

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062022\
 Data File : VU049300.D
 Acq On : 20 Jun 2022 13:04
 Operator : SY/MD
 Sample : N3395-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0156

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\SFAMULM061022WMA.M

Title : VOC Analysis

Signal : TIC: VU049300.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	38	46	62	rBV	14218	37108	3.75%	0.441%
2	1.597	74	80	101	rVB	119227	136711	13.82%	1.625%
3	1.912	170	178	191	rVB	95770	120203	12.15%	1.429%
4	2.568	370	382	396	rBV	187813	302272	30.56%	3.594%
5	2.922	488	492	496	rBV3	226	208	0.02%	0.002%
6	2.999	511	516	518	rBV2	335	240	0.02%	0.003%
7	3.038	526	528	533	rVV5	488	401	0.04%	0.005%
8	3.118	546	553	555	rBV3	261	318	0.03%	0.004%
9	3.279	598	603	608	rBV3	265	259	0.03%	0.003%
10	3.356	624	627	630	rBV3	259	178	0.02%	0.002%
11	3.446	653	655	657	rBV	291	196	0.02%	0.002%
12	3.501	670	672	677	rBV2	416	345	0.03%	0.004%
13	3.591	695	700	701	rBV	328	201	0.02%	0.002%
14	3.623	707	710	713	rBV2	501	400	0.04%	0.005%
15	3.645	713	717	720	rVV2	321	323	0.03%	0.004%
16	3.706	732	736	739	rVV2	343	332	0.03%	0.004%
17	3.835	774	776	781	rVB2	339	259	0.03%	0.003%
18	3.893	790	794	799	rBV2	406	531	0.05%	0.006%
19	3.970	815	818	821	rVB2	483	338	0.03%	0.004%
20	4.173	879	881	887	rBV2	207	210	0.02%	0.002%
21	4.231	895	899	905	rBV2	413	452	0.05%	0.005%
22	4.311	919	924	931	rVB2	467	591	0.06%	0.007%
23	4.478	970	976	980	rBV2	284	260	0.03%	0.003%
24	4.568	1000	1004	1008	rBV2	274	278	0.03%	0.003%
25	4.623	1008	1021	1047	rBV2	119038	299911	30.32%	3.566%
26	4.903	1105	1108	1112	rVB2	319	218	0.02%	0.003%
27	4.983	1130	1133	1135	rBV3	234	197	0.02%	0.002%
28	5.063	1141	1158	1179	rBV	184065	399194	40.36%	4.746%
29	5.218	1204	1206	1212	rVB2	541	435	0.04%	0.005%
30	5.259	1216	1219	1222	rBV2	233	190	0.02%	0.002%
31	5.372	1239	1254	1273	rBV	210313	433065	43.78%	5.149%
32	5.520	1296	1300	1303	rBV	445	371	0.04%	0.004%
33	5.726	1341	1364	1396	rBV2	365899	989170	100.00%	11.761%
34	6.018	1452	1455	1461	rVB2	341	340	0.03%	0.004%
35	6.054	1461	1466	1469	rBV2	316	261	0.03%	0.003%
36	6.073	1469	1472	1476	rVB	284	208	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
 Title : VOC Analysis

37	6.250	1510	1527	1546	rBV	332418	634396	64.13%	7.543%
38	6.382	1565	1568	1570	rBV	318	229	0.02%	0.003%
39	6.398	1570	1573	1579	rVV3	410	439	0.04%	0.005%
40	6.530	1607	1614	1622	rVB6	2179	3413	0.35%	0.041%
41	6.616	1639	1641	1644	rBV	288	184	0.02%	0.002%
42	6.690	1650	1664	1683	rBV	247186	475885	48.11%	5.658%
43	7.041	1770	1773	1779	rBV2	400	513	0.05%	0.006%
44	7.185	1811	1818	1829	rVB3	1477	2059	0.21%	0.024%
45	7.501	1913	1916	1920	rBV3	211	209	0.02%	0.002%
46	7.565	1923	1936	1957	rBV	105834	191302	19.34%	2.275%
47	7.684	1967	1973	1975	rBV3	774	849	0.09%	0.010%
48	7.755	1992	1995	1998	rVB2	363	234	0.02%	0.003%
49	7.793	2005	2007	2010	rBV3	358	283	0.03%	0.003%
50	7.896	2025	2039	2057	rBV	444226	776479	78.50%	9.232%
51	8.179	2115	2127	2145	rBV	73550	125721	12.71%	1.495%
52	8.298	2160	2164	2165	rBV2	380	270	0.03%	0.003%
53	8.375	2183	2188	2190	rBV2	362	415	0.04%	0.005%
54	8.391	2191	2193	2196	rVV	267	183	0.02%	0.002%
55	8.475	2214	2219	2222	rBV2	428	409	0.04%	0.005%
56	8.533	2232	2237	2240	rBV2	274	249	0.03%	0.003%
57	8.632	2255	2268	2297	rBV3	344233	672996	68.04%	8.002%
58	8.857	2335	2338	2341	rBV	275	209	0.02%	0.002%
59	8.883	2342	2346	2349	rVB3	418	393	0.04%	0.005%
60	9.166	2432	2434	2440	rBV2	264	284	0.03%	0.003%
61	9.259	2461	2463	2468	rVB3	318	229	0.02%	0.003%
62	9.417	2497	2512	2550	rBV	457965	774227	78.27%	9.205%
63	9.568	2555	2559	2561	rBV3	485	349	0.04%	0.004%
64	9.581	2561	2563	2566	rVB2	377	208	0.02%	0.002%
65	9.658	2582	2587	2591	rVB2	397	327	0.03%	0.004%
66	9.693	2591	2598	2605	rBV4	1267	1850	0.19%	0.022%
67	9.751	2612	2616	2619	rBV	431	363	0.04%	0.004%
68	9.832	2636	2641	2644	rBV2	277	243	0.02%	0.003%
69	9.947	2674	2677	2678	rBV2	310	219	0.02%	0.003%
70	10.102	2723	2725	2728	rVV2	412	260	0.03%	0.003%
71	10.166	2742	2745	2749	rBV3	258	254	0.03%	0.003%
72	10.246	2765	2770	2772	rBV2	332	295	0.03%	0.004%
73	10.426	2823	2826	2829	rVV	338	221	0.02%	0.003%
74	10.449	2829	2833	2837	rVB3	305	276	0.03%	0.003%
75	10.565	2863	2869	2875	rBV3	336	415	0.04%	0.005%
76	10.597	2875	2879	2883	rVB2	205	186	0.02%	0.002%

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Min Area: 0 % of largest Peak

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Peak Location: TOP

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

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 Title : VOC Analysis

77	10.664	2897	2900	2903	rBV	436	315	0.03%	0.004%
78	10.754	2916	2928	2954	rVB	345730	558660	56.48%	6.642%
79	10.867	2958	2963	2965	rBV2	322	340	0.03%	0.004%
80	10.889	2965	2970	2974	rBV3	651	653	0.07%	0.008%
81	11.015	3007	3009	3018	rVB3	227	230	0.02%	0.003%
82	11.076	3022	3028	3029	rBV	323	311	0.03%	0.004%
83	11.140	3043	3048	3050	rBV	306	239	0.02%	0.003%
84	11.327	3101	3106	3108	rBV	436	390	0.04%	0.005%
85	11.397	3124	3128	3132	rVB2	383	368	0.04%	0.004%
86	11.417	3132	3134	3139	rBV	234	178	0.02%	0.002%
87	11.745	3230	3236	3244	rBV4	1693	2225	0.22%	0.026%
88	11.812	3244	3257	3280	rBV	446310	716762	72.46%	8.522%
89	11.925	3290	3292	3297	rBV2	436	339	0.03%	0.004%
90	11.976	3304	3308	3311	rBV3	262	238	0.02%	0.003%
91	12.073	3336	3338	3342	rBV	209	179	0.02%	0.002%
92	12.192	3362	3375	3391	rBV	447575	727569	73.55%	8.651%
93	12.690	3527	3530	3533	rBV2	381	328	0.03%	0.004%
94	13.208	3688	3691	3693	rBV2	375	279	0.03%	0.003%
95	13.491	3774	3779	3782	rBV3	401	487	0.05%	0.006%
96	13.738	3854	3856	3860	rVB2	341	211	0.02%	0.003%
97	13.848	3882	3890	3898	rBV4	1672	2430	0.25%	0.029%
98	14.098	3958	3968	3978	rBV4	1583	2932	0.30%	0.035%
99	14.336	4034	4042	4043	rBV5	798	870	0.09%	0.010%
100	14.844	4197	4200	4203	rBV3	383	346	0.03%	0.004%

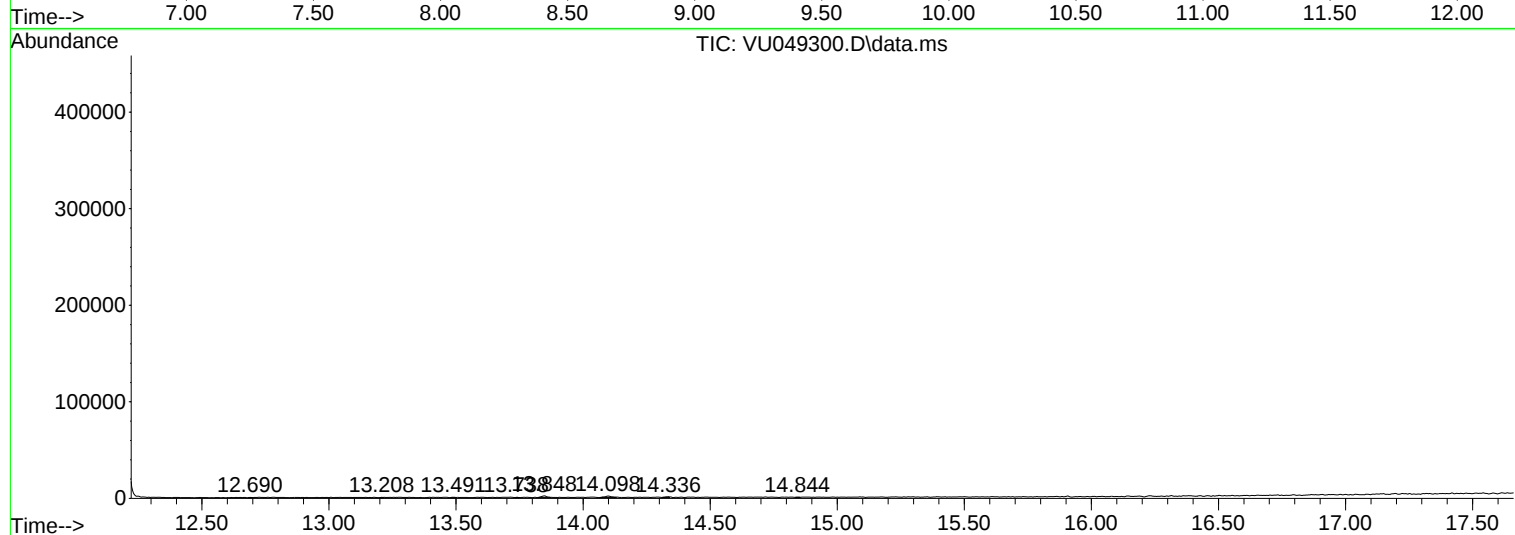
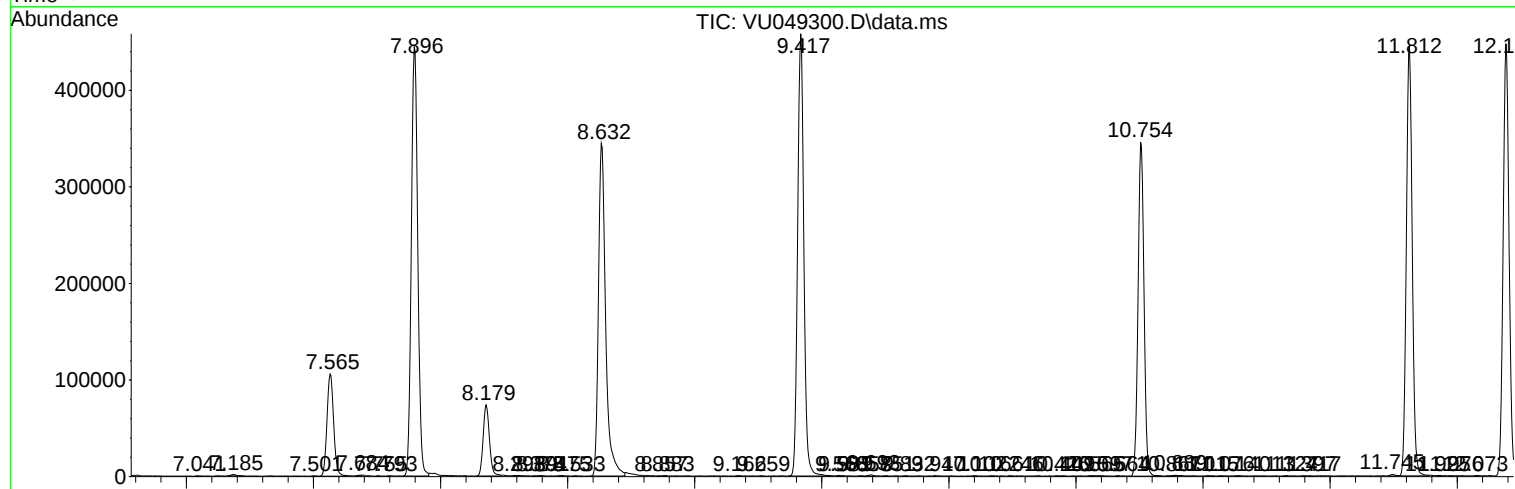
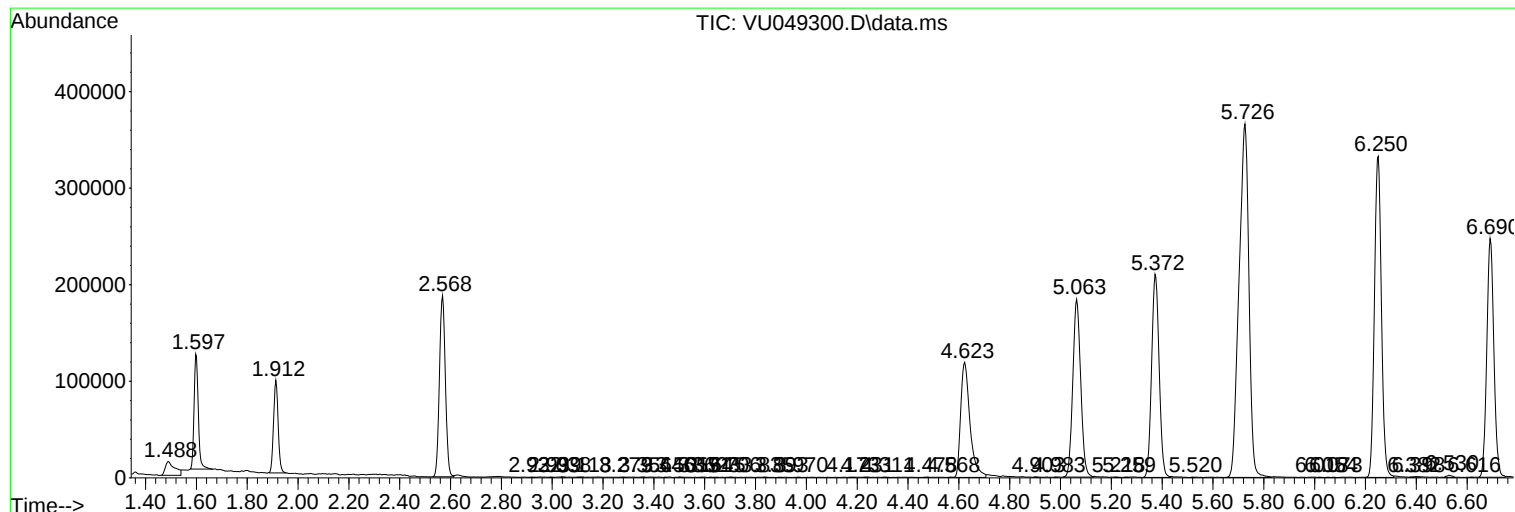
Sum of corrected areas: 8410578

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



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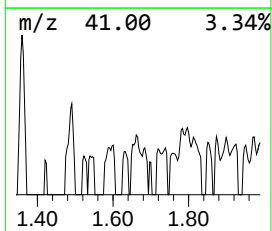
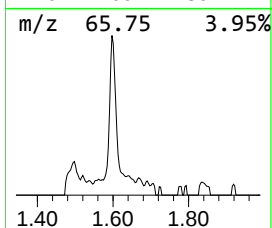
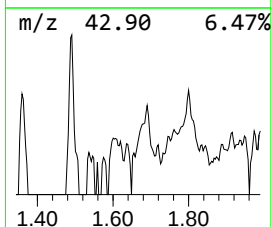
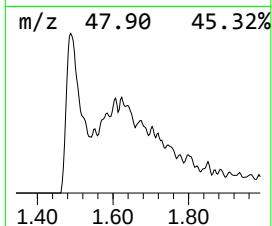
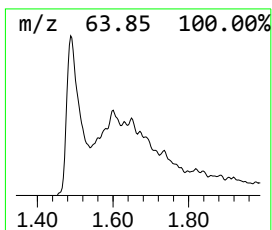
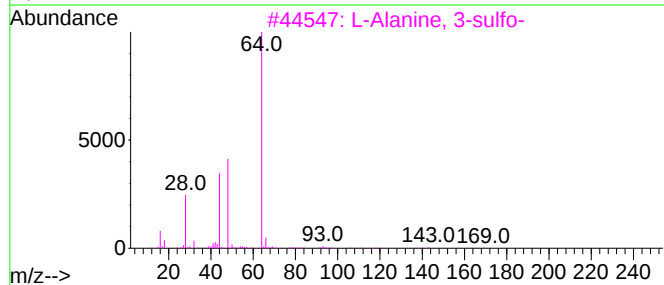
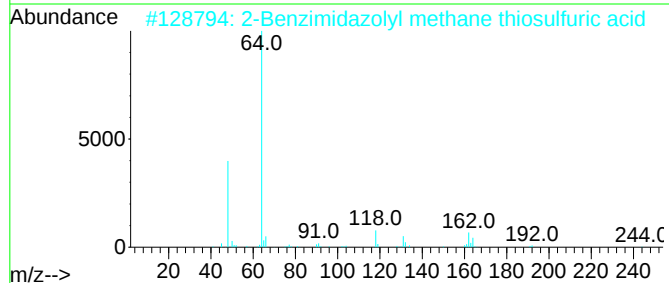
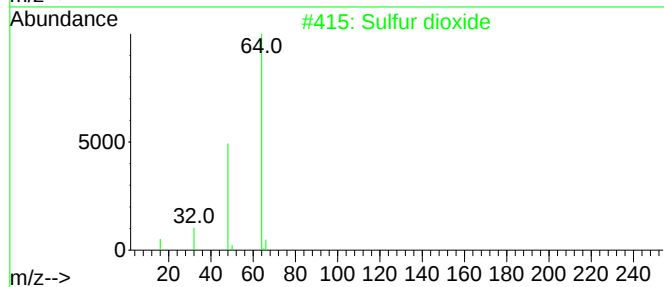
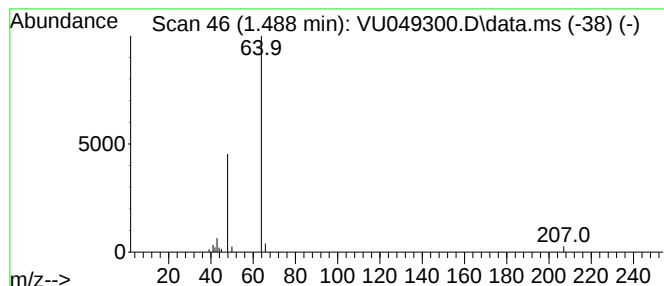
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.488	2.92 ug/L	37108	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
4			S-2-[4-Glutarimidobutylamino]eth...	324	C11H20N2O5S2	031701-78-7	9
5			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.488	2.9	ug/L	37108	1	6.250	634396	50.0