Interprotein®

Small molecule SARS-CoV-2 inhibitor (drug discovery)

Background and Concept:

- 3-chymotrypsin-like protease (3CLpro) is one of the main enzymes involved in replication of SARS-CoV-2.
- Although there are many types of coronavirus, structure of this enzyme is relatively conserved among the types, which means 3CLpro inhibitor would be effective for not only SARS-CoV-2 but also the next generation of HCoV.
- Interprotein has established a structure-based drug discovery (SBDD) strategy, INTerprotein's Engine for New Drug Design (INTENDD®) and an artificial intelligence (AI)-introduced activity prediction system (AI-guided INTENDD®).

Present Status:

- Identification of repurposing drug candidates for SARS-CoV-2 is being conducted and several potential 3CLpro inhibitors have been selected.

Key Factor for Success:

- Financial support by sponsors and/or investors and Participation and commitment of excellent medicinal chemists.
- Preparation of assay systems in collaboration with academia/public lab. and/or pharma/biotech.

Step for Accelerated Collaboration:

- Disclosure of confidential information on INTENDD® and AI-guided INTENDD® including predicted activity of known compounds under CDA.
- Activity prediction of newly designed and virtual compounds and assay of selected high-potency compounds.

Compare with General Drug Discovery

- Short-time and low-cost drug discovery is achieved by:
  - ✓ Efficient hit identification by INTENDD® and speedy lead generation/optimization by AI-guided INTENDD®.
  - ✓ Proposal of 200- hit candidates by INTENDD® in a half year.
  - ✓ Selection of small number of highly potent compounds by AI-guided INTENDD® prior to compound synthesis (identified from not greater than 5 cycles and 100 compounds in 1 – 2 years).

Process of INTENDD® and AI-guided INTENDD®