LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049681.D
Acq On : 11 Jul 2022 17:19
Operator : SY/MD
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

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: VU049681.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	72	80	97	rBV	135238	153066	15.06%	1.868%
2	1.906	168	176	197	rVB	99750	133015	13.09%	1.623%
3	2.327	304	307	313	rBV5	656	796	0.08%	0.010%
4	2.565	368	381	393	rBV	202922	325710	32.05%	3.975%
5	2.623	395	399	412	rVB	4965	7674	0.76%	0.094%
6	2.748	435	438	441	rBV2	246	185	0.02%	0.002%
7	2.941	492	498	502	rBV3	374	488	0.05%	0.006%
8	3.041	518	529	542	rVB2	11321	20362	2.00%	0.248%
9	3.182	559	573	591	rVV2	12529	27851	2.74%	0.340%
10	3.333	614	620	626	rVB2	316	361	0.04%	0.004%
11	3.401	638	641	648	rBV2	281	324	0.03%	0.004%
12	3.549	683	687	694	rBV	207	229	0.02%	0.003%
13	3.973	815	819	822	rBV2	290	199	0.02%	0.002%
14	4.070	845	849	856	rBV2	216	285	0.03%	0.003%
15	4.269	908	911	916	rVB	241	193	0.02%	0.002%
16	4.340	930	933	939	rBV2	211	209	0.02%	0.003%
17	4.620	1007	1020	1056	rBV	126525	308195	30.33%	3.761%
18	4.880	1099	1101	1106	rBV3	275	207	0.02%	0.003%
19	5.063	1140	1158	1183	rVV	183074	399396	39.31%	4.874%
20	5.234	1208	1211	1216	rBV2	194	223	0.02%	0.003%
21	5.285	1220	1227	1238	rVB3	732	1391	0.14%	0.017%
22	5.369	1249	1253	1254	rBV2	424	277	0.03%	0.003%
23	5.449	1276	1278	1284	rBV2	216	221	0.02%	0.003%
24	5.497	1289	1293	1296	rVV	226	243	0.02%	0.003%
25	5.565	1308	1314	1318	rBV	184	216	0.02%	0.003%
26	5.722	1341	1363	1389	rBV2	377839	1016139	100.00%	12.400%
27	5.912	1411	1422	1435	rBV2	8891	18213	1.79%	0.222%
28	6.018	1451	1455	1459	rBV2	281	315	0.03%	0.004%
29	6.083	1470	1475	1477	rBV2	284	247	0.02%	0.003%
30	6.111	1481	1484	1488	rVV2	197	197	0.02%	0.002%
31	6.176	1501	1504	1508	rBV2	402	251	0.02%	0.003%
32	6.246	1512	1526	1549	rBV	309550	588129	57.88%	7.177%
33	6.372	1563	1565	1569	rVB2	343	184	0.02%	0.002%
34	6.449	1583	1589	1593	rBV2	364	411	0.04%	0.005%
35	6.542	1607	1618	1631	rVB6	5921	10713	1.05%	0.131%
36	6.597	1631	1635	1638	rBV2	277	228	0.02%	0.003%

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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

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	6.690	1650	1664	1683	rVV	246782	471007	46.35%	5.748%
38	6.777	1688	1691	1694	rBV2	540	463	0.05%	0.006%
39	6.925	1725	1737	1760	rVB	4989	10283	1.01%	0.125%
40	7.037	1760	1772	1794	rBV	103159	183301	18.04%	2.237%
41	7.185	1811	1818	1819	rBV4	589	615	0.06%	0.008%
42	7.394	1880	1883	1892	rBV2	323	243	0.02%	0.003%
43	7.459	1898	1903	1906	rVB2	230	196	0.02%	0.002%
44	7.478	1906	1909	1913	rBV2	236	236	0.02%	0.003%
45	7.565	1924	1936	1957	rBV	124459	214949	21.15%	2.623%
46	7.684	1966	1973	1974	rBV3	275	288	0.03%	0.004%
47	7.738	1979	1990	2001	rBV	19166	31361	3.09%	0.383%
48	7.896	2025	2039	2065	rBV	437417	759282	74.72%	9.266%
49	8.025	2077	2079	2083	rBV3	323	199	0.02%	0.002%
50	8.047	2083	2086	2089	rVB2	603	421	0.04%	0.005%
51	8.179	2111	2127	2144	rBV2	86729	177103	17.43%	2.161%
52	8.262	2150	2153	2161	rVB4	689	623	0.06%	0.008%
53	8.369	2184	2186	2192	rVB2	338	241	0.02%	0.003%
54	8.465	2202	2216	2229	rBV	22491	37160	3.66%	0.453%
55	8.513	2229	2231	2235	rVB2	331	187	0.02%	0.002%
56	8.552	2236	2243	2246	rBV5	3546	4306	0.42%	0.053%
57	8.632	2256	2268	2289	rBV2	336374	616122	60.63%	7.519%
58	8.725	2290	2297	2314	rVB3	41410	69593	6.85%	0.849%
59	8.835	2322	2331	2341	rBV2	25640	37881	3.73%	0.462%
60	9.008	2381	2385	2387	rBV	297	242	0.02%	0.003%
61	9.211	2435	2448	2463	rBV	64868	100750	9.91%	1.230%
62	9.282	2467	2470	2473	rVV3	439	336	0.03%	0.004%
63	9.340	2483	2488	2489	rBV	340	271	0.03%	0.003%
64	9.365	2489	2496	2499	rVV3	1094	1251	0.12%	0.015%
65	9.417	2499	2512	2529	rVV	425650	702992	69.18%	8.579%
66	9.587	2559	2565	2568	rBV2	162	207	0.02%	0.003%
67	9.629	2574	2578	2579	rBV	381	250	0.02%	0.003%
68	9.642	2579	2582	2583	rBV2	371	227	0.02%	0.003%
69	9.703	2597	2601	2602	rVV	404	219	0.02%	0.003%
70	9.713	2602	2604	2610	rVB	362	253	0.02%	0.003%
71	9.918	2662	2668	2681	rVV2	956	1522	0.15%	0.019%
72	9.976	2681	2686	2694	rVV2	247	417	0.04%	0.005%
73	10.073	2709	2716	2729	rVB5	4193	6642	0.65%	0.081%
74	10.140	2734	2737	2742	rVB2	377	313	0.03%	0.004%
75	10.179	2742	2749	2753	rBV2	197	251	0.02%	0.003%
76	10.304	2784	2788	2793	rVB2	232	216	0.02%	0.003%

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Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

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

77	10.487	2842	2845	2848	rBV2	349	209	0.02%	0.003%
78	10.758	2916	2929	2952	rBV	314501	508525	50.04%	6.206%
79	10.864	2959	2962	2968	rBV2	510	616	0.06%	0.008%
80	11.050	3016	3020	3023	rBV2	302	280	0.03%	0.003%
81	11.221	3069	3073	3080	rBV2	286	311	0.03%	0.004%
82	11.471	3147	3151	3154	rBV2	275	216	0.02%	0.003%
83	11.741	3232	3235	3238	rBV	561	389	0.04%	0.005%
84	11.812	3244	3257	3280	rBV	389463	618312	60.85%	7.546%
85	11.970	3303	3306	3315	rBV2	419	459	0.05%	0.006%
86	12.192	3362	3375	3393	rBV	372596	612812	60.31%	7.478%
87	12.442	3451	3453	3456	rVV2	293	190	0.02%	0.002%
88	12.462	3456	3459	3462	rVB	301	207	0.02%	0.003%
89	12.603	3500	3503	3508	rBV	223	212	0.02%	0.003%
90	12.674	3520	3525	3527	rBV2	316	299	0.03%	0.004%
91	13.121	3661	3664	3667	rBV	311	243	0.02%	0.003%
92	13.285	3709	3715	3718	rBV	252	356	0.04%	0.004%
93	13.362	3736	3739	3741	rBV	249	189	0.02%	0.002%
94	13.481	3773	3776	3782	rBV	294	226	0.02%	0.003%
95	13.539	3790	3794	3795	rBV	258	196	0.02%	0.002%
96	13.802	3873	3876	3878	rBV	300	221	0.02%	0.003%
97	13.909	3906	3909	3912	rBV2	290	204	0.02%	0.002%
98	14.336	4040	4042	4045	rVB3	539	303	0.03%	0.004%
99	14.577	4115	4117	4122	rBV2	317	191	0.02%	0.002%
100	15.921	4533	4535	4541	rBV3	471	419	0.04%	0.005%

Sum of corrected areas: 8194347

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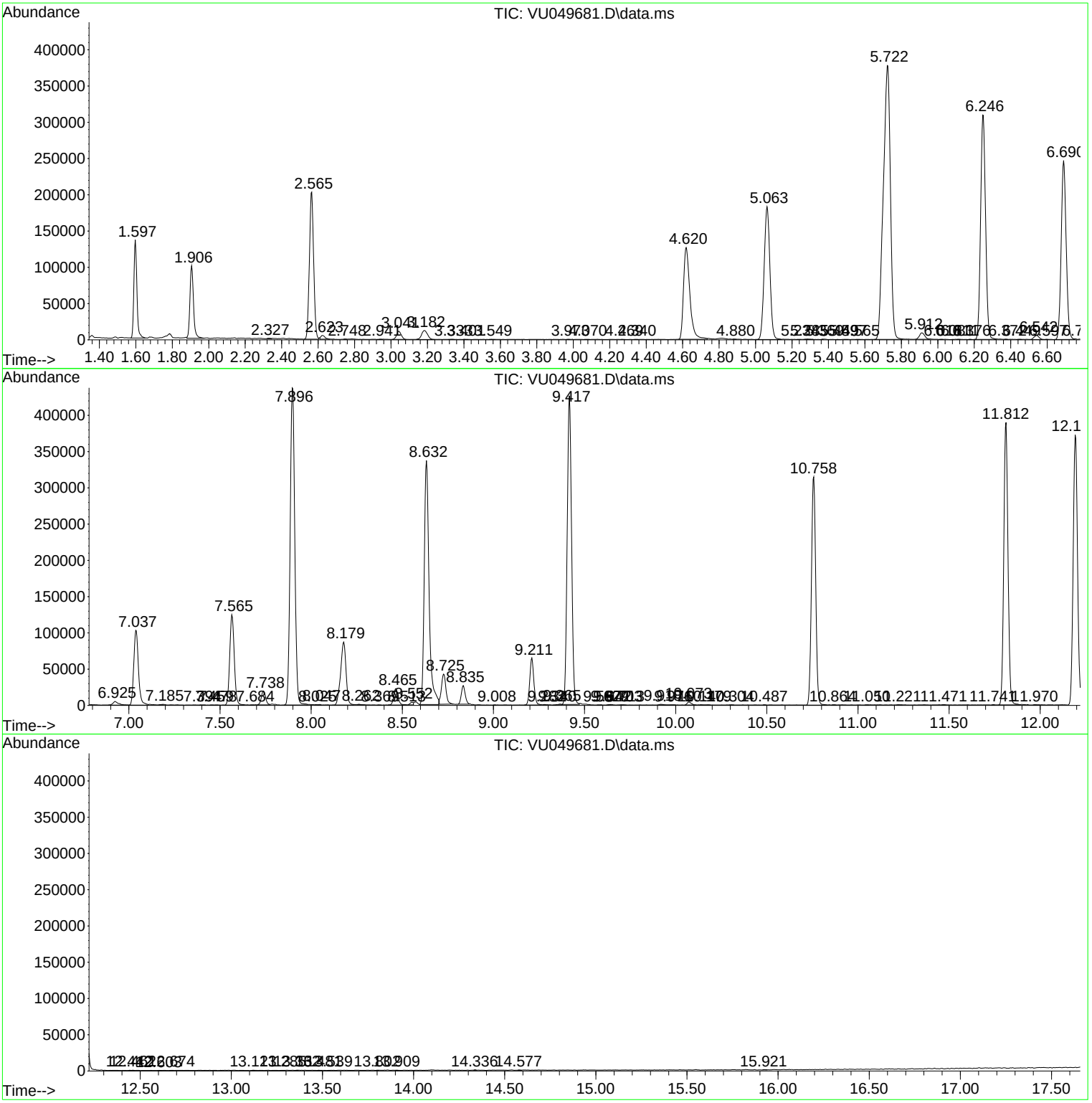
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

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\
Data File : VU049681.D
Acq On : 11 Jul 2022 17:19
Operator : SY/MD
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

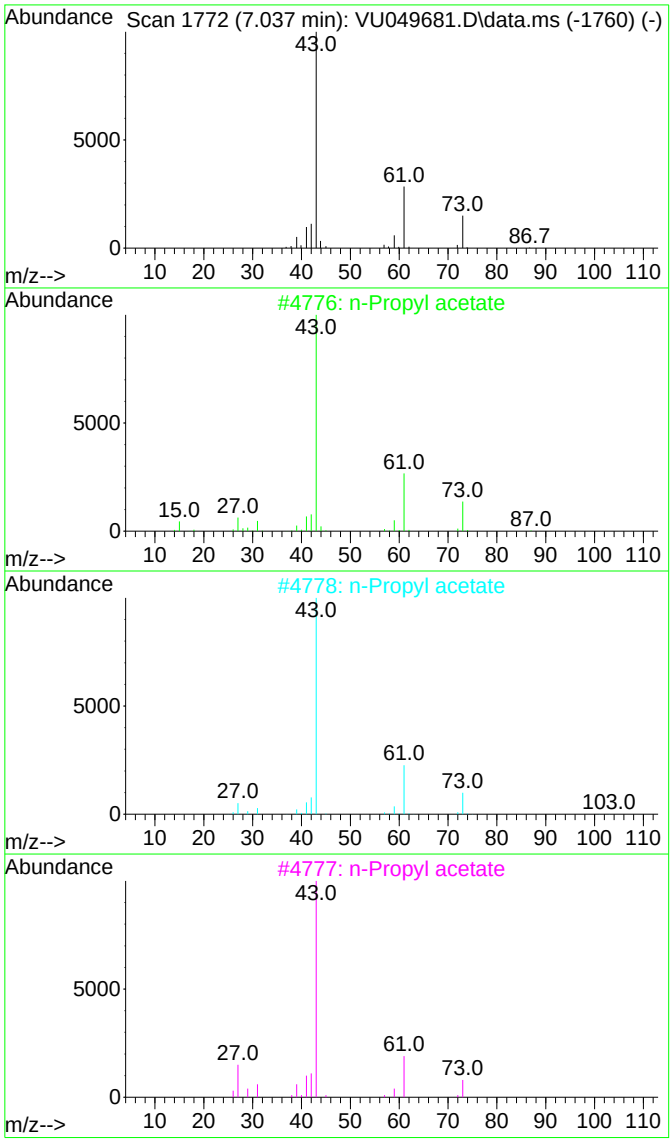
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

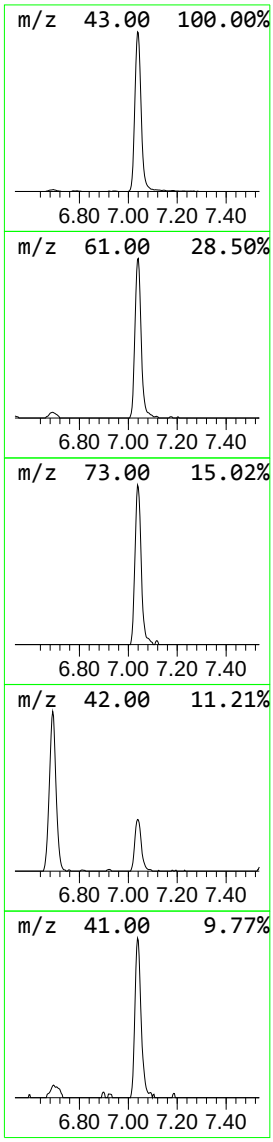
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.037	15.58 ug/L	183301	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	78
5	n-Propyl acetate	102	C5H10O2	000109-60-4	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
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Acq On : 11 Jul 2022 17:19
Operator : SY/MD
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

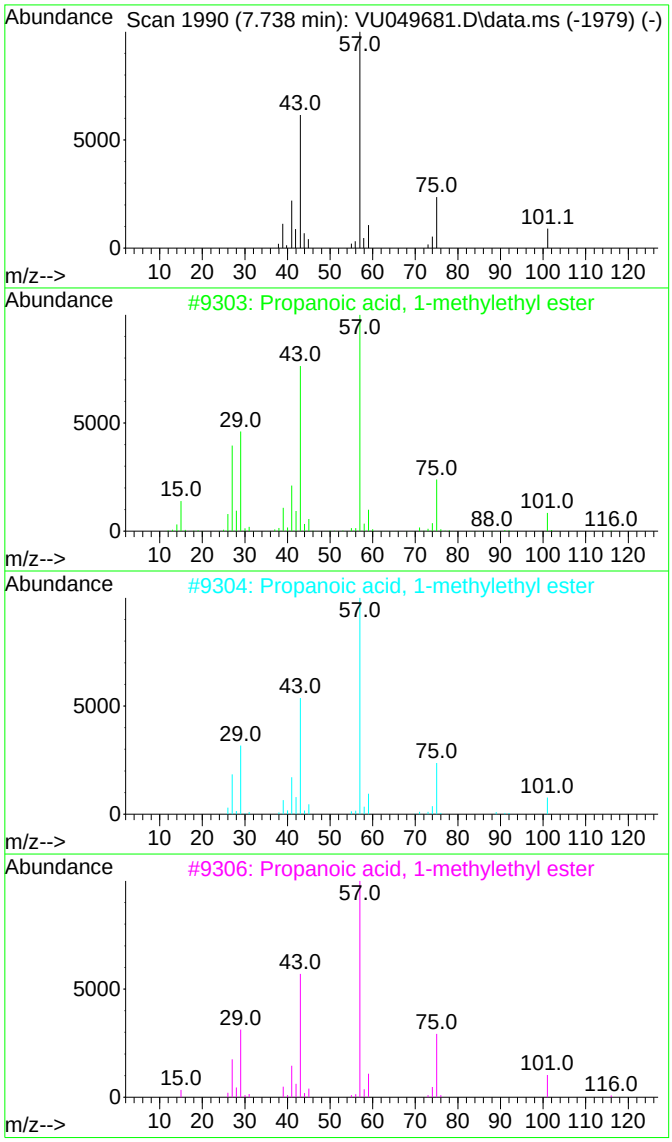
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

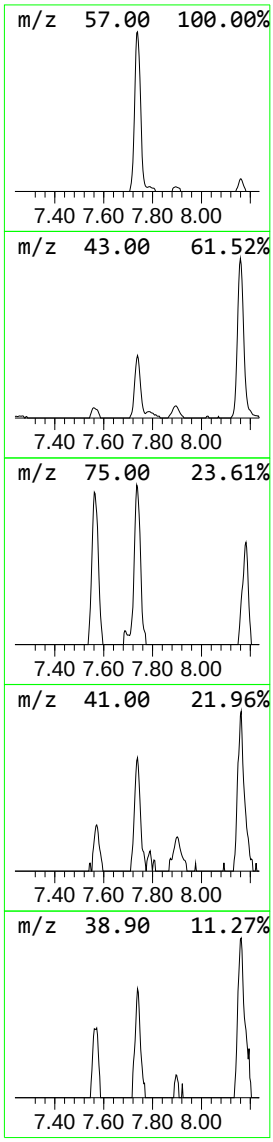
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.67 ug/L	31361	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	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	50





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Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

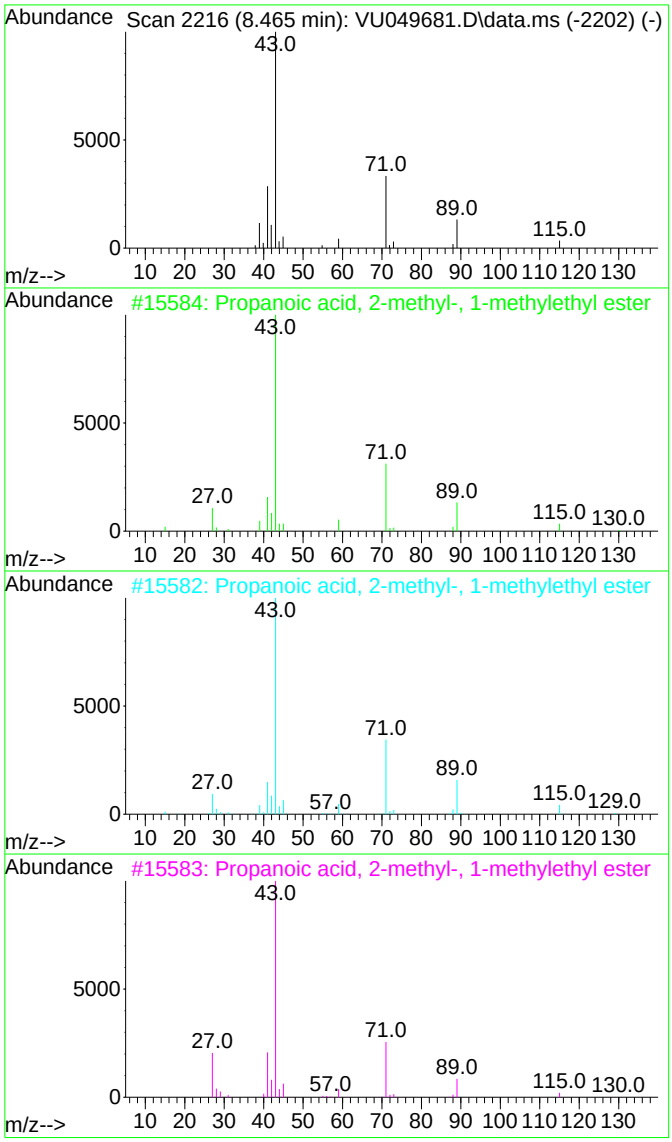
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

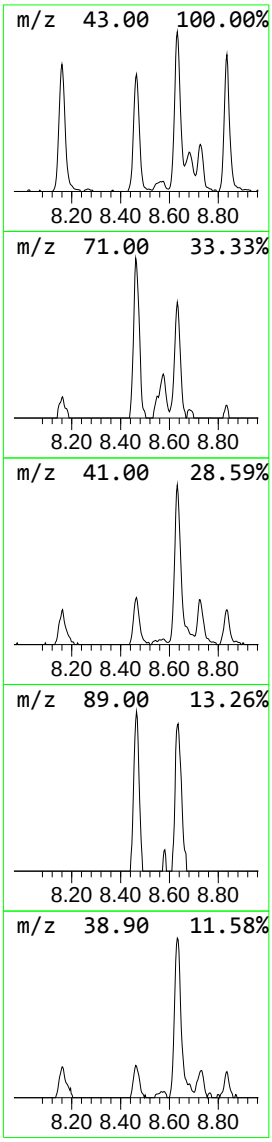
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.64 ug/L	37160	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	78
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





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Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

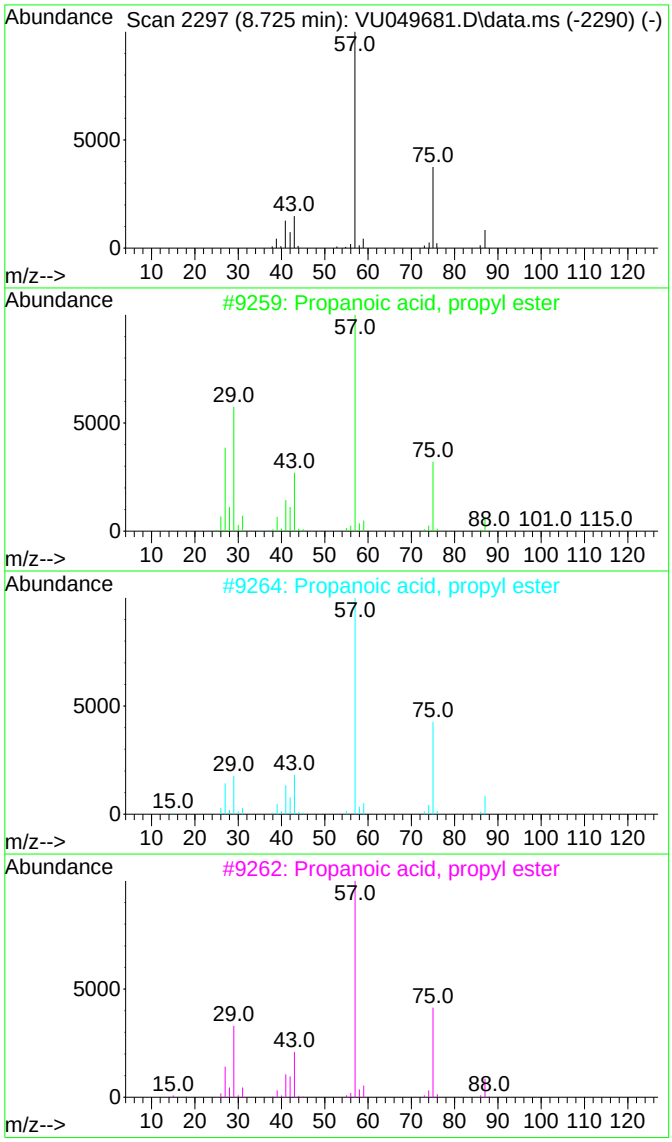
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

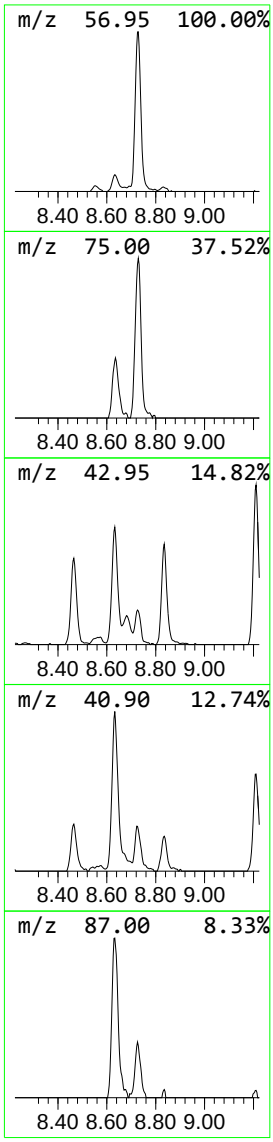
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.725	4.95 ug/L	69593	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049681.D
Acq On : 11 Jul 2022 17:19
Operator : SY/MD
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

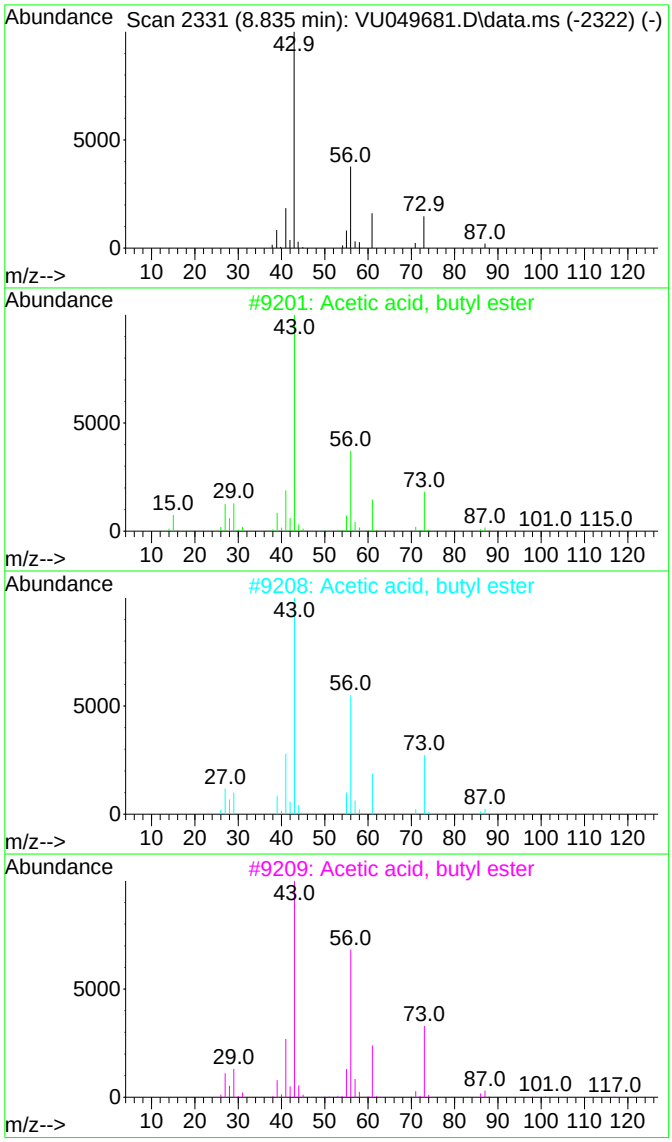
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

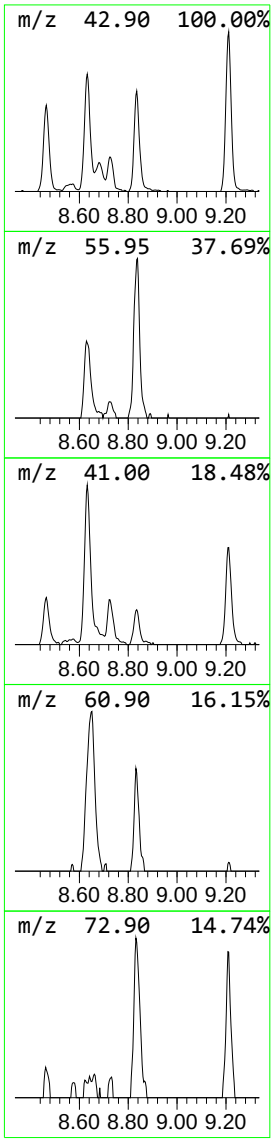
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	2.69 ug/L	37881	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	45
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	42
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049681.D
Acq On : 11 Jul 2022 17:19
Operator : SY/MD
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

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

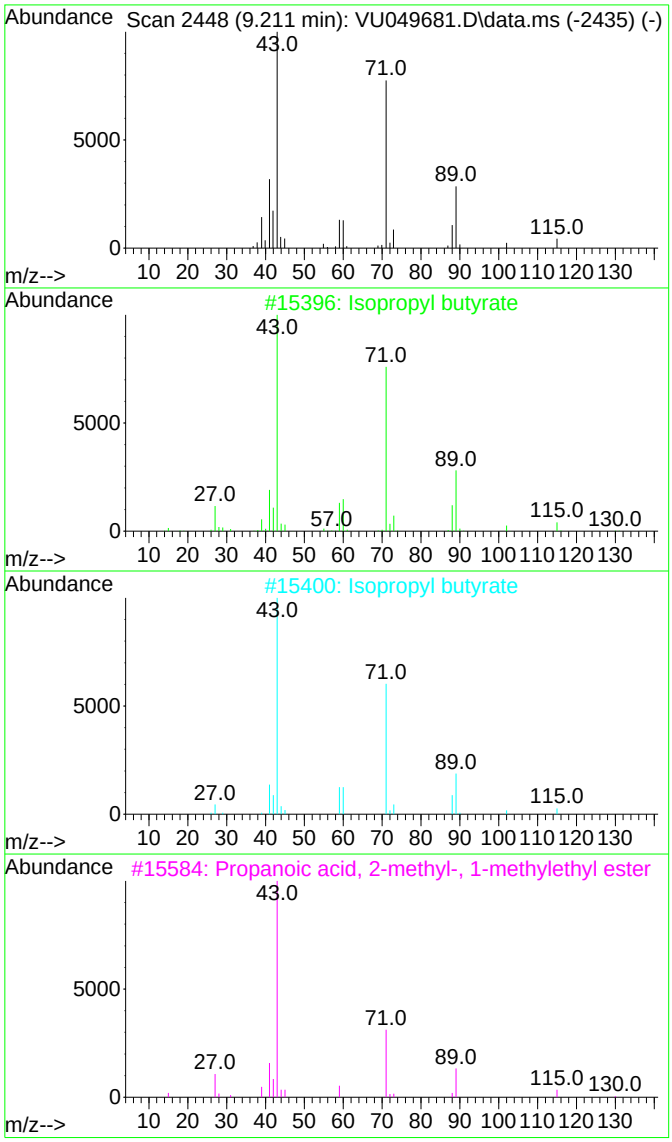
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

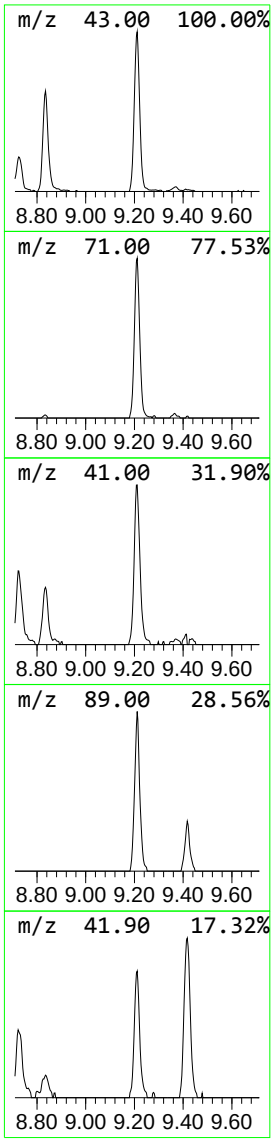
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	7.17 ug/L	100750	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	83
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4	Isopropyl butyrate	130	C7H14O2	000638-11-9	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049681.D
Acq On : 11 Jul 2022 17:19
Operator : SY/MD
Sample : N3625-06 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC2

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	7.037	15.6	ug/L	183301	1	6.250	588129	50.0
Propanoic acid,...	7.738	2.7	ug/L	31361	1	6.250	588129	50.0
Propanoic acid,...	8.465	2.6	ug/L	37160	2	9.417	702992	50.0
Propanoic acid,...	8.725	5.0	ug/L	69593	2	9.417	702992	50.0
Acetic acid, bu...	8.835	2.7	ug/L	37881	2	9.417	702992	50.0
Isopropyl butyrate	9.211	7.2	ug/L	100750	2	9.417	702992	50.0