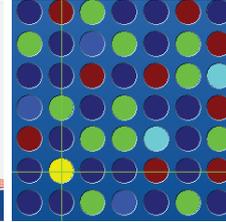
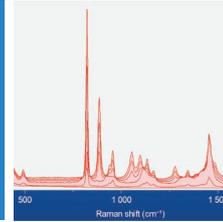


High Throughput Chemical Screening with the LabSpec 6 MultiWell Module



Technical Note
SO-TN06

The HORIBA Raman systems are fully compatible with high throughput screening experiments using well plates, micro-titre plates and other regularly arrayed sampling devices using the LabSpec 6 MultiWell module. Such experiments allow the known advantages of Raman spectroscopy (i.e., non-destructive, detailed chemical analysis, including insight into crystallinity, polymorphism and stress/strain) to be successfully integrated into industrial laboratory environments where sample throughput remains a top priority.



High throughput Raman systems use a combination of automated sample movement, autofocus devices, and automated data acquisition procedures to acquire spectra from hundreds of samples sequentially. Such screening and automated measurements can even be integrated with full robot handling, removing the need for expertise and operator intervention.

Typical applications include analysis of liquids/powders in multiwell plates, tablet content/uniformity assays with HORIBA's Transmission Raman accessory and biological assays with micro-spotted materials (such as DNA/RNA). More generally, any measurement of regularly arrayed samples will be greatly improved with the MultiWell module.

All the experiments benefit from the many advantages of Raman spectroscopy, which include:

- Non-destructive analysis, allowing samples to be re-analyzed in the future, whether with Raman or other complementary techniques
- Fast data acquisitions with second or sub-second measurement times per spectrum using optimized systems
- Detailed chemical information, including subtle structural information such as crystallinity, polymorphism and stress/strain
- Unequivocal chemical identification using extensive Raman spectral databases and search tools

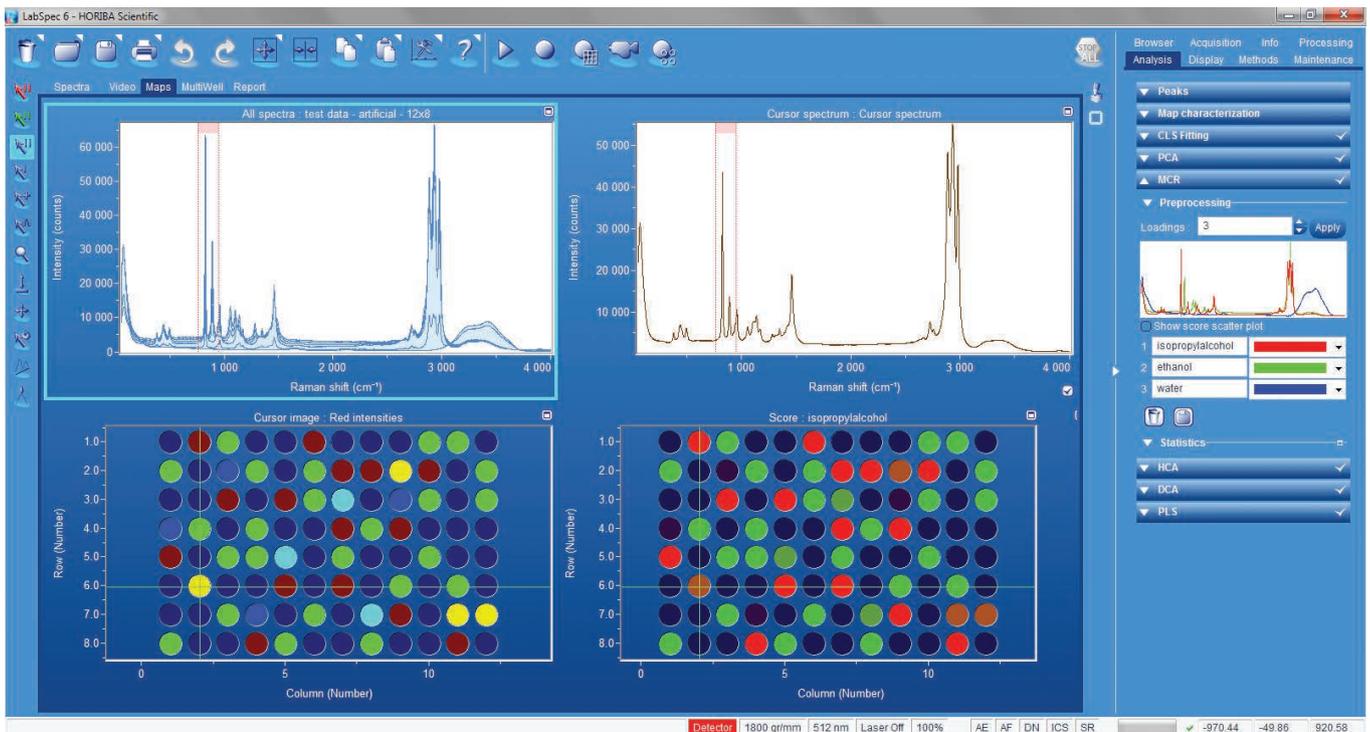


Figure 1 - LabSpec 6 screenshot, showing the MultiWell results interface, with plate schematics based on peak intensity (left) and MCR multivariate classification (right)

Plate Setup

The MultiWell module is compatible with plates of any size and shape, limited only by the physical capabilities of the automated XY stage – typical standard 96 well plates are easily accommodated, and options for larger stages are available for non-standard plates. A simple Plate Wizard makes light work of setting up a new plate within the software, directing the user through a small number of manual operations to allow calculation of the key plate parameters, such as plate dimensions, well size and spacing, and reference marker location.

Reference markers on the plate can be used to ensure easy relocation of the plate, with options to compensate for shift, rotation and/or tilt of the plate. Such options have minor impact on typical bulk measurements, but become increasingly important when working with micro-arrays or micro-spot arrays. Such tools allow plates to be reloaded time and time again, for verification of results, repeated measurements, or long time-based experiments.

Data Acquisition

The integrated plate schematic offers an interactive tool for navigating around the plate, and can be used to include/exclude rows, columns or individual cells from the experiment. Once set, the automated Raman acquisition can be started.

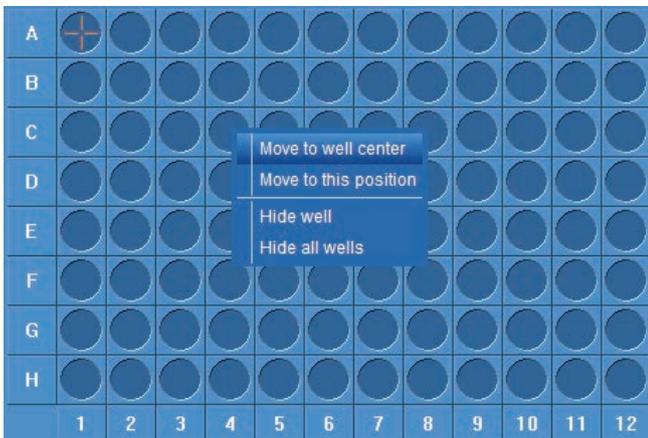


Figure 2 - The plate schematic allows easy manual movement to individual wells; additionally specific wells can be hidden, so that they will be excluded from the automated screening measurement.

The full capabilities of the advanced HORIBA Raman instrumentation is available for data acquisition, and can be optimized for different sample/measurement types (with options for multiple and varied laser wavelengths, extended spectral range analyses, high spectral resolution), and configured with various software tools such as FLAT correction (for fluorescence removal), AutoExposure, and AutoFocus.

Such capabilities ensure that standard screening measurements are dispatched with ease, whilst more challenging samples or measurement protocols are nonetheless possible with considered method development.

Data analysis

Once data has been acquired, it is available for processing and analysis using the full suite of functionality available within LabSpec 6. In particular, the spectral array can be analyzed for standard peak characteristics (height, position, width, area) with the results plotted both on individual spectra, and in graphical overview. Furthermore, advanced multivariate analysis including CLS fitting, PCA, MCR, clustering and PLS quantitative methods can be used via the LabSpec 6 Multivariate Analysis module. Even the most subtle of information can be clearly viewed using such tools.

Conclusion

The LabSpec 6 MultiWell module opens up high throughput screening experiments to the HORIBA Raman spectrometers, maximizing sample throughput and laboratory efficiency, whilst benefitting from the unique advantages of Raman spectroscopy.

The MultiWell module combines with other data acquisition, analysis and display modules within the LabSpec 6 Spectroscopy Suite to offer advanced capabilities underpinned by an intuitive, easy-to-use interface.



HORIBA
Scientific

info.sci@horiba.com

USA: +1 732 494 8660
UK: +44 (0)20 8204 8142
China: +86 (0)21 6289 6060

France: +33 (0)1 69 74 72 00
Italy: +39 2 5760 3050
Brazil: +55 (0)11 2923 5400

www.horiba.com/scientific

Germany: +49 (0)89 4623 17-0
Japan: +81 (0)3 6206 4721
Other: +33 (0)1 69 74 72 00