

JHU  O

# 日本ヒトプロテオーム機構 (JHUPPO) 第7回大会

日時：2009年7月27日(月)～28日(火)

プログラム・予稿集

基礎研究からさまざまな応用研究へ飛躍する最先端プロテオミクス  
～医学・薬学・農学への応用～

会場：北里大学薬学部（東京都港区白金）  
主催：日本ヒトプロテオーム機構  
北里大学理学部/北里大学薬学部  
大会委員長：前田忠計（北里大学名誉教授）



7th JHUPPO Conference

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**シンポジウム7 Symposium 7**  
**プロテオミクスの薬学への応用**  
**Pharmacological Applications of Proteomics**

社 長：檀原宏文（北里大学薬学部）  
山田陽城（北里大学）

日 時：7月28日 9:15～11:45

会 場：B会場（1501大講義室）

**S7-1** プロテオーム解析によるサルモネラ病原因子の同定

9:15～ Identification and characterization of novel virulence factors controlled by ppGpp in *Salmonella enteica* via proteome approach

○岡田信彦

北里大学薬学部微生物学教室

○Nobuhiko Okada

Kitasato University School of Pharmacy Department of Microbiology

**S7-2** プロテオミクス技術による細胞内シグナル伝達系の解析

9:40～ Proteomic analyses of signal transduction

○服部成介

北里大学薬学部生化学

○Seisuke Hattori

Div. Biochem., Colledge Pharm. Sci., Kitasato Univ.

**S7-3** プロテオミクスの漢方薬の薬効解析への応用

－香蘇散の抗うつ様活性に関与する脳及び血清タンパク質の解析－

10:05～ Application of proteomics for analysis of antidepressant-like activity of a Kampo (Japanese herbal) medicine, kososan

○永井隆之<sup>1,2)</sup>

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○Takayuki Nagai<sup>1,2)</sup>

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- S7-4** 漢方医学における「証」の科学的解明を目指したプロテミクス解析  
10:30~ Proteomic analysis of pathogenic alteration (SHO) diagnosed by Kampo medicine  
○ 濟木育夫  
富山大学和漢医薬学総合研究所  
○ Ikuo Saiki  
Institute of Natural Medicine, University of Toyama
- S7-5** In Silico 創薬技術に基づく Structure-Based Drug Design の実際  
10:55~ Practical in silico structure-based drug design  
○ 広野修一  
北里大学薬学部  
○ Shuichi Hirono  
School of Pharmacy, Kitasato University
- S7-6** タンパク質立体構造のホモロジーモデリング研究と将来への展望  
11:20~ Study and future view on homology modeling of 3-dimensional protein structure  
○ 梅山秀明、加納和彦、寺師玄記、竹田-志鷹真由子  
北里大学薬学部  
○ Hideaki Umeyama, Kazuhiko Kanou, Genki Terashi, Mayuko Takeda-Shitaka  
School of Pharmacy, Kitasato University

## S7-6

### タンパク質立体構造のホモロジーモデリング研究と将来への展望

#### Study and future view on homology modeling of 3-dimensional protein structure

○梅山秀明、加納和彦、寺師玄記、竹田志鷹真由子

北里大学薬学部

○Hideaki Umeyama, Kazuhiko Kanou, Genki Terashi, Mayuko Takeda-Shitaka

School of Pharmacy, Kitasato University

For anti-hypertension drug, the authors started "Structure Based Drug Design (SBDD) based upon homology modeling study on 3-dimensional protein structure" in 1985 before the computer graphics study is generally performed. The protein modeling of human renin which is the target angiotensinogenase for hypertension was carried out by using HGS Molecular models. Its target enzyme is containing aspartic acids in the catalytic site, and it has the 25% sequence identity for penicillopepsin determined experimentally. The inhibitor KRI-1230 was designed based upon the shape of the modeled active site. It was ascertained from the intravenous injection to marmoset that this drug is effective for the hypertension disease. At that time, we believed firmly that the homological protein modeling would become a greatly necessary tool in the SBDD study in recent future. Then we began making the soft programs such as sequence alignment and production of 3-dimensional protein structure. Thus, the system what is called BIOCES was made as the fundamental graphic system on which various application programs were executed. Moreover, we made the chimera modeling system in order to perform the homology modeling using some reference proteins determined from the X-ray and NMR experiments. From the use of those systems we have published 19 papers during 14 years since 1988. And it became possible that the plural proteins forming complex or multimer were made from the complex or multimer in the PDB database. Consequently, the FAMS (Full Automatic Modeling System) was developed. Using its FAMS, all the proteins coded on the genomes of various species had been modeled, and those modeling data were published to open from the RIKEN website as the name of FAMSBASE. Moreover, the FAMS program was developed to model the complex proteins as if the complex appears to be single protein in the proposal of a new organism. We have continuously had the excellent results during recent 8 years until 2008 in the CASP contests of protein modeling. Also we have had good results in the CAPRI contests in relation to the docking prediction of the protein-protein interaction. Recently, we have had developed a new SBDD program based upon bioinformatics using the 3-dimensional coordinates of proteins and binding ligand molecules in the PDB database.

Keywords : Homology modeling, protein structure prediction, FAMS, structure based drug design, CASP