LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

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\SFAMVLM092022WMA.M
Title : VOC Analysis

Signal : TIC: VV028018.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	101	rVB	187745	193007	13.72%	1.641%
2	1.561	155	162	173	rBV	158922	180881	12.85%	1.538%
3	2.098	318	329	347	rBV	325929	472029	33.55%	4.013%
4	2.268	378	382	383	rBV4	739	608	0.04%	0.005%
5	2.439	432	435	437	rBV3	1034	622	0.04%	0.005%
6	2.500	445	454	467	rVB3	9121	16051	1.14%	0.136%
7	2.760	532	535	537	rBV4	1044	744	0.05%	0.006%
8	2.886	570	574	576	rVV2	811	533	0.04%	0.005%
9	3.166	655	661	663	rBV4	1140	1048	0.07%	0.009%
10	3.178	663	665	668	rVV	1059	626	0.04%	0.005%
11	3.198	668	671	675	rVV5	646	699	0.05%	0.006%
12	3.365	719	723	727	rVB3	690	558	0.04%	0.005%
13	3.879	872	883	923	rBV2	132602	455496	32.37%	3.872%
14	4.339	1011	1026	1056	rBV	234956	574212	40.81%	4.882%
15	4.522	1080	1083	1087	rBV4	950	872	0.06%	0.007%
16	4.571	1094	1098	1102	rVB4	871	702	0.05%	0.006%
17	4.760	1154	1157	1162	rVB4	599	460	0.03%	0.004%
18	4.828	1174	1178	1179	rBV2	899	486	0.03%	0.004%
19	4.863	1186	1189	1191	rBV3	657	501	0.04%	0.004%
20	4.911	1201	1204	1208	rBV4	618	591	0.04%	0.005%
21	5.040	1227	1244	1272	rBV2	547504	1407130	100.00%	11.963%
22	5.227	1300	1302	1307	rVB6	792	567	0.04%	0.005%
23	5.284	1310	1320	1332	rBV4	9305	22270	1.58%	0.189%
24	5.384	1348	1351	1353	rBV3	1008	639	0.05%	0.005%
25	5.554	1401	1404	1405	rBV3	761	524	0.04%	0.004%
26	5.609	1409	1421	1440	rBV	446782	990885	70.42%	8.424%
27	6.063	1550	1562	1585	rVB	311716	629234	44.72%	5.349%
28	6.461	1676	1686	1711	rBV	122757	239957	17.05%	2.040%
29	6.982	1837	1848	1868	rBV	172688	314006	22.32%	2.670%
30	7.185	1901	1911	1924	rBV	25804	46552	3.31%	0.396%
31	7.313	1939	1951	1970	rBV	612731	1063395	75.57%	9.040%
32	7.619	2035	2046	2069	rBV2	153134	274997	19.54%	2.338%
33	7.924	2132	2141	2155	rBV	31160	53620	3.81%	0.456%
34	8.033	2164	2175	2181	rBV5	6131	11873	0.84%	0.101%
35	8.085	2181	2191	2215	rVV	451171	799192	56.80%	6.794%
36	8.191	2216	2224	2238	rVB	56692	96467	6.86%	0.820%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

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\SFAMVLM092022WMA.M
Title : VOC Analysis

37	8.304	2251	2259	2275	rVB	31324	51218	3.64%	0.435%
38	8.416	2289	2294	2306	rVB7	3809	6804	0.48%	0.058%
39	8.641	2359	2364	2365	rBV3	635	517	0.04%	0.004%
40	8.680	2365	2376	2397	rVV	97095	166134	11.81%	1.412%
41	8.847	2417	2428	2450	rBV	644313	1055657	75.02%	8.975%
42	9.213	2539	2542	2546	rVB5	759	656	0.05%	0.006%
43	9.503	2628	2632	2636	rVB6	834	686	0.05%	0.006%
44	9.551	2637	2647	2663	rVV6	8514	15135	1.08%	0.129%
45	9.818	2726	2730	2732	rBV4	667	548	0.04%	0.005%
46	10.046	2799	2801	2805	rVB3	1025	589	0.04%	0.005%
47	10.082	2809	2812	2816	rBV5	733	537	0.04%	0.005%
48	10.123	2818	2825	2827	rBV5	2016	1916	0.14%	0.016%
49	10.210	2840	2852	2874	rVV	473004	750484	53.33%	6.380%
50	10.329	2886	2889	2892	rBV3	899	541	0.04%	0.005%
51	10.365	2897	2900	2903	rBV5	862	526	0.04%	0.004%
52	10.590	2969	2970	2977	rVB5	1350	1054	0.07%	0.009%
53	10.638	2980	2985	2986	rBV3	860	546	0.04%	0.005%
54	10.648	2986	2988	2991	rVB3	771	448	0.03%	0.004%
55	10.721	3007	3011	3014	rBV4	878	675	0.05%	0.006%
56	10.741	3014	3017	3019	rVB3	711	436	0.03%	0.004%
57	10.757	3019	3022	3025	rBV4	718	537	0.04%	0.005%
58	10.776	3025	3028	3034	rVB4	725	555	0.04%	0.005%
59	10.831	3041	3045	3047	rBV4	662	554	0.04%	0.005%
60	10.853	3049	3052	3056	rVB4	570	502	0.04%	0.004%
61	10.914	3066	3071	3075	rBV7	1966	2071	0.15%	0.018%
62	11.008	3096	3100	3102	rBV3	712	605	0.04%	0.005%
63	11.098	3124	3128	3130	rBV3	757	577	0.04%	0.005%
64	11.156	3141	3146	3152	rVB5	1015	1241	0.09%	0.011%
65	11.246	3162	3174	3194	rBV	582048	896031	63.68%	7.618%
66	11.377	3213	3215	3217	rBV2	1130	598	0.04%	0.005%
67	11.464	3239	3242	3244	rBV3	1025	511	0.04%	0.004%
68	11.567	3271	3274	3276	rBV3	737	502	0.04%	0.004%
69	11.622	3278	3291	3313	rVV	595197	927097	65.89%	7.882%
70	11.828	3351	3355	3357	rBV3	728	505	0.04%	0.004%
71	12.252	3482	3487	3490	rBV5	1538	1156	0.08%	0.010%
72	12.303	3498	3503	3506	rBV4	746	783	0.06%	0.007%
73	12.361	3517	3521	3524	rBV4	809	626	0.04%	0.005%
74	12.490	3557	3561	3567	rVB4	947	952	0.07%	0.008%
75	12.551	3575	3580	3582	rBV2	887	811	0.06%	0.007%
76	12.692	3622	3624	3629	rVB4	857	504	0.04%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

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\SFAMVLM092022WMA.M
Title : VOC Analysis

77	12.728	3629	3635	3640	rVB4	1002	1231	0.09%	0.010%
78	12.924	3692	3696	3700	rBV3	571	626	0.04%	0.005%
79	13.104	3750	3752	3758	rBV5	455	483	0.03%	0.004%
80	13.139	3758	3763	3764	rBV2	629	570	0.04%	0.005%
81	13.300	3809	3813	3816	rBV4	767	792	0.06%	0.007%
82	13.519	3878	3881	3883	rBV3	787	471	0.03%	0.004%
83	13.583	3899	3901	3906	rVB3	802	484	0.03%	0.004%
84	13.625	3910	3914	3917	rBV6	848	830	0.06%	0.007%
85	13.660	3920	3925	3927	rBV4	833	752	0.05%	0.006%
86	13.776	3959	3961	3966	rVB3	953	687	0.05%	0.006%
87	13.818	3966	3974	3977	rBV4	952	1149	0.08%	0.010%
88	13.908	3999	4002	4004	rBV3	885	645	0.05%	0.005%
89	13.998	4028	4030	4031	rBV2	1175	527	0.04%	0.004%
90	14.290	4116	4121	4124	rBV4	590	631	0.04%	0.005%
91	14.371	4143	4146	4150	rBV4	781	686	0.05%	0.006%
92	14.393	4150	4153	4157	rVB3	914	606	0.04%	0.005%
93	14.509	4185	4189	4190	rBV3	732	527	0.04%	0.004%
94	14.631	4223	4227	4231	rBV4	1054	932	0.07%	0.008%
95	14.692	4242	4246	4247	rVV3	750	533	0.04%	0.005%
96	14.840	4288	4292	4295	rBV4	1401	1308	0.09%	0.011%
97	14.892	4305	4308	4311	rVV3	831	675	0.05%	0.006%
98	15.094	4368	4371	4374	rBV4	977	604	0.04%	0.005%
99	15.390	4458	4463	4467	rBV6	1211	1282	0.09%	0.011%
100	15.940	4628	4634	4635	rBV4	1565	1816	0.13%	0.015%

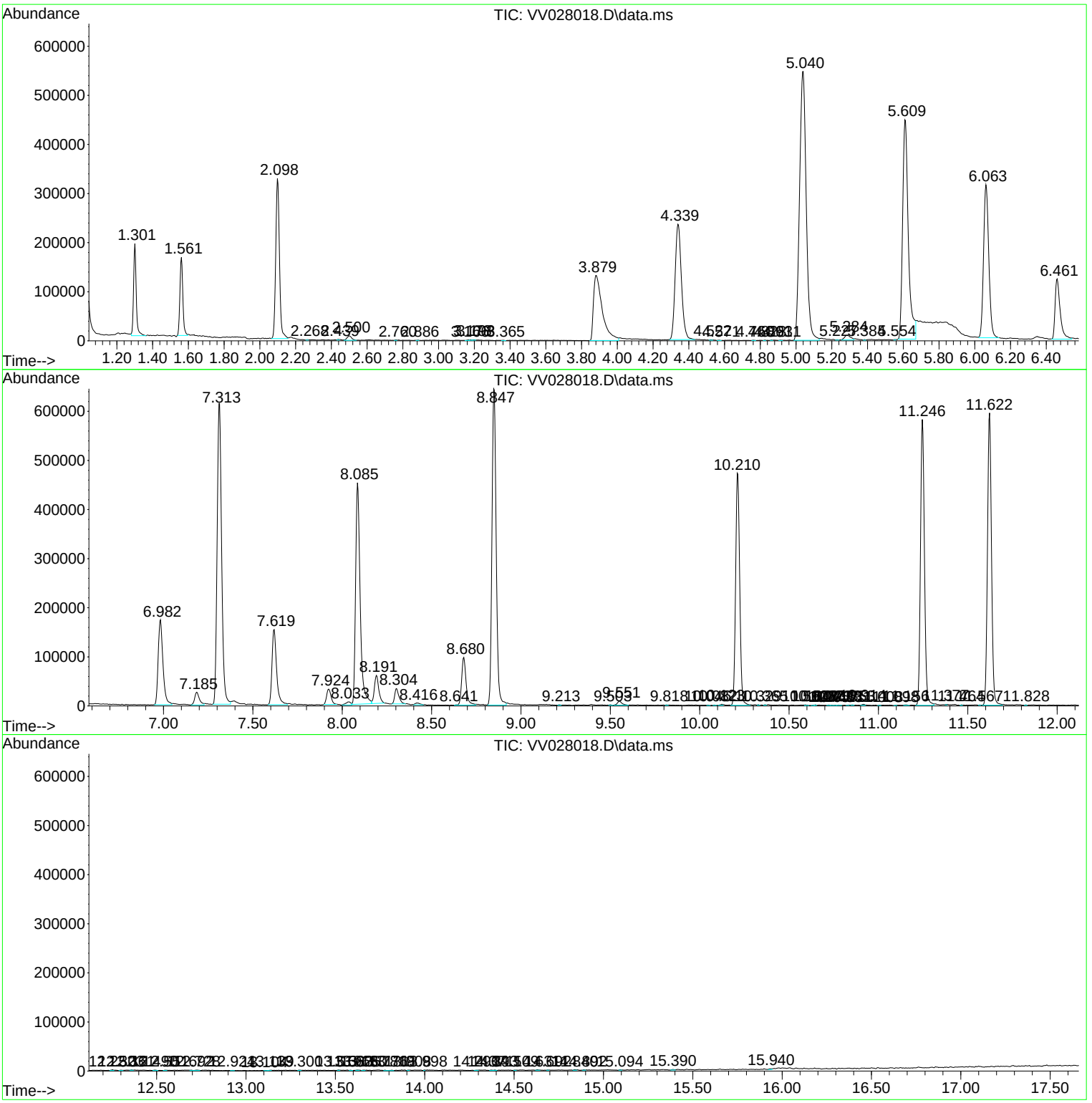
Sum of corrected areas: 11762706

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

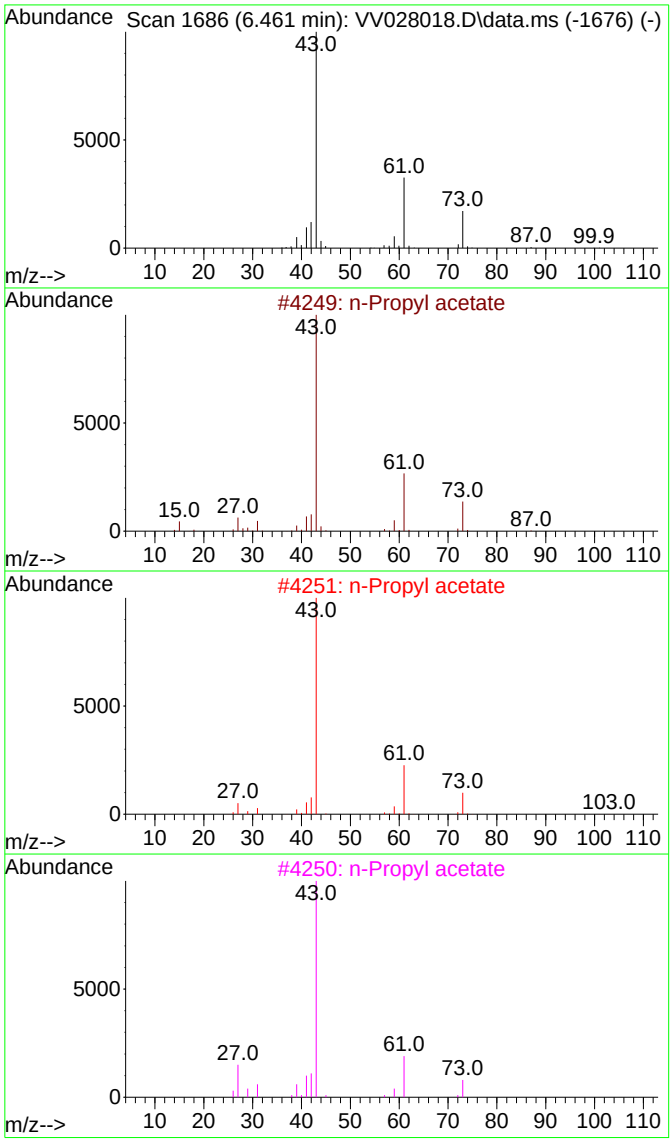
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

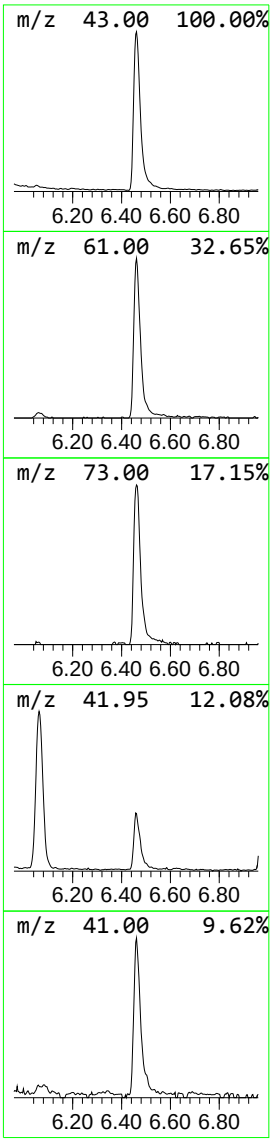
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	12.11 ug/L	239957	1,4-Difluorobenzene	5.612

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	1-Butanamine	73	C4H11N	000109-73-9	9
5	Isobutylamine	73	C4H11N	000078-81-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

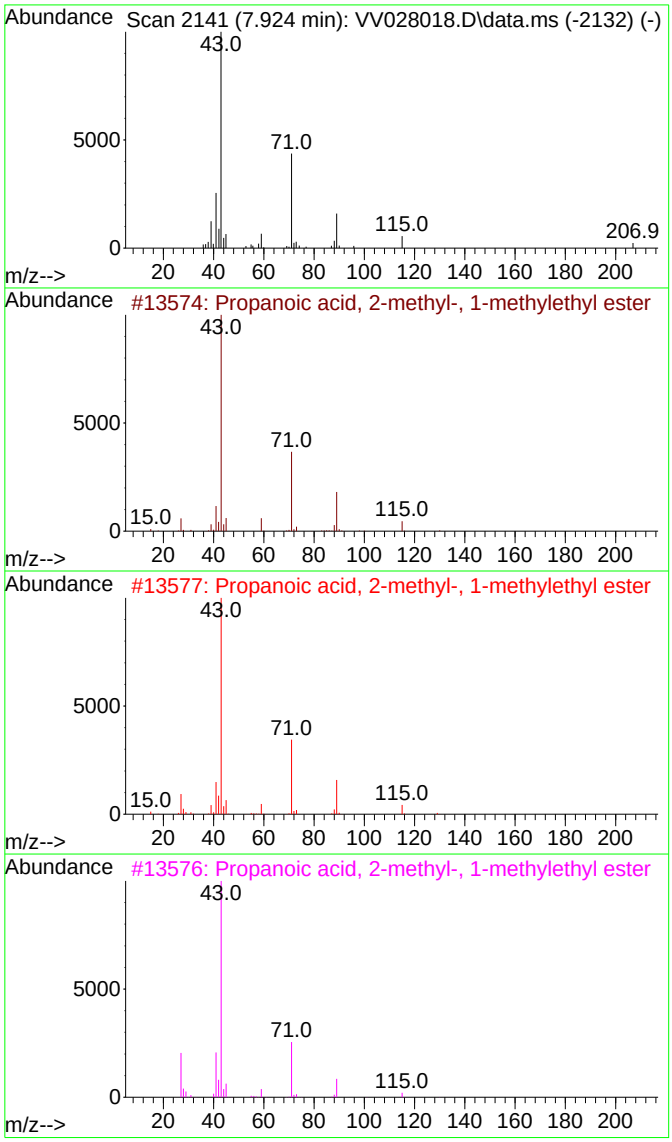
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

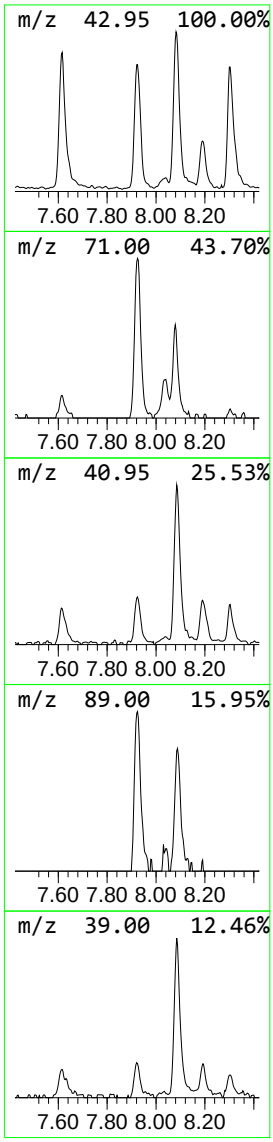
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.924	2.54 ug/L	53620	Chlorobenzene-d5	8.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
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	47
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	45
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

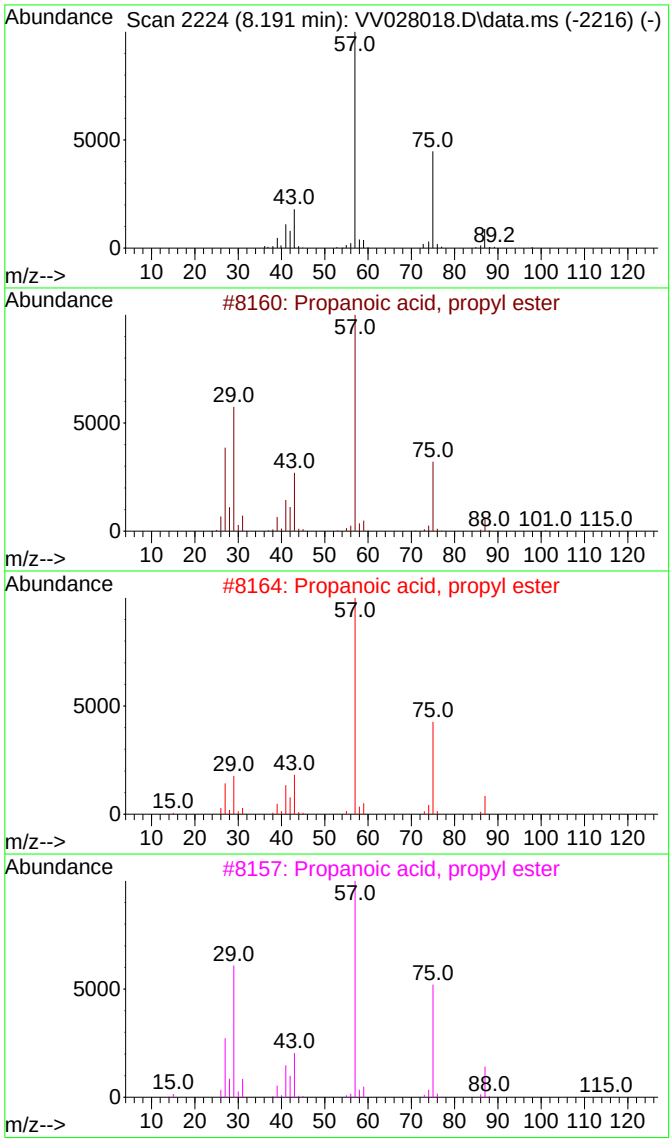
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

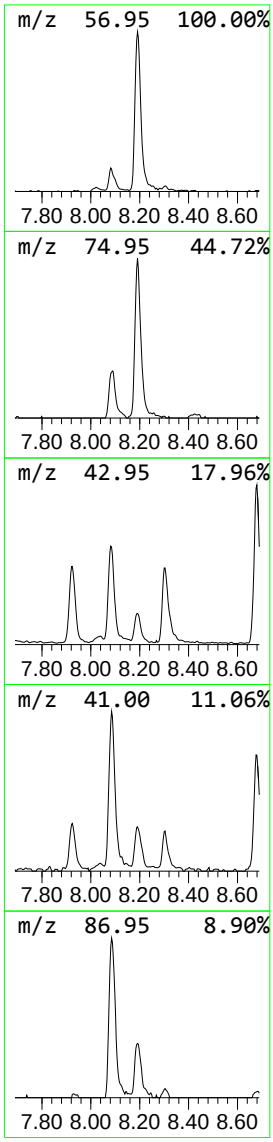
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	4.57 ug/L	96467	Chlorobenzene-d5	8.850

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	72
3	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	64
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
5	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

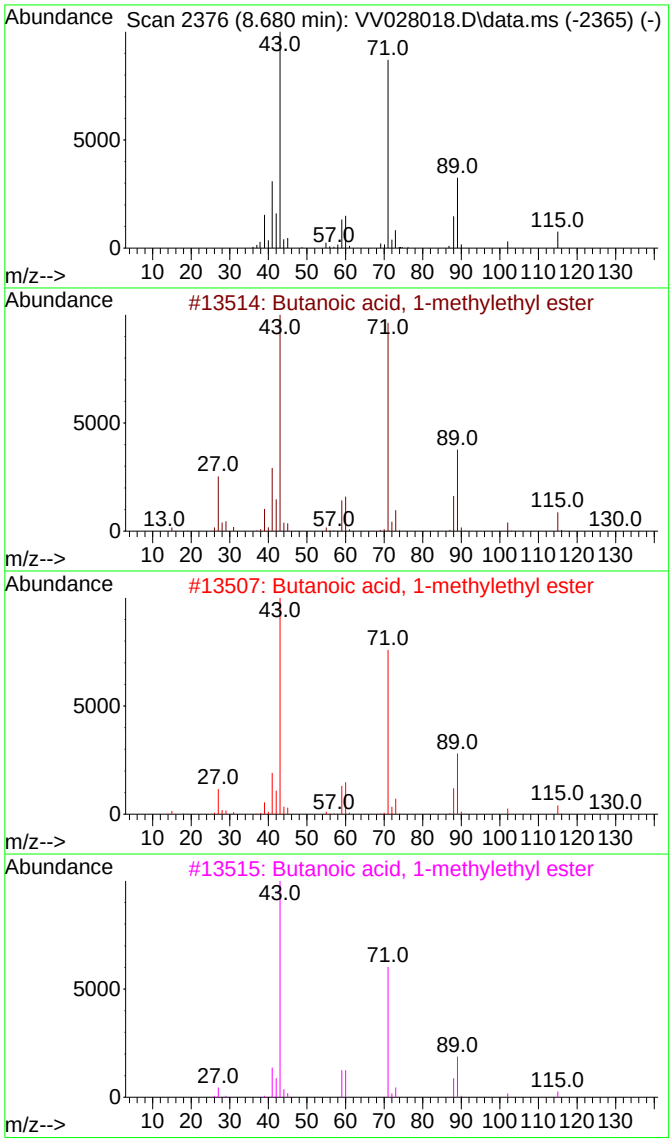
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

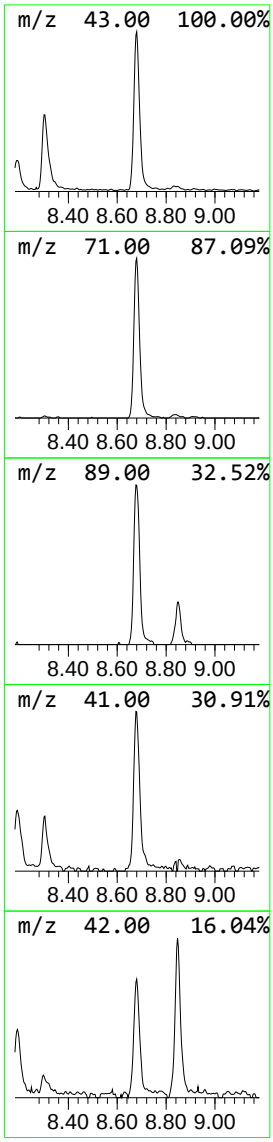
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	7.87 ug/L	166134	Chlorobenzene-d5	8.850

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092122\
Data File : VV028018.D
Acq On : 21 Sep 2022 15:55
Operator : SY/MD
Sample : N4689-03 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	6.461	12.1	ug/L	239957	1	5.612	990885	50.0
Propanoic acid,...	7.924	2.5	ug/L	53620	2	8.850	1055660	50.0
Propanoic acid,...	8.191	4.6	ug/L	96467	2	8.850	1055660	50.0
Butanoic acid, ...	8.680	7.9	ug/L	166134	2	8.850	1055660	50.0