

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072322\
 Data File : VV026928.D
 Acq On : 23 Jul 2022 17:40
 Operator : SY/MD
 Sample : N3766-06ME
 Misc : 6.15g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0ZD1ME

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_V\Method\SFAMVLM072222WMA.M
 Title : VOC Analysis

Signal : TIC: VV026928.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.208	48	52	60	rBV2	7992	8589	0.33%	0.043%
2	1.301	74	81	117	rVB	188992	310288	11.80%	1.552%
3	1.532	149	153	155	rBV	19526	16730	0.64%	0.084%
4	1.558	156	161	170	rVB	99220	110235	4.19%	0.551%
5	2.079	313	323	338	rVB	548657	767257	29.18%	3.837%
6	2.433	420	433	446	rBV	70809	140817	5.36%	0.704%
7	2.606	480	487	500	rVB5	4641	9737	0.37%	0.049%
8	2.921	583	585	588	rBV2	610	422	0.02%	0.002%
9	2.953	588	595	596	rBV4	1221	1380	0.05%	0.007%
10	3.182	663	666	671	rVV3	421	395	0.02%	0.002%
11	3.211	671	675	679	rVV4	503	405	0.02%	0.002%
12	3.281	694	697	704	rBV4	460	494	0.02%	0.002%
13	3.416	734	739	742	rVB2	367	400	0.02%	0.002%
14	3.468	753	755	762	rVB3	474	459	0.02%	0.002%
15	3.741	837	840	847	rBV4	471	498	0.02%	0.002%
16	3.841	866	871	874	rBV2	428	445	0.02%	0.002%
17	3.899	876	889	942	rBV	156264	639826	24.33%	3.200%
18	4.339	1006	1026	1058	rBV	417956	1059403	40.29%	5.298%
19	4.712	1138	1142	1147	rVB4	596	592	0.02%	0.003%
20	4.777	1158	1162	1165	rBV	703	448	0.02%	0.002%
21	4.934	1208	1211	1216	rVB2	538	387	0.01%	0.002%
22	5.034	1223	1242	1273	rBV2	1061821	2629475	100.00%	13.150%
23	5.272	1313	1316	1319	rVB2	772	455	0.02%	0.002%
24	5.294	1319	1323	1327	rBV4	472	499	0.02%	0.002%
25	5.349	1327	1340	1349	rBV10	3181	6995	0.27%	0.035%
26	5.477	1376	1380	1381	rBV3	634	422	0.02%	0.002%
27	5.513	1388	1391	1392	rBV2	749	514	0.02%	0.003%
28	5.609	1408	1421	1452	rBV	739067	1516621	57.68%	7.585%
29	5.902	1502	1512	1530	rBV2	16095	35397	1.35%	0.177%
30	5.979	1533	1536	1537	rBV3	939	556	0.02%	0.003%
31	5.995	1538	1541	1548	rVB5	1658	1714	0.07%	0.009%
32	6.063	1548	1562	1590	rBV	581385	1210609	46.04%	6.054%
33	6.262	1622	1624	1630	rVB3	871	691	0.03%	0.003%
34	6.297	1634	1635	1640	rVB4	818	378	0.01%	0.002%
35	6.468	1684	1688	1692	rBV6	525	498	0.02%	0.002%
36	6.645	1731	1743	1749	rBV8	3950	8001	0.30%	0.040%

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 Title : VOC Analysis

37	6.699	1757	1760	1764	rBV4	622	420	0.02%	0.002%
38	6.722	1764	1767	1770	rBV5	691	527	0.02%	0.003%
39	6.809	1788	1794	1797	rBV3	763	915	0.03%	0.005%
40	6.825	1797	1799	1805	rVB2	552	512	0.02%	0.003%
41	6.982	1832	1848	1875	rBV	256189	495180	18.83%	2.476%
42	7.310	1938	1950	1978	rBV	1106642	1964418	74.71%	9.824%
43	7.619	2036	2046	2080	rBV	176748	335828	12.77%	1.680%
44	7.937	2141	2145	2149	rVV3	1000	998	0.04%	0.005%
45	7.976	2152	2157	2163	rVB7	1410	1430	0.05%	0.007%
46	8.095	2182	2194	2227	rBV2	427804	1351519	51.40%	6.759%
47	8.471	2309	2311	2317	rBV4	693	544	0.02%	0.003%
48	8.661	2364	2370	2378	rVB7	1612	2336	0.09%	0.012%
49	8.850	2414	2429	2466	rBV	1103011	1904260	72.42%	9.524%
50	9.014	2477	2480	2482	rBV3	1120	779	0.03%	0.004%
51	9.133	2513	2517	2520	rBV4	827	846	0.03%	0.004%
52	9.153	2521	2523	2529	rVB6	1491	951	0.04%	0.005%
53	9.233	2545	2548	2553	rVB4	781	697	0.03%	0.003%
54	9.291	2561	2566	2568	rBV2	723	666	0.03%	0.003%
55	9.342	2578	2582	2589	rBV2	340	373	0.01%	0.002%
56	9.828	2730	2733	2735	rBV2	805	489	0.02%	0.002%
57	9.905	2751	2757	2761	rVV4	743	758	0.03%	0.004%
58	9.953	2766	2772	2775	rBV6	814	919	0.03%	0.005%
59	10.040	2793	2799	2802	rBV3	489	448	0.02%	0.002%
60	10.217	2841	2854	2878	rBV	818753	1412973	53.74%	7.067%
61	10.381	2894	2905	2920	rVB	88988	148389	5.64%	0.742%
62	10.548	2954	2957	2961	rVV3	577	514	0.02%	0.003%
63	10.580	2962	2967	2977	rVB6	1648	2638	0.10%	0.013%
64	11.033	3105	3108	3111	rBV2	572	406	0.02%	0.002%
65	11.249	3163	3175	3196	rBV	1086787	1721767	65.48%	8.611%
66	11.429	3229	3231	3237	rVB3	1066	769	0.03%	0.004%
67	11.625	3279	3292	3320	rBV	1138863	1779304	67.67%	8.899%
68	11.786	3338	3342	3350	rVB4	2995	4199	0.16%	0.021%
69	11.837	3353	3358	3368	rVB9	2005	2465	0.09%	0.012%
70	11.902	3374	3378	3385	rVB4	928	939	0.04%	0.005%
71	11.940	3386	3390	3393	rVB4	686	501	0.02%	0.003%
72	12.249	3475	3486	3499	rVB	68215	111716	4.25%	0.559%
73	12.377	3514	3526	3537	rVB2	9393	15338	0.58%	0.077%
74	12.496	3559	3563	3566	rBV3	608	512	0.02%	0.003%
75	12.570	3582	3586	3588	rBV2	766	567	0.02%	0.003%
76	12.599	3590	3595	3599	rVV4	707	796	0.03%	0.004%

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 Title : VOC Analysis

77	12.677	3615	3619	3626	rVB3	825	854	0.03%	0.004%
78	12.757	3640	3644	3648	rVB3	435	389	0.01%	0.002%
79	12.876	3678	3681	3682	rBV2	1141	553	0.02%	0.003%
80	13.069	3733	3741	3749	rBV5	3692	5175	0.20%	0.026%
81	13.230	3788	3791	3794	rBV2	514	424	0.02%	0.002%
82	13.435	3848	3855	3862	rBV7	2424	3360	0.13%	0.017%
83	13.522	3879	3882	3885	rBV3	781	555	0.02%	0.003%
84	13.850	3981	3984	3987	rBV3	591	401	0.02%	0.002%
85	14.043	4035	4044	4053	rBV2	7443	11105	0.42%	0.056%
86	14.165	4080	4082	4086	rBV3	755	585	0.02%	0.003%
87	14.188	4086	4089	4091	rVB3	873	426	0.02%	0.002%
88	14.348	4131	4139	4143	rBV4	1429	1679	0.06%	0.008%
89	14.413	4148	4159	4174	rVV	79024	117001	4.45%	0.585%
90	14.615	4219	4222	4226	rVB4	787	562	0.02%	0.003%
91	14.789	4273	4276	4279	rBV4	845	618	0.02%	0.003%
92	15.011	4339	4345	4351	rBV5	6779	8200	0.31%	0.041%
93	15.133	4379	4383	4387	rBV5	859	956	0.04%	0.005%
94	15.336	4438	4446	4453	rBV7	7466	10903	0.41%	0.055%
95	15.712	4559	4563	4564	rBV3	1347	1032	0.04%	0.005%
96	15.892	4613	4619	4620	rBV4	3532	3135	0.12%	0.016%
97	16.062	4667	4672	4680	rVB8	8837	11125	0.42%	0.056%
98	16.123	4685	4691	4693	rBV5	2536	2769	0.11%	0.014%
99	16.200	4706	4715	4727	rVB	34058	50940	1.94%	0.255%
100	16.538	4817	4820	4824	rBV	19459	10977	0.42%	0.055%

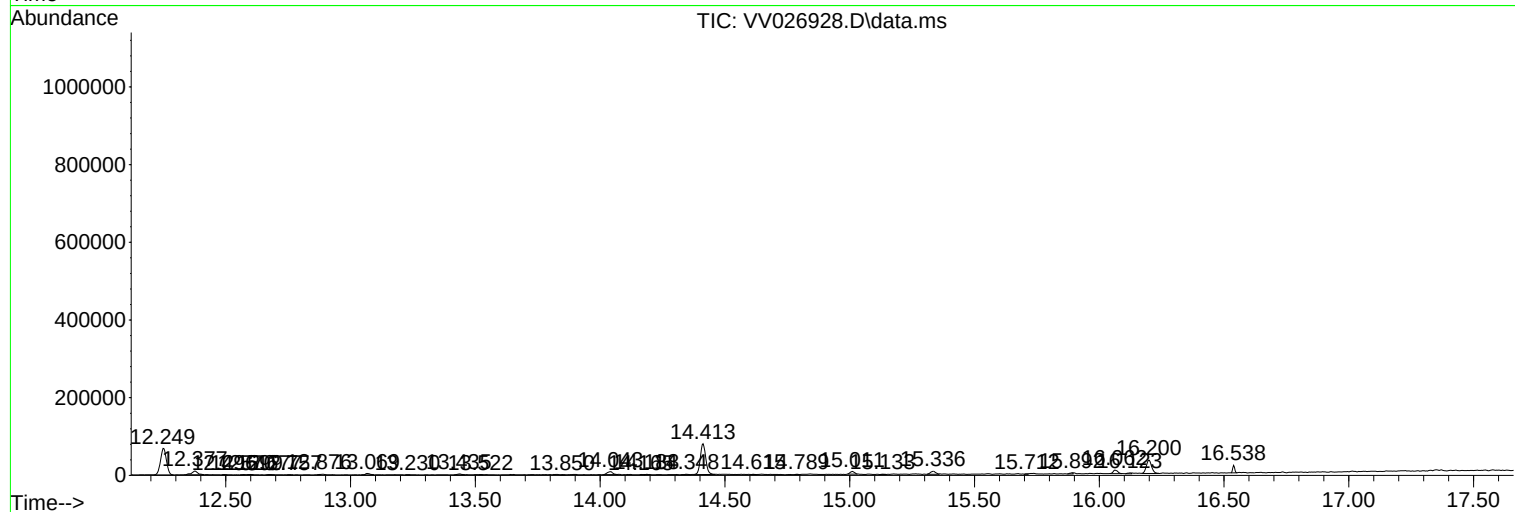
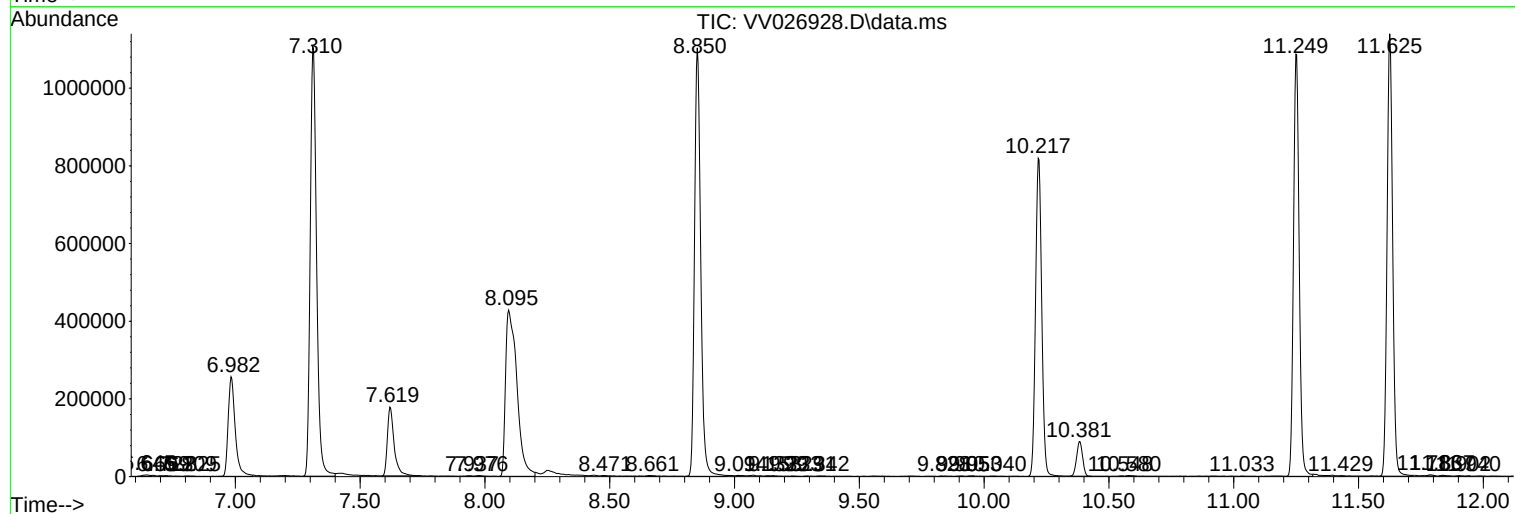
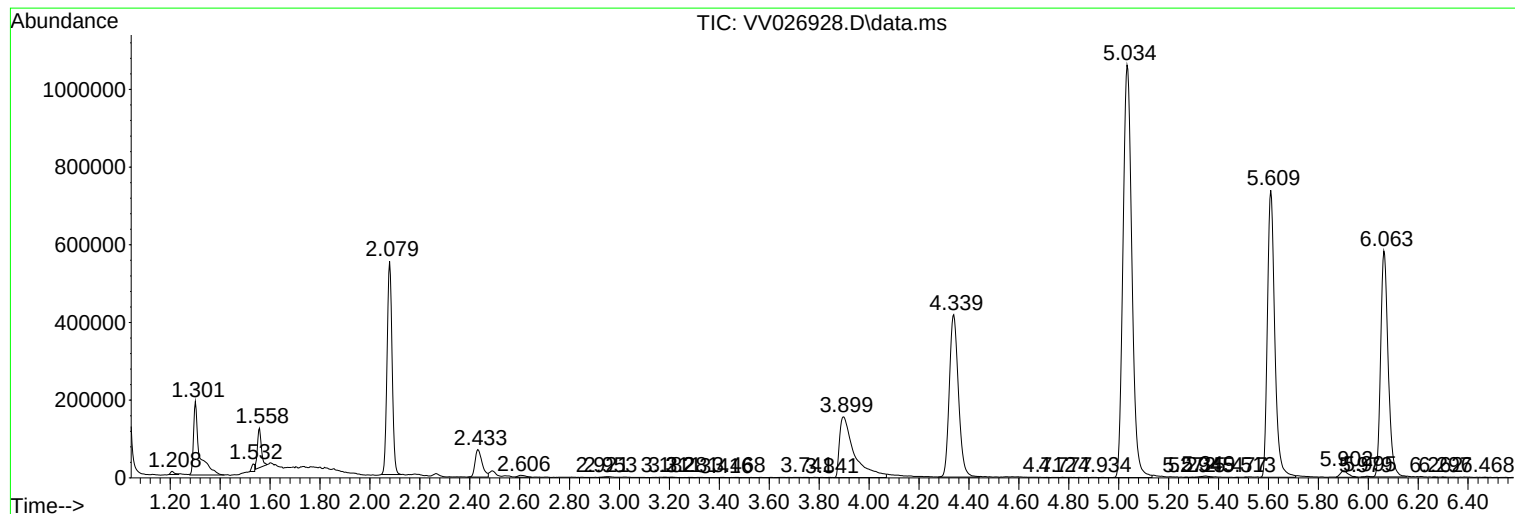
Sum of corrected areas: 19995362

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072222WMA.M
Quant Title : VOC Analysis

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



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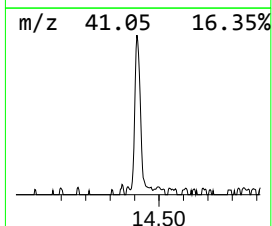
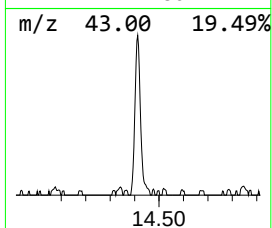
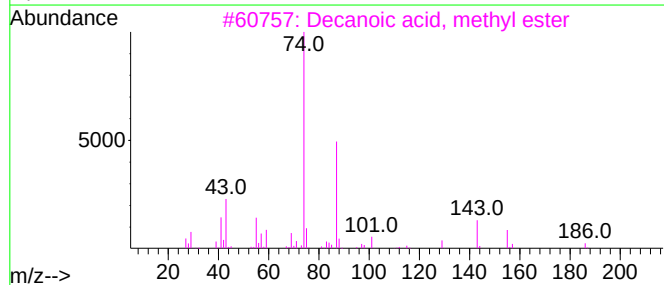
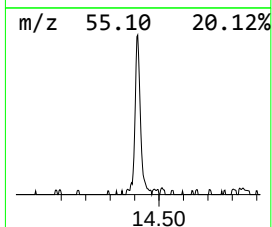
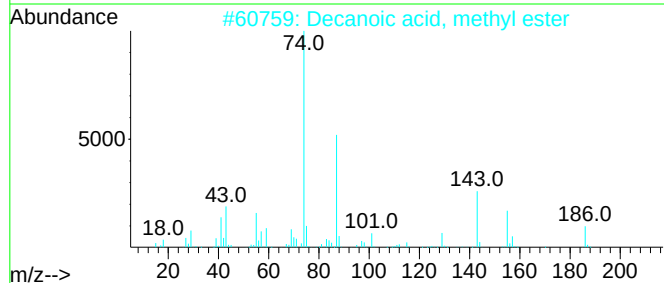
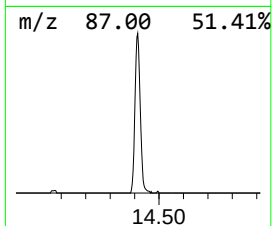
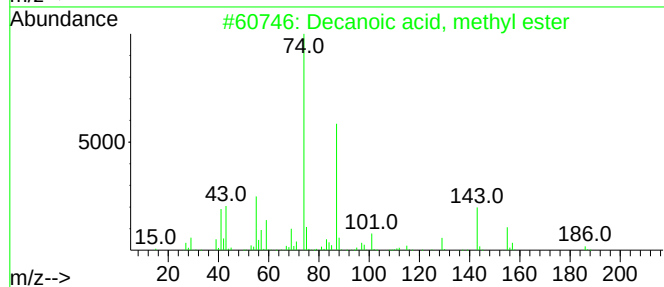
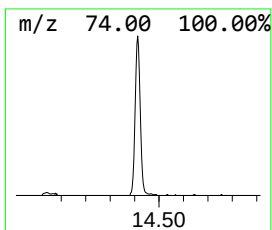
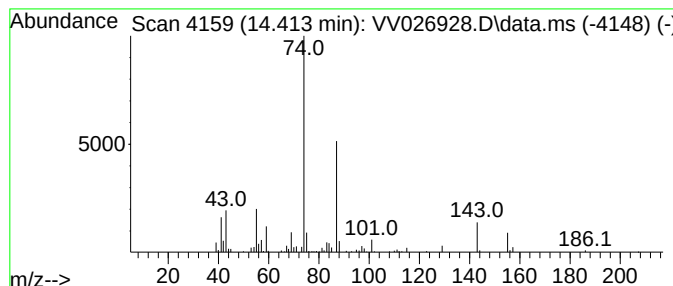
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072222WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Decanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.413	3.40 ug/L	117001	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	93
2			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	91
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	91
4			Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	86
5			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decanoic acid, ...	14.413	3.4	ug/L	117001	3	11.252	1721770	50.0