Product Note R37 - 01/17

BRAVO
- Next Level

The possibility for a quick on-site material analysis without extensive efforts, like sampling and subsequent transportation to a laboratory for analysis, is an attractive capability for product control. Optics based vibrational spectroscopy techniques like Raman, now available in a smart handheld format utilize modern technologies and innovations allowing a classical laboratory based analysis to be conducted in the field. Most importantly, handheld Raman spectroscopic analysis can be readily performed on materials through transparent barriers such as packaging material.

In accordance with Bruker's principle Innovation with Integrity, the first next generation handheld Raman spectrometer BRAVO introduced in 2015 was designed to overcome existing limitations, like fluorescence interference with new technologies and concepts [1, 2]. The BRAVO has proven its unique capabilities typically only found with a benchtop sys-

tem integrated in a handheld instrument for the first time [3]. New software functions aim to further increase performance for routine material control applications.

New Features

- Supports material identification and verification workflows
- Advanced method setup
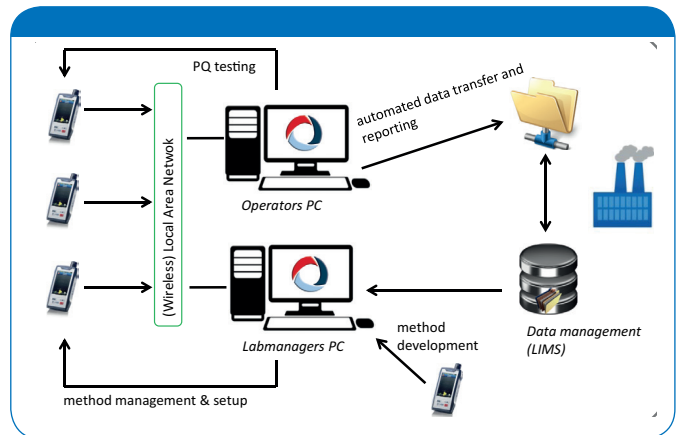- Fully automated data transfer and reporting

Figure 1: Schematics on the integration of multiple BRAVO systems into a network.

Fully automated data transfer and reporting

For any routine application, the automation of processes is a central point to facilitate efficient operation and ensure robustness in minimizing operational errors. Consequently, the BRAVO now features an automated network connection that includes data transfer and report generation. The transfer and reporting configuration is done by an administrator user and can be silently run as a background task during BRAVO's operation. A basic scheme of how to incorporate multiple spectrometers in a network is shown in Figure 1.

Material identification and verification

The BRAVO is dedicated for material verification, where the main task is to confirm the identity of a material that has been previously characterized. In order to generate an Accepted or Rejected result, prior measurement a presumption of the material to be analyzed is performed. Often it is also required to identify an unknown material, e.g. being not labeled. In the new software, the ability to run identifications through for library searching is added to the existing verification workflow.

Advanced method setup

Raman spectroscopy generally allows for unambiguous material verification based on library matching owing to the highly selective nature of Raman spectroscopy, where each compound has fingerprint signature. In general, the approach correlating a measurement towards a single spectrum of a reference material is appropriate, but in some cases a more dedicated approach is required. Now, the full flexibility at method setup is added, e.g. enabling the definition of spectral ranges and acceptance thresholds that are material specific. Proven OPUS software packages such as IDENT assist the user in setting up methods properly.

The benefits are many and range from a further increase in selectivity (see Figure 2), to the possibility to exclude a possible contribution of the PE packaging material from the analysis.
The BRAVO can distinguish differences based on hardly discernible contributions from additional compounds as well depicted in Figure 2 for a methanol (black spectrum) impurity in ethanol.

Software Update

The new software release is compatible with all BRAVO units and does not require any hardware adaptations. Previously generated methods are compatible with the new software, but will also benefit from the new advanced method setup.

The software can be installed locally on any BRAVO spectrometer by certified Bruker service engineers. This is essential for maintaining system validation for operation in the pharmaceutical industry.
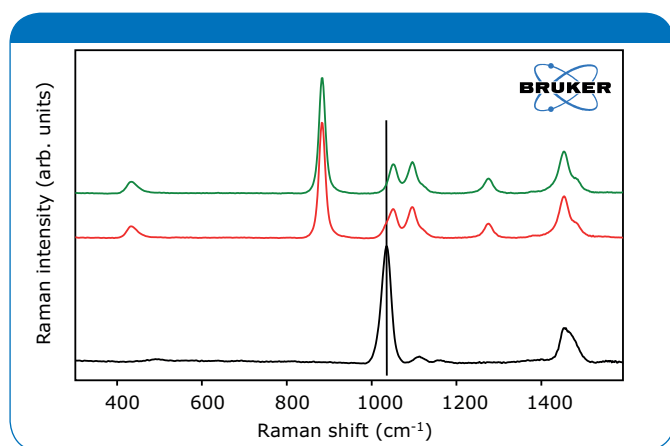

Figure 2: Raman spectra of ethanol. Pure (green) and laced with methanol impurity (red).

References

[1] Bruker Product Note T29 12/15, Efficient mitigation of fluorescence in Raman spectroscopy using SSE™.
[2] Bruker Product Note T30 03/16, Accuracy is crucial: The starting point for a robust transfer of methods.
[3] Bruker Product Note R34 05/16, Advanced data acquisition and evaluation in handheld Raman spectroscopy.