

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122718\
 Data File : VU028963.D
 Acq On : 27 Dec 2018 12:44
 Operator : MD/SY
 Sample : J6506-01ME
 Misc : 6.05g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEZX8ME

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\SOMULM122018WMA.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	82	rVB	78433	92810	11.96%	1.285%
2	2.231	319	329	344	rVB	164173	254011	32.74%	3.516%
3	2.347	357	365	375	rBV6	2153	4276	0.55%	0.059%
4	2.588	438	440	444	rBV2	270	252	0.03%	0.003%
5	2.623	444	451	461	rVV2	2430	4269	0.55%	0.059%
6	2.829	504	515	531	rVB	8699	18518	2.39%	0.256%
7	2.977	558	561	564	rBV2	288	177	0.02%	0.002%
8	2.996	564	567	570	rVV2	296	169	0.02%	0.002%
9	3.064	585	588	591	rBV	193	145	0.02%	0.002%
10	3.115	601	604	609	rVB	222	142	0.02%	0.002%
11	3.144	611	613	616	rVB	176	105	0.01%	0.001%
12	3.424	697	700	705	rBV	132	116	0.01%	0.002%
13	3.504	723	725	728	rBV	198	112	0.01%	0.002%
14	3.665	769	775	778	rBV	114	134	0.02%	0.002%
15	3.910	848	851	854	rBV	131	106	0.01%	0.001%
16	3.929	854	857	861	rVB2	309	208	0.03%	0.003%
17	4.135	917	921	924	rVB2	169	102	0.01%	0.001%
18	4.192	924	939	975	rBV2	56145	191631	24.70%	2.652%
19	4.546	1045	1049	1055	rBV2	181	261	0.03%	0.004%
20	4.639	1062	1078	1102	rBV	123541	295770	38.13%	4.094%
21	4.781	1119	1122	1126	rVB	170	108	0.01%	0.001%
22	4.887	1148	1155	1159	rBV2	509	706	0.09%	0.010%
23	4.974	1177	1182	1184	rBV3	602	482	0.06%	0.007%
24	5.041	1199	1203	1207	rVB	150	161	0.02%	0.002%
25	5.138	1230	1233	1236	rVB2	171	135	0.02%	0.002%
26	5.328	1269	1292	1320	rBV2	276813	775778	100.00%	10.738%
27	5.610	1371	1380	1382	rBV3	1454	1501	0.19%	0.021%
28	5.736	1415	1419	1422	rBV2	241	231	0.03%	0.003%
29	5.881	1449	1464	1499	rBV	259960	535405	69.02%	7.411%
30	6.070	1520	1523	1526	rBV3	235	144	0.02%	0.002%
31	6.106	1532	1534	1536	rBV	252	144	0.02%	0.002%
32	6.183	1548	1558	1571	rBV4	7156	13402	1.73%	0.185%
33	6.250	1573	1579	1588	rVV4	1587	2674	0.34%	0.037%
34	6.324	1588	1602	1627	rVV	167127	347573	44.80%	4.811%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Title : VOC Analysis

35	6.459	1642	1644	1649	rVB3	525	390	0.05%	0.005%
36	6.482	1649	1651	1657	rVB	137	112	0.01%	0.002%
37	6.553	1669	1673	1676	rBV	234	159	0.02%	0.002%
38	6.565	1676	1677	1682	rVB	219	114	0.01%	0.002%
39	6.601	1685	1688	1691	rVB2	161	119	0.02%	0.002%
40	6.623	1691	1695	1697	rVB	166	101	0.01%	0.001%
41	6.646	1697	1702	1703	rBV	188	134	0.02%	0.002%
42	6.884	1768	1776	1778	rBV3	789	879	0.11%	0.012%
43	6.971	1800	1803	1805	rBV	163	116	0.01%	0.002%
44	7.070	1831	1834	1837	rVB	181	101	0.01%	0.001%
45	7.122	1846	1850	1853	rVB	276	169	0.02%	0.002%
46	7.160	1857	1862	1864	rBV2	288	230	0.03%	0.003%
47	7.225	1870	1882	1910	rVB	95911	186410	24.03%	2.580%
48	7.331	1914	1915	1919	rVB	343	145	0.02%	0.002%
49	7.353	1919	1922	1925	rVB2	327	214	0.03%	0.003%
50	7.456	1947	1954	1955	rBV2	330	351	0.05%	0.005%
51	7.562	1974	1987	2013	rBV	348931	642499	82.82%	8.893%
52	7.848	2066	2076	2105	rBV	63336	123843	15.96%	1.714%
53	8.025	2127	2131	2135	rBV2	342	334	0.04%	0.005%
54	8.067	2142	2144	2148	rBV	125	105	0.01%	0.001%
55	8.093	2148	2152	2155	rBV2	160	143	0.02%	0.002%
56	8.173	2168	2177	2181	rBV3	572	812	0.10%	0.011%
57	8.225	2181	2193	2211	rBV	124129	214428	27.64%	2.968%
58	8.324	2211	2224	2250	rBV	241321	477274	61.52%	6.606%
59	8.633	2314	2320	2329	rVB4	1175	1944	0.25%	0.027%
60	8.694	2334	2339	2343	rBV2	245	260	0.03%	0.004%
61	8.739	2351	2353	2358	rVB	147	133	0.02%	0.002%
62	8.861	2389	2391	2394	rVV	305	184	0.02%	0.003%
63	8.884	2396	2398	2405	rVB	218	130	0.02%	0.002%
64	9.003	2432	2435	2438	rBV	157	137	0.02%	0.002%
65	9.089	2449	2462	2486	rBV	368376	661186	85.23%	9.152%
66	9.234	2505	2507	2511	rBV3	350	289	0.04%	0.004%
67	9.324	2531	2535	2538	rVB2	199	151	0.02%	0.002%
68	9.372	2547	2550	2551	rBV	446	269	0.03%	0.004%
69	9.530	2595	2599	2602	rBV	256	153	0.02%	0.002%
70	9.784	2671	2678	2681	rBV2	450	514	0.07%	0.007%
71	9.884	2705	2709	2714	rBV	169	154	0.02%	0.002%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE
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 Title : VOC Analysis

72	9.925	2718	2722	2725	rVV2	192	138	0.02%	0.002%
73	10.157	2790	2794	2796	rBV2	396	356	0.05%	0.005%
74	10.250	2821	2823	2827	rVB2	228	127	0.02%	0.002%
75	10.437	2868	2881	2898	rBV	295119	476156	61.38%	6.590%
76	10.607	2924	2934	2946	rBV4	3500	5726	0.74%	0.079%
77	10.665	2949	2952	2953	rBV	386	169	0.02%	0.002%
78	10.835	2997	3005	3014	rVB5	3793	6338	0.82%	0.088%
79	10.877	3015	3018	3023	rVB	238	210	0.03%	0.003%
80	10.909	3023	3028	3035	rBV2	1014	1384	0.18%	0.019%
81	10.999	3052	3056	3057	rBV	300	176	0.02%	0.002%
82	11.218	3122	3124	3127	rBV2	283	178	0.02%	0.002%
83	11.324	3151	3157	3160	rBV2	236	280	0.04%	0.004%
84	11.366	3168	3170	3173	rVB	278	115	0.01%	0.002%
85	11.427	3181	3189	3195	rBV3	639	806	0.10%	0.011%
86	11.485	3195	3207	3228	rBV	429240	680766	87.75%	9.423%
87	11.810	3294	3308	3313	rBV2	14206	23694	3.05%	0.328%
88	11.861	3314	3324	3345	rVB	422858	707613	91.21%	9.794%
89	12.147	3403	3413	3418	rBV	17631	27641	3.56%	0.383%
90	12.250	3436	3445	3460	rVB	41457	61678	7.95%	0.854%
91	12.395	3476	3490	3505	rVB6	14960	35886	4.63%	0.497%
92	12.482	3505	3517	3529	rBV5	11378	23867	3.08%	0.330%
93	12.552	3532	3539	3551	rVB	11375	16292	2.10%	0.225%
94	12.700	3578	3585	3596	rVB	66387	95550	12.32%	1.323%
95	12.784	3604	3611	3616	rBV	24193	34665	4.47%	0.480%
96	12.964	3659	3667	3679	rVB2	30908	46872	6.04%	0.649%
97	13.031	3681	3688	3696	rBV	14434	19615	2.53%	0.271%
98	13.083	3696	3704	3710	rBV3	25447	44248	5.70%	0.612%
99	13.237	3744	3752	3762	rBV	28217	41342	5.33%	0.572%
100	13.507	3828	3836	3843	rBV3	9623	16559	2.13%	0.229%

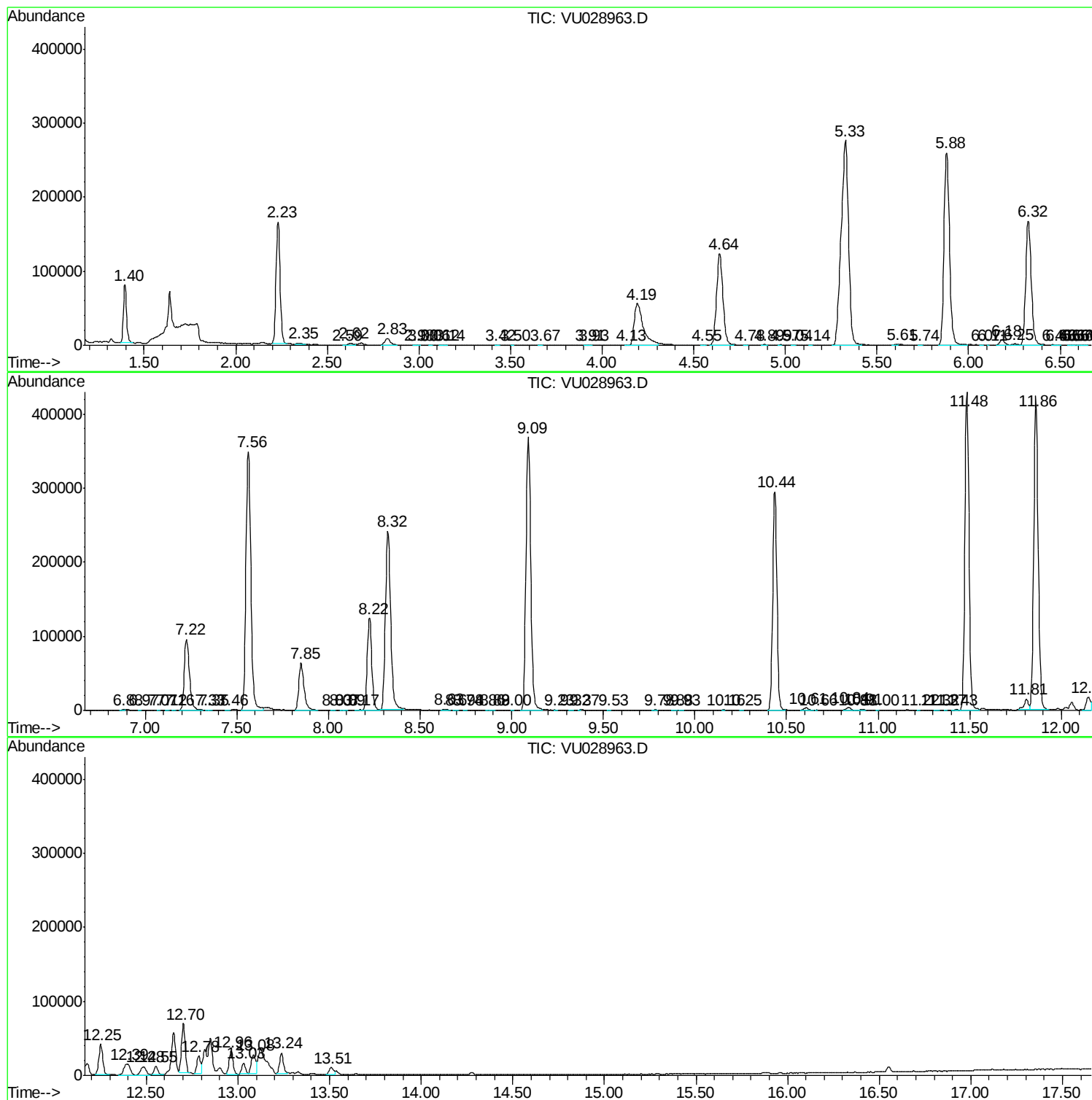
Sum of corrected areas: 7224891

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Instrument :
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ClientSampled :
BEZX8ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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ClientSampleId :
BEZX8ME

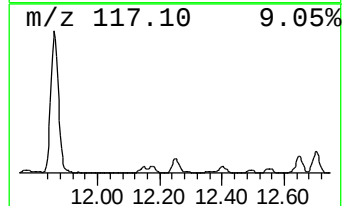
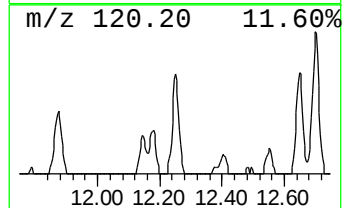
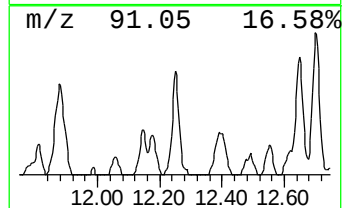
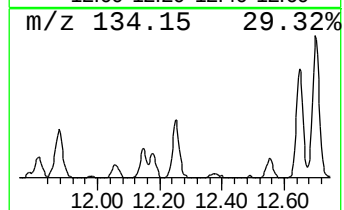
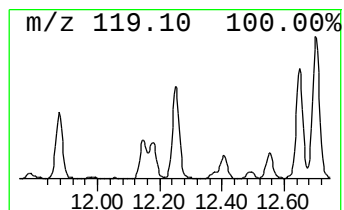
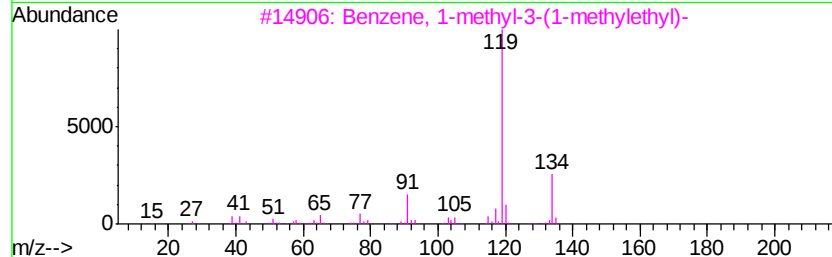
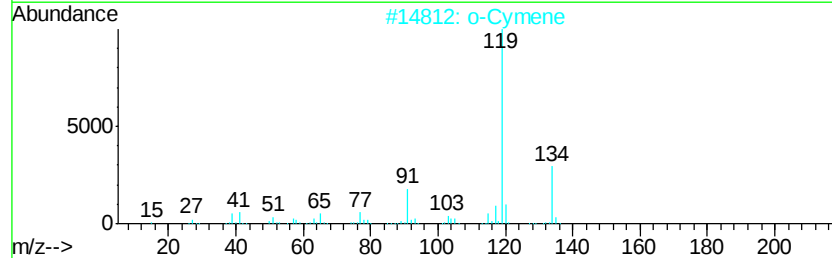
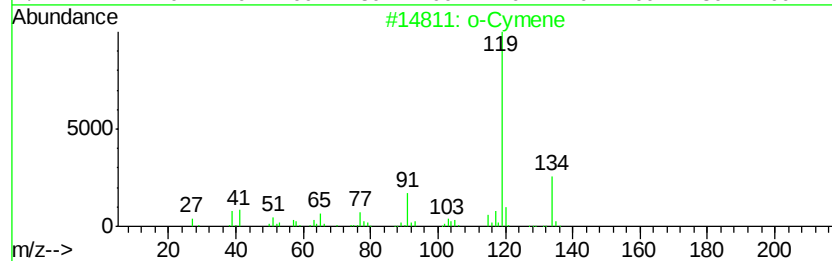
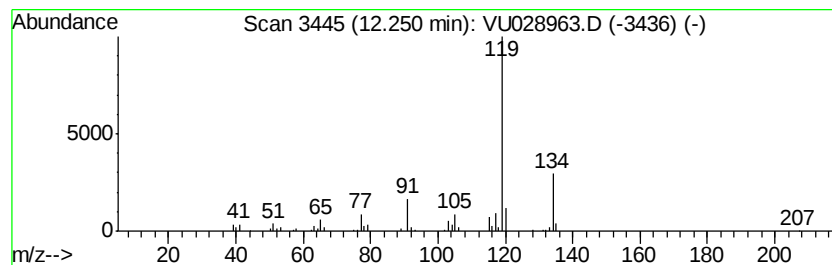
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 o-Cymene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	4.53 ug/L	61678	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	97
2		o-Cymene	134	C10H14	000527-84-4	97
3		Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95
4		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5		Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	95



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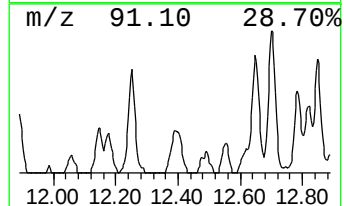
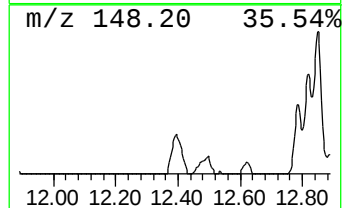
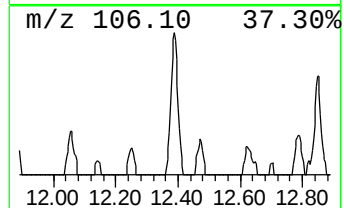
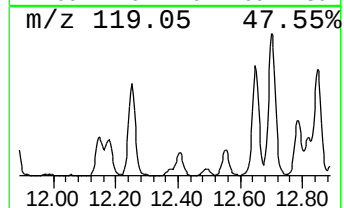
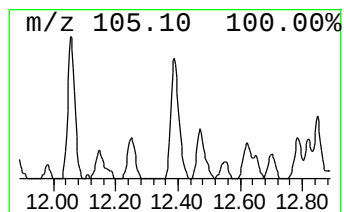
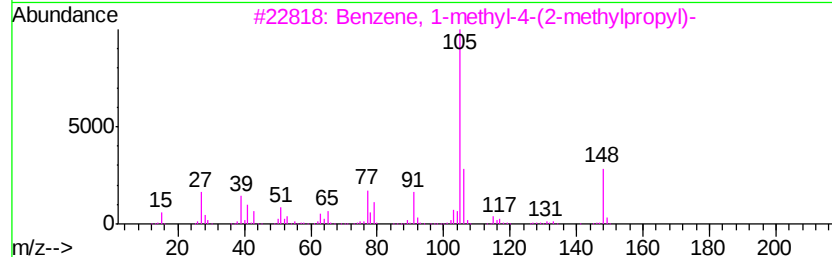
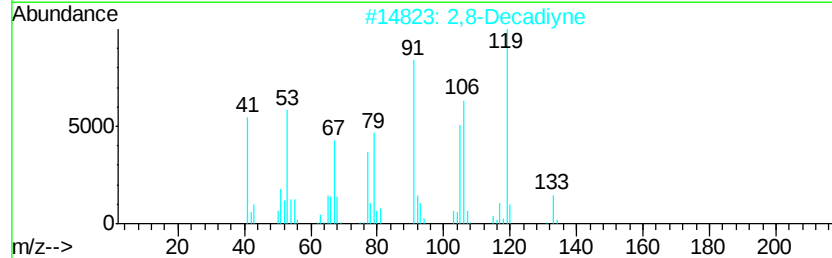
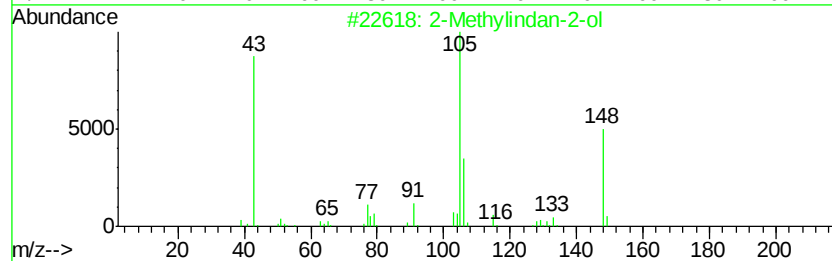
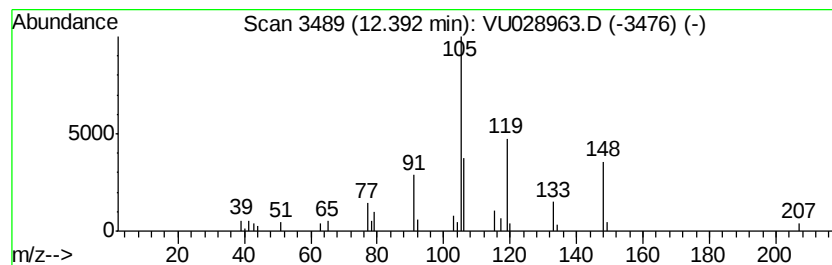
Instrument :
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ClientSampleId :
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.39	2.64 ug/L	35886	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindan-2-ol	148	C10H12O	033223-84-6	49
2	2,8-Decadiyne	134	C10H14	004116-93-2	47
3	Benzene, 1-methyl-4-(2-methylpro...	148	C11H16	005161-04-6	47
4	Benzene, (2-methoxy-2-propenyl)-	148	C10H12O	026473-60-9	46
5	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	43



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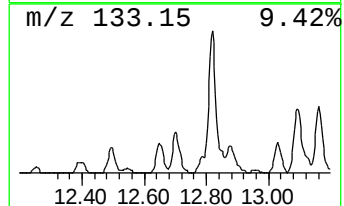
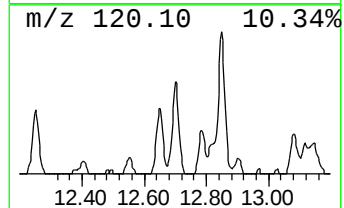
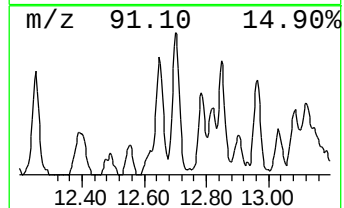
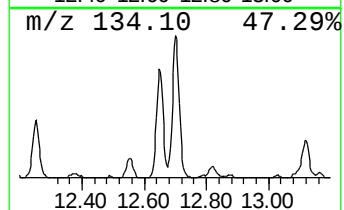
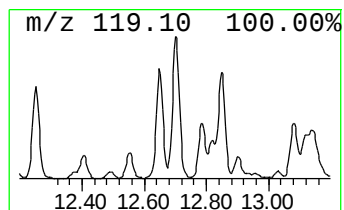
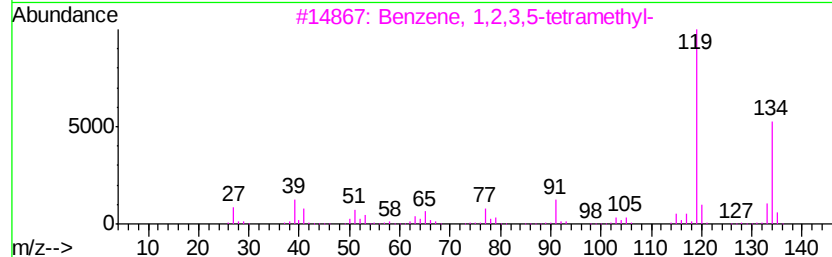
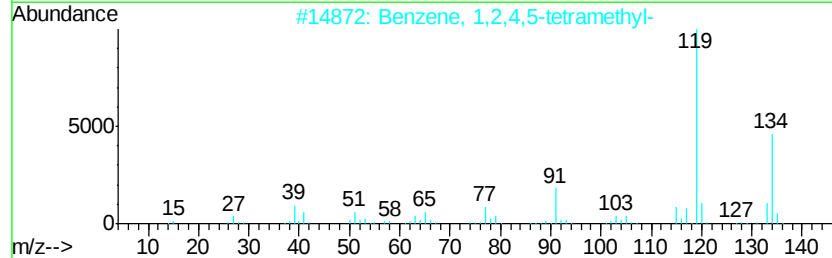
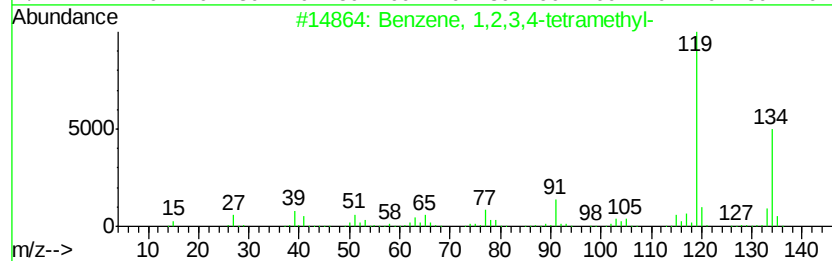
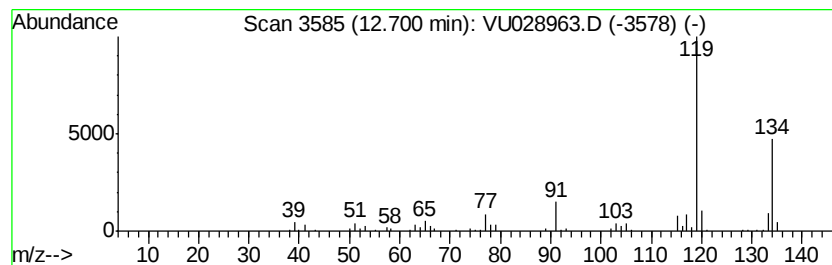
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	7.02 ug/L	95550	1,4-Dichlorobenzene-d4	11.48

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU122718\
Data File : VU028963.D
Acq On : 27 Dec 2018 12:44
Operator : MD/SY
Sample : J6506-01ME
Misc : 6.05a/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEZX8ME

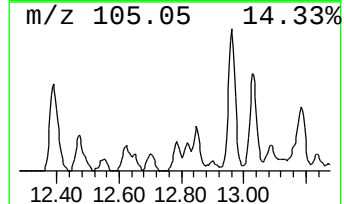
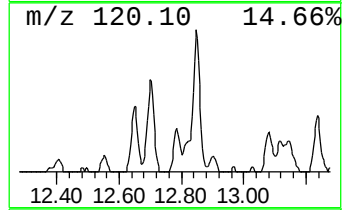
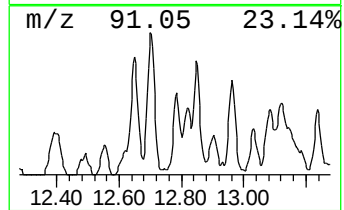
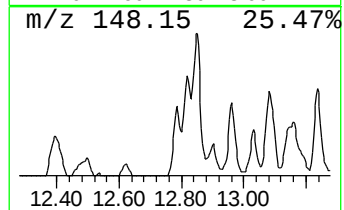
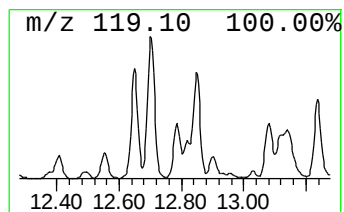
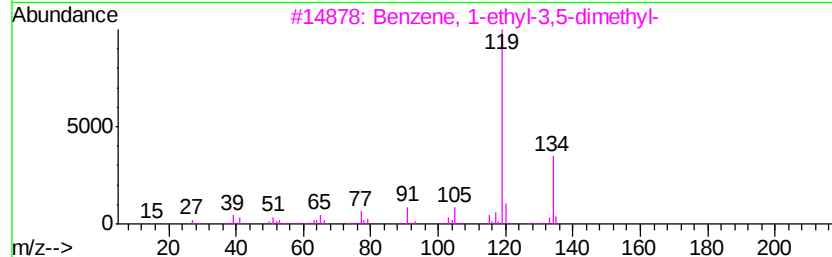
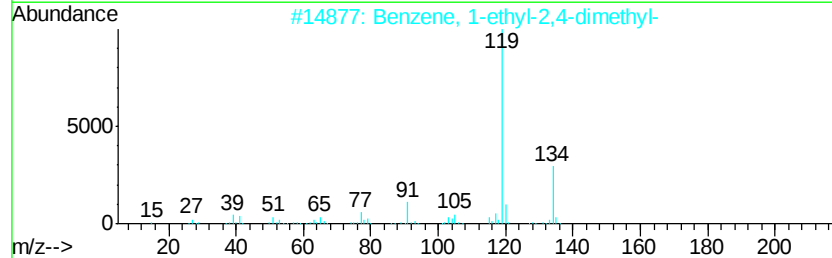
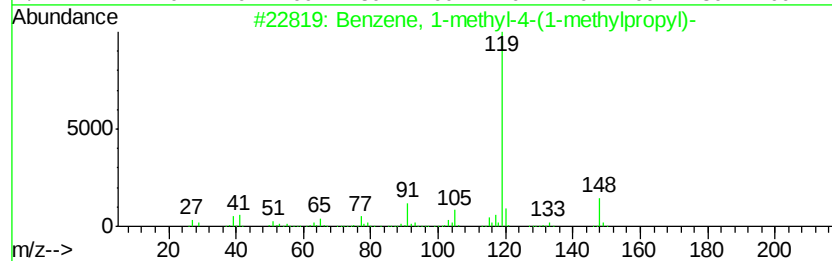
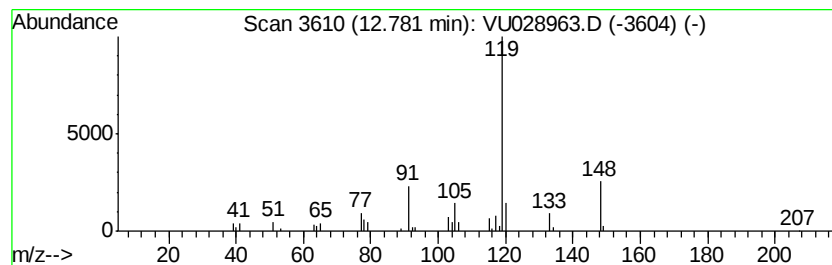
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Quant Title : VOC Analysis

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

Peak Number 5 Benzene, 1-methyl-4-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.55 ug/L	34665	1,4-Dichlorobenzene-d4	11.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene,	1-methyl-4-(1-methylpro...	148	C11H16		001595-16-0	87
2	Benzene,	1-ethyl-2,4-dimethyl-	134	C10H14		000874-41-9	68
3	Benzene,	1-ethyl-3,5-dimethyl-	134	C10H14		000934-74-7	68
4	o-Cymene		134	C10H14		000527-84-4	64
5	Benzene,	(1,1-dimethylpropyl)-	148	C11H16		002049-95-8	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU122718\
 Data File : VU028963.D
 Acq On : 27 Dec 2018 12:44
 Operator : MD/SY
 Sample : J6506-01ME
 Misc : 6.05µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEZX8ME

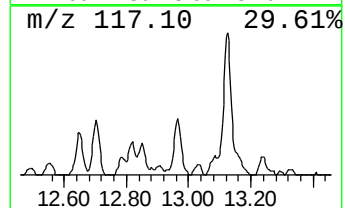
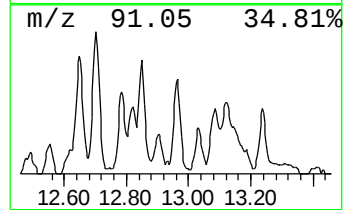
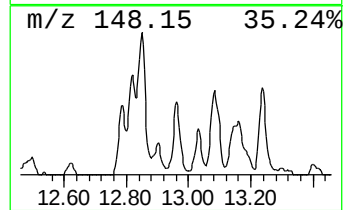
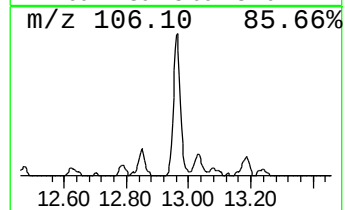
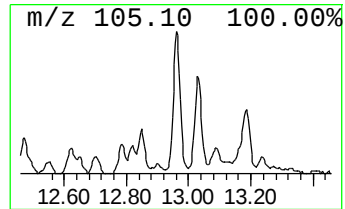
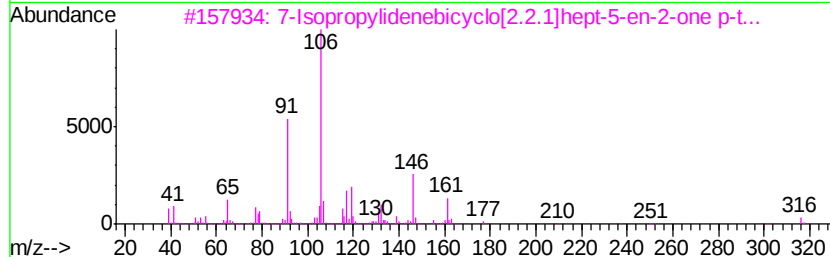
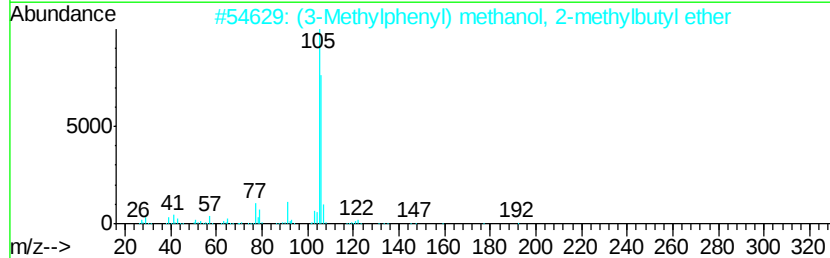
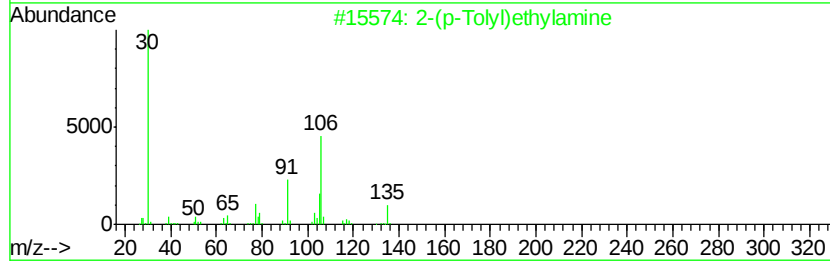
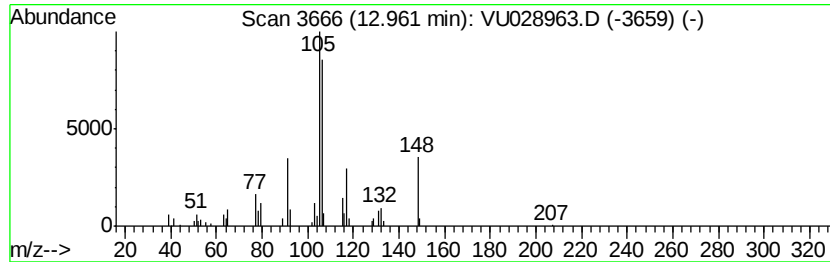
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Quant Title : VOC Analysis

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

 Peak Number 6 2-(p-Tolyl)ethylamine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	3.44 ug/L	46872	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	50
2		(3-Methylphenyl) methanol, 2-met...	192	C13H20O	1000374-43-9	47
3		7-Isopropylidenebicvclo[2.2.1]he...	316	C17H20N2O2S	165401-76-3	47
4		Benzene, (1-cyclohexylethyl)-	188	C14H20	004413-16-5	47
5		Benzene, 1-methyl-4-(2-methylpro...	148	C11H16	005161-04-6	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU122718\
Data File : VU028963.D
Acq On : 27 Dec 2018 12:44
Operator : MD/SY
Sample : J6506-01ME
Misc : 6.05g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEZX8ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.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
o-Cymene	12.25	4.5	ug/L	61678	3	11.48	680766	50.0
unknown-01	12.39	2.6	ug/L	35886	3	11.48	680766	50.0
Benzene, 1,2,3,4-...	12.70	7.0	ug/L	95550	3	11.48	680766	50.0
Benzene, 1-methyl...	12.78	2.5	ug/L	34665	3	11.48	680766	50.0
2-(p-Tolyl)ethyla...	12.96	3.4	ug/L	46872	3	11.48	680766	50.0