

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045292.D
 Acq On : 12 Oct 2021 15:22
 Operator : SY/MD
 Sample : M4103-07ME
 Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AC1ME

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: VU045292.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	31	37	51	rBV	36074	56896	4.33%	0.577%
2	1.597	73	80	102	rVB	102952	136774	10.41%	1.386%
3	1.870	159	165	177	rBV	41970	54820	4.17%	0.556%
4	2.520	354	367	388	rBV	191666	345699	26.30%	3.503%
5	2.613	388	396	413	rVV	5243	13328	1.01%	0.135%
6	2.964	497	505	510	rBV3	1822	2906	0.22%	0.029%
7	3.031	516	526	545	rVB2	5635	12546	0.95%	0.127%
8	3.163	562	567	569	rBV2	302	284	0.02%	0.003%
9	3.729	739	743	748	rBV2	262	258	0.02%	0.003%
10	4.208	887	892	897	rBV2	252	335	0.03%	0.003%
11	4.652	1013	1030	1074	rBV	110896	376299	28.63%	3.813%
12	5.066	1140	1159	1188	rVV	211192	507333	38.60%	5.141%
13	5.285	1222	1227	1229	rBV4	559	546	0.04%	0.006%
14	5.369	1248	1253	1254	rBV2	595	476	0.04%	0.005%
15	5.481	1284	1288	1293	rVB	302	324	0.02%	0.003%
16	5.719	1341	1362	1386	rBV2	518998	1314434	100.00%	13.320%
17	5.989	1435	1446	1459	rBV3	4865	11144	0.85%	0.113%
18	6.250	1511	1527	1550	rBV	346384	698866	53.17%	7.082%
19	6.468	1591	1595	1599	rVV2	267	292	0.02%	0.003%
20	6.529	1605	1614	1624	rVV4	3674	7084	0.54%	0.072%
21	6.610	1625	1639	1651	rBV2	3882	9020	0.69%	0.091%
22	6.693	1651	1665	1695	rVB	294516	617767	47.00%	6.260%
23	7.060	1770	1779	1785	rBV2	453	724	0.06%	0.007%
24	7.192	1810	1820	1831	rBV4	4043	9057	0.69%	0.092%
25	7.430	1886	1894	1899	rBV2	212	383	0.03%	0.004%
26	7.571	1923	1938	1959	rBV	148395	287456	21.87%	2.913%
27	7.697	1969	1977	1988	rVB4	1581	3494	0.27%	0.035%
28	7.816	2007	2014	2017	rBV	293	334	0.03%	0.003%
29	7.902	2020	2041	2056	rVV	549451	1004358	76.41%	10.178%
30	7.973	2057	2063	2086	rVB3	8769	23621	1.80%	0.239%
31	8.185	2117	2129	2154	rBV	98141	197013	14.99%	1.996%
32	8.362	2175	2184	2196	rBV5	956	1788	0.14%	0.018%
33	8.471	2214	2218	2219	rBV	338	243	0.02%	0.002%
34	8.652	2259	2274	2305	rBV	406086	785622	59.77%	7.961%
35	8.864	2336	2340	2343	rBV5	482	475	0.04%	0.005%
36	8.925	2352	2359	2367	rVB4	1981	2675	0.20%	0.027%

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

37	9.121	2415	2420	2428	rVB5	670	834	0.06%	0.008%
38	9.426	2501	2515	2536	rBV	472310	855023	65.05%	8.664%
39	9.584	2554	2564	2568	rBV3	497	775	0.06%	0.008%
40	9.703	2594	2601	2606	rBV4	1198	1531	0.12%	0.016%
41	9.748	2608	2615	2618	rBV2	428	617	0.05%	0.006%
42	9.886	2652	2658	2660	rBV2	206	253	0.02%	0.003%
43	10.021	2696	2700	2702	rVV2	378	292	0.02%	0.003%
44	10.037	2703	2705	2712	rVB2	372	311	0.02%	0.003%
45	10.250	2763	2771	2778	rBV5	931	1319	0.10%	0.013%
46	10.365	2799	2807	2811	rBV4	634	722	0.05%	0.007%
47	10.394	2811	2816	2824	rVB3	1399	1975	0.15%	0.020%
48	10.494	2844	2847	2852	rVB2	324	288	0.02%	0.003%
49	10.529	2852	2858	2862	rVB3	534	494	0.04%	0.005%
50	10.629	2884	2889	2892	rBV2	497	469	0.04%	0.005%
51	10.674	2893	2903	2912	rVV2	3791	6328	0.48%	0.064%
52	10.767	2918	2932	2949	rBV	453186	733209	55.78%	7.430%
53	10.828	2949	2951	2955	rVB	493	339	0.03%	0.003%
54	10.873	2960	2965	2969	rBV3	796	1022	0.08%	0.010%
55	10.999	3000	3004	3006	rBV2	384	318	0.02%	0.003%
56	11.069	3023	3026	3028	rBV2	537	374	0.03%	0.004%
57	11.114	3030	3040	3053	rVV8	3892	7248	0.55%	0.073%
58	11.204	3064	3068	3077	rVB2	777	915	0.07%	0.009%
59	11.375	3112	3121	3122	rBV3	652	686	0.05%	0.007%
60	11.420	3127	3135	3140	rVV3	2771	3892	0.30%	0.039%
61	11.462	3142	3148	3163	rVB6	3507	7416	0.56%	0.075%
62	11.581	3179	3185	3193	rVB5	1143	1733	0.13%	0.018%
63	11.629	3197	3200	3201	rBV2	466	250	0.02%	0.003%
64	11.700	3214	3222	3232	rBV7	2684	4644	0.35%	0.047%
65	11.819	3246	3259	3273	rBV	494018	783415	59.60%	7.939%
66	11.912	3282	3288	3290	rBV5	1162	1216	0.09%	0.012%
67	11.976	3304	3308	3316	rVB3	2858	3492	0.27%	0.035%
68	12.124	3352	3354	3358	rVB2	422	274	0.02%	0.003%
69	12.198	3360	3377	3396	rBV	564030	892243	67.88%	9.041%
70	12.269	3396	3399	3403	rVV4	521	428	0.03%	0.004%
71	12.327	3410	3417	3428	rBV5	5412	8546	0.65%	0.087%
72	12.404	3435	3441	3448	rVB7	1336	2170	0.17%	0.022%
73	12.542	3474	3484	3489	rBV5	1160	2054	0.16%	0.021%
74	12.600	3500	3502	3505	rBV2	366	250	0.02%	0.003%
75	12.642	3509	3515	3516	rBV5	588	489	0.04%	0.005%
76	12.732	3540	3543	3548	rVB2	459	356	0.03%	0.004%

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 Title : VOC Analysis

77	12.844	3576	3578	3582	rVB4	818	455	0.03%	0.005%
78	12.909	3594	3598	3600	rBV3	532	427	0.03%	0.004%
79	13.011	3626	3630	3635	rBV4	728	816	0.06%	0.008%
80	13.053	3635	3643	3645	rBV4	1406	1691	0.13%	0.017%
81	13.140	3661	3670	3676	rBV5	1503	2115	0.16%	0.021%
82	13.198	3685	3688	3693	rVB3	596	561	0.04%	0.006%
83	13.352	3732	3736	3738	rBV3	628	400	0.03%	0.004%
84	13.433	3754	3761	3772	rBV4	4822	8223	0.63%	0.083%
85	13.565	3799	3802	3803	rBV	578	280	0.02%	0.003%
86	13.593	3803	3811	3818	rVV3	2760	4504	0.34%	0.046%
87	13.847	3885	3890	3891	rBV2	285	234	0.02%	0.002%
88	13.886	3899	3902	3908	rVB4	575	482	0.04%	0.005%
89	13.954	3920	3923	3926	rBV2	493	372	0.03%	0.004%
90	14.050	3947	3953	3959	rVB4	1727	2265	0.17%	0.023%
91	14.095	3959	3967	3973	rBV4	2345	3651	0.28%	0.037%
92	14.195	3988	3998	4006	rBV5	4640	7010	0.53%	0.071%
93	14.452	4073	4078	4086	rVB5	3558	4499	0.34%	0.046%
94	14.577	4113	4117	4129	rVB5	1847	2632	0.20%	0.027%
95	14.777	4175	4179	4182	rVB3	501	367	0.03%	0.004%
96	15.211	4305	4314	4328	rBV8	3399	7348	0.56%	0.074%
97	15.404	4370	4374	4380	rBV4	1982	2231	0.17%	0.023%
98	15.503	4400	4405	4411	rBV6	1187	1772	0.13%	0.018%
99	15.745	4478	4480	4481	rBV	540	245	0.02%	0.002%
100	15.979	4549	4553	4560	rVB6	2233	2883	0.22%	0.029%

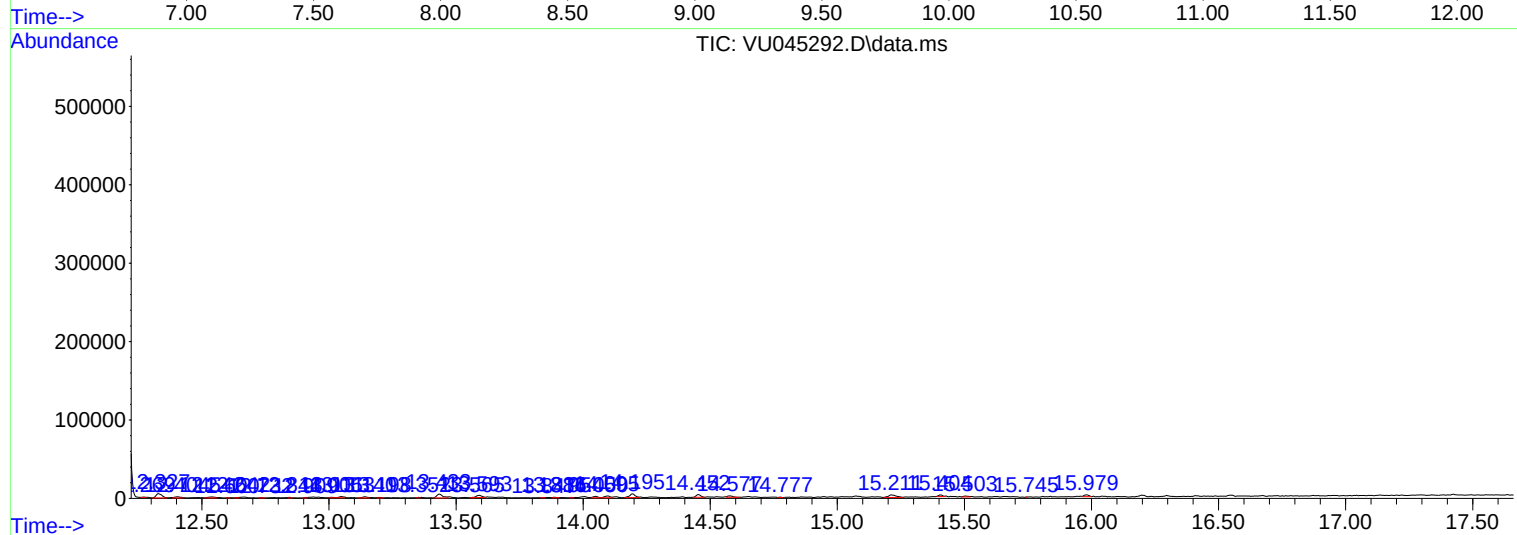
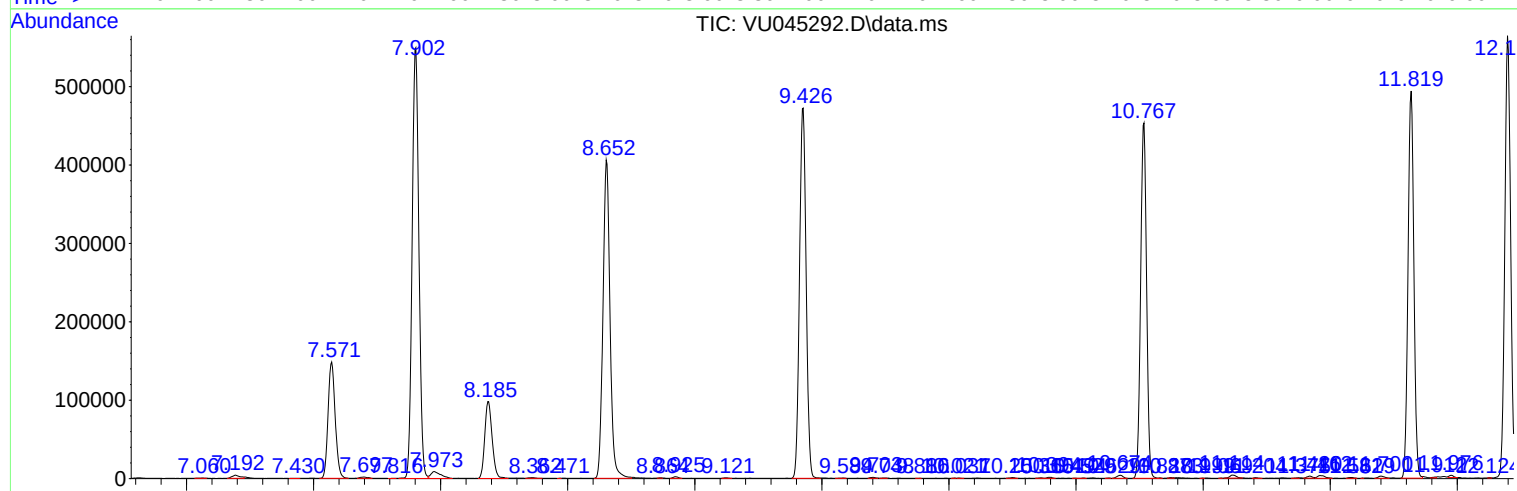
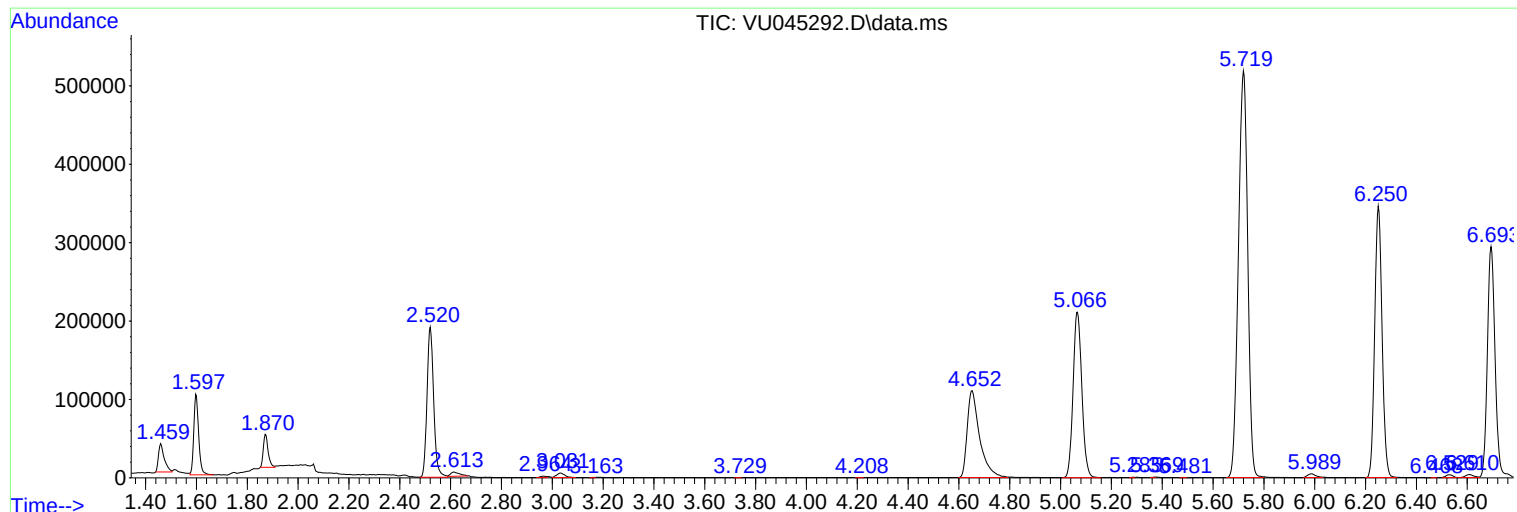
Sum of corrected areas: 9868347

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Instrument :
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ClientSampleId :
C0AC1ME

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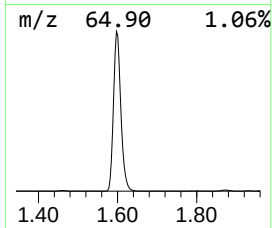
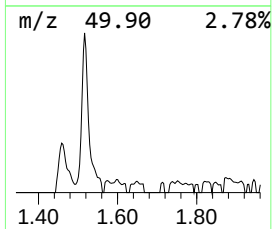
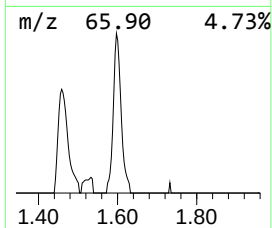
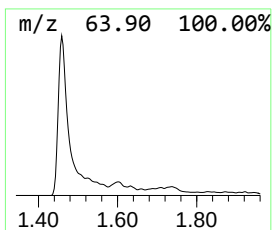
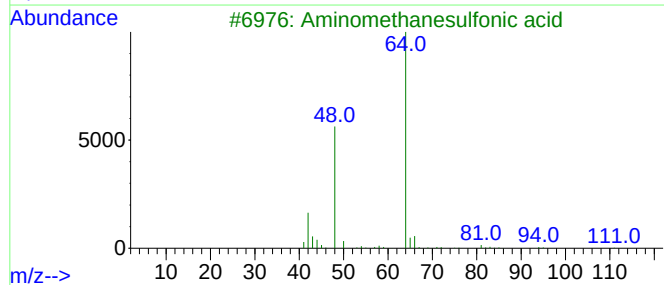
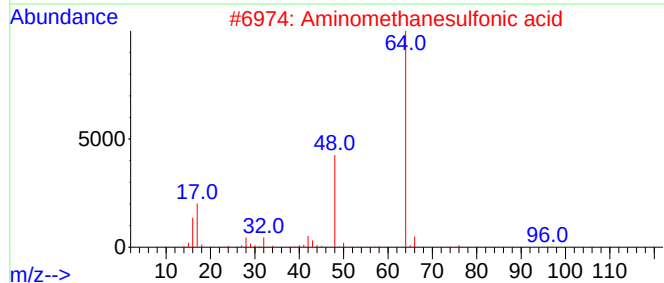
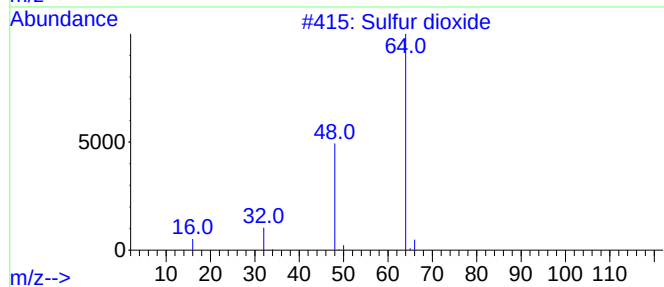
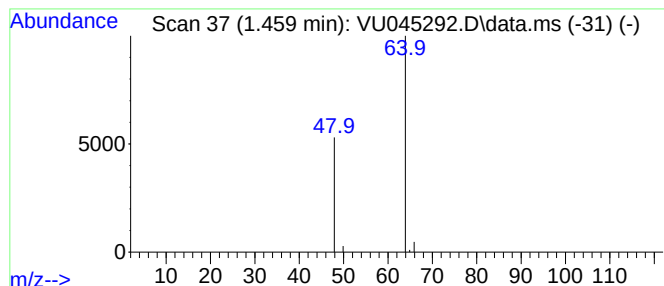
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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.
1.459	4.07 ug/L	56896	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			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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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	4.1	ug/L	56896	1	6.250	698866	50.0