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Correlation Queries for Mass Spectrometry Imaging

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Abstract

Supplemental material:

1. Pseudocode for the Pearson correlation calculation

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1. Pseudocode to calculate the correlation of two slices:
 - a. Given two “slices,” A and B, of the mass-spectrometry imaging data set, each consisting of a rectangular array of “pixels” corresponding to scan points, and the value at each pixel representing the total ion count in some small range of m/z
 - b. Find mean of all pixel intensities in SliceA and SliceB
 - c. Subtract the mean from each pixel value of each slice so the mean intensity of each slice is zero
 - d. Find the sum of the squares of each slice
 - e. Divide each pixel by the sum of squares in (d) so the “norm” of each slice is one
 - f. The correlation is then the dot product of the two slices, or the sum of the products of each pixel in A with the corresponding pixel in B
 - g. The correlation will range from -1 to 1 and is independent of the range of intensity values in each slice. 1 means fully correlated; -1 means anti-correlated.
 - h. If a mask is involved, perform the above calculation but only using the pixels covered by the mask