LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

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\SFAMVLM082323WMA.M
Title : VOC Analysis

Signal : TIC: VV032116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	88	rVB	135460	140748	15.43%	1.956%
2	1.532	146	153	168	rVB	109571	129065	14.15%	1.793%
3	2.060	308	317	328	rBV	206048	295557	32.41%	4.107%
4	2.449	429	438	451	rBV2	8652	15056	1.65%	0.209%
5	2.552	465	470	471	rBV2	773	655	0.07%	0.009%
6	2.693	512	514	517	rBV	370	255	0.03%	0.004%
7	2.744	525	530	531	rBV2	292	206	0.02%	0.003%
8	2.944	590	592	595	rBV2	222	126	0.01%	0.002%
9	2.963	595	598	601	rVV3	467	266	0.03%	0.004%
10	2.986	602	605	610	rVB2	365	277	0.03%	0.004%
11	3.031	615	619	622	rBV	200	144	0.02%	0.002%
12	3.060	622	628	631	rBV	159	171	0.02%	0.002%
13	3.121	645	647	651	rBV3	322	279	0.03%	0.004%
14	3.140	651	653	657	rVB2	553	336	0.04%	0.005%
15	3.159	657	659	664	rVB	479	342	0.04%	0.005%
16	3.185	664	667	670	rVB2	397	301	0.03%	0.004%
17	3.211	670	675	677	rBV2	128	127	0.01%	0.002%
18	3.249	685	687	689	rVB	233	98	0.01%	0.001%
19	3.265	689	692	695	rBV2	498	277	0.03%	0.004%
20	3.291	695	700	702	rBV2	220	135	0.01%	0.002%
21	3.416	737	739	744	rVB2	270	132	0.01%	0.002%
22	3.449	744	749	752	rBV3	331	319	0.03%	0.004%
23	3.558	780	783	785	rBV	264	183	0.02%	0.003%
24	3.680	819	821	824	rBV2	214	88	0.01%	0.001%
25	3.751	840	843	845	rBV	145	110	0.01%	0.002%
26	3.793	845	856	890	rBV2	72033	209437	22.97%	2.910%
27	4.252	984	999	1028	rBV	135724	351043	38.49%	4.878%
28	4.577	1097	1100	1102	rVB2	408	253	0.03%	0.004%
29	4.764	1156	1158	1160	rVB	241	84	0.01%	0.001%
30	4.786	1163	1165	1167	rVB	296	100	0.01%	0.001%
31	4.805	1167	1171	1174	rBV2	180	153	0.02%	0.002%
32	4.825	1175	1177	1180	rVB	204	93	0.01%	0.001%
33	4.841	1180	1182	1185	rVB2	261	164	0.02%	0.002%
34	4.860	1185	1188	1191	rBV2	243	209	0.02%	0.003%
35	4.960	1202	1219	1247	rBV2	345902	911931	100.00%	12.671%
36	5.448	1367	1371	1373	rBV2	380	250	0.03%	0.003%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

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\SFAMVLM082323WMA.M
Title : VOC Analysis

37	5.539	1385	1399	1419	rBV	241343	499104	54.73%	6.935%
38	5.831	1479	1490	1512	rVB3	9886	21593	2.37%	0.300%
39	5.992	1523	1540	1567	rBV	197481	419177	45.97%	5.825%
40	6.297	1626	1635	1636	rBV3	2465	2738	0.30%	0.038%
41	6.400	1658	1667	1697	rBV	73215	152320	16.70%	2.117%
42	6.918	1817	1828	1866	rBV	106977	209157	22.94%	2.906%
43	7.127	1884	1893	1903	rBV	19113	33178	3.64%	0.461%
44	7.246	1919	1930	1965	rBV	411499	737765	80.90%	10.251%
45	7.558	2016	2027	2051	rBV2	84883	159375	17.48%	2.215%
46	7.780	2093	2096	2097	rBV2	437	218	0.02%	0.003%
47	7.818	2105	2108	2109	rBV2	202	101	0.01%	0.001%
48	7.866	2112	2123	2138	rBV	25680	45730	5.01%	0.635%
49	7.979	2150	2158	2163	rBV6	4505	6646	0.73%	0.092%
50	8.027	2164	2173	2199	rVV	203326	388055	42.55%	5.392%
51	8.551	2334	2336	2339	rBV2	320	252	0.03%	0.004%
52	8.571	2339	2342	2348	rVV3	258	225	0.02%	0.003%
53	8.625	2348	2359	2383	rBV	60115	102157	11.20%	1.419%
54	8.786	2398	2409	2432	rBV	375900	631966	69.30%	8.781%
55	9.005	2474	2477	2480	rBV	319	203	0.02%	0.003%
56	9.172	2527	2529	2533	rVB	308	149	0.02%	0.002%
57	9.194	2534	2536	2538	rBV	299	131	0.01%	0.002%
58	9.249	2548	2553	2555	rBV2	240	260	0.03%	0.004%
59	9.304	2568	2570	2574	rVB	289	217	0.02%	0.003%
60	9.323	2574	2576	2578	rVB	238	112	0.01%	0.002%
61	9.349	2578	2584	2586	rBV2	509	530	0.06%	0.007%
62	9.599	2659	2662	2663	rBV	284	165	0.02%	0.002%
63	9.622	2667	2669	2673	rBV	329	231	0.03%	0.003%
64	9.696	2689	2692	2695	rVB2	252	101	0.01%	0.001%
65	9.821	2729	2731	2736	rVB2	264	188	0.02%	0.003%
66	9.915	2757	2760	2765	rVB2	414	275	0.03%	0.004%
67	9.943	2765	2769	2772	rBV2	216	185	0.02%	0.003%
68	9.972	2774	2778	2784	rVV2	375	291	0.03%	0.004%
69	10.014	2788	2791	2792	rBV	189	124	0.01%	0.002%
70	10.075	2806	2810	2815	rBV	334	286	0.03%	0.004%
71	10.111	2819	2821	2823	rBV	216	98	0.01%	0.001%
72	10.156	2823	2835	2865	rBV	252565	404416	44.35%	5.619%
73	10.426	2916	2919	2920	rBV	213	99	0.01%	0.001%
74	10.448	2924	2926	2928	rBV2	175	103	0.01%	0.001%
75	10.532	2950	2952	2954	rBV	236	92	0.01%	0.001%
76	10.680	2992	2998	2999	rBV2	330	267	0.03%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

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\SFAMVLM082323WMA.M
Title : VOC Analysis

77	10.776	3026	3028	3029	rBV2	229	113	0.01%	0.002%
78	10.863	3051	3055	3058	rBV3	552	424	0.05%	0.006%
79	11.059	3109	3116	3118	rBV2	265	281	0.03%	0.004%
80	11.117	3132	3134	3137	rBV2	358	229	0.03%	0.003%
81	11.130	3137	3138	3145	rVB2	616	507	0.06%	0.007%
82	11.188	3145	3156	3180	rBV	422416	653993	71.72%	9.087%
83	11.464	3239	3242	3251	rVB2	795	1006	0.11%	0.014%
84	11.522	3257	3260	3261	rBV	166	96	0.01%	0.001%
85	11.564	3261	3273	3299	rVV	412334	654497	71.77%	9.094%
86	11.750	3327	3331	3332	rBV2	241	142	0.02%	0.002%
87	11.815	3349	3351	3352	rBV2	193	89	0.01%	0.001%
88	12.204	3461	3472	3480	rVV5	1567	2724	0.30%	0.038%
89	12.406	3533	3535	3536	rBV	238	86	0.01%	0.001%
90	12.461	3550	3552	3558	rVB	195	101	0.01%	0.001%
91	12.490	3559	3561	3564	rBV2	191	104	0.01%	0.001%
92	12.596	3589	3594	3597	rBV3	663	417	0.05%	0.006%
93	12.638	3604	3607	3608	rBV	292	137	0.02%	0.002%
94	13.049	3733	3735	3739	rVB	216	106	0.01%	0.001%
95	13.204	3780	3783	3787	rBV4	710	561	0.06%	0.008%
96	13.455	3855	3861	3868	rVB4	1605	2177	0.24%	0.030%
97	13.689	3929	3934	3945	rVB4	754	1013	0.11%	0.014%
98	13.818	3972	3974	3979	rVB2	701	336	0.04%	0.005%
99	13.876	3989	3992	3993	rBV	303	164	0.02%	0.002%
100	14.156	4077	4079	4081	rBV2	393	207	0.02%	0.003%

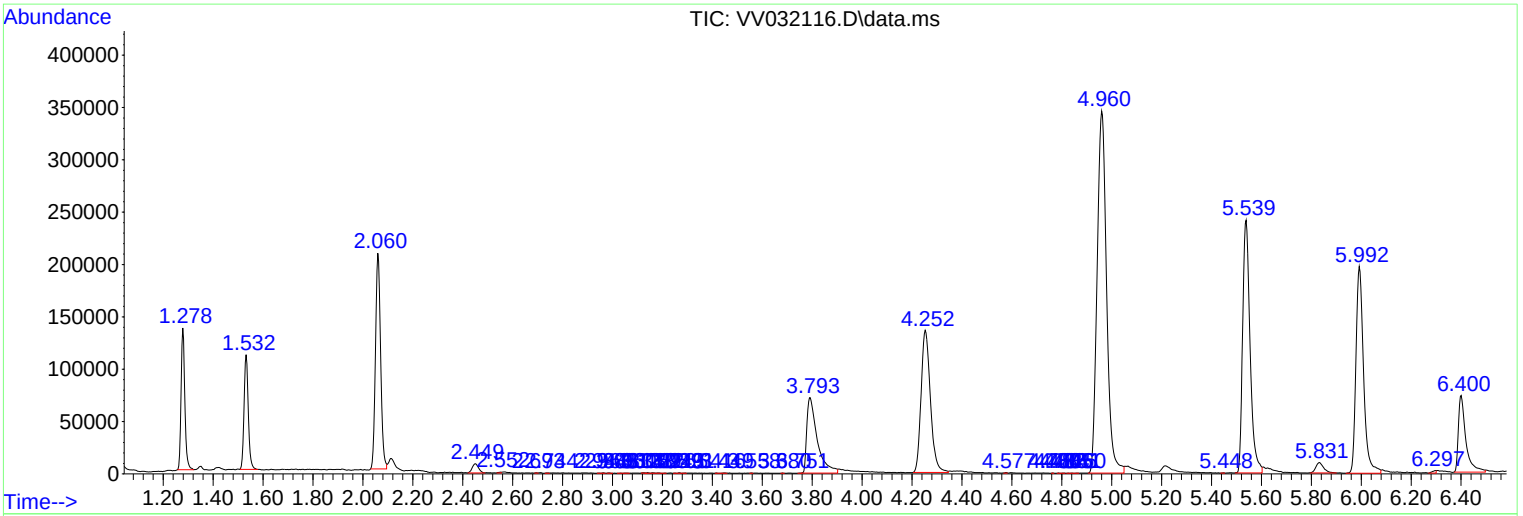
Sum of corrected areas: 7196760

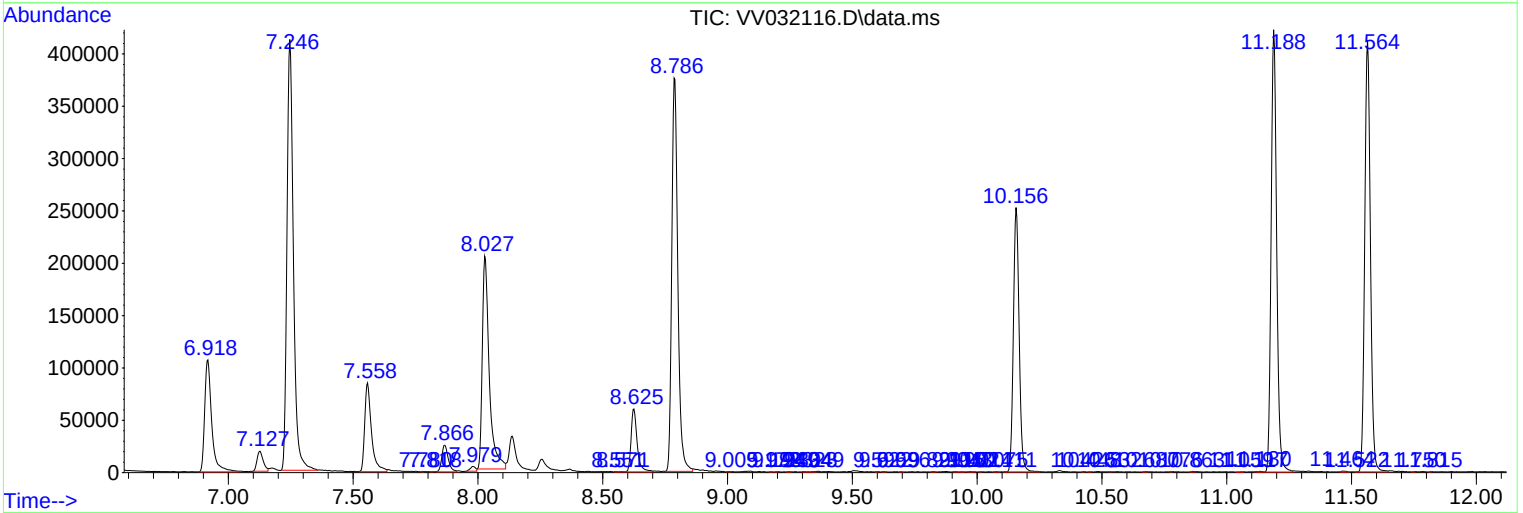
Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

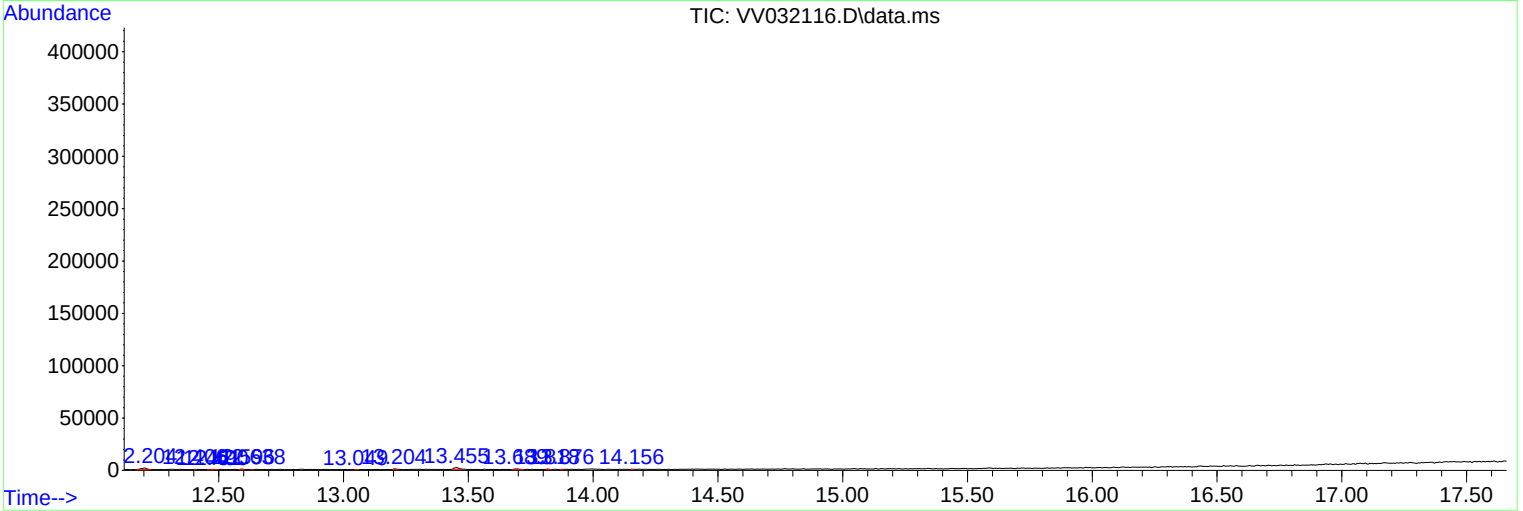
Instrument :
MSVOA_V
ClientSampleId :
JYCA3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

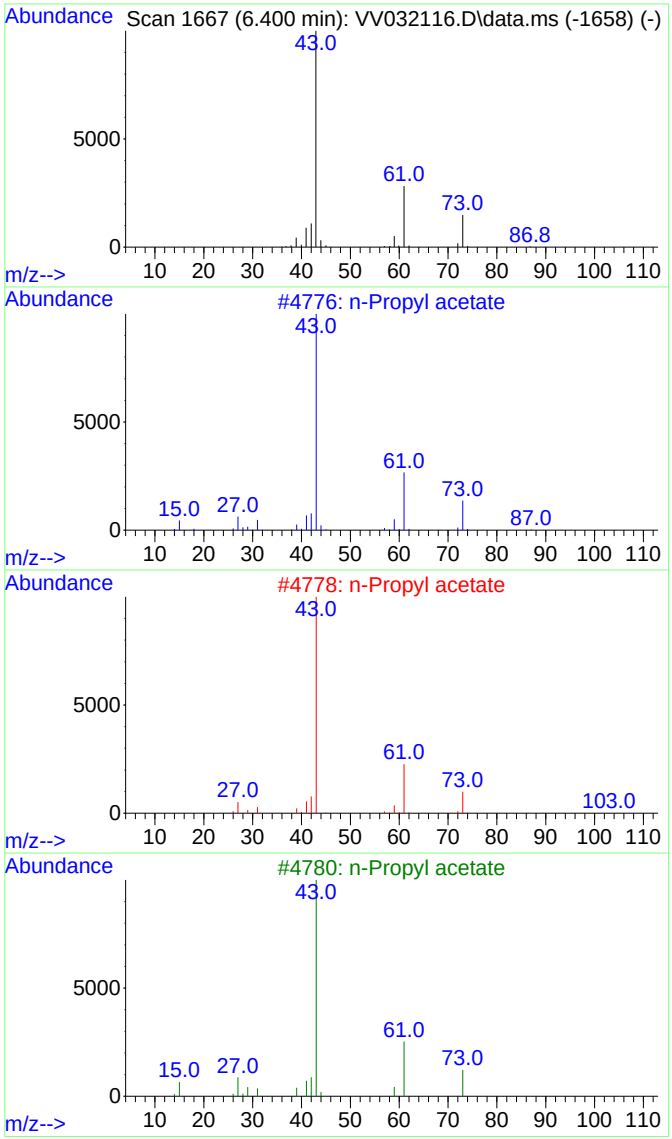
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

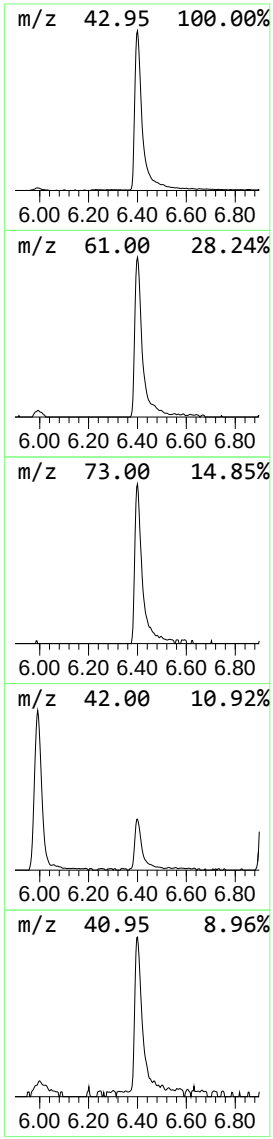
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.400	15.26 ug/L	152320	1,4-Difluorobenzene	5.539

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	72
4	n-Propyl acetate	102	C5H10O2	000109-60-4	64
5	Isopropyl acetate	102	C5H10O2	000108-21-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

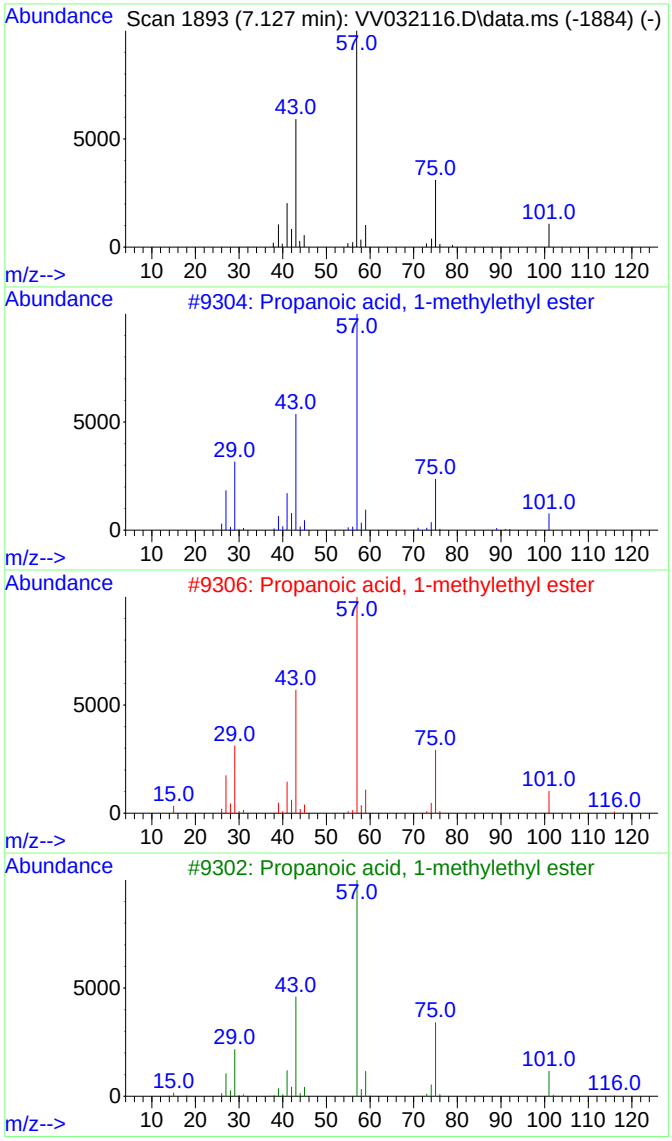
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

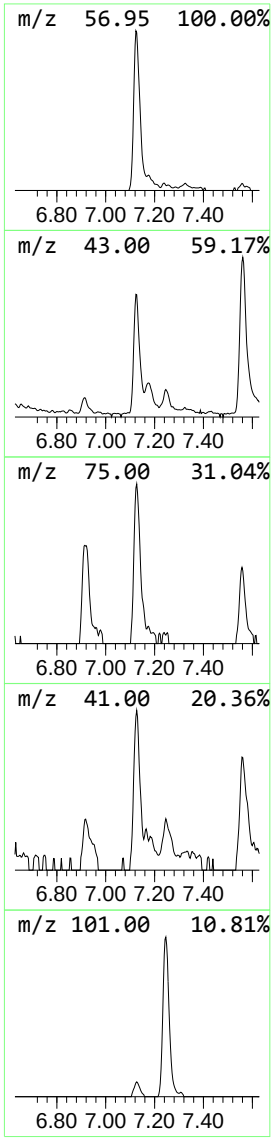
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.32 ug/L	33178	1,4-Difluorobenzene	5.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
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	74
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

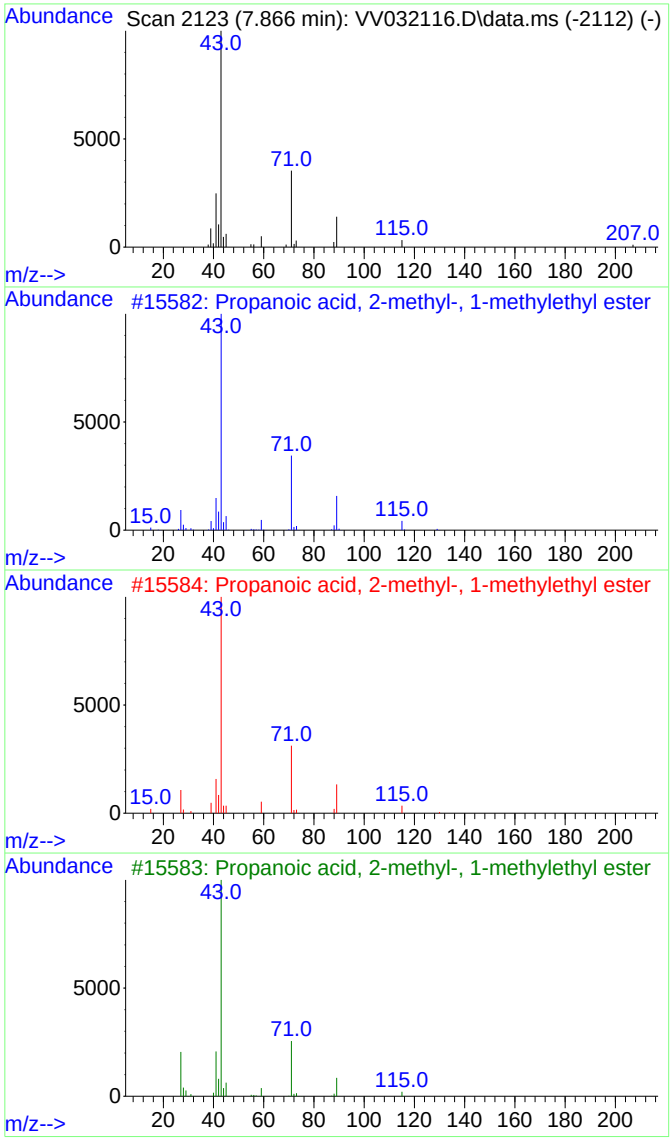
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

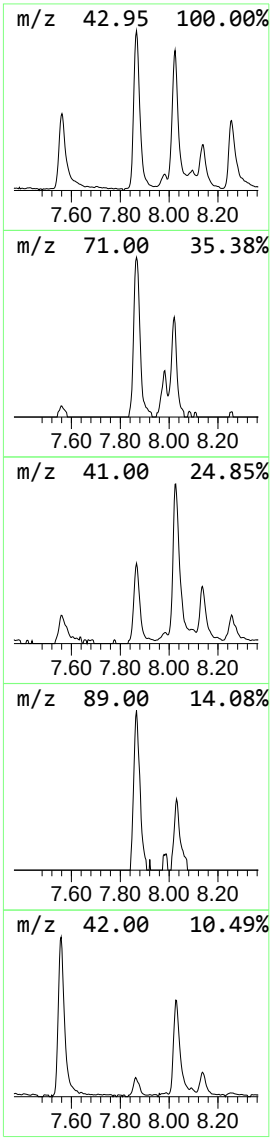
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	3.62 ug/L	45730	Chlorobenzene-d5	8.789

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	83
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

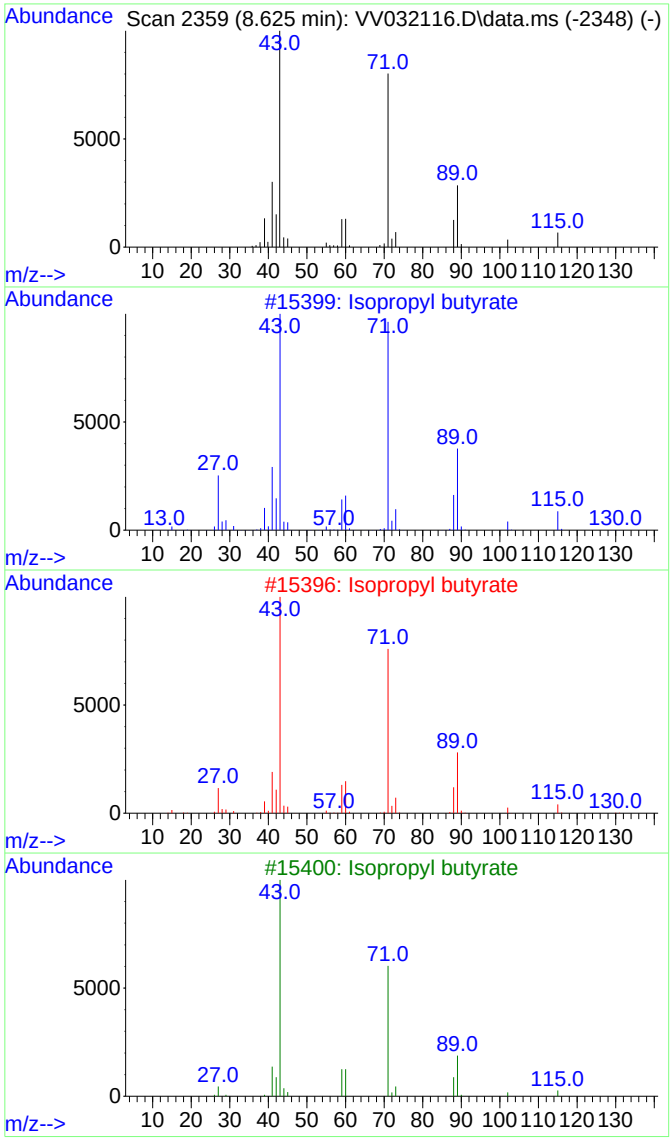
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

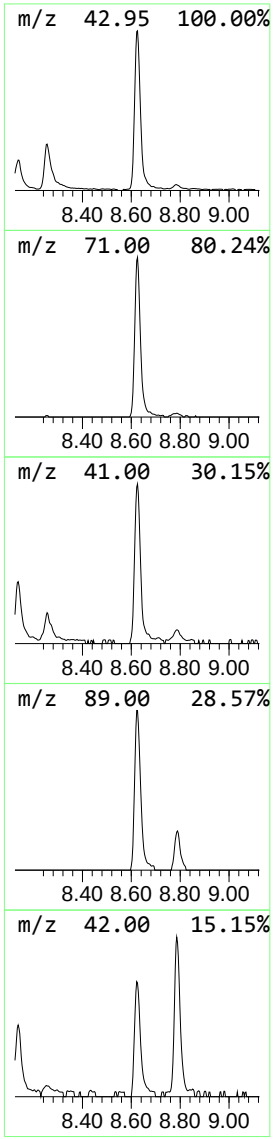
****

Peak Number 5 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.625	8.08 ug/L	102157	Chlorobenzene-d5	8.789

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	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032116.D
Acq On : 15 Sep 2023 13:07
Operator : SY/MD
Sample : 04359-02 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
JYCA3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.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	6.400	15.3	ug/L	152320	1	5.539	499104	50.0
Propanoic acid,...	7.127	3.3	ug/L	33178	1	5.539	499104	50.0
Propanoic acid,...	7.866	3.6	ug/L	45730	2	8.789	631966	50.0
Isopropyl butyrate	8.625	8.1	ug/L	102157	2	8.789	631966	50.0