Screening procedures to study homogeneity in pharmaceutical tablets

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Scope and aim

NIR Chemical Imaging is used, in combination with several Chemometric tools, to obtain chemical sample characteristics. The main problem is that extra information about the tablet (e.g. pure spectra of the components) are needed.

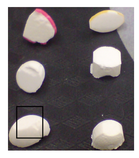
Alternatively, other tools can be used to extract image features without any previous information, as Principal Component Analysis (PCA) and autocorrelation coefficients.

In this study, a combination of PCA, autocorrelation coefficients mapping and Enhanced contrast function is introduced for screening and studying pharmaceutical tablets without any prior knowledge.

The methodology has been developed in MatLab (1) and tested with commercial tablets of Ibuprofen.

Experimental

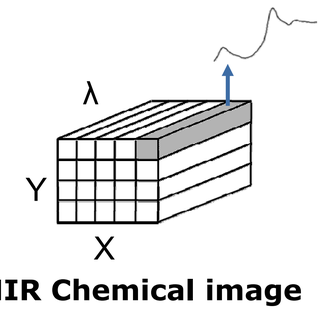
- **Sectioned commercial ibuprofen tablets**



Perkin Elmer Mapping System

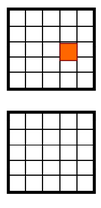
Matlab from Mathworks

Procedure



NIR Chemical image

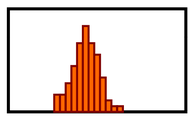
PCA analysis



Select one pixel from scores map

Autocorrelation coefficient

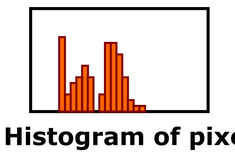
Correlation coefficient between the spectrum of the selected pixel and each spectrum on image



Histogram of pixel distribution

Enhanced contrast function

$$af1 = \left(\frac{c_i - c\min}{c\max - c_i} \right)$$



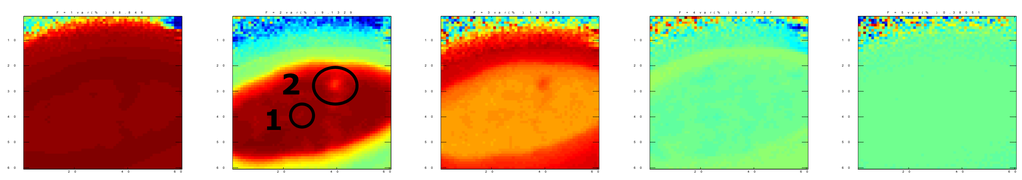
Enhanced Histogram of pixel distribution

Screening areas of interest in tablets

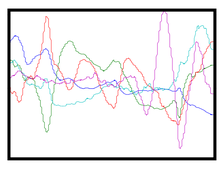
Getting statistic information

Results

1st step: Screening the image. PCA analysis and visualization of the scores maps

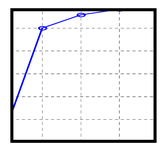


PC1 PC2 PC3 PC4 PC5



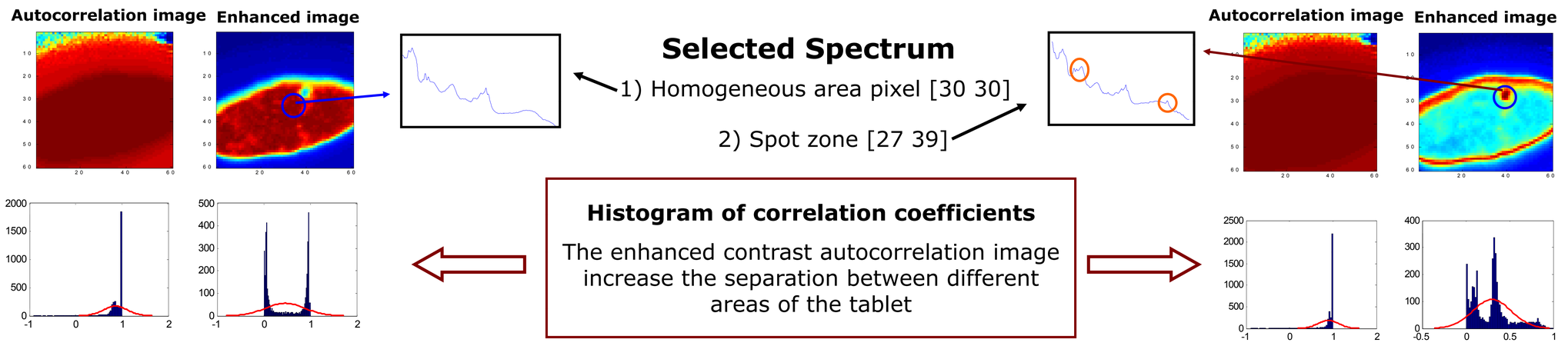
Loadings

Cumulative variance

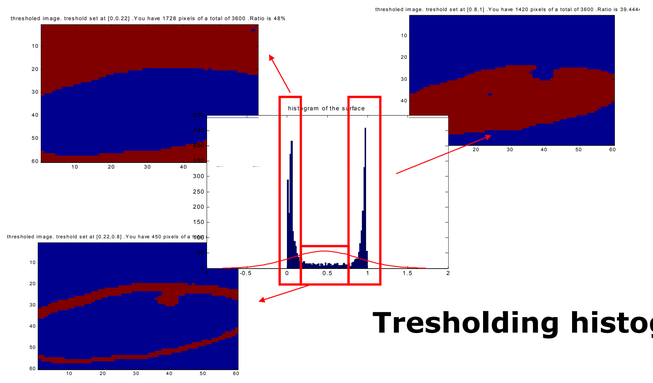


N. PC

2nd step: Selection of one pixel and calculation of autocorrelation coefficient (and enhanced contrast image)



3rd step: Getting information



Tresholding histogram

Standard Deviation of the distribution of pixel intensities as represented by the histogram of autocorrelation images

Spatial information obtained by simple pixel counting:

$$\frac{number\ of\ pixel\ of\ coating}{number\ of\ pixel\ of\ ibuprofen\ zone} = \frac{437}{1617}$$

Conclusions

A simple procedure had been described to extract information from near infrared hyperspectral image without any previous knowledge of the image.

Each zone is located using a chemical criterion (correlation coefficient with specific image spectrum of interest)

Quantitative information about the different zones in the tablet can be obtained in terms of spatial dimensions.

The routine is freely available in Reference (2)

References

(1) The Mathworks, version 7.0, The Matworks, Inc. Massachusetts.

(2) ttp://www.models.life.ku.dk/users/jose_manuel_amigo/index.htm

Acknowledges

Carlos Cairós wants to thank Prof. Robert Watt from the School of Pharmacy of London for all his help and suggestions.