

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU031519\
 Data File : VU030064.D
 Acq On : 14 Mar 2019 11:22
 Operator : JC/SP
 Sample : K1784-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0962

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\SOMULM031319WMA.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	25	29	38	rVB2	11136	10499	0.12%	0.039%
2	1.399	89	96	109	rVB	223308	237323	2.72%	0.884%
3	1.476	114	120	133	rVB	34094	40436	0.46%	0.151%
4	1.682	176	184	200	rVB	169233	211456	2.43%	0.787%
5	2.190	337	342	351	rVB6	4433	6059	0.07%	0.023%
6	2.273	355	368	378	rVV	381587	606338	6.96%	2.258%
7	2.331	378	386	405	rVB	94310	171086	1.96%	0.637%
8	2.450	419	423	425	rBV3	1312	1091	0.01%	0.004%
9	2.479	425	432	442	rVV4	4681	10492	0.12%	0.039%
10	2.701	486	501	562	rBV	4832033	8717657	100.00%	32.459%
11	2.984	585	589	590	rBV2	982	673	0.01%	0.003%
12	3.058	610	612	616	rBV4	410	294	0.00%	0.001%
13	3.132	627	635	638	rBV5	785	1287	0.01%	0.005%
14	3.190	641	653	662	rBV3	4907	8912	0.10%	0.033%
15	3.280	675	681	683	rBV2	825	799	0.01%	0.003%
16	3.698	807	811	815	rBV2	721	733	0.01%	0.003%
17	3.717	815	817	819	rVV2	613	317	0.00%	0.001%
18	3.862	854	862	863	rBV	467	600	0.01%	0.002%
19	3.910	871	877	881	rVB3	1004	973	0.01%	0.004%
20	4.000	893	905	919	rBV4	9400	25311	0.29%	0.094%
21	4.183	949	962	969	rBV	133181	317951	3.65%	1.184%
22	4.383	1012	1024	1052	rVB	78300	188150	2.16%	0.701%
23	4.582	1081	1086	1087	rBV4	1042	889	0.01%	0.003%
24	4.650	1090	1107	1140	rVV3	284417	841039	9.65%	3.131%
25	4.887	1178	1181	1184	rBV2	915	666	0.01%	0.002%
26	5.129	1252	1256	1259	rBV4	578	411	0.00%	0.002%
27	5.338	1297	1321	1356	rBV2	530570	1552265	17.81%	5.780%
28	5.540	1381	1384	1387	rBV3	528	428	0.00%	0.002%
29	5.592	1392	1400	1401	rBV4	1552	1338	0.02%	0.005%
30	5.659	1418	1421	1423	rVB2	566	304	0.00%	0.001%
31	5.675	1423	1426	1430	rVB4	971	715	0.01%	0.003%
32	5.698	1430	1433	1435	rBV2	540	320	0.00%	0.001%
33	5.768	1448	1455	1456	rBV4	2082	2347	0.03%	0.009%
34	5.884	1474	1491	1522	rBV	514605	1109944	12.73%	4.133%

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 Title : VOC Analysis

35	6.183	1569	1584	1615	rBV	2086507	4032487	46.26%	15.014%
36	6.328	1617	1629	1652	rVB	331732	656697	7.53%	2.445%
37	6.717	1744	1750	1755	rBV3	3495	5202	0.06%	0.019%
38	6.817	1777	1781	1783	rBV4	941	702	0.01%	0.003%
39	7.000	1836	1838	1840	rBV	551	313	0.00%	0.001%
40	7.093	1862	1867	1870	rBV3	1197	1244	0.01%	0.005%
41	7.225	1893	1908	1932	rBV	190264	355834	4.08%	1.325%
42	7.466	1974	1983	1995	rVB2	10299	17993	0.21%	0.067%
43	7.563	2000	2013	2032	rBV	718229	1270601	14.58%	4.731%
44	7.813	2087	2091	2092	rBV2	1064	698	0.01%	0.003%
45	7.849	2092	2102	2127	rVV	133273	235168	2.70%	0.876%
46	7.974	2139	2141	2144	rBV4	883	663	0.01%	0.002%
47	8.067	2162	2170	2183	rVB3	14504	24808	0.28%	0.092%
48	8.174	2189	2203	2215	rBV2	64312	132215	1.52%	0.492%
49	8.309	2234	2245	2271	rVB	486373	843279	9.67%	3.140%
50	8.579	2326	2329	2331	rBV3	1153	758	0.01%	0.003%
51	8.649	2349	2351	2356	rVB3	719	555	0.01%	0.002%
52	8.685	2357	2362	2364	rBV3	795	614	0.01%	0.002%
53	8.858	2414	2416	2419	rVB3	672	294	0.00%	0.001%
54	8.874	2419	2421	2424	rBV3	514	287	0.00%	0.001%
55	8.903	2424	2430	2438	rBV6	3686	5986	0.07%	0.022%
56	8.977	2450	2453	2455	rBV3	391	317	0.00%	0.001%
57	9.087	2473	2487	2507	rBV	748758	1252175	14.36%	4.662%
58	9.247	2532	2537	2544	rBV4	1695	2229	0.03%	0.008%
59	9.296	2549	2552	2553	rBV2	996	489	0.01%	0.002%
60	9.328	2554	2562	2572	rVV4	8842	14046	0.16%	0.052%
61	9.453	2592	2601	2604	rBV7	922	1462	0.02%	0.005%
62	9.543	2625	2629	2631	rBV2	529	394	0.00%	0.001%
63	9.614	2644	2651	2654	rBV4	818	977	0.01%	0.004%
64	9.646	2659	2661	2665	rBV4	558	393	0.00%	0.001%
65	9.665	2665	2667	2672	rVB2	679	467	0.01%	0.002%
66	9.723	2681	2685	2688	rBV5	630	505	0.01%	0.002%
67	9.778	2691	2702	2711	rBV2	21205	36753	0.42%	0.137%
68	9.929	2736	2749	2752	rBV7	2967	4325	0.05%	0.016%
69	10.042	2773	2784	2789	rBV7	1721	2895	0.03%	0.011%
70	10.087	2789	2798	2802	rBV5	1927	2667	0.03%	0.010%
71	10.164	2816	2822	2824	rBV6	1930	1955	0.02%	0.007%

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72	10.231	2841	2843	2847	rVB4	557	362	0.00%	0.001%
73	10.373	2884	2887	2889	rBV3	477	315	0.00%	0.001%
74	10.427	2889	2904	2924	rVV	499055	805287	9.24%	2.998%
75	10.608	2947	2960	2972	rBV	19377	35025	0.40%	0.130%
76	10.733	2987	2999	3011	rBV4	35354	61369	0.70%	0.228%
77	10.833	3028	3030	3033	rBV2	530	348	0.00%	0.001%
78	10.878	3038	3044	3051	rVB7	1978	2918	0.03%	0.011%
79	10.971	3070	3073	3076	rVB2	576	334	0.00%	0.001%
80	10.990	3076	3079	3081	rBV3	722	466	0.01%	0.002%
81	11.064	3096	3102	3103	rBV3	1091	958	0.01%	0.004%
82	11.109	3112	3116	3119	rVB2	459	315	0.00%	0.001%
83	11.154	3125	3130	3134	rBV5	1043	972	0.01%	0.004%
84	11.254	3141	3161	3175	rBV	65740	125862	1.44%	0.469%
85	11.411	3208	3210	3212	rBV3	863	350	0.00%	0.001%
86	11.479	3219	3231	3250	rVB	804722	1273497	14.61%	4.742%
87	11.678	3291	3293	3298	rVB4	796	595	0.01%	0.002%
88	11.743	3299	3313	3332	rBV	167474	310023	3.56%	1.154%
89	11.855	3337	3348	3371	rVB	728806	1191792	13.67%	4.437%
90	12.382	3505	3512	3524	rBV7	3857	6383	0.07%	0.024%
91	12.472	3531	3540	3557	rBV6	17665	42867	0.49%	0.160%
92	12.890	3664	3670	3679	rBV8	5364	9240	0.11%	0.034%
93	13.357	3811	3815	3817	rBV3	883	812	0.01%	0.003%
94	13.434	3836	3839	3842	rBV2	1070	936	0.01%	0.003%
95	14.115	4048	4051	4054	rVB5	890	609	0.01%	0.002%
96	14.170	4066	4068	4071	rBV2	688	390	0.00%	0.001%
97	14.279	4094	4102	4111	rVB3	3653	6171	0.07%	0.023%
98	14.389	4132	4136	4138	rBV2	814	741	0.01%	0.003%
99	14.511	4170	4174	4177	rBV4	1027	924	0.01%	0.003%
100	15.209	4389	4391	4394	rVB3	653	322	0.00%	0.001%

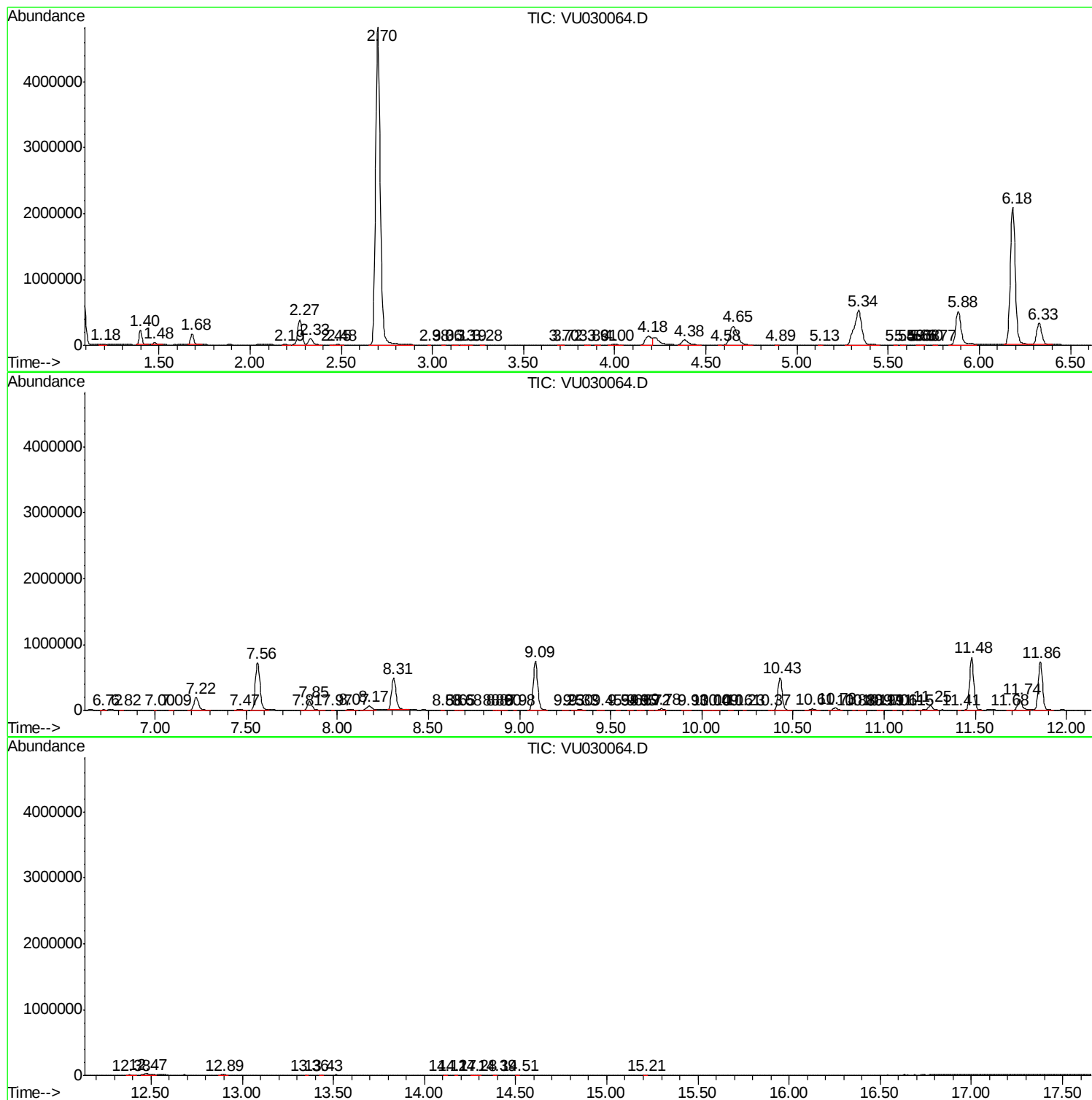
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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



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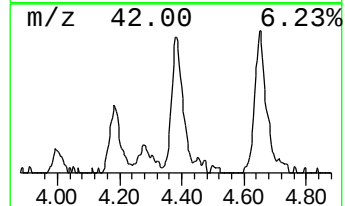
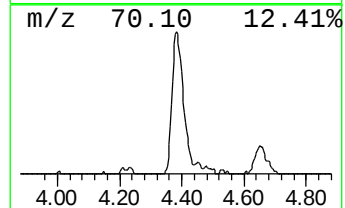
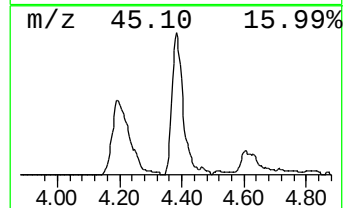
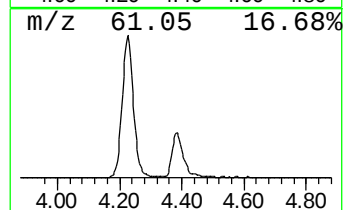
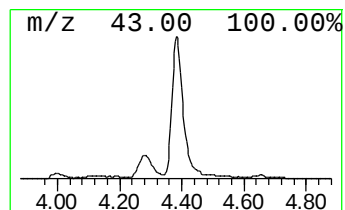
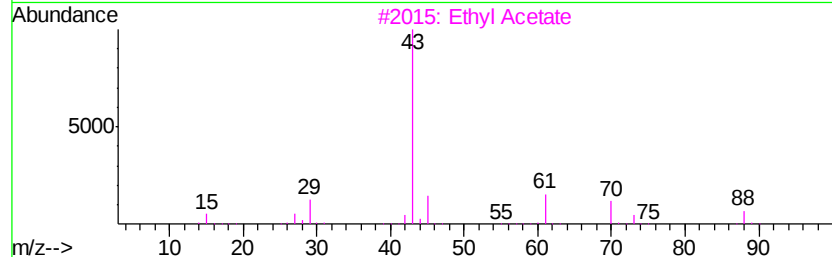
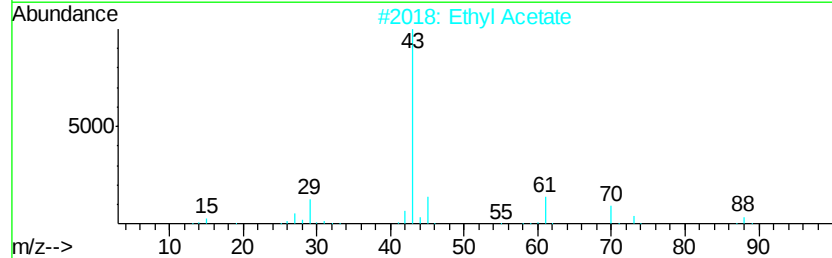
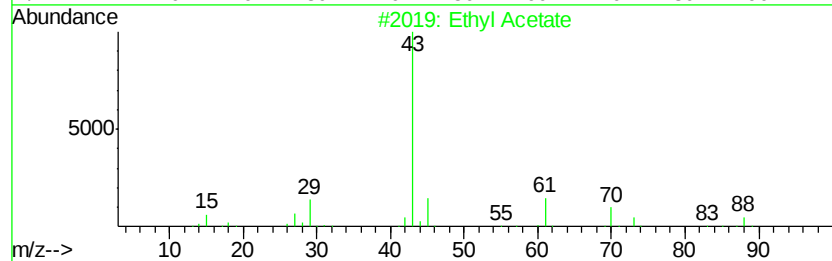
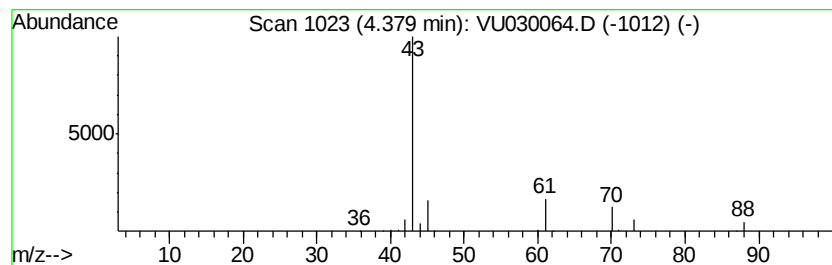
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	8.48 ug/L	188150	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	83
4			Ethyl Acetate	88	C4H8O2	000141-78-6	45
5			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9



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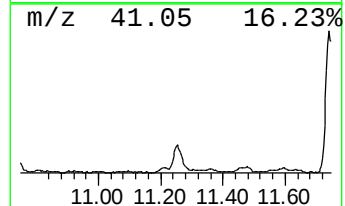
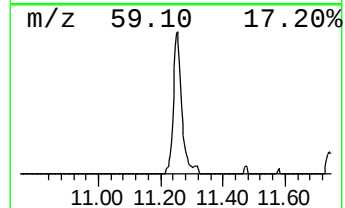
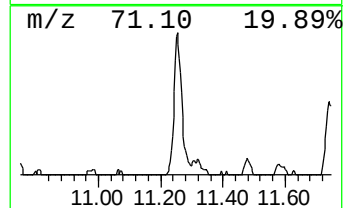
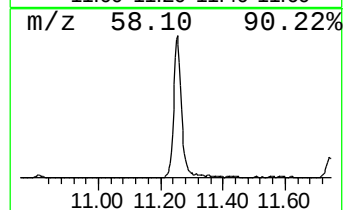
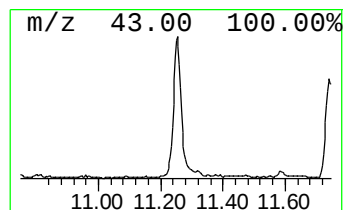
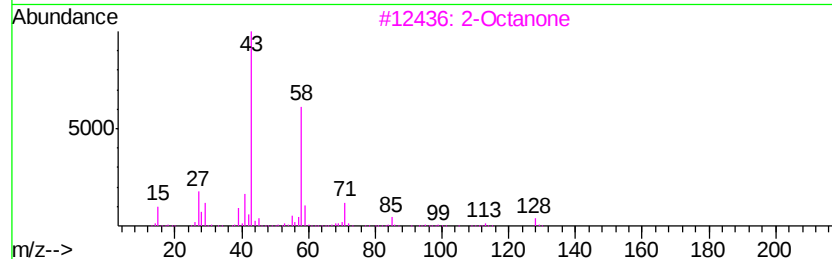
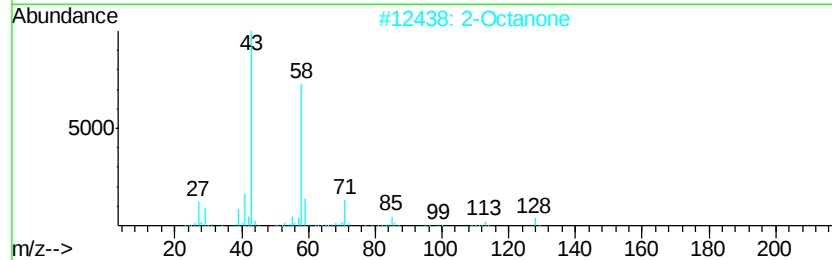
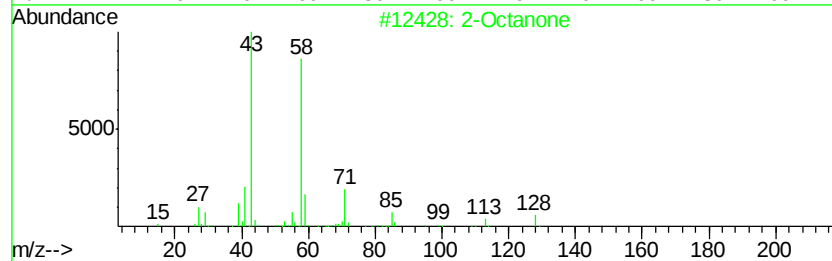
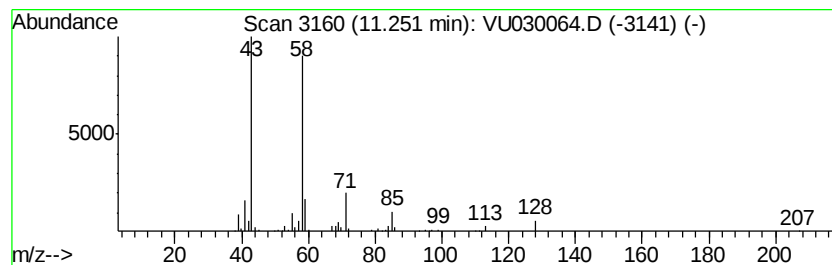
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Quant Title : VOC Analysis

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

Peak Number 4 2-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	4.94 ug/L	125862	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanone	128	C8H16O	000111-13-7	91
2		2-Octanone	128	C8H16O	000111-13-7	91
3		2-Octanone	128	C8H16O	000111-13-7	91
4		2-Octanone	128	C8H16O	000111-13-7	81
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72



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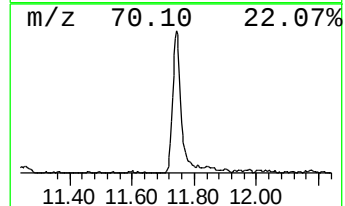
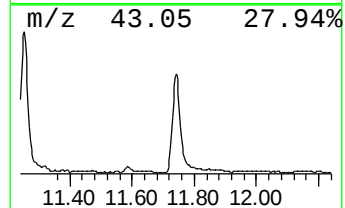
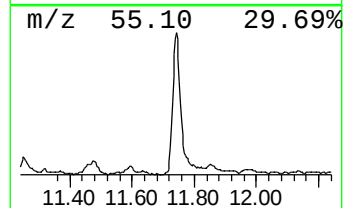
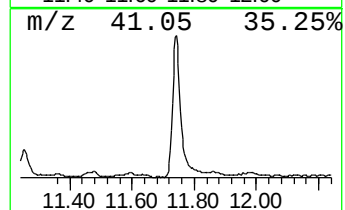
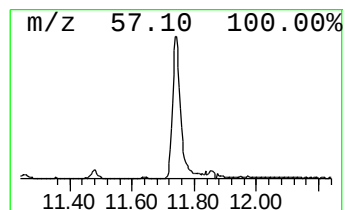
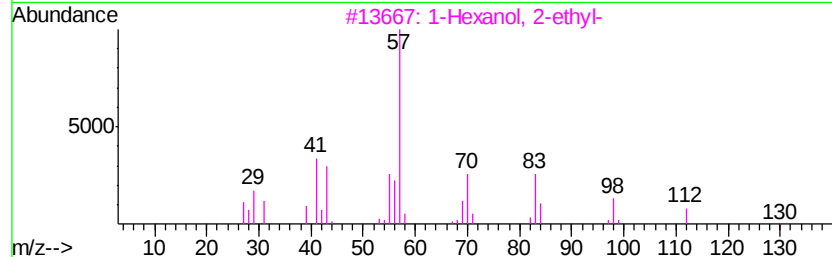
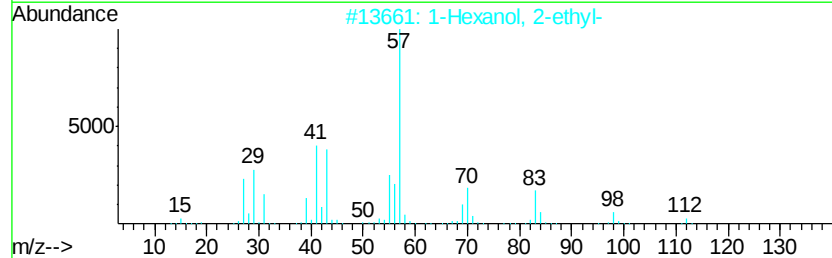
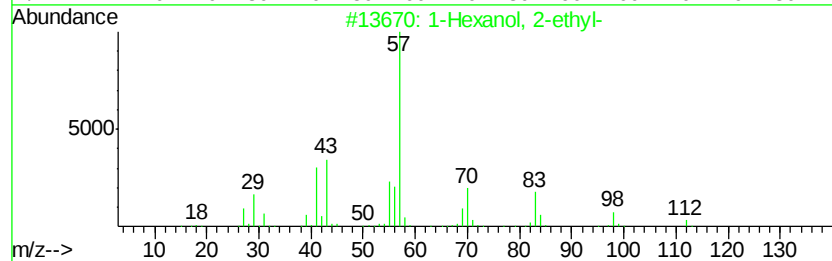
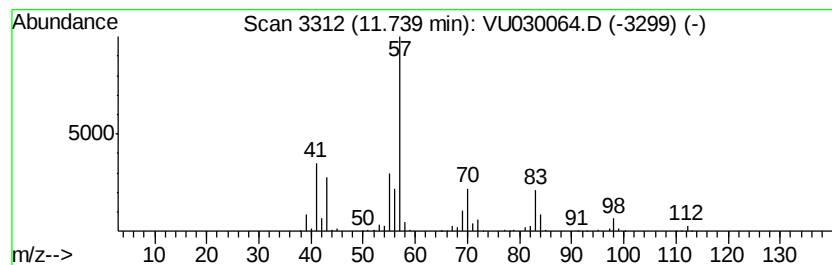
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Quant Title : VOC Analysis

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.74	12.17 ug/L	310023	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU031519\
Data File : VU030064.D
Acq On : 14 Mar 2019 11:22
Operator : JC/SP
Sample : K1784-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0962

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM031319WMA.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
Ethyl Acetate	4.38	8.5	ug/L	188150	1	5.88	1109940	50.0
2-Octanone	11.25	4.9	ug/L	125862	3	11.48	1273500	50.0
1-Hexanol, 2-ethyl-	11.74	12.2	ug/L	310023	3	11.48	1273500	50.0