Can These Two Drugs Be the Same?

A deep learning approach to identify drugs from their chemical fingerprints





Introduction

- Forensic drug detection
- Mass spectrometry
- Limitation of traditional methods
- Challenge: new & similar compounds
- Need: fast, scalable, accurate approach
- Solution: Siamese Neural Network (SNN)
- Task: Compare spectra

Method

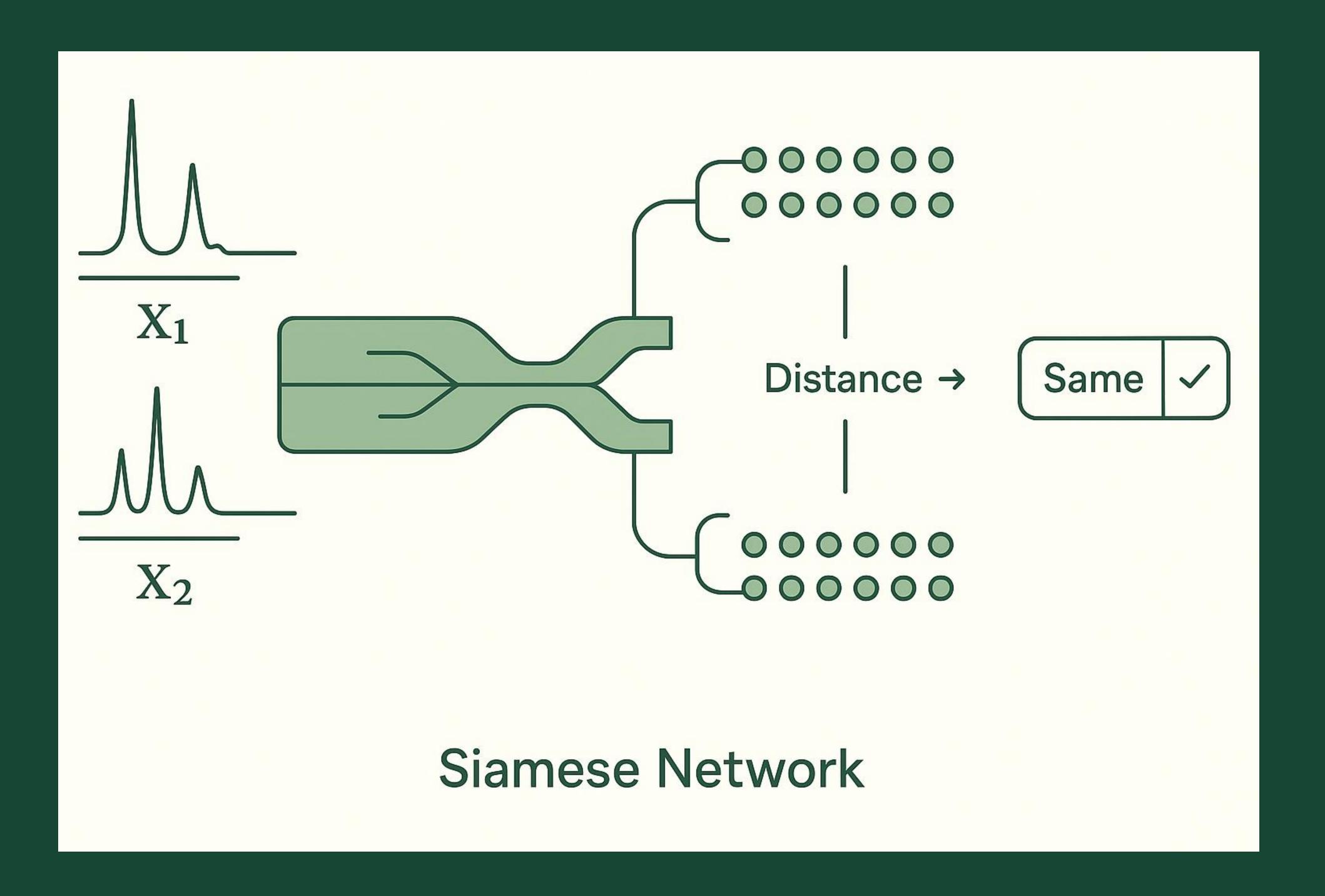
- Input data: 136 spectra (3 drug families)
- Neural Network: CNN + LSTM
- Siamese model
- Training: Balanced same/different pairs
- Prediction: Same or Different

Results

- Confirms strong model accuracy
- Very few misclassifications
- Balanced, unbiased results
- Supported by perfect family classification

GROUP
A-04

Our model compares drug fingerprints to tell if they match, even when the data looks slightly different.

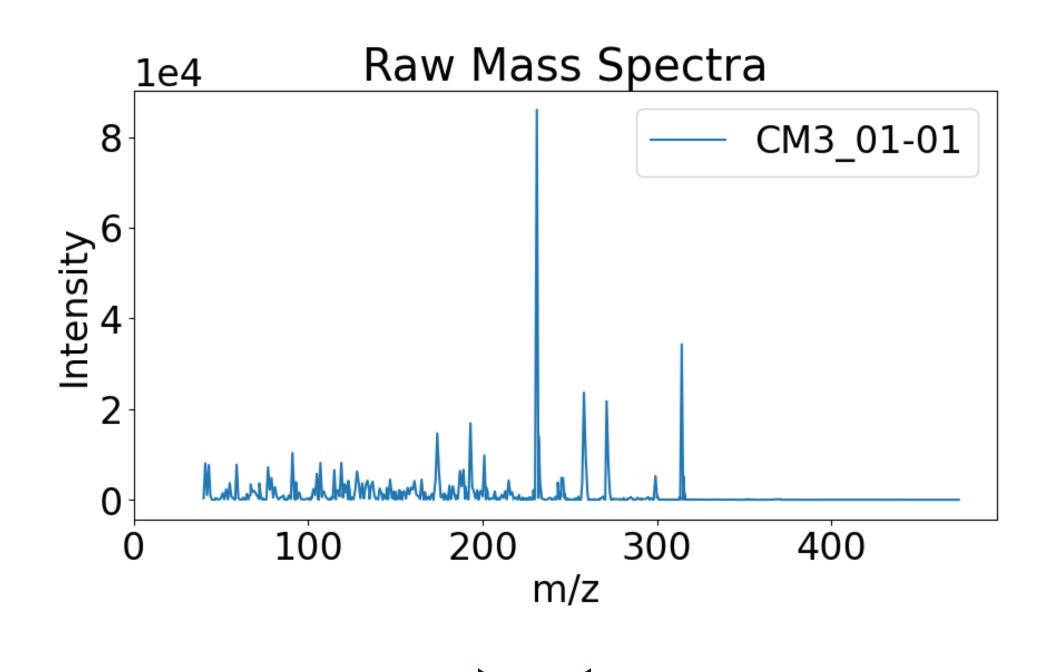


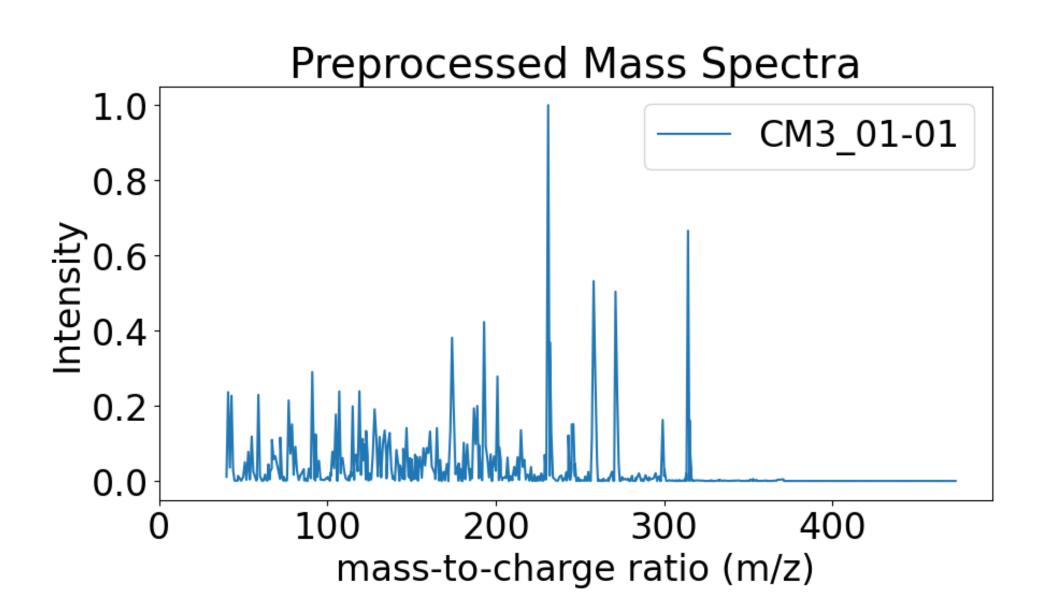


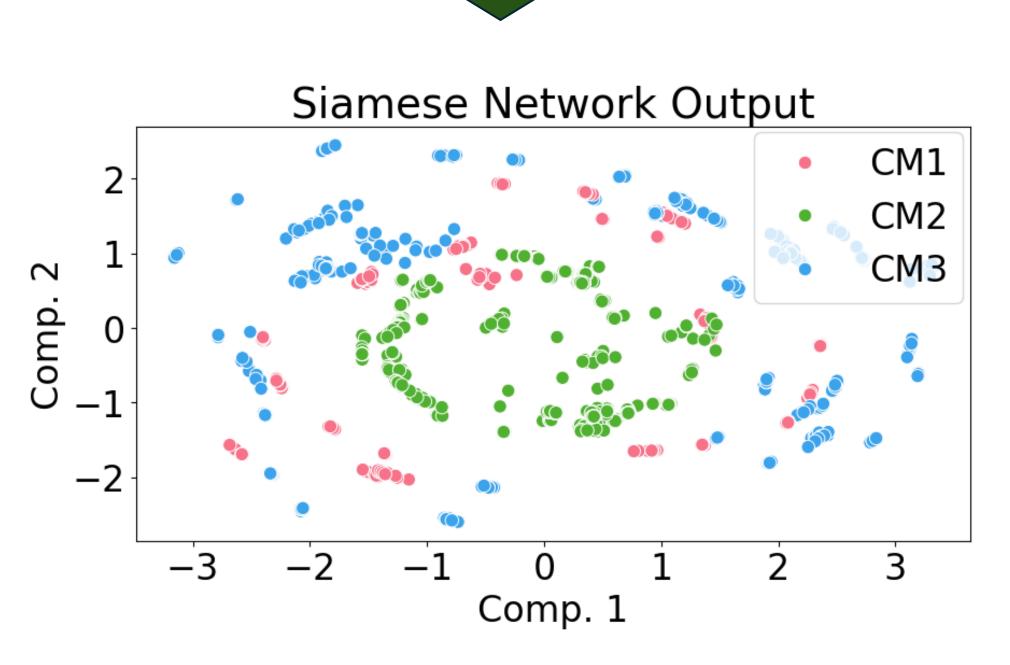
Scan the QR code to access:

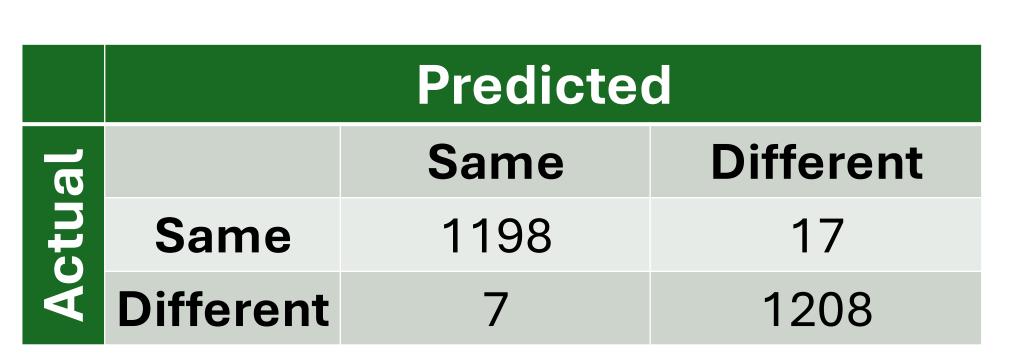
- Application
- Full project paper
- Raw dataset











Accuracy: 0.9901