

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110921\
 Data File : VX025122.D
 Acq On : 09 Nov 2021 15:20
 Operator : JC/MD
 Sample : PB140605TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB605

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\SFAMXML110821WMA.M

Title : VOC Analysis

Signal : TIC: VX025122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	57	rVB	83655	89796	14.51%	1.744%
2	1.666	91	95	103	rVB	68121	89044	14.38%	1.730%
3	2.306	194	200	209	rBV	136738	218073	35.23%	4.236%
4	2.477	227	228	231	rVB2	534	335	0.05%	0.007%
5	2.587	244	246	247	rBV2	454	296	0.05%	0.006%
6	2.666	255	259	260	rBV	288	352	0.06%	0.007%
7	2.788	273	279	285	rBV2	2588	5145	0.83%	0.100%
8	2.861	285	291	294	rVB2	469	829	0.13%	0.016%
9	2.940	303	304	305	rBV2	791	478	0.08%	0.009%
10	2.989	310	312	314	rBV	411	353	0.06%	0.007%
11	3.160	337	340	343	rVB	302	419	0.07%	0.008%
12	3.398	377	379	380	rBV	461	342	0.06%	0.007%
13	3.520	398	399	402	rBV3	404	334	0.05%	0.006%
14	3.757	436	438	439	rVB3	550	368	0.06%	0.007%
15	3.946	467	469	472	rBV	501	526	0.08%	0.010%
16	4.026	480	482	486	rBV2	496	527	0.09%	0.010%
17	4.087	490	492	495	rBV2	466	526	0.08%	0.010%
18	4.117	495	497	500	rVV2	338	329	0.05%	0.006%
19	4.190	508	509	515	rVB	432	572	0.09%	0.011%
20	4.257	518	520	525	rVB	653	625	0.10%	0.012%
21	4.464	545	554	569	rBV	47772	137085	22.14%	2.663%
22	5.068	640	653	666	rBV2	89448	275511	44.50%	5.352%
23	5.251	679	683	684	rBV	310	361	0.06%	0.007%
24	5.379	702	704	705	rBV	734	414	0.07%	0.008%
25	5.452	714	716	719	rBV	373	291	0.05%	0.006%
26	5.702	752	757	760	rBV	420	805	0.13%	0.016%
27	5.818	775	776	779	rBV	429	335	0.05%	0.007%
28	5.976	791	802	817	rVB2	207054	619061	100.00%	12.026%
29	6.184	833	836	837	rBV2	313	365	0.06%	0.007%
30	6.482	881	885	891	rVB2	348	611	0.10%	0.012%
31	6.543	891	895	900	rBV2	522	908	0.15%	0.018%
32	6.592	900	903	904	rBV2	446	452	0.07%	0.009%
33	6.684	916	918	920	rVB2	600	391	0.06%	0.008%
34	6.763	923	931	944	rVV	156180	374250	60.45%	7.270%
35	6.885	947	951	952	rBV	543	559	0.09%	0.011%
36	6.934	957	959	963	rBV	277	312	0.05%	0.006%

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 Title : VOC Analysis

37	7.086	982	984	985	rVV	674	531	0.09%	0.010%
38	7.110	986	988	996	rVB5	2575	4696	0.76%	0.091%
39	7.312	1013	1021	1034	rBV2	132015	293517	47.41%	5.702%
40	7.543	1057	1059	1061	rBV2	458	306	0.05%	0.006%
41	7.750	1092	1093	1094	rBV2	496	301	0.05%	0.006%
42	7.805	1095	1102	1111	rVV	67338	116298	18.79%	2.259%
43	8.135	1151	1156	1157	rBV2	399	445	0.07%	0.009%
44	8.189	1163	1165	1169	rVB	319	311	0.05%	0.006%
45	8.330	1182	1188	1197	rBV	93888	153586	24.81%	2.983%
46	8.464	1208	1210	1211	rBV	306	289	0.05%	0.006%
47	8.555	1220	1225	1233	rVB3	13014	20342	3.29%	0.395%
48	8.653	1235	1241	1248	rBV	297160	470186	75.95%	9.134%
49	8.951	1284	1290	1297	rBV	71998	110090	17.78%	2.139%
50	9.110	1314	1316	1319	rVB	371	398	0.06%	0.008%
51	9.165	1320	1325	1328	rBV	430	848	0.14%	0.016%
52	9.250	1336	1339	1346	rVB3	3987	5866	0.95%	0.114%
53	9.317	1346	1350	1351	rBV2	913	948	0.15%	0.018%
54	9.348	1351	1355	1357	rBV2	8924	12415	2.01%	0.241%
55	9.384	1357	1361	1373	rVV	213020	310440	50.15%	6.030%
56	9.488	1373	1378	1383	rVV	134761	174490	28.19%	3.390%
57	9.586	1389	1394	1402	rVB	13675	19131	3.09%	0.372%
58	9.793	1426	1428	1429	rBV	444	418	0.07%	0.008%
59	9.915	1441	1448	1456	rBV	90528	115312	18.63%	2.240%
60	10.055	1466	1471	1482	rBV	327163	446936	72.20%	8.682%
61	10.183	1490	1492	1493	rBV2	622	415	0.07%	0.008%
62	10.238	1500	1501	1504	rVB2	706	453	0.07%	0.009%
63	10.348	1517	1519	1521	rBV	431	398	0.06%	0.008%
64	10.646	1564	1568	1573	rVB2	2849	3479	0.56%	0.068%
65	10.732	1580	1582	1585	rVB2	439	435	0.07%	0.008%
66	10.829	1597	1598	1602	rVB2	429	440	0.07%	0.009%
67	10.872	1602	1605	1607	rBV	338	412	0.07%	0.008%
68	10.927	1612	1614	1618	rVB	409	504	0.08%	0.010%
69	10.994	1623	1625	1627	rBV	531	320	0.05%	0.006%
70	11.030	1629	1631	1633	rBV2	452	451	0.07%	0.009%
71	11.085	1638	1640	1641	rBV2	475	437	0.07%	0.008%
72	11.195	1652	1658	1666	rVB	224816	288741	46.64%	5.609%
73	11.378	1687	1688	1691	rBV2	577	410	0.07%	0.008%
74	11.835	1761	1763	1767	rBV3	658	793	0.13%	0.015%
75	11.933	1776	1779	1783	rBV2	1272	1749	0.28%	0.034%
76	12.024	1789	1794	1803	rVV	301691	377821	61.03%	7.339%

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 Title : VOC Analysis

77	12.201	1821	1823	1824	rVB	725	341	0.06%	0.007%
78	12.219	1824	1826	1828	rBV	520	420	0.07%	0.008%
79	12.323	1837	1843	1850	rVB	301390	377219	60.93%	7.328%
80	12.475	1866	1868	1873	rVB3	742	989	0.16%	0.019%
81	12.591	1884	1887	1889	rBV2	378	436	0.07%	0.008%
82	12.951	1944	1946	1948	rBV	485	308	0.05%	0.006%
83	12.993	1950	1953	1955	rBV	644	579	0.09%	0.011%
84	13.274	1997	1999	2001	rVV2	542	500	0.08%	0.010%
85	13.317	2004	2006	2011	rBV	722	1039	0.17%	0.020%
86	13.634	2054	2058	2060	rBV	299	468	0.08%	0.009%
87	13.999	2116	2118	2120	rBV2	366	372	0.06%	0.007%
88	14.079	2128	2131	2132	rBV	438	377	0.06%	0.007%
89	14.176	2144	2147	2149	rBV	348	389	0.06%	0.008%
90	14.255	2158	2160	2165	rVB2	671	700	0.11%	0.014%
91	14.560	2207	2210	2213	rBV	671	1093	0.18%	0.021%
92	14.633	2219	2222	2223	rBV	393	383	0.06%	0.007%
93	14.713	2230	2235	2237	rBV	454	757	0.12%	0.015%
94	15.030	2284	2287	2290	rBV	717	893	0.14%	0.017%
95	15.121	2300	2302	2306	rVB	777	699	0.11%	0.014%
96	15.182	2308	2312	2313	rBV	658	770	0.12%	0.015%
97	15.298	2329	2331	2334	rBV2	733	854	0.14%	0.017%
98	15.566	2373	2375	2378	rBV3	728	1131	0.18%	0.022%
99	15.981	2440	2443	2445	rBV	384	401	0.06%	0.008%
100	16.676	2554	2557	2558	rBV	388	437	0.07%	0.008%

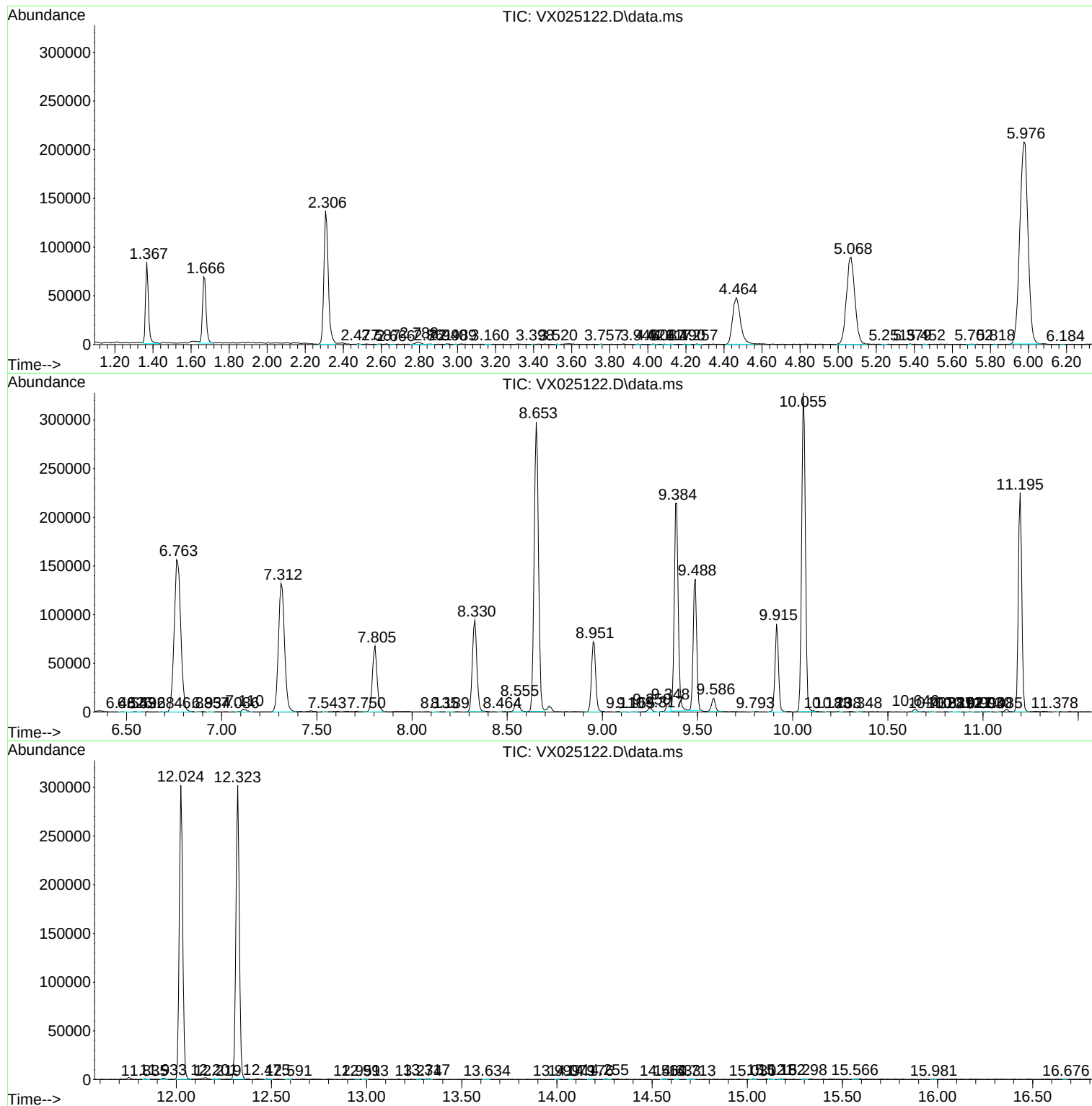
Sum of corrected areas: 5147893

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

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



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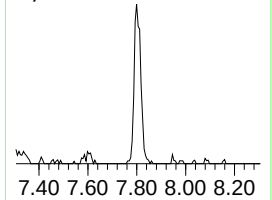
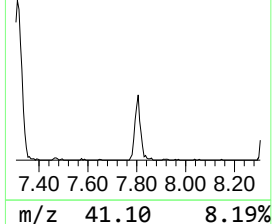
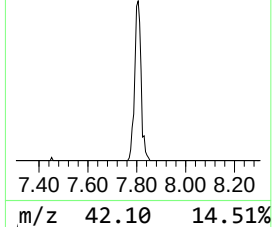
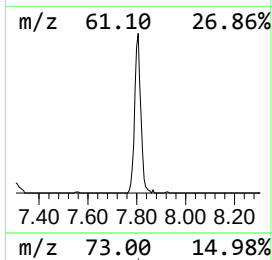
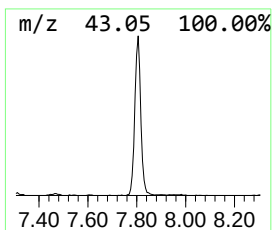
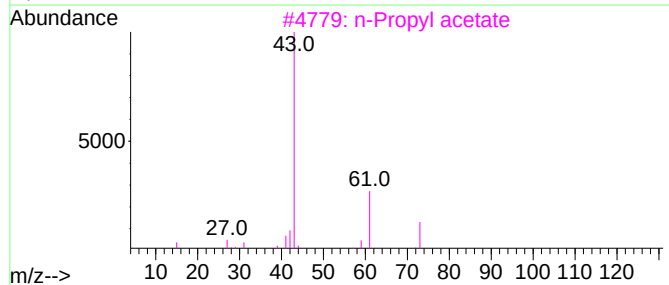
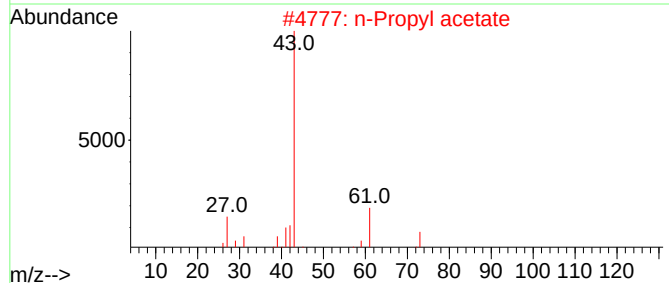
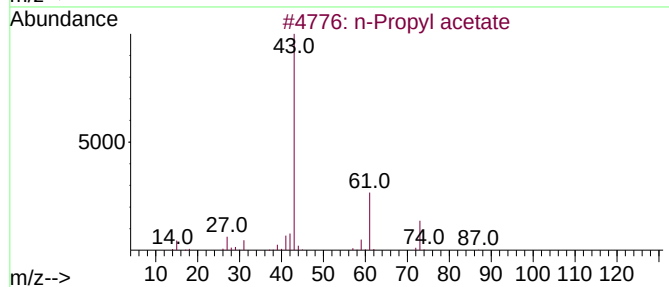
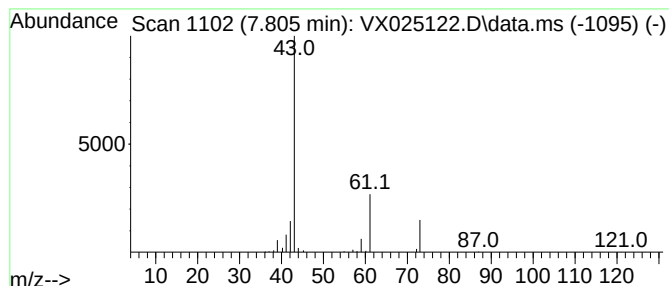
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.805	15.54 ug/L	116298	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	78
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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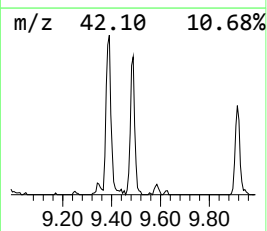
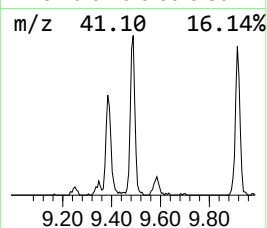
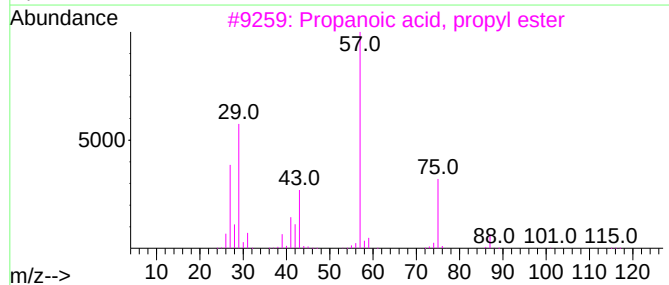
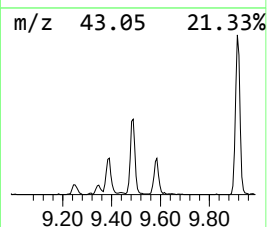
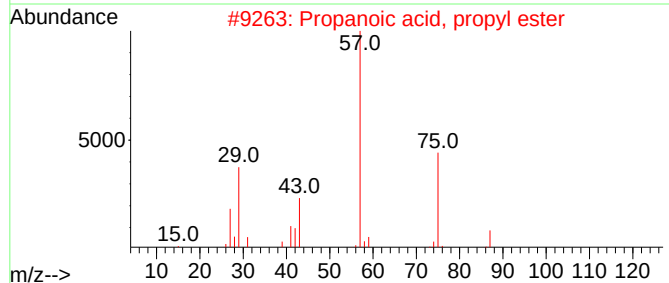
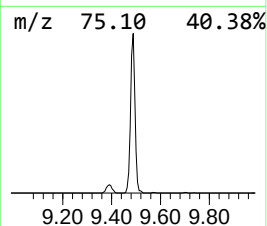
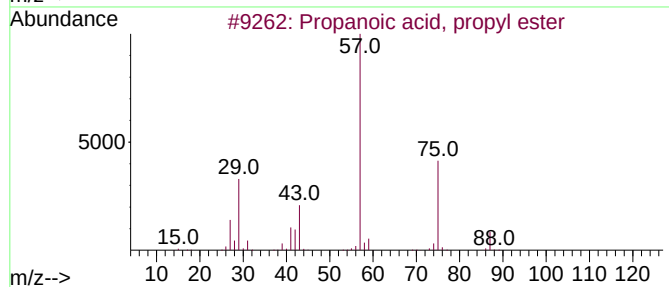
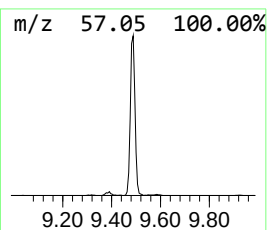
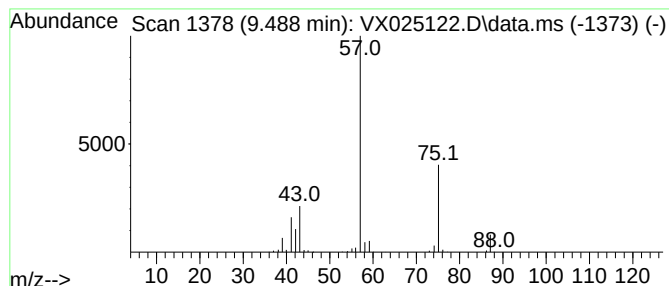
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110821WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	19.52 ug/L	174490	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	74
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72



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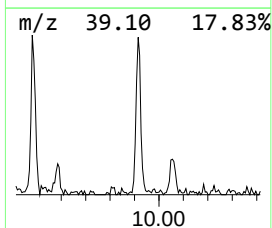
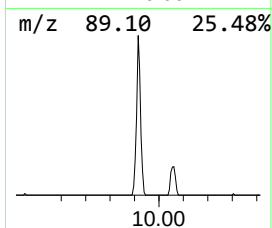
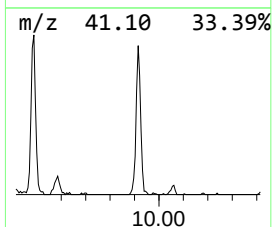
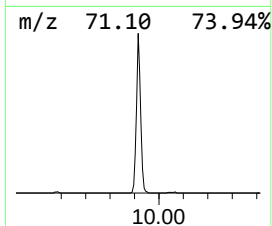
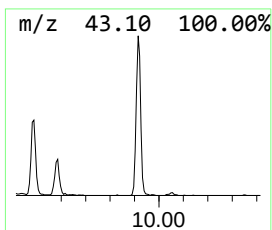
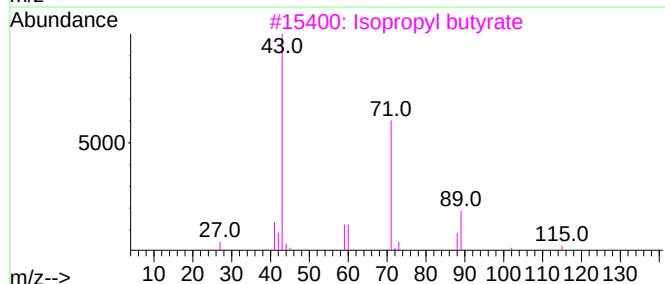
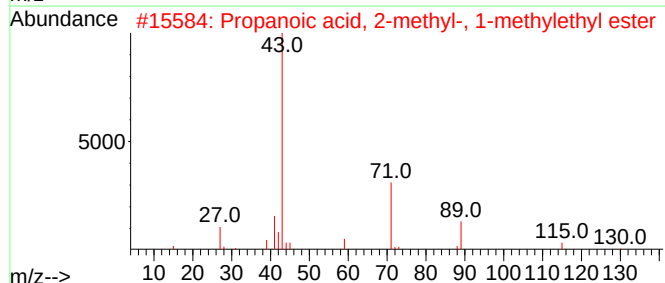
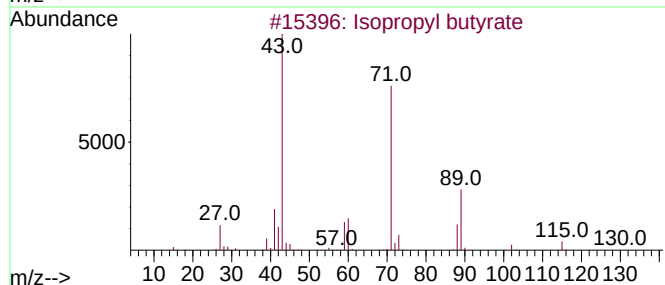
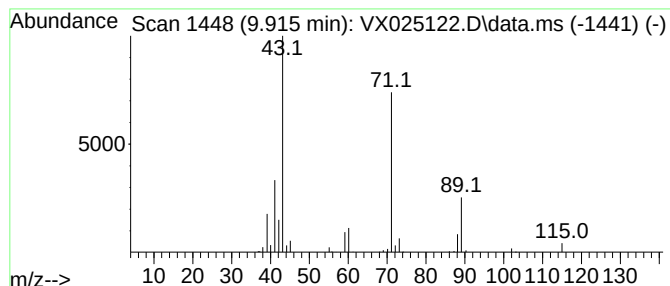
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	12.90 ug/L	115312	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



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ClientSampleId :
VLEB605

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110821WMA.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	15.5	ug/L	116298	1	6.763	374250	50.0
Propanoic acid,...	9.488	19.5	ug/L	174490	2	10.055	446936	50.0
Isopropyl butyrate	9.915	12.9	ug/L	115312	2	10.055	446936	50.0