

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AD1ME

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\SFAMULM092321WMA.M  
 Title : VOC Analysis

Signal : TIC: VU045295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	30	37	51	rBV2	35572	61433	4.65%	0.596%
2	1.597	73	80	101	rVB	102472	136278	10.30%	1.322%
3	1.871	159	165	179	rBV	40482	53026	4.01%	0.514%
4	2.517	354	366	385	rBV	194146	348070	26.32%	3.377%
5	2.610	390	395	423	rVB2	6341	19092	1.44%	0.185%
6	2.967	497	506	516	rBV3	1850	3529	0.27%	0.034%
7	3.031	516	526	544	rVV2	4266	9546	0.72%	0.093%
8	3.170	566	569	571	rBV	403	345	0.03%	0.003%
9	3.613	702	707	714	rVB	155	247	0.02%	0.002%
10	3.662	714	722	723	rBV3	1020	1064	0.08%	0.010%
11	3.916	797	801	805	rVB2	224	241	0.02%	0.002%
12	3.945	805	810	813	rBV2	183	180	0.01%	0.002%
13	4.073	842	850	856	rBV2	236	391	0.03%	0.004%
14	4.163	873	878	883	rVB2	171	191	0.01%	0.002%
15	4.546	993	997	1000	rBV2	213	201	0.02%	0.002%
16	4.652	1013	1030	1080	rBV	109675	385787	29.17%	3.743%
17	4.912	1107	1111	1113	rBV	238	225	0.02%	0.002%
18	4.941	1117	1120	1122	rBV	252	185	0.01%	0.002%
19	5.067	1138	1159	1185	rBV	212748	513969	38.86%	4.987%
20	5.292	1221	1229	1241	rBV4	591	1223	0.09%	0.012%
21	5.372	1247	1254	1256	rBV3	411	436	0.03%	0.004%
22	5.549	1305	1309	1314	rVB2	216	252	0.02%	0.002%
23	5.594	1314	1323	1326	rBV	247	433	0.03%	0.004%
24	5.719	1342	1362	1385	rBV2	520463	1322555	100.00%	12.832%
25	5.983	1434	1444	1466	rBV5	4509	12172	0.92%	0.118%
26	6.108	1478	1483	1484	rBV	339	347	0.03%	0.003%
27	6.121	1484	1487	1494	rVB4	586	715	0.05%	0.007%
28	6.250	1511	1527	1561	rVV	352235	714927	54.06%	6.937%
29	6.382	1566	1568	1575	rVB	222	226	0.02%	0.002%
30	6.539	1603	1617	1629	rBV3	16025	33661	2.55%	0.327%
31	6.610	1629	1639	1650	rVV2	3850	8771	0.66%	0.085%
32	6.694	1650	1665	1689	rVV	296592	620628	46.93%	6.022%
33	6.809	1696	1701	1710	rBV2	600	862	0.07%	0.008%
34	6.899	1726	1729	1734	rVB2	283	235	0.02%	0.002%
35	6.935	1734	1740	1742	rBV	219	245	0.02%	0.002%
36	6.973	1746	1752	1755	rBV	180	242	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AD1ME

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\SFAMULM092321WMA.M  
 Title : VOC Analysis

37	7.041	1768	1773	1774	rBV2	435	318	0.02%	0.003%
38	7.192	1805	1820	1827	rBV6	4100	8412	0.64%	0.082%
39	7.571	1924	1938	1960	rVB	148139	289287	21.87%	2.807%
40	7.694	1968	1976	1989	rBV2	1779	3776	0.29%	0.037%
41	7.899	2025	2040	2056	rVV	559270	1010139	76.38%	9.801%
42	7.973	2057	2063	2084	rVV2	9758	25089	1.90%	0.243%
43	8.047	2084	2086	2089	rVB	319	200	0.02%	0.002%
44	8.089	2093	2099	2102	rBV2	231	276	0.02%	0.003%
45	8.131	2107	2112	2115	rBV2	393	429	0.03%	0.004%
46	8.189	2115	2130	2149	rBV	98469	196843	14.88%	1.910%
47	8.356	2178	2182	2192	rVB6	980	1141	0.09%	0.011%
48	8.475	2212	2219	2221	rBV2	207	281	0.02%	0.003%
49	8.555	2241	2244	2250	rBV4	764	706	0.05%	0.007%
50	8.652	2259	2274	2315	rBV	417394	807420	61.05%	7.834%
51	8.970	2369	2373	2375	rBV2	266	240	0.02%	0.002%
52	9.173	2431	2436	2441	rBV2	175	232	0.02%	0.002%
53	9.346	2487	2490	2493	rBV2	307	259	0.02%	0.003%
54	9.423	2499	2514	2533	rBV	477148	875358	66.19%	8.493%
55	9.581	2553	2563	2571	rBV3	930	1493	0.11%	0.014%
56	9.700	2591	2600	2609	rBV2	3450	6007	0.45%	0.058%
57	9.745	2610	2614	2618	rVV2	355	317	0.02%	0.003%
58	10.047	2705	2708	2712	rVB	198	189	0.01%	0.002%
59	10.070	2712	2715	2719	rBV2	196	223	0.02%	0.002%
60	10.108	2719	2727	2734	rVV2	1192	1532	0.12%	0.015%
61	10.375	2806	2810	2815	rBV2	508	603	0.05%	0.006%
62	10.472	2837	2840	2849	rVB4	873	1162	0.09%	0.011%
63	10.533	2856	2859	2862	rBV	371	274	0.02%	0.003%
64	10.674	2894	2903	2911	rBV3	2996	4296	0.32%	0.042%
65	10.764	2917	2931	2949	rBV	463447	758717	57.37%	7.361%
66	10.867	2960	2963	2970	rVB4	581	523	0.04%	0.005%
67	10.899	2970	2973	2974	rBV2	381	196	0.01%	0.002%
68	10.992	2994	3002	3019	rBV4	5936	9791	0.74%	0.095%
69	11.057	3019	3022	3023	rBV2	346	243	0.02%	0.002%
70	11.105	3029	3037	3048	rBV8	2207	4212	0.32%	0.041%
71	11.198	3064	3066	3072	rVB2	381	384	0.03%	0.004%
72	11.301	3091	3098	3102	rBV2	435	580	0.04%	0.006%
73	11.472	3141	3151	3160	rVB4	3104	5708	0.43%	0.055%
74	11.584	3180	3186	3187	rBV2	411	399	0.03%	0.004%
75	11.697	3215	3221	3228	rVB4	1175	1671	0.13%	0.016%
76	11.758	3236	3240	3244	rBV	216	192	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AD1ME

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\SFAMULM092321WMA.M  
 Title : VOC Analysis

77	11.819	3246	3259	3274	rBV	524147	828953	62.68%	8.043%
78	11.947	3294	3299	3300	rBV3	777	639	0.05%	0.006%
79	12.066	3327	3336	3351	rBV5	2677	5687	0.43%	0.055%
80	12.198	3363	3377	3400	rVB	584152	925083	69.95%	8.976%
81	12.333	3412	3419	3423	rBV4	765	1088	0.08%	0.011%
82	12.378	3430	3433	3434	rBV2	300	193	0.01%	0.002%
83	12.407	3440	3442	3450	rBV2	480	455	0.03%	0.004%
84	12.471	3459	3462	3466	rBV	351	269	0.02%	0.003%
85	12.777	3551	3557	3564	rBV2	329	463	0.04%	0.004%
86	13.021	3630	3633	3635	rBV	293	215	0.02%	0.002%
87	13.150	3666	3673	3682	rVB5	1766	2821	0.21%	0.027%
88	13.436	3759	3762	3767	rBV3	431	393	0.03%	0.004%
89	13.841	3884	3888	3896	rBV4	693	862	0.07%	0.008%
90	14.092	3958	3966	3981	rVB	7484	12512	0.95%	0.121%
91	14.192	3994	3997	4002	rVB2	706	599	0.05%	0.006%
92	15.098	4274	4279	4285	rBV6	1625	2161	0.16%	0.021%
93	15.224	4307	4318	4336	rVB3	11076	22255	1.68%	0.216%
94	15.410	4368	4376	4391	rBV3	7024	11695	0.88%	0.113%
95	15.603	4429	4436	4445	rVB4	2052	2777	0.21%	0.027%
96	16.262	4636	4641	4648	rBV4	2044	2789	0.21%	0.027%
97	16.410	4682	4687	4694	rBV4	3760	4975	0.38%	0.048%
98	16.774	4789	4800	4819	rBV5	62034	136945	10.35%	1.329%
99	17.182	4919	4927	4940	rVB3	18883	29319	2.22%	0.284%
100	17.584	5043	5052	5065	rVB4	25347	42399	3.21%	0.411%

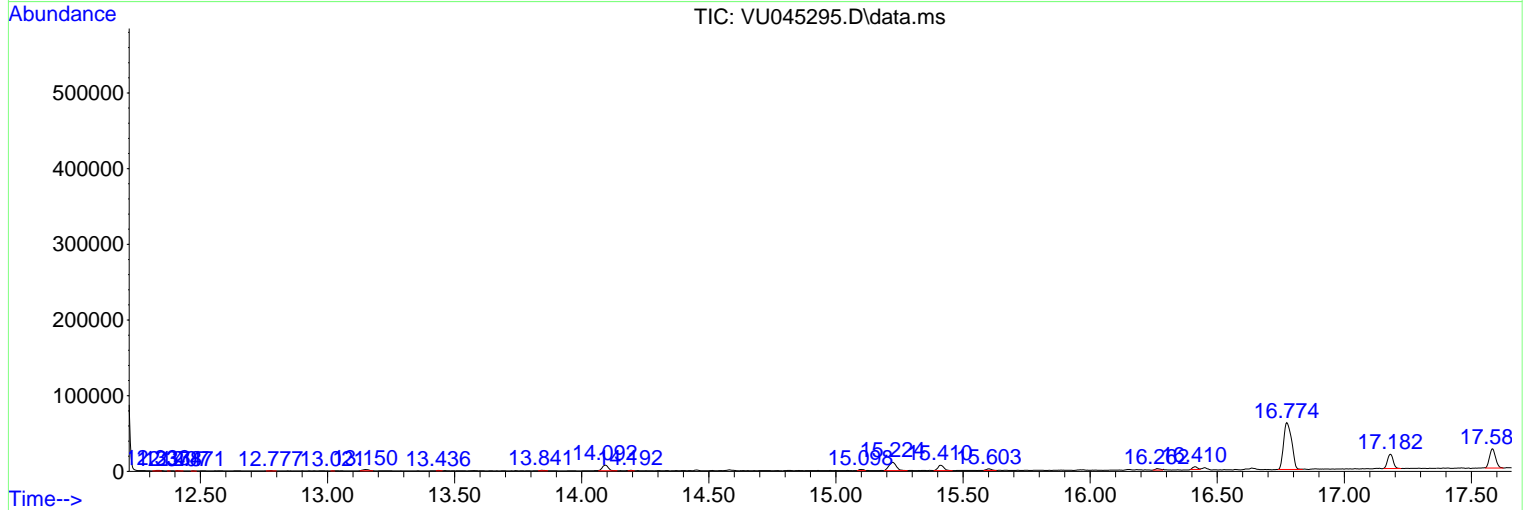
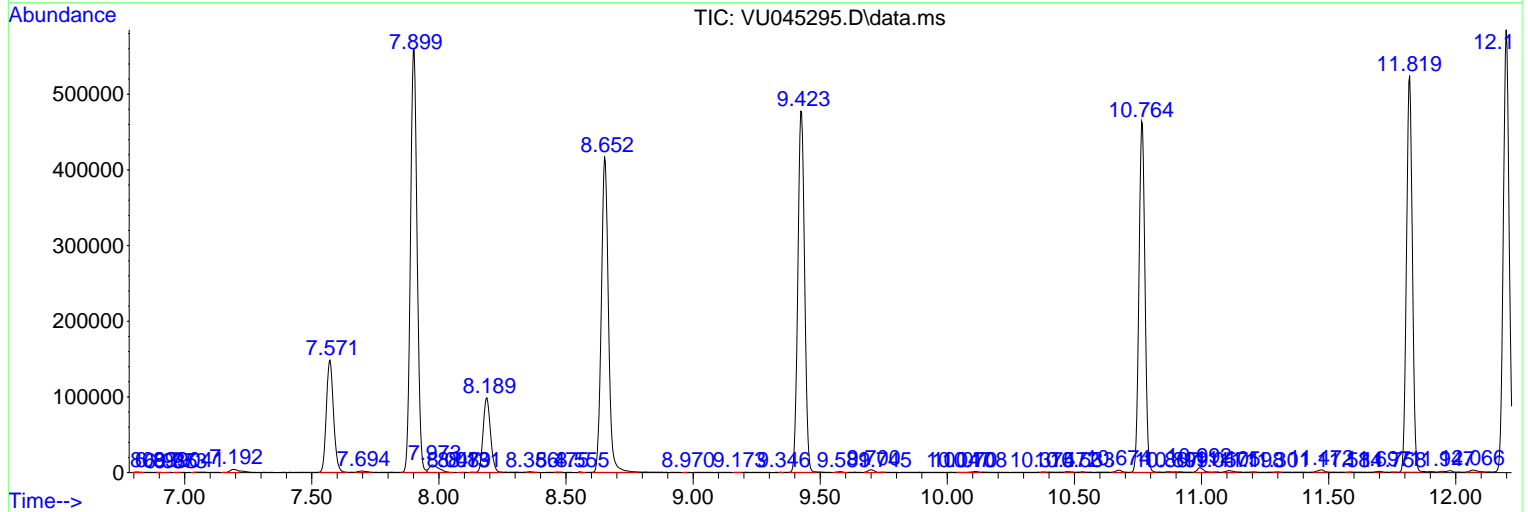
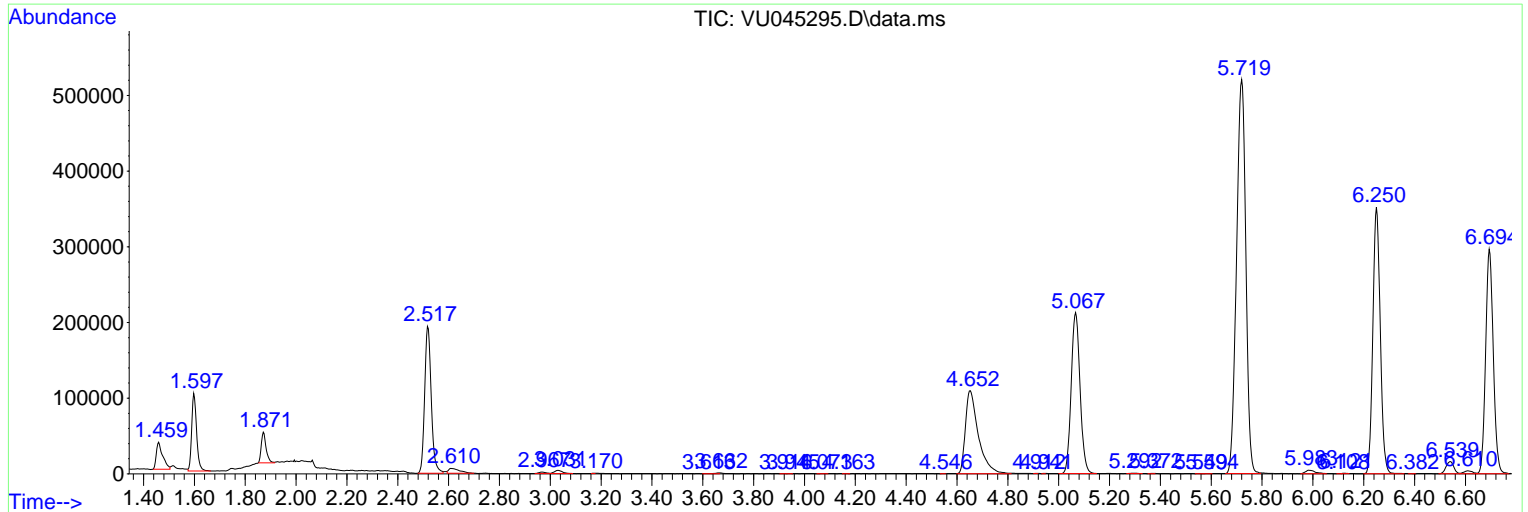
Sum of corrected areas: 10306595

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

**Instrument :**  
 MSVOA\_U  
**Client Sampled :**  
 C0AD1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AD1ME

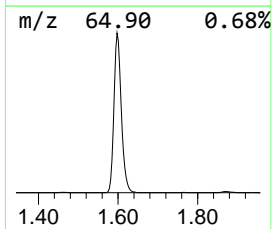
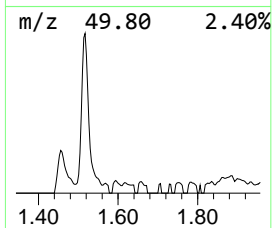
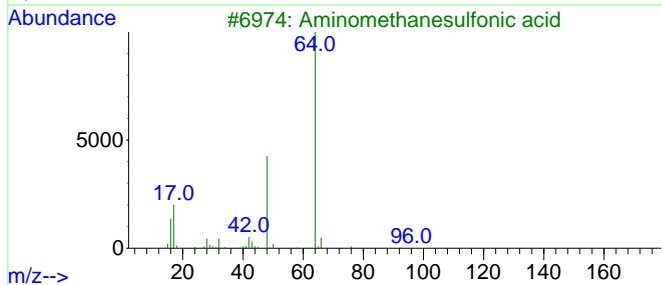
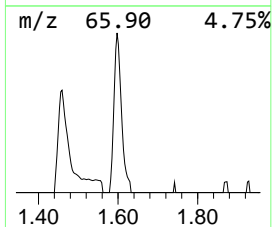
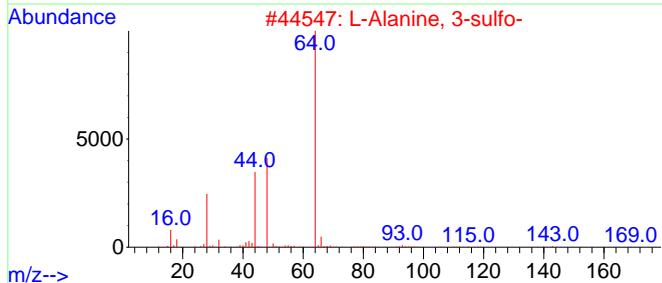
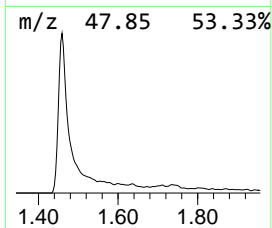
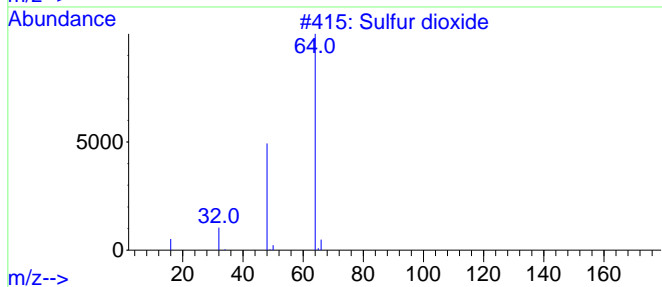
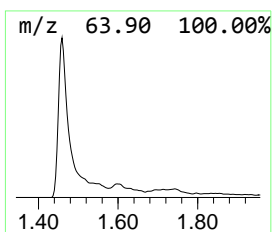
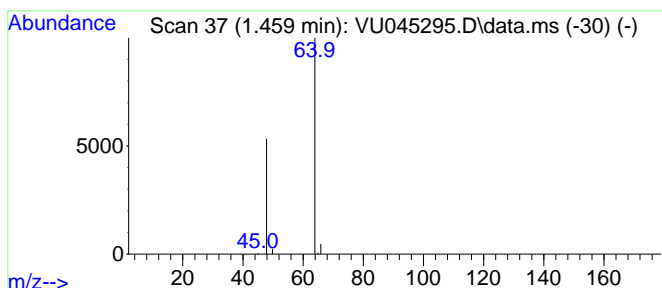
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Quant Title : VOC Analysis

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.
1.459	4.30 ug/L	61433	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
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



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AD1ME

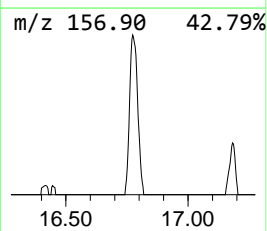
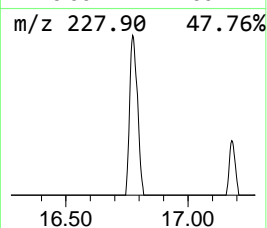
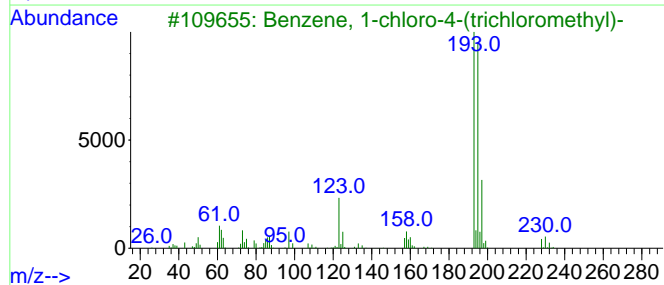
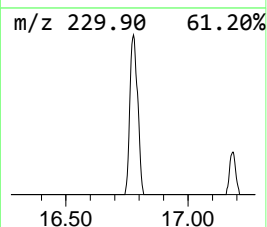
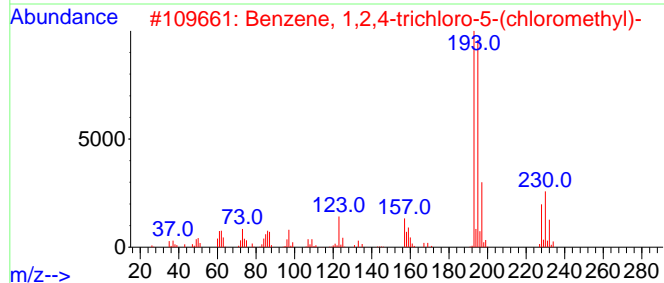
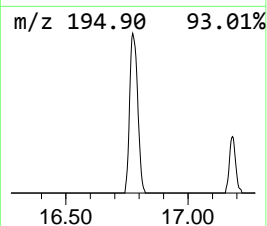
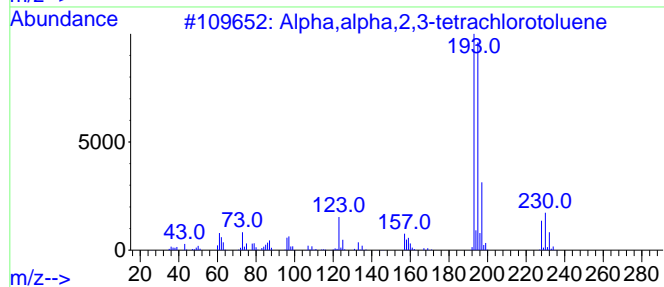
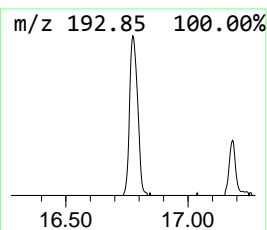
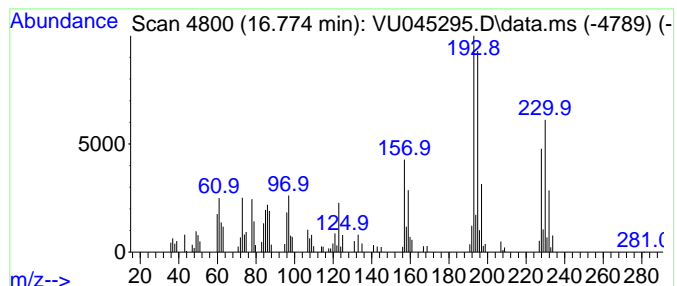
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Quant Title : VOC Analysis

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

\*\*\*\*\*  
 Peak Number 3 Alpha,alpha,2,3-tetrachloro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	8.26 ug/L	136945	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Alpha,alpha,2,3-tetrachlorotoluene	228	C7H4Cl4	057058-14-7	97
2			Benzene, 1,2,4-trichloro-5-(chlo...	228	C7H4Cl4	003955-26-8	93
3			Benzene, 1-chloro-4-(trichlorome...	228	C7H4Cl4	005216-25-1	46
4			Benzene, 1-chloro-2-(trichlorome...	228	C7H4Cl4	002136-89-2	46
5			Benzene, 1-chloro-2-(trichlorome...	228	C7H4Cl4	002136-89-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
 Data File : VU045295.D  
 Acq On : 12 Oct 2021 16:34  
 Operator : SY/MD  
 Sample : M4126-16ME  
 Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleID :  
 C0AD1ME

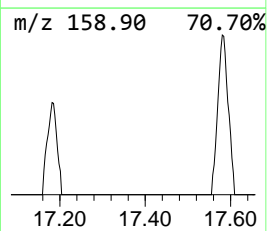
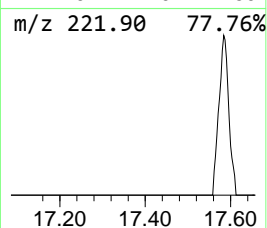
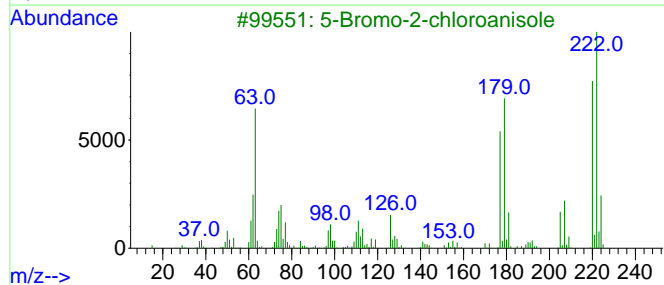
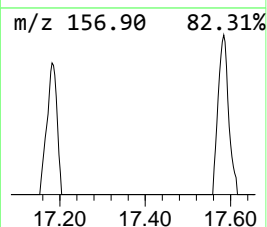
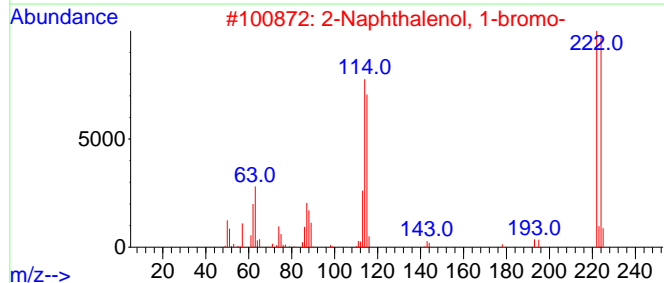
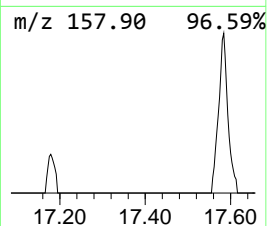
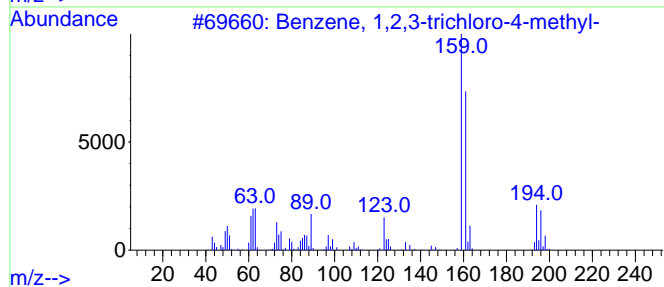
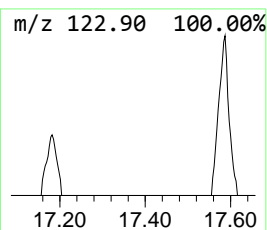
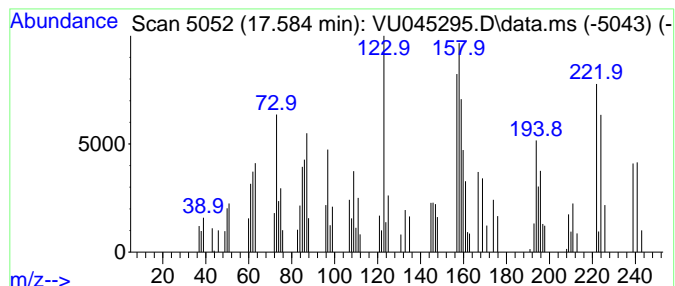
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.M  
 Quant Title : VOC Analysis

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

\*\*\*\*\*  
 Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.584	2.56 ug/L	42399	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trichloro-4-methyl-	194	C7H5Cl3	007359-72-0	42
2			2-Naphthalenol, 1-bromo-	222	C10H7BrO	000573-97-7	38
3			5-Bromo-2-chloroanisole	220	C7H6BrClO	016817-43-9	27
4			2-Chloro-3-methoxy-1,4-naphthoqu...	222	C11H7ClO3	015707-32-1	25
5			Carbonic acid, methyl 4-nitrophe...	197	C8H7NO5	017175-16-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU101221\  
Data File : VU045295.D  
Acq On : 12 Oct 2021 16:34  
Operator : SY/MD  
Sample : M4126-16ME  
Misc : 3.79g/10.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
C0AD1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092321WMA.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	1.459	4.3	ug/L	61433	1	6.250	714927	50.0
Alpha,alpha,2,3...	16.774	8.3	ug/L	136945	3	11.819	828953	50.0
unknown-01	17.584	2.6	ug/L	42399	3	11.819	828953	50.0