

Astellas Initiates Collaborative Research with National Institute of Advanced Industrial Science and Technology by Utilizing Highly Advanced IT Drug-Discovery Technologies

- Aiming for early discovery of compounds in the areas of Ophthalmology and Nephrology by merging approximately 10,000 of protein-ligand complex structural information and highly advanced IT drug-discovery technologies -

Tokyo, Japan, July 23, 2015 – Astellas Pharma Inc. (“Astellas”; TSE 4503, headquarters: Tokyo; President and CEO Yoshihiko Hatanaka) announced that it has initiated a collaborative research with the National Institute of Advanced Industrial Science and Technology (“AIST”; Tokyo; President Ryoji Chubachi) utilizing Astellas’ own protein-ligand complex structural information¹⁾ and AIST’s highly advanced IT drug-discovery technologies.

A candidate compound is a compound which has the potential to become a drug that plays a role by acting on proteins that cause diseases.

Astellas has accumulated rich structural information of pharmaceutical target proteins complexed with candidate compounds, and the number of protein-ligand complex structures becomes approximately 10,000. Furthermore, the candidate compounds included in these complex structures have highly desirable attributes as a drug (drug-likeness²⁾).

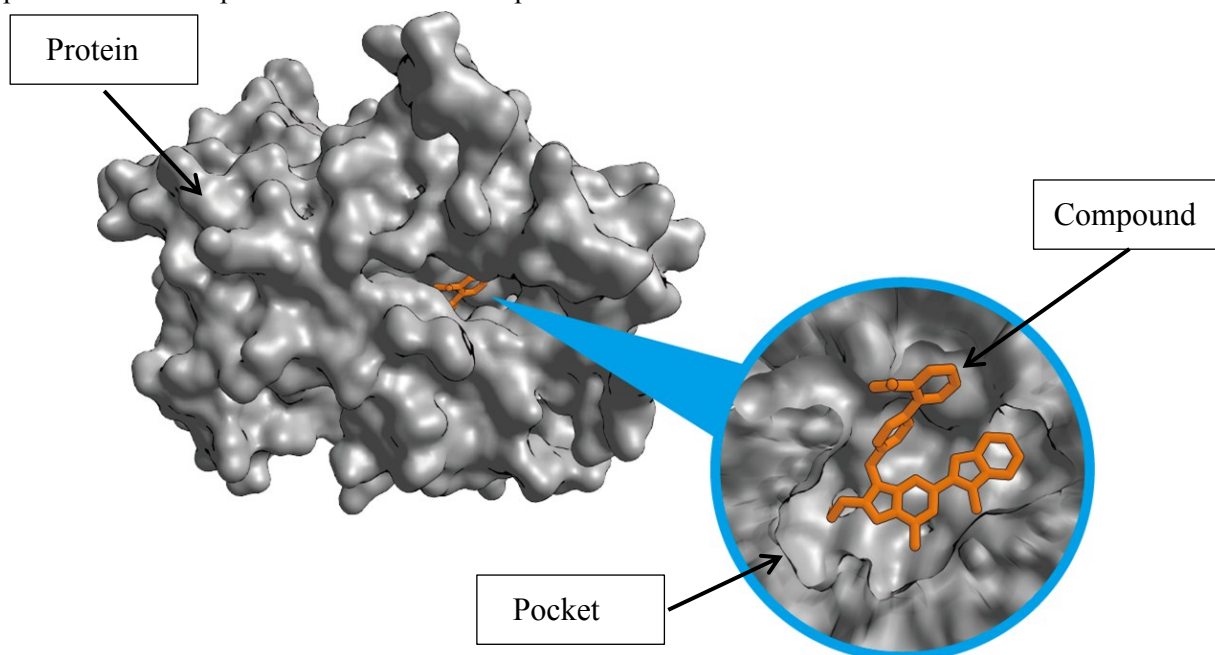
Meanwhile, AIST has technologies and calculation methods that enable the analysis of protein-ligand complex structures comprehensively, and also has state-of-the-art IT drug-discovery technologies analyzing structural fluctuations³⁾ of a protein that contribute to the protein function.

This collaboration focuses on early discovery of compounds in the therapeutic areas of Ophthalmology and Nephrology not only by utilizing highly advanced IT drug-discovery technologies at AIST, but also by accumulating know-how of medicinal chemists, computational chemists and X-ray crystallographers at Astellas.

Astellas is actively pursuing open innovation in drug discovery through collaboration with external partners having strong expertise. Through this collaborative research, we expect the efficiency of candidate compound search will be significantly improved and the opportunity for drug discovery will be extended.

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1) Protein-ligand complex structural information: 3-dimensional structural information of a protein complexed with a compound which acts on the protein.



<An example of protein-ligand complex structural information>

2) Drug-likeness: A qualitative concept used in drug design to outline how “druglike” a substance is. It is estimated from the molecular structure. QED (quantitative estimate of drug-likeness) and Lipinski’s Rule of Five are widely known indicators for drug-likeness.

3) Structural fluctuation: Proteins exist in living organisms perform their functions by fluctuating or changing their structures over time. One can observe the conformational changes of a protein by molecular simulations of static (snapshot) structures obtained from X-ray crystallographic analysis.

About Astellas Pharma Inc.

Astellas Pharma Inc., based in Tokyo, Japan, is a company dedicated to improving the health of people around the world through the provision of innovative and reliable pharmaceutical products. We focus on Urology, Oncology, Immunology, Nephrology and Neuroscience as prioritized therapeutic areas while advancing new therapeutic areas and discovery research leveraging new technologies/modalities. We are also creating new value by combining internal capabilities and external expertise in the medical/healthcare business. Astellas is on the forefront of healthcare change to turn innovative science into value for patients. For more information, please visit our website at www.astellas.com/en.

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