

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046112.D
 Acq On : 06 Dec 2021 15:19
 Operator : SY/MD
 Sample : M4938-03 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8D9

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: VU046112.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	14	rVB3	3205	3052	0.34%	0.041%
2	1.601	73	81	92	rVB	110258	120698	13.28%	1.610%
3	1.916	170	179	193	rBV	78923	100193	11.03%	1.336%
4	2.417	333	335	340	rVB2	309	215	0.02%	0.003%
5	2.456	344	347	349	rBV	262	190	0.02%	0.003%
6	2.510	360	364	370	rBV2	182	251	0.03%	0.003%
7	2.572	370	383	400	rBV	194448	323421	35.59%	4.314%
8	2.742	433	436	442	rVB	216	170	0.02%	0.002%
9	2.838	458	466	469	rBV2	338	571	0.06%	0.008%
10	3.051	521	532	542	rVB2	5296	8834	0.97%	0.118%
11	3.189	564	575	590	rVB2	2556	5542	0.61%	0.074%
12	3.440	650	653	659	rBV2	157	154	0.02%	0.002%
13	3.835	770	776	781	rBV3	601	825	0.09%	0.011%
14	4.063	844	847	850	rVV2	201	147	0.02%	0.002%
15	4.282	912	915	918	rBV	209	174	0.02%	0.002%
16	4.369	938	942	946	rBV	320	301	0.03%	0.004%
17	4.633	1009	1024	1049	rBV	89128	229981	25.31%	3.068%
18	4.912	1107	1111	1114	rVB2	374	304	0.03%	0.004%
19	5.067	1140	1159	1181	rBV	156277	357397	39.33%	4.767%
20	5.186	1190	1196	1200	rVV3	329	399	0.04%	0.005%
21	5.247	1211	1215	1219	rBV2	289	217	0.02%	0.003%
22	5.292	1224	1229	1232	rBV3	300	281	0.03%	0.004%
23	5.334	1237	1242	1246	rBB	176	213	0.02%	0.003%
24	5.362	1246	1251	1254	rBV	208	246	0.03%	0.003%
25	5.379	1254	1256	1258	rBV2	256	138	0.02%	0.002%
26	5.729	1342	1365	1382	rBV2	339423	908749	100.00%	12.122%
27	5.912	1413	1422	1431	rBV5	1390	2478	0.27%	0.033%
28	6.018	1452	1455	1457	rVB	249	183	0.02%	0.002%
29	6.034	1457	1460	1465	rBV3	376	351	0.04%	0.005%
30	6.250	1512	1527	1546	rBV	228804	430779	47.40%	5.746%
31	6.536	1605	1616	1630	rBV5	4952	10533	1.16%	0.140%
32	6.694	1650	1665	1681	rBV	208399	403302	44.38%	5.380%
33	6.925	1727	1737	1741	rBV3	1012	1434	0.16%	0.019%
34	6.993	1755	1758	1760	rBV	168	143	0.02%	0.002%
35	7.041	1760	1773	1791	rBV	107560	188020	20.69%	2.508%
36	7.179	1813	1816	1817	rBV2	437	255	0.03%	0.003%

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 Title : VOC Analysis

37	7.378	1874	1878	1881	rBV2	179	191	0.02%	0.003%
38	7.446	1896	1899	1901	rBV	288	194	0.02%	0.003%
39	7.568	1920	1937	1959	rBV	121745	212039	23.33%	2.828%
40	7.739	1980	1990	2002	rBV	15904	26199	2.88%	0.349%
41	7.793	2003	2007	2012	rVB3	634	538	0.06%	0.007%
42	7.899	2027	2040	2056	rBV	447491	767963	84.51%	10.244%
43	8.179	2114	2127	2145	rBV	83997	139336	15.33%	1.859%
44	8.279	2155	2158	2159	rBV2	378	176	0.02%	0.002%
45	8.465	2207	2216	2226	rVB2	3676	5646	0.62%	0.075%
46	8.565	2232	2247	2248	rBV3	12956	18625	2.05%	0.248%
47	8.632	2257	2268	2288	rBV	268246	471374	51.87%	6.288%
48	8.729	2288	2298	2318	rVV	174307	274188	30.17%	3.657%
49	8.835	2322	2331	2349	rVB	16629	26987	2.97%	0.360%
50	8.915	2349	2356	2363	rBV3	1277	1789	0.20%	0.024%
51	9.102	2410	2414	2417	rVB2	229	149	0.02%	0.002%
52	9.163	2430	2433	2437	rBV2	224	138	0.02%	0.002%
53	9.211	2437	2448	2467	rVV	83784	130501	14.36%	1.741%
54	9.420	2500	2513	2533	rBV	323578	541759	59.62%	7.226%
55	9.571	2554	2560	2561	rBV2	500	424	0.05%	0.006%
56	9.629	2575	2578	2583	rVB2	185	174	0.02%	0.002%
57	9.697	2591	2599	2606	rVB	997	1462	0.16%	0.020%
58	9.812	2632	2635	2640	rBV2	163	144	0.02%	0.002%
59	9.835	2640	2642	2649	rVB	211	144	0.02%	0.002%
60	9.928	2668	2671	2676	rVB2	266	228	0.03%	0.003%
61	10.076	2709	2717	2723	rBV	2765	3498	0.38%	0.047%
62	10.192	2751	2753	2758	rVB2	267	181	0.02%	0.002%
63	10.382	2810	2812	2818	rVB	206	176	0.02%	0.002%
64	10.478	2839	2842	2847	rVB2	211	181	0.02%	0.002%
65	10.581	2871	2874	2878	rVB2	181	168	0.02%	0.002%
66	10.671	2894	2902	2912	rBV5	2149	3355	0.37%	0.045%
67	10.758	2916	2929	2948	rBV	295460	469241	51.64%	6.259%
68	10.857	2957	2960	2961	rBV	278	148	0.02%	0.002%
69	10.870	2961	2964	2967	rVB	327	231	0.03%	0.003%
70	10.999	3001	3004	3007	rBV2	321	245	0.03%	0.003%
71	11.086	3026	3031	3032	rBV2	273	201	0.02%	0.003%
72	11.115	3037	3040	3042	rBV2	427	247	0.03%	0.003%
73	11.150	3047	3051	3056	rVB2	300	311	0.03%	0.004%
74	11.201	3065	3067	3074	rVB2	304	192	0.02%	0.003%
75	11.462	3139	3148	3156	rVB4	1987	3094	0.34%	0.041%
76	11.587	3179	3187	3188	rBV2	265	335	0.04%	0.004%

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 Title : VOC Analysis

77	11.697	3214	3221	3231	rVB4	961	1241	0.14%	0.017%
78	11.812	3244	3257	3277	rBV	361599	567201	62.42%	7.566%
79	11.935	3287	3295	3296	rBV	483	372	0.04%	0.005%
80	11.970	3303	3306	3317	rVB3	1675	2196	0.24%	0.029%
81	12.195	3361	3376	3394	rVV	448282	716171	78.81%	9.553%
82	12.333	3413	3419	3424	rVB3	558	610	0.07%	0.008%
83	12.372	3429	3431	3439	rVB2	272	304	0.03%	0.004%
84	12.478	3461	3464	3468	rBV2	140	137	0.02%	0.002%
85	12.594	3496	3500	3504	rVB	244	203	0.02%	0.003%
86	12.645	3510	3516	3519	rBV	395	441	0.05%	0.006%
87	12.767	3551	3554	3557	rBV2	272	199	0.02%	0.003%
88	13.108	3656	3660	3665	rBV	213	282	0.03%	0.004%
89	13.629	3816	3822	3825	rBV2	243	268	0.03%	0.004%
90	14.053	3951	3954	3957	rVB	250	163	0.02%	0.002%
91	14.092	3959	3966	3972	rVV2	714	1083	0.12%	0.014%
92	14.465	4079	4082	4084	rBV2	227	145	0.02%	0.002%
93	14.581	4110	4118	4121	rBV2	531	774	0.09%	0.010%
94	14.983	4241	4243	4248	rVB	276	153	0.02%	0.002%
95	15.137	4288	4291	4295	rBV2	309	279	0.03%	0.004%
96	15.230	4316	4320	4325	rVB2	1400	1350	0.15%	0.018%
97	15.410	4373	4376	4381	rVB4	515	435	0.05%	0.006%
98	15.902	4527	4529	4533	rVB	336	171	0.02%	0.002%
99	15.957	4543	4546	4549	rBV2	390	223	0.02%	0.003%
100	16.057	4574	4577	4579	rBV3	377	214	0.02%	0.003%

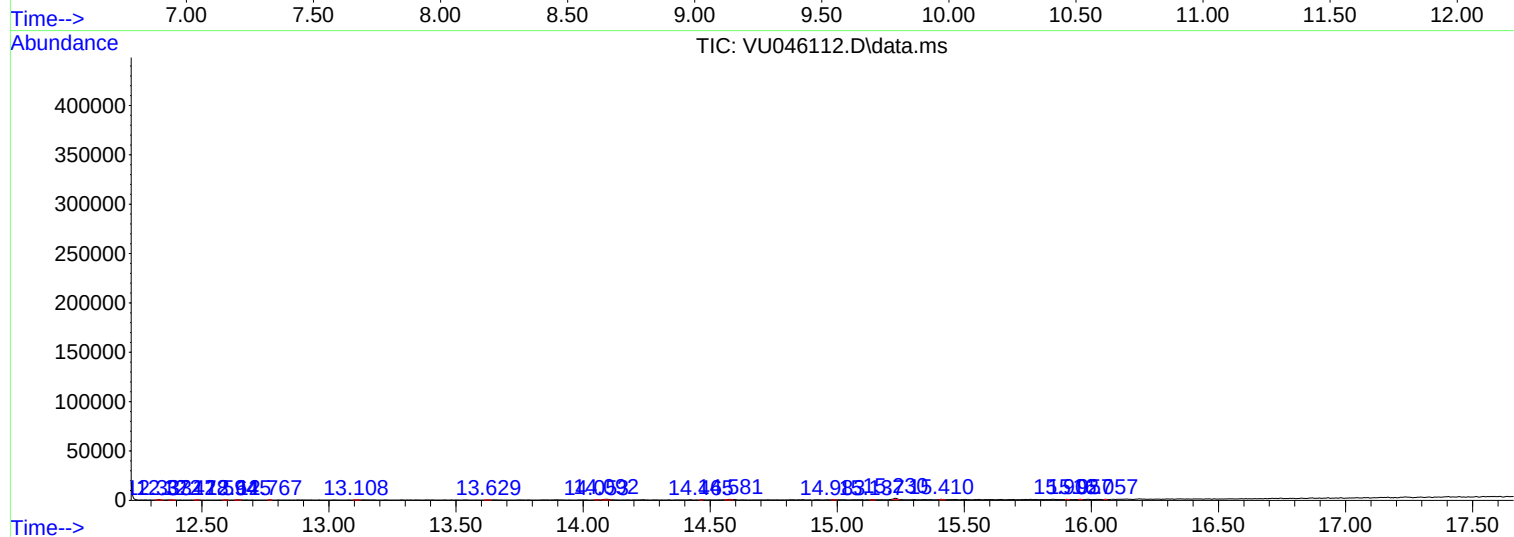
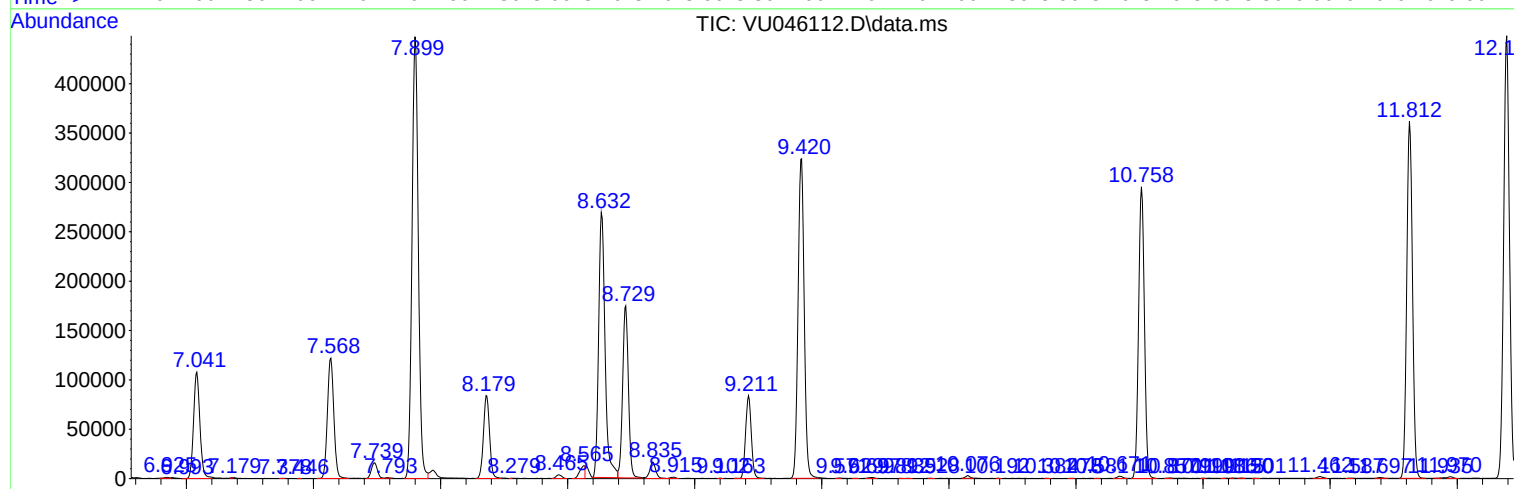
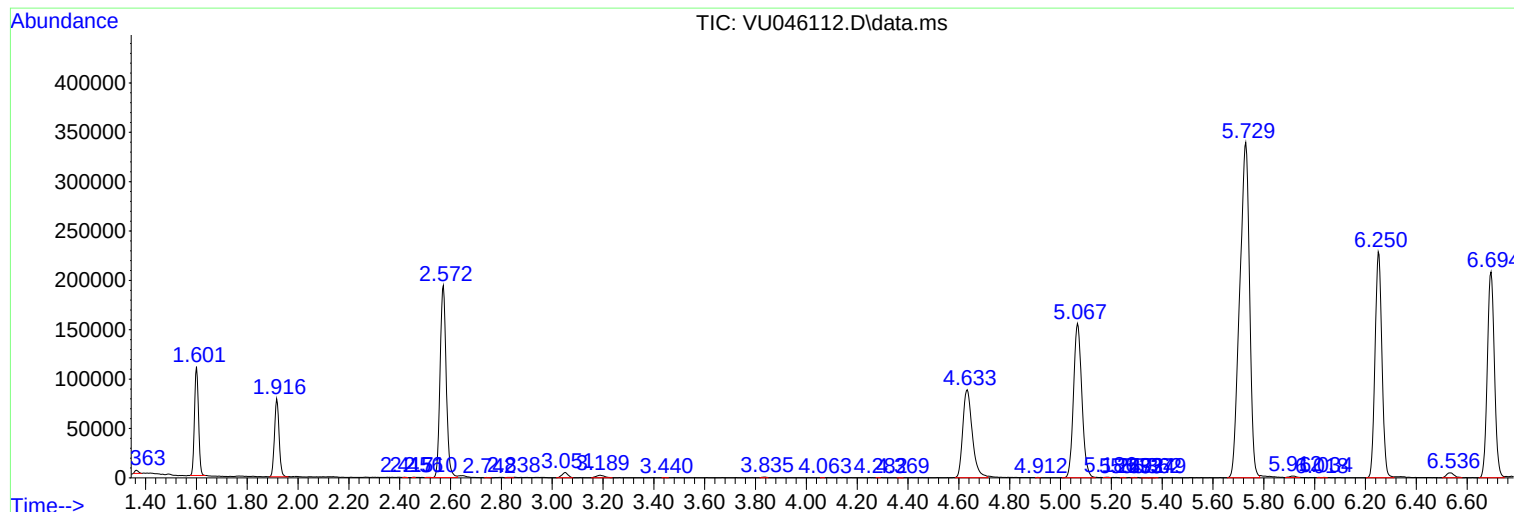
Sum of corrected areas: 7496928

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ClientSampleId :
EX8D9

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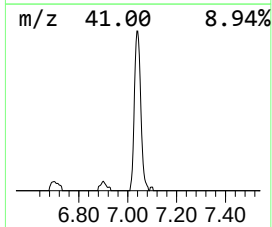
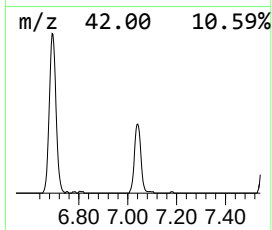
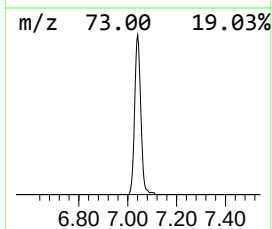
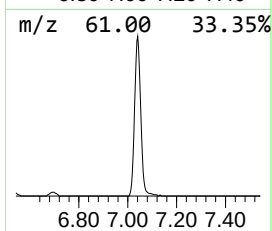
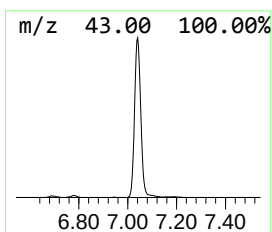
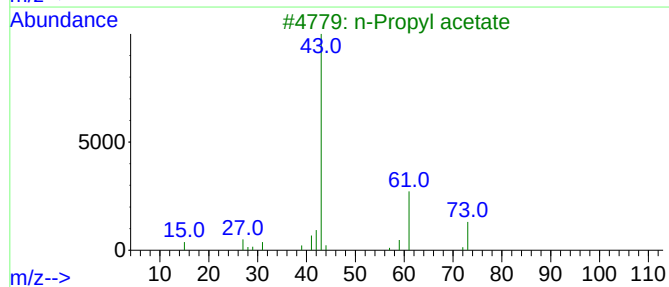
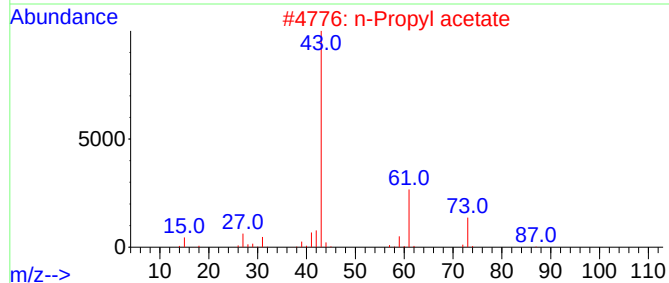
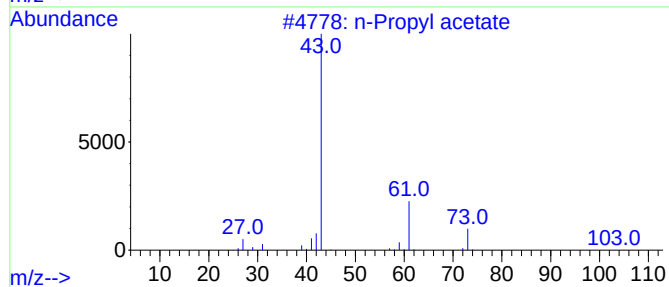
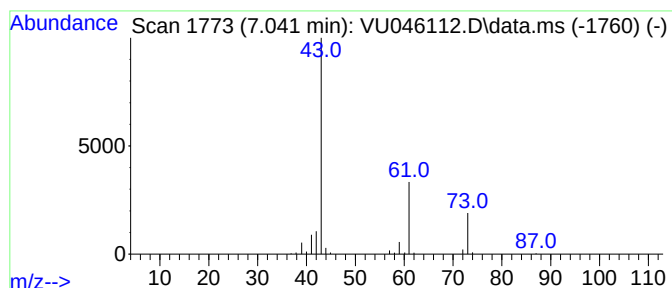
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	21.82 ug/L	188020	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	72
5		Isopropyl acetate	102	C5H10O2	000108-21-4	28



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Instrument :
MSVOA_U
ClientSampleId :
EX8D9

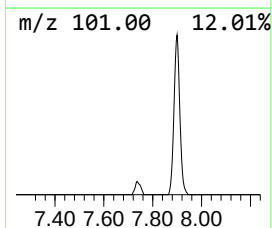
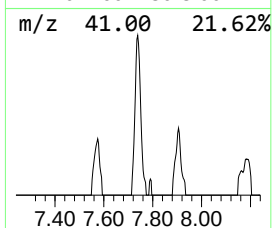
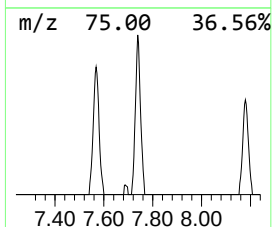
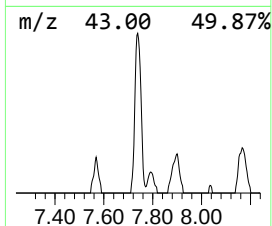
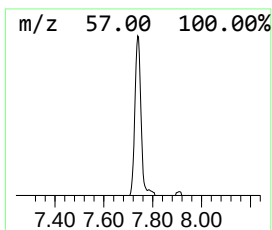
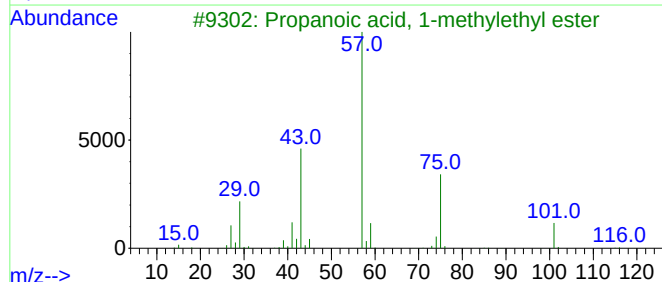
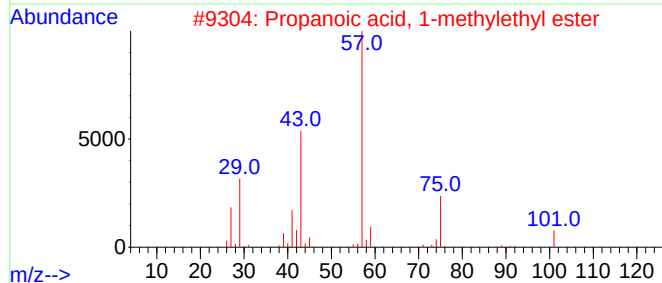
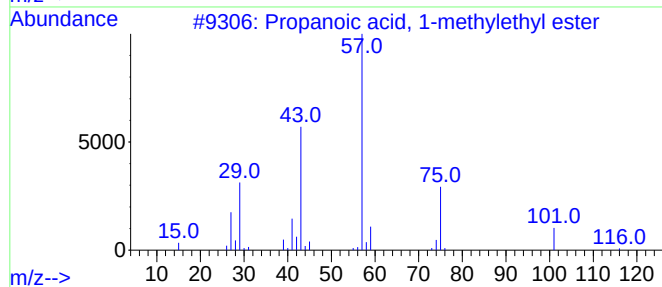
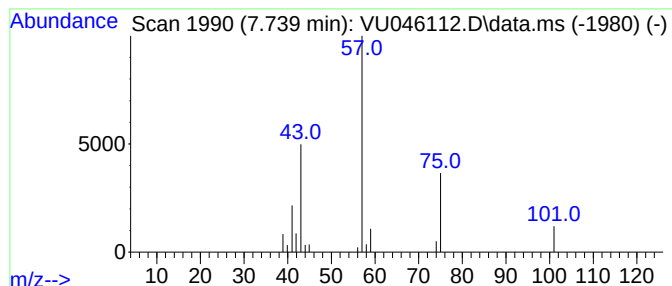
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
7.739	3.04 ug/L	26199	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	74
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42



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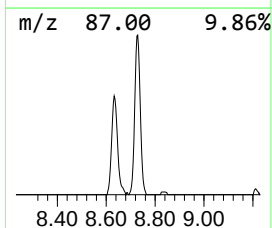
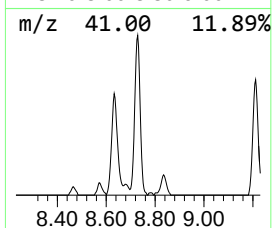
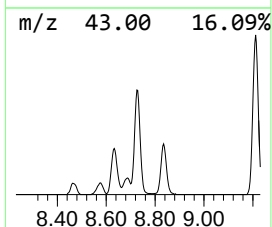
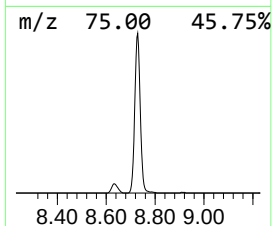
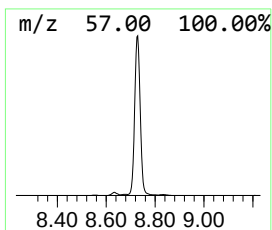
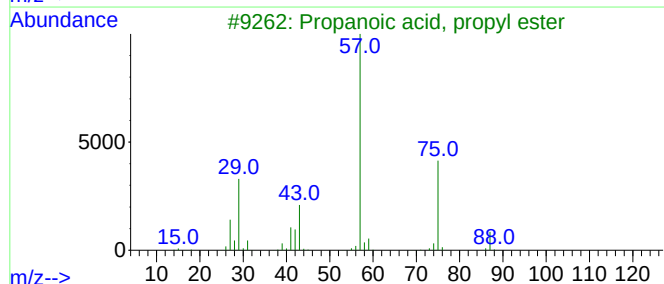
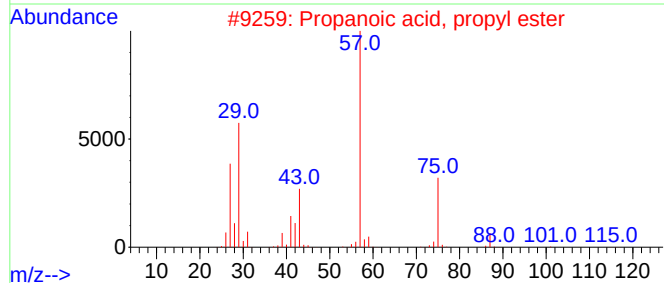
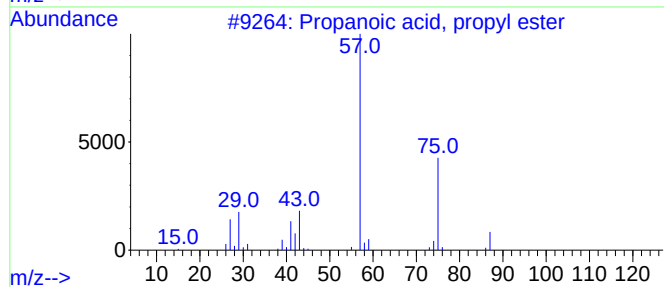
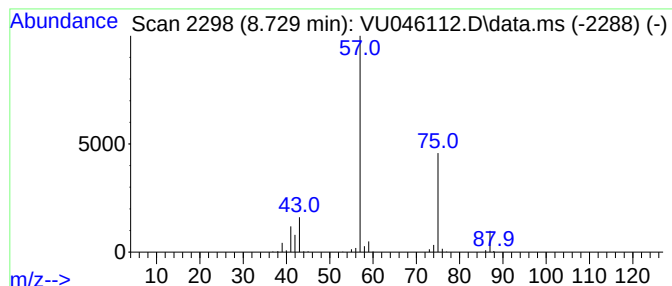
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	25.31 ug/L	274188	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	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046112.D
Acq On : 06 Dec 2021 15:19
Operator : SY/MD
Sample : M4938-03 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8D9

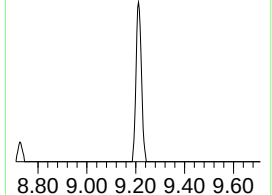
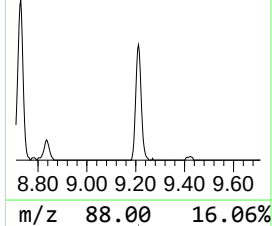
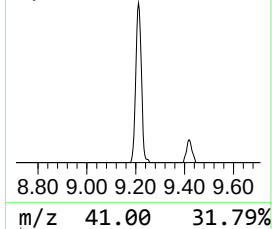
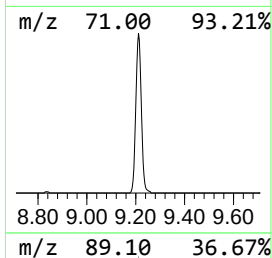
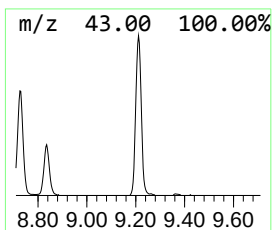
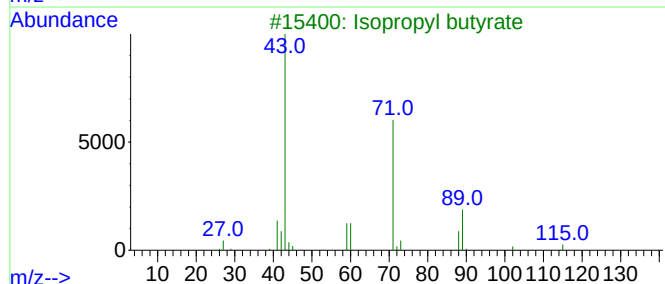
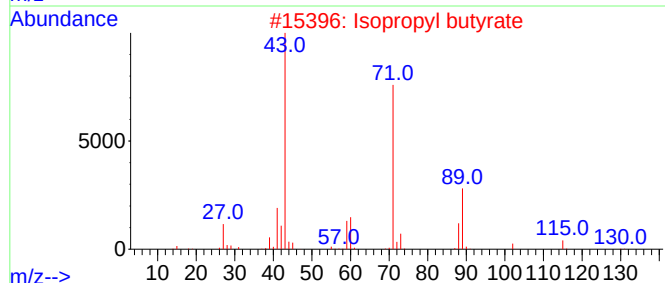
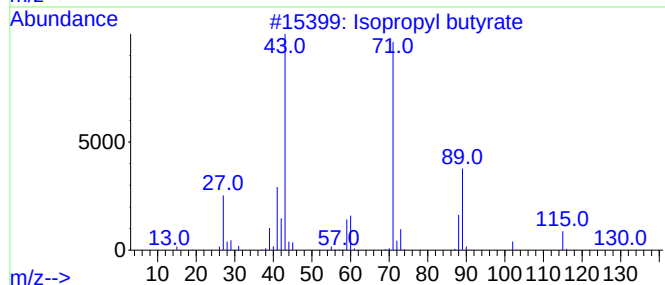
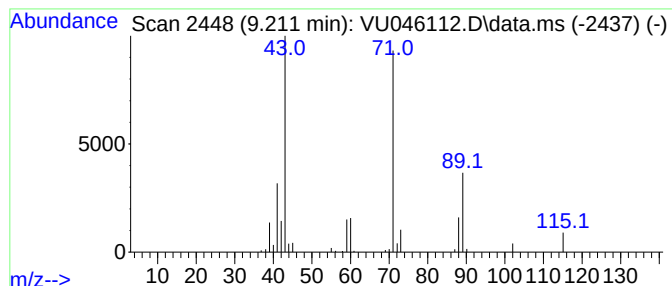
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Quant Title : VOC Analysis

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	12.04 ug/L	130501	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046112.D
Acq On : 06 Dec 2021 15:19
Operator : SY/MD
Sample : M4938-03 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8D9

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	21.8	ug/L	188020	1	6.250	430779	50.0
Propanoic acid,...	7.739	3.0	ug/L	26199	1	6.250	430779	50.0
Propanoic acid,...	8.729	25.3	ug/L	274188	2	9.420	541759	50.0
Isopropyl butyrate	9.211	12.0	ug/L	130501	2	9.420	541759	50.0