

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042319\
 Data File : VU031455.D
 Acq On : 23 Apr 2019 22:36
 Operator : JC/SP
 Sample : K2536-04
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0X24

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\SOMULM042319WMA.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	22	27	36	rVB2	57107	54476	0.62%	0.186%
2	1.289	58	62	69	rBV	15481	13165	0.15%	0.045%
3	1.395	87	95	109	rBV	327829	363554	4.13%	1.242%
4	1.678	175	183	194	rBV	275737	334144	3.80%	1.141%
5	1.881	238	246	260	rVB	103394	144240	1.64%	0.493%
6	2.267	356	366	379	rVV	562835	856349	9.74%	2.925%
7	2.334	379	387	408	rVB4	27047	65600	0.75%	0.224%
8	2.833	530	542	552	rBV4	7263	15083	0.17%	0.052%
9	2.897	559	562	565	rVB4	885	617	0.01%	0.002%
10	2.945	572	577	582	rBV4	1024	896	0.01%	0.003%
11	2.974	582	586	587	rBV3	929	603	0.01%	0.002%
12	3.090	619	622	626	rVB2	831	599	0.01%	0.002%
13	3.257	669	674	681	rVB3	860	1084	0.01%	0.004%
14	3.338	693	699	702	rBV5	800	854	0.01%	0.003%
15	3.399	714	718	721	rBV3	697	633	0.01%	0.002%
16	3.485	742	745	754	rVB2	972	950	0.01%	0.003%
17	3.791	834	840	844	rBV3	1118	1064	0.01%	0.004%
18	3.878	859	867	871	rBV3	956	1185	0.01%	0.004%
19	4.000	900	905	909	rVB4	834	857	0.01%	0.003%
20	4.186	949	963	998	rBV	233280	735845	8.37%	2.513%
21	4.389	1016	1026	1058	rVB2	54883	144995	1.65%	0.495%
22	4.643	1088	1105	1128	rBV	405481	951873	10.82%	3.251%
23	4.829	1157	1163	1167	rVB6	1402	1581	0.02%	0.005%
24	4.952	1197	1201	1204	rBV4	1394	1270	0.01%	0.004%
25	4.987	1204	1212	1215	rVV6	1797	2692	0.03%	0.009%
26	5.045	1224	1230	1232	rBV3	926	912	0.01%	0.003%
27	5.116	1247	1252	1253	rBV4	1460	948	0.01%	0.003%
28	5.231	1283	1288	1293	rBV4	829	1013	0.01%	0.003%
29	5.334	1297	1320	1348	rBV3	830409	2488356	28.29%	8.498%
30	5.630	1410	1412	1416	rBV	936	638	0.01%	0.002%
31	5.665	1419	1423	1430	rBV8	1347	1881	0.02%	0.006%
32	5.707	1434	1436	1439	rVV2	1186	662	0.01%	0.002%
33	5.800	1460	1465	1469	rBV5	734	885	0.01%	0.003%
34	5.881	1476	1490	1529	rBV	824222	1708466	19.42%	5.835%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042319WMA.M
 Title : VOC Analysis

35	6.180	1568	1583	1616	rBV	4462553	8796142	100.00%	30.041%
36	6.328	1618	1629	1651	rVB	547139	1127994	12.82%	3.852%
37	6.591	1709	1711	1715	rBV4	852	645	0.01%	0.002%
38	6.624	1717	1721	1724	rVB3	1105	841	0.01%	0.003%
39	6.656	1728	1731	1738	rVB5	783	874	0.01%	0.003%
40	6.894	1802	1805	1810	rVV4	995	744	0.01%	0.003%
41	6.929	1814	1816	1821	rVB3	815	652	0.01%	0.002%
42	7.022	1842	1845	1850	rVB3	787	667	0.01%	0.002%
43	7.225	1896	1908	1931	rBV	302218	563495	6.41%	1.924%
44	7.421	1966	1969	1972	rBV3	993	735	0.01%	0.003%
45	7.476	1982	1986	1994	rVB8	1723	1727	0.02%	0.006%
46	7.562	1999	2013	2047	rBV	1034578	1919595	21.82%	6.556%
47	7.849	2091	2102	2131	rBV	195749	360569	4.10%	1.231%
48	8.077	2169	2173	2175	rBV3	679	624	0.01%	0.002%
49	8.173	2191	2203	2208	rBV3	10994	17049	0.19%	0.058%
50	8.225	2208	2219	2235	rVV	183587	317876	3.61%	1.086%
51	8.312	2235	2246	2275	rBV	836093	1539401	17.50%	5.257%
52	8.591	2330	2333	2337	rBV5	716	673	0.01%	0.002%
53	8.755	2382	2384	2387	rBV4	785	646	0.01%	0.002%
54	8.826	2403	2406	2410	rBV3	1130	1045	0.01%	0.004%
55	9.086	2474	2487	2530	rVV	1157715	2014189	22.90%	6.879%
56	9.308	2554	2556	2557	rBV2	1446	651	0.01%	0.002%
57	9.382	2577	2579	2585	rVB5	1106	1007	0.01%	0.003%
58	9.466	2597	2605	2611	rBV4	3017	3763	0.04%	0.013%
59	9.543	2625	2629	2631	rBV3	805	675	0.01%	0.002%
60	9.556	2631	2633	2636	rVV2	857	564	0.01%	0.002%
61	9.585	2640	2642	2645	rBV3	972	663	0.01%	0.002%
62	9.713	2678	2682	2686	rBV3	1234	1210	0.01%	0.004%
63	9.784	2698	2704	2708	rVB5	915	931	0.01%	0.003%
64	9.852	2720	2725	2729	rVB2	611	638	0.01%	0.002%
65	9.890	2730	2737	2740	rBV3	1390	1372	0.02%	0.005%
66	9.945	2747	2754	2756	rBV2	871	1064	0.01%	0.004%
67	9.990	2764	2768	2771	rVB3	1091	922	0.01%	0.003%
68	10.016	2771	2776	2780	rBV3	1140	827	0.01%	0.003%
69	10.180	2824	2827	2831	rVB3	1210	907	0.01%	0.003%
70	10.212	2831	2837	2851	rBV6	5812	11356	0.13%	0.039%
71	10.318	2866	2870	2874	rBV3	852	704	0.01%	0.002%

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72	10.427	2889	2904	2932	rBV	761375	1248833	14.20%	4.265%
73	10.607	2950	2960	2966	rVV3	9937	15633	0.18%	0.053%
74	10.739	2997	3001	3006	rBV4	882	889	0.01%	0.003%
75	10.771	3006	3011	3014	rBV3	791	817	0.01%	0.003%
76	10.897	3048	3050	3056	rVB4	718	626	0.01%	0.002%
77	10.922	3056	3058	3062	rBV3	954	626	0.01%	0.002%
78	10.964	3069	3071	3073	rBV2	1011	650	0.01%	0.002%
79	10.996	3077	3081	3087	rVV4	855	1140	0.01%	0.004%
80	11.041	3092	3095	3097	rBV2	781	614	0.01%	0.002%
81	11.080	3103	3107	3111	rBV3	1194	1125	0.01%	0.004%
82	11.199	3141	3144	3147	rBV2	864	612	0.01%	0.002%
83	11.482	3219	3232	3252	rBV	1032134	1682007	19.12%	5.744%
84	11.746	3304	3314	3334	rBV3	61184	140457	1.60%	0.480%
85	11.855	3337	3348	3372	rVB	949438	1580057	17.96%	5.396%
86	12.292	3481	3484	3485	rBV3	1332	826	0.01%	0.003%
87	12.382	3509	3512	3515	rBV3	1293	872	0.01%	0.003%
88	12.440	3528	3530	3531	rBV2	1238	564	0.01%	0.002%
89	12.559	3565	3567	3569	rBV3	1210	654	0.01%	0.002%
90	12.601	3578	3580	3586	rVB5	1138	853	0.01%	0.003%
91	12.636	3588	3591	3594	rBV4	1242	903	0.01%	0.003%
92	12.762	3623	3630	3636	rBV8	1827	2565	0.03%	0.009%
93	12.826	3648	3650	3656	rBV4	1259	1238	0.01%	0.004%
94	13.012	3705	3708	3709	rBV3	1489	894	0.01%	0.003%
95	13.051	3716	3720	3725	rVB4	1377	1265	0.01%	0.004%
96	13.720	3926	3928	3931	rBV3	847	561	0.01%	0.002%
97	13.987	4008	4011	4013	rBV3	1313	1051	0.01%	0.004%
98	14.057	4030	4033	4035	rBV3	1294	878	0.01%	0.003%
99	14.414	4142	4144	4146	rVB2	1461	589	0.01%	0.002%
100	15.073	4346	4349	4350	rBV	2682	1657	0.02%	0.006%

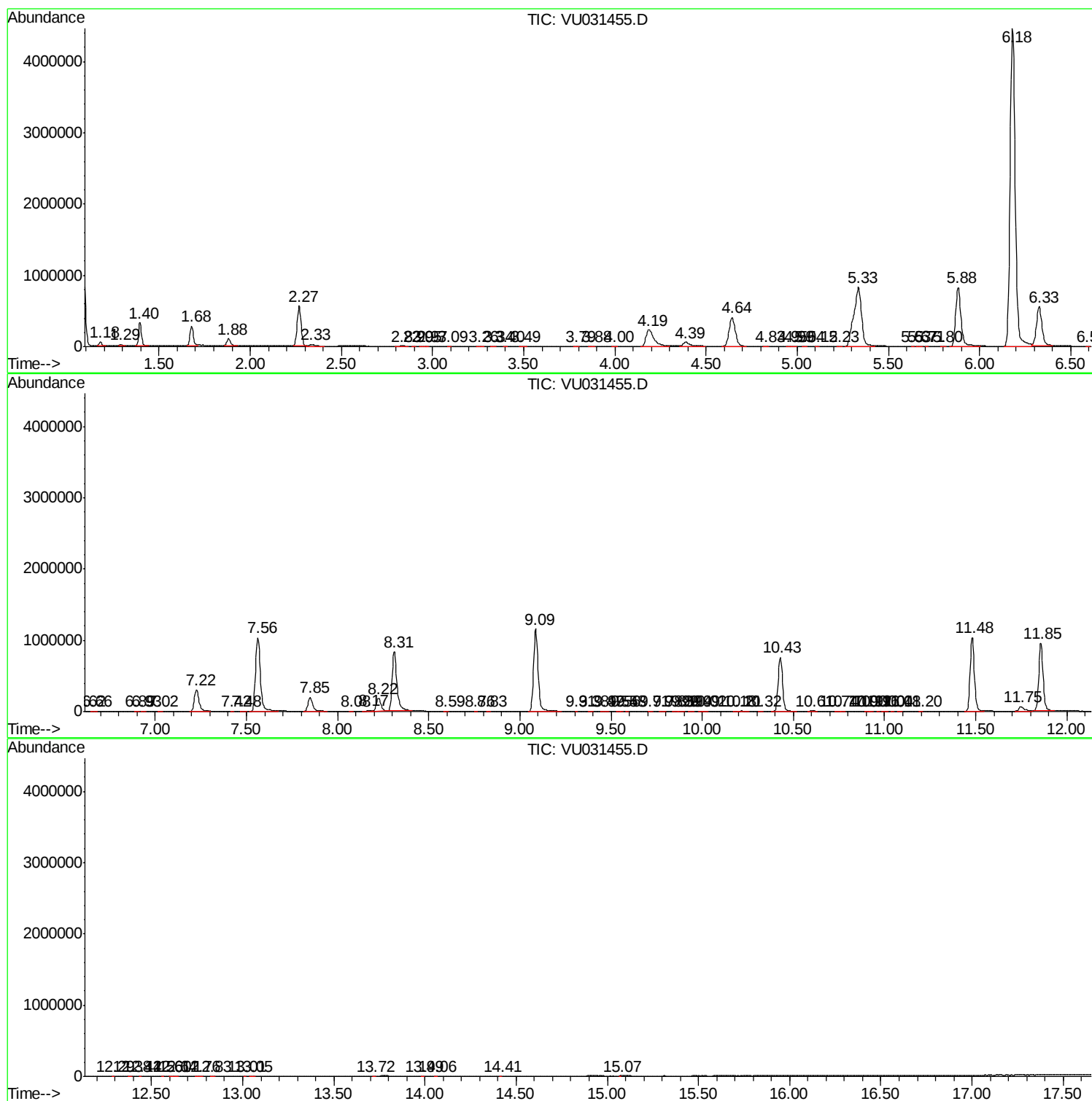
Sum of corrected areas: 29280863

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042319WMA.M
Quant Title : VOC Analysis

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



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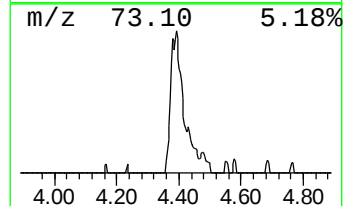
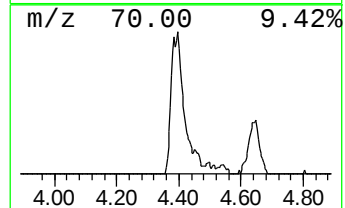
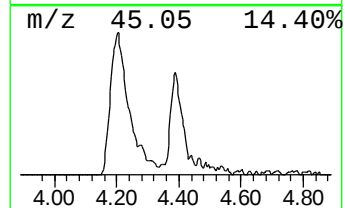
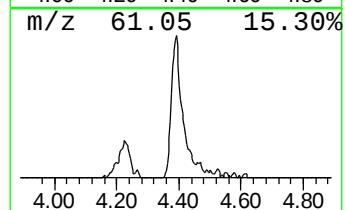
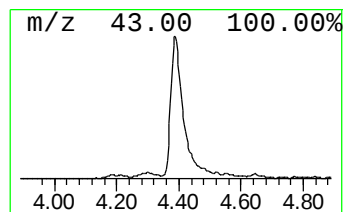
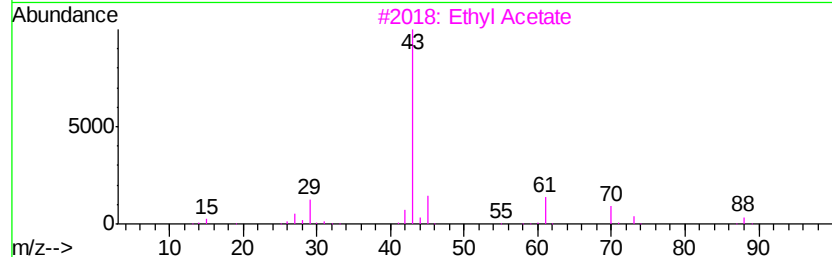
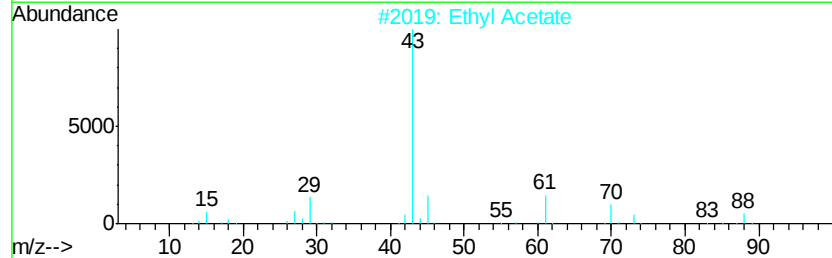
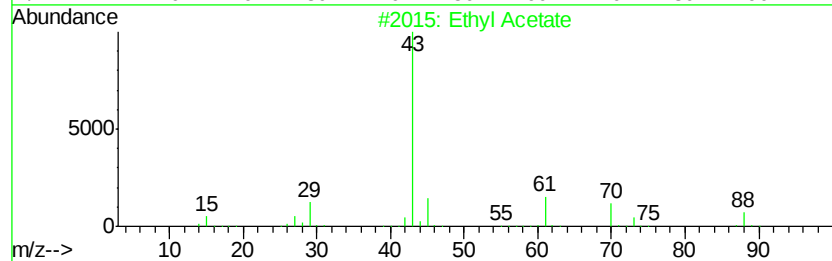
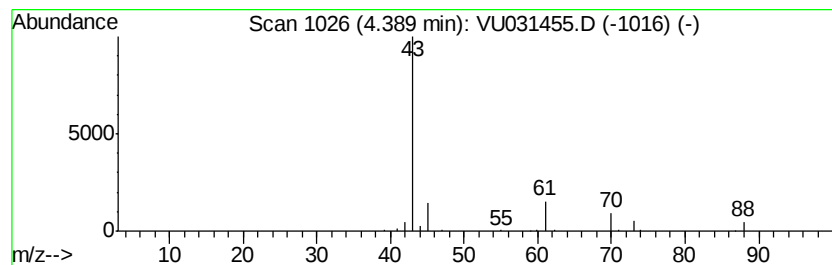
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042319WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	4.24 ug/L	144995	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	86
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	72
4		Ethyl Acetate	88	C4H8O2	000141-78-6	42
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9



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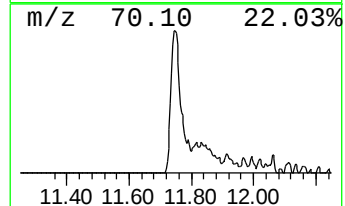
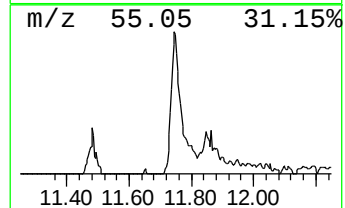
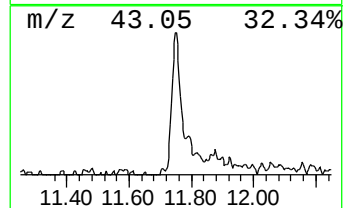
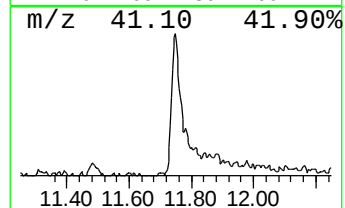
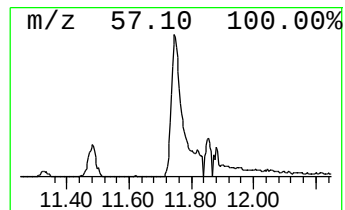
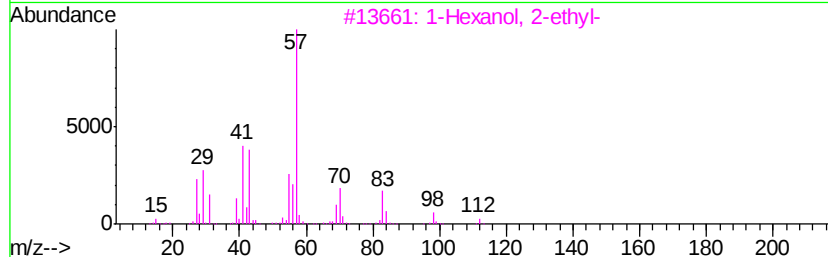
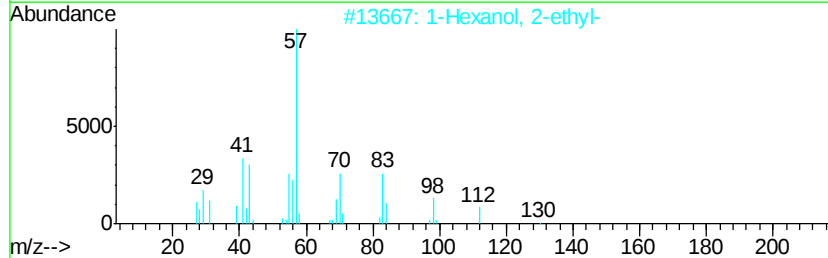
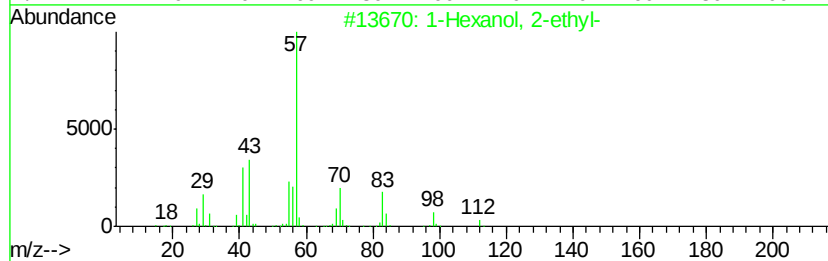
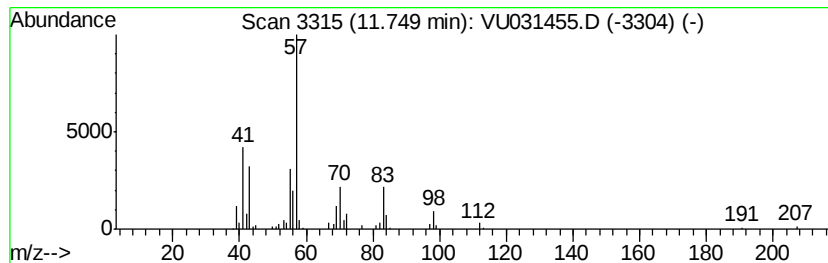
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.18 ug/L	140457	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		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5		Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.39	4.2	ug/L	144995	1	5.88	1708470	50.0
1-Hexanol, 2-ethyl-	11.75	4.2	ug/L	140457	3	11.48	1682010	50.0