Development of protein-ligand binding prediction method by deep learning

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Virtual screening is a promising computational method for obtaining novel hit compounds in drug discovery. It aims to enrich potentially active compounds from a large chemical library for further biological experiments. However, the accuracy of current virtual screening methods is insufficient.

Drug discovery requires to find molecules that interact with targets with high affinity and specificity. Virtual screening application has been developed to this goal. However, current methods still show relatively weak predictive power.

In this work, we proposed a new virtual screening method named Visual Inspection Network (VisINet) inspired by image classification. We will show how recent advances in computer vision can be applied to structure-based virtual screening by adopting a CNN model based on the ResNet architecture.