

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049359.D
 Acq On : 22 Jun 2022 18:07
 Operator : SY/MD
 Sample : N3392-14 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEY9

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\SFAMULM061022WMA.M

Title : VOC Analysis

Signal : TIC: VU049359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	74	80	94	rBV	67114	75786	10.92%	1.130%
2	1.903	168	175	193	rVB	56828	78474	11.31%	1.170%
3	2.562	369	380	393	rBV	111417	179314	25.85%	2.673%
4	2.716	425	428	431	rBV	252	137	0.02%	0.002%
5	2.764	434	443	445	rBV2	1803	2553	0.37%	0.038%
6	2.838	460	466	471	rBV2	432	494	0.07%	0.007%
7	2.944	494	499	500	rBV2	621	505	0.07%	0.008%
8	3.044	520	530	544	rVB	5075	8731	1.26%	0.130%
9	3.186	558	574	589	rBV	27607	64226	9.26%	0.958%
10	3.308	610	612	613	rBV	282	132	0.02%	0.002%
11	3.430	647	650	653	rBV	213	158	0.02%	0.002%
12	3.565	690	692	694	rBV2	170	85	0.01%	0.001%
13	3.739	741	746	747	rBV	142	135	0.02%	0.002%
14	3.777	752	758	760	rBV2	195	215	0.03%	0.003%
15	3.790	760	762	766	rVB	366	203	0.03%	0.003%
16	3.906	795	798	800	rBV	216	129	0.02%	0.002%
17	4.173	879	881	883	rBV	163	75	0.01%	0.001%
18	4.298	914	920	921	rBV2	284	234	0.03%	0.003%
19	4.417	955	957	961	rVB3	345	239	0.03%	0.004%
20	4.440	961	964	965	rBV	112	60	0.01%	0.001%
21	4.497	980	982	986	rVB2	212	104	0.01%	0.002%
22	4.514	986	987	988	rVB	124	24	0.00%	0.000%
23	4.526	989	991	992	rBV	190	70	0.01%	0.001%
24	4.562	998	1002	1003	rBV2	225	170	0.02%	0.003%
25	4.616	1007	1019	1047	rVV	125946	300534	43.32%	4.481%
26	5.002	1135	1139	1141	rBV2	272	243	0.04%	0.004%
27	5.063	1143	1158	1178	rVB	137486	301723	43.49%	4.498%
28	5.282	1221	1226	1230	rBV3	535	510	0.07%	0.008%
29	5.398	1259	1262	1264	rBV	220	123	0.02%	0.002%
30	5.488	1288	1290	1291	rBV2	170	53	0.01%	0.001%
31	5.565	1311	1314	1316	rBV	241	149	0.02%	0.002%
32	5.722	1342	1363	1390	rBV2	248671	693748	100.00%	10.343%
33	5.912	1409	1422	1434	rBV	9809	18684	2.69%	0.279%
34	6.025	1451	1457	1458	rBV2	232	204	0.03%	0.003%
35	6.076	1470	1473	1476	rBV2	162	112	0.02%	0.002%
36	6.099	1477	1480	1483	rBV	313	260	0.04%	0.004%

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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\SFAMULM061022WMA.M
 Title : VOC Analysis

37	6.163	1491	1500	1501	rBV3	956	1258	0.18%	0.019%
38	6.247	1514	1526	1549	rBV	301014	562349	81.06%	8.384%
39	6.690	1650	1664	1680	rBV2	182777	353116	50.90%	5.265%
40	6.857	1711	1716	1719	rBV2	462	319	0.05%	0.005%
41	6.925	1727	1737	1750	rBV	5104	10359	1.49%	0.154%
42	7.038	1761	1772	1789	rBV	106273	184532	26.60%	2.751%
43	7.382	1874	1879	1883	rVB2	353	329	0.05%	0.005%
44	7.404	1883	1886	1891	rBV2	303	254	0.04%	0.004%
45	7.430	1891	1894	1898	rBV2	307	237	0.03%	0.004%
46	7.472	1903	1907	1911	rBV2	423	382	0.06%	0.006%
47	7.507	1916	1918	1920	rBV	135	60	0.01%	0.001%
48	7.565	1923	1936	1951	rBV	95545	165582	23.87%	2.469%
49	7.738	1982	1990	2000	rVB3	18251	29134	4.20%	0.434%
50	7.896	2026	2039	2060	rBV	291548	502113	72.38%	7.486%
51	8.102	2100	2103	2105	rBV2	181	119	0.02%	0.002%
52	8.176	2110	2126	2142	rVV2	71669	147685	21.29%	2.202%
53	8.423	2200	2203	2204	rBV	252	146	0.02%	0.002%
54	8.465	2206	2216	2230	rVV2	23501	38787	5.59%	0.578%
55	8.632	2256	2268	2288	rBV	329045	591844	85.31%	8.824%
56	8.835	2322	2331	2348	rVB	27680	45311	6.53%	0.676%
57	8.986	2376	2378	2380	rBV2	181	79	0.01%	0.001%
58	9.002	2380	2383	2389	rVB2	383	302	0.04%	0.005%
59	9.066	2401	2403	2406	rBV2	176	56	0.01%	0.001%
60	9.086	2407	2409	2413	rVB2	330	208	0.03%	0.003%
61	9.111	2414	2417	2420	rVB3	240	155	0.02%	0.002%
62	9.208	2437	2447	2464	rBV	65866	103945	14.98%	1.550%
63	9.343	2484	2489	2491	rBV2	713	625	0.09%	0.009%
64	9.417	2500	2512	2537	rVB	402281	661035	95.28%	9.855%
65	9.565	2557	2558	2560	rBV	229	100	0.01%	0.001%
66	9.648	2577	2584	2589	rVB2	975	1081	0.16%	0.016%
67	9.767	2619	2621	2622	rBV	171	50	0.01%	0.001%
68	9.790	2626	2628	2631	rVB2	211	90	0.01%	0.001%
69	9.918	2661	2668	2676	rVB6	1000	1694	0.24%	0.025%
70	9.963	2676	2682	2688	rBV2	463	624	0.09%	0.009%
71	10.073	2708	2716	2727	rVB4	4815	7067	1.02%	0.105%
72	10.449	2831	2833	2837	rVB2	344	218	0.03%	0.003%
73	10.754	2916	2928	2950	rVB	290479	467535	67.39%	6.970%
74	11.111	3036	3039	3041	rBV	354	208	0.03%	0.003%
75	11.433	3136	3139	3144	rBV	409	335	0.05%	0.005%
76	11.812	3245	3257	3272	rBV	375515	604272	87.10%	9.009%

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ClientSampleId :
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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\SFAMULM061022WMA.M
Title : VOC Analysis

77	12.192	3363	3375	3398	rBV	300447	494524	71.28%	7.373%
78	12.549	3482	3486	3489	rBV3	384	358	0.05%	0.005%
79	13.767	3861	3865	3869	rBV3	381	409	0.06%	0.006%

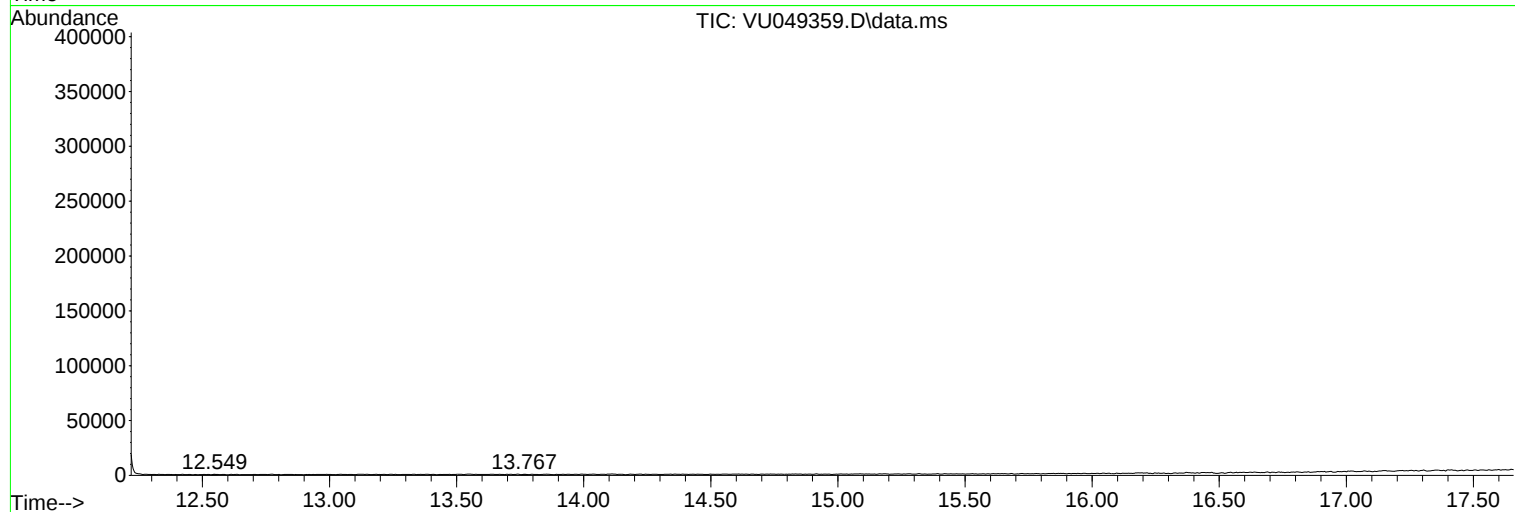
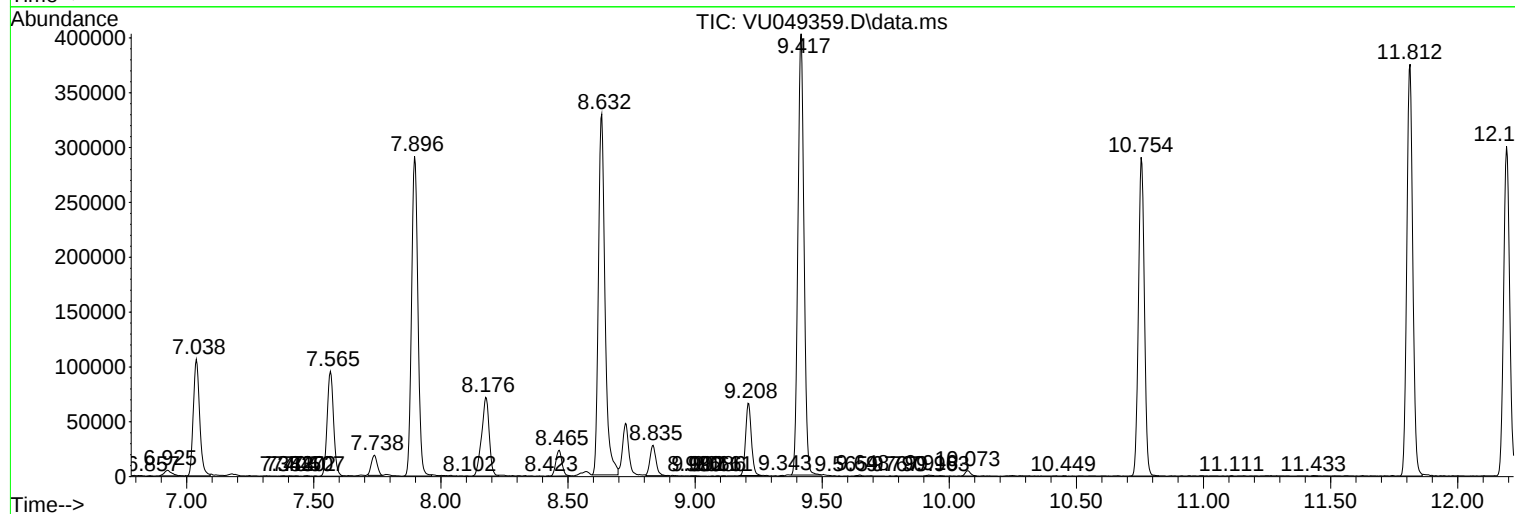
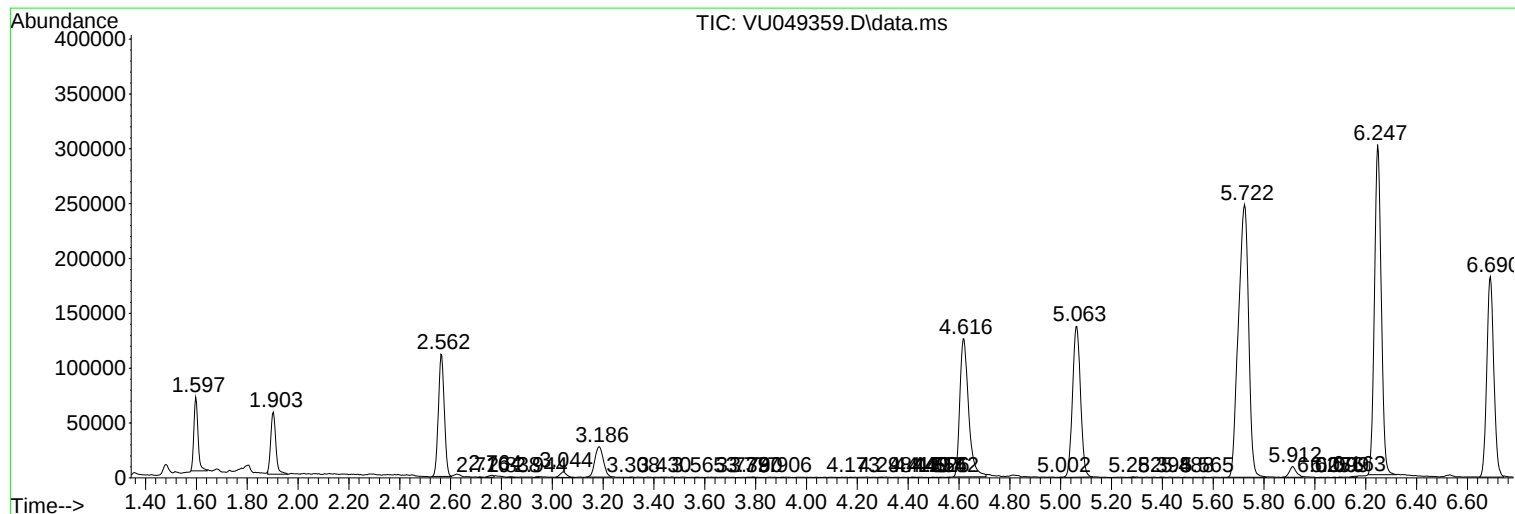
Sum of corrected areas: 6707482

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Instrument :
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ClientSampleId :
EXEY9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY9

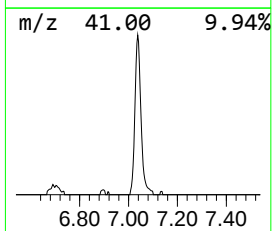
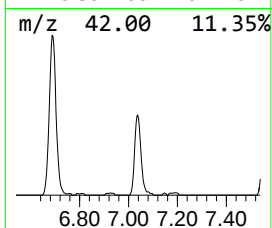
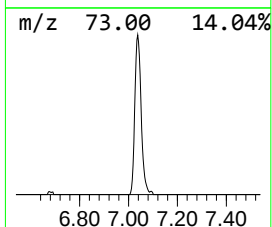
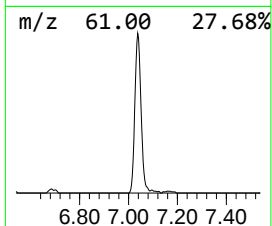
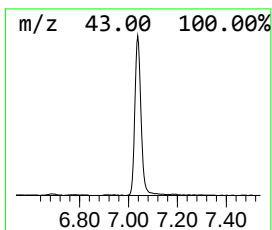
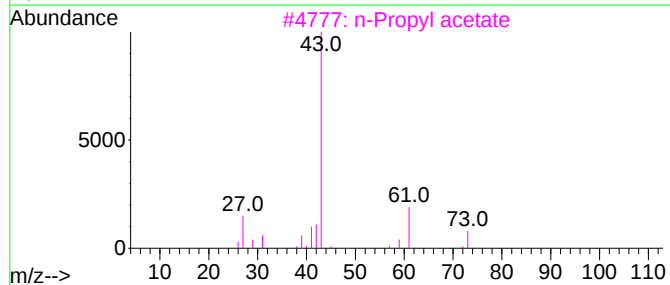
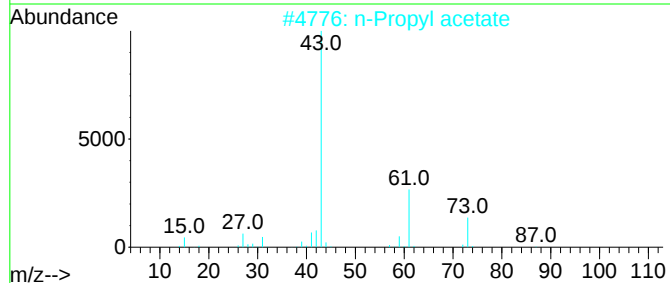
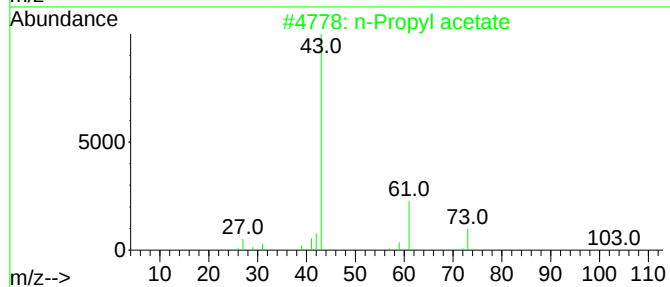
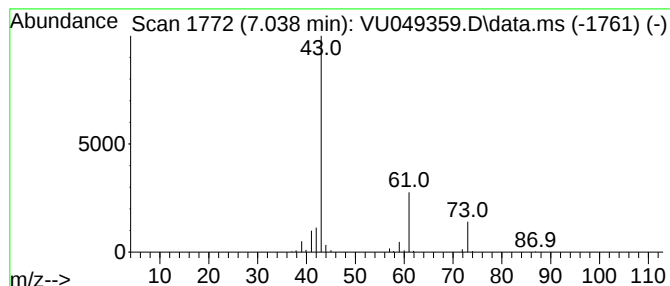
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	16.41 ug/L	184532	1,4-Difluorobenzene	6.247

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	78
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY9

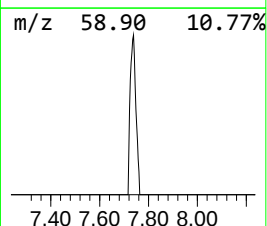
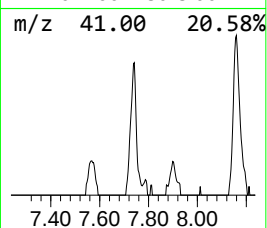
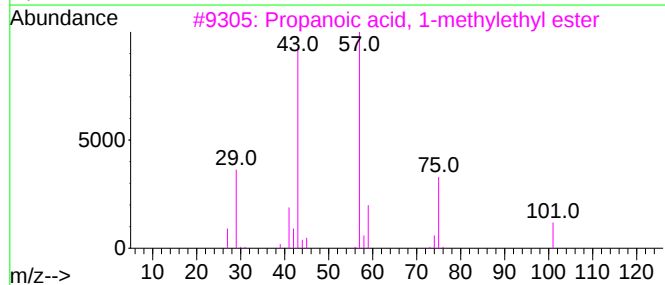
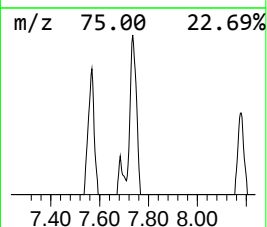
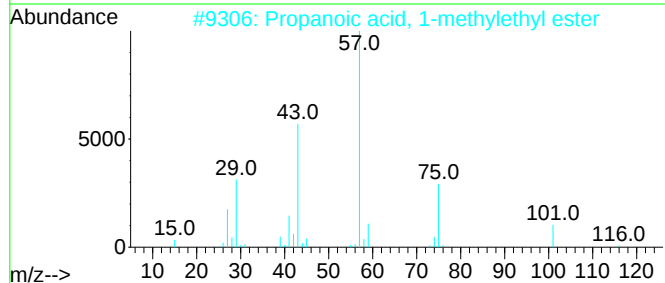
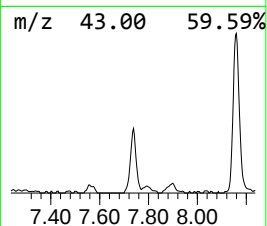
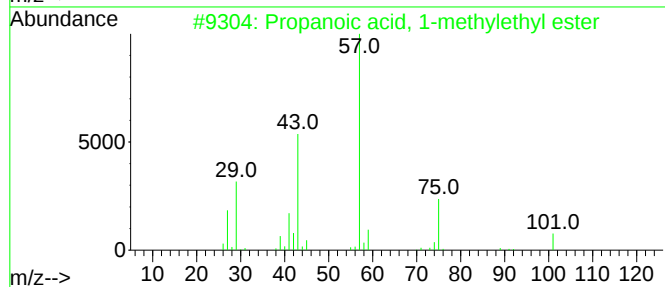
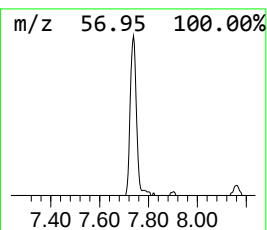
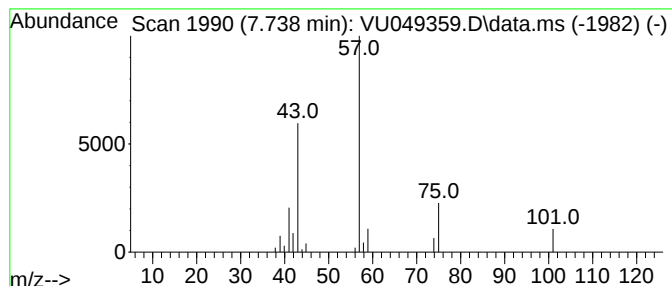
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.59 ug/L	29134	1,4-Difluorobenzene	6.247

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	56
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



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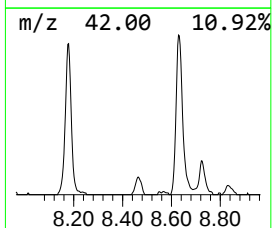
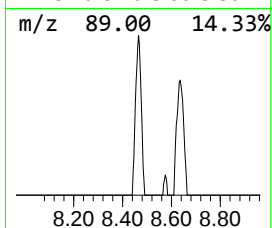
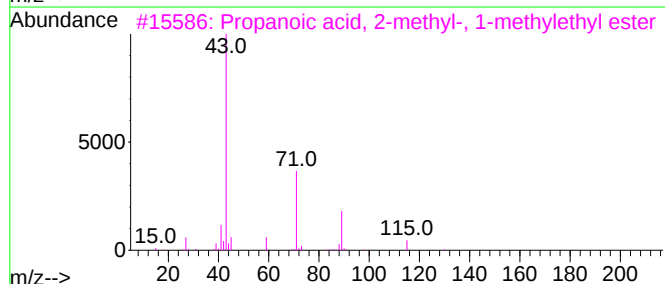
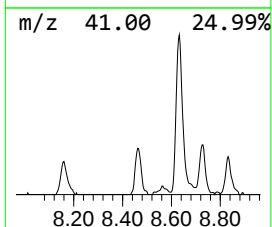
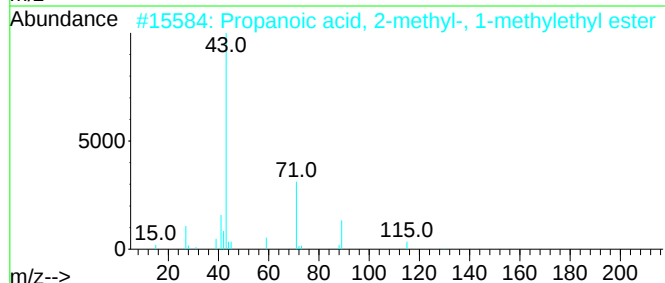
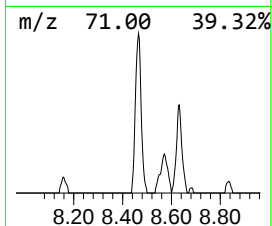
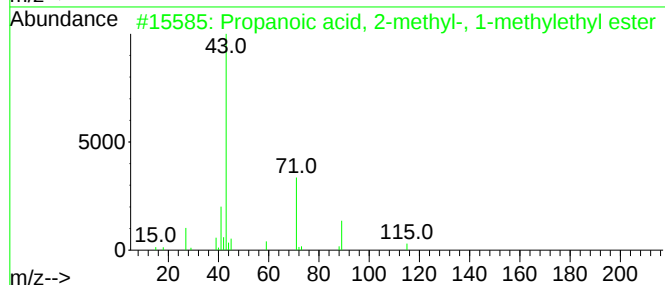
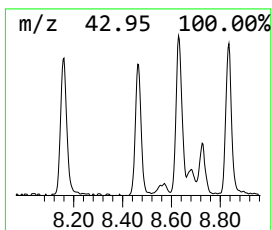
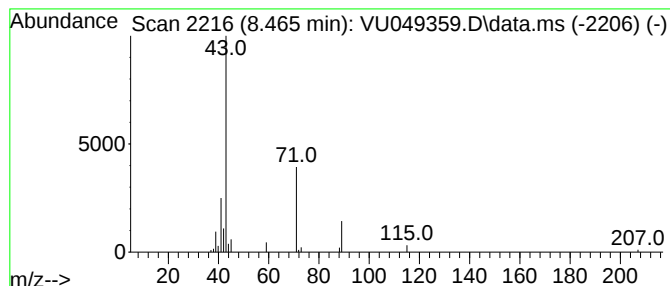
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.93 ug/L	38787	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	72
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



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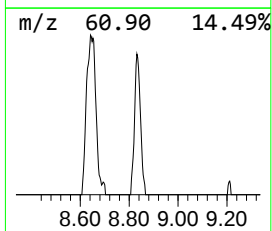
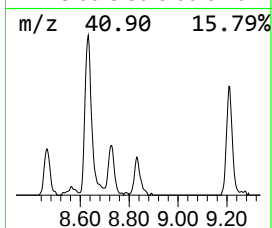
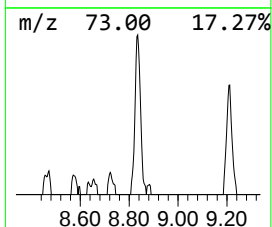
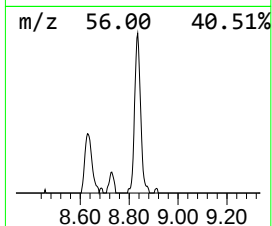
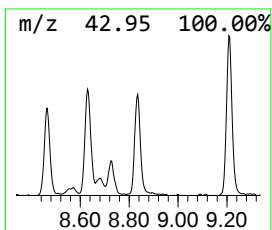
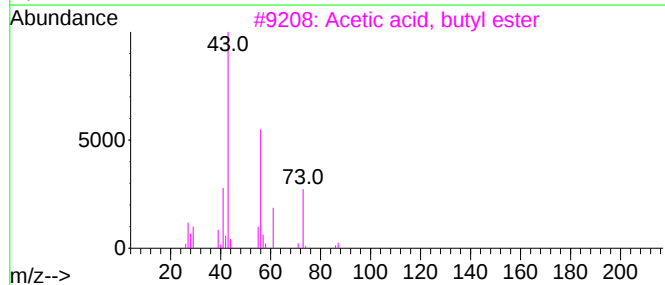
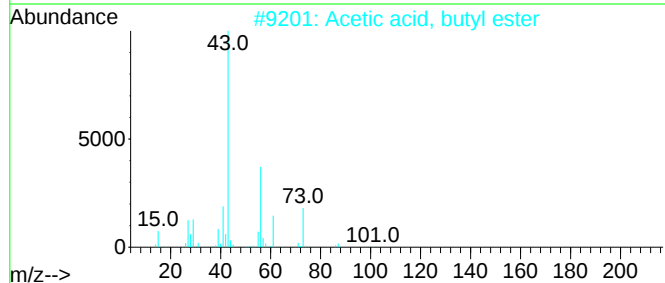
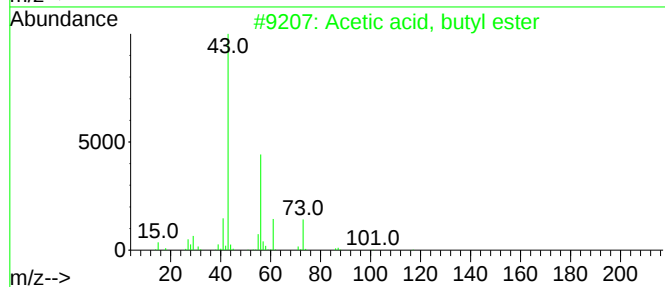
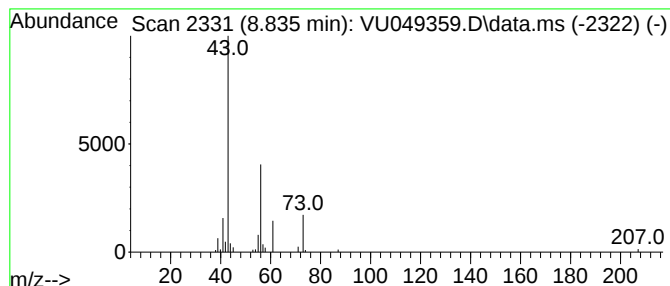
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.43 ug/L	45311	Chlorobenzene-d5	9.417

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	74
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Isobutyl acetate	116	C6H12O2	000110-19-0	39
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049359.D
Acq On : 22 Jun 2022 18:07
Operator : SY/MD
Sample : N3392-14 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY9

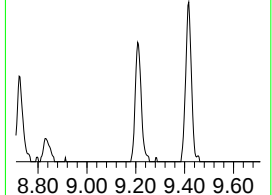
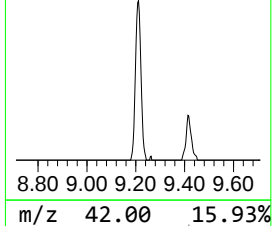
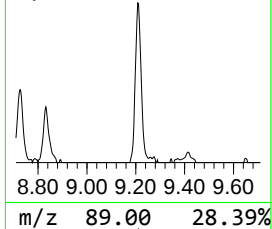
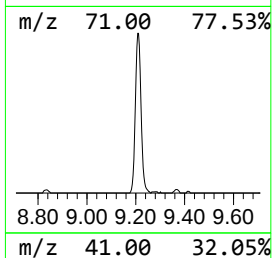
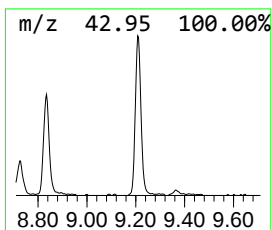
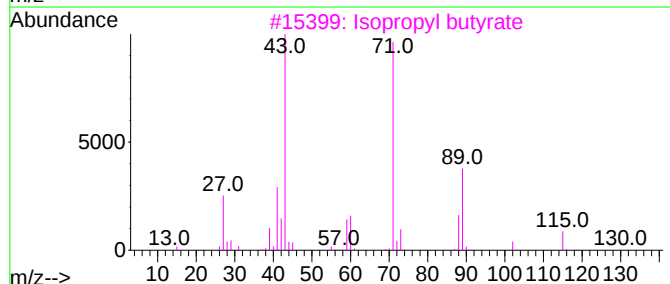
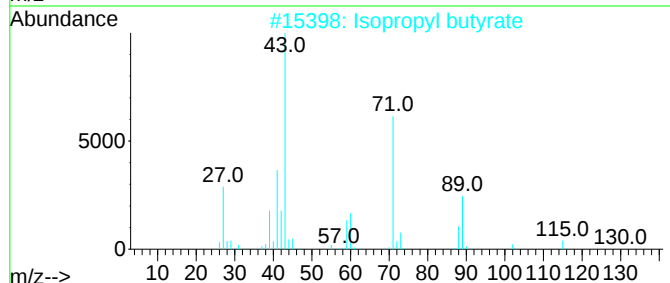
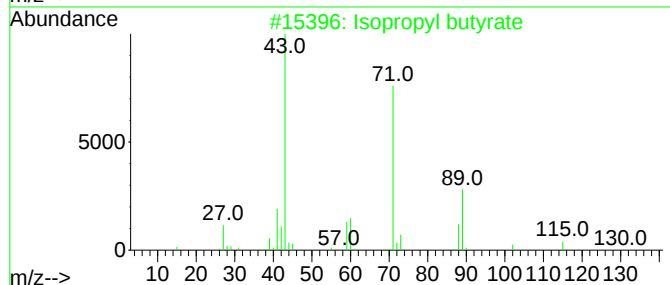
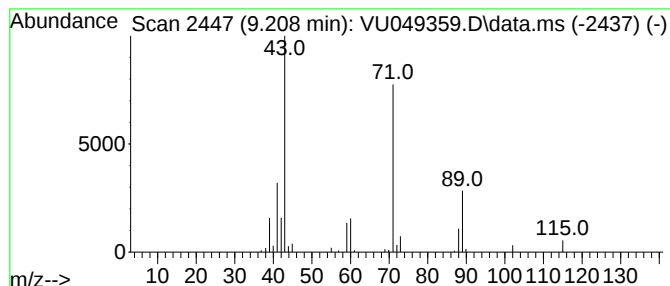
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Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.208	7.86 ug/L	103945	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	83
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049359.D
Acq On : 22 Jun 2022 18:07
Operator : SY/MD
Sample : N3392-14 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.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	7.038	16.4	ug/L	184532	1	6.247	562349	50.0
Propanoic acid,...	7.738	2.6	ug/L	29134	1	6.247	562349	50.0
Propanoic acid,...	8.465	2.9	ug/L	38787	2	9.417	661035	50.0
Acetic acid, bu...	8.835	3.4	ug/L	45311	2	9.417	661035	50.0
Isopropyl butyrate	9.208	7.9	ug/L	103945	2	9.417	661035	50.0