

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042919\
 Data File : VU031575.D
 Acq On : 29 Apr 2019 10:53
 Operator : JC/SP
 Sample : K2590-06
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0X96

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	23	28	36	rVB2	58791	55661	1.63%	0.221%
2	1.292	59	63	67	rBV	19943	14708	0.43%	0.058%
3	1.395	88	95	106	rBV	462851	504947	14.79%	2.007%
4	1.682	176	184	201	rVB	359589	464262	13.60%	1.845%
5	1.884	241	247	257	rVB2	76589	102661	3.01%	0.408%
6	2.270	357	367	379	rBV	769545	1170795	34.30%	4.653%
7	2.337	381	388	400	rVB2	39189	74237	2.17%	0.295%
8	2.836	531	543	557	rBV2	15994	36714	1.08%	0.146%
9	2.984	586	589	592	rBV5	1657	1134	0.03%	0.005%
10	3.003	592	595	598	rVB2	1542	1045	0.03%	0.004%
11	3.022	598	601	606	rVB3	1464	1323	0.04%	0.005%
12	3.048	606	609	614	rBV3	1819	1892	0.06%	0.008%
13	3.144	636	639	641	rBV3	1956	1321	0.04%	0.005%
14	3.196	650	655	661	rBV4	2551	3298	0.10%	0.013%
15	3.257	669	674	676	rBV	1653	1648	0.05%	0.007%
16	3.273	677	679	686	rVV5	2338	2843	0.08%	0.011%
17	3.305	686	689	692	rVV2	1506	1005	0.03%	0.004%
18	3.334	696	698	702	rVB2	1394	942	0.03%	0.004%
19	3.399	713	718	721	rBV3	1119	1090	0.03%	0.004%
20	3.485	740	745	748	rBV3	1093	1077	0.03%	0.004%
21	3.614	781	785	790	rBV3	1359	1427	0.04%	0.006%
22	3.813	844	847	850	rBV2	1173	1017	0.03%	0.004%
23	3.887	867	870	874	rVB2	1572	1141	0.03%	0.005%
24	4.058	919	923	925	rBV	1093	836	0.02%	0.003%
25	4.183	949	962	1013	rBV	318995	1052872	30.85%	4.184%
26	4.392	1019	1027	1056	rVB2	38885	109963	3.22%	0.437%
27	4.643	1089	1105	1134	rVB	546600	1293029	37.88%	5.139%
28	4.890	1174	1182	1187	rVB10	1913	3142	0.09%	0.012%
29	5.070	1235	1238	1240	rBV2	1553	820	0.02%	0.003%
30	5.135	1253	1258	1266	rVB7	1542	2066	0.06%	0.008%
31	5.206	1278	1280	1283	rVB3	1618	805	0.02%	0.003%
32	5.234	1283	1289	1293	rBV2	1266	1399	0.04%	0.006%
33	5.337	1297	1321	1355	rBV2	1121247	3413363	100.00%	13.566%
34	5.781	1456	1459	1461	rBV3	1627	995	0.03%	0.004%

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 Title : VOC Analysis

35	5.884	1477	1491	1523	rBV	756572	1601864	46.93%	6.366%
36	6.186	1572	1585	1605	rBV5	56177	128751	3.77%	0.512%
37	6.328	1615	1629	1665	rBV	750034	1557991	45.64%	6.192%
38	6.636	1722	1725	1731	rVB5	1312	1255	0.04%	0.005%
39	6.691	1740	1742	1746	rVB2	1848	943	0.03%	0.004%
40	6.720	1746	1751	1754	rBV4	988	810	0.02%	0.003%
41	6.787	1767	1772	1779	rVB6	1780	2288	0.07%	0.009%
42	6.839	1785	1788	1790	rBV2	1642	1068	0.03%	0.004%
43	6.910	1804	1810	1812	rVV5	1861	1938	0.06%	0.008%
44	6.922	1812	1814	1817	rVB3	2060	1001	0.03%	0.004%
45	6.964	1823	1827	1831	rBV4	1153	938	0.03%	0.004%
46	7.061	1854	1857	1860	rBV3	1070	786	0.02%	0.003%
47	7.099	1864	1869	1871	rBV2	1135	1021	0.03%	0.004%
48	7.225	1896	1908	1930	rBV	383797	734187	21.51%	2.918%
49	7.504	1989	1995	2000	rBV	3040	4000	0.12%	0.016%
50	7.562	2000	2013	2049	rBV	1310928	2470870	72.39%	9.820%
51	7.848	2091	2102	2125	rBV	259109	492683	14.43%	1.958%
52	8.173	2192	2203	2210	rVV2	29869	55085	1.61%	0.219%
53	8.225	2210	2219	2234	rVV2	179860	312218	9.15%	1.241%
54	8.308	2235	2245	2284	rVV	1034428	2036754	59.67%	8.095%
55	8.845	2406	2412	2413	rBV5	1761	1747	0.05%	0.007%
56	8.897	2424	2428	2433	rBV7	2283	2617	0.08%	0.010%
57	9.012	2461	2464	2467	rBV2	1344	1070	0.03%	0.004%
58	9.086	2474	2487	2527	rBV	1107523	2001402	58.63%	7.954%
59	9.302	2551	2554	2557	rBV3	1690	1242	0.04%	0.005%
60	9.382	2576	2579	2580	rBV2	1393	845	0.02%	0.003%
61	9.453	2596	2601	2603	rBV3	2340	1832	0.05%	0.007%
62	9.546	2628	2630	2635	rVB4	1419	963	0.03%	0.004%
63	9.604	2644	2648	2650	rBV5	1139	1011	0.03%	0.004%
64	9.623	2651	2654	2660	rVB5	1523	1419	0.04%	0.006%
65	9.675	2667	2670	2673	rVB4	1791	1214	0.04%	0.005%
66	9.701	2673	2678	2681	rBV3	1981	1788	0.05%	0.007%
67	9.771	2696	2700	2702	rBV2	1120	786	0.02%	0.003%
68	9.845	2721	2723	2728	rVB4	2593	1811	0.05%	0.007%
69	9.881	2728	2734	2739	rBV5	1943	2611	0.08%	0.010%
70	9.906	2739	2742	2745	rVB4	1285	843	0.02%	0.003%
71	9.929	2745	2749	2752	rBV4	1722	1386	0.04%	0.006%

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72	9.967	2757	2761	2764	rBV2	1478	1348	0.04%	0.005%
73	10.212	2831	2837	2844	rBV4	4812	8232	0.24%	0.033%
74	10.427	2891	2904	2926	rBV	979508	1593290	46.68%	6.332%
75	10.604	2950	2959	2969	rVB2	25963	42866	1.26%	0.170%
76	10.729	2991	2998	3001	rBV3	2421	2660	0.08%	0.011%
77	10.745	3001	3003	3009	rVV5	1993	1591	0.05%	0.006%
78	10.813	3020	3024	3029	rBV5	1201	1337	0.04%	0.005%
79	10.909	3048	3054	3055	rBV5	1155	1218	0.04%	0.005%
80	11.131	3117	3123	3126	rVB3	1419	1037	0.03%	0.004%
81	11.151	3126	3129	3132	rBV2	1606	1293	0.04%	0.005%
82	11.356	3190	3193	3197	rVB	1989	1224	0.04%	0.005%
83	11.479	3219	3231	3262	rBV	951833	1585268	46.44%	6.300%
84	11.749	3306	3315	3334	rBV2	49713	120396	3.53%	0.478%
85	11.855	3337	3348	3378	rVB	1180557	2003614	58.70%	7.963%
86	12.472	3533	3540	3550	rBV3	10682	17282	0.51%	0.069%
87	12.646	3592	3594	3598	rBV3	1660	1206	0.04%	0.005%
88	12.778	3633	3635	3640	rVB3	1938	1532	0.04%	0.006%
89	12.919	3676	3679	3685	rVB5	2422	2464	0.07%	0.010%
90	12.948	3685	3688	3690	rBV2	1968	1139	0.03%	0.005%
91	12.983	3697	3699	3705	rBV3	1731	1852	0.05%	0.007%
92	13.160	3750	3754	3759	rBV3	2734	3041	0.09%	0.012%
93	13.247	3778	3781	3787	rBV2	2075	1969	0.06%	0.008%
94	13.411	3828	3832	3835	rBV4	1306	1617	0.05%	0.006%
95	13.479	3849	3853	3856	rBV5	1546	1559	0.05%	0.006%
96	13.524	3865	3867	3869	rBV3	1545	802	0.02%	0.003%
97	13.765	3939	3942	3944	rBV2	1618	1030	0.03%	0.004%
98	13.961	4001	4003	4006	rBV	1814	1395	0.04%	0.006%
99	14.089	4040	4043	4045	rBV3	2255	1479	0.04%	0.006%
100	14.427	4146	4148	4154	rVB5	2128	1379	0.04%	0.005%

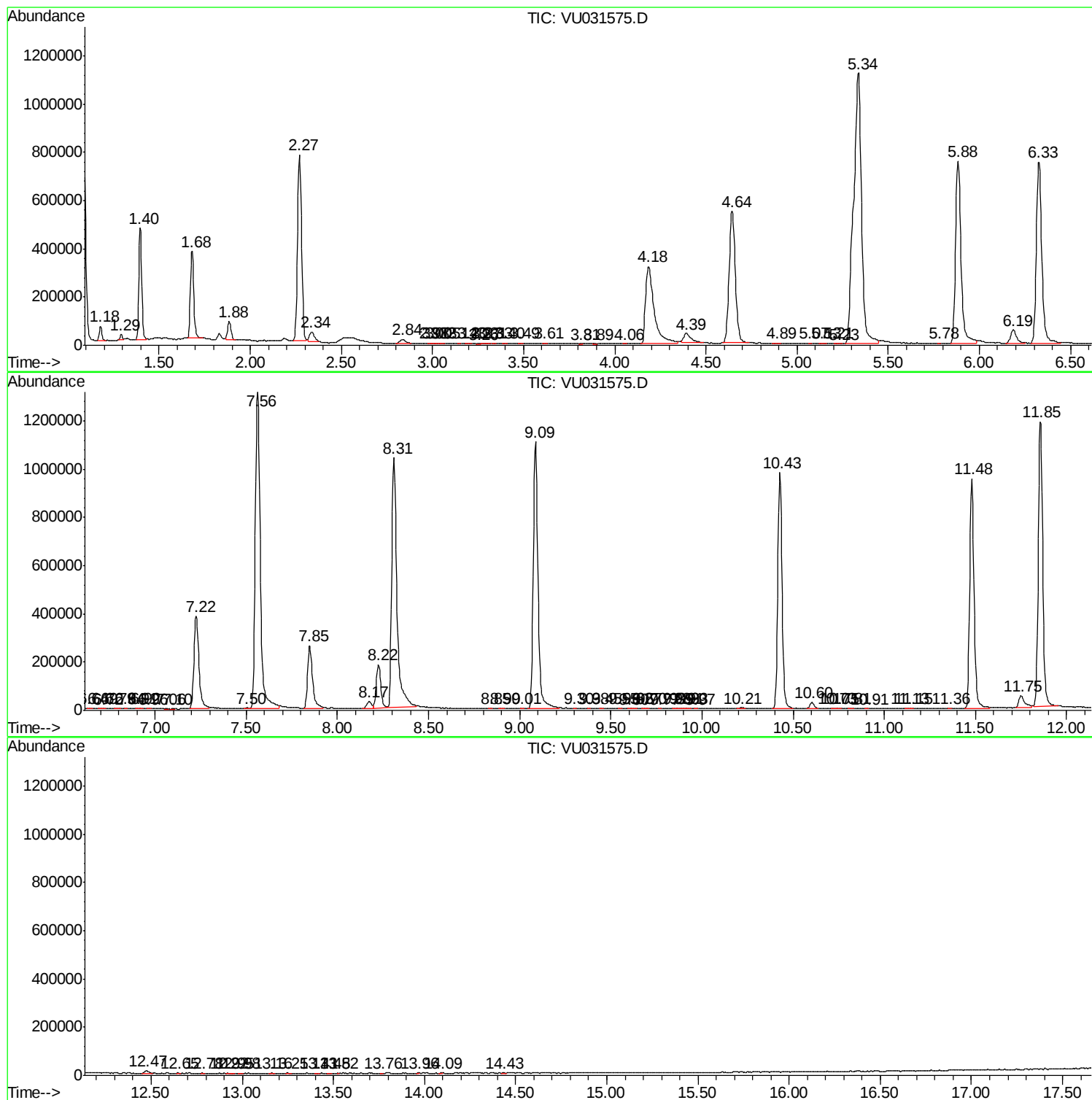
Sum of corrected areas: 25161636

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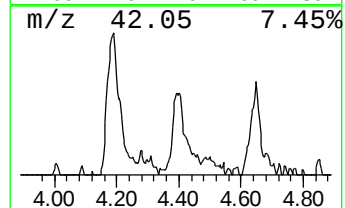
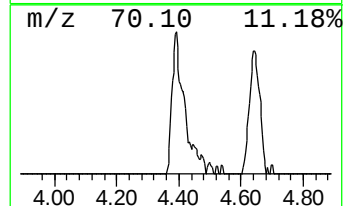
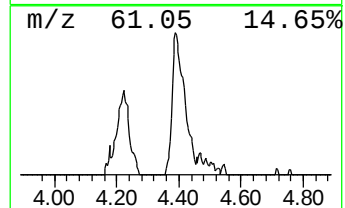
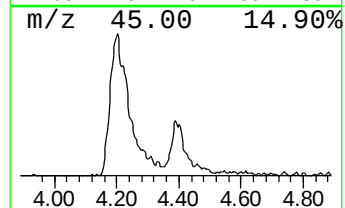
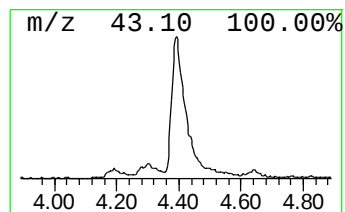
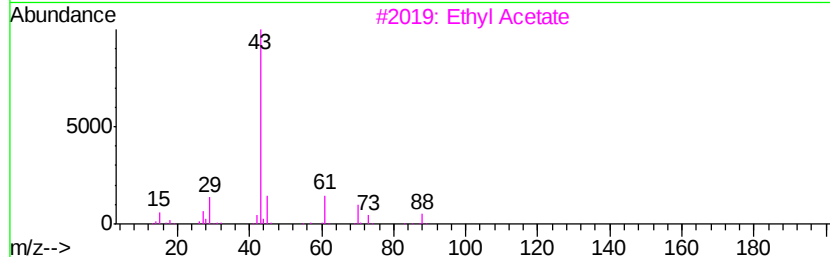
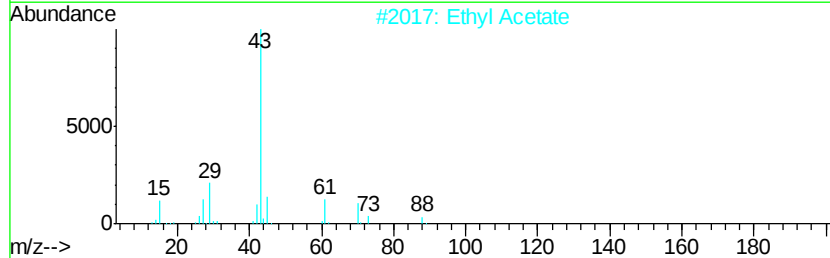
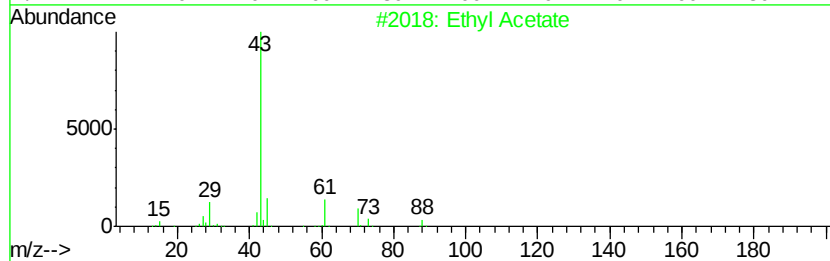
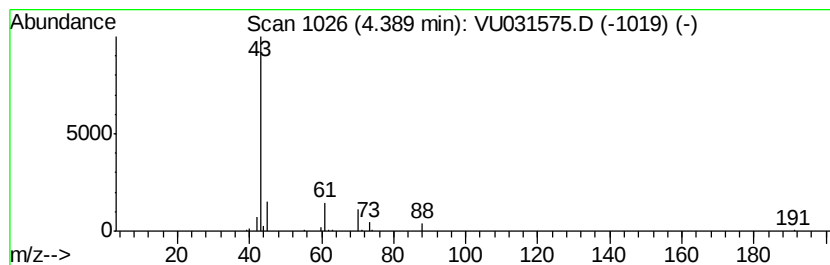
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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	3.43 ug/L	109963	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	90
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	78
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	33



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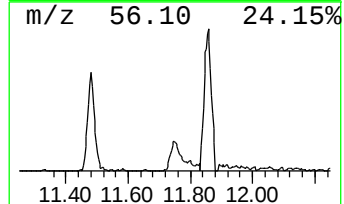
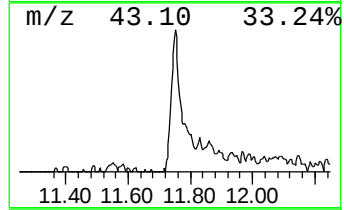
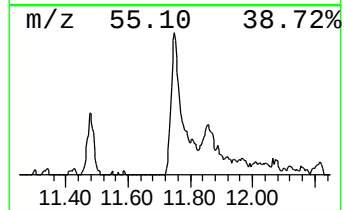
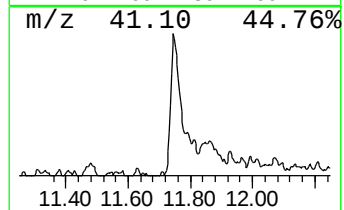
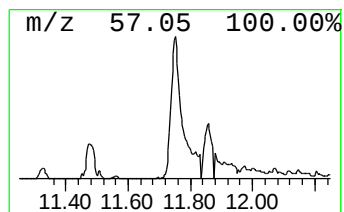
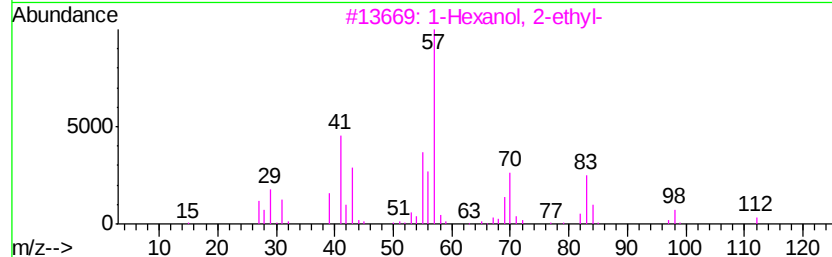
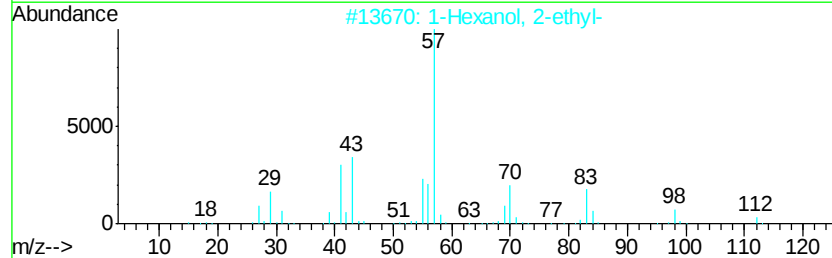
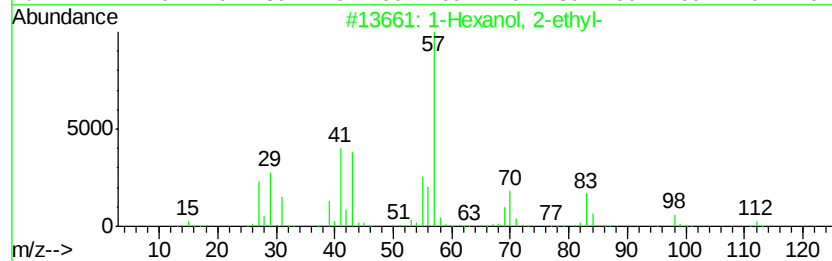
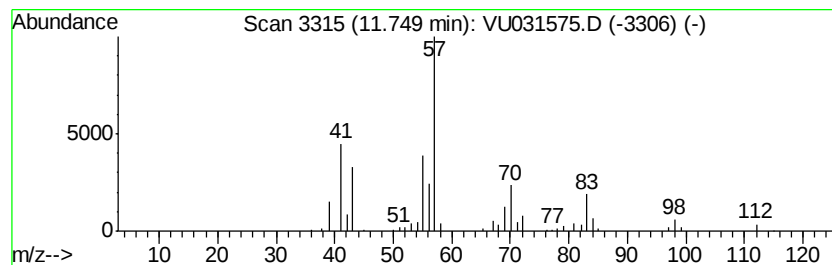
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.80 ug/L	120396	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 78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 72
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 64
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3 53
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.39	3.4	ug/L	109963	1	5.88	1601860	50.0
1-Hexanol, 2-ethyl-	11.75	3.8	ug/L	120396	3	11.48	1585270	50.0