

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
 Data File : VU047237.D
 Acq On : 22 Feb 2022 17:44
 Operator : SY/MD
 Sample : PB142839TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB839

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\SFAMULM021022WMA.M

Title : VOC Analysis

Signal : TIC: VU047237.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	104	rVB	203887	245738	15.67%	1.769%
2	1.916	171	179	204	rVB	171326	238117	15.19%	1.715%
3	2.572	369	383	401	rBV	351152	587605	37.47%	4.231%
4	2.742	433	436	439	rBV3	185	159	0.01%	0.001%
5	2.803	446	455	463	rVV2	1493	2535	0.16%	0.018%
6	2.864	470	474	475	rBV	364	229	0.01%	0.002%
7	2.900	481	485	488	rBV2	286	232	0.01%	0.002%
8	2.941	494	498	501	rBV2	765	602	0.04%	0.004%
9	3.054	523	533	545	rVB	6051	11317	0.72%	0.081%
10	3.186	570	574	576	rBV3	535	390	0.02%	0.003%
11	3.266	590	599	604	rBV2	461	617	0.04%	0.004%
12	3.340	618	622	624	rBV2	309	172	0.01%	0.001%
13	3.359	624	628	634	rVV3	804	854	0.05%	0.006%
14	3.414	641	645	649	rVV4	289	269	0.02%	0.002%
15	3.533	679	682	685	rVB	300	200	0.01%	0.001%
16	3.800	761	765	769	rVB2	250	228	0.01%	0.002%
17	3.822	769	772	778	rBV5	508	569	0.04%	0.004%
18	3.961	812	815	821	rVB2	226	191	0.01%	0.001%
19	4.002	825	828	831	rBV	298	184	0.01%	0.001%
20	4.035	836	838	842	rVB	290	202	0.01%	0.001%
21	4.076	842	851	857	rVB3	412	535	0.03%	0.004%
22	4.108	857	861	866	rBV2	385	428	0.03%	0.003%
23	4.160	873	877	880	rBV3	257	238	0.02%	0.002%
24	4.182	882	884	888	rVV2	243	183	0.01%	0.001%
25	4.218	892	895	901	rVV3	212	155	0.01%	0.001%
26	4.250	902	905	908	rVB4	230	164	0.01%	0.001%
27	4.285	912	916	919	rBV2	290	264	0.02%	0.002%
28	4.414	951	956	961	rVV3	324	353	0.02%	0.003%
29	4.462	968	971	974	rVB2	262	152	0.01%	0.001%
30	4.565	998	1003	1004	rBV3	250	191	0.01%	0.001%
31	4.629	1004	1023	1051	rBV	172582	436226	27.82%	3.141%
32	4.948	1119	1122	1124	rBV2	412	237	0.02%	0.002%
33	4.986	1131	1134	1137	rVB2	356	191	0.01%	0.001%
34	5.009	1137	1141	1142	rBV	637	357	0.02%	0.003%
35	5.067	1142	1159	1182	rVV	280231	611026	38.97%	4.400%
36	5.285	1223	1227	1229	rBV2	379	361	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
 Title : VOC Analysis

37	5.324	1237	1239	1244	rVB	274	195	0.01%	0.001%
38	5.391	1257	1260	1267	rBV4	401	415	0.03%	0.003%
39	5.462	1278	1282	1284	rBV	262	175	0.01%	0.001%
40	5.565	1311	1314	1318	rVB2	269	194	0.01%	0.001%
41	5.623	1329	1332	1342	rVB3	345	490	0.03%	0.004%
42	5.729	1342	1365	1387	rBV2	590383	1568038	100.00%	11.291%
43	5.915	1411	1423	1433	rVB4	3415	6492	0.41%	0.047%
44	5.957	1433	1436	1437	rBV2	310	170	0.01%	0.001%
45	5.993	1445	1447	1452	rVB3	308	156	0.01%	0.001%
46	6.018	1452	1455	1457	rBV	262	161	0.01%	0.001%
47	6.089	1473	1477	1478	rBV3	921	596	0.04%	0.004%
48	6.105	1478	1482	1483	rBV	1181	735	0.05%	0.005%
49	6.250	1514	1527	1549	rBV	421000	793372	50.60%	5.713%
50	6.694	1650	1665	1683	rBV	360184	694384	44.28%	5.000%
51	6.803	1695	1699	1710	rVB5	1635	2555	0.16%	0.018%
52	6.845	1710	1712	1718	rBV5	376	325	0.02%	0.002%
53	6.919	1733	1735	1736	rBV	1123	520	0.03%	0.004%
54	7.041	1757	1773	1797	rBV	214205	373007	23.79%	2.686%
55	7.182	1809	1817	1825	rBV4	3526	5545	0.35%	0.040%
56	7.272	1841	1845	1848	rVB3	333	299	0.02%	0.002%
57	7.343	1863	1867	1871	rBV3	383	335	0.02%	0.002%
58	7.401	1881	1885	1887	rBV2	569	345	0.02%	0.002%
59	7.565	1922	1936	1958	rBV	222946	388875	24.80%	2.800%
60	7.684	1966	1973	1979	rBV3	1457	2218	0.14%	0.016%
61	7.739	1979	1990	2002	rVV	31527	50871	3.24%	0.366%
62	7.793	2002	2007	2015	rVB5	1766	2304	0.15%	0.017%
63	7.899	2025	2040	2055	rBV	770445	1336501	85.23%	9.624%
64	7.970	2056	2062	2074	rVB2	11965	20509	1.31%	0.148%
65	8.079	2091	2096	2102	rBV5	910	1325	0.08%	0.010%
66	8.121	2107	2109	2113	rBV3	248	241	0.02%	0.002%
67	8.179	2113	2127	2149	rBV	157780	269818	17.21%	1.943%
68	8.317	2168	2170	2174	rBV4	438	251	0.02%	0.002%
69	8.359	2179	2183	2185	rBV3	447	300	0.02%	0.002%
70	8.472	2206	2218	2230	rBV4	16908	30504	1.95%	0.220%
71	8.575	2236	2250	2257	rBV	23275	37266	2.38%	0.268%
72	8.632	2257	2268	2286	rVV	599827	994505	63.42%	7.161%
73	8.726	2287	2297	2315	rVB	342276	531158	33.87%	3.825%
74	8.835	2321	2331	2343	rVB	36551	57134	3.64%	0.411%
75	8.899	2349	2351	2353	rBV	269	178	0.01%	0.001%
76	8.919	2355	2357	2359	rVB3	412	212	0.01%	0.002%

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Title : VOC Analysis

77	8.944	2361	2365	2369	rBV4	466	455	0.03%	0.003%
78	9.115	2413	2418	2423	rBV5	306	374	0.02%	0.003%
79	9.211	2435	2448	2464	rBV	198860	309316	19.73%	2.227%
80	9.417	2500	2512	2532	rVB	609246	985481	62.85%	7.096%
81	10.073	2708	2716	2724	rBV2	8570	12797	0.82%	0.092%
82	10.671	2895	2902	2911	rVB3	7911	11647	0.74%	0.084%
83	10.758	2916	2929	2947	rBV	518331	822945	52.48%	5.926%
84	10.896	2965	2972	2990	rVB	10832	19529	1.25%	0.141%
85	11.459	3139	3147	3158	rVB3	7418	13489	0.86%	0.097%
86	11.504	3158	3161	3167	rBV3	395	396	0.03%	0.003%
87	11.571	3179	3182	3184	rBV2	903	645	0.04%	0.005%
88	11.700	3213	3222	3230	rBV4	3429	5719	0.36%	0.041%
89	11.748	3231	3237	3243	rVB5	2234	2954	0.19%	0.021%
90	11.812	3243	3257	3271	rBV	719331	1119276	71.38%	8.060%
91	11.970	3303	3306	3317	rVB2	5092	6583	0.42%	0.047%
92	12.192	3362	3375	3393	rVB	761623	1226972	78.25%	8.835%
93	12.330	3414	3418	3428	rVB7	2470	3024	0.19%	0.022%
94	12.635	3509	3513	3522	rVB4	1548	2143	0.14%	0.015%
95	12.774	3547	3556	3570	rVB2	5528	9292	0.59%	0.067%
96	13.221	3689	3695	3704	rVB4	2601	3322	0.21%	0.024%
97	13.841	3882	3888	3898	rVB7	3087	4593	0.29%	0.033%
98	14.086	3957	3964	3973	rBV2	4977	6938	0.44%	0.050%
99	14.333	4034	4041	4050	rVB6	3621	5076	0.32%	0.037%
100	14.687	4148	4151	4153	rBV3	669	441	0.03%	0.003%

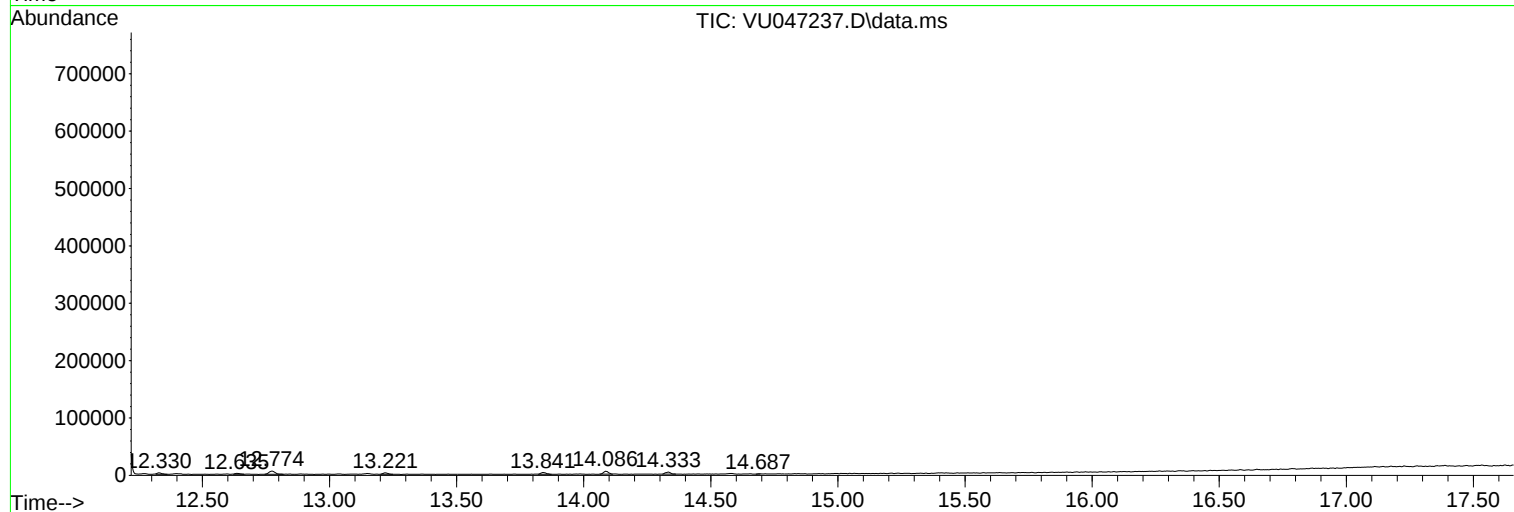
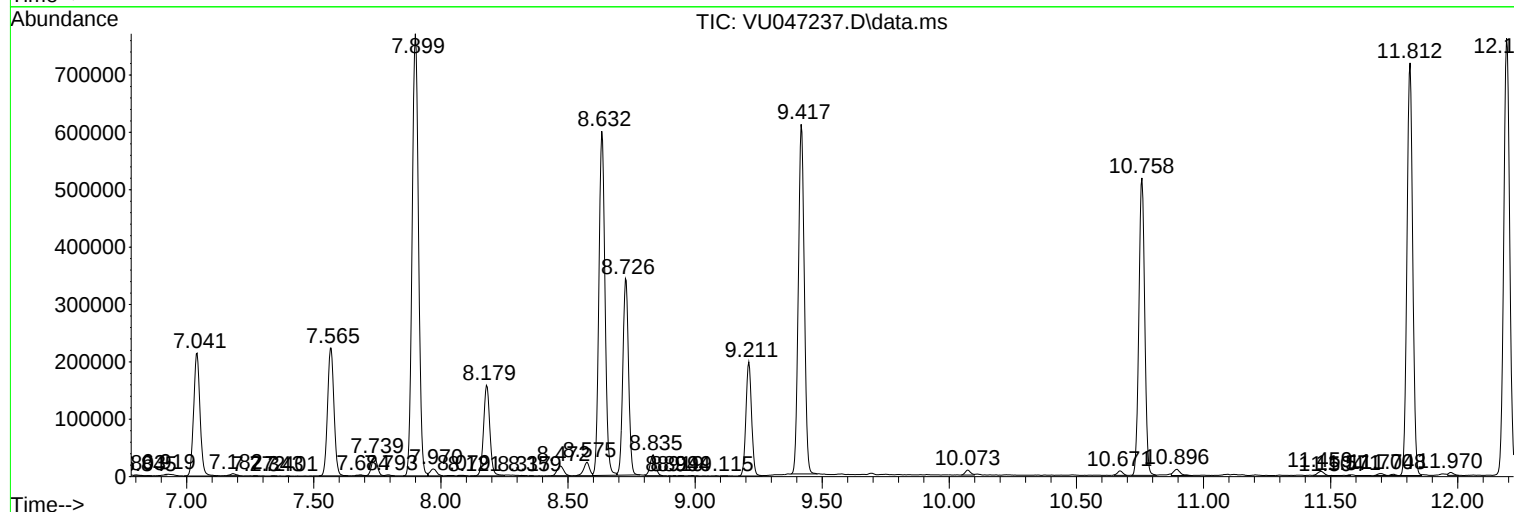
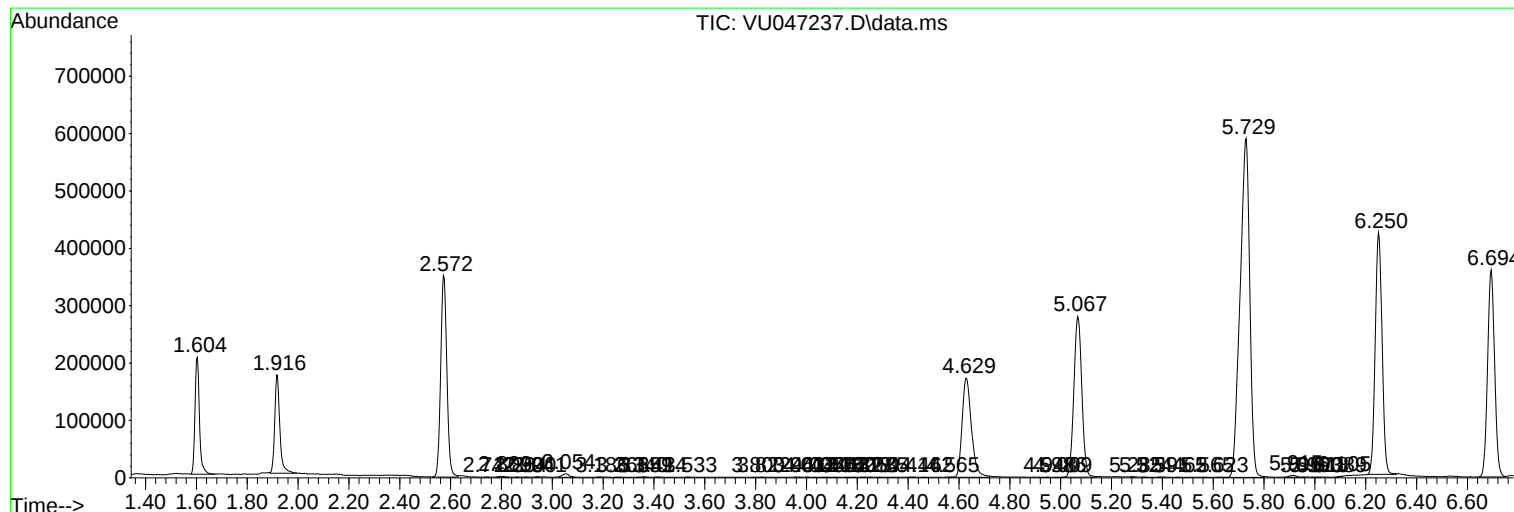
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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



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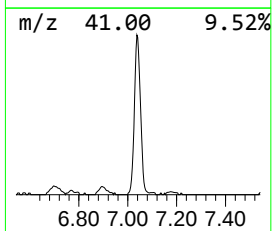
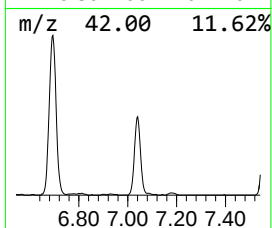
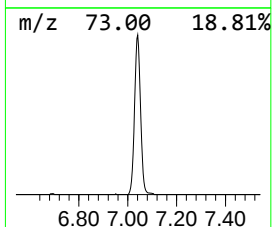
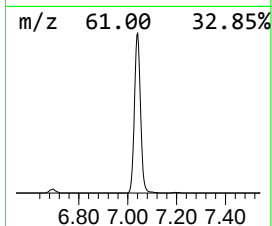
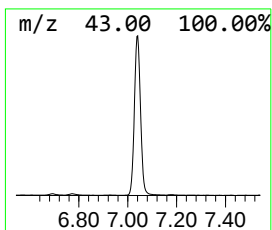
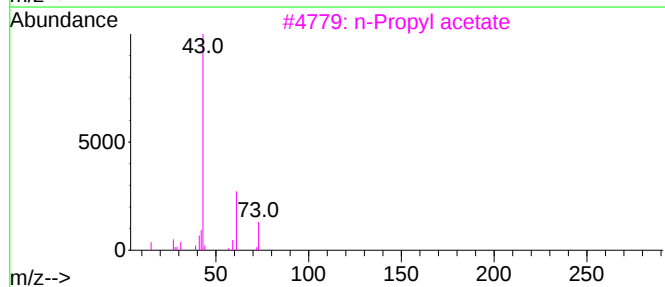
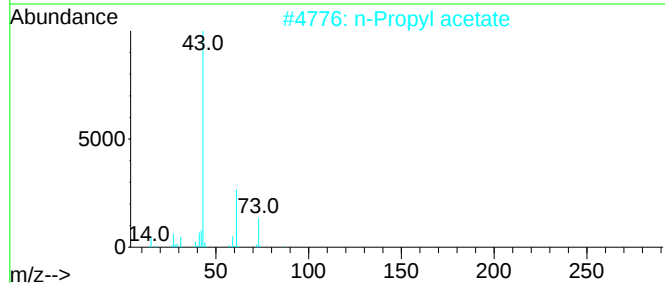
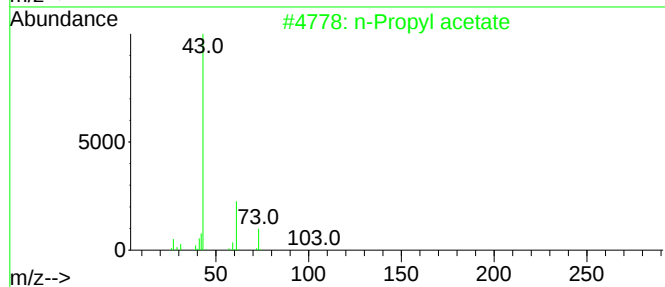
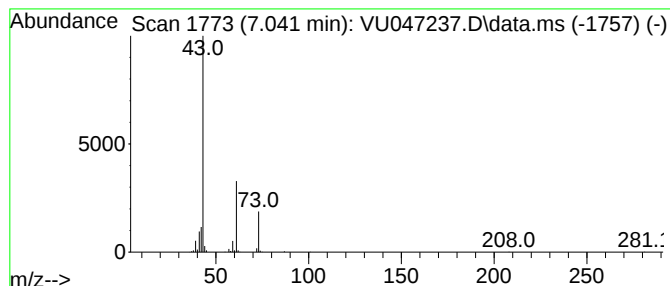
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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.
7.041	23.51 ug/L	373007	1,4-Difluorobenzene	6.250

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	83
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	78
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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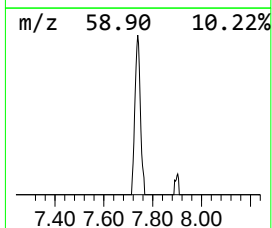
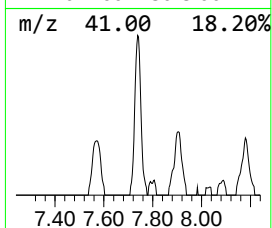
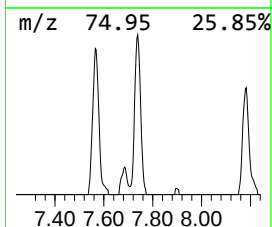
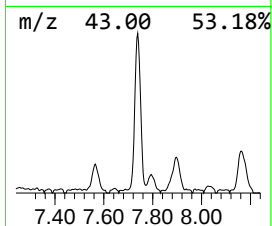
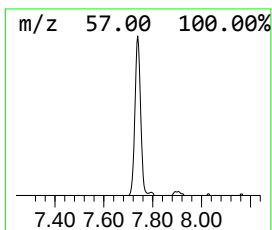
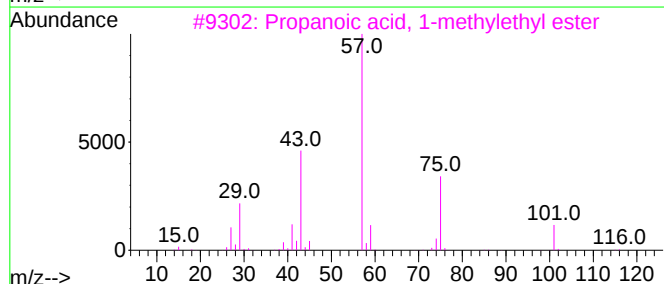
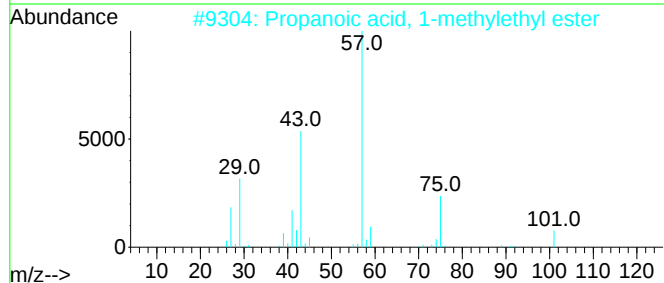
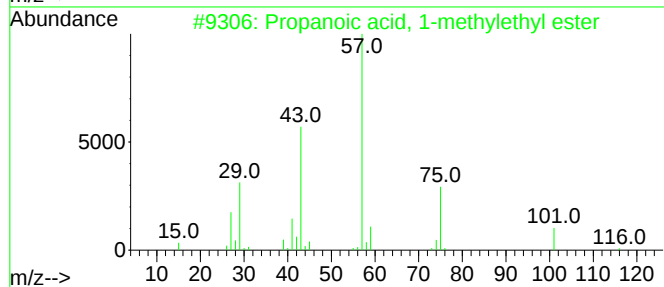
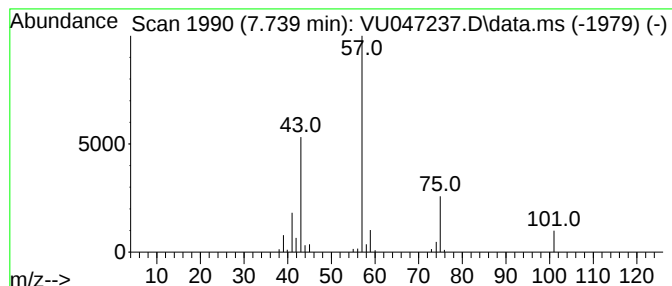
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	3.21 ug/L	50871	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53



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VLEB839

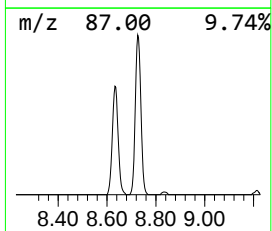
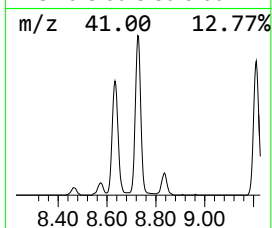
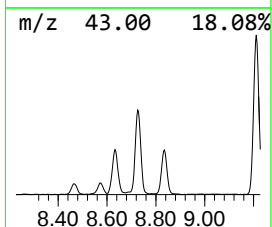
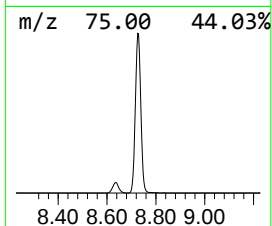
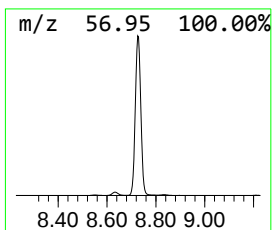
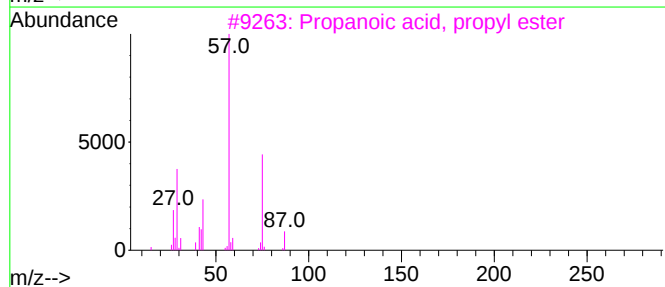
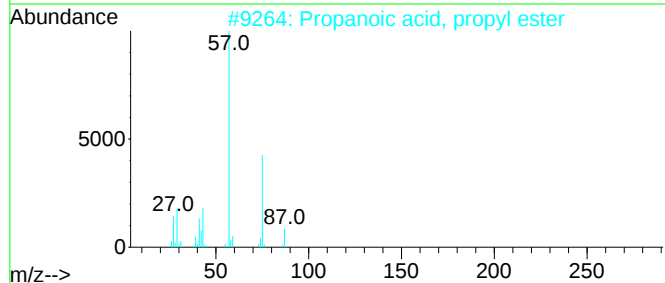
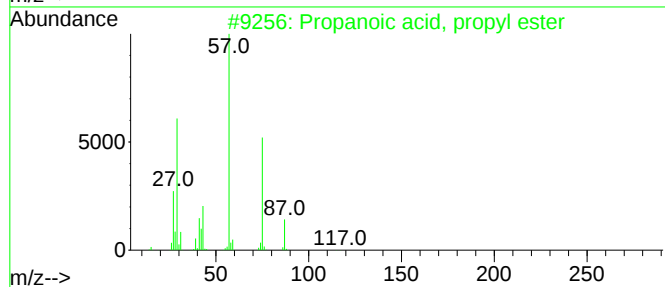
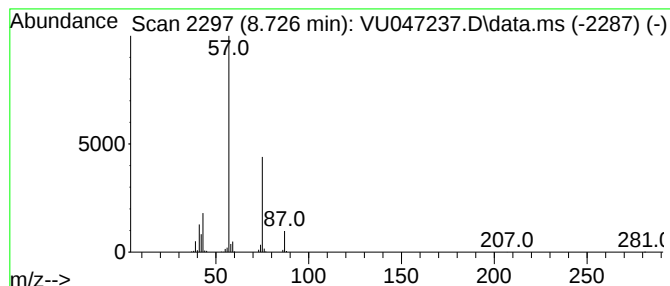
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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.
8.726	26.95 ug/L	531158	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\VU022222\
Data File : VU047237.D
Acq On : 22 Feb 2022 17:44
Operator : SY/MD
Sample : PB142839TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB839

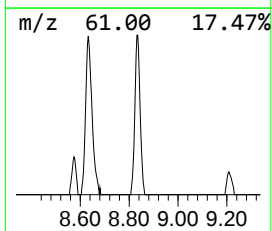
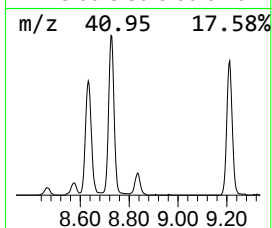
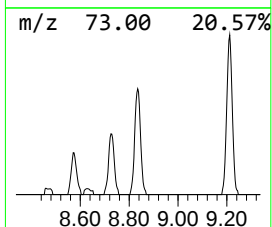
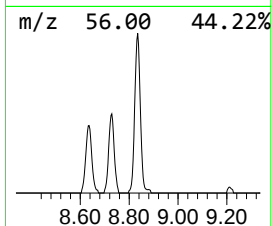
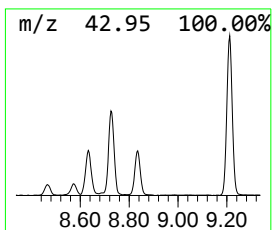
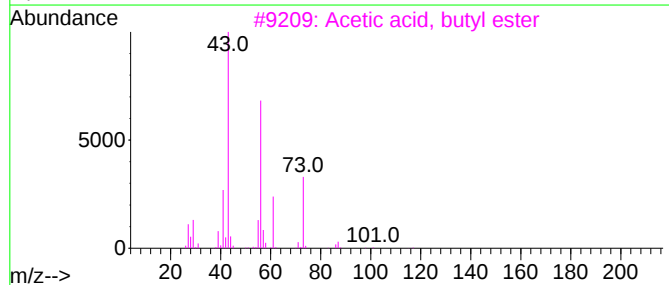
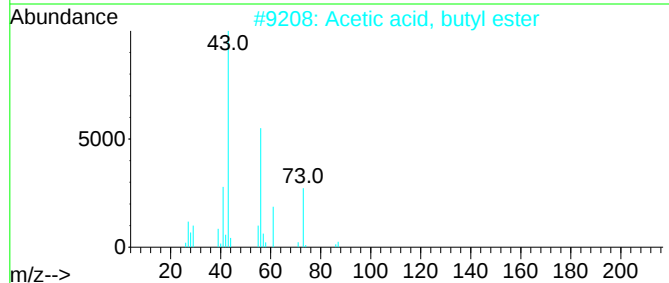
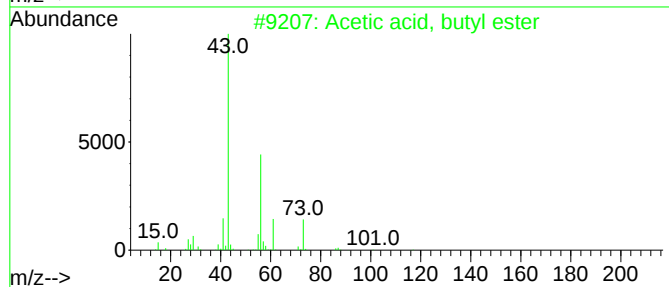
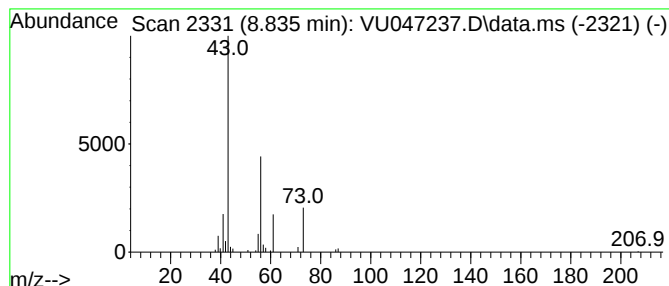
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	2.90 ug/L	57134	Chlorobenzene-d5	9.417

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	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	53
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047237.D
Acq On : 22 Feb 2022 17:44
Operator : SY/MD
Sample : PB142839TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB839

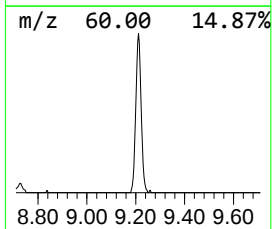
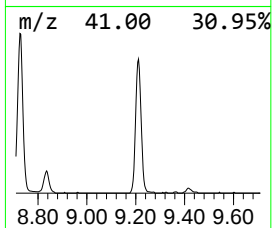
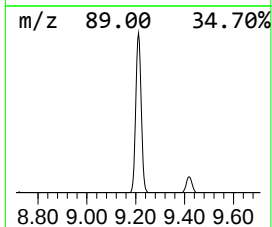
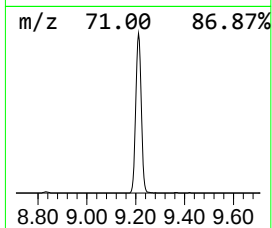
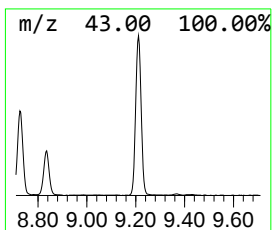
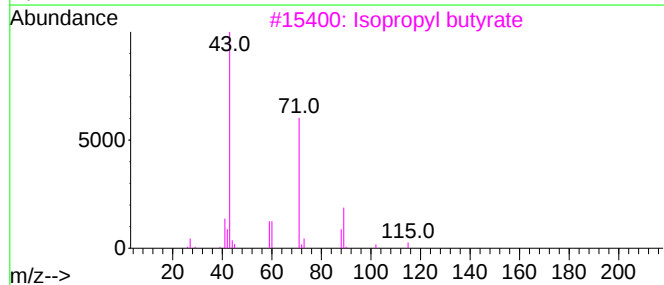
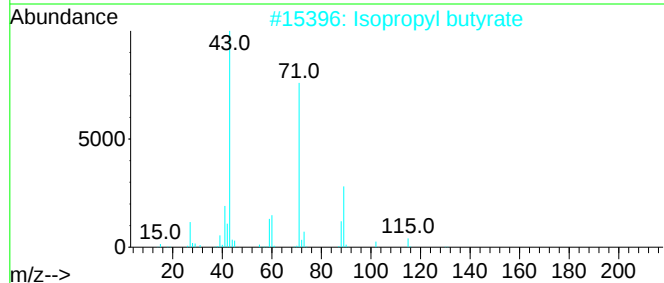
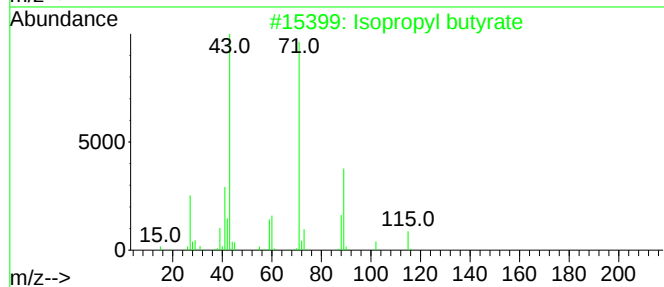
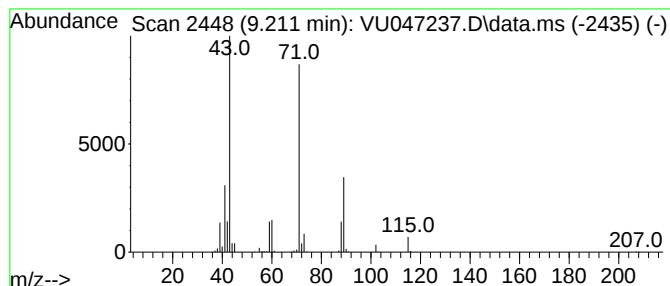
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Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	15.69 ug/L	309316	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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022222\
Data File : VU047237.D
Acq On : 22 Feb 2022 17:44
Operator : SY/MD
Sample : PB142839TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB839

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.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	23.5	ug/L	373007	1	6.250	793372	50.0
Propanoic acid,...	7.739	3.2	ug/L	50871	1	6.250	793372	50.0
Propanoic acid,...	8.726	26.9	ug/L	531158	2	9.417	985481	50.0
Acetic acid, bu...	8.835	2.9	ug/L	57134	2	9.417	985481	50.0
Isopropyl butyrate	9.211	15.7	ug/L	309316	2	9.417	985481	50.0