

# CHEMICAL IMAGING AND CHEMOMETRICS: USEFUL TOOLS FOR PROCESS ANALYTICAL TECHNOLOGY

YVES ROGGO AND MICHEL ULMSCHNEIDER

*F. Hoffmann-La Roche Ltd, Basel, Switzerland*

## Contents

- 1 Introduction
- 2 Definition of Hyperspectral Imaging
- 3 Hyperspectral Image Acquisition and Instrumentation
  - 3.1 Principles of Hyperspectral Image Acquisition
  - 3.2 Spectroscopic Instrumentation
- 4 Chemometric for Imaging
  - 4.1 Data Preprocessing
  - 4.2 Pixel Classification
- 5 Practical At-Line and Offline Chemical Imaging
  - 5.1 Practical Tools for Distribution Map Analysis
  - 5.2 Wavelength Selection and Chemical Interpretation
  - 5.3 Unsupervised Classification for Process Troubleshooting
  - 5.4 Supervised Classification, NIR Imaging, and Process Development
  - 5.5 Further Developments: Online Analysis by Hyperspectral Imaging
- 6 Conclusions
- References

## 1 INTRODUCTION

Chemical compound homogeneity is an important issue for pharmaceutical solid forms. A classical spectrometer [1–3] integrates spatial information. However, use of a mean spectrum on a surface can be a drawback in solid-form analysis. For example, in the pharmaceutical industry, it is important to map the distribution of active ingredients and excipients in a tablet as this reveals physical interaction