

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033248.D
 Acq On : 12 Dec 2023 05:16
 Operator : SY/MD
 Sample : 05751-17
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHF9

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: VV033248.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	55	rBV	58185	73923	7.69%	0.889%
2	1.278	67	74	89	rBV	142000	162262	16.89%	1.952%
3	1.532	146	153	167	rVB	95486	114329	11.90%	1.375%
4	2.063	308	318	329	rBV3	324509	551916	57.44%	6.638%
5	2.214	355	365	387	rBV	134344	232443	24.19%	2.796%
6	2.445	431	437	440	rBV6	1034	1332	0.14%	0.016%
7	2.558	466	472	484	rVB3	4279	8047	0.84%	0.097%
8	2.674	504	508	509	rBV2	507	303	0.03%	0.004%
9	2.783	539	542	547	rVB2	312	276	0.03%	0.003%
10	2.912	579	582	586	rBB	350	224	0.02%	0.003%
11	2.937	586	590	594	rBB	349	331	0.03%	0.004%
12	2.960	594	597	601	rBV	397	415	0.04%	0.005%
13	3.043	621	623	626	rBV	368	240	0.02%	0.003%
14	3.114	632	645	660	rBV2	11392	23690	2.47%	0.285%
15	3.243	681	685	687	rBV2	258	203	0.02%	0.002%
16	3.375	722	726	730	rBV	153	203	0.02%	0.002%
17	3.404	731	735	739	rVV2	369	286	0.03%	0.003%
18	3.551	774	781	785	rBB	313	331	0.03%	0.004%
19	3.786	843	854	859	rBV	54525	115292	12.00%	1.387%
20	4.153	965	968	970	rBV	473	322	0.03%	0.004%
21	4.246	981	997	1026	rBV2	155700	412030	42.88%	4.956%
22	4.593	1102	1105	1109	rBV3	619	519	0.05%	0.006%
23	4.657	1119	1125	1128	rBV3	701	646	0.07%	0.008%
24	4.956	1200	1218	1248	rBV2	360157	960938	100.00%	11.558%
25	5.378	1344	1349	1350	rBV	318	249	0.03%	0.003%
26	5.532	1384	1397	1423	rBV	290409	604858	62.94%	7.275%
27	5.834	1479	1491	1522	rBV2	132407	275850	28.71%	3.318%
28	5.985	1526	1538	1561	rBV	195643	407236	42.38%	4.898%
29	6.272	1623	1627	1631	rVB2	506	417	0.04%	0.005%
30	6.291	1631	1633	1635	rBV	325	192	0.02%	0.002%
31	6.355	1649	1653	1655	rBV	304	191	0.02%	0.002%
32	6.500	1692	1698	1702	rBV3	451	471	0.05%	0.006%
33	6.657	1744	1747	1751	rVB	433	367	0.04%	0.004%
34	6.690	1751	1757	1760	rBV	366	515	0.05%	0.006%
35	6.738	1769	1772	1775	rBV	309	230	0.02%	0.003%
36	6.831	1798	1801	1805	rBV2	242	254	0.03%	0.003%

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 Title : VOC Analysis

37	6.911	1816	1826	1852	rBV	110638	207051	21.55%	2.490%
38	7.136	1893	1896	1899	rBV	243	189	0.02%	0.002%
39	7.243	1918	1929	1959	rBV	465347	816589	84.98%	9.822%
40	7.551	2016	2025	2048	rBV	79550	145664	15.16%	1.752%
41	7.751	2084	2087	2091	rBV3	405	347	0.04%	0.004%
42	7.786	2095	2098	2101	rVB2	520	379	0.04%	0.005%
43	7.853	2116	2119	2121	rVV	609	378	0.04%	0.005%
44	7.876	2121	2126	2136	rVB4	2152	3272	0.34%	0.039%
45	8.024	2162	2172	2208	rBV	182130	351063	36.53%	4.222%
46	8.407	2289	2291	2292	rBV2	451	209	0.02%	0.003%
47	8.455	2303	2306	2309	rBV2	601	340	0.04%	0.004%
48	8.471	2309	2311	2315	rVV2	316	245	0.03%	0.003%
49	8.506	2317	2322	2324	rVV2	282	241	0.03%	0.003%
50	8.654	2363	2368	2373	rBV3	353	478	0.05%	0.006%
51	8.783	2397	2408	2432	rBV	469821	766756	79.79%	9.222%
52	9.095	2503	2505	2512	rVB4	390	479	0.05%	0.006%
53	9.185	2530	2533	2536	rBV	328	232	0.02%	0.003%
54	9.207	2538	2540	2543	rBV2	278	194	0.02%	0.002%
55	9.313	2569	2573	2577	rBV2	274	293	0.03%	0.004%
56	9.432	2608	2610	2616	rVB	479	408	0.04%	0.005%
57	9.474	2621	2623	2626	rVB	385	180	0.02%	0.002%
58	9.542	2641	2644	2649	rBV2	470	444	0.05%	0.005%
59	9.596	2658	2661	2665	rBB	313	221	0.02%	0.003%
60	9.628	2666	2671	2675	rBV2	335	452	0.05%	0.005%
61	9.680	2683	2687	2691	rBV	242	239	0.02%	0.003%
62	9.960	2768	2774	2776	rBV3	1747	1904	0.20%	0.023%
63	10.030	2793	2796	2802	rVB	336	274	0.03%	0.003%
64	10.152	2819	2834	2862	rBV	284983	452958	47.14%	5.448%
65	10.268	2867	2870	2873	rVB2	297	205	0.02%	0.002%
66	10.323	2880	2887	2895	rVB4	2488	3356	0.35%	0.040%
67	10.374	2901	2903	2906	rBV2	265	192	0.02%	0.002%
68	10.538	2947	2954	2956	rBV2	216	278	0.03%	0.003%
69	10.615	2975	2978	2980	rBV	207	171	0.02%	0.002%
70	10.757	3016	3022	3024	rBV2	249	241	0.03%	0.003%
71	10.895	3063	3065	3068	rBV2	306	228	0.02%	0.003%
72	11.004	3093	3099	3103	rBV2	302	413	0.04%	0.005%
73	11.069	3113	3119	3124	rBV2	366	509	0.05%	0.006%
74	11.123	3133	3136	3142	rVB2	292	268	0.03%	0.003%
75	11.185	3143	3155	3176	rBV	510330	784785	81.67%	9.439%
76	11.496	3248	3252	3253	rVB	341	210	0.02%	0.003%

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 Title : VOC Analysis

77	11.561	3259	3272	3293	rBV	516177	813897	84.70%	9.789%
78	11.857	3361	3364	3368	rBV3	356	361	0.04%	0.004%
79	11.914	3381	3382	3387	rVB2	348	208	0.02%	0.003%
80	11.940	3388	3390	3393	rBV	254	190	0.02%	0.002%
81	11.976	3398	3401	3403	rBV3	270	175	0.02%	0.002%
82	12.030	3415	3418	3419	rBV	346	220	0.02%	0.003%
83	12.136	3448	3451	3456	rBV2	256	209	0.02%	0.003%
84	12.165	3456	3460	3462	rBV	318	214	0.02%	0.003%
85	12.300	3499	3502	3505	rBV2	323	300	0.03%	0.004%
86	12.545	3575	3578	3583	rVB	280	217	0.02%	0.003%
87	12.574	3583	3587	3589	rBV2	316	234	0.02%	0.003%
88	12.853	3667	3674	3677	rBV2	389	465	0.05%	0.006%
89	12.930	3693	3698	3701	rBV2	596	457	0.05%	0.005%
90	12.950	3701	3704	3706	rBV2	253	181	0.02%	0.002%
91	12.975	3706	3712	3716	rBV3	479	557	0.06%	0.007%
92	13.175	3770	3774	3776	rBV3	297	207	0.02%	0.002%
93	13.184	3776	3777	3780	rVV	357	202	0.02%	0.002%
94	13.213	3784	3786	3790	rVB2	421	290	0.03%	0.003%
95	13.455	3857	3861	3862	rBV2	487	371	0.04%	0.004%
96	13.535	3883	3886	3888	rBV2	296	216	0.02%	0.003%
97	13.918	4002	4005	4008	rBV2	398	257	0.03%	0.003%
98	14.059	4046	4049	4053	rVB2	682	487	0.05%	0.006%
99	14.082	4053	4056	4058	rBV2	335	223	0.02%	0.003%
100	14.146	4072	4076	4080	rBV3	412	420	0.04%	0.005%

Sum of corrected areas: 8314224

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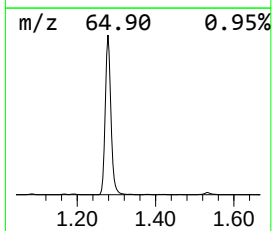
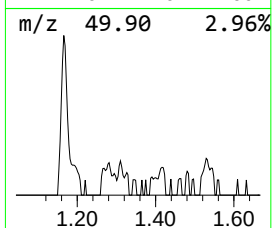
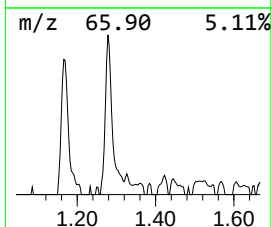
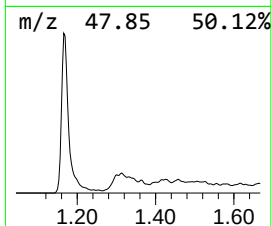
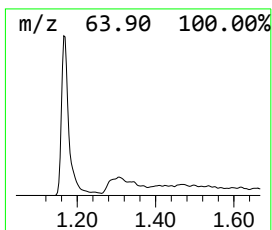
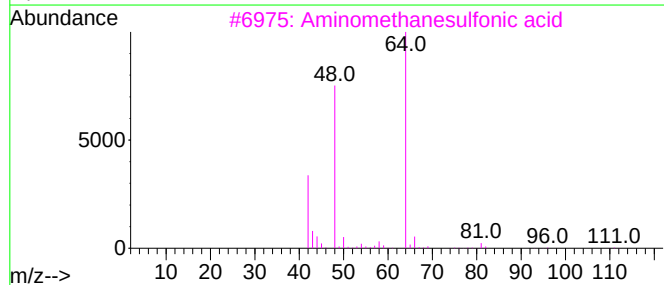
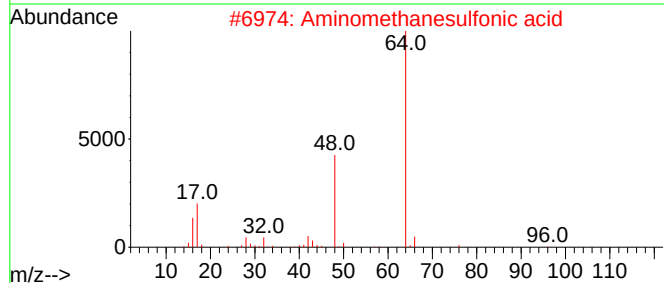
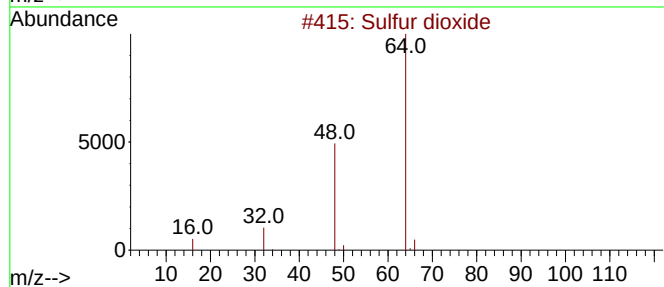
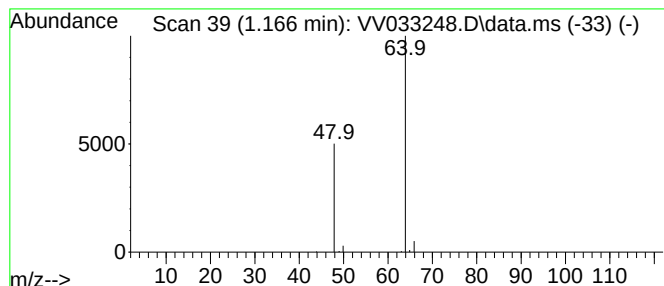
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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	6.11 ug/L	73923	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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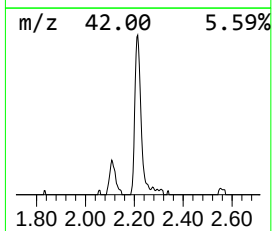
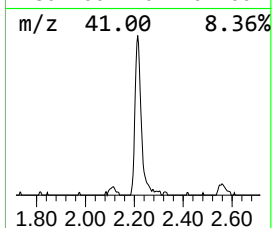
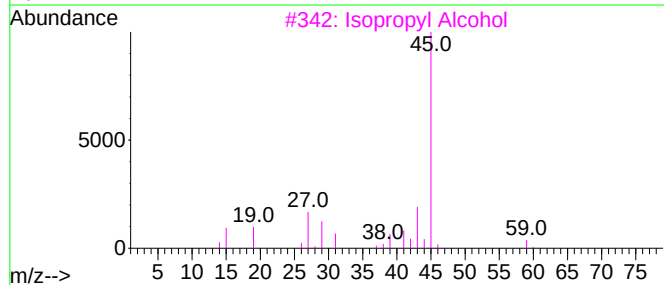
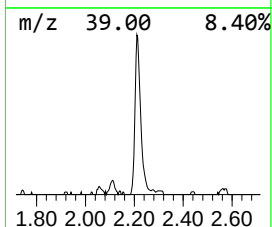
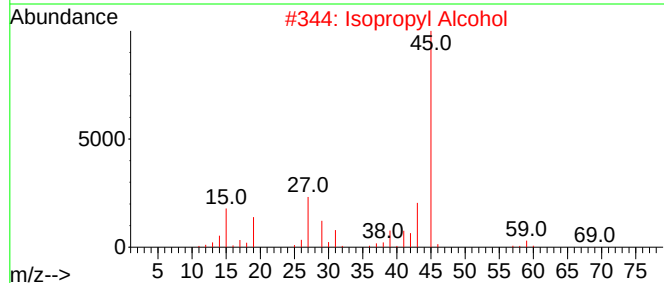
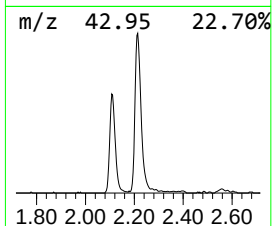
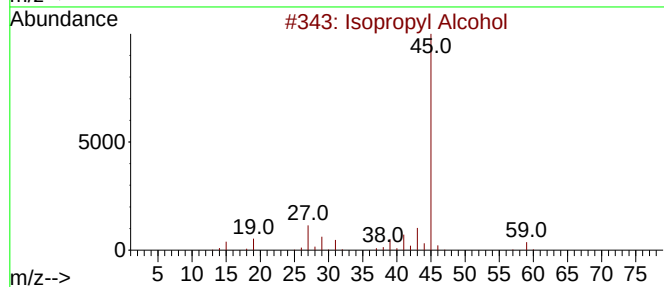
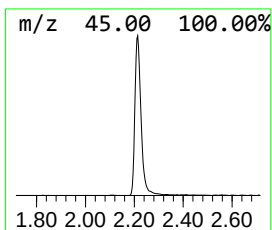
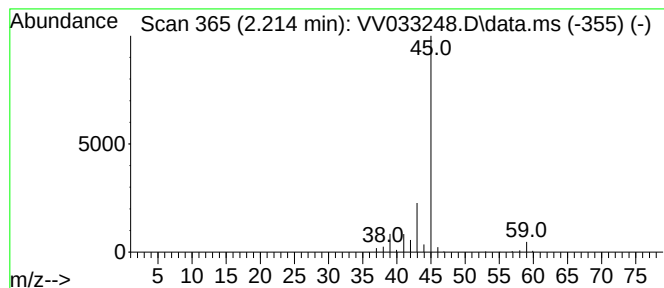
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.214	19.21 ug/L	232443	1,4-Difluorobenzene	5.532

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	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.166	6.1	ug/L	73923	1	5.532	604858	50.0
Isopropyl Alcohol	2.214	19.2	ug/L	232443	1	5.532	604858	50.0