LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049354.D
Acq On : 22 Jun 2022 16:09
Operator : SY/MD
Sample : N3392-08 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

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: VU049354.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	68641	76298	10.10%	1.071%
2	1.909	171	177	192	rVB	60507	78294	10.36%	1.099%
3	2.565	370	381	396	rBV	120062	190296	25.18%	2.671%
4	2.636	396	403	417	rVB	6078	11245	1.49%	0.158%
5	2.732	430	433	434	rBV	243	151	0.02%	0.002%
6	3.044	522	530	545	rVB4	3481	6233	0.82%	0.087%
7	3.118	550	553	555	rBV	234	193	0.03%	0.003%
8	3.186	559	574	589	rBV	16320	38058	5.04%	0.534%
9	3.346	621	624	627	rVB2	214	135	0.02%	0.002%
10	3.462	657	660	662	rBV2	274	150	0.02%	0.002%
11	3.578	687	696	712	rVB4	1458	3632	0.48%	0.051%
12	3.678	723	727	731	rBV2	297	279	0.04%	0.004%
13	3.745	744	748	749	rBV2	225	144	0.02%	0.002%
14	3.787	758	761	767	rVB2	238	231	0.03%	0.003%
15	3.819	767	771	775	rBV2	345	342	0.05%	0.005%
16	3.915	799	801	806	rBV	233	195	0.03%	0.003%
17	4.089	849	855	858	rBV2	339	262	0.03%	0.004%
18	4.141	869	871	875	rVB2	348	208	0.03%	0.003%
19	4.256	904	907	912	rBV2	309	229	0.03%	0.003%
20	4.308	916	923	925	rBV2	295	334	0.04%	0.005%
21	4.414	953	956	959	rBV	180	149	0.02%	0.002%
22	4.462	968	971	973	rBV	161	129	0.02%	0.002%
23	4.517	985	988	991	rVB2	339	208	0.03%	0.003%
24	4.539	991	995	997	rBV	199	127	0.02%	0.002%
25	4.555	997	1000	1001	rBV	342	211	0.03%	0.003%
26	4.626	1009	1022	1054	rBV2	126744	334580	44.27%	4.696%
27	4.906	1107	1109	1112	rBV4	389	276	0.04%	0.004%
28	5.063	1142	1158	1178	rBV	147649	321905	42.60%	4.518%
29	5.182	1193	1195	1198	rBV2	300	144	0.02%	0.002%
30	5.202	1199	1201	1210	rVB3	284	268	0.04%	0.004%
31	5.243	1210	1214	1216	rBV	203	143	0.02%	0.002%
32	5.285	1224	1227	1230	rBV3	269	217	0.03%	0.003%
33	5.362	1246	1251	1253	rBV	185	135	0.02%	0.002%
34	5.507	1293	1296	1301	rBV	225	181	0.02%	0.003%
35	5.607	1323	1327	1330	rVV2	315	265	0.04%	0.004%
36	5.726	1342	1364	1393	rBV2	272769	755708	100.00%	10.607%

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

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	5.874	1407	1410	1412	rVB2	435	259	0.03%	0.004%
38	5.915	1412	1423	1434	rBV3	8162	16631	2.20%	0.233%
39	6.050	1462	1465	1467	rBV	178	129	0.02%	0.002%
40	6.111	1482	1484	1486	rBV	213	147	0.02%	0.002%
41	6.250	1514	1527	1545	rBV	295408	559185	73.99%	7.849%
42	6.690	1650	1664	1684	rBV	196179	380723	50.38%	5.344%
43	6.780	1690	1692	1696	rVB4	454	319	0.04%	0.004%
44	6.851	1710	1714	1716	rBV3	343	261	0.03%	0.004%
45	6.922	1730	1736	1753	rVB2	3982	8281	1.10%	0.116%
46	7.041	1761	1773	1796	rBV	107416	197455	26.13%	2.771%
47	7.362	1871	1873	1879	rVB3	208	159	0.02%	0.002%
48	7.391	1880	1882	1886	rVB2	344	176	0.02%	0.002%
49	7.459	1899	1903	1905	rBV3	206	194	0.03%	0.003%
50	7.565	1924	1936	1958	rVB	106555	184061	24.36%	2.583%
51	7.639	1958	1959	1962	rBV	313	180	0.02%	0.003%
52	7.738	1981	1990	2002	rBV2	18603	30934	4.09%	0.434%
53	7.896	2026	2039	2059	rBV	319782	552610	73.12%	7.756%
54	8.108	2102	2105	2107	rBV	283	167	0.02%	0.002%
55	8.179	2112	2127	2144	rBV2	76168	152693	20.21%	2.143%
56	8.359	2181	2183	2184	rBV2	396	163	0.02%	0.002%
57	8.423	2198	2203	2206	rVV2	497	553	0.07%	0.008%
58	8.465	2206	2216	2231	rVB2	21457	35292	4.67%	0.495%
59	8.574	2236	2250	2257	rVV7	5233	10800	1.43%	0.152%
60	8.632	2257	2268	2289	rVV	334689	629687	83.32%	8.838%
61	8.729	2291	2298	2320	rVV	67883	113002	14.95%	1.586%
62	8.835	2323	2331	2344	rVB	24535	39153	5.18%	0.550%
63	9.005	2381	2384	2388	rBV2	270	232	0.03%	0.003%
64	9.092	2408	2411	2414	rBV2	261	226	0.03%	0.003%
65	9.211	2434	2448	2467	rBV	75067	120365	15.93%	1.689%
66	9.369	2489	2497	2499	rBV2	1265	1724	0.23%	0.024%
67	9.417	2500	2512	2535	rVV	400225	664983	87.99%	9.334%
68	9.571	2558	2560	2563	rBV	389	191	0.03%	0.003%
69	9.645	2575	2583	2585	rBV	669	928	0.12%	0.013%
70	9.690	2595	2597	2599	rBV2	315	179	0.02%	0.003%
71	9.732	2605	2610	2616	rBV2	381	525	0.07%	0.007%
72	9.780	2621	2625	2627	rBV2	214	136	0.02%	0.002%
73	9.925	2663	2670	2682	rVB4	771	1464	0.19%	0.021%
74	10.076	2709	2717	2729	rVB4	3700	5822	0.77%	0.082%
75	10.150	2736	2740	2744	rBV2	295	279	0.04%	0.004%
76	10.188	2749	2752	2757	rVB2	311	223	0.03%	0.003%

LSC Area Percent Report

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Operator : SY/MD
Sample : N3392-08 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

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	10.243	2766	2769	2770	rBV	266	148	0.02%	0.002%
78	10.307	2787	2789	2792	rBV2	254	173	0.02%	0.002%
79	10.533	2856	2859	2862	rVB	263	146	0.02%	0.002%
80	10.565	2862	2869	2870	rBV	321	369	0.05%	0.005%
81	10.693	2904	2909	2912	rBV3	321	304	0.04%	0.004%
82	10.754	2916	2928	2945	rBV	304212	485686	64.27%	6.817%
83	10.960	2989	2992	2995	rBV2	180	174	0.02%	0.002%
84	11.063	3021	3024	3026	rBV3	201	139	0.02%	0.002%
85	11.092	3030	3033	3034	rBV2	281	166	0.02%	0.002%
86	11.118	3039	3041	3045	rBB	270	139	0.02%	0.002%
87	11.288	3085	3094	3098	rBV2	420	568	0.08%	0.008%
88	11.375	3118	3121	3125	rVB3	299	208	0.03%	0.003%
89	11.423	3132	3136	3139	rBV2	251	179	0.02%	0.003%
90	11.729	3228	3231	3236	rBV3	375	300	0.04%	0.004%
91	11.812	3245	3257	3272	rBV	369783	587679	77.77%	8.249%
92	12.192	3362	3375	3392	rBV	316468	513844	68.00%	7.212%
93	12.317	3410	3414	3416	rBV2	528	343	0.05%	0.005%
94	12.864	3581	3584	3586	rBV2	244	155	0.02%	0.002%
95	12.928	3601	3604	3609	rVB	498	405	0.05%	0.006%
96	13.057	3642	3644	3648	rVB	332	170	0.02%	0.002%
97	13.214	3689	3693	3697	rBV2	328	291	0.04%	0.004%
98	13.413	3753	3755	3757	rBV	328	152	0.02%	0.002%
99	13.947	3918	3921	3928	rBV3	485	522	0.07%	0.007%
100	14.465	4080	4082	4085	rBV	362	231	0.03%	0.003%

Sum of corrected areas: 7124537

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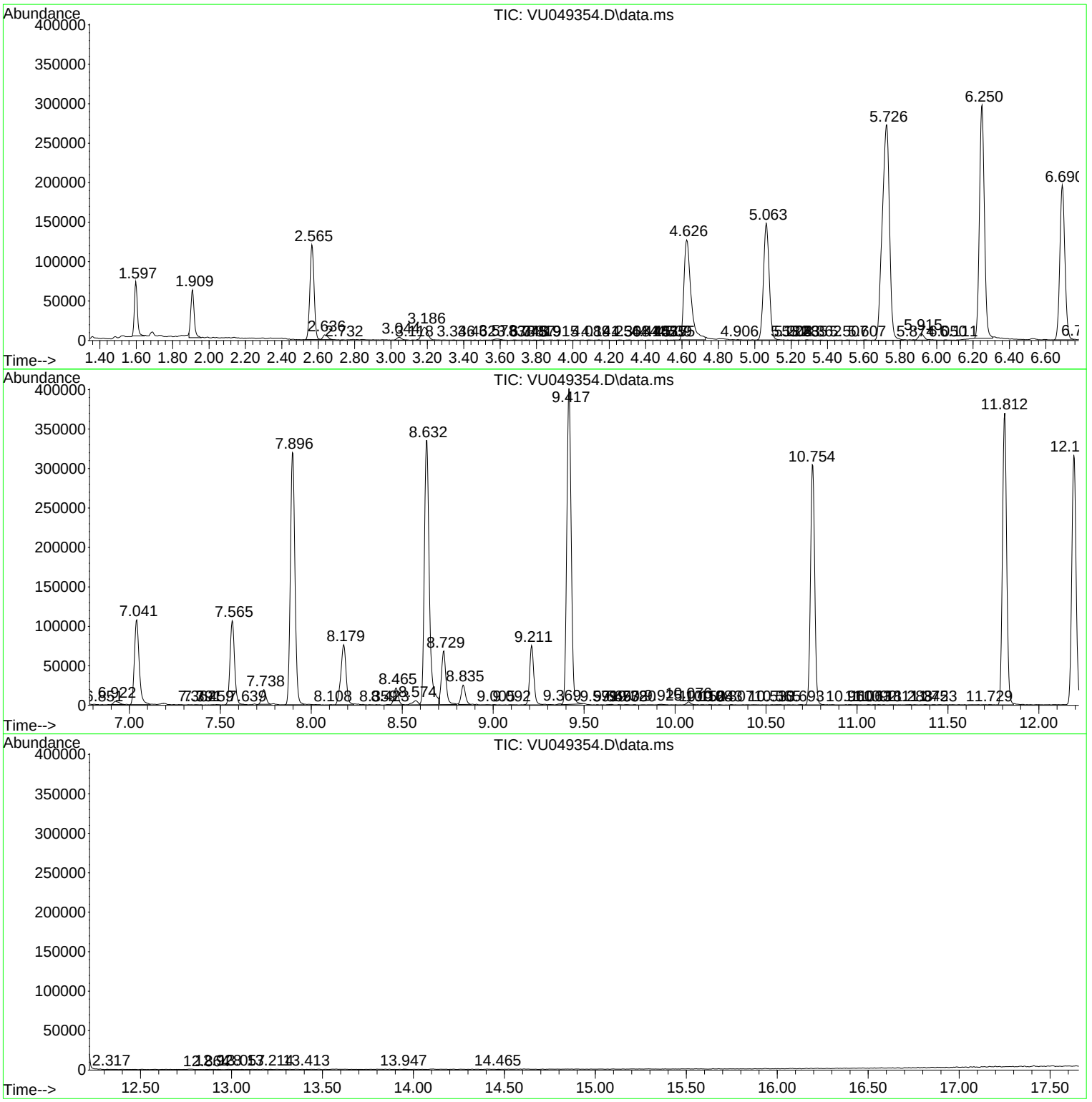
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

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



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Acq On : 22 Jun 2022 16:09
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Instrument :
MSVOA_U
ClientSampleId :
EXEY3

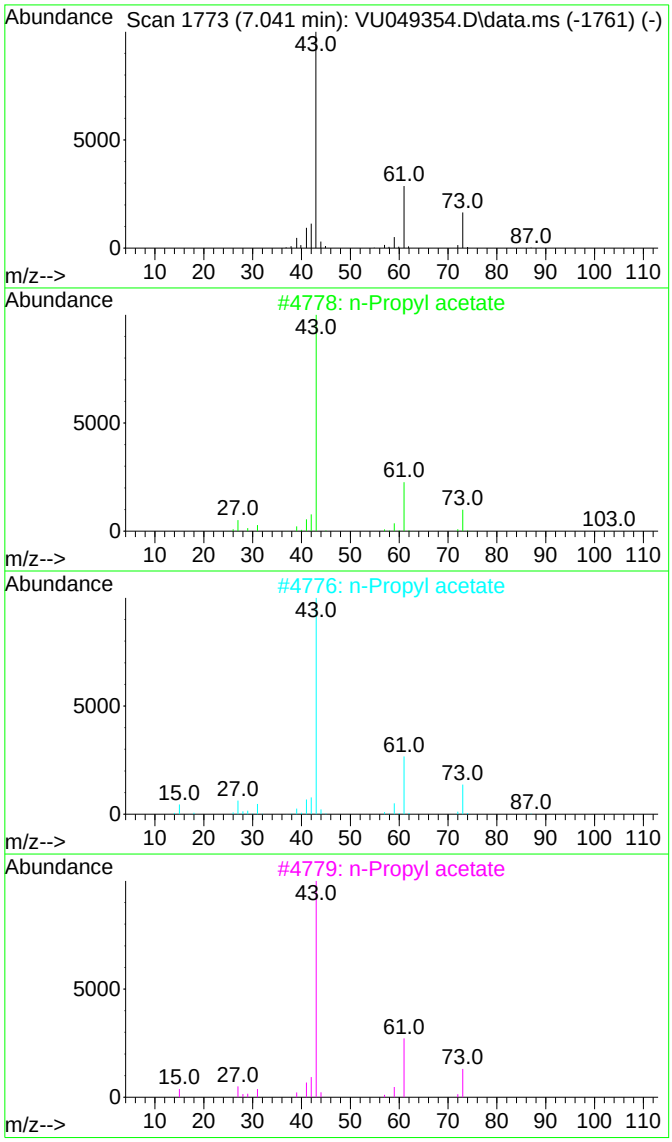
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

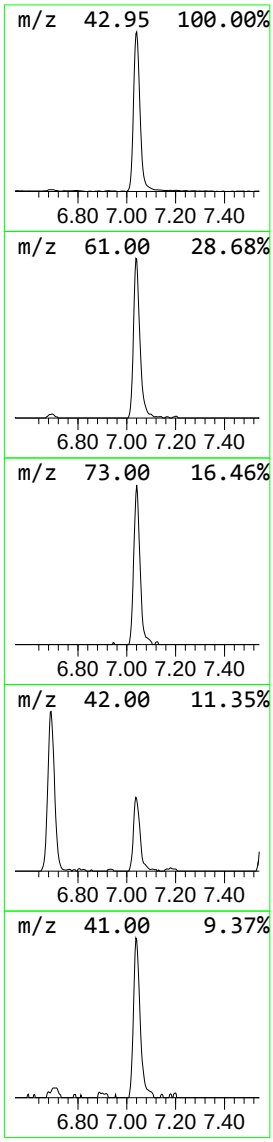
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	17.66 ug/L	197455	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





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Data File : VU049354.D
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Operator : SY/MD
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

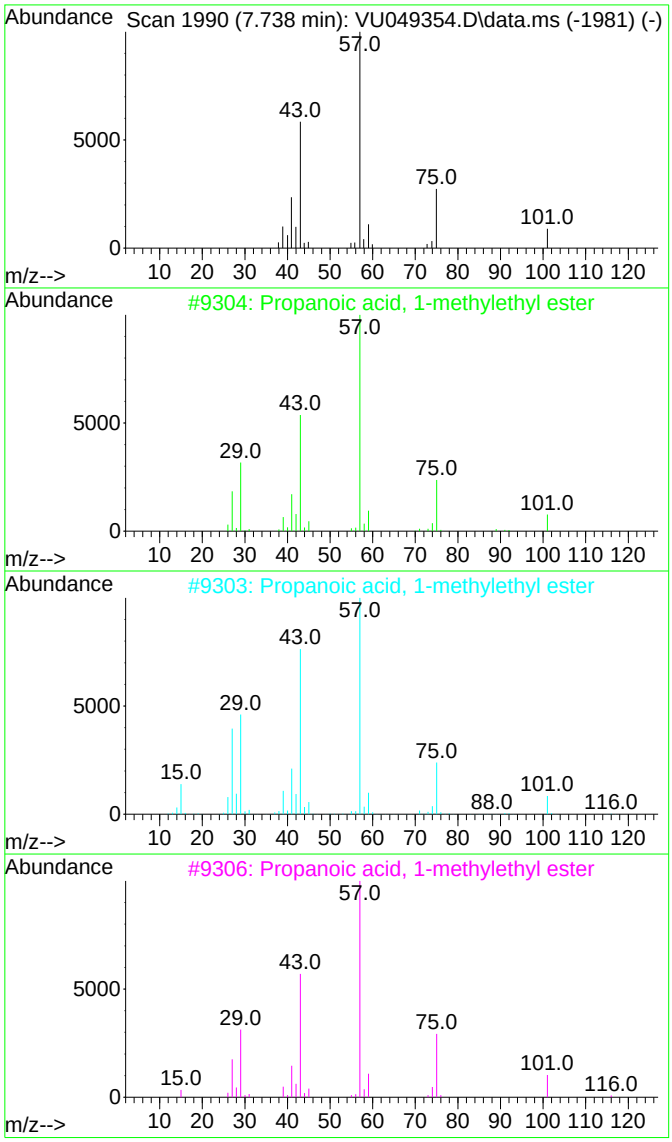
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

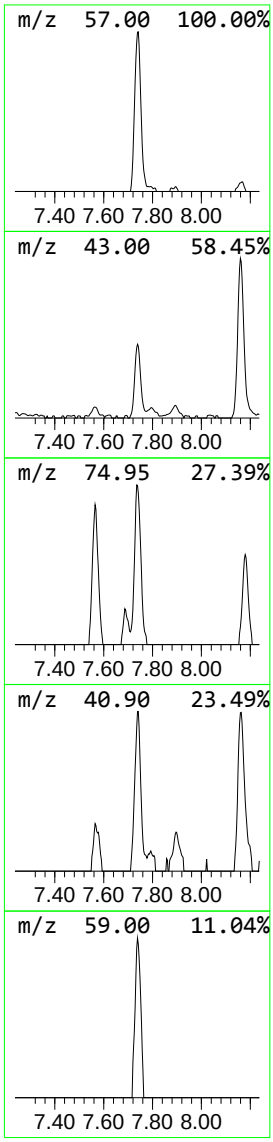
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.738	2.77 ug/L	30934	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	56
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	38





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MSVOA_U
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EXEY3

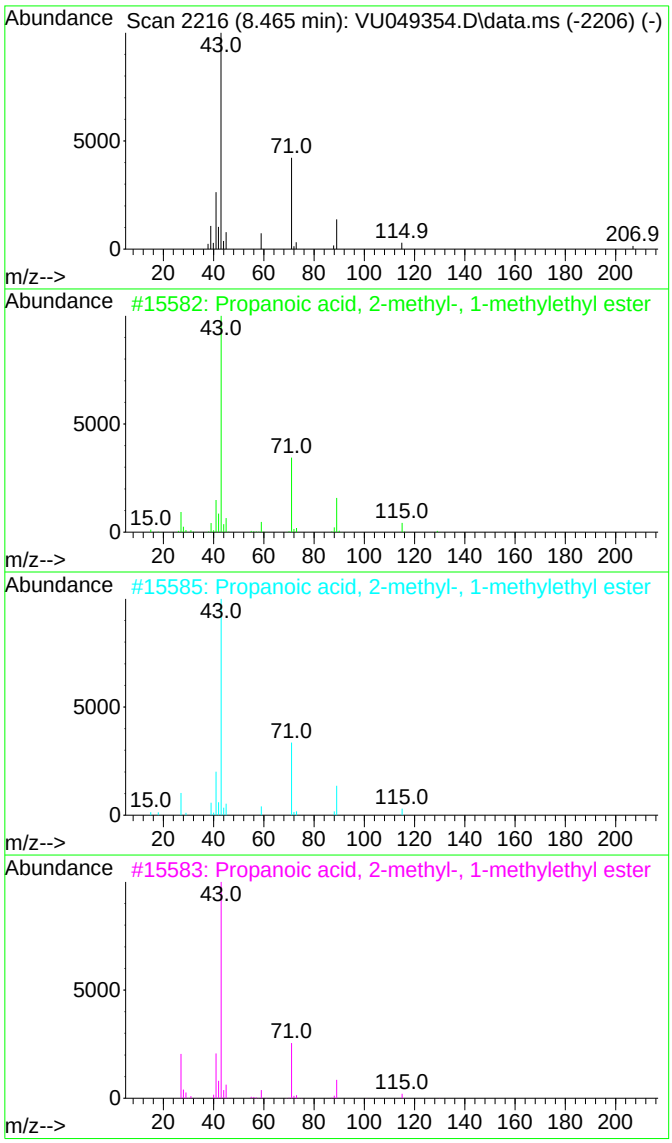
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

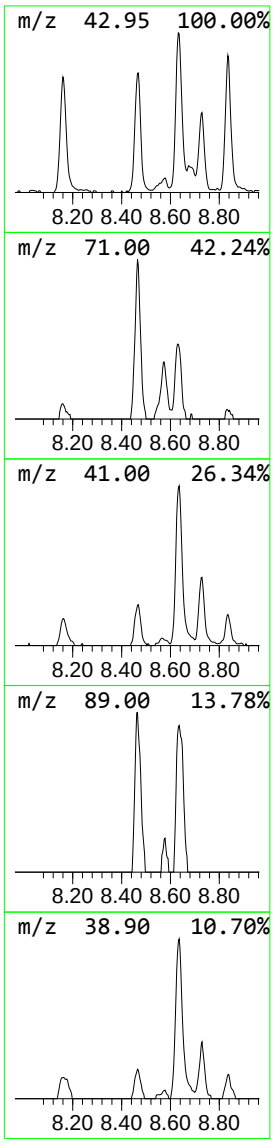
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.465	2.65 ug/L	35292	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	59
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





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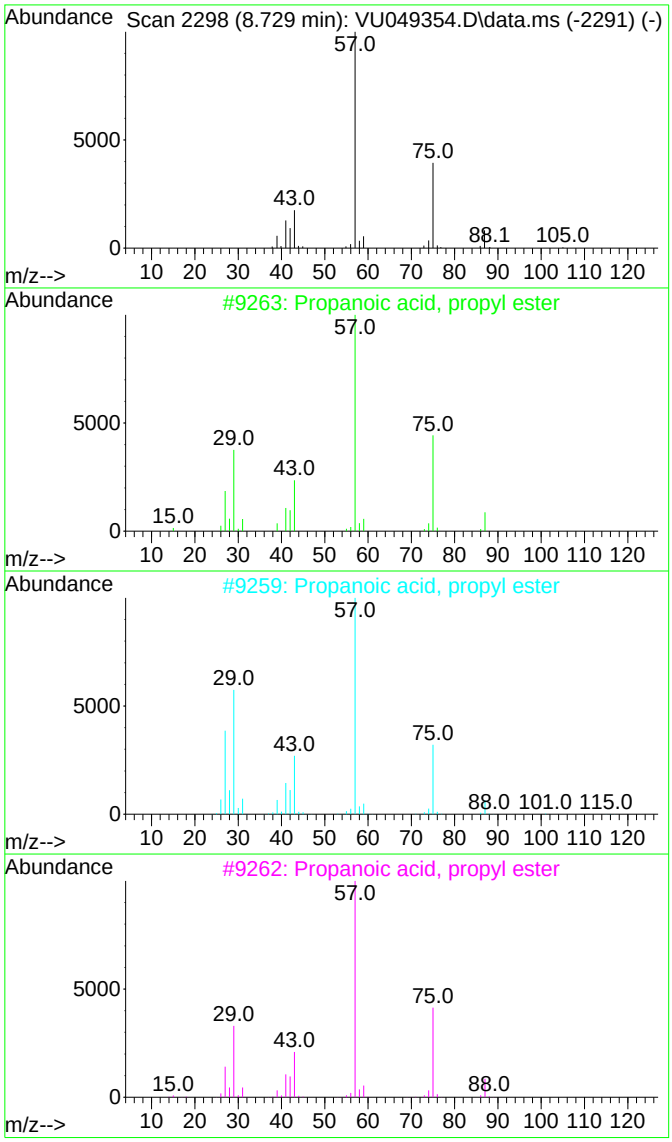
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

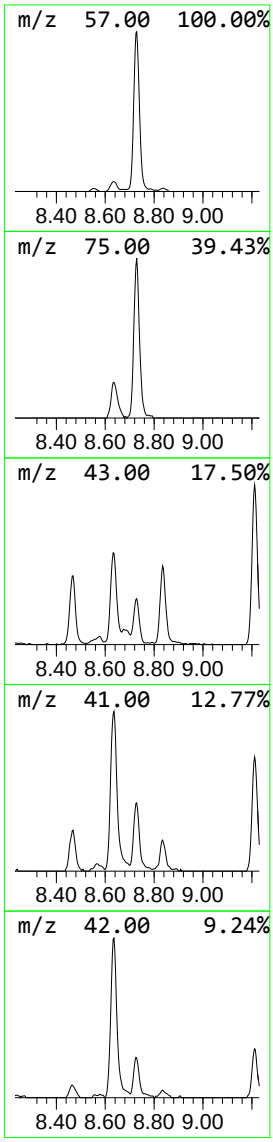
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	8.50 ug/L	113002	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	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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Data File : VU049354.D
Acq On : 22 Jun 2022 16:09
Operator : SY/MD
Sample : N3392-08 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

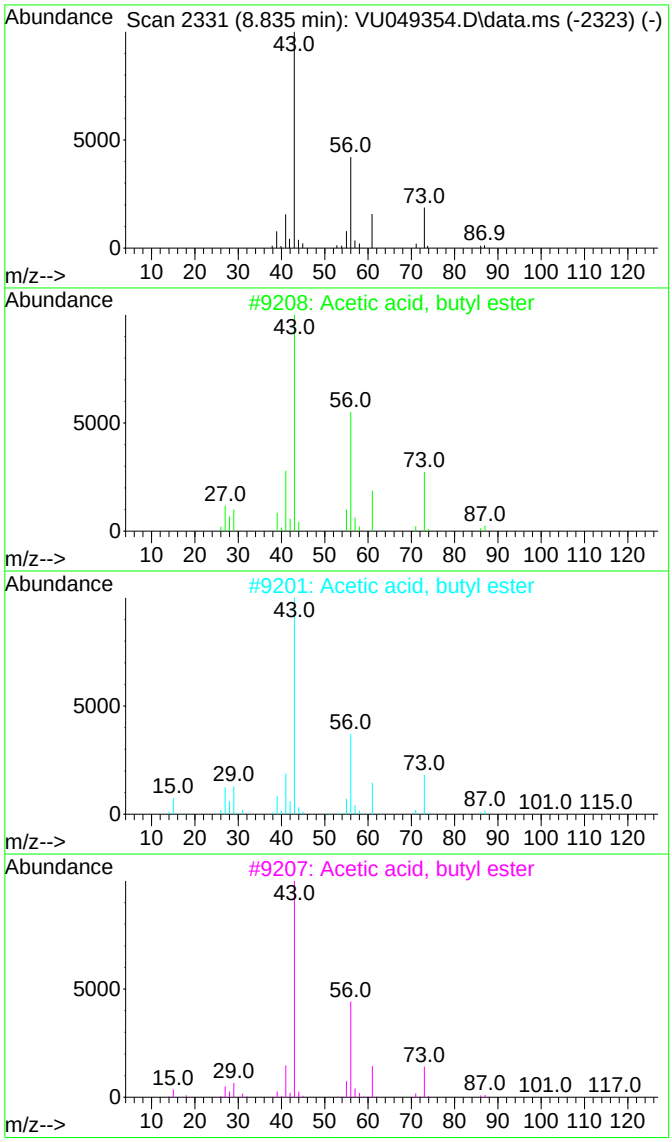
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

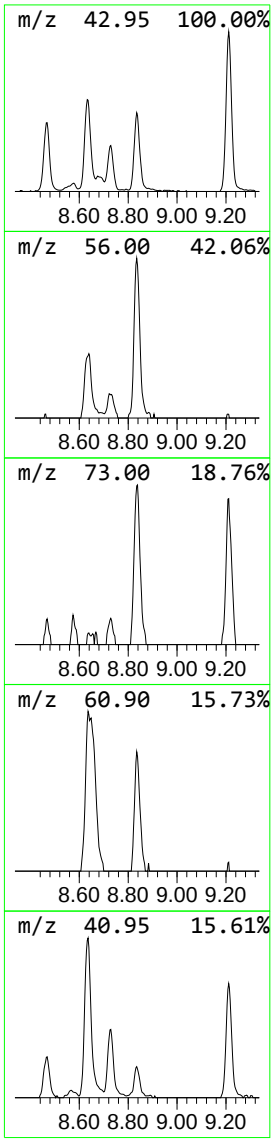
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	2.94 ug/L	39153	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049354.D
Acq On : 22 Jun 2022 16:09
Operator : SY/MD
Sample : N3392-08 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

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

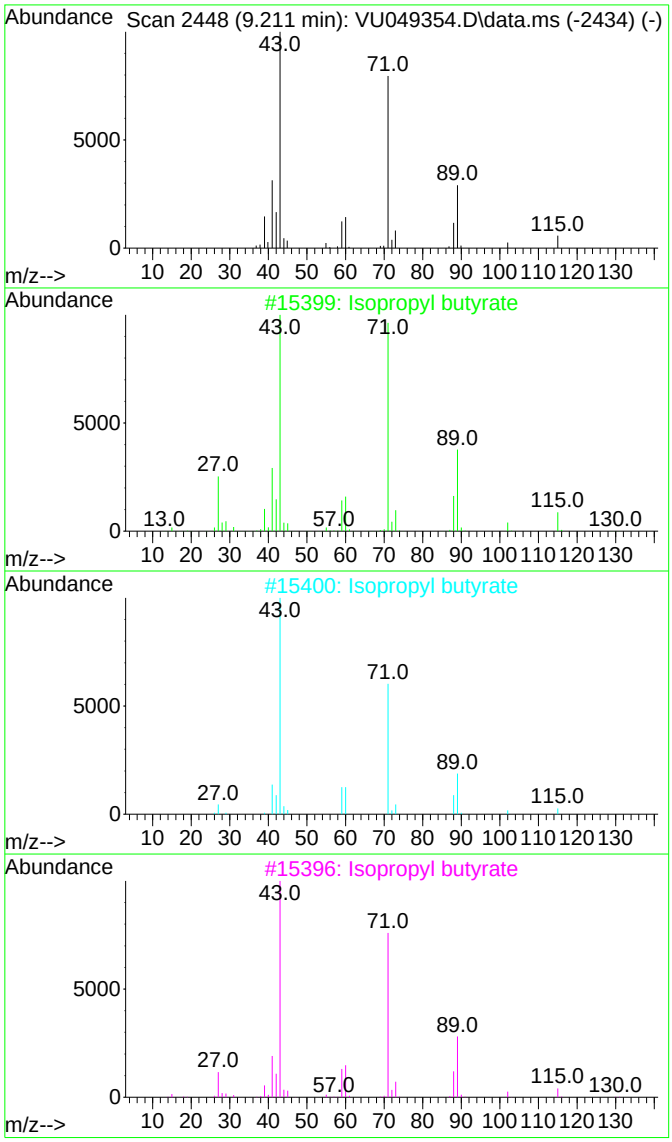
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

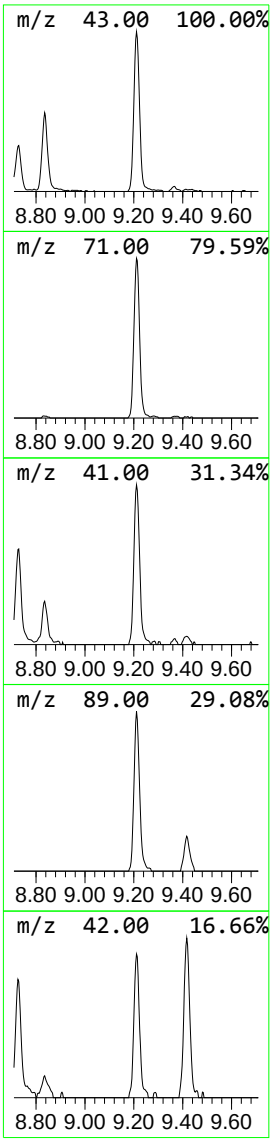
****

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	9.05 ug/L	120365	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062222\
Data File : VU049354.D
Acq On : 22 Jun 2022 16:09
Operator : SY/MD
Sample : N3392-08 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEY3

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	7.041	17.7	ug/L	197455	1	6.250	559185	50.0
Propanoic acid,...	7.738	2.8	ug/L	30934	1	6.250	559185	50.0
Propanoic acid,...	8.465	2.6	ug/L	35292	2	9.417	664983	50.0
Propanoic acid,...	8.729	8.5	ug/L	113002	2	9.417	664983	50.0
Acetic acid, bu...	8.835	2.9	ug/L	39153	2	9.417	664983	50.0
Isopropyl butyrate	9.211	9.1	ug/L	120365	2	9.417	664983	50.0