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NEWS RELEASE

Interprotein Corporation

# AI-guided INTENDD®, Interprotein's AI drug discovery platform based on deep learning of binding structures of small molecules and target proteins, is transitioning to a practical stage

Interprotein Corporation (CEO: Masato Hosoda, headquarters: Osaka, Japan) announced extremely positive updates on the recent progress regarding the pharmacological activity and subsequent value prediction system of compounds using artificial intelligence (AI).

Interprotein focuses on protein-protein interactions (PPIs), which have thought to have been difficult drug targets, and has developed a system supported by AI that enables pharmacological activity prediction of small molecules (AI-guided INTENDD®).

Mr. Hosoda stated that Interprotein has reached a stage where the prediction of ligand activity can be achieved with an accuracy of about 80%. Specifically, activity was divided into 8 classes from 3-digit pM to single-digit mM and AI-guided INTENDD® was trained to correctly classify the ligands that target PPI. They then performed a test prediction of ligands whose activities have been experimentally determined. The measured values matched the class predicted by AI-guided INTENDD® with an accuracy of about 80%. When Interprotein only focus on the ligands with high activity, the probability reaches > 90%.

Mr. Hosoda went to add that AI-guided INTENDD® can now be used as a technique to dramatically increase the success probability of small molecule drugs targeting PPI discovery.

With this technique, Interprotein can categorically say that it is possible to synthesize and evaluate only highly active compounds and we no longer need to repeat synthesis and evaluation of thousands of compounds. The system can contribute to the rapid optimization of compounds by effectively utilizing existing compound libraries, designed but not yet synthesized or evaluated compound, and virtual libraries containing many patentable compounds. In addition, this system can be applied not only to PPI but also to various types of other drug targets such as enzymes and receptors (that do not use proteins as ligands).

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