

## Analytica Chimica Acta

Available online 21 November 2018 https://doi.org/10.1016/j.aca.2018.11.032



## Denoising influence on discrete frequency classification results for quantum cascade laser based infrared microscopy

PaulinaKoziol<sup>®</sup> Magda K.Raczkowska<sup>®</sup> JustynaSkibinska<sup>®</sup> Nicholas J.McCollum<sup>d</sup> SlawkaUrbaniak-Wasik<sup>®</sup> CzeslawaPaluszkiewicz<sup>®</sup> Wojciech M.Kwiatek<sup>®</sup> Tomasz P.Wrobel<sup>®</sup>

<sup>a</sup> Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland

<sup>b</sup> Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Mickiewicza 30, Krakow, Poland

<sup>°</sup> Faculty of Electrical Engineering, Automatics, Computer Science and Biomedical Engineering, AGH University of Science and Technology, Mickiewicza 30, Krakow, Poland

<sup>d</sup> DRS Daylight Solutions, 15378 Avenue of Science, Suite 200, San Diego, USA

° NZOZ Pathology Department, Jagiellonska 70, Kielce, Poland

## Highlights

- QCL approach enables a truly Discrete Frequency approach speeding up IR imaging by a factor of 100–1000.
- Effects of spatial and spectral denoising on classification accuracy of QCL data were studied.
- Most important factor in classification accuracy is the number of experimental spectral variables.
- Only MNF has significantly improved classification results, but only when more than 20 variables were denoised.

## Abstract

Currently, there is great interest in bringing the application of IR spectroscopy into the clinic. This however will require a significant reduction in measurement time as Fourier Transform Infrared (FT-IR) imaging takes hours to days to scan a clinically relevant specimen. A potential remedy for this issue is the use of Quantum Cascade Laser Infrared (QCL IR) microscopy performed in Discrete Frequency (DF) mode for maximum speed gain. This gain could be furthermore improved by applying a proper denoising algorithm that takes into account the specific data structure. We have recently compared spectral and spatial denoising techniques in the context of Fourier Transform IR (FT-IR) imaging and showed that the optimal methods depend heavily on the exact data structure. In general multivariate denoising methods such as Principal Component Analysis (PCA) and Minimum Noise Fraction (MNF) are the most effective for a dataset containing multiple bands. Histologic classification of QCL IR images of pancreatic tissue using Random Forest was therefore performed to investigate which denoising schemes are the most optimal for such experimental data structure. This work is the first to show the effects of denoising on classification accuracy of QCL data and is likely to be transferable to other QCL microscopes and other modalities using DF imaging, e.g. AFM-IR or CARS/SRS imaging.