Drug Discovery Directly from Protein 3D-Structures

Takao Matsuzaki (Zoegene Corp.)

The conventional drug design is considered as a success when it gives a few active compounds among 100 proposed compounds. A new method, CPADD (Closest Packing Approach for denovo Drug Design) invented by the author, gave extraordinary improved situation, such as (1) 44 active compounds with IC50 < 5 microM among 100 proposed ones, and (2) 55 compounds with IC50 < 1 mM among 61 proposed ones. They can not be called “hit compounds” any more, since non-active compounds are only exceptions. This means that drug design has entered into a new era and has become “an engineering process”, where designed compounds normally have activity. The talk will include the explanation of CPADD, success stories on all 7 targets including PPI (Protein-Protein Interaction) and comparison with “docking methods”.