



UNIVERSITY OF
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An explainable machine learning method for predicting and understanding protein interactions

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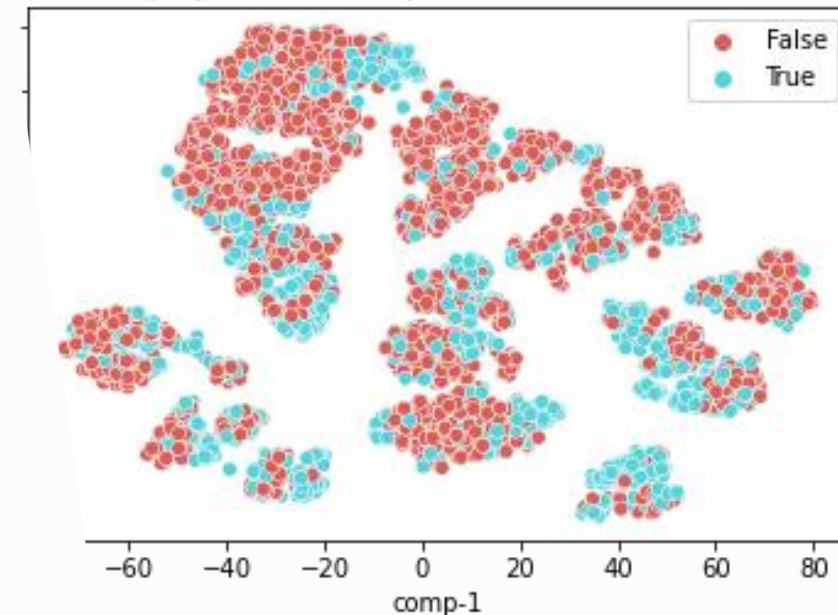
SUCCESSFUL R&I IN EUROPE 2025: 12TH EUROPEAN NETWORKING EVENT MAR/6-7/2025

Topics of interest

- Current EU project **Long-range electrodynamic interactions between proteins** (Links)
- Consequence: Protein composition is linked to its function and interactions
 - Predictive and generative machine learning tools
 - One patent

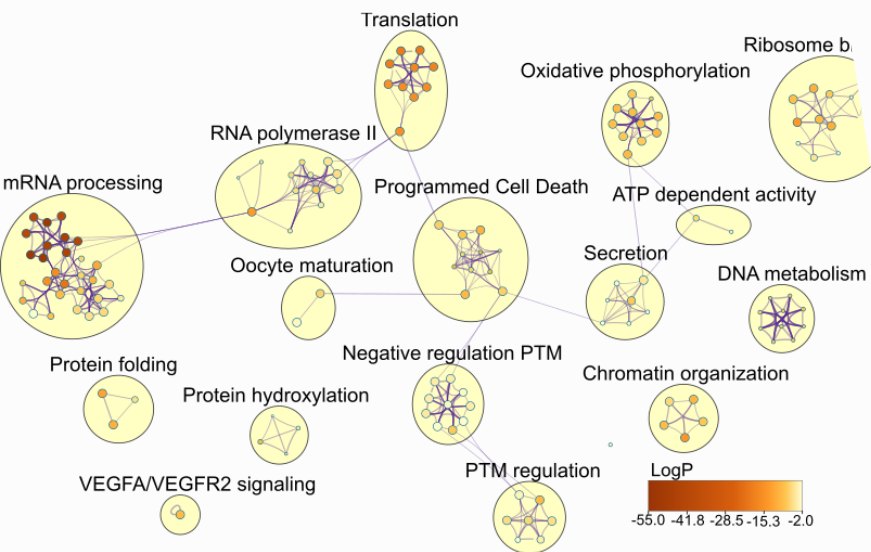
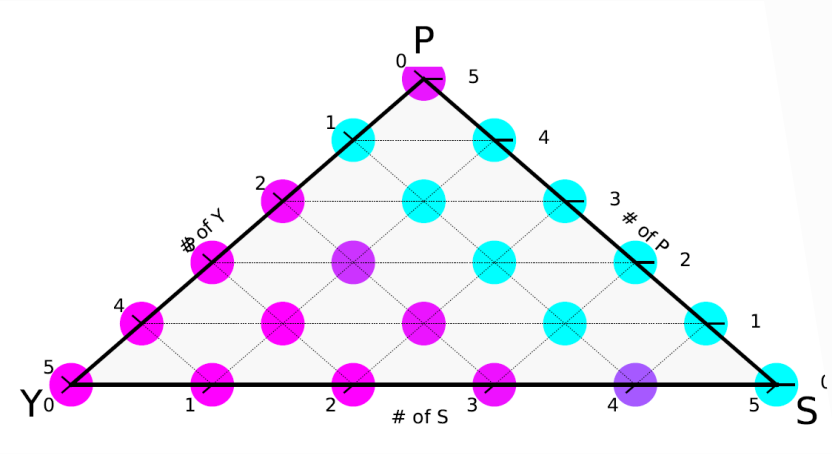


T-SNE projection of composition-based classification



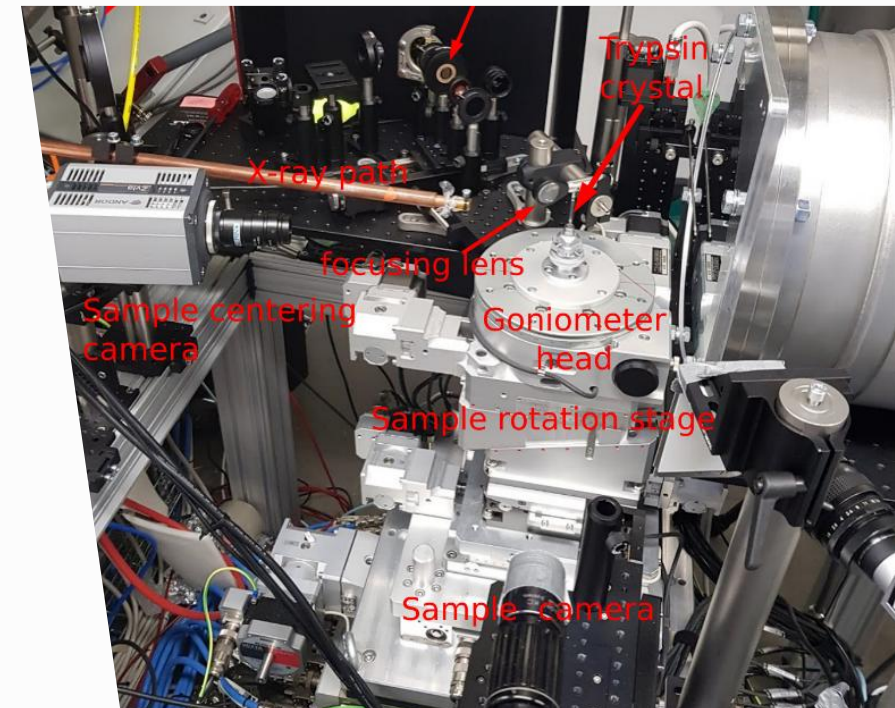
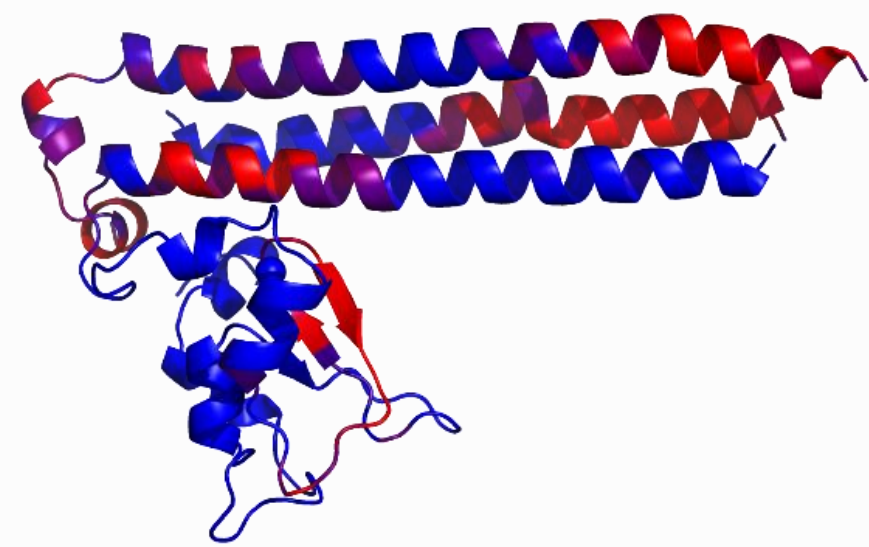
Partner profiles

- Pharmaceutical companies
 - Apply method to peptide fitness data sets
 - Biological drug development
 - targeting function, instead of genes/proteins
- Data centres
 - Annotation tasks
- Biotech startups, assay developers
 - Added value to high throughput screening
 - Affinity, interactions, localization



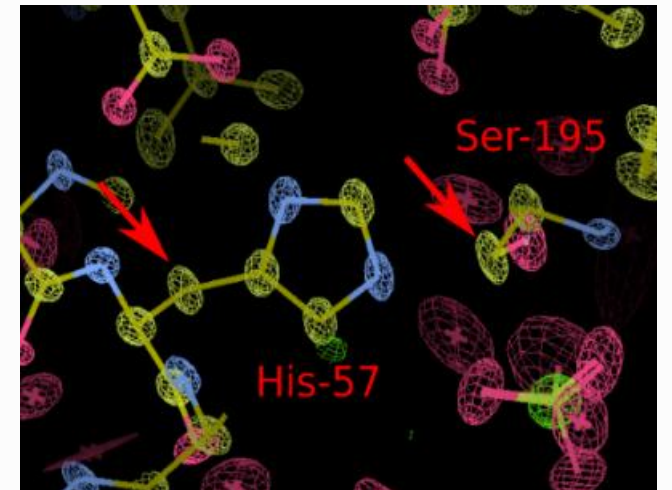
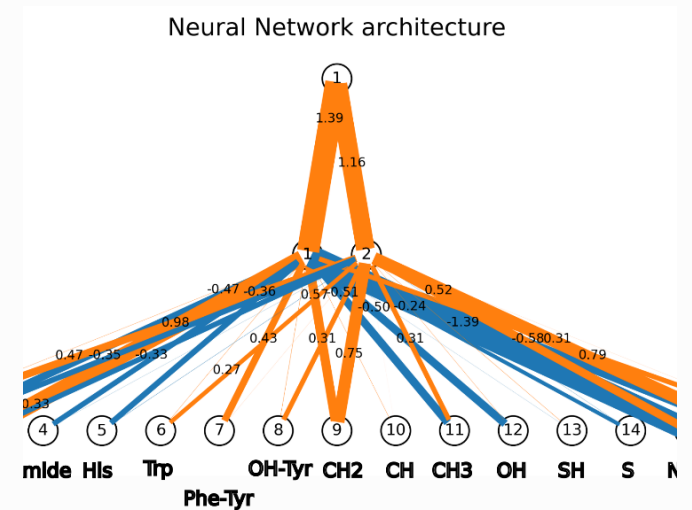
Previous scientific and technological expertise

- Structural biology (time-resolved crystallography)
 - Pioneering developer of femtosecond serial crystallography
- Molecular biology and biophysics
 - Protein-protein interactions
- Bioinformatics & machine learning
 - Bayesian and neural networks
 - Predictive and generative AI for biological data



Conclusions – NO STRUCTURE, NO PROBLEM! Composition behind the SYSTEM of interactions

- **Simple model** predicts which composition of a peptide binds survivin
 - What is the likely effect of a mutation?
- **Functional links** between compositionally similar proteins
- **What This Method Can Do for You:**
 - **Determine the function of your protein** based on specific sequence regions, including intrinsically disordered proteins (IDPs).
 - Identify which peptides are likely to **bind to your protein**.
 - Predict the likely **effects of mutations** on your protein interaction.
 - **Rank proteins** that are most likely to bind to your protein.



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