



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

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## 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:**
  - Protein sequence
  - Per-residue energy terms
  - Global energy term
- Input dimensions:**
  - x observations
  - y peptide positions
  - z channels, including sequence embedding and energy terms
- Pre-training with a transformer, Evolutionary Scale Modeling (ESM)

IMAGE OF TCR-PMHC COMPLEX

## Methods

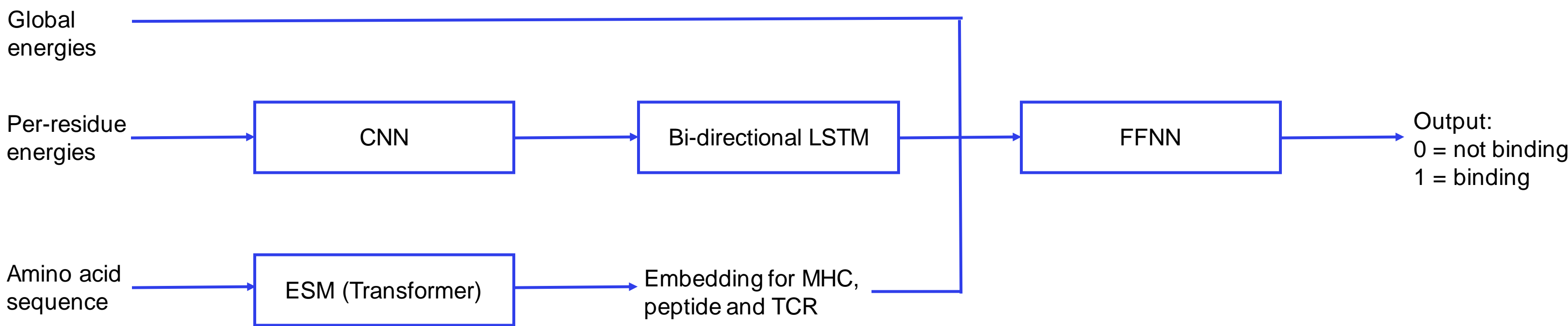


IMAGE OF THE NETWORK BY HENRIETTA

## Results

## References

- Magnus H. Høie. (2021). T-cell binding prediction challenge (TCR-pMHC). Github repository, Link: <https://github.com/CBH2021/tcr-pmhc>
- Ida Kristine Sandford Meitil. (2021). Using deep learning for improving TCR homology modeling and its application to immunogenicity prediction [Master's Thesis, DTU]
- 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).