LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049674.D
Acq On : 11 Jul 2022 14:35
Operator : SY/MD
Sample : PB146119TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

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\SFAMULM071122WMA.M
Title : VOC Analysis

Signal : TIC: VU049674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	3	5	11	rVB2	2788	2234	0.22%	0.027%
2	1.523	51	57	60	rBV2	1358	1844	0.18%	0.022%
3	1.597	73	80	99	rVV	136556	153151	14.92%	1.829%
4	1.678	102	105	112	rVB4	1678	1482	0.14%	0.018%
5	1.906	168	176	194	rVB	99123	129932	12.66%	1.551%
6	2.240	278	280	281	rBV	577	258	0.03%	0.003%
7	2.565	368	381	394	rBV	205671	332383	32.37%	3.969%
8	2.684	415	418	428	rBV3	414	447	0.04%	0.005%
9	2.793	446	452	460	rVB2	875	1357	0.13%	0.016%
10	2.925	490	493	496	rVB2	332	250	0.02%	0.003%
11	2.951	496	501	508	rBV3	446	777	0.08%	0.009%
12	2.983	508	511	517	rVV	403	471	0.05%	0.006%
13	3.044	519	530	542	rVB2	8579	15331	1.49%	0.183%
14	3.186	559	574	590	rBV2	9070	19569	1.91%	0.234%
15	3.311	610	613	621	rVV	301	342	0.03%	0.004%
16	3.366	627	630	633	rVB2	415	228	0.02%	0.003%
17	3.414	640	645	649	rBV	289	300	0.03%	0.004%
18	3.514	672	676	680	rVB2	329	254	0.02%	0.003%
19	3.710	729	737	740	rBV2	277	405	0.04%	0.005%
20	4.031	834	837	842	rVB2	302	240	0.02%	0.003%
21	4.282	910	915	921	rBV2	227	243	0.02%	0.003%
22	4.559	998	1001	1007	rVB3	275	234	0.02%	0.003%
23	4.620	1007	1020	1050	rBV2	118934	290687	28.31%	3.471%
24	4.813	1075	1080	1093	rVB3	1722	3127	0.30%	0.037%
25	4.944	1117	1121	1126	rVB2	268	247	0.02%	0.003%
26	5.063	1141	1158	1178	rBV2	185670	404591	39.41%	4.831%
27	5.147	1182	1184	1194	rVB3	583	752	0.07%	0.009%
28	5.295	1220	1230	1237	rBV3	614	1224	0.12%	0.015%
29	5.362	1247	1251	1253	rBV	502	346	0.03%	0.004%
30	5.436	1271	1274	1280	rVB2	270	241	0.02%	0.003%
31	5.533	1298	1304	1312	rBV2	414	731	0.07%	0.009%
32	5.726	1342	1364	1389	rVV2	377242	1026691	100.00%	12.258%
33	5.915	1411	1423	1434	rBV3	9776	20141	1.96%	0.240%
34	5.977	1440	1442	1449	rVB2	580	471	0.05%	0.006%
35	6.038	1457	1461	1466	rVB3	265	253	0.02%	0.003%
36	6.247	1509	1526	1548	rBV	309036	590909	57.55%	7.055%

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

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\SFAMULM071122WMA.M
Title : VOC Analysis

37	6.481	1596	1599	1604	rBV2	206	228	0.02%	0.003%
38	6.526	1609	1613	1618	rBV3	879	1082	0.11%	0.013%
39	6.620	1637	1642	1645	rBV2	252	231	0.02%	0.003%
40	6.690	1650	1664	1691	rBV	246232	473448	46.11%	5.653%
41	6.896	1726	1728	1729	rVV	484	234	0.02%	0.003%
42	6.922	1729	1736	1759	rVV2	5073	10890	1.06%	0.130%
43	7.038	1759	1772	1798	rVV	114816	201322	19.61%	2.404%
44	7.131	1798	1801	1808	rVB4	525	592	0.06%	0.007%
45	7.185	1813	1818	1826	rVB4	1366	1739	0.17%	0.021%
46	7.459	1897	1903	1906	rBV2	254	293	0.03%	0.003%
47	7.565	1924	1936	1960	rBV	133304	230958	22.50%	2.758%
48	7.687	1972	1974	1978	rVB2	464	278	0.03%	0.003%
49	7.739	1979	1990	2001	rBV	21530	34523	3.36%	0.412%
50	7.896	2026	2039	2057	rVV	446128	769598	74.96%	9.189%
51	8.179	2110	2127	2145	rBV2	93566	193972	18.89%	2.316%
52	8.465	2205	2216	2232	rBV	27422	44597	4.34%	0.532%
53	8.574	2232	2250	2256	rBV3	5074	10566	1.03%	0.126%
54	8.632	2256	2268	2289	rVV2	329163	612921	59.70%	7.318%
55	8.726	2290	2297	2314	rVB	50555	83270	8.11%	0.994%
56	8.835	2321	2331	2346	rVB2	30727	48984	4.77%	0.585%
57	9.160	2429	2432	2436	rVB2	363	299	0.03%	0.004%
58	9.211	2436	2448	2464	rBV	77286	123655	12.04%	1.476%
59	9.333	2483	2486	2488	rBV2	348	234	0.02%	0.003%
60	9.369	2488	2497	2499	rVV5	1523	2096	0.20%	0.025%
61	9.417	2499	2512	2546	rVB	431383	716342	69.77%	8.553%
62	9.574	2553	2561	2568	rVB5	571	854	0.08%	0.010%
63	9.645	2575	2583	2593	rVV3	1256	1685	0.16%	0.020%
64	9.690	2594	2597	2604	rVB3	405	454	0.04%	0.005%
65	9.880	2651	2656	2660	rBV2	213	262	0.03%	0.003%
66	9.922	2662	2669	2672	rBV3	806	1104	0.11%	0.013%
67	9.970	2680	2684	2689	rBV2	320	375	0.04%	0.004%
68	10.073	2707	2716	2725	rBV2	6198	8939	0.87%	0.107%
69	10.108	2725	2727	2730	rVV2	915	580	0.06%	0.007%
70	10.124	2730	2732	2737	rVB2	603	508	0.05%	0.006%
71	10.150	2737	2740	2749	rVB2	259	278	0.03%	0.003%
72	10.394	2812	2816	2818	rBV2	373	269	0.03%	0.003%
73	10.433	2825	2828	2831	rVB	328	249	0.02%	0.003%
74	10.484	2839	2844	2850	rVB3	641	678	0.07%	0.008%
75	10.754	2915	2928	2944	rBV	319741	513913	50.06%	6.136%
76	10.893	2968	2971	2976	rVB2	287	251	0.02%	0.003%

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VLEB119

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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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Title : VOC Analysis

77	11.645	3199	3205	3211	rBV2	380	585	0.06%	0.007%
78	11.745	3231	3236	3240	rBV3	969	910	0.09%	0.011%
79	11.812	3245	3257	3278	rVV	387499	628062	61.17%	7.499%
80	11.893	3280	3282	3285	rVV2	640	375	0.04%	0.004%
81	11.909	3285	3287	3292	rVB2	591	332	0.03%	0.004%
82	12.031	3322	3325	3329	rBV2	319	247	0.02%	0.003%
83	12.192	3363	3375	3395	rBV	390988	632296	61.59%	7.549%
84	12.433	3446	3450	3452	rBV2	329	235	0.02%	0.003%
85	12.992	3621	3624	3631	rBV2	247	236	0.02%	0.003%
86	13.063	3641	3646	3650	rBV2	424	586	0.06%	0.007%
87	13.471	3770	3773	3779	rBV2	284	289	0.03%	0.003%
88	13.504	3780	3783	3786	rBV	396	292	0.03%	0.003%
89	13.603	3810	3814	3817	rBV	319	315	0.03%	0.004%
90	13.671	3831	3835	3837	rBV2	425	336	0.03%	0.004%
91	13.806	3874	3877	3880	rBV2	359	232	0.02%	0.003%
92	13.844	3883	3889	3898	rVB6	2133	2579	0.25%	0.031%
93	13.931	3910	3916	3920	rBV	379	483	0.05%	0.006%
94	14.095	3958	3967	3978	rBV4	4315	7254	0.71%	0.087%
95	14.172	3988	3991	3994	rBV2	380	264	0.03%	0.003%
96	14.240	4009	4012	4016	rBV2	428	376	0.04%	0.004%
97	14.333	4036	4041	4049	rVB5	2029	2770	0.27%	0.033%
98	14.475	4082	4085	4088	rBV2	378	319	0.03%	0.004%
99	15.883	4518	4523	4525	rBV2	663	617	0.06%	0.007%
100	16.256	4637	4639	4642	rBV3	699	462	0.04%	0.006%

Sum of corrected areas: 8375346

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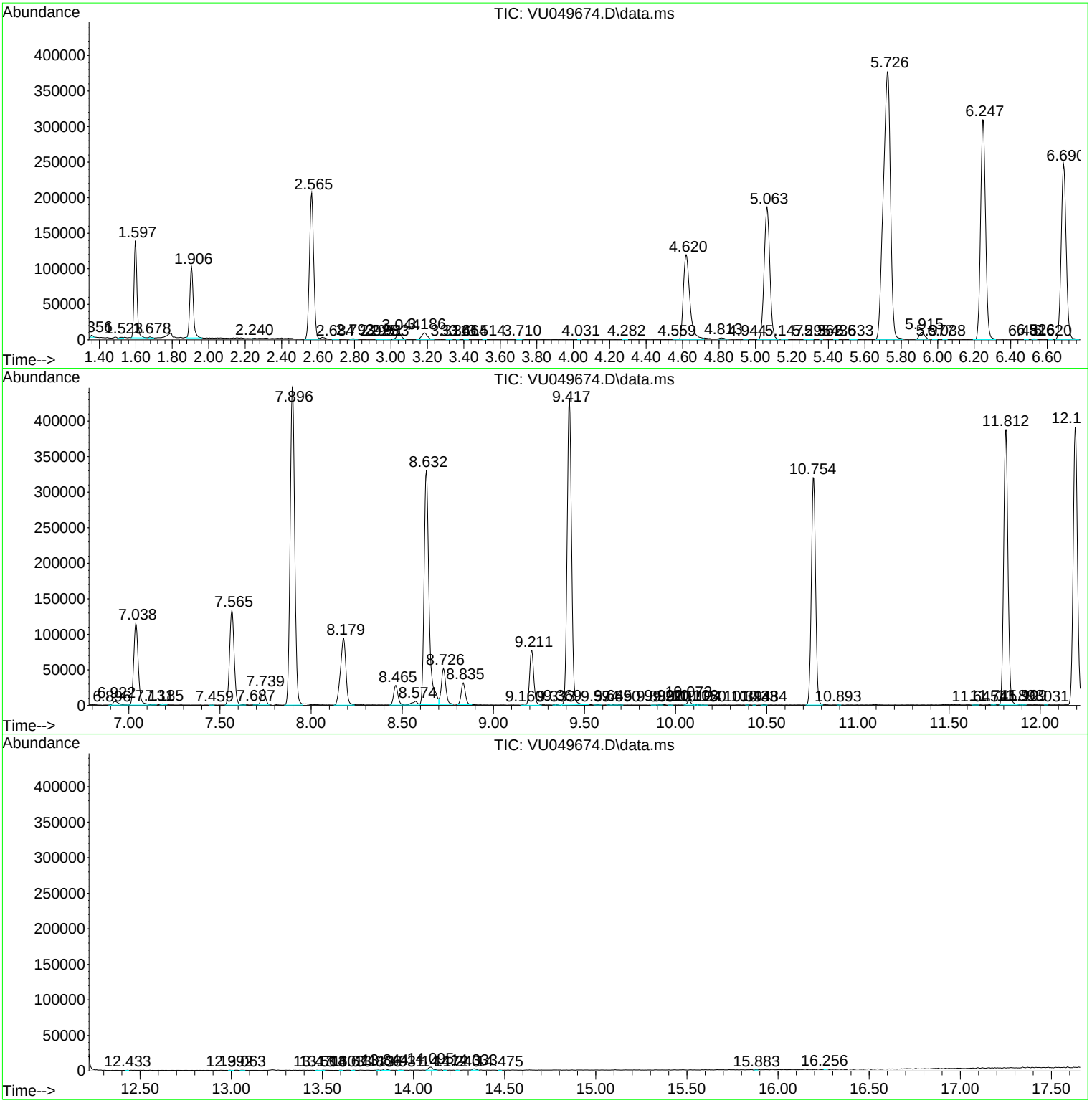
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VLEB119

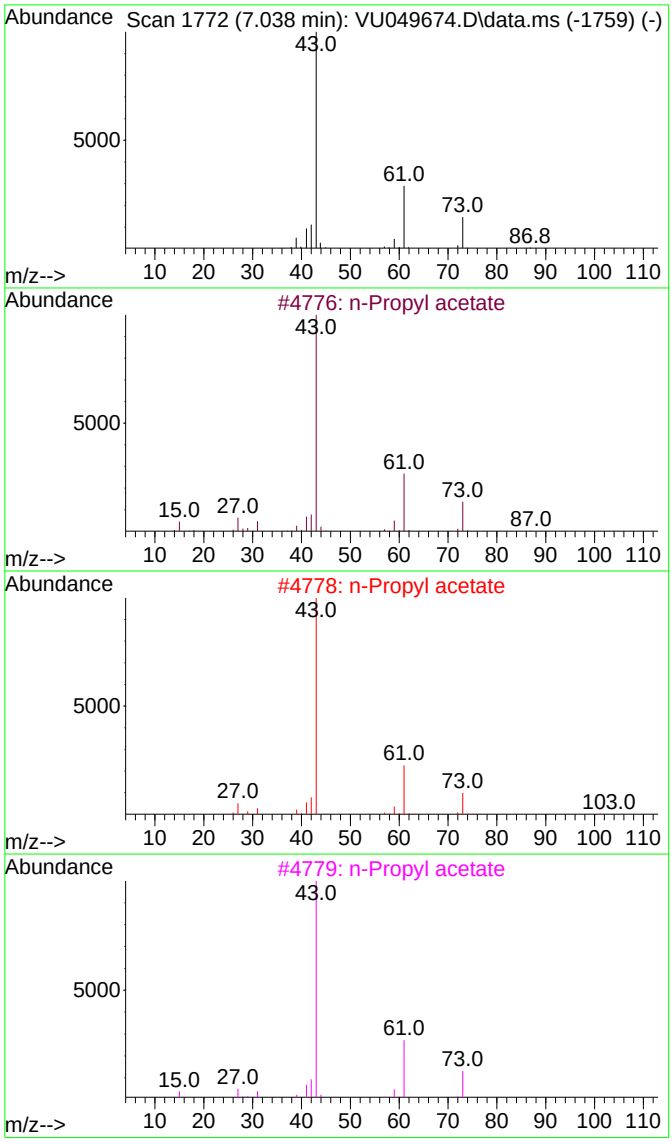
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

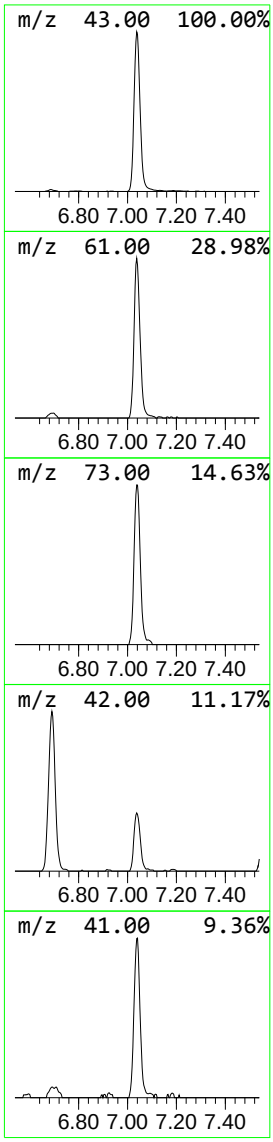
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	17.03 ug/L	201322	1,4-Difluorobenzene	6.250

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	64
5	n-Propyl acetate	102	C5H10O2	000109-60-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
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Operator : SY/MD
Sample : PB146119TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

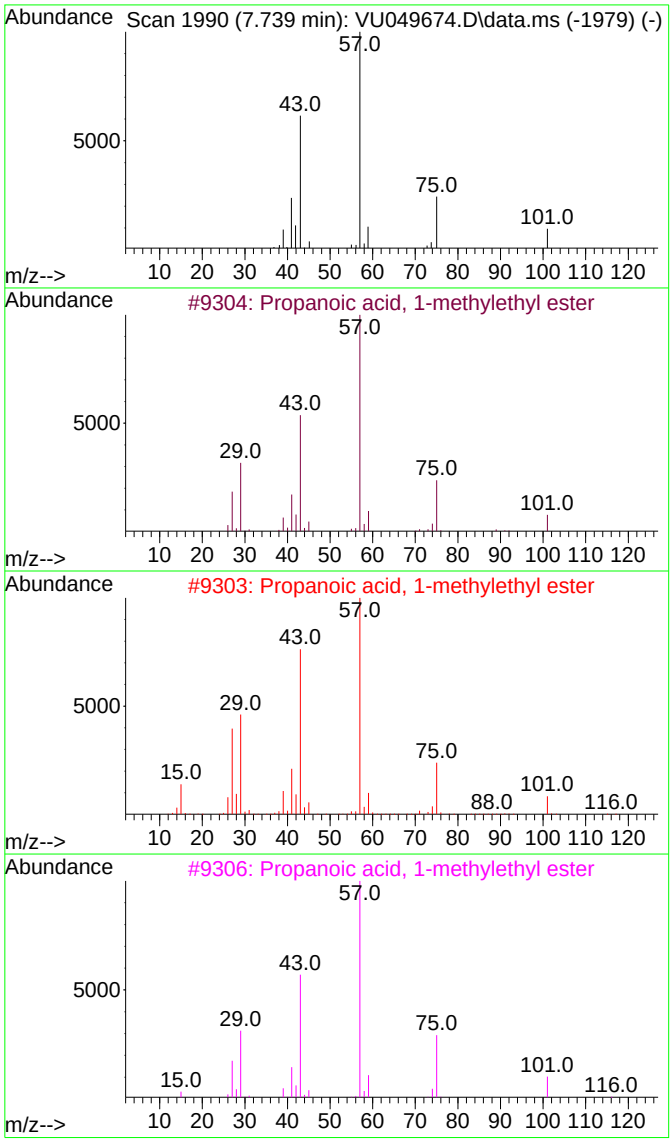
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

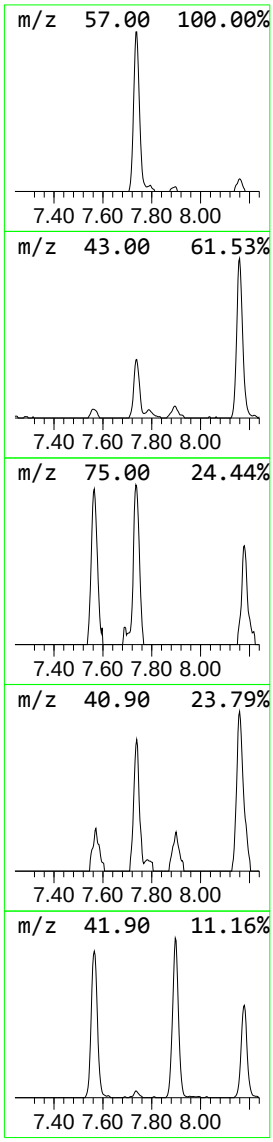
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	2.92 ug/L	34523	1,4-Difluorobenzene	6.250

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	64
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	38
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36





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ALS Vial : 12 Sample Multiplier: 1

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MSVOA_U
ClientSampleId :
VLEB119

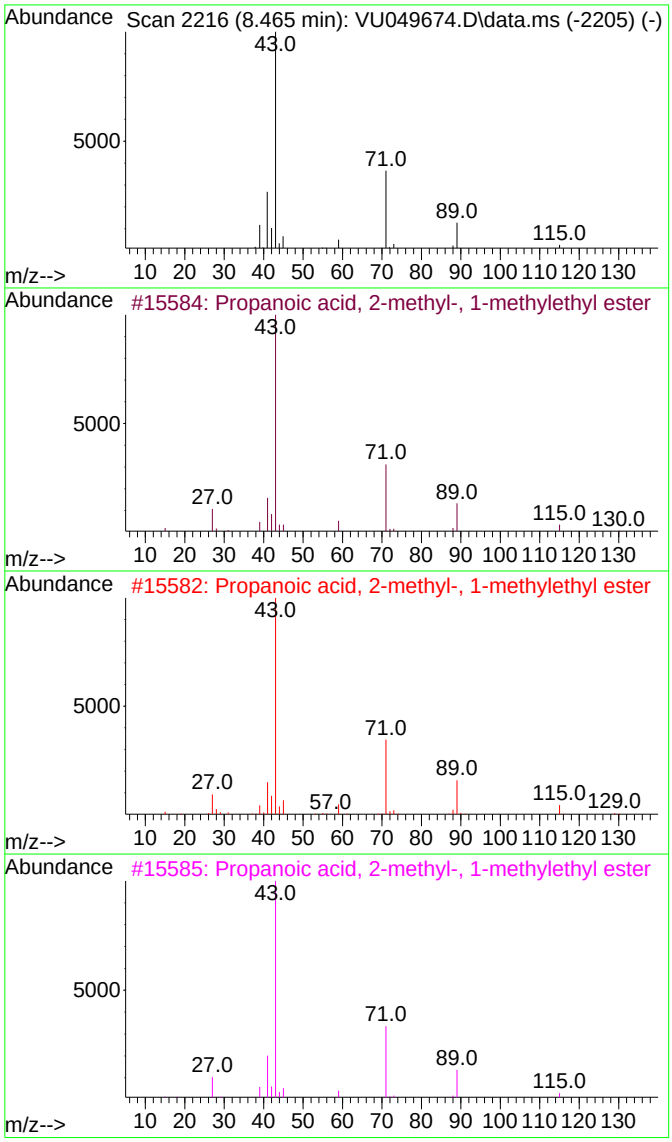
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

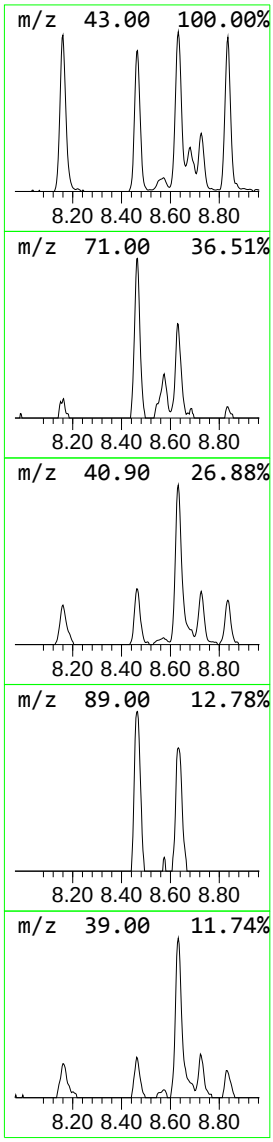
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.11 ug/L	44597	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	74
5	Isopropyl butyrate	130	C7H14O2	000638-11-9	56





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ClientSampleId :
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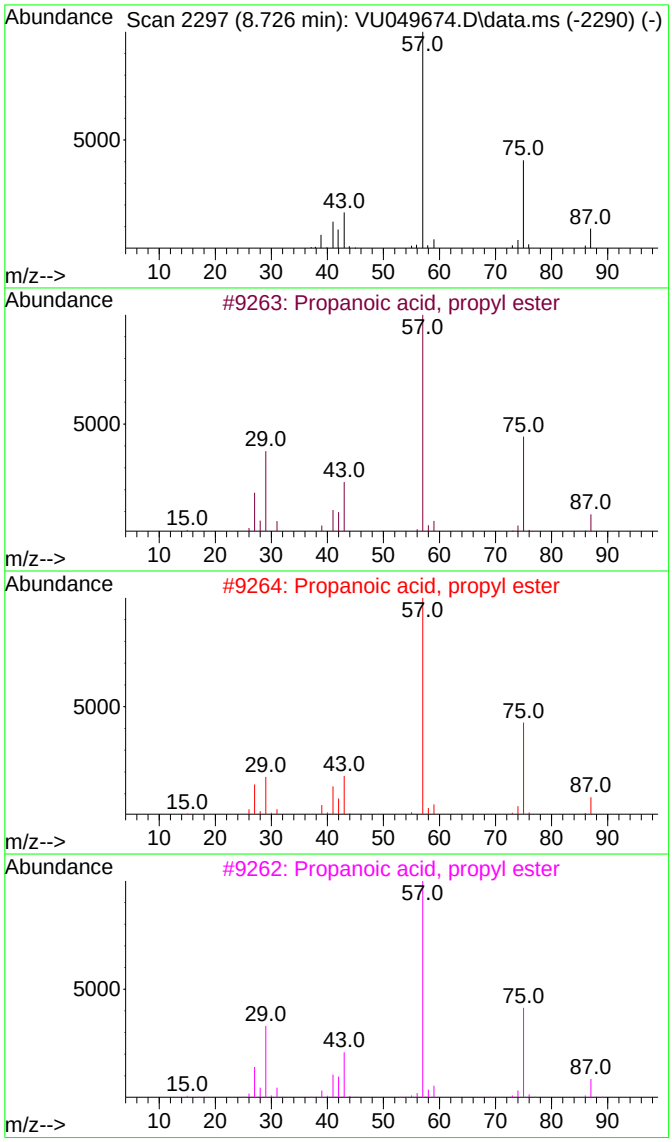
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

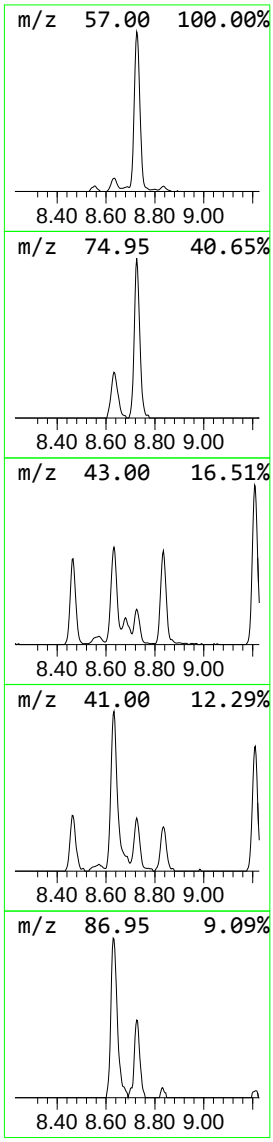
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	5.81 ug/L	83270	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	74
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40





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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

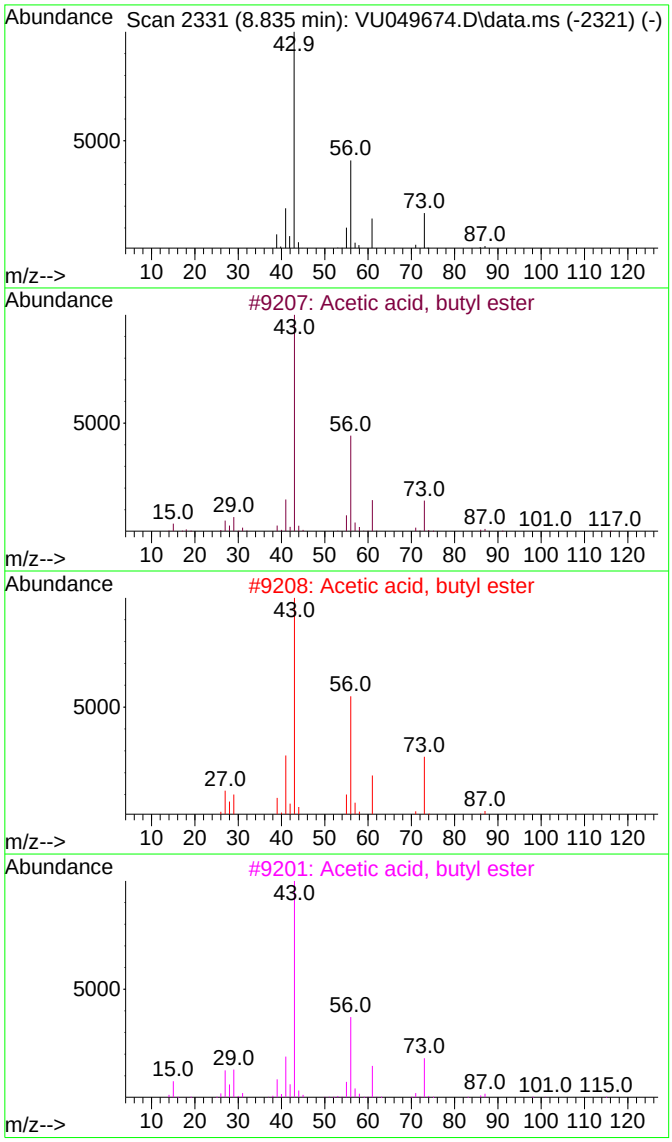
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

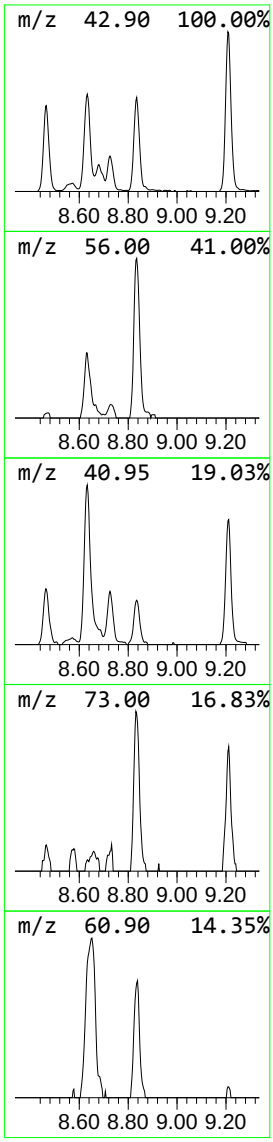
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.42 ug/L	48984	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	64
4	Isobutyl acetate	116	C6H12O2	000110-19-0	39
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	33





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Acq On : 11 Jul 2022 14:35
Operator : SY/MD
Sample : PB146119TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

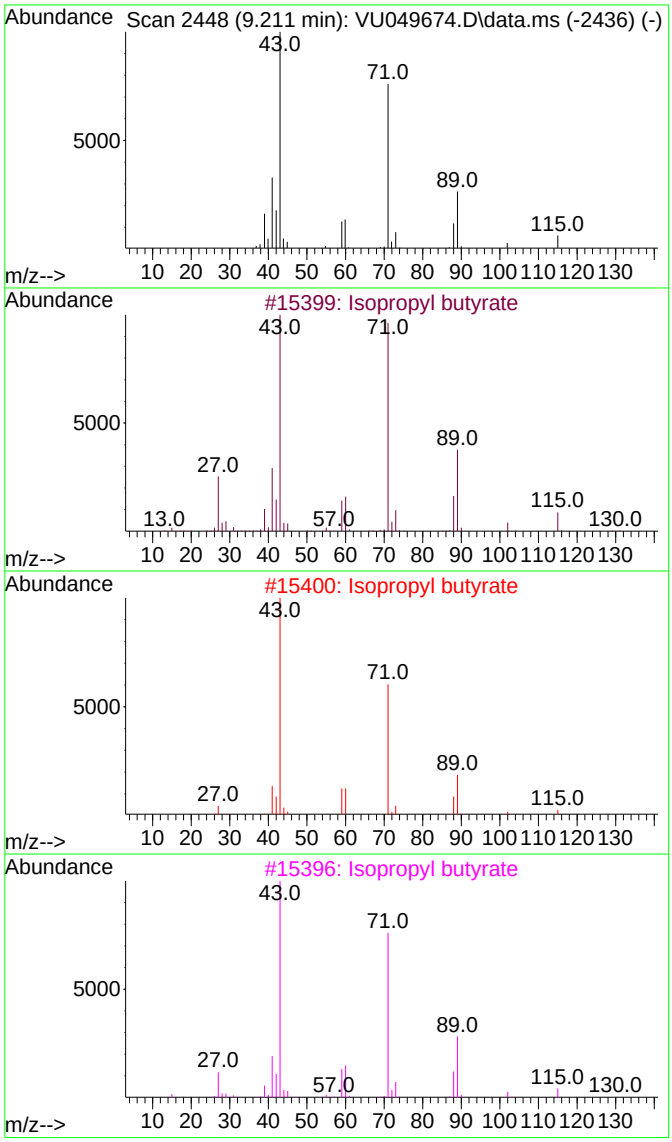
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

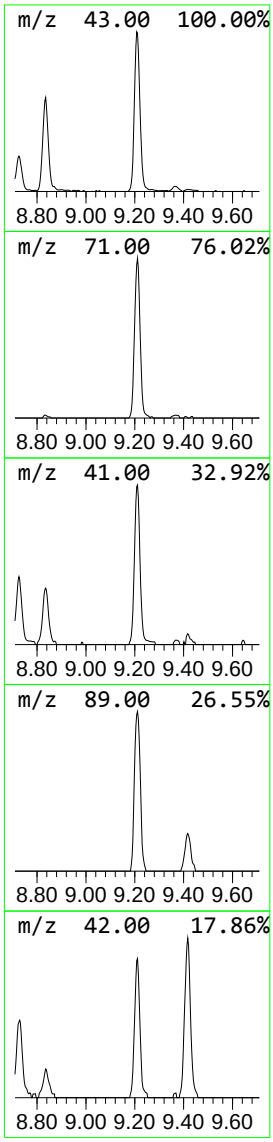
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	8.63 ug/L	123655	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	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049674.D
Acq On : 11 Jul 2022 14:35
Operator : SY/MD
Sample : PB146119TB 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VLEB119

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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	7.038	17.0	ug/L	201322	1	6.250	590909	50.0
Propanoic acid,...	7.739	2.9	ug/L	34523	1	6.250	590909	50.0
Propanoic acid,...	8.465	3.1	ug/L	44597	2	9.417	716342	50.0
Propanoic acid,...	8.726	5.8	ug/L	83270	2	9.417	716342	50.0
Acetic acid, bu...	8.835	3.4	ug/L	48984	2	9.417	716342	50.0
Isopropyl butyrate	9.211	8.6	ug/L	123655	2	9.417	716342	50.0