

ABSTRACT OF THE DOCTORAL DISSERTATION

*Changes in the secondary metabolism of selected living organisms
as a source of signals in analytical measurements*

MSc Eng. Marianna Kostina-Bednarz

Supervisor: Hanna Barchańska, DSc, PhD, Eng, Prof. SUT

Co-supervisor: Joanna Płonka, PhD, Eng.

The presented dissertation addresses the contemporary challenges of analytical chemistry in assessing the effects of exposing living organisms to exogenous compounds, redefining the approach from the traditional measurement of the cause (xenobiotic concentration) to the analysis of the effect (the organism's metabolic response). This complements classical analytical methods, which, although providing precise quantitative data, do not capture the full complexity of interactions at the metabolome level. The main research hypothesis posits that the metabolic profile, and in particular the pattern of changes in secondary metabolism, constitutes a sensitive and reliable source of an analytical signal, enabling a comprehensive assessment of the effects of xenobiotic exposure. The verification of this hypothesis, which was the main objective of the work, was conducted through a multi-stage research strategy that integrated advanced techniques based on the LC-MS platform with chemometric tools. Preliminary studies on the model organism *Saccharomyces cerevisiae* confirmed that contact with xenobiotics and their transformation products induces characteristic and measurable changes in the metabolic profile. In the subsequent stage, the research was extended to crop plants (wheat and barley), comparing the effects of biopesticides (hinokitiol, scopoletin, umbelliferone) with synthetic pesticides (tebuconazole, 2,4-dichlorophenoxyacetic acid). Metabolomic analysis proved to be a highly sensitive tool capable of differentiating the subtle biological effects caused by compounds with different mechanisms of action. Furthermore, tracking the fate of the parent substances and their transformation products within plant tissues confirmed the effectiveness of the adopted approach, even in complex biological matrices. The developed methodologies served as the basis for creating and applying a screening method for the analysis of real samples of edible plants, which allowed for the validation of its diagnostic potential. As a result, this doctoral dissertation, founded on a series of five scientific publications, provides science and practice with validated analytical procedures for broad application in environmental toxicology, sustainable agriculture, and public health, thereby making a significant contribution to the advancement of interdisciplinary research.