

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053633.D
 Acq On : 11 Apr 2023 14:23
 Operator : JC/MD
 Sample : 02251-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD5

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: VU053633.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	34	40	56	rBV	15712	28577	3.26%	0.419%
2	1.597	74	80	97	rVB	95541	110181	12.56%	1.616%
3	1.909	170	177	191	rVB	80504	110570	12.61%	1.621%
4	2.565	369	381	397	rBV	151164	243710	27.79%	3.574%
5	2.694	419	421	423	rBV	321	194	0.02%	0.003%
6	2.845	466	468	470	rBV	358	170	0.02%	0.002%
7	2.890	479	482	490	rBV2	311	404	0.05%	0.006%
8	3.035	524	527	528	rBV	548	307	0.04%	0.005%
9	3.167	562	568	569	rBV	1017	885	0.10%	0.013%
10	3.244	588	592	596	rBV	355	308	0.04%	0.005%
11	3.495	664	670	672	rBV2	258	261	0.03%	0.004%
12	3.916	795	801	803	rBV2	188	133	0.02%	0.002%
13	4.022	830	834	840	rBV	131	149	0.02%	0.002%
14	4.105	856	860	865	rBV2	251	281	0.03%	0.004%
15	4.131	865	868	872	rVB2	241	177	0.02%	0.003%
16	4.308	920	923	929	rBV2	207	245	0.03%	0.004%
17	4.353	932	937	939	rBV	346	222	0.03%	0.003%
18	4.523	985	990	997	rBV	304	271	0.03%	0.004%
19	4.568	1001	1004	1007	rBV2	225	154	0.02%	0.002%
20	4.613	1007	1018	1045	rBV	64739	157551	17.97%	2.310%
21	4.954	1122	1124	1128	rBV2	201	168	0.02%	0.002%
22	4.999	1134	1138	1141	rBV	324	268	0.03%	0.004%
23	5.057	1141	1156	1176	rVV2	143159	311470	35.52%	4.567%
24	5.253	1215	1217	1221	rVB2	255	166	0.02%	0.002%
25	5.633	1332	1335	1337	rBV	288	187	0.02%	0.003%
26	5.720	1341	1362	1391	rBV2	275596	784644	89.48%	11.506%
27	5.932	1425	1428	1432	rVB	277	183	0.02%	0.003%
28	5.974	1438	1441	1445	rBV	180	152	0.02%	0.002%
29	6.115	1482	1485	1489	rBV	495	418	0.05%	0.006%
30	6.170	1499	1502	1506	rVB2	300	208	0.02%	0.003%
31	6.244	1510	1525	1546	rBV	287150	549026	62.61%	8.051%
32	6.530	1608	1614	1617	rBV3	908	1016	0.12%	0.015%
33	6.594	1630	1634	1637	rVV2	351	315	0.04%	0.005%
34	6.684	1647	1662	1682	rBV	173156	342928	39.11%	5.029%
35	6.793	1694	1696	1697	rBV	361	160	0.02%	0.002%
36	6.835	1707	1709	1714	rVB	395	237	0.03%	0.003%

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

37	6.999	1758	1760	1765	rVB	252	156	0.02%	0.002%
38	7.064	1777	1780	1786	rBV	200	171	0.02%	0.003%
39	7.092	1786	1789	1791	rBV	210	137	0.02%	0.002%
40	7.189	1811	1819	1824	rBV4	843	1268	0.14%	0.019%
41	7.346	1862	1868	1869	rBV	239	218	0.02%	0.003%
42	7.475	1905	1908	1912	rBV	222	166	0.02%	0.002%
43	7.562	1922	1935	1951	rBV	97004	172381	19.66%	2.528%
44	7.687	1969	1974	1978	rBV2	645	623	0.07%	0.009%
45	7.793	2003	2007	2010	rBV2	381	328	0.04%	0.005%
46	7.835	2016	2020	2025	rBV3	373	388	0.04%	0.006%
47	7.893	2025	2038	2066	rBV	352067	614608	70.09%	9.012%
48	8.176	2114	2126	2148	rBV	67936	114477	13.05%	1.679%
49	8.462	2209	2215	2225	rBV2	759	1349	0.15%	0.020%
50	8.555	2237	2244	2247	rBV2	248	291	0.03%	0.004%
51	8.626	2255	2266	2296	rBV	192536	353077	40.26%	5.177%
52	8.845	2332	2334	2338	rVB2	266	173	0.02%	0.003%
53	8.932	2360	2361	2366	rVB2	285	149	0.02%	0.002%
54	8.977	2370	2375	2378	rBV	282	246	0.03%	0.004%
55	9.150	2426	2429	2432	rBV	245	147	0.02%	0.002%
56	9.414	2498	2511	2544	rBV2	400484	767837	87.56%	11.259%
57	9.568	2556	2559	2564	rVB2	514	387	0.04%	0.006%
58	9.613	2566	2573	2580	rBV2	379	564	0.06%	0.008%
59	9.649	2580	2584	2588	rBV	261	290	0.03%	0.004%
60	9.700	2594	2600	2604	rVB	292	355	0.04%	0.005%
61	9.877	2652	2655	2658	rVB2	181	145	0.02%	0.002%
62	9.935	2670	2673	2678	rVB	235	191	0.02%	0.003%
63	9.960	2678	2681	2683	rBV	226	170	0.02%	0.002%
64	10.051	2706	2709	2711	rBV	266	157	0.02%	0.002%
65	10.285	2775	2782	2784	rBV2	192	254	0.03%	0.004%
66	10.366	2804	2807	2813	rBV2	273	244	0.03%	0.004%
67	10.407	2817	2820	2824	rVB	227	173	0.02%	0.003%
68	10.552	2860	2865	2870	rVV2	257	287	0.03%	0.004%
69	10.751	2914	2927	2944	rBV	267507	424015	48.35%	6.218%
70	10.854	2956	2959	2963	rBV2	232	210	0.02%	0.003%
71	10.880	2963	2967	2968	rBV	652	474	0.05%	0.007%
72	11.063	3022	3024	3028	rBV2	248	190	0.02%	0.003%
73	11.517	3163	3165	3171	rVB	268	200	0.02%	0.003%
74	11.610	3189	3194	3198	rBV2	255	291	0.03%	0.004%
75	11.674	3210	3214	3216	rBV	245	232	0.03%	0.003%
76	11.742	3226	3235	3244	rBV2	22024	33778	3.85%	0.495%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : VOC Analysis

77	11.809	3244	3256	3278	rVV2	447600	876896	100.00%	12.858%
78	11.938	3294	3296	3300	rVB2	268	178	0.02%	0.003%
79	12.079	3336	3340	3341	rBV2	479	322	0.04%	0.005%
80	12.189	3362	3374	3397	rBV2	404056	768323	87.62%	11.266%
81	12.311	3410	3412	3418	rVB3	595	426	0.05%	0.006%
82	12.382	3432	3434	3438	rVB2	257	140	0.02%	0.002%
83	12.629	3509	3511	3515	rBV	284	166	0.02%	0.002%
84	12.854	3573	3581	3585	rBV2	417	532	0.06%	0.008%
85	12.973	3614	3618	3622	rBV2	255	256	0.03%	0.004%
86	13.073	3645	3649	3652	rBV2	225	183	0.02%	0.003%
87	13.250	3702	3704	3708	rBV	269	178	0.02%	0.003%
88	13.340	3730	3732	3734	rBV	212	135	0.02%	0.002%
89	13.420	3754	3757	3760	rBV	318	185	0.02%	0.003%
90	13.465	3768	3771	3772	rBV	329	144	0.02%	0.002%
91	13.629	3818	3822	3825	rBV	525	547	0.06%	0.008%
92	13.774	3865	3867	3871	rVB	286	136	0.02%	0.002%
93	13.838	3878	3887	3901	rBV4	13844	22695	2.59%	0.333%
94	13.902	3905	3907	3910	rBV2	287	178	0.02%	0.003%
95	13.964	3921	3926	3933	rBV3	435	635	0.07%	0.009%
96	14.047	3948	3952	3956	rBV2	405	289	0.03%	0.004%
97	14.076	3957	3961	3962	rBV2	366	267	0.03%	0.004%
98	14.253	4012	4016	4021	rBV	354	435	0.05%	0.006%
99	14.330	4032	4040	4050	rVB5	5361	9067	1.03%	0.133%
100	14.372	4050	4053	4056	rBV	392	205	0.02%	0.003%

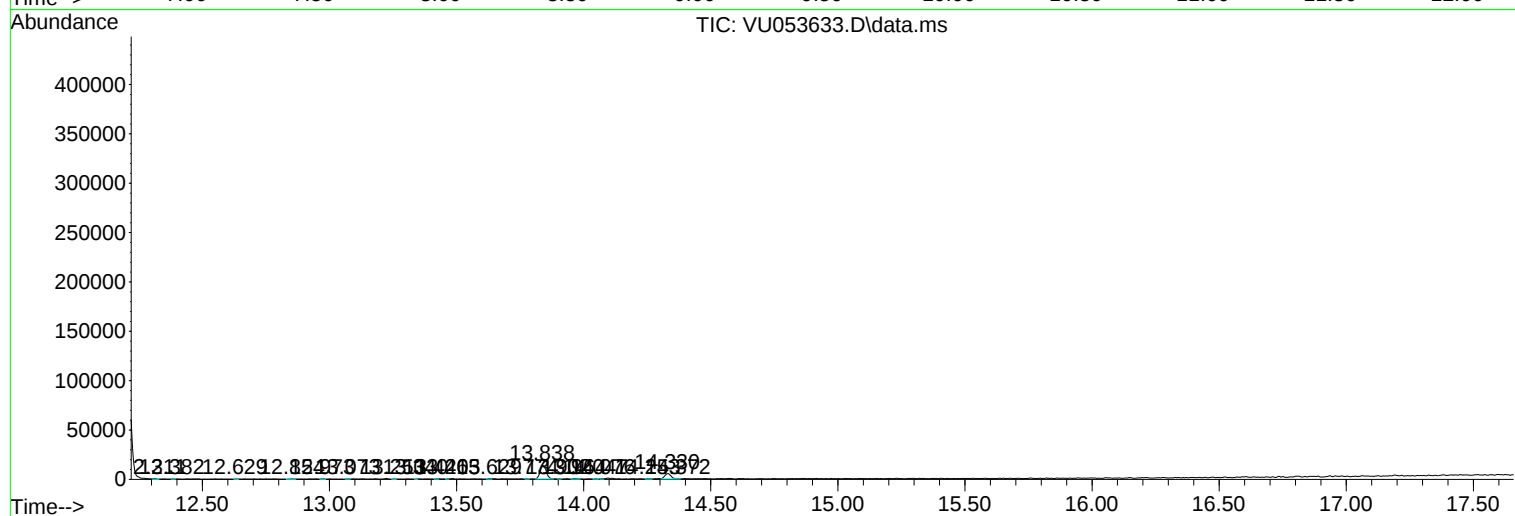
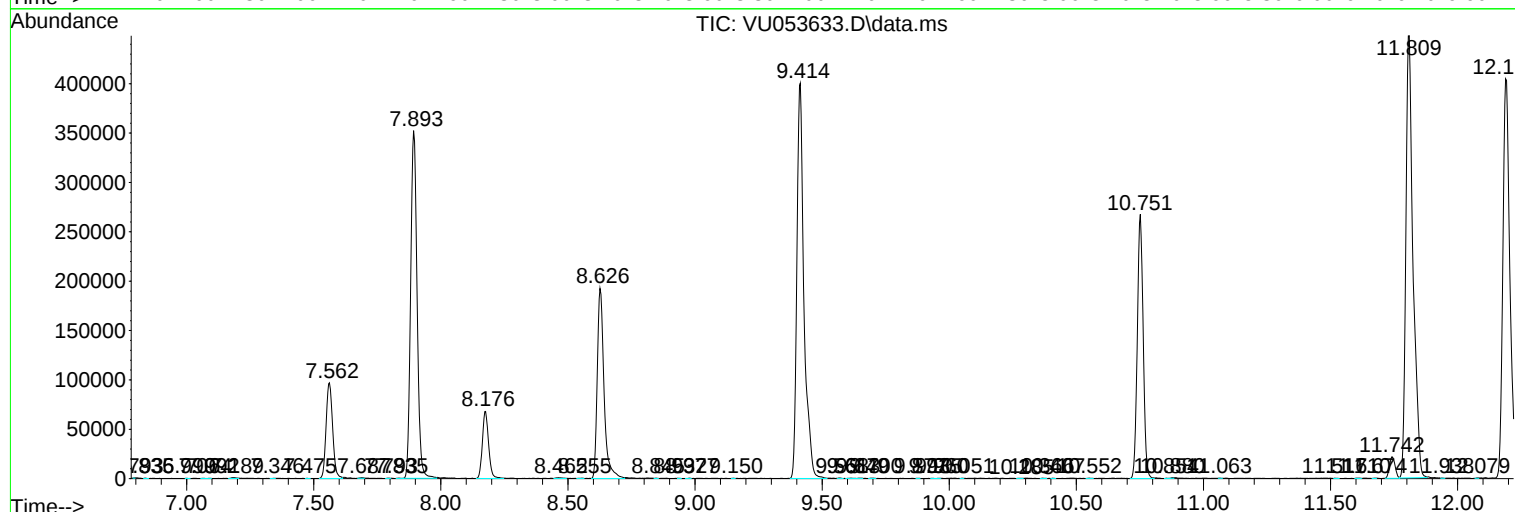
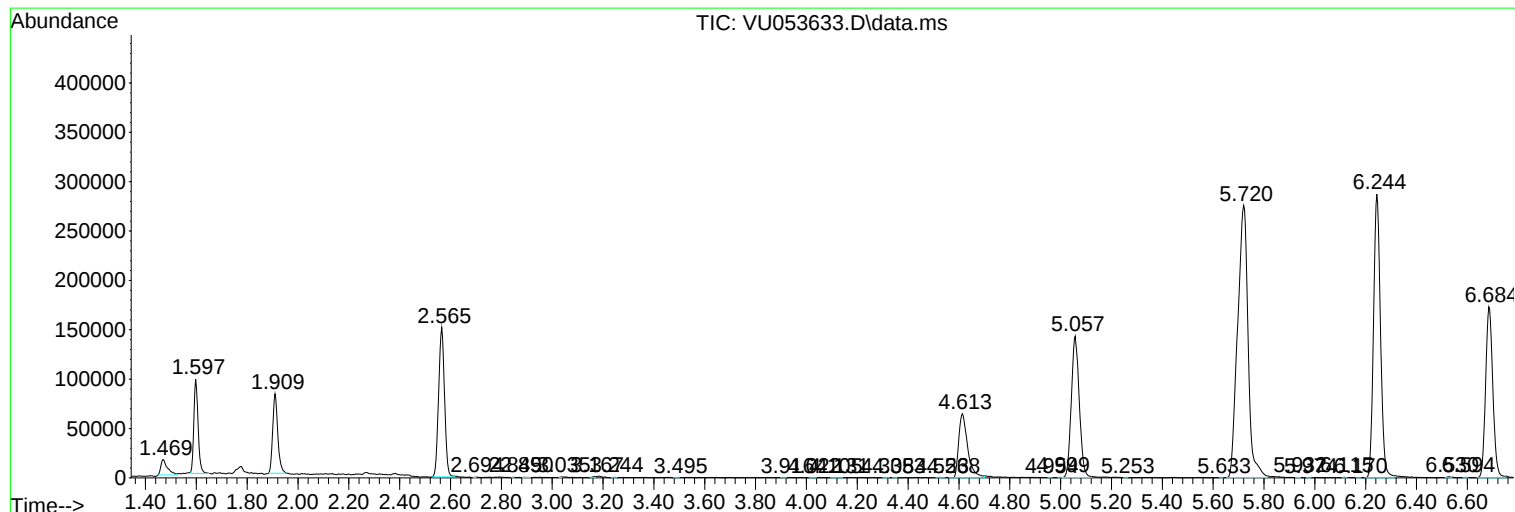
Sum of corrected areas: 6819611

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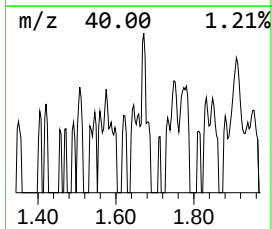
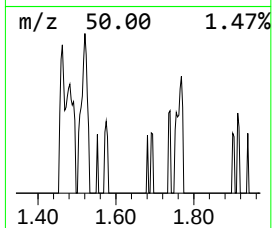
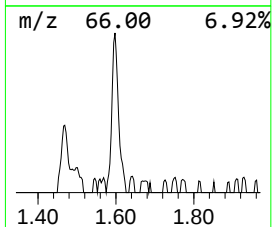
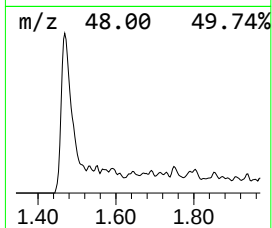
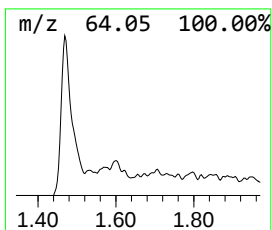
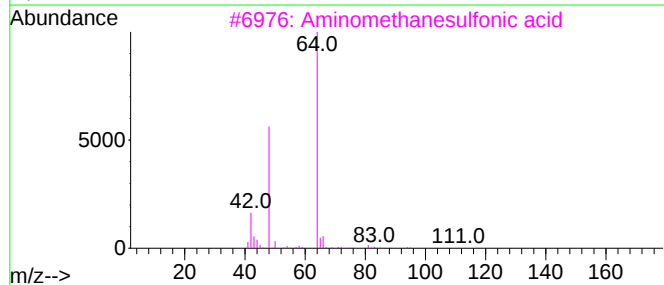
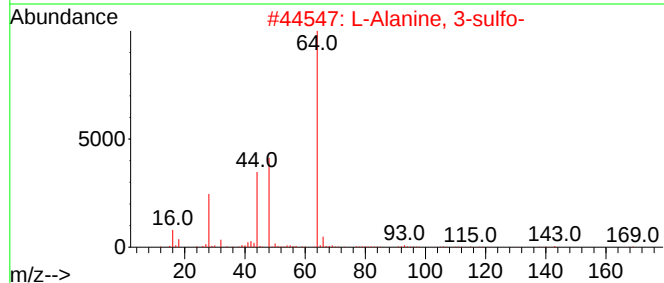
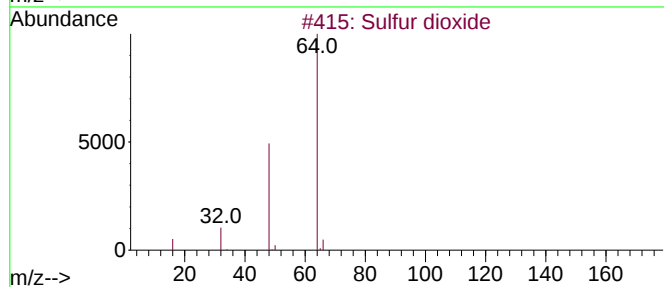
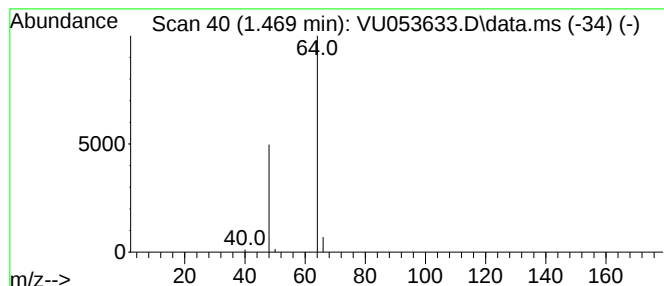
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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	2.60 ug/L	28577	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	2.6	ug/L	28577	1	6.244	549026	50.0