LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042219.D
Acq On : 05 Jul 2024 18:26
Operator : JC/MD
Sample : P3100-18ME
Misc : 4.27g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D13ME

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_X\Method\SFAMXLM070324WMA.M
Title : VOC Analysis

Signal : TIC: VX042219.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.257	24	28	38	rBV2	17524	21725	3.70%	0.422%
2	1.404	43	52	67	rVB2	15904	69243	11.79%	1.345%
3	2.269	189	194	213	rBV	83223	155891	26.54%	3.027%
4	2.721	262	268	274	rBV	14371	31108	5.30%	0.604%
5	2.946	299	305	314	rVB	5690	13944	2.37%	0.271%
6	3.221	347	350	353	rVB2	123	148	0.03%	0.003%
7	3.416	375	382	388	rVB3	783	1459	0.25%	0.028%
8	3.544	400	403	406	rBV2	143	209	0.04%	0.004%
9	3.605	411	413	415	rBV2	254	271	0.05%	0.005%
10	3.891	458	460	463	rBV2	130	141	0.02%	0.003%
11	3.964	471	472	474	rBV	176	166	0.03%	0.003%
12	4.025	479	482	483	rBV	163	147	0.03%	0.003%
13	4.208	509	512	514	rBV	136	123	0.02%	0.002%
14	4.306	524	528	530	rBV2	141	191	0.03%	0.004%
15	4.422	545	547	550	rVB	202	165	0.03%	0.003%
16	4.501	550	560	576	rBV	30248	108881	18.54%	2.114%
17	4.946	632	633	637	rBV3	280	266	0.05%	0.005%
18	5.056	640	651	667	rVV	68578	215095	36.62%	4.177%
19	5.281	686	688	690	rVB	239	184	0.03%	0.004%
20	5.385	701	705	710	rBV4	415	963	0.16%	0.019%
21	5.537	725	730	731	rBV3	422	426	0.07%	0.008%
22	5.702	756	757	762	rBV2	120	133	0.02%	0.003%
23	5.787	769	771	772	rBV2	134	109	0.02%	0.002%
24	5.872	782	785	787	rBV2	127	136	0.02%	0.003%
25	5.964	789	800	817	rBV2	198617	578159	98.44%	11.226%
26	6.330	855	860	861	rBV2	155	224	0.04%	0.004%
27	6.379	862	868	880	rVB5	1474	4513	0.77%	0.088%
28	6.470	880	883	887	rBV2	211	311	0.05%	0.006%
29	6.543	893	895	899	rVB2	198	211	0.04%	0.004%
30	6.653	911	913	916	rBV3	199	276	0.05%	0.005%
31	6.756	921	930	951	rBV	209281	511974	87.17%	9.941%
32	7.116	984	989	991	rBV4	831	1559	0.27%	0.030%
33	7.220	1001	1006	1013	rBV5	1985	4621	0.79%	0.090%
34	7.305	1013	1020	1037	rVB	113946	256496	43.67%	4.980%
35	7.494	1046	1051	1055	rVB4	339	590	0.10%	0.011%
36	7.549	1058	1060	1063	rVB2	163	162	0.03%	0.003%

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Instrument :
MSVOA_X
ClientSampleId :
A4D13ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Title : VOC Analysis

37	7.573	1063	1064	1066	rBV	131	135	0.02%	0.003%
38	7.628	1071	1073	1075	rBV2	93	121	0.02%	0.002%
39	7.689	1081	1083	1086	rBV2	116	136	0.02%	0.003%
40	7.787	1097	1099	1102	rBV2	149	193	0.03%	0.004%
41	7.970	1125	1129	1133	rBV4	1062	1829	0.31%	0.036%
42	8.043	1140	1141	1143	rBV	160	119	0.02%	0.002%
43	8.250	1171	1175	1178	rVB2	328	407	0.07%	0.008%
44	8.329	1182	1188	1205	rBV	59324	107196	18.25%	2.081%
45	8.646	1233	1240	1256	rBV	290992	467142	79.54%	9.071%
46	8.951	1285	1290	1303	rBV	41620	68883	11.73%	1.338%
47	9.116	1314	1317	1322	rVB2	476	633	0.11%	0.012%
48	9.280	1338	1344	1349	rVB4	1835	2981	0.51%	0.058%
49	9.347	1352	1355	1357	rBV2	102	108	0.02%	0.002%
50	9.396	1357	1363	1384	rBV	123454	277339	47.22%	5.385%
51	9.713	1411	1415	1423	rVB3	2476	4588	0.78%	0.089%
52	9.951	1450	1454	1458	rVB2	141	300	0.05%	0.006%
53	9.982	1458	1459	1460	rBV	239	144	0.02%	0.003%
54	10.055	1465	1471	1492	rVV	417788	587323	100.00%	11.404%
55	10.201	1492	1495	1499	rVV3	719	1288	0.22%	0.025%
56	10.244	1499	1502	1508	rVV2	1277	2081	0.35%	0.040%
57	10.305	1508	1512	1521	rVB	2619	4343	0.74%	0.084%
58	10.518	1546	1547	1549	rBV2	169	132	0.02%	0.003%
59	10.646	1564	1568	1571	rBV4	610	1061	0.18%	0.021%
60	10.969	1614	1621	1627	rBV3	1286	2463	0.42%	0.048%
61	11.091	1638	1641	1645	rVB3	382	637	0.11%	0.012%
62	11.195	1653	1658	1666	rVV	228874	299140	50.93%	5.809%
63	11.280	1670	1672	1673	rVV	285	241	0.04%	0.005%
64	11.317	1673	1678	1683	rVV	3406	4452	0.76%	0.086%
65	11.487	1699	1706	1713	rBV4	1469	2905	0.49%	0.056%
66	11.628	1728	1729	1734	rVB2	200	211	0.04%	0.004%
67	11.676	1734	1737	1738	rBV2	90	125	0.02%	0.002%
68	11.707	1738	1742	1744	rBV	1167	1596	0.27%	0.031%
69	11.762	1748	1751	1759	rVB	5084	7675	1.31%	0.149%
70	11.835	1759	1763	1765	rVB3	285	343	0.06%	0.007%
71	11.859	1765	1767	1773	rVB4	505	634	0.11%	0.012%
72	11.932	1777	1779	1780	rBV	243	138	0.02%	0.003%
73	11.981	1784	1787	1789	rBV3	1777	2185	0.37%	0.042%
74	12.024	1789	1794	1805	rVB	432643	546282	93.01%	10.607%
75	12.231	1825	1828	1832	rBV2	252	404	0.07%	0.008%
76	12.280	1834	1836	1837	rBV	182	157	0.03%	0.003%

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A4D13ME

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Title : VOC Analysis

77	12.323	1837	1843	1852	rBV	320423	416689	70.95%	8.091%
78	12.426	1858	1860	1864	rVB4	720	715	0.12%	0.014%
79	12.524	1875	1876	1880	rBV2	166	133	0.02%	0.003%
80	12.566	1880	1883	1885	rBV	118	133	0.02%	0.003%
81	12.768	1911	1916	1919	rVB2	894	1102	0.19%	0.021%
82	12.871	1929	1933	1943	rVV	4453	6755	1.15%	0.131%
83	12.950	1945	1946	1948	rVB2	256	137	0.02%	0.003%
84	13.097	1966	1970	1971	rBV2	194	178	0.03%	0.003%
85	13.164	1979	1981	1983	rBV2	225	179	0.03%	0.003%
86	13.408	2015	2021	2030	rBV2	3767	5787	0.99%	0.112%
87	13.505	2035	2037	2038	rBV2	169	142	0.02%	0.003%
88	13.566	2045	2047	2049	rBV2	200	203	0.03%	0.004%
89	13.603	2049	2053	2054	rVB2	376	410	0.07%	0.008%
90	13.682	2063	2066	2073	rVB3	764	1292	0.22%	0.025%
91	13.786	2081	2083	2090	rVB3	974	1105	0.19%	0.021%
92	13.889	2098	2100	2102	rVB2	317	179	0.03%	0.003%
93	14.042	2123	2125	2130	rBV	393	491	0.08%	0.010%
94	14.255	2158	2160	2162	rBV2	257	230	0.04%	0.004%
95	14.340	2173	2174	2175	rBV	205	121	0.02%	0.002%
96	14.426	2184	2188	2204	rBV	254135	326355	55.57%	6.337%
97	14.755	2239	2242	2244	rBV3	500	568	0.10%	0.011%
98	14.816	2251	2252	2257	rVB3	836	932	0.16%	0.018%
99	15.182	2308	2312	2315	rBV4	813	1130	0.19%	0.022%
100	15.956	2434	2439	2445	rBV2	4206	6769	1.15%	0.131%

Sum of corrected areas: 5150025

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MSVOA_X
ClientSampleId :
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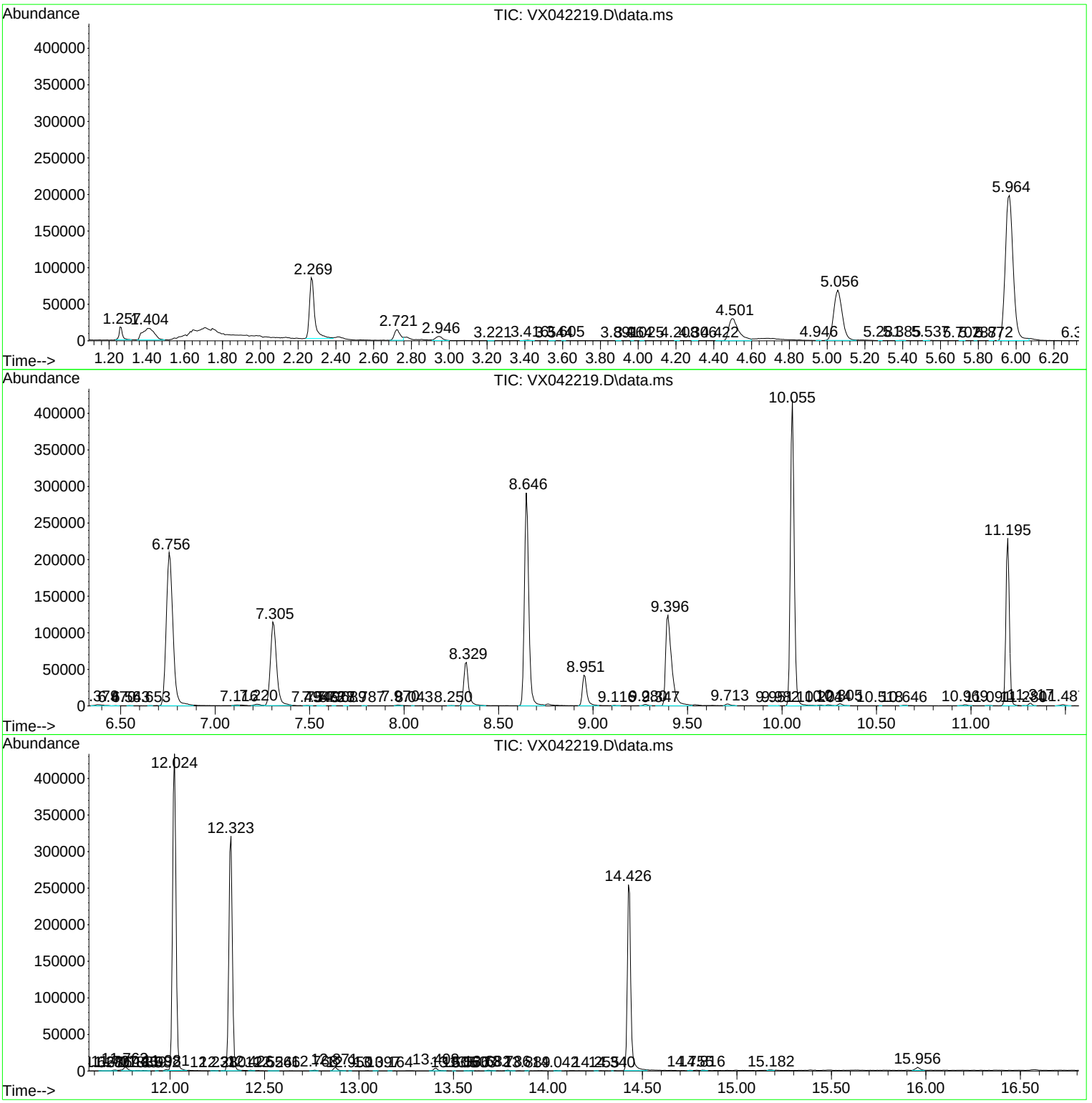
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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



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A4D13ME

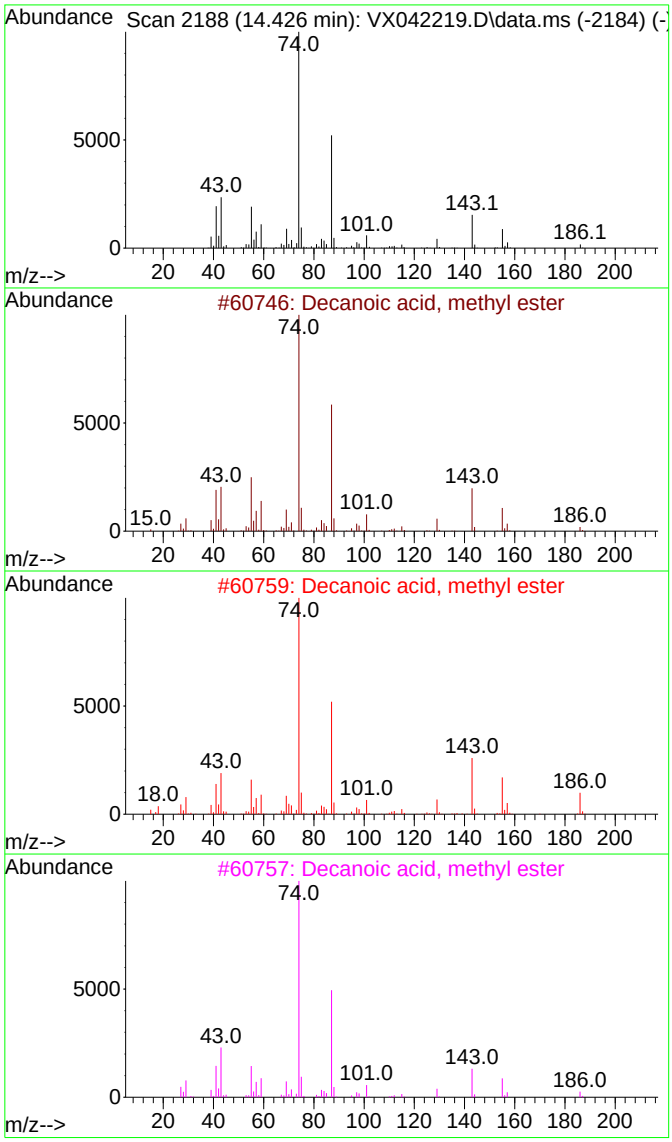
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

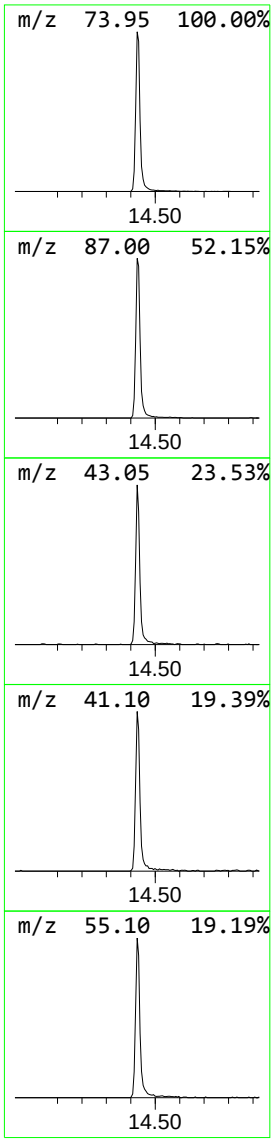
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Decanoic acid, methyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	29.87 ug/L	326355	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	98
2	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	97
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	90
4	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	86
5	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	78





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Decanoic acid, ...	14.426	29.9	ug/L	326355	3	12.024	546282	50.0