AI-powered drug discovery and development

남호정†
광주과학기술원
(hjnam@gist.ac.kr†)

The process of drug discovery is a challenging process considering its required time and efforts. Traditionally, developing one promising drug requires more than 10,000 initial compounds to be selected as candidates. Then these candidates undergo pre-clinical and clinical tests to be passed for several years. In recent years, the paradigm in drug development has been re-shaped in several ways. Many studies have shown the efficiency of artificial intelligence (AI) based drug development approaches that further increase the ability to predict and model the most relevant pharmacokinetic, metabolic, and toxicity endpoints, thereby accelerating the drug discovery process. This talk covers studies about developing AI models for drug discovery and development. The first part of the talk is about the AI model that suggests hit compounds using CNN & Transformer. The second part of the talk is about drug repurposing. We describe an interpretable AI model of use in predicting drug responses in cancer cells at the gene, molecular pathway, and drug level.