

## Tutorial-3 #2 Document

# Structural modeling of proteins: Principle and application to an ion channel

**Haruki Nakamura**

*PDBj, Institute for Protein Research, Osaka University*

**Daron M. Standley**

*Immunology Frontier Research Center, Osaka University*

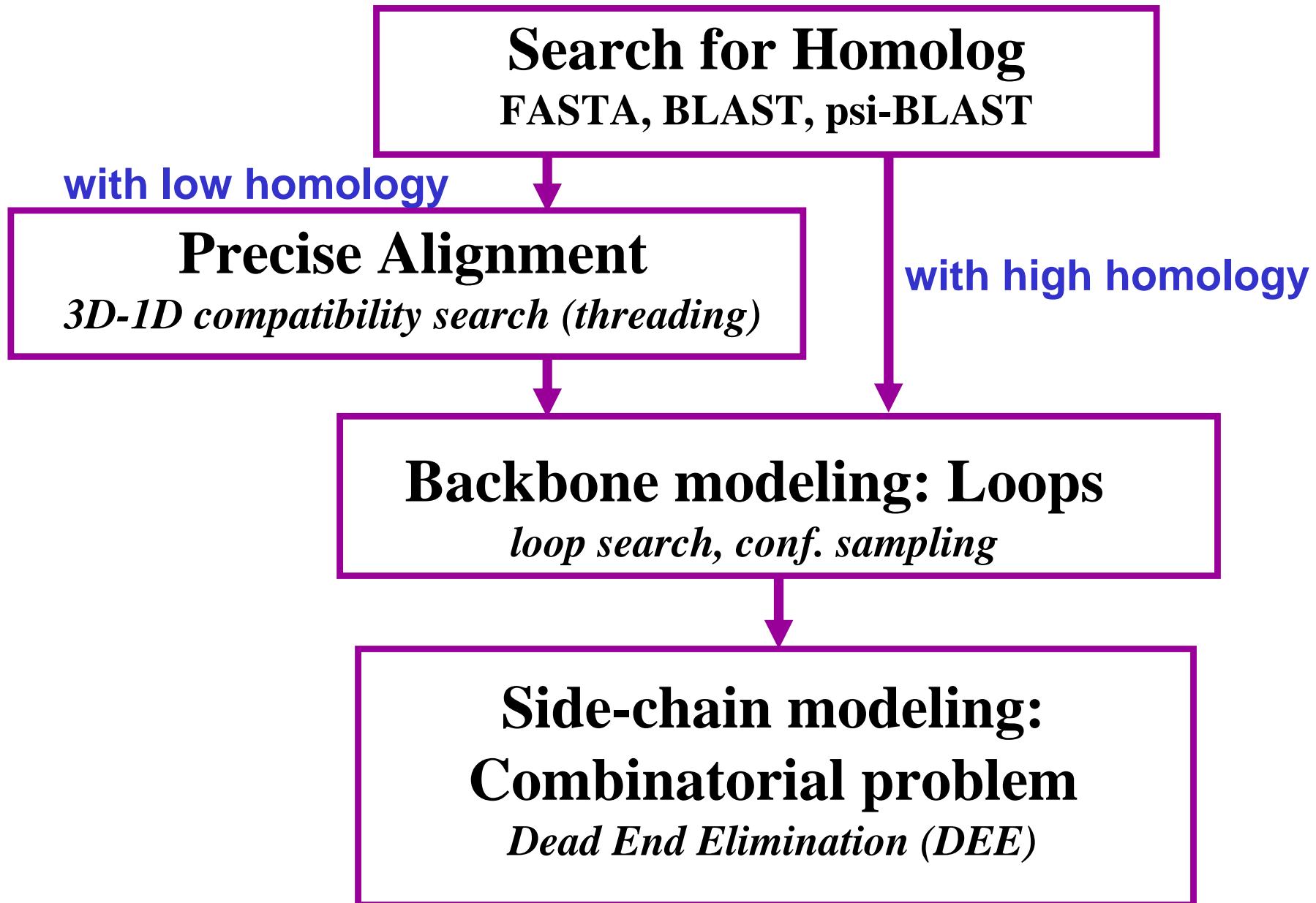
**Narutoshi Kamiya**

*The center for Advanced Medical Engineering and Informatics,  
Osaka University*

*<http://www.protein.osaka-u.ac.jp/rcsfp/pi/>  
<http://www.pdbj.org/>*

# Goal of the Tutorial:

To construct the homology model of hERG channel



## **Step 1. Get amino-acid sequence of hERG channel from NCBI.**

Access to NCBI (<http://www.ncbi.nlm.nih.gov/>), and get an amino acid sequence of **Q12809** (region from S5 to S6: residues from 550 to 671).

## **Step 2. Make the alignment by threading.**

Access to SFAS: Sequence to Function Annotation Server (<http://sysimm100.protein.osaka-u.ac.jp/sfas/>), and get the best alignment to the putative template structure.

The query may take several minutes to hours depending on the status of the Web site, please visit the example result page: ([http://sysimm100.protein.osaka-u.ac.jp/tmp/SFAS16483/hERG\\_top.html](http://sysimm100.protein.osaka-u.ac.jp/tmp/SFAS16483/hERG_top.html))

## **Step 3. Make the tetramer structure and see the result.**

Access to Quarternary Structure Service ([http://sysimm100.protein.osaka-u.ac.jp/pdb\\_quat/](http://sysimm100.protein.osaka-u.ac.jp/pdb_quat/)), and get & see the tetramer model structure of hERG channel.

# Step1: Get amino-acid sequence of hERG channel from NCBI (<http://www.ncbi.nlm.nih.gov/>)

The screenshot shows the NCBI Protein search results for the protein Q12809. The top navigation bar includes links for All Databases, PubMed, Nucleotide, Protein, Genome, Structure, OMIM, PMC, Journals, and Books. The search bar is set to "Protein". The main content area displays the following details:

**RecName:** Full=Potassium voltage-gated channel subfamily H member 2;  
**AltName:** Full=Voltage-gated potassium channel subunit Kv11.1;  
**AltName:** Full=Ether-a-go-go-related gene potassium channel 1; Short=H-ERG; Short=Erg1; Short=Ether-a-go-go-related protein 1; Shor...

**Comment Features Sequence**

**LOCUS** Q12809 1159 aa linear PRI 07-JUL-2009  
**DEFINITION** RecName: Full=Potassium voltage-gated channel subfamily H member 2;  
AltName: Full=Voltage-gated potassium channel subunit Kv11.1;  
AltName: Full=Ether-a-go-go-related gene potassium channel 1;  
Short=H-ERG; Short=Erg1; Short=Ether-a-go-go-related protein 1;  
Short=Eag-related protein 1; AltName: Full=eag homolog.

**ACCESSION** Q12809  
**VERSION** Q12809.1 GI:7531135  
**DBSOURCE** UniProtKB: locus KCNH2\_HUMAN, accession [Q12809](#);  
class: standard.  
extra accessions:075418,075680,Q9BT72,Q9BUT7,Q9H3P0  
created: May 30, 2000.  
sequence updated: Nov 1, 1996.  
annotation updated: Jul 7, 2009.  
xrefs: [U04270.1](#), [AAA62473.1](#), [AB009071.2](#), [BAA37096.1](#), [AF363636.1](#),  
[AAL37559.1](#), [AB044806.1](#), [BAB19682.1](#), [AJ512214.1](#), [CAD54447.1](#),  
[AJ010538.1](#), [CAA09232.1](#), [AJ010539.1](#), [AJ010540.1](#), [AJ010541.1](#),  
[AJ010542.1](#), [AJ010543.1](#), [AJ010544.1](#), [AJ010545.1](#), [AJ010546.1](#),  
[AJ010547.1](#), [AJ010548.1](#), [AJ010549.1](#), [AJ010550.1](#), [AJ010551.1](#),  
[AF052728.1](#), [AAC69709.1](#), [BC001914.1](#), [AAH01914.2](#), [BC004311.2](#),  
[AAH04311.2](#), [I38465](#), [NP\\_000229.1](#), [NP\\_742053.1](#), [NP\\_742054.1](#), [1BYW\\_A](#),  
[1UJL\\_A](#)  
xrefs (non-sequence databases): IPI:IPI00029662, IPI:IPI00172614,  
IPI:IPI00221190, IPI:IPI00221191, UniGene:Hs.647099, PDBsum:1BYW,  
PDBsum:1UJL, IntAct:Q12809, TCDB:1.A.1.20.1, PhosphoSite:Q12809,  
PRIDE:Q12809, Ensembl:ENSG00000055118, GeneID:[3757](#), KEGG:hsa:3757,  
UCSC:uc003wib.1, UCSC:uc003wic.1, UCSC:uc003wie.1,  
GeneCards:GC07M150272, H-InvDB:[HIX0007217](#), HGNC:[6251](#),  
HPA:CAB006838, MIM:[152427](#), MIM:[609620](#), Orphanet:130, Orphanet:768,  
Orphanet:51083, PharmGKB:PA212, HOGENOM:Q12809, HOVERGEN:Q12809,  
OMA:Q12809, DrugBank:DB01118, DrugBank:DB00276, DrugBank:DB00637,  
DrugBank:DB01136, DrugBank:DB00604, DrugBank:DB00204,  
DrugBank:DB01218, DrugBank:DB00308, DrugBank:DB01100,

**Download ▾ Save ▾ Links ▾**

**Change Region Shown**  
**Customize View**

**Sequence Analysis Tools**

- ▶ BLAST Sequence
- ▶ Conserved Domains

**Articles about the KCNH2 gene**

- ▶ Genetic Polymorphism of KCNH2 Confers Predispos [J Cardiovasc Electrophysiol. 2009]
- ▶ Breaking the gene barrier in schizophrenia. [Nat Med. 2009]
- ▶ Interactions of H562 in the S5 helix with T618 and S621 in the pore helix a [Biophys J. 2009]

» See all...

**Identical Proteins for Q12809.1**

- ▶ Sequence 2 from patent US 7541[ACS12627]
- ▶ Sequence 5 from patent US 7537[ACS08477]
- ▶ Sequence 2 from patent US 7510[ACQ19114]

» See all...

**RefSeq Protein Isoforms**

See 3 reference sequence protein isoforms for the KCNH2 gene.

**More about the KCNH2 gene**

This gene encodes a voltage-activated potassium channel belonging to the eag family. It shares sequence similarity with the Drosophila ether...

Also Known As: ERG1, HERG, HERG1, Kv11...

**Homologs of the KCNH2 gene**

The KCNH2 gene is conserved in chimpanzee,

## Step2: Get homologs in PDB and have alignments with 3D modes. (<http://sysimm100.protein.osaka-u.ac.jp/sfas/>)

**PDBj**

**iFReC**

### Sequence to Function Annotation Server

Please enter your query

Name: hERG(550-67)

Sequeunce:

```
>hERG | Q12809 | residues 550-671
LFLLMCTALIAHWLACIWAIGNMEQPHMDSRIGWLHNLGDQIGKPYNNSGLGGPSIKDKY
VTALYFTFSSLTSVFGNVPNTNSEKIFSCIVMLIGSLMYASIFGNVSAAIQRLYSGTA
```

Or

Upload a FASTA-formatted sequence file: (ファイルを選択) ファイルが選...ていません

Select Alignment methods

Blast       Whole PDB       Rep. Domains  
 PsiBlast       Whole PDB       Rep. Domains  
 HHpred       PDB + SCOP

Send results to this email address

[Send feedback](#)    [About SFAS](#)

### hERG Results

Method	Template	E-value	Coverage	Alignment	Model
HHpred	<a href="#">2r9rB</a>	<a href="#">jV</a>	1.10e-19	75	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">1orqC</a>	<a href="#">jV</a>	9.70e-20	46	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">3behA</a>	<a href="#">jV</a>	2.20e-19	75	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">1xl4A</a>	<a href="#">jV</a>	8.20e-17	47	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">2a9hA</a>	<a href="#">jV</a>	3.70e-17	49	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">2ih3C</a>	<a href="#">jV</a>	4.10e-16	48	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">2q67A</a>	<a href="#">jV</a>	2.40e-16	67	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
HHpred	<a href="#">2qksA</a>	<a href="#">jV</a>	5.60e-13	45	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqG</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqH</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqB</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqA</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqF</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqE</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqC</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1lnqD</a>	<a href="#">jV</a>	1.74e-08	40	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">1orqC</a>	<a href="#">jV</a>	1.67e-07	42	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Psiblast	<a href="#">2a01B</a>	<a href="#">jV</a>	4.19e-07	41	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">1ujlA</a>	<a href="#">jV</a>	8.03e-20	33	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">2q6aB</a>	<a href="#">jV</a>	7.93e-04	29	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">2q67B</a>	<a href="#">jV</a>	7.48e-04	29	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">2q67A</a>	<a href="#">jV</a>	7.24e-04	29	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">2ahzB</a>	<a href="#">jV</a>	8.62e-04	29	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">3e89B</a>	<a href="#">jV</a>	1.03e-03	31	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">3e8hB</a>	<a href="#">jV</a>	1.03e-03	31	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">2q6aA</a>	<a href="#">jV</a>	8.13e-04	29	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">2ahyA</a>	<a href="#">jV</a>	8.84e-04	29	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>
Blast	<a href="#">3e83B</a>	<a href="#">jV</a>	1.03e-03	31	<a href="#">Text</a> <a href="#">Jalview</a> <a href="#">Spanner</a>

([http://sysimm100.protein.osaka-u.ac.jp/tmp/SFAS16483/hERG\\_top.html](http://sysimm100.protein.osaka-u.ac.jp/tmp/SFAS16483/hERG_top.html))

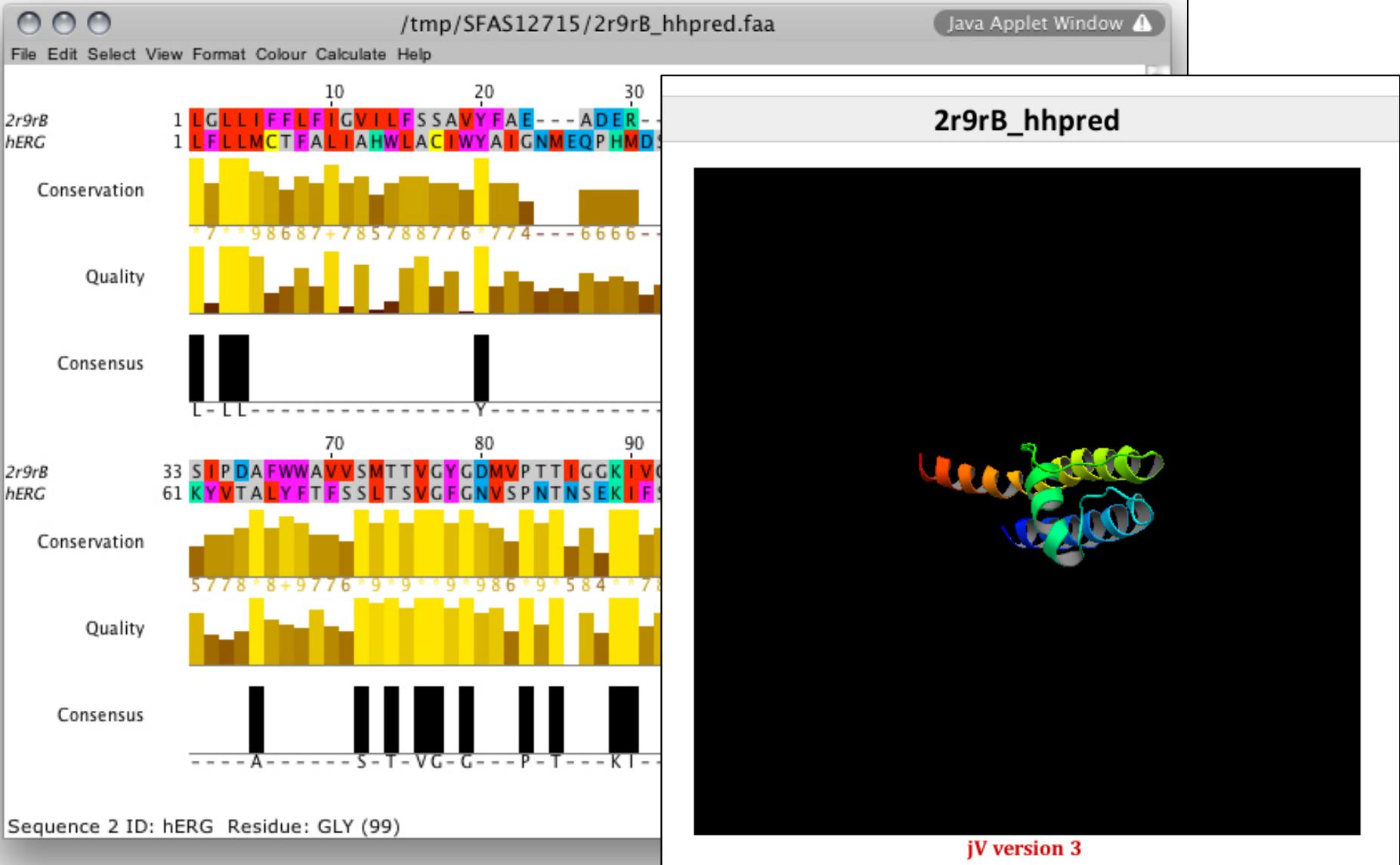
# Step2: Result of SFAS: The best template is 2r9rB

Jalview

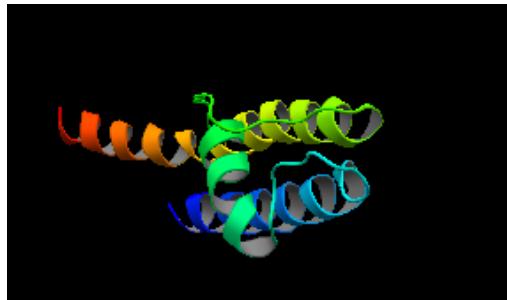
Start Jalview

[Return to SFAS Results](#)

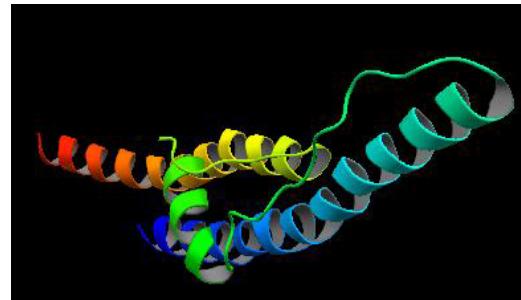
```
>2r9rB
LGLLIIFFLFIGVILFSSAVYFAE---ADER-----
DSQFPSIPDAFWAWVSMTTVGYGDMVPTTIGGKIVGSLCAIAGVLTIALPVPVI
VSNFNYFYHRET
>hERG
LFLLMCTFALIAHWLACIWYAIgnMEQPHMDSRIGWLHNLGDQIGKPYNSSGLGG
PSIKDKYVTALYFTFSSLTSVGFGNVSPNTNSEKIFSICVMLIGSLMYASIFGNV
SAIIQRLYSGTA
```



## Step3: Make the tetramer structure



Template: 2r9rB  
(550-670)



Model structure  
(monomer)

PDBj WPI Osaka University iFReC

### Quaternary Structure Service

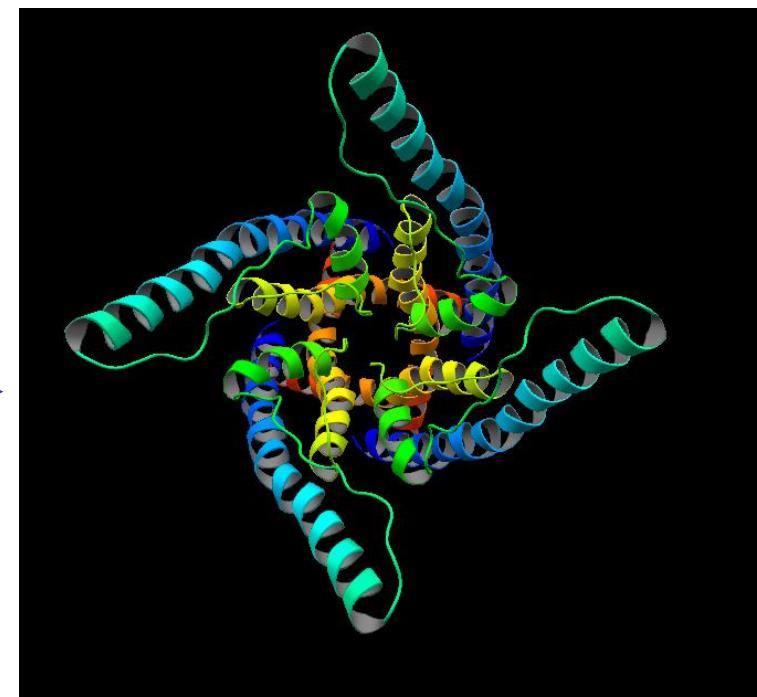
Please enter your query

Upload a PDB-formatted file:  ファイルを選択 ファイルが選...ていません

Please enter your template ID

PDB ID:  (template PDB file must contain the crystallographic symmetry info.)

[Send feedback](#)



([http://sysimm100.protein.osaka-u.ac.jp/pdb\\_quat/](http://sysimm100.protein.osaka-u.ac.jp/pdb_quat/))

Model structure  
(tetramer)

# Other options

**Step O1. Search PDB structures with similar amino acid sequences.**

Access to Sequence Navigator (<http://www.pdbj.org/>), and get the PDBID information for the homologs.

**Step O2. Collect the structural information of the homologs.**

Access to PDBj (<http://www.pdbj.org/>), and get the structural information for the above PDBIDs.

**Step O3. Make the sequences-structures multiple alignment.**

Access to MAFFTash (<http://www.pdbj.org/>), and input the PDBIDs and the sequence of the hERG channel, to get the multiple alignment.

**Step O4. Make the homology model with the alignment.**

Access to Spanner (<http://www.pdbj.org/spanner/>), and input the template structure with the above PDBID and the alignment information to get the homology model.

# Step 01: Search for a Homolog protein in PDB

## Use of Sequence Navigator at PDBj (<http://www.pdbj.org/>)

**PDBj** Protein Data Bank Japan

English

**Home**

Data Deposition >>  
ADIT: PDB Deposition  
ADIT-NMR

Search >>  
Search PDB (xPSSS)  
Latest Released Search  
**Sequence-Navigator** (circled)  
Structure-Navigator  
SeSAW  
Ligand Binding Sites (GIRAF)  
EM Navigator  
Search NMR Data (BMRB)  
Status Search

Service and Software >>  
Protein Globe  
ASH  
MAFFTash  
J/V: Graphic Viewer

Derived database >>  
eF-site/eF-seek/eF-surf  
eProtS  
ProMode  
Molecule of the Month

Download >>  
PDB Archive/Snapshot Archive

About Remediation Data

Links

PDBj (Protein Data Bank Japan) maintains a centralized archive of macromolecular structures in collaboration with the [RCSB](#) in USA and the [PDBe](#) in EU. PDBj is supported by [JS](#).

**Sequence Navigator**

**About Sequence Navigator**

**Sequence Navigator Soap Service**

To Enter Navigator, Input a PDB ID  and Chain ID

OR Input an AA Sequence

>Influenza A virus (A/Texas/04/2009(H1N1)) segment 6 neuraminidase(NA) gene, complete cds. FJ981614  
MNPQNQKIIITIGSVCMTIGMANLILQIGNIISIWISHSIQLGNQNQIETCNQSVITYENNTWV  
NQTYVNISNTNFAAGQSVSVKLAGNSSLCPVSGWAIYSKDNSVRIGSKGDVFIREPFIS  
CSPLECRTFFLTQGALLNDKHSNGTIKDRSPYRTLMSCPIGEVPSPYNSRFESVAWSASAC

**Clustering Options**  
 No Clustering    Cluster by E-value  $10^{\wedge}$

**PDBj** Protein Data Bank Japan

English

**Home**

Data Deposition >>  
ADIT: PDB Deposition  
ADIT-NMR

Search >>  
Search PDB (xPSSS)  
Latest Released Search  
**Sequence-Navigator**  
Structure-Navigator  
SeSAW  
Ligand Binding Sites (GIRAF)  
EM Navigator  
Search NMR Data (BMRB)  
Status Search

Service and Software >>  
Protein Globe  
ASH  
MAFFTash  
J/V: Graphic Viewer

Derived database >>  
eF-site/ eF-seek/ eF-surf  
eProtS  
ProMode  
Molecule of the Month

Download >>

PDBj (Protein Data Bank Japan) maintains a centralized archive of macromolecular structures in collaboration with the [RCSB](#) in USA and the [PDBe](#) in EU. PDBj is supported by [JST-BIRD](#).

**Sequence Navigator**

Query Sequence:  
[MNPQNQKIIITIGSVCMTIGMANLILQIGNIISIWISHSIQLGNQNQIETCNQSVITYENNTWV]  
Clustering Option: [No Clustering]

**Re-Clustering Options**  
 No Clustering    Cluster by E-value  $10^{\wedge}$

**Results (1-33) / 33**

Seq. Identity: 91% Seq. Positives: 97% E-value: 0.0 Score: 776 Compound: NEURAMINDASE

Query 83385 VKLAGNSSLCPVSGWAIYSKDNSVRIGSKGDVFIREPFISCSPLECRTFFLTQGALLNDKHSNG  
2HTYC 1385 VKLAGNSSLCPINGWAVYSKDNSIRIGSKGDVFIREPFISCSHLECRTFFLTQGALLNDKHSNG  
2HTYC Exact Matches: 2HU0F 2HU4C 2HTYG 2HU4G 2HU0B 2HU4A 2HTYA 2HU

Seq. Identity: 91% Seq. Positives: 97% E-value: 0.0 Score: 774 Compound: NEURAMINIDASE

Query 83385 VKLAGNSSLCPVSGWAIYSKDNSVRIGSKGDVFIREPFISCSPLECRTFFLTQGALLNDKHSNG  
3CL2B 1385 VKLAGNSSLCPINGWAVYSKDNSIRIGSKGDVFIREPFISCSHLECRTFFLTQGALLNDKHSNG  
3CL2B Exact Matches: 3CL2G 3CL2F 3CL2C 3CL2H 3CL2A 3CL2D 3CL2E

Seq. Identity: 91% Seq. Positives: 97% E-value: 0.0 Score: 774 Compound: NEURAMINIDASE

Query 83385 VKLAGNSSLCPVSGWAIYSKDNSVRIGSKGDVFIREPFISCSPLECRTFFLTQGALLNDKHSNG  
3CLOA 1385 VKLAGNSSLCPINGWAVYSKDNSIRIGSKGDVFIREPFISCSHLECRTFFLTQGALLNDKHSNG  
3CLOA Exact Matches: 3CKZA

Seq. Identity: 88% Seq. Positives: 95% E-value: 0.0 Score: 763 Compound: NEURAMINIDASE

Query 83385 VKLAGNSSLCPVSGWAIYSKDNSVRIGSKGDVFIREPFISCSPLECRTFFLTQGALLNDKHSNG  
3CYEA 1385 VILTGNSSLCPISGWAIYSKDNGIRIGSKGDVFIREPFISCSHLECRTFFLTQGALLNDKHSNG

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# Step O2: Get Entry Data from PDBj

(<http://www.pdbj.org/>)

PDBj (Protein Data Bank Japan) maintains a centralized archive of macromolecular structures and provides integrated tools, in collaboration with the RCSB in USA and the PDBe in EU. PDBj is supported by JST-BIRD.

**xPSSS**  
x-based Protein Structure Search Service

**Summary [1gof]**

**About xPSSS** [Update Information](#) [wwPDB Snapshot Mirror](#)

**Search**

PDB ID  keyword

**Summary** [Structural Details](#) [Experimental Details](#) [Functional Details](#) [Sequence Neighbor](#) [Download/Display](#) [Link](#)

**PDB ID** 1gof [sequence information \(FASTA format\)](#) [download PDB format file](#)

**Descriptor** GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5)  
NOVEL THIOETHER BOND REVEALED BY A 1.7 ANGSTROMS CRYSTAL STRUCTURE OF GALACTOSE OXIDASE

**Title** OXIDOREDUCTASE(OXYGEN(A))

**Functional Keywords** Hypomyces rosellus

**Biological source** [UNP - GAOA\_DACD] Secreted

**Cellular location**

**Total number of polymer chains** 1

**Total molecular weight** 68785.9 (the details in [Structural Details Page](#))

**Authors** Ito, N., Phillips, S.E., Knowles, P.F. (*deposition date* : 1993-09-30, *release date* : 1994-01-31)  
Ito, N., Phillips, S.E., Stevens, C., Ogel, Z.B., McPherson, M.J., Keen, J.N., Yadav, K.D., Knowles, P.F.  
Novel thioether bond revealed by a 1.7 Å crystal structure of galactose oxidase.  
*Nature*, 350:87 - 90, 1991. ([PubMed](#) : 2002850) (DOI: [10.1038/350087a0](https://doi.org/10.1038/350087a0))

**Primary citation**

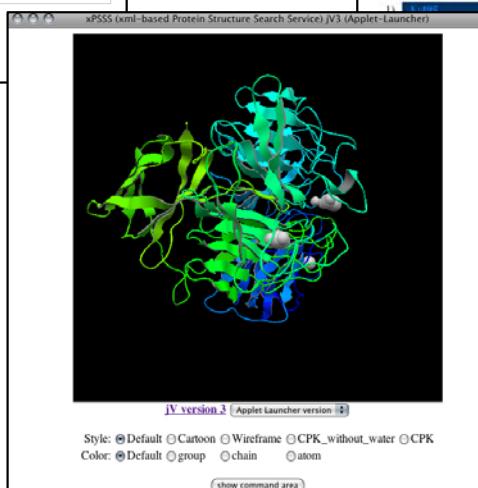
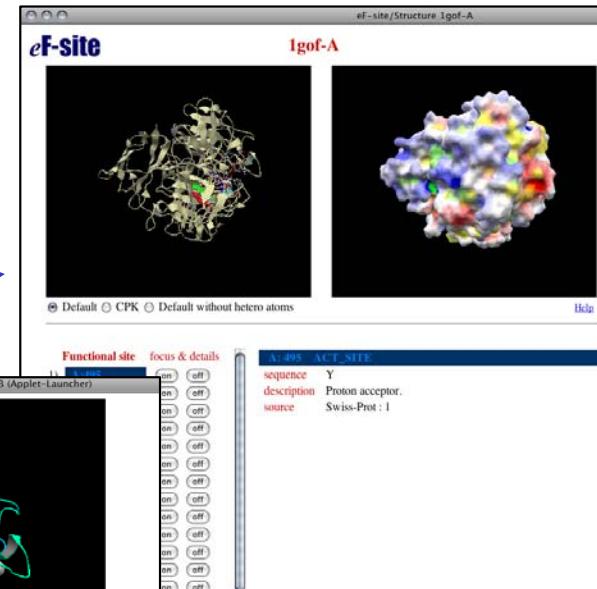
**Experimental method** X-RAY DIFFRACTION (1.7[Å])

**Other Database Information** CATH , CE , FSSP , SCOP , VAST , UniProt (UNP - Q01745) , eF-site , KEGG (EC 1.1.3.9) , EzCatDB

**Structure Viewers** **jV3 / Jmol**  
jV and Jmol require Java(TM)Plug-in 1.5 or later  
rotated about x by 90° 250X250 500X500  
rotated about y by 90° 250X250 500X500

Electron density map is available to be displayed from the Experimental Details page.

```
>1GOF:GALACTOSE OXIDASE
ASAPIGSIAISRNNAWAVTCDSAQSQNECNKAIIDGNKDTFWHTFYGANGDPKKPHTYTIDMK
TTQNVLNSLMLPRQDGQNQNGWIGRHEVYLSSDGTNNGSPVASGSWFADSITTKYNSFETRP
ARYVRVLVAITEANQGPWTISIAEINVFOASSTAPQPGPLGRWPFTIDLPIVAAAIEPTS
GRVLMWSYRNDAFGGSPGFGITLTLSMDPSTGIVSDRTVTVKTHDMPCGISMDDNGQIV
VTGNDAKKTSILYDSSDSWIPGPDQMVARGYQSSATMSDGRVFTIIGSNSSGGVFKNGE
VYSPSKTWTSILPNAKVNPMMLTADKQGLYRSNDHAMLFGWKGSVFOAGPSTMNNWYTS
GCGCCTGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGG
EGTSPNPNVFAFHNLQYFASPTPHTPSVLPDGSTFTITGGQRG1PFEDSTPFTVTFEIYYPHQ
DTFYQNPNNSIVRVYHSISLLPPGRVFNGGGLGDCTTNHFDQAQIFTPNLYNSNGNL
ATPKLITRTSTSQSVKVGGRTITISTDSSISKASLRIGYTAGHTVNTDQRRIPLTLNNNGGN
SYSTQVPSDSGVQALPGYWMLFVMNSAGVPSVASTIRVTL
```



Summary for each PDBID

Graphic viewer: **jV**  
<http://www.pdbj.org/jV/>

# Step O3: Alignment of Sequences and Structures(i)

(<http://sysimm100.protein.osaka-u.ac.jp/MAFFTash.3/>)

```
>PDBID  
2r9rB  
>PDBID  
1orqC  
>Q12809|hERG;550-671  
LFLLMCTFALIAHWLACIWy  
AIGNMEQPHMDSRIGWLHNL  
GDQIGKPYNSSLGGPSIKD  
KYVTALYFTFSSLTSVGFGN  
VSPNTNSEKIFSICVMLIGS  
LMYASIFGNVSAIIQRLYSG  
TA
```

**MAFFTash**

*alignment of multiple sequences and structures*

Paste your sequences and PDB IDs (plus chain IDs) here:

**(input here PDBID(s) and sequence(s))**

Example:

```
>PDBID  
3ygsC  
>Q6Q899|DDX58_MOUSE| 1-91  
MTAAQRQNLQAFRDYIKKILDPTYILSYMSSWLEDEEVQYIQAENNKGPMEAASLFLQY  
LLKLQSEGWFQAFLDALYHAGYCGLCEAIES  
>Q6Q899|DDX58_MOUSE| 101-176  
EEHRLLLRRLEPEFKATVDPNDILSELSECLINQECEEIRQIRDTKGRMAGAEKMAECLI  
RSOKENWPKVQLALE  
>PDBID  
2p1hA
```

Need help picking PDB IDs? Use [Prep-MAFFTash](#).

OR upload a file  ファイルを選択 ファイルが選...ていません

email address  (required)

**PDBj** [About MAFFTash](#) [Send feedback](#)

# Step O3: Alignment of Sequences and Structures(ii)

(<http://sysimm100.protein.osaka-u.ac.jp/MAFFTash.3/>)

Use “Prep-MAFFTash” for automatic search of sequences and structures.

**MAFFTash**  
*alignment of multiple sequences and structures*

Paste your sequences below. Missing PDB IDs will be automatically added. Example:

```
>hERG | Q12809 | residues 550-671  
LFLLMCTFALIAHWLACIWYAINMEQPHMDSRIGWLHNLGDQIKPYNSSLGGPSIKDKY  
VTALYFTSSLTSVGFGNVSPNTNSEKIFCIVMLIGSLMYASIFGNVSIIQLYSGTA
```

>PDBID  
1fanA  
>BPTI  
RPFDFCLEPPYTGPCKARIIRYFYNAKAGLCQTFVYGGCRAKRGNFKAEDCMRTCG  
>Alpha Dendrotoxin  
EPRRKLCILHRNPGRCYDKIPAFYYNQKKQCERFDWSGC GGNSNRFKTIEECRRTCIG

Note: You can add PDB IDs (plus chain IDs) too, if you want.

OR upload a file  ファイルを選択 ファイルが選...ていません

email address  (required)

Add structures

Use Blast to add structures (from PDB)  
Max seq ID between added structures   
Min seq ID from original input

Add ASH structural neighbors  
Max seq ID between added structures   
Min seq ID from original input

Add sequences

Use Blast to add sequences (from UniRef100)  
Max seq ID between added sequences   
Min seq ID from original input

# Step 04: Homology modeling with the alignment

(<http://www.pdbj.org/spanner/>)

## Spanner

Spanner is a structural homology modeling program—that is, it threads a specific amino-acid sequence onto a specific PDB structure, patching up the gaps as best it can.

To create a model, you must provide a template structure, as well as an alignment of the sequence you wish to model onto the template sequence. Spanner will replace matching residues, fill any gaps caused by inserted or deleted residues, and thermodynamically optimize the resulting structure.

The resulting PDB, as well as a log file, will be emailed to you when the modeling task finishes. If an error prevented a homology model from being generated (for example, when the alignment you provided does not match the template structure), the log file will explain which part of the modeling sequence failed.

Template PDB structure (PDB format):  
 ファイルが選...ていません

Sequence alignment (FASTA format; first sequence is the template, second sequence is the query):  
 ファイルが選...ていません

Model:  (not necessary if PDB file contains only one model)

Chain:  (not necessary if PDB file contains only one chain)

Email address for results:

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