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ATR-FTIR spectroscopy for non-invasive detection of fingernail biochemical alterations in paediatric patients with inflammatory bowel disease: a pilot study

Spektroskopia ATR-FTIR jako nieinwazyjna metoda wykrywania biochemicznych zmian w paznokciach u dzieci z nieswoistymi chorobami zapalnymi jelit: badanie pilotażowe

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Abstract

Introduction and objective: This pilot study aimed to evaluate the feasibility of attenuated total reflectance – Fourier transform infrared spectroscopy (ATR FTIR) as a rapid, non-invasive method for detecting biochemical alterations in the fingernails of paediatric patients with inflammatory bowel disease (IBD). **Materials and methods:** ATR FTIR spectra were acquired from fingernail clippings obtained from 10 children diagnosed with IBD and from 10 age-matched healthy controls. Spectral analysis focused on characteristic vibrational bands associated with keratin structure, including N–H stretching vibrations, asymmetric CH_2 and CH_3 stretching modes, and symmetric CH_3 vibrations. **Results:** Comparative spectral analysis revealed subtle but consistent differences between the IBD and control groups. Shifts in bands related to keratin-associated amino acids were observed, particularly in the regions corresponding to N–H and C–H stretching vibrations. The most pronounced difference was detected at 1,745 cm^{-1}, attributed to C = O stretching vibrations, suggesting alterations related to oxidative processes in the fingernails of children with IBD. **Conclusions:** ATR FTIR spectroscopy demonstrated potential for identifying disease-related biochemical changes in the fingernails of paediatric patients with IBD. The observed spectral differences indicate keratin derangements associated with oxidative stress and visible nail alterations. These preliminary findings justify further investigation of ATR FTIR fingernail analysis in larger cohorts and its potential role in monitoring disease-related biochemical changes and dietary interventions, including antioxidant strategies.

Keywords: attenuated total reflectance – Fourier transform infrared spectroscopy, children, inflammatory bowel disease, nails

Streszczenie

Wprowadzenie i cel: Celem niniejszego badania pilotażowego była ocena możliwości zastosowania spektroskopii w podczerwieni z transformacją Fouriera w technice osłabionego całkowitego odbicia jako szybkiej, nieinwazyjnej metody wykrywania biochemicznych zmian w paznokciach u dzieci z nieswoistymi chorobami zapalnymi jelit. **Materiał i metody:** Widma spektroskopii w podczerwieni z transformacją Fouriera w technice osłabionego całkowitego odbicia uzyskano z obciętych fragmentów paznokci pobranych od 10 dzieci z rozpoznaną nieswoistą chorobą zapalną jelit oraz od 10 zdrowych dzieci dobranych pod względem wieku. Analiza widmowa koncentrowała się na charakterystycznych pasmach drgań związanych ze strukturą keratyny, w tym drganiach rozciągających N–H, asymetrycznych drganiach rozciągających grup

CH_2 i CH_3 oraz symetrycznych drganiach grup CH_3. **Wyniki:** Porównawcza analiza widmowa wykazała subtelne, lecz powtarzalne różnice pomiędzy grupą dzieci z nieswoistą chorobą zapalną jelit a grupą kontrolną. Zaobserwowano przesunięcia pasm związanych z aminokwasami budującymi keratynę, szczególnie w obszarach odpowiadających drganiom rozciągającym N–H oraz C–H. Najbardziej wyraźną różnicę stwierdzono przy 1745 cm^{-1}, przypisywaną drganiom rozciągającym grupy C = O, co może wskazywać na zmiany związane z procesami oksydacyjnymi w paznokciach dzieci z nieswoistą chorobą zapalną jelit. **Wnioski:** Spektroskopia w podczerwieni z transformacją Fouriera w technice osłabionego całkowitego odbicia wykazała potencjał w identyfikacji zmian biochemicznych związanych z chorobą w paznokciach dzieci z nieswoistą chorobą zapalną jelit. Zaobserwowane różnice widmowe mogą wskazywać na zaburzenia struktury keratyny związane ze stresem oksydacyjnym oraz widocznymi zmianami w obrębie paznokci. Uzyskane wstępne wyniki uzasadniają dalsze badania z wykorzystaniem analizy paznokci metodą spektroskopii w podczerwieni z transformacją Fouriera w technice osłabionego całkowitego odbicia w większych grupach pacjentów oraz ocenę jej potencjalnej roli w monitorowaniu biochemicznych zmian związanych z chorobą i interwencji dietetycznych, w tym strategii antyoksydacyjnych.

Słowa kluczowe: spektroskopia w podczerwieni z transformacją Fouriera w technice osłabionego całkowitego odbicia, dzieci, nieswoiste choroby zapalne jelit, paznokcie

INTRODUCTION

Inflammatory bowel disease (IBD) may be accompanied by numerous extraintestinal complications. The most common sites of involvement include the skin, eyes, kidneys, joints, vascular system, liver, biliary tract, and bone mineralisation[1,2]. Except for onychomycosis, the available data on the profile of nail changes in IBD patients remain limited. In the adult population, significantly more common changes include onychomycosis, subungual hyperkeratosis, and brownish discolouration of nails[2].

Nail keratin and bone collagen are related structural proteins that require disulphide bonds for stability. Several studies have revealed that spectroscopic methods, particularly Raman spectroscopy of keratin, have potential as a diagnostic tool to screen bone quality and identify patients at risk of fracture for reasons other than low bone mineral density (BMD) in the adult female population[3–5].

The prevalence of low BMD in paediatric patients with IBD ranges from 5 to 70%[6–8]. Crohn's disease (CD) patients are more likely to demonstrate lower BMD values than subjects with ulcerative colitis (UC)[9]. BMD measurements form the basis for bone mass estimation. It is known that, ideally, bone formation must be at its most intense in the early years of life to reach peak bone mass (PBM) around the age of 30 years, after which BMD slowly decreases. Early detection of bone disorders may therefore be helpful in the clinical management of patients with decreased PBM in young adulthood. Dual-energy X-ray absorptiometry remains the gold standard for BMD assessment. However, it involves exposure to ionising radiation and provides an estimation of bone density (bone mass) only.

A few studies conducted in recent years indicate the usefulness of quantitative ultrasound (QUS) at the hand phalanges in detecting skeletal changes in paediatric populations with type 1 diabetes, end-stage renal disease, and coeliac disease. Nevertheless, it has been shown that QUS is not an appropriate method for bone status assessments in paediatric IBD patients[10].

Therefore, searching for a method that does not expose patients to radiation, while providing deeper insights into biomechanical bone properties and remaining suitable for entire populations, especially children, is a desirable goal.

Another spectroscopic technique, namely attenuated total reflectance – Fourier transform infrared (ATR-FTIR) spectroscopy, is a non-destructive, cost-effective, and reproducible method for sample analysis. By measuring characteristic absorbance peaks in the mid-infrared range (MIR, 4,000–400 cm^{-1}), FTIR spectroscopy provides a holistic view of the chemical composition of biological samples, including the detection of macromolecules, such as nucleic acids, proteins, and lipids[11].

Regarding the paediatric population, numerous notable reports can be found in the literature dealing with the use of ATR-FTIR for gallstone characterisation[12], to discriminate patients with autism spectrum disorders from healthy controls[13], or to differentiate normal brain tissue from medulloblastoma in the 1,800–800 cm^{-1} region[14]. ATR-FTIR spectroscopy is also likely to offer promising potential for the early screening of B-cell precursor lymphoblastic leukaemia[15]. In the adult population, Coopman et al. found that glycated protein concentrations reflected average glycaemia levels the preceding few months[16]. Another study, conducted with participation of type 2 diabetes patients, showed that the fingernail compositional/material properties (assessed by the FTIR spectroscopy) might be a non-invasive surrogate marker of bone quality[17].

This pilot study aimed to identify and assess differences in ATR-FTIR spectra and elemental fingernail composition between children with IBD and healthy controls, evaluating the feasibility of these approaches for detecting disease-related biochemical alterations.

MATERIALS AND METHODS

Subjects

This study included ten (10) children with IBD: seven children with UC and three with CD. All patients were

Parameter	Patients ($n = 10$, ♂)	Controls ($n = 10$, ♂)
Age [years] ± *SD*	16.32	16.84
SDS-Weight [kg]*	−0.76	0.45
SDS-Height [mm]*	−0.81	0.55
* Significant difference ($p < 0.05$). ♂ – male.		

Tab. 1. Characteristic features of study and control participants

Parameter	Patients ($n = 10$, ♂)
Disease duration [years] ± *SD*	3.2
Ulcerative colitis Crohn's disease	7 3
Disease activity: • mild • moderate • severe	 3 6 1

Tab. 2. Characteristic features of patients with inflammatory bowel disease

hospitalised at the Public Clinical Hospital in Zabrze in 2023. The inclusion criteria comprised an age range of 6–18 years and an established diagnosis of IBD based on the Porto criteria[18].

The following clinical parameters were recorded for each patient: disease duration, disease activity, and treatment methods. The median age of the study group was 16.3 years (range: 14–18 years). Only boys were included in the study to avoid potential nail contamination from nail polish residue. All fingernail samples were obtained in the course of routine medical tests. The control group consisted of 10 healthy, age-matched boys. The characteristic features of the study and control group participants are summarised in Tabs. 1 and 2.

The study protocol was approved by the Ethics Committee of the Medical University of Silesia (Approval Code: PCN/CBN/0052/KB1/36/22; Approval Date: 21.06.2022). Informed consent for the participation of minors was obtained from their parents or legal guardians. All methods were performed in accordance with the relevant guidelines and regulations.

Nail material analysis

A single fragment of the thumbnail distal edge, at least 1 mm in length, was obtained from each subject using stainless steel scissors. The scissors were cleaned with sterile gauze before use. Each collected nail fragment was washed with distilled water to remove impurities, then coded and stored in zip-lock bags at room temperature until ATR-FTIR spectroscopic analysis. The ATR-FTIR spectroscopy analysis targeted both the inner and outer sides of the collected nail fragments.

ATR-FTIR spectroscopy

Infrared spectroscopy is increasingly used in the assessment of biological materials. This technique involves the interaction of scanned matter with electromagnetic radiation, analysing the intensity and position of vibrational bands characteristic of the various groups of atoms present in a molecule. The position of each band in the spectrum is closely related to its specific molecular structure and the presence of distinct bonds or functional groups[11].

FTIR spectroscopic nail examinations of the IBD patients and healthy controls were performed using a Thermo Nicolet 8700A FITR spectrometer equipped with a Smart Orbit™ diamond ATR attachment. The ATR method, which has been widely used for over a decade, is a highly useful analytical technique compared to transmission techniques. It is also widely recognised for its simplicity, rapid processing, and non-destructive nature. Furthermore, it requires no special sample preparation, which is a particularly important feature for nail analysis[19]. The use of the ATR technique enabled the direct examination of both the external and internal sides of the nail samples. Spectra were collected in the MIR range of 4,000–400 cm^{-1} with a resolution of 4 cm^{-1}, using a DTGS (deuterated triglycine sulfate) detector. Maximum pressure was applied to the diamond crystal for each tested sample. The resulting spectra were subjected to ATR correction, baseline correction, and scaled normalisation. After these steps, the obtained spectra were equivalent to transmission spectra.

Elemental composition SEM-EDS

The nail samples obtained from the patients and healthy controls were examined using a Quanta 3D FEG (FEI) scanning electron-ion microscope. The flexible vacuum and optical system of this microscope enables imaging of the topography and surface morphology of micro- and nanostructures of the examined materials in high- and low-vacuum modes, as well as in the environmental mode. Consequently, this microscope is well-suited for imaging material samples, polymers, and biological specimens. The Quanta 3D FEG microscope is equipped with an energy-dispersive X-ray spectroscopy (SEM-EDS) system featuring a fast Octane Elect Plus detector. Microanalysis (elemental composition) was performed on the tested samples using SEM-EDS. The tests were conducted under the following operating conditions: an acceleration voltage of HV = 20 kV, a high-vacuum environment, and data collection via the Octane Elect Plus EDS detector.

RESULTS

ATR-FTIR spectroscopy

The initial stage of the study involved a comparison of two sides of the nail samples from both the patients and the controls. For this purpose, tests were carried out on the ten samples from the healthy controls and the ten samples from the IBD patients. Fig. 1 shows examples of the averaged spectra obtained from the external and internal nail sides of all subjects.

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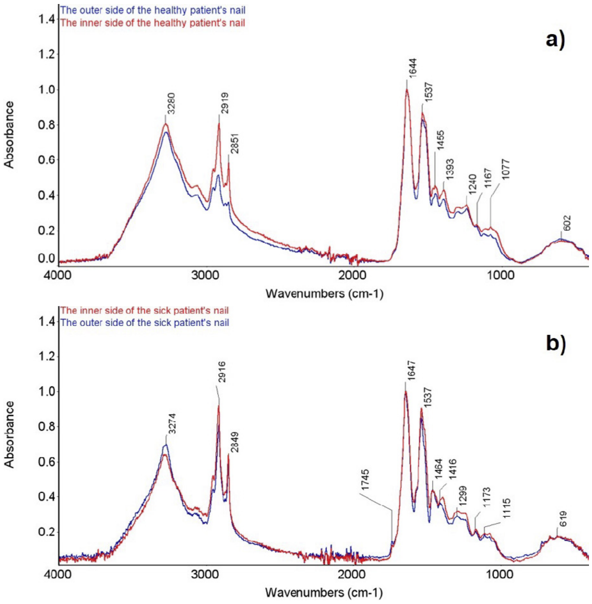

Fig. 1. Comparison of ATR-FTIR averaged spectra from the outer and inner nail sides in: **a)** *healthy controls,* **b)** *IBD patients*

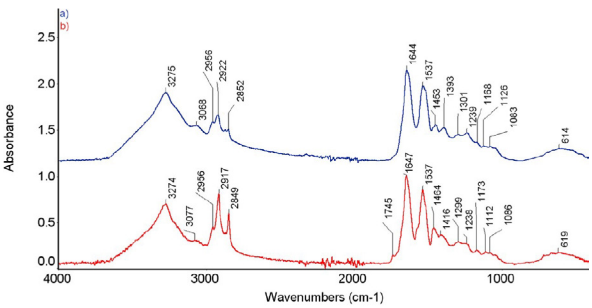

Fig. 2. Comparison of ATR-FTIR spectra of nails from: **a)** *healthy controls,* **b)** *IBD patients*

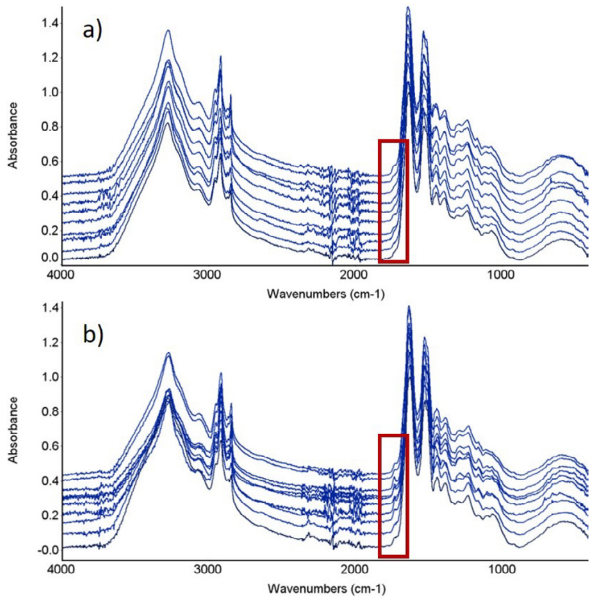

Fig. 3. ATR-FTIR spectra of nails from: **a)** *healthy controls,* **b)** *IBD patients*

The analyses revealed no significant differences between the healthy controls and the IBD patients regarding their nail spectra results. Furthermore, no significant differences in spectral band positions were observed.

The subsequent research stage involved the detailed spectral characterisation of human nails based on the spectra obtained from the study and control groups. Examples of these test results are presented in Fig. 2. To identify spectral features unique to IBD patients, the ATR-FTIR spectra of nails from the patients and healthy controls were compared. The interaction of electromagnetic radiation with the surface of human nails increases the vibrational amplitude of the molecules of chemical compounds present in nails. The resulting spectrum provides information about the key

Wavenumber [cm^{-1}]		Differences in band position [cm^{-1}]	Assignment	Description/Contributions
Healthy controls	Patients			
3,275	3,274	1	N–H stretching	Amide A (proteins, keratins)
3,086	3,077	9	=C–H stretching (olefinic/aromatic C–H)	Lipids and proteins
2,956	2,956	0	C–H asymmetric stretching of CH_3	Lipids and proteins
2,922	2,917	5	C–H asymmetric stretching of CH_3	Lipids and proteins
2,852	2,849	3	C–H symmetric stretching in CH_2	Lipids and proteins
-	1,745		C = 0 stretching (ester carbonyl)	Lipid esters; lipid peroxidation products
1,644	1,647	3	C = 0 stretching	Amide I
1,537	1,537	0	N–H bending coupled with C–N stretching	Amide II
1,453	1,464	12	CH_2, CH_3 asymmetric bending modes	Lipids and proteins
1,393	1,416	23	Symmetric mode of CH_3	Amino acids chains proteins
1,301	1,299	2	N–H bending	Amide III
1,239	1,238	1	C–N stretching, asymmetric stretching mode of PO_2	Amide III, nucleic acid
1,083	1,086	3	Symmetric stretching of PO_2	Nucleic acid

Tab. 3. Positions of characteristic peaks and their assigned chemical bonds in the ATR-FTIR spectra of human nails from patients and healthy controls[(21)]

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Healthy controls	1	2	3	4	5	6	7	8	9	10
	0.186	0.002	0.140	0.112	0.188	0.163	0.027	0.130	0.030	0.147
Patients	1	2	3	4	5	6	7	8	9	10
	0.317	0.266	0.820	0.490	0.393	0.103	0.370	0.472	0.133	0.227

Tab. 4. Values of the area under the peak determined for the region 1,767–1,721 cm^{-1} for healthy controls and patients

components of human nails. The main constituent of nails is a fibrous protein called keratin, formed by long chains of amino acids linked together by amide bonds.

The present study showed that, apart from these proteins, spectral bands characteristic of other components, such as nucleic acids (1,250–1,000 cm^{-1}), lipids (3,000–2,800 cm^{-1}), and carbohydrates (1,000–800 cm^{-1}), were also present[20]. Tab. 3 shows the assignment of specific chemical bonds to the peaks appearing in the ATR-FTIR spectra available compiled from the literature on the nails of both healthy subjects and patients with various pathologies.

The conducted tests showed that the most significant differences in the locations of spectral bands, exceeding the FTIR spectrometer's resolving capacity, occurred at 3,086 cm^{-1}, 1,453 cm^{-1}, and 1,393 cm^{-1}. The most significant difference between the ATR-FTIR spectra of the healthy controls and the patients was the appearance of an additional peak at 1,745 cm^{-1} in the spectra of IBD patients, which corresponded to the stretching vibrations of C = O groups.

The subsequent stage of the research involved obtaining the ATR-FTIR spectra for the ten healthy subjects and ten patients. The resulting ATR-FTIR spectra are shown in Fig. 3. The peak area values at 1,745 cm^{-1} were determined from the obtained spectra. The study results are presented in Tab. 4.

The data showed a significantly higher peak area value at 1,745 cm^{-1} in the patients compared to the healthy controls. Therefore, it may be assumed that an increased number of C = O groups is a characteristic feature of patients with IBD.

SEM-EDS

An analysis using the SEM-EDS technique was performed to compare the elemental composition of the nails between healthy subjects and patients. The test results for two healthy controls and two sick patients are presented in Tabs. 5 and 6. Two measurements were performed for each subject.

SEM-EDS studies of the nails did not show significant differences in the content of carbon, oxygen, and nitrogen between the healthy controls and the patients. Moreover, in the healthy subjects, the presence of iron was detected at levels below 1% by weight, and nickel was also detected at levels below 1% by weight.

DISCUSSION

While comparing the inner and outer sides of fingernails obtained from healthy children and paediatric IBD patients, no global or systematic spectral differences were observed between the two nail surfaces. To the best of our knowledge, there are no existing literature reports indicating side-dependent spectral differences in human fingernails, which supports the internal consistency of the present analysis.

Keratin, the major structural component of nails, is a fibrous protein composed of 18 different amino acids. The dominant amino acids forming the keratin polypeptide chain include glycine, alanine, serine, valine, and cysteine. The keratin structure is characterised by extensive folding stabilised by highly stable disulphide bonds, van der Waals interactions, hydrogen bonds, and coulombic forces. Disulphide bonds formed by cysteine residues provide structural strength, whereas other amino acids contribute to hydration, flexibility, and overall stability of the nail plate[22].

In the present study, subtle but reproducible differences were observed in selected spectral band positions exceeding the resolving capacity of the FTIR spectrometer, specifically at 3,086 cm^{-1}, 1,453 cm^{-1}, and 1,393 cm^{-1}. The band at 3,086 cm^{-1} was detected in healthy children, whereas a shifted band at 3,077 cm^{-1} was observed in IBD patients. These bands are commonly associated with C–H stretching vibrations present in aromatic rings of amino acids such as phenylalanine and tyrosine, which are integral components of nail keratin. Aromatic amino acid rings (phenol groups) contribute to hydrophobic interactions within the keratin structure, supporting the stability of its secondary and tertiary organisation and, consequently, increasing nail hardness and resistance to mechanical damage, alongside the critical role of cysteine-mediated disulphide bonds[22,23].

Similarly, the band at 1,453 cm^{-1} observed in healthy children and the corresponding band at 1,464 cm^{-1} in IBD patients are associated with asymmetric CH_2 and CH_3 bending modes characteristic of lipids and proteins. Amino acids containing methyl ($-CH_3$) and methylene ($-CH_2-$) groups in their side chains include alanine, valine, leucine, isoleucine, and serine, while tyrosine and phenylalanine may also contribute via their side chains. These amino acids are fundamental constituents of keratin[22]. Additionally, the band at 1,393 cm^{-1} observed in healthy children and the shifted band at 1,416 cm^{-1} in IBD patients correspond to symmetric CH_3 vibrational modes and may likewise reflect alterations in amino acid side-chain environments.

Taken together, these localised spectral shifts suggest subtle changes in keratin structure in the fingernails of children with IBD. Although these findings do not indicate global structural disruption, they may reflect early or mild biochemical modifications. Larger cohort studies are required

Element	Patient 5		Patient 6	
	Measurement 1	Measurement 2	Measurement 1	Measurement 2
	Wt%	Wt%	Wt%	Wt%
C	56.65	56.43	56.74	56.66
O	23.33	23.90	24.28	23.93
N	17.83	17.41	17.61	17.83
S	1.44	1.38	<1.00	<1.00
Cl	<1.00	<1.00	<1.00	<1.00
Na	<1.00	<1.00	<1.00	<1.00
Si	<1.00	<1.00	<1.00	<1.00
P	<1.00	<1.00	<1.00	<1.00
K	<1.00	<1.00	<1.00	<1.00
Ca	<1.00	<1.00	<1.00	<1.00

Wt% – weight percent.

Tab. 5. Elemental composition of the nails of patients obtained by SEM-EDS X-ray spectrometry

Element	Healthy subject 15		Healthy subject 16	
	Measurement 1	Measurement 2	Measurement 1	Measurement 2
	Wt%	Wt%	Wt%	Wt%
C	57.71	56.29	54.34	57.70
O	22.91	23.45	25.11	22.17
N	16.87	17.43	19.18	17.48
S	1.48	1.71	<1.00	<1.00
Cl	<1.00	<1.00	-	1.84
Si	<1.00	<1.00	<1.00	-
P	<1.00	<1.00	<1.00	<1.00
Na	<1.00	<1.00	<1.00	<1.00
K	<1.00	<1.00	<1.00	<1.00
Ca	<1.00	<1.00	<1.00	<1.00
Fe	<1.00	<1.00	<1.00	<1.00
Ni	<1.00	-	<1.00	-

Wt% – weight percent.

Tab. 6. Elemental composition of the nails of healthy controls obtained by SEM-EDS X-ray spectrometry

to further characterise the biological relevance and reproducibility of these observations.

In contrast to the findings reported by Towler et al., the present analysis did not detect changes in the disulphide (S–S) stretching vibration at approximately 510 cm^{-1}. Towler's Raman spectroscopy study assessed fingernail disulphide content in a cohort of 169 women and demonstrated significant associations between S–S bond intensity and fracture risk, suggesting that changes in keratin disulphide bonding may reflect clinically relevant alterations in bone protein integrity[3]. The absence of detectable S–S bond changes in the present paediatric cohort may reflect differences in underlying disease mechanisms, age-related factors, or methodological sensitivity.

Against this background, the most pronounced difference between healthy controls and IBD patients was observed in the C = O stretching region at 1,745 cm^{-1}. Quantitative peak area analysis revealed a significantly larger signal in the IBD group. Although lipid-associated bands in the 1,745–1,740 cm^{-1} range have been reported in various tissues, their presence is often interpreted as an indicator of lipid peroxidation and oxidative stress-related damage[24,25]. In general, the absence of these bands correlates with tissue integrity, whereas their emergence may serve as a spectral marker of oxidative injury.

Several studies support the interpretation of this band as a marker of oxidative stress. Kyriakidou et al. identified a band at 1,744 cm^{-1} in malignant skin regions, attributing it to aldehyde groups formed during lipid peroxidation initiated by reactive oxygen species (ROS)[26,27]. Similarly, Anastassopoulou et al. associated the 1,744 cm^{-1} band with malondialdehyde accumulation, proposing its application as a diagnostic indicator of cancer progression[28]. Kotoulas et al. reported an intensified 1,744 cm^{-1} band in the vascular tissues of patients with elevated serum glucose, linking it to oxidative stress-induced lipid hydroperoxidation and subsequent aldehyde formation[29]. Comparable findings have been reported in studies employing synchrotron radiation-based FTIR spectroscopy, where the appearance of a 1,743 cm^{-1} peak was associated with cellular death processes[30]. Altered lipid oxidation signatures in the 1,740 cm^{-1} region have also been reported in multiple sclerosis and Alzheimer's disease, further reinforcing the association between this spectral feature and oxidative stress-related pathology[31,32].

These mechanisms provide a plausible systemic link between intestinal inflammation and peripheral tissues such as the nail plate. Oxidative stress plays a well-documented role in the pathogenesis of IBD, where excessive production of ROS and reactive nitrogen species (RNS) contributes to mucosal injury and chronic inflammation[33]. ROS, including superoxide anion, nitric oxide, hydroxyl radicals, hydrogen peroxide, and singlet oxygen, are generated through the inflammation-mediated upregulation of enzymes such as lipoxygenases, myeloperoxidase, inducible nitric oxide synthase, cyclooxygenase-2, and NADPH oxidase[34]. RNS arise primarily from nitric oxide synthase activity and further contribute to oxidative and nitrosative stress[33].

To maintain cellular homeostasis, these oxidative processes must be counterbalanced by enzymatic and non-enzymatic antioxidant systems. Antioxidant enzymes – such as catalase, superoxide dismutase, glutathione peroxidase, peroxiredoxins, and paraoxonase – constitute the first line of defence, while non-enzymatic antioxidants, including glutathione, uric acid, bilirubin, carotenoids, and vitamins A, C, and E, provide additional protection[35,36]. Persistent oxidative imbalance results in lipid peroxidation, protein oxidation, and DNA damage, processes that are closely linked to IBD pathophysiology[37,38].

Lipid peroxidation, in particular, disrupts cellular membranes, thereby contributing to intestinal barrier dysfunction, increased permeability, and the activation of inflammatory cascades in IBD[39]. Secondary lipid peroxidation products, such as malondialdehyde, 4-hydroxy-2-nonenal, isoprostanes, and volatile alkanes, have been extensively investigated as biomarkers of oxidative stress[36]. While numerous studies have examined these markers in adult populations, data regarding paediatric IBD remain limited. Monasta et al. identified volatile organic compounds in alveolar air as potential non-invasive biomarkers of paediatric IBD, highlighting the need for accessible, child-friendly monitoring approaches[40].

The findings of the present study suggest that oxidative stress may contribute to the nail plate derangements observed in children with IBD. In adult populations, elevated oxidative stress markers have been reported in peripheral tissues, including nails, as demonstrated by Grešner et al. in occupational exposure studies[41]. However, to our knowledge, no previous studies have specifically investigated oxidative stress-related nail alterations in paediatric IBD using spectroscopic techniques.

Dietary modifications, including antioxidant supplementation, may modulate oxidative processes and aid in controlling inflammation in IBD. While antioxidant therapy has been proposed as a supportive treatment strategy, further clinical studies are required to establish standardised protocols and evaluate therapeutic efficacy. In this context, ATR-FTIR spectroscopy of fingernails represents a promising non-invasive approach for monitoring biochemical changes associated with oxidative stress. This is particularly relevant in paediatric populations, where invasive sampling methods are limited.

Additionally, elemental analysis of nail samples using SEM-EDS revealed no significant differences in mineral composition between healthy controls and IBD patients. Although elemental concentrations in nails are known to vary widely due to individual and environmental factors[22,42,43], the lack of consistent elemental alterations suggests that the observed spectral changes are primarily related to biochemical modifications rather than variations in mineral composition.

Several limitations of this pilot study should be acknowledged. The sample size was relatively small, reflecting the exploratory nature of the investigation, and only male participants were included to avoid potential contamination from nail cosmetics. Future studies involving larger, gender-balanced cohorts, longitudinal follow-ups, and structured assessments of dietary and pharmacological interventions are warranted to further evaluate the utility of ATR-FTIR spectroscopy for studying nail derangements associated with paediatric IBD.

CONCLUSIONS

This pilot study applied ATR-FTIR spectroscopy and EDS X-ray analysis to investigate the biochemical and elemental characteristics of fingernails collected from paediatric patients with IBD and age-matched healthy controls. While no global or systematic spectral differences were observed between the inner and outer nail surfaces across the study groups, localised and reproducible alterations in specific vibrational regions were successfully identified.

Differences in bands associated with N–H and C–H stretching vibrations suggested subtle changes in keratin structure, whereas the most pronounced alteration was observed in the C = O stretching region at 1,745 cm^{-1}. Quantitative peak area analysis revealed a significantly increased signal in the IBD group, which may reflect oxidative stress-related modifications affecting the nail plate. In contrast, no significant differences in elemental composition were detected among the groups.

These findings indicate that ATR-FTIR spectroscopy may provide valuable insights into disease-related biochemical alterations in fingernails and support its feasibility as a non-invasive analytical approach for studying nail derangements associated with paediatric IBD. Further studies involving larger cohorts and longitudinal designs are warranted to evaluate its potential role in monitoring biochemical changes and assessing the impact of therapeutic and dietary interventions, including targeted antioxidant strategies.

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Conflict of interest

The authors do not report any financial or personal connections with other persons or organisations which might negatively affect the content of this publication and/or claim authorship rights to this publication.

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Institutional review board statement

The study protocol was approved by the Ethics Committee of the Medical University of Silesia (Approval Code: PCN/CBN/0052/KB1/36/22; Approval Date: 21.06.2022).

Informed consent statement

Informed consent was obtained from all participants involved in the study.

Author contribution

Original concept of study: KKBD, UM, SB, WSC. Collection, recording and/or compilation of data; analysis and interpretation of data: KKBD, UM, NM, SB, NS, TT, WSC. Writing of manuscript: KKBD, UM, NM, SB, JK, NS, TT, WSC. Critical review of manuscript; final approval of manuscript: KKBD, JK, WSC.

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