LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049680.D
Acq On : 11 Jul 2022 16:55
Operator : SY/MD
Sample : N3625-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

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: VU049680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	11	rVB	2965	2454	0.24%	0.030%
2	1.485	41	45	50	rBV3	1953	1727	0.17%	0.021%
3	1.597	72	80	98	rBV	136309	155010	15.10%	1.919%
4	1.835	151	154	156	rBV3	1029	527	0.05%	0.007%
5	1.906	167	176	195	rVB	98337	132993	12.95%	1.646%
6	2.565	368	381	394	rBV	202783	330185	32.16%	4.088%
7	2.623	394	399	411	rVB2	4804	7973	0.78%	0.099%
8	2.684	416	418	423	rVB2	587	370	0.04%	0.005%
9	2.748	436	438	441	rBV2	341	233	0.02%	0.003%
10	2.851	467	470	474	rBV	292	190	0.02%	0.002%
11	3.044	519	530	543	rVB2	11438	20748	2.02%	0.257%
12	3.102	543	548	556	rVB2	299	406	0.04%	0.005%
13	3.182	556	573	588	rBV2	9910	21924	2.14%	0.271%
14	3.292	602	607	613	rBV2	147	234	0.02%	0.003%
15	3.829	771	774	779	rVB	399	377	0.04%	0.005%
16	3.858	779	783	785	rBV2	228	233	0.02%	0.003%
17	3.899	789	796	798	rBV2	240	232	0.02%	0.003%
18	4.237	897	901	907	rVB	308	241	0.02%	0.003%
19	4.459	965	970	973	rBV	233	203	0.02%	0.003%
20	4.552	996	999	1003	rBV3	385	278	0.03%	0.003%
21	4.620	1007	1020	1047	rBV	120914	290714	28.32%	3.599%
22	4.916	1109	1112	1115	rVB3	419	283	0.03%	0.004%
23	4.935	1115	1118	1119	rBV	343	212	0.02%	0.003%
24	4.948	1119	1122	1128	rVV2	496	555	0.05%	0.007%
25	4.977	1128	1131	1133	rVB2	295	195	0.02%	0.002%
26	4.996	1133	1137	1140	rBV2	269	207	0.02%	0.003%
27	5.063	1142	1158	1186	rVV	183714	399714	38.93%	4.948%
28	5.263	1215	1220	1223	rVB2	186	201	0.02%	0.002%
29	5.289	1223	1228	1237	rVB3	633	957	0.09%	0.012%
30	5.375	1250	1255	1263	rBV4	512	720	0.07%	0.009%
31	5.565	1310	1314	1318	rVB	277	263	0.03%	0.003%
32	5.723	1342	1363	1390	rBV2	376485	1026635	100.00%	12.710%
33	5.912	1409	1422	1436	rBV3	9181	18435	1.80%	0.228%
34	5.999	1447	1449	1453	rVB	275	184	0.02%	0.002%
35	6.186	1499	1507	1510	rBV	256	342	0.03%	0.004%
36	6.250	1513	1527	1545	rBV	311437	584409	56.92%	7.235%

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Sample : N3625-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

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	6.530	1612	1614	1616	rVV3	761	437	0.04%	0.005%
38	6.542	1616	1618	1622	rVB2	638	394	0.04%	0.005%
39	6.594	1631	1634	1636	rBV	317	182	0.02%	0.002%
40	6.690	1649	1664	1688	rBV	243886	470549	45.83%	5.825%
41	6.925	1722	1737	1753	rBV2	5430	11322	1.10%	0.140%
42	6.986	1753	1756	1760	rBV3	247	227	0.02%	0.003%
43	7.038	1760	1772	1796	rBV	87225	156309	15.23%	1.935%
44	7.153	1805	1808	1810	rBV	249	179	0.02%	0.002%
45	7.179	1812	1816	1819	rBV3	490	473	0.05%	0.006%
46	7.436	1891	1896	1901	rBV2	230	247	0.02%	0.003%
47	7.497	1910	1915	1918	rBV2	333	263	0.03%	0.003%
48	7.565	1924	1936	1952	rBV	123533	216345	21.07%	2.678%
49	7.661	1962	1966	1970	rVB2	527	437	0.04%	0.005%
50	7.697	1970	1977	1979	rBV3	704	828	0.08%	0.010%
51	7.739	1979	1990	2002	rBV2	19903	32446	3.16%	0.402%
52	7.896	2026	2039	2059	rBV	443444	767387	74.75%	9.500%
53	8.015	2073	2076	2080	rVB4	551	369	0.04%	0.005%
54	8.076	2092	2095	2099	rVB2	367	278	0.03%	0.003%
55	8.179	2109	2127	2145	rBV3	86283	163719	15.95%	2.027%
56	8.388	2186	2192	2196	rVB3	299	271	0.03%	0.003%
57	8.465	2204	2216	2231	rVB	24220	38701	3.77%	0.479%
58	8.523	2231	2234	2236	rBV2	387	198	0.02%	0.002%
59	8.562	2236	2246	2247	rBV3	2996	4255	0.41%	0.053%
60	8.632	2256	2268	2289	rBV2	333036	603091	58.74%	7.466%
61	8.726	2290	2297	2316	rVB	36246	62496	6.09%	0.774%
62	8.835	2322	2331	2347	rVB2	13083	21873	2.13%	0.271%
63	8.964	2367	2371	2374	rBV	368	287	0.03%	0.004%
64	9.092	2406	2411	2413	rBV2	214	193	0.02%	0.002%
65	9.211	2432	2448	2461	rBV2	58943	91400	8.90%	1.132%
66	9.369	2487	2497	2498	rBV2	1391	1777	0.17%	0.022%
67	9.417	2500	2512	2533	rVB	421806	693397	67.54%	8.584%
68	9.642	2576	2582	2584	rBV2	719	592	0.06%	0.007%
69	9.919	2663	2668	2669	rBV2	668	546	0.05%	0.007%
70	10.005	2690	2695	2698	rBV2	225	220	0.02%	0.003%
71	10.076	2710	2717	2727	rVB4	2030	2966	0.29%	0.037%
72	10.134	2733	2735	2742	rVB2	533	396	0.04%	0.005%
73	10.166	2742	2745	2748	rBV	277	229	0.02%	0.003%
74	10.263	2772	2775	2783	rVB2	198	246	0.02%	0.003%
75	10.295	2783	2785	2789	rBV	326	181	0.02%	0.002%
76	10.584	2871	2875	2877	rBV	237	186	0.02%	0.002%

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Acq On : 11 Jul 2022 16:55
Operator : SY/MD
Sample : N3625-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

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	10.755	2913	2928	2949	rBV	315341	505527	49.24%	6.258%
78	10.928	2979	2982	2985	rBV2	319	209	0.02%	0.003%
79	11.144	3046	3049	3056	rBV2	269	322	0.03%	0.004%
80	11.218	3068	3072	3073	rBV	275	206	0.02%	0.003%
81	11.391	3123	3126	3133	rVB2	333	329	0.03%	0.004%
82	11.517	3161	3165	3168	rBV2	221	182	0.02%	0.002%
83	11.600	3185	3191	3193	rBV2	294	338	0.03%	0.004%
84	11.690	3216	3219	3224	rBV2	462	510	0.05%	0.006%
85	11.812	3244	3257	3276	rBV	378624	602217	58.66%	7.455%
86	12.131	3353	3356	3359	rBV2	283	220	0.02%	0.003%
87	12.192	3362	3375	3398	rVV	373664	616522	60.05%	7.633%
88	12.809	3565	3567	3572	rVB2	520	389	0.04%	0.005%
89	12.861	3579	3583	3588	rBV2	304	247	0.02%	0.003%
90	13.018	3629	3632	3638	rVB2	376	362	0.04%	0.004%
91	13.584	3805	3808	3812	rBV3	404	292	0.03%	0.004%
92	13.783	3867	3870	3873	rBV2	392	238	0.02%	0.003%
93	14.031	3944	3947	3950	rVB2	476	294	0.03%	0.004%
94	14.362	4047	4050	4052	rBV2	343	250	0.02%	0.003%
95	14.394	4057	4060	4065	rBV2	381	382	0.04%	0.005%
96	14.539	4098	4105	4107	rBV3	598	709	0.07%	0.009%
97	14.983	4239	4243	4246	rBV3	492	485	0.05%	0.006%
98	15.237	4319	4322	4327	rBV	457	385	0.04%	0.005%
99	15.793	4493	4495	4497	rBV3	538	231	0.02%	0.003%
100	15.873	4518	4520	4522	rBV2	502	256	0.02%	0.003%

Sum of corrected areas: 8077558

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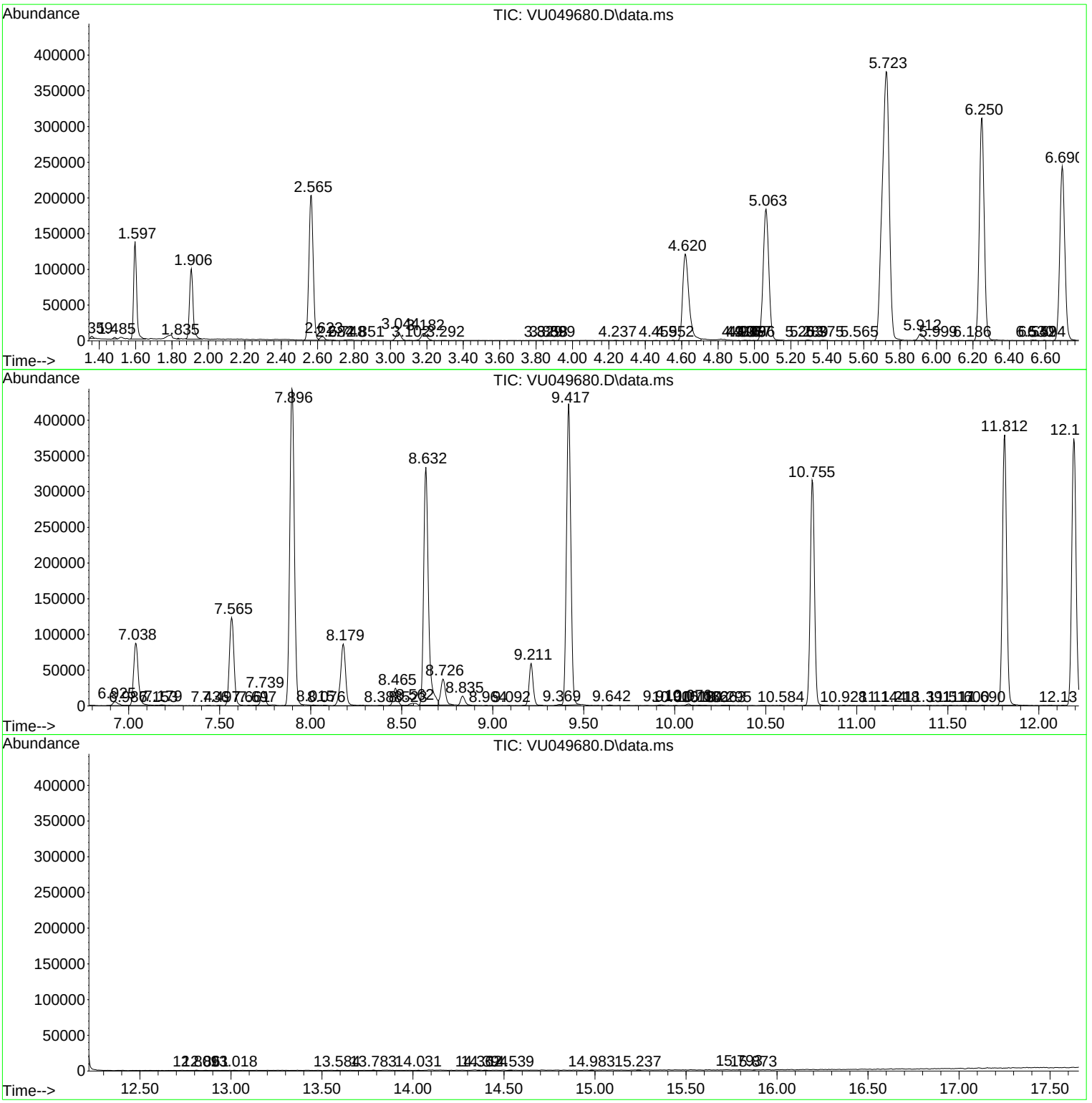
Acq On : 11 Jul 2022 16:55
Operator : SY/MD
Sample : N3625-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

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 : VU049680.D
Acq On : 11 Jul 2022 16:55
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

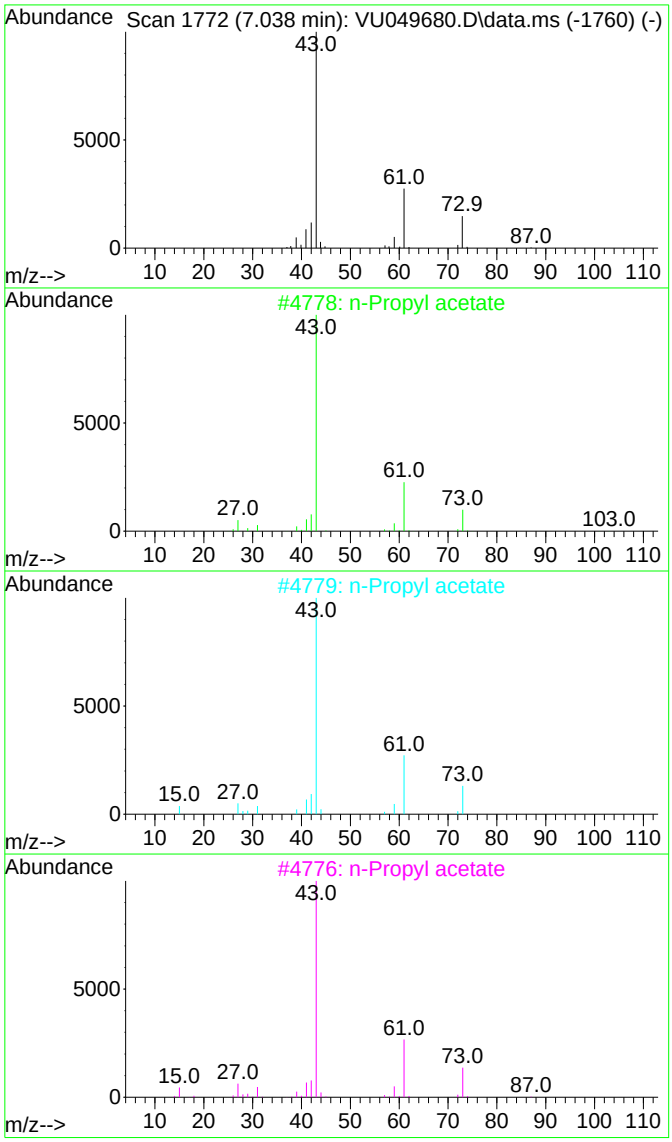
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

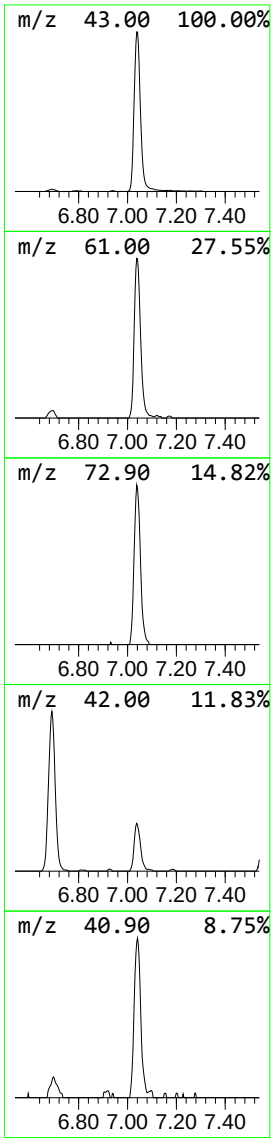
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	13.37 ug/L	156309	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	78
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_U\Data\VU071122\
Data File : VU049680.D
Acq On : 11 Jul 2022 16:55
Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

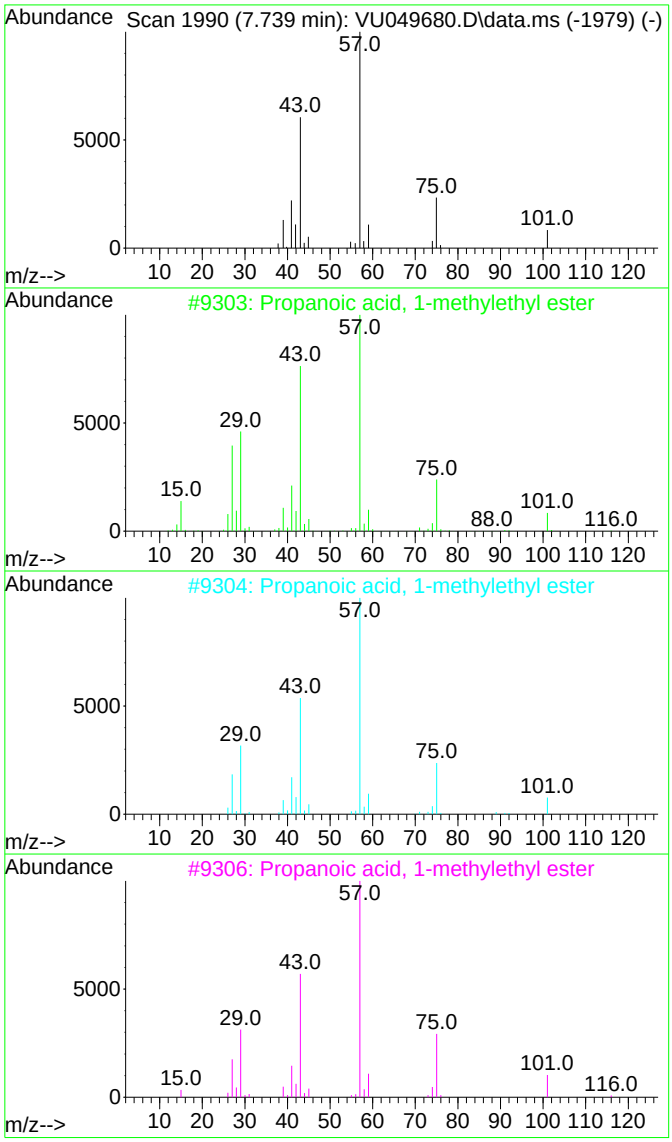
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

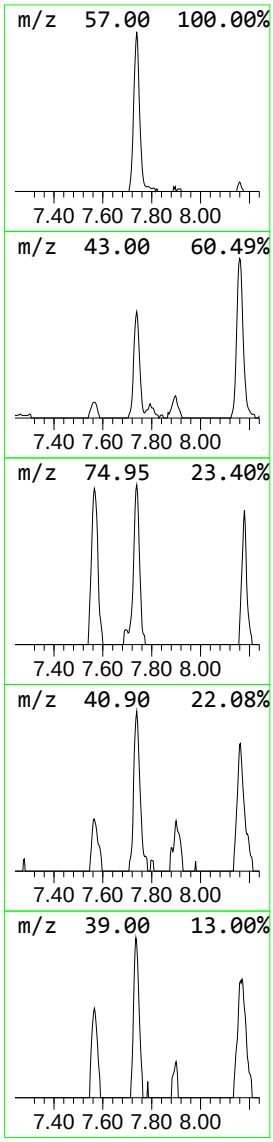
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	2.78 ug/L	32446	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	56
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	38





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Instrument :
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ClientSampleId :
C0ZC1

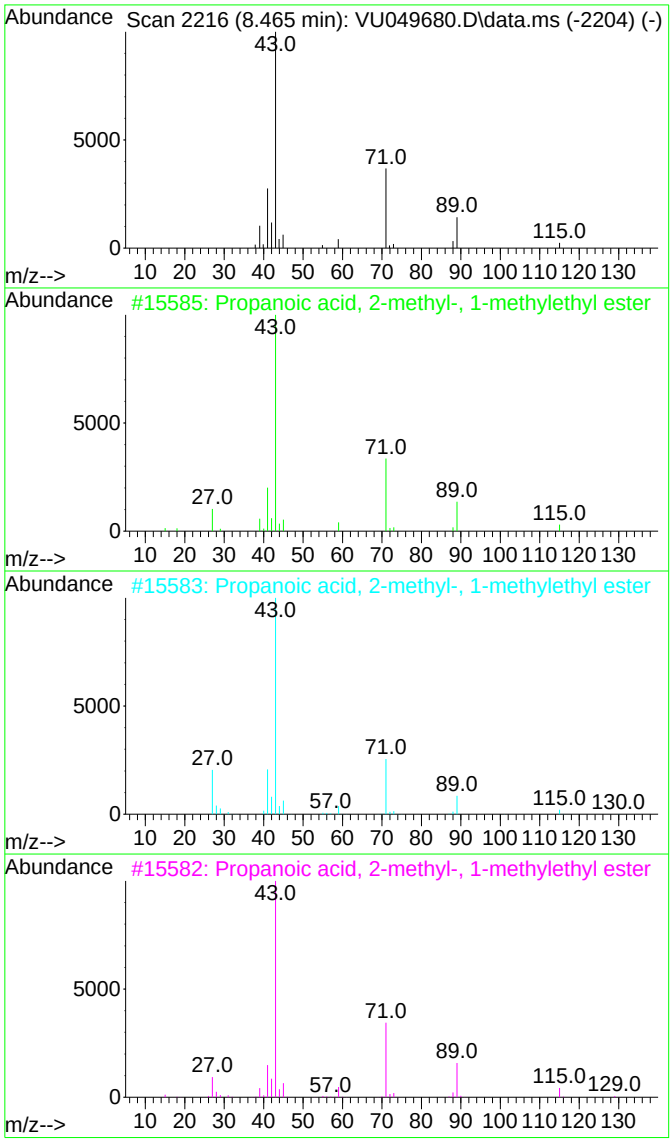
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

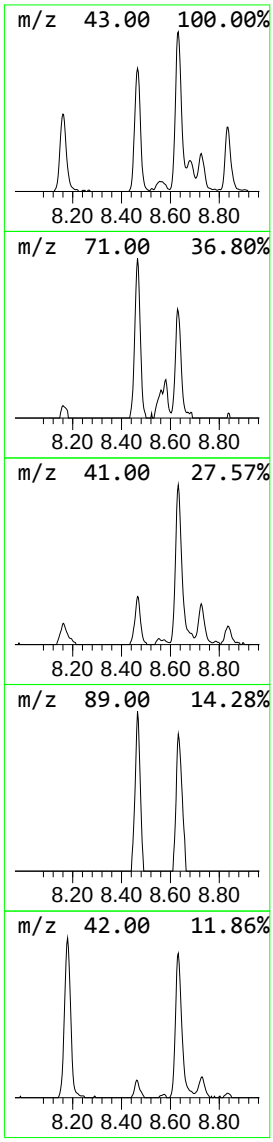
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.79 ug/L	38701	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	56
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	53





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Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

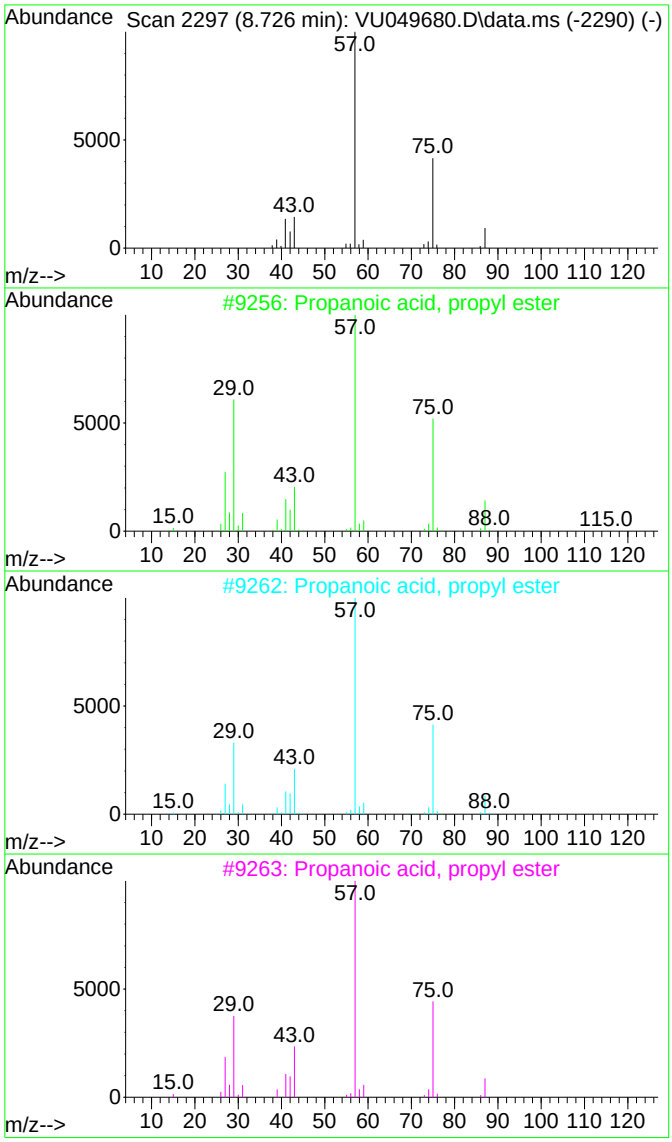
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

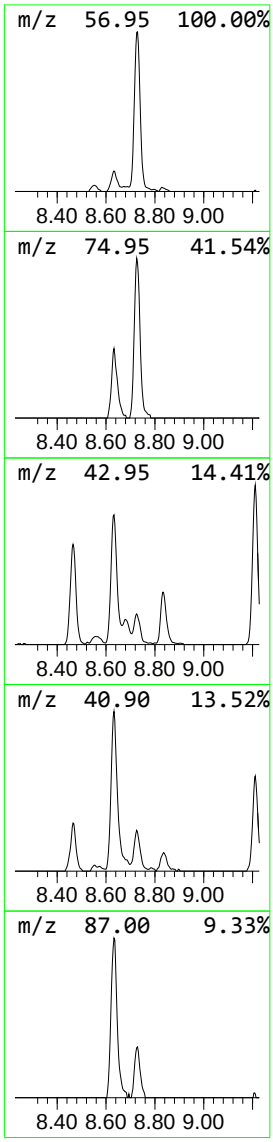
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.726	4.51 ug/L	62496	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	78
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049680.D
Acq On : 11 Jul 2022 16:55
Operator : SY/MD
Sample : N3625-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

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

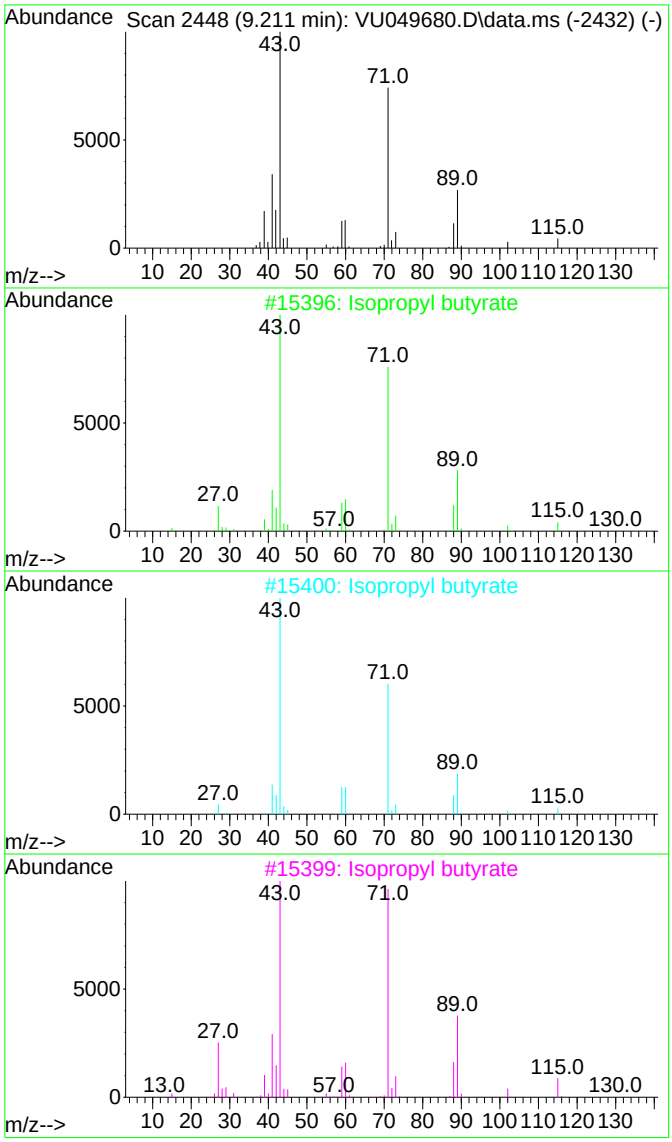
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

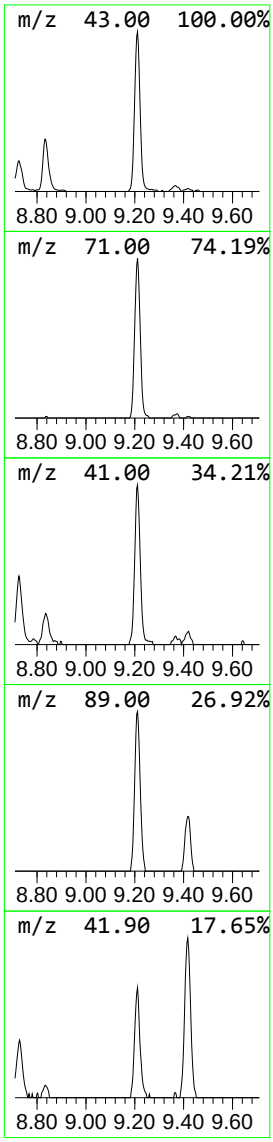
****

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	6.59 ug/L	91400	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	Isopropyl butyrate	130	C7H14O2	000638-11-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071122\
Data File : VU049680.D
Acq On : 11 Jul 2022 16:55
Operator : SY/MD
Sample : N3625-05 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0ZC1

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	13.4	ug/L	156309	1	6.250	584409	50.0
Propanoic acid,...	7.739	2.8	ug/L	32446	1	6.250	584409	50.0
Propanoic acid,...	8.465	2.8	ug/L	38701	2	9.417	693397	50.0
Propanoic acid,...	8.726	4.5	ug/L	62496	2	9.417	693397	50.0
Isopropyl butyrate	9.211	6.6	ug/L	91400	2	9.417	693397	50.0