

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110722\
 Data File : VU051768.D
 Acq On : 07 Nov 2022 15:07
 Operator : JC/MD
 Sample : VU1107MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK007

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\SFAMULM102022WMA.M
 Title : VOC Analysis

Signal : TIC: VU051768.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	54	rBV	90424	165442	7.67%	1.021%
2	1.597	73	80	96	rVB	302622	334404	15.51%	2.063%
3	1.912	169	178	195	rBV	239015	322703	14.97%	1.991%
4	2.510	361	364	367	rVB2	746	418	0.02%	0.003%
5	2.565	367	381	398	rBV	457781	750193	34.80%	4.628%
6	2.787	445	450	460	rVB2	2104	3037	0.14%	0.019%
7	2.928	491	494	496	rBV2	496	312	0.01%	0.002%
8	3.044	519	530	547	rVV	37040	71323	3.31%	0.440%
9	3.186	561	574	585	rBV	5699	11382	0.53%	0.070%
10	3.346	619	624	626	rBV4	870	747	0.03%	0.005%
11	3.420	644	647	652	rVB2	481	324	0.02%	0.002%
12	3.604	701	704	710	rVB2	404	342	0.02%	0.002%
13	3.732	740	744	748	rBV2	483	490	0.02%	0.003%
14	3.771	752	756	760	rBV	347	412	0.02%	0.003%
15	3.793	760	763	772	rVB2	650	788	0.04%	0.005%
16	3.874	779	788	792	rBV4	849	1153	0.05%	0.007%
17	3.973	816	819	827	rVB3	448	527	0.02%	0.003%
18	4.047	838	842	845	rBV2	562	397	0.02%	0.002%
19	4.115	859	863	866	rBV2	519	424	0.02%	0.003%
20	4.144	866	872	874	rBV2	435	442	0.02%	0.003%
21	4.218	891	895	899	rBV2	495	492	0.02%	0.003%
22	4.237	899	901	907	rVB2	528	485	0.02%	0.003%
23	4.311	922	924	928	rVB	536	410	0.02%	0.003%
24	4.501	979	983	987	rBV2	372	362	0.02%	0.002%
25	4.620	1006	1020	1051	rBV	208914	512409	23.77%	3.161%
26	4.909	1107	1110	1114	rBV3	776	649	0.03%	0.004%
27	5.060	1141	1157	1184	rBV	373765	834581	38.71%	5.148%
28	5.279	1219	1225	1226	rBV3	1042	984	0.05%	0.006%
29	5.366	1248	1252	1253	rBV	711	531	0.02%	0.003%
30	5.613	1326	1329	1333	rBV2	403	373	0.02%	0.002%
31	5.722	1341	1363	1404	rBV2	801171	2155953	100.00%	13.300%
32	5.925	1422	1426	1429	rVB	879	698	0.03%	0.004%
33	5.999	1446	1449	1452	rBV3	580	394	0.02%	0.002%
34	6.034	1455	1460	1462	rBV3	709	672	0.03%	0.004%
35	6.247	1510	1526	1561	rBV	603038	1169345	54.24%	7.214%
36	6.533	1606	1615	1626	rVB8	4690	8421	0.39%	0.052%

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 Title : VOC Analysis

37	6.574	1626	1628	1634	rVB3	768	690	0.03%	0.004%
38	6.603	1634	1637	1639	rBV	664	430	0.02%	0.003%
39	6.690	1645	1664	1693	rBV	490321	972955	45.13%	6.002%
40	6.890	1723	1726	1728	rBV2	573	347	0.02%	0.002%
41	7.028	1765	1769	1772	rVB2	669	455	0.02%	0.003%
42	7.066	1777	1781	1784	rBV2	467	378	0.02%	0.002%
43	7.105	1790	1793	1795	rBV2	526	316	0.01%	0.002%
44	7.185	1806	1818	1832	rBV3	5132	10973	0.51%	0.068%
45	7.275	1842	1846	1849	rBV2	605	509	0.02%	0.003%
46	7.356	1868	1871	1875	rVV	496	389	0.02%	0.002%
47	7.410	1885	1888	1892	rVB2	453	345	0.02%	0.002%
48	7.443	1892	1898	1905	rBV2	658	902	0.04%	0.006%
49	7.507	1912	1918	1921	rBV2	585	564	0.03%	0.003%
50	7.565	1921	1936	1963	rBV	234801	424335	19.68%	2.618%
51	7.693	1969	1976	1986	rVB4	3207	5611	0.26%	0.035%
52	7.793	1999	2007	2010	rBV7	2024	3080	0.14%	0.019%
53	7.896	2025	2039	2071	rBV	942173	1660073	77.00%	10.241%
54	8.179	2115	2127	2147	rBV	169078	288528	13.38%	1.780%
55	8.288	2156	2161	2163	rBV	623	559	0.03%	0.003%
56	8.472	2212	2218	2225	rBV6	905	1143	0.05%	0.007%
57	8.552	2234	2243	2252	rBV4	1522	2536	0.12%	0.016%
58	8.632	2256	2268	2305	rBV	610346	1121721	52.03%	6.920%
59	9.066	2400	2403	2409	rBV2	553	470	0.02%	0.003%
60	9.102	2411	2414	2419	rBV	468	450	0.02%	0.003%
61	9.295	2471	2474	2477	rBV2	531	403	0.02%	0.002%
62	9.417	2498	2512	2535	rBV	864058	1441753	66.87%	8.894%
63	9.562	2553	2557	2559	rBV3	1022	871	0.04%	0.005%
64	9.645	2581	2583	2589	rVB2	718	658	0.03%	0.004%
65	9.674	2589	2592	2593	rBV2	499	312	0.01%	0.002%
66	9.700	2593	2600	2608	rVB5	1578	2188	0.10%	0.013%
67	9.915	2664	2667	2672	rVB2	525	360	0.02%	0.002%
68	10.108	2722	2727	2738	rVB6	1816	3400	0.16%	0.021%
69	10.214	2756	2760	2764	rBV3	488	534	0.02%	0.003%
70	10.356	2801	2804	2812	rVV3	819	847	0.04%	0.005%
71	10.465	2832	2838	2839	rBV3	426	455	0.02%	0.003%
72	10.478	2839	2842	2843	rBV2	737	408	0.02%	0.003%
73	10.574	2867	2872	2874	rBV3	525	482	0.02%	0.003%
74	10.655	2895	2897	2903	rBV2	291	326	0.02%	0.002%
75	10.754	2915	2928	2946	rBV	723304	1144653	53.09%	7.061%
76	10.967	2991	2994	2997	rBV	431	361	0.02%	0.002%

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 Title : VOC Analysis

77	10.986	2997	3000	3010	rVB2	488	679	0.03%	0.004%
78	11.060	3020	3023	3026	rVB	493	330	0.02%	0.002%
79	11.086	3026	3031	3034	rBV3	1006	1059	0.05%	0.007%
80	11.471	3143	3151	3153	rBV3	1293	1590	0.07%	0.010%
81	11.619	3192	3197	3200	rBV2	429	418	0.02%	0.003%
82	11.745	3229	3236	3244	rBV6	2559	3764	0.17%	0.023%
83	11.809	3244	3256	3284	rBV	783916	1261228	58.50%	7.780%
84	12.069	3334	3337	3342	rVB4	474	346	0.02%	0.002%
85	12.127	3353	3355	3358	rVB2	547	316	0.01%	0.002%
86	12.192	3360	3375	3409	rVV	876114	1436001	66.61%	8.859%
87	12.388	3432	3436	3440	rBV3	635	616	0.03%	0.004%
88	13.005	3622	3628	3631	rBV6	773	787	0.04%	0.005%
89	13.163	3674	3677	3683	rBV3	469	558	0.03%	0.003%
90	13.224	3690	3696	3705	rVB4	3840	4997	0.23%	0.031%
91	13.301	3717	3720	3722	rBV	708	510	0.02%	0.003%
92	13.590	3804	3810	3811	rBV2	523	429	0.02%	0.003%
93	13.806	3873	3877	3880	rBV2	800	665	0.03%	0.004%
94	13.841	3880	3888	3902	rVV4	7266	12237	0.57%	0.075%
95	13.896	3902	3905	3910	rVB3	678	550	0.03%	0.003%
96	14.089	3955	3965	3984	rBV2	10956	20136	0.93%	0.124%
97	14.204	3995	4001	4005	rBV3	996	1151	0.05%	0.007%
98	14.330	4033	4040	4054	rVB6	8107	13182	0.61%	0.081%
99	14.529	4099	4102	4105	rVB2	970	602	0.03%	0.004%
100	14.632	4131	4134	4137	rBV2	649	470	0.02%	0.003%

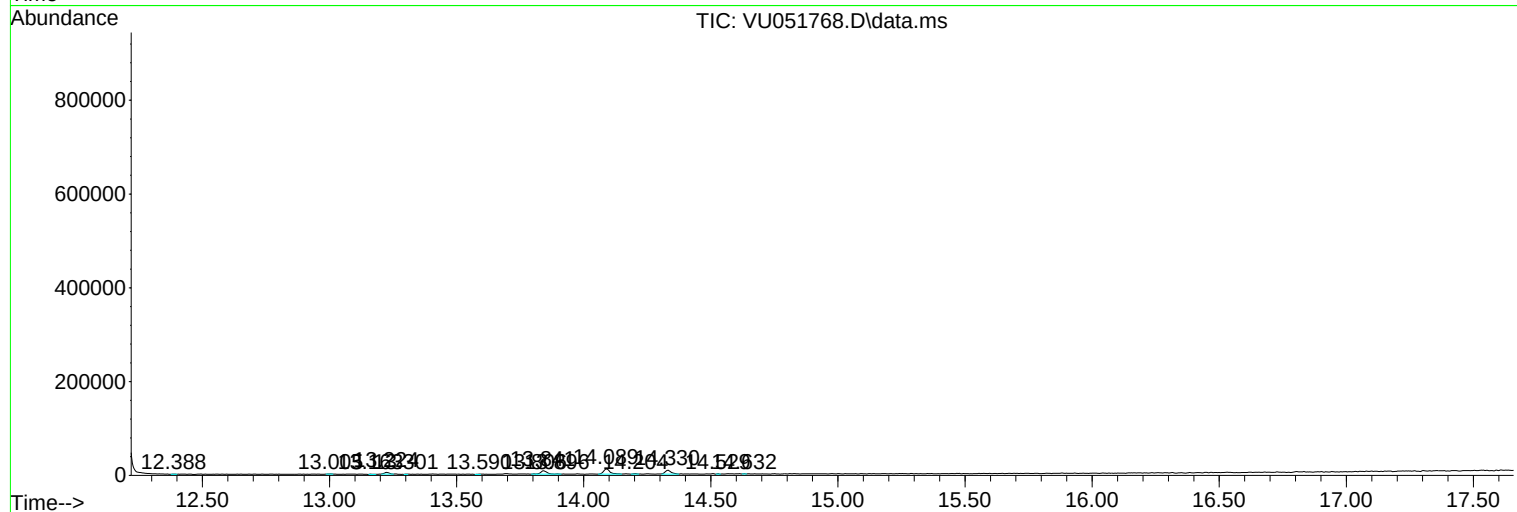
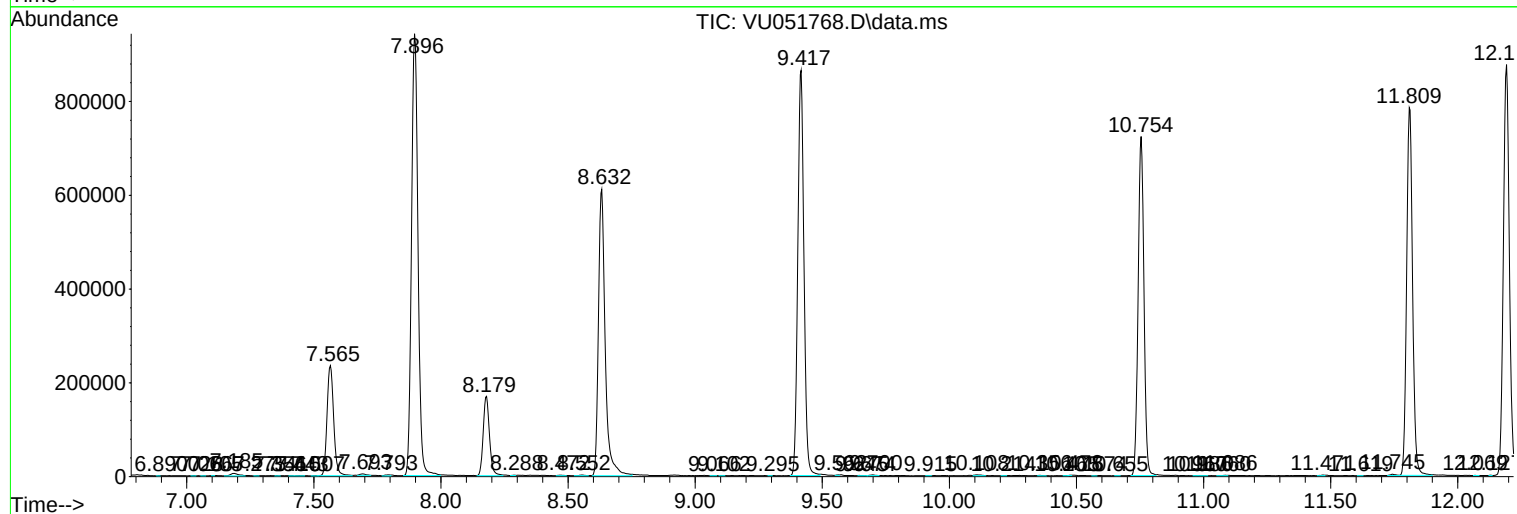
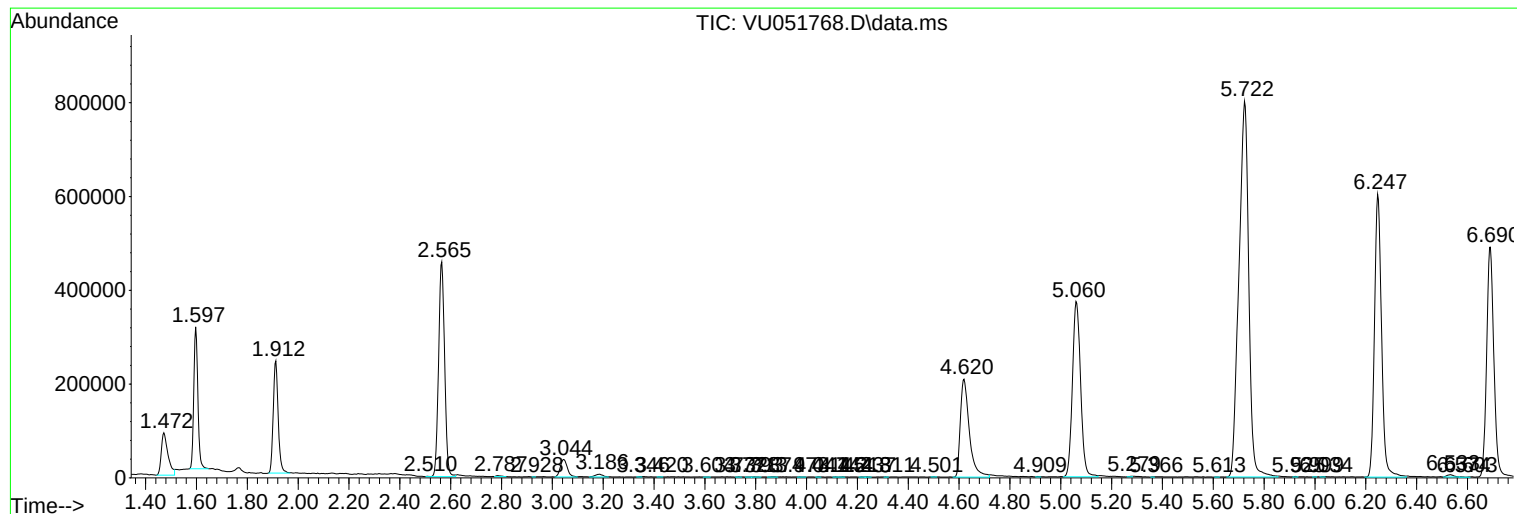
Sum of corrected areas: 16210410

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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



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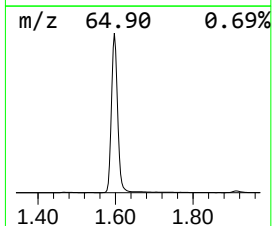
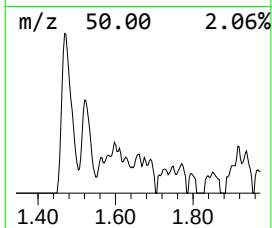
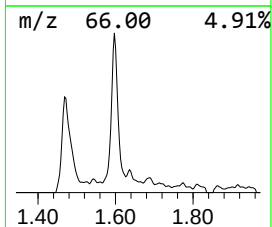
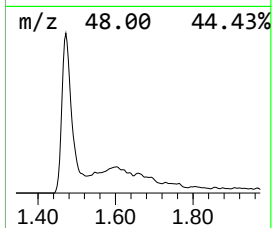
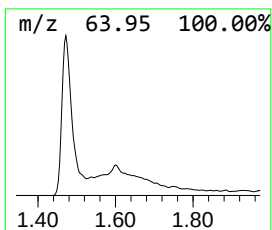
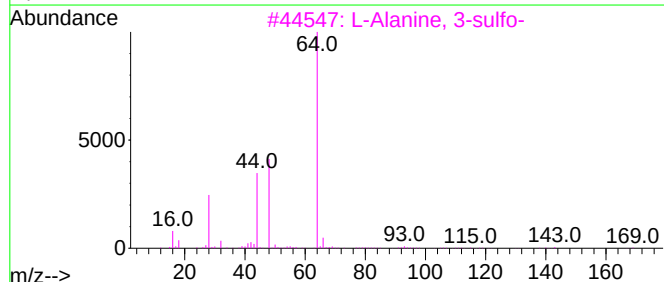
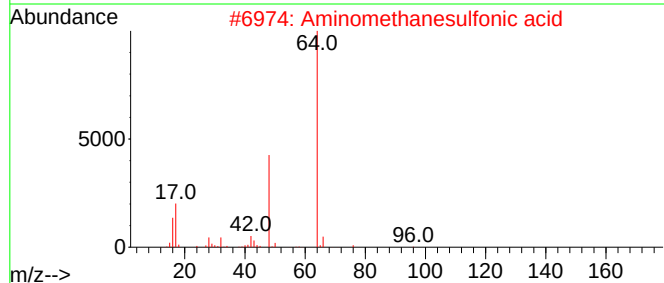
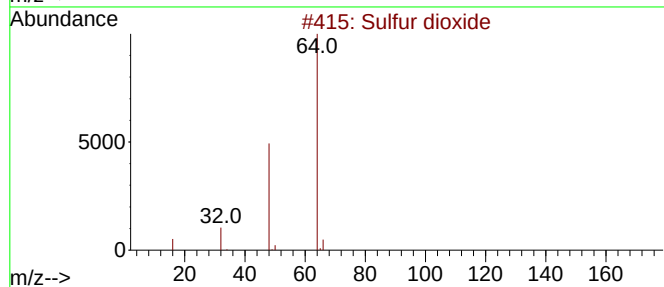
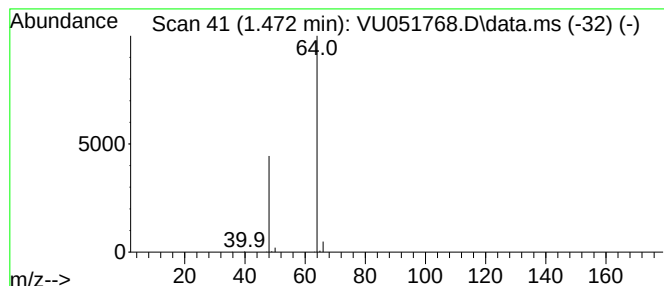
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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.
1.472	7.07 ug/L	165442	1,4-Difluorobenzene	6.247

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	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
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	1.472	7.1	ug/L	165442	1	6.247	1169350	50.0