

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046116.D
 Acq On : 06 Dec 2021 17:12
 Operator : SY/MD
 Sample : M4938-04 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8E0

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: VU046116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	4	7	15	rVB3	3228	2713	0.34%	0.038%
2	1.600	73	81	90	rBV	98291	107458	13.38%	1.497%
3	1.916	170	179	192	rBV	69383	88847	11.06%	1.238%
4	2.137	244	248	249	rBV	630	465	0.06%	0.006%
5	2.202	266	268	273	rVB3	309	233	0.03%	0.003%
6	2.375	319	322	328	rBV3	349	378	0.05%	0.005%
7	2.571	371	383	400	rBV	172027	284847	35.46%	3.967%
8	2.797	445	453	466	rVV	1908	3413	0.42%	0.048%
9	2.867	472	475	481	rVB2	334	217	0.03%	0.003%
10	2.961	498	504	510	rBV	271	366	0.05%	0.005%
11	3.051	522	532	543	rVV3	5535	10054	1.25%	0.140%
12	3.189	564	575	586	rBV	1952	3939	0.49%	0.055%
13	3.359	621	628	635	rVB2	864	1374	0.17%	0.019%
14	3.568	689	693	695	rBV	214	197	0.02%	0.003%
15	3.832	769	775	776	rBV2	720	787	0.10%	0.011%
16	3.967	814	817	822	rVB2	278	231	0.03%	0.003%
17	4.263	903	909	910	rVV2	168	180	0.02%	0.003%
18	4.523	987	990	993	rBV2	317	261	0.03%	0.004%
19	4.632	1009	1024	1049	rBV	79500	203274	25.31%	2.831%
20	4.970	1126	1129	1132	rBV	174	183	0.02%	0.003%
21	5.067	1142	1159	1183	rBV	136571	311642	38.80%	4.341%
22	5.173	1189	1192	1194	rBV3	284	187	0.02%	0.003%
23	5.279	1222	1225	1226	rBV	439	268	0.03%	0.004%
24	5.388	1256	1259	1265	rVV3	225	282	0.04%	0.004%
25	5.530	1298	1303	1304	rBV2	402	340	0.04%	0.005%
26	5.729	1342	1365	1387	rBV2	295517	803184	100.00%	11.187%
27	5.822	1392	1394	1397	rBV3	412	304	0.04%	0.004%
28	5.915	1417	1423	1434	rVB3	1469	2216	0.28%	0.031%
29	6.115	1481	1485	1490	rVB2	324	267	0.03%	0.004%
30	6.250	1512	1527	1550	rBV	240459	451738	56.24%	6.292%
31	6.542	1605	1618	1633	rVB	42887	82490	10.27%	1.149%
32	6.694	1650	1665	1682	rBV	182600	353809	44.05%	4.928%
33	6.890	1721	1726	1728	rBV2	424	444	0.06%	0.006%
34	6.928	1733	1738	1740	rBV2	625	602	0.07%	0.008%
35	7.041	1761	1773	1789	rBV	106450	185095	23.05%	2.578%
36	7.420	1889	1891	1896	rVB2	302	276	0.03%	0.004%

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

37	7.568	1922	1937	1950	rBV	108122	184353	22.95%	2.568%
38	7.738	1980	1990	2000	rBV	15386	25428	3.17%	0.354%
39	7.796	2002	2008	2018	rVB5	1617	2362	0.29%	0.033%
40	7.899	2026	2040	2056	rBV	390917	669587	83.37%	9.326%
41	8.179	2111	2127	2147	rBV	73894	125174	15.58%	1.743%
42	8.340	2172	2177	2180	rBV3	275	240	0.03%	0.003%
43	8.401	2192	2196	2198	rBV2	689	592	0.07%	0.008%
44	8.465	2208	2216	2225	rVB	4101	5625	0.70%	0.078%
45	8.555	2234	2244	2257	rVV4	33810	70466	8.77%	0.981%
46	8.632	2257	2268	2287	rVV	243306	421180	52.44%	5.866%
47	8.729	2288	2298	2320	rVV	174738	273962	34.11%	3.816%
48	8.835	2320	2331	2342	rVB	16745	26709	3.33%	0.372%
49	8.918	2348	2357	2366	rBV7	1247	2049	0.26%	0.029%
50	9.160	2429	2432	2433	rBV7	306	179	0.02%	0.002%
51	9.211	2438	2448	2464	rVV	88770	133033	16.56%	1.853%
52	9.356	2491	2493	2496	rBV	260	222	0.03%	0.003%
53	9.417	2496	2512	2535	rVV	338949	566546	70.54%	7.891%
54	9.571	2551	2560	2569	rBV2	2700	4130	0.51%	0.058%
55	9.648	2581	2584	2588	rVB2	308	211	0.03%	0.003%
56	9.697	2588	2599	2610	rBV3	3650	5898	0.73%	0.082%
57	10.076	2708	2717	2721	rBV3	2701	4113	0.51%	0.057%
58	10.115	2722	2729	2737	rVB4	3572	6079	0.76%	0.085%
59	10.439	2826	2830	2835	rBV2	218	207	0.03%	0.003%
60	10.488	2835	2845	2851	rBV	2168	3072	0.38%	0.043%
61	10.671	2896	2902	2909	rBB2	1843	2352	0.29%	0.033%
62	10.758	2916	2929	2945	rBV	261154	417801	52.02%	5.819%
63	10.825	2947	2950	2956	rVB3	814	895	0.11%	0.012%
64	10.999	3001	3004	3010	rBV3	461	503	0.06%	0.007%
65	11.089	3025	3032	3042	rBV3	2099	3265	0.41%	0.045%
66	11.468	3139	3150	3162	rVB3	3806	6530	0.81%	0.091%
67	11.539	3167	3172	3176	rVB3	606	658	0.08%	0.009%
68	11.578	3178	3184	3187	rBV	490	451	0.06%	0.006%
69	11.700	3214	3222	3229	rVB4	1001	1308	0.16%	0.018%
70	11.748	3229	3237	3244	rVB5	3042	4021	0.50%	0.056%
71	11.812	3244	3257	3273	rBV	385592	607517	75.64%	8.462%
72	11.941	3294	3297	3300	rVV3	835	747	0.09%	0.010%
73	11.970	3303	3306	3315	rVB4	1383	1749	0.22%	0.024%
74	12.063	3331	3335	3336	rBV	242	180	0.02%	0.003%
75	12.195	3359	3376	3392	rBV	398735	642362	79.98%	8.947%
76	12.324	3406	3416	3424	rVB6	1136	1955	0.24%	0.027%

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 Title : VOC Analysis

77	12.397	3436	3439	3443	rVB	275	226	0.03%	0.003%
78	12.549	3482	3486	3489	rBV2	265	236	0.03%	0.003%
79	13.002	3621	3627	3633	rVB4	836	904	0.11%	0.013%
80	13.060	3641	3645	3651	rVB2	263	295	0.04%	0.004%
81	13.153	3671	3674	3679	rVB2	268	236	0.03%	0.003%
82	13.221	3687	3695	3703	rBV2	4042	5630	0.70%	0.078%
83	13.368	3737	3741	3744	rBV2	313	232	0.03%	0.003%
84	13.844	3880	3889	3899	rVB3	5521	8215	1.02%	0.114%
85	14.089	3953	3965	3978	rBV	13128	20553	2.56%	0.286%
86	14.333	4032	4041	4052	rBV2	6634	9577	1.19%	0.133%
87	14.468	4080	4083	4088	rBV2	207	193	0.02%	0.003%
88	14.568	4111	4114	4115	rBV2	478	277	0.03%	0.004%
89	14.616	4127	4129	4133	rVB2	365	191	0.02%	0.003%
90	14.648	4136	4139	4142	rBV2	237	200	0.02%	0.003%
91	14.809	4186	4189	4198	rBV3	259	337	0.04%	0.005%
92	14.909	4216	4220	4222	rBV2	271	192	0.02%	0.003%
93	15.057	4262	4266	4268	rBV	352	303	0.04%	0.004%
94	15.230	4312	4320	4328	rVB3	1673	2650	0.33%	0.037%
95	15.413	4372	4377	4384	rVB5	932	1232	0.15%	0.017%
96	15.526	4410	4412	4415	rBV2	303	183	0.02%	0.003%
97	15.725	4471	4474	4477	rBV3	319	210	0.03%	0.003%
98	15.960	4545	4547	4552	rVB3	756	588	0.07%	0.008%
99	16.108	4590	4593	4596	rBV2	380	285	0.04%	0.004%
100	16.262	4638	4641	4642	rBV	587	298	0.04%	0.004%

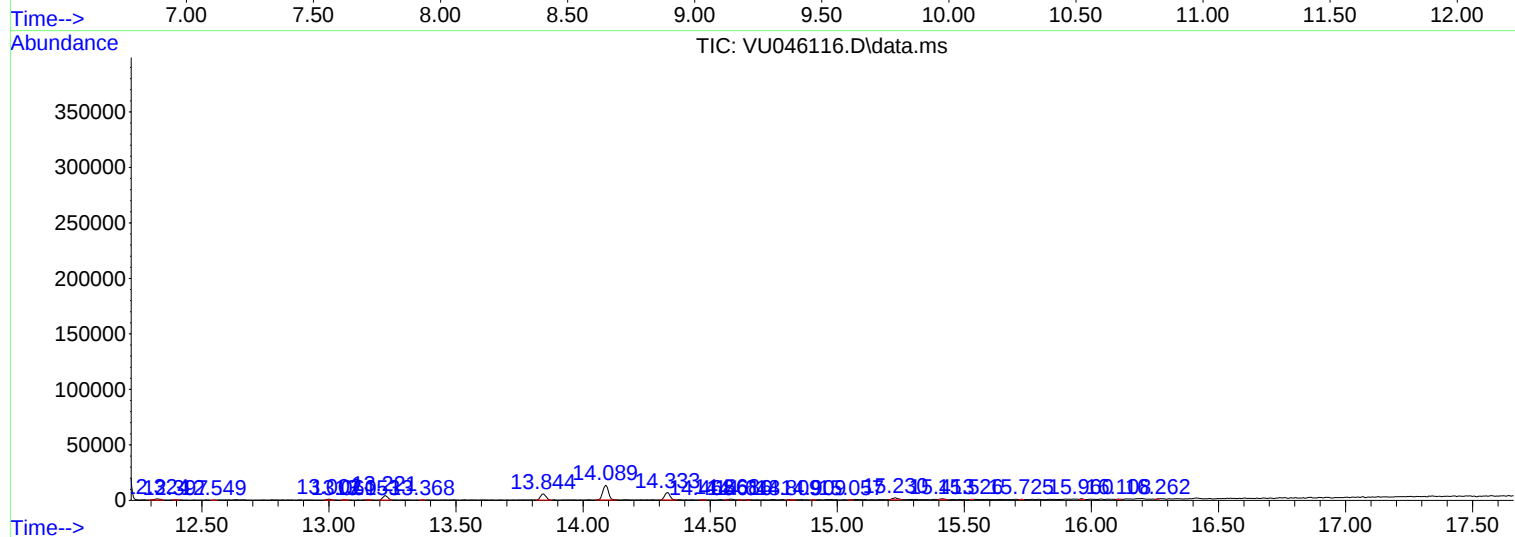
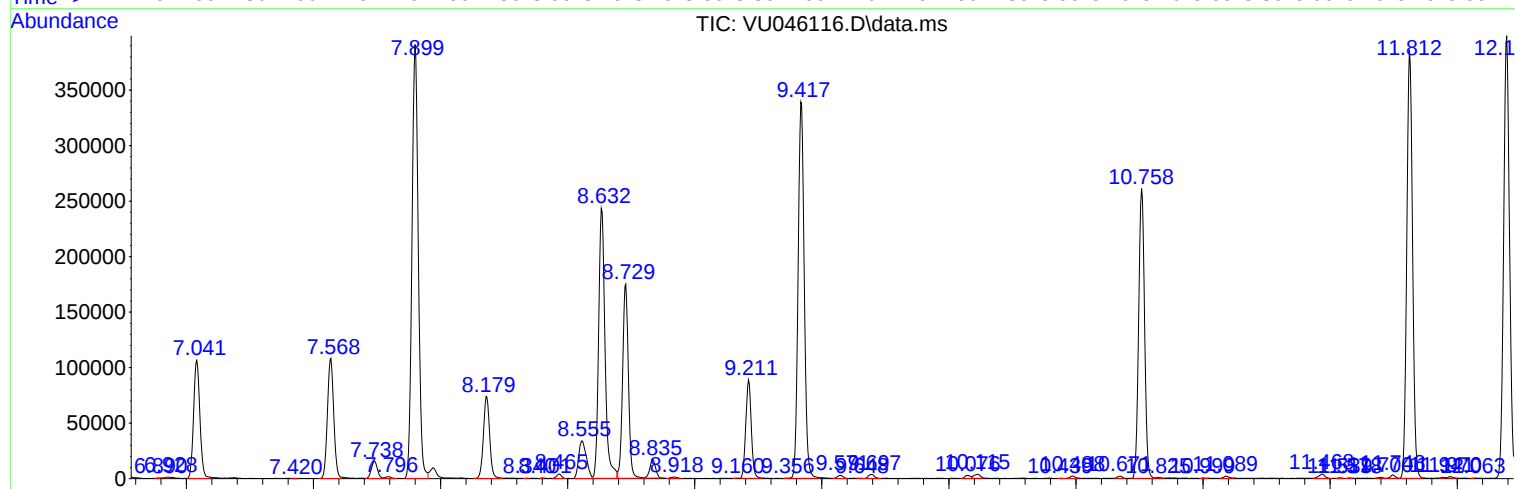
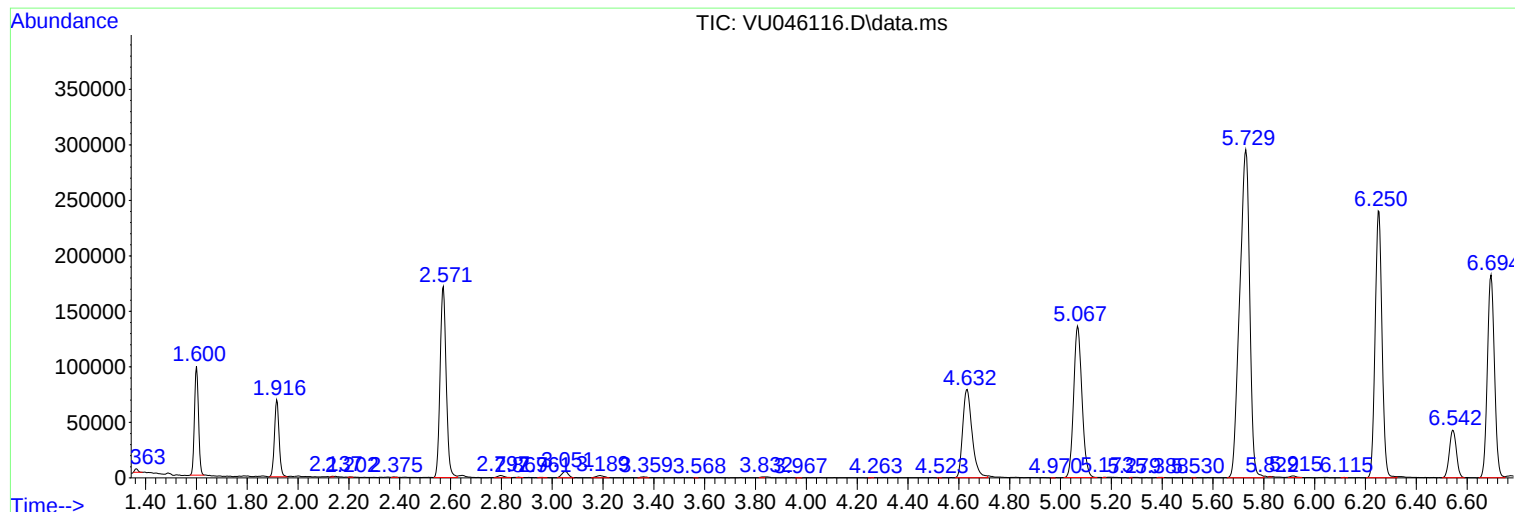
Sum of corrected areas: 7179515

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Instrument :
MSVOA_U
ClientSampleId :
EX8E0

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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EX8E0

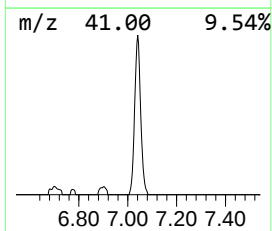
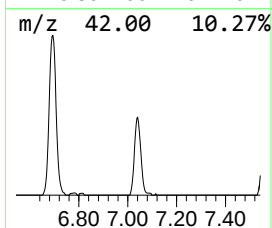
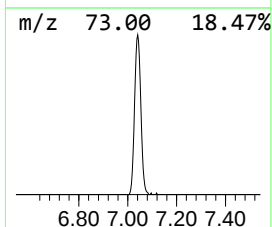
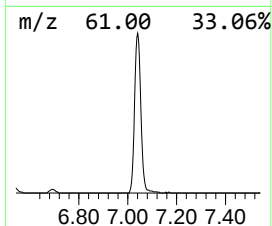
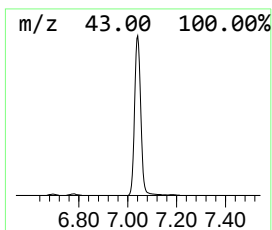
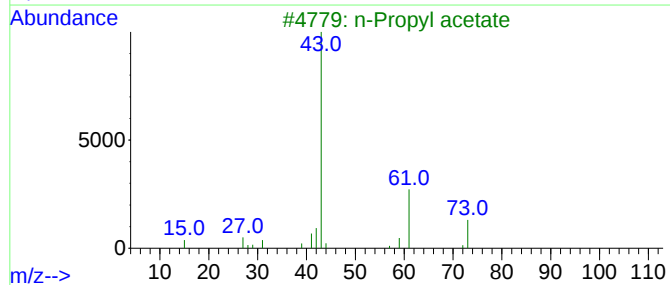
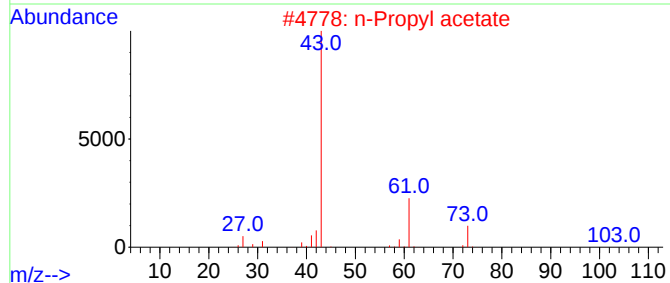
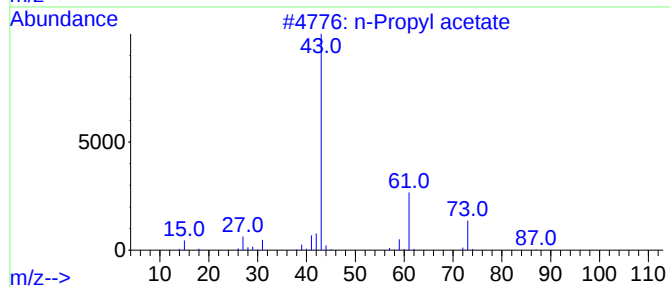
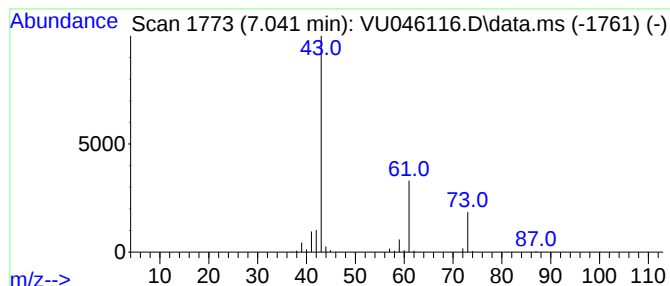
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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	20.49 ug/L	185095	1,4-Difluorobenzene	6.253

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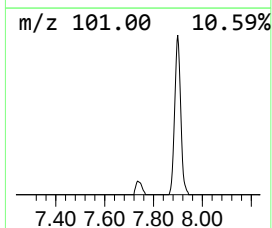
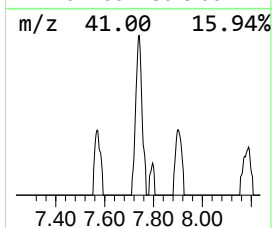
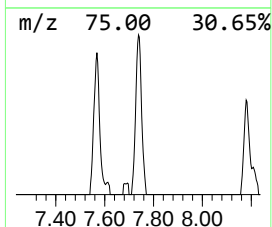
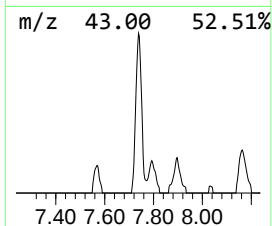
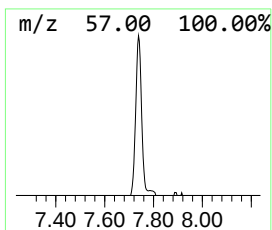
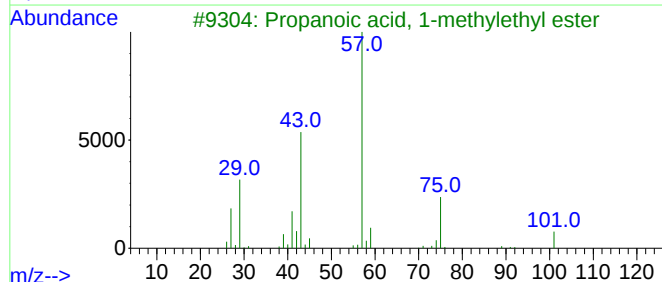
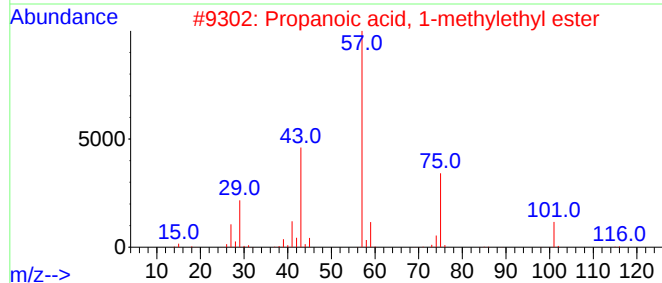
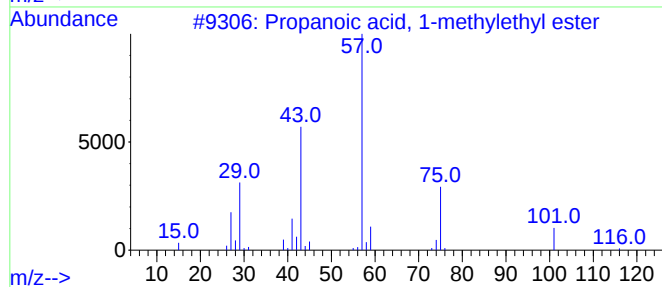
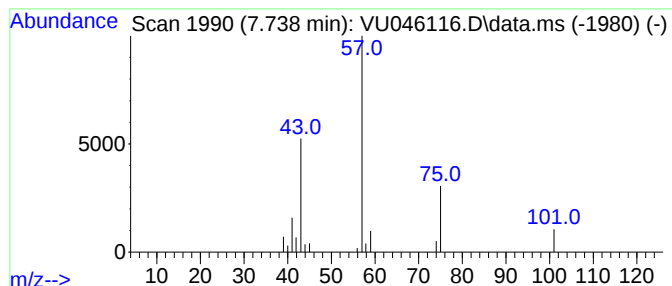
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.81 ug/L	25428	1,4-Difluorobenzene	6.253

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	83
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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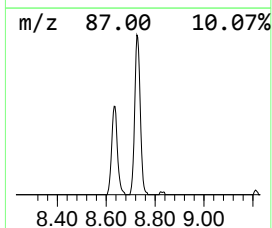
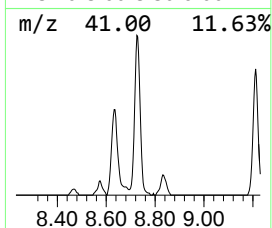
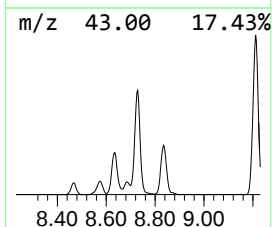
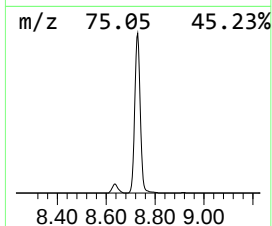
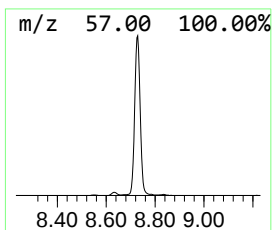
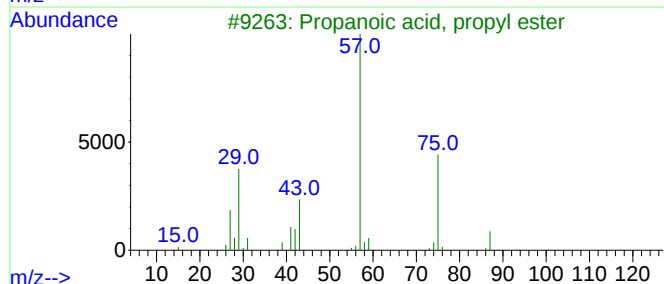
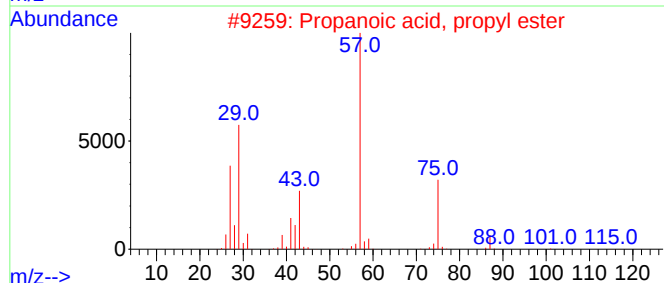
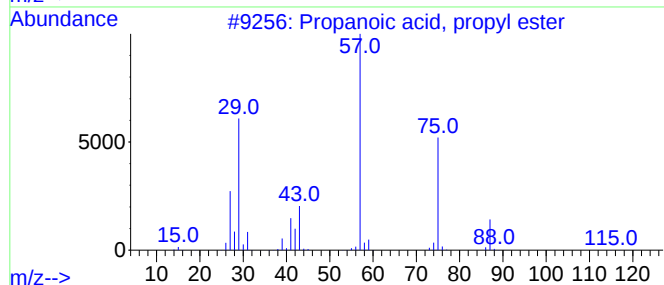
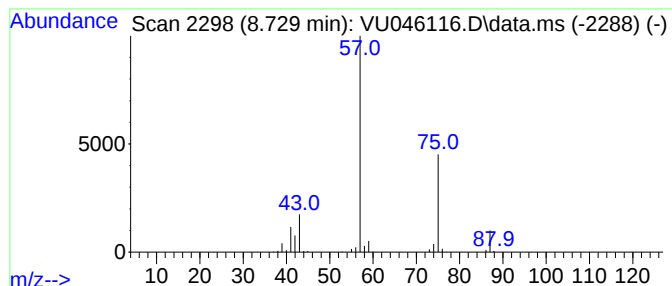
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	24.18 ug/L	273962	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\VU120621\
Data File : VU046116.D
Acq On : 06 Dec 2021 17:12
Operator : SY/MD
Sample : M4938-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8E0

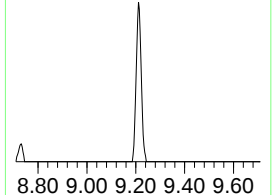
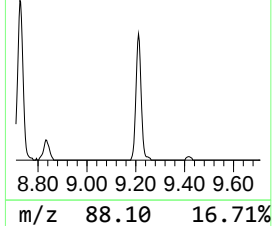
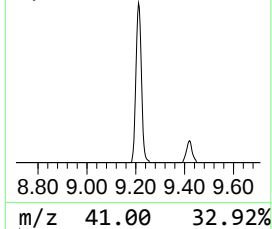
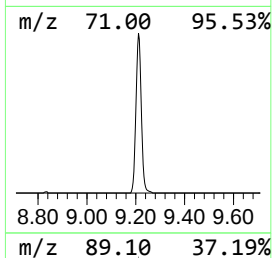
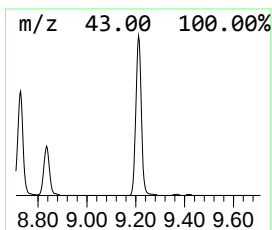
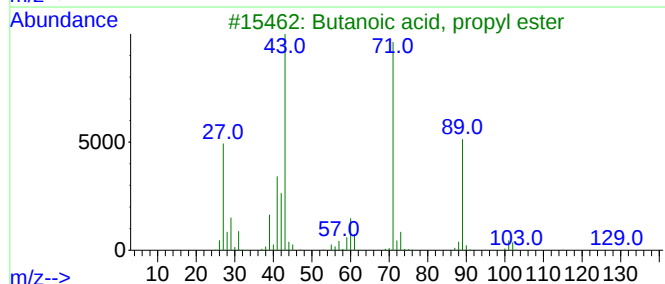
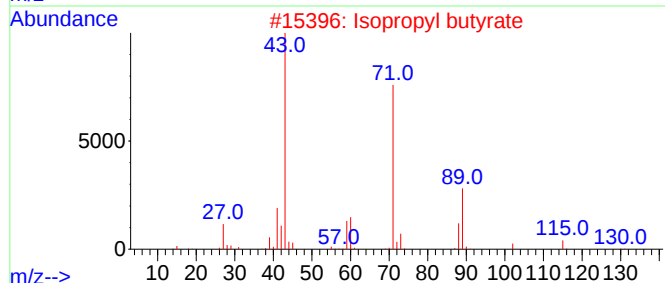
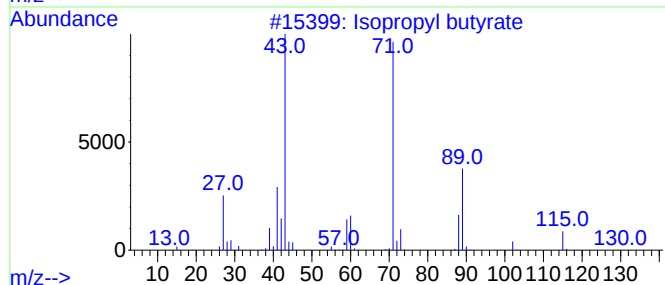
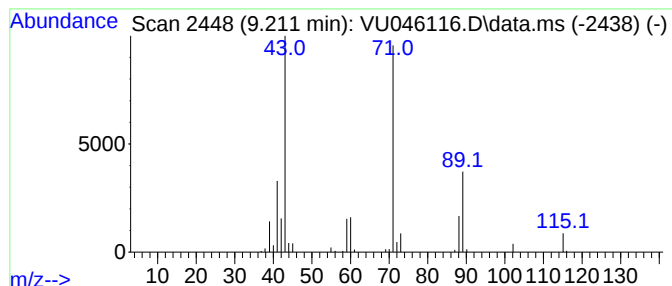
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	11.74 ug/L	133033	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			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046116.D
Acq On : 06 Dec 2021 17:12
Operator : SY/MD
Sample : M4938-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8E0

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	20.5	ug/L	185095	1	6.253	451738	50.0
Propanoic acid,...	7.738	2.8	ug/L	25428	1	6.253	451738	50.0
Propanoic acid,...	8.729	24.2	ug/L	273962	2	9.417	566546	50.0
Isopropyl butyrate	9.211	11.7	ug/L	133033	2	9.417	566546	50.0