

## Abstract

# Bioinformatics Supported Liquid Chromatography–Mass Spectrometry for Characterization of Bacterial Metabolites <sup>†</sup>

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## 1. Introduction

Metabolomics enables the comprehensive characterization of the set of low-molecular-weight compounds that are starting, intermediate, or end products of metabolic transformations in living organisms. Therefore, metabolomics provides information about the mechanisms of action of new potential drugs [1]. Metabolomic fingerprinting or footprinting supported by bioinformatics provides a powerful tool for a comprehensive description of perturbations observed within bacteria, indicating up- or down-regulated bacterial molecules, and altered metabolic pathways [2]. In this sense, metabolomics depicts the metabolic response of bacteria to stress induced by natural products.

## 2. Materials and Methods

Because this field is poorly explored, new findings of the influence of plant-based and medicinal plant-derived compounds on the bacteria metabolism studied with LC-MS metabolomics will be presented.

## 3. Results

This research provides insights into novel molecular targets within bacteria, identifies biomarkers of cellular stress and indicates how the reorganization of the cell envelope impacts bacteria survival under the influence of inhibiting agents.

## 4. Conclusions

LC-MS metabolomics supported by bioinformatics is a powerful tool for the determination of changes in bacterial metabolism.

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## References

1. Sieniawska, E.; Georgiev, M.I. Metabolomics: Towards acceleration of antibacterial plant-based leads discovery. *Phytochem. Rev.* **2021**, 1–17. [[CrossRef](#)]
2. Sieniawska, E.; Sawicki, R.; Golus, J.; Georgiev, M.I. Untargetted metabolomic exploration of the Mycobacterium tuberculosis stress response to cinnamon essential oil. *Biomolecules* **2020**, *10*, 357. [[CrossRef](#)] [[PubMed](#)]