Developing new drugs that bind exclusively to target cells in diseases such as cancer is crucial. Masumi Taki and co-workers at the University of Electro-Communications in Tokyo, together with scientists at Kagoshima University, Japan, have expanded on current drug discovery methods to create a hybrid-drug generating system for this purpose.

Their system uses ‘artificial-molecule evolution’ - taking non-natural core molecules and adapting and optimizing them to make new ‘pharmacophores’. A pharmacophore is a molecular model which can be manipulated to bind molecules for targets such as cancer cells.

Taki’s team designed an artificial core molecule using salicylic acid, a readily available drug-like molecule known never to bind to a target protein on its own. They then used a common technique in drug discovery called ‘phage display’ to manipulate peptides to surround the artificial core molecule. Phage display involves inserting gene fragments into surface protein genes on bacteriophages - naturally-occurring viruses that infect bacteria. A new, non-natural protein or peptide hybrid then appears on the phage surface, and its biological properties can be exploited.

Publication and Affiliation

Yuuki Tokunaga¹, Yuuki Azetsu¹, Keisuke Fukunaga¹, Takaaki Hatanaka², Yuji Ito² & Masumi Taki¹*. Pharmacophore generation from a drug-like core molecule surrounded by a library peptide via the 10BASEd-T on bacteriophage T7. *Molecules* 19 2481-2496 (2014)

1. Department of Engineering Science, Bioscience and Technology Program, The Graduate School of Informatics and Engineering, The University of Electro-Communications (UEC), 1-5-1 Chofugaoka, Chofu, Tokyo 182-8585, Japan.

2. Department of Chemistry and Bioscience, Graduate School of Science and Engineering, Kagoshima University, 1-21-35 Korimoto, Kagoshima, Kagoshima 890-0065, Japan

*corresponding author, e-mail address: taki@pc.uec.ac.jp
Researchers from the University of Electro-Communications in Tokyo have developed a new method for generating pharmacophores from artificial core molecules linked to T7 phages.