

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU083018\
 Data File : VU026441.D
 Acq On : 30 Aug 2018 13:02
 Operator : MD/SY
 Sample : J4649-01
 Misc : 5.33g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAB88

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\SOMULM082918WMA.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	0.722	38	41	43	rBV	144	125	0.002%	0.0002%
2	0.838	73	77	81	rBB	256	220	0.003%	0.0003%
3	1.082	136	153	172	rBV	501363	562249	87.89%	8.756%
4	1.394	243	250	269	rVB	54074	78146	12.22%	1.217%
5	1.641	288	327	341	rBV	77427	236472	36.96%	3.683%
6	2.111	471	473	475	rBV2	761	426	0.007%	0.0007%
7	2.230	500	510	527	rBV	154632	246902	38.60%	3.845%
8	2.342	542	545	547	rBV2	412	269	0.004%	0.0004%
9	2.535	596	605	606	rBV2	355	431	0.007%	0.0007%
10	2.622	621	632	673	rVB	64427	131309	20.53%	2.045%
11	2.828	685	696	710	rBV2	3544	8090	1.26%	0.126%
12	3.397	870	873	877	rBV	180	188	0.003%	0.0003%
13	3.542	915	918	921	rBV	155	150	0.002%	0.0002%
14	3.686	960	963	965	rBV	279	187	0.003%	0.0003%
15	3.786	991	994	998	rBV	145	175	0.003%	0.0003%
16	3.812	999	1002	1005	rVV2	204	156	0.002%	0.0002%
17	4.079	1082	1085	1087	rBV	160	134	0.002%	0.0002%
18	4.095	1088	1090	1092	rVB	271	129	0.002%	0.0002%
19	4.201	1107	1123	1177	rBV2	33828	147473	23.05%	2.297%
20	4.644	1242	1261	1297	rVB	95376	252451	39.46%	3.931%
21	4.783	1297	1304	1305	rBV	368	446	0.007%	0.0007%
22	4.805	1306	1311	1315	rBV3	637	877	0.14%	0.014%
23	4.953	1350	1357	1375	rVB3	1104	2866	0.45%	0.045%
24	5.201	1430	1434	1441	rBV	172	288	0.005%	0.0004%
25	5.333	1451	1475	1504	rBV2	220813	639719	100.00%	9.962%
26	5.767	1607	1610	1613	rBV	123	134	0.002%	0.0002%
27	5.882	1632	1646	1675	rBV	179763	380863	59.54%	5.931%
28	6.175	1734	1737	1739	rVB2	223	143	0.002%	0.0002%
29	6.329	1770	1785	1812	rBV	135658	297896	46.57%	4.639%
30	6.461	1824	1826	1829	rVB	283	124	0.002%	0.0002%
31	6.802	1928	1932	1935	rBV	175	189	0.003%	0.0003%
32	6.876	1944	1955	1971	rVB6	2706	6539	1.02%	0.102%
33	6.940	1971	1975	1976	rBV6	223	171	0.003%	0.0003%
34	7.136	2033	2036	2038	rBV	145	124	0.002%	0.0002%

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 Title : VOC Analysis

35	7.165	2043	2045	2047	rVV	327	179	0.03%	0.003%
36	7.181	2047	2050	2052	rVV	157	130	0.02%	0.002%
37	7.230	2052	2065	2093	rVB	72479	148105	23.15%	2.306%
38	7.339	2093	2099	2104	rBV	219	356	0.06%	0.006%
39	7.564	2153	2169	2185	rVV	286501	524452	81.98%	8.167%
40	7.638	2185	2192	2207	rVV	13629	24615	3.85%	0.383%
41	7.689	2207	2208	2212	rVV	278	129	0.02%	0.002%
42	7.792	2235	2240	2243	rBV3	505	649	0.10%	0.010%
43	7.853	2243	2259	2278	rVV	51192	104665	16.36%	1.630%
44	8.043	2314	2318	2321	rVV	226	165	0.03%	0.003%
45	8.188	2348	2363	2367	rBV3	12235	23316	3.64%	0.363%
46	8.326	2395	2406	2430	rVB	197200	360063	56.28%	5.607%
47	8.484	2444	2455	2468	rBV5	6262	13265	2.07%	0.207%
48	8.535	2468	2471	2472	rBV3	329	158	0.02%	0.002%
49	8.606	2488	2493	2499	rBV3	886	1408	0.22%	0.022%
50	8.689	2509	2519	2535	rBV4	4012	7576	1.18%	0.118%
51	8.821	2553	2560	2562	rBV	144	213	0.03%	0.003%
52	8.850	2564	2569	2573	rVB3	627	798	0.12%	0.012%
53	8.905	2580	2586	2595	rBV4	1864	2464	0.39%	0.038%
54	9.030	2616	2625	2632	rBV4	1285	1771	0.28%	0.028%
55	9.094	2632	2645	2665	rVV	273810	477622	74.66%	7.438%
56	9.255	2685	2695	2709	rBV2	13860	22298	3.49%	0.347%
57	9.377	2721	2733	2748	rBV	65272	111835	17.48%	1.742%
58	9.445	2748	2754	2762	rVB5	2511	3006	0.47%	0.047%
59	9.721	2838	2840	2844	rVB2	280	185	0.03%	0.003%
60	9.786	2849	2860	2872	rBV	27622	45101	7.05%	0.702%
61	9.866	2881	2885	2889	rBV	120	128	0.02%	0.002%
62	9.956	2911	2913	2917	rVB	294	152	0.02%	0.002%
63	10.043	2931	2940	2952	rVB3	1779	2492	0.39%	0.039%
64	10.159	2966	2976	2994	rBV	40445	60252	9.42%	0.938%
65	10.352	3032	3036	3041	rBV	362	440	0.07%	0.007%
66	10.438	3050	3063	3078	rBV	232282	364522	56.98%	5.677%
67	10.525	3087	3090	3093	rBV2	174	154	0.02%	0.002%
68	10.545	3094	3096	3100	rVB2	205	140	0.02%	0.002%
69	10.570	3100	3104	3107	rBV	267	242	0.04%	0.004%
70	10.615	3107	3118	3135	rVB	7905	15171	2.37%	0.236%
71	10.686	3136	3140	3142	rBV2	213	148	0.02%	0.002%

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72	10.763	3161	3164	3167	rBV	162	159	0.02%	0.002%
73	10.818	3175	3181	3187	rVB2	720	947	0.15%	0.015%
74	11.075	3258	3261	3266	rBV2	211	184	0.03%	0.003%
75	11.152	3280	3285	3291	rVB2	551	623	0.10%	0.010%
76	11.377	3348	3355	3365	rVB3	3650	5207	0.81%	0.081%
77	11.442	3366	3375	3378	rBV4	4832	6015	0.94%	0.094%
78	11.487	3379	3389	3409	rVB	312208	481752	75.31%	7.502%
79	11.750	3467	3471	3472	rBV	316	236	0.04%	0.004%
80	11.863	3494	3506	3525	rVV	341826	539643	84.36%	8.404%
81	12.020	3552	3555	3556	rBV	848	402	0.06%	0.006%
82	12.078	3568	3573	3580	rVB4	600	803	0.13%	0.013%
83	12.332	3648	3652	3658	rVB	194	146	0.02%	0.002%
84	12.435	3681	3684	3687	rBV	194	164	0.03%	0.003%
85	12.480	3687	3698	3710	rVV	4913	8527	1.33%	0.133%
86	12.573	3718	3727	3729	rBV4	6524	8031	1.26%	0.125%
87	12.599	3730	3735	3749	rVB3	17320	25869	4.04%	0.403%
88	12.763	3784	3786	3791	rVB	273	161	0.03%	0.003%
89	12.895	3823	3827	3830	rVB	475	338	0.05%	0.005%
90	12.972	3849	3851	3854	rBV	232	130	0.02%	0.002%
91	13.207	3918	3924	3933	rVB5	979	1290	0.20%	0.020%
92	13.271	3940	3944	3948	rVB2	186	198	0.03%	0.003%
93	13.458	3997	4002	4003	rBV2	345	277	0.04%	0.004%
94	13.506	4014	4017	4023	rVB4	464	449	0.07%	0.007%
95	13.667	4059	4067	4078	rBV4	3512	6426	1.00%	0.100%
96	13.747	4086	4092	4107	rVB2	4055	5866	0.92%	0.091%
97	14.245	4244	4247	4249	rBV	196	138	0.02%	0.002%
98	14.281	4252	4258	4267	rVB2	1857	2804	0.44%	0.044%
99	14.654	4367	4374	4387	rBV4	3188	5748	0.90%	0.090%
100	15.885	4747	4757	4765	rBV2	2575	4489	0.70%	0.070%

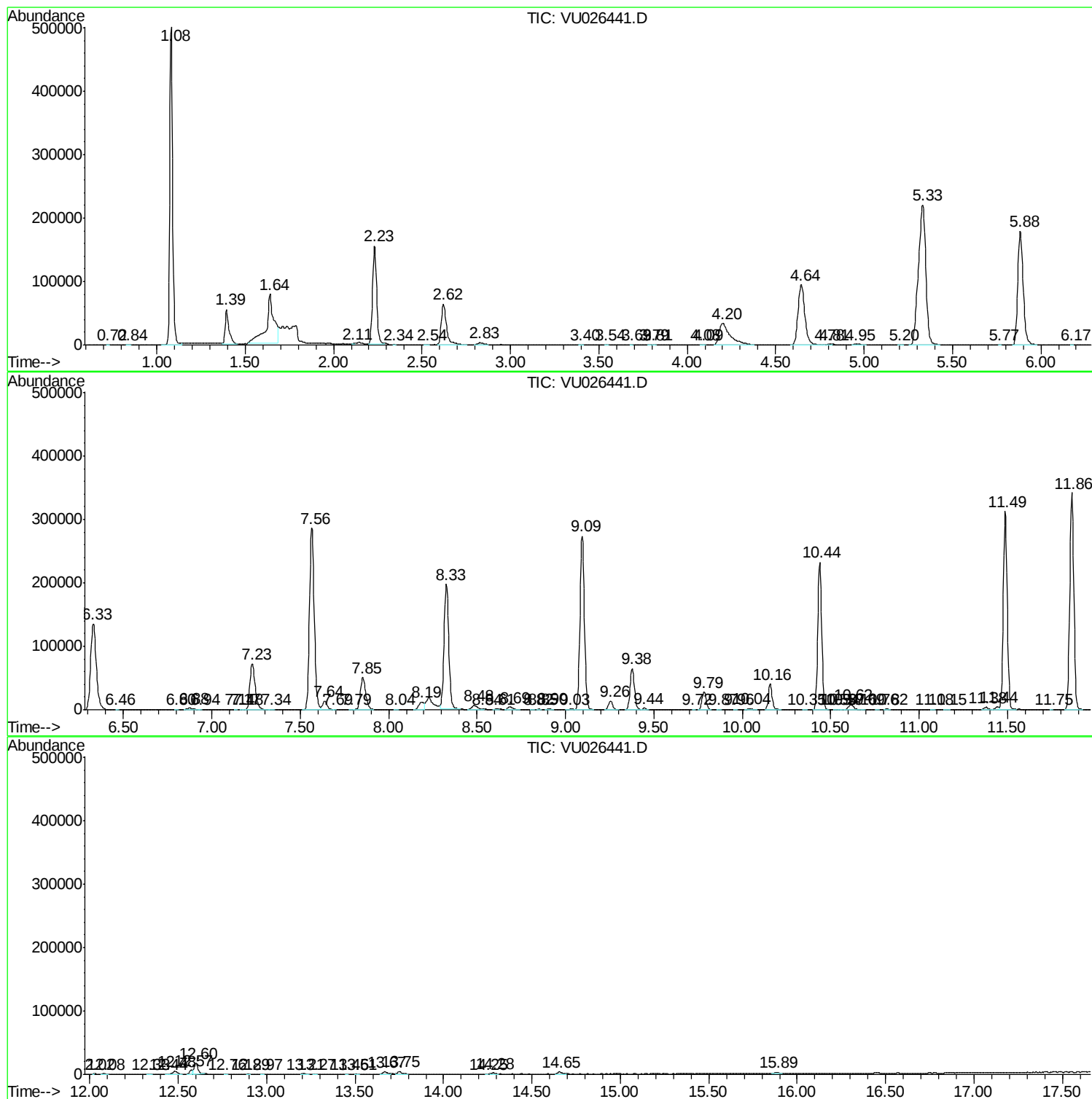
Sum of corrected areas: 6421448

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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



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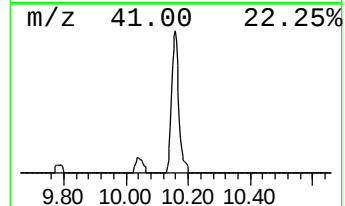
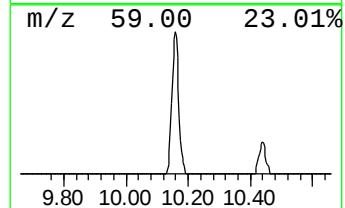
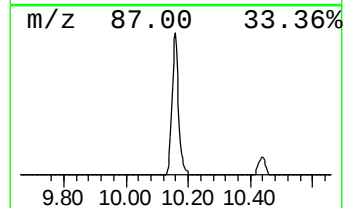
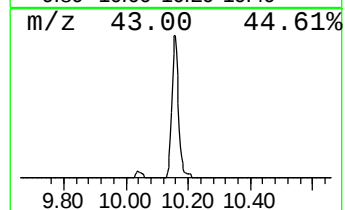
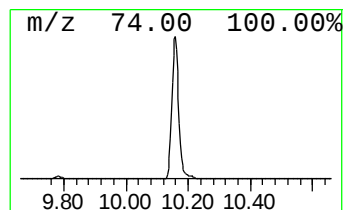
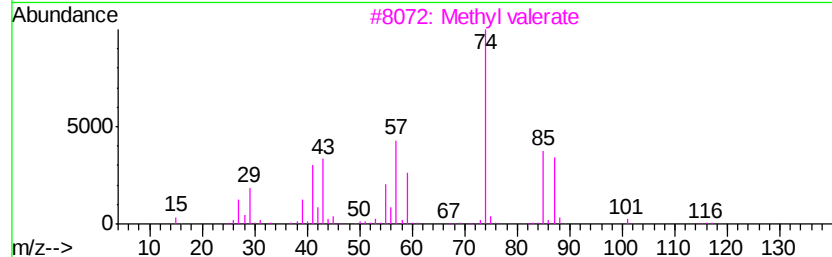
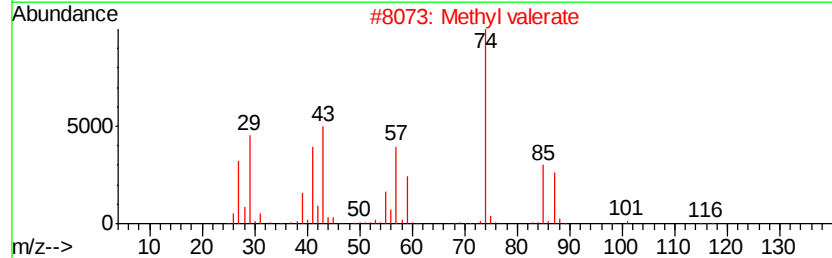
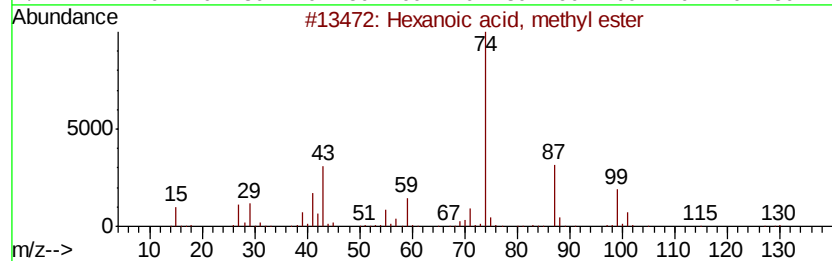
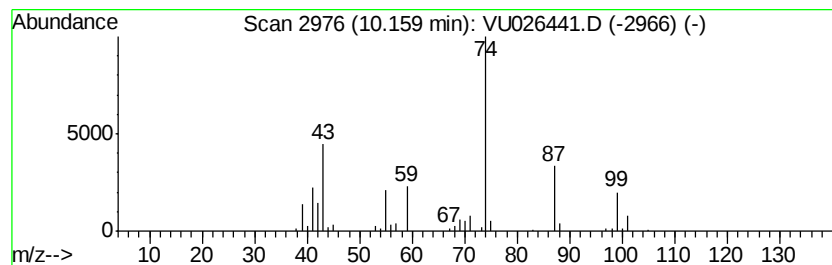
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.16	6.31 ug/L	60252	Chlorobenzene-d5	9.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	72	
2	Methyl valerate	116	C6H12O2	000624-24-8	59	
3	Methyl valerate	116	C6H12O2	000624-24-8	59	
4	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	56	
5	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	53	



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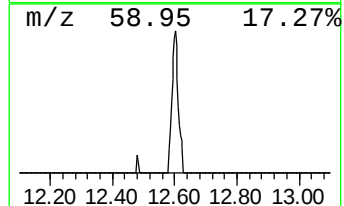
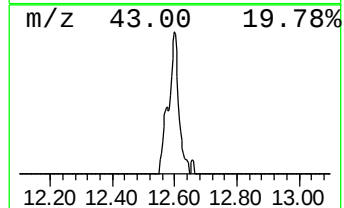
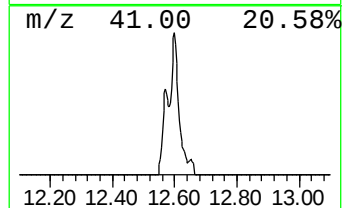
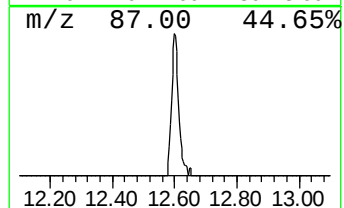
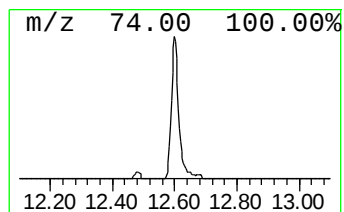
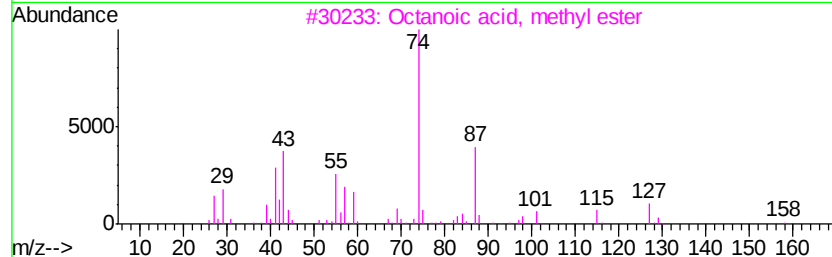
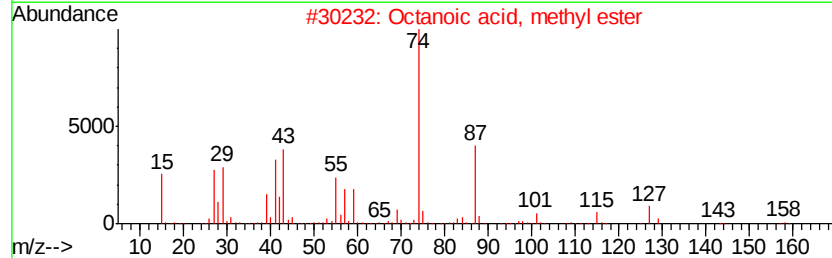
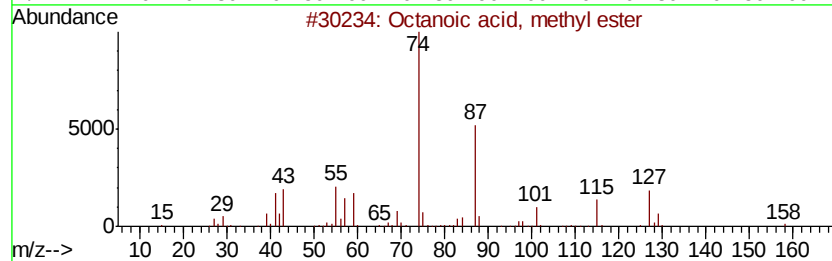
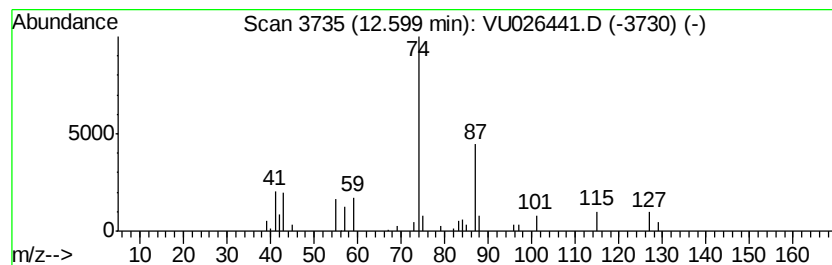
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Quant Title : VOC Analysis

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

Peak Number 4 Octanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	2.68 ug/L	25869	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	90
2		Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	83
3		Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	64
4		Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	64
5		Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid, me...	10.16	6.3	ug/L	60252	2	9.09	477622	50.0
Octanoic acid, me...	12.60	2.7	ug/L	25869	3	11.49	481752	50.0