

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
 Data File : VV037467.D
 Acq On : 23 Sep 2024 09:32
 Operator : SY/MD
 Sample : VV0923MBL01
 Misc : 5.0G/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK208

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: VV037467.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	55	rBV	111742	166762	6.11%	0.833%
2	1.278	68	74	90	rVB	391976	428480	15.70%	2.142%
3	1.532	146	153	169	rVB	331032	391782	14.35%	1.958%
4	2.059	307	317	331	rBV	683261	984133	36.05%	4.919%
5	3.378	722	727	732	rVB5	1293	1107	0.04%	0.006%
6	3.403	732	735	740	rVB5	985	729	0.03%	0.004%
7	3.432	740	744	747	rBV5	1020	832	0.03%	0.004%
8	3.567	784	786	791	rVB2	1274	884	0.03%	0.004%
9	3.789	847	855	882	rBV	108172	307274	11.26%	1.536%
10	4.043	932	934	939	rVB5	1239	789	0.03%	0.004%
11	4.137	959	963	964	rBV4	956	662	0.02%	0.003%
12	4.239	978	995	1030	rBV	434296	1111664	40.72%	5.556%
13	4.497	1072	1075	1078	rBV3	1037	680	0.02%	0.003%
14	4.558	1088	1094	1095	rBV4	1246	1025	0.04%	0.005%
15	4.696	1130	1137	1138	rBV4	542	568	0.02%	0.003%
16	4.947	1199	1215	1247	rBV2	1059126	2729688	100.00%	13.643%
17	5.391	1349	1353	1355	rBV4	884	766	0.03%	0.004%
18	5.403	1355	1357	1362	rVB6	1047	906	0.03%	0.005%
19	5.526	1383	1395	1427	rBV	781101	1614045	59.13%	8.067%
20	5.780	1471	1474	1478	rVB5	1458	898	0.03%	0.004%
21	5.831	1480	1490	1499	rBV5	6909	14033	0.51%	0.070%
22	5.937	1520	1523	1524	rBV2	1174	684	0.03%	0.003%
23	5.982	1524	1537	1566	rVV	586960	1226425	44.93%	6.130%
24	6.227	1611	1613	1617	rVB4	1069	572	0.02%	0.003%
25	6.374	1656	1659	1663	rBV3	1585	1243	0.05%	0.006%
26	6.416	1668	1672	1675	rVV4	973	986	0.04%	0.005%
27	6.432	1675	1677	1681	rVV4	1487	863	0.03%	0.004%
28	6.474	1685	1690	1694	rBV5	1584	1498	0.05%	0.007%
29	6.567	1712	1719	1724	rVB7	861	1019	0.04%	0.005%
30	6.641	1739	1742	1746	rBV5	757	590	0.02%	0.003%
31	6.680	1750	1754	1758	rVB4	1267	1001	0.04%	0.005%
32	6.718	1758	1766	1769	rBV7	1419	1760	0.06%	0.009%
33	6.905	1814	1824	1855	rBV	311270	605939	22.20%	3.029%
34	7.175	1901	1908	1909	rBV6	3422	2986	0.11%	0.015%
35	7.236	1916	1927	1952	rBV	1244658	2162632	79.23%	10.809%
36	7.548	2014	2024	2047	rBV2	203094	380461	13.94%	1.902%

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 Title : VOC Analysis

37	7.898	2128	2133	2134	rBV3	2177	1548	0.06%	0.008%
38	7.985	2157	2160	2163	rVB4	886	580	0.02%	0.003%
39	8.024	2163	2172	2210	rBV2	311089	718881	26.34%	3.593%
40	8.693	2376	2380	2382	rBV6	1022	621	0.02%	0.003%
41	8.776	2394	2406	2433	rBV	1213257	2005737	73.48%	10.025%
42	9.169	2525	2528	2532	rVB4	1073	852	0.03%	0.004%
43	9.191	2532	2535	2539	rVB5	828	719	0.03%	0.004%
44	9.329	2575	2578	2584	rVB4	712	587	0.02%	0.003%
45	9.371	2589	2591	2595	rVB2	1301	663	0.02%	0.003%
46	9.484	2617	2626	2632	rBV9	3344	6824	0.25%	0.034%
47	9.558	2646	2649	2652	rBV4	828	581	0.02%	0.003%
48	9.648	2674	2677	2681	rVB4	1142	779	0.03%	0.004%
49	9.673	2681	2685	2687	rBV4	1033	756	0.03%	0.004%
50	9.728	2699	2702	2704	rBV3	1070	753	0.03%	0.004%
51	9.741	2704	2706	2713	rVB5	861	659	0.02%	0.003%
52	9.866	2738	2745	2746	rBV5	3675	3057	0.11%	0.015%
53	9.937	2764	2767	2772	rBV5	626	569	0.02%	0.003%
54	10.043	2797	2800	2802	rVB4	1151	663	0.02%	0.003%
55	10.146	2818	2832	2850	rBV	650835	1037865	38.02%	5.187%
56	10.316	2880	2885	2886	rBV4	2005	1413	0.05%	0.007%
57	10.442	2920	2924	2926	rBV4	1099	894	0.03%	0.004%
58	10.480	2926	2936	2941	rVV8	3718	5499	0.20%	0.027%
59	10.535	2950	2953	2955	rVB4	984	665	0.02%	0.003%
60	10.554	2955	2959	2963	rVB5	739	643	0.02%	0.003%
61	10.635	2979	2984	2988	rBV4	939	875	0.03%	0.004%
62	10.779	3025	3029	3031	rBV3	1453	891	0.03%	0.004%
63	10.853	3045	3052	3055	rBV5	4693	5137	0.19%	0.026%
64	10.988	3092	3094	3097	rVB3	1210	647	0.02%	0.003%
65	11.127	3128	3137	3142	rBV3	8467	13740	0.50%	0.069%
66	11.178	3142	3153	3193	rVB	1225375	1915032	70.16%	9.572%
67	11.365	3208	3211	3215	rVB6	1846	1394	0.05%	0.007%
68	11.390	3215	3219	3224	rVV4	982	864	0.03%	0.004%
69	11.458	3238	3240	3244	rVB5	1169	735	0.03%	0.004%
70	11.506	3251	3255	3258	rBV5	1326	954	0.03%	0.005%
71	11.554	3258	3270	3298	rBV	1186739	1918019	70.27%	9.587%
72	11.680	3307	3309	3316	rVB8	1323	1288	0.05%	0.006%
73	11.879	3367	3371	3373	rBV4	1314	1084	0.04%	0.005%
74	11.937	3386	3389	3396	rVB6	1777	1581	0.06%	0.008%
75	12.104	3434	3441	3442	rBV5	997	956	0.04%	0.005%
76	12.178	3461	3464	3467	rBV4	818	626	0.02%	0.003%

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

77	12.197	3467	3470	3475	rBV5	957	607	0.02%	0.003%
78	12.326	3507	3510	3512	rBV2	892	580	0.02%	0.003%
79	12.371	3516	3524	3525	rBV4	1467	1797	0.07%	0.009%
80	12.541	3574	3577	3579	rBV3	898	584	0.02%	0.003%
81	12.583	3581	3590	3602	rVV5	11759	20985	0.77%	0.105%
82	12.715	3629	3631	3635	rVB2	1078	835	0.03%	0.004%
83	12.744	3635	3640	3642	rBV4	950	727	0.03%	0.004%
84	12.824	3662	3665	3667	rBV2	940	565	0.02%	0.003%
85	12.953	3702	3705	3709	rVB3	1338	854	0.03%	0.004%
86	13.201	3774	3782	3796	rVB2	18137	32523	1.19%	0.163%
87	13.323	3816	3820	3821	rBV4	950	675	0.02%	0.003%
88	13.438	3847	3856	3874	rBV	51230	95224	3.49%	0.476%
89	13.680	3922	3931	3950	rVB3	22964	39994	1.47%	0.200%
90	13.763	3955	3957	3962	rVB3	1189	869	0.03%	0.004%
91	13.792	3962	3966	3967	rBV4	929	745	0.03%	0.004%
92	14.281	4115	4118	4121	rBV4	1139	794	0.03%	0.004%
93	14.332	4131	4134	4138	rBV5	1043	976	0.04%	0.005%
94	14.448	4168	4170	4173	rVB3	1340	617	0.02%	0.003%
95	14.551	4200	4202	4206	rVB4	2031	1278	0.05%	0.006%
96	14.580	4207	4211	4213	rBV5	959	827	0.03%	0.004%
97	14.725	4254	4256	4259	rBV3	1298	664	0.02%	0.003%
98	15.049	4353	4357	4359	rBV4	1460	964	0.04%	0.005%
99	15.168	4391	4394	4395	rBV	1500	749	0.03%	0.004%
100	15.490	4492	4494	4498	rBV4	1796	1019	0.04%	0.005%

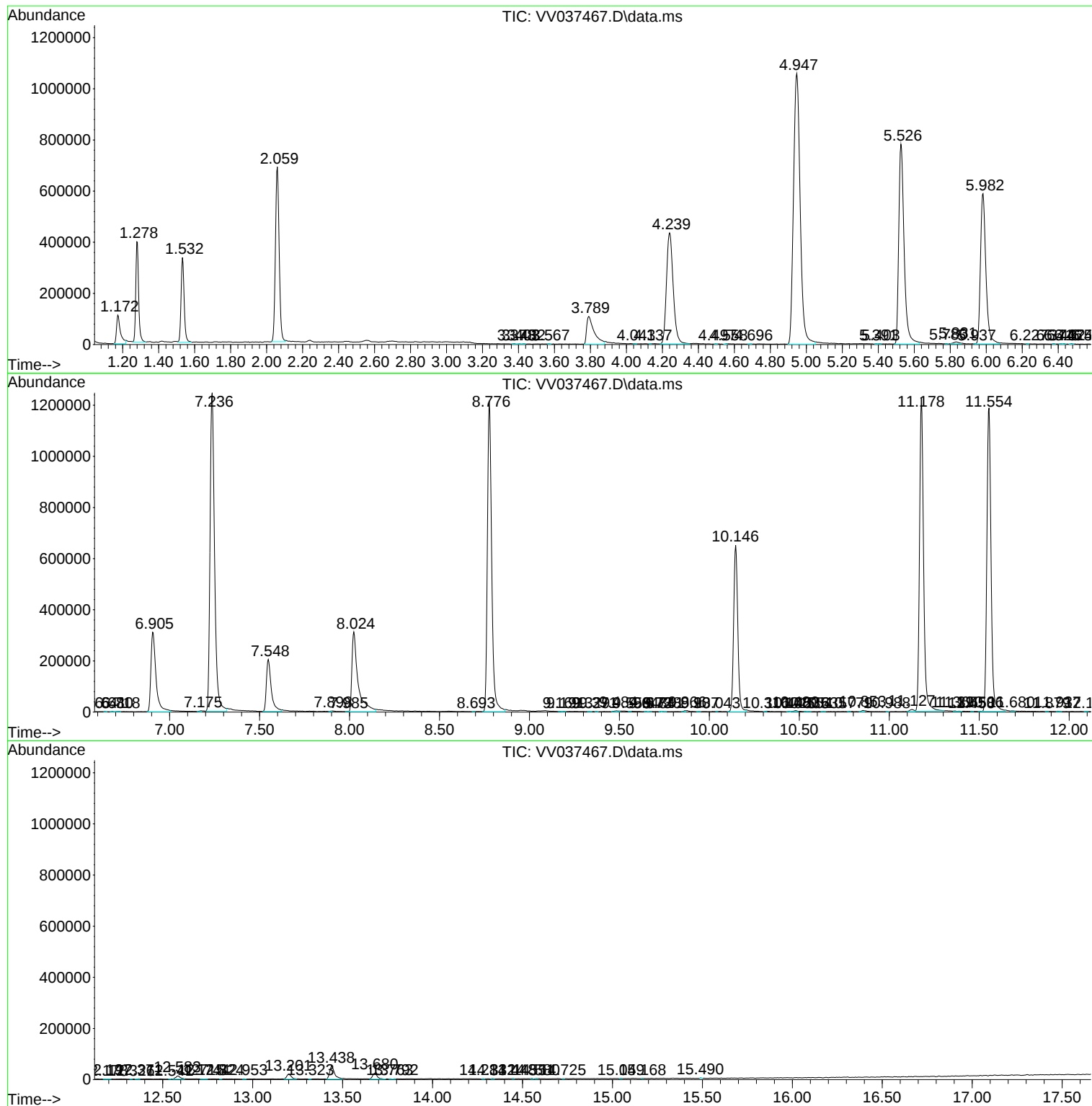
Sum of corrected areas: 20007449

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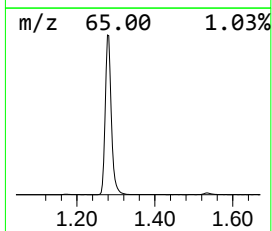
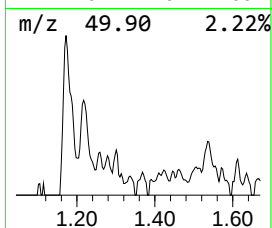
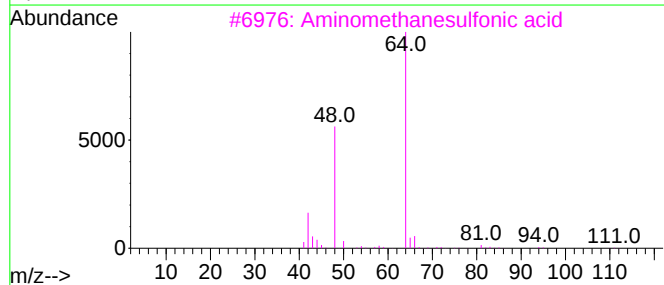
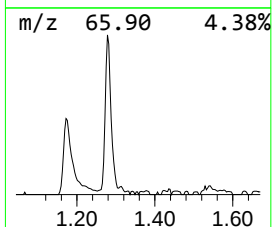
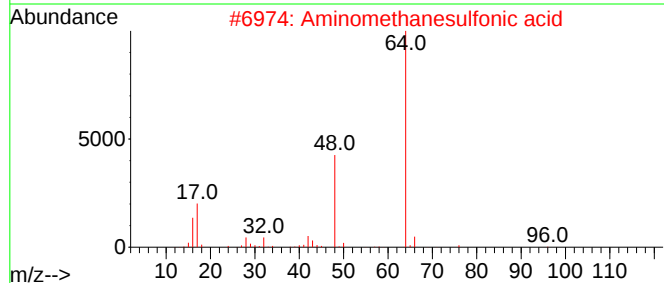
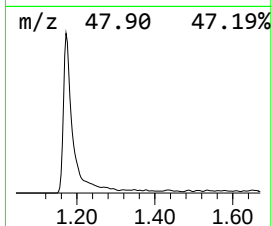
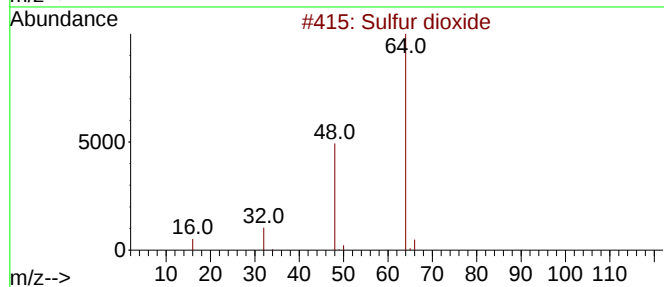
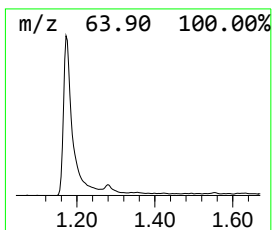
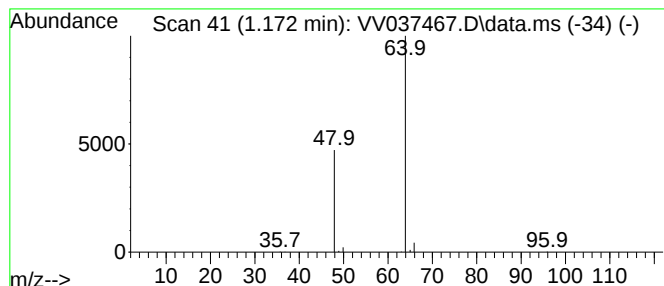
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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	5.17 ug/L	166762	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
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	1.172	5.2	ug/L	166762	1	5.526	1614050	50.0