

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
 Data File : VX041135.D
 Acq On : 17 Apr 2024 19:11
 Operator : JC/MD
 Sample : P2039-08 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1CX7

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: VX041135.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	25	28	32	rVB	4324	4323	0.41%	0.054%
2	1.368	42	46	59	rBV	92323	146463	13.80%	1.814%
3	1.648	88	92	112	rVB	49326	106540	10.04%	1.319%
4	2.288	191	197	209	rVV	223160	352611	33.23%	4.367%
5	2.398	212	215	223	rVB	2636	4861	0.46%	0.060%
6	2.715	263	267	272	rVB2	519	896	0.08%	0.011%
7	2.782	272	278	286	rBV3	3474	7883	0.74%	0.098%
8	2.940	299	304	312	rBV2	455	1298	0.12%	0.016%
9	3.026	316	318	321	rVB	162	165	0.02%	0.002%
10	3.355	371	372	377	rVB	283	246	0.02%	0.003%
11	3.422	381	383	390	rVV2	132	211	0.02%	0.003%
12	3.520	397	399	402	rVV	130	147	0.01%	0.002%
13	3.581	407	409	411	rVB	132	115	0.01%	0.001%
14	3.642	417	419	420	rBV	168	128	0.01%	0.002%
15	3.678	423	425	428	rVB2	115	136	0.01%	0.002%
16	3.770	438	440	443	rBV2	203	187	0.02%	0.002%
17	3.879	455	458	459	rBV2	137	150	0.01%	0.002%
18	3.946	467	469	471	rBV	132	139	0.01%	0.002%
19	3.971	471	473	474	rBV2	123	120	0.01%	0.001%
20	4.032	481	483	486	rVB2	180	167	0.02%	0.002%
21	4.135	498	500	503	rVB2	153	117	0.01%	0.001%
22	4.172	505	506	509	rVV	198	206	0.02%	0.003%
23	4.227	513	515	518	rVV2	160	172	0.02%	0.002%
24	4.349	531	535	536	rBV2	161	198	0.02%	0.002%
25	4.471	545	555	576	rBV	60928	223810	21.09%	2.772%
26	4.867	618	620	624	rVB2	294	363	0.03%	0.004%
27	4.928	626	630	633	rBV2	195	227	0.02%	0.003%
28	5.056	637	651	670	rBV	133748	417814	39.38%	5.174%
29	5.324	692	695	697	rBV	166	181	0.02%	0.002%
30	5.373	700	703	705	rBV3	354	445	0.04%	0.006%
31	5.507	723	725	727	rBV2	162	132	0.01%	0.002%
32	5.556	727	733	734	rBV3	415	827	0.08%	0.010%
33	5.964	789	800	819	rBV2	370484	1061059	100.00%	13.141%
34	6.355	854	864	876	rBV2	5863	17697	1.67%	0.219%
35	6.659	911	914	915	rBV2	168	186	0.02%	0.002%
36	6.757	920	930	950	rBV	255627	629006	59.28%	7.790%

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Integrator: RTE

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	7.117	984	989	999	rVB5	1800	4649	0.44%	0.058%
38	7.214	999	1005	1011	rBV2	1146	2820	0.27%	0.035%
39	7.306	1012	1020	1034	rBV	211819	466720	43.99%	5.780%
40	7.598	1065	1068	1069	rVB2	257	223	0.02%	0.003%
41	7.659	1072	1078	1084	rBV	2985	5982	0.56%	0.074%
42	7.805	1096	1102	1121	rBV	34565	72241	6.81%	0.895%
43	8.068	1143	1145	1148	rVB2	240	144	0.01%	0.002%
44	8.251	1171	1175	1179	rBV2	194	222	0.02%	0.003%
45	8.324	1181	1187	1207	rBV	128394	212813	20.06%	2.636%
46	8.555	1219	1225	1234	rBV	15556	27814	2.62%	0.344%
47	8.647	1234	1240	1258	rBV	528065	851187	80.22%	10.541%
48	8.903	1280	1282	1284	rVB3	363	249	0.02%	0.003%
49	8.952	1284	1290	1301	rBV	88204	136835	12.90%	1.695%
50	9.147	1321	1322	1325	rBV	155	170	0.02%	0.002%
51	9.250	1333	1339	1347	rBV	22186	35023	3.30%	0.434%
52	9.323	1347	1351	1352	rVV2	1984	2553	0.24%	0.032%
53	9.391	1356	1362	1374	rVV	302577	494297	46.59%	6.122%
54	9.488	1374	1378	1396	rVB	29840	51496	4.85%	0.638%
55	9.744	1418	1420	1422	rBV	142	127	0.01%	0.002%
56	9.915	1443	1448	1457	rBV	44863	64174	6.05%	0.795%
57	10.055	1465	1471	1491	rBV	519468	721297	67.98%	8.933%
58	10.311	1508	1513	1518	rVB3	801	1244	0.12%	0.015%
59	10.524	1544	1548	1552	rBV4	564	1131	0.11%	0.014%
60	10.646	1565	1568	1569	rBV3	235	216	0.02%	0.003%
61	10.695	1575	1576	1579	rVB2	161	139	0.01%	0.002%
62	10.732	1579	1582	1584	rVB2	255	199	0.02%	0.002%
63	10.805	1592	1594	1596	rVB	164	144	0.01%	0.002%
64	10.957	1618	1619	1626	rBV3	255	423	0.04%	0.005%
65	11.043	1631	1633	1634	rBV	233	146	0.01%	0.002%
66	11.067	1634	1637	1638	rBV2	151	171	0.02%	0.002%
67	11.098	1640	1642	1646	rVB2	446	328	0.03%	0.004%
68	11.195	1652	1658	1670	rBV	400998	530386	49.99%	6.569%
69	11.354	1682	1684	1686	rBV	200	198	0.02%	0.002%
70	11.427	1695	1696	1698	rBV2	191	158	0.01%	0.002%
71	11.451	1698	1700	1704	rVV3	288	377	0.04%	0.005%
72	11.482	1704	1705	1708	rVB	234	158	0.01%	0.002%
73	11.719	1742	1744	1746	rVV2	217	237	0.02%	0.003%
74	11.762	1748	1751	1757	rVV3	279	398	0.04%	0.005%
75	11.811	1757	1759	1762	rVB2	117	121	0.01%	0.001%
76	11.896	1770	1773	1777	rBV	134	207	0.02%	0.003%

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 Title : VOC Analysis

77	11.975	1781	1786	1788	rBV3	527	733	0.07%	0.009%
78	12.024	1788	1794	1812	rVV	501208	644608	60.75%	7.983%
79	12.317	1837	1842	1861	rBV	585278	756016	71.25%	9.363%
80	12.561	1880	1882	1884	rVB2	224	181	0.02%	0.002%
81	12.664	1898	1899	1903	rVB2	130	119	0.01%	0.001%
82	12.701	1903	1905	1907	rVB2	192	158	0.01%	0.002%
83	12.768	1909	1916	1920	rBV4	901	1219	0.11%	0.015%
84	12.963	1945	1948	1951	rVB2	254	262	0.02%	0.003%
85	13.115	1972	1973	1975	rBV	269	184	0.02%	0.002%
86	13.164	1977	1981	1982	rBV2	100	123	0.01%	0.002%
87	13.225	1990	1991	1994	rBV	149	132	0.01%	0.002%
88	13.335	2006	2009	2010	rBV2	203	161	0.02%	0.002%
89	13.506	2035	2037	2039	rVB2	166	121	0.01%	0.001%
90	13.554	2043	2045	2049	rVB2	273	274	0.03%	0.003%
91	13.597	2049	2052	2054	rBV2	457	418	0.04%	0.005%
92	13.652	2059	2061	2064	rVB2	260	229	0.02%	0.003%
93	13.689	2064	2067	2068	rBV2	192	221	0.02%	0.003%
94	13.908	2101	2103	2106	rVB2	223	200	0.02%	0.002%
95	13.945	2106	2109	2110	rBV2	218	228	0.02%	0.003%
96	14.012	2116	2120	2121	rBV2	202	200	0.02%	0.002%
97	14.048	2125	2126	2128	rBV	164	149	0.01%	0.002%
98	14.134	2136	2140	2145	rVB3	1343	1742	0.16%	0.022%
99	14.262	2159	2161	2163	rBV2	170	119	0.01%	0.001%
100	14.365	2175	2178	2179	rBV3	200	242	0.02%	0.003%

Sum of corrected areas: 8074682

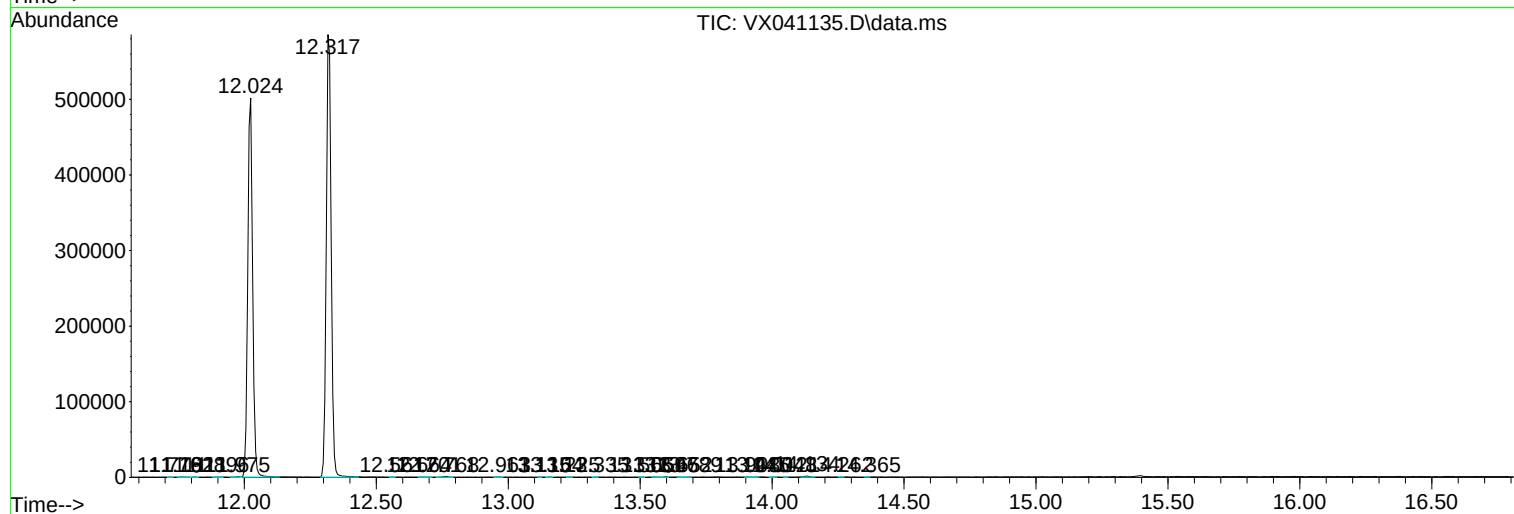
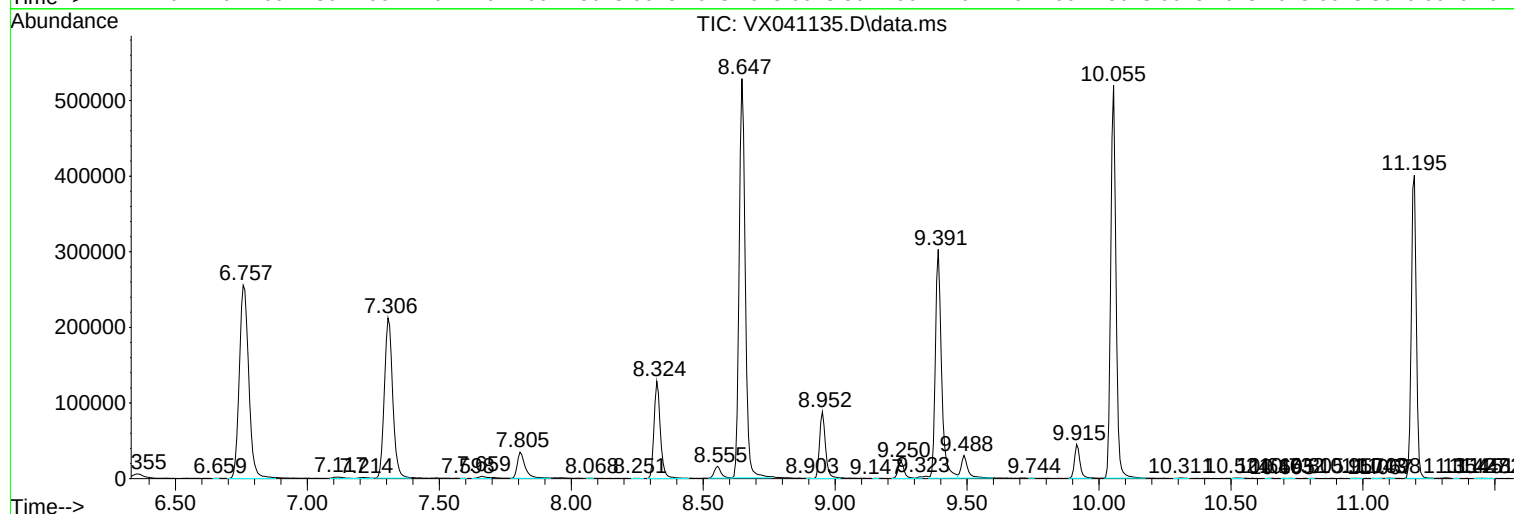
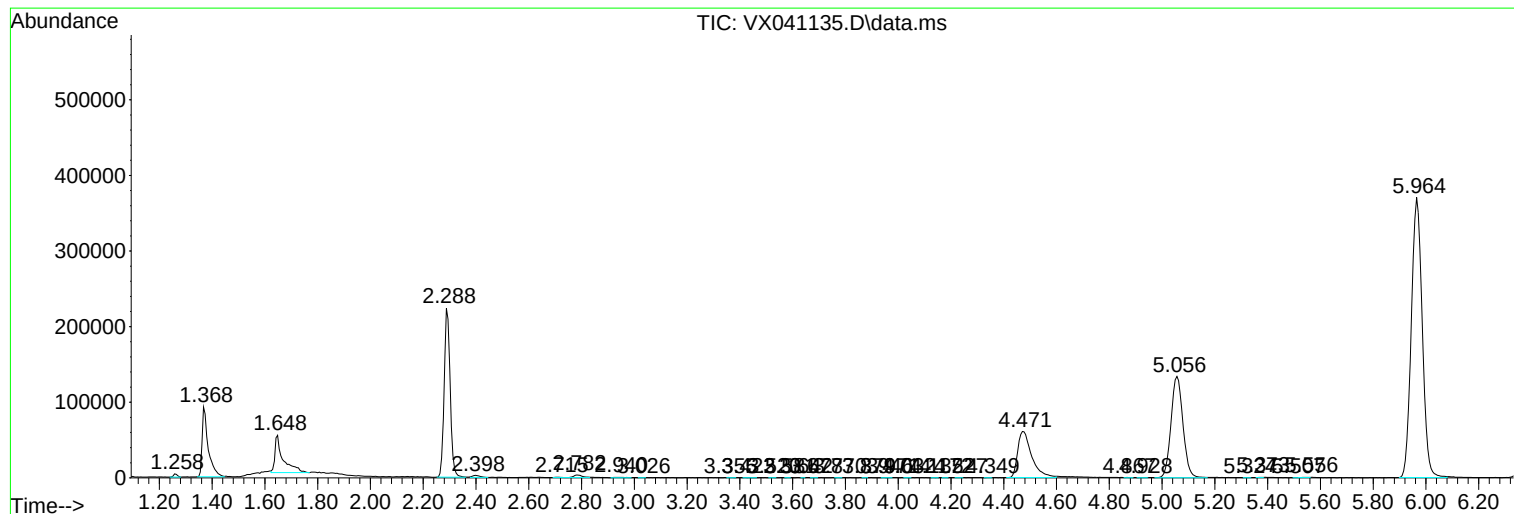
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Instrument :
MSVOA_X
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E1CX7

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX041724\
Data File : VX041135.D
Acq On : 17 Apr 2024 19:11
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Sample : P2039-08 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1CX7

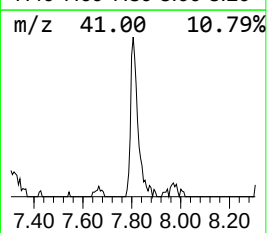
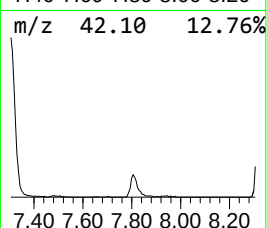
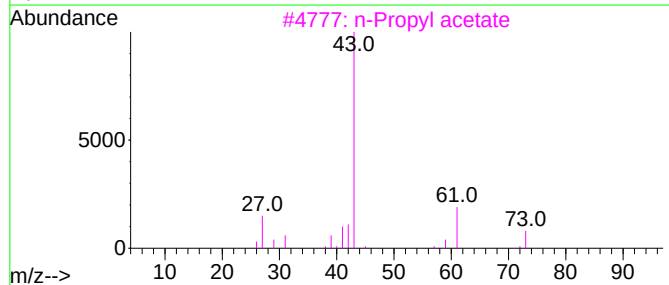
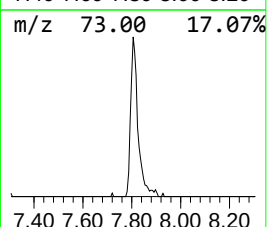
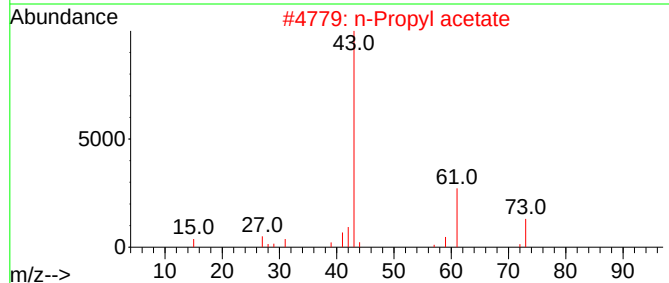
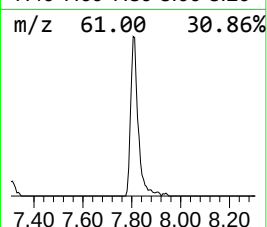
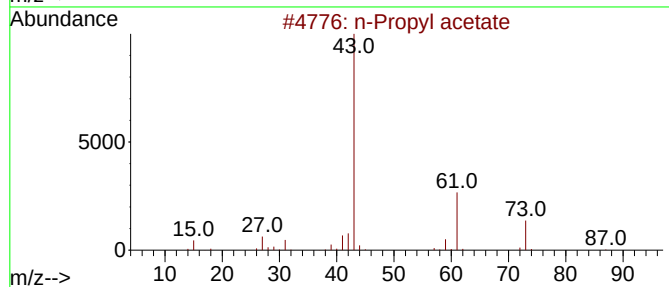
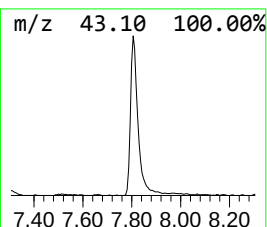
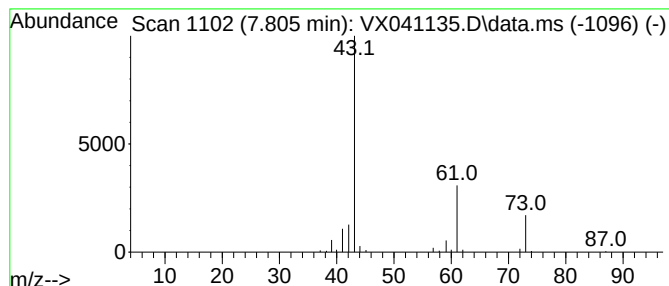
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041724WMA.M
Quant Title : VOC Analysis

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	5.74 ug/L	72241	1,4-Difluorobenzene	6.757

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	74
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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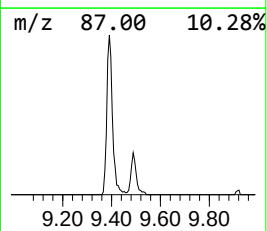
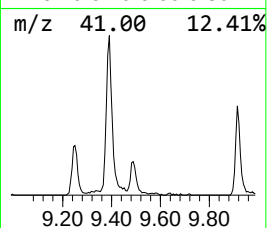
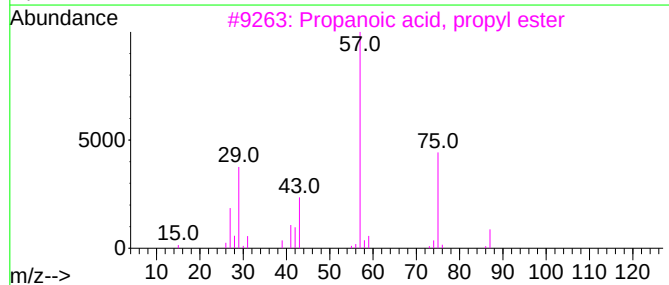
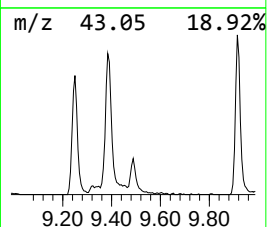
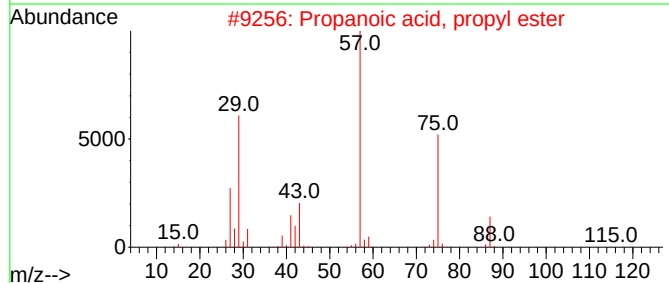
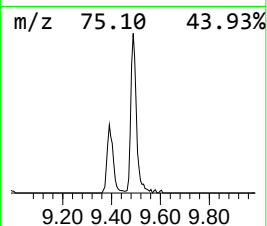
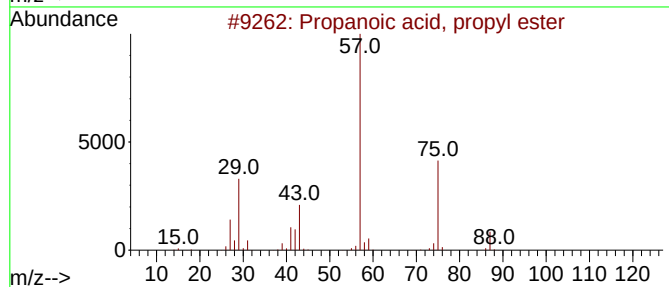
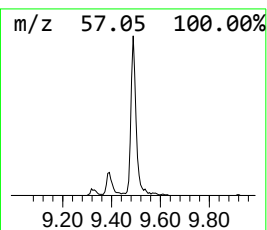
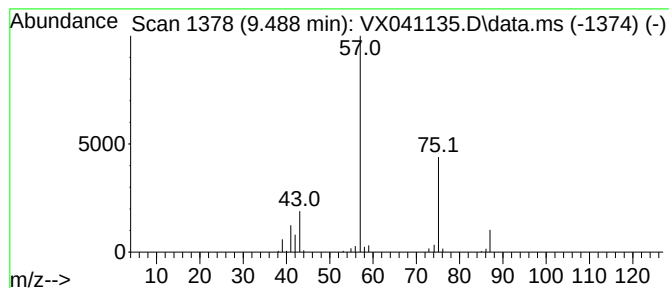
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041724WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	3.57 ug/L	51496	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	38



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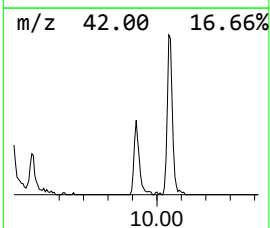
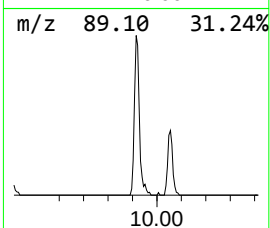
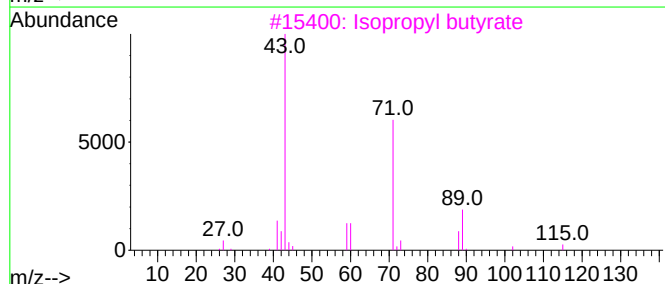
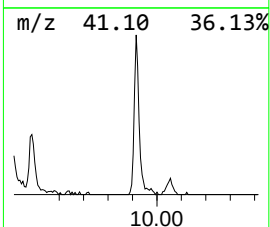
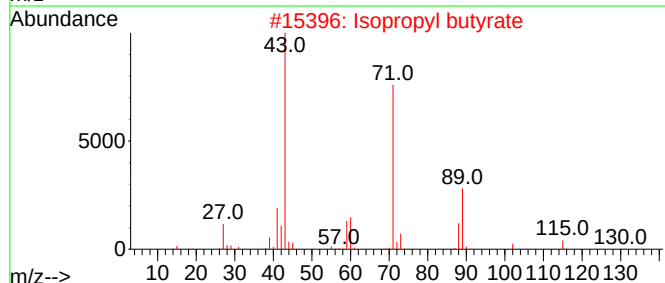
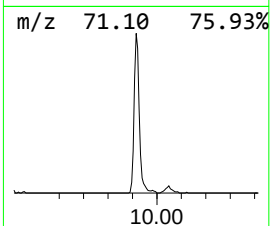
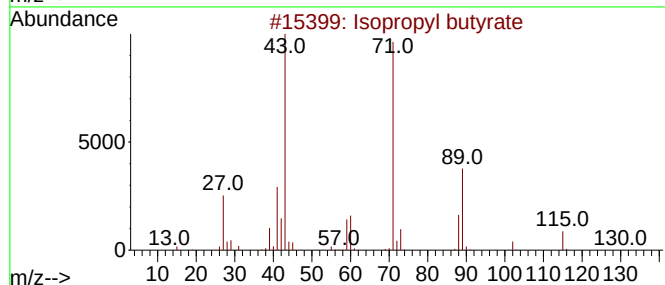
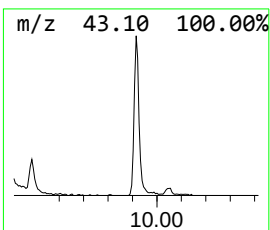
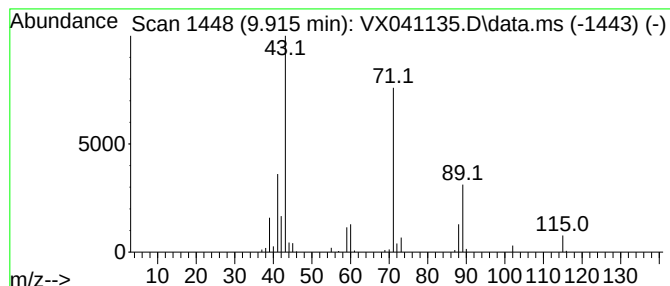
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041724WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	4.45 ug/L	64174	Chlorobenzene-d5	10.055

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041724\
Data File : VX041135.D
Acq On : 17 Apr 2024 19:11
Operator : JC/MD
Sample : P2039-08 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1CX7

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	5.7	ug/L	72241	1	6.757	629006	50.0
Propanoic acid,...	9.488	3.6	ug/L	51496	2	10.055	721297	50.0
Isopropyl butyrate	9.915	4.5	ug/L	64174	2	10.055	721297	50.0