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Predicting Physical Properties of Proteins Using 3D Convolutional Neural Networks. TALANT RUZMETOV, Department of Chemistry, Rutgers University, Camden, Center for Computational and Integrative Biology, Joint Health Sciences Center, Camden, NJ, SIDDHARTH BHADRA-LOBO, Center for Computational and Integrative Biology, Joint Health Sciences Center, Camden, NJ, DEVLINA CHAKRAVARTY, GUILLAUME LAMOUREUX, Department of Chemistry, Rutgers University, Camden, Center for Computational and Integrative Biology, Joint Health Sciences Center, Camden, NJ — Convolutional neural networks (CNNs) have gained widespread popularity by achieving state-of-the-art results on various image analysis tasks such as handwriting recognition, object detection, and medical diagnosis. An inherent property of CNNs is the so-called "translational equivariance", which enables the network to recognize an object (or pattern) irrespective of its position in the image. We use 3D CNNs as well as their rotationally equivariant versions, called SE(3)-CNNs, to predict spatially-resolved physical properties of proteins, such as the electrostatic potential, the density of solvent molecules, or the binding free energy of small molecular fragments. The binding free energies of small molecular fragments are obtained from molecular dynamics-based methods such as Site Identification by Ligand Competitive Saturation (SILCS). In this talk, we demonstrate how feature representations learned from protein atomic densities can be used to predict various physical properties of molecular interactions with 3D CNN-based architectures.

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