

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053278.D
 Acq On : 17 Mar 2023 19:35
 Operator : JC/MD
 Sample : 01930-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EYFC4

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\SFAMULM031523WMA.M
 Title : VOC Analysis

Signal : TIC: VU053278.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	32	39	53	rBV	15394	26897	5.72%	0.613%
2	1.597	73	80	94	rVB	76089	86392	18.36%	1.969%
3	1.909	169	177	195	rBV	59083	81591	17.34%	1.859%
4	2.565	369	381	394	rBV	113801	183144	38.92%	4.174%
5	3.170	565	569	572	rVB3	387	315	0.07%	0.007%
6	3.465	658	661	662	rBV	223	136	0.03%	0.003%
7	3.562	685	691	695	rBV	271	423	0.09%	0.010%
8	3.594	699	701	702	rBV	190	84	0.02%	0.002%
9	3.983	820	822	826	rVB2	198	125	0.03%	0.003%
10	4.308	920	923	924	rBV	170	81	0.02%	0.002%
11	4.433	960	962	964	rVB	155	79	0.02%	0.002%
12	4.498	979	982	984	rBV	182	105	0.02%	0.002%
13	4.613	1006	1018	1040	rBV	47625	113830	24.19%	2.594%
14	4.819	1079	1082	1083	rBB	57	74	0.02%	0.002%
15	4.932	1115	1117	1120	rVB	195	87	0.02%	0.002%
16	5.057	1140	1156	1177	rBV	105639	228780	48.62%	5.214%
17	5.153	1183	1186	1189	rBV	128	76	0.02%	0.002%
18	5.263	1218	1220	1224	rBV	292	214	0.05%	0.005%
19	5.285	1224	1227	1228	rBV	207	122	0.03%	0.003%
20	5.369	1250	1253	1256	rBV	346	254	0.05%	0.006%
21	5.388	1256	1259	1265	rVV	313	286	0.06%	0.007%
22	5.485	1286	1289	1290	rBV	202	96	0.02%	0.002%
23	5.510	1294	1297	1299	rBV	185	145	0.03%	0.003%
24	5.723	1341	1363	1365	rBV2	217340	470577	100.00%	10.724%
25	6.015	1444	1454	1471	rVB2	32630	62559	13.29%	1.426%
26	6.243	1512	1525	1541	rBV2	173448	325546	69.18%	7.419%
27	6.382	1566	1568	1572	rBV	171	92	0.02%	0.002%
28	6.417	1577	1579	1581	rBV	165	90	0.02%	0.002%
29	6.459	1590	1592	1593	rBV	164	88	0.02%	0.002%
30	6.517	1607	1610	1616	rBV3	447	472	0.10%	0.011%
31	6.684	1649	1662	1680	rBV	136983	262715	55.83%	5.987%
32	6.935	1738	1740	1744	rVB	171	82	0.02%	0.002%
33	6.980	1752	1754	1758	rVB	139	79	0.02%	0.002%
34	7.121	1796	1798	1799	rBV	125	71	0.02%	0.002%
35	7.144	1803	1805	1806	rBV	243	96	0.02%	0.002%
36	7.179	1811	1816	1824	rBV4	1096	1410	0.30%	0.032%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
 Title : VOC Analysis

37	7.259	1838	1841	1844	rBV	233	183	0.04%	0.004%
38	7.330	1859	1863	1864	rBV	135	116	0.02%	0.003%
39	7.340	1864	1866	1870	rVV	189	131	0.03%	0.003%
40	7.417	1885	1890	1893	rBV2	331	418	0.09%	0.010%
41	7.507	1914	1918	1920	rVV	234	164	0.03%	0.004%
42	7.562	1923	1935	1953	rVV	77287	132454	28.15%	3.018%
43	7.687	1969	1974	1980	rBV3	400	511	0.11%	0.012%
44	7.893	2025	2038	2052	rBV	268127	454326	96.55%	10.353%
45	7.967	2053	2061	2074	rVB	30627	51549	10.95%	1.175%
46	8.095	2099	2101	2104	rVB	329	161	0.03%	0.004%
47	8.176	2114	2126	2141	rBV	51374	86770	18.44%	1.977%
48	8.269	2148	2155	2166	rVB4	873	1278	0.27%	0.029%
49	8.385	2188	2191	2193	rBV	181	149	0.03%	0.003%
50	8.507	2226	2229	2230	rBV	181	123	0.03%	0.003%
51	8.626	2254	2266	2294	rBV	153677	280655	59.64%	6.396%
52	8.780	2308	2314	2315	rBV3	741	567	0.12%	0.013%
53	8.806	2320	2322	2327	rVB	386	241	0.05%	0.005%
54	8.915	2352	2356	2358	rBV	214	189	0.04%	0.004%
55	9.018	2386	2388	2390	rBV2	135	79	0.02%	0.002%
56	9.189	2439	2441	2443	rBV	177	71	0.02%	0.002%
57	9.275	2465	2468	2471	rBV	180	181	0.04%	0.004%
58	9.356	2491	2493	2499	rVB	294	251	0.05%	0.006%
59	9.411	2499	2510	2531	rBV	237730	392605	83.43%	8.947%
60	9.546	2549	2552	2554	rBV	206	170	0.04%	0.004%
61	9.558	2554	2556	2558	rBV2	333	162	0.03%	0.004%
62	9.652	2582	2585	2589	rVB	272	175	0.04%	0.004%
63	9.902	2661	2663	2666	rBV	181	99	0.02%	0.002%
64	9.976	2683	2686	2695	rVB3	1207	1112	0.24%	0.025%
65	10.134	2731	2735	2745	rVB2	263	319	0.07%	0.007%
66	10.214	2751	2760	2771	rBV2	9251	13842	2.94%	0.315%
67	10.285	2774	2782	2789	rVB5	3825	5846	1.24%	0.133%
68	10.356	2802	2804	2807	rBV	173	85	0.02%	0.002%
69	10.407	2812	2820	2826	rVB3	741	859	0.18%	0.020%
70	10.455	2833	2835	2837	rBV2	718	367	0.08%	0.008%
71	10.533	2856	2859	2862	rVB	191	124	0.03%	0.003%
72	10.568	2866	2870	2871	rBV	165	104	0.02%	0.002%
73	10.648	2893	2895	2902	rVB	221	170	0.04%	0.004%
74	10.751	2915	2927	2949	rVB	181907	286955	60.98%	6.539%
75	10.912	2974	2977	2980	rBV3	497	319	0.07%	0.007%
76	11.060	3018	3023	3031	rVB3	753	1020	0.22%	0.023%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Min Area: 0 % of largest Peak

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Peak Location: TOP

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 Title : VOC Analysis

77	11.173	3056	3058	3062	rBV	167	115	0.02%	0.003%
78	11.253	3081	3083	3085	rBV	159	76	0.02%	0.002%
79	11.314	3098	3102	3106	rBV2	349	363	0.08%	0.008%
80	11.475	3150	3152	3157	rVB	229	125	0.03%	0.003%
81	11.581	3183	3185	3189	rVB	239	115	0.02%	0.003%
82	11.806	3244	3255	3277	rBV	238799	377102	80.14%	8.594%
83	11.915	3287	3289	3291	rBV	194	86	0.02%	0.002%
84	11.960	3298	3303	3306	rBV2	331	333	0.07%	0.008%
85	12.060	3331	3334	3336	rBV	238	157	0.03%	0.004%
86	12.073	3336	3338	3341	rBV2	583	417	0.09%	0.010%
87	12.189	3362	3374	3393	rBV	243177	388651	82.59%	8.857%
88	12.314	3404	3413	3424	rBV6	2798	4620	0.98%	0.105%
89	12.809	3564	3567	3572	rVB4	381	341	0.07%	0.008%
90	12.918	3593	3601	3612	rVB5	1858	2719	0.58%	0.062%
91	13.073	3646	3649	3653	rBV	320	285	0.06%	0.006%
92	13.417	3746	3756	3773	rBV	23359	39490	8.39%	0.900%
93	13.561	3799	3801	3803	rBV	223	154	0.03%	0.004%
94	13.883	3898	3901	3905	rBV2	198	115	0.02%	0.003%
95	13.938	3910	3918	3927	rBV5	4287	7843	1.67%	0.179%
96	14.086	3957	3964	3972	rBV2	1573	2156	0.46%	0.049%
97	15.176	4300	4303	4306	rBV2	360	242	0.05%	0.006%
98	15.221	4314	4317	4319	rBV2	334	237	0.05%	0.005%
99	15.304	4341	4343	4350	rVB2	294	178	0.04%	0.004%
100	15.594	4432	4433	4436	rBV	250	168	0.04%	0.004%

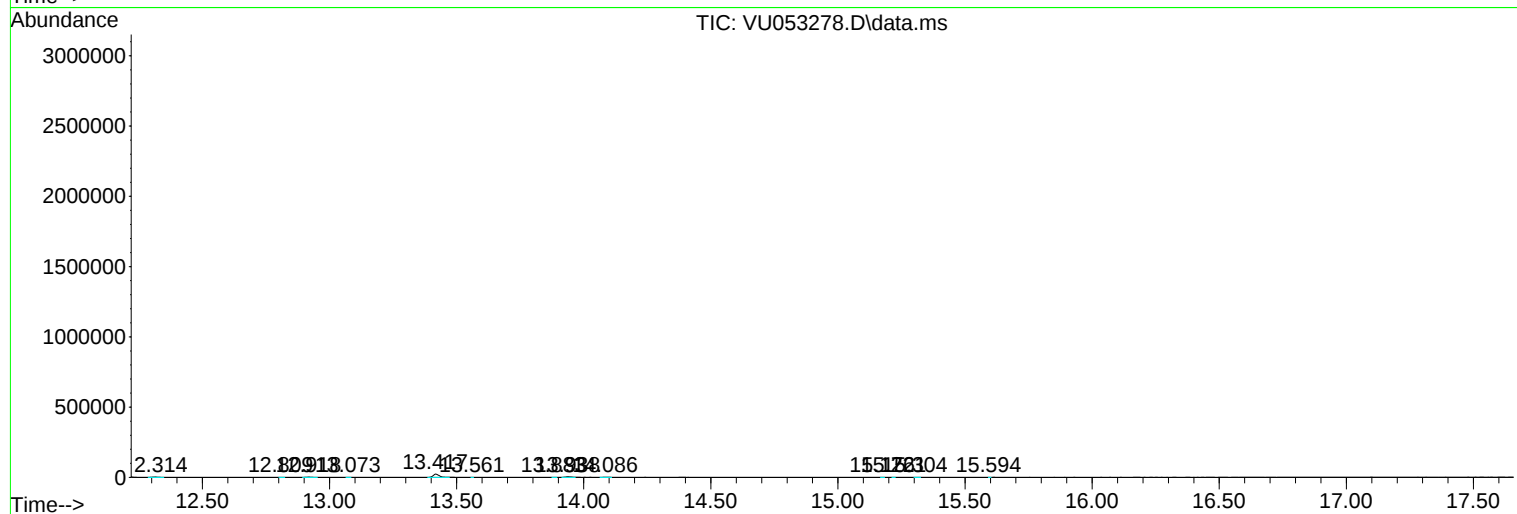
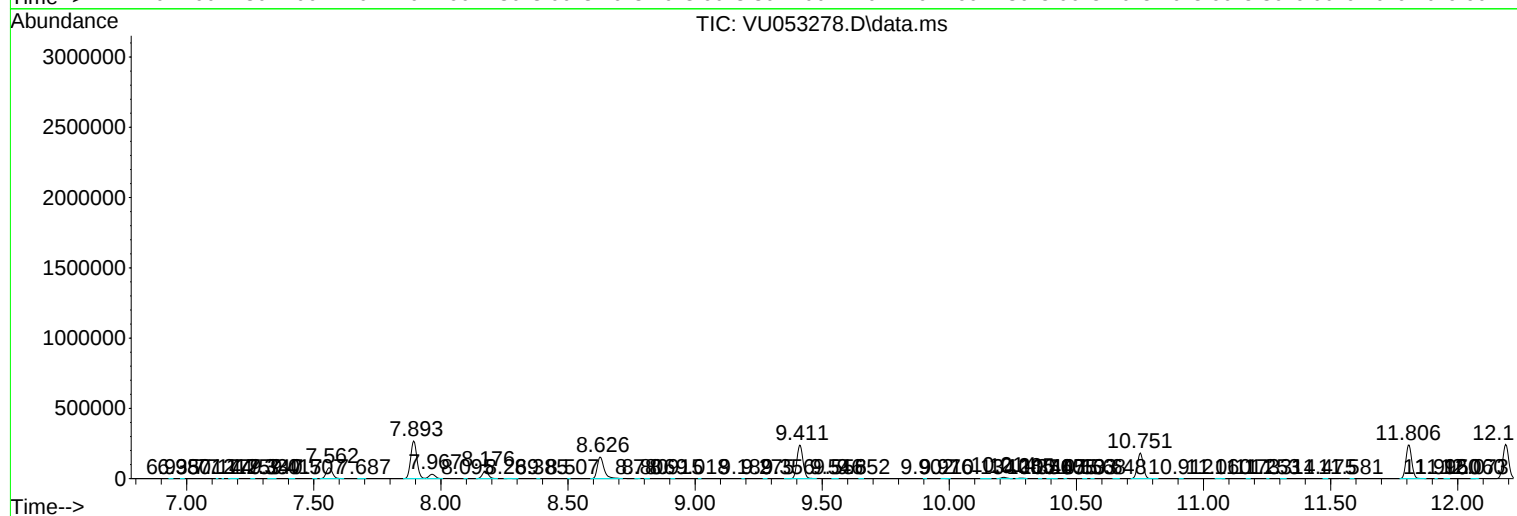
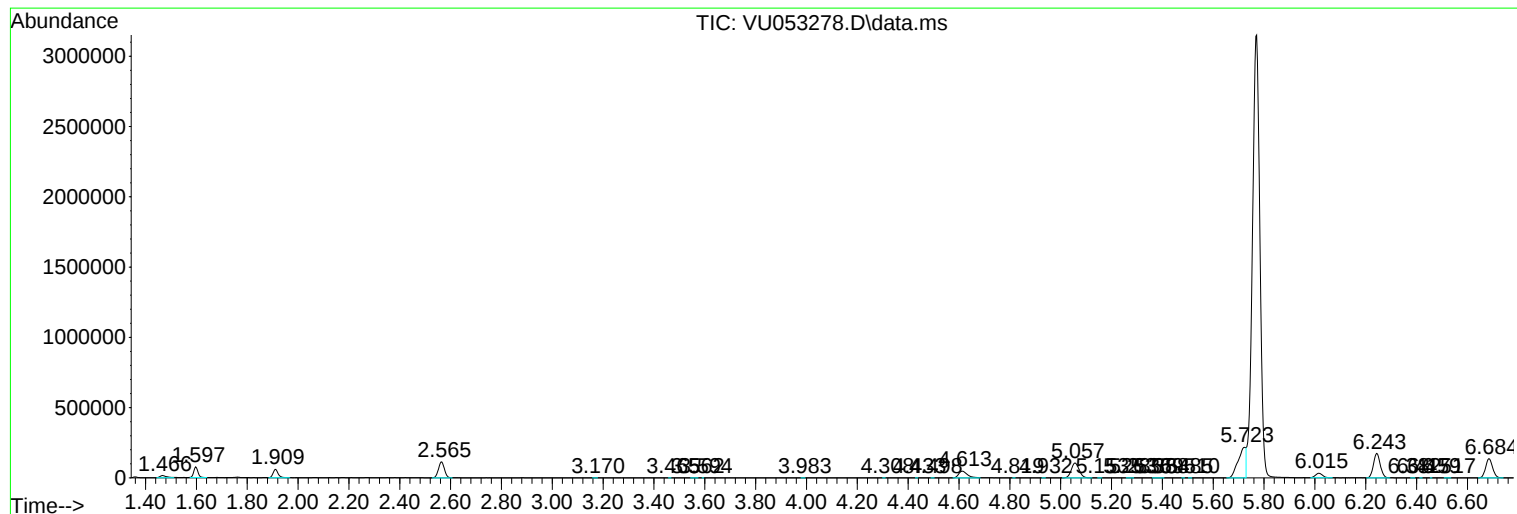
Sum of corrected areas: 4388201

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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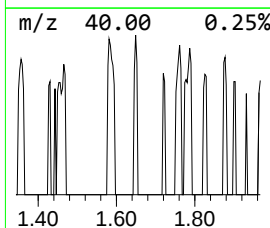
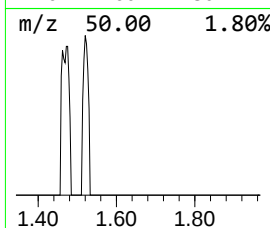
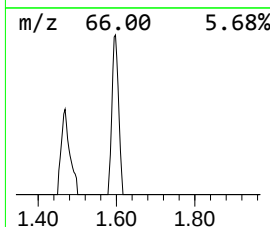
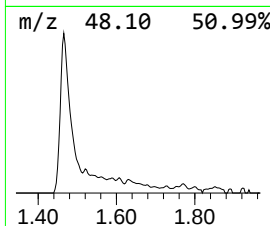
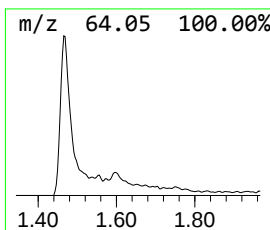
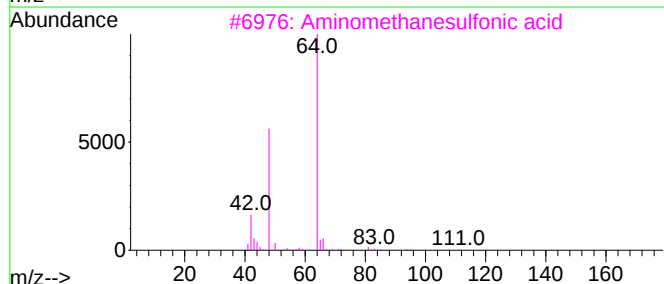
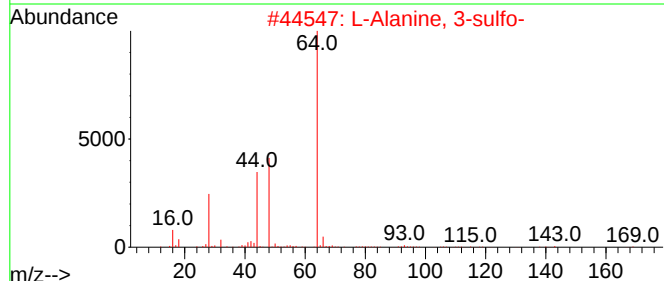
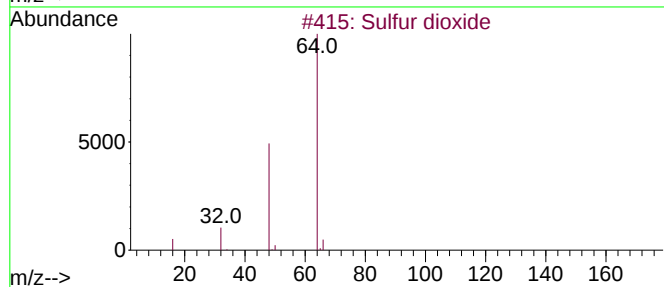
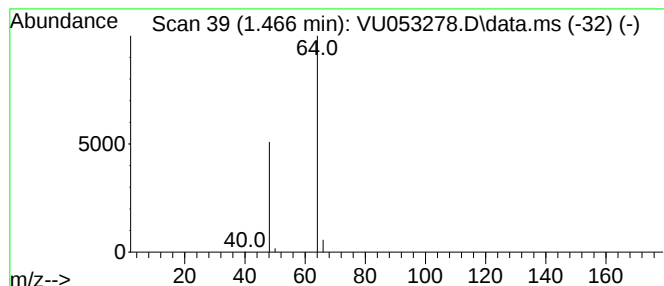
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	4.13 ug/L	26897	1,4-Difluorobenzene	6.243

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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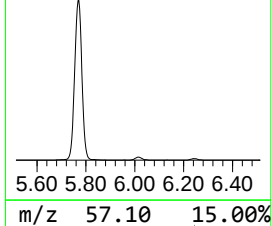
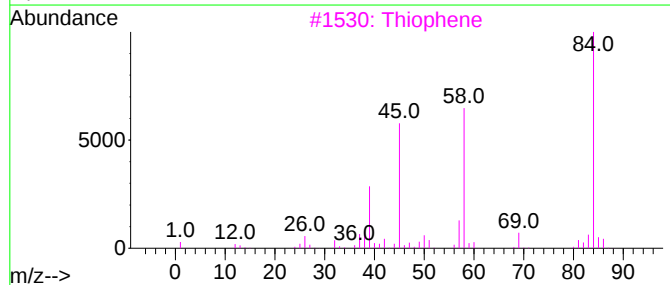
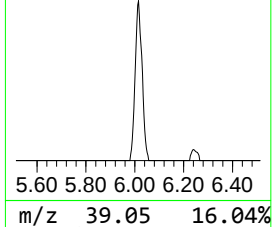
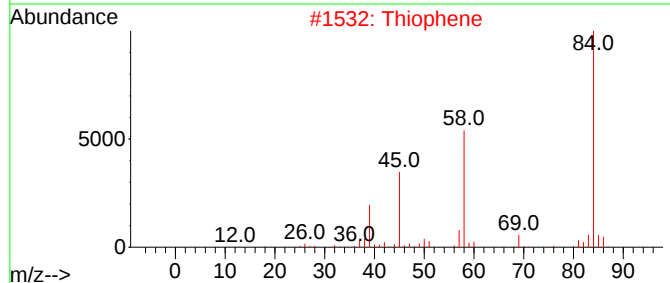
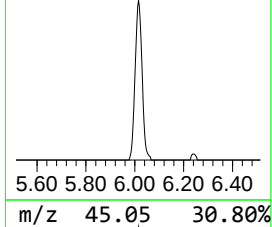
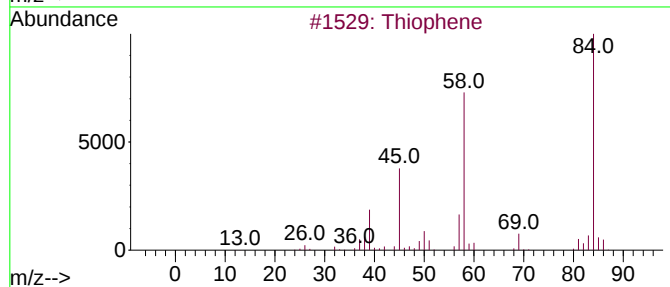
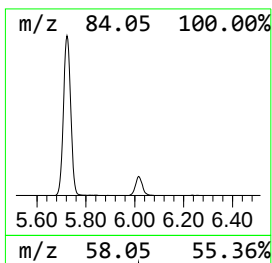
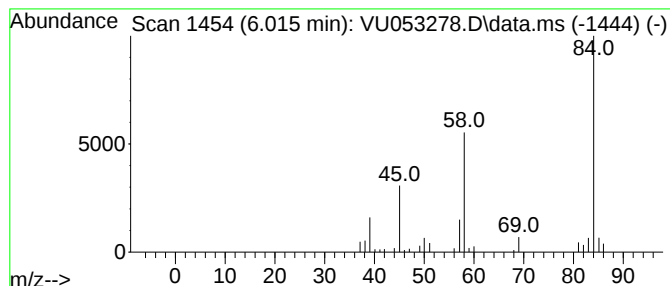
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Thiophene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.015	9.61 ug/L	62559	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene	84	C4H4S	000110-02-1	94
2			Thiophene	84	C4H4S	000110-02-1	94
3			Thiophene	84	C4H4S	000110-02-1	91
4			Thiophene	84	C4H4S	000110-02-1	91
5			4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	37



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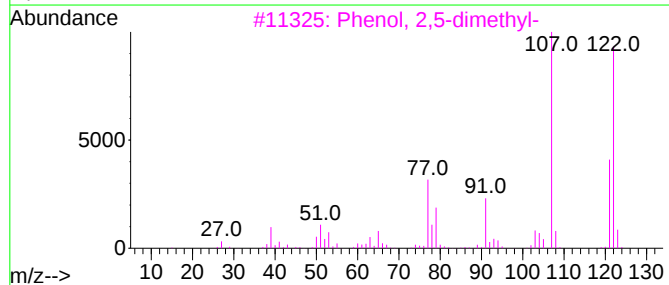
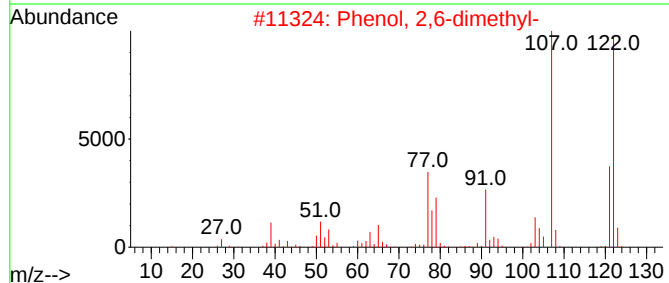
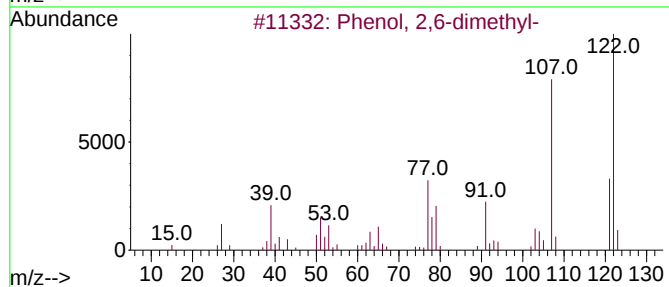
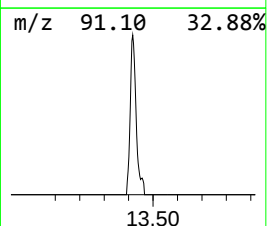
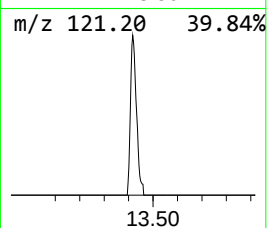
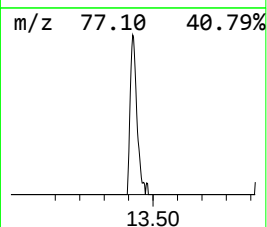
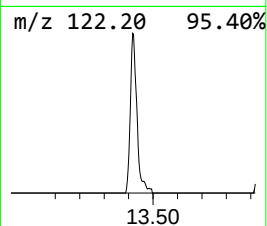
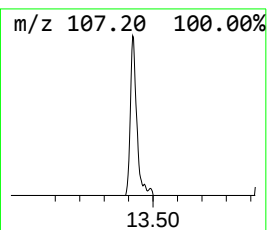
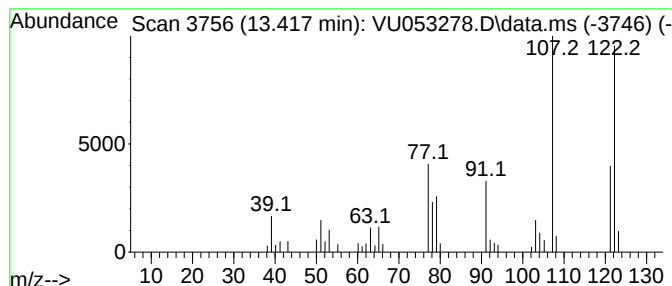
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Phenol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.417	5.24 ug/L	39490	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	96
2			Phenol, 2,6-dimethyl-	122	C8H10O	000576-26-1	96
3			Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	96
4			Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	94
5			Phenol, 2,5-dimethyl-	122	C8H10O	000095-87-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053278.D
Acq On : 17 Mar 2023 19:35
Operator : JC/MD
Sample : 01930-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EYFC4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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	1.466	4.1	ug/L	26897	1	6.243	325546	50.0
Thiophene	6.015	9.6	ug/L	62559	1	6.243	325546	50.0
Phenol, 2,6-dim...	13.417	5.2	ug/L	39490	3	11.809	377102	50.0