

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045230.D
 Acq On : 08 Oct 2021 00:15
 Operator : SY/MD
 Sample : M4138-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7F4

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_U\Method\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	13	rVB2	4731	4361	0.34%	0.045%
2	1.465	31	39	54	rBV	107987	182623	14.24%	1.879%
3	1.597	75	80	96	rVB	178766	199520	15.56%	2.053%
4	1.893	165	172	185	rVB	132811	178552	13.93%	1.837%
5	2.562	368	380	396	rBV	249167	420182	32.77%	4.323%
6	2.700	421	423	432	rVV	199	196	0.02%	0.002%
7	2.780	435	448	465	rBV3	5357	11897	0.93%	0.122%
8	2.957	496	503	505	rBV2	429	596	0.05%	0.006%
9	3.054	525	533	537	rBV3	547	695	0.05%	0.007%
10	3.150	560	563	565	rBV	228	171	0.01%	0.002%
11	3.195	565	577	587	rVV	2635	5729	0.45%	0.059%
12	3.253	591	595	597	rBV	212	179	0.01%	0.002%
13	3.292	604	607	610	rBV2	190	149	0.01%	0.002%
14	3.314	610	614	618	rVB	240	251	0.02%	0.003%
15	3.350	621	625	629	rBV2	211	195	0.02%	0.002%
16	3.436	649	652	655	rBV2	197	135	0.01%	0.001%
17	3.488	664	668	670	rBV	185	122	0.01%	0.001%
18	3.649	711	718	723	rBV2	280	322	0.03%	0.003%
19	3.687	726	730	736	rBV2	153	250	0.02%	0.003%
20	3.874	772	788	805	rBV	10147	23268	1.81%	0.239%
21	3.964	813	816	821	rVB2	234	183	0.01%	0.002%
22	4.005	826	829	831	rBV	271	164	0.01%	0.002%
23	4.079	849	852	854	rBV	183	124	0.01%	0.001%
24	4.169	874	880	882	rBV	191	208	0.02%	0.002%
25	4.324	925	928	932	rVB2	157	142	0.01%	0.001%
26	4.346	932	935	937	rBV2	198	157	0.01%	0.002%
27	4.501	981	983	988	rVB	164	120	0.01%	0.001%
28	4.629	1007	1023	1048	rBV	146148	344845	26.90%	3.548%
29	4.890	1102	1104	1107	rBV2	191	130	0.01%	0.001%
30	4.951	1119	1123	1124	rBV2	168	119	0.01%	0.001%
31	4.960	1124	1126	1133	rVV2	319	390	0.03%	0.004%
32	5.067	1143	1159	1177	rBV	227678	491520	38.34%	5.057%
33	5.211	1201	1204	1209	rVB2	488	373	0.03%	0.004%
34	5.298	1222	1231	1237	rBV2	575	969	0.08%	0.010%
35	5.378	1253	1256	1259	rVB2	225	136	0.01%	0.001%
36	5.729	1343	1365	1399	rBV2	481496	1282117	100.00%	13.192%

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 Title : VOC Analysis

37	5.931	1425	1428	1433	rBV3	213	211	0.02%	0.002%
38	5.973	1438	1441	1442	rBV2	203	136	0.01%	0.001%
39	6.105	1480	1482	1487	rVB2	289	237	0.02%	0.002%
40	6.166	1495	1501	1509	rVB2	459	615	0.05%	0.006%
41	6.253	1513	1528	1547	rBV	370515	686473	53.54%	7.063%
42	6.529	1608	1614	1623	rBV5	1551	2806	0.22%	0.029%
43	6.581	1628	1630	1633	rVV2	269	127	0.01%	0.001%
44	6.697	1651	1666	1687	rBV	305051	590704	46.07%	6.078%
45	6.800	1693	1698	1699	rBV2	514	419	0.03%	0.004%
46	6.854	1713	1715	1719	rBV	225	167	0.01%	0.002%
47	7.009	1759	1763	1765	rBV2	130	134	0.01%	0.001%
48	7.041	1768	1773	1775	rBV2	303	251	0.02%	0.003%
49	7.089	1784	1788	1793	rVB2	220	260	0.02%	0.003%
50	7.124	1793	1799	1801	rBV2	190	243	0.02%	0.003%
51	7.182	1811	1817	1826	rBV6	1395	1927	0.15%	0.020%
52	7.269	1841	1844	1850	rVB2	228	229	0.02%	0.002%
53	7.465	1903	1905	1911	rBV	129	165	0.01%	0.002%
54	7.568	1924	1937	1960	rBV	159571	279349	21.79%	2.874%
55	7.690	1969	1975	1980	rBV	743	1045	0.08%	0.011%
56	7.793	2004	2007	2011	rVB	299	207	0.02%	0.002%
57	7.816	2011	2014	2020	rVB2	125	120	0.01%	0.001%
58	7.902	2026	2041	2055	rBV	569671	970155	75.67%	9.982%
59	7.973	2056	2063	2073	rVB	10950	18112	1.41%	0.186%
60	8.182	2116	2128	2152	rBV	114127	186206	14.52%	1.916%
61	8.404	2193	2197	2200	rVB2	176	147	0.01%	0.002%
62	8.423	2200	2203	2206	rBV	186	190	0.01%	0.002%
63	8.478	2212	2220	2233	rVB	528	999	0.08%	0.010%
64	8.636	2256	2269	2304	rBV	431982	758730	59.18%	7.807%
65	8.986	2375	2378	2382	rBV	203	209	0.02%	0.002%
66	9.182	2436	2439	2442	rVB	254	189	0.01%	0.002%
67	9.201	2442	2445	2448	rBV2	242	206	0.02%	0.002%
68	9.336	2484	2487	2489	rBV	135	124	0.01%	0.001%
69	9.420	2500	2513	2549	rBV	510716	828062	64.59%	8.520%
70	9.574	2552	2561	2571	rVB	10013	15009	1.17%	0.154%
71	9.697	2588	2599	2612	rVB2	30408	48979	3.82%	0.504%
72	9.764	2617	2620	2626	rBV2	391	355	0.03%	0.004%
73	9.947	2671	2677	2683	rVB2	267	350	0.03%	0.004%
74	9.976	2683	2686	2688	rBV2	229	186	0.01%	0.002%
75	10.034	2700	2704	2708	rBV2	211	213	0.02%	0.002%
76	10.105	2717	2726	2736	rVB2	7203	10717	0.84%	0.110%

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 Title : VOC Analysis

77	10.674	2893	2903	2910	rBV4	2059	3062	0.24%	0.032%
78	10.761	2917	2930	2948	rVB	428075	685373	53.46%	7.052%
79	10.864	2959	2962	2966	rBV3	347	275	0.02%	0.003%
80	10.912	2975	2977	2980	rVB	278	131	0.01%	0.001%
81	11.127	3042	3044	3048	rVB3	231	163	0.01%	0.002%
82	11.365	3115	3118	3122	rBV2	236	166	0.01%	0.002%
83	11.468	3141	3150	3161	rBV5	1989	3390	0.26%	0.035%
84	11.545	3170	3174	3175	rBV	137	121	0.01%	0.001%
85	11.629	3193	3200	3205	rVB3	1086	1260	0.10%	0.013%
86	11.703	3219	3223	3227	rVB2	586	528	0.04%	0.005%
87	11.815	3245	3258	3279	rBV	438454	683094	53.28%	7.029%
88	11.899	3279	3284	3289	rVB4	514	695	0.05%	0.007%
89	11.973	3303	3307	3316	rVB4	1370	1552	0.12%	0.016%
90	12.069	3328	3337	3343	rBV3	2112	3269	0.25%	0.034%
91	12.198	3363	3377	3395	rBV	480049	776303	60.55%	7.988%
92	12.262	3395	3397	3403	rVB3	307	314	0.02%	0.003%
93	12.571	3488	3493	3495	rBV2	347	315	0.02%	0.003%
94	12.632	3510	3512	3515	rBV	197	136	0.01%	0.001%
95	12.957	3609	3613	3615	rBV	265	224	0.02%	0.002%
96	13.137	3666	3669	3672	rBV2	171	119	0.01%	0.001%
97	13.163	3672	3677	3679	rBV	297	321	0.03%	0.003%
98	13.339	3725	3732	3736	rBV2	286	446	0.03%	0.005%
99	13.455	3762	3768	3773	rBV3	547	734	0.06%	0.008%
100	14.092	3962	3966	3973	rVB3	634	845	0.07%	0.009%

Sum of corrected areas: 9718889

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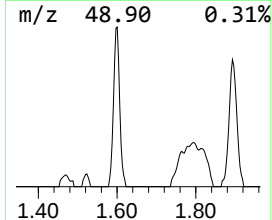
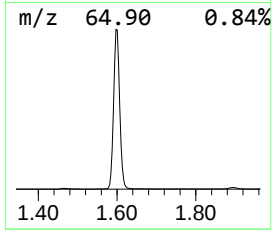
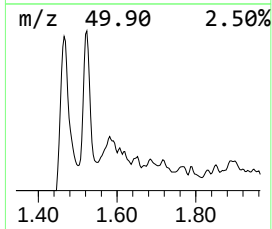
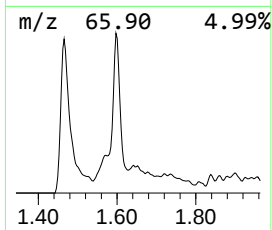
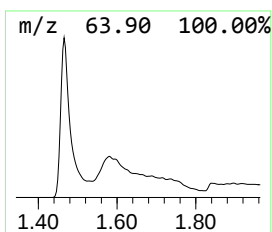
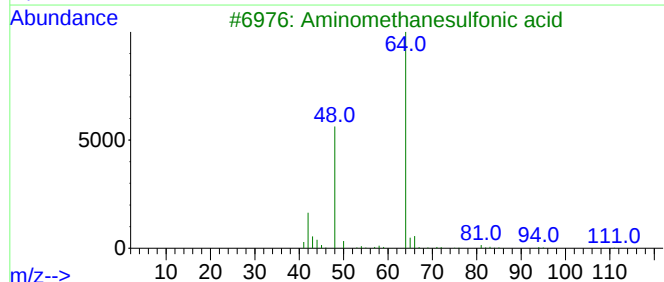
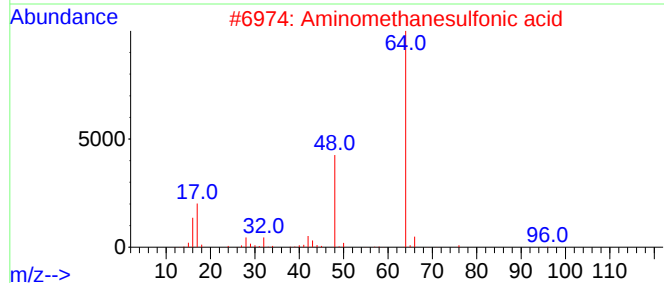
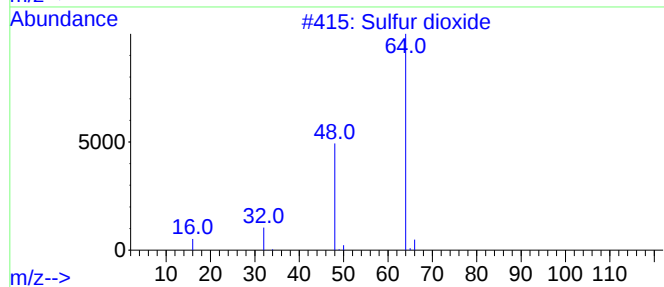
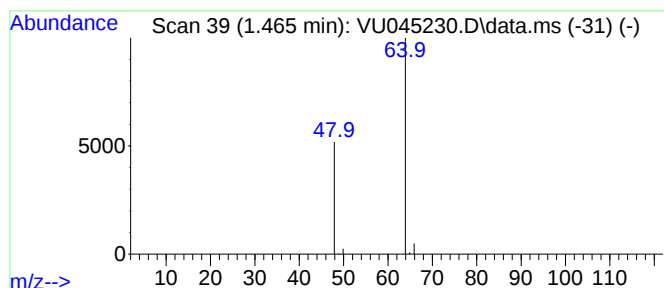
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.465	13.30 ug/L	182623	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
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	1.465	13.3	ug/L	182623	1	6.253	686473	50.0