

Tutorial Actividad Práctica 1.4

Modelado estructural de proteínas

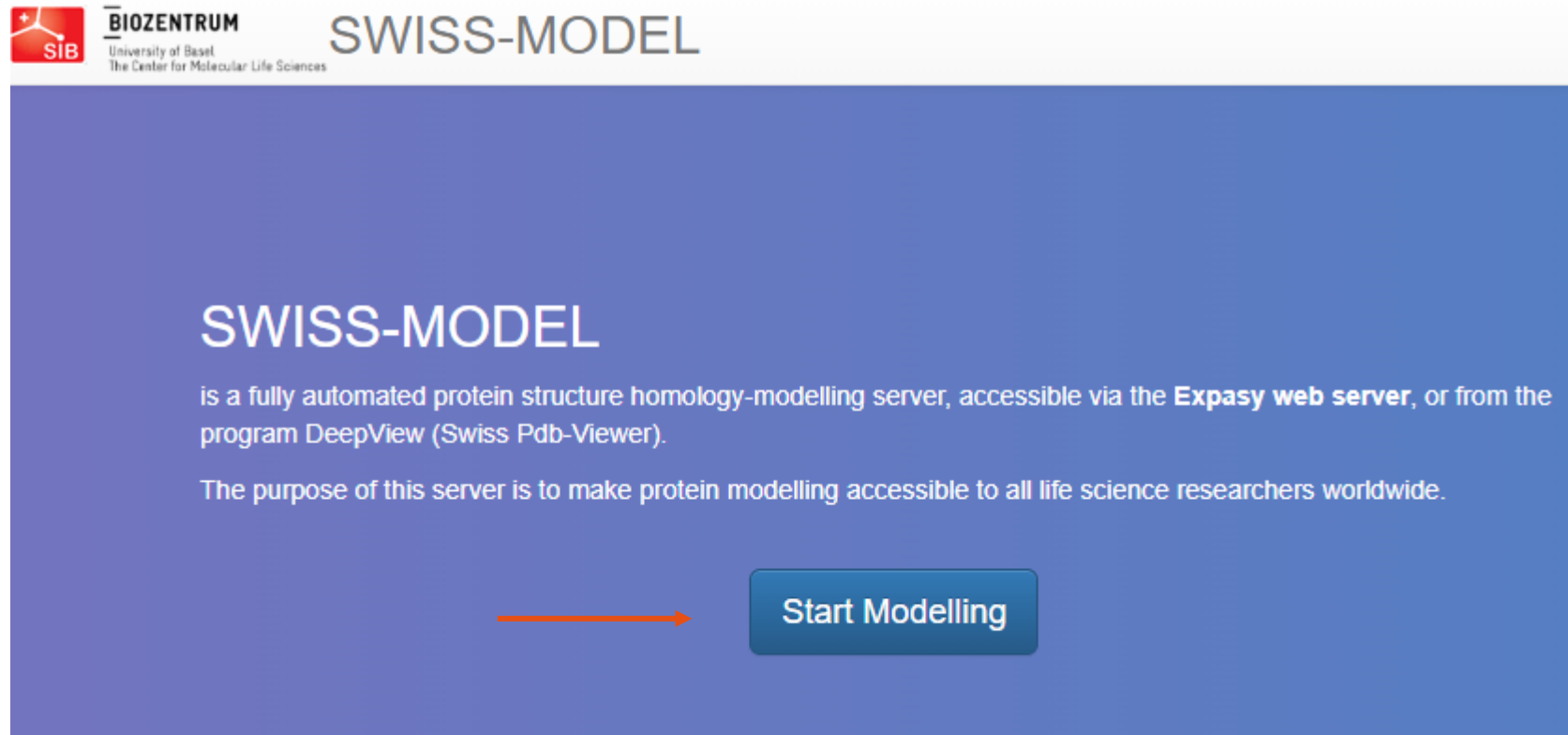


Universidad
Internacional
de Valencia

Modelado por homología

Swiss Model

<https://swissmodel.expasy.org>



Modelado por homología

Swiss Model

Crear un modelo nuevo. Podemos o bien pegar directamente la secuencia FASTA de nuestra proteína (1) o subir un archivo FASTA que la contenga (2). Buscar estructuras molde (3).

The screenshot shows the 'Start a New Modelling Project' page of the Swiss-Model server. The interface includes a header with logos for SIB, BIOZENTRUM, and SWISS-MODEL. The main form has three numbered steps: 1. A text area for pasting the target sequence, with a note that the format must be FASTA, Clustal, plain string, or a valid UniProtKB AC. 2. A green button to upload a target sequence file and a grey 'Validate' button. 3. A 'Project Title' field (labeled 'Untitled Project') and an 'Email' field (labeled 'Optional'). At the bottom, there are two large blue buttons: 'Search For Templates' and 'Build Model'.

Start a New Modelling Project

Target Sequence(s):
(Format must be FASTA, Clustal, plain string, or a valid UniProtKB AC)

Paste your target sequence(s) or UniProtKB AC here

1

2 + Upload Target Sequence File... Validate

Project Title: Untitled Project




Email: Optional

3 Search For Templates Build Model

Modelado por homología

Swiss Model

Crear un modelo nuevo. Podemos o bien pegar directamente la secuencia FASTA de nuestra proteína (1) o del alineamiento deseado empleando formato FASTA (2) o Clustal (3).



Start a New Modelling Project

Target Sequence(s):
(Format must be FASTA, Clustal,
plain string, or a valid UniProtKB AC)

1

Paste your target sequence(s) or UniProtKB AC here

+ Upload Target Sequence File...

Validate

Example for FASTA:

```
>THN_DENCL
KSCCPTTAARNQYNICRLPGTTPRPVCAALSGCKIISGTGCPGGRH-
>1crnA
TTCCPSIVARSNFNVCRLPGTPEALCATYTGCIIPGATCPGDYAN-
```

Example for Clustal:

```
CLUSTAL W (1.82) multiple sequence alignment
THN_DENCL      KSCCPTTAARNQYNICRLPGTTPRPVCAALSGCKIISGTGCPGGRH- 46
1crnA          TTCCPSIVARSNFNVCRLPGTPEALCATYTGCIIPGATCPGDYAN- 46
               ..***  ..*  :  **: * .. :**  :** **...: ** *
```

Modelado por homología

Swiss Model

Esperar mientras el servidor busca la secuencia molde más apropiada. Puede tardar varios minutos dependiendo de la longitud de la secuencia. Mientras tanto, verá una ventana parecida a la que se muestra aquí.

trpv1 Created: today at 09:00

Summary

Templates

Models

Project Data

Template Results

The search for templates matching your target sequence is currently running. Please wait.

...running HHblits against SMTL
...reusing cached query alignment
...predicting residue burial status with ACCpro
...searching PDB profile database with previously built query profile

Aquí se especifica cada paso que tiene lugar en la búsqueda del molde.

If you want to come back later, bookmark this link:

<https://swissmodel.expasy.org/interactive/RR8NvZ/>

MKKWSSTDLGAAADPLQKDTCPDPLDGDPSNRPPPAKQQLSTAKSRTLFGKGDSEEAFPVDCPHEEGELDSCPTITVSPVITIQRPGDGPTGARLLSQDSVAASTEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQKSKHLT
DNEFKDPETGKTCLLKAMLNLDHGQNTTIPLLLEIARQTDLSKELVNASYTDSYYKGQTALHIAIERRNMALVTLLVENGADVQAAAHGDFFKTKGRPGFYFGELPLSLAACTNQLGIVKFLQLNSWQTADISARDSVGNTVLH
ALVEVADNTADNTKFVTSMYNEILMLGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRHLSRKFTWAYGVPVHSSLYDLSCIDTCEKNSVLEVIAYSSSETPNRHDMLLVEPLNRLQLQDKWDRFVKRIF
YFNFLVYCLYMIIFTMAAYYRPVDGLPPFKMEKTGDYFRVTGEILSVLGGVYFFFRGIQYFLQRRPSMKTLFVDSYSEMLFFLQSLFMLATVVLYFSLHKEYYVASMVFSALGWTNMLYYTRGFQQMGIYAVMIEKMILRDLCRF
MFVYIVFLFGFSTAVVTLIEDGKNDSLPSSESTSHRWGPACRPPDSSYNSLYSTCLELFKFTIGMGDLEFTENYDFKAVFIILLLAYVILTYILLNMLIALMGETVNKIAQESKNIWKLQRAITILDTEKSFLKCMRKAFRSGK
LLQVGYPDGDYRWCFRVDENVNTTWNNTNNGIINEDPGNCEGVKRTL SFSLRSSRVSGRHWKNFALVPLLREASARDQSAQPEEVYLRQFSGSLKPDAEVFKSPAASGEK

Modelado por homología

Swiss Model

Esperar mientras el servidor busca la secuencia molde más apropiada. Puede tardar varios minutos dependiendo de la longitud de la secuencia. Mientras tanto, verá una ventana parecida a la que se muestra aquí.

The search for templates matching your target sequence is currently running. Please wait.

```
...running HHblits against SMTL
...reusing cached query alignment
...predicting residue burial status with ACCpro
...searching PDB profile database with previously built query profile
...running BLAST against SMTL
...running AFDB template search
...searching AFDB sequence database with target sequence
...getting AFDB templates
...extracting distance constraints from 4960 templates
...filtering list of templates
...structurally superpose templates
...predicting oligomeric state conservation
```

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Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:

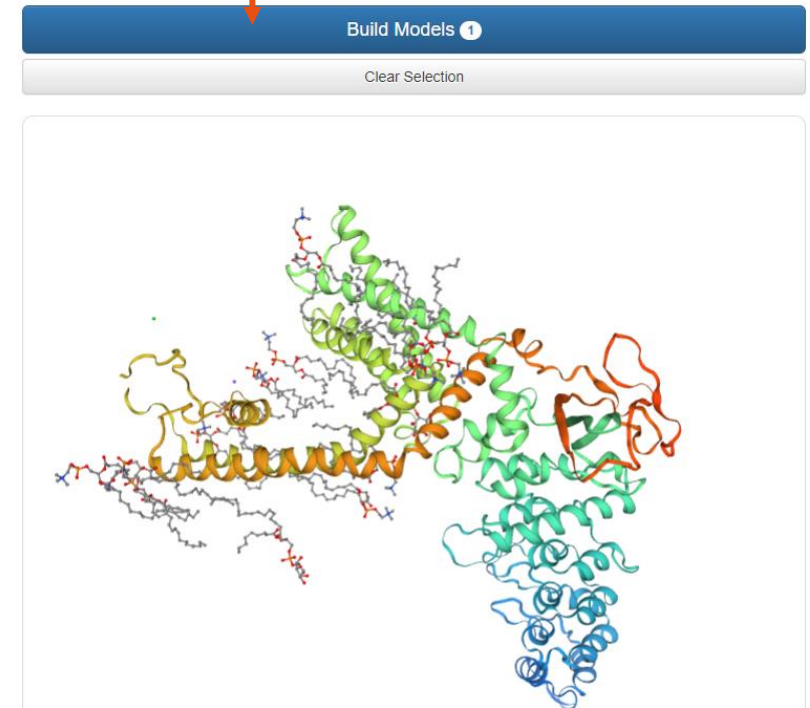
Summary **Templates 23** Models Project Data ▾

Template Results ⓘ

Templates Quaternary Structure Sequence Similarity Alignment More ▾

Sort	Coverage	GMQE	QSQE	Identity	Method	Oligo State	Ligands
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	0.78	0.95	85.35	EM	homo-tetramer ✓	32 x POV [Ⓢ] , 4 x YBG [Ⓢ]
7lqy.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in apo state							
<input type="checkbox"/>	<input type="checkbox"/>	0.78	0.95	89.26	EM	homo-tetramer ✓	32 x POV [Ⓢ] , 4 x YBG [Ⓢ]
7lqy.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in apo state							
<input type="checkbox"/>	<input type="checkbox"/>	0.76	0.95	86.14	EM, 2.6Å	homo-tetramer ✓	4 x T7X [Ⓢ] , 8 x LBN [Ⓢ] , 28 x 6OU [Ⓢ] , 4 x YFP [Ⓢ]
7lp9.1.A Transient receptor potential cation channel subfamily V member 1 Cryo-EM structure of full-length TRPV1 at 4 degrees Celsius							
<input type="checkbox"/>	<input type="checkbox"/>	0.73	0.96	86.14	EM, 3.4Å	homo-tetramer ✓	8 x LBN [Ⓢ] , 12 x 6OU [Ⓢ] , 4 x 4DY [Ⓢ] , 4 x YFP [Ⓢ]
7lpa.1.A Transient receptor potential cation channel subfamily V member 1 Cryo-EM structure of full-length TRPV1 with capsaicin at 4 degrees Celsius							
<input type="checkbox"/>	<input type="checkbox"/>	0.75	0.94	86.14	EM	homo-tetramer ✓	4 x 6EU [Ⓢ] , 8 x LBN [Ⓢ] , 20 x 6OU [Ⓢ] , 4 x YFP [Ⓢ]
7rqu.1.B Transient receptor potential cation channel subfamily V member 1 Cryo-EM structure of the full-length TRPV1 with RTX at 4 degrees Celsius, in a closed state, class I							
<input type="checkbox"/>	<input type="checkbox"/>	0.76	0.92	85.35	EM	homo-tetramer ✓	32 x POV [Ⓢ] , 4 x 6EU [Ⓢ]
7lqz.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in complex with RTX							
<input type="checkbox"/>	<input type="checkbox"/>	0.76	0.92	89.26	EM	homo-tetramer ✓	32 x POV [Ⓢ] , 4 x 6EU [Ⓢ]
7lqz.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in complex with RTX							

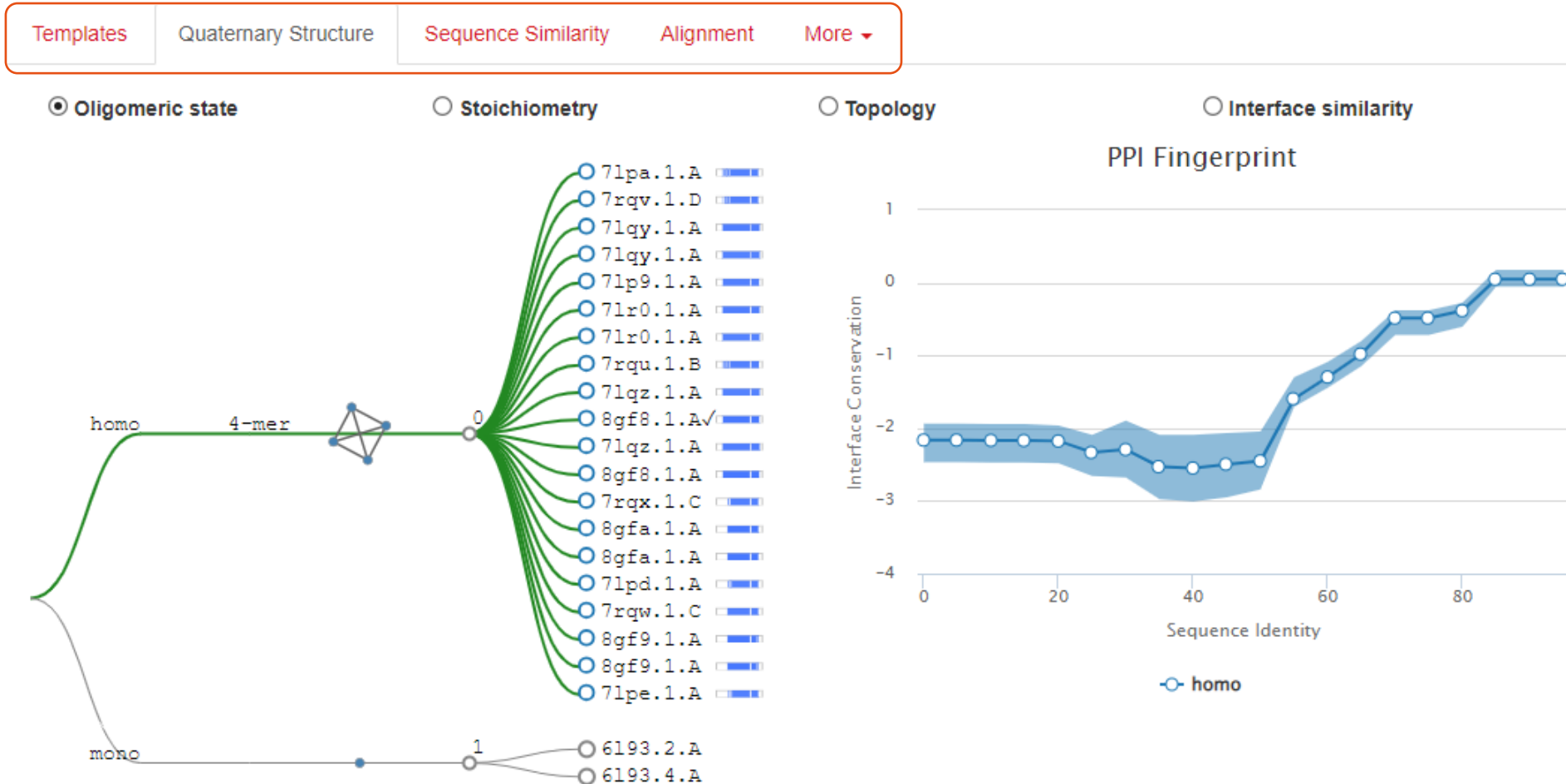
Construir modelo según molde
seleccionado



Modelado por homología

Swiss Model

Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:



Modelado por homología

Swiss Model

Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:


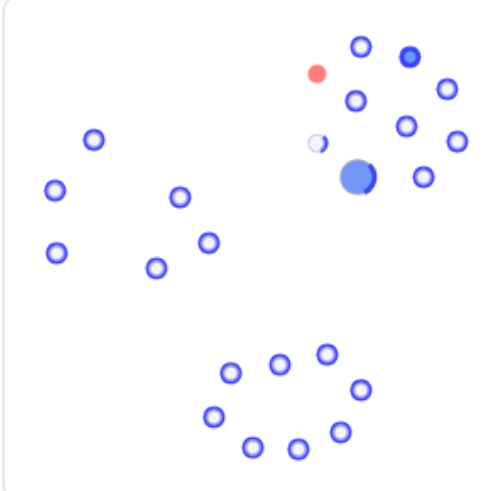
Templates

Quaternary Structure

Sequence Similarity

Alignment


More ▾



Template

6I93.2.A Transient receptor potential cation channel subfamily V member 1
X-ray structure of the ligand-free human TRPV1 ankyrin repeat domain

Coverage



Identity

100.00

Similarity

0.61

Ligands

-

Method

X-ray 4.47Å

Oligo State

monomer

Found By

BLAST

Modelado por homología

Swiss Model

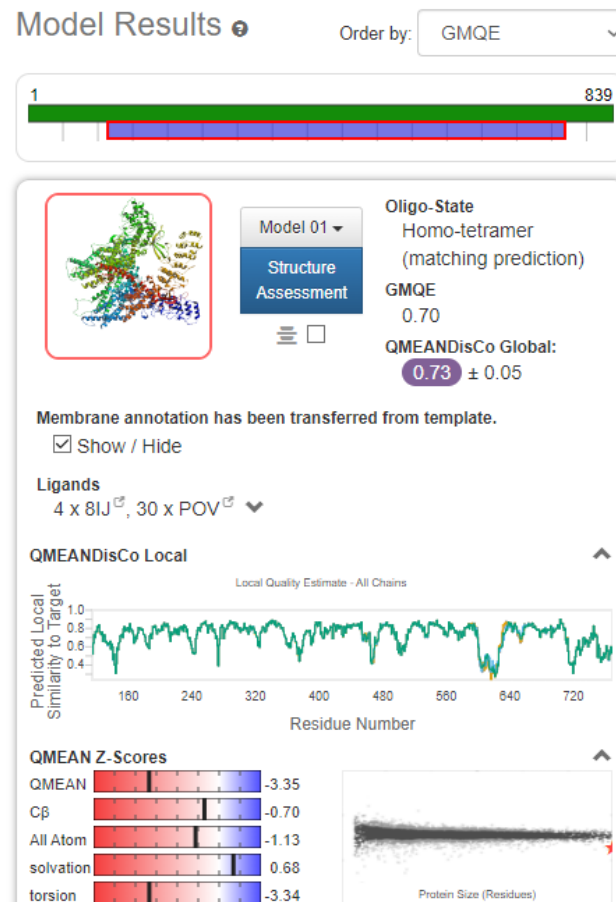
Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:

	Templates	Quaternary Structure	Sequence Similarity	Alignment	More ▾
⚙ Target	MKKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPPAKPQLSTAKSRTLFGKGDSEEAFPVDCPHEEGELDSCPTITVSPVITIQRPGDGPTGARLLSQDSVAAS				
8gf8.1.A	-KKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPPAKPQLSTAKSRTLFGKGDSEEAFPVDCPHEEGELDSCPTITVSPVITIQRPGDGPTGARLLSQDSVAAS				
6193.2.A	-----SVAAS				
Target	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQSKKKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIPLLLEIARQTDSLKELVNASYTDSEYKGGQTALHIAI				
8gf8.1.A	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQSKKKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIPLLLEIARQTDSLKELVNASYTDSEYKGGQTALHIAI				
6193.2.A	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQSKKKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIPLLLEIARQTDSLKELVNASYTDSEYKGGQTALHIAI				
Target	ERRNMALVTLLVENGADVQAAAHGDFFKKTGRPGFYFGELPLSLAACTNQLGIVKFLLQNSWQTADISARDSVGNTVLHALVEVADNTADNTKFVTSMYNEILM				
8gf8.1.A	ERRNMALVTLLVENGADVQAAAHGDFFKKTGRPGFYFGELPLSLAACTNQLGIVKFLLQNSWQTADISARDSVGNTVLHALVEVADNTADNTKFVTSMYNEILM				
6193.2.A	ERRNMALVTLLVENGADVQAAAHGDFFKKTGRPGFYFGELPLSLAACTNQLGIVKFLLQNSWQTADISARDSVGNTVLHALVEVADNTADNTKFVTSMYNEILM				
Target	LGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRHLSRKFTWAYGVPVHSSLYDLSCIDTCEKNSVLEVIAYSSSETPNRHDMLLVEPLN				
8gf8.1.A	LGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRHLSRKFTWAYGVPVHSSLYDLSCIDTCEKNSVLEVIAYSSSETPNRHDMLLVEPLN				
6193.2.A	LGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRH				
Target	RLQDKWDRFVKRIFYFNFLVYCLYMIIFTMAAYYRPVDGLPPFKMEKTGDYFRVTGEILSVLGGVYFFFRGIQYFLQRRPSMKTLFVDSYSEMLFFLQSLFMLA				
8gf8.1.A	RLQDKWDRFVKRIFYFNFLVYCLYMIIFTMAAYYRPVDGLPPFKMEKTGDYFRVTGEILSVLGGVYFFFRGIQYFLQRRPSMKTLFVDSYSEMLFFLQSLFMLA				
6193.2.A	-----				
Target	TVVLYFSHLKEYVASMVFSALGWTNMLYYTRGFQQMGIYAVMIEKMILRDLCRFMFVYIVFLFGFSTAVVTIIEDGKNDSLPESESTSHRWRGACRPPDSSYNS				
8gf8.1.A	TVVLYFSHLKEYVASMVFSALGWTNMLYYTRGFQQMGIYAVMIEKMILRDLCRFMFVYIVFLFGFSTAVVTIIEDGKNDSLPESESTSHRWRGACRPPDSSYNS				
6193.2.A	-----				
Target	LYSTCLELFKFTIGMGDLEFTENYDFKAVFIILLAYVILTYILLNMLIALMGETVNKIAQESKNIWKLQRAITILDTEKSFLKCMRKAFRSGKLLQVGYTPDG				
8gf8.1.A	LYSTCLELFKFTIGMGDLEFTENYDFKAVFIILLAYVILTYILLNMLIALMGETVNKIAQESKNIWKLQRAITILDTEKSFLKCMRKAFRSGKLLQVGYTPDG				
6193.2.A	-----				
Target	KDDYRWCFRVDEVNWTNTWNTNNGIINEDPGNCEGVKRTLFSLSRSSRVSGRHWKNFALVPLLREASARDRQSAQPEEVYLRQFSGSLKPEDAEEVFKSPAASGEK				
8gf8.1.A	KDDYRWCFRVDEVNWTNTWNTNNGIINEDPGNCEGVKRTLFSLSRSSRVSGRHWKNFALVPLLREASARDRQSAQPEEVYLRQFSGSLKPEDAEEVFKSPAASGEK				
6193.2.A	-----				

Modelado por homología


Swiss Model


Construcción del modelo según selección anterior.



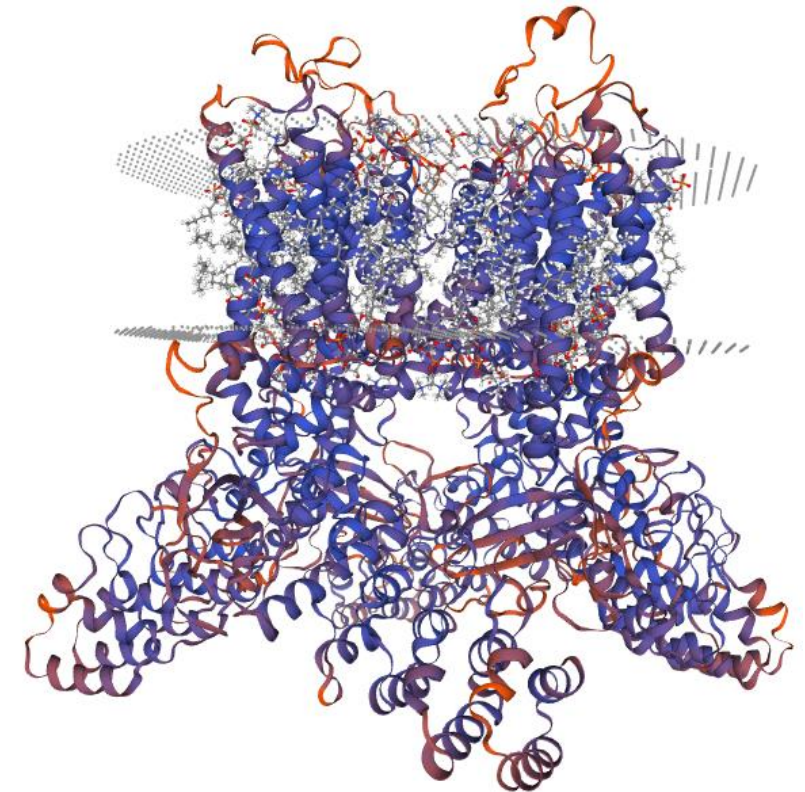
Template
8gf8.1.A Transient receptor potential cation channel subfamily V member 1
Cryo-EM structure of human TRPV1 in cNW11 nanodisc and soybean lipids

Seq Identity
100.00%

Coverage 

Model-Template Alignment 

Model_01:A	MKKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPP	35
Model_01:B	MKKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPP	35
Model_01:C	MKKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPP	35
Model_01:D	MKKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPP	35
8gf8.1.A	-KKWSSTDLGAAADPLQKDTCPDPLDGDPNRPPP	37
Model_01:A	AKPQLSTAKSRTLFGKGDSEEAFFVDCPHEEGEL	70
Model_01:B	AKPQLSTAKSRTLFGKGDSEEAFFVDCPHEEGEL	70
Model_01:C	AKPQLSTAKSRTLFGKGDSEEAFFVDCPHEEGEL	70
Model_01:D	AKPQLSTAKSRTLFGKGDSEEAFFVDCPHEEGEL	70
8gf8.1.A	AKPQLSTAKSRTLFGKGDSEEAFFVDCPHEEGEL	72
Model_01:A	DSCPTITVSPVITIQRPDGPPTGARLLSQDSVAAS	185
Model_01:B	DSCPTITVSPVITIQRPDGPPTGARLLSQDSVAAS	185
Model_01:C	DSCPTITVSPVITIQRPDGPPTGARLLSQDSVAAS	185
Model_01:D	DSCPTITVSPVITIQRPDGPPTGARLLSQDSVAAS	185
8gf8.1.A	DSCPTITVSPVITIQRPDGPPTGARLLSQDSVAAS	187
Model_01:A	TEKTLRLYD RRSIFEAVAQNN CDLESLLFLQKS	140
Model_01:B	TEKTLRLYD RRSIFEAVAQNN CDLESLLFLQKS	140
Model_01:C	TEKTLRLYD RRSIFEAVAQNN CDLESLLFLQKS	140
Model_01:D	TEKTLRLYD RRSIFEAVAQNN CDLESLLFLQKS	140
8gf8.1.A	TEKTLRLYD RRSIFEAVAQNN CDLESLLFLQKS	142
Model_01:A	KKHLTDNEFKDP ETGKTCLLKAMNLHDGONTTIP	175
Model_01:B	KKHLTDNEFKDP ETGKTCLLKAMNLHDGONTTIP	175
Model_01:C	KKHLTDNEFKDP ETGKTCLLKAMNLHDGONTTIP	175
Model_01:D	KKHLTDNEFKDP ETGKTCLLKAMNLHDGONTTIP	175
8gf8.1.A	KKHLTDNEFKDP ETGKTCLLKAMNLHDGONTTIP	177
Model_01:A	LLLEIARQ TD SLKELVNASY TD SY YKGQTALHIAI	210
Model_01:B	LLLEIARQ TD SLKELVNASY TD SY YKGQTALHIAI	210
Model_01:C	LLLEIARQ TD SLKELVNASY TD SY YKGQTALHIAI	210
Model_01:D	LLLEIARQ TD SLKELVNASY TD SY YKGQTALHIAI	210
8gf8.1.A	LLLEIARQ TD SLKELVNASY TD SY YKGQTALHIAI	212



Modelado por homología

Swiss Model

Error en proporcionar un modelo fiable.





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