

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU043019\
 Data File : VU031655.D
 Acq On : 01 May 2019 00:15
 Operator : JC/SP
 Sample : K2604-11
 Misc : 5.08g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAJ85

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	1.180	24	28	36	rBV4	10704	11722	0.41%	0.049%
2	1.293	59	63	68	rVB2	12522	10986	0.39%	0.046%
3	1.396	88	95	114	rBV	276525	415944	14.58%	1.745%
4	1.675	176	182	195	rBV	173535	302762	10.61%	1.271%
5	2.241	348	358	373	rBV	578175	943407	33.06%	3.959%
6	2.582	461	464	468	rBV3	1188	1104	0.04%	0.005%
7	2.691	490	498	511	rVB4	10567	20423	0.72%	0.086%
8	2.814	533	536	540	rBV4	1677	1269	0.04%	0.005%
9	2.836	540	543	546	rVB2	1651	1006	0.04%	0.004%
10	2.978	578	587	590	rBV7	2636	3871	0.14%	0.016%
11	3.026	599	602	608	rVB6	2003	1506	0.05%	0.006%
12	3.106	624	627	631	rVB4	1510	1047	0.04%	0.004%
13	3.135	631	636	641	rVB4	1137	1045	0.04%	0.004%
14	3.164	641	645	648	rBV3	1816	1228	0.04%	0.005%
15	3.228	658	665	671	rBV5	1188	1830	0.06%	0.008%
16	3.273	676	679	682	rBV4	1576	1420	0.05%	0.006%
17	3.383	711	713	716	rVB3	1852	986	0.03%	0.004%
18	3.537	756	761	765	rBV6	1105	1219	0.04%	0.005%
19	3.598	777	780	785	rVB3	1487	1166	0.04%	0.005%
20	3.630	785	790	793	rBV5	997	1065	0.04%	0.004%
21	3.698	808	811	816	rVB5	1436	1337	0.05%	0.006%
22	3.797	836	842	845	rBV3	1022	1015	0.04%	0.004%
23	3.990	897	902	905	rBV5	1279	1365	0.05%	0.006%
24	4.145	945	950	954	rVB3	1038	1001	0.04%	0.004%
25	4.212	958	971	1000	rBV2	139112	654965	22.95%	2.749%
26	4.643	1088	1105	1141	rBV	395599	1109200	38.87%	4.655%
27	4.836	1162	1165	1168	rBV3	1890	1233	0.04%	0.005%
28	4.945	1195	1199	1204	rBV5	1317	1626	0.06%	0.007%
29	4.981	1204	1210	1213	rBV6	1936	2336	0.08%	0.010%
30	5.167	1265	1268	1272	rVB4	1453	1038	0.04%	0.004%
31	5.206	1277	1280	1285	rVB5	1469	988	0.03%	0.004%
32	5.328	1295	1318	1348	rBV2	963281	2853470	100.00%	11.974%
33	5.614	1402	1407	1408	rBV4	2447	1889	0.07%	0.008%
34	5.881	1476	1490	1543	rBV2	921373	2239921	78.50%	9.400%

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 Title : VOC Analysis

35	6.186	1570	1585	1600	rBV10	26225	66204	2.32%	0.278%
36	6.328	1615	1629	1662	rVB	568497	1332573	46.70%	5.592%
37	6.540	1692	1695	1698	rVB3	2498	1613	0.06%	0.007%
38	6.585	1703	1709	1712	rBV6	1293	1313	0.05%	0.006%
39	6.608	1712	1716	1719	rVB4	1546	1373	0.05%	0.006%
40	6.694	1740	1743	1744	rBV3	1749	1027	0.04%	0.004%
41	6.739	1754	1757	1760	rVB2	1929	1113	0.04%	0.005%
42	6.768	1760	1766	1767	rBV2	1580	1424	0.05%	0.006%
43	6.846	1786	1790	1793	rVB4	1609	1316	0.05%	0.006%
44	6.894	1801	1805	1807	rBV2	1943	1481	0.05%	0.006%
45	6.923	1811	1814	1820	rVV6	2591	2686	0.09%	0.011%
46	7.119	1871	1875	1878	rBV3	1869	1181	0.04%	0.005%
47	7.228	1894	1909	1940	rBV	255761	598134	20.96%	2.510%
48	7.463	1975	1982	1984	rBV3	1347	1436	0.05%	0.006%
49	7.563	2001	2013	2040	rBV	987764	2015779	70.64%	8.459%
50	7.855	2092	2104	2138	rBV2	166406	402850	14.12%	1.691%
51	8.029	2155	2158	2160	rBV2	2078	1475	0.05%	0.006%
52	8.106	2178	2182	2186	rBV3	1408	1056	0.04%	0.004%
53	8.164	2196	2200	2203	rBV3	1839	1539	0.05%	0.006%
54	8.225	2207	2219	2229	rBV7	6594	11748	0.41%	0.049%
55	8.344	2238	2256	2301	rBV	656638	1778122	62.31%	7.462%
56	8.653	2349	2352	2356	rVB3	1495	1184	0.04%	0.005%
57	8.701	2364	2367	2371	rVB4	1441	1083	0.04%	0.005%
58	8.723	2371	2374	2377	rBV3	1608	986	0.03%	0.004%
59	8.784	2391	2393	2397	rBV4	1510	940	0.03%	0.004%
60	8.907	2419	2431	2435	rBV9	6369	10401	0.36%	0.044%
61	9.093	2475	2489	2522	rBV	1325664	2695280	94.46%	11.310%
62	9.386	2577	2580	2582	rBV2	1870	1302	0.05%	0.005%
63	9.402	2582	2585	2589	rVB6	2764	1875	0.07%	0.008%
64	9.492	2610	2613	2616	rVB2	1577	1083	0.04%	0.005%
65	9.537	2621	2627	2634	rVB5	1941	2270	0.08%	0.010%
66	9.595	2641	2645	2650	rBV4	1621	1650	0.06%	0.007%
67	9.810	2710	2712	2718	rVB5	1630	1184	0.04%	0.005%
68	9.842	2718	2722	2726	rVB5	1975	1564	0.05%	0.007%
69	9.865	2726	2729	2732	rBV3	1916	1501	0.05%	0.006%
70	9.916	2742	2745	2750	rVB2	1491	1007	0.04%	0.004%
71	9.945	2750	2754	2755	rBV3	2049	1139	0.04%	0.005%

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 Title : VOC Analysis

72	10.096	2796	2801	2807	rVB5	1833	2171	0.08%	0.009%
73	10.141	2812	2815	2818	rBV4	1650	1172	0.04%	0.005%
74	10.222	2836	2840	2842	rBV2	1509	1115	0.04%	0.005%
75	10.437	2891	2907	2928	rBV	777004	1306301	45.78%	5.482%
76	10.653	2967	2974	2977	rBV5	1585	2016	0.07%	0.008%
77	10.691	2979	2986	2989	rVB7	1831	2098	0.07%	0.009%
78	10.765	3006	3009	3012	rVV4	1902	1093	0.04%	0.005%
79	10.794	3016	3018	3028	rVB4	1614	2064	0.07%	0.009%
80	10.977	3070	3075	3078	rBV3	1374	1456	0.05%	0.006%
81	11.186	3137	3140	3144	rVB2	2351	1748	0.06%	0.007%
82	11.215	3144	3149	3153	rBV5	2235	2522	0.09%	0.011%
83	11.244	3153	3158	3162	rBV4	1753	1699	0.06%	0.007%
84	11.283	3167	3170	3173	rBV2	1578	1098	0.04%	0.005%
85	11.337	3185	3187	3193	rVB3	1500	1189	0.04%	0.005%
86	11.386	3197	3202	3204	rBV2	1343	1260	0.04%	0.005%
87	11.427	3209	3215	3220	rBV6	1846	2233	0.08%	0.009%
88	11.485	3220	3233	3263	rBV	1279328	2067318	72.45%	8.675%
89	11.861	3335	3350	3375	rBV	940591	1571508	55.07%	6.595%
90	12.151	3437	3440	3442	rBV3	1623	961	0.03%	0.004%
91	12.212	3454	3459	3463	rVB5	1949	1894	0.07%	0.008%
92	12.296	3482	3485	3488	rBV3	1368	1050	0.04%	0.004%
93	12.418	3520	3523	3525	rBV3	1602	979	0.03%	0.004%
94	12.543	3559	3562	3564	rBV3	1808	1028	0.04%	0.004%
95	13.032	3710	3714	3716	rBV5	2693	2123	0.07%	0.009%
96	13.212	3765	3770	3773	rBV6	3173	2798	0.10%	0.012%
97	13.279	3783	3791	3801	rBV3	32799	52801	1.85%	0.222%
98	13.746	3928	3936	3943	rBV3	66298	113574	3.98%	0.477%
99	13.881	3969	3978	3992	rVB	196513	293330	10.28%	1.231%
100	14.890	4287	4292	4302	rVB	633150	843014	29.54%	3.538%

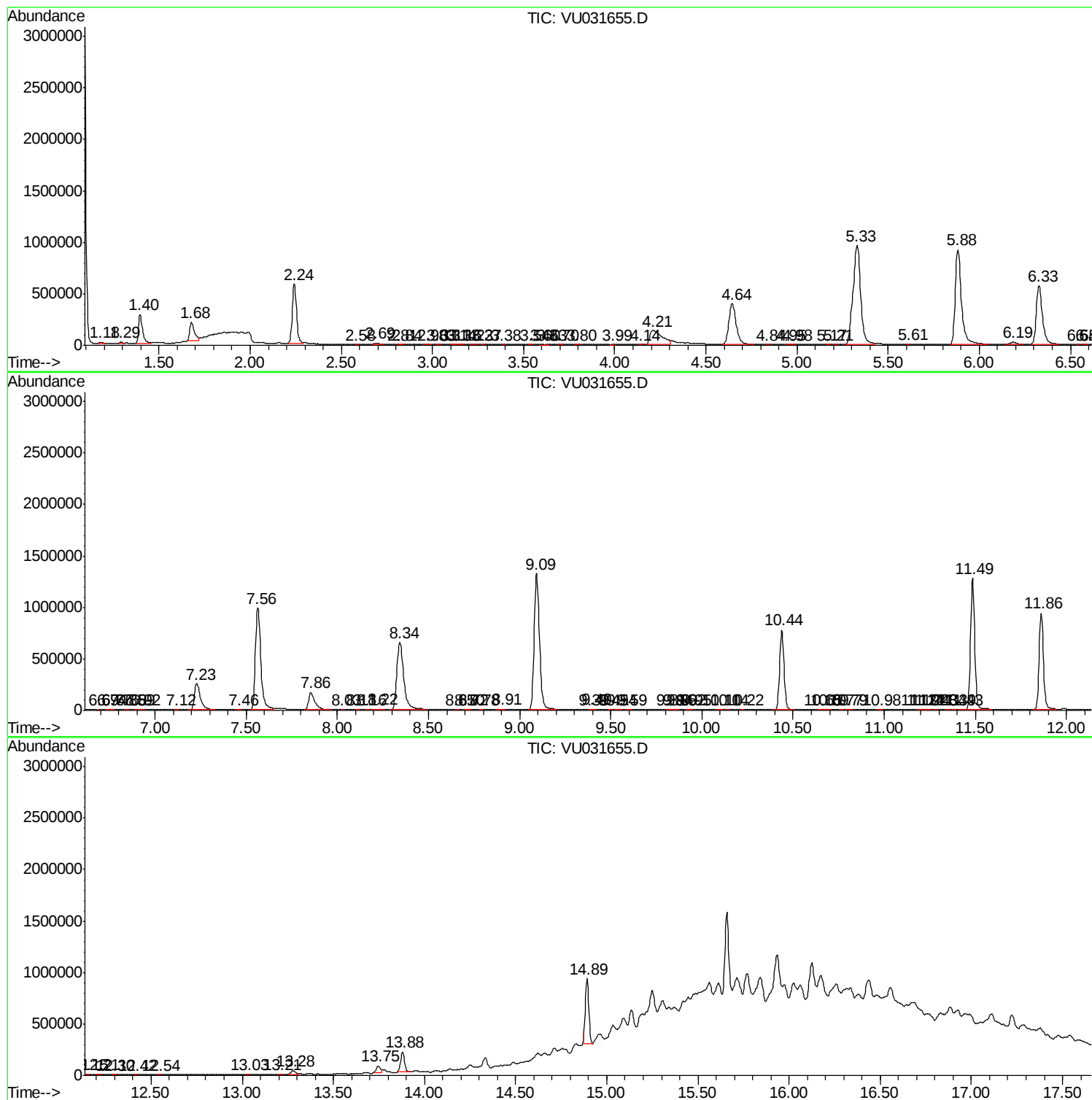
Sum of corrected areas: 23829895

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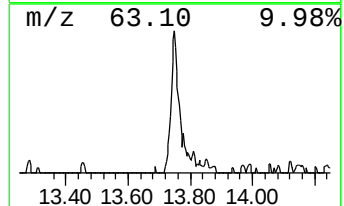
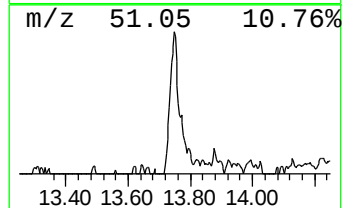
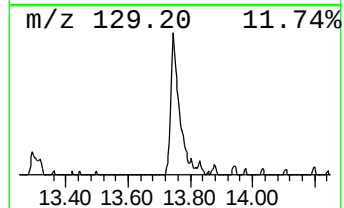
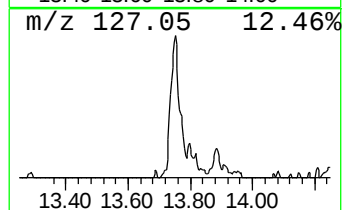
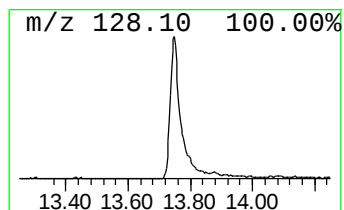
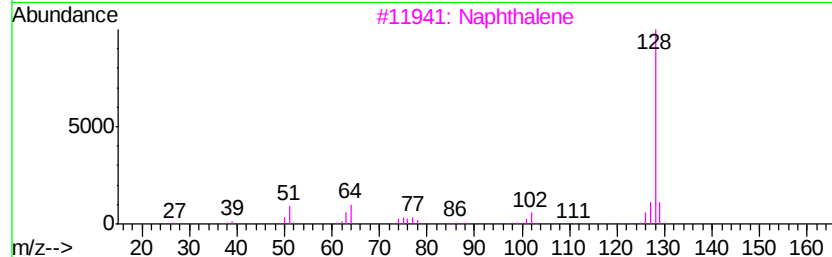
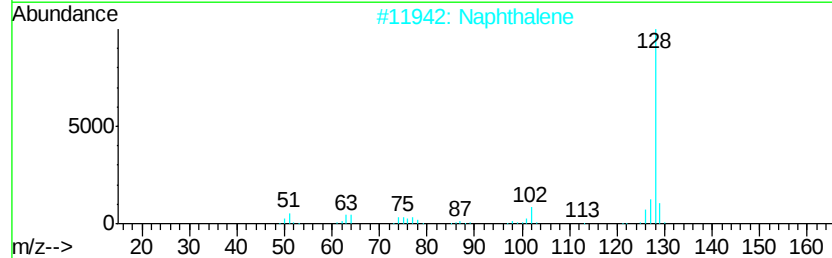
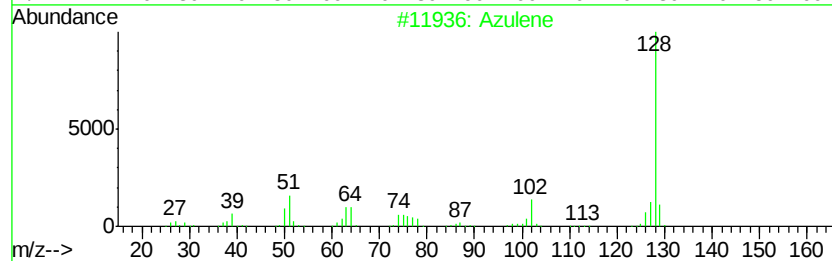
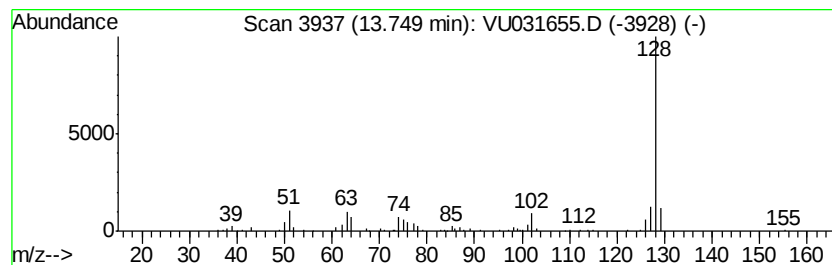
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.75 ug/L	113574	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene		128	C10H8	000275-51-4	94
2	Naphthalene		128	C10H8	000091-20-3	94
3	Naphthalene		128	C10H8	000091-20-3	91
4	Naphthalene		128	C10H8	000091-20-3	91
5	Azulene		128	C10H8	000275-51-4	91



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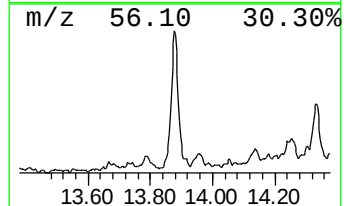
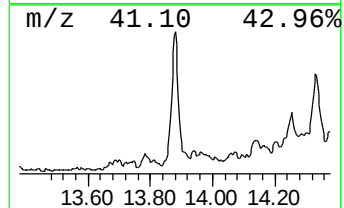
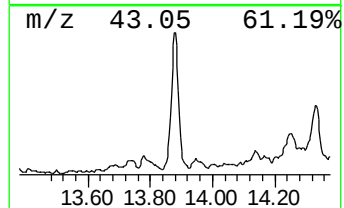
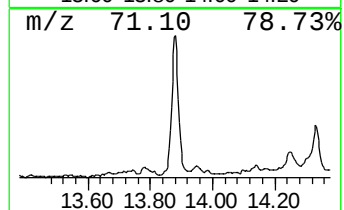
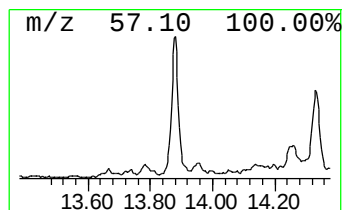
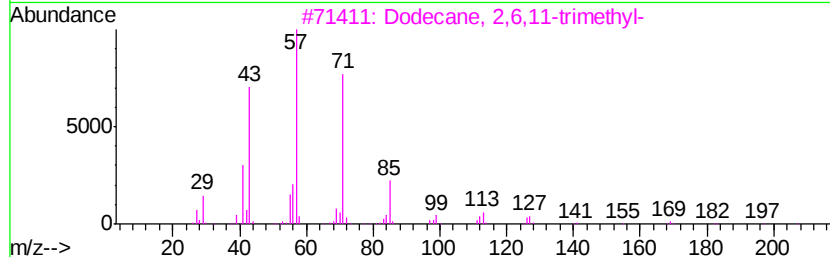
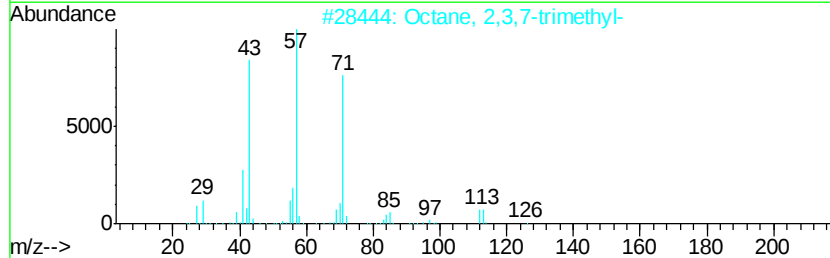
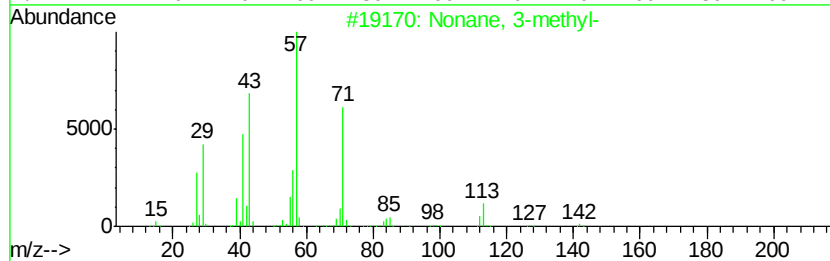
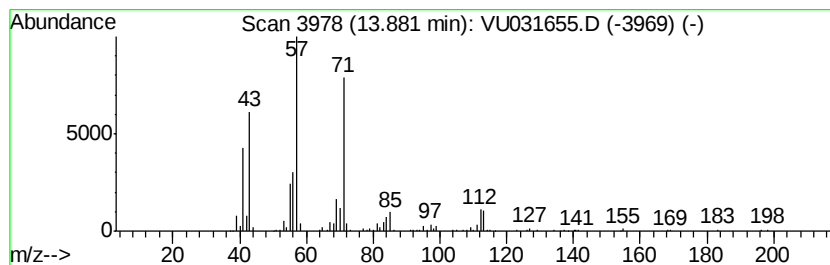
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Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.09 ug/L	293330	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 3-methyl-	142	C10H22	005911-04-6	83
2		Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	78
3		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	78
4		Tridecane, 7-methyl-	198	C14H30	026730-14-3	78
5		Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	64



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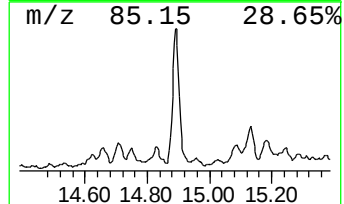
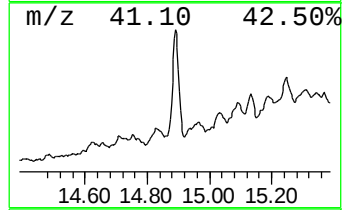
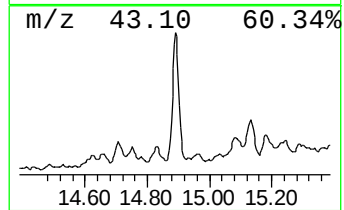
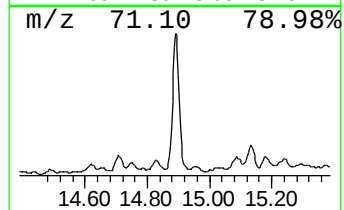
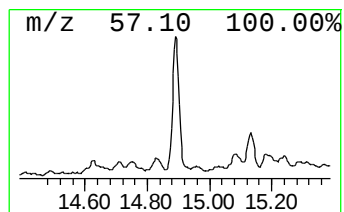
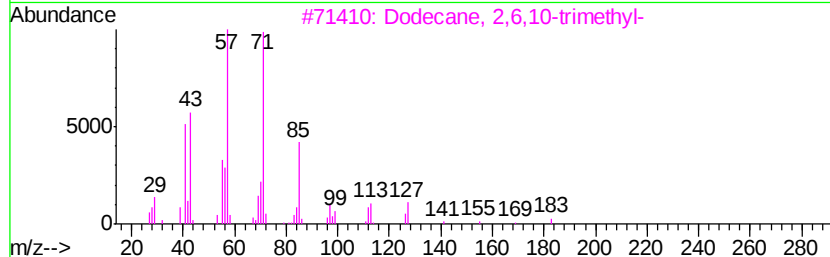
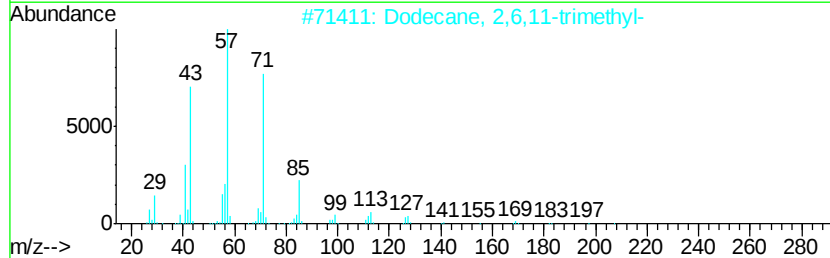
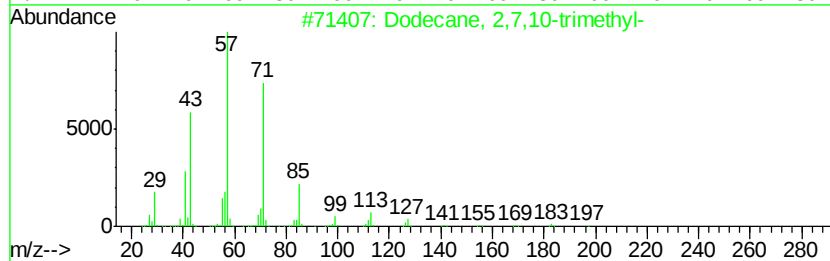
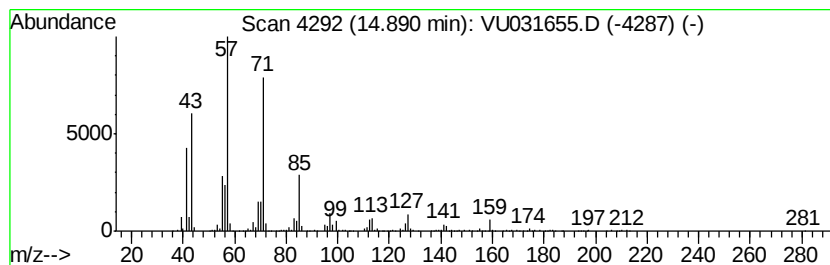
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	20.39 ug/L	843014	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
2		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	90
3		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	87
4		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
5		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU043019\
Data File : VU031655.D
Acq On : 01 May 2019 00:15
Operator : JC/SP
Sample : K2604-11
Misc : 5.08g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAJ85

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
Azulene	13.75	2.8	ug/L	113574	3	11.49	2067320	50.0
(DEL) Alkane: Str...	13.88	7.1	ug/L	293330	3	11.49	2067320	50.0
(DEL) Alkane: Str...	14.89	20.4	ug/L	843014	3	11.49	2067320	50.0