

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045258.D
 Acq On : 08 Oct 2021 17:50
 Operator : SY/MD
 Sample : M4023-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AJ2

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: VU045258.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	54	rBV	29730	54433	1.57%	0.315%
2	1.600	74	81	98	rVB	223776	247660	7.13%	1.435%
3	1.890	163	171	187	rVB	145361	194670	5.61%	1.128%
4	2.565	367	381	399	rBV3	402261	804078	23.15%	4.658%
5	2.780	436	448	463	rBV2	6964	13487	0.39%	0.078%
6	2.954	495	502	506	rBV2	430	613	0.02%	0.004%
7	3.047	521	531	542	rVB3	4666	8263	0.24%	0.048%
8	3.192	560	576	595	rVB2	12717	29232	0.84%	0.169%
9	3.353	614	626	638	rBV2	7556	14719	0.42%	0.085%
10	3.591	698	700	709	rVB2	289	383	0.01%	0.002%
11	3.639	709	715	717	rBV2	172	212	0.01%	0.001%
12	3.870	772	787	805	rBV2	25815	59843	1.72%	0.347%
13	4.173	873	881	883	rBV2	178	248	0.01%	0.001%
14	4.539	991	995	999	rBV2	245	227	0.01%	0.001%
15	4.668	1007	1035	1066	rBV2	1420191	3473081	100.00%	20.119%
16	5.066	1139	1159	1179	rBV	232009	515799	14.85%	2.988%
17	5.166	1188	1190	1197	rVB2	513	458	0.01%	0.003%
18	5.317	1219	1237	1263	rVB	374680	855134	24.62%	4.954%
19	5.729	1342	1365	1397	rVV2	504371	1348574	38.83%	7.812%
20	5.935	1426	1429	1433	rBV2	237	207	0.01%	0.001%
21	6.253	1513	1528	1551	rBV	367886	689797	19.86%	3.996%
22	6.546	1603	1619	1651	rBV	1478213	2744488	79.02%	15.898%
23	6.693	1651	1665	1684	rVB	313523	609716	17.56%	3.532%
24	6.809	1696	1701	1702	rBV5	618	432	0.01%	0.003%
25	6.845	1710	1712	1715	rVB3	431	203	0.01%	0.001%
26	7.050	1769	1776	1787	rBV4	661	1288	0.04%	0.007%
27	7.182	1809	1817	1827	rVB3	1046	1730	0.05%	0.010%
28	7.430	1891	1894	1898	rVB2	280	248	0.01%	0.001%
29	7.465	1898	1905	1908	rBV2	228	292	0.01%	0.002%
30	7.491	1908	1913	1915	rBV2	286	255	0.01%	0.001%
31	7.568	1923	1937	1956	rBV	173762	302124	8.70%	1.750%
32	7.687	1969	1974	1977	rBV3	640	664	0.02%	0.004%
33	7.774	1997	2001	2008	rBV2	183	264	0.01%	0.002%
34	7.899	2025	2040	2056	rVV	609970	1047671	30.17%	6.069%
35	7.973	2056	2063	2076	rVB	9124	15031	0.43%	0.087%
36	8.182	2116	2128	2143	rBV	122914	200672	5.78%	1.162%

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 Title : VOC Analysis

37	8.404	2183	2197	2209	rBV2	8674	14428	0.42%	0.084%
38	8.478	2212	2220	2231	rVB3	896	1534	0.04%	0.009%
39	8.635	2257	2269	2300	rBV	434882	759130	21.86%	4.398%
40	8.877	2343	2344	2350	rVB2	337	238	0.01%	0.001%
41	8.906	2350	2353	2358	rBV	226	258	0.01%	0.001%
42	9.285	2467	2471	2482	rBV3	473	770	0.02%	0.004%
43	9.333	2482	2486	2495	rBV3	356	617	0.02%	0.004%
44	9.420	2500	2513	2534	rBV	539492	860170	24.77%	4.983%
45	9.536	2545	2549	2555	rVB2	716	876	0.03%	0.005%
46	9.574	2555	2561	2568	rVB2	583	644	0.02%	0.004%
47	9.693	2591	2598	2611	rBV3	1804	2925	0.08%	0.017%
48	9.825	2636	2639	2644	rBV2	202	215	0.01%	0.001%
49	10.028	2699	2702	2709	rVB2	269	274	0.01%	0.002%
50	10.105	2720	2726	2734	rBV3	458	672	0.02%	0.004%
51	10.253	2769	2772	2776	rBV3	522	372	0.01%	0.002%
52	10.674	2894	2903	2911	rVB4	3311	5290	0.15%	0.031%
53	10.761	2916	2930	2948	rBV	428189	692748	19.95%	4.013%
54	11.002	3001	3005	3009	rBV2	260	301	0.01%	0.002%
55	11.118	3038	3041	3048	rVB4	792	915	0.03%	0.005%
56	11.388	3121	3125	3130	rVV2	344	354	0.01%	0.002%
57	11.417	3130	3134	3139	rVV2	795	832	0.02%	0.005%
58	11.462	3139	3148	3158	rVB5	2474	4337	0.12%	0.025%
59	11.577	3181	3184	3191	rVB4	573	592	0.02%	0.003%
60	11.635	3200	3202	3205	rVB	338	221	0.01%	0.001%
61	11.700	3216	3222	3225	rBV4	1434	1563	0.05%	0.009%
62	11.815	3245	3258	3281	rBV	491658	770707	22.19%	4.465%
63	11.909	3285	3287	3290	rBV2	411	250	0.01%	0.001%
64	11.976	3304	3308	3316	rVB7	2062	2618	0.08%	0.015%
65	12.085	3339	3342	3344	rVV	375	242	0.01%	0.001%
66	12.121	3348	3353	3359	rBV4	555	513	0.01%	0.003%
67	12.195	3360	3376	3396	rBV	543511	874664	25.18%	5.067%
68	12.304	3408	3410	3414	rVB2	357	255	0.01%	0.001%
69	12.330	3414	3418	3428	rBV4	1064	1414	0.04%	0.008%
70	12.397	3437	3439	3444	rBV2	544	435	0.01%	0.003%
71	12.616	3503	3507	3509	rBV2	254	207	0.01%	0.001%
72	12.748	3543	3548	3550	rBV	292	248	0.01%	0.001%
73	12.944	3606	3609	3611	rVV3	373	243	0.01%	0.001%
74	13.011	3625	3630	3635	rVV3	422	453	0.01%	0.003%
75	13.040	3637	3639	3647	rVB2	429	510	0.01%	0.003%
76	13.140	3665	3670	3682	rBV5	731	1274	0.04%	0.007%

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 Title : VOC Analysis

77	13.214	3686	3693	3697	rBV2	340	404	0.01%	0.002%
78	13.282	3709	3714	3716	rBV2	275	256	0.01%	0.001%
79	13.439	3758	3763	3764	rBV3	554	399	0.01%	0.002%
80	13.500	3777	3782	3785	rBV2	280	253	0.01%	0.001%
81	13.587	3798	3809	3820	rVB5	2084	2981	0.09%	0.017%
82	13.973	3926	3929	3930	rBV5	472	260	0.01%	0.002%
83	14.005	3937	3939	3944	rVV2	641	438	0.01%	0.003%
84	14.037	3945	3949	3951	rVV3	598	522	0.02%	0.003%
85	14.050	3951	3953	3959	rVV4	888	759	0.02%	0.004%
86	14.095	3961	3967	3974	rVB3	1541	2103	0.06%	0.012%
87	14.191	3989	3997	4004	rVB4	1949	3097	0.09%	0.018%
88	14.449	4076	4077	4083	rVB4	440	342	0.01%	0.002%
89	14.497	4088	4092	4095	rBV2	516	451	0.01%	0.003%
90	14.574	4112	4116	4121	rBV5	808	775	0.02%	0.004%
91	14.790	4180	4183	4187	rBV2	345	243	0.01%	0.001%
92	14.809	4187	4189	4192	rBV2	324	226	0.01%	0.001%
93	14.889	4211	4214	4215	rBV	469	226	0.01%	0.001%
94	14.937	4226	4229	4231	rBV2	709	530	0.02%	0.003%
95	14.966	4236	4238	4241	rBV2	357	247	0.01%	0.001%
96	15.069	4262	4270	4271	rBV5	1265	1464	0.04%	0.008%
97	15.220	4308	4317	4327	rVB6	2168	4265	0.12%	0.025%
98	15.404	4371	4374	4375	rBV2	1331	725	0.02%	0.004%
99	15.857	4513	4515	4521	rBV2	391	443	0.01%	0.003%
100	16.265	4639	4642	4648	rVB3	957	830	0.02%	0.005%

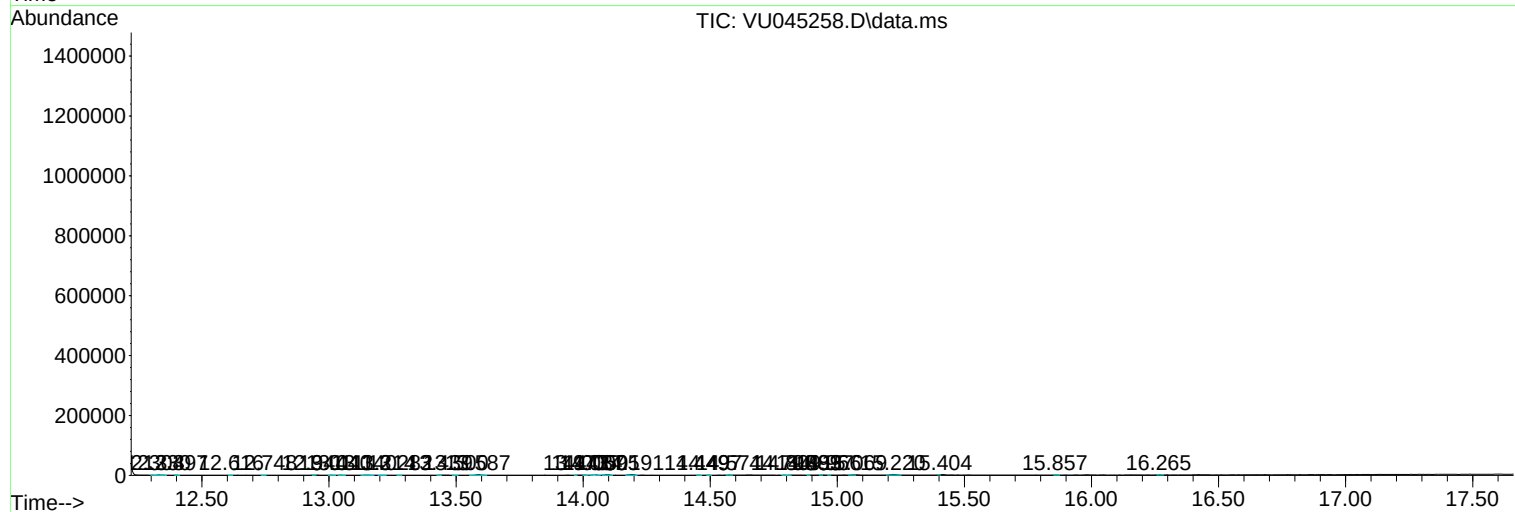
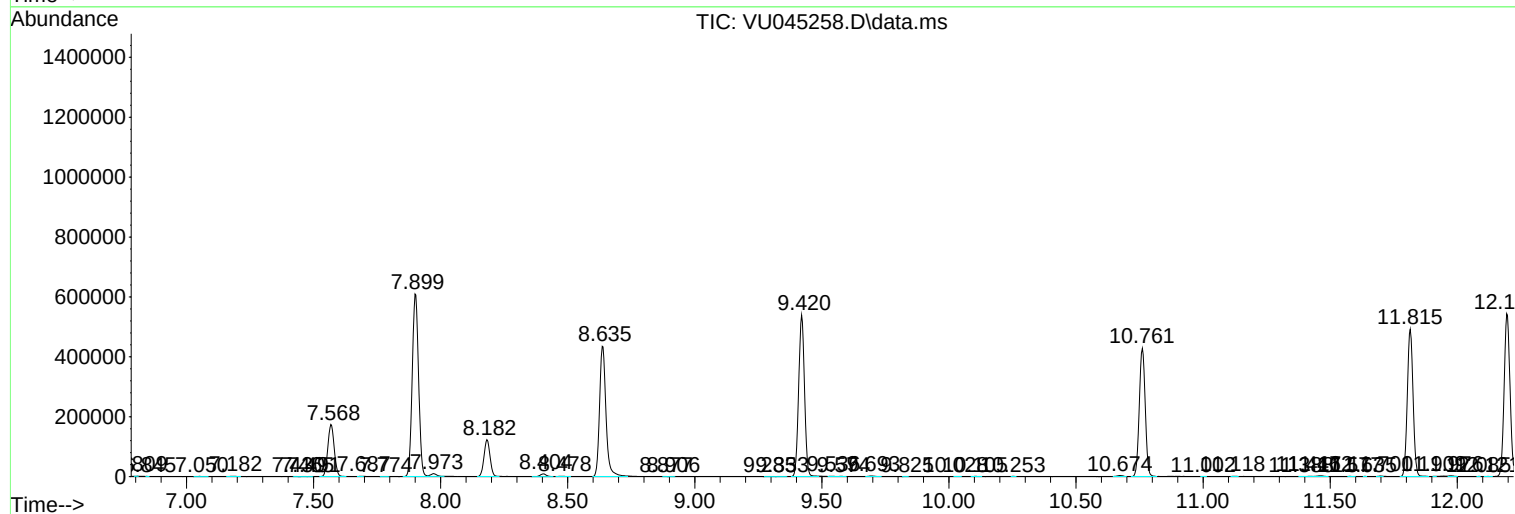
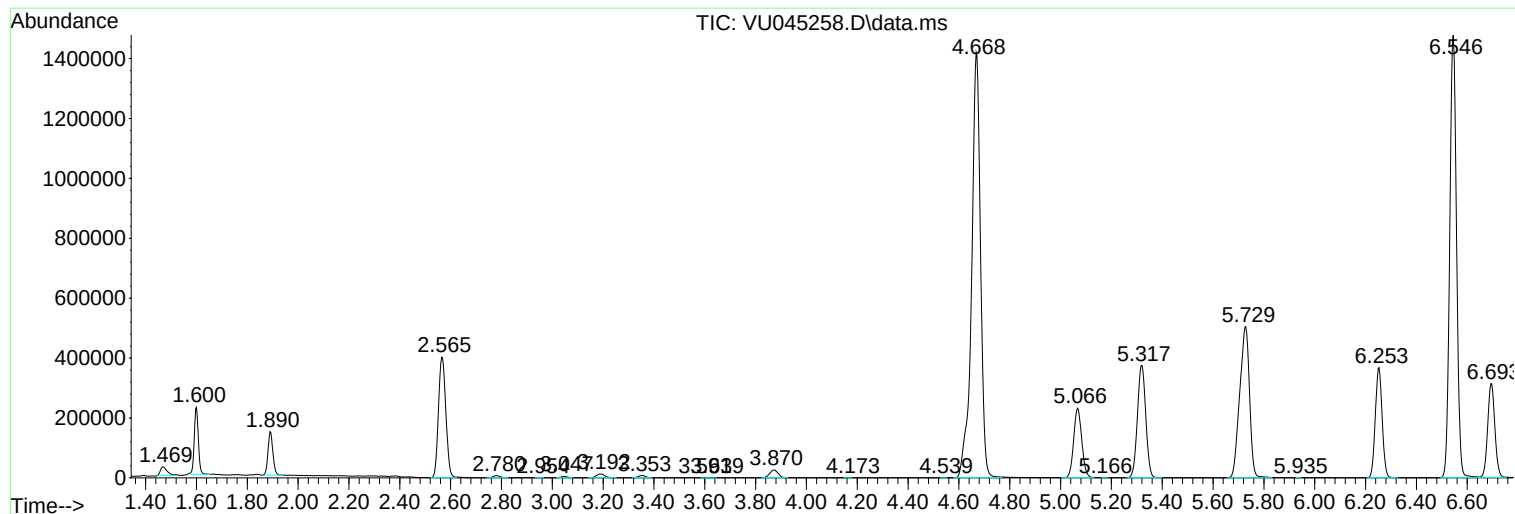
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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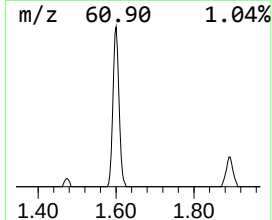
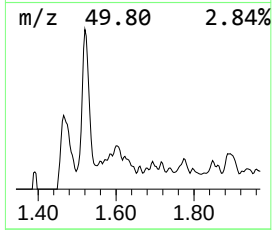
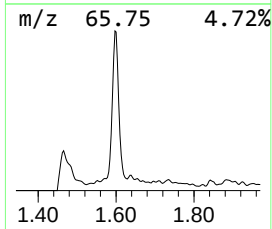
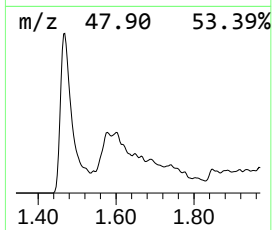
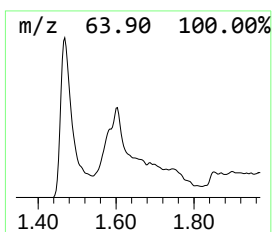
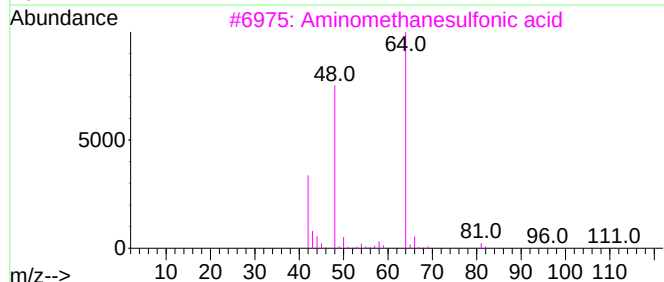
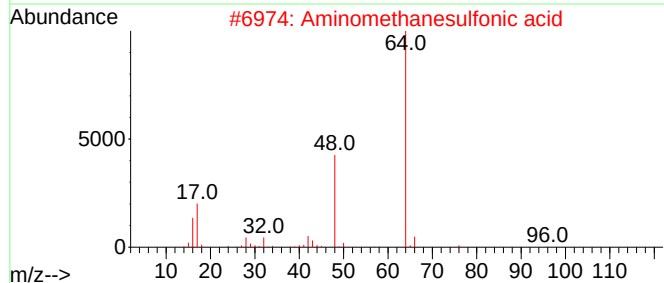
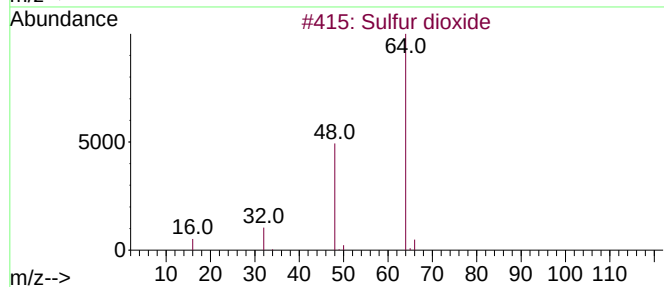
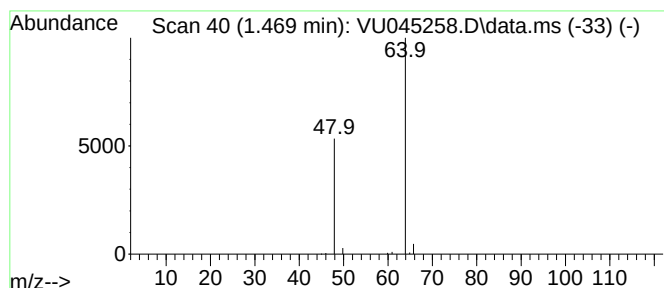
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	3.95 ug/L	54433	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	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	4.0	ug/L	54433	1	6.253	689797	50.0