

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037071.D
 Acq On : 27 Aug 2024 09:37
 Operator : SY/MD
 Sample : P3691-17
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K68

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: VV037071.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	34	41	59	rBV	103319	180202	8.58%	1.146%
2	1.278	68	74	88	rVB	279647	294560	14.02%	1.873%
3	1.529	146	152	166	rVB	238841	284051	13.52%	1.806%
4	2.056	307	316	329	rBV	498241	713334	33.96%	4.536%
5	3.497	760	764	766	rBV4	1016	810	0.04%	0.005%
6	3.648	807	811	813	rBV3	1257	870	0.04%	0.006%
7	3.670	817	818	819	rBV	957	295	0.01%	0.002%
8	3.696	823	826	827	rBV3	1059	666	0.03%	0.004%
9	3.793	847	856	884	rBV	108131	310044	14.76%	1.971%
10	4.088	946	948	949	rBV	869	250	0.01%	0.002%
11	4.240	979	995	1027	rBV	333101	842233	40.10%	5.355%
12	4.477	1065	1069	1070	rBV2	1253	898	0.04%	0.006%
13	4.603	1106	1108	1112	rVB3	1703	889	0.04%	0.006%
14	4.622	1112	1114	1117	rVB3	696	336	0.02%	0.002%
15	4.645	1117	1121	1122	rBV3	1031	644	0.03%	0.004%
16	4.677	1126	1131	1136	rBV8	2053	1857	0.09%	0.012%
17	4.728	1145	1147	1149	rVB3	580	188	0.01%	0.001%
18	4.799	1167	1169	1171	rBV3	719	301	0.01%	0.002%
19	4.844	1181	1183	1185	rBV3	879	425	0.02%	0.003%
20	4.879	1193	1194	1199	rVB5	1195	792	0.04%	0.005%
21	4.947	1199	1215	1247	rBV2	823672	2100366	100.00%	13.355%
22	5.400	1349	1356	1358	rBV6	1756	1899	0.09%	0.012%
23	5.471	1375	1378	1380	rBV3	983	668	0.03%	0.004%
24	5.526	1384	1395	1428	rBV	643565	1331439	63.39%	8.466%
25	5.738	1458	1461	1463	rBV3	2123	1162	0.06%	0.007%
26	5.982	1525	1537	1562	rBV	458627	940234	44.77%	5.978%
27	6.375	1657	1659	1662	rVB3	1318	511	0.02%	0.003%
28	6.526	1702	1706	1709	rBV6	1545	1661	0.08%	0.011%
29	6.638	1738	1741	1747	rBV7	1229	1227	0.06%	0.008%
30	6.677	1752	1753	1755	rBV2	789	335	0.02%	0.002%
31	6.757	1776	1778	1779	rBV2	1212	505	0.02%	0.003%
32	6.802	1790	1792	1794	rBV4	552	376	0.02%	0.002%
33	6.841	1799	1804	1806	rBV6	687	507	0.02%	0.003%
34	6.857	1807	1809	1812	rBV4	627	291	0.01%	0.002%
35	6.908	1815	1825	1852	rBV	235992	455712	21.70%	2.898%
36	7.236	1915	1927	1949	rBV	929997	1638864	78.03%	10.420%

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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

37	7.551	2016	2025	2049	rBV	152572	284545	13.55%	1.809%
38	7.940	2143	2146	2149	rVB4	1340	871	0.04%	0.006%
39	7.956	2149	2151	2153	rBV3	1439	766	0.04%	0.005%
40	8.024	2164	2172	2214	rBV	288114	626617	29.83%	3.984%
41	8.780	2394	2407	2429	rBV	1005602	1663599	79.21%	10.578%
42	9.236	2547	2549	2552	rVB4	1057	433	0.02%	0.003%
43	9.278	2559	2562	2565	rBV5	1287	1034	0.05%	0.007%
44	9.487	2624	2627	2628	rBV3	1313	658	0.03%	0.004%
45	9.927	2762	2764	2767	rBV3	981	502	0.02%	0.003%
46	10.005	2786	2788	2790	rBV3	1128	673	0.03%	0.004%
47	10.072	2805	2809	2810	rBV4	1270	893	0.04%	0.006%
48	10.146	2821	2832	2847	rBV	550236	875050	41.66%	5.564%
49	10.300	2879	2880	2888	rVB7	1280	748	0.04%	0.005%
50	10.445	2923	2925	2927	rBV3	1171	571	0.03%	0.004%
51	10.484	2934	2937	2940	rBV4	1131	809	0.04%	0.005%
52	10.548	2953	2957	2959	rBV5	1406	992	0.05%	0.006%
53	10.619	2975	2979	2981	rBV5	1621	1149	0.05%	0.007%
54	10.696	2999	3003	3004	rBV4	1595	1048	0.05%	0.007%
55	10.770	3023	3026	3028	rBV3	838	625	0.03%	0.004%
56	10.934	3075	3077	3079	rVV3	683	261	0.01%	0.002%
57	10.956	3082	3084	3086	rBV2	858	365	0.02%	0.002%
58	11.027	3102	3106	3108	rBV3	981	678	0.03%	0.004%
59	11.040	3108	3110	3112	rBV3	717	402	0.02%	0.003%
60	11.178	3143	3153	3187	rBV	1007909	1631846	77.69%	10.376%
61	11.442	3232	3235	3237	rBV3	1098	679	0.03%	0.004%
62	11.487	3247	3249	3250	rBV2	944	366	0.02%	0.002%
63	11.554	3259	3270	3295	rBV	935335	1498608	71.35%	9.529%
64	11.950	3390	3393	3395	rBV3	1289	909	0.04%	0.006%
65	12.316	3501	3507	3510	rBV7	2104	2503	0.12%	0.016%
66	12.413	3534	3537	3540	rBV3	2088	1400	0.07%	0.009%
67	12.490	3560	3561	3562	rBV	1056	360	0.02%	0.002%
68	12.657	3610	3613	3614	rBV2	1321	724	0.03%	0.005%
69	12.744	3637	3640	3642	rBV3	1781	1261	0.06%	0.008%
70	12.860	3673	3676	3679	rBV5	1834	1200	0.06%	0.008%
71	12.943	3698	3702	3704	rBV3	831	545	0.03%	0.003%
72	12.963	3706	3708	3711	rBV4	736	522	0.02%	0.003%
73	13.146	3763	3765	3766	rBV2	1052	369	0.02%	0.002%
74	13.210	3775	3785	3789	rBV9	5048	8814	0.42%	0.056%
75	13.509	3876	3878	3881	rBV3	1600	1133	0.05%	0.007%
76	13.850	3981	3984	3987	rBV4	1073	1034	0.05%	0.007%

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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

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Peak separation: 5

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

77	14.014	4031	4035	4039	rBV8	1657	1184	0.06%	0.008%
78	14.683	4239	4243	4245	rBV5	1656	1333	0.06%	0.008%

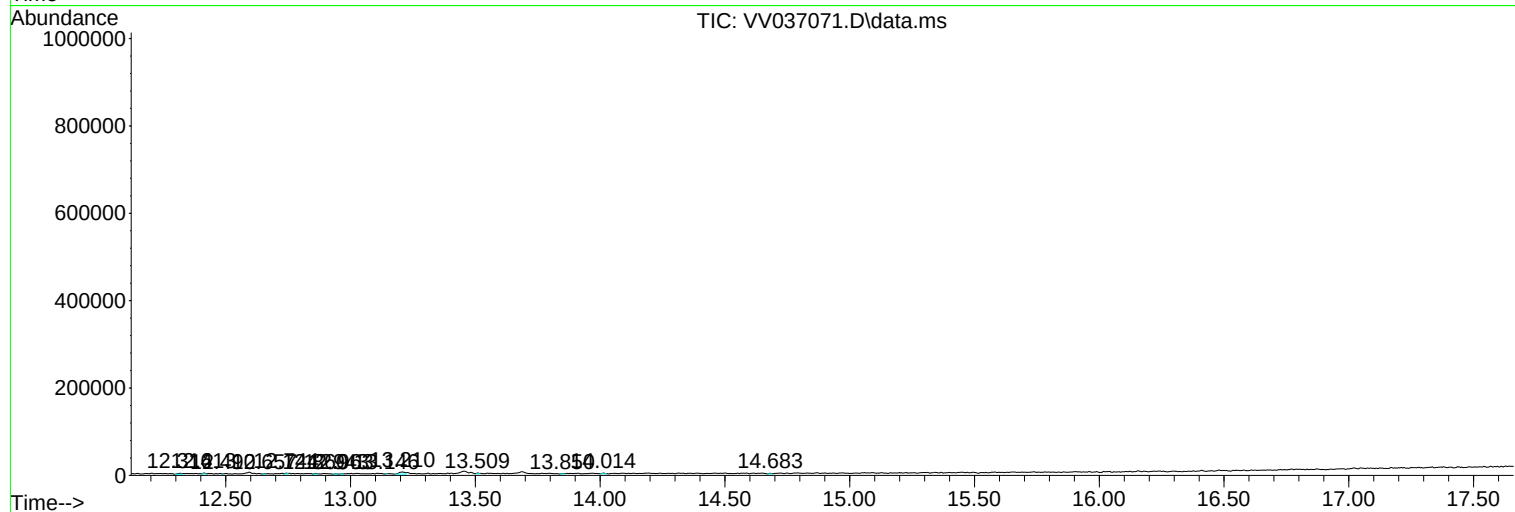
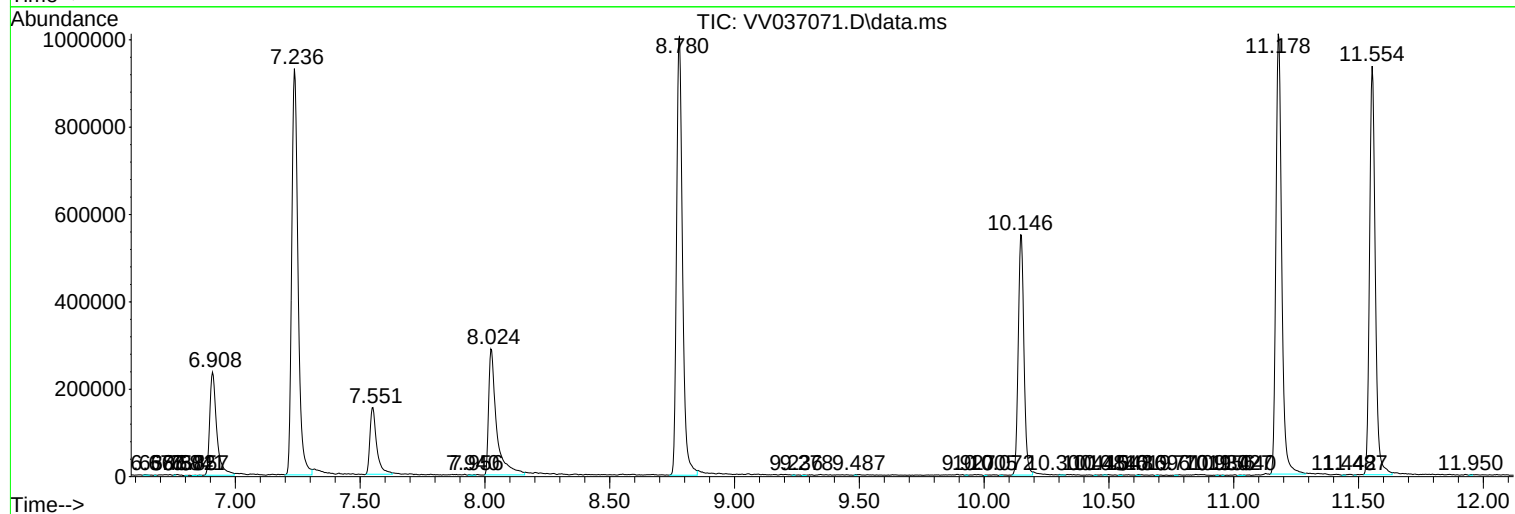
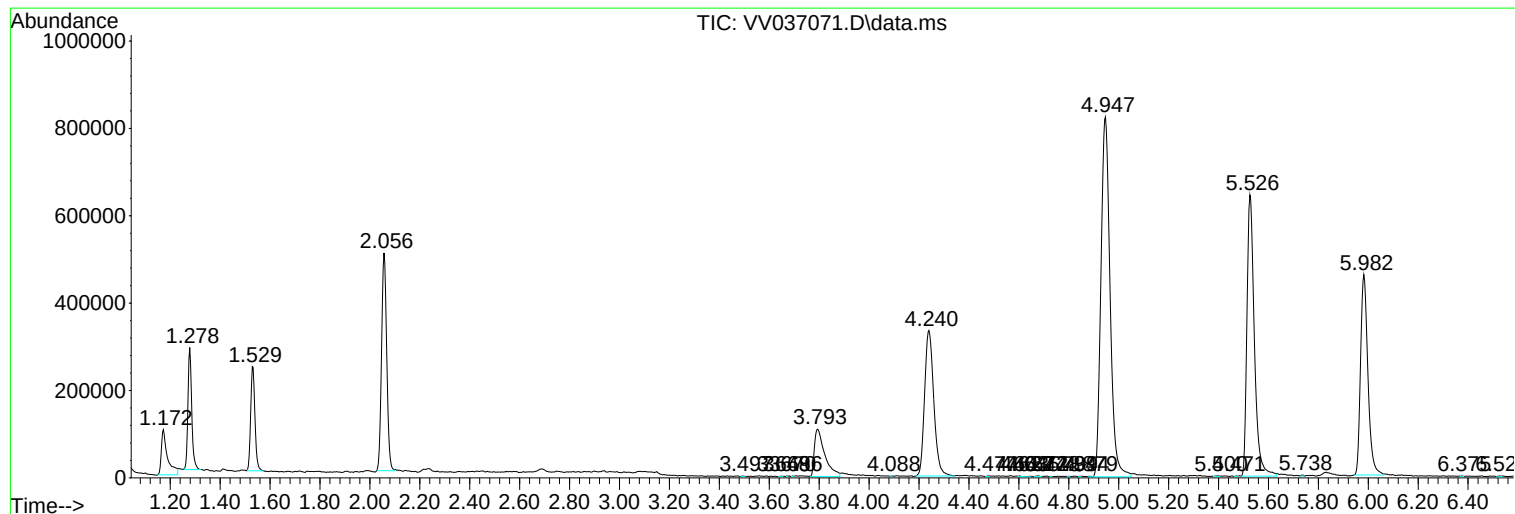
Sum of corrected areas: 15727481

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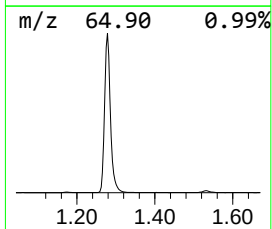
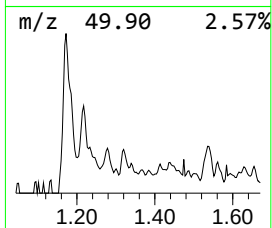
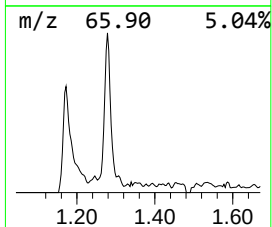
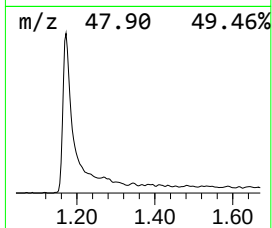
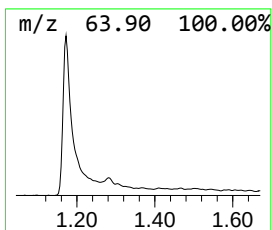
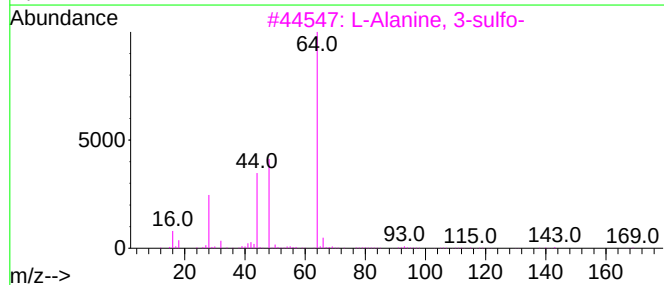
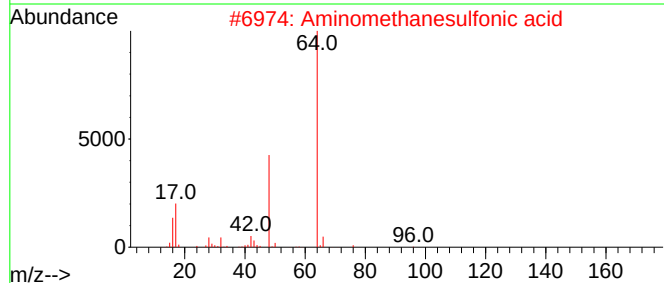
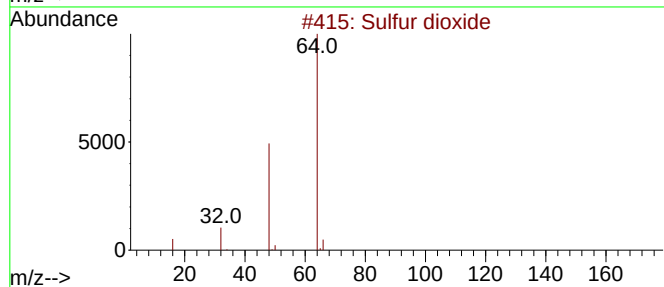
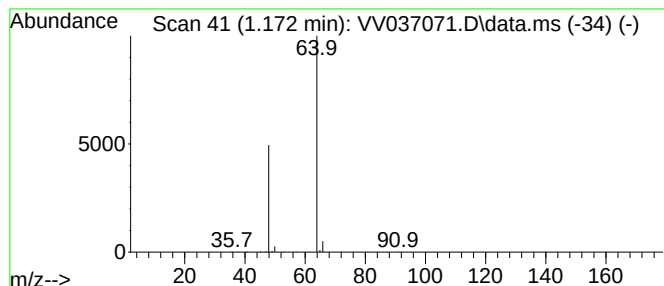
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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	6.77 ug/L	180202	1,4-Difluorobenzene	5.526

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	1.172	6.8	ug/L	180202	1	5.526	1331440	50.0