

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU043019\
 Data File : VU031656.D
 Acq On : 01 May 2019 00:39
 Operator : JC/SP
 Sample : K2604-05
 Misc : 5.08g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAJ79

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\SOMULM042719WMA.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	1.177	23	27	37	rVB3	13672	16232	0.60%	0.077%
2	1.219	37	40	41	rBV	3999	2458	0.09%	0.012%
3	1.289	58	62	67	rBV2	13592	13234	0.49%	0.063%
4	1.395	86	95	114	rBV	218452	342909	12.63%	1.627%
5	1.675	175	182	196	rBV	134726	283690	10.45%	1.346%
6	2.241	347	358	385	rVB	451082	784959	28.90%	3.724%
7	2.498	436	438	441	rVB4	2877	1465	0.05%	0.007%
8	2.530	441	448	455	rBV6	2231	3491	0.13%	0.017%
9	2.691	485	498	510	rVV4	12455	29829	1.10%	0.142%
10	2.833	540	542	547	rVB5	1918	1403	0.05%	0.007%
11	2.891	558	560	567	rVB4	1853	1847	0.07%	0.009%
12	2.926	567	571	574	rBV3	1279	1139	0.04%	0.005%
13	3.045	605	608	614	rVB5	1506	1323	0.05%	0.006%
14	3.193	652	654	661	rVB5	1267	1246	0.05%	0.006%
15	3.254	663	673	675	rBV5	2838	3635	0.13%	0.017%
16	3.267	675	677	678	rVV3	2107	1102	0.04%	0.005%
17	3.280	678	681	686	rVV6	3190	3269	0.12%	0.016%
18	3.437	727	730	735	rVB4	1726	1762	0.06%	0.008%
19	3.466	735	739	741	rBV3	1864	1498	0.06%	0.007%
20	3.527	752	758	763	rVB3	806	1117	0.04%	0.005%
21	3.633	786	791	796	rVB4	1201	1301	0.05%	0.006%
22	3.701	807	812	815	rBV3	1443	1562	0.06%	0.007%
23	3.720	815	818	824	rBV4	1414	1180	0.04%	0.006%
24	3.862	857	862	866	rBV5	1430	1377	0.05%	0.007%
25	4.128	939	945	948	rBV3	1523	1463	0.05%	0.007%
26	4.212	959	971	1018	rBV	95108	537661	19.80%	2.551%
27	4.643	1088	1105	1137	rBV3	297140	847926	31.22%	4.023%
28	4.881	1171	1179	1185	rVB8	1996	3216	0.12%	0.015%
29	4.984	1209	1211	1215	rVB4	1949	1247	0.05%	0.006%
30	5.006	1215	1218	1222	rVB6	1462	1244	0.05%	0.006%
31	5.051	1230	1232	1239	rVB5	1174	1154	0.04%	0.005%
32	5.328	1296	1318	1358	rBV2	751069	2220279	81.76%	10.533%
33	5.630	1399	1412	1419	rBV10	5595	12837	0.47%	0.061%
34	5.743	1441	1447	1451	rVB7	1734	1513	0.06%	0.007%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
 Title : VOC Analysis

35	5.881	1473	1490	1523	rBV	926490	2217262	81.65%	10.519%
36	6.032	1535	1537	1541	rVB3	2760	1908	0.07%	0.009%
37	6.119	1561	1564	1568	rVB6	2016	1629	0.06%	0.008%
38	6.183	1571	1584	1598	rBV9	24089	57345	2.11%	0.272%
39	6.260	1603	1608	1614	rVV9	4635	6288	0.23%	0.030%
40	6.328	1614	1629	1657	rVV	439295	1015177	37.38%	4.816%
41	6.495	1679	1681	1685	rVB3	2239	1383	0.05%	0.007%
42	6.517	1685	1688	1692	rVB3	1722	1219	0.04%	0.006%
43	6.562	1696	1702	1703	rBV5	1356	1135	0.04%	0.005%
44	6.607	1712	1716	1723	rBV6	1987	2140	0.08%	0.010%
45	6.749	1755	1760	1765	rVB7	1658	1851	0.07%	0.009%
46	6.800	1770	1776	1778	rBV2	1243	1123	0.04%	0.005%
47	6.868	1793	1797	1800	rBV3	1590	1273	0.05%	0.006%
48	6.890	1801	1804	1808	rBV4	1388	1150	0.04%	0.005%
49	6.980	1827	1832	1837	rBV6	1534	1699	0.06%	0.008%
50	7.022	1842	1845	1848	rVB3	1958	1179	0.04%	0.006%
51	7.067	1855	1859	1864	rVB6	1389	1310	0.05%	0.006%
52	7.093	1864	1867	1871	rVB4	1335	1127	0.04%	0.005%
53	7.160	1884	1888	1890	rBV4	1634	1233	0.05%	0.006%
54	7.228	1896	1909	1936	rBV2	197956	466554	17.18%	2.213%
55	7.562	2000	2013	2037	rBV	759747	1547032	56.97%	7.339%
56	7.855	2093	2104	2134	rBV2	122337	307868	11.34%	1.461%
57	8.058	2164	2167	2170	rVB4	2323	1607	0.06%	0.008%
58	8.077	2170	2173	2180	rVB9	1320	1130	0.04%	0.005%
59	8.228	2217	2220	2225	rVB5	5023	4315	0.16%	0.020%
60	8.276	2232	2235	2240	rVB7	1469	1322	0.05%	0.006%
61	8.344	2240	2256	2291	rBV	458423	1257442	46.30%	5.965%
62	8.527	2310	2313	2315	rBV2	1871	1499	0.06%	0.007%
63	8.704	2364	2368	2372	rBV5	1874	1536	0.06%	0.007%
64	8.839	2407	2410	2414	rBV4	1776	1672	0.06%	0.008%
65	8.906	2424	2431	2437	rVB9	4855	5634	0.21%	0.027%
66	9.093	2475	2489	2525	rBV	1312853	2715711	100.00%	12.883%
67	9.340	2561	2566	2572	rVB8	1818	2230	0.08%	0.011%
68	9.376	2572	2577	2583	rBV8	2185	3067	0.11%	0.015%
69	9.434	2593	2595	2598	rVB3	2050	1132	0.04%	0.005%
70	9.549	2626	2631	2635	rBV3	3490	4314	0.16%	0.020%
71	9.607	2640	2649	2656	rBV3	2271	3662	0.13%	0.017%

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72	9.646	2657	2661	2663	rBV4	1949	1352	0.05%	0.006%
73	9.691	2672	2675	2677	rBV5	1619	1106	0.04%	0.005%
74	9.707	2677	2680	2686	rVB8	3498	2677	0.10%	0.013%
75	9.826	2713	2717	2719	rBV5	1708	1257	0.05%	0.006%
76	9.935	2748	2751	2753	rVB3	2538	1544	0.06%	0.007%
77	9.948	2753	2755	2761	rBV7	1832	1729	0.06%	0.008%
78	10.025	2774	2779	2782	rBV6	1410	1392	0.05%	0.007%
79	10.102	2798	2803	2806	rBV6	2003	1668	0.06%	0.008%
80	10.202	2832	2834	2838	rVB4	1999	1202	0.04%	0.006%
81	10.289	2857	2861	2865	rVB6	2095	1357	0.05%	0.006%
82	10.369	2883	2886	2892	rVB7	1801	1808	0.07%	0.009%
83	10.437	2895	2907	2923	rBV	577473	979935	36.08%	4.649%
84	10.565	2943	2947	2952	rBV8	4098	5013	0.18%	0.024%
85	10.694	2982	2987	2992	rBV9	3757	4081	0.15%	0.019%
86	11.109	3113	3116	3118	rBV3	3156	2310	0.09%	0.011%
87	11.154	3125	3130	3131	rBV5	4127	3699	0.14%	0.018%
88	11.324	3180	3183	3186	rBV5	2833	1617	0.06%	0.008%
89	11.485	3221	3233	3252	rBV	1409403	2248594	82.80%	10.667%
90	11.861	3339	3350	3371	rBV	727952	1230995	45.33%	5.840%
91	12.688	3603	3607	3610	rBV5	6951	6690	0.25%	0.032%
92	13.128	3737	3744	3745	rBV6	18853	22336	0.82%	0.106%
93	13.749	3930	3937	3944	rBV2	48044	79491	2.93%	0.377%
94	14.138	4053	4058	4066	rBV3	28880	36928	1.36%	0.175%
95	14.877	4278	4288	4319	rBV2	232369	531559	19.57%	2.522%
96	15.060	4336	4345	4361	rBV2	174565	369891	13.62%	1.755%
97	15.659	4523	4531	4540	rVB	174772	244148	8.99%	1.158%
98	15.916	4603	4611	4623	rBV3	77103	158462	5.84%	0.752%
99	16.057	4648	4655	4662	rBV2	113239	172344	6.35%	0.818%
100	17.218	5011	5016	5031	rVB2	110191	187644	6.91%	0.890%

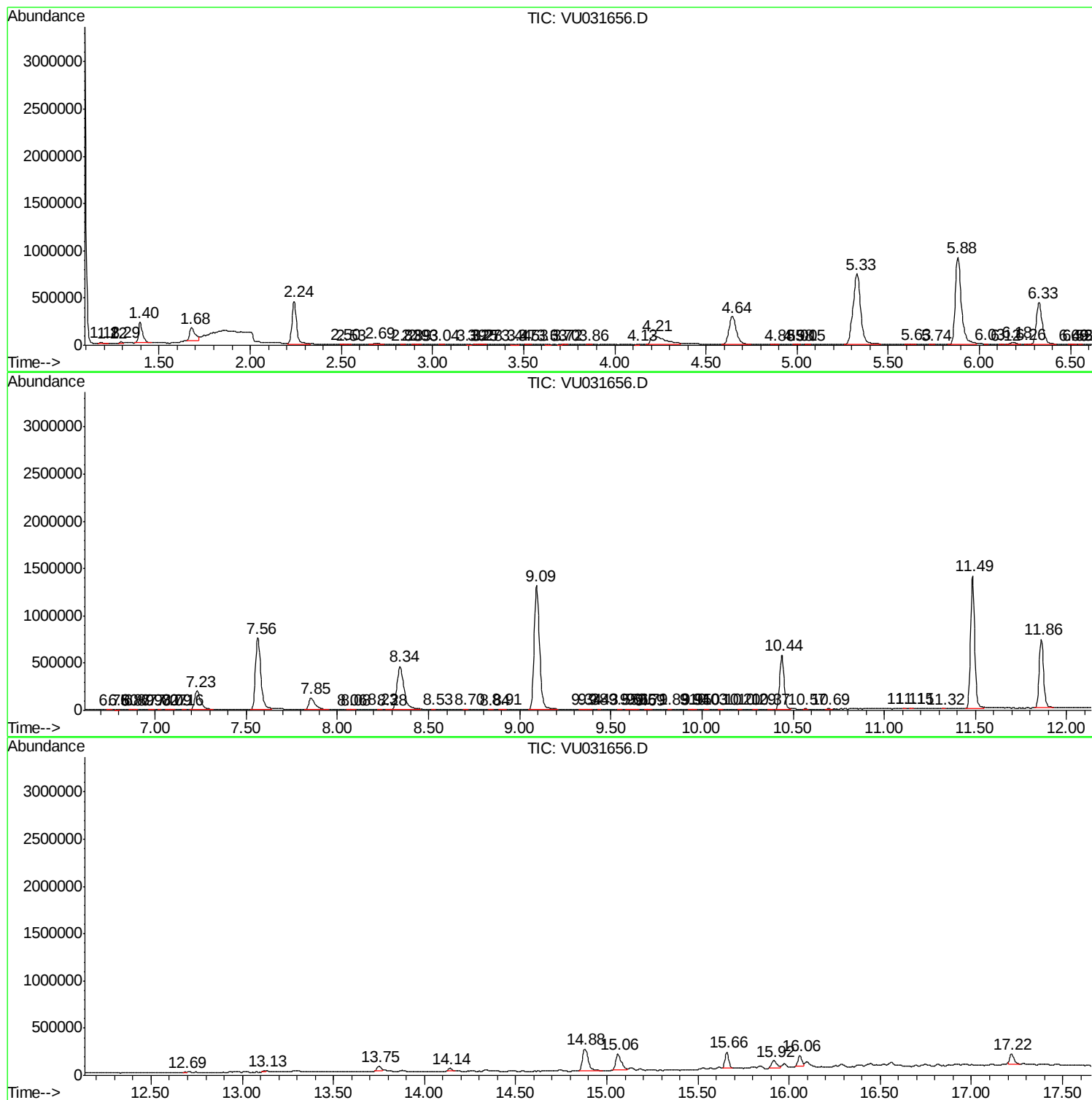
Sum of corrected areas: 21079555

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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



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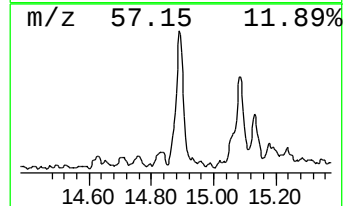
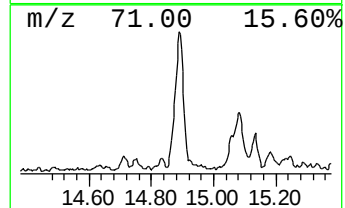
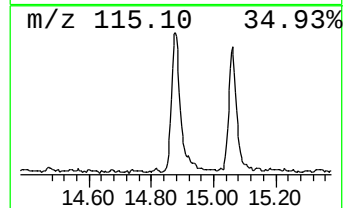
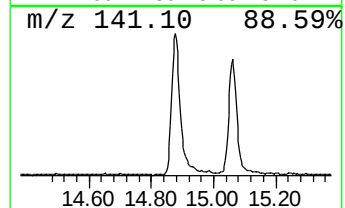
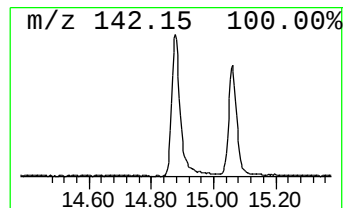
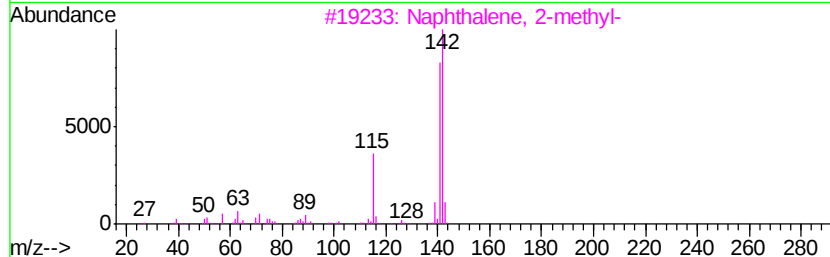
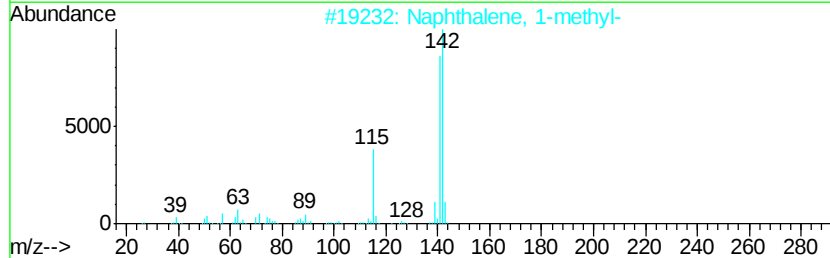
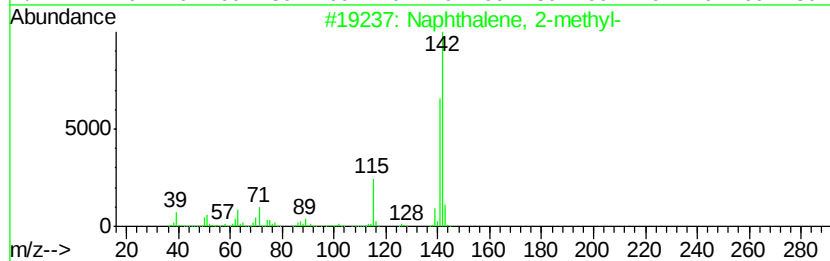
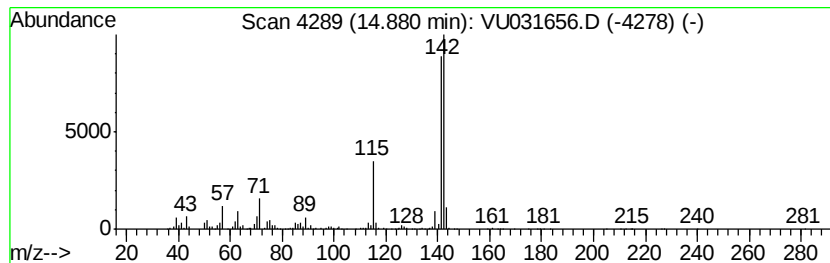
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Naphthalene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.88	11.82 ug/L	531559	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94



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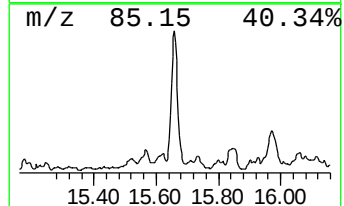
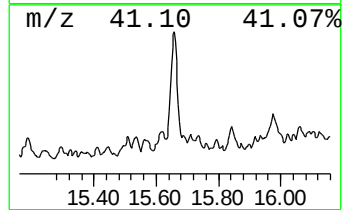
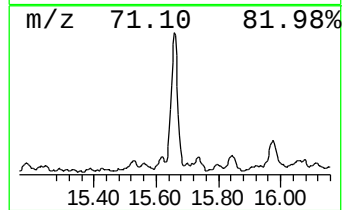
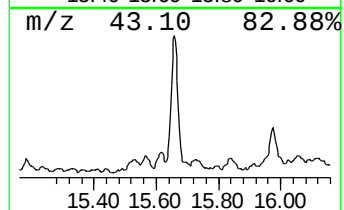
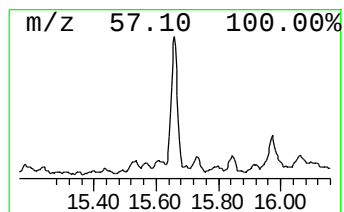
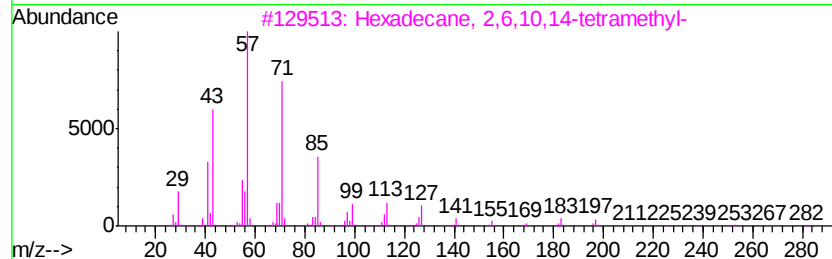
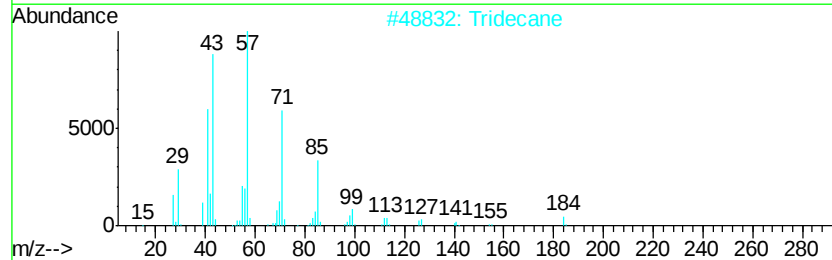
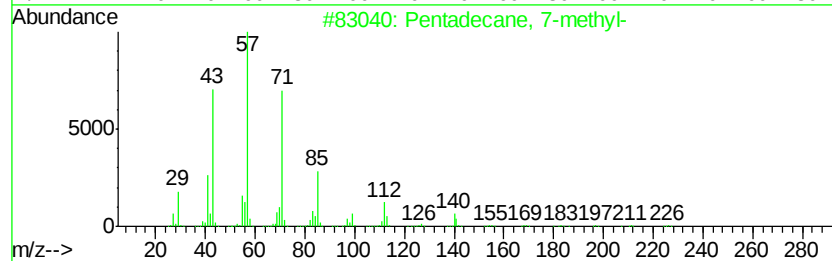
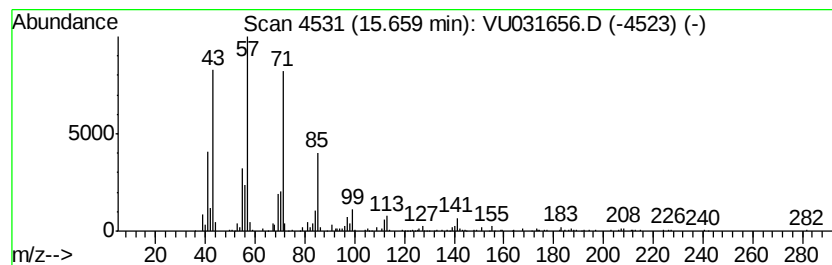
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	5.43 ug/L	244148	1,4-Dichlorobenzene-d4	11.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 7-methyl-	226	C16H34	006165-40-8	93
2			Tridecane	184	C13H28	000629-50-5	90
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
4			Nonadecane	268	C19H40	000629-92-5	86
5			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	86



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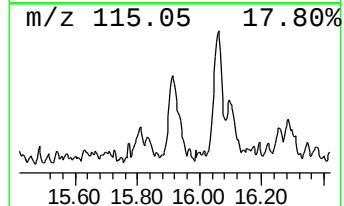
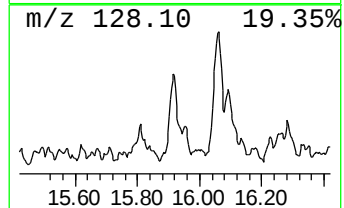
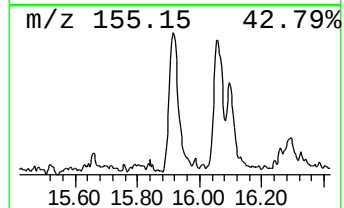
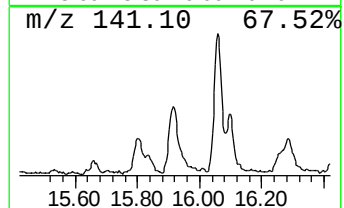
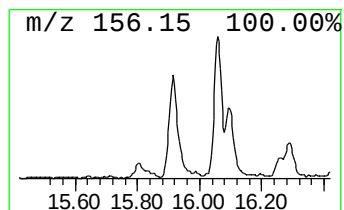
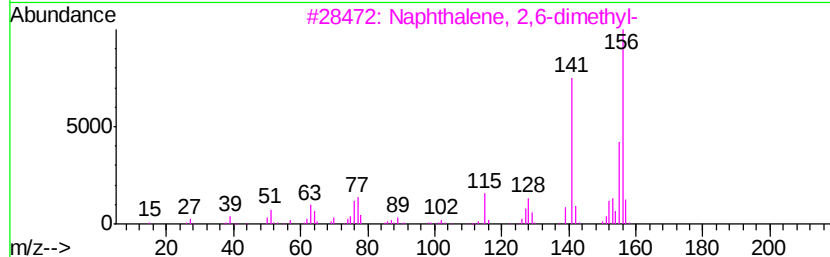
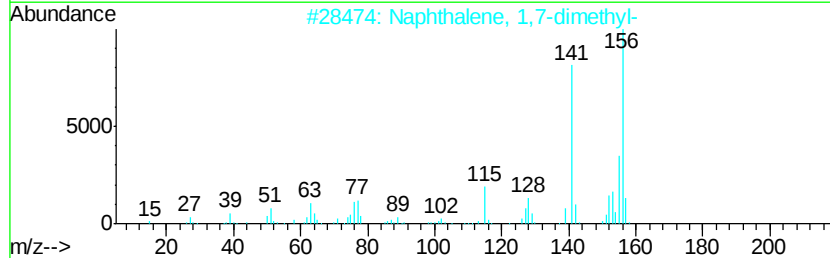
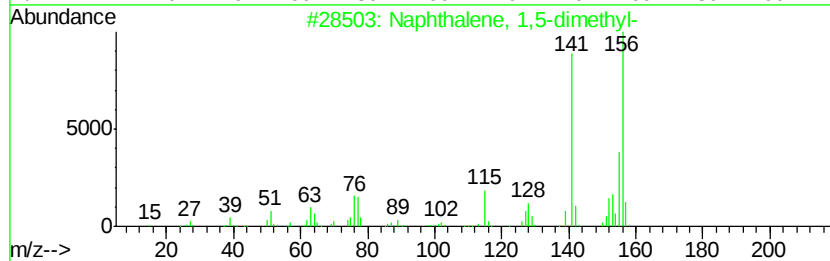
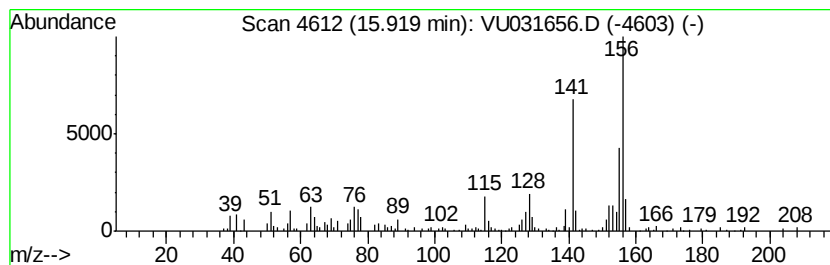
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.52 ug/L	158462	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,5-dimethyl-	156 C12H12	000571-61-9 98
2		Naphthalene, 1,7-dimethyl-	156 C12H12	000575-37-1 96
3		Naphthalene, 2,6-dimethyl-	156 C12H12	000581-42-0 96
4		Naphthalene, 2,7-dimethyl-	156 C12H12	000582-16-1 96
5		Naphthalene, 1,6-dimethyl-	156 C12H12	000575-43-9 95



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU043019\
Data File : VU031656.D
Acq On : 01 May 2019 00:39
Operator : JC/SP
Sample : K2604-05
Misc : 5.08g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

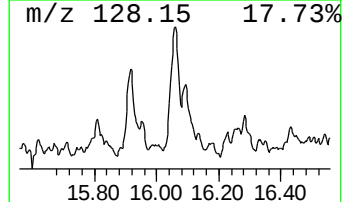
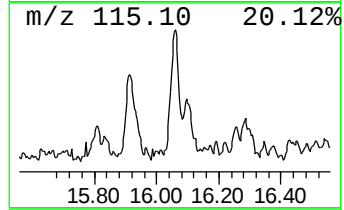
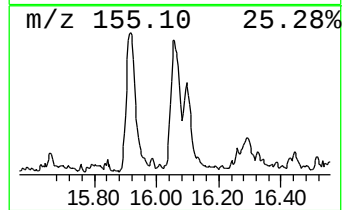
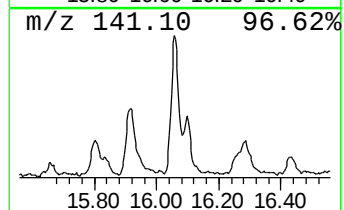
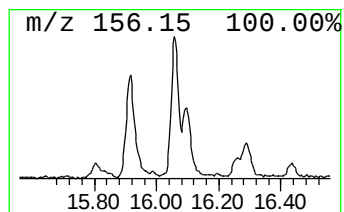
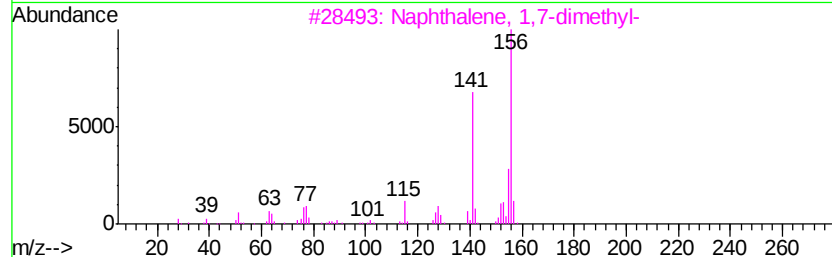
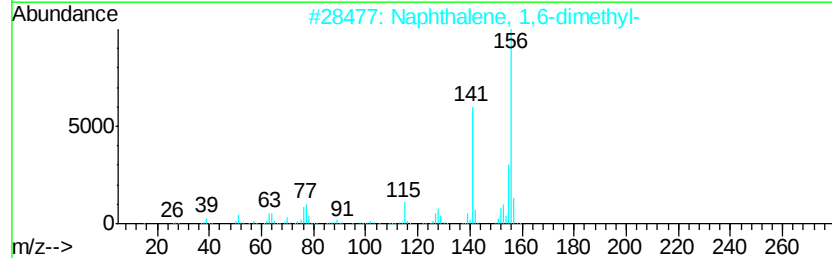
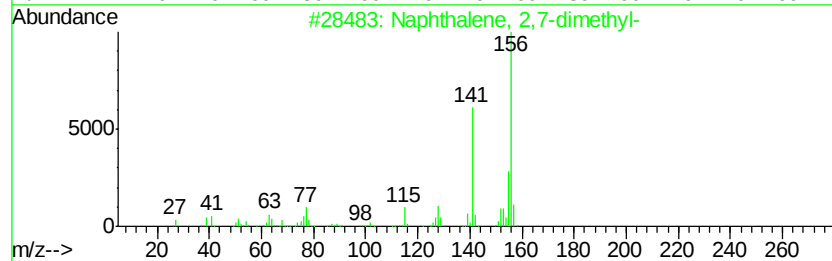
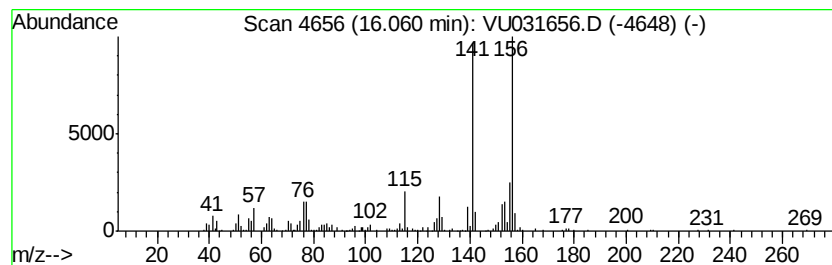
Instrument :
MSVOA_U
ClientSampleId :
GAJ79

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.06	3.83 ug/L	172344	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU043019\
Data File : VU031656.D
Acq On : 01 May 2019 00:39
Operator : JC/SP
Sample : K2604-05
Misc : 5.08g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAJ79

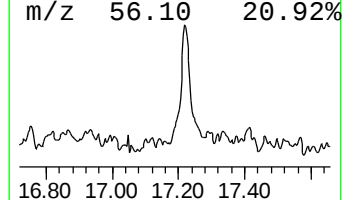
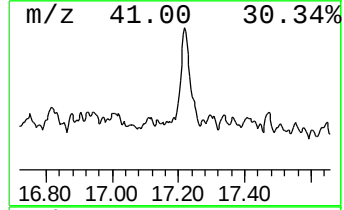
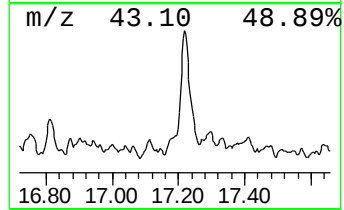
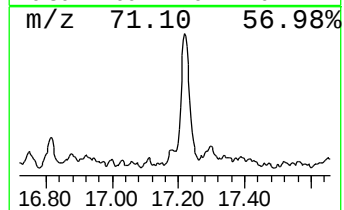
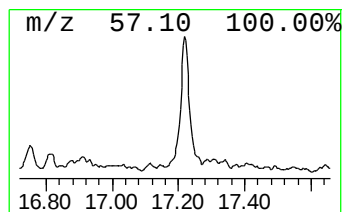
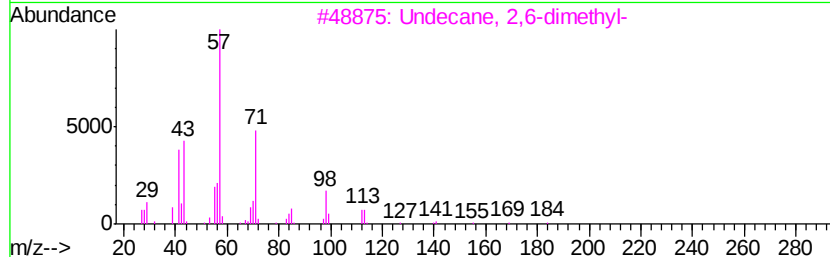
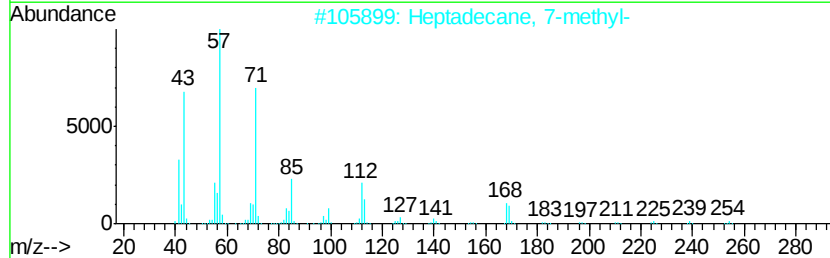
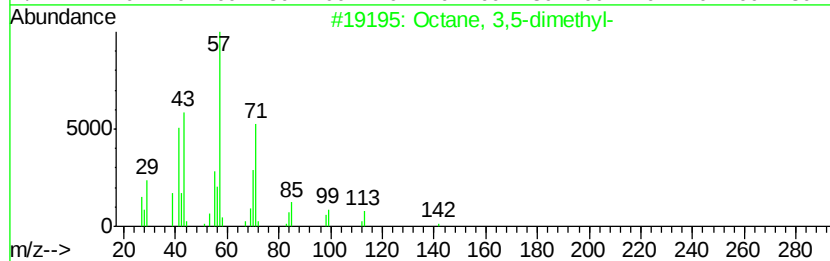
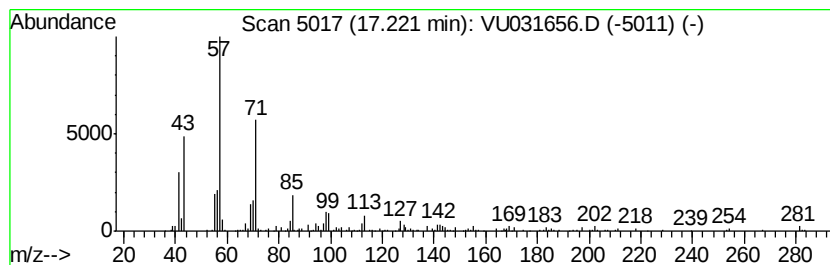
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.22	4.17 ug/L	187644	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	83
2		Heptadecane, 7-methyl-	254	C18H38	020959-33-5	62
3		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
4		Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	53
5		Heptadecane	240	C17H36	000629-78-7	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU043019\
Data File : VU031656.D
Acq On : 01 May 2019 00:39
Operator : JC/SP
Sample : K2604-05
Misc : 5.08g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAJ79

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.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
Naphthalene, 1-me...	14.88	11.8	ug/L	531559	3	11.48	2248590	50.0
(DEL) Alkane: Str...	15.66	5.4	ug/L	244148	3	11.48	2248590	50.0
Naphthalene, 1,5-...	15.92	3.5	ug/L	158462	3	11.48	2248590	50.0
Naphthalene, 2,7-...	16.06	3.8	ug/L	172344	3	11.48	2248590	50.0
(DEL) Alkane: Str...	17.22	4.2	ug/L	187644	3	11.48	2248590	50.0