

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
 Data File : VU055769.D
 Acq On : 16 Oct 2023 14:00
 Operator : MD/SY
 Sample : PB156381TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB381

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055769.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	110	rBV	206382	244075	13.10%	1.661%
2	1.891	179	187	205	rVB	174869	250548	13.45%	1.705%
3	2.560	381	395	409	rBV	359831	591527	31.75%	4.025%
4	2.779	460	463	465	rBV2	914	582	0.03%	0.004%
5	2.875	490	493	495	rVB	465	290	0.02%	0.002%
6	2.946	512	515	520	rBV3	613	511	0.03%	0.003%
7	2.969	520	522	525	rVB2	500	289	0.02%	0.002%
8	3.039	533	544	557	rBV3	9868	18748	1.01%	0.128%
9	3.181	578	588	596	rBV4	5091	9944	0.53%	0.068%
10	3.460	672	675	678	rBV3	452	282	0.02%	0.002%
11	3.505	685	689	694	rVB2	348	322	0.02%	0.002%
12	3.592	712	716	720	rBV3	294	268	0.01%	0.002%
13	3.644	727	732	735	rBV2	437	383	0.02%	0.003%
14	3.689	743	746	750	rBV2	365	320	0.02%	0.002%
15	3.753	762	766	771	rVB2	494	438	0.02%	0.003%
16	3.808	776	783	787	rBV3	332	411	0.02%	0.003%
17	3.843	787	794	795	rBV2	592	595	0.03%	0.004%
18	3.949	823	827	831	rBV2	454	485	0.03%	0.003%
19	4.190	899	902	907	rBV2	379	272	0.01%	0.002%
20	4.415	968	972	976	rVB	439	349	0.02%	0.002%
21	4.615	1022	1034	1064	rBV	134754	359094	19.27%	2.444%
22	4.952	1137	1139	1143	rVB3	535	368	0.02%	0.003%
23	5.055	1155	1171	1193	rBV	343837	765821	41.10%	5.212%
24	5.325	1244	1255	1256	rBV3	1290	1933	0.10%	0.013%
25	5.351	1262	1263	1267	rVB2	1029	514	0.03%	0.003%
26	5.718	1355	1377	1400	rBV2	667713	1863304	100.00%	12.680%
27	5.910	1428	1437	1458	rVV3	12805	28172	1.51%	0.192%
28	6.084	1489	1491	1495	rVB3	445	273	0.01%	0.002%
29	6.126	1502	1504	1508	rVB2	700	413	0.02%	0.003%
30	6.171	1515	1518	1523	rVB3	510	493	0.03%	0.003%
31	6.245	1527	1541	1563	rBV	506799	990712	53.17%	6.742%
32	6.483	1613	1615	1618	rBV	333	273	0.01%	0.002%
33	6.528	1618	1629	1643	rVV2	18532	36675	1.97%	0.250%
34	6.685	1664	1678	1704	rBV	432629	858376	46.07%	5.841%
35	6.930	1744	1754	1755	rBV	5459	6287	0.34%	0.043%
36	7.036	1776	1787	1810	rBV	131725	243176	13.05%	1.655%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	7.187	1825	1834	1842	rBV3	6167	12243	0.66%	0.083%
38	7.277	1859	1862	1864	rBV2	688	406	0.02%	0.003%
39	7.370	1886	1891	1894	rBV3	301	307	0.02%	0.002%
40	7.560	1937	1950	1978	rBV	227523	414832	22.26%	2.823%
41	7.695	1987	1992	1995	rBV4	2497	2830	0.15%	0.019%
42	7.737	1996	2005	2016	rVB2	29669	49147	2.64%	0.334%
43	7.894	2039	2054	2076	rBV	816422	1434258	76.97%	9.760%
44	8.103	2115	2119	2124	rVB6	461	443	0.02%	0.003%
45	8.174	2124	2141	2163	rBV2	174419	346792	18.61%	2.360%
46	8.299	2177	2180	2183	rBV3	401	324	0.02%	0.002%
47	8.373	2198	2203	2206	rBV3	590	491	0.03%	0.003%
48	8.425	2214	2219	2220	rBV2	485	401	0.02%	0.003%
49	8.463	2220	2231	2247	rBV	38937	65201	3.50%	0.444%
50	8.573	2251	2265	2273	rBV9	7238	16270	0.87%	0.111%
51	8.634	2273	2284	2305	rVV3	344778	826525	44.36%	5.625%
52	8.724	2307	2312	2333	rVB2	71794	121538	6.52%	0.827%
53	8.833	2338	2346	2361	rVB	37931	62153	3.34%	0.423%
54	8.984	2390	2393	2397	rVV	681	462	0.02%	0.003%
55	9.029	2403	2407	2409	rVB3	411	298	0.02%	0.002%
56	9.042	2409	2411	2417	rVB2	370	297	0.02%	0.002%
57	9.087	2419	2425	2428	rBV4	590	597	0.03%	0.004%
58	9.209	2451	2463	2475	rBV	107288	177818	9.54%	1.210%
59	9.367	2505	2512	2514	rBV3	1942	1951	0.10%	0.013%
60	9.412	2514	2526	2550	rVV	758846	1299592	69.75%	8.844%
61	9.570	2572	2575	2578	rBV4	857	560	0.03%	0.004%
62	9.621	2588	2591	2592	rBV2	510	289	0.02%	0.002%
63	9.643	2593	2598	2600	rBV3	1165	1139	0.06%	0.008%
64	9.692	2610	2613	2615	rBV2	848	624	0.03%	0.004%
65	9.798	2641	2646	2652	rBV4	654	798	0.04%	0.005%
66	9.869	2662	2668	2672	rBV2	499	400	0.02%	0.003%
67	9.923	2678	2685	2687	rBV3	1313	1439	0.08%	0.010%
68	10.023	2712	2716	2720	rBV3	492	400	0.02%	0.003%
69	10.074	2724	2732	2748	rBV5	7343	14570	0.78%	0.099%
70	10.139	2748	2752	2759	rVB3	861	951	0.05%	0.006%
71	10.422	2836	2840	2843	rBV	438	347	0.02%	0.002%
72	10.479	2855	2858	2860	rBV	419	297	0.02%	0.002%
73	10.531	2871	2874	2879	rVB2	400	347	0.02%	0.002%
74	10.650	2908	2911	2917	rVB	617	506	0.03%	0.003%
75	10.753	2930	2943	2967	rVV	643902	1063564	57.08%	7.238%
76	10.881	2981	2983	2988	rVB2	305	295	0.02%	0.002%

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Peak Location: TOP

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 Title : VOC Analysis

77	10.910	2988	2992	2993	rBV2	463	291	0.02%	0.002%
78	11.467	3162	3165	3169	rBV2	473	380	0.02%	0.003%
79	11.512	3177	3179	3185	rVB	432	287	0.02%	0.002%
80	11.669	3225	3228	3230	rBV2	611	475	0.03%	0.003%
81	11.749	3249	3253	3254	rBV2	593	361	0.02%	0.002%
82	11.811	3259	3272	3293	rBV	726597	1190297	63.88%	8.100%
83	12.106	3360	3364	3367	rVB3	667	474	0.03%	0.003%
84	12.126	3367	3370	3373	rVB	430	269	0.01%	0.002%
85	12.190	3377	3390	3410	rBV	778707	1296470	69.58%	8.823%
86	12.399	3451	3455	3456	rBV3	456	328	0.02%	0.002%
87	12.534	3494	3497	3500	rBV3	634	582	0.03%	0.004%
88	12.598	3512	3517	3521	rVV3	821	805	0.04%	0.005%
89	12.663	3534	3537	3539	rBV2	515	315	0.02%	0.002%
90	12.885	3603	3606	3612	rBV3	398	406	0.02%	0.003%
91	12.981	3633	3636	3642	rBV2	587	435	0.02%	0.003%
92	13.081	3664	3667	3670	rBV2	466	355	0.02%	0.002%
93	13.299	3732	3735	3741	rBV3	419	574	0.03%	0.004%
94	13.518	3800	3803	3806	rBV2	671	404	0.02%	0.003%
95	13.573	3818	3820	3824	rVB	741	410	0.02%	0.003%
96	13.634	3835	3839	3842	rVB2	437	347	0.02%	0.002%
97	13.650	3842	3844	3849	rBV2	810	775	0.04%	0.005%
98	13.756	3874	3877	3880	rBV	570	454	0.02%	0.003%
99	13.859	3906	3909	3914	rBV4	746	748	0.04%	0.005%
100	14.187	4009	4011	4013	rBV2	548	295	0.02%	0.002%

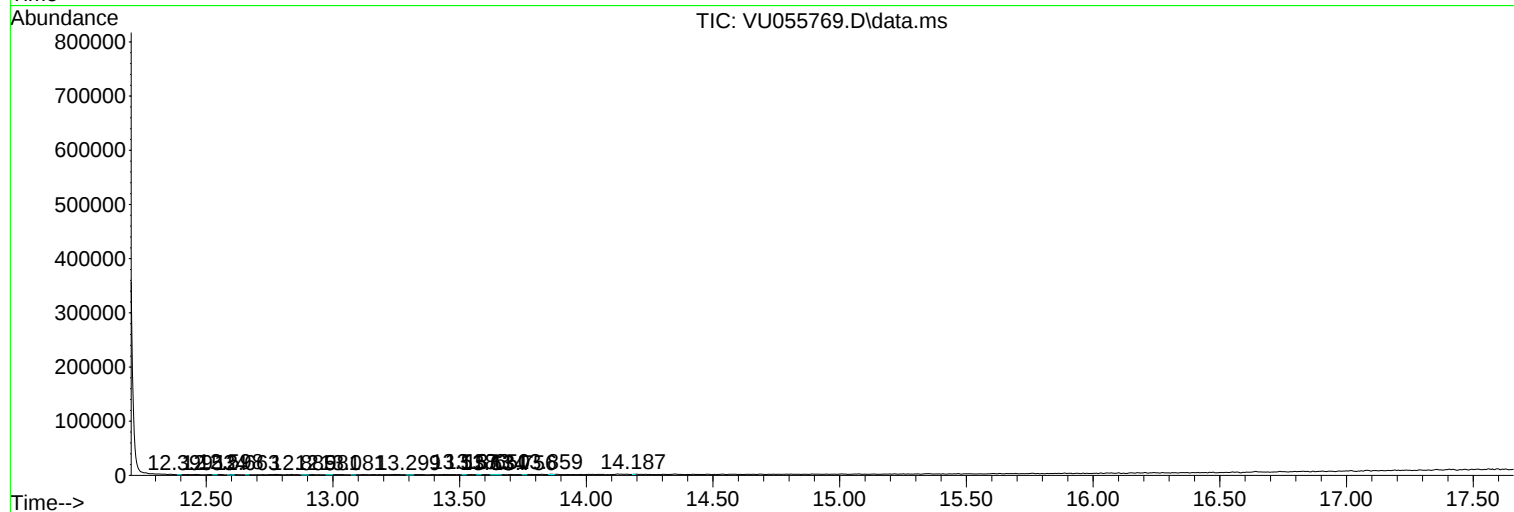
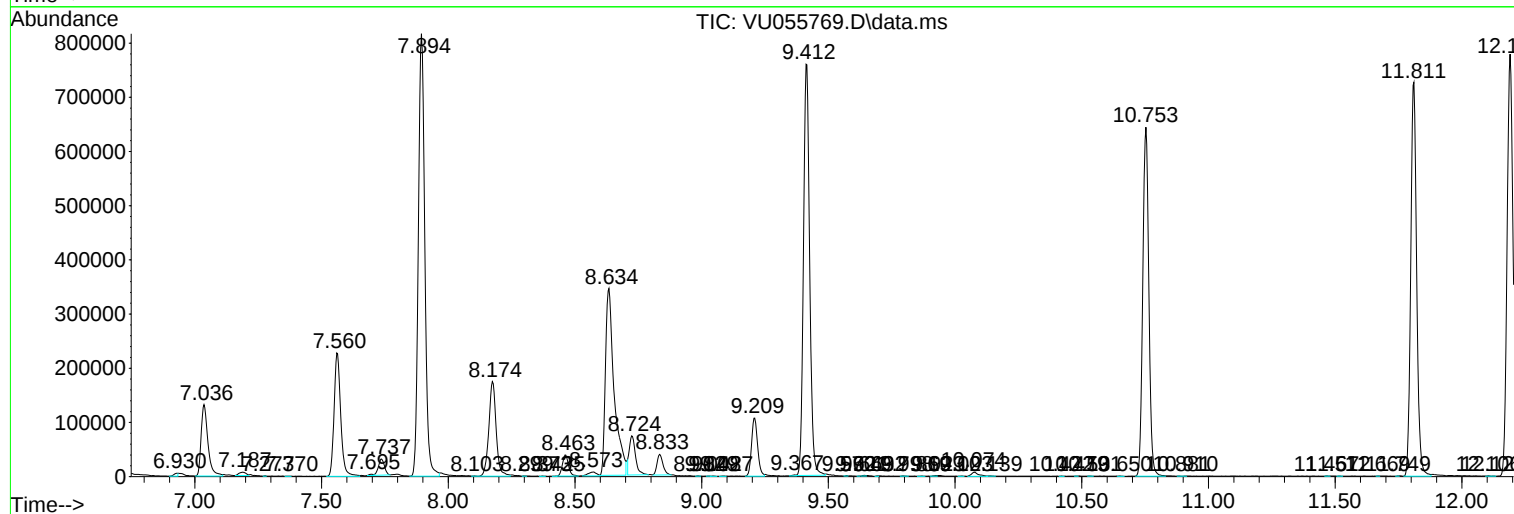
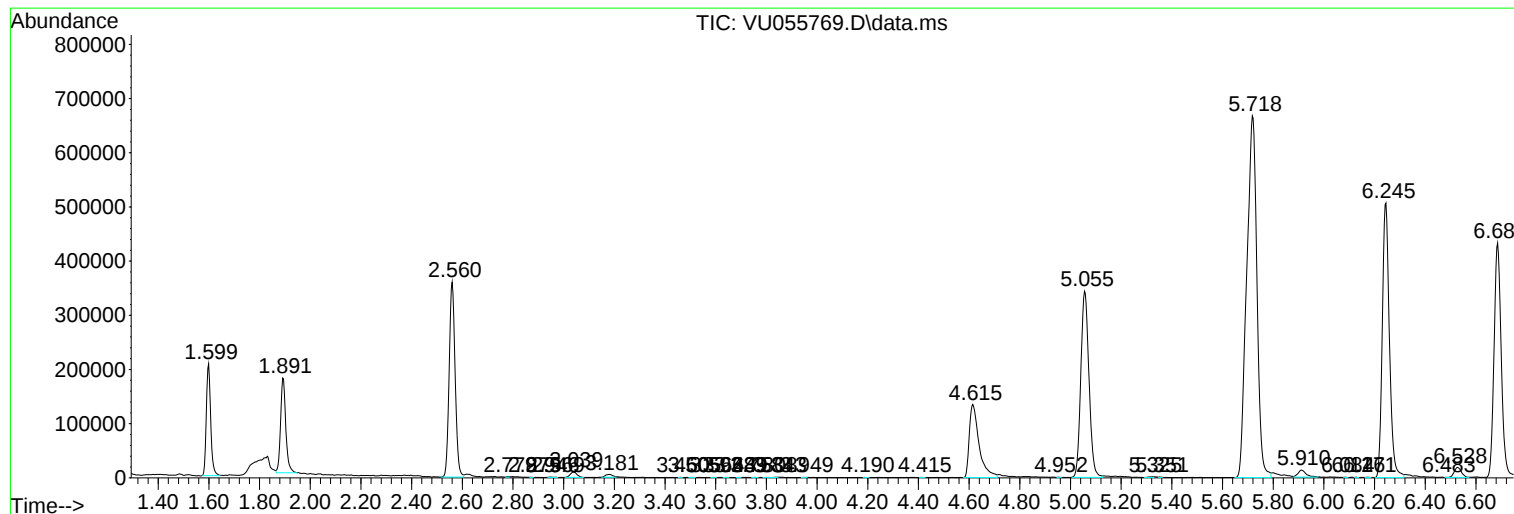
Sum of corrected areas: 14694762

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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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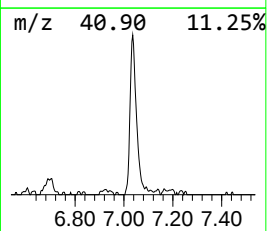
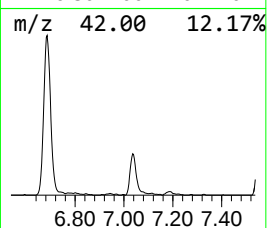
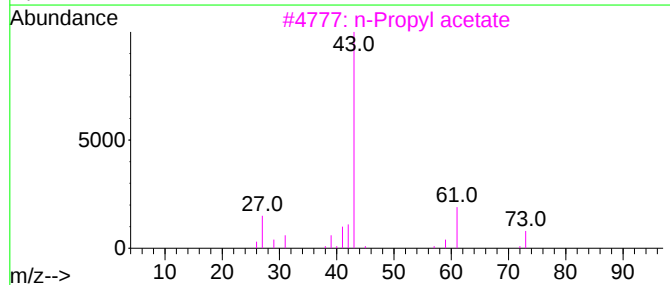
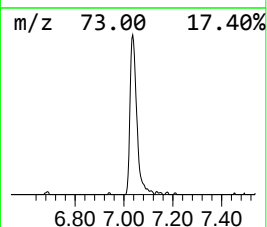
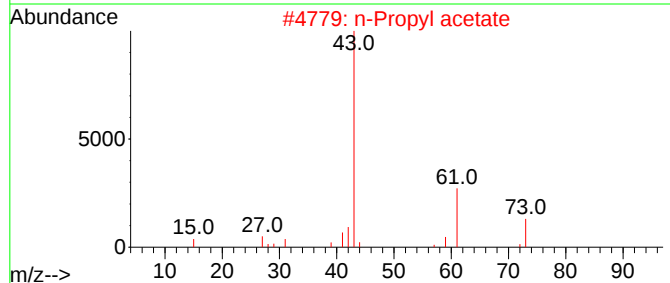
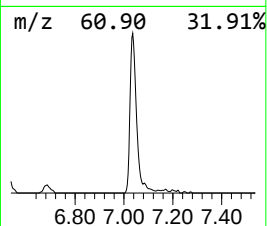
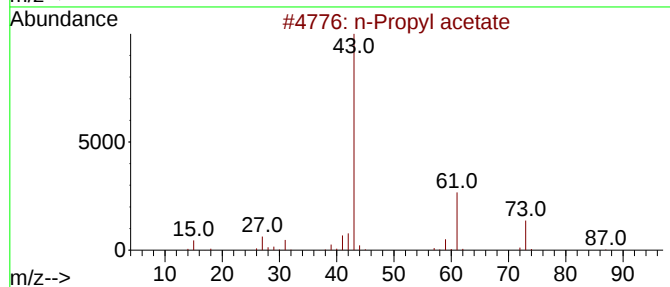
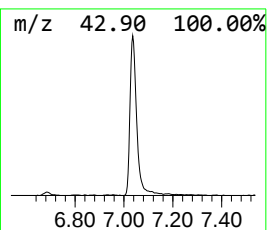
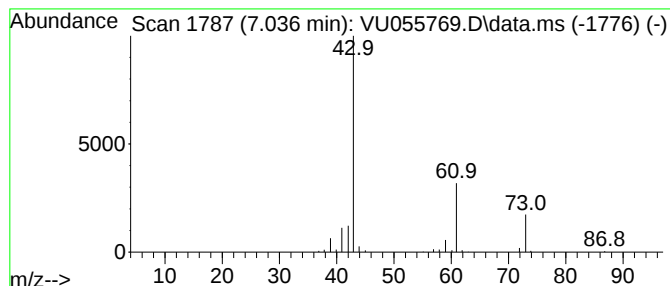
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
7.036	12.27 ug/L	243176	1,4-Difluorobenzene	6.245

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	72
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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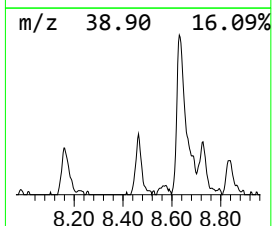
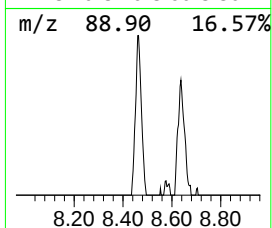
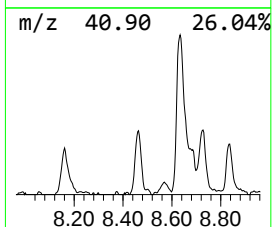
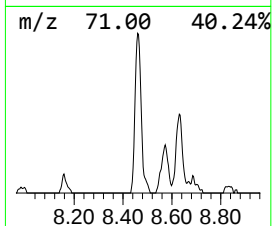
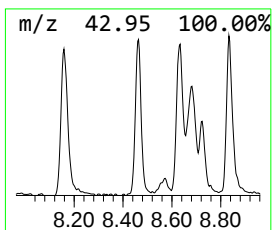
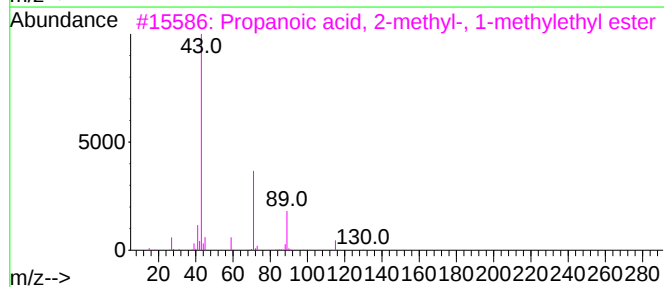
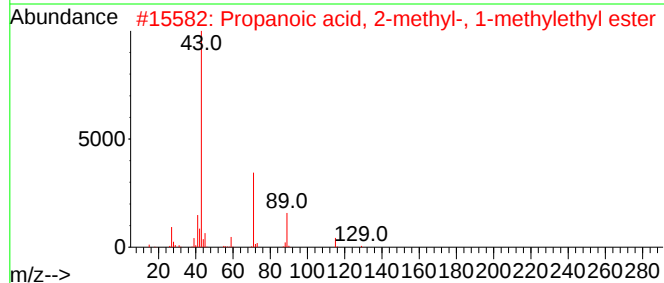
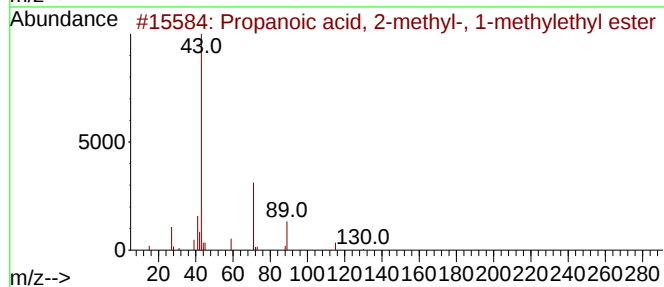
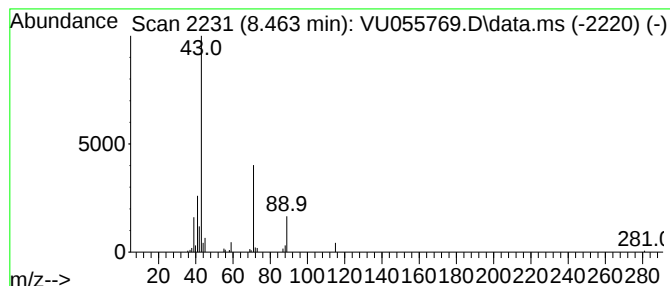
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.51 ug/L	65201	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	78
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



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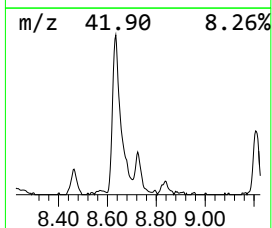
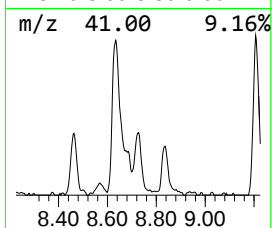
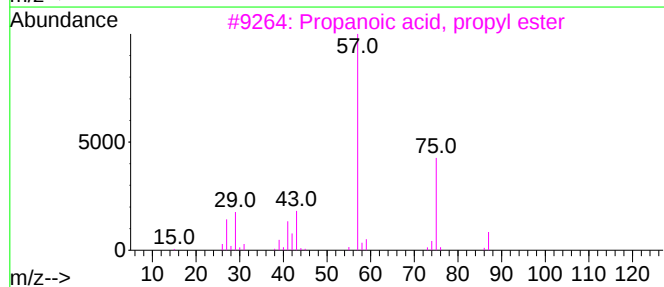
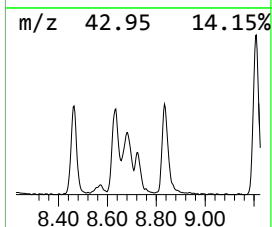
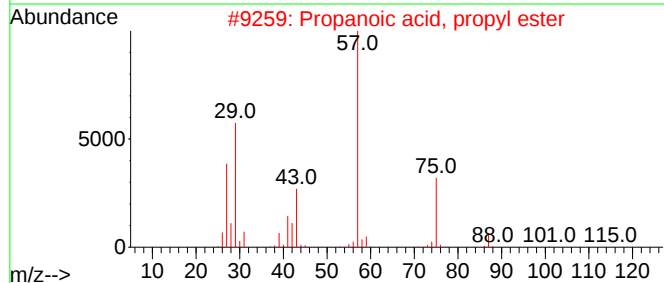
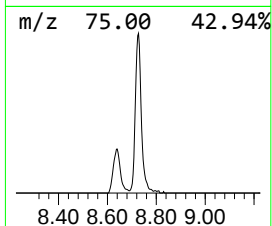
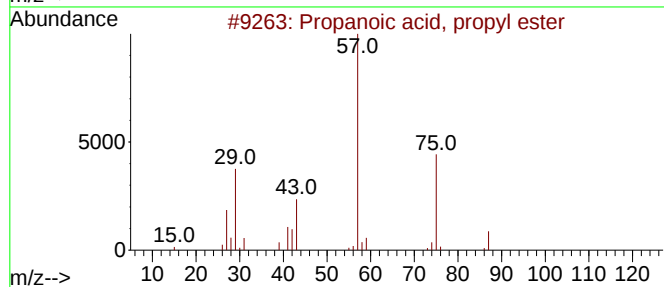
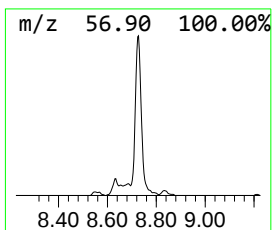
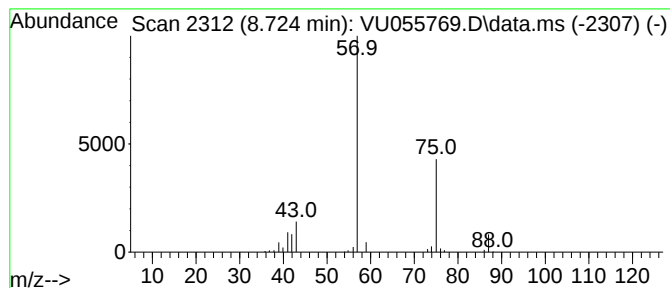
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.724	4.68 ug/L	121538	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	74		
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74		
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055769.D
Acq On : 16 Oct 2023 14:00
Operator : MD/SY
Sample : PB156381TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB381

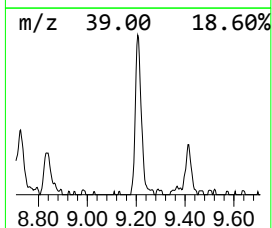
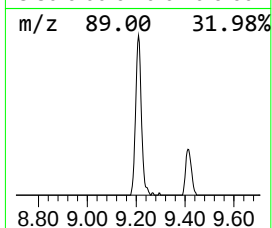
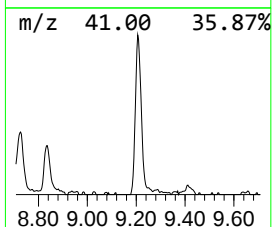
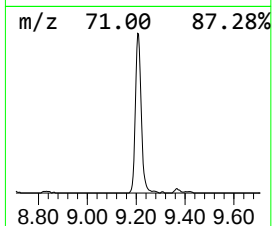
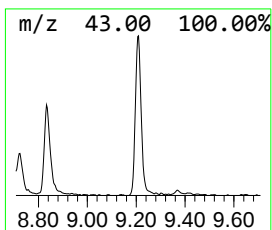
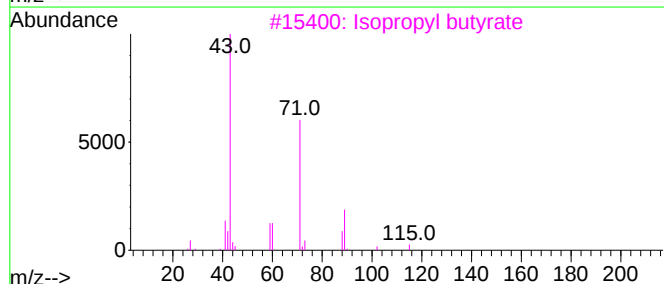
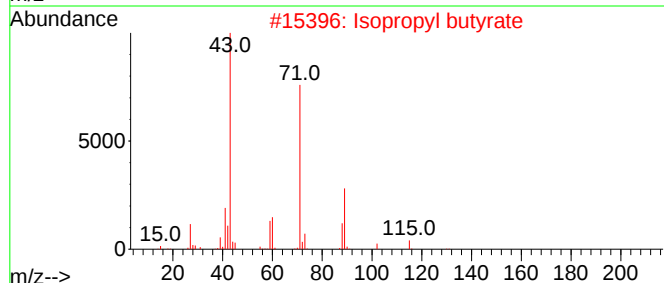
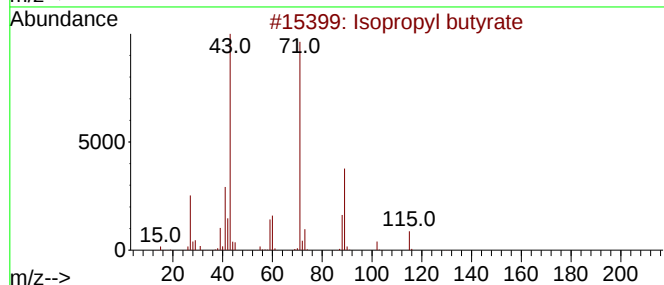
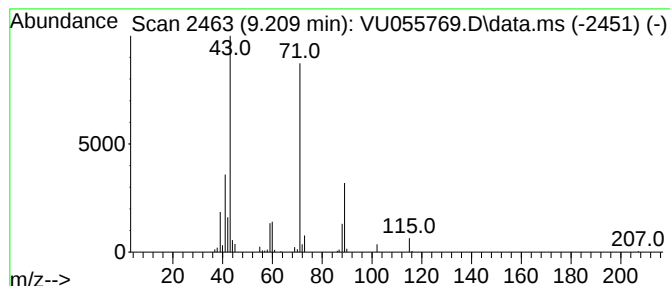
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Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.209	6.84 ug/L	177818	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-, 1-met...	130	C7H14O2	000617-50-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101623\
Data File : VU055769.D
Acq On : 16 Oct 2023 14:00
Operator : MD/SY
Sample : PB156381TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB381

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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	7.036	12.3	ug/L	243176	1	6.245	990712	50.0
Propanoic acid,...	8.463	2.5	ug/L	65201	2	9.412	1299590	50.0
Propanoic acid,...	8.724	4.7	ug/L	121538	2	9.412	1299590	50.0
Isopropyl butyrate	9.209	6.8	ug/L	177818	2	9.412	1299590	50.0