

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101921\
 Data File : VU045333.D
 Acq On : 19 Oct 2021 16:44
 Operator : SY/MD
 Sample : VU1019MBL03
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK027

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\SFAMULM101921WMA.M

Title : VOC Analysis

Signal : TIC: VU045333.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.462	32	38	52	rBV	25249	45618	4.93%	0.553%
2	1.600	74	81	95	rBV	82368	90363	9.77%	1.096%
3	1.874	160	166	183	rVB	41466	54709	5.91%	0.664%
4	2.485	354	356	363	rVB2	292	262	0.03%	0.003%
5	2.552	365	377	402	rBV2	114787	199009	21.51%	2.415%
6	2.777	441	447	458	rVB2	1005	1876	0.20%	0.023%
7	2.825	458	462	467	rBV2	188	231	0.02%	0.003%
8	2.954	494	502	516	rVB2	2352	4183	0.45%	0.051%
9	3.041	522	529	537	rVB4	1554	2726	0.29%	0.033%
10	3.076	537	540	544	rBV2	224	200	0.02%	0.002%
11	3.115	547	552	555	rBV	202	242	0.03%	0.003%
12	3.263	593	598	601	rBV	238	291	0.03%	0.004%
13	3.311	610	613	617	rVB2	206	164	0.02%	0.002%
14	3.407	638	643	647	rVB2	233	246	0.03%	0.003%
15	3.430	647	650	652	rBV2	215	176	0.02%	0.002%
16	3.706	732	736	743	rVB2	219	315	0.03%	0.004%
17	3.739	743	746	750	rBV2	194	220	0.02%	0.003%
18	3.870	784	787	790	rBV2	176	166	0.02%	0.002%
19	3.890	790	793	797	rVB	229	171	0.02%	0.002%
20	3.935	800	807	810	rBV	242	348	0.04%	0.004%
21	4.009	825	830	834	rBV2	220	276	0.03%	0.003%
22	4.124	862	866	872	rBV2	232	257	0.03%	0.003%
23	4.263	904	909	912	rBV2	157	182	0.02%	0.002%
24	4.343	932	934	937	rBV	192	163	0.02%	0.002%
25	4.420	954	958	961	rBV2	184	197	0.02%	0.002%
26	4.440	961	964	969	rVB2	212	170	0.02%	0.002%
27	4.632	1009	1024	1063	rBV	124908	315925	34.15%	3.833%
28	4.899	1098	1107	1110	rBV3	273	399	0.04%	0.005%
29	4.977	1129	1131	1135	rVB2	339	201	0.02%	0.002%
30	5.002	1135	1139	1142	rBV2	254	201	0.02%	0.002%
31	5.067	1142	1159	1184	rVB	167480	371632	40.17%	4.509%
32	5.288	1220	1228	1238	rVB4	621	1141	0.12%	0.014%
33	5.427	1268	1271	1276	rBV	166	206	0.02%	0.002%
34	5.722	1339	1363	1390	rBV2	305169	842073	91.03%	10.217%
35	5.983	1433	1444	1454	rVB5	1333	2264	0.24%	0.027%
36	6.034	1457	1460	1463	rBV2	327	297	0.03%	0.004%

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 Title : VOC Analysis

37	6.118	1482	1486	1492	rVB3	334	378	0.04%	0.005%
38	6.160	1492	1499	1502	rVB2	138	172	0.02%	0.002%
39	6.250	1512	1527	1547	rBV	366385	691679	74.77%	8.392%
40	6.436	1578	1585	1590	rBV3	313	422	0.05%	0.005%
41	6.530	1606	1614	1626	rVB4	3051	5716	0.62%	0.069%
42	6.603	1626	1637	1648	rBV4	1308	2719	0.29%	0.033%
43	6.693	1648	1665	1688	rBV	225256	432039	46.71%	5.242%
44	7.025	1764	1768	1770	rBV2	204	184	0.02%	0.002%
45	7.041	1770	1773	1775	rVV2	318	220	0.02%	0.003%
46	7.054	1775	1777	1785	rVB3	476	483	0.05%	0.006%
47	7.185	1807	1818	1825	rVV3	1789	3170	0.34%	0.038%
48	7.227	1829	1831	1836	rBV2	165	179	0.02%	0.002%
49	7.568	1924	1937	1956	rBV	125743	220288	23.81%	2.673%
50	7.690	1970	1975	1982	rVB4	681	858	0.09%	0.010%
51	7.803	2002	2010	2018	rVB4	1162	1730	0.19%	0.021%
52	7.902	2027	2041	2055	rVV	338197	575016	62.16%	6.977%
53	7.976	2056	2064	2079	rVV3	5110	11200	1.21%	0.136%
54	8.185	2116	2129	2146	rBV	94821	161544	17.46%	1.960%
55	8.250	2146	2149	2152	rVB2	242	187	0.02%	0.002%
56	8.394	2191	2194	2198	rBV2	195	204	0.02%	0.002%
57	8.594	2253	2256	2258	rBV	253	169	0.02%	0.002%
58	8.642	2258	2271	2304	rVV	440371	806583	87.19%	9.786%
59	8.931	2358	2361	2365	rBV	216	191	0.02%	0.002%
60	9.073	2399	2405	2408	rBV2	258	304	0.03%	0.004%
61	9.150	2425	2429	2435	rBV	229	216	0.02%	0.003%
62	9.218	2446	2450	2453	rBV2	257	230	0.02%	0.003%
63	9.320	2479	2482	2488	rVB2	262	261	0.03%	0.003%
64	9.423	2500	2514	2532	rBV	563342	925034	100.00%	11.223%
65	9.571	2555	2560	2568	rVB3	574	933	0.10%	0.011%
66	9.697	2594	2599	2600	rBV2	796	606	0.07%	0.007%
67	9.758	2614	2618	2624	rBV2	199	278	0.03%	0.003%
68	9.851	2641	2647	2652	rVB2	253	307	0.03%	0.004%
69	9.877	2652	2655	2658	rBV	194	166	0.02%	0.002%
70	9.970	2680	2684	2687	rBV2	227	212	0.02%	0.003%
71	10.102	2721	2725	2727	rBV2	359	307	0.03%	0.004%
72	10.118	2727	2730	2737	rVB3	810	754	0.08%	0.009%
73	10.414	2817	2822	2826	rVB	210	207	0.02%	0.003%
74	10.494	2842	2847	2851	rVB2	462	557	0.06%	0.007%
75	10.536	2855	2860	2866	rVB2	236	310	0.03%	0.004%
76	10.642	2887	2893	2897	rVV4	614	666	0.07%	0.008%

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Title : VOC Analysis

77	10.761	2918	2930	2949	rBV	455916	736040	79.57%	8.930%
78	10.996	3000	3003	3010	rVB2	280	301	0.03%	0.004%
79	11.098	3033	3035	3038	rVB	342	193	0.02%	0.002%
80	11.153	3048	3052	3058	rBV	220	241	0.03%	0.003%
81	11.250	3077	3082	3085	rBV2	250	217	0.02%	0.003%
82	11.394	3124	3127	3132	rBV2	232	276	0.03%	0.003%
83	11.475	3145	3152	3159	rBV2	944	1289	0.14%	0.016%
84	11.751	3233	3238	3245	rVB3	1288	1509	0.16%	0.018%
85	11.815	3245	3258	3280	rBV	544646	866191	93.64%	10.509%
86	11.970	3304	3306	3310	rVB	310	186	0.02%	0.002%
87	12.198	3364	3377	3395	rBV	519619	827033	89.41%	10.034%
88	12.446	3451	3454	3457	rBV2	207	168	0.02%	0.002%
89	12.603	3500	3503	3506	rBV2	227	171	0.02%	0.002%
90	12.841	3573	3577	3580	rBV2	347	284	0.03%	0.003%
91	12.954	3608	3612	3613	rBV	254	197	0.02%	0.002%
92	12.999	3624	3626	3630	rVB2	351	184	0.02%	0.002%
93	13.227	3690	3697	3703	rBV2	1514	1702	0.18%	0.021%
94	13.848	3883	3890	3897	rBV4	2841	4073	0.44%	0.049%
95	14.095	3956	3967	3981	rBV	7133	11843	1.28%	0.144%
96	14.198	3993	3999	4002	rBV	332	431	0.05%	0.005%
97	14.336	4035	4042	4052	rVB4	2924	4541	0.49%	0.055%
98	14.597	4118	4123	4128	rBV2	391	524	0.06%	0.006%
99	14.867	4204	4207	4211	rBV2	419	350	0.04%	0.004%
100	15.060	4261	4267	4270	rBV3	326	418	0.05%	0.005%

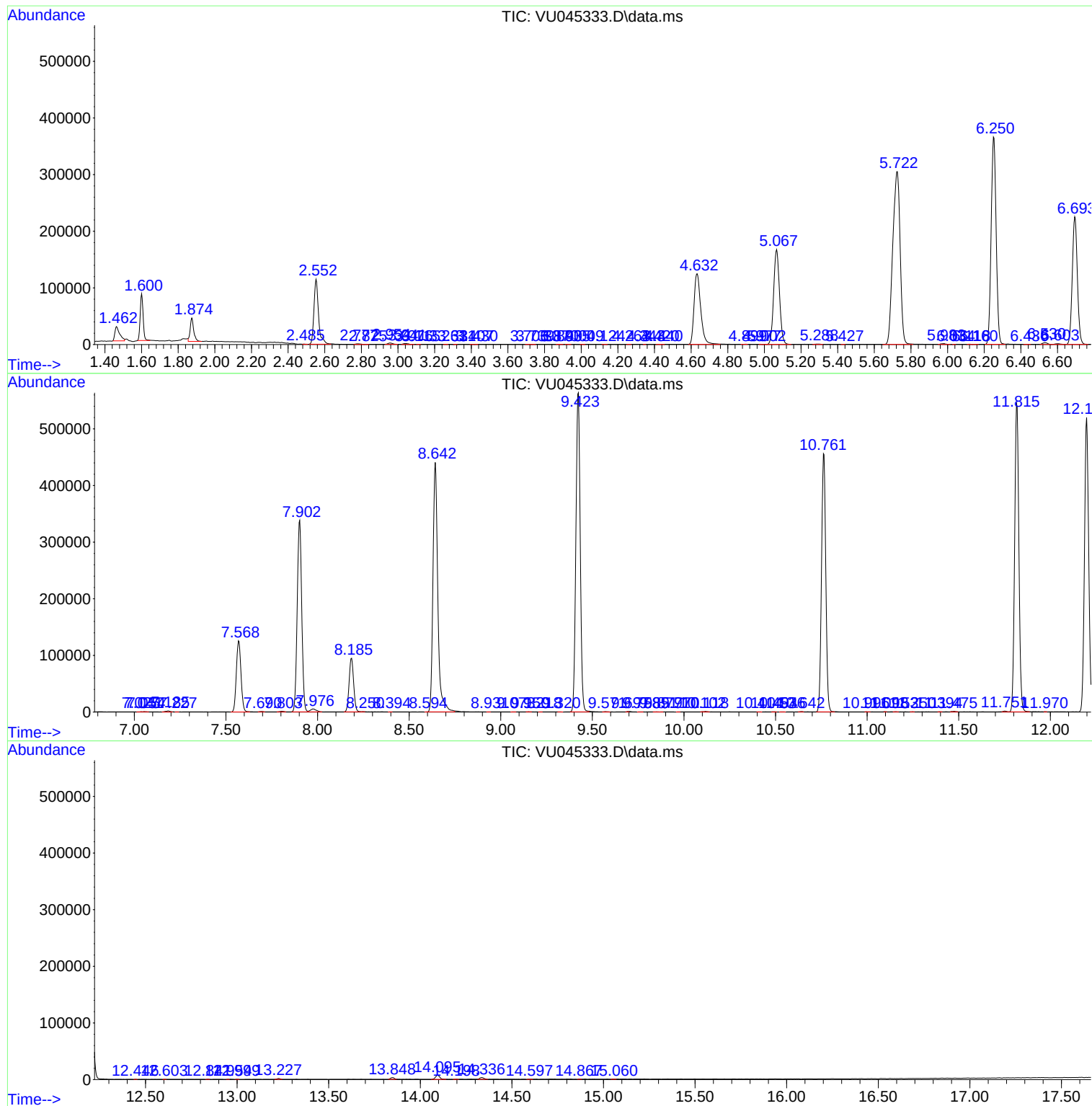
Sum of corrected areas: 8242141

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101921WMA.M
Quant Title : VOC Analysis

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



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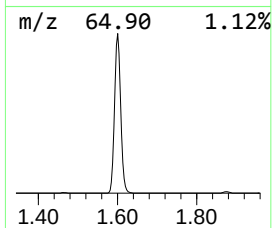
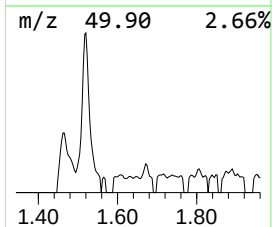
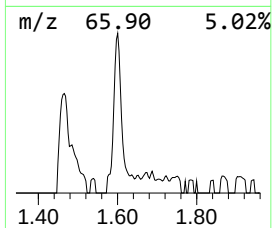
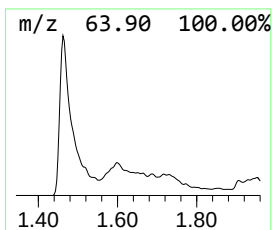
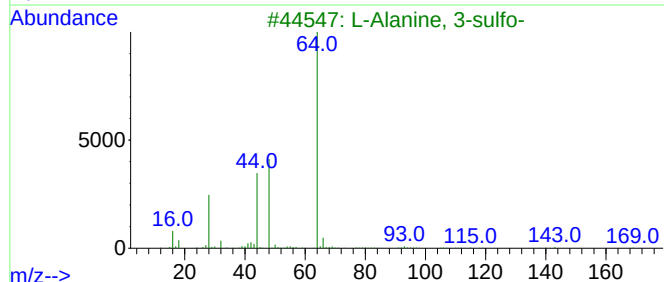
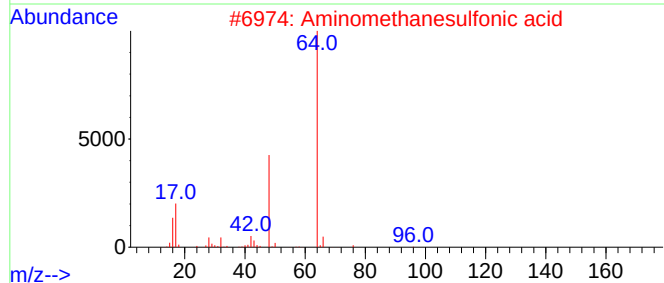
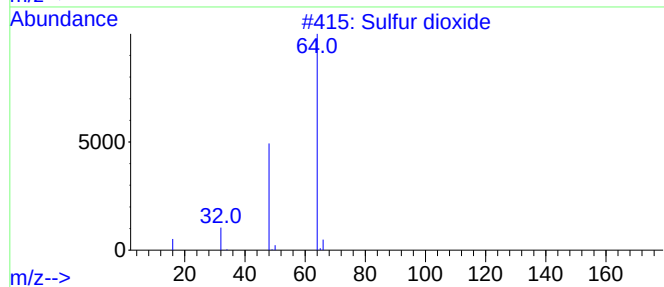
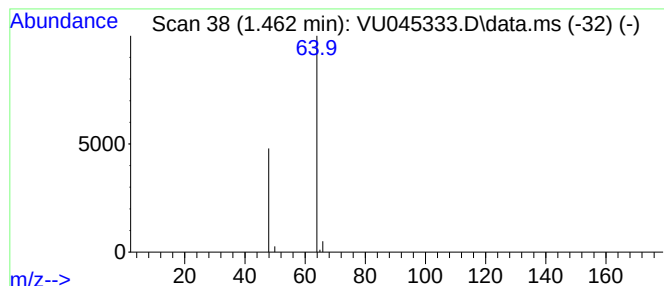
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101921WMA.M
Quant Title : VOC Analysis

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.
1.462	3.30 ug/L	45618	1,4-Difluorobenzene	6.250

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.462	3.3	ug/L	45618	1	6.250	691679	50.0