

Introduction to 3D-Structure Visualization and Homology Modeling using the Swiss-Model Workspace

Lorenza Bordoli

Biozentrum of the University of Basel and
Swiss Institute of Bioinformatics

Lecture 4

May 2009



Lecture 4: Outline

- Homology Modeling using the Swiss-Model Workspace (Part II)
- The Swiss-Model Repository
- The Protein Model Portal

Swiss-Model Repository

Swiss-Model Repository

- SWISS-MODEL Repository (<http://swissmodel.expasy.org/repository/>) is a database of 3D protein structure models generated by the SWISS-MODEL homology-modeling pipeline.
- The aim of the SWISS-MODEL Repository is to provide access to an up-to-date collection of annotated 3D protein models generated by automated homology modeling for all sequences in Swiss-Prot and for relevant models organisms.

Swiss-Model Repository

- As of May 2009, the database contains 3.4 million entries for 2.7 million different protein sequences from the UniProt database.

Swiss-Model Repository: query

SWISS-MODEL Repository

[\[Workspace \]](#) [\[Repository \]](#) [\[Modelling \]](#) [\[Tools \]](#)

Welcome to the SWISS-MODEL Repository

The SWISS-MODEL Repository is a database of annotated three-dimensional comparative protein structure models generated by the fully automated homology-modelling pipeline SWISS-MODEL.

Example Queries:

[\[P24723\]](#) [\[DNAK_PROM5\]](#) [\[PII00518769\]](#) [\[NP_536733\]](#) [\[GI:26454606\]](#) [\[ENTREZ:54401\]](#) [\[Sequence\]](#)

SEARCH



The current release of the SWISSMODEL-Repository (8.9) consists of 3'454'191 model entries for 2'728'637 unique sequences in the UniProt database (Version 13.7.; SwissProt 56.0).

NOTE: The SWISS-MODEL repository contains theoretically calculated models, which may contain significant errors.

Swiss-Model Repository: entry

SWISS-MODEL Repository


[Workspace] [Repository] [Modelling] [Tools]

SWISS-MODEL Repository Model Details

Model Overview [+/-]

Click on the bars to get more details about individual [Models](#) or experimental [structures](#)

1 683

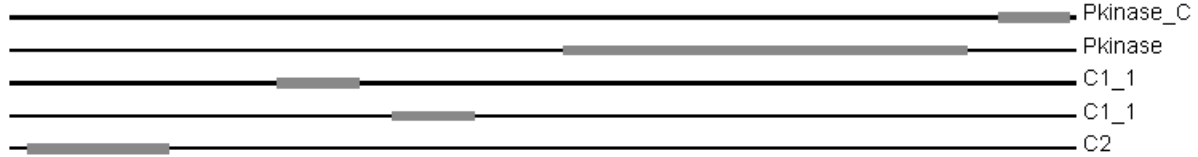


Sequence [+/-]


P24723 Protein kinase C eta type (nPKC-eta)
Homo sapiens (Human).
Database: Swiss-Prot (Reviewed) ★

Domain [+/-]

Link to: [InterPro]



Model 3D Structure [+/-]



Based on template: 2i0e [SMTL] [PDB] [SCOP] [CATH]

Sequence identity: 60%
Residue range: 352 to 683
Model date: 2008-08-30
Revision date: 2008-08-30

[display] [download] [download project]

Swiss-Model Repository: entry

Alignment [+/-]

```

TARGET      352      IDNFEFIR VLGKGSFGKV MLARVKETGD LYAVKVLKGD VILQDDVVEC
2i0eA      339      ltdfnflm vlgkgsfgkv mlserkgtde lyavkilkkd vviqdddvec

TARGET      352      ssssss sssss sss ssssss s sssssssssh hhh hhhh
2i0eA      339      ssssss sssss sss ssssss s sssssssssh hhh hhhh

TARGET      400      TMTEKRILSL ARNHPFLTQL FCCFQTPDRL FFVMEFVNGG DLMFHIQKSR
2i0eA      387      tmvekrvial pgkppfltql hscfqtmdrl yfvmevngg dlmyhiqqvg

TARGET      400      hhhhhhhh          ss ssssss sss sssss s sshhhhh
2i0eA      387      hhhhhhhh          ss ssssss sss sssss s sshhhhh

TARGET      450      RFDEARARFY AAEIISALMF LHDKGIIYRD LKLDNVLLDH EGHCKLADFG
2i0eA      437      rfkephavfy aaeiaiglff lqskgiyrd lkldnvmls eghikiadfg

TARGET      450      hhhhhhh hhhhhhhhhh hhh sss          sssss sssss
2i0eA      437      hhhhhhh hhhhhhhhhh hhh sss          sssss sssss

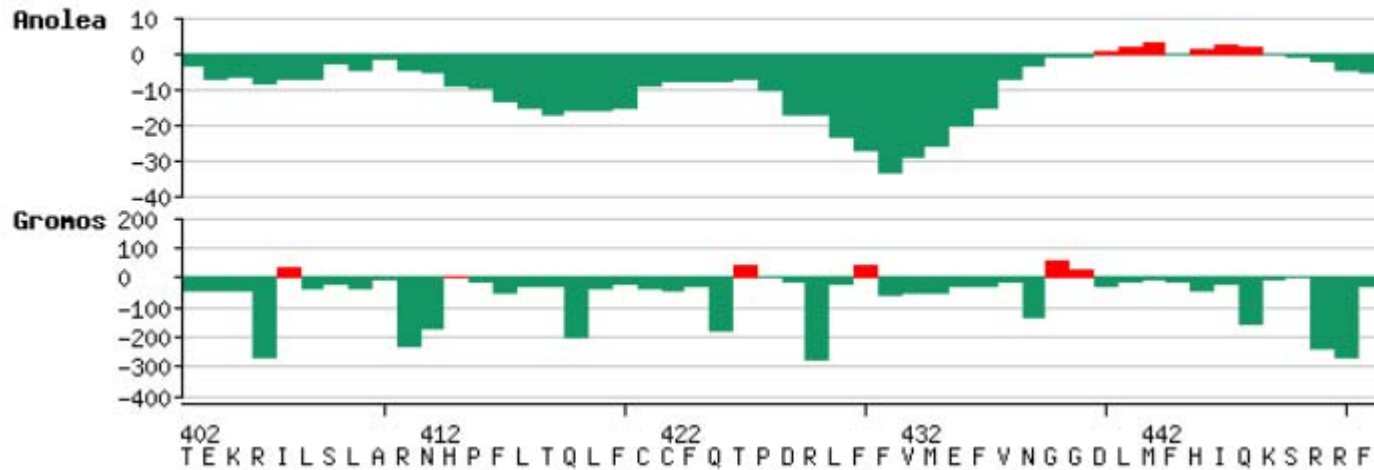
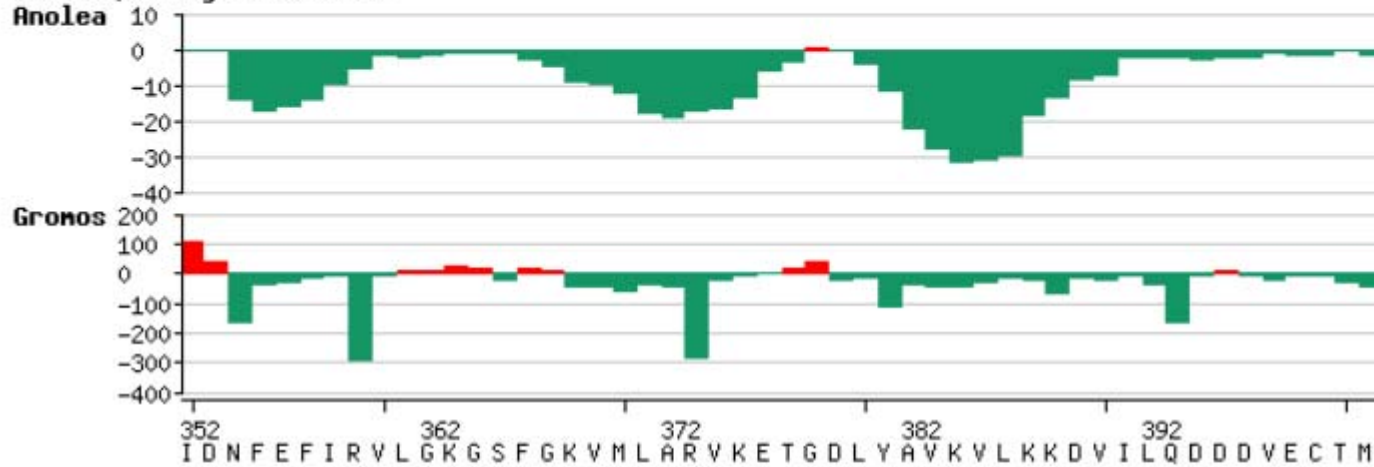
```


Swiss-Model Repository: entry

Quality [+/-]

[start new quality assessment in Workspace]

Model Quality Assessment



Swiss-Model Repository: entry

Template Selection [+/-]

START PIPELINE ON ID: e9db53770a288ad0b22b3394ccl7623d on BC2-cluster at Sat Aug 30 20:22:17 2008
BLAST_TEMPLATE_SELECTION SUCCESSFUL TEMPLATES FOUND: 2 BUT STILL ROOM FOR IMPROVEMENT GO TO
HHSEARCH

TEMPLATES SELECTED

```
>e9db53770a288ad0b22b3394ccl7623d
*****
>2i0eA Evalue: 1.45075e-116 SeqID: 60.060 Method: BLAST Type: MODEL
-----
>2fk9A Evalue: 1.4928e-75 SeqID: 96.403 Method: BLAST Type: MODEL
-----
>2eliA Evalue: 3E-14 SeqID: 50.000 Method: HHSEARCH Type: MODEL
-----
>2ernA Evalue: 5.5E-14 SeqID: 43.284 Method: HHSEARCH Type: MODEL
-----
>lb6cB Evalue: 3.6E-33 SeqID: 20.312 Method: HHSEARCH Type: MODEL
-----
>lxa6A Evalue: 3.7E-14 SeqID: 22.000 Method: HHSEARCH Type: MODEL
-----
*****
```

TEMPLATE ID	START	STOP	METHOD	STATUS
2i0eA	352	683	BLAST	BUILT
2fk9A	2	137	BLAST	NOT BUILT
2eliA	239	302	HHSEARCH	BUILT
2ernA	157	223	HHSEARCH	BUILT
lb6cB	326	557	HHSEARCH	BUILT
lxa6A	117	266	HHSEARCH	BUILT

FINISHED PIPELINE ON ID: e9db53770a288ad0b22b3394ccl7623d on gopt-76.cluster.bc2.ch BC2-Cluster at
Sat Aug 30 20:28:34 2008

Template Search [+/-]

[start new template identification in Workspace]

Model	From-To	PDB-ID	Resolution	Sequence ID	Type
	352-683	2i0eA	2.60	60%	BLAST
	350-679	2jedA	2.32	56%	BLAST
	352-683	2i0eB	2.60	56%	BLAST
	350-682	2jedB	2.32	53%	BLAST
	350-679	1zrZA	3.00	50%	BLAST

The Protein Model Portal

The Protein Model Portal

- The goal of the Protein Model Portal (PMP) is to provide a **single portal** which gives access to the various models that can be leveraged from experimental protein structures.
- A single interface allows all existing pre-computed models across various sites to be queried simultaneously, and provides links to interactive services for template selection, target-template alignment, model building, and quality assessment.
- The current release of the portal consists of 8.1 million model structures provided by different partner resources (CSMP, JCSG, MCSG, NESG, NYSGXRC, JCMM, ModBase, SWISS-MODEL Repository).
- The PMP is available at <http://www.proteinmodelportal.org> and from the PSI Structural Genomics Knowledgebase (<http://kb.psi-structuralgenomics.org/>)

The Protein Model Portal: query

The screenshot displays the Protein Model Portal (PMP) website. At the top, the PSI logo and the text "The Protein Model Portal" are visible. The main content area is titled "PMP | The Protein Model Portal" and includes a description of the portal's capabilities. A search bar is present with a red arrow pointing to it, and a "run query" button is highlighted with a red circle. Below the search bar, there is a section for "PSI Partner Resources" which lists various centers and their contributions to the portal. A "Release notes" section provides details about the current release, including the number of models and the release date.

PSI | The Protein Model Portal

YLDVGFDTTRVAVIQFVYLSK
SDFSNDVFPPEFADRSG
SVVVKRGGAVPIGIGI

models menu

- PMP home
- advanced search
- modeling service
- related tools
- news and events
- documentation
- about PMP
- contact Us

psi sgkb menu

- PSI SGKB home
- structural genomics update
- about this site
- about PSI
- PSI centers
- PSI resources
- NPG resources

PMP | The Protein Model Portal

The Protein Model Portal (PMP) gives access to the various models that can be leveraged from PSI targets and other experimental protein structures by comparative modeling methods. The current release of the portal allows searching 8.1 million precomputed model structures provided by different partner sites, and provides access to various interactive services for template selection, target-template alignment, model building, and quality assessment.

Query the Protein Model Portal by amino acid sequence:

run query [Example] [Reset]

PSI Partner Resources

- CSMP - Center for Structures of Membrane Proteins
- JCSG - Joint Center for Structural Genomics
- MCSG - Midwest Center for Structural Genomics
- NESG - Northeast Structural Genomics Consortium
- NMHRM - New Methods for High-Resolution Comparative Modeling
- NYSGXRC - New York SGX Research Center for Structural Genomics
- JCMM - Joint Center for Molecular Modeling
- ModBase - ModBase
- SWISS-MODEL - The SWISS-MODEL Repository

Release notes:

The current release consists of 8.1 million comparative protein models for 3.1 million distinct UniProt entries.

Portal version: 2.10-27.1233
Release date: 2009/05/14 (**statistics**)
Based on UniProt release 15.2

PMP is developed by the **Computational Structural Biology Group** at the **Swiss Institute of Bioinformatics (SIB)** and the **Biozentrum of the University of Basel**.

The Protein Model Portal: query

PSI | The Protein Model Portal

YLDVGFDTTRVAVIQFVLSSE
SDFSNDVFPFADRSG
SVVVKRGGAVPIGIG

PMP | Advanced Query:

models menu

- PMP home
- advanced search
- modeling service
- related tools
- news and events
- documentation
- about PMP
- contact Us

psi sgkb menu

- PSI SGKB home
- structural genomics update
- about this site
- about PSI
- PSI centers
- PSI resources
- NPG resources

Query by Database Accession Codes

Query the model portal by sequence database accession code (e.g. UniProt: **Q6LTE1**)

UniProt

Query by Amino Acid Sequence

Query the model portal by protein sequence (single letter code) or fragments of protein sequences (e.g. individual domains) for models matching, or similar to the query. [\[Example\]](#) [\[Reset\]](#)

Query by Template Structure:

Search for models build on a specific template structure using PDB accession codes (e.g. "1mw7", "1nrw", or "1s7j").

Search for models build on a specific template structure using structural genomics target codes (e.g. "NYSGXRC-T1648", "PpR6", or "APC80860").

The Protein Model Portal: results

PSI | The Protein Model Portal

YLDVGFDTTRVAVIQELVLSK
SDFSNDVFPFADRSQ
SVVVKRGGAVPIGIGADIS

models menu

- PMP home
- advanced search
- modeling service
- related tools
- news and events
- documentation
- about PMP
- contact Us

psi sgkb menu

- PSI SGKB home
- structural genomics update
- about this site
- about PSI
- PSI centers
- PSI resources
- NPG resources

PMP | Query Result:

Summary: 0

Your Query was: Q6LTE1

1 214

Colors: [Query](#) | [Sequence](#) | [Structures](#) | [Models](#)

Q6LTE1 Adenylate kinase; AK; EC=2.7.4.3; ATP-AMP transphosphorylase; Photobacterium profundum (Photobacterium sp. (strain SS9)).

Models found: 3
Experimental Structures: 0

Models:

Model	Provider	Type	Templates	%Seq id	from	to
[Show]	SWISSMODEL	SC	1akeB	72.89	1	214
[Show]	MODBASE	SC	1e4vA	72.00	1	214
[Show]	NYSGXRC	TC	1kagA	12.00	1	168

[1 - 3]


Experimental Structures:

No experimental structures found. (>90%).

The Protein Model Portal: results

models menu

- PMP home
- advanced search
- modeling service
- related tools
- news and events
- documentation
- about PMP
- contact Us

psi sgkb menu 

- PSI SGKB home
- structural genomics update
- about this site
- about PSI
- PSI centers
- PSI resources
- NPG resources

PMP | Model Details

Summary:

1 214

Model from 1 to 214

Colors: [Query](#) | [Sequence](#) | [Structures](#) | [Models](#)


Q6LTE1 Adenylate kinase; AK; EC=2.7.4.3; ATP-AMP transphosphorylase; Photobacterium profundum (Photobacterium sp. (strain S59)).

Domain Annotation:

[[InterPro](#)]

ADK
ADK_lid

Structure Model:

Model provided by:  MODBASE

Based on template: 1e4vA [[PDB](#)] * [[SCOP](#)] *
[[CATH](#)] *

Sequence identity: 72.00%


Residue range: 1 to 214

Resolution: 1.85 (X-RAY)

Model creation date: 2004-12-07

Template verification: 2004-12-07

[[display](#)] [[download](#)]



Target - Template Alignment:

Model	MRILLGAPG	AGKGTQAQFI	MAKFGIPQIS	TGDMLRRAAIK	AGTELKQAK
Template	MRILLGAPV	AGKGTQAQFI	MEKYGIPQIS	TGDMLRRAAVK	SGSELGKQAK

The Protein Model Portal: services

models menu

- PMP home
- advanced search
- modeling service**
- related tools
- news and events
- documentation
- about PMP
- contact Us

psi sgkb menu

- PSI SGKB home
- structural genomics update
- about this site
- about PSI
- PSI centers
- PSI resources
- NPG resources

PMP | Modeling Service

Name:

Request Title:

Email:

Amino Acid Sequence:
[Example]

SWISS-MODEL

Server Policy: Usage of SWISS-MODEL Server and Workspace are free of charge.

ModWeb

Server Policy: By checking this box, I assert that I am part of an academic institution (not a government research lab such as the NIH, or a commercial entity) and agree to the terms of the **Modeller license** *.

I have a MODELLER access key:

M4T

Server Policy: I am a non-profit/academic user and this server will be used solely for educational purposes or for basic research intended to advance scientific knowledge.

References

- Kiefer, F., Arnold, K., Kunzli, M., Bordoli, L. and Schwede, T. (2009). The SWISS-MODEL Repository and associated resources. *Nucleic Acids Res*, 37, D387–92.
- Arnold, K., Kiefer, F., Kopp, J., Battey, J. N., Podvinec, M., Westbrook, J. D., Berman, H. M., Bordoli, L. and Schwede, T. (2009). The Protein Model Portal. *J Struct Funct Genomics*, 10, 1–8.