LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041223\
Data File : VU053666.D
Acq On : 12 Apr 2023 16:53
Operator : JC/MD
Sample : PB152205TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

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\SFAMULM033123WMA.M
Title : VOC Analysis

Signal : TIC: VU053666.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	98	rVB	111054	134937	16.99%	1.929%
2	1.909	169	177	196	rVB	85971	122207	15.38%	1.747%
3	2.562	368	380	395	rBV	172819	280077	35.26%	4.004%
4	3.038	517	528	529	rBV3	3121	3060	0.39%	0.044%
5	3.173	566	570	574	rBV2	375	317	0.04%	0.005%
6	3.195	575	577	581	rVB2	360	197	0.02%	0.003%
7	3.382	630	635	639	rBV2	330	308	0.04%	0.004%
8	3.645	715	717	722	rVB2	218	196	0.02%	0.003%
9	3.755	748	751	757	rVB	261	239	0.03%	0.003%
10	3.784	757	760	765	rBV	247	270	0.03%	0.004%
11	3.999	823	827	830	rBV2	236	185	0.02%	0.003%
12	4.038	836	839	842	rBV2	392	282	0.04%	0.004%
13	4.089	848	855	857	rBV2	216	248	0.03%	0.004%
14	4.128	863	867	872	rBV	309	296	0.04%	0.004%
15	4.179	878	883	887	rBV2	236	334	0.04%	0.005%
16	4.250	899	905	908	rBV	256	327	0.04%	0.005%
17	4.346	930	935	939	rVV2	202	224	0.03%	0.003%
18	4.613	1006	1018	1040	rBV	62147	145966	18.37%	2.087%
19	4.925	1112	1115	1121	rVB3	368	296	0.04%	0.004%
20	5.057	1139	1156	1178	rBV	142536	323673	40.74%	4.627%
21	5.282	1225	1226	1230	rVB2	579	257	0.03%	0.004%
22	5.330	1234	1241	1244	rBV2	300	412	0.05%	0.006%
23	5.491	1289	1291	1296	rVB2	252	195	0.02%	0.003%
24	5.520	1296	1300	1306	rBV2	271	348	0.04%	0.005%
25	5.636	1332	1336	1341	rBV2	240	201	0.03%	0.003%
26	5.719	1341	1362	1387	rBV2	293138	794428	100.00%	11.356%
27	5.909	1413	1421	1436	rVB4	8357	15911	2.00%	0.227%
28	6.002	1447	1450	1452	rBV2	356	225	0.03%	0.003%
29	6.015	1452	1454	1458	rVV2	372	325	0.04%	0.005%
30	6.169	1500	1502	1507	rVB2	292	193	0.02%	0.003%
31	6.243	1512	1525	1559	rBV	292459	559178	70.39%	7.993%
32	6.449	1585	1589	1592	rVB2	333	292	0.04%	0.004%
33	6.472	1592	1596	1597	rBV	258	185	0.02%	0.003%
34	6.526	1602	1613	1622	rBV6	3478	6127	0.77%	0.088%
35	6.613	1636	1640	1644	rBV2	173	198	0.02%	0.003%
36	6.684	1648	1662	1685	rBV	180158	353442	44.49%	5.052%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

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\SFAMULM033123WMA.M
Title : VOC Analysis

37	6.822	1702	1705	1708	rBV	528	321	0.04%	0.005%
38	6.883	1720	1724	1726	rVB	367	223	0.03%	0.003%
39	6.919	1726	1735	1740	rBV2	3569	5803	0.73%	0.083%
40	7.034	1760	1771	1791	rBV	85751	155756	19.61%	2.227%
41	7.279	1844	1847	1852	rVB	277	252	0.03%	0.004%
42	7.311	1852	1857	1863	rVB2	255	268	0.03%	0.004%
43	7.562	1922	1935	1958	rBV	101085	179854	22.64%	2.571%
44	7.735	1980	1989	2002	rVB2	18774	31444	3.96%	0.449%
45	7.893	2023	2038	2064	rBV	384165	664527	83.65%	9.499%
46	8.063	2089	2091	2096	rBV2	284	200	0.03%	0.003%
47	8.089	2096	2099	2102	rVB2	369	244	0.03%	0.003%
48	8.108	2102	2105	2109	rBV	308	303	0.04%	0.004%
49	8.172	2109	2125	2146	rBV2	78860	160218	20.17%	2.290%
50	8.359	2179	2183	2186	rBV2	249	206	0.03%	0.003%
51	8.462	2205	2215	2234	rVB2	25135	41690	5.25%	0.596%
52	8.574	2235	2250	2255	rBV8	3762	7903	0.99%	0.113%
53	8.626	2255	2266	2287	rVV	198455	355631	44.77%	5.084%
54	8.722	2289	2296	2311	rVB	43369	69627	8.76%	0.995%
55	8.799	2317	2320	2321	rBV2	565	312	0.04%	0.004%
56	8.832	2321	2330	2347	rVB	26137	42804	5.39%	0.612%
57	8.980	2372	2376	2378	rBV2	313	221	0.03%	0.003%
58	9.034	2388	2393	2397	rBV2	186	261	0.03%	0.004%
59	9.205	2436	2446	2462	rBV	72930	114619	14.43%	1.638%
60	9.324	2479	2483	2485	rBV	208	181	0.02%	0.003%
61	9.365	2490	2496	2499	rBV4	1148	1481	0.19%	0.021%
62	9.414	2499	2511	2535	rVB	411124	687925	86.59%	9.834%
63	9.574	2558	2561	2564	rBV2	365	275	0.03%	0.004%
64	9.642	2574	2582	2586	rBV3	959	1262	0.16%	0.018%
65	9.729	2605	2609	2615	rVB2	333	323	0.04%	0.005%
66	9.812	2632	2635	2639	rBV	265	192	0.02%	0.003%
67	9.867	2648	2652	2655	rBV	263	207	0.03%	0.003%
68	9.979	2683	2687	2691	rBV2	250	273	0.03%	0.004%
69	10.073	2707	2716	2726	rVV4	6144	9577	1.21%	0.137%
70	10.121	2726	2731	2734	rVB2	343	240	0.03%	0.003%
71	10.224	2759	2763	2768	rBV	242	278	0.03%	0.004%
72	10.288	2777	2783	2784	rBV	245	209	0.03%	0.003%
73	10.307	2787	2789	2793	rBV2	211	179	0.02%	0.003%
74	10.539	2857	2861	2864	rBV	268	186	0.02%	0.003%
75	10.751	2914	2927	2945	rVV	254143	406499	51.17%	5.811%
76	10.902	2971	2974	2976	rBV	306	200	0.03%	0.003%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
LEB205

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Title : VOC Analysis

77	11.092	3030	3033	3034	rBV	312	188	0.02%	0.003%
78	11.182	3057	3061	3063	rVV2	337	178	0.02%	0.003%
79	11.221	3069	3073	3078	rBV2	410	366	0.05%	0.005%
80	11.295	3092	3096	3100	rBV2	266	257	0.03%	0.004%
81	11.426	3133	3137	3139	rBV2	245	206	0.03%	0.003%
82	11.581	3182	3185	3190	rVV2	308	245	0.03%	0.004%
83	11.706	3219	3224	3226	rBV2	264	209	0.03%	0.003%
84	11.806	3244	3255	3274	rBV	423499	686107	86.36%	9.808%
85	12.102	3345	3347	3351	rBV	253	198	0.02%	0.003%
86	12.188	3362	3374	3398	rBV	374197	615829	77.52%	8.803%
87	12.516	3473	3476	3480	rBV2	301	251	0.03%	0.004%
88	12.597	3498	3501	3503	rBV2	266	201	0.03%	0.003%
89	12.687	3527	3529	3532	rBV	285	177	0.02%	0.003%
90	12.774	3552	3556	3562	rBV3	402	400	0.05%	0.006%
91	12.979	3615	3620	3623	rVB2	285	264	0.03%	0.004%
92	12.999	3623	3626	3630	rBV2	247	261	0.03%	0.004%
93	13.063	3642	3646	3648	rBV2	263	196	0.02%	0.003%
94	13.298	3716	3719	3724	rBV2	286	324	0.04%	0.005%
95	13.574	3802	3805	3809	rBV	421	290	0.04%	0.004%
96	13.703	3841	3845	3848	rBV2	406	353	0.04%	0.005%
97	14.111	3969	3972	3976	rBV3	426	391	0.05%	0.006%
98	14.211	4000	4003	4007	rVB2	376	240	0.03%	0.003%
99	14.265	4017	4020	4023	rBV2	412	239	0.03%	0.003%
100	14.433	4067	4072	4073	rBV	421	344	0.04%	0.005%

Sum of corrected areas: 6995444

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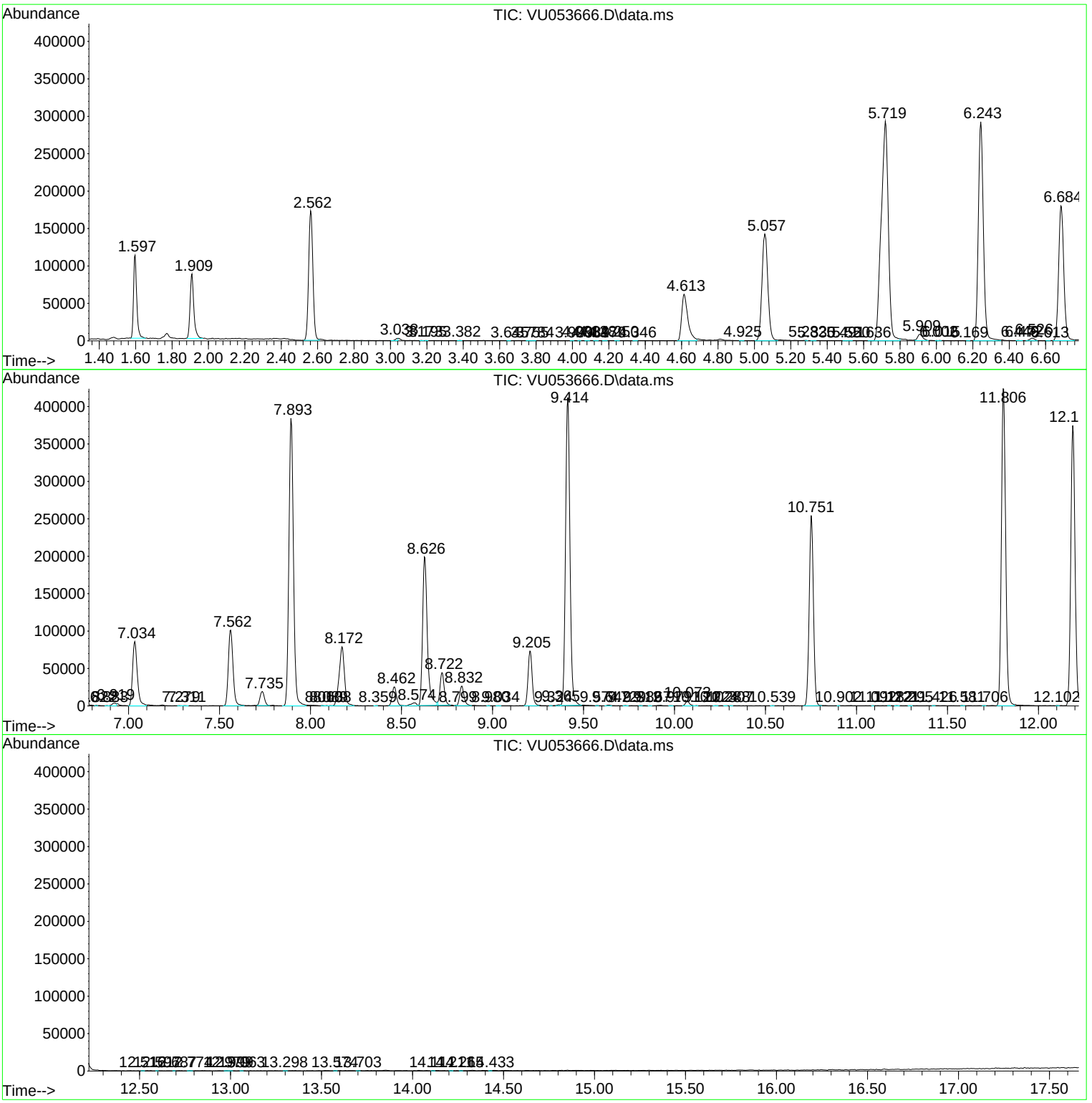
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

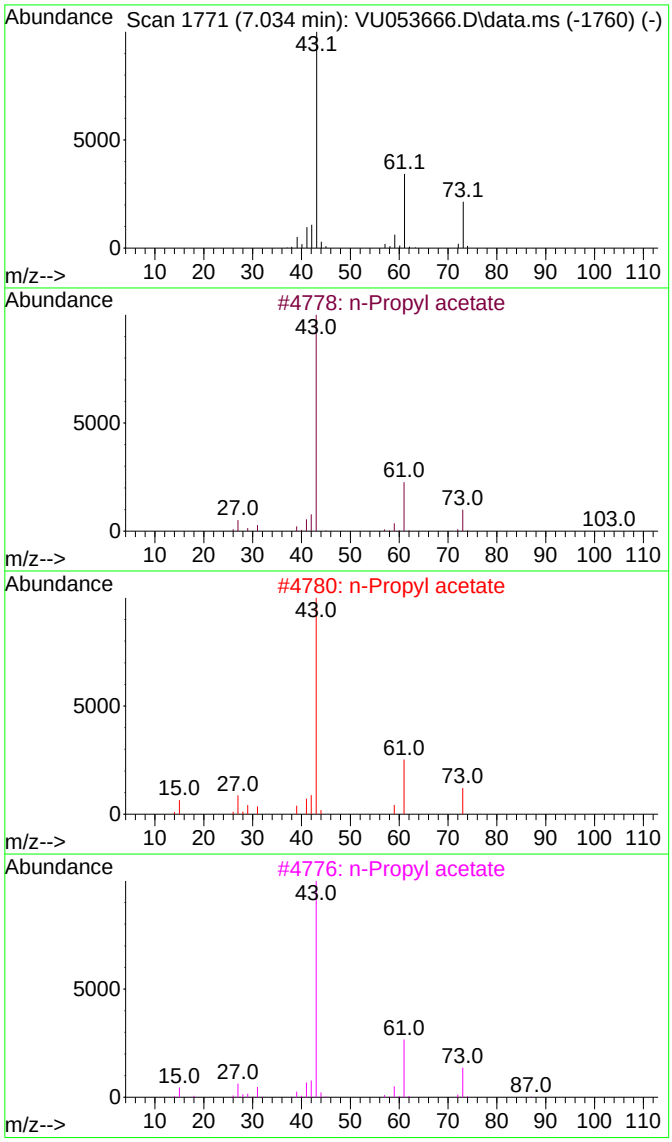
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

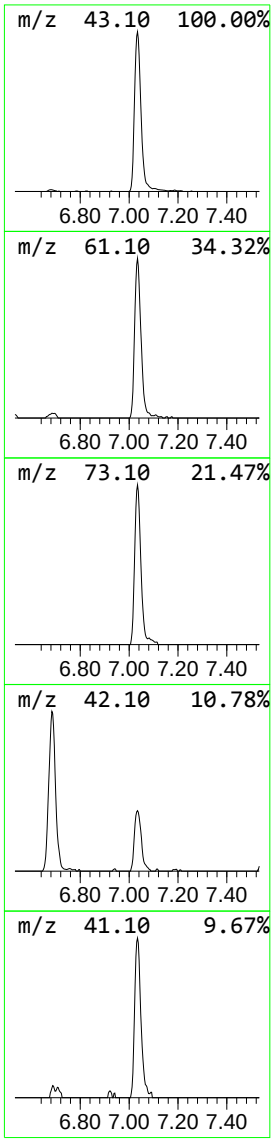
****

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	13.93 ug/L	155756	1,4-Difluorobenzene	6.243

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	72
3	n-Propyl acetate	102	C5H10O2	000109-60-4	64
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041223\
Data File : VU053666.D
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Sample : PB152205TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

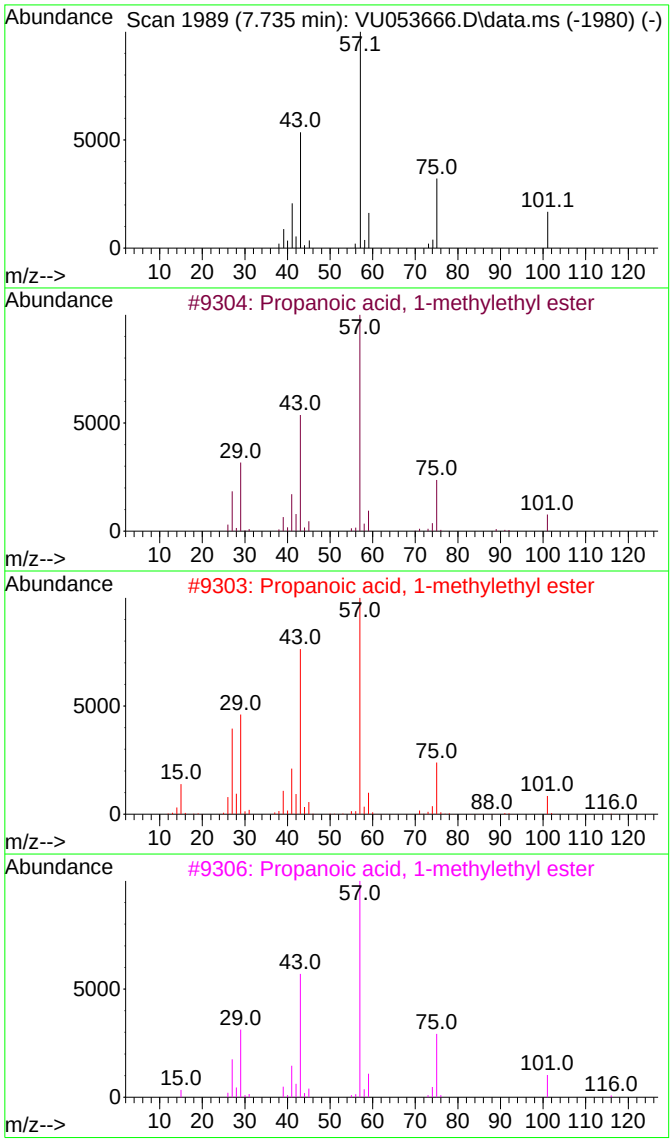
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

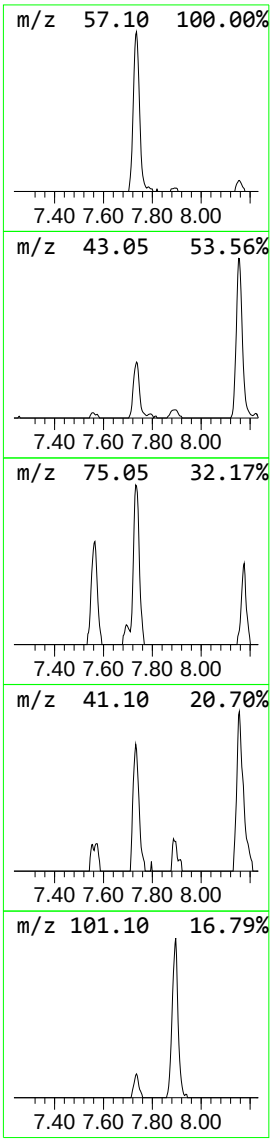
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.735	2.81 ug/L	31444	1,4-Difluorobenzene	6.243

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	78
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	45





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MSVOA_U
ClientSampleId :
LEB205

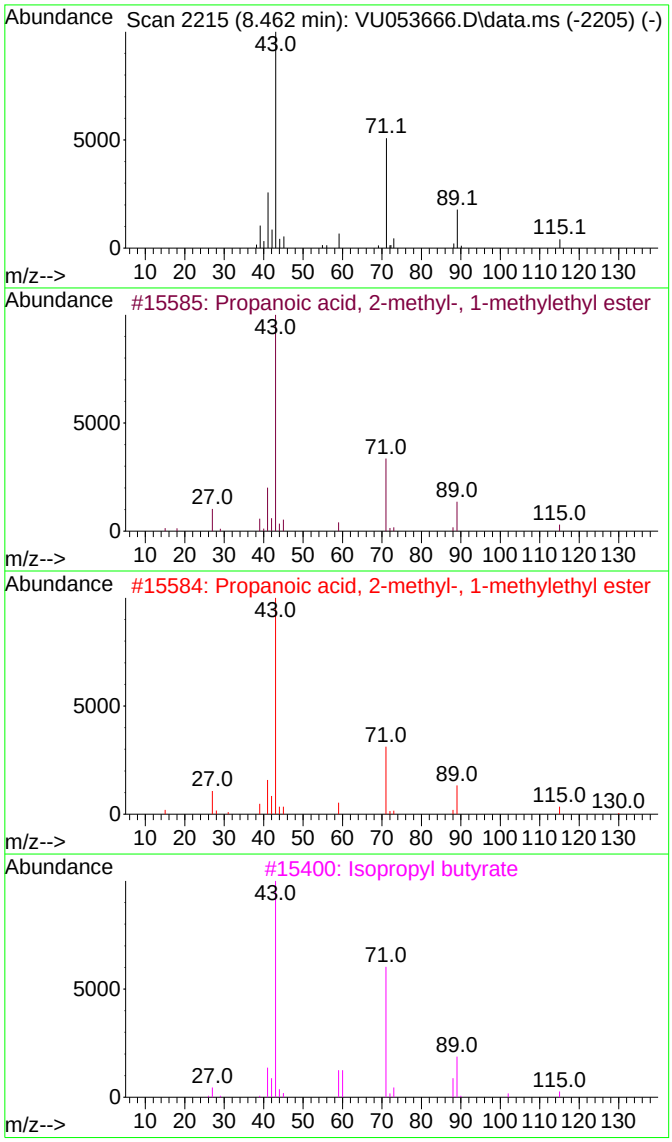
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

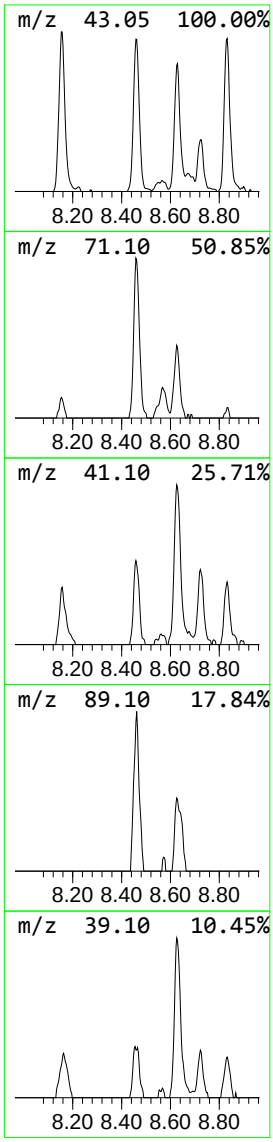
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.462	3.03 ug/L	41690	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	78
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72





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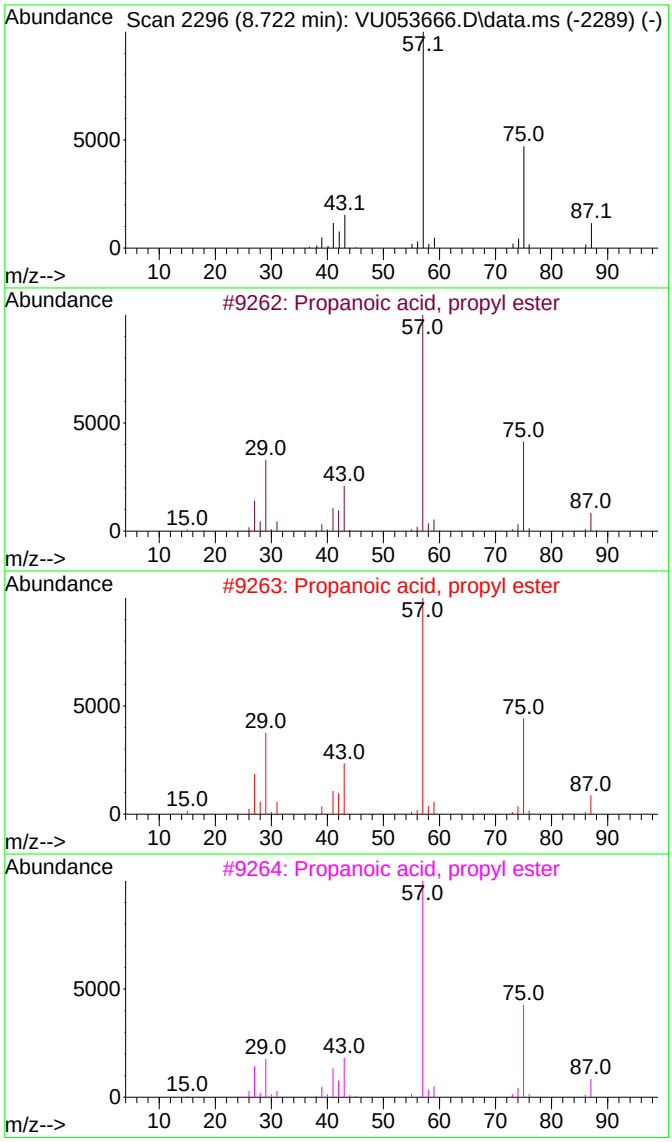
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

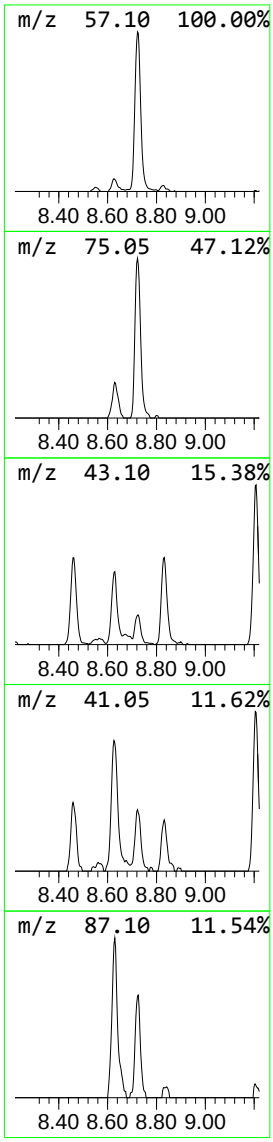
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.722	5.06 ug/L	69627	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	83





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Acq On : 12 Apr 2023 16:53
Operator : JC/MD
Sample : PB152205TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

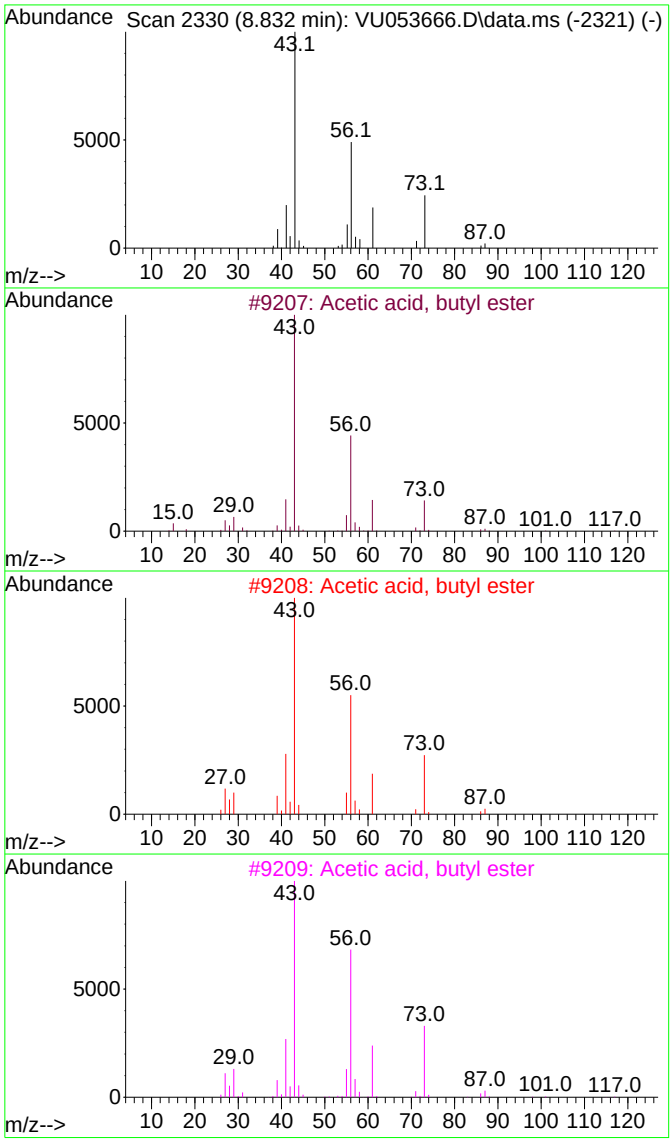
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

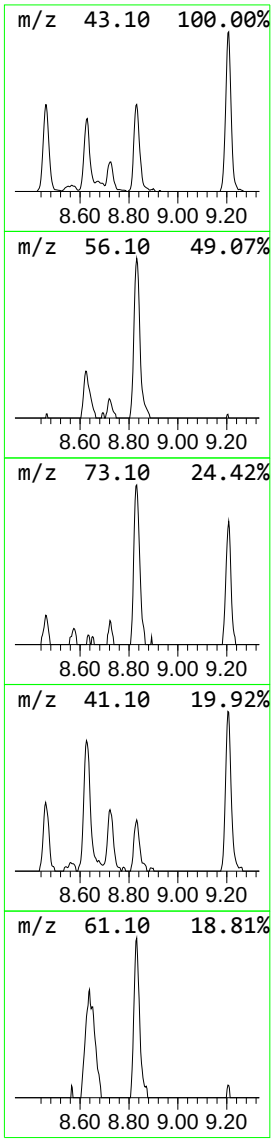
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.832	3.11 ug/L	42804	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	83
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041223\
Data File : VU053666.D
Acq On : 12 Apr 2023 16:53
Operator : JC/MD
Sample : PB152205TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

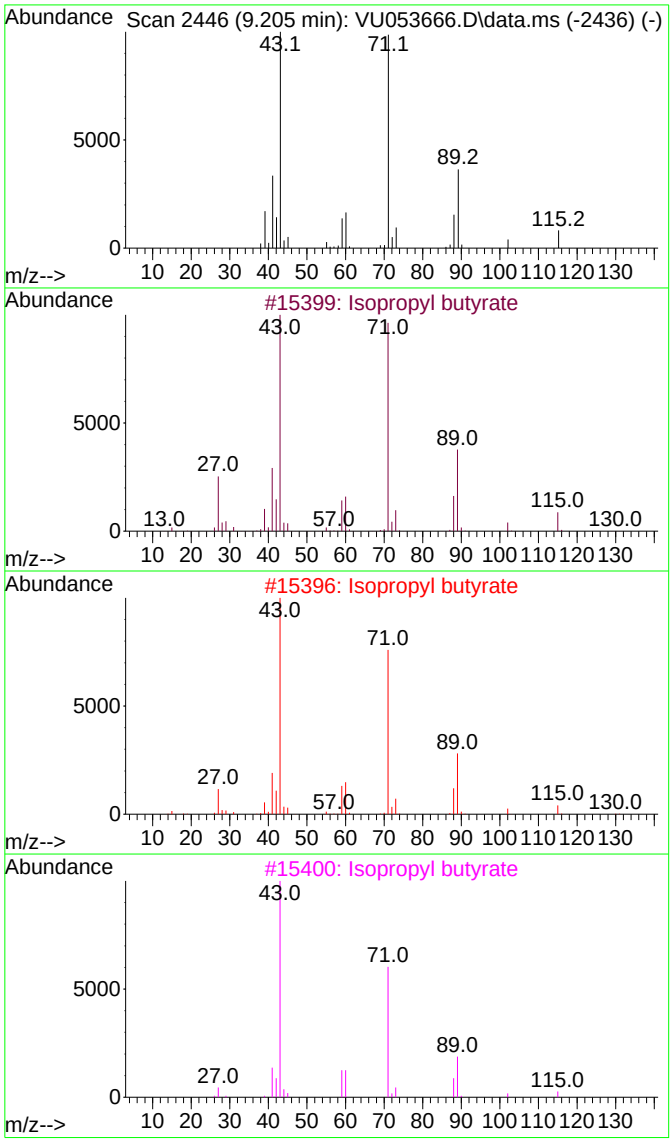
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

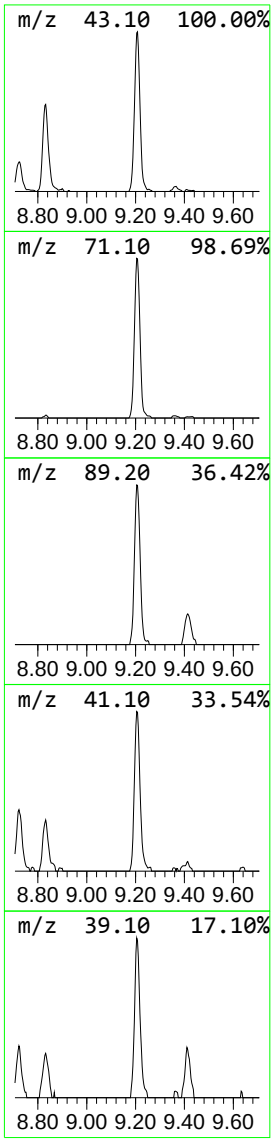
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.205	8.33 ug/L	114619	Chlorobenzene-d5	9.414

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041223\
Data File : VU053666.D
Acq On : 12 Apr 2023 16:53
Operator : JC/MD
Sample : PB152205TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
LEB205

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.034	13.9	ug/L	155756	1	6.243	559178	50.0
Propanoic acid,...	7.735	2.8	ug/L	31444	1	6.243	559178	50.0
Propanoic acid,...	8.462	3.0	ug/L	41690	2	9.414	687925	50.0
Propanoic acid,...	8.722	5.1	ug/L	69627	2	9.414	687925	50.0
Acetic acid, bu...	8.832	3.1	ug/L	42804	2	9.414	687925	50.0
Isopropyl butyrate	9.205	8.3	ug/L	114619	2	9.414	687925	50.0