

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045255.D
 Acq On : 08 Oct 2021 16:40
 Operator : SY/MD
 Sample : M4027-03DL 20X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AT7DL

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: VU045255.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	32	41	52	rBV2	105708	148729	11.04%	1.253%
2	1.600	74	81	98	rVB	225564	241983	17.95%	2.038%
3	1.890	163	171	188	rVB	149233	204277	15.16%	1.720%
4	2.562	367	380	399	rBV	281386	472101	35.03%	3.976%
5	2.793	443	452	461	rVB	800	1359	0.10%	0.011%
6	2.893	478	483	484	rBV	218	169	0.01%	0.001%
7	2.960	496	504	513	rVB2	825	1404	0.10%	0.012%
8	3.047	521	531	544	rVB2	4822	8504	0.63%	0.072%
9	3.186	563	574	589	rVB3	1912	4398	0.33%	0.037%
10	3.350	613	625	626	rBV5	2141	2804	0.21%	0.024%
11	3.661	719	722	724	rBV2	172	143	0.01%	0.001%
12	3.758	744	752	757	rBV2	321	460	0.03%	0.004%
13	3.864	780	785	786	rBV	216	197	0.01%	0.002%
14	3.970	807	818	823	rBV2	907	1680	0.12%	0.014%
15	4.565	999	1003	1008	rVB2	219	275	0.02%	0.002%
16	4.629	1008	1023	1032	rBV	148536	359370	26.66%	3.026%
17	5.067	1142	1159	1186	rBV	236823	511224	37.93%	4.305%
18	5.224	1203	1208	1215	rVB3	367	291	0.02%	0.002%
19	5.288	1222	1228	1231	rBV2	512	694	0.05%	0.006%
20	5.382	1253	1257	1259	rBV2	562	461	0.03%	0.004%
21	5.465	1278	1283	1286	rVB2	318	323	0.02%	0.003%
22	5.729	1343	1365	1390	rBV2	502001	1347775	100.00%	11.350%
23	5.912	1420	1422	1426	rBV3	306	196	0.01%	0.002%
24	6.083	1473	1475	1481	rBV2	157	182	0.01%	0.002%
25	6.124	1482	1488	1491	rVV3	343	355	0.03%	0.003%
26	6.173	1499	1503	1509	rVB2	204	234	0.02%	0.002%
27	6.253	1509	1528	1544	rBV	359379	670383	49.74%	5.646%
28	6.546	1603	1619	1650	rBV	583533	1088056	80.73%	9.163%
29	6.693	1651	1665	1683	rVV	317612	609509	45.22%	5.133%
30	6.803	1695	1699	1707	rVB4	741	1084	0.08%	0.009%
31	6.967	1745	1750	1751	rBV2	402	314	0.02%	0.003%
32	7.050	1766	1776	1787	rVB4	1296	2204	0.16%	0.019%
33	7.179	1809	1816	1828	rBV6	1023	1709	0.13%	0.014%
34	7.298	1850	1853	1861	rBV2	119	155	0.01%	0.001%
35	7.481	1908	1910	1915	rVB2	180	160	0.01%	0.001%
36	7.568	1924	1937	1960	rBV	170729	298543	22.15%	2.514%

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 Title : VOC Analysis

37	7.687	1971	1974	1976	rBV3	468	313	0.02%	0.003%
38	7.796	1998	2008	2019	rBV3	8616	14092	1.05%	0.119%
39	7.902	2027	2041	2055	rBV	606081	1037784	77.00%	8.740%
40	7.973	2056	2063	2075	rVB	10177	16330	1.21%	0.138%
41	8.182	2116	2128	2145	rBV	120785	199190	14.78%	1.677%
42	8.275	2153	2157	2160	rBV3	270	179	0.01%	0.002%
43	8.340	2172	2177	2181	rVB3	705	684	0.05%	0.006%
44	8.404	2191	2197	2201	rBV5	595	575	0.04%	0.005%
45	8.468	2209	2217	2220	rBV3	490	684	0.05%	0.006%
46	8.555	2231	2244	2257	rBV	383637	637683	47.31%	5.370%
47	8.639	2257	2270	2302	rVB	423297	767611	56.95%	6.464%
48	8.793	2316	2318	2323	rVB	362	186	0.01%	0.002%
49	8.812	2323	2324	2327	rVV2	248	148	0.01%	0.001%
50	8.841	2328	2333	2341	rVB2	1284	1771	0.13%	0.015%
51	8.880	2341	2345	2348	rBV2	169	154	0.01%	0.001%
52	8.896	2348	2350	2355	rVB	276	207	0.02%	0.002%
53	8.935	2358	2362	2363	rVV	267	168	0.01%	0.001%
54	9.015	2383	2387	2391	rVB	223	172	0.01%	0.001%
55	9.041	2391	2395	2397	rBV	253	227	0.02%	0.002%
56	9.420	2499	2513	2534	rBV	526344	842060	62.48%	7.091%
57	9.542	2547	2551	2553	rVB3	435	354	0.03%	0.003%
58	9.574	2553	2561	2571	rBB2	1769	2615	0.19%	0.022%
59	9.697	2586	2599	2612	rVB	6538	10455	0.78%	0.088%
60	9.764	2612	2620	2623	rBV3	612	814	0.06%	0.007%
61	9.934	2670	2673	2678	rVB	196	196	0.01%	0.002%
62	9.957	2678	2680	2683	rBV2	199	155	0.01%	0.001%
63	10.108	2718	2727	2735	rBV6	2140	3291	0.24%	0.028%
64	10.237	2763	2767	2771	rBV2	203	229	0.02%	0.002%
65	10.327	2790	2795	2803	rVB3	564	737	0.05%	0.006%
66	10.381	2809	2812	2814	rBV	250	185	0.01%	0.002%
67	10.488	2841	2845	2849	rBV2	358	358	0.03%	0.003%
68	10.674	2895	2903	2914	rBV2	3611	4810	0.36%	0.041%
69	10.761	2917	2930	2948	rBV	448411	716194	53.14%	6.031%
70	10.873	2959	2965	2966	rBV2	455	394	0.03%	0.003%
71	10.899	2971	2973	2978	rBV5	567	484	0.04%	0.004%
72	10.996	2996	3003	3012	rVB4	573	974	0.07%	0.008%
73	11.047	3015	3019	3025	rBV2	227	307	0.02%	0.003%
74	11.092	3027	3033	3036	rBV2	623	658	0.05%	0.006%
75	11.211	3065	3070	3073	rBV2	215	235	0.02%	0.002%
76	11.381	3120	3123	3128	rVV2	270	259	0.02%	0.002%

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 Title : VOC Analysis

77	11.426	3134	3137	3140	rVV	343	242	0.02%	0.002%
78	11.462	3140	3148	3162	rVB5	2512	4418	0.33%	0.037%
79	11.639	3201	3203	3208	rBV	235	208	0.02%	0.002%
80	11.700	3216	3222	3228	rVB4	1333	1678	0.12%	0.014%
81	11.745	3233	3236	3238	rBV2	259	192	0.01%	0.002%
82	11.815	3245	3258	3273	rBV	478560	739413	54.86%	6.227%
83	11.915	3285	3289	3291	rBV2	394	287	0.02%	0.002%
84	11.976	3303	3308	3318	rVB4	2482	3483	0.26%	0.029%
85	12.195	3359	3376	3397	rBV	536062	874106	64.86%	7.361%
86	12.333	3414	3419	3426	rVB3	851	1105	0.08%	0.009%
87	12.381	3432	3434	3437	rBV2	202	163	0.01%	0.001%
88	12.401	3437	3440	3445	rVB4	431	451	0.03%	0.004%
89	12.555	3485	3488	3493	rBV2	186	182	0.01%	0.002%
90	12.622	3505	3509	3510	rBV2	240	183	0.01%	0.002%
91	12.716	3533	3538	3541	rBV2	225	221	0.02%	0.002%
92	12.738	3541	3545	3548	rVV	250	227	0.02%	0.002%
93	12.774	3553	3556	3560	rVV2	183	186	0.01%	0.002%
94	13.034	3633	3637	3639	rBV2	223	230	0.02%	0.002%
95	13.073	3645	3649	3651	rBV2	218	189	0.01%	0.002%
96	13.288	3712	3716	3718	rBV2	232	203	0.02%	0.002%
97	14.085	3959	3964	3965	rBV2	665	486	0.04%	0.004%
98	14.520	4096	4099	4107	rVB3	334	350	0.03%	0.003%
99	14.854	4197	4203	4205	rBV2	297	311	0.02%	0.003%
100	15.037	4257	4260	4262	rBV	280	207	0.02%	0.002%

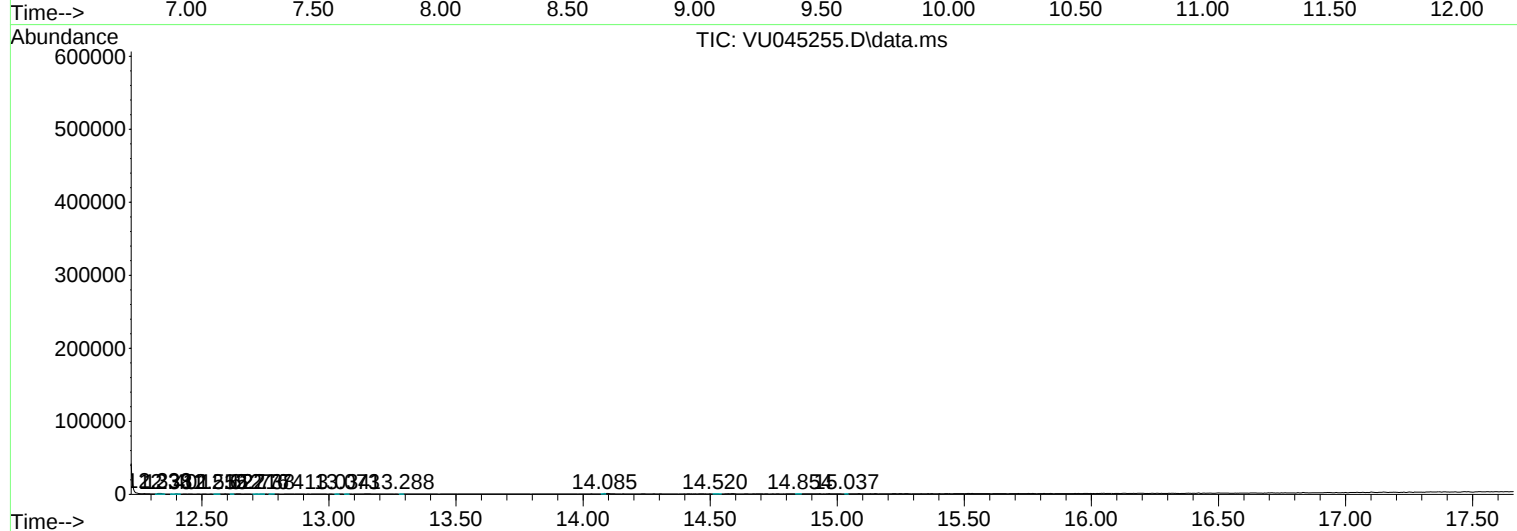
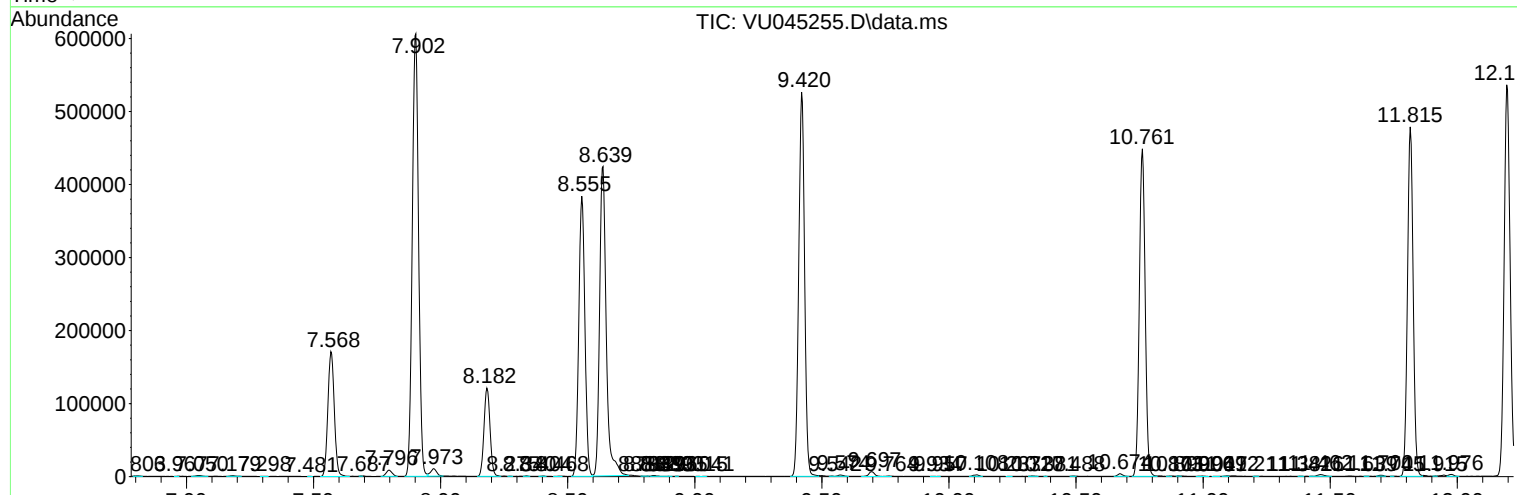
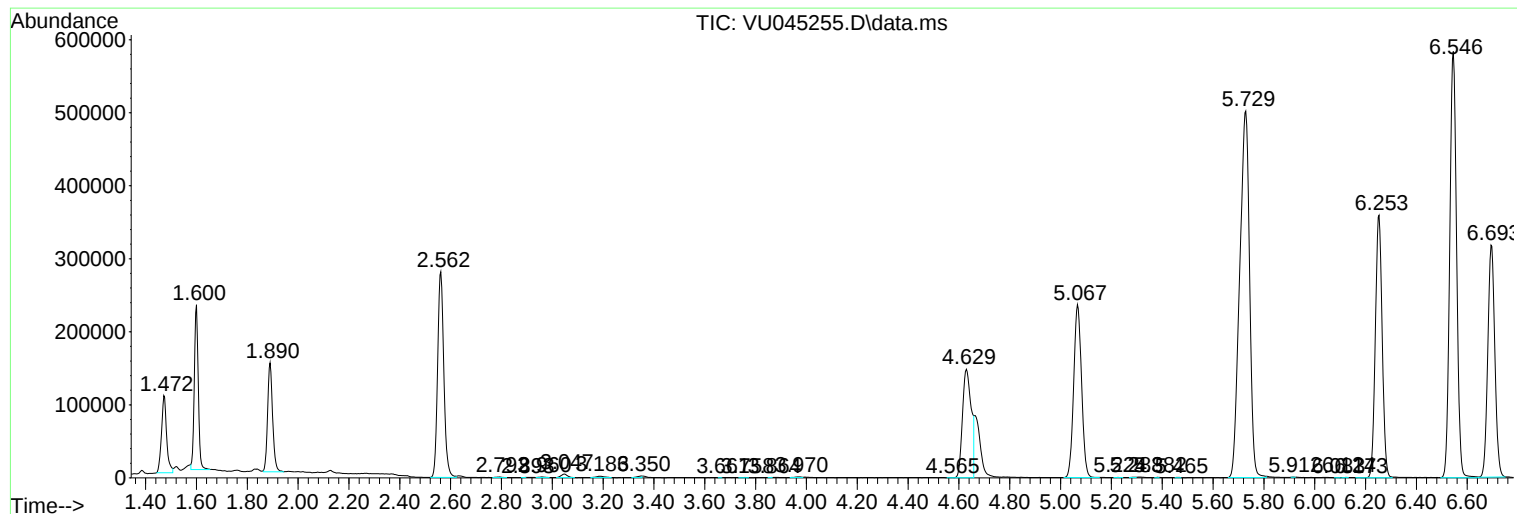
Sum of corrected areas: 11874348

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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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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



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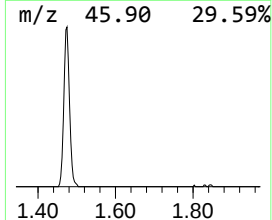
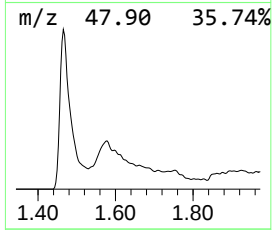
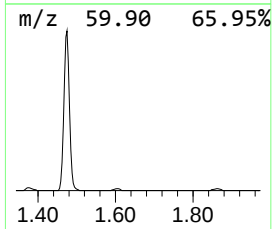
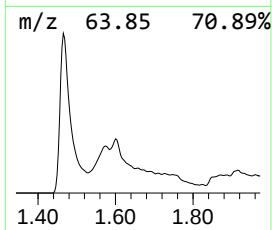
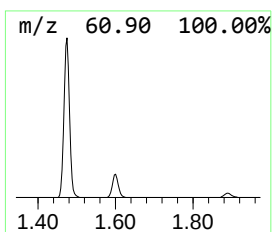
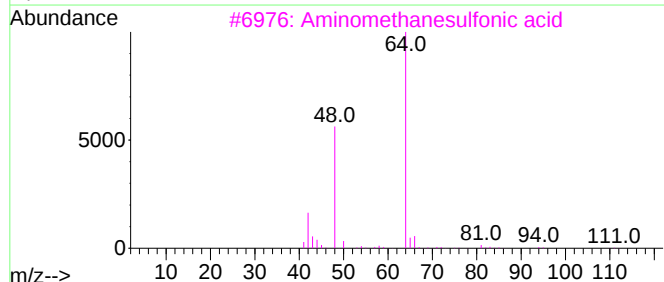
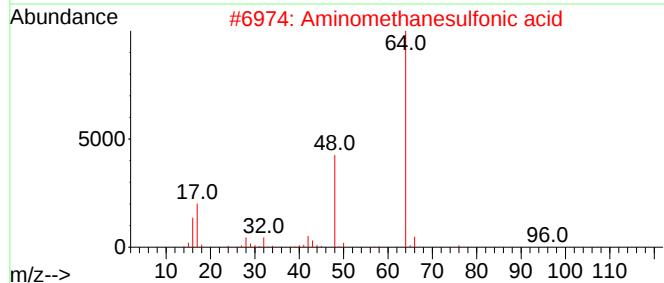
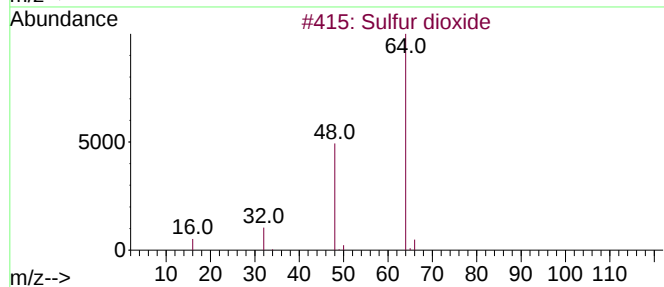
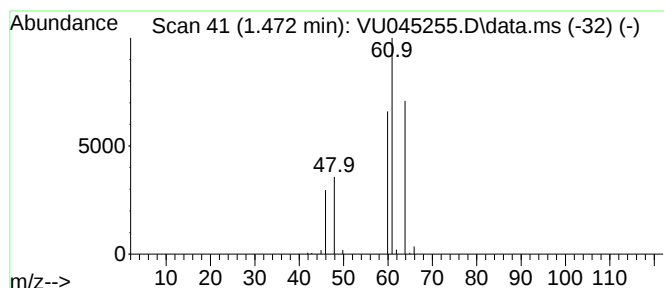
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.472	11.09 ug/L	148729	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	46
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	25
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	25
4			Pentaborane(11)	66	B5H11	018433-84-6	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
unknown-01	1.472	11.1	ug/L	148729	1	6.253	670383	50.0