

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049353.D
 Acq On : 22 Jun 2022 15:45
 Operator : SY/MD
 Sample : N3392-07 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEY2

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: VU049353.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	98	rBV	71818	82058	10.96%	1.142%
2	1.900	167	174	191	rVB	59942	79718	10.65%	1.109%
3	2.562	368	380	393	rBV	123479	198193	26.48%	2.758%
4	2.912	487	489	490	rBV	244	116	0.02%	0.002%
5	3.041	522	529	541	rVB2	3996	6604	0.88%	0.092%
6	3.183	554	573	591	rBV2	23514	53977	7.21%	0.751%
7	3.285	602	605	606	rBV	298	145	0.02%	0.002%
8	3.446	653	655	658	rBV	169	87	0.01%	0.001%
9	3.536	681	683	687	rVB2	390	229	0.03%	0.003%
10	3.629	709	712	713	rBV2	199	126	0.02%	0.002%
11	3.655	717	720	723	rBV	136	74	0.01%	0.001%
12	3.832	773	775	777	rBV	238	119	0.02%	0.002%
13	4.076	849	851	852	rBV	139	73	0.01%	0.001%
14	4.134	865	869	871	rBV	168	130	0.02%	0.002%
15	4.186	881	885	889	rBV2	252	228	0.03%	0.003%
16	4.237	898	901	902	rBV	192	105	0.01%	0.001%
17	4.272	909	912	916	rVB2	204	110	0.01%	0.002%
18	4.343	931	934	936	rBV2	151	94	0.01%	0.001%
19	4.356	936	938	939	rBV	206	86	0.01%	0.001%
20	4.488	977	979	981	rVB2	197	63	0.01%	0.001%
21	4.546	994	997	998	rBV	173	105	0.01%	0.001%
22	4.617	1005	1019	1048	rBV	120991	295014	39.42%	4.105%
23	4.999	1136	1138	1139	rBV	189	78	0.01%	0.001%
24	5.060	1141	1157	1181	rVV	145640	316576	42.30%	4.405%
25	5.170	1190	1191	1193	rBV	209	63	0.01%	0.001%
26	5.247	1205	1215	1217	rBV	252	337	0.05%	0.005%
27	5.266	1219	1221	1225	rVB2	228	124	0.02%	0.002%
28	5.292	1225	1229	1238	rVB3	757	921	0.12%	0.013%
29	5.330	1238	1241	1242	rBV	117	72	0.01%	0.001%
30	5.337	1242	1243	1245	rVB	152	32	0.00%	0.000%
31	5.350	1245	1247	1249	rBV	66	40	0.01%	0.001%
32	5.382	1252	1257	1261	rVB2	451	460	0.06%	0.006%
33	5.491	1284	1291	1294	rBV2	351	370	0.05%	0.005%
34	5.536	1304	1305	1308	rBV2	150	73	0.01%	0.001%
35	5.578	1313	1318	1322	rVB2	262	247	0.03%	0.003%
36	5.610	1322	1328	1334	rBV2	213	294	0.04%	0.004%

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Integrator: RTE

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

37	5.723	1342	1363	1387	rBV2	272227	748448	100.00%	10.414%
38	5.912	1403	1422	1434	rBV3	10071	21529	2.88%	0.300%
39	6.038	1459	1461	1463	rVB2	130	51	0.01%	0.001%
40	6.083	1472	1475	1479	rBV2	366	299	0.04%	0.004%
41	6.102	1479	1481	1487	rVB2	201	118	0.02%	0.002%
42	6.125	1487	1488	1490	rBV	244	109	0.01%	0.002%
43	6.170	1490	1502	1504	rBV3	1335	2415	0.32%	0.034%
44	6.247	1514	1526	1552	rVB	300609	559681	74.78%	7.788%
45	6.584	1627	1631	1632	rBV3	576	386	0.05%	0.005%
46	6.690	1650	1664	1686	rBV	193546	374312	50.01%	5.208%
47	7.038	1761	1772	1798	rBV	120050	208266	27.83%	2.898%
48	7.337	1863	1865	1866	rBV	175	49	0.01%	0.001%
49	7.350	1867	1869	1871	rBV2	330	136	0.02%	0.002%
50	7.382	1876	1879	1882	rBV	334	197	0.03%	0.003%
51	7.459	1898	1903	1907	rBV2	320	317	0.04%	0.004%
52	7.481	1907	1910	1913	rBV2	241	136	0.02%	0.002%
53	7.565	1923	1936	1951	rBV2	100598	178264	23.82%	2.480%
54	7.652	1959	1963	1967	rBV3	445	436	0.06%	0.006%
55	7.681	1969	1972	1976	rBV4	850	862	0.12%	0.012%
56	7.735	1981	1989	2000	rVB	23151	37988	5.08%	0.529%
57	7.896	2026	2039	2057	rBV	322700	553133	73.90%	7.697%
58	8.063	2087	2091	2093	rBV2	296	216	0.03%	0.003%
59	8.112	2103	2106	2110	rVB	215	145	0.02%	0.002%
60	8.176	2110	2126	2141	rBV2	75537	152206	20.34%	2.118%
61	8.382	2186	2190	2193	rBV2	377	304	0.04%	0.004%
62	8.465	2204	2216	2230	rBV	26346	42975	5.74%	0.598%
63	8.575	2235	2250	2256	rBV6	6645	13729	1.83%	0.191%
64	8.632	2256	2268	2288	rVV	346693	617191	82.46%	8.588%
65	8.726	2290	2297	2314	rVB	83454	130790	17.47%	1.820%
66	8.835	2323	2331	2344	rVB	23954	37001	4.94%	0.515%
67	8.951	2366	2367	2372	rVB2	288	192	0.03%	0.003%
68	9.057	2397	2400	2403	rBV2	345	260	0.03%	0.004%
69	9.095	2409	2412	2413	rBV2	192	97	0.01%	0.001%
70	9.128	2420	2422	2424	rBV	160	73	0.01%	0.001%
71	9.169	2432	2435	2437	rBV	256	145	0.02%	0.002%
72	9.211	2437	2448	2467	rVV	90887	145159	19.39%	2.020%
73	9.417	2500	2512	2536	rVB	409152	669451	89.45%	9.315%
74	9.565	2557	2558	2559	rBV	288	79	0.01%	0.001%
75	9.735	2608	2611	2613	rBV	151	101	0.01%	0.001%
76	9.755	2613	2617	2621	rVV2	304	258	0.03%	0.004%

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 Title : VOC Analysis

77	9.922	2661	2669	2676	rBV5	899	1592	0.21%	0.022%
78	10.073	2708	2716	2726	rBV2	5246	7872	1.05%	0.110%
79	10.394	2810	2816	2819	rBV3	320	378	0.05%	0.005%
80	10.494	2845	2847	2850	rBV	226	179	0.02%	0.002%
81	10.613	2881	2884	2887	rBV	201	158	0.02%	0.002%
82	10.755	2916	2928	2948	rBV	304125	492919	65.86%	6.859%
83	10.960	2990	2992	2993	rBV	182	82	0.01%	0.001%
84	11.111	3036	3039	3042	rBV3	264	243	0.03%	0.003%
85	11.131	3043	3045	3048	rVV2	370	244	0.03%	0.003%
86	11.218	3070	3072	3076	rVB	208	100	0.01%	0.001%
87	11.256	3082	3084	3085	rBV	164	58	0.01%	0.001%
88	11.587	3184	3187	3188	rBV	231	123	0.02%	0.002%
89	11.812	3244	3257	3283	rBV	384407	615113	82.19%	8.559%
90	12.070	3335	3337	3341	rBV2	330	220	0.03%	0.003%
91	12.192	3363	3375	3398	rBV	331247	532290	71.12%	7.407%
92	13.410	3750	3754	3759	rBV3	448	531	0.07%	0.007%

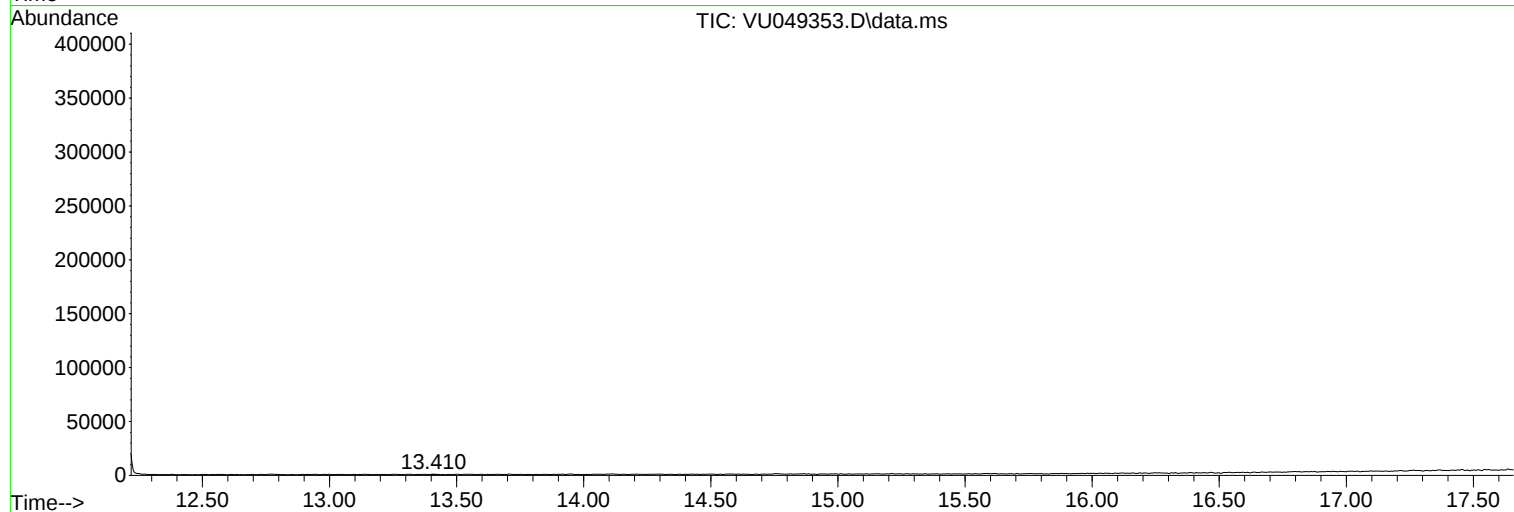
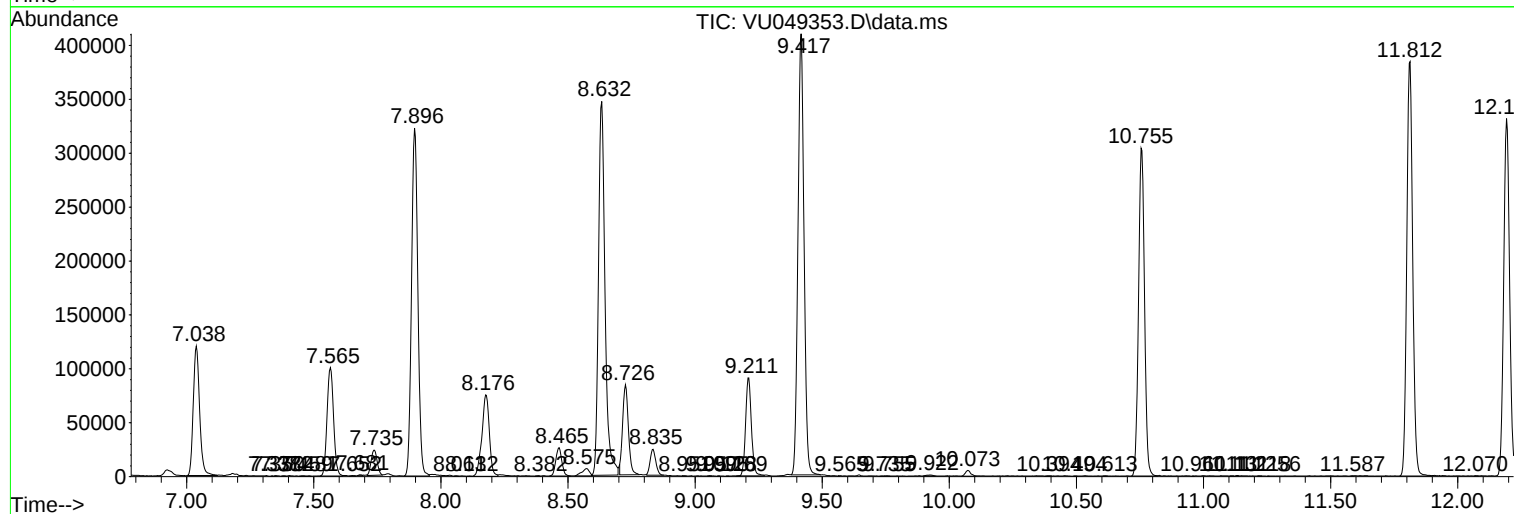
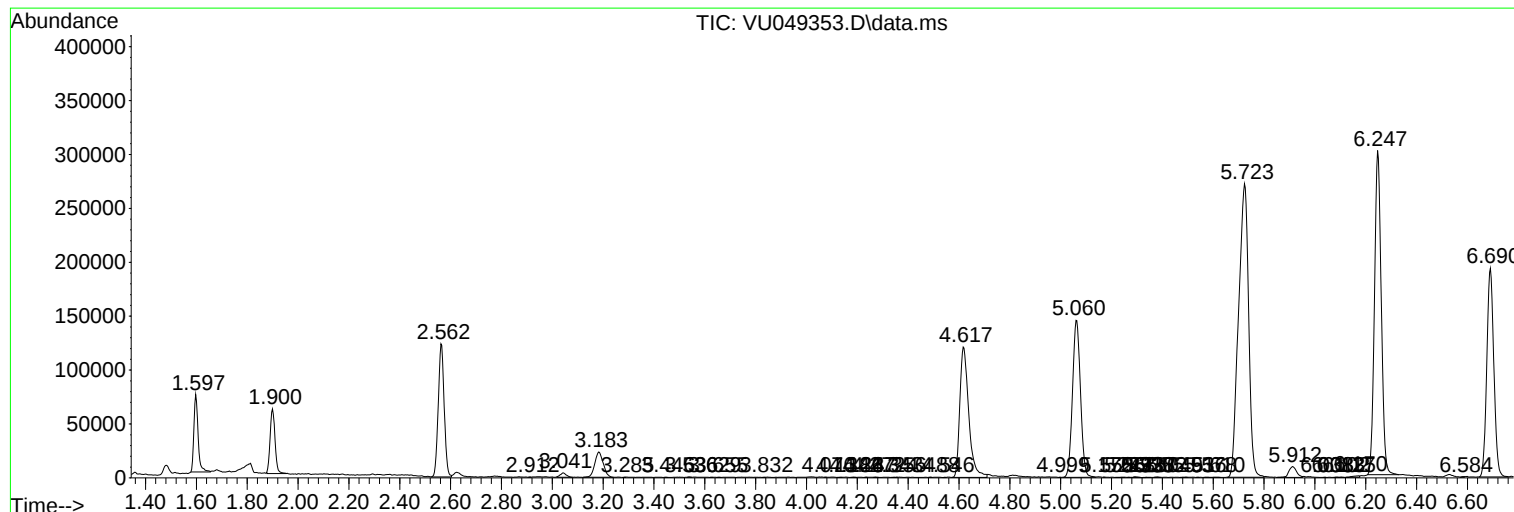
Sum of corrected areas: 7186747

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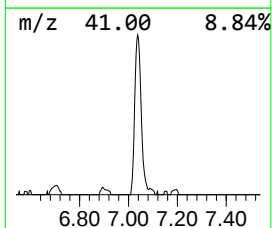
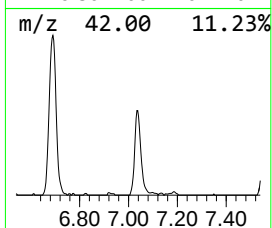
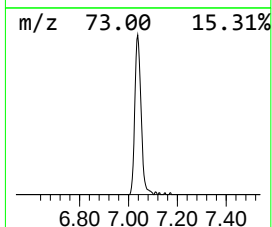
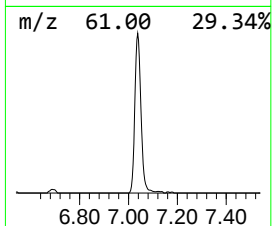
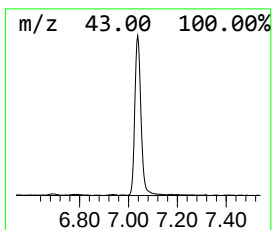
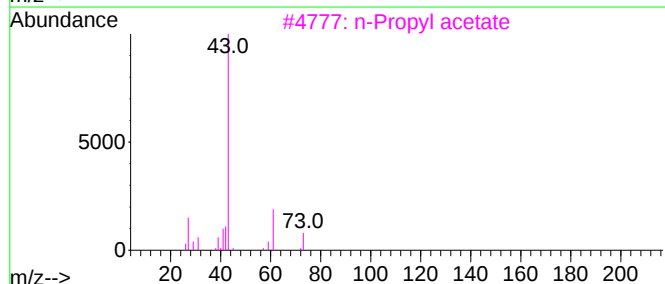
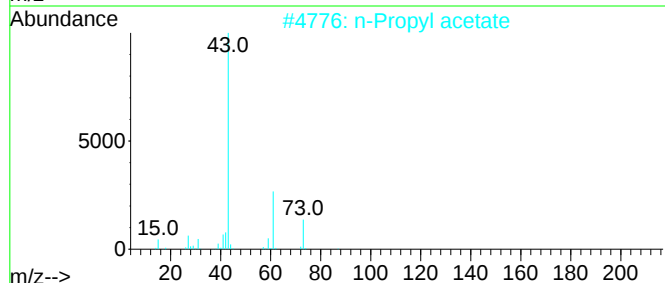
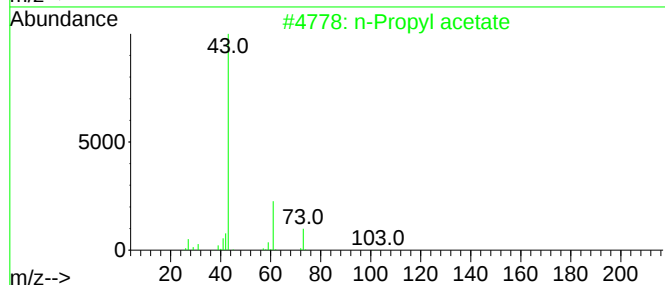
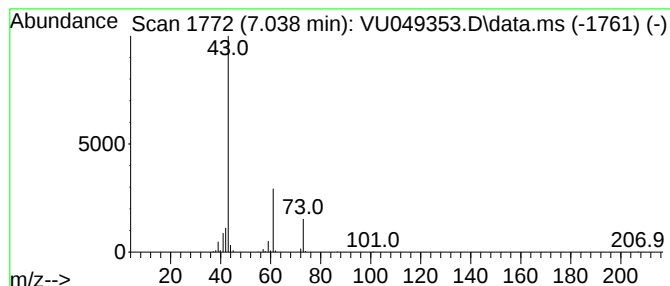
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	18.61 ug/L	208266	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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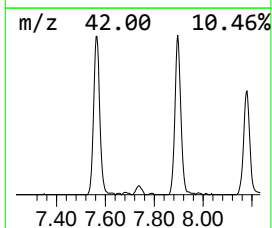
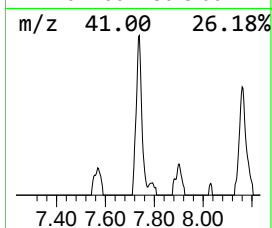
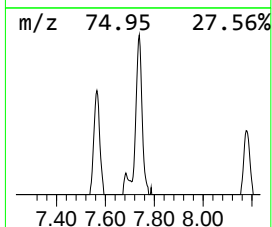
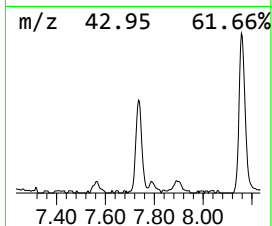
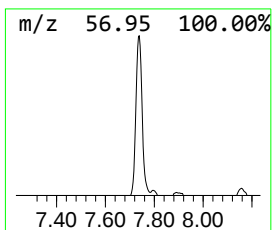
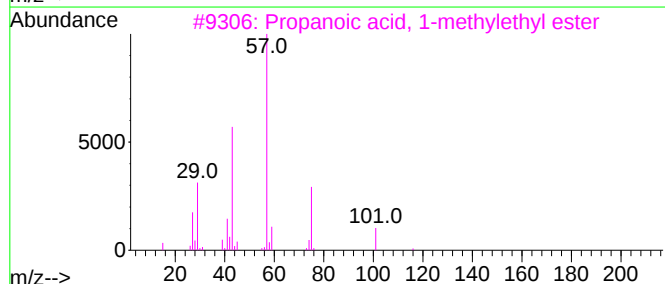
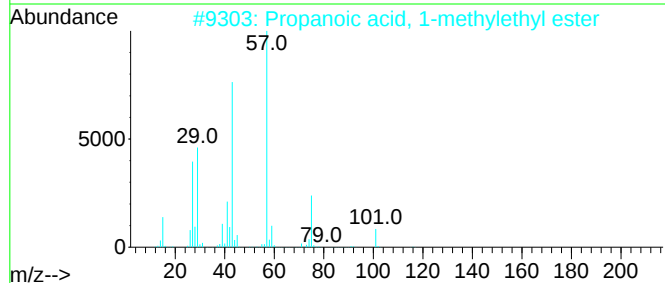
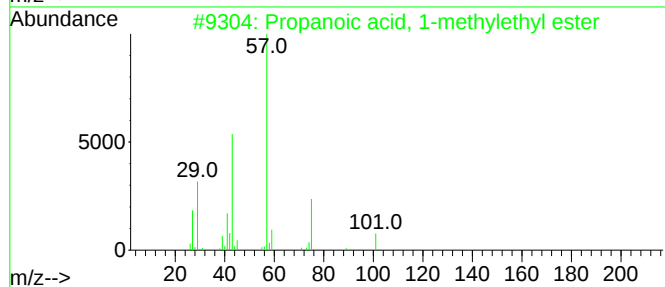
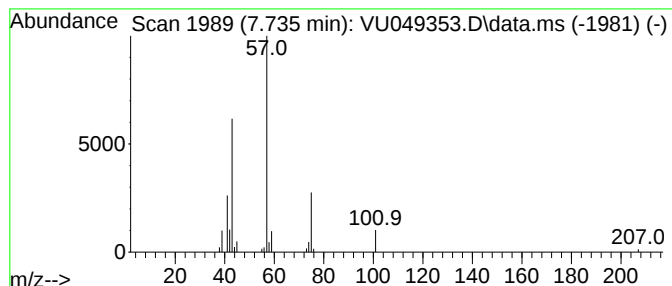
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
7.735	3.39 ug/L	37988	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	90
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	56



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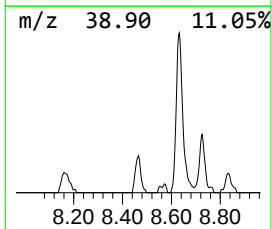
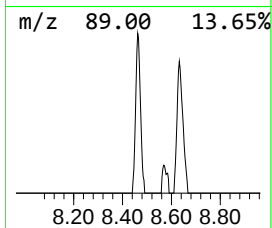
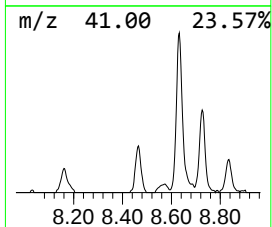
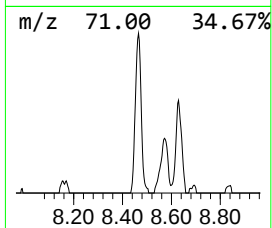
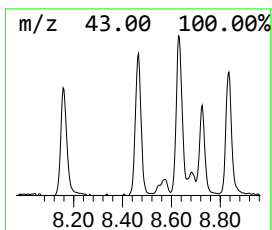
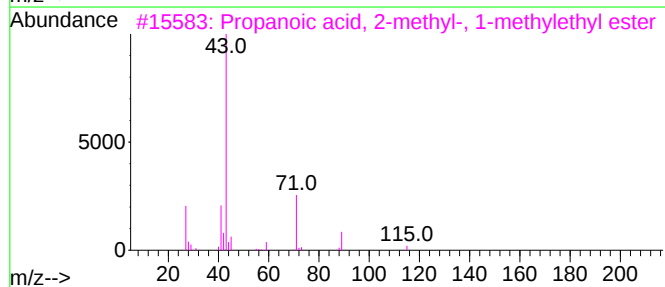
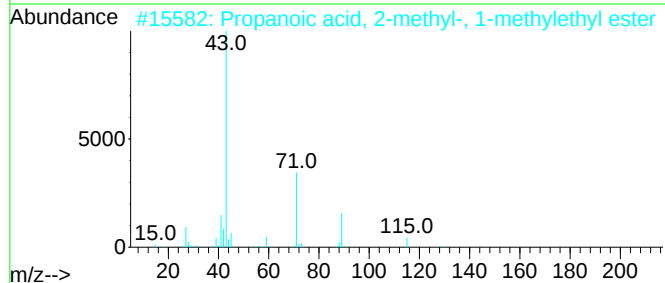
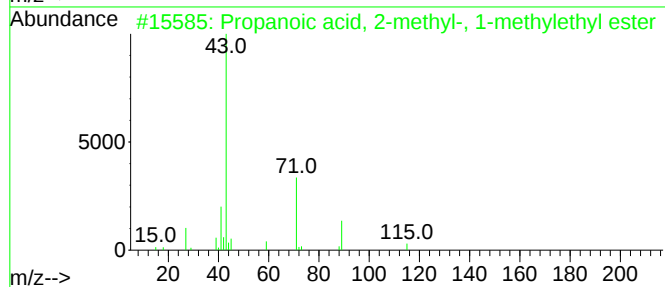
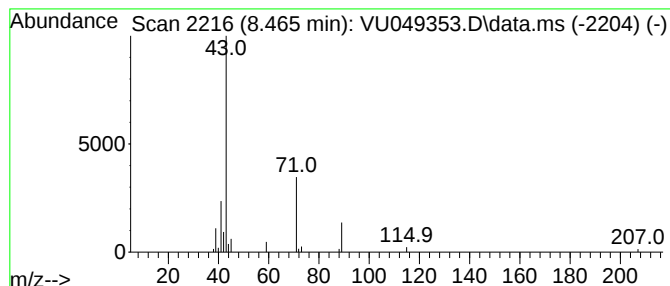
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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.
8.465	3.21 ug/L	42975	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-, 1-met...	130	C7H14O2	000617-50-5	72



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Instrument :
MSVOA_U
ClientSampleId :
EXEY2

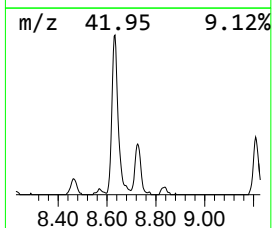
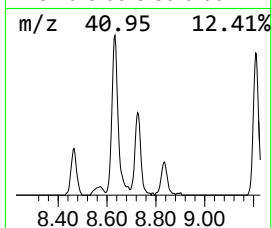
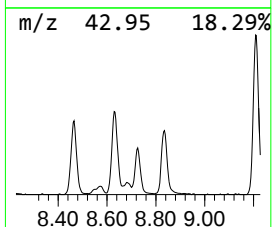
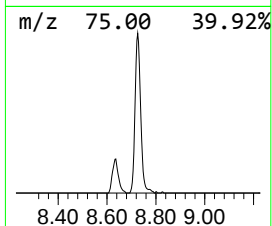
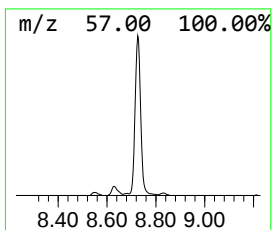
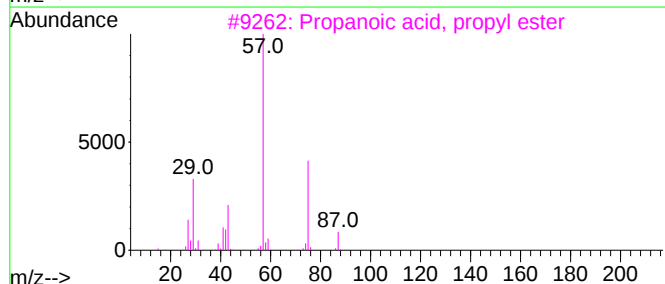
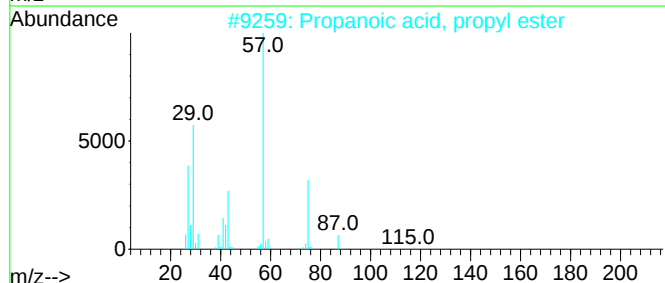
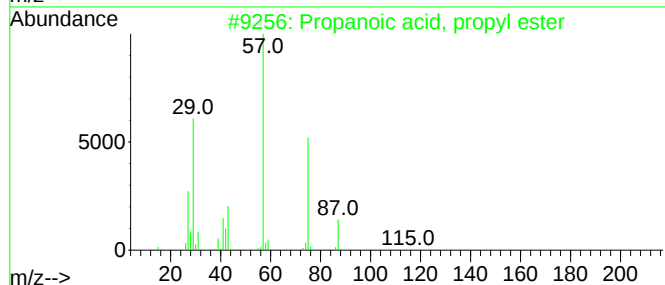
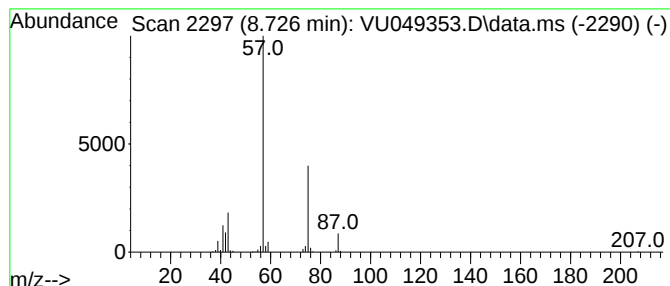
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Quant Title : VOC Analysis

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	9.77 ug/L	130790	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	78
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049353.D
Acq On : 22 Jun 2022 15:45
Operator : SY/MD
Sample : N3392-07 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY2

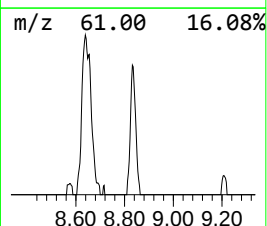
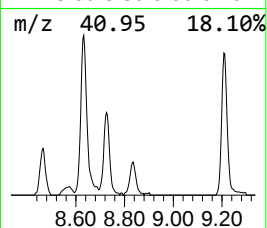
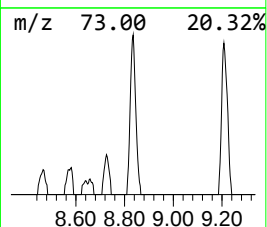
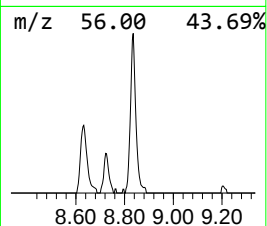
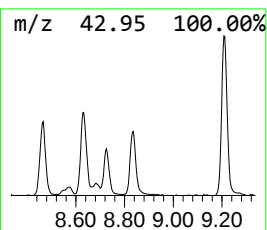
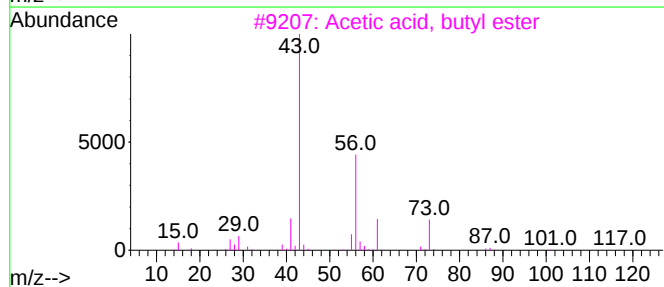
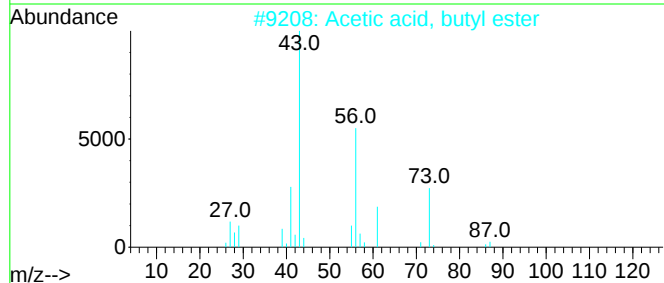
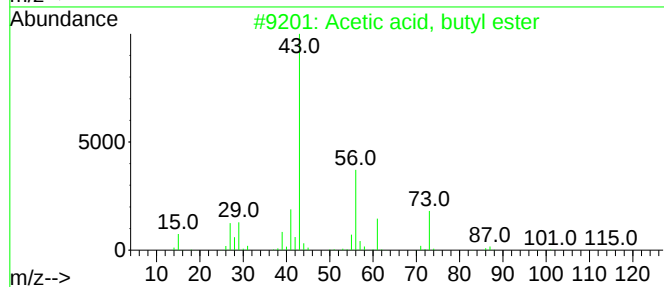
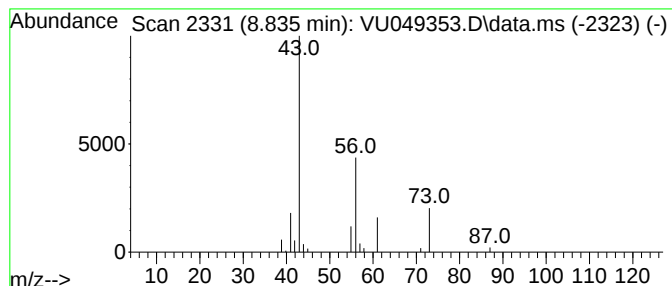
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Quant Title : VOC Analysis

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	2.76 ug/L	37001	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	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049353.D
Acq On : 22 Jun 2022 15:45
Operator : SY/MD
Sample : N3392-07 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY2

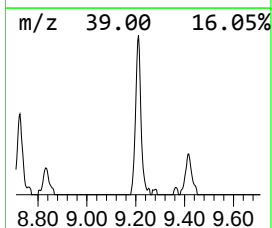
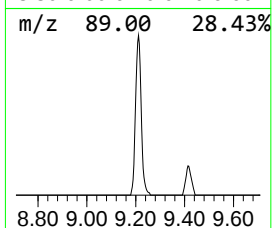
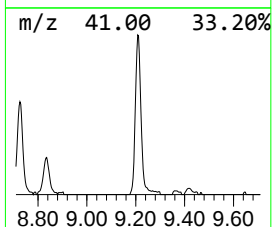
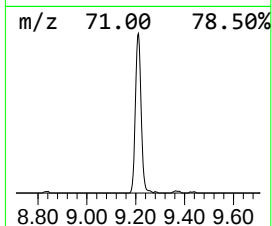
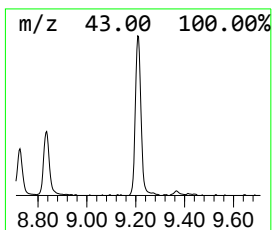
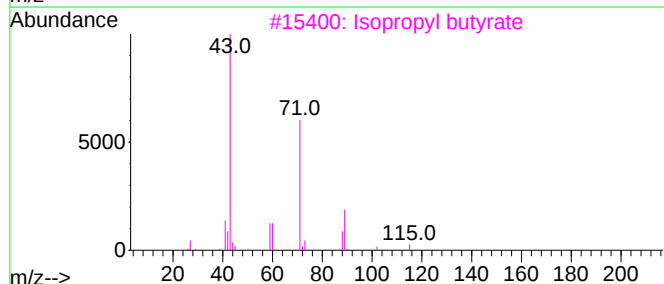
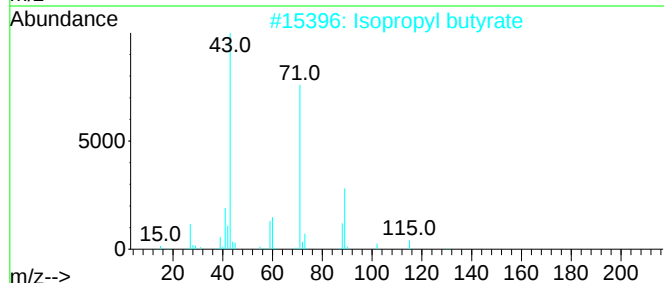
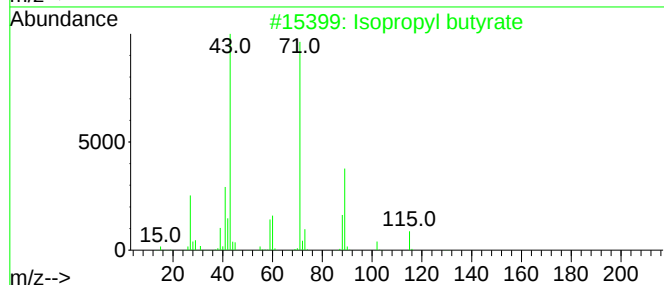
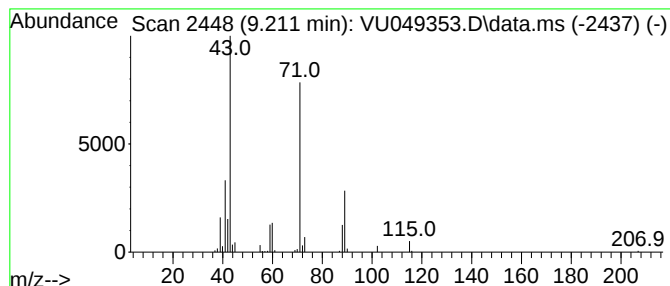
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	10.84 ug/L	145159	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-, 1-met...	130	C7H14O2	000617-50-5	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049353.D
Acq On : 22 Jun 2022 15:45
Operator : SY/MD
Sample : N3392-07 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY2

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	18.6	ug/L	208266	1	6.247	559681	50.0
Propanoic acid,...	7.735	3.4	ug/L	37988	1	6.247	559681	50.0
Propanoic acid,...	8.465	3.2	ug/L	42975	2	9.417	669451	50.0
Propanoic acid,...	8.726	9.8	ug/L	130790	2	9.417	669451	50.0
Acetic acid, bu...	8.835	2.8	ug/L	37001	2	9.417	669451	50.0
Isopropyl butyrate	9.211	10.8	ug/L	145159	2	9.417	669451	50.0