

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021519\
 Data File : VU029494.D
 Acq On : 15 Feb 2019 13:49
 Operator : JC/SP
 Sample : K1455-01 20X
 Misc : 4.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE801

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\SOMULM021519WMA.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	1.183	23	29	37	rBV	5962	6382	0.06%	0.022%
2	1.395	88	95	110	rBV	245574	264270	2.48%	0.918%
3	1.672	174	181	199	rVB	191378	249424	2.34%	0.867%
4	2.267	356	366	381	rVB	427025	642349	6.02%	2.232%
5	2.476	423	431	441	rBV	2569	4351	0.04%	0.015%
6	2.698	492	500	508	rVB5	2739	4319	0.04%	0.015%
7	2.739	508	513	517	rBV4	628	651	0.01%	0.002%
8	2.833	539	542	544	rBV3	693	424	0.00%	0.001%
9	2.981	578	588	600	rBV6	4342	8768	0.08%	0.030%
10	3.170	645	647	652	rVB2	406	335	0.00%	0.001%
11	3.209	654	659	666	rVB2	352	440	0.00%	0.002%
12	3.444	721	732	747	rVV2	6029	13901	0.13%	0.048%
13	3.505	747	751	754	rVV	411	337	0.00%	0.001%
14	3.739	822	824	829	rVV2	335	335	0.00%	0.001%
15	3.958	889	892	899	rBV3	367	431	0.00%	0.001%
16	4.051	917	921	925	rBV3	331	330	0.00%	0.001%
17	4.109	936	939	942	rBV2	486	324	0.00%	0.001%
18	4.222	946	974	1004	rBV3	543283	1618149	15.16%	5.624%
19	4.399	1027	1029	1034	rVB4	773	405	0.00%	0.001%
20	4.473	1049	1052	1055	rBV3	650	508	0.00%	0.002%
21	4.537	1069	1072	1076	rVB2	583	368	0.00%	0.001%
22	4.643	1087	1105	1132	rBV	229570	577995	5.41%	2.009%
23	4.910	1174	1188	1203	rVV5	15598	39470	0.37%	0.137%
24	4.990	1203	1213	1225	rVB7	2024	4155	0.04%	0.014%
25	5.132	1255	1257	1262	rVB3	576	461	0.00%	0.002%
26	5.215	1275	1283	1293	rVB5	1146	2064	0.02%	0.007%
27	5.334	1293	1320	1356	rBV2	504221	1490004	13.96%	5.178%
28	5.527	1377	1380	1386	rVB3	687	614	0.01%	0.002%
29	5.553	1386	1388	1393	rVB2	684	413	0.00%	0.001%
30	5.579	1393	1396	1398	rBV3	605	378	0.00%	0.001%
31	5.669	1421	1424	1427	rVB4	530	348	0.00%	0.001%
32	5.681	1427	1428	1434	rVB3	604	467	0.00%	0.002%
33	5.714	1434	1438	1443	rBV2	373	425	0.00%	0.001%
34	5.781	1453	1459	1465	rBV4	1437	1824	0.02%	0.006%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
 Title : VOC Analysis

35	5.881	1474	1490	1523	rBV	470330	942090	8.82%	3.274%
36	6.183	1568	1584	1605	rBV	198560	398260	3.73%	1.384%
37	6.328	1614	1629	1646	rBV	325471	651757	6.10%	2.265%
38	6.534	1689	1693	1699	rVB4	1120	1205	0.01%	0.004%
39	6.636	1722	1725	1728	rBV2	406	353	0.00%	0.001%
40	6.907	1805	1809	1813	rBV5	980	1069	0.01%	0.004%
41	7.103	1864	1870	1873	rBV5	979	1101	0.01%	0.004%
42	7.177	1884	1893	1897	rBV5	4433	7182	0.07%	0.025%
43	7.225	1897	1908	1934	rVV	206340	371790	3.48%	1.292%
44	7.341	1937	1944	1956	rVB5	4728	9099	0.09%	0.032%
45	7.460	1978	1981	1984	rBV2	657	575	0.01%	0.002%
46	7.562	1991	2013	2028	rBV	767848	1350969	12.65%	4.695%
47	7.845	2083	2101	2116	rBV	142346	253548	2.37%	0.881%
48	8.042	2153	2162	2170	rBV9	2947	5097	0.05%	0.018%
49	8.112	2179	2184	2186	rBV3	359	389	0.00%	0.001%
50	8.160	2194	2199	2204	rVV5	1437	1916	0.02%	0.007%
51	8.225	2204	2219	2235	rVV	6428501	10676831	100.00%	37.107%
52	8.308	2236	2245	2279	rVB	464493	849392	7.96%	2.952%
53	8.450	2284	2289	2293	rBV3	5269	6240	0.06%	0.022%
54	8.543	2309	2318	2326	rVB4	10052	18087	0.17%	0.063%
55	8.607	2326	2338	2346	rBV5	11959	24375	0.23%	0.085%
56	8.717	2368	2372	2373	rBV3	571	404	0.00%	0.001%
57	8.810	2393	2401	2406	rBV2	6952	12080	0.11%	0.042%
58	8.906	2425	2431	2444	rVB2	21910	35451	0.33%	0.123%
59	9.029	2460	2469	2476	rBV4	18845	30665	0.29%	0.107%
60	9.086	2476	2487	2509	rVV2	743789	1442850	13.51%	5.015%
61	9.247	2526	2537	2550	rBV	112656	182842	1.71%	0.635%
62	9.373	2563	2576	2592	rBV	228409	415913	3.90%	1.445%
63	9.562	2627	2635	2646	rVB7	6575	11094	0.10%	0.039%
64	9.646	2654	2661	2667	rBV7	3246	5329	0.05%	0.019%
65	9.717	2670	2683	2692	rVV6	30415	64109	0.60%	0.223%
66	9.778	2693	2702	2722	rVB	80940	152050	1.42%	0.528%
67	9.951	2737	2756	2765	rBV5	44259	91663	0.86%	0.319%
68	10.041	2777	2784	2793	rBV5	33174	55392	0.52%	0.193%
69	10.160	2812	2821	2830	rVB5	23918	43439	0.41%	0.151%
70	10.225	2833	2841	2846	rBV6	12727	22393	0.21%	0.078%
71	10.427	2894	2904	2917	rBV	530865	864839	8.10%	3.006%

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72	10.588	2945	2954	2961	rBV	39488	60548	0.57%	0.210%
73	10.681	2976	2983	2987	rBV2	48907	74371	0.70%	0.258%
74	10.971	3065	3073	3081	rBV3	44353	75231	0.70%	0.261%
75	11.112	3111	3117	3119	rBV2	29177	34050	0.32%	0.118%
76	11.144	3120	3127	3153	rVB	289739	494174	4.63%	1.717%
77	11.482	3222	3232	3251	rVB	852067	1452838	13.61%	5.049%
78	11.569	3252	3259	3267	rVB	67289	91138	0.85%	0.317%
79	11.775	3312	3323	3328	rBV4	30985	60650	0.57%	0.211%
80	11.858	3338	3349	3371	rVB	937120	1662291	15.57%	5.777%
81	12.144	3430	3438	3442	rBV2	36448	52324	0.49%	0.182%
82	12.247	3463	3470	3479	rVB	57028	81668	0.76%	0.284%
83	12.356	3496	3504	3508	rBV3	18209	29969	0.28%	0.104%
84	12.617	3575	3585	3586	rBV7	14216	17352	0.16%	0.060%
85	12.646	3589	3594	3603	rVV	49759	75441	0.71%	0.262%
86	12.701	3603	3611	3628	rVB	69384	117009	1.10%	0.407%
87	12.787	3629	3638	3643	rBV3	15974	24575	0.23%	0.085%
88	12.887	3662	3669	3676	rBV5	13220	19149	0.18%	0.067%
89	12.961	3686	3692	3706	rVB3	22589	35198	0.33%	0.122%
90	13.032	3706	3714	3720	rBV3	9305	13663	0.13%	0.047%
91	13.083	3722	3730	3734	rBV3	10863	17576	0.16%	0.061%
92	13.118	3735	3741	3758	rVB3	34140	64111	0.60%	0.223%
93	13.237	3771	3778	3786	rBV	9999	16385	0.15%	0.057%
94	13.408	3824	3831	3838	rBV7	5074	8306	0.08%	0.029%
95	13.456	3841	3846	3851	rVB5	4659	5618	0.05%	0.020%
96	13.504	3851	3861	3870	rBV2	60125	100700	0.94%	0.350%
97	13.704	3918	3923	3925	rBV4	2176	2241	0.02%	0.008%
98	13.742	3925	3935	3960	rVB	71578	141918	1.33%	0.493%
99	13.948	3995	3999	4001	rBV4	3370	2890	0.03%	0.010%
100	14.479	4157	4164	4171	rVB8	2962	4364	0.04%	0.015%

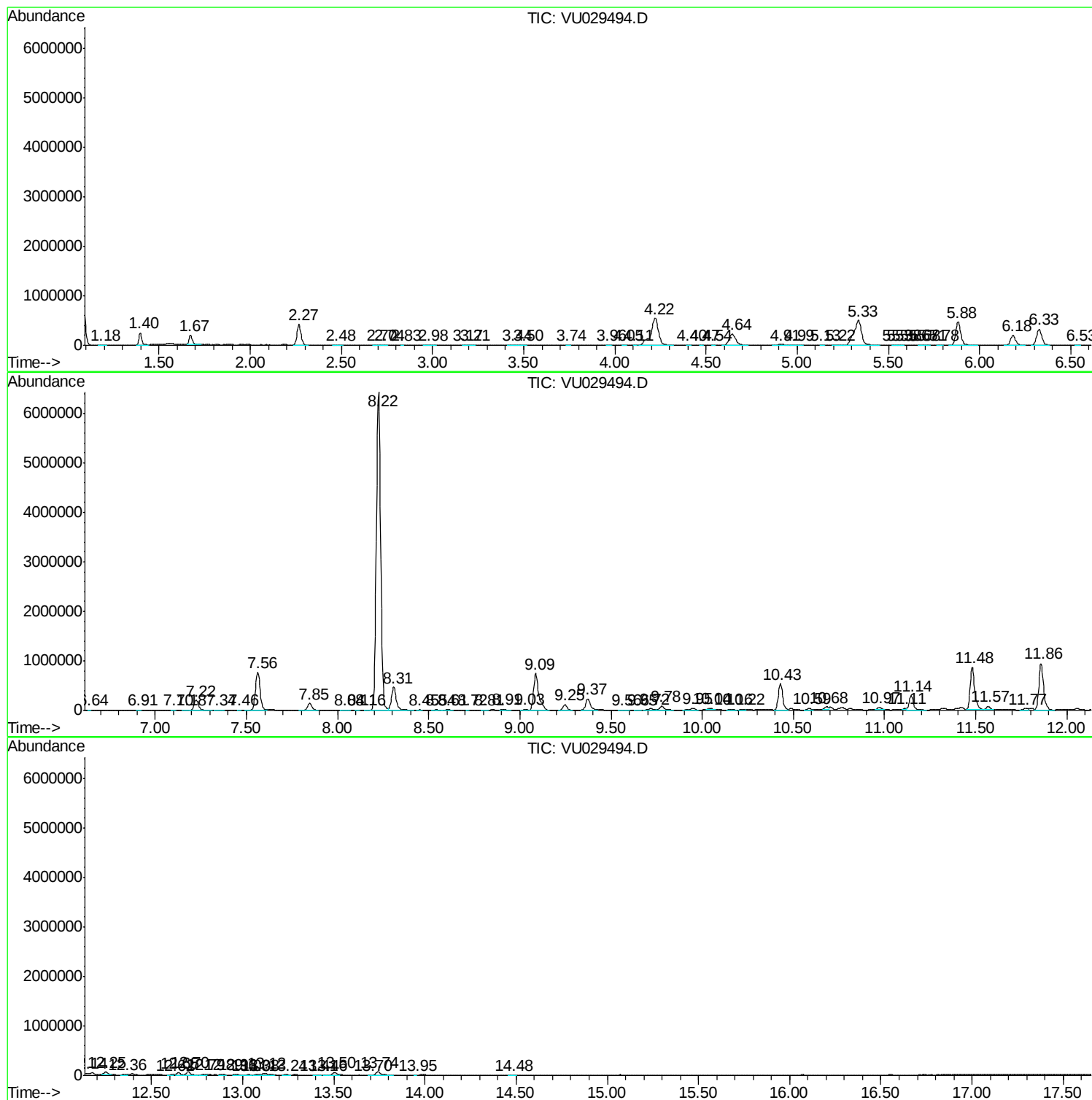
Sum of corrected areas: 28773005

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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



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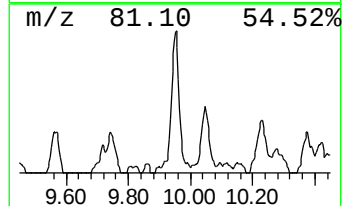
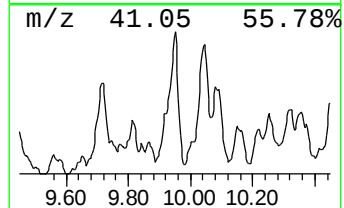
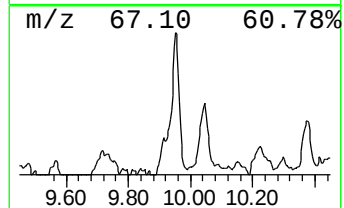
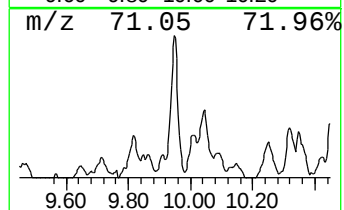
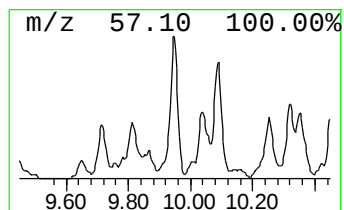
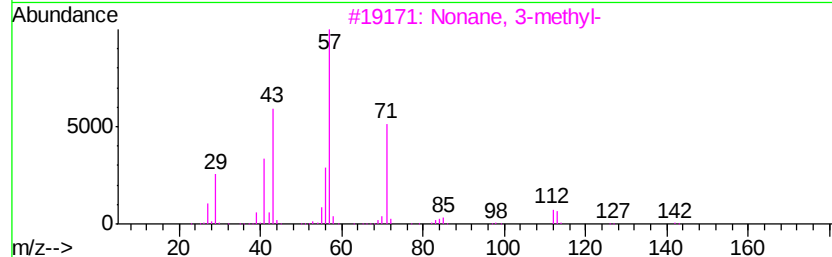
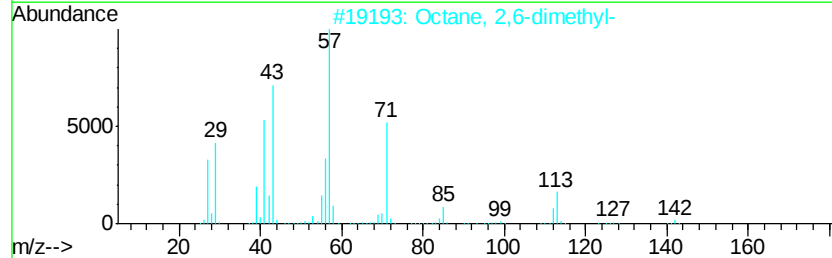
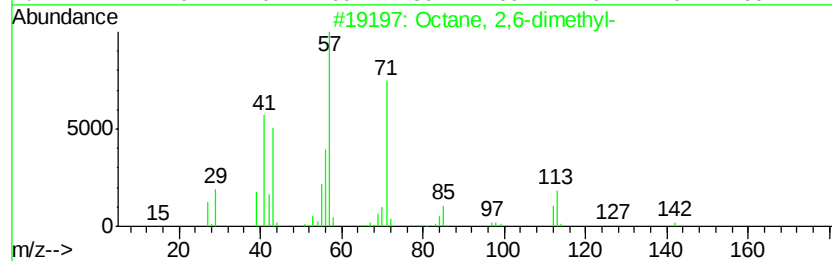
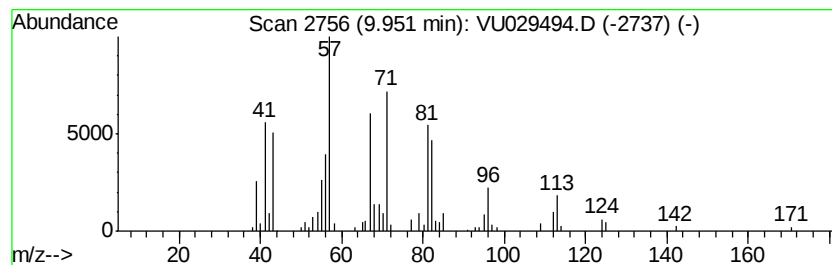
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.95	3.18 ug/L	91663	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	70
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	55
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	45
4			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	42
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	38



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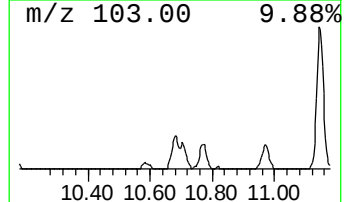
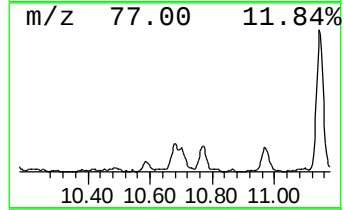
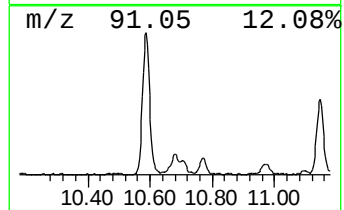
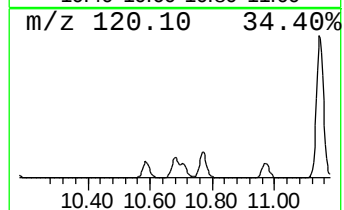
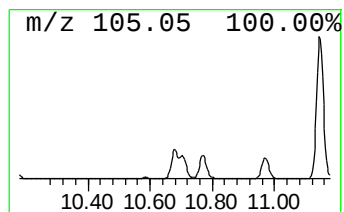
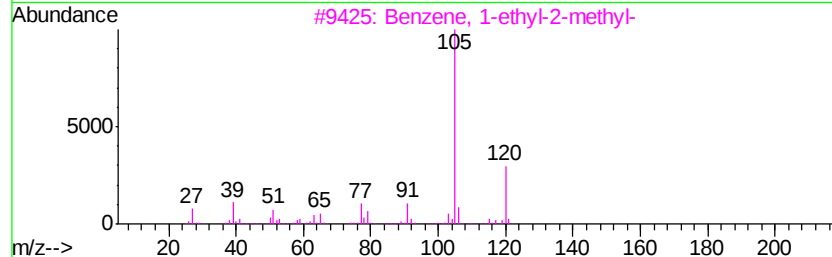
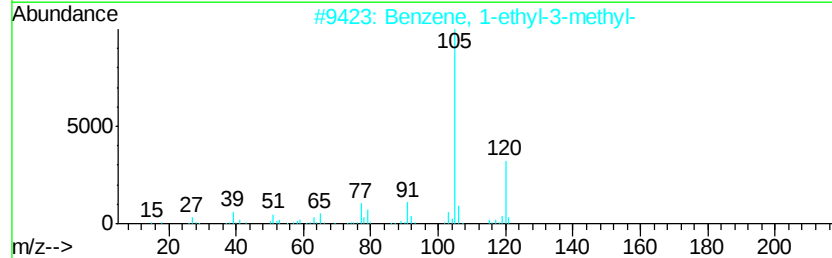
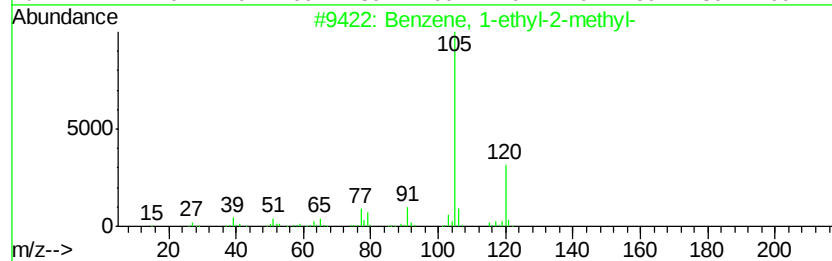
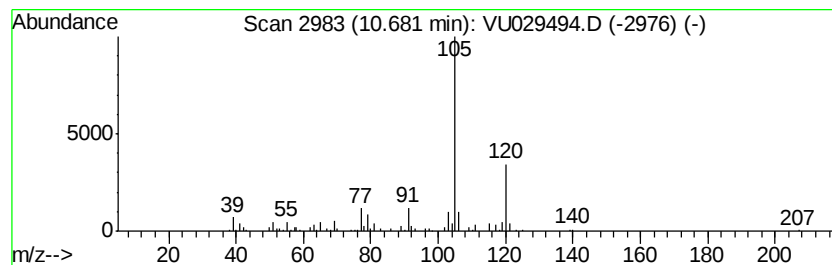
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Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.56 ug/L	74371	1,4-Dichlorobenzene-d4	11.48

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-3-methyl-	120	C9H12	000620-14-4	91
3		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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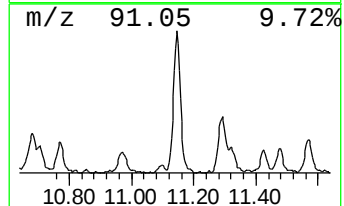
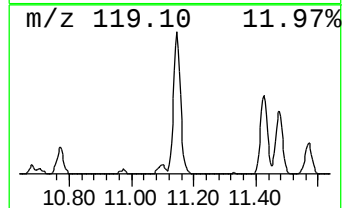
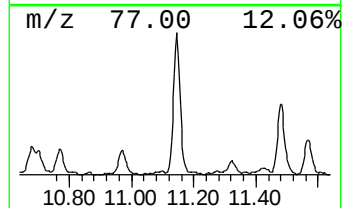
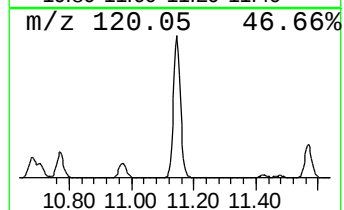
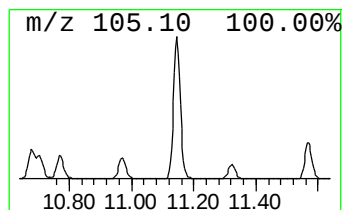
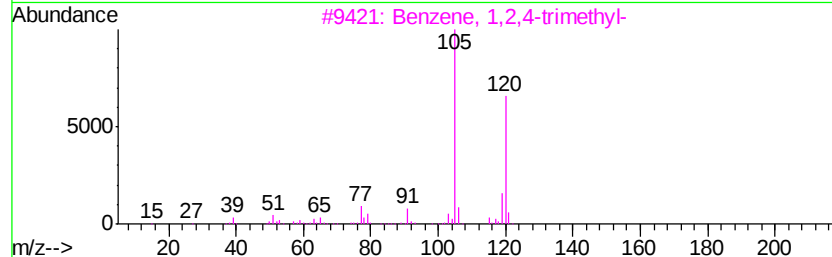
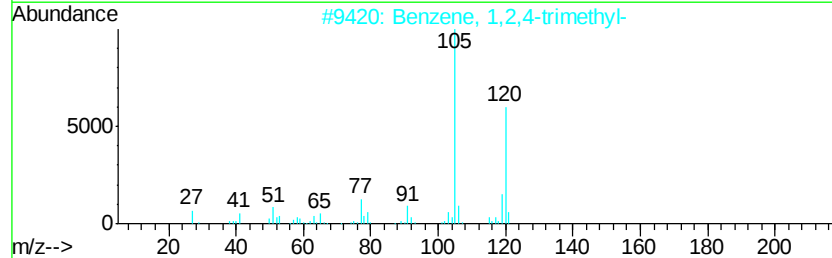
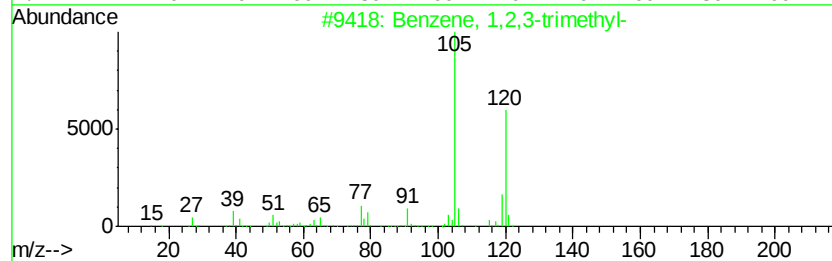
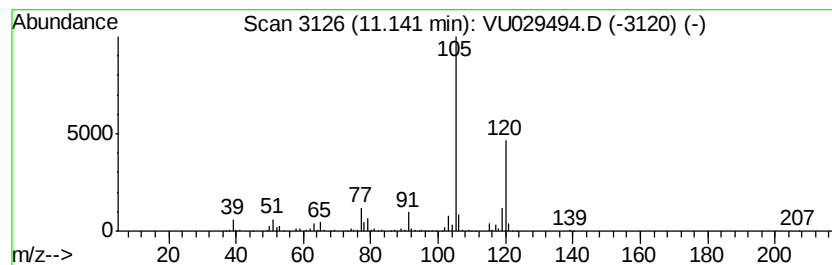
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	17.01 ug/L	494174	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Mesitylene	120	C9H12	000108-67-8	94
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU021519\
Data File : VU029494.D
Acq On : 15 Feb 2019 13:49
Operator : JC/SP
Sample : K1455-01 20X
Misc : 4.86µ/5.0mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE801

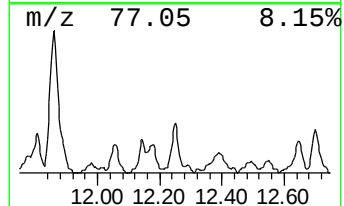
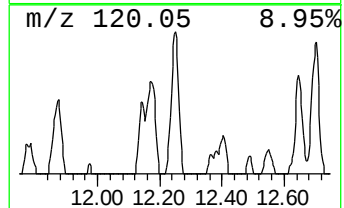
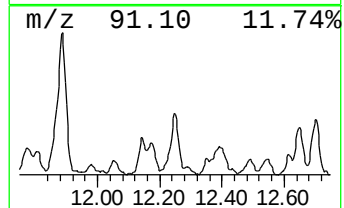
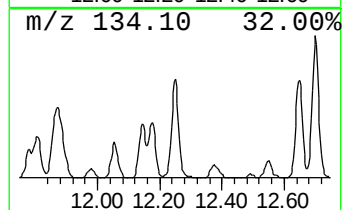
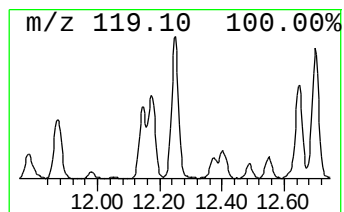
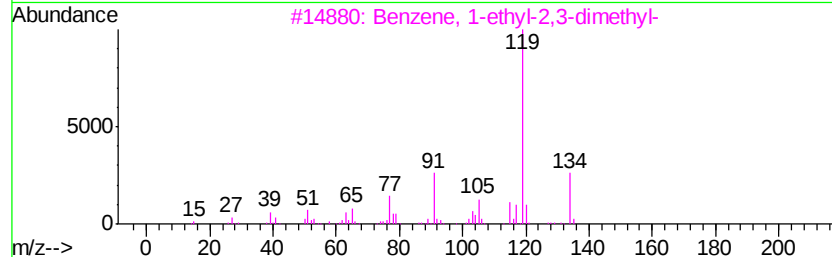
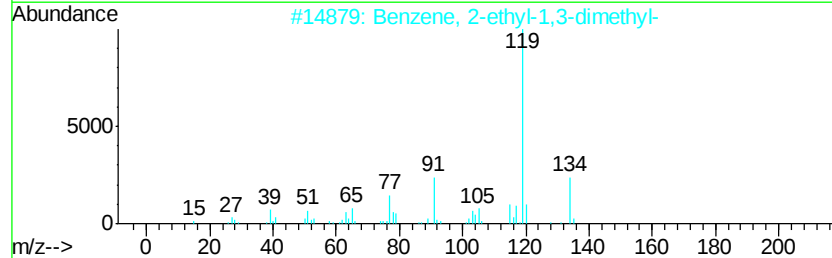
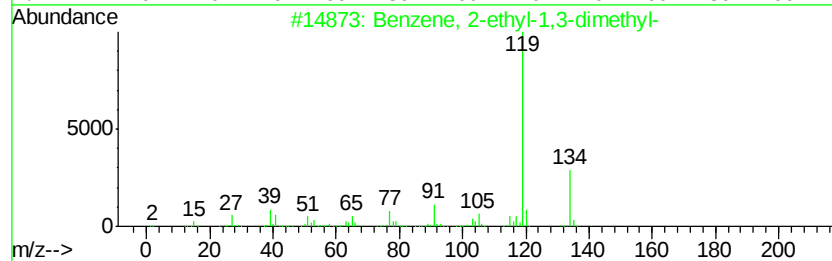
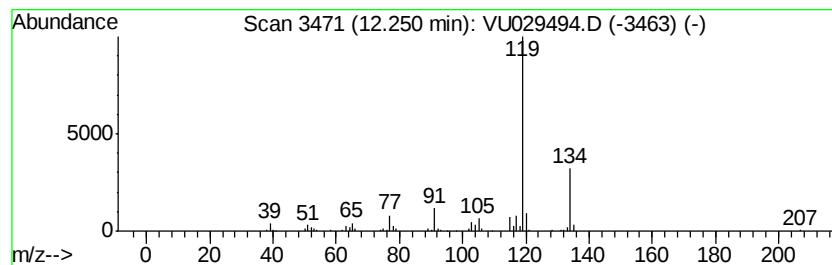
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Quant Title : VOC Analysis

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

Peak Number 7 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	2.81 ug/L	81668	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU021519\
Data File : VU029494.D
Acq On : 15 Feb 2019 13:49
Operator : JC/SP
Sample : K1455-01 20X
Misc : 4.86µ/5.0mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE801

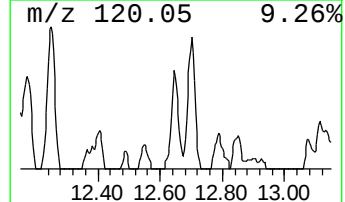
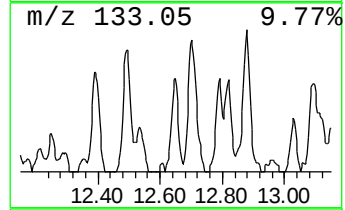
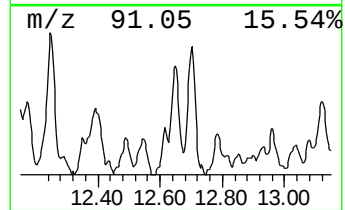
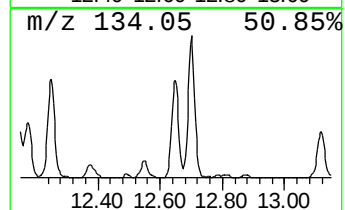
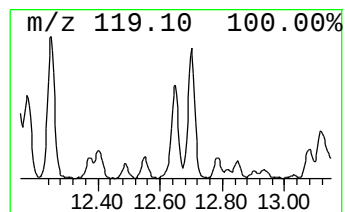
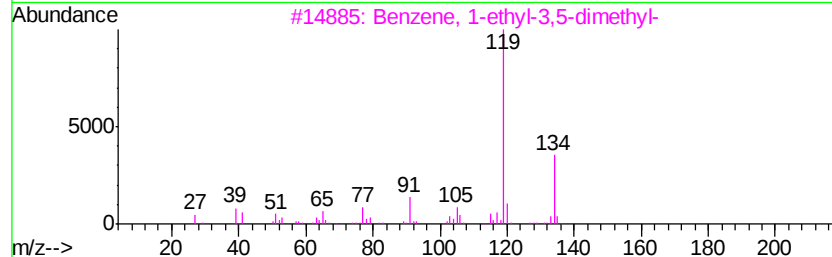
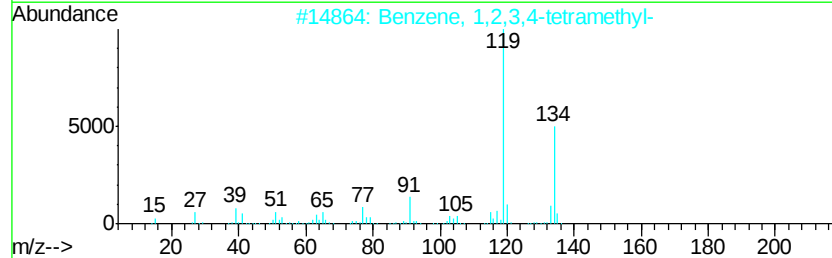
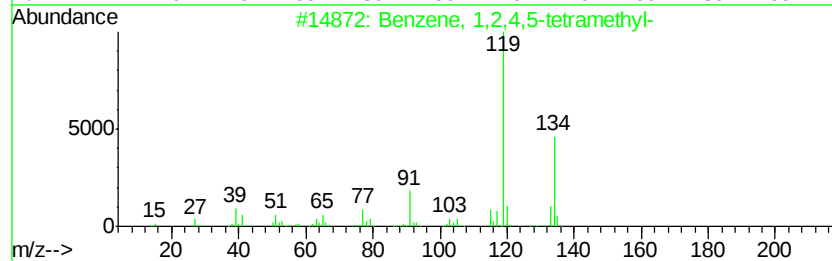
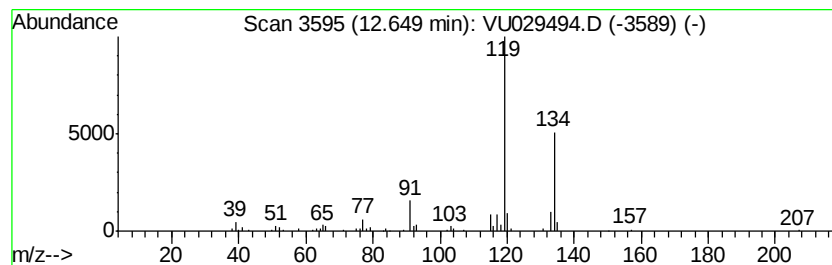
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Quant Title : VOC Analysis

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.60 ug/L	75441	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
3		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
4		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	91
5		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU021519\
Data File : VU029494.D
Acq On : 15 Feb 2019 13:49
Operator : JC/SP
Sample : K1455-01 20X
Misc : 4.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE801

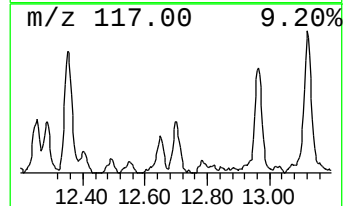
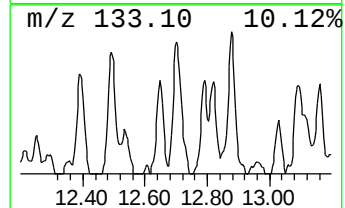
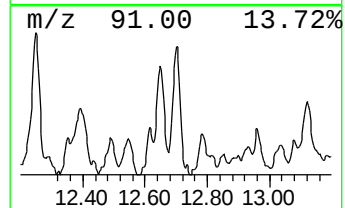
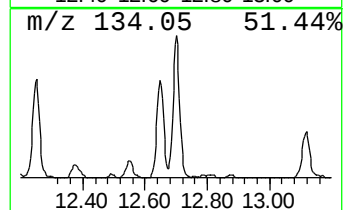
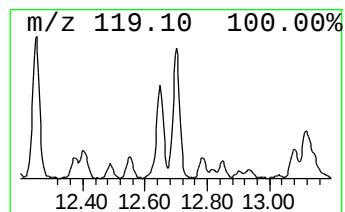
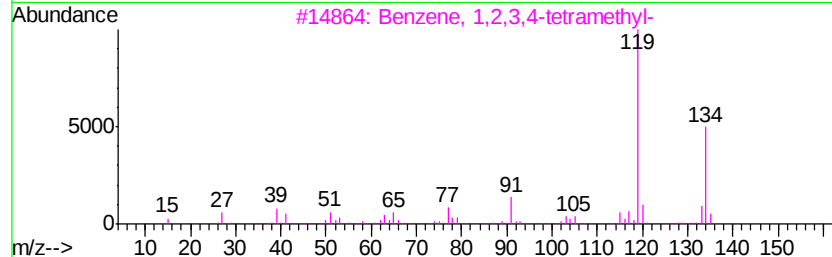
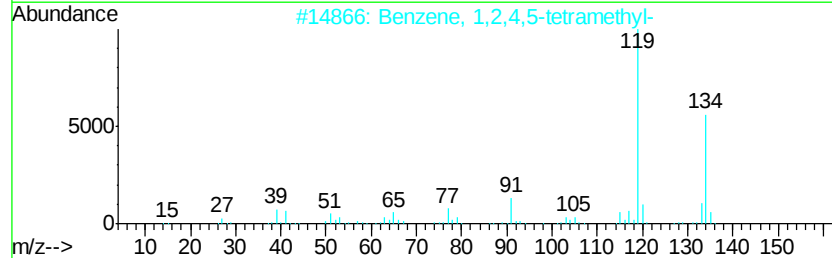
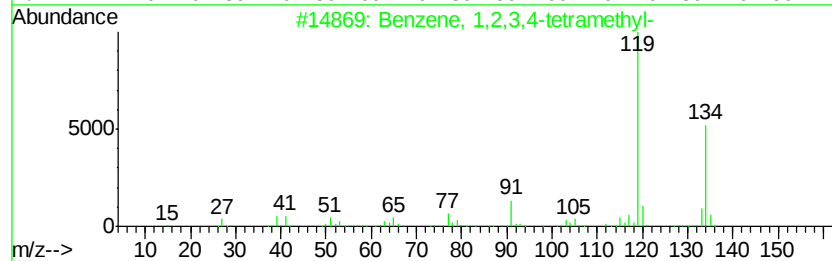
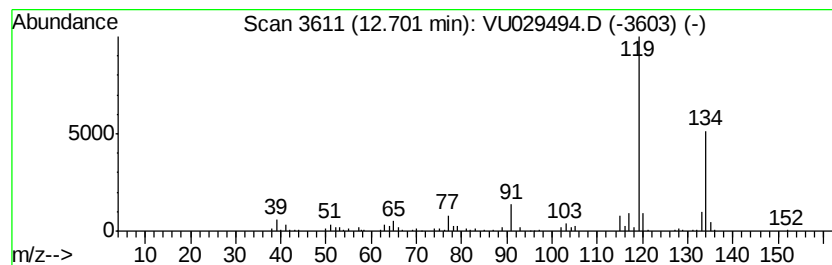
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.03 ug/L	117009	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, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU021519\
Data File : VU029494.D
Acq On : 15 Feb 2019 13:49
Operator : JC/SP
Sample : K1455-01 20X
Misc : 4.86g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE801

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.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
(DEL) Alkane: Str...	9.95	3.2	ug/L	91663	2	9.09	1442850	50.0
Benzene, 1-ethyl-...	10.68	2.6	ug/L	74371	3	11.48	1452840	50.0
Benzene, 1,2,3-tr...	11.14	17.0	ug/L	494174	3	11.48	1452840	50.0
Benzene, 2-ethyl-...	12.25	2.8	ug/L	81668	3	11.48	1452840	50.0
Benzene, 1,2,4,5-...	12.65	2.6	ug/L	75441	3	11.48	1452840	50.0
Benzene, 1,2,3,4-...	12.70	4.0	ug/L	117009	3	11.48	1452840	50.0