

Raj Shekhor Roy

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Professional Profile:   

Research Interest

To build highly accurate deep learning methods for the prediction of protein structures and drug-discovery.

Education

University of Missouri-Columbia,
Ph.D. in Computer Science

Missouri , USA

2019 - Present

University of Missouri-Columbia,
MS in Computer Science

Missouri , USA

2023

BRAC University,
B.Sc. in Computer Science and Engineering

Dhaka, Bangladesh

2017

Research Experience

Bioinformatics and Machine Learning Lab
Graduate Research Assistant, University of Missouri

August 2019 - Present
Columbia, Missouri

Protein Structure Prediction

- Developed DRCon, a deep learning tool for the interchain contact prediction of homodimers.
- Developed ConComplex, a simulated annealing based tool to reconstruct protein structure.
- Co-developed DeepComplex, a web server to predict protein structure.
- Co-developed DRLcomplex, a novel approach to reconstruct protein dimeric structure utilizing reinforcement learning.
- Contributed to GDFold, a gradient descent based method to reconstruct protein structure.

Protein Quality Assessment

- Developed MULTICOM_qa, a tool to estimate the global fold quality of a protein using a hybrid approach.
 - The average TM-score of the first predictions submitted by MULTICOM_qa for CASP15 assembly targets is 5.3% higher than that of the standard AlphaFold-Multimer.
 - It was ranked first in estimating the global fold accuracy of protein assembly structures in the 2022 CASP15 experiment.

Activities and Impacts

Presentation: At the ICIBM	2023
Media: Bangladeshi student wins prestigious award in computational biology competition https://www.thedailystar.net/tech-startup/news/bangladeshi-student-wins-prestigious-award-computational-biology-competition-3268431	2023
Media: MIZZOU TEAM RANKS FIRST IN CATEGORY AT CASP15 PROTEIN PREDICTION COMPETITION. https://engineering.missouri.edu/2023/mizzou-team-ranks-first-in-category-at-casp15-protein-prediction-competition/	2023
Patent : “DEEP LEARNING SYSTEMS AND METHODS FOR PREDICTING STRUCTURAL ASPECTS OF PROTEIN-RELATED COMPLEXES” Application Serial No. 17/988,461 and case number 21UMC093, filed on November 16, 2022 and entitled	2022
Competition: Ranked Top in the CASP15 in EMA category. https://predictioncenter.org/casp15/zscores_EMA.cgi	2022
Participation: The Critical Assessment of protein Structure Prediction and Critical Assessment of PRedicted Interactions (CASP15)	2022
Participation: The 2021 ARPA-E Energy Innovation Summit.	2021
Poster Presentation: The CASP14 Virtual Symposium.	2020
Participation: The Critical Assessment of protein Structure Prediction and Critical Assessment of PRedicted Interactions (CASP14-CAPRI50)	2020

Peer-Reviewed Publications and Presentations

Soltanikazemi, E., Roy, R. S (Equal Contribution) ., Quadir, F., Giri, N., Morehead, A. & Cheng, J. A deep reinforcement learning approach to reconstructing quaternary structures of protein dimers through self-learning. (Presented in ICIBM,2023)	2023
Liu J, Guo Z, Wu T, Roy RS , Quadir F, Chen C, Cheng J. Enhancing AlphaFold-Multimer-based Protein Complex Structure Prediction with MULTICOM in CASP15. doi: 10.1101/2023.05.16.541055.	2023
Lensink, M. F., Brysbaert, G., Raouraoua, N., Bates, P. A., Giulini, M., Honorato, R. V., C. Teixeira, J. M., J. Bonvin, M. J., Kong, R., Shi, H., Lu, X., Chang, S., Liu, J., Guo, Z., Chen, X., Morehead, A., Roy, R. S. , Wu, T., Giri, N., . . . Wodak, S. J. Impact of AlphaFold on structure prediction of protein complexes: The CASP15-CAPRI experiment. <i>Proteins: Structure, Function, and Bioinformatics</i> . https://doi.org/10.1002/prot.26609	2023
Liu, J., Guo, Z., Wu, T., Roy, R.S. , Chen Chen & Cheng, J. Improving AlphaFold2-based protein tertiary structure prediction with MULTICOM in CASP15. <i>Commun Chem</i> 6, 188 (2023). https://doi.org/10.1038/s42004-023-00991-6	2023
Roy, R. S. , Liu,J., Giri,N., Guo, Z.,and Cheng,J. Combining pairwise structural similarity and deep learning interface contact prediction to	2023

estimate protein complex model accuracy in CASP15. *Proteins*. 2023; 1-14.
doi:10.1002/prot.26542

- Giri, N., **Roy, R. S.**, & Cheng, J. (2023). Deep learning for reconstructing protein structures from cryo-EM density maps: Recent advances and future directions. *Current Opinion in Structural Biology*, 79, 102536. <https://doi.org/10.1016/j.sbi.2023.102536> 2023
- Roy, R. S.**, Quadir, F., Soltanikazemi, E., & Cheng, J. (2022). A deep dilated convolutional residual network for predicting interchain contacts of protein homodimers. *Bioinformatics*, btac063. <https://doi.org/10.1093/bioinformatics/btac063> 2022
- Soltanikazemi, E., Quadir, F., **Roy, R. S.**, Guo, Z., & Cheng, J. (2022). Distance-based reconstruction of protein quaternary structures from inter-chain contacts. *Proteins: Structure, Function, and Bioinformatics*, 90(3), 720–731. <https://doi.org/10.1002/prot.26269> 2022
- Gao, M., Lund-Andersen, P., Morehead, A., Mahmud, S., Chen, C., Chen, X., Giri, N., **Roy, R. S.**, Quadir, F., Effler, T. C., Prout, R., Abraham, S., Elwasif, W., Haas, N. Q., Skolnick, J., Cheng, J., & Sedova, A. (2021). High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function. 46–57. <https://doi.org/10.1109/MLHPC54614.2021.00010> 2021
- Quadir, F., **Roy, R. S. (Equal Contribution)**, Soltanikazemi, E., & Cheng, J. (2021). DeepComplex: A Web Server of Predicting Protein Complex Structures by Deep Learning Inter-chain Contact Prediction and Distance-Based Modelling. *Frontiers in Molecular Biosciences*, 8. <https://www.frontiersin.org/article/10.3389/fmolb.2021.716973> 2021
- Lensink, M. F., Brysbaert, G., Mauri, T., Nadzirin, N., Velankar, S., Chaleil, R. A. G., Clarence, T., Bates, P. A., Kong, R., Liu, B., Yang, G., Liu, M., Shi, H., Lu, X., Chang, S., **Roy, R. S.**, Quadir, F., Liu, J., Cheng, J., ... Wodak, S. J. (2021). Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function, and Bioinformatics*, 89(12), 1800–1823. <https://doi.org/10.1002/prot.26222> 2021
- Quadir, F., **Roy, R. S.**, Halfmann, R., & Cheng, J. (2021). DNCON2_Inter: Predicting interchain contacts for homodimeric and homomultimeric protein complexes using multiple sequence alignments of monomers and deep learning. *Scientific Reports*, 11(1), 12295. <https://doi.org/10.1038/s41598-021-91827-7> 2021
- Rashid, M.R., Shuvra, N.K., **Roy, R.S.**, & Sarker, S.A Theoretical Approach of Fall Control System for Disable People Using Double Inverted Pendulum, 2018 4th International Conference on Electrical Engineering and Information & Communication Technology (iCEEICT), 2018, pp. 49-53, doi: 10.1109/CEEICT.2018.8628130. 2018

Publications in Progress

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- Soltanikazemi, E., **Roy, R. S (Equal Contribution)**., Quadir, F., Giri, N., Morehead, A. & Cheng, J. (2022) 2023
- A deep reinforcement learning approach to reconstructing quaternary structures of protein dimers through self-learning.
- Bioarxiv link: <https://doi.org/10.1101/2022.04.17.488609>