LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049361.D
Acq On : 22 Jun 2022 18:54
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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: VU049361.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	74	80	95	rBV	59302	68951	10.42%	1.033%
2	1.896	166	173	186	rVB	50207	65643	9.92%	0.984%
3	2.562	369	380	392	rBV	98650	157382	23.78%	2.359%
4	2.858	470	472	476	rVB	310	169	0.03%	0.003%
5	2.922	489	492	495	rVB2	438	264	0.04%	0.004%
6	2.945	495	499	502	rBV3	628	591	0.09%	0.009%
7	3.041	518	529	539	rBV	6103	10353	1.56%	0.155%
8	3.183	558	573	595	rVB2	32992	80608	12.18%	1.208%
9	3.285	602	605	606	rBV	346	185	0.03%	0.003%
10	3.388	635	637	638	rBV	164	74	0.01%	0.001%
11	3.443	653	654	657	rBV	151	77	0.01%	0.001%
12	3.549	681	687	689	rBV2	260	283	0.04%	0.004%
13	3.584	693	698	711	rVB3	448	891	0.13%	0.013%
14	3.687	727	730	735	rVB2	249	207	0.03%	0.003%
15	3.716	736	739	741	rBV2	257	117	0.02%	0.002%
16	3.745	746	748	751	rBV	170	84	0.01%	0.001%
17	3.877	787	789	793	rBV2	208	96	0.01%	0.001%
18	3.896	793	795	796	rBV2	169	68	0.01%	0.001%
19	3.964	811	816	823	rVB2	333	400	0.06%	0.006%
20	3.993	823	825	828	rBV2	161	119	0.02%	0.002%
21	4.012	828	831	834	rBV2	356	183	0.03%	0.003%
22	4.118	862	864	867	rBV	293	133	0.02%	0.002%
23	4.401	949	952	953	rBV	151	79	0.01%	0.001%
24	4.620	1007	1020	1052	rBV	118160	291670	44.07%	4.371%
25	4.928	1114	1116	1119	rBV	285	217	0.03%	0.003%
26	4.970	1126	1129	1130	rBV	187	111	0.02%	0.002%
27	5.060	1140	1157	1178	rBV	131280	284502	42.99%	4.264%
28	5.176	1189	1193	1194	rBV	158	96	0.01%	0.001%
29	5.211	1201	1204	1208	rBV3	374	323	0.05%	0.005%
30	5.234	1208	1211	1214	rVB	391	239	0.04%	0.004%
31	5.337	1235	1243	1245	rBV	216	256	0.04%	0.004%
32	5.408	1262	1265	1267	rBV	152	109	0.02%	0.002%
33	5.478	1279	1287	1292	rBV2	244	366	0.06%	0.005%
34	5.530	1301	1303	1308	rVB2	133	99	0.01%	0.001%
35	5.604	1323	1326	1332	rVB2	159	172	0.03%	0.003%
36	5.633	1332	1335	1337	rBV2	191	115	0.02%	0.002%

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Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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

37	5.723	1341	1363	1382	rBV2	238207	661848	100.00%	9.919%
38	5.912	1410	1422	1436	rBV3	9622	19428	2.94%	0.291%
39	6.018	1453	1455	1459	rVB2	396	169	0.03%	0.003%
40	6.041	1459	1462	1464	rBV	314	146	0.02%	0.002%
41	6.076	1469	1473	1479	rVB2	310	337	0.05%	0.005%
42	6.108	1479	1483	1485	rBV	206	132	0.02%	0.002%
43	6.147	1491	1495	1497	rBV	232	166	0.03%	0.002%
44	6.186	1498	1507	1510	rBV3	922	1427	0.22%	0.021%
45	6.247	1514	1526	1545	rBV	288457	538295	81.33%	8.067%
46	6.523	1608	1612	1622	rBV8	1433	2323	0.35%	0.035%
47	6.690	1650	1664	1685	rVB	175485	341246	51.56%	5.114%
48	6.764	1685	1687	1688	rBV2	236	77	0.01%	0.001%
49	6.922	1724	1736	1751	rBV2	5336	11742	1.77%	0.176%
50	7.038	1761	1772	1793	rBV	112471	197304	29.81%	2.957%
51	7.449	1896	1900	1905	rBV2	438	450	0.07%	0.007%
52	7.565	1924	1936	1951	rBV	90930	157934	23.86%	2.367%
53	7.687	1967	1974	1979	rBV5	879	1250	0.19%	0.019%
54	7.735	1980	1989	2001	rVV2	19829	33736	5.10%	0.506%
55	7.896	2025	2039	2060	rBV	271741	473855	71.60%	7.101%
56	8.176	2108	2126	2144	rBV3	70422	149419	22.58%	2.239%
57	8.362	2181	2184	2187	rBV	394	285	0.04%	0.004%
58	8.401	2194	2196	2200	rVB2	358	218	0.03%	0.003%
59	8.423	2200	2203	2205	rBV2	261	108	0.02%	0.002%
60	8.465	2205	2216	2229	rBV2	26120	43104	6.51%	0.646%
61	8.575	2236	2250	2256	rBV7	4054	9219	1.39%	0.138%
62	8.632	2257	2268	2289	rVV	325285	591425	89.36%	8.863%
63	8.726	2291	2297	2314	rVB	50458	80054	12.10%	1.200%
64	8.835	2321	2331	2345	rVB	30224	48141	7.27%	0.721%
65	8.948	2362	2366	2370	rBV3	621	587	0.09%	0.009%
66	9.002	2381	2383	2386	rBV2	193	86	0.01%	0.001%
67	9.047	2393	2397	2399	rBV	465	292	0.04%	0.004%
68	9.092	2409	2411	2414	rVB	246	100	0.02%	0.001%
69	9.208	2435	2447	2461	rBV	74869	118060	17.84%	1.769%
70	9.372	2489	2498	2499	rBV5	1440	1789	0.27%	0.027%
71	9.417	2500	2512	2545	rVB	396906	658448	99.49%	9.868%
72	9.616	2570	2574	2577	rVB2	402	317	0.05%	0.005%
73	9.642	2577	2582	2590	rBV5	979	1471	0.22%	0.022%
74	9.694	2596	2598	2602	rVB2	311	168	0.03%	0.003%
75	9.716	2603	2605	2611	rVB2	217	185	0.03%	0.003%
76	9.777	2621	2624	2629	rVB3	303	241	0.04%	0.004%

LSC Area Percent Report

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Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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

77	9.813	2633	2635	2637	rBV3	153	90	0.01%	0.001%
78	9.922	2662	2669	2677	rVB4	975	1595	0.24%	0.024%
79	10.073	2707	2716	2730	rVB2	5674	8835	1.33%	0.132%
80	10.140	2735	2737	2739	rBV	179	71	0.01%	0.001%
81	10.292	2781	2784	2786	rVB2	413	261	0.04%	0.004%
82	10.337	2796	2798	2800	rBV2	183	83	0.01%	0.001%
83	10.452	2832	2834	2837	rVB2	346	189	0.03%	0.003%
84	10.475	2837	2841	2845	rBV3	401	304	0.05%	0.005%
85	10.523	2850	2856	2860	rBV	160	201	0.03%	0.003%
86	10.546	2860	2863	2864	rBV3	177	101	0.02%	0.002%
87	10.575	2870	2872	2876	rBV2	181	133	0.02%	0.002%
88	10.755	2916	2928	2950	rBV	291418	470343	71.07%	7.049%
89	11.111	3038	3039	3042	rVB2	281	109	0.02%	0.002%
90	11.128	3042	3044	3047	rBV2	165	71	0.01%	0.001%
91	11.147	3048	3050	3055	rBV3	250	204	0.03%	0.003%
92	11.205	3066	3068	3070	rBV	198	80	0.01%	0.001%
93	11.745	3233	3236	3240	rBV2	311	218	0.03%	0.003%
94	11.767	3240	3243	3244	rBV	301	182	0.03%	0.003%
95	11.812	3244	3257	3278	rVV	365152	595028	89.90%	8.917%
96	12.192	3363	3375	3394	rBV	292790	482465	72.90%	7.230%
97	12.841	3572	3577	3585	rBV2	359	528	0.08%	0.008%
98	12.877	3585	3588	3590	rBV2	297	174	0.03%	0.003%
99	13.037	3635	3638	3645	rBV3	345	281	0.04%	0.004%
100	13.208	3687	3691	3694	rBV2	374	329	0.05%	0.005%

Sum of corrected areas: 6672689

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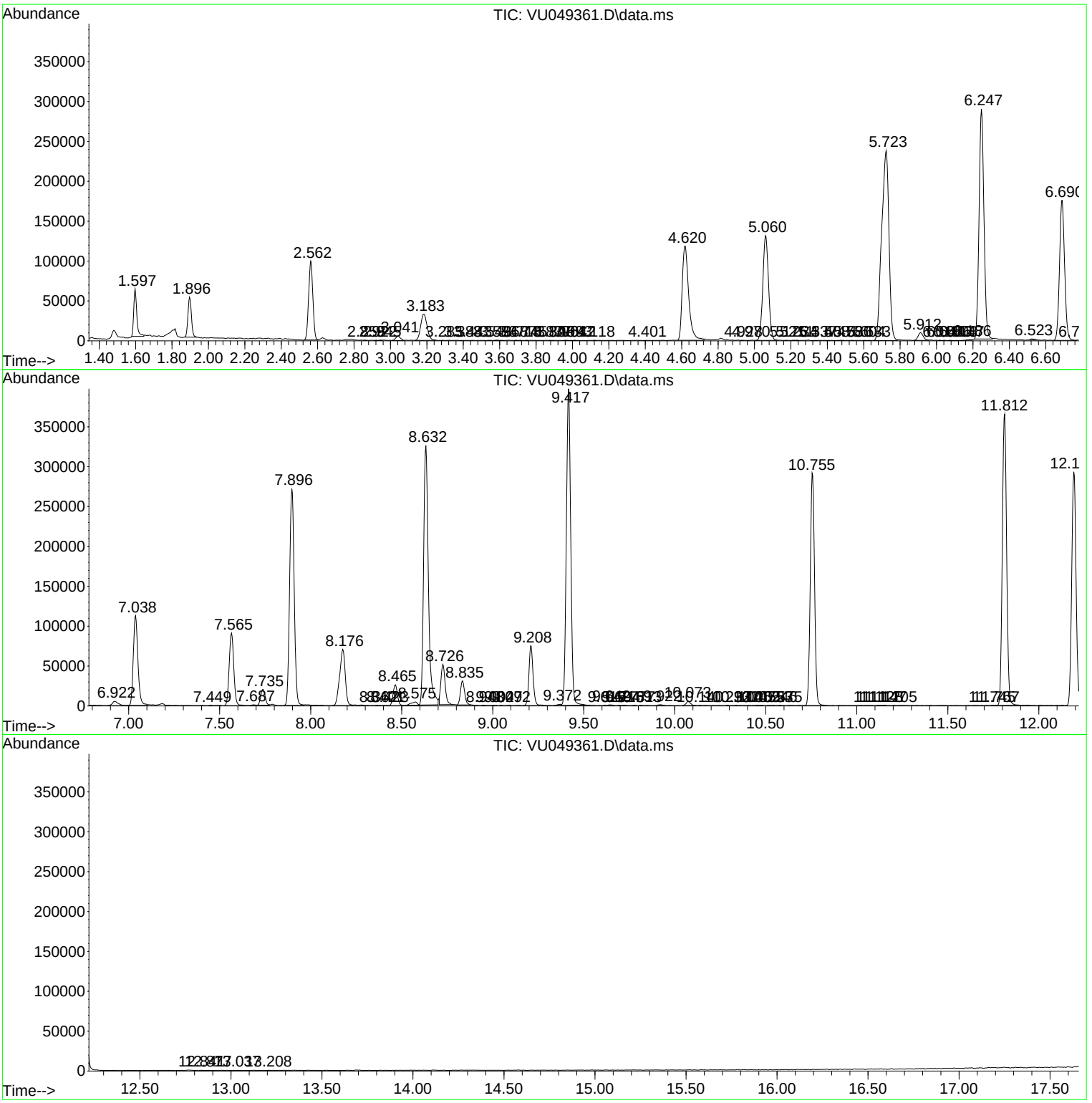
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049361.D
Acq On : 22 Jun 2022 18:54
Operator : SY/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

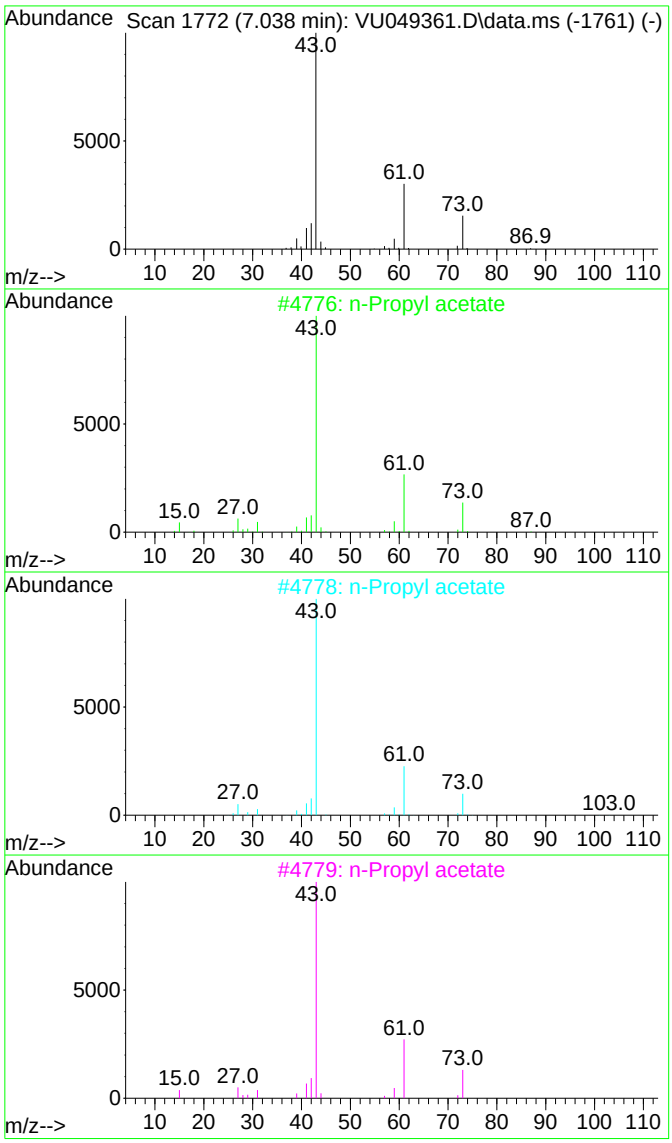
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

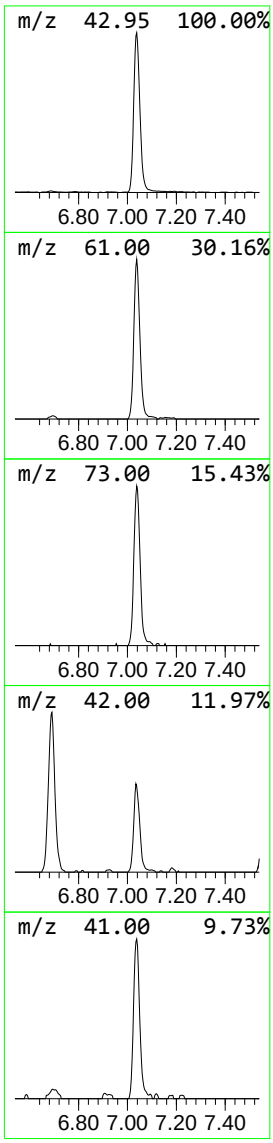
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	18.33 ug/L	197304	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	72
5	n-Propyl acetate	102	C5H10O2	000109-60-4	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049361.D
Acq On : 22 Jun 2022 18:54
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

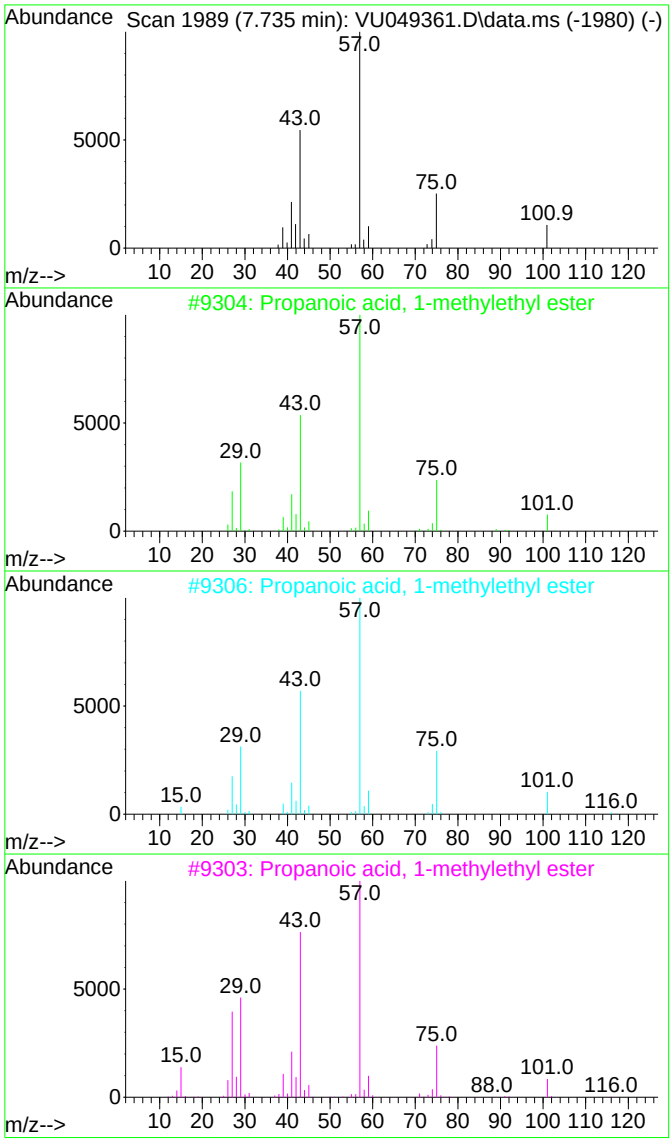
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

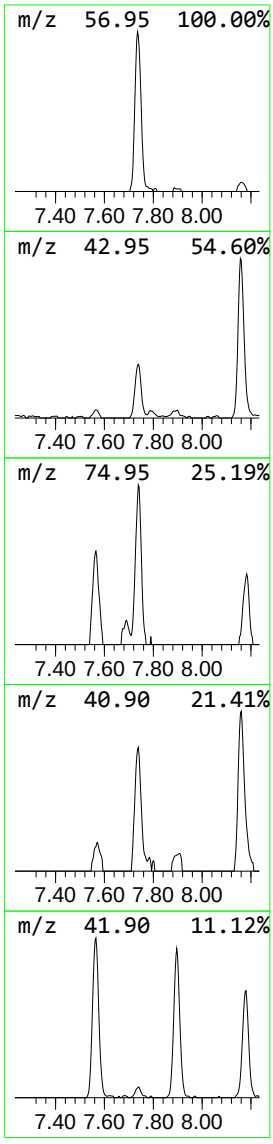
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.735	3.13 ug/L	33736	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	78
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	56
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

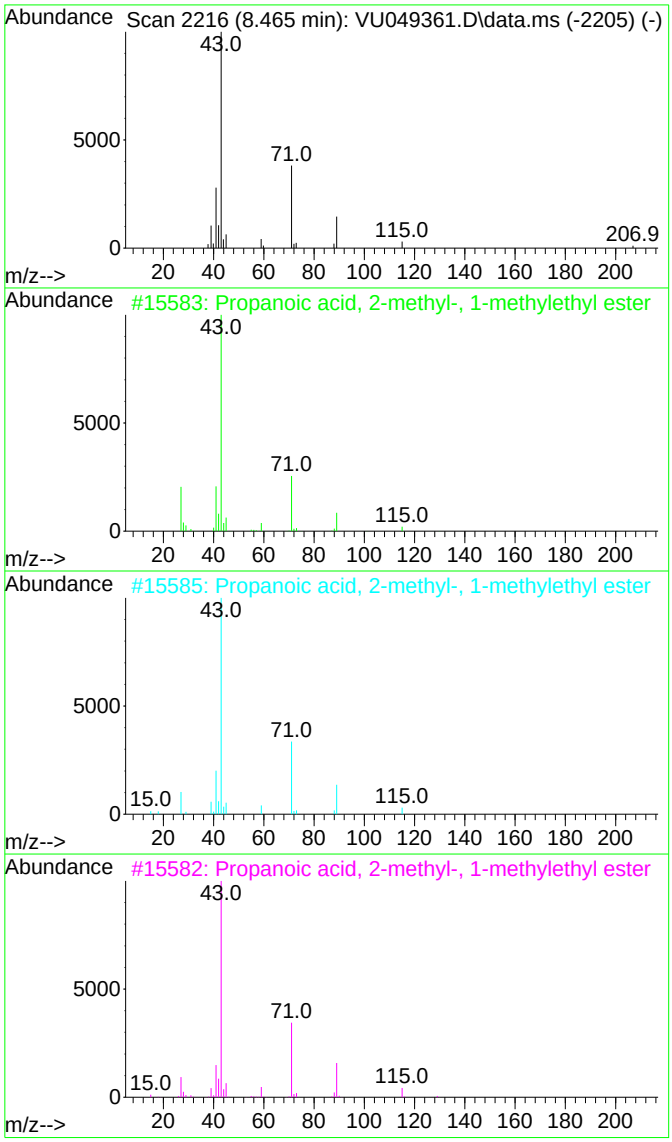
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

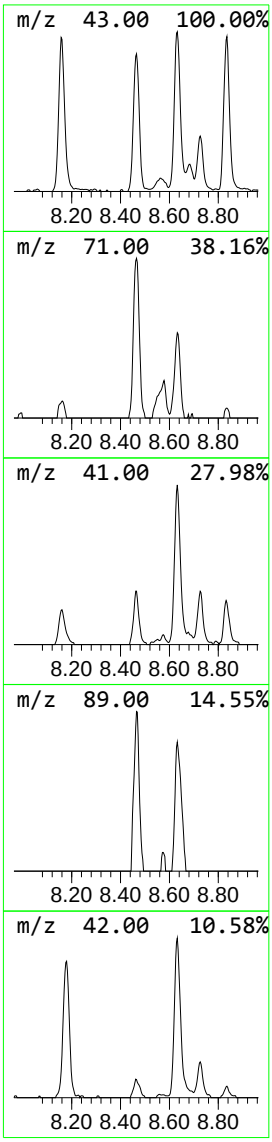
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	3.27 ug/L	43104	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-, propy...	130	C7H14O2	000644-49-5	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64





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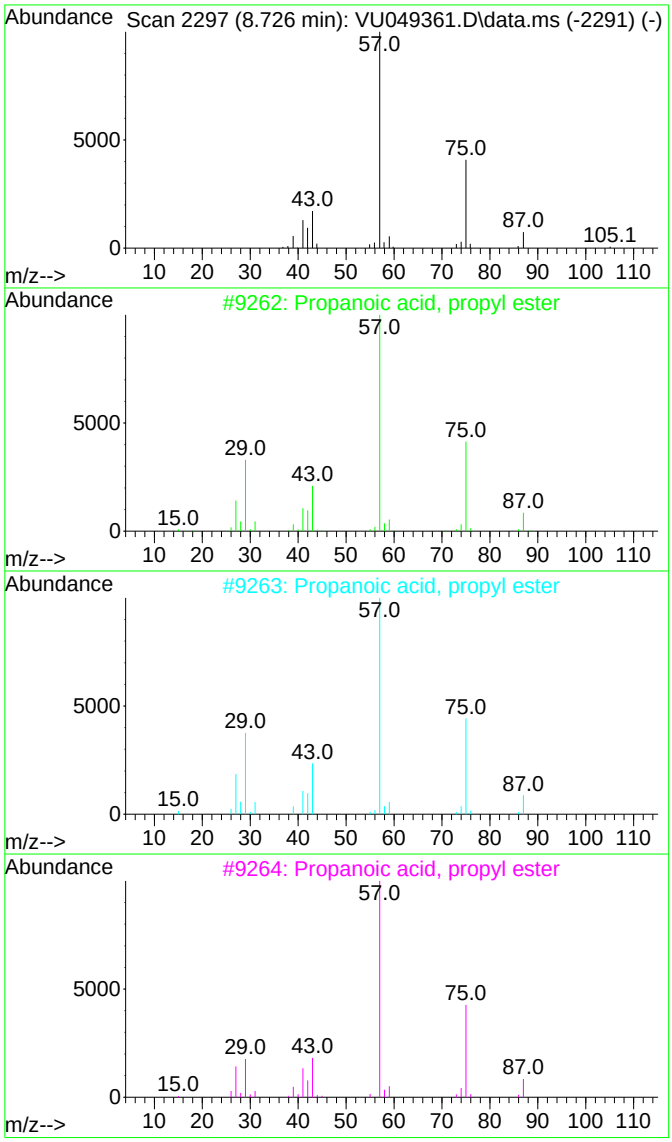
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

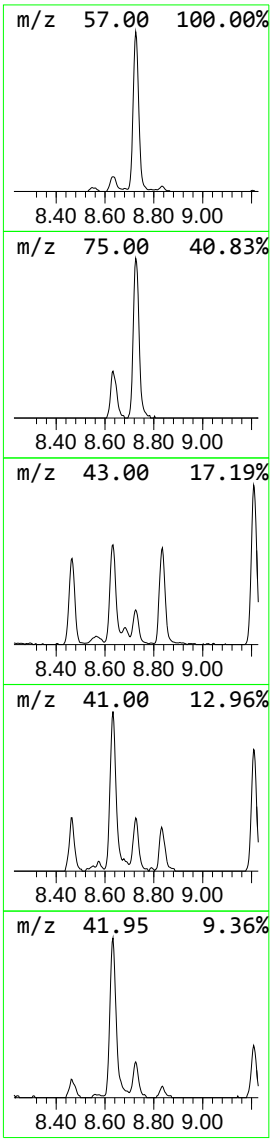
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	6.08 ug/L	80054	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, propyl ester	116	C6H12O2	000106-36-5	74





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Data File : VU049361.D
Acq On : 22 Jun 2022 18:54
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

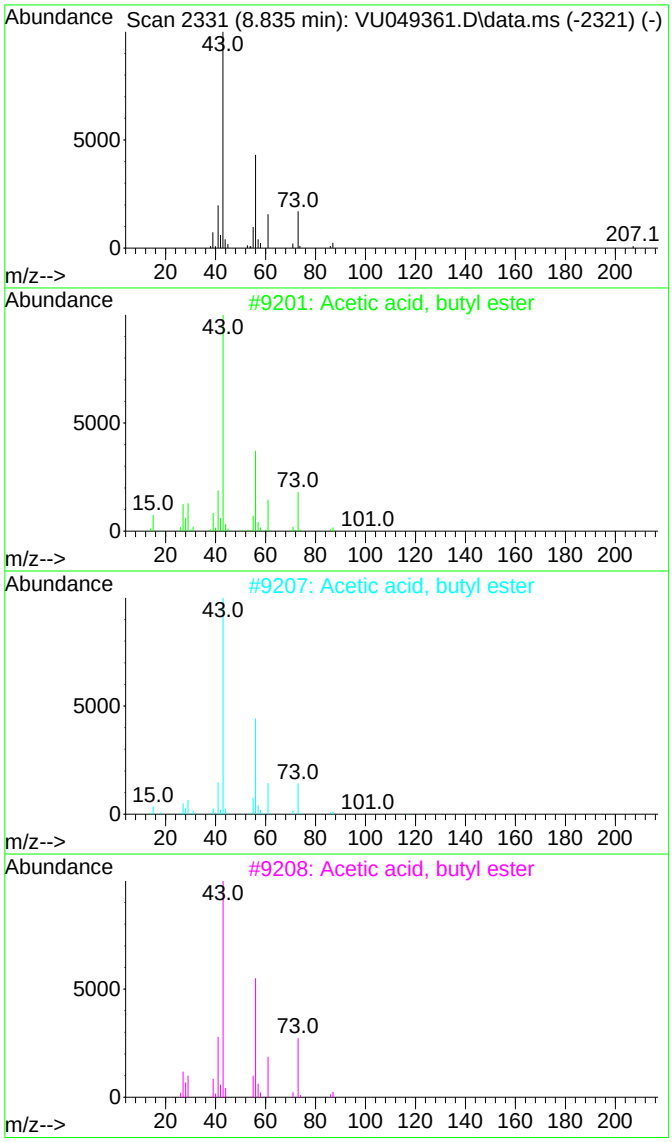
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

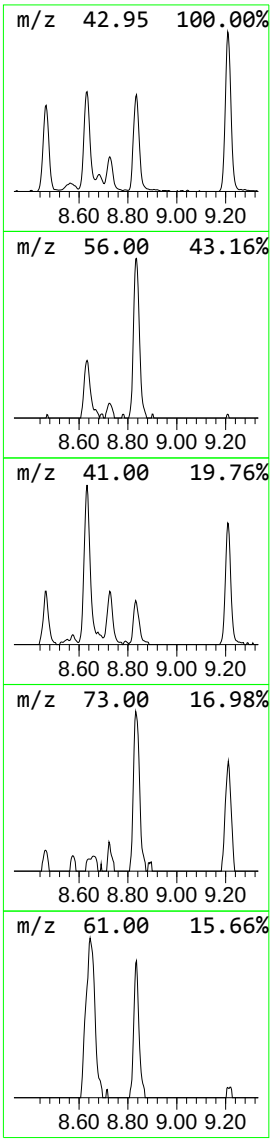
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	3.66 ug/L	48141	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	83
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049361.D
Acq On : 22 Jun 2022 18:54
Operator : SY/MD
Sample : N3392-16 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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

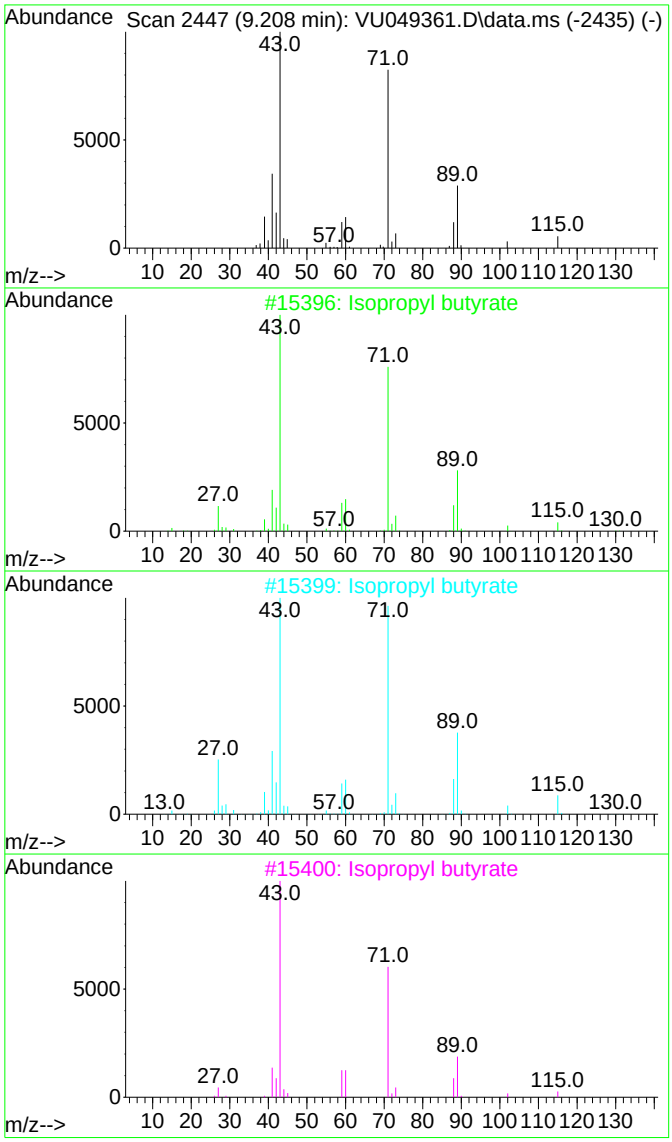
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

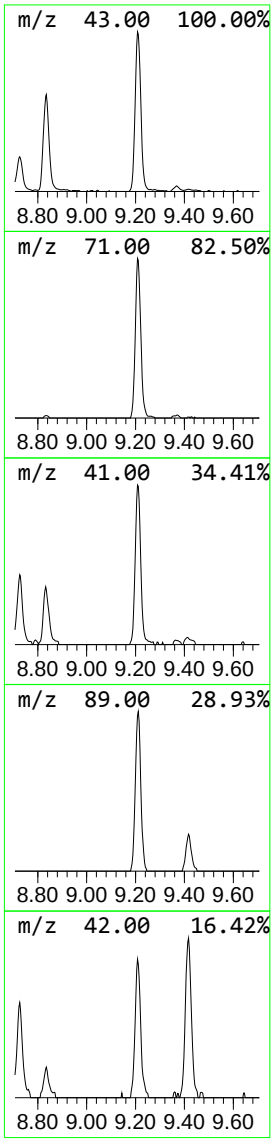
****

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.208	8.97 ug/L	118060	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	83
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049361.D
Acq On : 22 Jun 2022 18:54
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEZ1

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	7.038	18.3	ug/L	197304	1	6.247	538295	50.0
Propanoic acid,...	7.735	3.1	ug/L	33736	1	6.247	538295	50.0
Propanoic acid,...	8.465	3.3	ug/L	43104	2	9.417	658448	50.0
Propanoic acid,...	8.726	6.1	ug/L	80054	2	9.417	658448	50.0
Acetic acid, bu...	8.835	3.7	ug/L	48141	2	9.417	658448	50.0
Isopropyl butyrate	9.208	9.0	ug/L	118060	2	9.417	658448	50.0