

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053545.D
 Acq On : 04 Apr 2023 01:55
 Operator : JC/MD
 Sample : 02158-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-2(20230330)

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	42	47	57	rVB	24126	23470	0.22%	0.082%
2	1.600	73	81	90	rBV2	193325	233810	2.16%	0.816%
3	1.909	170	177	192	rVB	99296	139703	1.29%	0.487%
4	2.369	310	320	336	rVB2	181629	297635	2.74%	1.038%
5	2.578	369	385	410	rBV3	1179659	2094774	19.31%	7.307%
6	3.044	520	530	539	rBV7	4129	7709	0.07%	0.027%
7	3.350	612	625	642	rBV2	36386	72262	0.67%	0.252%
8	3.549	685	687	690	rBV	157	60	0.00%	0.000%
9	3.742	744	747	748	rBV	189	88	0.00%	0.000%
10	3.864	761	785	810	rBV	4599086	10847810	100.00%	37.840%
11	4.327	926	929	931	rBV2	480	327	0.00%	0.001%
12	4.520	981	989	990	rBV4	1806	1971	0.02%	0.007%
13	4.661	1007	1033	1057	rBV2	1023204	2470322	22.77%	8.617%
14	5.057	1141	1156	1183	rBV2	170157	375846	3.46%	1.311%
15	5.311	1221	1235	1250	rBV2	49216	108320	1.00%	0.378%
16	5.472	1282	1285	1289	rVB	250	171	0.00%	0.001%
17	5.501	1290	1294	1297	rVB2	333	252	0.00%	0.001%
18	5.552	1307	1310	1313	rBV2	305	217	0.00%	0.001%
19	5.575	1315	1317	1325	rVB2	359	350	0.00%	0.001%
20	5.719	1341	1362	1373	rBV2	329114	901773	8.31%	3.146%
21	5.906	1418	1420	1422	rBV2	502	291	0.00%	0.001%
22	5.960	1435	1437	1439	rBV	255	99	0.00%	0.000%
23	6.102	1478	1481	1486	rVB3	384	324	0.00%	0.001%
24	6.121	1486	1487	1489	rBV3	143	60	0.00%	0.000%
25	6.153	1493	1497	1501	rBV2	323	294	0.00%	0.001%
26	6.243	1512	1525	1546	rBV	296652	562053	5.18%	1.961%
27	6.468	1594	1595	1597	rVB	373	74	0.00%	0.000%
28	6.536	1601	1616	1650	rBV	2759505	5185398	47.80%	18.088%
29	6.684	1653	1662	1680	rVB	208662	404103	3.73%	1.410%
30	6.877	1720	1722	1725	rVB2	513	258	0.00%	0.001%
31	6.896	1725	1728	1732	rVB2	370	287	0.00%	0.001%
32	6.919	1733	1735	1737	rBV	282	122	0.00%	0.000%
33	6.960	1738	1748	1759	rBV3	7239	13895	0.13%	0.048%
34	7.240	1833	1835	1839	rBV	558	489	0.00%	0.002%
35	7.314	1855	1858	1860	rVV	307	222	0.00%	0.001%
36	7.404	1879	1886	1894	rBV5	2371	3377	0.03%	0.012%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.478	1905	1909	1913	rBV2	296	245	0.00%	0.001%
38	7.497	1913	1915	1917	rBV2	157	85	0.00%	0.000%
39	7.562	1921	1935	1952	rBV2	117222	209951	1.94%	0.732%
40	7.655	1962	1964	1967	rBV	239	111	0.00%	0.000%
41	7.761	1994	1997	2000	rBV3	305	198	0.00%	0.001%
42	7.893	2024	2038	2055	rBV	431036	750656	6.92%	2.619%
43	8.176	2115	2126	2147	rBV	83838	141774	1.31%	0.495%
44	8.288	2159	2161	2163	rBV2	219	119	0.00%	0.000%
45	8.401	2187	2196	2205	rVB6	2137	3643	0.03%	0.013%
46	8.475	2211	2219	2223	rBV2	633	1020	0.01%	0.004%
47	8.552	2233	2243	2251	rVB2	7957	12106	0.11%	0.042%
48	8.626	2255	2266	2304	rVV	223509	417120	3.85%	1.455%
49	9.073	2403	2405	2409	rVB	261	134	0.00%	0.000%
50	9.272	2465	2467	2472	rVB	371	189	0.00%	0.001%
51	9.304	2472	2477	2479	rBV2	411	361	0.00%	0.001%
52	9.414	2497	2511	2535	rBV2	404201	798728	7.36%	2.786%
53	9.690	2593	2597	2611	rVB3	1481	2112	0.02%	0.007%
54	9.745	2611	2614	2618	rVB	376	218	0.00%	0.001%
55	9.761	2618	2619	2621	rBV	217	90	0.00%	0.000%
56	9.848	2643	2646	2648	rBV	265	192	0.00%	0.001%
57	9.931	2670	2672	2677	rVB	381	203	0.00%	0.001%
58	9.999	2690	2693	2695	rBV2	222	148	0.00%	0.001%
59	10.099	2719	2724	2727	rBV2	1035	1042	0.01%	0.004%
60	10.198	2753	2755	2759	rBV	162	70	0.00%	0.000%
61	10.269	2775	2777	2780	rBV	228	145	0.00%	0.001%
62	10.304	2785	2788	2791	rBV2	245	172	0.00%	0.001%
63	10.343	2793	2800	2807	rBV5	3075	3921	0.04%	0.014%
64	10.433	2825	2828	2832	rBV2	320	244	0.00%	0.001%
65	10.488	2838	2845	2849	rVB2	374	562	0.01%	0.002%
66	10.517	2852	2854	2858	rVB	228	109	0.00%	0.000%
67	10.539	2858	2861	2865	rVB2	317	259	0.00%	0.001%
68	10.639	2883	2892	2902	rBV	9478	14193	0.13%	0.050%
69	10.703	2909	2912	2914	rBV	233	114	0.00%	0.000%
70	10.751	2914	2927	2945	rBV	300998	488183	4.50%	1.703%
71	10.883	2965	2968	2969	rBV	525	248	0.00%	0.001%
72	10.893	2969	2971	2977	rVB2	519	403	0.00%	0.001%
73	11.070	3024	3026	3027	rBV2	216	99	0.00%	0.000%
74	11.137	3044	3047	3051	rBV2	395	267	0.00%	0.001%
75	11.243	3078	3080	3082	rVB	352	117	0.00%	0.000%
76	11.414	3122	3133	3145	rBV	42410	64788	0.60%	0.226%

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 Title : VOC Analysis

77	11.742	3225	3235	3244	rBV	52395	80659	0.74%	0.281%
78	11.809	3245	3256	3281	rVB2	469430	985658	9.09%	3.438%
79	11.983	3307	3310	3311	rBV	392	214	0.00%	0.001%
80	12.095	3338	3345	3352	rVB4	6481	8146	0.08%	0.028%
81	12.131	3352	3356	3359	rBV	256	182	0.00%	0.001%
82	12.188	3361	3374	3398	rBV	459075	755080	6.96%	2.634%
83	12.307	3409	3411	3414	rVB	318	93	0.00%	0.000%
84	12.362	3419	3428	3438	rVB5	4957	7544	0.07%	0.026%
85	12.883	3588	3590	3594	rBV	242	203	0.00%	0.001%
86	12.938	3604	3607	3608	rBV	270	129	0.00%	0.000%
87	13.002	3625	3627	3631	rVB2	456	288	0.00%	0.001%
88	13.131	3664	3667	3670	rVB	513	263	0.00%	0.001%
89	13.487	3776	3778	3782	rVB2	380	199	0.00%	0.001%
90	13.520	3785	3788	3792	rBV3	517	346	0.00%	0.001%
91	13.581	3802	3807	3816	rBV4	2008	2443	0.02%	0.009%
92	13.668	3832	3834	3836	rBV	349	157	0.00%	0.001%
93	13.700	3842	3844	3846	rBV	362	144	0.00%	0.001%
94	13.838	3876	3887	3906	rBV2	91173	150779	1.39%	0.526%
95	13.947	3920	3921	3924	rBV2	408	169	0.00%	0.001%
96	13.963	3924	3926	3927	rBV2	386	111	0.00%	0.000%
97	14.089	3961	3965	3973	rVB5	3980	4792	0.04%	0.017%
98	14.774	4174	4178	4185	rBV8	1882	2578	0.02%	0.009%
99	15.015	4248	4253	4258	rBV4	1495	1371	0.01%	0.005%
100	15.208	4306	4313	4325	rVB6	2074	3166	0.03%	0.011%

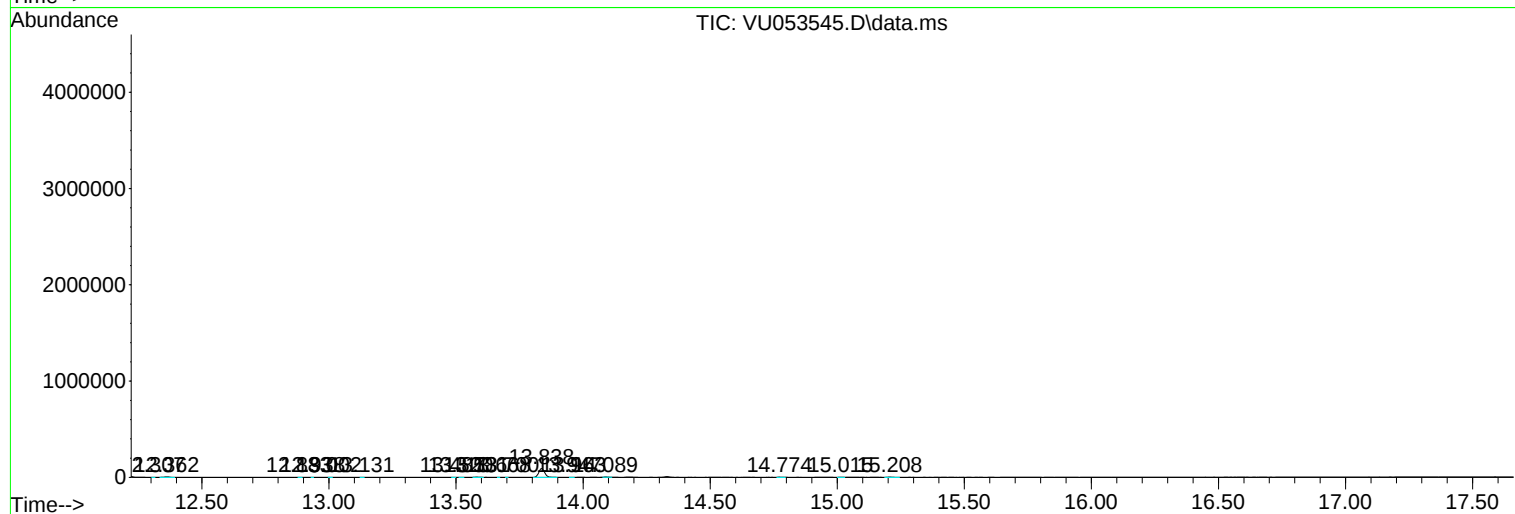
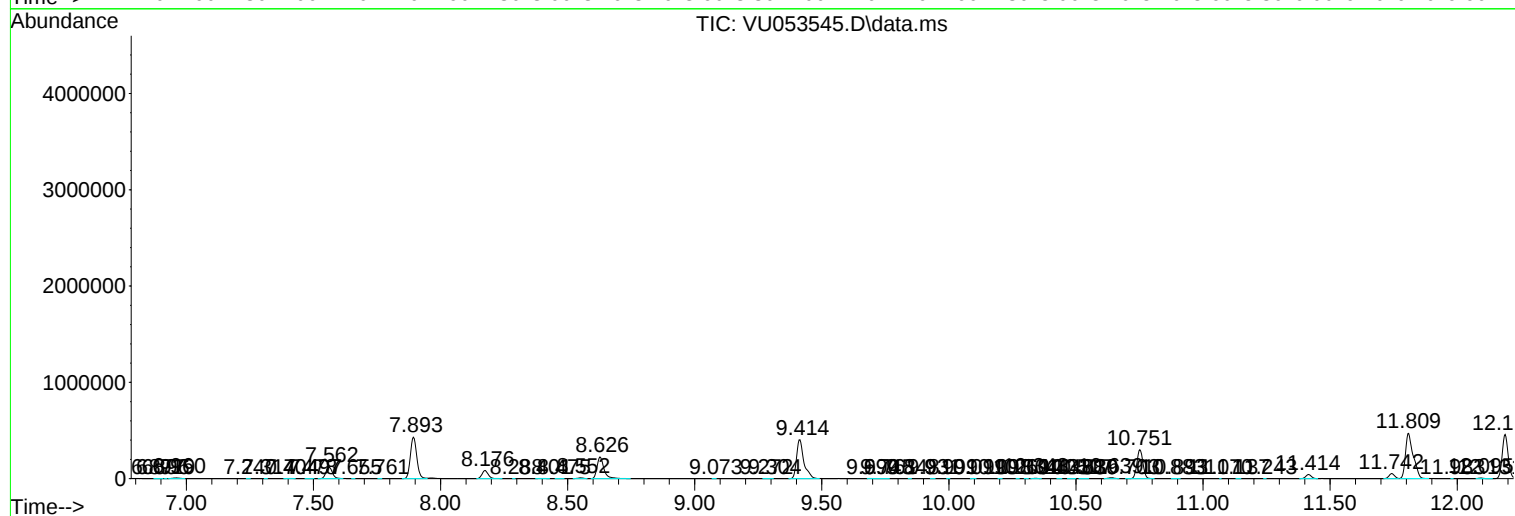
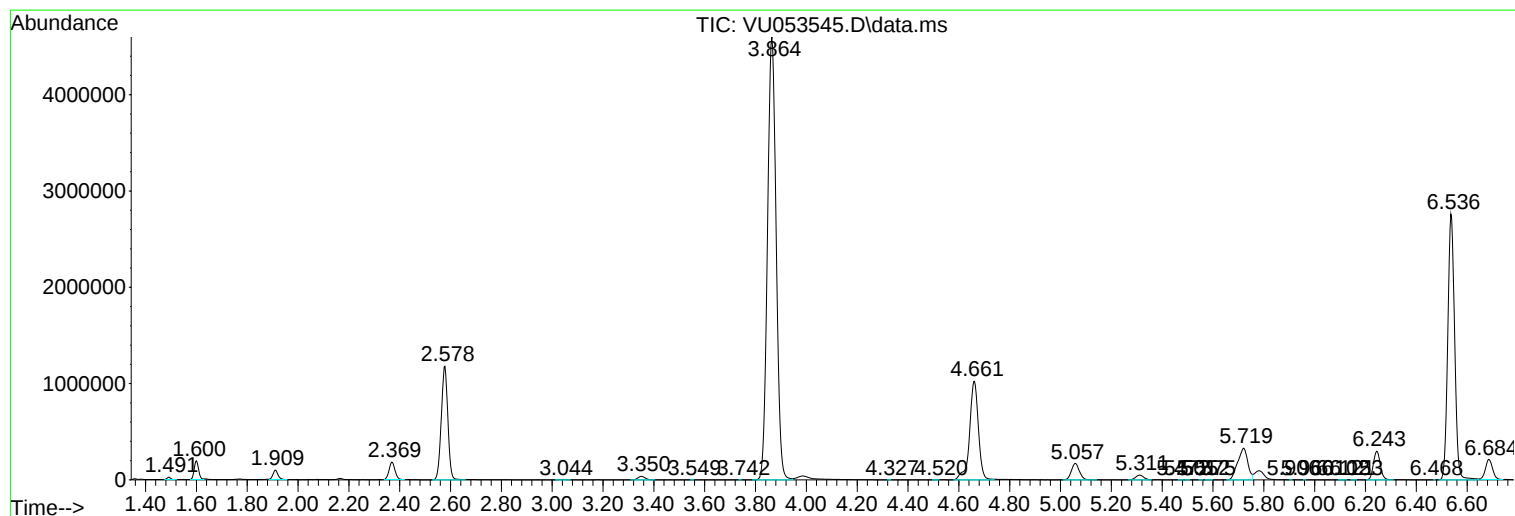
Sum of corrected areas: 28667269

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Instrument :
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ClientSampleId :
PMW-2(20230330)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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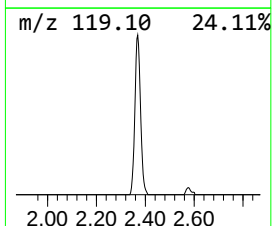
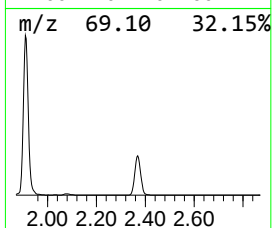
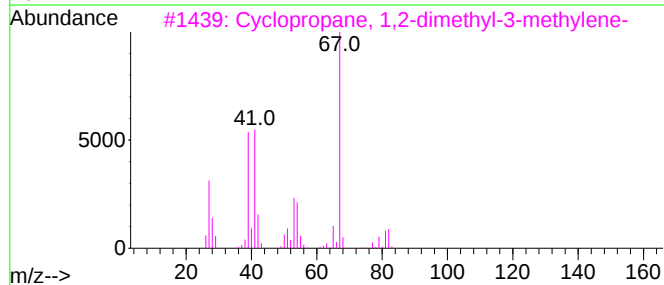
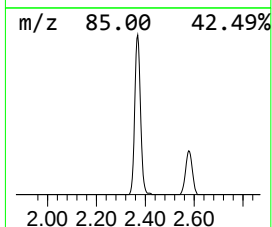
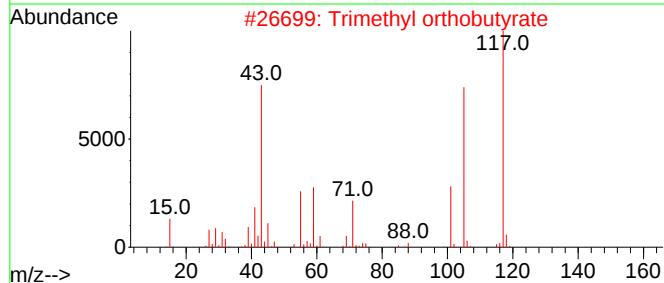
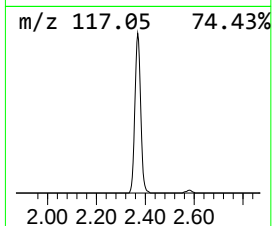
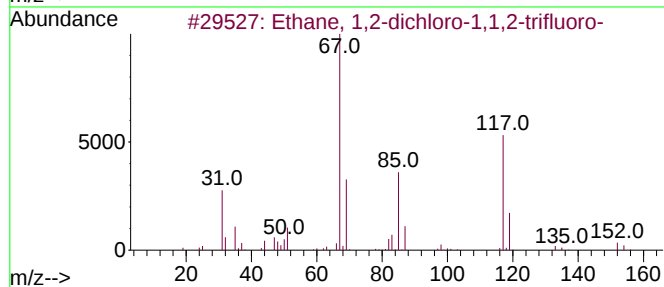
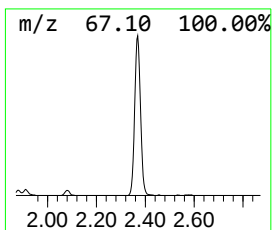
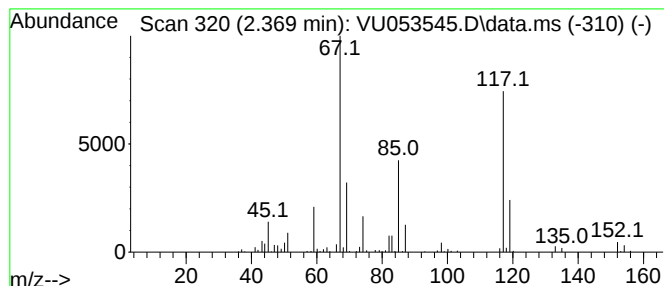
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethane, 1,2-dichloro-1,1,2-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.369	26.48 ug/L	297635	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	87
2			Trimethyl orthobutyrate	148	C7H16O3	043083-12-1	10
3			Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	10
4			1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	10
5			3-Chloro-5-propyl-1H-1,2,4-triazole	145	C5H8ClN3	063580-18-7	10



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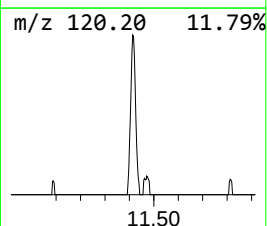
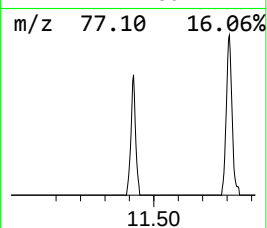
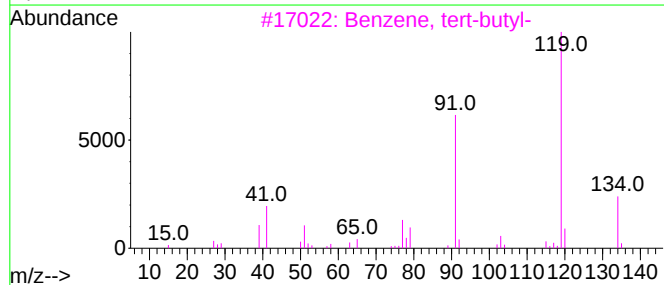
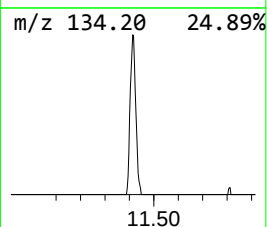
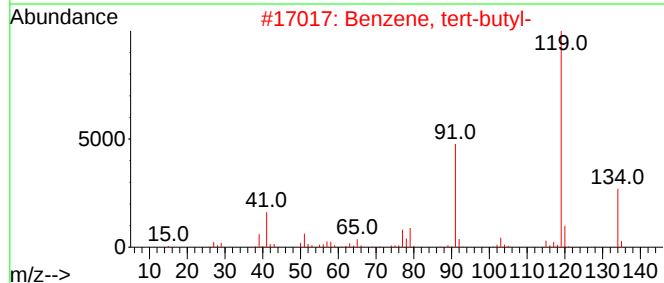
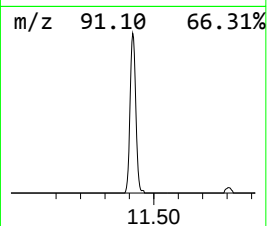
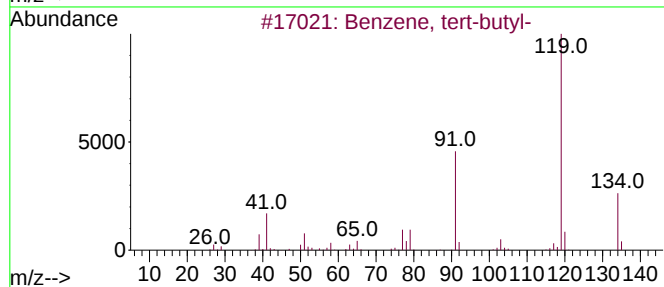
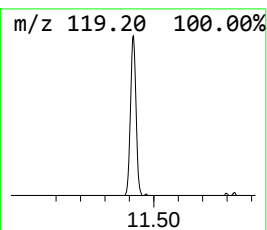
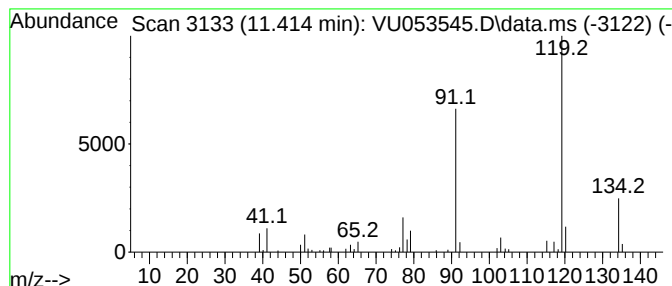
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Quant Title : VOC Analysis

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

Peak Number 3 Benzene, tert-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.414	3.29 ug/L	64788	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, tert-butyl-	134	C10H14	000098-06-6	95
2			Benzene, tert-butyl-	134	C10H14	000098-06-6	94
3			Benzene, tert-butyl-	134	C10H14	000098-06-6	94
4			Benzene, tert-butyl-	134	C10H14	000098-06-6	94
5			o-Cymene	134	C10H14	000527-84-4	86



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1,2-dic...	2.369	26.5	ug/L	297635	1	6.243	562053	50.0
Benzene, tert-b...	11.414	3.3	ug/L	64788	3	11.806	985658	50.0