



Prediction of TCR-pMHC interactions using molecular modeling and recurrent networks

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<https://github.com/HenriettaHolze/TCR-pMHC-prediction>

Hex code
color
#990000
#2F3EEA

Introduction

- Adaptive immune system is a key element for fighting diseases
- T cells are responsible for cell-mediated immune response
- T cell receptors (TCR) bind to pMHC complexes (protein – Major Histocompatibility Complex) to trigger immune response
- **Problem:** Predict TCR-pMHC binding
- **Input data [1]:**
 - Protein sequence
 - Per-residue energy terms
 - Global energy term
- **Input dimensions:**
 - x observations
 - y peptide positions
 - z channels, including sequence embedding and energy terms

IMAGE OF TCR-PMHC
COMPLEX

Methods

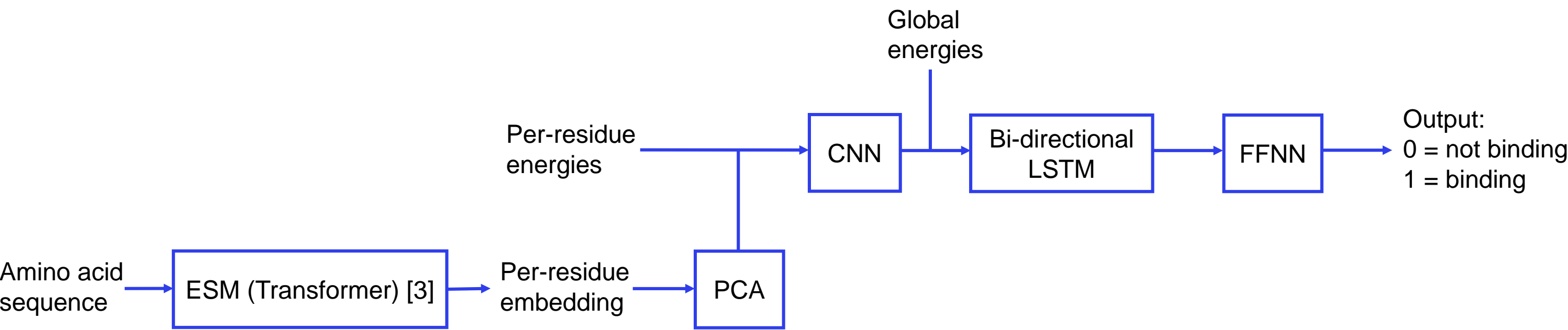


Figure 2. Pipeline for the data.

IMAGE OF ARCHITECTURE
FROM HENRIETTA

Results

MCC on test
Confusion matrix
AUC plot

Comparison with Ida [2]

Discussion

High number of negative
BERT
Graph based approach

References

[1] Magnus H. Høie. (2021). T-cell binding prediction challenge (TCR-pMHC). Github repository, Link: <https://github.com/CBH2021/tcr-pmhc>
[2] Ida Kristine Sandford Meitil. (2021). Using deep learning for improving TCR homology modeling and its application to immunogenicity prediction [Master's Thesis, DTU]
[3] Rives, A. et al. (2021). Biological structure and function emerge from scaling unsupervised learning to 250 million protein sequences. *Proceedings of the National Academy of Sciences*, 118(15).