LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041723\
Data File : VV030591.D
Acq On : 17 Apr 2023 16:11
Operator : SY/MD
Sample : PB152132TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB132

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\SFAMVLM041723WMA.M
Title : VOC Analysis

Signal : TIC: VV030591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.285	70	76	85	rVB	39035	42241	5.57%	1.200%
2	1.539	150	155	163	rVB	40117	45185	5.96%	1.284%
3	2.066	311	319	331	rBV	71332	97977	12.92%	2.784%
4	2.558	469	472	475	rBV5	1885	1007	0.13%	0.029%
5	2.619	488	491	493	rBV4	980	595	0.08%	0.017%
6	2.789	542	544	546	rVB2	1461	506	0.07%	0.014%
7	2.805	546	549	551	rBV2	795	523	0.07%	0.015%
8	2.828	554	556	559	rBV3	1248	759	0.10%	0.022%
9	2.850	559	563	565	rBV5	1447	1106	0.15%	0.031%
10	2.886	570	574	577	rVB5	1228	1091	0.14%	0.031%
11	2.918	582	584	585	rBV2	944	433	0.06%	0.012%
12	2.995	604	608	611	rBV6	1370	1121	0.15%	0.032%
13	3.140	652	653	656	rVB3	1306	399	0.05%	0.011%
14	3.320	707	709	712	rVB4	1058	406	0.05%	0.012%
15	3.336	712	714	716	rBV3	926	527	0.07%	0.015%
16	3.375	721	726	727	rBV4	1179	782	0.10%	0.022%
17	3.513	768	769	770	rBV2	1035	348	0.05%	0.010%
18	3.558	781	783	785	rBV3	1173	711	0.09%	0.020%
19	3.603	794	797	799	rBV4	1214	694	0.09%	0.020%
20	3.635	804	807	809	rVB4	1197	541	0.07%	0.015%
21	3.696	823	826	829	rBV4	1273	659	0.09%	0.019%
22	3.715	829	832	835	rBV5	860	626	0.08%	0.018%
23	3.735	835	838	840	rBV4	972	679	0.09%	0.019%
24	3.799	847	858	887	rBV	113910	326605	43.08%	9.279%
25	4.259	990	1001	1022	rVB2	49689	131243	17.31%	3.729%
26	4.538	1086	1088	1089	rBV2	1102	367	0.05%	0.010%
27	4.561	1093	1095	1096	rBV2	1017	425	0.06%	0.012%
28	4.654	1123	1124	1127	rBV4	1001	344	0.05%	0.010%
29	4.670	1127	1129	1133	rVB4	1613	989	0.13%	0.028%
30	4.879	1192	1194	1196	rVB3	1007	392	0.05%	0.011%
31	4.969	1207	1222	1245	rBV3	116222	313141	41.31%	8.896%
32	5.545	1392	1401	1425	rVB	47606	104132	13.74%	2.958%
33	5.998	1531	1542	1559	rBV2	70083	146453	19.32%	4.161%
34	6.400	1658	1667	1690	rBV	103632	198759	26.22%	5.647%
35	6.722	1765	1767	1769	rBV3	1365	738	0.10%	0.021%
36	6.821	1795	1798	1801	rVB3	1368	967	0.13%	0.027%

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Instrument :
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ClientSampleId :
LEB132

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\SFAMVLM041723WMA.M
Title : VOC Analysis

37	6.837	1801	1803	1806	rBV4	1528	884	0.12%	0.025%
38	6.876	1813	1815	1817	rBV4	1303	878	0.12%	0.025%
39	6.924	1821	1830	1846	rVB	34414	67862	8.95%	1.928%
40	7.127	1887	1893	1905	rVB2	22581	34639	4.57%	0.984%
41	7.252	1922	1932	1946	rBV	124219	220069	29.03%	6.252%
42	7.484	2002	2004	2005	rBV2	1197	499	0.07%	0.014%
43	7.561	2019	2028	2047	rBV2	53019	98876	13.04%	2.809%
44	7.870	2116	2124	2137	rVB	31353	51471	6.79%	1.462%
45	8.034	2165	2175	2199	rBV	408404	758080	100.00%	21.537%
46	8.625	2350	2359	2375	rBV	94400	153801	20.29%	4.370%
47	8.796	2403	2412	2428	rVB	80537	133385	17.60%	3.790%
48	9.284	2562	2564	2565	rBV2	1235	412	0.05%	0.012%
49	9.496	2624	2630	2638	rBV7	8315	11538	1.52%	0.328%
50	9.628	2669	2671	2675	rBV4	1286	888	0.12%	0.025%
51	9.927	2762	2764	2767	rBV4	1139	875	0.12%	0.025%
52	10.162	2827	2837	2853	rVB	104454	165445	21.82%	4.700%
53	10.480	2934	2936	2938	rBV4	2182	1186	0.16%	0.034%
54	10.519	2946	2948	2952	rVB4	1697	996	0.13%	0.028%
55	10.590	2968	2970	2976	rVB7	1536	1074	0.14%	0.031%
56	10.615	2976	2978	2982	rBV6	1151	649	0.09%	0.018%
57	10.696	3001	3003	3004	rBV	996	376	0.05%	0.011%
58	10.722	3010	3011	3016	rVB5	1750	678	0.09%	0.019%
59	10.950	3079	3082	3084	rBV4	1621	1064	0.14%	0.030%
60	10.988	3091	3094	3095	rBV3	1094	497	0.07%	0.014%
61	11.094	3125	3127	3133	rBV6	1109	709	0.09%	0.020%
62	11.194	3149	3158	3176	rVB	80077	131657	17.37%	3.740%
63	11.371	3209	3213	3218	rVB7	1452	1323	0.17%	0.038%
64	11.394	3218	3220	3221	rBV2	1293	503	0.07%	0.014%
65	11.522	3258	3260	3263	rBV3	1172	653	0.09%	0.019%
66	11.570	3263	3275	3293	rBV	136283	224970	29.68%	6.392%
67	11.667	3303	3305	3306	rBV3	1092	488	0.06%	0.014%
68	11.853	3357	3363	3365	rBV4	1394	1338	0.18%	0.038%
69	11.889	3372	3374	3376	rBV3	1157	595	0.08%	0.017%
70	11.937	3387	3389	3391	rBV2	1469	538	0.07%	0.015%
71	11.988	3403	3405	3409	rBV4	1186	689	0.09%	0.020%
72	12.008	3409	3411	3414	rVB4	1498	656	0.09%	0.019%
73	12.030	3414	3418	3422	rBV7	1372	1265	0.17%	0.036%
74	12.046	3422	3423	3427	rVV4	973	419	0.06%	0.012%
75	12.123	3445	3447	3448	rBV2	1308	414	0.05%	0.012%
76	12.242	3482	3484	3485	rBV2	987	368	0.05%	0.010%

LSC Area Percent Report

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Instrument :
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ClientSampleId :
LEB132

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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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Title : VOC Analysis

77	12.352	3516	3518	3524	rBV7	1143	636	0.08%	0.018%
78	12.641	3606	3608	3609	rBV2	1251	436	0.06%	0.012%
79	12.738	3635	3638	3641	rBV5	1628	1415	0.19%	0.040%
80	12.776	3647	3650	3652	rBV4	1346	874	0.12%	0.025%
81	12.956	3704	3706	3707	rBV2	945	322	0.04%	0.009%
82	13.082	3740	3745	3747	rBV5	1087	1040	0.14%	0.030%
83	13.104	3751	3752	3754	rBV2	962	405	0.05%	0.012%
84	13.352	3824	3829	3830	rBV5	1793	1237	0.16%	0.035%
85	13.422	3846	3851	3854	rBV6	1815	1923	0.25%	0.055%
86	13.455	3857	3861	3864	rBV6	2565	2708	0.36%	0.077%
87	13.554	3889	3892	3895	rBV4	1033	702	0.09%	0.020%
88	13.593	3902	3904	3908	rBV4	634	407	0.05%	0.012%
89	13.615	3908	3911	3914	rBV5	1547	934	0.12%	0.027%
90	13.670	3926	3928	3932	rBV5	927	613	0.08%	0.017%
91	13.689	3932	3934	3935	rBV2	1634	773	0.10%	0.022%
92	13.728	3943	3946	3947	rBV2	1526	756	0.10%	0.021%
93	13.779	3958	3962	3964	rBV5	1508	1023	0.13%	0.029%
94	13.873	3989	3991	3992	rBV2	876	326	0.04%	0.009%
95	13.882	3992	3994	4001	rVV7	1863	1761	0.23%	0.050%
96	13.911	4001	4003	4007	rVV4	1278	731	0.10%	0.021%
97	13.946	4012	4014	4020	rVB6	1460	1368	0.18%	0.039%
98	14.242	4098	4106	4108	rBV7	1564	1744	0.23%	0.050%
99	14.329	4131	4133	4136	rBV4	1514	749	0.10%	0.021%
100	14.847	4292	4294	4296	rBV3	1577	769	0.10%	0.022%

Sum of corrected areas: 3519830

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041723\
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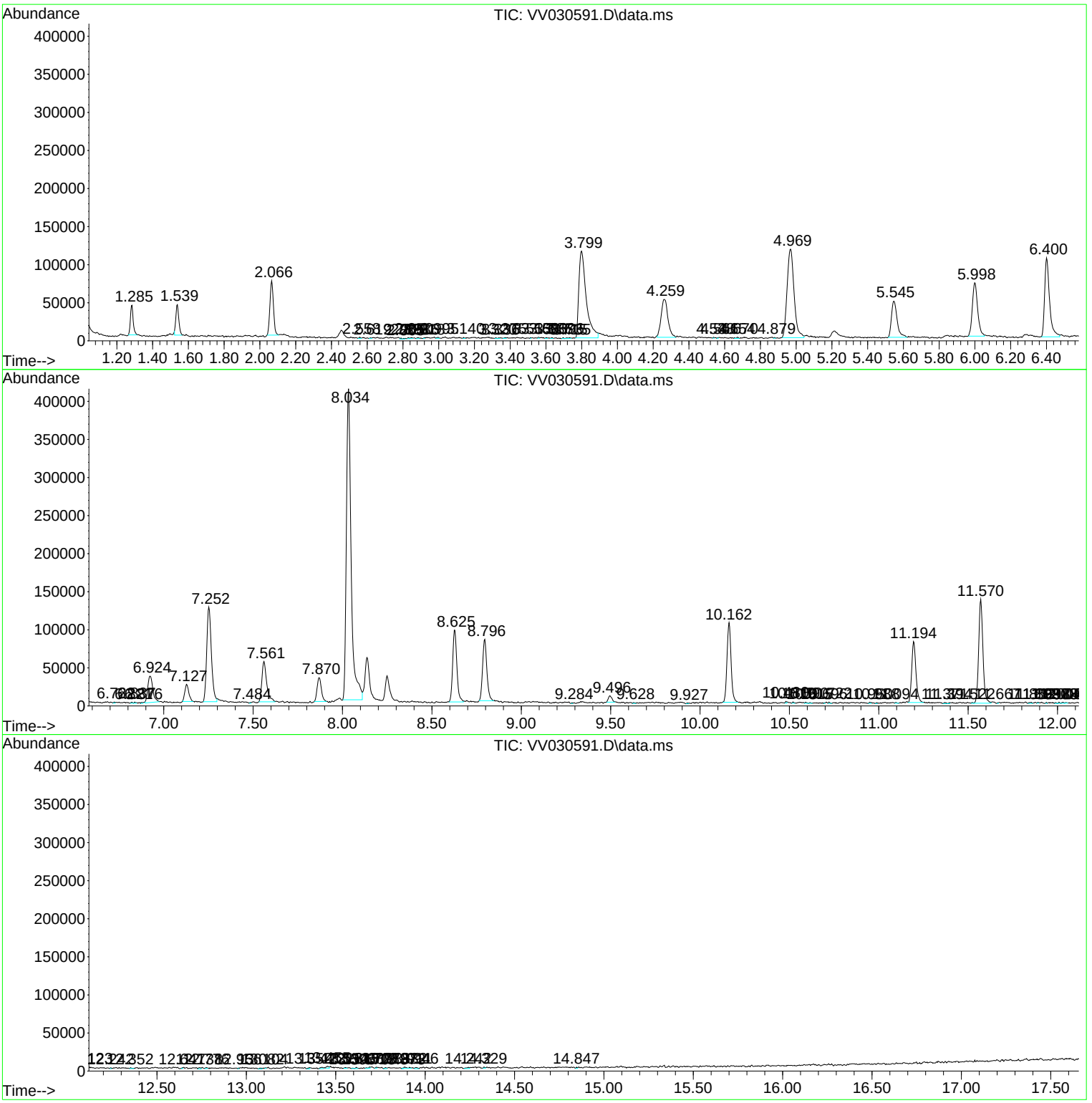
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041723\
Data File : VV030591.D
Acq On : 17 Apr 2023 16:11
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB132

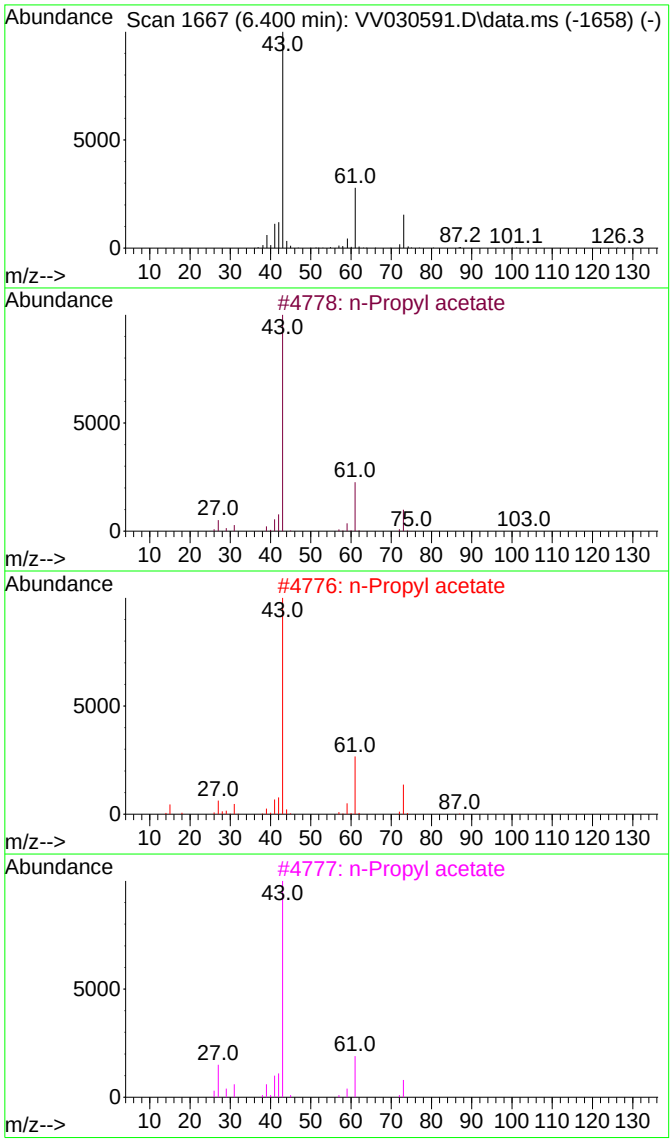
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Quant Title : VOC Analysis

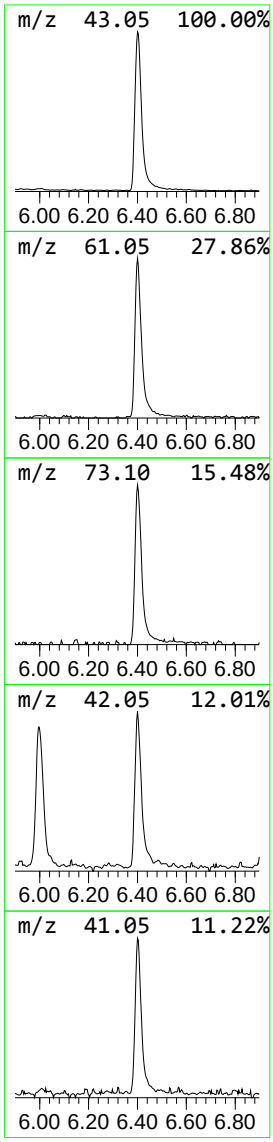
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.400	95.44 ug/L	198759	1,4-Difluorobenzene	5.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
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	72
5	n-Propyl acetate	102	C5H10O2	000109-60-4	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041723\
Data File : VV030591.D
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Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB132

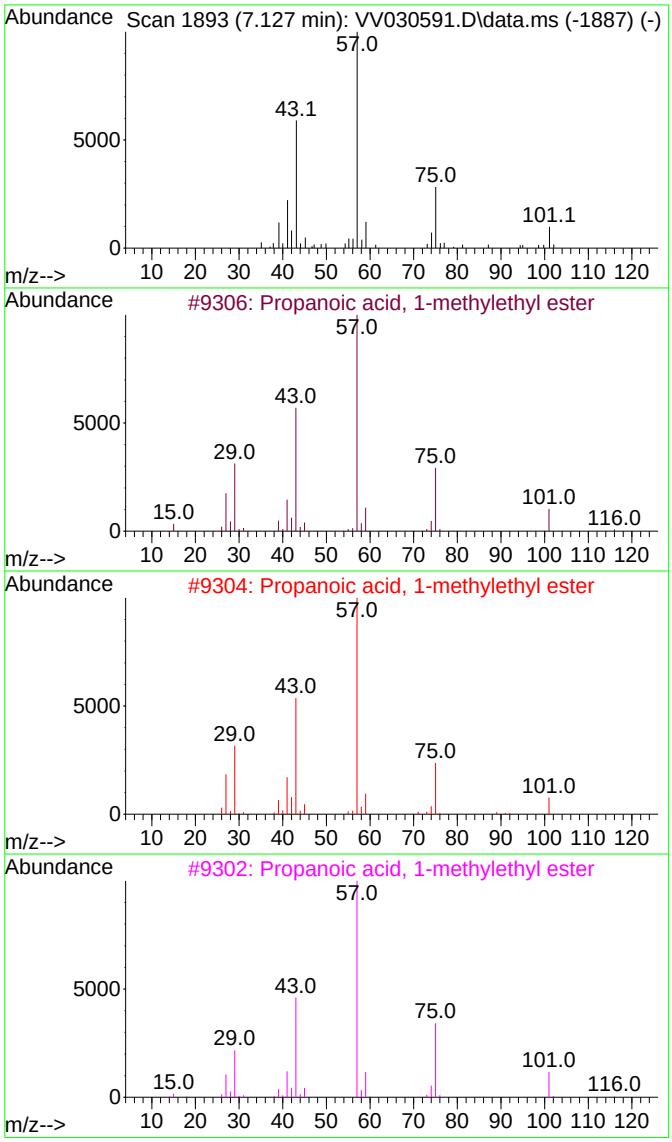
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Quant Title : VOC Analysis

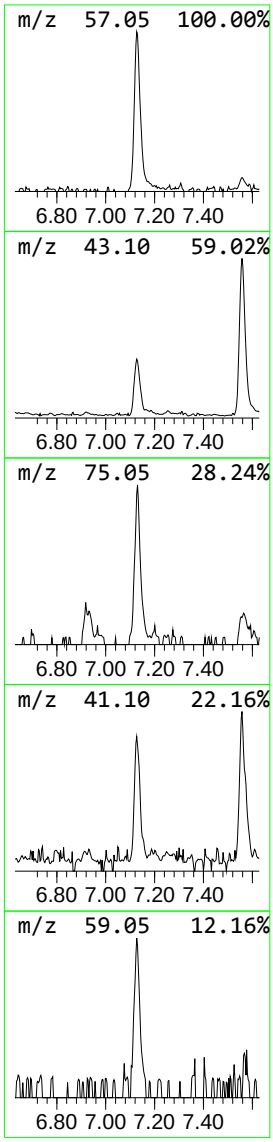
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	16.63 ug/L	34639	1,4-Difluorobenzene	5.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
2	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	53
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50
5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	38





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Instrument :
MSVOA_V
ClientSampleId :
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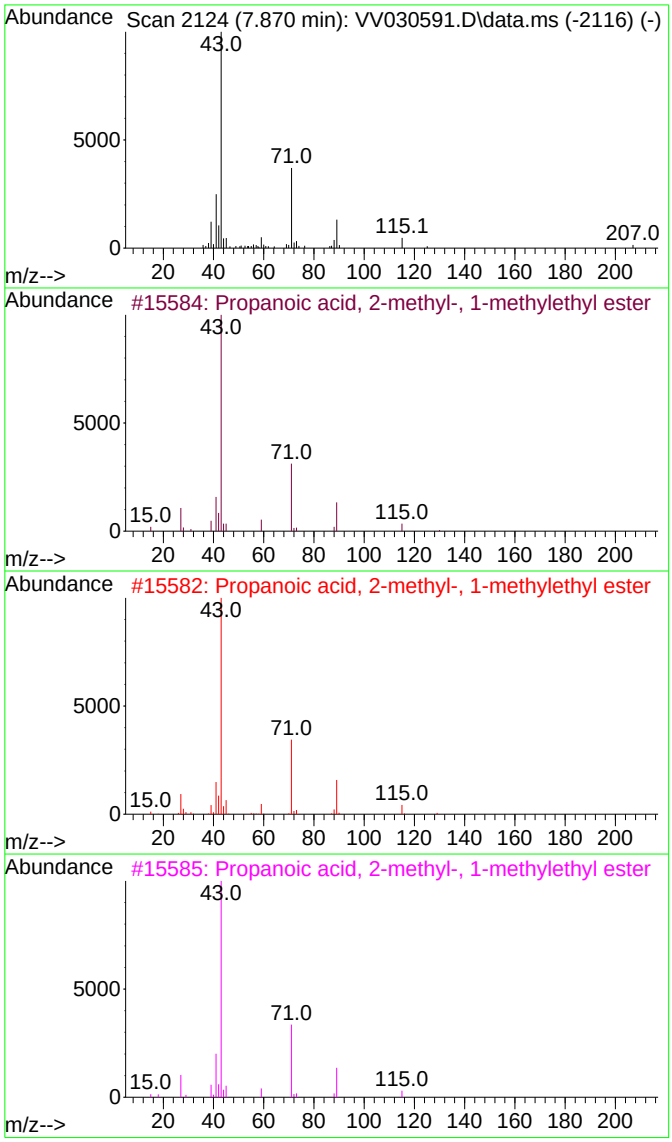
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Quant Title : VOC Analysis

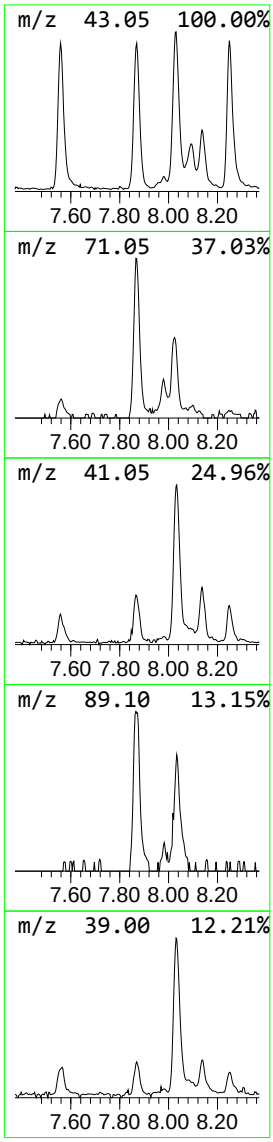
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.870	19.29 ug/L	51471	Chlorobenzene-d5	8.796

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	72
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59





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Instrument :
MSVOA_V
ClientSampleId :
LEB132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Quant Title : VOC Analysis

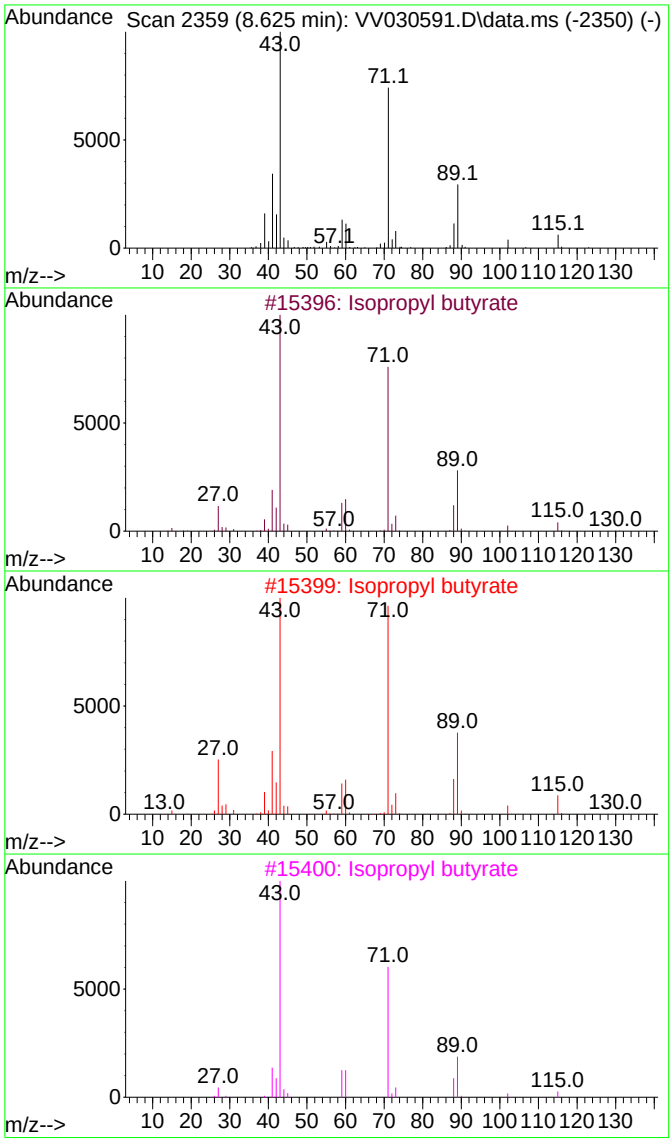
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

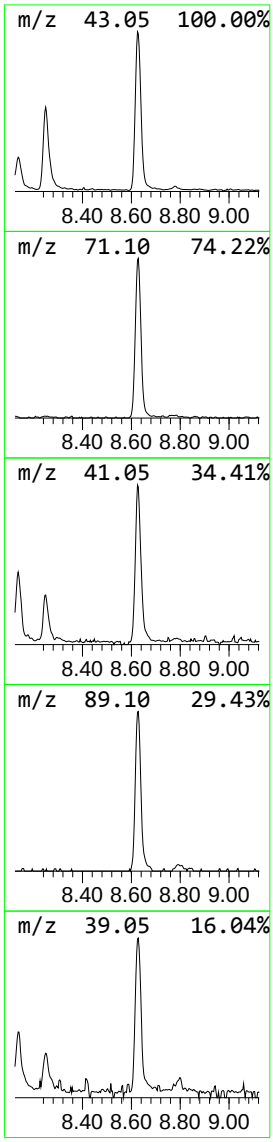
****

Peak Number 5 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.625	57.65 ug/L	153801	Chlorobenzene-d5	8.796

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	83
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





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Data File : VV030591.D
Acq On : 17 Apr 2023 16:11
Operator : SY/MD
Sample : PB152132TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.M
Quant Title : VOC Analysis

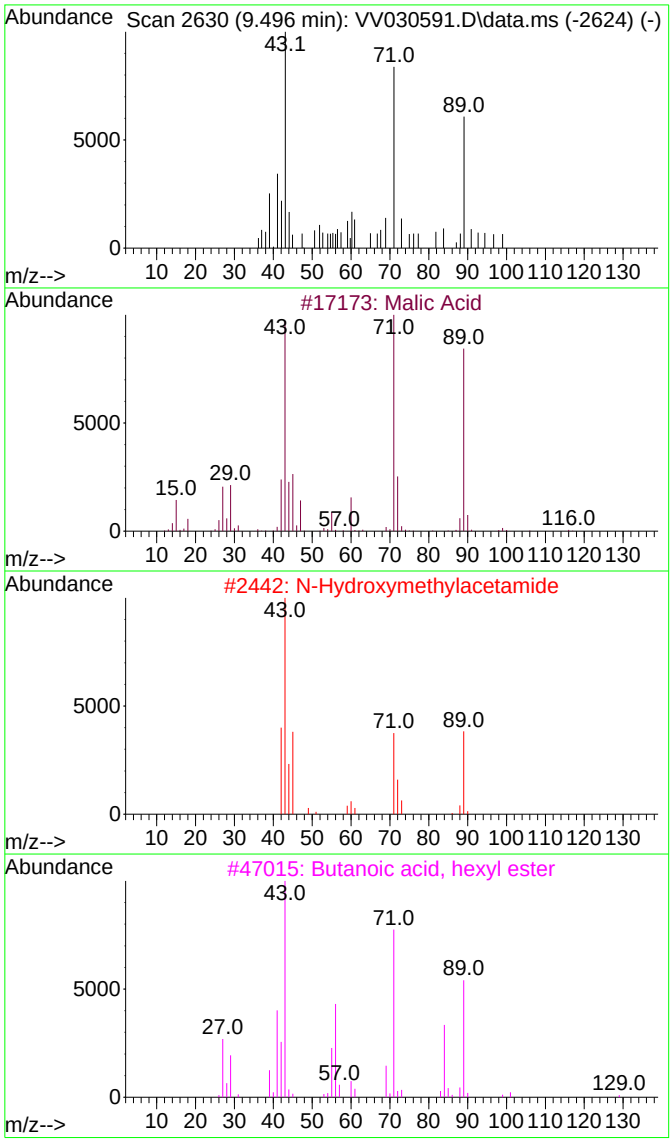
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

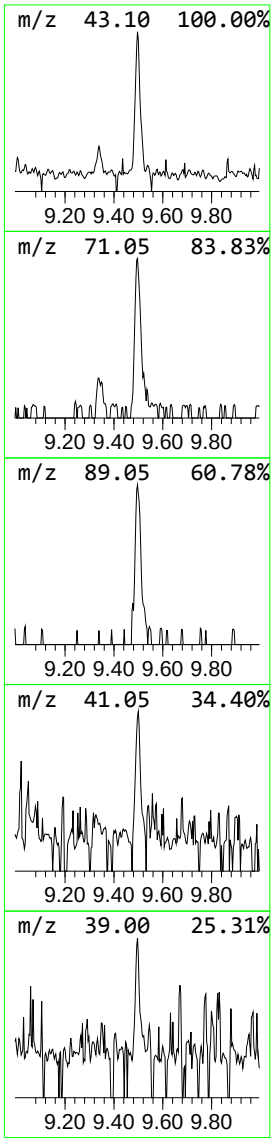
****

Peak Number 6 Malic Acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.496	4.33 ug/L	11538	Chlorobenzene-d5	8.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malic Acid	134	C4H6O5	006915-15-7	53
2	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	47
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	42
4	Malic Acid	134	C4H6O5	006915-15-7	36
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	36





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041723\
Data File : VV030591.D
Acq On : 17 Apr 2023 16:11
Operator : SY/MD
Sample : PB152132TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
LEB132

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041723WMA.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	95.4	ug/L	198759	1	5.545	104132	50.0
Propanoic acid,...	7.127	16.6	ug/L	34639	1	5.545	104132	50.0
Propanoic acid,...	7.870	19.3	ug/L	51471	2	8.796	133385	50.0
Isopropyl butyrate	8.625	57.6	ug/L	153801	2	8.796	133385	50.0
Malic Acid	9.496	4.3	ug/L	11538	2	8.796	133385	50.0