

Role of Artificial Intelligence in Nano Proteomics

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Abstract : Recent advances in single-molecule protein identification (ID) and quantification techniques are poised to revolutionize proteomics, enabling researchers to delve into single-cell proteomics and identify low-abundance proteins crucial for biomedical and clinical research. This paper introduces a different approach to single-molecule protein ID and quantification using tri-color amino acid tags and a plasmonic nanopore device. A comprehensive simulator incorporating various physical phenomena was designed to predict and model the device's behavior under diverse experimental conditions, providing insights into its feasibility and limitations. The study employs a whole-proteome single-molecule identification algorithm based on convolutional neural networks, achieving high accuracies (>90%), particularly in challenging conditions (95-97%). To address potential challenges in clinical samples, where post-translational modifications affecting labeling efficiency, the paper evaluates protein identification accuracy under partial labeling conditions. Solid-state nanopores, capable of processing tens of individual proteins per second, are explored as a platform for this method. Unlike techniques relying solely on ion-current measurements, this approach enables parallel readout using high-density nanopore arrays and multi-pixel single-photon sensors. Convolutional neural networks contribute to the method's versatility and robustness, simplifying calibration procedures and potentially allowing protein ID based on partial reads. The study also discusses the efficacy of the approach in real experimental conditions, resolving functionally similar proteins. The theoretical analysis, protein labeler program, finite difference time domain calculation of plasmonic fields, and simulation of nanopore-based optical sensing are detailed in the methods section. The study anticipates further exploration of temporal distributions of protein translocation dwell-times and the impact on convolutional neural network identification accuracy. Overall, the research presents a promising avenue for advancing single-molecule protein identification and quantification with broad applications in proteomics research. The contributions made in methodology, accuracy, robustness, and technological exploration collectively position this work at the forefront of transformative developments in the field.

Keywords : nano proteomics, nanopore-based optical sensing, deep learning, artificial intelligence

Conference Title : ICALRAI 2024 : International Conference on Artificial Life, Robotics and Artificial Intelligence

Conference Location : New York, United States

Conference Dates : January 29-30, 2024