

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
 Data File : VU048307.D
 Acq On : 27 Apr 2022 12:20
 Operator : SY/MD
 Sample : PB144390TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB390

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_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048307.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	40	45	52	rBV3	4312	5754	0.35%	0.043%
2	1.600	73	81	100	rBV	196227	250893	15.15%	1.873%
3	1.899	165	174	188	rBV	133787	199508	12.05%	1.490%
4	2.565	368	381	396	rBV	341937	559915	33.82%	4.181%
5	2.758	434	441	442	rVV2	442	461	0.03%	0.003%
6	2.787	442	450	457	rVB3	954	1714	0.10%	0.013%
7	2.960	501	504	507	rVB2	575	326	0.02%	0.002%
8	3.044	520	530	551	rVV	9252	19932	1.20%	0.149%
9	3.186	559	574	600	rVV	20786	52636	3.18%	0.393%
10	3.362	626	629	632	rBV	277	207	0.01%	0.002%
11	3.555	687	689	694	rBV2	196	188	0.01%	0.001%
12	3.690	728	731	736	rVV	192	165	0.01%	0.001%
13	3.787	757	761	764	rBV	234	233	0.01%	0.002%
14	3.877	786	789	793	rBV2	247	247	0.01%	0.002%
15	4.028	832	836	840	rBV2	221	266	0.02%	0.002%
16	4.076	848	851	857	rBV2	181	207	0.01%	0.002%
17	4.288	913	917	922	rVB2	191	193	0.01%	0.001%
18	4.433	956	962	968	rBV2	245	356	0.02%	0.003%
19	4.542	993	996	1001	rBV2	249	260	0.02%	0.002%
20	4.620	1006	1020	1051	rBV	167693	409772	24.75%	3.060%
21	5.063	1137	1158	1183	rBV	295451	644193	38.91%	4.810%
22	5.224	1203	1208	1212	rBV2	637	574	0.03%	0.004%
23	5.282	1220	1226	1228	rBV2	591	496	0.03%	0.004%
24	5.449	1275	1278	1282	rBV2	233	251	0.02%	0.002%
25	5.539	1303	1306	1310	rBV	199	214	0.01%	0.002%
26	5.581	1316	1319	1324	rBV2	246	285	0.02%	0.002%
27	5.636	1333	1336	1340	rBV	186	192	0.01%	0.001%
28	5.726	1340	1364	1392	rBV2	618813	1655749	100.00%	12.364%
29	5.864	1405	1407	1413	rVB3	499	358	0.02%	0.003%
30	5.915	1416	1423	1434	rVB4	2284	3698	0.22%	0.028%
31	6.038	1457	1461	1462	rBV2	537	339	0.02%	0.003%
32	6.073	1469	1472	1477	rBV2	157	169	0.01%	0.001%
33	6.118	1481	1486	1492	rVV2	526	574	0.03%	0.004%
34	6.250	1511	1527	1554	rBV	408167	782747	47.27%	5.845%
35	6.378	1565	1567	1576	rVB3	631	620	0.04%	0.005%
36	6.529	1608	1614	1622	rBV3	1064	1743	0.11%	0.013%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
 Data File : VU048307.D
 Acq On : 27 Apr 2022 12:20
 Operator : SY/MD
 Sample : PB144390TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB390

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_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

37	6.626	1641	1644	1646	rBV2	384	257	0.02%	0.002%
38	6.690	1650	1664	1683	rBV	377456	739356	44.65%	5.521%
39	6.931	1734	1739	1742	rBV3	1213	1045	0.06%	0.008%
40	7.041	1757	1773	1797	rBV	161443	288606	17.43%	2.155%
41	7.179	1808	1816	1828	rVB8	3151	6479	0.39%	0.048%
42	7.240	1832	1835	1841	rVB3	291	265	0.02%	0.002%
43	7.269	1841	1844	1850	rVB3	380	397	0.02%	0.003%
44	7.375	1873	1877	1879	rBV2	312	239	0.01%	0.002%
45	7.394	1880	1883	1886	rVB	269	179	0.01%	0.001%
46	7.417	1886	1890	1896	rBV2	157	190	0.01%	0.001%
47	7.565	1922	1936	1953	rBV	206126	361180	21.81%	2.697%
48	7.738	1981	1990	2000	rBV	24448	37942	2.29%	0.283%
49	7.899	2025	2040	2056	rBV	779729	1337606	80.79%	9.988%
50	8.092	2096	2100	2109	rVB4	910	1217	0.07%	0.009%
51	8.179	2114	2127	2145	rBV	143412	243441	14.70%	1.818%
52	8.404	2194	2197	2200	rBV3	460	304	0.02%	0.002%
53	8.465	2208	2216	2227	rVB4	6164	9650	0.58%	0.072%
54	8.542	2235	2240	2241	rBV	512	375	0.02%	0.003%
55	8.574	2241	2250	2257	rVV4	16241	24536	1.48%	0.183%
56	8.636	2257	2269	2288	rVV	506258	921561	55.66%	6.881%
57	8.729	2288	2298	2321	rVV	293100	478528	28.90%	3.573%
58	8.835	2322	2331	2348	rVB	28114	47124	2.85%	0.352%
59	8.925	2356	2359	2363	rVB2	527	381	0.02%	0.003%
60	8.951	2363	2367	2371	rVB3	394	328	0.02%	0.002%
61	8.976	2371	2375	2376	rBV	370	219	0.01%	0.002%
62	9.012	2383	2386	2390	rBV2	449	325	0.02%	0.002%
63	9.031	2390	2392	2398	rVB2	260	239	0.01%	0.002%
64	9.060	2398	2401	2405	rBV2	369	260	0.02%	0.002%
65	9.211	2436	2448	2469	rBV	144615	230689	13.93%	1.723%
66	9.346	2488	2490	2491	rBV	515	252	0.02%	0.002%
67	9.417	2500	2512	2536	rBV	612698	1022527	61.76%	7.635%
68	9.645	2577	2583	2587	rVB3	606	624	0.04%	0.005%
69	9.690	2593	2597	2602	rBV4	613	740	0.04%	0.006%
70	9.835	2637	2642	2644	rBV2	223	224	0.01%	0.002%
71	9.864	2648	2651	2656	rVV	295	277	0.02%	0.002%
72	9.922	2666	2669	2674	rBV2	375	338	0.02%	0.003%
73	9.983	2684	2688	2690	rBV	206	179	0.01%	0.001%
74	10.076	2709	2717	2728	rBV2	3879	6600	0.40%	0.049%
75	10.243	2764	2769	2780	rBV2	666	1351	0.08%	0.010%
76	10.362	2803	2806	2809	rVB3	275	170	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
 Data File : VU048307.D
 Acq On : 27 Apr 2022 12:20
 Operator : SY/MD
 Sample : PB144390TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB390

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_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

77	10.671	2894	2902	2910	rBV3	2589	3410	0.21%	0.025%
78	10.758	2915	2929	2947	rBV	599239	964775	58.27%	7.204%
79	10.918	2977	2979	2983	rBV3	405	297	0.02%	0.002%
80	11.092	3029	3033	3035	rBV3	585	394	0.02%	0.003%
81	11.124	3041	3043	3046	rVB3	379	182	0.01%	0.001%
82	11.301	3094	3098	3103	rBV2	224	243	0.01%	0.002%
83	11.346	3109	3112	3115	rVB2	390	219	0.01%	0.002%
84	11.417	3131	3134	3136	rBV2	407	220	0.01%	0.002%
85	11.462	3140	3148	3159	rVB5	1666	2983	0.18%	0.022%
86	11.696	3215	3221	3224	rBV3	989	979	0.06%	0.007%
87	11.812	3244	3257	3279	rBV	570868	913682	55.18%	6.823%
88	12.008	3316	3318	3323	rVB2	547	398	0.02%	0.003%
89	12.195	3359	3376	3395	rBV	694961	1136539	68.64%	8.487%
90	12.401	3438	3440	3446	rVB3	383	274	0.02%	0.002%
91	12.430	3446	3449	3450	rBV	349	221	0.01%	0.002%
92	12.468	3457	3461	3462	rBV2	245	173	0.01%	0.001%
93	12.500	3468	3471	3473	rBV2	209	161	0.01%	0.001%
94	12.635	3511	3513	3518	rBV3	546	456	0.03%	0.003%
95	12.690	3527	3530	3532	rBV	434	234	0.01%	0.002%
96	12.706	3532	3535	3540	rVB2	353	349	0.02%	0.003%
97	12.770	3549	3555	3564	rBV3	1094	1906	0.12%	0.014%
98	12.870	3583	3586	3590	rBV3	481	329	0.02%	0.002%
99	13.655	3825	3830	3833	rBV2	374	396	0.02%	0.003%
100	14.105	3963	3970	3978	rVB4	1111	1685	0.10%	0.013%

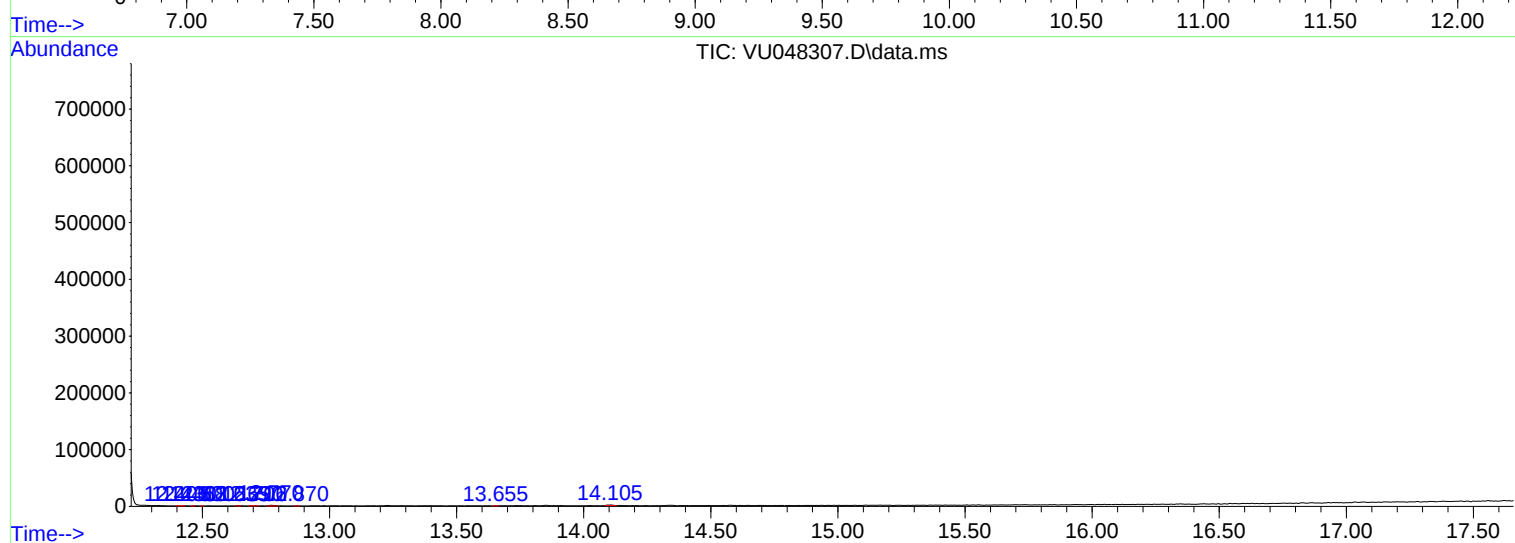
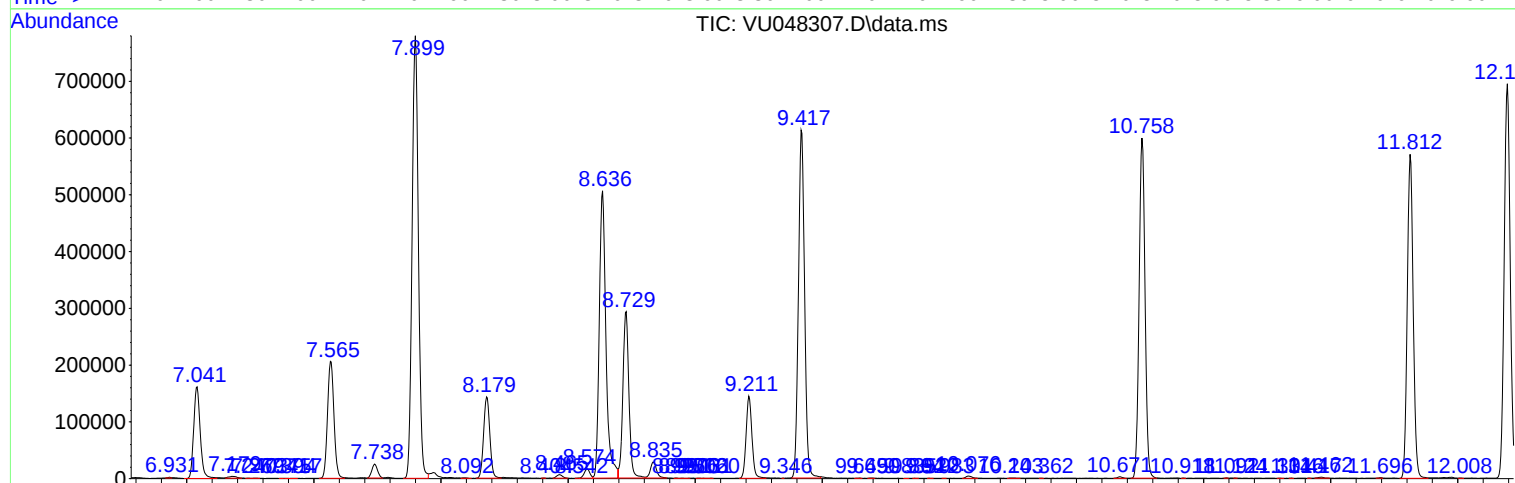
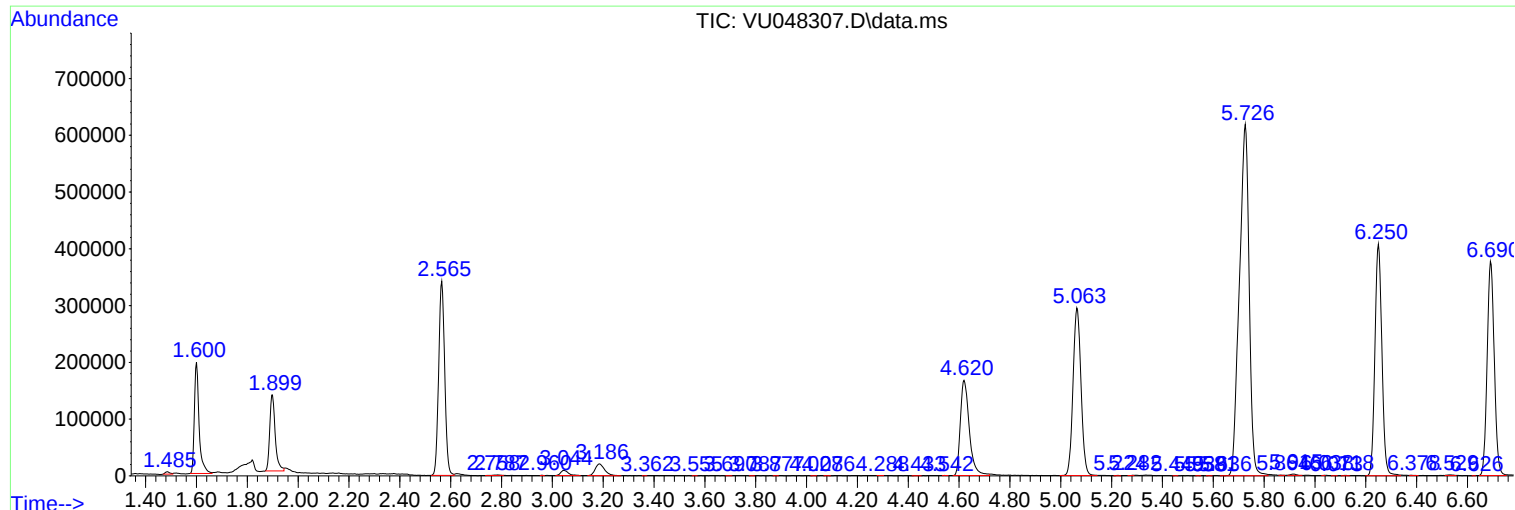
Sum of corrected areas: 13392140

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
Data File : VU048307.D
Acq On : 27 Apr 2022 12:20
Operator : SY/MD
Sample : PB144390TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB390

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
Data File : VU048307.D
Acq On : 27 Apr 2022 12:20
Operator : SY/MD
Sample : PB144390TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB390

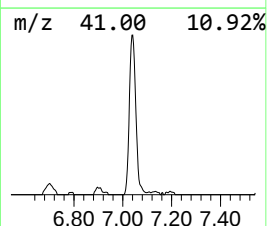
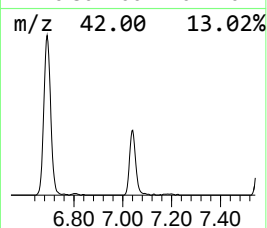
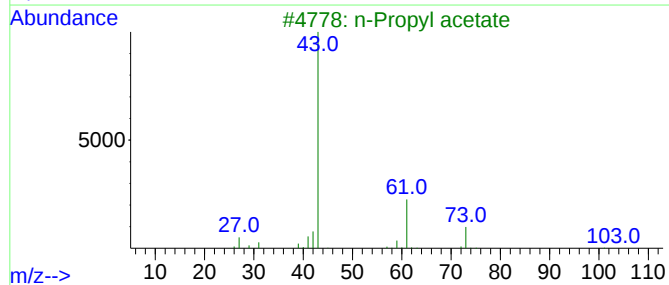
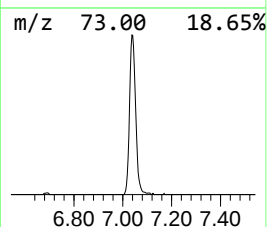
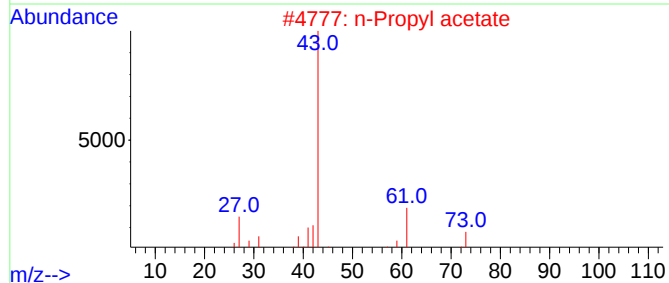
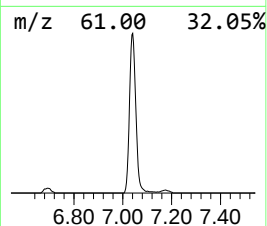
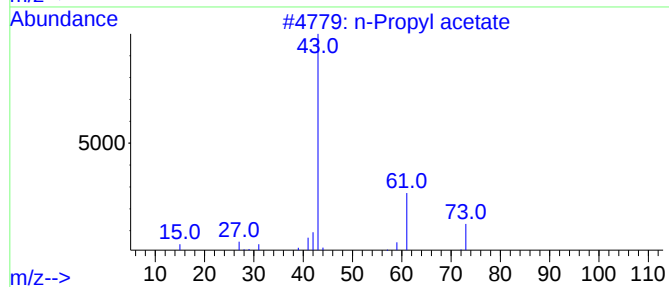
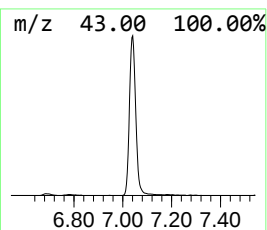
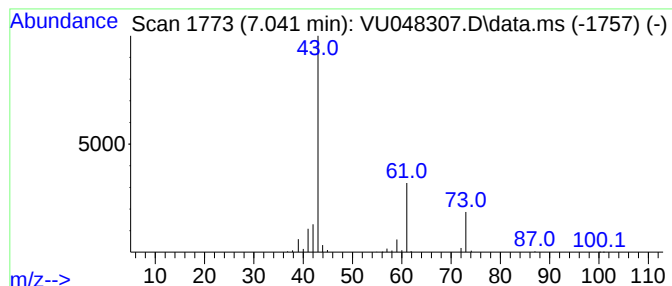
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	18.44 ug/L	288606	1,4-Difluorobenzene	6.250

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	74
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
Data File : VU048307.D
Acq On : 27 Apr 2022 12:20
Operator : SY/MD
Sample : PB144390TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB390

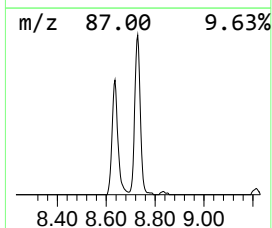
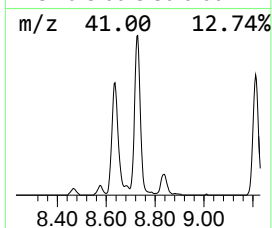
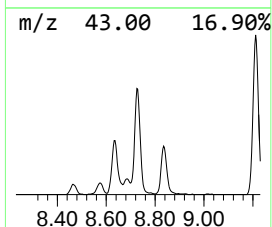
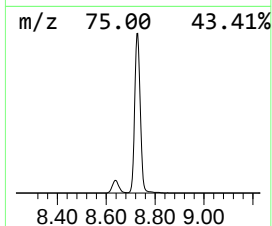
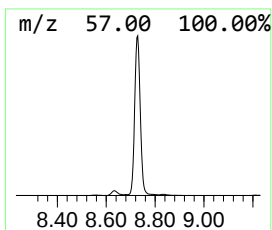
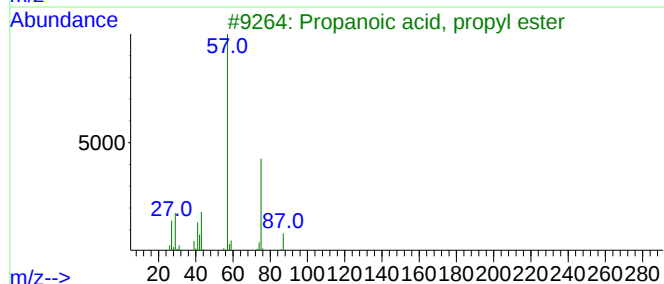
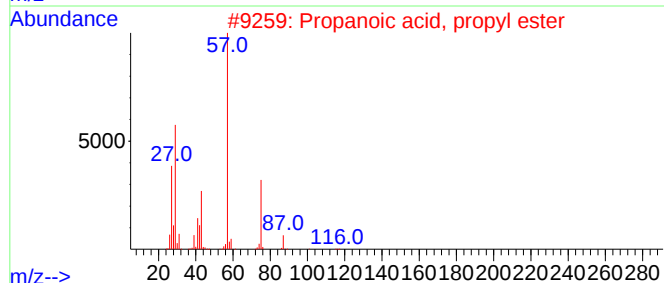
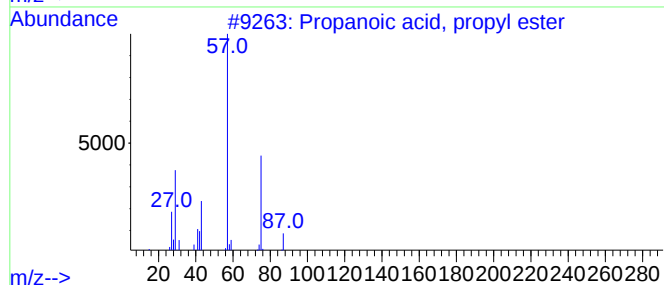
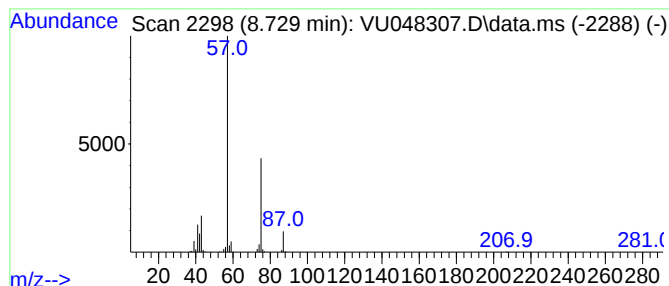
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	23.40 ug/L	478528	Chlorobenzene-d5	9.417

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_U\Data\VU042722\
Data File : VU048307.D
Acq On : 27 Apr 2022 12:20
Operator : SY/MD
Sample : PB144390TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB390

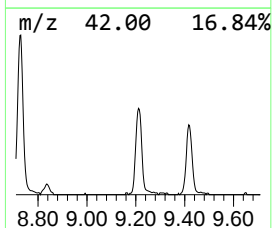
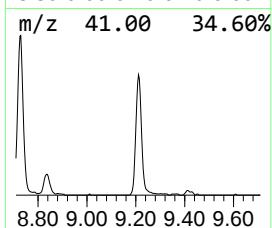
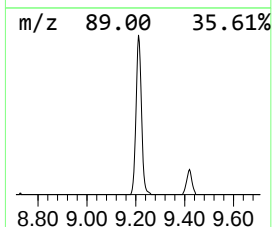
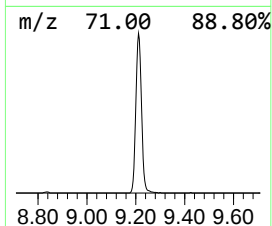
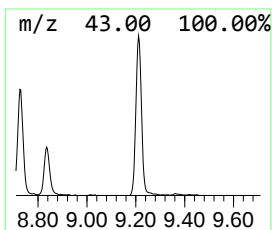
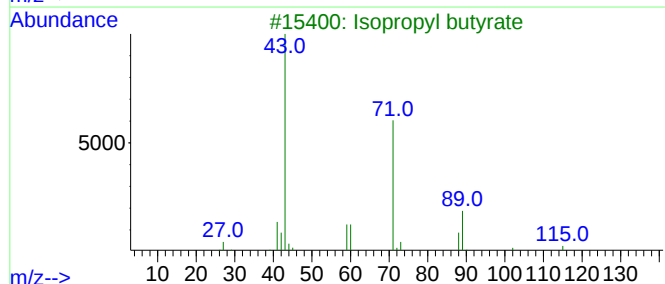
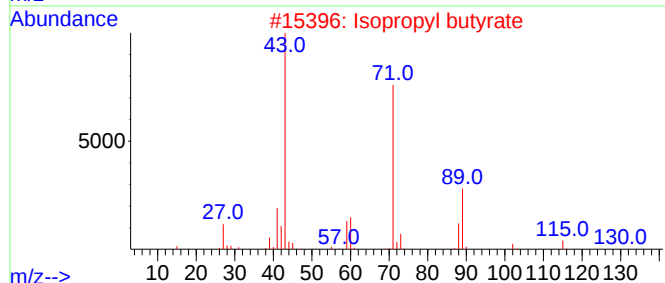
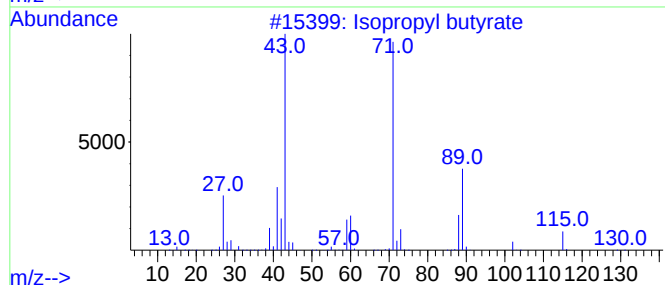
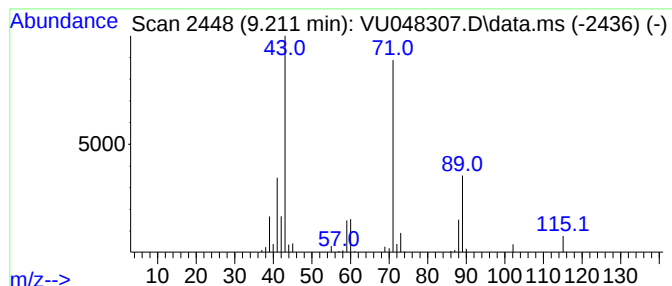
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	11.28 ug/L	230689	Chlorobenzene-d5	9.417

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	78
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
Data File : VU048307.D
Acq On : 27 Apr 2022 12:20
Operator : SY/MD
Sample : PB144390TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB390

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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	7.041	18.4	ug/L	288606	1	6.250	782747	50.0
Propanoic acid,...	8.729	23.4	ug/L	478528	2	9.417	1022530	50.0
Isopropyl butyrate	9.211	11.3	ug/L	230689	2	9.417	1022530	50.0