

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070424\
 Data File : VX042196.D
 Acq On : 04 Jul 2024 04:45
 Operator : JC/MD
 Sample : P3088-17ME
 Misc : 4.52g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D12ME

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: VX042196.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	40	rBV2	20996	27281	4.91%	0.631%
2	1.404	43	52	67	rVB	17401	65673	11.81%	1.519%
3	2.276	189	195	209	rBV	77522	144624	26.01%	3.346%
4	2.721	262	268	273	rBV2	11372	24292	4.37%	0.562%
5	2.947	299	305	316	rVB	4207	10186	1.83%	0.236%
6	3.416	376	382	388	rVV5	825	1579	0.28%	0.037%
7	3.514	396	398	400	rBV2	143	175	0.03%	0.004%
8	3.593	407	411	413	rVB3	123	145	0.03%	0.003%
9	3.623	413	416	417	rBV	162	139	0.03%	0.003%
10	3.849	447	453	455	rBV3	186	358	0.06%	0.008%
11	3.983	472	475	477	rVB	179	141	0.03%	0.003%
12	4.093	490	493	496	rBV2	126	195	0.04%	0.005%
13	4.190	508	509	513	rVV2	130	136	0.02%	0.003%
14	4.245	516	518	520	rVB2	179	142	0.03%	0.003%
15	4.276	520	523	526	rBV2	213	235	0.04%	0.005%
16	4.495	551	559	576	rBV	21896	83362	14.99%	1.929%
17	5.056	640	651	670	rBV	56798	177447	31.92%	4.106%
18	5.373	700	703	705	rBV2	295	366	0.07%	0.008%
19	5.440	712	714	717	rBV	131	130	0.02%	0.003%
20	5.532	725	729	731	rBV2	199	266	0.05%	0.006%
21	5.696	753	756	759	rBV2	157	172	0.03%	0.004%
22	5.727	759	761	766	rVB2	172	214	0.04%	0.005%
23	5.885	785	787	789	rBV2	125	147	0.03%	0.003%
24	5.958	789	799	817	rBV2	166886	487690	87.72%	11.284%
25	6.312	854	857	860	rVB2	145	149	0.03%	0.003%
26	6.373	862	867	872	rBV5	1112	2779	0.50%	0.064%
27	6.470	881	883	885	rVB	191	184	0.03%	0.004%
28	6.489	885	886	889	rBV	163	138	0.02%	0.003%
29	6.550	893	896	897	rBV	159	135	0.02%	0.003%
30	6.757	921	930	952	rBV	196348	479408	86.23%	11.092%
31	7.111	983	988	989	rBV4	879	1278	0.23%	0.030%
32	7.214	999	1005	1012	rBV3	2016	4824	0.87%	0.112%
33	7.306	1012	1020	1041	rVB	94737	213718	38.44%	4.945%
34	7.476	1046	1048	1052	rVB3	220	291	0.05%	0.007%
35	7.513	1052	1054	1057	rVB	186	208	0.04%	0.005%
36	7.964	1124	1128	1137	rVB4	734	1811	0.33%	0.042%

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Integrator: RTE

Smoothing : OFF

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37	8.080	1144	1147	1148	rBV	162	155	0.03%	0.004%
38	8.214	1167	1169	1170	rBV	112	114	0.02%	0.003%
39	8.245	1172	1174	1175	rBV2	217	222	0.04%	0.005%
40	8.324	1181	1187	1203	rBV	45958	82885	14.91%	1.918%
41	8.580	1225	1229	1230	rBV2	172	185	0.03%	0.004%
42	8.647	1234	1240	1255	rBV	250971	401472	72.21%	9.289%
43	8.952	1285	1290	1305	rBV	32483	52492	9.44%	1.215%
44	9.275	1338	1343	1349	rVB2	3704	5861	1.05%	0.136%
45	9.342	1349	1354	1357	rBV	143	199	0.04%	0.005%
46	9.397	1357	1363	1383	rBV	82796	205230	36.91%	4.748%
47	9.714	1409	1415	1423	rVB3	1634	3175	0.57%	0.073%
48	9.775	1423	1425	1429	rVB	161	120	0.02%	0.003%
49	9.805	1429	1430	1434	rBV2	165	156	0.03%	0.004%
50	9.897	1442	1445	1446	rVB	202	140	0.03%	0.003%
51	9.988	1459	1460	1465	rBV	91	136	0.02%	0.003%
52	10.055	1465	1471	1487	rVV	391957	555981	100.00%	12.864%
53	10.201	1491	1495	1498	rVV3	769	1190	0.21%	0.028%
54	10.244	1499	1502	1507	rVV2	1138	1720	0.31%	0.040%
55	10.305	1508	1512	1519	rVV2	3499	5121	0.92%	0.118%
56	10.586	1553	1558	1559	rBV2	150	172	0.03%	0.004%
57	10.647	1565	1568	1577	rVB3	777	1380	0.25%	0.032%
58	10.781	1588	1590	1592	rVB	199	147	0.03%	0.003%
59	10.970	1617	1621	1631	rVB3	1439	2364	0.43%	0.055%
60	11.104	1641	1643	1645	rVV	243	189	0.03%	0.004%
61	11.153	1649	1651	1652	rBV	176	140	0.03%	0.003%
62	11.195	1652	1658	1670	rVV	174281	230789	41.51%	5.340%
63	11.311	1673	1677	1682	rVB	3221	4526	0.81%	0.105%
64	11.451	1698	1700	1701	rBV2	205	175	0.03%	0.004%
65	11.482	1701	1705	1712	rVB3	1511	2450	0.44%	0.057%
66	11.628	1726	1729	1733	rVB3	241	350	0.06%	0.008%
67	11.701	1737	1741	1744	rBV	2981	4358	0.78%	0.101%
68	11.732	1744	1746	1748	rVV3	4194	5597	1.01%	0.129%
69	11.762	1748	1751	1762	rVV3	14588	23816	4.28%	0.551%
70	11.860	1763	1767	1777	rVB2	2805	5186	0.93%	0.120%
71	11.939	1777	1780	1783	rBV2	380	602	0.11%	0.014%
72	11.976	1784	1786	1788	rBV2	896	921	0.17%	0.021%
73	12.024	1789	1794	1803	rVB	412859	537517	96.68%	12.437%
74	12.317	1837	1842	1852	rBV	268069	355193	63.89%	8.218%
75	12.427	1858	1860	1864	rVB4	588	740	0.13%	0.017%
76	12.463	1864	1866	1870	rVB	484	380	0.07%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

77	12.524	1874	1876	1877	rVB2	163	109	0.02%	0.003%
78	12.762	1910	1915	1919	rVB3	757	1287	0.23%	0.030%
79	12.872	1928	1933	1939	rBV3	3542	5506	0.99%	0.127%
80	13.042	1957	1961	1964	rVB2	964	1167	0.21%	0.027%
81	13.158	1978	1980	1983	rBV3	198	200	0.04%	0.005%
82	13.268	1995	1998	2000	rBV2	434	498	0.09%	0.012%
83	13.353	2010	2012	2016	rVB3	240	209	0.04%	0.005%
84	13.408	2017	2021	2024	rVB3	719	930	0.17%	0.022%
85	13.445	2024	2027	2029	rBV2	230	187	0.03%	0.004%
86	13.530	2038	2041	2043	rBV2	138	124	0.02%	0.003%
87	13.555	2043	2045	2046	rBV	144	109	0.02%	0.003%
88	13.591	2050	2051	2052	rBV	361	231	0.04%	0.005%
89	13.683	2063	2066	2073	rVB5	758	1036	0.19%	0.024%
90	13.786	2079	2083	2090	rVB2	933	1748	0.31%	0.040%
91	13.835	2090	2091	2096	rBV3	192	246	0.04%	0.006%
92	13.878	2096	2098	2100	rBV	207	218	0.04%	0.005%
93	13.969	2111	2113	2114	rBV2	225	154	0.03%	0.004%
94	14.036	2121	2124	2127	rVV3	499	496	0.09%	0.011%
95	14.256	2159	2160	2161	rBV	283	121	0.02%	0.003%
96	14.426	2182	2188	2199	rBV	55012	74079	13.32%	1.714%
97	14.756	2240	2242	2244	rBV2	750	571	0.10%	0.013%
98	15.036	2284	2288	2291	rBV4	922	1289	0.23%	0.030%
99	15.341	2337	2338	2341	rVB3	793	533	0.10%	0.012%
100	15.957	2434	2439	2445	rVB3	4449	7479	1.35%	0.173%

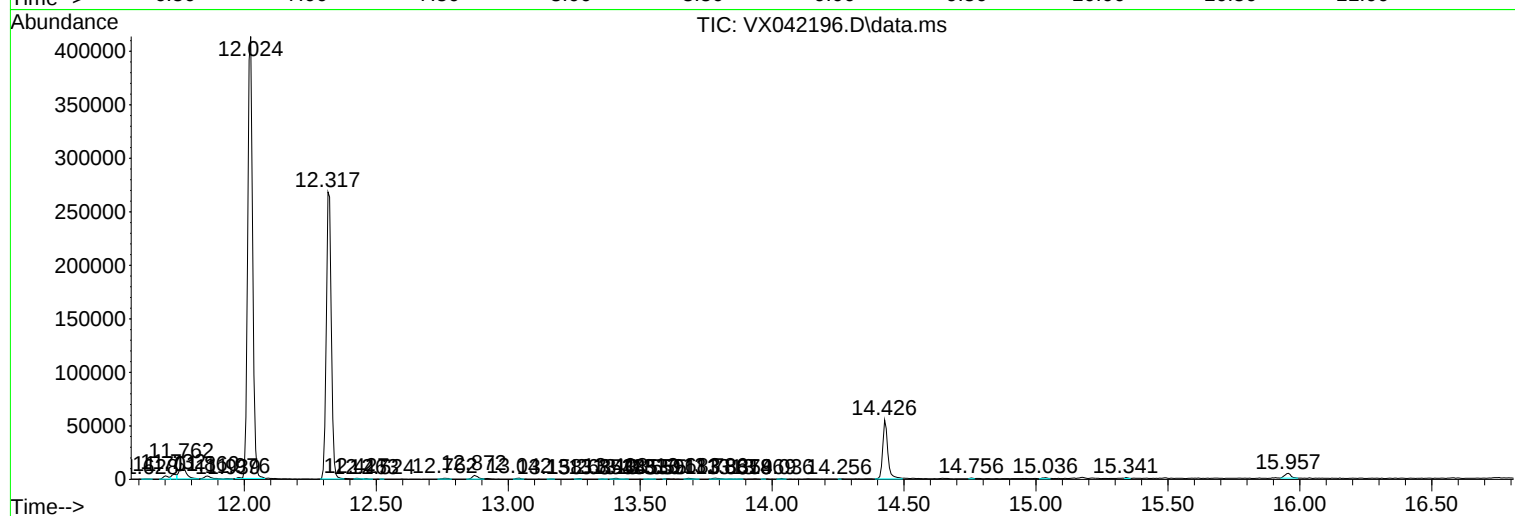
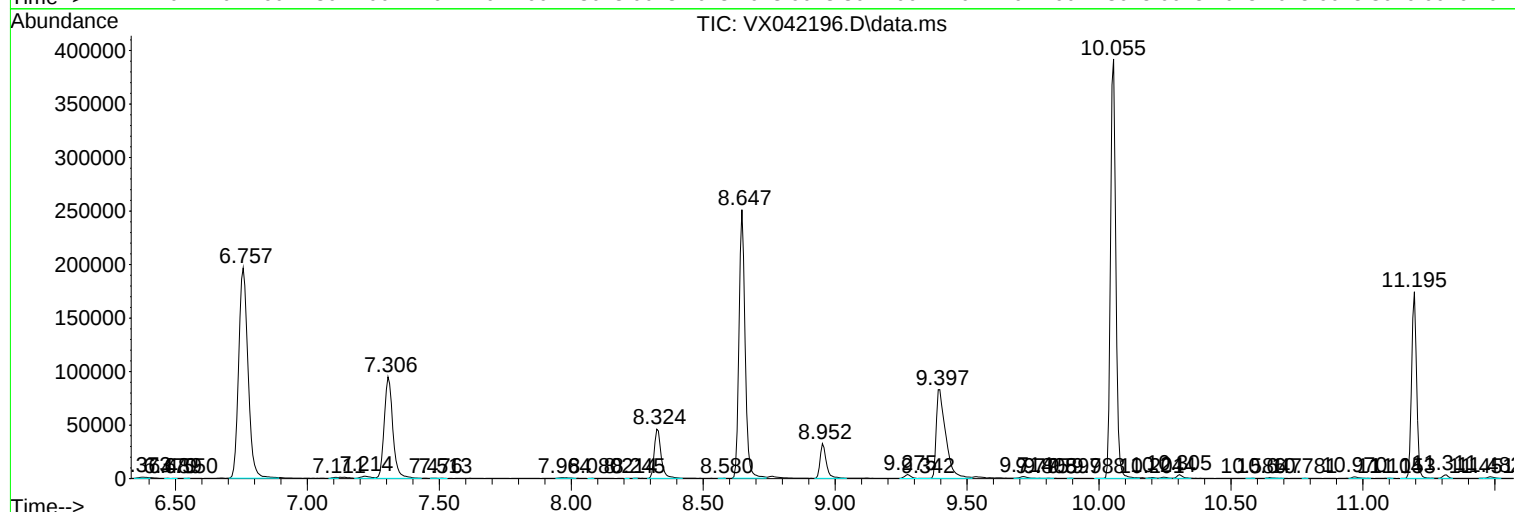
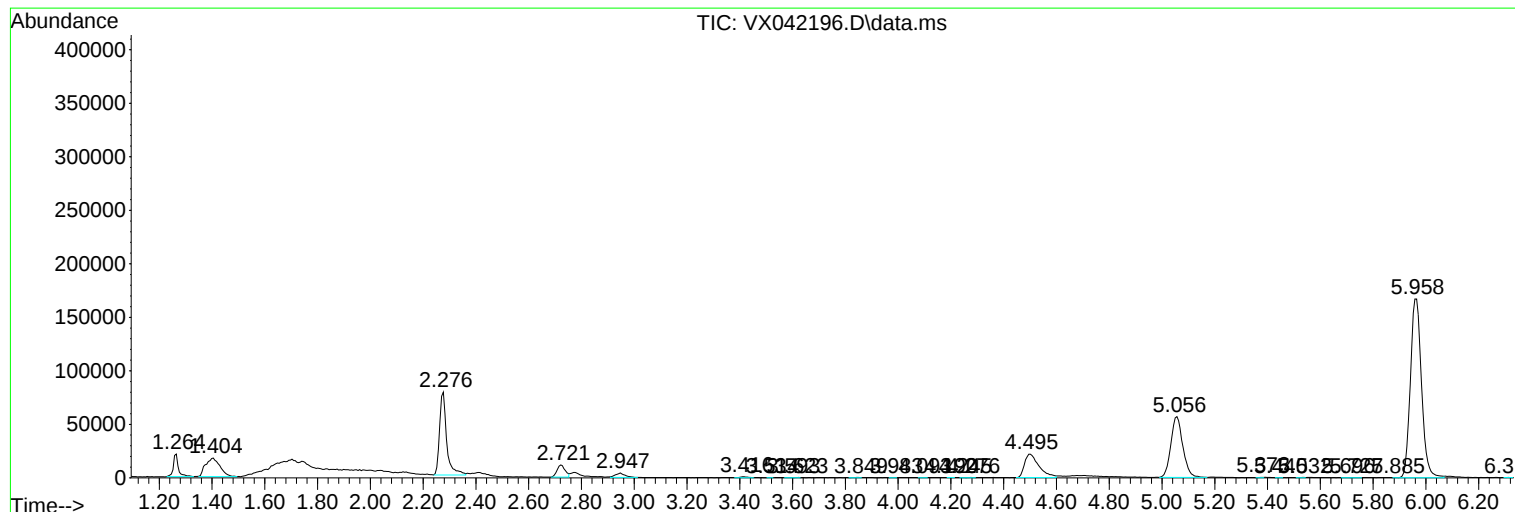
Sum of corrected areas: 4322091

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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A4D12ME

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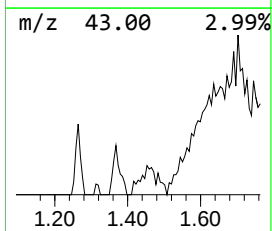
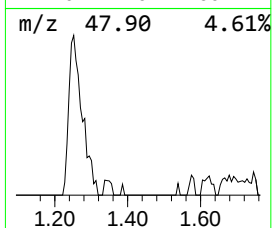
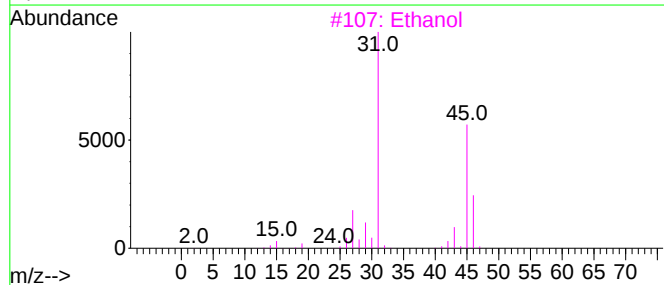
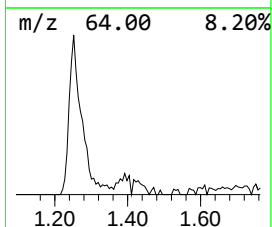
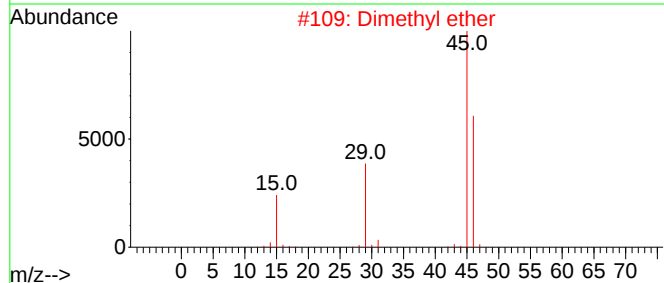
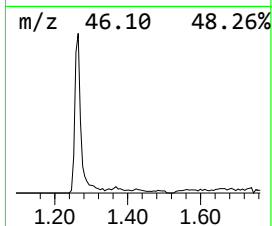
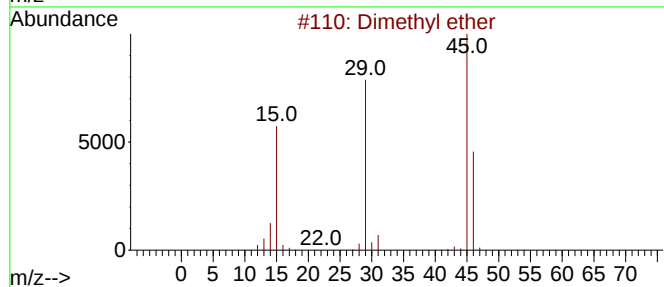
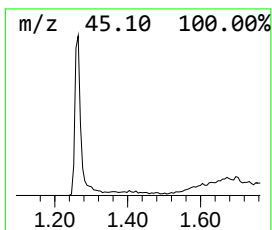
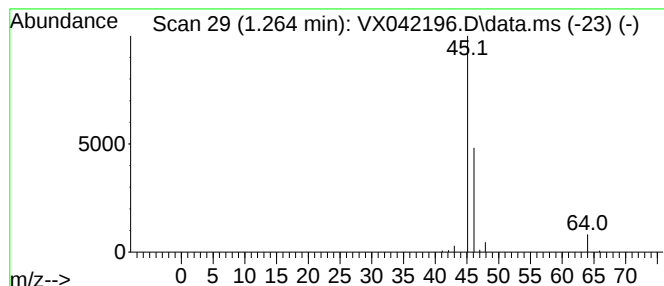
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	2.85 ug/L	27281	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Ethanol	46	C2H6O	000064-17-5	7
4			Dimethyl ether	46	C2H6O	000115-10-6	7
5			Ethanol	46	C2H6O	000064-17-5	7



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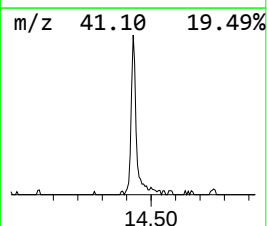
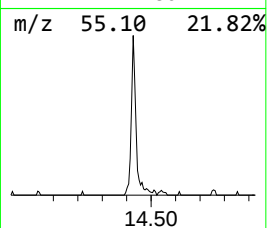
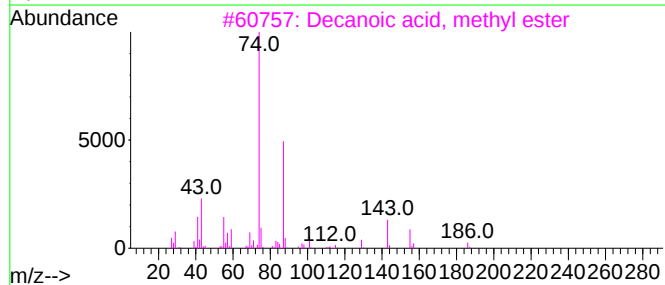
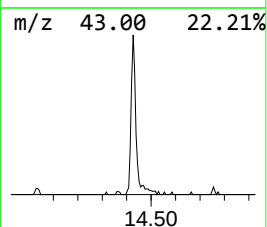
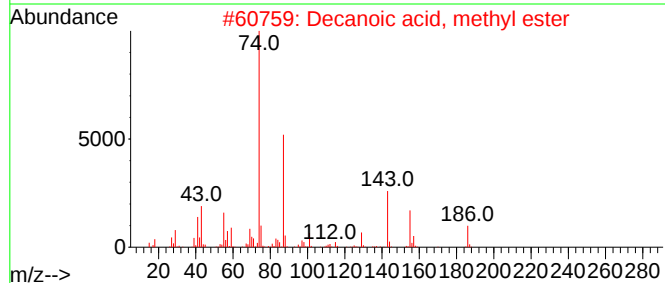
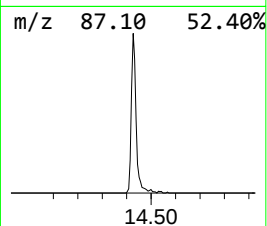
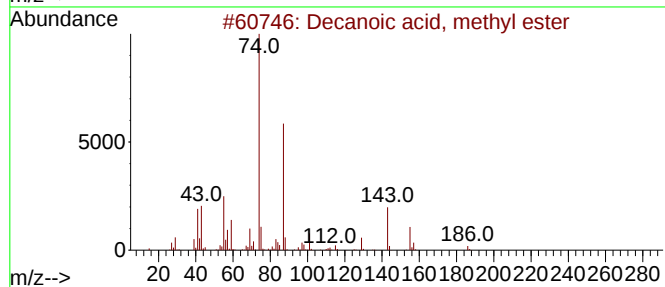
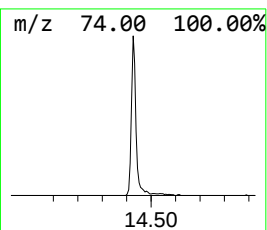
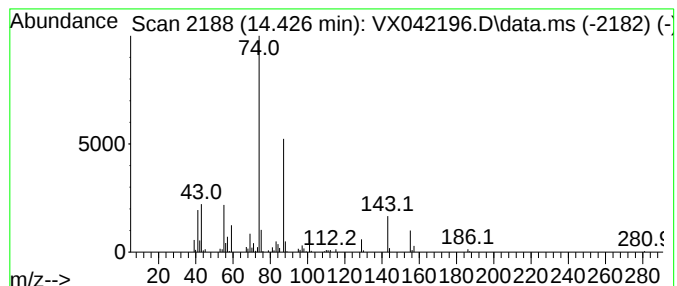
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Decanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	6.89 ug/L	74079	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	95
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	86



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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	2.9	ug/L	27281	1	6.757	479408	50.0
Decanoic acid, ...	14.426	6.9	ug/L	74079	3	12.024	537517	50.0