

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050522\
 Data File : VU048437.D
 Acq On : 05 May 2022 15:10
 Operator : SY/MD
 Sample : N2710-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXL85

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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	33	43	53	rBV	61726	125911	7.79%	1.009%
2	1.600	74	81	105	rVB	186551	251016	15.53%	2.012%
3	1.893	164	172	187	rVB	126373	183937	11.38%	1.474%
4	2.562	367	380	396	rBV	327993	535689	33.15%	4.293%
5	2.681	414	417	419	rBV2	517	333	0.02%	0.003%
6	2.780	440	448	461	rVB6	1926	4368	0.27%	0.035%
7	2.832	461	464	469	rVV2	199	197	0.01%	0.002%
8	3.044	523	530	540	rVB4	1137	1936	0.12%	0.016%
9	3.186	560	574	590	rBV	8197	19049	1.18%	0.153%
10	3.427	643	649	652	rVV2	261	200	0.01%	0.002%
11	3.607	698	705	707	rBV2	173	195	0.01%	0.002%
12	4.015	826	832	841	rBV2	225	281	0.02%	0.002%
13	4.227	893	898	901	rVV2	235	220	0.01%	0.002%
14	4.343	931	934	942	rVB	215	208	0.01%	0.002%
15	4.620	1005	1020	1047	rBV	191038	457246	28.30%	3.664%
16	5.002	1135	1139	1141	rVV2	291	218	0.01%	0.002%
17	5.063	1141	1158	1182	rVV	282986	633393	39.20%	5.076%
18	5.288	1220	1228	1231	rBV4	620	807	0.05%	0.006%
19	5.337	1235	1243	1254	rVB4	1027	2235	0.14%	0.018%
20	5.440	1270	1275	1282	rVB2	223	261	0.02%	0.002%
21	5.488	1287	1290	1296	rVB	200	207	0.01%	0.002%
22	5.536	1302	1305	1311	rVB	216	205	0.01%	0.002%
23	5.726	1341	1364	1395	rBV2	600413	1615969	100.00%	12.950%
24	5.967	1433	1439	1444	rBV5	557	664	0.04%	0.005%
25	6.034	1456	1460	1461	rBV2	337	227	0.01%	0.002%
26	6.115	1480	1485	1491	rVB3	341	408	0.03%	0.003%
27	6.166	1497	1501	1504	rVB2	383	320	0.02%	0.003%
28	6.247	1512	1526	1558	rBV	393083	750906	46.47%	6.018%
29	6.369	1561	1564	1571	rVB3	415	504	0.03%	0.004%
30	6.420	1576	1580	1584	rBV2	238	208	0.01%	0.002%
31	6.536	1606	1616	1627	rVB9	3634	7153	0.44%	0.057%
32	6.607	1636	1638	1641	rVB2	376	223	0.01%	0.002%
33	6.690	1646	1664	1685	rBV	368874	721571	44.65%	5.783%
34	7.047	1768	1775	1777	rBV2	393	402	0.02%	0.003%
35	7.095	1786	1790	1791	rBV2	850	471	0.03%	0.004%
36	7.179	1807	1816	1829	rVV5	4315	9050	0.56%	0.073%

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 Title : VOC Analysis

37	7.311	1852	1857	1860	rBV	218	216	0.01%	0.002%
38	7.356	1866	1871	1873	rVB2	248	200	0.01%	0.002%
39	7.565	1923	1936	1955	rBV	191731	336960	20.85%	2.700%
40	7.687	1966	1974	1984	rBV5	2635	4355	0.27%	0.035%
41	7.758	1993	1996	2000	rVB2	287	202	0.01%	0.002%
42	7.806	2004	2011	2014	rBV3	483	504	0.03%	0.004%
43	7.899	2025	2040	2057	rBV	748658	1298277	80.34%	10.404%
44	8.118	2104	2108	2114	rVB4	601	808	0.05%	0.006%
45	8.179	2114	2127	2147	rBV	137003	227258	14.06%	1.821%
46	8.311	2165	2168	2171	rBV2	293	256	0.02%	0.002%
47	8.410	2197	2199	2202	rVB	476	239	0.01%	0.002%
48	8.436	2202	2207	2208	rBV	371	252	0.02%	0.002%
49	8.465	2208	2216	2217	rBV4	668	714	0.04%	0.006%
50	8.555	2232	2244	2256	rBV	81480	134645	8.33%	1.079%
51	8.636	2256	2269	2304	rBV2	573044	1060009	65.60%	8.495%
52	8.783	2313	2315	2327	rVB6	1378	1711	0.11%	0.014%
53	8.832	2327	2330	2332	rBV3	292	226	0.01%	0.002%
54	8.963	2367	2371	2374	rBV3	460	383	0.02%	0.003%
55	9.070	2399	2404	2407	rVB	374	243	0.02%	0.002%
56	9.086	2407	2409	2413	rBV3	417	314	0.02%	0.003%
57	9.211	2444	2448	2452	rBV3	263	200	0.01%	0.002%
58	9.317	2479	2481	2487	rVB2	298	233	0.01%	0.002%
59	9.417	2498	2512	2549	rBV	574008	959304	59.36%	7.688%
60	9.603	2566	2570	2574	rVB3	364	319	0.02%	0.003%
61	9.671	2586	2591	2593	rBV	390	283	0.02%	0.002%
62	9.700	2593	2600	2607	rVB3	866	1295	0.08%	0.010%
63	9.806	2630	2633	2637	rVB	331	228	0.01%	0.002%
64	9.864	2647	2651	2655	rBV2	203	199	0.01%	0.002%
65	9.928	2665	2671	2674	rBV3	665	725	0.04%	0.006%
66	10.102	2720	2725	2728	rBV	626	472	0.03%	0.004%
67	10.459	2833	2836	2839	rBV	354	199	0.01%	0.002%
68	10.491	2840	2846	2848	rBV2	181	213	0.01%	0.002%
69	10.671	2894	2902	2910	rBV3	2386	3159	0.20%	0.025%
70	10.758	2916	2929	2954	rBV	619740	990081	61.27%	7.934%
71	10.848	2954	2957	2961	rBV2	356	247	0.02%	0.002%
72	10.893	2962	2971	2979	rVV	2101	3226	0.20%	0.026%
73	11.031	3011	3014	3019	rBV3	251	214	0.01%	0.002%
74	11.115	3037	3040	3048	rVB2	704	808	0.05%	0.006%
75	11.304	3095	3099	3102	rBV2	229	193	0.01%	0.002%
76	11.381	3120	3123	3127	rVB2	483	286	0.02%	0.002%

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Peak Location: TOP

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 Title : VOC Analysis

77	11.414	3130	3133	3136	rVV3	303	215	0.01%	0.002%
78	11.459	3138	3147	3160	rVB5	1614	3061	0.19%	0.025%
79	11.581	3177	3185	3189	rBV3	424	624	0.04%	0.005%
80	11.642	3202	3204	3208	rBV2	237	200	0.01%	0.002%
81	11.693	3212	3220	3226	rVB4	1100	1579	0.10%	0.013%
82	11.748	3235	3237	3240	rVB2	589	331	0.02%	0.003%
83	11.812	3244	3257	3281	rBV	582859	924570	57.21%	7.409%
84	11.973	3302	3307	3314	rVB4	1559	2038	0.13%	0.016%
85	12.063	3331	3335	3337	rBV	450	371	0.02%	0.003%
86	12.147	3358	3361	3362	rBV	412	194	0.01%	0.002%
87	12.195	3362	3376	3398	rVV	722959	1181444	73.11%	9.468%
88	12.333	3415	3419	3424	rVB5	771	638	0.04%	0.005%
89	12.397	3435	3439	3443	rVB3	574	560	0.03%	0.004%
90	12.587	3495	3498	3501	rVB3	310	217	0.01%	0.002%
91	12.626	3508	3510	3516	rBV2	317	317	0.02%	0.003%
92	12.741	3543	3546	3549	rBV2	436	364	0.02%	0.003%
93	12.761	3549	3552	3553	rVV2	638	406	0.03%	0.003%
94	12.777	3553	3557	3563	rVV3	1235	1417	0.09%	0.011%
95	12.822	3567	3571	3574	rBV	257	242	0.01%	0.002%
96	13.433	3755	3761	3764	rBV4	1170	1151	0.07%	0.009%
97	13.584	3805	3808	3809	rBV2	444	245	0.02%	0.002%
98	14.192	3995	3997	4000	rBV3	505	333	0.02%	0.003%
99	14.330	4038	4040	4041	rBV2	593	271	0.02%	0.002%
100	14.455	4071	4079	4084	rBV5	1501	1736	0.11%	0.014%

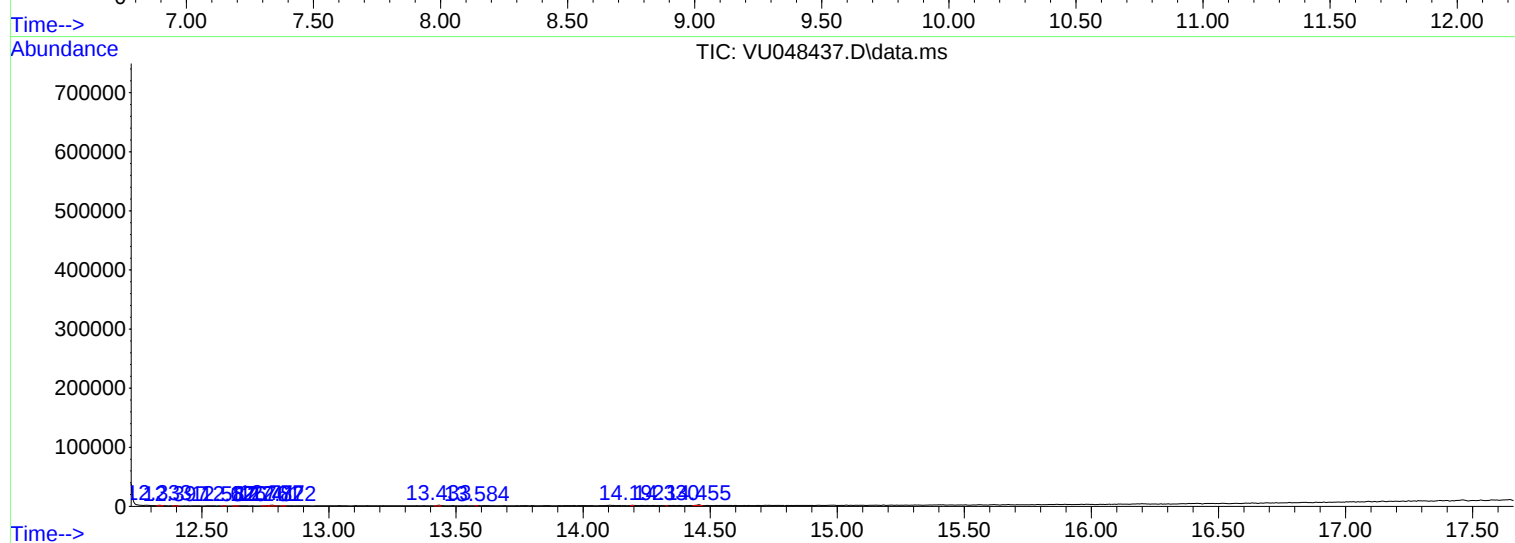
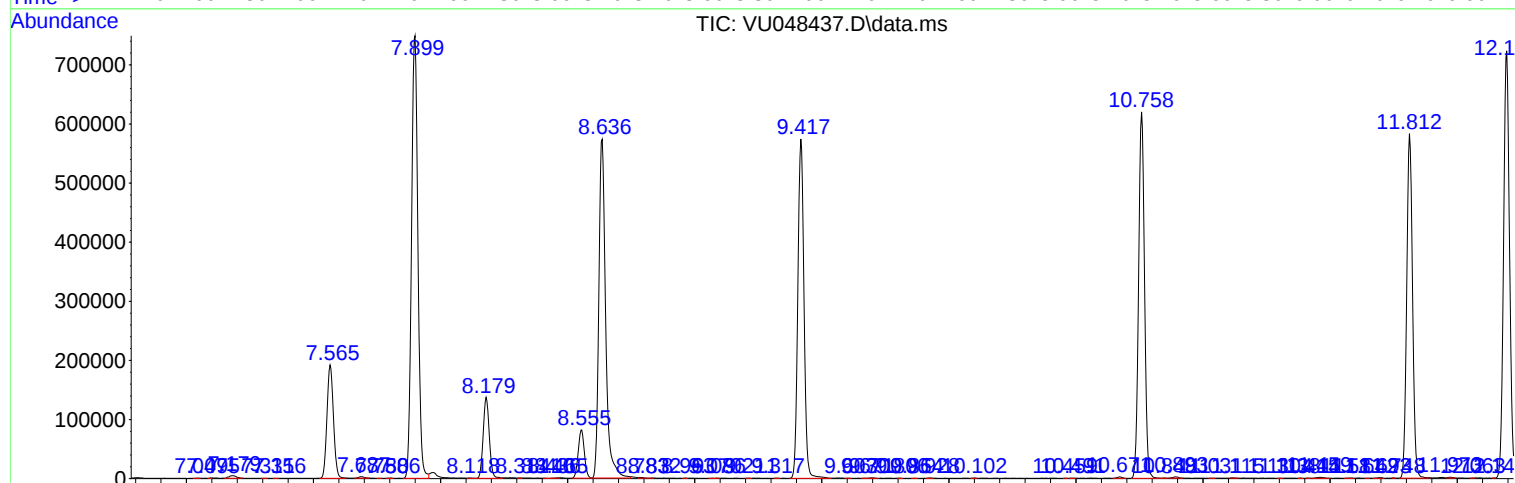
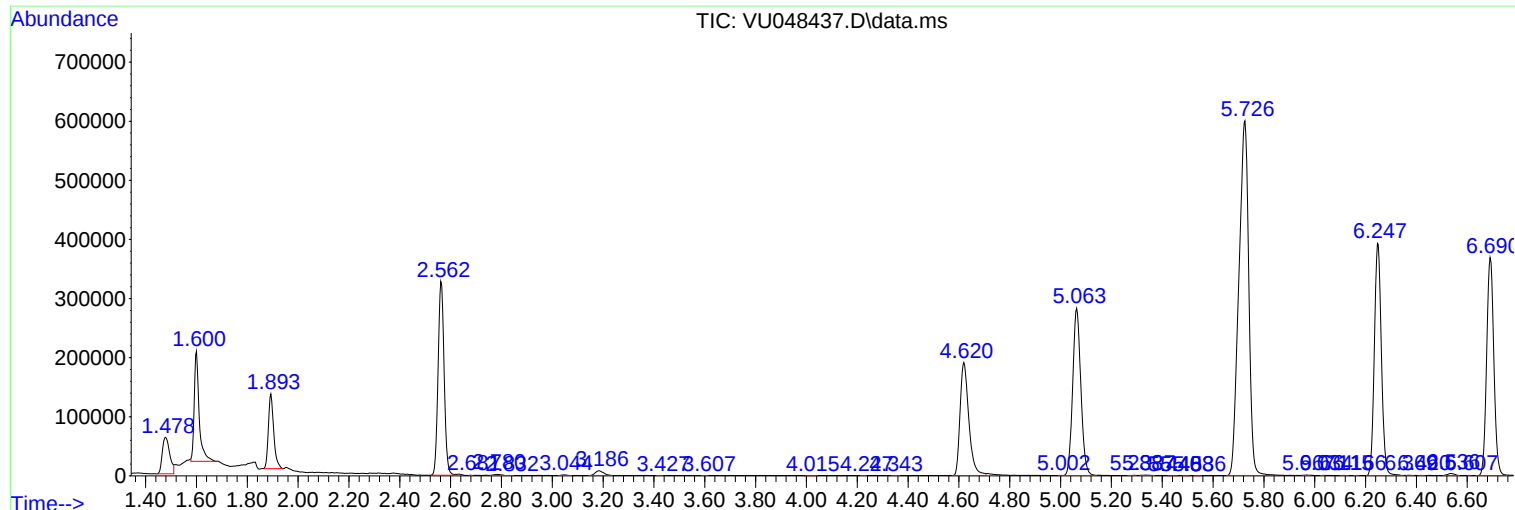
Sum of corrected areas: 12478368

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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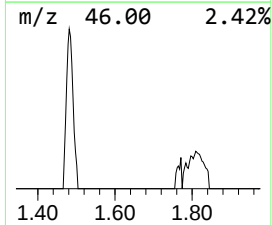
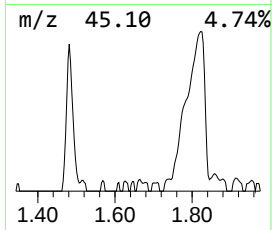
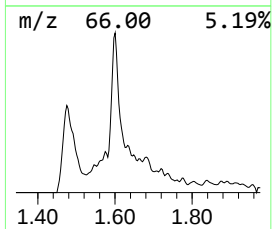
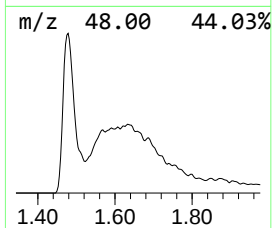
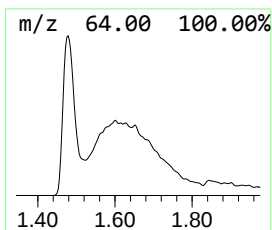
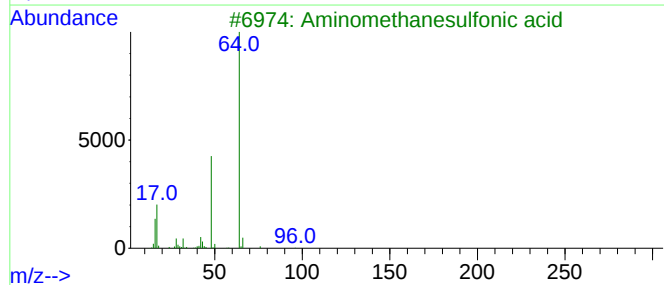
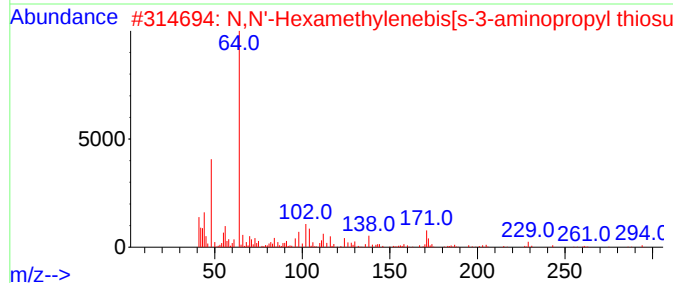
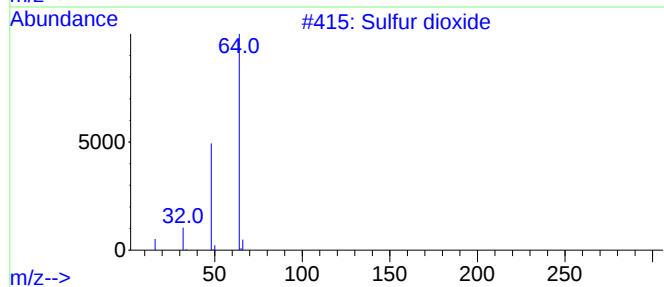
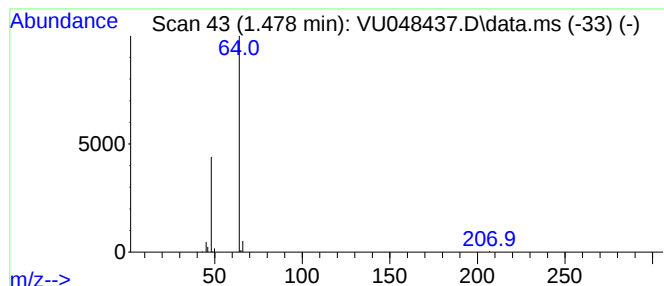
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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.
1.478	8.38 ug/L	125911	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64
5			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.478	8.4	ug/L	125911	1	6.250	750906	50.0