

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
 Data File : VU057838.D
 Acq On : 07 Feb 2024 14:22
 Operator : MD/SY
 Sample : PB158871TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB871

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\SFAMULM020724WMA.M

Title : VOC Analysis

Signal : TIC: VU057838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	88	95	110	rVB	129410	156491	15.79%	1.899%
2	1.888	179	186	202	rVB	96647	137512	13.88%	1.669%
3	2.557	382	394	408	rBV	210687	342158	34.53%	4.152%
4	2.673	428	430	435	rVB2	505	317	0.03%	0.004%
5	2.698	435	438	443	rVB2	287	214	0.02%	0.003%
6	2.769	456	460	461	rVV	393	305	0.03%	0.004%
7	2.782	461	464	473	rVB2	1072	1263	0.13%	0.015%
8	2.817	473	475	478	rVB2	356	191	0.02%	0.002%
9	2.914	501	505	509	rVB2	383	276	0.03%	0.003%
10	2.946	511	515	517	rBV2	493	399	0.04%	0.005%
11	3.036	534	543	558	rVB4	4306	8213	0.83%	0.100%
12	3.177	574	587	600	rBV2	1659	4016	0.41%	0.049%
13	3.248	604	609	613	rVB2	203	197	0.02%	0.002%
14	3.351	635	641	649	rVB4	1041	1528	0.15%	0.019%
15	3.740	759	762	771	rVB2	258	310	0.03%	0.004%
16	3.820	782	787	791	rBV	238	243	0.02%	0.003%
17	3.856	794	798	800	rBV2	287	216	0.02%	0.003%
18	3.949	823	827	832	rBV2	202	239	0.02%	0.003%
19	4.367	955	957	964	rVB	241	195	0.02%	0.002%
20	4.611	1022	1033	1063	rBV	67018	178376	18.00%	2.164%
21	5.052	1155	1170	1195	rVV	173698	382270	38.58%	4.638%
22	5.200	1214	1216	1221	rVB3	478	416	0.04%	0.005%
23	5.299	1244	1247	1249	rBV	341	218	0.02%	0.003%
24	5.319	1249	1253	1254	rBV2	446	274	0.03%	0.003%
25	5.373	1267	1270	1275	rBV3	278	258	0.03%	0.003%
26	5.714	1354	1376	1414	rBV2	358516	990907	100.00%	12.024%
27	5.910	1429	1437	1448	rBV3	7861	15679	1.58%	0.190%
28	5.971	1455	1456	1465	rVB3	722	441	0.04%	0.005%
29	6.036	1473	1476	1482	rBV3	351	431	0.04%	0.005%
30	6.087	1489	1492	1497	rVB3	288	213	0.02%	0.003%
31	6.116	1497	1501	1502	rBV	321	208	0.02%	0.003%
32	6.242	1527	1540	1570	rBV	303592	581248	58.66%	7.053%
33	6.451	1603	1605	1609	rBV3	248	189	0.02%	0.002%
34	6.492	1613	1618	1619	rBV3	265	248	0.03%	0.003%
35	6.537	1624	1632	1644	rVB8	2814	5791	0.58%	0.070%
36	6.592	1644	1649	1652	rBV2	700	755	0.08%	0.009%

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Title : VOC Analysis

37	6.682	1664	1677	1698	rBV	221301	434897	43.89%	5.277%
38	6.849	1727	1729	1733	rVB3	341	195	0.02%	0.002%
39	6.930	1745	1754	1756	rBV2	2978	4086	0.41%	0.050%
40	7.033	1776	1786	1816	rBV	95180	174418	17.60%	2.116%
41	7.348	1882	1884	1890	rVB3	203	192	0.02%	0.002%
42	7.560	1935	1950	1972	rBV	127828	229405	23.15%	2.784%
43	7.659	1978	1981	1989	rVB3	407	500	0.05%	0.006%
44	7.733	1994	2004	2017	rBV2	20895	35550	3.59%	0.431%
45	7.891	2038	2053	2072	rBV	454945	782014	78.92%	9.489%
46	8.042	2097	2100	2104	rVV3	414	327	0.03%	0.004%
47	8.084	2111	2113	2119	rVB3	497	398	0.04%	0.005%
48	8.174	2122	2141	2163	rBV2	95375	198459	20.03%	2.408%
49	8.280	2173	2174	2177	rBV2	377	253	0.03%	0.003%
50	8.335	2185	2191	2193	rBV	300	290	0.03%	0.004%
51	8.348	2193	2195	2200	rBV2	230	191	0.02%	0.002%
52	8.393	2204	2209	2213	rBV3	391	365	0.04%	0.004%
53	8.460	2219	2230	2247	rBV	29689	48132	4.86%	0.584%
54	8.573	2252	2265	2272	rBV9	5188	10369	1.05%	0.126%
55	8.627	2272	2282	2303	rBV	261066	483448	48.79%	5.866%
56	8.724	2304	2312	2327	rVB	44998	77762	7.85%	0.944%
57	8.833	2337	2346	2366	rVB	28233	48959	4.94%	0.594%
58	8.920	2369	2373	2376	rVB4	623	577	0.06%	0.007%
59	8.962	2384	2386	2390	rVB2	380	228	0.02%	0.003%
60	9.206	2451	2462	2487	rVV	86355	138786	14.01%	1.684%
61	9.370	2506	2513	2514	rVV4	1135	1288	0.13%	0.016%
62	9.412	2514	2526	2559	rVB	422870	708466	71.50%	8.596%
63	9.569	2567	2575	2582	rBV2	2753	3720	0.38%	0.045%
64	9.630	2591	2594	2595	rBV	398	214	0.02%	0.003%
65	9.643	2595	2598	2603	rVV3	783	868	0.09%	0.011%
66	9.692	2607	2613	2625	rVB5	3001	4698	0.47%	0.057%
67	9.936	2678	2689	2698	rBV5	906	2088	0.21%	0.025%
68	10.071	2724	2731	2736	rBV3	5596	8560	0.86%	0.104%
69	10.245	2775	2785	2789	rBV2	390	466	0.05%	0.006%
70	10.476	2854	2857	2859	rBV	326	227	0.02%	0.003%
71	10.656	2907	2913	2918	rVB2	206	226	0.02%	0.003%
72	10.749	2929	2942	2958	rBV	298478	489847	49.43%	5.944%
73	10.817	2960	2963	2973	rVB6	4176	5702	0.58%	0.069%
74	10.881	2979	2983	2993	rVB3	832	1286	0.13%	0.016%
75	11.093	3040	3049	3059	rVB6	2250	3523	0.36%	0.043%
76	11.402	3136	3145	3146	rBV	225	249	0.03%	0.003%

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 Title : VOC Analysis

77	11.437	3151	3156	3158	rBV2	227	210	0.02%	0.003%
78	11.470	3158	3166	3174	rVV2	4473	5895	0.59%	0.072%
79	11.563	3191	3195	3199	rBV2	219	208	0.02%	0.003%
80	11.746	3242	3252	3260	rBV2	8150	11909	1.20%	0.145%
81	11.807	3260	3271	3291	rVV	436402	693098	69.95%	8.410%
82	11.994	3325	3329	3335	rVB2	229	280	0.03%	0.003%
83	12.036	3335	3342	3345	rBV2	276	352	0.04%	0.004%
84	12.190	3377	3390	3411	rVV	421131	707906	71.44%	8.590%
85	12.765	3564	3569	3576	rVB	931	1285	0.13%	0.016%
86	12.997	3634	3641	3651	rBV3	3116	5201	0.52%	0.063%
87	13.235	3711	3715	3718	rBV2	507	472	0.05%	0.006%
88	13.412	3766	3770	3773	rBV2	342	264	0.03%	0.003%
89	13.839	3897	3903	3904	rBV3	1191	842	0.08%	0.010%
90	14.087	3968	3980	3999	rBV	51805	95508	9.64%	1.159%
91	14.289	4040	4043	4049	rVB2	526	420	0.04%	0.005%
92	14.315	4049	4051	4052	rBV	579	272	0.03%	0.003%
93	14.331	4052	4056	4067	rVB5	1608	1708	0.17%	0.021%
94	14.441	4087	4090	4095	rBV3	228	267	0.03%	0.003%
95	14.489	4102	4105	4108	rBV3	304	244	0.02%	0.003%
96	14.537	4116	4120	4123	rBV2	325	232	0.02%	0.003%
97	14.875	4217	4225	4227	rBV3	420	545	0.06%	0.007%
98	15.283	4348	4352	4354	rBV2	334	309	0.03%	0.004%
99	15.331	4363	4367	4368	rBV	394	301	0.03%	0.004%
100	15.897	4541	4543	4546	rVB2	558	246	0.02%	0.003%

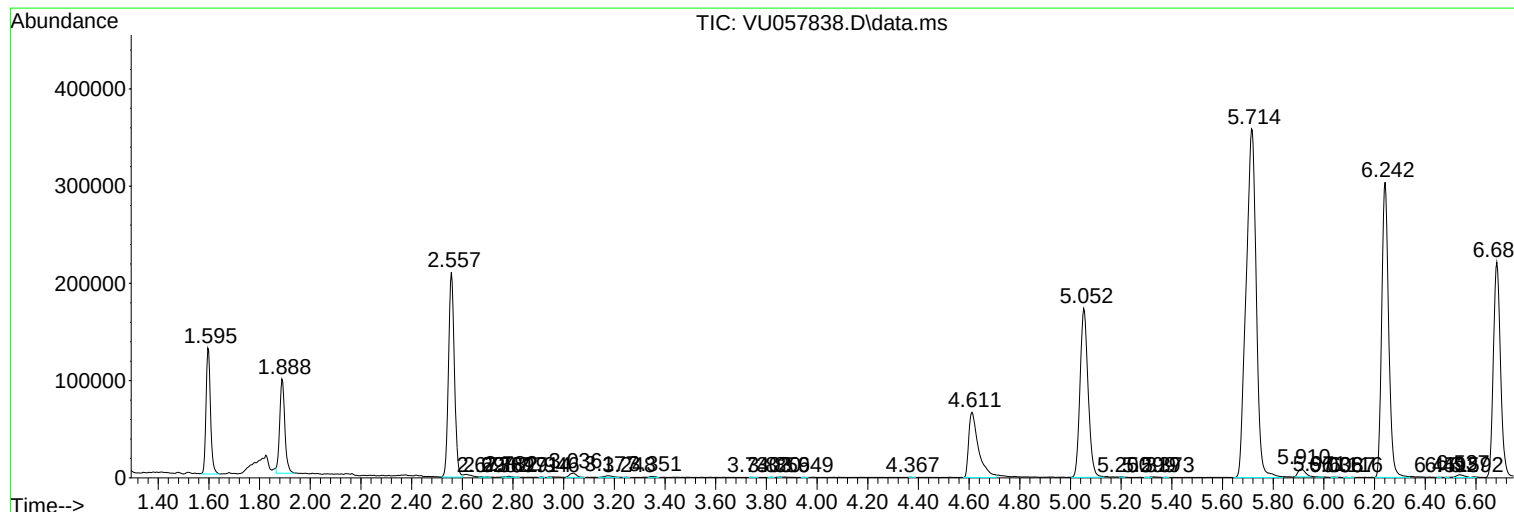
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
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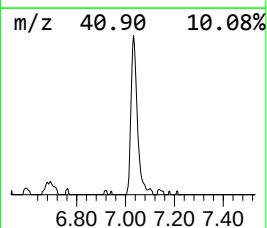
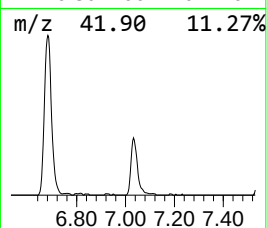
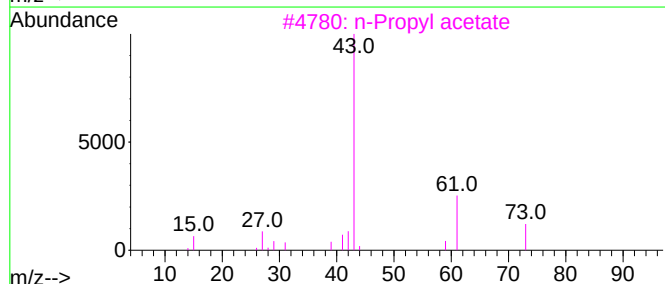
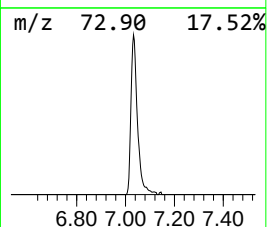
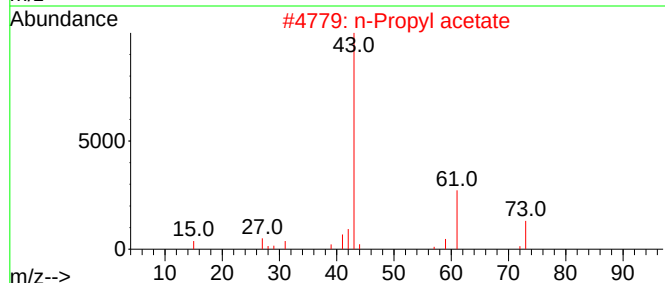
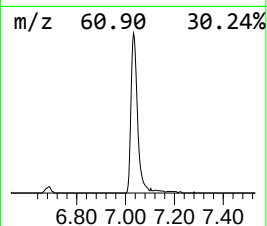
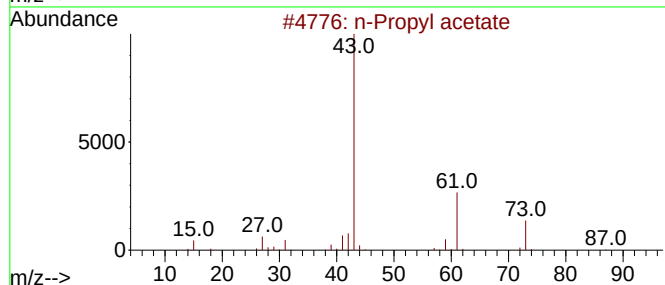
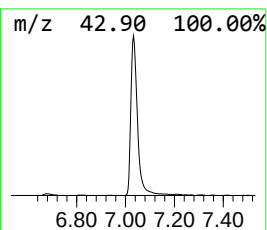
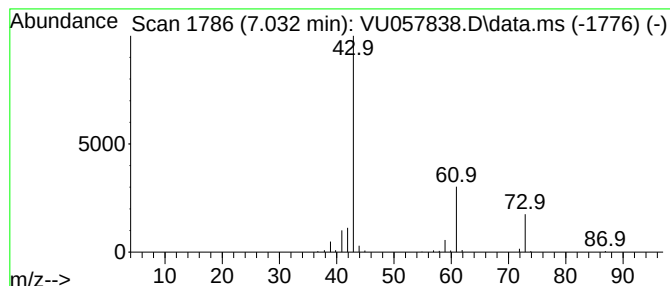
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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.
7.032	15.00 ug/L	174418	1,4-Difluorobenzene	6.242

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	72	
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64	
5	Isopropyl acetate	102	C5H10O2	000108-21-4	38	



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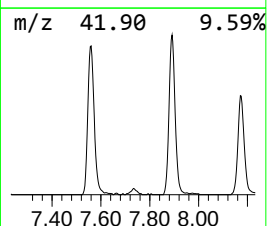
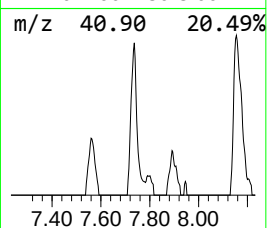
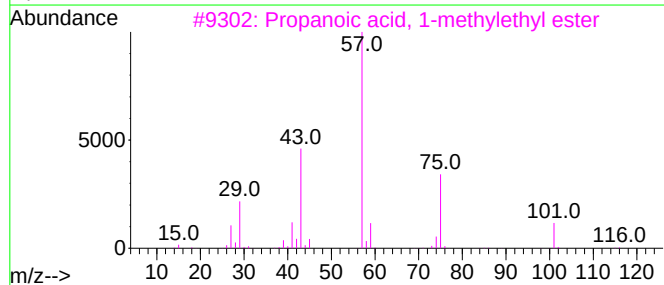
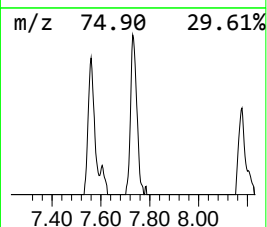
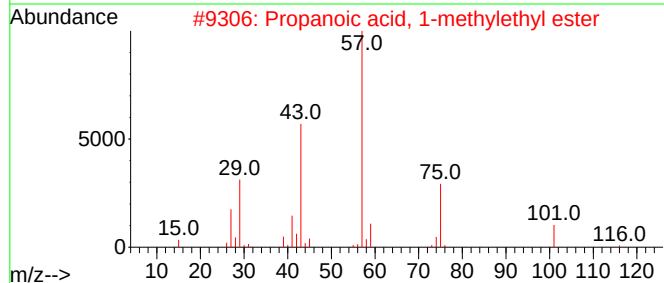
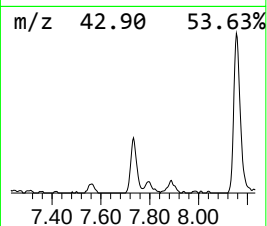
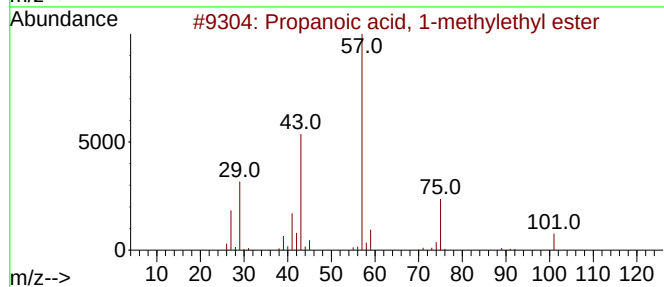
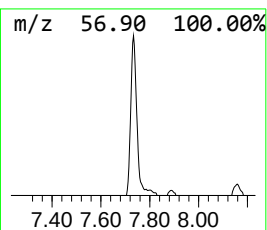
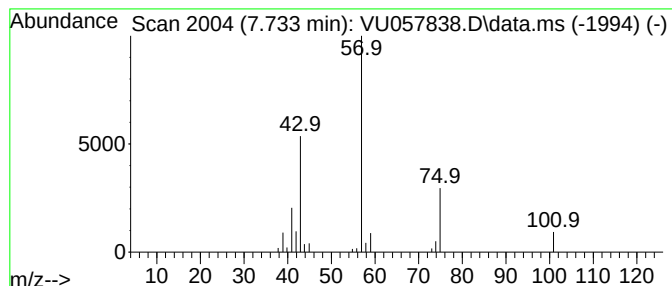
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.733	3.06 ug/L	35550	1,4-Difluorobenzene	6.242

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	72
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64



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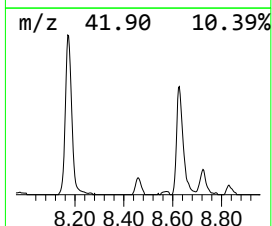
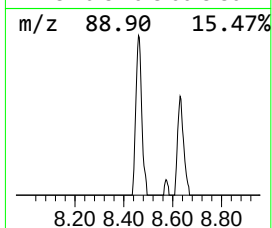
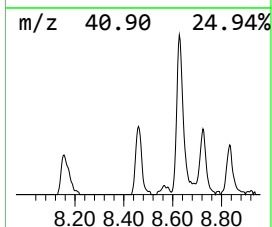
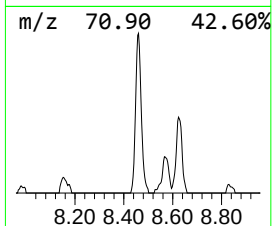
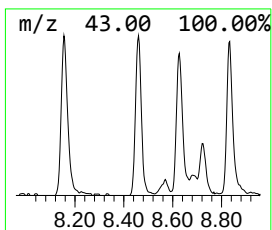
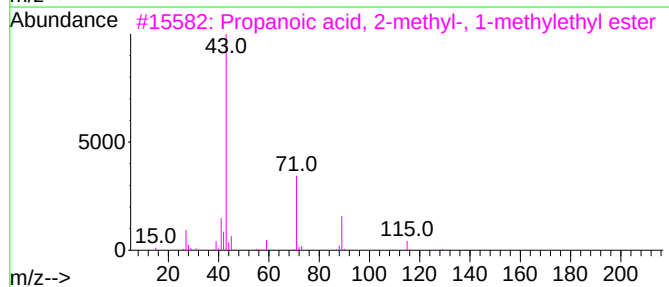
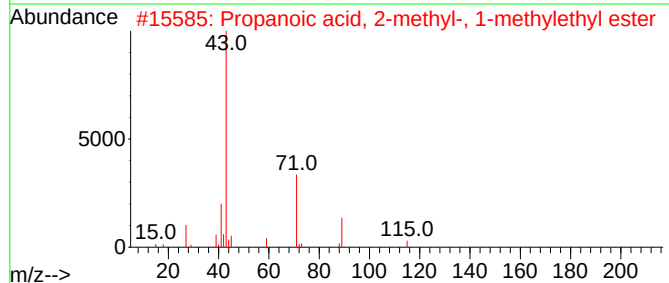
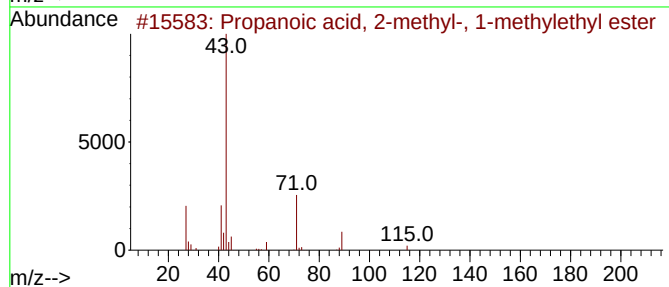
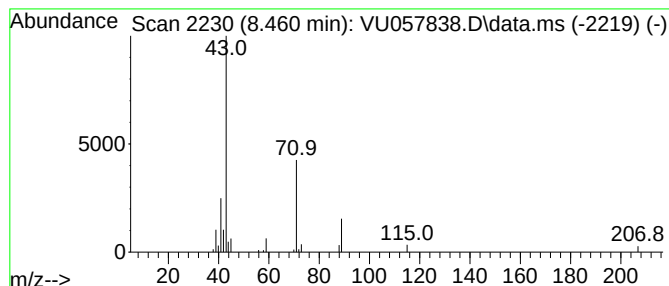
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.460	3.40 ug/L	48132	Chlorobenzene-d5	9.412

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	78
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
Data File : VU057838.D
Acq On : 07 Feb 2024 14:22
Operator : MD/SY
Sample : PB158871TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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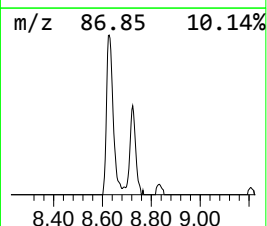
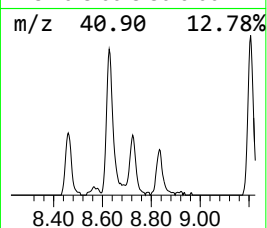
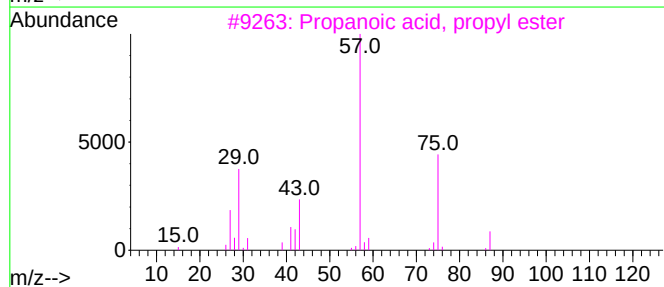
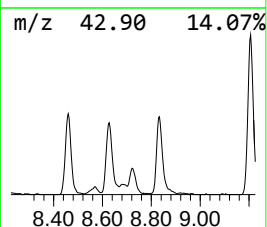
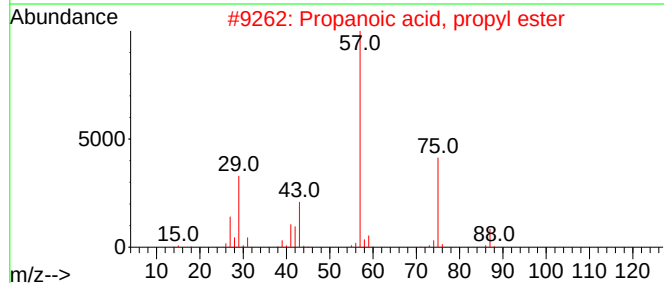
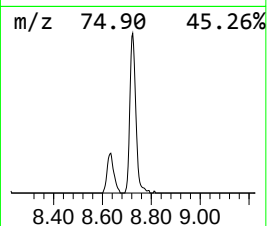
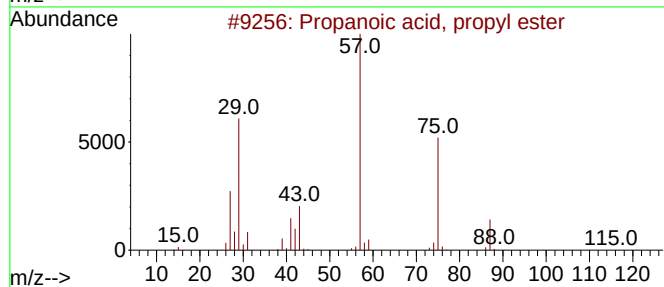
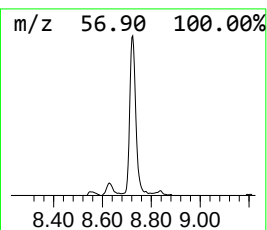
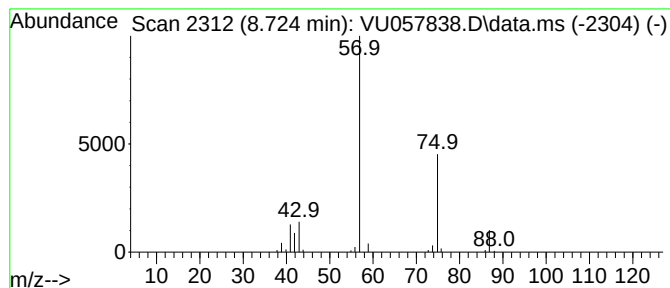
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.724	5.49 ug/L	77762	Chlorobenzene-d5	9.412

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	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
Data File : VU057838.D
Acq On : 07 Feb 2024 14:22
Operator : MD/SY
Sample : PB158871TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB871

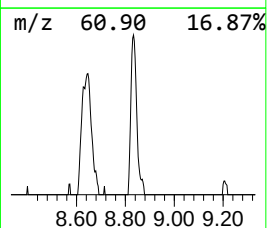
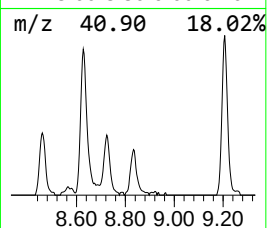
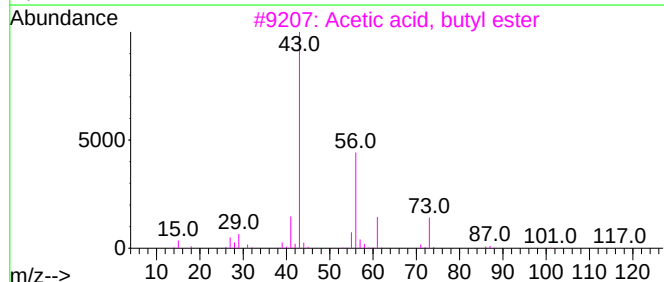
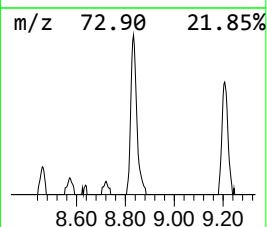
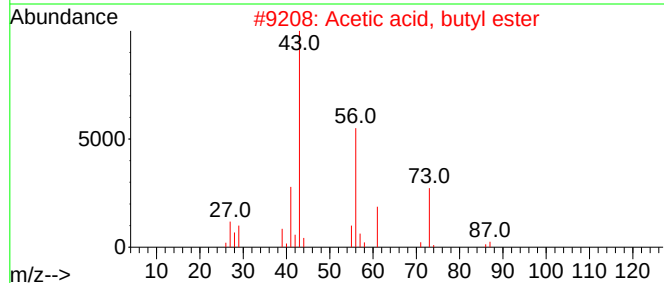
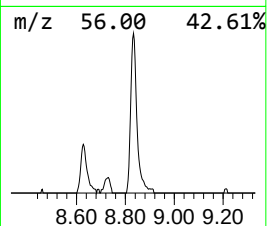
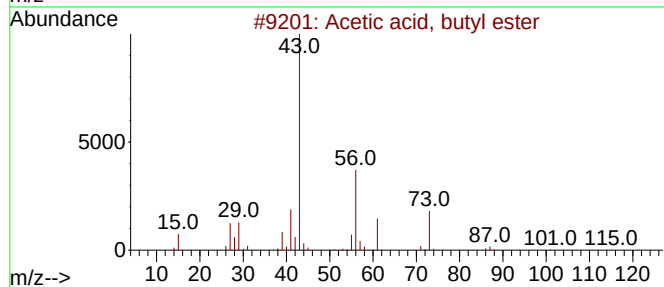
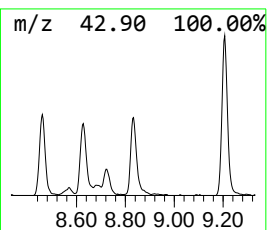
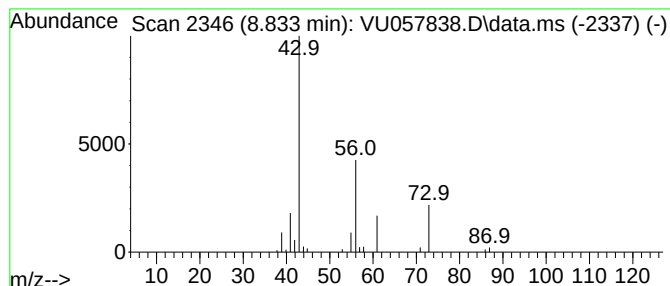
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.833	3.46 ug/L	48959	Chlorobenzene-d5	9.412

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	72		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56		
5	Isobutyl acetate	116	C6H12O2	000110-19-0	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
Data File : VU057838.D
Acq On : 07 Feb 2024 14:22
Operator : MD/SY
Sample : PB158871TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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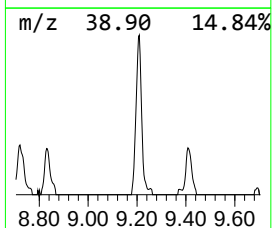
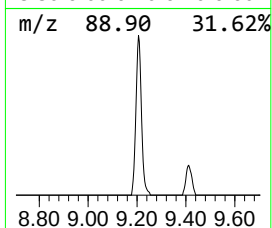
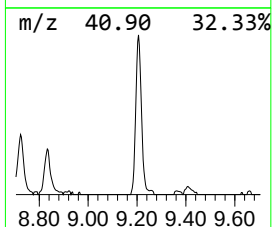
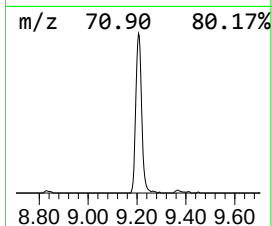
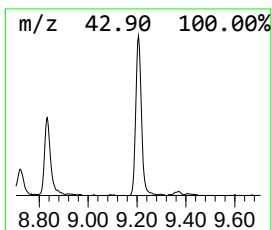
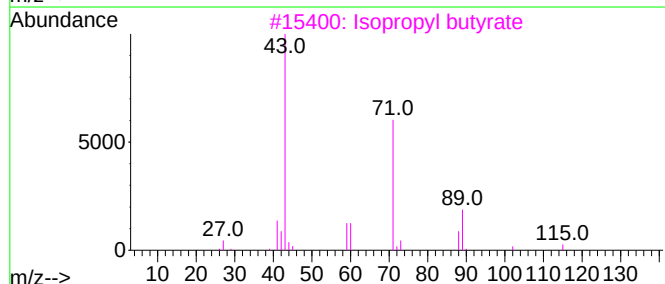
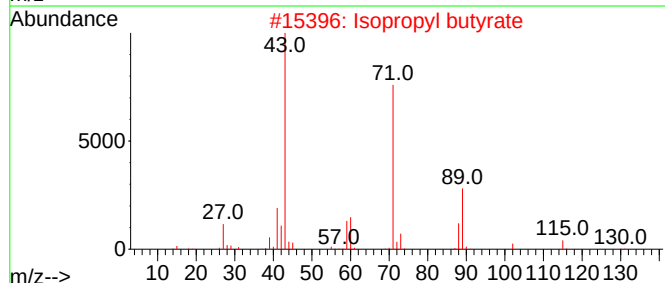
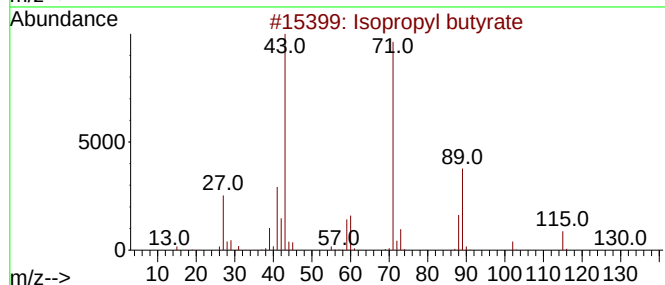
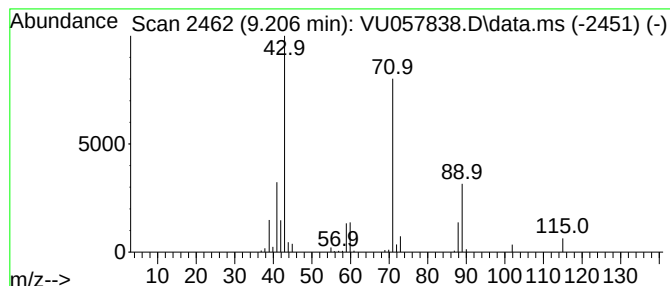
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Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.206	9.79 ug/L	138786	Chlorobenzene-d5	9.412

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-, propy...	130	C7H14O2	000644-49-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
Data File : VU057838.D
Acq On : 07 Feb 2024 14:22
Operator : MD/SY
Sample : PB158871TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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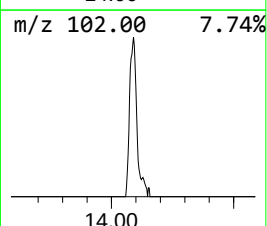
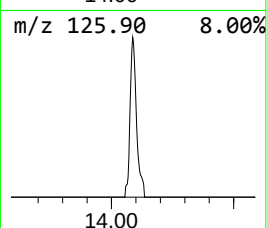
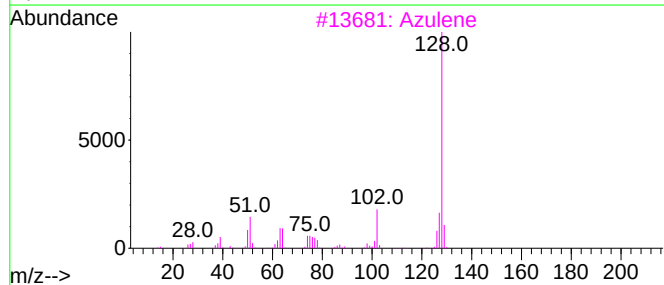
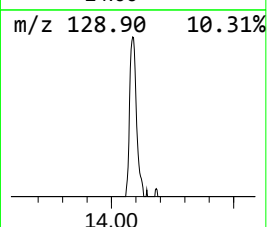
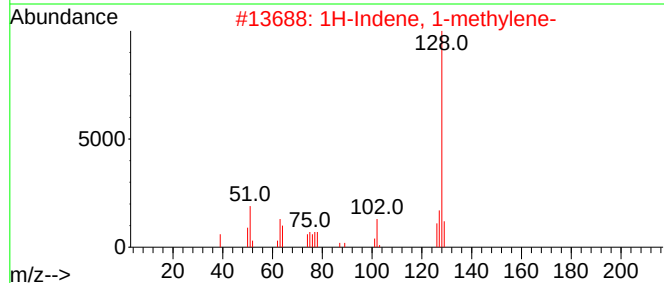
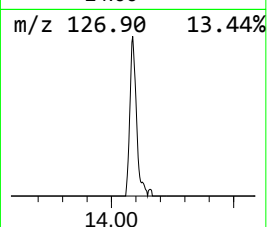
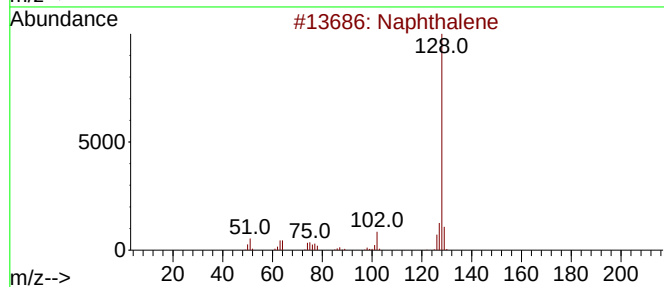
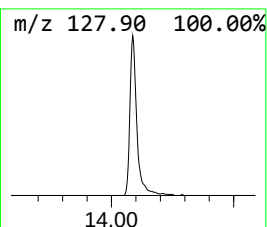
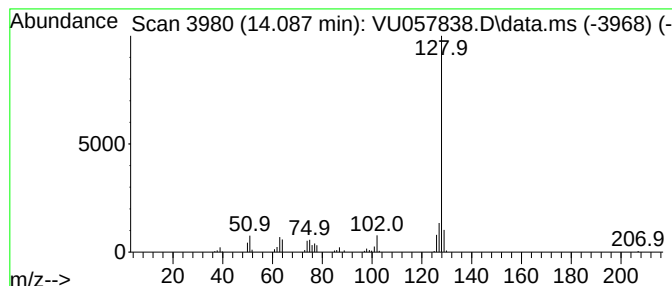
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Quant Title : VOC Analysis

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

Peak Number 8 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.087	6.89 ug/L	95508	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
3			Azulene	128	C10H8	000275-51-4	91
4			Naphthalene	128	C10H8	000091-20-3	91
5			Naphthalene	128	C10H8	000091-20-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
Data File : VU057838.D
Acq On : 07 Feb 2024 14:22
Operator : MD/SY
Sample : PB158871TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB871

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.032	15.0	ug/L	174418	1	6.242	581248	50.0
Propanoic acid,...	7.733	3.1	ug/L	35550	1	6.242	581248	50.0
Propanoic acid,...	8.460	3.4	ug/L	48132	2	9.412	708466	50.0
Propanoic acid,...	8.724	5.5	ug/L	77762	2	9.412	708466	50.0
Acetic acid, bu...	8.833	3.5	ug/L	48959	2	9.412	708466	50.0
Isopropyl butyrate	9.206	9.8	ug/L	138786	2	9.412	708466	50.0
Azulene	14.087	6.9	ug/L	95508	3	11.807	693098	50.0