

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070424\
 Data File : VX042195.D
 Acq On : 04 Jul 2024 04:22
 Operator : JC/MD
 Sample : P3088-14ME
 Misc : 4.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D02ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	39	rBV2	23894	32306	4.70%	0.574%
2	1.404	43	52	68	rVB	22375	88339	12.87%	1.570%
3	2.276	189	195	212	rBV	102590	194037	28.26%	3.448%
4	2.721	262	268	273	rBV	9247	20239	2.95%	0.360%
5	2.946	298	305	316	rVB2	5332	14790	2.15%	0.263%
6	3.324	365	367	370	rBV2	135	157	0.02%	0.003%
7	3.422	377	383	387	rVB5	726	1380	0.20%	0.025%
8	3.654	420	421	426	rBV	128	179	0.03%	0.003%
9	3.757	437	438	441	rBV	184	135	0.02%	0.002%
10	3.830	446	450	451	rBV2	652	649	0.09%	0.012%
11	3.952	465	470	472	rBV2	130	159	0.02%	0.003%
12	4.062	487	488	492	rVB	190	153	0.02%	0.003%
13	4.129	496	499	500	rBV	233	161	0.02%	0.003%
14	4.428	546	548	550	rBV	159	179	0.03%	0.003%
15	4.495	550	559	580	rBV	33932	128676	18.74%	2.286%
16	5.056	639	651	666	rBV	81745	255329	37.19%	4.537%
17	5.367	699	702	703	rBV2	197	209	0.03%	0.004%
18	5.556	727	733	736	rBV2	402	741	0.11%	0.013%
19	5.739	761	763	767	rBV2	125	142	0.02%	0.003%
20	5.958	788	799	817	rBV2	238364	686645	100.00%	12.200%
21	6.379	861	868	877	rBV5	1633	4150	0.60%	0.074%
22	6.464	880	882	885	rBV2	139	182	0.03%	0.003%
23	6.525	889	892	893	rBV2	141	146	0.02%	0.003%
24	6.549	893	896	899	rBV2	278	322	0.05%	0.006%
25	6.659	910	914	916	rBV2	384	481	0.07%	0.009%
26	6.757	921	930	946	rBV	216941	529277	77.08%	9.404%
27	7.104	983	987	988	rBV	1310	1396	0.20%	0.025%
28	7.220	999	1006	1012	rBV3	1891	4574	0.67%	0.081%
29	7.305	1012	1020	1045	rVB	136187	308569	44.94%	5.482%
30	7.476	1046	1048	1051	rBV4	267	221	0.03%	0.004%
31	7.854	1108	1110	1114	rVB2	121	152	0.02%	0.003%
32	7.891	1114	1116	1119	rBV	203	162	0.02%	0.003%
33	7.964	1124	1128	1136	rVV5	1005	2376	0.35%	0.042%
34	8.043	1138	1141	1144	rVV2	187	211	0.03%	0.004%
35	8.074	1144	1146	1149	rVB2	208	224	0.03%	0.004%
36	8.165	1157	1161	1162	rBV2	100	135	0.02%	0.002%

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 Title : VOC Analysis

37	8.256	1172	1176	1181	rBV2	249	394	0.06%	0.007%
38	8.324	1181	1187	1203	rBV	69594	121875	17.75%	2.165%
39	8.647	1232	1240	1254	rBV	345551	553708	80.64%	9.838%
40	8.909	1280	1283	1285	rBV	185	191	0.03%	0.003%
41	8.951	1285	1290	1308	rVV	50164	78929	11.49%	1.402%
42	9.110	1314	1316	1317	rBV2	330	214	0.03%	0.004%
43	9.153	1321	1323	1325	rBV2	199	221	0.03%	0.004%
44	9.232	1333	1336	1337	rBV	151	138	0.02%	0.002%
45	9.275	1337	1343	1349	rVB2	2371	3584	0.52%	0.064%
46	9.390	1357	1362	1381	rBV	133280	317751	46.28%	5.646%
47	9.714	1410	1415	1423	rVB2	3222	5669	0.83%	0.101%
48	9.842	1434	1436	1438	rBV2	182	140	0.02%	0.002%
49	9.896	1443	1445	1450	rVB3	284	335	0.05%	0.006%
50	10.055	1465	1471	1484	rVV	429041	609882	88.82%	10.836%
51	10.305	1508	1512	1524	rVB2	2793	4958	0.72%	0.088%
52	10.433	1531	1533	1539	rVB2	200	213	0.03%	0.004%
53	10.646	1565	1568	1571	rBV	783	848	0.12%	0.015%
54	10.890	1604	1608	1615	rBV2	332	562	0.08%	0.010%
55	10.963	1617	1620	1632	rVB3	2163	3543	0.52%	0.063%
56	11.097	1640	1642	1644	rBV	364	319	0.05%	0.006%
57	11.195	1652	1658	1672	rBV	254166	346227	50.42%	6.152%
58	11.311	1673	1677	1684	rVB	6434	8974	1.31%	0.159%
59	11.439	1694	1698	1701	rBV2	1556	2068	0.30%	0.037%
60	11.481	1702	1705	1712	rVB3	2285	3497	0.51%	0.062%
61	11.634	1729	1730	1733	rVB	356	238	0.03%	0.004%
62	11.701	1737	1741	1743	rBV2	4417	6047	0.88%	0.107%
63	11.731	1743	1746	1748	rVV	13079	16751	2.44%	0.298%
64	11.762	1748	1751	1762	rVB	17837	26940	3.92%	0.479%
65	11.853	1762	1766	1775	rBV2	3477	5937	0.86%	0.105%
66	11.939	1775	1780	1784	rBV3	1074	1908	0.28%	0.034%
67	11.975	1784	1786	1788	rBV2	1260	1437	0.21%	0.026%
68	12.024	1789	1794	1804	rVB	448371	579336	84.37%	10.293%
69	12.195	1820	1822	1824	rVB3	195	182	0.03%	0.003%
70	12.225	1824	1827	1832	rBV3	400	663	0.10%	0.012%
71	12.317	1837	1842	1852	rBV	382353	495930	72.23%	8.811%
72	12.420	1857	1859	1862	rVB2	668	677	0.10%	0.012%
73	12.609	1887	1890	1896	rVB3	406	600	0.09%	0.011%
74	12.762	1911	1915	1920	rVB2	2578	3512	0.51%	0.062%
75	12.871	1928	1933	1941	rBV3	5626	8619	1.26%	0.153%
76	12.981	1948	1951	1953	rBV2	195	238	0.03%	0.004%

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 A4D02ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

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 Title : VOC Analysis

77	13.036	1955	1960	1965	rVV2	1551	1893	0.28%	0.034%
78	13.164	1977	1981	1985	rBV2	283	386	0.06%	0.007%
79	13.262	1995	1997	2004	rVB4	395	507	0.07%	0.009%
80	13.347	2009	2011	2014	rBV2	195	193	0.03%	0.003%
81	13.371	2014	2015	2017	rVB	266	157	0.02%	0.003%
82	13.408	2017	2021	2025	rBV2	1018	1679	0.24%	0.030%
83	13.487	2031	2034	2036	rBV2	214	209	0.03%	0.004%
84	13.512	2036	2038	2042	rVV2	246	289	0.04%	0.005%
85	13.554	2042	2045	2046	rVV2	193	161	0.02%	0.003%
86	13.603	2049	2053	2055	rBV2	403	513	0.07%	0.009%
87	13.652	2059	2061	2062	rBV	326	227	0.03%	0.004%
88	13.682	2062	2066	2074	rBV3	2452	3792	0.55%	0.067%
89	13.780	2079	2082	2088	rBV	1445	1920	0.28%	0.034%
90	13.884	2096	2099	2103	rBV3	1040	1305	0.19%	0.023%
91	14.036	2121	2124	2128	rVB2	500	625	0.09%	0.011%
92	14.072	2128	2130	2131	rBV	170	159	0.02%	0.003%
93	14.127	2135	2139	2143	rVB2	523	802	0.12%	0.014%
94	14.158	2143	2144	2147	rBV	198	229	0.03%	0.004%
95	14.365	2176	2178	2182	rBV2	254	330	0.05%	0.006%
96	14.426	2182	2188	2205	rBV	83687	111303	16.21%	1.978%
97	14.761	2238	2243	2245	rBV4	758	1199	0.17%	0.021%
98	14.987	2279	2280	2282	rBV2	457	405	0.06%	0.007%
99	15.176	2308	2311	2315	rVB3	1660	1908	0.28%	0.034%
100	15.956	2435	2439	2446	rVB2	4380	7645	1.11%	0.136%

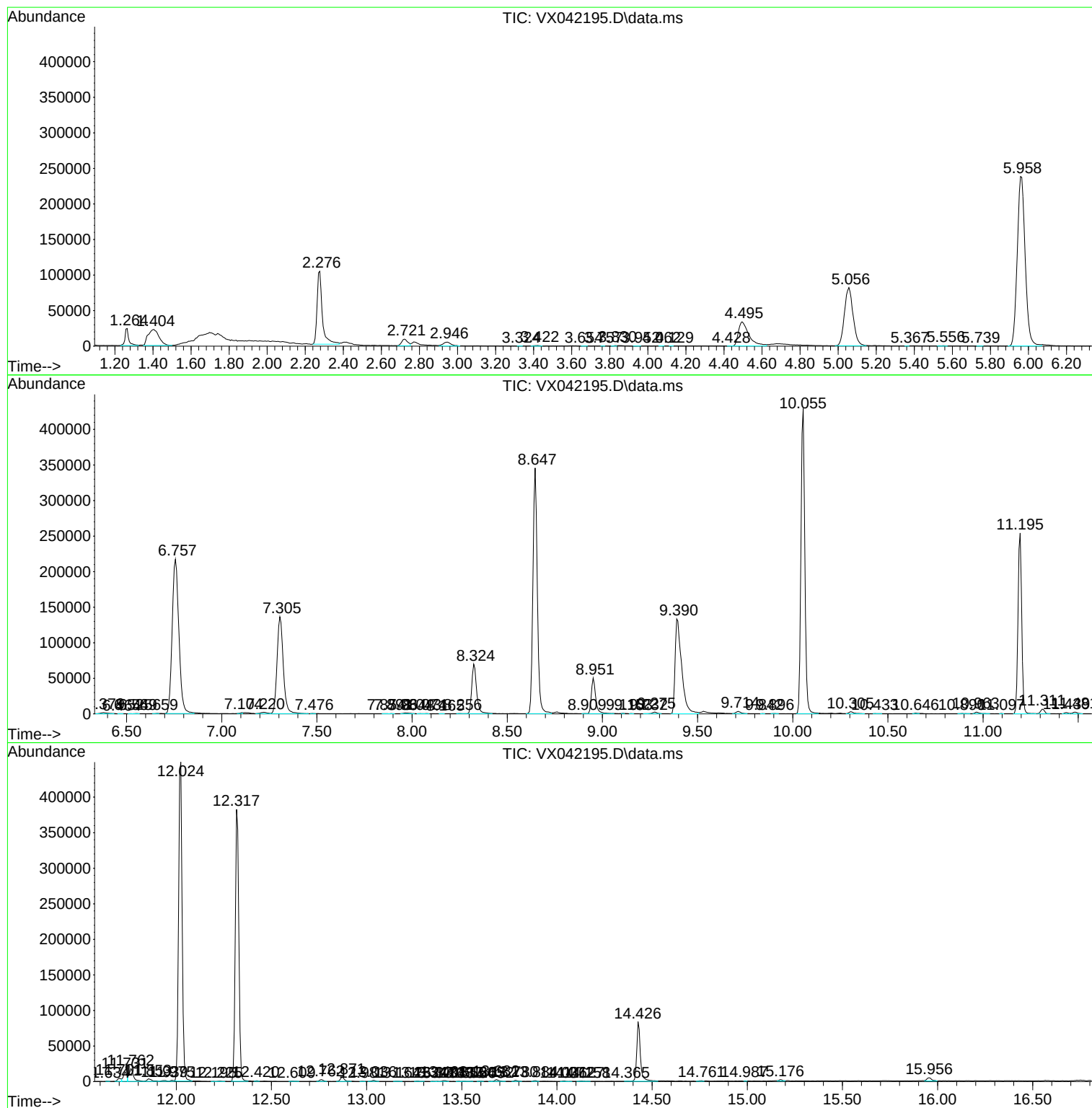
Sum of corrected areas: 5628274

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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D02ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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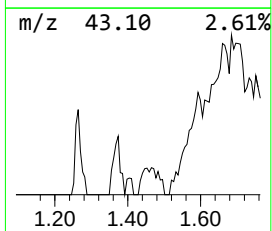
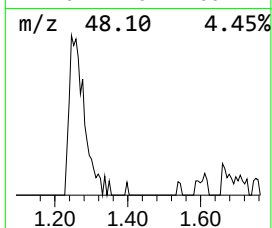
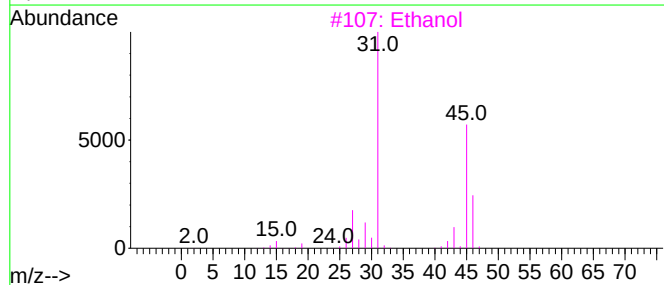
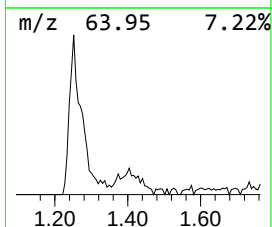
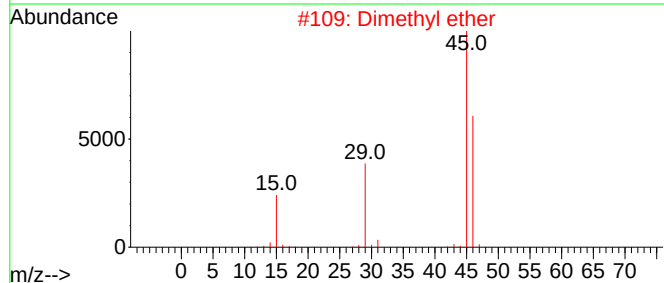
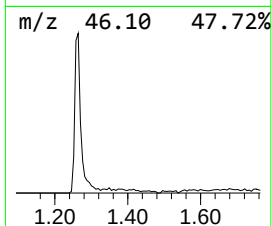
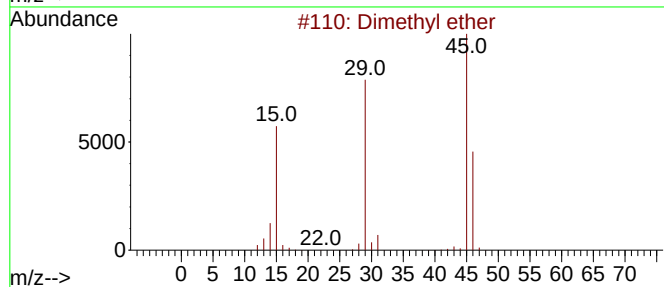
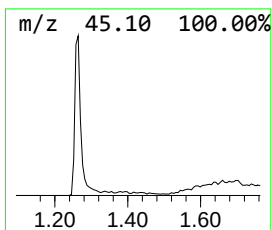
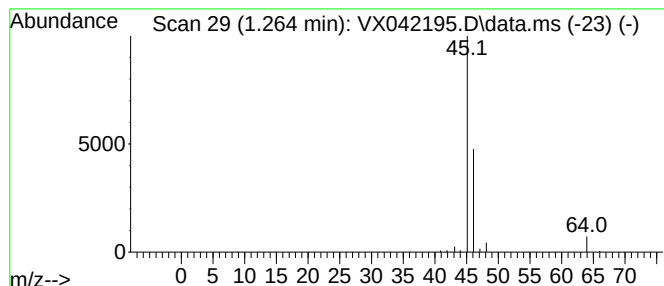
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	3.05 ug/L	32306	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	86
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Ethanol	46	C2H6O	000064-17-5	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



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Misc : 4.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D02ME

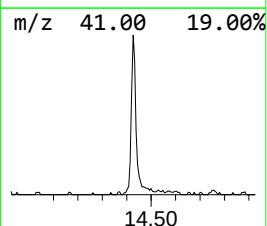
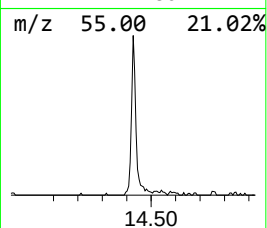
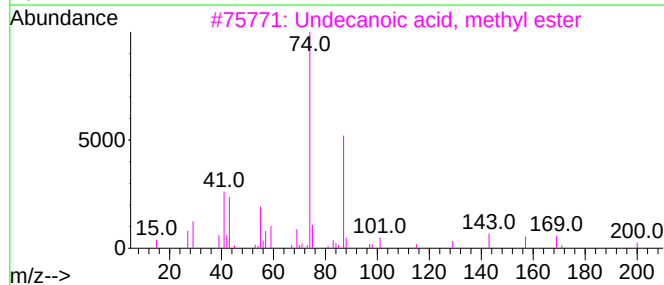
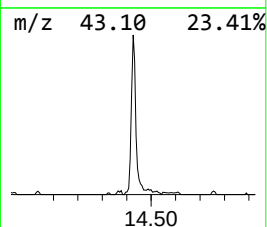
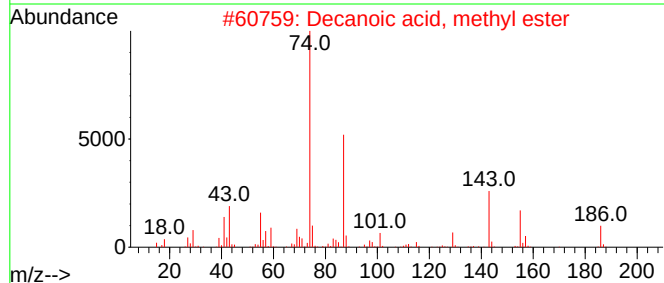
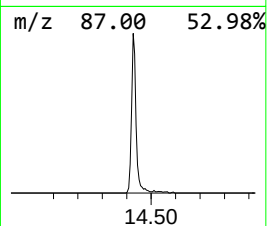
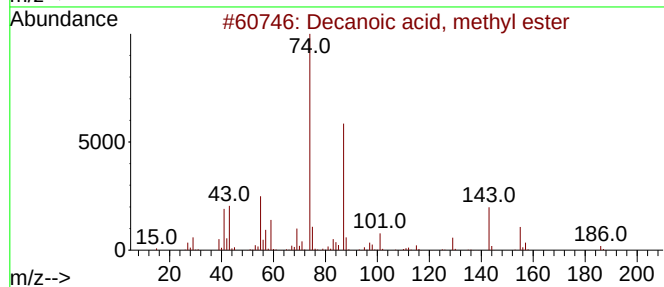
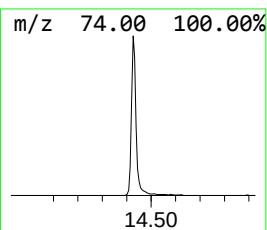
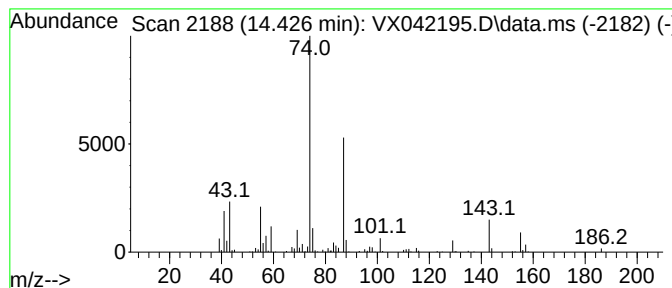
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Decanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	9.61 ug/L	111303	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			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	80
4			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	80
5			Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	80



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.264	3.0	ug/L	32306	1	6.757	529277	50.0
Decanoic acid, ...	14.426	9.6	ug/L	111303	3	12.024	579336	50.0