Transfer of active pharmaceutical ingredients (API) Raman library from benchtop towards handheld spectrometers

Matthieu Clavaud[1,2], Pierre-Yves Sacré[2], Philippe Hubert[2], Eric Ziemons[2]

[1]F. Hoffmann-La Roche Ltd., Wurmisweg, 4303 Kaiseraugst, Switzerland.
[2]University of Liege (ULiege), CIRM, VibraSanté Hub, Department of Pharmacy, Laboratory of Pharmaceutical Analytical Chemistry, Quartier Hôpital, Avenue Hippocrate 15, B36, B-4000 Liege, Belgium

Over the last few years, manufacturers have made progress miniaturizing Raman spectrometers and trying to meet the practical needs of the end-users for raw material and finished goods identification.

In this study, library transfer from a donor benchtop Raman towards different Raman receiver devices, benchtop and handheld, was evaluated. The aim was to create a library of active pharmaceutical ingredients (API) on a lab spectrometer and to show that a transfer to different Raman systems using the Hit Quality Index (HQI) algorithm is possible. Consequently, library creation would be faster as well as the set-up of a device for routine measurements avoiding the acquisition of hundreds sample on each system, and allow optimizing method update strategy.

A donor benchtop DXR SmartRaman (Thermo Fisher Scientific®) and receivers composed of a benchtop RXN1 (Kaiser Optical System®), and two handheld spectrometers respectively Truscan (Thermo Fisher Scientific®) and MIRA M-1 (Metrohm AG®) were selected. All spectrometers were equipped with a 785 nm near infrared excitation laser to avoid variation in laser differences.

The Orbital-Raster-Scanning (ORS) technology available on the MIRA M-1 was initially evaluated. Understanding the effect of the ORS technique on APIs was a previous step before setting up a database transfer experiment. Subsequently, acetaminophen was used for library standardization to calibrate the x-axis of the Raman spectrometers. Finally, Raman spectra were pre-processed prior to computation of the HQI method.

The results showed that transferring an API library from a benchtop Raman system towards handheld systems with HQI values higher than 90% is possible. Additionally, an HQI of maximum 75% was observed between the different APIs suggesting that the APIs were different enough allowing a transfer.