

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046109.D
 Acq On : 06 Dec 2021 14:12
 Operator : SY/MD
 Sample : PB141182TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB182

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\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046109.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	95	rBV	106945	116389	13.46%	1.570%
2	1.915	171	179	196	rVB	76320	95807	11.08%	1.292%
3	2.459	346	348	354	rVB	296	241	0.03%	0.003%
4	2.571	371	383	400	rBV	186625	308080	35.64%	4.155%
5	2.796	447	453	458	rVB3	404	583	0.07%	0.008%
6	2.928	492	494	498	rVB2	287	208	0.02%	0.003%
7	2.954	498	502	503	rBV	275	188	0.02%	0.003%
8	3.047	522	531	543	rVB2	4642	8377	0.97%	0.113%
9	3.189	562	575	585	rBV	1884	3899	0.45%	0.053%
10	3.784	757	760	766	rBB	164	217	0.03%	0.003%
11	3.829	769	774	784	rBV3	948	1706	0.20%	0.023%
12	3.931	802	806	812	rBV	199	286	0.03%	0.004%
13	4.115	858	863	870	rBV	225	403	0.05%	0.005%
14	4.202	886	890	893	rBV	175	198	0.02%	0.003%
15	4.349	932	936	938	rBV	182	172	0.02%	0.002%
16	4.465	967	972	975	rBV	324	298	0.03%	0.004%
17	4.632	1009	1024	1051	rBV	82001	215641	24.95%	2.908%
18	4.902	1105	1108	1111	rVB2	187	153	0.02%	0.002%
19	5.066	1142	1159	1184	rBV	150507	335282	38.79%	4.522%
20	5.298	1225	1231	1235	rVV3	447	548	0.06%	0.007%
21	5.340	1241	1244	1250	rVB2	206	178	0.02%	0.002%
22	5.620	1327	1331	1335	rVB	223	196	0.02%	0.003%
23	5.729	1342	1365	1386	rBV2	324872	864417	100.00%	11.658%
24	5.912	1414	1422	1424	rBV3	1468	1650	0.19%	0.022%
25	6.121	1480	1487	1488	rBV2	296	233	0.03%	0.003%
26	6.250	1513	1527	1545	rBV	251029	477521	55.24%	6.440%
27	6.533	1604	1615	1625	rBV3	4205	8073	0.93%	0.109%
28	6.693	1651	1665	1683	rBV	194747	377341	43.65%	5.089%
29	6.761	1683	1686	1687	rBV2	482	324	0.04%	0.004%
30	6.835	1707	1709	1714	rVB2	200	164	0.02%	0.002%
31	6.883	1720	1724	1725	rBV	239	161	0.02%	0.002%
32	6.896	1725	1728	1729	rVV	305	167	0.02%	0.002%
33	6.931	1731	1739	1748	rVB2	1170	2124	0.25%	0.029%
34	7.041	1759	1773	1797	rBV	112346	199246	23.05%	2.687%
35	7.176	1811	1815	1818	rBV2	671	571	0.07%	0.008%
36	7.259	1838	1841	1845	rBV	180	212	0.02%	0.003%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.568	1923	1937	1954	rBV	115324	199164	23.04%	2.686%
38	7.668	1965	1968	1972	rBV2	252	173	0.02%	0.002%
39	7.687	1972	1974	1978	rVB	357	215	0.02%	0.003%
40	7.738	1979	1990	2001	rBV2	16662	27230	3.15%	0.367%
41	7.899	2025	2040	2056	rBV	417663	725236	83.90%	9.781%
42	8.082	2095	2097	2104	rVB3	299	292	0.03%	0.004%
43	8.179	2112	2127	2145	rBV	77576	130715	15.12%	1.763%
44	8.279	2156	2158	2161	rVB2	258	152	0.02%	0.002%
45	8.298	2161	2164	2169	rVB3	332	306	0.04%	0.004%
46	8.465	2206	2216	2225	rBV2	4120	6323	0.73%	0.085%
47	8.574	2237	2250	2257	rBV3	11809	18562	2.15%	0.250%
48	8.632	2257	2268	2288	rVV	249438	447686	51.79%	6.038%
49	8.729	2288	2298	2321	rVV	189912	300684	34.78%	4.055%
50	8.835	2322	2331	2343	rVB	18816	29120	3.37%	0.393%
51	8.915	2349	2356	2363	rVB4	763	1133	0.13%	0.015%
52	8.979	2370	2376	2383	rVB2	243	380	0.04%	0.005%
53	9.211	2437	2448	2468	rVB	96105	147931	17.11%	1.995%
54	9.314	2477	2480	2485	rVB2	177	175	0.02%	0.002%
55	9.369	2494	2497	2500	rVV	470	288	0.03%	0.004%
56	9.420	2500	2513	2544	rVB	353051	595828	68.93%	8.036%
57	9.571	2555	2560	2566	rBV2	509	535	0.06%	0.007%
58	9.658	2584	2587	2590	rVV	284	211	0.02%	0.003%
59	9.677	2590	2593	2594	rVV	300	182	0.02%	0.002%
60	9.693	2594	2598	2606	rVB	855	1155	0.13%	0.016%
61	10.073	2708	2716	2724	rBV2	3098	4291	0.50%	0.058%
62	10.134	2730	2735	2744	rVB2	467	461	0.05%	0.006%
63	10.674	2896	2903	2911	rVB3	2312	3189	0.37%	0.043%
64	10.758	2917	2929	2949	rVB	273731	437945	50.66%	5.906%
65	10.870	2959	2964	2968	rBV3	499	628	0.07%	0.008%
66	10.999	3001	3004	3008	rBV2	185	202	0.02%	0.003%
67	11.092	3026	3033	3040	rVV3	503	646	0.07%	0.009%
68	11.127	3041	3044	3048	rVB3	434	269	0.03%	0.004%
69	11.153	3049	3052	3057	rBV3	243	160	0.02%	0.002%
70	11.233	3074	3077	3080	rVV	220	153	0.02%	0.002%
71	11.459	3138	3147	3158	rBV4	2080	3498	0.40%	0.047%
72	11.584	3181	3186	3192	rVB2	523	491	0.06%	0.007%
73	11.661	3207	3210	3214	rBV	260	195	0.02%	0.003%
74	11.696	3214	3221	3226	rBV5	883	945	0.11%	0.013%
75	11.748	3233	3237	3243	rVB2	212	207	0.02%	0.003%
76	11.812	3243	3257	3273	rBV	396381	625025	72.31%	8.429%

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Integration Parameters: LSCINT.P

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Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	11.973	3303	3307	3315	rVB3	1570	2045	0.24%	0.028%
78	12.082	3332	3341	3343	rBV2	386	426	0.05%	0.006%
79	12.195	3359	3376	3397	rBV	412188	668679	77.36%	9.018%
80	12.272	3397	3400	3402	rBV	324	216	0.02%	0.003%
81	12.333	3413	3419	3422	rVB4	622	540	0.06%	0.007%
82	12.545	3482	3485	3488	rBV	204	162	0.02%	0.002%
83	12.587	3495	3498	3501	rBV2	313	175	0.02%	0.002%
84	12.774	3554	3556	3560	rVB	328	152	0.02%	0.002%
85	13.455	3765	3768	3773	rBV2	229	271	0.03%	0.004%
86	13.844	3885	3889	3894	rVB2	472	361	0.04%	0.005%
87	13.909	3906	3909	3913	rVV	240	198	0.02%	0.003%
88	13.989	3931	3934	3936	rBV2	223	186	0.02%	0.003%
89	14.092	3958	3966	3975	rVB	1172	1789	0.21%	0.024%
90	14.220	4004	4006	4012	rVB2	214	176	0.02%	0.002%
91	14.282	4021	4025	4028	rBV2	303	237	0.03%	0.003%
92	14.339	4038	4043	4048	rBV2	344	318	0.04%	0.004%
93	14.581	4110	4118	4128	rVB2	996	1549	0.18%	0.021%
94	14.645	4135	4138	4140	rBV	334	154	0.02%	0.002%
95	14.954	4231	4234	4237	rVB	276	180	0.02%	0.002%
96	14.999	4246	4248	4253	rVB2	374	289	0.03%	0.004%
97	15.224	4312	4318	4330	rBV3	1642	2541	0.29%	0.034%
98	15.529	4410	4413	4418	rBV2	350	319	0.04%	0.004%
99	16.021	4564	4566	4571	rBV3	385	288	0.03%	0.004%
100	16.298	4649	4652	4654	rBV3	589	416	0.05%	0.006%

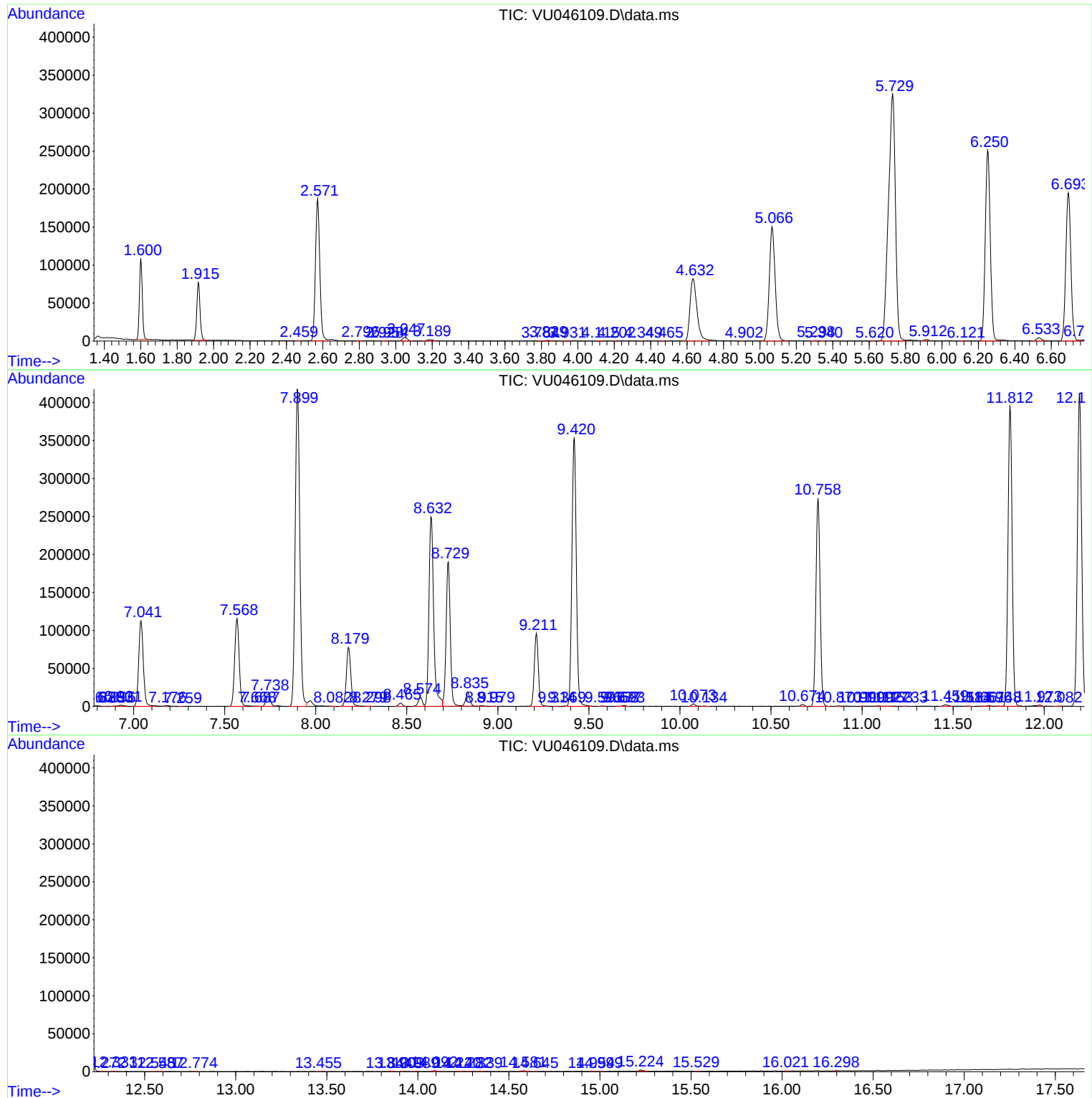
Sum of corrected areas: 7414902

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
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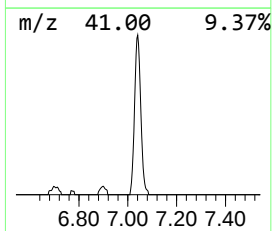
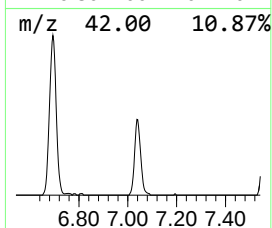
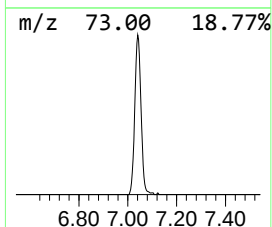
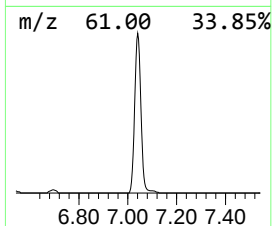
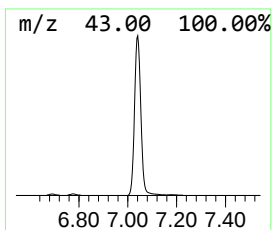
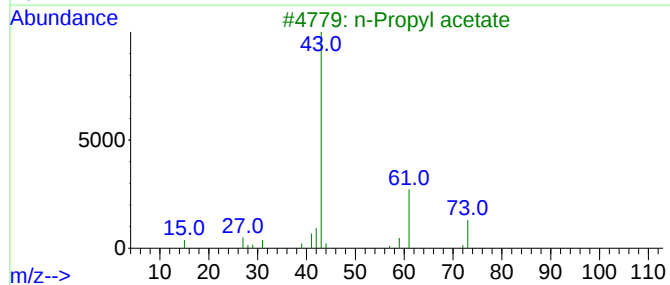
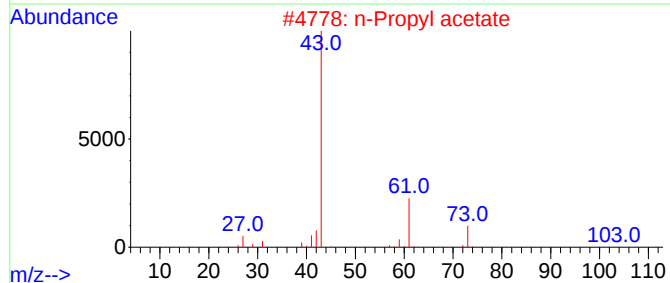
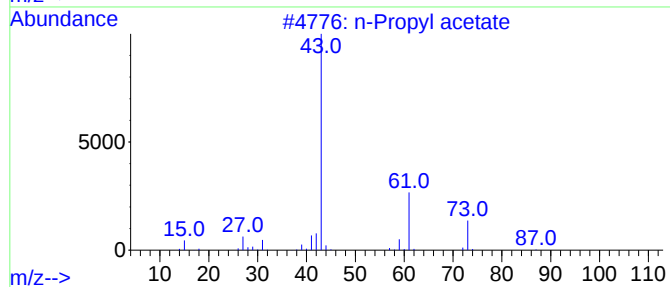
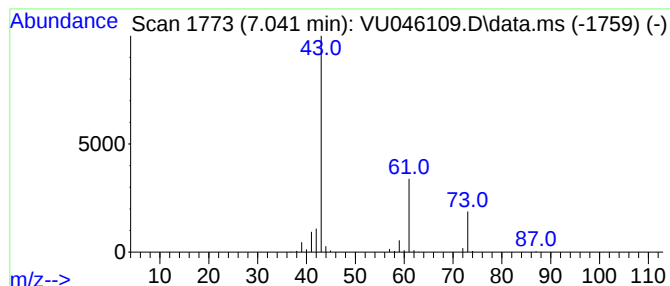
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
7.041	20.86 ug/L	199246	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	64
5	Isopropyl acetate			102	C5H10O2	000108-21-4	36



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Instrument :
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ClientSampleId :
VLEB182

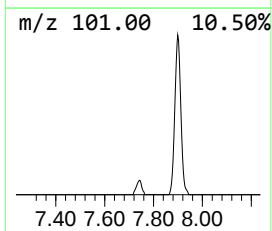
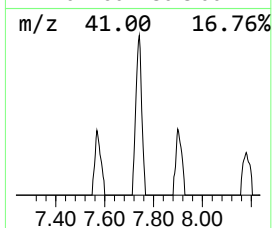
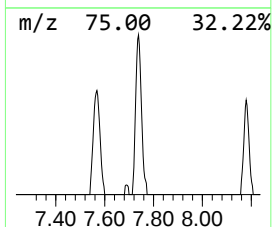
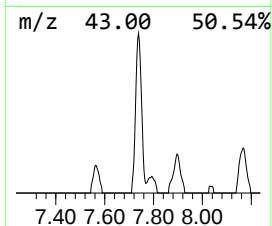
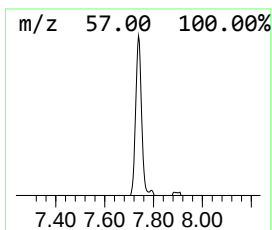
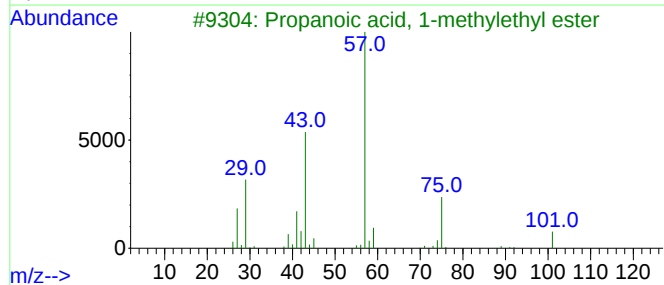
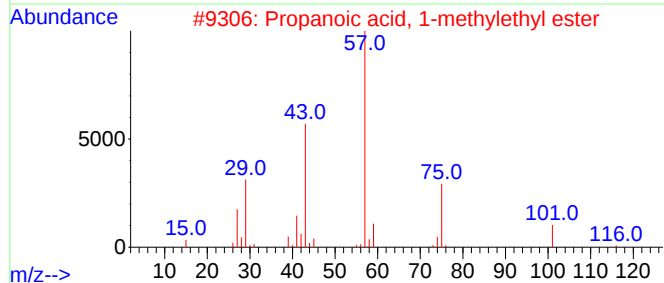
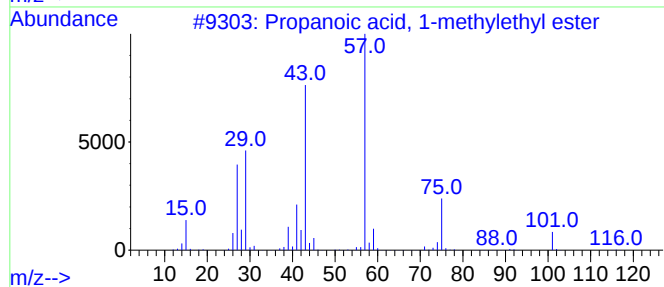
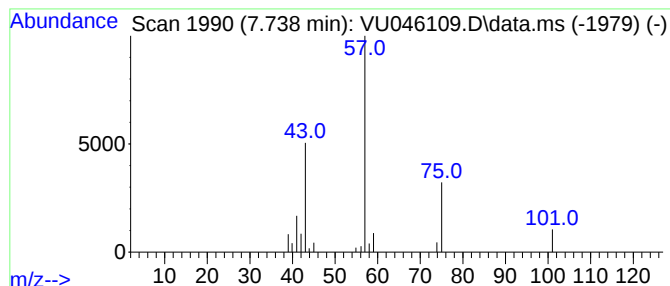
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.85 ug/L	27230	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	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45



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ClientSampleId :
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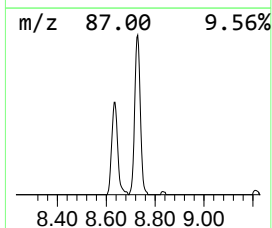
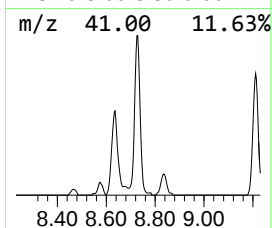
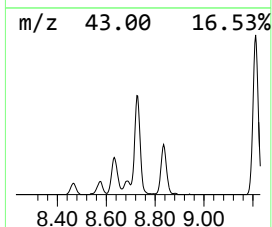
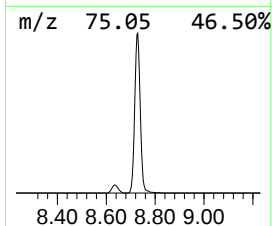
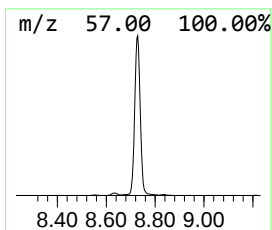
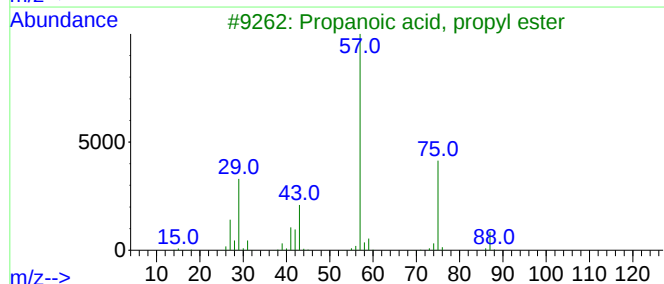
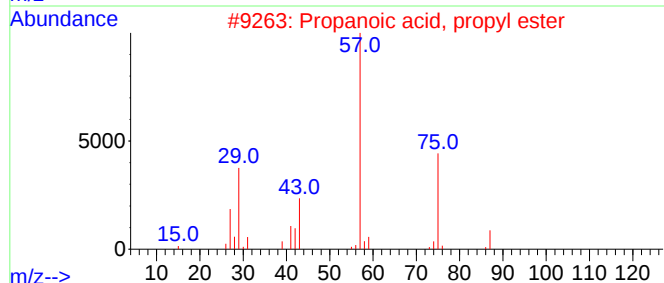
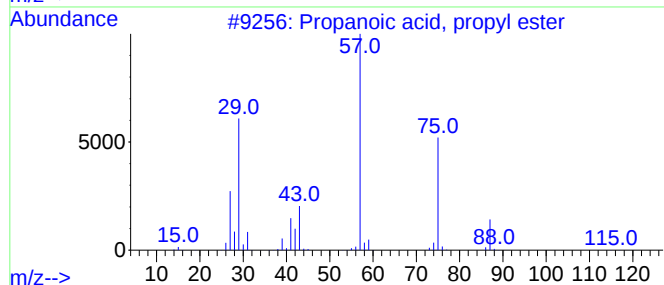
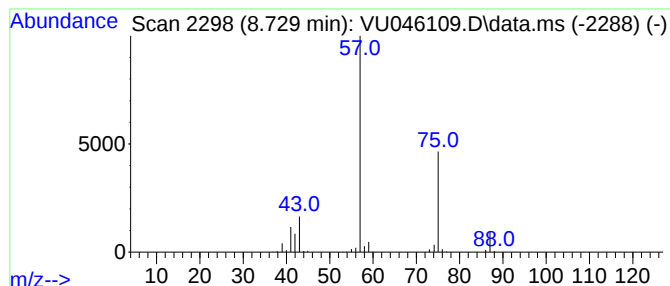
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	25.23 ug/L	300684	Chlorobenzene-d5	9.420

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\VU120621\
Data File : VU046109.D
Acq On : 06 Dec 2021 14:12
Operator : SY/MD
Sample : PB141182TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB182

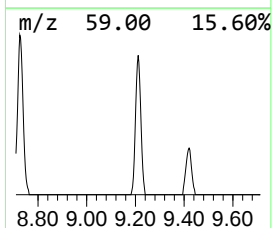
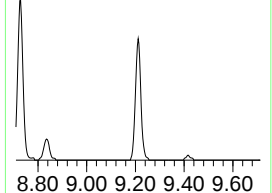
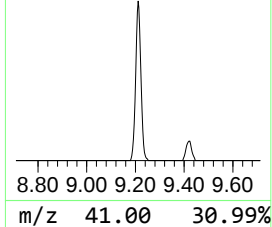
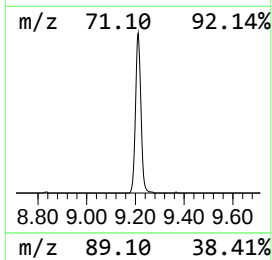
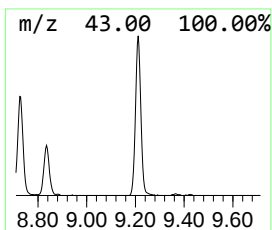
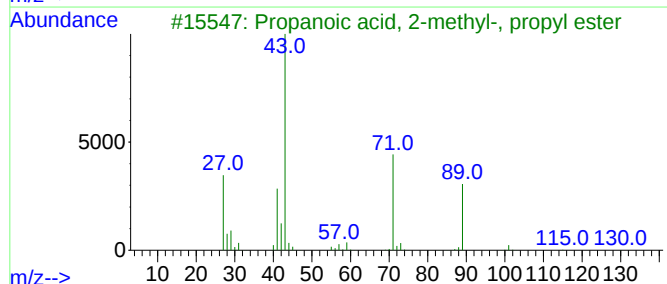
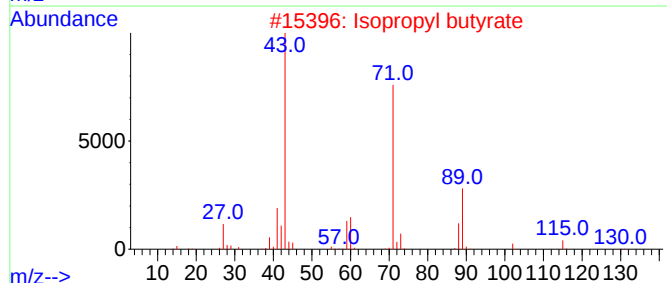
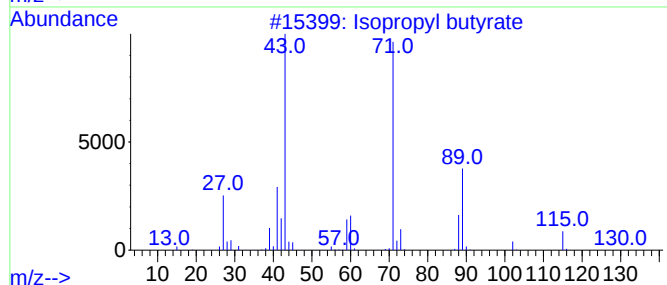
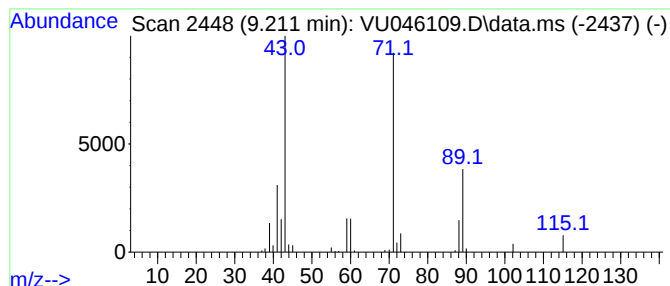
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Quant Title : VOC Analysis

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.
9.211	12.41 ug/L	147931	Chlorobenzene-d5	9.420

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			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046109.D
Acq On : 06 Dec 2021 14:12
Operator : SY/MD
Sample : PB141182TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB182

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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	20.9	ug/L	199246	1	6.250	477521	50.0
Propanoic acid,...	7.738	2.9	ug/L	27230	1	6.250	477521	50.0
Propanoic acid,...	8.729	25.2	ug/L	300684	2	9.420	595828	50.0
Isopropyl butyrate	9.211	12.4	ug/L	147931	2	9.420	595828	50.0