LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020298.D
Acq On : 11 Feb 2021 14:53
Operator : SY/MD
Sample : M1375-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ2

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\SOMVLM020521WMA.M
Title : VOC Analysis

Signal : TIC: VV020298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	98	rVB	284061	291724	6.34%	1.010%
2	1.568	156	164	179	rVB	256079	289070	6.29%	1.001%
3	2.108	321	332	346	rBV	505757	756257	16.45%	2.619%
4	2.301	386	392	397	rBV4	1479	2363	0.05%	0.008%
5	2.506	447	456	468	rBV2	17165	28567	0.62%	0.099%
6	2.648	496	500	506	rBV5	977	975	0.02%	0.003%
7	2.728	521	525	528	rBV	420	382	0.01%	0.001%
8	2.754	528	533	535	rBV3	439	416	0.01%	0.001%
9	2.947	589	593	597	rBV3	925	1069	0.02%	0.004%
10	3.175	656	664	665	rBV5	1052	1160	0.03%	0.004%
11	3.452	734	750	752	rBV7	2191	4274	0.09%	0.015%
12	3.545	777	779	782	rVB3	697	380	0.01%	0.001%
13	3.876	870	882	929	rBV	156314	452752	9.85%	1.568%
14	4.349	1011	1029	1058	rBV	313192	832072	18.10%	2.881%
15	4.548	1088	1091	1095	rVB4	542	374	0.01%	0.001%
16	4.606	1104	1109	1111	rVB3	545	486	0.01%	0.002%
17	4.619	1111	1113	1119	rVB4	412	400	0.01%	0.001%
18	5.047	1228	1246	1272	rBV2	800671	2071617	45.05%	7.174%
19	5.204	1293	1295	1301	rVB6	801	813	0.02%	0.003%
20	5.281	1308	1319	1338	rBV2	17903	41651	0.91%	0.144%
21	5.391	1350	1353	1358	rBV3	976	717	0.02%	0.002%
22	5.481	1377	1381	1385	rVB3	633	549	0.01%	0.002%
23	5.506	1385	1389	1391	rBV2	472	358	0.01%	0.001%
24	5.545	1399	1401	1404	rVB3	701	362	0.01%	0.001%
25	5.616	1409	1423	1454	rBV	697925	1403217	30.52%	4.859%
26	5.905	1486	1513	1529	rBV5	35108	102360	2.23%	0.354%
27	6.069	1550	1564	1586	rBV	459645	927161	20.16%	3.211%
28	6.188	1594	1601	1620	rVB3	9179	20247	0.44%	0.070%
29	6.336	1635	1647	1648	rBV2	15044	18651	0.41%	0.065%
30	6.458	1672	1685	1719	rBV	1705977	2987575	64.97%	10.346%
31	6.857	1806	1809	1814	rBV3	838	932	0.02%	0.003%
32	6.924	1828	1830	1834	rVB4	931	569	0.01%	0.002%
33	6.985	1838	1849	1870	rBV	264631	473758	10.30%	1.641%
34	7.185	1899	1911	1923	rBV	253009	431731	9.39%	1.495%
35	7.317	1940	1952	1977	rBV	998286	1728657	37.59%	5.986%
36	7.474	1997	2001	2017	rVB	4032	7380	0.16%	0.026%

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Instrument : MSVOA_V
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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

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Title : VOC Analysis

37	7.622	2036	2047	2069	rBV2	200637	352027	7.66%	1.219%
38	7.860	2119	2121	2126	rVB4	702	517	0.01%	0.002%
39	7.924	2129	2141	2156	rBV	68530	117279	2.55%	0.406%
40	8.034	2161	2175	2183	rVV	178261	283043	6.16%	0.980%
41	8.088	2183	2192	2212	rVV	614388	1100760	23.94%	3.812%
42	8.191	2213	2224	2248	rVV	2974712	4598292	100.00%	15.923%
43	8.300	2249	2258	2286	rVB	271328	450245	9.79%	1.559%
44	8.680	2364	2376	2403	rBV	1761919	2663580	57.93%	9.224%
45	8.853	2418	2430	2458	rBV	1141486	1830186	39.80%	6.338%
46	9.194	2533	2536	2539	rBV3	609	569	0.01%	0.002%
47	9.210	2539	2541	2546	rVV4	664	588	0.01%	0.002%
48	9.397	2592	2599	2608	rVV6	2628	4574	0.10%	0.016%
49	9.551	2637	2647	2663	rBV	49015	80882	1.76%	0.280%
50	9.648	2675	2677	2683	rVB6	669	528	0.01%	0.002%
51	9.718	2695	2699	2701	rBV4	1264	1177	0.03%	0.004%
52	9.812	2726	2728	2731	rBV2	780	379	0.01%	0.001%
53	9.908	2754	2758	2762	rBV3	654	579	0.01%	0.002%
54	9.934	2762	2766	2770	rVV6	594	566	0.01%	0.002%
55	10.127	2822	2826	2830	rVB3	630	520	0.01%	0.002%
56	10.220	2843	2855	2874	rBV	642324	1010013	21.96%	3.498%
57	10.358	2896	2898	2901	rBV4	653	367	0.01%	0.001%
58	10.419	2913	2917	2921	rBV3	540	530	0.01%	0.002%
59	10.458	2927	2929	2933	rVB2	615	376	0.01%	0.001%
60	10.487	2933	2938	2940	rBV4	669	524	0.01%	0.002%
61	10.545	2949	2956	2963	rVB8	1548	2364	0.05%	0.008%
62	10.587	2965	2969	2971	rBV	528	344	0.01%	0.001%
63	10.648	2984	2988	2991	rVB5	532	507	0.01%	0.002%
64	10.689	2996	3001	3004	rBV2	897	828	0.02%	0.003%
65	10.847	3045	3050	3052	rBV3	487	493	0.01%	0.002%
66	11.095	3124	3127	3128	rBV3	746	474	0.01%	0.002%
67	11.168	3147	3150	3153	rVB3	851	473	0.01%	0.002%
68	11.194	3156	3158	3163	rVB5	1117	945	0.02%	0.003%
69	11.255	3163	3177	3199	rBV	1178219	1791120	38.95%	6.202%
70	11.541	3259	3266	3276	rBV6	3703	6781	0.15%	0.023%
71	11.631	3281	3294	3318	rVV	1067942	1672853	36.38%	5.793%
72	11.824	3351	3354	3357	rVB3	618	470	0.01%	0.002%
73	11.931	3383	3387	3389	rVB4	647	479	0.01%	0.002%
74	11.947	3389	3392	3395	rBV3	583	347	0.01%	0.001%
75	12.017	3409	3414	3417	rVV6	779	831	0.02%	0.003%
76	12.111	3440	3443	3446	rBV2	461	343	0.01%	0.001%

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ClientSampleId : C0BJ2

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Title : VOC Analysis

77	12.255	3481	3488	3491	rBV5	1247	1594	0.03%	0.006%
78	12.323	3505	3509	3512	rVB4	636	460	0.01%	0.002%
79	12.355	3512	3519	3530	rBV6	2629	4504	0.10%	0.016%
80	12.474	3554	3556	3563	rVB3	733	524	0.01%	0.002%
81	12.750	3639	3642	3646	rVB4	798	621	0.01%	0.002%
82	12.882	3677	3683	3685	rBV3	655	671	0.01%	0.002%
83	13.072	3735	3742	3744	rBV4	502	638	0.01%	0.002%
84	13.159	3767	3769	3772	rVV3	549	427	0.01%	0.001%
85	13.275	3800	3805	3813	rBV6	1467	1835	0.04%	0.006%
86	13.590	3898	3903	3905	rBV3	673	588	0.01%	0.002%
87	13.625	3910	3914	3916	rVB2	559	463	0.01%	0.002%
88	13.664	3923	3926	3932	rBV5	443	438	0.01%	0.002%
89	13.856	3983	3986	3990	rBV3	471	348	0.01%	0.001%
90	13.975	4020	4023	4026	rBV4	718	484	0.01%	0.002%
91	14.049	4044	4046	4051	rBV4	625	539	0.01%	0.002%
92	14.210	4090	4096	4100	rBV4	1000	1117	0.02%	0.004%
93	14.265	4109	4113	4114	rBV2	652	376	0.01%	0.001%
94	14.387	4148	4151	4156	rBV3	642	554	0.01%	0.002%
95	14.458	4170	4173	4175	rBV2	584	363	0.01%	0.001%
96	14.696	4245	4247	4252	rVB3	596	424	0.01%	0.001%
97	14.889	4304	4307	4310	rVB	662	367	0.01%	0.001%
98	15.159	4388	4391	4393	rBV2	1024	601	0.01%	0.002%
99	15.374	4455	4458	4462	rVB2	697	438	0.01%	0.002%
100	15.471	4484	4488	4491	rBV4	642	551	0.01%	0.002%

Sum of corrected areas: 28877704

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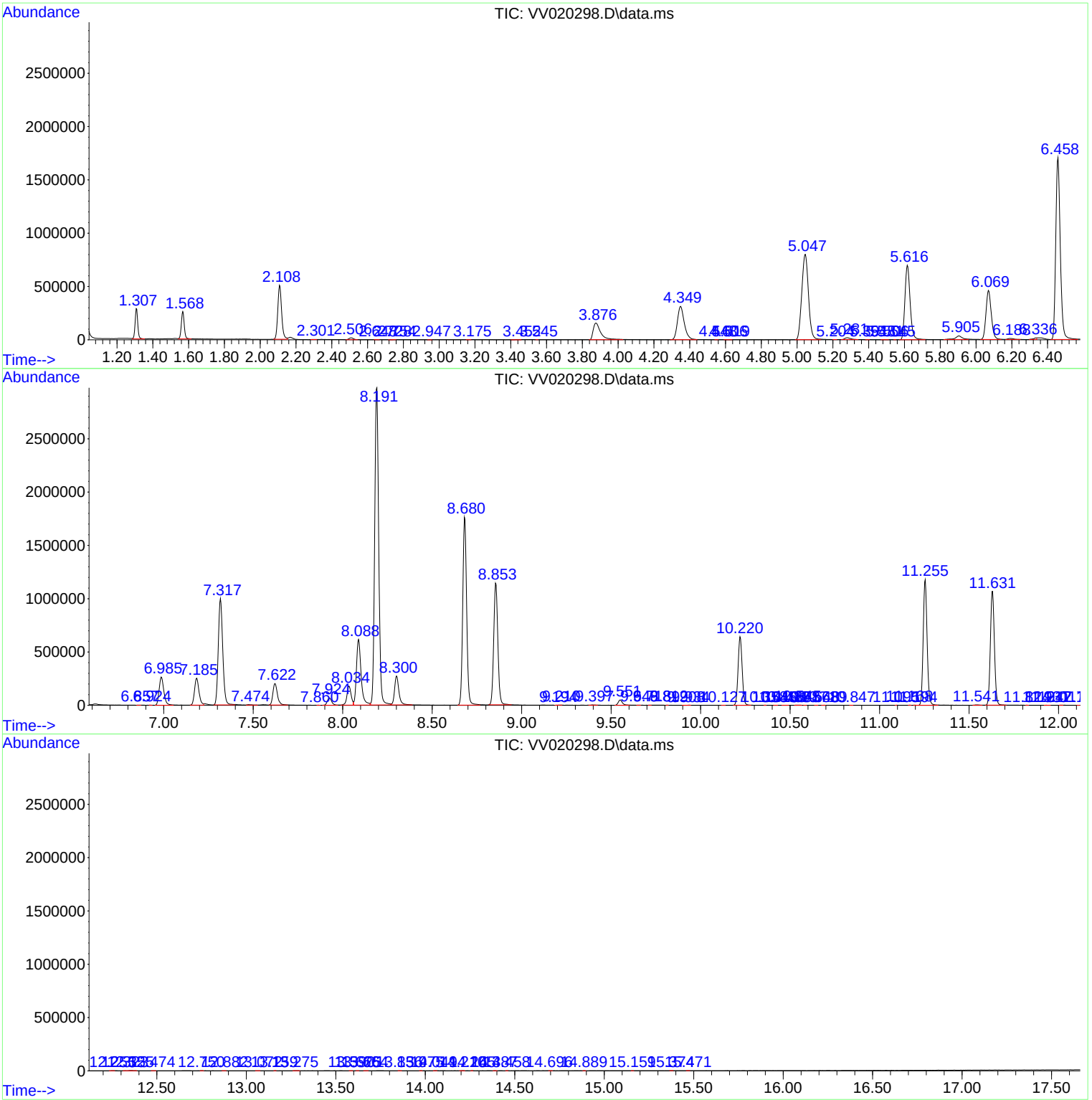
Instrument :
MSVOA_V
ClientSampleId :
C0BJ2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId : C0BJ2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

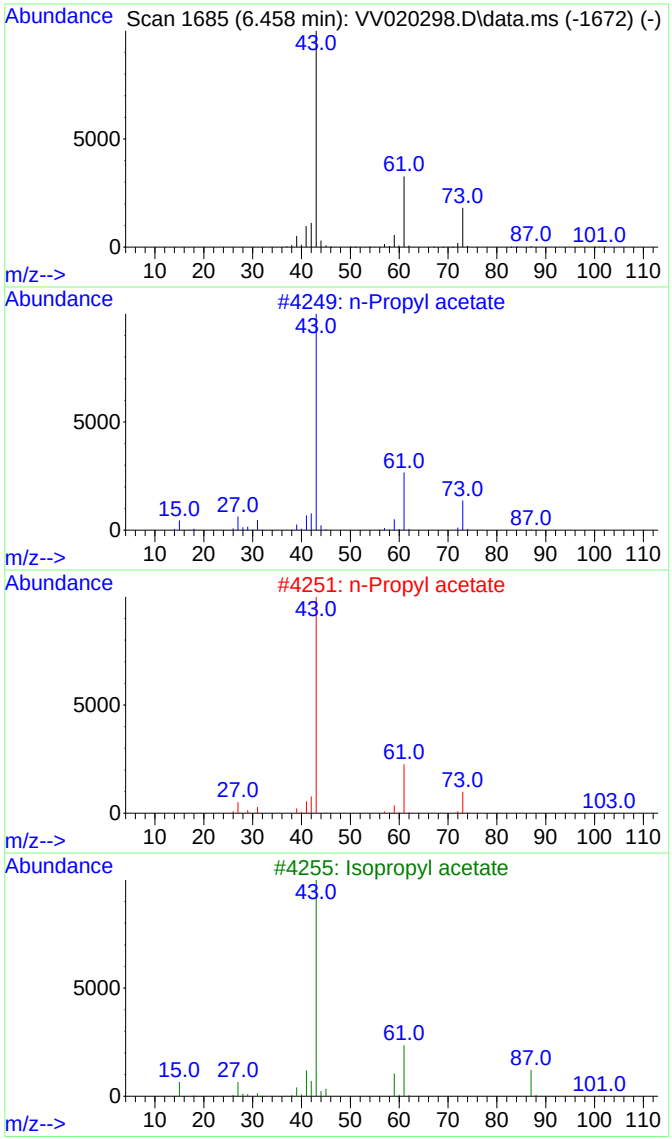
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

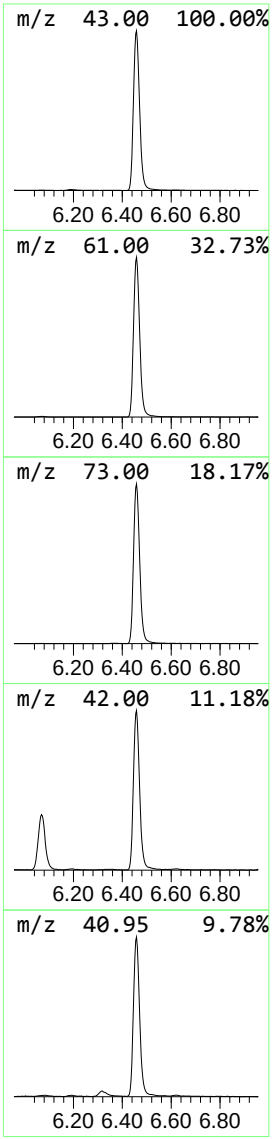
****

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.458	106.45 ug/L	2987580	1,4-Difluorobenzene	5.616

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	Isopropyl acetate	102	C5H10O2	000108-21-4	36
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Isobutyl acetate	116	C6H12O2	000110-19-0	9





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Sample : M1375-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ2

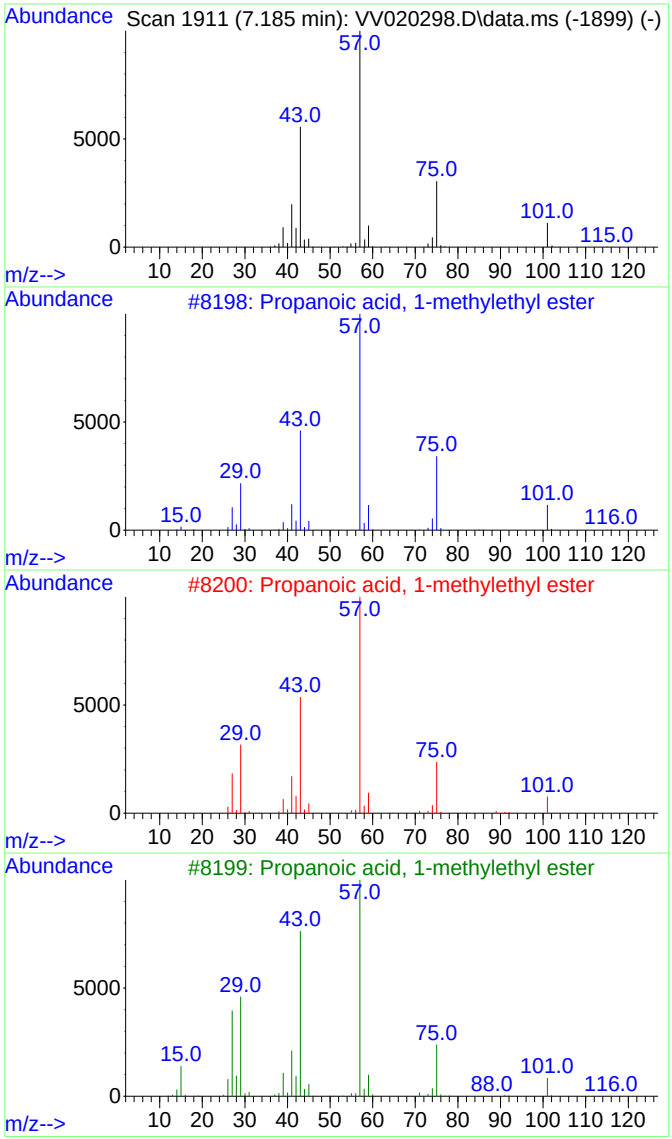
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

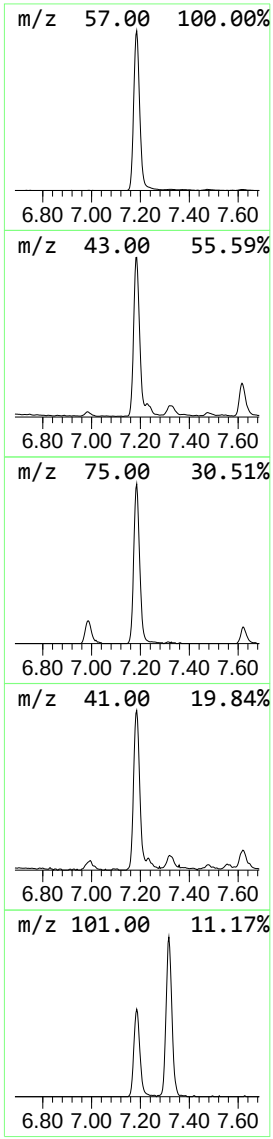
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	15.38 ug/L	431731	1,4-Difluorobenzene	5.616

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	78
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	40





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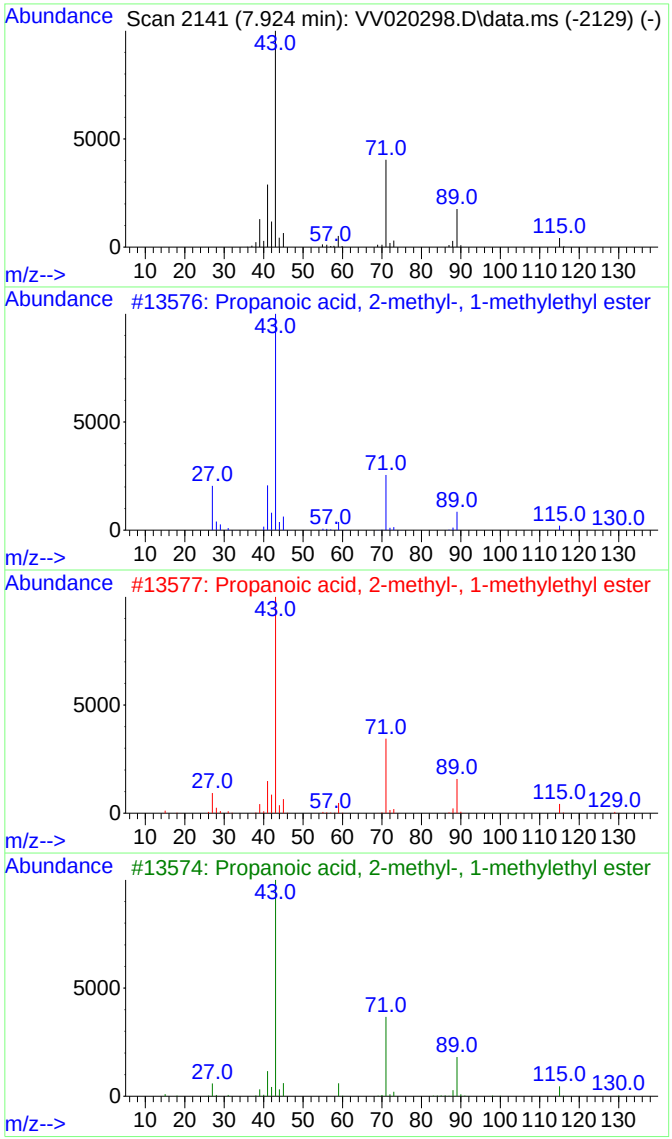
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

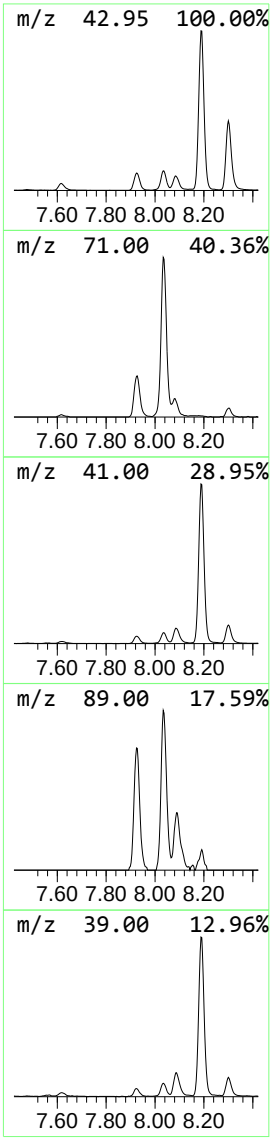
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.924	3.20 ug/L	117279	Chlorobenzene-d5	8.853

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	78
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56





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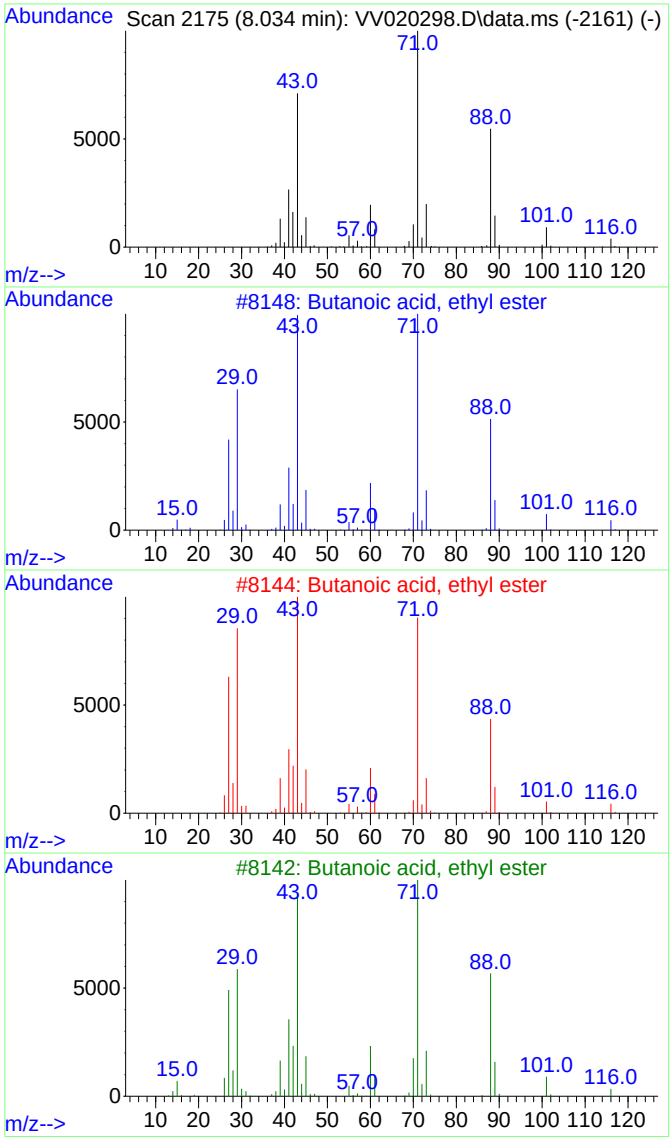
Quant Title : VOC Analysis

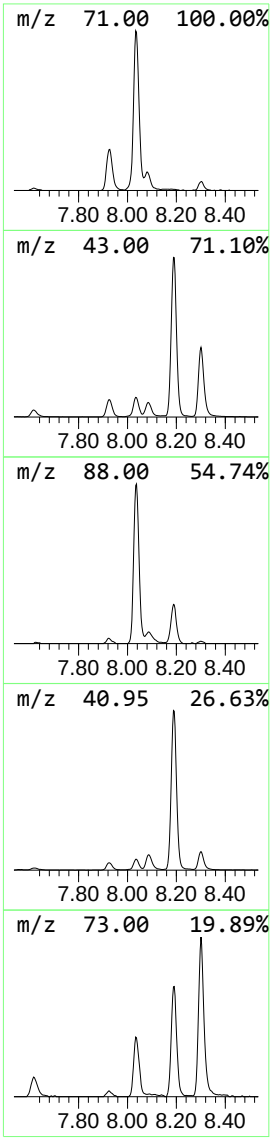
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	7.73 ug/L	283043	Chlorobenzene-d5	8.853

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
3	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
4	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	47
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ2

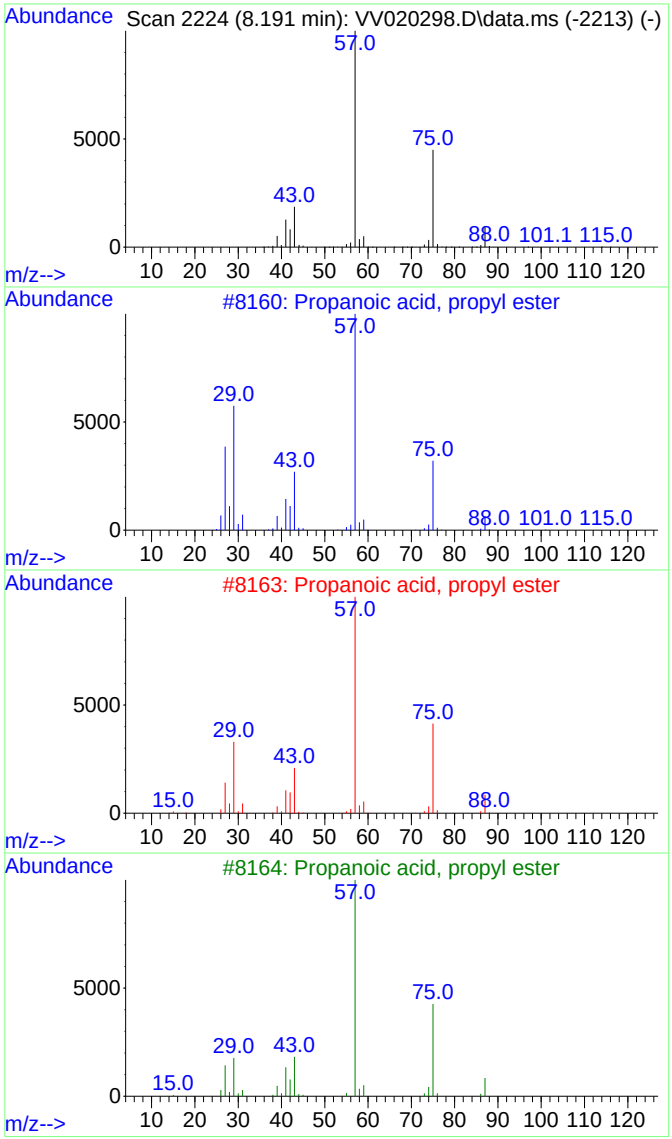
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

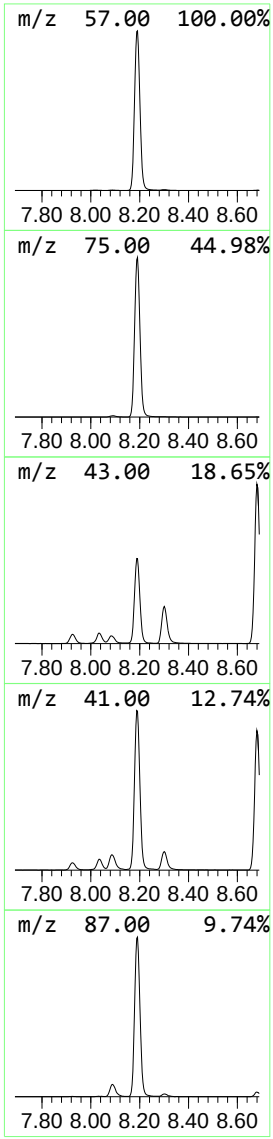
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	125.62 ug/L	4598290	Chlorobenzene-d5	8.853

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, butyl ester	130	C7H14O2	000590-01-2	28





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Acq On : 11 Feb 2021 14:53
Operator : SY/MD
Sample : M1375-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

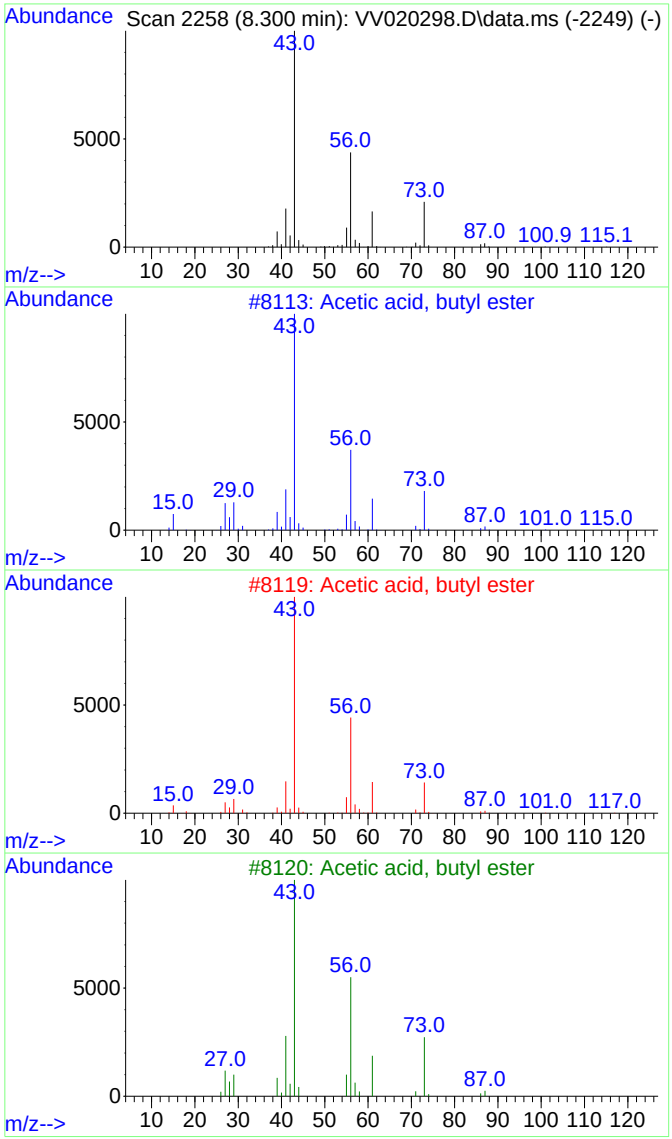
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

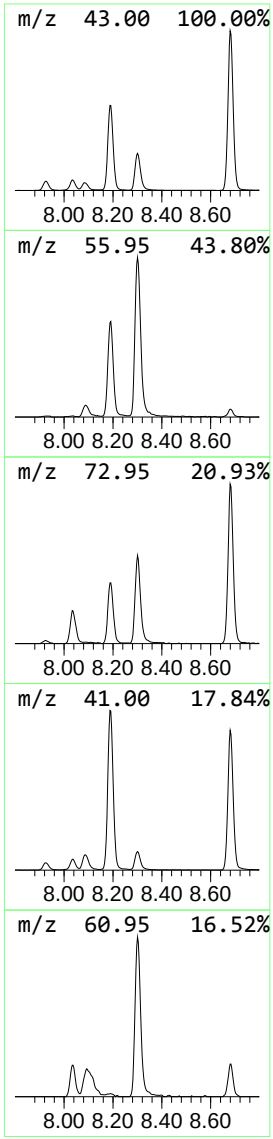
****

Peak Number 8 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.300	12.30 ug/L	450245	Chlorobenzene-d5	8.853

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020298.D
Acq On : 11 Feb 2021 14:53
Operator : SY/MD
Sample : M1375-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ2

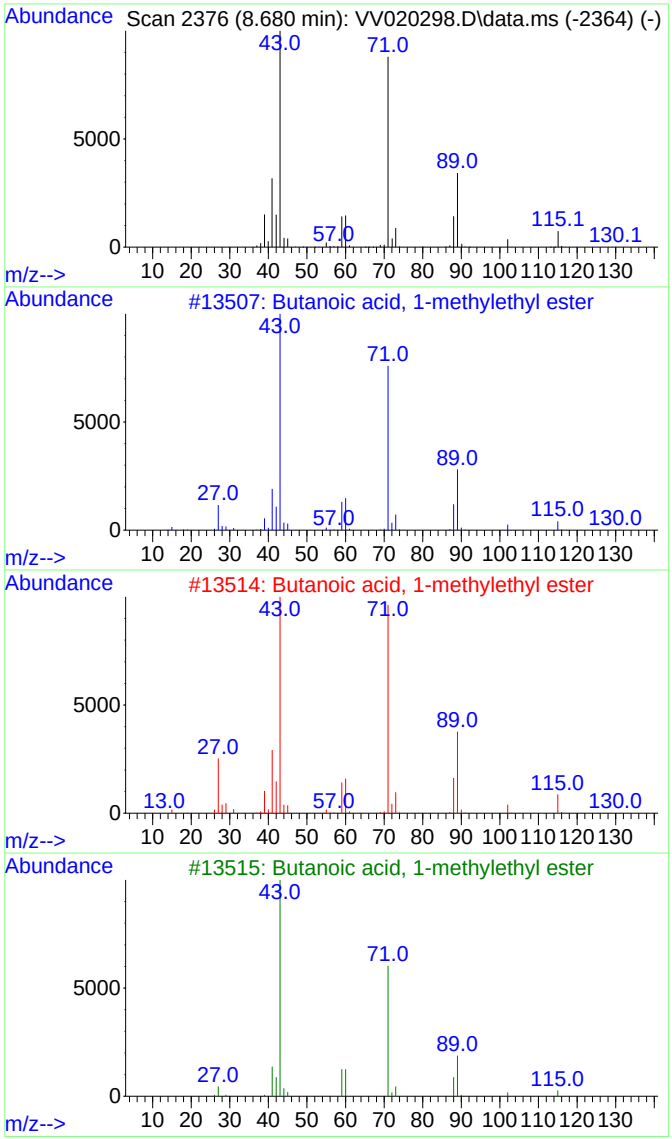
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

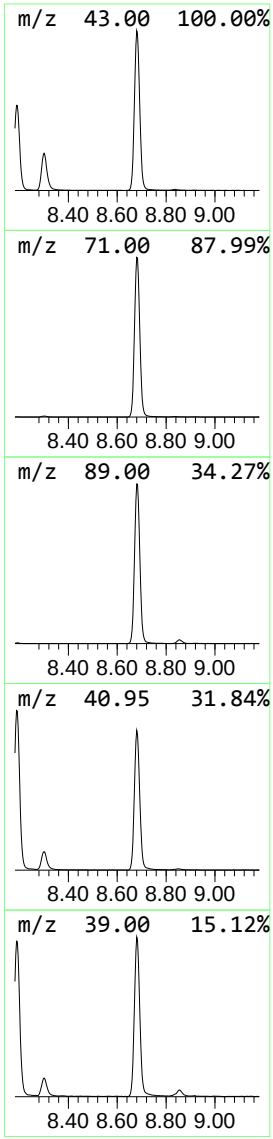
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	72.77 ug/L	2663580	Chlorobenzene-d5	8.853

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	91
3	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020298.D
Acq On : 11 Feb 2021 14:53
Operator : SY/MD
Sample : M1375-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.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	6.458	106.5	ug/L	2987580	1	5.616	1403220	50.0
Propanoic acid,...	7.185	15.4	ug/L	431731	1	5.616	1403220	50.0
Propanoic acid,...	7.924	3.2	ug/L	117279	2	8.853	1830190	50.0
Butanoic acid, ...	8.034	7.7	ug/L	283043	2	8.853	1830190	50.0
Propanoic acid,...	8.191	125.6	ug/L	4598290	2	8.853	1830190	50.0
Acetic acid, bu...	8.300	12.3	ug/L	450245	2	8.853	1830190	50.0
Butanoic acid, ...	8.680	72.8	ug/L	2663580	2	8.853	1830190	50.0