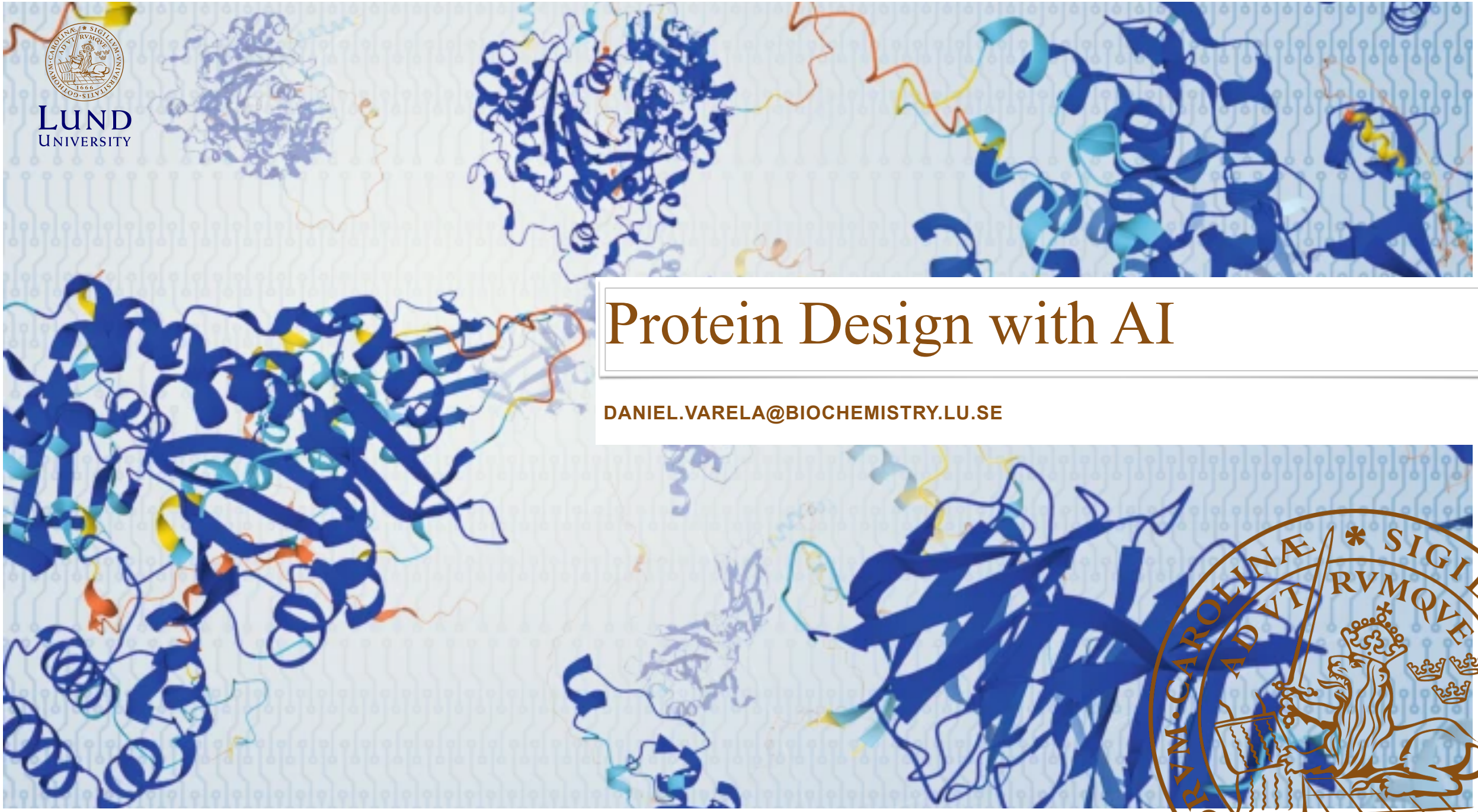
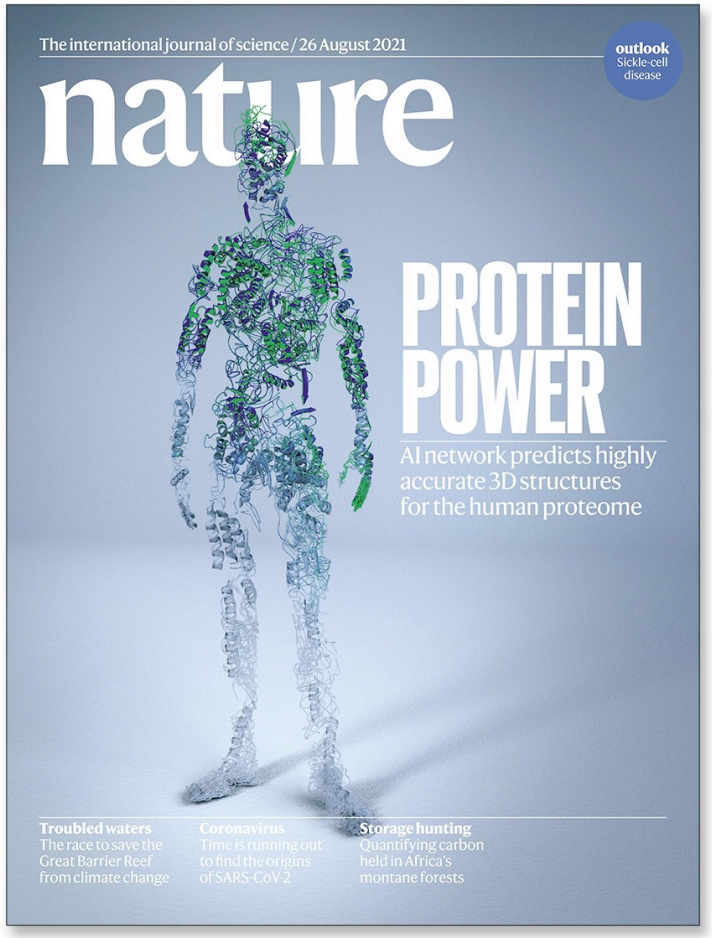


Protein Design with AI

DANIEL.VARELA@BIOCHEMISTRY.LU.SE

Computational structural biology

Best Nature method 2021



Computational Challenge

Google

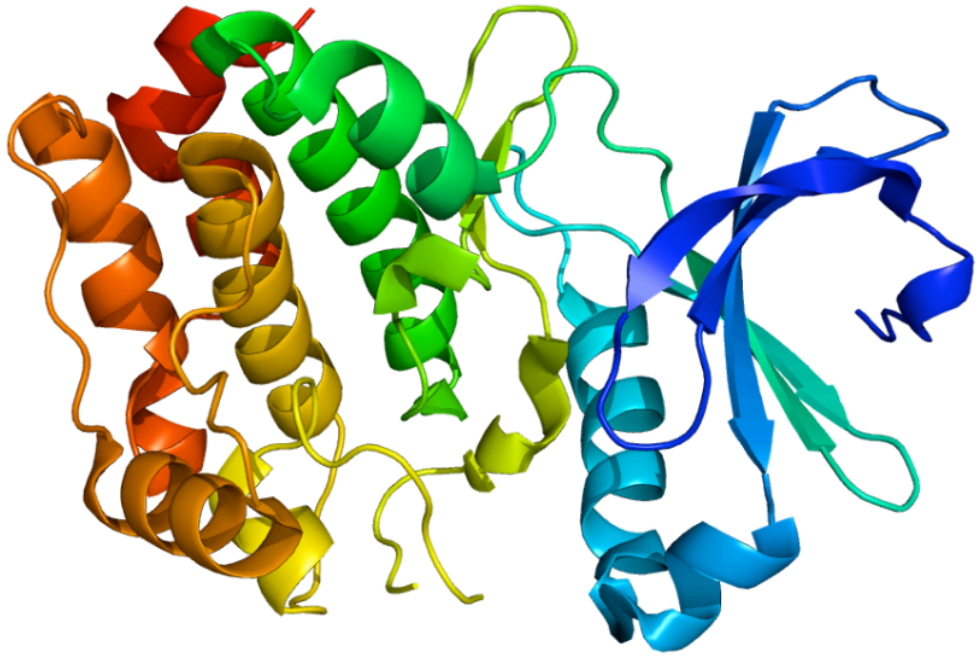
NVIDIA

Microsoft

AstraZeneca

novo nordisk®

Protein Design and Drug Development



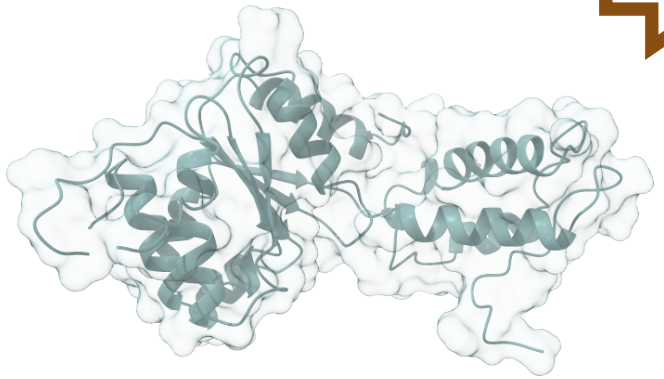
Protein Structure

Drug Development

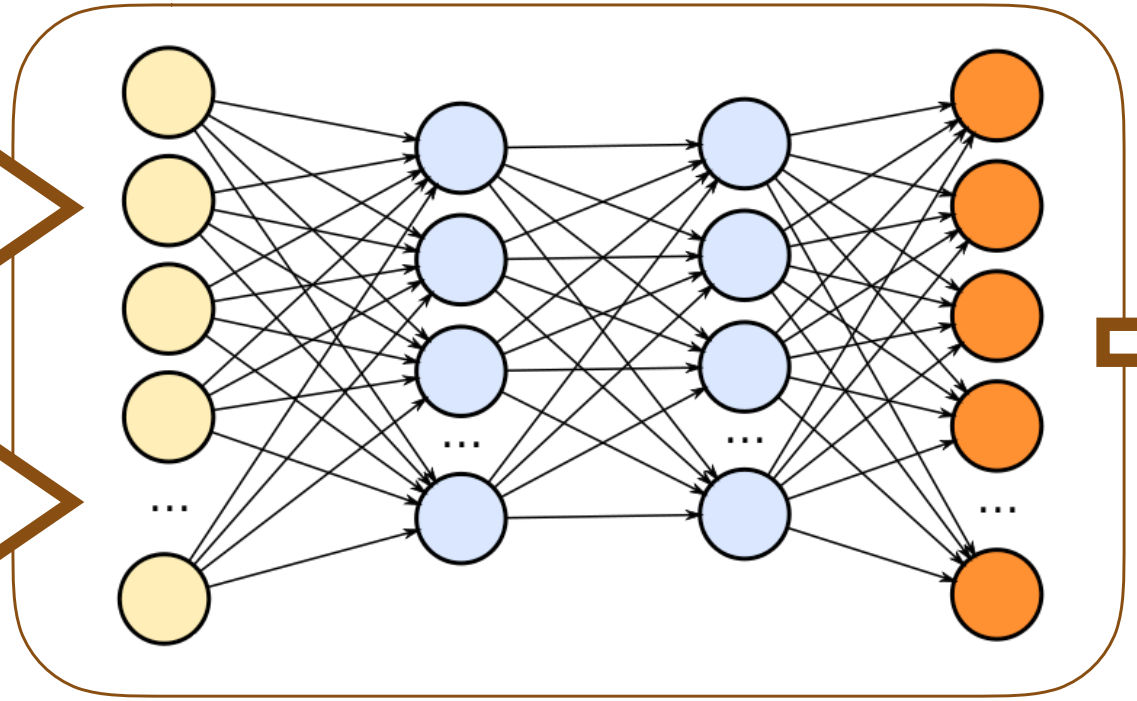
Protein Superimposition with Deep Learning

Input 1

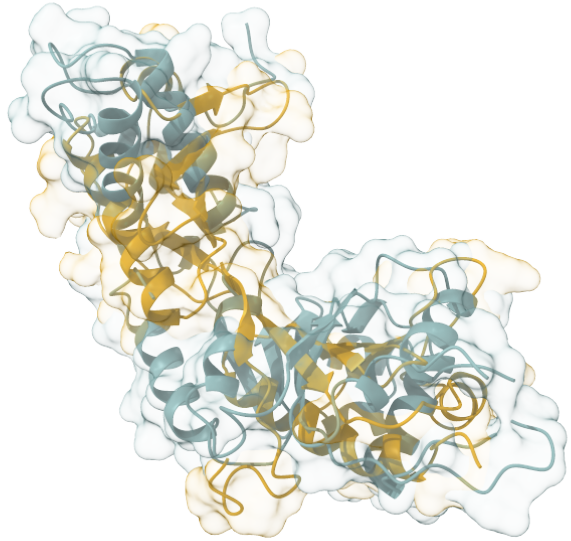
Input 2



Deep Learning method



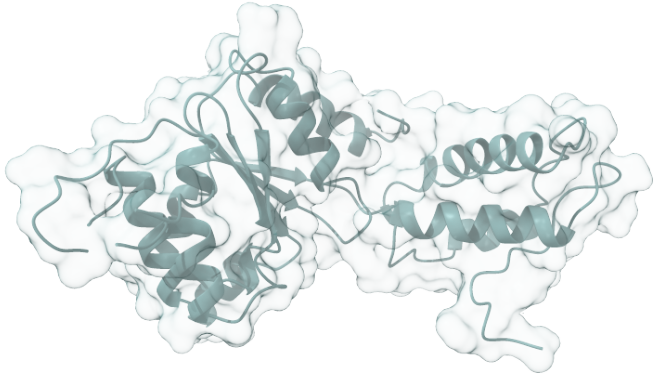
Aligned Proteins



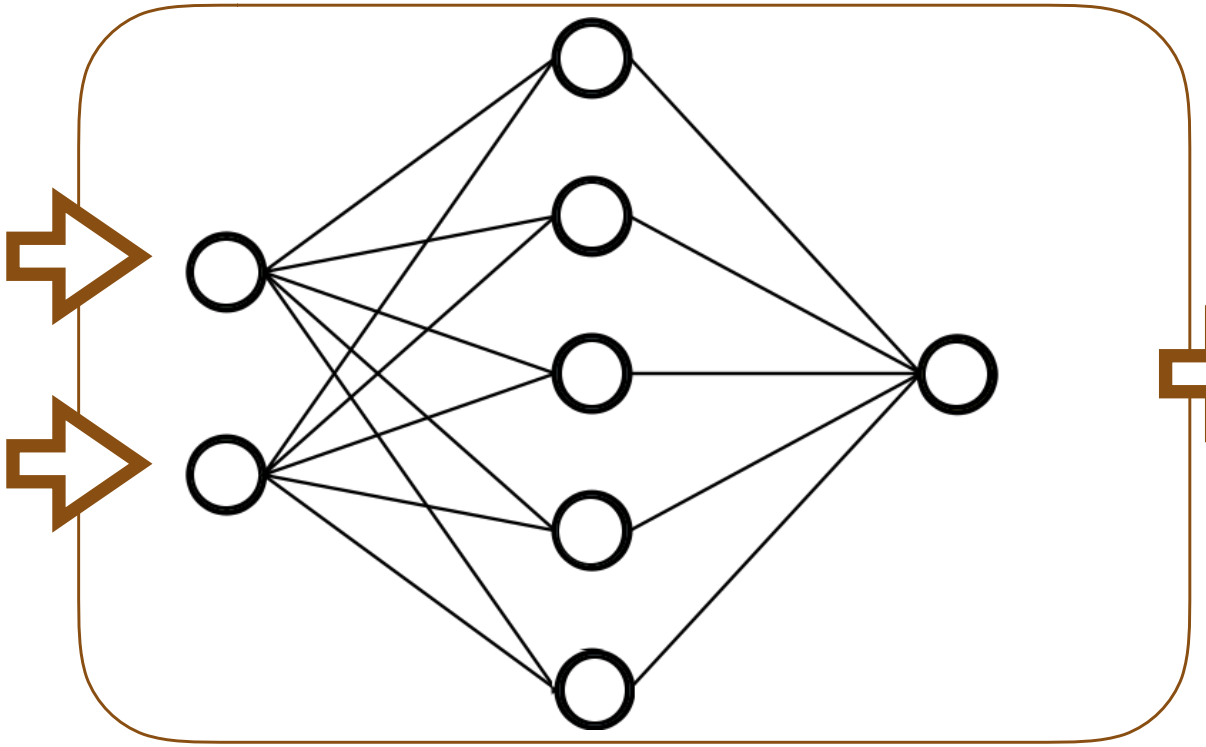
Protein similarity score with Deep Learning

Input 1

Input 2



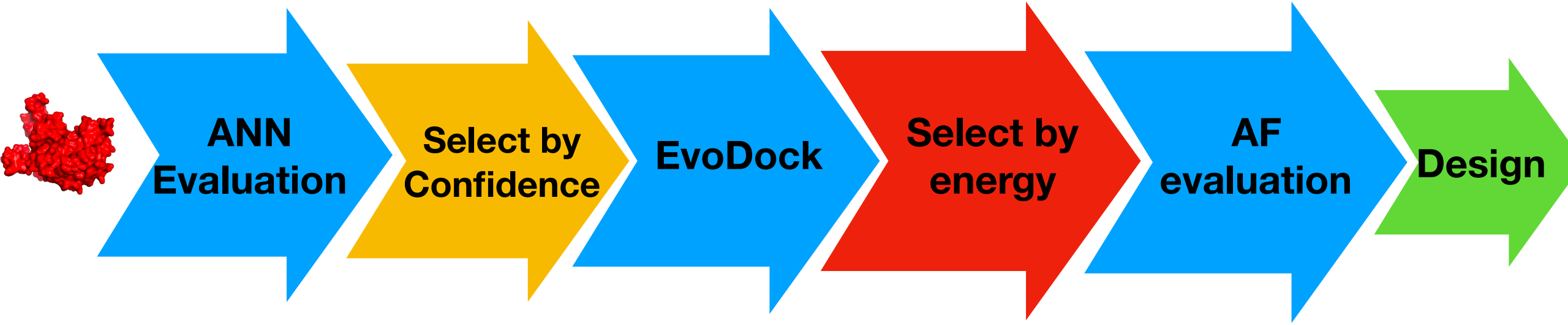
Deep Learning method



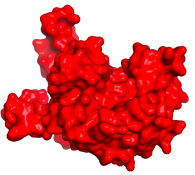
Similarity Score

0.96

AndreLab protein design approach



AndreLab protein design approach



ANN Evaluation

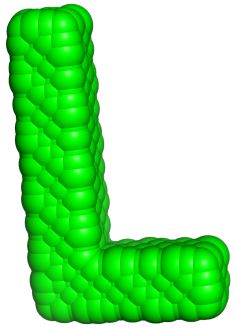
Select by Confidence

EvoDock

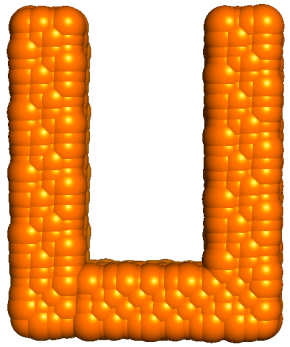
Select by energy

AF evaluation

Design

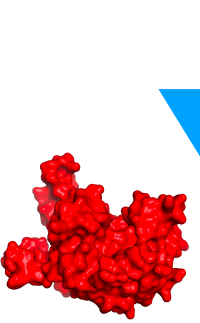


und



niversity

AndreLab protein design approach



ANN Evaluation

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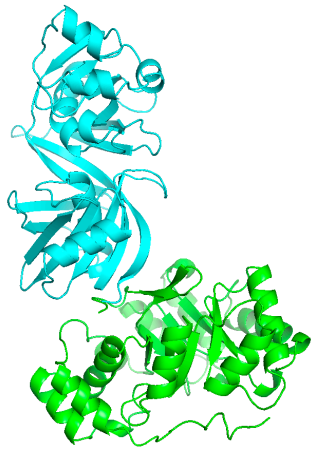

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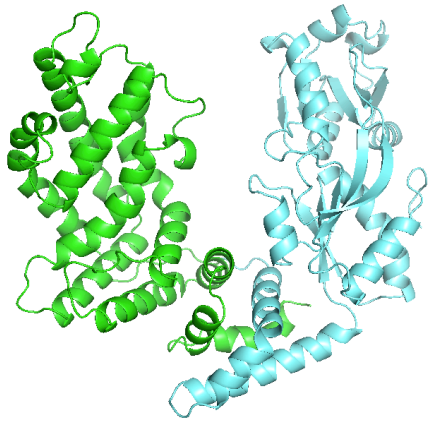

niversity

Outcome

- Introduction to an emergent field as computational drug development
- Real example of a Deep Learning application
- Learning of widely used software frameworks and tools
  - Python, PyTorch, Pandas, Scipy, Sklearn,…

Contact

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Website

- More Info: https://andrelab.biochemistry.lu.se/