

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100518\
 Data File : VU027449.D
 Acq On : 05 Oct 2018 13:34
 Operator : MD/SY
 Sample : J5180-20ME
 Misc : 4.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JLC29ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.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	1.395	62	69	85	rVB	78127	102751	12.84%	1.462%
2	1.640	140	145	163	rBV	57253	90866	11.35%	1.293%
3	2.151	297	304	311	rVB4	2038	3176	0.40%	0.045%
4	2.231	318	329	346	rBV	138769	216727	27.08%	3.083%
5	2.344	358	364	375	rVB2	2295	4095	0.51%	0.058%
6	2.437	386	393	405	rVB3	1412	2517	0.31%	0.036%
7	2.566	431	433	436	rVB2	291	149	0.02%	0.002%
8	2.588	436	440	443	rBV2	315	271	0.03%	0.004%
9	2.620	445	450	462	rVV4	1159	2070	0.26%	0.029%
10	2.681	462	469	480	rVB3	2036	3770	0.47%	0.054%
11	2.833	503	516	528	rBV3	4507	9718	1.21%	0.138%
12	3.029	574	577	580	rVB	181	124	0.02%	0.002%
13	3.058	582	586	588	rVB	180	119	0.01%	0.002%
14	3.077	588	592	595	rBV	127	121	0.02%	0.002%
15	3.099	595	599	602	rVB2	145	125	0.02%	0.002%
16	3.161	615	618	623	rVV	167	147	0.02%	0.002%
17	3.196	623	629	632	rVV2	183	217	0.03%	0.003%
18	3.273	643	653	663	rVB6	1745	3349	0.42%	0.048%
19	3.402	689	693	696	rBV2	195	129	0.02%	0.002%
20	3.424	696	700	702	rBV	160	160	0.02%	0.002%
21	3.640	764	767	772	rVB2	186	164	0.02%	0.002%
22	3.884	839	843	845	rVV	197	137	0.02%	0.002%
23	4.199	926	941	994	rBV3	41043	187428	23.42%	2.666%
24	4.488	1027	1031	1033	rBV2	224	188	0.02%	0.003%
25	4.643	1062	1079	1111	rVV	102892	268571	33.56%	3.820%
26	4.810	1120	1131	1135	rBV2	484	821	0.10%	0.012%
27	4.942	1168	1172	1173	rBV	563	372	0.05%	0.005%
28	4.961	1174	1178	1179	rVV	990	782	0.10%	0.011%
29	4.974	1179	1182	1188	rVB3	1249	1088	0.14%	0.015%
30	5.331	1270	1293	1319	rVV3	248743	718768	89.81%	10.224%
31	5.498	1342	1345	1348	rVB	260	205	0.03%	0.003%
32	5.620	1381	1383	1390	rVB	147	138	0.02%	0.002%
33	5.675	1397	1400	1408	rVB	94	128	0.02%	0.002%
34	5.781	1423	1433	1437	rBV2	1102	1535	0.19%	0.022%

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 ClientSampleId :
 JLC29ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
 Title : VOC Analysis

35	5.881	1449	1464	1488	rBV	264019	558411	69.77%	7.943%
36	6.164	1550	1552	1554	rBV	278	153	0.02%	0.002%
37	6.215	1563	1568	1572	rVB	124	132	0.02%	0.002%
38	6.328	1589	1603	1626	rBV	156162	339525	42.42%	4.829%
39	6.450	1637	1641	1643	rBV	256	159	0.02%	0.002%
40	6.466	1643	1646	1648	rVB	275	126	0.02%	0.002%
41	6.495	1653	1655	1657	rVB2	252	123	0.02%	0.002%
42	6.826	1752	1758	1761	rBV	120	123	0.02%	0.002%
43	6.887	1767	1777	1788	rBV7	2107	4778	0.60%	0.068%
44	7.038	1818	1824	1827	rVB2	219	197	0.02%	0.003%
45	7.083	1836	1838	1843	rVB2	153	135	0.02%	0.002%
46	7.157	1858	1861	1863	rBV	186	121	0.02%	0.002%
47	7.170	1863	1865	1871	rVB3	444	347	0.04%	0.005%
48	7.228	1871	1883	1905	rBV	84392	169127	21.13%	2.406%
49	7.334	1910	1916	1926	rVB5	1545	2692	0.34%	0.038%
50	7.389	1926	1933	1939	rVB2	202	330	0.04%	0.005%
51	7.562	1963	1987	2004	rBV	302195	558351	69.77%	7.942%
52	7.639	2005	2011	2025	rVB2	7244	13092	1.64%	0.186%
53	7.742	2038	2043	2045	rBV2	323	291	0.04%	0.004%
54	7.852	2059	2077	2100	rVV	57777	119825	14.97%	1.704%
55	8.125	2158	2162	2169	rBV3	547	657	0.08%	0.009%
56	8.186	2169	2181	2186	rBV5	2519	5192	0.65%	0.074%
57	8.231	2189	2195	2203	rVB6	1727	3093	0.39%	0.044%
58	8.328	2213	2225	2253	rVB	229097	432035	53.98%	6.145%
59	8.614	2302	2314	2329	rBV	3612	11064	1.38%	0.157%
60	8.675	2331	2333	2338	rVB3	754	593	0.07%	0.008%
61	8.736	2349	2352	2353	rBV2	538	246	0.03%	0.003%
62	8.758	2353	2359	2365	rVB6	1415	2128	0.27%	0.030%
63	8.803	2369	2373	2374	rBV2	627	468	0.06%	0.007%
64	8.848	2381	2387	2388	rBV4	2175	2020	0.25%	0.029%
65	8.909	2399	2406	2415	rVB5	3529	5550	0.69%	0.079%
66	8.951	2415	2419	2422	rBV2	277	258	0.03%	0.004%
67	9.032	2434	2444	2451	rBV5	3835	6429	0.80%	0.091%
68	9.093	2451	2463	2488	rVV	405519	712720	89.06%	10.138%
69	9.196	2492	2495	2497	rBV3	802	520	0.06%	0.007%
70	9.254	2505	2513	2525	rVB4	6703	11370	1.42%	0.162%
71	9.318	2531	2533	2535	rVB2	379	143	0.02%	0.002%

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Instrument :
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 ClientSampleId :
 JLC29ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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 Title : VOC Analysis

72	9.379	2537	2552	2566	rBV	18472	36177	4.52%	0.515%
73	9.453	2567	2575	2577	rBV5	3075	4185	0.52%	0.060%
74	9.569	2601	2611	2616	rBV4	2034	3080	0.38%	0.044%
75	9.591	2616	2618	2622	rVB2	194	136	0.02%	0.002%
76	9.655	2632	2638	2645	rBV7	1807	2787	0.35%	0.040%
77	9.717	2649	2657	2666	rBV7	6855	11024	1.38%	0.157%
78	9.784	2672	2678	2685	rBV2	6708	9517	1.19%	0.135%
79	9.922	2712	2721	2722	rBV4	3822	4275	0.53%	0.061%
80	10.154	2789	2793	2806	rVB8	5034	9164	1.15%	0.130%
81	10.253	2807	2824	2833	rBV6	8619	17500	2.19%	0.249%
82	10.369	2852	2860	2870	rVB2	18467	32382	4.05%	0.461%
83	10.437	2870	2881	2893	rBV	240996	398953	49.85%	5.675%
84	10.684	2950	2958	2973	rBV	17978	41528	5.19%	0.591%
85	10.774	2979	2986	2994	rVB2	24323	33400	4.17%	0.475%
86	10.977	3040	3049	3057	rBV	18505	32642	4.08%	0.464%
87	11.118	3087	3093	3096	rBV4	5015	5789	0.72%	0.082%
88	11.154	3097	3104	3114	rVB3	18684	27782	3.47%	0.395%
89	11.276	3134	3142	3147	rBV4	5435	9215	1.15%	0.131%
90	11.392	3169	3178	3185	rBV3	19362	30366	3.79%	0.432%
91	11.434	3186	3191	3197	rVV4	10770	13534	1.69%	0.193%
92	11.488	3197	3208	3227	rVB	511657	800312	100.00%	11.384%
93	11.575	3227	3235	3244	rBV	27634	38521	4.81%	0.548%
94	11.784	3289	3300	3303	rBV4	18638	30888	3.86%	0.439%
95	11.864	3315	3325	3344	rVB2	397711	681080	85.10%	9.688%
96	12.147	3408	3413	3415	rBV4	4781	5015	0.63%	0.071%
97	12.179	3418	3423	3431	rVB3	15463	22141	2.77%	0.315%
98	12.356	3474	3478	3485	rBV2	9098	13293	1.66%	0.189%
99	12.704	3579	3586	3594	rBV	34814	54605	6.82%	0.777%
100	13.125	3710	3717	3736	rBV4	42578	77495	9.68%	1.102%

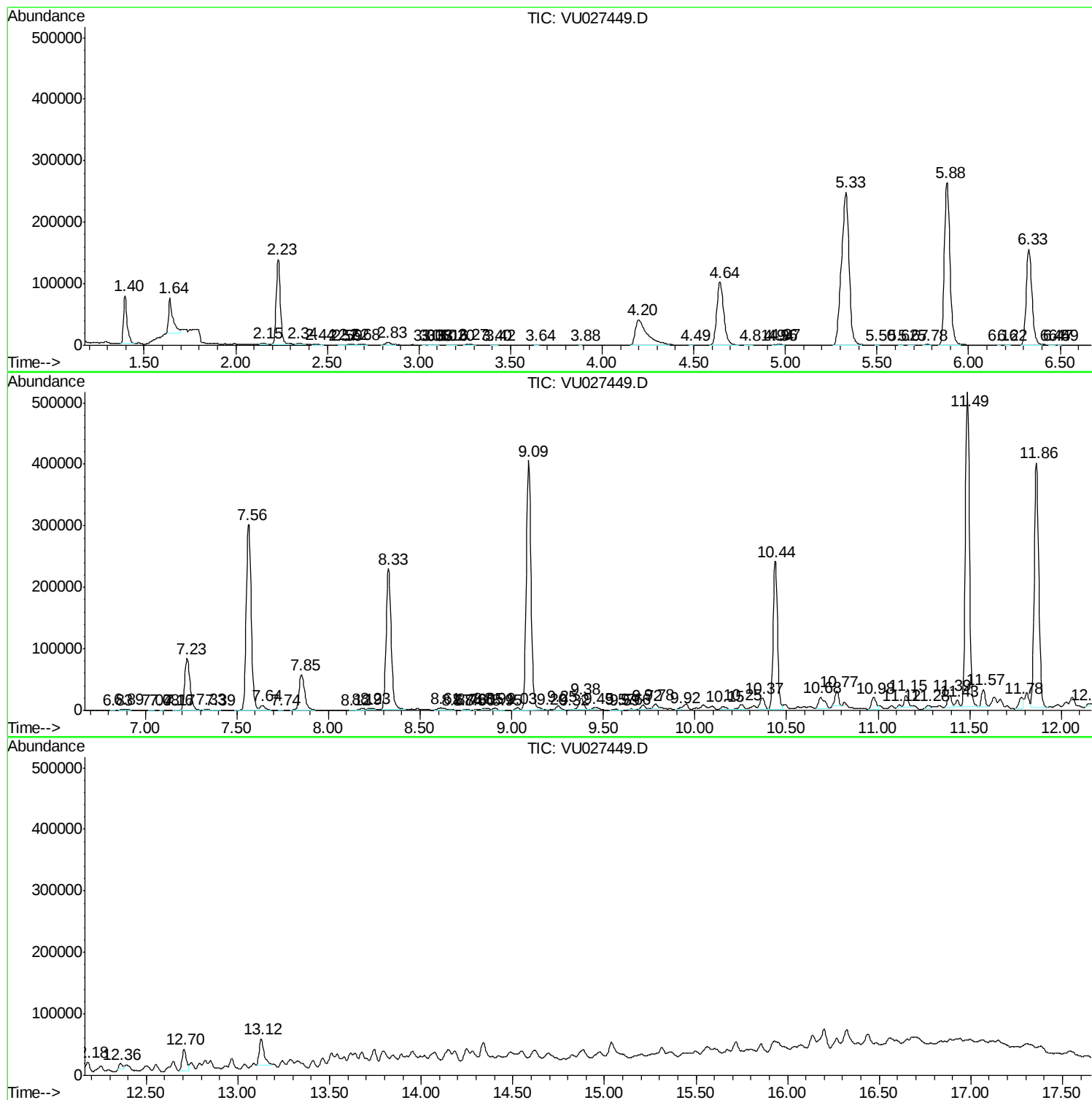
Sum of corrected areas: 7030236

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Misc : 4.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
JLC29ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JLC29ME

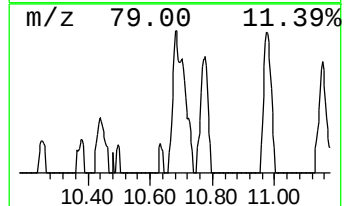
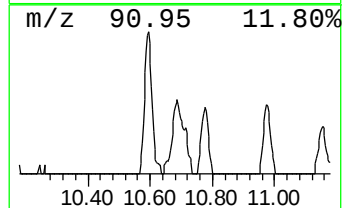
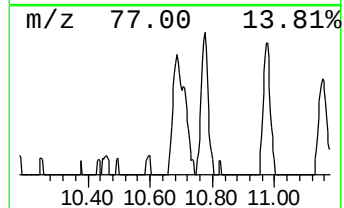
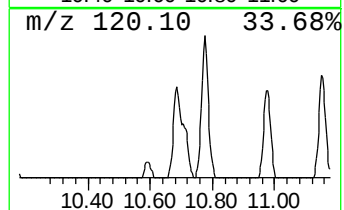
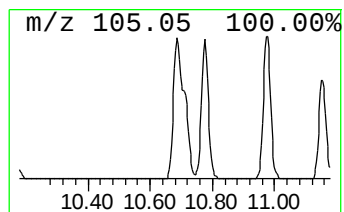
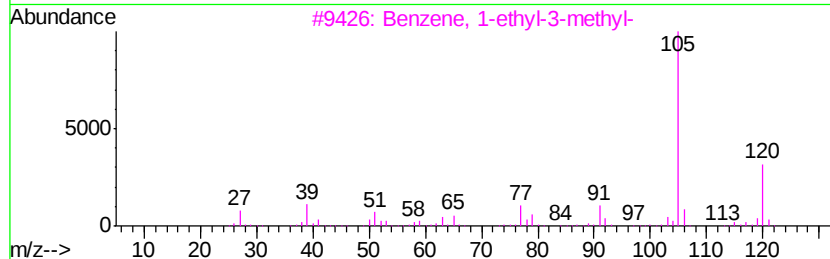
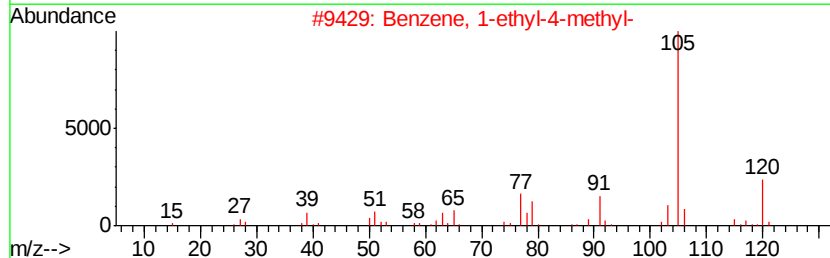
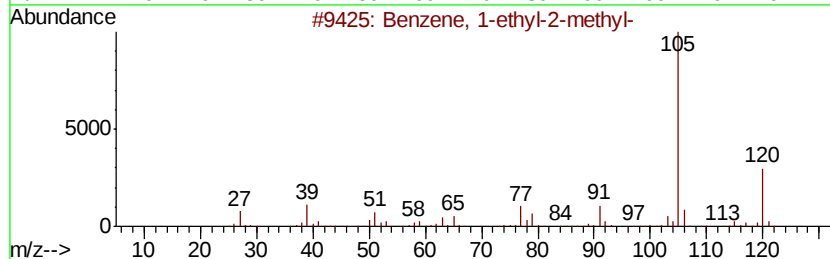
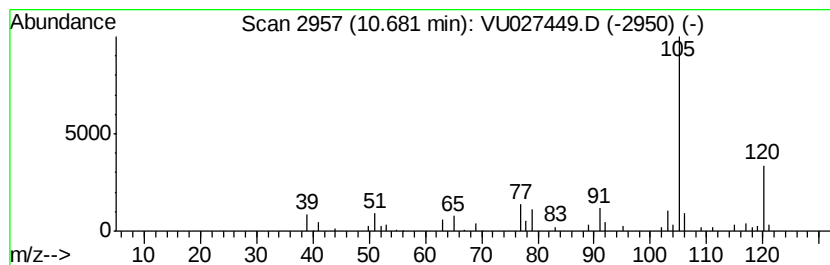
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.59 ug/L	41528	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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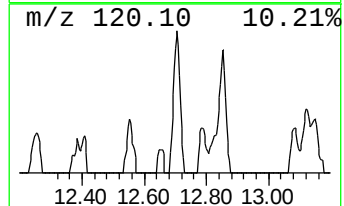
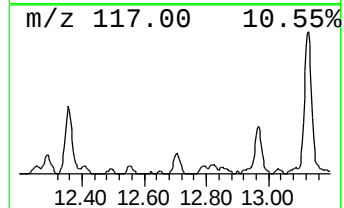
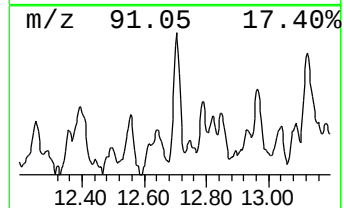
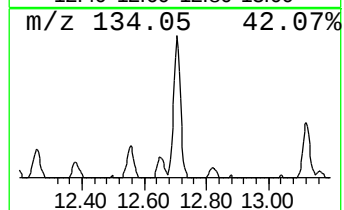
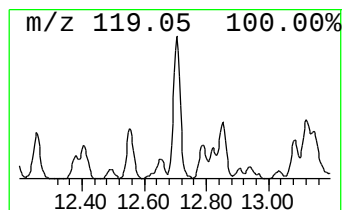
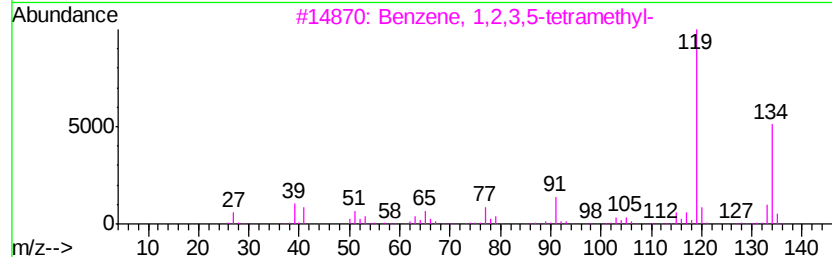
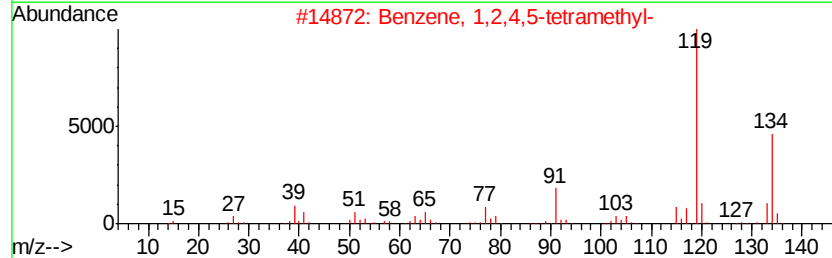
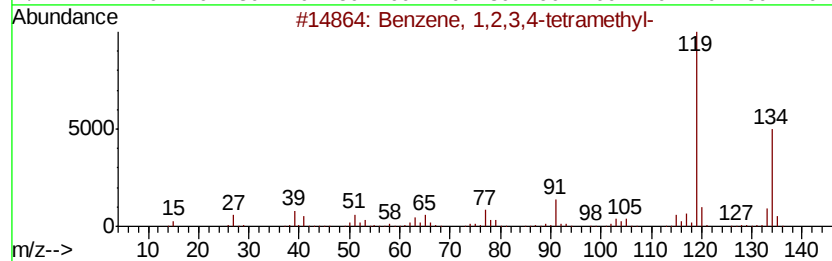
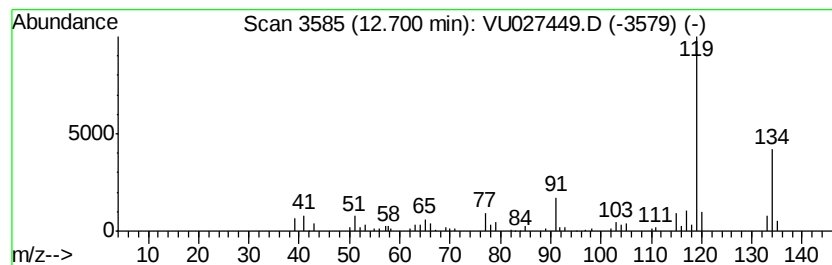
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.41 ug/L	54605	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
5		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95



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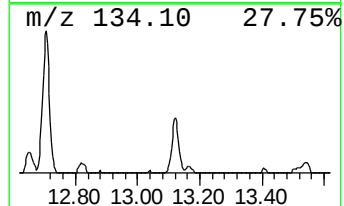
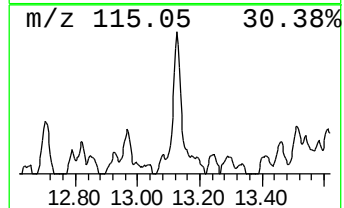
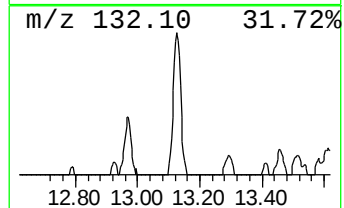
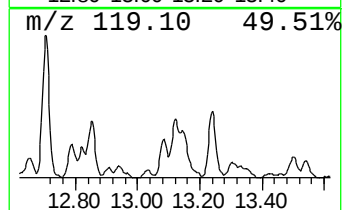
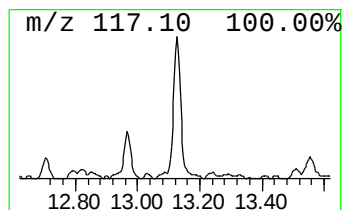
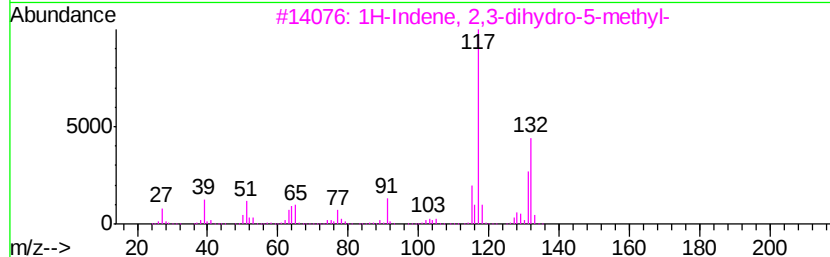
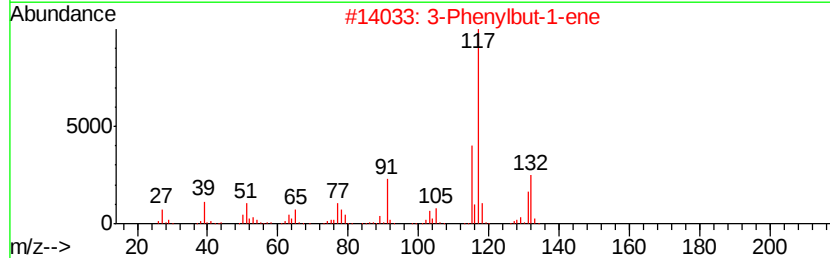
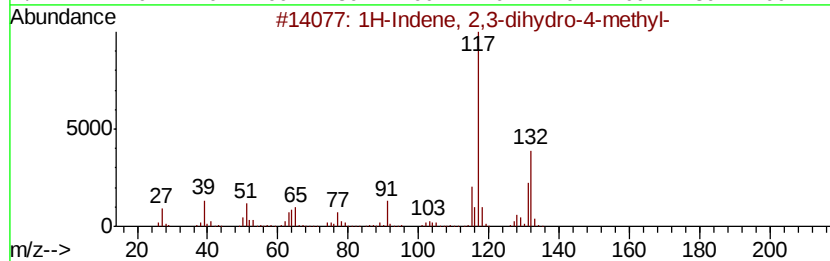
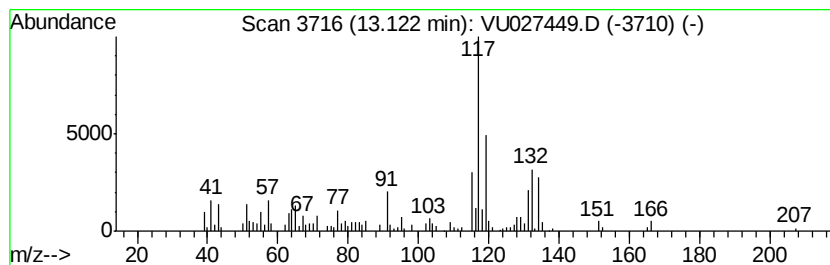
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	4.84 ug/L	77495	1,4-Dichlorobenzene-d4	11.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	64
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	58
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100518\
Data File : VU027449.D
Acq On : 05 Oct 2018 13:34
Operator : MD/SY
Sample : J5180-20ME
Misc : 4.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JLC29ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.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-ethyl-...	10.68	2.6	ug/L	41528	3	11.49	800312	50.0
Benzene, 1,2,3,4-...	12.70	3.4	ug/L	54605	3	11.49	800312	50.0
1H-Indene, 2,3-di...	13.12	4.8	ug/L	77495	3	11.49	800312	50.0