

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037080.D
 Acq On : 27 Aug 2024 13:03
 Operator : SY/MD
 Sample : P3691-15DL 200X
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K61DL

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: VV037080.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	35	41	53	rBV	53432	94816	4.03%	0.506%
2	1.282	68	75	89	rVB2	594256	665293	28.31%	3.552%
3	1.532	146	153	171	rVB	272856	323541	13.77%	1.727%
4	2.056	308	316	333	rVB	556904	803206	34.18%	4.288%
5	3.490	757	762	768	rBV8	1185	1745	0.07%	0.009%
6	3.642	807	809	812	rBV4	1032	810	0.03%	0.004%
7	3.687	820	823	826	rBV4	1369	971	0.04%	0.005%
8	3.722	830	834	838	rVB6	1102	793	0.03%	0.004%
9	3.744	838	841	843	rBV2	763	477	0.02%	0.003%
10	3.806	846	860	893	rBV2	534615	1400732	59.60%	7.478%
11	4.243	982	996	1022	rBV2	370900	930087	39.58%	4.965%
12	4.561	1092	1095	1096	rBV3	1289	590	0.03%	0.003%
13	4.629	1114	1116	1120	rVB6	1413	788	0.03%	0.004%
14	4.809	1170	1172	1174	rBV3	1266	534	0.02%	0.003%
15	4.841	1178	1182	1184	rBV6	1007	594	0.03%	0.003%
16	4.870	1188	1191	1194	rBV4	1111	784	0.03%	0.004%
17	4.950	1201	1216	1246	rBV2	941472	2350078	100.00%	12.546%
18	5.310	1326	1328	1330	rBV3	1076	489	0.02%	0.003%
19	5.384	1347	1351	1352	rBV4	1089	591	0.03%	0.003%
20	5.413	1357	1360	1366	rVB7	2203	2292	0.10%	0.012%
21	5.439	1366	1368	1372	rBV4	1309	989	0.04%	0.005%
22	5.529	1385	1396	1427	rBV	690759	1406529	59.85%	7.509%
23	5.985	1526	1538	1565	rBV	526607	1084437	46.14%	5.790%
24	6.297	1633	1635	1638	rBV4	1211	704	0.03%	0.004%
25	6.365	1654	1656	1661	rVB5	1792	1318	0.06%	0.007%
26	6.391	1661	1664	1666	rBV3	1135	827	0.04%	0.004%
27	6.542	1710	1711	1715	rVB4	1034	578	0.02%	0.003%
28	6.564	1715	1718	1721	rBV4	1115	809	0.03%	0.004%
29	6.619	1732	1735	1738	rBV5	1788	1217	0.05%	0.006%
30	6.818	1793	1797	1800	rBV4	1287	1033	0.04%	0.006%
31	6.912	1816	1826	1857	rBV	257704	505234	21.50%	2.697%
32	7.239	1917	1928	1957	rBV	1046325	1859990	79.15%	9.930%
33	7.551	2016	2025	2046	rBV	170758	311561	13.26%	1.663%
34	7.931	2141	2143	2146	rVB3	1555	888	0.04%	0.005%
35	8.024	2163	2172	2207	rBV	388465	798040	33.96%	4.261%
36	8.516	2323	2325	2326	rBV3	1436	508	0.02%	0.003%

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 Title : VOC Analysis

37	8.725	2384	2390	2392	rBV6	1605	1757	0.07%	0.009%
38	8.780	2396	2407	2439	rVV	1059472	1747296	74.35%	9.328%
39	9.136	2515	2518	2519	rBV3	963	500	0.02%	0.003%
40	9.352	2583	2585	2589	rVB4	1265	778	0.03%	0.004%
41	9.374	2589	2592	2593	rBV3	973	592	0.03%	0.003%
42	9.551	2643	2647	2649	rBV4	1088	768	0.03%	0.004%
43	9.686	2685	2689	2693	rBV5	1232	1098	0.05%	0.006%
44	9.760	2710	2712	2716	rVB5	1228	832	0.04%	0.004%
45	9.828	2731	2733	2736	rVB3	1150	699	0.03%	0.004%
46	9.847	2736	2739	2741	rBV4	1040	652	0.03%	0.003%
47	9.895	2751	2754	2756	rBV3	978	579	0.02%	0.003%
48	9.915	2758	2760	2762	rVB3	1113	483	0.02%	0.003%
49	9.979	2776	2780	2783	rBV5	1024	964	0.04%	0.005%
50	10.030	2792	2796	2798	rBV4	1178	747	0.03%	0.004%
51	10.043	2798	2800	2802	rVB3	1081	525	0.02%	0.003%
52	10.149	2821	2833	2851	rBV	658363	1043872	44.42%	5.573%
53	10.284	2872	2875	2880	rVB6	1923	1775	0.08%	0.009%
54	10.310	2880	2883	2885	rBV2	829	538	0.02%	0.003%
55	10.378	2898	2904	2905	rBV6	1482	1442	0.06%	0.008%
56	10.574	2962	2965	2967	rBV3	1064	618	0.03%	0.003%
57	10.632	2979	2983	2984	rBV3	740	550	0.02%	0.003%
58	10.677	2994	2997	3000	rBV5	1524	1043	0.04%	0.006%
59	10.728	3008	3013	3015	rBV5	889	644	0.03%	0.003%
60	10.754	3015	3021	3025	rBV8	1982	2025	0.09%	0.011%
61	10.776	3025	3028	3029	rBV3	1229	623	0.03%	0.003%
62	10.847	3047	3050	3053	rBV4	1055	714	0.03%	0.004%
63	10.921	3069	3073	3077	rVB7	1433	1435	0.06%	0.008%
64	10.950	3077	3082	3085	rBV4	1814	1356	0.06%	0.007%
65	11.098	3126	3128	3130	rBV3	1280	556	0.02%	0.003%
66	11.120	3131	3135	3136	rBV4	2160	1184	0.05%	0.006%
67	11.181	3143	3154	3183	rBV	1040631	1659698	70.62%	8.861%
68	11.464	3238	3242	3243	rBV4	1240	693	0.03%	0.004%
69	11.554	3259	3270	3302	rBV	1059186	1674484	71.25%	8.940%
70	11.873	3368	3369	3371	rBV2	1134	527	0.02%	0.003%
71	11.982	3400	3403	3405	rBV5	1397	912	0.04%	0.005%
72	12.053	3422	3425	3427	rVB4	1680	883	0.04%	0.005%
73	12.069	3427	3430	3431	rBV3	965	606	0.03%	0.003%
74	12.152	3452	3456	3457	rBV4	693	487	0.02%	0.003%
75	12.181	3463	3465	3468	rVB3	1240	655	0.03%	0.003%
76	12.284	3493	3497	3498	rBV3	985	599	0.03%	0.003%

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

77	12.294	3498	3500	3503	rVB3	1134	616	0.03%	0.003%
78	12.368	3518	3523	3526	rVB5	1415	869	0.04%	0.005%
79	12.397	3529	3532	3536	rVB5	1676	1185	0.05%	0.006%
80	12.496	3560	3563	3565	rBV4	776	568	0.02%	0.003%
81	12.542	3573	3577	3579	rBV4	1259	994	0.04%	0.005%
82	12.725	3632	3634	3635	rBV	958	473	0.02%	0.003%
83	12.754	3640	3643	3644	rBV3	929	451	0.02%	0.002%
84	12.886	3682	3684	3686	rVB2	1015	547	0.02%	0.003%
85	12.902	3686	3689	3692	rBV4	636	495	0.02%	0.003%
86	12.947	3701	3703	3707	rVB4	1194	897	0.04%	0.005%
87	12.969	3707	3710	3711	rBV3	1032	707	0.03%	0.004%
88	13.091	3745	3748	3751	rBV4	1057	674	0.03%	0.004%
89	13.152	3761	3767	3769	rBV6	1572	1166	0.05%	0.006%
90	13.165	3769	3771	3773	rBV2	1281	736	0.03%	0.004%
91	13.287	3807	3809	3810	rBV2	1189	449	0.02%	0.002%
92	13.336	3821	3824	3827	rVB6	1617	843	0.04%	0.005%
93	13.448	3857	3859	3864	rBV6	1761	1194	0.05%	0.006%
94	13.570	3892	3897	3899	rBV5	1419	1114	0.05%	0.006%
95	13.834	3976	3979	3983	rBV4	1165	928	0.04%	0.005%
96	13.885	3992	3995	3997	rBV5	1703	1391	0.06%	0.007%
97	14.072	4050	4053	4055	rBV4	1187	582	0.02%	0.003%
98	14.268	4109	4114	4117	rBV5	1877	1448	0.06%	0.008%
99	14.902	4308	4311	4314	rBV4	1627	1288	0.05%	0.007%
100	14.982	4334	4336	4342	rBV7	1809	1361	0.06%	0.007%

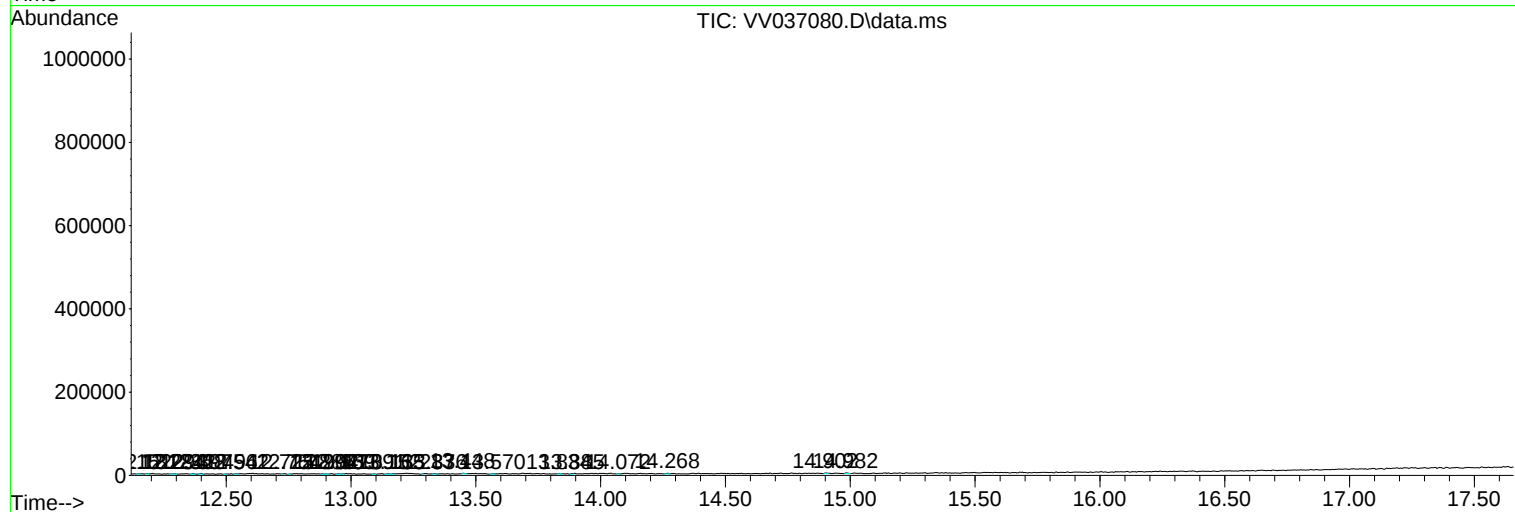
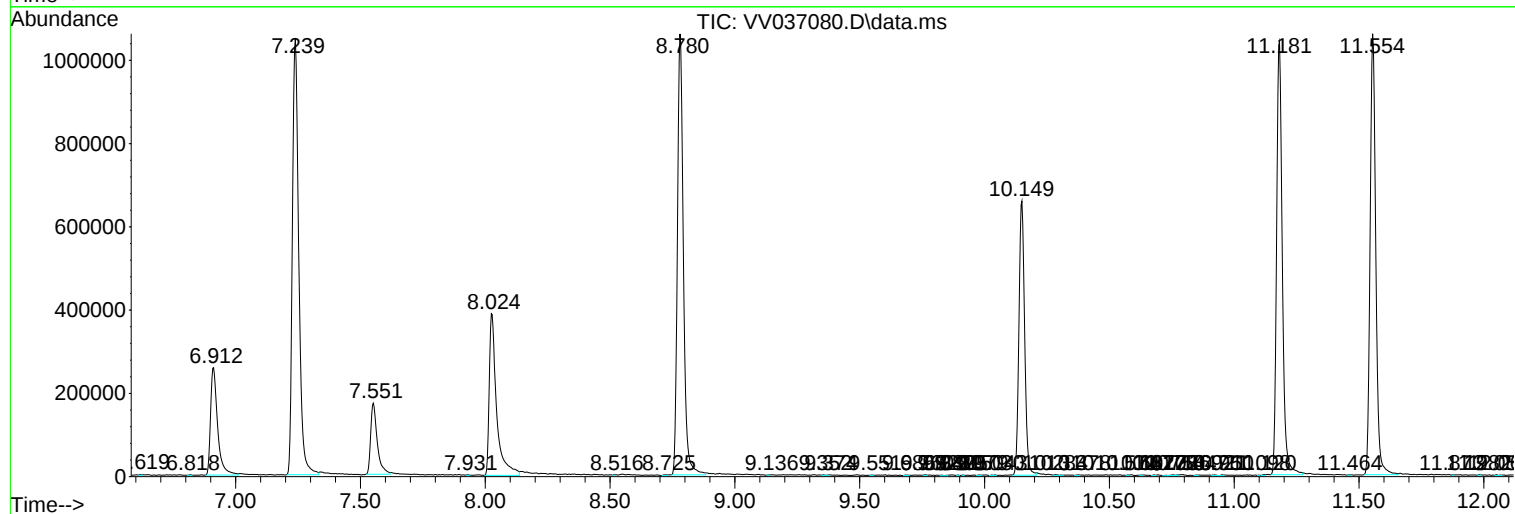
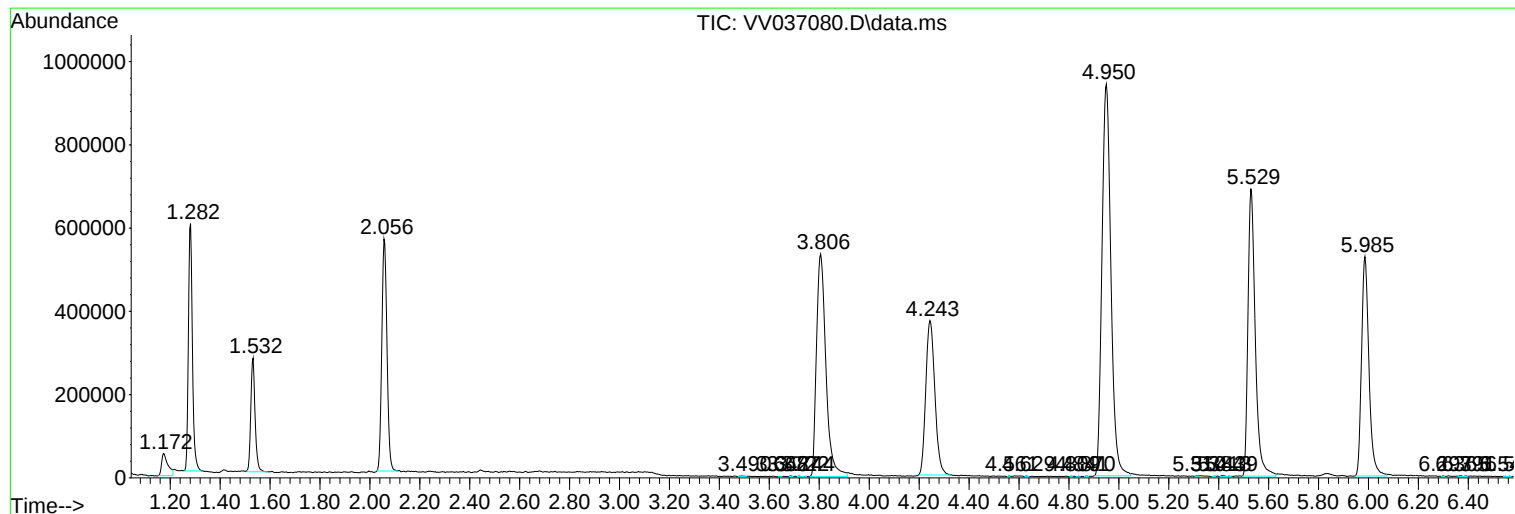
Sum of corrected areas: 18731038

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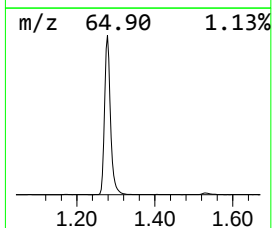
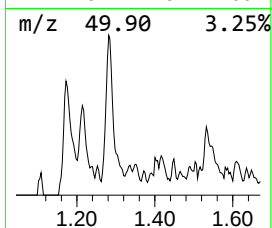
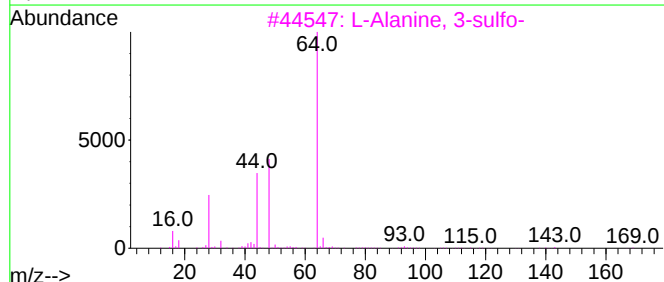
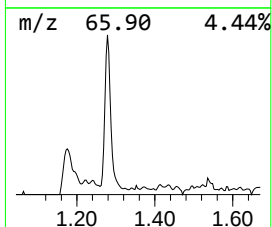
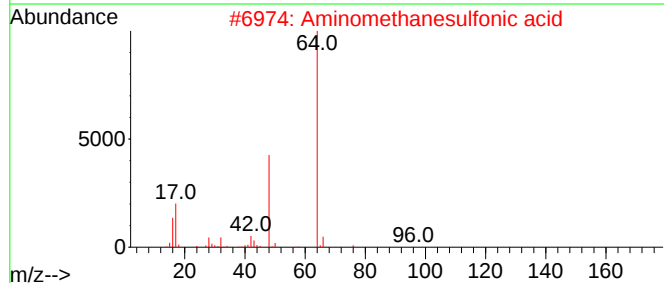
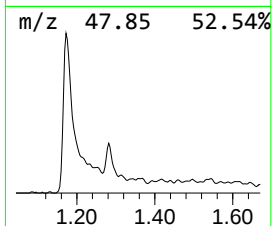
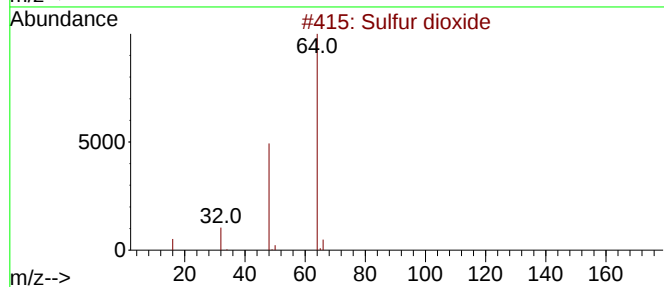
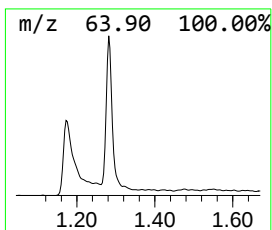
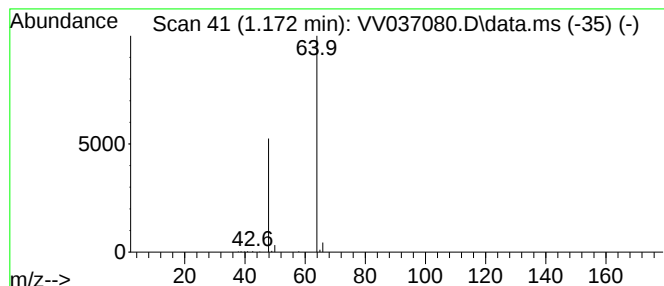
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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.
1.172	3.37 ug/L	94816	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.172	3.4	ug/L	94816	1	5.529	1406530	50.0