

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
 Data File : VX041133.D
 Acq On : 17 Apr 2024 18:25
 Operator : JC/MD
 Sample : PB160244TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB244

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\SFAMXML041724WMA.M

Title : VOC Analysis

Signal : TIC: VX041133.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	26	29	32	rBV2	2930	2904	0.28%	0.034%
2	1.373	43	47	63	rBV	94560	150293	14.26%	1.760%
3	1.648	88	92	109	rVB	54673	101044	9.59%	1.184%
4	2.294	191	198	209	rBV	228776	352091	33.40%	4.124%
5	2.398	211	215	223	rVB	3908	7839	0.74%	0.092%
6	2.599	243	248	250	rBV3	376	689	0.07%	0.008%
7	2.715	265	267	270	rVB2	478	464	0.04%	0.005%
8	2.782	273	278	289	rBV	4792	10492	1.00%	0.123%
9	2.904	296	298	299	rBV	343	161	0.02%	0.002%
10	2.940	299	304	311	rVB3	872	1892	0.18%	0.022%
11	3.062	323	324	329	rVB	151	185	0.02%	0.002%
12	3.123	332	334	335	rVB	234	129	0.01%	0.002%
13	3.141	335	337	338	rBV	225	138	0.01%	0.002%
14	3.239	351	353	356	rBV2	134	200	0.02%	0.002%
15	3.343	367	370	373	rVB2	142	209	0.02%	0.002%
16	3.538	399	402	403	rBV2	127	146	0.01%	0.002%
17	3.593	403	411	420	rVB4	2224	6104	0.58%	0.071%
18	3.763	437	439	442	rVB2	138	138	0.01%	0.002%
19	3.788	442	443	444	rBV	327	151	0.01%	0.002%
20	3.891	458	460	463	rBV	163	141	0.01%	0.002%
21	4.032	480	483	484	rBV	198	138	0.01%	0.002%
22	4.470	546	555	574	rBV2	61842	223142	21.17%	2.614%
23	5.056	638	651	668	rBV	132821	409822	38.88%	4.800%
24	5.391	698	706	709	rBV3	597	1462	0.14%	0.017%
25	5.458	715	717	720	rVB3	200	193	0.02%	0.002%
26	5.556	725	733	735	rBV3	719	1348	0.13%	0.016%
27	5.623	742	744	747	rBV2	130	133	0.01%	0.002%
28	5.860	781	783	787	rVB2	128	172	0.02%	0.002%
29	5.964	787	800	818	rBV2	361836	1054127	100.00%	12.347%
30	6.360	856	865	876	rBV2	6854	20797	1.97%	0.244%
31	6.501	885	888	889	rBV	183	161	0.02%	0.002%
32	6.586	901	902	904	rBV	231	170	0.02%	0.002%
33	6.757	921	930	958	rVV	265809	657739	62.40%	7.704%
34	7.116	984	989	991	rBV4	1026	1758	0.17%	0.021%
35	7.208	997	1004	1011	rBV	1236	2787	0.26%	0.033%
36	7.305	1011	1020	1036	rBV	209727	463346	43.96%	5.427%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
 Title : VOC Analysis

37	7.543	1058	1059	1061	rBV2	269	212	0.02%	0.002%
38	7.659	1070	1078	1084	rBV	2985	7284	0.69%	0.085%
39	7.805	1096	1102	1122	rBV	88591	174135	16.52%	2.040%
40	8.141	1156	1157	1161	rVB2	138	144	0.01%	0.002%
41	8.232	1170	1172	1174	rBV	236	287	0.03%	0.003%
42	8.323	1181	1187	1200	rBV	126780	214173	20.32%	2.509%
43	8.512	1215	1218	1219	rBV2	474	509	0.05%	0.006%
44	8.555	1219	1225	1234	rVV	18686	33478	3.18%	0.392%
45	8.647	1234	1240	1256	rBV	531039	854575	81.07%	10.009%
46	8.951	1285	1290	1306	rBV2	108013	178338	16.92%	2.089%
47	9.104	1311	1315	1317	rBV4	412	397	0.04%	0.005%
48	9.146	1320	1322	1323	rBV2	188	145	0.01%	0.002%
49	9.250	1333	1339	1347	rBV	26298	41293	3.92%	0.484%
50	9.317	1347	1350	1351	rVV3	1825	1949	0.18%	0.023%
51	9.348	1352	1355	1356	rVV2	4916	5845	0.55%	0.068%
52	9.390	1356	1362	1374	rVV	299094	510282	48.41%	5.977%
53	9.488	1374	1378	1390	rVV	49878	78299	7.43%	0.917%
54	9.585	1390	1394	1409	rVB	29700	47079	4.47%	0.551%
55	9.793	1426	1428	1430	rBV	191	152	0.01%	0.002%
56	9.915	1443	1448	1462	rBV	83951	115899	10.99%	1.358%
57	10.055	1465	1471	1492	rVV	552120	773964	73.42%	9.065%
58	10.201	1493	1495	1498	rVB2	640	467	0.04%	0.005%
59	10.415	1528	1530	1532	rBV	272	193	0.02%	0.002%
60	10.524	1543	1548	1550	rBV4	639	1069	0.10%	0.013%
61	10.646	1562	1568	1578	rVB	5498	9057	0.86%	0.106%
62	10.725	1578	1581	1583	rBV2	142	165	0.02%	0.002%
63	10.817	1592	1596	1597	rBV2	245	273	0.03%	0.003%
64	10.957	1618	1619	1621	rBV	215	212	0.02%	0.002%
65	11.067	1636	1637	1640	rBV	205	176	0.02%	0.002%
66	11.091	1640	1641	1645	rBV2	355	455	0.04%	0.005%
67	11.146	1648	1650	1652	rBV	209	139	0.01%	0.002%
68	11.195	1652	1658	1673	rVV	412237	539601	51.19%	6.320%
69	11.311	1673	1677	1682	rVV3	907	1637	0.16%	0.019%
70	11.353	1682	1684	1685	rVB2	263	154	0.01%	0.002%
71	11.427	1694	1696	1699	rVV2	161	156	0.01%	0.002%
72	11.463	1699	1702	1703	rVV2	311	299	0.03%	0.004%
73	11.713	1741	1743	1745	rVB	427	252	0.02%	0.003%
74	11.756	1748	1750	1753	rVB2	269	233	0.02%	0.003%
75	11.798	1756	1757	1760	rVB2	147	136	0.01%	0.002%
76	11.859	1766	1767	1770	rVB	291	158	0.01%	0.002%

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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\SFAMXLM041724WMA.M
 Title : VOC Analysis

77	11.890	1770	1772	1775	rBV	222	179	0.02%	0.002%
78	11.920	1775	1777	1780	rVB	191	172	0.02%	0.002%
79	11.969	1780	1785	1788	rBV3	539	750	0.07%	0.009%
80	12.024	1788	1794	1811	rBV	544730	697321	66.15%	8.168%
81	12.317	1837	1842	1855	rBV	594536	765905	72.66%	8.971%
82	12.542	1878	1879	1883	rVB	232	174	0.02%	0.002%
83	12.689	1901	1903	1905	rBV	190	132	0.01%	0.002%
84	12.719	1906	1908	1911	rVV	174	154	0.01%	0.002%
85	12.762	1911	1915	1921	rVB2	969	1297	0.12%	0.015%
86	13.115	1971	1973	1978	rVV2	237	302	0.03%	0.004%
87	13.310	2003	2005	2006	rBV2	168	129	0.01%	0.002%
88	13.463	2027	2030	2031	rBV	187	141	0.01%	0.002%
89	13.560	2044	2046	2047	rBV	214	133	0.01%	0.002%
90	13.597	2047	2052	2054	rBV	505	741	0.07%	0.009%
91	13.640	2058	2059	2061	rBV	185	154	0.01%	0.002%
92	13.755	2076	2078	2080	rBV2	151	130	0.01%	0.002%
93	13.792	2080	2084	2087	rBV4	331	645	0.06%	0.008%
94	13.957	2110	2111	2112	rBV	205	131	0.01%	0.002%
95	14.072	2129	2130	2132	rBV2	210	182	0.02%	0.002%
96	14.133	2135	2140	2143	rBV2	1349	1703	0.16%	0.020%
97	14.225	2152	2155	2156	rBV2	203	156	0.01%	0.002%
98	14.396	2182	2183	2186	rBV2	199	172	0.02%	0.002%
99	14.597	2214	2216	2217	rBV	317	199	0.02%	0.002%
100	14.963	2273	2276	2278	rBV3	449	680	0.06%	0.008%

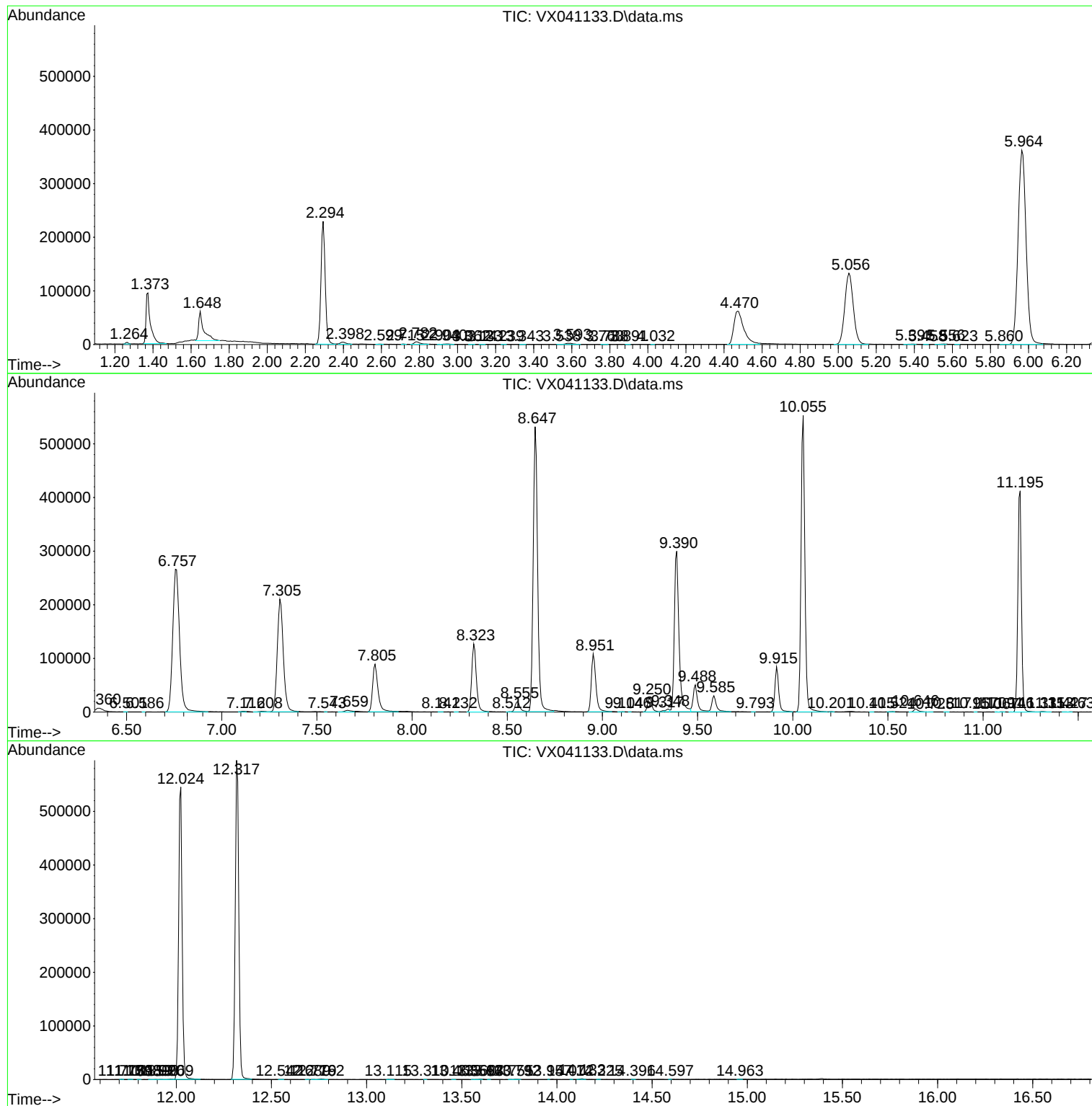
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Instrument :
MSVOA_X
ClientSampleId :
VLEB244

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.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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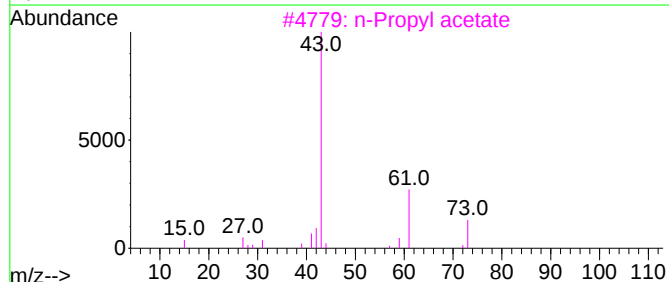
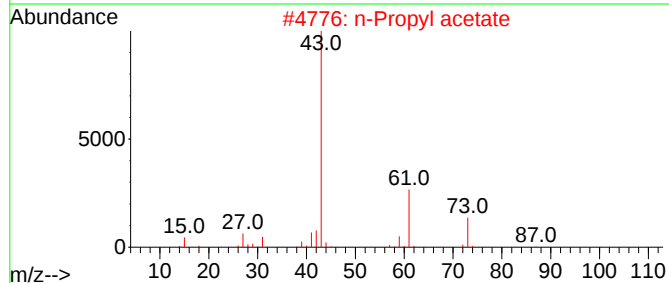
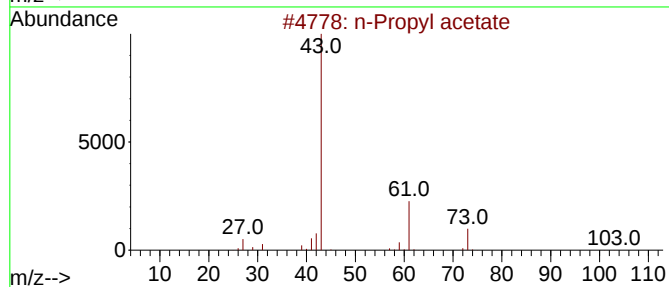
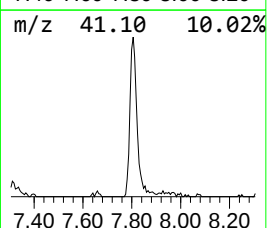
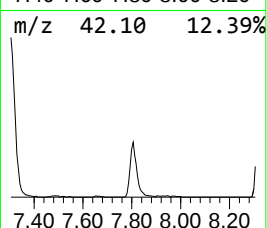
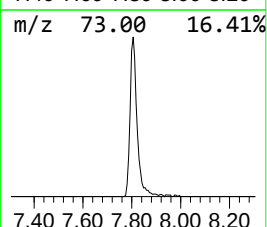
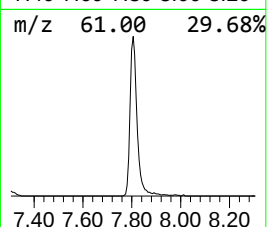
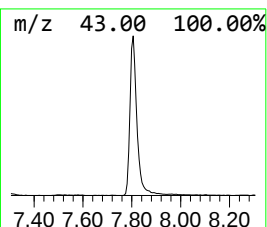
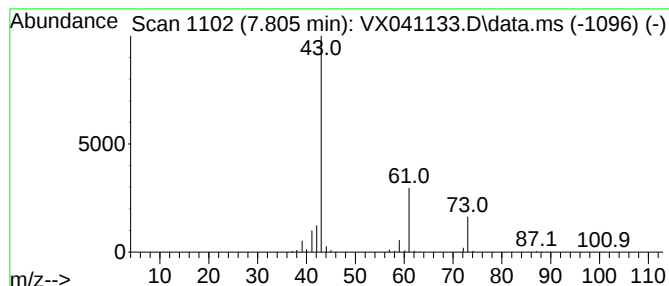
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.805	13.24 ug/L	174135	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VLEB244

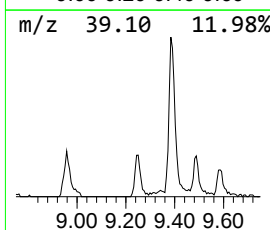
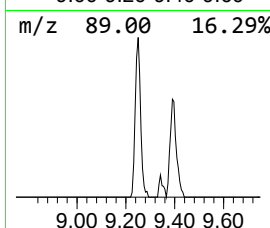
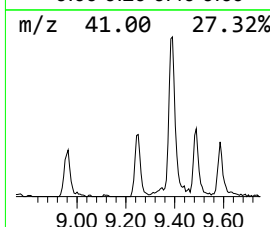
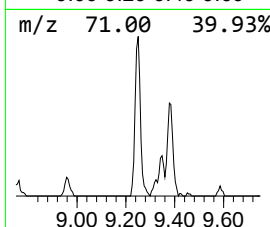
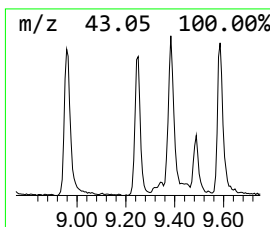
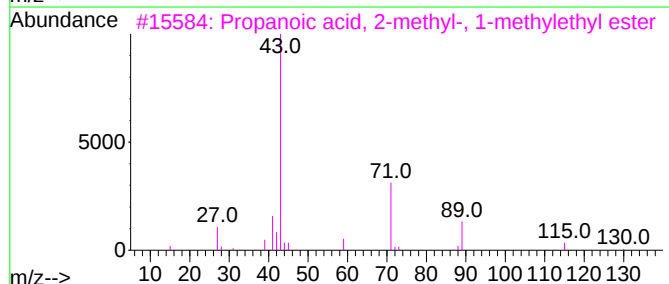
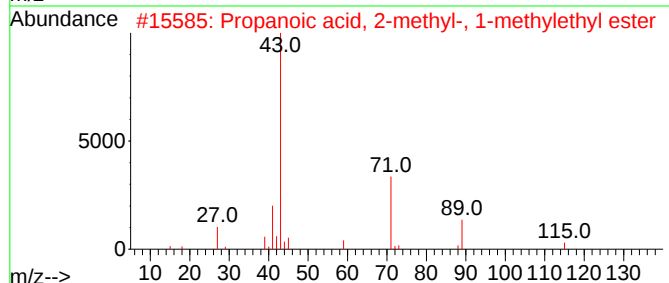
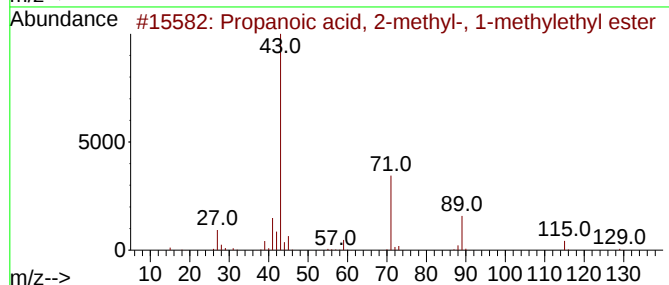
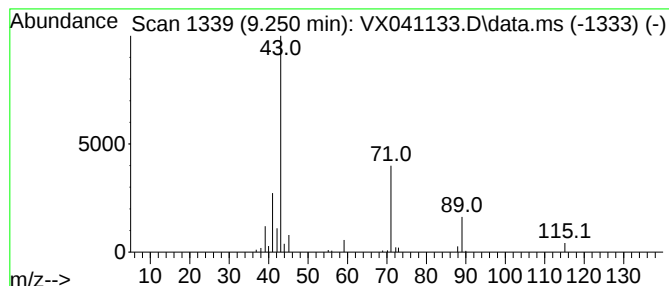
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	2.67 ug/L	41293	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



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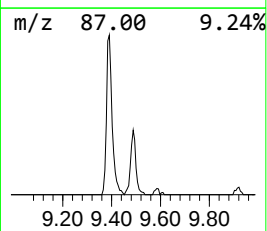
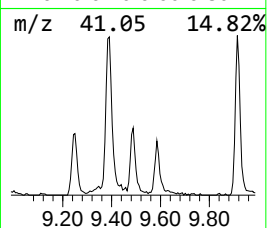
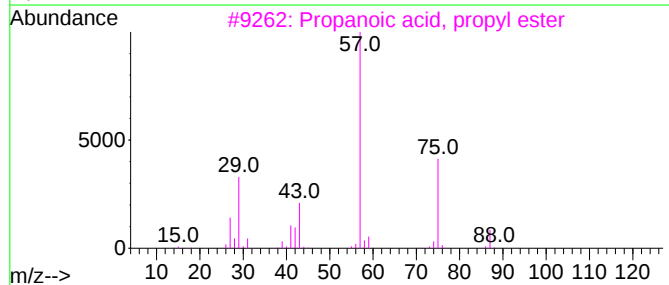
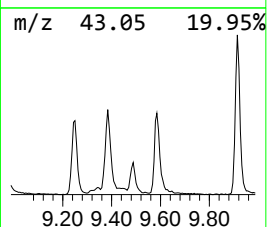
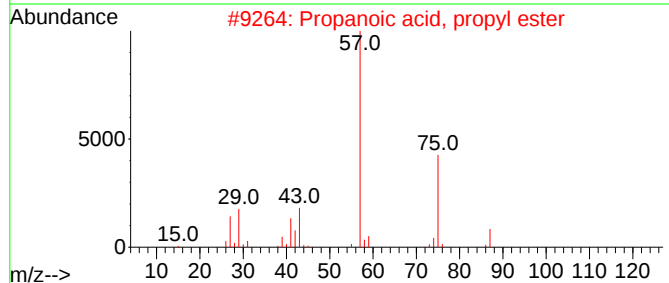
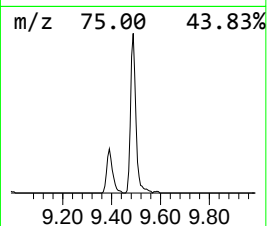
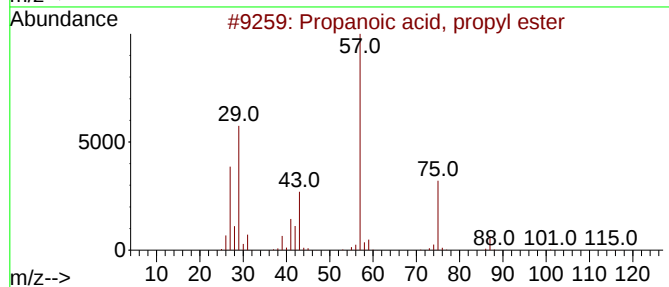
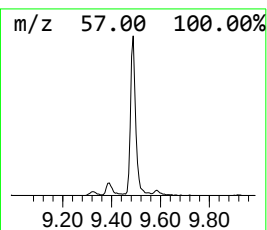
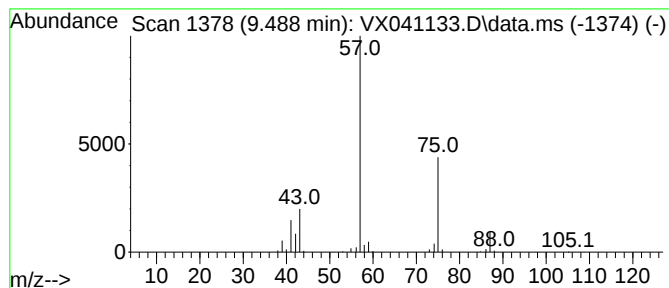
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	5.06 ug/L	78299	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
Data File : VX041133.D
Acq On : 17 Apr 2024 18:25
Operator : JC/MD
Sample : PB160244TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB244

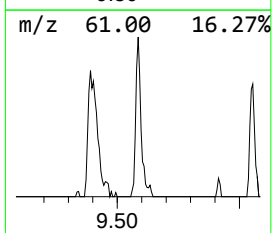
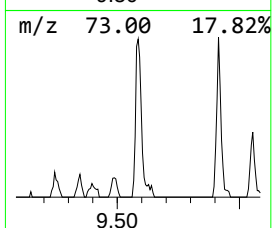
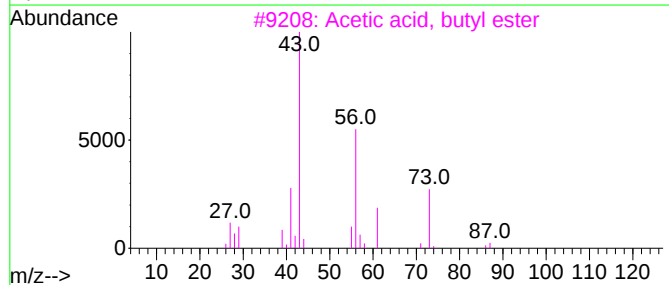
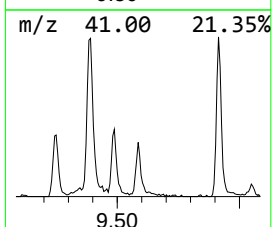
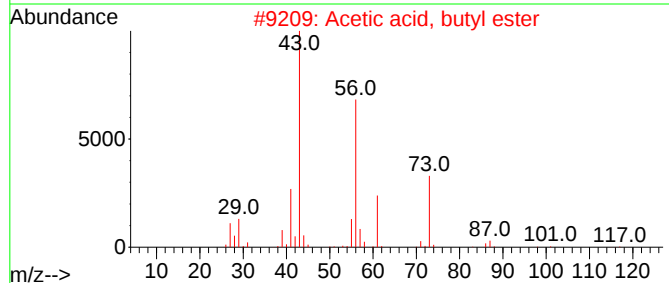
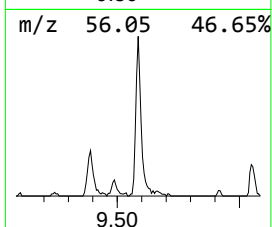
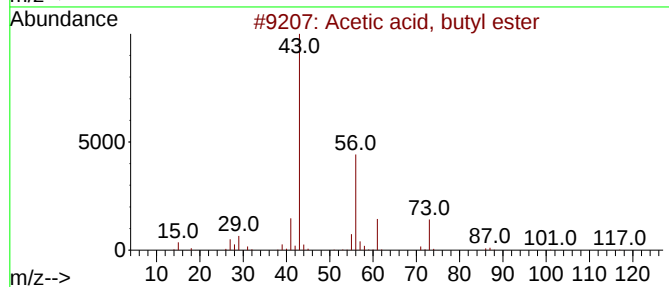
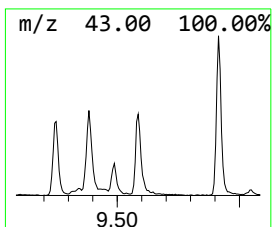
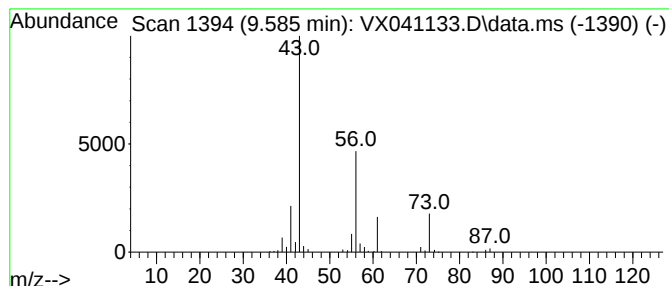
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.585	3.04 ug/L	47079	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



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Operator : JC/MD
Sample : PB160244TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB244

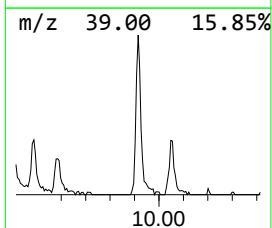
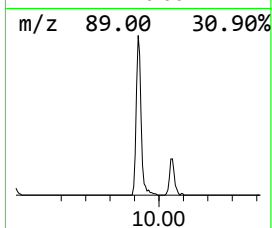
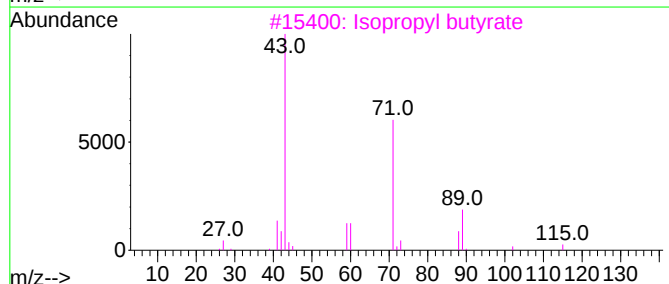
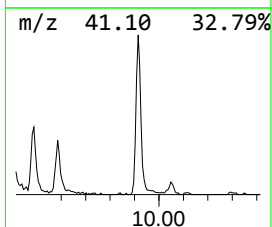
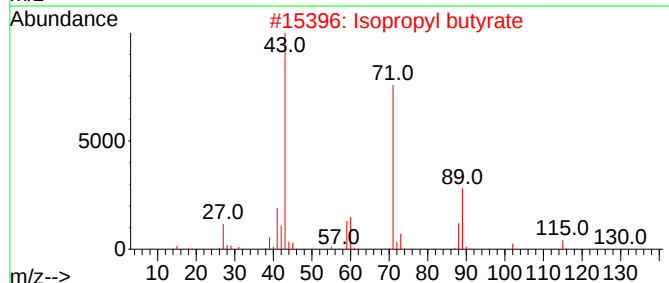
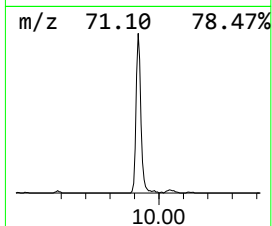
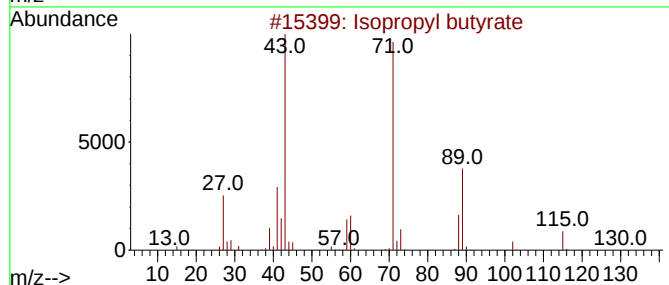
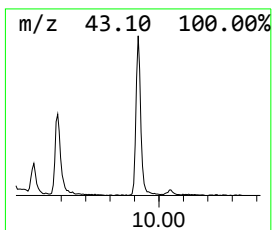
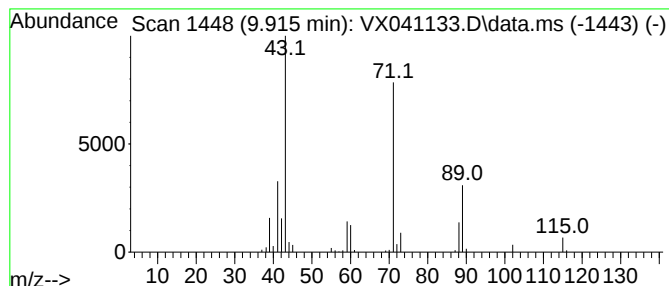
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	7.49 ug/L	115899	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



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Data File : VX041133.D
Acq On : 17 Apr 2024 18:25
Operator : JC/MD
Sample : PB160244TB 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VLEB244

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
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
n-Propyl acetate	7.805	13.2	ug/L	174135	1	6.763	657739	50.0
Propanoic acid,...	9.250	2.7	ug/L	41293	2	10.055	773964	50.0
Propanoic acid,...	9.488	5.1	ug/L	78299	2	10.055	773964	50.0
Acetic acid, bu...	9.585	3.0	ug/L	47079	2	10.055	773964	50.0
Isopropyl butyrate	9.915	7.5	ug/L	115899	2	10.055	773964	50.0