

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
 Data File : VV033873.D
 Acq On : 26 Jan 2024 09:31
 Operator : SY/MD
 Sample : VV0126MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK224

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\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033873.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	32	39	51	rBV	68292	78002	10.02%	1.219%
2	1.278	68	74	92	rBV	115357	138281	17.76%	2.160%
3	1.516	141	148	162	rVB	86615	109654	14.08%	1.713%
4	2.053	306	315	336	rVB	205217	304199	39.07%	4.753%
5	2.175	351	353	354	rBV2	514	194	0.02%	0.003%
6	2.240	363	373	377	rBV2	1478	2245	0.29%	0.035%
7	2.381	414	417	420	rBV3	400	285	0.04%	0.004%
8	2.445	432	437	445	rVB3	814	867	0.11%	0.014%
9	2.558	466	472	481	rVB3	389	503	0.06%	0.008%
10	3.011	606	613	620	rBV2	235	363	0.05%	0.006%
11	3.111	636	644	646	rBV2	146	203	0.03%	0.003%
12	3.159	653	659	666	rVB2	200	276	0.04%	0.004%
13	3.433	740	744	747	rBV2	222	202	0.03%	0.003%
14	3.783	845	853	884	rBV2	52736	139510	17.92%	2.180%
15	4.246	977	997	1030	rBV	120254	310741	39.91%	4.855%
16	4.497	1073	1075	1078	rVB2	367	176	0.02%	0.003%
17	4.532	1082	1086	1088	rVV2	239	186	0.02%	0.003%
18	4.561	1092	1095	1097	rBV2	241	186	0.02%	0.003%
19	4.661	1121	1126	1132	rBV2	229	312	0.04%	0.005%
20	4.953	1200	1217	1254	rBV2	295580	778689	100.00%	12.166%
21	5.333	1332	1335	1337	rBV	294	208	0.03%	0.003%
22	5.391	1349	1353	1356	rBV2	214	206	0.03%	0.003%
23	5.458	1371	1374	1378	rVB2	218	145	0.02%	0.002%
24	5.532	1386	1397	1432	rBV	253772	524205	67.32%	8.190%
25	5.760	1466	1468	1475	rVB	333	241	0.03%	0.004%
26	5.799	1475	1480	1484	rBV2	199	252	0.03%	0.004%
27	5.831	1484	1490	1491	rBV3	1274	1379	0.18%	0.022%
28	5.985	1526	1538	1560	rBV	169395	346313	44.47%	5.411%
29	6.111	1575	1577	1582	rVB2	307	177	0.02%	0.003%
30	6.137	1582	1585	1590	rVB4	480	426	0.05%	0.007%
31	6.159	1590	1592	1596	rVB2	388	227	0.03%	0.004%
32	6.455	1681	1684	1690	rVB	211	131	0.02%	0.002%
33	6.532	1705	1708	1711	rVV2	227	139	0.02%	0.002%
34	6.564	1715	1718	1720	rBV	261	206	0.03%	0.003%
35	6.645	1740	1743	1750	rVB2	261	231	0.03%	0.004%
36	6.911	1814	1826	1852	rBV	102650	191743	24.62%	2.996%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

37	7.243	1918	1929	1956	rBV	361321	636625	81.76%	9.946%
38	7.551	2015	2025	2050	rBV	71846	126618	16.26%	1.978%
39	7.751	2083	2087	2090	rVB2	280	247	0.03%	0.004%
40	7.844	2113	2116	2120	rBV	156	132	0.02%	0.002%
41	8.024	2163	2172	2209	rBV	202861	371088	47.66%	5.798%
42	8.310	2258	2261	2264	rBV2	212	144	0.02%	0.002%
43	8.371	2277	2280	2284	rBV2	388	364	0.05%	0.006%
44	8.474	2308	2312	2313	rBV2	281	172	0.02%	0.003%
45	8.783	2397	2408	2445	rBV	389538	641566	82.39%	10.023%
46	8.960	2458	2463	2471	rVB4	480	790	0.10%	0.012%
47	9.085	2497	2502	2507	rBV3	238	339	0.04%	0.005%
48	9.481	2622	2625	2627	rBV3	245	172	0.02%	0.003%
49	9.522	2634	2638	2640	rBV3	402	318	0.04%	0.005%
50	9.606	2661	2664	2670	rBV2	155	166	0.02%	0.003%
51	9.757	2707	2711	2714	rVB	281	204	0.03%	0.003%
52	9.844	2734	2738	2741	rBV	200	144	0.02%	0.002%
53	9.879	2741	2749	2753	rBV2	699	931	0.12%	0.015%
54	9.947	2767	2770	2774	rVB2	160	150	0.02%	0.002%
55	10.153	2822	2834	2860	rBV	230678	357613	45.93%	5.587%
56	10.345	2891	2894	2897	rBV	225	140	0.02%	0.002%
57	10.448	2920	2926	2930	rBV2	138	188	0.02%	0.003%
58	10.487	2930	2938	2942	rBV3	645	862	0.11%	0.013%
59	10.525	2947	2950	2952	rBV2	196	133	0.02%	0.002%
60	10.635	2976	2984	2989	rBV2	263	454	0.06%	0.007%
61	10.673	2993	2996	2998	rBV2	253	183	0.02%	0.003%
62	10.754	3015	3021	3024	rBV2	156	168	0.02%	0.003%
63	10.866	3050	3056	3062	rVV2	564	827	0.11%	0.013%
64	10.915	3067	3071	3073	rBV	247	165	0.02%	0.003%
65	11.046	3106	3112	3115	rBV	206	181	0.02%	0.003%
66	11.101	3125	3129	3132	rBV2	151	147	0.02%	0.002%
67	11.130	3132	3138	3144	rBV4	1256	1897	0.24%	0.030%
68	11.185	3144	3155	3180	rBV	415858	646949	83.08%	10.107%
69	11.297	3187	3190	3194	rVB2	507	355	0.05%	0.006%
70	11.561	3260	3272	3296	rBV	381710	598346	76.84%	9.348%
71	12.162	3456	3459	3467	rVB2	224	294	0.04%	0.005%
72	12.249	3484	3486	3492	rVB2	208	164	0.02%	0.003%
73	12.358	3517	3520	3522	rBV2	172	130	0.02%	0.002%
74	12.442	3543	3546	3549	rBV2	204	143	0.02%	0.002%
75	12.493	3558	3562	3567	rVB	336	304	0.04%	0.005%
76	12.522	3567	3571	3573	rBV2	166	137	0.02%	0.002%

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 Title : VOC Analysis

77	12.593	3580	3593	3603	rBV5	2613	4228	0.54%	0.066%
78	12.641	3605	3608	3616	rVB2	222	236	0.03%	0.004%
79	12.869	3675	3679	3683	rBV2	207	204	0.03%	0.003%
80	12.947	3700	3703	3706	rBV	221	165	0.02%	0.003%
81	13.082	3740	3745	3748	rBV2	176	197	0.03%	0.003%
82	13.207	3775	3784	3799	rVB3	5429	9094	1.17%	0.142%
83	13.339	3820	3825	3828	rBV	284	320	0.04%	0.005%
84	13.445	3846	3858	3882	rBV	27911	48036	6.17%	0.750%
85	13.583	3897	3901	3904	rBV2	167	146	0.02%	0.002%
86	13.628	3911	3915	3917	rBV	273	192	0.02%	0.003%
87	13.686	3922	3933	3946	rBV4	8113	13228	1.70%	0.207%
88	14.014	4031	4035	4039	rBV2	273	277	0.04%	0.004%
89	14.104	4060	4063	4067	rVB3	318	253	0.03%	0.004%
90	14.130	4067	4071	4076	rBV3	369	447	0.06%	0.007%
91	14.390	4148	4152	4159	rVB2	369	364	0.05%	0.006%
92	14.419	4159	4161	4164	rBV3	200	136	0.02%	0.002%
93	14.738	4258	4260	4263	rVB2	412	195	0.03%	0.003%
94	14.824	4284	4287	4288	rBV	291	151	0.02%	0.002%
95	14.876	4300	4303	4304	rBV2	345	228	0.03%	0.004%
96	14.911	4311	4314	4317	rBV2	285	214	0.03%	0.003%
97	14.972	4331	4333	4336	rBV2	209	144	0.02%	0.002%
98	15.220	4406	4410	4413	rBV2	331	306	0.04%	0.005%
99	15.406	4466	4468	4471	rBV2	395	273	0.04%	0.004%
100	15.477	4487	4490	4492	rBV2	581	414	0.05%	0.006%

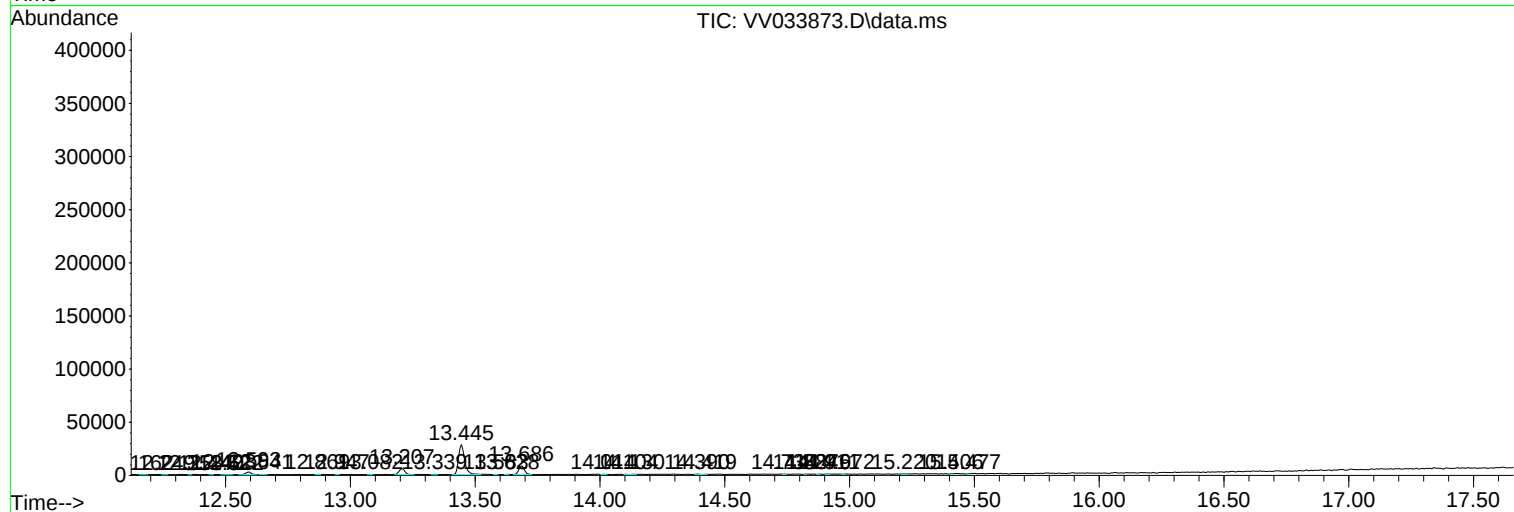
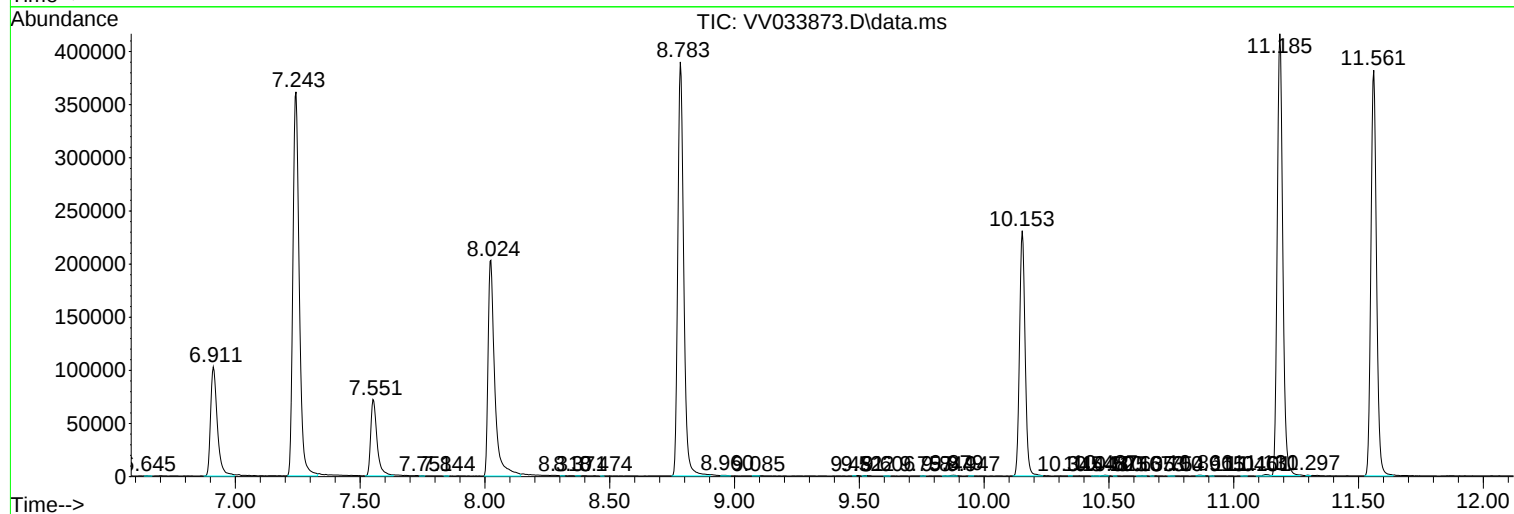
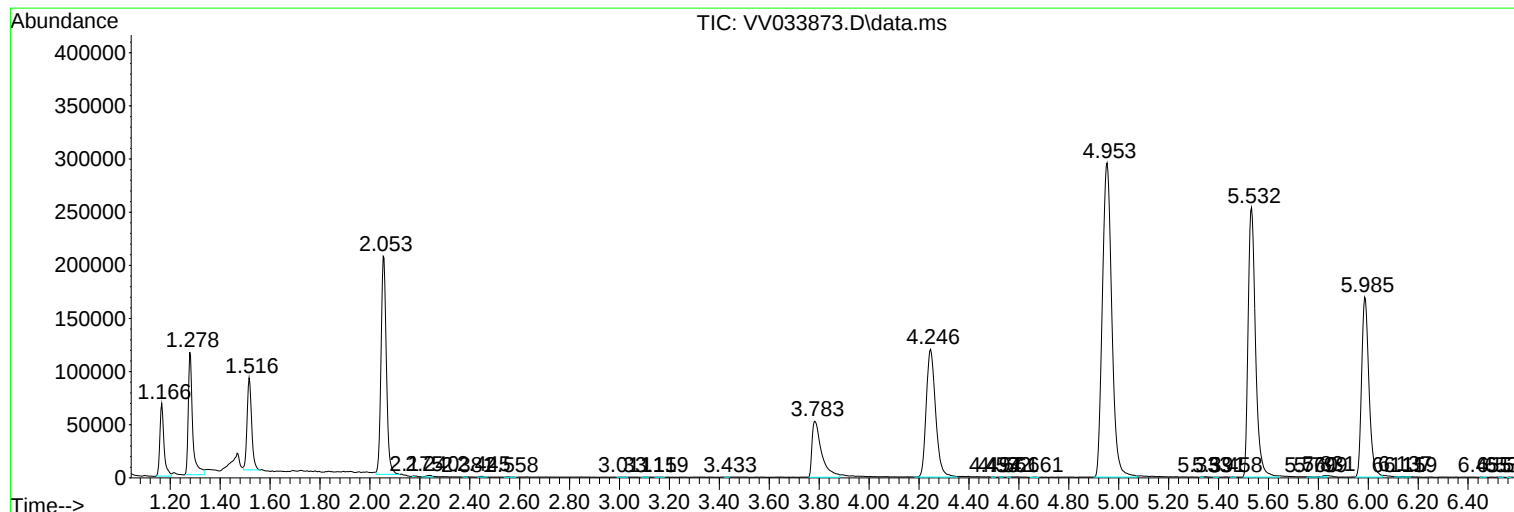
Sum of corrected areas: 6400701

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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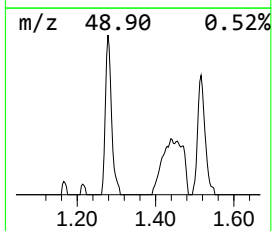
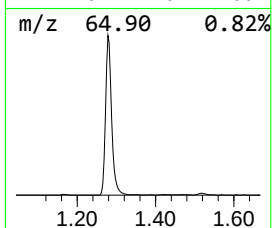
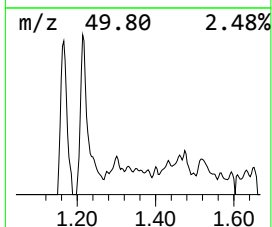
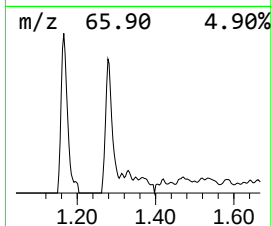
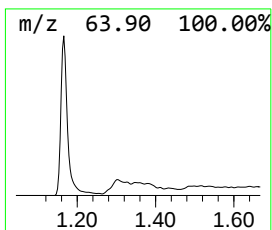
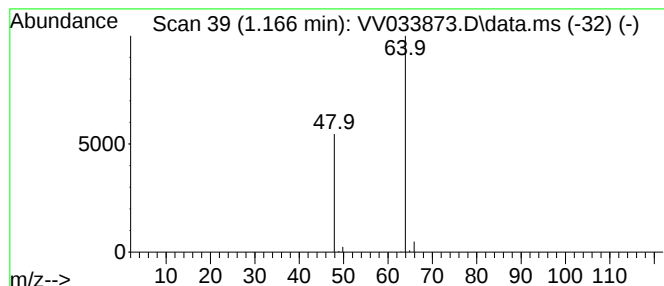
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
1.166	7.44 ug/L	78002	1,4-Difluorobenzene	5.532

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	7.4	ug/L	78002	1	5.532	524205	50.0