SERS-based study combined with chemometric methods for recognition of the molecular pattern of vaginal fluids: towards a differential diagnosis of vaginal infections

Popular science summary

In this project's framework, we intend to exploit Surface-enhanced Raman spectroscopy (SERS) assisted by chemometric analysis to study clinical materials (vaginal fluids) for vaginitis caused by bacteria, fungi, and protozoa. The currently used diagnostic technique marked as ‘gold standard’ is a microscopic examination of Gram-stained vaginal discharge. It is also recommended to use the Amsel criteria, e.g., determination of the discharge consistency and detection of characteristic odor (whiff test). These methods are based on visual and organoleptic evaluation of the material and impose a heavy workload on the trained staff. Therefore, in the proposed project, we intend to understand how inflammatory conditions of various etiological backgrounds (bacterial, fungal, protozoal) affect changes in the spectral images of study materials. Additionally, with the use of chemometric methods (supervised and unsupervised), we will create a model for classifying samples of unknown origin and validate it.

Raman spectroscopy is a technique that exploits the phenomena of inelastic scattering of photons (the source is a laser beam) by molecules of the tested substance. The obtained spectral image consists of many bands encoding information about unique molecular oscillations in a given material. Since only one photon per million undergoes Raman scattering, the received signal is feeble. The situation was changed in 1974 when Martin Fleischmann proved that this Raman signal could be enhanced by up to 6 orders of magnitude when the tested substance is placed on a rough silver surface, and such a modified technique was called SERS. Since then, this method has gained the interest of many scientists, especially in medicine and biology, due to its non-destructive and ultra-sensitive nature. Its application potential has been presented in many articles related to the imaging of biological materials such as animal and human tissues, tumor cells, fungi, viruses, species, and strains of bacteria. Trying to discover new possibilities of the SERS technique, the proposed project includes research in an aspect that has never been reported before. Thus, for spectral characterization of vaginal swabs, we will exploit SERS performed under an intrinsic format where the information-rich spectra are produced upon indirect interaction with SERS-active substrate. Since SERS registers at the molecular level both quantitative and qualitative changes in biochemical components, we demonstrate that apart from binary differentiation (healthy, sick), it will be possible to determine the etiological agent causing an inflammation (bacterial vaginosis, candidiasis, trichomoniasis). We aim to designate the marker bands for each type of infection. Then, based on the reference spectra of biochemical compounds produced by the female reproductive system and the vaginal microbiome, we will identify them. Currently, it is supposed that vaginal infections result from the overgrowth of a given type of pathogen above the rest of the microflora. For this reason, we will record reference spectra of a number of microorganisms (bacteria, yeast, protozoa), both pathogenic and commensals. This will allow for the designation of characteristic futures for them and the determination of their possible impact on the spectra of clinical samples.

In summary, the topic of the proposed project is one of the most developing sciences in the world. This project involves spectroscopic research on the clinical materials for the diagnosis of vaginal infections and has not only purely cognitive but also practical significance. Examinations performed using a portable Raman spectrometer in conjunction with a chemometric algorithm can notably contribute to streamlining the point-of-care diagnostics as the visual and sensory evaluation of preparations will no longer be needed. In addition, the possibility of frequent screening tests and accurate diagnostics will facilitate the introduction of appropriate treatment, which is the only guarantee against recurrent infections.