

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049371.D
 Acq On : 23 Jun 2022 12:01
 Operator : SY/MD
 Sample : PB145709TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB709

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: VU049371.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	37	44	51	rBV2	7956	12059	1.40%	0.154%
2	1.597	72	80	94	rBV	101619	121785	14.13%	1.558%
3	1.903	167	175	189	rVB	78404	100702	11.69%	1.288%
4	2.565	369	381	394	rBV	159665	258870	30.05%	3.312%
5	2.626	394	400	409	rVB2	2158	3381	0.39%	0.043%
6	2.752	435	439	444	rBV4	329	362	0.04%	0.005%
7	2.832	461	464	467	rVB2	399	295	0.03%	0.004%
8	2.890	478	482	486	rBV2	324	353	0.04%	0.005%
9	2.919	489	491	495	rVV	340	268	0.03%	0.003%
10	2.945	496	499	501	rVV	467	301	0.03%	0.004%
11	2.957	501	503	510	rVB2	495	463	0.05%	0.006%
12	3.044	518	530	538	rBV6	2575	5135	0.60%	0.066%
13	3.076	538	540	545	rVB3	321	224	0.03%	0.003%
14	3.186	561	574	589	rVV	13360	30376	3.53%	0.389%
15	3.314	611	614	620	rVB2	313	278	0.03%	0.004%
16	3.491	665	669	671	rBV2	239	218	0.03%	0.003%
17	3.594	698	701	704	rBV2	267	203	0.02%	0.003%
18	4.472	968	974	977	rBV2	202	260	0.03%	0.003%
19	4.530	987	992	993	rBV2	383	285	0.03%	0.004%
20	4.617	1005	1019	1049	rBV	123039	294007	34.12%	3.761%
21	4.790	1070	1073	1074	rBV2	408	227	0.03%	0.003%
22	4.816	1079	1081	1093	rVB3	1613	1672	0.19%	0.021%
23	4.935	1114	1118	1122	rVB3	259	198	0.02%	0.003%
24	5.060	1140	1157	1182	rBV	166183	358013	41.55%	4.580%
25	5.295	1227	1230	1234	rVB2	394	342	0.04%	0.004%
26	5.324	1234	1239	1243	rBV2	359	338	0.04%	0.004%
27	5.346	1243	1246	1252	rVB3	375	261	0.03%	0.003%
28	5.462	1277	1282	1285	rBV2	273	261	0.03%	0.003%
29	5.597	1320	1324	1328	rVB	306	244	0.03%	0.003%
30	5.723	1340	1363	1388	rBV2	318128	861597	100.00%	11.022%
31	5.912	1412	1422	1436	rBV	8851	17603	2.04%	0.225%
32	5.996	1446	1448	1451	rVB2	377	221	0.03%	0.003%
33	6.015	1451	1454	1458	rVB2	410	364	0.04%	0.005%
34	6.038	1458	1461	1464	rBV2	362	271	0.03%	0.003%
35	6.160	1496	1499	1503	rBV2	269	225	0.03%	0.003%
36	6.247	1510	1526	1548	rBV	293594	559279	64.91%	7.154%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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

37	6.382	1566	1568	1574	rVB3	444	349	0.04%	0.004%
38	6.523	1608	1612	1613	rBV3	1415	1047	0.12%	0.013%
39	6.690	1648	1664	1682	rBV	218090	421752	48.95%	5.395%
40	6.925	1727	1737	1754	rVB	4791	10831	1.26%	0.139%
41	7.038	1758	1772	1795	rBV	133013	237749	27.59%	3.041%
42	7.179	1811	1816	1827	rVB7	2542	4347	0.50%	0.056%
43	7.388	1879	1881	1886	rVB3	286	198	0.02%	0.003%
44	7.465	1902	1905	1910	rBV2	403	326	0.04%	0.004%
45	7.565	1923	1936	1961	rVB2	113913	200782	23.30%	2.568%
46	7.652	1961	1963	1968	rBV2	328	213	0.02%	0.003%
47	7.690	1968	1975	1979	rBV3	1428	1985	0.23%	0.025%
48	7.739	1979	1990	2001	rBV	24190	39703	4.61%	0.508%
49	7.896	2025	2039	2060	rBV	381034	656375	76.18%	8.397%
50	8.054	2086	2088	2094	rBV2	395	249	0.03%	0.003%
51	8.083	2094	2097	2100	rBV2	270	206	0.02%	0.003%
52	8.099	2100	2102	2106	rVB	431	231	0.03%	0.003%
53	8.176	2107	2126	2143	rBV2	84080	172987	20.08%	2.213%
54	8.411	2195	2199	2202	rBV	312	280	0.03%	0.004%
55	8.462	2204	2215	2234	rVB	23862	40474	4.70%	0.518%
56	8.571	2234	2249	2256	rBV5	7928	15096	1.75%	0.193%
57	8.629	2256	2267	2288	rVV	332428	609085	70.69%	7.792%
58	8.726	2288	2297	2312	rVB	99476	159318	18.49%	2.038%
59	8.832	2321	2330	2346	rVV	32344	53011	6.15%	0.678%
60	8.973	2371	2374	2379	rVV4	416	311	0.04%	0.004%
61	8.996	2379	2381	2385	rVB2	353	216	0.03%	0.003%
62	9.208	2434	2447	2466	rBV2	101703	164526	19.10%	2.105%
63	9.372	2488	2498	2499	rBV3	1422	1834	0.21%	0.023%
64	9.417	2499	2512	2534	rVV	406548	667222	77.44%	8.535%
65	9.629	2575	2578	2579	rVV	558	271	0.03%	0.003%
66	9.642	2579	2582	2591	rVB3	1088	1342	0.16%	0.017%
67	9.919	2662	2668	2676	rBV4	754	1336	0.16%	0.017%
68	10.070	2707	2715	2728	rVB3	5668	9149	1.06%	0.117%
69	10.292	2779	2784	2789	rVB2	310	291	0.03%	0.004%
70	10.755	2914	2928	2949	rBV	313258	508879	59.06%	6.510%
71	10.915	2977	2978	2984	rVB	248	199	0.02%	0.003%
72	10.947	2984	2988	2993	rBV	231	215	0.02%	0.003%
73	11.041	3013	3017	3022	rBV2	297	290	0.03%	0.004%
74	11.086	3029	3031	3035	rBV	357	265	0.03%	0.003%
75	11.295	3091	3096	3099	rBV3	399	396	0.05%	0.005%
76	11.382	3118	3123	3126	rBV2	186	199	0.02%	0.003%

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77	11.812	3244	3257	3275	rBV	375868	604399	70.15%	7.732%
78	12.121	3351	3353	3359	rBV2	266	236	0.03%	0.003%
79	12.192	3361	3375	3391	rBV	360633	590929	68.59%	7.559%
80	12.295	3405	3407	3410	rBV	345	212	0.02%	0.003%
81	12.423	3443	3447	3449	rBV2	263	217	0.03%	0.003%
82	12.507	3469	3473	3479	rBV3	407	500	0.06%	0.006%
83	12.697	3529	3532	3537	rVB2	331	250	0.03%	0.003%
84	12.761	3549	3552	3557	rBV3	416	460	0.05%	0.006%
85	12.912	3596	3599	3604	rBV2	312	336	0.04%	0.004%
86	13.057	3641	3644	3646	rBV	314	200	0.02%	0.003%
87	13.263	3705	3708	3713	rBV3	317	377	0.04%	0.005%
88	13.410	3751	3754	3759	rVB2	279	252	0.03%	0.003%
89	13.735	3852	3855	3860	rBV3	317	313	0.04%	0.004%
90	13.812	3877	3879	3884	rVB2	384	276	0.03%	0.004%
91	13.848	3886	3890	3892	rBV3	719	488	0.06%	0.006%
92	13.902	3903	3907	3911	rVV2	282	273	0.03%	0.003%
93	13.941	3911	3919	3923	rBV3	396	596	0.07%	0.008%
94	13.970	3925	3928	3932	rBV	344	256	0.03%	0.003%
95	14.089	3961	3965	3968	rBV2	769	786	0.09%	0.010%
96	14.275	4020	4023	4026	rBV	327	241	0.03%	0.003%
97	14.513	4093	4097	4102	rBV3	331	360	0.04%	0.005%
98	14.703	4153	4156	4161	rBV2	249	320	0.04%	0.004%
99	15.070	4268	4270	4273	rBV2	349	221	0.03%	0.003%
100	15.143	4291	4293	4295	rBV	320	196	0.02%	0.003%

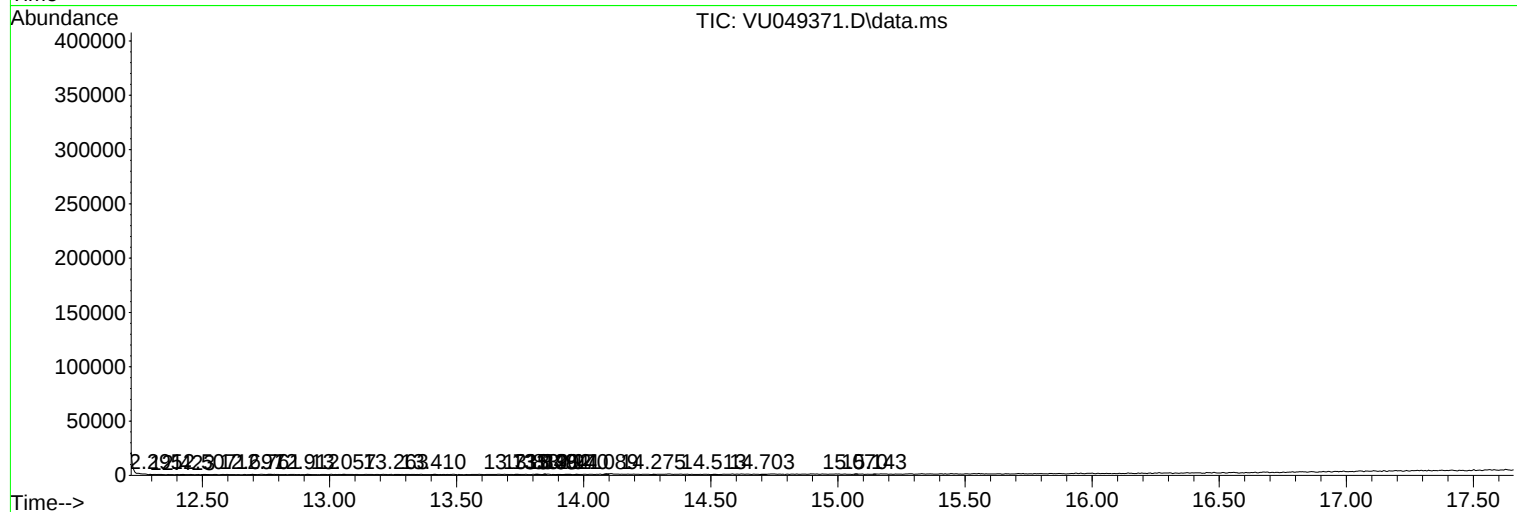
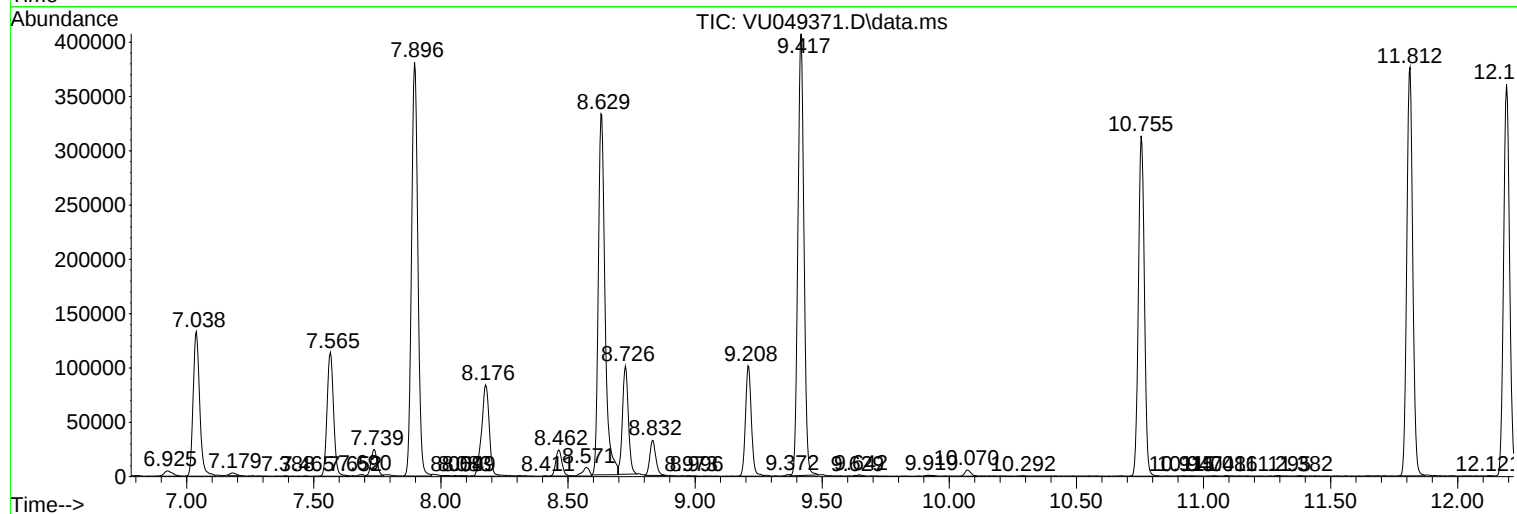
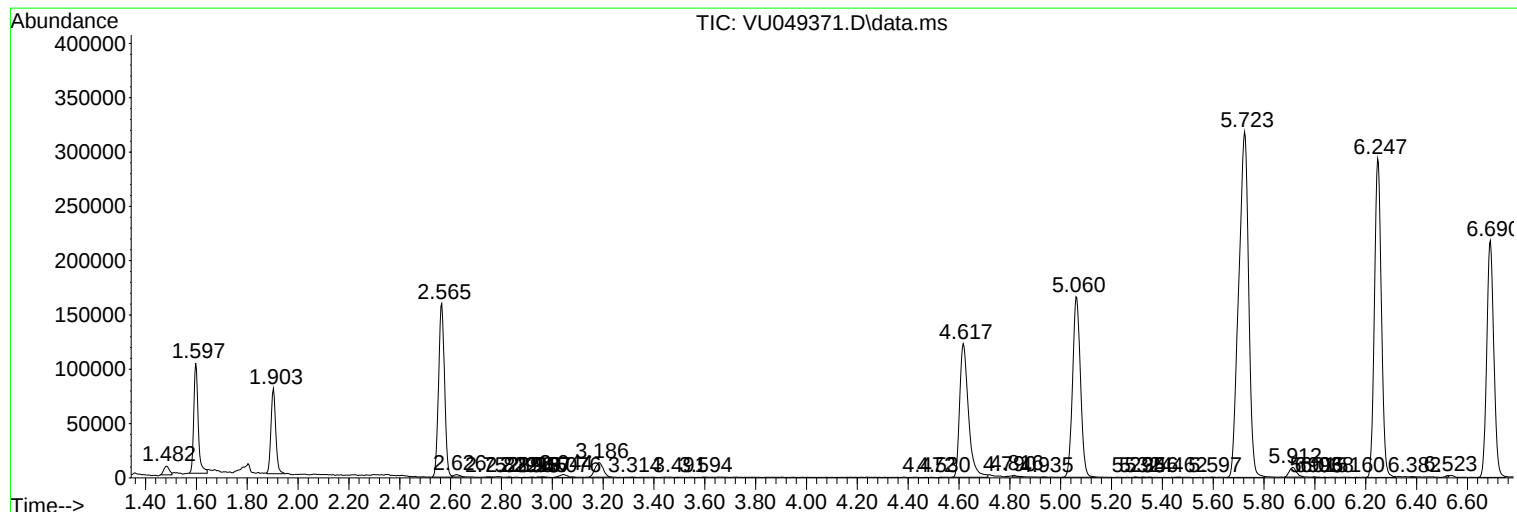
Sum of corrected areas: 7817170

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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



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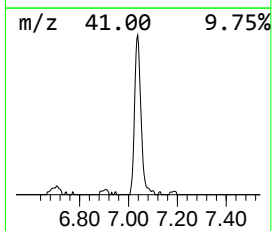
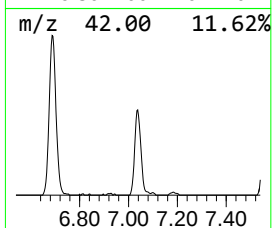
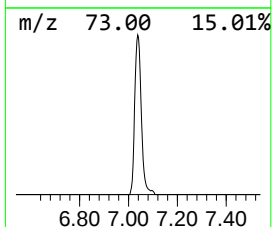
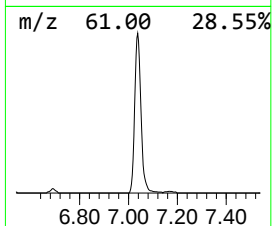
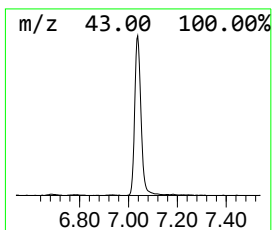
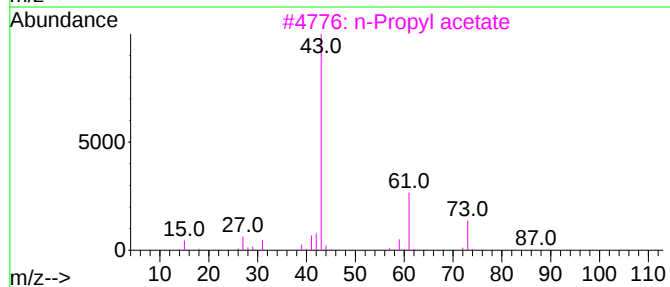
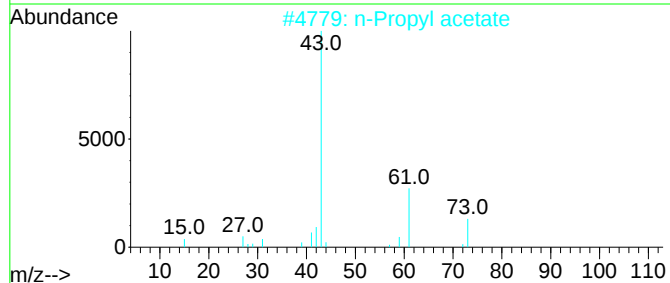
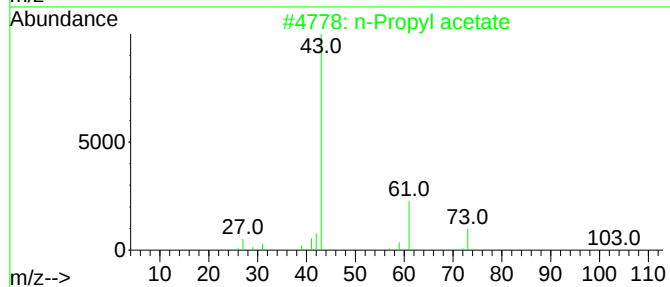
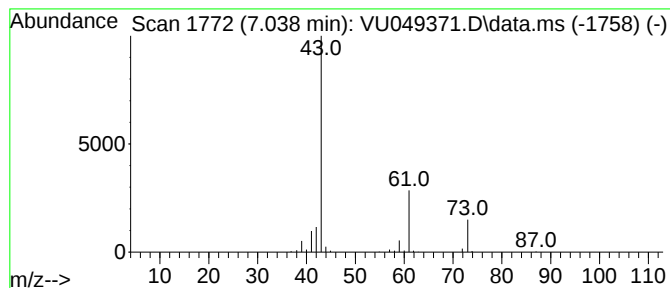
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	21.25 ug/L	237749	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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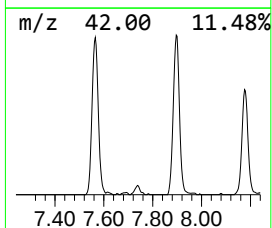
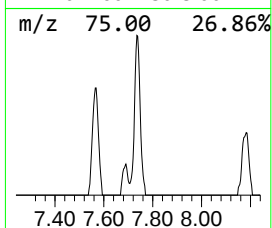
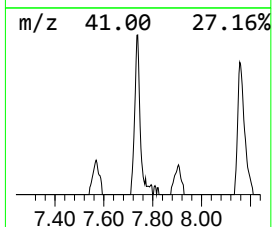
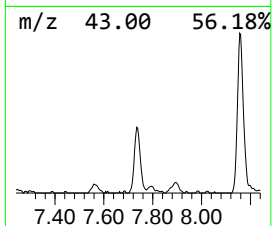
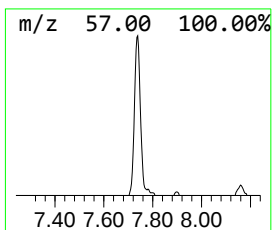
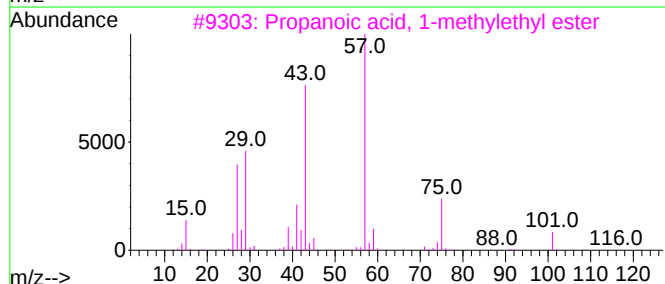
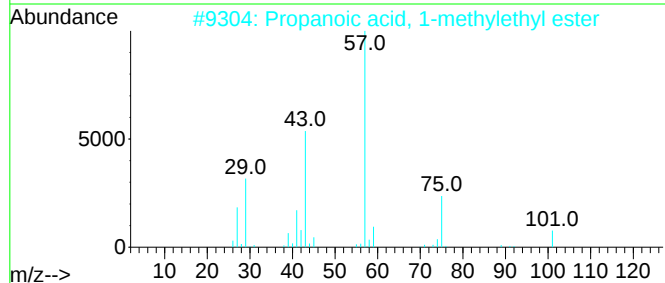
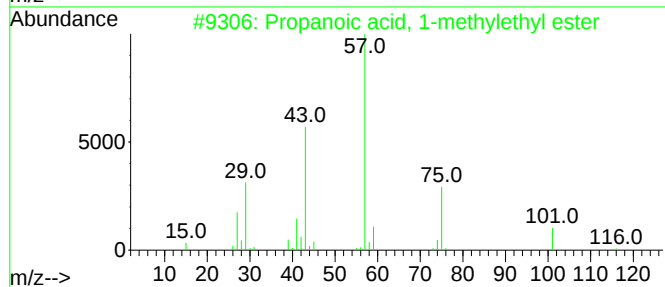
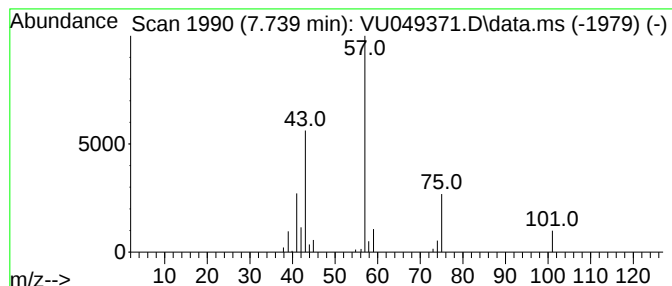
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	3.55 ug/L	39703	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	74
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56



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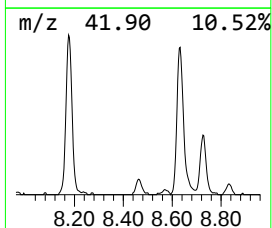
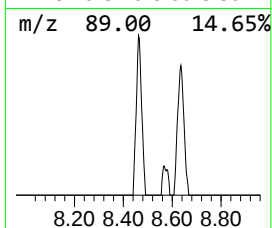
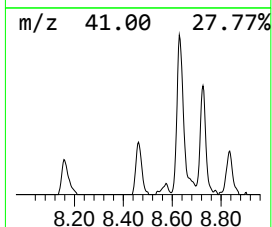
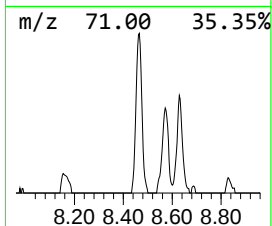
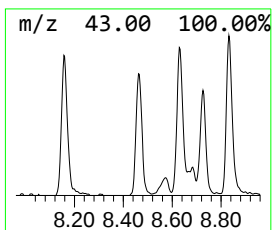
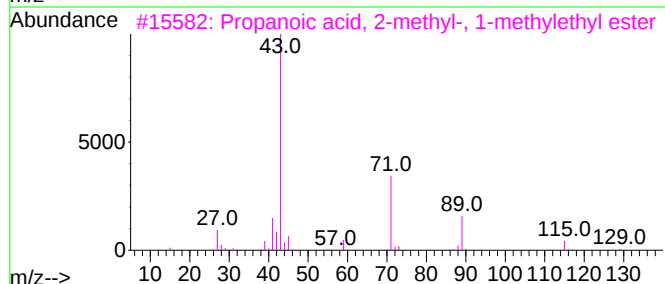
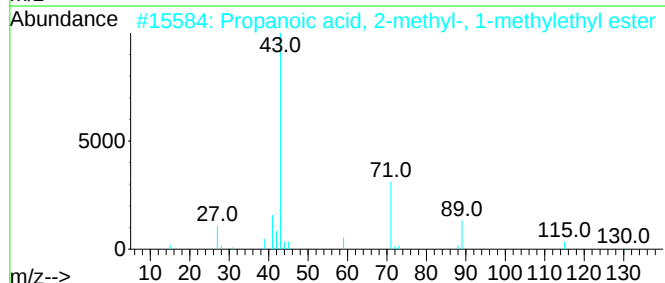
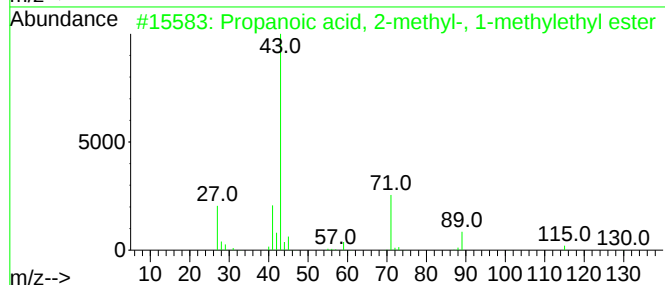
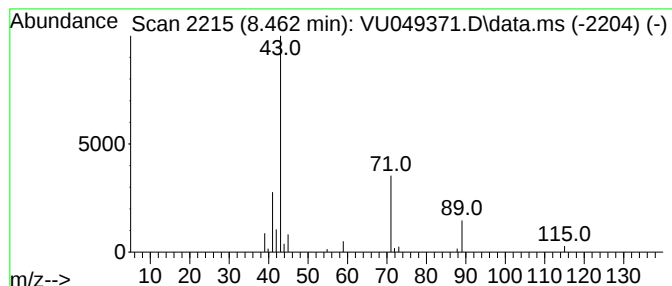
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
8.462	3.03 ug/L	40474	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	83
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049371.D
Acq On : 23 Jun 2022 12:01
Operator : SY/MD
Sample : PB145709TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB709

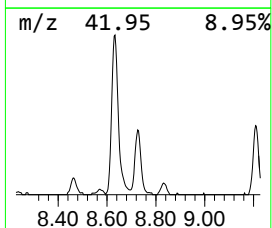
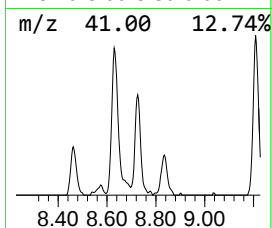
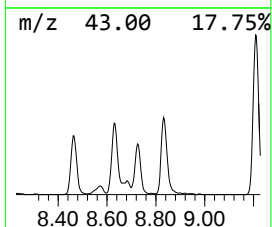
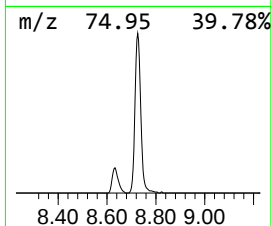
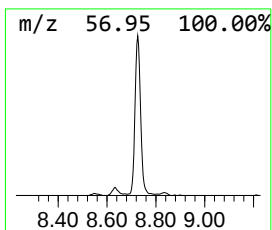
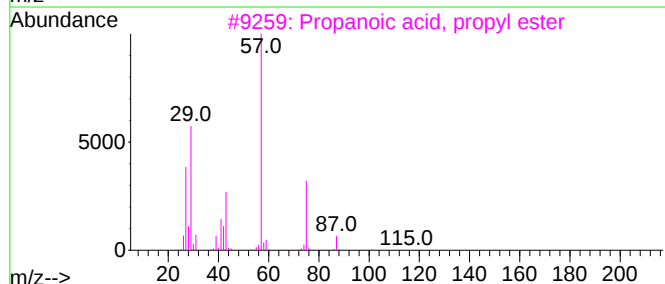
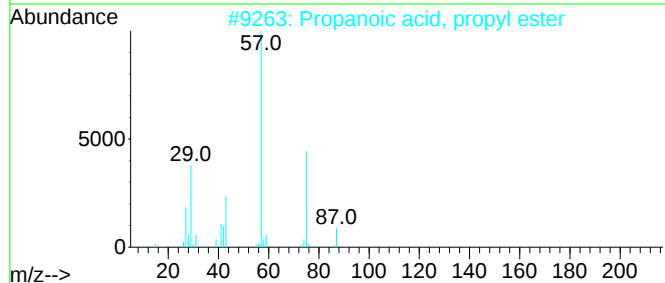
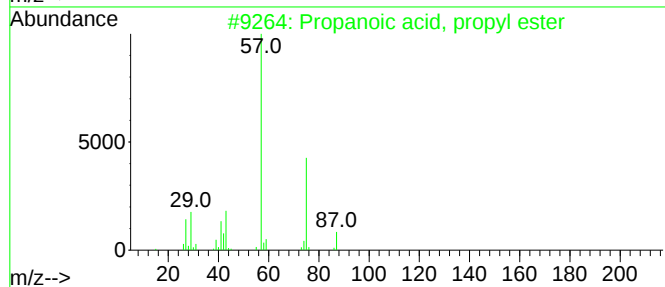
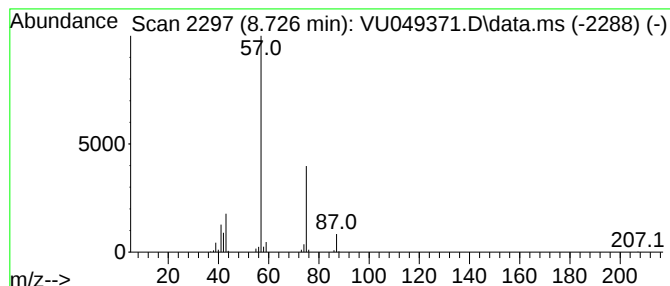
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Quant Title : VOC Analysis

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.
8.726	11.94 ug/L	159318	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	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049371.D
Acq On : 23 Jun 2022 12:01
Operator : SY/MD
Sample : PB145709TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB709

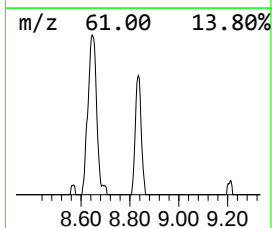
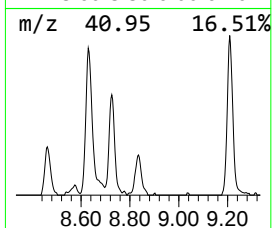
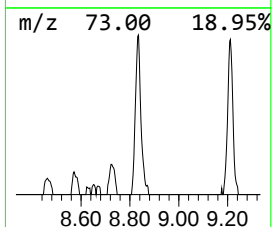
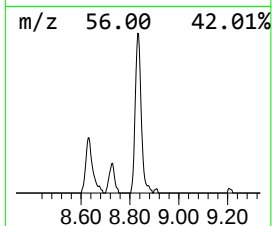
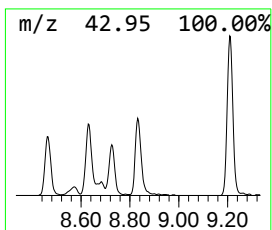
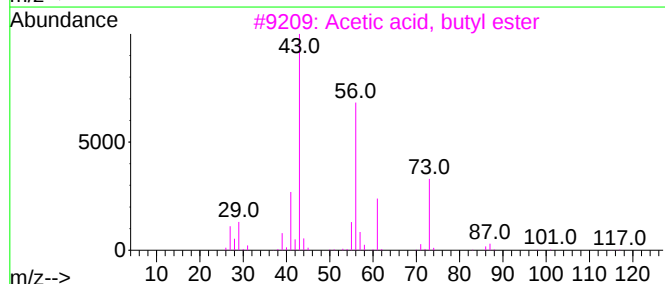
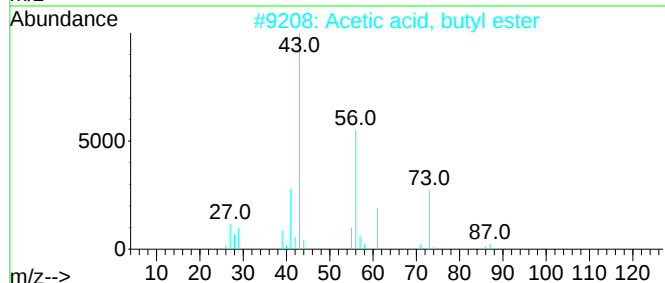
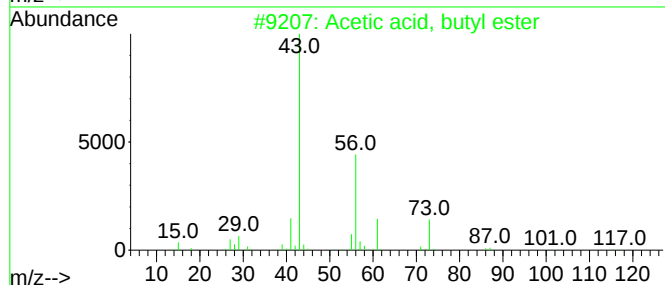
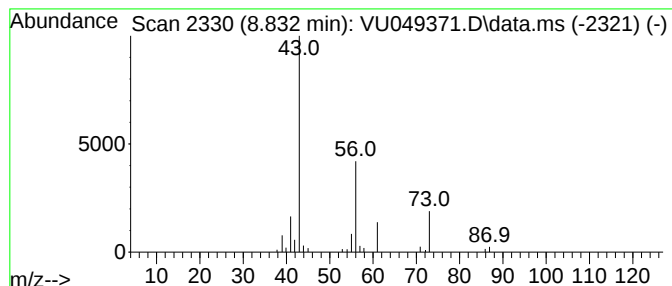
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Quant Title : VOC Analysis

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.
8.832	3.97 ug/L	53011	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	74		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	59		
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049371.D
Acq On : 23 Jun 2022 12:01
Operator : SY/MD
Sample : PB145709TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB709

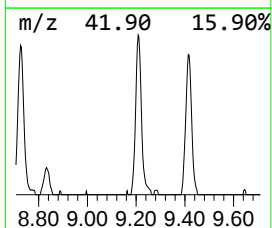
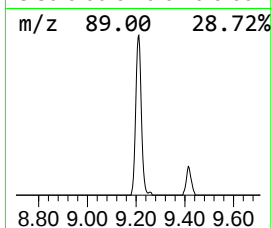
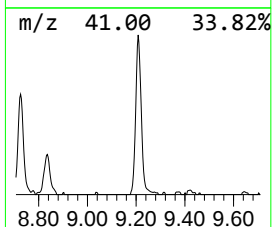
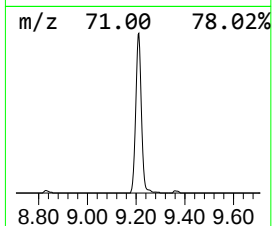
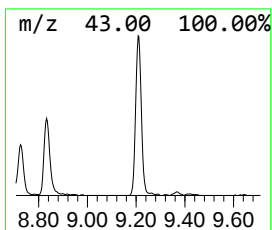
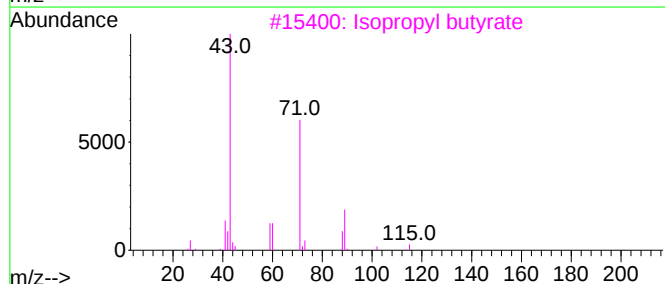
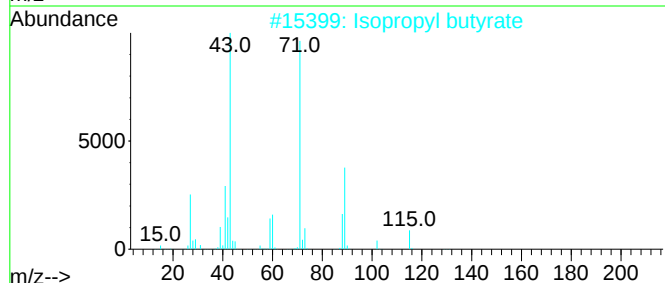
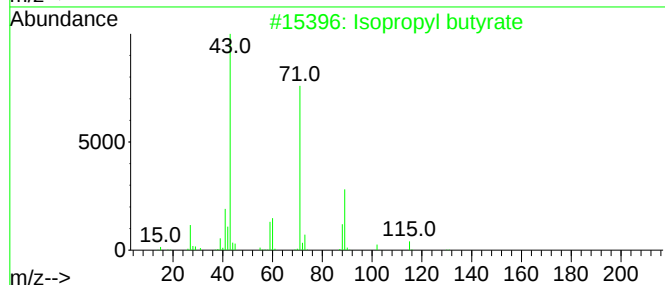
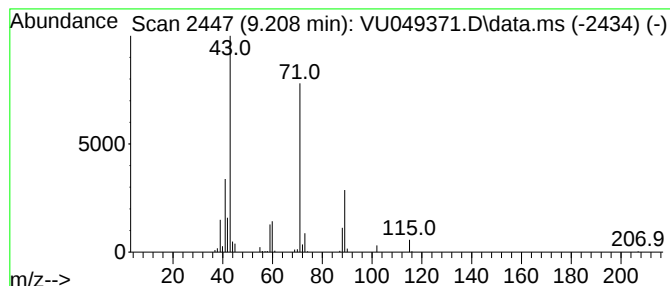
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
9.208	12.33 ug/L	164526	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	83
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049371.D
Acq On : 23 Jun 2022 12:01
Operator : SY/MD
Sample : PB145709TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB709

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	21.3	ug/L	237749	1	6.247	559279	50.0
Propanoic acid,...	7.739	3.5	ug/L	39703	1	6.247	559279	50.0
Propanoic acid,...	8.462	3.0	ug/L	40474	2	9.417	667222	50.0
Propanoic acid,...	8.726	11.9	ug/L	159318	2	9.417	667222	50.0
Acetic acid, bu...	8.832	4.0	ug/L	53011	2	9.417	667222	50.0
Isopropyl butyrate	9.208	12.3	ug/L	164526	2	9.417	667222	50.0