

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
 Data File : VU049351.D
 Acq On : 22 Jun 2022 14:58
 Operator : SY/MD
 Sample : N3392-05 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEY0

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: VU049351.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	11	rVB2	1898	1565	0.20%	0.021%
2	1.597	73	80	96	rBV	73876	86336	10.82%	1.149%
3	1.903	168	175	189	rVB	65874	86723	10.87%	1.154%
4	2.565	368	381	394	rBV	132901	212271	26.60%	2.825%
5	2.636	395	403	417	rVB	2649	5085	0.64%	0.068%
6	2.784	441	449	452	rBV5	883	1235	0.15%	0.016%
7	2.916	487	490	495	rBB2	305	238	0.03%	0.003%
8	2.944	495	499	501	rBV2	440	280	0.04%	0.004%
9	3.047	520	531	540	rVB4	3707	6808	0.85%	0.091%
10	3.186	558	574	589	rBV2	18711	45319	5.68%	0.603%
11	3.407	640	643	646	rBV	308	292	0.04%	0.004%
12	3.533	678	682	686	rBV	228	212	0.03%	0.003%
13	3.588	693	699	705	rVB3	349	513	0.06%	0.007%
14	3.777	755	758	762	rVB2	275	248	0.03%	0.003%
15	3.919	797	802	807	rBV3	310	288	0.04%	0.004%
16	4.038	836	839	843	rVB2	489	356	0.04%	0.005%
17	4.070	843	849	851	rBV2	303	311	0.04%	0.004%
18	4.102	855	859	865	rVB3	253	272	0.03%	0.004%
19	4.170	874	880	883	rBV	270	297	0.04%	0.004%
20	4.198	887	889	893	rVV	358	208	0.03%	0.003%
21	4.623	1007	1021	1068	rBV2	125963	329181	41.26%	4.381%
22	4.925	1112	1115	1120	rVB3	324	236	0.03%	0.003%
23	5.009	1138	1141	1142	rBV2	516	252	0.03%	0.003%
24	5.063	1142	1158	1182	rVV	155014	334595	41.93%	4.453%
25	5.446	1274	1277	1284	rVB	240	232	0.03%	0.003%
26	5.491	1284	1291	1293	rBV	338	291	0.04%	0.004%
27	5.575	1314	1317	1324	rBV	211	230	0.03%	0.003%
28	5.722	1342	1363	1391	rBV2	292160	797904	100.00%	10.620%
29	5.912	1409	1422	1436	rBV3	8848	18852	2.36%	0.251%
30	5.967	1436	1439	1442	rVV3	594	580	0.07%	0.008%
31	6.018	1450	1455	1457	rVB2	266	236	0.03%	0.003%
32	6.128	1481	1489	1490	rBV3	1242	1473	0.18%	0.020%
33	6.140	1490	1493	1495	rVV3	728	545	0.07%	0.007%
34	6.247	1513	1526	1548	rBV	306859	587357	73.61%	7.818%
35	6.526	1607	1613	1622	rVB6	1964	3419	0.43%	0.046%
36	6.690	1650	1664	1683	rBV	203604	396074	49.64%	5.272%

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Integrator: RTE

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Peak separation: 5

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

37	6.829	1704	1707	1711	rVB	375	236	0.03%	0.003%
38	6.925	1727	1737	1756	rVB	4493	10995	1.38%	0.146%
39	7.041	1760	1773	1797	rBV2	123651	225582	28.27%	3.002%
40	7.189	1812	1819	1831	rVB6	2308	4304	0.54%	0.057%
41	7.247	1835	1837	1846	rVB3	261	287	0.04%	0.004%
42	7.353	1865	1870	1874	rBV2	343	320	0.04%	0.004%
43	7.378	1874	1878	1881	rBV2	277	229	0.03%	0.003%
44	7.497	1913	1915	1921	rVB3	511	331	0.04%	0.004%
45	7.565	1922	1936	1953	rBV	107756	188828	23.67%	2.513%
46	7.687	1969	1974	1975	rBV2	938	760	0.10%	0.010%
47	7.738	1980	1990	2001	rVV2	21052	34993	4.39%	0.466%
48	7.899	2025	2040	2059	rBV	335773	587467	73.63%	7.819%
49	8.179	2110	2127	2142	rBV2	81278	169463	21.24%	2.256%
50	8.288	2158	2161	2167	rBV5	429	447	0.06%	0.006%
51	8.314	2167	2169	2174	rVB3	350	286	0.04%	0.004%
52	8.465	2204	2216	2227	rVV	23320	38040	4.77%	0.506%
53	8.574	2235	2250	2257	rBV4	13406	23496	2.94%	0.313%
54	8.632	2257	2268	2289	rVV	357742	638667	80.04%	8.500%
55	8.729	2289	2298	2314	rVB	75993	124848	15.65%	1.662%
56	8.835	2322	2331	2348	rVB	31686	49937	6.26%	0.665%
57	9.163	2427	2433	2436	rBV2	458	407	0.05%	0.005%
58	9.211	2436	2448	2462	rBV	84992	133633	16.75%	1.779%
59	9.343	2484	2489	2490	rVV2	247	227	0.03%	0.003%
60	9.369	2490	2497	2499	rVV4	1186	1405	0.18%	0.019%
61	9.417	2500	2512	2535	rVV	414710	684222	85.75%	9.107%
62	9.568	2554	2559	2562	rBV3	587	456	0.06%	0.006%
63	9.639	2576	2581	2583	rBV2	888	762	0.10%	0.010%
64	9.697	2596	2599	2602	rBV2	344	266	0.03%	0.004%
65	9.922	2662	2669	2675	rVB5	781	1268	0.16%	0.017%
66	10.073	2709	2716	2726	rVB3	5189	7670	0.96%	0.102%
67	10.240	2762	2768	2770	rBV2	417	368	0.05%	0.005%
68	10.388	2809	2814	2815	rBV	316	222	0.03%	0.003%
69	10.459	2831	2836	2841	rVB2	238	292	0.04%	0.004%
70	10.565	2863	2869	2870	rBV3	289	240	0.03%	0.003%
71	10.645	2892	2894	2898	rBV2	308	220	0.03%	0.003%
72	10.754	2916	2928	2951	rBV	308212	508658	63.75%	6.770%
73	10.835	2951	2953	2957	rVB2	414	246	0.03%	0.003%
74	10.989	2997	3001	3003	rBV	366	237	0.03%	0.003%
75	11.053	3018	3021	3027	rVB2	233	269	0.03%	0.004%
76	11.115	3037	3040	3043	rVB2	385	250	0.03%	0.003%

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 Title : VOC Analysis

77	11.420	3132	3135	3139	rVB2	341	228	0.03%	0.003%
78	11.478	3147	3153	3159	rBV3	492	574	0.07%	0.008%
79	11.549	3171	3175	3178	rBV2	318	252	0.03%	0.003%
80	11.600	3188	3191	3194	rBV	340	292	0.04%	0.004%
81	11.616	3194	3196	3200	rVB2	332	209	0.03%	0.003%
82	11.812	3245	3257	3281	rBV	382664	610852	76.56%	8.130%
83	12.047	3327	3330	3335	rBV2	369	314	0.04%	0.004%
84	12.192	3363	3375	3393	rBV	331927	533125	66.82%	7.096%
85	12.404	3437	3441	3445	rBV2	299	236	0.03%	0.003%
86	12.690	3526	3530	3532	rVV2	330	274	0.03%	0.004%
87	12.703	3532	3534	3539	rVV3	315	245	0.03%	0.003%
88	12.735	3541	3544	3550	rVB2	322	323	0.04%	0.004%
89	12.774	3550	3556	3563	rBV3	612	958	0.12%	0.013%
90	13.037	3635	3638	3641	rBV2	402	320	0.04%	0.004%
91	13.307	3718	3722	3726	rVB2	423	312	0.04%	0.004%
92	13.645	3823	3827	3828	rBV	308	250	0.03%	0.003%
93	13.713	3845	3848	3850	rBV	312	222	0.03%	0.003%
94	13.799	3873	3875	3879	rVB2	464	286	0.04%	0.004%
95	13.825	3880	3883	3885	rBV2	361	227	0.03%	0.003%
96	14.176	3988	3992	3995	rBV2	313	334	0.04%	0.004%
97	14.883	4209	4212	4215	rBV3	317	279	0.03%	0.004%
98	14.983	4238	4243	4247	rBV3	413	418	0.05%	0.006%
99	15.237	4314	4322	4325	rBV3	542	847	0.11%	0.011%
100	16.359	4669	4671	4676	rBV4	807	775	0.10%	0.010%

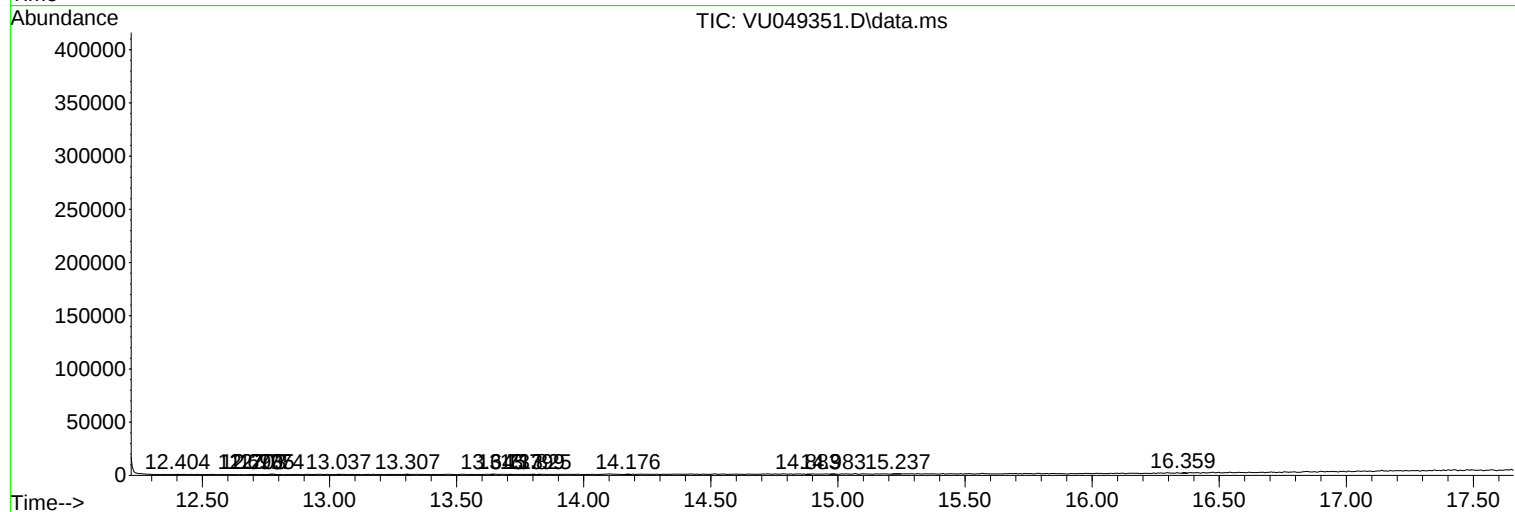
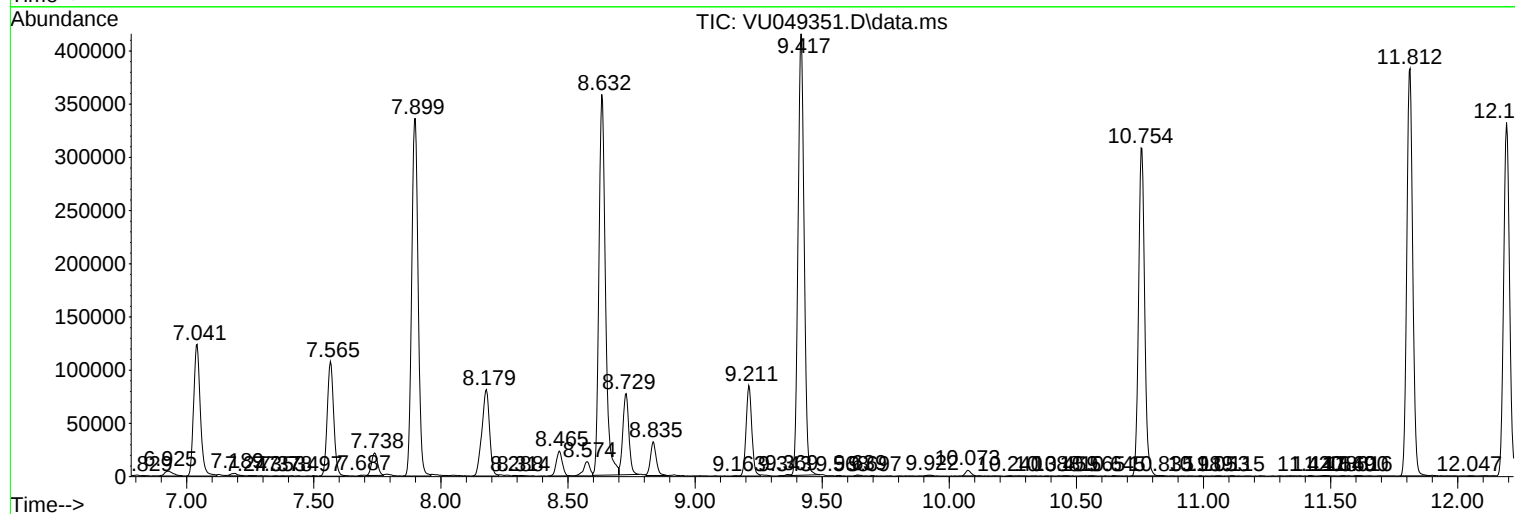
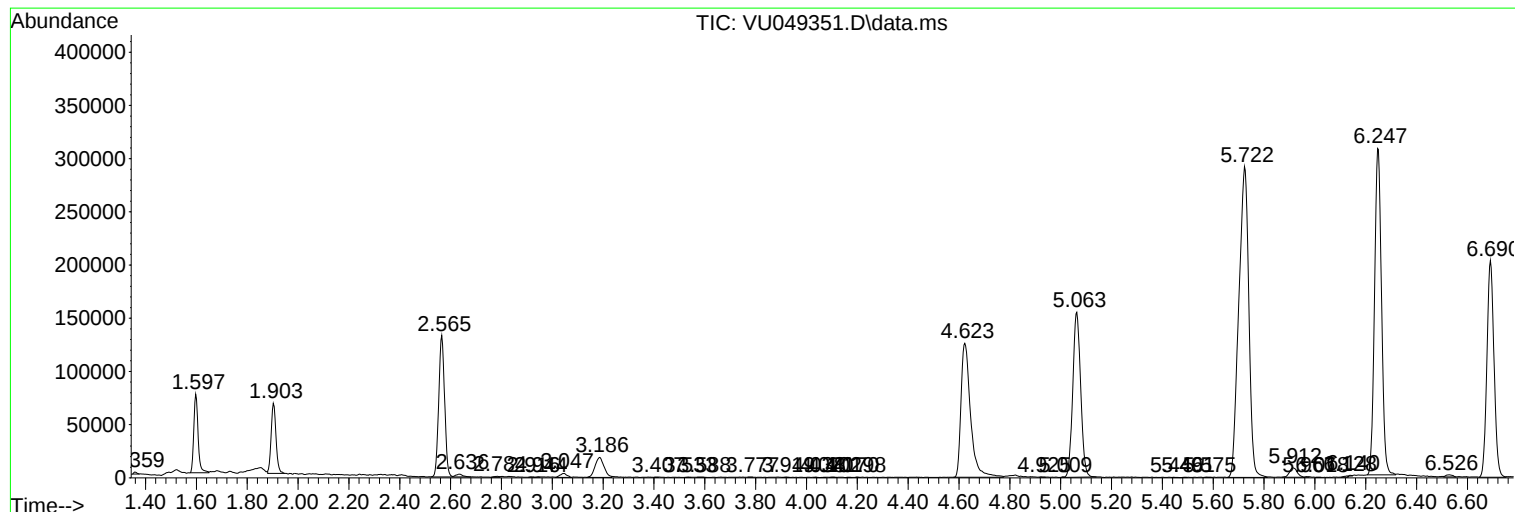
Sum of corrected areas: 7513300

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY0

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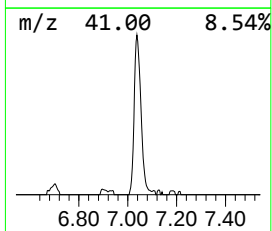
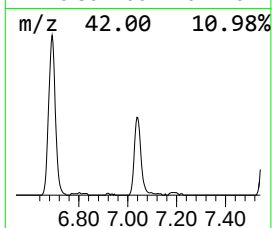
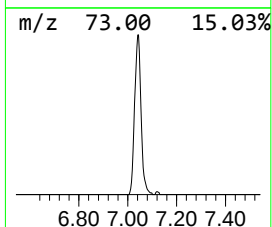
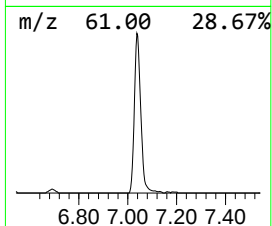
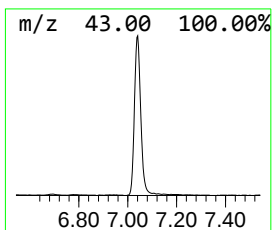
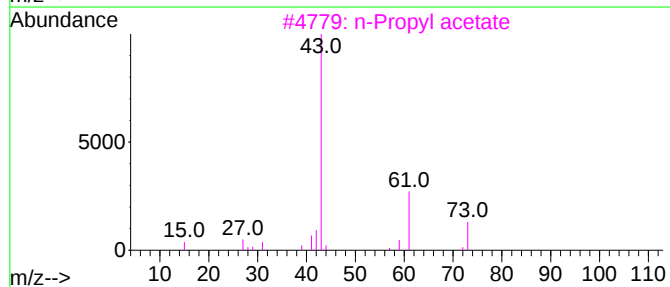
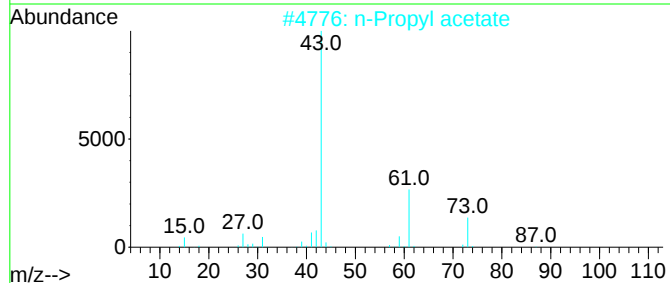
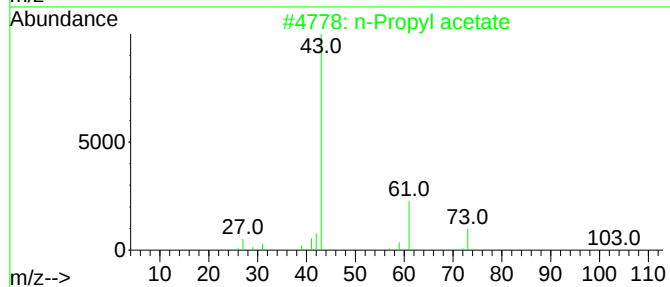
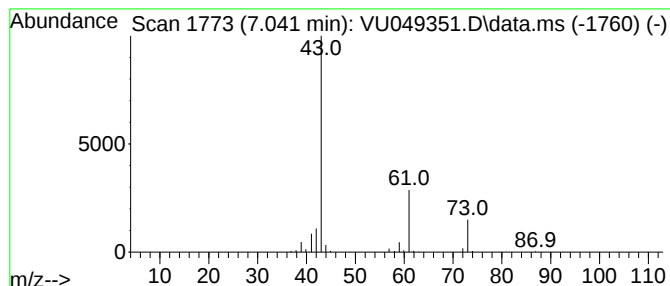
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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	19.20 ug/L	225582	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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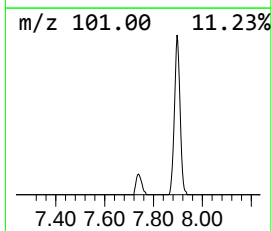
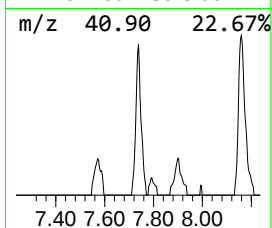
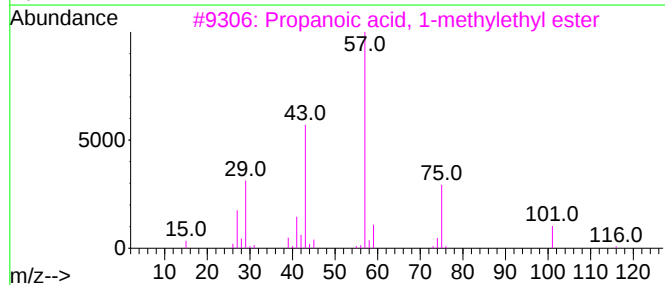
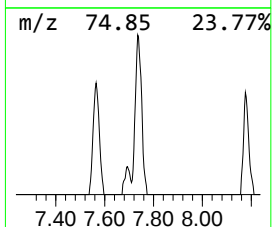
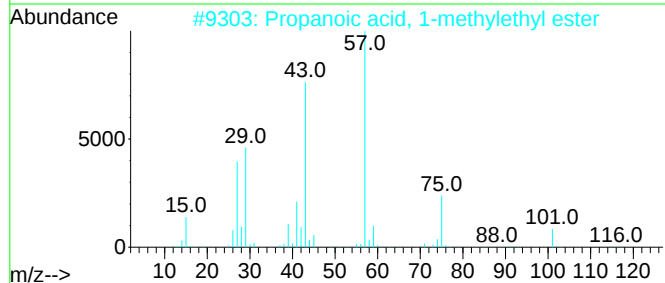
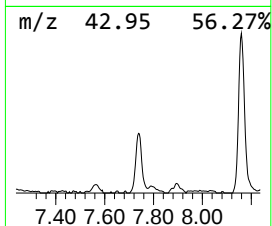
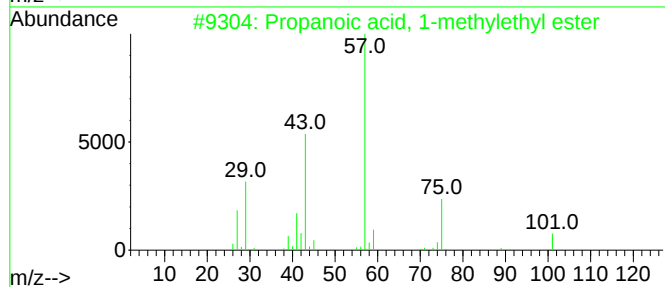
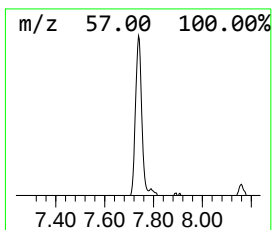
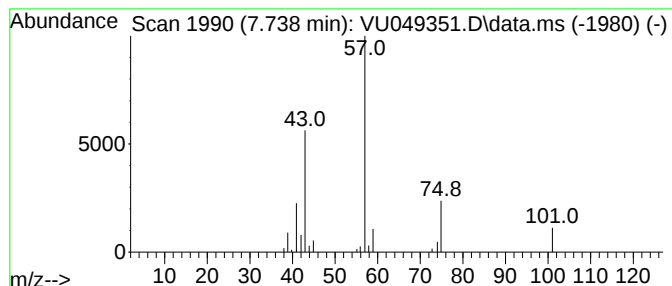
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.98 ug/L	34993	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	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72



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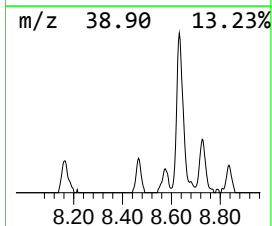
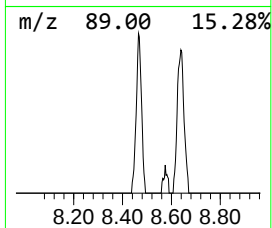
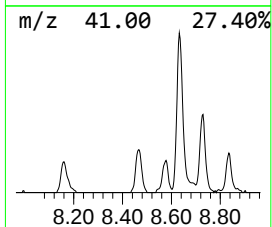
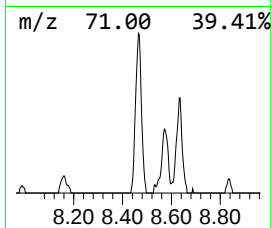
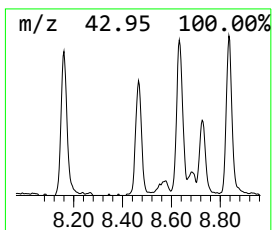
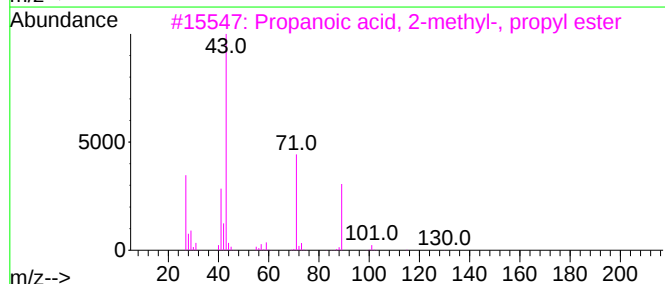
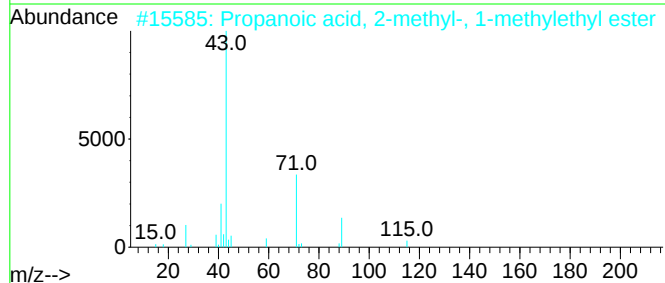
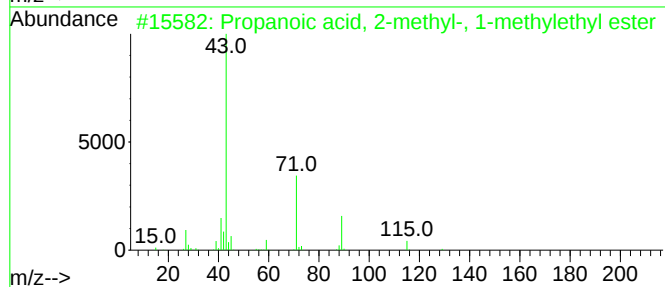
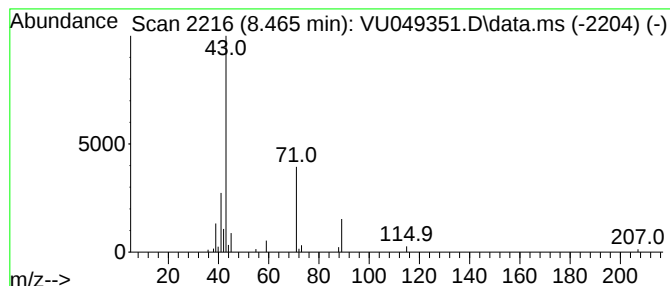
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.78 ug/L	38040	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-, propy...	130	C7H14O2	000644-49-5	64
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049351.D
Acq On : 22 Jun 2022 14:58
Operator : SY/MD
Sample : N3392-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY0

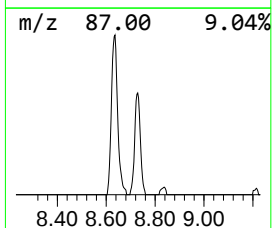
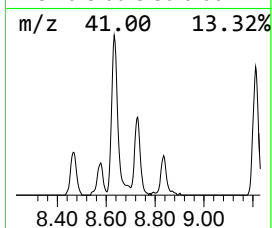
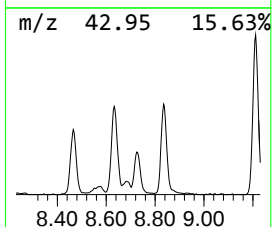
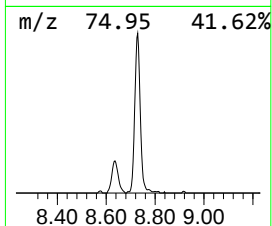
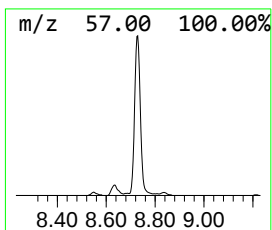
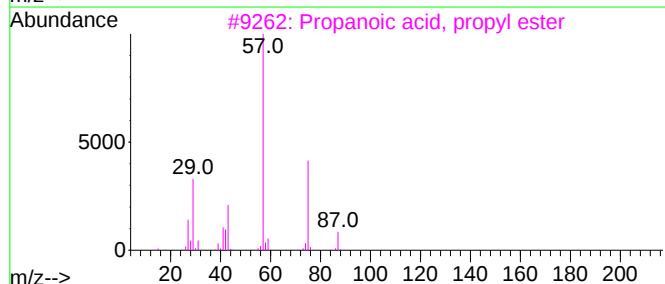
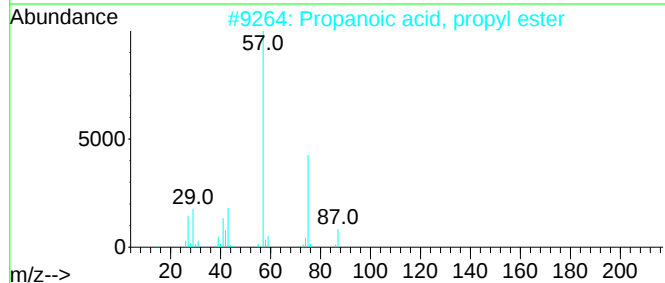
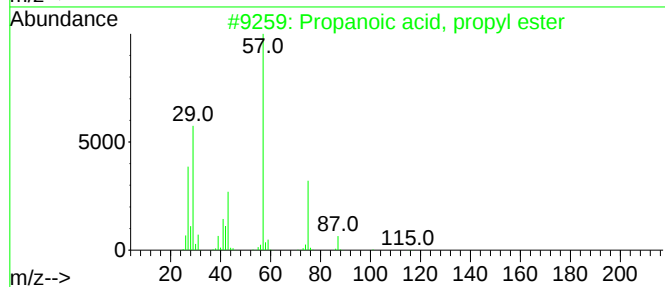
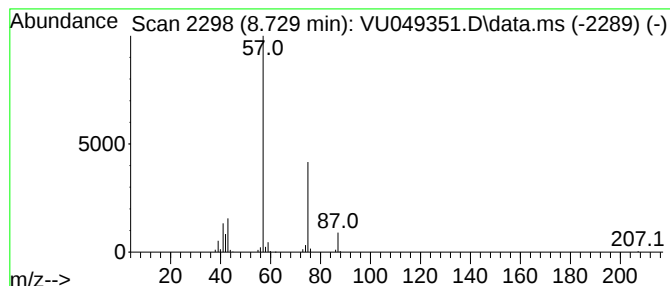
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Quant Title : VOC Analysis

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	9.12 ug/L	124848	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	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049351.D
Acq On : 22 Jun 2022 14:58
Operator : SY/MD
Sample : N3392-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY0

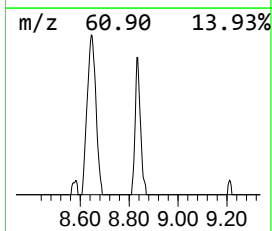
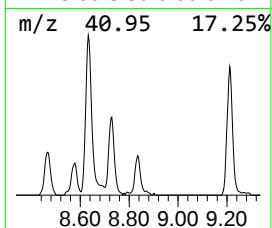
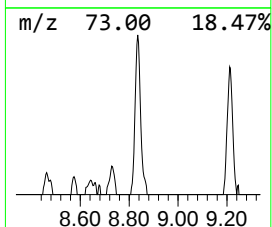
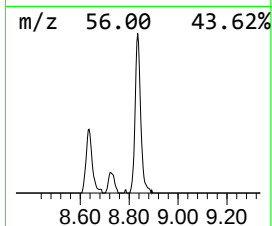
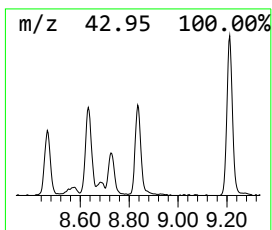
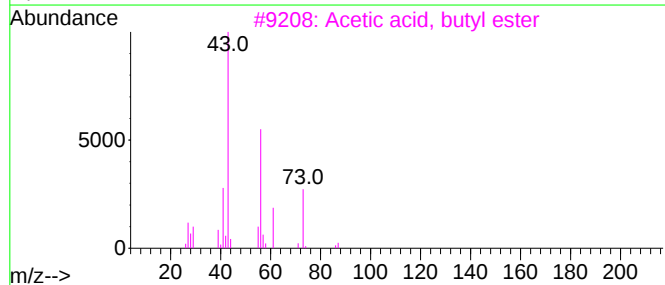
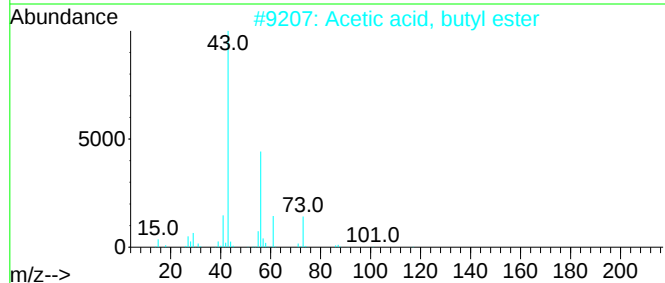
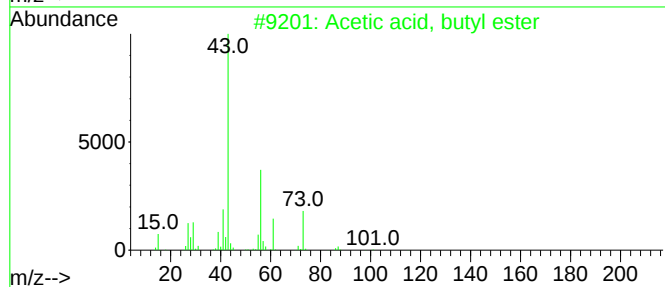
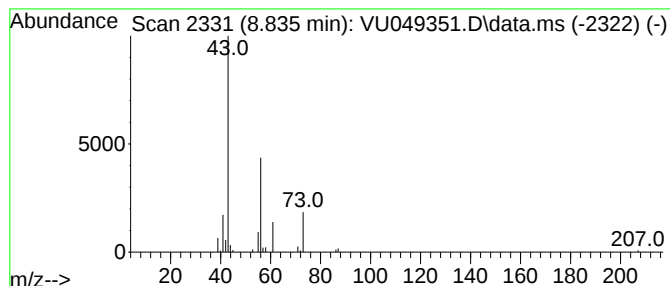
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Quant Title : VOC Analysis

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	3.65 ug/L	49937	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	72	
4	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	72	
5	1-Butanol, 4-chloro-, acetate		150	C6H11ClO2	006962-92-1	23	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049351.D
Acq On : 22 Jun 2022 14:58
Operator : SY/MD
Sample : N3392-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY0

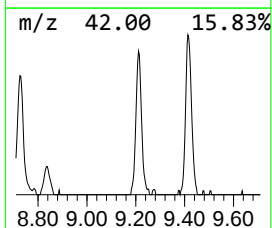
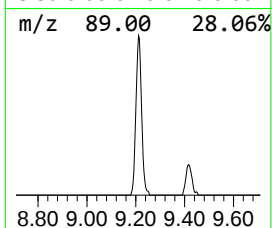
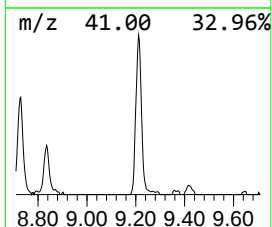
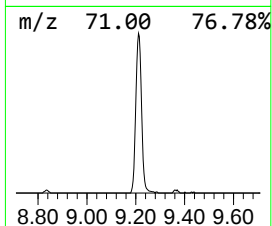
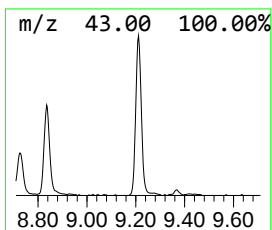
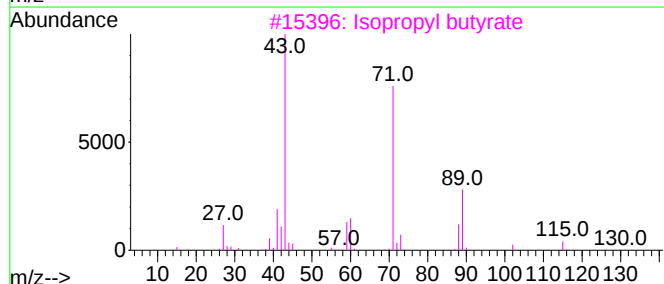
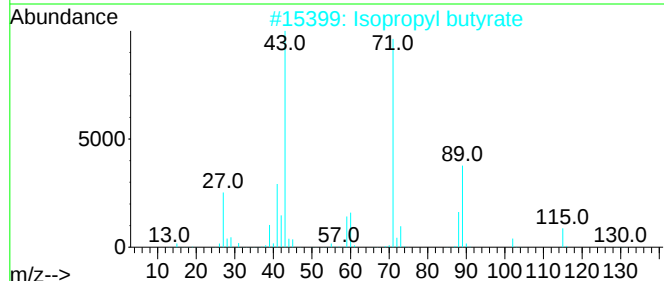
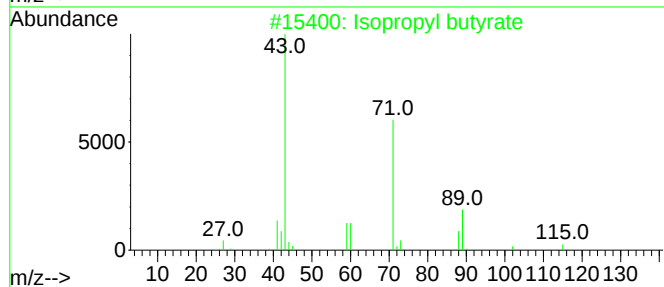
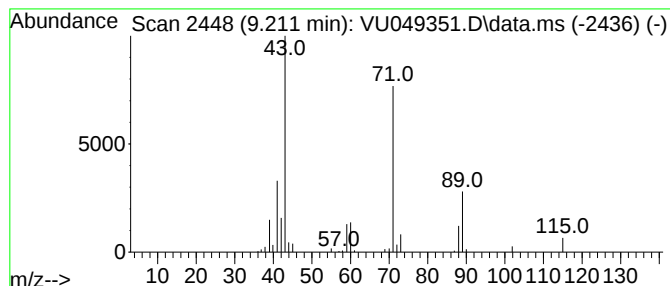
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Quant Title : VOC Analysis

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	9.77 ug/L	133633	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	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049351.D
Acq On : 22 Jun 2022 14:58
Operator : SY/MD
Sample : N3392-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY0

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	19.2	ug/L	225582	1	6.247	587357	50.0
Propanoic acid,...	7.738	3.0	ug/L	34993	1	6.247	587357	50.0
Propanoic acid,...	8.465	2.8	ug/L	38040	2	9.417	684222	50.0
Propanoic acid,...	8.729	9.1	ug/L	124848	2	9.417	684222	50.0
Acetic acid, bu...	8.835	3.6	ug/L	49937	2	9.417	684222	50.0
Isopropyl butyrate	9.211	9.8	ug/L	133633	2	9.417	684222	50.0