

Dr. Arijit Roy

Scientist – Life Sciences Research Area

TCS Research & Innovation

Education

- PhD (Chemistry) Indian Institute of Technology Kharagpur (2009)

Research Interests

- Drug discovery using deep learning based methods
- Understanding disease mechanism and drug repurposing using network-based approaches
- Multi-scale simulations of biomolecules

Selected Publications:

1. Network analysis of hydroxymethylbilane synthase dynamics, Chakrabarty B, Das D, Bung N, Roy A, Bulusu G *Journal of Molecular Graphics and Modelling* (2020) 99, 107641.
2. Human aminolevulinate synthase structure reveals a eukaryotic-specific autoinhibitory loop regulating substrate binding and product release. Bailey HJ, Bezerra GA, Marcero JR, Padhi S, Foster WR, Rembeza E, Roy A, Bishop DF, Desnick RJ, Bulusu G, Dailey HA. *Nature Communications* (2020) 11, 2813.
3. Network-based analysis of fatal comorbidities of COVID-19 and potential therapeutics Chakrabarty B, Das D, Bulusu G, Roy A, (2020) (under review)
<https://doi.org/10.26434/chemrxiv.12136470.v1>
4. De novo design of new chemical entities (NCEs) for SARS-CoV-2 using artificial intelligence, Bung N, Krishnan SR, Bulusu G, Roy A, (2020) (under review)
<https://doi.org/10.26434/chemrxiv.11998347.v2>
5. Computational predictions of host-pathogen interactions using domain and sequence signature Das D, Krishnan SR, Bulusu G, Roy A, 2019 IEEE International Conference on



Bioinformatics and Biomedicine (BIBM), San Diego, CA, USA, 2019, pp. 935-938, doi: 10.1109/BIBM47256.2019.8983364.

6. A network-based approach reveals novel invasion and Maurer's cleft-related proteins in *Plasmodium falciparum* Das D, Krishnan S R, Roy A and Bulusu G.. Mol Omics. (2019) 15, 431– 441.
7. Computational modeling of the catalytic mechanism of hydroxymethylbilane synthase. Bung N, Roy A, Priyakumar UD, Bulusu G Phys Chem Chem Phys, (2019) 21, 7932-7940.
8. TPP riboswitch aptamer: Role of Mg²⁺ ions, ligand unbinding, and allostery. Padhi S, Pradhan M, Bung N, Roy A, Bulusu G, J Mol Graph Model (2019) 88, 282-291.
9. Human hydroxymethylbilane synthase: Molecular dynamics of the pyrrole chain elongation identifies step-specific residues that cause AIP. Bung N, Roy A, Chen B, Das D, Pradhan M, Yasuda M, New MI, Desnick RJ, Bulusu G, PNAS (2018) 115, E4071-E4080.