

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120121\
 Data File : VU046039.D
 Acq On : 01 Dec 2021 17:11
 Operator : SY/MD
 Sample : M4878-02 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0G21

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046039.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	36	42	54	rVB	30990	31169	4.24%	0.514%
2	1.601	74	81	100	rVB	95988	106640	14.50%	1.759%
3	1.919	171	180	192	rBV	73046	94713	12.88%	1.563%
4	1.999	201	205	210	rVB3	806	836	0.11%	0.014%
5	2.141	246	249	250	rBV	409	213	0.03%	0.004%
6	2.208	263	270	276	rVV3	831	1190	0.16%	0.020%
7	2.334	306	309	310	rBV	303	157	0.02%	0.003%
8	2.572	371	383	399	rBV	153325	251445	34.20%	4.148%
9	2.797	450	453	457	rVB2	311	256	0.03%	0.004%
10	3.054	527	533	534	rBV3	668	669	0.09%	0.011%
11	3.086	538	543	552	rVV3	479	745	0.10%	0.012%
12	3.192	565	576	587	rVB2	1266	3043	0.41%	0.050%
13	3.363	624	629	630	rBV2	586	464	0.06%	0.008%
14	3.494	667	670	675	rBB	155	175	0.02%	0.003%
15	3.703	729	735	738	rVV3	418	552	0.08%	0.009%
16	3.723	739	741	745	rVB	263	173	0.02%	0.003%
17	4.035	836	838	842	rBV	157	158	0.02%	0.003%
18	4.539	985	995	1002	rBB5	1014	1802	0.25%	0.030%
19	4.642	1010	1027	1071	rBV	58277	204853	27.86%	3.380%
20	4.790	1071	1073	1077	rVB2	376	202	0.03%	0.003%
21	4.928	1111	1116	1121	rBV	287	414	0.06%	0.007%
22	5.067	1141	1159	1183	rBV	131036	289300	39.34%	4.773%
23	5.195	1195	1199	1201	rVV2	241	199	0.03%	0.003%
24	5.247	1212	1215	1218	rBB	248	201	0.03%	0.003%
25	5.292	1227	1229	1233	rVB	404	237	0.03%	0.004%
26	5.375	1251	1255	1256	rVV	514	320	0.04%	0.005%
27	5.391	1256	1260	1268	rVB	879	1063	0.14%	0.018%
28	5.729	1343	1365	1388	rBV2	273188	735315	100.00%	12.131%
29	5.970	1438	1440	1442	rVV	335	191	0.03%	0.003%
30	5.986	1442	1445	1449	rVB4	490	424	0.06%	0.007%
31	6.253	1513	1528	1546	rBV	235600	445615	60.60%	7.352%
32	6.321	1546	1549	1555	rVB4	585	783	0.11%	0.013%
33	6.398	1567	1573	1582	rVB3	571	804	0.11%	0.013%
34	6.542	1604	1618	1632	rBV5	9511	21732	2.96%	0.359%
35	6.694	1650	1665	1683	rBV	170463	329748	44.84%	5.440%
36	7.018	1761	1766	1769	rBV	171	224	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.041	1769	1773	1775	rBV	265	204	0.03%	0.003%
38	7.186	1809	1818	1825	rBV4	1299	2306	0.31%	0.038%
39	7.240	1830	1835	1839	rBB	148	176	0.02%	0.003%
40	7.568	1923	1937	1954	rVV	91655	159583	21.70%	2.633%
41	7.629	1954	1956	1959	rVV2	407	341	0.05%	0.006%
42	7.655	1962	1964	1969	rVV2	325	285	0.04%	0.005%
43	7.684	1969	1973	1981	rVV3	1094	1424	0.19%	0.023%
44	7.899	2027	2040	2056	rBV	332980	592052	80.52%	9.768%
45	8.182	2116	2128	2147	rBV	63390	106914	14.54%	1.764%
46	8.304	2163	2166	2169	rVB	297	218	0.03%	0.004%
47	8.350	2175	2180	2185	rBV	162	256	0.03%	0.004%
48	8.472	2213	2218	2224	rBV2	263	357	0.05%	0.006%
49	8.555	2234	2244	2257	rBV2	40969	68913	9.37%	1.137%
50	8.636	2257	2269	2306	rVV	206164	383058	52.09%	6.320%
51	9.137	2422	2425	2428	rBV	179	167	0.02%	0.003%
52	9.176	2433	2437	2440	rBV	169	195	0.03%	0.003%
53	9.420	2500	2513	2542	rBV	334483	563782	76.67%	9.301%
54	9.571	2551	2560	2571	rVB	4833	7248	0.99%	0.120%
55	9.693	2589	2598	2611	rBV	9553	15210	2.07%	0.251%
56	9.925	2664	2670	2672	rBV	222	272	0.04%	0.004%
57	10.041	2698	2706	2709	rBV	172	323	0.04%	0.005%
58	10.105	2718	2726	2736	rVB3	1558	2441	0.33%	0.040%
59	10.491	2840	2846	2852	rVB2	342	503	0.07%	0.008%
60	10.671	2896	2902	2909	rVB2	1499	1823	0.25%	0.030%
61	10.758	2916	2929	2946	rVB	241741	382207	51.98%	6.306%
62	10.861	2957	2961	2965	rBV2	202	235	0.03%	0.004%
63	10.902	2968	2974	2984	rVB3	1936	2970	0.40%	0.049%
64	10.999	2994	3004	3021	rBV3	7324	14961	2.03%	0.247%
65	11.089	3024	3032	3041	rBV2	3965	5633	0.77%	0.093%
66	11.292	3086	3095	3108	rVB2	4217	6030	0.82%	0.099%
67	11.468	3138	3150	3162	rBV	25170	37568	5.11%	0.620%
68	11.697	3216	3221	3226	rBV2	664	590	0.08%	0.010%
69	11.812	3245	3257	3274	rBV	356430	560709	76.25%	9.251%
70	11.896	3275	3283	3291	rVB	5033	6940	0.94%	0.114%
71	11.941	3292	3297	3300	rVV3	365	391	0.05%	0.006%
72	11.973	3303	3307	3314	rVB2	1092	1178	0.16%	0.019%
73	12.099	3337	3346	3354	rBV2	4857	7458	1.01%	0.123%
74	12.195	3361	3376	3395	rVB	342145	559432	76.08%	9.230%
75	12.330	3413	3418	3423	rVB2	267	230	0.03%	0.004%
76	12.375	3428	3432	3438	rVB	492	476	0.06%	0.008%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

77	12.462	3453	3459	3460	rBV	1010	722	0.10%	0.012%
78	12.497	3466	3470	3476	rVB2	1069	1173	0.16%	0.019%
79	12.571	3485	3493	3501	rVB	2890	3632	0.49%	0.060%
80	12.613	3501	3506	3512	rVB3	695	747	0.10%	0.012%
81	12.684	3519	3528	3537	rVB2	3314	4687	0.64%	0.077%
82	12.883	3583	3590	3599	rVB2	299	428	0.06%	0.007%
83	12.973	3610	3618	3627	rBV	1684	2434	0.33%	0.040%
84	13.028	3627	3635	3642	rVB3	2164	2889	0.39%	0.048%
85	13.140	3667	3670	3676	rBV2	239	218	0.03%	0.004%
86	13.295	3710	3718	3725	rVB3	1924	2537	0.35%	0.042%
87	13.455	3759	3768	3777	rVB4	5134	7377	1.00%	0.122%
88	13.558	3796	3800	3804	rBV	480	335	0.05%	0.006%
89	13.626	3818	3821	3824	rBV2	505	344	0.05%	0.006%
90	13.780	3863	3869	3873	rBV2	428	617	0.08%	0.010%
91	13.838	3883	3887	3896	rVB3	552	683	0.09%	0.011%
92	14.089	3955	3965	3976	rVB	5443	7607	1.03%	0.126%
93	15.169	4299	4301	4306	rVB2	238	198	0.03%	0.003%
94	15.227	4311	4319	4325	rBV2	987	1499	0.20%	0.025%
95	15.407	4371	4375	4379	rBV2	719	738	0.10%	0.012%
96	15.497	4399	4403	4407	rVB2	237	223	0.03%	0.004%
97	15.574	4424	4427	4429	rBV2	228	170	0.02%	0.003%
98	16.690	4772	4774	4777	rBV2	463	367	0.05%	0.006%
99	16.754	4792	4794	4796	rBV2	344	200	0.03%	0.003%
100	16.973	4859	4862	4864	rBV	476	373	0.05%	0.006%

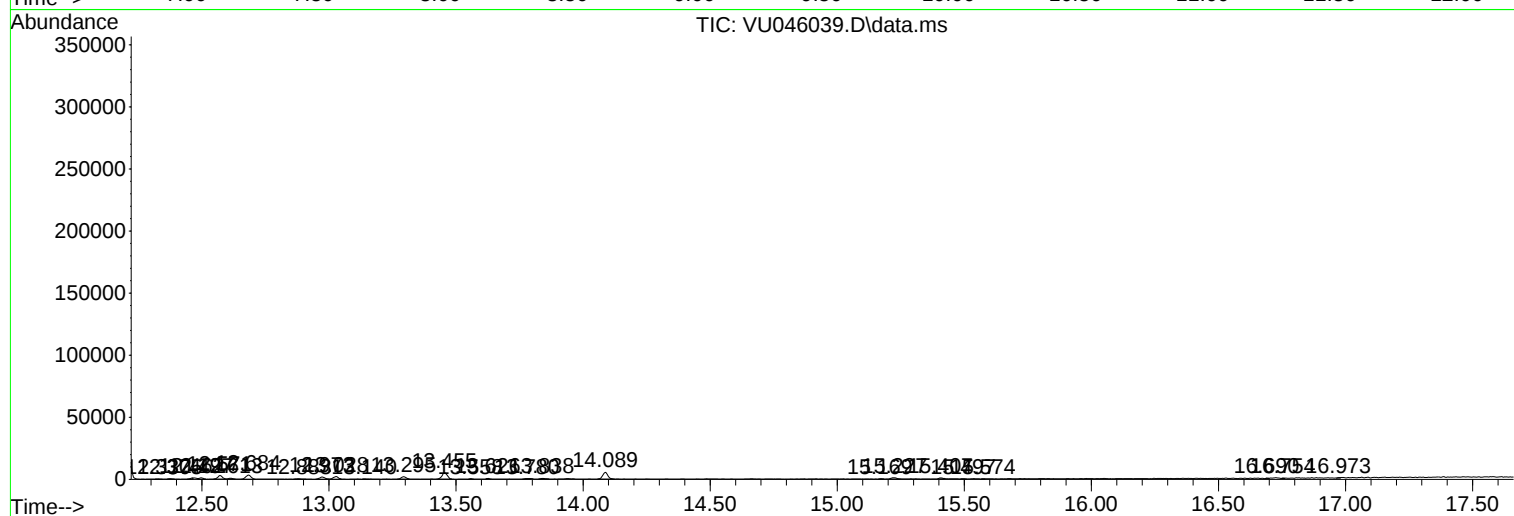
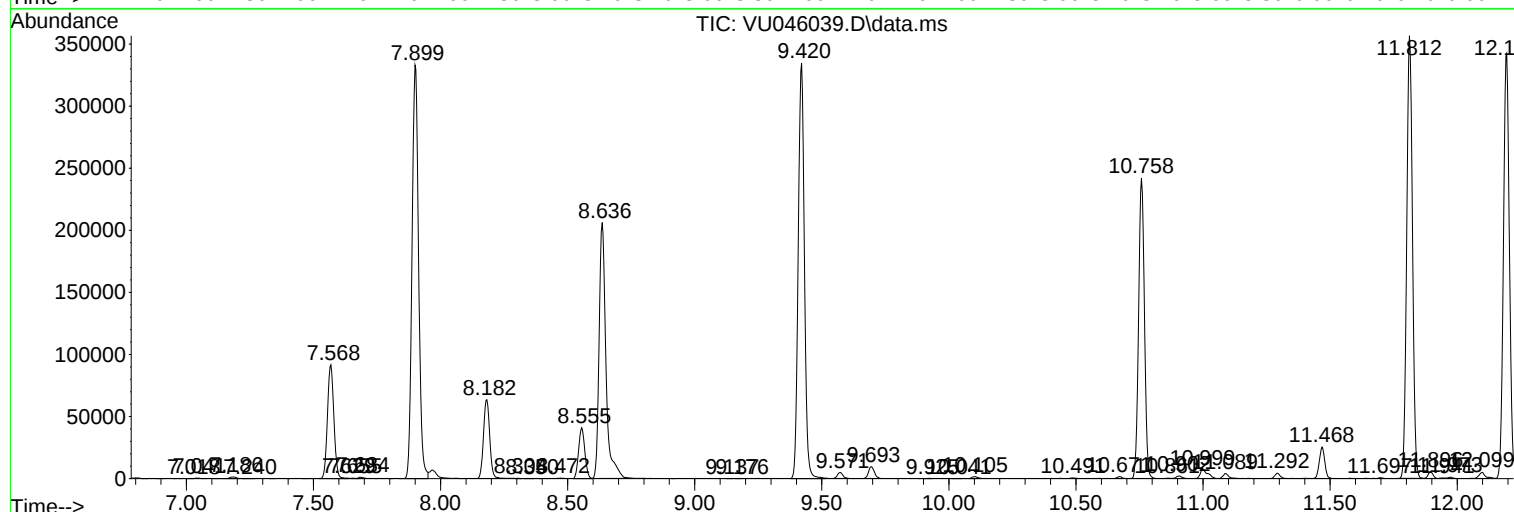
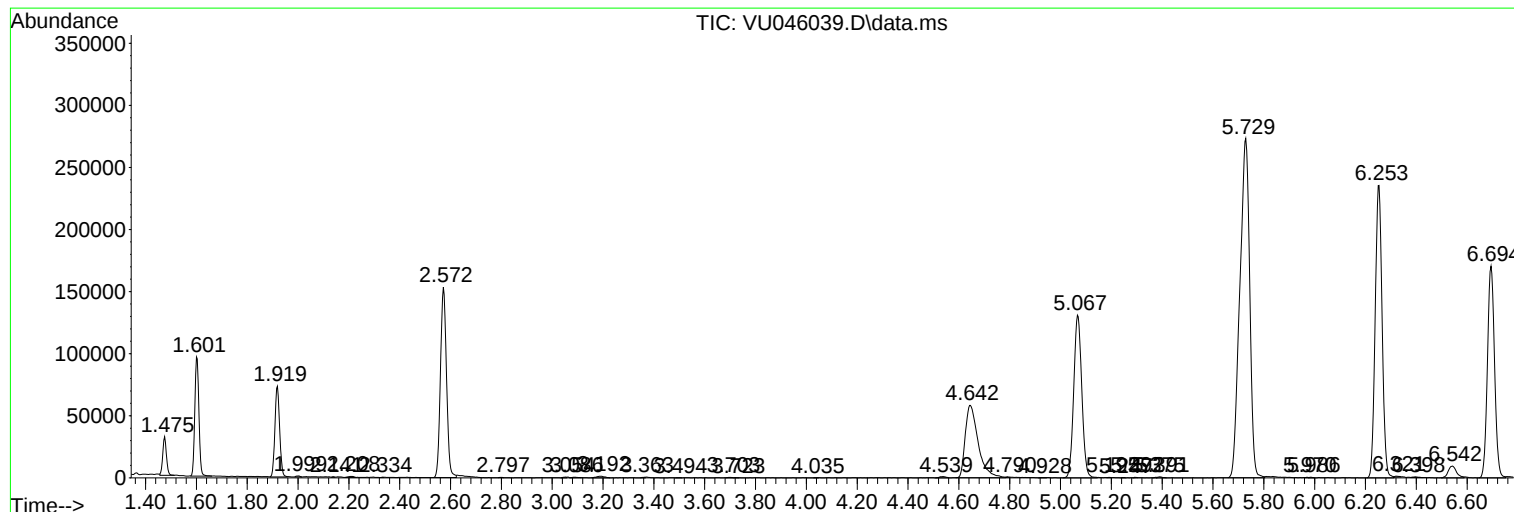
Sum of corrected areas: 6061282

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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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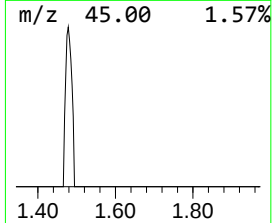
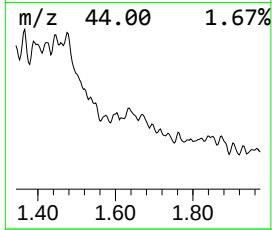
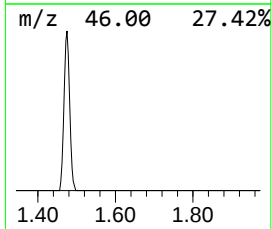
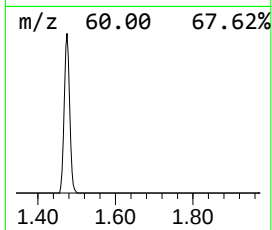
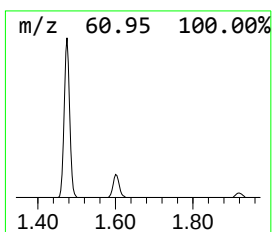
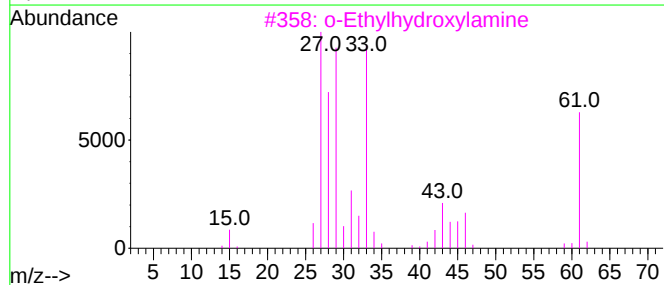
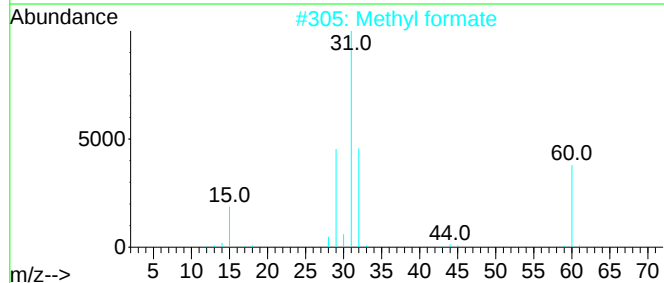
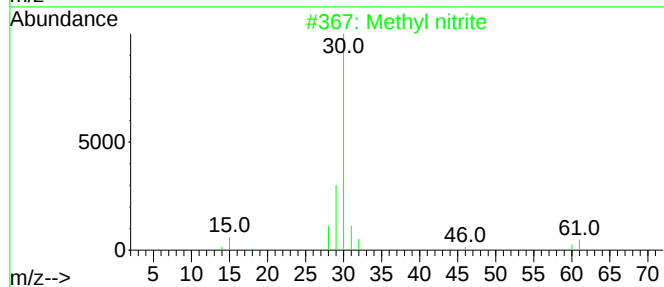
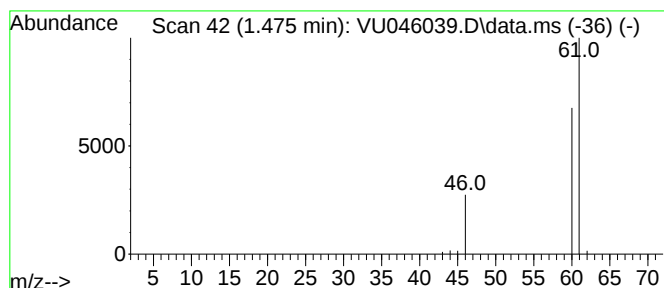
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	3.50 ug/L	31169	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			Methyl formate	60	C2H4O2	000107-31-3	4
3			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
4			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4
5			Carbonyl sulfide	60	COS	000463-58-1	3



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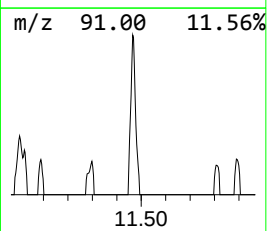
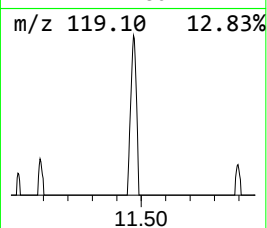
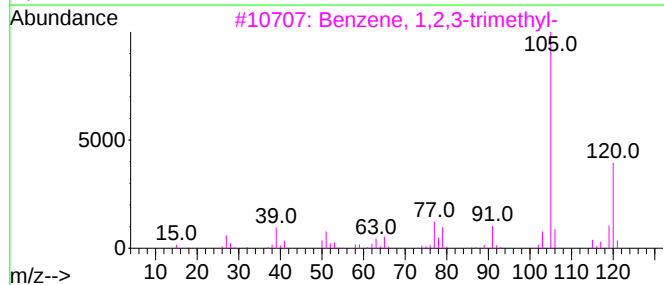
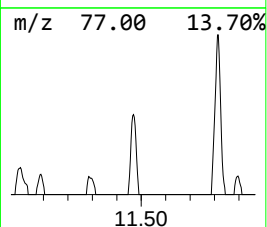
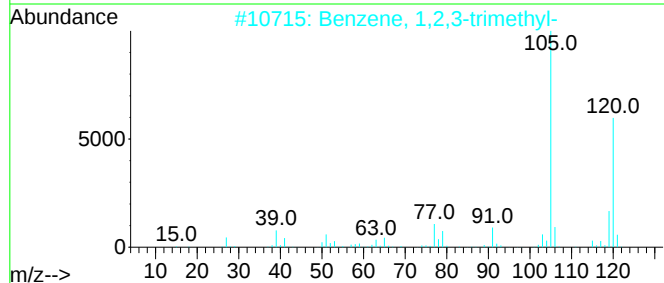
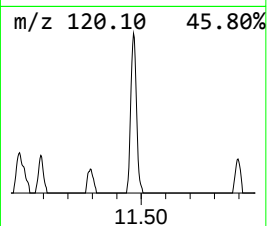
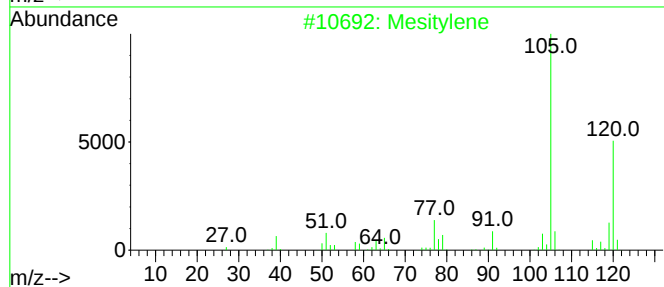
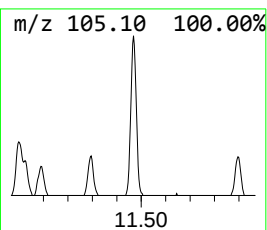
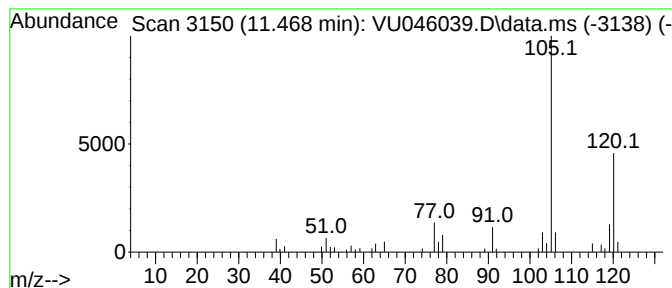
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.468	3.35 ug/L	37568	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
4			Mesitylene	120	C9H12	000108-67-8	94
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94



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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
unknown-01	1.475	3.5	ug/L	31169	1	6.253	445615	50.0
Benzene, 1,2,4-...	11.468	3.4	ug/L	37568	3	11.812	560709	50.0