

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042919\
 Data File : VU031576.D
 Acq On : 29 Apr 2019 11:16
 Operator : JC/SP
 Sample : K2590-12
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0XB3

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	22	28	36	rVB3	53884	53779	1.53%	0.179%
2	1.293	59	63	68	rBV	17123	14684	0.42%	0.049%
3	1.395	88	95	112	rBV	452273	501388	14.29%	1.664%
4	1.682	176	184	200	rVB	360751	457899	13.05%	1.520%
5	1.884	241	247	260	rVB	85615	121471	3.46%	0.403%
6	2.270	357	367	380	rBV	774688	1173921	33.46%	3.896%
7	2.337	382	388	405	rVB4	38746	85582	2.44%	0.284%
8	2.913	563	567	570	rBV4	1916	1451	0.04%	0.005%
9	2.990	588	591	593	rBV3	1424	918	0.03%	0.003%
10	3.051	606	610	613	rVB3	1506	1027	0.03%	0.003%
11	3.186	647	652	655	rBV	2059	1730	0.05%	0.006%
12	3.212	655	660	662	rBV2	1036	831	0.02%	0.003%
13	3.235	662	667	675	rVB6	2241	2992	0.09%	0.010%
14	3.273	675	679	681	rBV2	1297	1088	0.03%	0.004%
15	3.341	698	700	705	rVB3	1253	949	0.03%	0.003%
16	3.373	705	710	712	rBV3	1070	1073	0.03%	0.004%
17	3.595	775	779	781	rBV2	1393	1210	0.03%	0.004%
18	3.675	801	804	808	rVB2	1455	878	0.03%	0.003%
19	3.752	822	828	830	rBV4	939	841	0.02%	0.003%
20	3.800	840	843	845	rBV2	1157	859	0.02%	0.003%
21	3.845	852	857	863	rBV4	838	1130	0.03%	0.004%
22	4.093	930	934	938	rBV3	1385	1233	0.04%	0.004%
23	4.186	945	963	1001	rBV	292227	993563	28.32%	3.298%
24	4.389	1019	1026	1056	rVB	55437	149572	4.26%	0.496%
25	4.643	1089	1105	1131	rBV	550484	1294500	36.90%	4.297%
26	4.816	1155	1159	1160	rBV4	1173	894	0.03%	0.003%
27	4.878	1173	1178	1180	rBV5	2178	2022	0.06%	0.007%
28	4.977	1204	1209	1211	rBV4	2067	2155	0.06%	0.007%
29	5.083	1238	1242	1246	rBV5	2388	2495	0.07%	0.008%
30	5.119	1251	1253	1255	rBV2	1377	870	0.02%	0.003%
31	5.180	1269	1272	1275	rVB4	1648	1095	0.03%	0.004%
32	5.222	1279	1285	1288	rBV6	921	969	0.03%	0.003%
33	5.334	1292	1320	1353	rBV2	1106196	3377163	96.27%	11.209%
34	5.691	1429	1431	1435	rVB4	2142	1258	0.04%	0.004%

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 Title : VOC Analysis

35	5.881	1475	1490	1530	rBV	860079	1828180	52.11%	6.068%
36	6.080	1550	1552	1555	rBV3	1956	1091	0.03%	0.004%
37	6.183	1568	1584	1615	rBV	1732036	3508005	100.00%	11.644%
38	6.324	1617	1628	1664	rVB	743224	1566383	44.65%	5.199%
39	6.633	1718	1724	1728	rBV6	2043	1788	0.05%	0.006%
40	6.659	1728	1732	1736	rVV4	1277	1054	0.03%	0.003%
41	6.697	1742	1744	1748	rVB3	1120	796	0.02%	0.003%
42	6.775	1764	1768	1770	rBV2	1206	868	0.02%	0.003%
43	6.900	1805	1807	1809	rVV3	1102	729	0.02%	0.002%
44	6.929	1812	1816	1821	rVB4	1611	1736	0.05%	0.006%
45	7.103	1866	1870	1875	rBV3	1352	1438	0.04%	0.005%
46	7.164	1884	1889	1891	rBV3	1050	857	0.02%	0.003%
47	7.177	1891	1893	1896	rBV2	1053	856	0.02%	0.003%
48	7.225	1896	1908	1930	rBV	383698	727884	20.75%	2.416%
49	7.392	1954	1960	1967	rVB6	2277	2994	0.09%	0.010%
50	7.511	1994	1997	1999	rBV3	1992	1181	0.03%	0.004%
51	7.562	1999	2013	2047	rBV	1334919	2489169	70.96%	8.262%
52	7.848	2091	2102	2124	rBV	259499	482410	13.75%	1.601%
53	8.093	2176	2178	2181	rBV3	996	752	0.02%	0.002%
54	8.176	2194	2204	2207	rVV4	18369	26953	0.77%	0.089%
55	8.221	2208	2218	2235	rVV	775462	1362629	38.84%	4.523%
56	8.312	2236	2246	2289	rVB	1031752	2060939	58.75%	6.841%
57	8.646	2347	2350	2353	rBV4	1944	1580	0.05%	0.005%
58	8.704	2364	2368	2371	rBV2	1979	1724	0.05%	0.006%
59	8.955	2442	2446	2449	rBV5	1738	1442	0.04%	0.005%
60	8.996	2456	2459	2463	rBV4	1574	1067	0.03%	0.004%
61	9.019	2463	2466	2471	rBV5	1425	1327	0.04%	0.004%
62	9.086	2474	2487	2523	rBV	1266938	2251457	64.18%	7.473%
63	9.305	2552	2555	2557	rBV2	1495	924	0.03%	0.003%
64	9.411	2585	2588	2591	rBV4	1166	874	0.02%	0.003%
65	9.463	2600	2604	2606	rBV4	2195	1720	0.05%	0.006%
66	9.591	2642	2644	2650	rVB3	1720	1465	0.04%	0.005%
67	9.620	2650	2653	2657	rVB2	1839	1126	0.03%	0.004%
68	9.717	2680	2683	2687	rVB4	1990	1629	0.05%	0.005%
69	9.739	2687	2690	2692	rBV3	1461	1032	0.03%	0.003%
70	9.774	2698	2701	2708	rBV4	2121	1723	0.05%	0.006%
71	9.910	2741	2743	2749	rVB4	1052	1097	0.03%	0.004%

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72	9.971	2759	2762	2766	rVB2	1995	1248	0.04%	0.004%
73	9.993	2766	2769	2772	rBV4	1428	1258	0.04%	0.004%
74	10.064	2789	2791	2792	rBV	1660	755	0.02%	0.003%
75	10.131	2808	2812	2813	rBV2	1638	1149	0.03%	0.004%
76	10.215	2827	2838	2840	rBV6	5084	6345	0.18%	0.021%
77	10.308	2865	2867	2871	rVB3	1493	809	0.02%	0.003%
78	10.340	2872	2877	2880	rBV2	1854	1299	0.04%	0.004%
79	10.376	2884	2888	2890	rBV3	1282	937	0.03%	0.003%
80	10.427	2890	2904	2932	rVV	968353	1574227	44.88%	5.225%
81	10.601	2947	2958	2968	rBV5	17054	32221	0.92%	0.107%
82	10.678	2979	2982	2985	rVB3	1482	849	0.02%	0.003%
83	10.700	2985	2989	2994	rBV3	1306	1470	0.04%	0.005%
84	10.951	3063	3067	3070	rBV3	1199	999	0.03%	0.003%
85	11.035	3088	3093	3095	rBV3	1163	1042	0.03%	0.003%
86	11.064	3099	3102	3104	rBV2	1169	739	0.02%	0.002%
87	11.212	3145	3148	3154	rBV3	1059	1050	0.03%	0.003%
88	11.315	3178	3180	3183	rBV3	1327	953	0.03%	0.003%
89	11.482	3219	3232	3258	rBV	1077414	1778143	50.69%	5.902%
90	11.749	3306	3315	3331	rBV	68919	148285	4.23%	0.492%
91	11.855	3337	3348	3376	rVB	1188713	1966835	56.07%	6.528%
92	12.527	3553	3557	3559	rBV3	2617	1921	0.05%	0.006%
93	12.678	3602	3604	3606	rBV2	1667	928	0.03%	0.003%
94	12.729	3616	3620	3623	rBV3	1428	1356	0.04%	0.005%
95	12.993	3698	3702	3706	rBV5	2467	2437	0.07%	0.008%
96	13.163	3752	3755	3759	rVB3	1634	1231	0.04%	0.004%
97	13.221	3771	3773	3777	rVB3	1806	1155	0.03%	0.004%
98	13.980	4007	4009	4012	rBV2	1540	791	0.02%	0.003%
99	14.086	4038	4042	4048	rBV6	2506	3089	0.09%	0.010%
100	14.495	4165	4169	4172	rBV4	2106	2096	0.06%	0.007%

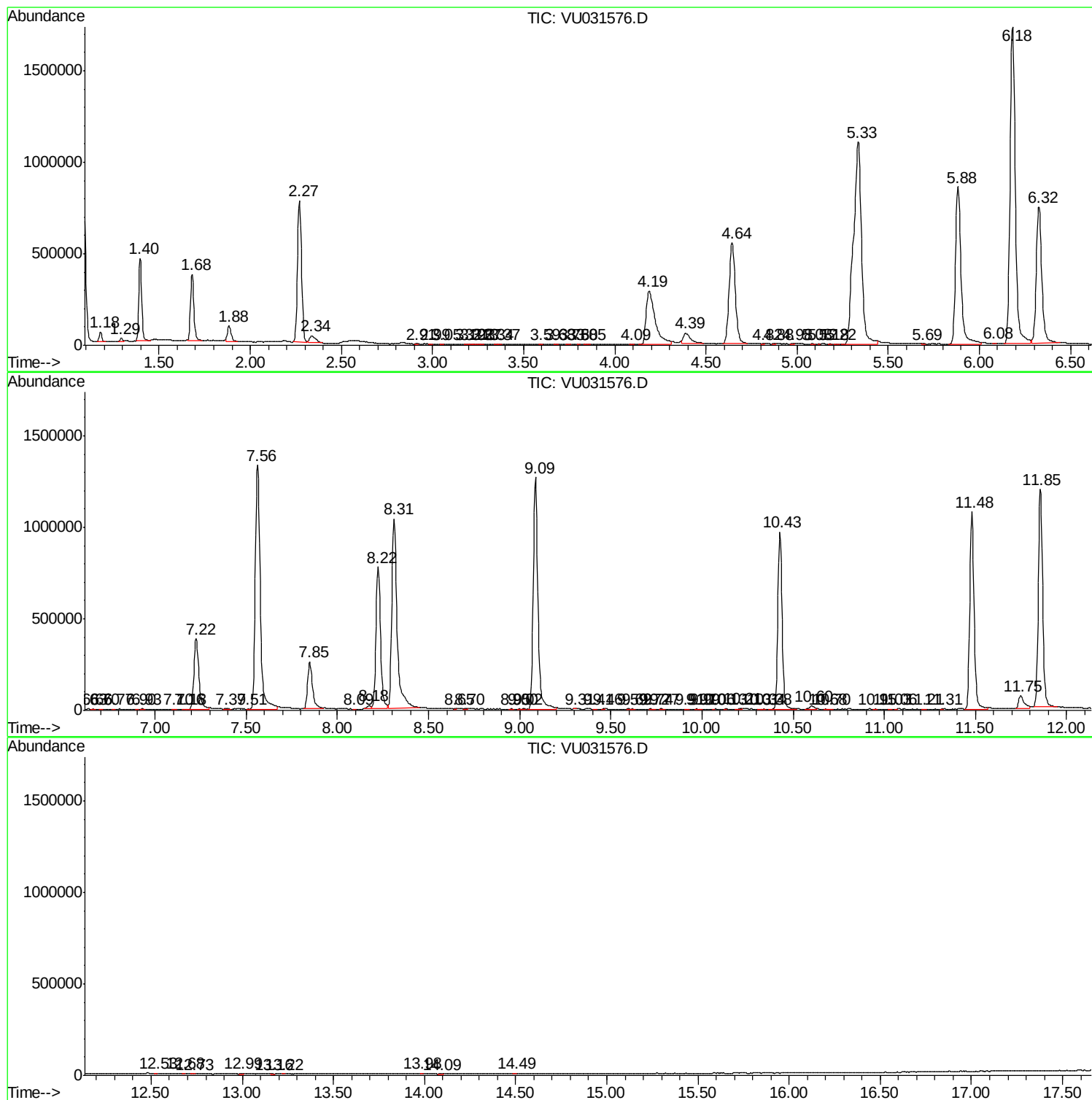
Sum of corrected areas: 30127986

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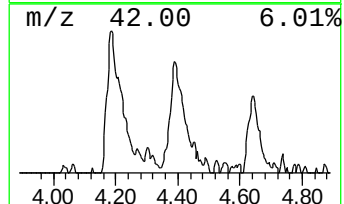
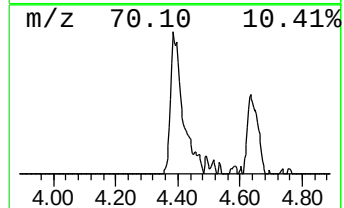
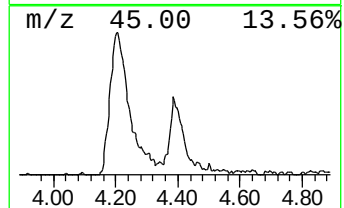
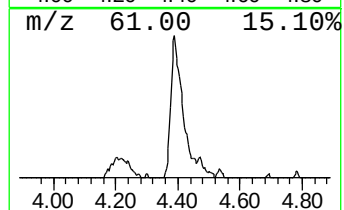
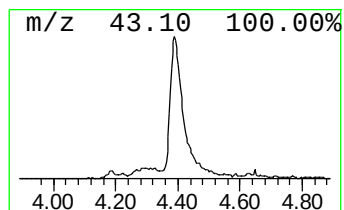
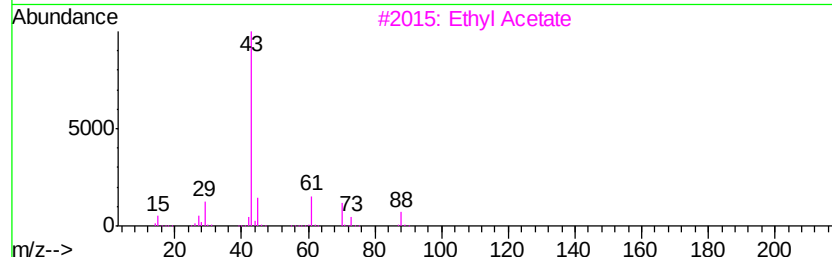
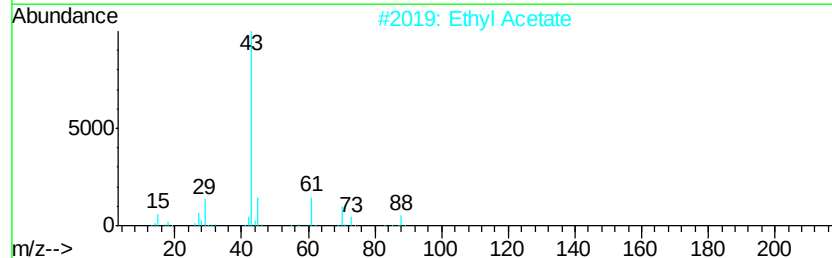
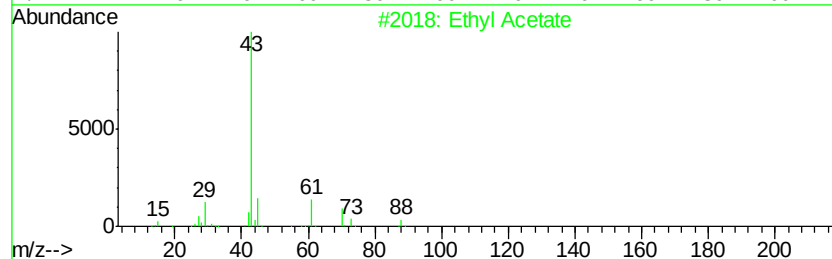
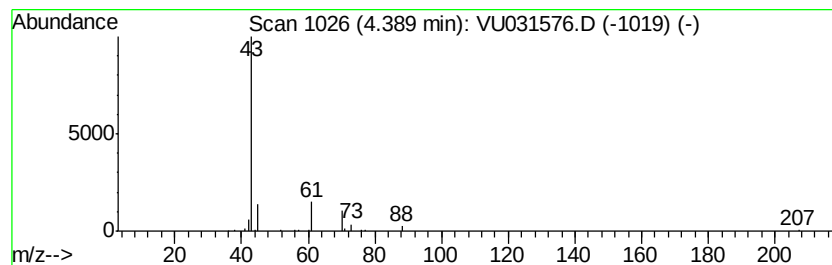
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	4.09 ug/L	149572	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	80
2		Ethyl Acetate	88	C4H8O2	000141-78-6	72
3		Ethyl Acetate	88	C4H8O2	000141-78-6	72
4		Ethyl Acetate	88	C4H8O2	000141-78-6	59
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9



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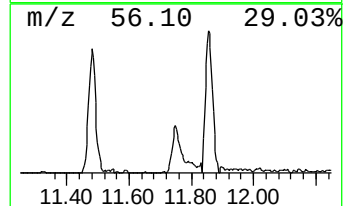
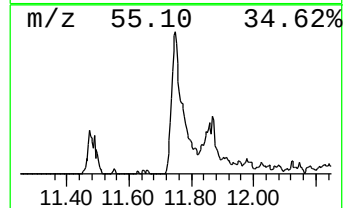
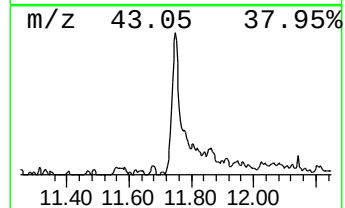
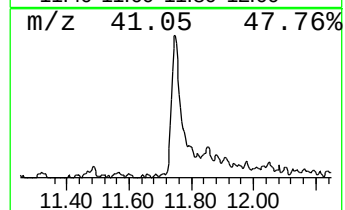
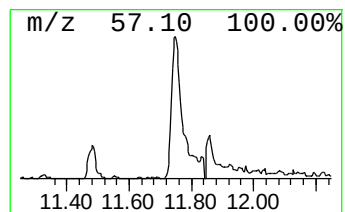
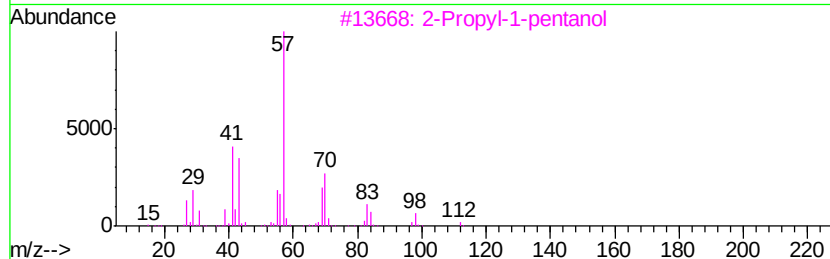
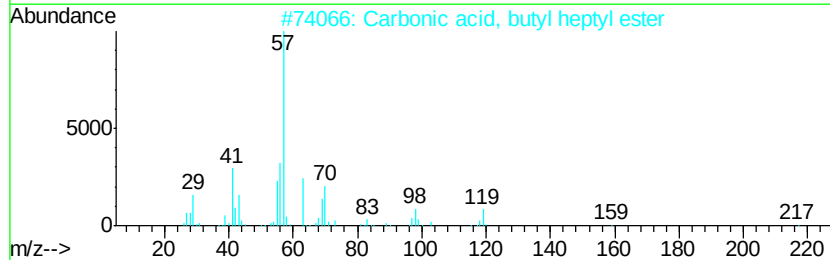
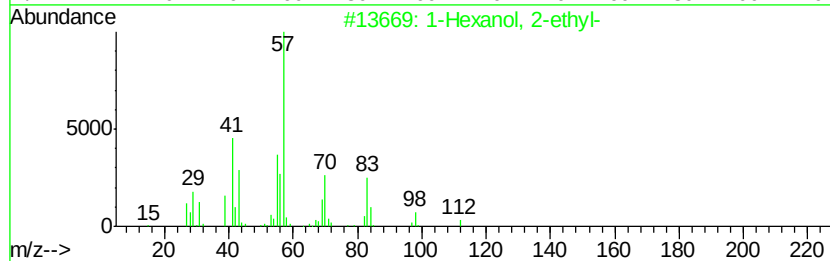
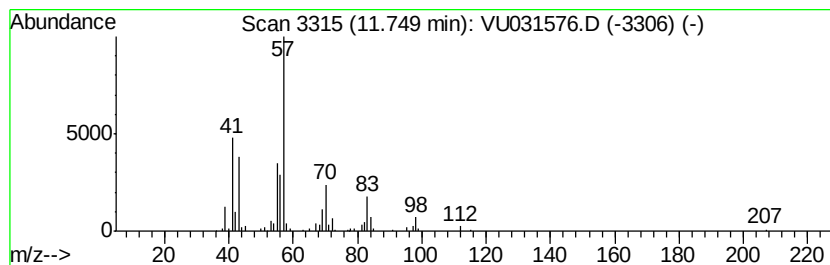
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Quant Title : VOC Analysis

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.17 ug/L	148285	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	64
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
5		1-Hexanethiol, 2-ethyl-	146	C8H18S	007341-17-5	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.39	4.1	ug/L	149572	1	5.88	1828180	50.0
1-Hexanol, 2-ethyl-	11.75	4.2	ug/L	148285	3	11.48	1778140	50.0