



Principal Investigator

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Adopted Theme

Drug discovery platform targeting membrane proteins through the integration of Cryo-EM and computer science

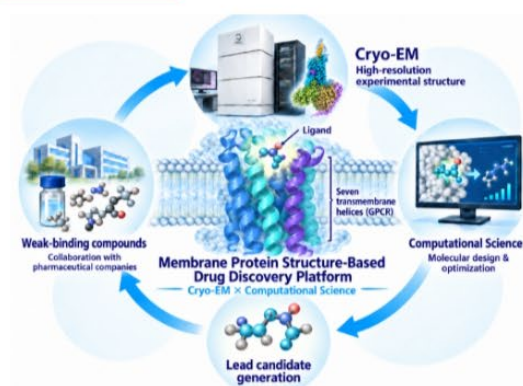
Subject of Research

Drug discovery platform targeting membrane proteins through the integration of Cryo-EM and computer science

GTIE VC Collective

Kyoto University Innovation Capital Co.,Ltd. (KYOTO-ICAP)

Overview



G protein-coupled receptors (GPCRs), which are located on cell membranes, account for around 30 % of all drug targets. However, rational drug design based on structural information (SGDD: structure-guided drug development) has only been achieved for a limited number of these targets, because analyzing their structure is difficult. Although AI-based structure prediction has advanced in recent years, precise drug design still requires high-resolution structural information based on actual analyses. In particular, it is challenging to analyze the binding structures of low-affinity compounds held by pharmaceutical companies. Consequently, these developments must proceed without binding structural information. In this project, we will combine the high-resolution analysis using a Cryo-electron microscopy (Cryo-EM) system developed by the principal investigator with computational molecular design to create a structure-guided discovery platform targeting membrane proteins, including GPCRs. Furthermore, we aim to generate new drug candidates in collaboration with pharmaceutical companies using this platform.

Business Models (when applying)

Our business model is based on collaborating with pharmaceutical companies. First, we will perform high-resolution structural analyses of compounds with weak binding affinity, which are owned by pharmaceutical companies, using Cryo-EM. We then optimize these compounds through computational science to identify lead candidate compounds. We then license the lead compounds to pharmaceutical companies during the preclinical stage through joint development agreements, generating milestone payments and royalties. Our aim is to operate a low-fixed-cost business model while bearing no clinical development risks ourselves.

Activity Planning (when applying)

During the GTIE GAP funding period, we will advance R & D and business development in parallel. We will conduct a structural analysis of compound complexes for the Class B receptor family, a task that is particularly challenging. At the same time, we will use computational science to integrate in silico screening and structural dynamics analysis in order to identify lead compounds and establish a screening evaluation system. By validating these platforms, we will demonstrate the superiority of our technologies. In terms of business development, we will collaborate with Kyoto-ICAP to verify customer needs through interviews with pharmaceutical companies, recruitment of potential executives, formulation of business plans and capital strategies, and securing partners for contract and joint research. These efforts will gradually reduce the technical and business risks, with the aim of establishing the start-up in April 2029 and commencing operations immediately afterwards.