

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059391.D
 Acq On : 20 Jun 2024 19:51
 Operator : MD/SY
 Sample : P2909-01ME
 Misc : 3.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4B75ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	114	rBV	57399	85729	11.12%	1.211%
2	1.846	136	173	175	rBV5	55352	222060	28.80%	3.137%
3	2.493	372	374	378	rVB2	356	211	0.03%	0.003%
4	2.544	378	390	406	rBV	134352	218179	28.30%	3.082%
5	2.624	410	415	416	rBV3	1818	1352	0.18%	0.019%
6	2.724	442	446	448	rBV	260	223	0.03%	0.003%
7	2.769	455	460	466	rBV3	936	1338	0.17%	0.019%
8	2.943	504	514	529	rBV2	16175	31913	4.14%	0.451%
9	3.026	532	540	552	rVB4	5131	9928	1.29%	0.140%
10	3.165	577	583	585	rBV3	433	412	0.05%	0.006%
11	3.714	751	754	757	rVB	262	184	0.02%	0.003%
12	3.814	781	785	792	rVB2	288	346	0.04%	0.005%
13	4.026	847	851	854	rBV	214	186	0.02%	0.003%
14	4.065	858	863	867	rBV2	172	240	0.03%	0.003%
15	4.145	885	888	896	rVB2	332	410	0.05%	0.006%
16	4.377	956	960	963	rBV	292	280	0.04%	0.004%
17	4.618	1025	1035	1077	rBV2	83902	239191	31.02%	3.379%
18	4.936	1131	1134	1138	rVB2	304	263	0.03%	0.004%
19	4.962	1138	1142	1146	rVB3	311	312	0.04%	0.004%
20	4.988	1146	1150	1154	rBV2	303	309	0.04%	0.004%
21	5.052	1154	1170	1193	rBV	141716	311749	40.43%	4.403%
22	5.213	1215	1220	1223	rBV2	274	231	0.03%	0.003%
23	5.261	1229	1235	1237	rBV2	353	436	0.06%	0.006%
24	5.531	1316	1319	1322	rBV	296	267	0.03%	0.004%
25	5.714	1353	1376	1405	rBV2	286843	771001	100.00%	10.890%
26	5.894	1429	1432	1438	rBV2	412	558	0.07%	0.008%
27	5.975	1454	1457	1464	rVB2	204	212	0.03%	0.003%
28	6.023	1467	1472	1475	rVB2	293	235	0.03%	0.003%
29	6.187	1520	1523	1527	rBV2	227	207	0.03%	0.003%
30	6.242	1527	1540	1557	rBV	283959	546495	70.88%	7.719%
31	6.525	1619	1628	1641	rVB4	5135	9019	1.17%	0.127%
32	6.599	1649	1651	1656	rBV	292	292	0.04%	0.004%
33	6.682	1663	1677	1696	rBV	180798	351937	45.65%	4.971%
34	6.775	1704	1706	1709	rVB2	347	223	0.03%	0.003%
35	6.808	1713	1716	1719	rBV2	630	438	0.06%	0.006%
36	7.197	1827	1837	1848	rBV4	2950	5745	0.75%	0.081%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	7.351	1883	1885	1892	rVB2	195	219	0.03%	0.003%
38	7.560	1939	1950	1965	rBV	88315	156418	20.29%	2.209%
39	7.698	1984	1993	2004	rBV5	1823	3326	0.43%	0.047%
40	7.804	2024	2026	2031	rBV	190	203	0.03%	0.003%
41	7.891	2036	2053	2067	rBV	328631	576662	74.79%	8.145%
42	7.965	2068	2076	2091	rVB	36283	64627	8.38%	0.913%
43	8.087	2110	2114	2121	rVB2	344	397	0.05%	0.006%
44	8.177	2131	2142	2161	rBV	60831	106258	13.78%	1.501%
45	8.335	2181	2191	2194	rBV	254	357	0.05%	0.005%
46	8.470	2225	2233	2238	rBV2	353	604	0.08%	0.009%
47	8.550	2254	2258	2262	rBV3	551	554	0.07%	0.008%
48	8.634	2272	2284	2324	rBV	257613	520092	67.46%	7.346%
49	8.807	2330	2338	2355	rVB9	2622	5824	0.76%	0.082%
50	9.081	2419	2423	2426	rBV	267	256	0.03%	0.004%
51	9.235	2465	2471	2476	rBV2	203	326	0.04%	0.005%
52	9.412	2513	2526	2550	rBV	420193	704782	91.41%	9.955%
53	9.573	2573	2576	2579	rBV2	537	484	0.06%	0.007%
54	9.717	2619	2621	2624	rVB	373	186	0.02%	0.003%
55	9.746	2627	2630	2632	rVB	364	210	0.03%	0.003%
56	9.766	2632	2636	2638	rBV	279	203	0.03%	0.003%
57	9.814	2645	2651	2653	rBV	219	248	0.03%	0.004%
58	9.875	2665	2670	2673	rBV2	383	404	0.05%	0.006%
59	10.110	2739	2743	2748	rBV3	243	307	0.04%	0.004%
60	10.171	2756	2762	2766	rBV2	269	305	0.04%	0.004%
61	10.470	2848	2855	2859	rBV4	1162	1561	0.20%	0.022%
62	10.753	2930	2943	2961	rBV	328591	537405	69.70%	7.591%
63	10.891	2982	2986	2991	rVB2	356	236	0.03%	0.003%
64	11.338	3122	3125	3130	rBV	239	186	0.02%	0.003%
65	11.412	3144	3148	3154	rBV3	264	289	0.04%	0.004%
66	11.692	3232	3235	3237	rBV2	289	201	0.03%	0.003%
67	11.753	3250	3254	3257	rBV3	377	357	0.05%	0.005%
68	11.811	3257	3272	3302	rVV	452364	737903	95.71%	10.423%
69	11.920	3302	3306	3311	rVV5	411	430	0.06%	0.006%
70	12.026	3335	3339	3342	rBV2	406	297	0.04%	0.004%
71	12.190	3377	3390	3415	rBV	395037	645565	83.73%	9.118%
72	12.495	3481	3485	3491	rVB2	317	292	0.04%	0.004%
73	12.907	3602	3613	3628	rBV	54249	90038	11.68%	1.272%
74	13.135	3681	3684	3693	rBV3	635	675	0.09%	0.010%
75	13.450	3775	3782	3785	rBV2	369	433	0.06%	0.006%
76	13.618	3831	3834	3840	rVB4	659	557	0.07%	0.008%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

77	13.682	3850	3854	3860	rBV3	305	315	0.04%	0.004%
78	13.724	3863	3867	3871	rBV	375	332	0.04%	0.005%
79	13.804	3889	3892	3895	rBV2	395	283	0.04%	0.004%
80	13.849	3903	3906	3910	rVB3	544	390	0.05%	0.006%
81	13.987	3940	3949	3959	rVB5	1707	3171	0.41%	0.045%
82	14.032	3959	3963	3967	rBV3	433	407	0.05%	0.006%
83	14.093	3971	3982	3997	rBV	13533	25441	3.30%	0.359%
84	14.245	4025	4029	4031	rBV2	227	189	0.02%	0.003%
85	14.450	4087	4093	4098	rBV3	817	1087	0.14%	0.015%
86	14.621	4141	4146	4154	rVB6	1341	1906	0.25%	0.027%
87	14.772	4191	4193	4195	rBV	303	183	0.02%	0.003%
88	14.823	4207	4209	4212	rBV2	284	217	0.03%	0.003%
89	14.865	4220	4222	4228	rBV3	333	301	0.04%	0.004%
90	14.913	4234	4237	4242	rVB4	517	464	0.06%	0.007%
91	14.968	4247	4254	4263	rBV5	2703	4279	0.55%	0.060%
92	15.045	4276	4278	4280	rBV	354	194	0.03%	0.003%
93	15.225	4325	4334	4348	rBV2	15998	28498	3.70%	0.403%
94	15.415	4382	4393	4405	rBV3	6806	12865	1.67%	0.182%
95	15.508	4418	4422	4425	rBV2	473	429	0.06%	0.006%
96	15.958	4555	4562	4572	rVB5	3855	5909	0.77%	0.083%
97	16.148	4615	4621	4631	rVB4	3437	4762	0.62%	0.067%
98	16.267	4650	4658	4670	rBV9	5499	11116	1.44%	0.157%
99	16.447	4710	4714	4724	rVB5	3191	4738	0.61%	0.067%
100	16.772	4813	4815	4816	rBV2	1095	477	0.06%	0.007%

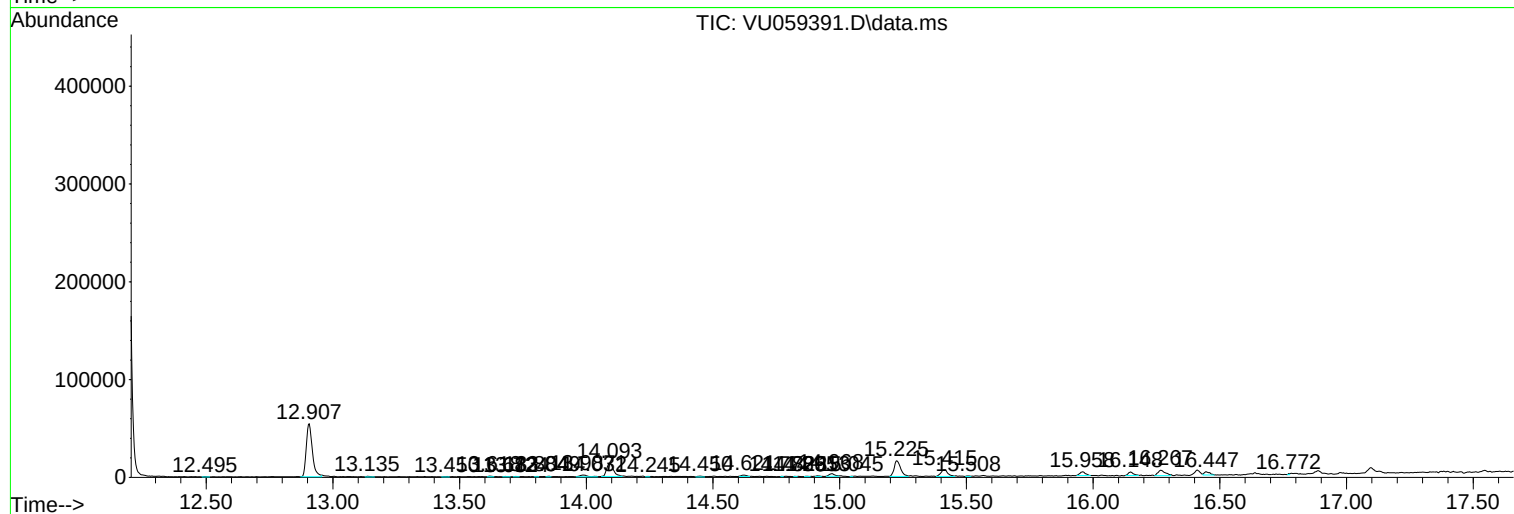
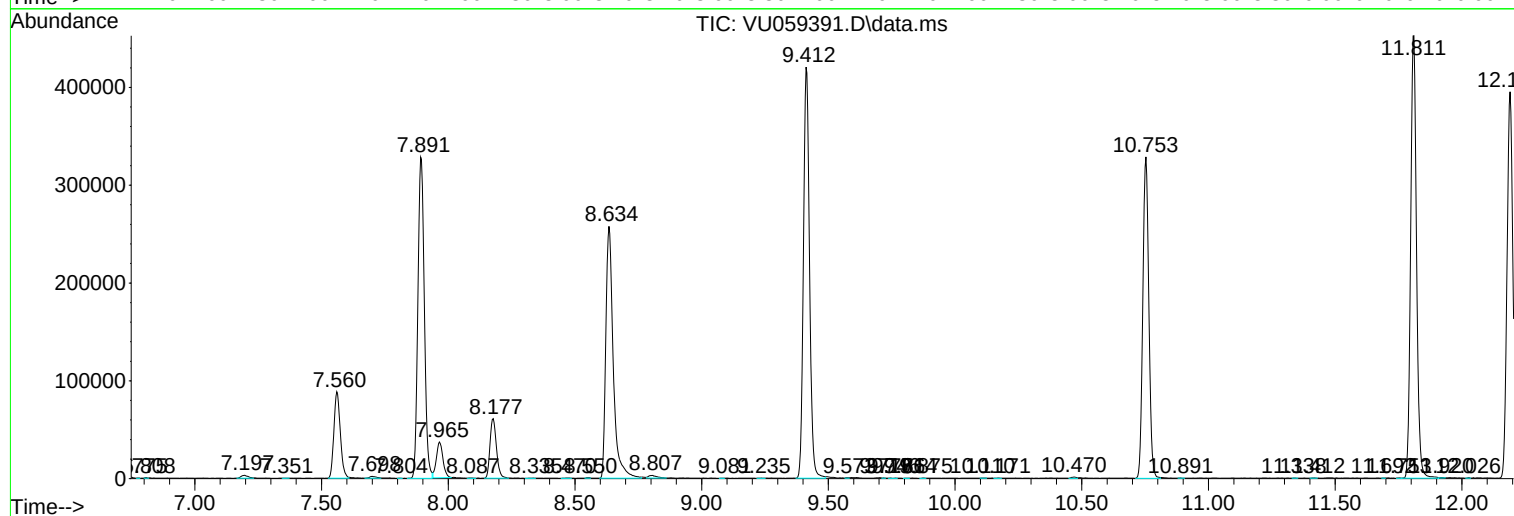
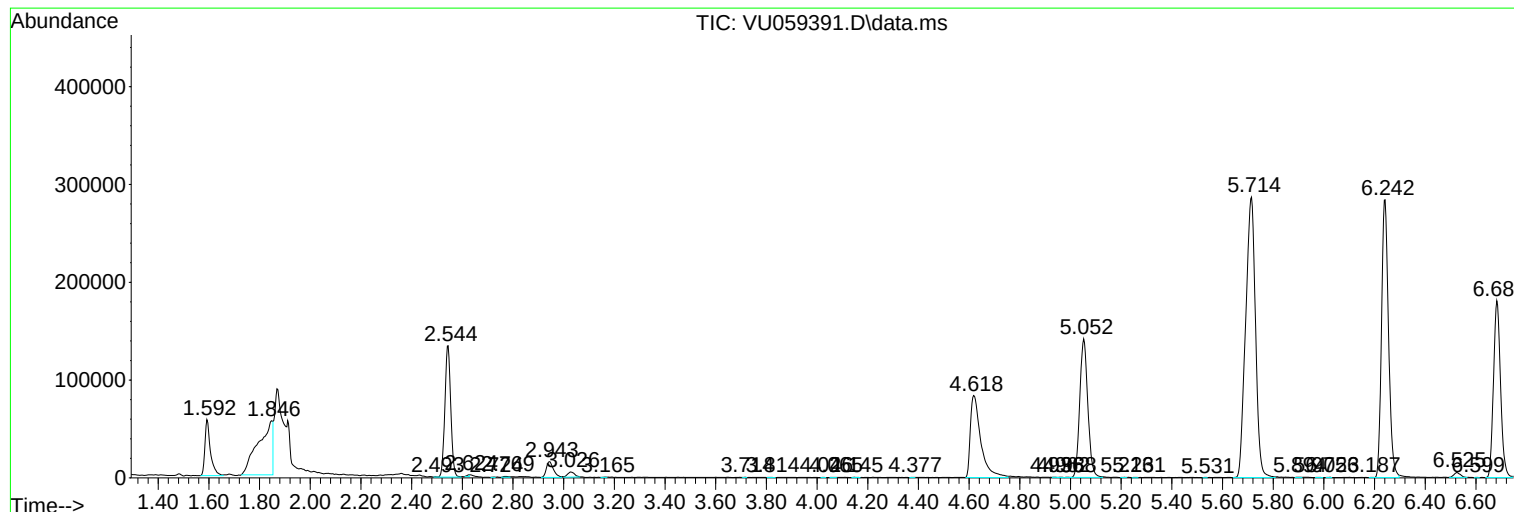
Sum of corrected areas: 7079741

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Instrument :
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A4B75ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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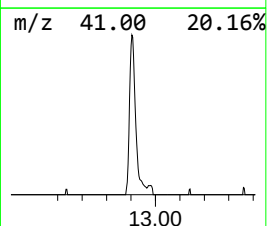
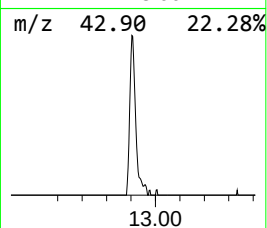
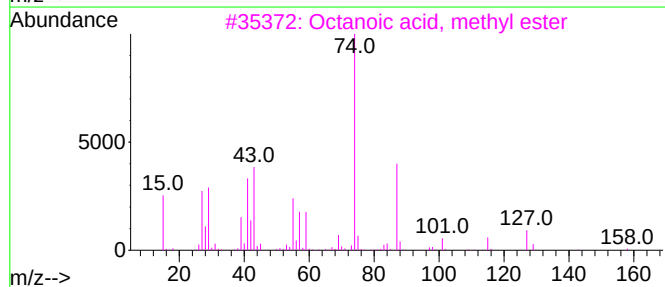
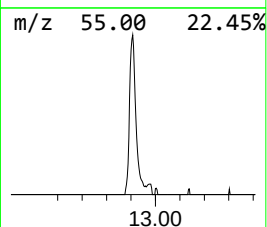
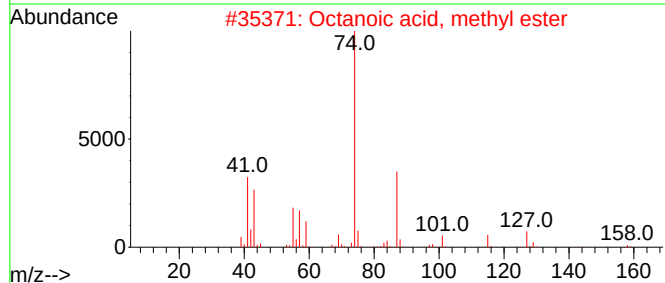
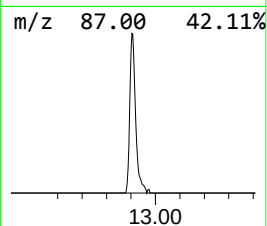
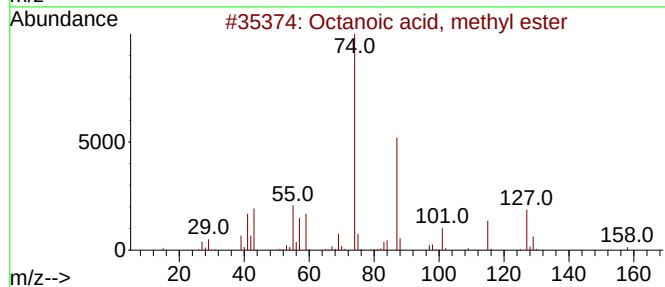
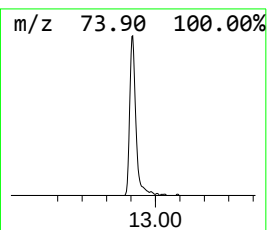
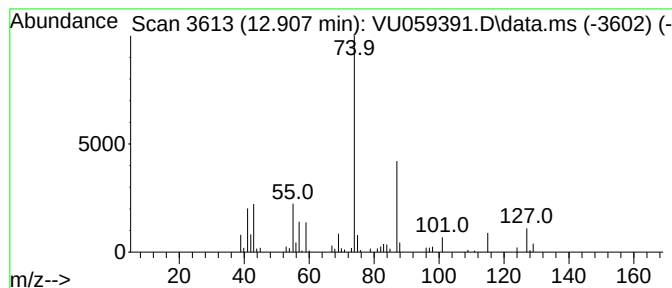
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.907	6.10 ug/L	90038	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	90
2			Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	90
3			Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	83
4			Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	59
5			Methyl 6-methyl heptanoate	158	C9H18O2	002519-37-1	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octanoic acid, ...	12.907	6.1	ug/L	90038	3	11.810	737903	50.0