

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
 Data File : VV037472.D
 Acq On : 23 Sep 2024 11:37
 Operator : SY/MD
 Sample : P4106-04 400X
 Misc : 5mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0SX9

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: VV037472.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	61	rBV	80492	137350	3.43%	0.615%
2	1.278	67	74	89	rVB	370525	394253	9.84%	1.765%
3	1.532	145	153	168	rVB	317097	370037	9.23%	1.657%
4	2.060	307	317	338	rBV	648282	934934	23.33%	4.187%
5	3.429	740	743	748	rVB6	629	607	0.02%	0.003%
6	3.548	776	780	782	rBV4	758	546	0.01%	0.002%
7	3.655	804	813	816	rBV7	1353	1924	0.05%	0.009%
8	3.674	816	819	824	rVB5	971	1061	0.03%	0.005%
9	3.754	842	844	848	rVB3	1157	695	0.02%	0.003%
10	3.793	848	856	890	rBV	109317	334751	8.35%	1.499%
11	4.108	951	954	957	rBV2	1208	926	0.02%	0.004%
12	4.153	963	968	973	rVB5	1189	1173	0.03%	0.005%
13	4.179	973	976	978	rBV3	1002	666	0.02%	0.003%
14	4.243	979	996	1029	rVV2	419208	1073915	26.80%	4.809%
15	4.455	1061	1062	1067	rVB3	822	527	0.01%	0.002%
16	4.523	1081	1083	1087	rBV4	905	554	0.01%	0.002%
17	4.577	1097	1100	1103	rVB3	1078	687	0.02%	0.003%
18	4.613	1109	1111	1117	rVB4	1047	785	0.02%	0.004%
19	4.658	1121	1125	1128	rVB4	939	725	0.02%	0.003%
20	4.709	1135	1141	1144	rBV5	901	855	0.02%	0.004%
21	4.728	1144	1147	1156	rVV8	1965	2905	0.07%	0.013%
22	4.780	1159	1163	1166	rBV3	1058	797	0.02%	0.004%
23	4.841	1178	1182	1187	rVB3	1456	1271	0.03%	0.006%
24	4.950	1200	1216	1230	rBV2	1027867	2660288	66.38%	11.913%
25	5.262	1309	1313	1317	rBV5	1283	1373	0.03%	0.006%
26	5.314	1326	1329	1333	rBV7	1058	1042	0.03%	0.005%
27	5.333	1333	1335	1340	rVB4	1587	1061	0.03%	0.005%
28	5.359	1340	1343	1345	rBV2	837	570	0.01%	0.003%
29	5.400	1354	1356	1360	rVB4	1555	1055	0.03%	0.005%
30	5.484	1378	1382	1385	rBV4	1006	958	0.02%	0.004%
31	5.529	1385	1396	1435	rVV	790041	1627689	40.61%	7.289%
32	5.831	1484	1490	1492	rBV7	4298	4790	0.12%	0.021%
33	5.986	1524	1538	1567	rBV	573039	1193945	29.79%	5.346%
34	6.294	1630	1634	1638	rVV5	992	679	0.02%	0.003%
35	6.336	1642	1647	1651	rBV3	996	1079	0.03%	0.005%
36	6.654	1743	1746	1749	rVV3	1041	641	0.02%	0.003%

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 Title : VOC Analysis

37	6.706	1759	1762	1765	rVB3	735	539	0.01%	0.002%
38	6.786	1785	1787	1793	rVB5	1004	694	0.02%	0.003%
39	6.908	1810	1825	1862	rBV	299667	590093	14.72%	2.642%
40	7.236	1916	1927	1957	rBV	1184325	2085276	52.03%	9.338%
41	7.551	2015	2025	2055	rBV	194819	367959	9.18%	1.648%
42	7.748	2083	2086	2089	rVB3	1196	782	0.02%	0.004%
43	7.767	2089	2092	2096	rVB6	764	553	0.01%	0.002%
44	7.834	2111	2113	2117	rVB3	1303	669	0.02%	0.003%
45	7.857	2117	2120	2121	rBV3	1057	653	0.02%	0.003%
46	7.966	2151	2154	2157	rBV4	966	619	0.02%	0.003%
47	8.024	2163	2172	2202	rBV2	324338	712028	17.77%	3.188%
48	8.532	2328	2330	2334	rBV3	1443	1250	0.03%	0.006%
49	8.609	2353	2354	2360	rVB4	1073	641	0.02%	0.003%
50	8.693	2376	2380	2381	rBV3	998	593	0.01%	0.003%
51	8.780	2396	2407	2410	rBV	1352659	1913139	47.73%	8.567%
52	9.182	2529	2532	2534	rBV3	1327	670	0.02%	0.003%
53	9.259	2552	2556	2558	rBV4	663	527	0.01%	0.002%
54	9.384	2594	2595	2599	rBV3	804	533	0.01%	0.002%
55	9.407	2599	2602	2605	rVV5	731	560	0.01%	0.003%
56	9.465	2615	2620	2626	rBV7	1531	1928	0.05%	0.009%
57	9.551	2644	2647	2649	rVV3	829	569	0.01%	0.003%
58	9.751	2703	2709	2712	rBV7	987	1006	0.03%	0.005%
59	9.802	2722	2725	2728	rVB3	877	645	0.02%	0.003%
60	9.831	2728	2734	2736	rBV4	1179	784	0.02%	0.004%
61	9.899	2753	2755	2758	rVB3	953	596	0.01%	0.003%
62	10.011	2785	2790	2795	rBV4	982	1016	0.03%	0.005%
63	10.059	2800	2805	2807	rBV5	956	797	0.02%	0.004%
64	10.146	2818	2832	2854	rBV	654062	1031762	25.74%	4.620%
65	10.368	2897	2901	2903	rVB3	1061	559	0.01%	0.003%
66	10.416	2913	2916	2919	rVB2	834	517	0.01%	0.002%
67	10.558	2958	2960	2964	rBV3	726	598	0.01%	0.003%
68	10.609	2969	2976	2977	rBV5	670	711	0.02%	0.003%
69	10.760	3020	3023	3027	rBV5	691	560	0.01%	0.003%
70	10.786	3027	3031	3037	rVV8	1334	1527	0.04%	0.007%
71	10.892	3060	3064	3068	rBV5	921	891	0.02%	0.004%
72	10.921	3071	3073	3076	rBV2	660	547	0.01%	0.002%
73	10.979	3087	3091	3099	rVB7	742	738	0.02%	0.003%
74	11.043	3108	3111	3114	rVB3	782	634	0.02%	0.003%
75	11.066	3114	3118	3124	rBV6	1176	1386	0.03%	0.006%
76	11.114	3124	3133	3143	rBV	114034	186246	4.65%	0.834%

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Title : VOC Analysis

77	11.182	3143	3154	3158	rBV	1348264	2220865	55.41%	9.945%
78	11.387	3214	3218	3223	rVB7	1380	1442	0.04%	0.006%
79	11.500	3252	3253	3256	rBV2	790	512	0.01%	0.002%
80	11.567	3256	3274	3302	rBV2	1680033	4007884	100.00%	17.947%
81	12.034	3416	3419	3424	rBV6	1647	1321	0.03%	0.006%
82	12.120	3443	3446	3450	rBV5	798	549	0.01%	0.002%
83	12.230	3476	3480	3482	rBV4	984	725	0.02%	0.003%
84	12.487	3557	3560	3563	rBV5	1019	593	0.01%	0.003%
85	12.516	3566	3569	3573	rVB	759	545	0.01%	0.002%
86	12.574	3580	3587	3588	rBV5	1377	1198	0.03%	0.005%
87	12.915	3689	3693	3696	rVB5	1001	782	0.02%	0.004%
88	12.931	3696	3698	3700	rBV2	951	585	0.01%	0.003%
89	13.117	3753	3756	3758	rBV3	993	583	0.01%	0.003%
90	13.194	3768	3780	3804	rBV	208441	344466	8.59%	1.543%
91	13.374	3833	3836	3842	rBV6	1403	1070	0.03%	0.005%
92	13.423	3846	3851	3853	rBV3	1050	1040	0.03%	0.005%
93	13.445	3853	3858	3861	rBV7	1855	1804	0.05%	0.008%
94	13.677	3920	3930	3943	rBV2	42329	71569	1.79%	0.320%
95	13.972	4020	4022	4024	rBV3	1079	577	0.01%	0.003%
96	14.059	4047	4049	4051	rBV3	857	506	0.01%	0.002%
97	14.091	4057	4059	4061	rBV3	919	605	0.02%	0.003%
98	14.178	4084	4086	4091	rVB5	1176	689	0.02%	0.003%
99	14.760	4261	4267	4268	rBV6	1618	1434	0.04%	0.006%
100	16.033	4661	4663	4665	rBV3	2385	1312	0.03%	0.006%

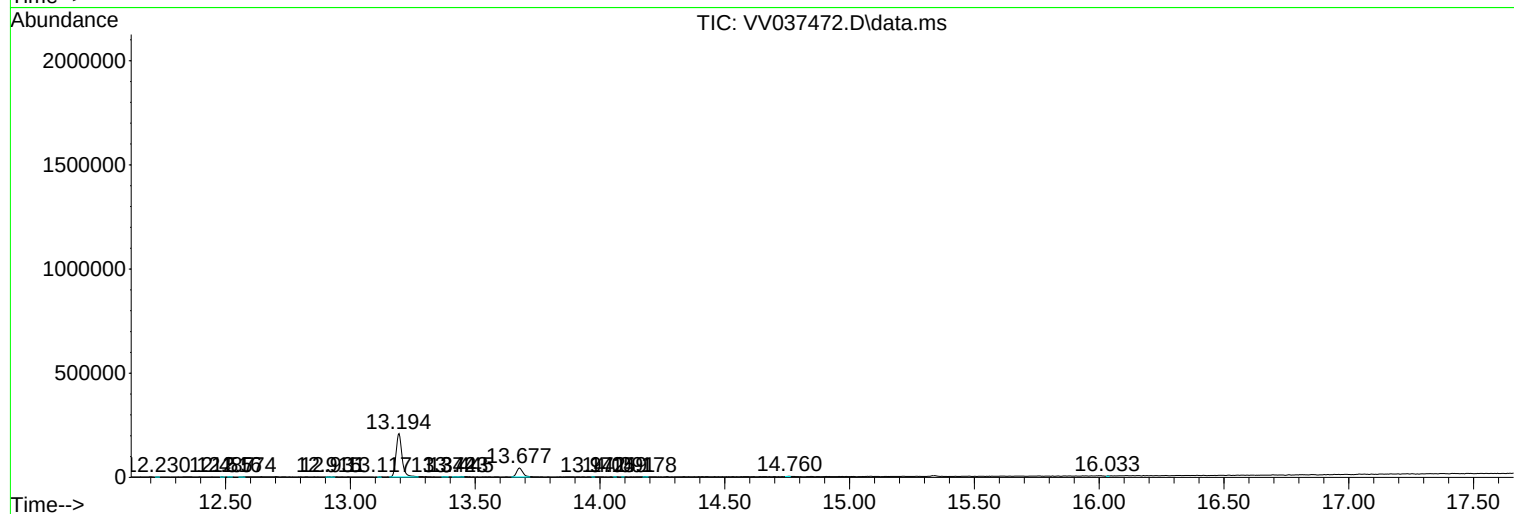
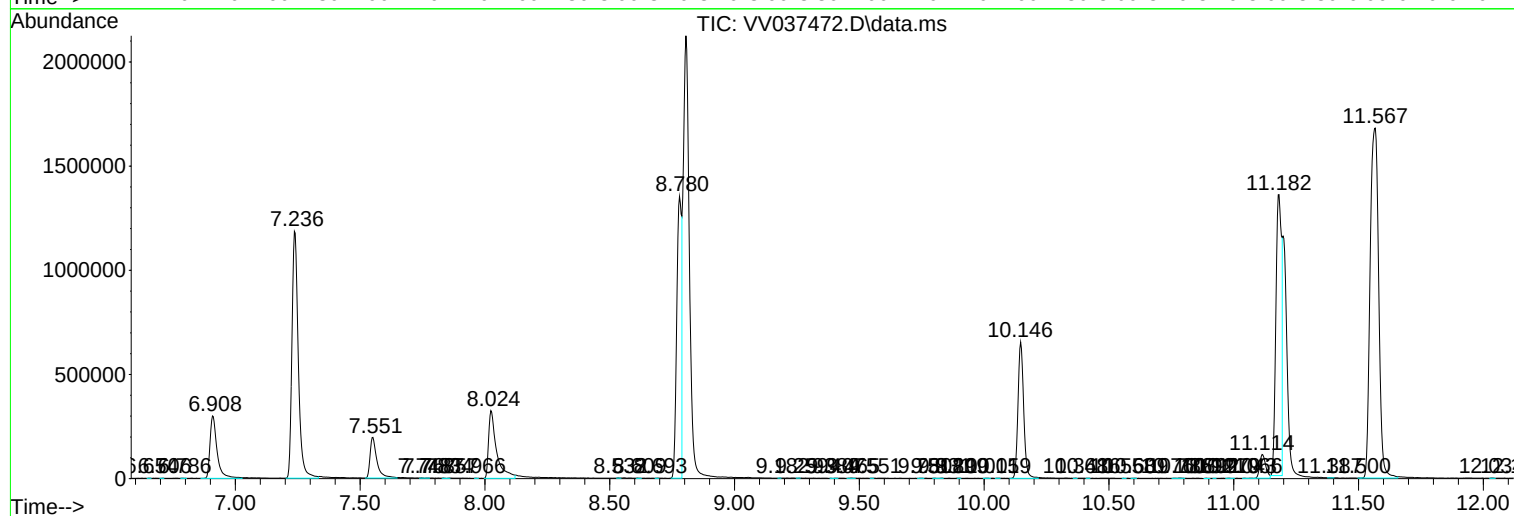
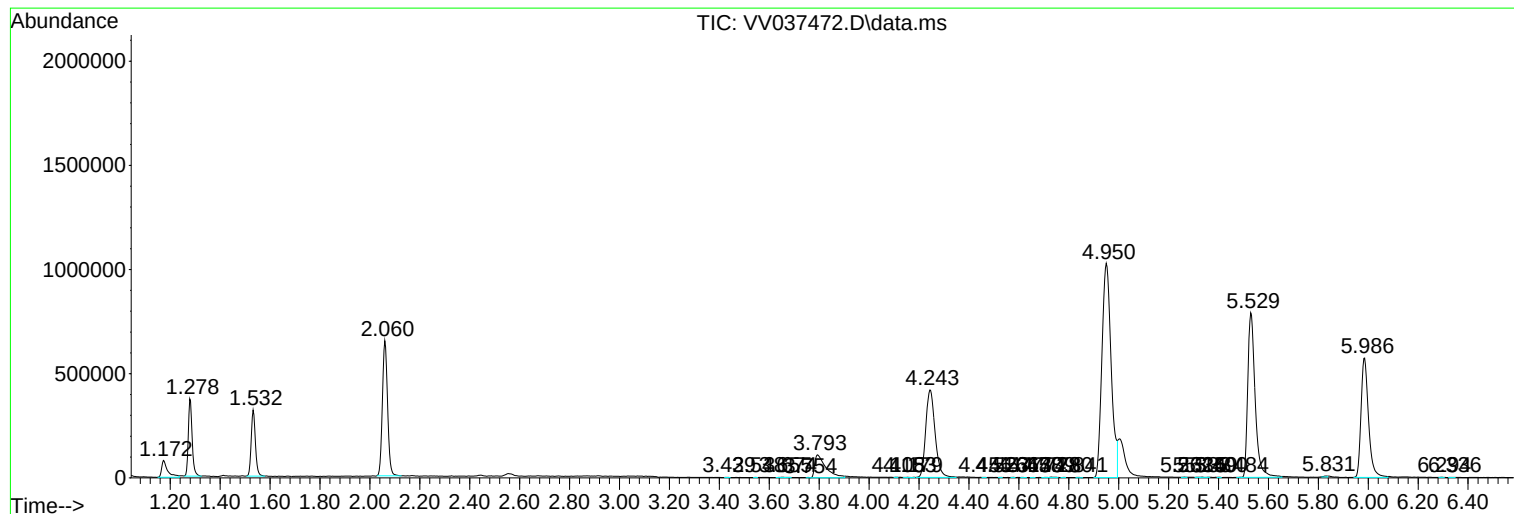
Sum of corrected areas: 22331565

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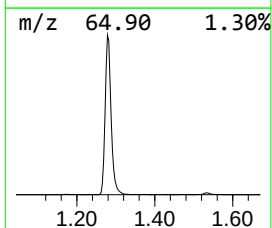
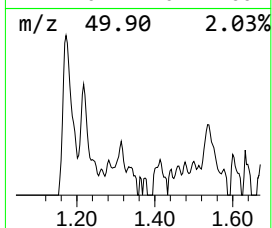
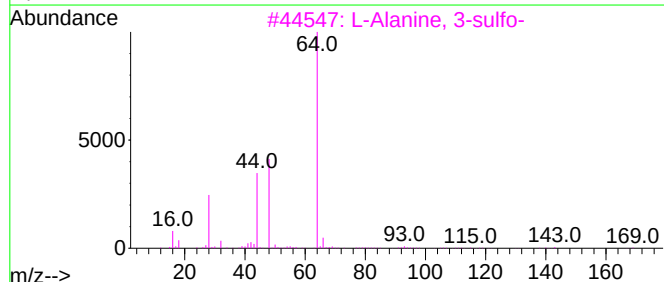
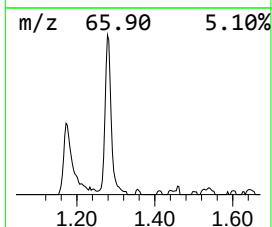
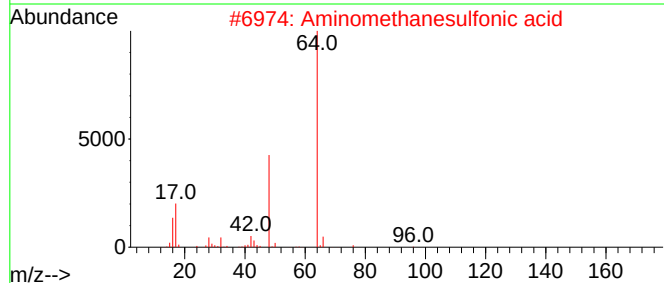
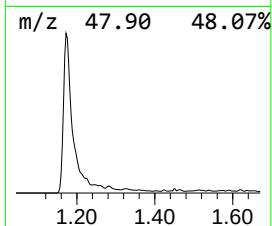
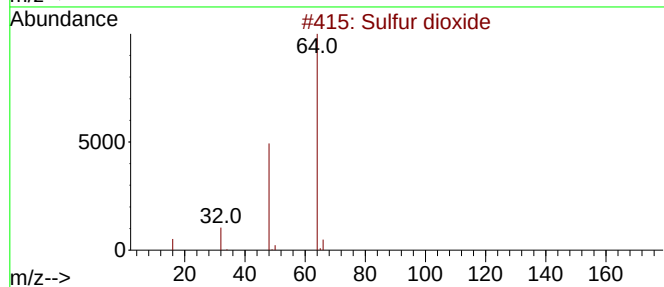
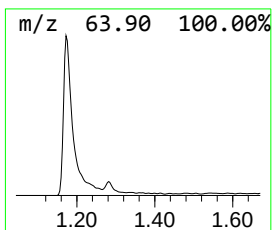
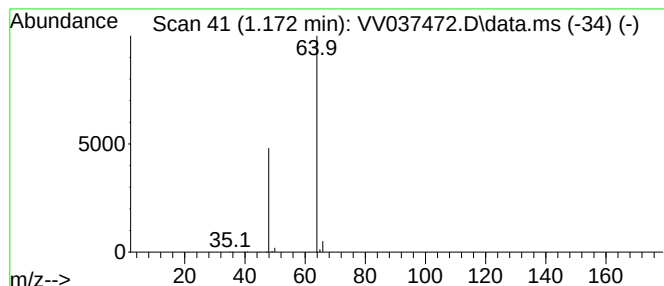
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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	4.22 ug/L	137350	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			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	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	1.172	4.2	ug/L	137350	1	5.529	1627690	50.0