

PROCESS ANALYTICAL TECHNOLOGY

MICHEL ULMSCHNEIDER AND YVES ROGGO

F. Hoffmann-La Roche Ltd, Basel, Switzerland

Contents

- 1 Basic Concepts and Impact
 - 1.1 Definition
 - 1.2 What Motivated PAT?
 - 1.3 Root-Cause Analysis and Process Control
 - 1.4 When to Introduce PAT
 - 1.5 PAT Enhances Process Understanding
 - 1.6 Changing Current Practice Using PAT
 - 1.7 Promoting Physical Pharmacy and Pharmaceutical Sciences
 - 1.8 Data Mining
 - 1.9 Data Warehousing
 - 1.10 Data-Mining Methods for Pharmaceutical Processes
 - 1.11 Data-Mining Practice
 - 1.12 Comments about Data Mining
 - 1.13 PAT Methods
 - 1.14 Conclusion
- 2 Vibrational Spectroscopy
 - 2.1 Introduction
 - 2.2 IR Spectroscopy Theory
 - 2.3 Mechanical Model of IR Vibration
 - 2.4 Quantum Mechanical Model
 - 2.5 Anharmonicity
 - 2.6 Structure Elucidation Using MIRS
 - 2.7 Extending Use of MIRS
 - 2.8 Raman Spectroscopy
 - 2.9 Introducing NIRS
 - 2.10 Benefits of NIRS
 - 2.11 Introducing MIR/NIR Chemical Imaging
 - 2.12 Design of MIR Instruments
 - 2.13 Conclusion