LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020299.D
Acq On : 11 Feb 2021 15:17
Operator : SY/MD
Sample : M1375-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

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: VV020299.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	77	83	97	rVB	267949	270420	5.75%	0.953%
2	1.381	101	106	117	rBV	16368	19394	0.41%	0.068%
3	1.568	157	164	179	rVB	245239	273868	5.82%	0.965%
4	2.108	321	332	346	rBV	470745	719637	15.30%	2.535%
5	2.510	446	457	471	rVB	36399	60844	1.29%	0.214%
6	2.642	488	498	499	rBV3	2333	2764	0.06%	0.010%
7	2.799	545	547	551	rBV4	473	361	0.01%	0.001%
8	2.899	574	578	581	rBV3	493	396	0.01%	0.001%
9	2.944	590	592	594	rBV	730	428	0.01%	0.002%
10	2.999	604	609	615	rBV2	426	464	0.01%	0.002%
11	3.027	616	618	623	rVV2	551	480	0.01%	0.002%
12	3.108	638	643	648	rBV3	643	590	0.01%	0.002%
13	3.211	673	675	680	rVB3	445	331	0.01%	0.001%
14	3.236	680	683	688	rVB3	332	374	0.01%	0.001%
15	3.278	688	696	698	rBV3	379	354	0.01%	0.001%
16	3.343	709	716	720	rVB5	570	528	0.01%	0.002%
17	3.400	729	734	738	rBV4	504	605	0.01%	0.002%
18	3.433	738	744	746	rBV2	1491	1366	0.03%	0.005%
19	3.719	823	833	834	rBV4	2421	3214	0.07%	0.011%
20	3.880	872	883	907	rBV	154381	421405	8.96%	1.484%
21	4.162	968	971	975	rVB5	793	414	0.01%	0.001%
22	4.352	1012	1030	1061	rBV	298337	790769	16.81%	2.786%
23	4.613	1107	1111	1113	rBV3	449	321	0.01%	0.001%
24	4.709	1137	1141	1147	rVB4	323	369	0.01%	0.001%
25	4.741	1149	1151	1156	rVB3	478	350	0.01%	0.001%
26	4.963	1213	1220	1225	rBV3	544	654	0.01%	0.002%
27	5.050	1227	1247	1279	rBV2	762976	1979537	42.08%	6.973%
28	5.281	1310	1319	1337	rBV2	20728	47057	1.00%	0.166%
29	5.423	1358	1363	1365	rBV5	707	530	0.01%	0.002%
30	5.484	1380	1382	1386	rBV2	771	422	0.01%	0.001%
31	5.503	1386	1388	1393	rVB3	438	351	0.01%	0.001%
32	5.529	1393	1396	1397	rBV3	774	414	0.01%	0.001%
33	5.619	1411	1424	1447	rBV	661580	1342198	28.53%	4.728%
34	6.072	1552	1565	1590	rVV	442251	886437	18.84%	3.122%
35	6.188	1594	1601	1615	rVB	12640	25450	0.54%	0.090%
36	6.339	1634	1648	1670	rVB2	22907	76883	1.63%	0.271%

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

37	6.461	1674	1686	1722	rBV	1807262	3186089	67.73%	11.223%
38	6.899	1820	1822	1826	rBV5	654	544	0.01%	0.002%
39	6.989	1838	1850	1877	rBV	249934	450820	9.58%	1.588%
40	7.188	1900	1912	1940	rBV	274885	486511	10.34%	1.714%
41	7.320	1940	1953	1972	rBV	951513	1640933	34.88%	5.780%
42	7.622	2037	2047	2069	rVB2	194466	340860	7.25%	1.201%
43	7.928	2130	2142	2155	rBV	74637	127693	2.71%	0.450%
44	8.037	2161	2176	2184	rBV	186971	306302	6.51%	1.079%
45	8.088	2184	2192	2209	rVB	576932	964922	20.51%	3.399%
46	8.191	2214	2224	2249	rVV	3110786	4704217	100.00%	16.571%
47	8.304	2250	2259	2290	rVB	275051	454574	9.66%	1.601%
48	8.683	2364	2377	2406	rBV	1791801	2677186	56.91%	9.430%
49	8.857	2418	2431	2464	rVB	1065001	1715915	36.48%	6.044%
50	9.120	2508	2513	2520	rBV7	1639	2387	0.05%	0.008%
51	9.175	2526	2530	2532	rBV5	715	593	0.01%	0.002%
52	9.239	2548	2550	2553	rVB2	1078	564	0.01%	0.002%
53	9.400	2592	2600	2608	rBV6	3291	5322	0.11%	0.019%
54	9.551	2638	2647	2656	rBV	48211	71826	1.53%	0.253%
55	9.603	2656	2663	2675	rVB2	30280	46528	0.99%	0.164%
56	9.719	2693	2699	2710	rVB4	3779	5596	0.12%	0.020%
57	9.792	2720	2722	2725	rVB2	737	335	0.01%	0.001%
58	9.947	2762	2770	2772	rBV6	817	894	0.02%	0.003%
59	10.223	2843	2856	2873	rBV	618891	973576	20.70%	3.429%
60	10.342	2891	2893	2895	rBV2	796	330	0.01%	0.001%
61	10.542	2951	2955	2956	rBV3	545	361	0.01%	0.001%
62	10.770	3020	3026	3037	rVB8	2035	3614	0.08%	0.013%
63	10.828	3042	3044	3048	rVB3	643	382	0.01%	0.001%
64	10.850	3048	3051	3052	rBV	711	310	0.01%	0.001%
65	10.866	3053	3056	3058	rBV4	619	362	0.01%	0.001%
66	10.944	3068	3080	3090	rBV6	8981	13937	0.30%	0.049%
67	11.018	3101	3103	3106	rVB2	767	370	0.01%	0.001%
68	11.050	3106	3113	3123	rBV5	3209	5705	0.12%	0.020%
69	11.104	3128	3130	3136	rVB4	704	508	0.01%	0.002%
70	11.162	3140	3148	3150	rBV3	1418	1623	0.03%	0.006%
71	11.194	3155	3158	3164	rVB5	1446	1126	0.02%	0.004%
72	11.255	3164	3177	3201	rBV	1100036	1668610	35.47%	5.878%
73	11.497	3249	3252	3256	rBV3	807	614	0.01%	0.002%
74	11.545	3256	3267	3270	rBV5	3751	6141	0.13%	0.022%
75	11.632	3282	3294	3311	rBV	1010497	1570590	33.39%	5.532%
76	11.812	3347	3350	3351	rBV2	680	350	0.01%	0.001%

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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Title : VOC Analysis

77	11.860	3363	3365	3371	rVB5	820	625	0.01%	0.002%
78	11.895	3374	3376	3382	rVB5	581	452	0.01%	0.002%
79	11.940	3388	3390	3394	rBV2	429	306	0.01%	0.001%
80	11.982	3397	3403	3407	rBV5	2845	3476	0.07%	0.012%
81	12.156	3454	3457	3458	rBV3	620	316	0.01%	0.001%
82	12.214	3473	3475	3481	rVB3	489	435	0.01%	0.002%
83	12.252	3481	3487	3488	rBV3	1789	1833	0.04%	0.006%
84	12.355	3514	3519	3527	rVB8	2779	3902	0.08%	0.014%
85	12.583	3588	3590	3594	rVB2	745	454	0.01%	0.002%
86	12.747	3639	3641	3646	rVB3	922	494	0.01%	0.002%
87	12.927	3694	3697	3699	rBV2	494	360	0.01%	0.001%
88	13.262	3797	3801	3803	rBV2	607	535	0.01%	0.002%
89	13.442	3852	3857	3859	rBV4	617	531	0.01%	0.002%
90	13.738	3946	3949	3951	rBV3	593	367	0.01%	0.001%
91	14.001	4029	4031	4036	rVB3	708	511	0.01%	0.002%
92	14.088	4055	4058	4065	rVB5	1182	1047	0.02%	0.004%
93	14.413	4157	4159	4163	rVB3	1059	619	0.01%	0.002%
94	14.525	4190	4194	4196	rBV3	593	526	0.01%	0.002%
95	14.564	4203	4206	4209	rVB2	616	310	0.01%	0.001%
96	14.731	4255	4258	4260	rBV3	518	369	0.01%	0.001%
97	14.914	4313	4315	4319	rBV2	589	341	0.01%	0.001%
98	15.075	4362	4365	4367	rBV	1028	543	0.01%	0.002%
99	15.381	4458	4460	4466	rBV5	744	821	0.02%	0.003%
100	15.783	4583	4585	4586	rBV	1152	450	0.01%	0.002%

Sum of corrected areas: 28388722

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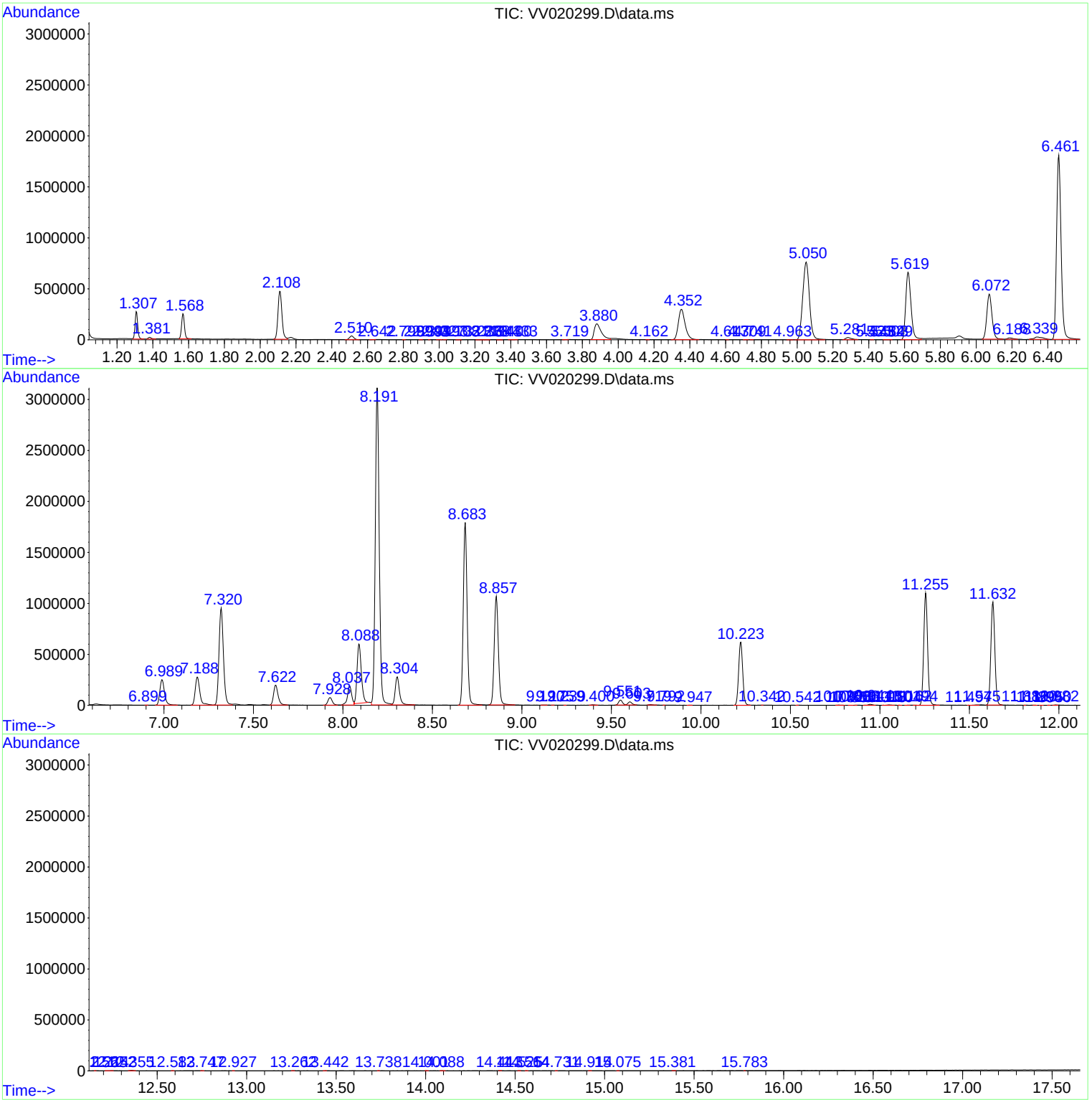
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BJ3

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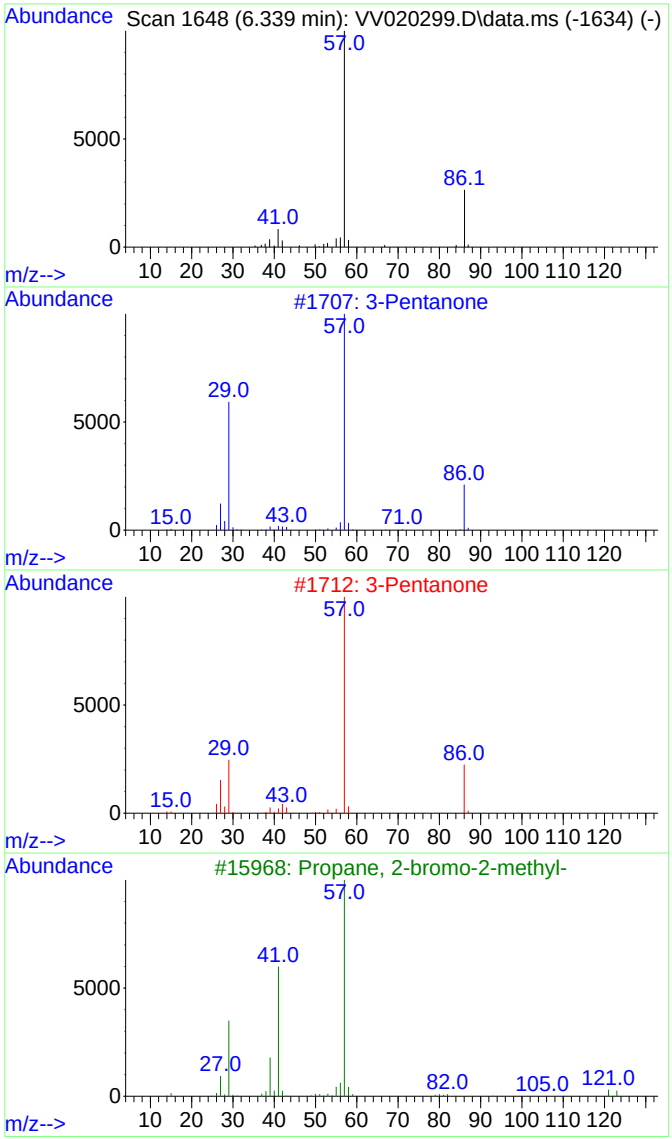
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

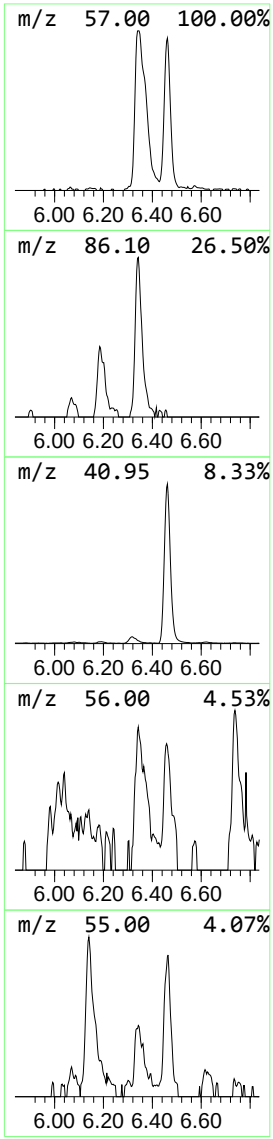
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.339	2.86 ug/L	76883	1,4-Difluorobenzene	5.619

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
2	3-Pentanone	86	C5H10O	000096-22-0	58
3	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	23
4	3-Pentanone	86	C5H10O	000096-22-0	9
5	Azetidine	57	C3H7N	000503-29-7	9





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Sample : M1375-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

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

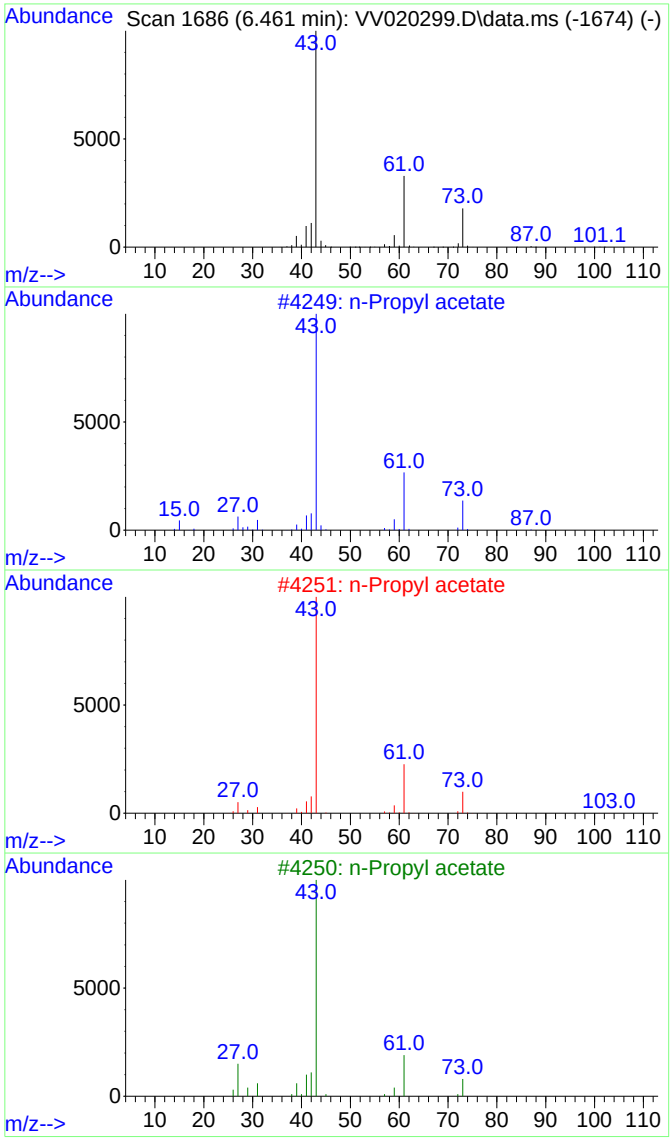
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

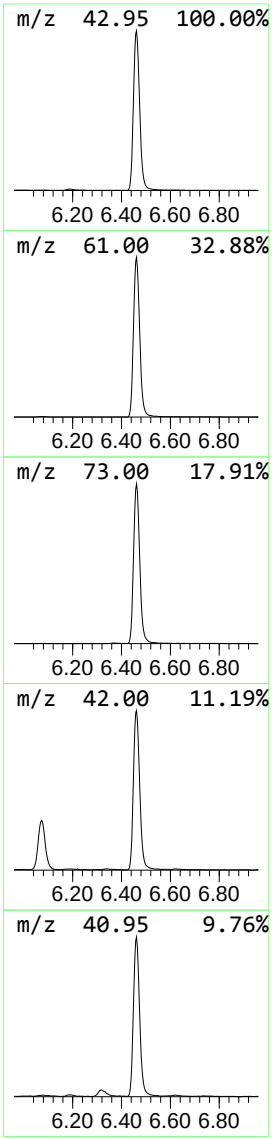
****

Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.461	118.69 ug/L	3186090	1,4-Difluorobenzene	5.619

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	Isopropyl acetate	102	C5H10O2	000108-21-4	36
5	Isobutylamine	73	C4H11N	000078-81-9	9





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ClientSampleId : C0BJ3

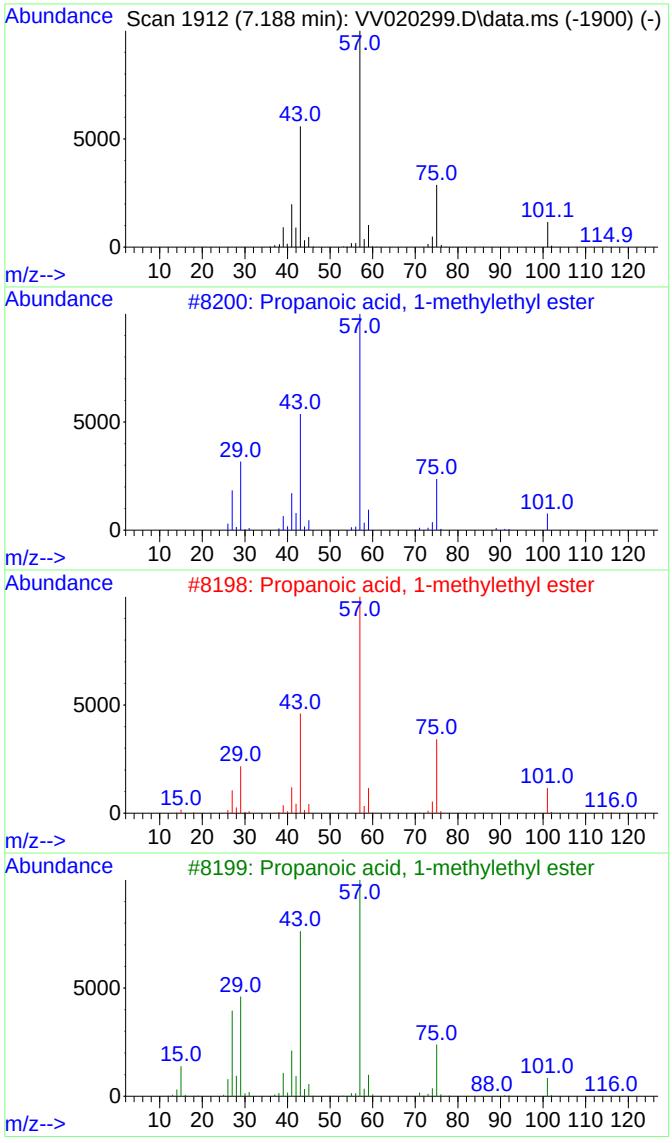
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

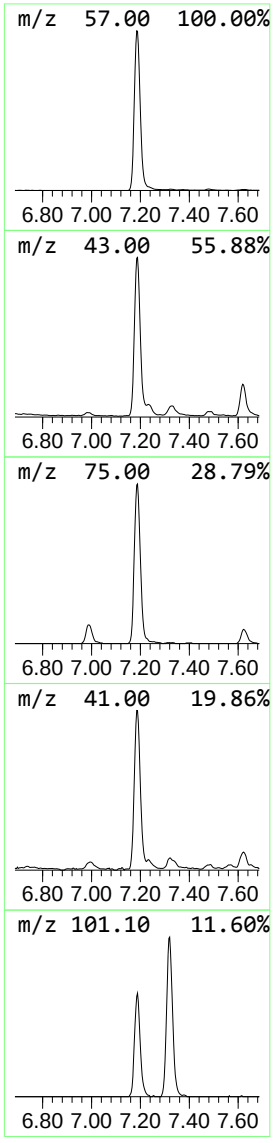
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.188	18.12 ug/L	486511	1,4-Difluorobenzene	5.619

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	78
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	74
4	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53





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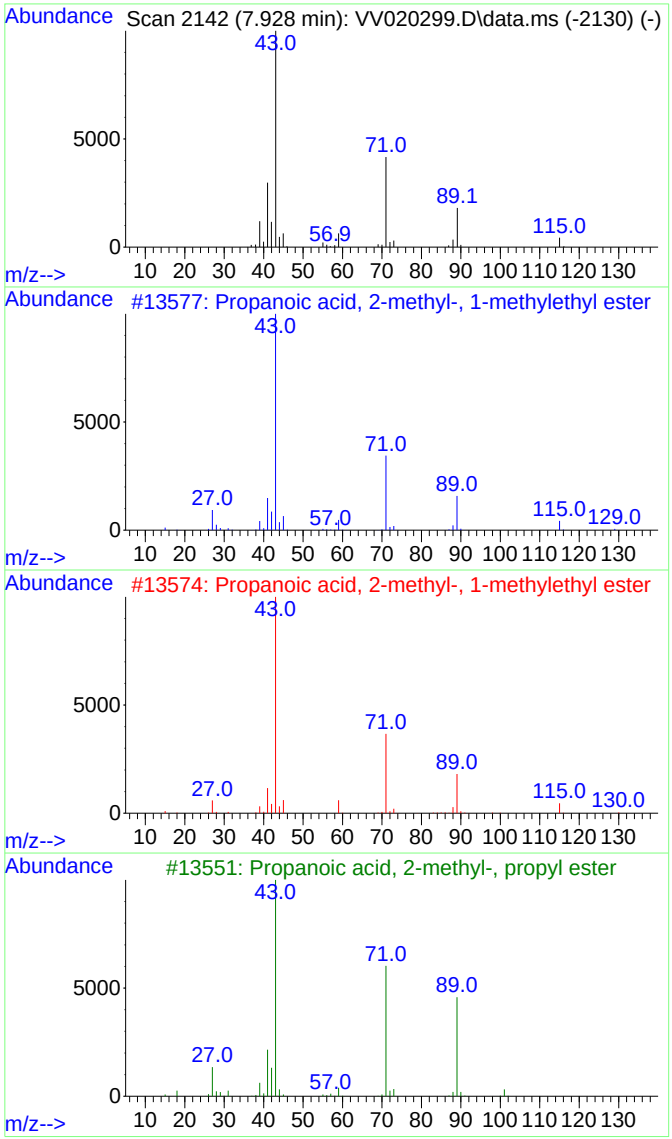
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

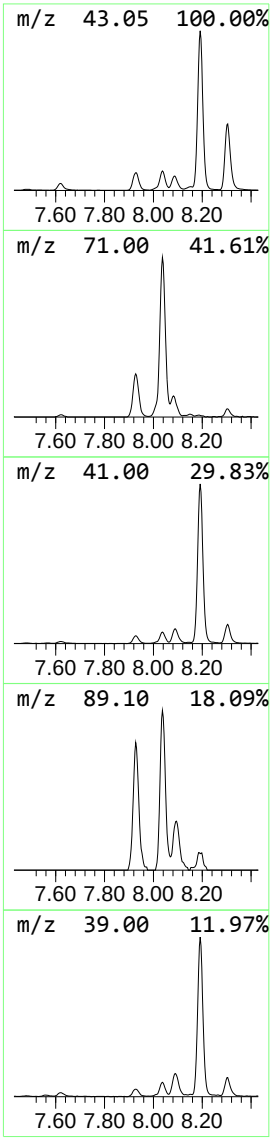
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.928	3.72 ug/L	127693	Chlorobenzene-d5	8.857

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	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	64





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

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

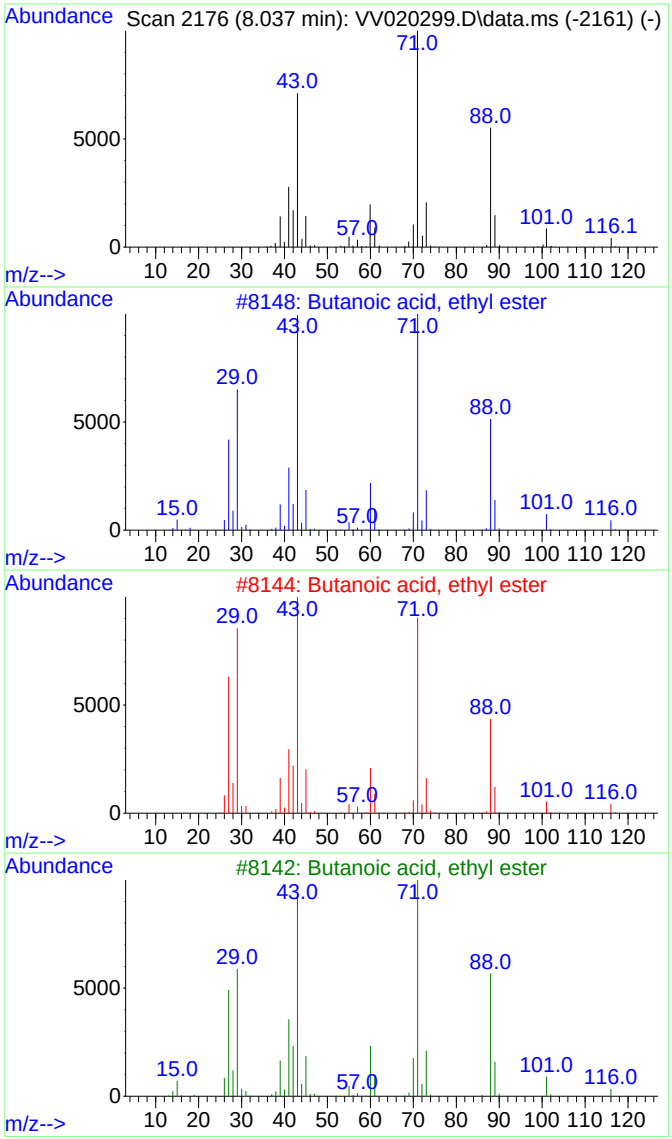
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

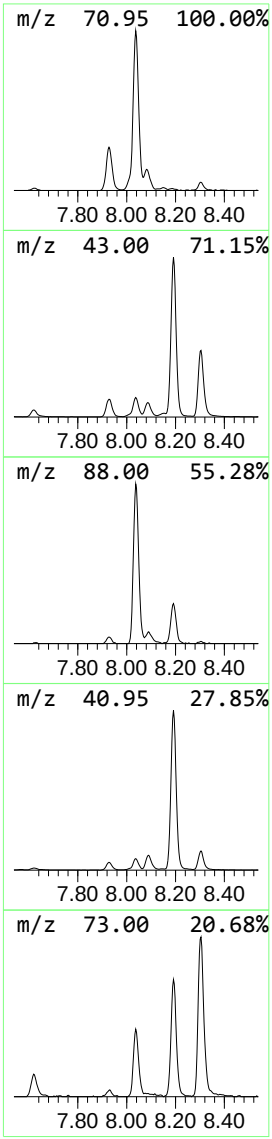
****

Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.037	8.93 ug/L	306302	Chlorobenzene-d5	8.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	93
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020299.D
Acq On : 11 Feb 2021 15:17
Operator : SY/MD
Sample : M1375-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

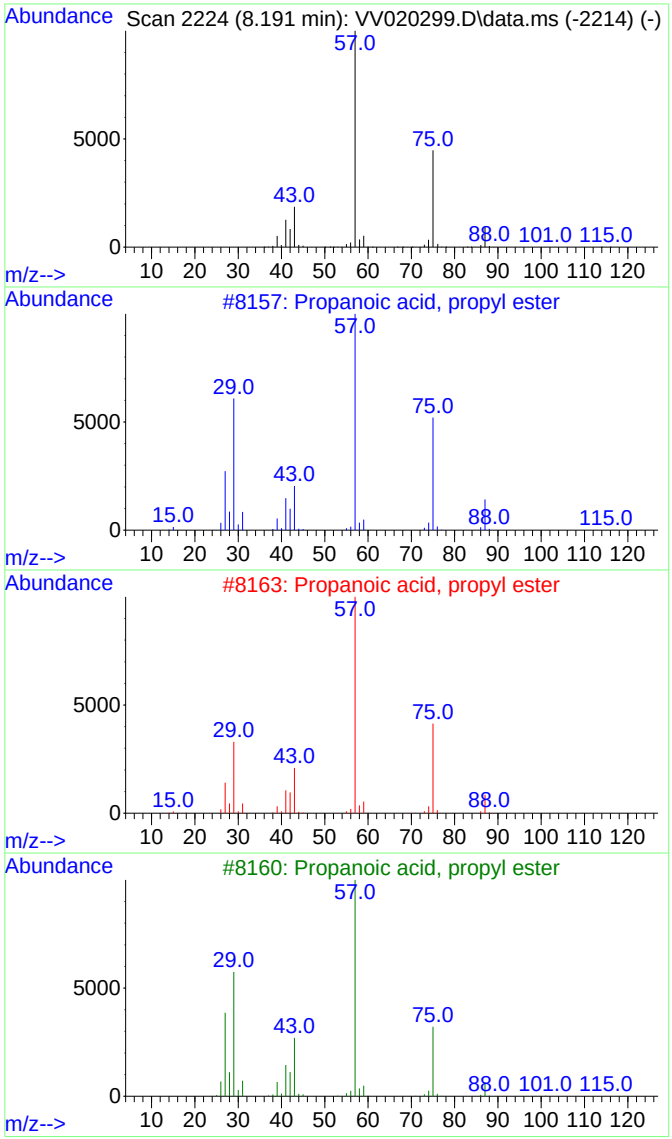
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

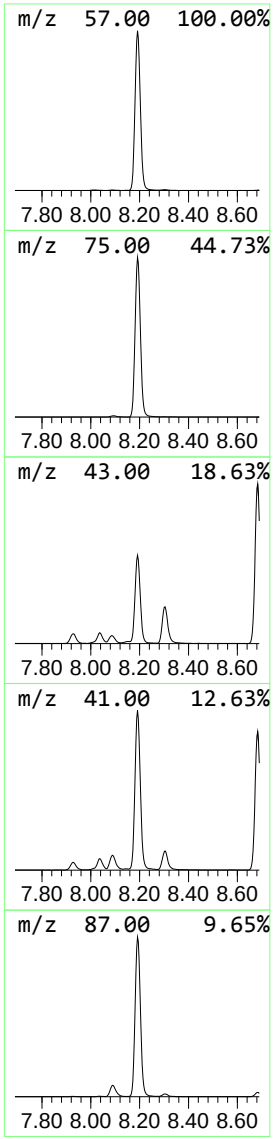
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.191	137.08 ug/L	4704220	Chlorobenzene-d5	8.857

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020299.D
Acq On : 11 Feb 2021 15:17
Operator : SY/MD
Sample : M1375-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

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

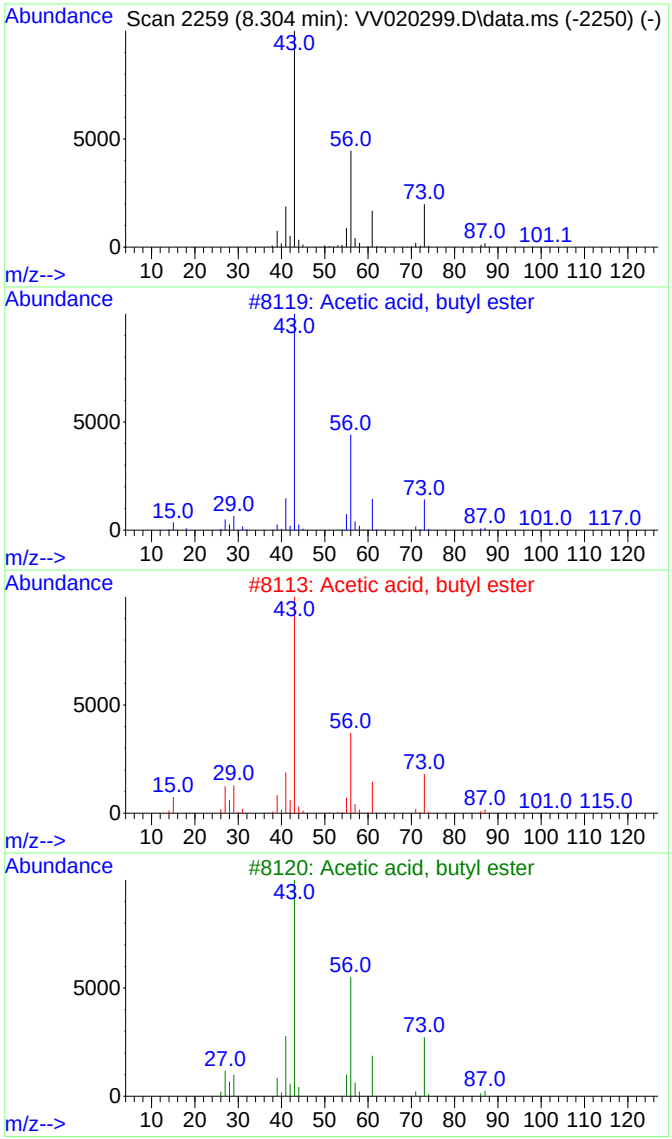
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

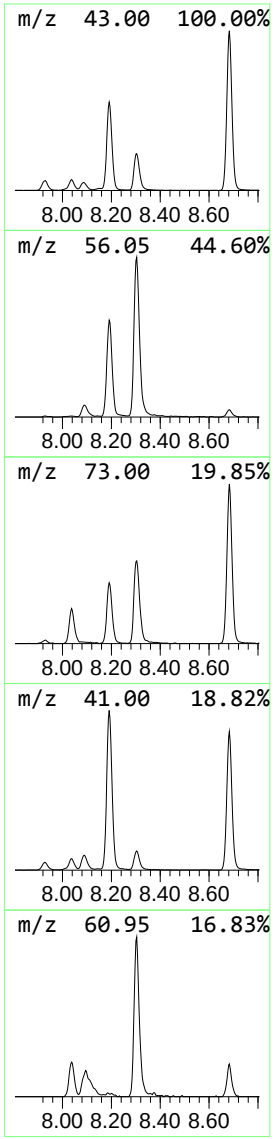
****

Peak Number 8 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	13.25 ug/L	454574	Chlorobenzene-d5	8.857

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	83
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021121\
Data File : VV020299.D
Acq On : 11 Feb 2021 15:17
Operator : SY/MD
Sample : M1375-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

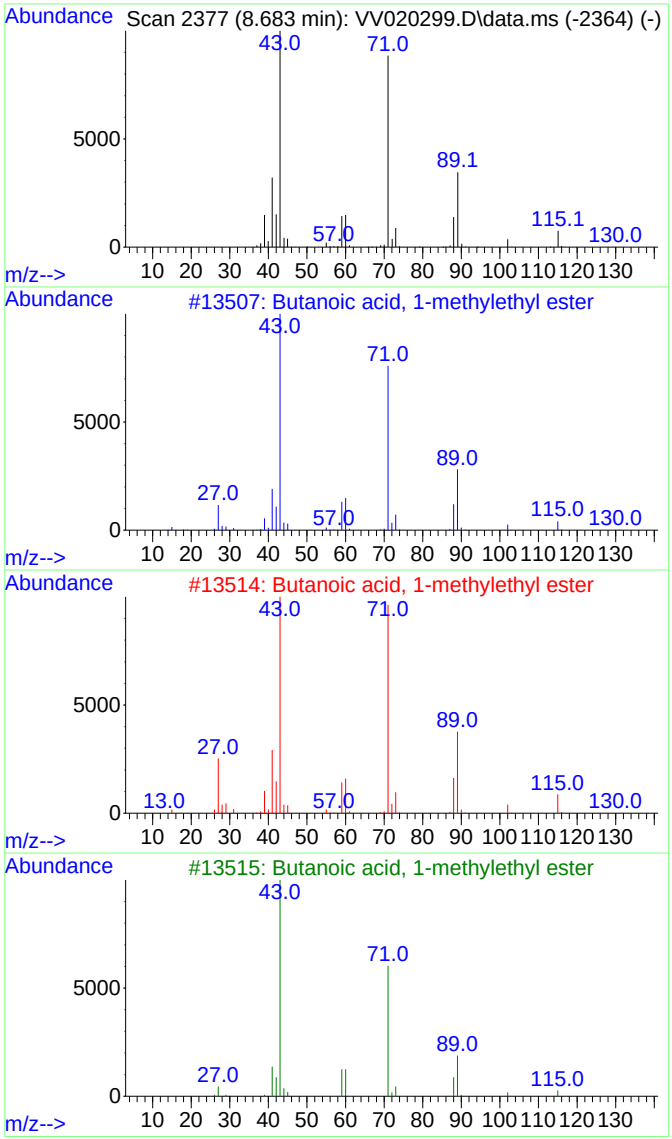
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM020521WMA.M
Quant Title : VOC Analysis

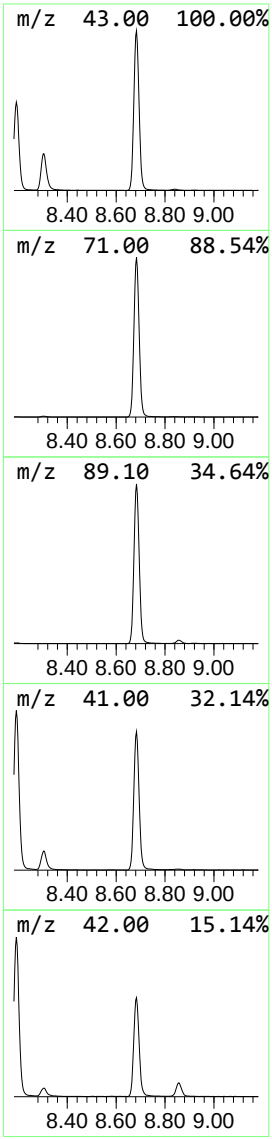
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.683	78.01 ug/L	2677190	Chlorobenzene-d5	8.857

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	83
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 : VV020299.D
Acq On : 11 Feb 2021 15:17
Operator : SY/MD
Sample : M1375-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BJ3

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
3-Pentanone	6.339	2.9	ug/L	76883	1	5.619	1342200	50.0
n-Propyl acetate	6.461	118.7	ug/L	3186090	1	5.619	1342200	50.0
Propanoic acid,...	7.188	18.1	ug/L	486511	1	5.619	1342200	50.0
Propanoic acid,...	7.928	3.7	ug/L	127693	2	8.857	1715920	50.0
Butanoic acid, ...	8.037	8.9	ug/L	306302	2	8.857	1715920	50.0
Propanoic acid,...	8.191	137.1	ug/L	4704220	2	8.857	1715920	50.0
Acetic acid, bu...	8.304	13.3	ug/L	454574	2	8.857	1715920	50.0
Butanoic acid, ...	8.683	78.0	ug/L	2677190	2	8.857	1715920	50.0