Reg. No: 2019/35/N/ST4/02481; Principal Investigator: mgr inż. Paulina Klaudia Kozioł

Improving 3D macromolecule orientation determination based on polarized IR chemical imaging by optimization of scattering removal algorithms

Paulina Koziol

Abstract

Fourier Transform Infrared Spectroscopy (FT-IR) is a powerful imaging modality, with a wide range of biomedical applications. It gives full insight into sample's chemical composition using its ability to absorb infrared (IR) light. Tremendous progress was done through the last decade towards implementation of this technique into the clinic, especially in the area of cancer detection and diagnosis using combination of FT-IR and Machine Learning methods. One of the latest discoveries is a possibility to determine molecular 3D orientation using polarized IR light. Polarization is one of the light's characteristics that, in this case, changes its absorbing properties, therefore might give additional information about the structure of sample. Unfortunately, as every experimental technique, FT-IR is not free from effects hindering its effectiveness and accuracy. An optical effect called scattering has a great impact in this case. It causes the light passing by the sample to change direction, thus it does not reach the detector and is mistaken with the true signal coming from light absorbed by the sample. One way to reduce the impact of this effect on performed analysis is to introduce signal processing methods making corrections for the artificial signal. Methods correcting light scattering effect are called Extended Multiplicative Signal Correction (EMSC), and are well developed if applied to data collected for spherical samples (for example cells), but are still early in the development when it comes to applying for tissue samples. This is caused by tissue heterogeneity, that makes scattering characteristic very complicated. Another reason is algorithm's complexity that makes the time frame needed for performing calculations very extended.

The main goal of this project is optimization of existing one and implementation of new EMSC based algorithms for light scattering correction for FT-IR, in order to improve 3D macromolecular orientation determination based on polarized light. Recently developed new version of EMSC algorithm, available as an open source code, will be implemented on multi-core platforms like GPU or AGH's Cyfronet Supercomputers. Hopefully, this will make the timescale needed to perform calculations for tissue samples much shorter. An EMSC algorithm will also be implemented for samples with cylindrical shape, which will be ideal to execute on fibrous tissue. Fibrous tissue is rich in collagen fibers that have a cylindrical shape and is perfect to determine molecular orientation using absorption of light with different polarization.