

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050618\
 Data File : VU023690.D
 Acq On : 06 May 2018 15:04
 Operator : MD/SY
 Sample : J2721-01DL 200X
 Misc : 6.42g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.089	134	155	178	rBV	1263559	1428930	100.00%	9.481%
2	1.182	180	184	192	rVB2	7392	7368	0.52%	0.049%
3	1.397	245	251	267	rVB	170146	174709	12.23%	1.159%
4	1.680	331	339	356	rVB	128201	161630	11.31%	1.072%
5	2.188	494	497	505	rVB5	3135	3786	0.26%	0.025%
6	2.272	512	523	538	rBV	271181	413530	28.94%	2.744%
7	2.703	650	657	665	rVB4	755	1015	0.07%	0.007%
8	2.838	689	699	713	rVB2	2061	4173	0.29%	0.028%
9	2.998	741	749	753	rBV4	493	595	0.04%	0.004%
10	3.310	837	846	856	rVB5	1441	2627	0.18%	0.017%
11	4.018	1061	1066	1073	rBV2	779	1077	0.08%	0.007%
12	4.178	1100	1116	1156	rBV	119845	320599	22.44%	2.127%
13	4.651	1246	1263	1299	rBV	203252	484852	33.93%	3.217%
14	4.992	1357	1369	1382	rVB5	4382	9858	0.69%	0.065%
15	5.079	1389	1396	1398	rBV3	1211	1392	0.10%	0.009%
16	5.220	1430	1440	1453	rBV4	5081	11530	0.81%	0.077%
17	5.342	1454	1478	1514	rBV2	428419	1286130	90.01%	8.534%
18	5.555	1539	1544	1551	rVB5	1027	1317	0.09%	0.009%
19	5.616	1557	1563	1565	rBV3	1106	1018	0.07%	0.007%
20	5.789	1605	1617	1633	rVB2	14149	28587	2.00%	0.190%
21	5.889	1634	1648	1690	rBV	441593	896575	62.74%	5.949%
22	6.178	1730	1738	1748	rVB3	2121	3286	0.23%	0.022%
23	6.336	1772	1787	1803	rBV	283593	578328	40.47%	3.837%
24	6.532	1844	1848	1849	rBV2	900	624	0.04%	0.004%
25	6.645	1878	1883	1889	rVB5	1126	1075	0.08%	0.007%
26	6.738	1905	1912	1914	rBV3	1371	1496	0.10%	0.010%
27	6.895	1958	1961	1963	rBV3	824	616	0.04%	0.004%
28	7.104	2018	2026	2033	rBV5	1051	1542	0.11%	0.010%
29	7.185	2041	2051	2055	rBV3	5701	8988	0.63%	0.060%
30	7.230	2055	2065	2087	rVB	152674	275365	19.27%	1.827%
31	7.346	2093	2101	2109	rVB4	3313	5390	0.38%	0.036%
32	7.567	2149	2170	2183	rBV	583984	1037112	72.58%	6.882%
33	7.641	2184	2193	2223	rVB	150791	277842	19.44%	1.844%
34	7.854	2240	2259	2275	rBV2	104264	205542	14.38%	1.364%

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Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
 Title : VOC Analysis

35	8.050	2314	2320	2328	rVB4	1381	1868	0.13%	0.012%
36	8.172	2352	2358	2361	rBV3	460	572	0.04%	0.004%
37	8.233	2370	2377	2380	rBV5	622	580	0.04%	0.004%
38	8.313	2390	2402	2435	rBV	398018	695715	48.69%	4.616%
39	8.490	2454	2457	2466	rVB5	2385	2710	0.19%	0.018%
40	8.548	2466	2475	2484	rVB6	4907	8053	0.56%	0.053%
41	8.612	2485	2495	2506	rBV4	2111	4158	0.29%	0.028%
42	8.821	2554	2560	2564	rBV4	1285	1320	0.09%	0.009%
43	8.863	2566	2573	2577	rVV7	1334	1837	0.13%	0.012%
44	8.915	2581	2589	2598	rVB5	5927	9872	0.69%	0.066%
45	9.037	2619	2627	2632	rBV3	4323	5782	0.40%	0.038%
46	9.095	2632	2645	2682	rVB	641138	1074971	75.23%	7.133%
47	9.252	2682	2694	2714	rBV	261377	426511	29.85%	2.830%
48	9.378	2719	2733	2749	rVV	533742	878305	61.47%	5.828%
49	9.445	2749	2754	2768	rVB2	11993	19607	1.37%	0.130%
50	9.718	2832	2839	2846	rBV4	1746	2463	0.17%	0.016%
51	9.783	2847	2859	2879	rVV	188414	303027	21.21%	2.011%
52	9.953	2905	2912	2920	rVV3	3074	4094	0.29%	0.027%
53	10.050	2934	2942	2949	rVV5	2451	3680	0.26%	0.024%
54	10.088	2950	2954	2968	rVB4	1364	2167	0.15%	0.014%
55	10.172	2968	2980	2991	rBV3	4486	7188	0.50%	0.048%
56	10.259	3001	3007	3015	rBV4	1181	1664	0.12%	0.011%
57	10.326	3016	3028	3033	rBV7	2121	3974	0.28%	0.026%
58	10.355	3033	3037	3049	rVB7	2640	3439	0.24%	0.023%
59	10.435	3049	3062	3080	rBV	391164	628936	44.01%	4.173%
60	10.593	3102	3111	3122	rBV2	7327	11351	0.79%	0.075%
61	10.686	3129	3140	3156	rBV	20724	43046	3.01%	0.286%
62	10.776	3156	3168	3174	rVV	10284	16940	1.19%	0.112%
63	10.818	3174	3181	3193	rVB2	17786	26215	1.83%	0.174%
64	10.979	3221	3231	3238	rBV2	7497	11141	0.78%	0.074%
65	11.079	3256	3262	3266	rBV6	1125	1540	0.11%	0.010%
66	11.117	3268	3274	3278	rVV3	4897	6579	0.46%	0.044%
67	11.152	3278	3285	3297	rVB	40096	59923	4.19%	0.398%
68	11.275	3317	3323	3325	rBV2	1626	1765	0.12%	0.012%
69	11.400	3354	3362	3366	rBV6	2505	3588	0.25%	0.024%
70	11.487	3377	3389	3409	rBV	700527	1111559	77.79%	7.376%
71	11.574	3409	3416	3424	rBV	21149	30424	2.13%	0.202%

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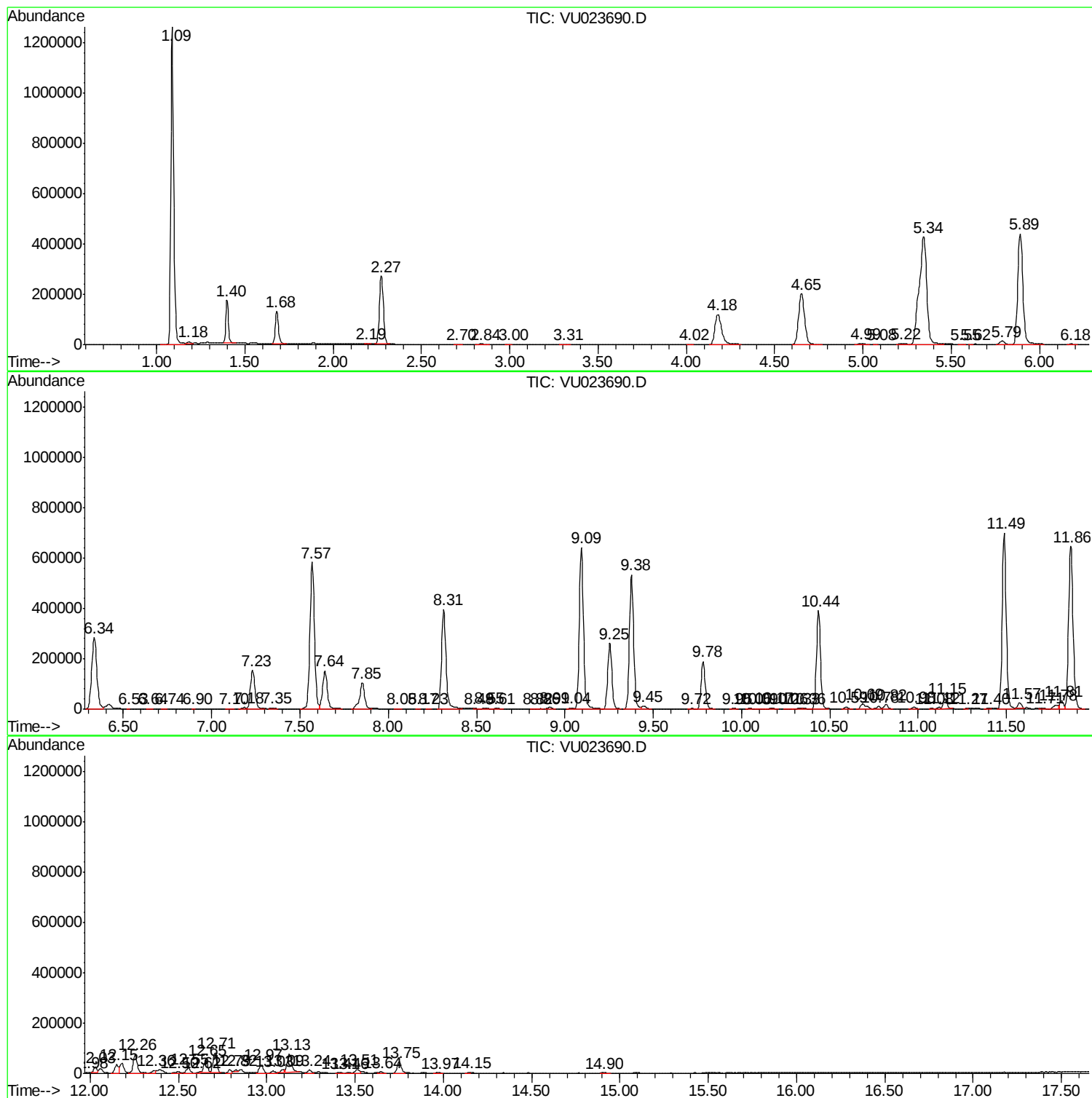
72	11.706	3451	3457	3466	rVB3	4240	5925	0.41%	0.039%
73	11.783	3468	3481	3484	rBV4	14863	26301	1.84%	0.175%
74	11.812	3486	3490	3496	rVV	31262	42213	2.95%	0.280%
75	11.863	3496	3506	3530	rVB	646603	1113817	77.95%	7.391%
76	11.982	3537	3543	3549	rBV5	3100	4661	0.33%	0.031%
77	12.027	3550	3557	3562	rBV	21677	29896	2.09%	0.198%
78	12.149	3585	3595	3599	rBV	35546	49823	3.49%	0.331%
79	12.255	3616	3628	3650	rVB	72899	119679	8.38%	0.794%
80	12.361	3653	3661	3664	rBV3	10368	14183	0.99%	0.094%
81	12.496	3692	3703	3710	rBV7	5822	10067	0.70%	0.067%
82	12.554	3713	3721	3732	rVB	20777	32271	2.26%	0.214%
83	12.622	3734	3742	3743	rBV5	4856	5333	0.37%	0.035%
84	12.654	3744	3752	3760	rVV	51083	78107	5.47%	0.518%
85	12.705	3760	3768	3779	rVB	79678	118610	8.30%	0.787%
86	12.789	3787	3794	3799	rBV3	12449	17000	1.19%	0.113%
87	12.824	3801	3805	3809	rVV3	6401	7045	0.49%	0.047%
88	12.969	3841	3850	3863	rVB3	33718	53435	3.74%	0.355%
89	13.033	3863	3870	3878	rBV3	8408	12139	0.85%	0.081%
90	13.091	3879	3888	3890	rBV4	11692	16277	1.14%	0.108%
91	13.127	3891	3899	3916	rVB3	70344	121959	8.53%	0.809%
92	13.242	3926	3935	3943	rBV	12515	17841	1.25%	0.118%
93	13.410	3981	3987	3996	rVB6	2257	3126	0.22%	0.021%
94	13.458	3998	4002	4010	rVB6	1668	1893	0.13%	0.013%
95	13.512	4010	4019	4025	rBV2	14779	24712	1.73%	0.164%
96	13.644	4054	4060	4069	rVB	5652	7627	0.53%	0.051%
97	13.750	4082	4093	4103	rBV	44955	74567	5.22%	0.495%
98	13.969	4153	4161	4169	rBV6	1488	2711	0.19%	0.018%
99	14.149	4209	4217	4218	rBV4	2822	2874	0.20%	0.019%
100	14.898	4447	4450	4465	rVB4	1282	1594	0.11%	0.011%

Sum of corrected areas: 15070754

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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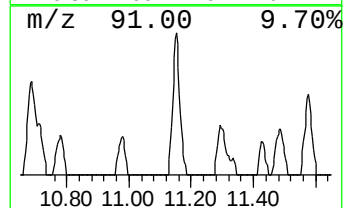
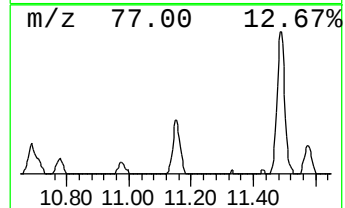
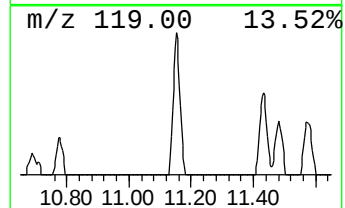
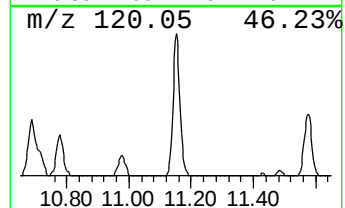
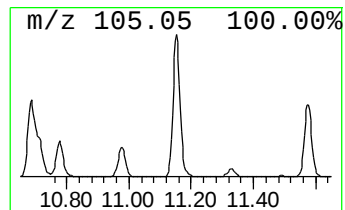
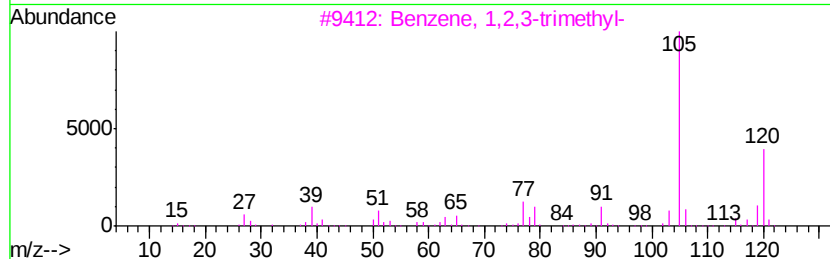
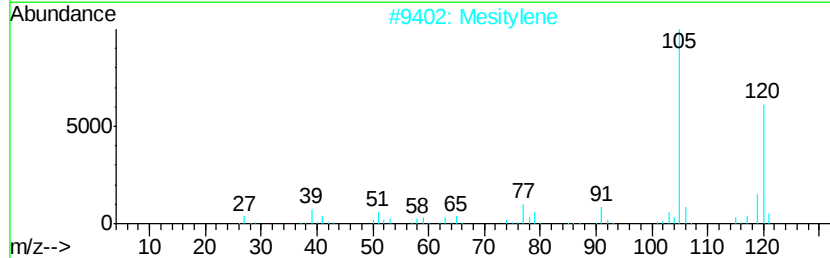
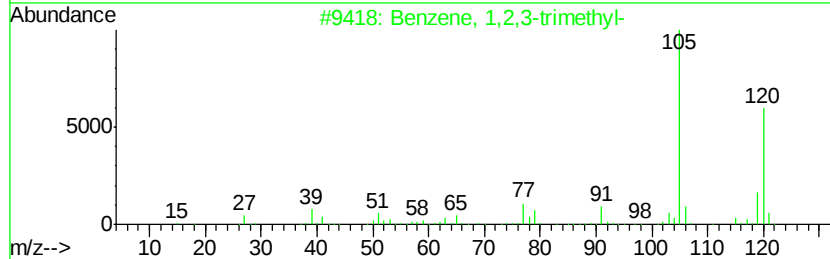
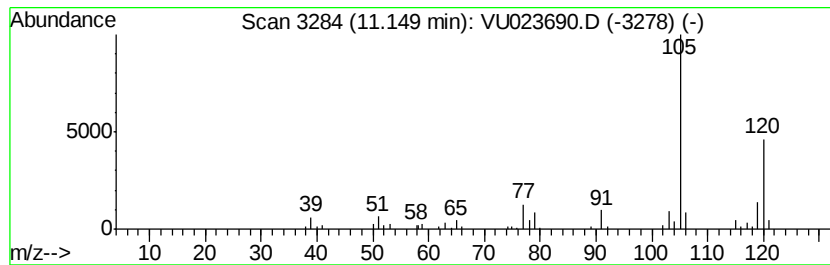
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	2.70 ug/L	59923	1,4-Dichlorobenzene-d4	11.49

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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91	
4	Mesitylene	120	C9H12	000108-67-8	91	
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91	



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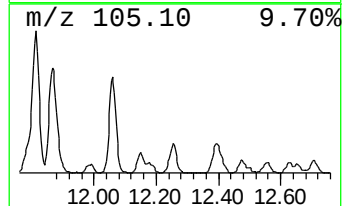
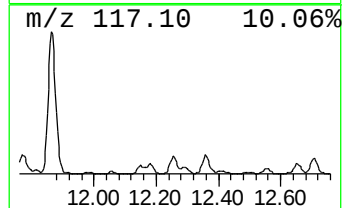
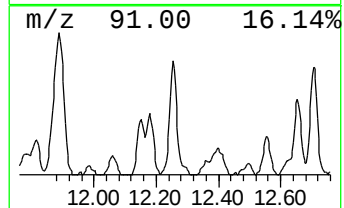
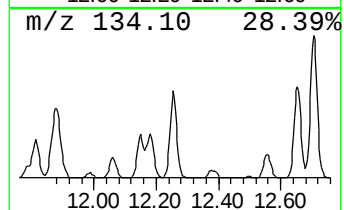
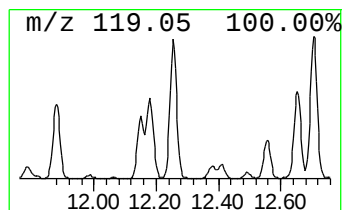
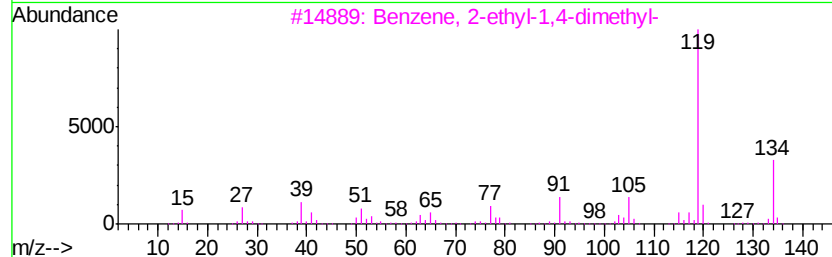
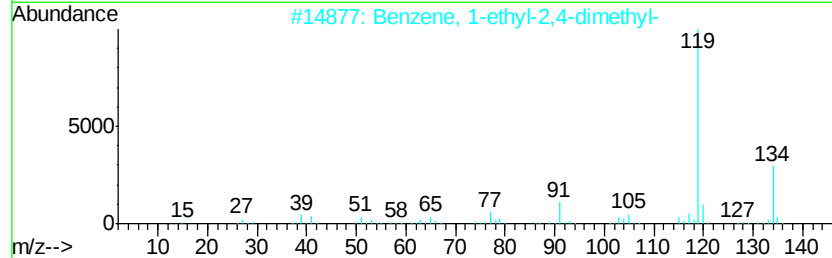
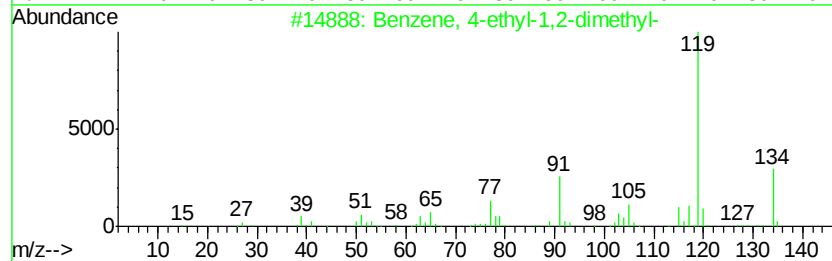
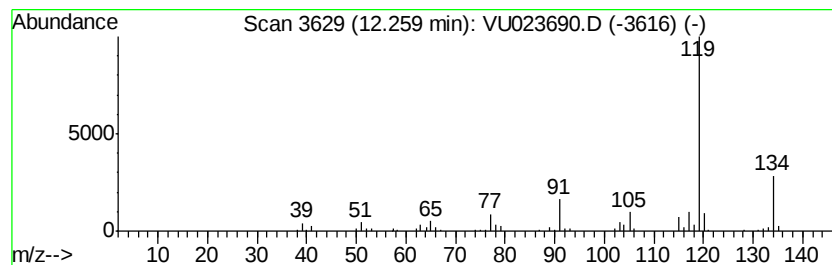
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	5.38 ug/L	119679	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
3		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
4		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5		p-Cymene	134	C10H14	000099-87-6	94



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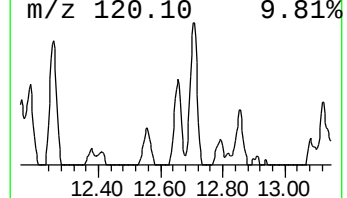
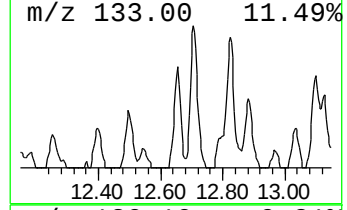
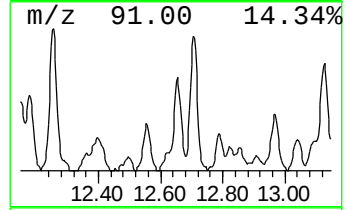
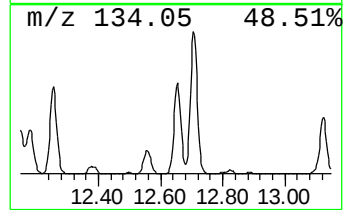
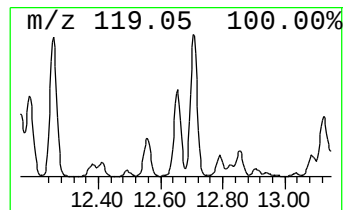
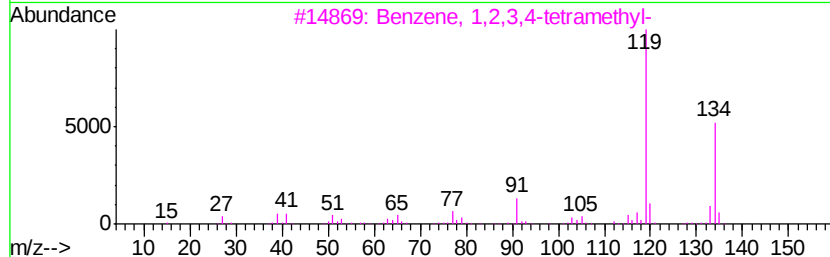
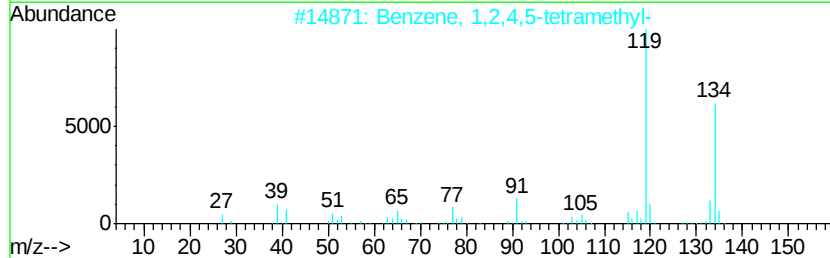
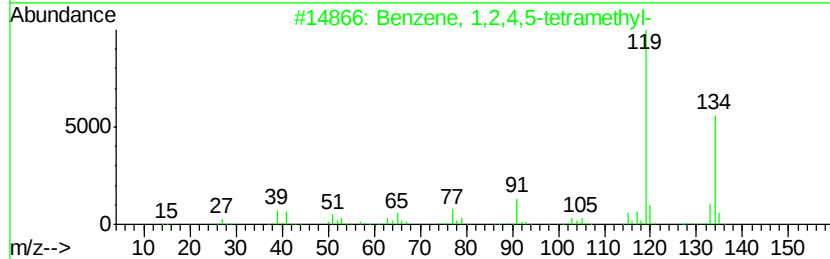
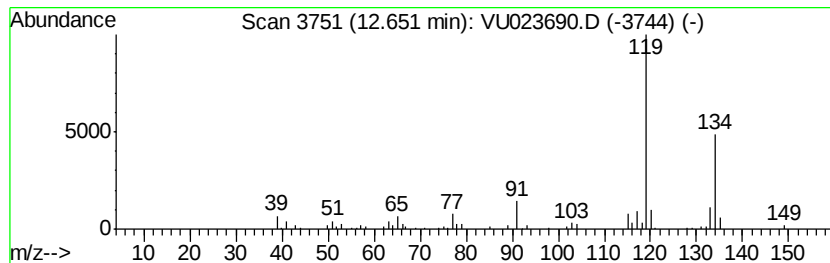
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Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.51 ug/L	78107	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94



Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050618\
Data File : VU023690.D
Acq On : 06 May 2018 15:04
Operator : MD/SY
Sample : J2721-01DL 200X
Misc : 6.42g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

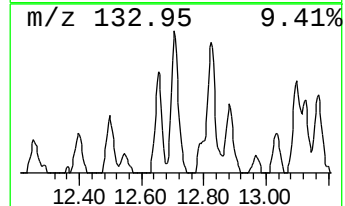
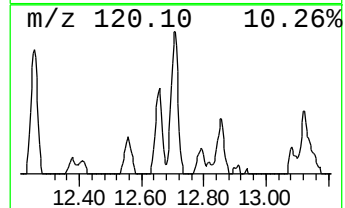
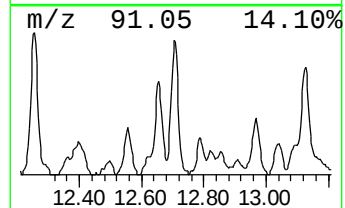
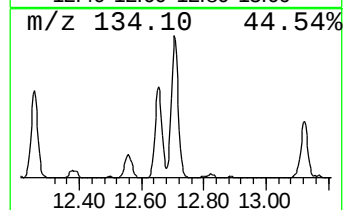
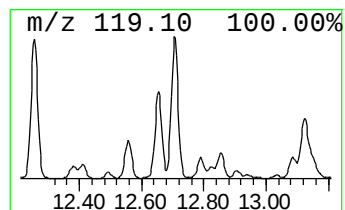
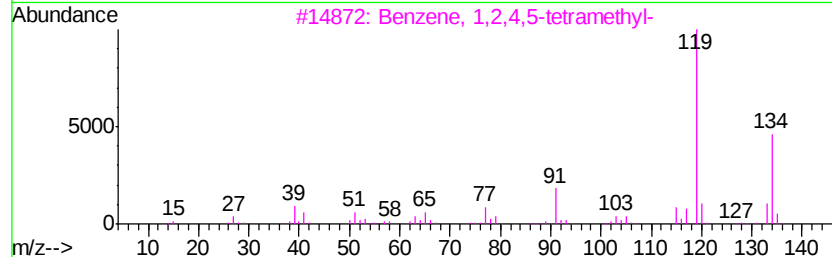
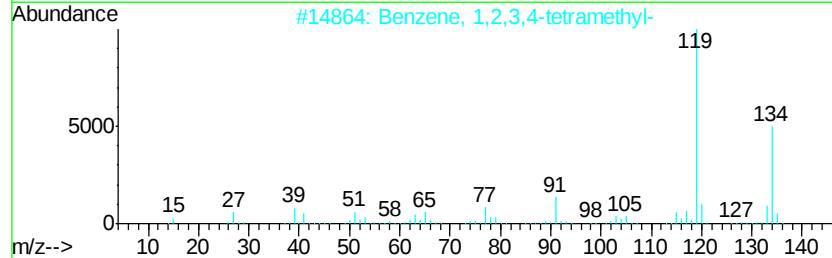
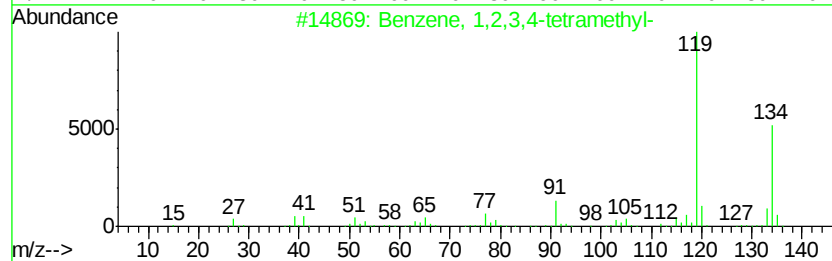
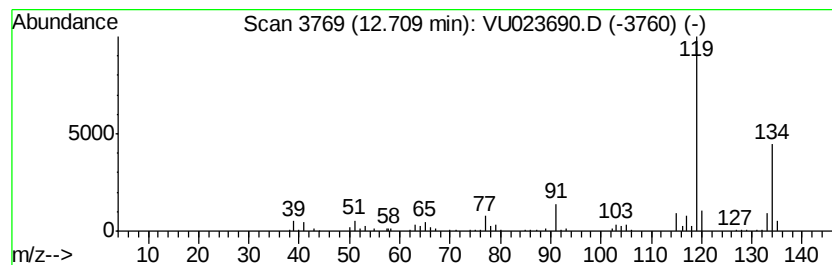
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	5.34 ug/L	118610	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4		o-Cymene	134	C10H14	000527-84-4	95
5		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94



Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050618\
Data File : VU023690.D
Acq On : 06 May 2018 15:04
Operator : MD/SY
Sample : J2721-01DL 200X
Misc : 6.42g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

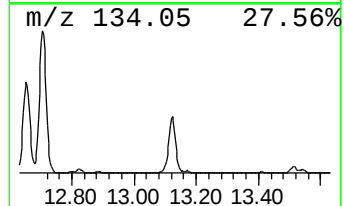
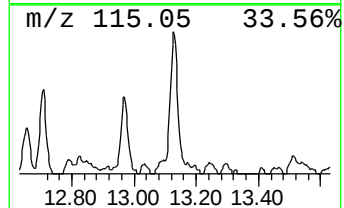
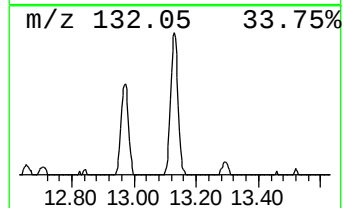
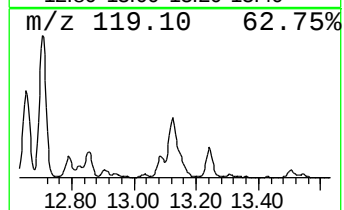
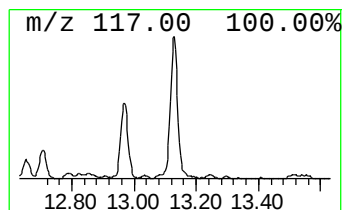
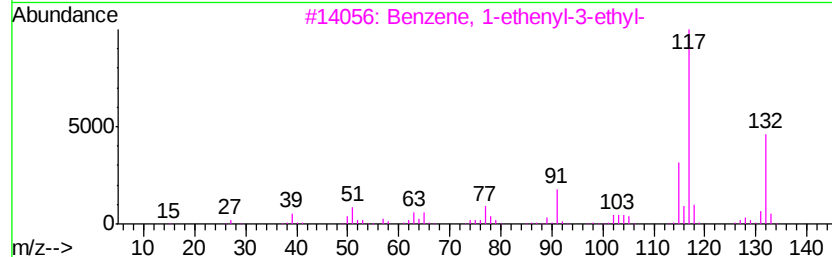
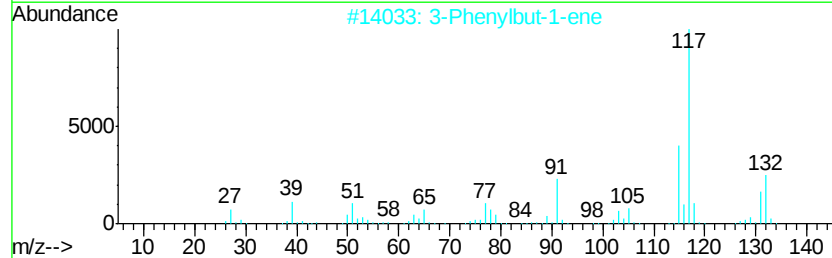
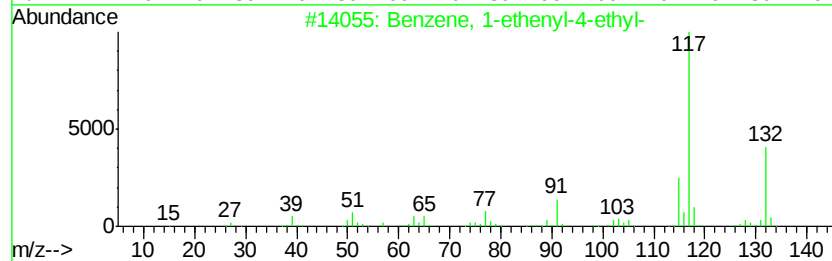
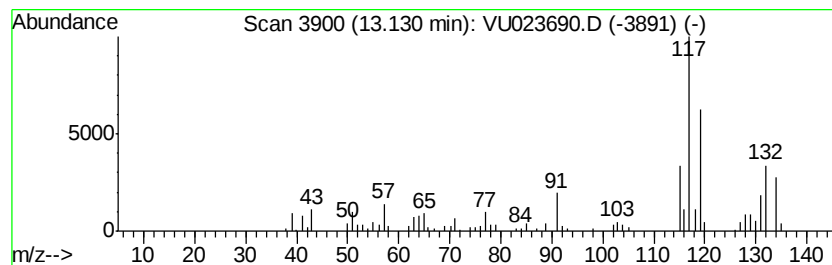
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	5.49 ug/L	121959	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	55
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	55
3		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	49
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	49
5		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	49



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050618\
Data File : VU023690.D
Acq On : 06 May 2018 15:04
Operator : MD/SY
Sample : J2721-01DL 200X
Misc : 6.42g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,2,3-tr...	11.15	2.7	ug/L	59923	3	11.49	1111560	50.0
Benzene, 4-ethyl-...	12.26	5.4	ug/L	119679	3	11.49	1111560	50.0
Benzene, 1,2,4,5-...	12.65	3.5	ug/L	78107	3	11.49	1111560	50.0
Benzene, 1,2,3,4-...	12.71	5.3	ug/L	118610	3	11.49	1111560	50.0
Benzene, 1-etheny...	13.13	5.5	ug/L	121959	3	11.49	1111560	50.0