一般社団法人日本生物物理学会　第 6 回 Biophysics and Physicobiology 論文賞受賞講演会
The 6th Award Seminar for outstanding Biophysics and Physicobiology paper

オーガナイザー：日本生物物理学会 Biophysics and Physicobiology 論文賞選考委員会

Organizers: Award committee for outstanding Biophysics and Physicobiology paper

日　時：9 月 19 日（火）12:50 〜 13:20 ／ Sept. 19 Tue.

場　所：A 会場（全学教育棟 E107）／ Room A (General Education Building E107)

形　式：講演会／ Lecture

第 6 回 Biophysics and Physicobiology 論文賞受賞者

BPPB Outstanding Paper Awardee

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LigandBox : 化合物の立体構造のデータベース

LigandBox: A database for 3D structures of chemical compounds

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A database for the 3D structures of available compounds is essential for the virtual screening by molecular docking. In 2013, we opened the web server for the LigandBox database containing four million available compounds, collected from the catalogues of commercial suppliers, and approved drugs and biochemical compounds. Each chemical compound in the database has several 3D conformers with hydrogen atoms and atomic charges, which are ready to be docked into receptors using docking programs. The 3D conformations were generated using our molecular simulation program package, myPresto. Various physical properties, such as aqueous solubility (LogS) have also been calculated to characterize the ADME-Tox properties of the compounds. The Web database provides two services for compound searches: a property/chemical ID search and a chemical structure search. The chemical structure search is performed by a descriptor search and a maximum common substructure (MCS) search combination, using our program *kcombu*. By specifying a query chemical structure, users can find similar compounds among the millions of compounds in the database within a few minutes. In 2017, the LigandBox stores more than 10 million compounds. Our database is expected to assist a wide range of researchers, in the fields of medical science, chemical biology, and biochemistry, who are seeking to discover active chemical compounds by the virtual screening.