

# Development of an R Toolbox for Near-Infrared Spectroscopy Data Processing and Analysis of Plant Metabolic Phenotypes

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MSC. LIFE SCIENCE INFORMATICS

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December 11, 2024

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# Chapter 1

## Introduction

The advancement and widespread use of high-throughput experimental technologies in the field of plant biology have introduced significant challenges in managing and analysing the vast datasets effectively. Addressing these challenges require innovative methods that maximize the data utility while minimizing computational inefficiencies and resource consumption, ensuring robust insights into complex biological systems (<https://www.frontiersin.org/research-topics/6856/machine-learning-in-plant-science/articles>). Machine learning has rapidly evolved and is now widely applied in science in general and in plant genotyping and phenotyping in particular.

### 1.1 Related Work

The related work include, the followings

# Chapter 2

## Background

The background of this study include

### 2.1 Near Infrared Spectroscopy (NIRS)

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#### 2.1.1 Introduction

### 2.2 Metabolomics

#### 2.2.1 Introduction

#### 2.2.2 Mass Spectrometry

### 2.3 Machine Learning

#### 2.3.1 Introduction

#### 2.3.2 Partial Least Square Regression (PLS)

#### 2.3.3 Random Forest (RF)

#### 2.3.4 Convolutional Neural Network (CNN)



# Chapter 3

## Methods and Implementation

### 3.1 MSNovelist

#### 3.1.1 Basic Idea of the Software

#### 3.1.2 Deep Learning Architecture

#### 3.1.3 Preparation of Data

### 3.2 Data

#### 3.2.1 Data Records

#### 3.2.2 File Formats

### 3.3 Evaluation of the Training

### 3.4 Implementations in the TensorFlow Framework

#### 3.4.1 Preprocessing of Data

#### 3.4.2 Training

#### 3.4.3 Evaluation

#### 3.4.4 Termination Criterion

#### 3.4.5 Training on the Pubchem Dataset

### 3.5 Implementations in the PyTorch Framework

#### 3.5.1 Reimplementation of the LSTM Architecture

#### 3.5.2 Training with DeepSMILES and SELFIES

#### 3.5.3 Transformer Implementation

### 3.6 Software

### 3.7 Hardware

# Chapter 4

## Results and Discussion

### 4.1 Baseline Model

#### 4.1.1 Termination Criterion

#### 4.1.2 Impact of the Amount of Data

#### 4.1.3 Duplicates in the Fingerprints

### 4.2 Alternative Tokenization of SMILES Sequences

#### 4.2.1 QBMG Tokenization