

Supplementary Materials for

mQC: A Heuristic Quality-Control Metric for High-Throughput Drug Combination Screening

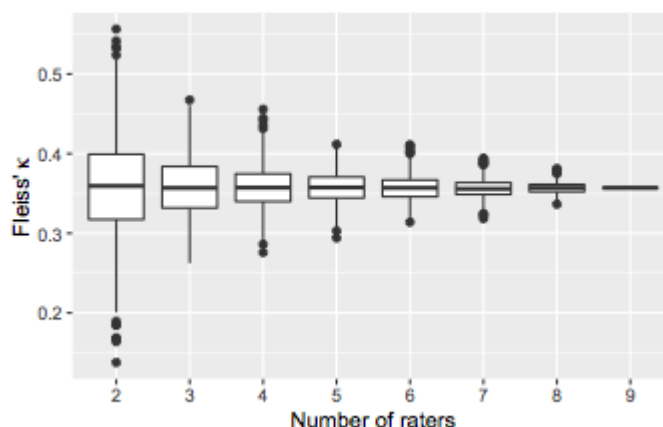
Lu Chen, Kelli Wilson, Ian Goldlust, Bryan T. Mott, Richard Eastman, Mindy I. Davis, Xiaohu Zhang, Crystal McKnight, Carleen Klumpp-Thomas, Paul Shinn, John Simmons, Mike Gormally, Sam Michael, Craig J. Thomas, Marc Ferrer, Rajarshi Guha

Supplementary Dataset S1. The 133 response matrices used for training and the survey results.

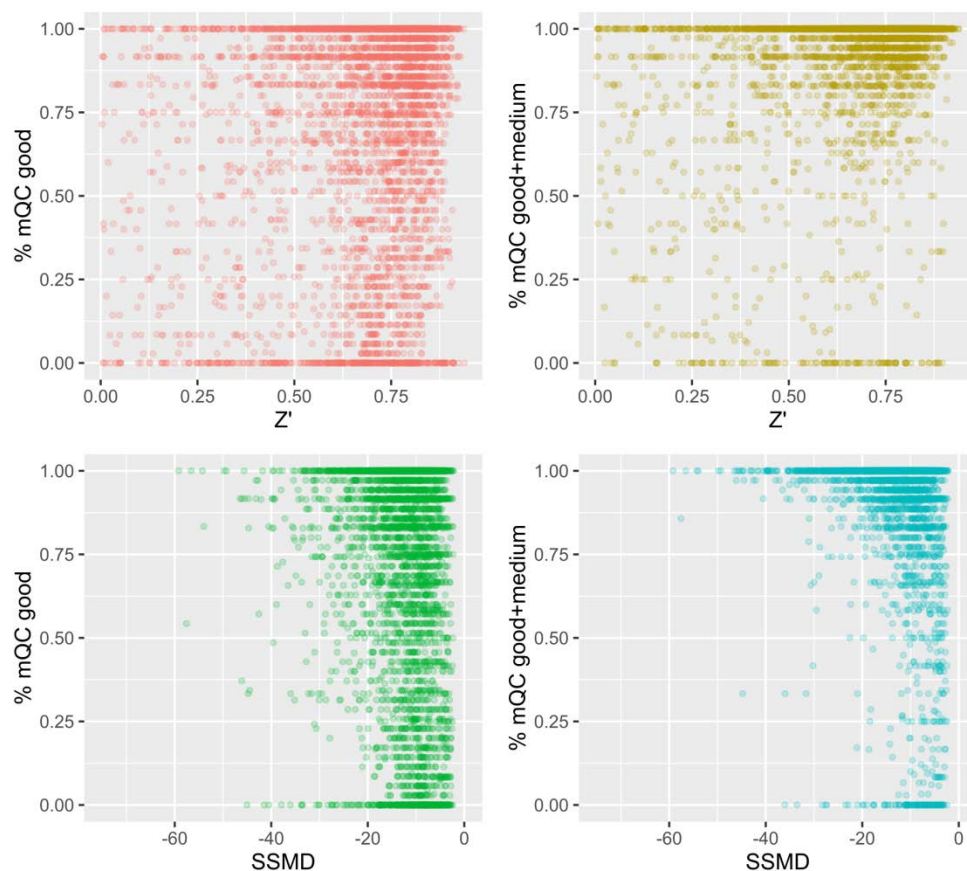
Supplementary Dataset S2. The layout for 6×6 and 10×10 screens (1536-well plate).

Supplementary Dataset S3. Plate-level and matrix-level QC metrics breakdown by plate.

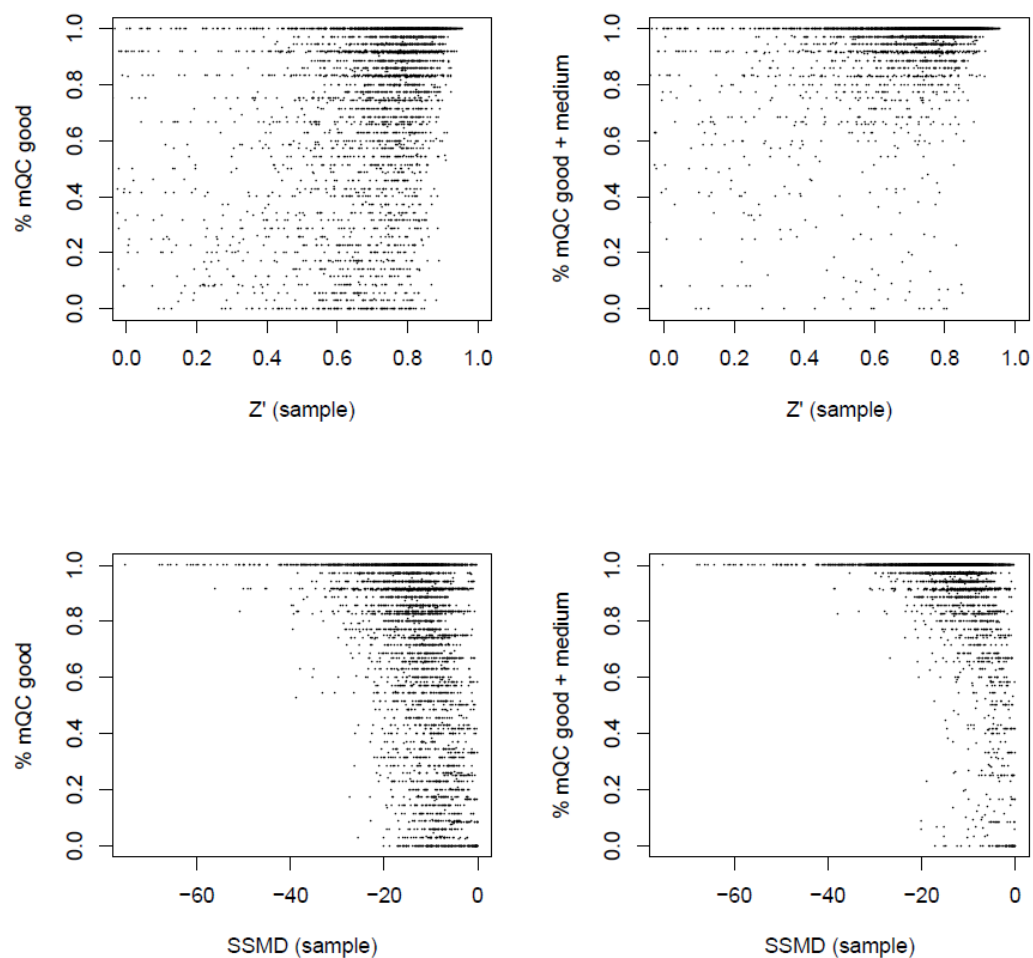
Supplementary Figure S1. Relationship between number of raters and the inter-rater agreement (measured by Fleiss' κ).



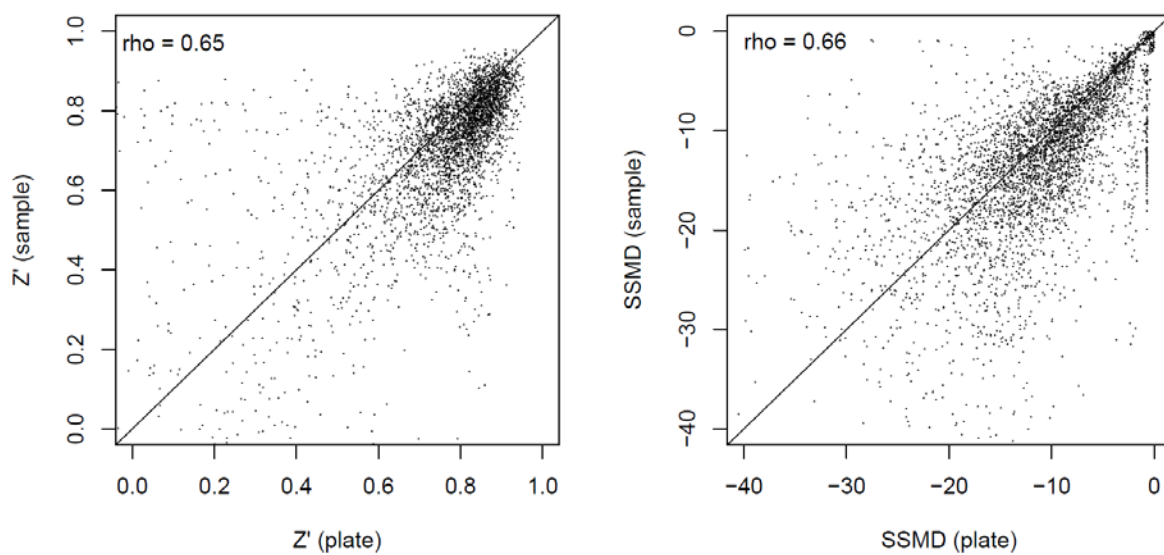
Supplementary Figure S2. Correlation between plate-level QC (i.e., Z' , SSMD) and matrix-level QC (mQC) (breakdown by assay plate). The plates with negative Z' or SSMD < -75 are excluded.



Supplementary Figure S3. Correlation between plate-level QC (i.e., Z' or SSMD calculated using plate-level positive controls and block DMSO controls) and matrix-level QC (mQC) (breakdown by assay plate). The plates with negative Z' or SSMD < -75 are excluded.

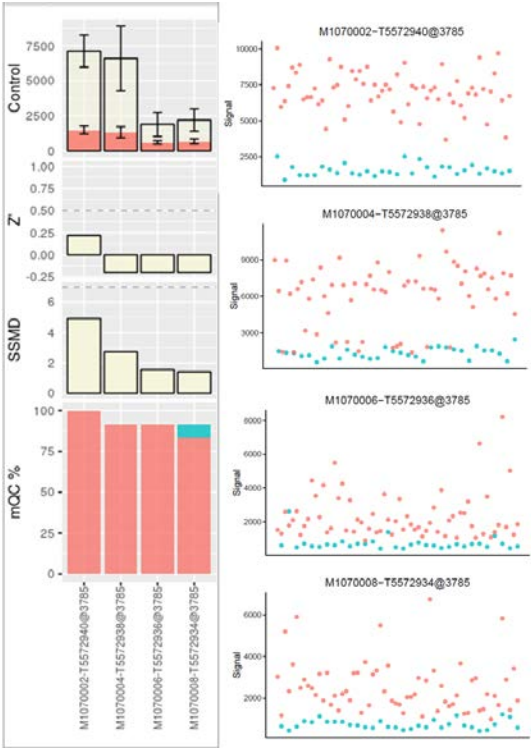


Supplementary Figure S4. Correlation between Z' (plate) or SSMD (plate) computed using plate-level positive and negative controls and Z' (sample) or SSMD (sample) computed using plate-level positive controls and block DMSO controls. The plates that hold less than 12 blocks or have negative Z' or $SSMD < -40$ are excluded in this analysis.

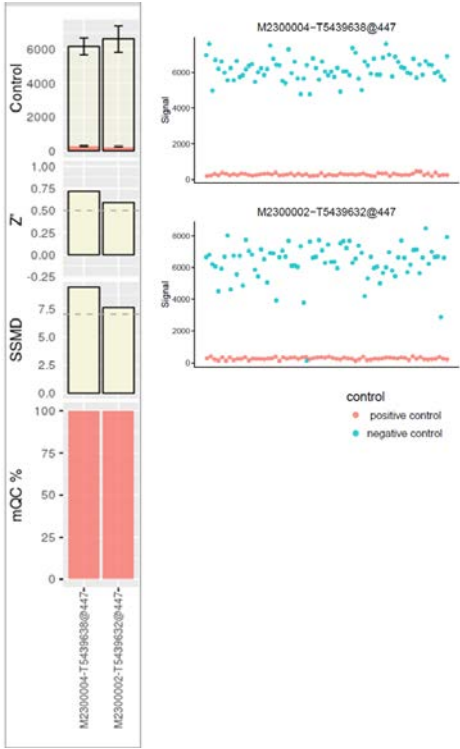


Supplementary Figure S5. Plate-level QC and mQC for 11 screens. For each assay, we show a bar plot summary comparing per-plate QC metrics (left) and scatter plots of the plate-level controls (right, red=positive controls, green=negative controls). (A) CaspaseGlo assay 3785: failed positive control, good mQC; (B) CellTiterGlo assay 447: excellent assay; (C) CellTiterGlo assay 241: excellent screen; (D) CellTiterGlo assay 5021: cell contamination; (E) CellTiterGlo assay 6028: cell contamination; (F) CellTiterGlo assay 2850: excellent screen; (G) CellTiterGlo assay 2852: low cell viability; (H) CellTiterGlo assay 702: drift; (I) CellTiterGlo assay 703: drift; (J) CellTiterGlo assay 704: drift; (K) CellTiterGlo assay 705: drift. Each assay was performed on various number of 1536-well plates, and we analyzed the quality of each plate using the median and standard deviation of positive control signals (red), negative control signals (yellow), Z'-factor, robust SSMD, and the proportion of “Good” (red) and “Medium” (green) response matrices (assessed by mQC). The dashed lines in Z' and SSMD plots are the empirical Z' or SSMD cutoffs (Z'=0.5 and SSMD=-7). For visualization purpose, we use the negative robust SSMD values.

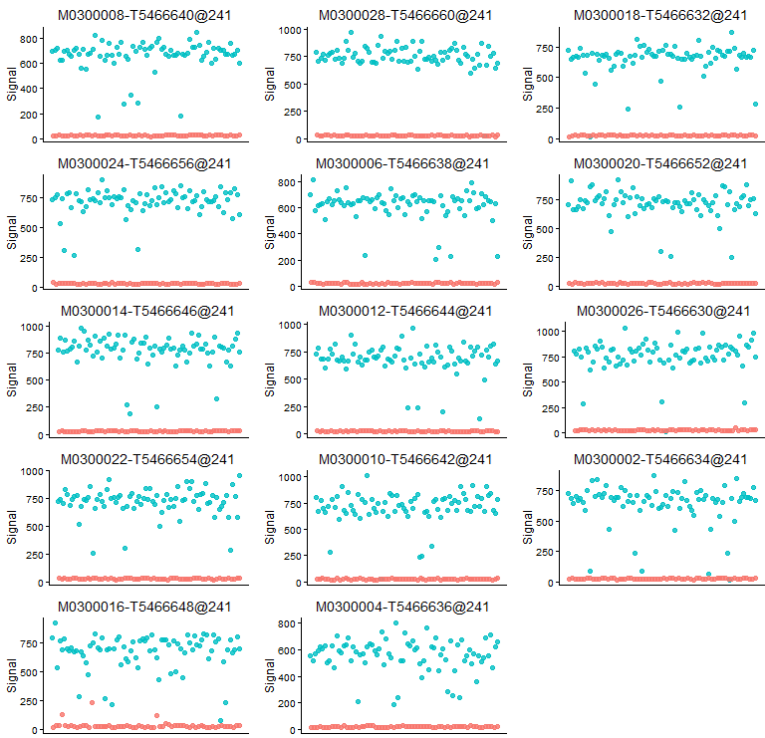
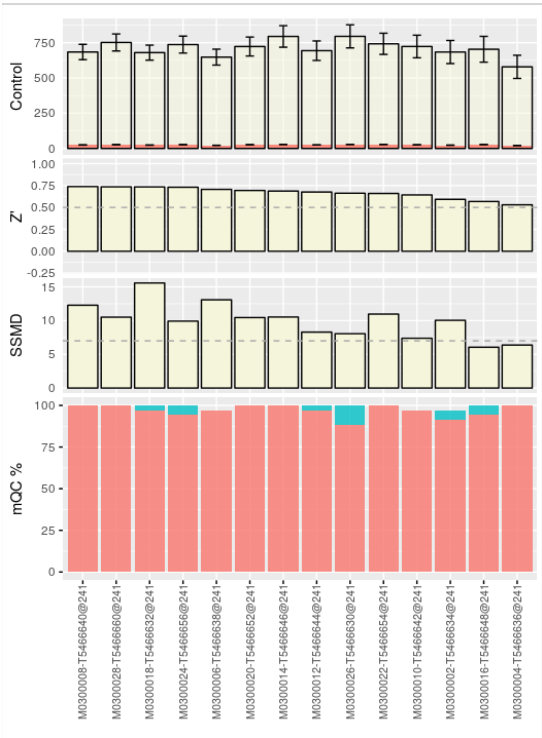
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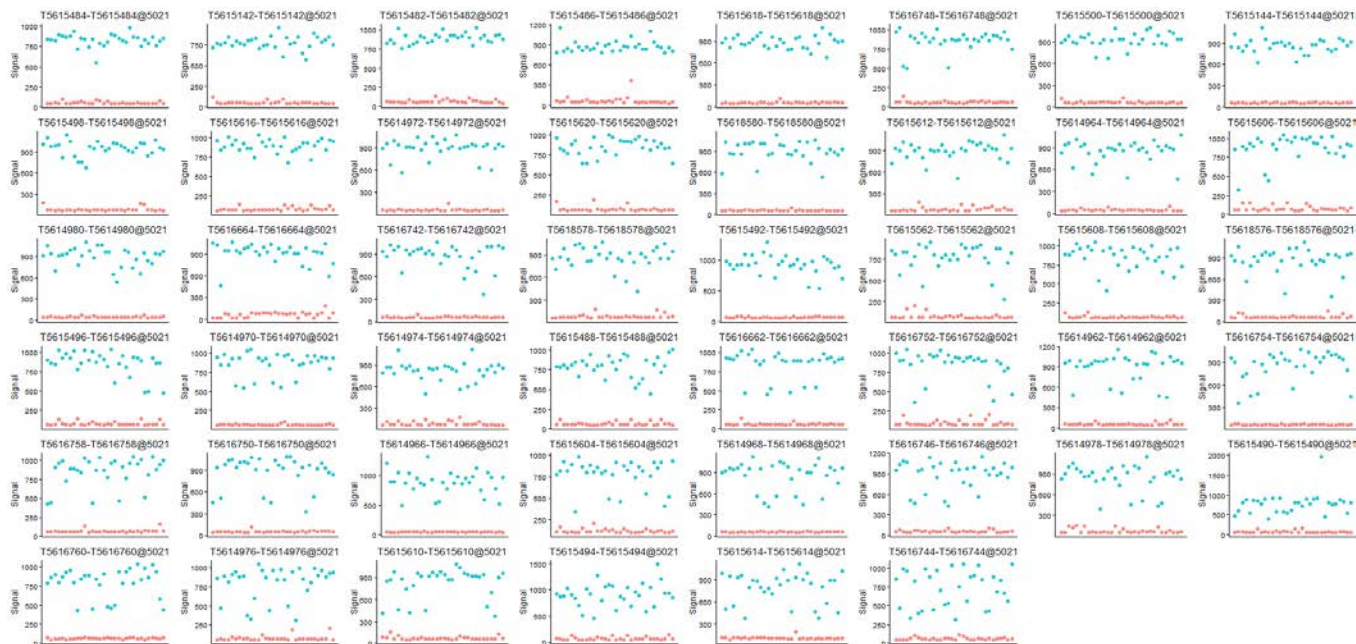
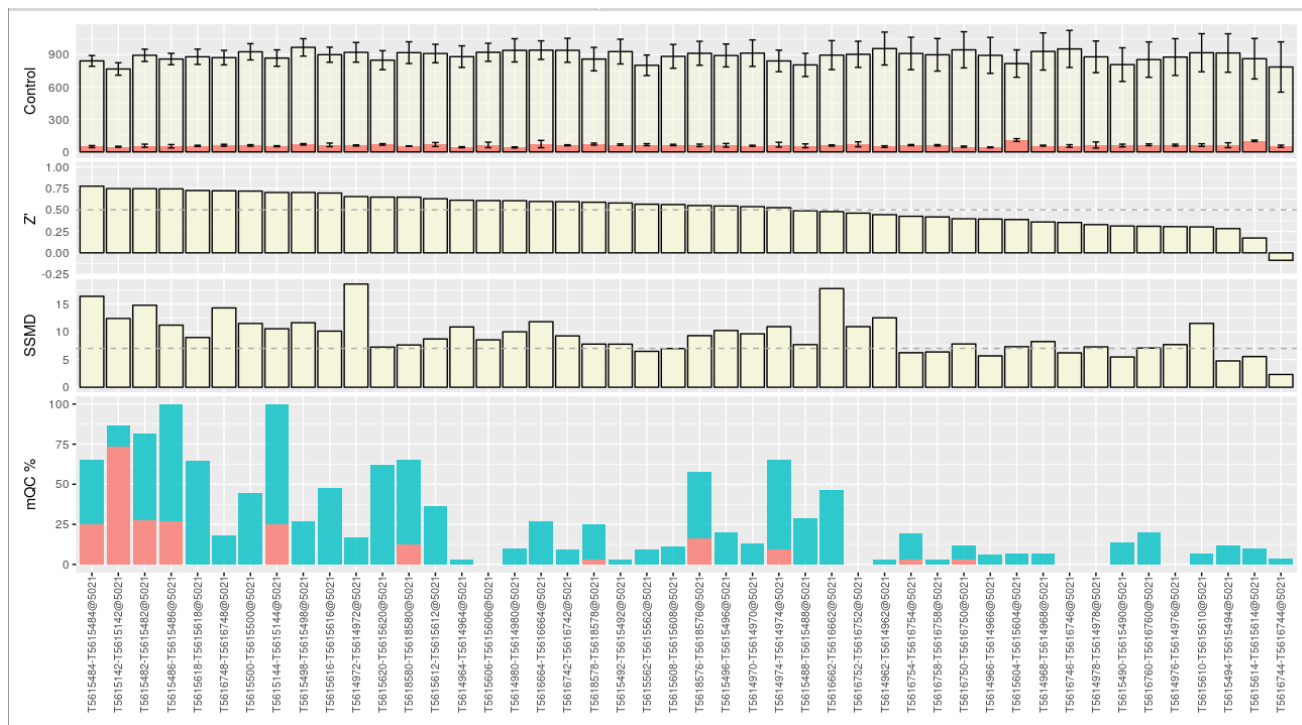
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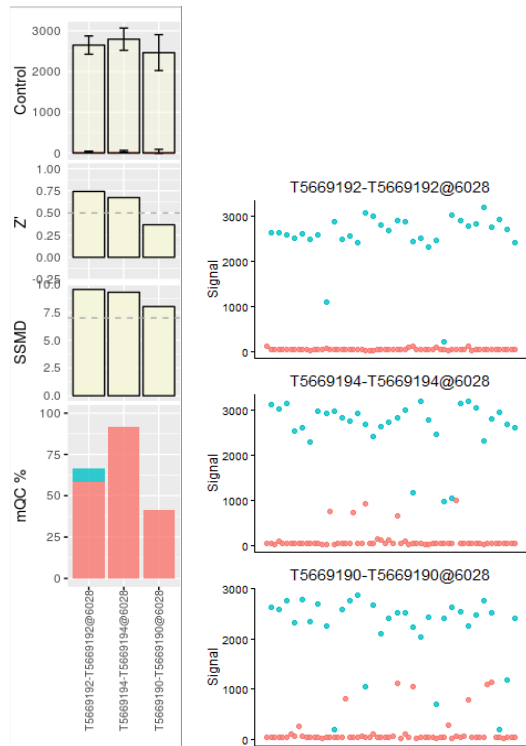
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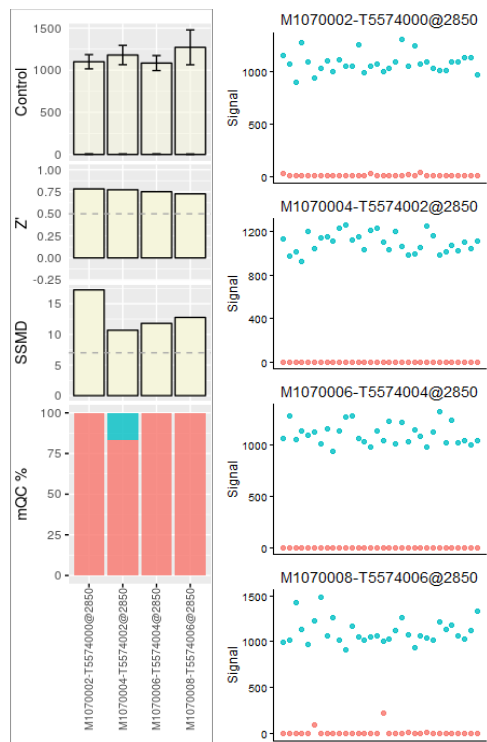
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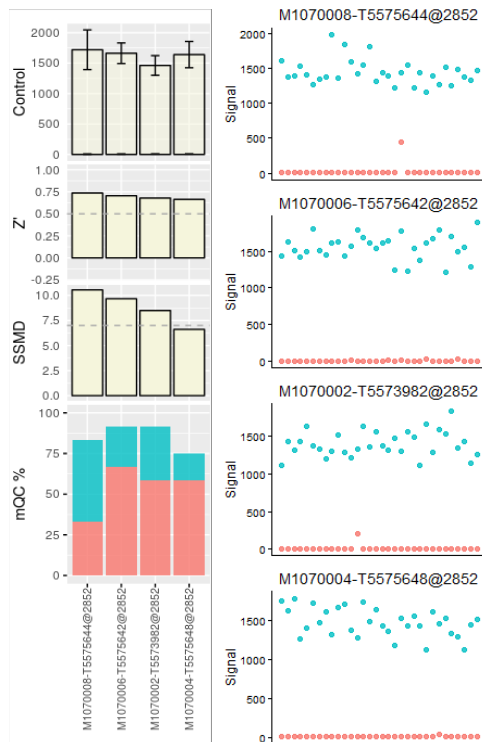
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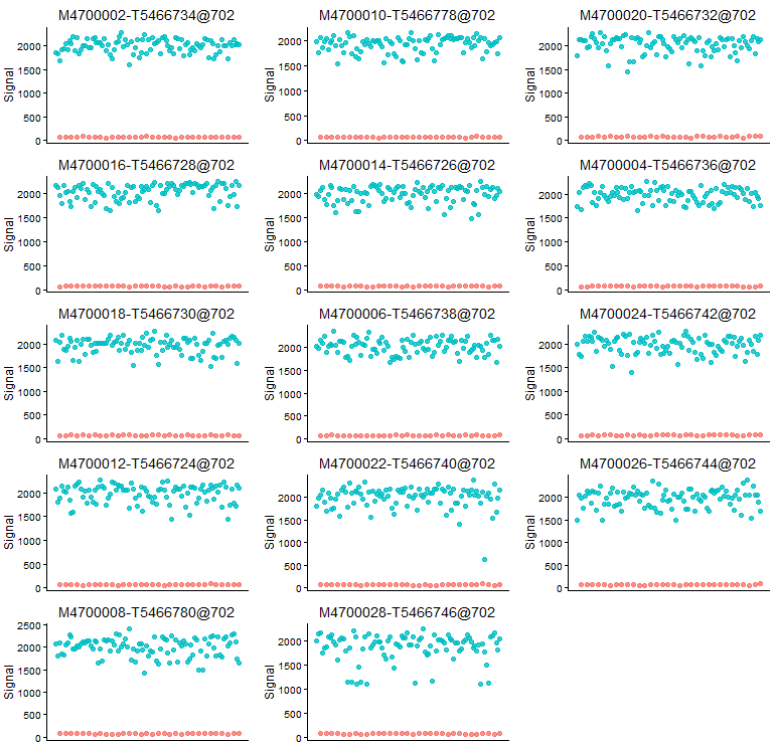
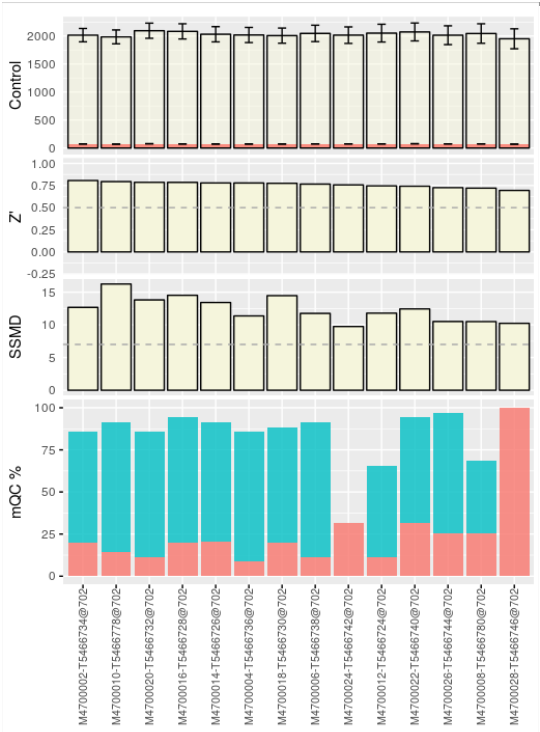
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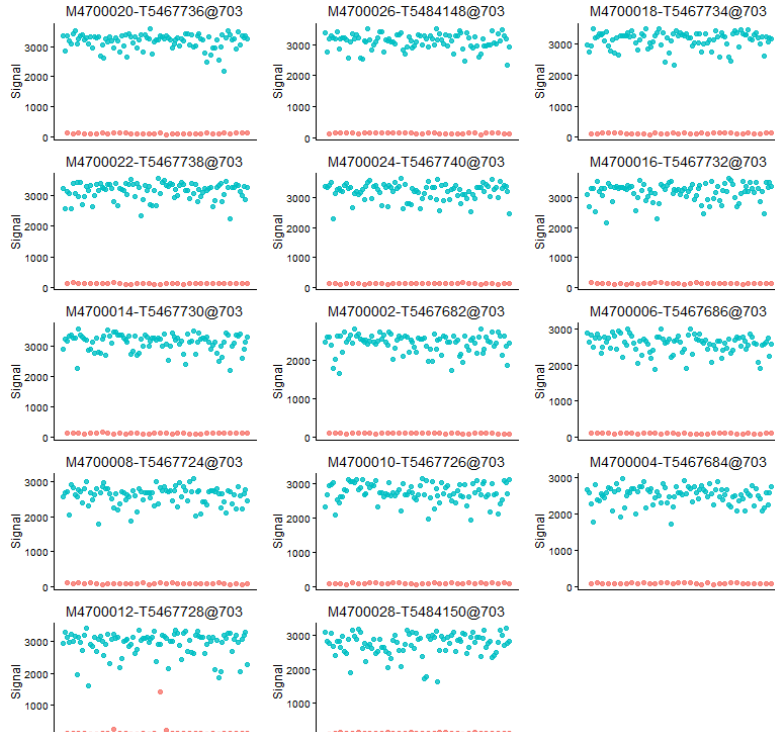
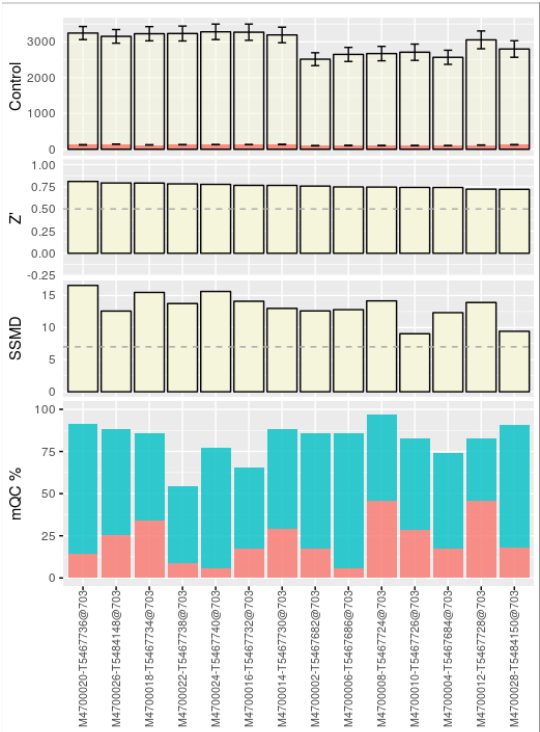
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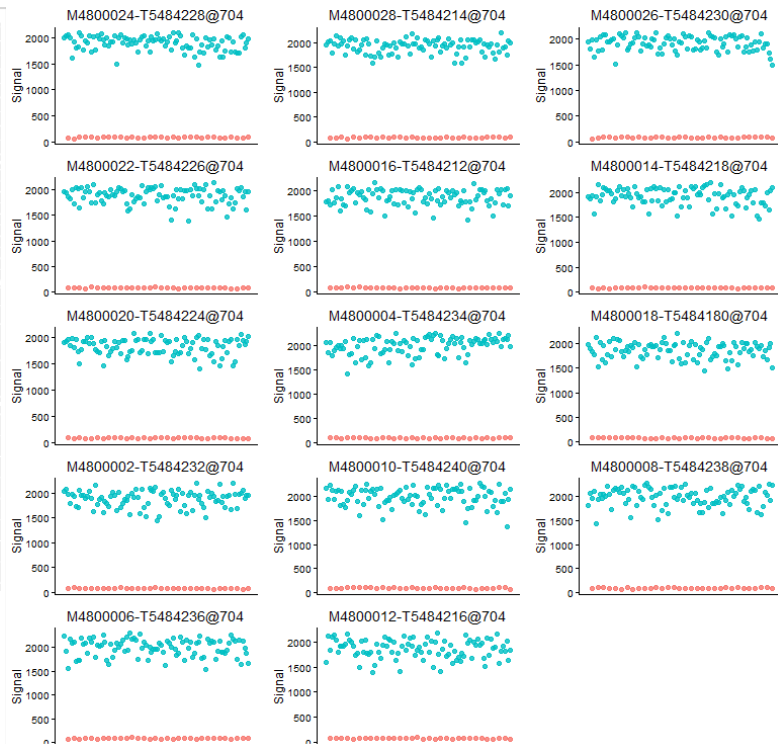
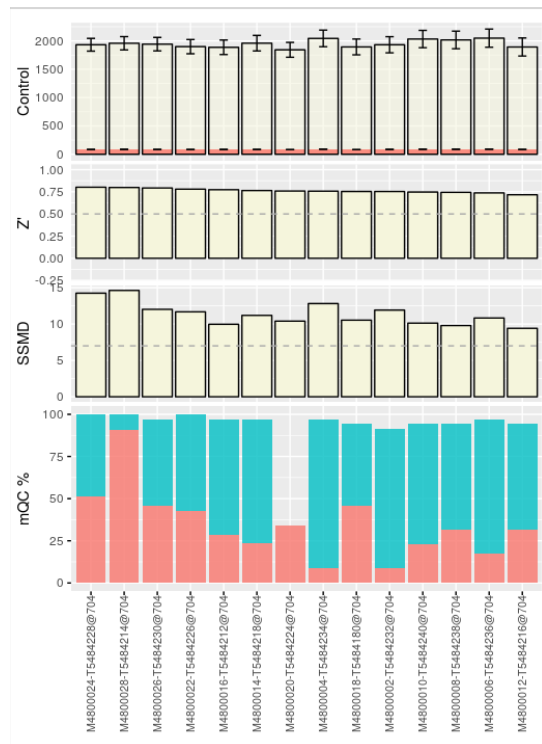
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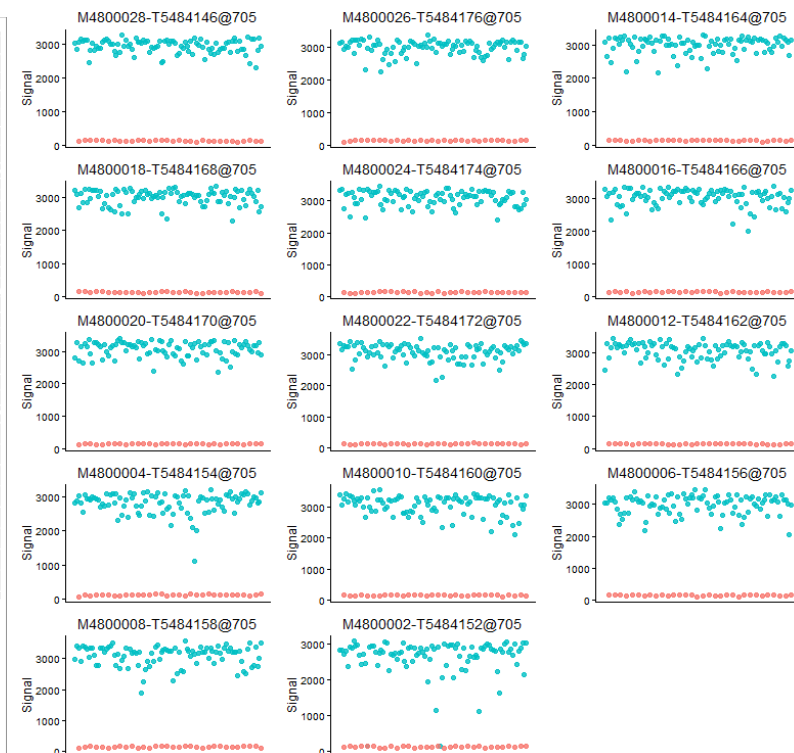
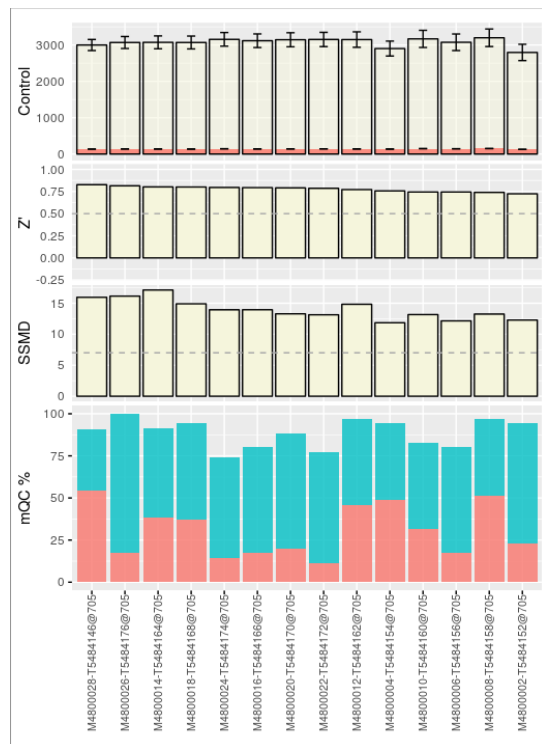
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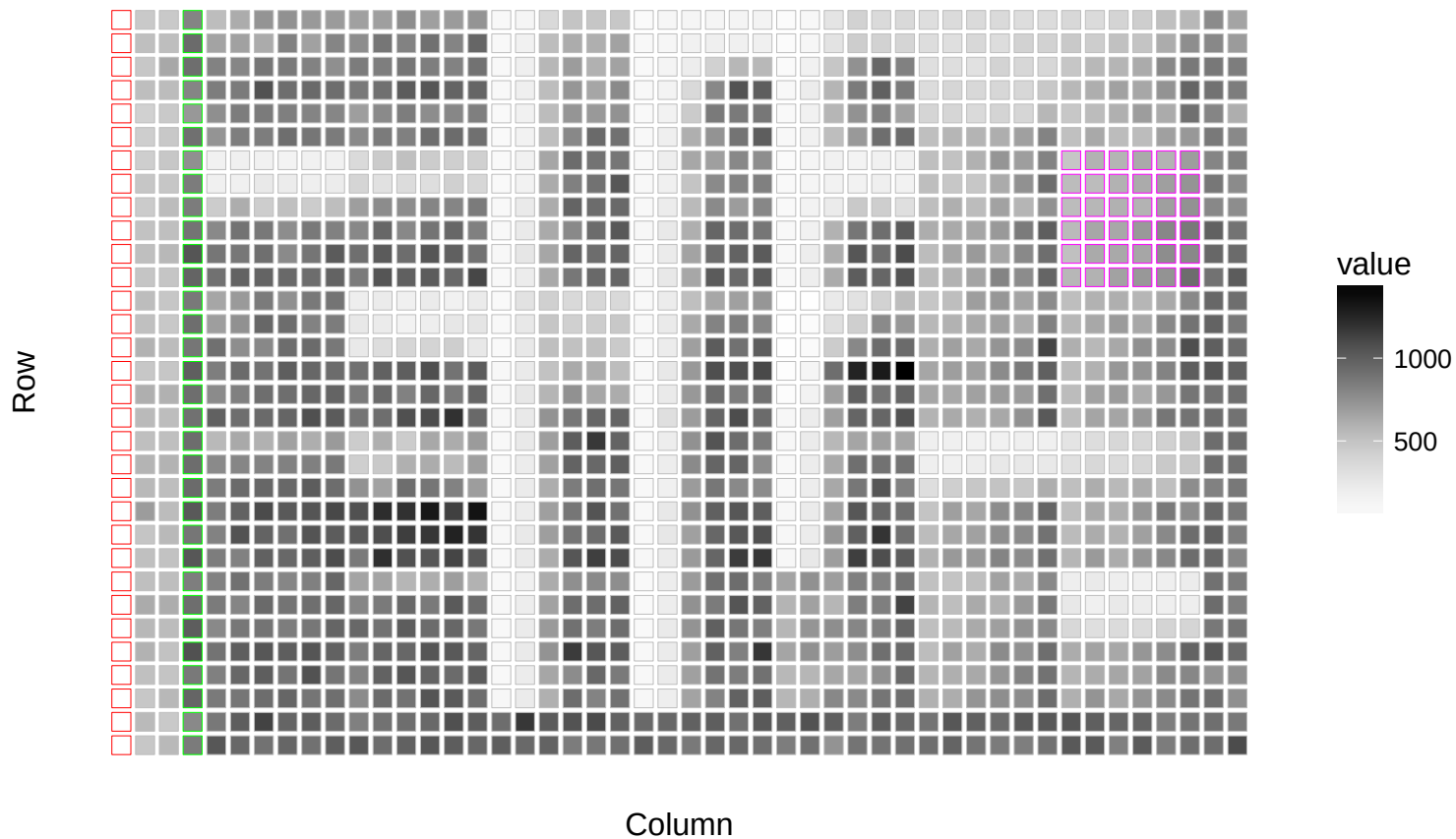


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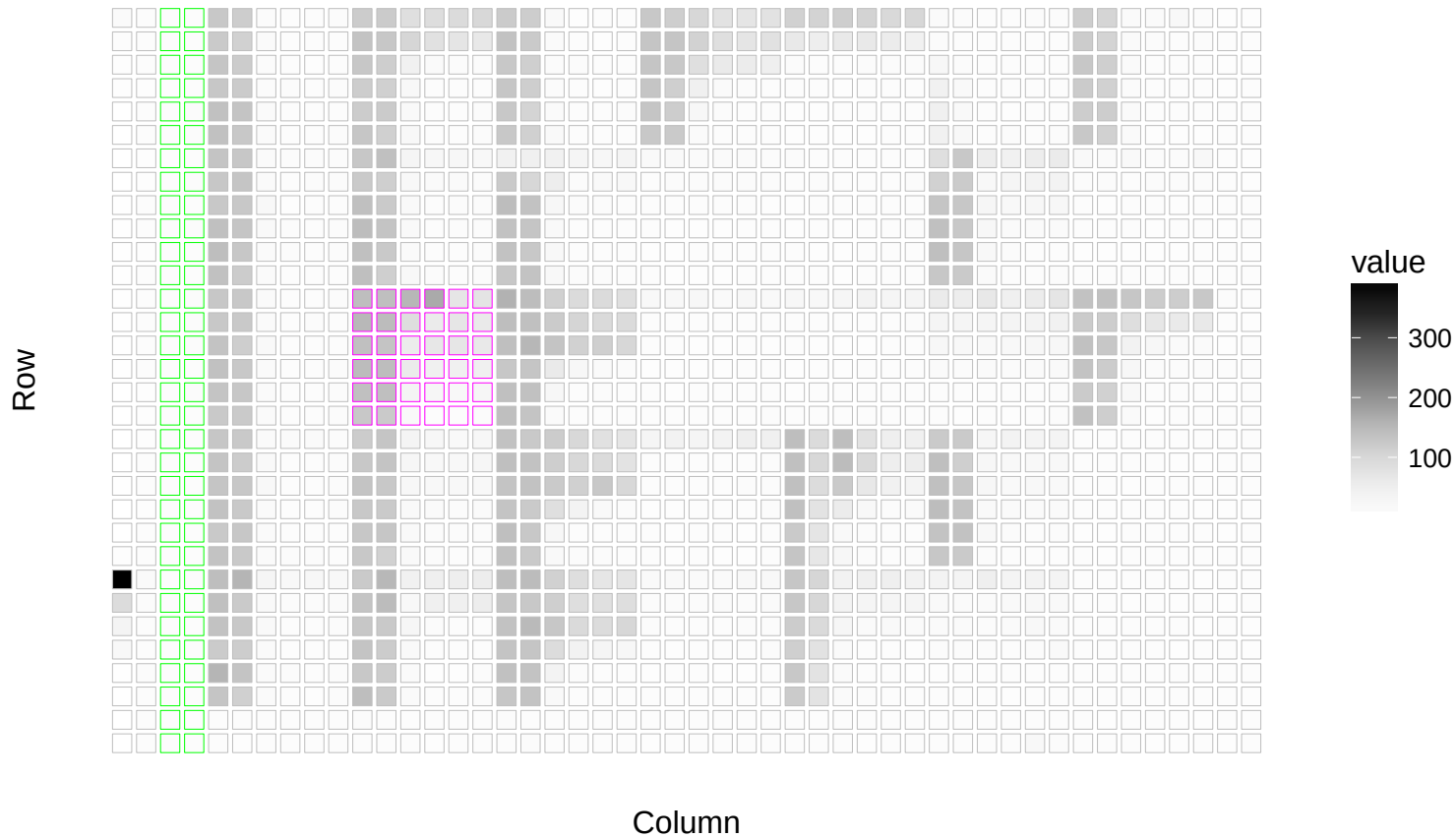


Supplementary Figure S6. The 133 blocks used to train mQC model and their corresponding plate data (shown as heatmap). Red: plate-level positive controls. Green: plate-level negative control (e.g., DMSO). Magenta: the selected block.

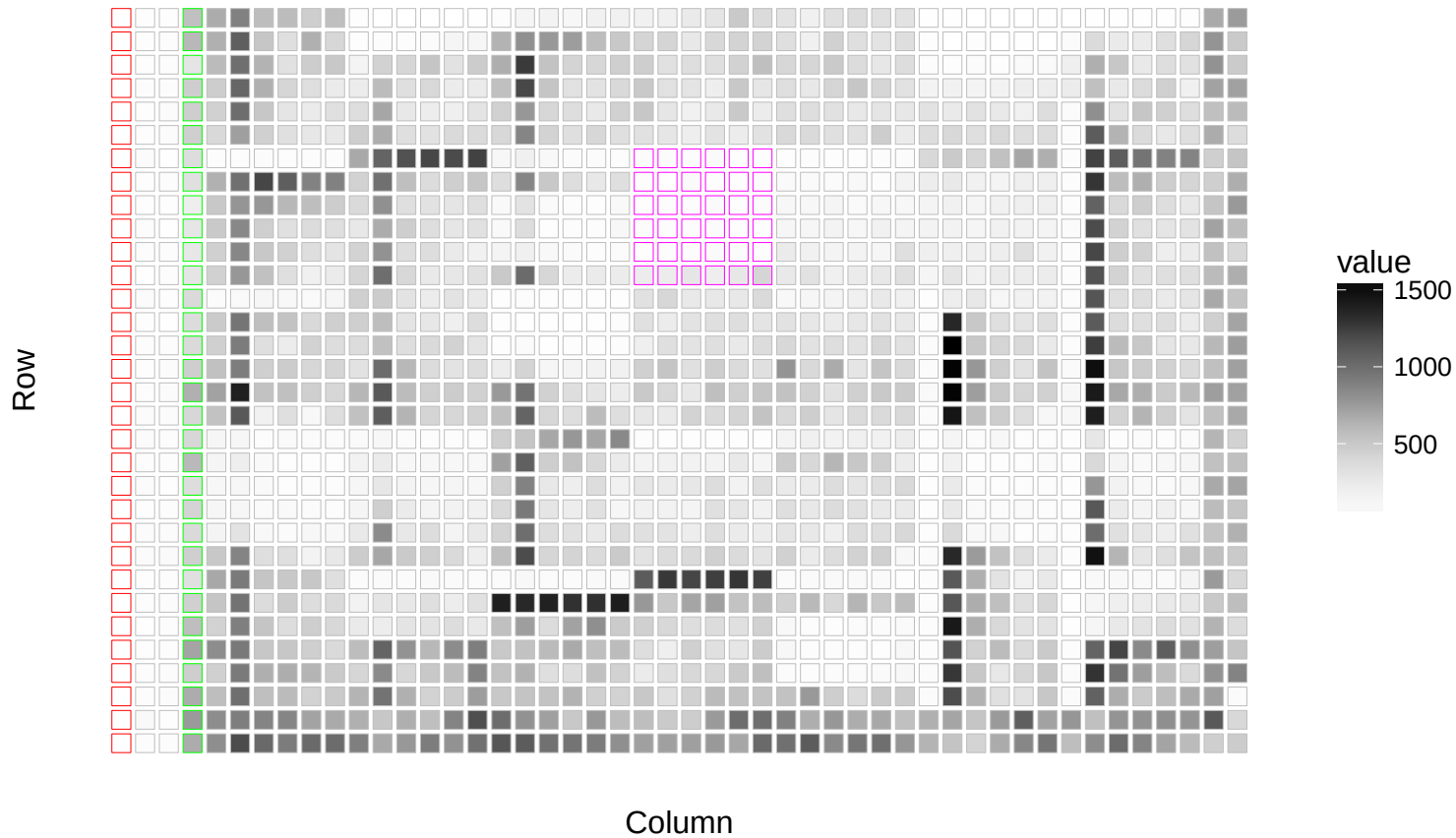
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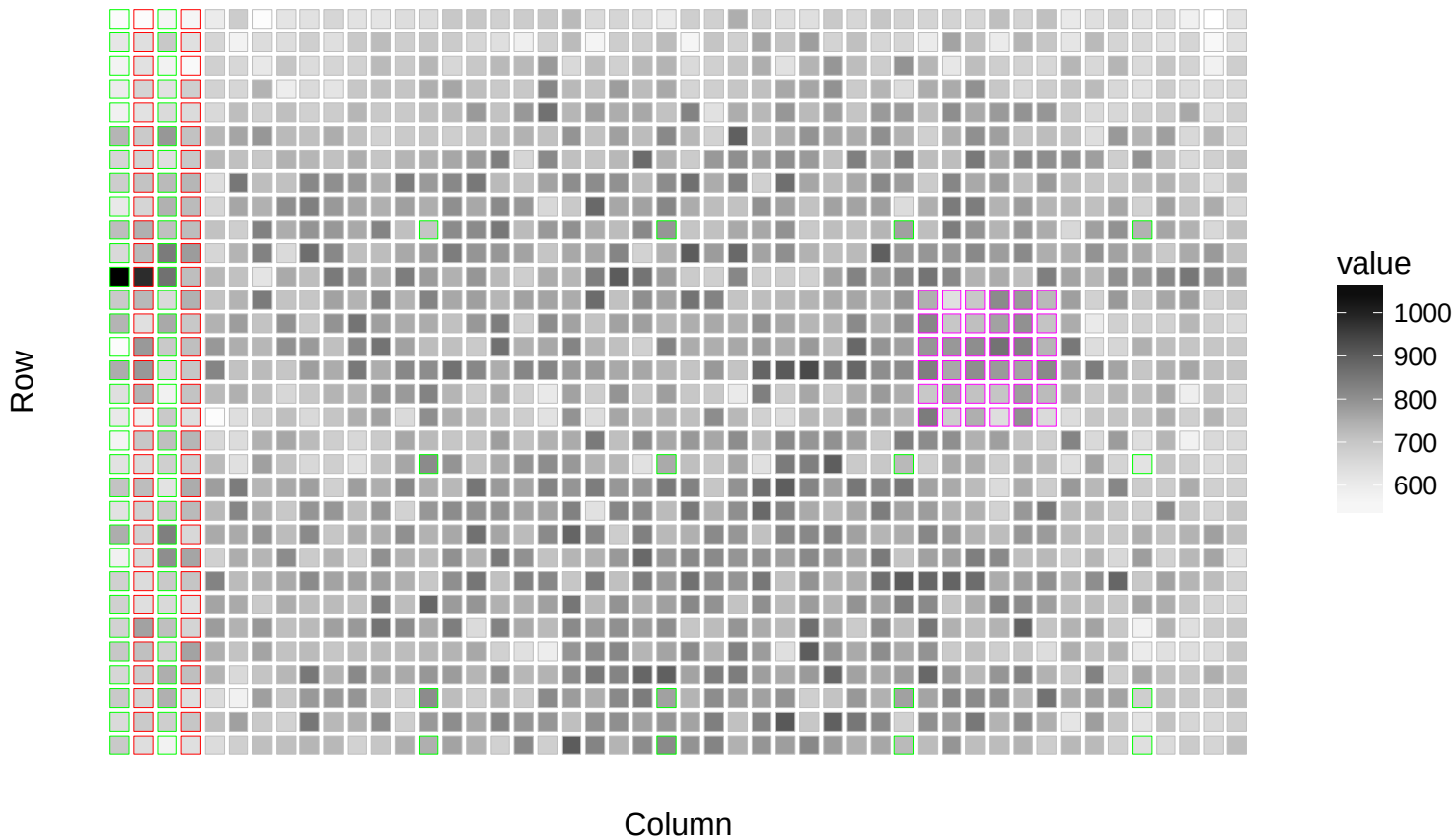
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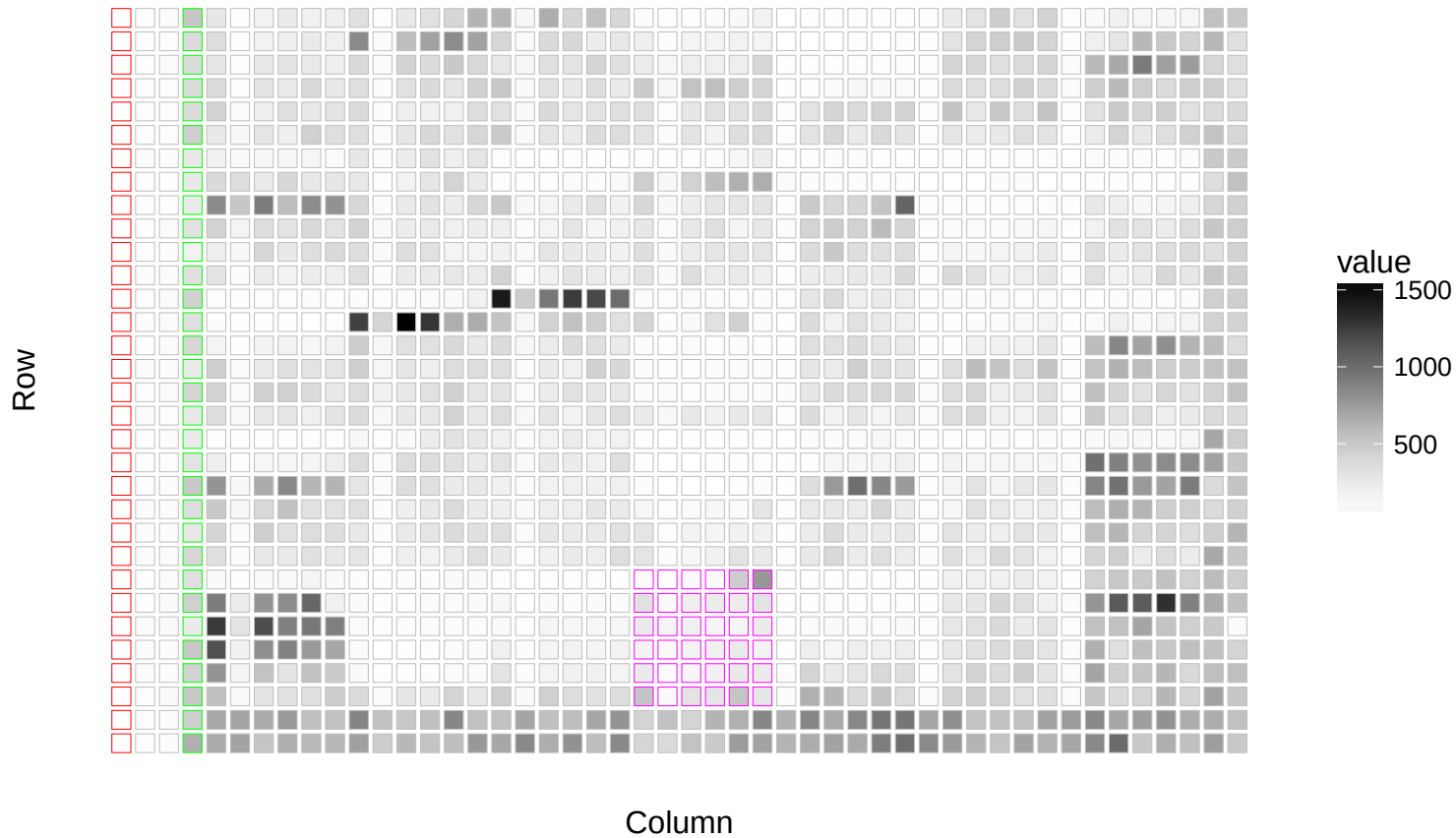
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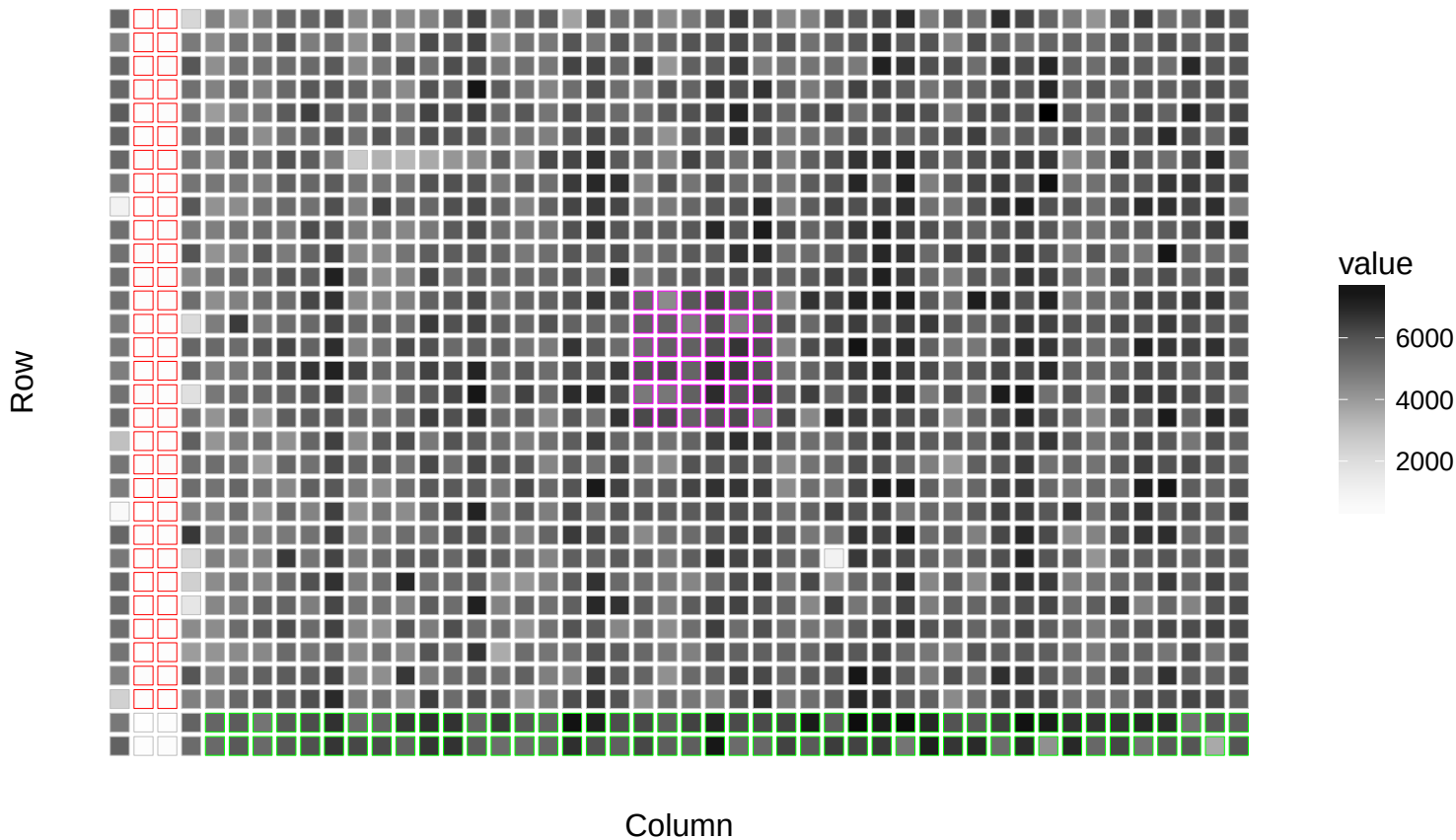
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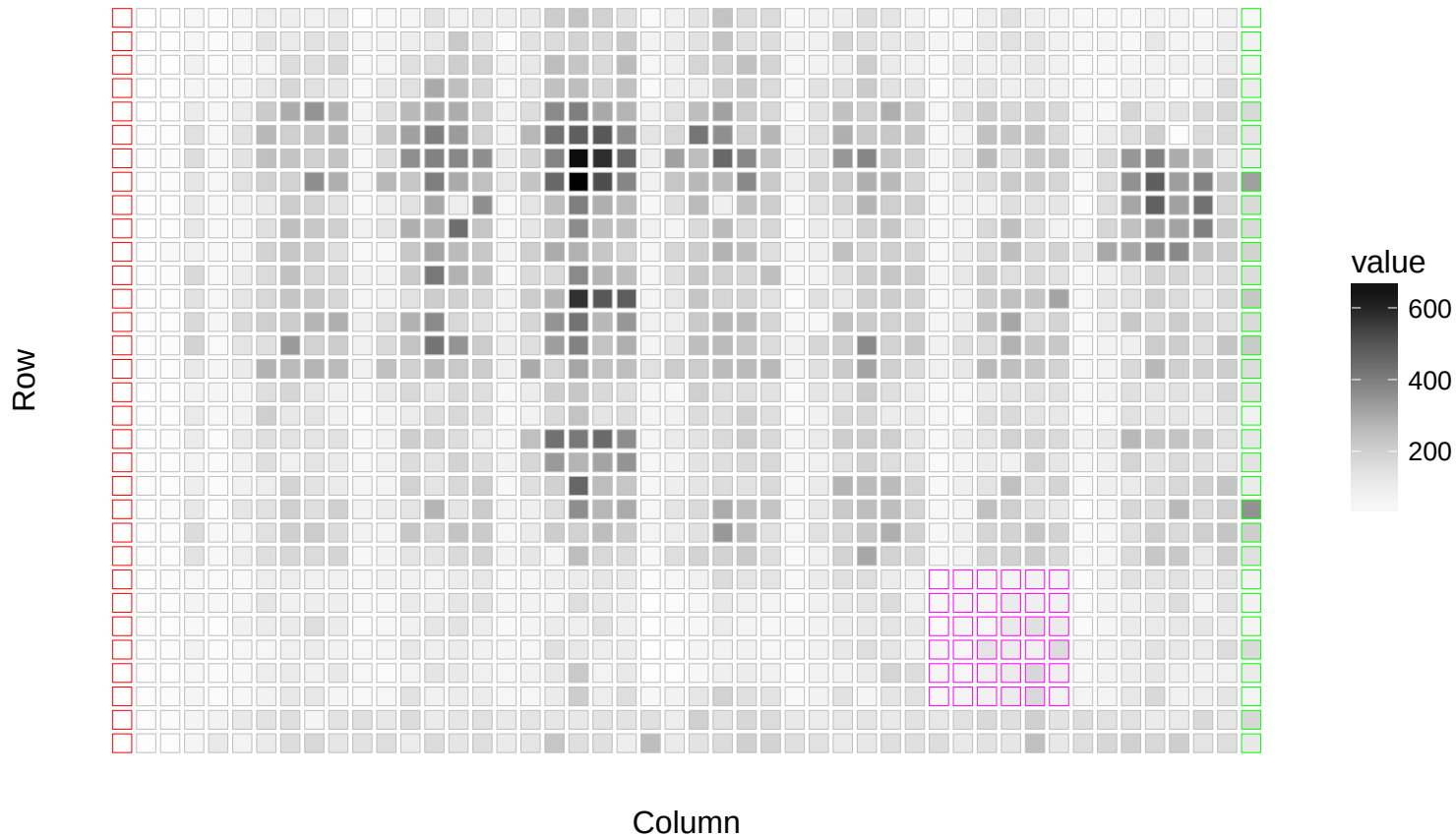
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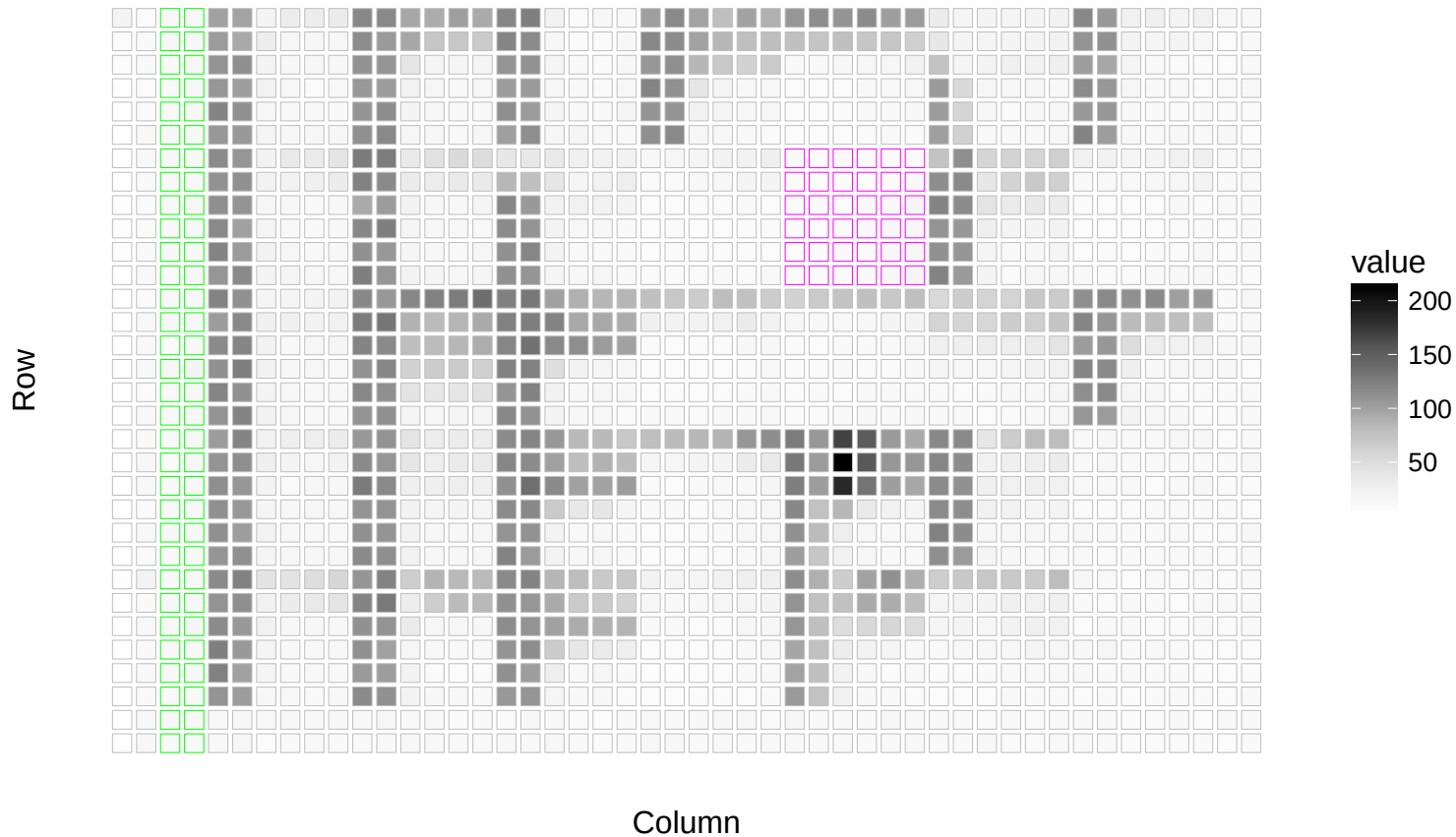
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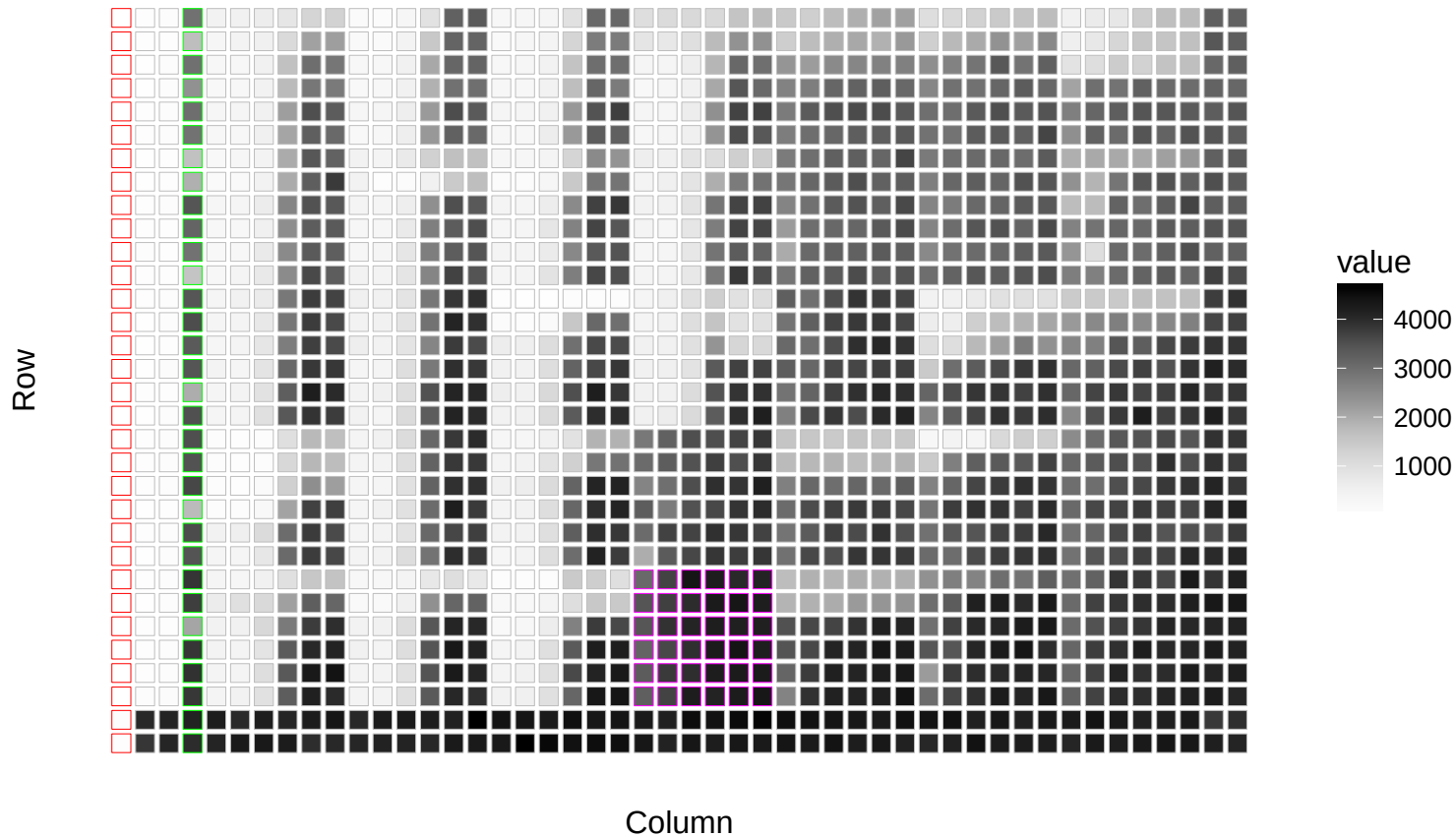
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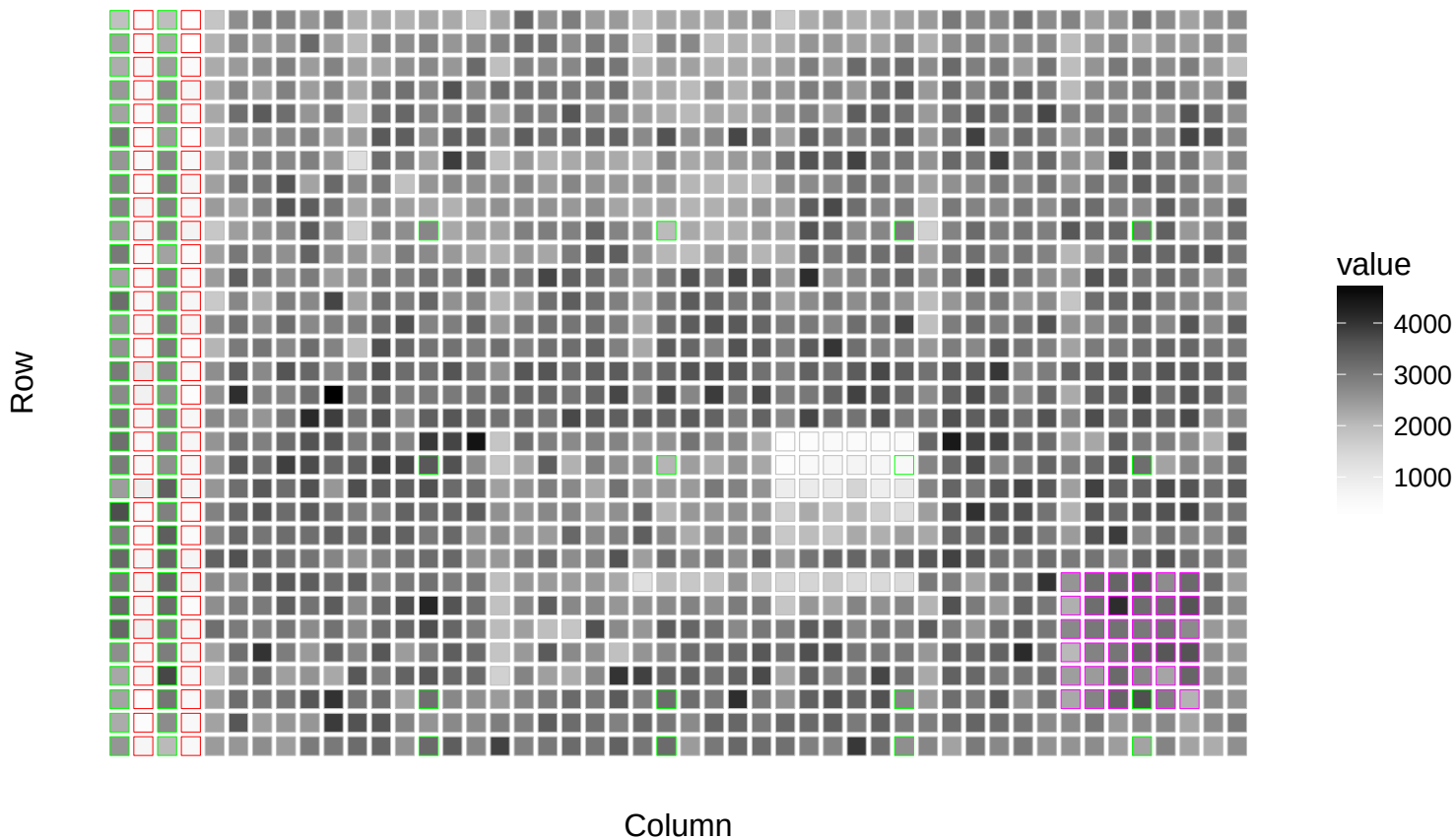
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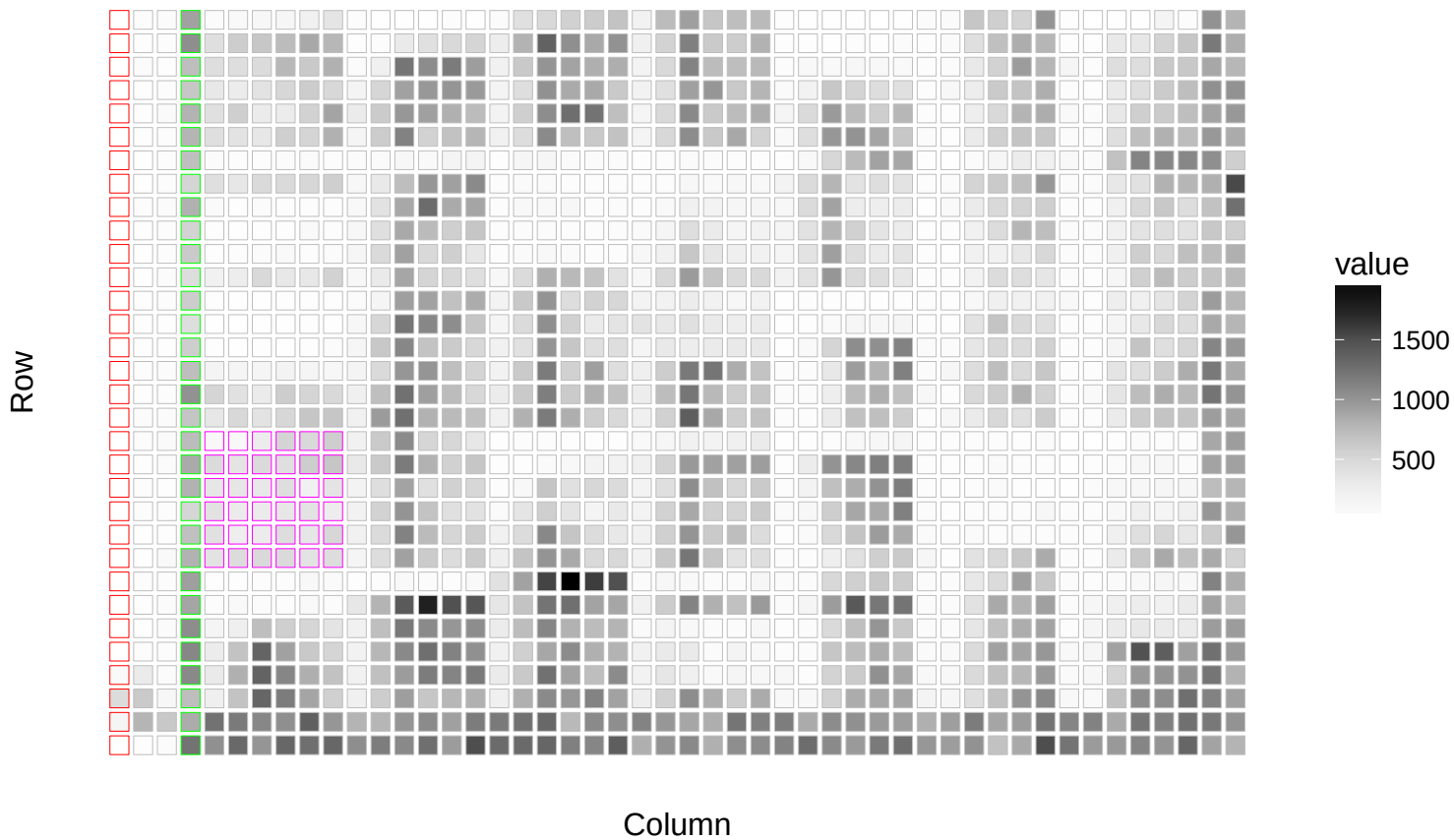
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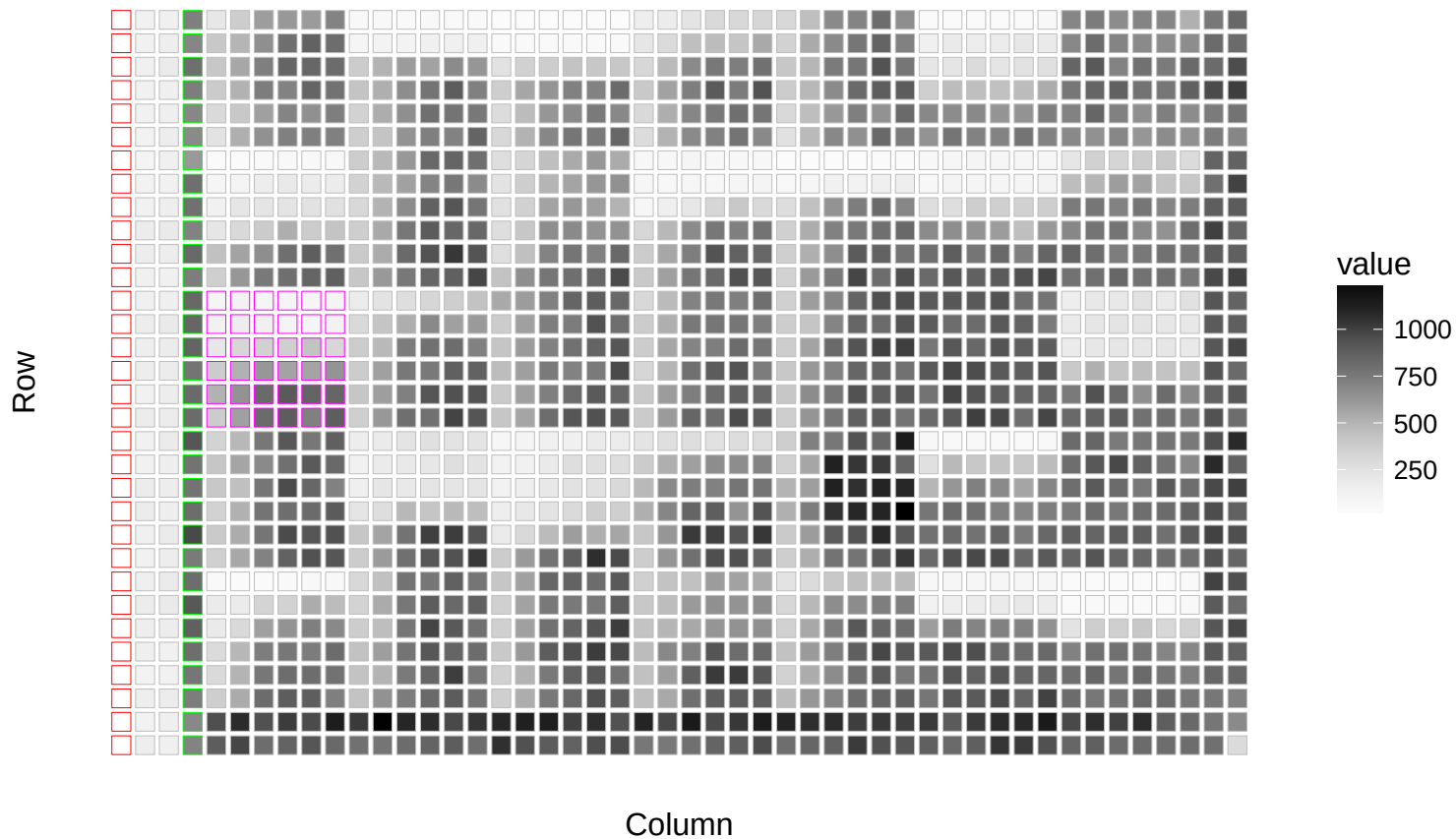
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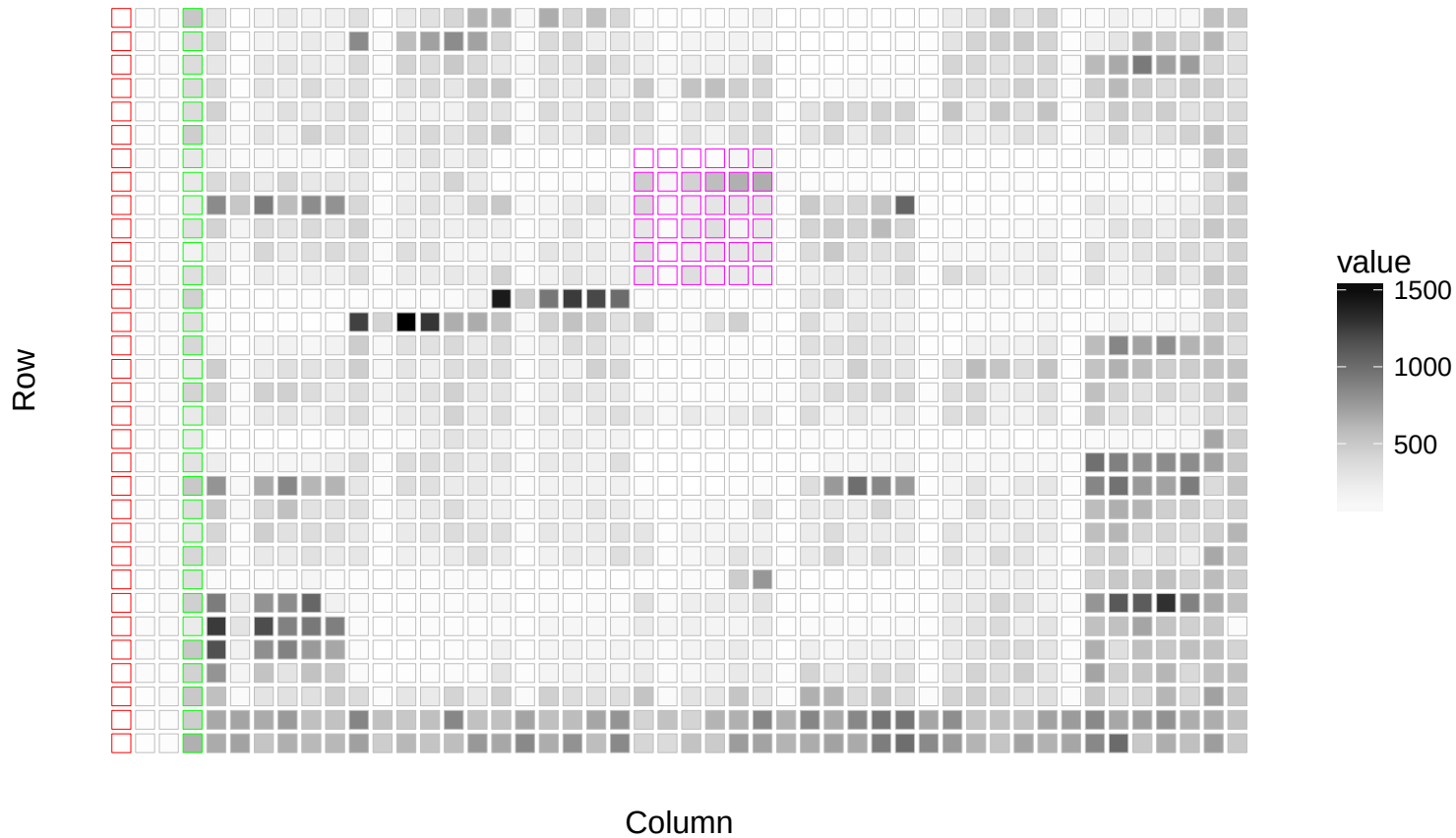
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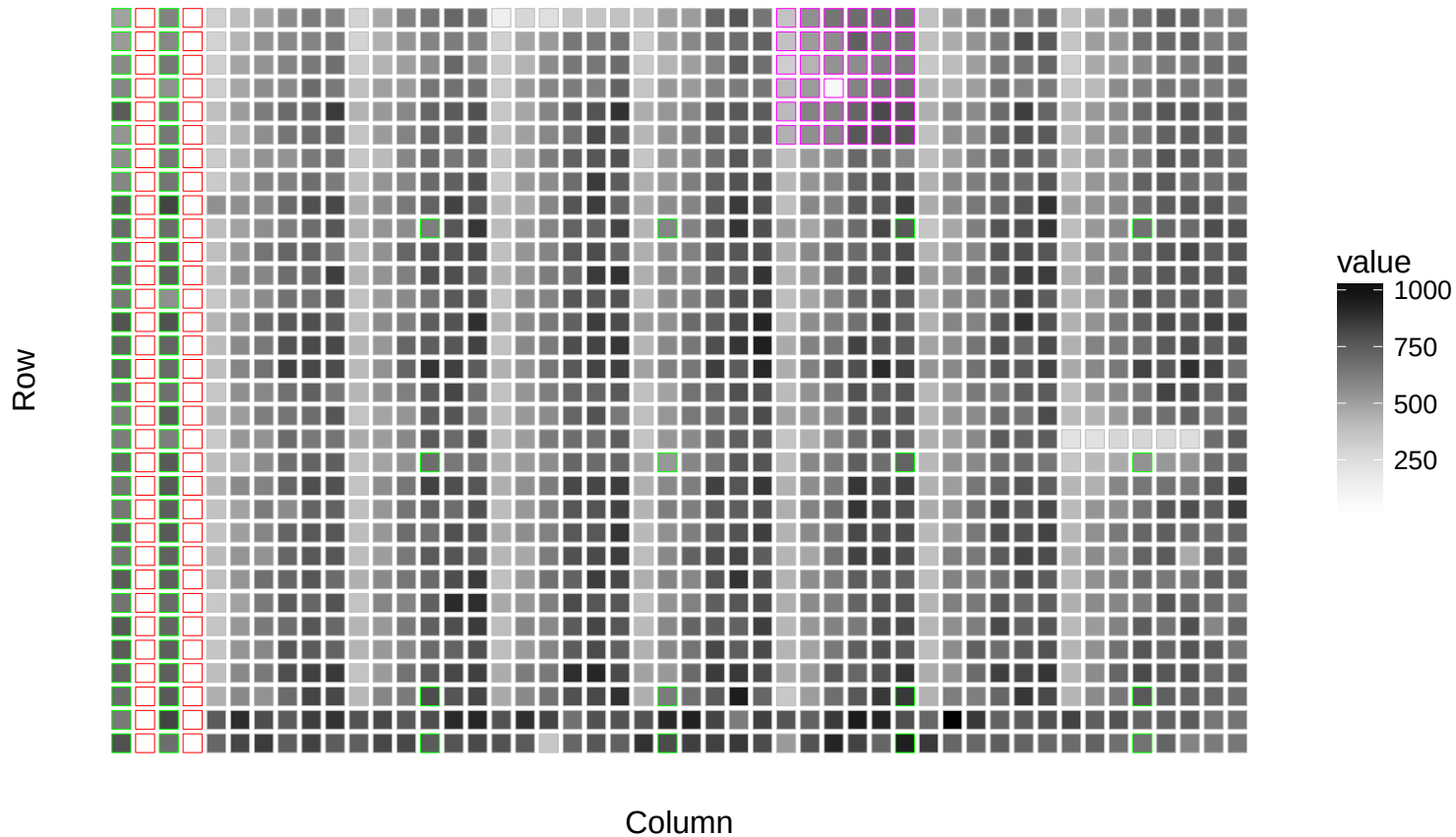
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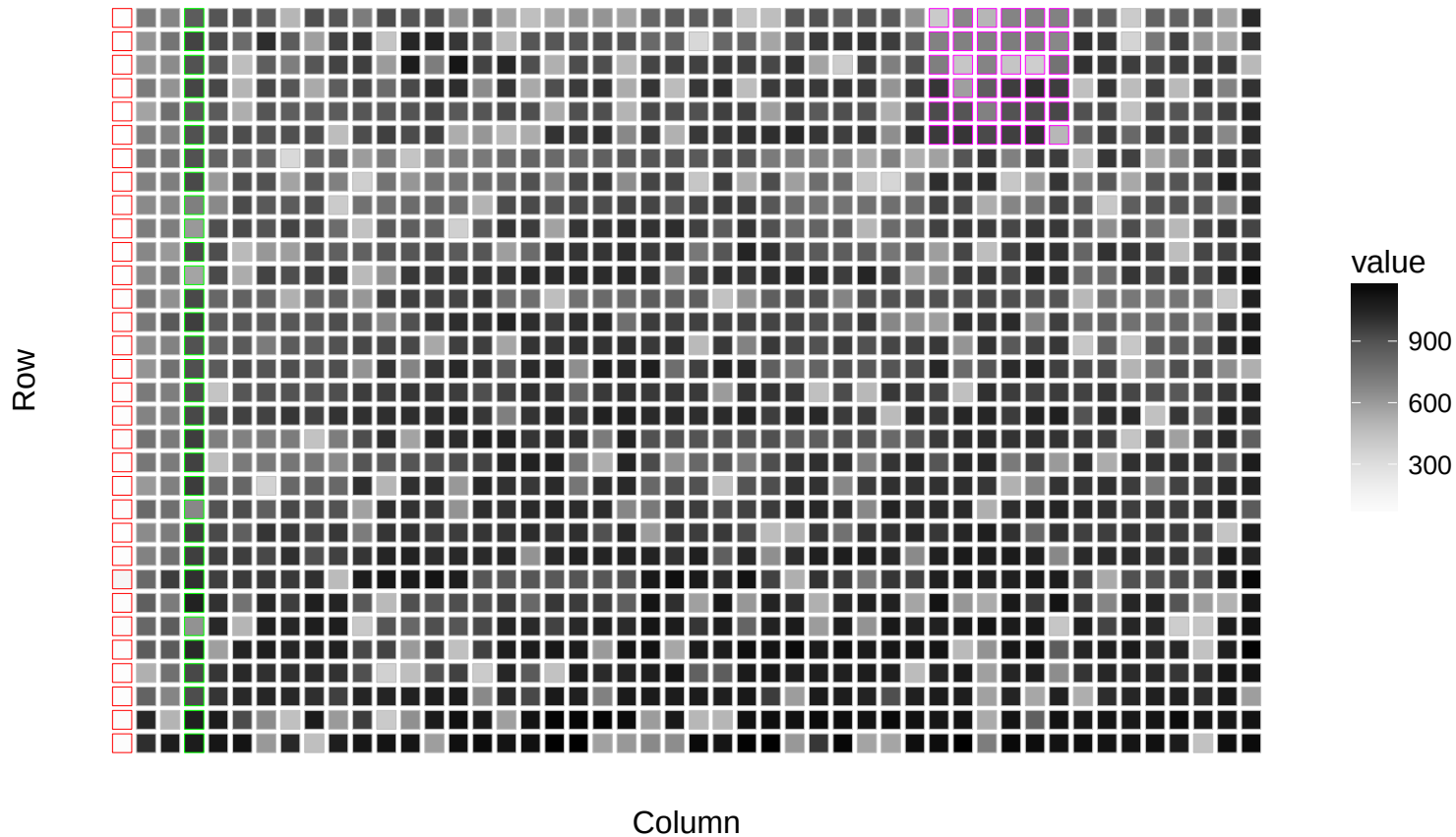
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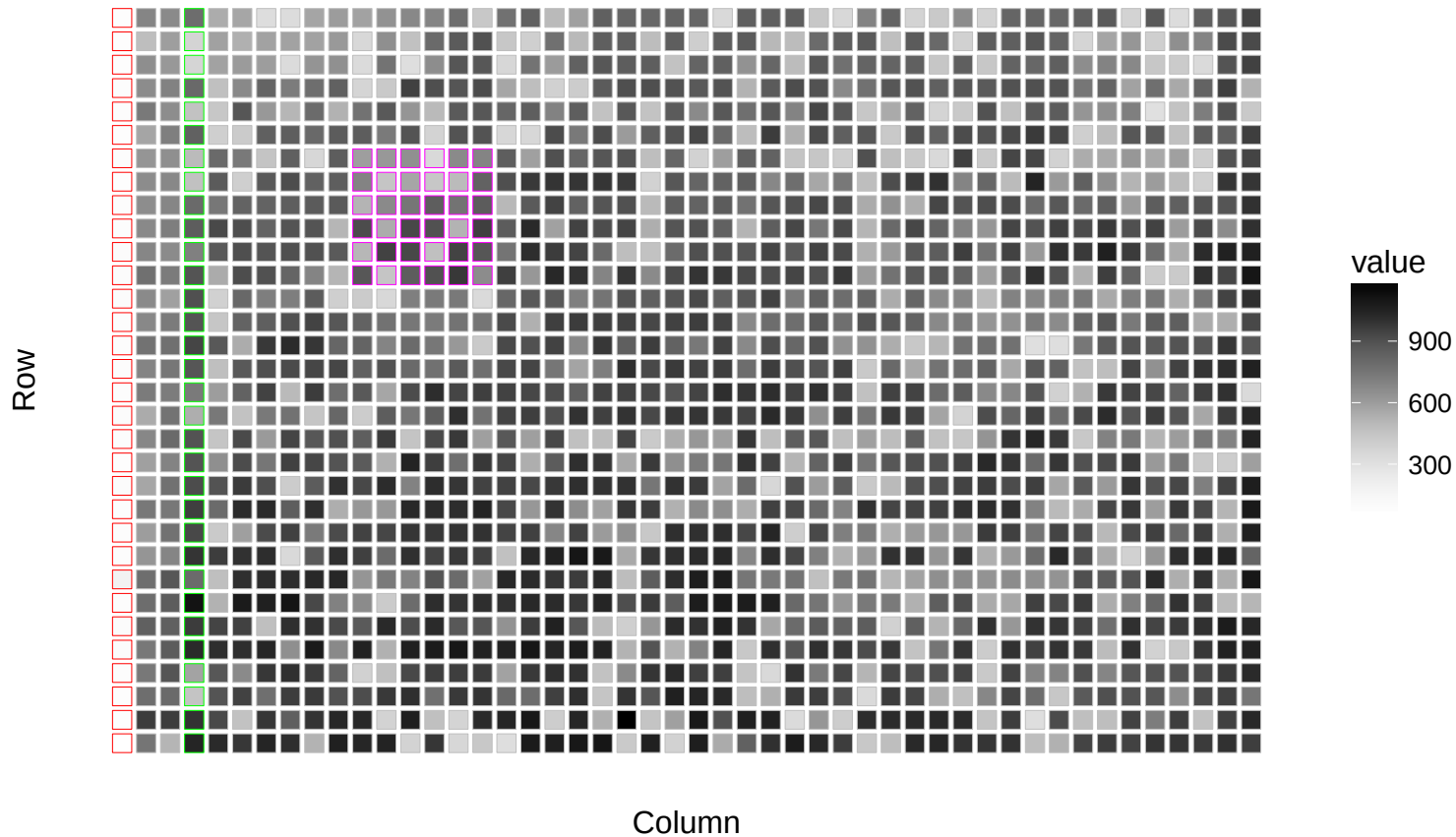
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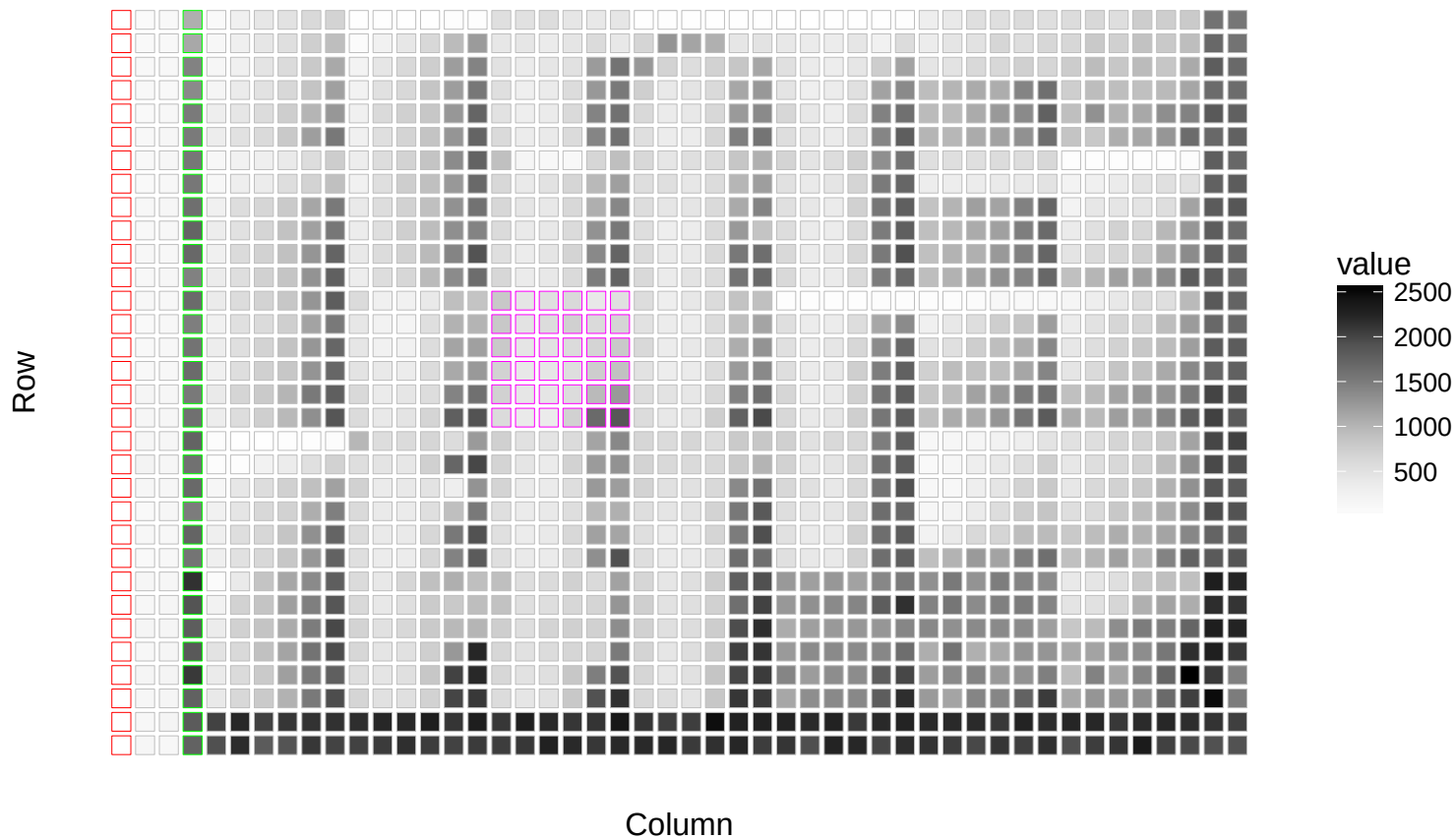
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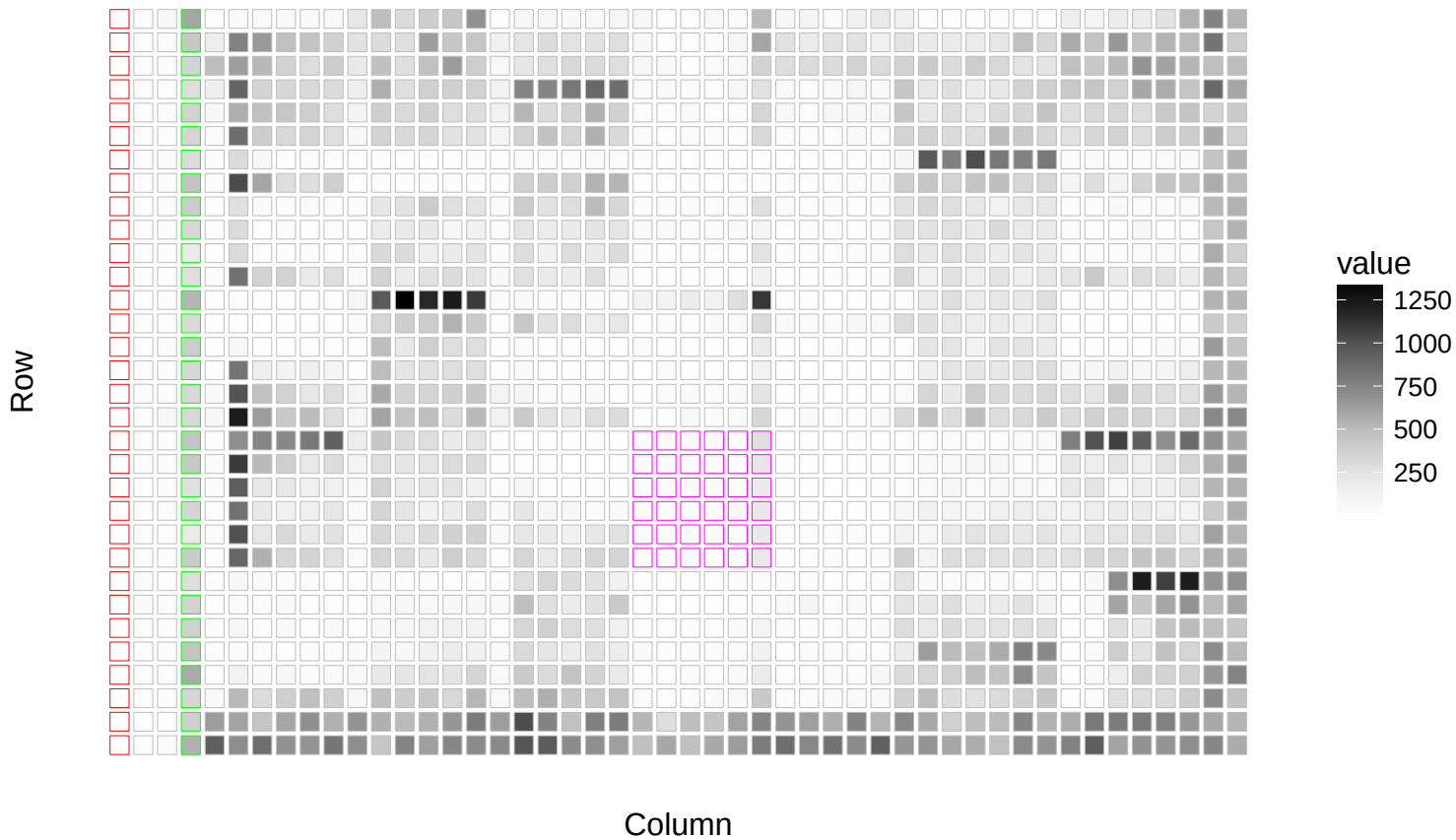
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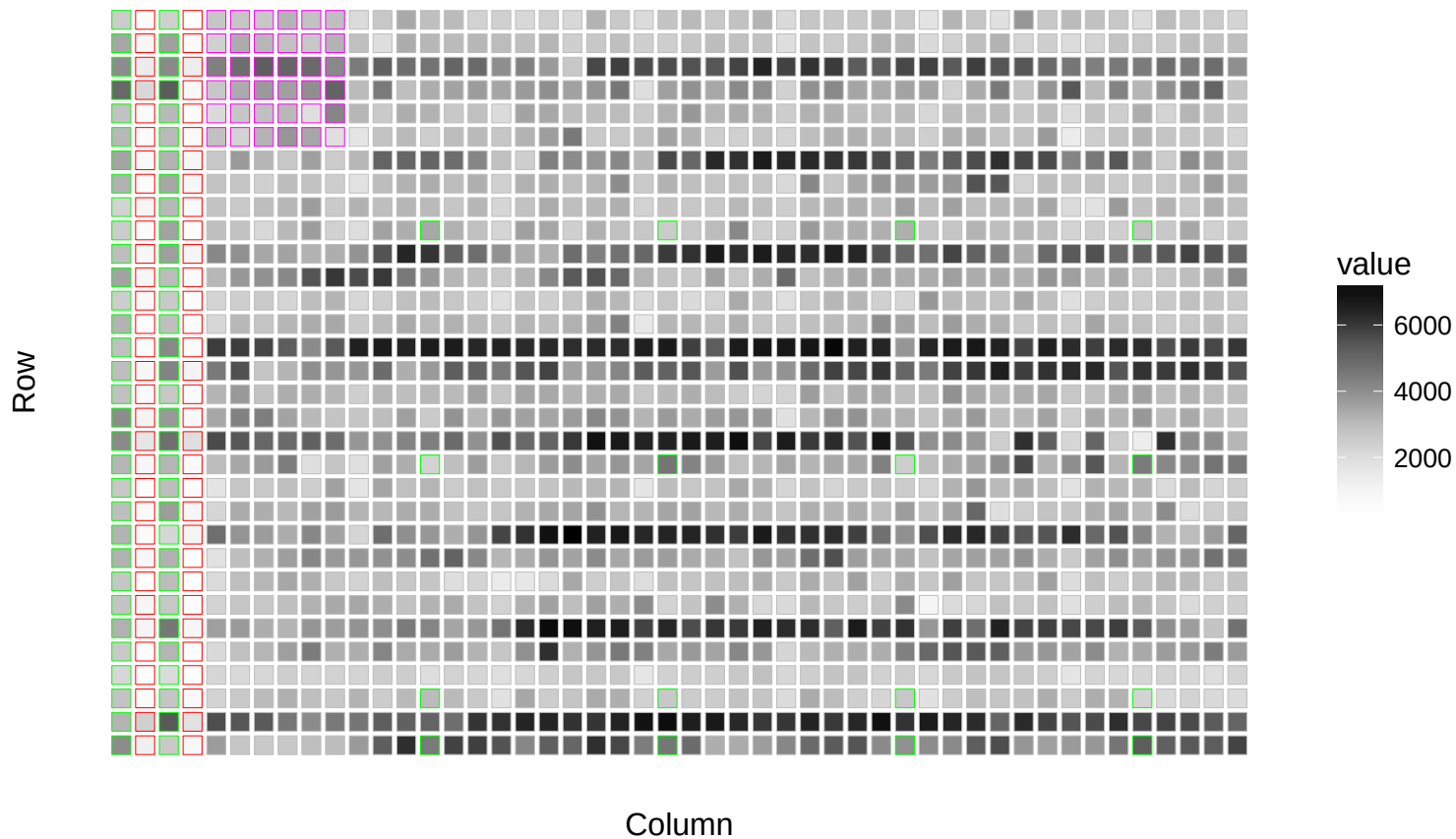
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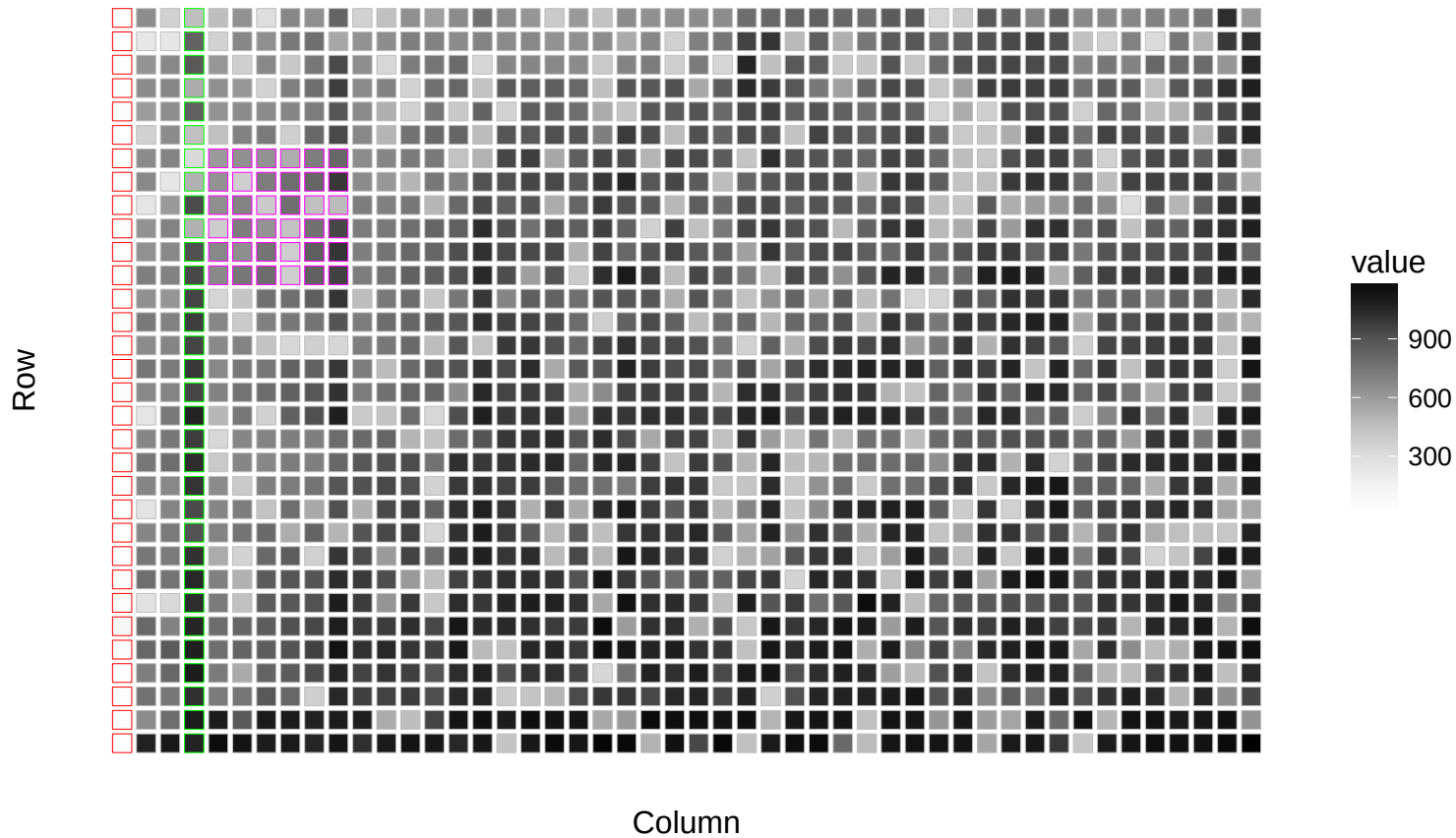
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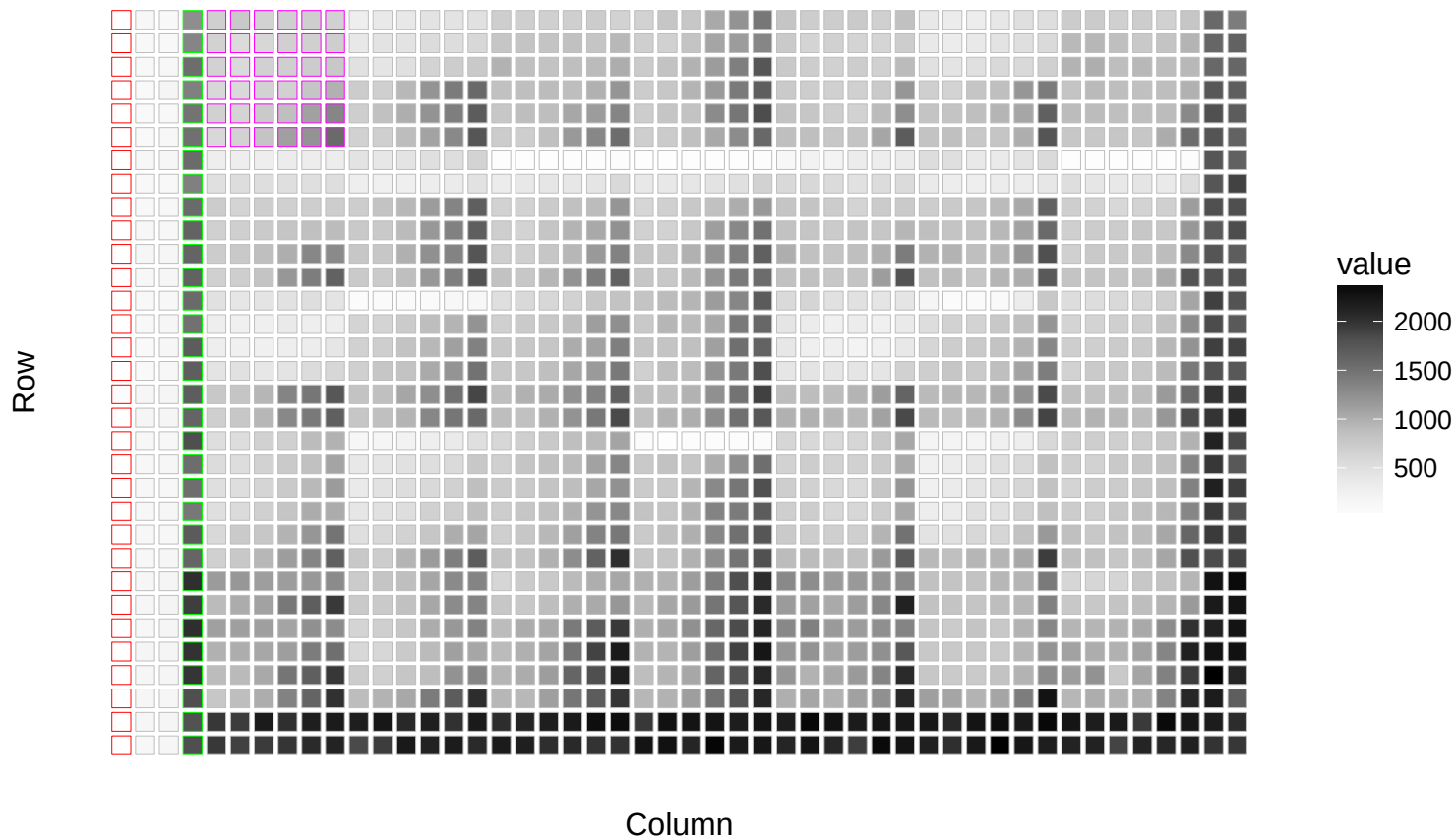
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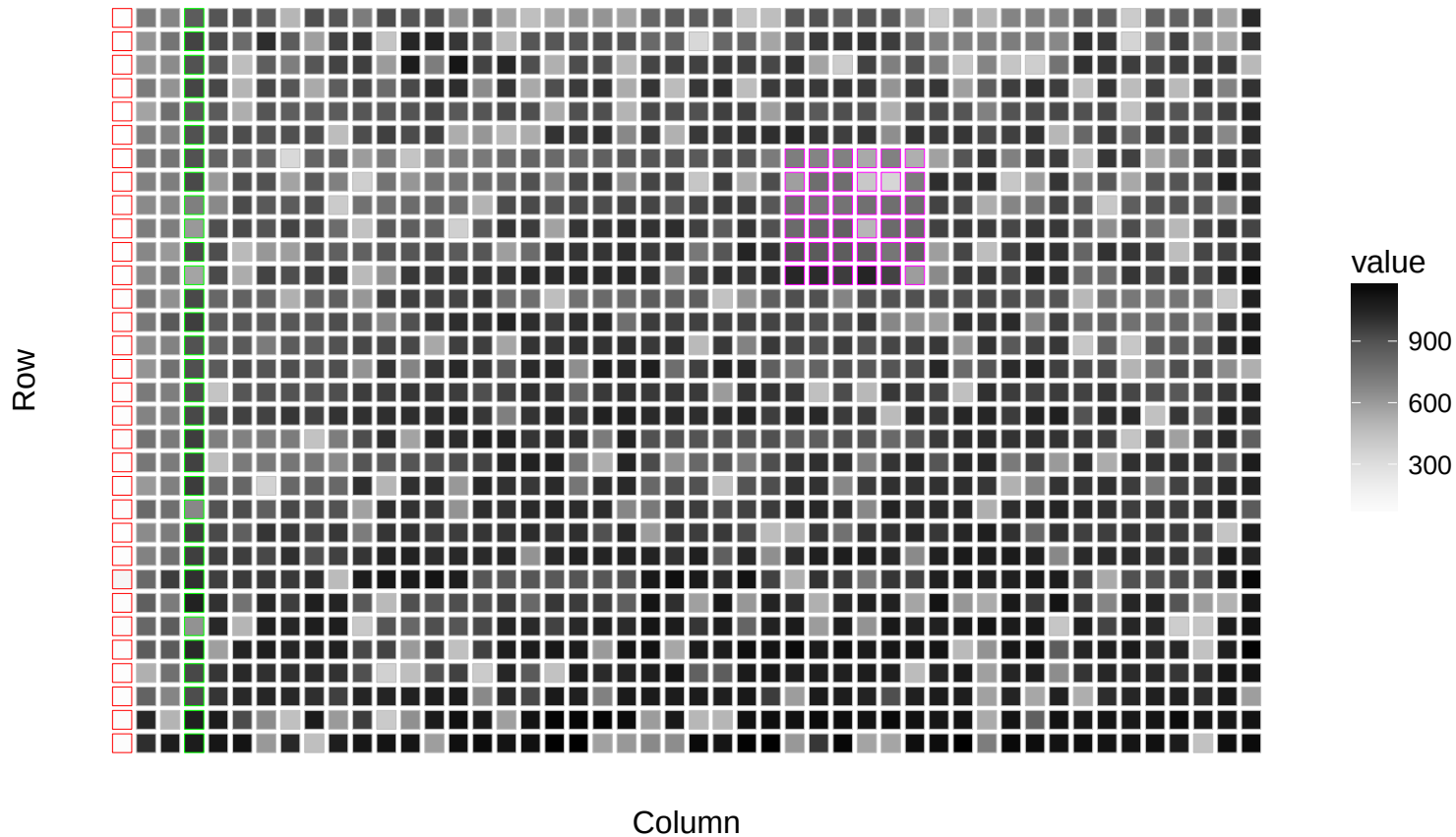
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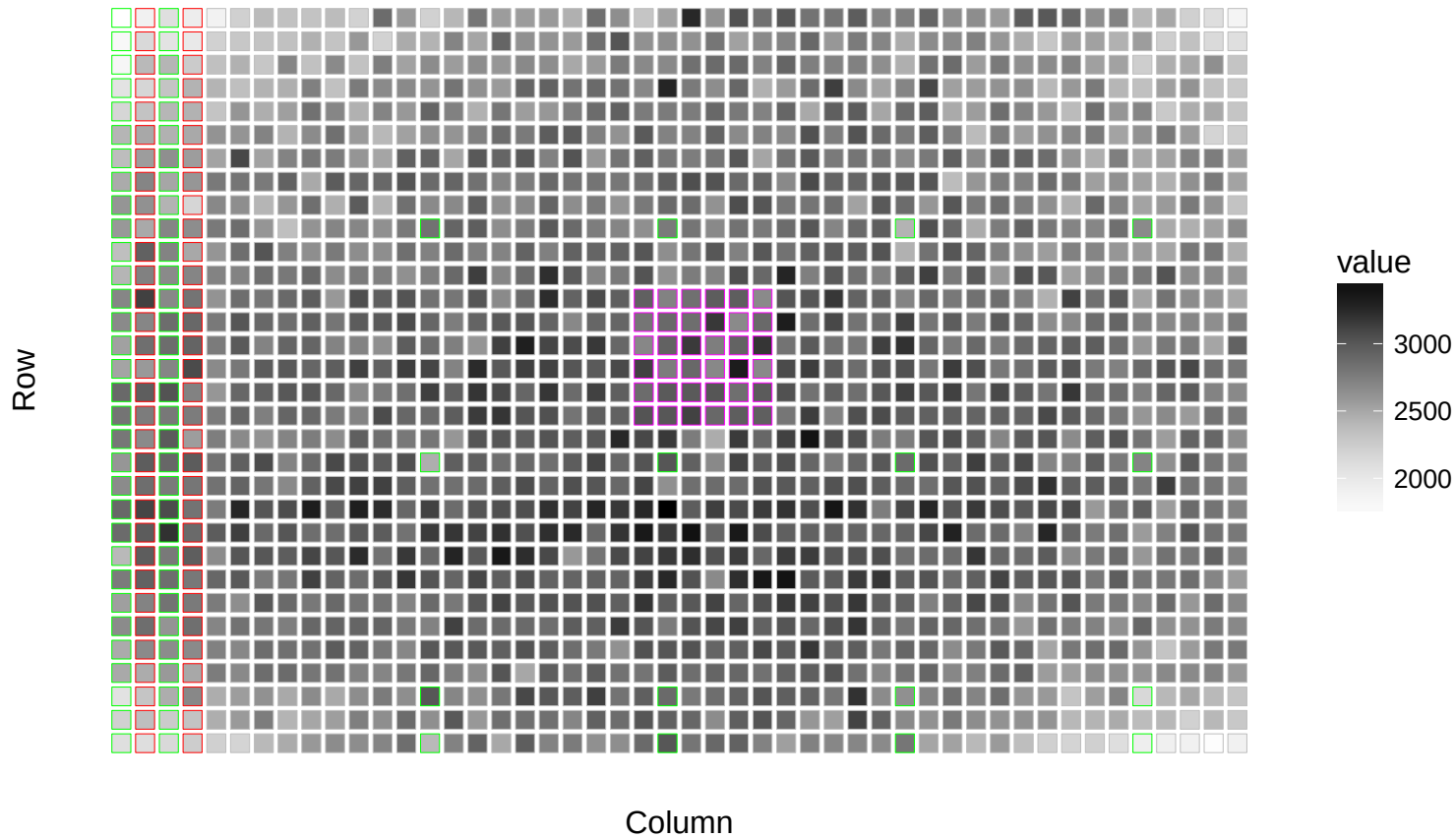
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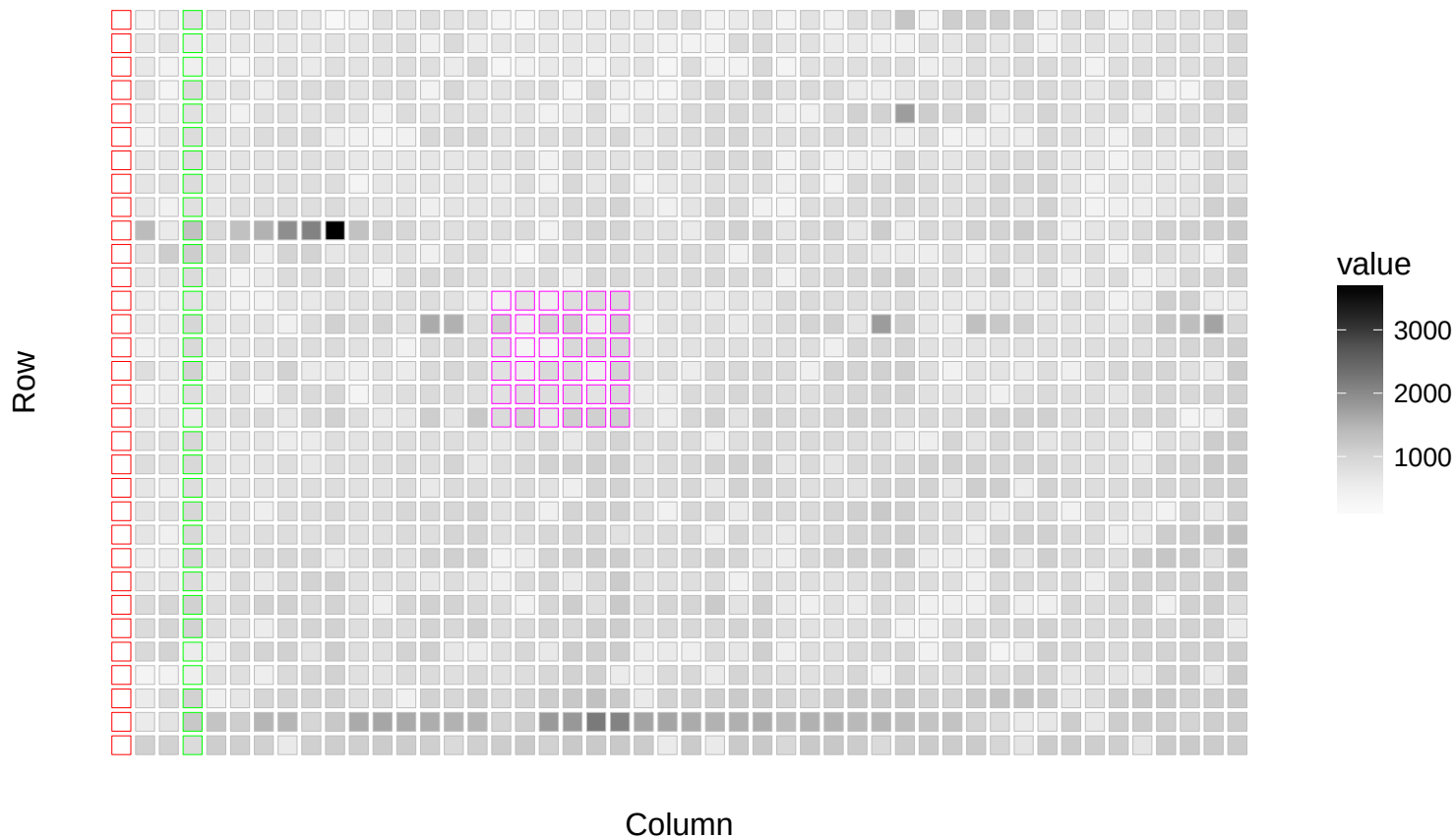
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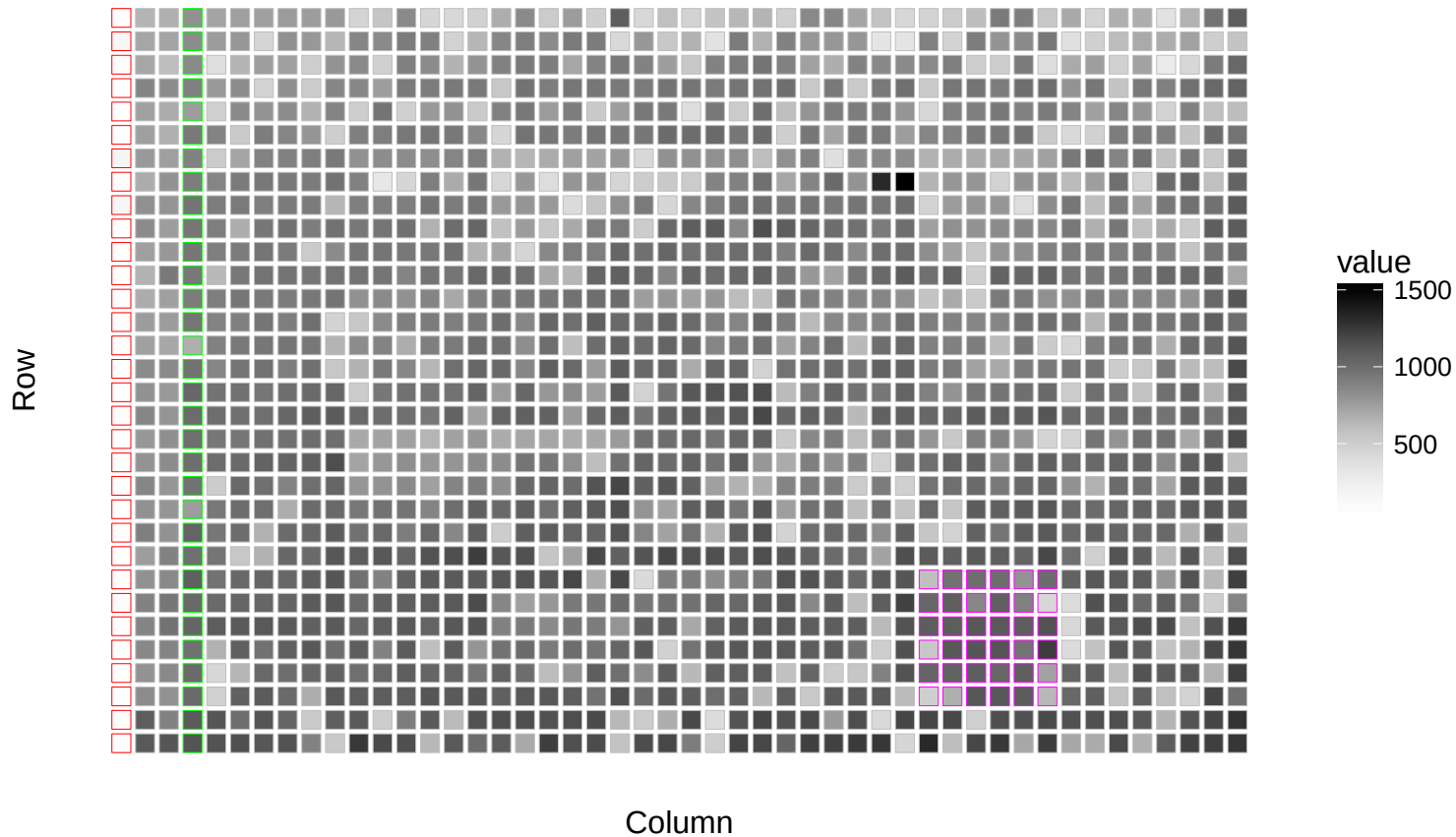
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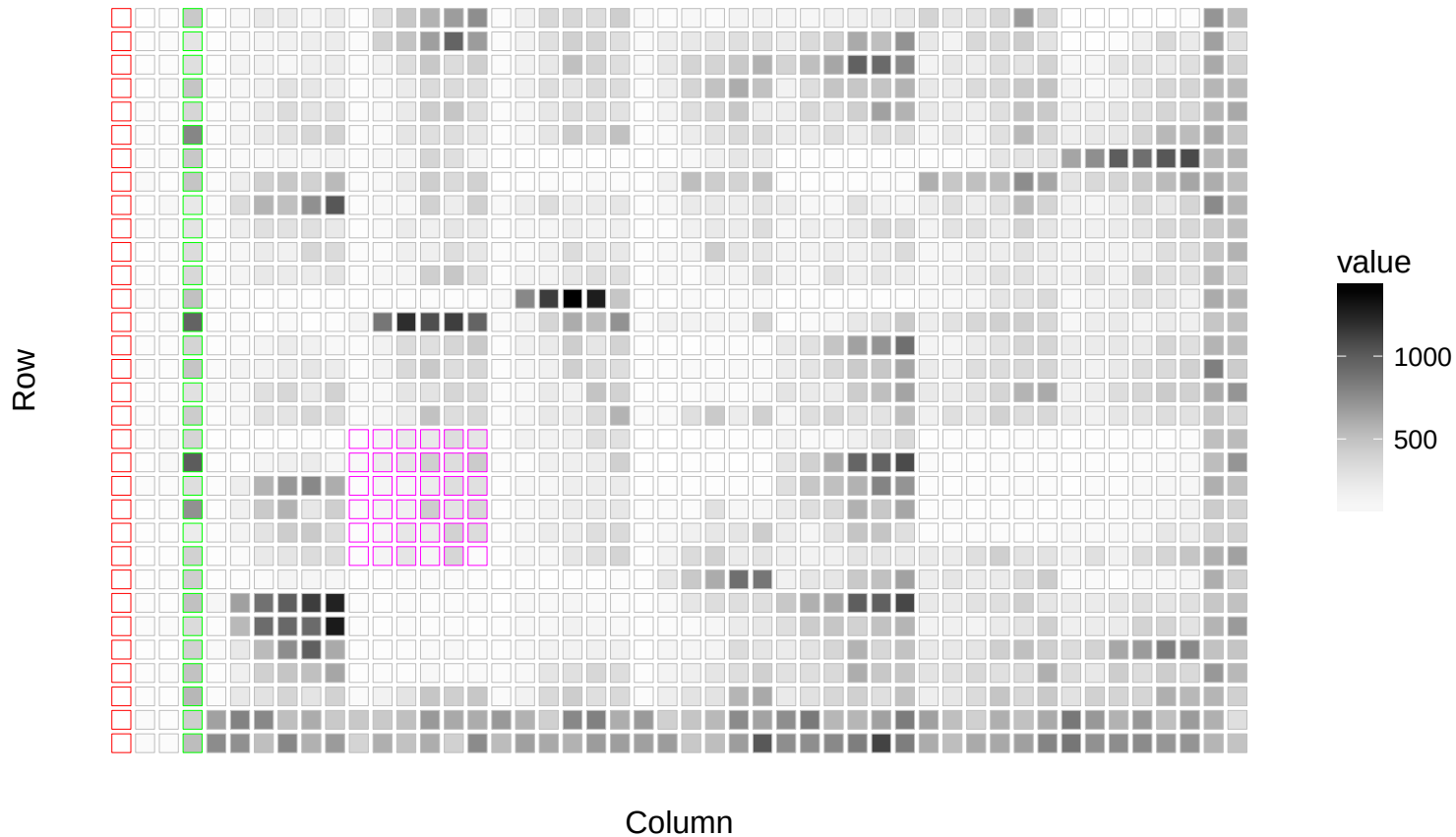
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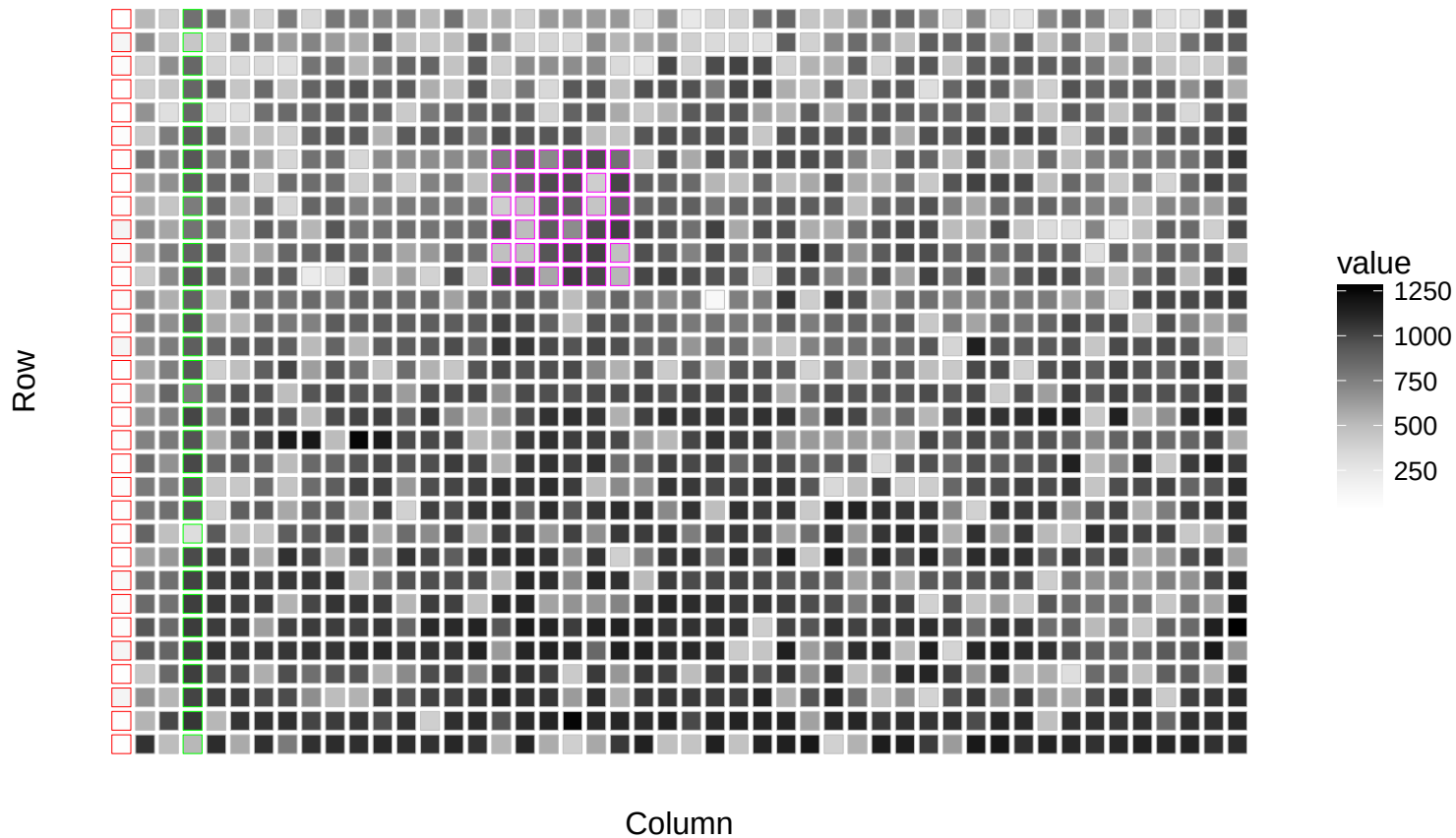
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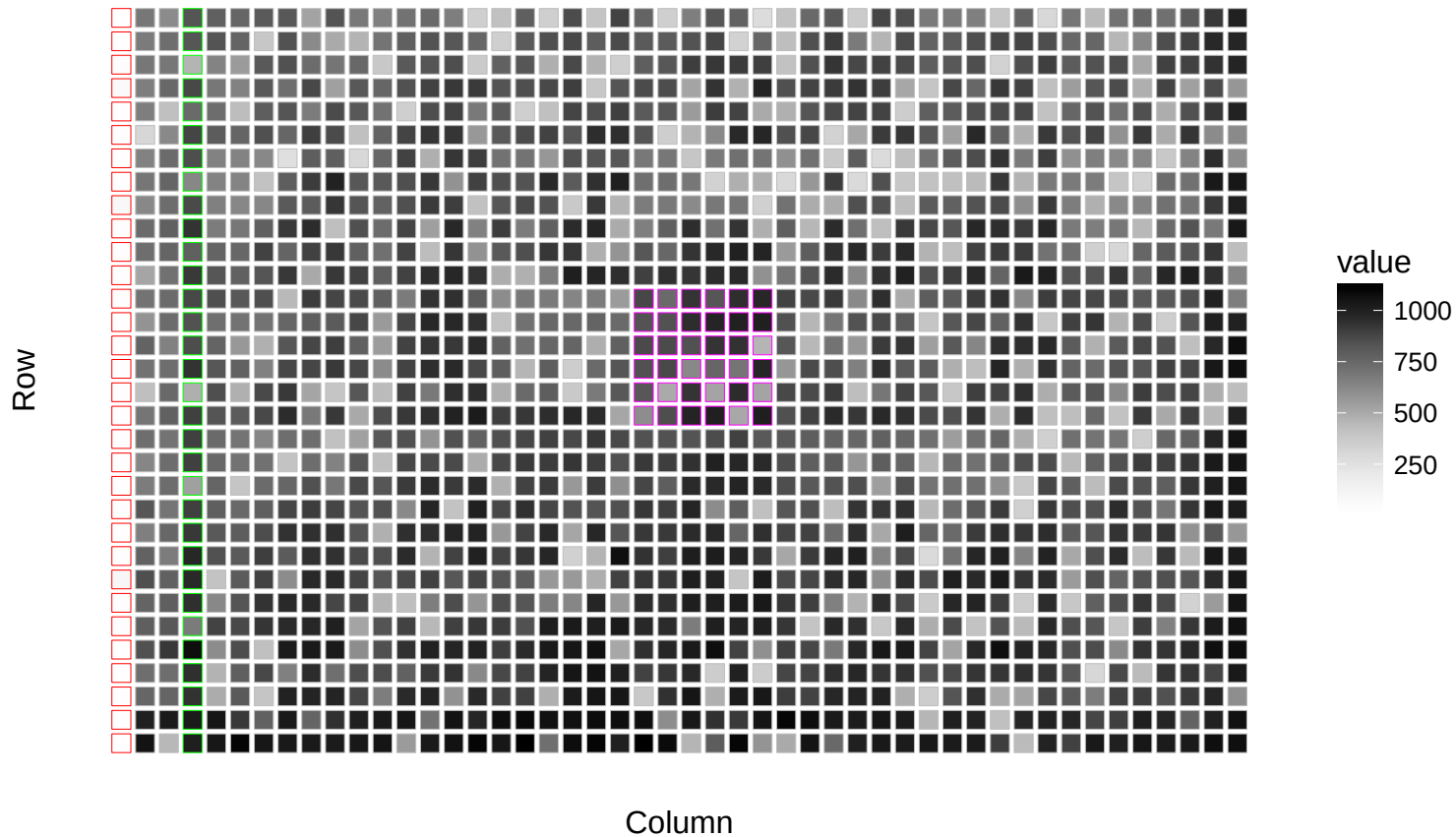
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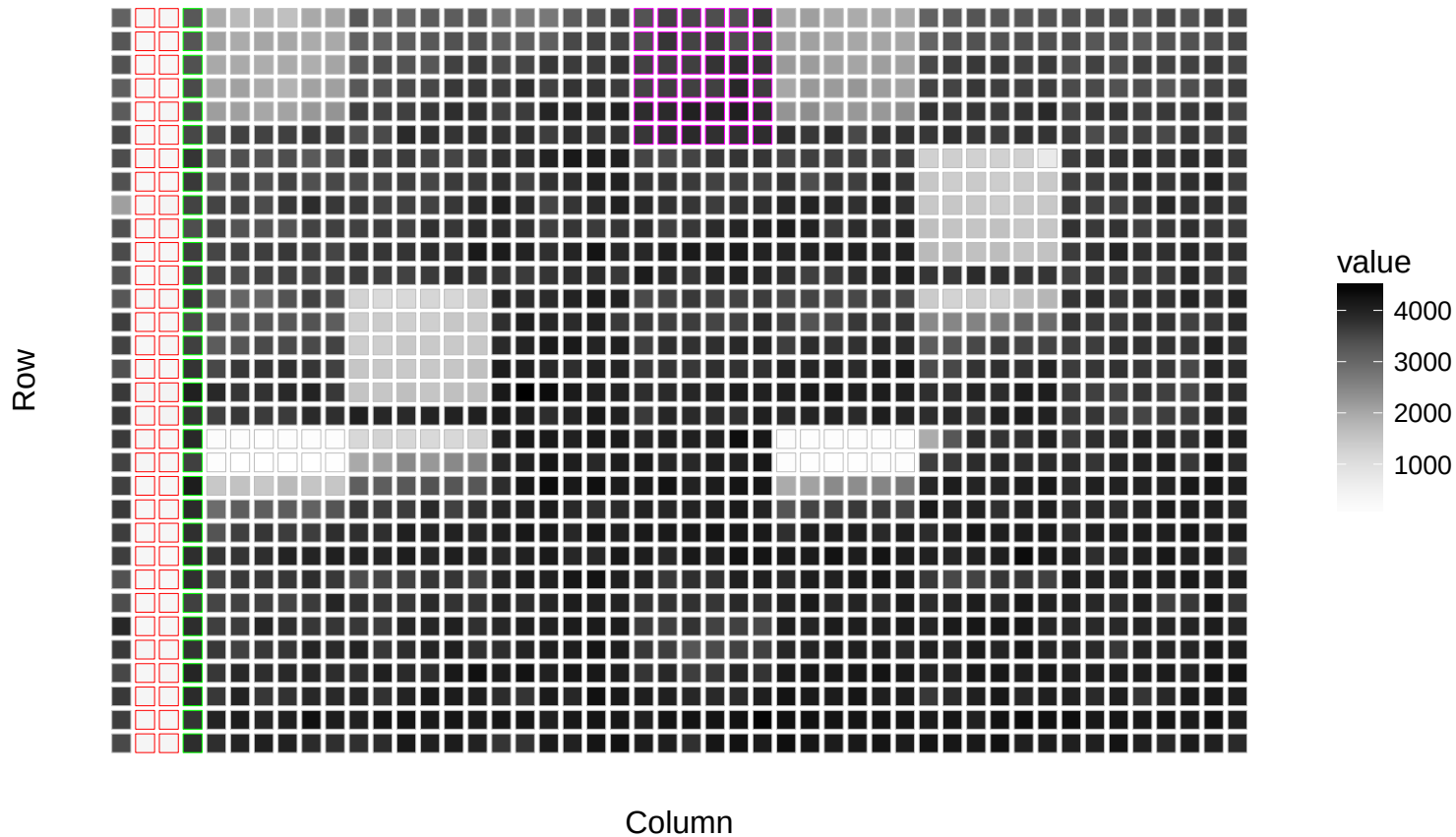
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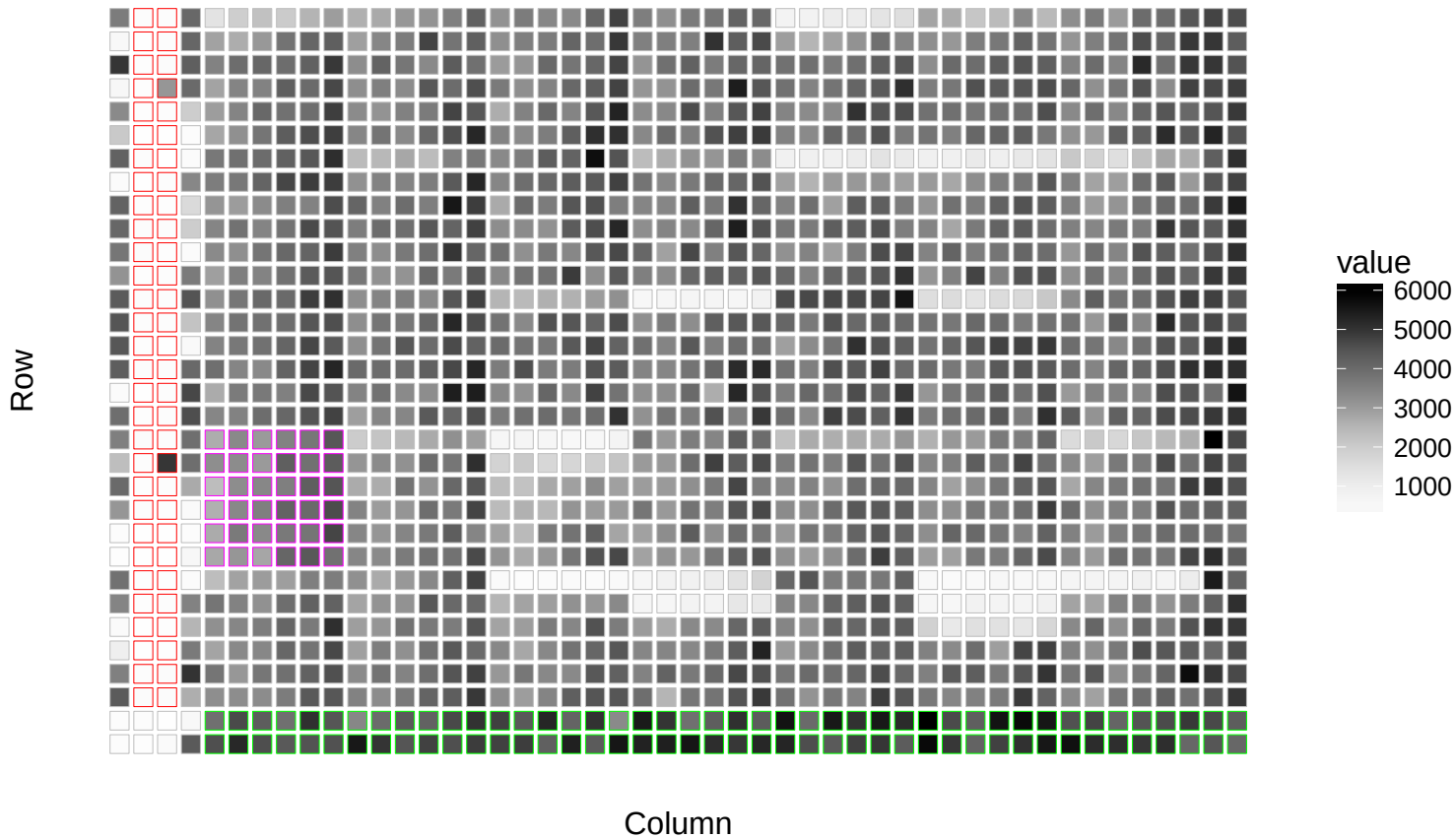
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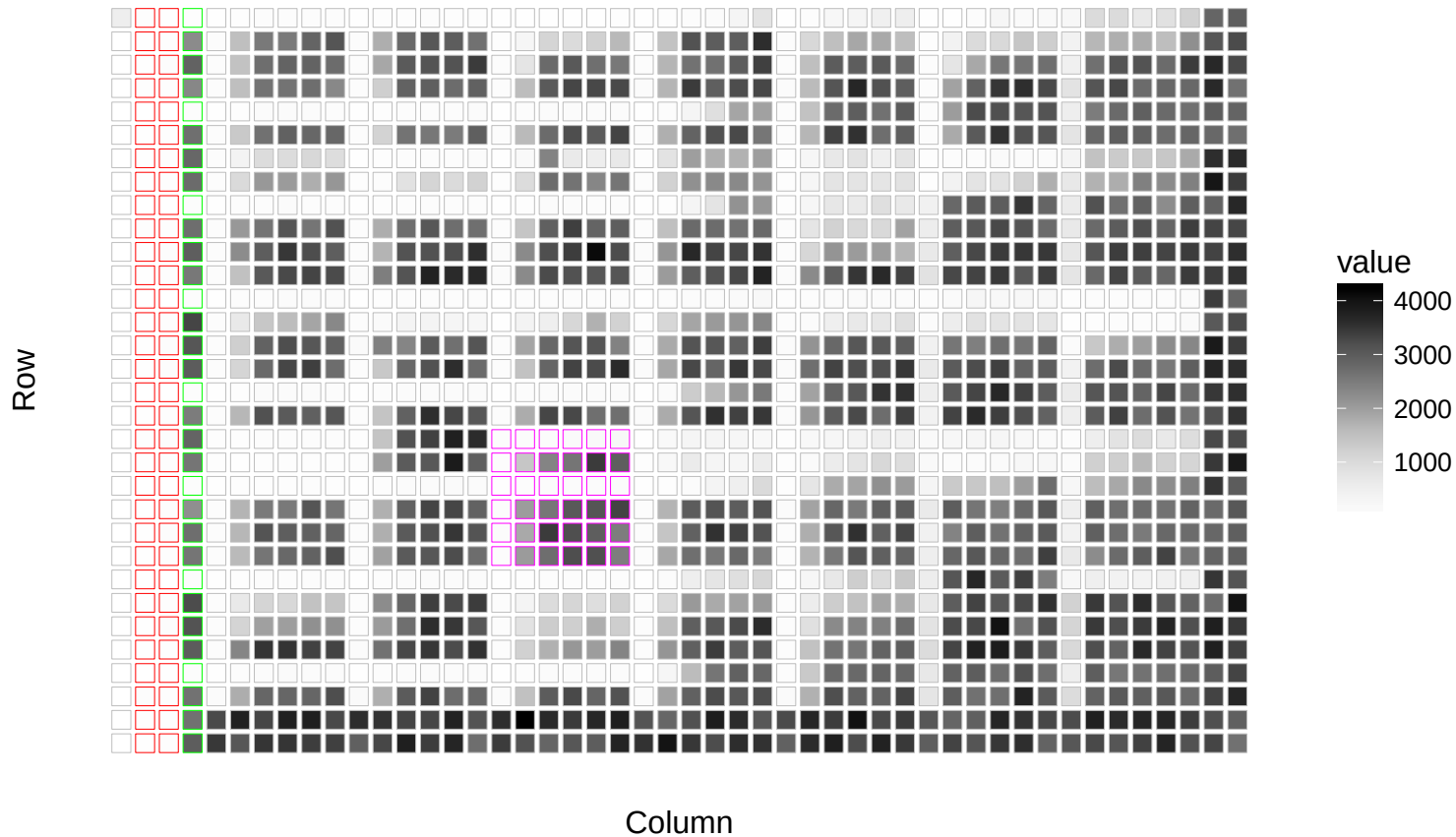
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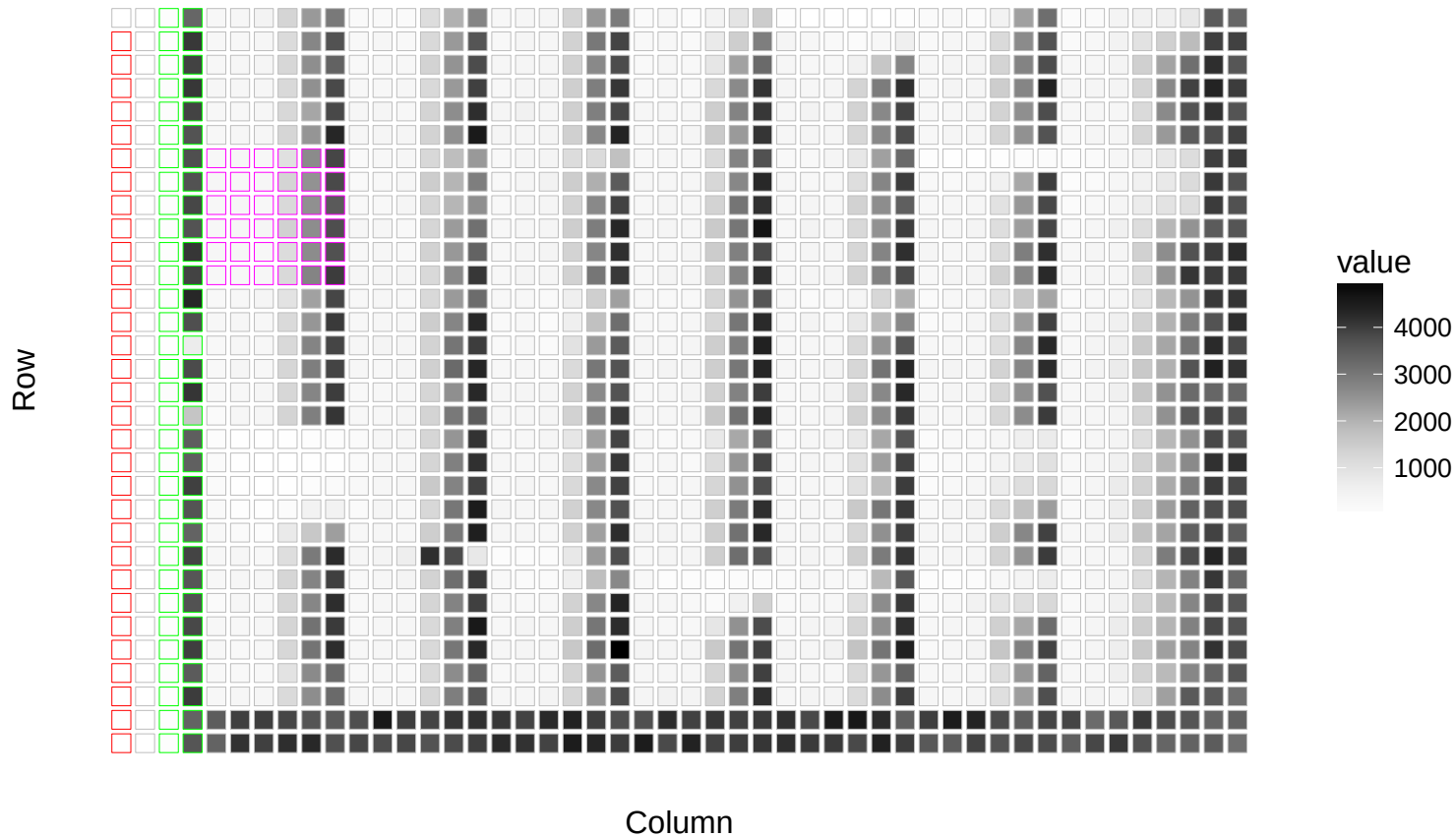
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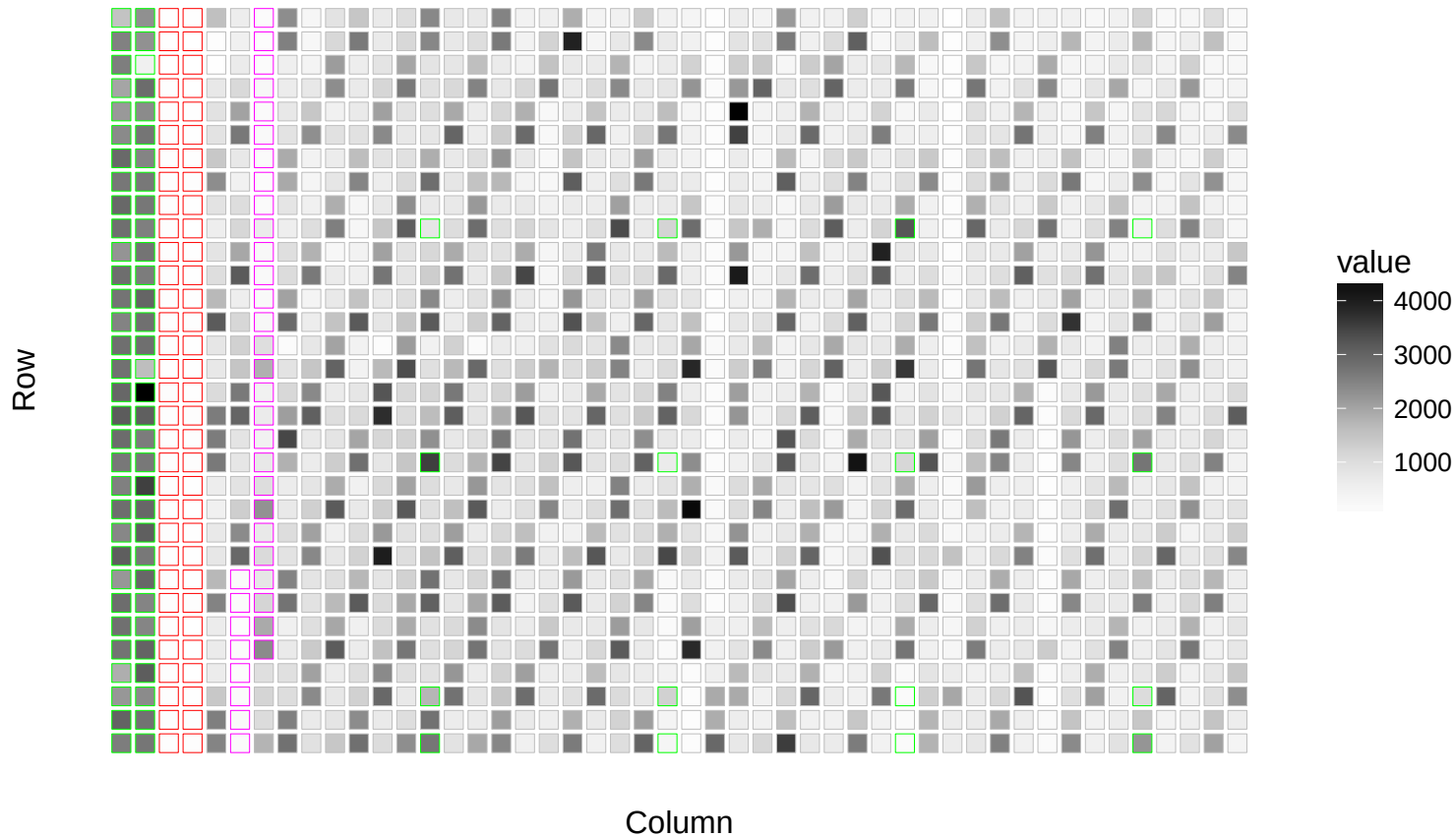
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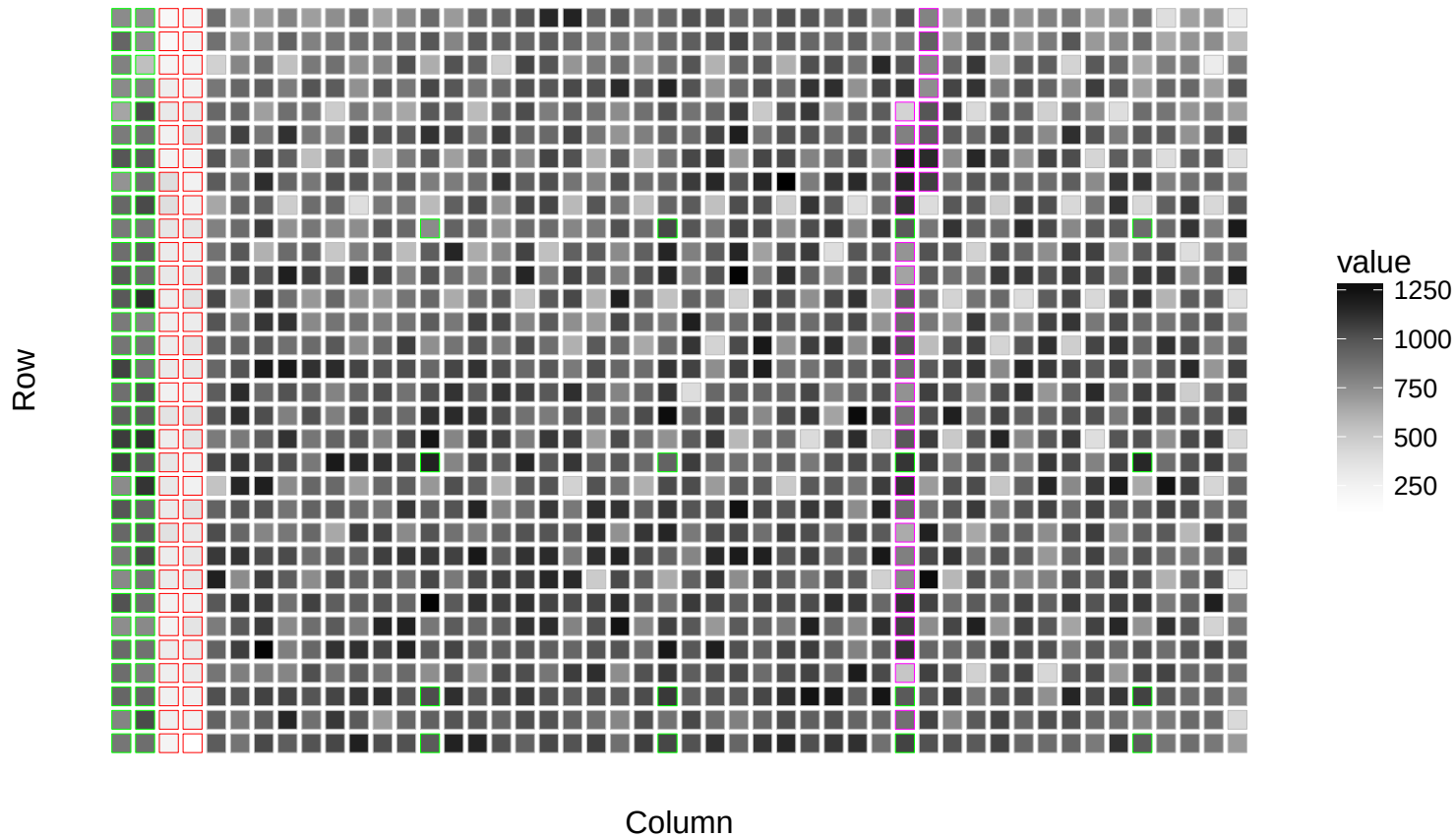
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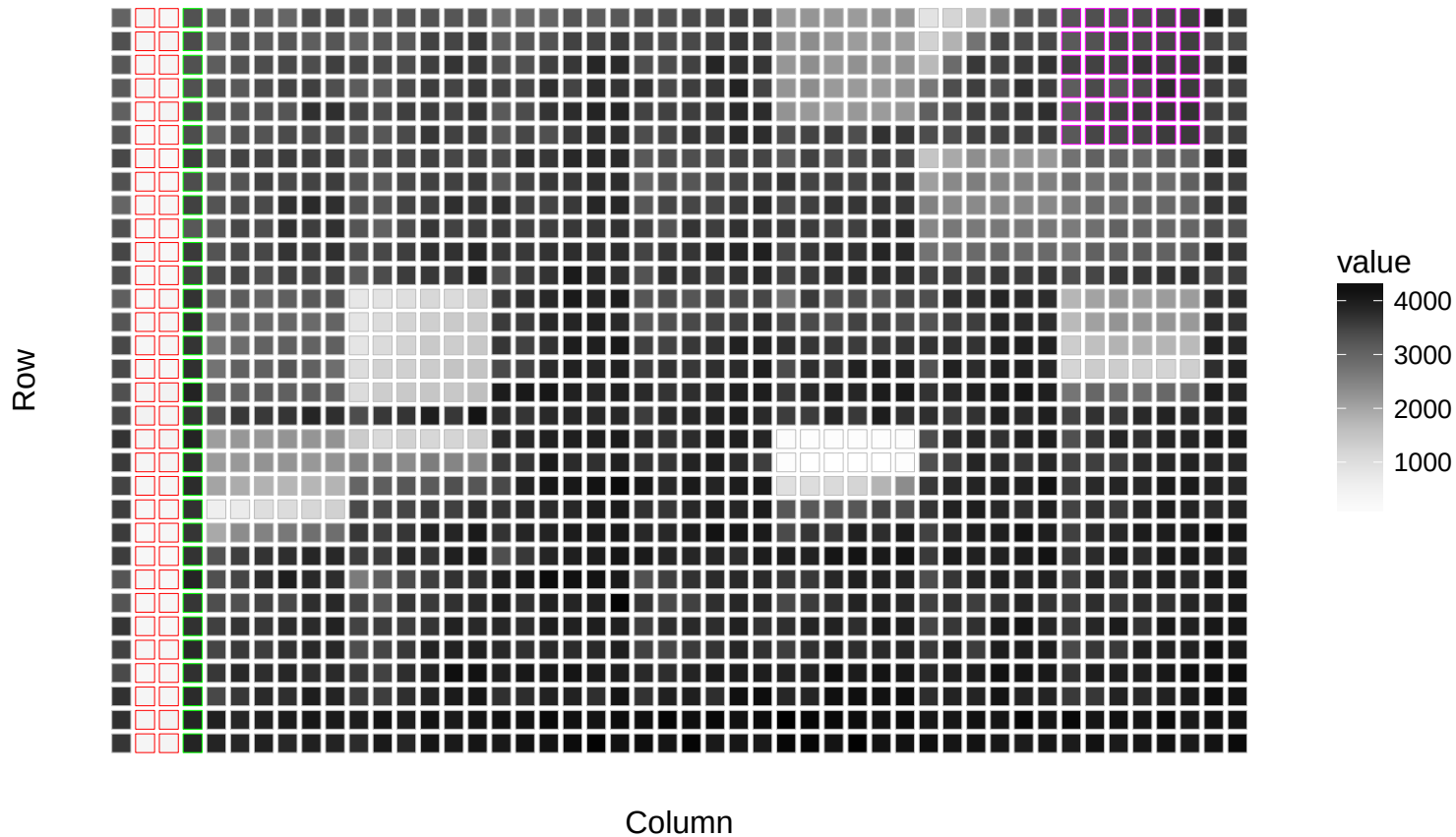
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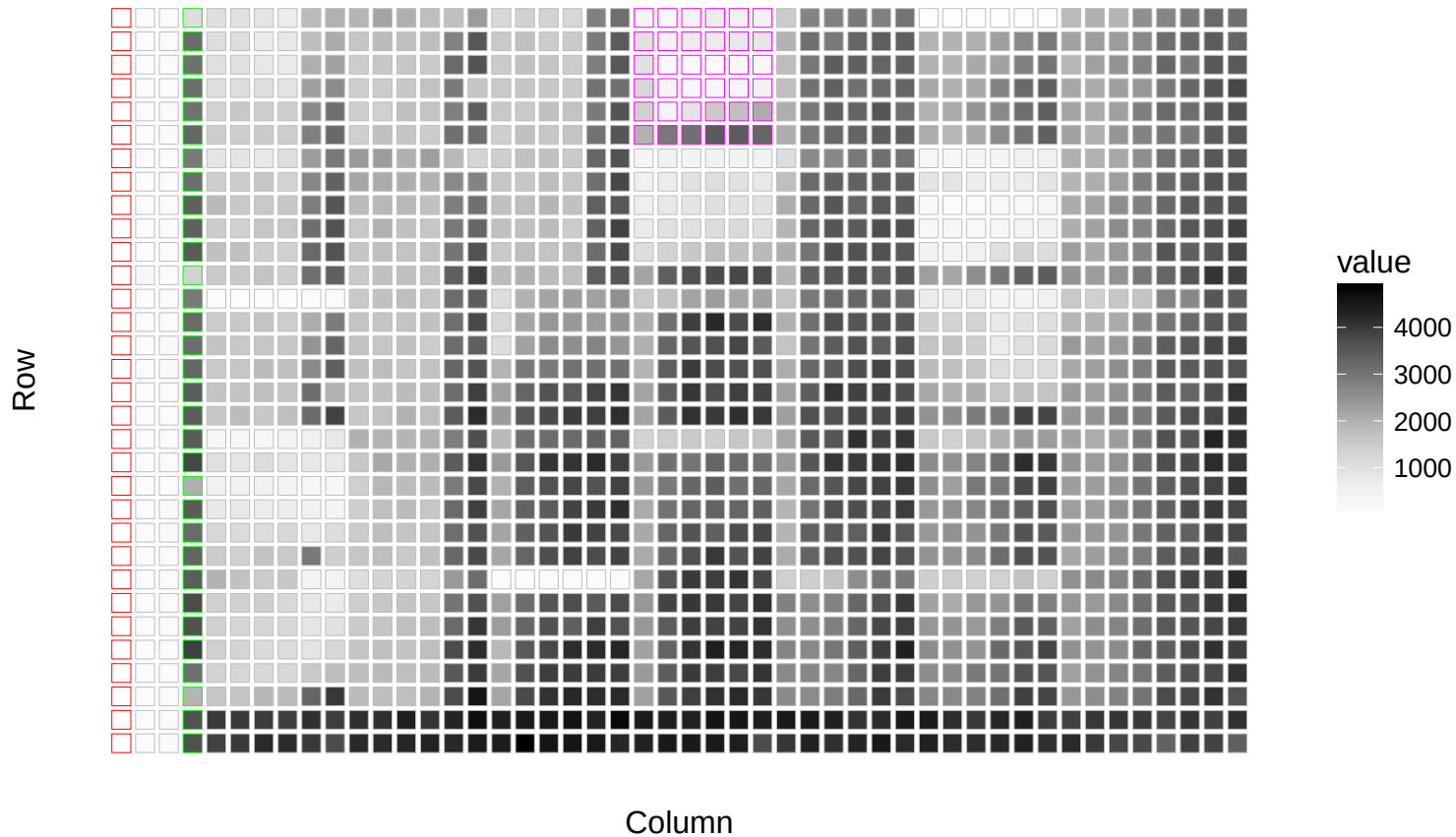
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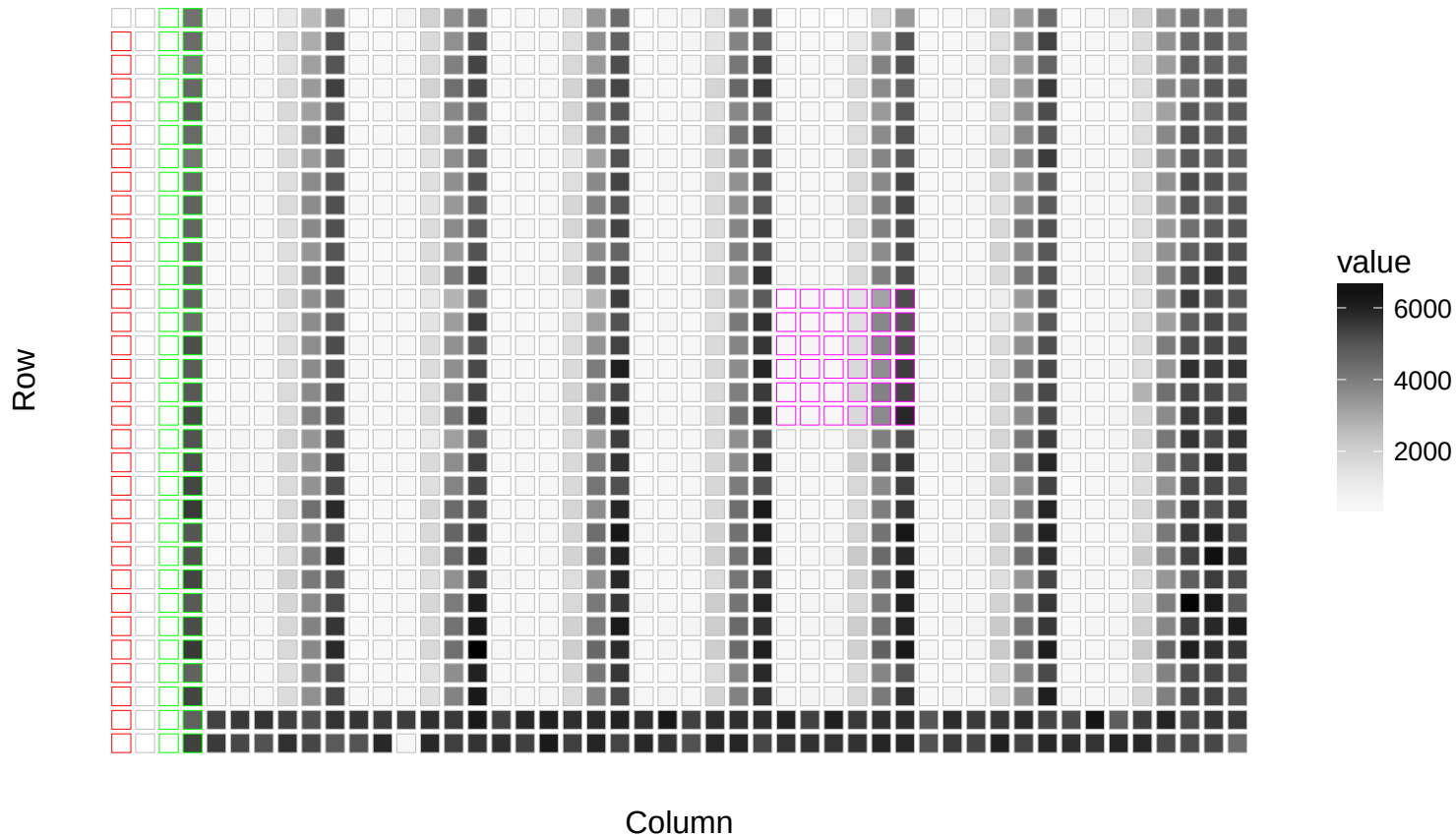
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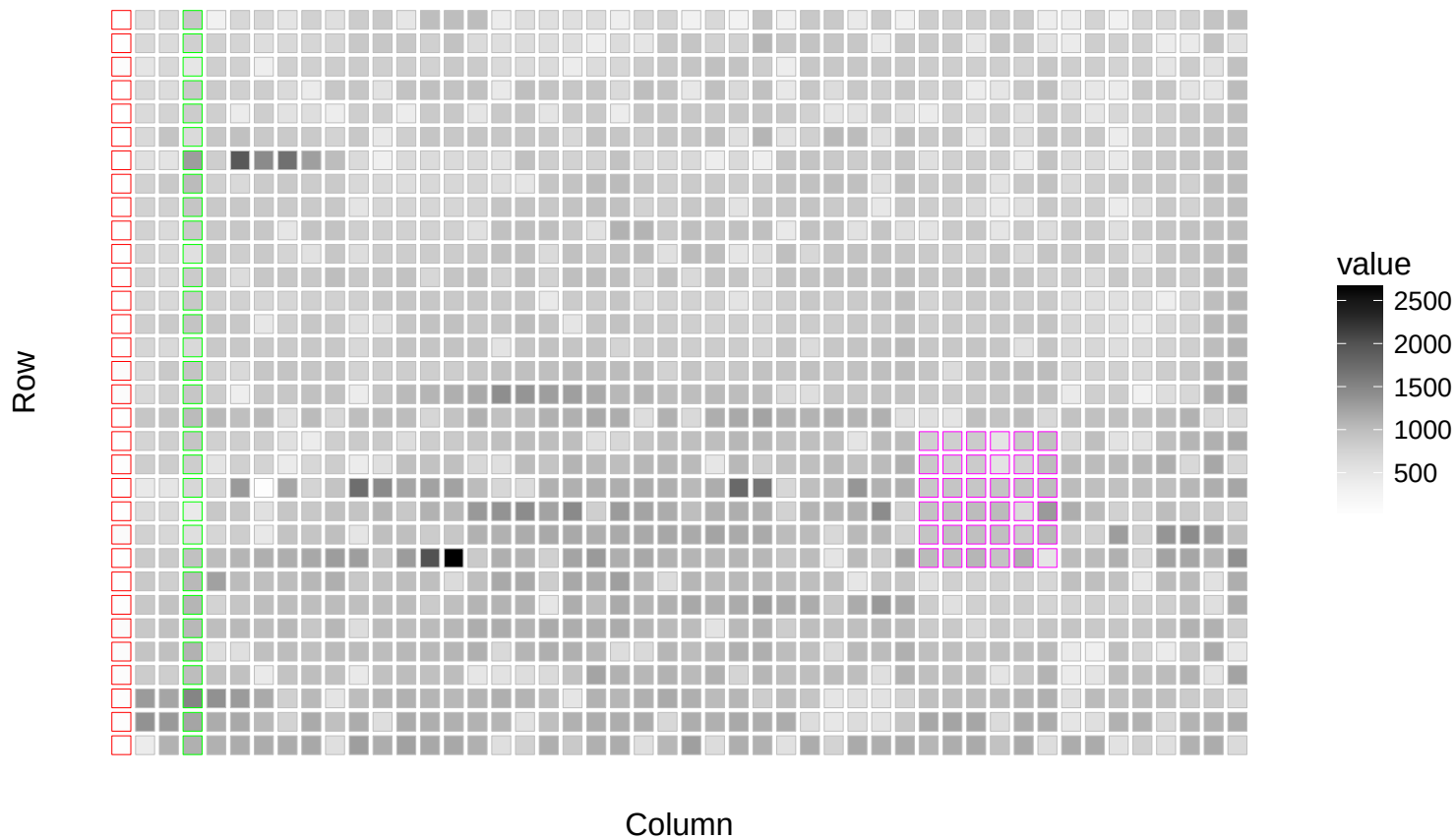
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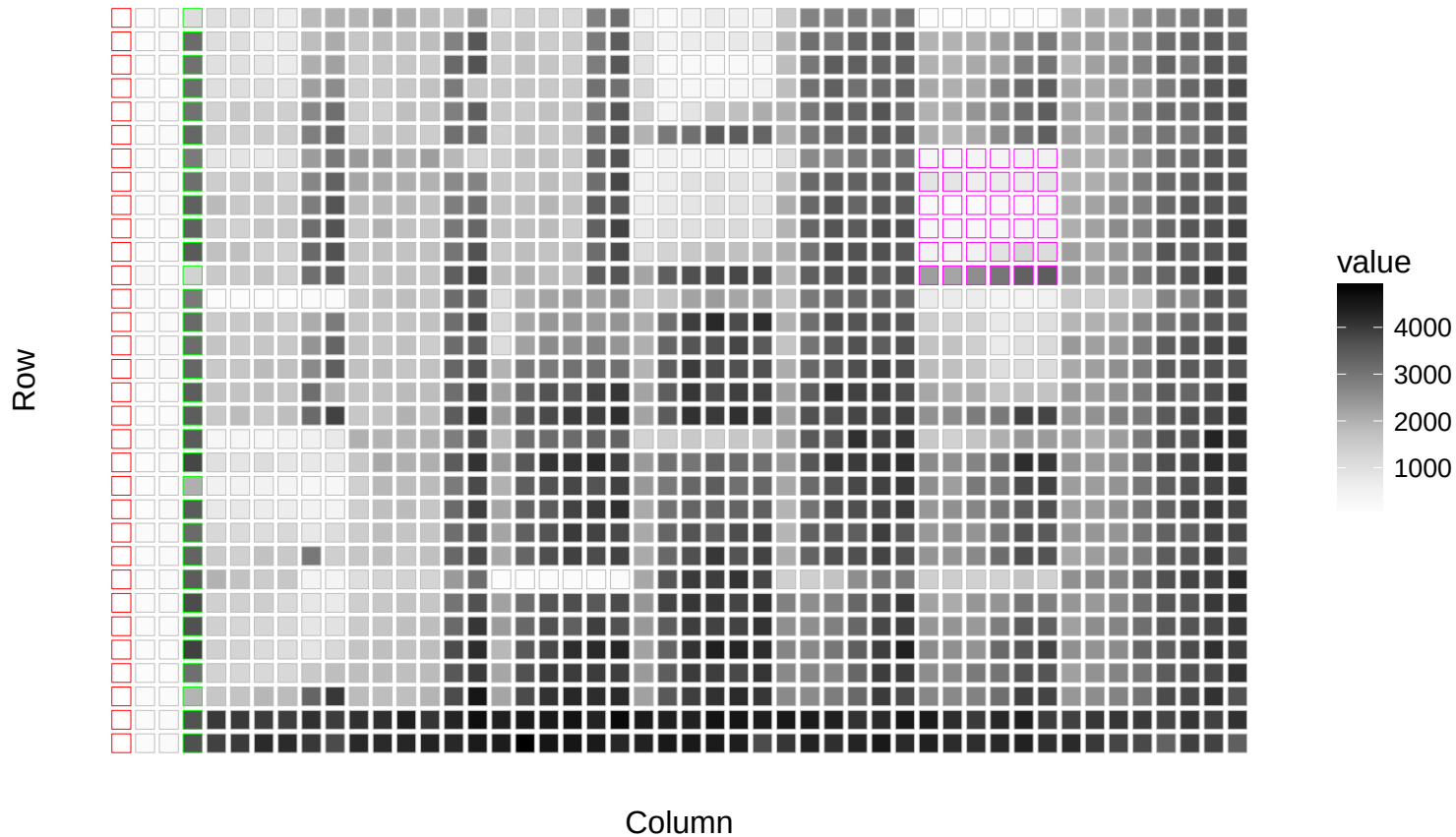
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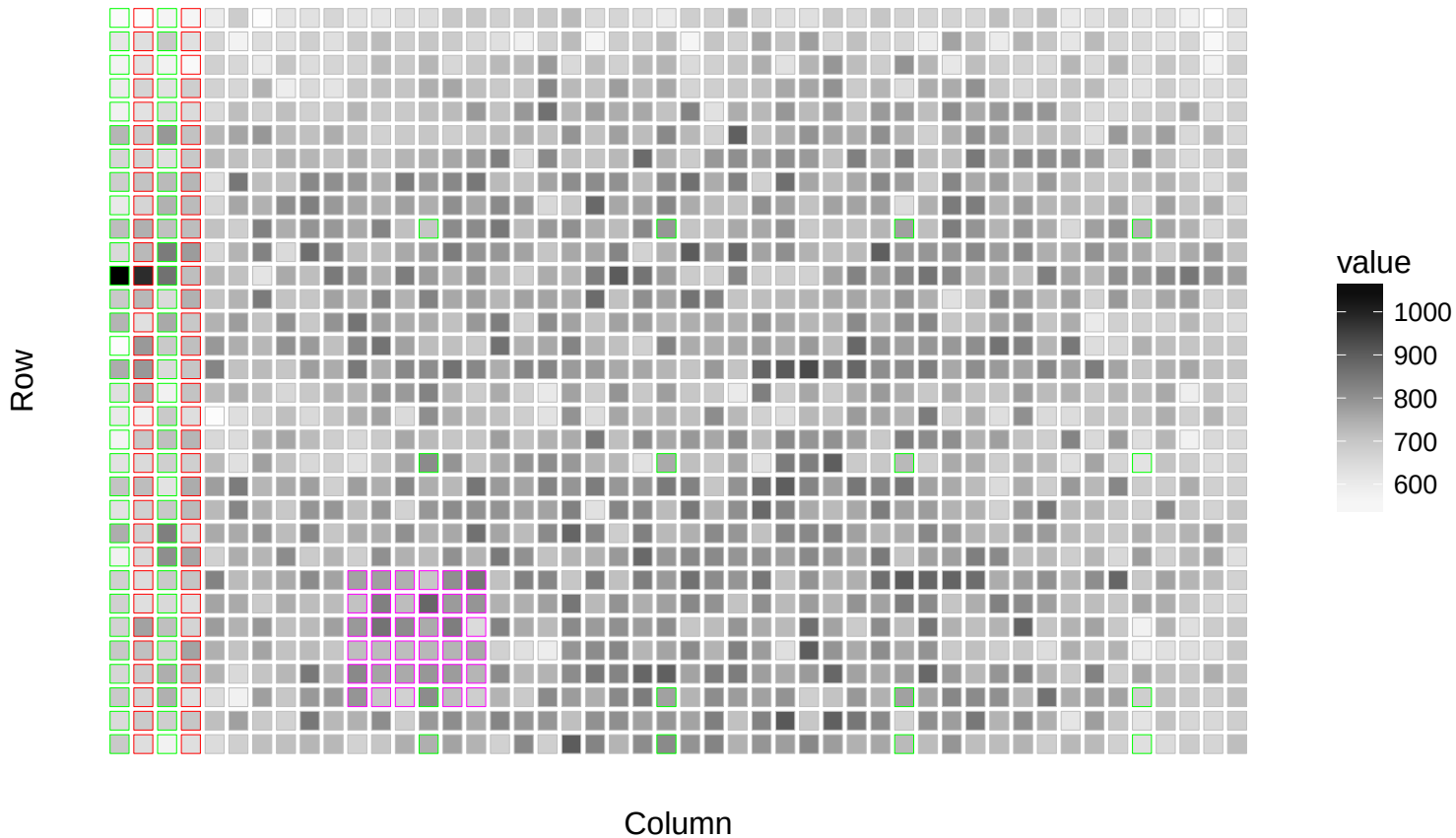
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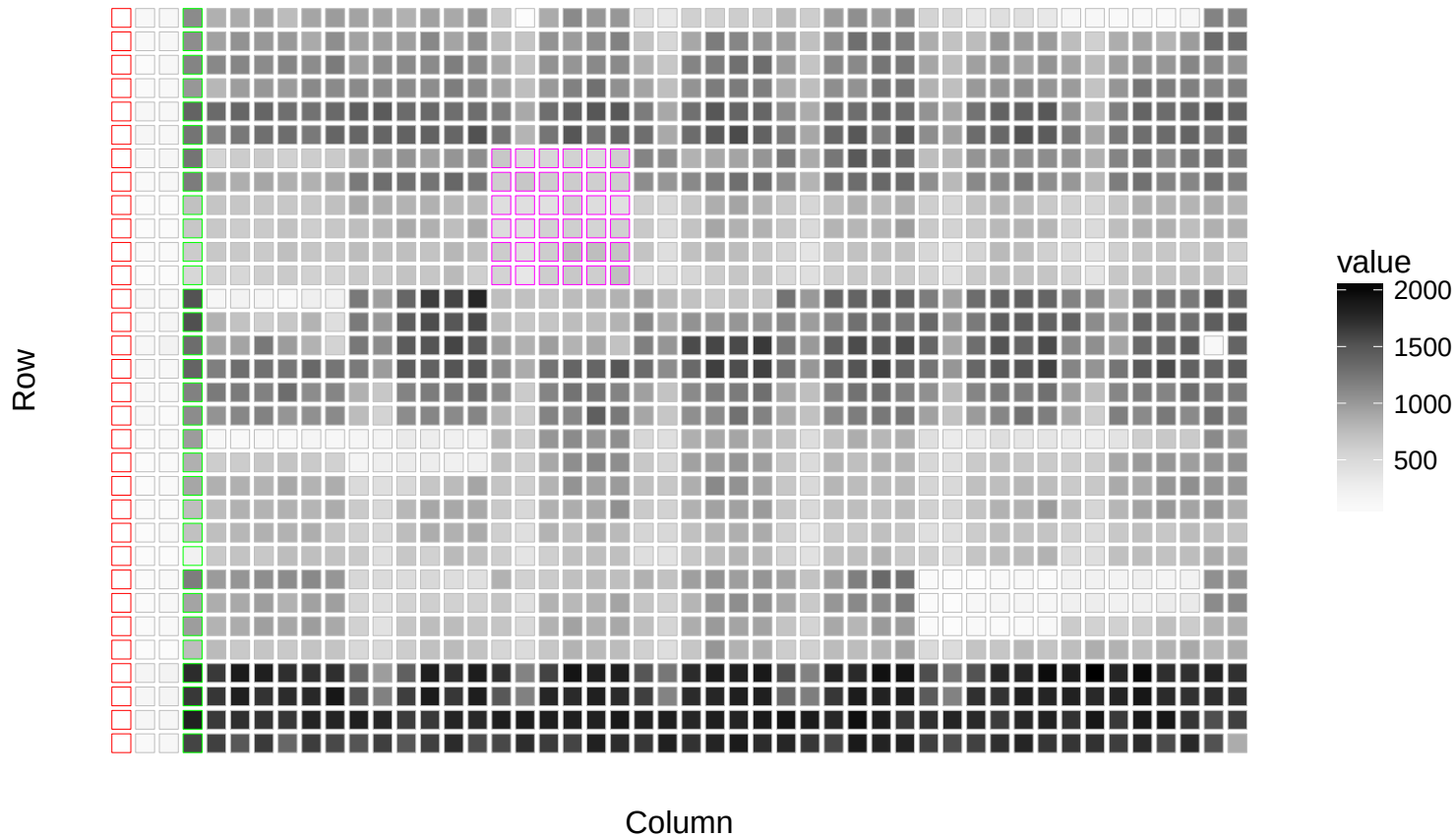
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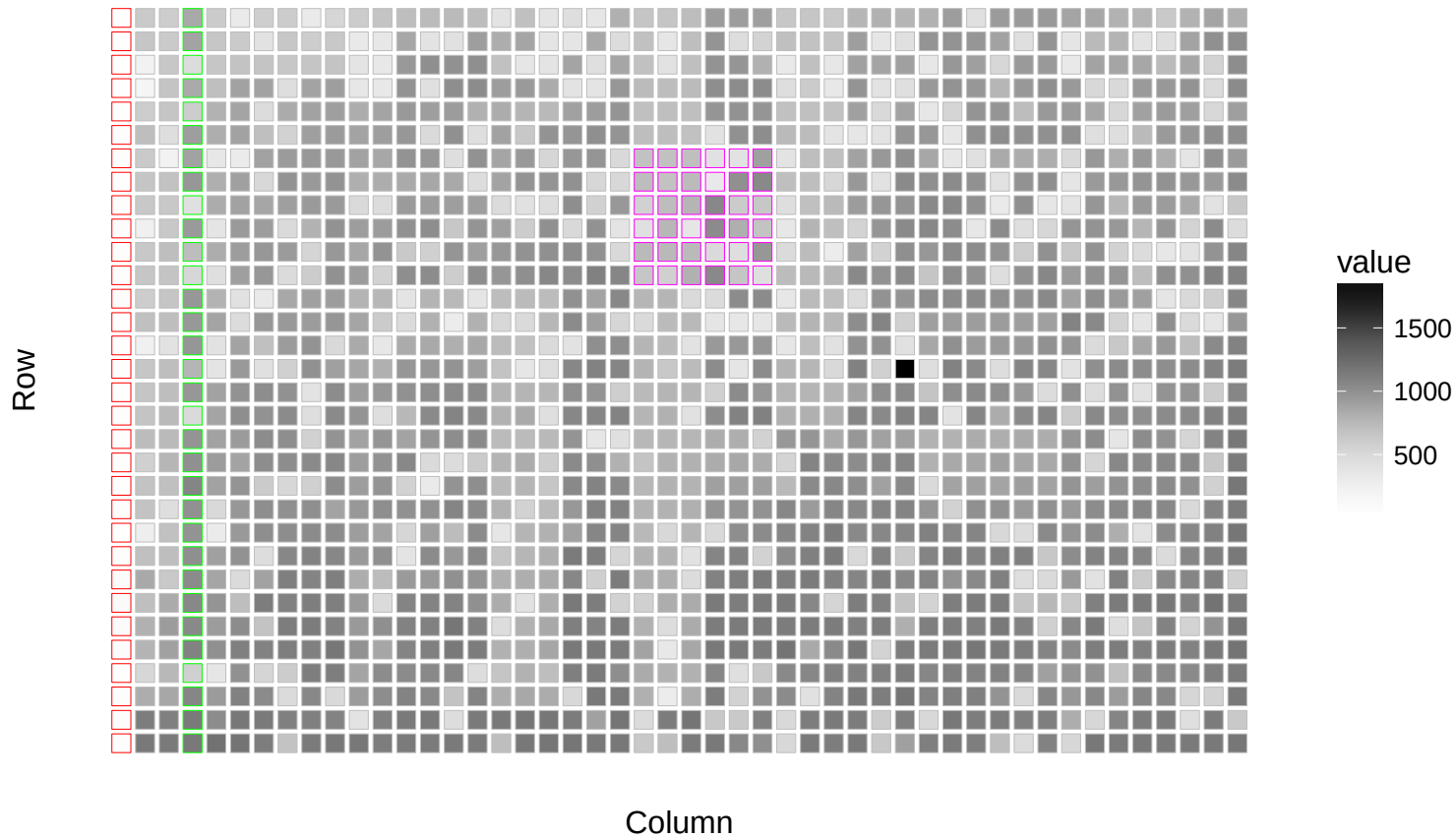
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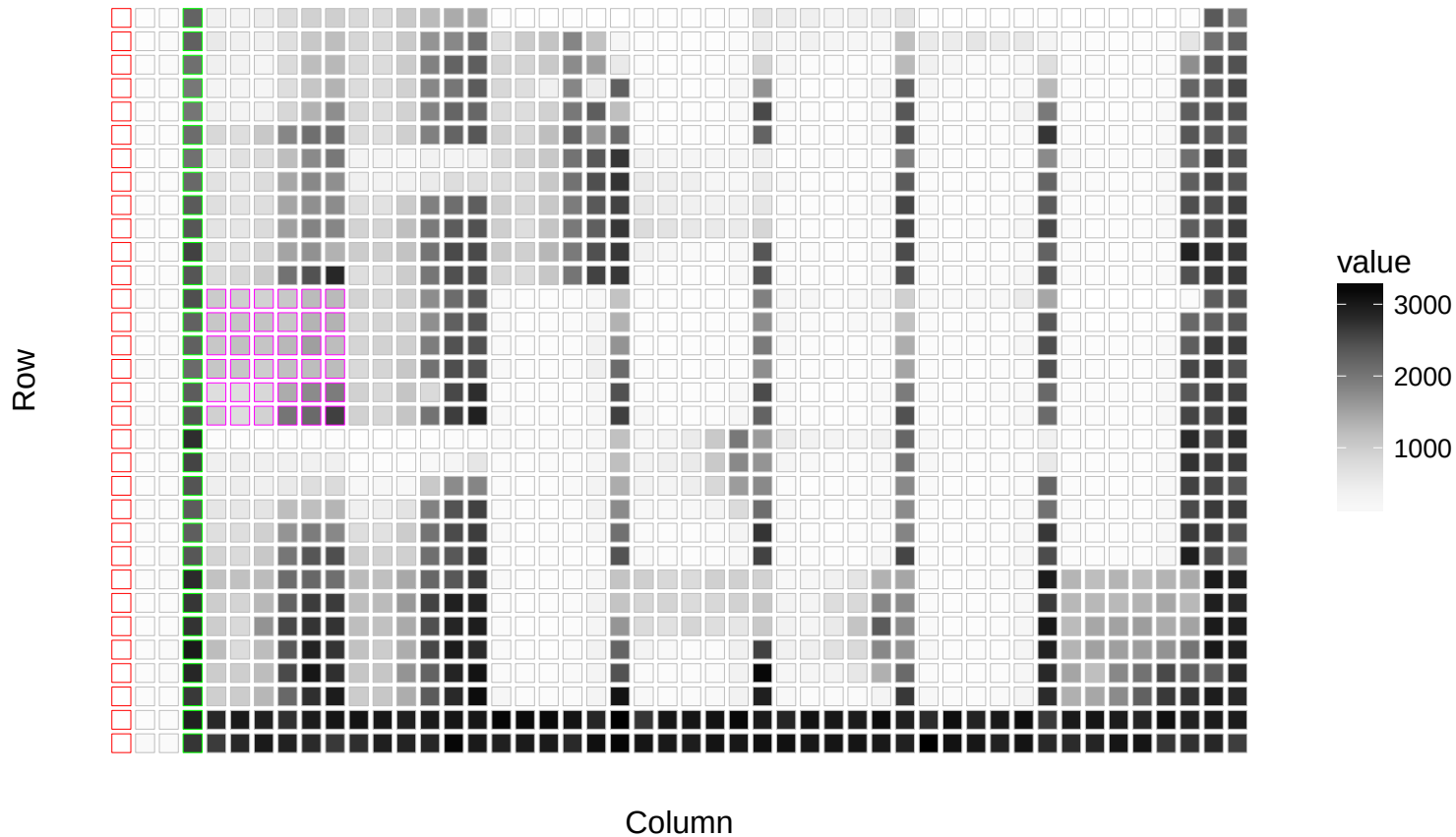
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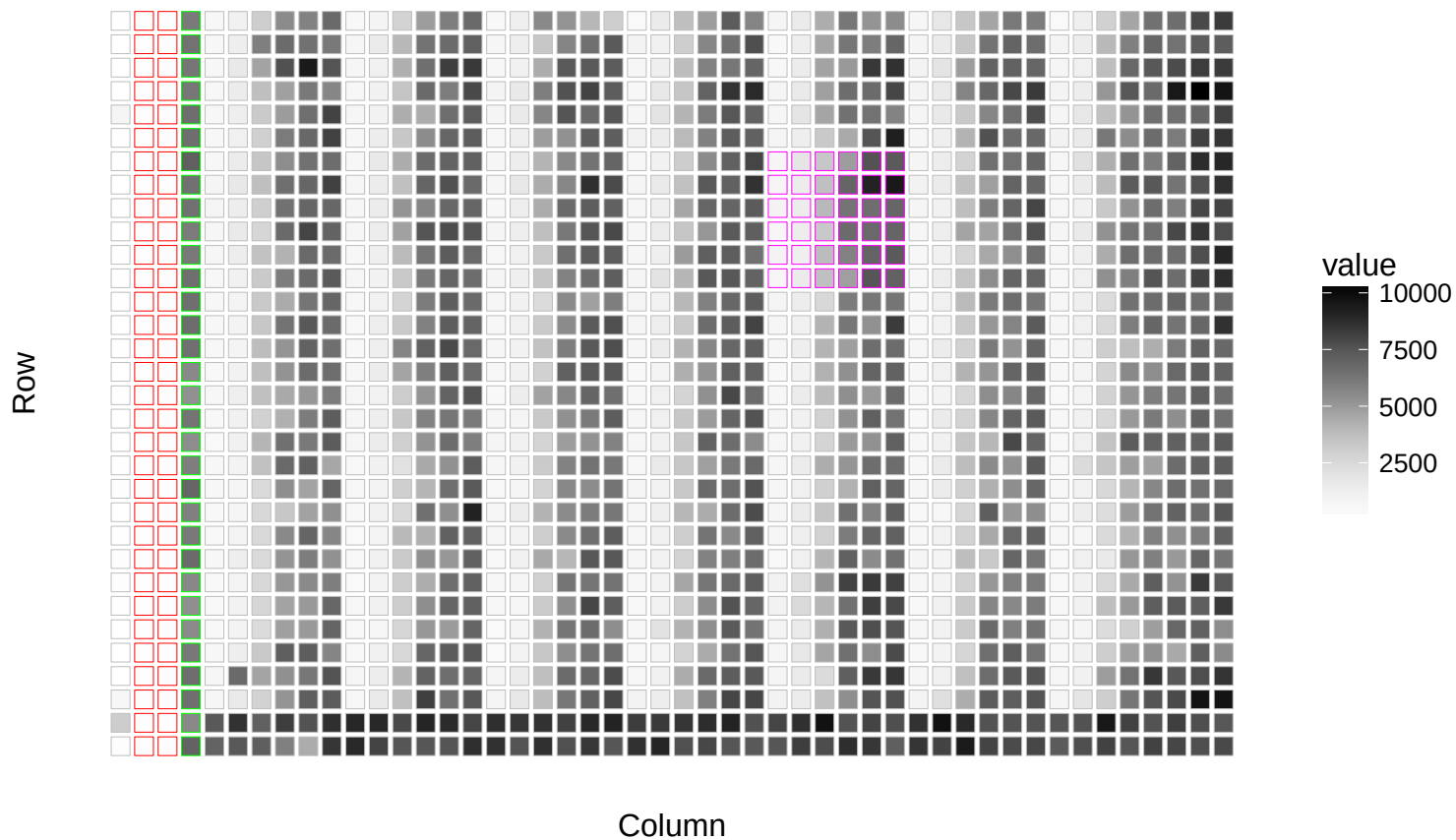
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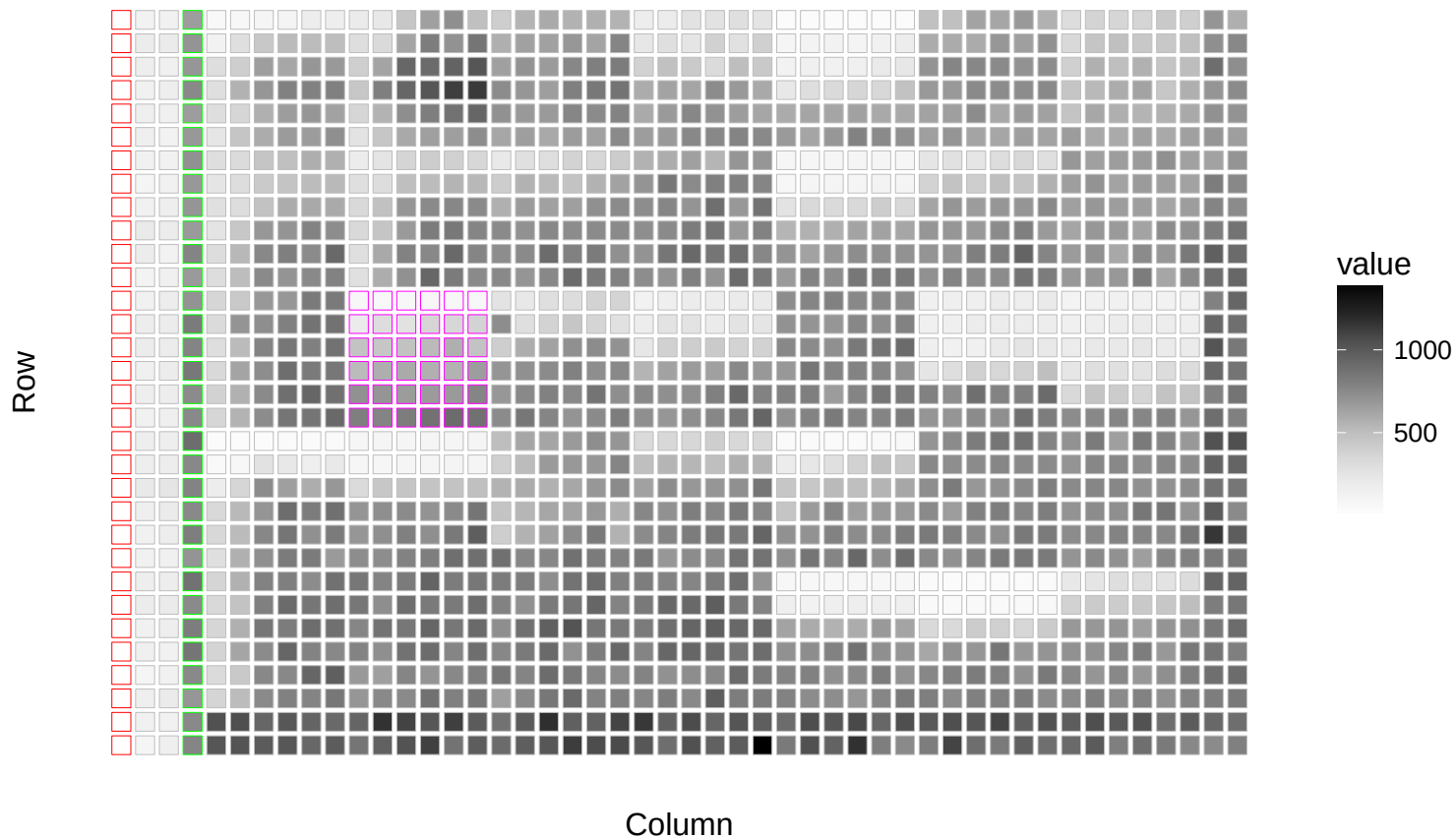
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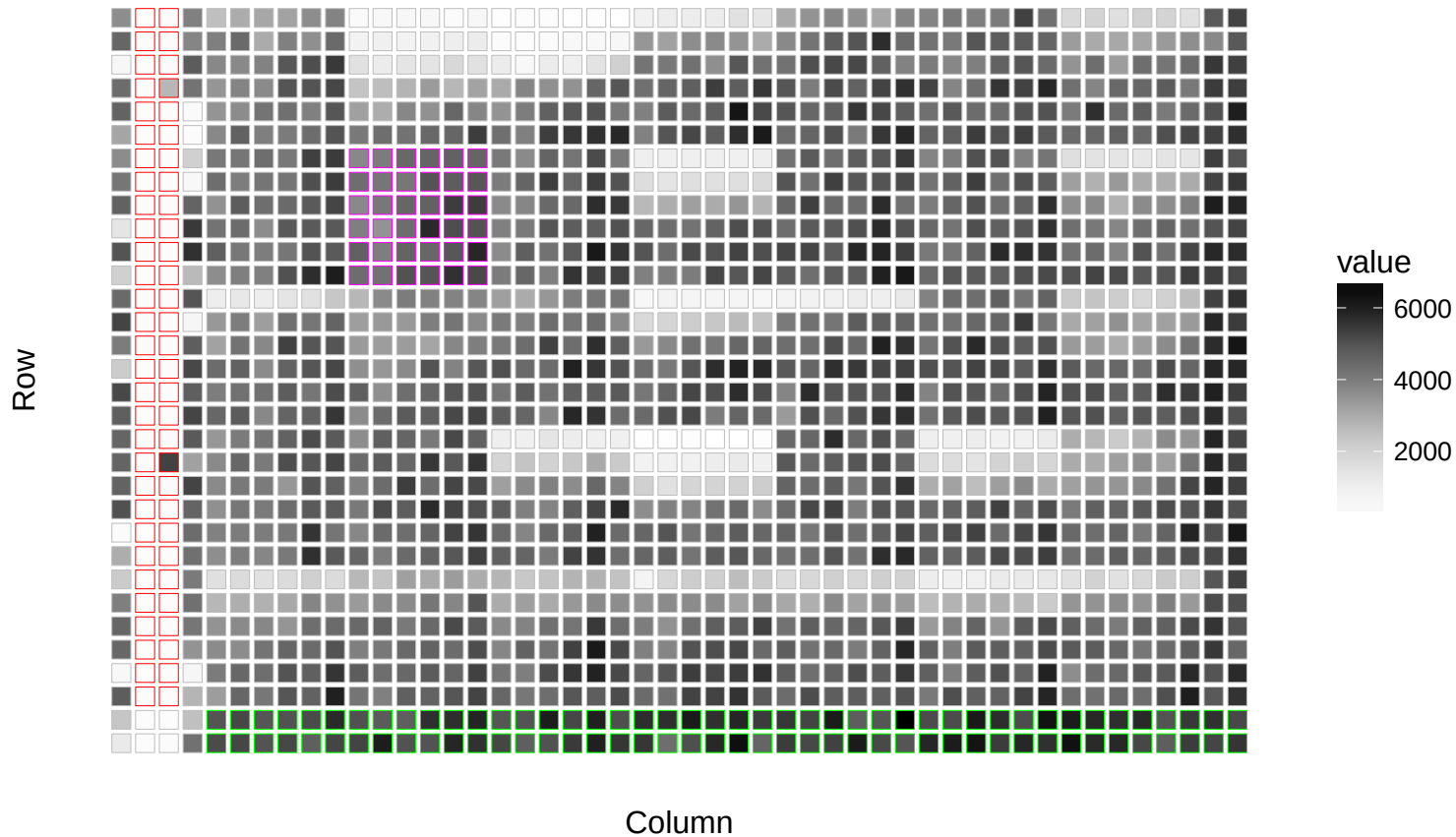
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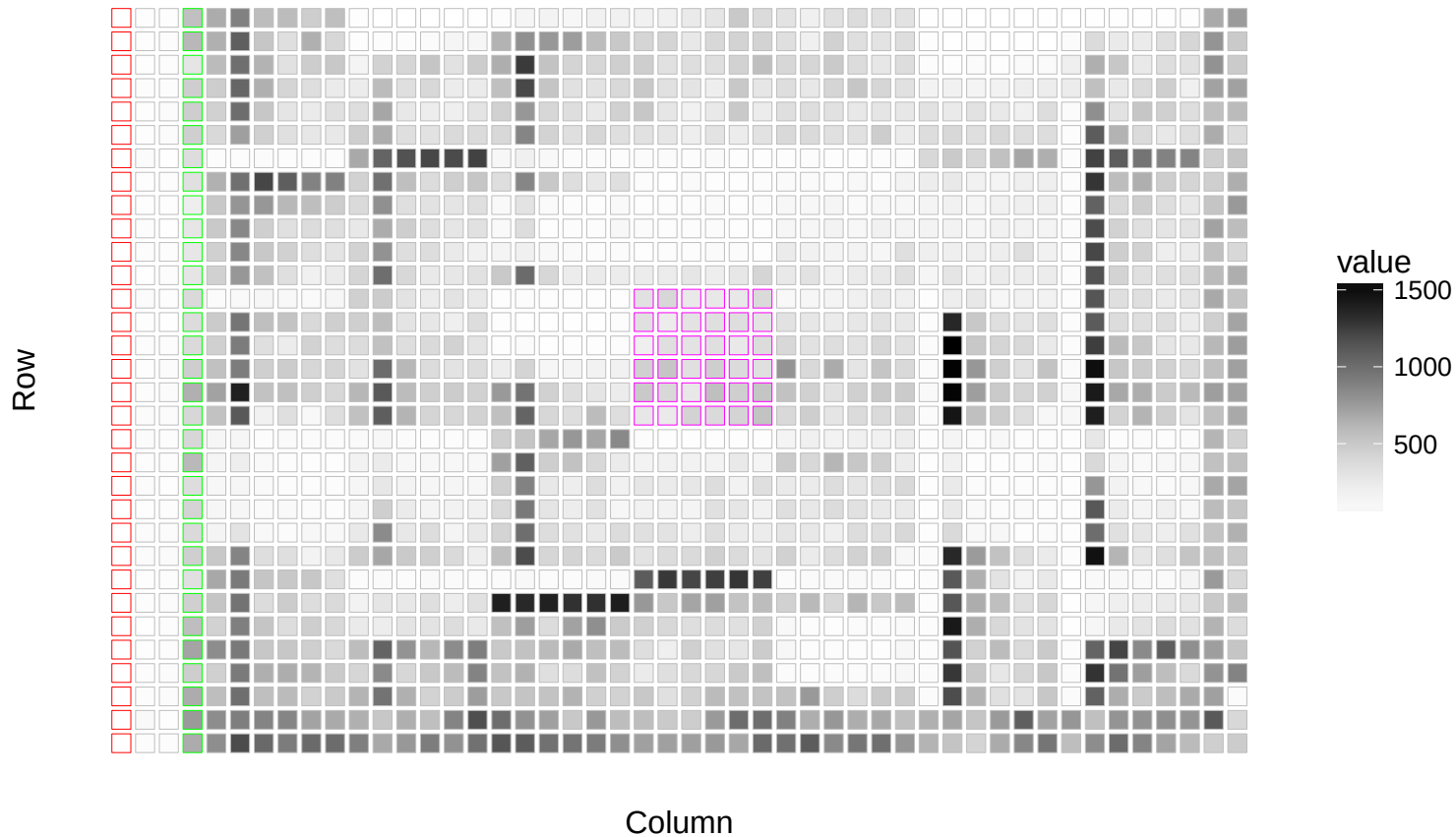
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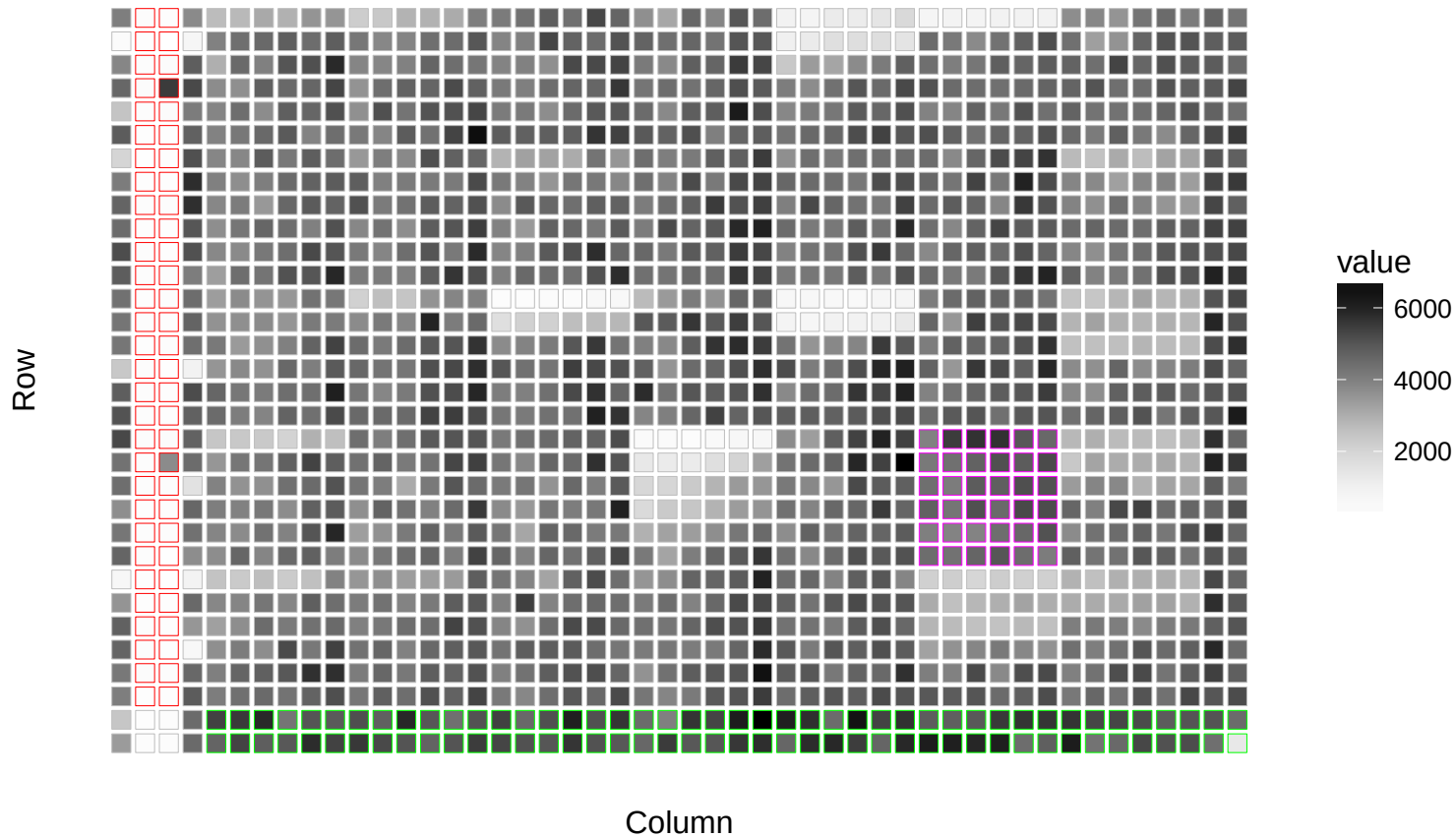
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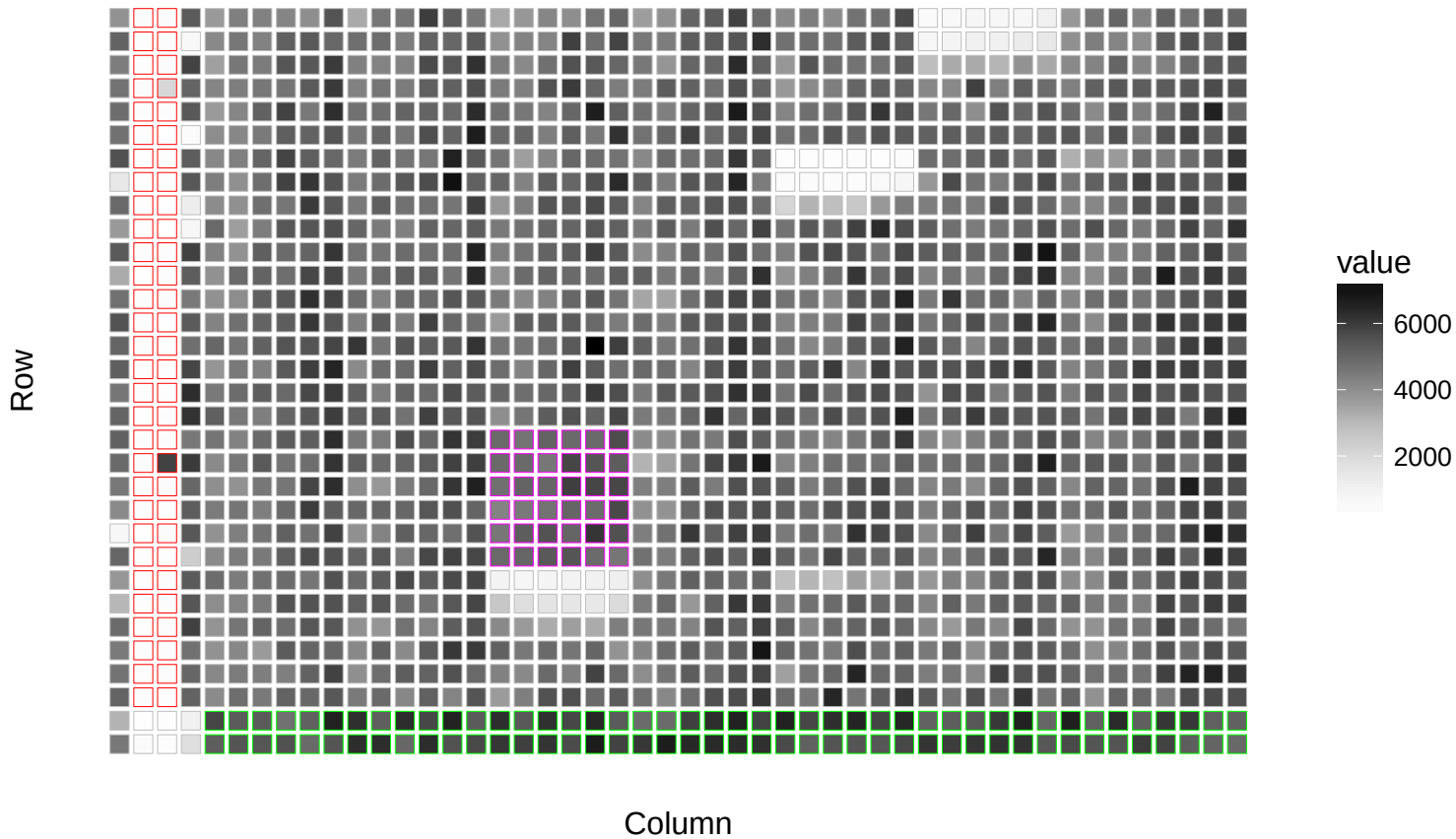
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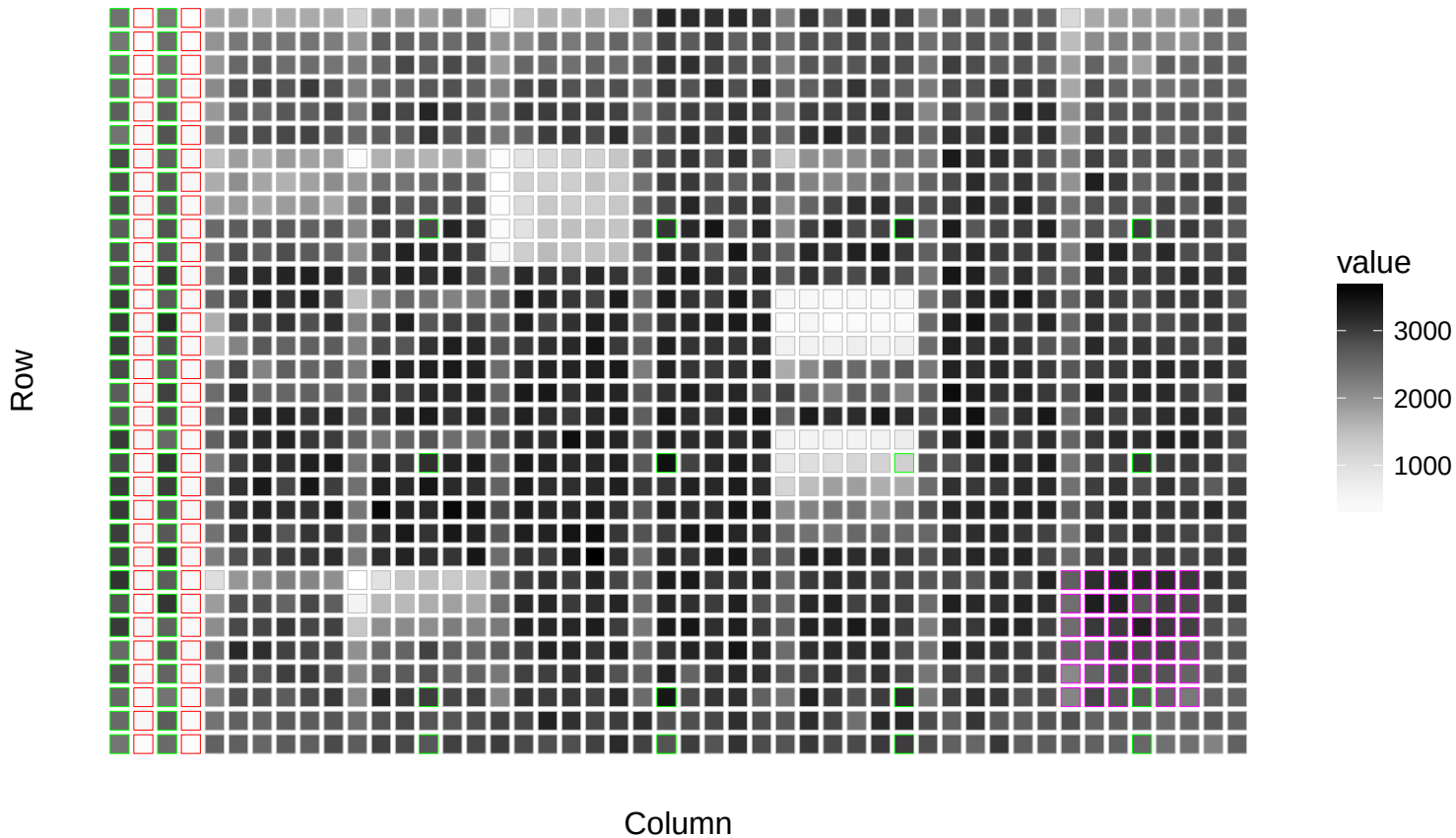
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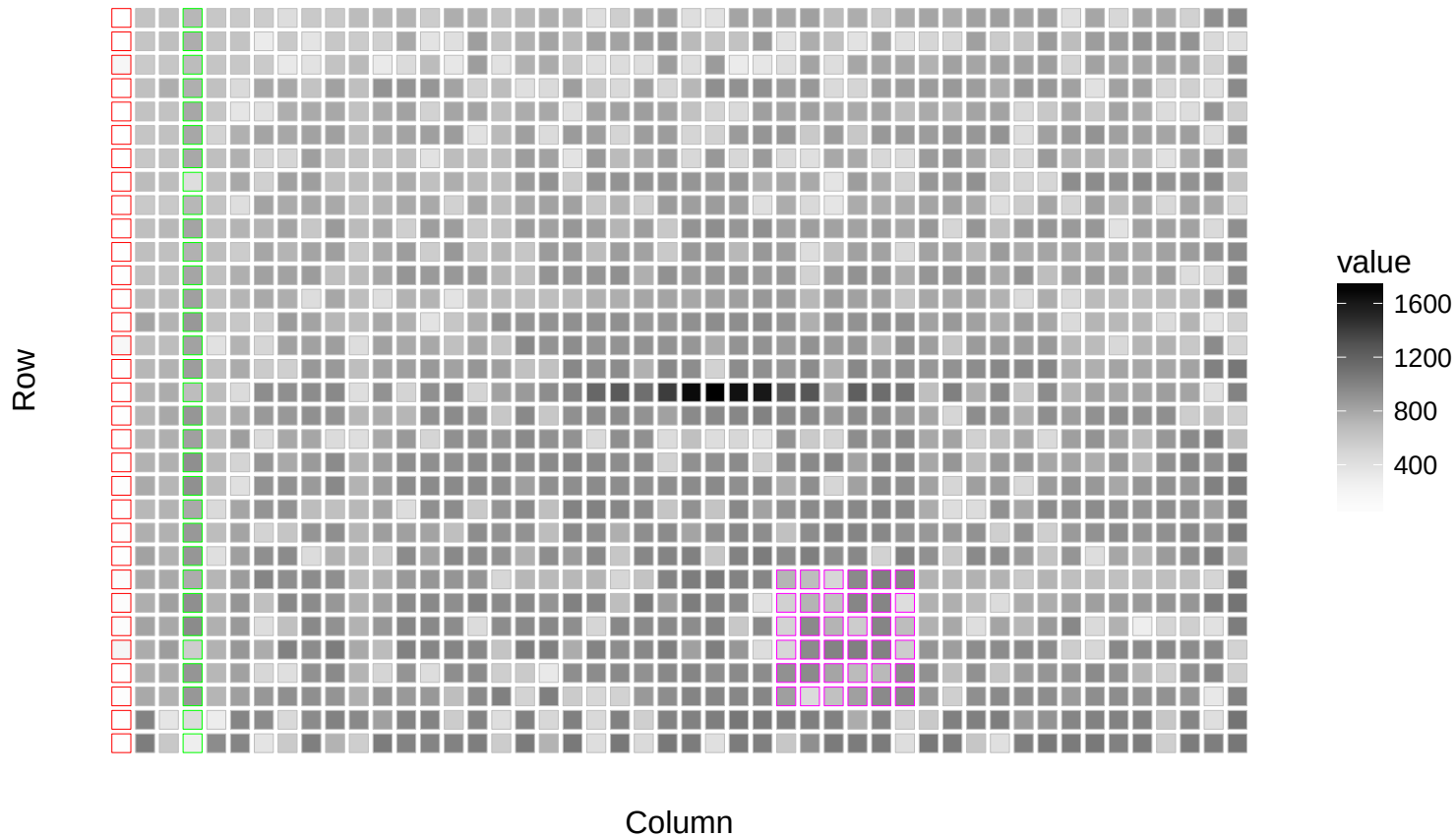
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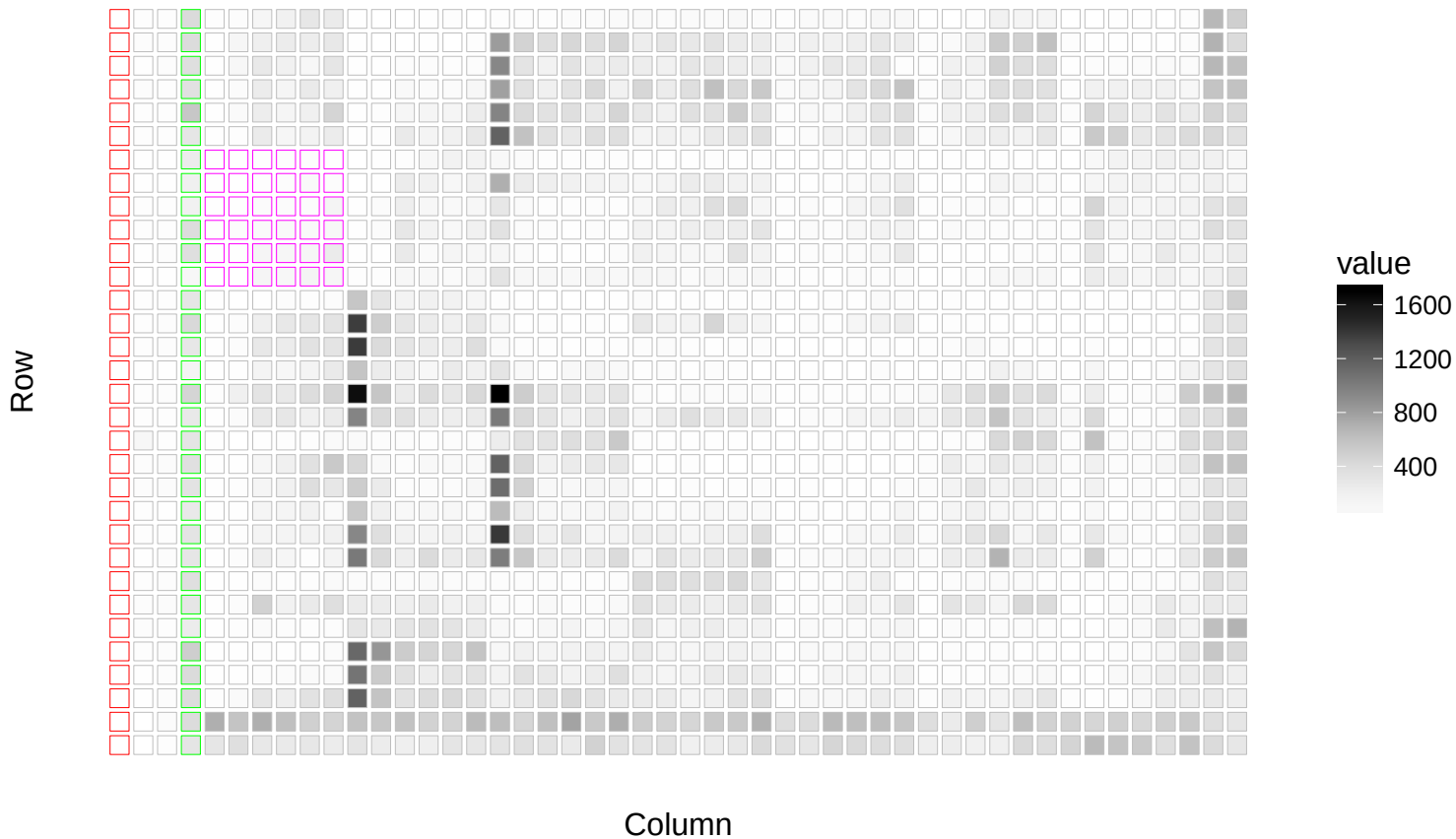
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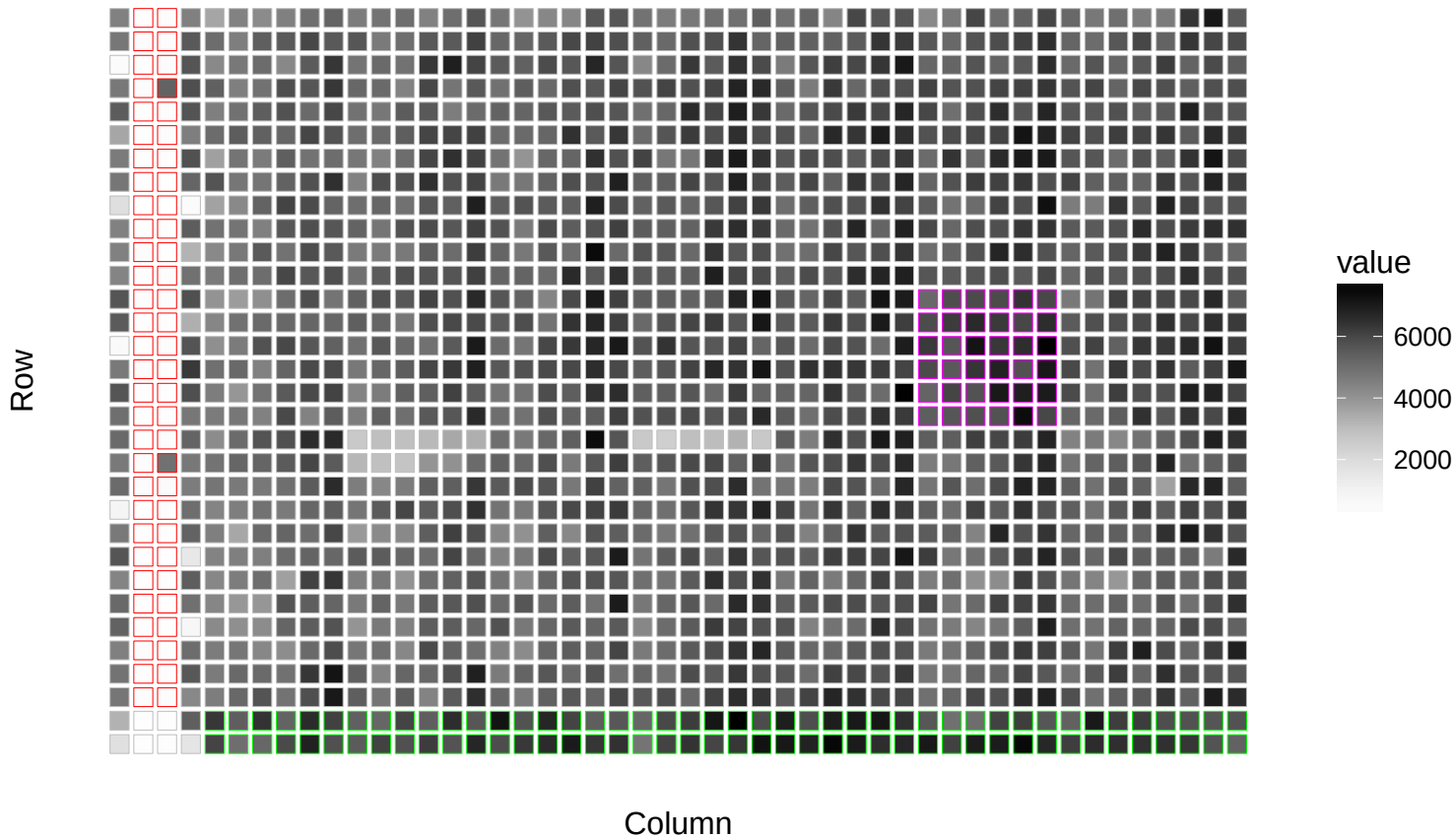
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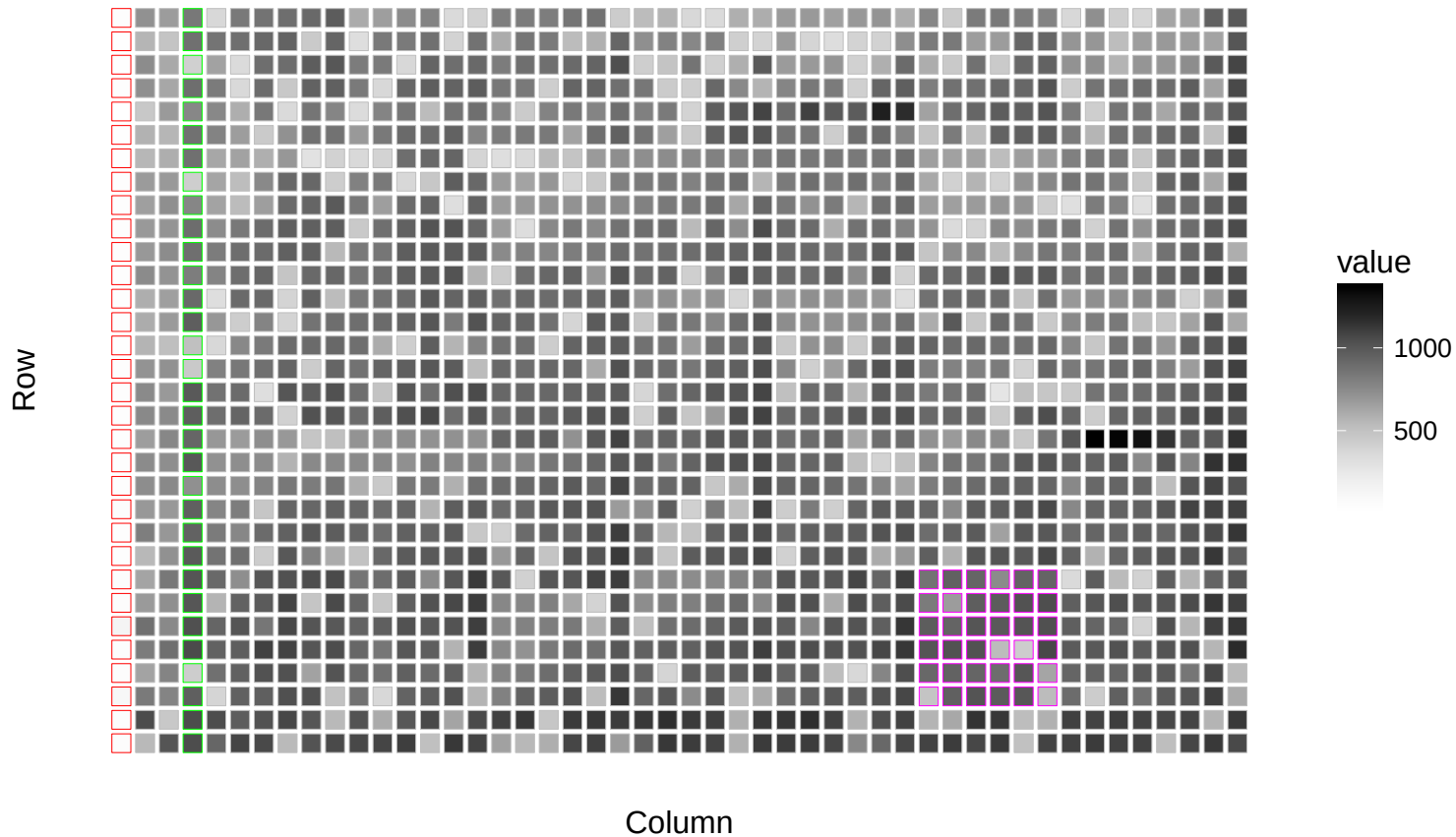
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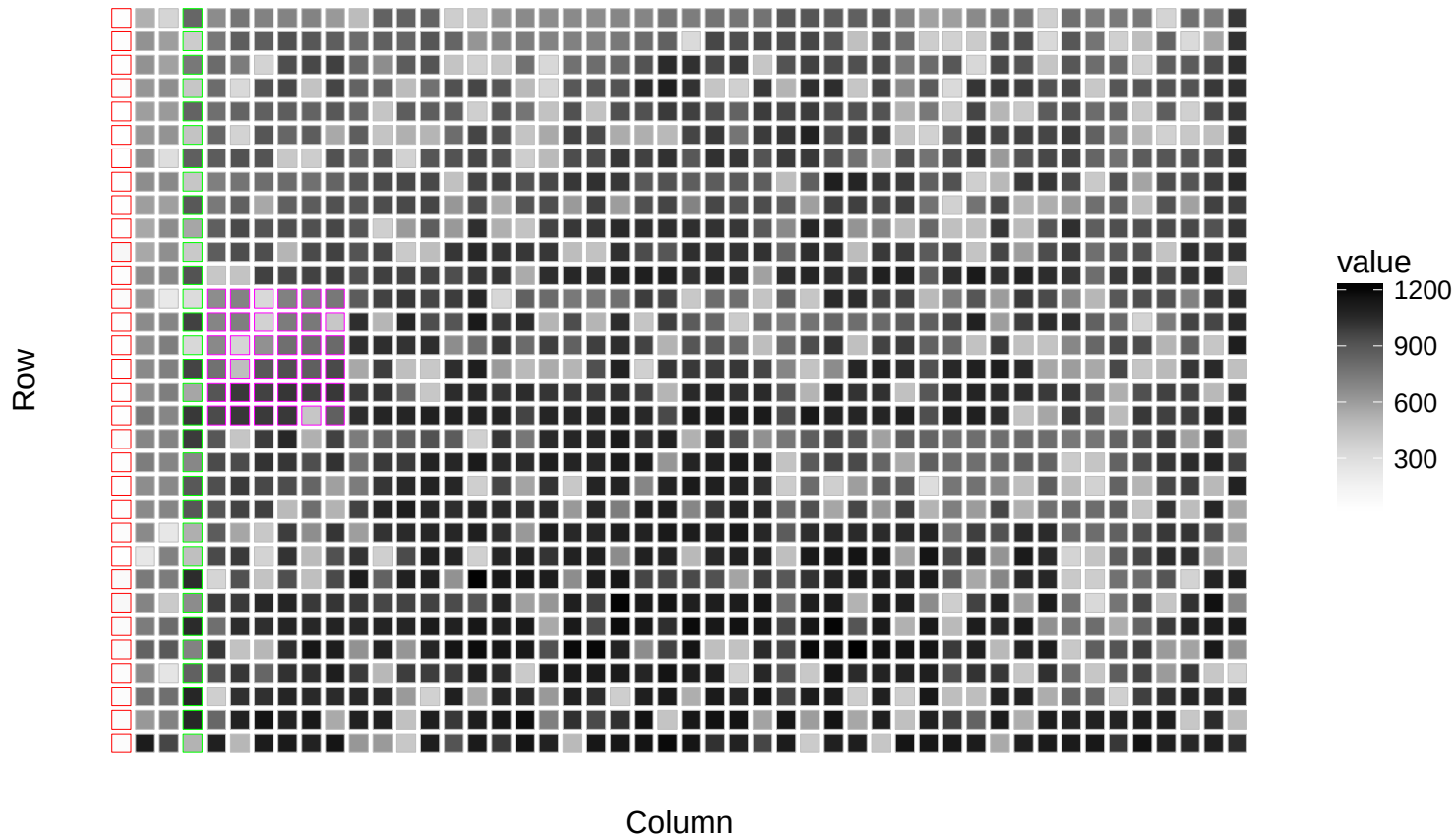
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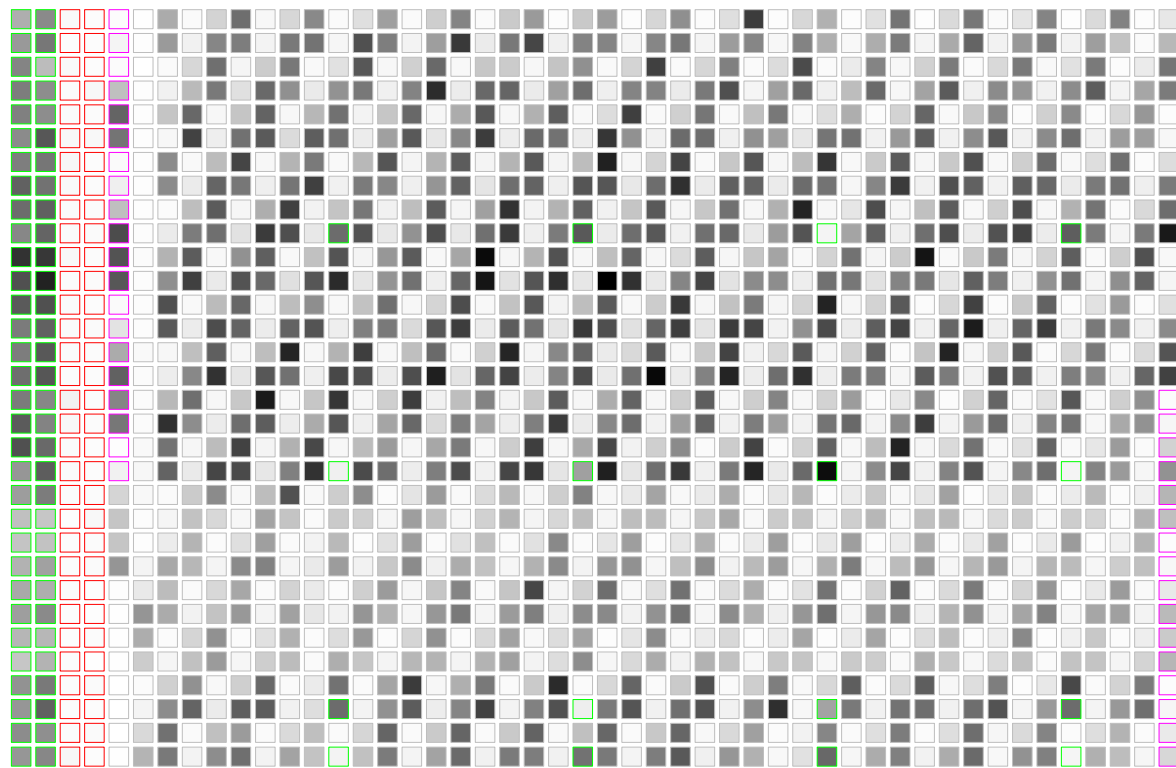


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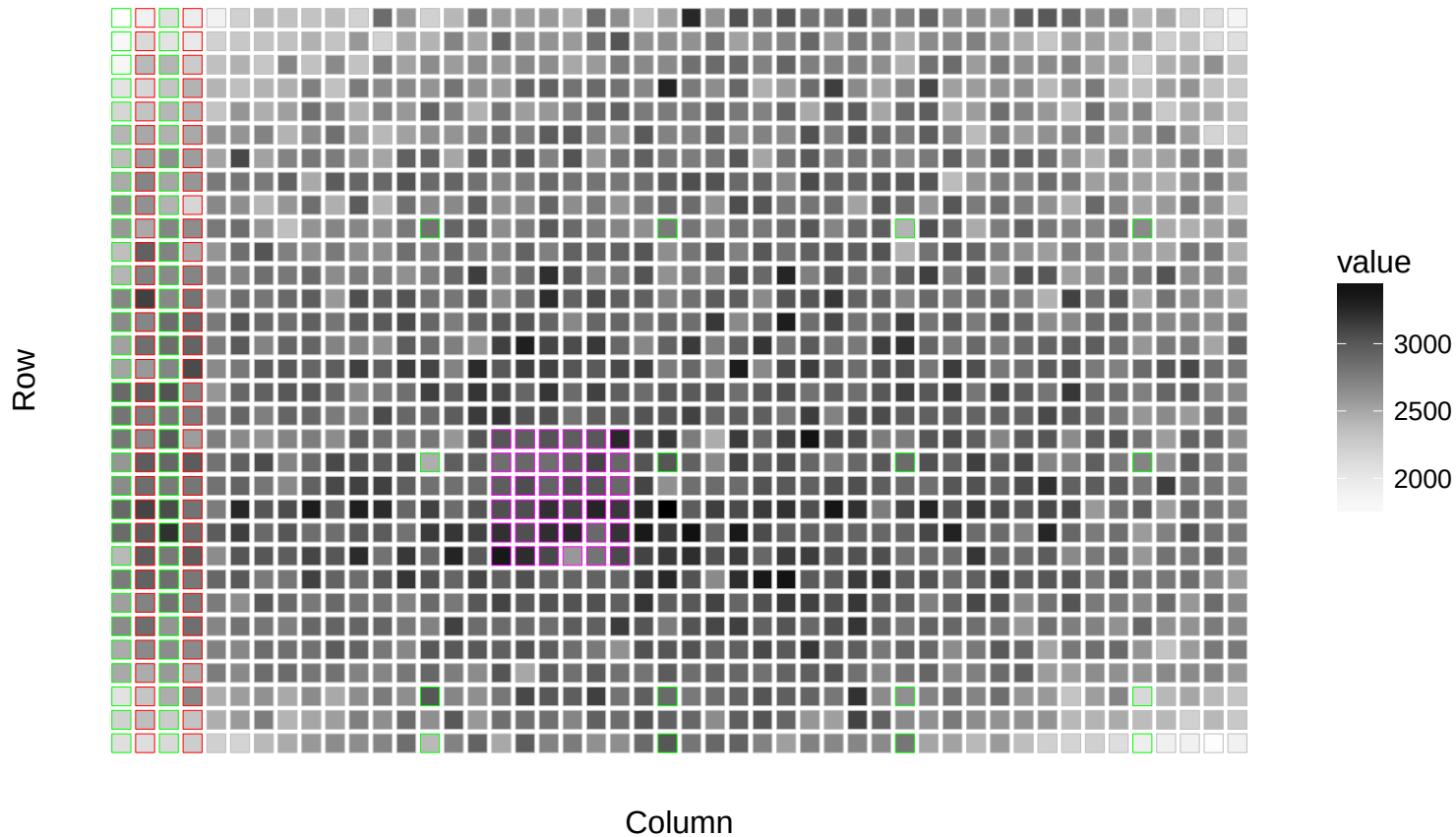
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Row

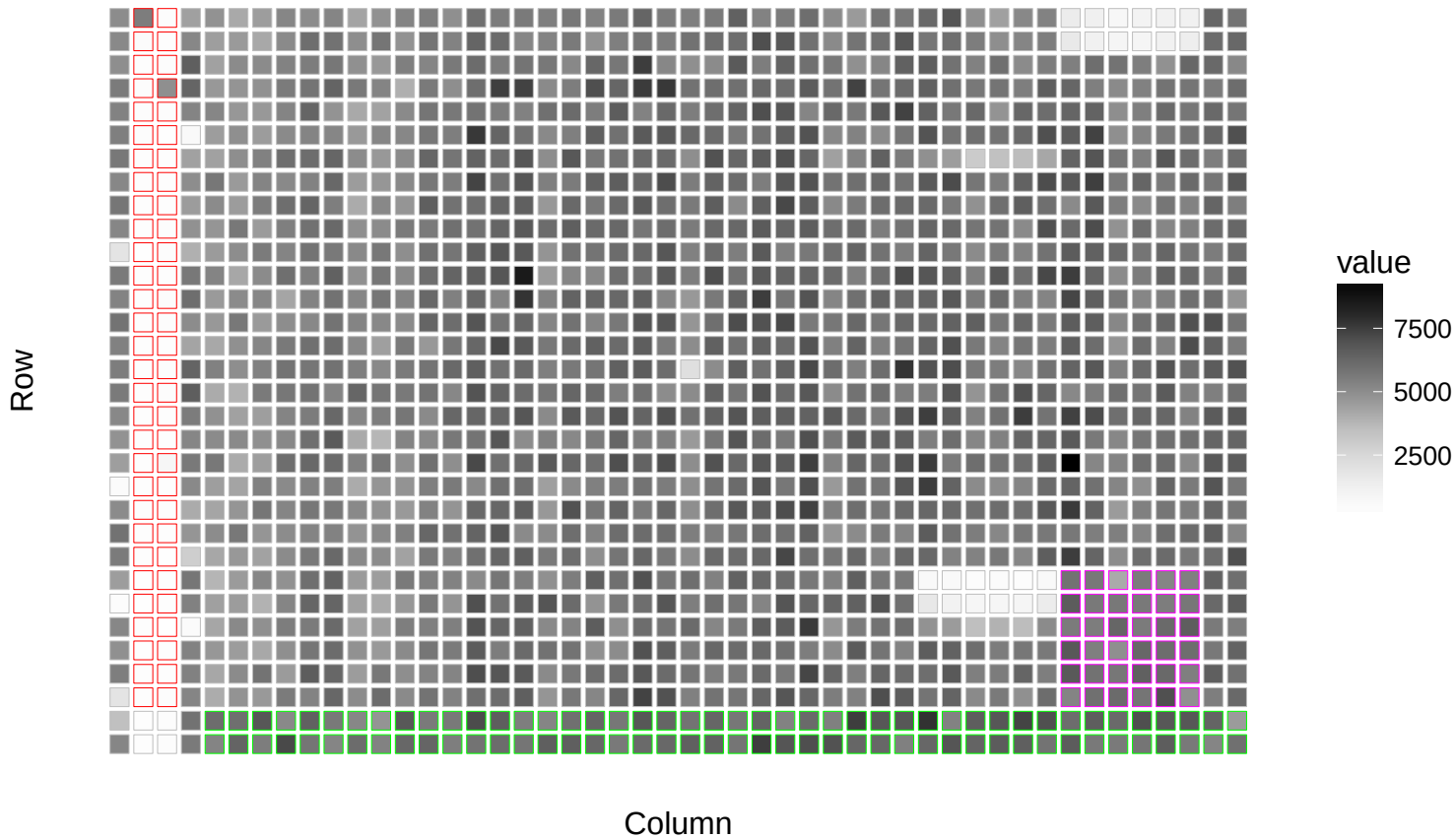


Column

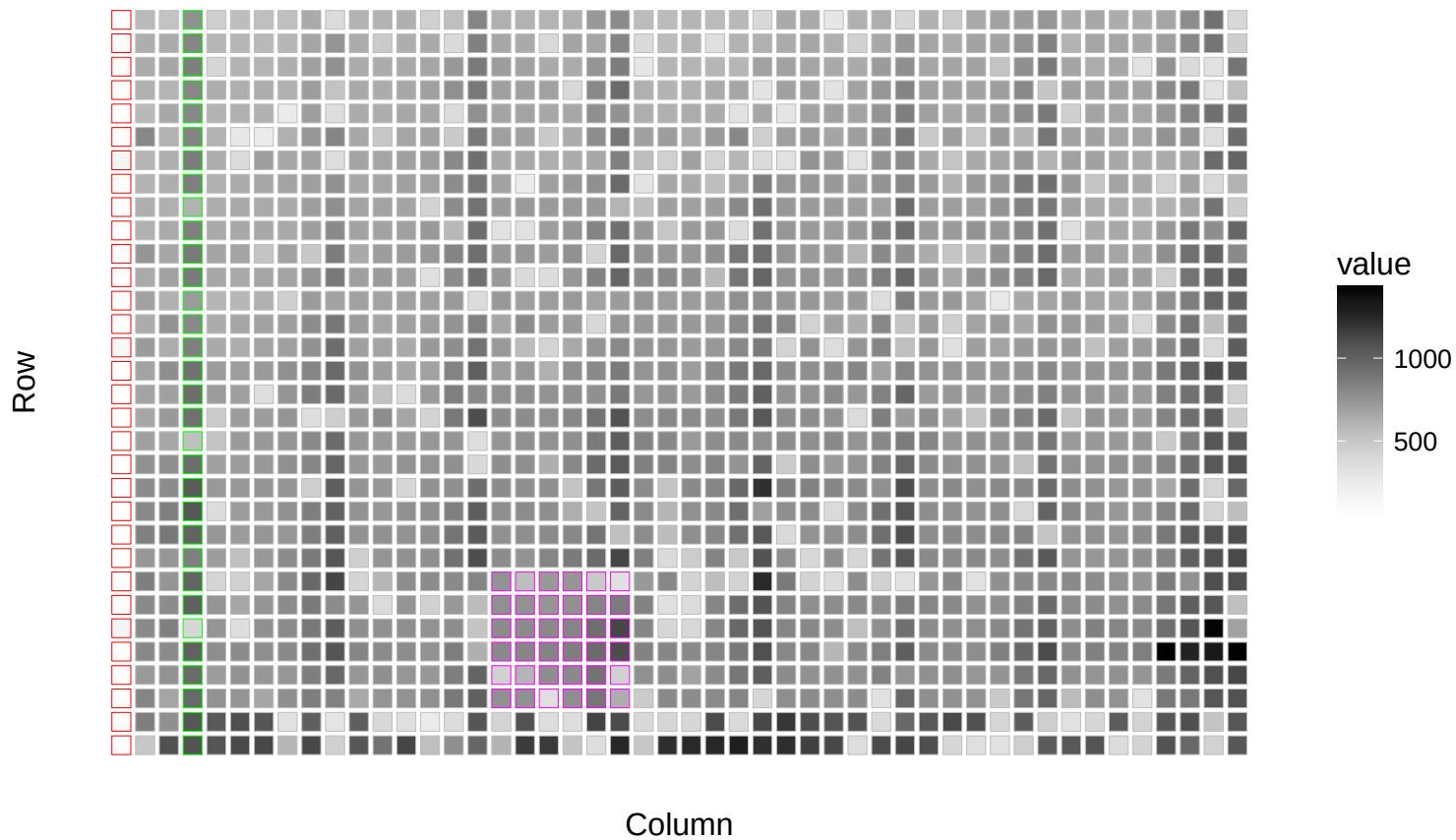
Block 59 (M1400026-T5436718)



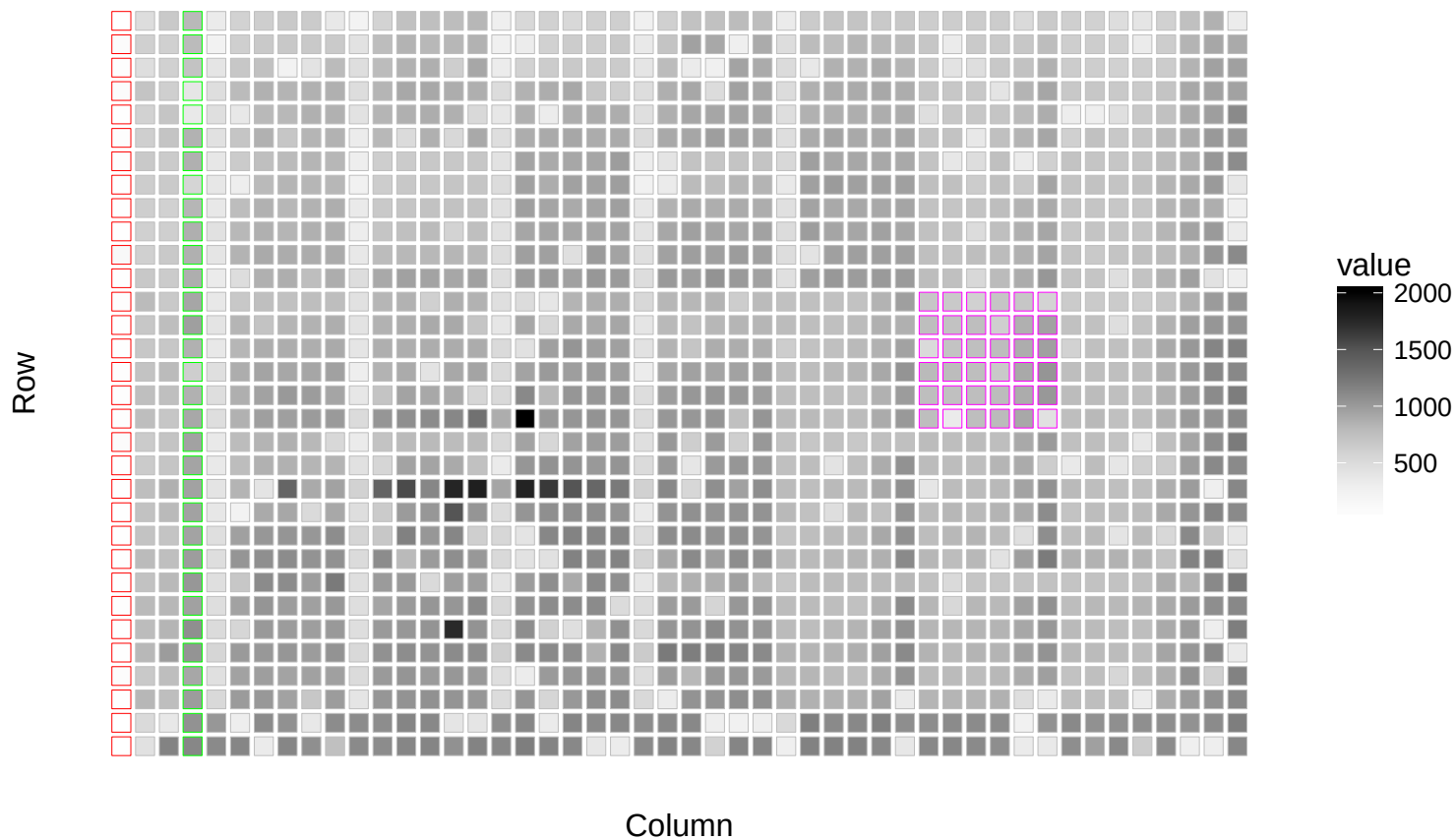
Block 60 (M8900086-T5510616)



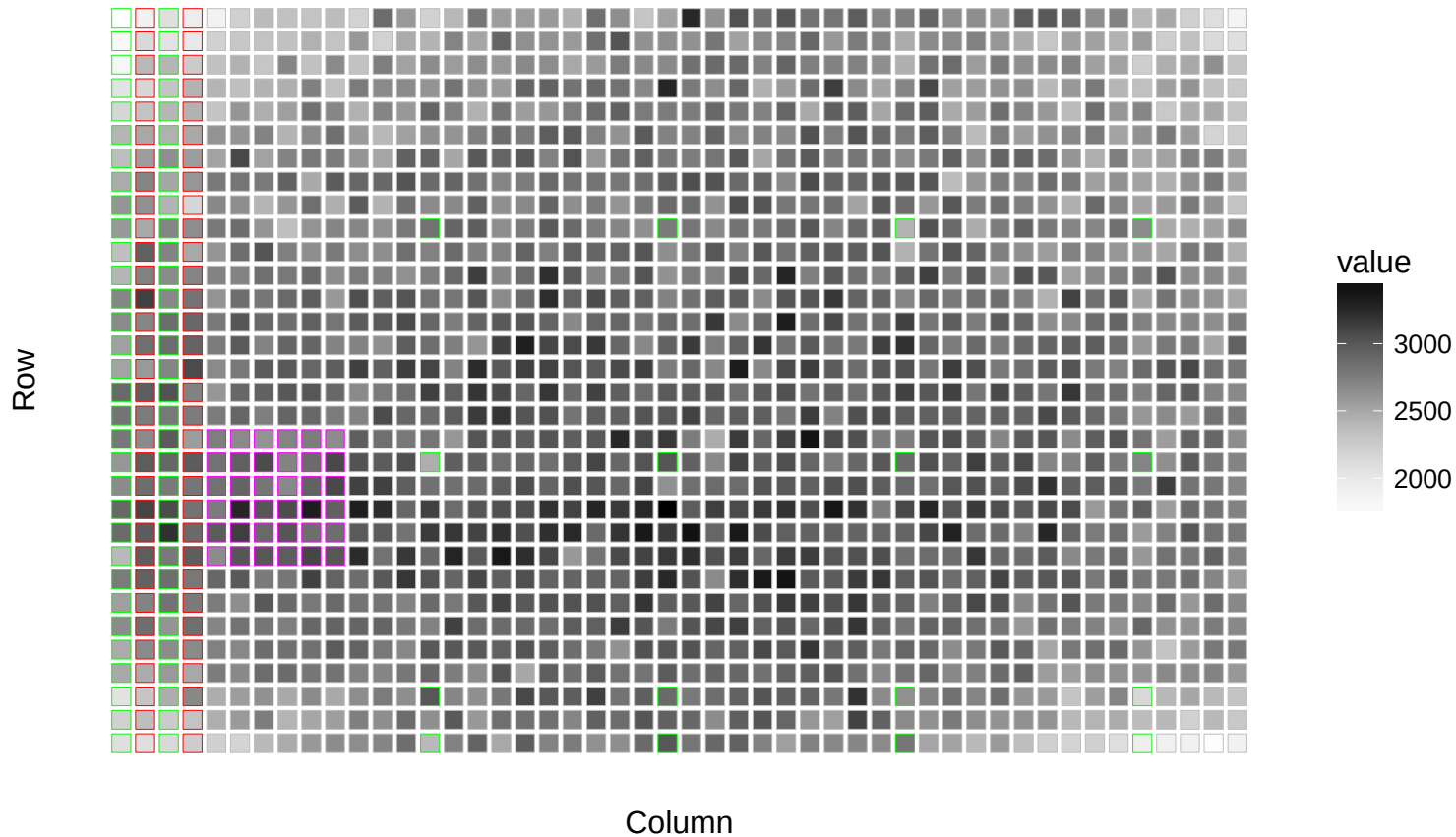
Block 61 (T5618578-T5618578)



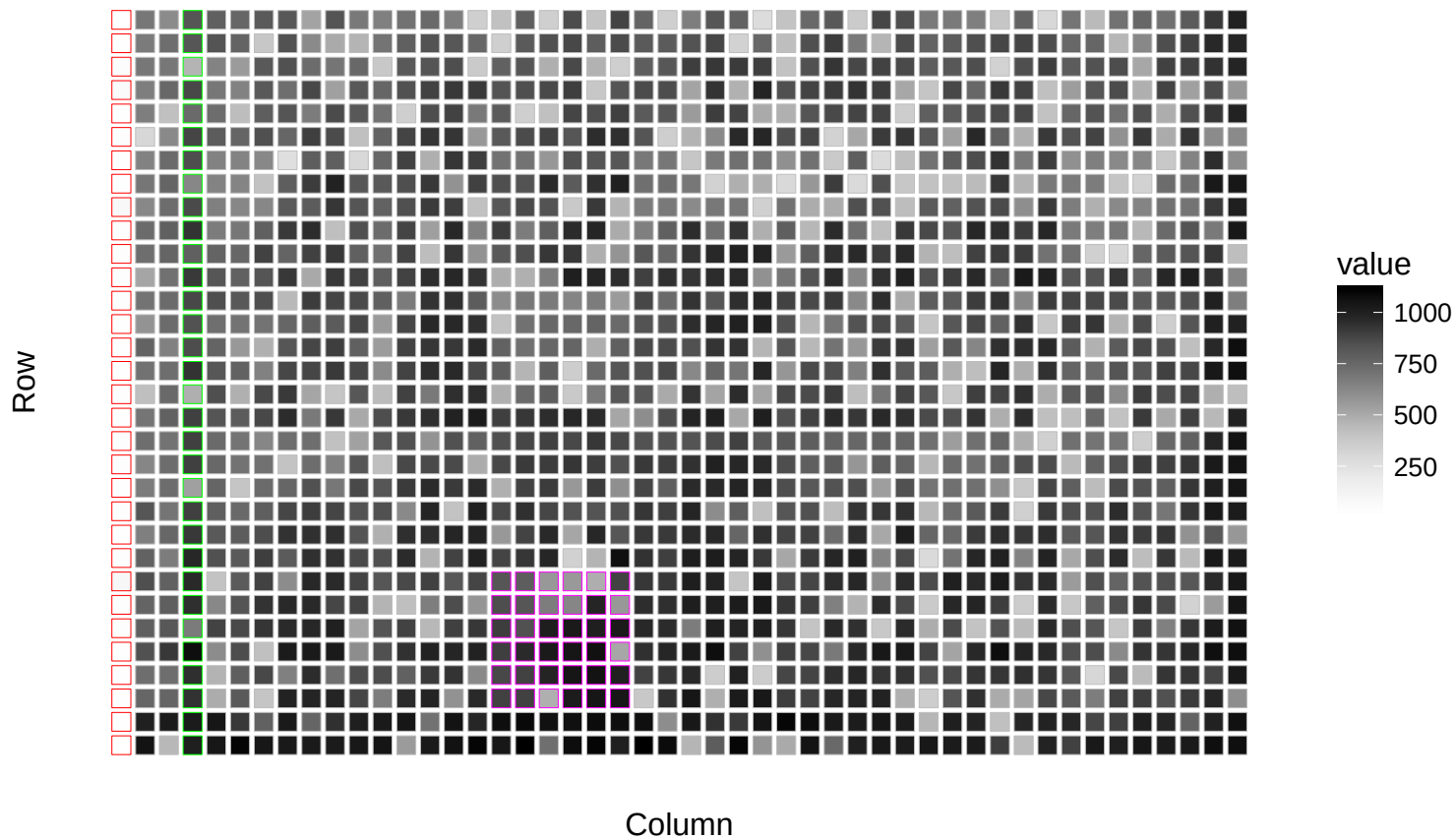
Block 62 (T5618576-T5618576)



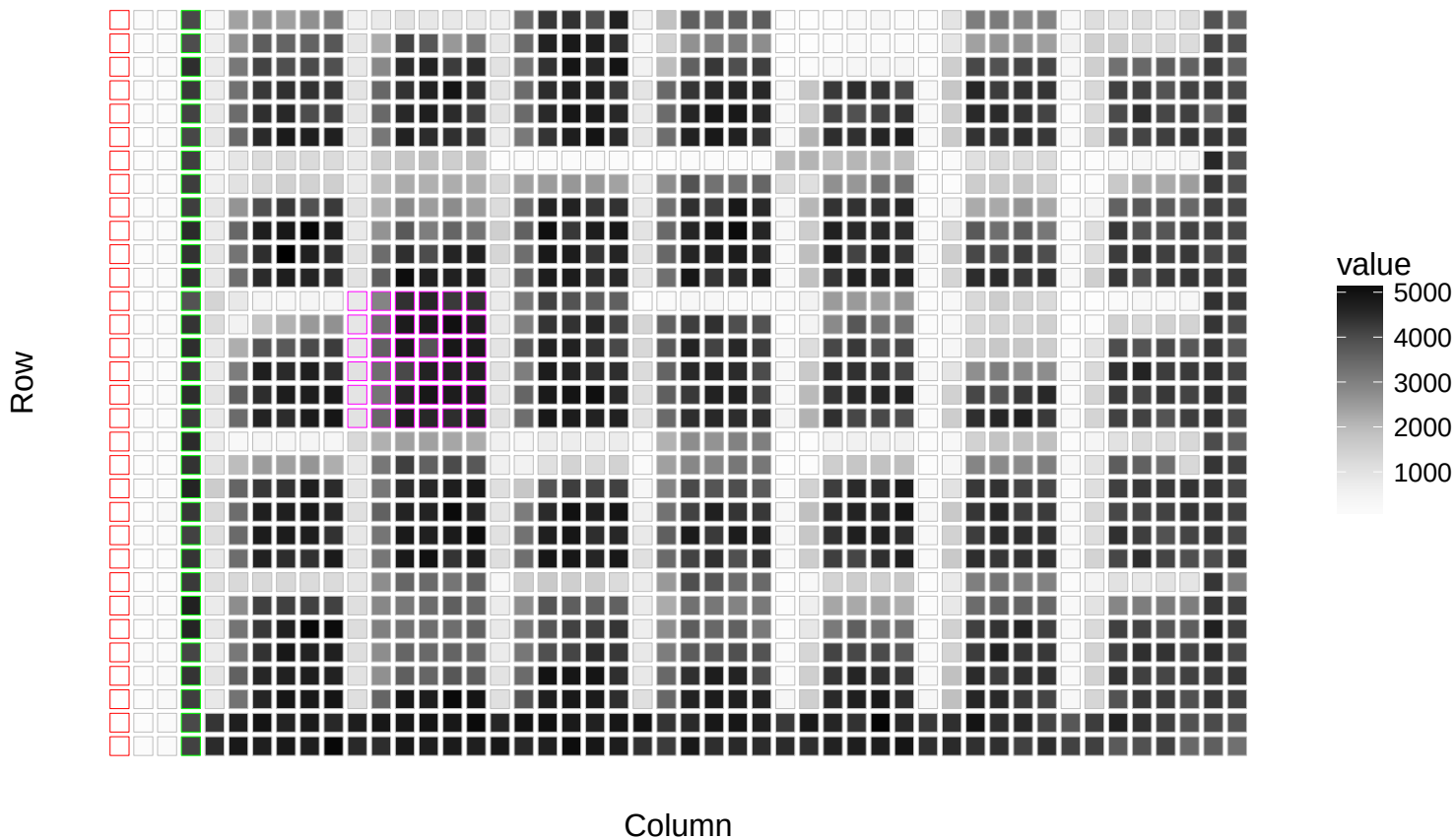
Block 63 (M1400026-T5436718)



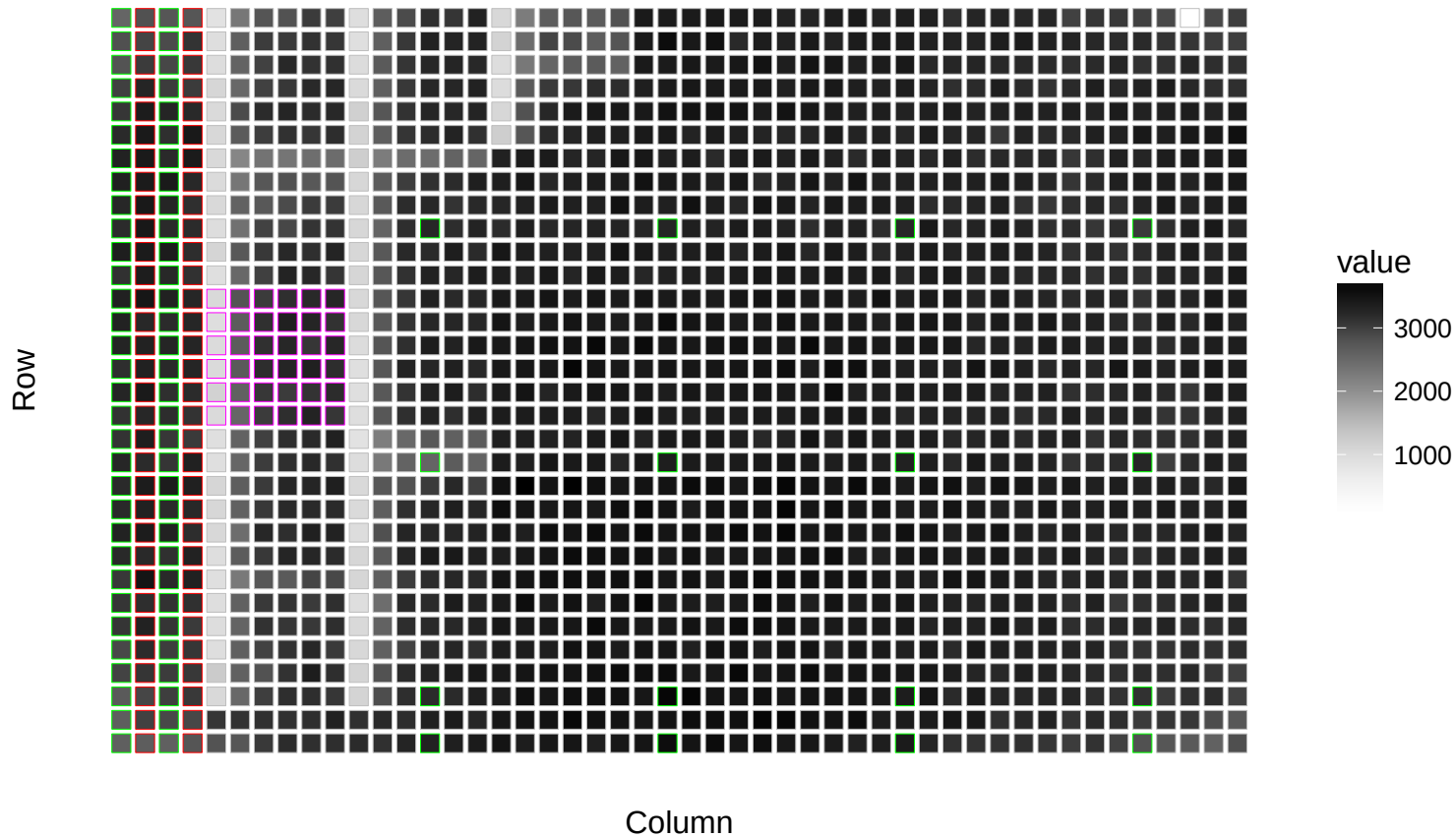
Block 64 (T5614964-T5614964)



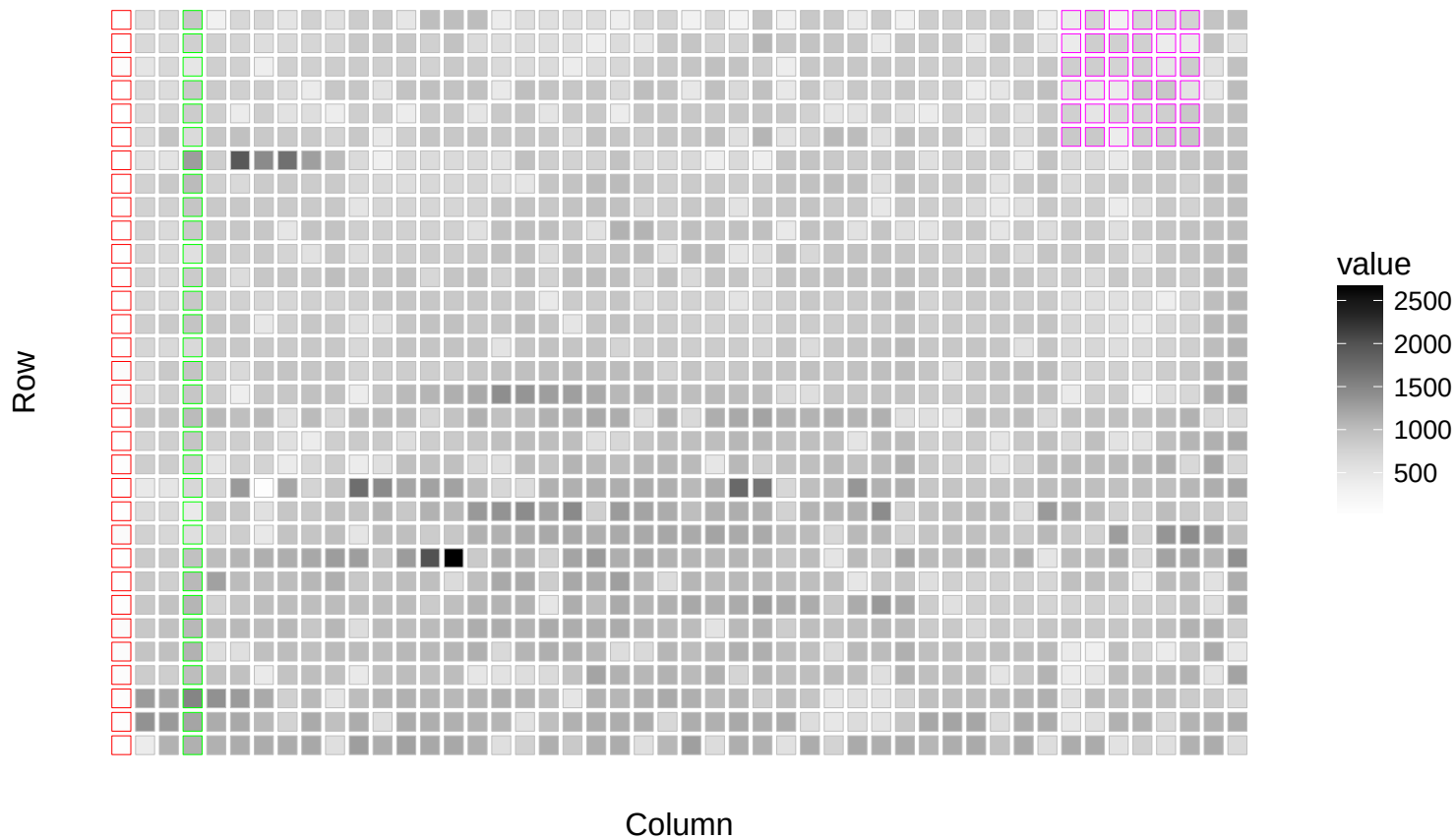
Block 65 (M1020010-T5571036)



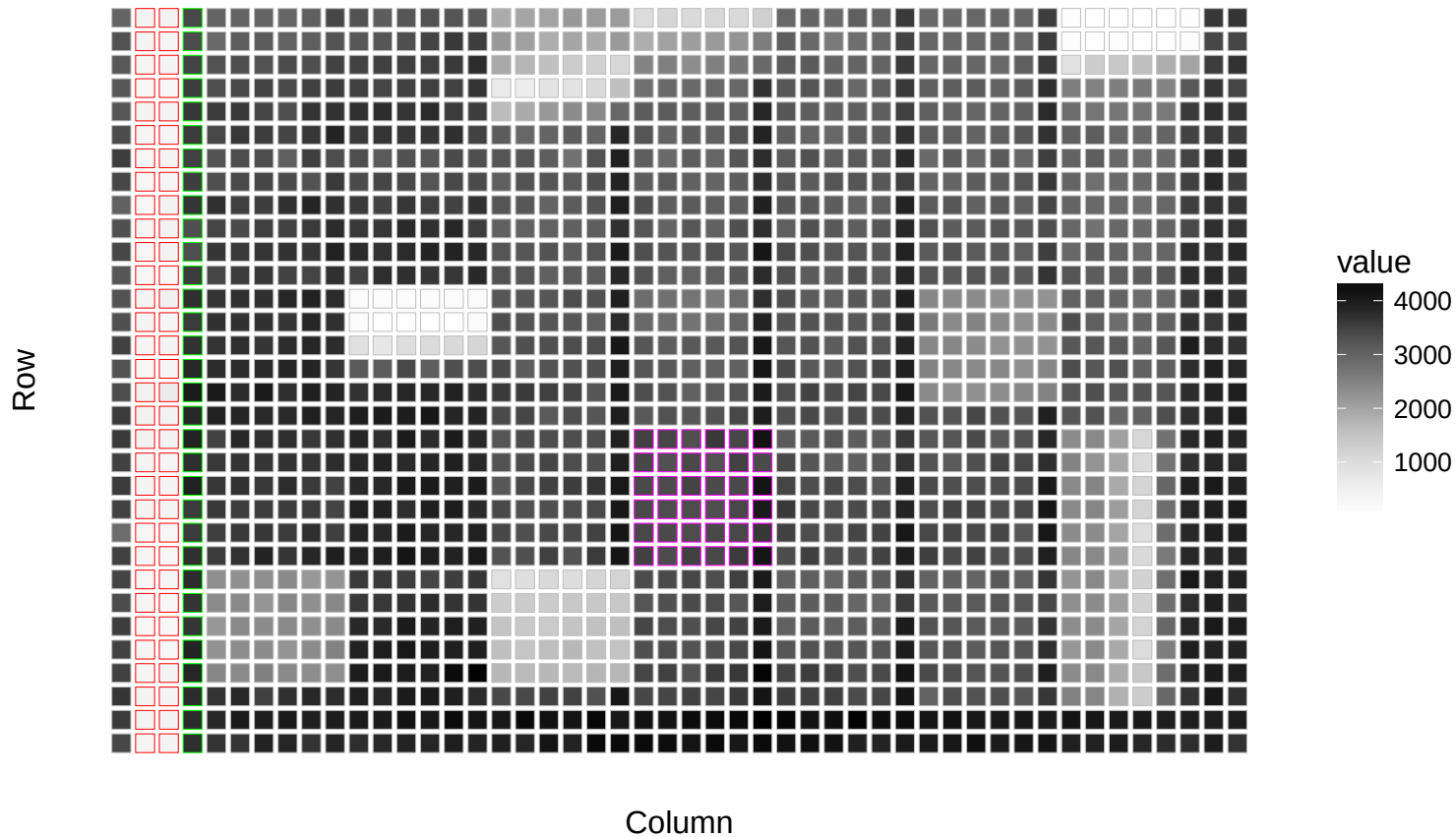
Block 66 (M2100028-T5470428)



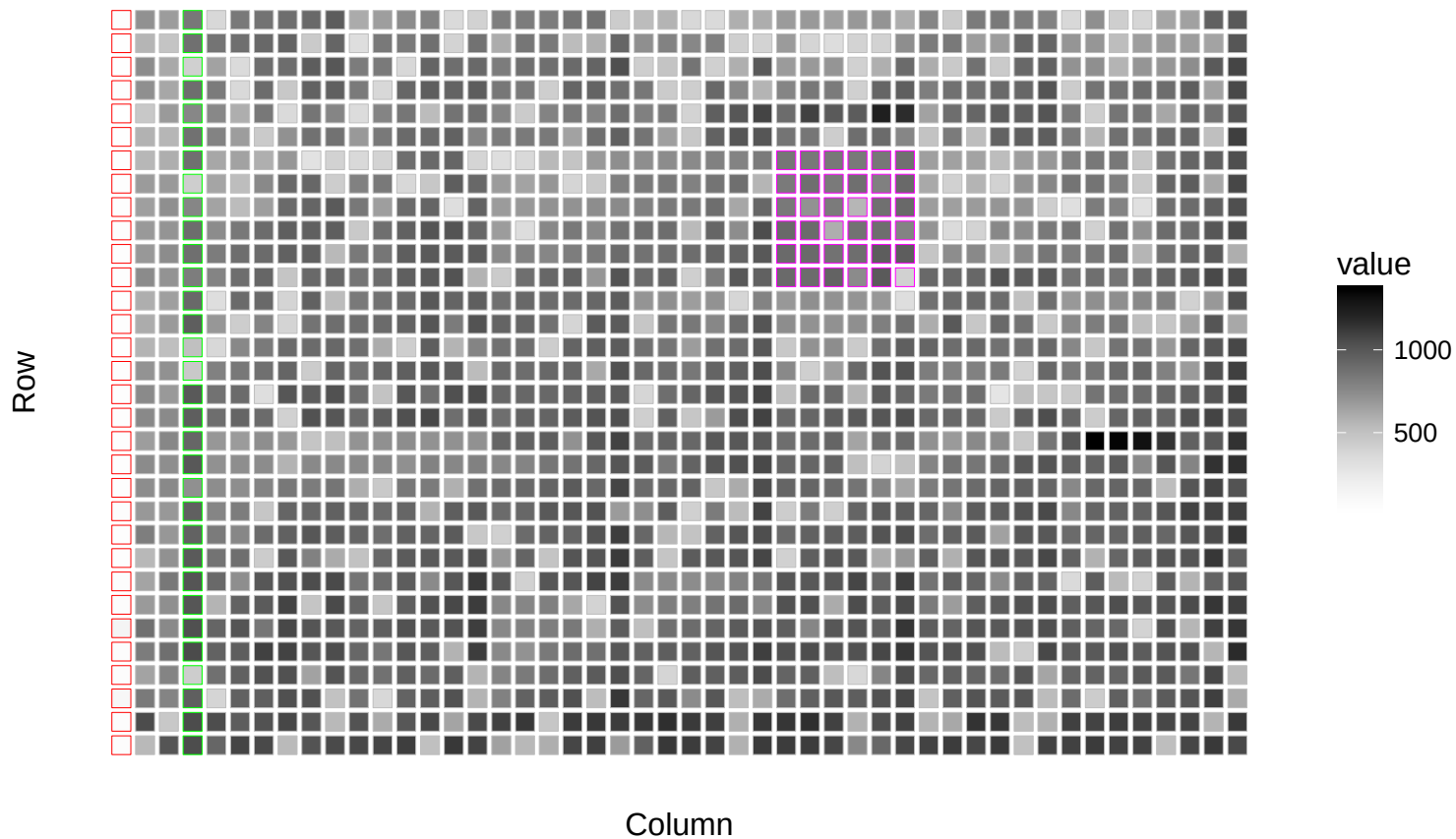
Block 67 (T5615494-T5615494)



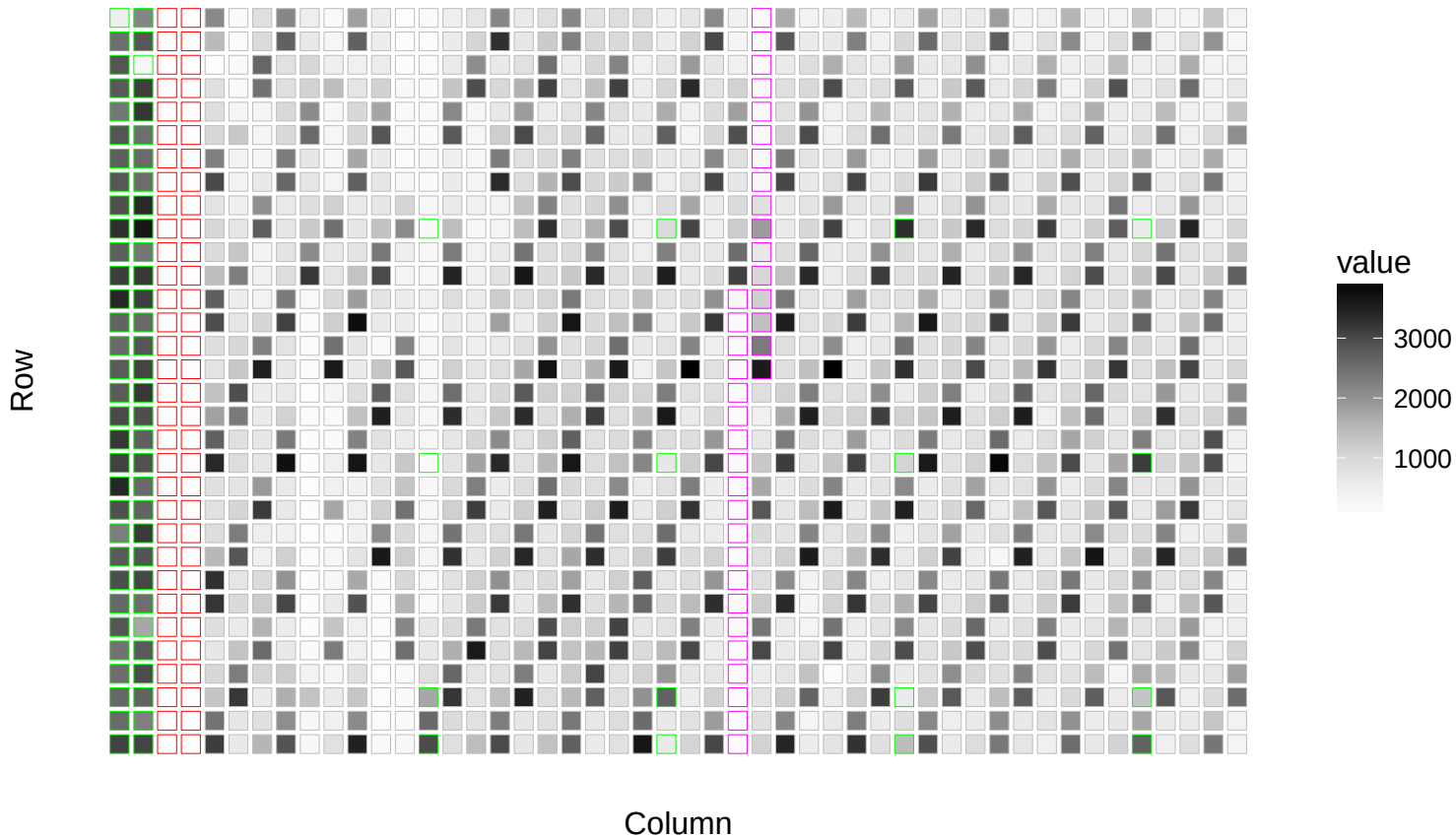
Block 68 (T5666294-T5666294)



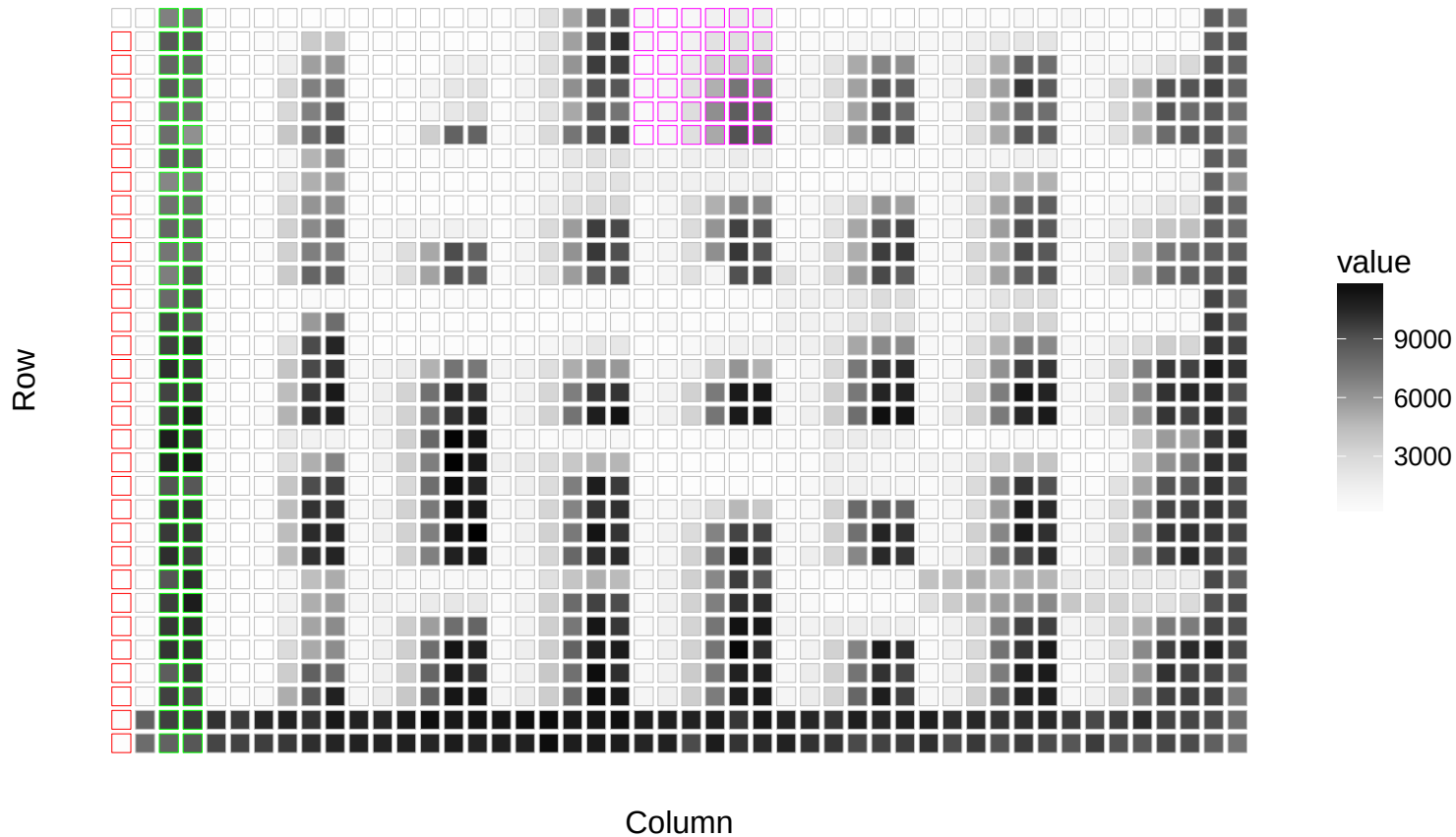
Block 69 (T5616758-T5616758)



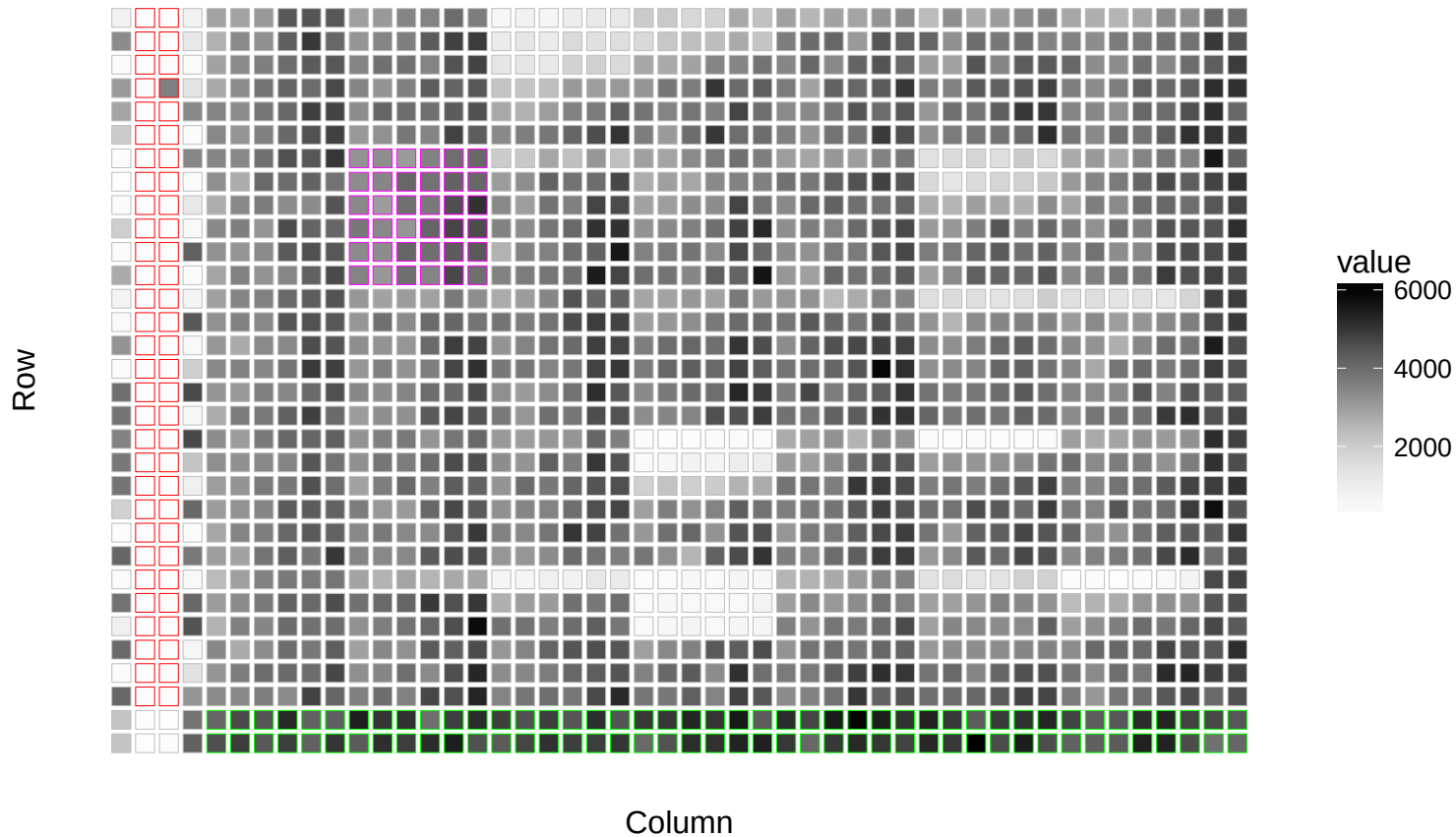
Block 70 (M0200022-T5423650)



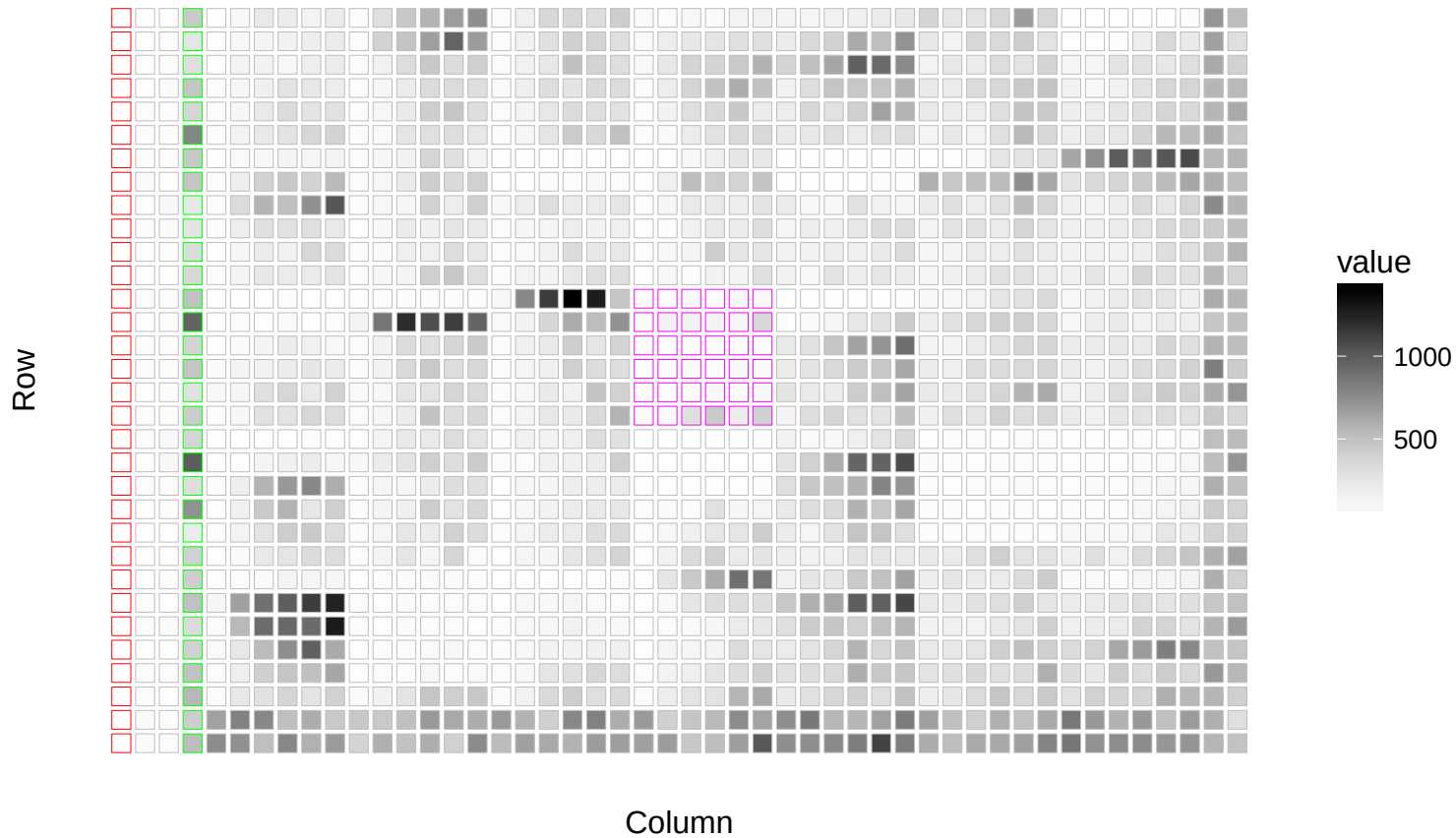
Block 71 (M9900004-T5574594)



Block 72 (M8900010-T5510708)

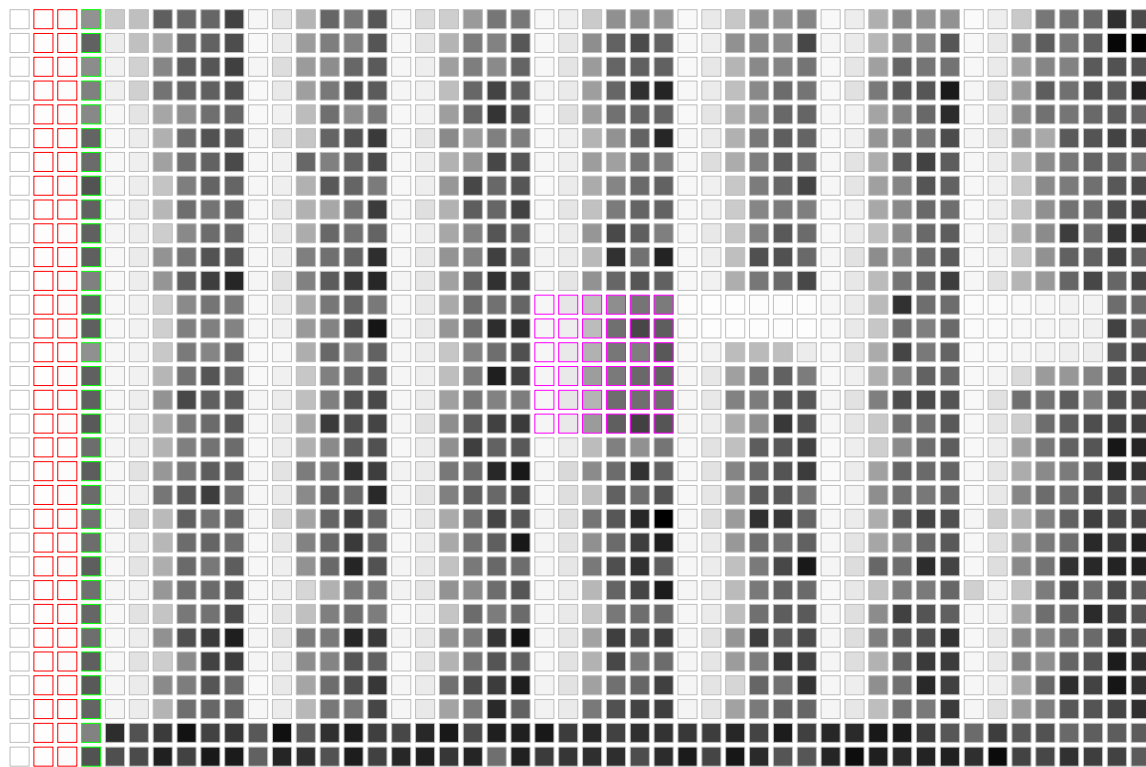


Block 73 (M1020024-T5571454)



Block 74 (T5570388-T5570388)

Row



value

12500

10000

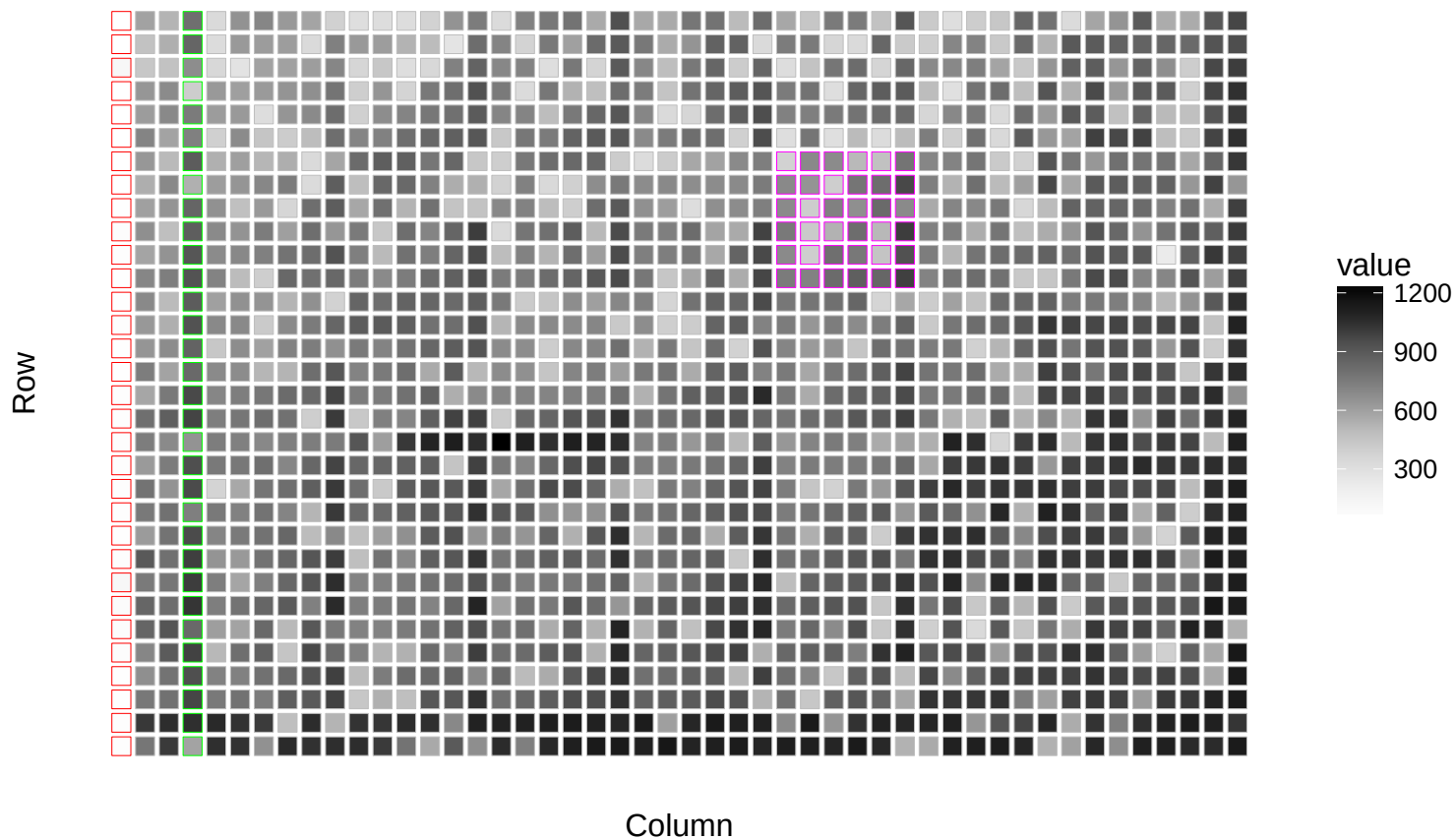
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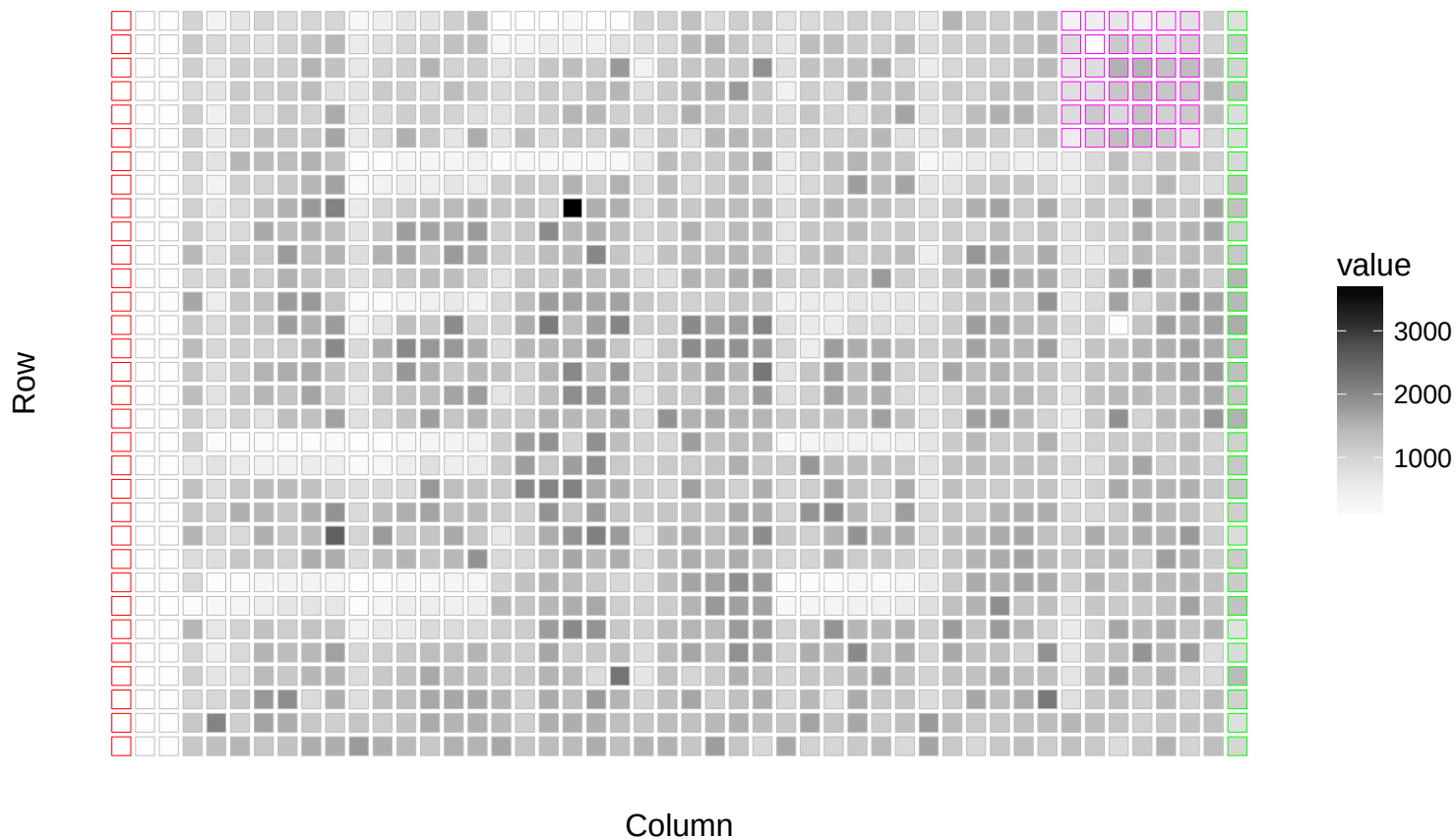
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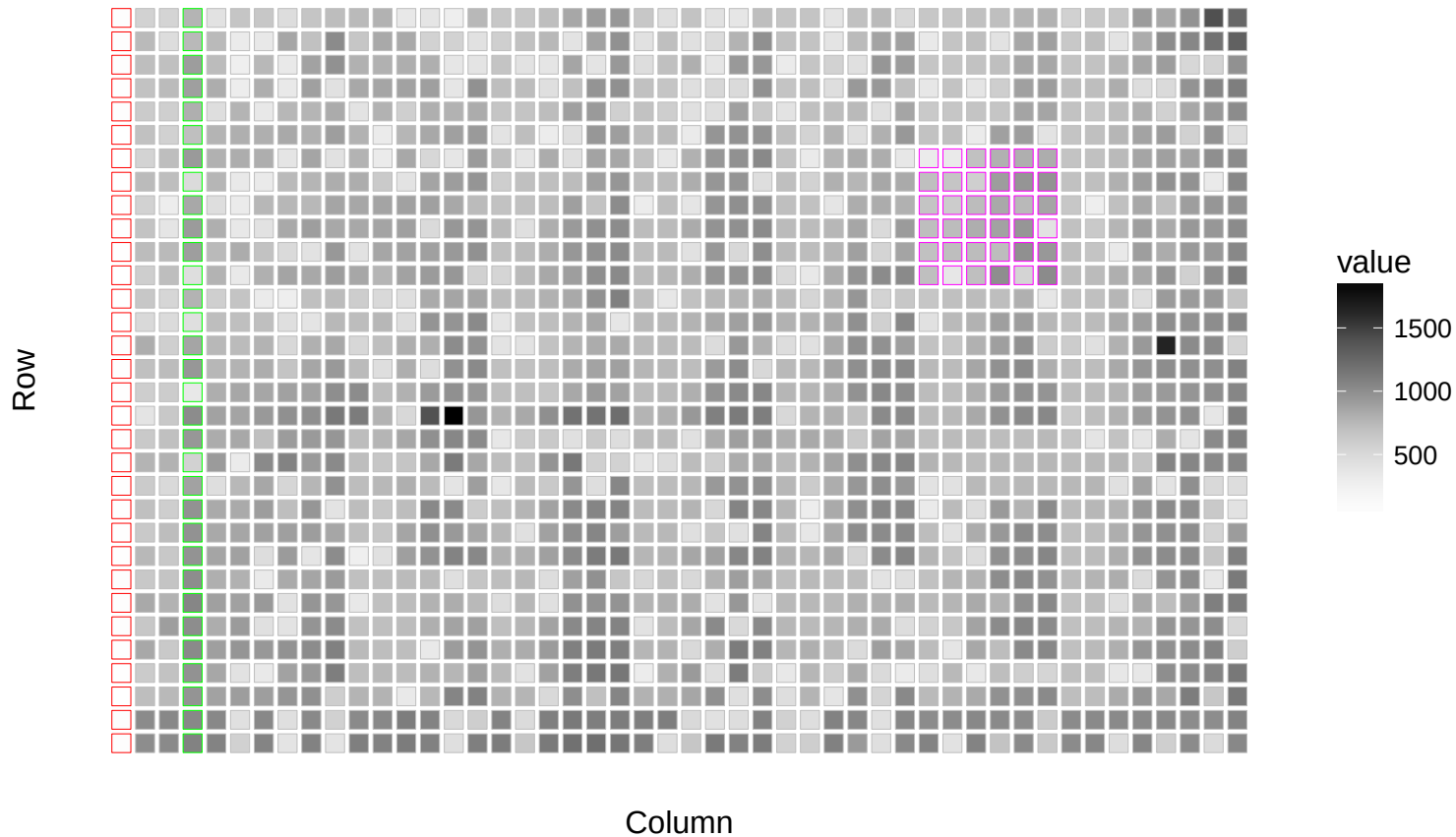
Block 75 (T5615608-T5615608)



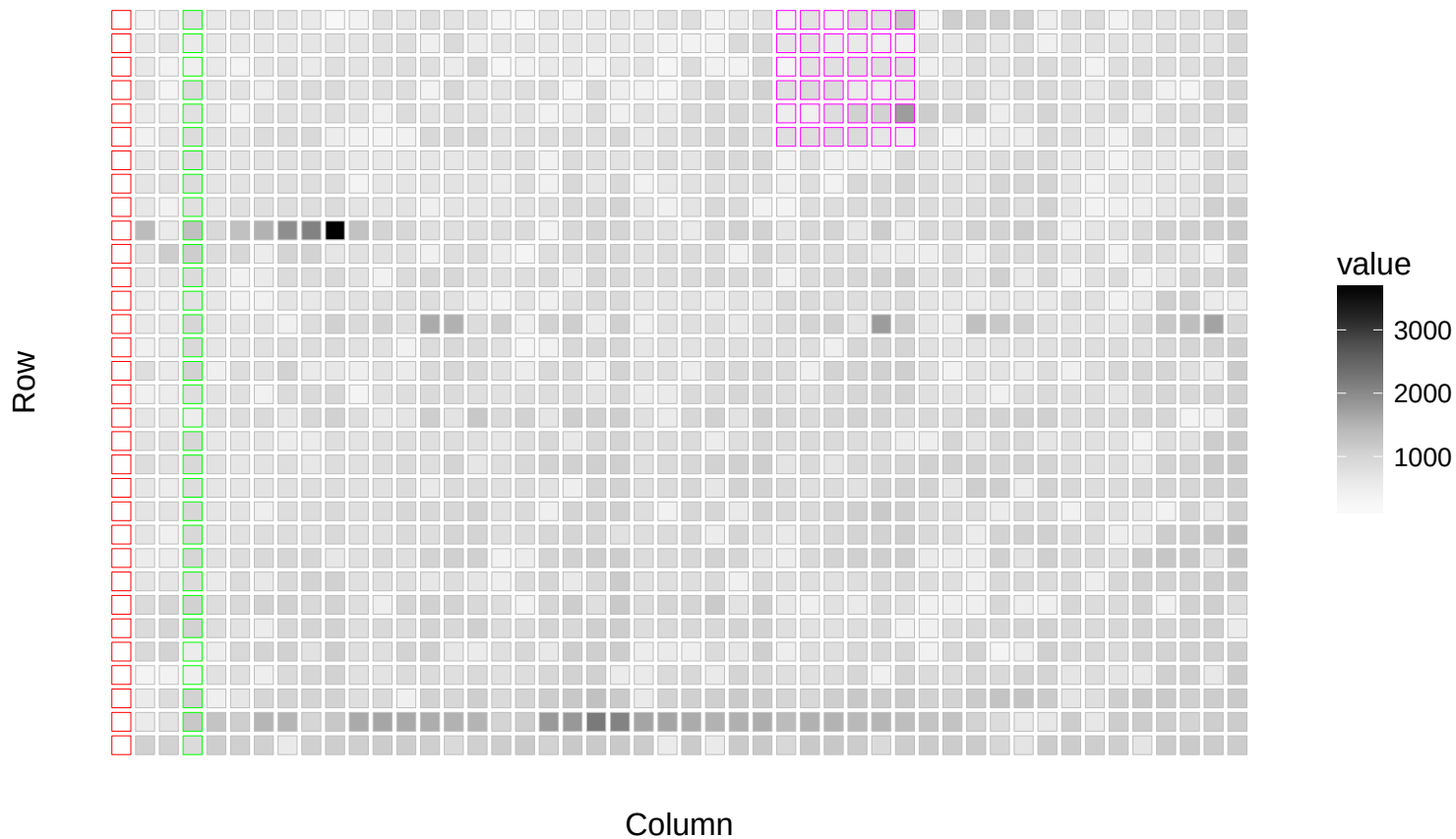
Block 76 (T5574276–T5574276)



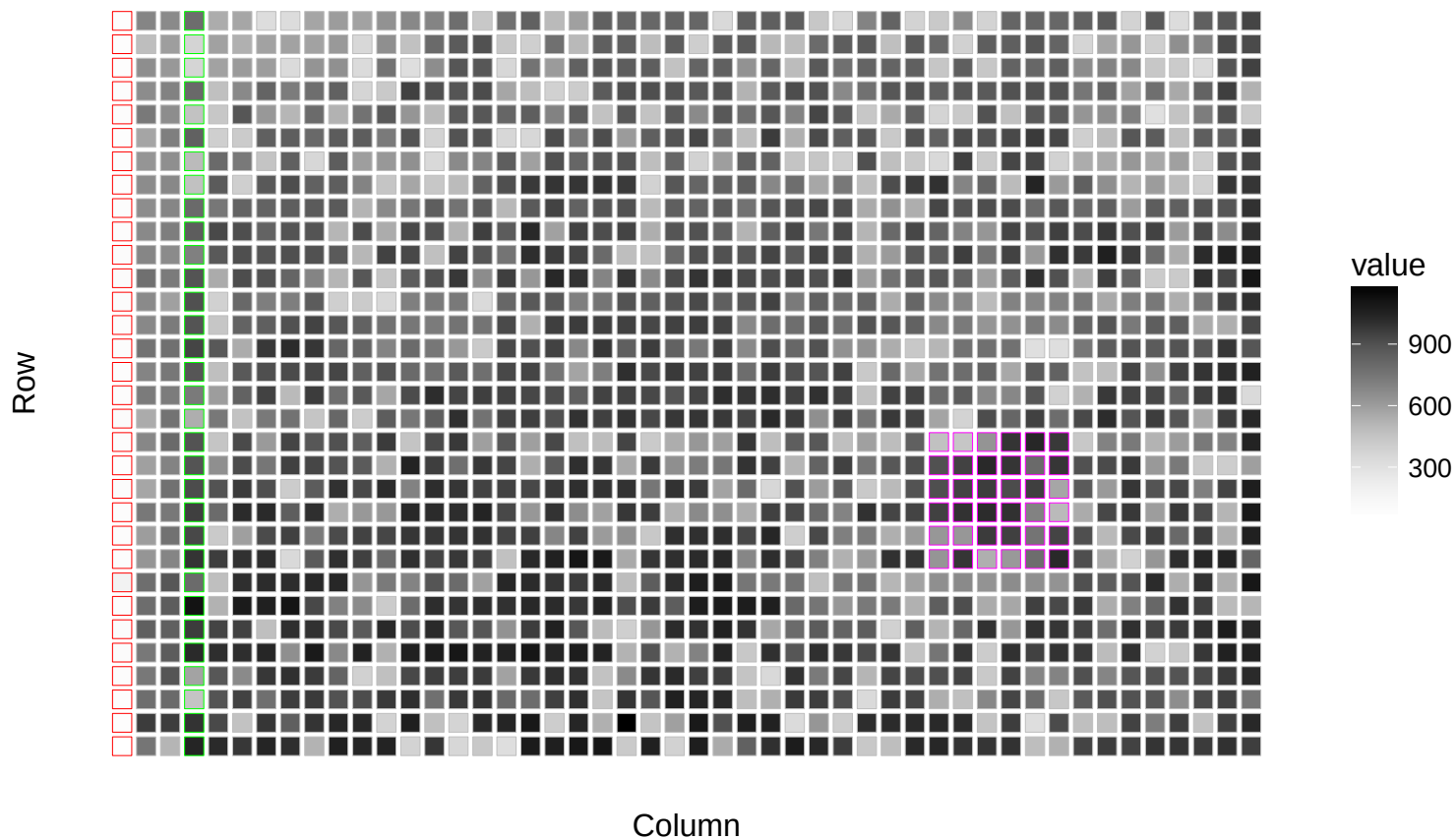
Block 77 (T5616754-T5616754)



Block 78 (T5614966–T5614966)

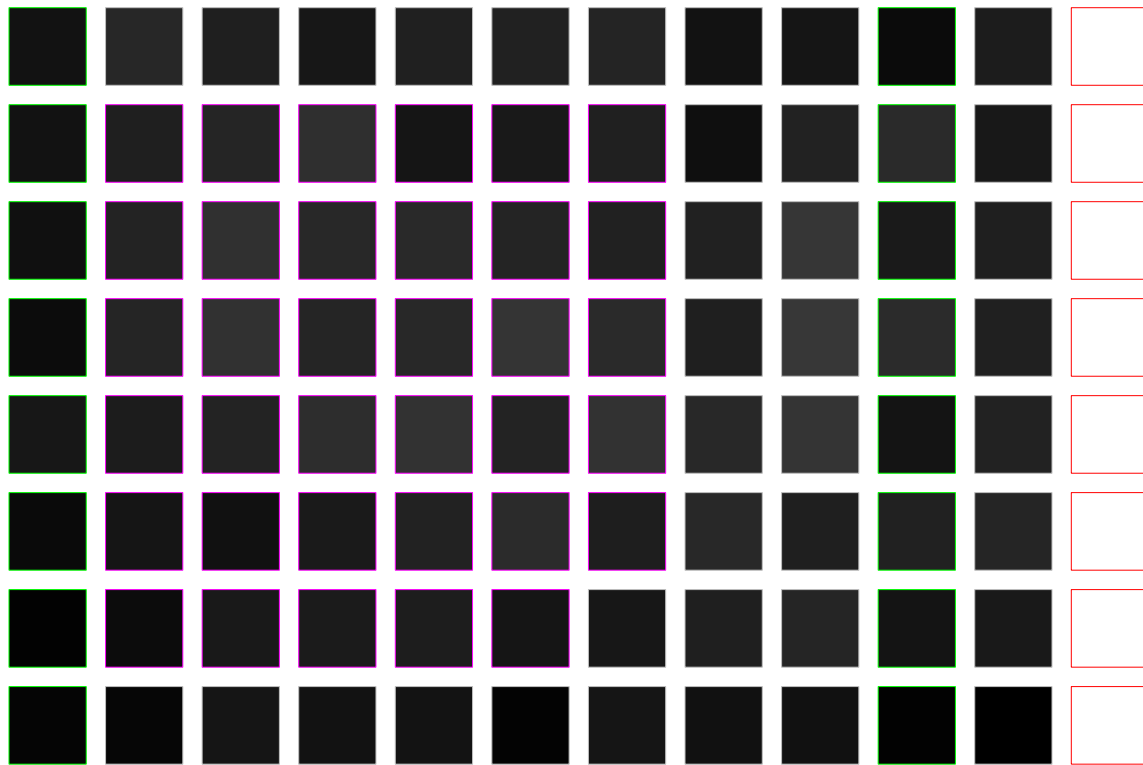


Block 79 (T5615614-T5615614)

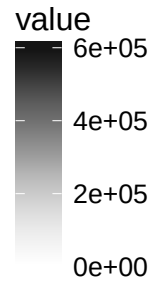


Block 80 (E2000008-E2000008)

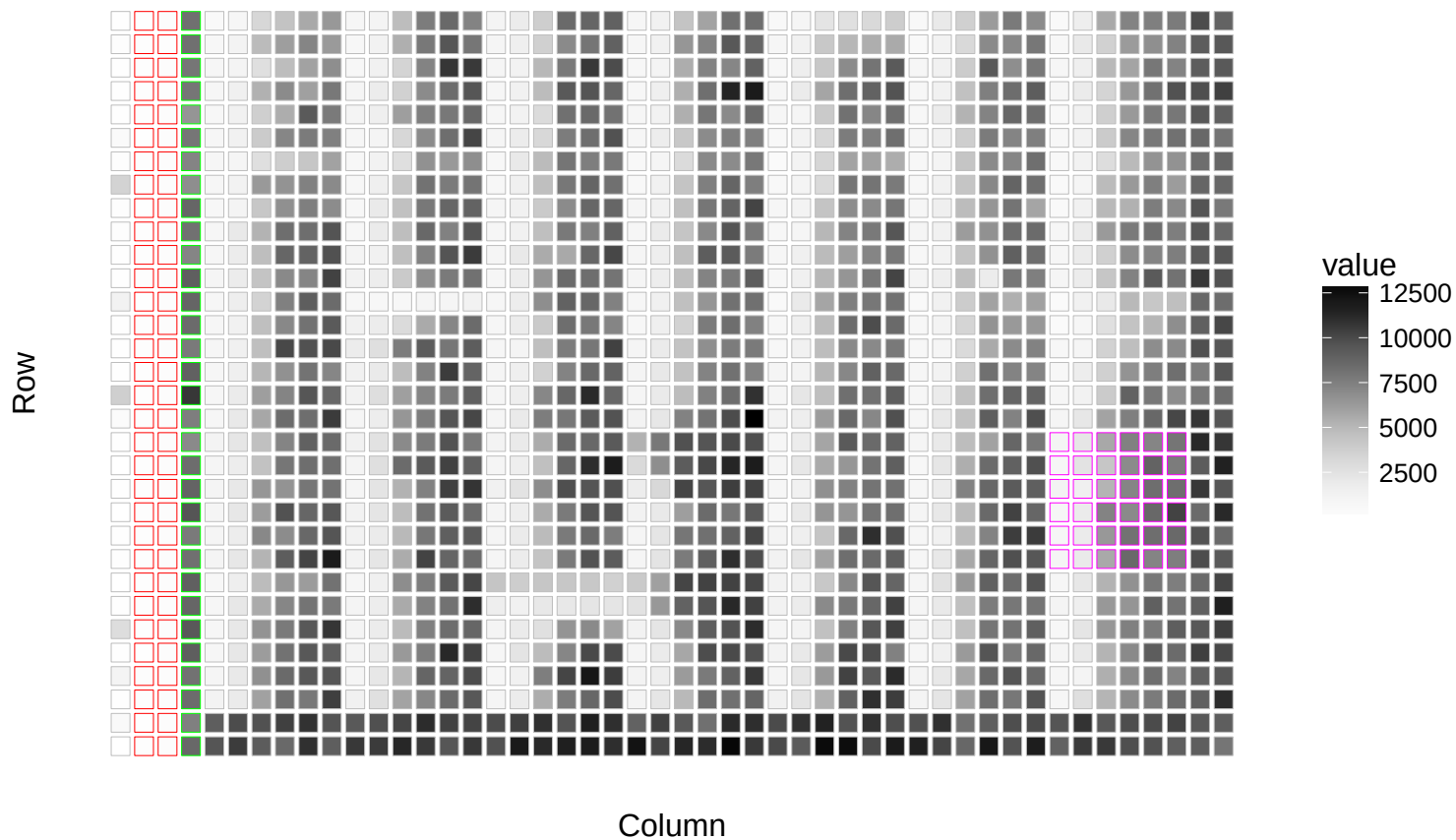
Row



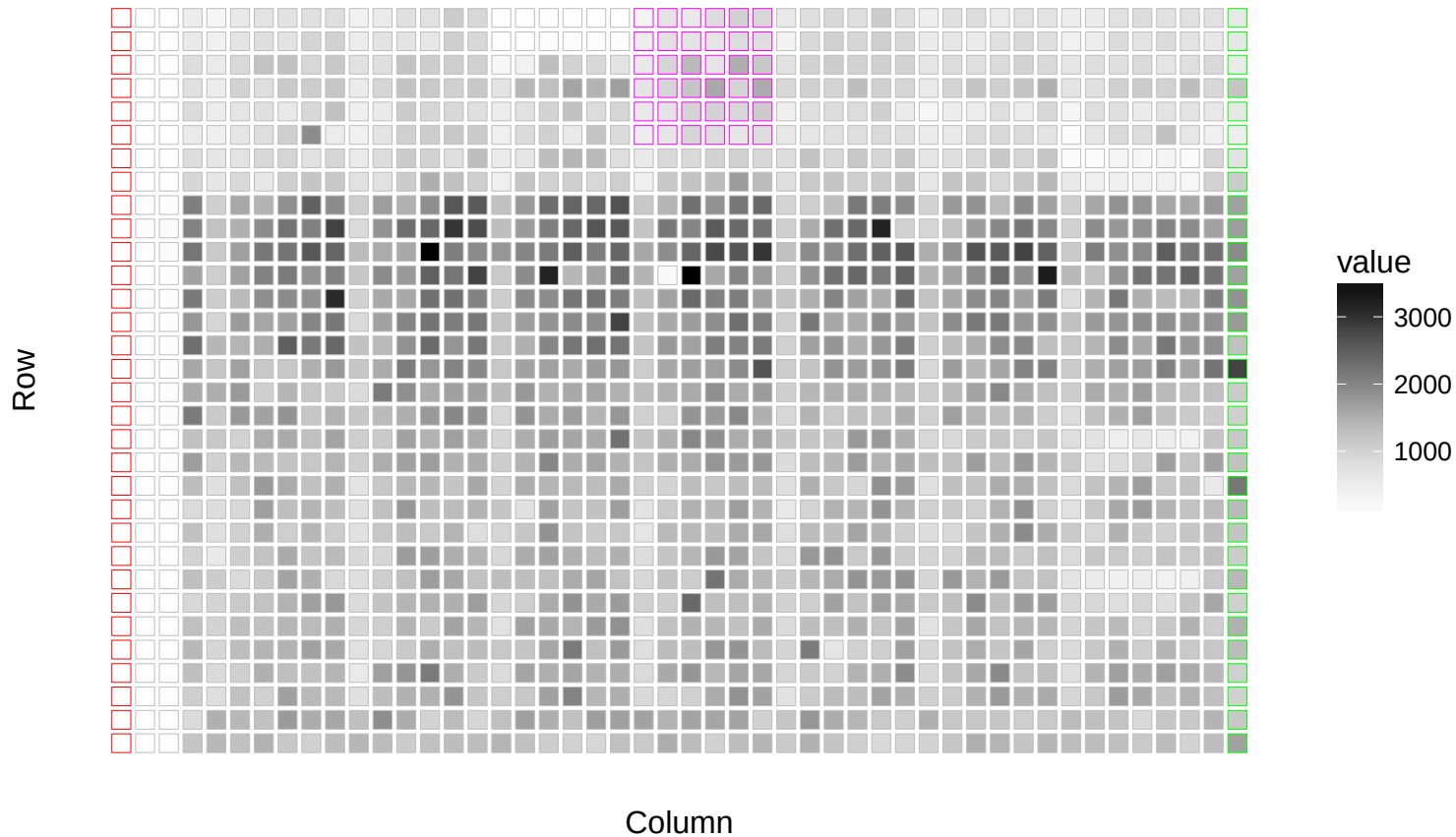
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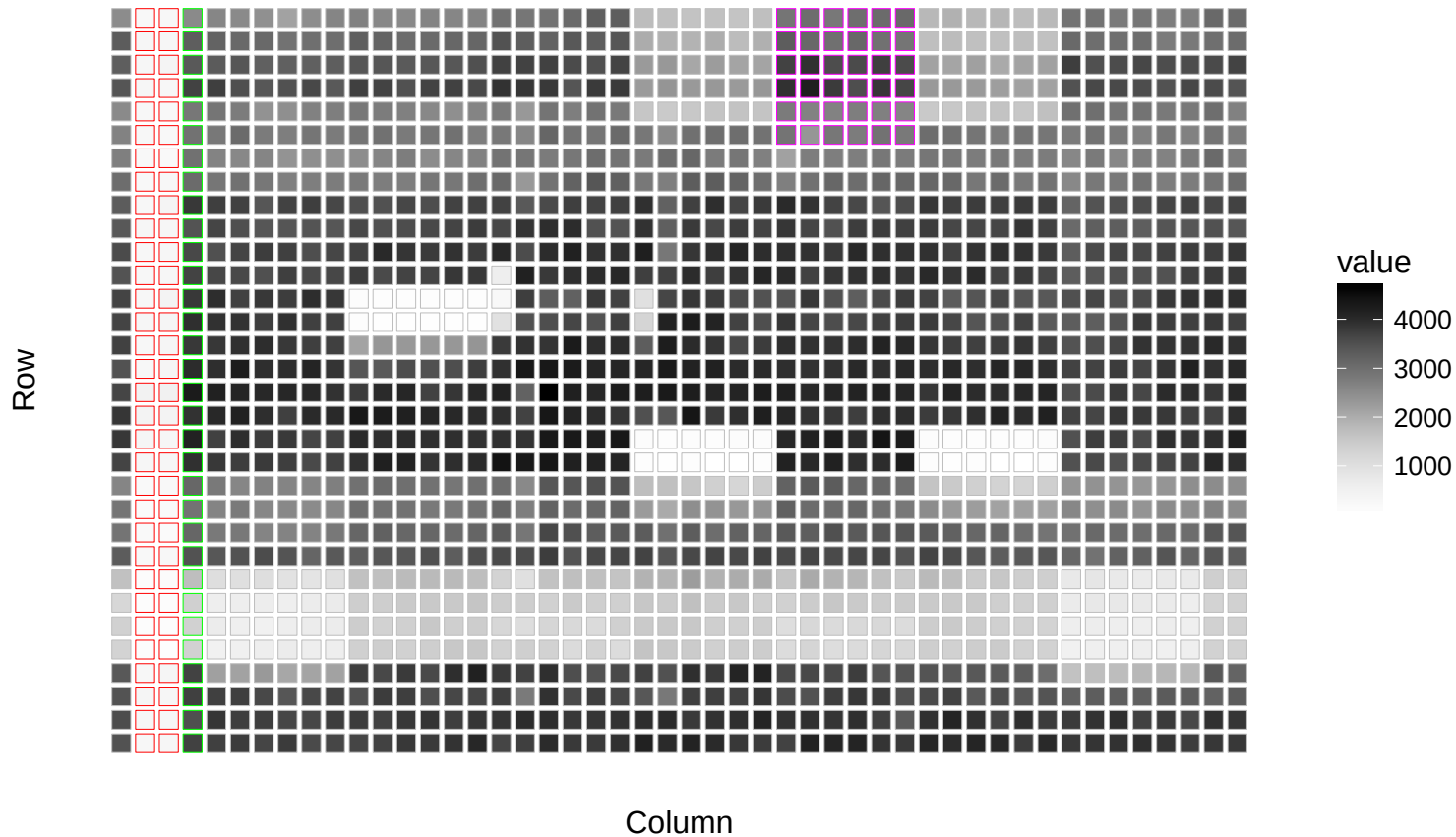
Block 81 (T5570430-T5570430)



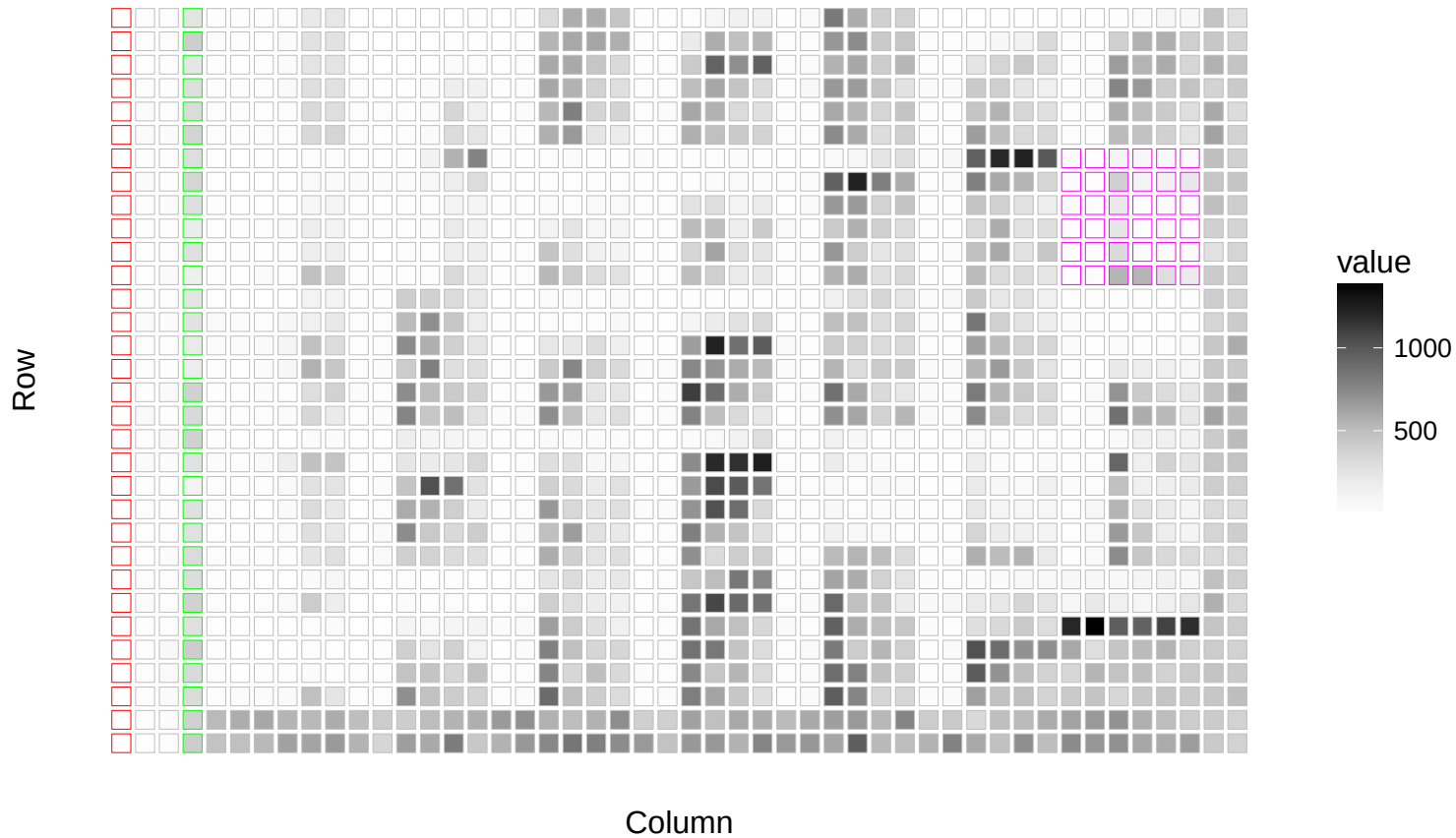
Block 82 (T5574270–T5574270)



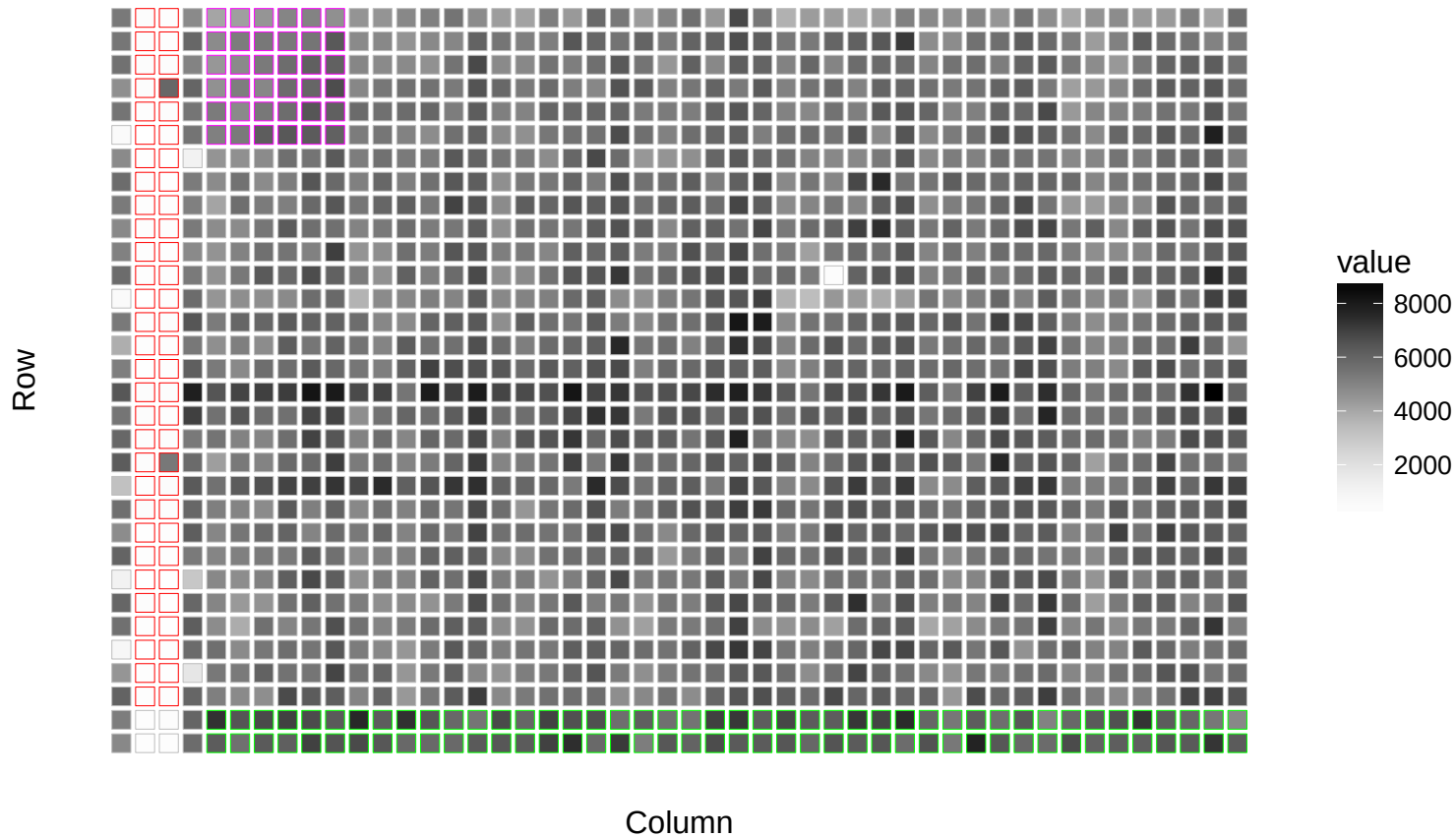
Block 83 (T5666306-T5666306)



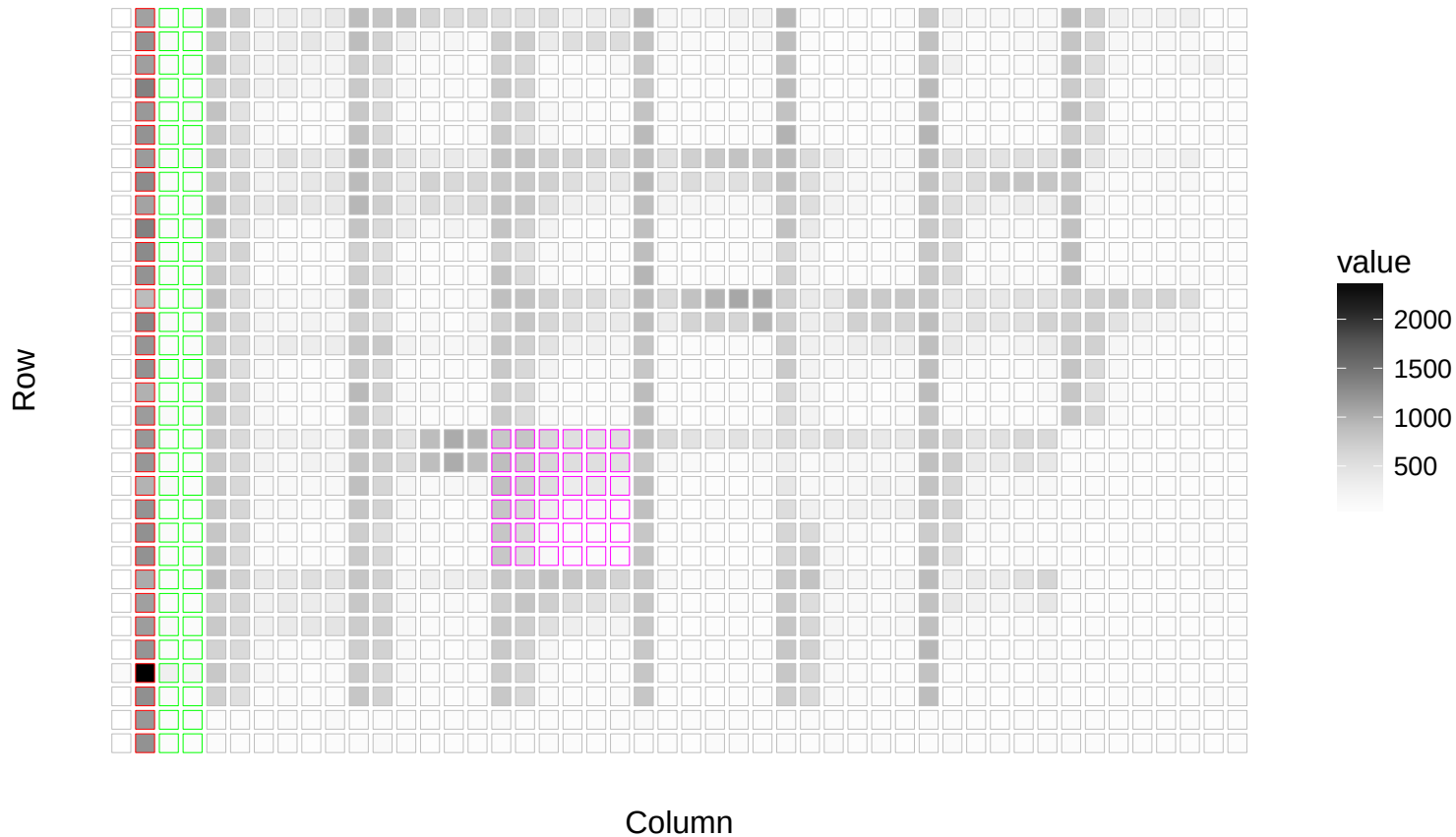
Block 84 (M1020014-T5571464)



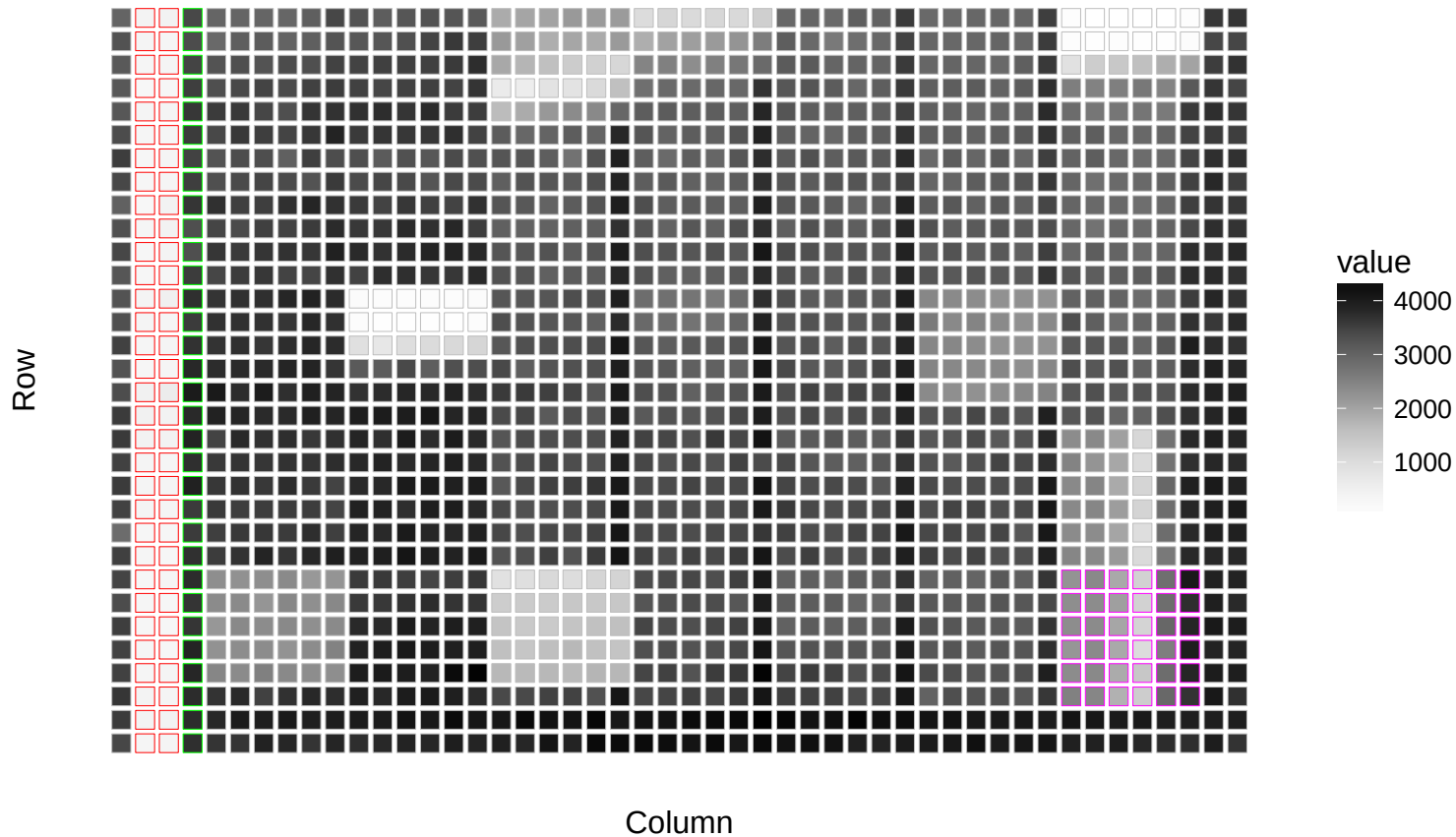
Block 85 (M8900066-T5510680)



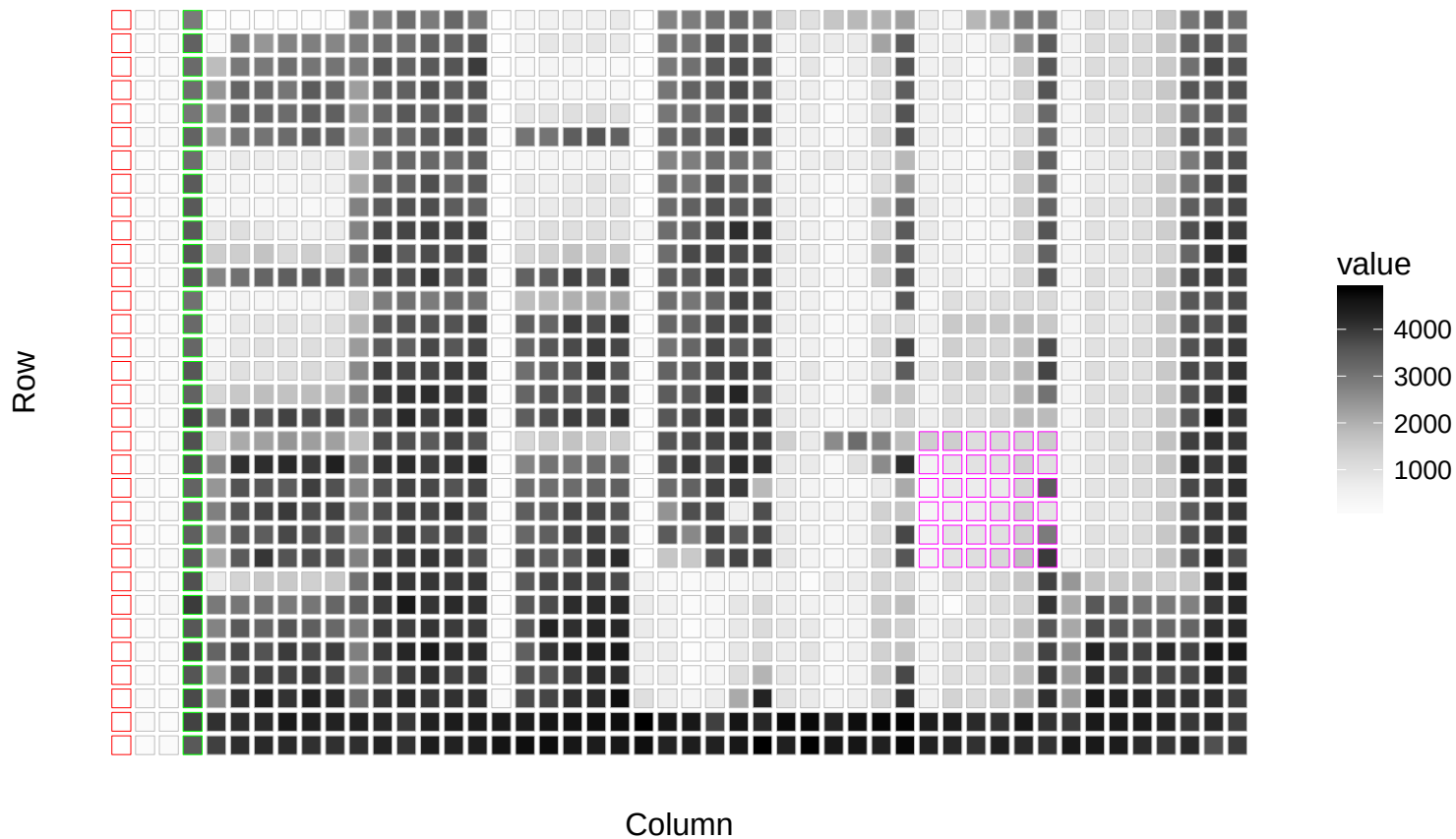
Block 86 (T5563358–T5563358)



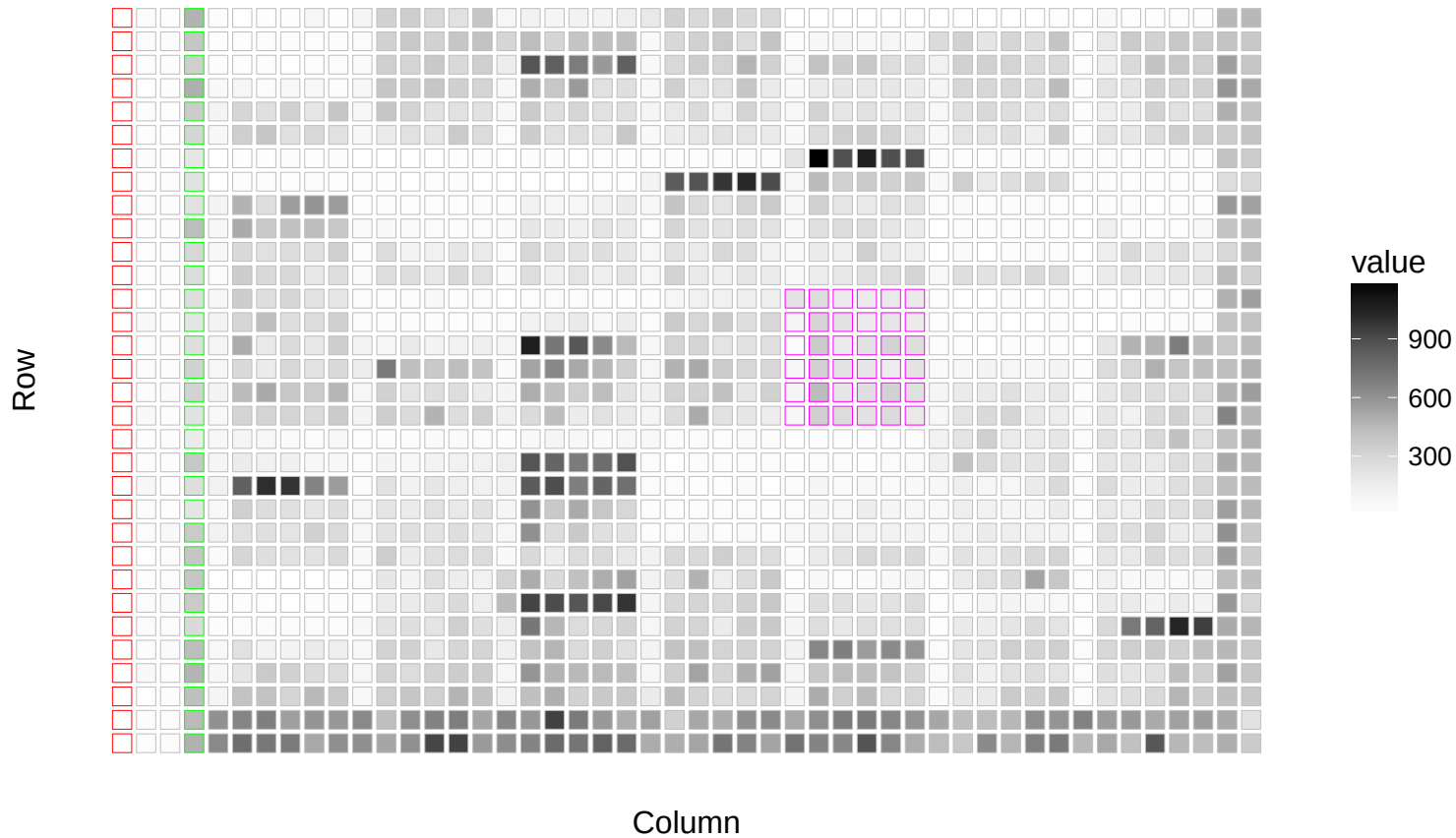
Block 87 (T5666294-T5666294)



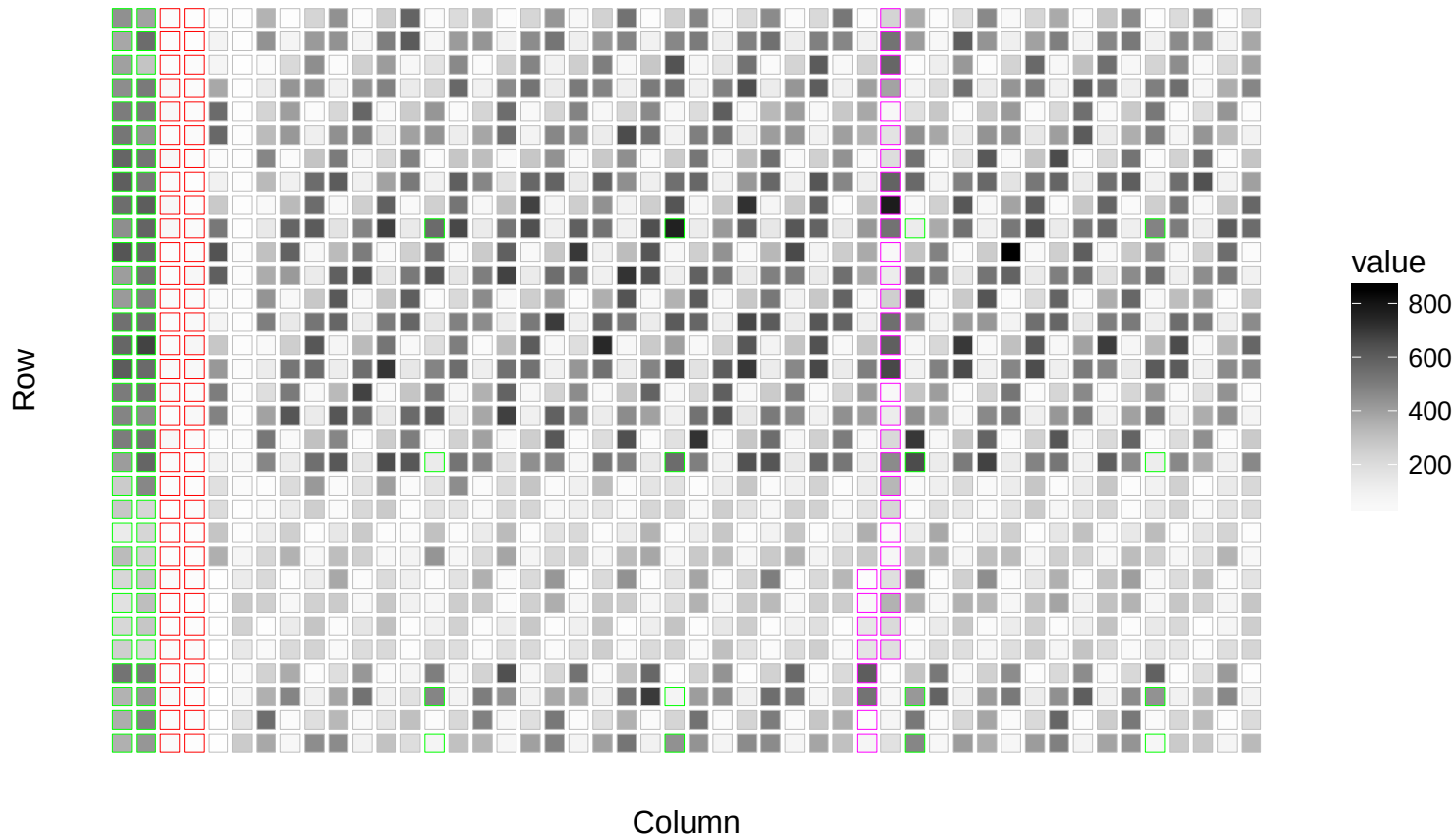
Block 88 (T5614752-T5614752)



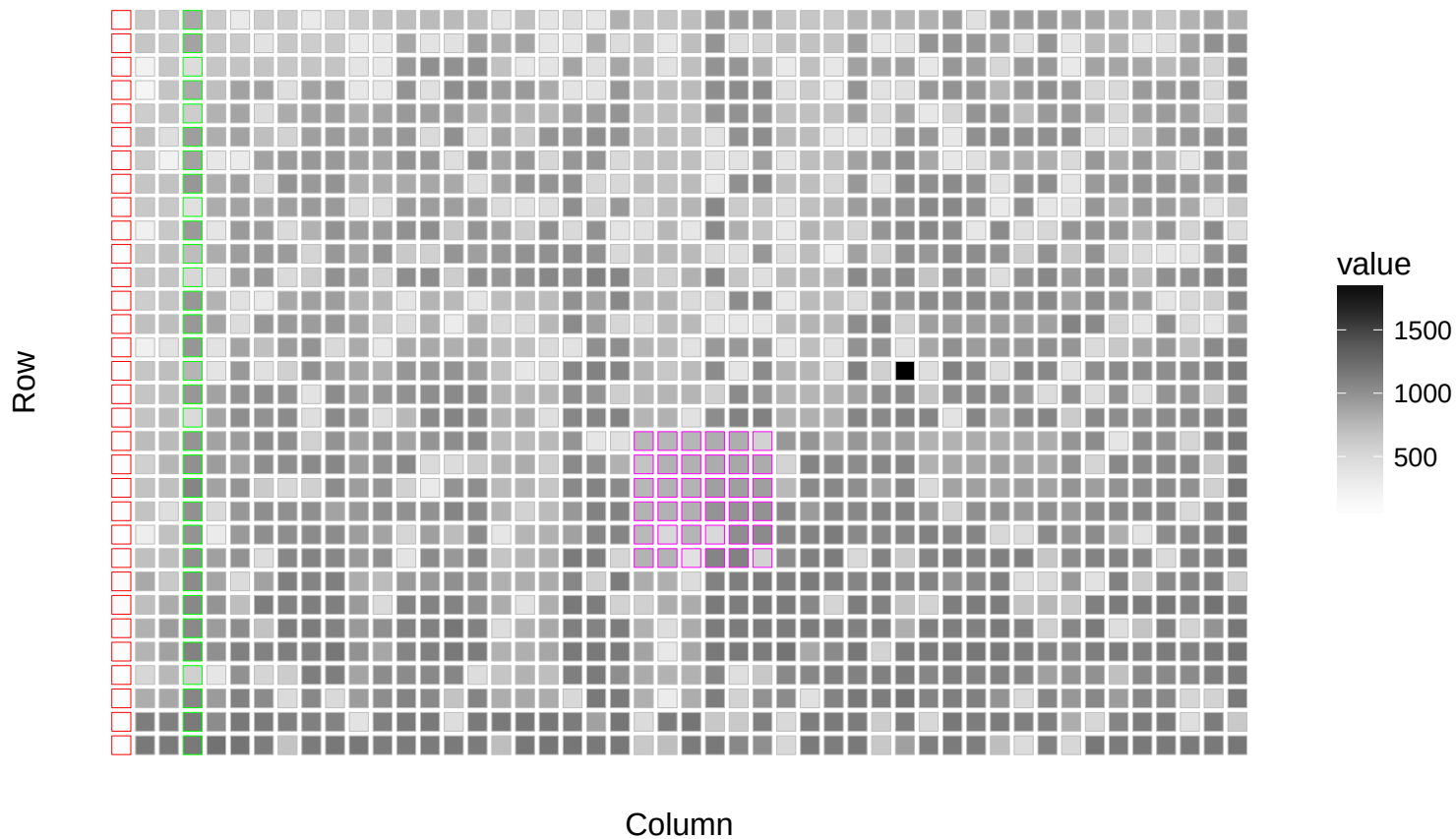
Block 89 (M1020006-T5571448)



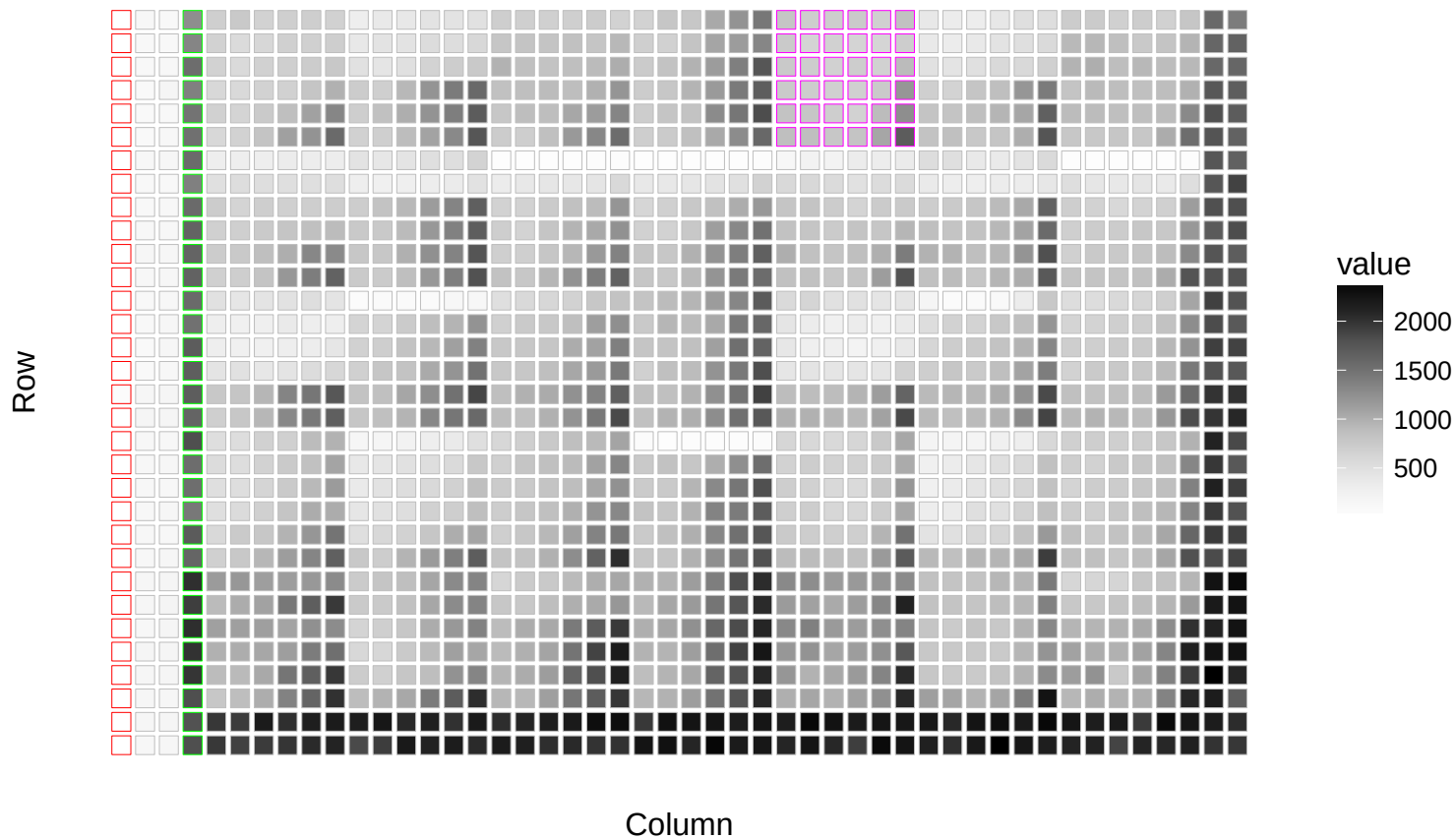
Block 90 (M0300042-T5423700)



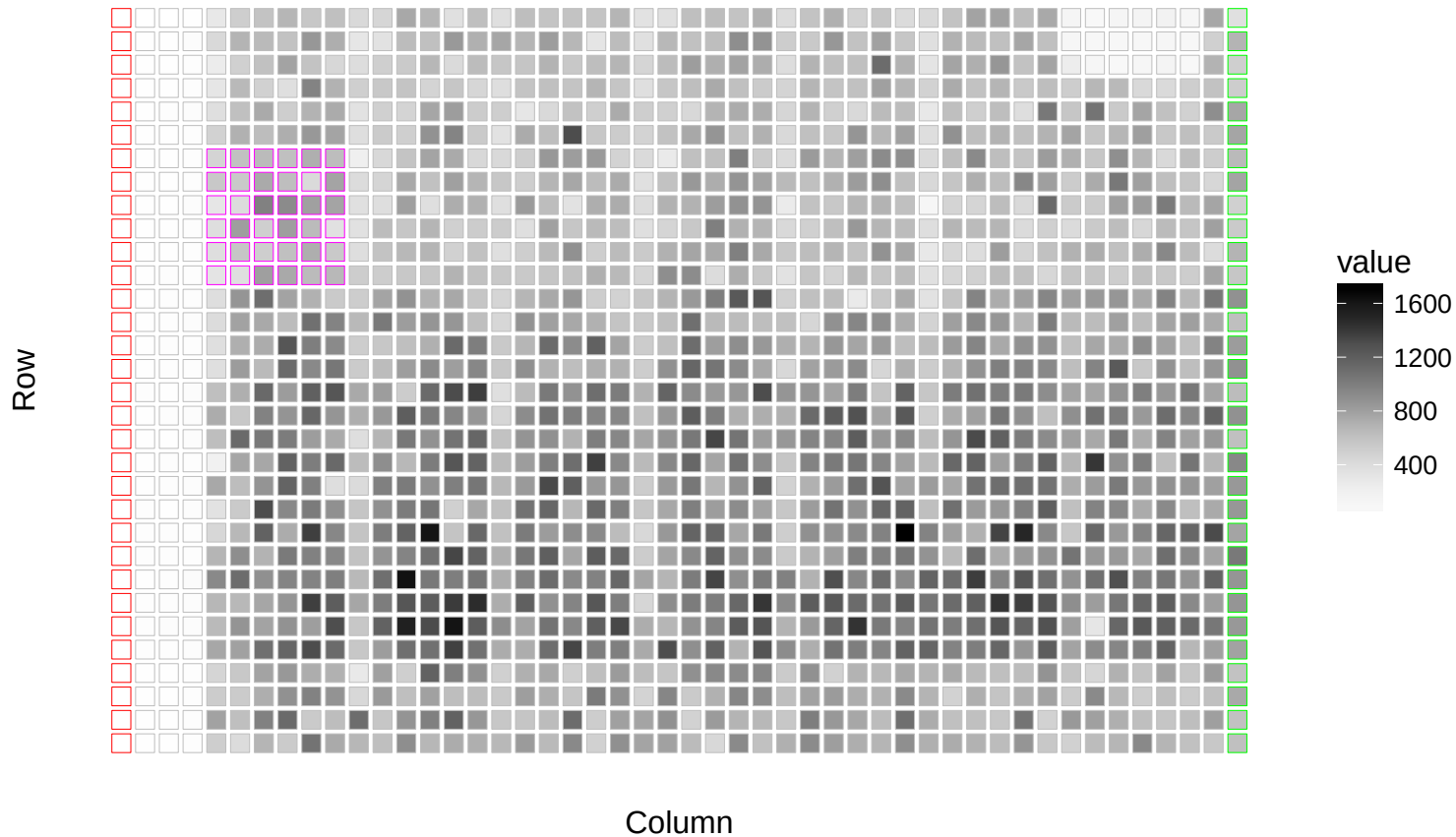
Block 91 (T5616746-T5616746)



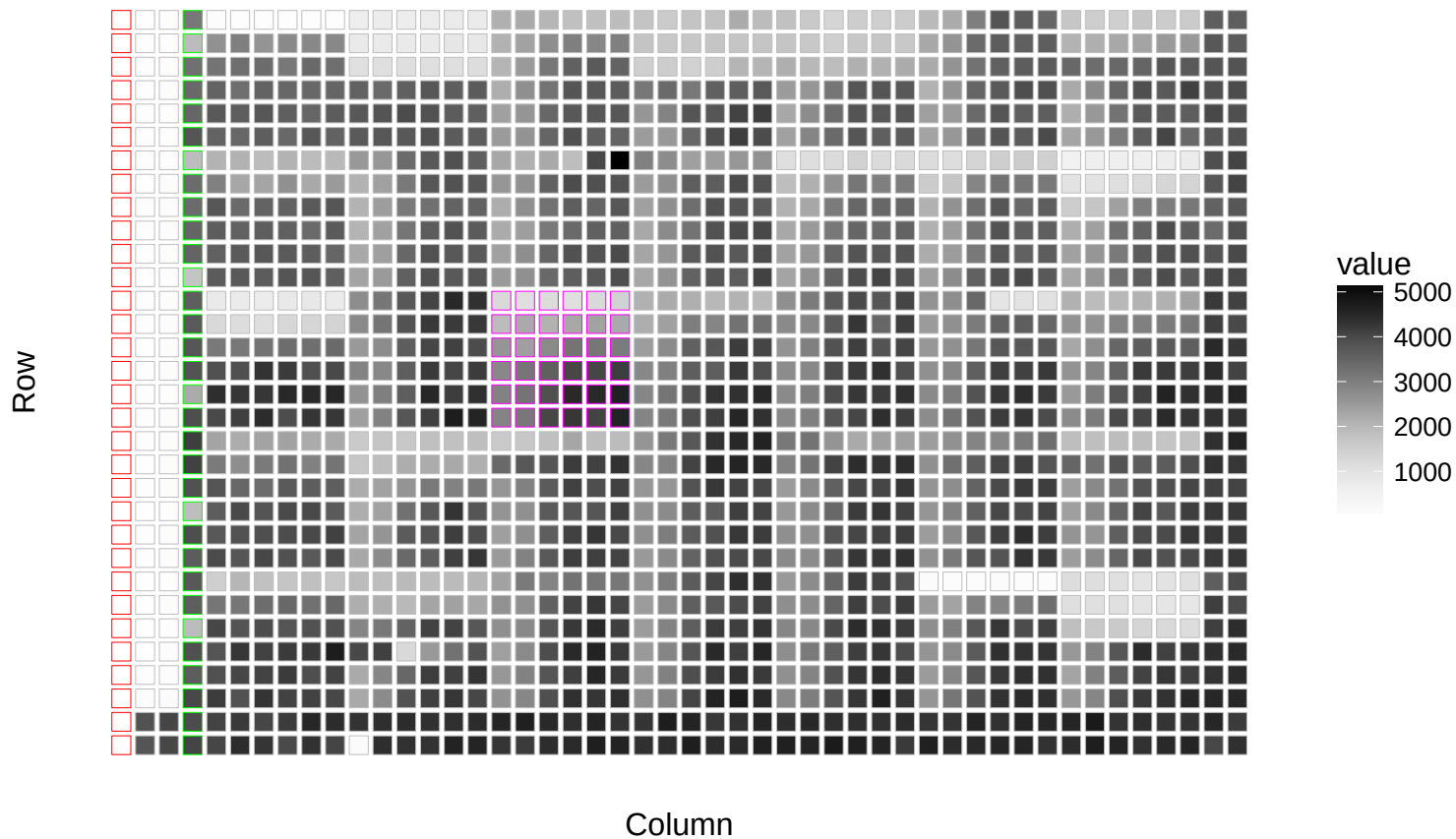
Block 92 (T5622510-T5622510)



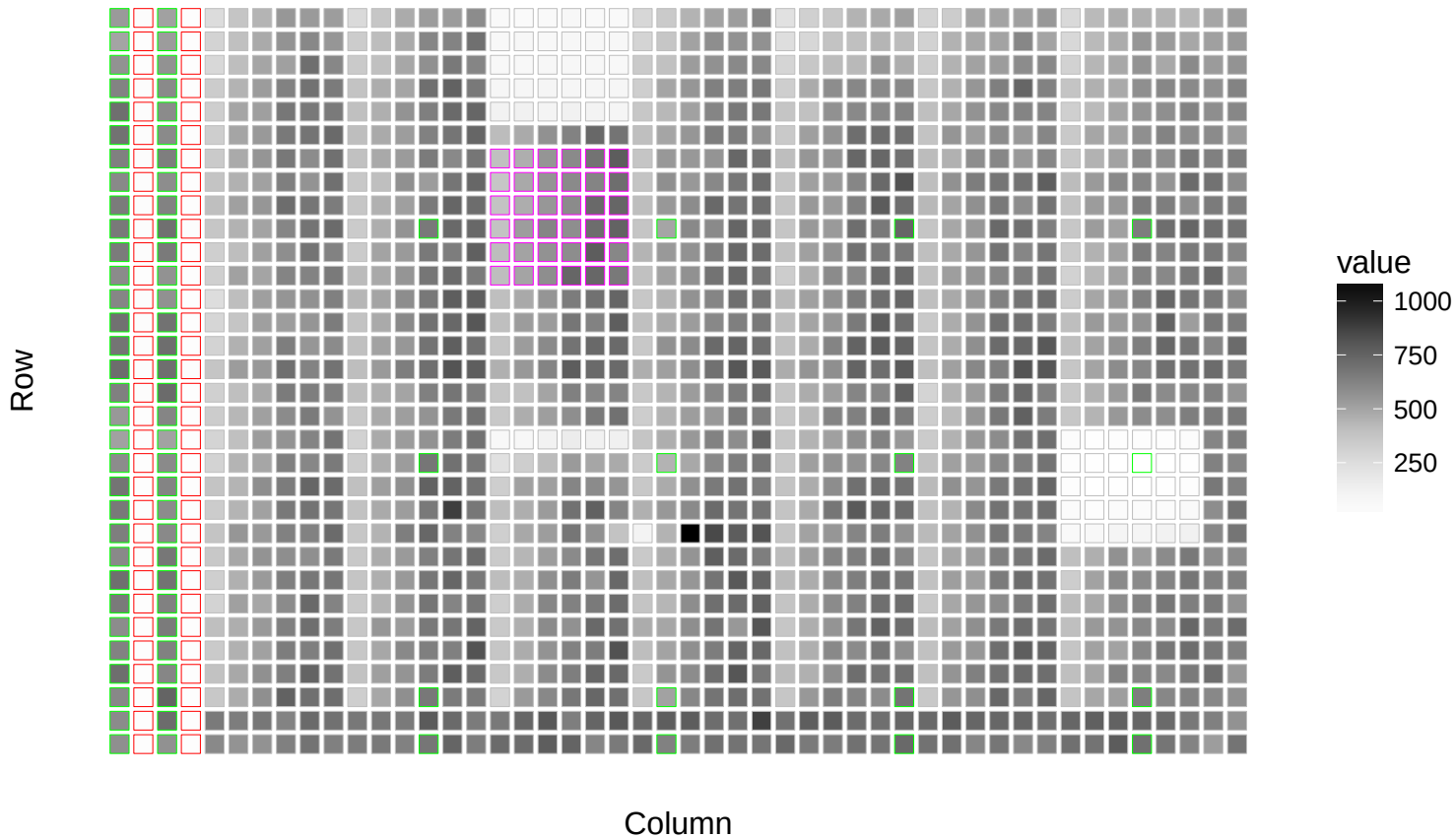
Block 93 (T5574244-T5574244)



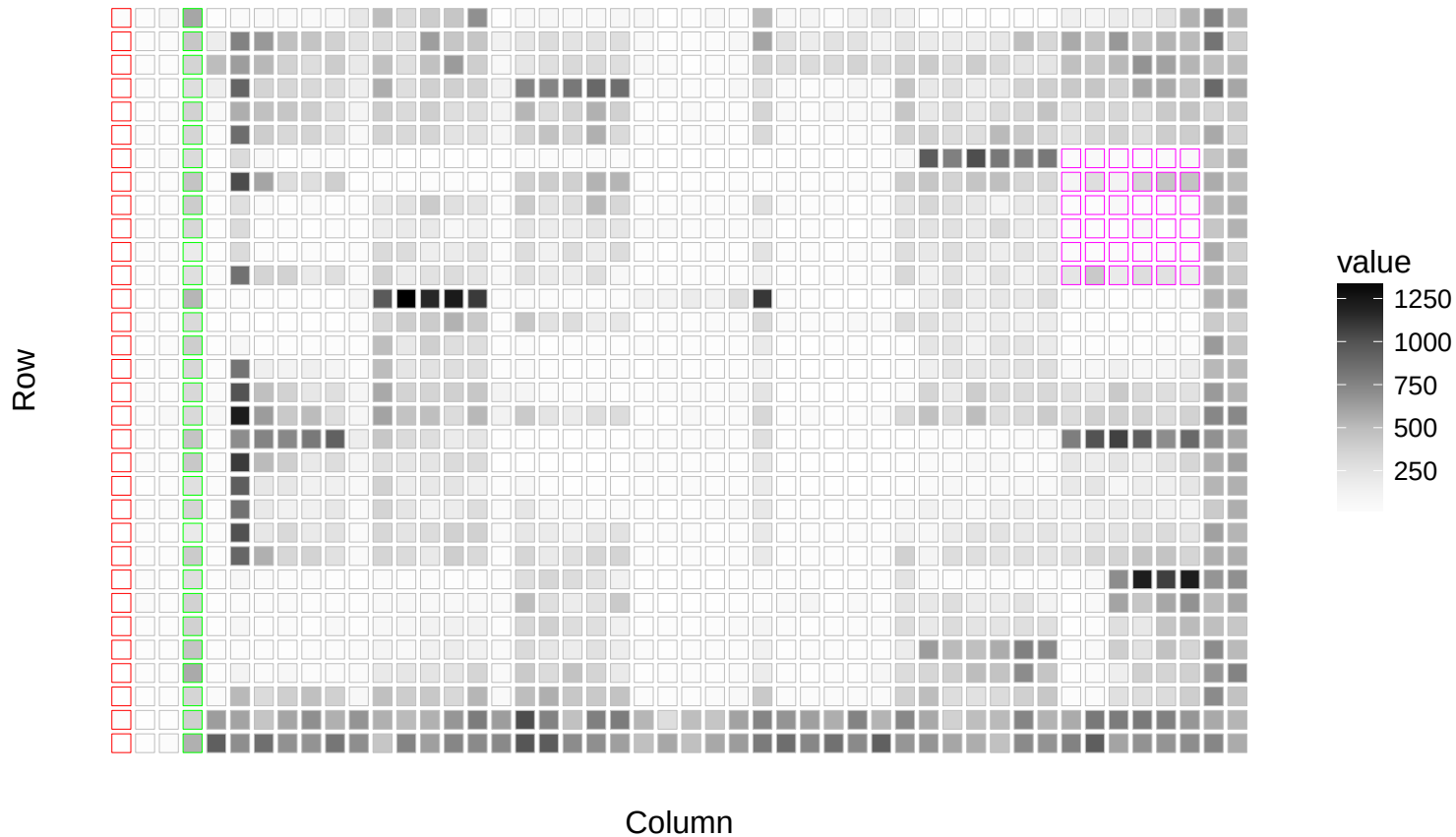
Block 94 (T5606798–T5606798)



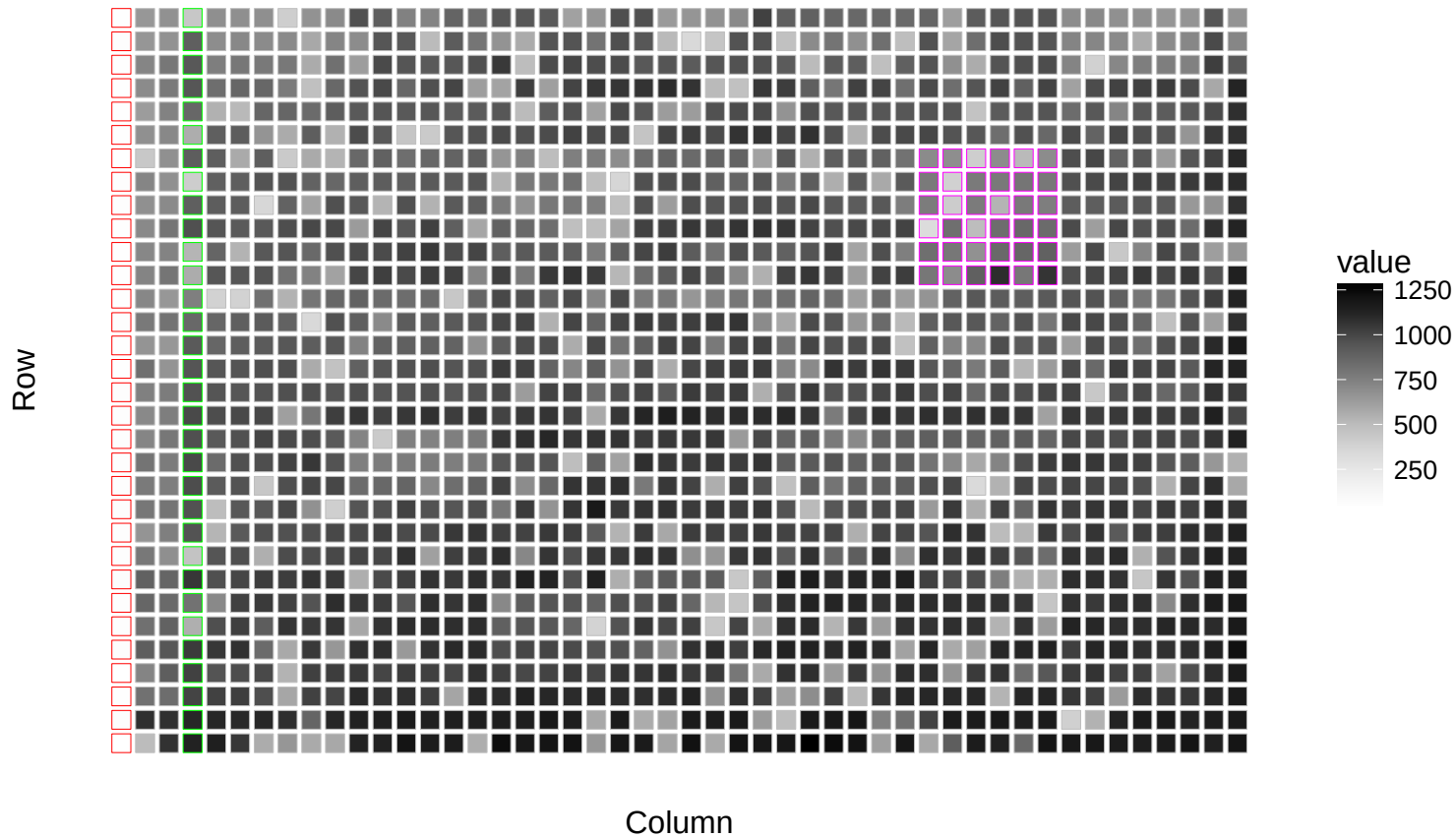
Block 95 (M0300026-T5470338)



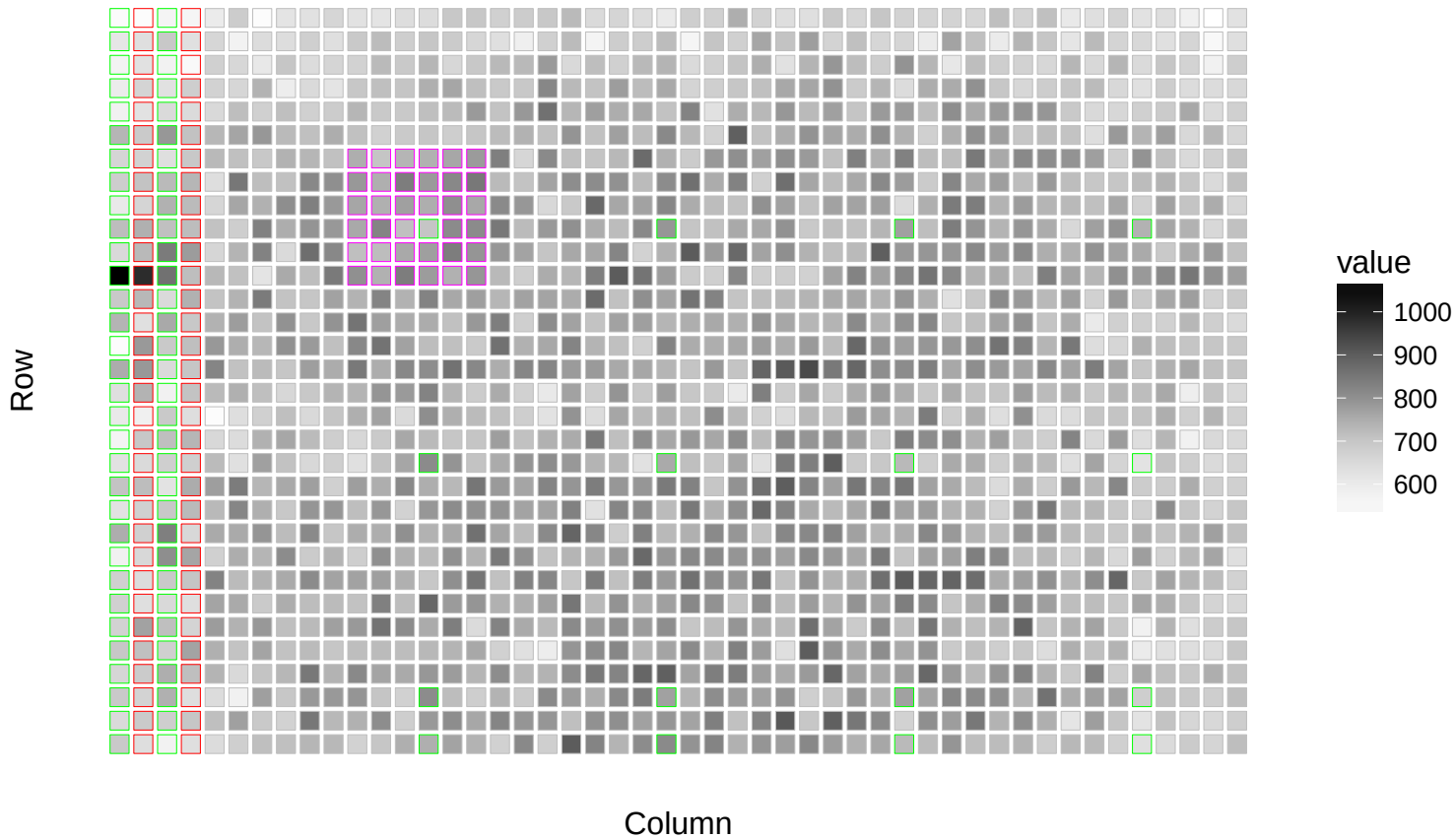
Block 96 (M1020032-T5571468)



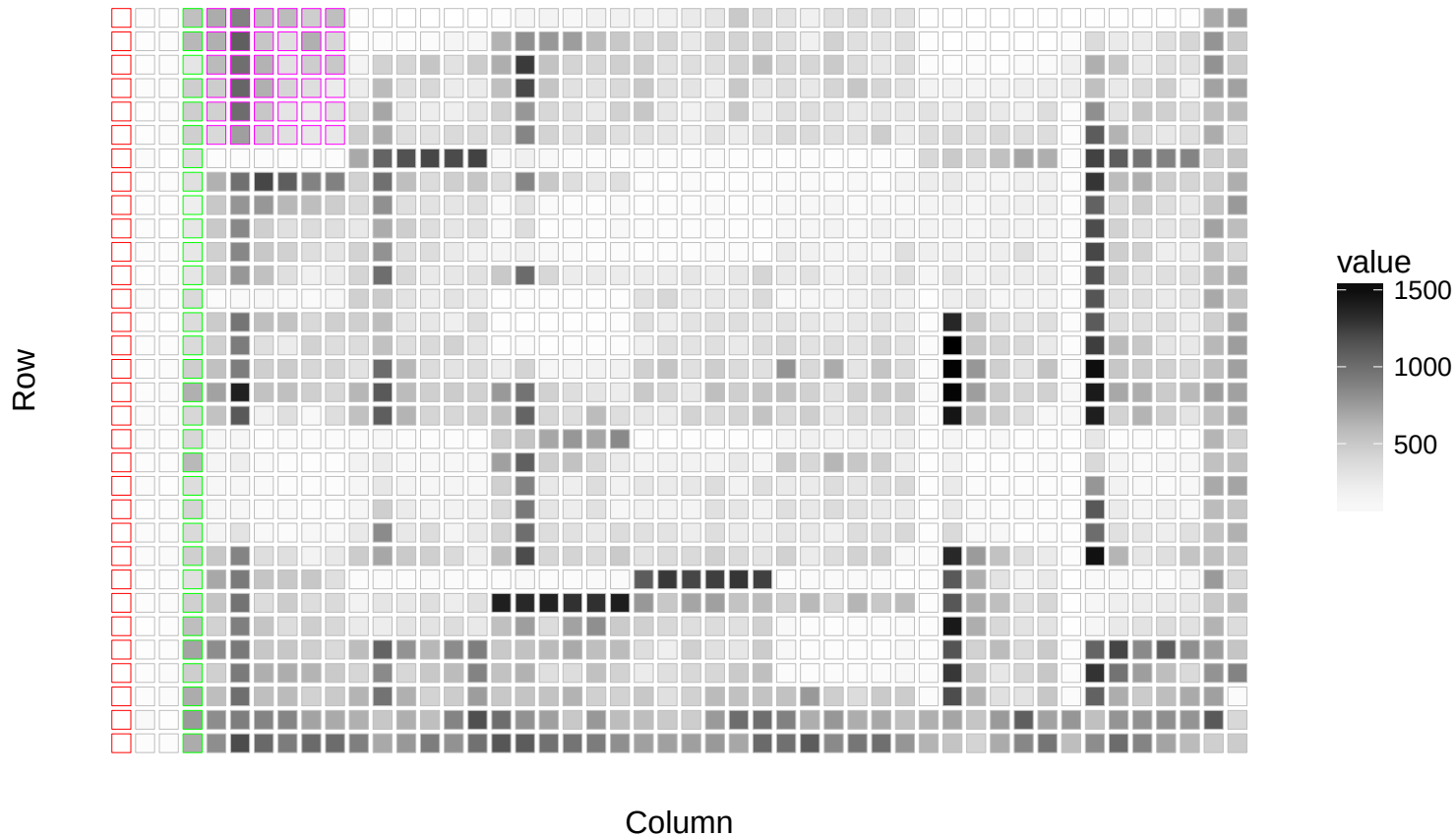
Block 97 (T5614968–T5614968)



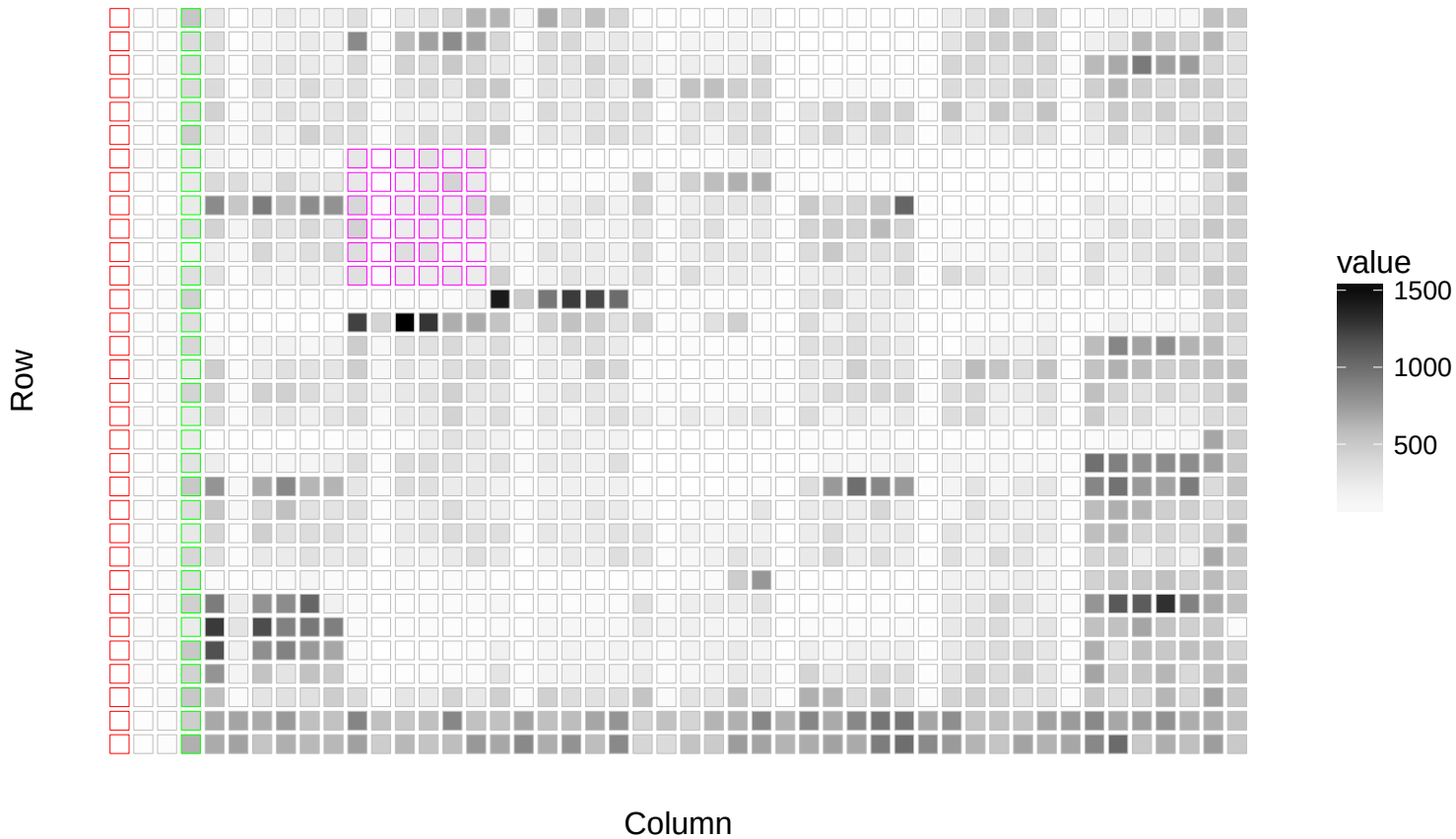
Block 98 (M0300020-T5470332)



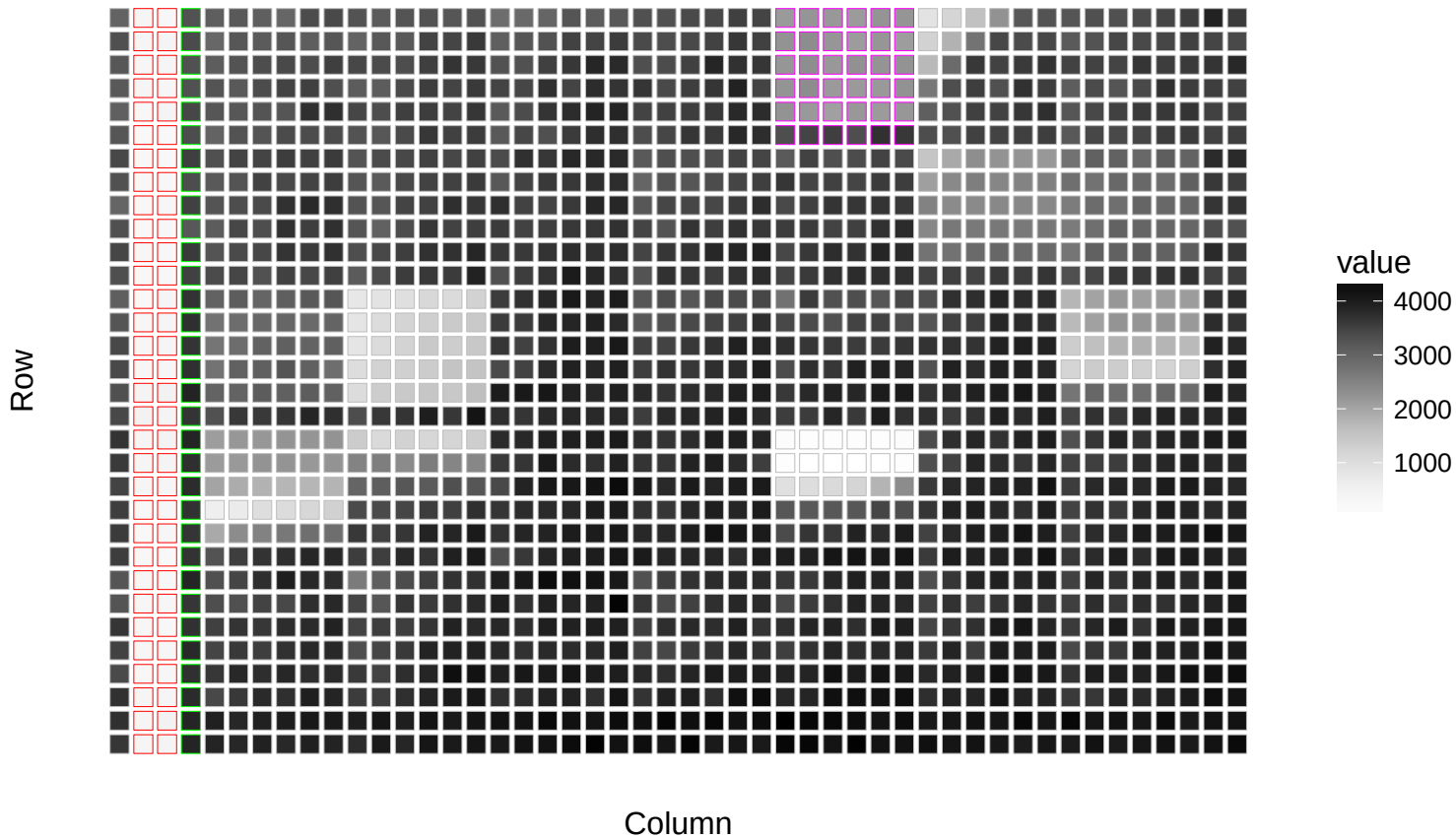
Block 99 (M1020030-T5571470)



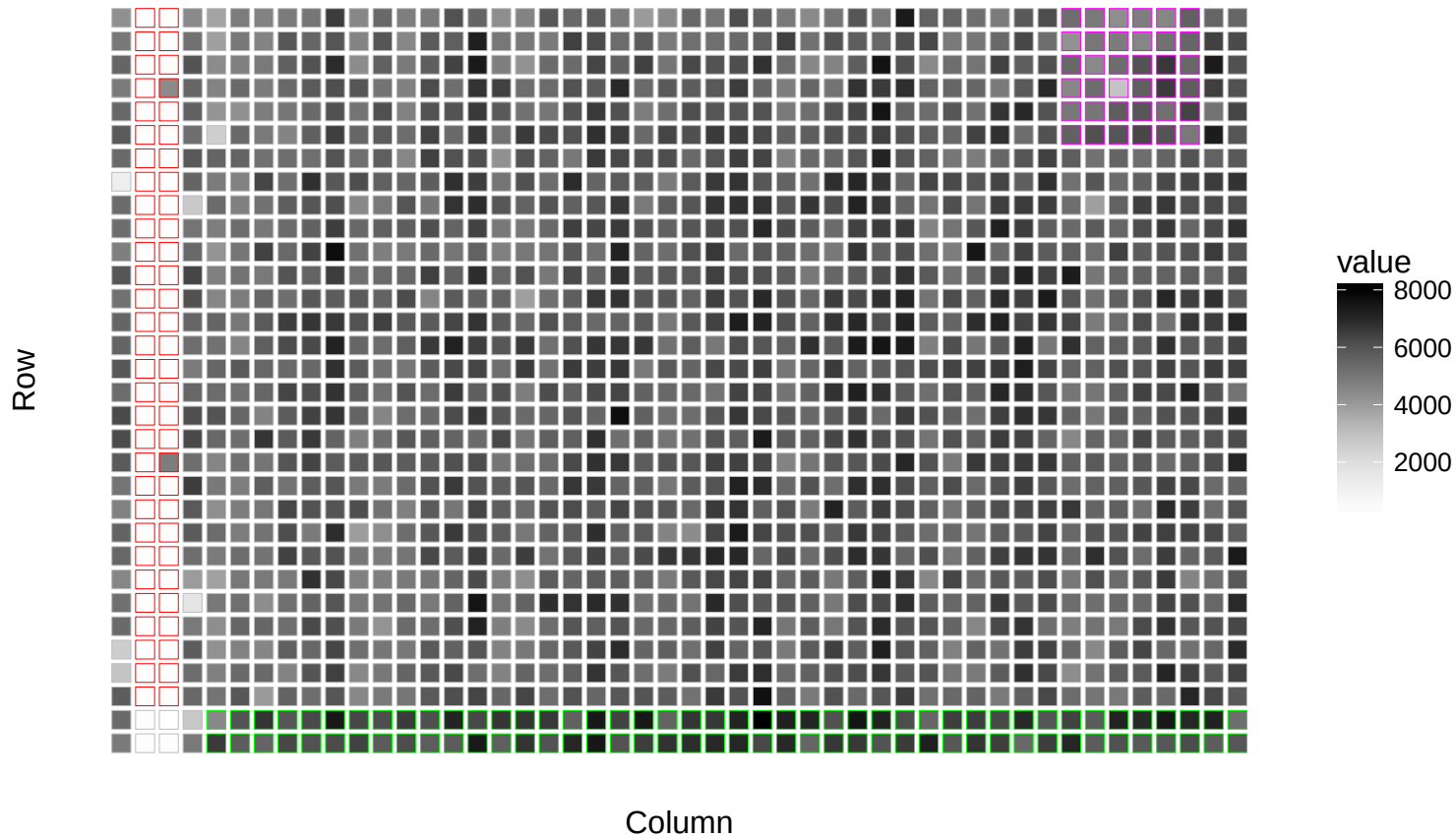
Block 100 (M1020010-T5571444)



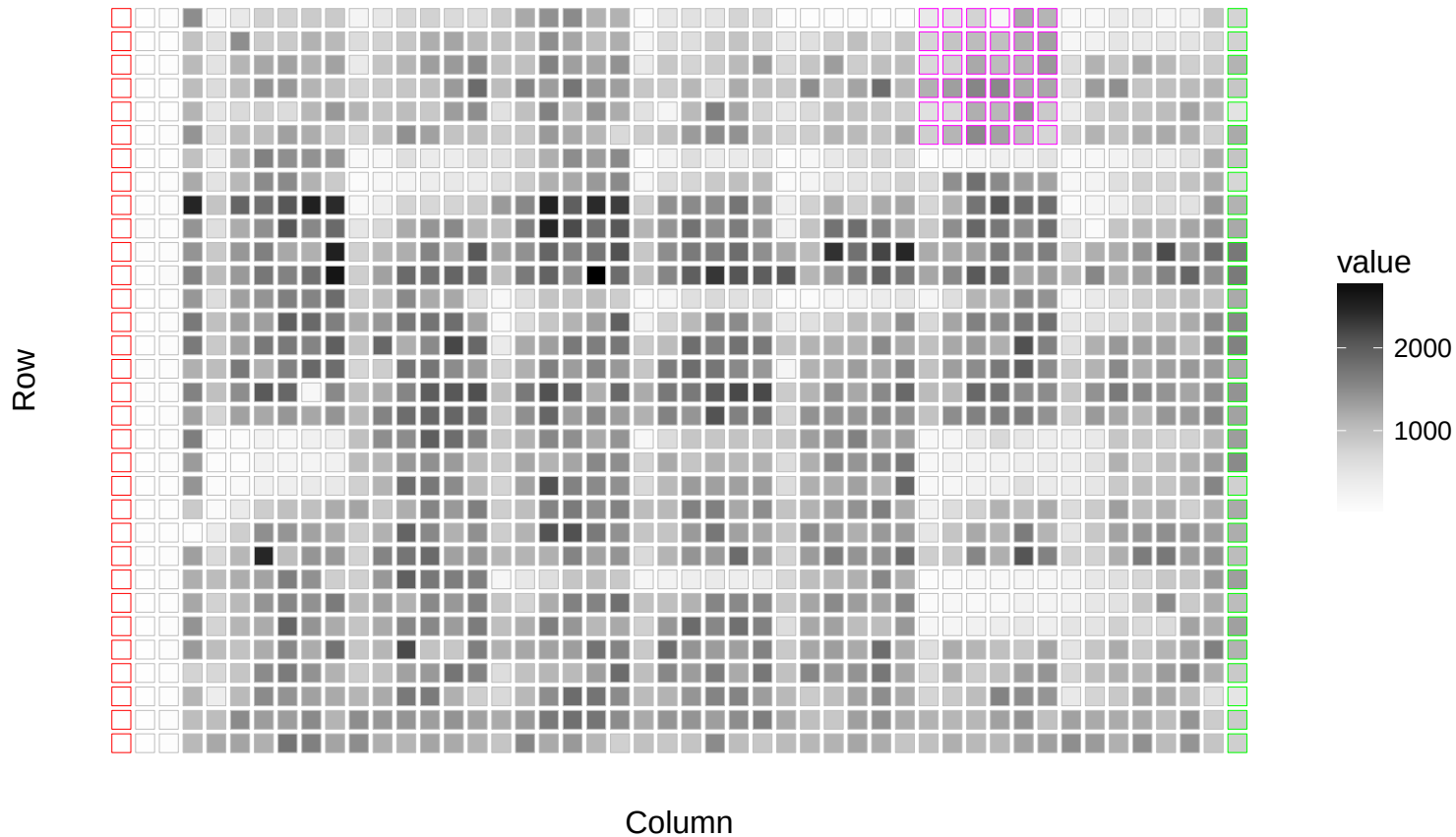
Block 101 (T5666284-T5666284)



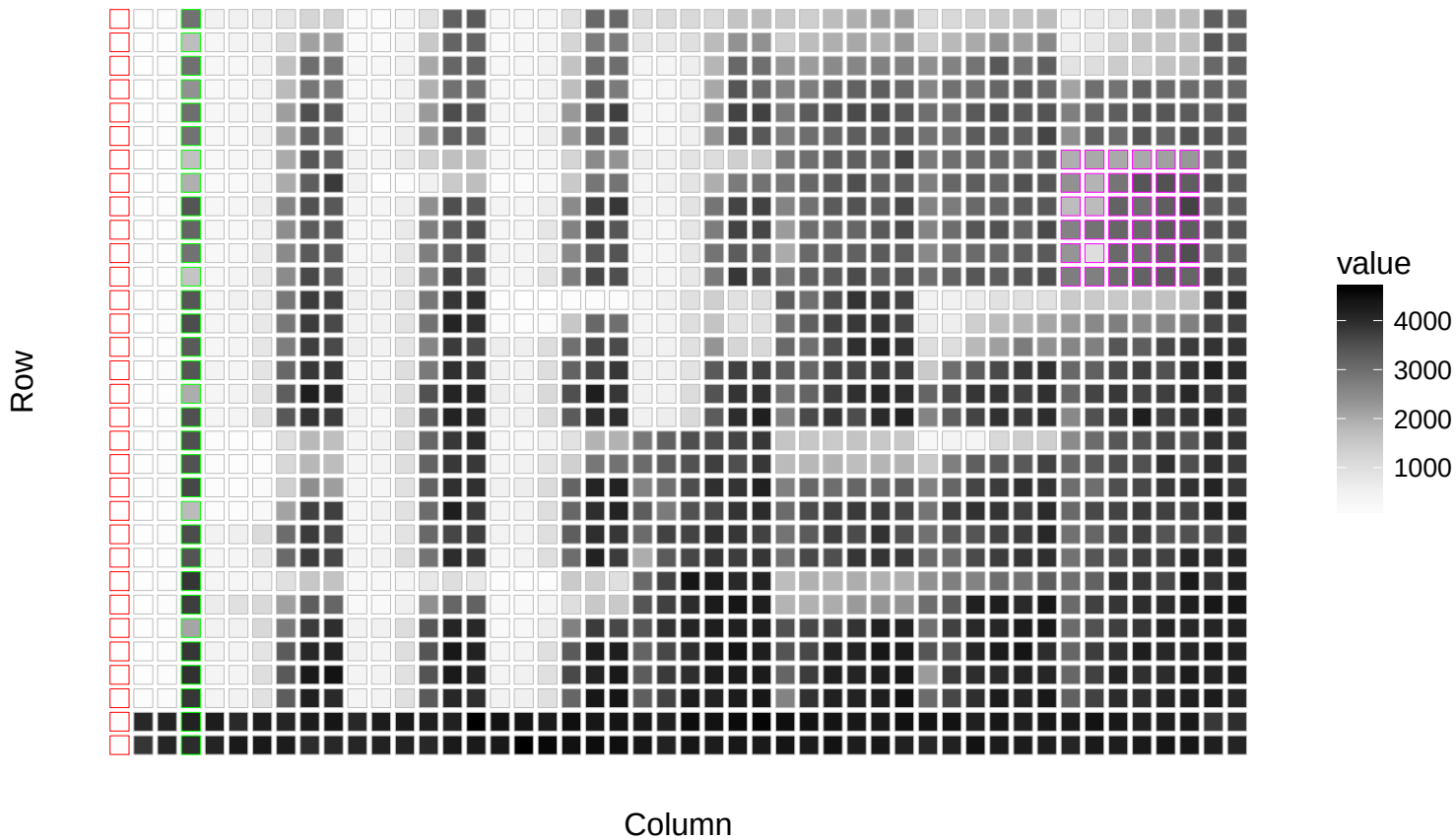
Block 102 (M8900102-T5510690)



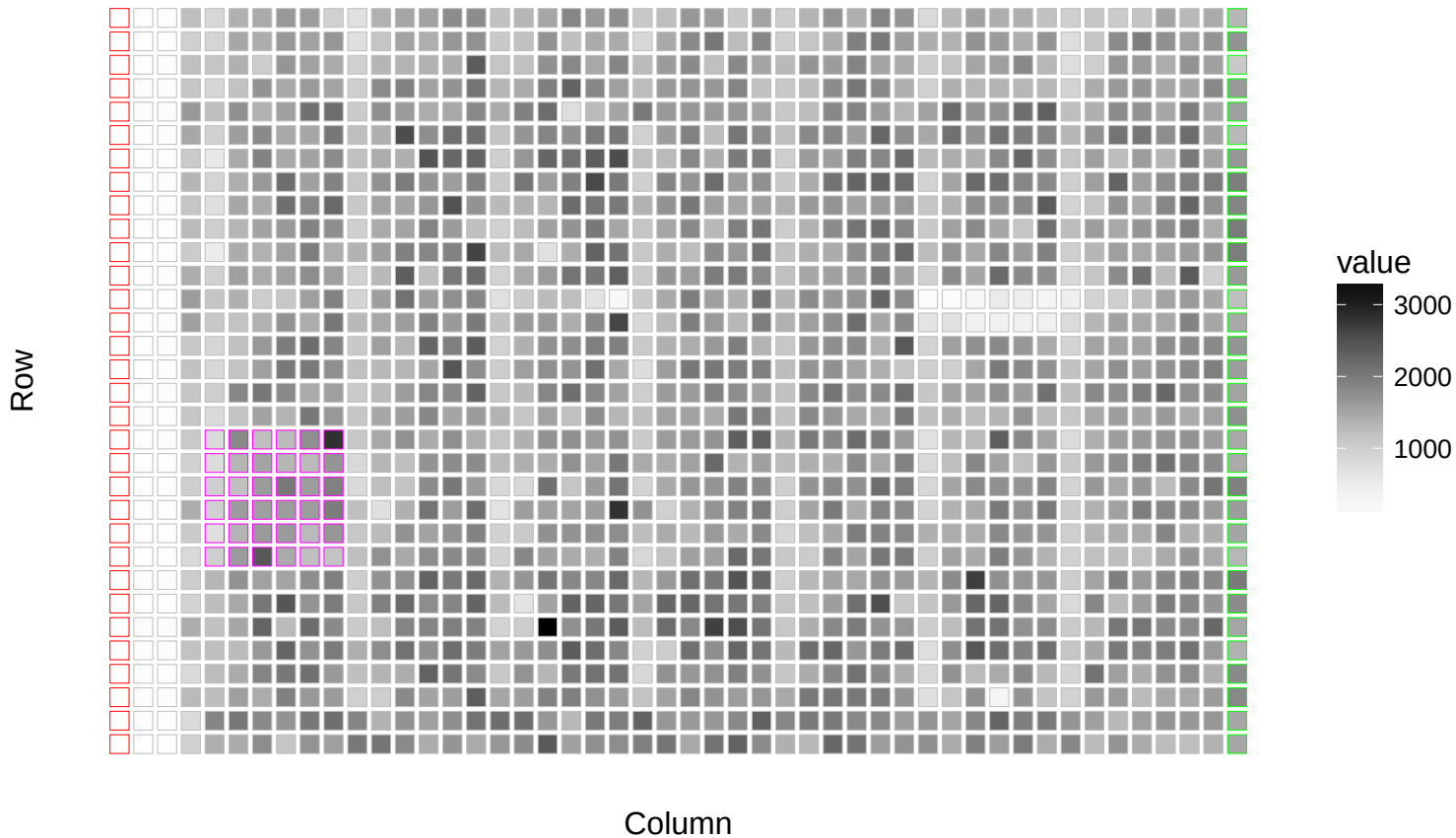
Block 103 (T5574272-T5574272)



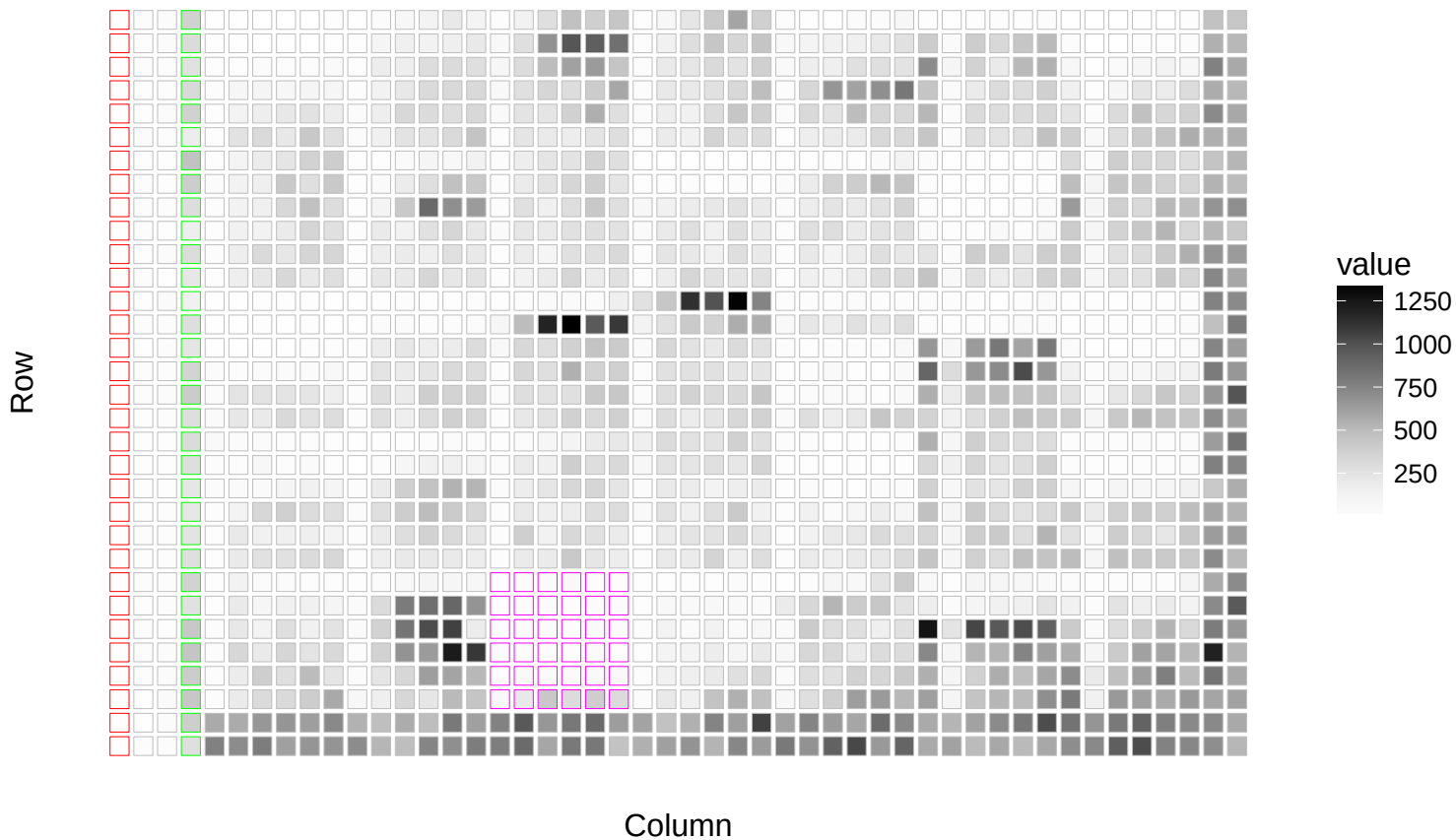
Block 104 (T5606792-T5606792)



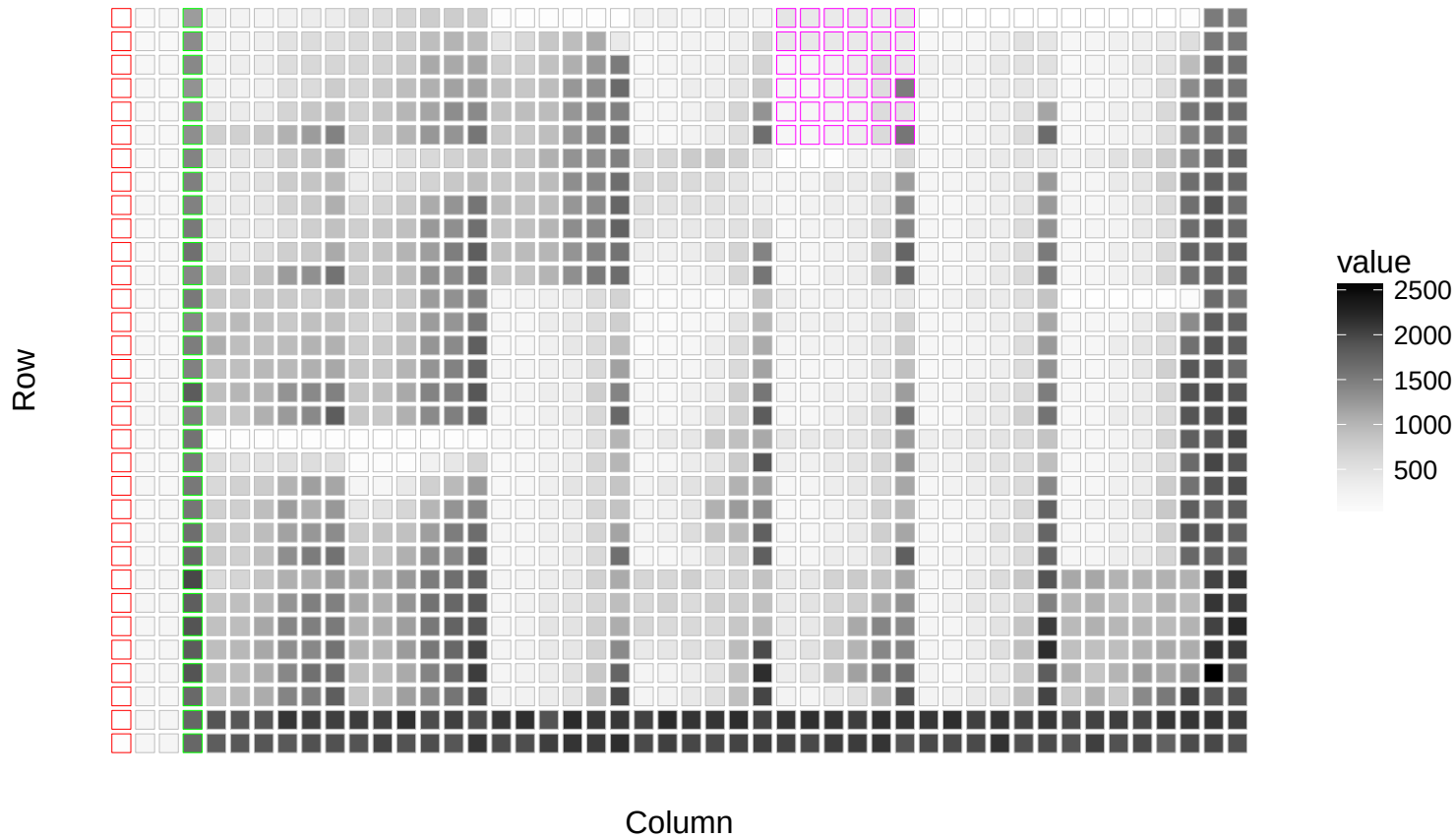
Block 105 (T5574254–T5574254)



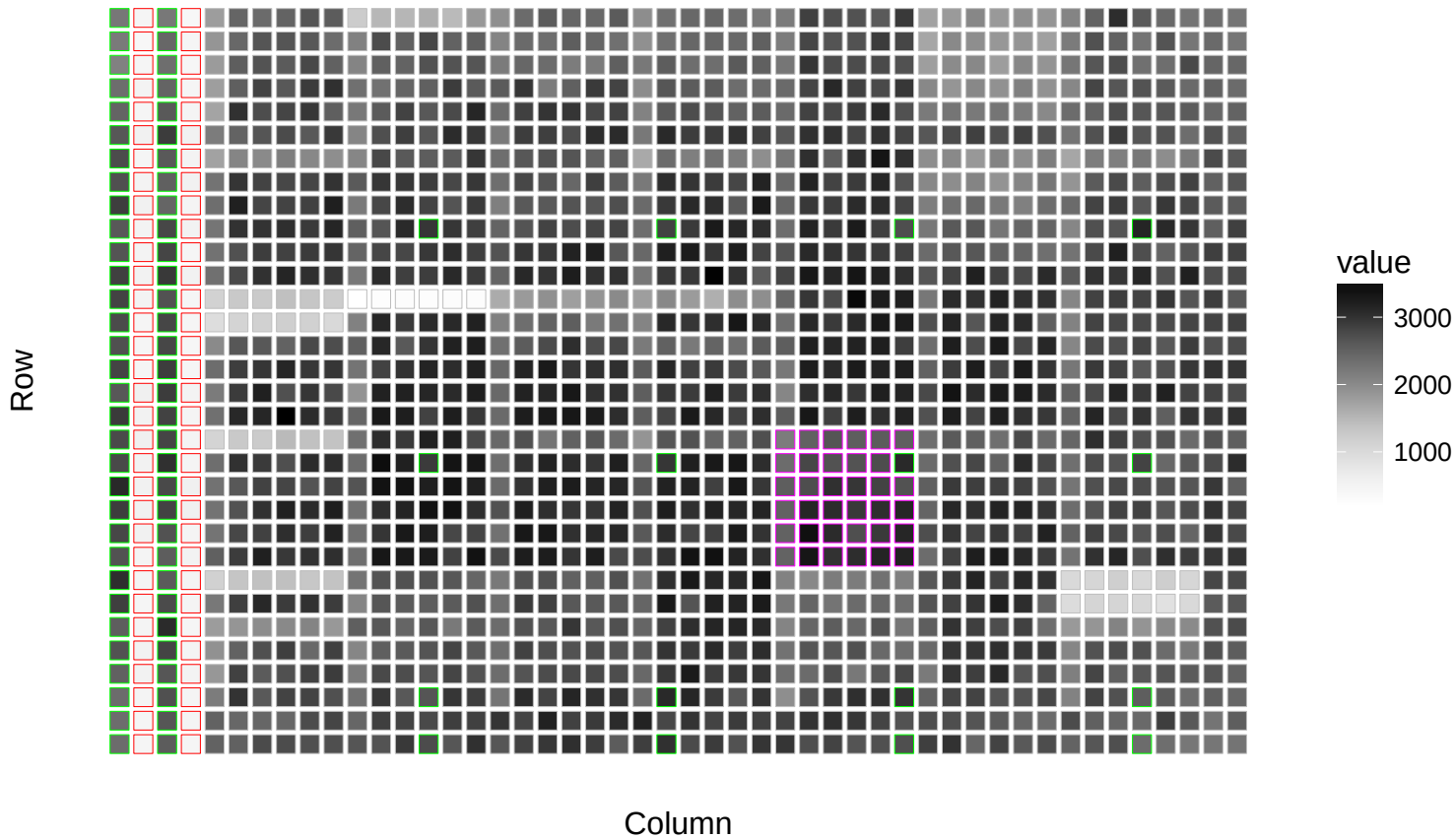
Block 106 (M1020008-T5571446)



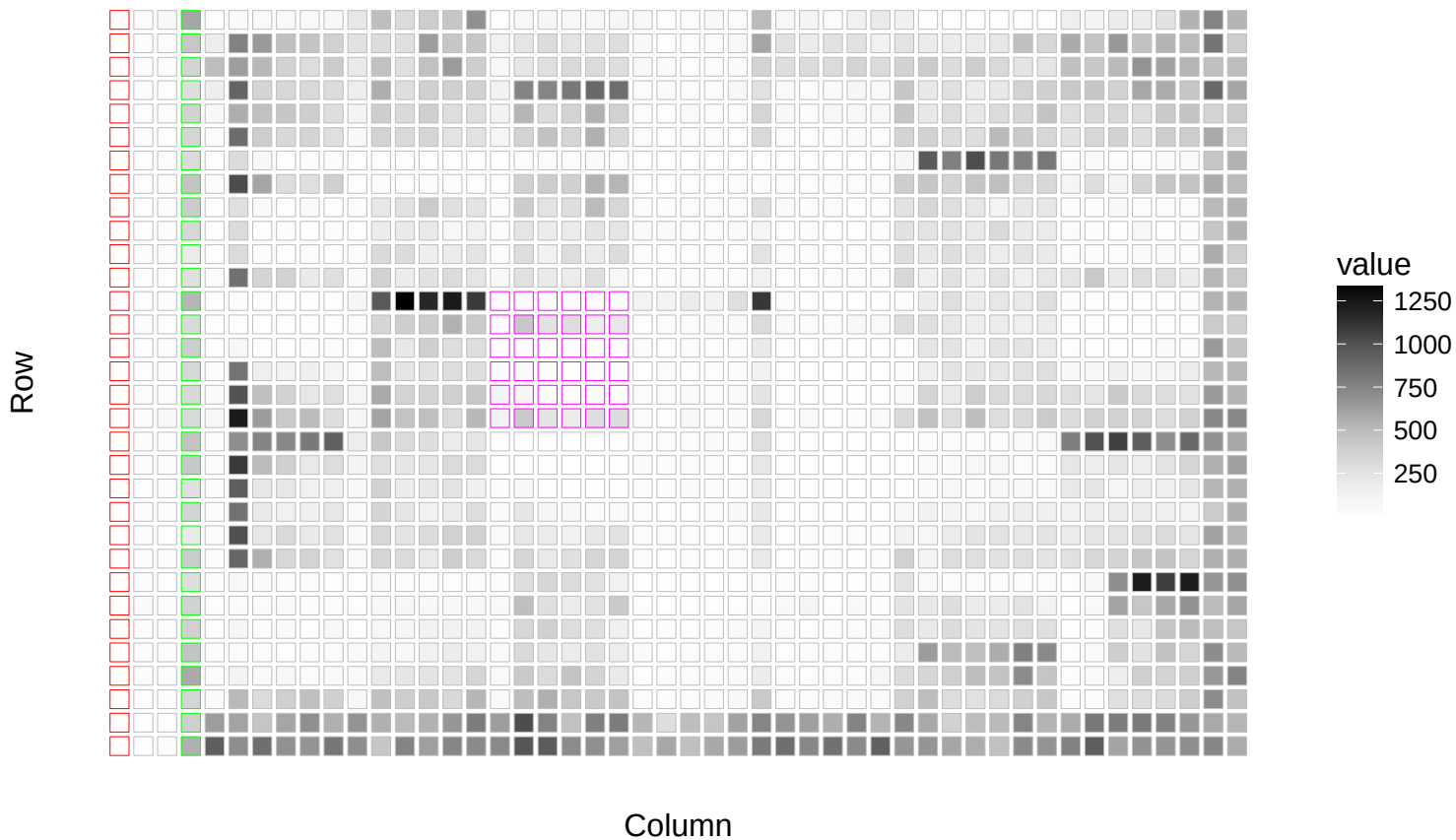
Block 107 (T5622508-T5622508)



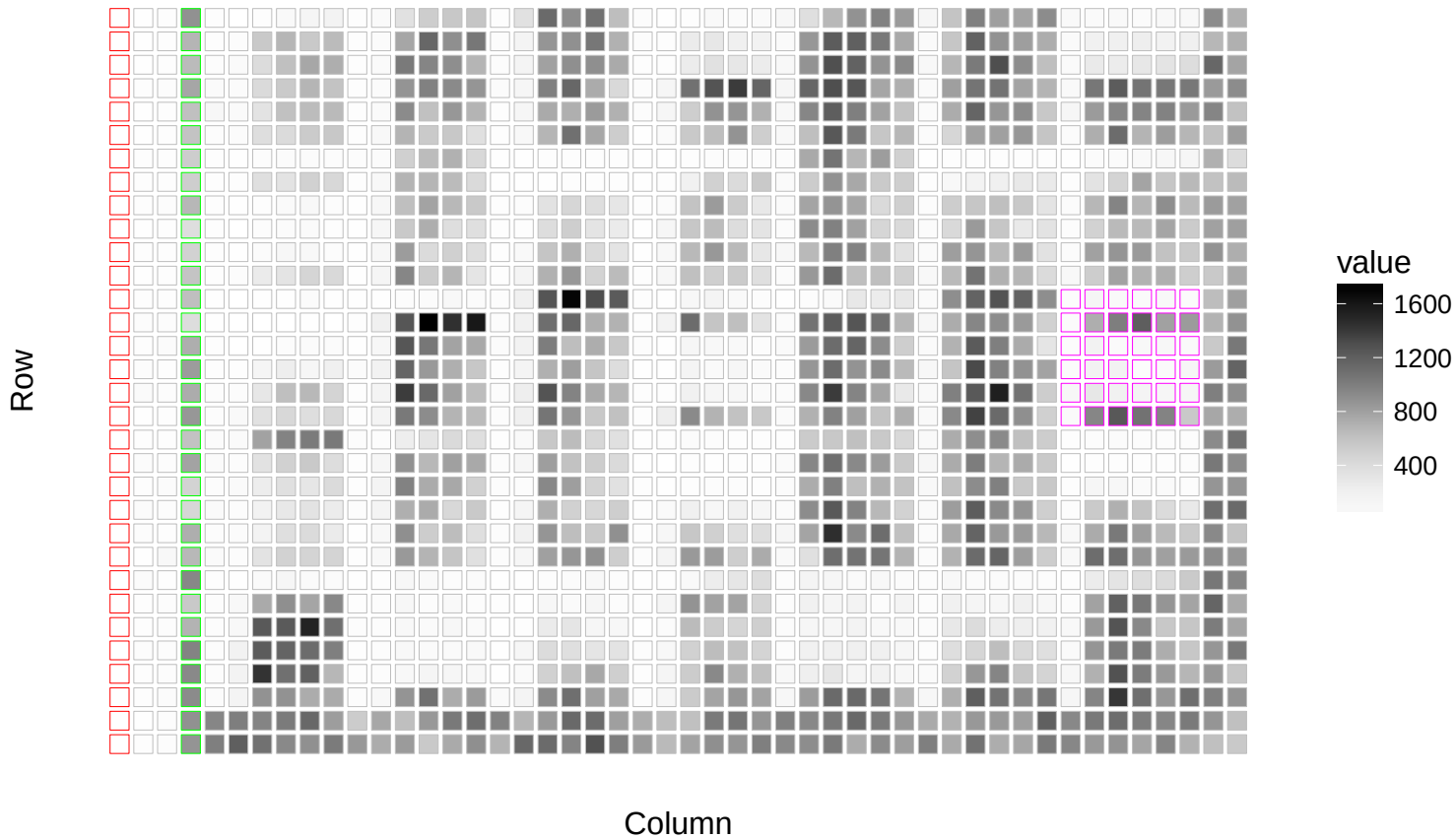
Block 108 (M1400012-T5436672)



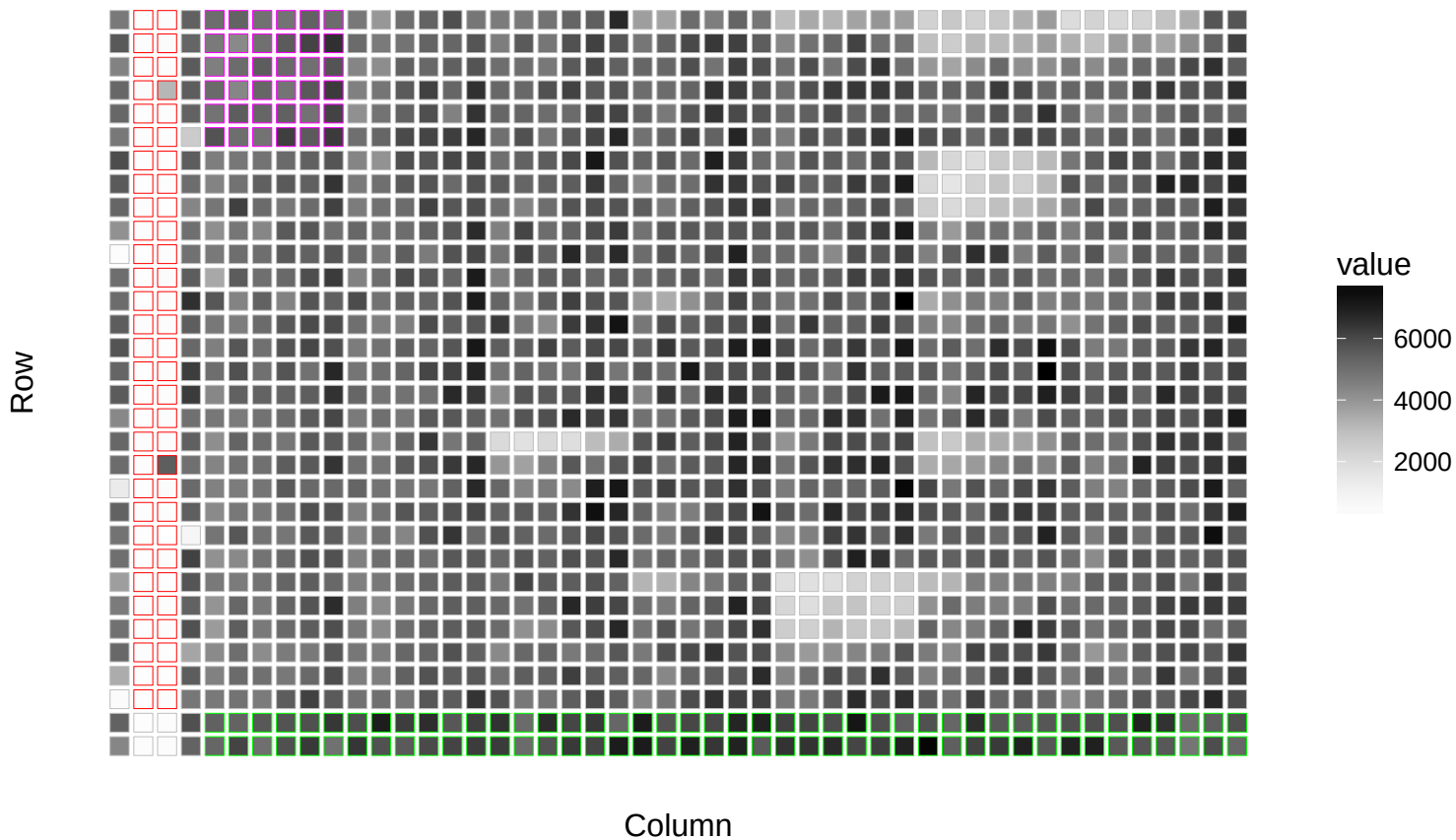
Block 109 (M1020032-T5571468)



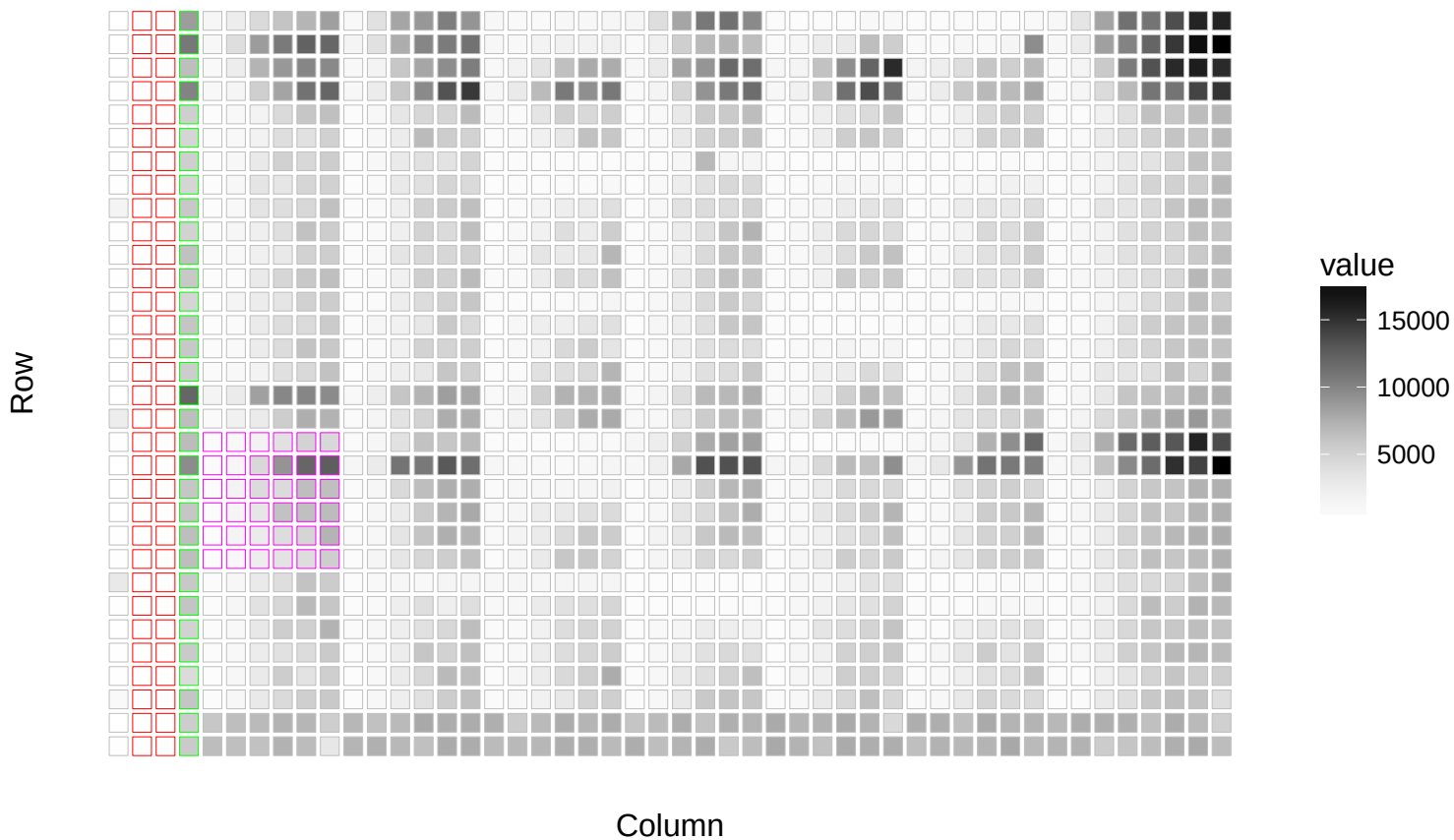
Block 110 (M1020028-T5571472)



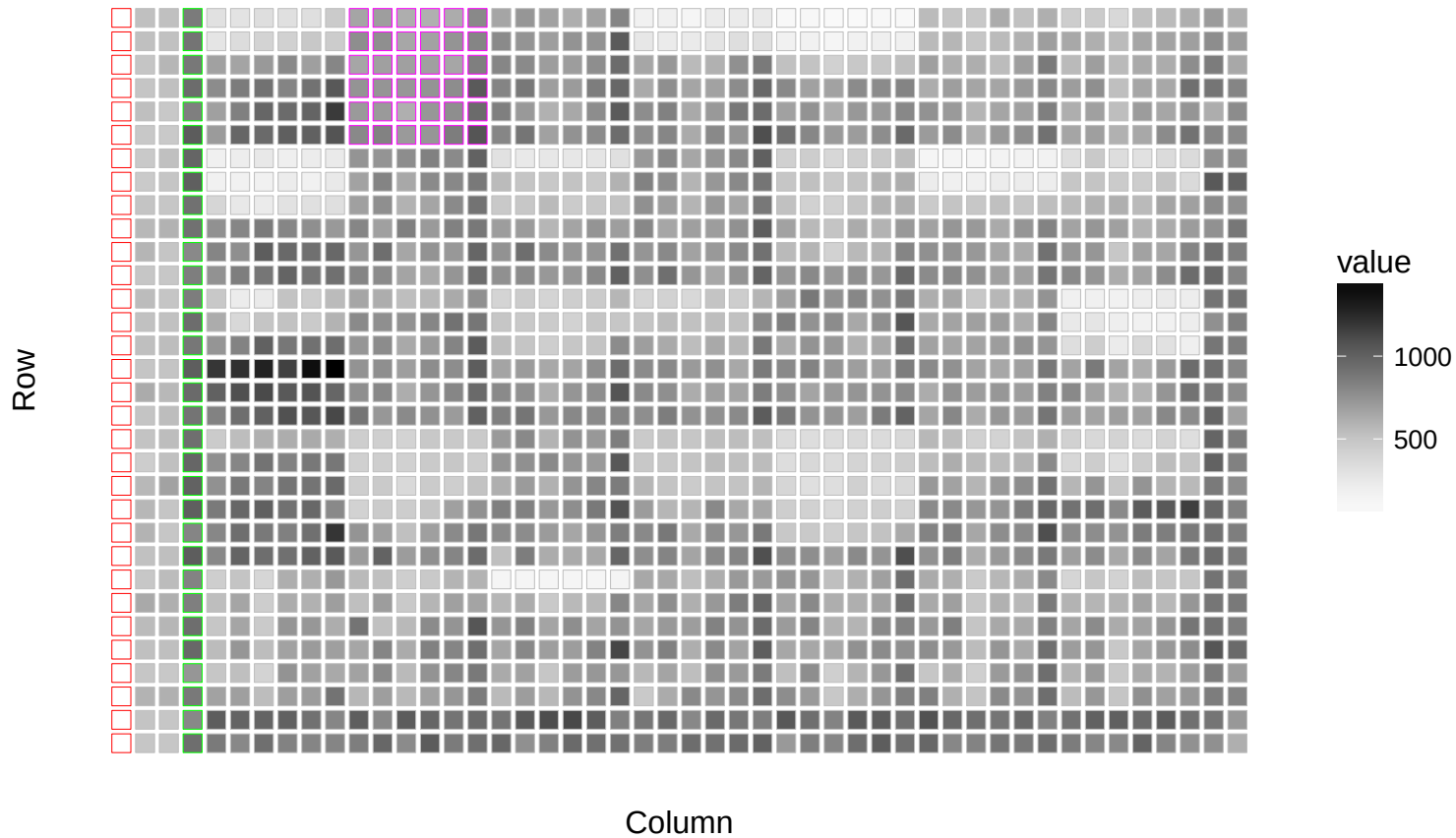
Block 111 (M8900078-T5510692)



Block 112 (T5570448–T5570448)

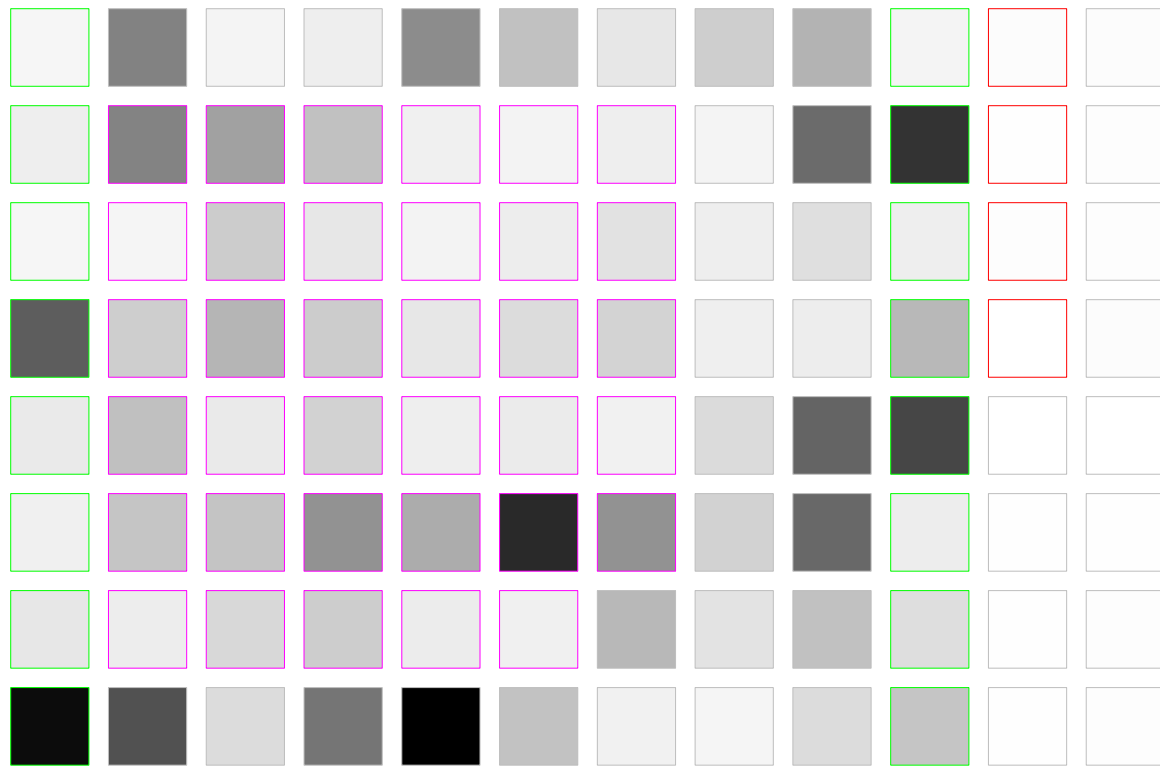


Block 113 (T5615536-T5615536)

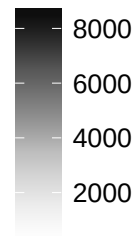


Block 114 (E2000068-E2000068)

Row

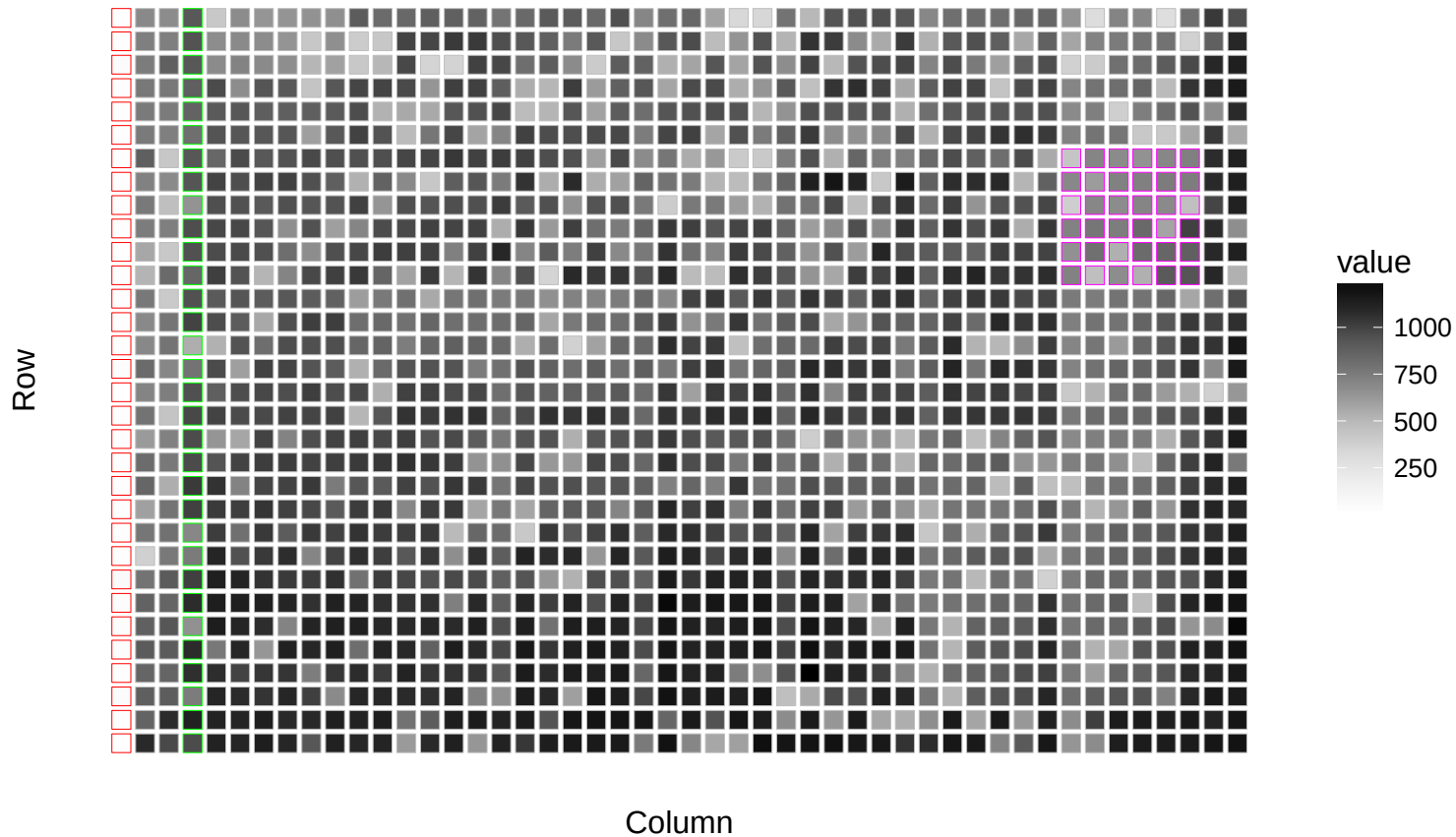


value

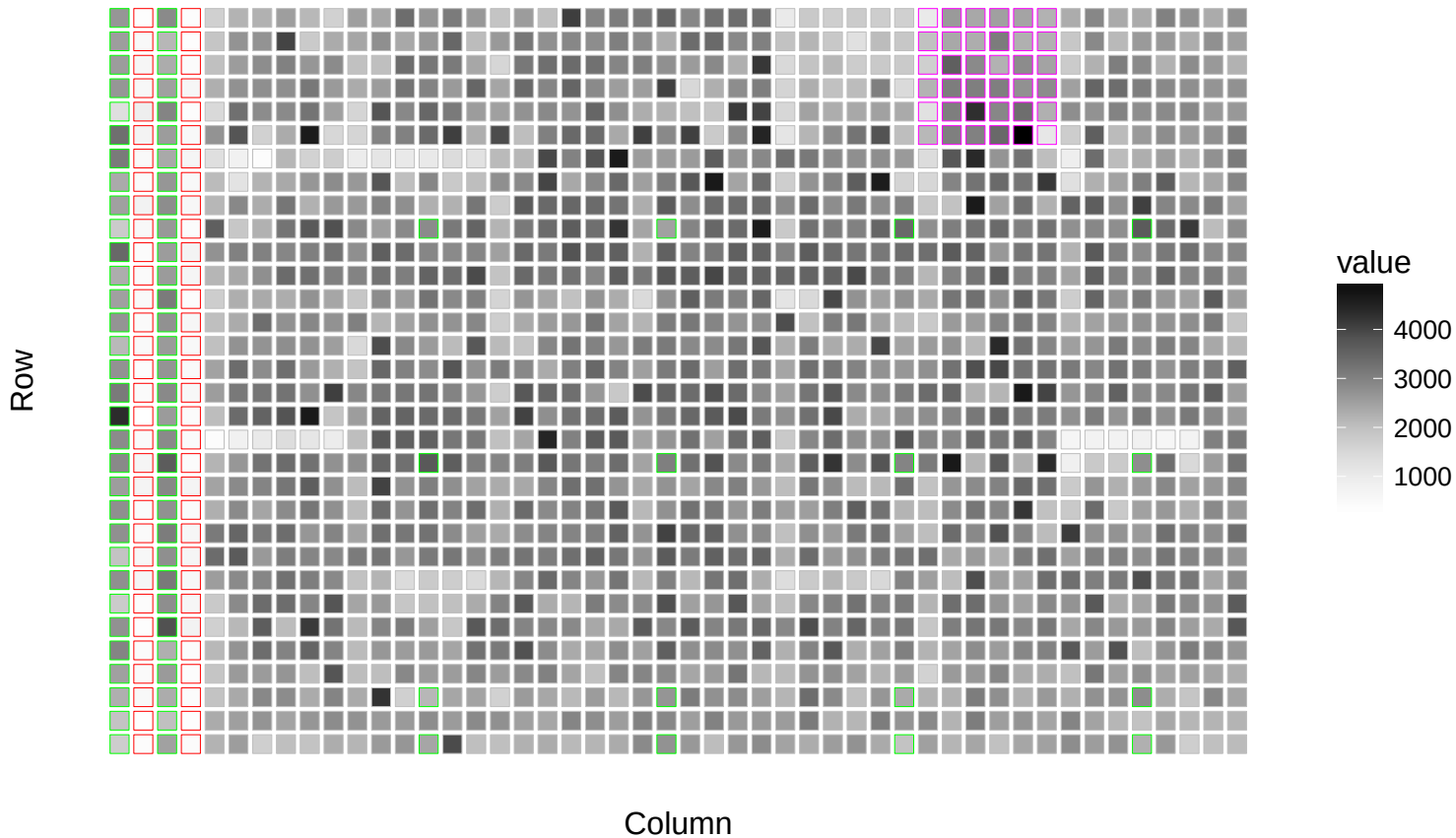


Column

Block 115 (T5614980-T5614980)

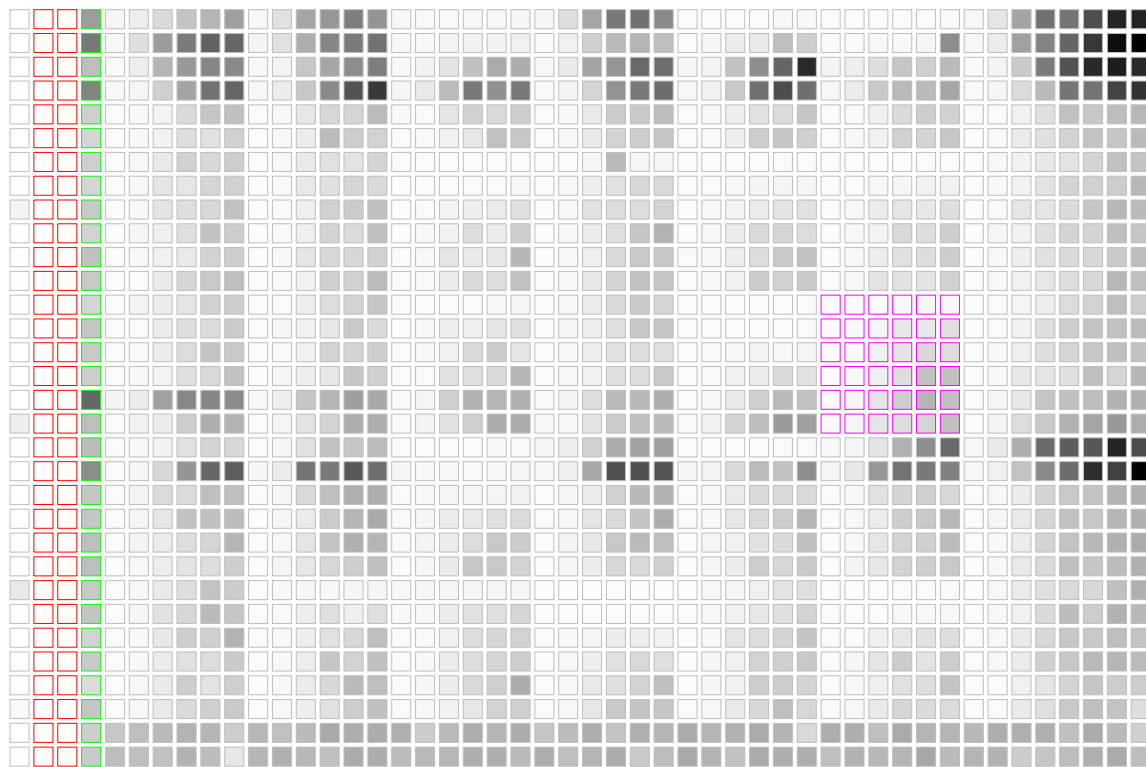


Block 116 (M2200010-T5436640)



Block 117 (T5570448–T5570448)

Row



value



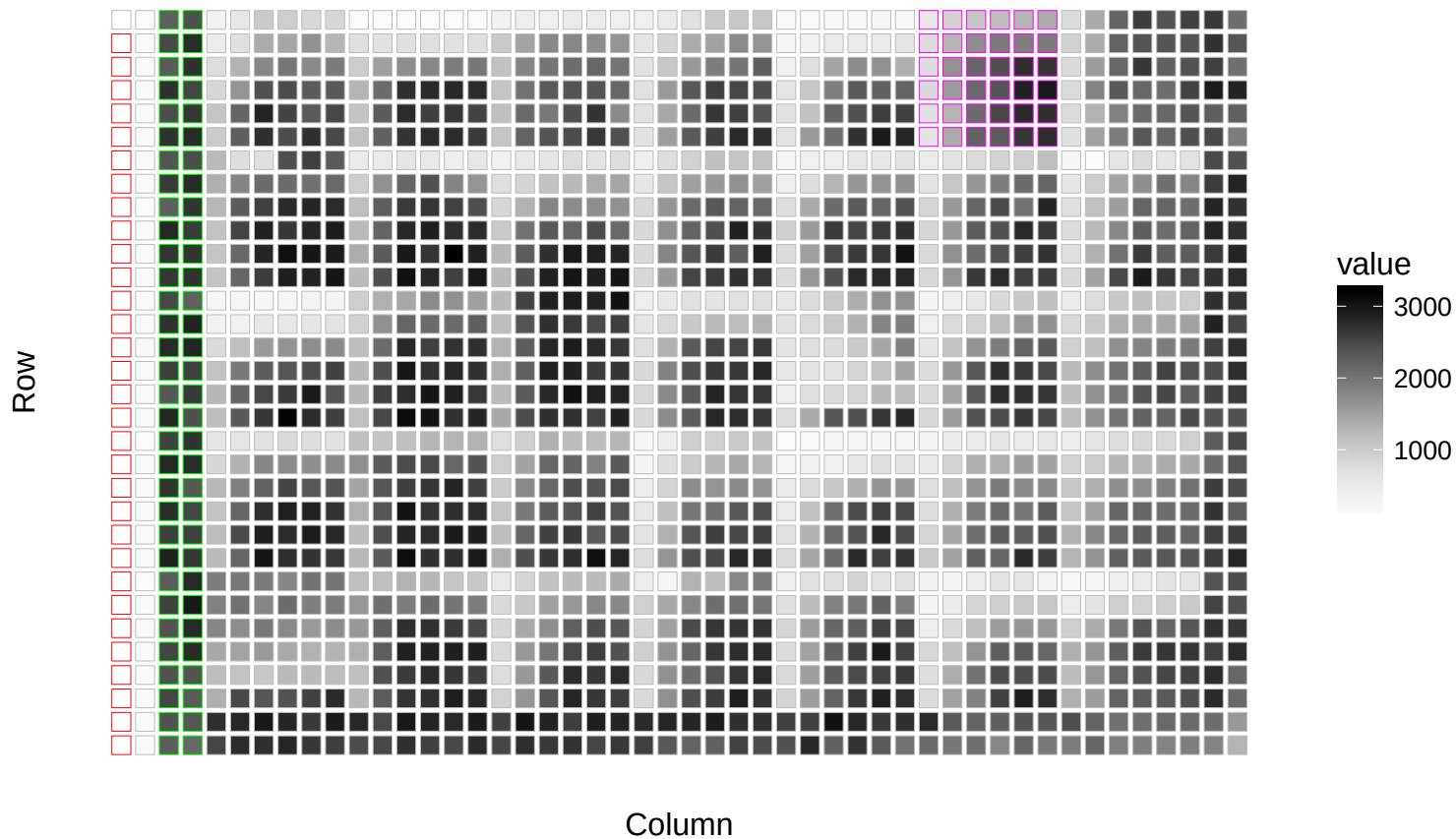
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10000

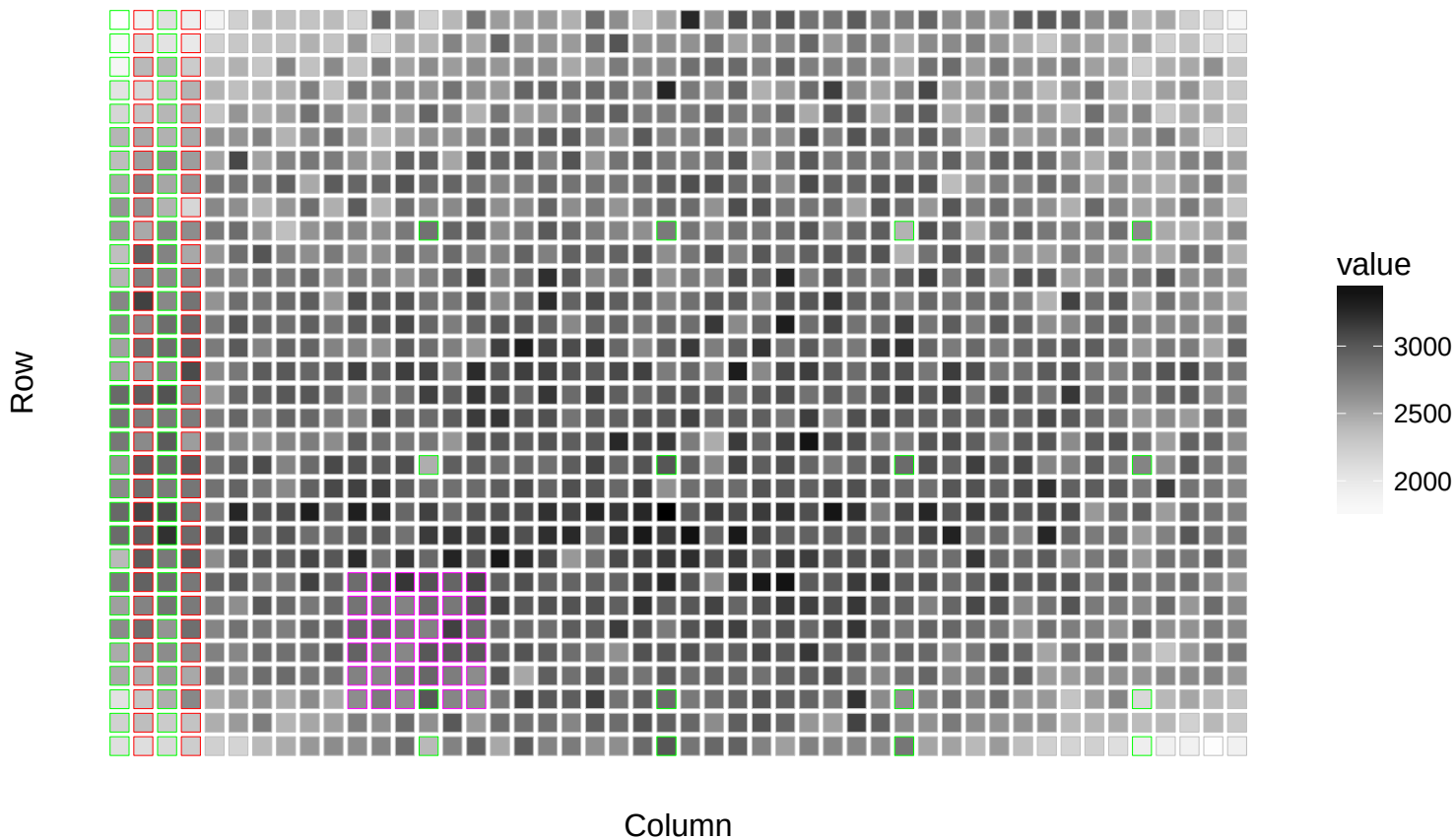
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Column

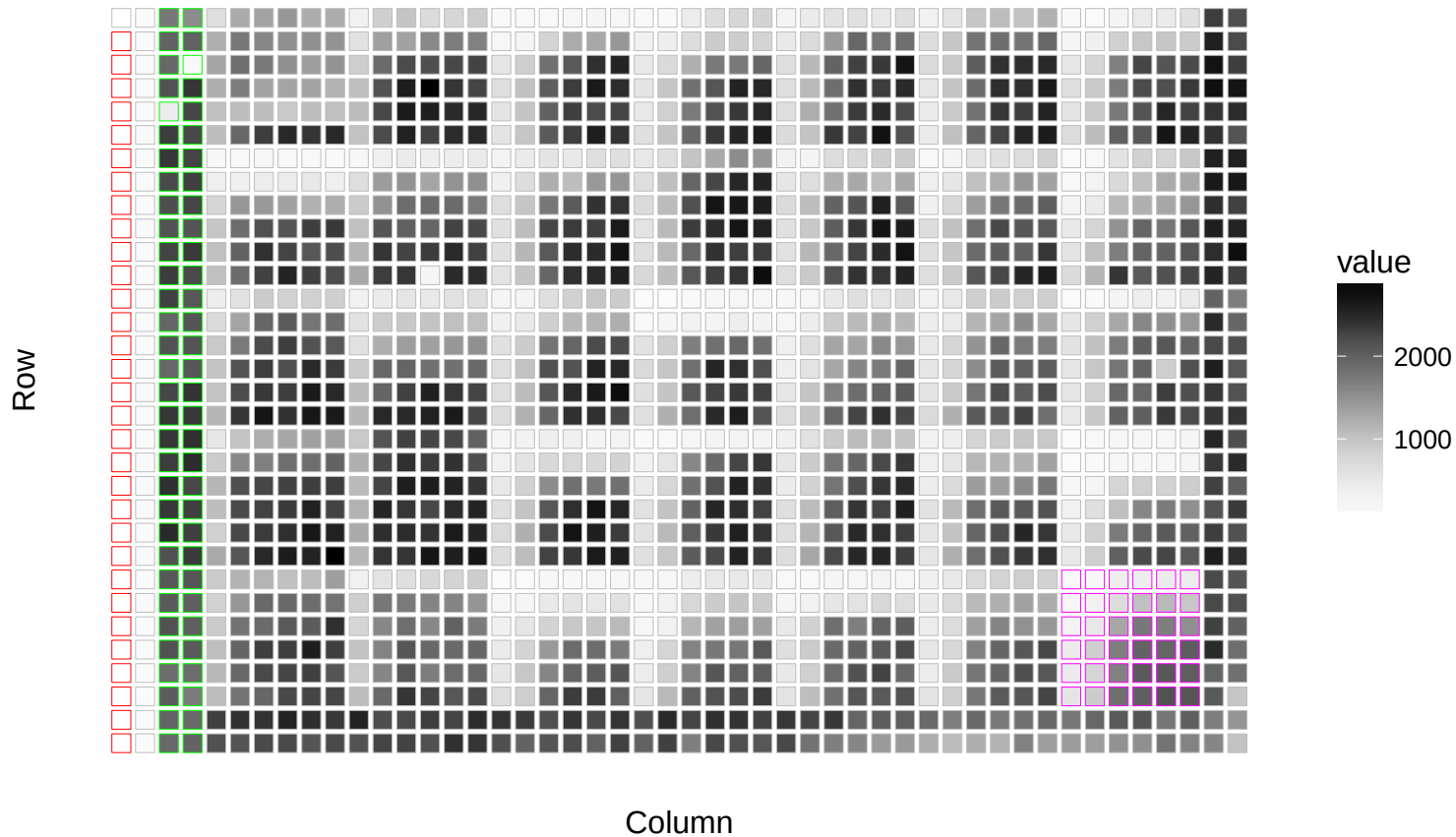
Block 118 (M9900004-T5570148)



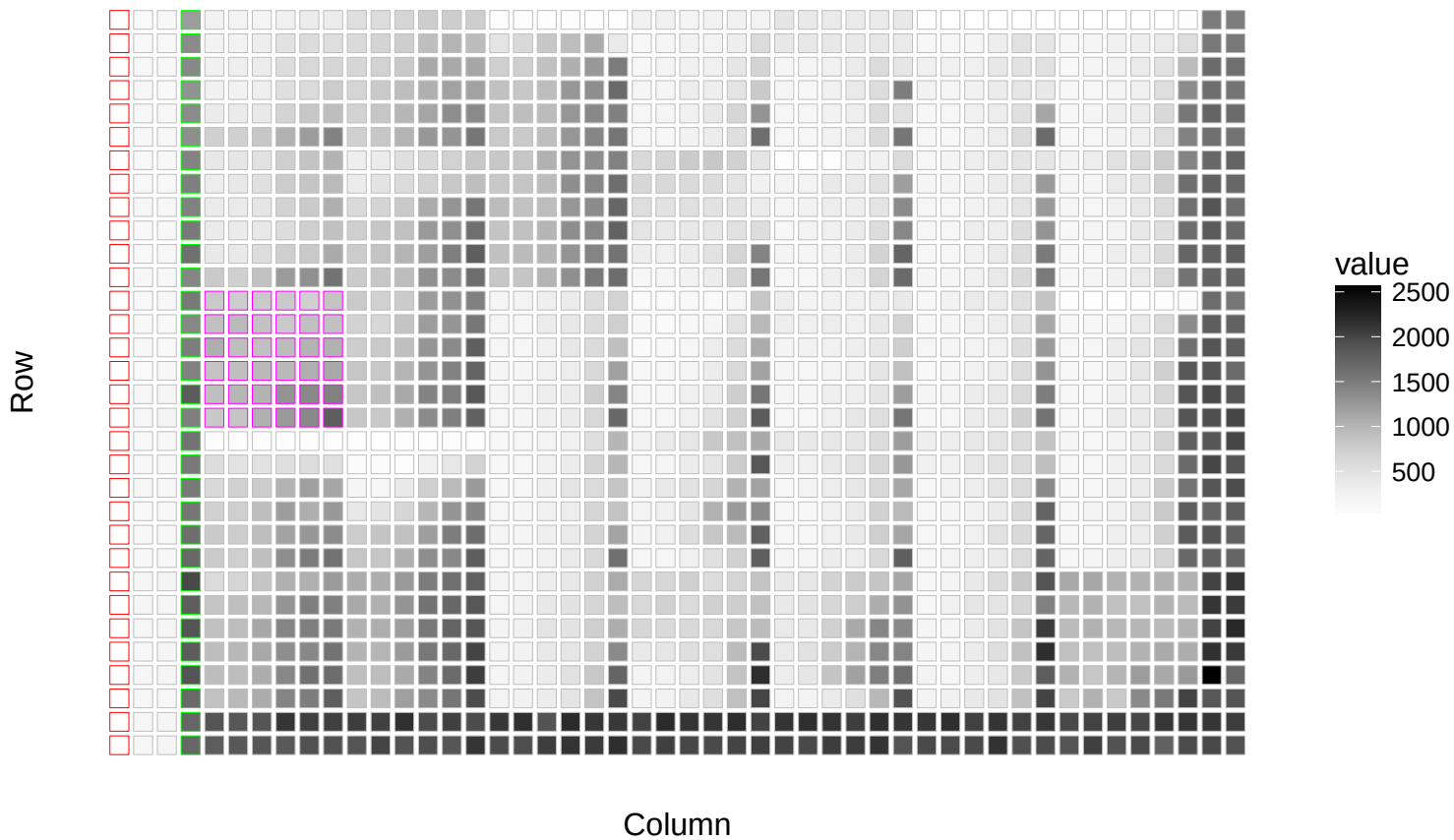
Block 119 (M1400026-T5436718)



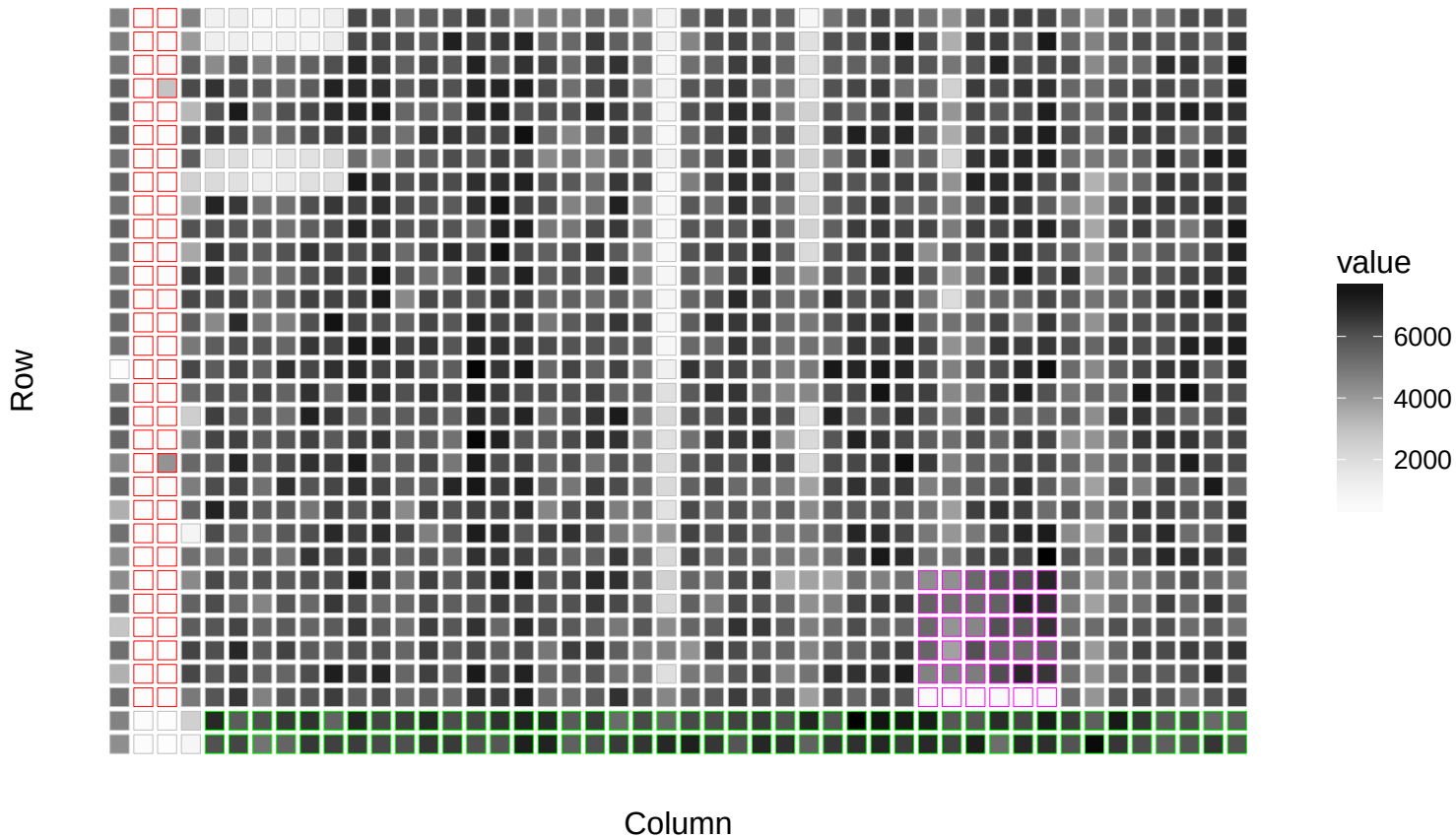
Block 120 (M9900048-T5574670)



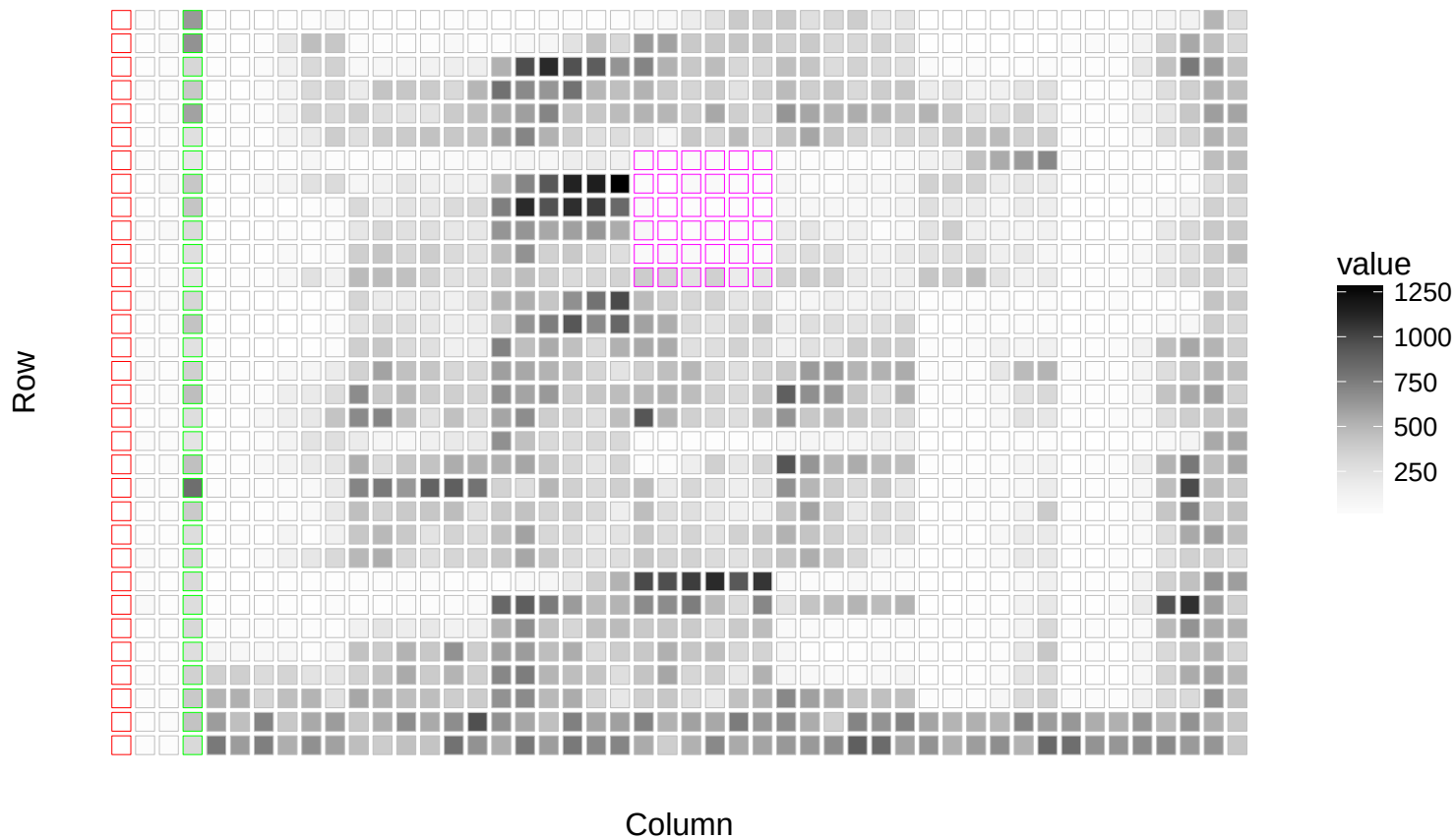
Block 121 (T5622508-T5622508)



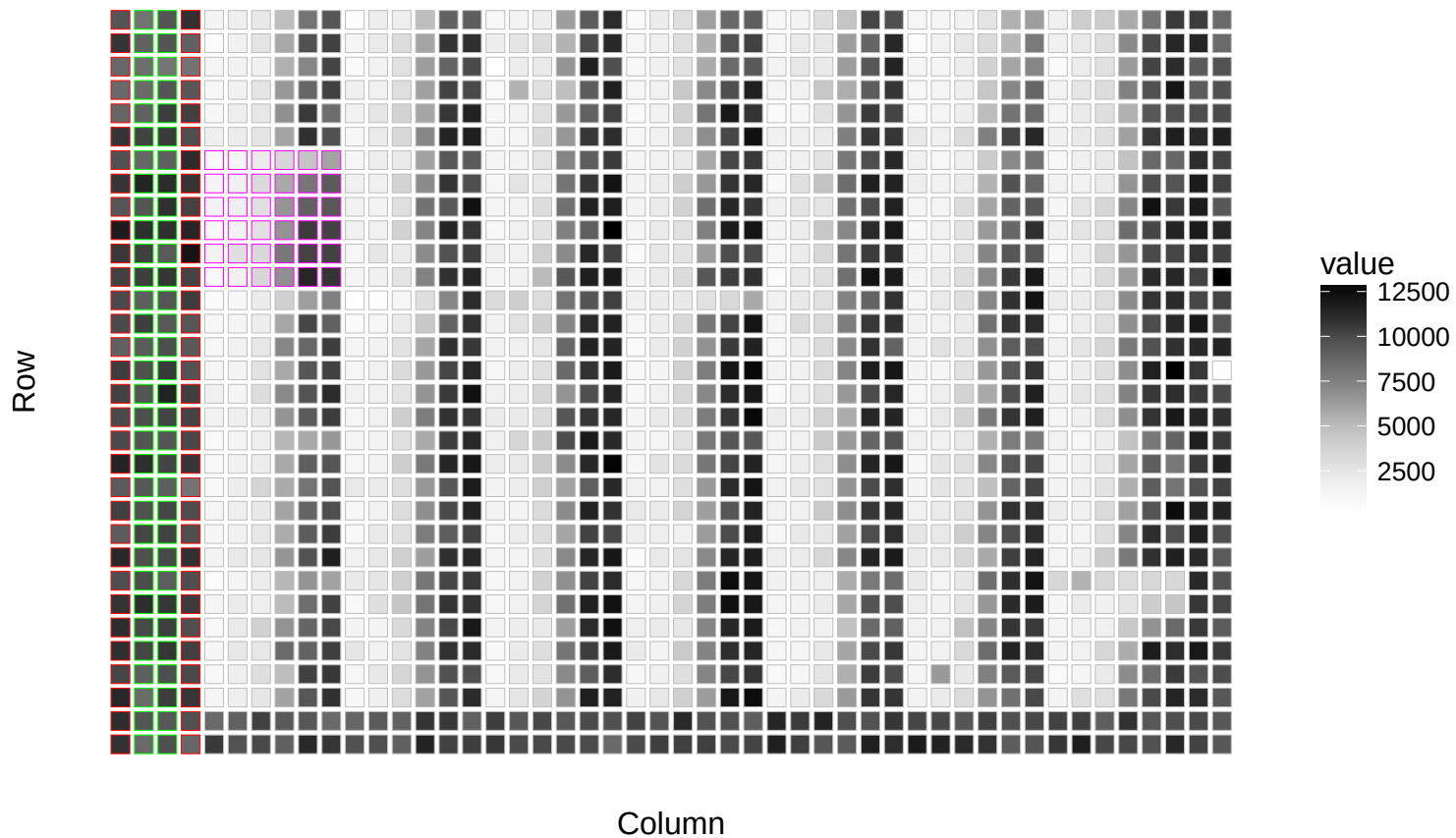
Block 122 (M8900088-T5510634)



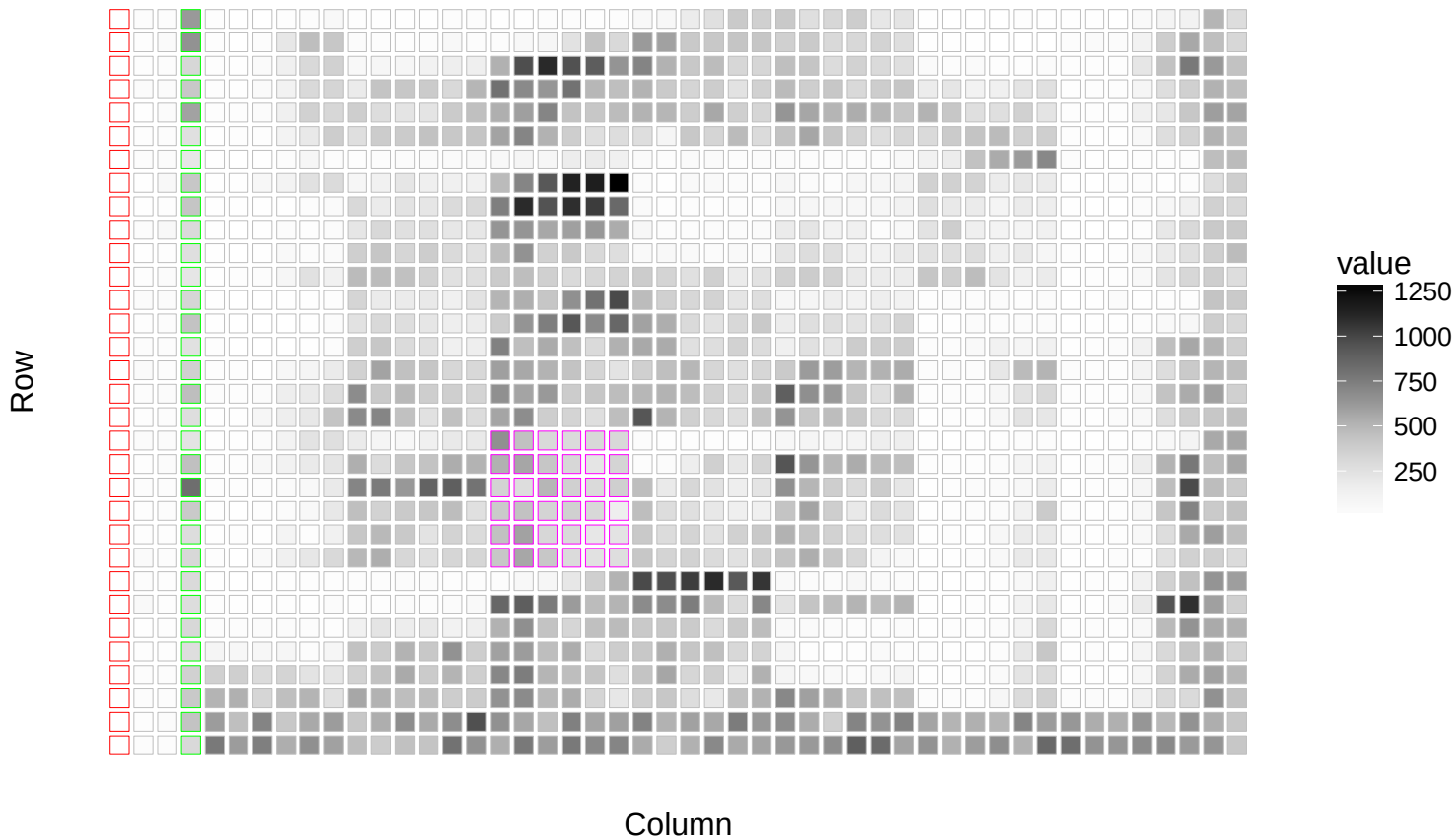
Block 123 (M1020020-T5571458)



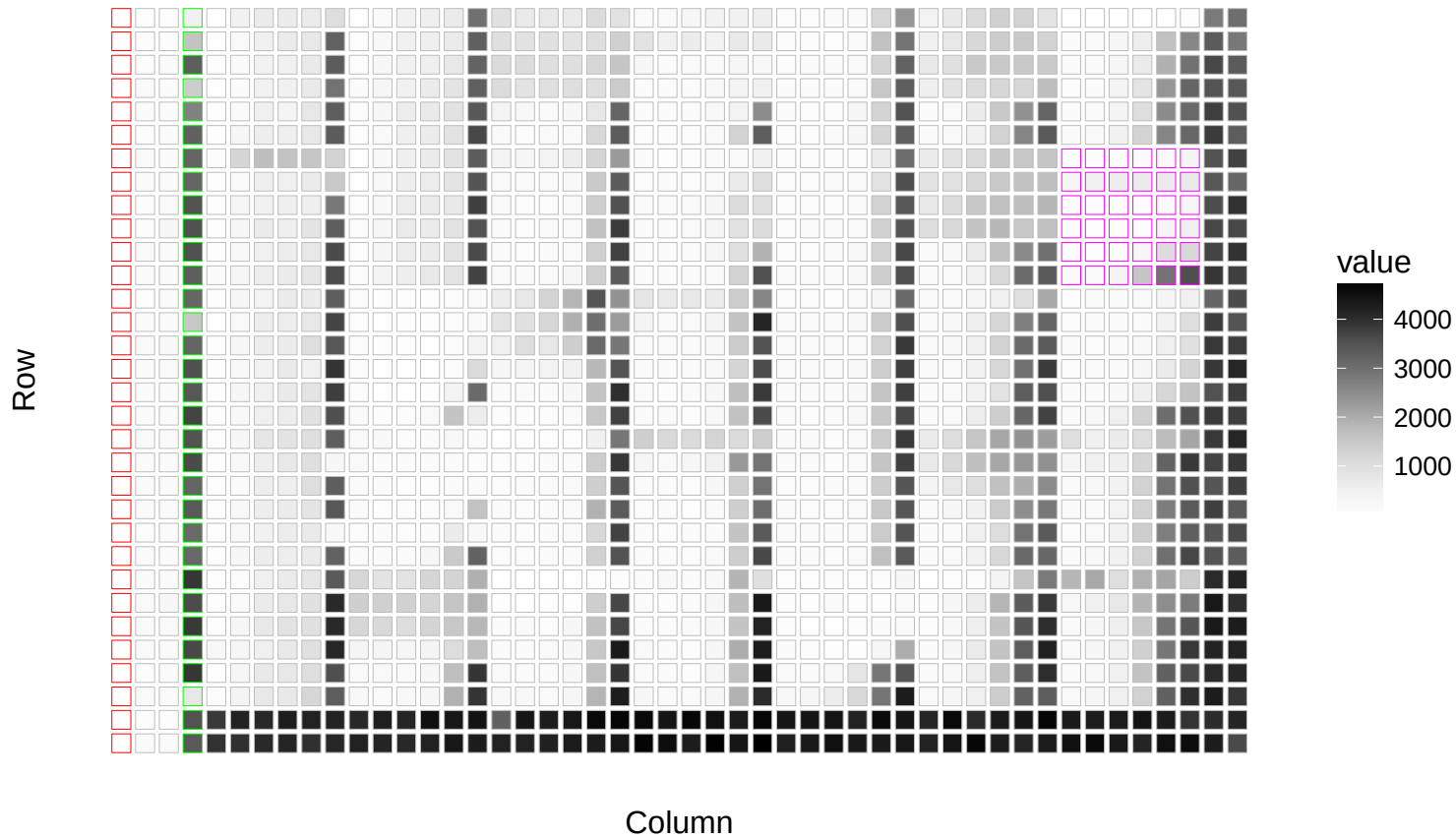
Block 124 (M7500040–T5516214)



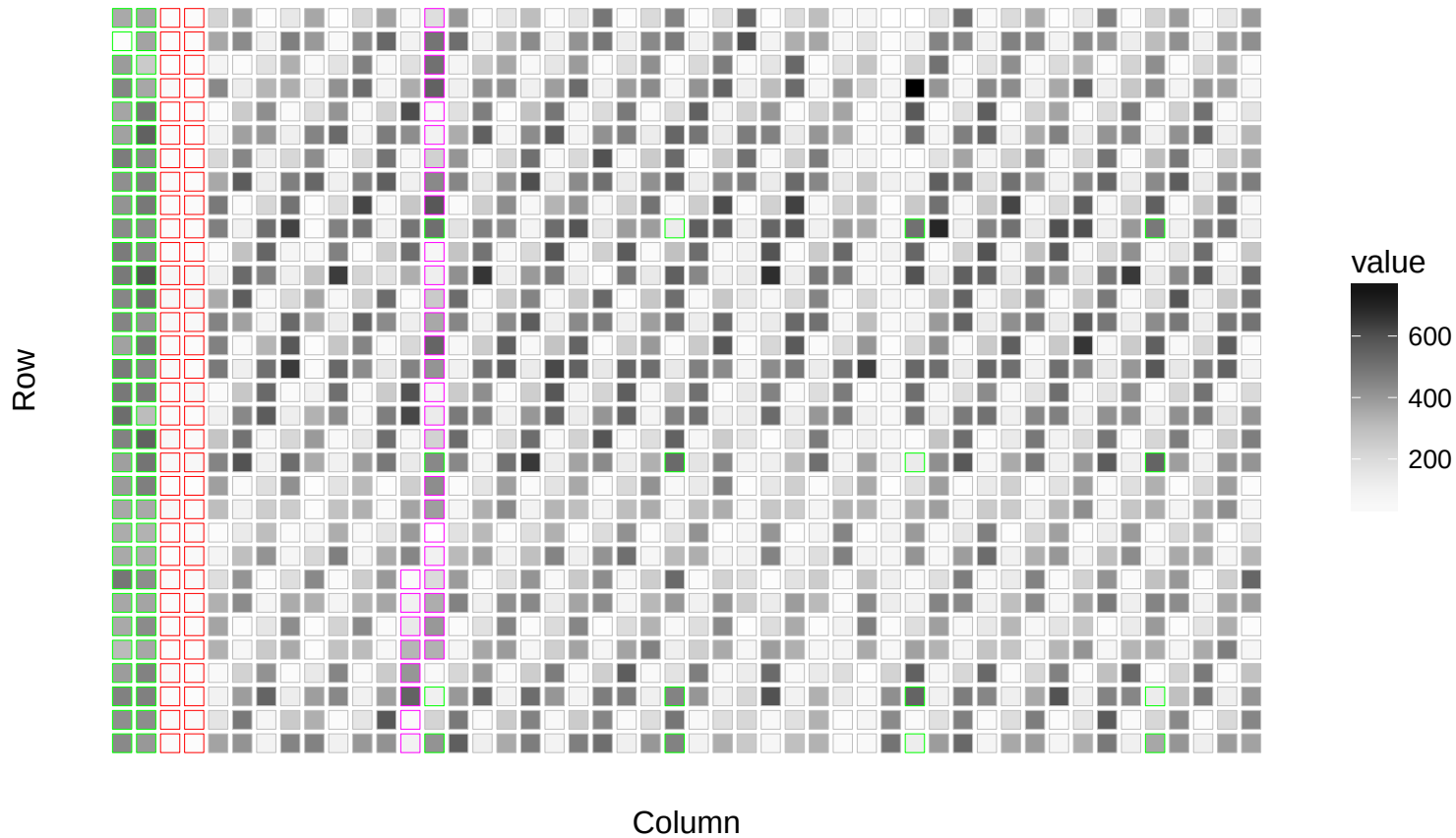
Block 125 (M1020020-T5571458)



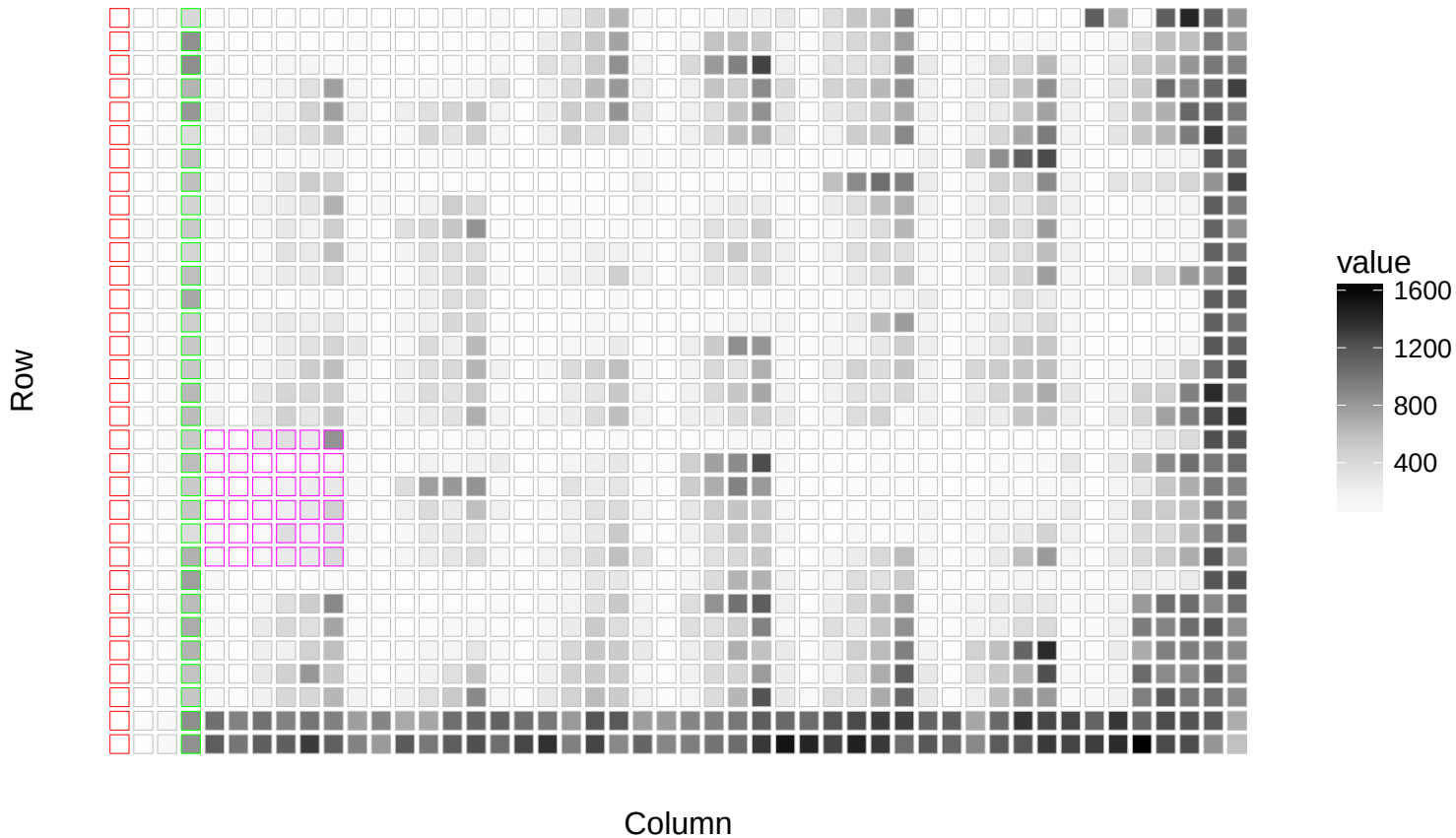
Block 126 (T5614758-T5614758)



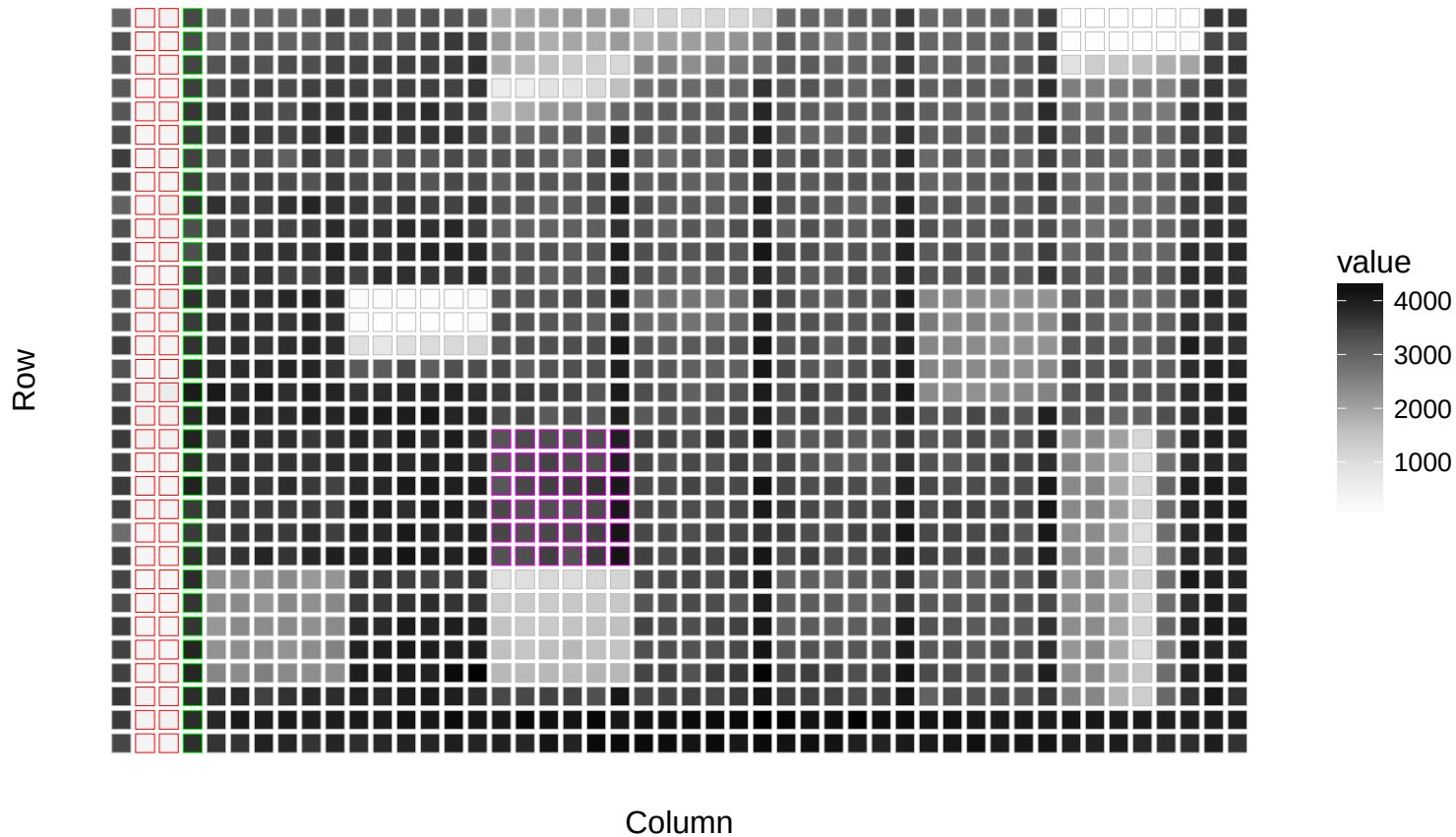
Block 127 (M0300032-T5423732)



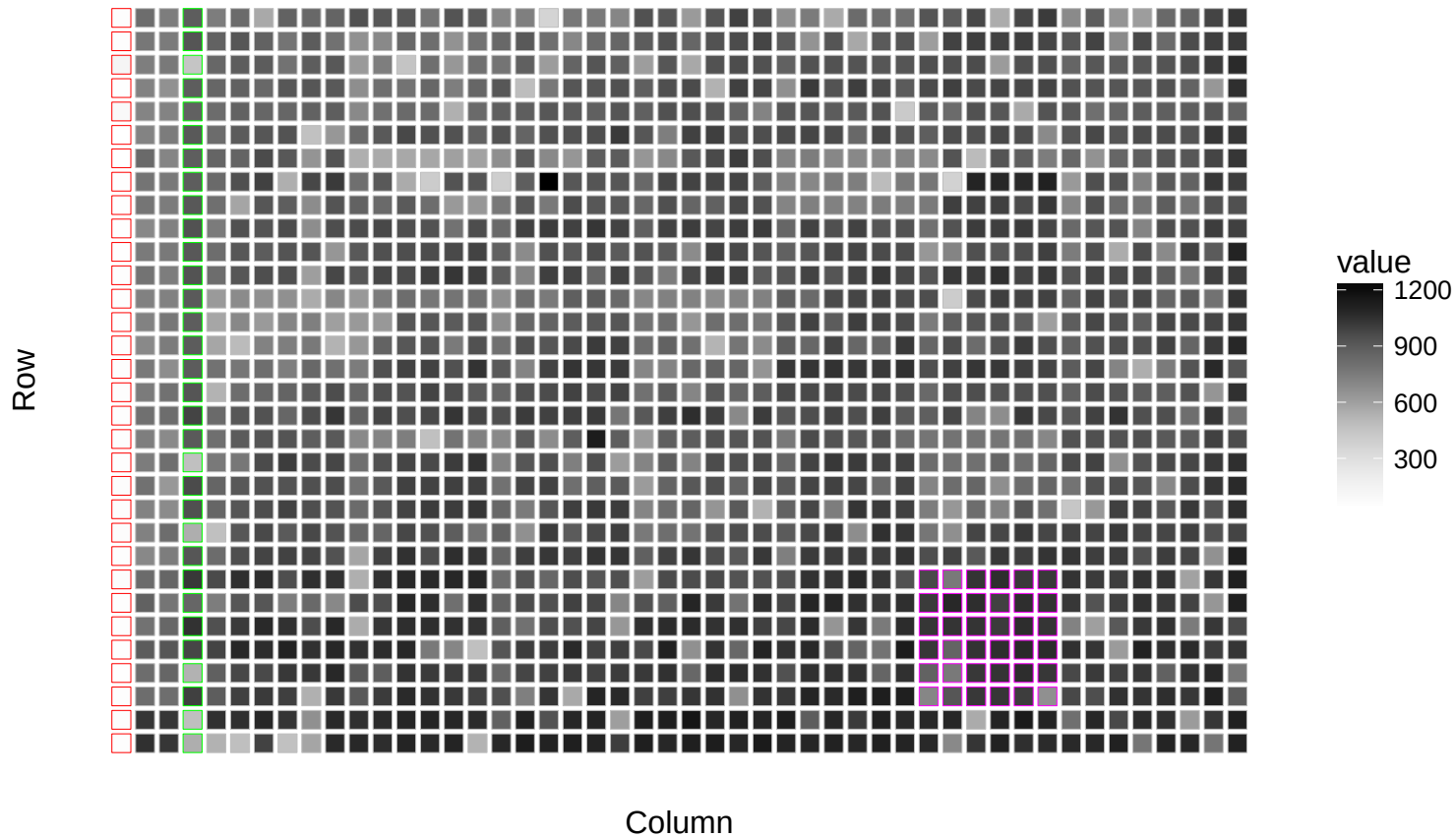
Block 128 (M1020002-T5571452)



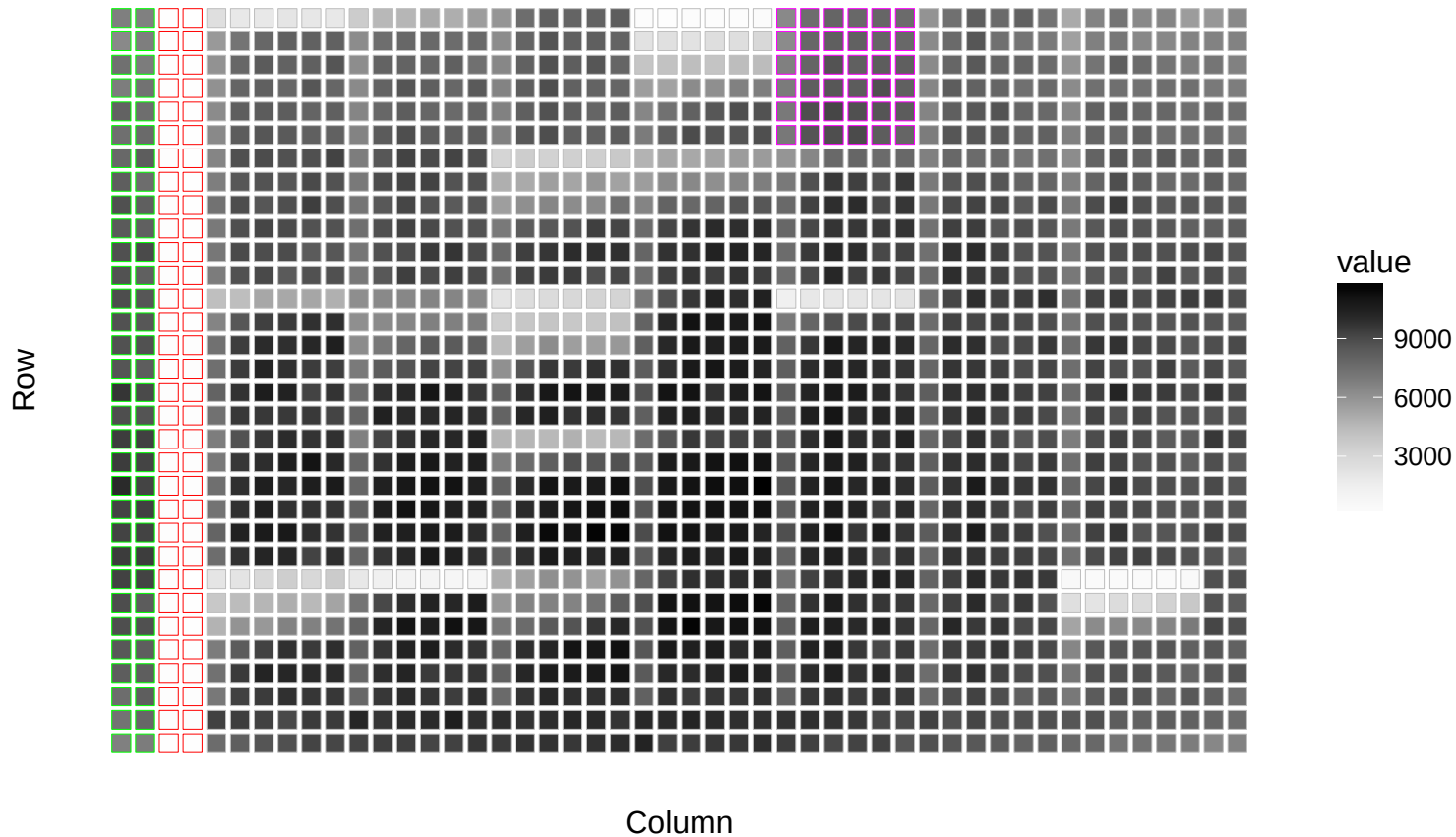
Block 129 (T5666294–T5666294)



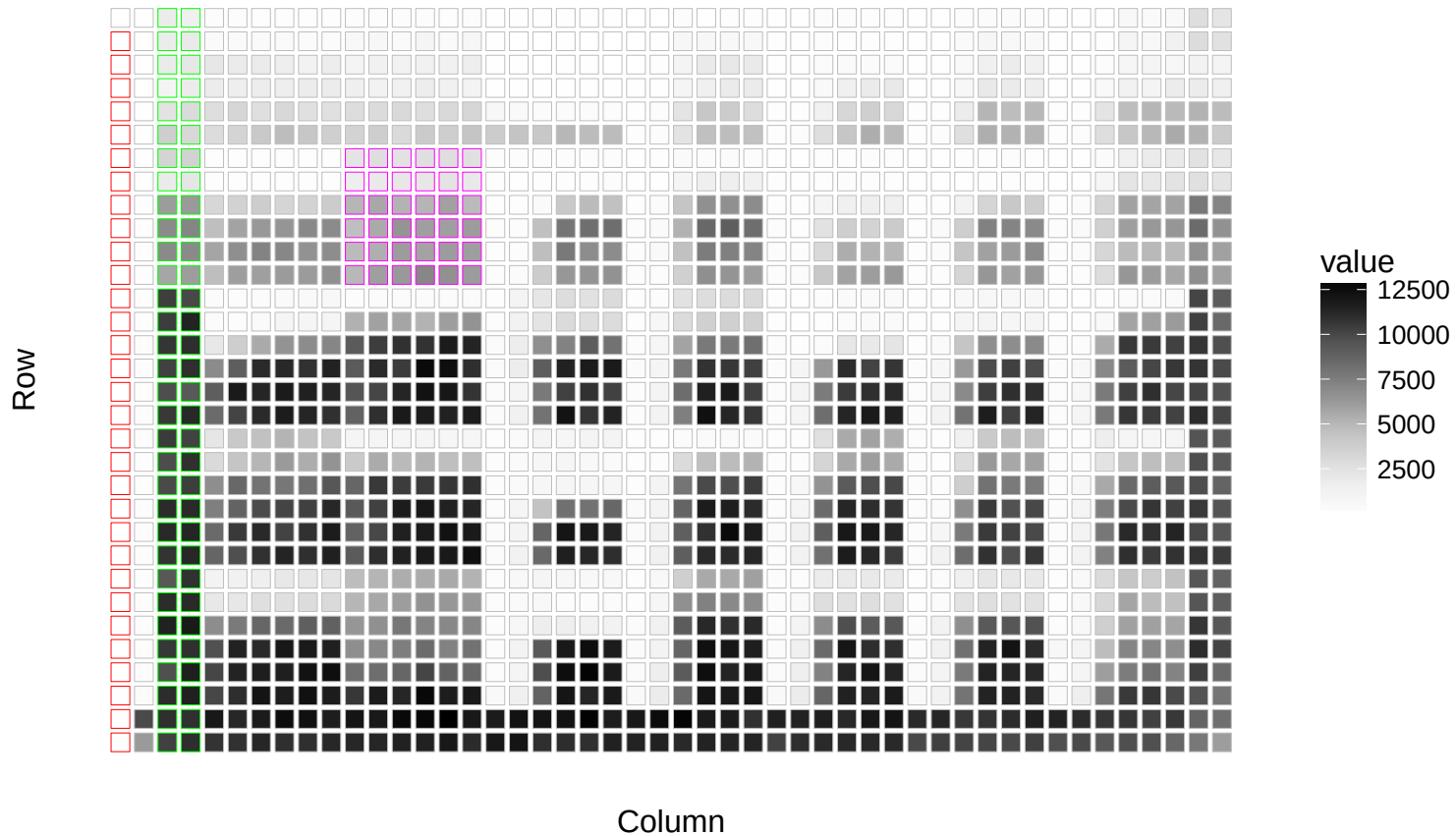
Block 130 (T5616662-T5616662)



Block 131 (M7900006-T5512018)



Block 132 (M9900032-T5574642)



Block 133 (T5622538-T5622538)

