

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033243.D
 Acq On : 12 Dec 2023 03:20
 Operator : SY/MD
 Sample : 05751-10
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHC5

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\SFAMVLM120123WMA.M
 Title : VOC Analysis

Signal : TIC: VV033243.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	33	39	54	rBV	103831	127605	12.87%	1.513%
2	1.281	67	75	99	rBV2	158015	219990	22.19%	2.609%
3	1.532	147	153	168	rVB	98956	117613	11.86%	1.395%
4	2.059	308	317	327	rBV2	220522	324890	32.77%	3.853%
5	2.214	355	365	394	rVB	109280	194347	19.61%	2.305%
6	2.387	417	419	422	rVB3	521	274	0.03%	0.003%
7	2.404	422	424	428	rVB2	654	392	0.04%	0.005%
8	2.452	430	439	445	rBV5	1416	2085	0.21%	0.025%
9	2.500	451	454	455	rBV	305	182	0.02%	0.002%
10	2.558	461	472	473	rBV3	4721	5522	0.56%	0.065%
11	2.731	523	526	529	rVB2	440	275	0.03%	0.003%
12	2.754	530	533	534	rBV	379	203	0.02%	0.002%
13	2.773	537	539	541	rBV2	408	183	0.02%	0.002%
14	2.812	546	551	554	rVB	286	254	0.03%	0.003%
15	2.886	570	574	576	rBV2	348	305	0.03%	0.004%
16	2.915	580	583	585	rBV2	297	187	0.02%	0.002%
17	2.992	605	607	610	rVB	400	224	0.02%	0.003%
18	3.114	635	645	658	rVV3	5718	12382	1.25%	0.147%
19	3.201	670	672	680	rVB2	416	518	0.05%	0.006%
20	3.236	680	683	686	rBV	194	180	0.02%	0.002%
21	3.265	689	692	696	rBV	259	231	0.02%	0.003%
22	3.358	718	721	723	rBV	261	178	0.02%	0.002%
23	3.548	776	780	784	rVB	399	340	0.03%	0.004%
24	3.780	843	852	873	rBV2	53172	140534	14.18%	1.667%
25	4.246	979	997	1022	rBV	164136	426114	42.99%	5.053%
26	4.513	1069	1080	1095	rVB7	3398	8443	0.85%	0.100%
27	4.583	1099	1102	1106	rBV2	401	304	0.03%	0.004%
28	4.619	1111	1113	1116	rBV	437	234	0.02%	0.003%
29	4.680	1129	1132	1138	rVB2	208	212	0.02%	0.003%
30	4.744	1149	1152	1154	rBV	285	223	0.02%	0.003%
31	4.844	1181	1183	1186	rVB2	326	173	0.02%	0.002%
32	4.956	1201	1218	1241	rBV2	370077	991306	100.00%	11.755%
33	5.165	1281	1283	1287	rBV3	732	586	0.06%	0.007%
34	5.262	1310	1313	1316	rBV	664	503	0.05%	0.006%
35	5.407	1351	1358	1362	rBV3	433	553	0.06%	0.007%
36	5.448	1370	1371	1375	rVB	370	248	0.03%	0.003%

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37	5.532	1386	1397	1420	rBV	324138	666103	67.19%	7.899%
38	5.837	1480	1492	1512	rBV5	67905	145515	14.68%	1.726%
39	5.989	1526	1539	1561	rBV	202157	415004	41.86%	4.921%
40	6.239	1611	1617	1618	rVB2	326	288	0.03%	0.003%
41	6.252	1618	1621	1623	rBV2	457	318	0.03%	0.004%
42	6.294	1630	1634	1640	rBV2	278	372	0.04%	0.004%
43	6.500	1694	1698	1700	rBV2	512	401	0.04%	0.005%
44	6.538	1707	1710	1713	rBV3	424	380	0.04%	0.005%
45	6.725	1764	1768	1771	rBV	235	240	0.02%	0.003%
46	6.767	1778	1781	1785	rBV2	253	200	0.02%	0.002%
47	6.873	1809	1814	1816	rBV2	315	328	0.03%	0.004%
48	6.911	1816	1826	1850	rBV	115218	211811	21.37%	2.512%
49	7.095	1880	1883	1885	rBV	429	238	0.02%	0.003%
50	7.111	1886	1888	1893	rVB3	381	230	0.02%	0.003%
51	7.191	1910	1913	1916	rVB2	330	204	0.02%	0.002%
52	7.243	1917	1929	1958	rBV	484021	844013	85.14%	10.009%
53	7.551	2016	2025	2052	rBV	86059	152293	15.36%	1.806%
54	7.696	2066	2070	2072	rBV2	613	364	0.04%	0.004%
55	7.776	2092	2095	2096	rBV2	385	187	0.02%	0.002%
56	7.815	2104	2107	2109	rVB	467	295	0.03%	0.003%
57	7.828	2109	2111	2114	rBV	573	410	0.04%	0.005%
58	7.879	2118	2127	2136	rVV5	1875	2870	0.29%	0.034%
59	8.024	2162	2172	2202	rBV	187997	361230	36.44%	4.284%
60	8.384	2282	2284	2290	rVB	401	313	0.03%	0.004%
61	8.419	2290	2295	2299	rBV	444	478	0.05%	0.006%
62	8.458	2305	2307	2312	rVV2	356	207	0.02%	0.002%
63	8.487	2314	2316	2320	rVB2	563	263	0.03%	0.003%
64	8.513	2320	2324	2327	rBV2	447	280	0.03%	0.003%
65	8.583	2341	2346	2350	rVV3	286	262	0.03%	0.003%
66	8.783	2397	2408	2438	rBV	523453	862717	87.03%	10.231%
67	9.017	2476	2481	2485	rBV3	531	526	0.05%	0.006%
68	9.159	2521	2525	2528	rBV2	445	419	0.04%	0.005%
69	9.175	2528	2530	2532	rVB	614	233	0.02%	0.003%
70	9.223	2543	2545	2548	rBV	335	222	0.02%	0.003%
71	9.313	2570	2573	2580	rVB2	470	391	0.04%	0.005%
72	9.455	2614	2617	2622	rVB3	331	267	0.03%	0.003%
73	9.490	2626	2628	2630	rBV3	521	319	0.03%	0.004%
74	9.677	2683	2686	2688	rBV	292	200	0.02%	0.002%
75	9.722	2696	2700	2701	rBV	247	180	0.02%	0.002%
76	9.773	2711	2716	2717	rBV	272	256	0.03%	0.003%

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 Title : VOC Analysis

77	9.834	2732	2735	2740	rBV2	410	220	0.02%	0.003%
78	10.040	2797	2799	2804	rVB2	731	505	0.05%	0.006%
79	10.114	2817	2822	2823	rBV2	758	591	0.06%	0.007%
80	10.152	2823	2834	2858	rVB	295930	464904	46.90%	5.513%
81	10.590	2966	2970	2973	rBV	200	172	0.02%	0.002%
82	10.670	2992	2995	2998	rBV2	374	298	0.03%	0.004%
83	10.770	3023	3026	3029	rBV2	499	475	0.05%	0.006%
84	10.943	3077	3080	3082	rBV	317	212	0.02%	0.003%
85	11.059	3113	3116	3123	rVB2	269	258	0.03%	0.003%
86	11.185	3144	3155	3188	rBV	563749	871915	87.96%	10.340%
87	11.561	3259	3272	3295	rBV	533572	839858	84.72%	9.959%
88	11.914	3378	3382	3384	rBV2	268	201	0.02%	0.002%
89	12.561	3581	3583	3592	rBV2	294	267	0.03%	0.003%
90	13.178	3769	3775	3779	rBV3	399	472	0.05%	0.006%
91	13.329	3820	3822	3827	rBV2	346	232	0.02%	0.003%
92	13.355	3827	3830	3833	rVB2	421	274	0.03%	0.003%
93	13.455	3857	3861	3863	rBV2	581	509	0.05%	0.006%
94	13.516	3875	3880	3884	rBV3	496	515	0.05%	0.006%
95	13.538	3884	3887	3889	rBV	330	232	0.02%	0.003%
96	14.027	4037	4039	4043	rBV2	443	358	0.04%	0.004%
97	14.432	4163	4165	4169	rBV2	420	332	0.03%	0.004%
98	14.503	4184	4187	4193	rVV4	734	544	0.05%	0.006%
99	14.776	4270	4272	4274	rBV	763	414	0.04%	0.005%
100	15.107	4373	4375	4378	rBV2	666	392	0.04%	0.005%

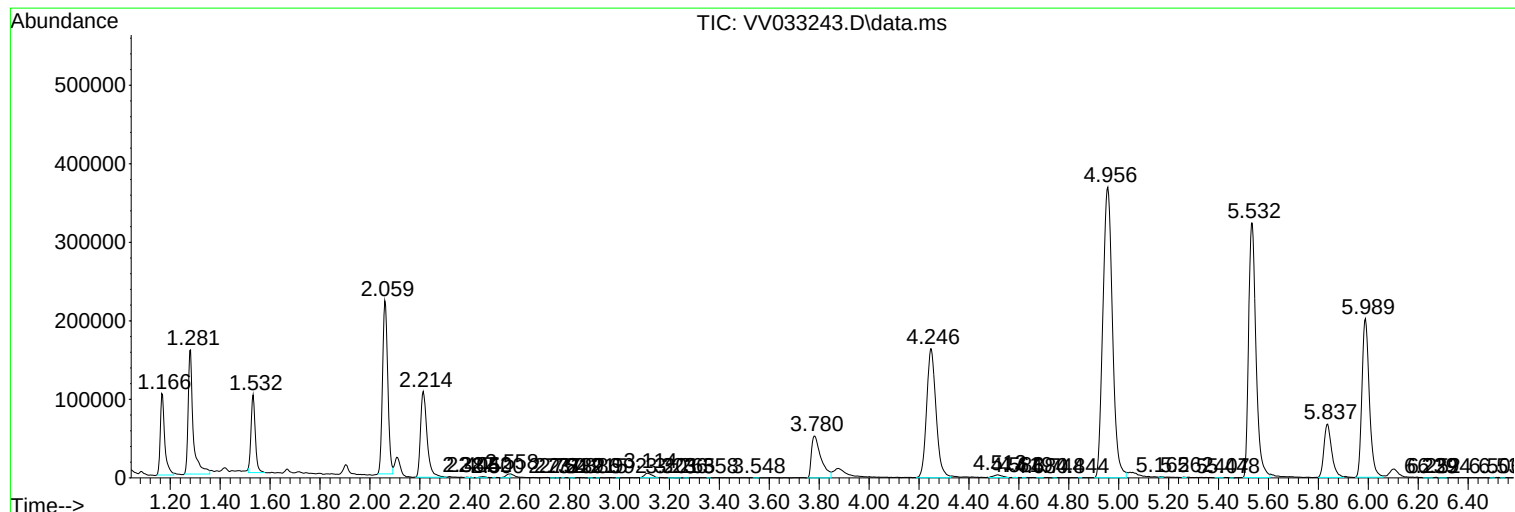
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P



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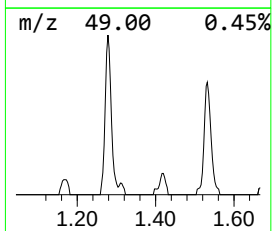
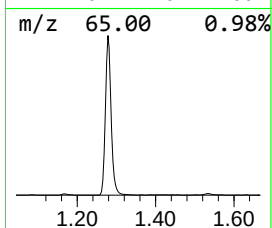
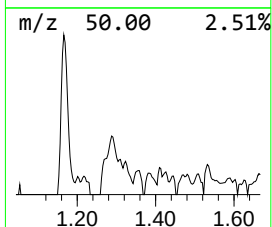
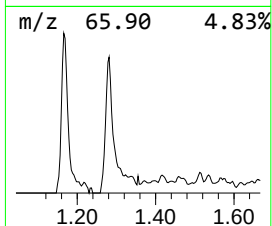
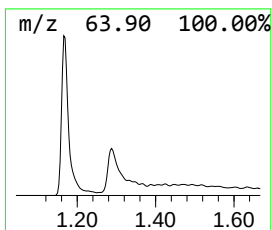
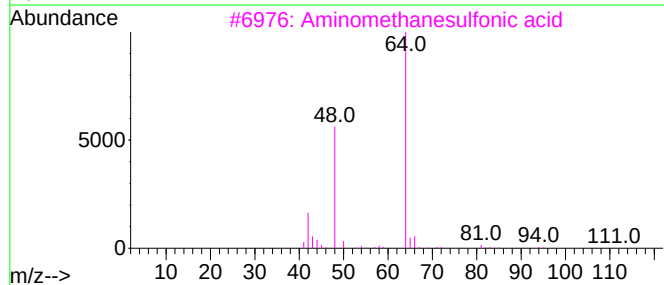
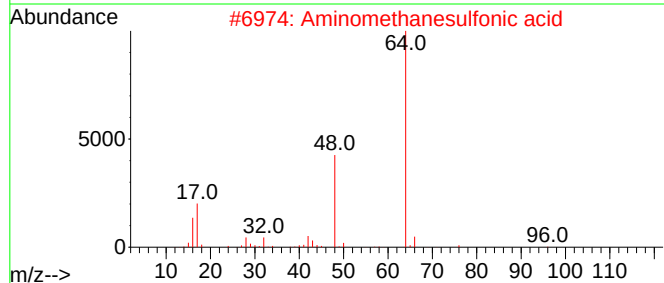
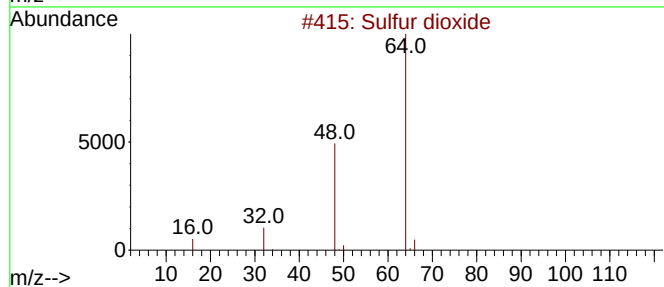
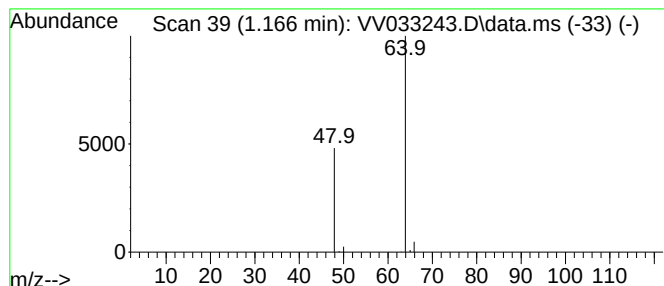
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	9.58 ug/L	127605	1,4-Difluorobenzene	5.535

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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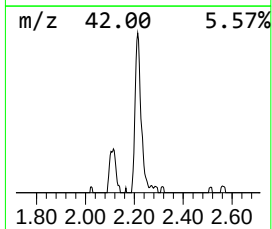
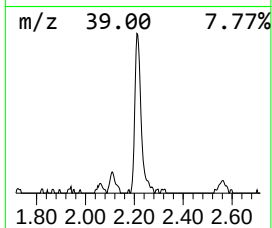
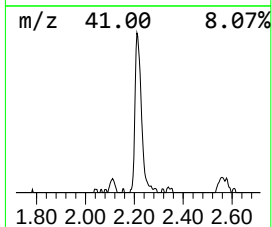
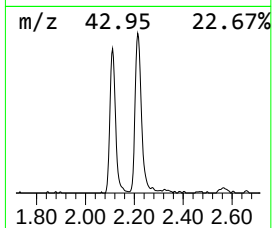
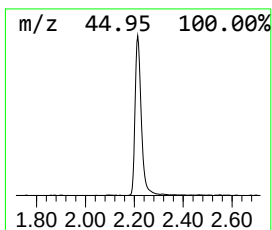
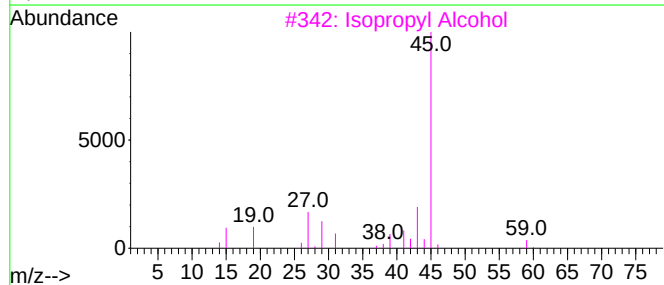
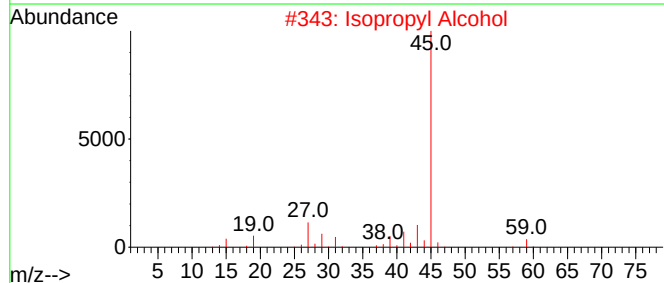
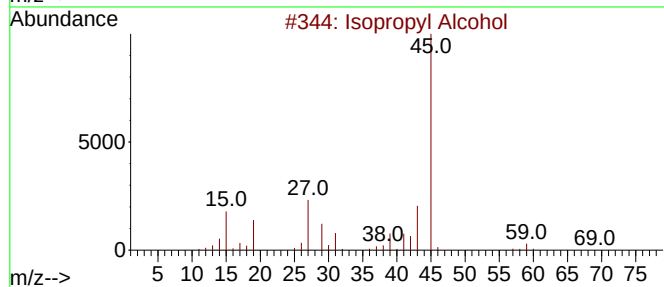
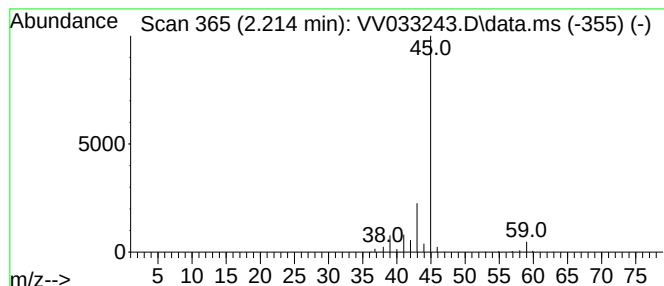
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.214	14.59 ug/L	194347	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	64



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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	9.6	ug/L	127605	1	5.535	666103	50.0
Isopropyl Alcohol	2.214	14.6	ug/L	194347	1	5.535	666103	50.0