

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012224\
 Data File : VV033800.D
 Acq On : 22 Jan 2024 14:12
 Operator : SY/MD
 Sample : P1189-24
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMM0

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: VV033800.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.085	11	14	31	rVB3	2914	3743	0.45%	0.051%
2	1.166	32	39	63	rBV	188339	222250	26.88%	3.021%
3	1.282	65	75	109	rBV3	298563	480414	58.11%	6.531%
4	1.532	147	153	170	rVB	98975	121461	14.69%	1.651%
5	2.060	308	317	334	rVB	199192	296266	35.84%	4.028%
6	2.246	365	375	386	rBV5	1496	3401	0.41%	0.046%
7	2.384	415	418	424	rVB3	317	287	0.03%	0.004%
8	2.410	424	426	429	rBV	266	153	0.02%	0.002%
9	2.436	431	434	435	rBV	219	116	0.01%	0.002%
10	2.442	435	436	439	rBV2	262	140	0.02%	0.002%
11	2.558	468	472	474	rBV2	440	367	0.04%	0.005%
12	2.703	507	517	532	rBV3	4803	8454	1.02%	0.115%
13	2.786	535	543	545	rBV3	212	322	0.04%	0.004%
14	2.857	563	565	568	rBV2	149	109	0.01%	0.001%
15	2.976	599	602	605	rBV2	250	221	0.03%	0.003%
16	3.031	616	619	623	rBV2	232	210	0.03%	0.003%
17	3.137	649	652	656	rVB2	208	142	0.02%	0.002%
18	3.246	679	686	690	rBV2	153	188	0.02%	0.003%
19	3.699	824	827	833	rVB	212	177	0.02%	0.002%
20	3.738	833	839	842	rVB2	203	251	0.03%	0.003%
21	3.812	845	862	894	rBV2	149242	471232	57.00%	6.406%
22	4.085	945	947	949	rBV3	286	166	0.02%	0.002%
23	4.098	949	951	954	rVB2	344	192	0.02%	0.003%
24	4.249	982	998	1028	rBV2	123901	320739	38.80%	4.360%
25	4.384	1038	1040	1041	rBV	287	108	0.01%	0.001%
26	4.462	1061	1064	1067	rBV3	166	147	0.02%	0.002%
27	4.494	1071	1074	1077	rVB2	388	267	0.03%	0.004%
28	4.526	1081	1084	1087	rVB	260	173	0.02%	0.002%
29	4.580	1097	1101	1103	rBV2	341	247	0.03%	0.003%
30	4.590	1103	1104	1107	rVB	303	138	0.02%	0.002%
31	4.638	1116	1119	1122	rVV2	209	163	0.02%	0.002%
32	4.664	1123	1127	1129	rVV	288	187	0.02%	0.003%
33	4.683	1131	1133	1136	rVV2	216	130	0.02%	0.002%
34	4.822	1170	1176	1177	rBV	341	250	0.03%	0.003%
35	4.957	1202	1218	1256	rBV2	310287	826684	100.00%	11.239%
36	5.249	1307	1309	1314	rVB2	307	228	0.03%	0.003%

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 Title : VOC Analysis

37	5.436	1363	1367	1370	rBV2	235	150	0.02%	0.002%
38	5.532	1386	1397	1437	rBV	269224	563162	68.12%	7.656%
39	5.789	1474	1477	1486	rVB3	892	863	0.10%	0.012%
40	5.844	1486	1494	1509	rVB9	2549	5735	0.69%	0.078%
41	5.918	1514	1517	1521	rVB3	210	189	0.02%	0.003%
42	5.941	1521	1524	1526	rBV2	227	165	0.02%	0.002%
43	5.989	1526	1539	1563	rBV	178103	366158	44.29%	4.978%
44	6.188	1597	1601	1605	rBV4	247	204	0.02%	0.003%
45	6.230	1612	1614	1617	rBV2	339	227	0.03%	0.003%
46	6.593	1724	1727	1730	rBV2	146	116	0.01%	0.002%
47	6.654	1744	1746	1749	rVB2	224	120	0.01%	0.002%
48	6.770	1778	1782	1788	rBV2	197	245	0.03%	0.003%
49	6.818	1793	1797	1801	rBV2	149	118	0.01%	0.002%
50	6.912	1816	1826	1848	rBV	98630	184423	22.31%	2.507%
51	7.137	1894	1896	1901	rVV3	406	426	0.05%	0.006%
52	7.159	1901	1903	1907	rVB3	296	199	0.02%	0.003%
53	7.243	1917	1929	1957	rBV	385049	667961	80.80%	9.081%
54	7.551	2016	2025	2056	rBV	66338	121651	14.72%	1.654%
55	7.725	2077	2079	2081	rBV	195	119	0.01%	0.002%
56	7.793	2096	2100	2101	rBV	352	169	0.02%	0.002%
57	7.847	2113	2117	2118	rBV	199	124	0.01%	0.002%
58	7.873	2118	2125	2130	rVV3	2008	3005	0.36%	0.041%
59	7.912	2130	2137	2148	rVB4	4349	7976	0.96%	0.108%
60	7.953	2148	2150	2153	rBV2	197	151	0.02%	0.002%
61	8.024	2162	2172	2210	rBV	174829	343595	41.56%	4.671%
62	8.339	2267	2270	2271	rBV	176	126	0.02%	0.002%
63	8.606	2350	2353	2357	rVB	238	139	0.02%	0.002%
64	8.635	2357	2362	2366	rBV2	130	151	0.02%	0.002%
65	8.783	2397	2408	2432	rBV	411595	671545	81.23%	9.130%
66	9.079	2498	2500	2503	rBV2	224	111	0.01%	0.002%
67	9.159	2521	2525	2526	rBV3	360	259	0.03%	0.004%
68	9.375	2588	2592	2597	rVV2	160	180	0.02%	0.002%
69	9.693	2689	2691	2696	rVB2	172	125	0.02%	0.002%
70	9.725	2696	2701	2703	rBV	154	149	0.02%	0.002%
71	10.153	2822	2834	2858	rBV	228839	357970	43.30%	4.867%
72	10.680	2994	2998	3001	rBV	147	108	0.01%	0.001%
73	10.879	3054	3060	3064	rVB2	109	135	0.02%	0.002%
74	11.185	3144	3155	3184	rBV	436776	676720	81.86%	9.200%
75	11.329	3198	3200	3204	rVB3	268	197	0.02%	0.003%
76	11.381	3214	3216	3221	rVV2	136	110	0.01%	0.001%

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : VOC Analysis

77	11.519	3254	3259	3260	rBV2	713	686	0.08%	0.009%
78	11.561	3260	3272	3300	rVV	386089	614241	74.30%	8.351%
79	11.661	3301	3303	3313	rVV3	772	796	0.10%	0.011%
80	11.706	3313	3317	3320	rVB3	281	245	0.03%	0.003%
81	12.001	3404	3409	3415	rBV2	216	216	0.03%	0.003%
82	12.034	3416	3419	3425	rVB2	143	133	0.02%	0.002%
83	12.487	3557	3560	3563	rBV	227	129	0.02%	0.002%
84	12.603	3593	3596	3602	rBV2	151	138	0.02%	0.002%
85	12.924	3692	3696	3702	rBV2	171	250	0.03%	0.003%
86	13.564	3893	3895	3899	rVB2	175	113	0.01%	0.002%
87	13.590	3899	3903	3907	rBV2	170	171	0.02%	0.002%
88	13.776	3958	3961	3963	rBV	204	118	0.01%	0.002%
89	13.988	4020	4027	4032	rBV3	458	659	0.08%	0.009%
90	14.053	4043	4047	4051	rBV	244	288	0.03%	0.004%
91	14.120	4065	4068	4073	rBV2	179	156	0.02%	0.002%
92	14.172	4081	4084	4087	rBV3	228	148	0.02%	0.002%
93	14.233	4102	4103	4107	rVB	233	132	0.02%	0.002%
94	14.294	4119	4122	4125	rBV2	283	248	0.03%	0.003%
95	14.316	4127	4129	4134	rVB2	364	223	0.03%	0.003%
96	14.448	4166	4170	4173	rBV2	174	154	0.02%	0.002%
97	14.773	4268	4271	4273	rBV2	317	195	0.02%	0.003%
98	14.992	4333	4339	4343	rBV4	429	601	0.07%	0.008%
99	15.181	4394	4398	4399	rBV2	469	303	0.04%	0.004%
100	15.474	4486	4489	4491	rBV2	388	287	0.03%	0.004%

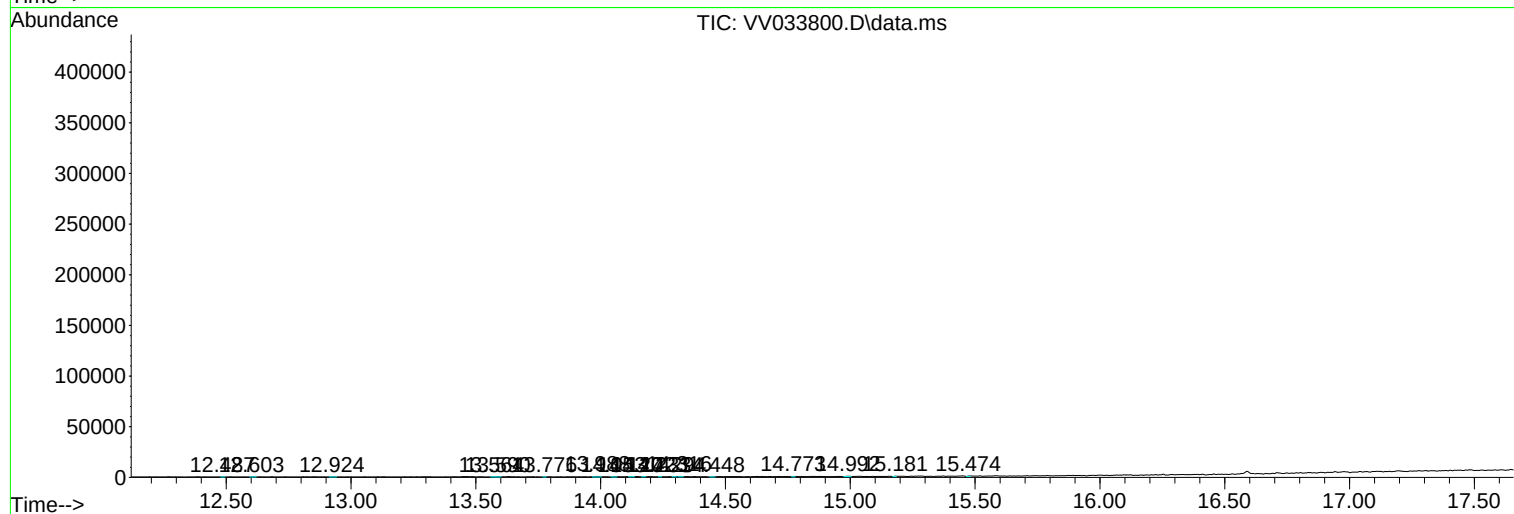
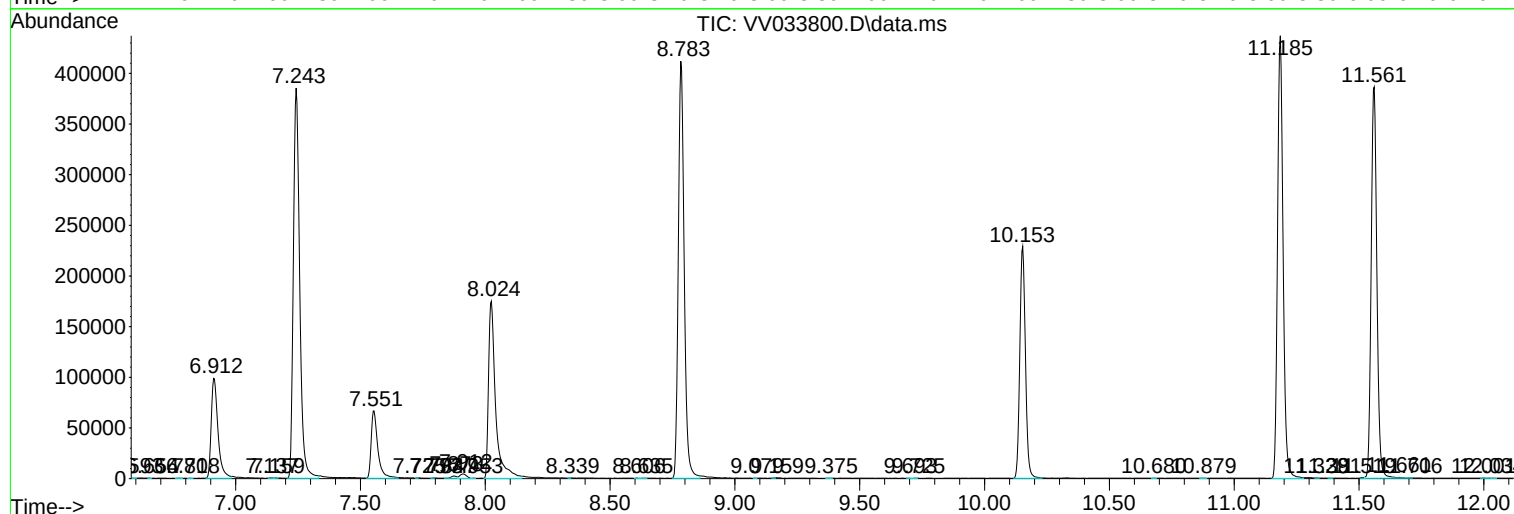
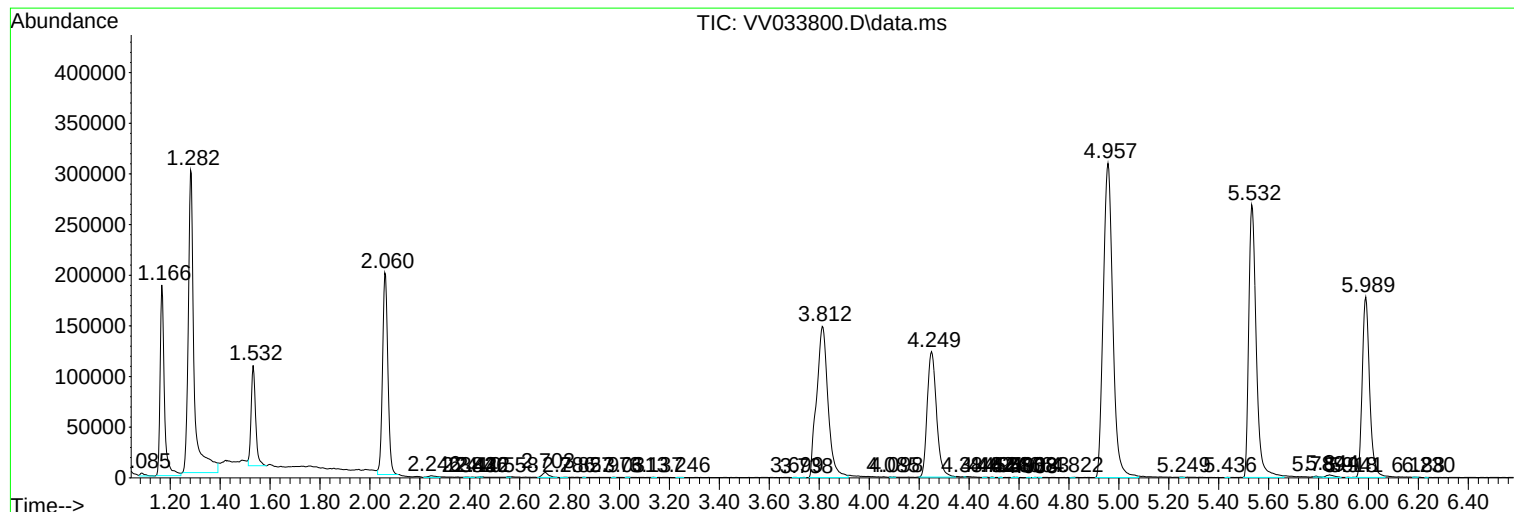
Sum of corrected areas: 7355629

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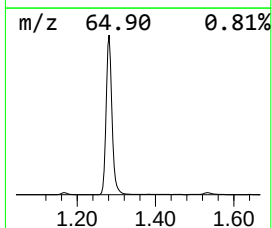
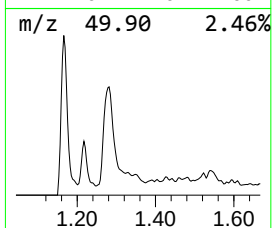
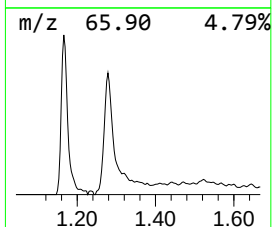
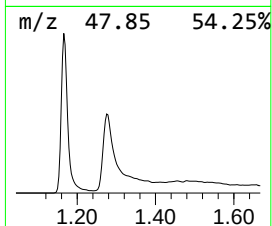
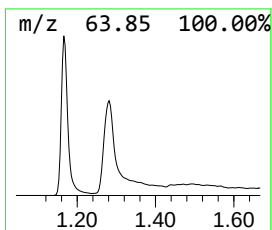
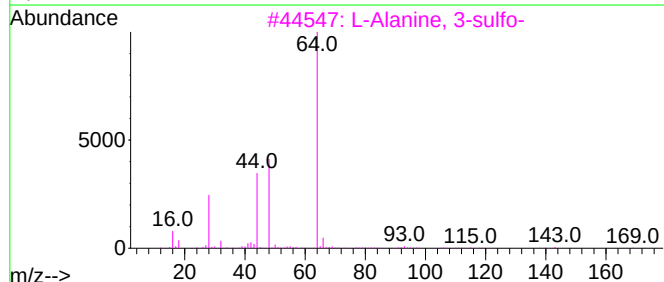
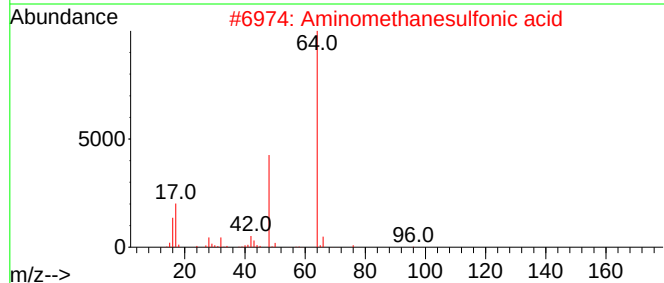
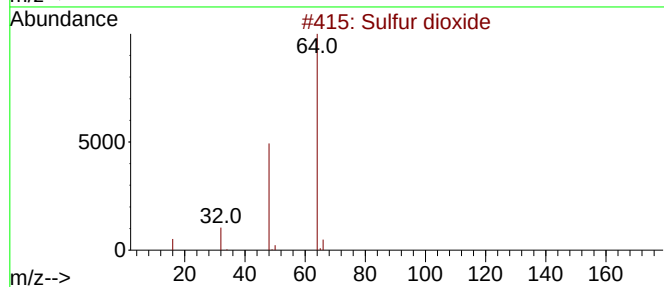
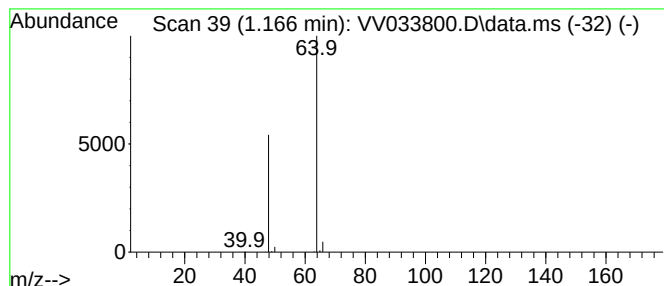
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	19.73 ug/L	222250	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			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 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	1.166	19.7	ug/L	222250	1	5.532	563162	50.0