Imaging MS: Defining Resolution in Imaging MS - A Quest for Solid Ground

Workshop Report

Monday 1st of June, 5:45 - 7:00, Room 120/127

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Introduction

The central envisioned topic of the workshop was "Spatial Resolution in Mass Spectrometry". Due to the recent introduction of a number of new technologies into Mass Spectrometric Imaging, a `War of Numbers' broke out on the field, where individual research groups keep claiming better and better spatial resolution for their techniques or experimental setups. In order to establish a solid ground, the workshop made an attempt to come up with a widely acceptable definition (and associated method of determining it) for spatial resolution claimed in a scientific publication.

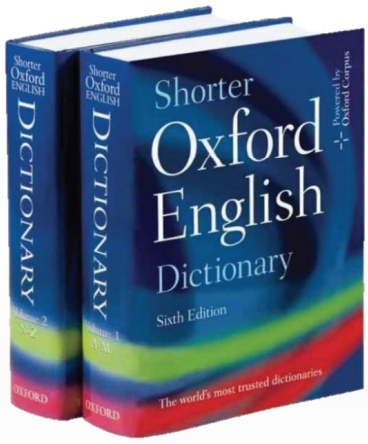
Agenda

The workshop started out by Imabiotech (Lille, France) presented the second Imabiotech award for innovation in Imaging MS, which was won by Richard Hsu (for his work of Nano DESI) of University of California, San Diego, CA. Hsu was selected out of the more than 50 students applied for the award. Note: Though the award was presented during the workshop there was never any ASMS endorsement of the award – as agreed in previous year.

The scientific discussion was started by a short overview on "Spatial Resolution of MSI" by Liam McDonnell (of Leiden University Medical Center, Leiden, The Netherlands). He started out by calling the help of dictionary:

Definitions

FPS Fondazione Pisana per la Scienza



Two relevant definitions

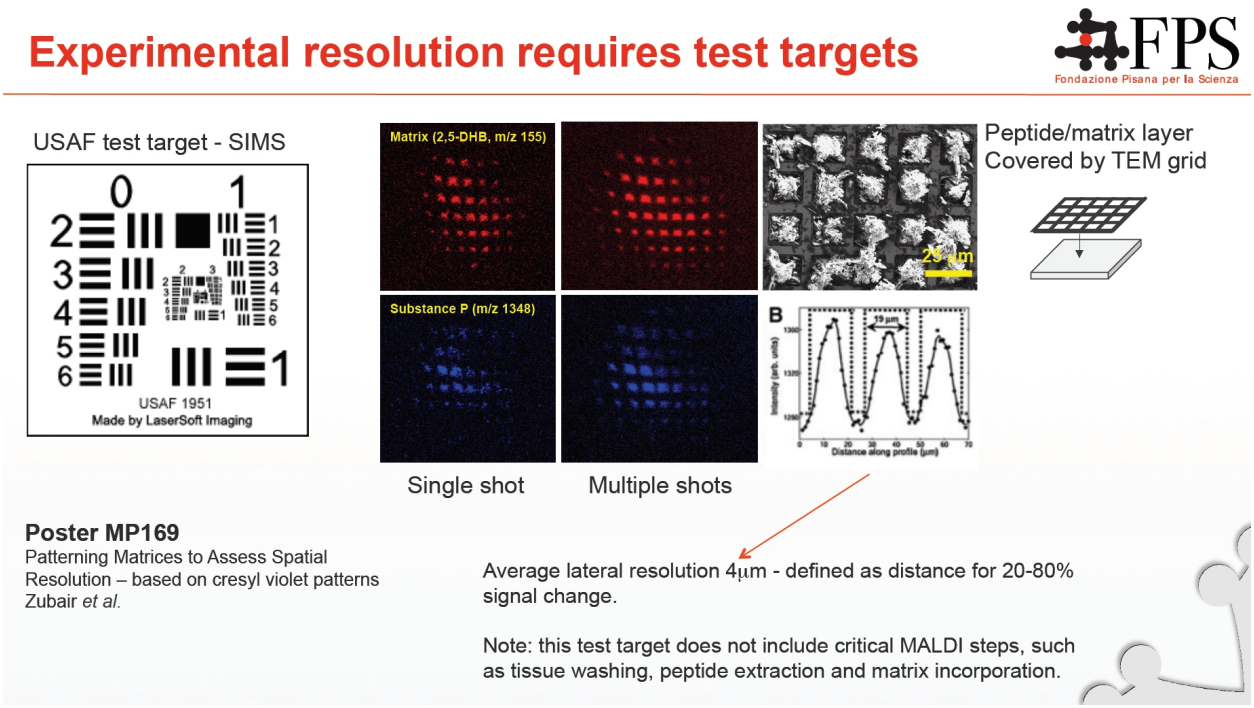
1. "the smallest interval measurable by a telescope or other scientific instrument",
2. "the degree of detail visible in a photographic or television image".

In MSI

1. pixel size (smallest measurable distance),
2. experimental spatial resolution based on detail visible in image.

The former is easier to specify but omits many crucial factors. The "experimental spatial resolution," or the length scale that can be distinguished, is a convolution of the inherent spatial distribution of the sample, sample preparation, the inherent capabilities of the instrument, and the signal intensity per pixel.

He brought up during this discussion-starting talk that an often forgotten, but very important fact that testing resolution requires correct, reproducible test targets:



Liam's talk was followed by four experts shortly (about 5 min each) discussing current best resolution and approaches how to improve these resolution in case of different imaging techniques:

I) *Spatial resolution in MALDI Imaging.* Andreas Römpp, Justus Liebig University, Giessen, Germany

II) *Spatial resolution in DESI-MSI – some personal considerations,* Christian Janfelt, University of Copenhagen, Denmark

III) *State-of-the-art molecular imaging in SIMS – and beyond…* Matthias Lorenz, National Physical Laboratory, Teddington, Middlesex, UK

IV) *Metabolite Imaging: From whole-body to a cell (LAESI),* Bindesh Shrestha, The George Washington University, Washington, DC, USA

Each presentation was followed by a short Q&A session. Some of these presentations started lively discussions between attendees what was the current best resolution achieved. These emotional discussions pointed out that the main point of the workshop, i.e. groups define resolution differently. However, the main take home messages of these talks were that a) sample preparation affecting analyte redistribution and b) sensitivity of the analysis affecting the smallest area where from an acceptable analytical signal derives are major factor in achievable spatial resolution. Also, during these talks two recent papers (Development of an Organic Lateral Resolution Test Device for Imaging Mass Spectrometry by MK Passarelli et al, *Anal. Chem*. **2014**, *86*, 9473–9480 and Resolution Pattern for Mass

Spectrometry Imaging by SR Fagerer et al., *RCM* **2015**, *29*, 1019–1024) were referenced and discussed that developed test devices for evaluating spatial resolution for imaging MS.

The discussion was followed by a short talk by Kristina Schwamborn (Technische Universität München, Munich, Germany) titled "Imaging MS – A Pathologist's Perspective" about the needed imaging resolution for pathology. Kristina has discussed many aspects of spatial resolution including structures of different cell/tissue types, the effect of tissue heterogeneity on resolving power using given a sampling area and the complex relationship between resolution/acquisition time/data file size.

The workshop ended with a lively discussion on "Which resolution?" to use: pixel size? so-called 20-to-80 rule? size of the smallest feature resolved? Unfortunately, as the time was running out, the attendees could not settle for one common definition. However, no one opposed when test devices with features of well-defined sizes were proposed to be able to evaluate resolving power of a given imaging MS platform. It was also established, that the surface patterns had to be built using different class of chemicals (e.g. lipids, proteins, small molecules) of different surface concentrations for the most comprehensive evaluation.

At the end of the workshop, Dr. Raf Van de Plas (Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN, USA/Delft Center for Systems and Control, Delft University of Technology, Delft, the Netherlands) was voted to be the next co-chair of the interest group, replacing Zoltan Takats.

Participation was estimated to be around 150 attendees.

Acknowledgements

We thank the ASMS for the opportunity to hold the workshop as part of the conference as well as all of their help and support in doing so. The presenters are gratefully acknowledged for stimulating the discussion and getting everyone involved and excited about the discussions.