2015-04-01

# Optical Diagnostics – Spectropathology for the Next Generation

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## Recommended Citation

"Optical diagnostics – spectropathology for the next generation", Malgorzata Baranska and Hugh J. Byrne, *Analyst*, Editorial, Special Issue "*Optical Diagnostics*", 140, 2064-2065 (2015) doi:10.1039/c5an90024g

Analyst

EDITORIAL

# Optical diagnostics – spectropathology for the next generation

Cite this: *Analyst*, 2015, **140**, 2064
DOI: 10.1039/c5an90024g
www.rsc.org/analyst

This latest Optical Diagnosis themed issue of *Analyst*, guest-edited by Prof. Malgorzata Baranska, Jagiellonian University, Krakow, Poland, and Prof. Hugh J. Byrne, Dublin Institute of Technology, Ireland, is drawn from the participants and proceedings of the International conference, SPEC 2014: Shedding New Light on Disease, which was held on the 17th–22nd August 2014 in Krakow, Poland. The conference was co-chaired by Prof. Baranska, Prof. Byrne and Prof. Anna Sulkowska, Medical University of Silesia, Katowice, Poland.

The event was the eighth in the series of biennial conferences, the aim of which is to bring together clinicians and scientists who have joined forces in the quest for novel biomedical applications of infrared and Raman spectroscopy to improve patient care. Recent advances in the biological sciences and medicine have led to an increasing demand for real-time and minimally invasive chemical and structural information on biological materials. Due to its unique fingerprinting capability, vibrational spectroscopy plays a significant role in histopathology, cytology, biopsy targeting, surgical targets, treatment-monitoring and drug studies.

The conference aimed to highlight further advances in state of the art and emerging biomedical applications of vibrational spectroscopy, while reviewing the challenges in the context of other emerging technologies. The programme was constructed in an attempt to prioritise real-world applications from the outset, systematically progressing from research towards *in-vivo*, *ex-vivo* and *in-vitro* applications, as well as emerging technologies and data processing.

A feature of the conference was the daily discussion sessions which were aimed at a critical assessment of the routes towards the further development of clinical applications, and were moderated by members of the SPEC International Advisory Board. The deliberations are summarised in the second editorial 'Spectropathology for the next generation: Quo vadis?' (Byrne *et al.*, c4an02036g), under the headings of (i) Translational research into *in-vivo* clinical applications, (ii) *Ex-vivo* tissue biopsies, body fluids and cytological samples for diagnostics and disease studies, and (iii) *In-vitro* cell culture and 3D models for research and medical applications. A number of critical concerns are highlighted under the respective headings, including (i) the need for the engagement with the clinical community and adherence to clinical standards in terms of statistical relevance, (ii) standardisation of protocols for sample preparation, presentation and measurement and data processing, and (iii) continued development of instrumentation and models to explore the limitations of the techniques.

The scope of the conference and the contents of this themed issue are indicative of the progress in the understanding of the complexity of spectroscopic characterisation of biological materials, and data preprocessing and postprocessing methods can increasingly be applied with confidence to give true biochemical representations of tissue, cells and bodily fluids. The issue contains a total of 51 contributed communications and articles, drawing from research activities across the globe, including Australia, India, Japan, US and across Europe with a notably strong representation from the host country, Poland.

The increased development of fibre probes shows great promise for *in-vivo* diagnosis and intra-operative applications, and although Raman probes – operating at visible or near-infrared wavelengths – are relatively well established, probes for FTIR spectroscopy are less so. The study by Padalkar and Pleshko (c4an01987c) details the development of such probes for the *in-vivo* analysis of cartilage.

For clinical applications, the research field remains dominated by *ex-vivo* applications of tissue, cells and biofluids. Spectrohistopathological studies using either FTIR or Raman profiling range from analysis of cancer markers in adrenal glands (Dudala *et al.*, c4an01891e), salivary tissue (Brozek-Pluska *et al.*, c4an01394h), lung tumour (Gerwert *et al.*, c4an01978d), breast tissue (Abramczyk *et al.*, c4an01876a; Brozek-Pluska *et al.*, c4an01877j), and primary and metastatic melanoma (Wald and Goormaghtigh, c4an01831a). Further studies include analysis of the pituitary gland (Banas *et al.*, c4an01985g), calcification of the aortic valve (Kaczor *et al.*, c4an01856g), the vitamin A content in murine lung and liver tissue (Marzec *et al.*, c4an01881h; Baranska *et al.*, c4an01878h) and endothelial function/dysfunction (Kaczor *et al.*, c4an01870b; Rygula *et al.*, c4an01998a). Animal models also feature strongly in

the studies of Chwiej *et al.* (c4an01857e) as epileptic models, and as obesity models in the work of Severcan *et al.* (c4an02008a).

Cytological studies, using FTIR and FTIR-ATR spectroscopy also feature strongly, in, for example, the study by Diem *et al.* (c4an01884b) of oesophageal cells. Abramczyk *et al.* (c4an01875c) demonstrate the role of lipid droplets and adipocytes in cancer by comparing the Raman spectral profiles of cell cultures to those of adipocytes in cancerous human breast tissue.

The contents of this issue reflect an increasing prominence of studies of blood cells (Wood *et al.*, c4an01904k) and peripheral blood lymphocytes (Goormaghtigh *et al.*, c4an01855a and c4an02247e), and indeed of bodily fluids themselves, using both FTIR and Raman spectroscopy, notably blood plasma (Šťovíčková *et al.*, c4an01874e; Malek *et al.*, c4an01864h; Garnotel *et al.*, c4an01942c; Tatarkovič *et al.*, c4an01880j) and serum (Chilakapati *et al.*, c4an01860e), potentially promising more accessible routine screening applications of vibrational spectroscopy.

Spectroscopic techniques remain a powerful tool for basic research and may find applications *in vitro* for toxicology and drug screening, as exemplified by the study of cellular uptake of doxorubicin by Chlopicki, Baranska and co-workers (c4an01882f), and the study of the biocompatibility of nanocomposites by Wesełucha-Birczyńska *et al.* (c4an02284j), Malek *et al.* (c4an01988a), and Campbell *et al.* (c4an02365j), demonstrate the use of SERS-based nanosensors to monitor the intracellular pH in endothelial cells. Equally, such *in-vitro* studies can provide valuable explorations for new 3D cell culture models (Smolina and Goormaghtigh, c4an01833h), developing neural systems (Sato *et al.*, c4an01961j) and disease models (malaria) (Hobro, Smith and co-workers, c4an01850h). Mosig *et al.* (c4an02153c) demonstrate the colocalization of fluorescence and Raman microscopic images for the identification of subcellular compartments, and thus the potential of the technique for *in-vitro* screening.

Although the proof of concept of a range of potential clinical applications of vibrational spectroscopy has been well demonstrated, there remains the need for standardisation of measurement protocols and data processing, as highlighted in the discussion editorial (Byrne *et al.*, c4an02036g). Exploration of the impact of tissue processing (Stone *et al.*, c4an02122c; Wood *et al.*, c4an02034k) as well as measurement configurations for FTIR spectroscopy (Gardner *et al.*, c4an01975j; Mignolet and Goormaghtigh, c4an01834f; Wood *et al.*, c4an01901f; Malek *et al.*, c4an01842g) feature strongly. Gardner *et al.* (c4an02053g) also propose protocols for enhanced FTIR bench-top imaging of single biological cells. The relative merit of different classification and data-mining algorithms continues to be a subject for investigation (Wood *et al.*, c4an01783h; Surowka *et al.*, c4an01867b; Gobinet *et al.*, c4an01937g; Diem *et al.*, c4an01832j and c4an01879f; Meade *et al.*, c4an01887g), while Keating *et al.* (c4an02167c) demonstrate the importance of simulated datasets for method validation.

Emerging technologies continue to push the performances in terms of spatial resolution (Gough *et al.*, c4an01982b), sampling depth (Ariese *et al.*, c4an01889c) and the emergence of quantum cascade lasers as IR sources promises increased scanning speeds for large area spectral mapping (Kröger-Lui *et al.*, c4an02001d). Meanwhile, Czepiel, Wesełucha-Birczyńska and co-workers (c4an01947d) give glimpses into applications beyond human pathologies.

The field of clinical applications of vibrational spectroscopy continues to engage a broad interdisciplinary research community across the world, including spectroscopists, chemists, biochemists *etc*. The field is furthermore becoming increasingly intersectoral, as instrument companies address the challenge of faster acquisition speeds over larger areas, and the medical community itself becomes more 'spectrophilic' and engaged in promoting the potential of spectropathology for the next generation. We hope you find the articles gathered in this themed issue of *Analyst* stimulating and inspiring.

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