## **Postgraduate Seminar Series**

Venue: Graduate Seminar Room Date & Time: May 4, 2024 at 2:30 PM

## **Speaker Information**

Ajmain Yasar Ahmed (Std No. 0422052013) is a full-time M.Sc. student in the department of CSE, BUET. He completed his undergraduate studies from CSE, BUET in 2022. His research interests lie in the application of machine learning and deep learning methods in biomolecule and cellular organelle analysis, and in any interesting problem in the field of computational biology, in a broader sense. He is currently doing his postgraduate thesis under the supervision of Dr. Md. Shamsuzzoha Bayzid. He will be speaking about his ongoing research in this talk.



## <u>Protein Secondary Structure and Backbone Torsion Angle Prediction using</u> <u>Multitask Learning</u>

Knowledge of protein structures in 3-dimensional (3D) space enables understanding of their functions inside living organisms, leading to their vast applications in modern therapeutics and agriculture. However, determining protein 3D structures in traditional wet-lab settings is both time-consuming and costly. Therefore, many computational methods have been proposed in recent years to accurately predict protein structural properties, resulting in reliable predictions of protein structures. But there still remain challenges in this arena due to the complex nature of proteins. In our ongoing research, we have developed a set of multitask learning-based protein 8-state (Q8) secondary structure and backbone torsion angle ( $\Phi$  and  $\Psi$ ) prediction methods. These methods are based on single-task learning-based Q8 and torsion angle predictors previously designed in our lab. In this study, we have investigated the change in predictive performance between single-task and multitask learning paradigms. Besides, our proposed methods are both evolutionary-feature-based and single-sequence-based, demonstrating comparable predictive performance with respect to other contemporary methods. This versatility allows reliable prediction of the structural properties of proteins using our methods, irrespective of their evolutionary nature. In this work, we have also conducted a comparative analysis of the contribution of protein sequence embeddings from various emerging protein language models to the accurate prediction of structural properties. We envision that the predictions from our proposed methods will assist in downstream analyses of proteins as well as in extremely challenging single-sequence-based protein structure prediction.