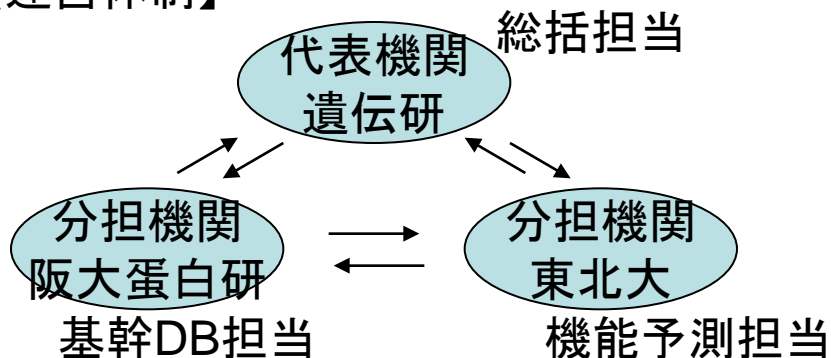


### 【課題概要】

タンパク質の立体構造に基づいて生物学的な機能を理解する上で必要な研究推進の支援と手法の高度化として、低分子結合部位の予測法の適用と高度化を行う。

### 【運営体制】



### 【連絡先】

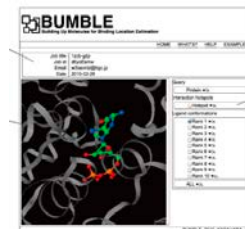
東北大  
木下賢吾(kengo@ecei.tohoku.ac.jp)  
城田松之(mshirota@ecei.tohoku.ac.jp)  
村上洋一(yoichi@ecei.tohoku.ac.jp)

### 【支援に供する技術】

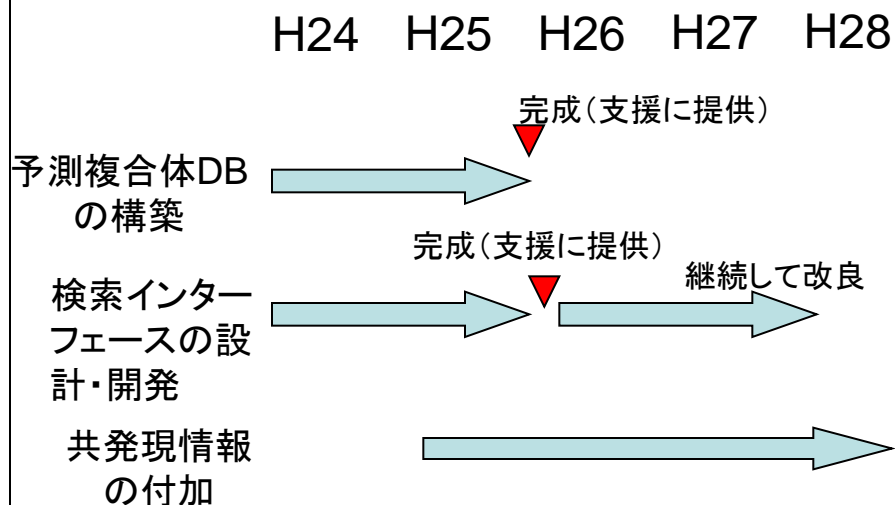
eF-seek+BUMBLE  
蛋白質低分子複合体モデリング

PDBj eF-seek

ABOUT eF-seek:  
Molecular function of proteins are determined by their three dimensional structures. But the similarity of protein structure can give some clues to infer their functions. In many cases, the molecular function are begun with the molecular interaction with small molecules (ligands). eF-seek is a web server to search for the similar ligand binding sites for the uploaded coordinate file with PDB format. The representative binding sites in eF-seek database are search by our own algorithm based on the close search algorithm.



### 【高度化研究】



# 【これまでの研究実績と創薬等PFにおける事業内容】

分子表面に着目した低分子結合予測＋フラグメント相互作用に着目した予測

**BUMBLE**  
Building Up Molecules for Binding Location Estimation

HOME WHAT'S? HELP EXAMPLE

Job title : 1zob-gdp  
Job id : d8yoEamw  
Email : w3iasmbi@hgc.jp

**PDBj eF-seek**

ABOUT eF-seek:  
Molecular function of proteins are determined by their three dimensional structures, thus the similarity of protein structure functions. In eF-seek, we began all protein structure data on the server to estimate the material. The database is on the server.

遺伝子共発現DB

**COXPRESdb ver. 4.7**  
last update: 2011.07.22

COXPRESdb provides co-regulated gene relationships to estimate gene functions.

Information  
 • Overview  
 • Publication  
 • Help

Target species  
 • Human (Hsa) Example: [gene page] [gene list]  
 • Mouse (Mmu) Example: [gene page] [gene list]  
 • Rat (Rno) Example: [gene page] [gene list]  
 • Chicken (Gga) Example: [gene list]  
 • Zebrafish (Dre) Example: [gene list]  
 • Fly (Dme) Example: [gene list]  
 • Nematoda (Cel) Example: [gene list] [statistics]

Search  
 • Gene Table  
 • EdgeAnnotation  
 • CoExSearch  
 • etc.

Draw  
 • NetworkDrawer  
 • HCluster  
 • CoexViewer  
 • etc.

Browse Bulk download

What's new  
 2010.11.17 \* COXPRESdb official reference is renewed. [Publication]  
 2010.10.16 \* Data statistics page is available. [statistics]  
 2010.09.15 \* Public annotations are updated. (ver.4.1)  
 2010.05.20 \* "NetworkDrawer" is renewed to draw larger gene networks. [Draw > NetworkDrawer]

twitter  
 27 Jul 2012 COXPRESdb mirror site: [Link]  
 13 Feb 2012 [Update Plan] Coexpression data will be updated in March (or April). [more]

**PDBj eF-site**  
electrostatic surface of Functional-site

About eF-site | Tools | References | Links | Acknowledgements | Feedback

396421 Entries, Last Update: 25-Dec-2010

Keyword Search  
  
 PDB code only @and ○or

Category Search  
 • Antibody  
 • Prosite  
 • Active Site  
 • Membrane  
 • Binding Site

Examples of molecular surface  
 1tup-C 1tup-A 1tup-B 1tup-ABCE  
 1tup-EF

For all pdb entries, molecular surfaces are generated for individual subunits of proteins and the complex of proteins. In addition, when double strands DNA is included in the entry, a molecular surface for each dsDNA is also stored.

選択) ファイルが選択されていません

of version 3, please make sure that the  
 rds to express the version (click here for

is a part of PDBj project.

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