

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049350.D
 Acq On : 22 Jun 2022 14:35
 Operator : SY/MD
 Sample : N3392-04 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEX9

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: VU049350.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	94	rBV	77233	87579	11.13%	1.169%
2	1.909	170	177	188	rVB	63194	77185	9.81%	1.030%
3	2.565	369	381	398	rBV	131172	213155	27.09%	2.845%
4	2.639	398	404	416	rBV	2635	4776	0.61%	0.064%
5	2.751	436	439	444	rBV	505	385	0.05%	0.005%
6	2.938	494	497	502	rBV3	482	497	0.06%	0.007%
7	3.041	520	529	545	rVB2	7247	13813	1.76%	0.184%
8	3.186	560	574	594	rVB	13159	30718	3.90%	0.410%
9	3.304	607	611	615	rVB2	316	249	0.03%	0.003%
10	3.385	634	636	641	rVB2	362	253	0.03%	0.003%
11	3.761	749	753	756	rVB3	292	241	0.03%	0.003%
12	3.951	808	812	814	rBV3	317	241	0.03%	0.003%
13	4.571	1000	1005	1008	rBV2	320	352	0.04%	0.005%
14	4.629	1009	1023	1053	rBV	122905	328442	41.74%	4.384%
15	5.063	1141	1158	1185	rBV	151845	331995	42.19%	4.431%
16	5.185	1193	1196	1203	rVB3	601	743	0.09%	0.010%
17	5.230	1207	1210	1213	rVB2	437	248	0.03%	0.003%
18	5.292	1227	1229	1232	rVB	447	294	0.04%	0.004%
19	5.314	1232	1236	1242	rBV2	556	638	0.08%	0.009%
20	5.343	1242	1245	1249	rVB3	307	222	0.03%	0.003%
21	5.726	1343	1364	1392	rBV2	284982	786913	100.00%	10.503%
22	5.848	1400	1402	1408	rVB3	428	310	0.04%	0.004%
23	5.912	1410	1422	1441	rBV	8749	18686	2.37%	0.249%
24	6.005	1449	1451	1458	rVB	312	222	0.03%	0.003%
25	6.047	1460	1464	1468	rVB3	234	218	0.03%	0.003%
26	6.147	1490	1495	1496	rBV3	392	314	0.04%	0.004%
27	6.160	1496	1499	1500	rBV	533	352	0.04%	0.005%
28	6.250	1513	1527	1551	rBV	309306	590044	74.98%	7.876%
29	6.526	1608	1613	1625	rVB4	2532	3955	0.50%	0.053%
30	6.690	1650	1664	1680	rBV	203554	393101	49.95%	5.247%
31	6.896	1725	1728	1729	rBV	640	342	0.04%	0.005%
32	6.928	1729	1738	1751	rVV	5021	10890	1.38%	0.145%
33	7.041	1761	1773	1806	rBV	121383	223927	28.46%	2.989%
34	7.185	1813	1818	1829	rVB4	1962	3071	0.39%	0.041%
35	7.266	1839	1843	1845	rBV3	356	270	0.03%	0.004%
36	7.372	1873	1876	1879	rVB2	390	225	0.03%	0.003%

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

37	7.427	1891	1893	1896	rVB2	413	249	0.03%	0.003%
38	7.452	1896	1901	1905	rBV3	303	274	0.03%	0.004%
39	7.565	1924	1936	1958	rBV	107199	189817	24.12%	2.534%
40	7.677	1967	1971	1972	rBV	696	454	0.06%	0.006%
41	7.738	1981	1990	2001	rBV2	21614	34289	4.36%	0.458%
42	7.896	2025	2039	2059	rBV	339533	587465	74.65%	7.841%
43	8.060	2088	2090	2094	rVB4	413	240	0.03%	0.003%
44	8.179	2108	2127	2146	rBV2	80725	169732	21.57%	2.265%
45	8.391	2189	2193	2195	rVB3	322	212	0.03%	0.003%
46	8.407	2196	2198	2201	rVB	549	283	0.04%	0.004%
47	8.465	2205	2216	2234	rVB2	23404	40143	5.10%	0.536%
48	8.574	2234	2250	2257	rBV5	7004	14261	1.81%	0.190%
49	8.635	2257	2269	2289	rVV	351354	645146	81.98%	8.611%
50	8.729	2289	2298	2315	rVB	74505	127446	16.20%	1.701%
51	8.835	2322	2331	2351	rVB	31073	50503	6.42%	0.674%
52	8.989	2376	2379	2383	rVB2	338	223	0.03%	0.003%
53	9.025	2386	2390	2393	rVB3	290	227	0.03%	0.003%
54	9.063	2400	2402	2406	rVB	264	192	0.02%	0.003%
55	9.092	2406	2411	2415	rBV2	317	405	0.05%	0.005%
56	9.211	2437	2448	2462	rBV2	85772	135779	17.25%	1.812%
57	9.365	2490	2496	2499	rBV4	1391	1522	0.19%	0.020%
58	9.417	2499	2512	2535	rVV	415814	697836	88.68%	9.314%
59	9.565	2555	2558	2560	rBV3	361	253	0.03%	0.003%
60	9.645	2579	2583	2588	rVB2	686	662	0.08%	0.009%
61	9.687	2593	2596	2598	rBV2	379	236	0.03%	0.003%
62	9.857	2645	2649	2655	rBV2	205	247	0.03%	0.003%
63	9.909	2661	2665	2666	rBV2	638	398	0.05%	0.005%
64	9.999	2690	2693	2697	rVB2	327	232	0.03%	0.003%
65	10.024	2697	2701	2705	rVB	236	223	0.03%	0.003%
66	10.073	2705	2716	2731	rBV3	5027	8399	1.07%	0.112%
67	10.140	2733	2737	2739	rBV2	286	208	0.03%	0.003%
68	10.333	2794	2797	2801	rVB3	286	222	0.03%	0.003%
69	10.359	2801	2805	2808	rBV	249	223	0.03%	0.003%
70	10.430	2822	2827	2832	rBV2	291	318	0.04%	0.004%
71	10.462	2832	2837	2839	rBV2	320	299	0.04%	0.004%
72	10.616	2878	2885	2888	rBV2	374	369	0.05%	0.005%
73	10.754	2915	2928	2951	rVB	310288	495964	63.03%	6.620%
74	10.941	2982	2986	2990	rBV2	266	227	0.03%	0.003%
75	10.963	2990	2993	2999	rVB3	401	344	0.04%	0.005%
76	11.478	3151	3153	3158	rVB2	405	284	0.04%	0.004%

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 Title : VOC Analysis

77	11.507	3158	3162	3164	rBV3	398	293	0.04%	0.004%
78	11.812	3244	3257	3278	rBV	388698	617887	78.52%	8.247%
79	11.938	3293	3296	3303	rVB2	527	525	0.07%	0.007%
80	12.079	3337	3340	3345	rBV3	258	192	0.02%	0.003%
81	12.118	3349	3352	3356	rVB2	377	259	0.03%	0.003%
82	12.192	3363	3375	3396	rBV	333845	535605	68.06%	7.149%
83	12.381	3429	3434	3441	rVB2	368	463	0.06%	0.006%
84	12.417	3441	3445	3449	rBV	401	374	0.05%	0.005%
85	12.622	3502	3509	3513	rBV2	341	507	0.06%	0.007%
86	12.709	3533	3536	3541	rBV	287	262	0.03%	0.003%
87	13.169	3676	3679	3683	rBV3	212	193	0.02%	0.003%
88	13.291	3714	3717	3719	rBV	293	231	0.03%	0.003%
89	13.362	3736	3739	3744	rVB	379	263	0.03%	0.004%
90	13.446	3762	3765	3768	rBV3	398	311	0.04%	0.004%
91	13.484	3774	3777	3783	rBV2	397	457	0.06%	0.006%
92	13.716	3844	3849	3851	rBV	357	361	0.05%	0.005%
93	13.918	3905	3912	3915	rBV3	534	632	0.08%	0.008%
94	13.992	3932	3935	3939	rBV3	385	317	0.04%	0.004%
95	14.156	3984	3986	3992	rBV3	290	269	0.03%	0.004%
96	14.317	4033	4036	4039	rBV3	513	381	0.05%	0.005%
97	14.519	4095	4099	4100	rBV	348	240	0.03%	0.003%
98	15.394	4369	4371	4377	rBV3	444	383	0.05%	0.005%
99	16.053	4573	4576	4579	rBV2	651	474	0.06%	0.006%
100	16.262	4638	4641	4643	rBV3	835	571	0.07%	0.008%

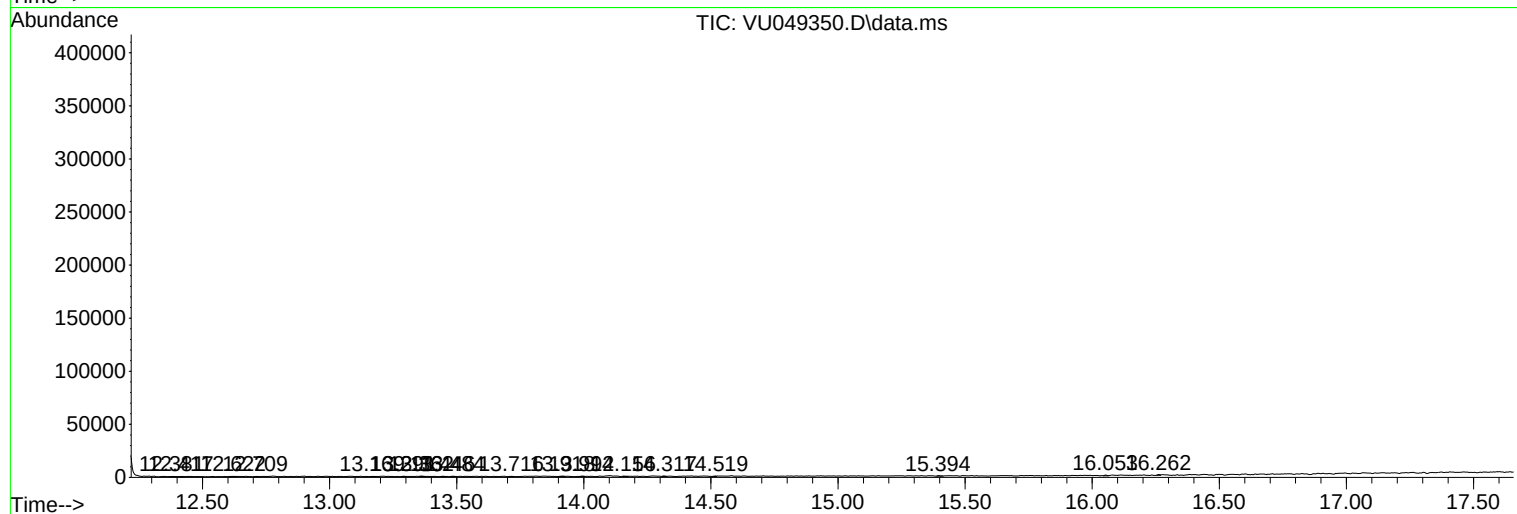
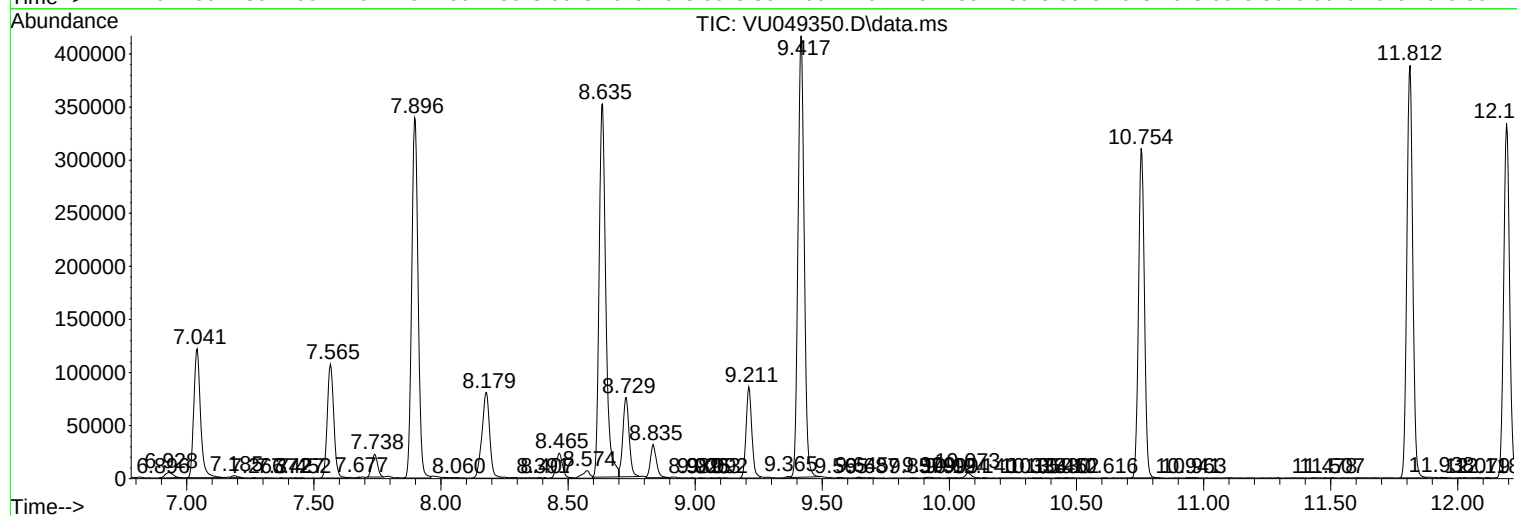
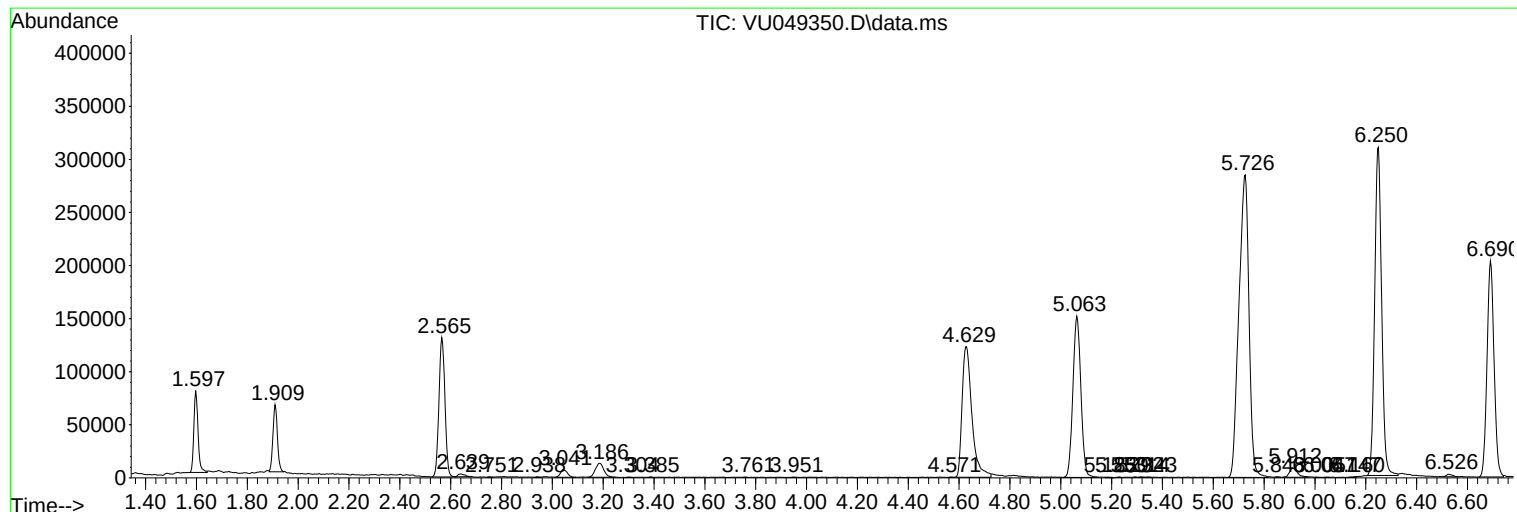
Sum of corrected areas: 7492122

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EXEX9

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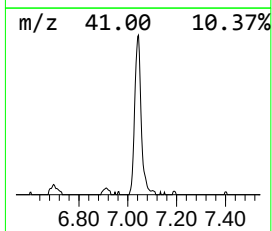
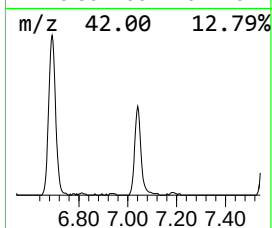
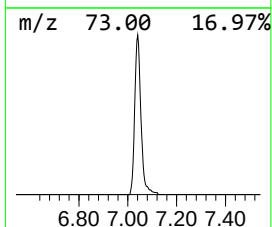
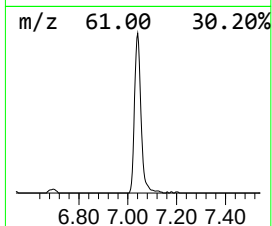
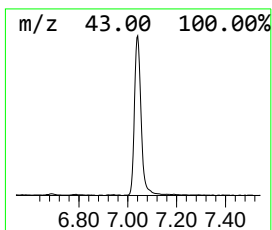
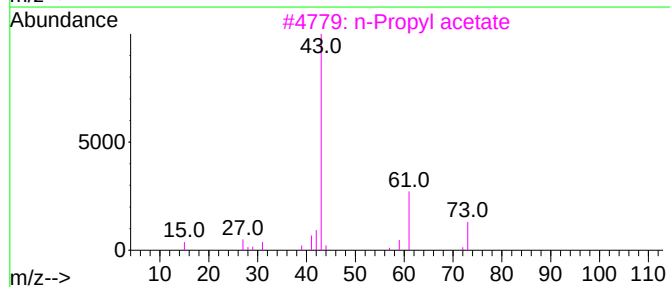
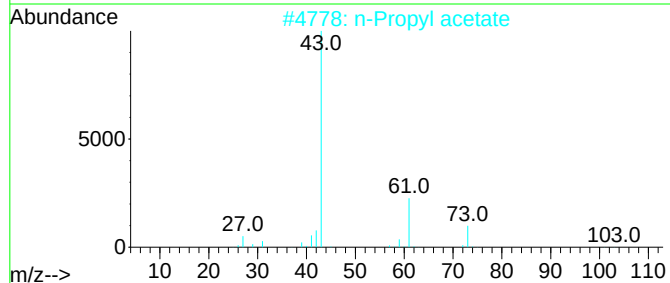
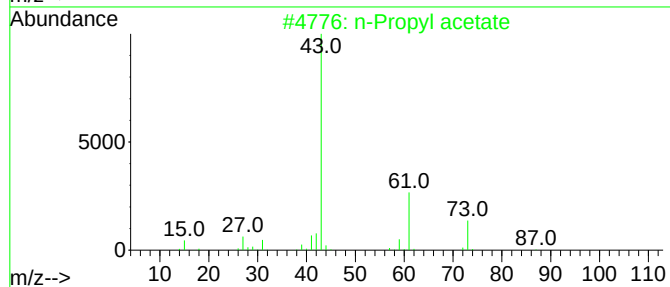
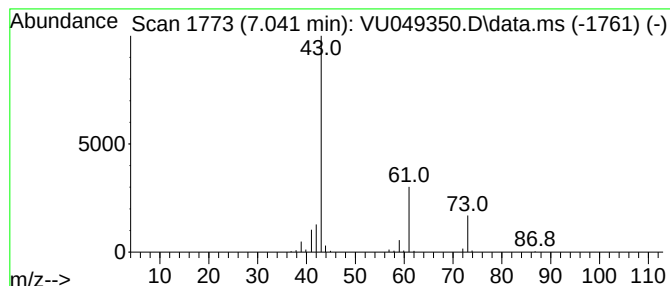
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
7.041	18.98 ug/L	223927	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	83
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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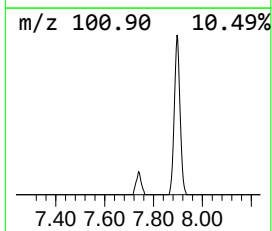
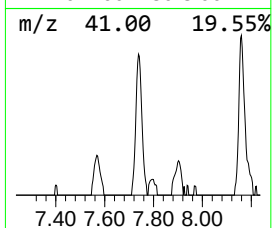
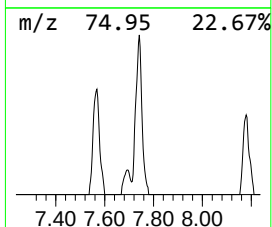
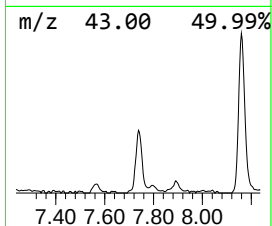
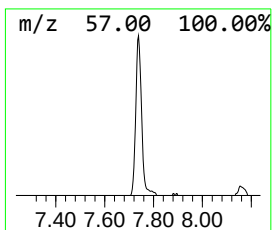
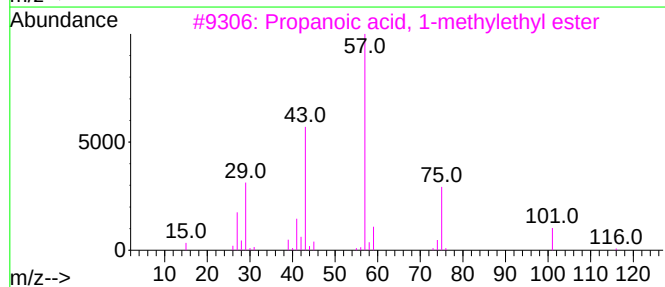
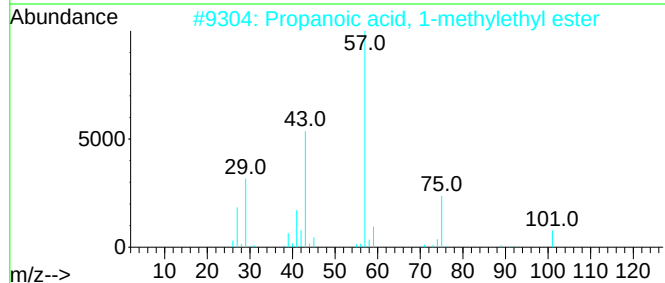
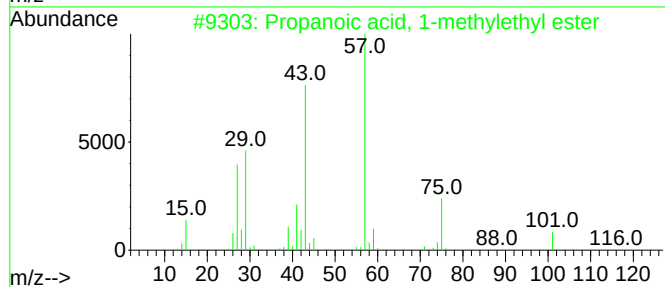
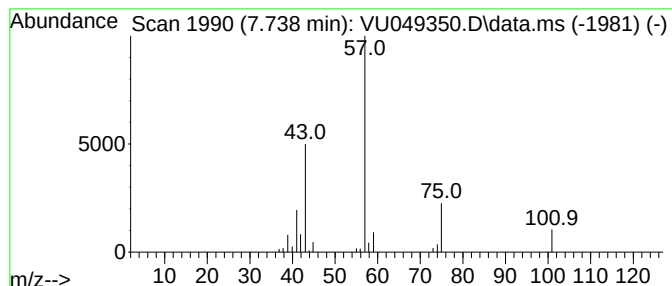
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.91 ug/L	34289	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	56
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45



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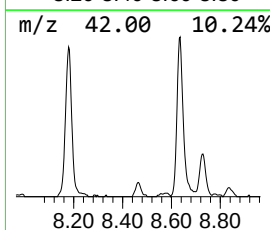
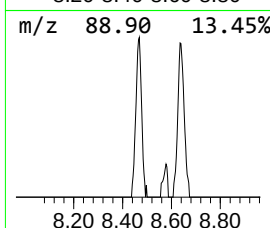
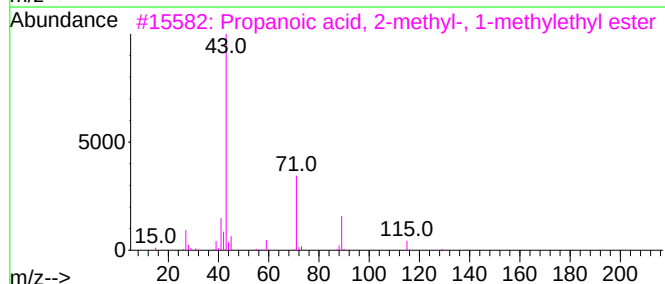
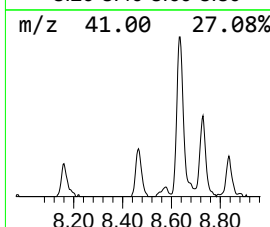
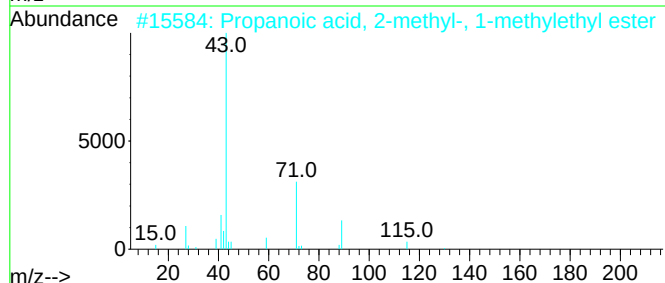
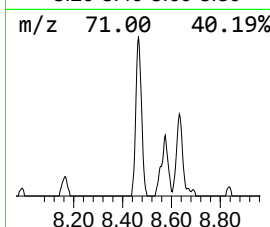
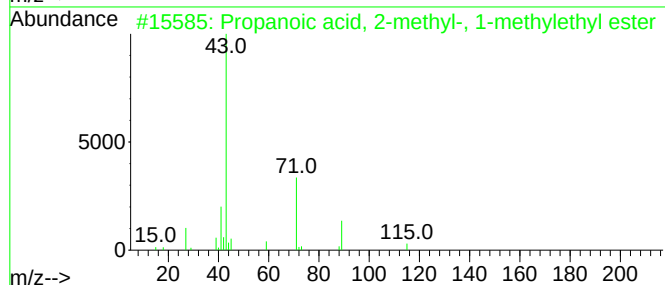
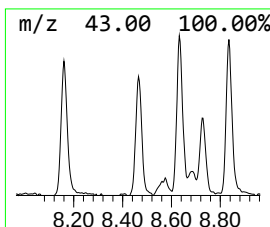
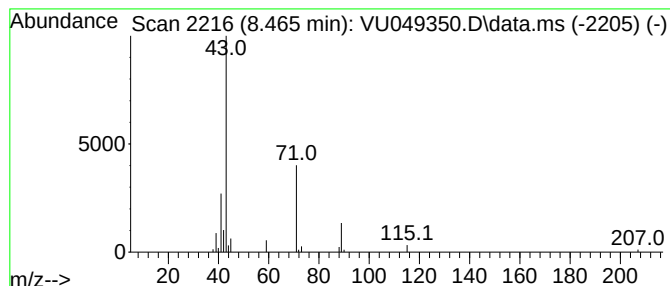
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.88 ug/L	40143	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	78
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049350.D
Acq On : 22 Jun 2022 14:35
Operator : SY/MD
Sample : N3392-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX9

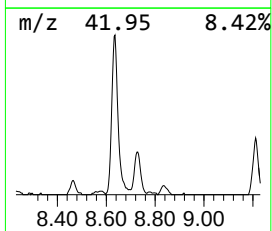
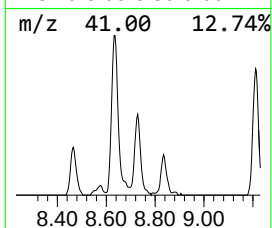
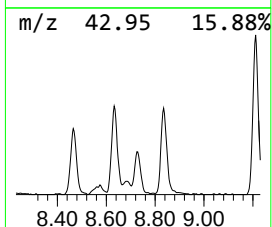
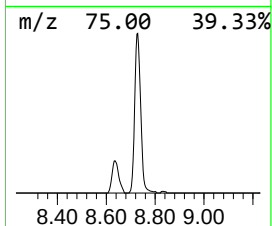
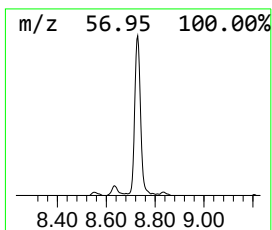
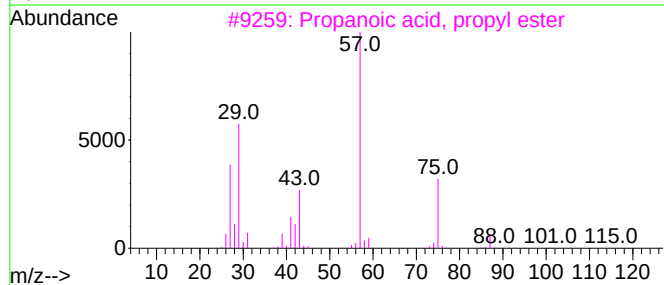
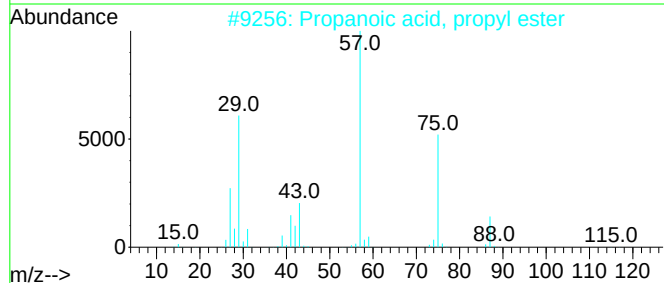
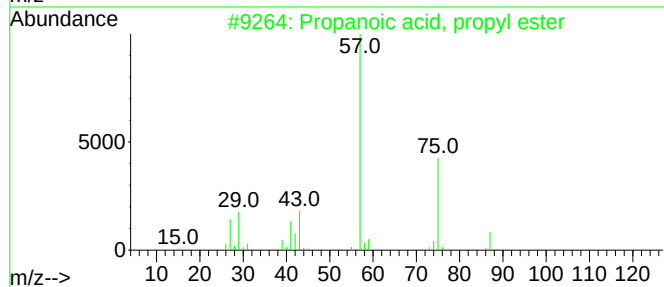
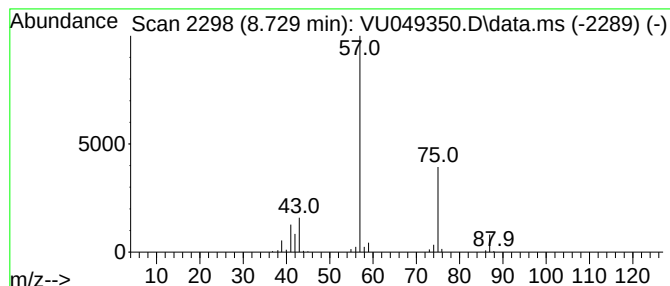
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Quant Title : VOC Analysis

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	9.13 ug/L	127446	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	78
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049350.D
Acq On : 22 Jun 2022 14:35
Operator : SY/MD
Sample : N3392-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX9

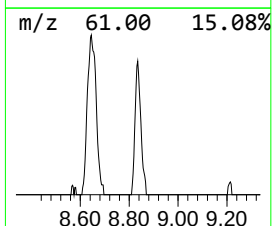
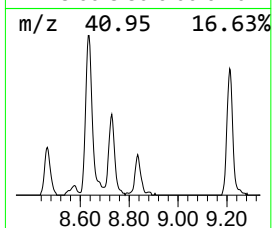
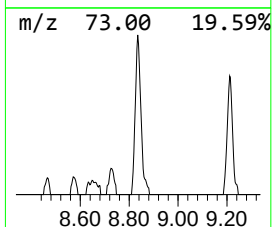
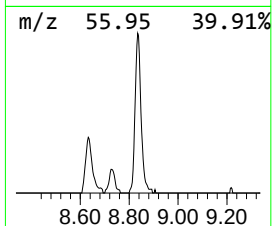
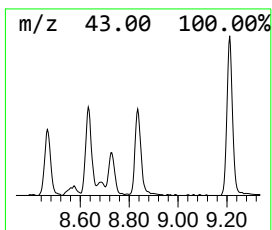
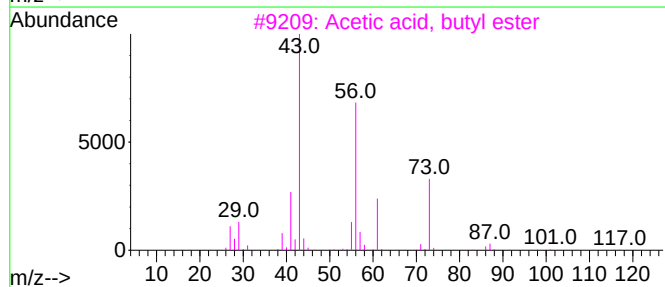
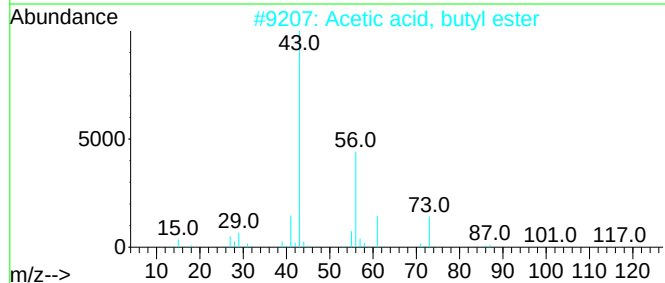
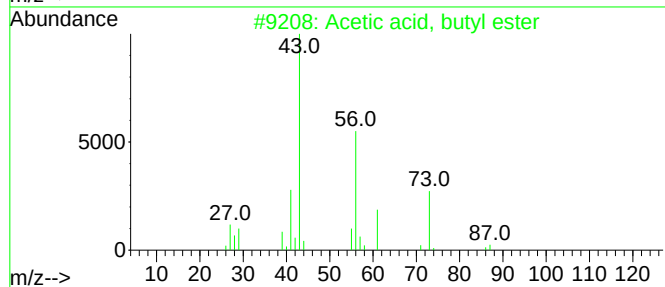
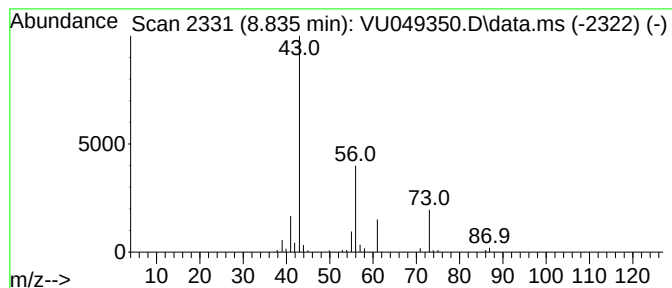
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Quant Title : VOC Analysis

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.62 ug/L	50503	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	64
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049350.D
Acq On : 22 Jun 2022 14:35
Operator : SY/MD
Sample : N3392-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX9

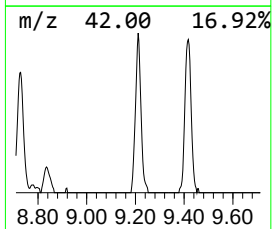
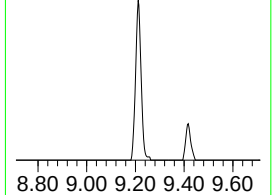
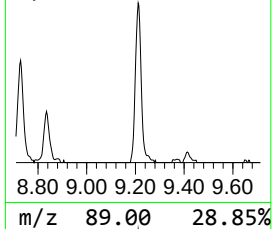
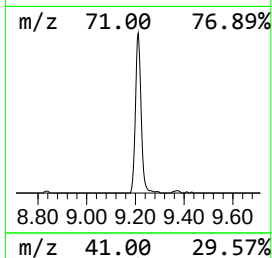
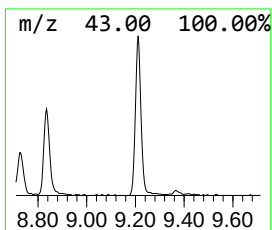
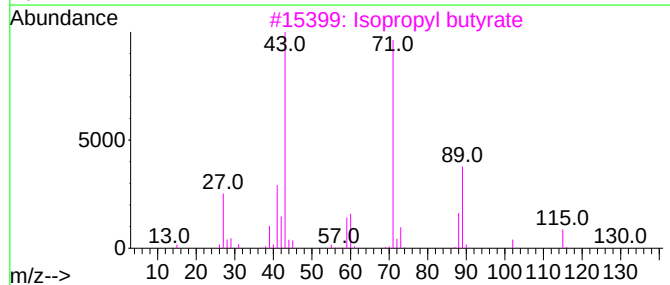
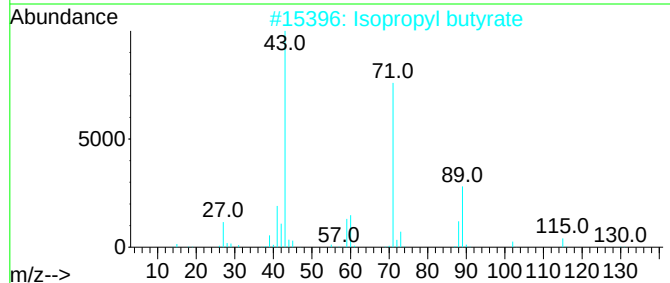
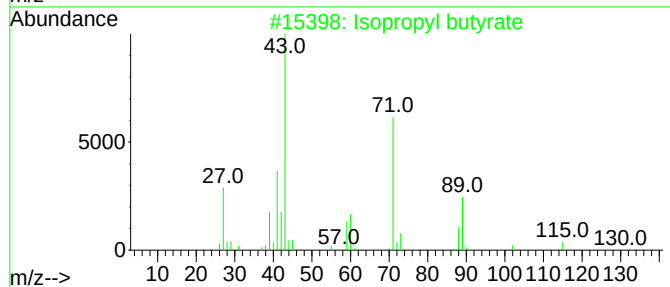
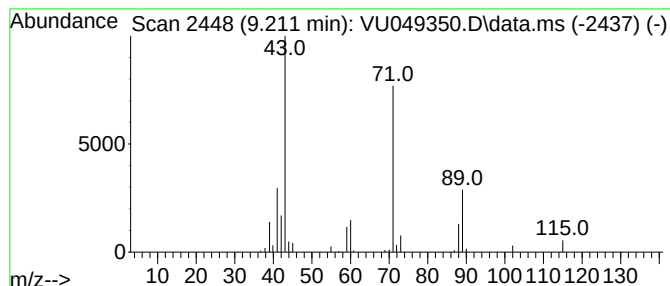
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	9.73 ug/L	135779	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049350.D
Acq On : 22 Jun 2022 14:35
Operator : SY/MD
Sample : N3392-04 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEX9

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	7.041	19.0	ug/L	223927	1	6.250	590044	50.0
Propanoic acid,...	7.738	2.9	ug/L	34289	1	6.250	590044	50.0
Propanoic acid,...	8.465	2.9	ug/L	40143	2	9.417	697836	50.0
Propanoic acid,...	8.729	9.1	ug/L	127446	2	9.417	697836	50.0
Acetic acid, bu...	8.835	3.6	ug/L	50503	2	9.417	697836	50.0
Isopropyl butyrate	9.211	9.7	ug/L	135779	2	9.417	697836	50.0