

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045101.D
 Acq On : 04 Oct 2021 17:08
 Operator : SY/MD
 Sample : M3996-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A27

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: VU045101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	35	42	53	rBV	22575	36682	0.16%	0.111%
2	1.601	74	81	92	rBV	137690	155247	0.67%	0.471%
3	1.906	168	176	195	rVB	110321	153692	0.66%	0.466%
4	2.469	344	351	361	rVB4	2149	3160	0.01%	0.010%
5	2.568	369	382	400	rBV	225889	374329	1.61%	1.135%
6	2.691	416	420	422	rBV2	291	154	0.00%	0.000%
7	2.758	436	441	445	rBV2	181	256	0.00%	0.001%
8	2.797	448	453	458	rVB2	453	515	0.00%	0.002%
9	3.047	524	531	538	rBB6	669	923	0.00%	0.003%
10	3.076	538	540	543	rBV	236	183	0.00%	0.001%
11	3.134	555	558	560	rBV3	309	209	0.00%	0.001%
12	3.192	563	576	592	rVB2	3282	7464	0.03%	0.023%
13	3.366	611	630	650	rBV2	81845	189235	0.81%	0.574%
14	3.665	720	723	730	rVB2	277	377	0.00%	0.001%
15	3.697	730	733	741	rVB2	267	378	0.00%	0.001%
16	3.742	741	747	753	rBV2	225	314	0.00%	0.001%
17	3.771	753	756	758	rBV	178	148	0.00%	0.000%
18	4.089	852	855	857	rBV	162	137	0.00%	0.000%
19	4.147	870	873	877	rBV2	192	174	0.00%	0.001%
20	4.218	891	895	900	rBV	120	143	0.00%	0.000%
21	4.526	987	991	993	rBV2	266	225	0.00%	0.001%
22	4.623	1005	1021	1050	rBV	158692	402362	1.73%	1.220%
23	4.925	1111	1115	1119	rBV2	203	154	0.00%	0.000%
24	4.967	1124	1128	1131	rVB2	266	221	0.00%	0.001%
25	4.993	1131	1136	1140	rBV3	392	525	0.00%	0.002%
26	5.067	1143	1159	1180	rBV	214379	468718	2.01%	1.422%
27	5.292	1224	1229	1232	rBV4	464	584	0.00%	0.002%
28	5.379	1251	1256	1262	rBV4	400	496	0.00%	0.002%
29	5.427	1267	1271	1274	rBV	157	151	0.00%	0.000%
30	5.526	1299	1302	1308	rVB2	160	179	0.00%	0.001%
31	5.591	1318	1322	1324	rBV	147	149	0.00%	0.000%
32	5.729	1342	1365	1402	rBV2	430516	1204100	5.18%	3.652%
33	5.890	1413	1415	1417	rBV3	311	168	0.00%	0.001%
34	6.083	1472	1475	1477	rBV2	208	140	0.00%	0.000%
35	6.115	1481	1485	1487	rBV2	207	178	0.00%	0.001%
36	6.153	1492	1497	1499	rBV	318	284	0.00%	0.001%

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 Title : VOC Analysis

37	6.179	1503	1505	1512	rVB2	363	358	0.00%	0.001%
38	6.253	1512	1528	1549	rBV	318187	597109	2.57%	1.811%
39	6.343	1554	1556	1559	rBV	443	247	0.00%	0.001%
40	6.546	1606	1619	1638	rBV	153479	288824	1.24%	0.876%
41	6.645	1646	1650	1651	rBV	225	144	0.00%	0.000%
42	6.694	1651	1665	1684	rVV	282696	548839	2.36%	1.665%
43	6.809	1696	1701	1703	rBV3	777	745	0.00%	0.002%
44	6.899	1727	1729	1732	rBV	169	137	0.00%	0.000%
45	6.938	1737	1741	1745	rVB	166	151	0.00%	0.000%
46	6.960	1745	1748	1752	rBV	149	139	0.00%	0.000%
47	7.034	1765	1771	1772	rVV2	362	327	0.00%	0.001%
48	7.047	1772	1775	1782	rVV2	786	793	0.00%	0.002%
49	7.096	1786	1790	1794	rBV	225	180	0.00%	0.001%
50	7.186	1807	1818	1828	rBV6	2418	4255	0.02%	0.013%
51	7.250	1835	1838	1842	rBV3	315	216	0.00%	0.001%
52	7.276	1842	1846	1849	rBV2	128	142	0.00%	0.000%
53	7.346	1863	1868	1871	rBV2	174	157	0.00%	0.000%
54	7.568	1922	1937	1955	rBV	155242	270912	1.16%	0.822%
55	7.687	1968	1974	1988	rVB4	1555	3102	0.01%	0.009%
56	7.903	2024	2041	2055	rBV	513184	886205	3.81%	2.688%
57	7.973	2055	2063	2077	rVB	15151	25852	0.11%	0.078%
58	8.118	2105	2108	2112	rVB2	222	197	0.00%	0.001%
59	8.182	2112	2128	2143	rBV	107821	180142	0.77%	0.546%
60	8.301	2163	2165	2170	rVB3	172	144	0.00%	0.000%
61	8.452	2210	2212	2214	rBV	280	182	0.00%	0.001%
62	8.475	2215	2219	2227	rVB3	912	1186	0.01%	0.004%
63	8.558	2228	2245	2259	rBV	14007171	23265796	100.00%	70.569%
64	8.636	2260	2269	2308	rVB	490696	958202	4.12%	2.906%
65	9.009	2380	2385	2387	rBV	201	180	0.00%	0.001%
66	9.034	2387	2393	2394	rVV2	148	182	0.00%	0.001%
67	9.144	2423	2427	2428	rVV	222	189	0.00%	0.001%
68	9.169	2432	2435	2441	rBV2	154	210	0.00%	0.001%
69	9.230	2450	2454	2458	rVB3	290	246	0.00%	0.001%
70	9.256	2460	2462	2467	rBV2	223	199	0.00%	0.001%
71	9.324	2481	2483	2486	rBV2	253	198	0.00%	0.001%
72	9.420	2499	2513	2529	rBV	453251	731780	3.15%	2.220%
73	9.571	2550	2560	2568	rBV	3350	4757	0.02%	0.014%
74	9.700	2591	2600	2611	rBV3	4037	6051	0.03%	0.018%
75	9.758	2613	2618	2621	rBV	174	197	0.00%	0.001%
76	9.870	2650	2653	2655	rBV2	187	145	0.00%	0.000%

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Integrator: RTE

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Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

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 Title : VOC Analysis

77	9.964	2679	2682	2687	rVB2	181	157	0.00%	0.000%
78	10.102	2717	2725	2736	rBV2	2005	3185	0.01%	0.010%
79	10.192	2750	2753	2755	rBV2	184	155	0.00%	0.000%
80	10.320	2788	2793	2796	rVB2	305	267	0.00%	0.001%
81	10.369	2803	2808	2809	rBV2	264	235	0.00%	0.001%
82	10.423	2822	2825	2830	rBV2	163	204	0.00%	0.001%
83	10.488	2842	2845	2846	rBV	301	166	0.00%	0.001%
84	10.671	2896	2902	2916	rVB4	1639	2522	0.01%	0.008%
85	10.758	2916	2929	2948	rBV	407700	655492	2.82%	1.988%
86	10.873	2961	2965	2967	rVV2	365	281	0.00%	0.001%
87	10.964	2989	2993	3000	rBV2	298	412	0.00%	0.001%
88	11.118	3039	3041	3045	rVB2	253	143	0.00%	0.000%
89	11.298	3090	3097	3101	rVB2	394	493	0.00%	0.001%
90	11.472	3140	3151	3164	rVB5	2449	4224	0.02%	0.013%
91	11.587	3180	3187	3192	rBV2	376	385	0.00%	0.001%
92	11.697	3218	3221	3228	rVB3	861	984	0.00%	0.003%
93	11.816	3245	3258	3273	rBV	438913	697868	3.00%	2.117%
94	11.935	3291	3295	3298	rBV3	440	392	0.00%	0.001%
95	12.095	3341	3345	3347	rBV2	379	288	0.00%	0.001%
96	12.195	3362	3376	3395	rBV	499814	814599	3.50%	2.471%
97	12.317	3411	3414	3418	rVB2	257	162	0.00%	0.000%
98	12.571	3491	3493	3499	rVB2	234	191	0.00%	0.001%
99	12.639	3511	3514	3516	rBV	236	157	0.00%	0.000%
100	14.092	3958	3966	3977	rBV2	2851	4424	0.02%	0.013%

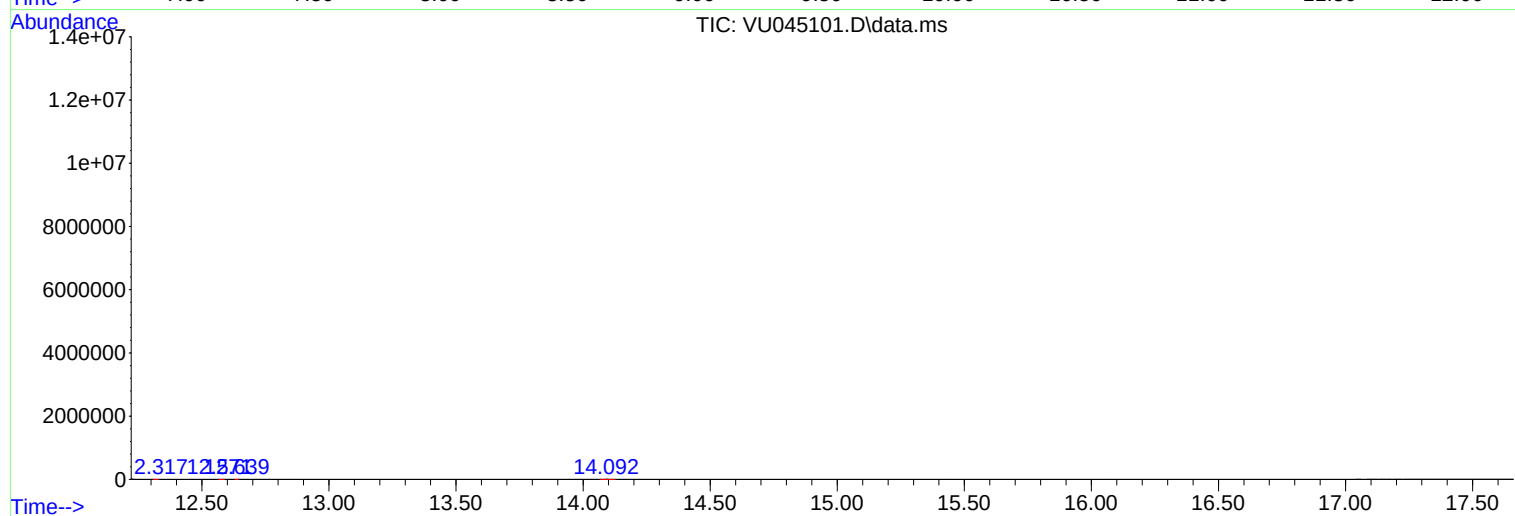
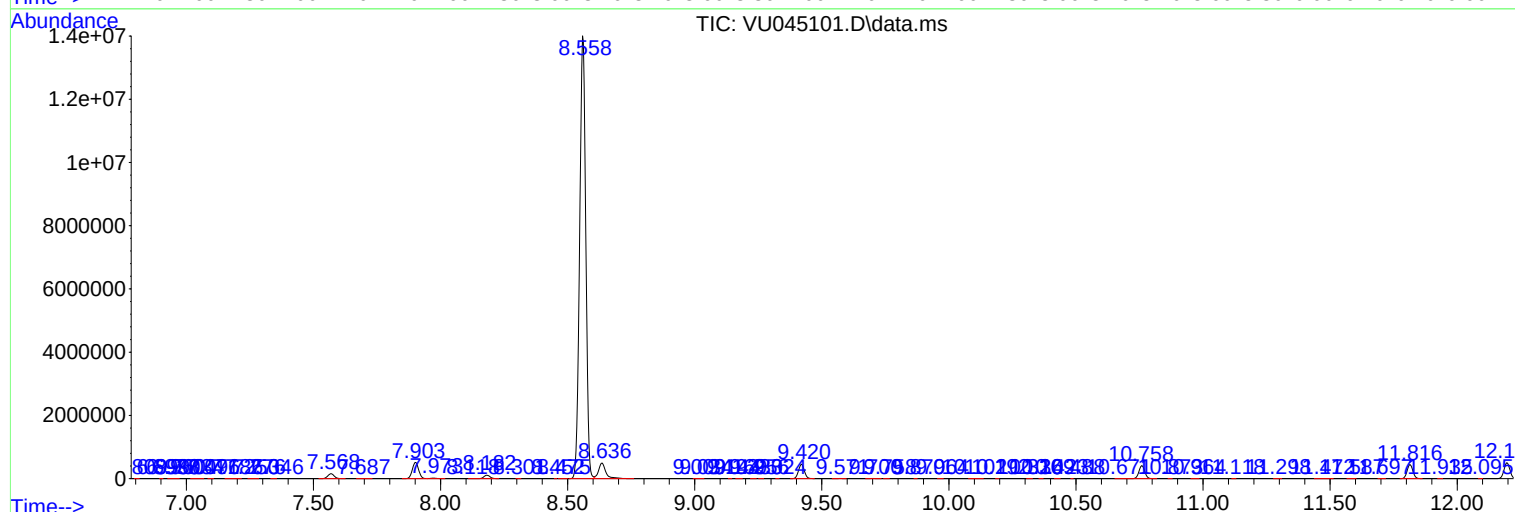
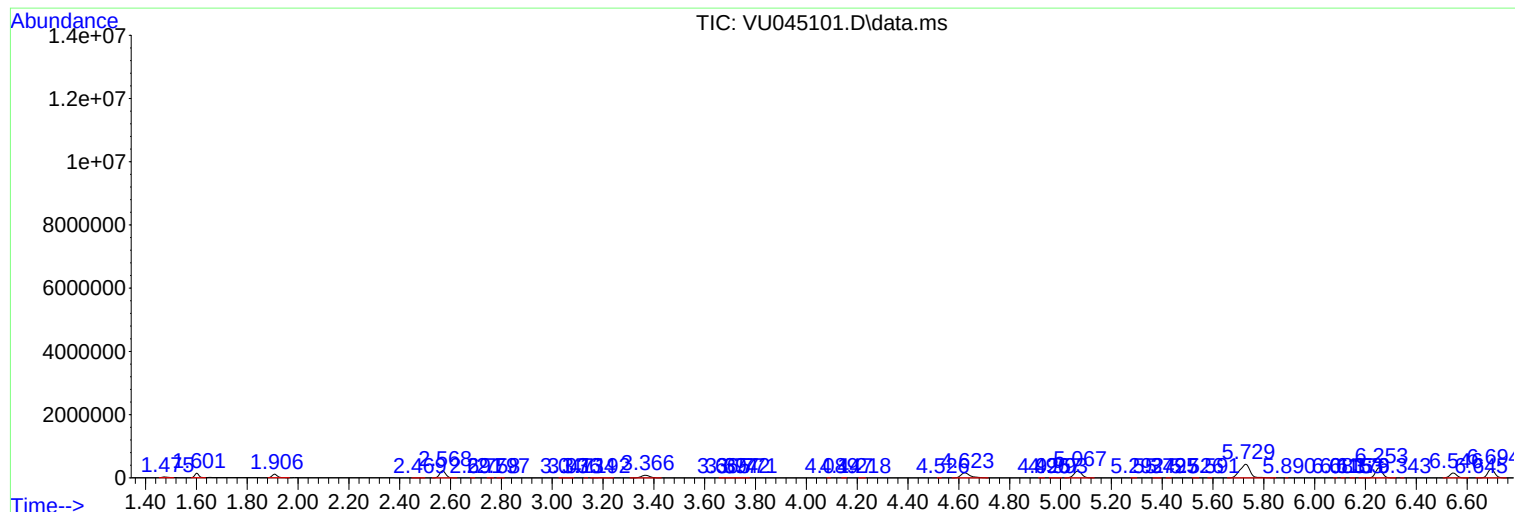
Sum of corrected areas: 32968757

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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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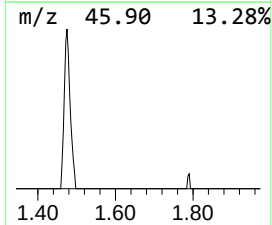
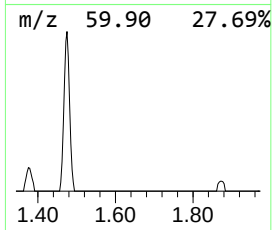
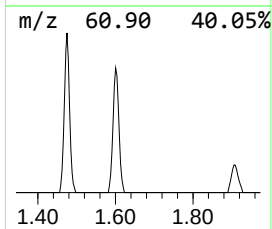
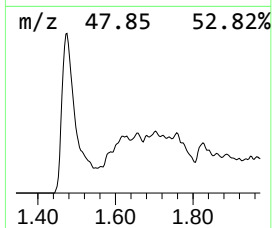
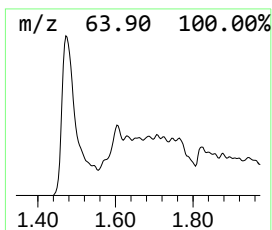
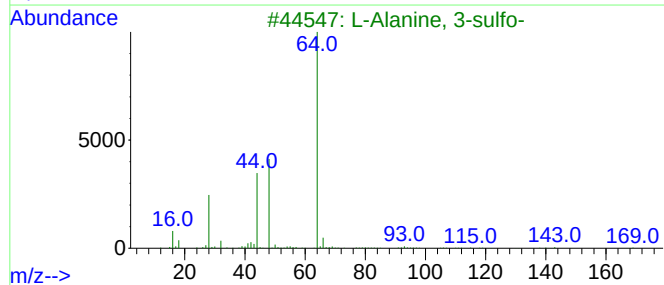
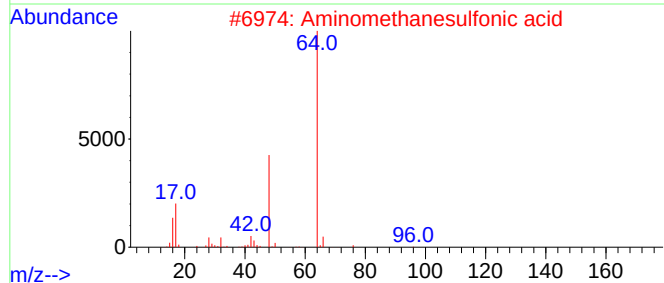
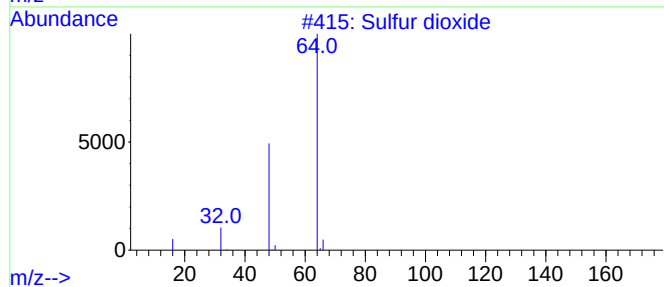
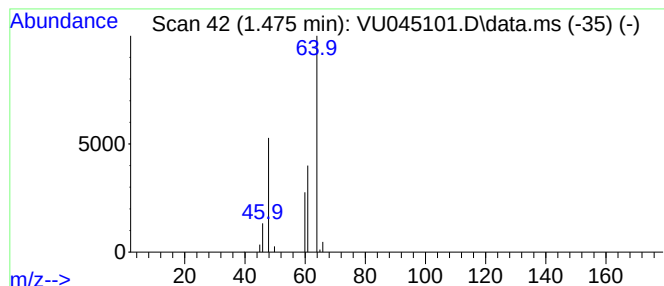
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	3.07 ug/L	36682	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	72
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	39
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.475	3.1	ug/L	36682	1	6.253	597109	50.0