

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
 Data File : VU050613.D
 Acq On : 03 Sep 2022 15:36
 Operator : SY/MD
 Sample : PB147438TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB438

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\SFAMULM090222WMA.M
 Title : VOC Analysis

Signal : TIC: VU050613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	40	45	51	rBV2	3083	3424	0.23%	0.031%
2	1.597	72	80	104	rBV	163910	205754	13.64%	1.840%
3	1.732	117	122	130	rVB3	3049	3646	0.24%	0.033%
4	1.906	168	176	189	rVB	123015	159329	10.56%	1.425%
5	2.163	253	256	260	rBV3	751	755	0.05%	0.007%
6	2.253	282	284	285	rBV	479	211	0.01%	0.002%
7	2.362	314	318	319	rBV2	490	350	0.02%	0.003%
8	2.382	322	324	327	rVB3	652	360	0.02%	0.003%
9	2.520	363	367	368	rBV	458	283	0.02%	0.003%
10	2.562	368	380	397	rVV	275008	448513	29.73%	4.010%
11	2.793	446	452	458	rVV5	1116	1483	0.10%	0.013%
12	2.909	486	488	493	rVB2	385	225	0.01%	0.002%
13	3.041	517	529	539	rBV2	5386	9121	0.60%	0.082%
14	3.186	561	574	591	rBV	12195	26781	1.78%	0.239%
15	3.633	708	713	717	rBV2	181	204	0.01%	0.002%
16	3.697	729	733	736	rBV	225	217	0.01%	0.002%
17	3.751	745	750	752	rBV2	371	302	0.02%	0.003%
18	4.205	886	891	895	rVB2	266	298	0.02%	0.003%
19	4.391	944	949	953	rBV2	234	230	0.02%	0.002%
20	4.555	997	1000	1005	rBV2	210	199	0.01%	0.002%
21	4.632	1010	1024	1061	rBV2	130899	421957	27.97%	3.773%
22	5.063	1141	1158	1181	rBV	270139	599625	39.74%	5.362%
23	5.234	1207	1211	1219	rVB4	668	844	0.06%	0.008%
24	5.285	1219	1227	1232	rBV4	1193	1724	0.11%	0.015%
25	5.356	1246	1249	1252	rBV	408	311	0.02%	0.003%
26	5.375	1252	1255	1256	rBV	435	224	0.01%	0.002%
27	5.626	1328	1333	1336	rBV	352	325	0.02%	0.003%
28	5.722	1342	1363	1395	rBV2	561566	1508774	100.00%	13.491%
29	5.835	1395	1398	1401	rBV4	501	349	0.02%	0.003%
30	5.915	1414	1423	1445	rVB	13471	28824	1.91%	0.258%
31	6.031	1456	1459	1462	rBV3	467	332	0.02%	0.003%
32	6.121	1482	1487	1490	rBV2	487	382	0.03%	0.003%
33	6.250	1511	1527	1553	rBV	403916	771993	51.17%	6.903%
34	6.439	1583	1586	1592	rVB3	346	337	0.02%	0.003%
35	6.533	1604	1615	1627	rVB10	1894	4662	0.31%	0.042%
36	6.578	1627	1629	1630	rBV	450	215	0.01%	0.002%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	6.600	1630	1636	1640	rVV3	651	757	0.05%	0.007%
38	6.690	1645	1664	1688	rBV	349293	689767	45.72%	6.168%
39	6.931	1726	1739	1753	rBV2	7304	17370	1.15%	0.155%
40	7.041	1762	1773	1806	rBV	143680	283505	18.79%	2.535%
41	7.353	1866	1870	1873	rBV	341	233	0.02%	0.002%
42	7.398	1882	1884	1888	rVV2	281	204	0.01%	0.002%
43	7.443	1892	1898	1899	rBV	344	211	0.01%	0.002%
44	7.565	1924	1936	1958	rBV	173511	310913	20.61%	2.780%
45	7.661	1964	1966	1971	rVB2	526	432	0.03%	0.004%
46	7.693	1971	1976	1979	rBV4	587	535	0.04%	0.005%
47	7.742	1979	1991	2003	rBV	28948	50504	3.35%	0.452%
48	7.899	2026	2040	2065	rBV	632844	1119702	74.21%	10.012%
49	8.179	2111	2127	2152	rBV4	127095	264039	17.50%	2.361%
50	8.269	2152	2155	2158	rBV4	652	435	0.03%	0.004%
51	8.314	2165	2169	2171	rBV2	321	243	0.02%	0.002%
52	8.468	2206	2217	2231	rBV2	34179	59633	3.95%	0.533%
53	8.578	2239	2251	2258	rVB7	5170	10678	0.71%	0.095%
54	8.639	2258	2270	2280	rBV4	278140	611909	40.56%	5.471%
55	8.835	2322	2331	2354	rVB	39299	68272	4.52%	0.610%
56	9.214	2437	2449	2469	rBV	98856	165488	10.97%	1.480%
57	9.340	2484	2488	2491	rBV2	379	390	0.03%	0.003%
58	9.372	2491	2498	2500	rVV5	1990	2476	0.16%	0.022%
59	9.417	2500	2512	2541	rVB	552684	928275	61.53%	8.300%
60	9.562	2553	2557	2559	rVB3	293	213	0.01%	0.002%
61	9.645	2576	2583	2588	rBV5	1066	1539	0.10%	0.014%
62	9.719	2604	2606	2610	rVB2	426	233	0.02%	0.002%
63	9.922	2661	2669	2678	rBV3	1270	2021	0.13%	0.018%
64	10.073	2708	2716	2727	rBV2	6846	11054	0.73%	0.099%
65	10.230	2761	2765	2769	rBV	317	267	0.02%	0.002%
66	10.333	2793	2797	2801	rBV2	321	253	0.02%	0.002%
67	10.423	2818	2825	2832	rBV2	305	524	0.03%	0.005%
68	10.484	2841	2844	2853	rVB2	587	663	0.04%	0.006%
69	10.526	2853	2857	2859	rBV	319	230	0.02%	0.002%
70	10.668	2898	2901	2908	rBV	225	206	0.01%	0.002%
71	10.754	2915	2928	2951	rBV	486692	797131	52.83%	7.128%
72	10.947	2981	2988	2990	rBV2	328	346	0.02%	0.003%
73	10.967	2990	2994	2998	rVV	372	269	0.02%	0.002%
74	11.018	3007	3010	3013	rBV2	314	233	0.02%	0.002%
75	11.095	3030	3034	3038	rVV2	635	568	0.04%	0.005%
76	11.230	3073	3076	3083	rBV2	222	228	0.02%	0.002%

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 Title : VOC Analysis

77	11.420	3131	3135	3138	rBV2	359	269	0.02%	0.002%
78	11.751	3231	3238	3244	rVB4	1060	1144	0.08%	0.010%
79	11.812	3244	3257	3282	rBV	431587	701479	46.49%	6.272%
80	12.002	3311	3316	3319	rBV3	490	432	0.03%	0.004%
81	12.041	3325	3328	3330	rBV2	412	276	0.02%	0.002%
82	12.192	3359	3375	3395	rBV	523913	865278	57.35%	7.737%
83	12.369	3426	3430	3434	rVB	670	506	0.03%	0.005%
84	12.391	3434	3437	3441	rBV2	259	229	0.02%	0.002%
85	12.410	3441	3443	3448	rVV	438	318	0.02%	0.003%
86	12.462	3456	3459	3464	rBV4	356	285	0.02%	0.003%
87	12.584	3494	3497	3500	rBV2	418	325	0.02%	0.003%
88	12.651	3516	3518	3524	rVB	626	401	0.03%	0.004%
89	12.732	3539	3543	3546	rBV	808	459	0.03%	0.004%
90	12.809	3563	3567	3570	rBV2	626	501	0.03%	0.004%
91	12.905	3593	3597	3601	rBV3	469	392	0.03%	0.004%
92	13.018	3628	3632	3639	rBV2	510	819	0.05%	0.007%
93	13.076	3647	3650	3656	rBV3	349	392	0.03%	0.004%
94	13.198	3686	3688	3690	rBV2	441	245	0.02%	0.002%
95	13.848	3885	3890	3899	rVB3	2717	3669	0.24%	0.033%
96	14.063	3954	3957	3960	rBV3	384	328	0.02%	0.003%
97	14.237	4008	4011	4018	rBV3	435	504	0.03%	0.005%
98	14.391	4056	4059	4061	rBV	429	220	0.01%	0.002%
99	15.095	4275	4278	4280	rBV3	596	483	0.03%	0.004%
100	15.963	4546	4548	4549	rBV2	785	375	0.02%	0.003%

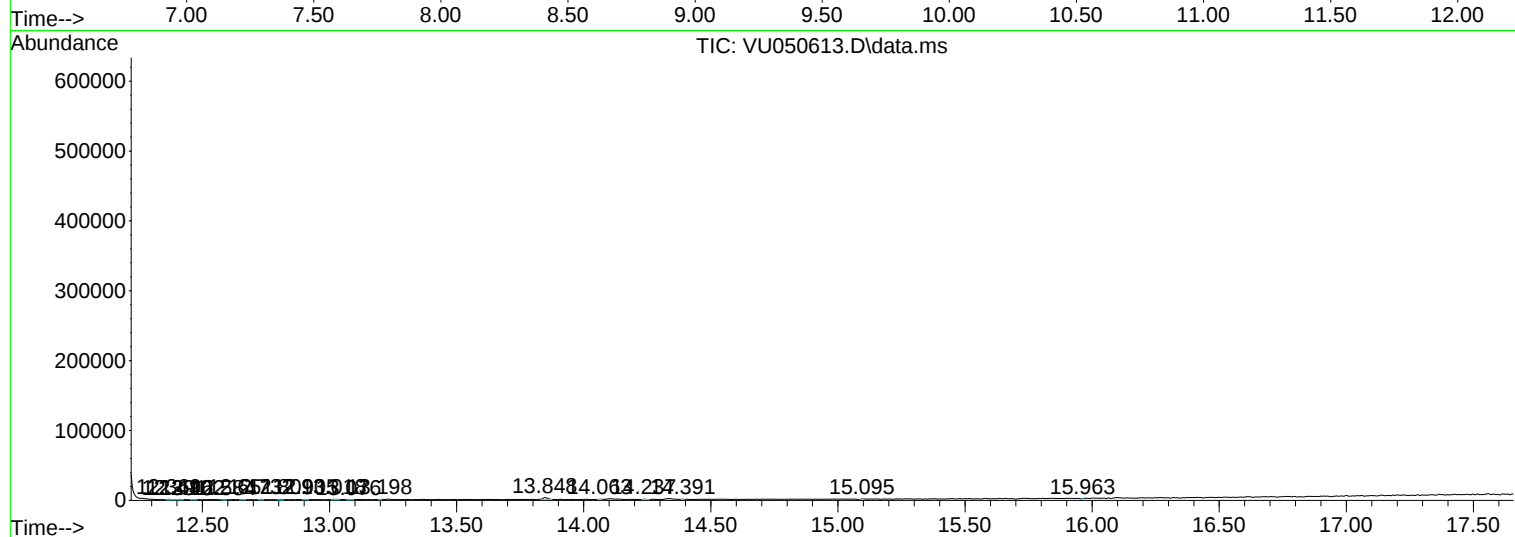
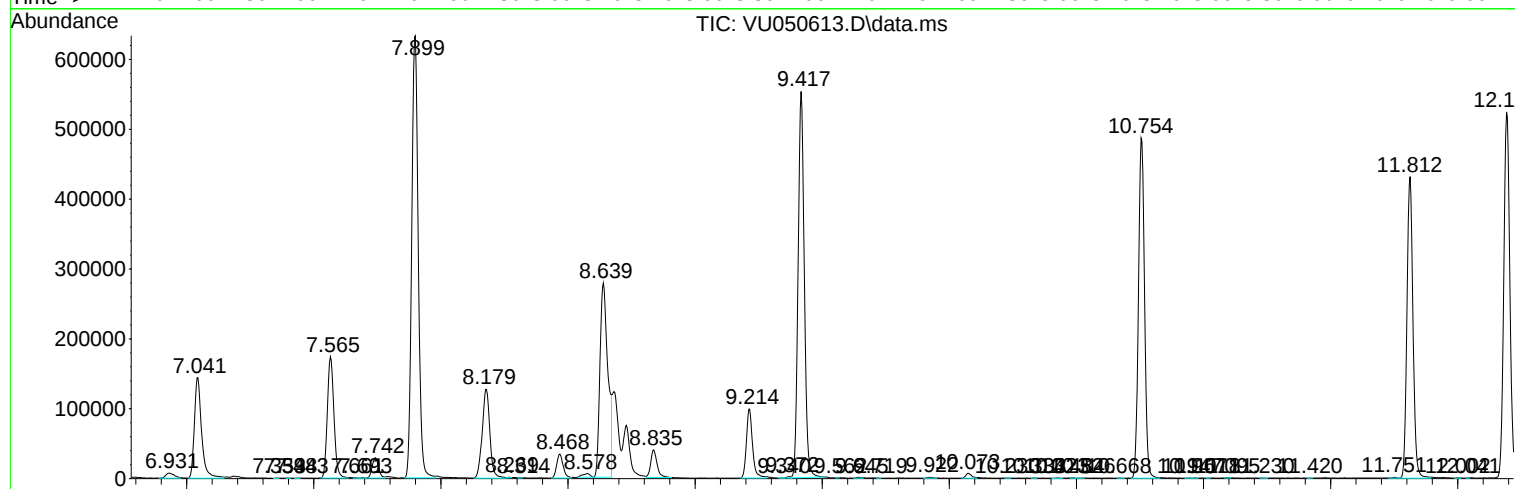
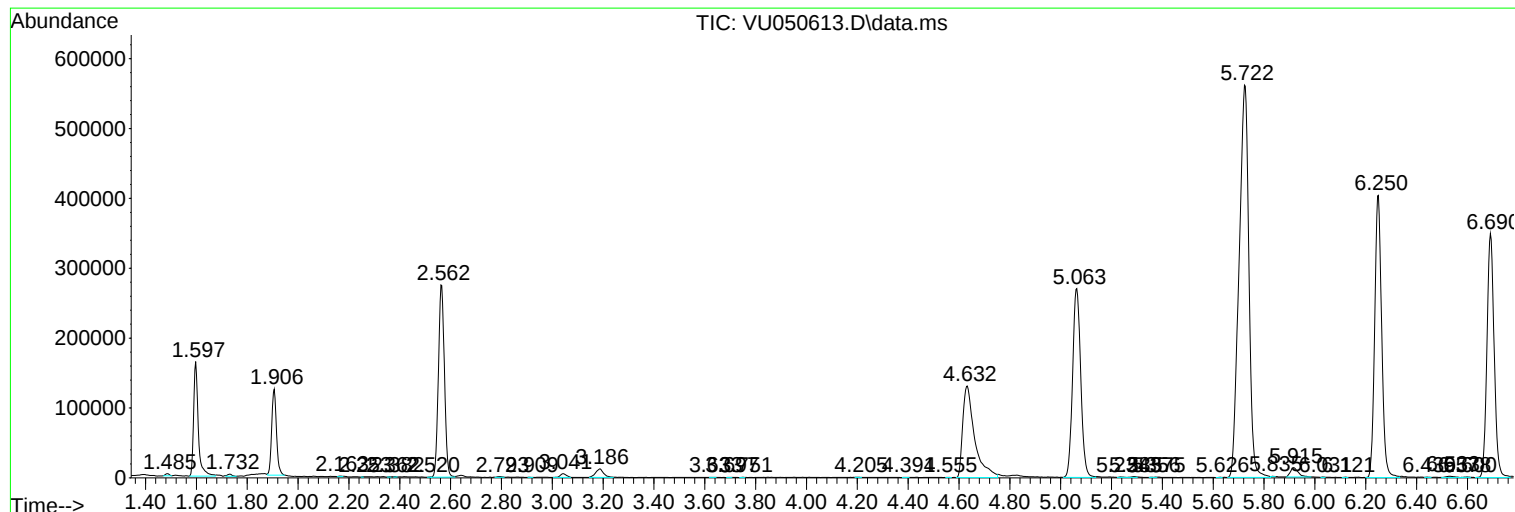
Sum of corrected areas: 11183841

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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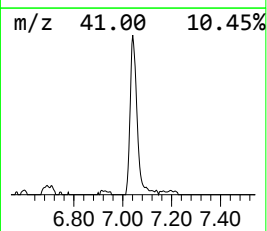
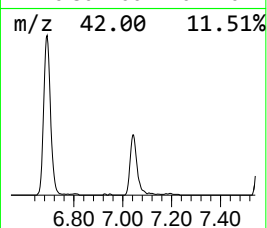
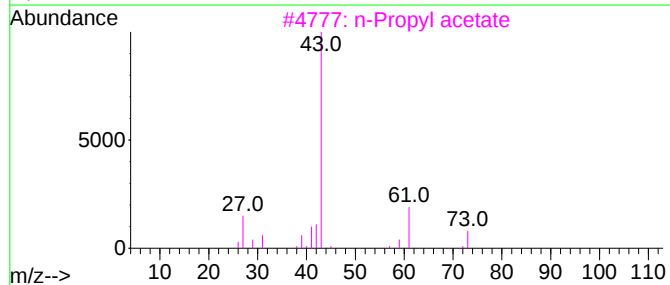
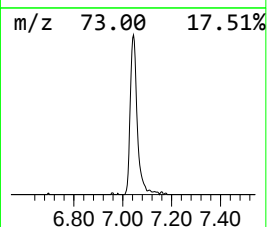
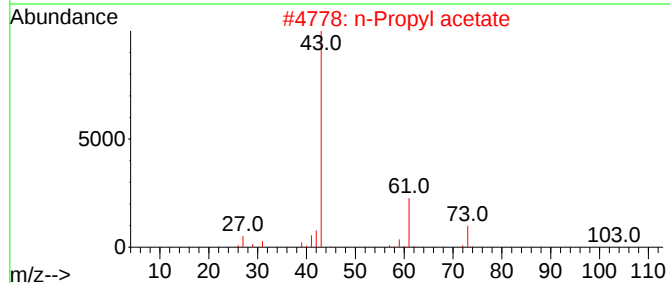
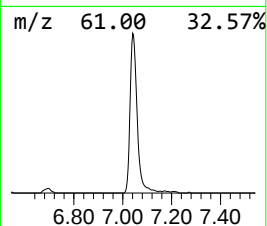
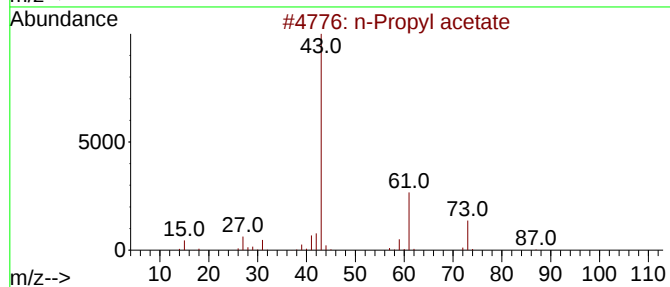
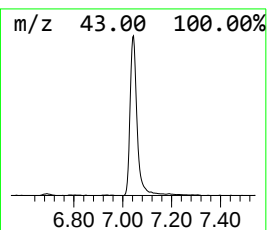
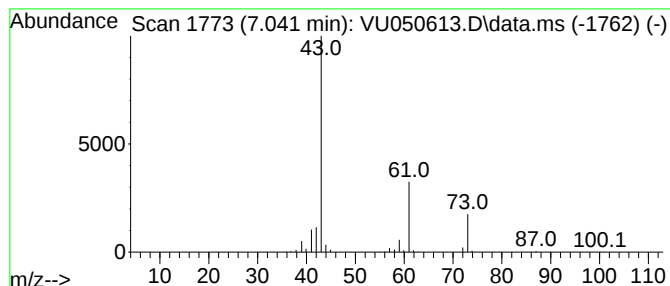
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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	18.36 ug/L	283505	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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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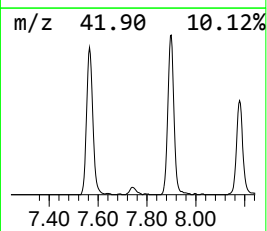
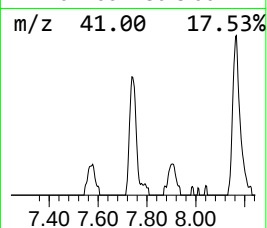
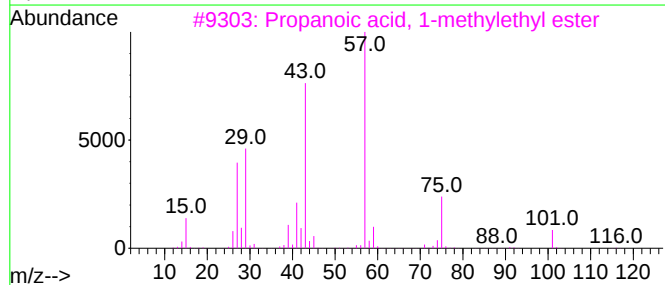
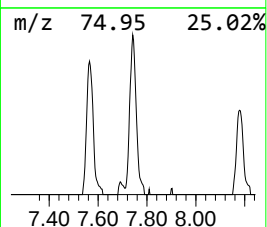
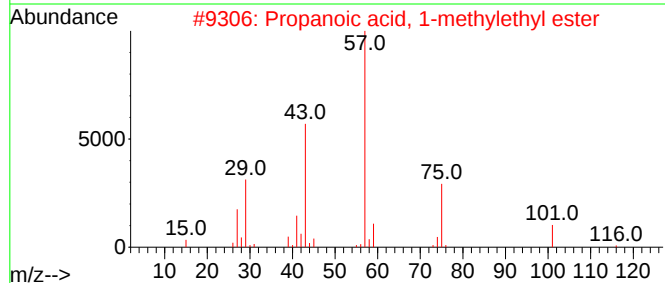
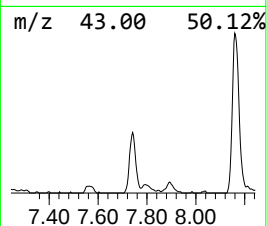
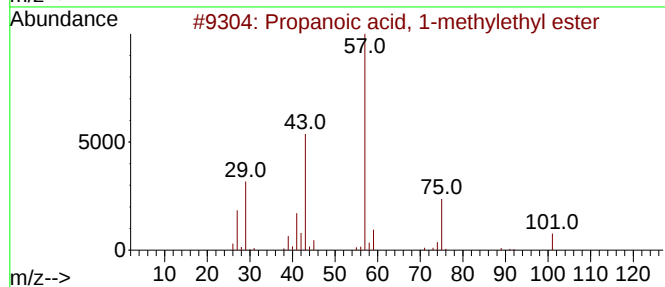
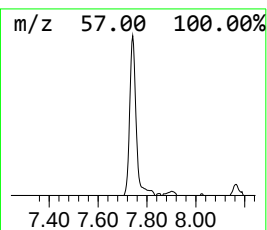
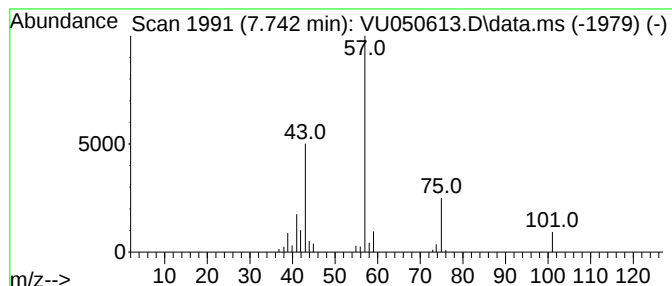
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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.
7.742	3.27 ug/L	50504	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	72
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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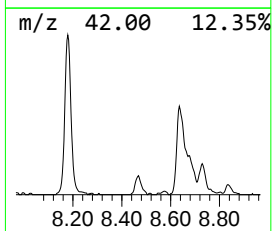
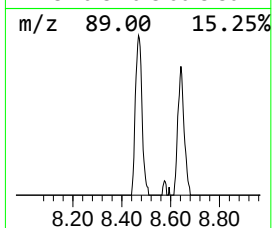
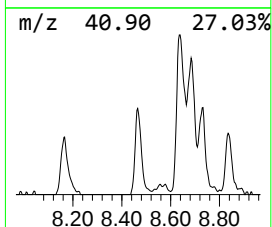
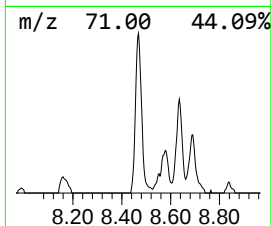
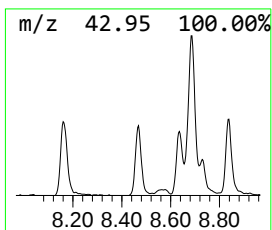
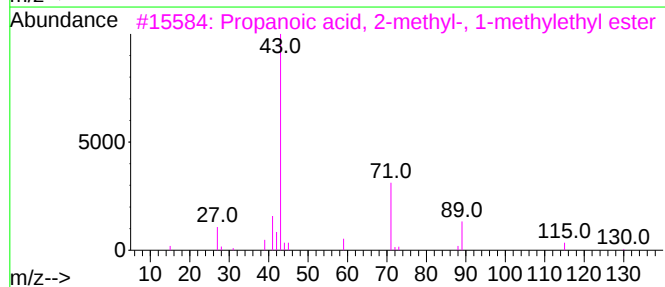
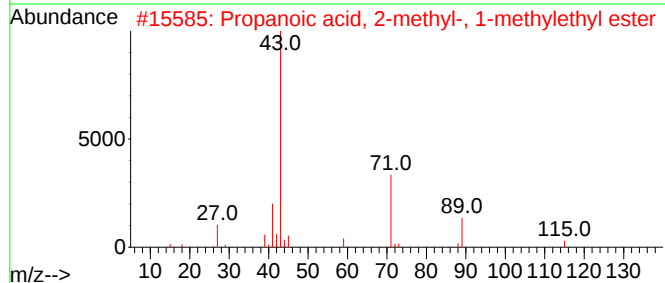
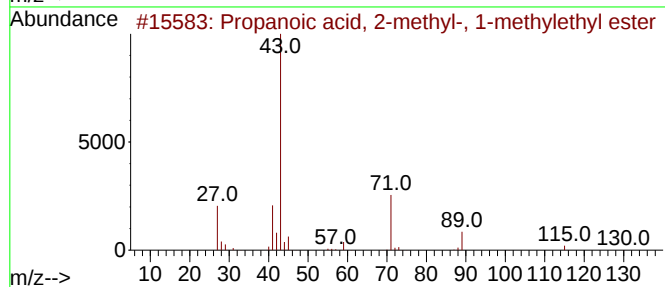
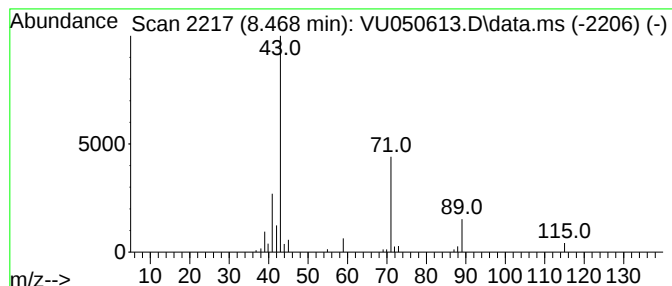
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.468	3.21 ug/L	59633	Chlorobenzene-d5	9.417

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	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
Data File : VU050613.D
Acq On : 03 Sep 2022 15:36
Operator : SY/MD
Sample : PB147438TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB438

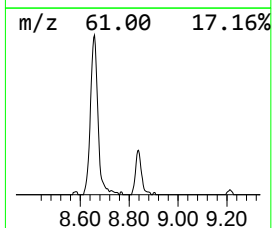
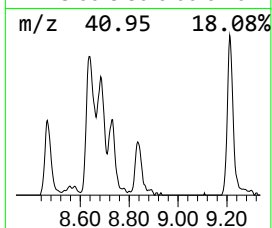
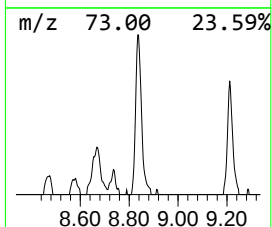
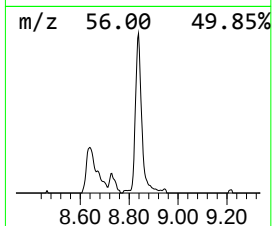
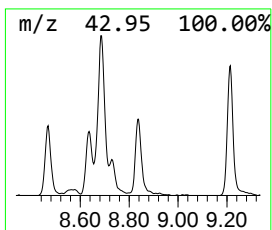
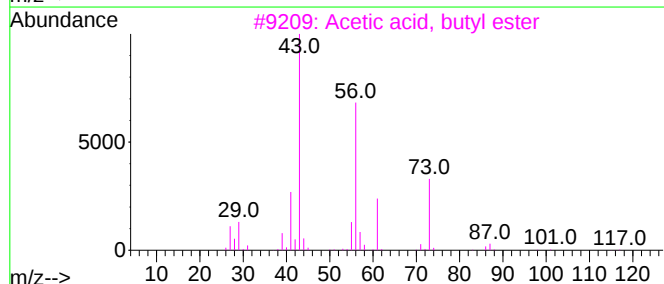
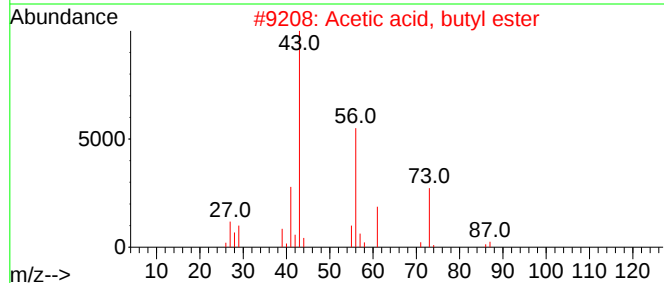
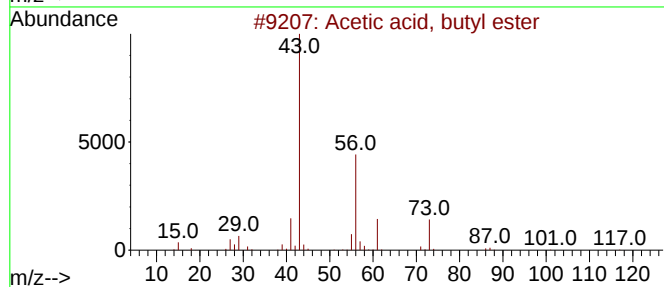
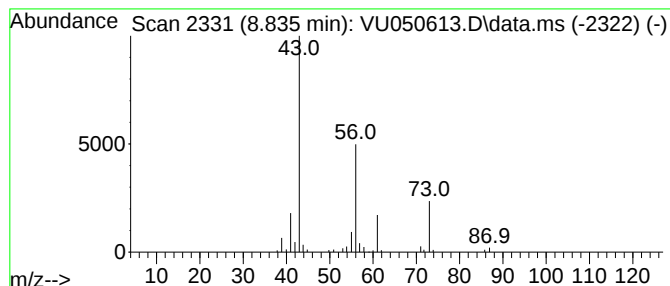
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Quant Title : VOC Analysis

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

Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.68 ug/L	68272	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
Data File : VU050613.D
Acq On : 03 Sep 2022 15:36
Operator : SY/MD
Sample : PB147438TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB438

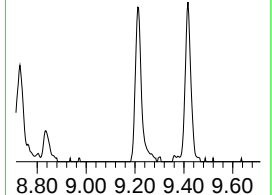
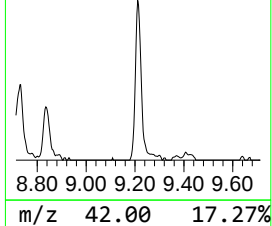
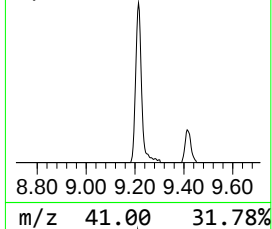
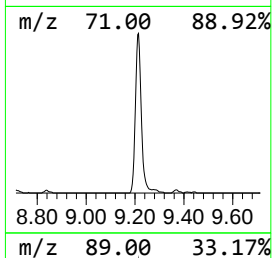
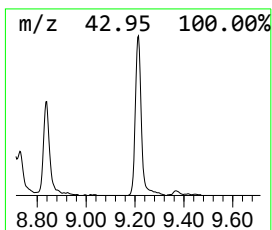
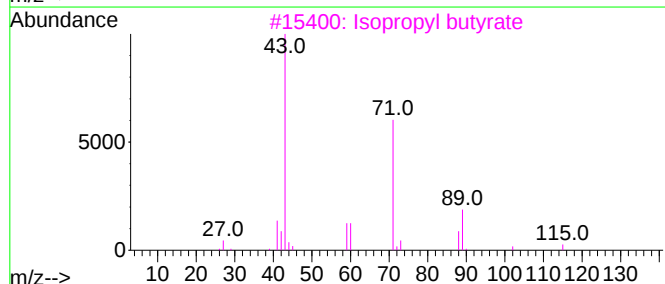
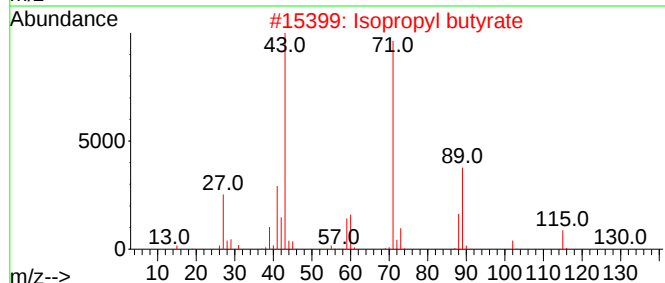
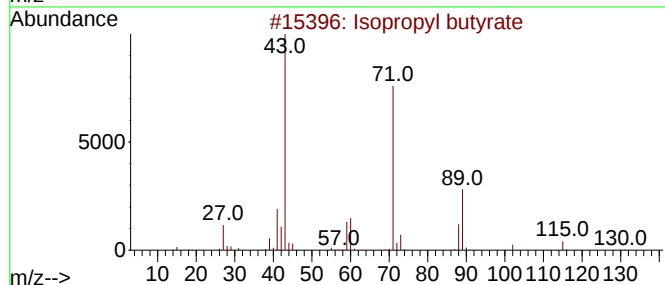
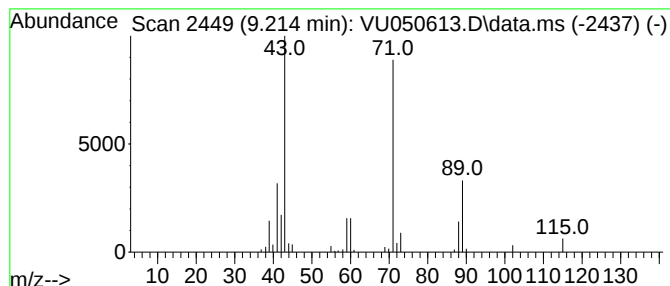
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Quant Title : VOC Analysis

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.
9.214	8.91 ug/L	165488	Chlorobenzene-d5	9.417

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			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090322\
Data File : VU050613.D
Acq On : 03 Sep 2022 15:36
Operator : SY/MD
Sample : PB147438TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB438

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.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	18.4	ug/L	283505	1	6.250	771993	50.0
Propanoic acid,...	7.742	3.3	ug/L	50504	1	6.250	771993	50.0
Propanoic acid,...	8.468	3.2	ug/L	59633	2	9.417	928275	50.0
Acetic acid, bu...	8.835	3.7	ug/L	68272	2	9.417	928275	50.0
Isopropyl butyrate	9.214	8.9	ug/L	165488	2	9.417	928275	50.0