Chapter 2
Role of Deep Learning and Machine Learning Algorithms in Identifying and Classifying Secondary Metabolites in Ashwagandha Plant

K. Kavitha
https://orcid.org/0000-0002-9159-9690
Velammal College of Engineering and Technology, Madurai, India

S. Rajkumar
https://orcid.org/0009-0002-0499-9619
Velammal College of Engineering and Technology, Madurai, India

N. Vijay
https://orcid.org/0000-0003-3337-815X
Kalasalingam Academy of Research and Education, India

S. Gandhimathi Alais Usha
Velammal College of Engineering and Technology, Madurai, India

P. Uma Maheswari
Velammal College of Engineering and Technology, Madurai, India

ABSTRACT

Ashwagandha plant (Withania somnifera), celebrated for its therapeutic properties,

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is rich in secondary metabolites like withanolides, alkaloids, and flavonoids, which contribute to its medicinal value. Identifying these metabolites using traditional methods can be labor-intensive and costly. This chapter explores the transformative role of deep learning (DL) and machine learning (ML) algorithms in metabolite identification and classification, integrating them with advanced spectral imaging techniques such as multispectral and hyperspectral cameras. These approaches enable rapid, non-invasive, and precise analysis of metabolite profiles, addressing limitations of conventional techniques. The chapter presents a comprehensive review of recent advancements, highlighting applications of ML/DL in enhancing accuracy and efficiency in metabolomics. Future research directions are discussed, focusing on personalized herbal medicine, biodiversity conservation, and sustainable agriculture.

INTRODUCTION

Ashwagandha (*Withaniasomnifera*), a prominent medicinal plant, is celebrated for its diverse therapeutic properties, largely attributed to its secondary metabolites such as alkaloids, flavonoids, and steroidal lactones. Traditional identification methods for these metabolites can be labor-intensive and less precise. The integration of deep learning (DL) and machine learning (ML) algorithms presents a transformative approach to enhance the identification and classification of secondary metabolites in Ashwagandha.

Medicinal Plant Analysis

The application of advanced computational techniques in medicinal plant analysis has gained traction. Ratnasekhar et al. (2025) demonstrated that deep learning approaches could significantly streamline the identification of secondary metabolites in Ashwagandha by employing neural networks for data classification. Agrahari et al. (2025) highlighted the potential of machine learning algorithms to predict metabolite profiles based on various input parameters, leading to more accurate analyses. Monib (2024) further emphasized the effectiveness of DL models in improving classification accuracy compared to traditional methods. Kalita et al. (2025) utilized machine learning techniques to enhance the detection of bioactive compounds, showcasing significant improvements in accuracy. Singh et al. (2025) provided insights into the applicability of DL in analyzing secondary metabolites, reinforcing the importance of computational techniques in the medicinal plant domain.