

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
 Data File : VU052135.D
 Acq On : 25 Nov 2022 11:38
 Operator : JC/MD
 Sample : PB149243TB 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VLEB243

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\SFAMULM112122WMA.M
 Title : VOC Analysis

Signal : TIC: VU052135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	35	42	51	rBV	11429	21182	1.22%	0.150%
2	1.601	73	81	99	rVB	258692	296610	17.02%	2.098%
3	1.909	168	177	200	rVB	174318	265747	15.25%	1.880%
4	2.565	367	381	393	rBV	380340	621443	35.66%	4.396%
5	2.623	394	399	415	rVB	18993	32603	1.87%	0.231%
6	2.777	445	447	450	rBV2	326	235	0.01%	0.002%
7	2.941	491	498	500	rBV3	315	366	0.02%	0.003%
8	2.977	506	509	516	rBV3	440	475	0.03%	0.003%
9	3.048	519	531	547	rBV2	19595	39074	2.24%	0.276%
10	3.186	561	574	589	rVV2	11369	25805	1.48%	0.183%
11	3.295	604	608	612	rBV3	313	339	0.02%	0.002%
12	3.366	627	630	635	rBV3	568	442	0.03%	0.003%
13	3.459	655	659	663	rBV3	301	251	0.01%	0.002%
14	3.613	698	707	712	rBV	408	587	0.03%	0.004%
15	3.655	713	720	723	rBV2	402	471	0.03%	0.003%
16	3.765	751	754	757	rVB2	433	256	0.01%	0.002%
17	3.835	767	776	777	rBV	3047	3192	0.18%	0.023%
18	3.999	825	827	832	rVV2	309	299	0.02%	0.002%
19	4.060	843	846	851	rBV2	382	270	0.02%	0.002%
20	4.137	868	870	876	rVV2	248	243	0.01%	0.002%
21	4.253	902	906	908	rBV	392	262	0.02%	0.002%
22	4.330	927	930	935	rBV3	299	235	0.01%	0.002%
23	4.617	1007	1019	1051	rBV	137825	344723	19.78%	2.439%
24	5.060	1141	1157	1185	rBV	307473	681583	39.11%	4.822%
25	5.285	1223	1227	1237	rVB3	1196	1672	0.10%	0.012%
26	5.372	1251	1254	1258	rVV2	505	548	0.03%	0.004%
27	5.391	1258	1260	1263	rVB	605	310	0.02%	0.002%
28	5.424	1263	1270	1275	rVB3	419	456	0.03%	0.003%
29	5.568	1312	1315	1320	rVB2	389	309	0.02%	0.002%
30	5.723	1341	1363	1389	rBV2	645050	1742644	100.00%	12.328%
31	5.912	1411	1422	1434	rBV2	15958	33318	1.91%	0.236%
32	6.051	1463	1465	1469	rVB3	364	241	0.01%	0.002%
33	6.102	1478	1481	1482	rBV	478	247	0.01%	0.002%
34	6.247	1511	1526	1555	rBV	546551	1052195	60.38%	7.444%
35	6.417	1577	1579	1582	rVB2	598	364	0.02%	0.003%
36	6.440	1582	1586	1588	rBV4	368	285	0.02%	0.002%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
 Title : VOC Analysis

37	6.520	1606	1611	1613	rBV4	982	881	0.05%	0.006%
38	6.536	1613	1616	1621	rVV5	1357	1278	0.07%	0.009%
39	6.604	1633	1637	1642	rVB3	366	346	0.02%	0.002%
40	6.687	1649	1663	1692	rBV	398004	787971	45.22%	5.574%
41	6.787	1692	1694	1696	rBV3	583	322	0.02%	0.002%
42	6.925	1728	1737	1759	rVB	8408	20277	1.16%	0.143%
43	7.038	1759	1772	1801	rBV	189148	346889	19.91%	2.454%
44	7.192	1816	1820	1827	rVB5	1510	1385	0.08%	0.010%
45	7.266	1841	1843	1846	rVB2	577	341	0.02%	0.002%
46	7.295	1846	1852	1854	rBV4	403	406	0.02%	0.003%
47	7.404	1883	1886	1889	rBV2	371	313	0.02%	0.002%
48	7.565	1922	1936	1951	rBV	202865	355722	20.41%	2.516%
49	7.735	1979	1989	2002	rBV	38494	66291	3.80%	0.469%
50	7.896	2026	2039	2063	rBV	782347	1348212	77.37%	9.538%
51	8.025	2076	2079	2086	rVB5	516	533	0.03%	0.004%
52	8.176	2110	2126	2147	rBV2	154107	322804	18.52%	2.284%
53	8.356	2179	2182	2186	rBV2	506	328	0.02%	0.002%
54	8.462	2202	2215	2232	rBV	47056	76477	4.39%	0.541%
55	8.571	2236	2249	2256	rVV5	8142	16299	0.94%	0.115%
56	8.629	2256	2267	2288	rVV	430514	796424	45.70%	5.634%
57	8.726	2288	2297	2315	rVB	94492	160444	9.21%	1.135%
58	8.832	2321	2330	2352	rVB2	57185	94984	5.45%	0.672%
59	8.964	2368	2371	2375	rVB3	443	336	0.02%	0.002%
60	8.989	2376	2379	2380	rBV	533	247	0.01%	0.002%
61	9.038	2391	2394	2401	rVB3	637	491	0.03%	0.003%
62	9.076	2403	2406	2408	rBV	538	332	0.02%	0.002%
63	9.208	2436	2447	2464	rBV	138024	220451	12.65%	1.560%
64	9.321	2478	2482	2483	rBV	386	266	0.02%	0.002%
65	9.362	2491	2495	2498	rBV3	1766	1699	0.10%	0.012%
66	9.414	2498	2511	2545	rVB	819346	1354617	77.73%	9.583%
67	9.639	2575	2581	2582	rBV2	924	783	0.04%	0.006%
68	9.694	2593	2598	2606	rVB4	782	995	0.06%	0.007%
69	9.893	2657	2660	2663	rBV2	352	260	0.01%	0.002%
70	9.925	2663	2670	2675	rVV4	1569	1868	0.11%	0.013%
71	10.073	2707	2716	2723	rBV2	9733	14886	0.85%	0.105%
72	10.472	2838	2840	2845	rBV2	400	322	0.02%	0.002%
73	10.523	2850	2856	2859	rBV2	326	318	0.02%	0.002%
74	10.636	2887	2891	2894	rBV2	574	462	0.03%	0.003%
75	10.755	2914	2928	2949	rBV	567445	909958	52.22%	6.437%
76	10.899	2968	2973	2974	rBV	496	360	0.02%	0.003%

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 ClientSampleId :
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Integrator: RTE

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

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 Title : VOC Analysis

77	10.993	2999	3002	3006	rBV3	291	264	0.02%	0.002%
78	11.083	3027	3030	3033	rBV	428	251	0.01%	0.002%
79	11.121	3039	3042	3047	rBV2	311	305	0.02%	0.002%
80	11.253	3080	3083	3088	rVB	420	306	0.02%	0.002%
81	11.417	3132	3134	3140	rVB	608	345	0.02%	0.002%
82	11.478	3146	3153	3161	rVB4	379	641	0.04%	0.005%
83	11.529	3166	3169	3173	rVB	327	251	0.01%	0.002%
84	11.552	3173	3176	3181	rBV2	407	392	0.02%	0.003%
85	11.671	3211	3213	3218	rVB	382	233	0.01%	0.002%
86	11.742	3232	3235	3243	rBV3	913	1030	0.06%	0.007%
87	11.809	3243	3256	3277	rBV	625857	1004457	57.64%	7.106%
88	12.189	3360	3374	3395	rBV	624993	1039901	59.67%	7.357%
89	12.610	3501	3505	3508	rBV2	735	629	0.04%	0.004%
90	12.841	3574	3577	3580	rVB	462	302	0.02%	0.002%
91	12.857	3580	3582	3587	rBV2	449	396	0.02%	0.003%
92	13.230	3692	3698	3701	rBV3	762	911	0.05%	0.006%
93	13.713	3845	3848	3852	rBV2	506	407	0.02%	0.003%
94	13.748	3857	3859	3862	rBV3	434	233	0.01%	0.002%
95	14.015	3938	3942	3944	rBV3	476	393	0.02%	0.003%
96	14.095	3962	3967	3979	rVB4	1499	2135	0.12%	0.015%
97	14.333	4037	4041	4049	rVB5	2292	2583	0.15%	0.018%
98	14.385	4054	4057	4063	rBV2	613	774	0.04%	0.005%
99	14.677	4146	4148	4152	rBV3	511	404	0.02%	0.003%
100	16.102	4586	4591	4597	rBV5	995	1316	0.08%	0.009%

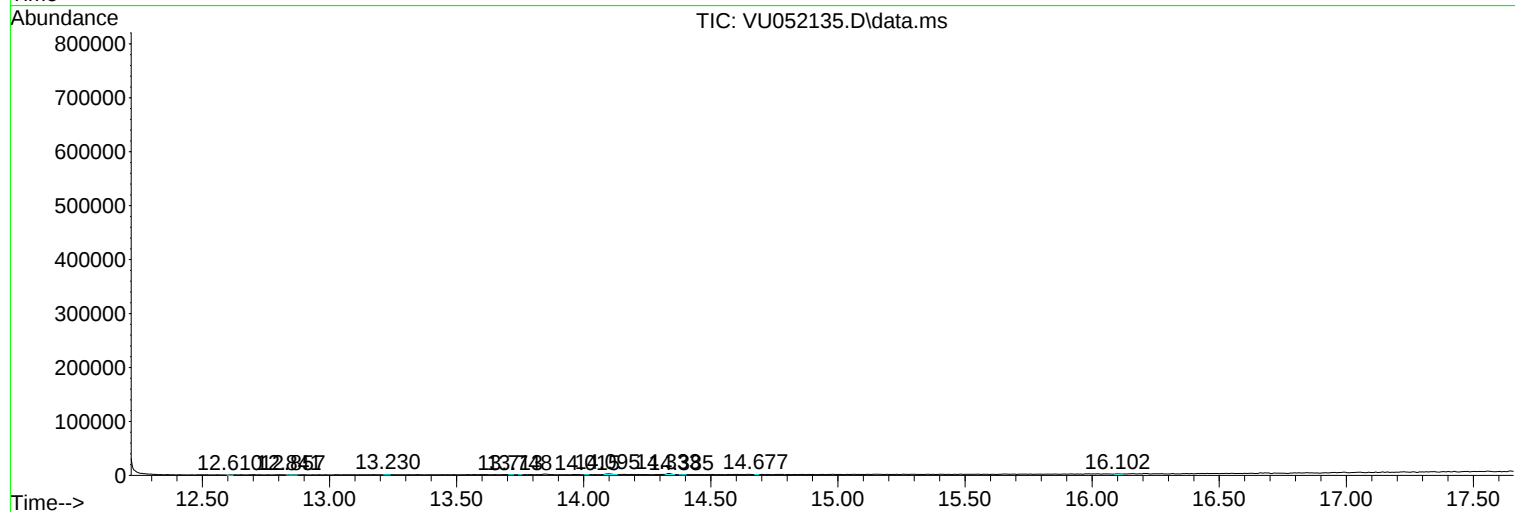
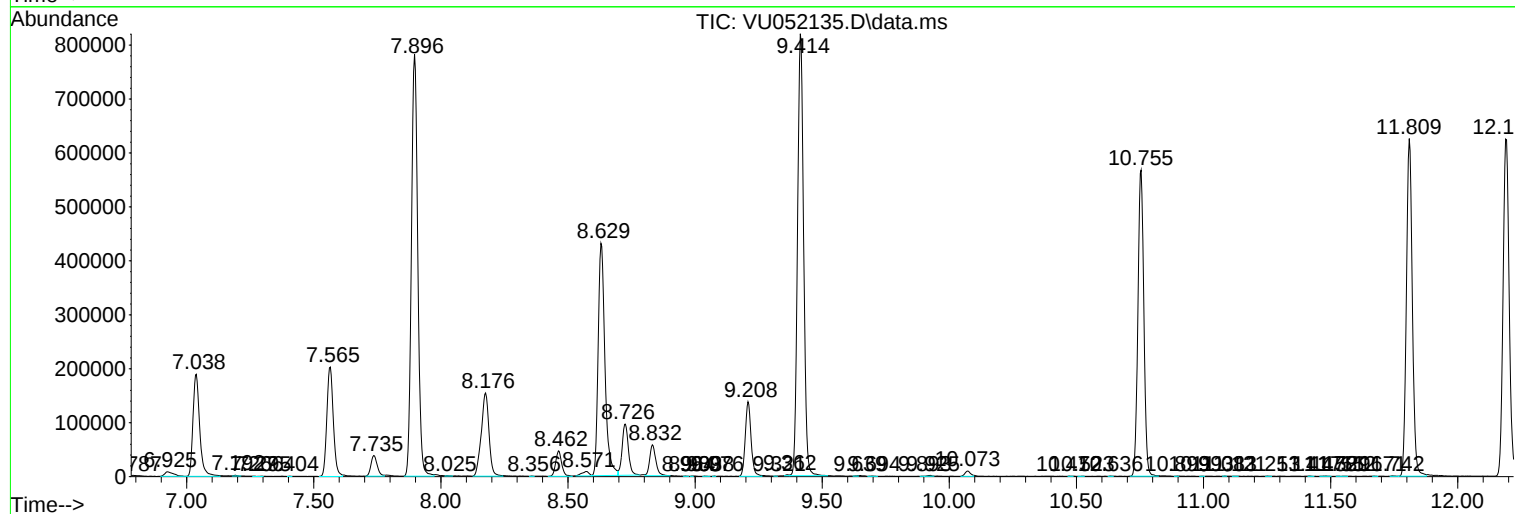
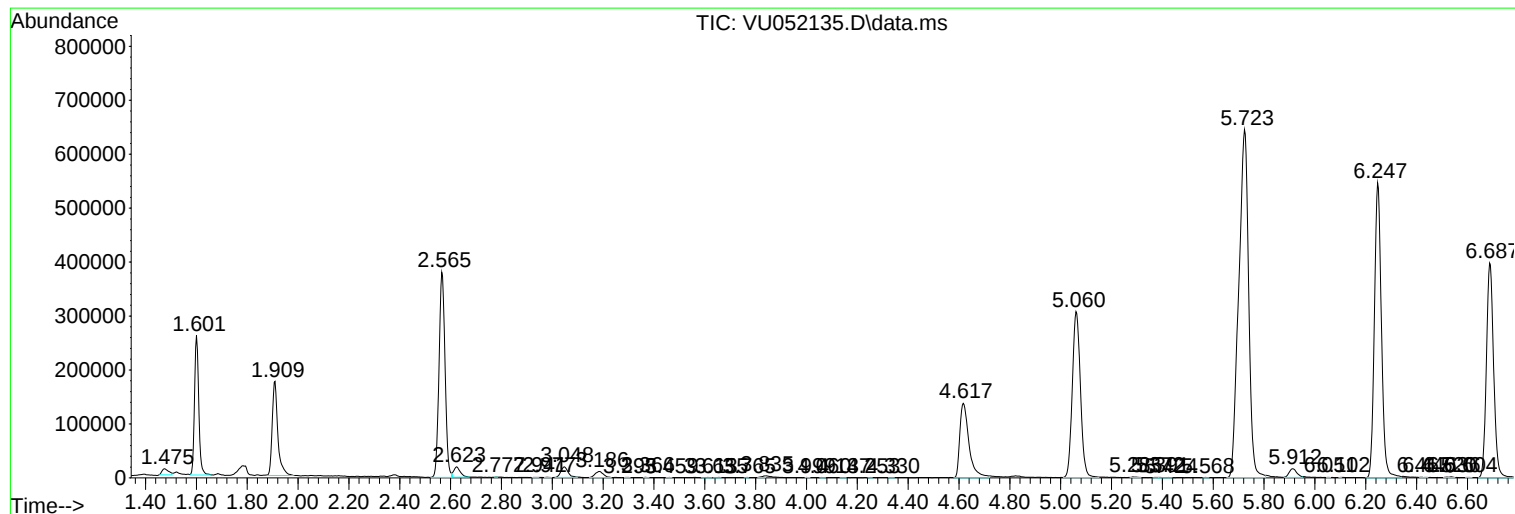
Sum of corrected areas: 14135719

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ClientSampleId :
VLEB243

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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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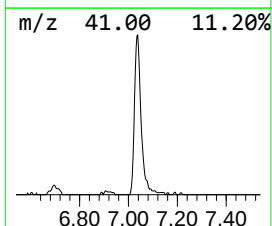
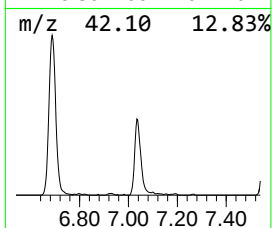
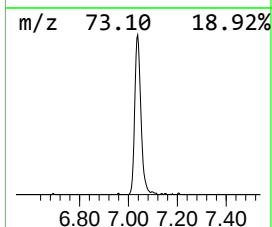
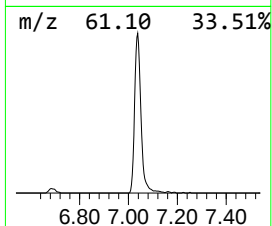
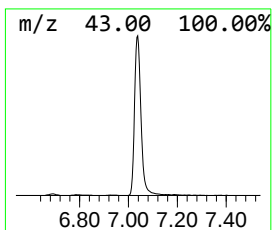
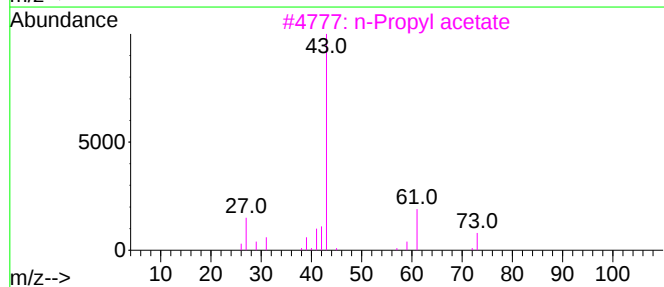
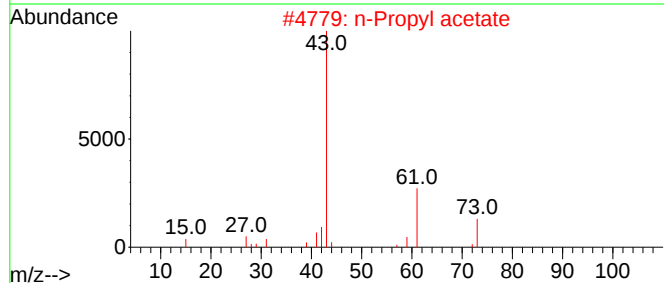
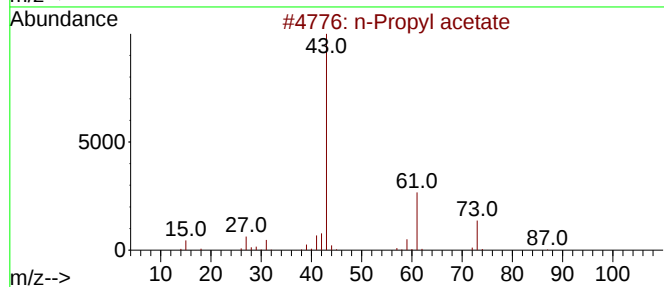
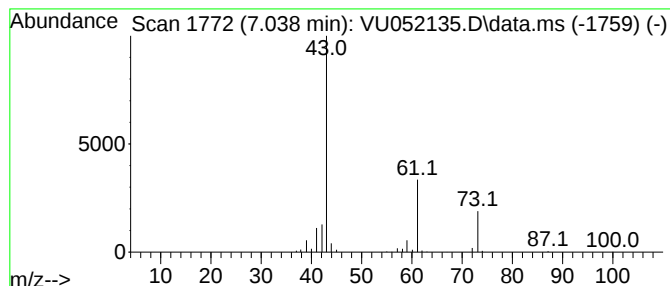
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	16.48 ug/L	346889	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	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	56



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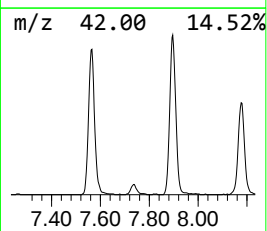
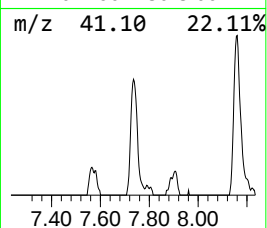
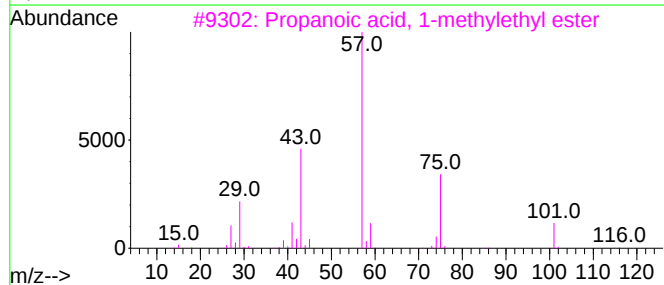
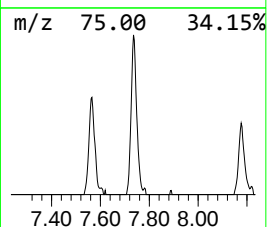
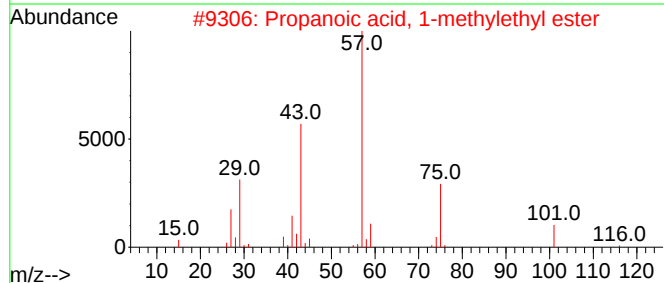
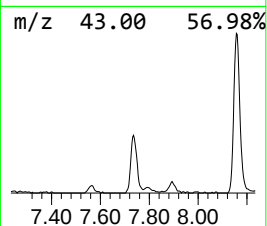
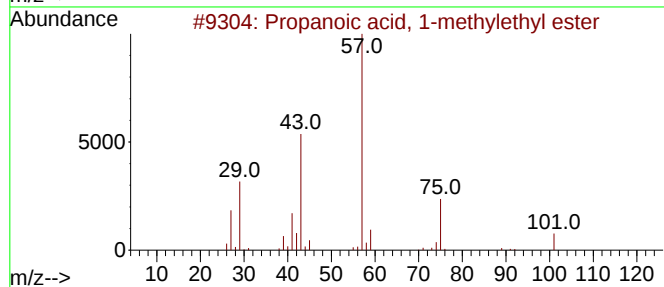
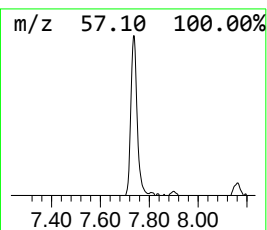
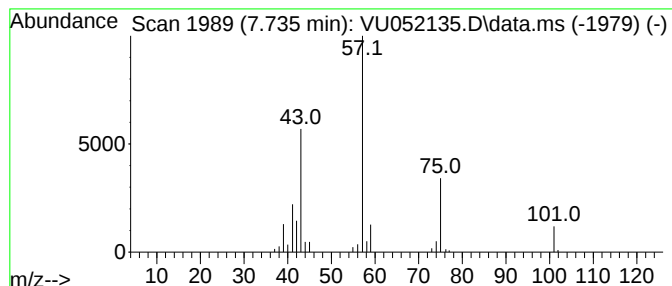
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.735	3.15 ug/L	66291	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	72
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	42



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ClientSampleId :
VLEB243

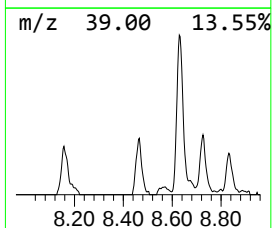
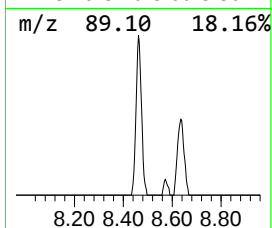
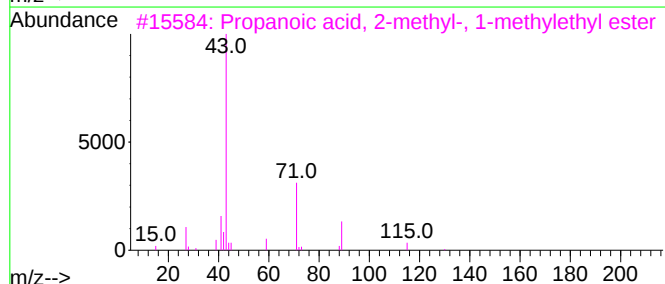
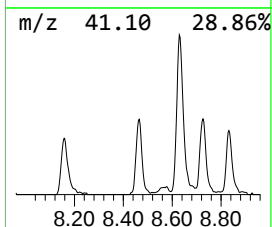
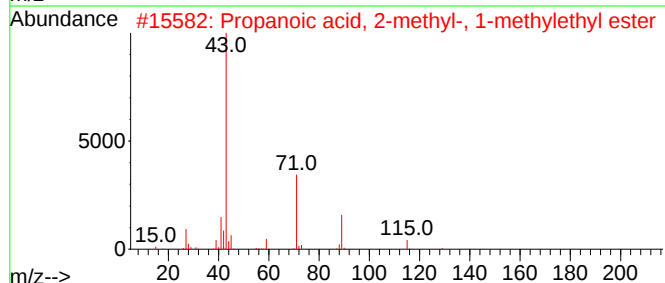
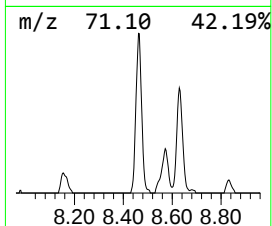
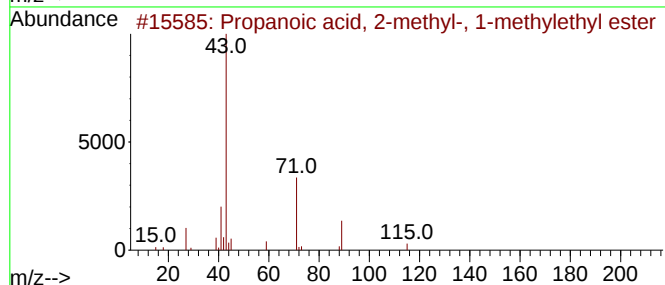
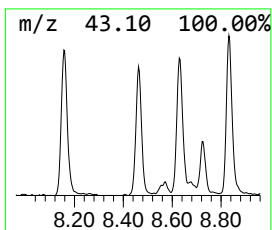
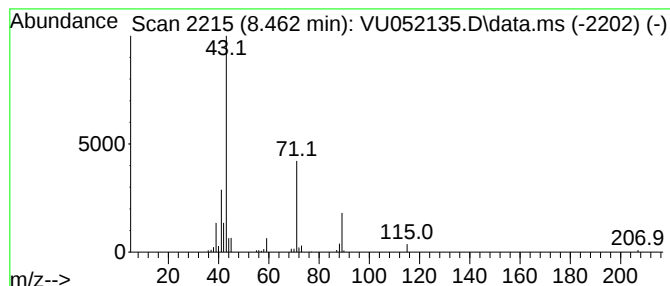
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.462	2.82 ug/L	76477	Chlorobenzene-d5	9.414

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			Isopropyl butyrate	130	C7H14O2	000638-11-9	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052135.D
Acq On : 25 Nov 2022 11:38
Operator : JC/MD
Sample : PB149243TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB243

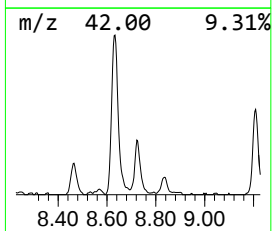
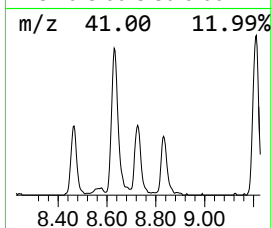
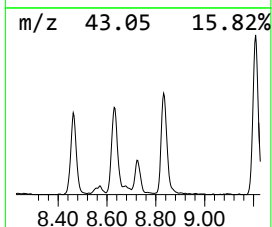
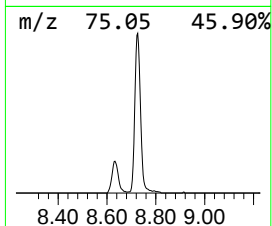
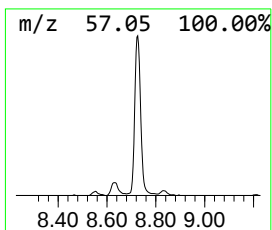
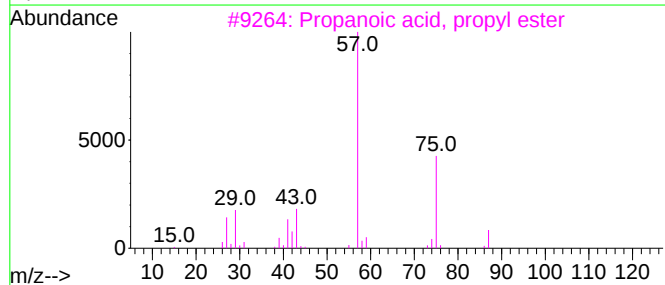
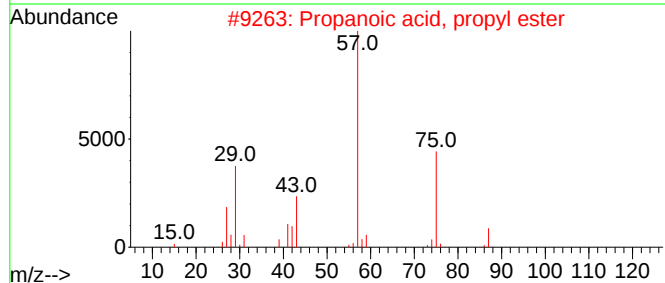
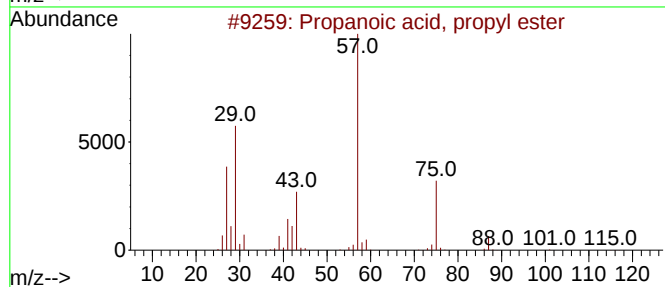
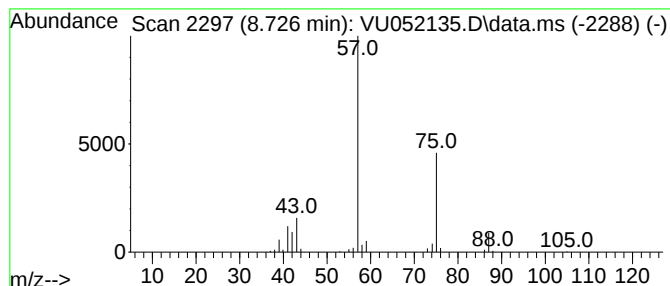
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	5.92 ug/L	160444	Chlorobenzene-d5	9.414

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	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052135.D
Acq On : 25 Nov 2022 11:38
Operator : JC/MD
Sample : PB149243TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB243

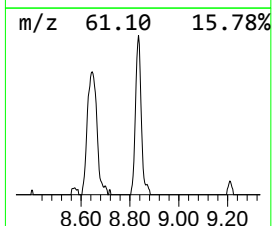
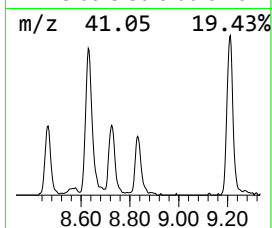
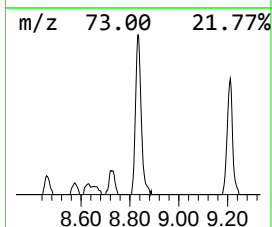
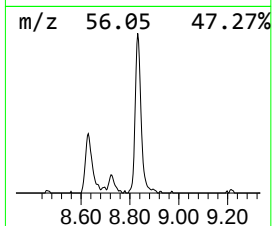
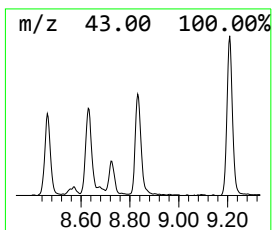
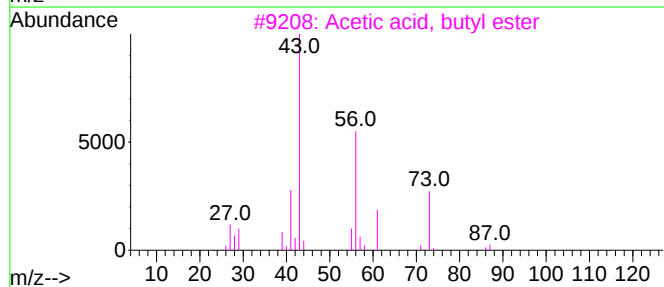
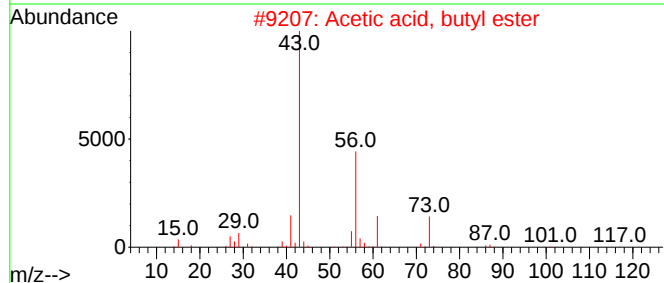
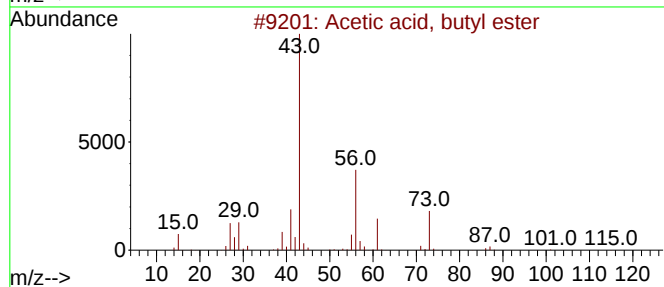
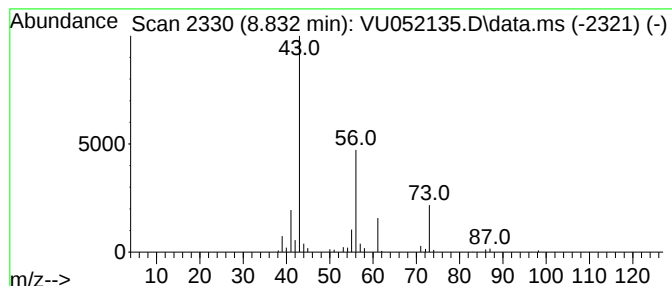
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.832	3.51 ug/L	94984	Chlorobenzene-d5	9.414

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	74
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\VU112522\
Data File : VU052135.D
Acq On : 25 Nov 2022 11:38
Operator : JC/MD
Sample : PB149243TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB243

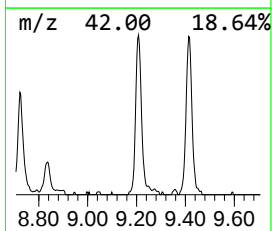
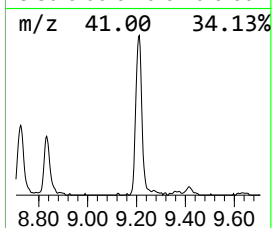
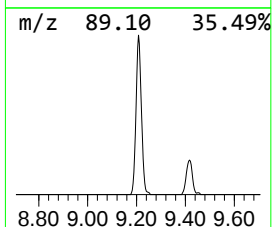
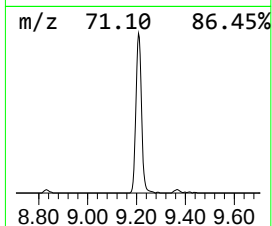
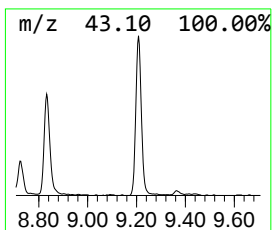
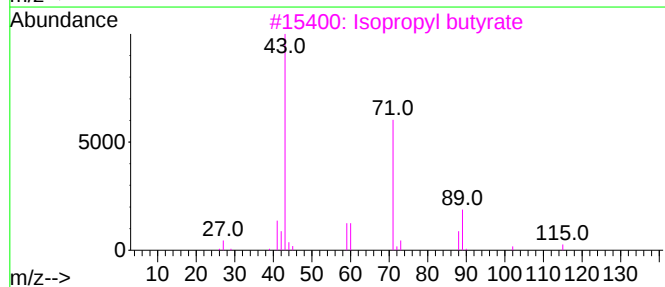
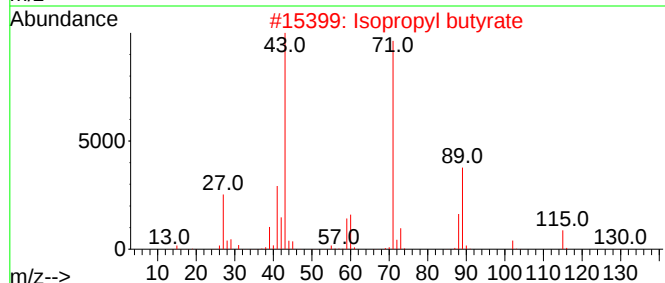
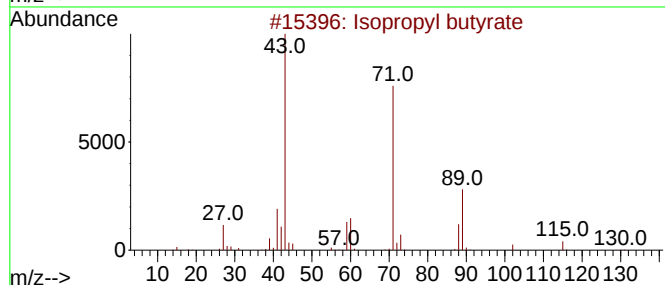
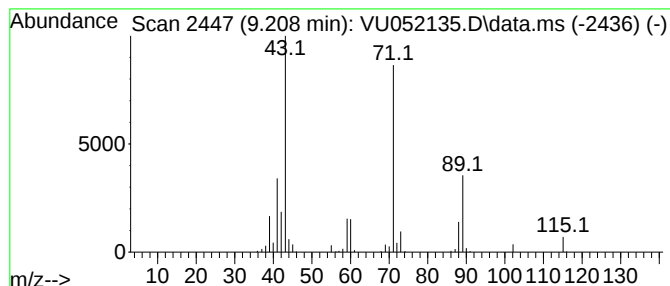
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Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.208	8.14 ug/L	220451	Chlorobenzene-d5	9.414

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	78
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112522\
Data File : VU052135.D
Acq On : 25 Nov 2022 11:38
Operator : JC/MD
Sample : PB149243TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB243

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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
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Propanoic acid,...	7.735	3.1	ug/L	66291	1	6.247	1052200	50.0
Propanoic acid,...	8.462	2.8	ug/L	76477	2	9.414	1354620	50.0
Propanoic acid,...	8.726	5.9	ug/L	160444	2	9.414	1354620	50.0
Acetic acid, bu...	8.832	3.5	ug/L	94984	2	9.414	1354620	50.0
Isopropyl butyrate	9.208	8.1	ug/L	220451	2	9.414	1354620	50.0