

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041023\
 Data File : VU053616.D
 Acq On : 10 Apr 2023 15:39
 Operator : JC/MD
 Sample : 02251-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD1

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053616.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	52	rBV	19460	34827	3.07%	0.471%
2	1.597	74	80	95	rVB	112792	127832	11.26%	1.728%
3	1.909	170	177	190	rVB	93603	127640	11.24%	1.725%
4	2.565	369	381	396	rBV	169824	283595	24.98%	3.833%
5	2.957	501	503	506	rVB2	337	168	0.01%	0.002%
6	2.980	506	510	512	rBV	370	258	0.02%	0.003%
7	3.022	520	523	524	rBV2	315	192	0.02%	0.003%
8	3.051	529	532	535	rBV	392	291	0.03%	0.004%
9	3.131	554	557	561	rBV2	238	223	0.02%	0.003%
10	3.182	570	573	578	rVB3	622	526	0.05%	0.007%
11	3.572	690	694	698	rVB2	359	271	0.02%	0.004%
12	3.600	698	703	706	rBV	287	337	0.03%	0.005%
13	3.883	787	791	792	rBV	264	195	0.02%	0.003%
14	3.928	800	805	809	rVB2	245	218	0.02%	0.003%
15	3.951	809	812	817	rBV2	254	237	0.02%	0.003%
16	4.453	964	968	974	rVB2	308	231	0.02%	0.003%
17	4.491	977	980	986	rVB2	272	221	0.02%	0.003%
18	4.523	988	990	996	rVB2	199	188	0.02%	0.003%
19	4.552	996	999	1004	rVB	281	189	0.02%	0.003%
20	4.613	1006	1018	1041	rBV	71507	171072	15.07%	2.312%
21	4.771	1065	1067	1070	rVB2	499	174	0.02%	0.002%
22	4.922	1111	1114	1118	rVB3	336	301	0.03%	0.004%
23	4.941	1118	1120	1123	rVB	360	174	0.02%	0.002%
24	4.964	1123	1127	1131	rBV2	457	387	0.03%	0.005%
25	5.057	1136	1156	1176	rBV	157977	347479	30.60%	4.697%
26	5.289	1226	1228	1232	rBV2	532	373	0.03%	0.005%
27	5.401	1258	1263	1265	rBV	298	264	0.02%	0.004%
28	5.719	1341	1362	1371	rBV2	306381	850338	74.89%	11.493%
29	6.022	1452	1456	1461	rVB4	590	546	0.05%	0.007%
30	6.044	1461	1463	1467	rBV	391	280	0.02%	0.004%
31	6.108	1479	1483	1486	rBV3	527	450	0.04%	0.006%
32	6.163	1496	1500	1502	rBV	367	285	0.03%	0.004%
33	6.243	1511	1525	1545	rBV	301790	572219	50.40%	7.734%
34	6.485	1596	1600	1603	rBV2	208	180	0.02%	0.002%
35	6.530	1606	1614	1617	rBV2	995	1058	0.09%	0.014%
36	6.575	1625	1628	1634	rVB2	266	223	0.02%	0.003%

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 Title : VOC Analysis

37	6.626	1641	1644	1649	rVB	291	202	0.02%	0.003%
38	6.687	1649	1663	1685	rBV	190831	380671	33.53%	5.145%
39	6.887	1721	1725	1730	rBV2	254	315	0.03%	0.004%
40	6.983	1752	1755	1760	rBV2	228	206	0.02%	0.003%
41	7.092	1784	1789	1793	rVB2	267	213	0.02%	0.003%
42	7.189	1811	1819	1823	rBV4	960	1370	0.12%	0.019%
43	7.276	1843	1846	1849	rVB	288	207	0.02%	0.003%
44	7.298	1849	1853	1857	rBV2	355	348	0.03%	0.005%
45	7.446	1894	1899	1902	rVB2	236	207	0.02%	0.003%
46	7.472	1902	1907	1910	rBV2	190	157	0.01%	0.002%
47	7.562	1922	1935	1959	rBV	110319	195789	17.24%	2.646%
48	7.822	2010	2016	2020	rBV2	263	286	0.03%	0.004%
49	7.893	2025	2038	2061	rBV	395933	689305	60.71%	9.317%
50	8.034	2079	2082	2086	rBV3	452	367	0.03%	0.005%
51	8.070	2091	2093	2095	rVB	441	204	0.02%	0.003%
52	8.173	2115	2125	2146	rBV2	75335	130498	11.49%	1.764%
53	8.420	2199	2202	2204	rBV	259	174	0.02%	0.002%
54	8.468	2209	2217	2219	rBV2	710	791	0.07%	0.011%
55	8.539	2236	2239	2240	rBV	300	185	0.02%	0.003%
56	8.626	2254	2266	2298	rVV	212063	392842	34.60%	5.310%
57	8.787	2314	2316	2320	rBV2	305	192	0.02%	0.003%
58	9.083	2406	2408	2411	rVB2	281	160	0.01%	0.002%
59	9.243	2453	2458	2463	rVV2	313	299	0.03%	0.004%
60	9.288	2468	2472	2474	rBV	277	221	0.02%	0.003%
61	9.349	2488	2491	2493	rBV	287	190	0.02%	0.003%
62	9.414	2498	2511	2514	rBV	429528	639103	56.29%	8.638%
63	9.645	2580	2583	2587	rBV	330	238	0.02%	0.003%
64	9.915	2663	2667	2672	rBV2	215	206	0.02%	0.003%
65	10.111	2726	2728	2731	rVV2	316	167	0.01%	0.002%
66	10.160	2737	2743	2746	rBV	176	204	0.02%	0.003%
67	10.202	2753	2756	2759	rVV2	337	215	0.02%	0.003%
68	10.224	2760	2763	2769	rBV2	222	245	0.02%	0.003%
69	10.304	2785	2788	2790	rBV	251	158	0.01%	0.002%
70	10.394	2814	2816	2818	rBV	315	158	0.01%	0.002%
71	10.436	2826	2829	2832	rBV2	181	156	0.01%	0.002%
72	10.581	2871	2874	2881	rBV2	288	301	0.03%	0.004%
73	10.751	2914	2927	2944	rBV	283628	457110	40.26%	6.178%
74	10.883	2964	2968	2969	rBV	839	540	0.05%	0.007%
75	10.970	2992	2995	2997	rBV2	281	181	0.02%	0.002%
76	11.047	3017	3019	3022	rBV	426	204	0.02%	0.003%

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 Title : VOC Analysis

77	11.099	3029	3035	3038	rVB2	319	339	0.03%	0.005%
78	11.115	3038	3040	3043	rBV	326	184	0.02%	0.002%
79	11.134	3043	3046	3049	rBV	224	178	0.02%	0.002%
80	11.179	3055	3060	3062	rBV	240	235	0.02%	0.003%
81	11.343	3105	3111	3114	rBV2	283	383	0.03%	0.005%
82	11.407	3128	3131	3135	rVB3	384	351	0.03%	0.005%
83	11.742	3224	3235	3244	rBV2	43165	67344	5.93%	0.910%
84	11.809	3244	3256	3259	rBV	474045	695428	61.25%	9.399%
85	12.070	3331	3337	3339	rBV2	674	611	0.05%	0.008%
86	12.192	3362	3375	3397	rBV2	477955	1135457	100.00%	15.347%
87	12.369	3427	3430	3437	rVB3	382	336	0.03%	0.005%
88	12.455	3456	3457	3460	rBV	358	226	0.02%	0.003%
89	12.777	3554	3557	3560	rBV	217	185	0.02%	0.003%
90	13.050	3640	3642	3645	rVB	353	169	0.01%	0.002%
91	13.108	3657	3660	3662	rBV	275	193	0.02%	0.003%
92	13.201	3686	3689	3691	rBV	395	231	0.02%	0.003%
93	13.362	3737	3739	3741	rBV	340	192	0.02%	0.003%
94	13.439	3758	3763	3766	rBV2	478	470	0.04%	0.006%
95	13.497	3778	3781	3787	rBV2	450	602	0.05%	0.008%
96	13.748	3856	3859	3860	rBV2	289	161	0.01%	0.002%
97	13.838	3877	3887	3901	rBV2	40919	66299	5.84%	0.896%
98	14.018	3940	3943	3946	rBV3	544	385	0.03%	0.005%
99	14.192	3994	3997	3999	rBV2	481	300	0.03%	0.004%
100	14.330	4032	4040	4050	rVB2	6889	10319	0.91%	0.139%

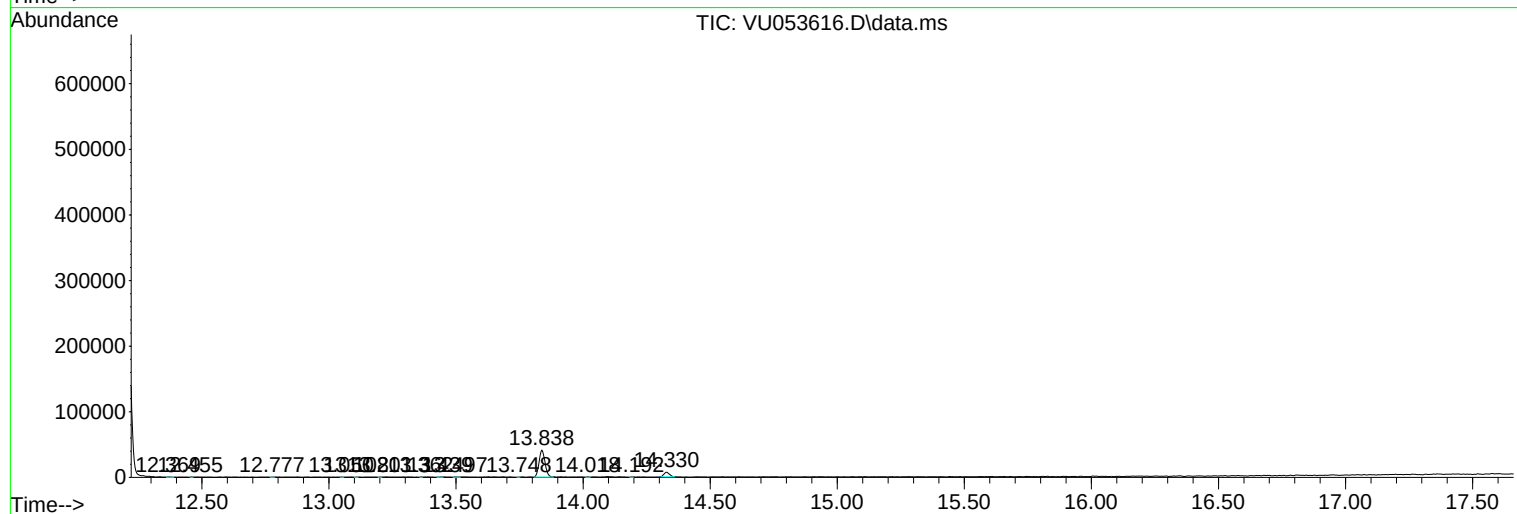
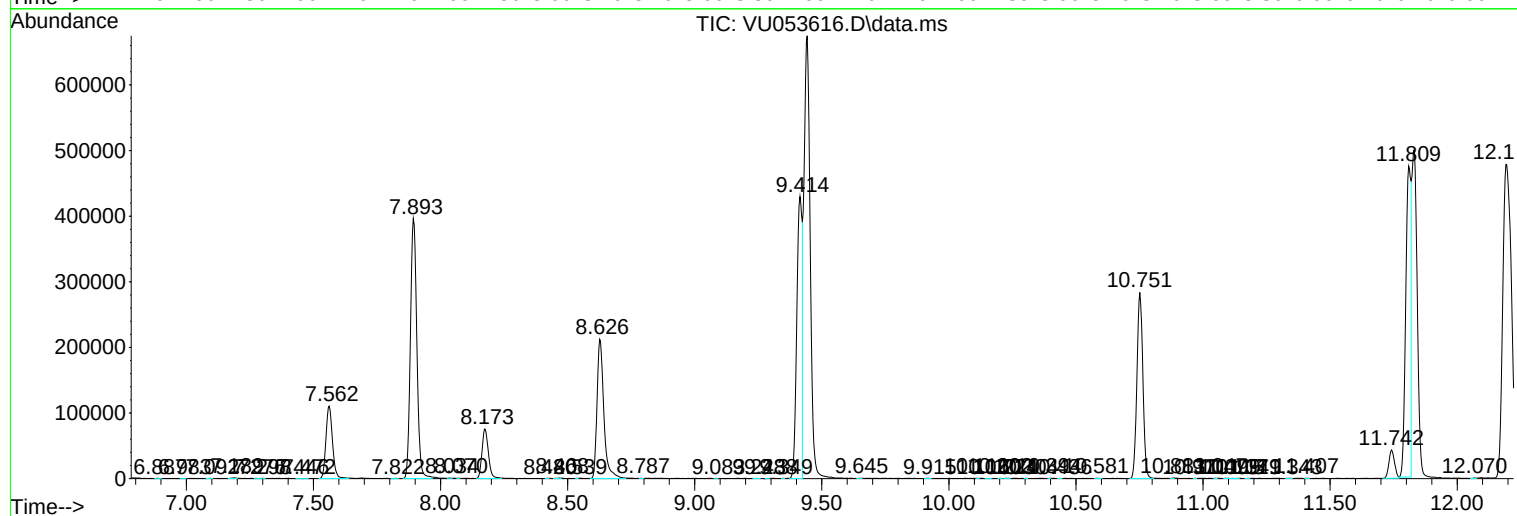
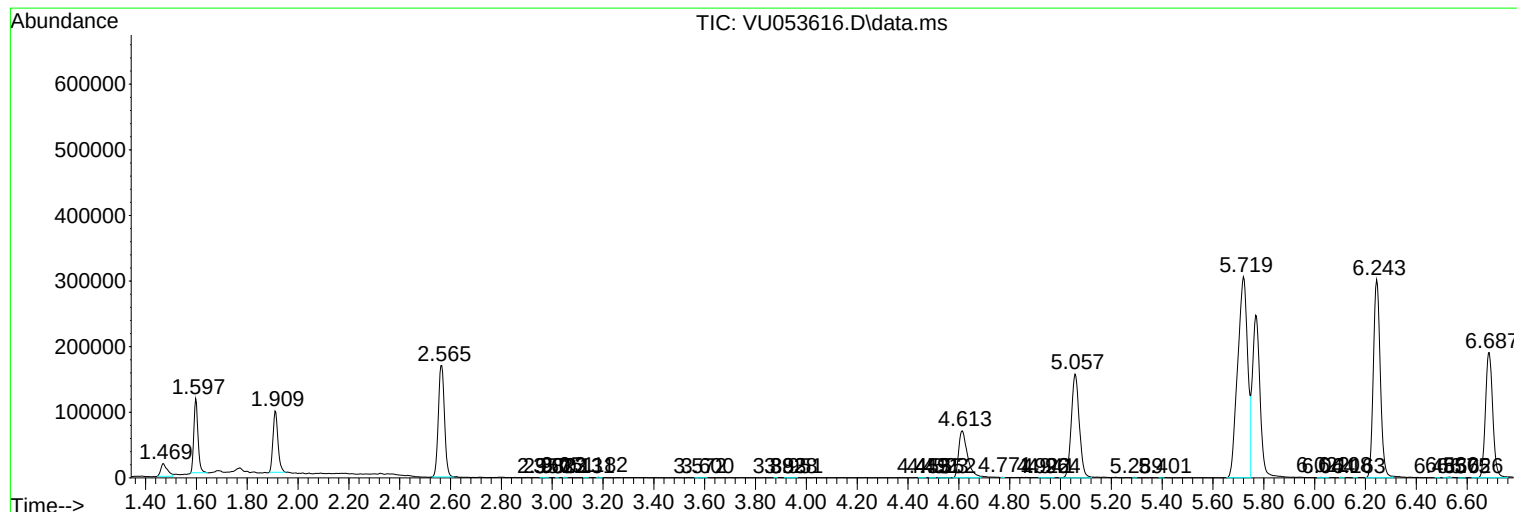
Sum of corrected areas: 7398605

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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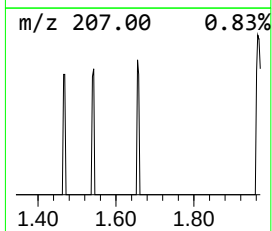
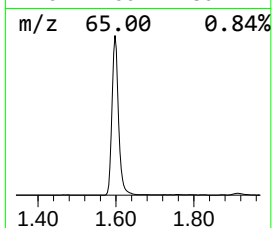
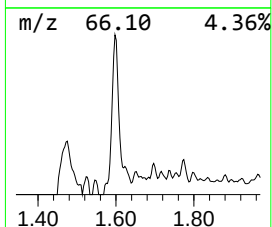
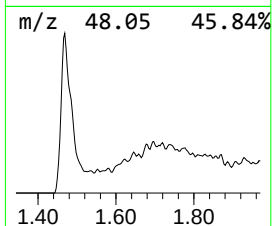
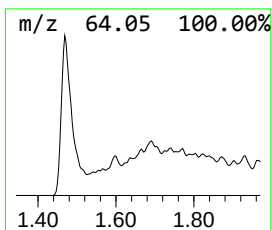
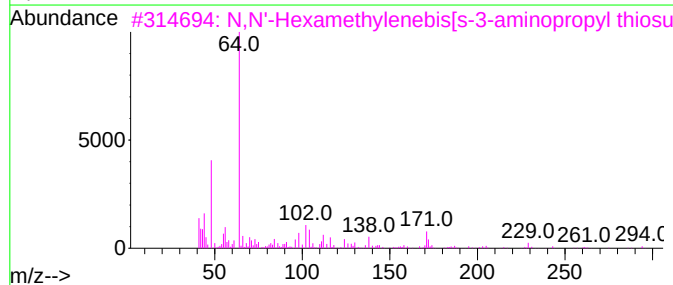
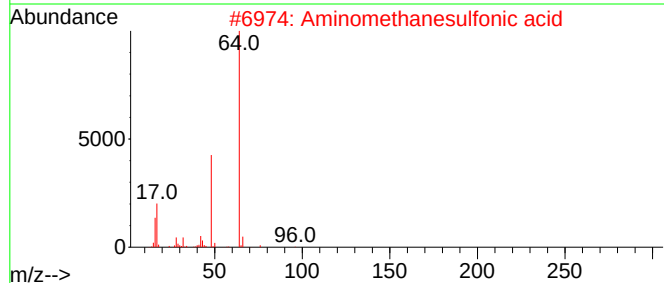
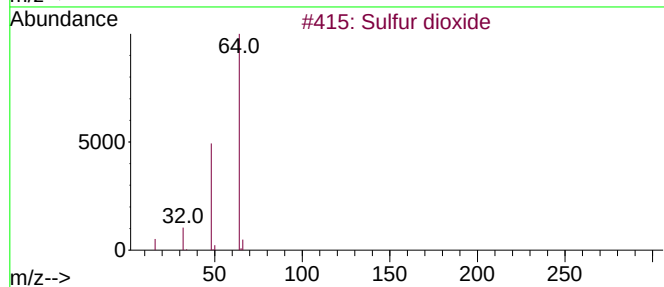
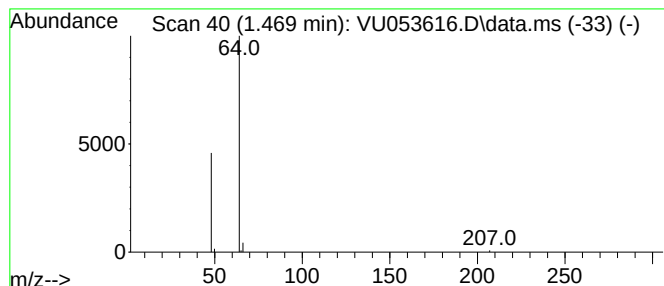
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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	3.04 ug/L	34827	1,4-Difluorobenzene	6.243

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			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	9
4			Benzenesulfonic acid, 2,5-diamino-	188	C6H8N2O3S	000088-45-9	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.0	ug/L	34827	1	6.243	572219	50.0