세미나 초록

발표주제	Developing structure-based drug discovery methods in the AI era
발표내용	While deep learning (DL) has brought a revolution in the protein structure prediction field, an important question remains: How can the revolution be transferred to advances in structure-based drug discovery. In the first half, a large-scale benchmark result will be shown for the best-practice DL-based receptor modeling and docking strategies in GPCR drug discovery. From our quantitative analysis, it is shown that substantial improvements in docking and virtual screening have been majorly driven by the improved receptor model quality generated by AlphaFold, while ligand docking tools remained to be improved in their prediction accuracy. This observation demonstrates the necessity of DL approaches for more advanced ligand docking and virtual screening to help real practice drug discovery problems. In the second half of the talk, two DL tools currently being developed in my lab will be introduced: 1) evaluation tools for AlphaFold model-ligand complex structure accuracy, and 2) a virtual screening and inverse-screening tool from the learned interaction patterns between receptor and ligands.