

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120221\
 Data File : VU046060.D
 Acq On : 02 Dec 2021 18:12
 Operator : SY/MD
 Sample : M4878-02 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 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: VU046060.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	51	rVB	30338	31068	3.71%	0.436%
2	1.601	73	81	97	rVB	100090	109441	13.09%	1.536%
3	1.916	170	179	192	rBV	74187	93372	11.16%	1.310%
4	2.208	265	270	275	rBV3	765	638	0.08%	0.009%
5	2.514	360	365	369	rBV2	368	396	0.05%	0.006%
6	2.572	369	383	401	rBV	167366	282487	33.78%	3.964%
7	2.967	501	506	509	rBV	301	203	0.02%	0.003%
8	3.051	525	532	539	rBV4	1612	2368	0.28%	0.033%
9	3.189	564	575	586	rBV2	1661	3703	0.44%	0.052%
10	3.298	606	609	616	rBV	302	320	0.04%	0.004%
11	3.427	645	649	652	rBB	216	195	0.02%	0.003%
12	3.472	658	663	667	rVB2	157	175	0.02%	0.002%
13	4.215	891	894	898	rVB	163	169	0.02%	0.002%
14	4.366	938	941	945	rBV	152	175	0.02%	0.002%
15	4.414	952	956	959	rBV	177	168	0.02%	0.002%
16	4.533	987	993	994	rBV2	347	350	0.04%	0.005%
17	4.543	994	996	1000	rVB2	491	331	0.04%	0.005%
18	4.633	1009	1024	1062	rBV	88318	239733	28.66%	3.364%
19	4.899	1104	1107	1112	rVB2	166	167	0.02%	0.002%
20	4.932	1114	1117	1121	rBV2	228	196	0.02%	0.003%
21	4.951	1121	1123	1126	rVB3	335	196	0.02%	0.003%
22	5.067	1143	1159	1178	rBV	151473	329485	39.40%	4.623%
23	5.218	1203	1206	1210	rVB2	350	196	0.02%	0.003%
24	5.285	1224	1227	1230	rBV	260	231	0.03%	0.003%
25	5.391	1252	1260	1266	rBV2	677	954	0.11%	0.013%
26	5.542	1300	1307	1310	rBV	161	260	0.03%	0.004%
27	5.729	1342	1365	1383	rBV2	312315	836344	100.00%	11.735%
28	6.044	1458	1463	1468	rVB2	403	484	0.06%	0.007%
29	6.118	1482	1486	1489	rBV	274	265	0.03%	0.004%
30	6.186	1504	1507	1511	rBV	172	200	0.02%	0.003%
31	6.250	1511	1527	1548	rBV	290892	555308	66.40%	7.792%
32	6.395	1566	1572	1578	rVB4	884	1169	0.14%	0.016%
33	6.539	1603	1617	1635	rBV5	10015	21766	2.60%	0.305%
34	6.694	1651	1665	1685	rBV	196502	374574	44.79%	5.256%
35	7.182	1807	1817	1826	rBV2	2035	3053	0.37%	0.043%
36	7.568	1923	1937	1951	rBV	108192	188205	22.50%	2.641%

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Integrator: RTE

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

37	7.684	1967	1973	1986	rVB3	1513	2463	0.29%	0.035%
38	7.899	2027	2040	2057	rBV	389707	679207	81.21%	9.530%
39	8.128	2107	2111	2115	rBV	188	226	0.03%	0.003%
40	8.179	2115	2127	2141	rBV	73716	121343	14.51%	1.703%
41	8.555	2233	2244	2256	rBV	43419	71903	8.60%	1.009%
42	8.632	2256	2268	2302	rVV	252428	450421	53.86%	6.320%
43	8.902	2351	2352	2357	rVB	263	184	0.02%	0.003%
44	8.928	2357	2360	2364	rBV	220	224	0.03%	0.003%
45	9.420	2499	2513	2533	rBV	414035	693225	82.89%	9.727%
46	9.571	2550	2560	2574	rVB	6571	9574	1.14%	0.134%
47	9.697	2588	2599	2610	rBV3	12347	20636	2.47%	0.290%
48	10.099	2718	2724	2734	rBV3	2106	3310	0.40%	0.046%
49	10.488	2839	2845	2850	rBV	509	587	0.07%	0.008%
50	10.629	2885	2889	2892	rVV	351	294	0.04%	0.004%
51	10.674	2892	2903	2911	rVB3	1786	2830	0.34%	0.040%
52	10.758	2917	2929	2947	rBV	274785	443650	53.05%	6.225%
53	10.864	2958	2962	2965	rBV	260	219	0.03%	0.003%
54	10.906	2968	2975	2984	rVB3	1916	3348	0.40%	0.047%
55	10.999	2995	3004	3009	rBV	9413	13908	1.66%	0.195%
56	11.089	3023	3032	3038	rBV	5550	8110	0.97%	0.114%
57	11.150	3049	3051	3053	rBV	356	207	0.02%	0.003%
58	11.291	3087	3095	3105	rVB2	5731	7978	0.95%	0.112%
59	11.417	3127	3134	3140	rVV4	1121	1562	0.19%	0.022%
60	11.468	3140	3150	3164	rVB	31975	48918	5.85%	0.686%
61	11.574	3178	3183	3190	rVB3	448	596	0.07%	0.008%
62	11.697	3215	3221	3227	rBV5	1426	1830	0.22%	0.026%
63	11.812	3245	3257	3272	rBV	460626	720801	86.18%	10.114%
64	11.896	3276	3283	3293	rVB2	6241	9161	1.10%	0.129%
65	11.938	3293	3296	3301	rBV6	774	914	0.11%	0.013%
66	12.002	3315	3316	3320	rVB2	501	285	0.03%	0.004%
67	12.095	3335	3345	3353	rBV2	6341	9912	1.19%	0.139%
68	12.195	3363	3376	3391	rVV	412887	653715	78.16%	9.173%
69	12.327	3412	3417	3427	rVB3	2334	3193	0.38%	0.045%
70	12.378	3427	3433	3439	rBV2	540	650	0.08%	0.009%
71	12.465	3455	3460	3465	rBV4	1169	1354	0.16%	0.019%
72	12.574	3485	3494	3501	rVV2	3714	5007	0.60%	0.070%
73	12.684	3519	3528	3539	rBV	4012	6017	0.72%	0.084%
74	12.877	3584	3588	3594	rBV2	366	454	0.05%	0.006%
75	12.973	3610	3618	3626	rVB3	2350	3112	0.37%	0.044%
76	13.031	3626	3636	3644	rBV3	2715	4044	0.48%	0.057%

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77	13.102	3656	3658	3663	rBV2	173	179	0.02%	0.003%
78	13.143	3666	3671	3678	rVV4	496	717	0.09%	0.010%
79	13.172	3678	3680	3684	rVB	333	227	0.03%	0.003%
80	13.253	3701	3705	3711	rVB	428	334	0.04%	0.005%
81	13.295	3711	3718	3726	rVB4	2348	3327	0.40%	0.047%
82	13.417	3753	3756	3757	rVV2	463	299	0.04%	0.004%
83	13.459	3759	3769	3780	rVB4	6472	10079	1.21%	0.141%
84	13.526	3785	3790	3796	rBV2	238	278	0.03%	0.004%
85	13.561	3796	3801	3807	rVV	370	456	0.05%	0.006%
86	13.626	3815	3821	3827	rVB4	602	755	0.09%	0.011%
87	13.783	3864	3870	3871	rBV	661	580	0.07%	0.008%
88	13.841	3881	3888	3893	rBV3	820	1122	0.13%	0.016%
89	13.912	3905	3910	3913	rBV2	336	333	0.04%	0.005%
90	13.941	3914	3919	3923	rVV4	659	628	0.08%	0.009%
91	14.089	3954	3965	3976	rVB	8604	12739	1.52%	0.179%
92	14.487	4084	4089	4093	rVB	548	515	0.06%	0.007%
93	14.581	4112	4118	4124	rBV2	548	596	0.07%	0.008%
94	14.690	4150	4152	4156	rVB2	411	280	0.03%	0.004%
95	14.954	4228	4234	4239	rVB2	298	369	0.04%	0.005%
96	15.224	4310	4318	4331	rBV	3212	5225	0.62%	0.073%
97	15.340	4351	4354	4356	rBV2	313	174	0.02%	0.002%
98	15.410	4369	4376	4386	rBV4	1794	2951	0.35%	0.041%
99	16.124	4595	4598	4600	rBV2	381	295	0.04%	0.004%
100	16.195	4615	4620	4623	rBV3	466	594	0.07%	0.008%

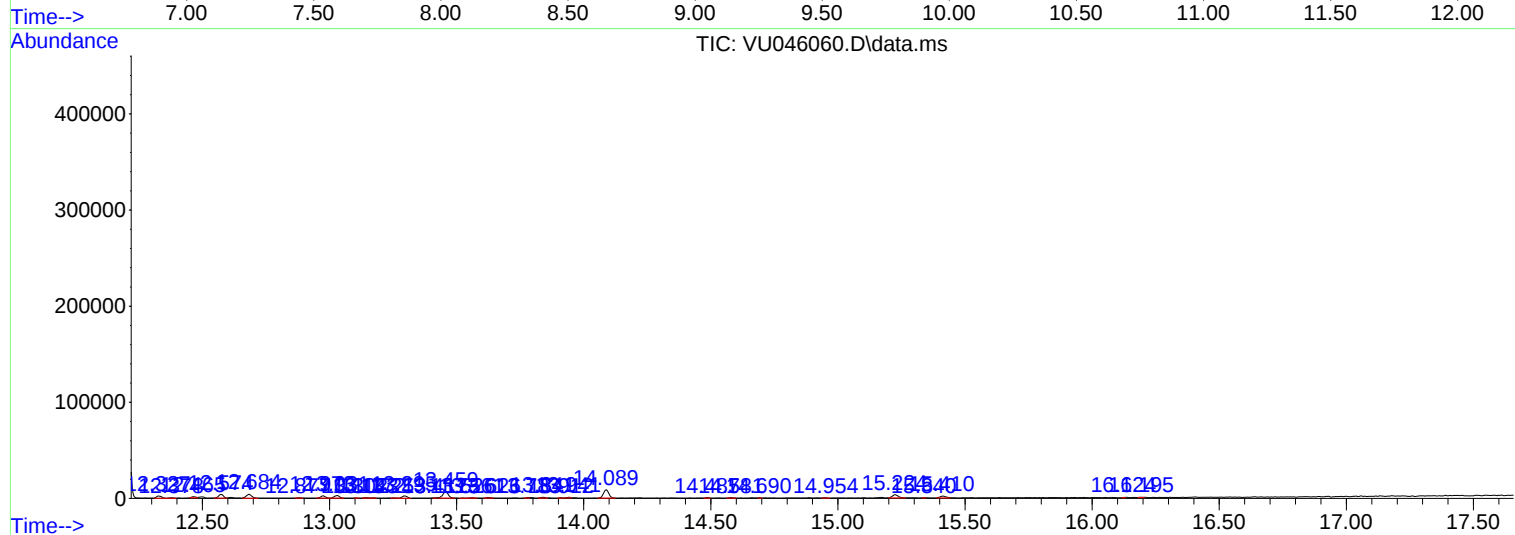
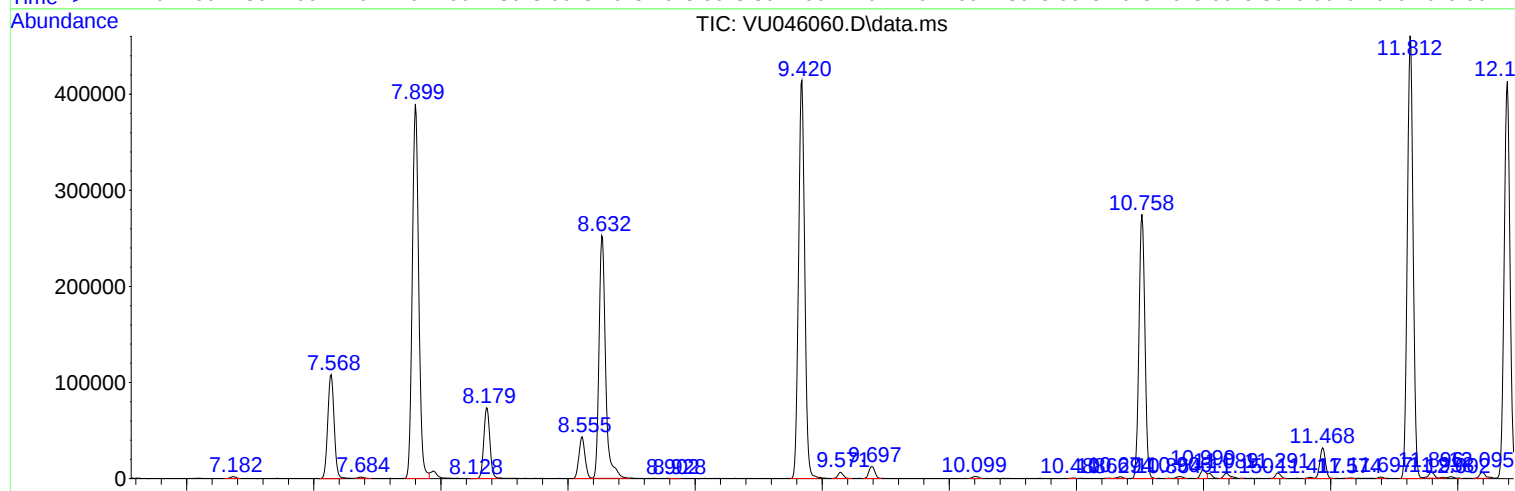
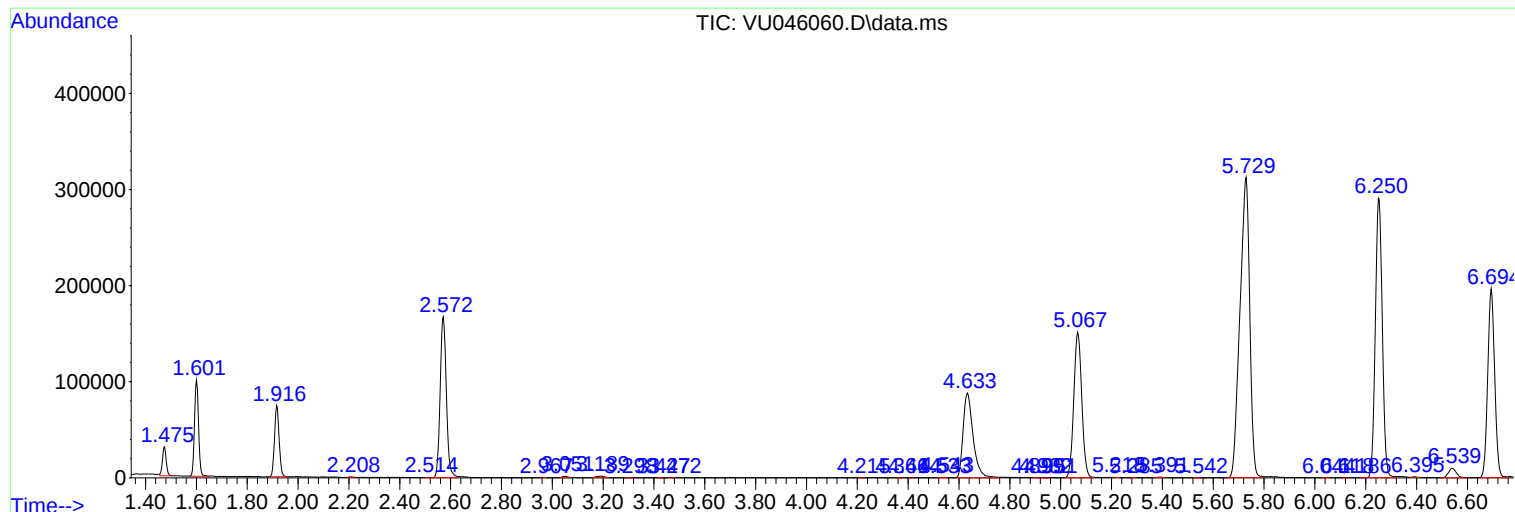
Sum of corrected areas: 7126769

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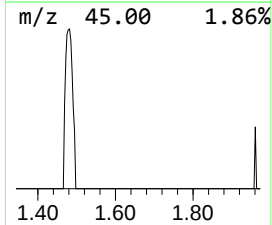
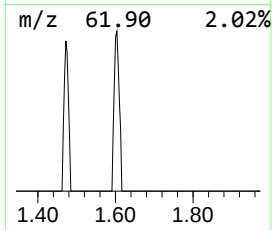
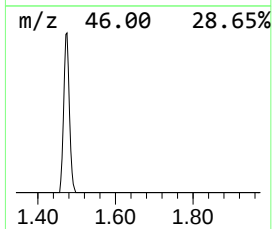
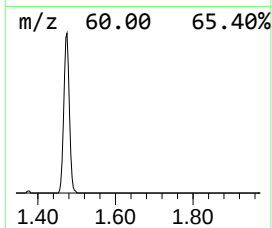
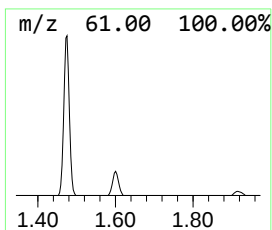
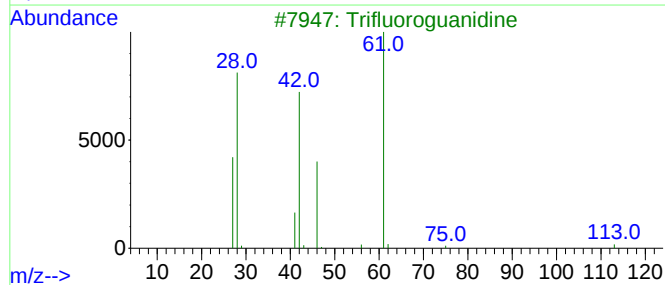
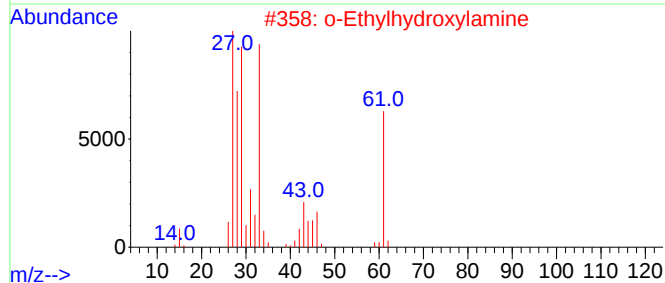
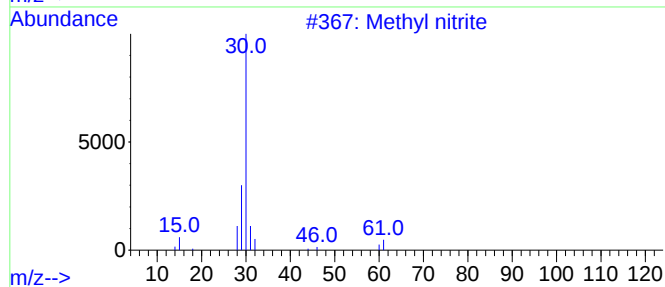
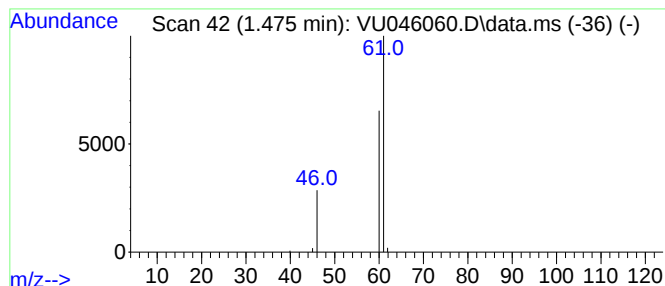
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	2.80 ug/L	31068	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3			Trifluoroguanidine	113	CH2F3N3	037950-72-4	4
4			Carbonyl sulfide	60	COS	000463-58-1	3
5			Thiirane	60	C2H4S	000420-12-2	3



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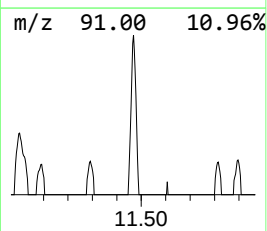
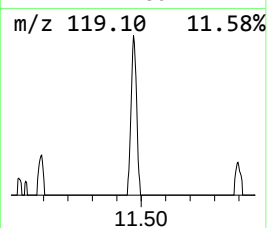
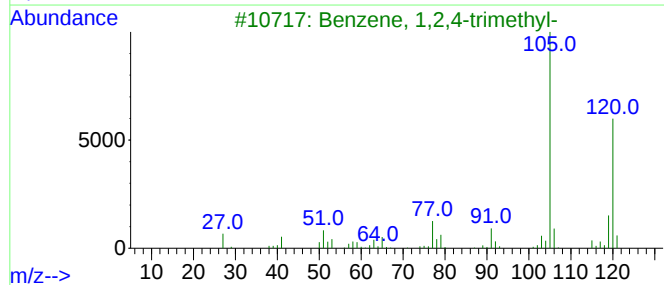
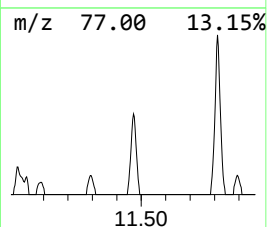
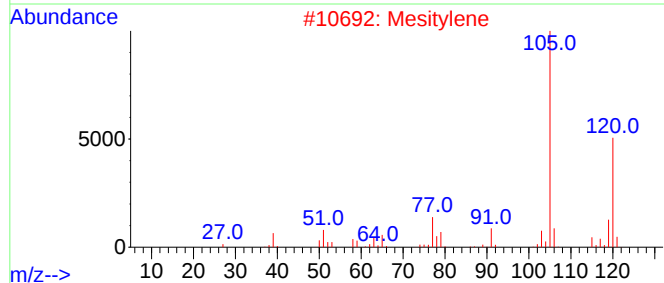
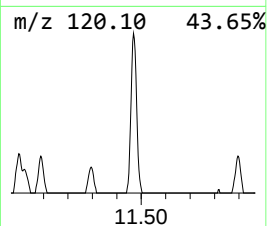
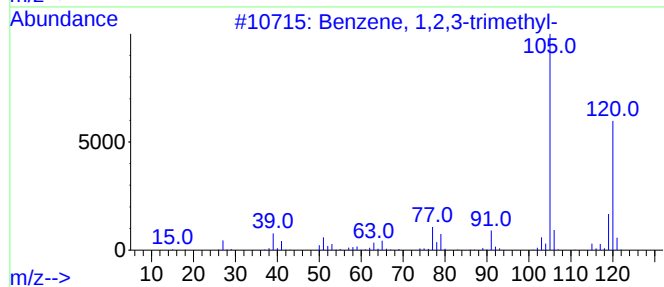
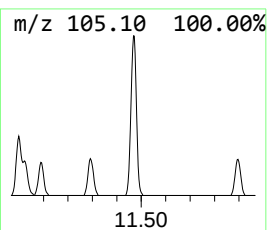
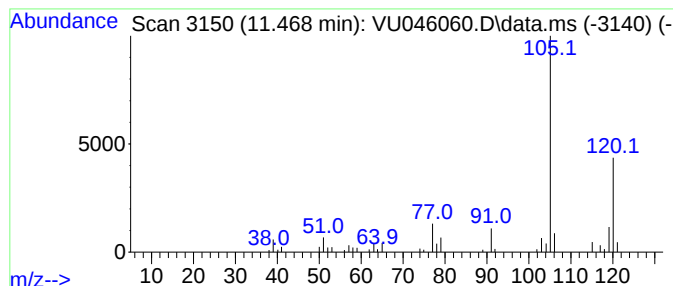
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.468	3.39 ug/L	48918	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	97
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Mesitylene	120	C9H12	000108-67-8	93
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93



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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	2.8	ug/L	31068	1	6.253	555308	50.0
Benzene, 1,2,4-...	11.468	3.4	ug/L	48918	3	11.812	720801	50.0