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Review article: Sample preparation and recent trends in volatolomics for diagnosing gastrointestinal diseases

Tomasz Majchrzak, Wojciech Wojnowski, Grażyna Piotrowicz, Jacek Gębicki, Jacek Namieśnik

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## ACCEPTED MANUSCRIPT

1 2	Review article: Sample preparation and recent trends in volatolomics for diagnosing gastrointestinal diseases
3	Tomasz Majchrzak* <sup>1</sup> , Wojciech Wojnowski* <sup>1</sup> , Grażyna Piotrowicz <sup>2</sup> , Jacek Gębicki <sup>3</sup> , and Jacek Namieśnik <sup>1</sup>
5 6 7 8	<sup>1</sup> Gdansk University of Technology, Faculty of Chemistry, Department of Analytical Chemistry <sup>2</sup> Gdansk Hospital of the Ministry of the Interior and Administration, Department of Gastroenterology <sup>3</sup> Gdansk University of Technology, Faculty of Chemistry, Department of Chemical and Process Engineering
9	*tomasz.majchrzak@pg.edu.pl, wojciech.wojnowski@pg.edu.pl
10	ABSTRACT
11 12 13 14 15 16 17 18	The analysis of the human volatilome can be successfully used for rapid and non-invasive diagnostics of gastrointestinal diseases. However, the introduction of techniques based on detection of volatiles is limited, among other factors, by difficulties which arise during the sampling stage and instrumental analysis. The aim of this article was to review and discuss medical and analytical literature on the analysis of volatiles in diagnostics of gastrointestinal disorders and to elaborate on technical aspects of sampling and analysis of volatile organic compounds in this context. The easily overlooked technical aspects of the sampling and analysis of volatiles can have a significant impact on the outcome of the classification. In order to introduce headspace analysis into clinical practice, it is necessary to standardise upon the best available techniques and to introduce external validation of the results.
20 21	<b>KEYWORDS:</b> gastrointestinal diseases; medical diagnostics; volatolomics; non-invasive diagnostics; breath analysis; sampling; faeces; urine
22	ABBREVIATIONS
23 24 25 26 27	ANNs- artificial neural networks CA- cluster analysis CP- conducting polymer CD- Crohn's disease CRC- colorectal cancer
28 29 30	DFA- discriminant function analysis DHS- dynamic headspace sampling DI- direct injection
31 32 33 34	DMS- differential ion mobility spectrometry DMAC- N,N-dimethyl acetamide FAIMS- field asymmetric ion mobility spectrometry FS- full scan
35 36 37 38	GC- gas chromatography GCxGC- multi-dimensional gas chromatography GI- gastrointestinal IBD- inflammatory bowel diseases
39 40 41	IBS- irritable bowel syndrome IMR-MS- ion-molecule reactions mass spectrometry IMS- ion mobility spectrometry
42 43 44	MIM- multiple ion monitoring MOS- metal-oxide semiconductors PCA- principal component analysis
45 46 47	PTR-MS- proton transfer reaction mass spectrometry QCM- quartz crystal microbalance SCFAs- short-chain fatty acids
48 49	SESI-MS- secondary electrospray ionisation mass spectrometry SHS- static headspace sampling

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