# Chapter 3
# Role of Secondary Metabolites in Essential Oils for Antimicrobial Activity and the Integration of Artificial Intelligence to Optimize Their Use

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## ABSTRACT

*This study investigates the antimicrobial properties of secondary metabolites found in essential oils (EOs) derived from aromatic and medicinal plants (AMP), with a particular focus on the integration of artificial intelligence (AI) into this area of research. Secondary metabolites, including phenols, terpenoids, and flavonoids, are key contributors to the biological activity of EOs, especially their capacity to inhibit pathogenic microorganisms. The research emphasized how AI, using methods such as machine learning (ML) and virtual screening, can improve the identification and analysis of bioactive compounds, simulate interactions between EOs and pathogens, and optimize antimicrobial formulations. By incorporating AI, researchers can accelerate discovery, identify novel metabolite combinations, and address the growing challenge of antimicrobial resistance.*

## INTRODUCTION

Artificial intelligence (AI) is reshaping various scientific disciplines, particularly in addressing the pressing issue of antimicrobial resistance (AMR). With AMR responsible for nearly five million deaths in 2019 and projected to cause 10 million deaths annually by 2050, the urgent need for innovative solutions is clear (Laxminarayan, 2022 ; Murray et al., 2022). Traditional antibiotic discovery faces significant challenges, including the dereplication problem, where previously