

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062724\
 Data File : VU059551.D
 Acq On : 27 Jun 2024 10:32
 Operator : MD/SY
 Sample : PB161741TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB741

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\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	112	rBV	74623	88831	14.11%	1.622%
2	1.907	184	192	207	rBV	61832	85962	13.65%	1.569%
3	2.560	383	395	408	rBV	123125	198167	31.47%	3.617%
4	2.692	434	436	440	rVB2	435	270	0.04%	0.005%
5	2.792	458	467	472	rVB2	627	1080	0.17%	0.020%
6	2.917	503	506	512	rBV2	199	192	0.03%	0.004%
7	2.981	521	526	529	rBV2	177	198	0.03%	0.004%
8	3.042	535	545	556	rBB4	4074	7933	1.26%	0.145%
9	3.171	578	585	588	rBV2	696	946	0.15%	0.017%
10	3.557	701	705	710	rBV2	182	214	0.03%	0.004%
11	3.721	751	756	759	rBV2	188	198	0.03%	0.004%
12	4.120	877	880	882	rBV2	251	196	0.03%	0.004%
13	4.396	961	966	973	rVB2	157	227	0.04%	0.004%
14	4.612	1023	1033	1064	rBV	57130	145570	23.12%	2.657%
15	5.055	1153	1171	1193	rBV	116232	258475	41.05%	4.718%
16	5.174	1205	1208	1214	rBV3	436	512	0.08%	0.009%
17	5.203	1214	1217	1221	rVB2	408	303	0.05%	0.006%
18	5.226	1221	1224	1228	rVB2	399	239	0.04%	0.004%
19	5.261	1228	1235	1239	rBV2	210	246	0.04%	0.004%
20	5.531	1314	1319	1321	rBV	222	190	0.03%	0.003%
21	5.605	1339	1342	1349	rVB	206	188	0.03%	0.003%
22	5.718	1358	1377	1410	rBV2	227145	629617	100.00%	11.493%
23	5.911	1428	1437	1450	rBV2	5643	11670	1.85%	0.213%
24	6.020	1466	1471	1474	rVB3	274	251	0.04%	0.005%
25	6.097	1490	1495	1502	rVB2	264	415	0.07%	0.008%
26	6.139	1502	1508	1510	rBV	427	364	0.06%	0.007%
27	6.242	1525	1540	1564	rBV	227310	447322	71.05%	8.166%
28	6.534	1619	1631	1639	rBV5	2050	3945	0.63%	0.072%
29	6.682	1664	1677	1703	rVV	144585	283469	45.02%	5.175%
30	6.814	1713	1718	1721	rVB3	209	215	0.03%	0.004%
31	6.846	1726	1728	1734	rBV2	277	266	0.04%	0.005%
32	6.927	1745	1753	1768	rBV2	2914	6112	0.97%	0.112%
33	7.033	1777	1786	1805	rBV	68488	124358	19.75%	2.270%
34	7.177	1829	1831	1833	rBV	357	227	0.04%	0.004%
35	7.197	1834	1837	1840	rVV3	634	431	0.07%	0.008%
36	7.341	1879	1882	1885	rBV	302	212	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	7.499	1925	1931	1938	rBV2	165	221	0.04%	0.004%
38	7.560	1938	1950	1974	rBV2	72647	132780	21.09%	2.424%
39	7.669	1982	1984	1990	rVB	490	364	0.06%	0.007%
40	7.734	1990	2004	2019	rBV	13583	23811	3.78%	0.435%
41	7.891	2041	2053	2086	rBV	270120	481933	76.54%	8.797%
42	8.084	2110	2113	2116	rVB3	441	347	0.06%	0.006%
43	8.110	2116	2121	2123	rBV2	340	273	0.04%	0.005%
44	8.174	2123	2141	2158	rBV2	56840	118194	18.77%	2.158%
45	8.460	2218	2230	2247	rVV	16963	28381	4.51%	0.518%
46	8.554	2250	2259	2260	rVV4	2005	1992	0.32%	0.036%
47	8.570	2260	2264	2272	rVV3	3379	4499	0.71%	0.082%
48	8.627	2272	2282	2304	rVV	159814	316264	50.23%	5.773%
49	8.724	2305	2312	2336	rVV	34858	65141	10.35%	1.189%
50	8.833	2337	2346	2366	rVV2	17727	35165	5.59%	0.642%
51	8.917	2370	2372	2374	rVV	502	261	0.04%	0.005%
52	8.930	2374	2376	2379	rVB	369	225	0.04%	0.004%
53	9.206	2451	2462	2479	rBV	49488	80623	12.81%	1.472%
54	9.303	2490	2492	2496	rVB2	532	284	0.05%	0.005%
55	9.361	2505	2510	2511	rBV3	642	551	0.09%	0.010%
56	9.412	2514	2526	2551	rBV	350374	589164	93.57%	10.755%
57	9.570	2570	2575	2578	rBV	589	606	0.10%	0.011%
58	9.772	2636	2638	2643	rVV2	202	187	0.03%	0.003%
59	9.798	2643	2646	2650	rVB2	256	183	0.03%	0.003%
60	9.901	2672	2678	2681	rBV2	183	196	0.03%	0.004%
61	9.917	2681	2683	2686	rBV	316	222	0.04%	0.004%
62	10.078	2724	2733	2747	rBV5	2566	5410	0.86%	0.099%
63	10.174	2760	2763	2769	rVB2	202	191	0.03%	0.003%
64	10.248	2783	2786	2794	rVB2	204	236	0.04%	0.004%
65	10.299	2797	2802	2808	rBV	235	298	0.05%	0.005%
66	10.489	2854	2861	2869	rVB3	447	783	0.12%	0.014%
67	10.563	2881	2884	2887	rBV	308	227	0.04%	0.004%
68	10.750	2929	2942	2962	rBV	223300	364121	57.83%	6.647%
69	10.888	2982	2985	2992	rVB2	498	519	0.08%	0.009%
70	11.023	3024	3027	3033	rBV	293	264	0.04%	0.005%
71	11.312	3112	3117	3120	rBV	286	305	0.05%	0.006%
72	11.412	3143	3148	3153	rBV2	254	251	0.04%	0.005%
73	11.457	3159	3162	3164	rBV2	292	189	0.03%	0.003%
74	11.473	3164	3167	3169	rVV	347	242	0.04%	0.004%
75	11.553	3189	3192	3196	rBV2	272	199	0.03%	0.004%
76	11.750	3246	3253	3260	rVB2	592	678	0.11%	0.012%

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 Title : VOC Analysis

77	11.807	3260	3271	3292	rBV	301937	490297	77.87%	8.950%
78	12.190	3378	3390	3412	rBV	251452	424978	67.50%	7.758%
79	12.724	3553	3556	3558	rBV2	257	188	0.03%	0.003%
80	12.762	3563	3568	3571	rBV2	297	223	0.04%	0.004%
81	13.238	3714	3716	3721	rVB2	588	453	0.07%	0.008%
82	13.534	3805	3808	3813	rVB2	242	198	0.03%	0.004%
83	13.859	3905	3909	3916	rBV3	640	855	0.14%	0.016%
84	14.119	3986	3990	3995	rBV2	514	669	0.11%	0.012%
85	14.331	4049	4056	4057	rBV	566	557	0.09%	0.010%
86	14.386	4069	4073	4081	rBV2	401	514	0.08%	0.009%
87	14.434	4086	4088	4093	rBV	217	191	0.03%	0.003%
88	14.492	4103	4106	4112	rBV2	331	230	0.04%	0.004%
89	14.611	4138	4143	4146	rBV3	418	356	0.06%	0.006%
90	14.647	4152	4154	4157	rVB	518	231	0.04%	0.004%
91	14.701	4169	4171	4176	rBV2	317	258	0.04%	0.005%
92	14.756	4186	4188	4190	rBV	345	214	0.03%	0.004%
93	14.894	4227	4231	4235	rVB2	413	405	0.06%	0.007%
94	15.045	4275	4278	4280	rBV3	416	271	0.04%	0.005%
95	15.129	4302	4304	4307	rBV	445	294	0.05%	0.005%
96	15.431	4394	4398	4401	rBV2	389	416	0.07%	0.008%
97	15.711	4481	4485	4487	rBV3	441	362	0.06%	0.007%
98	15.897	4540	4543	4547	rBV	583	509	0.08%	0.009%
99	15.936	4553	4555	4558	rBV3	458	329	0.05%	0.006%
100	16.126	4611	4614	4615	rBV3	560	369	0.06%	0.007%

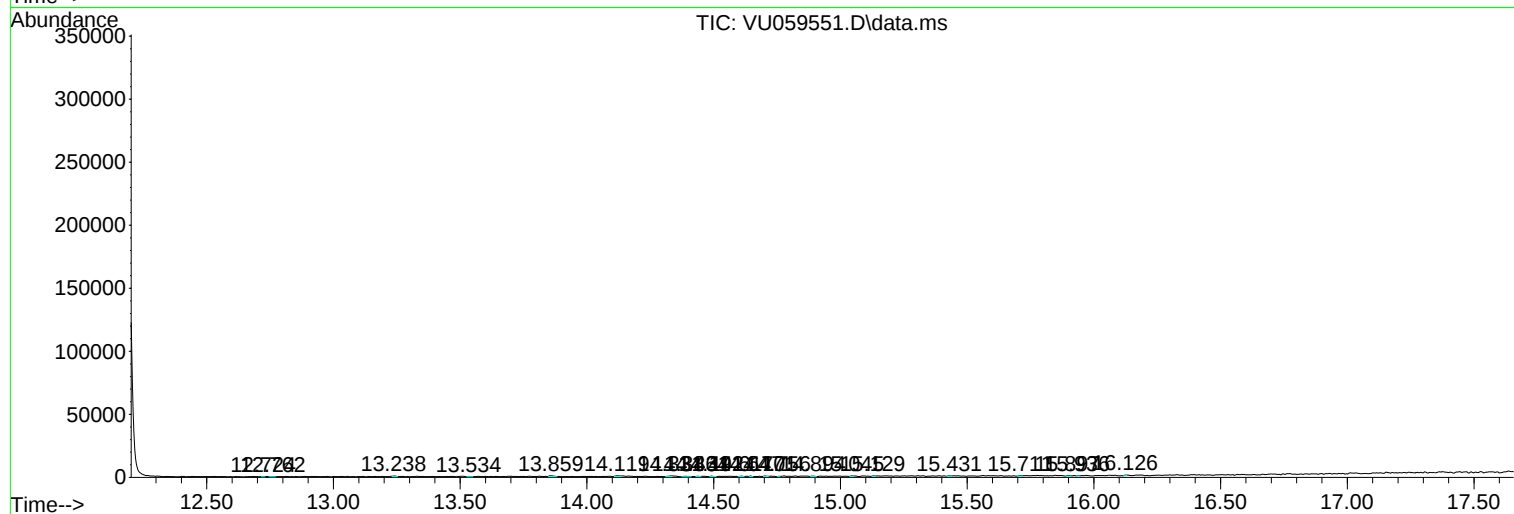
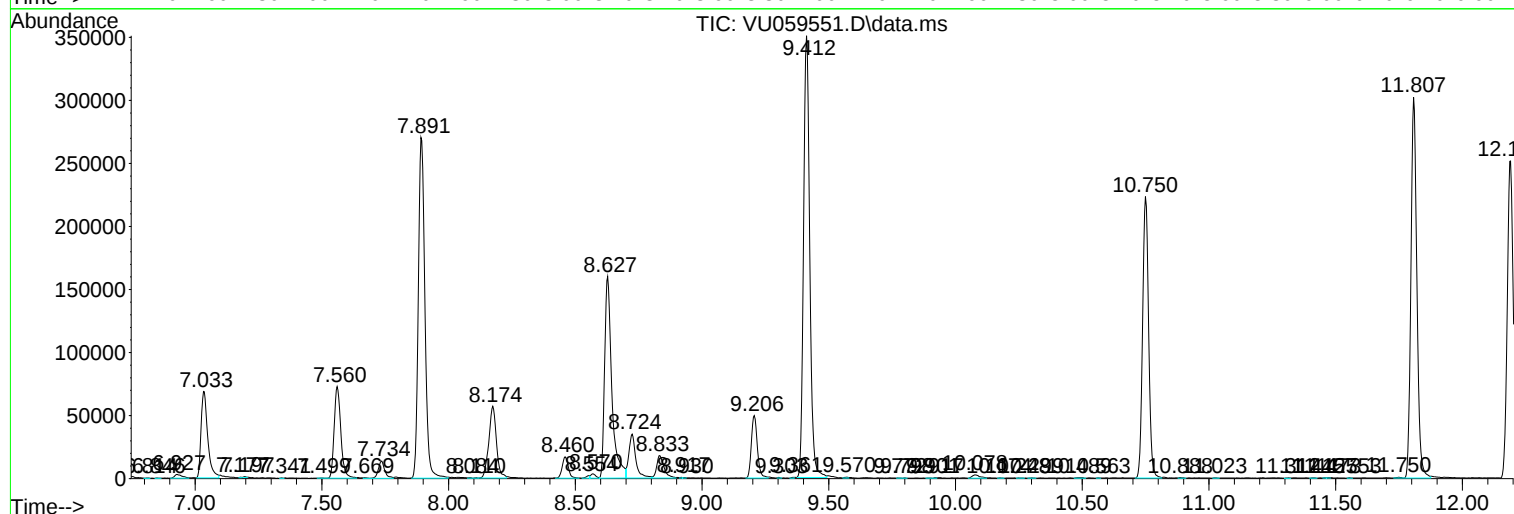
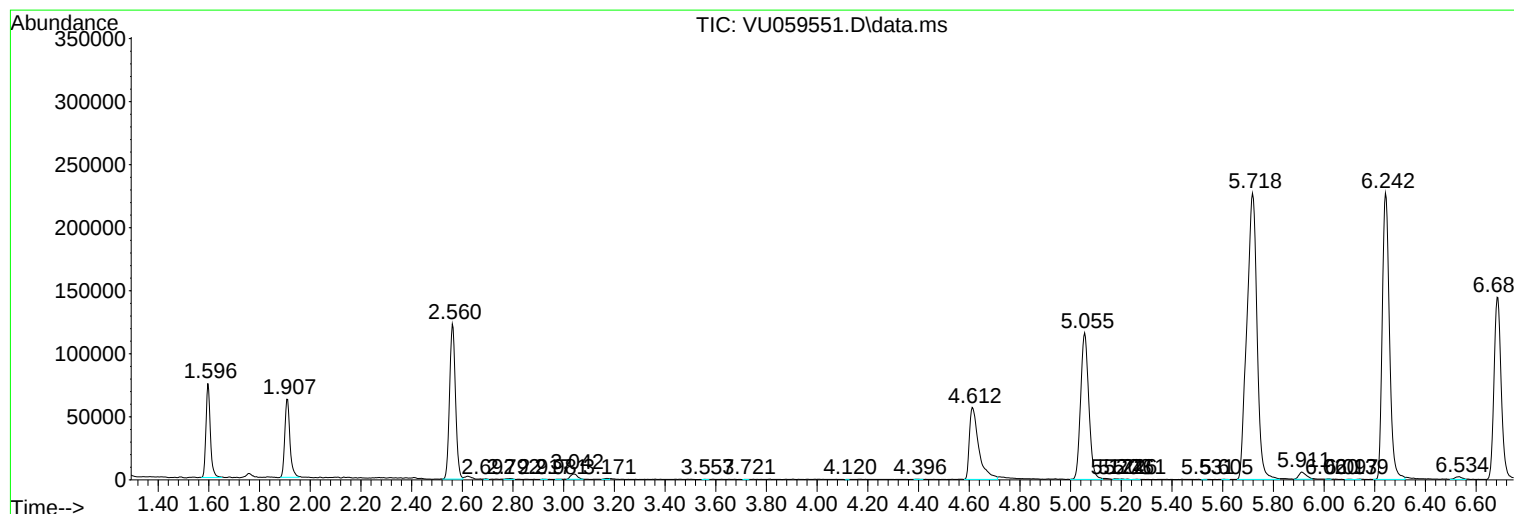
Sum of corrected areas: 5478158

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Instrument :
MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
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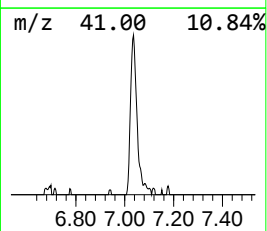
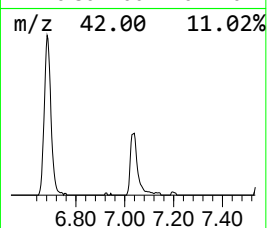
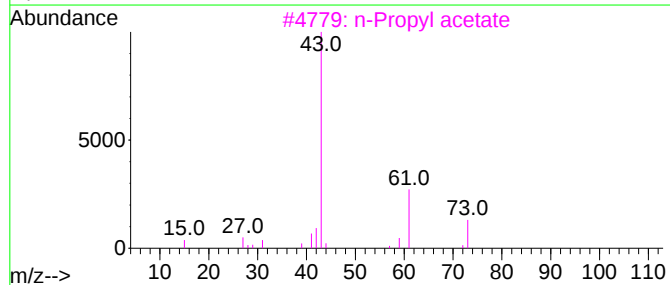
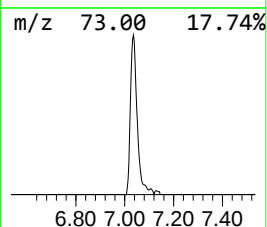
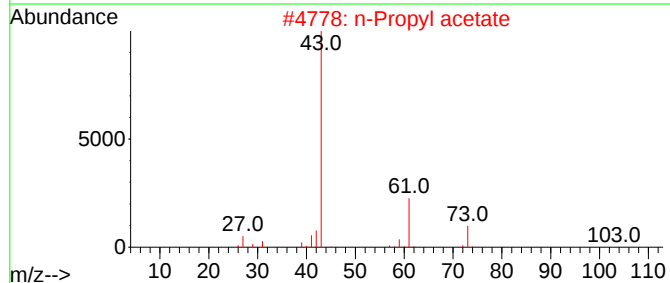
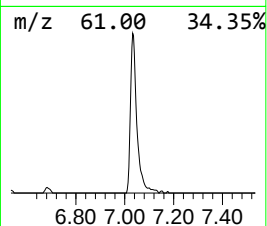
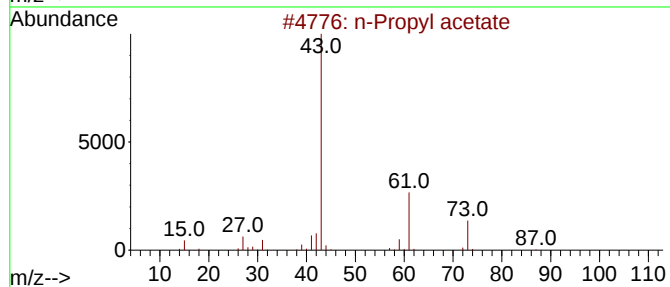
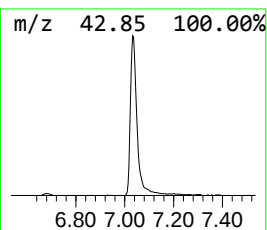
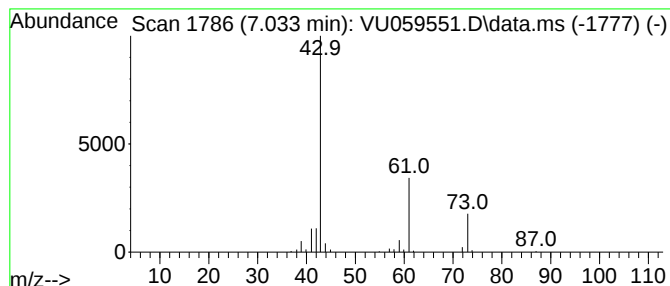
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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.
7.033	13.90 ug/L	124358	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	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	72



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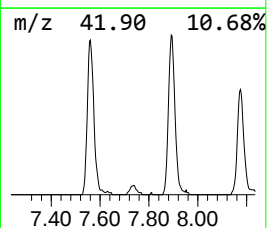
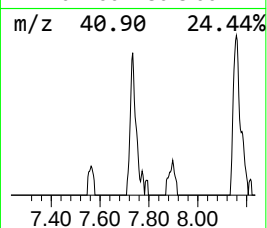
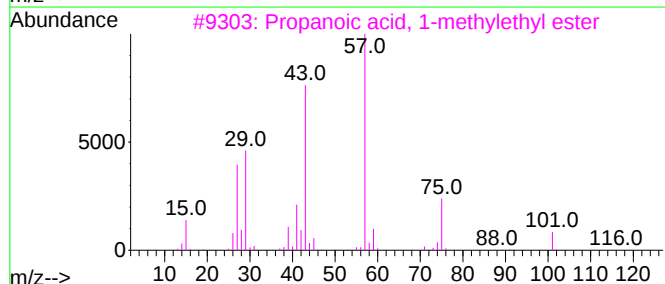
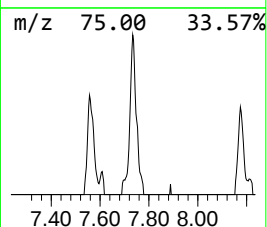
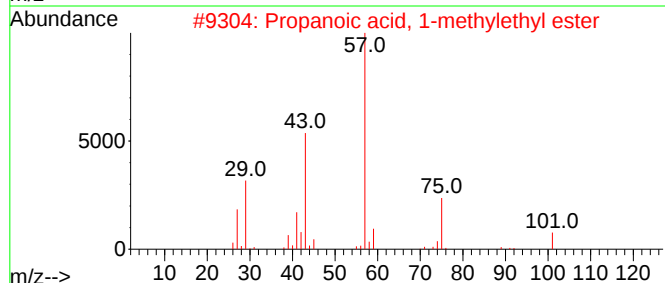
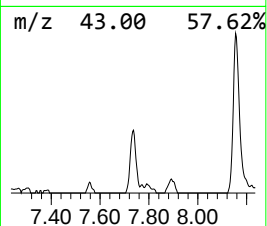
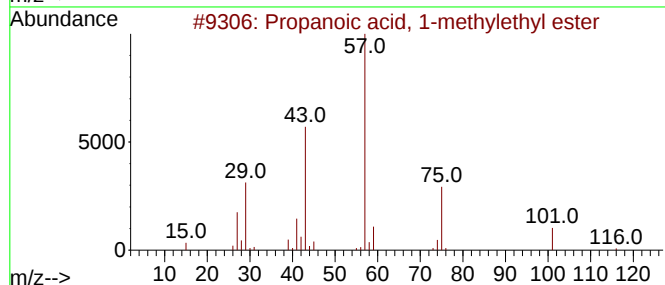
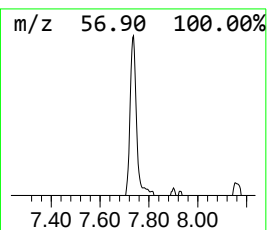
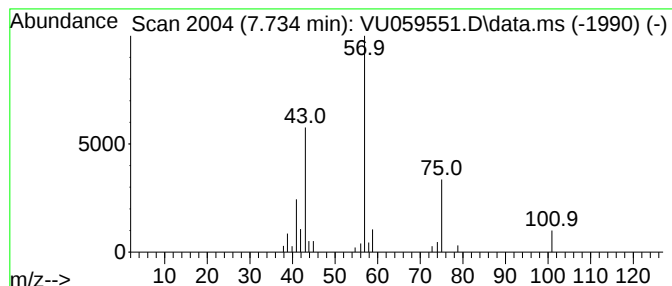
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.734	2.66 ug/L	23811	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	64
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



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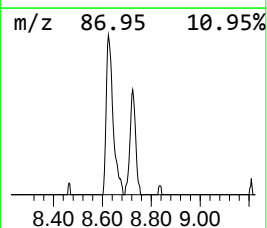
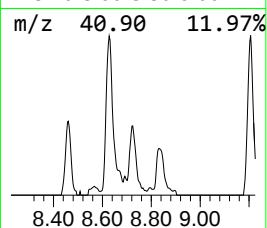
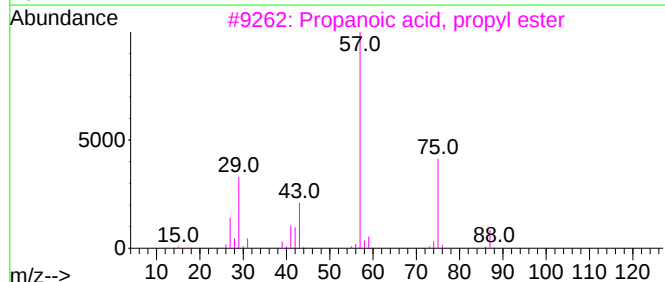
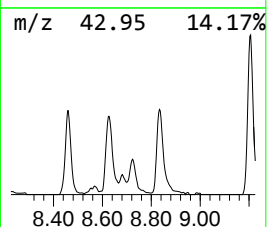
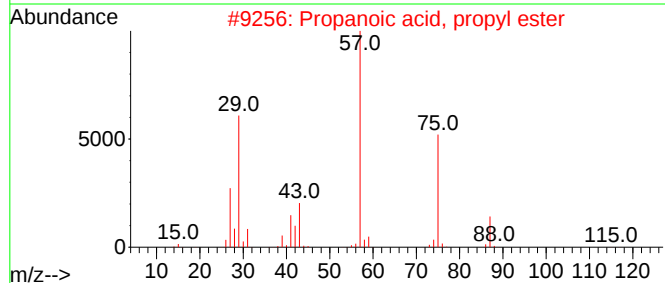
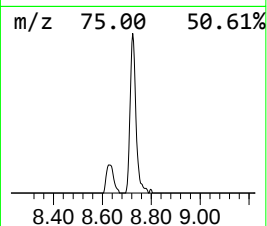
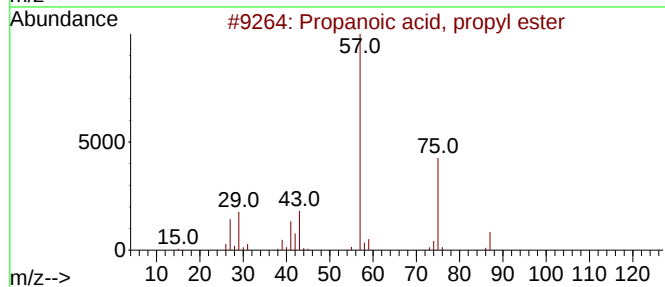
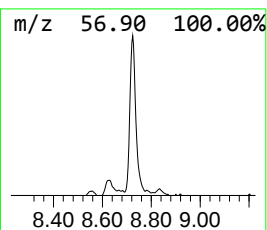
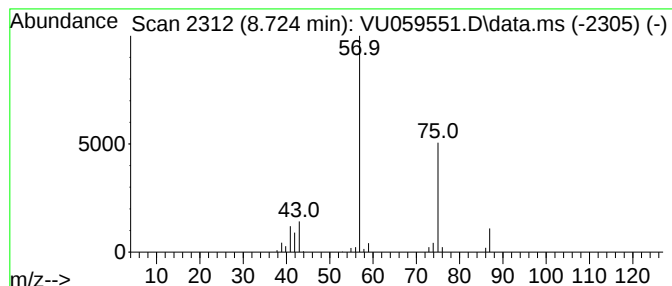
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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	5.53 ug/L	65141	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	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062724\
Data File : VU059551.D
Acq On : 27 Jun 2024 10:32
Operator : MD/SY
Sample : PB161741TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB741

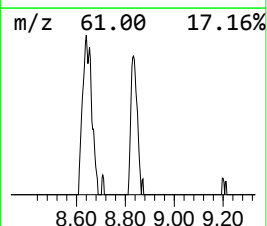
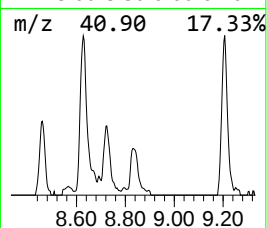
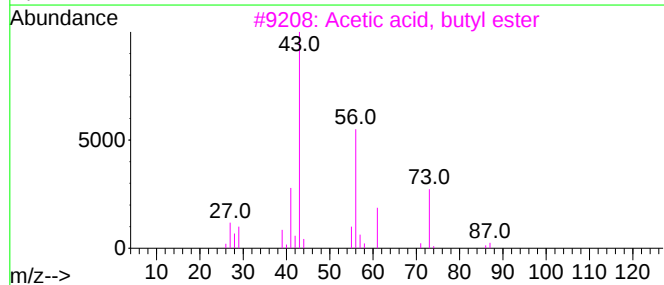
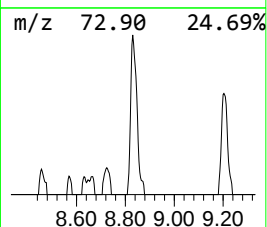
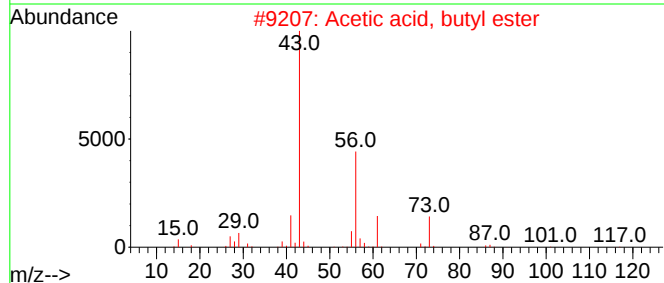
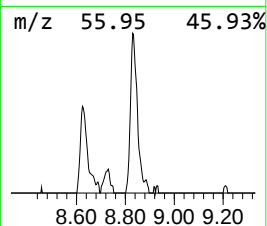
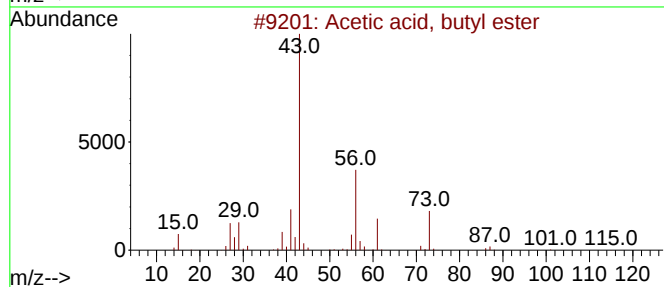
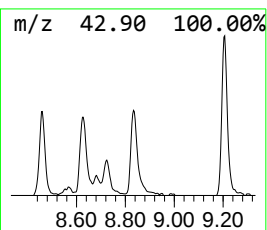
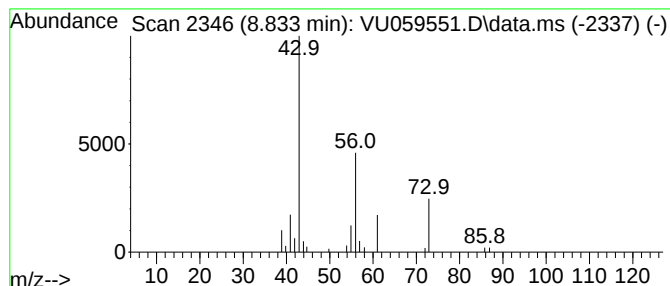
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.833	2.98 ug/L	35165	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	83
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5			Isobutyl acetate	116	C6H12O2	000110-19-0	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062724\
Data File : VU059551.D
Acq On : 27 Jun 2024 10:32
Operator : MD/SY
Sample : PB161741TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB741

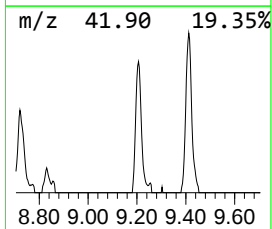
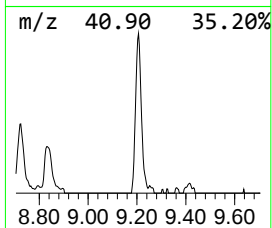
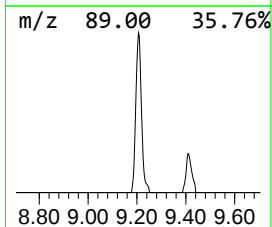
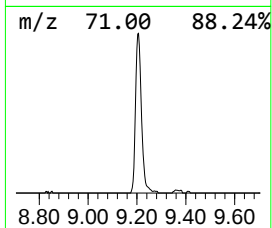
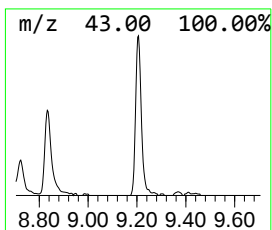
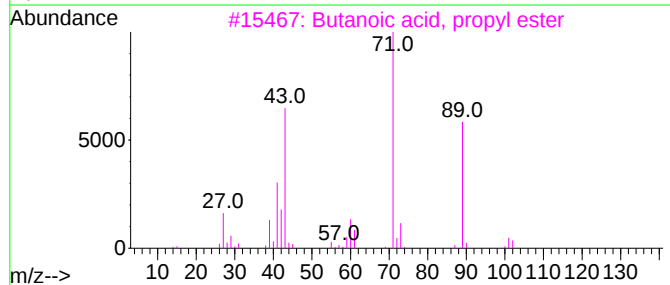
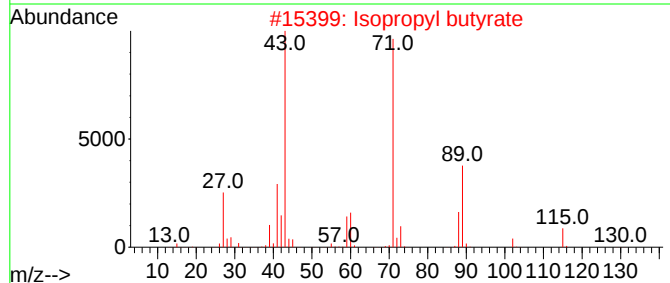
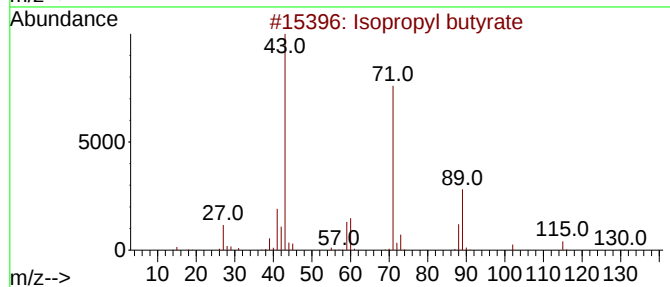
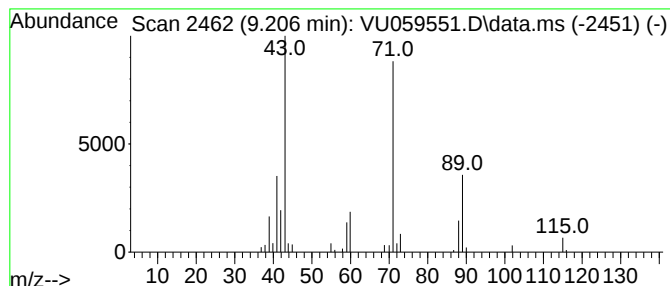
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Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.206	6.84 ug/L	80623	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062724\
Data File : VU059551.D
Acq On : 27 Jun 2024 10:32
Operator : MD/SY
Sample : PB161741TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB741

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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	7.033	13.9	ug/L	124358	1	6.242	447322	50.0
Propanoic acid,...	7.734	2.7	ug/L	23811	1	6.242	447322	50.0
Propanoic acid,...	8.724	5.5	ug/L	65141	2	9.412	589164	50.0
Acetic acid, bu...	8.833	3.0	ug/L	35165	2	9.412	589164	50.0
Isopropyl butyrate	9.206	6.8	ug/L	80623	2	9.412	589164	50.0