

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049364.D
 Acq On : 22 Jun 2022 20:04
 Operator : SY/MD
 Sample : N3392-19 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEZ4

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: VU049364.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	73	80	96	rBV	61851	72744	10.51%	1.046%
2	1.903	169	175	186	rVB	55096	71463	10.33%	1.027%
3	2.514	361	365	367	rBV	322	274	0.04%	0.004%
4	2.565	368	381	395	rVV	110360	176514	25.51%	2.538%
5	2.633	398	402	412	rVB3	2913	4242	0.61%	0.061%
6	2.989	511	513	518	rVB3	432	333	0.05%	0.005%
7	3.044	520	530	542	rBV4	3845	7232	1.04%	0.104%
8	3.092	542	545	547	rBV2	319	248	0.04%	0.004%
9	3.182	558	573	596	rBV2	21789	54854	7.93%	0.789%
10	3.356	623	627	630	rBV2	249	226	0.03%	0.003%
11	3.491	666	669	672	rBV	350	206	0.03%	0.003%
12	3.507	672	674	680	rVB2	278	247	0.04%	0.004%
13	3.623	704	710	713	rBV3	280	299	0.04%	0.004%
14	4.063	840	847	851	rBV3	331	346	0.05%	0.005%
15	4.372	939	943	952	rBV2	355	428	0.06%	0.006%
16	4.517	983	988	993	rVB2	203	284	0.04%	0.004%
17	4.626	1009	1022	1067	rBV	117175	313580	45.31%	4.508%
18	4.819	1074	1082	1096	rVB3	2187	4646	0.67%	0.067%
19	4.893	1102	1105	1109	rVB3	389	273	0.04%	0.004%
20	4.973	1125	1130	1132	rBV	299	253	0.04%	0.004%
21	5.063	1142	1158	1183	rVV	134998	296142	42.79%	4.258%
22	5.285	1221	1227	1230	rBV2	347	335	0.05%	0.005%
23	5.607	1319	1327	1330	rBV3	363	517	0.07%	0.007%
24	5.723	1342	1363	1392	rVV2	250273	692068	100.00%	9.950%
25	5.915	1413	1423	1435	rBV2	10331	20645	2.98%	0.297%
26	5.983	1443	1444	1449	rVB2	594	371	0.05%	0.005%
27	6.108	1478	1483	1486	rBV3	314	215	0.03%	0.003%
28	6.179	1492	1505	1506	rBV2	981	1493	0.22%	0.021%
29	6.247	1513	1526	1545	rBV	304468	580836	83.93%	8.351%
30	6.526	1609	1613	1621	rVB5	1561	2066	0.30%	0.030%
31	6.591	1629	1633	1634	rBV2	365	248	0.04%	0.004%
32	6.690	1651	1664	1682	rBV	181338	351929	50.85%	5.060%
33	6.755	1682	1684	1689	rVB4	409	304	0.04%	0.004%
34	6.809	1696	1701	1702	rVB2	445	306	0.04%	0.004%
35	6.829	1702	1707	1711	rVB2	368	285	0.04%	0.004%
36	6.931	1727	1739	1753	rBV	5701	12916	1.87%	0.186%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	7.038	1760	1772	1794	rBV2	120025	220790	31.90%	3.174%
38	7.182	1809	1817	1831	rVB9	2420	5238	0.76%	0.075%
39	7.247	1831	1837	1838	rBV2	369	370	0.05%	0.005%
40	7.417	1885	1890	1893	rVV2	385	363	0.05%	0.005%
41	7.565	1924	1936	1959	rBV	91758	161505	23.34%	2.322%
42	7.684	1966	1973	1974	rBV2	1316	1104	0.16%	0.016%
43	7.738	1979	1990	2001	rVV2	22829	38773	5.60%	0.557%
44	7.793	2001	2007	2013	rVB6	1343	1839	0.27%	0.026%
45	7.896	2026	2039	2058	rBV	286166	494977	71.52%	7.116%
46	8.044	2080	2085	2088	rBV4	466	533	0.08%	0.008%
47	8.176	2107	2126	2142	rBV2	73874	159850	23.10%	2.298%
48	8.362	2181	2184	2187	rVB2	392	215	0.03%	0.003%
49	8.388	2187	2192	2194	rBV3	507	411	0.06%	0.006%
50	8.465	2205	2216	2229	rBV	29023	47564	6.87%	0.684%
51	8.574	2235	2250	2257	rBV6	5119	11493	1.66%	0.165%
52	8.636	2257	2269	2289	rVV	323854	595739	86.08%	8.565%
53	8.729	2290	2298	2315	rVB	55385	90373	13.06%	1.299%
54	8.835	2322	2331	2348	rVV	34940	56112	8.11%	0.807%
55	8.964	2368	2371	2375	rVB3	394	252	0.04%	0.004%
56	9.102	2409	2414	2418	rBV2	265	275	0.04%	0.004%
57	9.211	2437	2448	2464	rBV2	84986	132567	19.16%	1.906%
58	9.327	2481	2484	2489	rVB3	238	218	0.03%	0.003%
59	9.365	2489	2496	2498	rBV4	1592	1699	0.25%	0.024%
60	9.417	2500	2512	2540	rVB	411805	687184	99.29%	9.880%
61	9.648	2577	2584	2591	rVB3	1076	1445	0.21%	0.021%
62	9.825	2635	2639	2642	rVB2	306	207	0.03%	0.003%
63	9.925	2661	2670	2677	rBV3	1163	1926	0.28%	0.028%
64	9.999	2690	2693	2695	rBV	305	221	0.03%	0.003%
65	10.076	2708	2717	2724	rBV3	5909	8689	1.26%	0.125%
66	10.298	2784	2786	2791	rVB2	525	312	0.05%	0.004%
67	10.372	2804	2809	2811	rBV2	267	248	0.04%	0.004%
68	10.446	2829	2832	2835	rBV	437	374	0.05%	0.005%
69	10.533	2856	2859	2863	rVV3	246	229	0.03%	0.003%
70	10.758	2914	2929	2952	rBV	279452	460266	66.51%	6.617%
71	11.021	3006	3011	3013	rBV	296	224	0.03%	0.003%
72	11.124	3040	3043	3048	rBV2	313	271	0.04%	0.004%
73	11.214	3068	3071	3076	rBV2	289	221	0.03%	0.003%
74	11.471	3145	3151	3152	rBV2	191	206	0.03%	0.003%
75	11.664	3209	3211	3215	rBV3	287	201	0.03%	0.003%
76	11.812	3244	3257	3279	rBV	375667	609180	88.02%	8.758%

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

77	12.192	3357	3375	3403	rBV	296090	484895	70.06%	6.971%
78	12.436	3448	3451	3456	rVB2	390	315	0.05%	0.005%
79	12.471	3459	3462	3466	rBV2	258	228	0.03%	0.003%
80	12.539	3479	3483	3485	rBV2	359	280	0.04%	0.004%
81	12.774	3554	3556	3561	rVB3	406	390	0.06%	0.006%
82	12.941	3606	3608	3611	rBV2	319	229	0.03%	0.003%
83	13.073	3646	3649	3655	rBV3	221	222	0.03%	0.003%
84	13.793	3870	3873	3876	rBV2	313	235	0.03%	0.003%
85	13.915	3908	3911	3913	rBV2	368	207	0.03%	0.003%
86	13.963	3923	3926	3932	rBV3	331	292	0.04%	0.004%
87	14.063	3954	3957	3960	rBV2	311	218	0.03%	0.003%
88	14.198	3996	3999	4003	rBV2	323	346	0.05%	0.005%
89	14.295	4026	4029	4035	rVB3	539	552	0.08%	0.008%
90	14.346	4042	4045	4047	rBV	312	204	0.03%	0.003%
91	14.436	4070	4073	4076	rVB3	411	240	0.03%	0.003%
92	14.925	4221	4225	4228	rBV2	357	351	0.05%	0.005%
93	14.999	4243	4248	4254	rVB3	580	748	0.11%	0.011%
94	15.031	4254	4258	4260	rBV2	314	290	0.04%	0.004%
95	15.433	4381	4383	4386	rBV2	479	326	0.05%	0.005%
96	15.809	4497	4500	4502	rBV3	655	428	0.06%	0.006%
97	15.876	4519	4521	4525	rBV	472	266	0.04%	0.004%
98	16.060	4575	4578	4580	rBV2	586	321	0.05%	0.005%
99	16.089	4585	4587	4592	rBV2	525	339	0.05%	0.005%
100	16.269	4640	4643	4644	rBV3	751	444	0.06%	0.006%

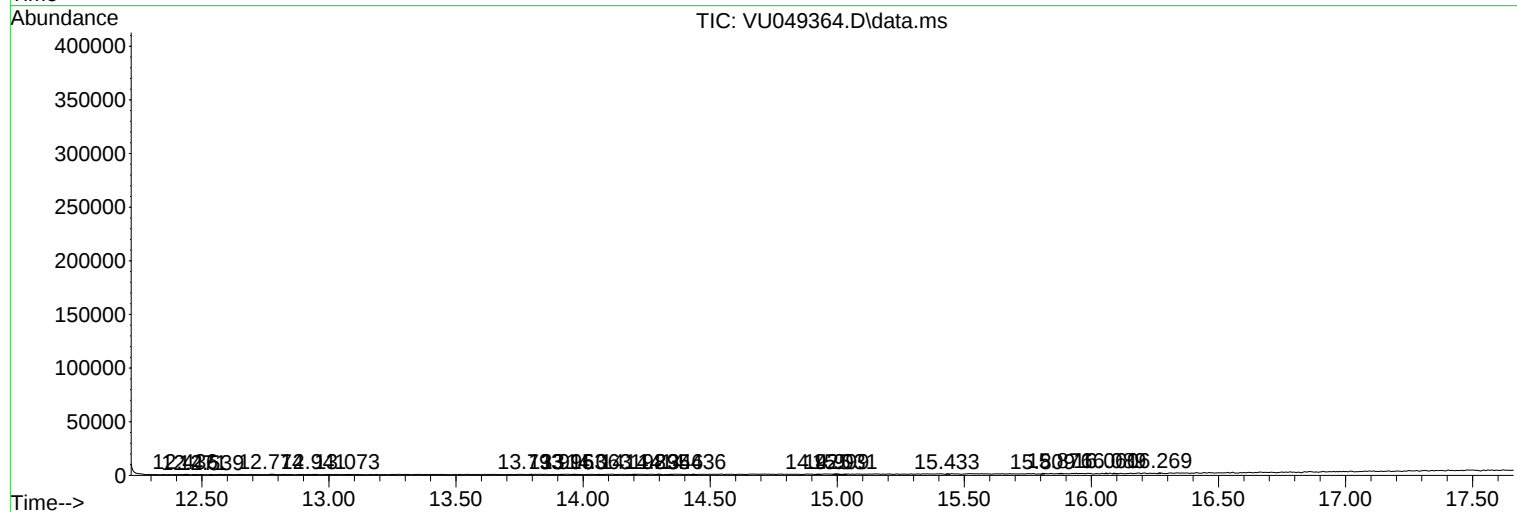
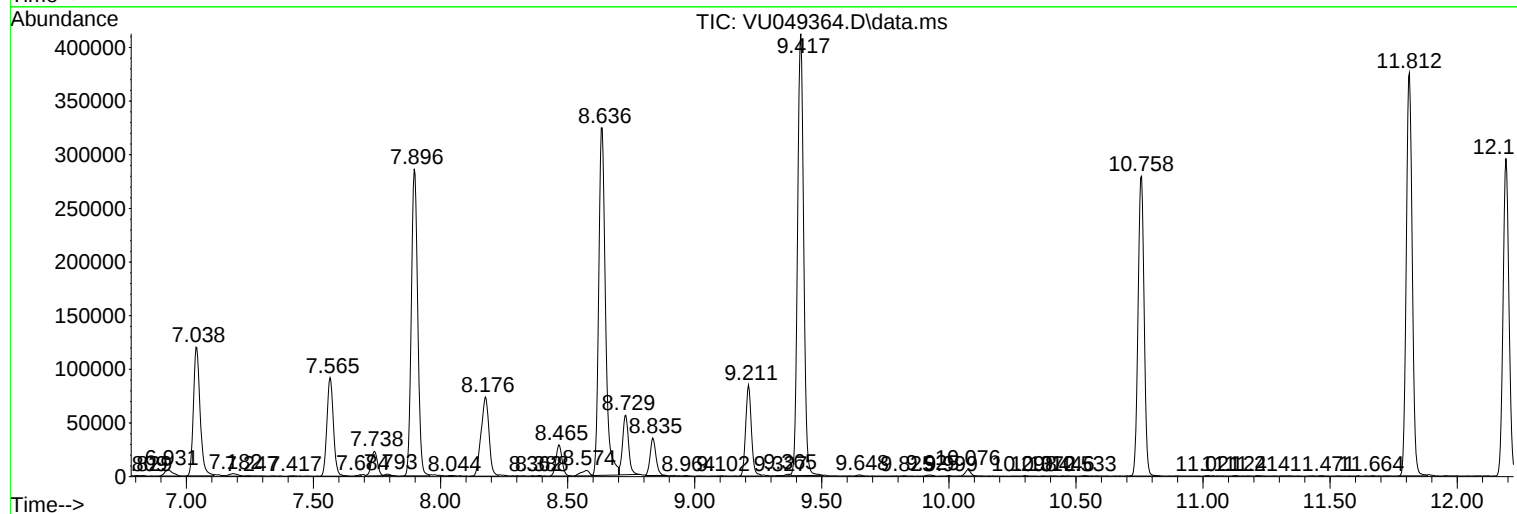
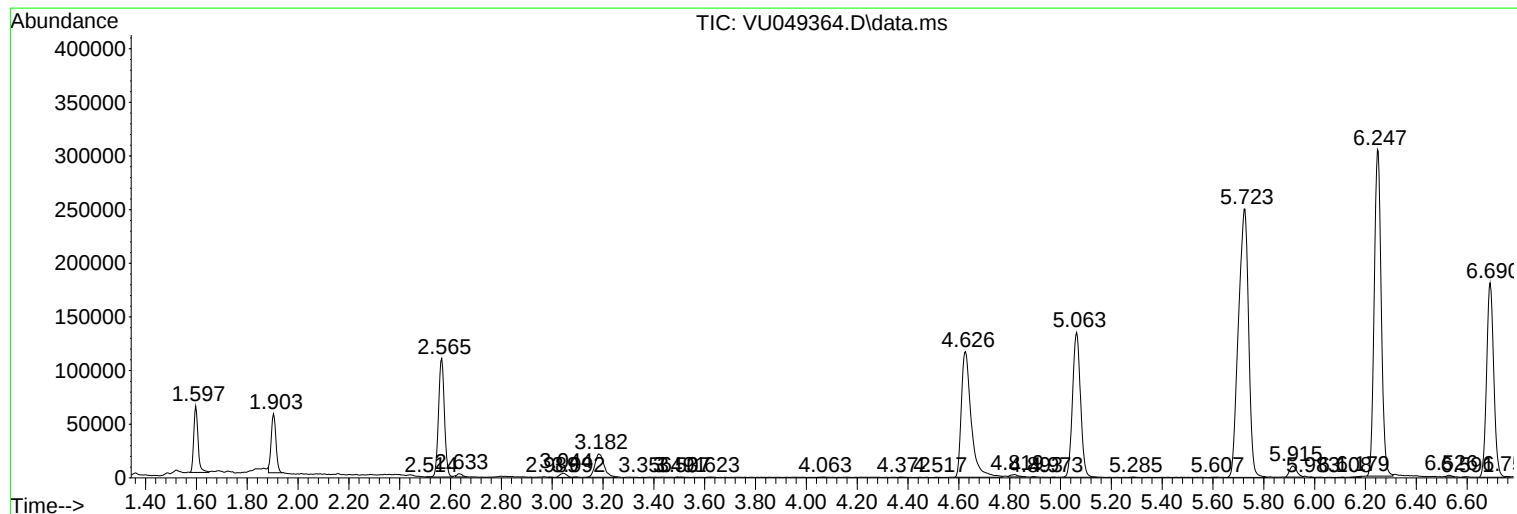
Sum of corrected areas: 6955398

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MSVOA_U
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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



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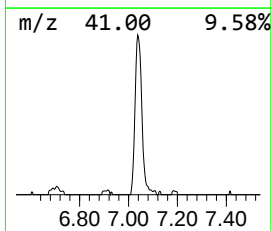
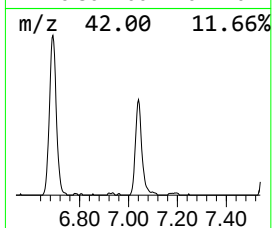
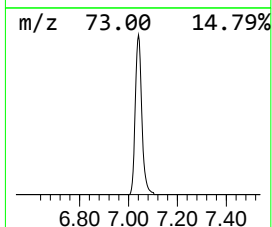
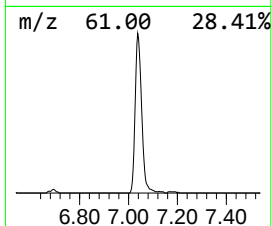
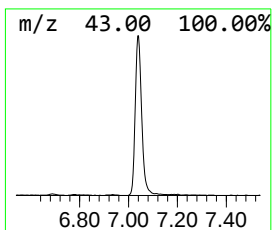
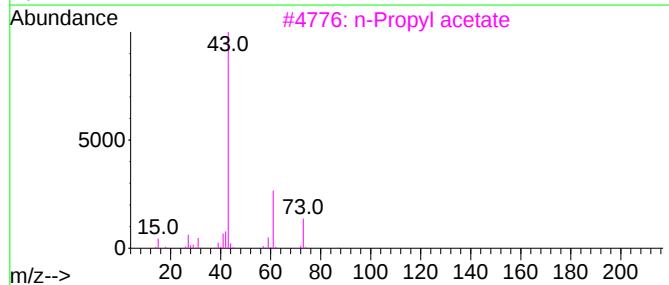
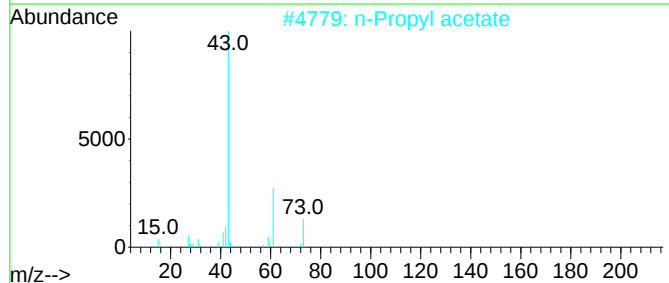
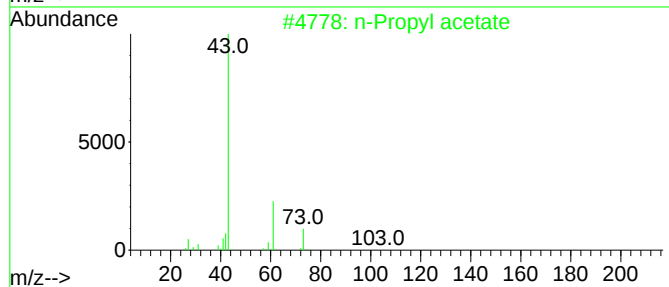
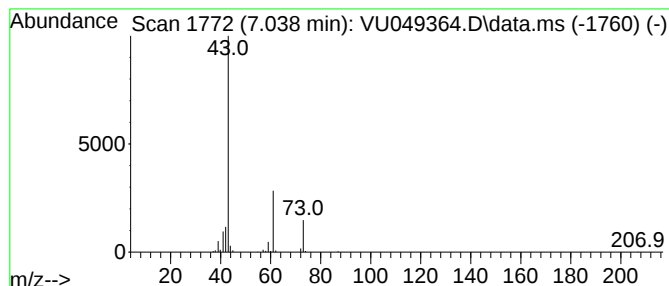
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	19.01 ug/L	220790	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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	64



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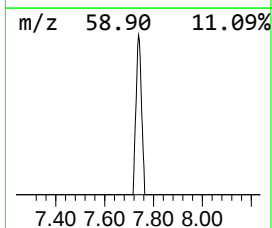
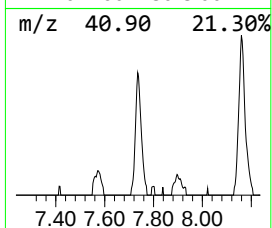
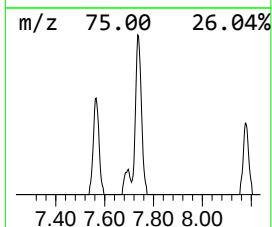
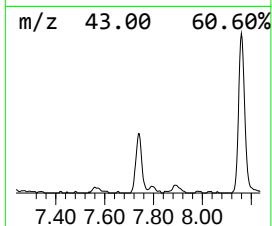
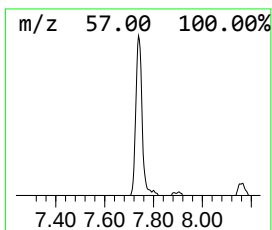
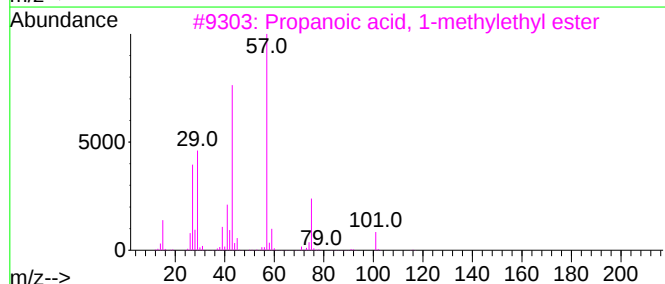
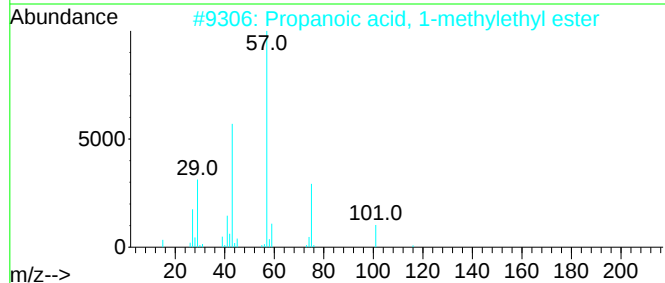
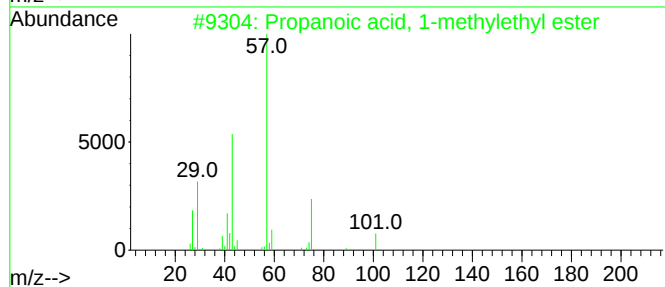
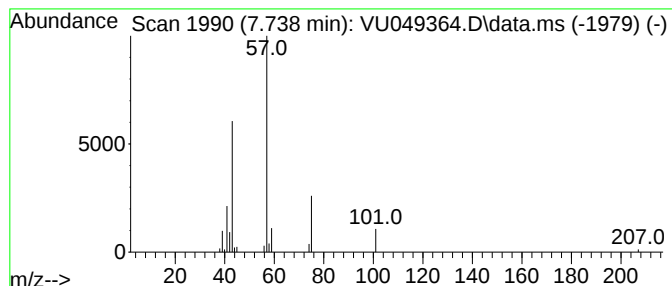
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	3.34 ug/L	38773	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	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36



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EXEZ4

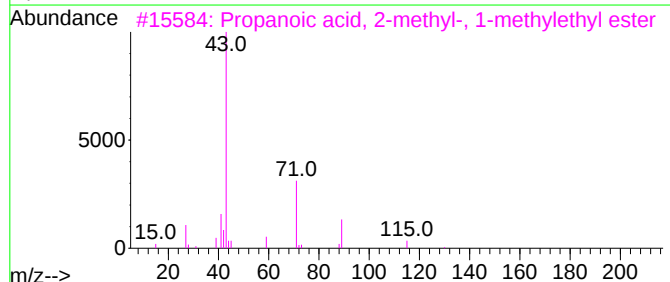
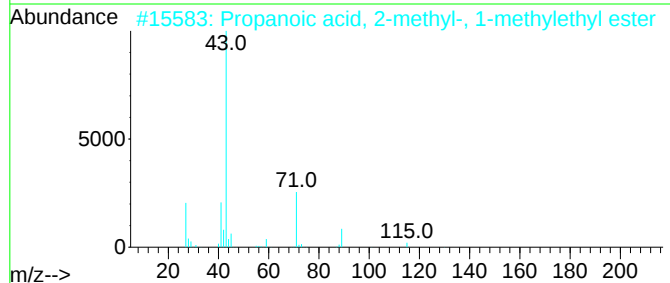
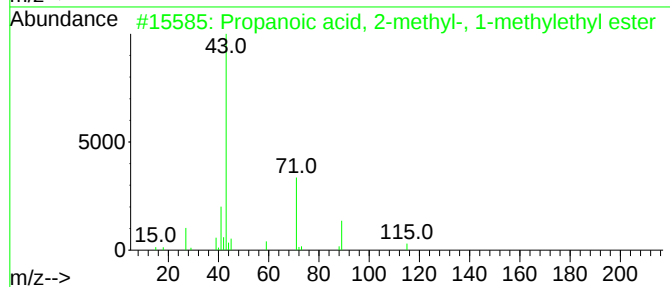
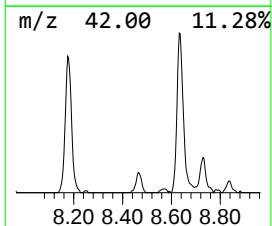
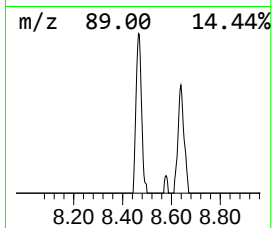
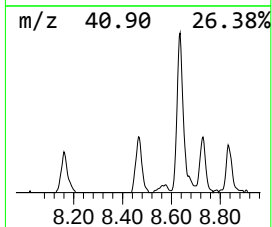
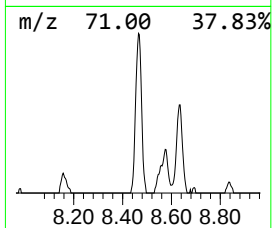
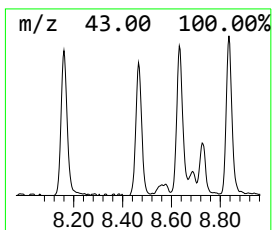
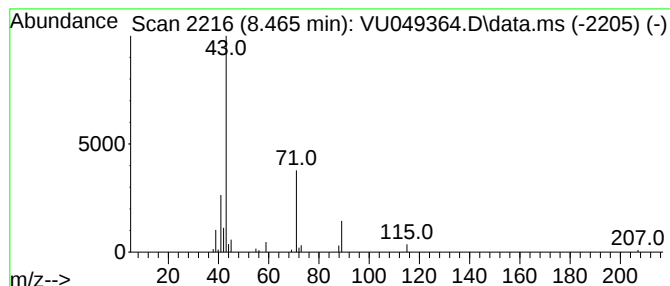
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.46 ug/L	47564	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	83
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049364.D
Acq On : 22 Jun 2022 20:04
Operator : SY/MD
Sample : N3392-19 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ4

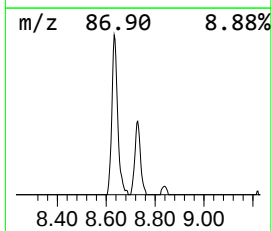
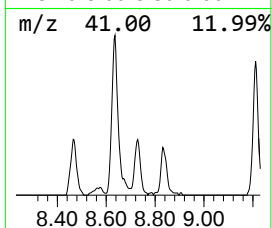
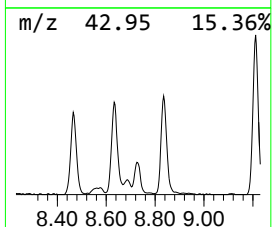
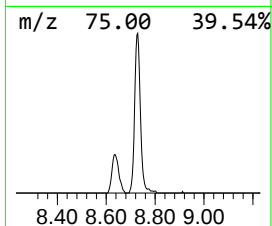
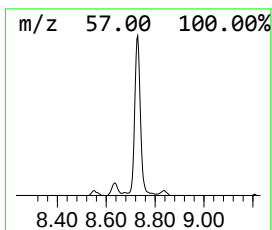
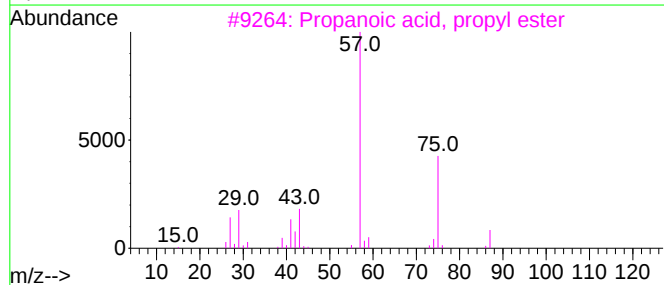
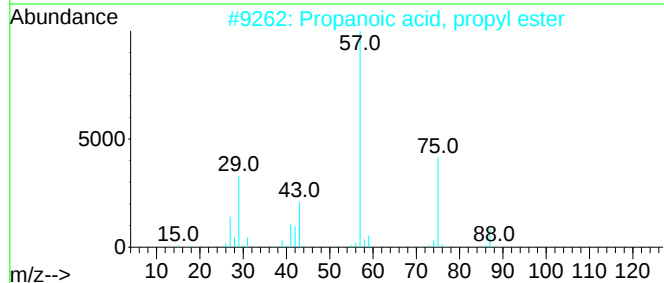
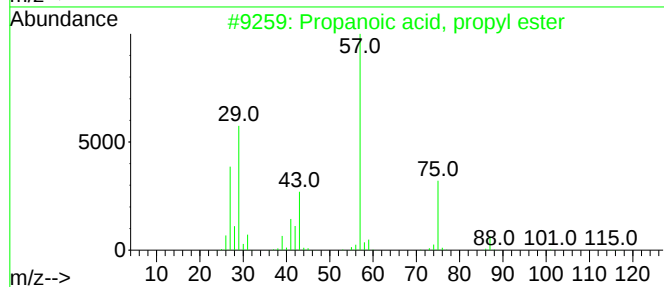
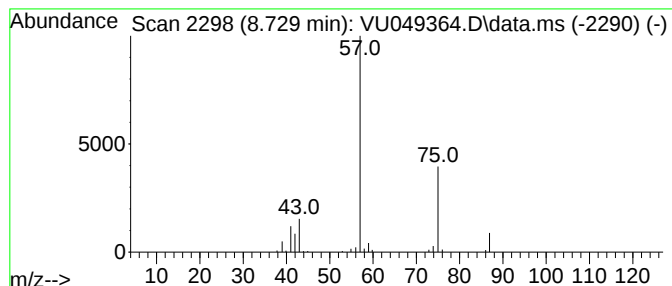
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	6.58 ug/L	90373	Chlorobenzene-d5	9.417

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	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049364.D
Acq On : 22 Jun 2022 20:04
Operator : SY/MD
Sample : N3392-19 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ4

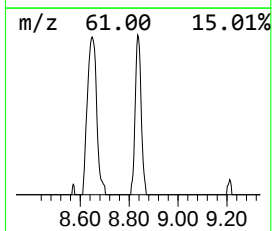
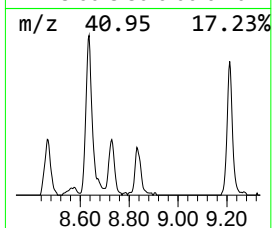
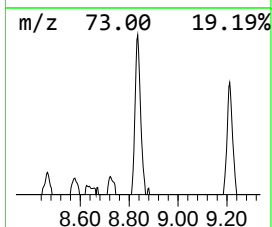
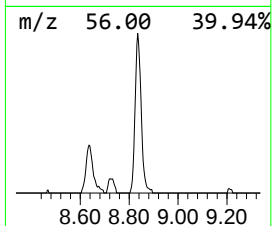
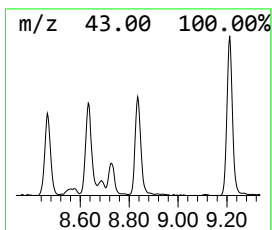
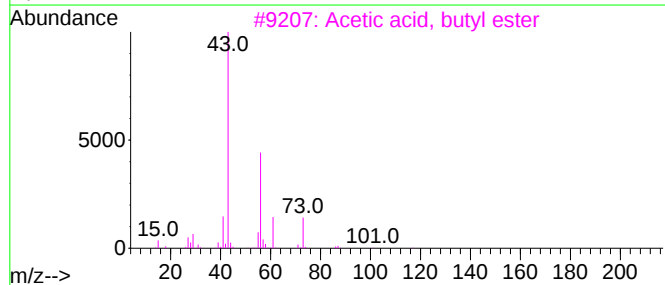
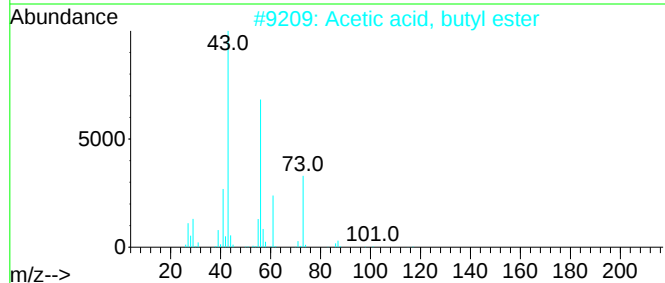
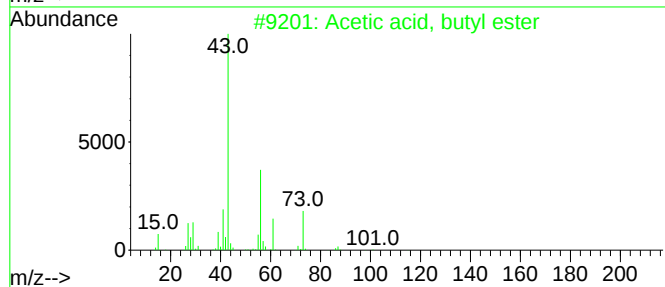
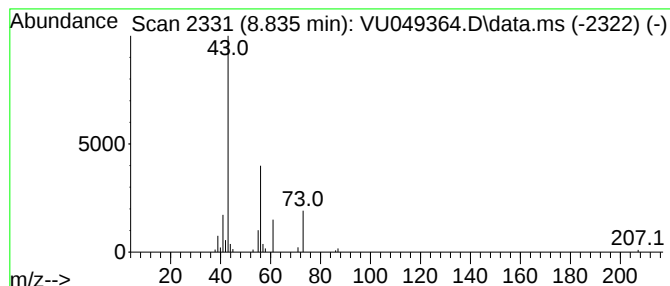
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Quant Title : VOC Analysis

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	4.08 ug/L	56112	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
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	72
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049364.D
Acq On : 22 Jun 2022 20:04
Operator : SY/MD
Sample : N3392-19 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ4

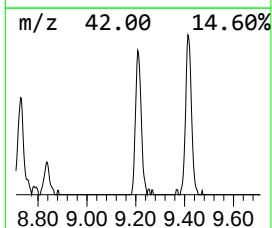
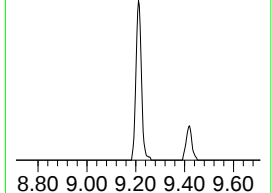
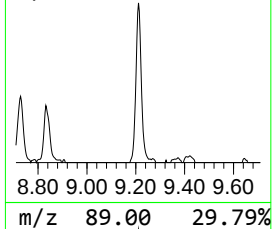
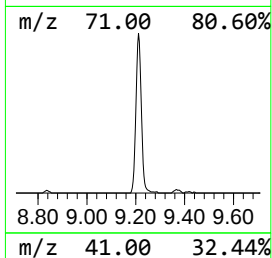
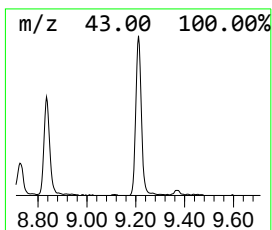
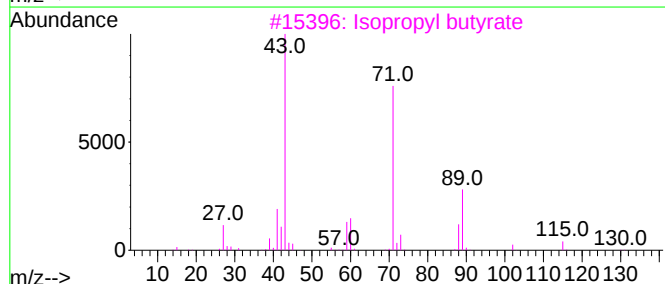
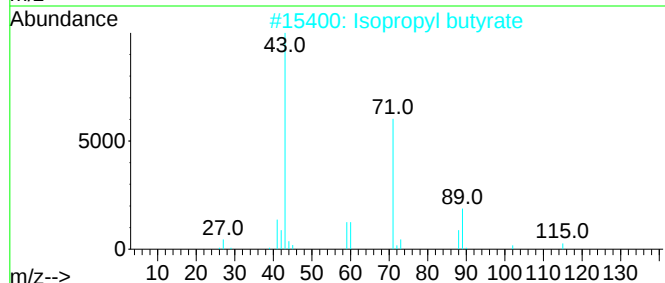
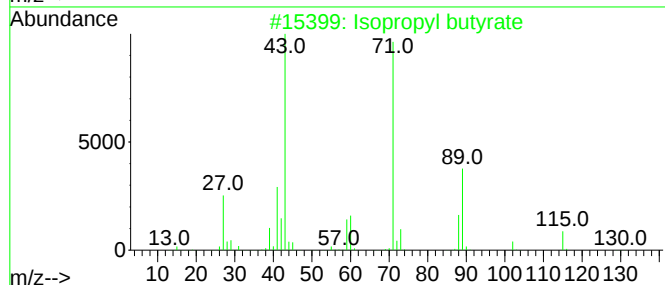
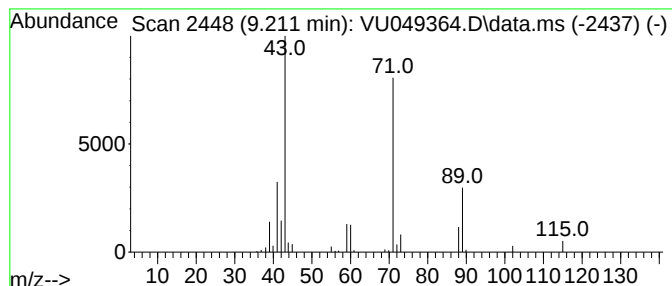
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	9.65 ug/L	132567	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	90
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049364.D
Acq On : 22 Jun 2022 20:04
Operator : SY/MD
Sample : N3392-19 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ4

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.038	19.0	ug/L	220790	1	6.247	580836	50.0
Propanoic acid,...	7.738	3.3	ug/L	38773	1	6.247	580836	50.0
Propanoic acid,...	8.465	3.5	ug/L	47564	2	9.417	687184	50.0
Propanoic acid,...	8.729	6.6	ug/L	90373	2	9.417	687184	50.0
Acetic acid, bu...	8.835	4.1	ug/L	56112	2	9.417	687184	50.0
Isopropyl butyrate	9.211	9.7	ug/L	132567	2	9.417	687184	50.0