LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042220.D
Acq On : 05 Jul 2024 18:49
Operator : JC/MD
Sample : P3100-20ME
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : A4D33ME

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: VX042220.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	38	rBV	19642	24705	4.13%	0.487%
2	1.416	43	54	68	rVB2	15919	71940	12.03%	1.417%
3	2.270	188	194	212	rVB	83922	160510	26.85%	3.161%
4	2.721	262	268	286	rBV	49414	128979	21.57%	2.540%
5	3.184	341	344	346	rBV	193	188	0.03%	0.004%
6	3.239	352	353	356	rBV	136	140	0.02%	0.003%
7	3.416	376	382	387	rBV4	708	1491	0.25%	0.029%
8	3.599	406	412	415	rBV3	965	1970	0.33%	0.039%
9	3.715	430	431	435	rBV2	139	181	0.03%	0.004%
10	4.276	519	523	526	rVB3	220	355	0.06%	0.007%
11	4.501	552	560	578	rBV	30177	112246	18.77%	2.211%
12	5.056	640	651	666	rBV	65809	214402	35.86%	4.223%
13	5.562	727	734	735	rBV3	413	861	0.14%	0.017%
14	5.800	771	773	778	rBV2	166	175	0.03%	0.003%
15	5.958	789	799	814	rBV2	209643	597852	100.00%	11.776%
16	6.379	862	868	879	rBV6	1270	4001	0.67%	0.079%
17	6.452	879	880	884	rVB2	298	183	0.03%	0.004%
18	6.757	921	930	958	rBV	193741	475959	79.61%	9.375%
19	7.220	1000	1006	1012	rBV5	1710	4414	0.74%	0.087%
20	7.305	1012	1020	1041	rVB	117409	275300	46.05%	5.422%
21	7.543	1056	1059	1062	rBV2	119	153	0.03%	0.003%
22	7.976	1124	1130	1136	rBV5	897	1690	0.28%	0.033%
23	8.061	1142	1144	1146	rVB2	190	153	0.03%	0.003%
24	8.263	1171	1177	1178	rBV2	308	454	0.08%	0.009%
25	8.324	1182	1187	1206	rBV	62715	110066	18.41%	2.168%
26	8.555	1223	1225	1227	rVB2	187	164	0.03%	0.003%
27	8.592	1229	1231	1232	rBV2	289	261	0.04%	0.005%
28	8.647	1233	1240	1251	rBV	305415	481888	80.60%	9.491%
29	8.872	1274	1277	1278	rBV2	218	198	0.03%	0.004%
30	8.909	1281	1283	1285	rBV2	358	367	0.06%	0.007%
31	8.951	1285	1290	1302	rBV	44378	72303	12.09%	1.424%
32	9.281	1338	1344	1348	rVB4	1285	2010	0.34%	0.040%
33	9.397	1357	1363	1381	rBV	127765	301784	50.48%	5.944%
34	9.714	1411	1415	1421	rBV2	3398	5242	0.88%	0.103%
35	9.817	1428	1432	1434	rBV2	234	341	0.06%	0.007%
36	9.903	1442	1446	1450	rBV2	361	479	0.08%	0.009%

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Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D33ME

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

37	10.006	1461	1463	1465	rVB	219	162	0.03%	0.003%
38	10.055	1465	1471	1481	rBV	386958	543876	90.97%	10.712%
39	10.195	1492	1494	1499	rVB	515	648	0.11%	0.013%
40	10.244	1500	1502	1508	rVB3	878	1201	0.20%	0.024%
41	10.305	1508	1512	1519	rBV2	3428	5071	0.85%	0.100%
42	10.530	1548	1549	1553	rVB2	117	142	0.02%	0.003%
43	10.646	1564	1568	1576	rVB2	1554	2622	0.44%	0.052%
44	10.780	1587	1590	1591	rBV3	207	249	0.04%	0.005%
45	10.829	1596	1598	1602	rVB3	216	310	0.05%	0.006%
46	10.872	1602	1605	1606	rBV	198	267	0.04%	0.005%
47	10.896	1606	1609	1614	rVB4	530	681	0.11%	0.013%
48	10.969	1616	1621	1627	rBV4	1804	2924	0.49%	0.058%
49	11.091	1638	1641	1648	rVB4	501	786	0.13%	0.015%
50	11.195	1652	1658	1668	rBV	240311	313864	52.50%	6.182%
51	11.317	1673	1678	1683	rVB2	5109	7271	1.22%	0.143%
52	11.390	1683	1690	1692	rBV2	180	367	0.06%	0.007%
53	11.433	1695	1697	1698	rBV	182	150	0.03%	0.003%
54	11.451	1698	1700	1701	rVV2	308	214	0.04%	0.004%
55	11.482	1701	1705	1713	rVB2	1920	3188	0.53%	0.063%
56	11.585	1720	1722	1724	rBV	131	138	0.02%	0.003%
57	11.701	1736	1741	1743	rBV	7871	11791	1.97%	0.232%
58	11.731	1743	1746	1749	rVV	24329	29887	5.00%	0.589%
59	11.860	1764	1767	1777	rVB3	2289	3208	0.54%	0.063%
60	11.939	1777	1780	1782	rBV2	1230	1355	0.23%	0.027%
61	11.981	1784	1787	1789	rVV3	2313	2382	0.40%	0.047%
62	12.024	1789	1794	1804	rVB	405711	518366	86.70%	10.210%
63	12.231	1825	1828	1832	rVB3	676	709	0.12%	0.014%
64	12.323	1837	1843	1856	rVV	331994	436879	73.07%	8.605%
65	12.426	1856	1860	1863	rVV5	1738	2346	0.39%	0.046%
66	12.469	1863	1867	1869	rVB3	582	690	0.12%	0.014%
67	12.591	1881	1887	1890	rBV3	1548	2574	0.43%	0.051%
68	12.762	1911	1915	1919	rVB4	1500	2296	0.38%	0.045%
69	12.798	1919	1921	1923	rBV	233	203	0.03%	0.004%
70	12.835	1925	1927	1929	rBV2	273	319	0.05%	0.006%
71	12.872	1929	1933	1940	rBV2	7243	10666	1.78%	0.210%
72	13.042	1956	1961	1964	rVB3	187	286	0.05%	0.006%
73	13.164	1978	1981	1985	rVB3	419	447	0.07%	0.009%
74	13.207	1985	1988	1989	rVB	150	142	0.02%	0.003%
75	13.268	1995	1998	2001	rVB	1009	989	0.17%	0.019%
76	13.402	2018	2020	2024	rVV3	1320	1747	0.29%	0.034%

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Sample : P3100-20ME
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : A4D33ME

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

77	13.451	2026	2028	2030	rVV2	387	281	0.05%	0.006%
78	13.554	2041	2045	2048	rBV2	206	350	0.06%	0.007%
79	13.597	2049	2052	2057	rBV2	691	884	0.15%	0.017%
80	13.682	2063	2066	2071	rVB3	808	1470	0.25%	0.029%
81	13.743	2074	2076	2077	rBV	294	157	0.03%	0.003%
82	13.780	2077	2082	2088	rBV2	3415	5637	0.94%	0.111%
83	13.841	2089	2092	2096	rVB4	626	951	0.16%	0.019%
84	13.884	2098	2099	2104	rVB4	483	396	0.07%	0.008%
85	13.926	2104	2106	2107	rBV2	173	185	0.03%	0.004%
86	14.036	2121	2124	2128	rBV2	976	1049	0.18%	0.021%
87	14.127	2137	2139	2145	rVB2	549	626	0.10%	0.012%
88	14.207	2150	2152	2154	rBV2	203	199	0.03%	0.004%
89	14.274	2161	2163	2165	rBV2	310	208	0.03%	0.004%
90	14.377	2177	2180	2181	rBV	306	358	0.06%	0.007%
91	14.408	2181	2185	2186	rVV	17771	19910	3.33%	0.392%
92	14.426	2186	2188	2202	rVB	29229	38485	6.44%	0.758%
93	14.755	2238	2242	2245	rBV3	1432	2224	0.37%	0.044%
94	14.822	2250	2253	2256	rVB4	1003	1345	0.22%	0.026%
95	14.932	2267	2271	2275	rBV3	6149	8284	1.39%	0.163%
96	15.176	2308	2311	2314	rBV3	930	1239	0.21%	0.024%
97	15.487	2360	2362	2367	rVB5	1494	1734	0.29%	0.034%
98	15.737	2398	2403	2411	rVB6	6637	12884	2.16%	0.254%
99	15.908	2427	2431	2435	rBV5	2205	3849	0.64%	0.076%
100	15.956	2435	2439	2447	rVB2	5643	9554	1.60%	0.188%

Sum of corrected areas: 5077077

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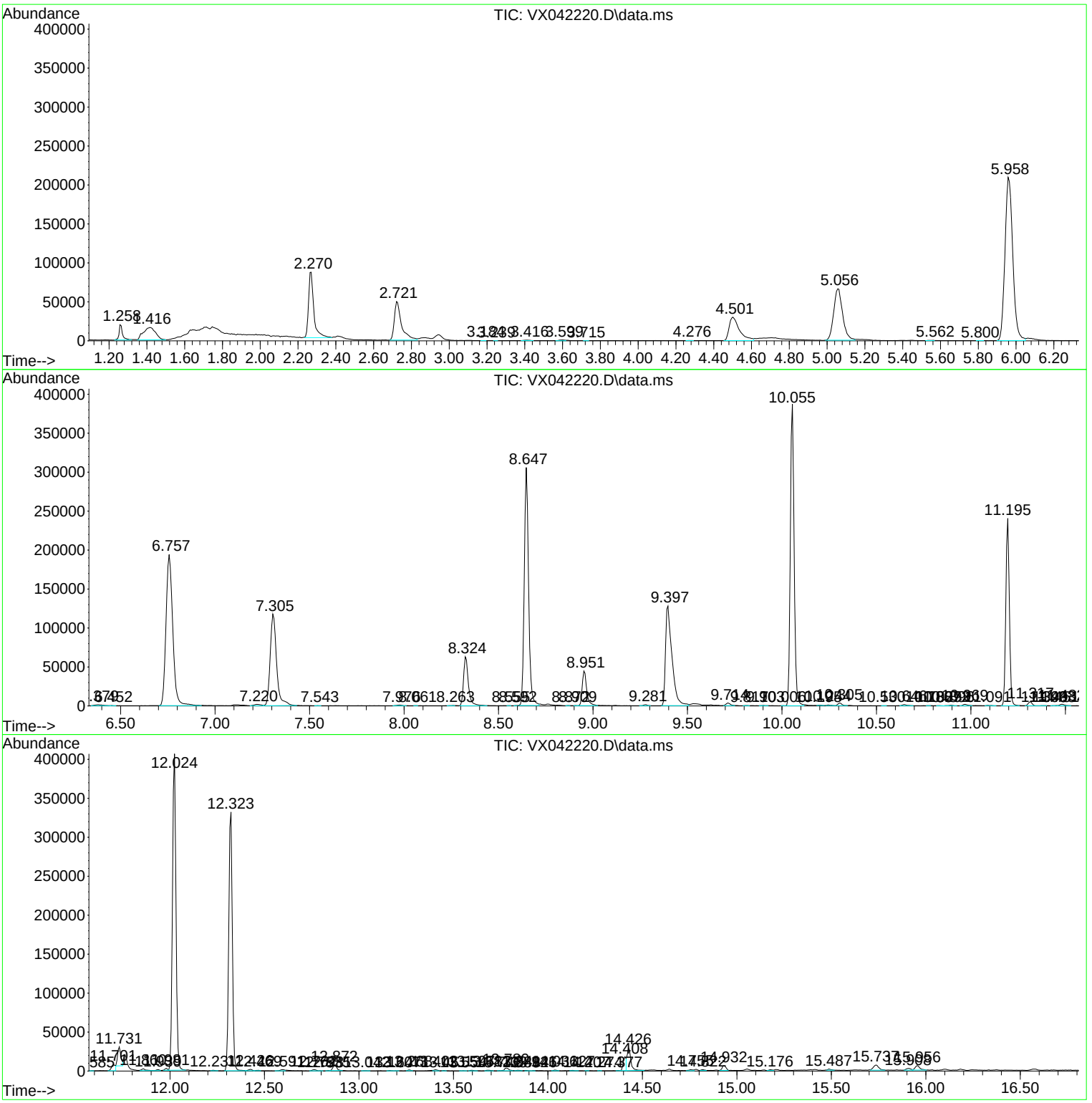
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D33ME

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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Data File : VX042220.D
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Instrument :
MSVOA_X
ClientSampleId :
A4D33ME

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

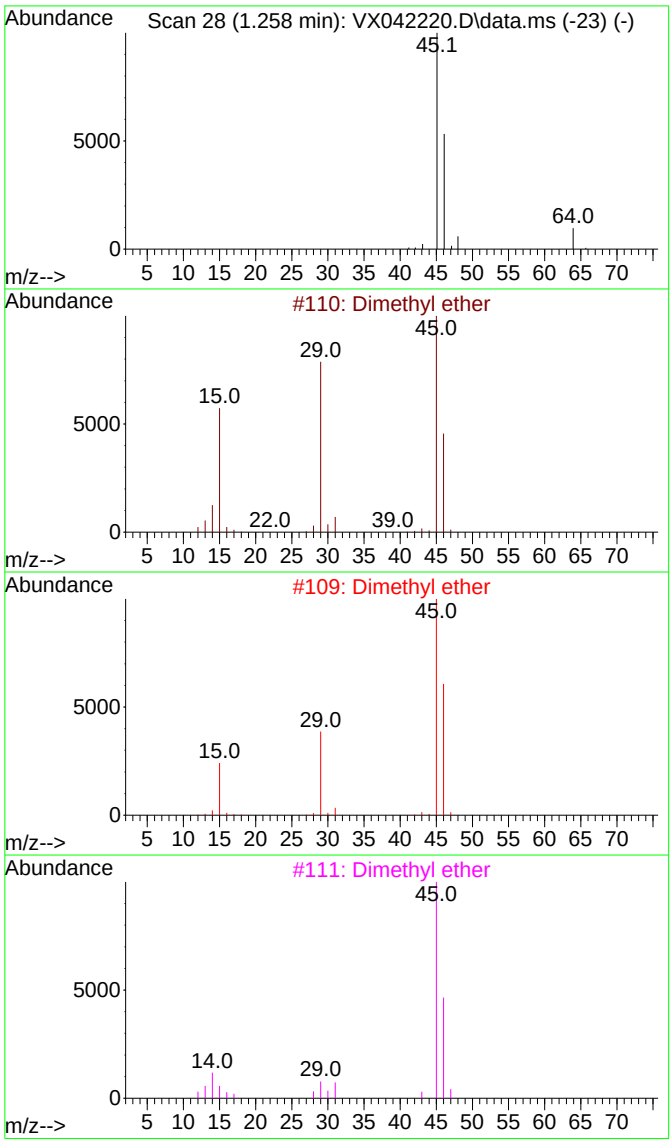
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

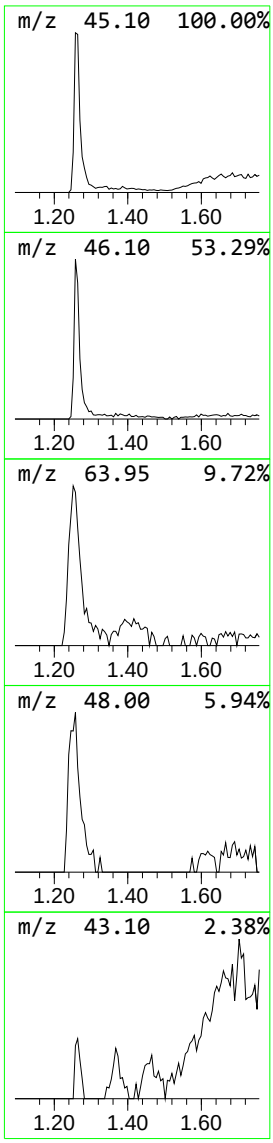
****

Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	2.60 ug/L	24705	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	56
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Dimethyl ether	46	C2H6O	000115-10-6	7
4	Ethanol	46	C2H6O	000064-17-5	7
5	Ethanol	46	C2H6O	000064-17-5	7





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Data File : VX042220.D
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Sample : P3100-20ME
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D33ME

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

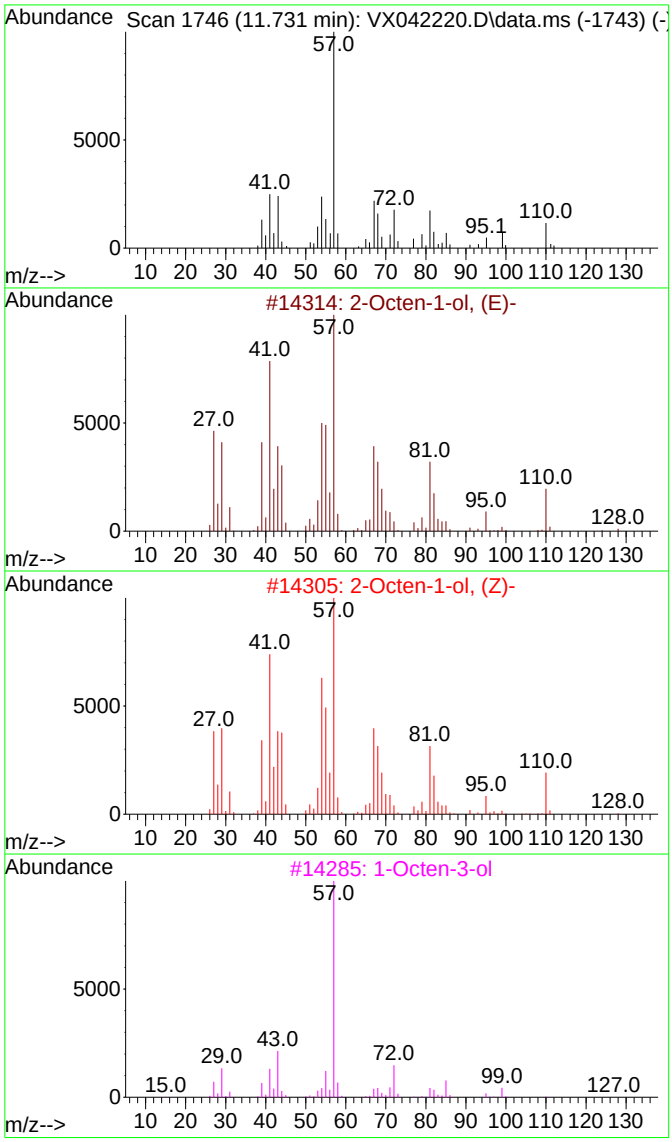
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

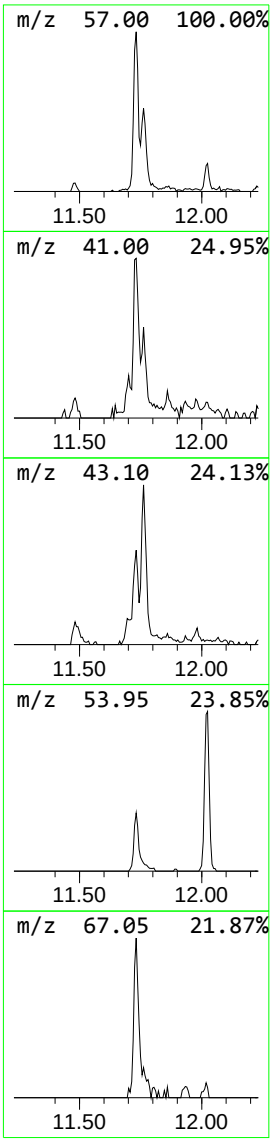
****

Peak Number 3 2-Octen-1-ol, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.732	2.88 ug/L	29887	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octen-1-ol, (E)-	128	C8H16O	018409-17-1	50
2	2-Octen-1-ol, (Z)-	128	C8H16O	026001-58-1	47
3	1-Octen-3-ol	128	C8H16O	003391-86-4	43
4	1-Octen-3-ol	128	C8H16O	003391-86-4	42
5	1-Octen-3-ol	128	C8H16O	003391-86-4	38





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Sample : P3100-20ME
Misc : 5.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D33ME

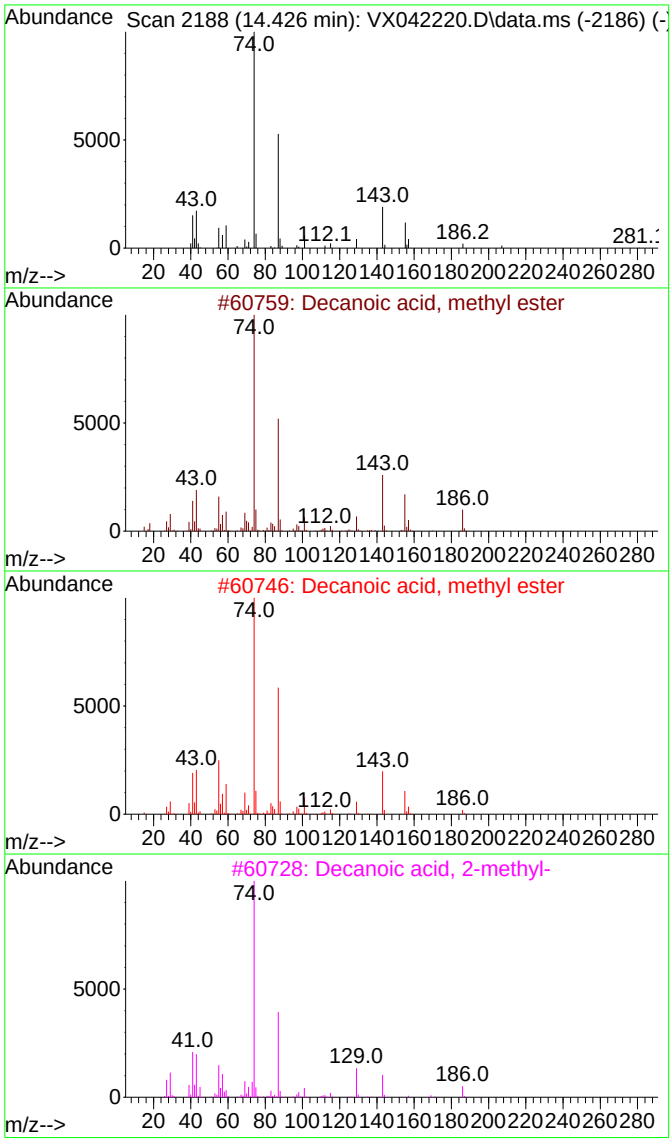
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

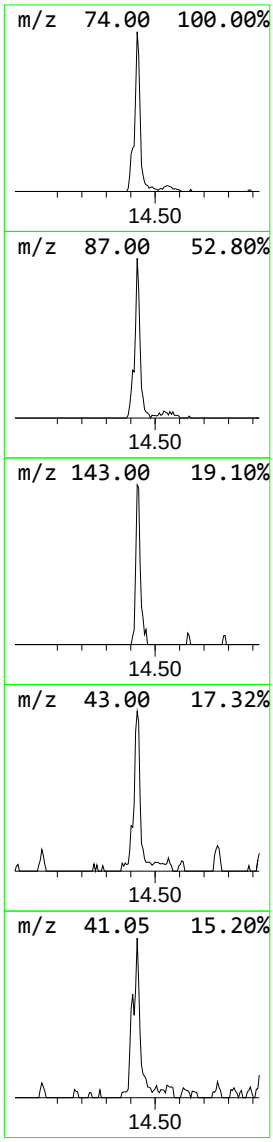
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Decanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	3.71 ug/L	38485	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	87
2	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	70
3	Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	59
4	Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	56
5	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	50





Tentatively Identified Compound (LSC) summary

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MSVOA_X
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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Dimethyl ether	1.258	2.6	ug/L	24705	1	6.757	475959	50.0
2-Octen-1-ol, (E)-	11.732	2.9	ug/L	29887	3	12.024	518366	50.0
Decanoic acid, ...	14.426	3.7	ug/L	38485	3	12.024	518366	50.0