

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045195.D
 Acq On : 06 Oct 2021 19:00
 Operator : SY/MD
 Sample : VIBLK011
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK005

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: VU0451195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	33	40	53	rBV	26553	48540	3.56%	0.463%
2	1.600	74	81	91	rVB	174213	186847	13.70%	1.780%
3	1.893	164	172	184	rVB	120981	162270	11.90%	1.546%
4	2.562	367	380	401	rBV	249025	422973	31.02%	4.030%
5	2.723	426	430	432	rBV2	200	177	0.01%	0.002%
6	2.777	444	447	451	rBV3	357	357	0.03%	0.003%
7	2.838	459	466	469	rBV2	188	253	0.02%	0.002%
8	2.864	469	474	479	rBV2	169	210	0.02%	0.002%
9	2.899	482	485	486	rBV	140	78	0.01%	0.001%
10	2.951	495	501	504	rBV3	483	548	0.04%	0.005%
11	3.012	517	520	521	rBV2	129	81	0.01%	0.001%
12	3.047	521	531	544	rVV2	8127	14576	1.07%	0.139%
13	3.128	552	556	559	rBV	92	86	0.01%	0.001%
14	3.189	564	575	587	rVB2	1556	3514	0.26%	0.033%
15	3.256	593	596	598	rBV	213	151	0.01%	0.001%
16	3.295	605	608	616	rVB2	222	284	0.02%	0.003%
17	3.346	616	624	626	rBV	228	325	0.02%	0.003%
18	3.395	636	639	642	rVB	163	104	0.01%	0.001%
19	3.430	646	650	653	rVV2	228	202	0.01%	0.002%
20	3.462	657	660	664	rVB2	130	102	0.01%	0.001%
21	3.613	704	707	709	rBV	114	102	0.01%	0.001%
22	3.697	729	733	738	rBV2	203	264	0.02%	0.003%
23	3.726	738	742	745	rVV2	240	214	0.02%	0.002%
24	3.745	745	748	754	rVB2	180	198	0.01%	0.002%
25	3.800	762	765	768	rBV	113	86	0.01%	0.001%
26	3.896	793	795	799	rBV2	131	136	0.01%	0.001%
27	4.083	848	853	859	rBV	102	145	0.01%	0.001%
28	4.214	892	894	898	rVB2	134	88	0.01%	0.001%
29	4.314	922	925	928	rVV	157	105	0.01%	0.001%
30	4.423	956	959	961	rVB2	189	125	0.01%	0.001%
31	4.517	985	988	992	rVB2	177	170	0.01%	0.002%
32	4.536	992	994	997	rBV2	129	100	0.01%	0.001%
33	4.559	998	1001	1004	rBV	157	108	0.01%	0.001%
34	4.626	1007	1022	1063	rBV	162235	381415	27.97%	3.634%
35	5.067	1143	1159	1184	rVV	233869	516050	37.84%	4.917%
36	5.237	1209	1212	1216	rBV2	230	184	0.01%	0.002%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Peak separation: 5

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

37	5.295	1222	1230	1241	rVB3	648	1232	0.09%	0.012%
38	5.382	1251	1257	1262	rVB3	647	897	0.07%	0.009%
39	5.414	1262	1267	1268	rBV	175	133	0.01%	0.001%
40	5.578	1315	1318	1320	rBV	153	94	0.01%	0.001%
41	5.729	1342	1365	1384	rBV2	503810	1363595	100.00%	12.993%
42	6.112	1480	1484	1486	rBV3	330	242	0.02%	0.002%
43	6.253	1512	1528	1551	rBV	387978	718246	52.67%	6.844%
44	6.533	1604	1615	1624	rBV4	5028	8429	0.62%	0.080%
45	6.693	1650	1665	1689	rBV	324038	633340	46.45%	6.035%
46	6.809	1697	1701	1713	rVB3	998	1525	0.11%	0.015%
47	6.886	1722	1725	1728	rBV2	182	135	0.01%	0.001%
48	7.005	1759	1762	1765	rBV2	137	131	0.01%	0.001%
49	7.047	1768	1775	1777	rBV2	581	575	0.04%	0.005%
50	7.156	1806	1809	1811	rBV	146	106	0.01%	0.001%
51	7.182	1811	1817	1827	rVV3	1018	1497	0.11%	0.014%
52	7.234	1831	1833	1841	rVB	186	183	0.01%	0.002%
53	7.292	1848	1851	1853	rVB2	136	91	0.01%	0.001%
54	7.317	1856	1859	1863	rBV2	191	185	0.01%	0.002%
55	7.340	1863	1866	1868	rBV	115	85	0.01%	0.001%
56	7.568	1923	1937	1958	rBV	184739	320756	23.52%	3.056%
57	7.687	1969	1974	1979	rBV3	660	632	0.05%	0.006%
58	7.800	2006	2009	2012	rBV3	313	258	0.02%	0.002%
59	7.902	2026	2041	2056	rBV	616067	1061558	77.85%	10.115%
60	7.970	2056	2062	2078	rVB	8523	14243	1.04%	0.136%
61	8.182	2116	2128	2152	rBV	131822	217914	15.98%	2.076%
62	8.391	2190	2193	2198	rBV2	148	121	0.01%	0.001%
63	8.475	2216	2219	2223	rVB2	176	121	0.01%	0.001%
64	8.494	2223	2225	2233	rVB2	149	127	0.01%	0.001%
65	8.562	2242	2246	2248	rVB2	148	87	0.01%	0.001%
66	8.587	2251	2254	2257	rBV	119	84	0.01%	0.001%
67	8.636	2257	2269	2298	rBV	501548	848953	62.26%	8.089%
68	8.822	2325	2327	2329	rBV	165	85	0.01%	0.001%
69	8.835	2329	2331	2333	rVB2	259	113	0.01%	0.001%
70	8.851	2333	2336	2338	rBV2	210	126	0.01%	0.001%
71	8.915	2354	2356	2360	rVB2	198	108	0.01%	0.001%
72	8.938	2360	2363	2367	rBV	231	167	0.01%	0.002%
73	9.160	2430	2432	2435	rVV	177	79	0.01%	0.001%
74	9.346	2486	2490	2492	rVB3	238	164	0.01%	0.002%
75	9.420	2499	2513	2532	rBV	567048	919110	67.40%	8.758%
76	9.562	2554	2557	2558	rBV	270	115	0.01%	0.001%

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 ALS Vial : 24 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 VIBLK005

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

77	9.693	2585	2598	2606	rBV5	1556	2542	0.19%	0.024%
78	9.754	2614	2617	2619	rBB2	224	94	0.01%	0.001%
79	9.777	2619	2624	2626	rBV2	252	148	0.01%	0.001%
80	9.835	2639	2642	2648	rBV2	286	128	0.01%	0.001%
81	9.890	2657	2659	2662	rVB	308	136	0.01%	0.001%
82	9.918	2662	2668	2672	rBV3	405	493	0.04%	0.005%
83	9.944	2674	2676	2679	rBV2	259	168	0.01%	0.002%
84	9.976	2684	2686	2690	rVB	219	110	0.01%	0.001%
85	10.002	2691	2694	2695	rBV2	190	111	0.01%	0.001%
86	10.021	2697	2700	2702	rBV2	193	108	0.01%	0.001%
87	10.050	2707	2709	2710	rBV2	288	117	0.01%	0.001%
88	10.095	2720	2723	2724	rBV2	347	204	0.01%	0.002%
89	10.195	2753	2754	2755	rBV2	244	91	0.01%	0.001%
90	10.465	2836	2838	2840	rBV3	445	212	0.02%	0.002%
91	10.491	2843	2846	2849	rBV3	371	236	0.02%	0.002%
92	10.603	2879	2881	2882	rBV	604	267	0.02%	0.003%
93	10.632	2887	2890	2893	rVV3	843	600	0.04%	0.006%
94	10.674	2896	2903	2913	rVB3	4265	6973	0.51%	0.066%
95	10.761	2918	2930	2945	rBV	464202	749115	54.94%	7.138%
96	10.873	2960	2965	2969	rBV8	1321	1682	0.12%	0.016%
97	11.420	3131	3135	3142	rBV7	1842	2093	0.15%	0.020%
98	11.465	3142	3149	3158	rBV7	4251	7741	0.57%	0.074%
99	11.815	3246	3258	3271	rBV	560882	886032	64.98%	8.443%
100	12.195	3364	3376	3394	rVB	604151	978363	71.75%	9.323%

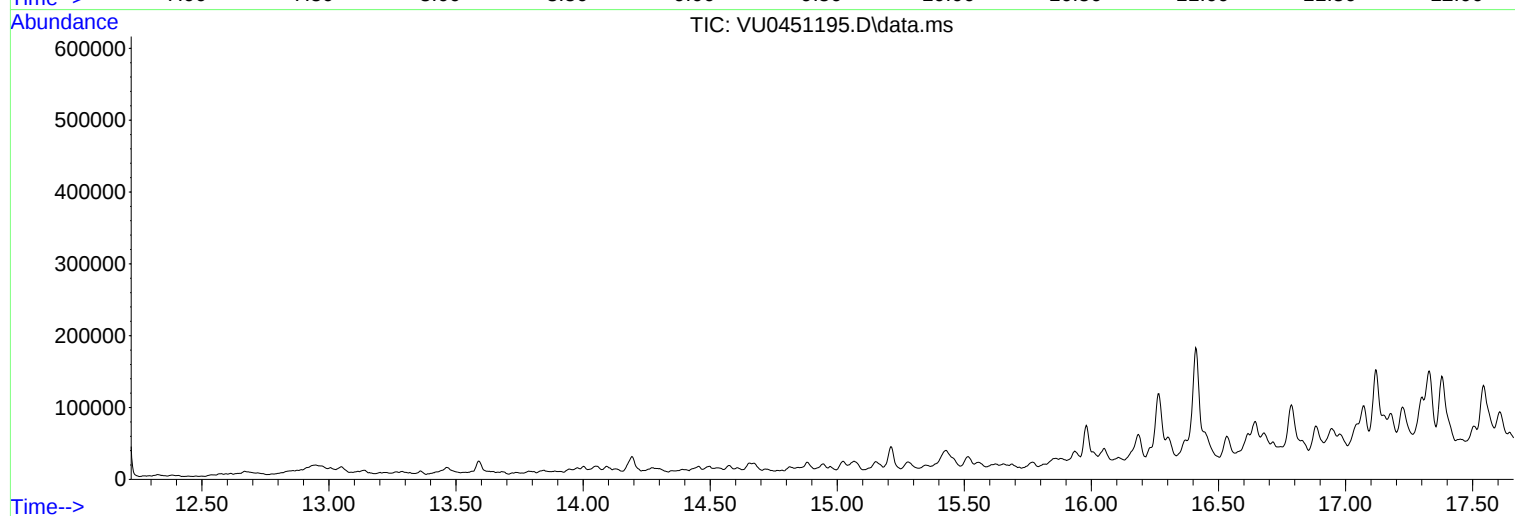
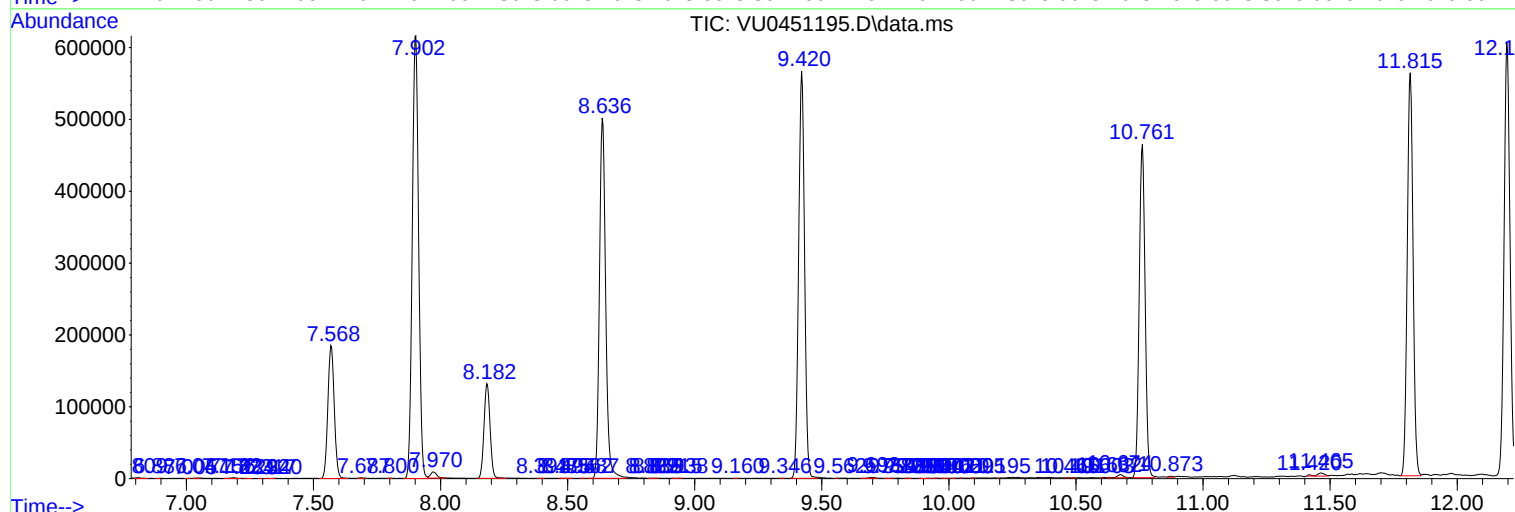
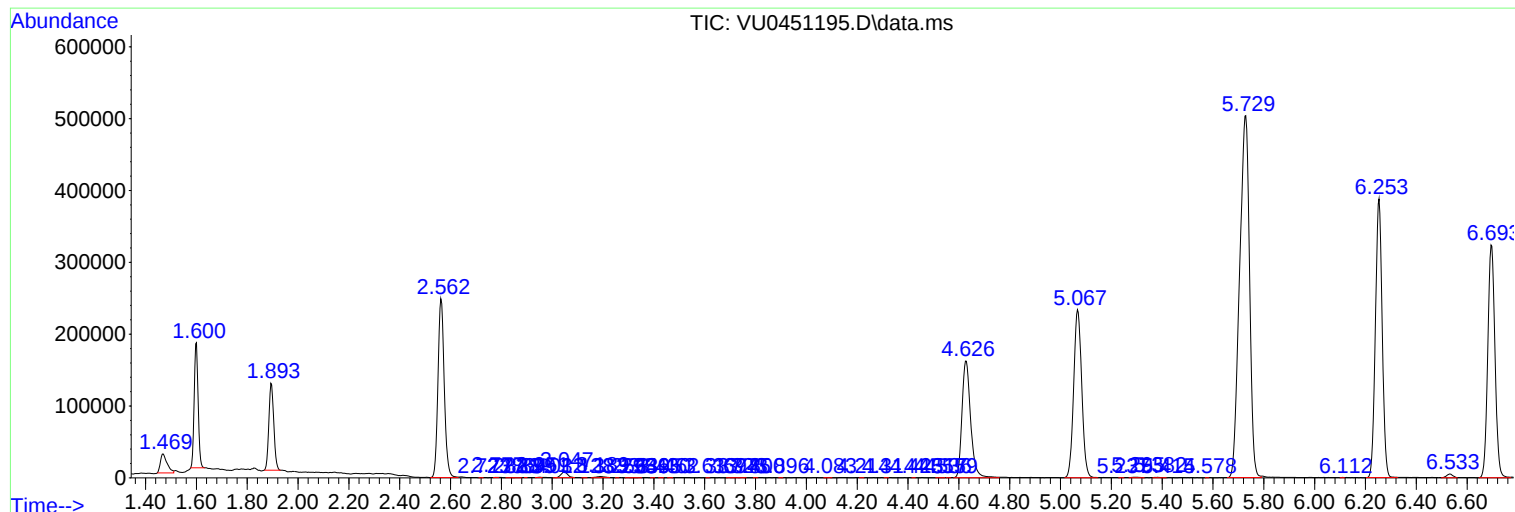
Sum of corrected areas: 10494574

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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK005

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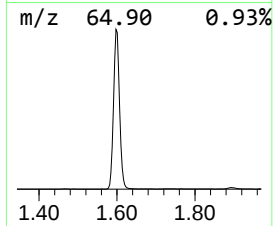
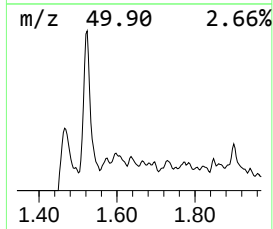
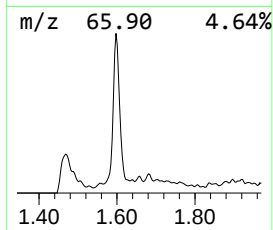
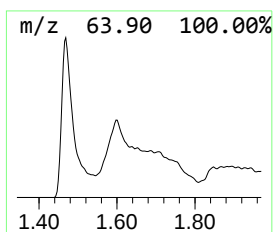
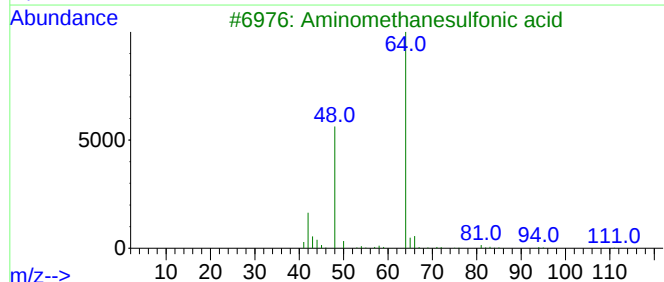
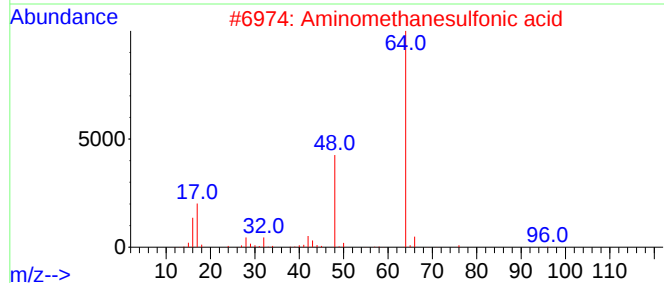
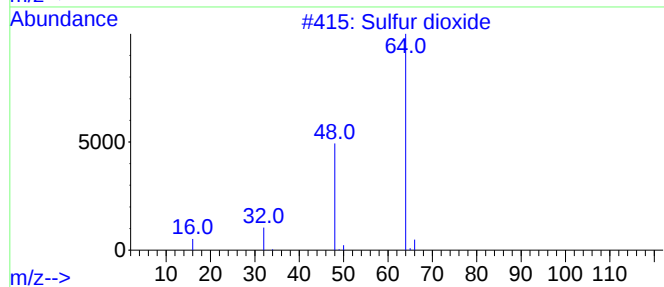
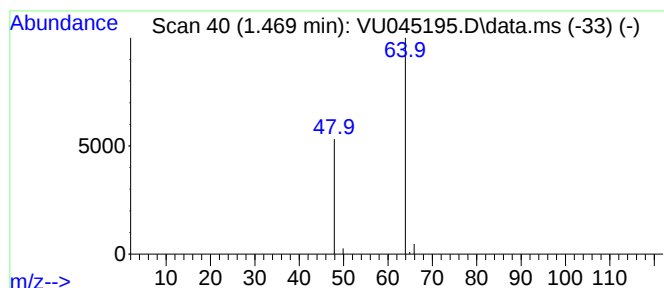
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	3.38 ug/L	48540	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			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_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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	1.469	3.4	ug/L	48540	1	6.253	718246	50.0