RECEP ADIYAMAN, PHD

POSTDOCTORAL RESEARCHER
Structural Bioinformatics Scientist / Protein Structure and Drug Design Researcher

Career Summary:

- **2023-Present** Collaborative Researcher, Instadeep, London,UK
  Development of the Protein Structure Prediction Pipeline for Structural Immunology
- **2020-Present** Research Fellow, McGuffin Lab, University of Reading, UK
  Improvement of the IntFOLD server for 3D protein model prediction, including quality assessment, refinement, ligand binding site prediction, disordered region identification, and protein-protein interactions.
- **2016-2020** PhD Studentship, McGuffin Lab, University of Reading, UK
  Refinement of protein 3D structures and ligand binding sites.

PROFESSIONAL EXPERIENCE

Instadeep **2023-Present**

Collaborative Researcher (Part-Time) in Industry Setting, focused on the development of a protein structure prediction pipeline for structural immunology, in collaboration with BioNTech to support cancer vaccine design. This project combines experimental and computational immunology to enhance personalized vaccine target identification and optimization. (Confidential project)

University of Reading **2020-Present**

Research Fellow at McGuffin Lab, University of Reading, UK, working on a BBSRC-funded project to enhance the IntFOLD server for 3D protein model prediction. As the main developer, I have led the refinement of protein 3D structures, prediction of protein-ligand interactions, and ensemble prediction, with a focus on improving model quality assessment, structural refinement, ligand binding site prediction, disordered region identification, and protein-protein interaction analysis.

Selected Achievement

Adapting ReFOLD4 to refine 3D predictions beyond AlphaFold2 accuracy, integrating local quality estimation and MD simulations, resulting in a recent publication. Contributing to MultiFOLD protocol development, achieving top rankings in CASP15.

In CASP16, I led the development of FunFOLD5, surpassing the capabilities of the AlphaFold3 server method in protein-ligand interaction prediction. FunFOLD5 efficiently utilizes blind docking and template-based docking methods to facilitate drug design, providing alternative poses, global scores, and accurate affinity predictions. This advancement addresses the specific limitations observed in AlphaFold3's approach to these critical aspects of protein-ligand interactions.

Education

University of Reading (2017-2021)

PhD

The research titled 'The Molecular Dynamics Based Refinement of the Predicted 3D models using different restraint strategies'. Supervisor: Professor Liam McGuffin, Biological Sciences, University of Reading.

The accuracy of predicted models is crucial for various biological applications, including drug design, protein docking, and protein function prediction. Improving the quality of predicted models refers to the refinement of the models, and the refinement of predicted models aims at bringing them closer to the native structure. In this study, our primary objective is to develop a refinement

protocol based on molecular dynamics (MD) simulations. By employing different restraint strategies to guide the MD-based refinements, we aim to achieve higher accuracy in the refined models, ultimately bringing them closer to the native structure.
MD-based refinement protocols were also used to improve the local quality of the protein-ligand binding site predictions in addition to the global accuracy.

Selected Achievements

Published a comprehensive review of the field in an invited special issue and a result paper as a book chapter, and co-authored two papers.
ReFOLD2 which was developed during the research, ranked among the top 10 refinement methods according to cumulative GDT-TS score in CASP13.
ReFOLD3 which was also developed during my PhD ranked among the top 5 refinement methods according to cumulative GDT-TS score in CASP13 for the highly accurate predictions which is difficult targets for the refinement category. Its server application was published in NAR Web Server Issue and it is live at and it has been the top refinement server application in CASP14. https://www.reading.ac.uk/bioinf/ReFOLD/ReFOLD3_form.html.

Yildiz Technical University (2012 –2014)

MSc in Bioengineering

The research titled 'In Silico Optimization of Zinc Binding Proteins for Biosensor Applications
In our research, we focused on using zinc binding peptides and attempted to increase their affinity for zinc ions by mutating single residues with the 20 standard amino acids. Through targeted mutagenesis, we systematically introduced substitutions in individual amino acid residues and assessed their impact on zinc binding. Our goal was to identify specific mutations that could enhance the interaction between the peptides and zinc ions. By conducting binding assays and structural studies, we aimed to uncover amino acid substitutions that would lead to a significant increase in zinc ion affinity. The findings from this research have the potential to inform the design of zinc binding peptides with improved properties, benefiting fields such as bioinorganic chemistry and molecular biology.
. Supervisor: Assistant Professor Gundog Yucesan and Assistant Professor Alper Yilmaz
GPA: 3.86 /4.00
Trakya University (2011-2013)
MSc in Physics
The dissertation titled 'GaAs/GaAlAs Quantum Well' Supervisor: Professor Hasan Akbas.GPA: 67/100
Trakya University (2007-2011)
BSc in Physics
Modules included Classical Mechanics & Relativity and the Quantum Mechanics and its Applications. GPA: 2.78/4.00

Publications

Google Scholar H-index: 9 Total Citations :469

- **Adiyaman, R.**, Edmunds, N. S., Genc, A. G., Alharbi, S. M. A., & McGuffin, L. J. (2023). *Improvement of protein tertiary and quaternary structure predictions using the ReFOLD refinement method and the AlphaFold2 recycling process.* Bioinformatics Advances (Total citations :19)
- **Adiyaman, R.**, & McGuffin, L. J. (2023). *Using local protein model quality estimates to guide a molecular dynamics-based refinement strategy.* In Homology Modeling: Methods and Protocols (pp. 119-140). Springer US. (Total citations :1)
- **Adiyaman, R**., & McGuffin, L. J. (2021). *ReFOLD3: refinement of 3D protein models with gradual restraints based on predicted local quality and residue contacts.* Nucleic Acids Research, **49**(W1). (Total citations :22)

- **Adiyaman, R.**, & McGuffin, L. J. (2019). *Methods for the Refinement of Protein Structure 3D Models.* International Journal of Molecular Sciences, **20**(9), 2301. (Total citations :80)
- Taylor, K. A., Elgheznawy, A., **Adiyaman, R.**, Horn, T. L., Parkes, S., Hughes, C. E., McGuffin, L. J., & Gibbins, J. M. (2025). Inter-platelet communication driving thrombus formation is regulated by extracellular calpain-1 cleavage of connexin 62. Haematologica, 110(8), 1822–1833. https://doi.org/10.3324/haematol.2024.286466
- McGuffin, L. J., Alhaddad, S. N., Behzadi, B., Edmunds, N. S., Genc, A. G., & **Adiyaman, R**. (2025). Prediction and quality assessment of protein quaternary structure models using the MultiFOLD2 and ModFOLDdock2 servers . Nucleic Acids Research, gkaf336.
- Fadini, A., Adiyaman, R., Alhaddad, S. N., et al. (2025). Highlights of model quality assessment in CASP16. Proteins: Structure, Function, and Bioinformatics, 1–16. https://doi.org/10.1002/prot.70035
- McGuffin, L. J., Edmunds, N. S., Genc, A. G., Alharbi, S. M. A., Salehe, B. R., & **Adiyaman, R.** (2023). *Prediction of protein structures, functions and interactions using the IntFOLD7, MultiFOLD and ModFOLDdock servers.* Nucleic Acids Research, **51**(W1), W274-W280. (Total citations :67)
- Edmunds, N. S., Alharbi, S. M. A., Genc, A. G., **Adiyaman, R.**, & McGuffin, L. J. (2023). *Estimation of model accuracy in CASP15 using the ModFOLDdock server.* Proteins: Structure, Function, and Bioinformatics. (Total citations :20)
- McGuffin, L. J., **Adiyaman, R**., Maghrabi, A. H. A., Shuid, A. N., Brackenridge, D. A., Nealon, J. O., & Philomina, L. S. (2019). *IntFOLD: An integrated web resource for high-performance protein structure and function prediction.* Nucleic Acids Research. (Total citations :145)
- McGuffin, L. J., Aldowsari, F. M. F., Alharbi, S. M. A., & **Adiyaman, R.** (2021). *ModFOLD8: Accurate global and local quality estimates for 3D protein models.* Nucleic Acids Research. (Total citations :78)
- Sahli, K. A., Flora, G. D., Sasikumar, P., Maghrabi, A. H., Holbrook, L. M., AlOuda, S. K., Elgheznawy, A., Sage, T., Stainer, A. R., **Adiyaman, R.,** & AboHassan, M. (2021). *Structural, functional, and mechanistic insights uncover the fundamental role of orphan connexin-62 in platelets.* Blood, **137**(6), 830-843. (Total citations :12)
- Kryshtafovych, A., Moult, J., Billings, W. M., Della Corte, D., Fidelis, K., Kwon, S., Olechnovič, K., Seok, C., Venclovas, Č., Won, J., & CASP-COVID participants (**Adiyaman, R.**). (2021). *Modelling SARS‐CoV‐2 proteins in the CASP‐commons experiment.* Proteins: Structure, Function, and Bioinformatics, **89**(12), 1987-1996. (Total citations :22)
- Yucesan, G., Yilmaz, A., & **Adiyaman, R**. (2014). *Design and synthesis of small peptide sequences to detect concentrations of free transition metal ions.* In Abstracts of Papers of the American Chemical Society, 247. Washington, DC: American Chemical Society.

Research skills

- Using Molecular Dynamics Simulations
- Analysis of data by R, python scripts, Shell scripting
- Application of Bioinformatics Tools(BLAST, NCBI, EMBOSS, Rosetta, SWISS-MODEL, Modeller, HHpred, PyMol, Chimera)
- Application of Machine Learning Tools (scikit-learn, TensorFlow , PyTorch)
- Using Cloud Services (AWS, MMM Hub Young Server-UCL)
- Protein ligand interactions (blind and redocking using Vina, gnina, SwissDock, DiffDock, Rosetta software family)

Conferences and presentations

Oral

- Adıyaman, R., Yılmaz, A., Yücesan, G., (2014). Design of metal ions binding small peptides, 1. National Biosensor Congress, Tekirdag, Turkey

- Recep Adiyaman ‘Molecular Dynamics Based Refinement of Protein Models with the Guidance of Local Quality Assessment’, University of Reading Biological Sciences Symposium, Reading, The UK
- Recep Adıyaman, Liam James McGuffin ‘ ReFOLD4 for the refinement of the AlphaFOLD2 predictions’, ISMB 2023 - (3D-SIG)
-

Poster

- Recep Adıyaman, Liam James McGuffin ‘ ReFOLD2’, 13th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, Cancun, Mexico 2018
- Recep Adıyaman, Liam James McGuffin ‘ The refinement of theoretical 3D models of proteins using the ReFOLD3 web server’, ISMB 2021 - (3D-SIG)
- ReFOLD3: refinement of 3D protein models with gradual restraints based on predicted local quality and residue contacts. 14th Community Wide Experiment on the Critical Assessment of Techniques for Protein Structure Prediction, Virtual due to COVID pandemic

Employment

Teaching assistant, Reading (2016-2020)

- Demonstrating in Bioinformatics practical of Molecular and Genetics and Introduction to Bioinformatics Modules. The practical included the application of the bioinformatics tools such as BLAST, PDB, CATH, PDBsum and PyMol. Around 150 students attended the practicals and the fundamentals of the tools were introduced to them.

Research Associate, Reading (2020-present)

- Working on the further improvement of the IntFOLD server for the prediction of protein 3D models, and their global and local assessment , refinement stages, protein ligand binding site and disordered region predictions.

References

Professor Liam McGuffin, School of Biological Sciences, The University of Reading, Whiteknights, PO Box 221 ,Reading RG6 6AS UK, l.j.mcguffin@reading.ac.uk
Assist.Prof.Dr. Alper YILMAZ, Yildiz Technical University Bioengineering Department, YTU Bioengineering Department, Room KM-A129, Esenler, Istanbul, Turkey, alperyilmaz@gmail.com