196	1199	rBV5	1348	1305	0.06%	0.008%
17	4.950	1199	1216	1250	rBV2	923210	2354968	100.00%	13.736%
18	5.339	1334	1337	1339	rBV3	1618	945	0.04%	0.006%
19	5.404	1353	1357	1359	rBV4	2493	1831	0.08%	0.011%
20	5.529	1384	1396	1432	rBV	602288	1259381	53.48%	7.346%
21	5.802	1478	1481	1483	rBV5	1742	1149	0.05%	0.007%
22	5.828	1483	1489	1499	rVV5	3954	7344	0.31%	0.043%
23	5.986	1525	1538	1568	rBV	519510	1074902	45.64%	6.270%
24	6.294	1630	1634	1636	rBV5	1012	709	0.03%	0.004%
25	6.307	1636	1638	1641	rVB4	1630	780	0.03%	0.005%
26	6.429	1672	1676	1678	rVV4	1933	1028	0.04%	0.006%
27	6.616	1732	1734	1738	rVB5	1657	794	0.03%	0.005%
28	6.645	1741	1743	1745	rBV2	1352	736	0.03%	0.004%
29	6.741	1769	1773	1776	rBV6	1428	1137	0.05%	0.007%
30	6.912	1814	1826	1856	rBV	243582	469437	19.93%	2.738%
31	7.143	1893	1898	1899	rBV4	1701	1307	0.06%	0.008%
32	7.240	1916	1928	1951	rBV	1007067	1795644	76.25%	10.474%
33	7.551	2014	2025	2048	rBV	156573	292455	12.42%	1.706%
34	7.690	2066	2068	2073	rBV5	1137	912	0.04%	0.005%
35	7.937	2142	2145	2148	rVB5	1987	1225	0.05%	0.007%
36	8.024	2163	2172	2211	rBV	407938	835530	35.48%	4.874%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

37	8.362	2274	2277	2279	rBV4	1728	1071	0.05%	0.006%
38	8.564	2339	2340	2347	rVB7	1475	1279	0.05%	0.007%
39	8.638	2358	2363	2366	rBV5	1816	1792	0.08%	0.010%
40	8.780	2396	2407	2430	rVV	957863	1568498	66.60%	9.149%
41	9.169	2524	2528	2530	rBV5	1834	1404	0.06%	0.008%
42	9.211	2538	2541	2545	rBV6	1363	1003	0.04%	0.006%
43	9.365	2587	2589	2597	rVB8	2134	2039	0.09%	0.012%
44	9.452	2612	2616	2619	rBV6	944	703	0.03%	0.004%
45	9.481	2620	2625	2628	rBV6	2221	2222	0.09%	0.013%
46	9.667	2681	2683	2688	rBV5	1125	1004	0.04%	0.006%
47	9.719	2695	2699	2701	rBV5	1576	982	0.04%	0.006%
48	9.738	2701	2705	2707	rBV4	1146	899	0.04%	0.005%
49	9.776	2714	2717	2718	rBV2	1297	777	0.03%	0.005%
50	10.040	2797	2799	2802	rBV5	1869	1086	0.05%	0.006%
51	10.059	2802	2805	2807	rBV5	823	683	0.03%	0.004%
52	10.085	2810	2813	2817	rBV4	1410	864	0.04%	0.005%
53	10.146	2819	2832	2849	rBV	683991	1087481	46.18%	6.343%
54	10.275	2870	2872	2877	rVB5	1639	1222	0.05%	0.007%
55	10.538	2950	2954	2957	rBV5	1223	894	0.04%	0.005%
56	10.600	2970	2973	2975	rBV4	2635	1939	0.08%	0.011%
57	10.612	2975	2977	2979	rBV3	1593	856	0.04%	0.005%
58	10.635	2982	2984	2986	rVB3	1465	749	0.03%	0.004%
59	10.651	2986	2989	2992	rBV5	1238	754	0.03%	0.004%
60	10.882	3057	3061	3064	rBV6	1281	852	0.04%	0.005%
61	10.908	3067	3069	3076	rVB6	1579	1099	0.05%	0.006%
62	11.018	3099	3103	3106	rVB4	1366	993	0.04%	0.006%
63	11.114	3126	3133	3136	rBV9	2799	3799	0.16%	0.022%
64	11.182	3143	3154	3176	rBV	957804	1518598	64.48%	8.858%
65	11.503	3250	3254	3256	rBV4	1671	1364	0.06%	0.008%
66	11.554	3259	3270	3303	rVV	1028002	1658092	70.41%	9.672%
67	11.837	3355	3358	3361	rBV4	2099	1505	0.06%	0.009%
68	12.014	3410	3413	3414	rVV3	1711	814	0.03%	0.005%
69	12.140	3449	3452	3457	rBV6	1703	1984	0.08%	0.012%
70	12.210	3472	3474	3477	rVB3	1597	780	0.03%	0.005%
71	12.239	3477	3483	3484	rBV4	1760	1515	0.06%	0.009%
72	12.329	3507	3511	3512	rBV4	1534	1279	0.05%	0.007%
73	12.390	3528	3530	3534	rVB5	1889	1126	0.05%	0.007%
74	12.416	3534	3538	3541	rBV5	1050	793	0.03%	0.005%
75	12.577	3585	3588	3591	rBV5	1697	1441	0.06%	0.008%
76	12.670	3614	3617	3622	rBV6	2177	2165	0.09%	0.013%

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 Title : VOC Analysis

77	12.744	3636	3640	3644	rBV6	2268	1912	0.08%	0.011%
78	12.818	3659	3663	3666	rBV6	1167	1043	0.04%	0.006%
79	12.898	3686	3688	3693	rVB5	1848	1342	0.06%	0.008%
80	13.095	3747	3749	3753	rBV6	1247	932	0.04%	0.005%
81	13.210	3778	3785	3790	rVB10	2215	2857	0.12%	0.017%
82	13.236	3790	3793	3796	rBV5	1119	989	0.04%	0.006%
83	13.323	3816	3820	3822	rBV4	1245	891	0.04%	0.005%
84	13.365	3830	3833	3838	rVB5	1406	1211	0.05%	0.007%
85	13.464	3861	3864	3868	rVV5	1829	1436	0.06%	0.008%
86	13.644	3916	3920	3921	rBV4	1041	820	0.03%	0.005%
87	13.805	3967	3970	3972	rBV5	1704	1189	0.05%	0.007%
88	13.931	4006	4009	4012	rVB4	1318	790	0.03%	0.005%
89	13.969	4018	4021	4028	rVB8	1734	1391	0.06%	0.008%
90	14.043	4041	4044	4046	rBV3	2380	1487	0.06%	0.009%
91	14.095	4057	4060	4063	rBV5	1394	894	0.04%	0.005%
92	14.191	4087	4090	4094	rBV5	1962	1684	0.07%	0.010%
93	14.313	4125	4128	4129	rBV2	1366	876	0.04%	0.005%
94	14.371	4144	4146	4150	rVB4	1555	997	0.04%	0.006%
95	14.632	4224	4227	4228	rBV2	1327	856	0.04%	0.005%
96	14.722	4252	4255	4258	rBV4	1367	1165	0.05%	0.007%
97	14.892	4306	4308	4312	rBV4	1603	1032	0.04%	0.006%
98	14.943	4322	4324	4327	rBV4	1533	1127	0.05%	0.007%
99	15.085	4365	4368	4369	rBV3	1638	917	0.04%	0.005%
100	15.786	4581	4586	4587	rBV4	2163	2063	0.09%	0.012%

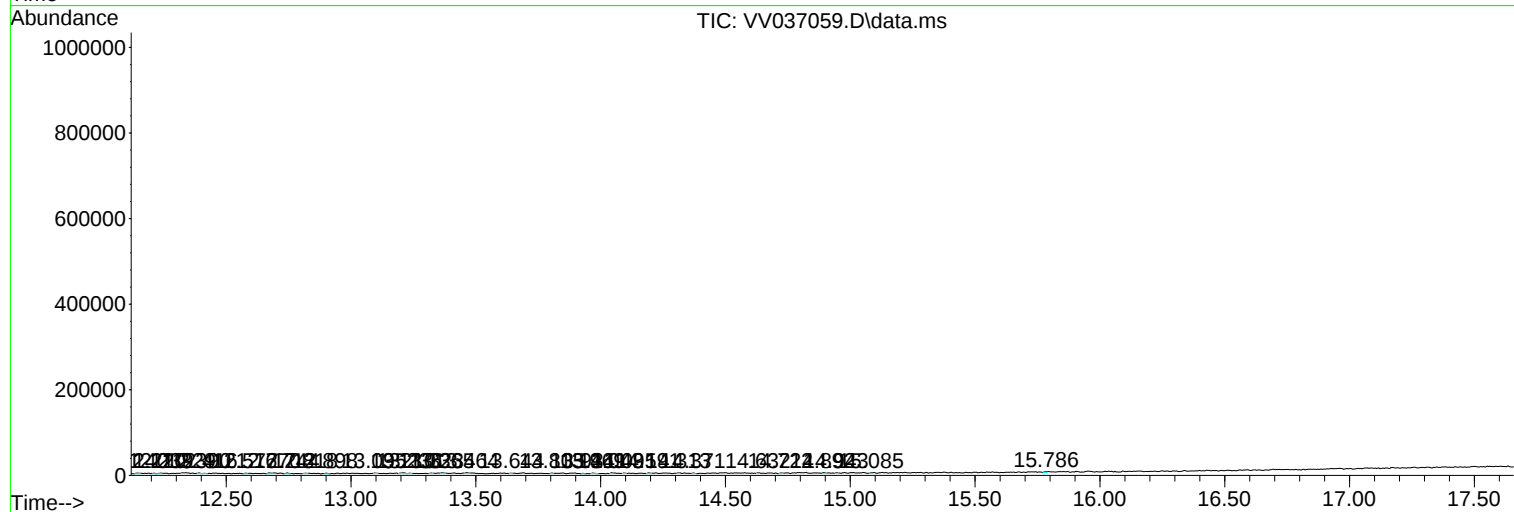
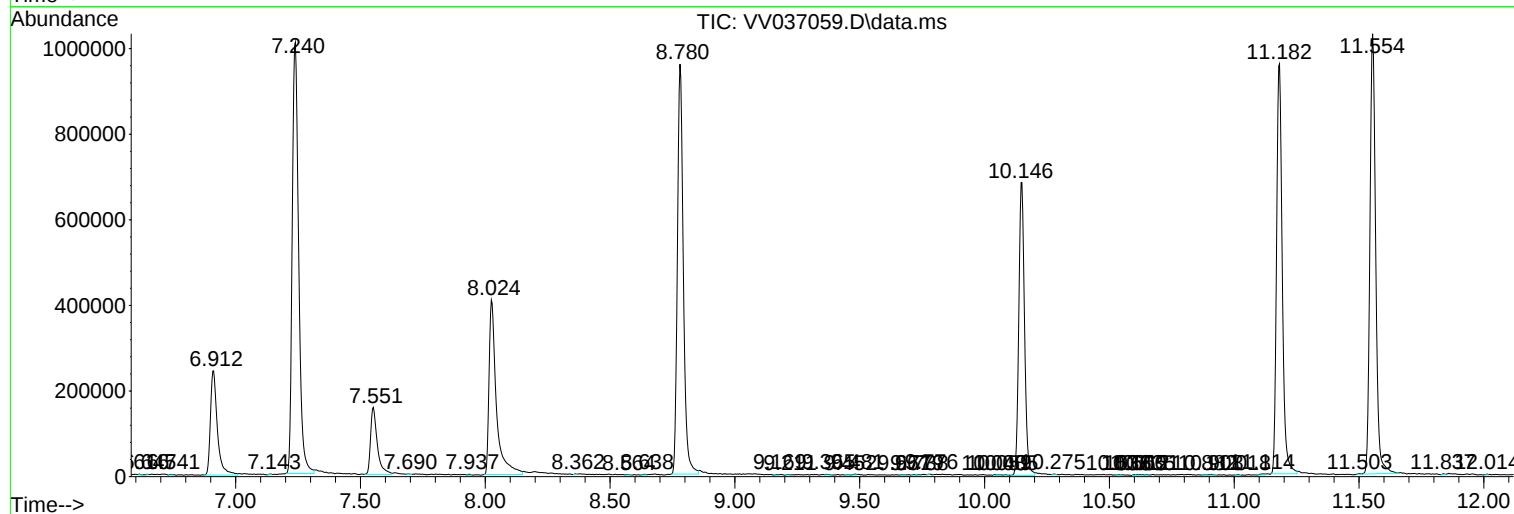
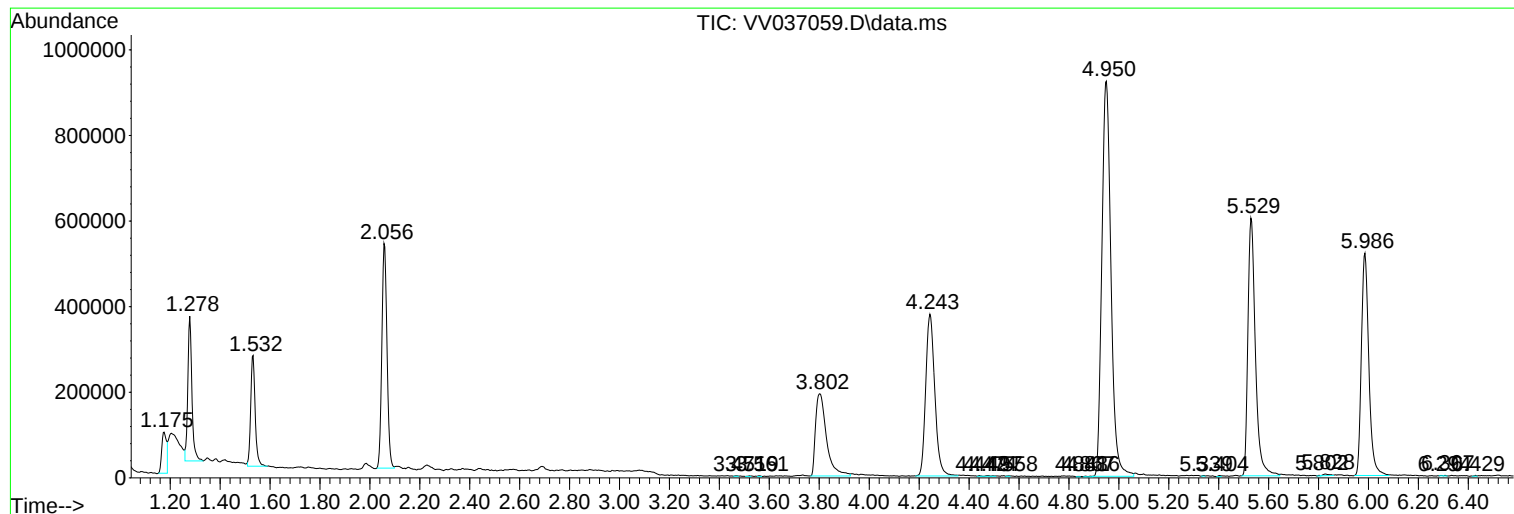
Sum of corrected areas: 17143925

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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



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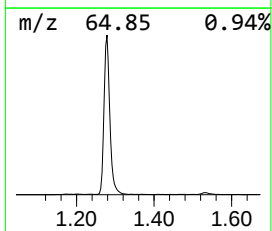
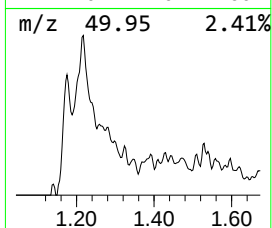
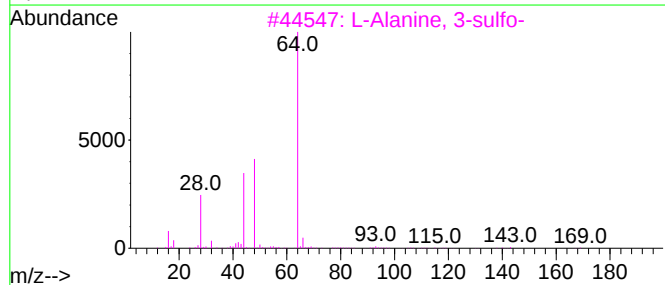
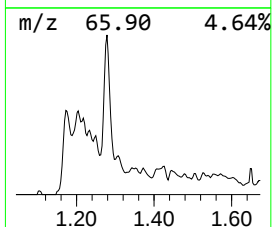
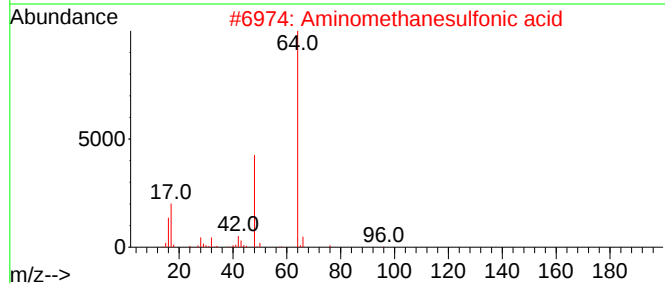
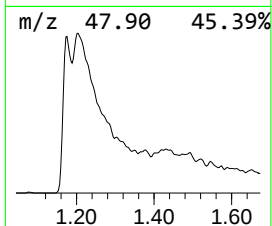
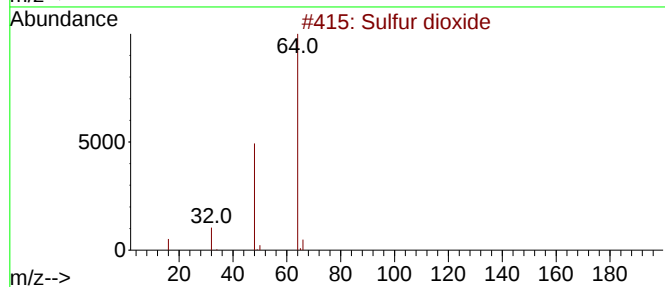
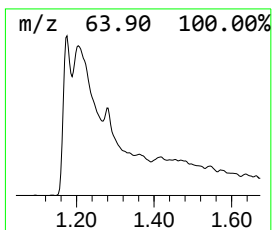
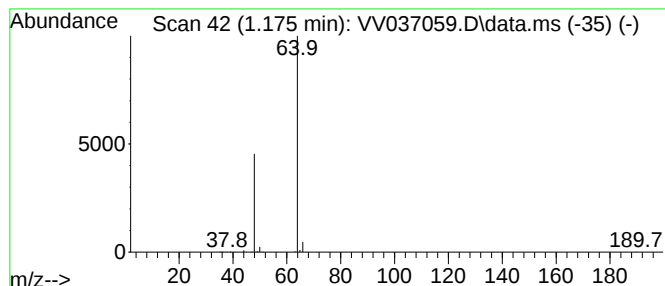
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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.
1.175	5.33 ug/L	134155	1,4-Difluorobenzene	5.529

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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.175	5.3	ug/L	134155	1	5.529	1259380	50.0