LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021931.D
Acq On : 23 Aug 2021 13:58
Operator : SY/MD
Sample : PB138622TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

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_V\Method\SFAMVLM081621WMA.M
Title : VOC Analysis

Signal : TIC: VV021931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	99	rVB	194163	197142	13.95%	1.692%
2	1.564	156	163	175	rVB	150856	174546	12.35%	1.498%
3	2.105	321	331	354	rVB	302399	444425	31.44%	3.814%
4	2.503	445	455	470	rBV	32776	55129	3.90%	0.473%
5	2.603	484	486	487	rBV	419	161	0.01%	0.001%
6	2.693	512	514	517	rBV	516	212	0.01%	0.002%
7	2.719	519	522	524	rBV3	385	225	0.02%	0.002%
8	2.883	571	573	575	rBV	376	106	0.01%	0.001%
9	2.953	593	595	598	rBV	404	211	0.01%	0.002%
10	2.992	605	607	609	rBV2	227	115	0.01%	0.001%
11	3.031	615	619	626	rBV4	664	683	0.05%	0.006%
12	3.101	637	641	642	rBV2	262	193	0.01%	0.002%
13	3.150	650	656	658	rBV2	491	400	0.03%	0.003%
14	3.162	658	660	661	rVB	226	72	0.01%	0.001%
15	3.220	675	678	682	rVB2	387	225	0.02%	0.002%
16	3.288	697	699	700	rBV	264	79	0.01%	0.001%
17	3.423	739	741	743	rBV	316	121	0.01%	0.001%
18	3.487	759	761	765	rVB	412	258	0.02%	0.002%
19	3.513	765	769	773	rBV2	207	204	0.01%	0.002%
20	3.555	780	782	783	rVB2	237	53	0.00%	0.000%
21	3.703	822	828	831	rBV	327	311	0.02%	0.003%
22	3.751	841	843	847	rVB2	490	359	0.03%	0.003%
23	3.777	847	851	854	rBV	301	263	0.02%	0.002%
24	3.799	854	858	859	rBV	204	153	0.01%	0.001%
25	3.870	871	880	924	rBV	108787	293554	20.77%	2.519%
26	4.346	1012	1028	1059	rBV	217108	553933	39.18%	4.754%
27	4.712	1136	1142	1143	rBV2	596	421	0.03%	0.004%
28	4.748	1151	1153	1154	rBV2	255	74	0.01%	0.001%
29	4.793	1165	1167	1170	rBV3	330	229	0.02%	0.002%
30	4.860	1186	1188	1190	rBV	161	65	0.00%	0.001%
31	4.876	1190	1193	1197	rVV	425	362	0.03%	0.003%
32	4.896	1198	1199	1201	rVB	301	101	0.01%	0.001%
33	5.043	1227	1245	1280	rBV2	551025	1413683	100.00%	12.132%
34	5.413	1358	1360	1362	rBV3	649	306	0.02%	0.003%
35	5.513	1389	1391	1393	rBV2	295	153	0.01%	0.001%
36	5.526	1393	1395	1397	rBV2	341	149	0.01%	0.001%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

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_V\Method\SFAMVLM081621WMA.M
Title : VOC Analysis

37	5.558	1403	1405	1407	rBV	305	153	0.01%	0.001%
38	5.613	1410	1422	1453	rBV	436503	896929	63.45%	7.697%
39	5.905	1504	1513	1528	rVB3	25743	52402	3.71%	0.450%
40	6.069	1551	1564	1591	rBV	309107	635142	44.93%	5.451%
41	6.326	1642	1644	1645	rBV	553	285	0.02%	0.002%
42	6.461	1677	1686	1718	rBV	100942	196867	13.93%	1.690%
43	6.847	1804	1806	1809	rBV2	365	163	0.01%	0.001%
44	6.985	1837	1849	1873	rBV	175744	321644	22.75%	2.760%
45	7.188	1904	1912	1922	rBV	16791	28195	1.99%	0.242%
46	7.313	1939	1951	1970	rBV	683453	1189321	84.13%	10.207%
47	7.622	2036	2047	2070	rBV	119059	213575	15.11%	1.833%
48	7.812	2104	2106	2109	rBV2	325	225	0.02%	0.002%
49	7.934	2129	2144	2150	rBV2	4922	9892	0.70%	0.085%
50	8.037	2168	2176	2182	rBV2	13973	19000	1.34%	0.163%
51	8.088	2183	2192	2214	rVV2	318999	597596	42.27%	5.129%
52	8.191	2216	2224	2251	rVB	187228	311937	22.07%	2.677%
53	8.442	2300	2302	2304	rBV	419	196	0.01%	0.002%
54	8.680	2366	2376	2395	rBV	112087	182504	12.91%	1.566%
55	8.854	2418	2430	2458	rBV	661816	1080025	76.40%	9.269%
56	9.236	2546	2549	2551	rBV2	278	198	0.01%	0.002%
57	9.262	2555	2557	2560	rVB2	330	128	0.01%	0.001%
58	9.368	2588	2590	2594	rBV2	251	177	0.01%	0.002%
59	9.555	2641	2648	2657	rBV5	3038	5375	0.38%	0.046%
60	9.619	2665	2668	2672	rVV2	337	210	0.01%	0.002%
61	9.638	2672	2674	2677	rVB2	335	154	0.01%	0.001%
62	9.760	2710	2712	2715	rVB2	196	72	0.01%	0.001%
63	9.892	2751	2753	2755	rVB	408	130	0.01%	0.001%
64	9.908	2755	2758	2762	rBV2	286	187	0.01%	0.002%
65	9.927	2762	2764	2765	rBV	285	126	0.01%	0.001%
66	10.130	2820	2827	2839	rVB3	3805	6738	0.48%	0.058%
67	10.217	2842	2854	2880	rVV	398160	627393	44.38%	5.384%
68	10.423	2915	2918	2921	rBV4	450	258	0.02%	0.002%
69	10.452	2925	2927	2928	rBV2	351	139	0.01%	0.001%
70	10.513	2944	2946	2948	rBV	522	222	0.02%	0.002%
71	10.529	2949	2951	2954	rBV2	287	156	0.01%	0.001%
72	10.657	2989	2991	2993	rBV	430	281	0.02%	0.002%
73	10.998	3095	3097	3101	rVB	382	179	0.01%	0.002%
74	11.037	3104	3109	3110	rBV2	568	542	0.04%	0.005%
75	11.149	3137	3144	3150	rBV7	1925	2457	0.17%	0.021%
76	11.249	3164	3175	3200	rBV	682793	1059333	74.93%	9.091%

LSC Area Percent Report

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Operator : SY/MD
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

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_V\Method\SFAMVLM081621WMA.M
Title : VOC Analysis

77	11.558	3269	3271	3274	rBV2	536	295	0.02%	0.003%
78	11.625	3280	3292	3319	rBV	670525	1071615	75.80%	9.197%
79	11.940	3387	3390	3391	rBV2	264	140	0.01%	0.001%
80	12.034	3416	3419	3421	rVB	427	226	0.02%	0.002%
81	12.050	3421	3424	3427	rBV3	834	587	0.04%	0.005%
82	12.143	3451	3453	3456	rBV2	583	320	0.02%	0.003%

Sum of corrected areas: 11652365

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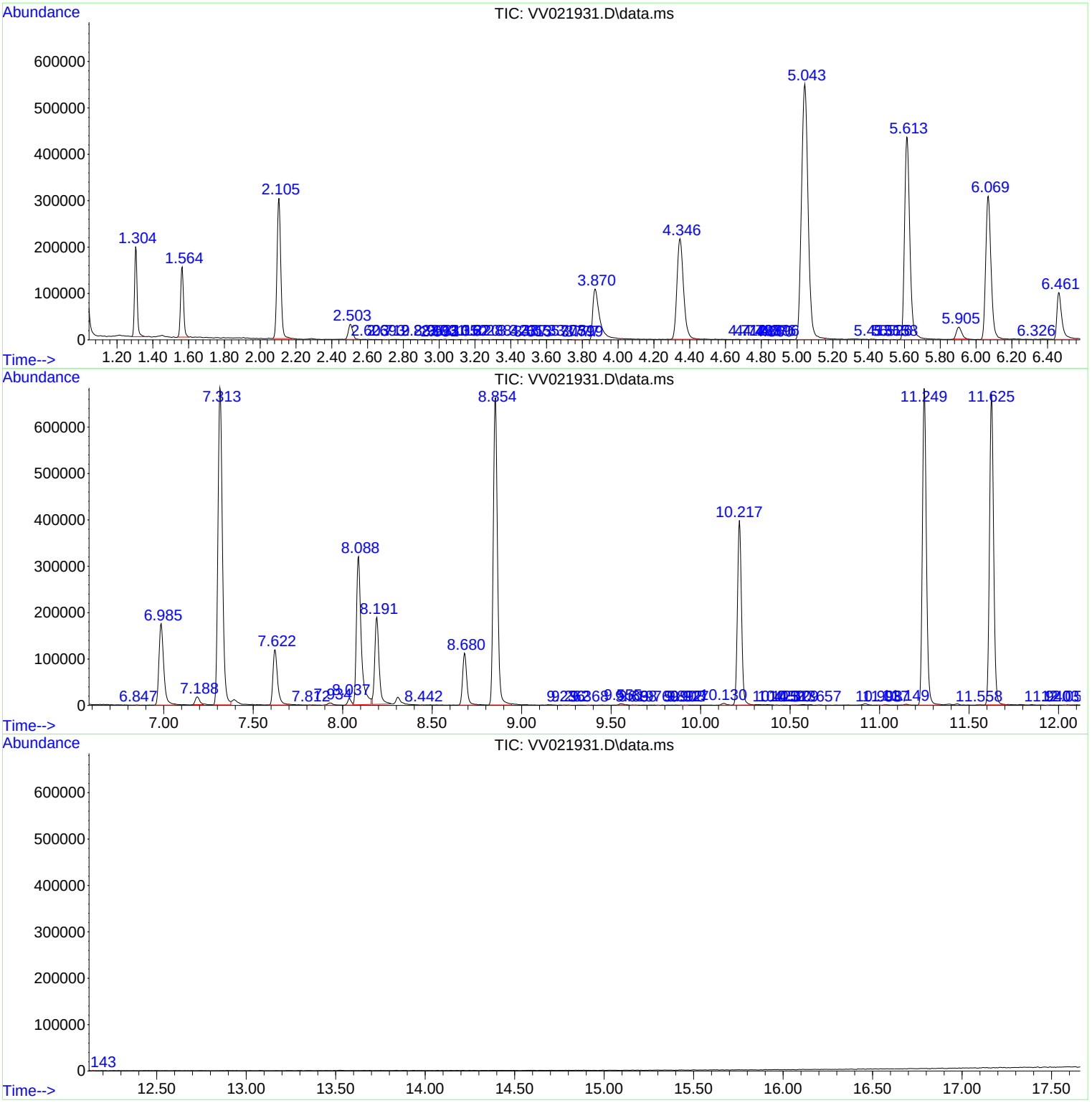
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB622

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021931.D
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Operator : SY/MD
Sample : PB138622TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

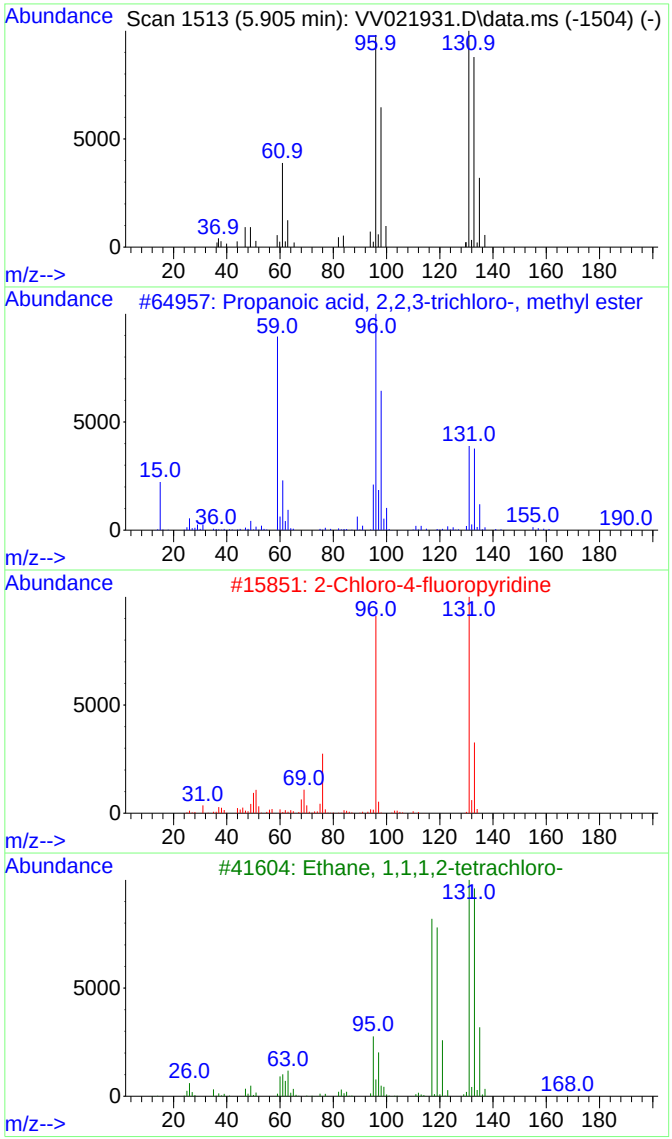
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

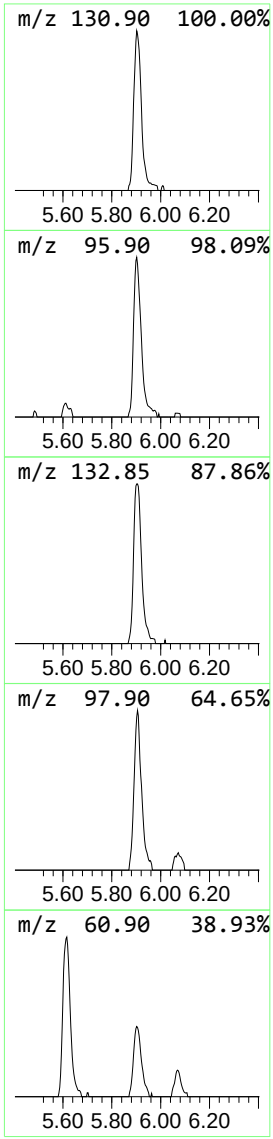
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	2.92 ug/L	52402	1,4-Difluorobenzene	5.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	50
2	2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
3	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	37
4	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
5	4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32





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Operator : SY/MD
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

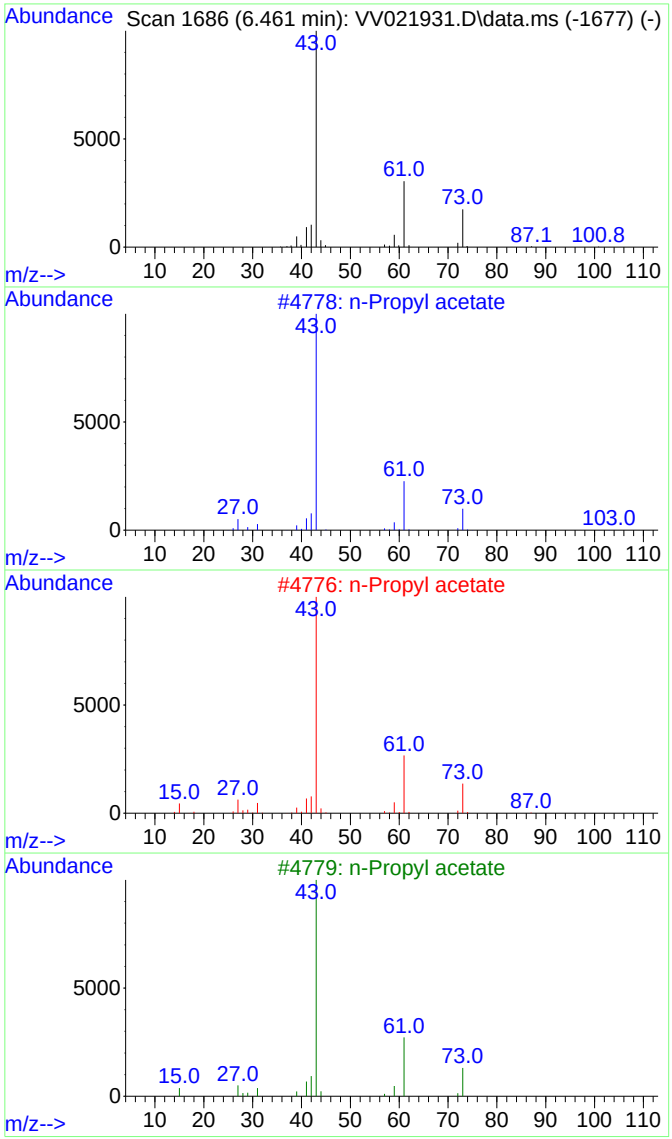
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

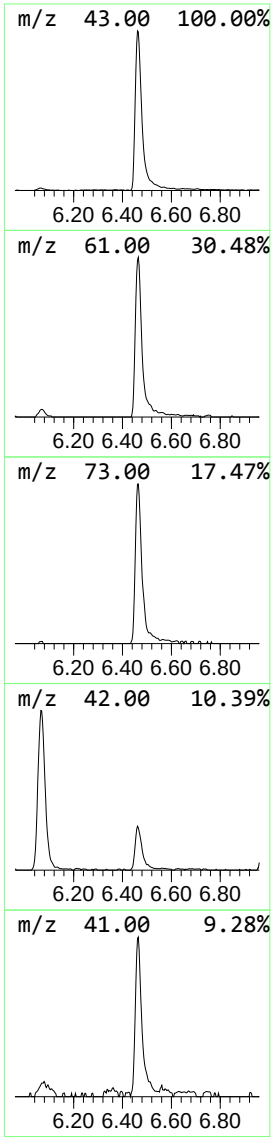
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	10.97 ug/L	196867	1,4-Difluorobenzene	5.616

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082321\
Data File : VV021931.D
Acq On : 23 Aug 2021 13:58
Operator : SY/MD
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB622

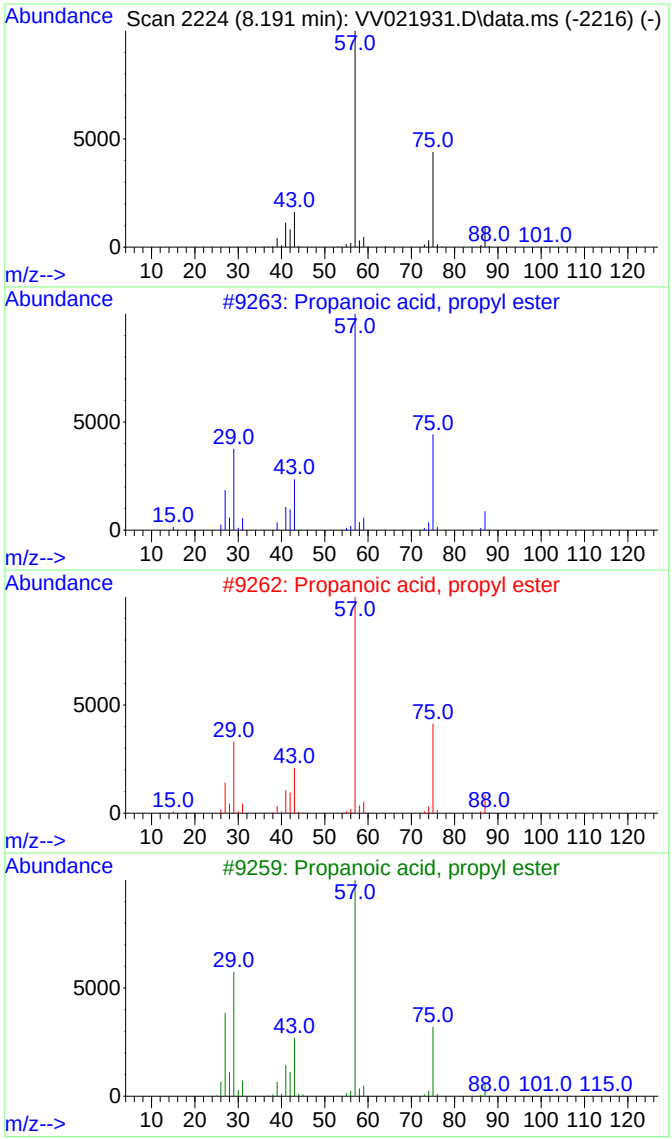
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

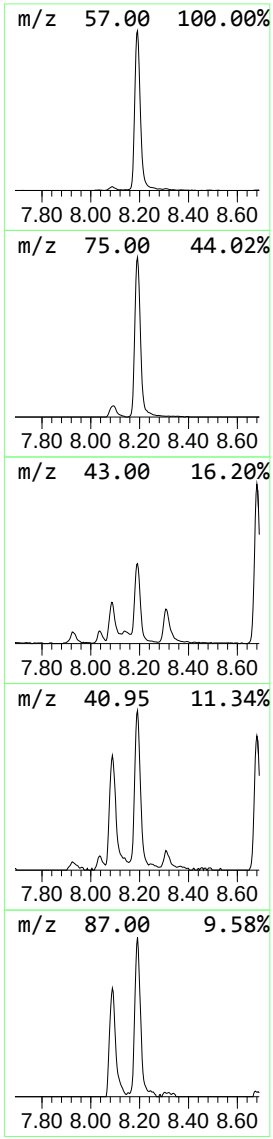
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	14.44 ug/L	311937	Chlorobenzene-d5	8.854

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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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

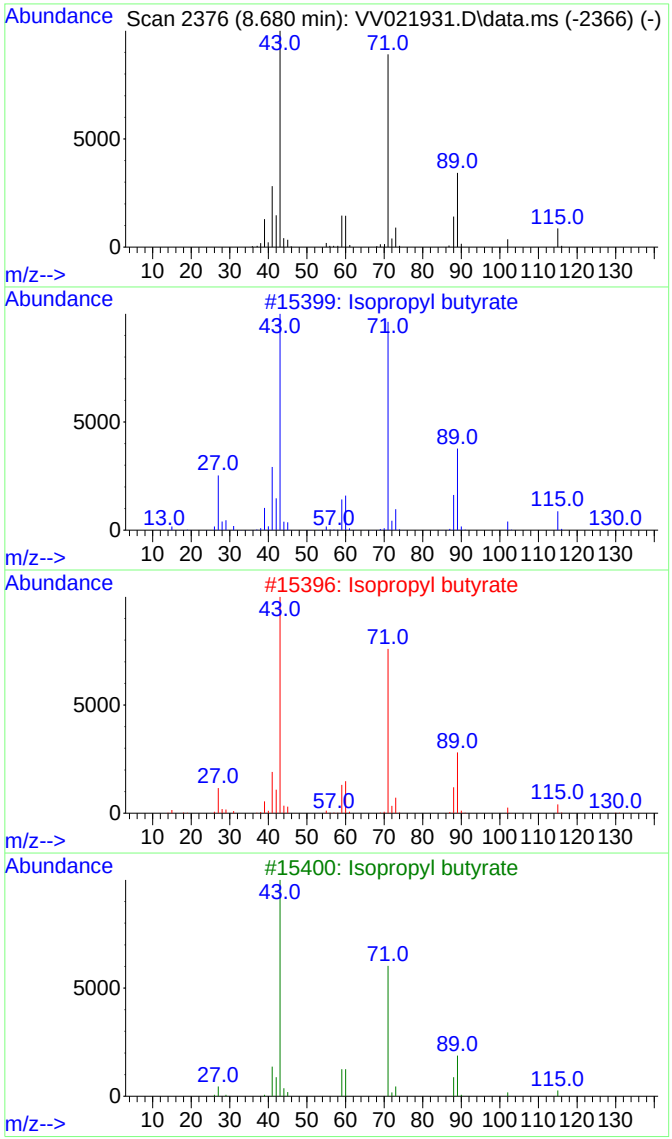
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

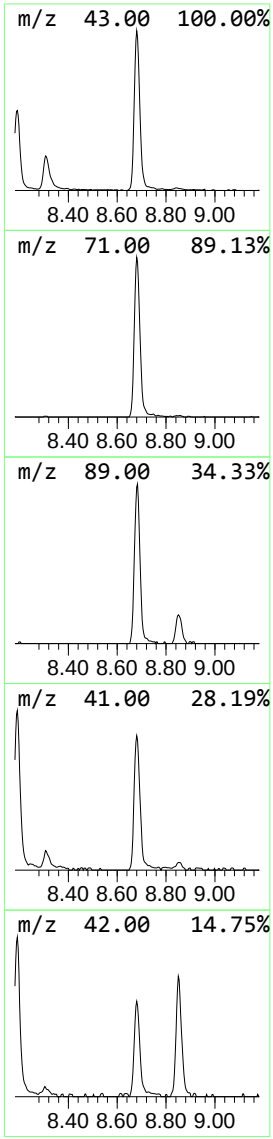
****

Peak Number 5 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	8.45 ug/L	182504	Chlorobenzene-d5	8.854

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	78
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

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Data File : VV021931.D
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Operator : SY/MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VLEB622

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.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
Propanoic acid,...	5.905	2.9	ug/L	52402	1	5.616	896929	50.0
n-Propyl acetate	6.461	11.0	ug/L	196867	1	5.616	896929	50.0
Propanoic acid,...	8.191	14.4	ug/L	311937	2	8.854	1080030	50.0
Isopropyl butyrate	8.680	8.4	ug/L	182504	2	8.854	1080030	50.0