

**WAB**

Provadis School of International Management and Technology

# **Examining Random Forest vs Neural Networks for LogP Prediction of Drug-like Compounds**

A Proof-of-Concept Implementation and Performance Analysis

Rubin Chempananickal James

rubin.chempananickal-james@stud-provadis-hochschule.de

Matriculation Number: D876

Department: Information Technology

Module: Fortgeschrittene Programmierung

Reviewer: Prof. Dr. Henrik Paul

February 18, 2026

# Abstract

# Contents

<b>Abstract</b>	<b>II</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Background . . . . .	1
1.2 Research Questions . . . . .	1
<b>2 Methods</b>	<b>2</b>
2.1 Design . . . . .	2
2.2 Data Collection . . . . .	2
<b>AI Declaration</b>	<b>i</b>
<b>Declaration of Authorship</b>	<b>iii</b>

# List of Figures

# List of Tables

# 1 Introduction

## 1.1 Background

## 1.2 Research Questions

## 2 Methods

### 2.1 Design

### 2.2 Data Collection

# AI Declaration

The usage of AI tools within this project is documented here. I solemnly declare that I have documented all interactions with AI tools, including the prompts used and the outputs received.

System	Prompt	Usage
GitHub Copilot 1	Asked to delete the existing project and provide a simple LaTeX template with a shared preamble, a Chapters subdirectory, TOC, glossary, abbreviations, and Roman numerals for non-content pages.	Template structure and LaTeX setup provided
GitHub Copilot 2	Requested additional title page lines (WAB header, reviewer, module) for the main document.	Title page metadata and layout updated
GitHub Copilot 3	Requested uppercase Roman numerals for front matter and lowercase Roman numerals for back matter page numbering.	Page numbering adjusted in main and exposee
GitHub Copilot 4	Requested exposee title page to include shared info fields (WAB header, department, module, reviewer).	Exposee title page updated to include shared metadata
GitHub Copilot 5	Requested adding the provadis-hochschule.pdf logo to the top right corner of both main and exposee title pages.	Logo added to top right of both title pages
GitHub Copilot 6	Reported that Glossary and Abbreviations sections were missing from compiled output.	Added example <code>\newacronym</code> entries to <code>abbreviations.tex</code> so the Abbreviations section displays properly



System	Prompt	Usage
GitHub Copilot 7	Reported that glossary section still not appearing in final PDF.	Updated <code>settings.tex</code> to include <code>automake</code> option in <code>glossaries</code> package to enable automatic glossary generation
GitHub Copilot 8	Asked for boilerplate to train a TFLite model for ESP32 to estimate logP from SMILES.	Provided a Python training script (RD-Kit + Keras) with TFLite export
GitHub Copilot 9	Asked how to run inference on an ESP32 with the trained model.	Provided a high-level TFLite Micro deployment workflow for ESP32
GitHub Copilot 10	Asked for a beginner-friendly README in Code/ with step-by-step setup and usage.	Added a novice-oriented Code/README.md with installation, training, and ESP32 notes
GitHub Copilot 11	Asked for a TFLite Micro skeleton and beginner ESP32 setup steps.	Added Code/tflite_micro_skeleton.cpp and expanded Code/README.md with ESP32 instructions
GitHub Copilot 12	Reported the TFLite Micro skeleton was incomplete.	Completed the skeleton with quantized support, Arduino setup, and a runnable loop
GitHub Copilot 13	Asked to avoid Roman-numbered pages in glossary references.	Explained how <code>\glsaddall</code> affects page references

# Declaration of Authorship

I hereby confirm that I have personally and independently prepared the present work and have not used any sources or aids other than those specified. All passages taken verbatim or in substance from other sources are identified as such. The drawings, illustrations and tables in this work are created by me or have been provided with an appropriate source reference. This work has not been submitted by me to any other university in the same or similar form for the acquisition of an academic degree.

Frankfurt, February 18, 2026 .....

Rubin Chempananickal James