RAPID TEST IN CLINICAL PHARMACOLOGY ACTIVITY USING FTIR SPECTROSCOPY

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Abstract

Background. *This research was aimed to investigate the pharmacological activity by using Fourier Transform Infra Red (FTIR) spectroscopy technique. Within an infrared spectrum from patient serum contributes qualitatively and quantitatively to the measurement.*

Methods. *Pathological patients and healthy controls serum were collected from Mannheim Hospital, Germany. The serum were dropped on the plate and were measured by FTIR. The spectra were applied a baseline correction and vector normalization and were performed the second derivative of the original spectra using the Savitzky-Golay algorithm with 9 smoothing points.*

Results. *In this work, we propose a novel technique for pharmacological activity test based on FTIR spectra that allows observing several parameters. Our results showed that major spectral differences were observed in between 1250-1228 (main marker for antisymmetric PO2- stretching-depicting adenine form of DNA), 1174-1164 and 1026-1014 cm^{-1} spectra region.*

Conclusions. *This preliminary finding constitutes a novel testing approach and suggest that FTIR spectroscopy can be applied for the detection several parameters in pharmacological activity.*

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INTRODUCTION:

In the field of clinical diagnosis and pharmacology activity, various medical imaging techniques such as computerized tomography, ultrasonography, magnetic resonance imaging, and positron emission tomography are utilized. With these techniques, information of size, shape, and location of disease dan activity can be observed. However, most pharmacological activity are caused by several biochemical processes with molecular pathways changes accompanied.

Infra red spectroscopy is known to be an accurate, fast, convenient and inexpensive method applicable for tissue pathology studies. In recent years infrared (IR) spectroscopy has caught the attention for the biomedical study of several diseases. In particular, near-infrared spectroscopy (NIRS) has been used for general tissue pathology studies and non-invasive or minimally invasive diagnostic applications due to the advances in fibreoptic probes (Heise, 2002). Fourier transform infrared (FTIR) spectroscopy, has already shown great potential for reliable screening analysis of some conditions such as cancer, alzheimers, myocard infarction, and eyes pressure [Weissbrodt et al., 2005; 2007, Griebe, 2007, Kondepati et al., 2010]. Kondepati et al. (2007) have reported the qualitative near-infrared spectral differences between diverticulitis and their adjacent normal tissues in electively resected colon sigma diverticulitis specimens using cluster analysis as a pattern recognition technique. In this study, FTIR spectroscopy [Henneges et al., 2010, Kondepati et al., 2005 and 2007] was applied for the first time to analyse pharmacological activity in serum and tissues patients.

METHODS

1. FTIR Spectroscopy

FTIR were recorded with a Tensor 37 FT-IR Spectrometer (Bruker Optics, Ettlingen, Germany) which was equipped with a HTS/XT unit for high throughput measurements. All serum samples (39 healthy and 58 sepsis patients) were measured in diffuse reflection. For the measurement in diffuse reflection a liquid nitrogen-cooled MTC (mercury cadmium telluride) detector was used. For each sample 64 interferogrammes were co-added to yield a spectrum with a nominal resolution of 4 cm^{-1}. the spectra were recorded in wavenumber range between 4000 an 400 cm^{-1}. A zero filling factor of 4 was used, yield a point spacing of 1 cm^{-1}.

2. Data processing

The spectra were evaluated in the same plate measured. The spectra were applied a baseline correction and vector normalization and were performed the second derivative of the original spectra using the Savitzky-Golay algorithm with 9 smoothing points.

RESULTS AND DISCUSSION

This study shows that the application of mid-infrared spectroscopy in pharmacology activity using serum patients. In addition, obtained spectra were analysed with a baseline correction and vector normalization and performed the second derivative of the original spectra using the Savitzky-Golay algorithm with 9 smoothing points.

Sepsis is infection accompanied by an acute inflammatory reaction with systemic manifestations associated with release into the bloodstream of numerous endogenous mediators of inflammation. Biomarkers may be used to diagnose patients with sepsis, and they may also help patients who would benefit from immunomodulatory therapies (Stearns-Kurosawa et al, 2010).

Figure 1 shows the second derivative average spectra from healthy, surviving and non surviving sepsis patient in the spectral region 1400-800 cm^{-1}. The spectra profile between pathological status and healthy controls give information that there is a significantly differences. This result can also indicate the type of sepsis disease.

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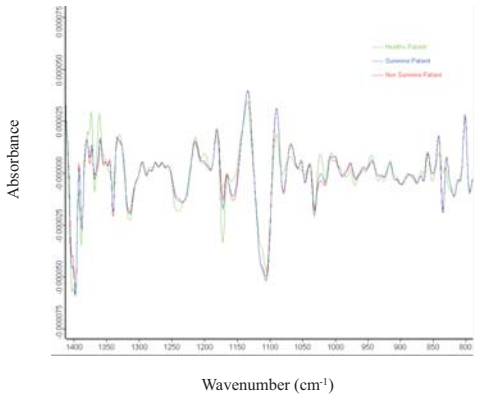

Figure.1 Second derivative average spectra from healthy and sepsis patient in the spectral region 1400-800 cm^{-1}

CONCLUSION

Based on FTIR spectra can be concluded that this FTIR approach offers considerable advantages over conventional methods of analysis. FTIR will therefore acquire increasing importance as a testing method in clinical pharmacology.

In the future, further quality control for clinical pharmacology activity can be calibrated and simultaneously determined with FTIR spectroscopy.

Table I. The wavenumbers and spectral assignments of major strong IR peaks in sepsis and healthy controls in the second derivative.

Peaks Position (cm^{-1})	Assignment	Moiety	References
1000-1050	Symmetric PO2 stretching-insensitive to B → A transition of DNA backbone	DNA	Dovbeshko et al, (2002)
1150-1170	Indication of A-form of helix. Sugar-phosphate backbone vibration with a high contribution from the sugar moiety in C3'-endo/anti-type of puckering	DNA-Phospholipid	Yoshida et al, (1997)
1230-1250	CH in-plane bend	phospholipid	Schulz, et al, (2007)
1350-1400	CO, CN	Amide III	Dovbeshko et al, (2002)

The result gave information about region of interest (ROI) were 1000—1050, 1150—1170, 1230—1250, 1350—1400 cm^{-1} which showed differences between spectra of healthy and sepsis patients. Furthermore, the spectral assigments of major strong peak in sepsis and helathy control are shown in Table I.

Based on our infrared spectra, FTIRspectroscopy appears to be a promising method to test pharmacological aspect from serum samples. The other reports support the reasons (Hass et al., 2010; Kondepati et al., 2007, 2008, 2009).

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