

Detection of protein-ligand binding sites plays key role not only in understanding of protein function but it also can be used for computer-aided drug design. Improving these detection can lead to faster drug development. In recent years, many machine learning methods were proposed for this task. Nowadays, transformer architecture became one of the most prominent one for non-biological data. Its extension for images, vision transformer, became comparable to state-of-the-art algorithms. Moreover, this vision transformer can be expanded into 3D space. The goal of this thesis is to evaluate possibilities of extending transformers into 3D, for biological data, specifically for protein-ligand binding site detection, exploiting the qualities of attention mechanism.